Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Polyketides with α-glucosidase inhibitory and neuroprotective activities from *Aspergillus versicolor* associated with *Pedicularis sylvatica*

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Table S42. Atomic coordinates (Å) of cpd-**6A**-5 obtained at the B3LYP/6-31G(d) level of theory in the gas phase.

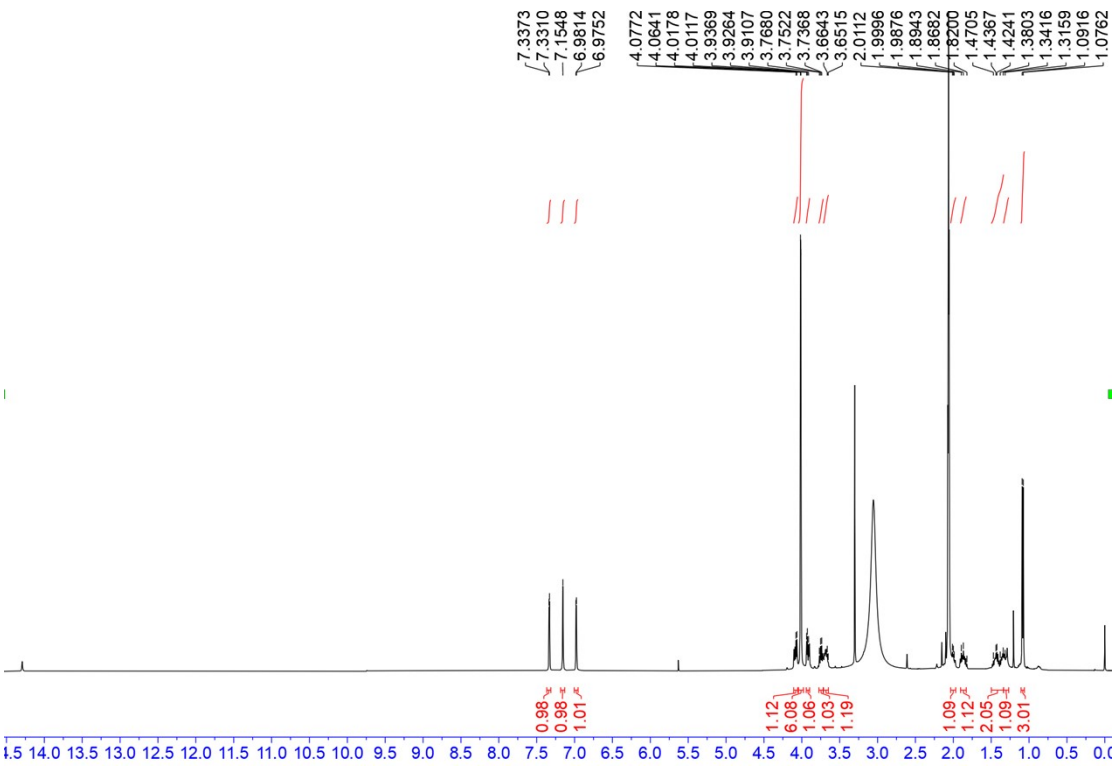


Figure S1. The ^{1}H NMR spectrum of **1** in $CDCl_3$ (400 MHz).

