Supplementary Material

A new terrein dimer and a new meroterpene from the mangrove endophytic fungus *Lichtheimia* sp.

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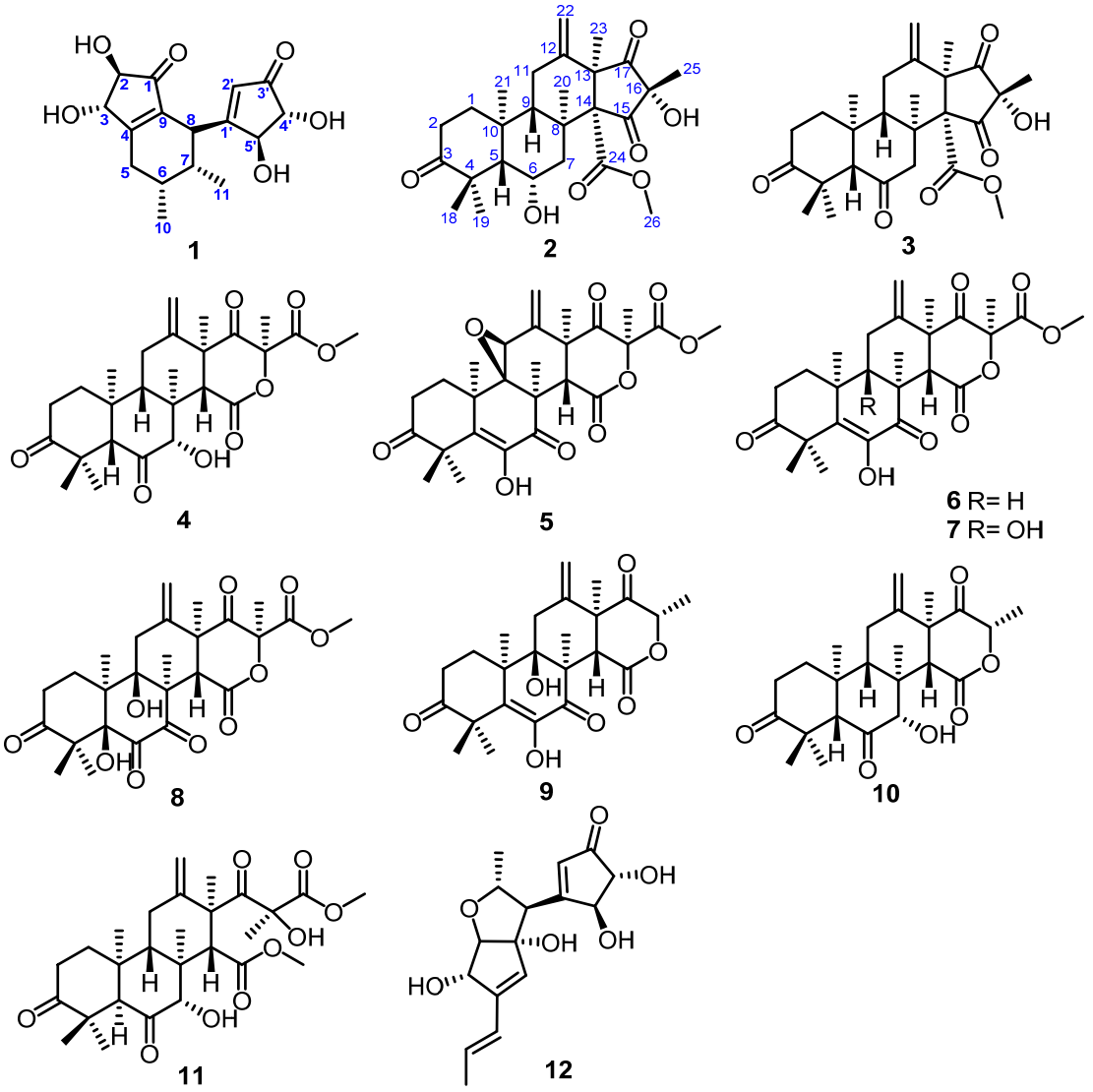


Figure S1. Structures of twelve compounds from the mangrove endophytic fungus J2B1

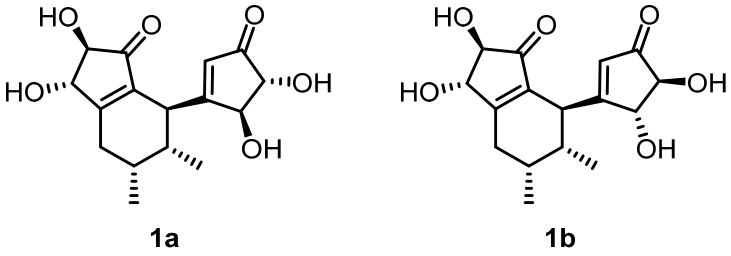


Figure S2. The two possible relative configurations of compound **1**

1. ECD calculations

Conformational searches were carried out by means of the Spartan 10 software using Molecular Merck force field (MMFF). Conformations in the 10 kal/mol energy range were

chosen to generate the initial set of conformations. The resultant conformers were optimized using DFT at the B3LYP/6-31+G(d,p) level in the gas phase by the GAUSSIAN 09 program. Gaussian 09 software was used with the CPCM solvent module at the CAM-B3LYP/6-31+G(d) level, the solvent environment of methanol was added. The calculated data were corrected by zero-point energy. Boltzmann statistical method was used to fit the theoretical calculation data of ECD.

Table S1. Key thermodynamic parameters (a.u.) of **1a** with simplified structures at B3LYP/6-31+G(d,p) level in the gas phase.

Conformers	E+ZPE	G
1a-1	-1072.719940	-1073.246286
1a-2	-1072.715610	-1073.245329
1a-3	-1072.715068	-1073.243339
1a-4	-1072.713008	-1073.241883
1a-5	-1072.715610	-1073.245325
1a-6	-1072.715298	-1073.245033
1a-7	-1072.715429	-1073.245519
1a-8	-1072.715068	-1073.243336
1a-9	-1072.713008	-1073.241886
1a-10	-1072.712174	-1073.244885

Table S2. Cartesian coordinates for the low-energy conformers of **1a** at B3LYP/6-31+G (d, p) level of theory in MeOH.

Conformer 1a-1							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	1.93716	0.196716	-0.49437	**O**	4.204736	-0.40014	-1.01221
C	2.103787	1.638172	-0.82483	**H**	2.293907	1.757035	-1.89799
C	0.894042	2.484725	-0.3885	**H**	3.028	1.981238	-0.33994
C	0.351899	2.037113	0.997064	**H**	0.098966	2.285278	-1.11435
C	-0.1178	0.555998	0.950235	**H**	-0.52725	2.651204	1.216248
C	0.96855	-0.29566	0.312902	**H**	-0.23755	0.198392	1.982005
C	1.216577	-1.7265	0.523232	**H**	3.319605	-2.00868	0.743982

C	2.585227	-2.05875	-0.07463	**H**	2.562573	-1.16018	-2.03144
C	2.866472	-0.87756	-1.01403	**H**	-2.06134	2.294347	-0.46307
C	-1.47878	0.340195	0.318905	**H**	-4.1715	-0.66466	0.892283
C	-2.27634	1.252225	-0.26983	**H**	-1.70065	-1.69073	-0.41137
C	-3.53428	0.625654	-0.69286	**H**	-1.23781	-2.15628	1.658808
C	-3.59543	-0.75632	-0.04086	**H**	-4.82374	-1.28213	-1.42939
C	-2.14336	-1.04365	0.355917	**H**	2.253489	1.645109	2.0307
O	-2.0688	-1.65459	1.628802	**H**	1.654371	3.294309	2.225199
O	-4.15658	-1.73096	-0.89149	**H**	0.891745	1.972785	3.102079
O	-4.381	1.054	-1.452	**H**	0.339661	4.583797	-0.17762
C	1.349314	2.248828	2.148218	**H**	2.038585	4.260171	0.190442
C	1.207749	3.982993	-0.46395	**H**	1.484988	4.26819	-1.48294
O	0.520223	-2.5713	1.066516	**H**	2.080133	-3.92281	-0.20813
O	2.624777	-3.3101	-0.72103	**H**	4.758328	-1.02663	-1.49

Conformer 1a-2							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	-2.06872	0.254133	0.384879	**O**	-4.45629	-0.05014	0.55828
C	-2.02008	1.619895	0.985047	**H**	-2.33218	1.585328	2.038241
C	-0.61012	2.249596	0.85831	**H**	-2.77538	2.245638	0.484772
C	0.0035	2.015995	-0.55386	**H**	0.04416	1.722504	1.56992
C	0.152383	0.468035	-0.83594	**H**	1.01354	2.440425	-0.55776
C	-1.10872	-0.2484	-0.4336	**H**	0.294079	0.352894	-1.91867
C	-1.49876	-1.59165	-0.87186	**H**	-3.6109	-1.56277	-1.30912
C	-2.95863	-1.80803	-0.45627	**H**	-3.06571	-1.22235	1.616159
C	-3.18556	-0.74261	0.633203	**H**	0.697831	-0.92182	1.723136
C	1.384833	-0.097	-0.17653	**H**	4.079472	0.649961	0.596328
C	1.503116	-0.68282	1.042435	**H**	2.770107	-0.91613	-1.61236
C	2.904766	-1.01947	1.298893	**H**	3.656428	1.141223	-2.19617
C	3.745173	-0.32884	0.217508	**H**	5.136573	-1.6902	0.563664
C	2.724824	-0.07639	-0.90329	**H**	-1.79105	2.243781	-1.80925
O	2.880399	1.183066	-1.60347	**H**	-0.90545	3.753914	-1.53158
O	4.864503	-1.12838	-0.19629	**H**	-0.25968	2.546409	-2.64698
O	3.400677	-1.75535	2.170865	**H**	0.377272	4.171855	1.187855
C	-0.79055	2.677952	-1.69753	**H**	-1.30147	4.320599	0.635462
C	-0.62423	3.733017	1.265988	**H**	-0.95946	3.845481	2.304084
O	-0.81411	-2.45823	-1.44696	**H**	-2.62274	-3.76005	-0.49607
O	-3.19884	-3.14699	0.011717	**H**	-5.1756	-0.63899	0.86086

Conformer 1a-3							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	-2.26046	0.052018	0.444377	**O**	-4.48491	-0.86249	0.199501
C	-2.68648	1.372954	0.995769	**H**	-2.62407	1.345011	2.096201

C	-1.80493	2.52039	0.436799	**H**	-3.74574	1.532497	0.759559
C	-0.29834	2.134582	0.550908	**H**	-1.95253	3.398442	1.081828
C	0.0412	0.8566	-0.29044	**H**	-0.12966	1.873766	1.607803
C	-1.06256	-0.16971	-0.15676	**H**	0.125448	1.151279	-1.34538
C	-1.02338	-1.54469	-0.6614	**H**	-2.96008	-2.0213	-1.4796
C	-2.43072	-2.13326	-0.52024	**H**	-3.04034	-1.67403	1.495182
C	-3.11035	-1.20424	0.50272	**H**	1.211932	-0.10982	2.24509
C	1.382548	0.27083	0.100034	**H**	4.238248	0.756284	-0.03258
C	1.795455	-0.1134	1.333914	**H**	2.207975	-0.9361	-1.47574
C	3.174804	-0.6001	1.265171	**H**	3.032215	0.870477	-2.65757
C	3.725324	-0.21531	-0.11326	**H**	5.024806	-1.68779	0.110699
C	2.452356	-0.00505	-0.94819	**H**	0.568817	3.570494	-0.85982
O	2.508642	1.114353	-1.86948	**H**	0.407482	4.183083	0.799973
O	4.6085	-1.21586	-0.64504	**H**	1.688345	3.027996	0.384335
O	3.830792	-1.25072	2.098776	**H**	-1.64279	3.735038	-1.38522
C	0.644195	3.297905	0.197892	**H**	-2.16124	2.067164	-1.68612
C	-2.24357	2.909905	-0.99012	**H**	-3.29106	3.232617	-0.98913
O	-0.05852	-2.19192	-1.11416	**H**	-1.6267	-3.945	-0.49925
O	-2.40917	-3.50773	-0.09716	**H**	-5.06432	-1.63174	0.367182

Conformer 1a-4							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	-2.16473	0.07165	0.320188	**O**	-4.34877	-0.96583	0.245986
C	-2.61316	1.36759	0.910625	**H**	-2.51528	1.309047	2.007095
C	-1.7847	2.556445	0.361622	**H**	-3.68361	1.503525	0.712065
C	-0.2662	2.197627	0.383728	**H**	-1.91571	3.402987	1.050929
C	0.042313	0.979885	-0.55411	**H**	-0.04366	1.867148	1.409299
C	-0.9951	-0.10515	-0.34427	**H**	-0.02974	1.326438	-1.59713
C	-0.89733	-1.5024	-0.77668	**H**	-2.84853	-2.06394	-1.51034
C	-2.27439	-2.14389	-0.57379	**H**	-2.77603	-1.65711	1.462885
C	-2.93948	-1.22356	0.464964	**H**	2.334224	0.753128	-2.33503
C	1.444783	0.455433	-0.36881	**H**	2.843611	-1.90115	0.375535
C	2.413482	0.397389	-1.3164	**H**	2.3437	0.82037	1.567144
C	3.608233	-0.24585	-0.76838	**H**	1.327683	-1.05961	2.560298
C	3.1976	-0.87602	0.565782	**H**	5.112569	-0.88557	1.051023
C	1.978798	-0.03318	0.975023	**H**	0.503308	3.73621	-0.97769
O	0.954801	-0.73821	1.715023	**H**	0.38972	4.250584	0.714227
O	4.256737	-0.85807	1.534844	**H**	1.690063	3.165846	0.199001
O	4.772384	-0.28694	-1.20617	**H**	-1.72876	3.838497	-1.42449
C	0.630107	3.404835	0.059577	**H**	-2.26469	2.178824	-1.75125
C	-2.30342	2.997394	-1.02312	**H**	-3.34911	3.317114	-0.94898
O	0.086225	-2.14349	-1.19297	**H**	-1.33841	-3.88287	-0.50544
O	-2.17677	-3.51292	-0.14867	**H**	-4.86916	-1.765	0.460654

Conformer 1a-5							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	-2.06852	0.254254	0.385005	**O**	-4.45602	-0.05003	0.559612
C	-2.01975	1.620083	0.985019	**H**	-2.33167	1.585634	2.038264
C	-0.60979	2.249729	0.857958	**H**	-2.7751	2.245825	0.484816
C	0.003568	2.015928	-0.55429	**H**	0.044598	1.7227	1.569515
C	0.152446	0.467939	-0.83608	**H**	1.013594	2.440396	-0.55844
C	-1.10866	-0.24841	-0.43357	**H**	0.294145	0.352567	-1.91879
C	-1.49885	-1.59168	-0.87168	**H**	-3.61083	-1.56127	-1.30909
C	-2.95885	-1.80763	-0.45628	**H**	-3.06489	-1.22246	1.616401
C	-3.1853	-0.74249	0.633598	**H**	0.697857	-0.92142	1.723337
C	1.384885	-0.09702	-0.17652	**H**	4.079857	0.649532	0.596169
C	1.503118	-0.68264	1.042524	**H**	2.770003	-0.91652	-1.6123
C	2.904749	-1.01932	1.299139	**H**	3.657552	1.141289	-2.1951
C	3.745216	-0.32923	0.217479	**H**	5.137301	-1.6899	0.563836
C	2.724872	-0.07668	-0.90334	**H**	-1.79136	2.243586	-1.80916
O	2.880539	1.182643	-1.60365	**H**	-0.90544	3.753668	-1.53223
O	4.864098	-1.12921	-0.19652	**H**	-0.26023	2.545733	-2.64748
O	3.400565	-1.75474	2.171565	**H**	0.377677	4.172048	1.187035
C	-0.79076	2.677643	-1.6979	**H**	-1.3012	4.320698	0.635027
C	-0.6238	3.733207	1.265467	**H**	-0.95878	3.845805	2.303628
O	-0.81438	-2.45846	-1.44667	**H**	-2.62357	-3.75972	-0.49655
O	-3.20003	-3.14658	0.010703	**H**	-5.17524	-0.63933	0.861572

Conformer 1a-6							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	2.241673	0.249083	-0.31988	**O**	4.536272	-0.45633	-0.06251
C	2.548703	1.600642	-0.87174	**H**	2.550038	1.533436	-1.97228
C	1.524269	2.66131	-0.39875	**H**	3.571365	1.88071	-0.5901
C	0.073452	2.09029	-0.49208	**H**	1.569935	3.506197	-1.10032
C	-0.10043	0.85295	0.462693	**H**	-0.05211	1.716597	-1.51978
C	1.056121	-0.105	0.24855	**H**	-0.02026	1.228002	1.495619
C	1.130046	-1.52003	0.611763	**H**	3.051387	-1.7739	1.562081
C	2.597483	-1.9414	0.572911	**H**	3.197083	-1.3599	-1.41103
C	3.208534	-0.91621	-0.40458	**H**	-2.33228	0.766551	2.285431
C	-1.4791	0.244493	0.34901	**H**	-3.26947	-2.07389	-0.33025
C	-2.43351	0.307886	1.3097	**H**	-2.18045	0.324532	-1.71779
C	-3.6771	-0.29688	0.831936	**H**	-0.87	-2.04448	-0.82404
C	-3.3765	-0.99081	-0.50141	**H**	-5.27477	-0.72997	-0.99465
C	-2.01121	-0.41632	-0.93046	**H**	-0.99628	3.502117	0.804105
O	-1.09862	-1.37431	-1.50757	**H**	-0.80027	4.047795	-0.87046
O	-4.41257	-0.72388	-1.46678	**H**	-1.99733	2.807977	-0.47351
O	-4.81756	-0.24222	1.327394	**H**	1.179467	3.942004	1.356119

C	-0.99154	3.171089	-0.241	**H**	1.952447	2.392281	1.743142
C	1.897374	3.196458	0.999685	**H**	2.882785	3.675028	0.967831
O	0.205458	-2.34006	0.818529	**H**	1.965732	-3.80983	0.410245
O	2.765841	-3.30104	0.150723	**H**	5.192813	-1.1539	-0.25678

Conformer 1a-7							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	1.963489	0.18476	-0.49668	**O**	4.298646	-0.49839	-0.99379
C	2.132816	1.623822	-0.85045	**H**	2.322054	1.726031	-1.92848
C	0.914158	2.478517	-0.42947	**H**	3.053241	1.993989	-0.37078
C	0.369804	2.049103	0.969706	**H**	0.11565	2.265588	-1.15379
C	-0.10816	0.563788	0.939273	**H**	-0.50836	2.672287	1.183702
C	0.977421	-0.2985	0.309989	**H**	-0.23909	0.216115	1.977374
C	1.207822	-1.72878	0.521155	**H**	3.301682	-2.19483	0.706934
C	2.555234	-2.10948	-0.10191	**H**	2.700213	-1.16045	-2.03426
C	2.907076	-0.90365	-0.99132	**H**	-2.0771	2.315445	-0.4637
C	-1.47243	0.356057	0.308079	**H**	-4.17782	-0.71833	0.916509
C	-2.28624	1.272038	-0.27127	**H**	-1.70396	-1.69521	-0.40032
C	-3.55738	0.644272	-0.64625	**H**	-1.22252	-2.17152	1.702672
C	-3.59446	-0.75019	-0.01579	**H**	-4.86207	-1.29829	-1.43261
C	-2.13562	-1.03008	0.3595	**H**	2.274145	1.648904	2.001912
O	-2.03623	-1.61513	1.674151	**H**	1.696833	3.314267	2.174687
O	-4.13	-1.72391	-0.93403	**H**	0.920071	2.011465	3.079168
O	-4.46172	1.090118	-1.37553	**H**	0.357998	4.585234	-0.24432
C	1.37737	2.269201	2.117049	**H**	2.059384	4.26352	0.136728
C	1.22972	3.981021	-0.52162	**H**	1.512789	4.254776	-1.54487
O	0.487631	-2.57929	1.092063	**H**	1.946255	-3.98411	-0.33405
O	2.469427	-3.33247	-0.8498	**H**	4.624818	-0.38365	-0.07702

Conformer 1a-8							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	-2.26033	0.051967	0.444492	**O**	-4.48472	-0.86292	0.200361
C	-2.68646	1.372914	0.995742	**H**	-2.62411	1.345101	2.09618
C	-1.80504	2.520388	0.436662	**H**	-3.74575	1.5323	0.759508
C	-0.29841	2.134741	0.550661	**H**	-1.95265	3.398458	1.081665
C	0.041195	0.856678	-0.29058	**H**	-0.12959	1.874044	1.607561
C	-1.06249	-0.1697	-0.15676	**H**	0.125454	1.151205	-1.34555
C	-1.02319	-1.54467	-0.66135	**H**	-2.95994	-2.02068	-1.47965
C	-2.43055	-2.13323	-0.52036	**H**	-3.03948	-1.67439	1.495309
C	-3.11008	-1.20441	0.502972	**H**	1.211827	-0.10944	2.245116
C	1.382538	0.270973	0.100016	**H**	4.238453	0.756032	-0.03275
C	1.795381	-0.11313	1.333957	**H**	2.207918	-0.93631	-1.47557
C	3.174739	-0.59979	1.265385	**H**	3.033162	0.870364	-2.65718

C	3.72526	-0.21544	-0.11318	**H**	5.02512	-1.6876	0.110931
C	2.452328	-0.0052	-0.94814	**H**	0.568578	3.570427	-0.86039
O	2.508646	1.114074	-1.86965	**H**	0.407104	4.183413	0.799258
O	4.608059	-1.21642	-0.64485	**H**	1.688152	3.028403	0.38391
O	3.830766	-1.2501	2.099204	**H**	-1.64319	3.735197	-1.38526
C	0.643969	3.298127	0.197397	**H**	-2.16116	2.067206	-1.68631
C	-2.24376	2.90987	-0.99024	**H**	-3.29134	3.232285	-0.98927
O	-0.05831	-2.19179	-1.1142	**H**	-1.62681	-3.94506	-0.49988
O	-2.40924	-3.50773	-0.09782	**H**	-5.06397	-1.63229	0.368013

Conformer 1a-9							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	-2.16457	0.071587	0.32039	**O**	-4.34858	-0.96606	0.246625
C	-2.61288	1.367479	0.911052	**H**	-2.51441	1.30894	2.007469
C	-1.78471	2.556399	0.361709	**H**	-3.68342	1.503413	0.713026
C	-0.26615	2.197786	0.383551	**H**	-1.91572	3.402973	1.05098
C	0.042349	0.979937	-0.55418	**H**	-0.04337	1.867492	1.409131
C	-0.99502	-0.10508	-0.34422	**H**	-0.02967	1.326367	-1.59724
C	-0.89725	-1.50227	-0.7769	**H**	-2.84842	-2.06348	-1.5105
C	-2.27431	-2.14376	-0.57392	**H**	-2.77544	-1.65732	1.462931
C	-2.93926	-1.22367	0.465081	**H**	2.334508	0.753578	-2.33482
C	1.444817	0.455528	-0.36877	**H**	2.843204	-1.90111	0.374992
C	2.41365	0.397662	-1.31624	**H**	2.34376	0.820384	1.567108
C	3.608345	-0.24566	-0.76817	**H**	1.328245	-1.06138	2.559419
C	3.197438	-0.87613	0.565752	**H**	5.112286	-0.88624	1.051405
C	1.978729	-0.03319	0.975072	**H**	0.502651	3.736566	-0.97804
O	0.954737	-0.73801	1.715164	**H**	0.389855	4.250701	0.713999
O	4.256332	-0.85885	1.535004	**H**	1.689986	3.166067	0.198001
O	4.772568	-0.28669	-1.20576	**H**	-1.72952	3.838389	-1.42447
C	0.629955	3.405049	0.059118	**H**	-2.26506	2.178557	-1.75104
C	-2.30386	2.99714	-1.02293	**H**	-3.34962	3.316585	-0.94858
O	0.086156	-2.14312	-1.1939	**H**	-1.33944	-3.8834	-0.50702
O	-2.17691	-3.51277	-0.14894	**H**	-4.8686	-1.76606	0.459212

Conformer 1a-10							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	1.962705	0.369966	-0.34646	**O**	4.333617	0.06517	-0.67462
C	1.882616	1.745204	-0.9183	**H**	2.134998	1.723839	-1.98735
C	0.479102	2.361969	-0.70671	**H**	2.660907	2.369416	-0.4533
C	-0.03611	2.106884	0.741491	**H**	-0.21114	1.83426	-1.38257
C	-0.18235	0.555528	1.019169	**H**	-1.03996	2.544601	0.814749
C	1.035514	-0.16347	0.491941	**H**	-0.18222	0.43732	2.113203
C	1.434001	-1.53101	0.819396	**H**	3.545873	-1.43834	1.246881

C	2.892177	-1.70736	0.402367	**H**	2.87061	-1.08617	-1.66015
C	3.059791	-0.61985	-0.68206	**H**	-2.78648	0.709575	2.195016
C	-1.52575	0.018664	0.555503	**H**	-3.33523	-2.20075	-0.51019
C	-2.68084	0.200733	1.24448	**H**	-1.63421	-0.0634	-1.63143
C	-3.8169	-0.34242	0.50078	**H**	-0.74685	-2.34696	-0.16268
C	-3.26345	-1.11895	-0.69871	**H**	-4.92444	-0.6892	-1.69197
C	-1.77543	-0.72027	-0.76776	**H**	1.846006	2.310738	1.8639
O	-0.87543	-1.83039	-0.99001	**H**	0.957276	3.830298	1.663611
O	-3.96817	-0.75943	-1.90645	**H**	0.389847	2.621428	2.818899
O	-5.03377	-0.18121	0.706004	**H**	-0.54456	4.278159	-0.95781
C	0.844671	2.754545	1.830444	**H**	1.163962	4.438003	-0.50742
C	0.454195	3.849064	-1.09958	**H**	0.723717	3.972453	-2.15507
O	0.7358	-2.46513	1.273686	**H**	2.544731	-3.65596	0.357583
O	3.177443	-3.03297	-0.06381	**H**	5.027489	-0.51296	-1.04828

Table S3. Key thermodynamic parameters (a.u.) of **1b** with simplified structures at B3LYP/6-31+G(d,p) level in the gas phase.

Conformers	E+ZPE	G
1b-1	-1073.009262	-1073.128789
1b-2	-1073.002225	-1073.122484
1b-3	-1073.009243	-1073.128789
1b-4	-1073.009052	-1073.127726
1b-5	-1073.004552	-1073.126019
1b-6	-1073.002214	-1073.122484
1b-7	-1073.009116	-1073.127726
1b-8	-1073.001767	-1073.124408
1b-9	-1073.008362	-1073.125464
1b-10	-1073.004561	-1073.126019
1b-11	-1073.001761	-1073.124408
1b-12	-1073.001976	-1073.122999
1b-13	-1073.002066	-1073.122417

Table S4. Cartesian coordinates for the low-energy conformers of **1b** at B3LYP/6-31+G (d, p) level of theory in MeOH.

