Supplementary Information

Lvsiyujin A-G, new sesquiterpenoids from *Curcuma phaeocaulis* Valeton root tuber and their preliminary pharmacological properties assessment based on ADME evaluation, molecular docking and *in vitro* experiment

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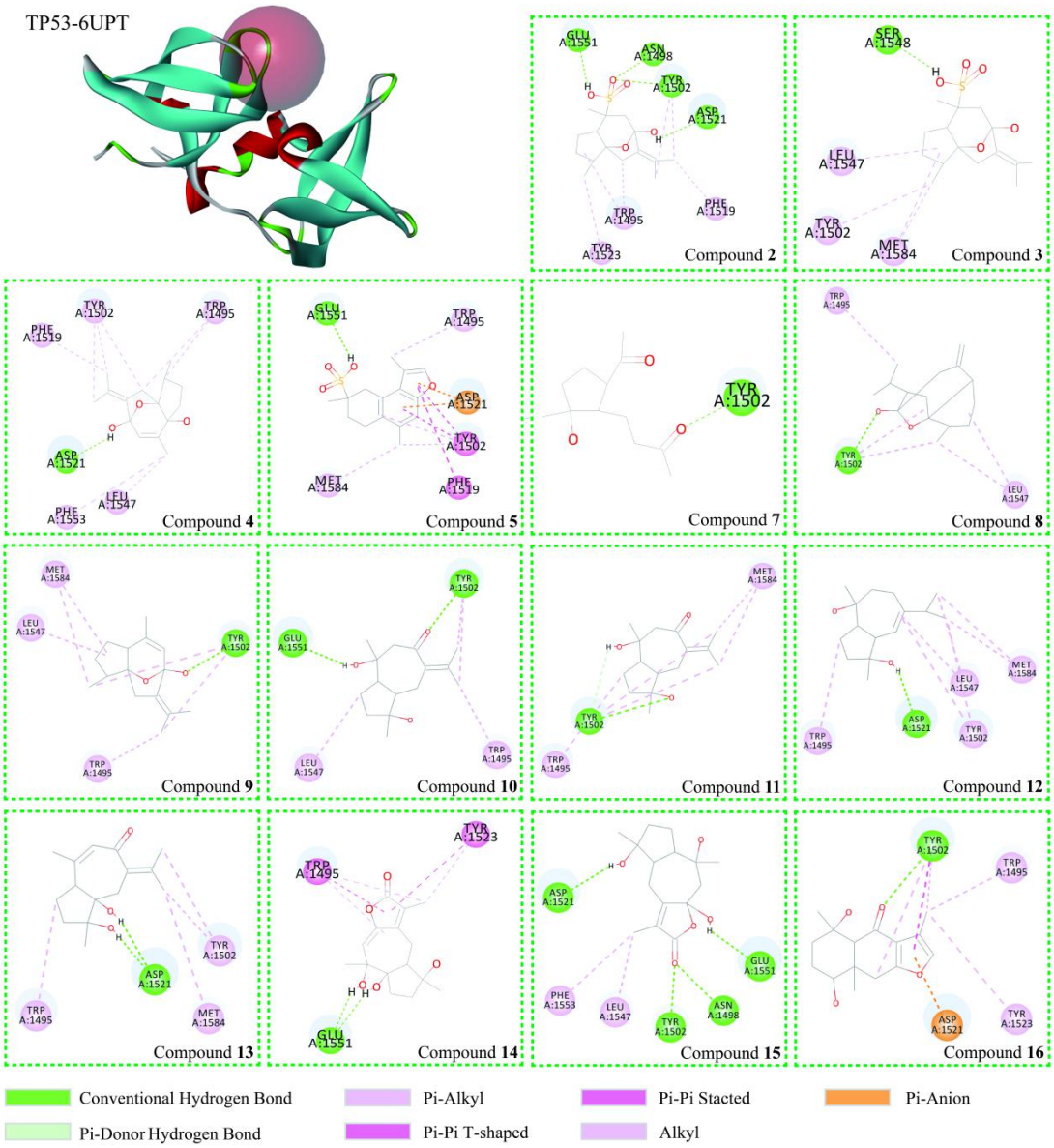


Figure S1. Docked interactions of compounds and TP53.

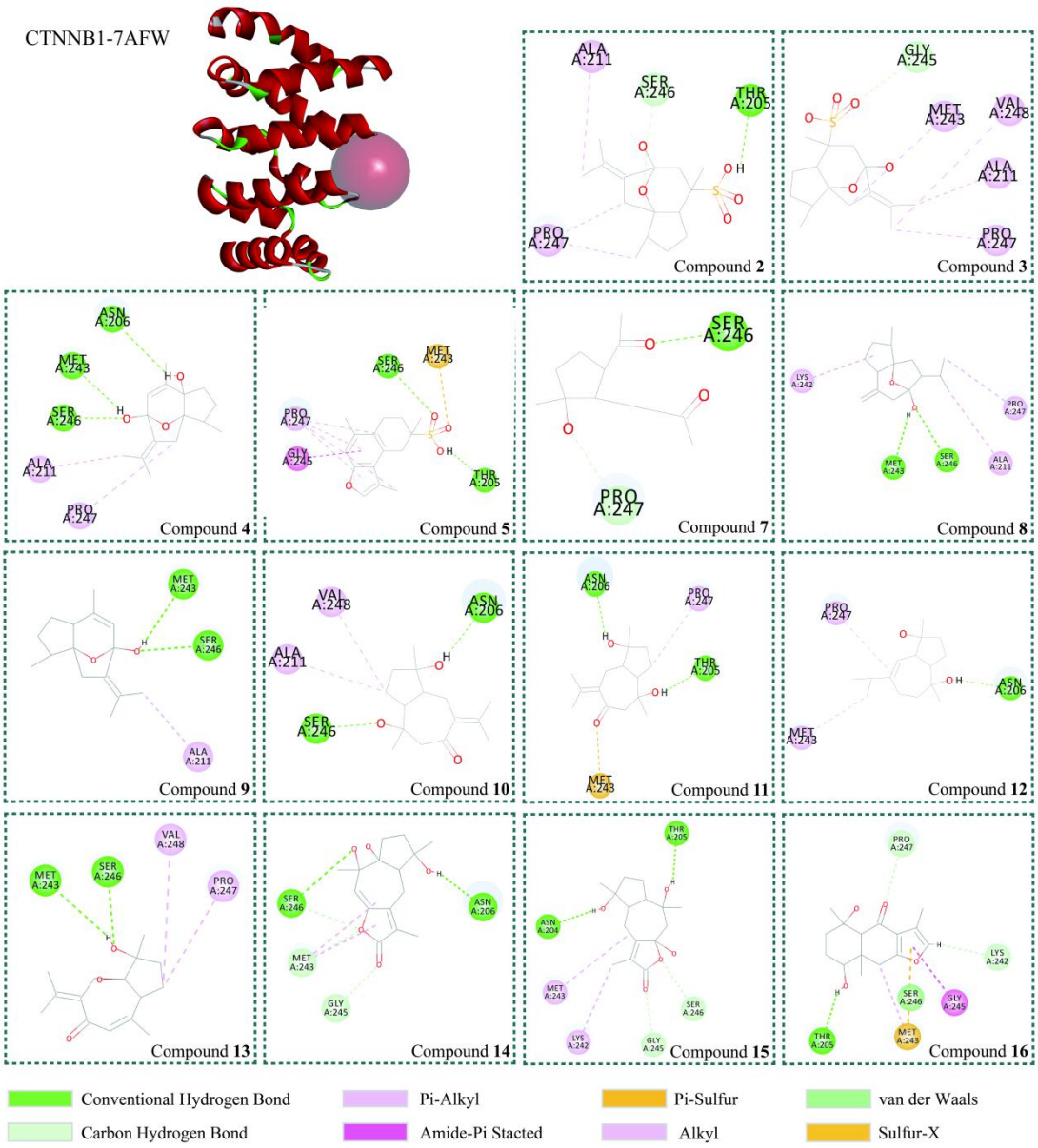


Figure S2. Docked interactions of compounds and CTNNB1.

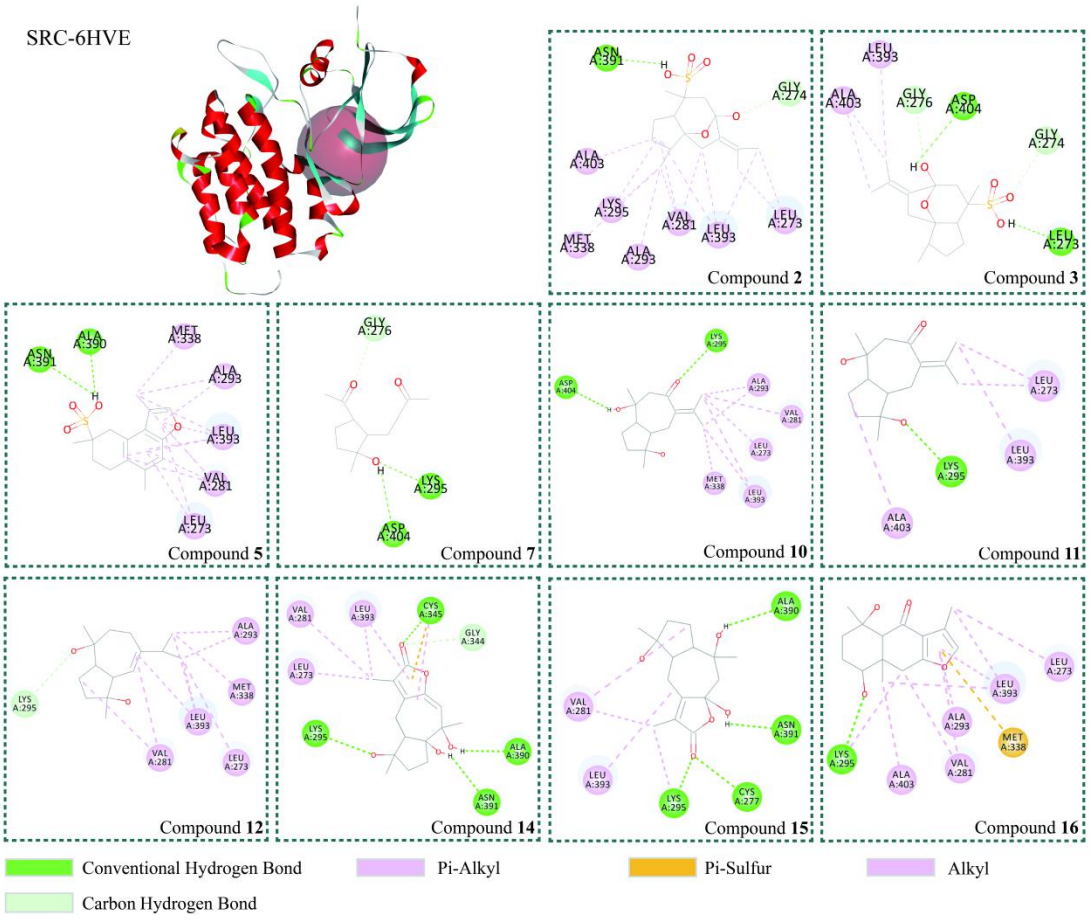


Figure S3. Docked interactions of compounds and SRC.

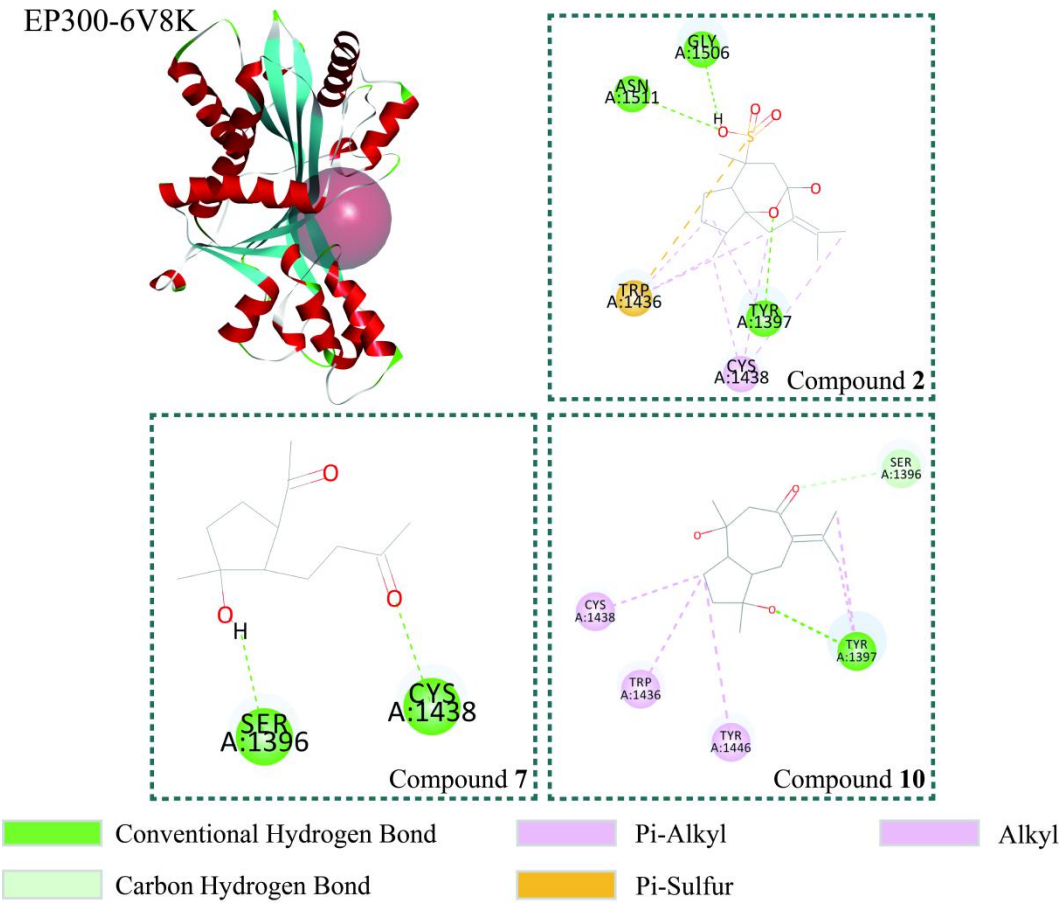


Figure S4. Docked interactions of compounds and EP300.

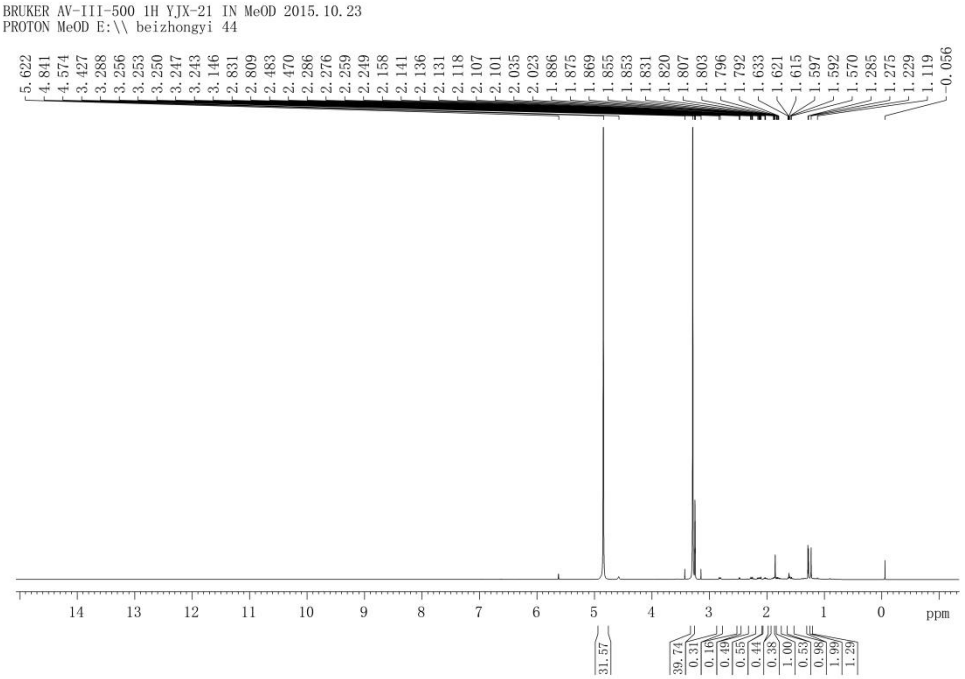


Figure S5. The ^{1}H NMR spectrum of **1** in CD_3OD

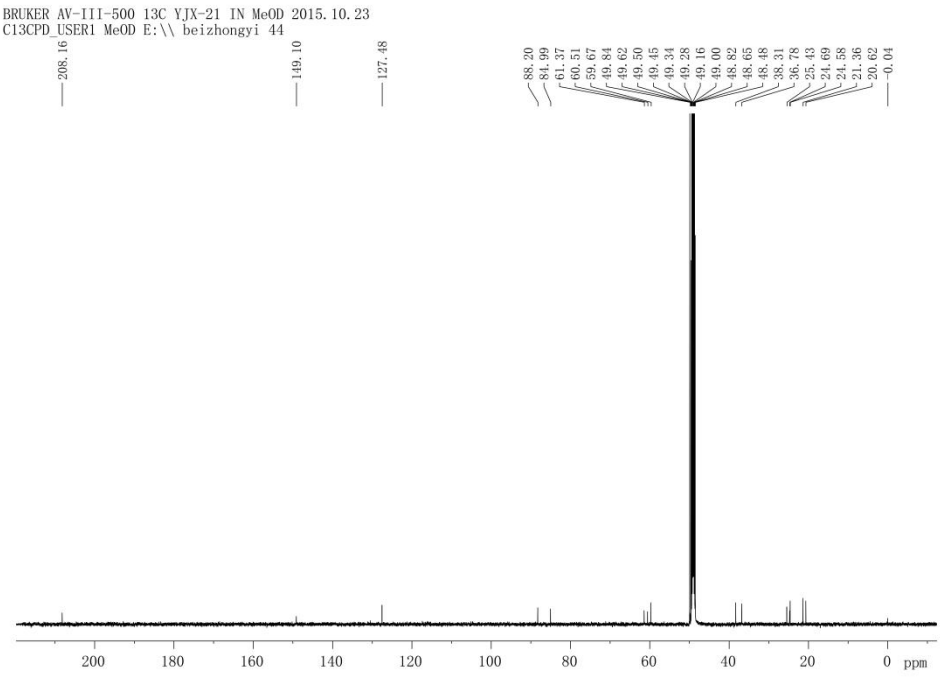


Figure S6. The ^{13}C NMR spectra of **1** in CD_3OD

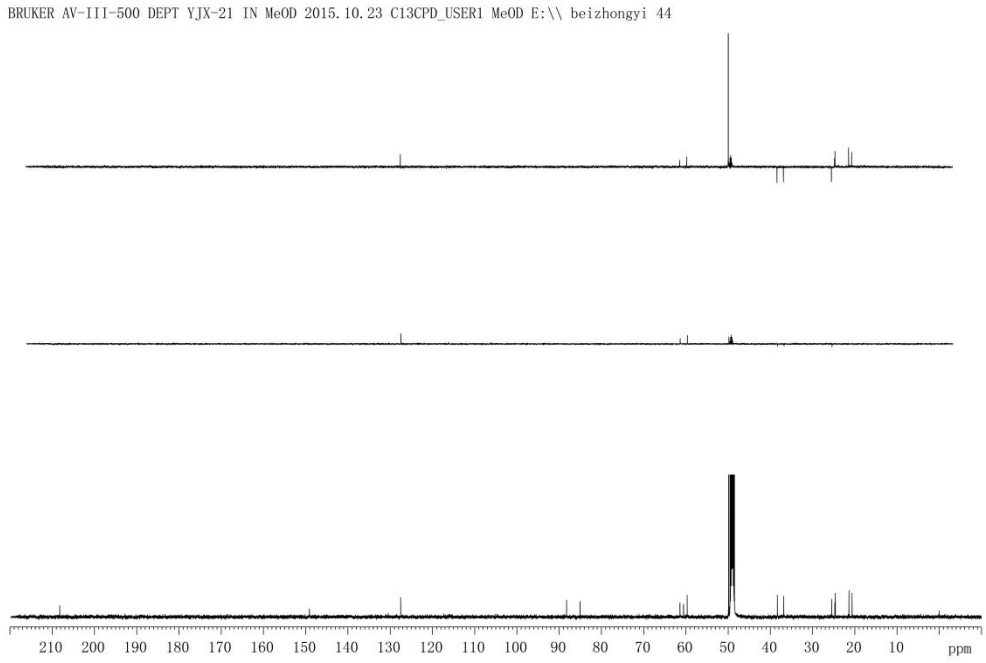


Figure S7. The DEPT spectra of **1** in CD_3OD

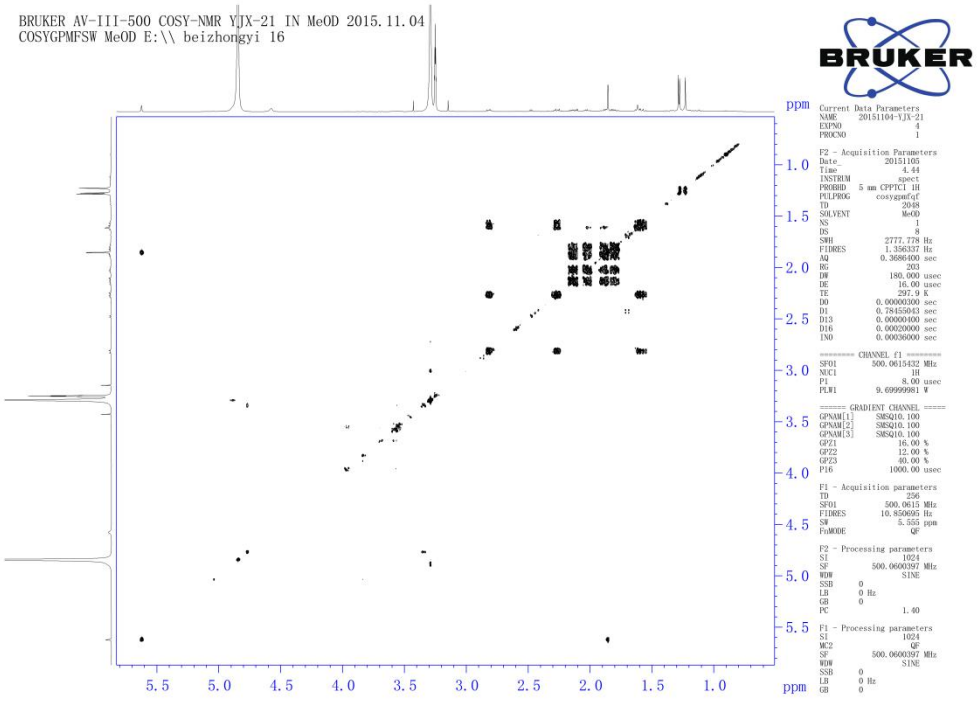


Figure S8. The ^1H-^1H COSY spectrum of **1** in CD_3OD

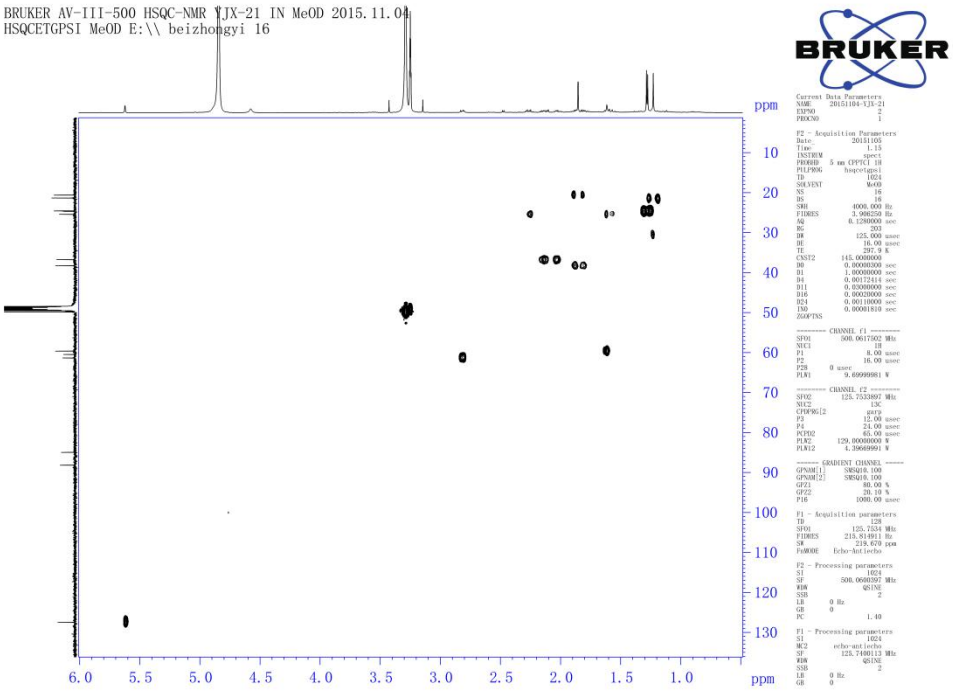


Figure S9. The HSQC spectrum of **1** in CD_3OD

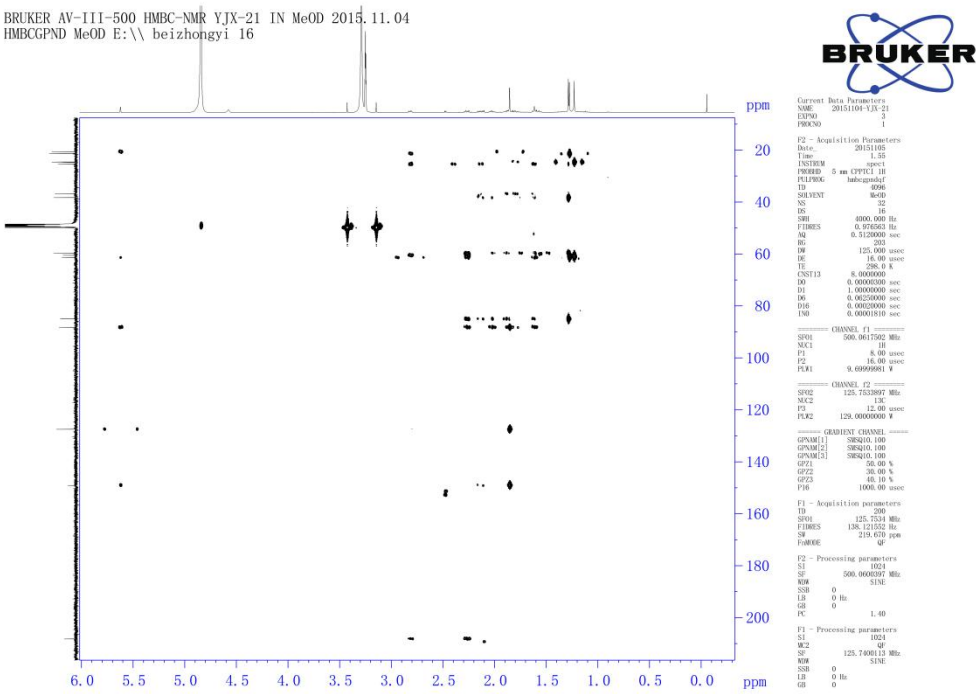


Figure S10. The HMBC spectrum of **1** in CD_3OD

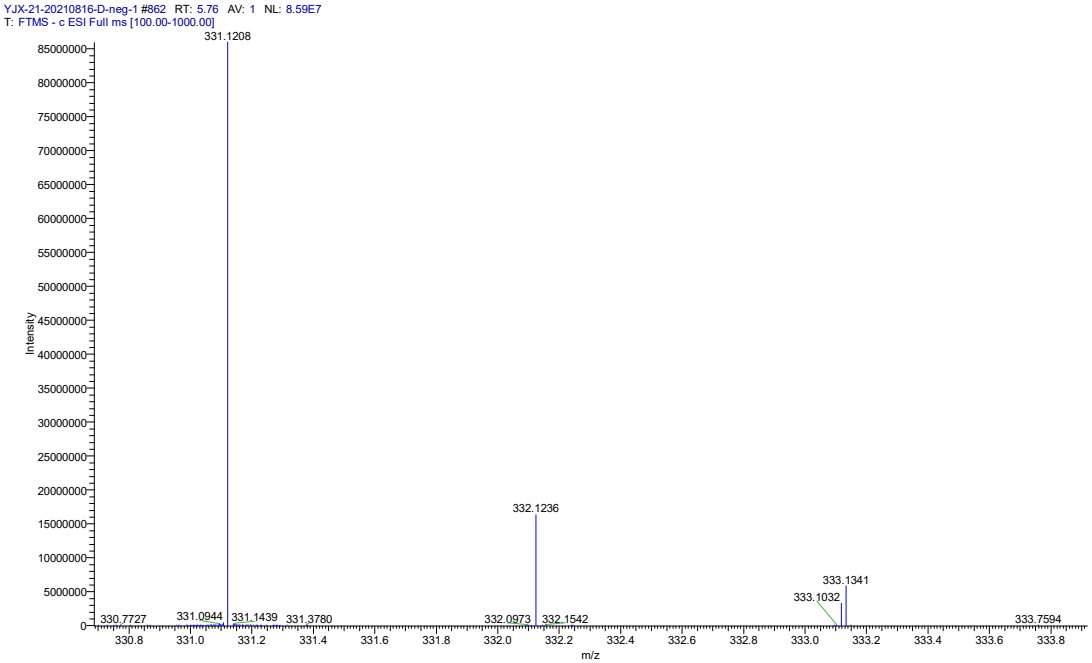


Figure S11. The HRESIMS spectrum of **1**

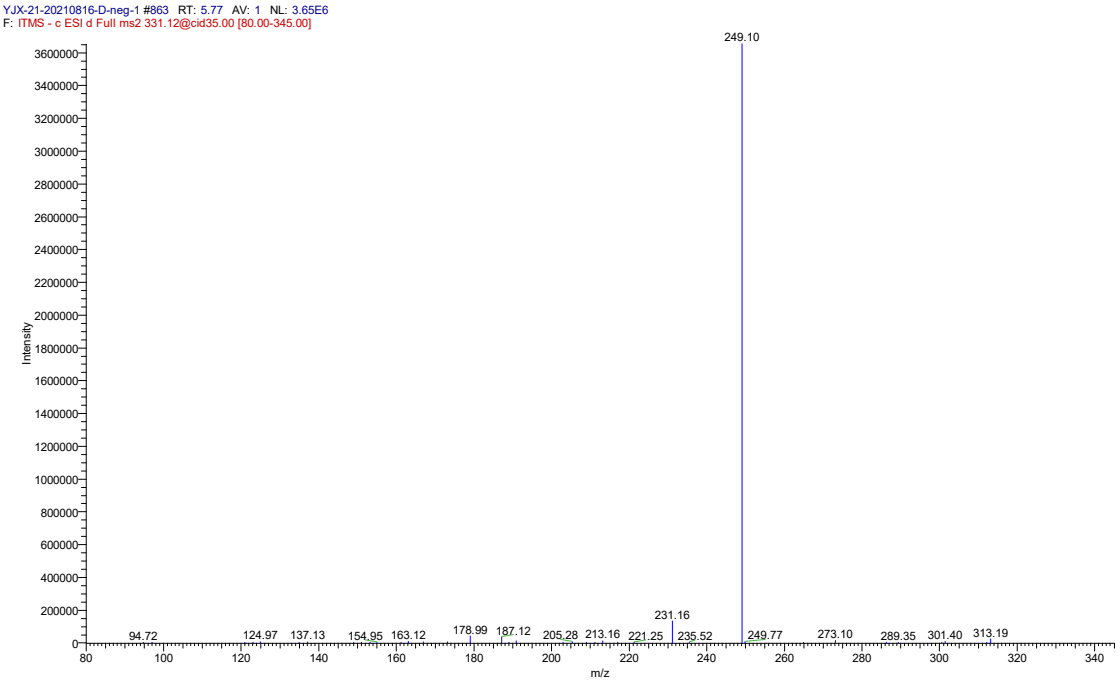


Figure S12. The MS/MS spectrum of **1**

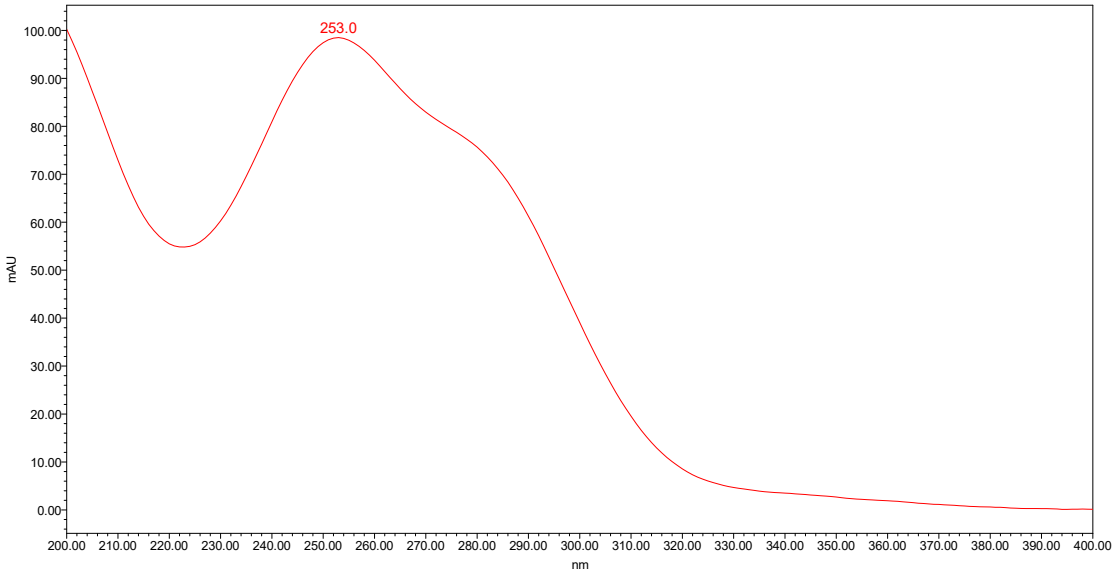


Figure S13. The UV-Vis spectrum of **1** in CH_3OH.