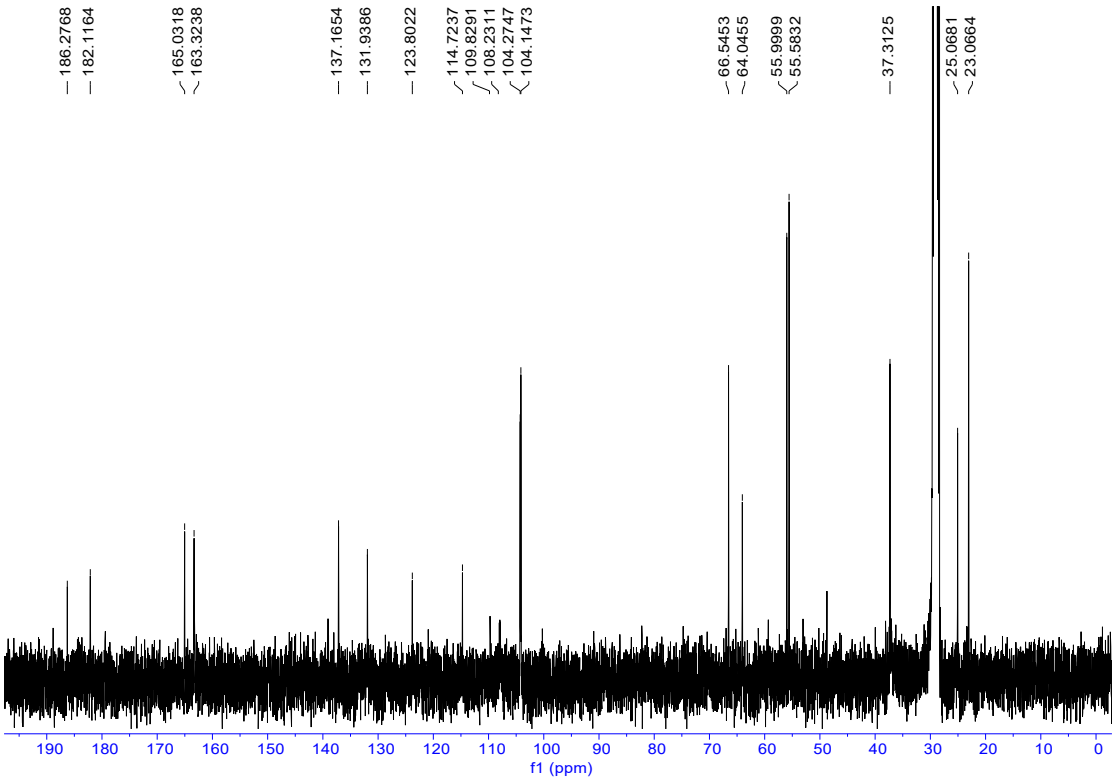


Figure S2. The ^{13}C NMR spectrum of **1** in $CDCl_3$ (100 MHz).