Conformer 1b-1							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	-2.22511	0.112977	0.457981	**O**	-4.41823	-0.87181	0.380392
C	-2.66079	1.471878	0.897333	**H**	-2.58399	1.527034	1.994695
C	-1.80632	2.577647	0.237943	**H**	-3.72588	1.597687	0.670348
C	-0.30028	2.222693	0.367838	**H**	-1.95984	3.499186	0.814944
C	0.051248	0.892184	-0.36857	**H**	-0.12256	2.050923	1.43891
C	-1.03535	-0.13821	-0.14192	**H**	0.107123	1.085622	-1.4485
C	-0.98597	-1.55207	-0.52529	**H**	-2.91794	-2.12056	-1.24772
C	-2.37433	-2.15198	-0.28881	**H**	-2.93242	-1.50147	1.690389
C	-3.05013	-1.14264	0.656173	**H**	1.283703	0.248553	2.229832
C	1.405257	0.351305	0.048975	**H**	3.331685	-1.82237	-0.36008
C	1.826624	0.084644	1.30502	**H**	2.949921	0.987196	-1.32738
C	3.200508	-0.42979	1.267741	**H**	1.414228	-1.31262	-1.88558
C	3.533633	-0.75054	-0.19433	**H**	5.395344	-0.57448	0.28286
C	2.48375	0.051457	-0.99334	**H**	0.559823	3.548018	-1.15122
O	1.981176	-0.56737	-2.15886	**H**	0.362287	4.296072	0.441646
O	4.867692	-0.4314	-0.52017	**H**	1.669051	3.141569	0.162932
O	3.999222	-0.55464	2.185361	**H**	-1.69058	3.658384	-1.66587
C	0.624181	3.365449	-0.07341	**H**	-2.18208	1.968048	-1.84236
C	-2.26917	2.853517	-1.20355	**H**	-3.32078	3.1589	-1.21183
O	-0.04481	-2.21102	-0.96298	**H**	-1.59794	-3.92754	-0.19217
O	-2.33482	-3.46164	0.234288	**H**	-4.94762	-1.63637	0.643147

Conformer 1b-2							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	1.921989	0.325546	-0.50094	**O**	4.265517	0.051835	-0.96319
C	1.911778	1.768913	-0.86896	**H**	2.048116	1.885087	-1.95271
C	0.633205	2.490699	-0.39881	**H**	2.812335	2.220736	-0.42681
C	0.158901	1.972454	0.989236	**H**	-0.15443	2.228846	-1.11542
C	-0.18939	0.453728	0.909634	**H**	-0.76226	2.50964	1.242007
C	1.002585	-0.27116	0.301205	**H**	-0.28802	0.069966	1.938283
C	1.474395	-1.62255	0.617927	**H**	3.588471	-1.51159	0.927146
C	2.905309	-1.76087	0.097786	**H**	2.778554	-1.03397	-1.92961
C	3.016543	-0.62614	-0.93547	**H**	-2.2777	2.154386	-0.28562
C	-1.54529	0.166686	0.271379	**H**	-3.30283	-1.44585	-1.5169
C	-2.41403	1.082353	-0.2151	**H**	-2.43322	-1.50142	1.32919
C	-3.68641	0.447078	-0.5743	**H**	-0.74922	-2.57365	0.340994
C	-3.48742	-1.06572	-0.49923	**H**	-5.38653	-1.23951	-0.18371
C	-2.18299	-1.23675	0.290728	**H**	2.115622	1.740121	1.979252

O	-1.39485	-2.2459	-0.30928	**H**	1.357376	3.316567	2.230469
O	-4.59004	-1.71899	0.096026	**H**	0.747103	1.901121	3.0848
O	-4.75523	0.9815	-0.8333	**H**	-0.11472	4.528369	-0.15103
C	1.156496	2.246362	2.129259	**H**	1.613892	4.359838	0.19734
C	0.804274	4.014503	-0.45444	**H**	1.043523	4.338578	-1.47338
O	0.893605	-2.53792	1.199904	**H**	2.696264	-3.68827	0.094892
O	3.18906	-3.03643	-0.42918	**H**	4.923429	-0.52262	-1.3765

Conformer 1b-3							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	-2.22535	0.112427	0.457451	**O**	-4.41814	-0.87277	0.377346
C	-2.66162	1.471087	0.896969	**H**	-2.58548	1.525808	1.994403
C	-1.80712	2.57727	0.238439	**H**	-3.72662	1.596749	0.669409
C	-0.30102	2.222555	0.368635	**H**	-1.96101	3.498553	0.815755
C	0.051011	0.892404	-0.36819	**H**	-0.12355	2.050457	1.439701
C	-1.0353	-0.13844	-0.14189	**H**	0.10675	1.08629	-1.44805
C	-0.98526	-1.55236	-0.5253	**H**	-2.9166	-2.12413	-1.24721
C	-2.37326	-2.15321	-0.28809	**H**	-2.93416	-1.50143	1.689944
C	-3.05031	-1.14328	0.655322	**H**	1.284237	0.249253	2.230075
C	1.405219	0.351933	0.049143	**H**	3.329886	-1.82206	-0.35987
C	1.826891	0.085357	1.305115	**H**	2.950172	0.988169	-1.32673
C	3.20077	-0.42912	1.267507	**H**	1.414409	-1.31121	-1.88637
C	3.533241	-0.7504	-0.1946	**H**	5.395156	-0.57544	0.281988
C	2.483616	0.052383	-0.99336	**H**	0.559412	3.548296	-1.14985
O	1.980969	-0.56552	-2.15931	**H**	0.360858	4.296166	0.442974
O	4.867384	-0.43298	-0.52105	**H**	1.668107	3.142046	0.16483
O	3.999817	-0.55357	2.184897	**H**	-1.69082	3.659014	-1.66475
C	0.623303	3.36566	-0.07202	**H**	-2.18186	1.968649	-1.84238
C	-2.26942	2.853756	-1.20313	**H**	-3.32111	3.158881	-1.21173
O	-0.04395	-2.21038	-0.96394	**H**	-1.59949	-3.93017	-0.19187
O	-2.33268	-3.46167	0.237942	**H**	-4.94788	-1.63694	0.640602

Conformer 1b-4							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	2.10461	0.093263	-0.31542	**O**	4.3259	-0.79327	-0.52191
C	2.417293	1.516974	-0.63628	**H**	2.842801	1.589549	-1.64533
C	1.168102	2.415969	-0.50667	**H**	3.218899	1.858443	0.035211
C	0.372039	2.120103	0.794369	**H**	0.504716	2.159536	-1.34269
C	-0.09223	0.623903	0.860075	**H**	-0.53169	2.741766	0.765915
C	0.996475	-0.29186	0.36061	**H**	-0.26504	0.378731	1.91472
C	0.994363	-1.75085	0.486738	**H**	2.989064	-2.3511	0.985192
C	2.37834	-2.25644	0.071957	**H**	2.777433	-1.29183	-1.81649
C	2.952904	-1.08429	-0.7495	**H**	-1.04467	0.740736	-1.96331

C	-1.40247	0.328222	0.156324	**H**	-3.45941	-1.74112	-0.20361
C	-1.69434	0.41036	-1.16116	**H**	-3.0629	0.678373	1.510401
C	-3.08929	0.010994	-1.38662	**H**	-1.62226	-1.75168	1.591585
C	-3.59282	-0.65091	-0.09893	**H**	-5.38293	-0.22229	-0.68022
C	-2.59982	-0.16132	0.976435	**H**	2.036238	1.854863	2.20671
O	-2.24503	-1.10227	1.969436	**H**	1.457818	3.522884	2.082126
O	-4.93754	-0.33041	0.176285	**H**	0.508652	2.322632	2.958611
O	-3.7872	0.186227	-2.37504	**H**	0.643027	4.534111	-0.58185
C	1.142478	2.47585	2.079228	**H**	2.258402	4.228574	0.078337
C	1.530829	3.898386	-0.67039	**H**	1.971262	4.079547	-1.65701
O	0.075783	-2.49498	0.823149	**H**	1.619517	-4.00789	-0.27334
O	2.337651	-3.47056	-0.64454	**H**	4.865597	-1.47189	-0.94872

Conformer 1b-5							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	2.039558	0.298387	-0.4174	**O**	4.417243	0.057945	-0.6589
C	1.944808	1.667026	-1.00703	**H**	2.217051	1.63727	-2.07051
C	0.539521	2.279429	-0.82458	**H**	2.7149	2.296244	-0.53677
C	-0.02517	2.005011	0.595589	**H**	-0.12874	1.759508	-1.52579
C	-0.16373	0.459565	0.825278	**H**	-1.03154	2.43914	0.634295
C	1.107499	-0.23227	0.40888	**H**	-0.31627	0.297187	1.900756
C	1.549191	-1.56963	0.834848	**H**	3.648806	-1.43176	1.255821
C	3.014183	-1.72635	0.403494	**H**	3.047081	-1.13227	-1.67177
C	3.185354	-0.65558	-0.68888	**H**	-0.65151	-1.31815	-1.49045
C	-1.39401	-0.10853	0.164454	**H**	-3.74241	-1.63631	0.756485
C	-1.47596	-0.941	-0.89754	**H**	-3.07053	1.251702	0.245508
C	-2.88126	-1.26028	-1.17148	**H**	-3.64906	0.64975	2.38386
C	-3.68969	-0.79577	0.044944	**H**	-5.24399	-0.79906	-1.10111
C	-2.78122	0.277087	0.6683	**H**	1.802425	2.232064	1.797449
O	-2.78204	0.341745	2.088183	**H**	0.876895	3.726994	1.60091
O	-4.97787	-0.33216	-0.29107	**H**	0.298595	2.468407	2.694682
O	-3.3911	-1.75403	-2.16637	**H**	-0.4769	4.192729	-1.09945
C	0.790057	2.644476	1.732383	**H**	1.211353	4.353381	-0.58685
C	0.52626	3.765188	-1.20686	**H**	0.8331	3.898029	-2.25032
O	0.919392	-2.44944	1.403375	**H**	2.766131	-3.64328	0.482625
O	3.32177	-3.03344	-0.03039	**H**	5.123108	-0.52704	-0.96448

Conformer 1b-6							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	1.921715	0.325401	-0.50119	**O**	4.265267	0.051652	-0.96352
C	1.91131	1.768634	-0.86968	**H**	2.046517	1.884272	-1.95365
C	0.633141	2.490748	-0.3988	**H**	2.812329	2.220618	-0.42869
C	0.159247	1.97252	0.989391	**H**	-0.15492	2.22922	-1.11507

C	-0.18929	0.453817	0.909833	**H**	-0.76172	2.509842	1.242516
C	1.002424	-0.2712	0.301167	**H**	-0.28766	0.070095	1.938523
C	1.474365	-1.62251	0.618158	**H**	3.588464	-1.512	0.926832
C	2.905076	-1.76094	0.097561	**H**	2.778191	-1.03414	-1.92979
C	3.016272	-0.62629	-0.93566	**H**	-2.27803	2.154728	-0.28439
C	-1.54535	0.166907	0.27186	**H**	-3.30168	-1.44498	-1.51741
C	-2.41419	1.082647	-0.21434	**H**	-2.43409	-1.50073	1.329472
C	-3.68638	0.447297	-0.57396	**H**	-0.74917	-2.57334	0.342391
C	-3.48707	-1.06547	-0.49967	**H**	-5.38631	-1.2398	-0.18549
C	-2.1831	-1.23659	0.291035	**H**	2.11662	1.740509	1.978184
O	-1.39484	-2.246	-0.30806	**H**	1.357786	3.316451	2.230737
O	-4.58996	-1.71942	0.094424	**H**	0.748658	1.900263	3.084624
O	-4.75531	0.981594	-0.83287	**H**	-0.11419	4.52864	-0.15093
C	1.157342	2.246216	2.129034	**H**	1.614423	4.359618	0.197255
C	0.804628	4.014498	-0.45441	**H**	1.043861	4.338541	-1.47338
O	0.893815	-2.53763	1.200767	**H**	2.697035	-3.68851	0.095323
O	3.18851	-3.0365	-0.42979	**H**	4.923154	-0.52298	-1.37664

Conformer 1b-7							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	2.10456	0.09286	-0.31523	**O**	4.325721	-0.79417	-0.52106
C	2.417534	1.516371	-0.63664	**H**	2.842848	1.588401	-1.64581
C	1.16862	2.41575	-0.50711	**H**	3.219416	1.857915	0.034503
C	0.372637	2.120322	0.794067	**H**	0.505049	2.159325	-1.343
C	-0.09221	0.624332	0.85996	**H**	-0.53082	2.742376	0.765715
C	0.996271	-0.29189	0.360737	**H**	-0.26516	0.379371	1.914631
C	0.993775	-1.75085	0.486923	**H**	2.988342	-2.35213	0.985487
C	2.377788	-2.25686	0.072245	**H**	2.777493	-1.29234	-1.81611
C	2.952686	-1.08495	-0.74902	**H**	-1.04482	0.741209	-1.96348
C	-1.40244	0.328812	0.156188	**H**	-3.46015	-1.74064	-0.203
C	-1.69439	0.410741	-1.16127	**H**	-3.06299	0.679539	1.509872
C	-3.08913	0.010665	-1.38686	**H**	-1.6235	-1.7512	1.592232
C	-3.59288	-0.65031	-0.09867	**H**	-5.38394	-0.22432	-0.67938
C	-2.59986	-0.16052	0.976488	**H**	2.036833	1.854317	2.206283
O	-2.24529	-1.10081	1.969968	**H**	1.459454	3.522672	2.081468
O	-4.9373	-0.32874	0.176895	**H**	0.509607	2.323179	2.958244
O	-3.78658	0.184562	-2.37581	**H**	0.643957	4.533953	-0.5831
C	1.143447	2.475837	2.07877	**H**	2.259033	4.228338	0.077771
C	1.531676	3.898041	-0.67112	**H**	1.972514	4.078835	-1.65763
O	0.075105	-2.4948	0.823438	**H**	1.618024	-4.00783	-0.27337
O	2.336468	-3.47091	-0.64457	**H**	4.865309	-1.47225	-0.94893

Conformer 1b-8							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	-2.14623	0.082693	0.368867	**O**	-4.37076	-0.83558	0.35081
C	-2.50592	1.394216	0.983294	**H**	-2.31263	1.33404	2.065655
C	-1.69343	2.546639	0.355423	**H**	-3.58432	1.56063	0.879818
C	-0.18535	2.173002	0.317455	**H**	-1.77779	3.411756	1.026555
C	0.070959	0.90084	-0.5673	**H**	0.092259	1.900516	1.341939
C	-1.00859	-0.13339	-0.33334	**H**	0.014655	1.209315	-1.62182
C	-1.01489	-1.51621	-0.83059	**H**	-3.01002	-1.92691	-1.5072
C	-2.41722	-2.08747	-0.59146	**H**	-2.81789	-1.63341	1.478816
C	-2.9943	-1.16673	0.497263	**H**	2.490194	1.069943	-2.14641
C	1.466213	0.357386	-0.36135	**H**	3.686483	0.391183	1.45242
C	2.51705	0.564088	-1.18764	**H**	1.568119	-1.56539	0.575747
C	3.719811	-0.07022	-0.64125	**H**	1.40833	-0.77362	2.697883
C	3.399878	-0.45559	0.806318	**H**	4.83683	-1.73853	0.671864
C	1.86339	-0.53374	0.809905	**H**	0.541737	3.623851	-1.1612
O	1.242223	-0.10462	2.020419	**H**	0.471871	4.236213	0.497908
O	4.041048	-1.63965	1.221336	**H**	1.758528	3.12662	0.017395
O	4.786955	-0.3206	-1.18243	**H**	-1.73451	3.802485	-1.44253
C	0.696631	3.353367	-0.11064	**H**	-2.26722	2.138722	-1.72881
C	-2.28054	2.961391	-1.00546	**H**	-3.32396	3.273099	-0.8887
O	-0.10338	-2.17131	-1.32003	**H**	-1.64305	-3.8572	-0.6885
O	-2.39871	-3.45177	-0.23177	**H**	-4.90145	-1.61676	0.555477

Conformer 1b-9							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	-2.2361	0.096543	0.458624	**O**	-4.45803	-0.9714	0.354135
C	-2.66537	1.450412	0.922189	**H**	-2.56891	1.48616	2.018747
C	-1.82028	2.566685	0.269406	**H**	-3.73501	1.586107	0.722048
C	-0.31237	2.215714	0.387531	**H**	-1.97448	3.481671	0.856432
C	0.040493	0.890961	-0.35886	**H**	-0.12803	2.038026	1.456382
C	-1.04214	-0.14561	-0.13665	**H**	0.091542	1.091899	-1.43781
C	-0.97802	-1.56024	-0.51533	**H**	-2.87601	-2.25058	-1.22522
C	-2.35079	-2.19294	-0.25442	**H**	-3.04147	-1.50243	1.670162
C	-3.0772	-1.16115	0.629355	**H**	1.288833	0.231043	2.22894
C	1.399407	0.354734	0.048378	**H**	3.337738	-1.80135	-0.38895
C	1.828374	0.080084	1.299936	**H**	2.933315	1.014525	-1.32927
C	3.206301	-0.4237	1.251175	**H**	1.414275	-1.29246	-1.90084
C	3.534069	-0.72963	-0.21538	**H**	5.397655	-0.547	0.252259
C	2.475079	0.0726	-1.00176	**H**	0.535391	3.553065	-1.12827
O	1.970563	-0.53831	-2.17086	**H**	0.34223	4.291409	0.469871
O	4.863885	-0.39908	-0.54583	**H**	1.651952	3.143673	0.178501
O	4.010549	-0.54983	2.163414	**H**	-1.72328	3.673219	-1.62074

C	0.605228	3.36478	-0.05174	**H**	-2.19436	1.981251	-1.81852
C	-2.29146	2.856553	-1.16655	**H**	-3.34606	3.152609	-1.16753
O	-0.03036	-2.20321	-0.96165	**H**	-1.51803	-3.93363	-0.08092
O	-2.25667	-3.46598	0.340525	**H**	-4.5782	-0.78962	-0.58856

Conformer 1b-10							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	2.039246	0.298619	-0.41771	**O**	4.416911	0.058552	-0.66032
C	1.944036	1.667214	-1.00739	**H**	2.215805	1.637406	-2.07099
C	0.538711	2.279391	-0.82444	**H**	2.714218	2.296583	-0.5375
C	-0.02545	2.004827	0.595889	**H**	-0.1297	1.759393	-1.52545
C	-0.16381	0.459361	0.825399	**H**	-1.03183	2.438922	0.63501
C	1.107492	-0.23221	0.408808	**H**	-0.31629	0.296768	1.900859
C	1.549757	-1.56931	0.835077	**H**	3.649122	-1.43007	1.255636
C	3.014656	-1.72556	0.40344	**H**	3.046453	-1.13216	-1.67202
C	3.185174	-0.6551	-0.68937	**H**	-0.65143	-1.31896	-1.48994
C	-1.39406	-0.10885	0.164579	**H**	-3.74341	-1.63607	0.756425
C	-1.47591	-0.9416	-0.8972	**H**	-3.07046	1.251618	0.24557
C	-2.88116	-1.26114	-1.17119	**H**	-3.6489	0.650476	2.383727
C	-3.68983	-0.79575	0.044681	**H**	-5.24498	-0.80019	-1.10033
C	-2.78128	0.276908	0.668224	**H**	1.80275	2.232182	1.796768
O	-2.78226	0.341321	2.088141	**H**	0.876532	3.726819	1.601245
O	-4.97752	-0.33116	-0.292	**H**	0.299342	2.467656	2.694947
O	-3.39059	-1.75609	-2.16569	**H**	-0.47804	4.192594	-1.09874
C	0.790188	2.644226	1.732425	**H**	1.210451	4.3534	-0.58696
C	0.525111	3.765169	-1.20666	**H**	0.831423	3.898085	-2.25026
O	0.920452	-2.44911	1.40416	**H**	2.76827	-3.64263	0.483746
O	3.323071	-3.03253	-0.02984	**H**	5.122836	-0.527	-0.96465

Conformer 1b-11							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	-2.14609	0.082653	0.368932	**O**	-4.3704	-0.83623	0.351881
C	-2.50615	1.394255	0.982974	**H**	-2.31348	1.334343	2.065457
C	-1.69359	2.546699	0.355235	**H**	-3.58454	1.560445	0.878959
C	-0.18551	2.17312	0.317476	**H**	-1.77807	3.411786	1.026395
C	0.07095	0.901056	-0.56729	**H**	0.091972	1.900589	1.341978
C	-1.00846	-0.1333	-0.33335	**H**	0.014822	1.209522	-1.62182
C	-1.01462	-1.51613	-0.83069	**H**	-3.00972	-1.92601	-1.50734
C	-2.41691	-2.08738	-0.5917	**H**	-2.8167	-1.63389	1.478805
C	-2.99385	-1.16695	0.497485	**H**	2.490506	1.070437	-2.146
C	1.466203	0.357546	-0.36124	**H**	3.68652	0.39039	1.452823
C	2.517129	0.564304	-1.18737	**H**	1.56761	-1.56541	0.575825
C	3.719817	-0.07018	-0.641	**H**	1.409543	-0.77264	2.698369

C	3.399643	-0.45604	0.80636	**H**	4.83678	-1.73887	0.672574
C	1.863155	-0.53382	0.809905	**H**	0.542297	3.623668	-1.16114
O	1.242021	-0.10447	2.020415	**H**	0.471401	4.236481	0.497758
O	4.040221	-1.64057	1.220991	**H**	1.758446	3.12686	0.018315
O	4.787133	-0.32009	-1.18205	**H**	-1.73462	3.80282	-1.4425
C	0.696606	3.35349	-0.11041	**H**	-2.26683	2.138971	-1.72919
C	-2.28054	2.961513	-1.00569	**H**	-3.32406	3.272922	-0.8891
O	-0.10306	-2.17097	-1.32033	**H**	-1.6436	-3.85745	-0.68954
O	-2.39897	-3.45169	-0.2327	**H**	-4.90077	-1.61781	0.555836

Conformer 1b-12							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	1.980552	0.159407	-0.28181	**O**	4.277388	-0.48142	-0.58414
C	2.08618	1.528831	-0.86438	**H**	2.351167	1.457884	-1.92755
C	0.778923	2.330106	-0.68783	**H**	2.937572	2.042751	-0.39348
C	0.191374	2.15357	0.737536	**H**	0.048762	1.892842	-1.37835
C	-0.14435	0.64438	1.021288	**H**	-0.75553	2.706231	0.770277
C	0.989089	-0.23162	0.552083	**H**	-0.20687	0.537401	2.112891
C	1.19384	-1.6378	0.913121	**H**	3.291391	-1.88305	1.30469
C	2.603636	-2.03161	0.455901	**H**	2.698578	-1.37737	-1.59816
C	2.939225	-0.96733	-0.60494	**H**	-2.75852	1.004032	2.130458
C	-1.51522	0.226935	0.518738	**H**	-3.44319	0.369038	-1.62445
C	-2.66851	0.505566	1.171139	**H**	-1.57163	-1.68111	-0.45562
C	-3.8126	-0.04933	0.444661	**H**	-1.10053	-0.87307	-2.52795
C	-3.3003	-0.47765	-0.93237	**H**	-4.81389	-1.67525	-1.01758
C	-1.78499	-0.63345	-0.71177	**H**	2.039882	2.163039	1.929995
O	-0.98724	-0.22404	-1.82055	**H**	1.326906	3.764084	1.690884
O	-3.93147	-1.63824	-1.42333	**H**	0.592188	2.632585	2.826515
O	-4.96402	-0.22152	0.817441	**H**	0.037697	4.365043	-0.96843
C	1.09299	2.708454	1.855263	**H**	1.741098	4.294996	-0.48543
C	0.969379	3.799913	-1.08506	**H**	1.272716	3.876955	-2.13523
O	0.411754	-2.42158	1.437236	**H**	2.020555	-3.87592	0.471513
O	2.672773	-3.35625	-0.02695	**H**	4.862771	-1.16702	-0.93206

Conformer 1b-13							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	2.268998	0.123408	-0.42638	**O**	4.506251	-0.72661	-0.18115
C	2.660778	1.467083	-0.9499	**H**	2.641827	1.434338	-2.05057
C	1.719386	2.573297	-0.42577	**H**	3.703735	1.668798	-0.67934
C	0.240767	2.123928	-0.57967	**H**	1.845771	3.449432	-1.07588
C	-0.06323	0.84637	0.272572	**H**	0.11609	1.833974	-1.6331
C	1.066787	-0.14952	0.134161	**H**	-0.12949	1.136718	1.329175
C	1.060654	-1.5522	0.588053	**H**	2.979187	-1.91727	1.474308

C	2.502031	-2.06877	0.491738	**H**	3.122859	-1.53521	-1.50415
C	3.167659	-1.09577	-0.49552	**H**	-1.05864	-0.62443	-2.06683
C	-1.3988	0.23933	-0.09222	**H**	-3.32699	-1.62874	0.841023
C	-1.71127	-0.43389	-1.22209	**H**	-3.09008	1.366427	0.62369
C	-3.10348	-0.88776	-1.15856	**H**	-3.0136	0.469894	2.723822
C	-3.56449	-0.70376	0.290983	**H**	-5.375	-0.76215	-0.37705
C	-2.61641	0.390038	0.810906	**H**	-0.77887	3.521577	0.768512
O	-2.23792	0.291426	2.1759	**H**	-0.47997	4.158192	-0.85645
O	-4.93265	-0.37998	0.39961	**H**	-1.76872	2.984103	-0.59431
O	-3.83318	-1.30357	-2.04743	**H**	1.452772	3.797407	1.374593
C	-0.75294	3.258447	-0.29423	**H**	2.049534	2.16509	1.709642
C	2.102382	2.999694	1.002371	**H**	3.130106	3.377452	1.021307
O	0.128405	-2.25133	0.955641	**H**	1.780103	-3.86134	0.440538
O	2.574664	-3.42075	0.095938	**H**	5.081885	-1.48725	-0.33577

Table S5. Key thermodynamic parameters (a.u.) of **2** with simplified structures at B3LYP/6-31+G(d,p) level in the gas phase.

Conformers	E+ZPE	G
2a	-1538.503733	-1538.954123
2b	-1538.503838	-1538.942894
2c	-1538.505274	-1538.952712
2d	-1538.501385	-1538.946164
2e	-1538.503135	-1538.943059
2f	-1538.500203	-1538.950819
2g	-1538.499764	-1538.939735
2h	-1538.500448	-1538.943495
2i	-1538.503135	-1538.943059
2j	-1538.501233	-1538.943499
2k	-1538.501803	-1538.949713
2l	-1538.499744	-1538.940269
2m	-1538.49722	-1538.939318

Table S6. Cartesian coordinates for the low-energy conformers of **2** at B3LYP/6-31+G (d, p) level of theory in MeOH.

Conformer 2a							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	4.144003	-2.11362	-0.29700	**H**	4.442706	-3.1228	0.002552
C	4.654663	-1.14652	0.751943	**H**	4.654871	-1.89794	-1.24586
C	4.202875	0.321734	0.633489	**H**	2.126573	-2.40562	0.418208
C	2.643484	0.336668	0.360102	**H**	2.337456	-2.70944	-1.30544
C	2.094939	-0.58653	-0.79099	**H**	2.370971	2.26874	1.261545
C	2.615982	-2.0299	-0.49182	**H**	0.093019	2.710355	0.359928
C	2.016353	1.741999	0.36632	**H**	0.25174	1.368833	1.484707
C	0.484253	1.692818	0.467818	**H**	-0.08342	-1.10569	-2.66699
C	-0.23843	0.756042	-0.55208	**H**	0.325347	-2.51188	-1.71201
C	0.513856	-0.62839	-0.62945	**H**	3.823758	0.720762	2.765425
C	-1.71085	0.426034	-0.03903	**H**	5.520638	0.797966	2.293123
C	-2.54141	-0.60808	-0.94339	**H**	4.429643	2.12775	1.857846
C	-1.64655	-1.79994	-1.38274	**H**	6.127183	1.013351	-0.11686
C	-0.17848	-1.54261	-1.66538	**H**	5.070912	0.440179	-1.41527
C	-1.77513	-0.30958	1.371286	**H**	4.740187	1.997869	-0.66073
C	-3.0231	-1.20436	1.470653	**H**	3.559104	-0.54136	-2.42886
C	-3.57863	-1.18582	0.046616	**H**	1.900037	-0.6398	-2.97762
O	5.43606	-1.52757	1.640669	**H**	2.550268	0.895642	-2.35918
C	4.506163	1.041815	1.969572	**H**	-0.58346	0.818698	-2.75157
C	5.089239	0.982252	-0.46793	**H**	-0.9572	2.322067	-1.90801
H	2.226032	-0.11557	1.277421	**H**	0.71975	1.851103	-2.1634
C	2.547	-0.18378	-2.22142	**H**	-2.57072	0.214865	-2.98381
C	-0.27532	1.471748	-1.93426	**H**	-3.98912	-0.74866	-2.52686
C	-3.26327	-0.01229	-2.17250	**H**	-3.81903	0.894897	-1.91572
O	-3.96313	-0.65856	2.430116	**H**	-4.31346	0.185703	2.067131
O	-4.69383	-1.60162	-0.27817	**H**	-3.22702	-3.23805	-1.44638
O	-0.96822	-0.17594	2.292274	**H**	-1.55715	-3.83469	-1.95143
H	0.373078	-1.10029	0.352806	**H**	-2.28128	-2.51271	2.991421
C	-2.17621	-3.01647	-1.59497	**H**	-3.62148	-3.18402	2.022571
C	-2.69315	-2.60867	1.983463	**H**	-1.97371	-3.11951	1.339876
C	-2.63599	1.63252	0.202062	**H**	-2.51146	4.876234	-0.2127
O	-2.17402	2.863344	-0.13398	**H**	-4.00443	3.888455	-0.41295
O	-3.77273	1.501479	0.699906	**H**	-3.27736	4.072578	1.20602
C	-3.07049	4.011701	0.136745	**H**	2.111591	3.412805	-0.76493
O	2.483447	2.508423	-0.8054				