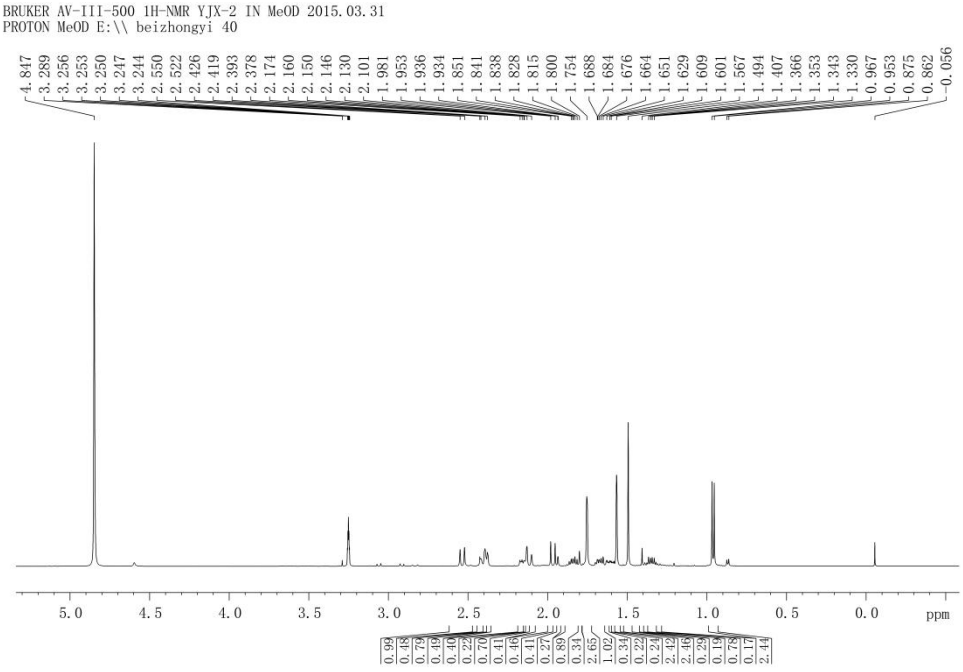


Figure S14. The ^1H NMR spectrum of **2** in CD_3OD

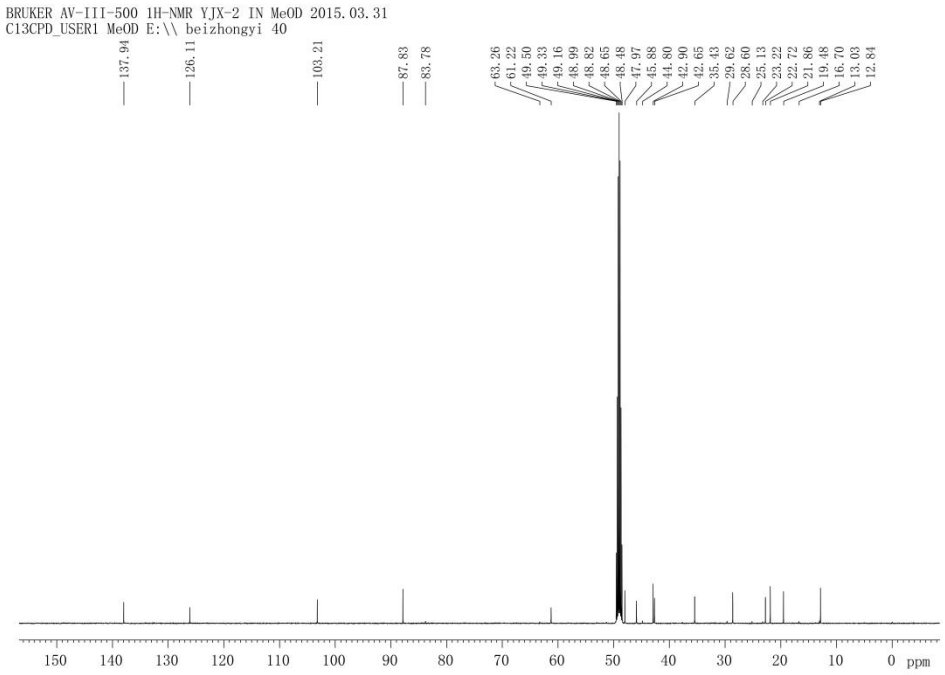


Figure S15. The ^{13}C NMR spectra of **2** in CD_3OD

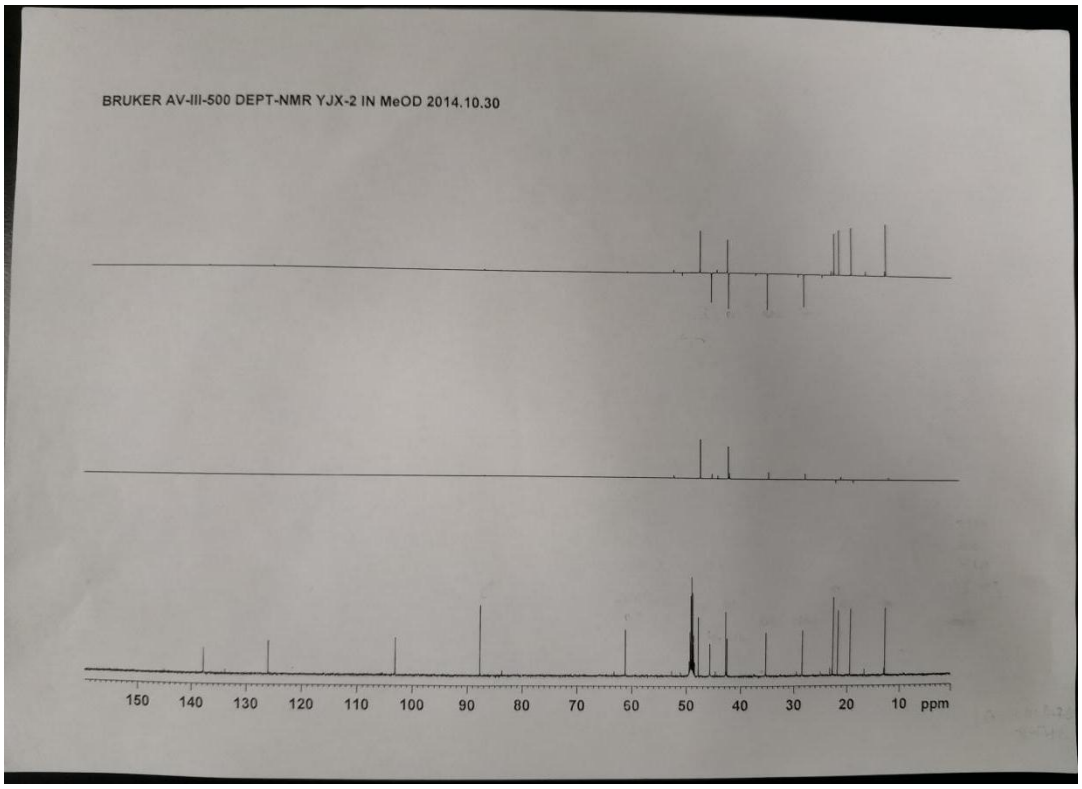


Figure S16. The DEPT spectra of **2** in CD_3OD

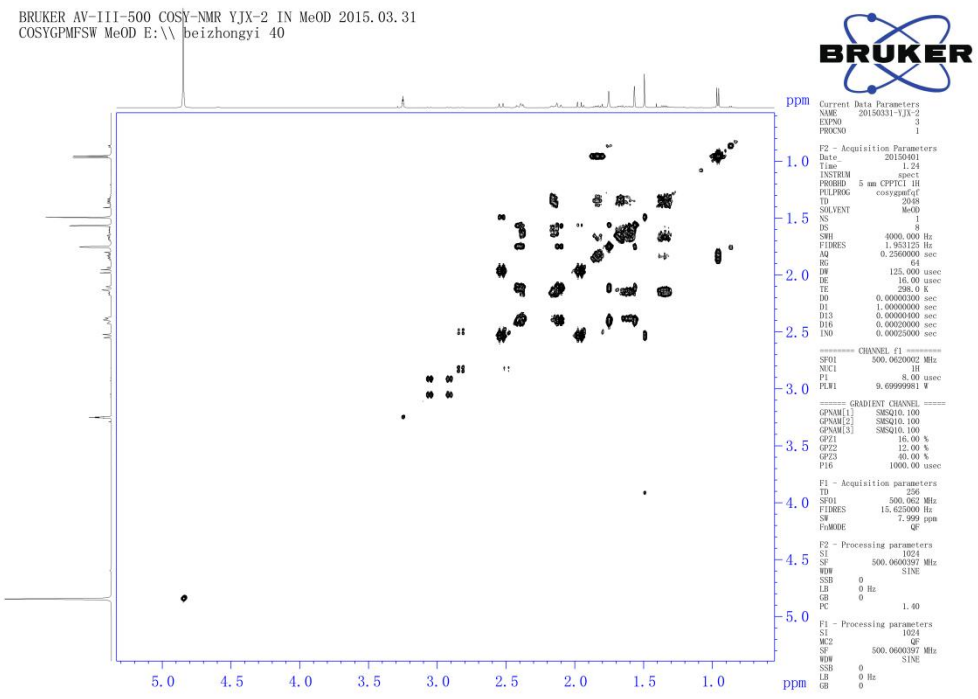


Figure S17. The ^{1}H-^{1}H COSY spectrum of **2** in CD_3OD

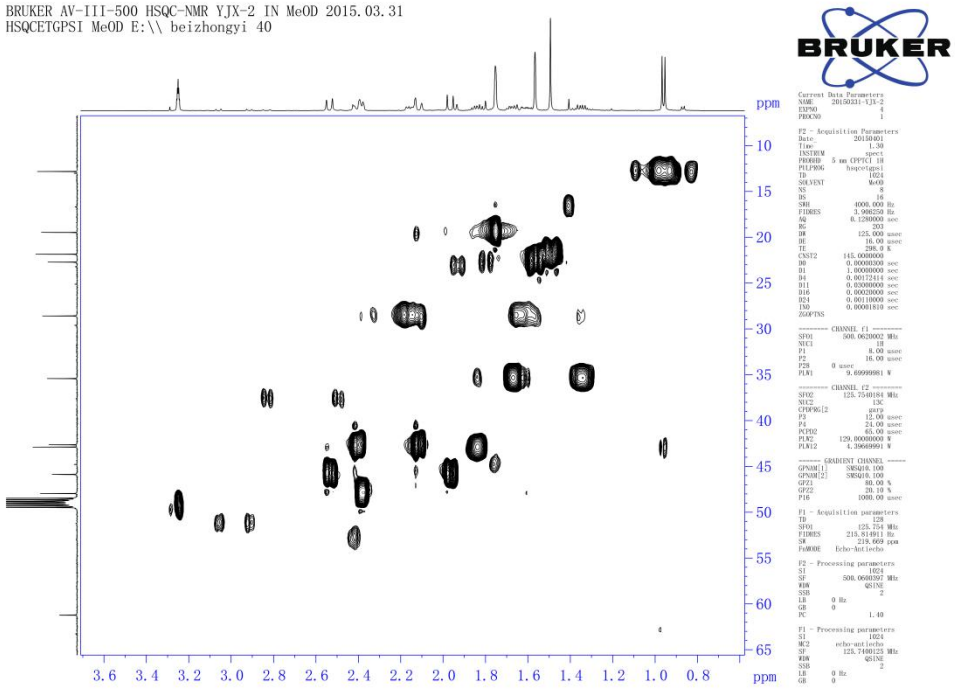


Figure S18. The HSQC spectrum of **2** in CD_3OD

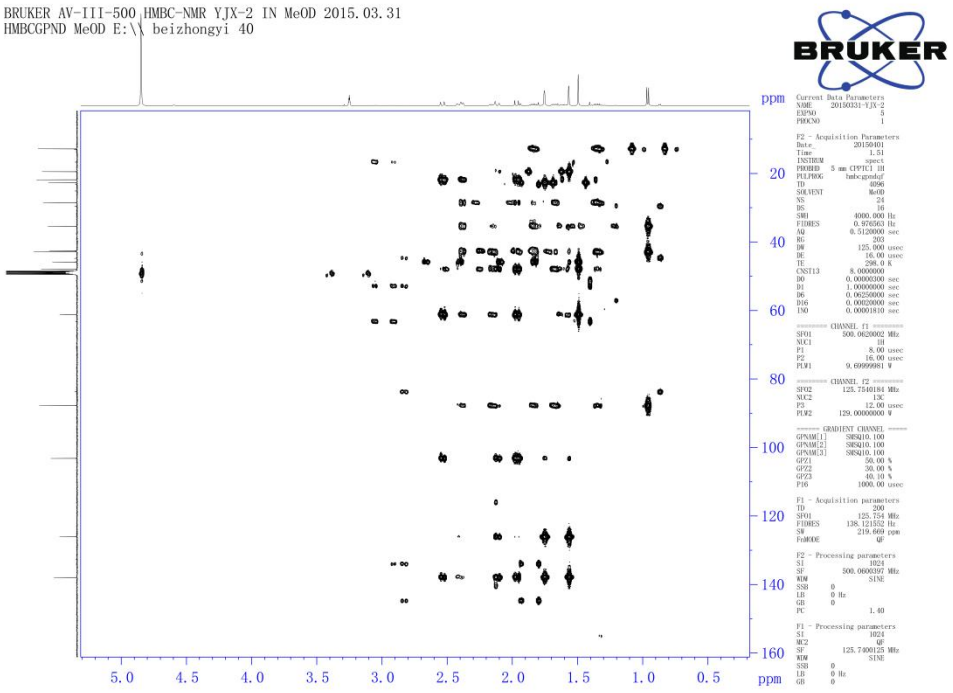


Figure S19. The HMBC spectrum of **2** in CD_3OD

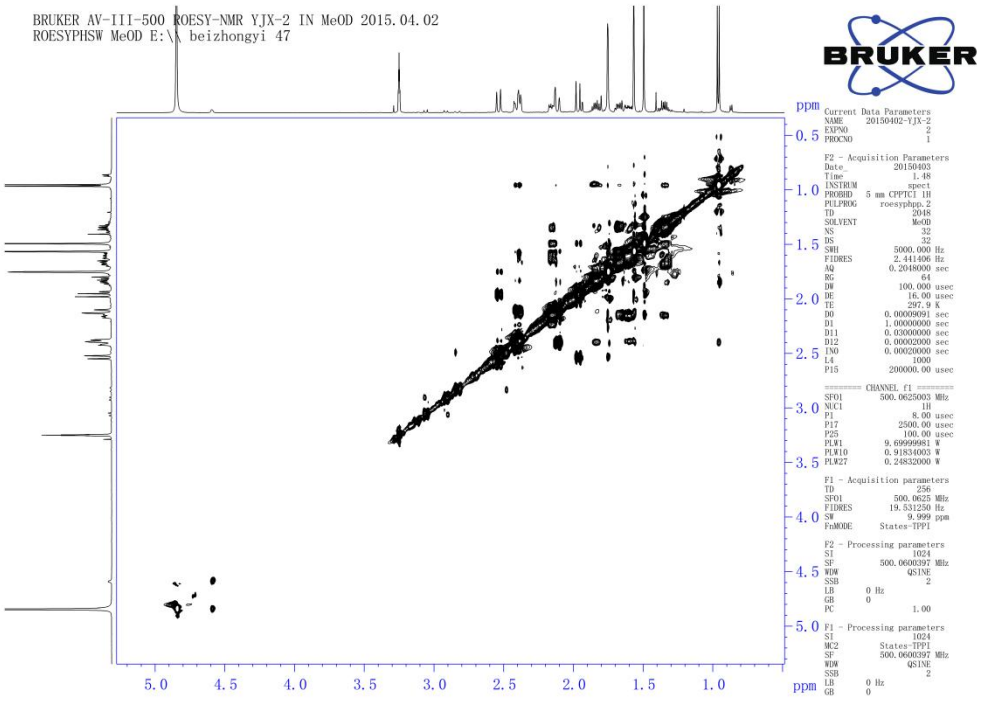


Figure S20. The ROESY spectrum of **2** in CD_3OD

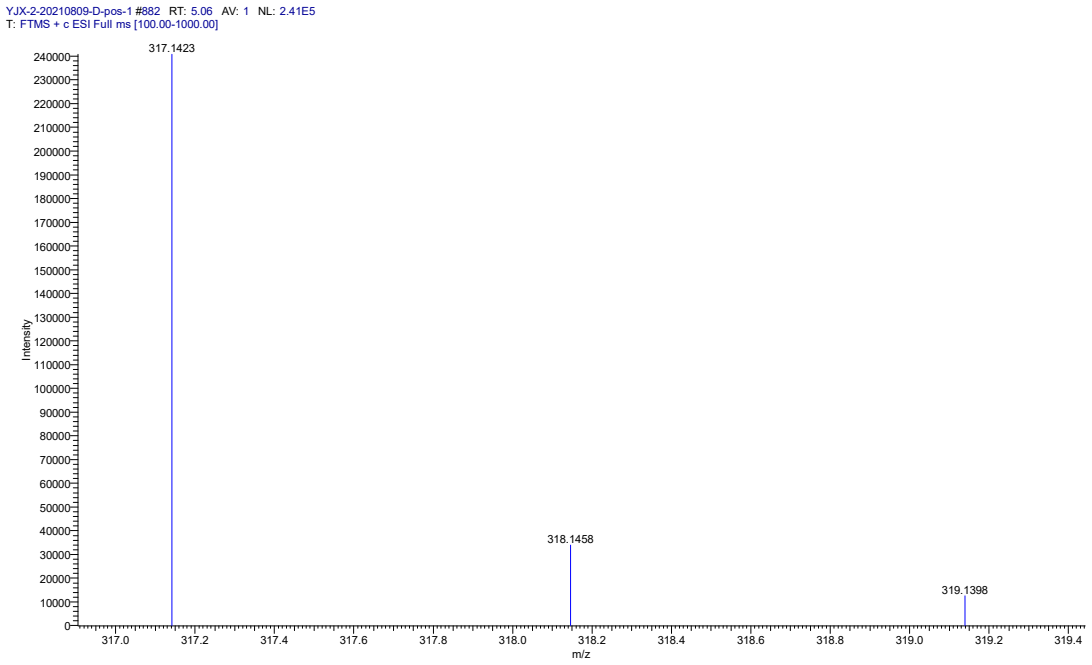


Figure S21. The HRESIMS spectrum of **2**

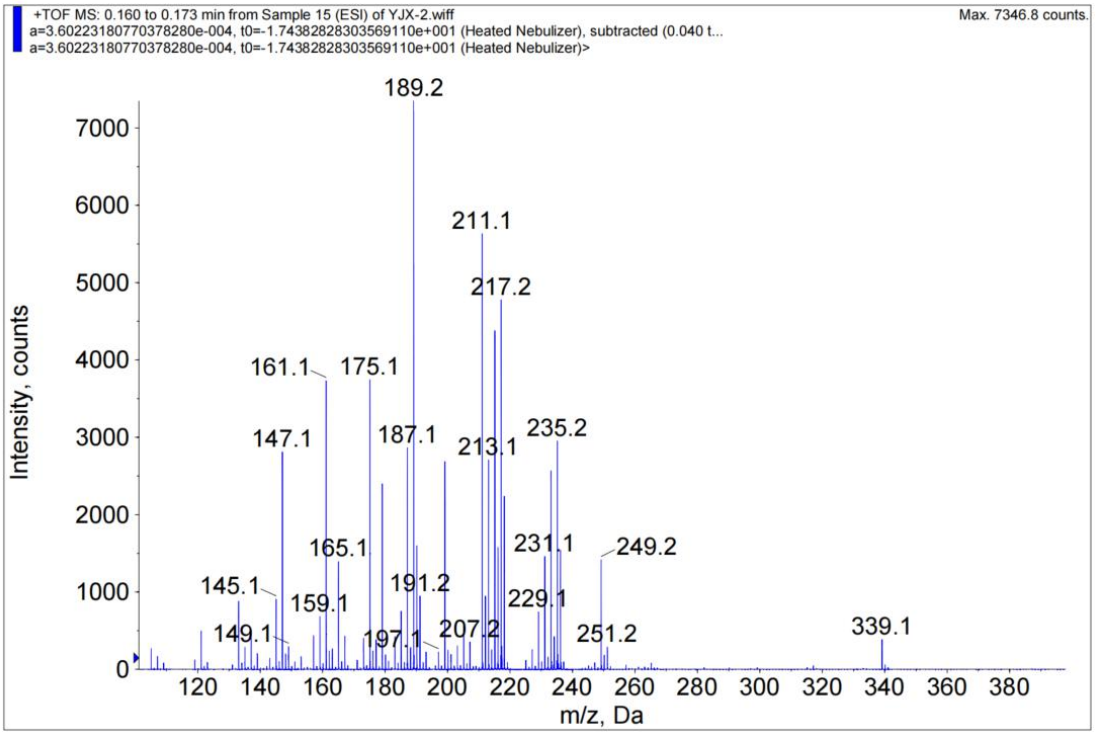


Figure S22. The MS/MS spectrum of **2**

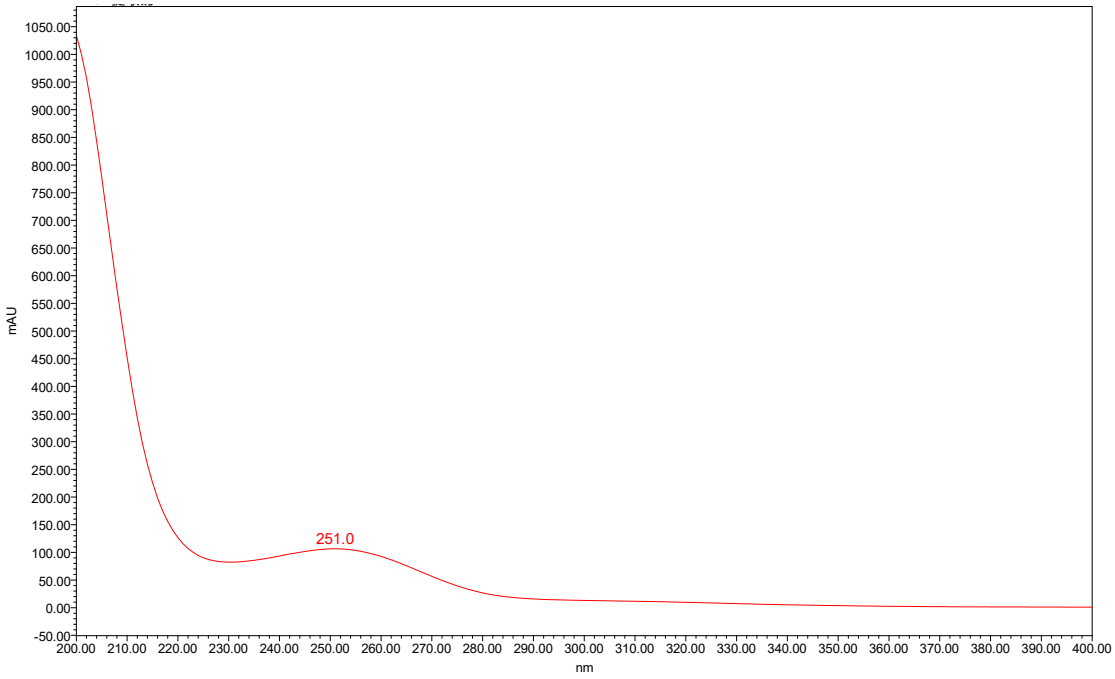


Figure S23. The UV-Vis spectrum of **2** in CH_3OH.

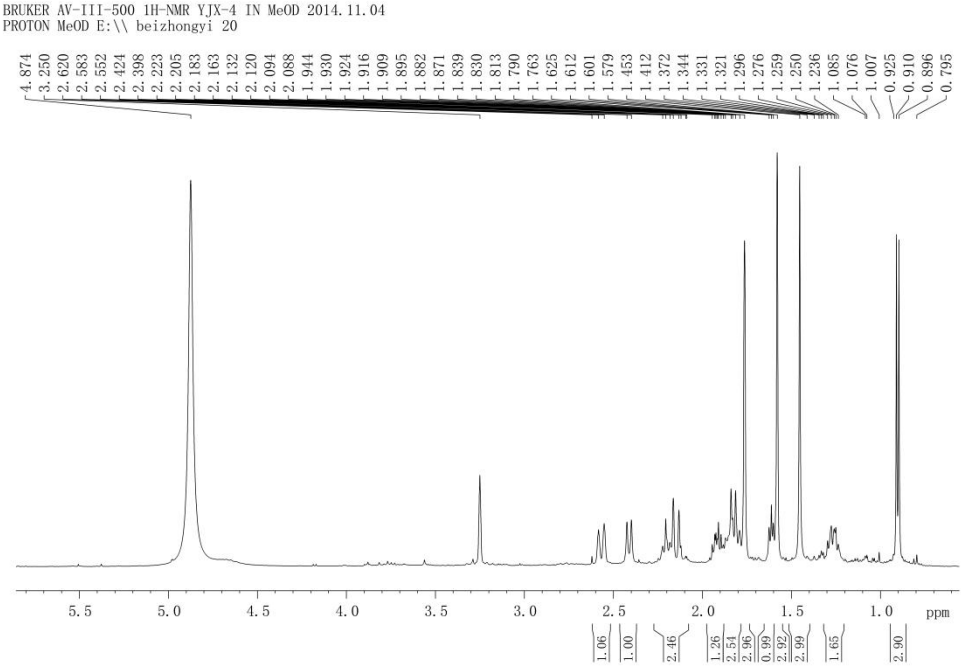


Figure S24. The ^1H NMR spectrum of **3** in CD_3OD

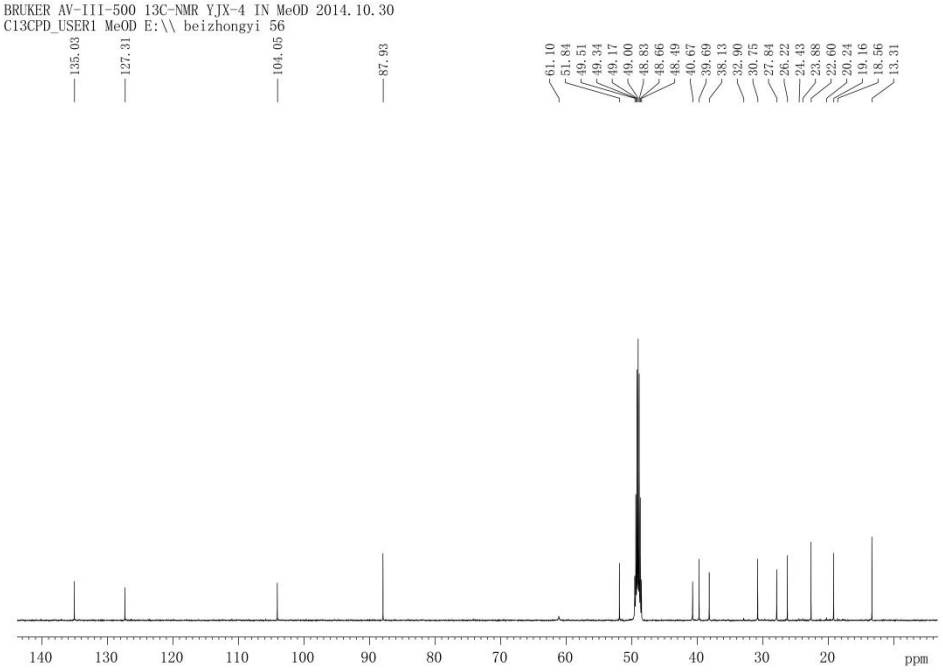


Figure S25. The ^{13}C NMR spectra of **3** in CD_3OD

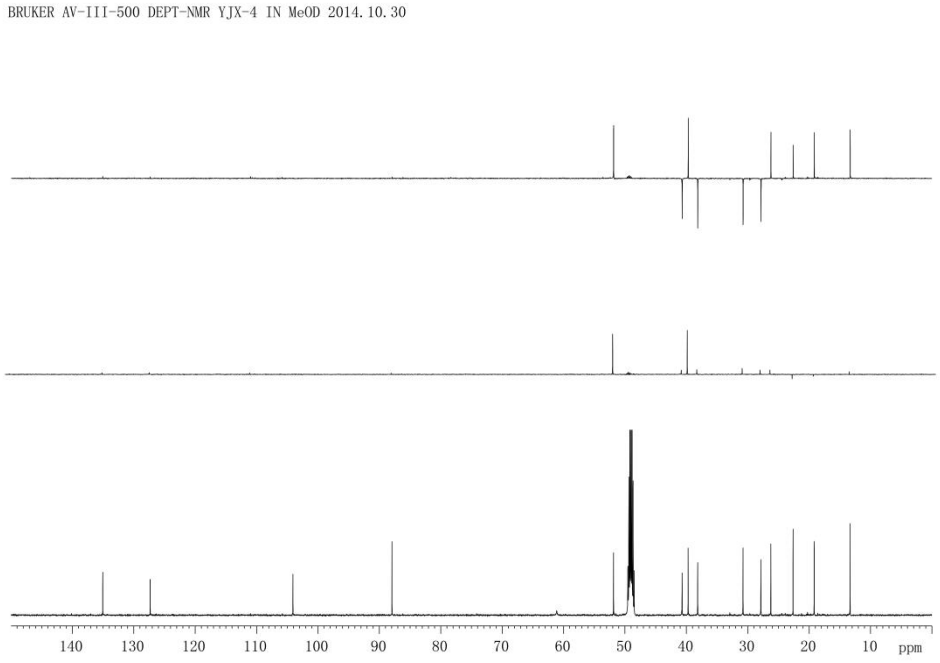


Figure S26. The DEPT spectra of **3** in CD_3OD

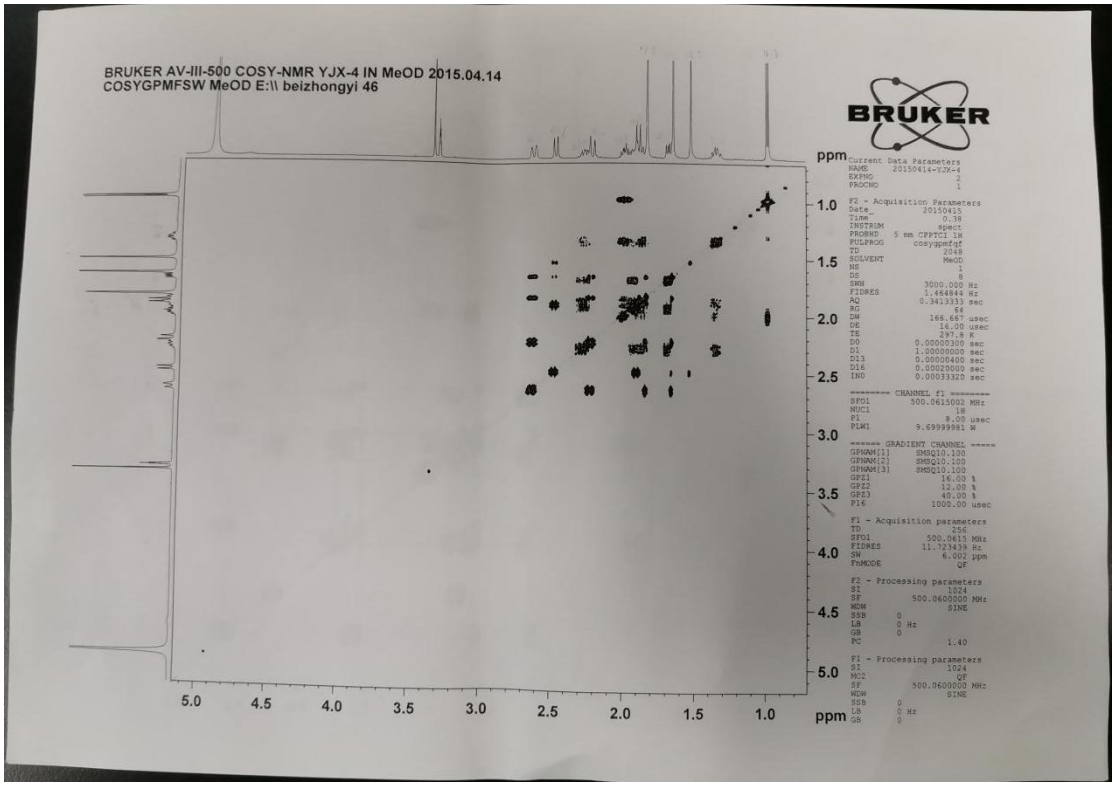


Figure S27. The ^{1}H-^{1}H COSY spectrum of **3** in CD_3OD

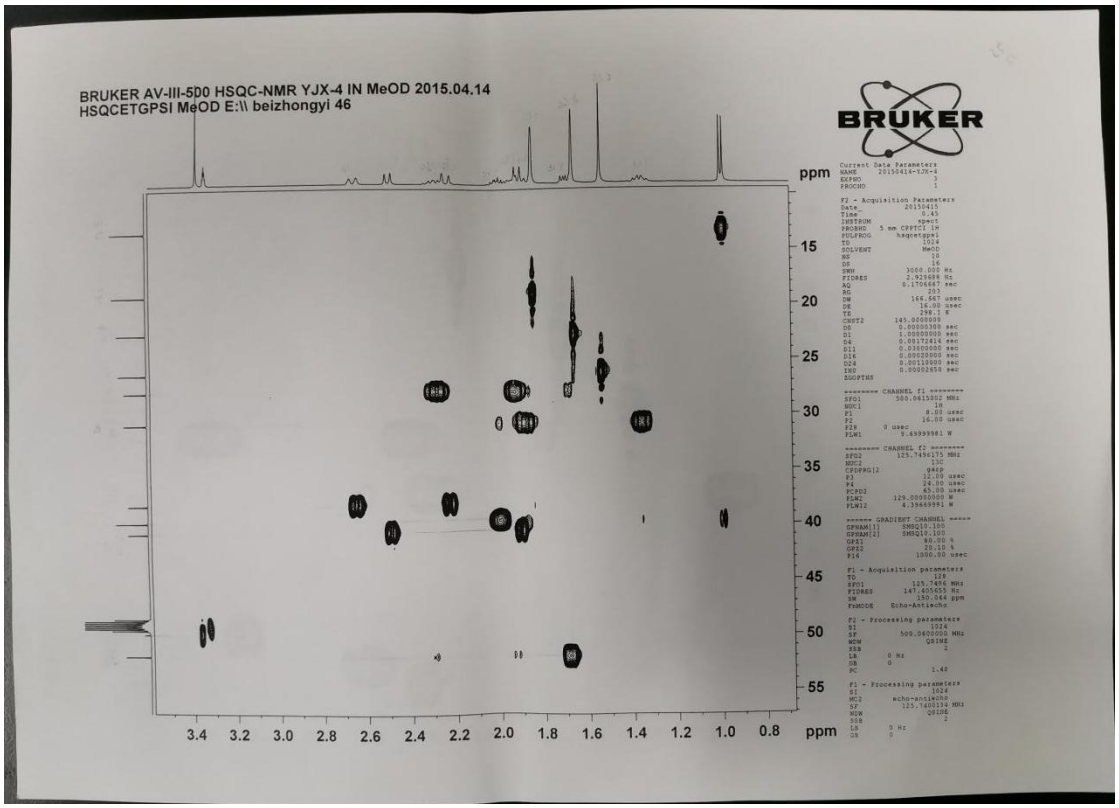


Figure S28. The HSQC spectrum of **3** in CD_3OD

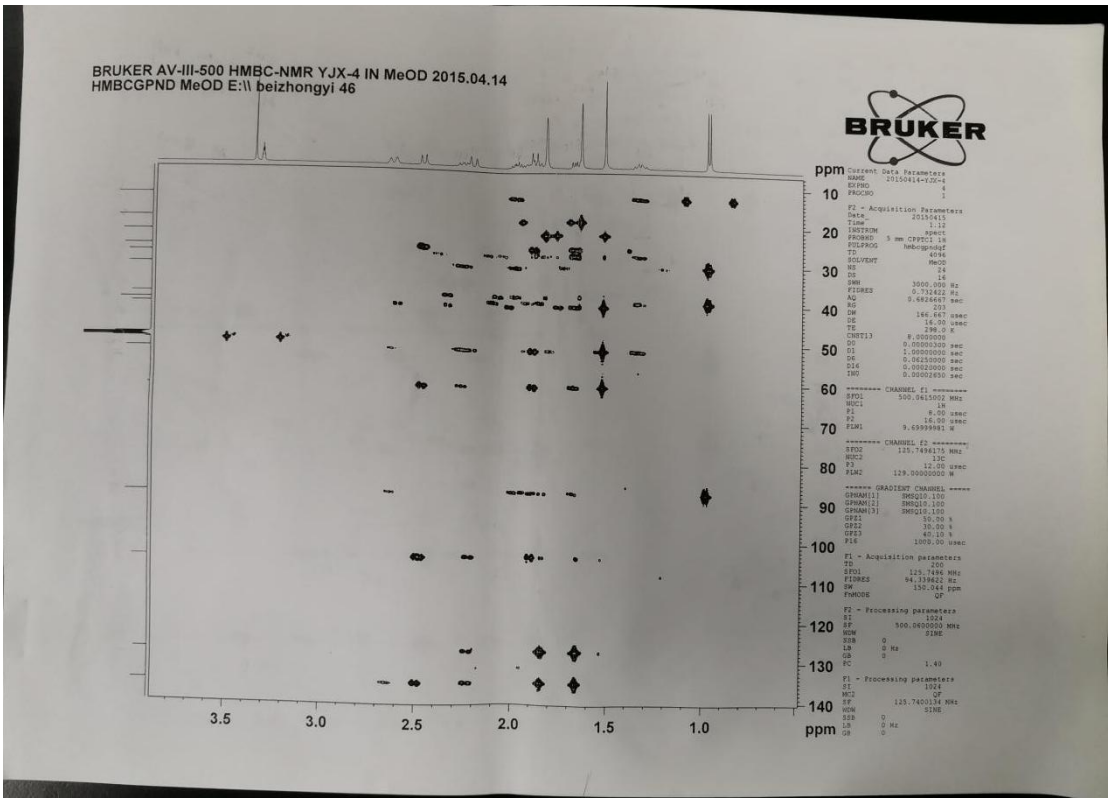


Figure S29. The HMBC spectrum of **3** in CD_3OD

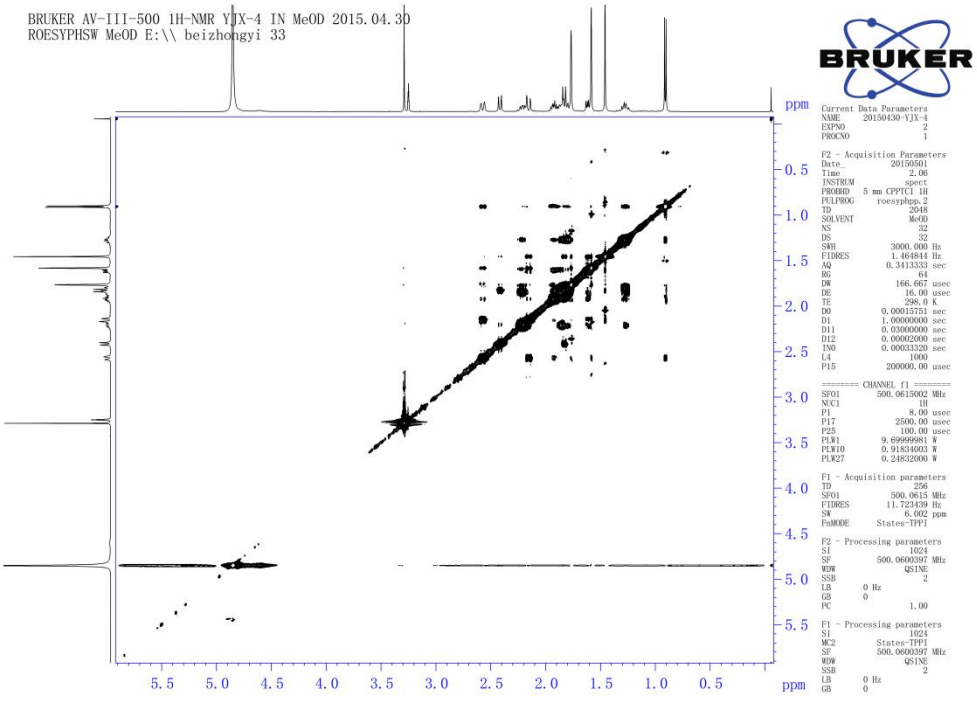


Figure S30. The ROESY spectrum of **3** in CD_3OD

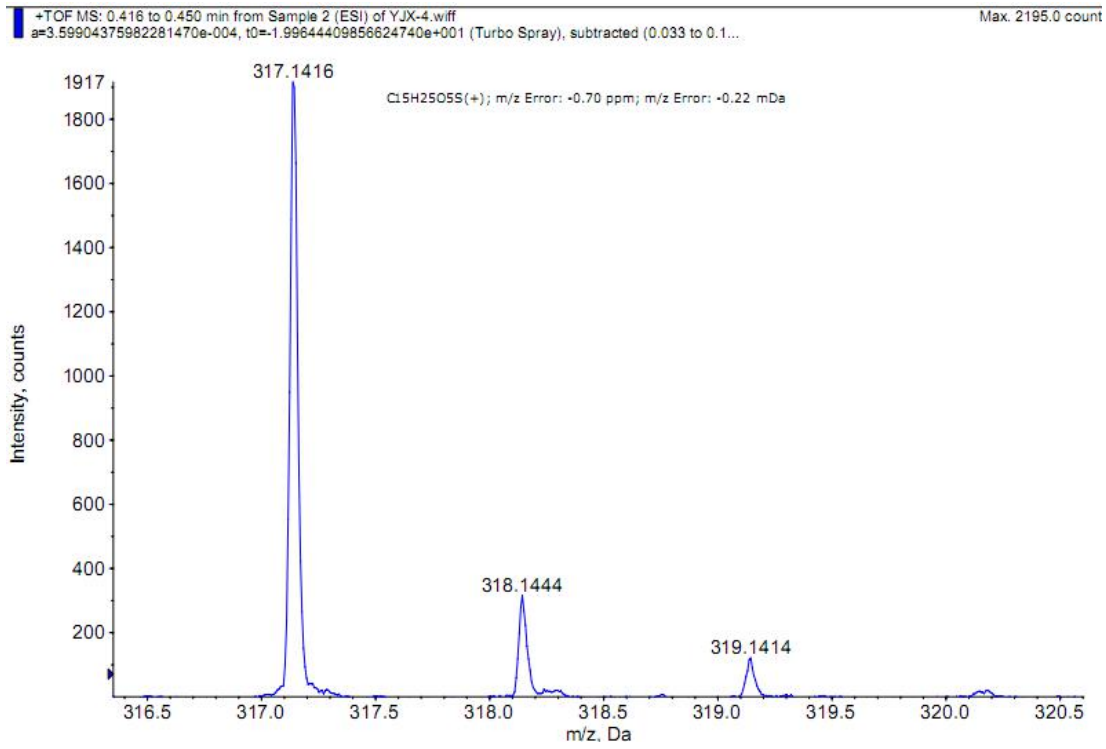


Figure S31. The HRESIMS spectrum of **3**

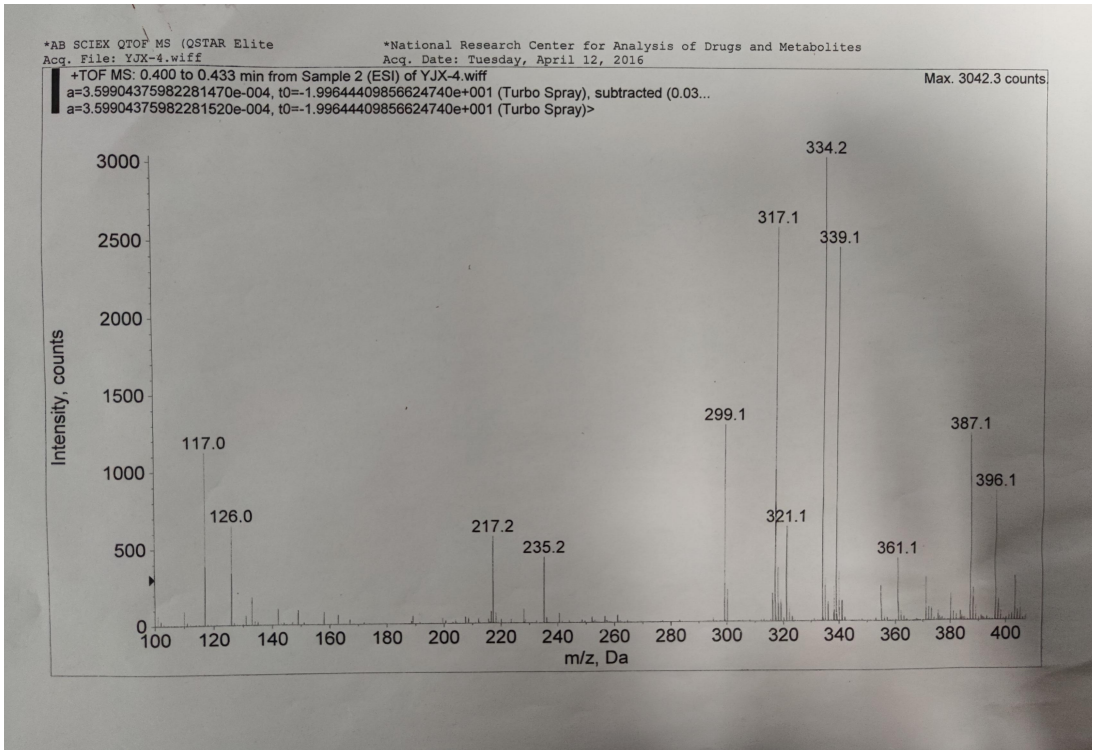


Figure S32. The MS/MS spectrum of **3**

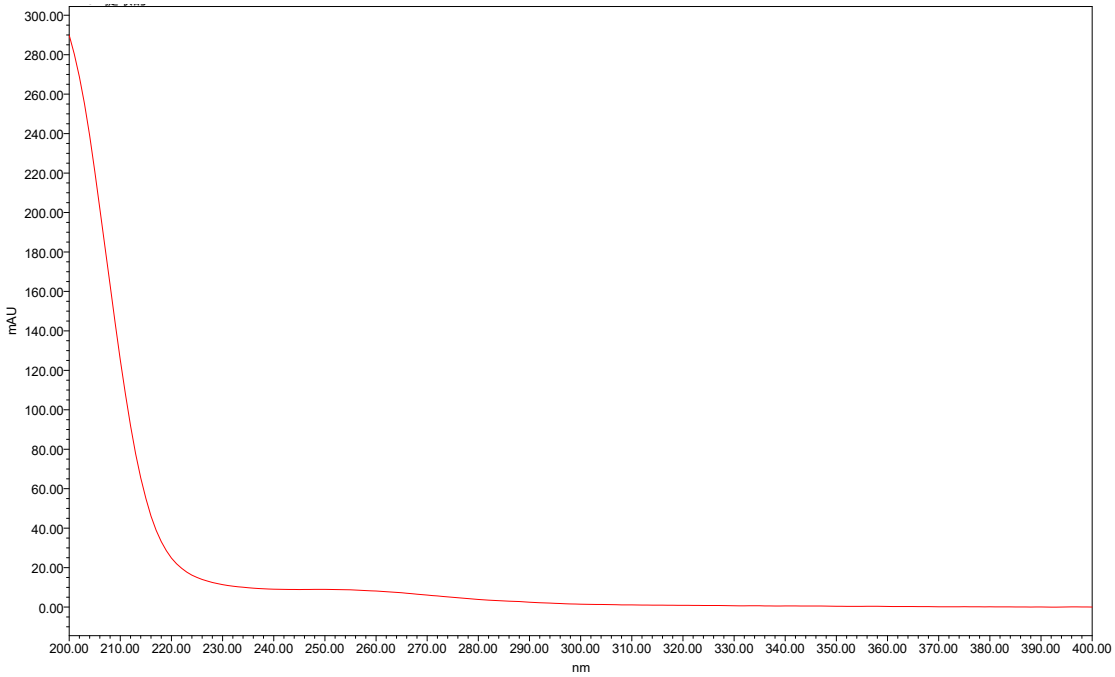


Figure S33. The UV-Vis spectrum of **3** in CH_3OH.