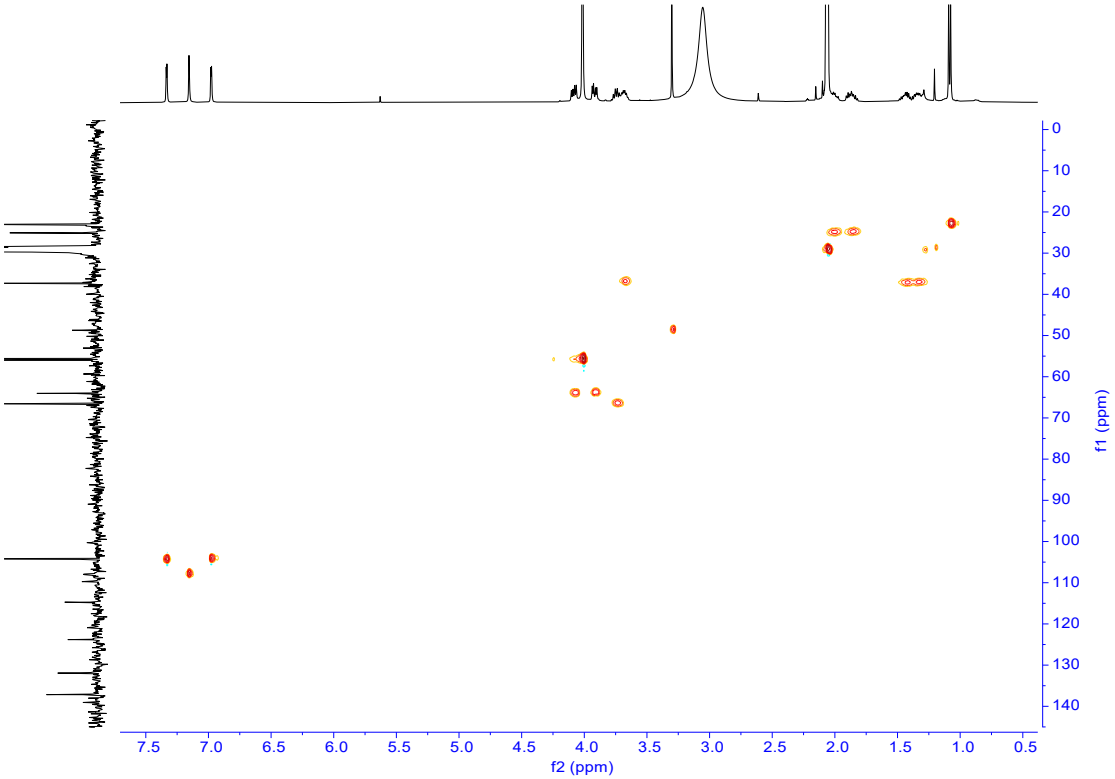


Figure S3. The HSQC spectrum of **1** in $CDCl_3$.

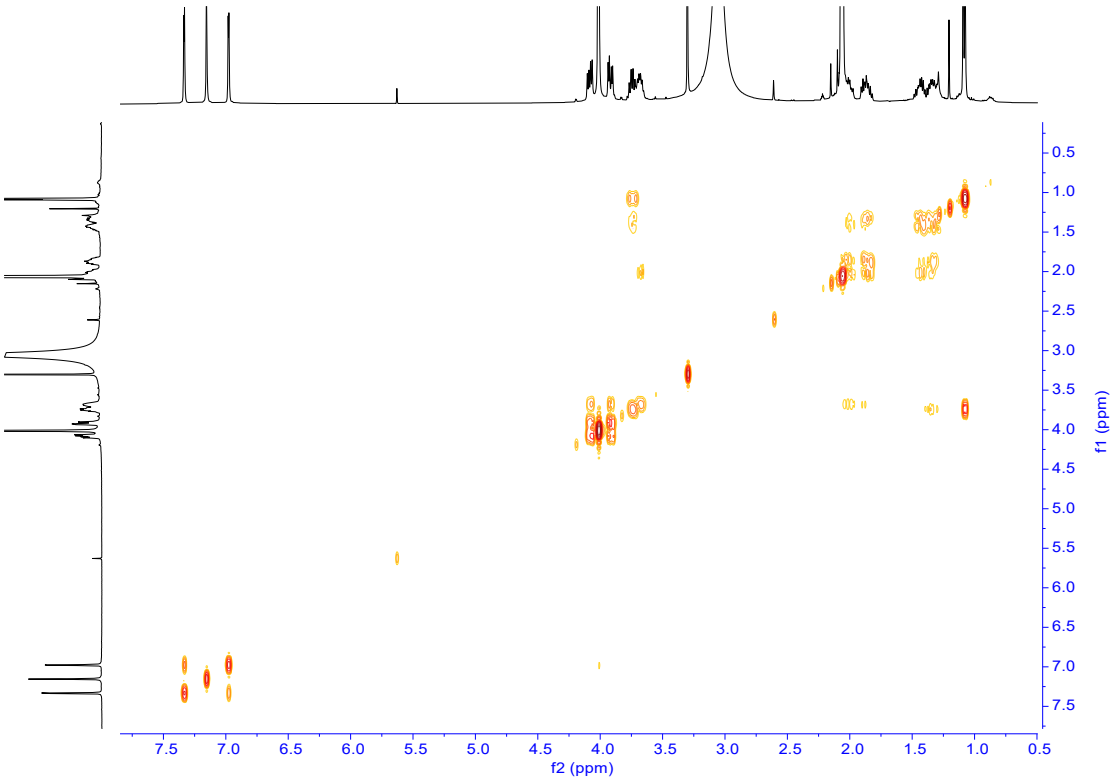


Figure S4. The $^1H-^1H$ COSY spectrum of **1** in $CDCl_3$.