Conformer 2b							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	4.242013	-2.0788	0.252371	**H**	4.566755	-2.97276	0.793471
C	4.722441	-0.86648	1.024032	**H**	4.749667	-2.09291	-0.72232
C	4.237047	0.511124	0.534812	**H**	2.228678	-2.24343	1.021948
C	2.676619	0.414302	0.285916	**H**	2.459126	-2.95506	-0.57489
C	2.152086	-0.7797	-0.59729	**H**	2.32683	2.489849	0.715665
C	2.712653	-2.08891	0.04692	**H**	0.057711	2.646342	-0.28037
C	2.005232	1.760624	-0.03887	**H**	0.22134	1.599716	1.11407
C	0.471528	1.687361	0.0549	**H**	-0.06109	-1.88487	-2.20717
C	-0.19614	0.520634	-0.73536	**H**	0.432663	-2.93876	-0.89604
C	0.575088	-0.81356	-0.4147	**H**	3.862278	1.436264	2.496974
C	-1.71162	0.317368	-0.24682	**H**	5.552151	1.43581	1.995417
C	-2.46474	-0.95983	-0.87938	**H**	4.417628	2.576864	1.247089
C	-1.54751	-2.19622	-0.69965	**H**	6.141013	1.020353	-0.39236
C	-0.1045	-2.01316	-1.11784	**H**	5.085836	0.115489	-1.48689
C	-1.90126	0.006846	1.270717	**H**	4.729953	1.808906	-1.15103
C	-3.3091	-0.57125	1.474173	**H**	3.59125	-1.14001	-2.21985
C	-3.64372	-1.12494	0.085041	**H**	1.921148	-1.35198	-2.70317
O	5.502935	-0.99099	1.983774	**H**	2.588498	0.280137	-2.48202
C	4.528383	1.559525	1.634828	**H**	-0.41398	0.04842	-2.89862
C	5.100964	0.8825	-0.71031	**H**	-0.95607	1.659187	-2.45124
H	2.278246	0.186277	1.290678	**H**	0.770045	1.302713	-2.52116
C	2.584217	-0.73441	-2.08828	**H**	-2.14683	-1.11222	-3.04825
C	-0.20038	0.894431	-2.24453	**H**	-3.70339	-1.71403	-2.46044
C	-2.9591	-0.92053	-2.34526	**H**	-3.42168	0.035189	-2.58473
O	-4.20959	0.579785	1.670666	**H**	-5.12507	0.266288	1.493623
O	-4.75924	-1.58256	-0.19124	**H**	-3.04968	-3.56024	-0.02169
O	-1.0706	0.103071	2.174243	**H**	-1.35176	-4.24545	-0.21582
H	0.443813	-0.97162	0.663553	**H**	-3.19695	-1.04119	3.560906
C	-2.01105	-3.38487	-0.27996	**H**	-4.44657	-1.95612	2.667013
C	-3.42764	-1.55717	2.62564	**H**	-2.73117	-2.39175	2.503935
C	-2.53029	1.608939	-0.46699	**H**	-2.70878	4.313265	1.385198
O	-2.28514	2.507697	0.536427	**H**	-3.0941	4.238272	-0.37377
O	-3.301	1.861052	-1.39849	**H**	-4.15371	3.413593	0.809997
C	-3.12943	3.712662	0.581874	**H**	2.09512	3.139375	-1.51416
O	2.473908	2.252066	-1.34908				

Conformer 2c							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	4.183435	-2.08348	-0.06024	**H**	4.471102	-3.0608	0.339174
C	4.677909	-1.02353	0.903769	**H**	4.714444	-1.95999	-1.01447
C	4.234495	0.42888	0.642123	**H**	2.15191	-2.29893	0.639636

C	2.681591	0.424451	0.334283	**H**	2.39201	-2.76511	-1.04362
C	2.153473	-0.60228	-0.73627	**H**	2.408448	2.438673	1.036602
C	2.660213	-2.013	-0.29252	**H**	0.138104	2.791913	0.068672
C	2.063307	1.82761	0.192845	**H**	0.285091	1.566214	1.319385
C	0.530612	1.790223	0.278979	**H**	0.039692	-1.25846	-2.61672
C	-0.17614	0.759564	-0.65683	**H**	0.377546	-2.58964	-1.53517
C	0.568721	-0.6258	-0.60732	**H**	3.81004	1.024305	2.71921
C	-1.6559	0.479035	-0.12361	**H**	5.517908	1.048292	2.281206
C	-2.48609	-0.60621	-0.95915	**H**	4.447066	2.338349	1.700875
C	-1.59317	-1.81814	-1.35624	**H**	6.175411	1.054776	-0.1234
C	-0.10632	-1.61014	-1.58833	**H**	5.154124	0.353972	-1.38642
C	-1.72672	-0.12431	1.334876	**H**	4.799817	1.975489	-0.79396
C	-2.905	-1.10124	1.483773	**H**	3.65978	-0.70017	-2.33229
C	-3.49653	-1.14884	0.075667	**H**	2.017742	-0.8692	-2.91254
O	5.441255	-1.32297	1.83833	**H**	2.638129	0.725878	-2.42733
C	4.512843	1.26697	1.913398	**H**	-0.5572	0.648861	-2.84948
C	5.146767	0.984904	-0.49553	**H**	-0.85294	2.233555	-2.12733
H	2.241695	0.063214	1.281043	**H**	0.79724	1.67146	-2.36886
C	2.63965	-0.33536	-2.18702	**H**	-2.5616	0.119214	-3.03427
C	-0.20823	1.354607	-2.09471	**H**	-3.96206	-0.83568	-2.50956
C	-3.23747	-0.07781	-2.20155	**H**	-3.79503	0.83794	-1.98083
O	-3.8567	-0.61213	2.460012	**H**	-4.20863	0.242786	2.134356
O	-4.62366	-1.56783	-0.20075	**H**	-3.20881	-3.21406	-1.45587
O	-0.97982	0.162974	2.273087	**H**	-1.53947	-3.86383	-1.89315
H	0.403649	-1.01951	0.406185	**H**	-2.02571	-2.3198	3.005538
C	-2.14763	-3.02318	-1.57174	**H**	-3.34668	-3.10605	2.098503
C	-2.46207	-2.46953	2.01439	**H**	-1.73248	-2.94693	1.357564
C	-2.48379	1.773777	-0.0437	**H**	-5.52423	2.300023	1.144405
O	-3.69399	1.556004	0.60514	**H**	-4.18483	3.496244	1.284875
O	-2.20052	2.893823	-0.46623	**H**	-4.83422	3.073588	-0.32385
C	-4.6262	2.702551	0.680465	**H**	2.162869	3.369385	-1.10735
O	2.548367	2.472104	-1.04205				

Conformer 2d							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	4.219359	-2.08812	0.257331	**H**	4.537714	-2.98382	0.799318
C	4.697237	-0.87831	1.034368	**H**	4.733505	-2.10227	-0.7139
C	4.220395	0.501786	0.543088	**H**	2.200913	-2.24573	1.014103
C	2.661484	0.411166	0.282421	**H**	2.437559	-2.95753	-0.58157
C	2.13981	-0.78136	-0.60534	**H**	2.320761	2.489866	0.708019
C	2.691345	-2.09276	0.04206	**H**	0.053994	2.652845	-0.30076
C	1.998702	1.761462	-0.04716	**H**	0.210141	1.607217	1.098985
C	0.464118	1.692868	0.040455	**H**	-0.07309	-1.85728	-2.24008

C	-0.20161	0.52594	-0.74969	**H**	0.408122	-2.92961	-0.94011
C	0.561862	-0.81161	-0.43333	**H**	3.835037	1.425807	2.50374
C	-1.71625	0.324503	-0.24741	**H**	5.528428	1.419233	2.014532
C	-2.48699	-0.9337	-0.88554	**H**	4.40423	2.565967	1.259534
C	-1.57078	-2.18052	-0.74537	**H**	6.132972	1.003932	-0.37019
C	-0.12266	-1.998	-1.15272	**H**	5.080815	0.106251	-1.47358
C	-1.88324	-0.01217	1.264266	**H**	4.731018	1.800606	-1.13691
C	-3.28298	-0.60738	1.487346	**H**	3.589526	-1.14667	-2.2173
C	-3.65802	-1.12703	0.096361	**H**	1.92224	-1.35187	-2.71301
O	5.468634	-1.00626	2.000989	**H**	2.594275	0.277456	-2.48671
C	4.507873	1.547597	1.646577	**H**	0.775004	1.289633	-2.53457
C	5.094457	0.871564	-0.69538	**H**	-0.42885	0.054197	-2.91113
H	2.254379	0.184476	1.284024	**H**	-0.94561	1.672906	-2.46731
C	2.583152	-0.7371	-2.09317	**H**	-2.21024	-1.03953	-3.063
C	-0.20247	0.897911	-2.25866	**H**	-3.75292	-1.66005	-2.45453
C	-3.00918	-0.86626	-2.33992	**H**	-3.47779	0.092816	-2.55414
O	-4.21427	0.506409	1.728831	**H**	-3.95153	0.960231	2.558391
O	-4.73774	-1.65419	-0.17355	**H**	-3.0786	-3.56659	-0.1267
O	-1.06597	0.141224	2.177237	**H**	-1.38089	-4.24692	-0.34278
H	0.424589	-0.97997	0.6427	**H**	-3.04458	-1.1928	3.548261
C	-2.0391	-3.38355	-0.37401	**H**	-4.40118	-1.98429	2.687277
C	-3.36732	-1.63997	2.601823	**H**	-2.71957	-2.49701	2.396839
C	-2.50521	1.632059	-0.46072	**H**	-2.84558	4.271897	1.465668
O	-2.36947	2.478114	0.615051	**H**	-2.89806	4.29444	-0.33349
O	-3.15204	1.958707	-1.45944	**H**	-4.20861	3.496944	0.579303
C	-3.14252	3.731929	0.569002	**H**	2.098603	3.134791	-1.52725
O	2.475184	2.247821	-1.35558				

Conformer 2e							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	4.170259	-2.09099	-0.06017	**H**	4.454167	-3.06914	0.339963
C	4.67154	-1.03219	0.901766	**H**	4.700057	-1.97123	-1.01554
C	4.233637	0.421702	0.640284	**H**	2.138769	-2.29491	0.643565
C	2.6807	0.424098	0.332389	**H**	2.374346	-2.76649	-1.03893
C	2.146836	-0.60129	-0.73585	**H**	2.416657	2.441196	1.029437
C	2.647042	-2.01366	-0.29016	**H**	0.144703	2.799973	0.071798
C	2.067792	1.828854	0.188159	**H**	0.290937	1.576434	1.318785
C	0.536138	1.797809	0.277969	**H**	0.034111	-1.23573	-2.62249
C	-0.17915	0.772089	-0.65761	**H**	0.375331	-2.5755	-1.55252
C	0.561375	-0.6161	-0.61026	**H**	3.81036	1.019186	2.71713
C	-1.66083	0.500101	-0.13151	**H**	5.518739	1.035987	2.280025
C	-2.48648	-0.59933	-0.95827	**H**	4.453218	2.330257	1.699111
C	-1.59588	-1.80809	-1.36739	**H**	6.176025	1.046859	-0.12221

C	-0.11097	-1.59675	-1.5972	**H**	5.158979	0.3415	-1.38586
C	-1.75333	-0.056	1.351152	**H**	4.801077	1.964342	-0.79911
C	-2.85579	-1.11071	1.483921	**H**	3.658369	-0.69247	-2.32695
C	-3.46961	-1.13632	0.092334	**H**	2.020122	-0.88323	-2.91084
O	5.435857	-1.33469	1.834623	**H**	2.622079	0.721695	-2.43264
C	4.514721	1.258697	1.911748	**H**	-0.58116	0.676035	-2.84798
C	5.148442	0.975048	-0.4968	**H**	-0.85754	2.258222	-2.11106
H	2.239776	0.066532	1.280163	**H**	0.786188	1.686444	-2.37581
C	2.633983	-0.33817	-2.18678	**H**	-2.58212	0.122099	-3.03126
C	-0.21817	1.374115	-2.09224	**H**	-3.96512	-0.85461	-2.50682
C	-3.25418	-0.08424	-2.19745	**H**	-3.82635	0.819778	-1.97301
O	-3.83889	-0.6857	2.463738	**H**	-4.72564	-0.91035	2.101271
O	-4.62641	-1.52196	-0.11952	**H**	-3.21779	-3.19522	-1.47695
O	-1.05468	0.298596	2.301161	**H**	-1.55263	-3.85069	-1.92055
H	0.389741	-1.00989	0.403584	**H**	-1.88917	-2.32318	2.95644
C	-2.15532	-3.00881	-1.59241	**H**	-3.08117	-3.20521	1.963139
C	-2.27695	-2.46333	1.943836	**H**	-1.47891	-2.8256	1.292037
C	-2.49523	1.7946	-0.06034	**H**	-5.46617	2.188603	1.296188
O	-3.72921	1.512904	0.472683	**H**	-4.14481	3.409688	1.294259
O	-2.16939	2.940677	-0.37535	**H**	-5.01084	3.036904	-0.2238
C	-4.65375	2.630714	0.724665	**H**	2.166913	3.364889	-1.11784
O	2.553683	2.468372	-1.04951				

Conformer 2f							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	3.773863	-2.20453	0.661682	**H**	3.449135	-2.13763	1.709523
C	4.747692	-1.08125	0.396892	**H**	4.289229	-3.16012	0.535273
C	4.212059	0.338096	0.655542	**H**	1.708329	-2.64263	0.229265
C	2.640311	0.336731	0.468641	**H**	2.74481	-2.65845	-1.18989
C	2.09281	-0.63978	-0.63476	**H**	2.381128	2.310126	1.280596
C	2.531516	-2.11254	-0.26408	**H**	0.087912	2.711722	0.41834
C	2.011256	1.740981	0.41376	**H**	0.238224	1.359745	1.533592
C	0.479251	1.693515	0.521794	**H**	0.013507	-1.07961	-2.62671
C	-0.22827	0.763976	-0.5166	**H**	0.36937	-2.49811	-1.66797
C	0.509676	-0.62625	-0.56211	**H**	4.073648	-0.1043	2.829733
C	-1.71609	0.440223	-0.04607	**H**	5.615589	0.618407	2.32026
C	-2.52246	-0.58987	-0.9799	**H**	4.160753	1.623214	2.438032
C	-1.61687	-1.77681	-1.41862	**H**	6.079329	1.149074	-0.05965
C	-0.13557	-1.52743	-1.63655	**H**	4.780927	1.277837	-1.25706
C	-1.82242	-0.29324	1.361698	**H**	4.797433	2.375685	0.115505
C	-3.0618	-1.20204	1.420153	**H**	3.739245	-0.56958	-2.06787
C	-3.57877	-1.18107	-0.01753	**H**	2.191137	-0.95097	-2.80367
O	5.917695	-1.29406	0.035944	**H**	2.564534	0.720667	-2.31017

C	4.53292	0.63123	2.158885	**H**	0.791694	1.75812	-2.15488
C	5.013095	1.351438	-0.19474	**H**	-0.60651	0.833866	-2.70632
H	2.240566	-0.06956	1.412929	**H**	-0.83603	2.371214	-1.87494
C	2.670666	-0.32844	-2.04021	**H**	-2.5301	0.237472	-3.02098
C	-0.22693	1.467052	-1.90434	**H**	-3.95724	-0.71687	-2.57582
C	-3.2294	0.014291	-2.21476	**H**	-3.78135	0.92491	-1.96183
O	-4.03368	-0.67364	2.356692	**H**	-4.36921	0.178752	1.998416
O	-4.68281	-1.60283	-0.37166	**H**	-3.20525	-3.19973	-1.56899
O	-1.05399	-0.14383	2.313215	**H**	-1.52363	-3.79808	-2.03246
H	0.306097	-1.09357	0.410919	**H**	-2.34149	-2.51579	2.947365
C	-2.14837	-2.98352	-1.67745	**H**	-3.65379	-3.19124	1.943585
C	-2.73017	-2.60722	1.929779	**H**	-1.99271	-3.10667	1.297382
C	-2.64374	1.647857	0.172234	**H**	-2.5154	4.88573	-0.2833
O	-2.17854	2.874095	-0.1746	**H**	-4.00509	3.894851	-0.49143
O	-3.7852	1.521014	0.660668	**H**	-3.30037	4.099675	1.134955
C	-3.07883	4.025411	0.069471	**H**	2.078439	3.353166	-0.79573
O	2.449593	2.447714	-0.80063				

Conformer 2g							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	3.882421	-1.96973	1.143313	**H**	3.5659	-1.6826	2.155991
C	4.822185	-0.90739	0.626213	**H**	4.424199	-2.91577	1.222499
C	4.247149	0.519448	0.565096	**H**	1.822666	-2.53199	0.856665
C	2.674781	0.432448	0.403636	**H**	2.842559	-2.85759	-0.53789
C	2.151711	-0.77875	-0.45201	**H**	2.331261	2.516398	0.800071
C	2.628486	-2.11658	0.240429	**H**	0.049536	2.664587	-0.14958
C	1.998468	1.772702	0.059786	**H**	0.204811	1.568038	1.208277
C	0.464332	1.696232	0.155338	**H**	0.016026	-1.78924	-2.22328
C	-0.18641	0.553721	-0.68598	**H**	0.478717	-2.89137	-0.94097
C	0.570878	-0.7859	-0.36956	**H**	4.134228	0.576298	2.784619
C	-1.71554	0.331274	-0.24917	**H**	5.653356	1.202119	2.106266
C	-2.4405	-0.93605	-0.93771	**H**	4.17383	2.172518	2.011946
C	-1.51928	-2.17346	-0.77496	**H**	6.088456	1.184564	-0.34081
C	-0.066	-1.96446	-1.14291	**H**	4.774424	1.021271	-1.51706
C	-1.95047	-0.01474	1.254071	**H**	4.782715	2.396487	-0.42316
C	-3.35691	-0.61155	1.400241	**H**	3.782801	-1.00526	-1.88925
C	-3.64373	-1.13648	-0.00996	**H**	2.228775	-1.55349	-2.50022
O	5.997679	-1.16319	0.314139	**H**	2.586175	0.187806	-2.38935
C	4.56967	1.152268	1.959511	**H**	0.842855	1.302665	-2.44945
C	5.016922	1.333413	-0.50133	**H**	-0.42511	0.140569	-2.85551
H	2.294934	0.227018	1.418584	**H**	-0.85484	1.776122	-2.37975
C	2.711285	-0.7754	-1.8977	**H**	-2.07962	-1.06542	-3.10254
C	-0.15427	0.956757	-2.18593	**H**	-3.66164	-1.6361	-2.55669

C	-2.9016	-0.86212	-2.41429	**H**	-3.33667	0.107289	-2.64983
O	-4.27303	0.526971	1.59656	**H**	-5.17956	0.212483	1.379651
O	-4.74557	-1.60057	-0.32762	**H**	-3.02984	-3.56723	-0.18116
O	-1.15172	0.071977	2.187242	**H**	-1.32368	-4.23704	-0.35792
H	0.378859	-0.9707	0.694958	**H**	-3.30069	-1.13212	3.477446
C	-1.98621	-3.37796	-0.40758	**H**	-4.51662	-2.03386	2.525406
C	-3.50031	-1.62632	2.523465	**H**	-2.79401	-2.45263	2.400788
C	-2.534	1.623458	-0.46473	**H**	-2.77108	4.288999	1.436807
O	-2.31726	2.50298	0.562654	**H**	-3.0993	4.252528	-0.33479
O	-3.28254	1.892112	-1.40928	**H**	-4.19559	3.401501	0.795226
C	-3.16466	3.705801	0.607352	**H**	2.063724	3.1263	-1.43521
O	2.43956	2.238837	-1.26477				

Conformer 2h							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	4.281553	-2.05535	-0.17549	**H**	4.601971	-3.03908	0.181014
C	4.791804	-1.01604	0.802202	**H**	4.773088	-1.89075	-1.14457
C	4.31818	0.433843	0.591031	**H**	2.278635	-2.34071	0.585938
C	2.752742	0.402348	0.357879	**H**	2.474158	-2.74041	-1.12019
C	2.197259	-0.59538	-0.72514	**H**	2.438628	2.364249	1.173729
C	2.74903	-2.00956	-0.35121	**H**	0.146931	2.719516	0.292548
C	2.092019	1.790137	0.30481	**H**	0.33982	1.422848	1.448457
C	0.562258	1.716479	0.420594	**H**	-0.04849	-1.31599	-2.49376
C	-0.14537	0.730904	-0.5645	**H**	0.46844	-2.62362	-1.44834
C	0.620556	-0.64641	-0.53175	**H**	3.988413	0.975769	2.699158
C	-1.64928	0.435875	-0.1076	**H**	5.669889	1.052022	2.174902
C	-2.42127	-0.7021	-0.93141	**H**	4.538637	2.3255	1.676584
C	-1.50798	-1.94778	-1.06356	**H**	6.21029	1.100859	-0.25768
C	-0.0726	-1.67418	-1.4563	**H**	5.132423	0.417684	-1.48295
C	-1.80925	-0.13314	1.347111	**H**	4.791134	2.020389	-0.83214
C	-3.14745	-0.86965	1.475138	**H**	3.607149	-0.66185	-2.41154
C	-3.58073	-1.07675	0.019028	**H**	1.927295	-0.74477	-2.89956
O	5.583739	-1.32994	1.708015	**H**	2.631705	0.800882	-2.37542
C	4.642093	1.252378	1.863453	**H**	0.809519	1.76703	-2.22514
C	5.164416	1.027196	-0.57785	**H**	-0.50391	0.712692	-2.76196
H	2.368641	-0.00769	1.309245	**H**	-0.86086	2.248197	-1.96614
C	2.610688	-0.27094	-2.18739	**H**	-2.19687	-0.54027	-3.11281
C	-0.1798	1.390782	-1.97145	**H**	-3.80308	-1.02002	-2.54351
C	-2.95247	-0.36044	-2.34559	**H**	-3.29922	0.669527	-2.42108
O	-4.08174	0.067533	2.109939	**H**	-3.91846	0.055104	3.077174
O	-4.65698	-1.56765	-0.32195	**H**	-3.00719	-3.43554	-0.73012
O	-1.0358	0.001781	2.3001	**H**	-1.31433	-4.05194	-1.11823
H	0.49865	-1.02056	0.495536	**H**	-2.68868	-1.95425	3.282408

C	-1.97159	-3.20342	-0.9514	**H**	-4.07368	-2.60027	2.34186
C	-3.07159	-2.16711	2.277556	**H**	-2.40091	-2.88998	1.807246
C	-2.49758	1.7325	-0.05141	**H**	-5.72996	2.174662	-0.43002
O	-3.81532	1.484935	-0.31524	**H**	-4.87521	2.626545	1.081481
O	-2.09254	2.856377	0.261051	**H**	-4.48755	3.4824	-0.44749
C	-4.79774	2.536045	-0.00268	**H**	2.127378	3.402522	-0.90935
O	2.538419	2.514196	-0.90188				

Conformer 2i							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	4.170325	-2.09103	-0.06011	**H**	4.454198	-3.06916	0.340121
C	4.671695	-1.03215	0.901701	**H**	4.700104	-1.9714	-1.0155
C	4.233744	0.421723	0.640131	**H**	2.138854	-2.29494	0.643686
C	2.680775	0.424036	0.332495	**H**	2.374395	-2.76653	-1.03881
C	2.146884	-0.60133	-0.73574	**H**	2.416622	2.440987	1.029848
C	2.647098	-2.01369	-0.29006	**H**	0.144629	2.799799	0.072337
C	2.067781	1.828779	0.18846	**H**	0.290938	1.576037	1.319061
C	0.536135	1.79761	0.278286	**H**	0.033962	-1.23556	-2.62249
C	-0.17907	0.772042	-0.65749	**H**	0.375486	-2.57544	-1.55275
C	0.561401	-0.61615	-0.61021	**H**	3.810914	1.019287	2.717049
C	-1.66084	0.500082	-0.13155	**H**	5.519169	1.03638	2.279494
C	-2.4864	-0.59946	-0.95827	**H**	4.453247	2.330398	1.698746
C	-1.59577	-1.80826	-1.36718	**H**	6.17597	1.046814	-0.12283
C	-0.11093	-1.59674	-1.59724	**H**	5.158644	0.341404	-1.38621
C	-1.75342	-0.05588	1.351144	**H**	4.800888	1.964312	-0.79941
C	-2.85602	-1.11042	1.484003	**H**	3.658231	-0.69317	-2.327
C	-3.46968	-1.13627	0.092346	**H**	2.019816	-0.88259	-2.91085
O	5.43599	-1.33459	1.834583	**H**	2.622907	0.721757	-2.43223
C	4.515015	1.258871	1.911462	**H**	-0.58137	0.676459	-2.84782
C	5.148292	0.975008	-0.49719	**H**	-0.85681	2.258699	-2.11071
H	2.240011	0.066395	1.280319	**H**	0.786567	1.686028	-2.37574
C	2.634099	-0.33819	-2.18665	**H**	-2.58186	0.121119	-3.03158
C	-0.21793	1.37424	-2.09204	**H**	-3.96513	-0.8549	-2.50664
C	-3.25394	-0.08461	-2.19764	**H**	-3.82584	0.819681	-1.97359
O	-3.83916	-0.68485	2.463576	**H**	-4.72583	-0.91058	2.101595
O	-4.6264	-1.52204	-0.1196	**H**	-3.2175	-3.19564	-1.47655
O	-1.05462	0.298527	2.301106	**H**	-1.55227	-3.85087	-1.9202
H	0.389709	-1.01003	0.40359	**H**	-1.88948	-2.32271	2.956786
C	-2.15507	-3.00907	-1.59205	**H**	-3.082	-3.20463	1.964048
C	-2.27752	-2.46302	1.944305	**H**	-1.47976	-2.82583	1.292463
C	-2.49528	1.794537	-0.06056	**H**	-5.46686	2.188218	1.294779
O	-3.72937	1.512769	0.472158	**H**	-4.14543	3.409216	1.294276
O	-2.16935	2.94066	-0.37534	**H**	-5.01045	3.037153	-0.22454

C	-4.65404	2.630533	0.723992	**H**	2.165309	3.364347	-1.11819
O	2.553631	2.468563	-1.04907				

Conformer 2j							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	4.157156	-2.0935	-0.03411	**H**	4.437716	-3.06734	0.37867
C	4.655343	-1.02419	0.917653	**H**	4.690626	-1.98582	-0.98879
C	4.224073	0.42763	0.63432	**H**	2.122782	-2.28456	0.66487
C	2.672107	0.429808	0.321334	**H**	2.36233	-2.77707	-1.0109
C	2.13934	-0.60808	-0.73549	**H**	2.412473	2.457374	0.990899
C	2.63478	-2.0159	-0.27061	**H**	0.139652	2.806008	0.029738
C	2.062768	1.834347	0.157754	**H**	0.284727	1.597043	1.290548
C	0.530958	1.805603	0.246767	**H**	0.032644	-1.25101	-2.62274
C	-0.1834	0.770838	-0.67781	**H**	0.360294	-2.58375	-1.54046
C	0.553616	-0.61774	-0.61551	**H**	3.796334	1.054296	2.701684
C	-1.66145	0.503575	-0.14376	**H**	5.505905	1.06067	2.269521
C	-2.4979	-0.59956	-0.94527	**H**	4.44568	2.349773	1.667806
C	-1.61019	-1.80546	-1.37359	**H**	6.169742	1.039928	-0.13038
C	-0.1206	-1.60269	-1.59553	**H**	5.156461	0.317107	-1.38705
C	-1.74819	-0.03228	1.331498	**H**	4.798042	1.948634	-0.82525
C	-2.8291	-1.10301	1.497175	**H**	3.656507	-0.72299	-2.31975
C	-3.48125	-1.15239	0.121166	**H**	2.019935	-0.91817	-2.90677
O	5.409766	-1.31733	1.861568	**H**	2.623433	0.691741	-2.4476
C	4.503644	1.281053	1.895122	**H**	0.779724	1.64107	-2.4208
C	5.143371	0.963465	-0.50737	**H**	-0.61806	0.656039	-2.85921
H	2.227669	0.084991	1.272365	**H**	-0.84808	2.252442	-2.13928
C	2.632364	-0.36486	-2.18798	**H**	-2.63436	0.104042	-3.02343
C	-0.22723	1.355401	-2.11879	**H**	-4.01076	-0.86012	-2.45612
C	-3.28876	-0.09036	-2.17249	**H**	-3.85178	0.819054	-1.9457
O	-3.80138	-0.67901	2.485936	**H**	-3.3166	-0.46728	3.3134
O	-4.59337	-1.61779	-0.12532	**H**	-3.23379	-3.18625	-1.5179
O	-1.11005	0.381705	2.30795	**H**	-1.56749	-3.83502	-1.97138
H	0.377635	-1.00203	0.40223	**H**	-1.71987	-2.32423	2.889962
C	-2.17112	-2.99974	-1.62773	**H**	-3.05531	-3.16727	2.05179
C	-2.23231	-2.45779	1.930296	**H**	-1.52211	-2.85796	1.204068
C	-2.50024	1.798896	-0.08114	**H**	-5.44811	2.138304	1.340422
O	-3.70275	1.51235	0.509078	**H**	-4.18745	3.424145	1.254626
O	-2.20157	2.935582	-0.45169	**H**	-5.06756	2.941756	-0.22395
C	-4.6714	2.596412	0.733216	**H**	2.157994	3.347398	-1.17503
O	2.549945	2.454785	-1.08813				