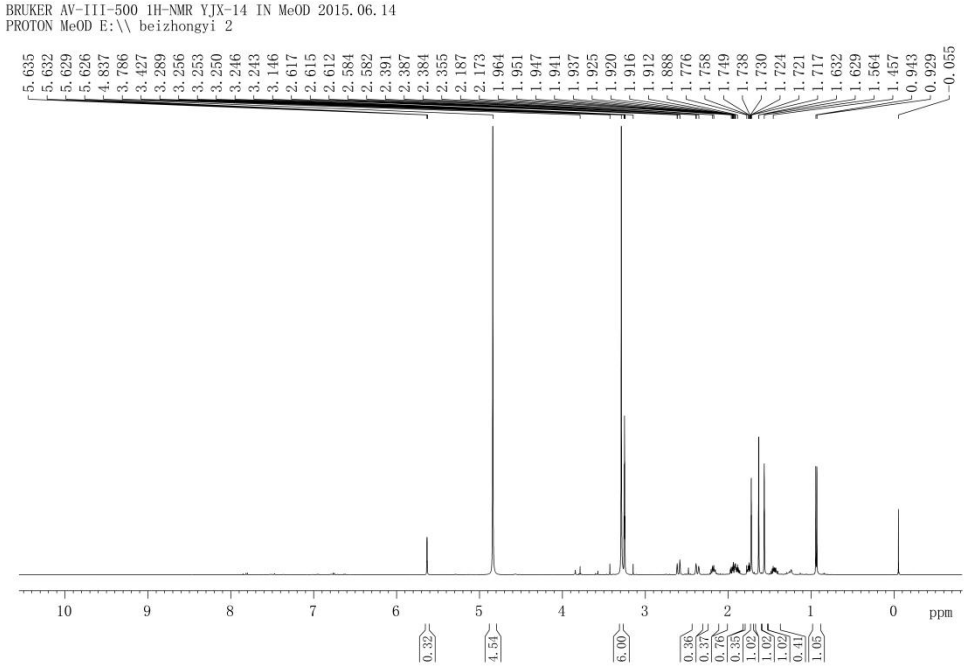


Figure S34. The ^1H NMR spectrum of **4** in CD_3OD

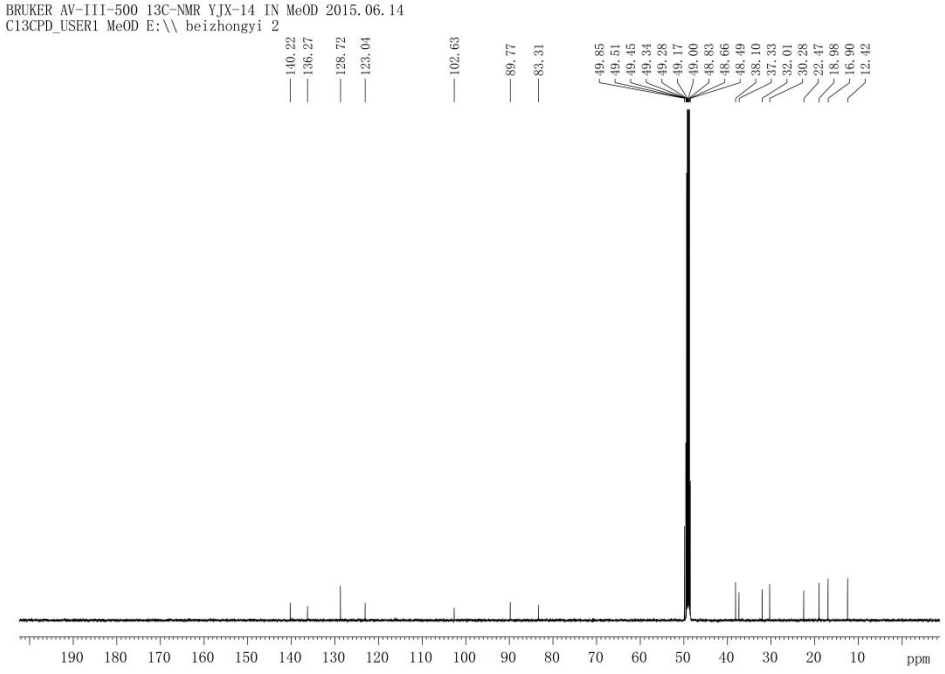


Figure S35. The ^{13}C NMR spectra of **4** in CD_3OD

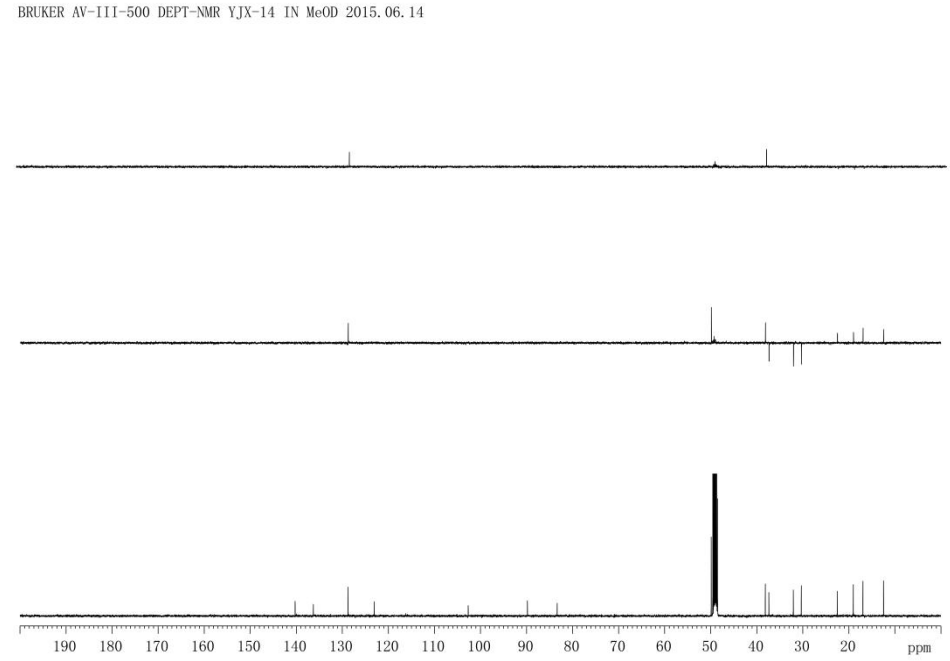


Figure S36. The DEPT spectra of **4** in CD_3OD

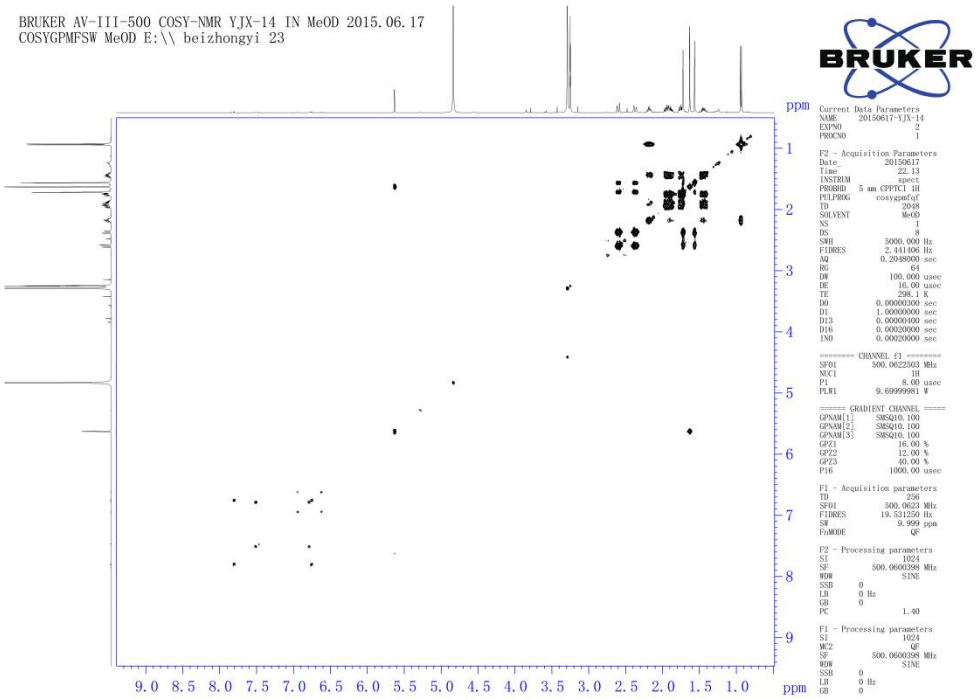


Figure S37. The ^{1}H-^{1}H COSY spectrum of **4** in CD_3OD

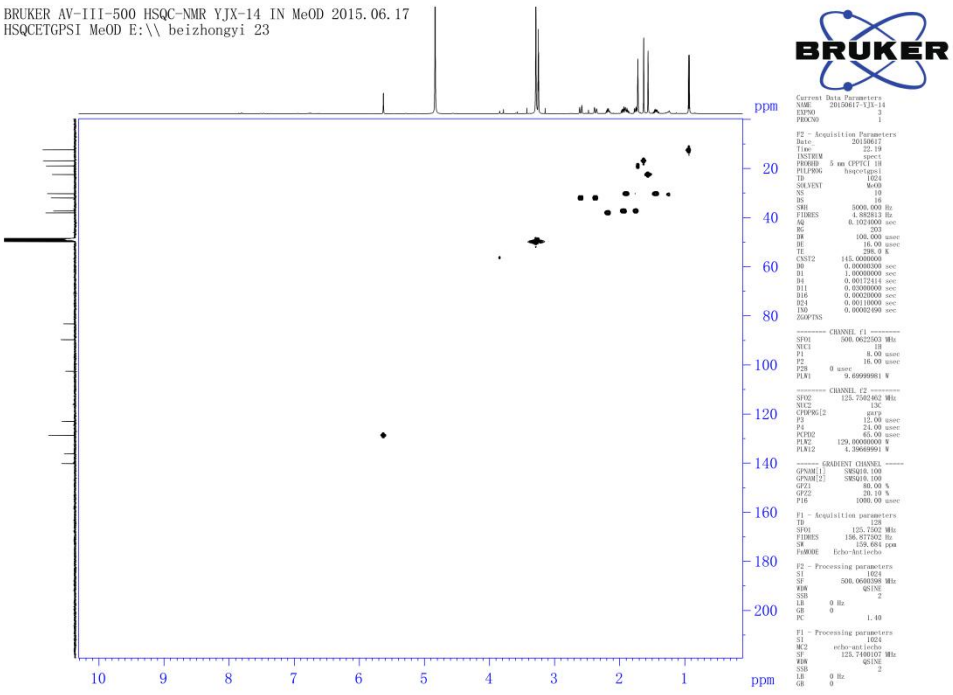


Figure S38. The HSQC spectrum of **4** in CD_3OD

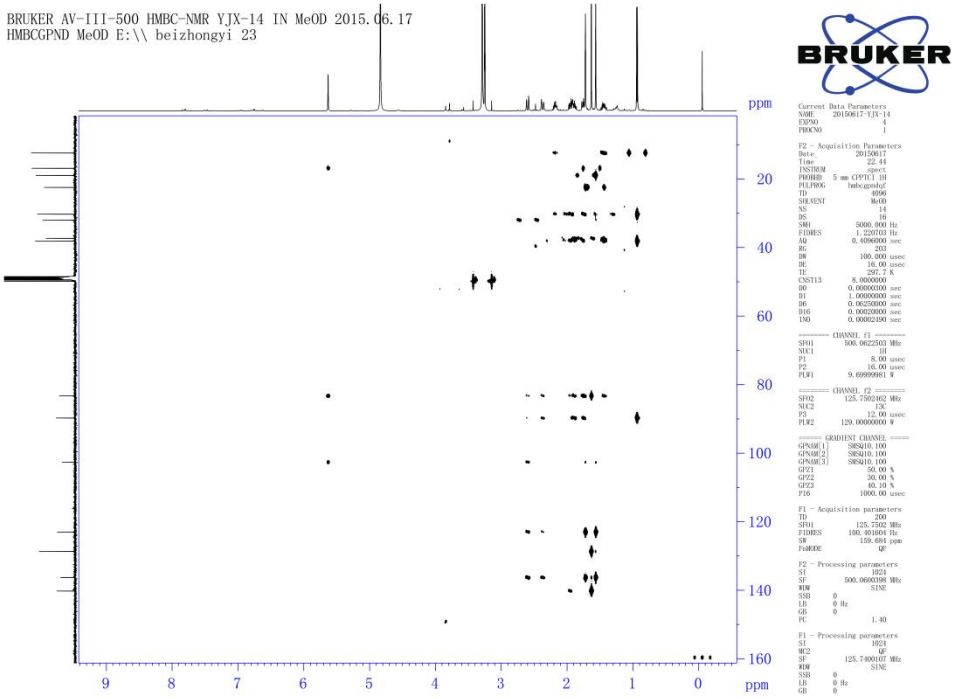


Figure S39. The HMBC spectrum of **4** in CD_3OD

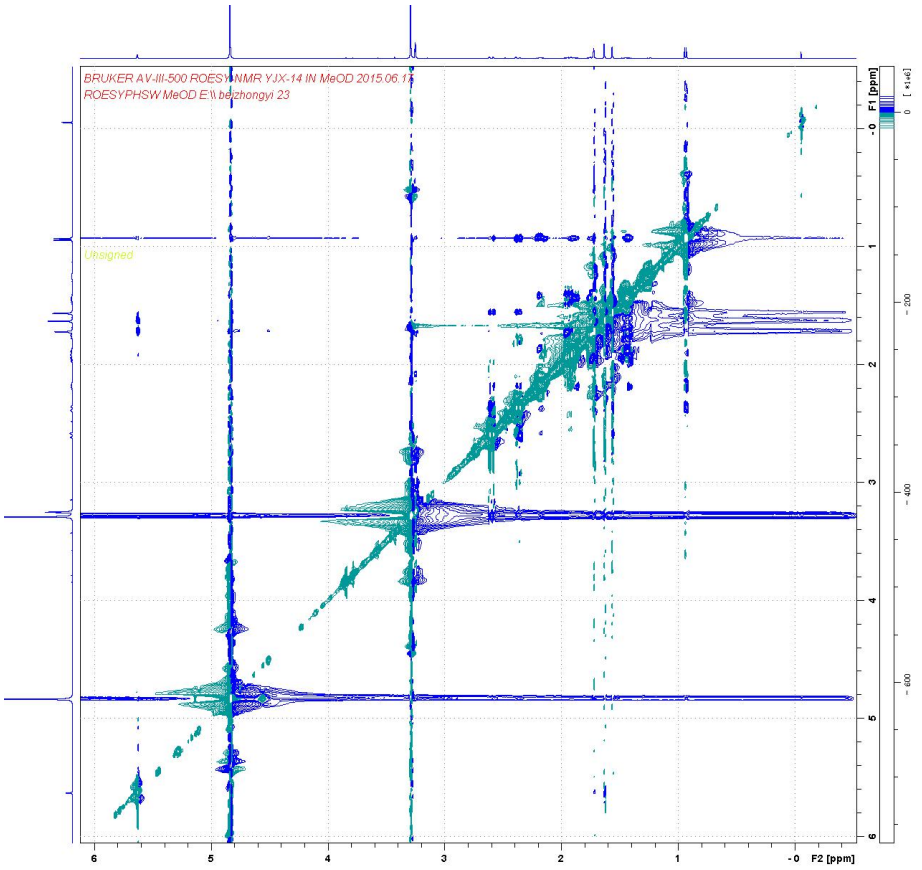


Figure S40. The ROESY spectrum of **4** in CD_3OD

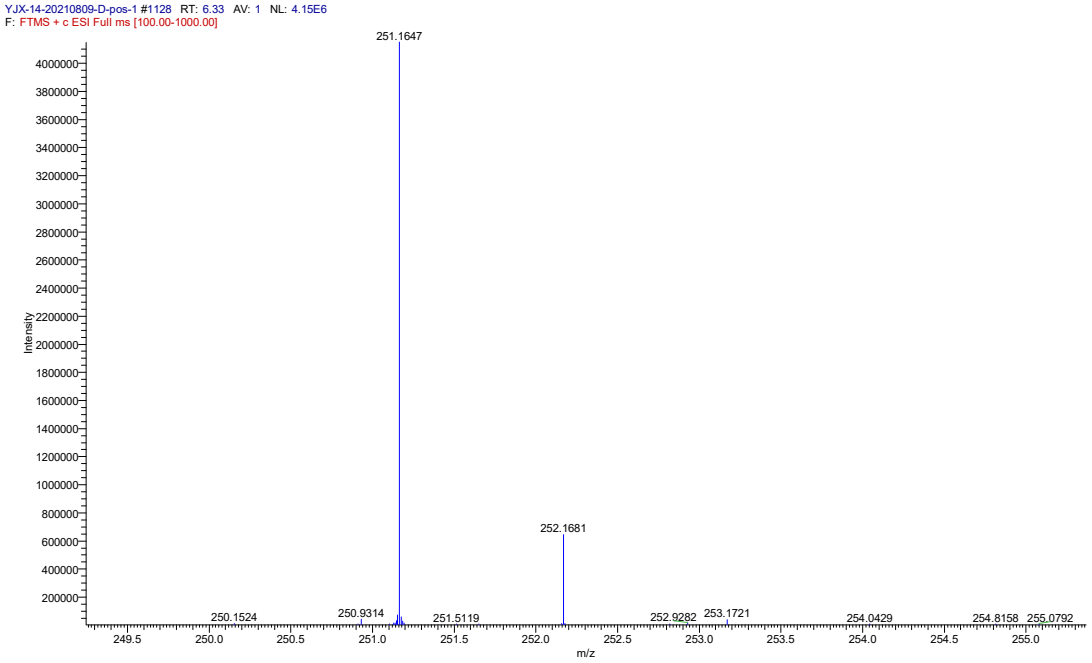


Figure S41. The HRESIMS spectrum of **4**

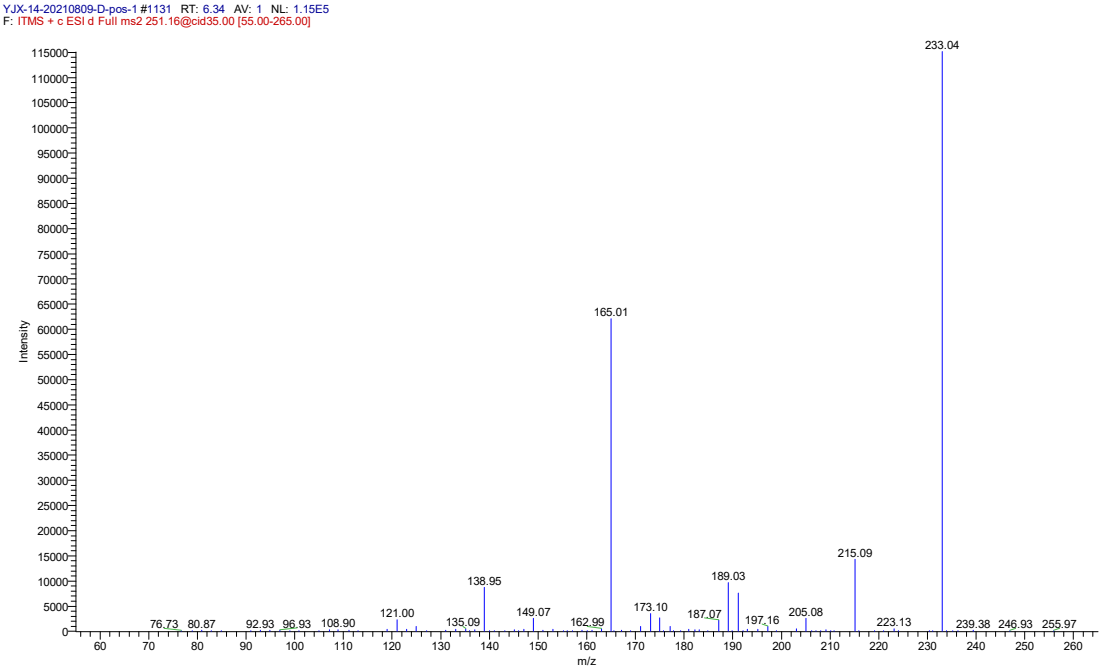


Figure S42. The MS/MS spectrum of **4**

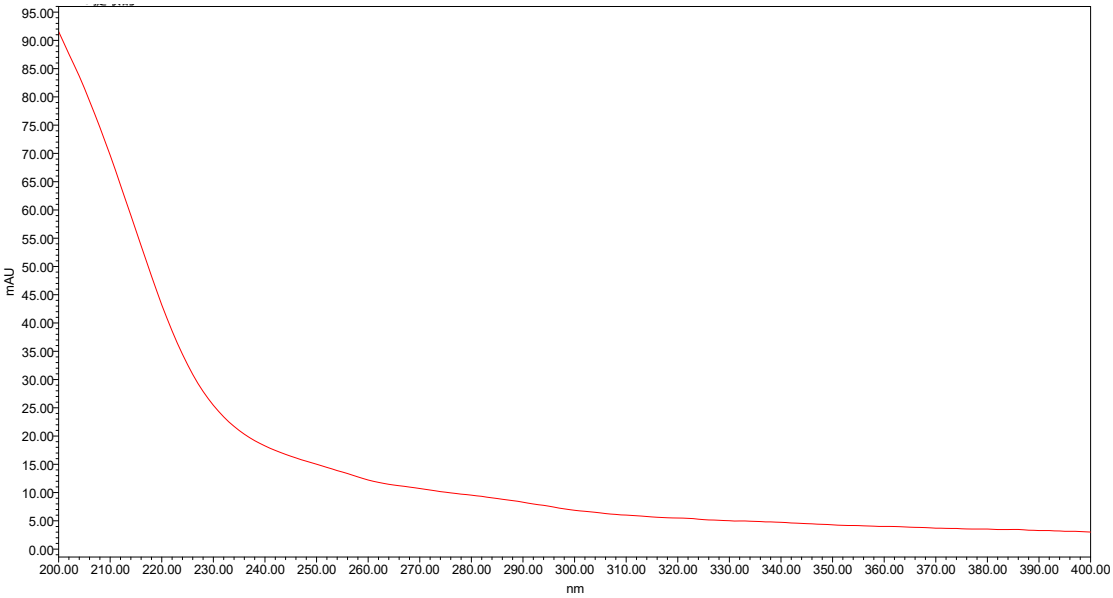


Figure S43. The UV-Vis spectrum of **4** in CH_3OH.