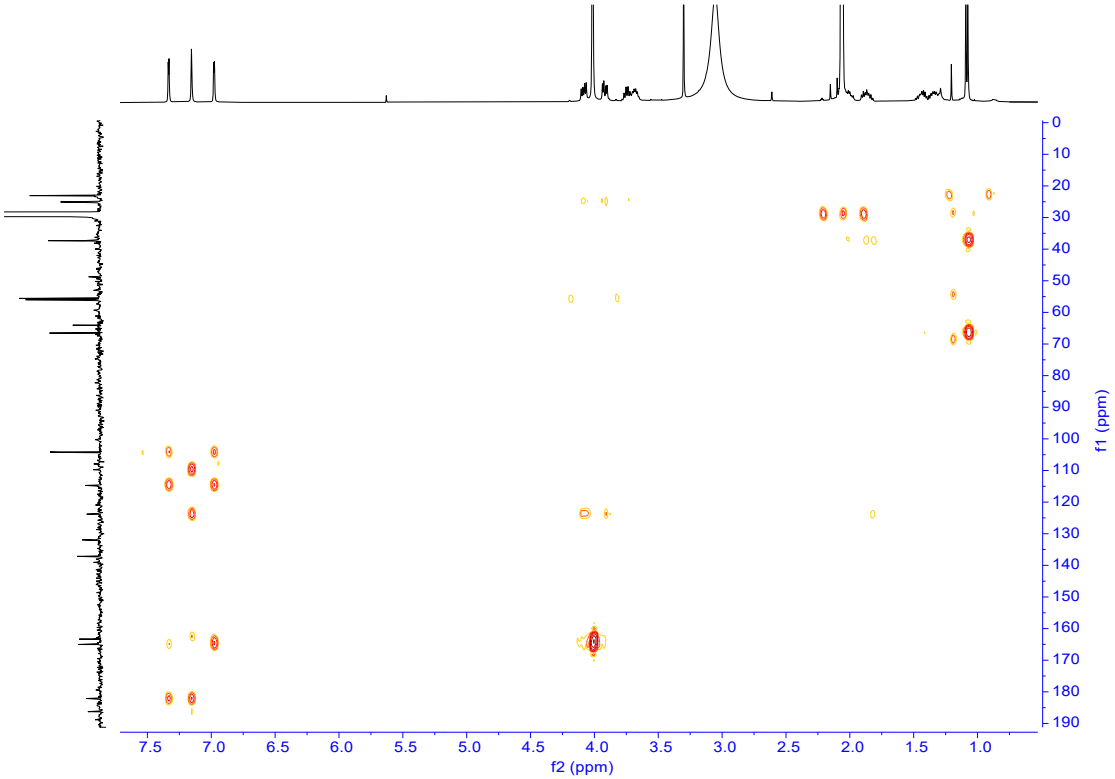


Figure S5. The HMBC spectrum of **1** in $CDCl_3$.