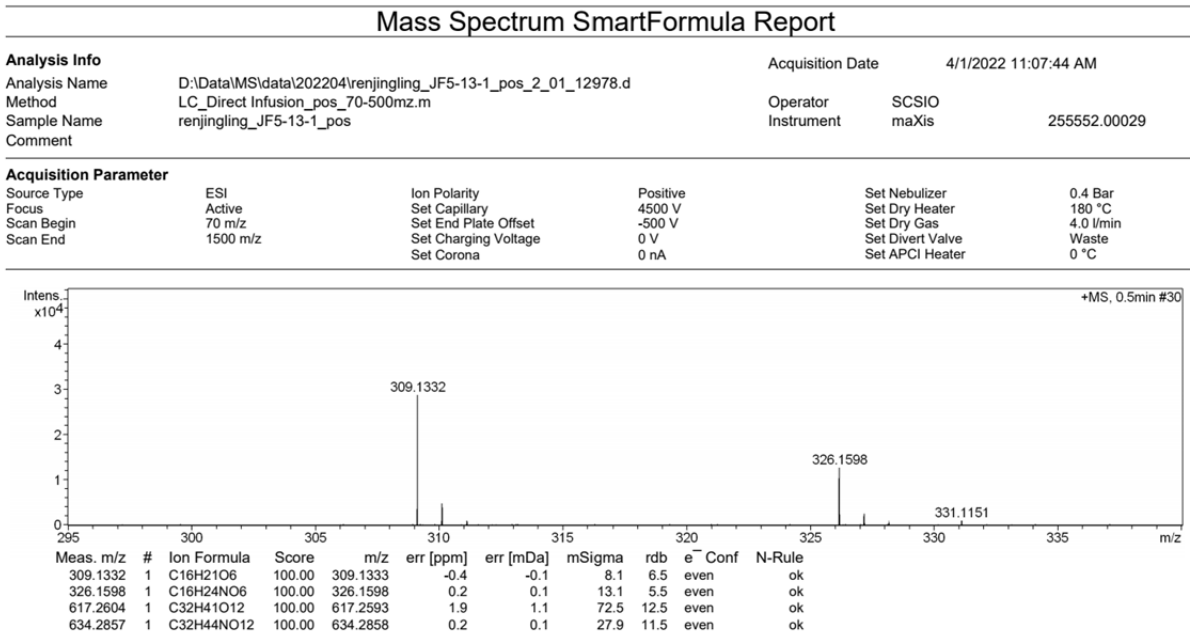
Conformer 2k							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	3.803905	-2.08878	0.871599	**H**	3.460858	-1.93343	1.904097
C	4.78514	-0.99238	0.530553	**H**	4.319358	-3.05199	0.835312
C	4.248807	0.443926	0.659867	**H**	1.745278	-2.56075	0.439599
C	2.680573	0.429482	0.446104	**H**	2.807357	-2.69499	-0.95412
C	2.15037	-0.63668	-0.58057	**H**	2.418863	2.467611	1.079637
C	2.578594	-2.07385	-0.08087	**H**	0.132532	2.793443	0.15904
C	2.058065	1.826196	0.260825	**H**	0.27197	1.54373	1.387786
C	0.525523	1.788801	0.354032	**H**	0.132904	-1.21341	-2.57758
C	-0.16573	0.773301	-0.61094	**H**	0.426525	-2.56328	-1.50522
C	0.565822	-0.61517	-0.54024	**H**	4.071298	0.185273	2.860805
C	-1.66207	0.491477	-0.12704	**H**	5.623198	0.86264	2.319981
C	-2.46362	-0.59045	-0.99833	**H**	4.167832	1.873784	2.326931
C	-1.55611	-1.79511	-1.39205	**H**	6.129841	1.195006	-0.08468
C	-0.06113	-1.58471	-1.56399	**H**	4.855646	1.219199	-1.31427
C	-1.78009	-0.11638	1.325493	**H**	4.843845	2.429201	-0.03982
C	-2.95092	-1.10693	1.429015	**H**	3.825747	-0.68167	-1.97968
C	-3.49788	-1.15036	0.0035	**H**	2.295735	-1.13186	-2.71316
O	5.960446	-1.23656	0.208786	**H**	2.653113	0.577919	-2.35533
C	4.54358	0.861908	2.138883	**H**	-0.56341	0.68748	-2.79749
C	5.066391	1.382845	-0.25753	**H**	-0.74355	2.289459	-2.07871
H	2.263217	0.105614	1.414414	**H**	0.863945	1.612185	-2.32767
C	2.756205	-0.44408	-1.99551	**H**	-2.50446	0.139826	-3.0747
C	-0.15961	1.368479	-2.04805	**H**	-3.9176	-0.80598	-2.57081
C	-3.19254	-0.05323	-2.2514	**H**	-3.74716	0.865896	-2.03781
O	-3.9379	-0.63623	2.378817	**H**	-4.28799	0.218343	2.050086
O	-4.61253	-1.57814	-0.30804	**H**	-3.16838	-3.18733	-1.57009
O	-1.07367	0.17923	2.292487	**H**	-1.48597	-3.82937	-1.9678
H	0.340438	-1.01118	0.460483	**H**	-2.10281	-2.33137	2.96435
C	-2.10404	-2.99501	-1.64886	**H**	-3.3899	-3.12148	2.012902
C	-2.50966	-2.47563	1.959885	**H**	-1.75765	-2.93999	1.318827
C	-2.49211	1.784775	-0.06575	**H**	-5.56694	2.301163	1.036455
O	-3.72177	1.560955	0.544393	**H**	-4.23221	3.49591	1.224634
O	-2.19544	2.907675	-0.47053	**H**	-4.83497	3.085797	-0.40529
C	-4.65583	2.70688	0.601677	**H**	2.125082	3.316478	-1.09485
O	2.513194	2.422595	-1.00444				

Conformer 2l							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	3.794135	-2.09281	0.871318	**H**	3.455912	-1.93541	1.905096
C	4.778539	-1.00027	0.526025	**H**	4.305905	-3.05794	0.833676
C	4.248048	0.43788	0.656131	**H**	1.731008	-2.55475	0.448704

C	2.67929	0.429626	0.44551	**H**	2.787125	-2.69859	-0.94872
C	2.14272	-0.63574	-0.57792	**H**	2.425323	2.469891	1.074462
C	2.565095	-2.07377	-0.07634	**H**	0.13725	2.800463	0.163135
C	2.061103	1.827491	0.257942	**H**	0.276032	1.553044	1.388643
C	0.529532	1.795629	0.354435	**H**	0.131766	-1.19904	-2.57828
C	-0.16916	0.784467	-0.61037	**H**	0.42175	-2.55342	-1.5104
C	0.557856	-0.60644	-0.5396	**H**	4.074123	0.180187	2.85759
C	-1.66743	0.512456	-0.13404	**H**	5.626797	0.853338	2.313627
C	-2.46526	-0.58232	-0.99732	**H**	4.173835	1.868118	2.322823
C	-1.56038	-1.78423	-1.40304	**H**	6.130371	1.183477	-0.09099
C	-0.0659	-1.57465	-1.56695	**H**	4.854739	1.210693	-1.31911
C	-1.80738	-0.051	1.34113	**H**	4.847538	2.421023	-0.04517
C	-2.89996	-1.12003	1.429685	**H**	3.818071	-0.68296	-1.97707
C	-3.47264	-1.13667	0.021034	**H**	2.289207	-1.13784	-2.7094
O	5.951756	-1.24975	0.20063	**H**	2.643281	0.573825	-2.35591
C	4.546844	0.855317	2.134529	**H**	-0.58001	0.707777	-2.79526
C	5.067207	1.374045	-0.26268	**H**	-0.75083	2.30712	-2.06621
H	2.262841	0.109536	1.415545	**H**	0.853505	1.627582	-2.33217
C	2.748196	-0.44716	-1.99365	**H**	-2.52538	0.148841	-3.07001
C	-0.16827	1.38424	-2.04549	**H**	-3.92005	-0.82289	-2.57031
C	-3.21037	-0.05712	-2.24699	**H**	-3.7819	0.848602	-2.02818
O	-3.91564	-0.71988	2.385657	**H**	-4.78925	-0.9439	1.992097
O	-4.62092	-1.52703	-0.226	**H**	-3.1815	-3.16278	-1.60027
O	-1.14935	0.310148	2.317641	**H**	-1.50328	-3.81404	-1.99938
H	0.326886	-1.00029	0.462091	**H**	-1.95807	-2.34132	2.911623
C	-2.11508	-2.9776	-1.67414	**H**	-3.1147	-3.2226	1.876848
C	-2.31822	-2.47227	1.887593	**H**	-1.50037	-2.81822	1.251418
C	-2.50198	1.806625	-0.08196	**H**	-5.51132	2.198353	1.189934
O	-3.74981	1.523847	0.418944	**H**	-4.19008	3.418923	1.231877
O	-2.16692	2.952975	-0.38533	**H**	-5.00885	3.050214	-0.31304
C	-4.68135	2.64142	0.644964	**H**	2.126617	3.312529	-1.10268
O	2.516473	2.419657	-1.00973				

Conformer 2m							
Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	3.853493	-1.97828	1.146814	**H**	3.527746	-1.69109	2.156574
C	4.800929	-0.91799	0.639494	**H**	4.392025	-2.92578	1.230535
C	4.230708	0.510716	0.574561	**H**	1.796191	-2.53879	0.837572
C	2.659577	0.42887	0.400353	**H**	2.82961	-2.85924	-0.54773
C	2.139703	-0.7803	-0.46112	**H**	2.325066	2.515752	0.793314
C	2.608372	-2.12114	0.231276	**H**	0.04538	2.670918	-0.16842
C	1.991604	1.773108	0.0522	**H**	0.193206	1.574386	1.193888
C	0.456677	1.701168	0.141692	**H**	0.006771	-1.76298	-2.25442

C	-0.19162	0.558736	-0.70013	**H**	0.456506	-2.88169	-0.98253
C	0.558589	-0.78392	-0.38822	**H**	4.100616	0.56635	2.793084
C	-1.72077	0.337834	-0.25042	**H**	5.627129	1.187343	2.127102
C	-2.46248	-0.91184	-0.9437	**H**	4.151987	2.163205	2.022036
C	-1.54029	-2.15763	-0.81976	**H**	4.775565	1.011649	-1.50317
C	-0.08219	-1.94943	-1.17659	**H**	4.778864	2.386708	-0.40895
C	-1.93369	-0.0321	1.247262	**H**	6.080771	1.171493	-0.3167
C	-3.3322	-0.6467	1.412667	**H**	3.780098	-1.01163	-1.88659
C	-3.65777	-1.14155	0.001102	**H**	2.22797	-1.55127	-2.51007
O	5.978617	-1.17646	0.338326	**H**	2.593167	0.187966	-2.39374
C	4.544463	1.141516	1.971859	**H**	0.849205	1.280955	-2.46503
C	5.010898	1.322984	-0.48553	**H**	-0.44803	0.150086	-2.86737
H	2.270773	0.223768	1.412	**H**	-0.8365	1.794769	-2.39346
C	2.709781	-0.77656	-1.90279	**H**	-2.14346	-0.99577	-3.11755
C	-0.15582	0.960182	-2.19971	**H**	-3.71088	-1.58744	-2.54879
C	-2.95251	-0.81172	-2.40858	**H**	-3.39518	0.160169	-2.61972
O	-4.28159	0.453573	1.646713	**H**	-4.04719	0.89545	2.491113
O	-4.72183	-1.67795	-0.31001	**H**	-3.05357	-3.57217	-0.2839
O	-1.15007	0.112226	2.191172	**H**	-1.34653	-4.2349	-0.48192
H	0.361052	-0.97843	0.673671	**H**	-3.15086	-1.2752	3.466927
C	-2.00965	-3.37486	-0.49959	**H**	-4.47398	-2.05834	2.547884
C	-3.44112	-1.70377	2.501581	**H**	-2.78041	-2.55113	2.296882
C	-2.50905	1.645971	-0.46064	**H**	-2.91439	4.24532	1.508365
O	-2.40862	2.46972	0.636871	**H**	-2.90388	4.306212	-0.29058
O	-3.12644	1.992387	-1.47091	**H**	-4.24569	3.49093	0.558317
C	-3.17977	3.724724	0.590587	**H**	2.063533	3.120074	-1.44884
O	2.440199	2.234524	-1.27063				



Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name	D:\Data\MS\data\202204\renjingling_JF5-13-1_pos_2_01_12978.d	Acquisition Date	4/1/2022 11:07:44 AM
Method	LC_Direct Infusion_pos_70-500mz.m	Operator	SCSIO
Sample Name	renjingling_JF5-13-1_pos	Instrument	maXis 255552.00029
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	70 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Charging Voltage	0 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C

Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	err [mDa]	mSigma	rdb	e⁻ Conf	N-Rule
309.1332	1	C16H21O6	100.00	309.1333	-0.4	-0.1	8.1	6.5	even	ok
326.1598	1	C16H24NO6	100.00	326.1598	0.2	0.1	13.1	5.5	even	ok
617.2604	1	C32H41O12	100.00	617.2593	1.9	1.1	72.5	12.5	even	ok
634.2857	1	C32H44NO12	100.00	634.2858	0.2	0.1	27.9	11.5	even	ok

Figure S3. HR-ESI-MS spectrum of compound **1**.

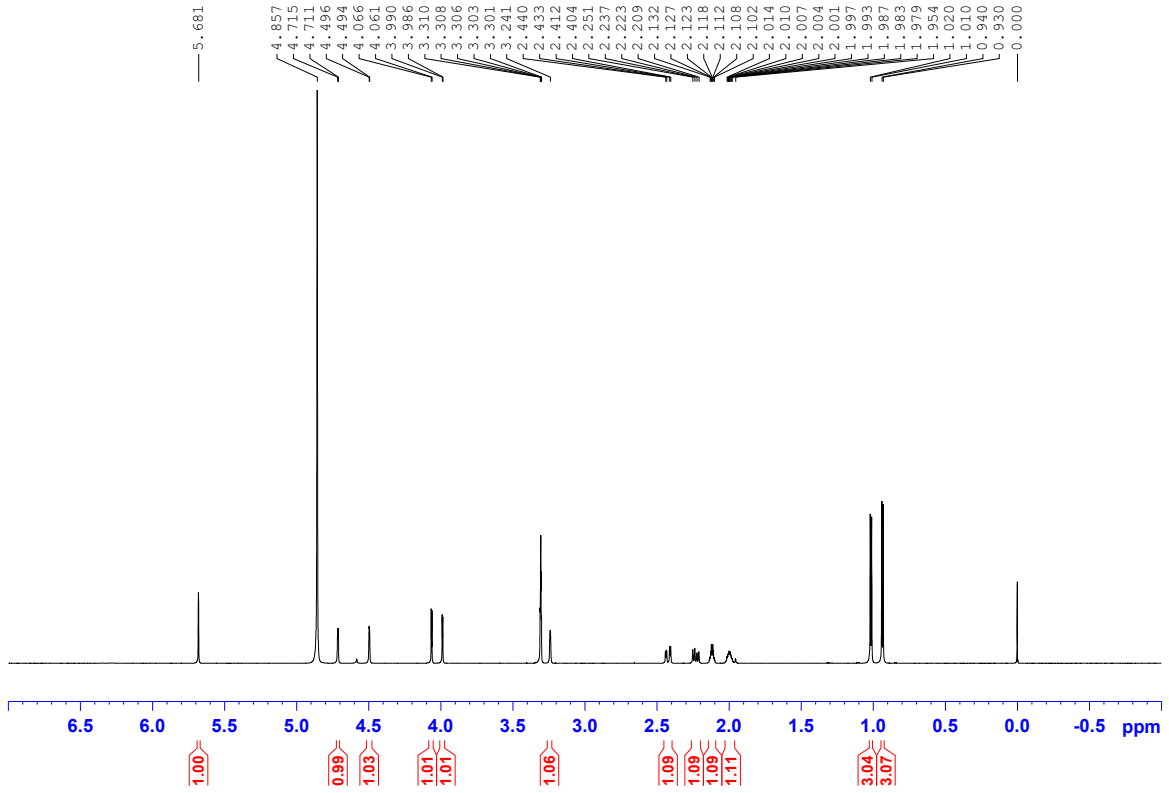


Figure S4. The ^{1}H-NMR spectrum of compound **1** in CD_3OD.

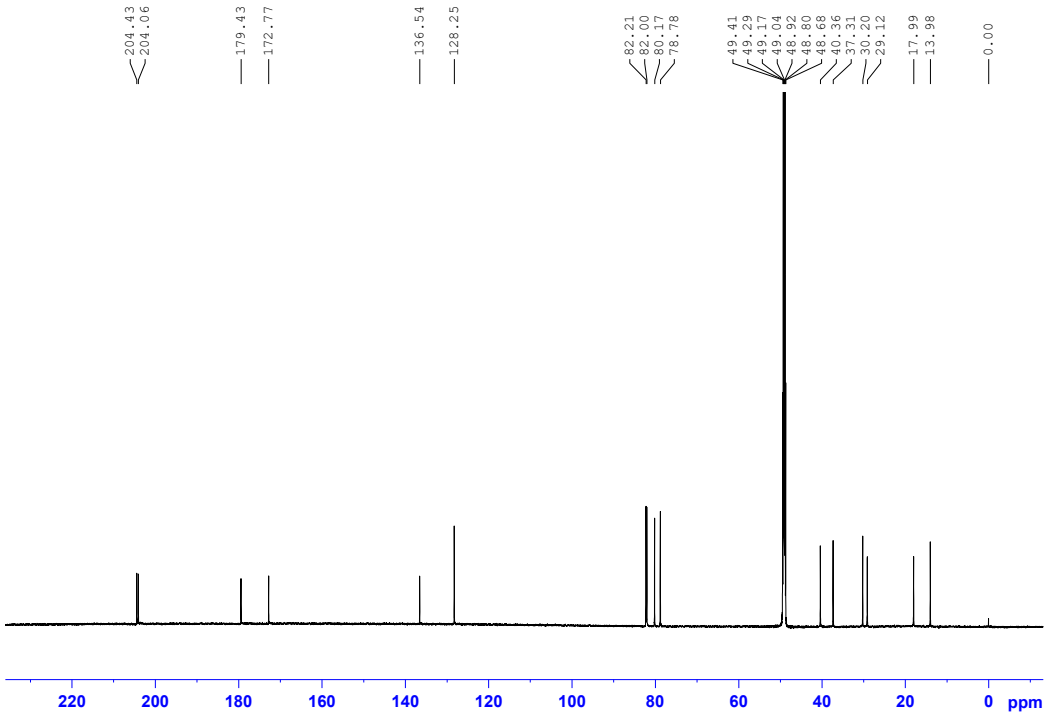


Figure S5. The ^{13}C NMR spectrum of compound **1** in CD_3OD.

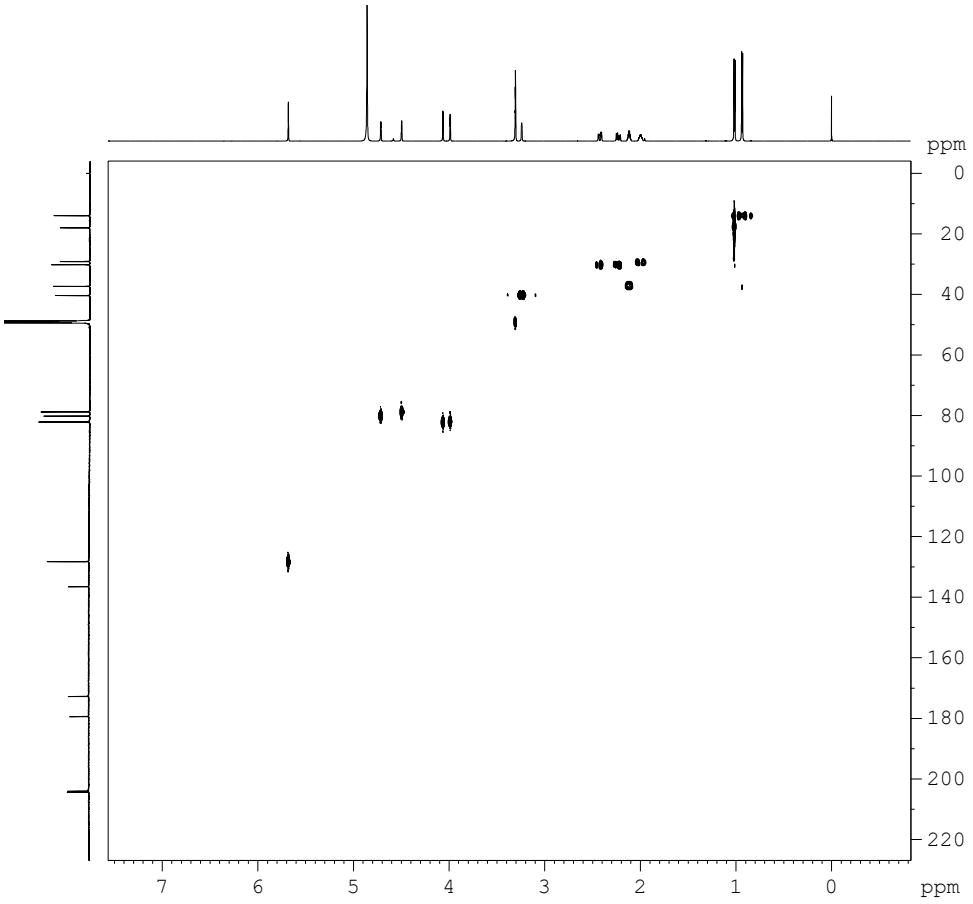


Figure S6. The HSQC spectrum of compound **1** in CD_3OD.

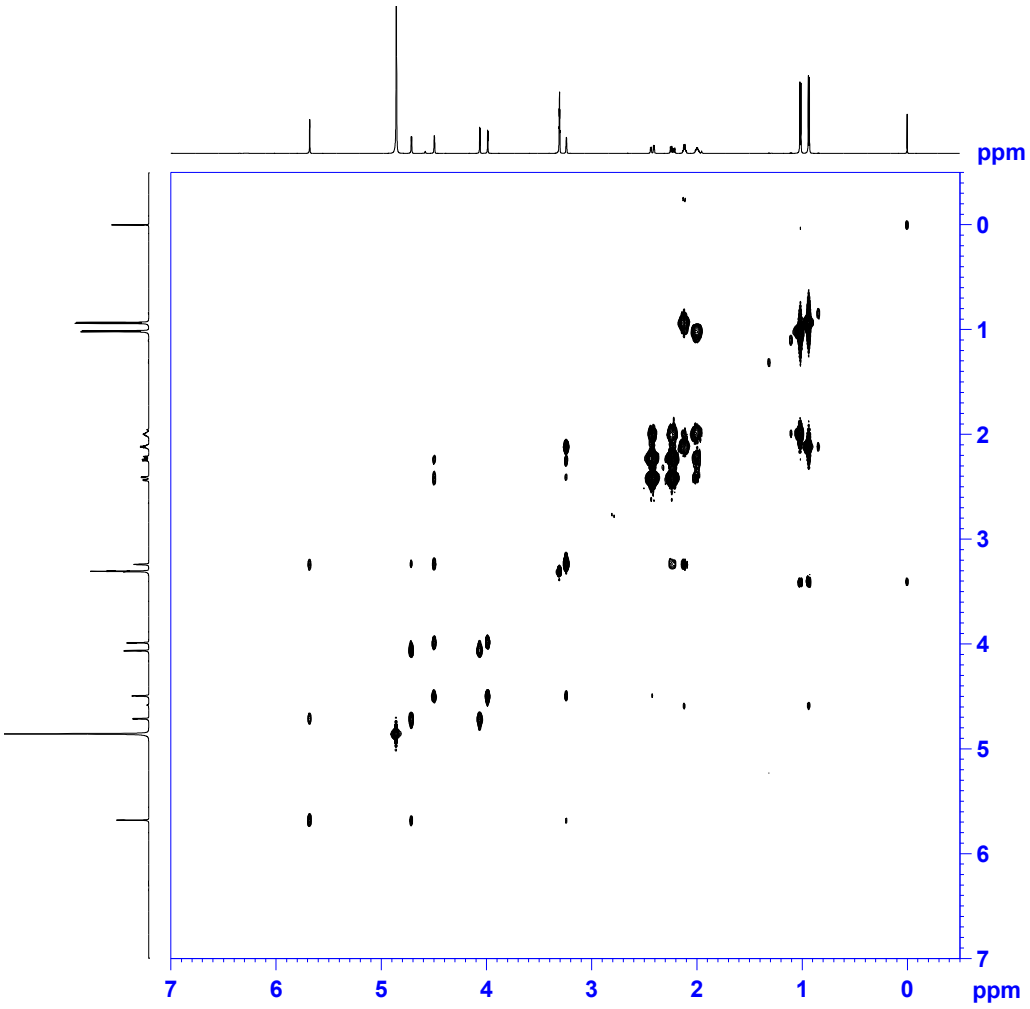


Figure S7. The ^{1}H-^{1}H COSY spectrum of compound **1** in CD_3OD.

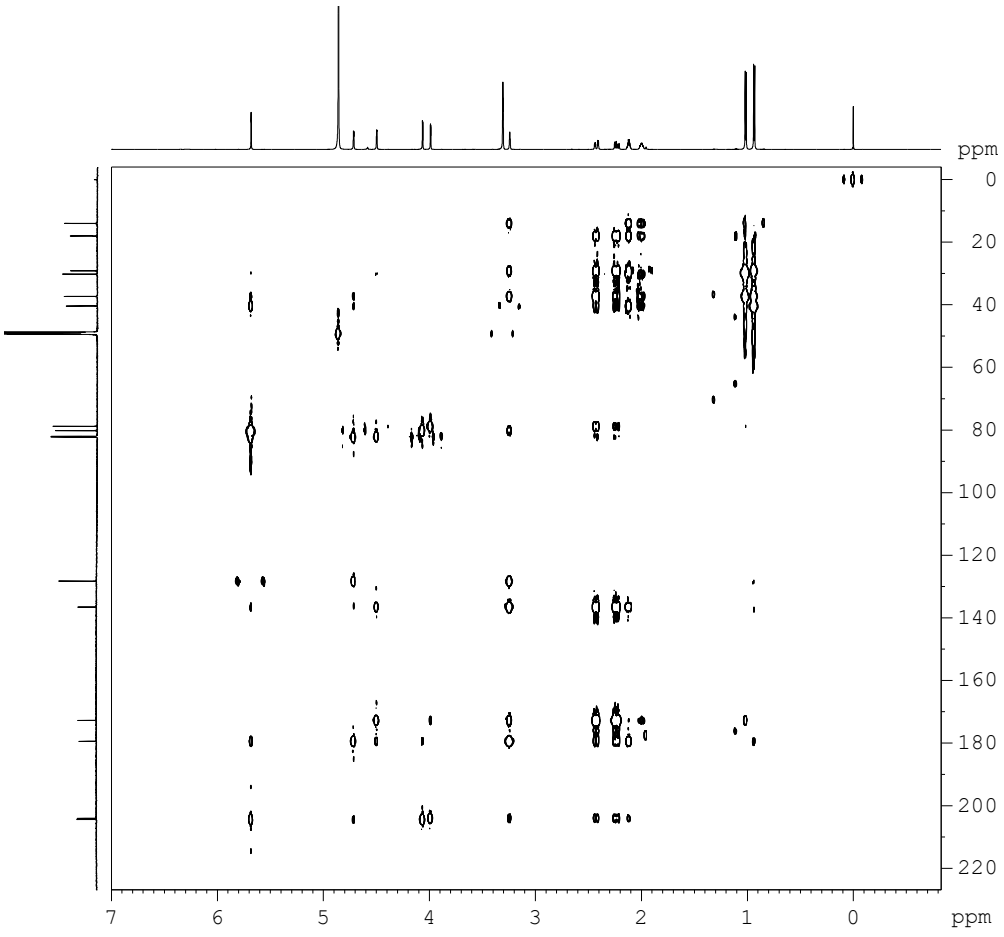


Figure S8. The HMBC spectrum of compound **1** in CD_3OD.

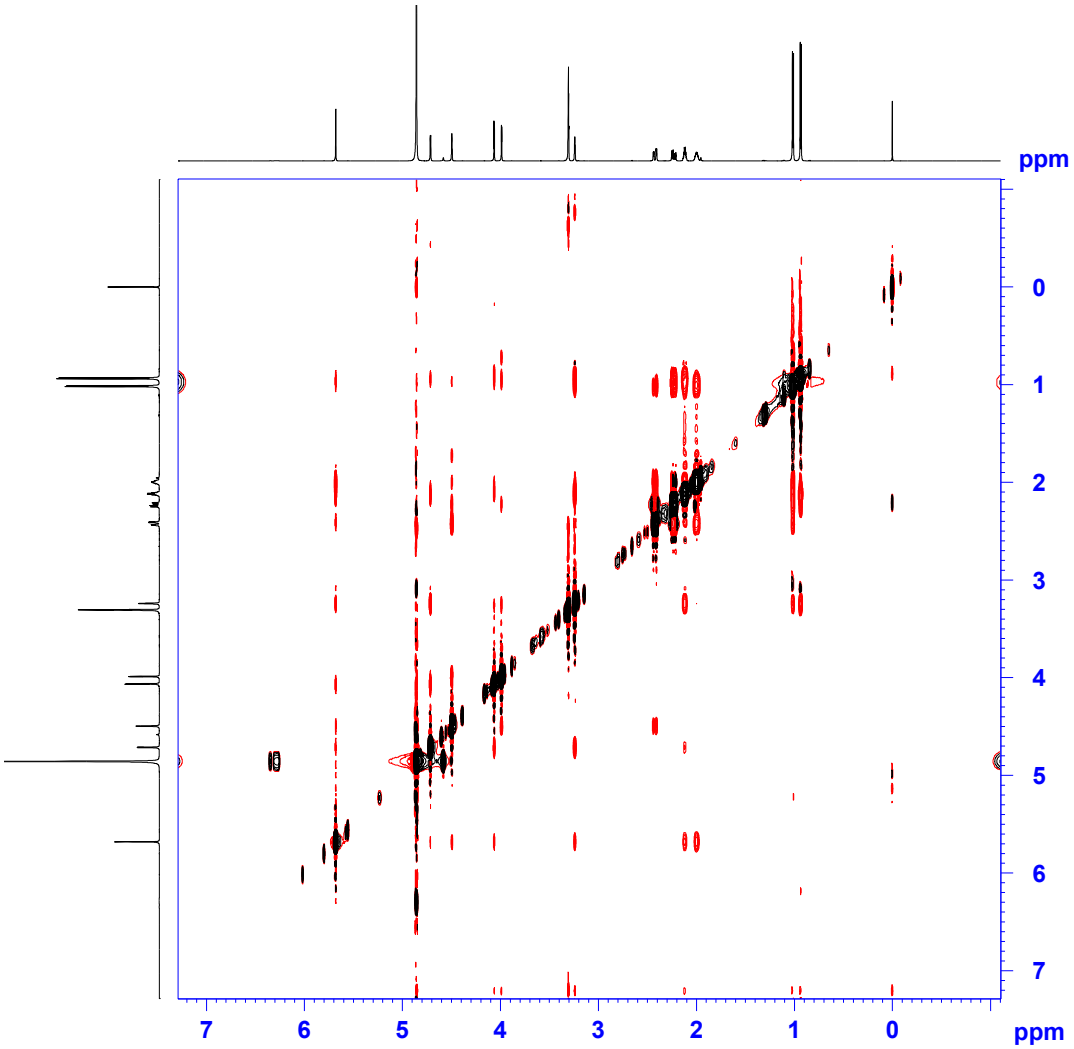


Figure S9. The NOESY spectrum of compound **1** in CD_3OD.