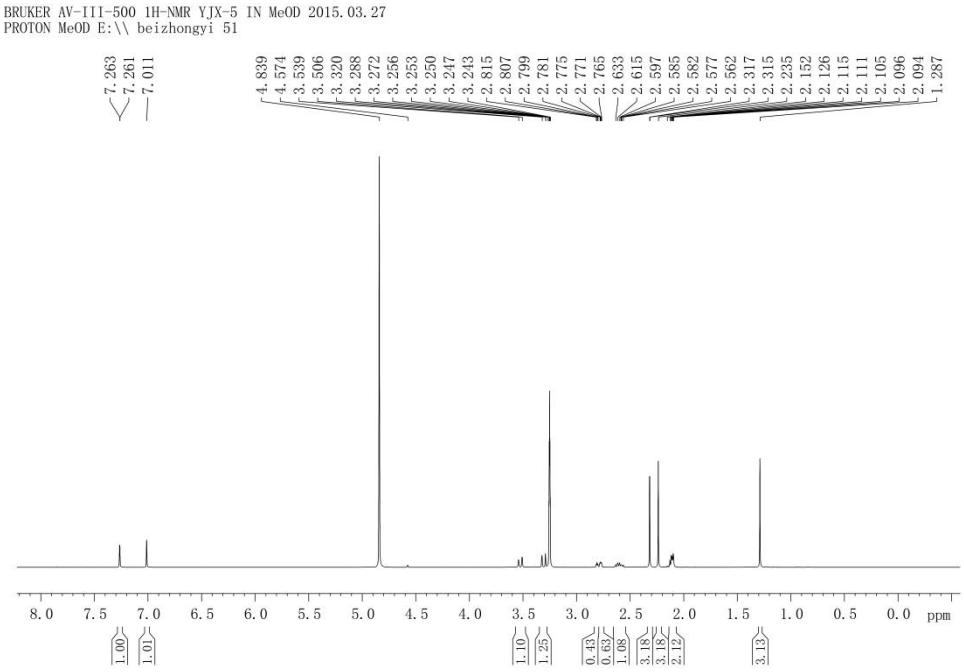


Figure S44. The ^1H NMR spectrum of **5** in CD_3OD

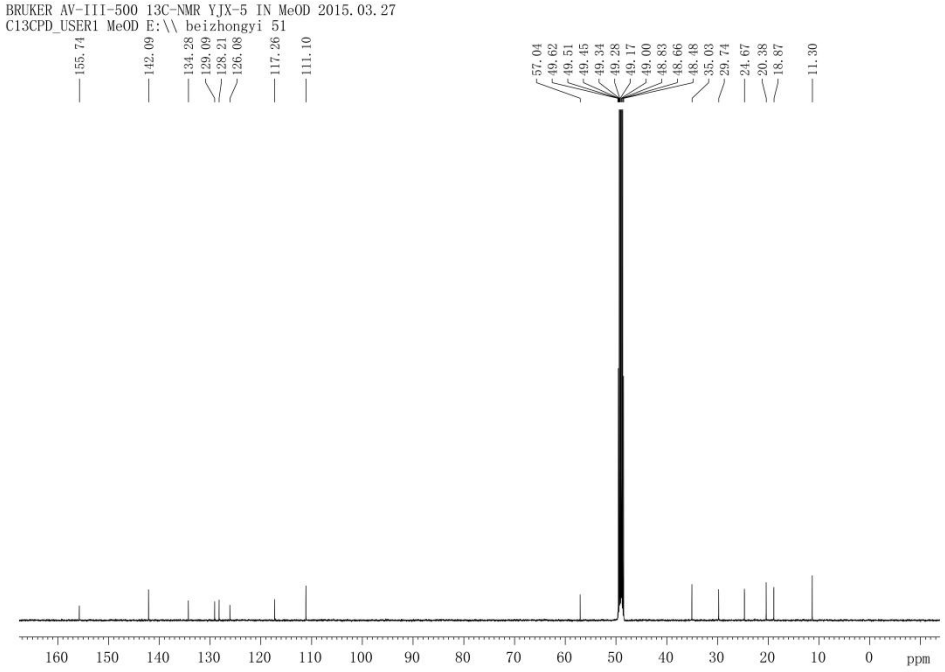


Figure S45. The ^{13}C NMRspectra of **5** in CD_3OD

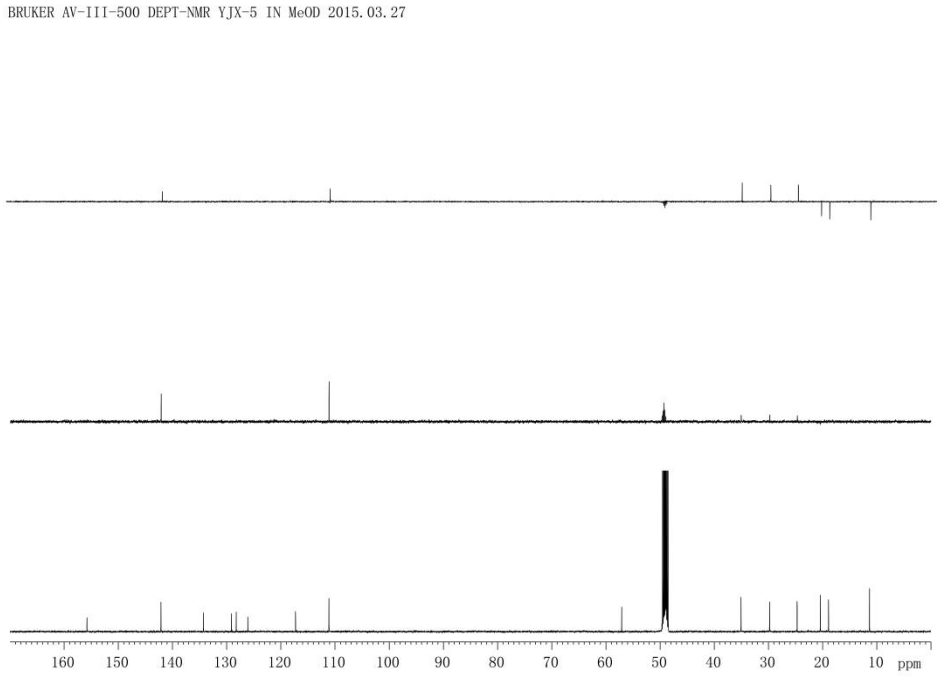


Figure S46. The DEPT spectra of **5** in CD_3OD

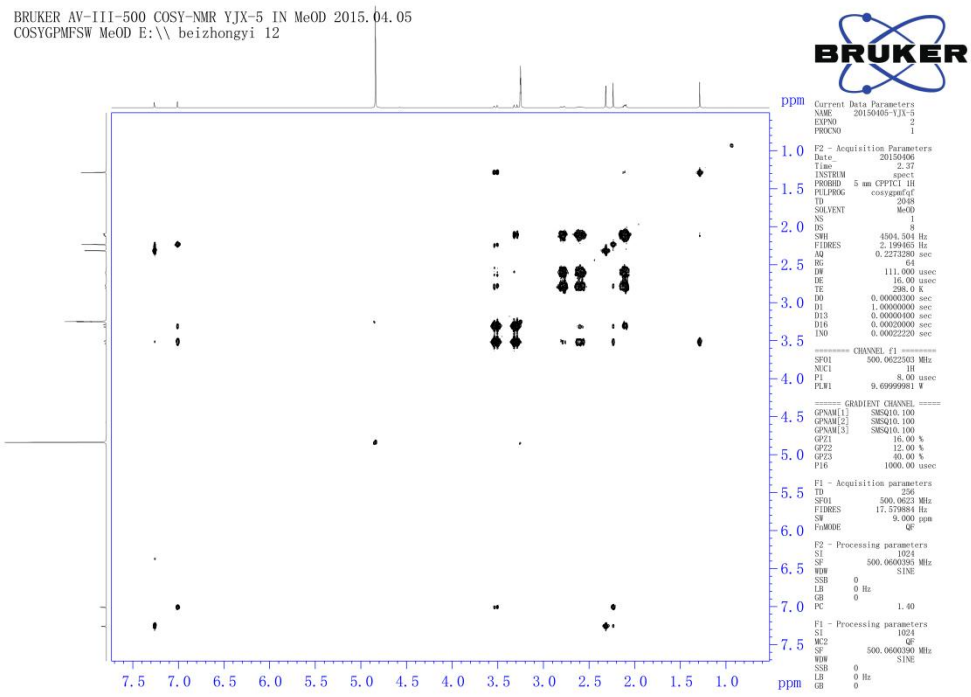


Figure S47. The ^{1}H-^{1}H COSY spectrum of **5** in CD_3OD

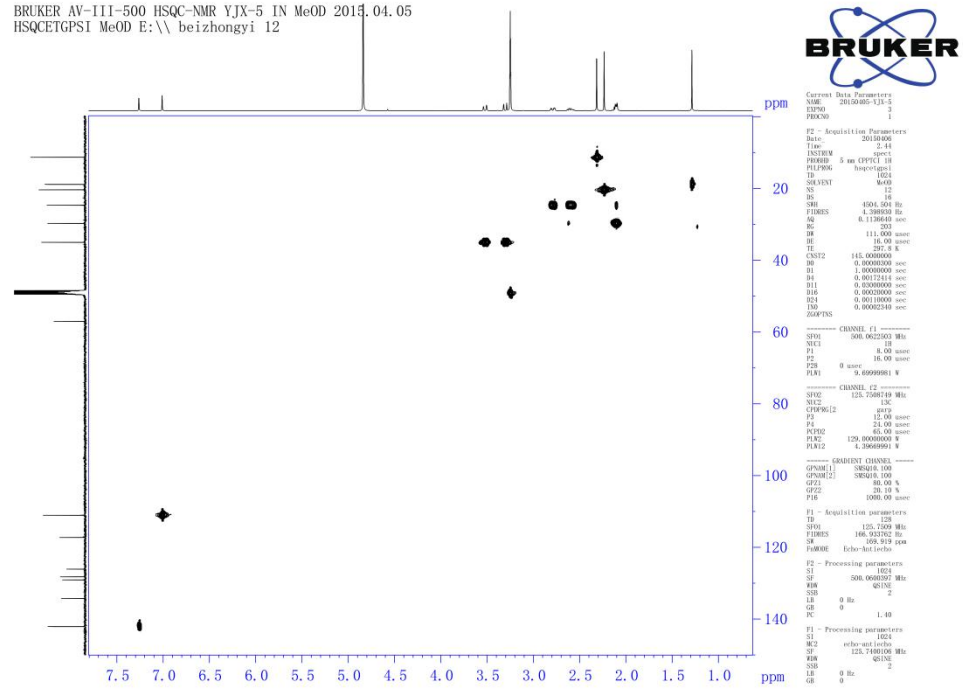


Figure S48. The HSQC spectrum of **5** in CD_3OD

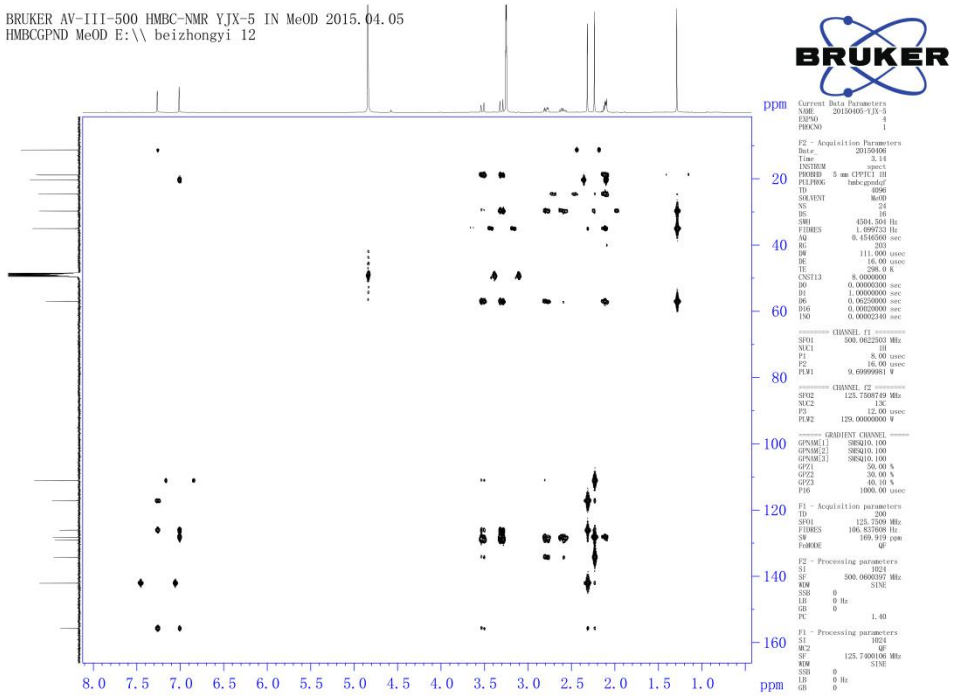


Figure S49. The HMBC spectrum of **5** in CD_3OD

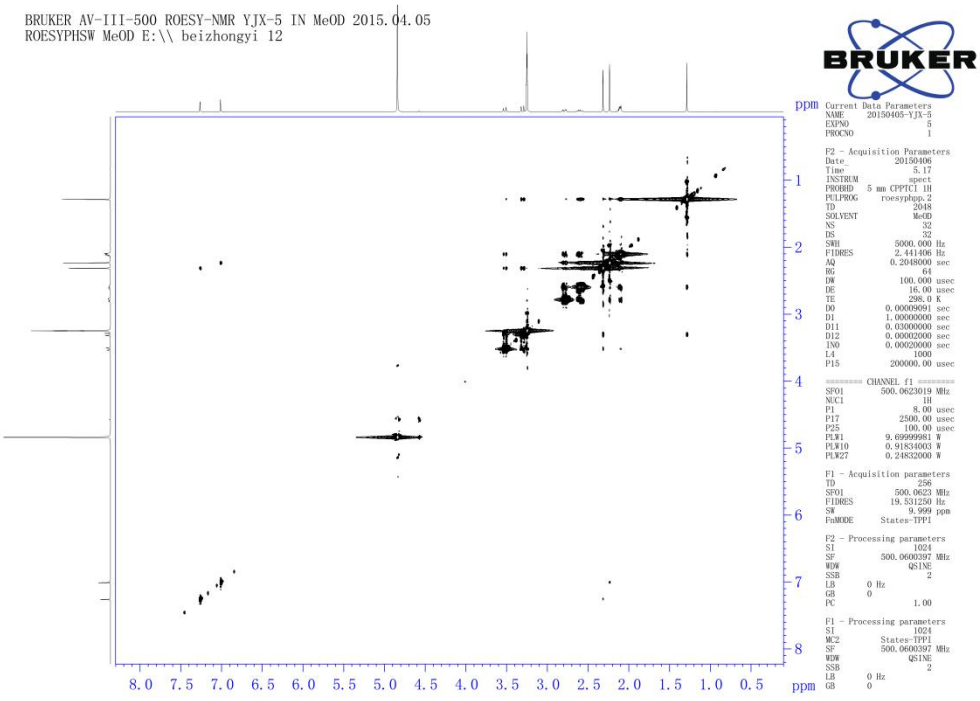


Figure S50. The ROESY spectrum of **5** in CD_3OD

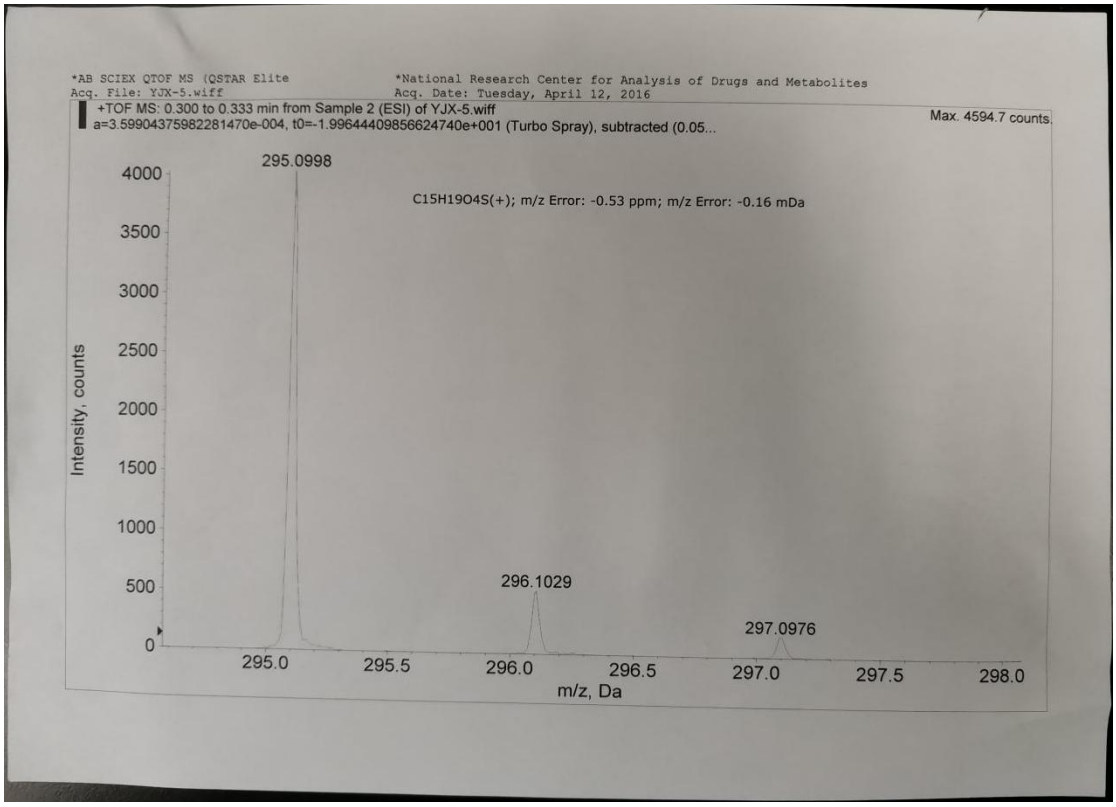


Figure S51. The HRESIMS spectrum of **5**

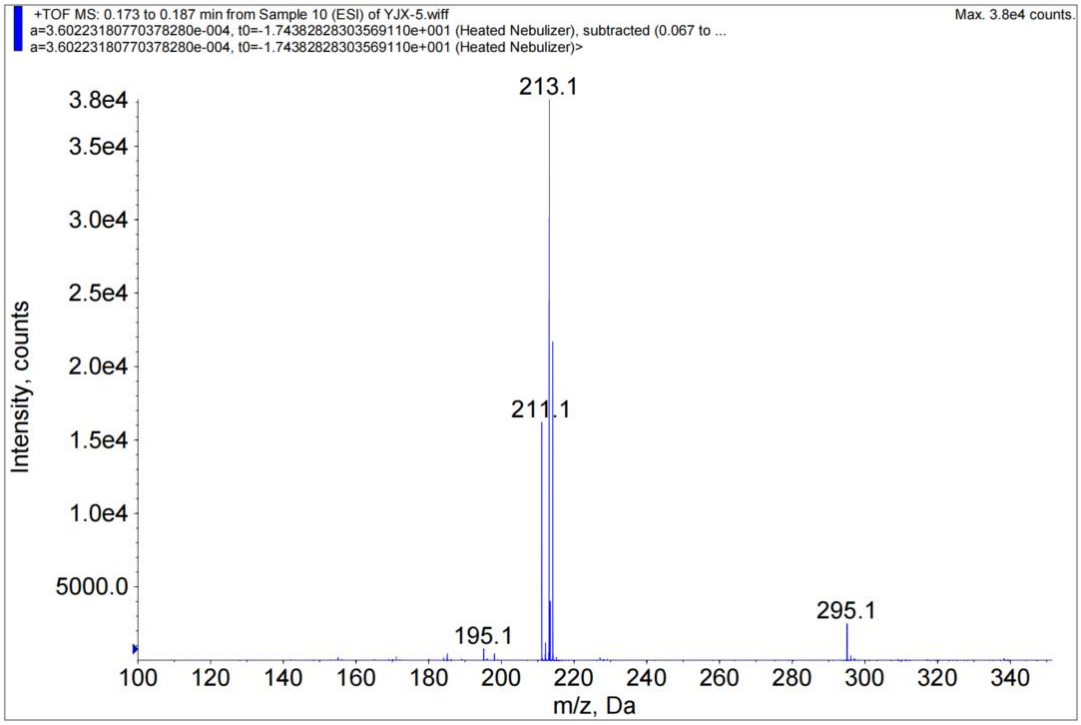


Figure S52. The MS/MS spectrum of **5**

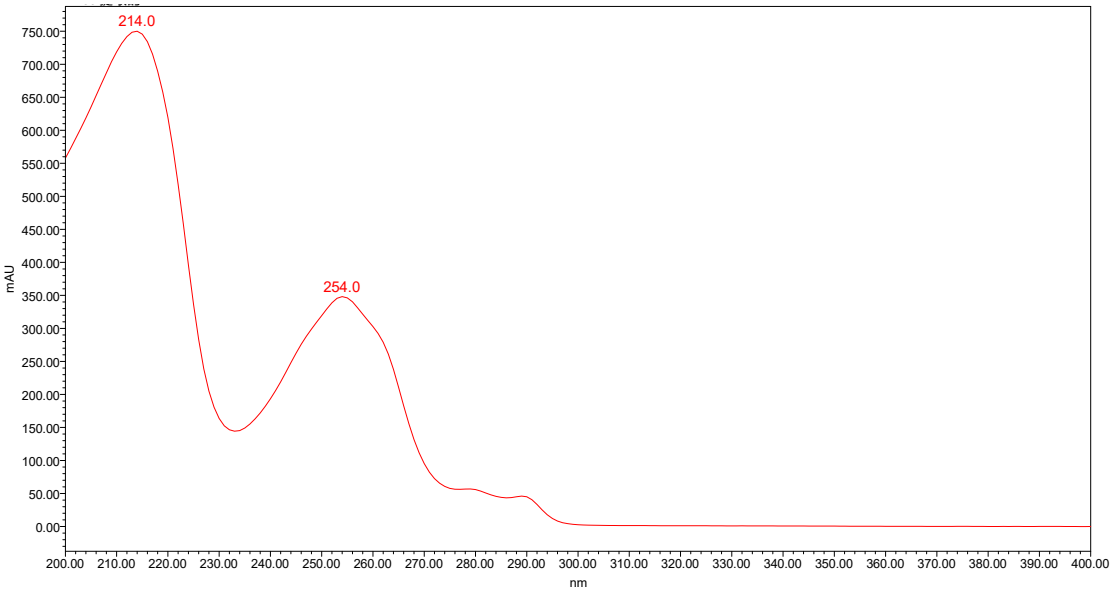


Figure S53. The UV-Vis spectrum of **5** in CH_3OH.

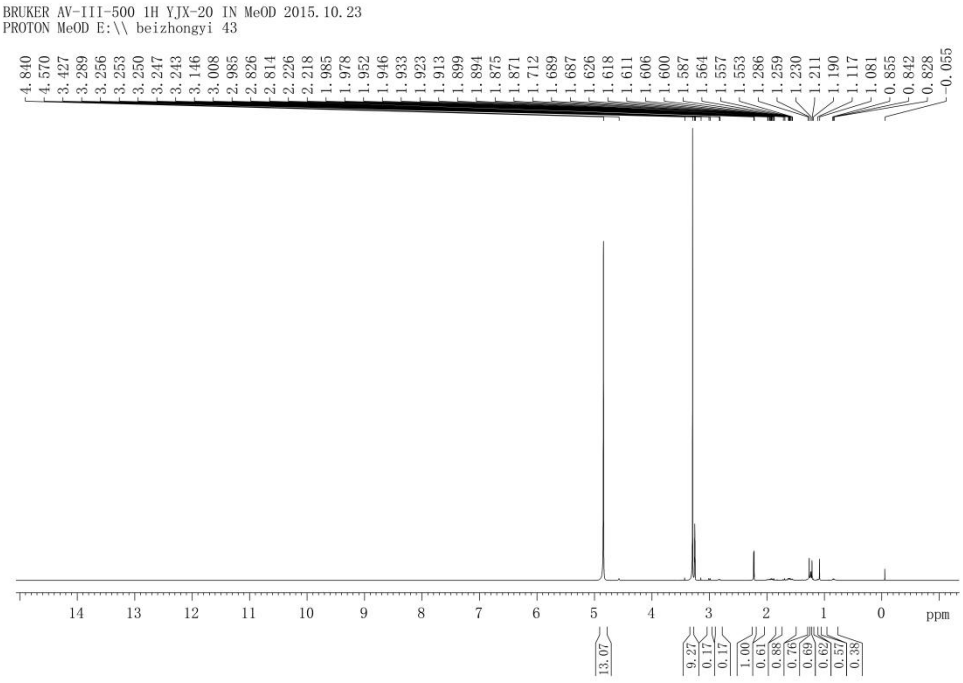


Figure S54. The ^1H NMR spectrum of **6** in CD_3OD

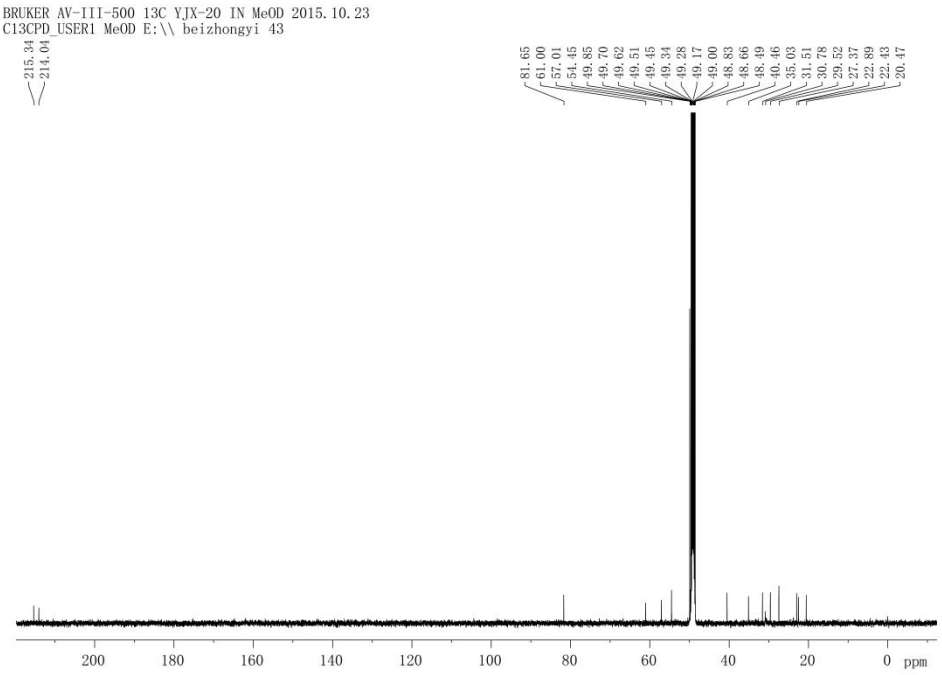


Figure S55. The ^{13}C NMR spectra of **6** in CD_3OD

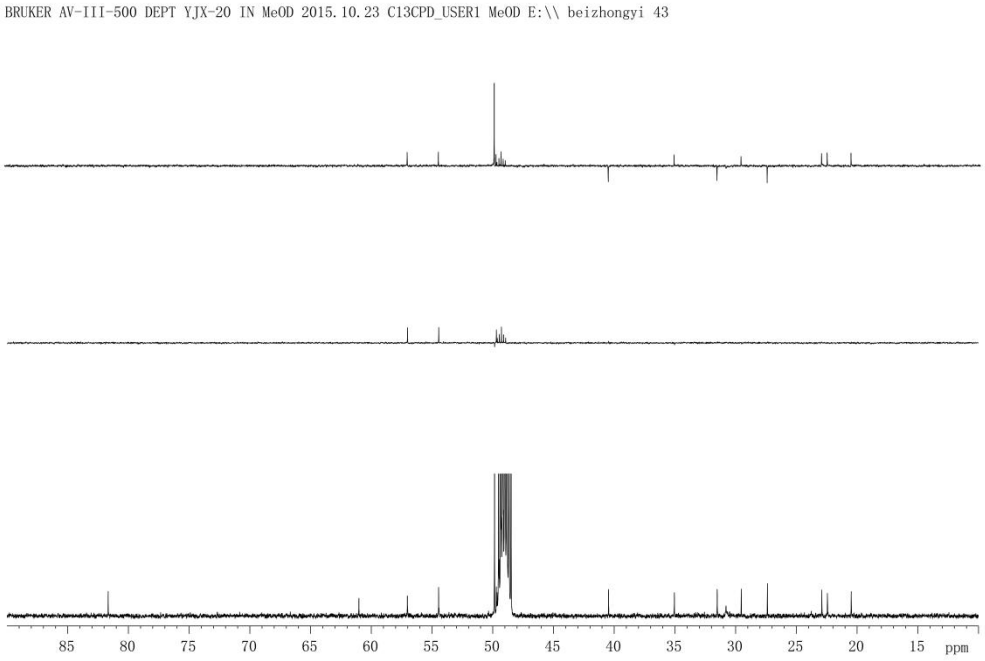


Figure S56. The DEPT spectra of **6** in CD_3OD

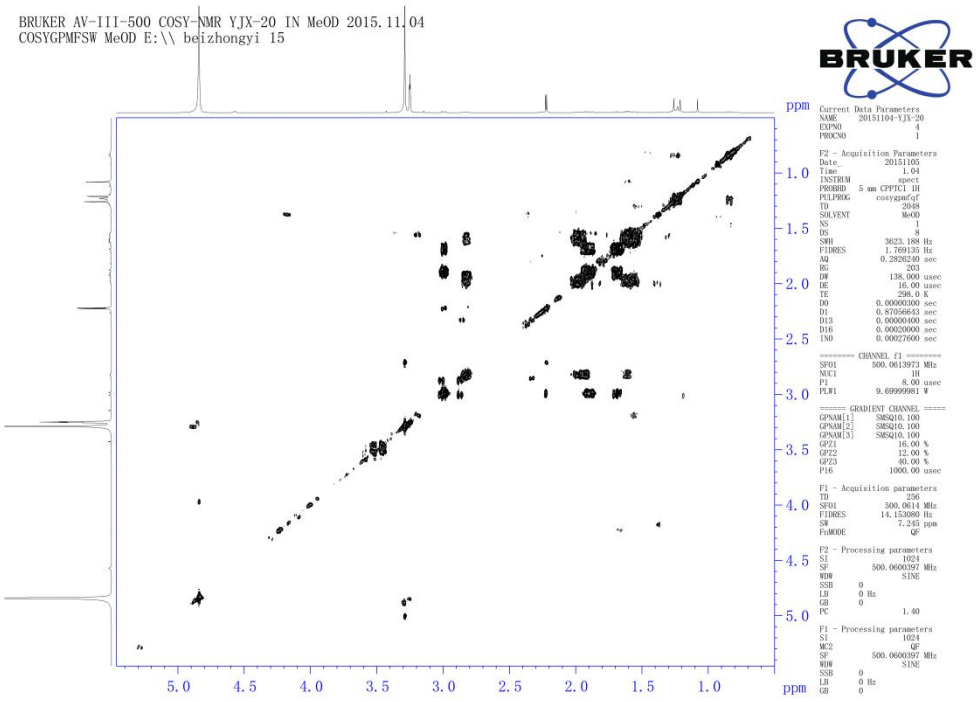


Figure S57. The ^{1}H-^{1}H COSY spectrum of **6** in CD_3OD

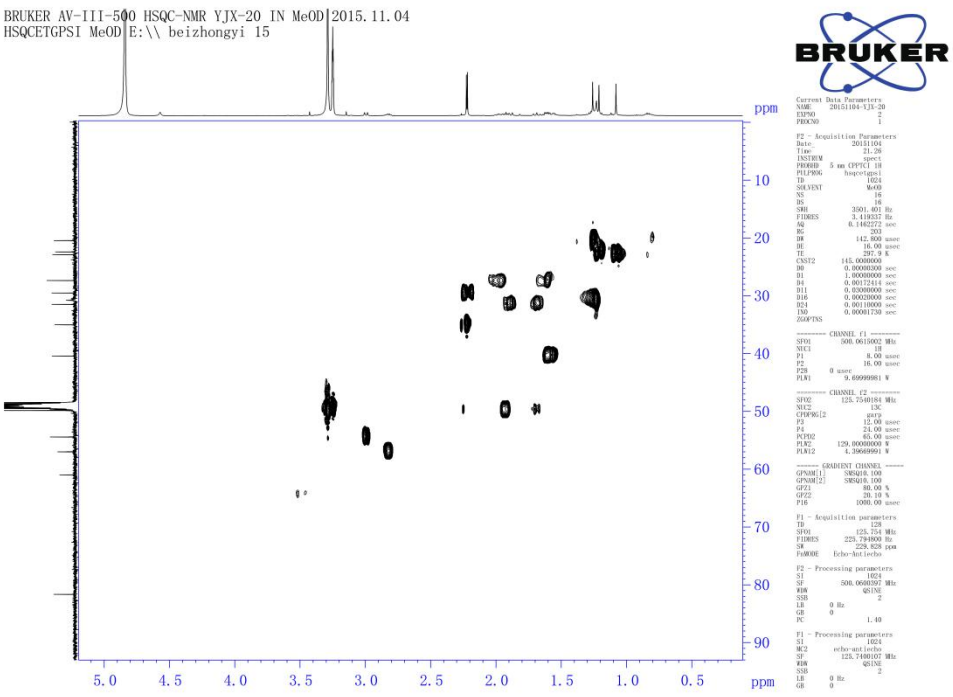


Figure S58. The HSQC spectrum of **6** in CD_3OD

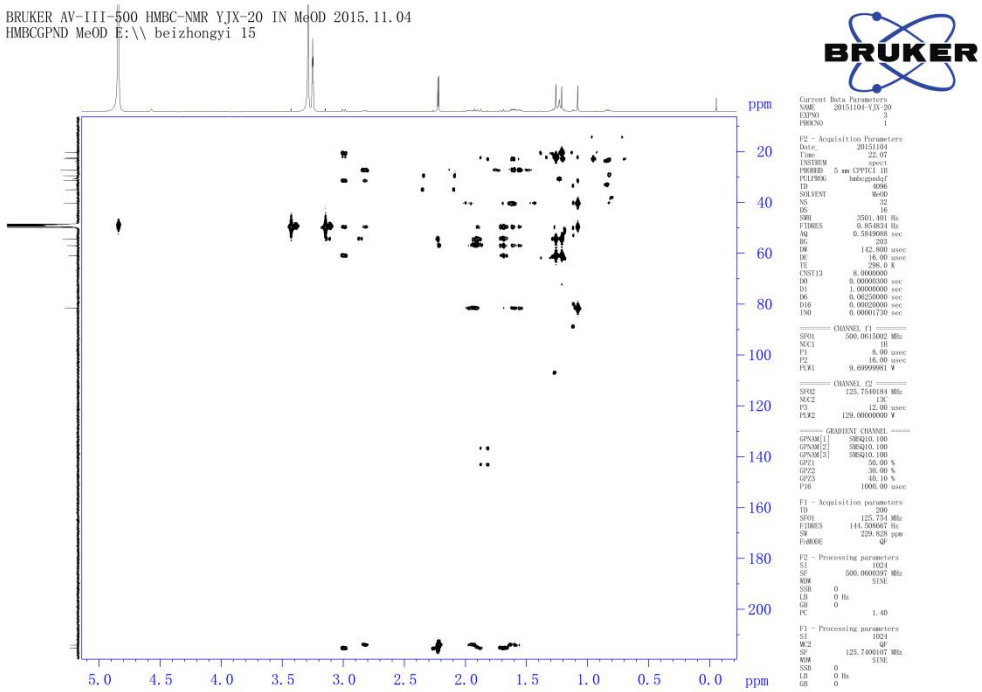


Figure S59. The HMBC spectrum of **6** in CD_3OD

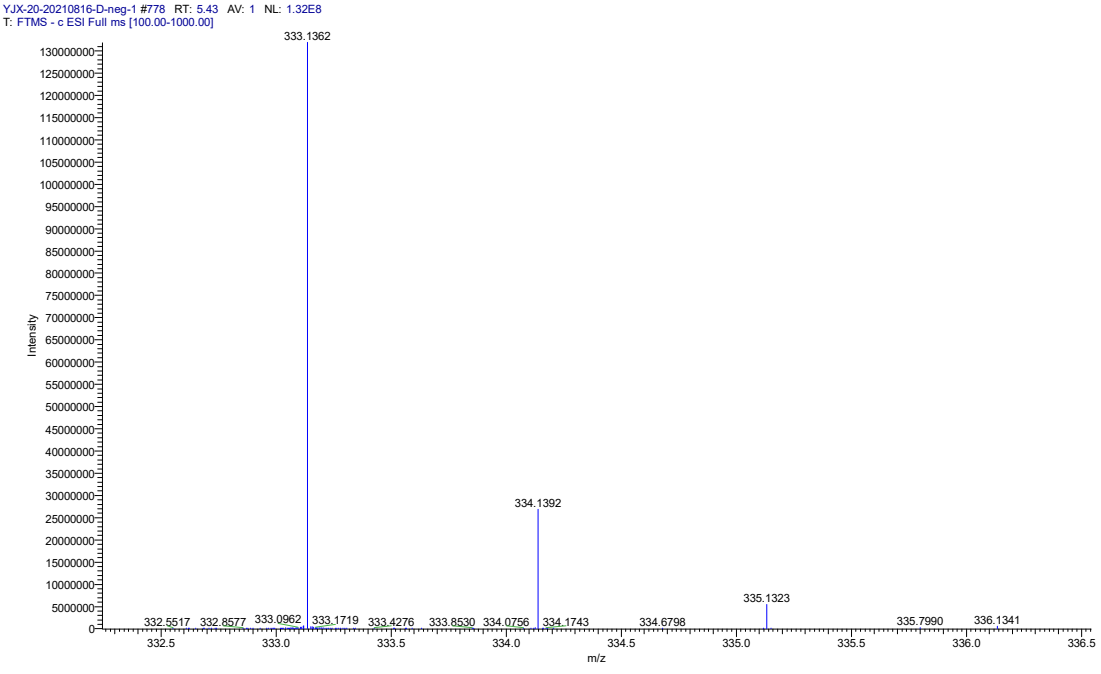


Figure S60. The HRESIMS spectrum of **6**

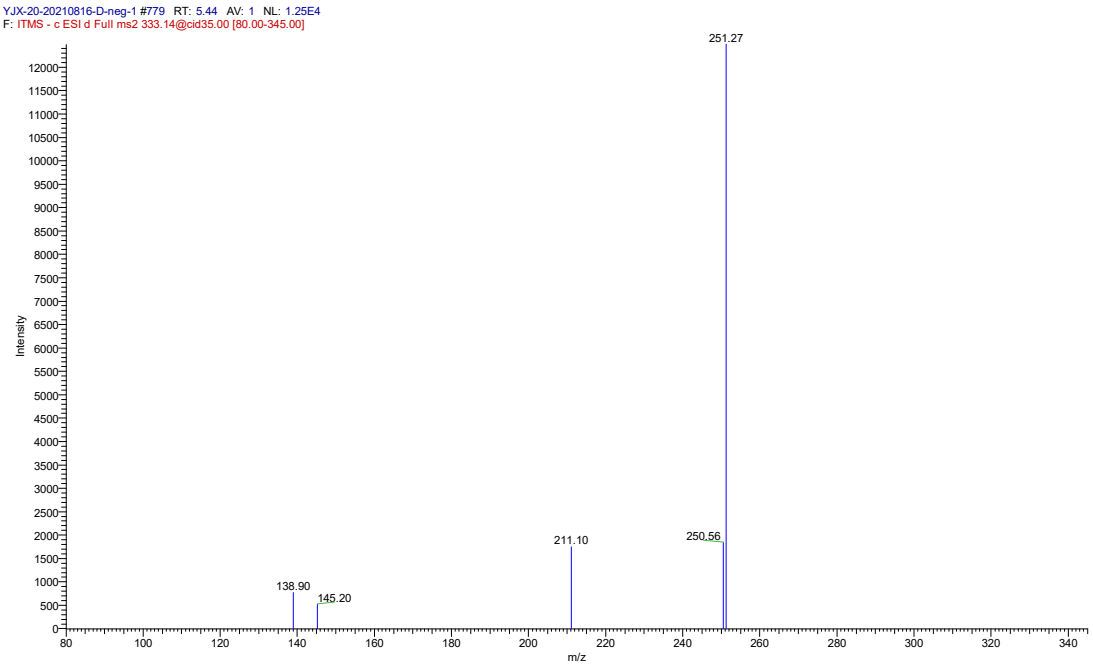


Figure S61. The MS/MS spectrum of **6**

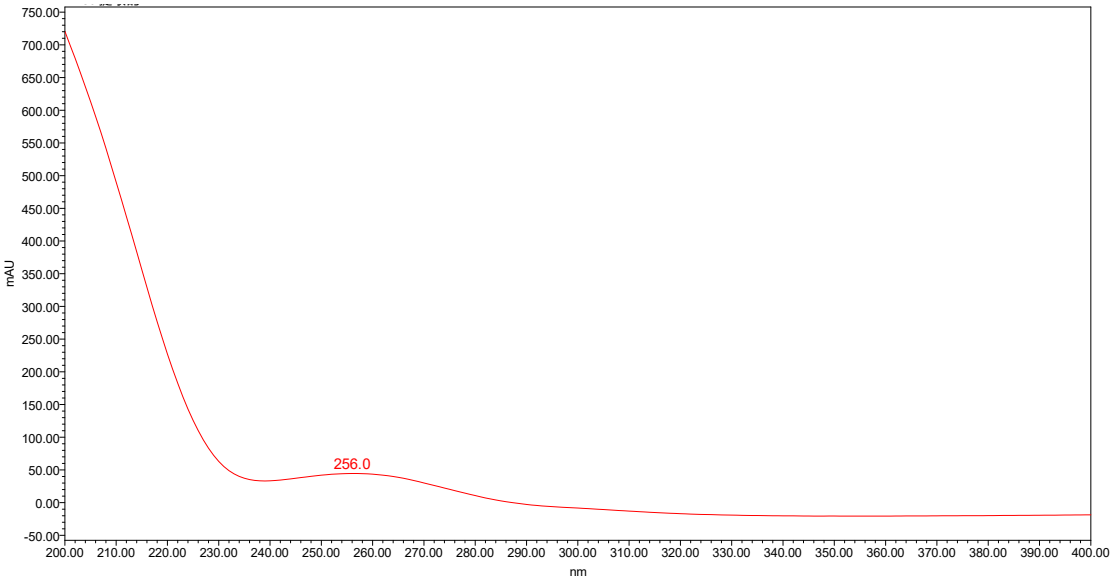


Figure S62. The UV-Vis spectrum of **6** in CH_3OH.