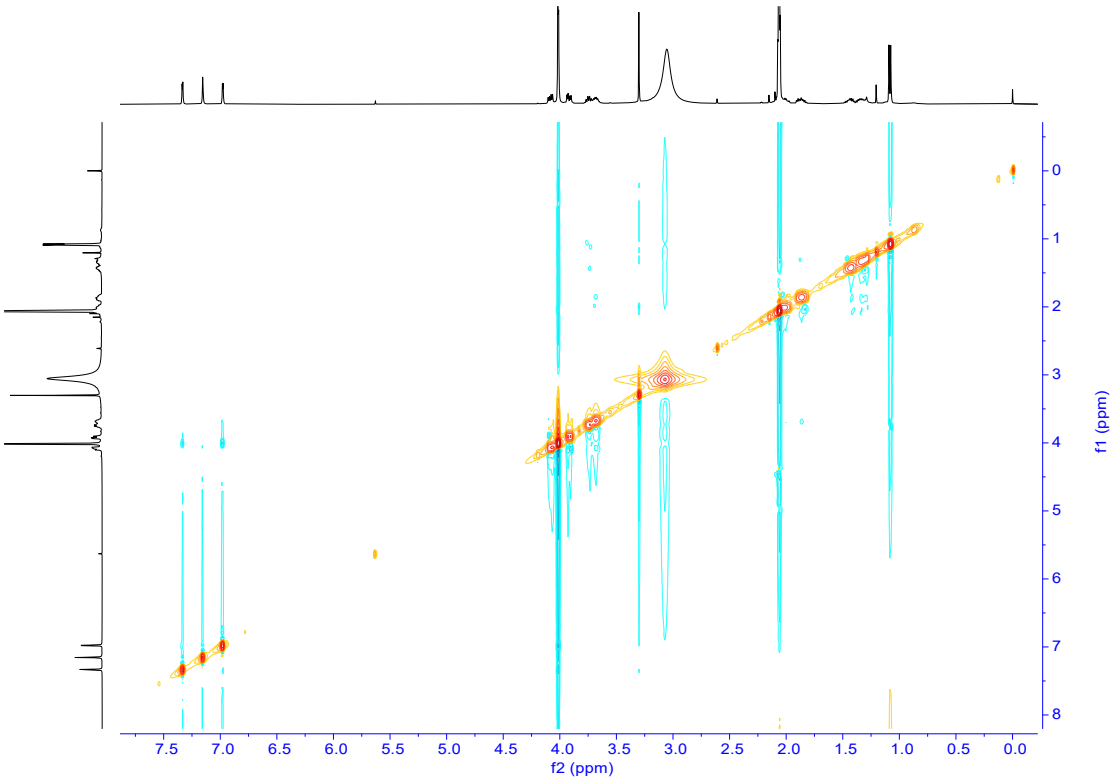


Figure S6. The NOESY spectrum of **1** in $CDCl_3$.