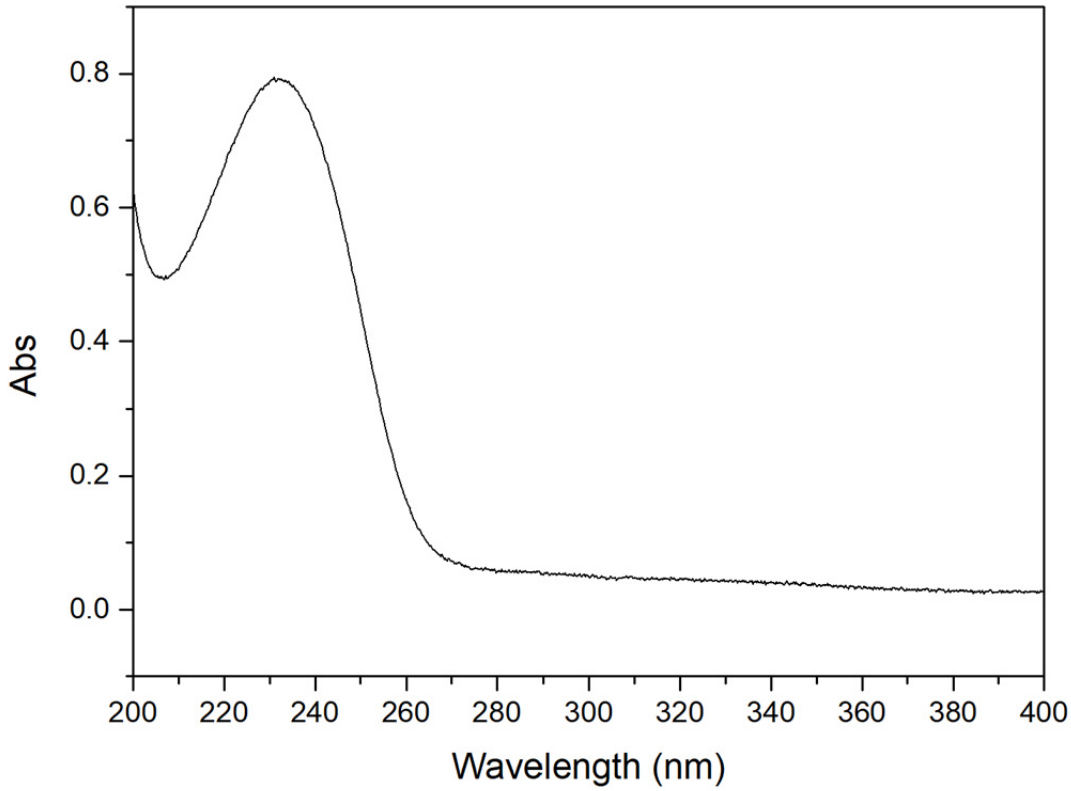


Figure S10. UV spectrum of compound **1**.

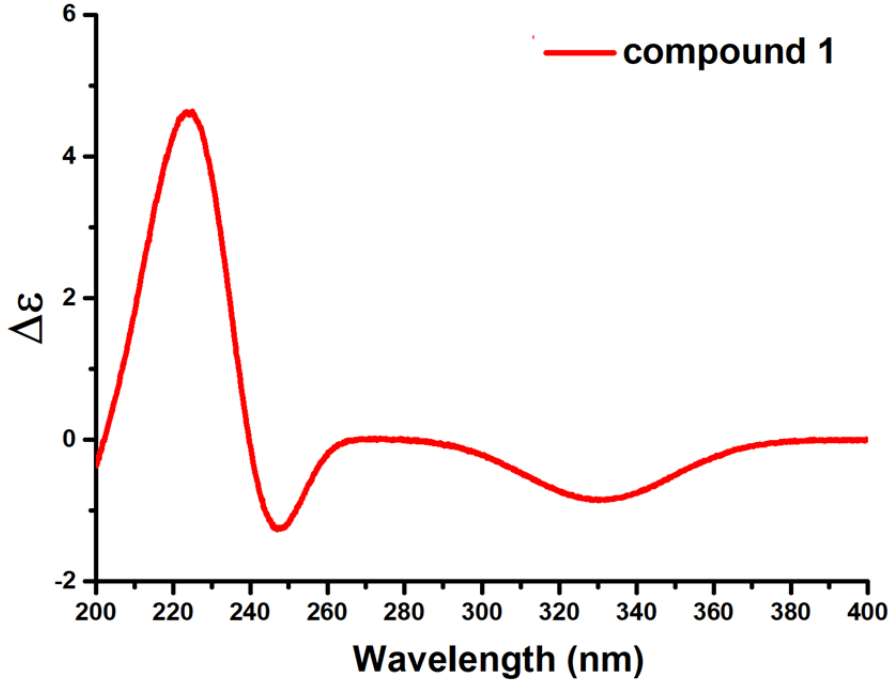


Figure S11. ECD curve of compound **1**.

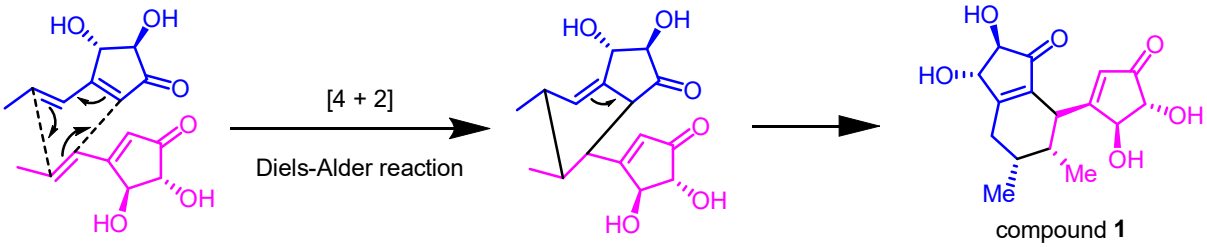


Figure S12. Possible biosynthetic pathways of compound **1**

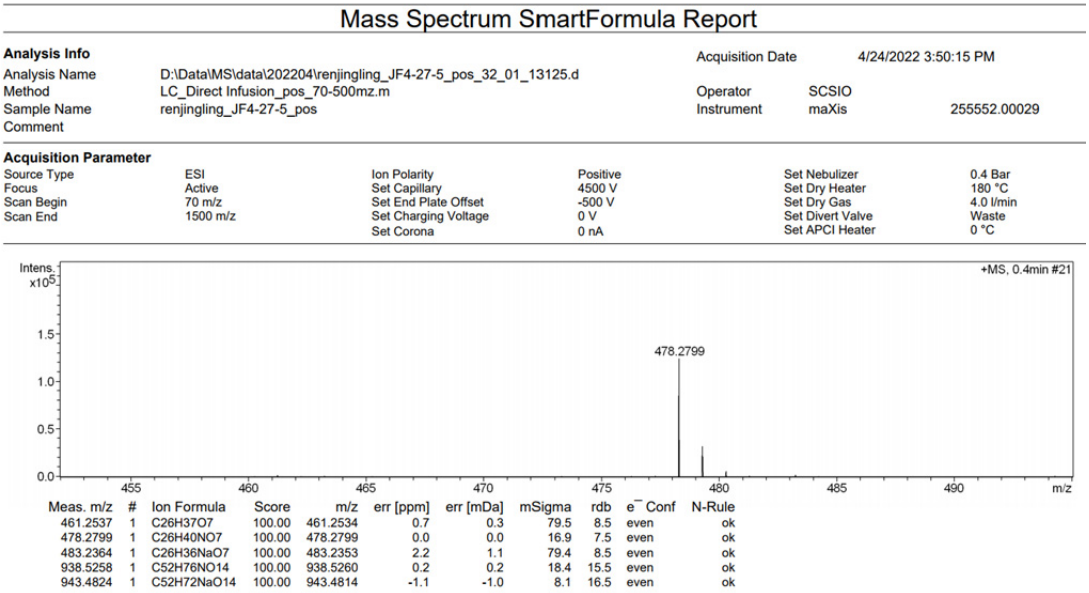


Figure S13. The HR-ESI-MS spectrum of compound **2**.

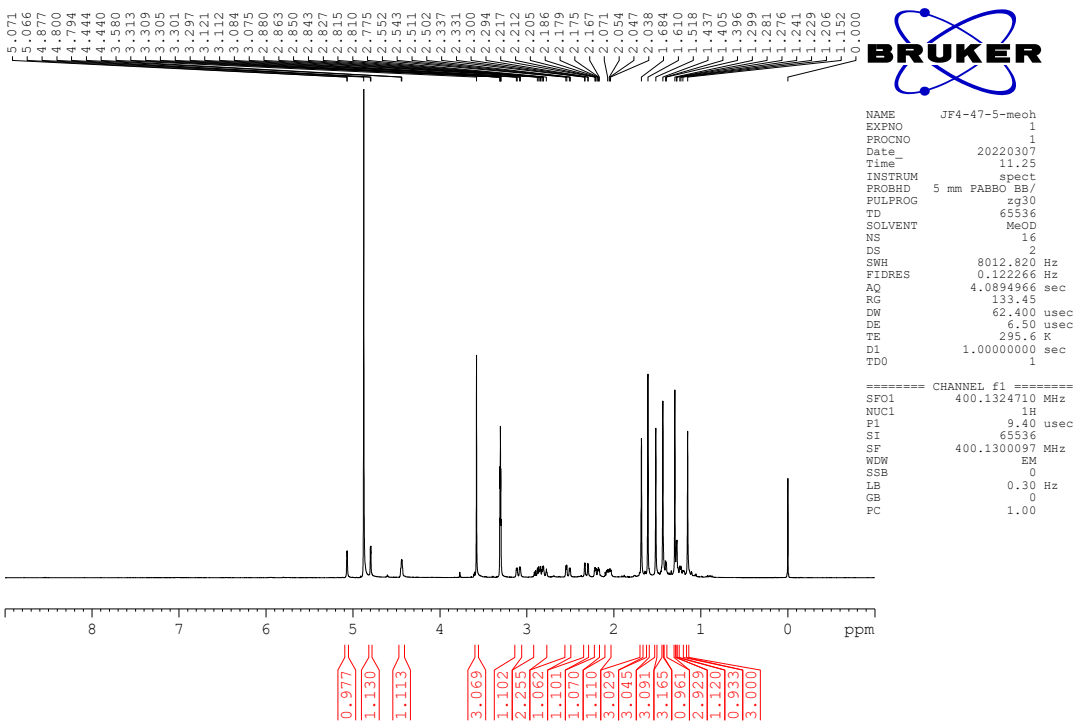


Figure S14. The ^{1}H-NMR spectrum of compound **2** in CD_3OD.

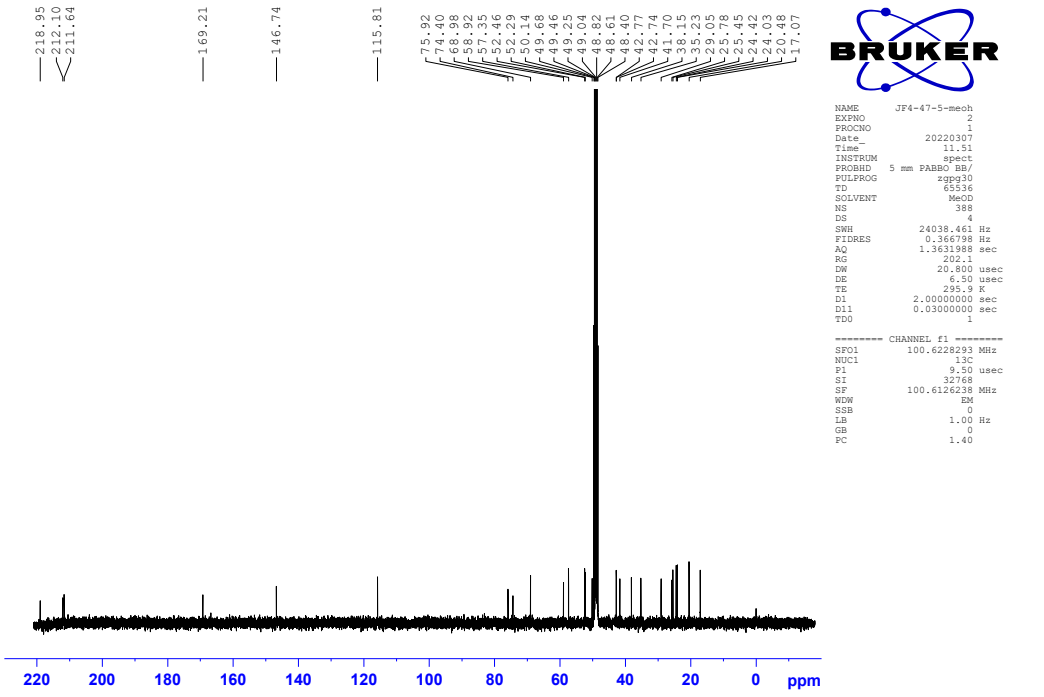


Figure S15. The ^{13}C-NMR spectrum of compound **2** in CD_3OD.

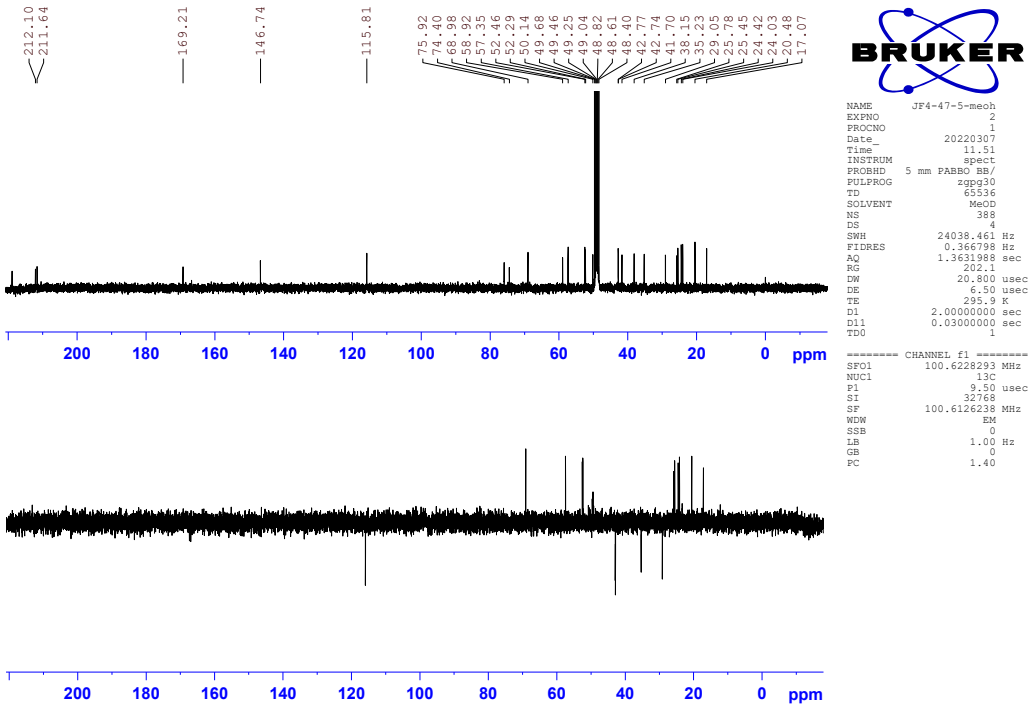


Figure S16. The DEPT135 spectrum of compound **2** in CD_3OD.

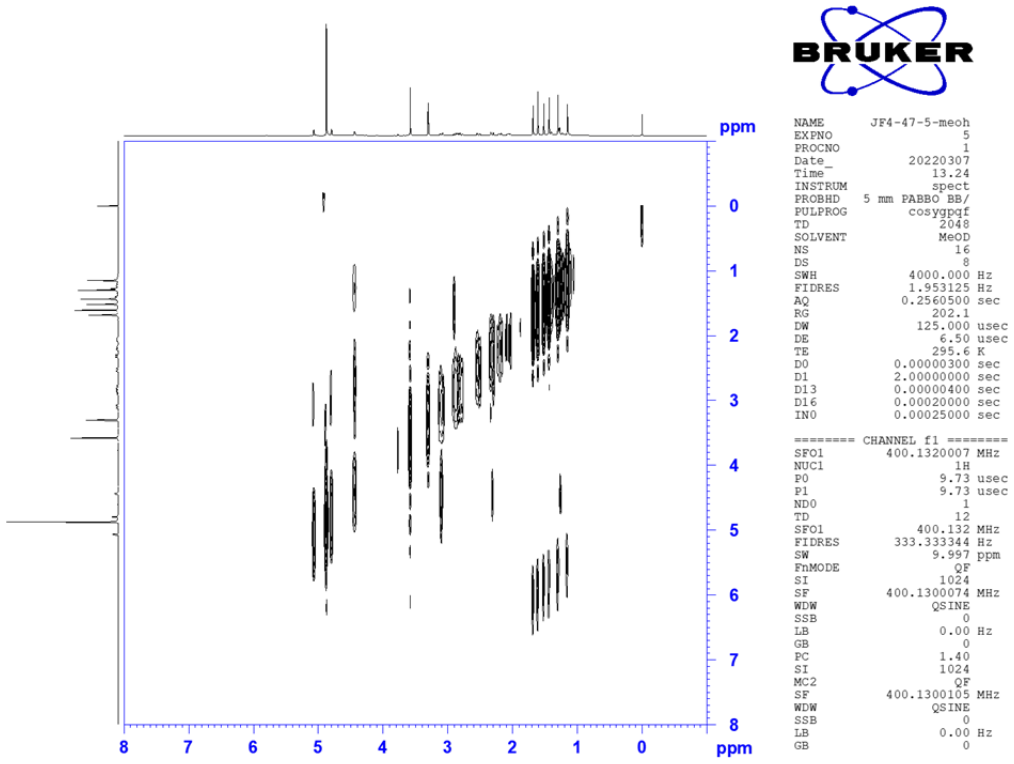
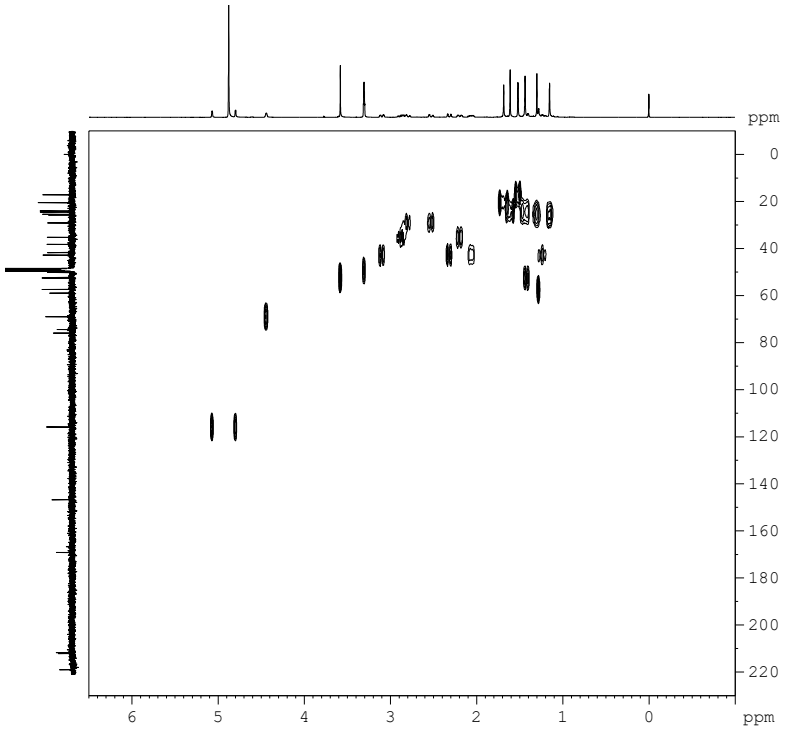


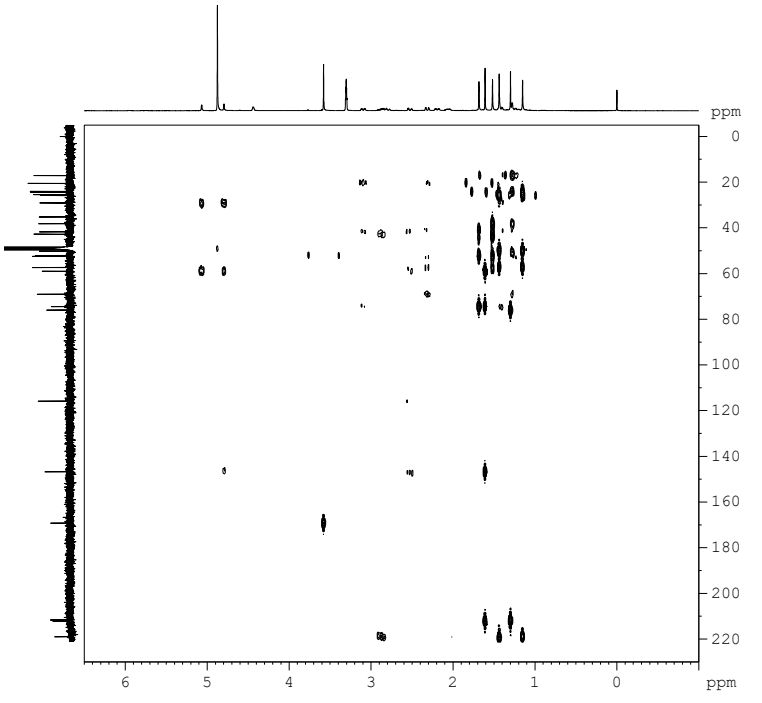
Figure S17. The ^{1}H-^{1}H COSY spectrum of compound **2** in CD_3OD.




```
NAME         JF4-47-5-meoh
EXPNO                   8
PROCNO                  1
Date_            20220311
Time                19.22
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG      hsqcetgpsi2
TD                   2048
SOLVENT              MeOD
NS                     24
DS                     16
SWH              4000.000 Hz
FIDRES           1.953125 Hz
AQ             0.2560500 sec
RG                 202.1
DW               125.000 usec
DE                  6.50 usec
TE                296.2 K
CNST2        145.0000000
D0            0.00000300 sec
D1            1.50000000 sec
D4            0.00172414 sec
D11           0.03000000 sec
D16           0.00020000 sec
D24           0.00110000 sec
IN0           0.00002160 sec
ZGOPTNS

======== CHANNEL f1 ========
SFO1          400.1322007 MHz
NUC1                    1H
P1                   9.73 usec
P2                  19.46 usec
P28               1000.00 usec
ND0                     2
TD                     33
SFO1            100.6233 MHz
FIDRES         701.459045 Hz
SW              230.048 ppm
FnMODE     Echo-Antiecho
SI                   1024
SF            400.1300065 MHz
WDW                 QSINE
SSB                     2
LB                   0.00 Hz
GB                      0
PC                   1.40
SI                   1024
MC2         echo-antiecho
SF           100.6126072 MHz
WDW                 QSINE
SSB                     2
LB                   0.00 Hz
GB                      0
```

Figure S18. The HSQC spectrum of compound **2** in CD_3OD.




```
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PROCNO                  1
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Time                13.46
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG     hmbcgplpndqf
TD                   2048
SOLVENT              MeOD
NS                     12
DS                     16
SWH              4000.000 Hz
FIDRES           1.953125 Hz
AQ             0.2560500 sec
RG                 202.1
DW               125.000 usec
DE                  6.50 usec
TE                295.5 K
CNST2        145.0000000
CNST13        10.0000000
D0            0.00000300 sec
D1            1.50000000 sec
D2            0.00344828 sec
D6            0.05000000 sec
D16           0.00020000 sec
IN0           0.00002160 sec

======== CHANNEL f1 ========
SFO1          400.1322007 MHz
NUC1                    1H
P1                   9.73 usec
P2                  19.46 usec
ND0                     2
TD                     69
SFO1            100.6233 MHz
FIDRES         335.480408 Hz
SW              230.048 ppm
FnMODE                 QF
SI                   2048
SF            400.1300088 MHz
WDW                 SINE
SSB                     0
LB                   0.00 Hz
GB                      0
PC                   1.40
SI                   1024
MC2                    QF
SF           100.6126163 MHz
WDW                 SINE
SSB                     0
LB                   0.00 Hz
GB                      0
```

Figure S19. The HMBC spectrum of compound **2** in CD_3OD.

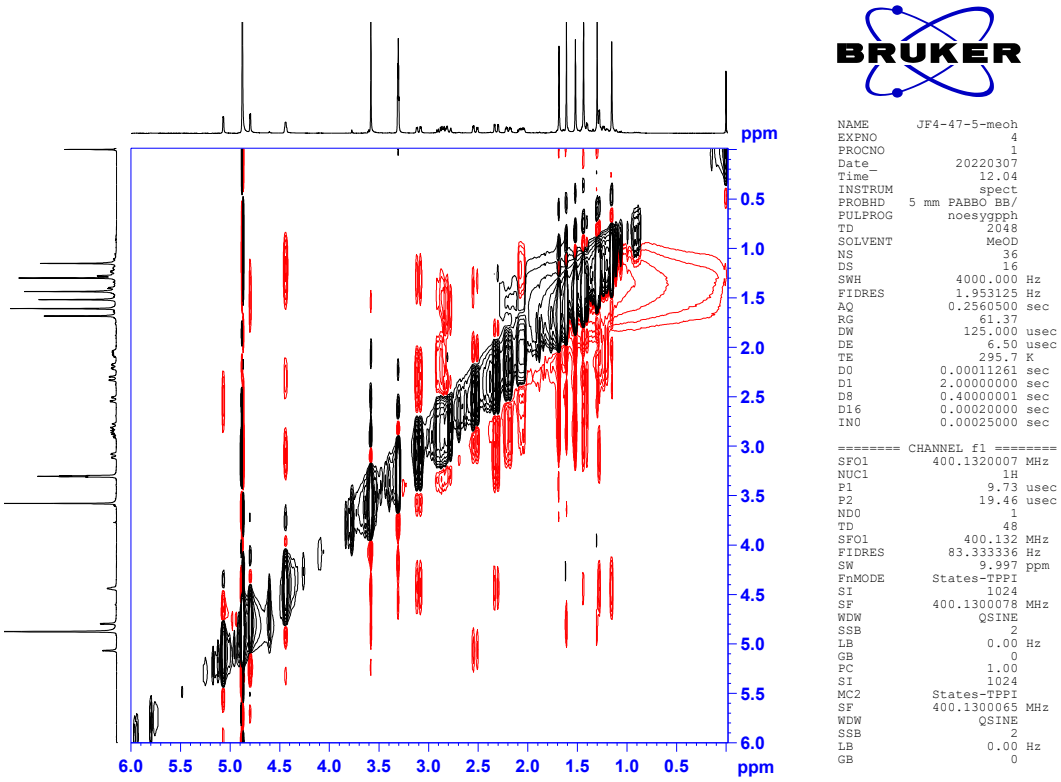

Figure S20. The NOESY spectrum of compound **2** in CD_3OD.