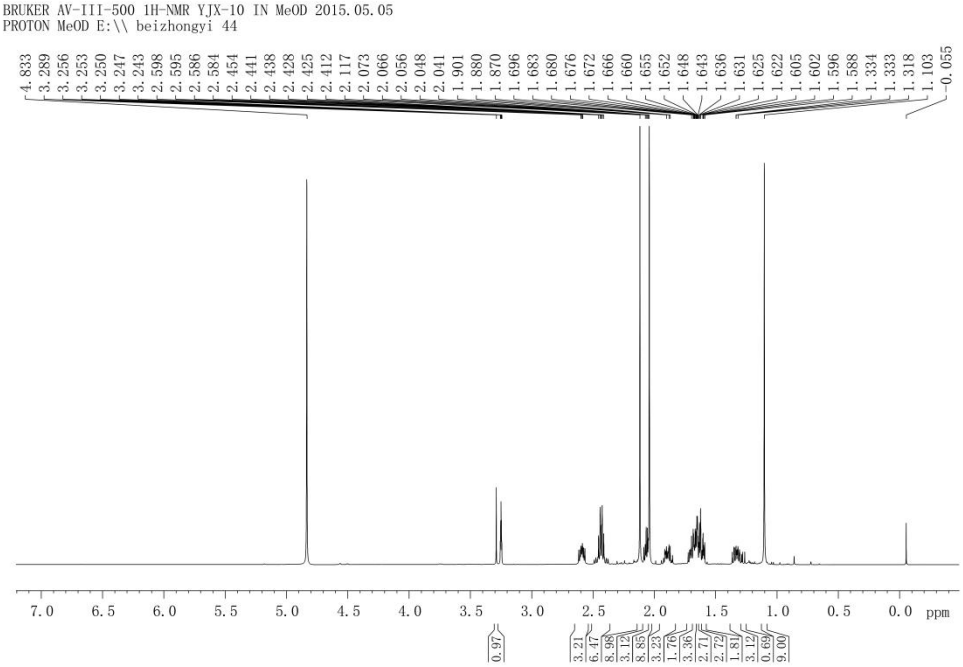


Figure S63. The ^{1}H NMR spectrum of **7** in CD_3OD

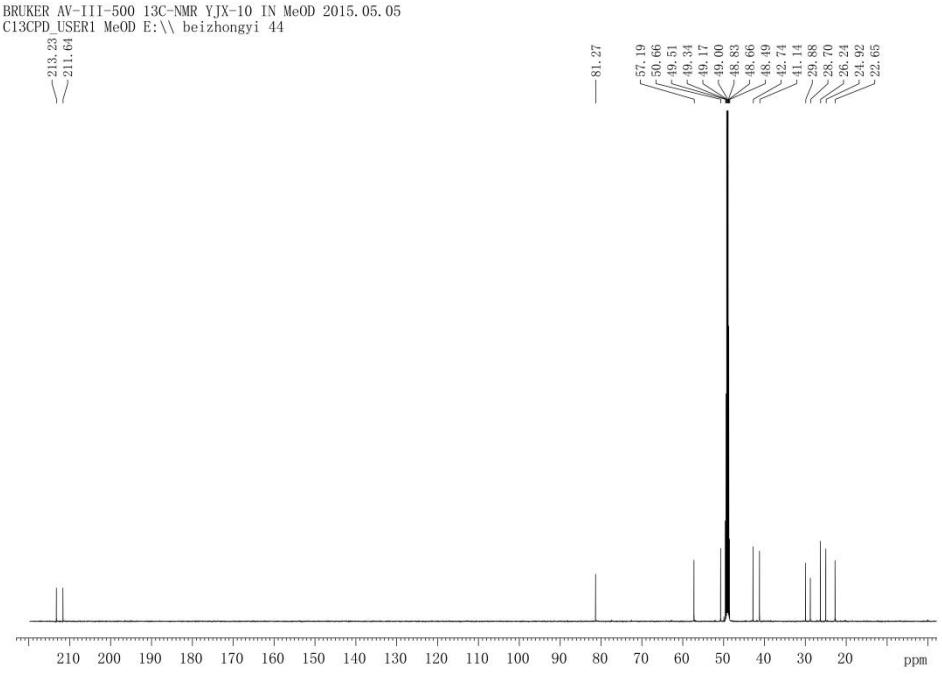


Figure S64. The ^{13}C NMR spectra of **7** in CD_3OD

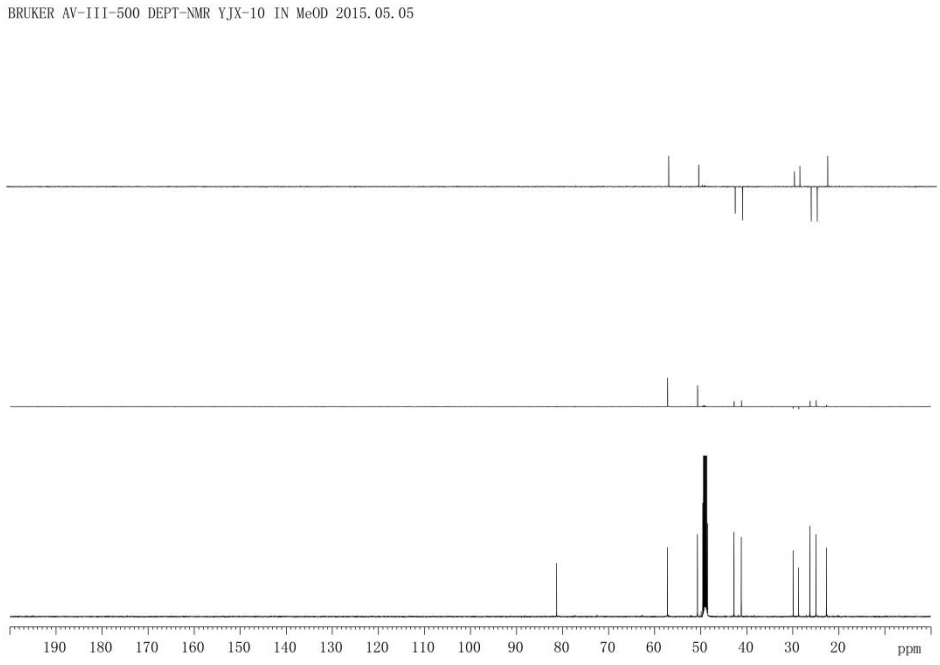


Figure S65. The DEPT spectra of **7** in CD_3OD

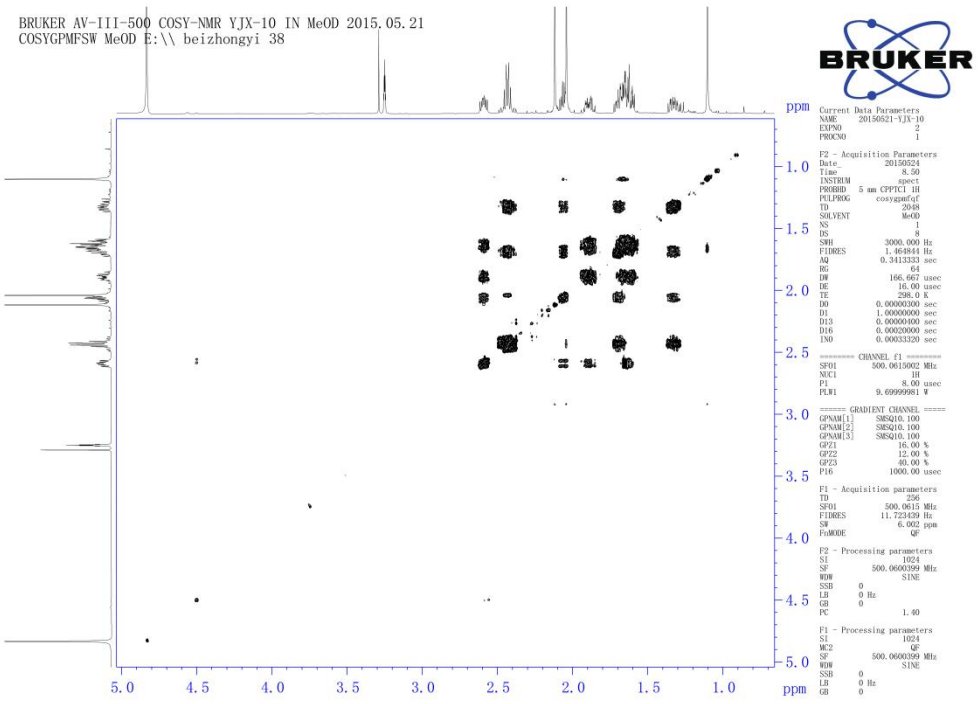


Figure S66. The ^{1}H-^{1}H COSY spectrum of **7** in CD_3OD

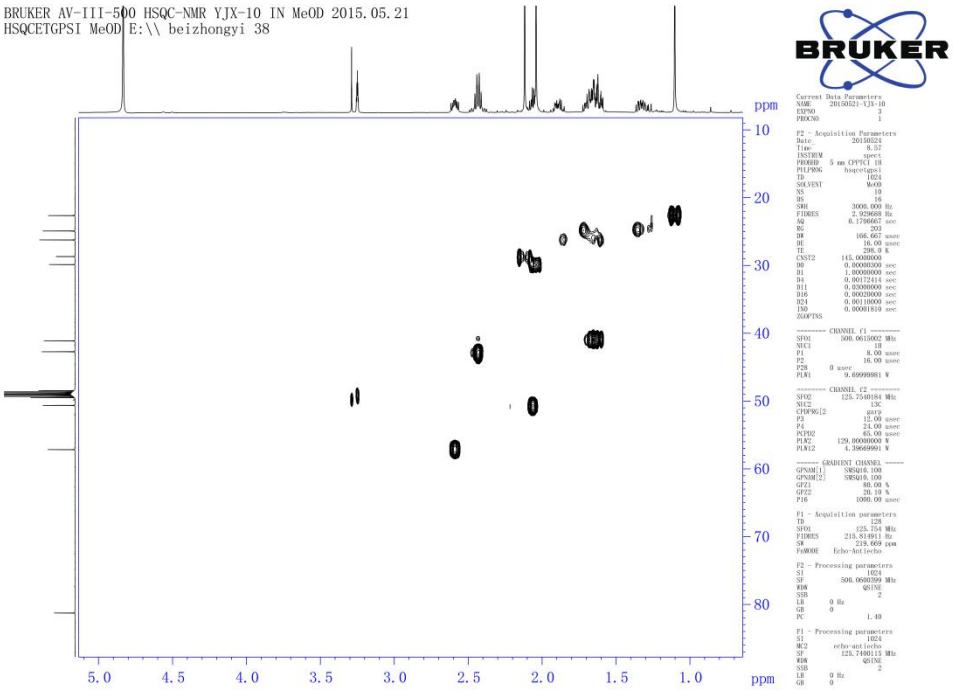


Figure S67. The HSQC spectrum of **7** in CD_3OD

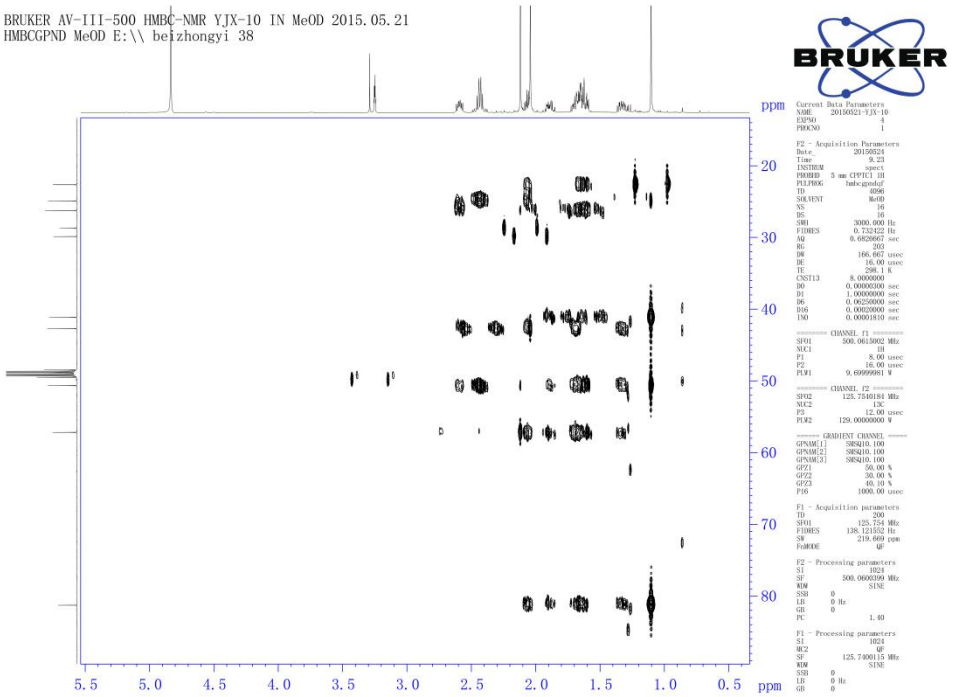


Figure S68. The HMBC spectrum of **7** in CD_3OD

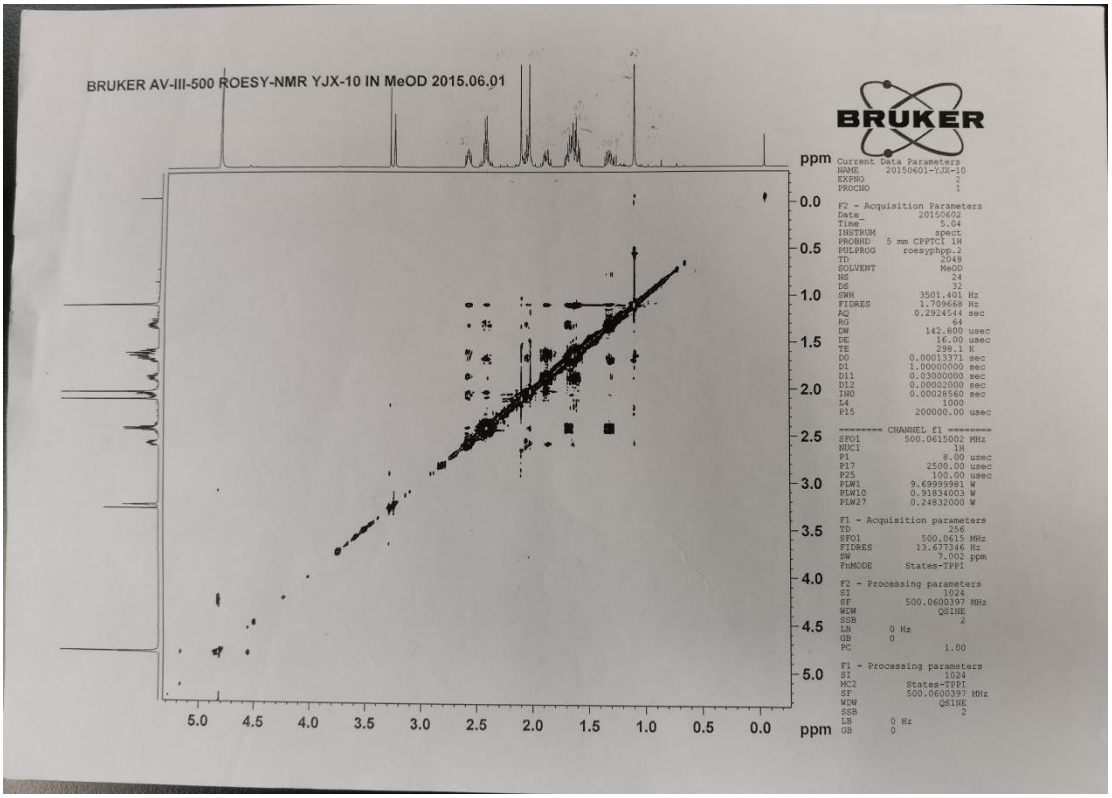


Figure S69. The ROESY spectrum of **7** in CD_3OD

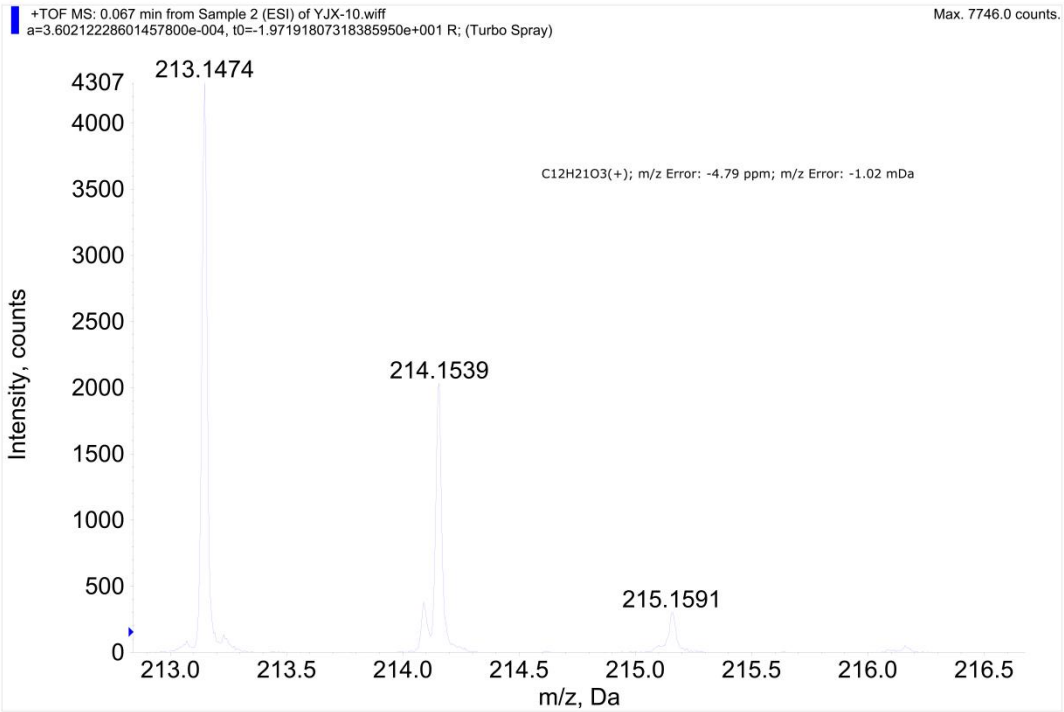


Figure S70. The HRESIMS spectrum of **7**

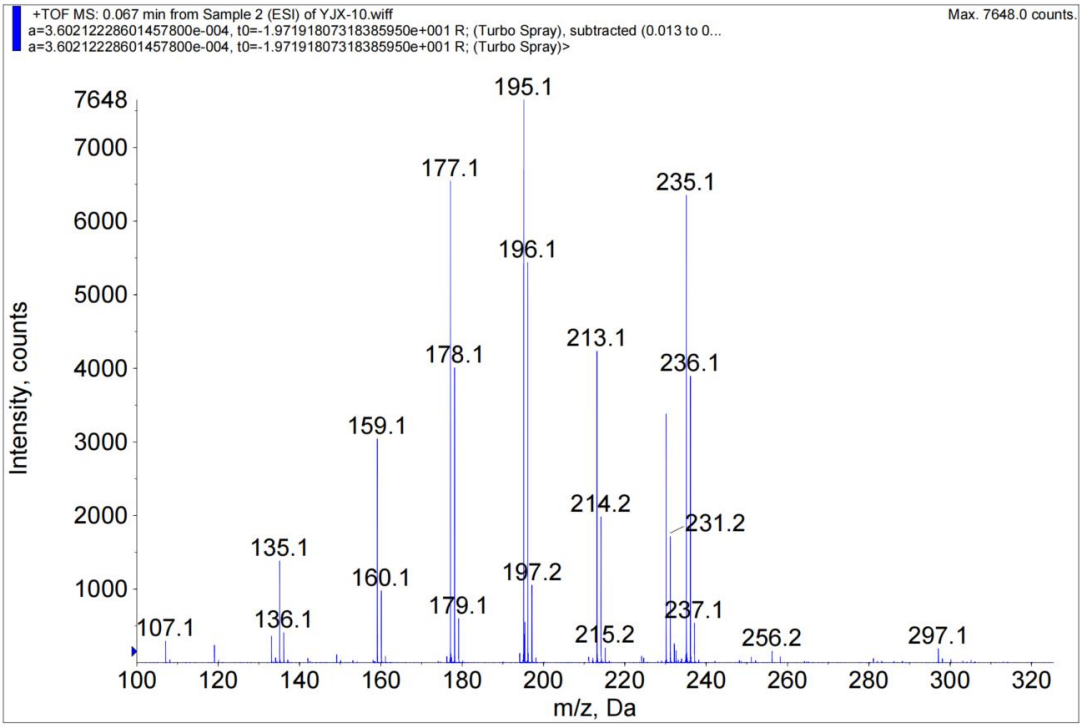


Figure S71. The MS/MS spectrum of **7**

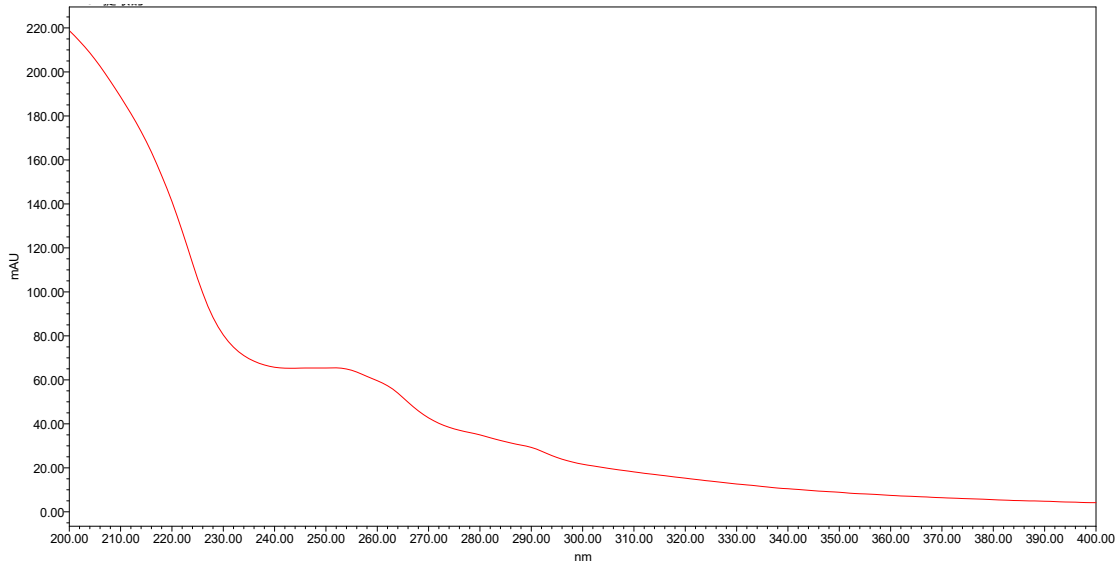


Figure S72. The UV-Vis spectrum of **7** in CH_3OH.

Table S1. Cartesian coordinates and geometries of optimized predominant conformers in CH_3OH for compound **2**.

(1*R*,4*R*,5*S*,8*R*,10*R*)-**2** conformer 1				(1*R*,4*R*,5*S*,8*R*,10*R*)-**2** conformer 2			
C	-0.90987165	-0.39100407	0.77225598	C	-0.83708153	-0.36619500	0.89609019

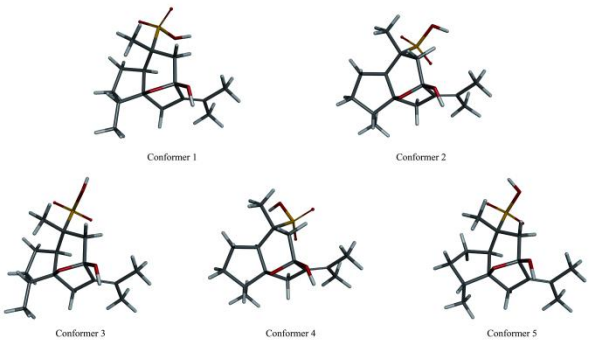
C	-0.11536844	-1.22838744	-0.30840952	C	-0.68776208	-1.36808182	-0.28143406
C	0.07919318	0.33832968	1.69181116	C	0.42616844	0.33822655	1.40383990
C	0.52718821	1.45237013	0.77616817	C	0.57525528	1.49481544	0.44626814
C	-0.52030853	1.53470452	-0.34140643	C	-0.67870502	1.49381667	-0.41273269
C	-0.04620673	0.92448797	-1.67609273	C	-0.52440178	0.77077453	-1.75051688
C	-0.30727322	-0.60375917	-1.70927629	C	-0.23672135	-0.74475657	-1.63588566
C	-1.65565112	-0.91854584	-2.37163567	C	-0.84485914	-1.45851361	-2.85377127
O	-1.01414735	2.81419674	-0.60811575	O	-1.24155435	2.74444013	-0.68448635
O	-1.59886531	0.71217418	0.15739378	O	-1.62042566	0.73935956	0.38452081
C	1.63025264	2.20300422	0.88347622	C	1.60808081	2.33954376	0.36058262
C	2.58237846	2.05215318	2.03749523	C	2.77840574	2.23578055	1.29782557
C	2.04508982	3.24776509	-0.11662922	C	1.75566390	3.40789113	-0.68785845
S	0.94682487	-1.33570386	-2.86810557	S	1.60411143	-1.11073734	-1.81007226
O	0.97914381	-0.55376616	-4.11466386	O	1.75322861	-2.54497341	-2.08782349
O	0.77780520	-2.79094866	-2.93184865	O	2.43428315	-0.51234136	-0.75772700
O	2.38862073	-1.13224819	-2.09983025	O	1.99434754	-0.37699755	-3.23426332
C	-0.55413762	-2.69281811	-0.09154006	C	-2.09711622	-1.99125452	-0.33074010
C	-1.13712905	-2.70287066	1.32703307	C	-2.45429937	-2.20342077	1.14496542
C	-1.89288763	-1.37313792	1.41162208	C	-1.67700183	-1.12228180	1.94282042
C	-2.39746157	-1.00606690	2.79989425	C	-0.83777451	-1.75884969	3.05247006
H	0.94846261	-1.13753697	-0.06172171	H	0.01614411	-2.15772694	0.02053856
H	-0.45166158	0.73332738	2.56731634	H	0.23779504	0.70090496	2.42314340
H	0.89060651	-0.30646678	2.04106509	H	1.29732096	-0.32070747	1.43439114
H	-0.59121166	1.39986363	-2.49708827	H	-1.48407536	0.87533310	-2.27137545

H	1.01445403	1.16082430	-1.79916715	H	0.22372261	1.27537182	-2.36983911
H	-1.74546068	-0.38516823	-3.32214900	H	-1.92286326	-1.28345381	-2.84985143
H	-1.78971093	-1.98609854	-2.55593706	H	-0.44289631	-1.04234759	-3.78209713
H	-2.44994843	-0.57377669	-1.70617800	H	-0.66273413	-2.53415177	-2.83152546
H	-1.06711345	3.28959529	0.23368320	H	-1.11994814	3.29443119	0.10281319
H	3.56343255	1.71313069	1.67855980	H	2.58736515	1.57040572	2.14257926
H	2.22800518	1.34890042	2.79319324	H	3.65871935	1.85979418	0.75854616
H	2.74694517	3.02422534	2.51969952	H	3.04667205	3.22613538	1.68673107
H	2.10495373	4.23156613	0.36695199	H	1.79566371	4.40284397	-0.22472183
H	1.36953335	3.32967294	-0.96820702	H	0.95225046	3.40408419	-1.42424902
H	3.05432727	3.02182745	-0.48568057	H	2.71257179	3.27066698	-1.20942302
H	2.79969553	-0.29673189	-2.38790327	H	2.36457621	0.50508570	-3.04763700
H	-1.33554554	-2.98096018	-0.80067061	H	-2.79364895	-1.28508062	-0.79431794
H	0.27651742	-3.39120157	-0.22120411	H	-2.12460256	-2.92035220	-0.90603752
H	-0.33388898	-2.71597791	2.07706151	H	-3.53371194	-2.15088071	1.31613537
H	-1.78436258	-3.56564837	1.51481522	H	-2.12293383	-3.19812281	1.46642715
H	-2.75033673	-1.43280434	0.72301252	H	-2.36232378	-0.39313339	2.39254753
H	-2.84097660	-0.00414899	2.81399939	H	-0.07931938	-2.43140005	2.63351379
H	-1.58725243	-1.03358406	3.53678677	H	-1.48549014	-2.35600141	3.70317089
H	-3.16515244	-1.71785778	3.12136625	H	-0.33269572	-1.01494329	3.67566578
(1*R*,4*R*,5*S*,8*R*,10*R*)-**2** conformer 3				(1*R*,4*R*,5*S*,8*R*,10*R*)-**2** conformer 4			
C	-0.90838337	-0.21496082	0.95124376	C	-0.84606547	-0.40419352	0.87888353
C	0.01577276	-1.00864115	-0.05454215	C	-0.72272228	-1.32432127	-0.36935440
C	-0.04123810	0.64933323	1.87643543	C	0.41875061	0.28336462	1.39825358

C	0.33348933	1.76557754	0.93048551	C	0.57261657	1.43966075	0.43991380
C	-0.65876994	1.69046508	-0.23532552	C	-0.73911973	1.52501830	-0.33208387
C	-0.06774314	1.07466550	-1.51963873	C	-0.68011977	0.88256729	-1.71266611
C	-0.18064599	-0.47290258	-1.49557665	C	-0.29742057	-0.61388235	-1.67754201
C	-1.45208139	-0.96492444	-2.19135516	C	-0.85208578	-1.28705303	-2.94047362
O	-1.26511173	2.90037565	-0.58397731	O	-1.28858077	2.80182040	-0.48317416
O	-1.67410064	0.78405297	0.25554420	O	-1.64683609	0.73114784	0.46684353
C	1.34097797	2.63738140	1.05735842	C	1.64838686	2.21798410	0.27170787
C	2.23690917	2.64066663	2.26484593	C	1.75836184	3.30892263	-0.75791601
C	1.69156671	3.68137873	0.03227550	C	2.88460350	2.04060578	1.10707434
S	1.26001631	-1.13917097	-2.45592431	S	1.60096596	-0.75233549	-1.86325317
O	1.11643182	-2.58391947	-2.69767134	O	2.30059969	-0.94829847	-0.58562774
O	2.53591787	-0.66957823	-1.88954672	O	2.07182033	0.27415042	-2.80172974
O	0.98473288	-0.33710590	-3.86676093	O	1.80003047	-2.15492551	-2.71112816
C	-0.27639995	-2.50160208	0.20959184	C	-2.14100483	-1.92727673	-0.43727257
C	-0.92463009	-2.51538901	1.59958017	C	-2.49019248	-2.22128420	1.02977743
C	-1.81420408	-1.26831388	1.59110622	C	-1.65179119	-1.23573269	1.88898148
C	-2.41955421	-0.90061200	2.93869308	C	-0.76219065	-1.98365612	2.88399982
H	1.05345793	-0.79265598	0.22785784	H	-0.01767737	-2.13654597	-0.14276266
H	-0.64740086	1.02385482	2.71108885	H	1.28406739	-0.37817538	1.43792278
H	0.81367375	0.10459987	2.28690729	H	0.21405604	0.64784243	2.41508112
H	0.97391940	1.39392546	-1.61463413	H	-1.68991665	0.94824600	-2.13630737
H	-0.62245230	1.45951074	-2.38056552	H	-0.00924158	1.43433184	-2.37700864
H	-1.58156297	-0.46087188	-3.15210142	H	-0.42399596	-0.83501455	-3.84105483

H	-2.30597980	-0.71995113	-1.55590768	H	-1.93186703	-1.12090339	-2.96462473
H	-1.44100244	-2.04283310	-2.36246077	H	-0.66316526	-2.36110156	-2.95589380
H	-1.40450364	3.40533623	0.23043078	H	-1.12867983	3.28890841	0.33795096
H	2.29138664	3.65055747	2.69084443	H	2.65805100	3.14632211	-1.36543716
H	3.26152502	2.36771823	1.97850130	H	1.88504394	4.28369548	-0.26819678
H	1.90109646	1.95523775	3.04514043	H	0.89413084	3.36820165	-1.41901622
H	2.75048203	3.58606309	-0.24118780	H	3.18184468	2.99902238	1.55207149
H	1.56968828	4.68593168	0.45852066	H	3.72212871	1.71561608	0.47517737
H	1.08742950	3.62232690	-0.87315419	H	2.75574328	1.31109791	1.90882406
H	1.65249958	-0.61504893	-4.52227709	H	1.76264804	-2.90748772	-2.09212637
H	-0.98870701	-2.89927084	-0.51900935	H	-2.18466644	-2.82209494	-1.06368638
H	0.62874652	-3.11218890	0.14944845	H	-2.83241840	-1.18829227	-0.85516655
H	-0.16298632	-2.41910110	2.38611594	H	-2.20834549	-3.25098792	1.27944685
H	-1.49158738	-3.43147517	1.79394766	H	-3.56372643	-2.12556331	1.21805478
H	-2.62785571	-1.44266083	0.86978140	H	-2.29700088	-0.54163504	2.44161059
H	-2.95954964	0.05146930	2.88899321	H	-0.19944609	-1.30275171	3.52969302
H	-1.64762714	-0.81891310	3.71168414	H	-0.04879450	-2.63113216	2.35982466
H	-3.12824207	-1.67323678	3.25509431	H	-1.38017827	-2.62178115	3.52440993
(1*R*,4*R*,5*S*,8*R*,10*R*)-**2** conformer 5							
C	-0.86856307	-0.17127285	0.94601872	H	0.82942051	0.24062599	2.28395642
C	0.01992395	-1.07392258	0.00286811	H	1.16987373	1.26678948	-1.58150998
C	-0.02003689	0.75503258	1.82595696	H	-0.35079730	1.32056394	-2.48651285
C	0.36895341	1.82560956	0.83918248	H	-1.18274216	-0.70306510	-3.31045138
C	-0.56357835	1.65920757	-0.36274715	H	-2.14702098	-0.55820596	-1.84128397

C	0.11728623	0.97122837	-1.56116296	H	-1.38799823	-2.11346020	-2.24957889
C	-0.04205649	-0.56549609	-1.46882127	H	-1.36007920	3.38498843	-0.05382299
C	-1.26009726	-1.03006680	-2.26872475	H	2.79846819	3.62334008	-0.33170161
O	-1.16551358	2.83287993	-0.82514187	H	1.57435018	4.74318431	0.25216806
O	-1.59594766	0.77992473	0.13912299	H	1.16346842	3.59447201	-1.03266116
C	1.34936307	2.72861373	0.96090051	H	2.19103216	3.85318050	2.58119733
C	1.72770420	3.71734132	-0.10821081	H	3.23331402	2.57047174	1.97914172
C	2.18839143	2.82207762	2.20518029	H	1.83903807	2.16516347	3.00398061
S	1.45845988	-1.29621281	-2.30441978	H	1.00568986	-0.98783210	-4.40952320
O	1.25532083	-2.72588742	-2.58468692	H	0.10401998	-2.98474634	1.00795221
O	2.67812909	-0.86445241	-1.61137921	H	-0.41544965	-3.14420865	-0.66063972
O	1.51694653	-0.49510887	-3.74176950	H	-2.32273363	-3.22514602	1.23022906
C	-0.49933228	-2.51110142	0.22581882	H	-2.60903911	-2.12309830	-0.12378017
C	-1.94104839	-2.33524277	0.71821167	H	-2.82484215	-0.60243345	1.73436728
C	-1.85917235	-1.11607915	1.65173086	H	-1.34804468	-0.66977045	3.73387677
C	-1.39851190	-1.52539654	3.05454602	H	-0.41040044	-1.99834601	3.03583130
H	1.06152239	-0.98467013	0.33052017	H	-2.10660718	-2.24634647	3.47565460
H	-0.64816319	1.16387351	2.62911715				



The optimized conformers of (1*R*,4*R*,5*S*,8*R*,10*R*)-**2**.

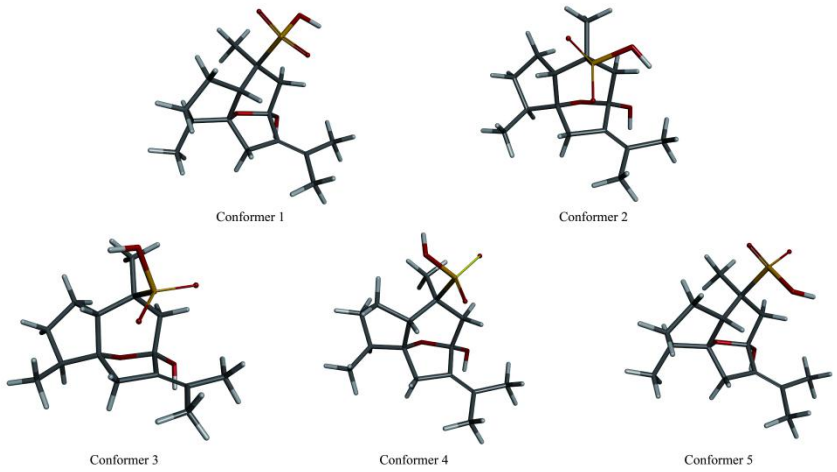
(1*S*,4*S*,5*R*,8*S*,10*S*)-**2** conformer 1				(1*S*,4*S*,5*R*,8*S*,10*S*)-**2** conformer 2			
C	-0.89887763	-0.27250319	-0.83578040	C	-0.84556082	-0.41680022	-0.87421274
C	-0.10998829	-1.23069016	0.14148574	C	-0.72046953	-1.35976949	0.35512286
C	0.09467207	0.53628263	-1.68032429	C	0.43785850	0.23253670	-1.40637815
C	0.56911461	1.53623400	-0.65258148	C	0.60840652	1.42994143	-0.50399768
C	-0.46705506	1.51243581	0.47783108	C	-0.65332871	1.50440840	0.34015286
C	0.00372440	0.75112133	1.73534476	C	-0.53054465	0.84981133	1.71470580
C	-0.29248910	-0.76615031	1.60706396	C	-0.27395245	-0.67543013	1.68182329
C	-1.63736733	-1.12958983	2.23868445	C	-0.91422661	-1.30968740	2.92644948
O	-0.93579677	2.76283439	0.88876438	O	-1.18781278	2.78099896	0.53924349
O	-1.56416765	0.76785132	-0.09815500	O	-1.60594538	0.73094741	-0.42465207
C	1.68336447	2.27715307	-0.68852365	C	1.66479448	2.24742652	-0.44290399
C	2.12483743	3.19556729	0.41816266	C	2.84366993	2.06700083	-1.35735425
C	2.62041012	2.24183744	-1.86373385	C	1.83003192	3.35755852	0.55837646
S	1.01358520	-1.65531676	2.58620478	S	1.55607962	-1.07182429	1.89858241
O	2.35219465	-1.32673331	2.07062504	O	1.66797194	-2.48302138	2.28862270
O	0.64007565	-3.06096607	2.77306126	O	2.40473119	-0.58030541	0.80644321
O	0.86384932	-1.00311339	4.09163085	O	1.95969583	-0.23971508	3.26305040
C	-0.56177586	-2.65933155	-0.22941221	C	-2.13428910	-1.96981177	0.41597070
C	-1.15767460	-2.50913351	-1.63491162	C	-2.44280421	-2.28251768	-1.05009534
C	-1.89957301	-1.17007909	-1.56604789	C	-1.70302952	-1.20595381	-1.88678562
C	-2.41487086	-0.65067324	-2.90065529	C	-0.89604161	-1.84852314	-3.01585612
H	0.95538995	-1.12163344	-0.09554400	H	-0.02334480	-2.17167438	0.09887049
H	0.89199780	-0.08109838	-2.10352575	H	1.29242633	-0.44817186	-1.39611462

H	-0.43574118	1.03257152	-2.50291065	H	0.26700064	0.55091069	-2.44304239
H	-0.52976695	1.14719058	2.60547739	H	0.21944841	1.36899283	2.31911329
H	1.07342511	0.94080896	1.87222574	H	-1.49487367	1.00090378	2.21550094
H	-2.42912608	-0.67358569	1.64038259	H	-1.98822543	-1.11313168	2.89499022
H	-1.70004231	-0.72904122	3.25413018	H	-0.51727455	-0.85112222	3.83709188
H	-1.80071652	-2.20746340	2.27905812	H	-0.75441503	-2.38820898	2.96684747
H	-0.99009715	3.32876486	0.10492246	H	-1.04486127	3.28643737	-0.27394082
H	2.19524359	4.22699039	0.04872865	H	2.64218187	1.37688178	-2.17960892
H	3.13365645	2.91413154	0.74792399	H	3.70223122	1.68153821	-0.79040261
H	1.45863625	3.18851489	1.28079988	H	3.15222346	3.03185769	-1.77902820
H	3.59903924	1.84796589	-1.55814536	H	2.77631432	3.21718740	1.09821723
H	2.79694447	3.25929210	-2.23545719	H	1.90411152	4.32918323	0.05191266
H	2.24507098	1.63446622	-2.68923567	H	1.01784785	3.40954347	1.28316368
H	1.39668820	-0.18904348	4.15224528	H	2.34848789	0.61814752	3.01171073
H	0.26371909	-3.37544832	-0.18507906	H	-2.18440055	-2.85653356	1.05331480
H	-1.34168646	-3.01649532	0.44941987	H	-2.83857653	-1.22796655	0.80722823
H	-0.36303362	-2.45037699	-2.39183153	H	-2.04242071	-3.27231733	-1.30263164
H	-1.81774626	-3.33910096	-1.90682420	H	-3.51756697	-2.30387576	-1.25436160
H	-2.74996997	-1.29534115	-0.87762217	H	-2.41446720	-0.49328894	-2.32206898
H	-1.61419855	-0.61225926	-3.64733757	H	-0.10374775	-2.49139234	-2.61324286
H	-2.84237977	0.35339213	-2.80215212	H	-0.43712240	-1.10882562	-3.67837610
H	-3.19769808	-1.31303836	-3.28518217	H	-1.55581122	-2.47734507	-3.62335056
(1*S*,4*S*,5*R*,8*S*,10*S*)-**2** conformer 3				(1*S*,4*S*,5*R*,8*S*,10*S*)-**2** conformer 4			
C	-0.84578216	-0.39641239	-0.94242178	C	-0.88312625	-0.19184297	-0.94499548

C	-0.74739721	-1.30849650	0.31324496	C	-0.00774914	-1.02056131	0.07604721
C	0.43750038	0.24901271	-1.47120440	C	-0.02796404	0.66988693	-1.88047906
C	0.62658348	1.40974927	-0.52440834	C	0.33852967	1.81712847	-0.97583249
C	-0.67964188	1.53939063	0.25066902	C	-0.61542618	1.74121730	0.21809328
C	-0.63457185	0.90653596	1.63669357	C	0.04944238	1.16307428	1.47845964
C	-0.29445037	-0.60029061	1.61296908	C	-0.05495723	-0.38903215	1.49828842
C	-0.86091501	-1.24648065	2.88487588	C	-1.24228673	-0.81897332	2.36137961
O	-1.19217063	2.83222945	0.39347650	O	-1.23523004	2.94297486	0.57312617
O	-1.61197813	0.76575304	-0.53951078	O	-1.62972751	0.81103631	-0.22094211
C	1.72391128	2.16013265	-0.36843716	C	1.32042203	2.70964916	-1.15136442
C	1.86840645	3.25618751	0.65126826	C	1.67630446	3.78548761	-0.16167419
C	2.95113344	1.93991174	-1.20669782	C	2.18572560	2.70136226	-2.38106281
S	1.60054054	-0.79174387	1.79101507	S	1.49536817	-0.90125505	2.40375587
O	2.28827780	-1.02288574	0.51285780	O	2.67771638	-0.61679931	1.58202300
O	2.10433252	0.23128418	2.71604125	O	1.44101851	-0.39371101	3.78371510
O	1.76289002	-2.18974898	2.65362868	O	1.44465463	-2.54175351	2.45447578
C	-2.18472049	-1.86373849	0.39417156	C	-0.55159809	-2.46520110	-0.02785565
C	-2.56530102	-2.14201218	-1.06945988	C	-1.97986407	-2.31666673	-0.56386845
C	-1.67723869	-1.21314496	-1.94204144	C	-1.86095370	-1.18579579	-1.59707116
C	-0.80824402	-2.01961455	-2.90903083	C	-1.36067456	-1.71780492	-2.94389935
H	-0.06962211	-2.14493146	0.09198980	H	1.03302963	-0.98144741	-0.26198223
H	1.28361650	-0.43706898	-1.50495366	H	0.83130954	0.12711641	-2.28400628
H	0.24083532	0.60862667	-2.49143208	H	-0.64501845	1.01090325	-2.72313075
H	-1.64083630	1.00437654	2.06268285	H	-0.45841737	1.55931458	2.36305518

H	0.05383511	1.44452234	2.29439608	H	1.08847044	1.50442811	1.50634797
H	-0.70317986	-2.32544050	2.90835390	H	-1.33671845	-1.90384639	2.44694418
H	-1.93519578	-1.04887832	2.91446632	H	-2.15150527	-0.42790058	1.89934101
H	-0.41423891	-0.79950670	3.77892330	H	-1.15919467	-0.39110020	3.36380997
H	-1.01991754	3.30931352	-0.43100408	H	-1.42554463	3.42765252	-0.24334591
H	2.76751118	3.07547346	1.25456596	H	1.54740537	4.77633557	-0.61677742
H	2.01687397	4.22344704	0.15286447	H	2.73841466	3.70177870	0.10387074
H	1.01001374	3.34250689	1.31686778	H	1.08197555	3.75198783	0.75158464
H	2.79250394	1.22212892	-2.01382672	H	2.19186475	3.69639072	-2.84404723
H	3.28690787	2.88880383	-1.64433947	H	3.22660677	2.47716545	-2.11153590
H	3.77516270	1.57583948	-0.57822760	H	1.85766139	1.97605029	-3.12784177
H	1.70395850	-2.94858987	2.04417339	H	0.89579314	-2.83217342	3.20635335
H	-2.24999182	-2.75767459	1.01989625	H	-0.49953071	-3.01951512	0.91010523
H	-2.84583300	-1.10350460	0.82246234	H	0.06007169	-3.01756413	-0.74937355
H	-2.35398324	-3.18820340	-1.31940253	H	-2.66346130	-2.02478558	0.24163949
H	-3.63249159	-1.97749310	-1.24555101	H	-2.36213328	-3.24382808	-1.00450322
H	-2.28553790	-0.50505989	-2.51824913	H	-2.81840126	-0.67393650	-1.75395944
H	-0.20944560	-1.37642438	-3.56088319	H	-2.05793210	-2.47327272	-3.32032537
H	-0.12905656	-2.68582917	-2.36328897	H	-0.37471586	-2.18715080	-2.85522591
H	-1.44505308	-2.64415197	-3.54428321	H	-1.28885390	-0.92532252	-3.69421572
(1*S*,4*S*,5*R*,8*S*,10*S*)-**2** conformer 5							
C	-0.89720367	-0.23682704	-0.90061658	H	0.83512335	-0.04791216	-2.24823562
C	-0.02559784	-1.09178801	0.10406455	H	1.10070595	1.26999111	1.64704363
C	0.02460199	0.55893204	-1.83517451	H	-0.47997682	1.42597515	2.42152028

C	0.48612831	1.64664326	-0.89490555	H	-2.30734406	-0.56230522	1.64572188
C	-0.50840845	1.65305141	0.27295845	H	-1.52470094	-0.43636943	3.23105798
C	0.04367914	1.00390902	1.55846543	H	-1.56886937	-1.99737148	2.38622514
C	-0.16765130	-0.53260718	1.53851654	H	-1.13028642	3.41466509	-0.20061296
C	-1.47098412	-0.91857776	2.25090977	H	3.46924688	2.04378276	-1.92861082
O	-1.02410691	2.90552171	0.61613600	H	2.09339302	1.66970097	-2.98966456
O	-1.58635763	0.81939968	-0.20844626	H	2.56512713	3.35233847	-2.67910362
C	1.56217178	2.43251150	-1.02232323	H	3.02668537	3.23458520	0.31427723
C	2.45990611	2.35815287	-2.22618381	H	2.00882465	4.45059448	-0.44541021
C	1.99622160	3.44727858	0.00016638	H	1.35831255	3.47724505	0.88360480
S	1.16503015	-1.27080194	2.60200256	H	2.96652527	-0.15295199	2.10627564
O	1.04949292	-2.73262497	2.60233781	H	-1.16767870	-2.90075112	0.57677194
O	1.23144173	-0.54862082	3.88283111	H	0.42612828	-3.23614624	-0.09514223
O	2.55858504	-0.97477125	1.77734819	H	-1.71092208	-3.40376854	-1.73624765
C	-0.42986544	-2.55935899	-0.15491424	H	-0.31708126	-2.48418172	-2.33127457
C	-1.08162781	-2.52900661	-1.54299593	H	-2.70072129	-1.33832246	-0.80605378
C	-1.88119857	-1.22247016	-1.53263343	H	-2.94006530	0.17254241	-2.82603125
C	-2.46649328	-0.81427300	-2.87714123	H	-3.22810981	-1.53637245	-3.18999632
H	1.02176685	-0.95599262	-0.18794422	H	-1.69459606	-0.78592075	-3.65396585
H	-0.55895088	0.97327315	-2.66700685				



The optimized conformers of (1*S*,4*S*,5*R*,8*S*,10*S*)-**2**.