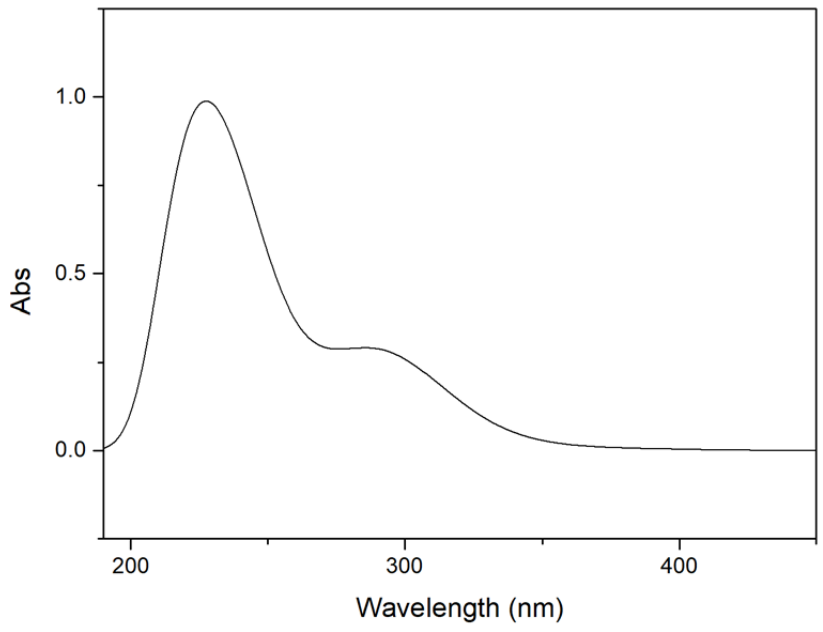

Figure S21. UV spectrum of compound **2**.

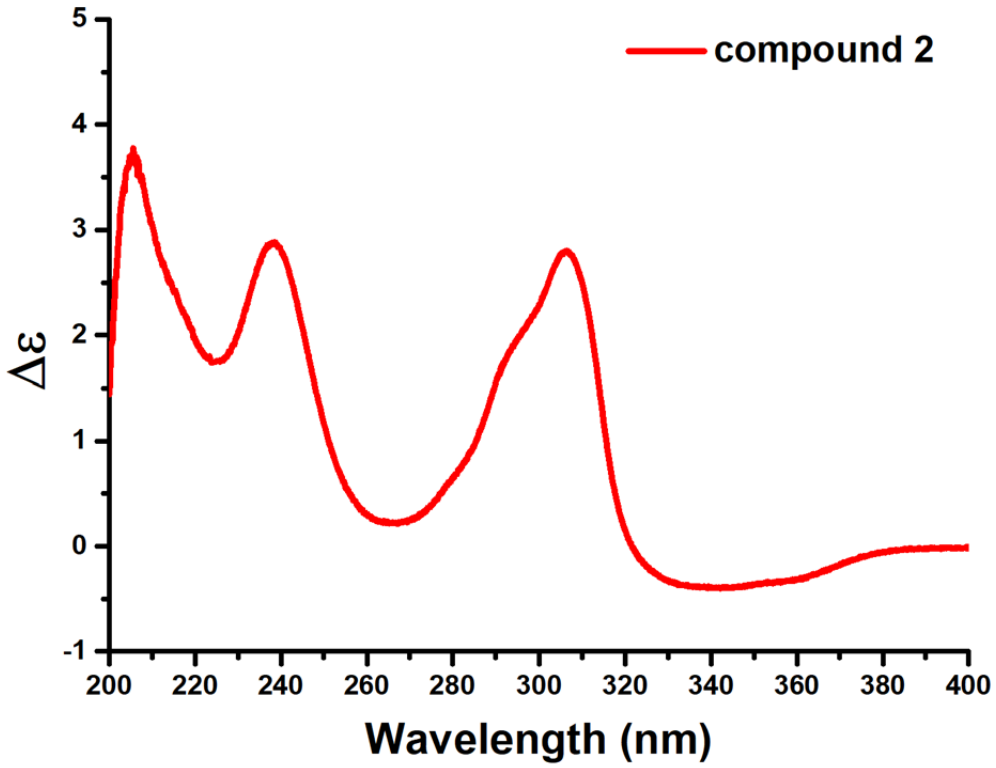

Figure S22. ECD curve of compound **2**.

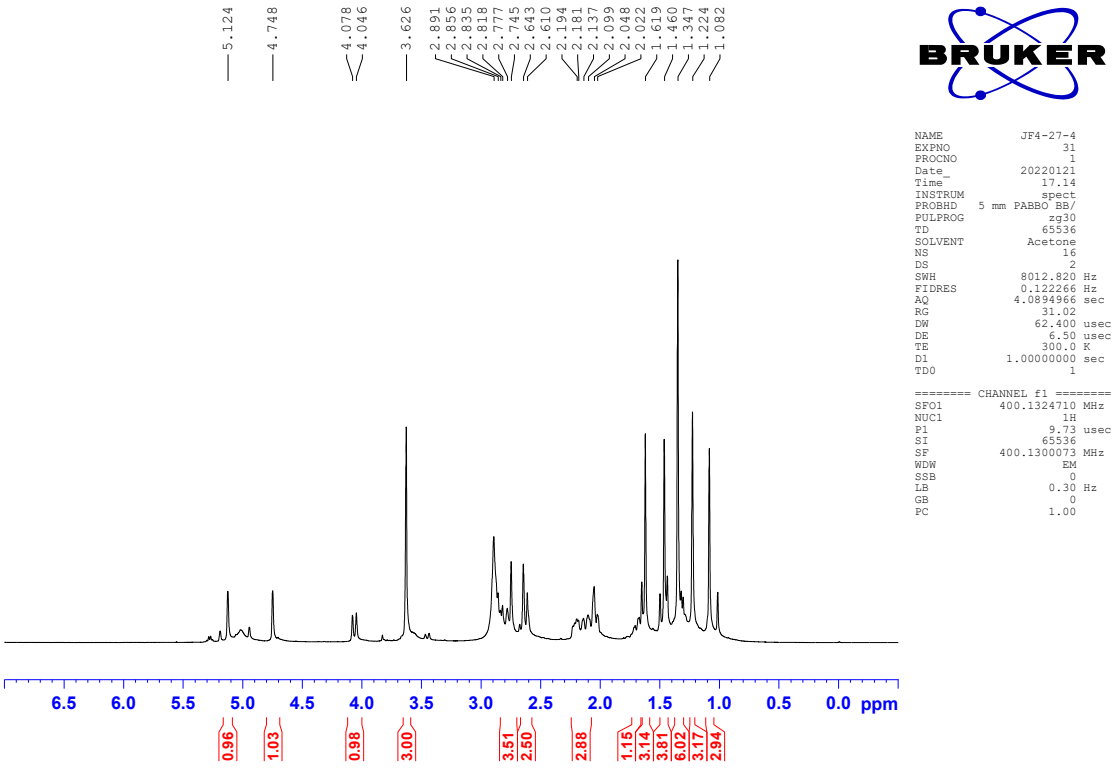

Figure S23. The ^{1}H-NMR spectrum of asperterpene C (**3**) in acetone-d_6.

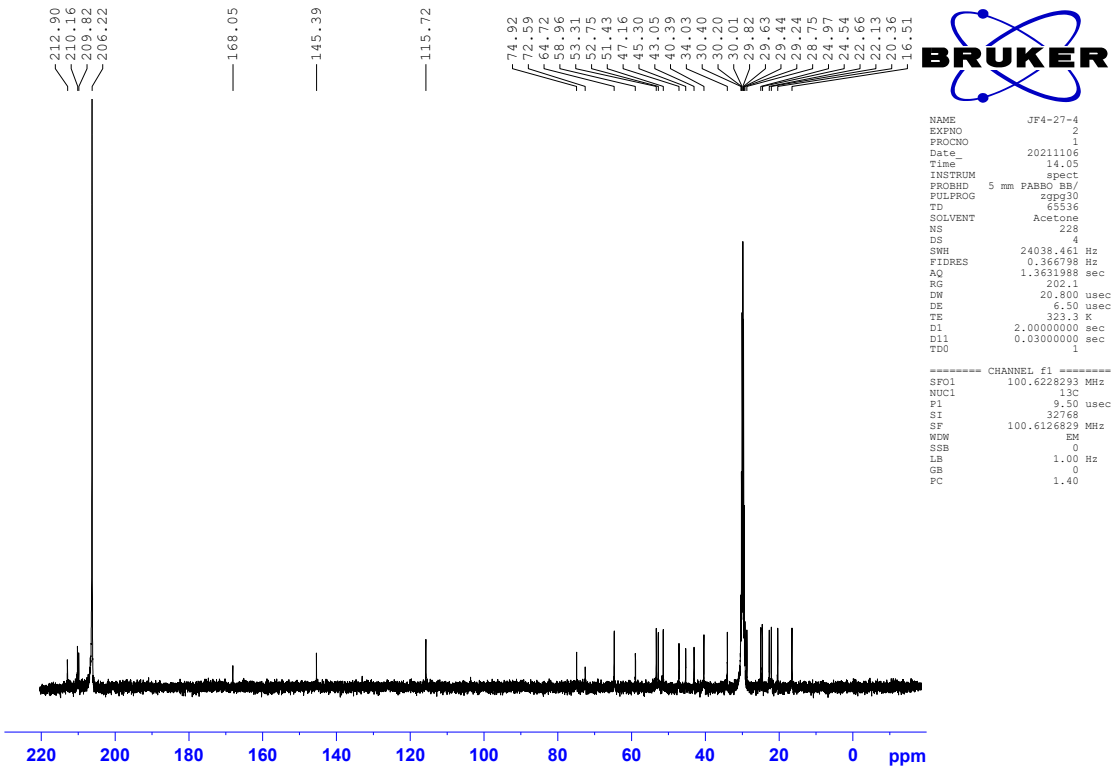

Figure S24. The ^{13}C-NMR spectrum of asperterpene C (**3**) in acetone-d_6.

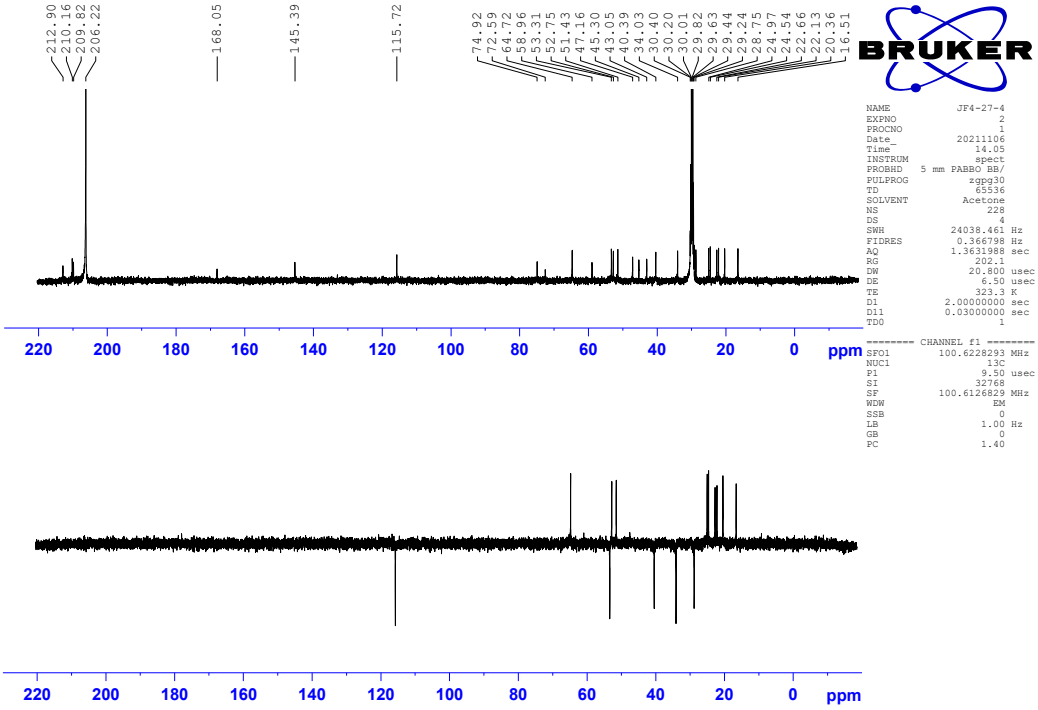

Figure S25. The DEPT 135 spectrum of asperterpene C (**3**) in acetone-d_6.

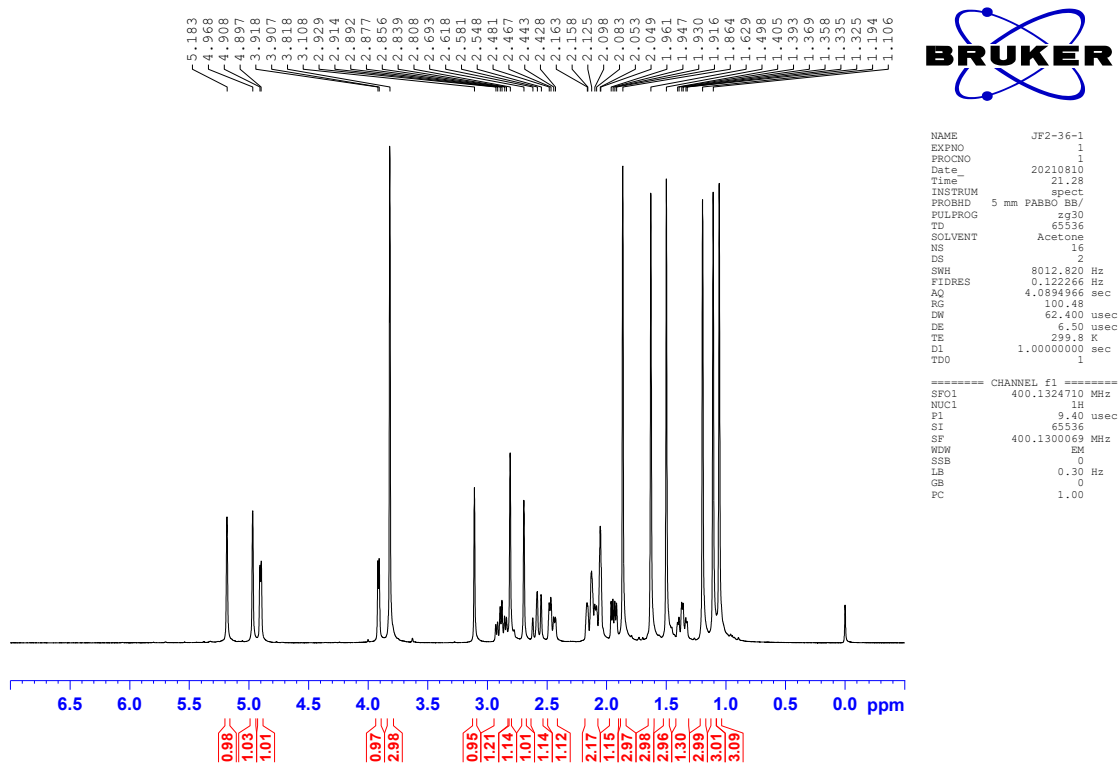

Figure S26. The ^{1}H-NMR spectrum of asperterpene D (**4**) in acetone-d_6.

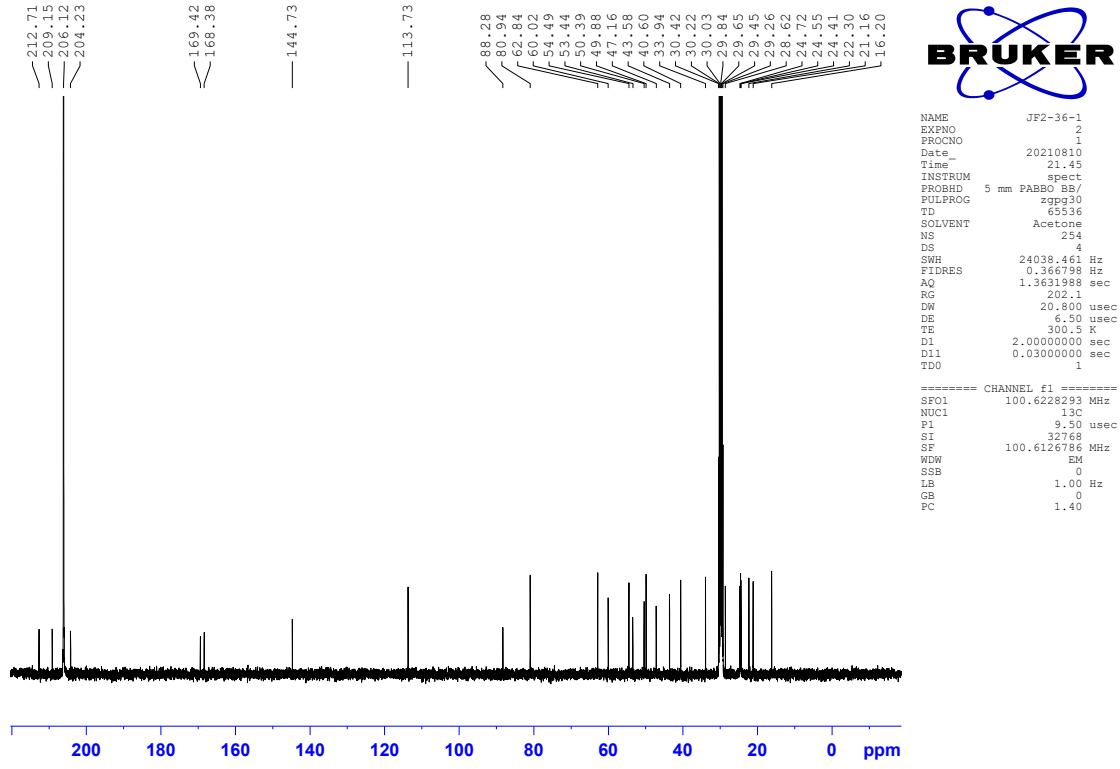

Figure S27. The ^{13}C-NMR spectrum of asperterpene D (**4**) in acetone-d_6.

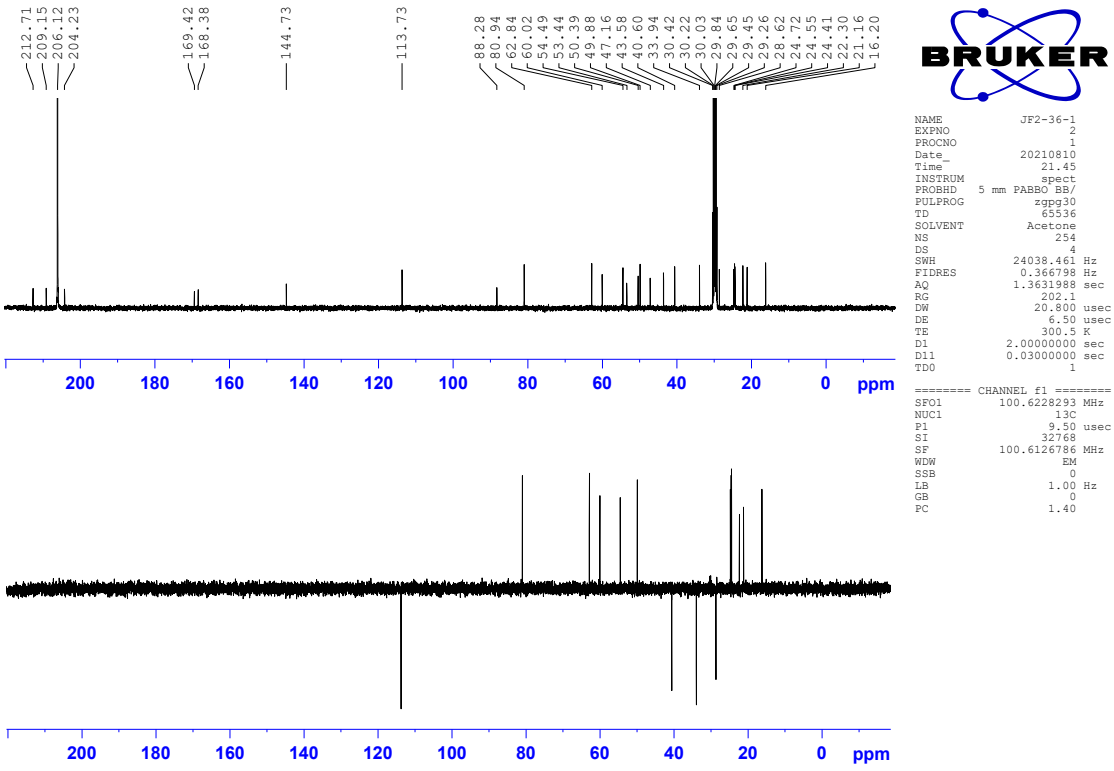

Figure S28. The DEPT 135 spectrum of asperterpene D (**4**) in acetone-d_6.

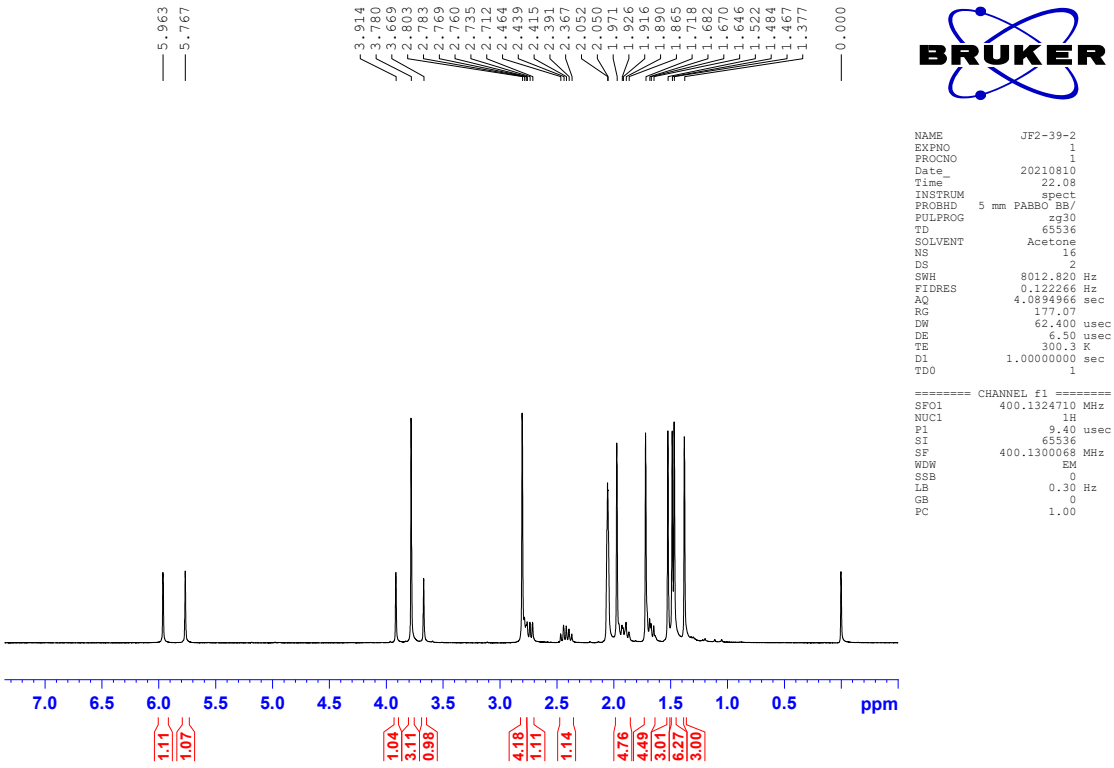

Figure S29. The ^{1}H-NMR spectrum of asperterpene E (**5**) in acetone-d_6.

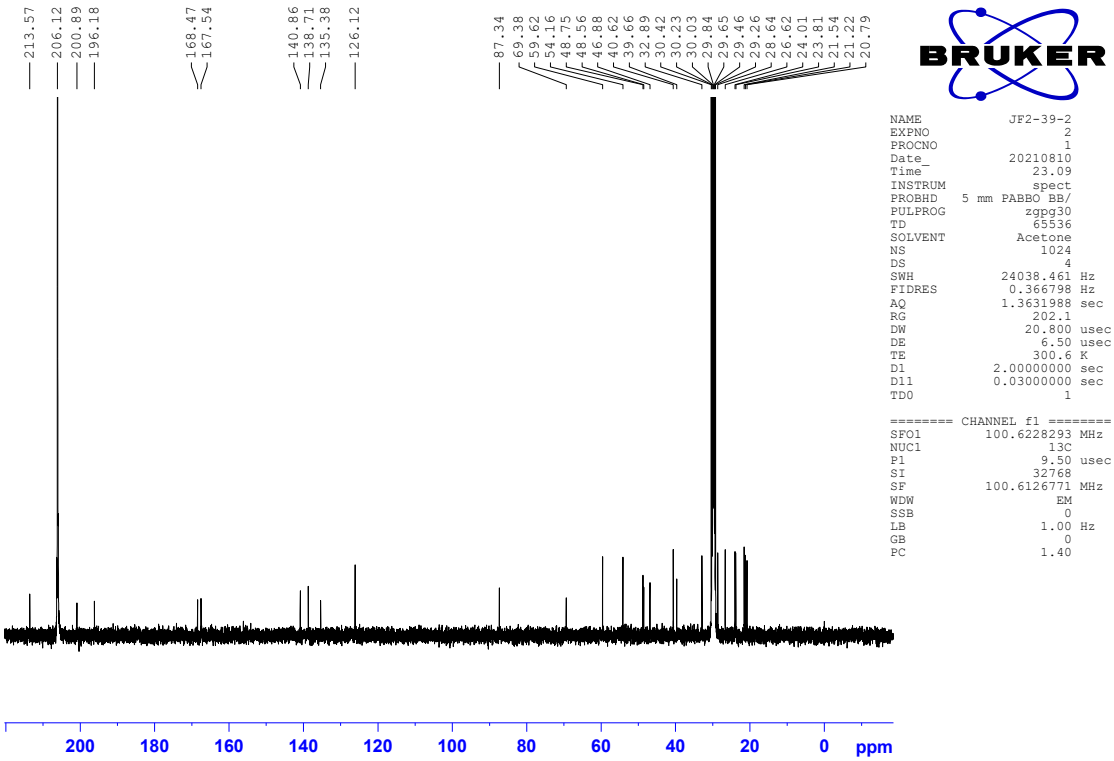

Figure S30. The ^{13}C-NMR spectrum of asperterpene E (**5**) in acetone-d_6.

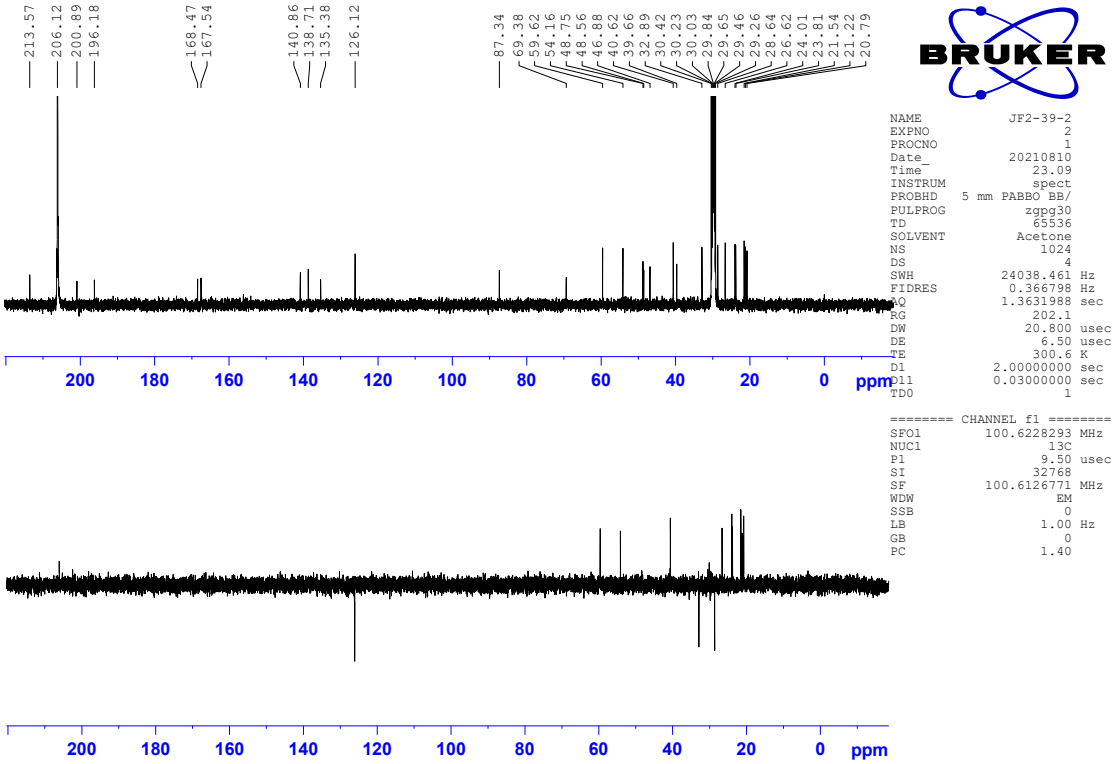

Figure S31. The DEPT 135 spectrum of asperterpene E (**5**) in acetone-d_6.