Table S2. Free energy summary of conformer set in CH_3OH of compound **2**

	Conformer No.	Energy (kcal/mol)	Relative Energy (kcal/mol)	proportion of various comformations
(1*R*,4*R*,5*S*,8*R*,10*R*)-**2**	1	-853450.429268515	0.000000000	54.08%
	2	-853448.467707571	1.961560944	1.97%
	3	-853450.211465944	0.217802571	37.44%
	4	-853448.889081036	1.540187478	4.01%
	5	-853448.609319128	1.819949387	2.50%
(1*S*,4*S*,5*R*,8*S*,10*S*)-**2**	1	-853450.789001398	0.000000000	52.91%
	2	-853448.653527873	2.135473525	1.44%
	3	-853448.853062896	1.935938502	2.01%
	4	-853448.737593045	2.051408353	1.66%
	5	-853450.652061787	0.136939610	41.99%

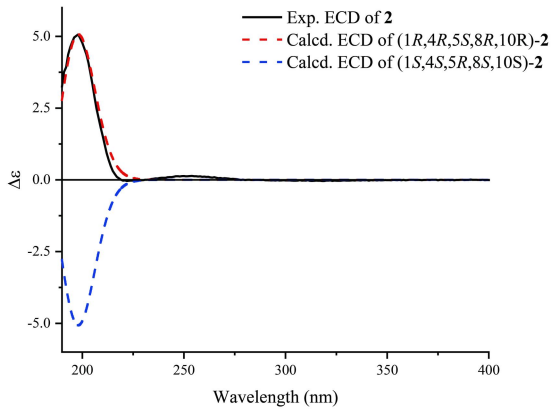


Figure S73. The experimental and calculated ECD spectra of **2** in CH_3OH

Table S3. Cartesian coordinates and geometries of optimized predominant conformers in CH_3OH for compound **3**

(1*R*,4*S*,5*S*,8*R*,10*S*)-**3** conformer 1				(1*R*,4*S*,5*S*,8*R*,10*S*)-**3** conformer 2			
C	2.67262958	-0.16784024	1.63772883	C	2.25611228	-1.20584295	1.88681614
C	2.14929885	-1.21482534	0.64732619	C	2.28819958	-1.18408597	0.34618137
C	0.77907515	-0.68292367	0.19930448	C	0.88418739	-0.65204384	0.02376163
C	0.30365030	0.32016633	1.30284825	C	0.46033082	0.26528824	1.22097306
C	1.41138517	0.27978361	2.38211381	C	1.58078051	0.11974694	2.27208082
C	-0.26691266	-1.74559378	-0.13719359	C	-0.16250329	-1.74137222	-0.23781933
C	-1.23177516	-0.98184594	-1.01091117	C	-1.25643379	-0.96326329	-0.92566339
C	-0.54530575	0.32479120	-1.39548405	C	-0.65375816	0.37288978	-1.34798726
C	-0.97787993	1.53064316	-0.54021737	C	-1.01254411	1.53715685	-0.40074930
C	-0.14056529	1.70066651	0.74792578	C	-0.05473637	1.66479855	0.80679030
C	3.10250205	-1.57261384	-0.48551715	C	3.43824447	-0.32936911	-0.18780142
C	-0.94366381	2.46412364	1.80831165	C	-0.74761307	2.34045226	1.99559985
O	-0.61131637	0.68428547	-2.73353506	O	-0.89705790	0.77465823	-2.65195554
O	0.86504936	0.02693829	-1.07478764	O	0.80003350	0.10481272	-1.21748149

S	1.25573725	2.90736372	0.34304076	S	1.25477778	2.93300590	0.30878837
C	-2.47064858	-1.34497048	-1.36329480	C	-2.52917959	-1.33559522	-1.10778594
C	-3.41125915	-0.48941425	-2.16667709	C	-3.02312305	-2.68634081	-0.67209180
C	-3.04432941	-2.67305646	-0.95554157	C	-3.58577439	-0.46902585	-1.73581735
O	2.12510190	3.12597429	1.51201066	O	0.56560529	4.20212884	0.01049664
O	0.65378739	4.11542990	-0.25293812	O	2.34636012	3.00470275	1.29739584
O	2.12286959	2.18346916	-0.80248176	O	1.84617993	2.39085493	-1.08449472
H	3.12479158	0.67038789	1.09479580	H	1.65333992	-2.05384690	2.23559514
H	3.43367061	-0.57946870	2.30868029	H	3.25816683	-1.30911761	2.31548750
H	1.92333671	-2.12810266	1.21884731	H	2.39306971	-2.19721016	-0.05979667
H	-0.63086126	-0.06446213	1.73165211	H	-0.44781786	-0.18354160	1.64934977
H	1.53131330	1.22522738	2.91360281	H	1.18272260	0.10753744	3.29073727
H	1.13941128	-0.48512483	3.11889093	H	2.29844254	0.93857768	2.20756011
H	0.21514917	-2.56818329	-0.68420554	H	0.26871109	-2.50410512	-0.90017054
H	-0.72284772	-2.15915107	0.76734832	H	-0.48311063	-2.23103389	0.68594512
H	-0.93614543	2.43965468	-1.14907789	H	-2.01891317	1.36387763	-0.00635072
H	-2.02195384	1.39393905	-0.24118194	H	-1.05028954	2.47149823	-0.97090729
H	3.40461161	-0.68039073	-1.04363301	H	3.40290163	-0.24381222	-1.27840198
H	2.64669979	-2.27731115	-1.18923386	H	3.43502290	0.68009510	0.23401176
H	4.00585203	-2.03803654	-0.07823564	H	4.38842531	-0.80100327	0.08280395
H	-1.80226315	1.84699789	2.09024429	H	-0.04792458	2.50715348	2.82018882
H	-1.31753512	3.41370339	1.41533487	H	-1.54084992	1.67376214	2.34760169
H	-0.34774563	2.65687405	2.70462956	H	-1.19796705	3.29353058	1.70746387
H	-0.57426127	-0.12563223	-3.26431431	H	-0.91688902	-0.01578546	-3.21223756

H	-4.37637997	-0.42496654	-1.64849998	H	-3.54482430	-3.18007348	-1.50152509
H	-3.61130939	-0.95596937	-3.14029231	H	-2.22284447	-3.34402996	-0.32779807
H	-3.03994874	0.52018286	-2.34411290	H	-3.75751169	-2.57789444	0.13720542
H	-3.46153357	-3.18612512	-1.83109610	H	-3.93188667	-0.91584596	-2.67701256
H	-3.87636467	-2.52719990	-0.25377832	H	-4.45936720	-0.42273618	-1.07315064
H	-2.30826249	-3.33014459	-0.48844590	H	-3.25035033	0.54678731	-1.94559346
H	1.68104572	1.26845037	-1.00494963	H	1.52025594	1.41735992	-1.21314229
(1*R*,4*S*,5*S*,8*R*,10*S*)-**3** conformer 3				(1*R*,4*S*,5*S*,8*R*,10*S*)-**3** conformer 4			
C	2.71574817	-0.10004984	1.61902101	C	2.41075439	-1.29823393	1.58104685
C	2.20298136	-1.12839140	0.60368689	C	2.35314800	-1.10634749	0.05300907
C	0.80539840	-0.62816095	0.20567641	C	0.91371299	-0.60531605	-0.13319918
C	0.32509736	0.32258016	1.35221291	C	0.52338712	0.15389406	1.17958593
C	1.45870287	0.28467005	2.40456760	C	1.70623833	-0.05527215	2.14790243
C	-0.21281004	-1.71321089	-0.14067383	C	-0.10250800	-1.70492858	-0.45875617
C	-1.22823978	-0.95439742	-0.95934713	C	-1.26930172	-0.90535520	-0.98133708
C	-0.58975517	0.37809173	-1.33122293	C	-0.74107418	0.48676569	-1.30533062
C	-1.03980913	1.54418797	-0.41904986	C	-1.08535459	1.53131374	-0.21369897
C	-0.17450080	1.70411890	0.85188865	C	-0.06760602	1.56582470	0.95229198
C	3.14079177	-1.41460250	-0.56189723	C	3.43843868	-0.15083880	-0.44474034
C	-0.97242816	2.41102550	1.95476689	C	-0.72205740	2.07763482	2.24061969
O	-0.71873172	0.65251526	-2.68392999	O	-1.09603146	0.88756694	-2.58312226
O	0.83660575	0.12194891	-1.04838375	O	0.72809107	0.27558999	-1.27831604
S	1.17299757	2.96679257	0.44997329	S	1.16282514	2.93718092	0.52974951
C	-2.47170713	-1.33767200	-1.26817807	C	-2.54070458	-1.30386361	-1.09803718

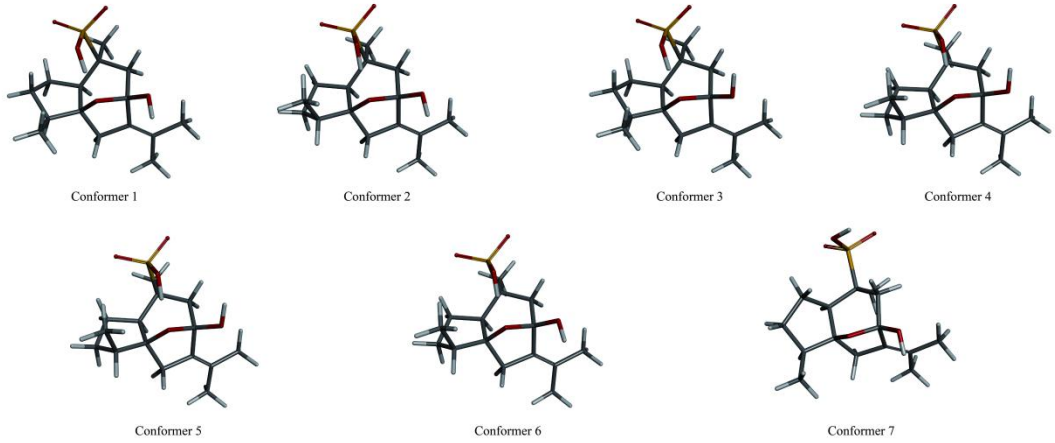
C	-2.99901553	-2.68798304	-0.86999464	C	-3.66931696	-0.42251911	-1.55633865
C	-3.46184860	-0.48850400	-2.01605335	C	-2.95977693	-2.70695359	-0.75749311
O	2.05890525	3.18253812	1.60668774	O	2.31531301	2.93835665	1.44891379
O	0.51841670	4.16841585	-0.10182811	O	0.41380677	4.20264777	0.42375343
O	2.03971655	2.30321006	-0.73283816	O	1.67672165	2.58340836	-0.95321317
H	3.13252899	0.76941186	1.09745905	H	1.86299961	-2.20602583	1.86350337
H	3.50242258	-0.51217984	2.25944880	H	3.43903319	-1.40178424	1.94227105
H	2.01970917	-2.06755577	1.14768105	H	2.47112909	-2.06317956	-0.46909265
H	-0.58636201	-0.10510851	1.79007451	H	-0.34060736	-0.38004961	1.60154378
H	1.56231369	1.21770921	2.96104056	H	2.38562388	0.79767025	2.13829495
H	1.22706751	-0.50871269	3.12478309	H	1.36731117	-0.19828938	3.17793099
H	0.28219090	-2.49814344	-0.73025788	H	-0.34047435	-2.31426239	0.41734637
H	-0.62739265	-2.17498196	0.76028652	H	0.31618997	-2.36244993	-1.23285359
H	-1.05896053	2.48497188	-0.98166535	H	-2.06334382	1.27714380	0.20699111
H	-2.06839406	1.35368719	-0.09634136	H	-1.18758154	2.52859547	-0.65874948
H	3.39889609	-0.49429432	-1.09592863	H	3.43085670	0.80458316	0.08901489
H	2.69319265	-2.11086534	-1.27910641	H	3.33353891	0.05480097	-1.51472542
H	4.06905589	-1.86104175	-0.19097044	H	4.41857976	-0.61168502	-0.28494510
H	-1.80763461	1.76198526	2.23534417	H	-1.45384953	1.33174576	2.56588839
H	-1.37975205	3.36281819	1.60265445	H	-1.24269674	3.02400993	2.07477001
H	-0.36015378	2.58950688	2.84289326	H	0.01419786	2.20755549	3.03983174
H	-0.46713239	1.57255759	-2.85127028	H	-0.90841259	1.83172236	-2.69022896
H	-2.23566535	-3.33179534	-0.42895361	H	-3.38216318	0.61986596	-1.69270397
H	-3.41782436	-3.19907264	-1.74616914	H	-4.49018375	-0.47297345	-0.82957125

H	-3.82151673	-2.57861482	-0.15064838	H	-4.07264371	-0.79040305	-2.50882075
H	-4.41167587	-0.46661441	-1.46680446	H	-3.53663387	-3.13679998	-1.58597634
H	-3.67780255	-0.93257026	-2.99665859	H	-3.62507738	-2.70236657	0.11623660
H	-3.12351705	0.53492958	-2.17749427	H	-2.11590191	-3.36656984	-0.54753929
H	1.62479085	1.37885043	-0.94868099	H	1.39750427	1.60949055	-1.16280634
(1*R*,4*S*,5*S*,8*R*,10*S*)-**3** conformer 5				(1*R*,4*S*,5*S*,8*R*,10*S*)-**3** conformer 6			
C	2.47566282	-1.28601726	1.34920584	C	2.26480378	-1.22984430	1.73805754
C	2.28530243	-1.13672639	-0.17290411	C	2.25381275	-1.09246775	0.20333120
C	0.82735773	-0.66070512	-0.24621351	C	0.82194966	-0.59678998	-0.04398476
C	0.54173974	0.13341212	1.07338424	C	0.39549682	0.21180034	1.22767783
C	1.80640398	-0.03499607	1.94071044	C	1.54829173	0.03420326	2.23831991
C	-0.19674009	-1.78246502	-0.44667088	C	-0.18750957	-1.70740430	-0.35846906
C	-1.41701264	-1.01293122	-0.88544786	C	-1.33102663	-0.92697194	-0.95708471
C	-0.93938108	0.37443216	-1.29844441	C	-0.79371621	0.45991748	-1.29571166
C	-1.19735380	1.45324206	-0.21718753	C	-1.17020883	1.53846576	-0.25803546
C	-0.08433605	1.53190817	0.85711030	C	-0.18377543	1.61615003	0.93085845
C	3.30780082	-0.17956884	-0.78671961	C	3.35427037	-0.15490118	-0.29491176
C	-0.63535698	2.07580126	2.18001342	C	-0.86766671	2.17741516	2.18268320
O	-1.41288186	0.72751491	-2.55218724	O	-1.08950295	0.94355952	-2.56063558
O	0.52847843	0.18183778	-1.39609924	O	0.67249431	0.24332794	-1.22290051
S	1.08945712	2.90231195	0.29073571	S	1.06288470	2.96832910	0.49236903
C	-2.68715942	-1.43183608	-0.88158386	C	-2.59244218	-1.33842812	-1.13382633
C	-3.05253763	-2.83176401	-0.47274332	C	-3.01796319	-2.73770732	-0.78799337
C	-3.86490064	-0.58045356	-1.26655561	C	-3.70187951	-0.47265934	-1.66430565

O	2.31660936	2.94422577	1.10674007	O	2.19066657	2.99748042	1.44179649
O	0.31752785	4.15615117	0.21231707	O	0.32246809	4.23218805	0.32441744
O	1.47716978	2.50598480	-1.21927174	O	1.61630043	2.56439731	-0.96347665
H	1.96326236	-2.19094834	1.69891574	H	3.28141827	-1.32321420	2.13344552
H	3.53189871	-1.37024670	1.62438881	H	1.70543955	-2.12562951	2.03585565
H	2.37279596	-2.10580342	-0.67820721	H	2.38708674	-2.06772360	-0.27974826
H	-0.27666860	-0.39613758	1.58276255	H	-0.48301619	-0.30341658	1.64289371
H	1.55994460	-0.15147777	2.99991999	H	2.23086992	0.88440690	2.21914995
H	2.47034548	0.82495884	1.84710234	H	1.17752694	-0.07088866	3.26193309
H	-0.34567299	-2.36733045	0.46514507	H	0.25509611	-2.40046549	-1.08662786
H	0.16024934	-2.45817078	-1.23589473	H	-0.46119865	-2.27696483	0.53410327
H	-1.34255496	2.43456060	-0.68542516	H	-2.15867449	1.29930589	0.14707241
H	-2.13488651	1.21117994	0.29346871	H	-1.25675142	2.50913518	-0.75781484
H	3.33018014	0.78861872	-0.27735711	H	3.32836284	0.81985558	0.20203989
H	3.10644523	-0.00236262	-1.84789909	H	3.28342472	0.01020448	-1.37463695
H	4.30573997	-0.62181364	-0.70254606	H	4.32916796	-0.60759159	-0.08688164
H	-1.33046630	1.33424436	2.58576436	H	-1.61278394	1.44853306	2.51617551
H	0.16195766	2.23543487	2.91243850	H	-0.15020091	2.33035144	2.99475122
H	-1.17735125	3.01283301	2.03006646	H	-1.37682240	3.12091506	1.97102036
H	-1.24711125	1.66913356	-2.70687867	H	-1.09027316	0.19556522	-3.17683126
H	-2.18282178	-3.46624273	-0.29294565	H	-2.18034912	-3.38629942	-0.52511596
H	-3.66622046	-2.81420941	0.43766919	H	-3.72412698	-2.72119360	0.05289521
H	-3.66587099	-3.30025131	-1.25284751	H	-3.55217388	-3.18708169	-1.63442636
H	-4.61766088	-0.61611865	-0.46862380	H	-4.06149278	-0.86344556	-2.62515674

H	-4.34478585	-0.98621613	-2.16671520	H	-3.41386050	0.56891815	-1.80775660
H	-3.60624427	0.45985957	-1.46238987	H	-4.55427941	-0.51128656	-0.97411070
H	1.18694678	1.52494748	-1.37399983	H	1.33696280	1.58695017	-1.14920419
(1*R*,4*S*,5*S*,8*R*,10*S*)-**3** conformer 7							
C	3.14165513	-0.54405401	1.21924580	H	1.72868013	-2.12646853	1.68949214
C	2.09442525	-1.60641772	0.79316778	H	0.69240888	0.26544096	2.14698675
C	0.89600670	-0.80541245	0.27660123	H	2.76582070	1.54837497	1.80823622
C	0.95404861	0.51070064	1.10869061	H	2.70610343	1.24913123	0.06825439
C	2.45968116	0.82800182	1.04604076	H	-0.96153656	-1.51571356	1.20847084
C	-0.44796312	-1.54013468	0.24128935	H	-0.27425267	-2.59481357	-0.01138545
C	-1.18500322	-0.82331540	-0.86830952	H	0.61686773	2.09030392	-1.41885232
C	-0.17291556	0.13295865	-1.49500794	H	-1.14979961	2.05315961	-1.21531495
C	-0.21286022	1.56270202	-0.93425650	H	3.03578282	-2.16712251	-1.08008293
C	-0.06198796	1.56118813	0.60072387	H	1.84871844	-3.35088941	-0.49816125
C	2.62749917	-2.64668996	-0.18527814	H	3.42983238	-3.22343713	0.28715833
C	-1.41901401	1.42060591	1.31566140	H	-1.85406816	0.45257692	1.06743751
O	-0.19987238	0.23649295	-2.88649098	H	-2.11939926	2.19183456	0.98462559
O	1.09304920	-0.44106717	-1.10446817	H	-1.29773381	1.47876046	2.40116802
S	0.44648458	3.29039457	1.11251522	H	-0.38686485	-0.64425607	-3.24277164
C	-2.47047203	-0.97715789	-1.20698751	H	-4.08635252	0.28596930	-1.79568744
C	-3.18704276	-0.15702053	-2.24364029	H	-3.53357148	-0.79625435	-3.06643074
C	-3.34363697	-1.97883234	-0.50287020	H	-2.57417643	0.64119140	-2.66162261
O	0.83752626	3.28078704	2.52680146	H	-3.94076562	-2.54272144	-1.22994263
O	-0.57548160	4.24321285	0.64742220	H	-4.05665190	-1.46046903	0.15354074

O	1.83129409	3.63795301	0.29930543	H	-2.77377977	-2.68597921	0.10358000
H	3.44312742	-0.70167496	2.26014762	H	1.60640377	4.10324784	-0.52759127
H	4.04678659	-0.61308686	0.60658923				



The optimized conformers of (1*R*,4*S*,5*S*,8*R*,10*S*)-**3**.

(1*S*,4*R*,5*R*,8*S*,10*R*)-**3** conformer 1				(1*S*,4*R*,5*R*,8*S*,10*R*)-**3** conformer 2			
C	1.17135303	-2.00110209	2.13232099	C	0.06859636	-2.39755771	2.05905948
C	-0.16503556	-1.25203414	2.19961682	C	-0.20203696	-0.92292729	2.41554225
C	-0.26240387	-0.49697220	0.86479292	C	-0.27489564	-0.28249143	1.02035165
C	0.70445242	-1.21796477	-0.13312127	C	0.63799371	-1.13988152	0.07829722
C	1.27460969	-2.41617602	0.66152588	C	1.11506607	-2.33011750	0.93623521
C	-1.67271490	-0.32240797	0.30363177	C	-1.69530765	-0.15618436	0.45727215
C	-1.49252940	0.83085365	-0.65219820	C	-1.50606089	0.85598140	-0.64461766
C	-0.14348781	1.46824045	-0.33235045	C	-0.14465664	1.50653668	-0.42278197
C	0.98865496	1.04235803	-1.28472033	C	0.96546580	0.94130381	-1.33260308
C	1.69702741	-0.26179923	-0.84973164	C	1.65075578	-0.32005949	-0.75719154
C	-0.36842858	-0.39404761	3.44126865	C	0.87776306	-0.35069093	3.33518544
C	2.32088712	-0.95843687	-2.06505812	C	2.23587753	-1.19216135	-1.87413193
O	-0.13048101	2.85040381	-0.21812785	O	-0.10559282	2.89007089	-0.48758264

O	0.15165207	0.89828403	0.99797815	O	0.15718444	1.10672910	0.97538411
S	3.21043971	0.24578695	0.15911696	S	3.19283294	0.28985671	0.15037932
C	-2.32160161	1.21234780	-1.63096495	C	-2.34395090	1.12829979	-1.65206577
C	-3.64371200	0.53220296	-1.85057446	C	-3.67899656	0.44767263	-1.76842691
C	-2.03150931	2.31860505	-2.60785503	C	-2.05280467	2.10358912	-2.75898587
O	3.98244961	1.21832256	-0.63789214	O	4.03044375	1.01804351	-0.82084083
O	3.95254220	-0.93375757	0.63680240	O	3.85724376	-0.79927395	0.88986712
O	2.62156318	1.02563993	1.43767490	O	2.64717828	1.37537817	1.20176133
H	1.99308828	-1.32998685	2.40779811	H	-0.85211930	-2.86760817	1.69121037
H	1.19855513	-2.85738327	2.81420294	H	0.41511929	-2.97069008	2.92507699
H	-0.96872967	-2.00266022	2.15541225	H	-1.17227174	-0.81068019	2.91372420
H	0.10603580	-1.59416689	-0.97310422	H	-0.01759199	-1.54512418	-0.70640043
H	2.28462269	-2.69557047	0.35720467	H	1.16968891	-3.25491918	0.35481476
H	0.62276230	-3.28026071	0.48688078	H	2.10427975	-2.14455263	1.35617541
H	-2.36047968	-0.07181371	1.12367276	H	-2.36126481	0.22424612	1.24346342
H	-2.02926898	-1.24037375	-0.17291789	H	-2.08631731	-1.11799357	0.11349153
H	1.71090083	1.86012376	-1.37740374	H	0.51963255	0.66615450	-2.29375870
H	0.56566420	0.87461662	-2.28021451	H	1.70197345	1.72573728	-1.53673610
H	-1.31782267	0.15086258	3.40460575	H	0.73984047	0.72260401	3.49952242
H	0.43999461	0.33550429	3.55465293	H	1.88632646	-0.50803294	2.94113940
H	-0.37761255	-1.02862618	4.33338805	H	0.81848546	-0.85077958	4.30721971
H	2.98257692	-0.28161122	-2.61269213	H	2.79157849	-2.04083093	-1.46414527
H	1.50856562	-1.26040020	-2.73291208	H	1.40394037	-1.58114029	-2.46912366
H	2.88175325	-1.85141875	-1.77606992	H	2.89195620	-0.61609361	-2.53158798

H	-0.97477133	3.12726065	0.16842593	H	-0.93888990	3.23235602	-0.13077084
H	-3.64497393	0.01089297	-2.81711970	H	-3.69467727	-0.20568681	-2.65101284
H	-4.44624599	1.27891387	-1.89836318	H	-4.46894625	1.19408793	-1.91847215
H	-3.88896493	-0.18802025	-1.06785873	H	-3.93159831	-0.15052157	-0.89096195
H	-2.75161238	3.13716817	-2.47850588	H	-2.74823233	2.95161523	-2.70886818
H	-2.16627045	1.94432252	-3.63071145	H	-2.22476630	1.61656225	-3.72725146
H	-1.02697008	2.73203371	-2.51558609	H	-1.03613873	2.49651170	-2.73912340
H	1.58837562	1.04294658	1.35118032	H	1.61329409	1.30996243	1.22326768
(1*S*,4*R*,5*R*,8*S*,10*R*)-**3** conformer 3				(1*S*,4*R*,5*R*,8*S*,10*R*)-**3** conformer 4			
C	1.00220400	-1.66536156	2.45475652	C	0.12130157	-2.63795419	1.65691296
C	-0.31263165	-0.87803677	2.40040448	C	-0.29643971	-1.25961576	2.20616084
C	-0.38156312	-0.32574474	0.96613212	C	-0.33606662	-0.42210304	0.91927175
C	0.56840626	-1.22154812	0.09911174	C	0.71072567	-1.04830750	-0.06354448
C	1.08561835	-2.30911143	1.06780215	C	1.22616668	-2.32274852	0.63596723
C	-1.78369606	-0.22921458	0.35363770	C	-1.72157180	-0.32812987	0.26945440
C	-1.54207432	0.75460276	-0.76427629	C	-1.54848958	0.84541891	-0.66189836
C	-0.18736760	1.41042563	-0.46653322	C	-0.27439991	1.56760565	-0.23652922
C	0.97001332	0.86420480	-1.32221502	C	0.94739941	1.24142442	-1.12061657
C	1.60406931	-0.41612393	-0.73361643	C	1.70433871	-0.03158968	-0.67410605
C	-0.48204166	0.16731237	3.49426419	C	0.67139533	-0.75535208	3.27693188
C	2.16662027	-1.30628078	-1.84978123	C	2.45200790	-0.66942473	-1.85109050
O	-0.16736982	2.80647678	-0.56342701	O	-0.36322920	2.94368298	-0.09887562
O	0.06291586	1.03912959	0.90138839	O	-0.03474387	0.98915246	1.11032089
S	3.13571846	0.08748321	0.26145773	S	3.10871141	0.55832134	0.44628031

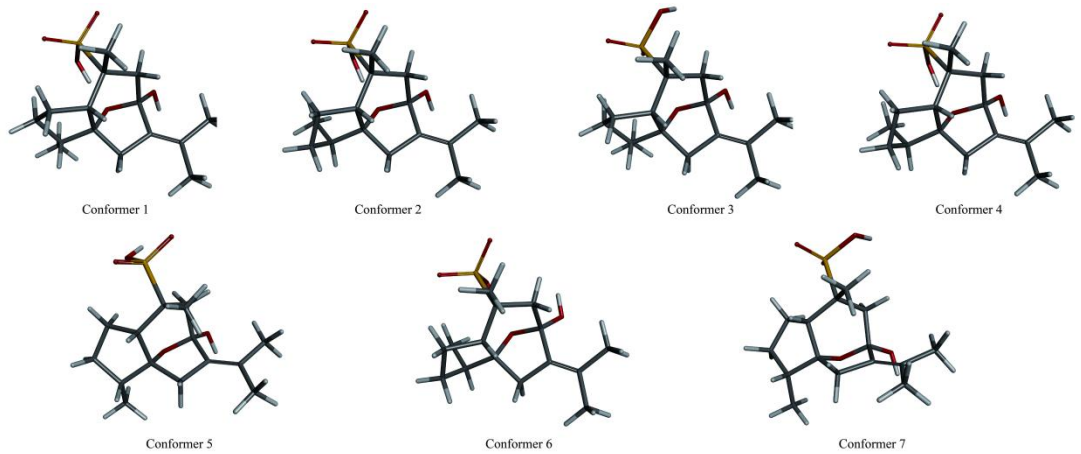
C	-2.32416577	0.99589443	-1.82319189	C	-2.33128504	1.18816248	-1.69192407
C	-3.65552075	0.31740868	-1.99327874	C	-2.05355044	2.33333175	-2.62650008
C	-1.96706855	1.93339937	-2.94439170	C	-3.58332742	0.42243639	-2.01550199
O	3.90133095	-1.11620404	0.61040564	O	3.96830317	1.45790144	-0.34492582
O	2.89345651	1.10246155	1.29517538	O	3.78756556	-0.56884532	1.11168828
O	4.05207506	0.81298365	-0.91025292	O	2.39262866	1.46719208	1.56223494
H	1.84112007	-0.97801144	2.62296599	H	0.46139547	-3.30923797	2.45208998
H	1.01199668	-2.40402276	3.26345448	H	-0.73183172	-3.11465004	1.15789496
H	-1.13605795	-1.60496276	2.47503757	H	-1.30232209	-1.29785542	2.64059760
H	-0.02871523	-1.69739161	-0.68980769	H	0.14962280	-1.36667398	-0.95414249
H	2.07892959	-2.68313535	0.81368614	H	2.17068309	-2.13945243	1.14966442
H	0.39249850	-3.15788906	1.02609523	H	1.38747462	-3.13932777	-0.07358960
H	-2.47761875	0.16839722	1.10847932	H	-2.46915467	-0.11960993	1.04667134
H	-2.16128135	-1.20104915	0.02063364	H	-2.00131666	-1.25712254	-0.23515362
H	1.71250544	1.65842172	-1.44979227	H	0.60004207	1.07488780	-2.14523400
H	0.60367973	0.62042531	-2.32474484	H	1.61871701	2.10636557	-1.14762292
H	-1.41634830	0.72680624	3.37540636	H	0.42963282	0.26471364	3.59167188
H	0.34635153	0.88221988	3.47889155	H	1.71208219	-0.77147392	2.93903017
H	-0.49970904	-0.31619349	4.47684787	H	0.59799680	-1.40429491	4.15563679
H	2.87889780	-0.76666568	-2.47856249	H	3.08301656	0.05980159	-2.36525662
H	1.32463276	-1.61572994	-2.47658033	H	1.70722578	-1.04493392	-2.55941925
H	2.64681723	-2.20225659	-1.44913282	H	3.06998097	-1.51137536	-1.52414988
H	-1.01734899	3.13389656	-0.23536752	H	-1.24849263	3.15770538	0.23206691
H	-3.63379964	-0.34930842	-2.86599424	H	-2.82932886	3.10330055	-2.52284557

H	-4.43686364	1.06245903	-2.19026719	H	-2.10576735	1.97746786	-3.66331735
H	-3.94923434	-0.26736195	-1.11938546	H	-1.08365608	2.80501640	-2.46629037
H	-2.68367581	2.76426436	-2.98858321	H	-3.47404287	-0.09077943	-2.98021780
H	-2.04608493	1.40468252	-3.90333965	H	-4.42831960	1.11382482	-2.12385880
H	-0.96536749	2.35398520	-2.85561995	H	-3.83859755	-0.31857589	-1.25588267
H	3.95564710	1.77926331	-0.83499206	H	1.37351946	1.29712070	1.50404619
(1*S*,4*R*,5*R*,8*S*,10*R*)-**3** conformer 5				(1*S*,4*R*,5*R*,8*S*,10*R*)-**3** conformer 6			
C	0.81561331	-1.78496589	2.84039611	C	-0.07347095	-2.06956714	2.37917686
C	-0.60458833	-1.51995488	2.27449649	C	-0.27536822	-0.54803911	2.52148549
C	-0.39008495	-0.63674606	1.04071434	C	-0.31358039	-0.11166970	1.04971224
C	1.02588385	-1.05004994	0.53725170	C	0.57306952	-1.12721345	0.25208244
C	1.79905061	-1.10663288	1.86745219	C	0.98221551	-2.21102311	1.27106514
C	-1.51921244	-0.63162487	0.00534698	C	-1.72085791	-0.01772843	0.44962292
C	-1.36531089	0.72684362	-0.64221830	C	-1.47622150	0.80655138	-0.78972078
C	-0.29939462	1.46001450	0.16842407	C	-0.10535655	1.45245747	-0.62753192
C	1.12408971	1.35104542	-0.39777752	C	1.00308871	0.72093718	-1.42696033
C	1.53064052	-0.12328027	-0.59416648	C	1.63235884	-0.47045788	-0.66432496
C	-1.58081625	-0.94596417	3.29519308	C	0.83167368	0.09700821	3.35624320
C	1.12448371	-0.65760434	-1.98066903	C	2.20449398	-1.50610426	-1.63871472
O	-0.53893302	2.81135418	0.42285187	O	-0.14677111	2.81713462	-0.86474950
O	-0.31125254	0.75073098	1.42561439	O	0.16689804	1.24335513	0.81498488
S	3.39982703	-0.17456721	-0.71670063	S	3.17842515	0.21099197	0.18632893
C	-2.01293719	1.17908890	-1.72242045	C	-2.27037331	0.92426909	-1.85934426
C	-1.74031629	2.49599015	-2.39522288	C	-3.61312709	0.25064625	-1.92144874

C	-3.06271584	0.34618954	-2.40485246	C	-1.92333682	1.71000788	-3.09315728
O	3.84680021	-1.57156366	-0.67092574	O	4.08143680	0.72604502	-0.85929435
O	3.82714147	0.68831279	-1.83099161	O	3.75994451	-0.76621548	1.12480615
O	3.98477693	0.49596283	0.66432655	O	2.66055776	1.48813420	1.01503679
H	0.92183066	-1.38238943	3.85330155	H	0.23800248	-2.53169817	3.32145076
H	1.00797315	-2.86157081	2.89807584	H	-1.01400259	-2.54110279	2.06795752
H	-1.01842534	-2.46236094	1.88968443	H	-1.23985687	-0.32001615	2.99040800
H	0.95885733	-2.06865372	0.13117439	H	-0.08998738	-1.60382500	-0.48449172
H	2.02314971	-0.09189912	2.20604278	H	1.97826296	-2.02150027	1.67236991
H	2.74331186	-1.64915034	1.77973092	H	0.98938909	-3.20850137	0.82242501
H	-2.48196227	-0.71822431	0.52701600	H	-2.37948730	0.50244844	1.15836906
H	-1.44919109	-1.47092216	-0.69504870	H	-2.14504438	-1.00476194	0.24654903
H	1.19532447	1.88487892	-1.35021497	H	0.55871506	0.32574543	-2.34577199
H	1.76976326	1.85188118	0.33306188	H	1.78212865	1.42867624	-1.73452412
H	-2.55533400	-0.72102883	2.84773835	H	0.73893625	1.18741428	3.37597712
H	-1.18568652	-0.02569461	3.73606065	H	0.75820556	-0.26586433	4.38652656
H	-1.74117618	-1.66816453	4.10278603	H	1.83041855	-0.15440489	2.98656989
H	1.51435516	-0.01869861	-2.77737886	H	1.36684620	-1.95854409	-2.17821480
H	0.03739436	-0.65857452	-2.06230100	H	2.87424241	-1.04039393	-2.36591866
H	1.48222245	-1.68110157	-2.12587816	H	2.74255909	-2.29947722	-1.11089179
H	-1.48982910	2.91725561	0.57217647	H	0.75565529	3.16187133	-0.93757606
H	-1.53283412	2.32169106	-3.45924973	H	-3.89851656	-0.22322156	-0.98043514
H	-2.62916501	3.13934352	-2.35414783	H	-3.61772430	-0.51181631	-2.71174082
H	-0.90201315	3.03873252	-1.95917498	H	-4.38679090	0.98124927	-2.18915911

H	-3.94855680	0.95499380	-2.62406443	H	-2.06620116	1.07947255	-3.98007569
H	-2.68633917	-0.01792817	-3.37103973	H	-0.90394828	2.09532628	-3.09375229
H	-3.37228936	-0.51715792	-1.81196410	H	-2.60767990	2.56147468	-3.20258187
H	4.16057470	1.44226422	0.50929051	H	1.62727938	1.44112968	1.05623299
(1*S*,4*R*,5*R*,8*S*,10*R*)-**3** conformer 7							
C	0.90535332	-1.41457971	3.00037554	H	-0.89578192	-2.24932729	2.11835270
C	-0.51867181	-1.25852181	2.40862989	H	0.96655998	-2.04671280	0.29026243
C	-0.32230827	-0.50201631	1.09312948	H	2.78629422	-1.56319634	1.85413734
C	1.06881908	-0.99781350	0.59989781	H	2.20166495	0.08447442	2.09933817
C	1.88634548	-0.94376315	1.90503920	H	-2.42726791	-0.57750815	0.62866759
C	-1.47342995	-0.56637764	0.08436427	H	-1.43840306	-1.47063895	-0.53271726
C	-1.29828134	0.71959117	-0.69268661	H	1.88560273	1.84517110	0.10997065
C	-0.20194352	1.50052783	0.02754422	H	1.26164941	1.74850828	-1.55399104
C	1.20376471	1.30289448	-0.55517928	H	-1.16569851	0.36171962	3.69689172
C	1.57317827	-0.19301749	-0.62774877	H	-2.50485712	-0.49615213	2.90811774
C	-1.51772237	-0.62040269	3.36668832	H	-1.63824033	-1.25310070	4.25259578
C	1.13668890	-0.85113048	-1.94375615	H	1.49336868	-0.28381447	-2.80629612
O	-0.40567830	2.87495895	0.15826030	H	0.04750909	-0.87500023	-1.99107880
O	-0.20134176	0.91192536	1.34570163	H	1.50524917	-1.87852939	-2.00601100
S	3.44669208	-0.28176985	-0.65934909	H	-1.35002448	3.01801376	0.31738350
C	-1.94581248	1.08029744	-1.80686763	H	-2.64951382	-0.26876425	-3.31869992
C	-3.01818573	0.20868119	-2.39992756	H	-3.35401922	-0.57630168	-1.71887050
C	-1.64814839	2.31918891	-2.60539955	H	-3.88551596	0.81465664	-2.68944705
O	3.86039367	-1.68330593	-0.79053041	H	-2.52050189	2.98590184	-2.61977579

O	4.06043500	0.56255260	0.37646190	H	-0.79292787	2.88007934	-2.22937037
O	3.82020358	0.38656676	-2.11931988	H	-1.45589494	2.03795931	-3.64924257
H	1.01766615	-0.81043154	3.90683410	H	3.91387674	1.35155997	-2.01536086
H	1.09275575	-2.45605252	3.28088193				



The optimized conformers of (1*S*,4*R*,5*R*,8*S*,10*R*)-**3**.