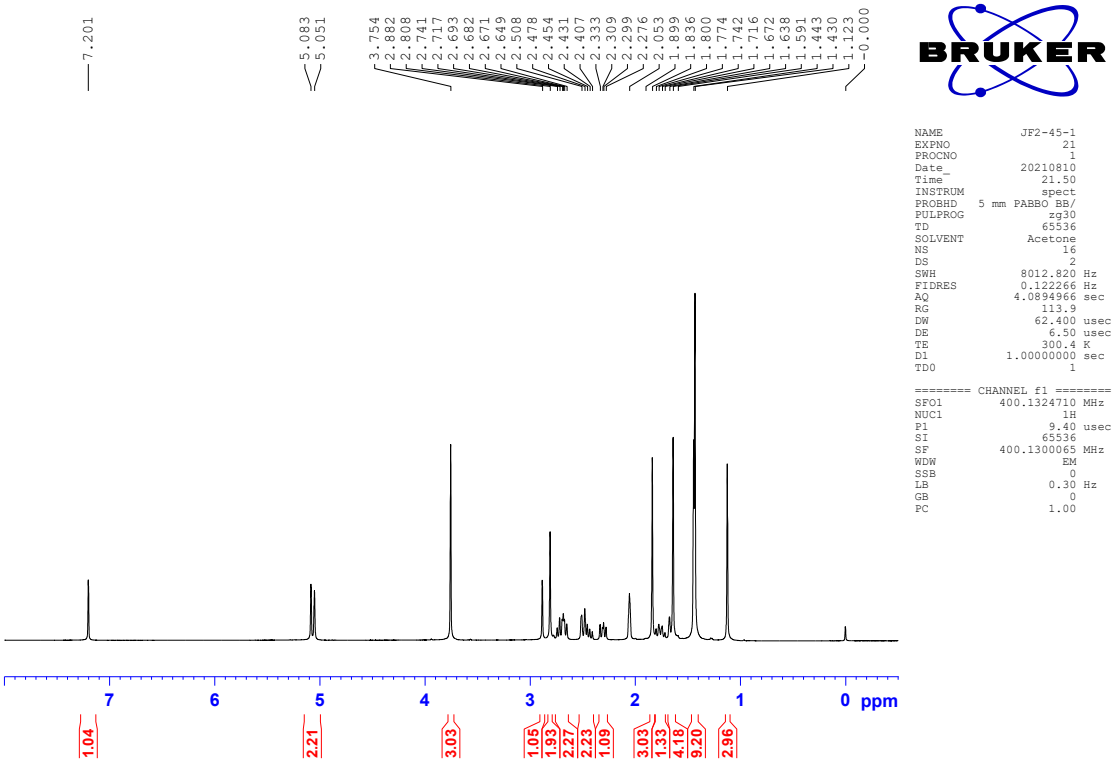

Figure S32. The ^{1}H-NMR spectrum of terretonin A (**6**) in acetone-d_6.

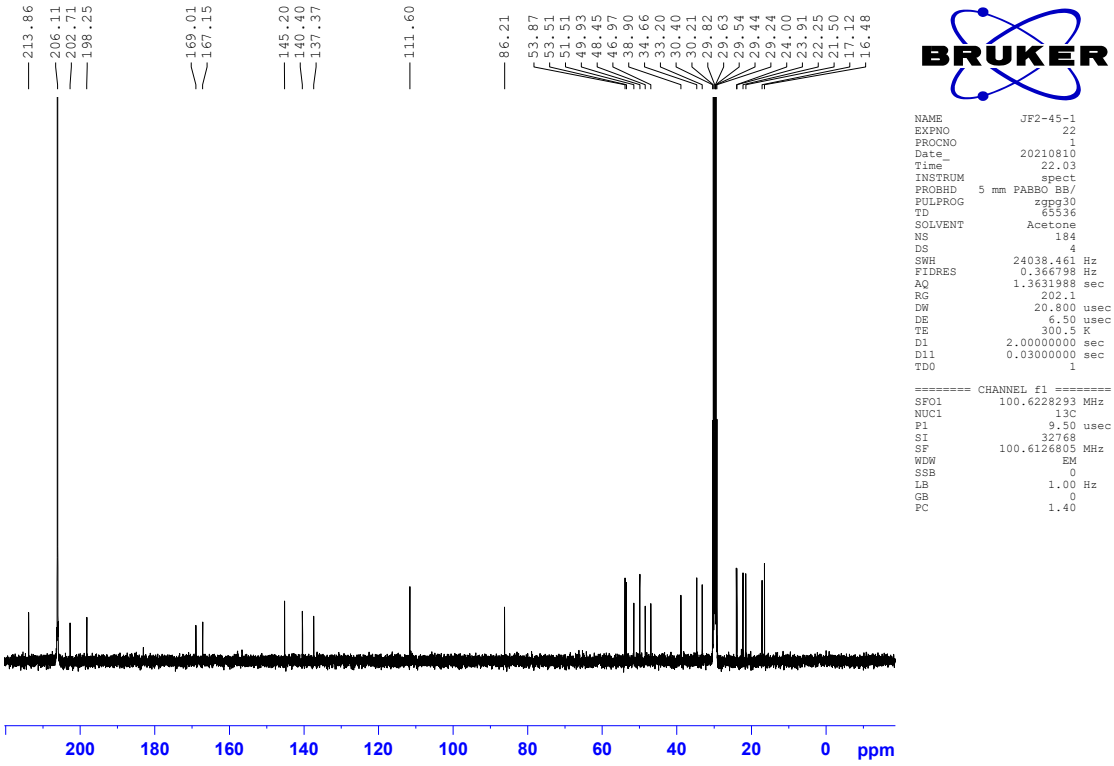

Figure S33. The ^{13}C-NMR spectrum of terretonin A (**6**) in acetone-d_6.

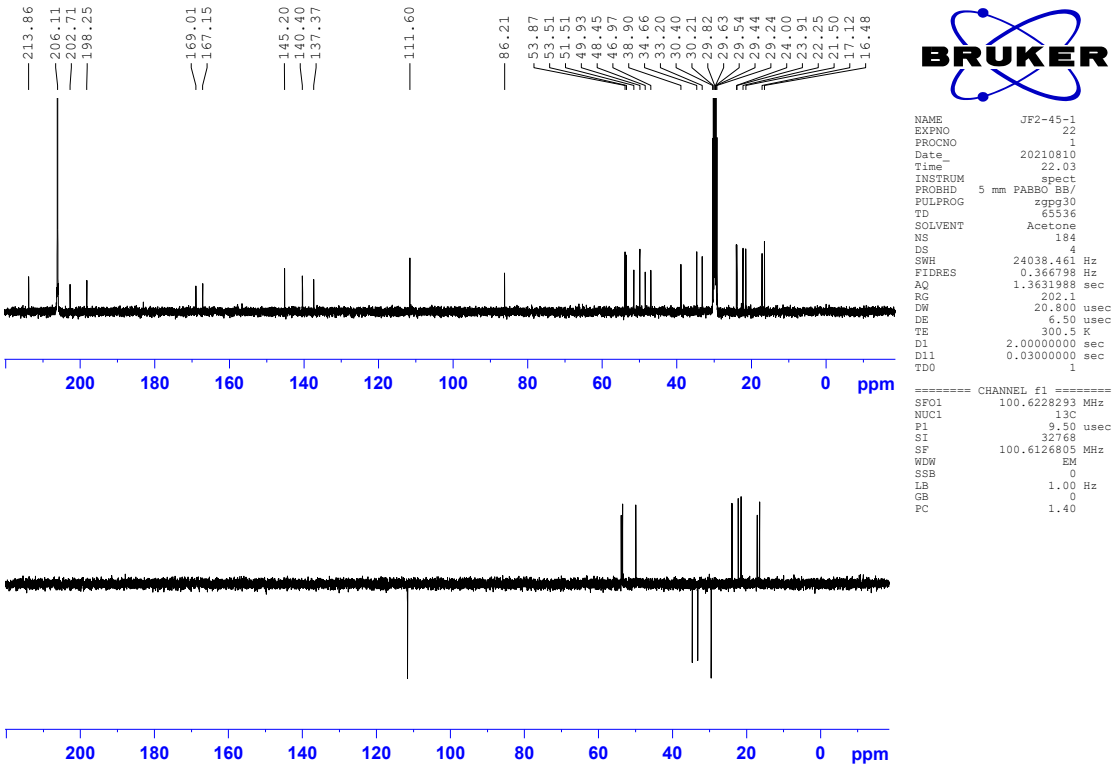

Figure S34. The DEPT 135 spectrum of terretonin A (**6**) in acetone-d_6.

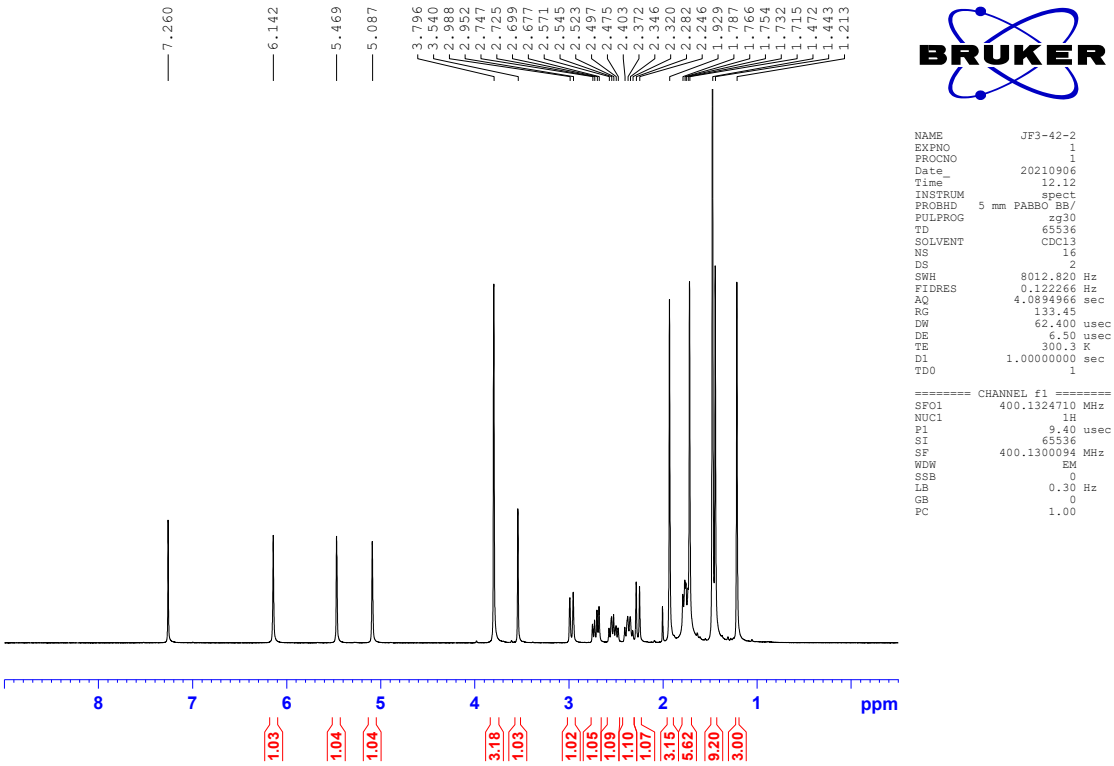

Figure S35. The ^{1}H-NMR spectrum of terretonin (**7**) in $CDCl_3$.

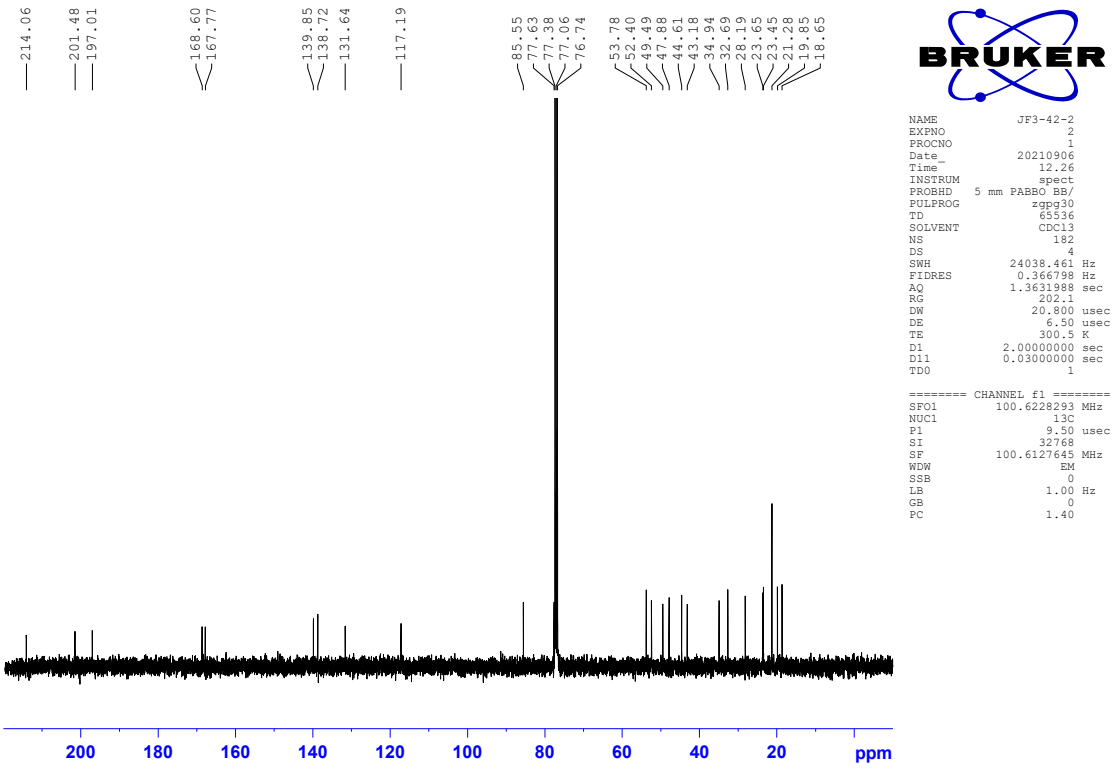

Figure S36. The ^{13}C-NMR spectrum of terretonin (**7**) in $CDCl_3$.

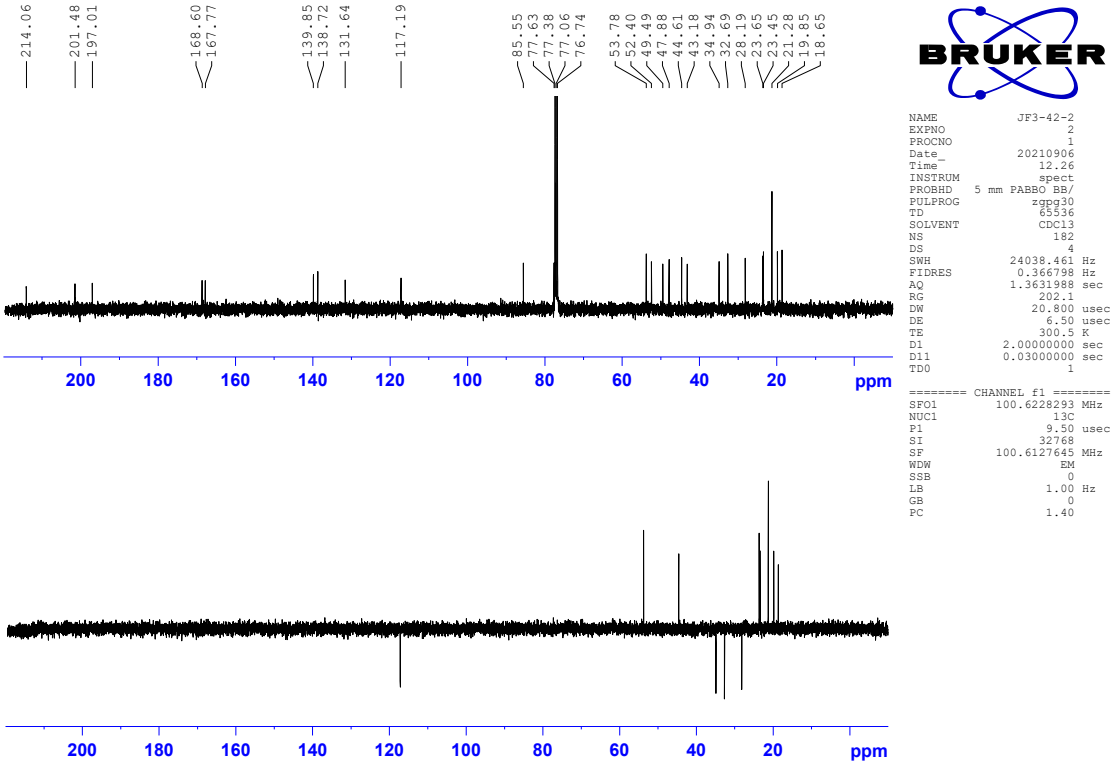

Figure S37. The DEPT 135 spectrum of terretonin (**7**) in $CDCl_3$.

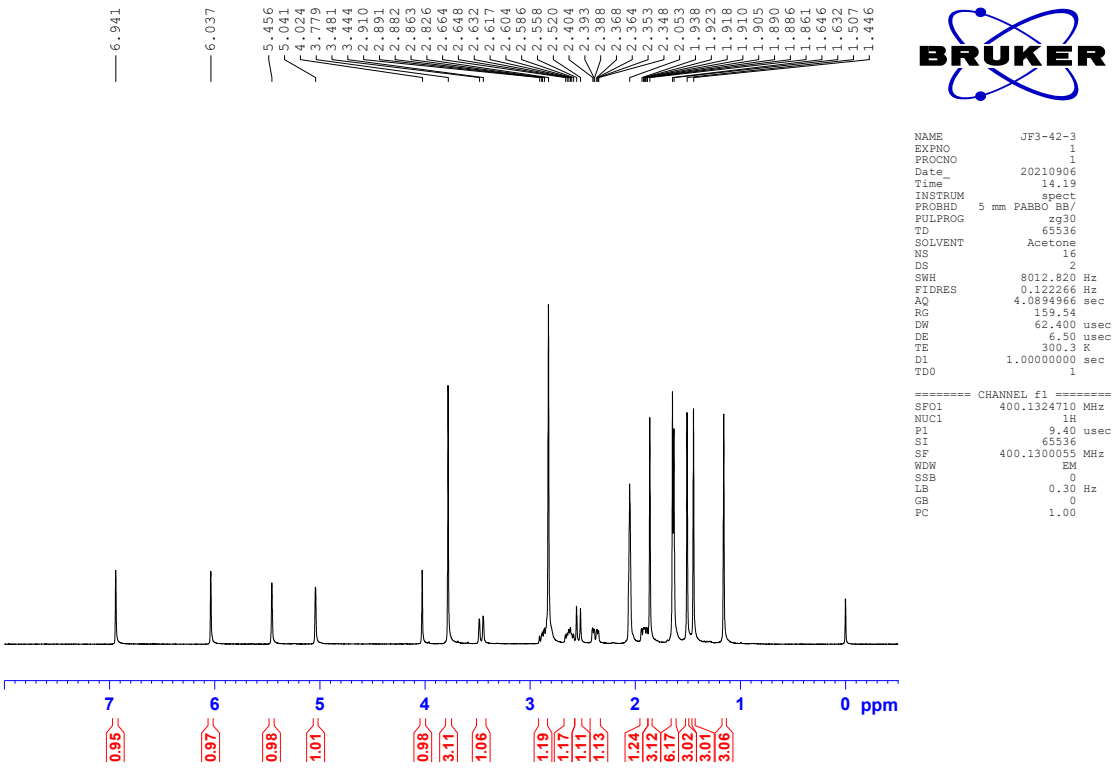

Figure S38. The ^{1}H-NMR spectrum of aperterpene O (**8**) in acetone-d_6.

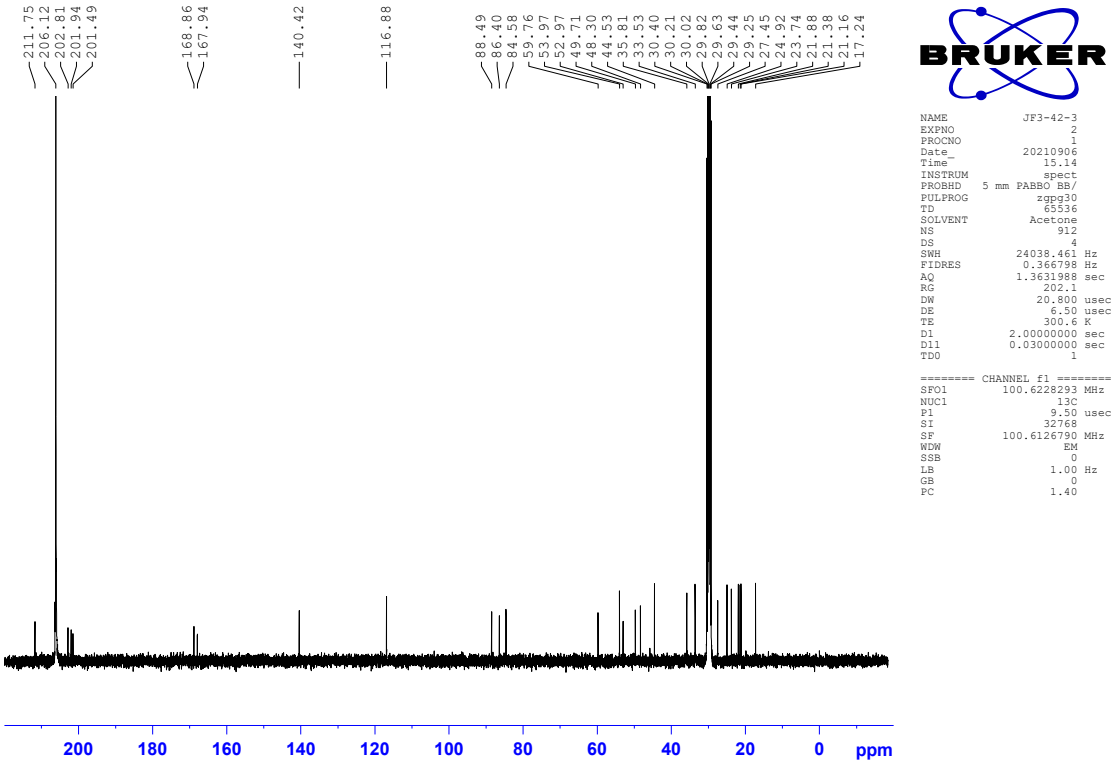

Figure S39. The ^{13}C-NMR spectrum of aperterpene O (**8**) in acetone-d_6.

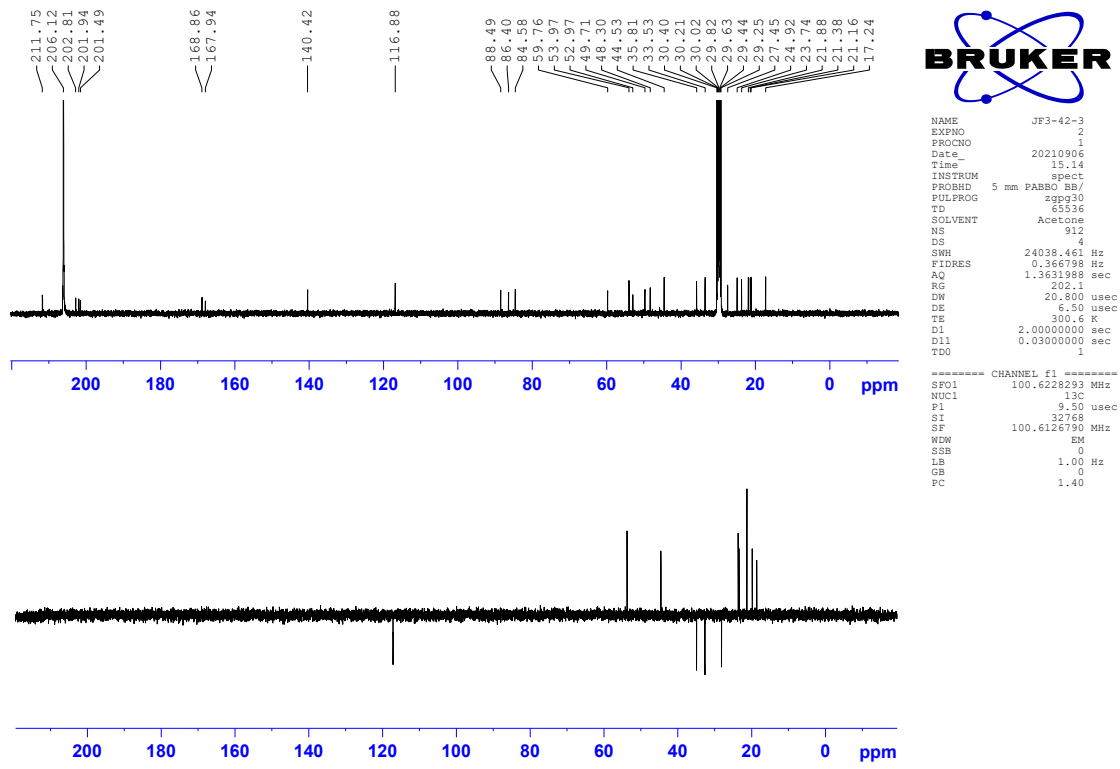

Figure S40. The DEPT 135 spectrum of aperterpene O (**8**) in acetone-d_6.

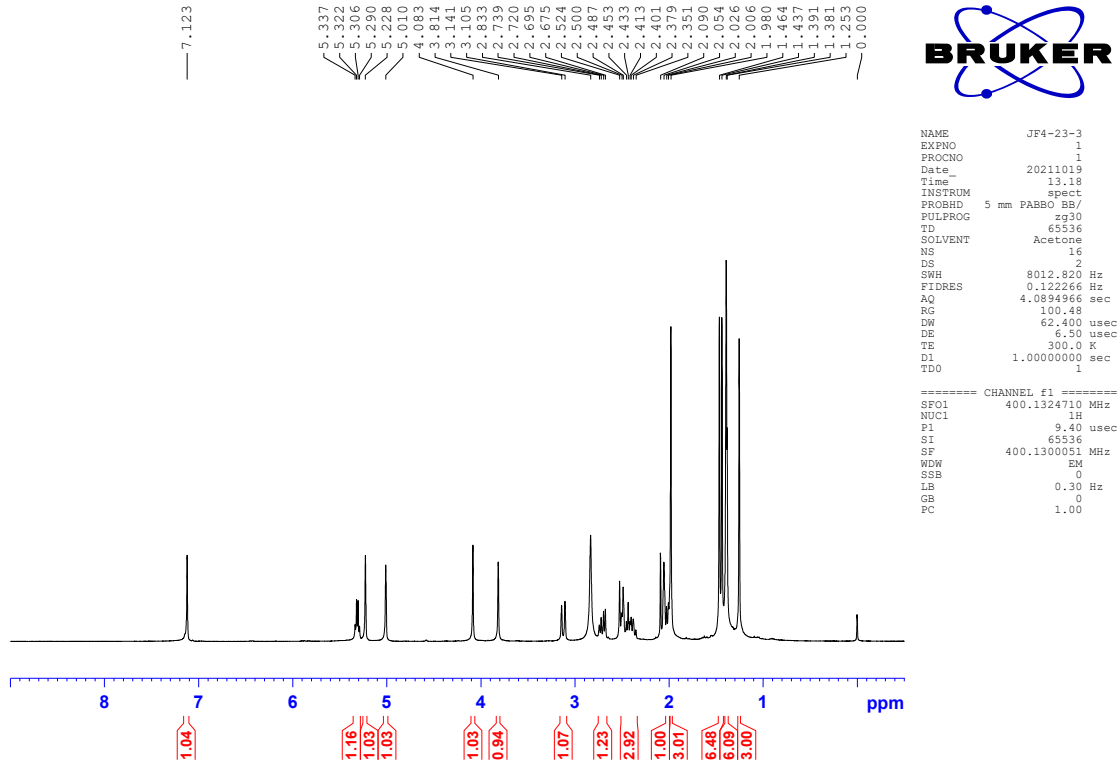

Figure S41. The ^{1}H-NMR spectrum of terretonin C (**9**) in acetone-d_6.

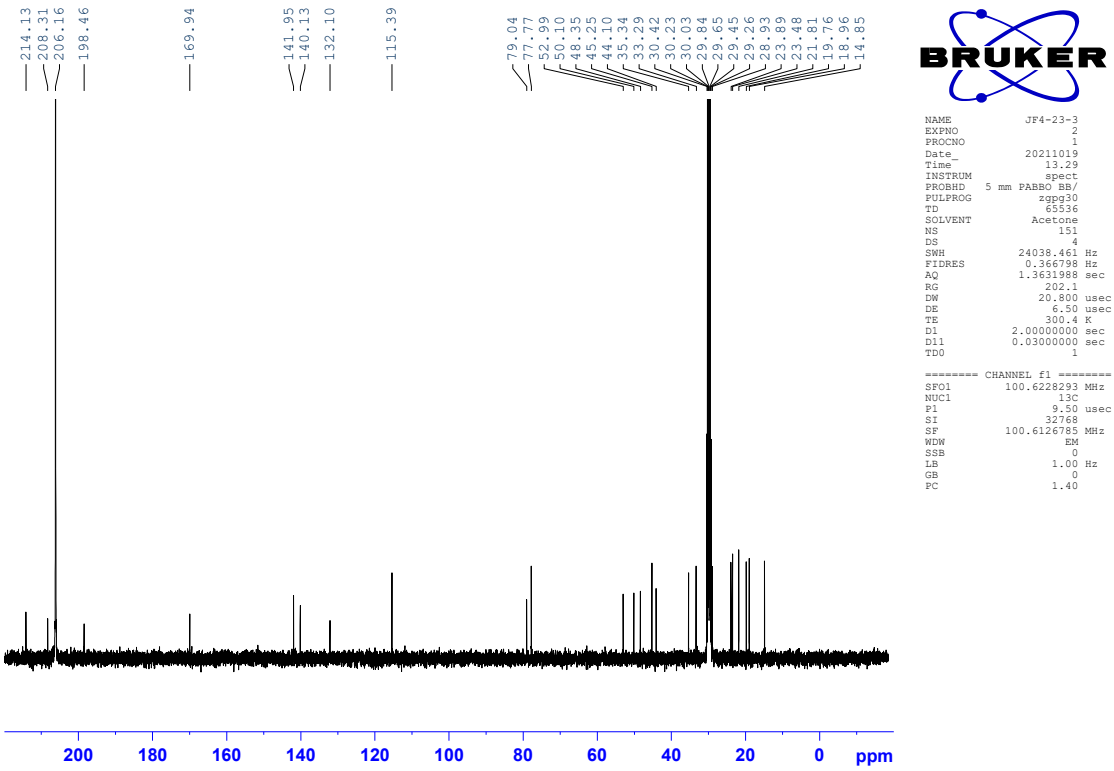

Figure S42. The ^{13}C-NMR spectrum of terretonin C (**9**) in acetone-d_6.

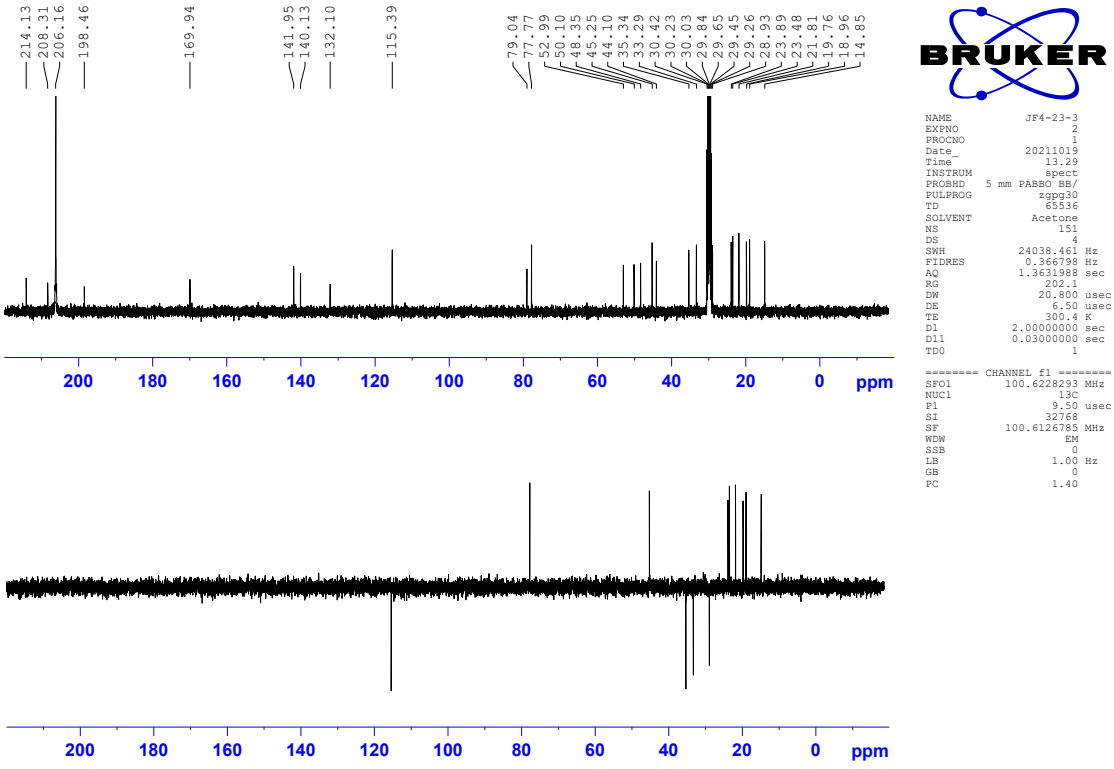

Figure S43. The DEPT 135 spectrum of terretonin C (**9**) in acetone-d_6.

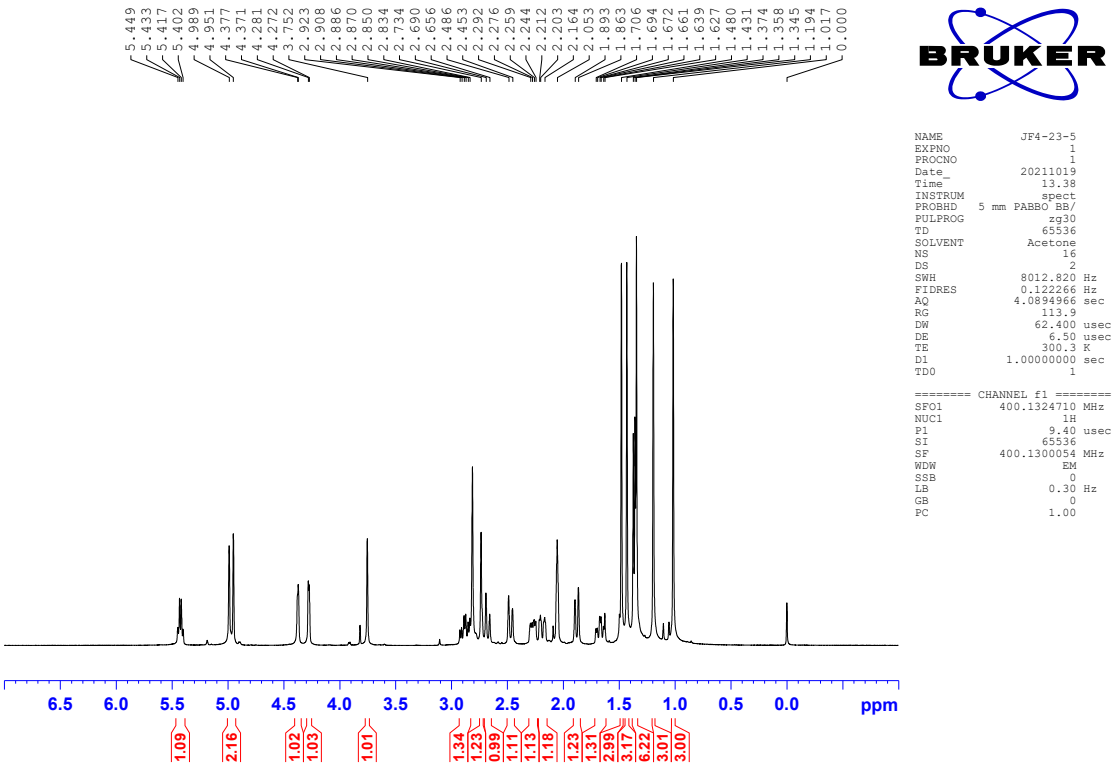

Figure S44. The ^{1}H-NMR spectrum of terretonin H (**10**) in acetone-d_6.

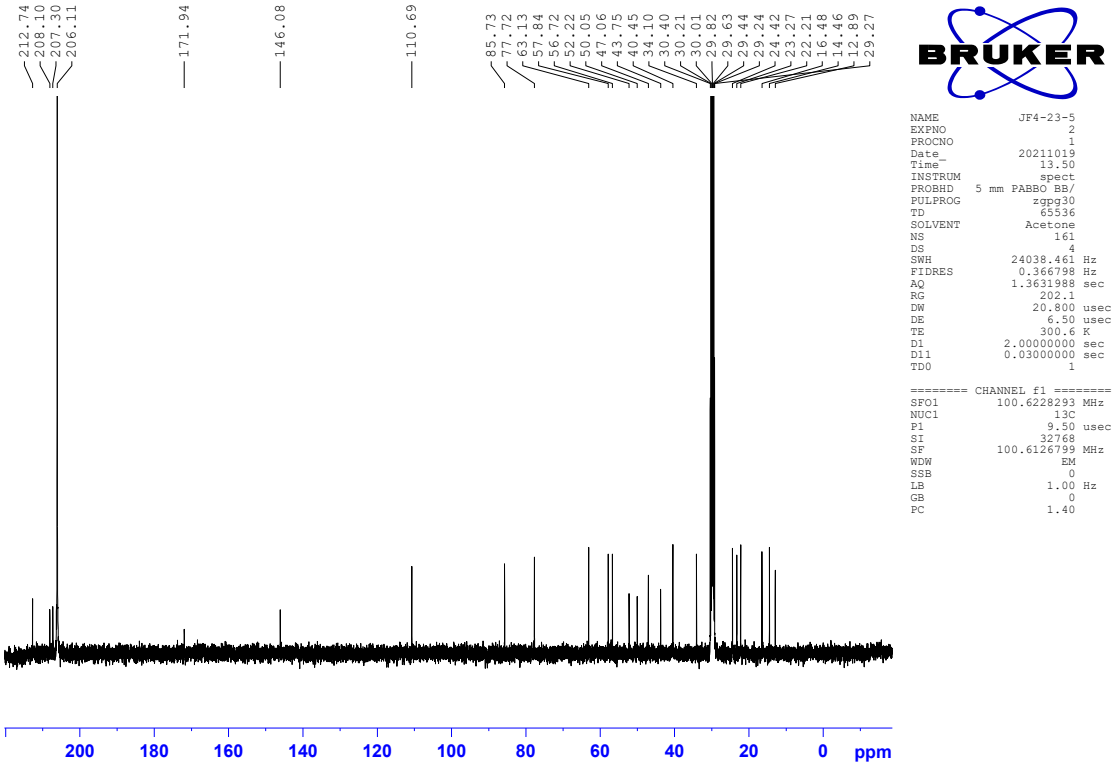

Figure S45. The ^{13}C-NMR spectrum of terretonin H (**10**) in acetone-d_6.

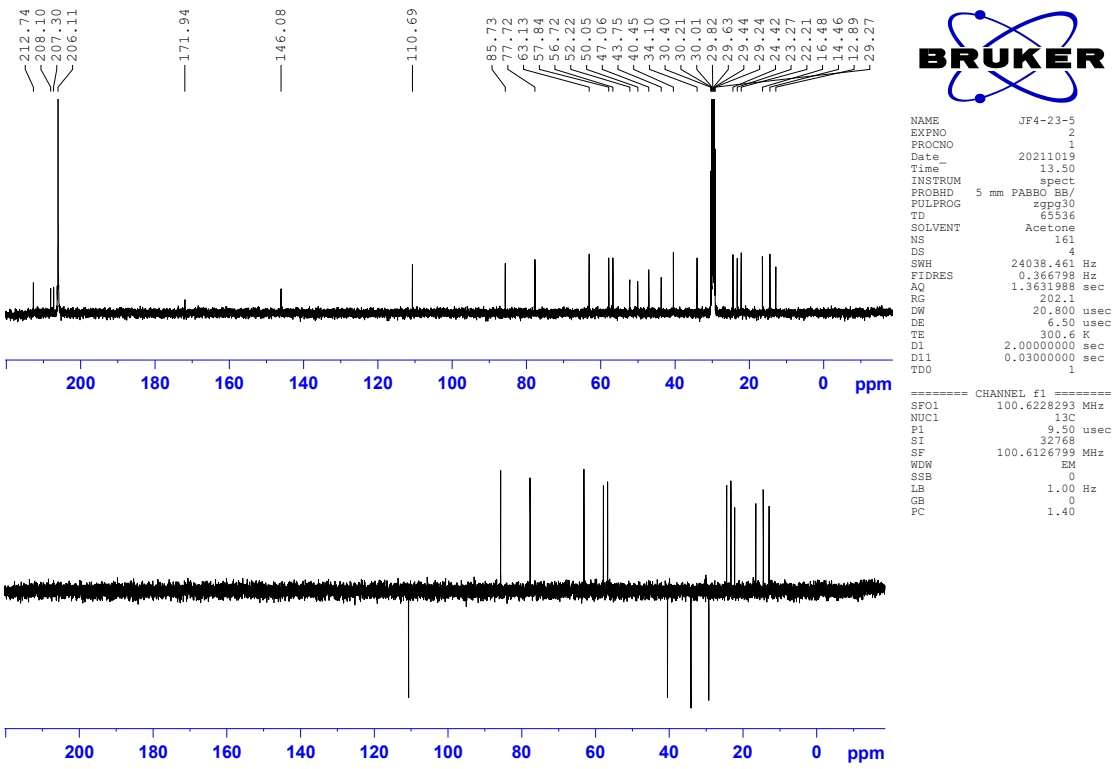

Figure S46. The DEPT 135 spectrum of terretonin H (**10**) in acetone-d_6.

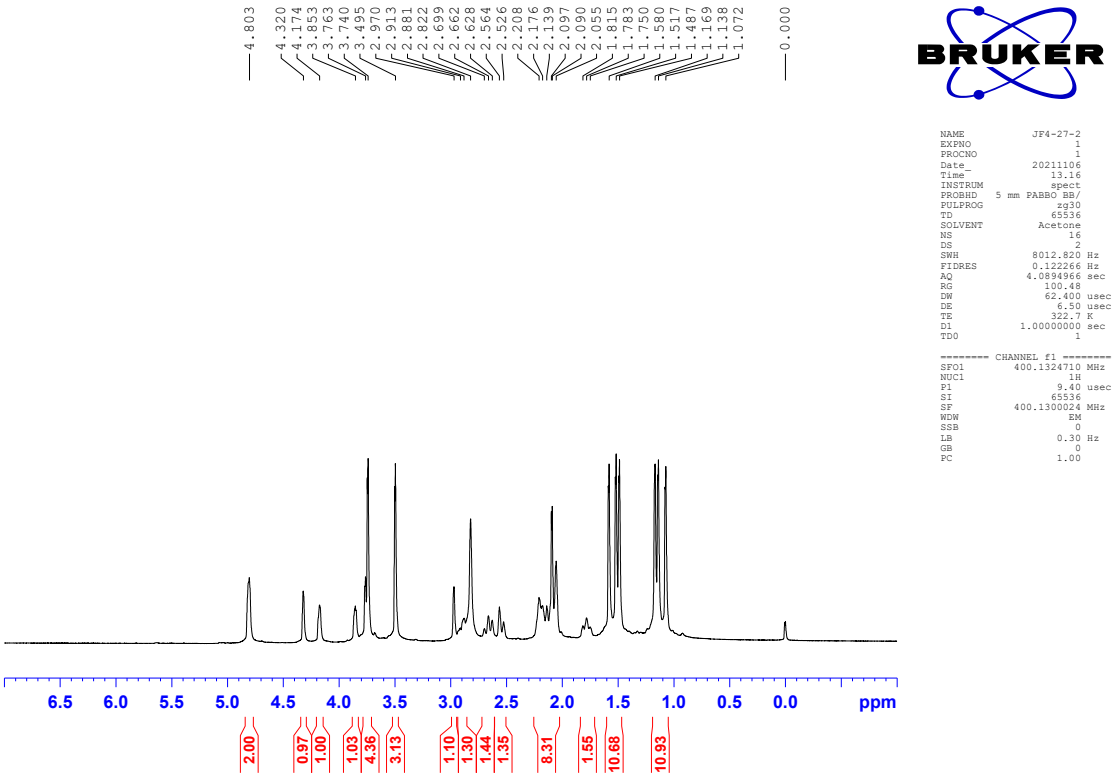

Figure S47. The ^{1}H-NMR spectrum of asperterpene J (**11**) in acetone-d_6.

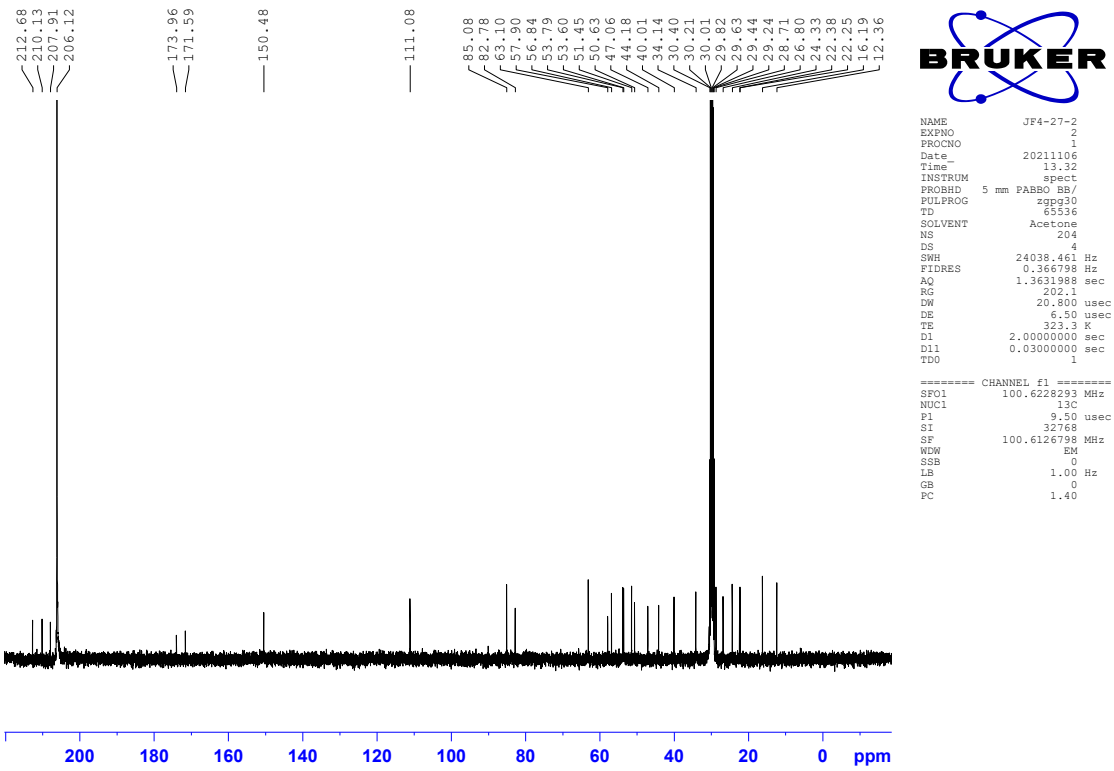

Figure S48. The ^{13}C-NMR spectrum of asperterpene J (**11**) in acetone-d_6.

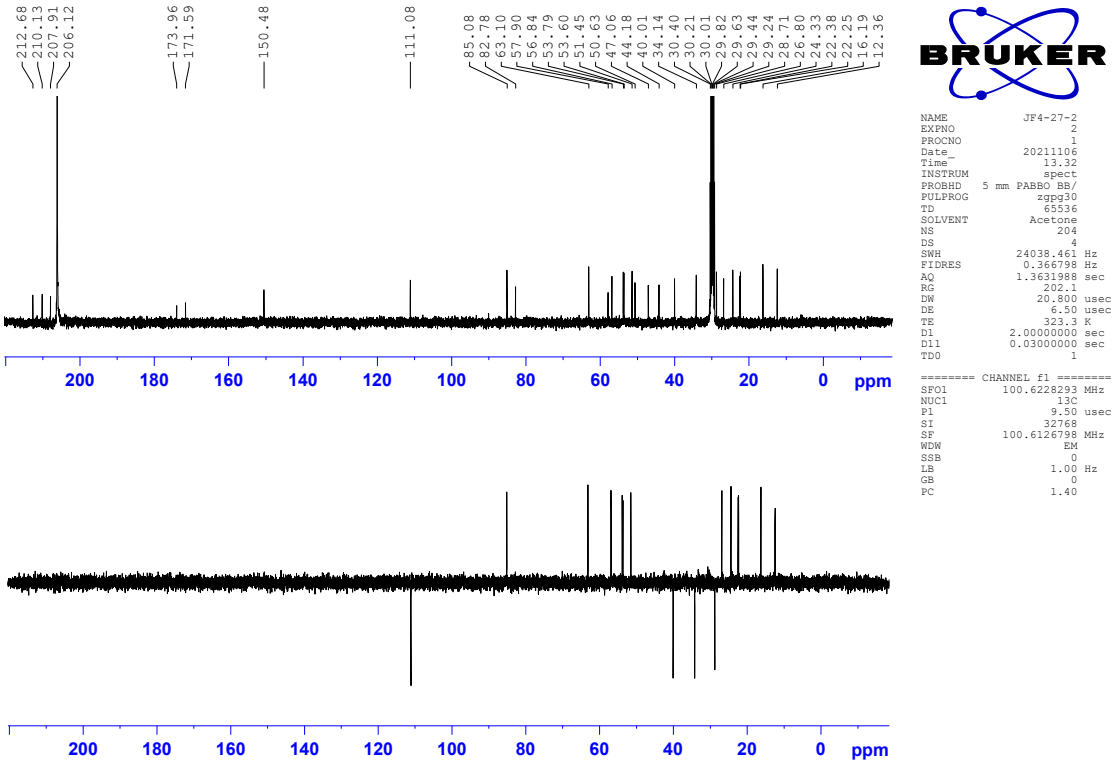

Figure S49. The DEPT 135 spectrum of asperterpene J (**11**) in acetone-d_6.

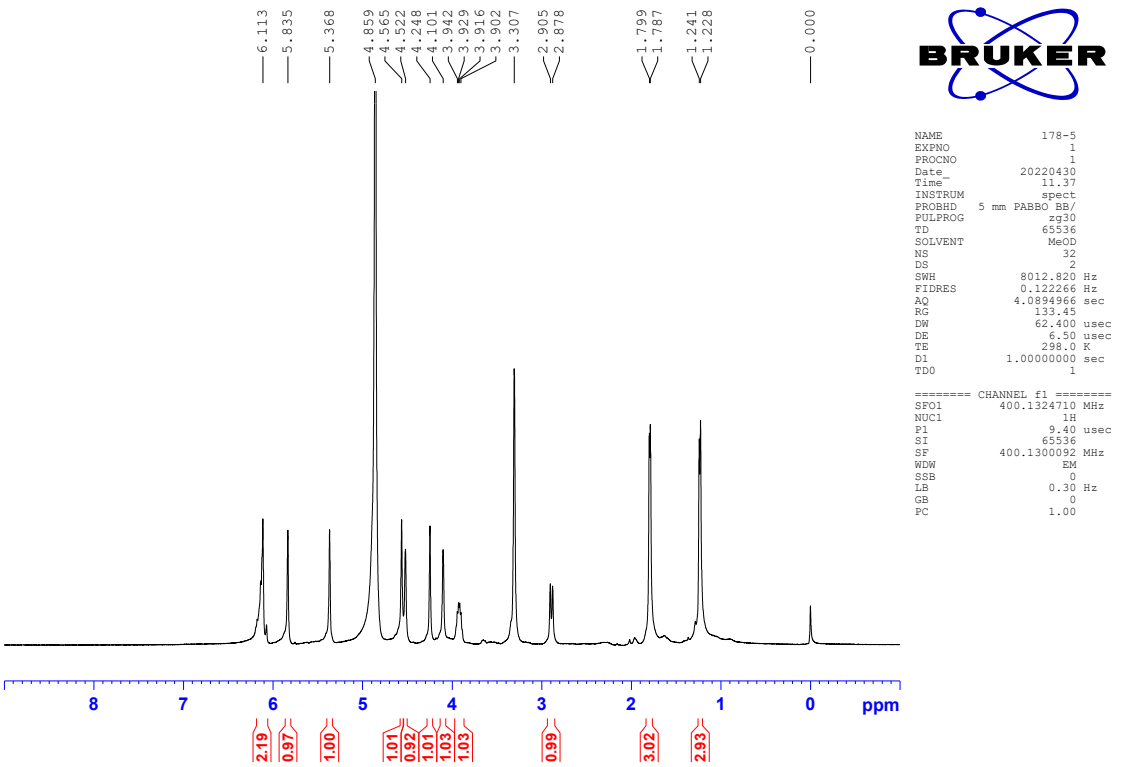

Figure S50. The ^{1}H-NMR spectrum of javanicol D (**12**) in CD_3OD.

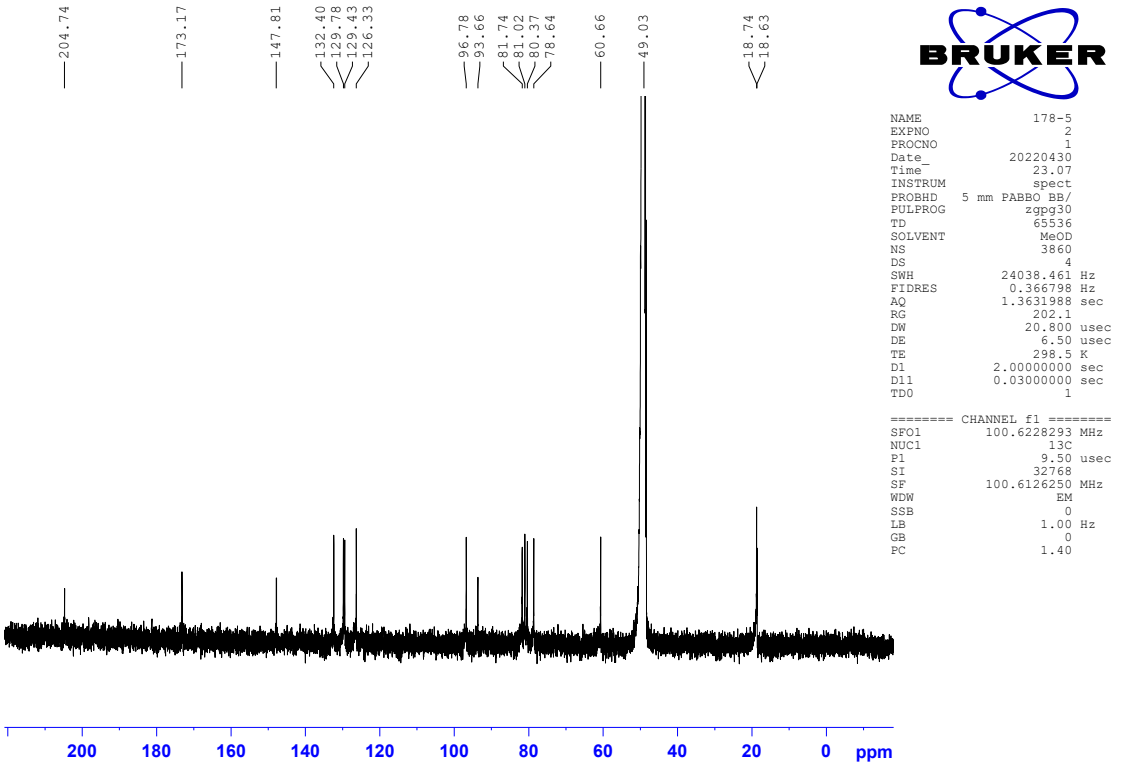

Figure S51. The ^{13}C-NMR spectrum of javanicol D (**12**) in CD_3OD.

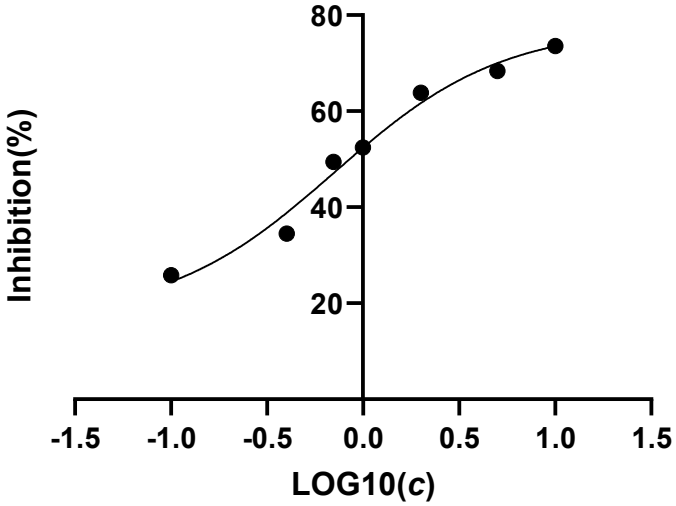

Figure S52. The BuChE inhibition curve of compound **4**.

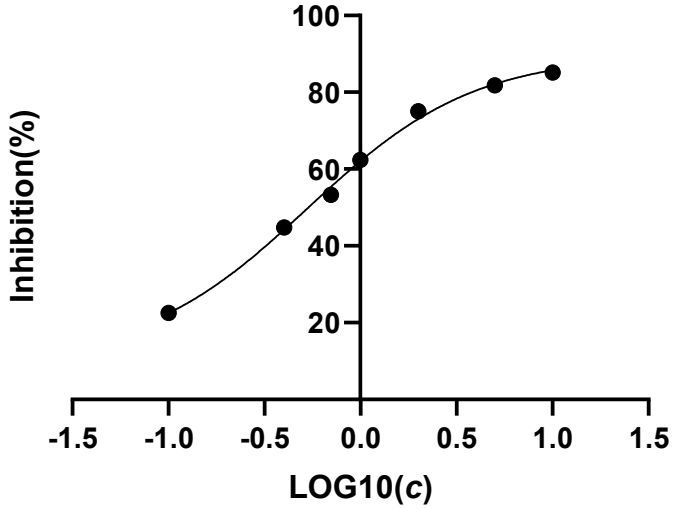

Figure S53. The BuChE inhibition curve of compound **5**.