Table S4. Free energy summary of conformer set in CH_3OH of compound **3**

	Conformer No.	Energy (kcal/mol)	Relative Energy (kcal/mol)	proportion of various comformations
(1*R*,4*S*,5*S*,8*R*,10*S*)-**3**	1	-853452.210183097	0.000000000	70.47%
	2	-853449.382900194	2.827282903	0.59%
	3	-853451.344381456	0.865801641	16.33%
	4	-853448.541342915	3.668840182	0.14%
	5	-853448.389812191	3.820370907	0.11%
	6	-853449.399599683	2.810583414	0.61%
	7	-853451.148691529	1.061491569	11.73%
(1*S*,4*R*,5*R*,8*S*,10*R*)-**3**	1	-853452.242976887	0.000000000	68.17%
	2	-853446.094618372	6.148358515	0.77%
	3	-853446.995470734	5.247506153	0.01%

	4	-853449.491739704	2.751237183	0.65%
	5	-853450.883541530	1.359435357	6.86%
	6	-853448.303354657	3.939622230	0.09%
	7	-853451.610992850	0.631984037	23.45%

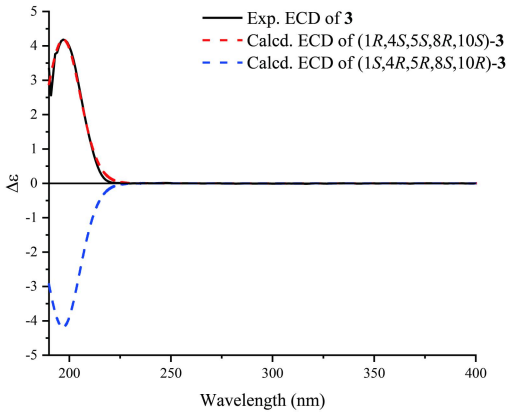


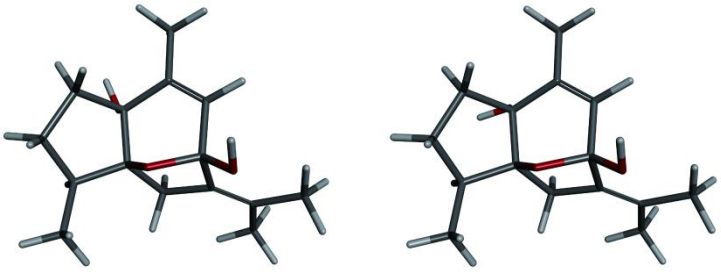
Figure S74. The experimental and calculated ECD spectra of **3** in CH_3OH

Table S5. Cartesian coordinates and geometries of optimized predominant conformers in CH_3OH for compound **4**

(1*R*,4*S*,5*S*,8*R*)-**4** conformer 1				(1*R*,4*S*,5*S*,8*R*)-**4** conformer 2			
C	-3.20146988	0.54316912	-0.51533896	C	-3.19182445	0.55508970	-0.37454443
C	-2.32244819	-0.71864476	-0.64882844	C	-2.34988443	-0.71297252	-0.60834433
C	-0.92122861	-0.24564011	-0.26518262	C	-0.93322747	-0.26240204	-0.25943037
C	-0.83328430	1.18256410	-0.85975476	C	-0.83539777	1.16367507	-0.87882124
C	-2.25081697	1.75882301	-0.63945908	C	-2.26048743	1.75225232	-0.68066081
C	-2.84333460	-1.91270402	0.14085546	C	-2.85789878	-1.93528343	0.14461247
O	-0.55837891	1.01431381	-2.26521718	O	-0.49497420	1.08969007	-2.27672715
C	0.25308437	-1.17674604	-0.60138506	C	0.23041415	-1.20331769	-0.59452710
C	1.24982466	-0.90838038	0.50799897	C	1.24081534	-0.91895313	0.49952568

C	0.58686363	0.14558316	1.38496873	C	0.58408810	0.13984330	1.37712388
C	0.91905742	1.52018720	0.84944824	C	0.90818663	1.51321580	0.83460701
C	0.25865555	2.01113061	-0.20395342	C	0.25208066	1.99444575	-0.22572491
C	2.47133202	-1.44079393	0.63004598	C	2.46780651	-1.44120195	0.60956983
C	3.47776936	-1.05695226	1.68033023	C	3.48487429	-1.03936051	1.64278129
O	0.85169364	-0.00644203	2.74547227	O	0.86103725	-0.00648980	2.73620142
O	-0.82478187	-0.09211922	1.16363660	O	-0.82748172	-0.09716727	1.16931666
C	0.54205400	3.35850091	-0.79391506	C	0.53512512	3.33863983	-0.82244293
C	2.96976687	-2.47559903	-0.34305885	C	2.96145520	-2.48205739	-0.35938254
H	-3.99344112	0.55548772	-1.27038883	H	-3.51025195	0.58145379	0.67362373
H	-3.69018415	0.54675911	0.46546573	H	-4.09656622	0.56025305	-0.99048660
H	-2.25577885	-0.99518456	-1.71007484	H	-2.33783102	-0.94430176	-1.68513475
H	-2.51993714	2.42966486	-1.46279377	H	-2.26369490	2.47427061	0.14130324
H	-2.26285755	2.35644517	0.27753775	H	-2.55524242	2.29433637	-1.58544479
H	-2.91423438	-1.67281851	1.20646961	H	-2.23814731	-2.81849302	-0.04315155
H	-2.19842228	-2.79095897	0.02791384	H	-3.87942848	-2.17277194	-0.17141885
H	-3.84344024	-2.18750904	-0.21173203	H	-2.87184374	-1.74671211	1.22267381
H	-0.79714804	1.83270342	-2.71879205	H	-1.27007451	0.77758639	-2.76117407
H	-0.09288201	-2.21790937	-0.57908558	H	0.62087245	-1.02154815	-1.60014463
H	0.65679840	-0.98423064	-1.59942266	H	-0.11521238	-2.24390613	-0.55332041
H	1.74709087	2.05647774	1.31171999	H	1.72447077	2.06284782	1.30144798
H	4.43982827	-0.83970424	1.19814169	H	4.43327303	-0.80051290	1.14387351
H	3.65765381	-1.89404057	2.36839556	H	3.69490882	-1.87476193	2.32429428
H	3.17475063	-0.19068256	2.26750323	H	3.17453697	-0.18130165	2.23802064

H	0.56956118	0.80215832	3.19679668	H	0.57722520	0.80131010	3.18786066
H	-0.36794346	3.97197651	-0.82019609	H	1.27091646	3.88533806	-0.22664658
H	0.89521659	3.26950801	-1.82887558	H	-0.38199396	3.93801539	-0.88434249
H	1.30279131	3.88995052	-0.21624157	H	0.91312018	3.23834836	-1.84589897
H	3.41356217	-3.32145537	0.19745200	H	3.76022461	-2.06743102	-0.98970691
H	3.76661604	-2.05480047	-0.97182011	H	3.40174841	-3.32742509	0.18489042
H	2.18424175	-2.85718722	-0.99883604	H	2.17408300	-2.86324035	-1.01305012



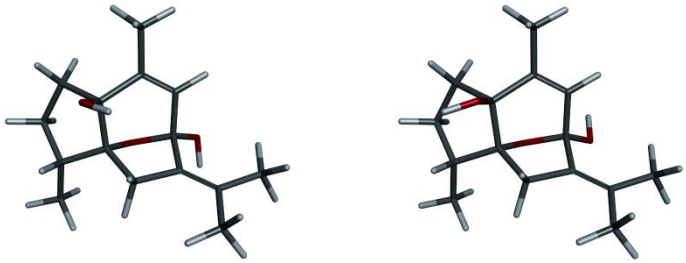
Conformer 1 Conformer 2

The optimized conformers of (1*R*,4*S*,5*S*,8*R*)-**4**.

(1*S*,4*R*,5*R*,8*S*)-**4** conformer 1				(1*S*,4*R*,5*R*,8*S*)-**4** conformer 2			
C	3.20220069	-0.22707097	0.52500187	C	3.20251936	-0.20714248	0.57176511
C	2.08565458	-1.27744568	0.64202977	C	2.08863266	-1.26660087	0.65675236
C	0.83474973	-0.50429082	0.23316373	C	0.83999973	-0.49556815	0.23612538
C	1.31060184	0.36614025	-0.97011177	C	1.33053854	0.38368256	-0.95295024
C	2.78097733	0.71403939	-0.62615740	C	2.78464706	0.76644313	-0.55620988
H	3.26756670	0.33036498	1.46662000	H	3.26044265	0.32448443	1.52817619
H	4.17898206	-0.68925308	0.35073652	H	4.18157646	-0.66175711	0.39105580
H	2.23048787	-2.04015858	-0.13702998	H	2.25368395	-2.02700635	-0.12301997
C	2.02205696	-1.95706618	2.00330611	C	2.00590764	-1.96526738	2.00738272
O	1.35766854	-0.42228123	-2.17702936	O	1.30880746	-0.36424353	-2.18374528

C	-0.45905232	-1.29987165	0.01101869	C	-0.44844449	-1.28494084	-0.02441997
H	-1.23907383	2.69053276	-0.46832913	H	-1.25056158	2.67073095	-0.47878599
C	-1.54310779	-0.31430707	0.39242313	C	-1.54259977	-0.32005070	0.38817384
H	3.39159212	0.57335624	-1.52294799	H	2.82680585	1.80548856	-0.21622436
H	2.86831059	1.76411585	-0.33250579	H	3.43004753	0.69050404	-1.43776958
C	-0.80237269	0.94196419	0.85066141	C	-0.80916756	0.93100848	0.85729840
C	-0.55856815	1.85339685	-0.32471307	C	-0.56093769	1.84209296	-0.32339284
C	0.43229492	1.58720565	-1.18143267	C	0.43422561	1.58612302	-1.17804121
H	-0.46578457	-2.17222556	0.67695389	H	-0.52278204	-1.60028004	-1.06951008
H	-0.55748690	-1.68360655	-1.00988348	H	-0.46051195	-2.18857076	0.59805350
C	-2.86526191	-0.49776618	0.29381849	C	-2.86192828	-0.51640794	0.28280032
C	-3.43732983	-1.81106920	-0.16700799	C	-3.41564055	-1.82493899	-0.21441413
O	-1.36336510	1.66679048	1.90074512	O	-1.42002071	1.56671745	1.93788313
O	0.47444190	0.41601957	1.28335966	O	0.46866435	0.41311417	1.29236997
H	0.45039359	-0.57057632	-2.47656268	H	2.03728186	-0.99829876	-2.16777085
H	-1.69912572	1.03007450	2.54855815	H	-1.01487112	2.43994154	2.03942703
H	1.22085194	-2.70204054	2.05252048	H	1.20679348	-2.71358319	2.03109709
C	0.72862294	2.44066889	-2.37756704	C	0.72393245	2.43769179	-2.37564466
H	1.85666863	-1.22132869	2.79677512	H	1.82253844	-1.24024241	2.80653074
H	2.96655166	-2.47205207	2.20994595	H	2.94914467	-2.47837693	2.22385447
H	1.77230218	2.77922299	-2.36399699	H	0.07811702	3.31964067	-2.39662296
H	0.59468302	1.87642044	-3.30763781	H	0.57630954	1.86985591	-3.30093255
H	0.07745677	3.31845152	-2.40433485	H	1.77028706	2.76826403	-2.37358939
C	-3.90094838	0.55756853	0.57466484	C	-3.91343895	0.51570225	0.58728448

H	-4.59055559	0.62233703	-0.27690005	H	-3.49708747	1.50145827	0.79159925
H	-4.50972179	0.28105656	1.44603777	H	-4.51771263	0.20967929	1.45192244
H	-3.47159369	1.54366106	0.75217322	H	-4.60392329	0.59049672	-0.26301022
H	-4.24493545	-2.12996932	0.50415436	H	-4.22086178	-2.17228708	0.44554763
H	-3.88520451	-1.70211067	-1.16436588	H	-3.86250752	-1.69578825	-1.20992403
H	-2.69092832	-2.60699738	-0.21325434	H	-2.65890600	-2.60966847	-0.28002165



Conformer 1 Conformer 2

The optimized conformers of (1*R*,4*S*,5*S*,8*R*)-**4**.

Table S6. Free energy summary of conformer set in CH_3OH of compound **4**

	Conformer No.	Energy (kcal/mol)	Relative Energy (kcal/mol)	proportion of various comformations
(1*R*,4*S*,5*S*,8*R*)-**4**	1	-508408.497722229	0.000000000	53.93%
	2	-508408.404415560	0.093306668	46.07%
(1*S*,4*R*,5*R*,8*S*)-**4**	1	-508409.294816700	0.000000000	86.60%
	2	-508408.190018030	1.104798669	13.40%

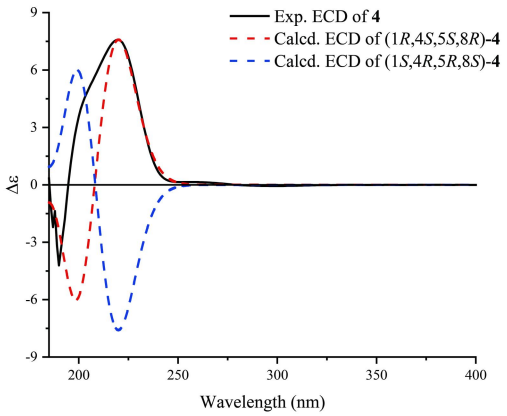


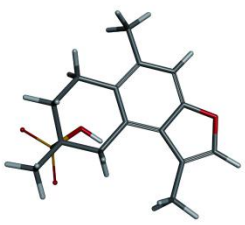
Figure S75. The experimental and calculated ECD spectra of **4** in CH_3OH

Table S7. Cartesian coordinates and geometries of optimized predominant conformers in CH_3OH for compound **5**

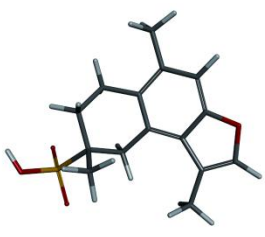
(2*R*)-**5** conformer 1				(2*R*)-**5** conformer 2			
C	0.03659926	2.57816826	0.00310188	C	0.72282667	2.14551082	0.09385248
C	-0.12047408	1.85425140	-1.32959713	C	0.35618082	1.36887510	-1.19554495
C	-0.82452325	0.51217601	-1.13064103	C	0.68095384	-0.14295486	-1.06941635
C	-0.44922335	-0.25010483	0.12047796	C	0.18899732	-0.65923740	0.25527836
C	0.27096176	0.32989605	1.16972555	C	0.61209672	0.03154368	1.39619022
C	0.73793489	1.76393811	1.08386979	C	1.43746691	1.26383263	1.13047283
C	-0.84963257	-1.59641537	0.24436903	C	-0.63784577	-1.78265761	0.40479697
C	-0.49595142	-2.29653656	1.40314405	C	-0.98712513	-2.16368976	1.70945529
C	0.23475673	-1.75384977	2.44428170	C	-0.57330508	-1.50608124	2.85300704
C	0.62426182	-0.42317907	2.32244447	C	0.23866840	-0.38086120	2.69542475
C	-1.59663593	-2.53746979	-0.57008590	C	-1.28805853	-2.73558249	-0.47292878
C	-1.62849607	-3.68814168	0.14681310	C	-1.95321269	-3.58505384	0.34814162
O	-0.96692129	-3.58077062	1.35338718	O	-1.79334665	-3.27102686	1.68323578
C	1.43300586	0.20655374	3.42493016	C	0.70313306	0.37045599	3.91563642

C	-2.22948279	-2.34953635	-1.91231666	C	-1.27198383	-2.81089682	-1.96520992
C	-0.86641103	2.72183666	-2.34822358	C	-1.10150607	1.57439440	-1.59984106
S	1.54643937	1.56624273	-2.11481990	S	1.42713087	1.95787466	-2.58393989
O	1.35186576	1.03900549	-3.47472921	O	1.07623119	1.23844954	-3.81358993
O	2.40032065	2.74139477	-1.90893786	O	2.83260700	2.00827871	-2.15070118
O	2.27707544	0.39562781	-1.22403215	O	0.91287443	3.49564558	-2.85873779
H	0.53546729	3.54177089	-0.14234689	H	1.33182083	3.03037707	-0.11894109
H	-0.99143495	2.79388716	0.32586216	H	-0.21226893	2.51061492	0.53238418
H	-1.90064915	0.73686569	-1.10366130	H	1.76946096	-0.29027619	-1.11726903
H	-0.68348892	-0.11693953	-2.01705157	H	0.23839238	-0.68035498	-1.90851990
H	0.57102261	2.26405863	2.04466855	H	1.59967629	1.84710572	2.03914057
H	1.82579987	1.78236649	0.92889690	H	2.43066634	0.98406014	0.74999005
H	0.49676414	-2.34223022	3.31887898	H	-0.87492676	-1.84932198	3.83848072
H	-2.07433418	-4.65213362	-0.05458054	H	-2.57476642	-4.44593430	0.14498036
H	2.37006492	0.62966363	3.04446620	H	1.79679496	0.42230022	3.96430247
H	1.67759621	-0.53261211	4.19159413	H	0.34550877	-0.11722712	4.82586717
H	0.88779407	1.02713851	3.90731659	H	0.33200679	1.40215033	3.91636501
H	-2.78684895	-3.24748934	-2.19361387	H	-1.68542287	-1.90150112	-2.41620588
H	-1.48095230	-2.16255422	-2.69013013	H	-1.86978858	-3.65997942	-2.30834295
H	-2.92437267	-1.50329481	-1.91363970	H	-0.25351445	-2.93571706	-2.34985649
H	-0.31509327	3.63902183	-2.57885883	H	-1.72402394	1.10221037	-0.83165119
H	-1.06116474	2.17479703	-3.27421995	H	-1.32486556	1.10295916	-2.56131042
H	-1.82497419	3.00495559	-1.90191539	H	-1.35852075	2.63591611	-1.64371440
H	1.92423445	-0.47975859	-1.47082683	H	1.42488742	4.11779908	-2.31028109

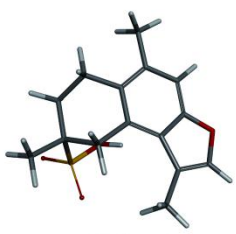
(2*R*)-**5** conformer 3							
C	0.97162396	2.35511822	0.11541232	O	1.81895720	-0.23514305	-1.38936821
C	0.09043897	1.92420490	-1.08245912	H	1.06156199	3.44588428	0.10964413
C	-1.07601719	1.00957917	-0.64906814	H	1.98614580	1.95511387	0.02224026
C	-0.64008395	-0.04049186	0.33330362	H	-1.80484761	1.67857285	-0.16849275
C	0.11299755	0.40229359	1.42777784	H	-1.56911475	0.58862641	-1.52651637
C	0.38890953	1.88240939	1.46051042	H	1.08544552	2.14819432	2.25799754
C	-0.90170380	-1.41453689	0.19505920	H	-0.54430798	2.42913882	1.66026135
C	-0.38984490	-2.27654850	1.17948012	H	0.72258431	-2.57691568	2.99884025
C	0.35083856	-1.86241381	2.27011951	H	-1.81040430	-4.47875566	-0.63741265
C	0.61001968	-0.49573369	2.39883939	H	2.34103473	0.48949710	3.24006315
C	-1.60184516	-2.26383091	-0.74988585	H	0.86138270	0.71900693	4.17060331
C	-1.45887867	-3.52412999	-0.27179723	H	1.70148232	-0.84063955	4.21862985
O	-0.72776346	-3.57217336	0.89897838	H	-3.15926183	-1.18616269	-1.76536065
C	1.42101332	-0.00714446	3.57000564	H	-1.68502926	-1.39960381	-2.71761853
C	-2.34454444	-1.88409041	-1.98920017	H	-2.77705121	-2.77199486	-2.45850897
C	-0.43682094	3.11719508	-1.88206129	H	0.38024160	3.73674514	-2.26212051
S	1.14297179	0.96654429	-2.28196384	H	-1.03966438	3.72680218	-1.20087708
O	2.29915819	1.77176244	-2.69282468	H	-1.07221296	2.79823513	-2.71389213
O	0.28800834	0.36222333	-3.31597880	H	1.11658072	-0.82683825	-1.04615933



Conformer 1



Conformer 2

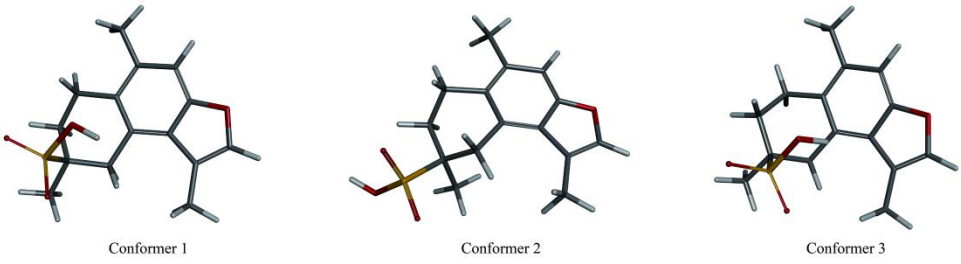


Conformer 3

The optimized conformers of (2*R*)-**5**.							
(2*S*)-**5** conformer 1				(2*S*)-**5** conformer 2			
C	2.35473201	0.92524658	0.20533186	C	1.88089856	1.21464804	0.03510047
C	1.77820015	0.55937308	-1.15804146	C	1.24769323	0.61425731	-1.24356385
C	0.73019788	-0.54488672	-1.01827012	C	-0.29287435	0.48553683	-1.12380363
C	-0.15885099	-0.46254534	0.20219985	C	-0.65967893	-0.07568756	0.22357002
C	0.11376471	0.38753605	1.27826612	C	-0.12805114	0.57222985	1.34408879
C	1.31038155	1.30792288	1.24743946	C	0.82765324	1.69812044	1.04337058
C	-1.29871393	-1.28967338	0.27194281	C	-1.51256386	-1.17389995	0.41097297
C	-2.11105343	-1.21573643	1.40870152	C	-1.79640135	-1.55943615	1.73008084
C	-1.87501399	-0.37041797	2.47724824	C	-1.29165796	-0.93153628	2.85354323
C	-0.74816464	0.44339437	2.40736434	C	-0.43558679	0.15455694	2.65889712
C	-1.91170807	-2.28808715	-0.58448869	C	-2.24334623	-2.09568126	-0.43617693
C	-3.00643342	-2.71869424	0.09043332	C	-2.88666483	-2.93297445	0.41430923
O	-3.16207687	-2.08723714	1.30777537	O	-2.64006970	-2.63866104	1.74074215
C	-0.45588678	1.38832542	3.54210415	C	0.14139009	0.86301177	3.85669663
C	-1.48566219	-2.78611401	-1.92887862	C	-2.30894537	-2.16158048	-1.92763847
C	2.88335144	0.14923041	-2.13651953	C	1.87391624	-0.72532699	-1.62459884
S	0.99854505	2.05645640	-1.95164448	S	1.51141663	1.79340150	-2.64082924
O	0.66309092	1.74322044	-3.34962505	O	1.13719246	3.16074013	-2.24199023
O	1.79702257	3.24979691	-1.65026456	O	0.94826551	1.23163375	-3.87486704
O	-0.40994289	2.31768894	-1.14728496	O	3.14690823	1.74822517	-2.82038440
H	2.87875249	0.01857645	0.53850485	H	2.57735144	2.02469130	-0.20461939
H	3.10872912	1.71230229	0.10294190	H	2.47322349	0.42318063	0.50736437

H	0.12468339	-0.60342875	-1.92990760	H	-0.75548343	1.47854044	-1.22064763
H	1.29149970	-1.48995093	-0.98548676	H	-0.66898928	-0.13119094	-1.94049905
H	0.96986963	2.34020742	1.08387369	H	1.33425453	2.05048825	1.94429502
H	1.79826550	1.31222606	2.22853933	H	0.28624697	2.55950850	0.62597581
H	-2.54232477	-0.34098474	3.33379795	H	-1.54939539	-1.27375478	3.85175653
H	-3.75997129	-3.45520149	-0.15119633	H	-3.54435599	-3.77308342	0.23999406
H	-1.25614699	1.35463711	4.28528095	H	1.23497128	0.78576338	3.88025583
H	-0.35711230	2.42201024	3.19056607	H	-0.24677927	0.43038957	4.78213221
H	0.48468656	1.13380541	4.04609395	H	-0.10528159	1.93074819	3.84997979
H	-0.45522572	-3.15566995	-1.91286374	H	-2.70022975	-1.23076264	-2.35324794
H	-2.13588134	-3.60463808	-2.25027004	H	-2.96325064	-2.97947696	-2.24225197
H	-1.54036211	-1.99721012	-2.68716879	H	-1.31858380	-2.33314341	-2.36495003
H	3.58193623	0.97076329	-2.32493659	H	1.50151910	-1.08932356	-2.58649499
H	2.46815899	-0.19711997	-3.08631792	H	1.59194250	-1.44848784	-0.85110430
H	3.44067339	-0.67345229	-1.67748144	H	2.96481165	-0.66315426	-1.65324285
H	-1.09900955	1.71442897	-1.48275903	H	3.51033449	2.63028997	-2.62131485
(2*S*)-**5** conformer 3							
C	1.87183540	1.73395939	0.16529734	O	-0.81057119	1.68849811	-1.44487719
C	1.78702594	0.77862445	-1.04989452	H	2.85904427	2.20638106	0.17366107
C	1.27673115	-0.62609293	-0.65862910	H	1.13591077	2.54007883	0.08369578
C	0.14145353	-0.57334665	0.32394590	H	2.13800681	-1.12856097	-0.19415549
C	0.31800726	0.24959482	1.44237067	H	1.03318040	-1.19947002	-1.55447989
C	1.62645466	0.99387015	1.49303058	H	2.45156405	0.28869273	1.67161904
C	-1.07180449	-1.26483503	0.16946424	H	1.64968960	1.71857400	2.30914157

C	-2.05033503	-1.09254984	1.16229039	H	-2.69096041	-0.19488509	3.01263955
C	-1.89747438	-0.29037244	2.27707177	H	-3.67506541	-3.09621968	-0.71301267
C	-0.69036692	0.39787997	2.42104932	H	0.38518225	0.98543073	4.20375669
C	-1.64950545	-2.17346822	-0.80294907	H	-0.32956265	2.33175810	3.31804698
C	-2.88598293	-2.46470284	-0.32948395	H	-1.36449108	1.25758257	4.27241993
O	-3.16552029	-1.82692876	0.86297442	H	-1.75669926	-3.38661609	-2.55652824
C	-0.48990376	1.28944316	3.61808823	H	-0.81916420	-1.89715152	-2.76740081
C	-1.05570486	-2.70537456	-2.06640598	H	-0.12795214	-3.25470600	-1.87034774
C	3.11431524	0.66959213	-1.80371015	H	3.86125881	0.29098680	-1.09802826
S	0.59012072	1.49040756	-2.28133117	H	3.45075411	1.64491392	-2.16630914
O	0.35929288	0.52025171	-3.36331487	H	3.04555449	-0.02955168	-2.64254587
O	0.97535292	2.86430928	-2.62348118	H	-1.16997081	0.81600288	-1.18187819



The optimized conformers of (2*S*)-**5**.

Table S8. Free energy summary of conformer set in CH_3OH of compound **5**

	Conformer No.	Energy (kcal/mol)	Relative Energy (kcal/mol)	proportion of various comformations
(2*R*)-**5**	1	-804032.988864250	0.000000000	81.19%
	2	-804031.516042882	1.472821368	6.75%
	3	-804031.859642942	1.129221308	12.06%
(2*S*)-**5**	1	-804032.978991116	0.000000000	66.22%

	2	-804032.309396313	0.669594803	21.37%
	3	-804031.987590655	0.991400461	12.41%

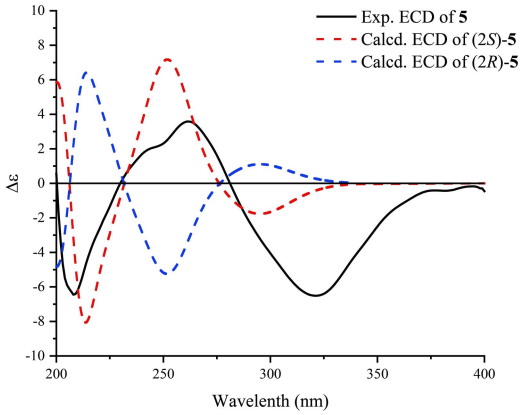


Figure S76. The experimental and calculated ECD spectra of **5** in CH_3OH

Table S9. Cartesian coordinates and geometries of optimized predominant conformers in CH_3OH for compound **7**

(1*R*, 4*S*, 5*S*)-**7** conformer 1				(1*R*, 4*S*, 5*S*)-**7** conformer 2			
C	-1.35044304	-2.08362614	-0.78235203	C	-1.28076580	-1.21098237	-0.72910255
C	-0.09329255	-2.75441073	-0.19086481	C	-0.15835454	-2.25192746	-0.74408185
C	0.45086356	-1.74742176	0.82703819	C	0.58653479	-2.01404968	0.57423843
C	0.18557149	-0.38661800	0.15890440	C	0.67878376	-0.46556676	0.64230794
C	-1.24682706	-0.58403078	-0.41554873	C	-0.66524511	0.02313370	0.02413167
C	-2.35303332	-0.09233221	0.50356936	C	-1.66267121	0.50553252	1.05206071
C	1.18980277	-0.02878735	-0.94452435	C	1.90223402	0.11955444	-0.07409922
C	1.04478520	1.41005137	-1.42831593	C	2.04064426	1.64396460	0.10650231
C	1.49576850	2.45806217	-0.43344025	C	1.21526633	2.52266528	-0.80616187
C	1.06625700	3.87107978	-0.72139649	C	1.34625378	2.29518390	-2.29143458
O	-3.36206871	-0.74376337	0.72845477	O	-1.80018456	-0.08690347	2.11889716
C	-2.19246104	1.29196553	1.08481364	C	-2.49753473	1.69347426	0.69202075

O	2.17409671	2.17814786	0.54357848	O	0.50896845	3.41807109	-0.36103927
C	1.88303344	-2.01032845	1.26592410	C	1.90271954	-2.76383338	0.67246517
O	-0.41285655	-1.72352862	1.99247942	O	-0.22549940	-2.48031010	1.67614664
H	-1.40487506	-2.22392378	-1.86568921	H	-1.62529417	-0.93246997	-1.72817914
H	-2.26707951	-2.49760047	-0.35388984	H	-2.14461214	-1.59918821	-0.17772816
H	0.66383920	-2.92762630	-0.96438939	H	-0.52909109	-3.27972052	-0.81737189
H	-0.30195592	-3.72173148	0.28131914	H	0.52157562	-2.07196427	-1.58634874
H	0.22165160	0.39159268	0.92845576	H	0.74660291	-0.17142880	1.69856649
H	-1.36549228	0.05192874	-1.30666954	H	-0.49721109	0.82512708	-0.69882726
H	2.21108718	-0.16240343	-0.57487431	H	1.89320467	-0.14082498	-1.14019182
H	1.06261408	-0.70744053	-1.79746962	H	2.80046893	-0.33866586	0.35127435
H	1.65758374	1.57714669	-2.32794705	H	3.08470610	1.91602791	-0.10956533
H	0.01914102	1.64803456	-1.74284934	H	1.83272876	1.92779512	1.14415529
H	0.00205526	3.96233219	-0.46669747	H	0.77803237	1.40275361	-2.58199815
H	1.15625448	4.09962463	-1.78855152	H	2.38937659	2.10610345	-2.56587500
H	1.63922245	4.58272492	-0.12409914	H	0.95297696	3.15316743	-2.83972386
H	-3.17471621	1.72627560	1.28378715	H	-2.94788784	1.53990441	-0.29653555
H	-1.60794207	1.94673835	0.43108799	H	-3.26894523	1.88293441	1.44011698
H	-1.65302735	1.21273180	2.03681100	H	-1.83821026	2.56593836	0.59627113
H	1.92712936	-2.94863358	1.83117820	H	2.44851710	-2.48004458	1.57881347
H	2.55648235	-2.10557374	0.40950583	H	2.53652780	-2.57022103	-0.19711184
H	2.24402384	-1.20162261	1.91079810	H	1.70142746	-3.83949274	0.71556199
H	-0.44029257	-2.62033352	2.35166350	H	-0.83214303	-1.76043739	1.93184561
(1*R*, 4*S*, 5*S*)-**7** conformer 3				(1*R*, 4*S*, 5*S*)-**7** conformer 4			

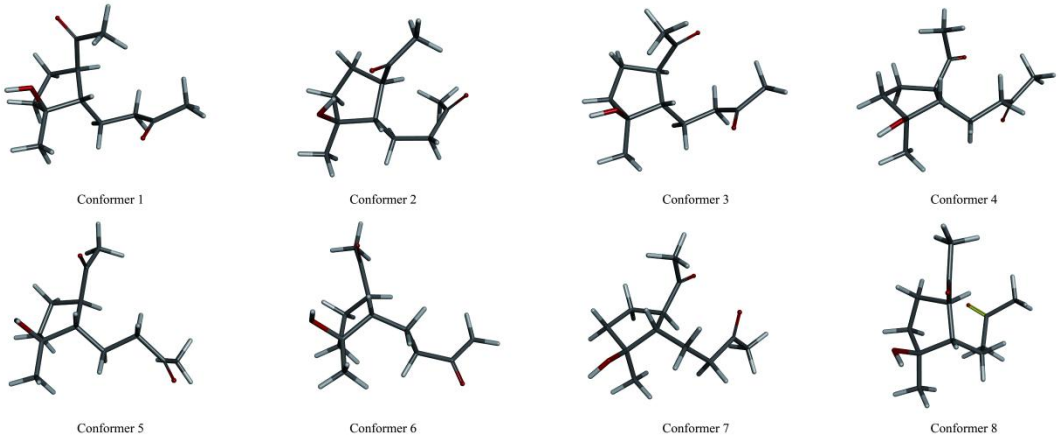
C	-1.56473980	-2.08138687	0.41377235	C	-0.74721891	-2.35653685	-0.09391078
C	-0.25039711	-2.85921656	0.39320455	C	-0.27650533	-2.49575951	1.35827869
C	0.76734808	-1.85259295	0.93950163	C	0.85409123	-1.46658130	1.49435582
C	0.35769577	-0.50905932	0.27272947	C	0.27572421	-0.25261281	0.73361725
C	-1.15288549	-0.69090248	-0.12126527	C	-0.42503756	-0.87278585	-0.50038298
C	-2.00400555	0.45315615	0.37713452	C	-1.70096506	-0.18490097	-0.92800750
C	1.20562275	-0.11161046	-0.94009136	C	1.28218851	0.85332221	0.42375446
C	0.78071688	1.21846658	-1.55538959	C	0.65309799	2.11093081	-0.17615116
C	1.01574160	2.43196093	-0.68219648	C	0.54686339	2.14414754	-1.68780850
C	0.24061644	3.66662010	-1.05156572	C	-0.40414576	3.16291769	-2.25436093
O	-2.50587059	1.25915989	-0.39763329	O	-1.90100730	0.10771267	-2.10033998
C	-2.22083090	0.58028229	1.86399051	C	-2.74785381	0.09941344	0.12147179
O	1.79307498	2.41478070	0.26098974	O	1.22167130	1.42117234	-2.40420149
C	2.21379920	-2.28181359	0.74327498	C	2.16132902	-1.98789409	0.90321352
O	0.52276437	-1.64429560	2.35447135	O	1.06298234	-1.05700414	2.85738868
H	-1.93623171	-2.01343184	1.44061524	H	-1.80995116	-2.59765519	-0.20484142
H	-2.34948850	-2.53004040	-0.20265502	H	-0.19816309	-3.02967055	-0.75860598
H	0.02179955	-3.12187415	-0.63789396	H	0.04638935	-3.51338485	1.60517367
H	-0.27267517	-3.78295536	0.98367758	H	-1.07701356	-2.21317346	2.05309093
H	0.46773479	0.27367104	1.03316133	H	-0.49087619	0.16166082	1.40522944
H	-1.23117048	-0.69703709	-1.21498800	H	0.25040854	-0.85887574	-1.36135967
H	2.25676777	-0.04072269	-0.64227106	H	1.78843819	1.11953607	1.35909985
H	1.13705431	-0.89273560	-1.70853053	H	2.04977694	0.48226549	-0.26509895
H	1.35374146	1.40923793	-2.47660775	H	1.26658200	2.99417414	0.06398878

H	-0.27014748	1.21500436	-1.87101939	H	-0.33047650	2.32935590	0.26149770
H	0.64151224	4.54839398	-0.54841440	H	-0.27603043	4.12893106	-1.75351034
H	0.23048590	3.80986010	-2.13741545	H	-1.42948252	2.83069953	-2.04882834
H	-0.80265691	3.51464980	-0.74419487	H	-0.26729655	3.26820585	-3.33211247
H	-3.16528931	0.07725662	2.10978580	H	-3.74076526	0.08737376	-0.33330335
H	-2.32310119	1.63375611	2.13526203	H	-2.70159084	-0.59736843	0.96263502
H	-1.42809965	0.10216984	2.44401634	H	-2.56939941	1.10631912	0.52053522
H	2.39405482	-3.21174380	1.29544821	H	2.05227726	-2.23132525	-0.15919252
H	2.90193304	-1.51867282	1.12149700	H	2.95942279	-1.24723758	1.00686775
H	2.43806188	-2.46718236	-0.31136063	H	2.46428528	-2.90137886	1.42858119
H	0.63186401	-2.49875248	2.79376014	H	1.49325088	-1.78709300	3.32133660
(1*R*, 4*S*, 5*S*)-**7** conformer 3				(1*R*, 4*S*, 5*S*)-**7** conformer 4			
C	-1.45037812	-1.72369401	-0.45724693	C	-0.90889055	-1.75126486	-0.44823636
C	-0.12691002	-2.48618312	-0.47309964	C	0.56548749	-2.05423590	-0.15564929
C	0.63990454	-1.91295124	0.71616727	C	0.82726472	-1.37752095	1.18818261
C	0.34752290	-0.38496905	0.64102432	C	0.06899474	-0.03038547	1.08128078
C	-1.01500837	-0.26994678	-0.08949200	C	-1.15756713	-0.34880641	0.19910107
C	-2.12158558	0.41809907	0.67975875	C	-2.49616648	-0.28950425	0.90787483
C	1.42845503	0.44312588	-0.06115301	C	0.87208812	1.18136531	0.57797636
C	1.12589034	1.95307819	0.02003429	C	1.43013353	1.10261998	-0.85877722
C	2.19254970	2.72286003	-0.72446679	C	1.99477853	2.45622360	-1.22906283
C	1.92428511	3.01848992	-2.17394670	C	1.07575199	3.39935768	-1.95373790
O	-2.08335238	0.57414367	1.89159637	O	-2.62032928	0.05564438	2.07313661
C	-3.29794787	0.88045495	-0.13837792	C	-3.69874884	-0.68790401	0.08696948

O	3.23037582	3.06207502	-0.17334675	O	3.13835027	2.76613711	-0.92611152
C	2.10727035	-2.30996199	0.75073949	C	2.29057572	-1.28434513	1.58846121
O	-0.02751791	-2.44716450	1.88617529	O	0.12438687	-2.20534600	2.15274520
H	-2.11147049	-2.13357857	0.31416475	H	-1.54134543	-2.50672273	0.02772653
H	-1.98168525	-1.75722746	-1.41232374	H	-1.13773835	-1.75416445	-1.51766886
H	0.42960787	-2.26323251	-1.39218729	H	0.78070469	-3.12740730	-0.11188550
H	-0.24549527	-3.57244986	-0.39711405	H	1.21304650	-1.61053051	-0.91836635
H	0.25134621	-0.00816688	1.66727759	H	-0.27254387	0.24169650	2.08816257
H	-0.88291156	0.27513080	-1.03471489	H	-1.24909460	0.39469242	-0.60720697
H	1.51514783	0.13386547	-1.11278788	H	0.20460249	2.05182758	0.64425207
H	2.40079027	0.26706914	0.41168824	H	1.70429343	1.37612082	1.26490166
H	1.12774829	2.26350191	1.07091208	H	2.23747461	0.36758526	-0.92416645
H	0.14254015	2.16962670	-0.41483046	H	0.63875682	0.82566918	-1.56515117
H	1.52937514	2.13132481	-2.68159274	H	0.92896175	3.01963829	-2.97341507
H	1.13892847	3.78378437	-2.22830010	H	1.49383751	4.40663109	-1.99575928
H	2.82198481	3.38206188	-2.67721002	H	0.08669462	3.41038166	-1.48200571
H	-2.97923776	1.73833850	-0.74464993	H	-4.59362174	-0.18822512	0.46423082
H	-4.12909785	1.17784408	0.50345381	H	-3.84410227	-1.77070841	0.18996440
H	-3.61459795	0.10107753	-0.83977125	H	-3.55575164	-0.47622285	-0.97644112
H	2.62967986	-1.99965368	-0.15928743	H	2.70850384	-2.29225830	1.67930567
H	2.18431801	-3.39875365	0.83743392	H	2.39219899	-0.77974465	2.55676725
H	2.61592023	-1.85843323	1.61101700	H	2.88432713	-0.73275495	0.85394970
H	0.37155544	-2.03058539	2.66135635	H	0.16768578	-1.75463862	3.00665278
(1*R*, 4*S*, 5*S*)-**7** conformer 5				(1*R*, 4*S*, 5*S*)-**7** conformer 6			

C	-1.39084245	-1.88605821	-0.24644285	C	-0.73116387	-0.97611365	-1.15438225
C	-0.46999589	-2.73390222	0.64835490	C	0.60694264	-1.64663969	-0.82685213
C	0.82741349	-1.91978342	0.78042628	C	0.68183892	-1.60925807	0.69734121
C	0.28230516	-0.47824131	0.89111743	C	0.13184025	-0.20428338	1.06247198
C	-0.80919323	-0.42474056	-0.19020371	C	-0.91561244	0.09930675	-0.03168702
C	-1.95887336	0.53956821	0.00312675	C	-2.35914894	0.12633179	0.43439871
C	1.33402617	0.64379482	0.89604038	C	1.16439701	0.92073343	1.25312463
C	1.72014287	1.22286821	-0.46406705	C	2.05984429	1.32540453	0.06117382
C	0.75752125	2.25551538	-1.00957970	C	1.36907102	1.96700020	-1.12255348
C	0.84625215	2.53145982	-2.48511095	C	0.72845666	3.31485916	-0.90472762
O	-2.55633122	0.98098930	-0.97020413	O	-2.70906267	-0.21267036	1.55415186
C	-2.39559758	0.86447350	1.40421350	C	-3.35604994	0.62974695	-0.57820445
O	-0.03564721	2.84525858	-0.29069158	O	1.39791278	1.45475712	-2.23363308
C	1.75896697	-2.15457209	-0.40480317	C	2.03911951	-1.96257391	1.28446860
O	1.52751869	-2.20098762	2.00491938	O	-0.28773190	-2.59938086	1.13005938
H	-2.42664933	-1.91862520	0.10810584	H	-1.54060216	-1.71302994	-1.10914399
H	-1.39644972	-2.23404282	-1.28291450	H	-0.74467892	-0.52425301	-2.15014604
H	-0.29363461	-3.73645328	0.24343922	H	1.43507485	-1.06727908	-1.24660854
H	-0.90188410	-2.84123459	1.64980726	H	0.67726409	-2.67171504	-1.20669876
H	-0.21063143	-0.46416632	1.87342766	H	-0.38013656	-0.29403781	2.02927522
H	-0.37138409	-0.19292605	-1.16774774	H	-0.74442103	1.09123431	-0.47009493
H	2.23144032	0.25784428	1.39375259	H	0.61959931	1.80674513	1.60254354
H	0.96967610	1.47073406	1.51540013	H	1.83329644	0.64112509	2.07531606
H	2.67921833	1.75903484	-0.37741263	H	2.64673666	0.48101517	-0.30903282

H	1.89524872	0.45825358	-1.22918444	H	2.76738604	2.07686533	0.44250175
H	1.89065799	2.58607107	-2.81053715	H	0.00574350	3.53061293	-1.69426473
H	0.31073598	3.44615384	-2.74582335	H	1.52831801	4.06643691	-0.94755173
H	0.39364923	1.68414336	-3.01746119	H	0.26060342	3.40089382	0.07972247
H	-3.33424128	1.42091654	1.38843121	H	-3.12794567	0.26897426	-1.58557233
H	-2.50730826	-0.04985171	1.99866576	H	-4.37343815	0.35670573	-0.29192072
H	-1.61965297	1.46676833	1.89212953	H	-3.27574218	1.72472843	-0.60661401
H	2.06793446	-3.20683209	-0.42298367	H	2.82909412	-1.29374428	0.93224517
H	1.26219437	-1.93950308	-1.35711334	H	2.00962967	-1.90887084	2.37948278
H	2.65720856	-1.53414147	-0.32731303	H	2.30411851	-2.98553799	0.99765248
H	1.94620588	-3.06668567	1.91333635	H	-0.37955325	-2.51798913	2.08865898



The optimized conformers of (1*R*, 4*S*, 5*S*)-**7**.

(1*S*, 4*R*, 5*R*)-**7** conformer 1				(1*S*, 4*R*, 5*R*)-**7** conformer 2			
C	1.66276288	-1.87412103	-0.35310918	C	1.52949855	-1.02021249	-0.61809387
C	0.39854998	-2.73533027	-0.28218453	C	0.51990070	-2.14465779	-0.86432992
C	-0.49132374	-1.98773445	0.71574715	C	-0.41060030	-2.07917797	0.35160798
C	-0.33745023	-0.50758691	0.27389716	C	-0.65447592	-0.55448678	0.51481795
C	1.15743737	-0.40373281	-0.19121224	C	0.70897279	0.09237685	0.12698473

C	1.99087143	0.34960847	0.82244560	C	1.50652592	0.56904113	1.32000065
C	-1.29680741	-0.07305136	-0.84089816	C	-1.82114936	-0.01865125	-0.32373684
C	-1.20169214	1.41591412	-1.15920636	C	-2.11021468	1.47592569	-0.08205537
C	-1.73999751	2.33138644	-0.08043199	C	-1.27375948	2.47299314	-0.85181537
C	-1.33283219	3.77655071	-0.17925620	C	-1.18837900	2.29945076	-2.34784144
O	2.05051549	-0.03682239	1.98681707	O	1.56672918	-0.10561440	2.34427883
C	2.71869291	1.57223661	0.35933500	C	2.24567198	1.86177343	1.17715658
O	-2.46816382	1.92711979	0.81348204	O	-0.72879087	3.41490435	-0.29106375
C	-1.91572812	-2.50722144	0.78137695	C	-1.65346936	-2.94007622	0.21613426
O	0.04729479	-2.13789102	2.04913139	O	0.28949819	-2.56787881	1.51927230
H	2.33746996	-2.13180048	0.47069815	H	2.34406110	-1.38160026	0.01981963
H	2.21791577	-2.00100640	-1.28618706	H	1.97743735	-0.63285270	-1.53668130
H	-0.09938960	-2.77251814	-1.25930377	H	-0.05721416	-1.95137607	-1.77735766
H	0.59539538	-3.76275942	0.04191245	H	0.99034092	-3.12892457	-0.95945209
H	-0.52245712	0.12860966	1.14893644	H	-0.89083994	-0.35378439	1.56866740
H	1.21355918	0.11339142	-1.15370728	H	0.56570049	0.93654390	-0.55159709
H	-2.32552953	-0.29299749	-0.53884270	H	-2.72314855	-0.57233638	-0.04531088
H	-1.09528275	-0.64830289	-1.75342901	H	-1.65590384	-0.20701639	-1.39199348
H	-1.79026179	1.65186633	-2.05988466	H	-2.04362836	1.71526315	0.98516397
H	-0.17915330	1.73136316	-1.40572678	H	-3.14411895	1.67560706	-0.40210761
H	-0.29339350	3.85996465	0.16545108	H	-0.46127231	1.51272377	-2.58571858
H	-1.96840340	4.40578606	0.44647203	H	-0.85806544	3.22905060	-2.81512150
H	-1.34909936	4.11930987	-1.21912255	H	-2.14882692	1.97707266	-2.76295748
H	3.37028964	1.30945844	-0.48331540	H	2.85586286	1.83238571	0.26545596

H	3.29861590	2.02385491	1.16575418	H	2.86911051	2.06622834	2.04893013
H	1.98769674	2.29196372	-0.03173146	H	1.51614814	2.66872168	1.03030602
H	-1.91291336	-3.51359439	1.21317776	H	-1.36040260	-3.99532913	0.21582903
H	-2.36455675	-2.56415851	-0.21374652	H	-2.18511455	-2.73433236	-0.71697875
H	-2.53680518	-1.86258133	1.41289722	H	-2.33629421	-2.77411739	1.05643195
H	0.80537338	-1.53017362	2.14056417	H	0.78801016	-1.82443689	1.90745564
(1*S*, 4*R*, 5*R*)-**7** conformer 1				(1*S*, 4*R*, 5*R*)-**7** conformer 2			
C	1.44879720	-1.83751601	-0.23286714	C	1.64254385	-2.00924645	0.39372668
C	0.52375690	-2.72828891	0.61425294	C	0.36938892	-2.84877526	0.29094629
C	-0.79703219	-1.94990750	0.73223456	C	-0.70997922	-1.93104675	0.86008519
C	-0.28799198	-0.49060544	0.87856250	C	-0.35450949	-0.52835459	0.27384538
C	0.82414545	-0.39303915	-0.17713510	C	1.17689052	-0.61067502	-0.07143004
C	1.94207156	0.60123614	0.04781683	C	1.94265686	0.54791108	0.52262923
C	-1.36792827	0.60302758	0.88366466	C	-1.17955110	-0.11364163	-0.95009550
C	-1.74499214	1.19392774	-0.47364657	C	-0.80767780	1.26543331	-1.48768333
C	-0.79740825	2.25682315	-0.98669923	C	-1.12958862	2.42084976	-0.56571108
C	-0.86683994	2.55292298	-2.45935676	C	-0.42828581	3.71703008	-0.86650157
O	2.54300219	1.07220040	-0.90930278	O	2.40713614	1.43402985	-0.18496138
C	2.34500319	0.92082334	1.46047211	C	2.11483109	0.59099727	2.01984162
O	-0.03026170	2.85299408	-0.24532257	O	-1.91635913	2.31320943	0.36373319
C	-1.69511228	-2.18295211	-0.47389548	C	-2.12937992	-2.41292776	0.59859155
O	-1.57797661	-2.35463825	1.86651304	O	-0.47242712	-1.91143158	2.28996751
H	1.50115521	-2.16892642	-1.27333194	H	1.98774860	-1.98639265	1.43148626
H	2.47179032	-1.84418483	0.15802061	H	2.46268642	-2.38196139	-0.22740913

H	0.37931920	-3.72334156	0.18095960	H	0.13555155	-3.05938583	-0.76028167
H	0.93887727	-2.85734947	1.62180803	H	0.41945853	-3.80000916	0.83117327
H	0.19049845	-0.47694521	1.86977493	H	-0.53372669	0.21360987	1.06277805
H	0.40034700	-0.16550983	-1.16181871	H	1.29140223	-0.54614364	-1.15985977
H	-1.03836046	1.42868747	1.52388495	H	-1.04237669	-0.85104808	-1.75192404
H	-2.26320491	0.18386530	1.35901112	H	-2.24273316	-0.11265698	-0.68853098
H	-2.71823271	1.70528723	-0.39662674	H	0.25030797	1.33027060	-1.77186535
H	-1.88807652	0.43704189	-1.25288667	H	-1.36413143	1.47186203	-2.41577117
H	-0.38281124	1.72538001	-2.99517343	H	0.61638462	3.61874039	-0.54251351
H	-1.90596179	2.58637954	-2.80377872	H	-0.40665557	3.90864774	-1.94462942
H	-0.34971422	3.48443881	-2.69668645	H	-0.89484517	4.54812595	-0.33450272
H	2.47094057	0.00314044	2.04673085	H	2.15074473	1.62857794	2.35998029
H	3.26834927	1.50249317	1.46810910	H	3.07812063	0.12309317	2.26187332
H	1.54467166	1.49687532	1.94057998	H	1.33494925	0.03326659	2.54421304
H	-2.61659488	-1.59771585	-0.39507652	H	-2.33007968	-2.51256059	-0.47210189
H	-1.96385210	-3.24308268	-0.52574342	H	-2.86345730	-1.71806117	1.02400675
H	-1.18693668	-1.91473716	-1.40500602	H	-2.26926561	-3.39198035	1.06844523
H	-1.02853658	-2.25480418	2.65585846	H	-1.09757243	-1.28515618	2.67864970
(1*S*, 4*R*, 5*R*)-**7** conformer 1				(1*S*, 4*R*, 5*R*)-**7** conformer 2			
C	0.77875557	-0.92492437	-1.16330563	C	1.55393379	-2.18872537	0.58942540
C	-0.54224756	-1.64449369	-0.87123528	C	0.41411684	-2.44755119	1.58061036
C	-0.64130346	-1.64336808	0.65213414	C	-0.83492462	-1.92750937	0.86911391
C	-0.14010102	-0.23113506	1.05710229	C	-0.32004077	-0.60351605	0.24495091
C	0.91402908	0.12855625	-0.01356695	C	1.10676435	-0.94400111	-0.25694892

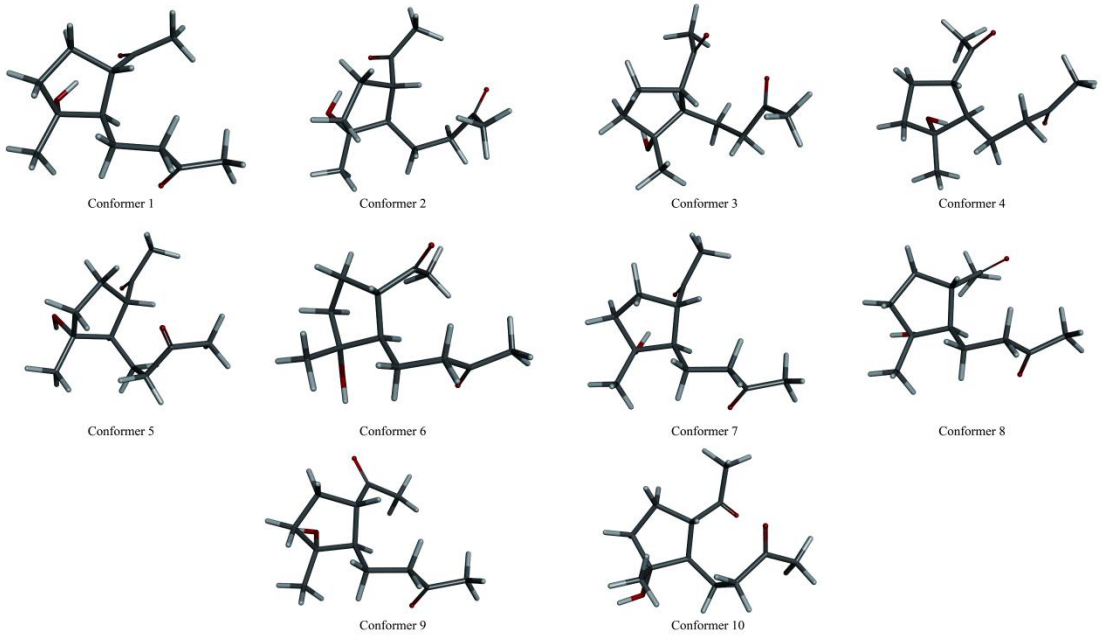
C	2.34898994	0.18450103	0.47570043	C	2.11622531	0.17055113	-0.10622296
C	-1.20805088	0.85904538	1.25574423	C	-1.22888402	0.00950546	-0.81793222
C	-2.10105460	1.25929111	0.06072083	C	-0.78931241	1.39487770	-1.28118588
C	-1.41669877	1.94310692	-1.10287005	C	-0.91348740	2.49405019	-0.24900884
C	-0.81841226	3.30470654	-0.85375325	C	-0.18574853	3.77376597	-0.56048957
O	2.69181788	-0.17506650	1.59119336	O	2.81304918	0.52860681	-1.04748725
C	3.34652723	0.74318752	-0.50695637	C	2.26724933	0.81816946	1.24895878
O	-1.41863492	1.45046985	-2.22327084	O	-1.57391901	2.35776467	0.77015115
C	-1.99619401	-2.05050912	1.20951721	C	-1.35179684	-2.91938063	-0.16982374
O	0.35142604	-2.61376077	1.07787774	O	-1.84728948	-1.68579998	1.86000971
H	1.61070835	-1.63672331	-1.12497973	H	2.50977992	-2.02450470	1.09787128
H	0.79062685	-0.44889906	-2.14780511	H	1.69397385	-3.03969841	-0.08342522
H	-1.38126312	-1.08170759	-1.29171467	H	0.55442880	-1.85774448	2.49505344
H	-0.57431484	-2.66244595	-1.27454070	H	0.32806474	-3.50157361	1.86495582
H	0.35892273	-0.32684484	2.03013130	H	-0.24708793	0.09225103	1.09111486
H	0.72005122	1.12514873	-0.43139566	H	1.07769473	-1.20452091	-1.32132073
H	-0.69320469	1.75379596	1.62762821	H	-1.26248007	-0.65101302	-1.69277452
H	-1.87803191	0.54542278	2.06476671	H	-2.25220351	0.07435047	-0.42544797
H	-2.65694233	0.40432006	-0.33240824	H	-1.40758657	1.72580269	-2.13069026
H	-2.83604816	1.98056394	0.44819986	H	0.23689910	1.39055273	-1.67267620
H	-0.09721552	3.55690300	-1.63383020	H	0.89248444	3.59533617	-0.45439508
H	-1.63977008	4.03324461	-0.88671804	H	-0.35326684	4.06935316	-1.60204250
H	-0.35931482	3.38521414	0.13530158	H	-0.49005382	4.57178431	0.11905430
H	3.13758709	0.41644404	-1.52991494	H	3.29108004	1.17747612	1.37457896

H	4.36585953	0.47960117	-0.21848407	H	1.59849619	1.68763605	1.29588899
H	3.24570454	1.83681199	-0.49527796	H	1.99017102	0.15200251	2.07020109
H	-2.80052759	-1.39926220	0.85677184	H	-1.57881118	-3.87515357	0.31332957
H	-1.98603554	-2.01731581	2.30570300	H	-2.26506463	-2.54606323	-0.64626956
H	-2.22462335	-3.07516081	0.89863995	H	-0.61146379	-3.09539304	-0.95761366
H	0.42888339	-2.54961787	2.03899502	H	-2.66899025	-1.46458795	1.40238656
(1*S*, 4*R*, 5*R*)-**7** conformer 1				(1*S*, 4*R*, 5*R*)-**7** conformer 2			
C	1.40399839	-2.01273233	-0.68172295	C	1.62310912	-2.04302962	0.39508761
C	0.66161974	-2.77043812	0.41937610	C	0.33327311	-2.85897177	0.33571166
C	-0.50033487	-1.84732228	0.89051733	C	-0.72228883	-1.89494943	0.88718916
C	-0.22844003	-0.45555248	0.20586797	C	-0.34350825	-0.52618035	0.25491534
C	1.23362380	-0.52229836	-0.28520529	C	1.17825321	-0.65412437	-0.11708114
C	2.25869561	-0.17940220	0.77050303	C	1.98613781	0.50461367	0.41819687
C	-1.16552534	-0.09063492	-0.95633843	C	-1.18268958	-0.12946620	-0.96428524
C	-1.04711308	1.37514284	-1.36495899	C	-0.79117072	1.22787180	-1.54086982
C	-1.64654536	2.35474946	-0.37819119	C	-1.08339226	2.41185781	-0.64479009
C	-1.25665687	3.79684451	-0.56026975	C	-0.34712871	3.68164854	-0.97285239
O	2.03733147	-0.32031992	1.96952699	O	2.47394712	1.34181579	-0.33210864
C	3.58130993	0.33369786	0.27809237	C	2.17648501	0.60742519	1.91043547
O	-2.40871099	2.00210771	0.50918738	O	-1.87441200	2.34569377	0.28479466
C	-1.85943440	-2.45618175	0.58606383	C	-2.15242371	-2.36216869	0.66062262
O	-0.47108506	-1.69374102	2.32560943	O	-0.50408784	-1.70929954	2.30950745
H	2.45150005	-2.31605683	-0.78486734	H	1.97560287	-1.98658859	1.42927238
H	0.92194058	-2.16077889	-1.65487103	H	2.43095258	-2.45460573	-0.21739374

H	0.29738796	-3.74451417	0.07698784	H	0.08531552	-3.10597306	-0.70530616
H	1.32663042	-2.95175906	1.27081857	H	0.37367183	-3.79459332	0.90610176
H	-0.34198257	0.31414422	0.97854485	H	-0.49111848	0.23682772	1.02891913
H	1.41962784	0.11921654	-1.15449413	H	1.27361756	-0.63476811	-1.20926874
H	-2.20380393	-0.27519894	-0.66753605	H	-2.24070146	-0.09967843	-0.68465679
H	-0.95994560	-0.72624908	-1.82707551	H	-1.07472963	-0.88992205	-1.74880603
H	-1.57950972	1.55368401	-2.31252212	H	-1.35265657	1.42155858	-2.46858595
H	-0.01095433	1.67777333	-1.56696461	H	0.26504557	1.26656356	-1.83587284
H	-1.92220689	4.45437400	0.00213147	H	-0.79283099	4.53772792	-0.46310479
H	-1.24731235	4.07051420	-1.62062425	H	-0.31601252	3.84641295	-2.05517200
H	-0.23014089	3.92254513	-0.19138558	H	0.69333089	3.56288383	-0.64197825
H	3.92073484	-0.23303062	-0.59504156	H	3.12877733	0.12220680	2.16174837
H	4.33174199	0.31315188	1.07021864	H	2.24867076	1.65745463	2.20372087
H	3.43625307	1.36940761	-0.05742600	H	1.38655021	0.09874032	2.46792520
H	-1.95390641	-3.40266777	1.12863104	H	-2.31354682	-3.30784205	1.19157127
H	-1.96676557	-2.66230134	-0.48298220	H	-2.86804496	-1.62699391	1.04322264
H	-2.67213001	-1.79400289	0.90208273	H	-2.35582215	-2.53263132	-0.40077660
H	0.36100859	-1.22527028	2.51421742	H	-0.59597500	-2.57521633	2.72986677
(1*S*, 4*R*, 5*R*)-**7** conformer 1				(1*S*, 4*R*, 5*R*)-**7** conformer 2			
C	1.43555745	-2.03120970	-0.79125727	C	1.33858453	-1.80970088	0.76133200
C	0.18133506	-2.74854298	-0.25275496	C	0.15177871	-2.58211815	1.37693329
C	-0.40906723	-1.78467844	0.78058268	C	-1.11030304	-1.77552914	1.01659845
C	-0.17439862	-0.40045058	0.14973686	C	-0.59344582	-0.32439191	1.08624776
C	1.27175778	-0.54073988	-0.40816669	C	0.76199526	-0.40395032	0.38225224

C	2.34813454	-0.02015554	0.53048017	C	1.71802158	0.71835089	0.70751281
C	-1.17537585	-0.04368340	-0.95700897	C	-1.57686871	0.76675183	0.63162324
C	-1.06474973	1.40917600	-1.40649967	C	-1.50269942	1.21803316	-0.84547116
C	-1.56343568	2.42171391	-0.39764943	C	-0.39043355	2.19771795	-1.15883691
C	-1.17049172	3.85251697	-0.64771444	C	-0.49194259	3.57477754	-0.55826110
O	3.37772219	-0.63685373	0.76017894	O	1.44121075	1.59059934	1.51964498
C	2.12849082	1.34891733	1.12815009	C	3.03901962	0.70163229	-0.01444914
O	-2.25007306	2.10125988	0.56097185	O	0.52328846	1.90874698	-1.92058878
C	-1.83943016	-2.10098281	1.18878058	C	-1.66081435	-2.18099390	-0.34733976
O	0.43515991	-1.76394885	1.96023459	O	-2.14372055	-1.90782295	2.00935737
H	1.53515273	-2.15617679	-1.87326429	H	1.74394327	-2.30735009	-0.12402104
H	2.34798098	-2.42197684	-0.33307851	H	2.15527302	-1.71928964	1.48477272
H	-0.55339682	-2.91315208	-1.04939999	H	0.23568568	-2.60161062	2.46885027
H	0.40103401	-3.72542826	0.19409705	H	0.09387049	-3.61733436	1.02374469
H	-0.24385961	0.35643144	0.93813939	H	-0.39311740	-0.15178305	2.15415715
H	1.37950017	0.10902424	-1.29077335	H	0.62779406	-0.37713112	-0.70700454
H	-2.19657914	-0.21264598	-0.60170790	H	-2.59369024	0.40414965	0.82353739
H	-1.02146164	-0.69925654	-1.82354362	H	-1.44862566	1.64533346	1.27105374
H	-1.66703761	1.57843481	-2.31281614	H	-2.44402647	1.73710398	-1.07576081
H	-0.04156108	1.68432854	-1.69796456	H	-1.41301202	0.36680750	-1.52588603
H	-0.11668816	3.96966367	-0.36197552	H	-0.84220225	3.54996487	0.47684075
H	-1.23874196	4.09938075	-1.71235241	H	0.46599213	4.09365682	-0.62484363
H	-1.77982280	4.53478188	-0.05218657	H	-1.24082718	4.13343364	-1.13559470
H	3.09064204	1.81557762	1.35050759	H	3.58711123	1.62833565	0.16524921

H	1.53210488	1.99139088	0.47307666	H	3.63740184	-0.14662326	0.34011810
H	1.57555979	1.23637615	2.06891059	H	2.88089634	0.55428526	-1.08791653
H	-1.86372517	-3.05303170	1.73179217	H	-0.89612124	-2.10523563	-1.12802729
H	-2.49532803	-2.19696929	0.31885559	H	-2.51635165	-1.55950162	-0.63064414
H	-2.23598520	-1.31876976	1.84534112	H	-1.99137182	-3.22611776	-0.31102203
H	0.47907693	-2.66712092	2.30137835	H	-2.52829301	-2.78949642	1.91984144



The optimized conformers of (1*S*, 4*R*, 5*R*)-**7**.

Table S10. Free energy summary of conformer set in CH_3OH of compound **7**

	Conformer No.	Energy (kcal/mol)	Relative Energy (kcal/mol)	proportion of various comformations
(1*R*, 4*S*, 5*S*)-**7**	1	-435961.242489801	0.000000000	41.59%
	2	-435959.719001851	1.523487950	3.17%
	3	-435961.078823430	0.163666371	31.54%
	4	-435960.537016559	0.705473242	12.63%
	5	-435960.374270206	0.868219595	9.60%
	6	-435958.417508329	2.824981472	0.35%

	7	-435959.032735703	2.209754098	1.00%
	8	-435957.758709635	3.483780166	0.12%
(1*S*, 4*R*, 5*R*)-**7**	1	-435961.500720786	0.000000000	29.33%
	2	-435959.155903245	2.344817540	0.56%
	3	-435959.006995503	2.493725283	0.43%
	4	-435961.172967056	0.327753730	16.86%
	5	-435957.800420450	3.700300336	0.06%
	6	-435961.109293971	0.391426815	15.14%
	7	-435959.301250282	2.199470504	0.71%
	8	-435961.146946669	0.353774117	16.14%
	9	-435961.282962602	0.217758184	20.31%
	10	-435959.023230829	2.477489957	0.45%

Table S11. Anticancer activity of the ethanol extract from the root tuber of *Curcuma phaeocaulis* Valeton (CP). (n = 3)

Cell line	Concentration (μg/mL)	Inhibition rate of cell growth (%)			IC_{50} (μg/mL)
		1	2	3	
4T1	125	9.39	12.48	13.75	789.40 ± 16.24
	500	39.45	40.26	39.45	
	1000	62.53	62.53	64.71	
	1500	67.24	66.49	69.68	
	2000	79.04	81.89	76.26	
	2500	83.40	84.15	83.40	
	3000	84.52	86.21	88.66	

	3500	87.72	88.47	86.96	
	4000	89.78	88.84	88.47	
CT26	500	14.74	14.74	15.92	2318.45 ± 46.70
	1000	28.29	29.68	32.16	
	1500	38.45	37.65	36.47	
	2000	46.41	45.22	45.88	
	2500	63.35	63.55	63.40	
	3000	70.55	70.92	70.90	
	3500	80.48	80.28	80.77	
	4000	90.24	90.62	90.49	
HepG2	500	12.44	9.33	10.88	1474.84 ± 45.03
	1000	31.09	34.72	32.64	
	1500	54.40	52.33	54.92	
	2000	68.91	67.88	67.36	
	2500	80.31	80.31	79.79	
	3000	87.56	89.12	87.56	
	3500	90.16	90.16	91.19	
	4000	93.78	93.26	93.26	
A549	500	12.98	9.63	11.47	2322.24 ± 15.95
	750	11.47	12.65	10.80	
	1000	12.31	13.49	10.13	
	1250	18.18	18.85	18.18	
	1500	28.75	22.71	30.26	
	2000	40.99	44.68	39.65	

	2500	58.44	58.94	59.61	
	3000	74.37	75.04	73.53	
	3500	88.80	90.47	89.30	
Hela	1500	3.86	2.60	2.60	3061.49 ± 16.31
	2000	9.11	9.39	9.31	
	2500	29.26	29.38	29.70	
	3000	43.67	43.80	43.22	
	3500	69.95	70.02	69.03	
	4000	82.53	83.28	82.78	

Table S12. The mortality rate at different concentrations of CP on 3-6 dpf zebrafish. (n = 9)

Concentration (μg/mL)	Mortality rate (%)								
	1	2	3	4	5	6	7	8	9
1200	100	100	100	100	100	100	100	100	100
1100	100	100	100	100	100	100	90	100	100
1000	100	100	100	90	90	100	100	95	100
900	100	95	90	85	90	95	80	95	75
850	65	35	75	70	70	35	90	95	85
800	40	50	55	60	60	65	70	35	45
750	50	65	30	10	15	10	15	30	25
700	5	5	10	10	10	20	20	25	5
600	0	0	5	5	0	0	10	10	20
500	0	5	0	0	0	0	5	5	0
400	0	0	0	0	0	0	0	0	0

LC_{50} (µg/mL)	789.4 ± 16.24

Table S13. Cell viability of 4T1 cells with different concentrations of compound **2**, **3**, **5**, **8**-**16**. (n = 3)

Compound \ Concentration (μM)		Cell viability (%)								IC_{50} (μM)
		0	50	100	200	400	600	800	1000	
2	1	101.99	95.69	97.02	101.99	96.91	100.88	96.69	97.68	-
	2	99.01	96.02	95.36	103.65	104.97	97.68	99.67	96.24	
	3	99.01	95.80	95.47	97.02	101.10	97.24	100.88	104.42	
3	1	99.93	98.75	99.50	103.25	86.86	92.64	92.43	101.86	-
	2	101.54	101.96	99.18	107.00	101.00	97.46	99.07	101.43	
	3	98.54	95.00	93.82	98.32	110.32	102.61	102.82	104.96	
5	1	100.28	97.59	94.29	94.50	86.65	69.31	47.43	43.10	942.26 ± 22.89
	2	100.07	97.80	96.35	88.51	84.59	69.52	46.81	43.31	
	3	99.66	97.59	92.23	82.52	84.79	64.36	49.29	45.99	
8	1	101.55	102.07	103.36	86.05	80.13	80.30	68.15	57.71	＞1000

	2	102.19	99.49	97.09	78.48	74.49	77.31	65.81	62.70	
	3	96.26	98.55	99.20	82.88	84.23	75.67	63.69	62.23	
9	1	95.49	104.79	99.82	98.93	63.78	18.23	0.05	0.21	371.84 ± 27.78
	2	96.44	101.41	92.43	93.43	55.96	14.06	0.26	0.16	
	3	108.07	93.43	97.18	94.65	56.70	16.70	0.11	0.16	
10	1	103.15	105.65	102.69	100.42	97.23	106.67	96.32	108.38	-
	2	98.14	93.93	101.10	95.75	95.98	95.30	100.64	111.34	
	3	98.71	93.14	88.25	87.22	96.44	99.39	104.06	104.74	
11	1	93.75	106.14	103.34	105.17	93.75	106.58	98.81	105.93	-
	2	106.58	95.69	101.83	98.81	91.70	109.81	98.38	94.83	
	3	99.68	90.30	94.72	98.71	99.68	83.19	97.84	103.56	
12	1	94.65	99.73	101.69	98.91	98.42	112.17	95.96	86.14	-
	2	100.87	99.24	104.48	105.46	95.63	92.69	98.09	115.94	
	3	104.48	98.91	97.43	95.80	94.16	100.22	103.49	111.03	

13	1	100.38	107.15	99.25	94.73	94.35	100.00	117.70	99.62	-
	2	97.74	100.75	106.78	97.74	105.65	94.73	100.75	97.74	
	3	101.88	92.47	93.60	96.61	102.64	105.65	88.70	100.38	
14	1	101.99	96.03	93.64	97.22	87.28	84.50	99.21	99.60	-
	2	102.78	101.19	101.99	98.41	81.72	115.50	94.44	105.17	
	3	95.23	96.82	95.63	90.86	110.73	82.91	100.00	100.79	
15	1	95.56	104.82	103.04	100.00	105.20	105.45	103.17	85.29	-
	2	105.83	103.17	95.69	95.82	105.83	92.39	81.36	96.58	
	3	98.61	109.00	100.76	104.95	91.50	100.51	98.35	109.51	
16	1	100.50	102.95	98.43	103.14	100.50	100.13	100.31	71.85	＞1000
	2	104.65	98.05	95.98	96.17	99.18	99.18	85.42	75.62	
	3	94.85	100.13	101.07	97.86	98.62	100.88	94.09	71.10	

"-" means that the compound did not show inhibitory activity on the growth of 4T1 cancer cells.

Table S14. Cell viability of 4T1 cells with different concentrations of cisplatin (positive control) and the equal mixture of compound **2**, **3**, **5**, **8-16**. (n = 3)

Drug	Concentration (μM)	Cell viability (%)			IC_{50} (μM)
		1	2	3	
Cisplatin	0	96.91	102.41	100.68	75.78 ± 5.38
	12.5	81.87	78.11	73.19	
	25	75.80	63.36	70.30	
	50	62.78	62.20	65.09	
	100	48.31	47.16	46.58	
	200	32.69	35.58	35.87	
	300	31.24	31.53	24.30	
	400	14.46	19.38	19.96	
	500	8.68	9.84	10.99	
Eaual mixture of tested compounds	0	106.66	96.67	96.67	188.92 ± 8.60
	50	89.98	89.64	90.33	

	100	85.81	74.87	75.91	
	200	60.10	56.63	65.14	
	300	36.65	37.00	32.83	
	400	17.37	15.81	17.89	
	500	7.12	7.99	8.34	
	600	1.91	0.69	0.00	
	800	0.69	0.52	0.69	