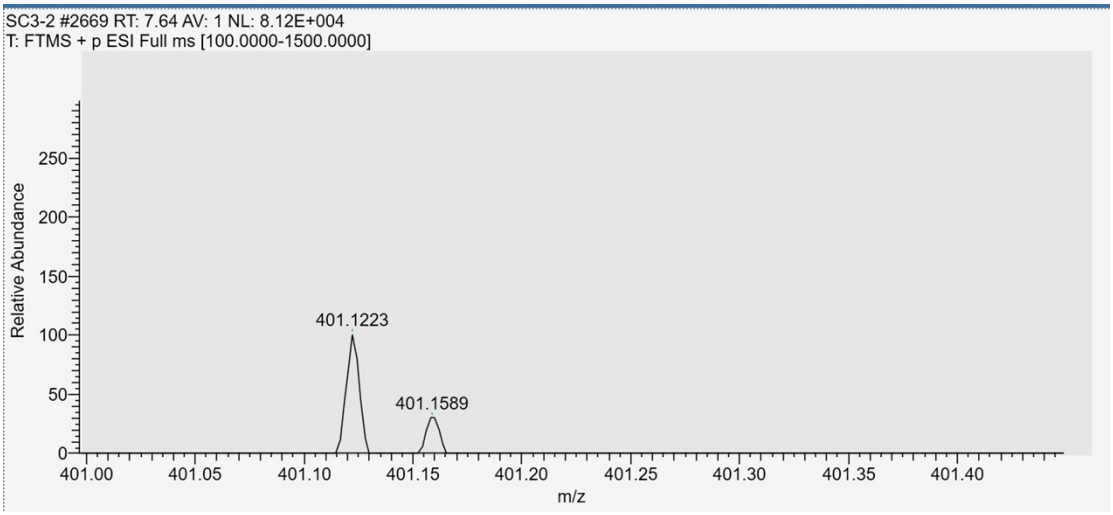


Figure S7. (+)-HRESIMS of compound **1**

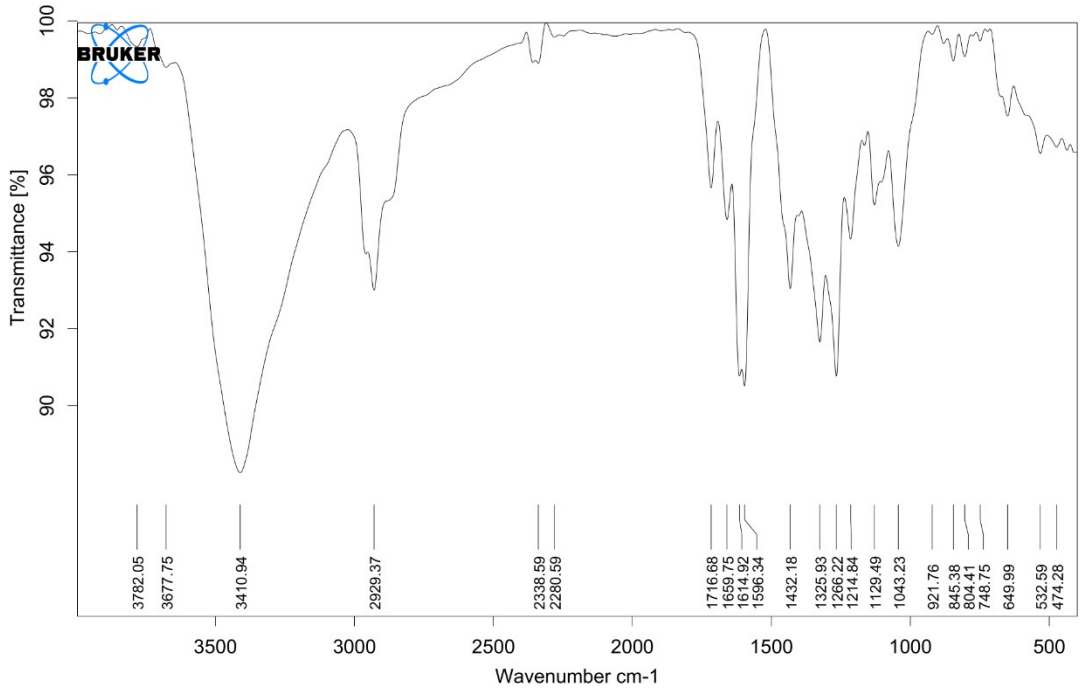


Figure S8. IR spectrum (film on KBr pellet) of compound **1**

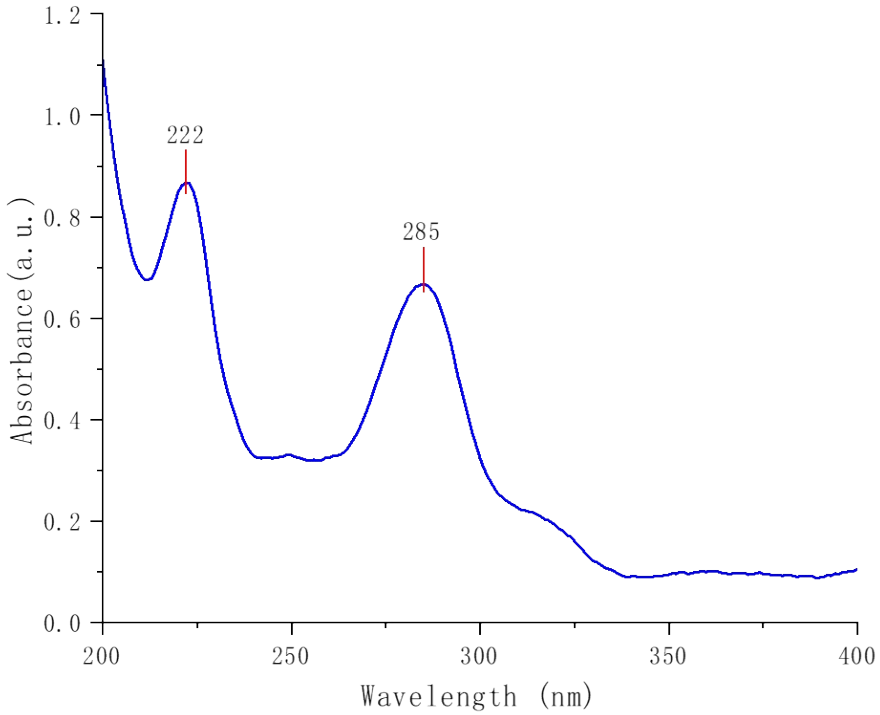


Figure S9. UV spectrum of compound **1** (MeOH)

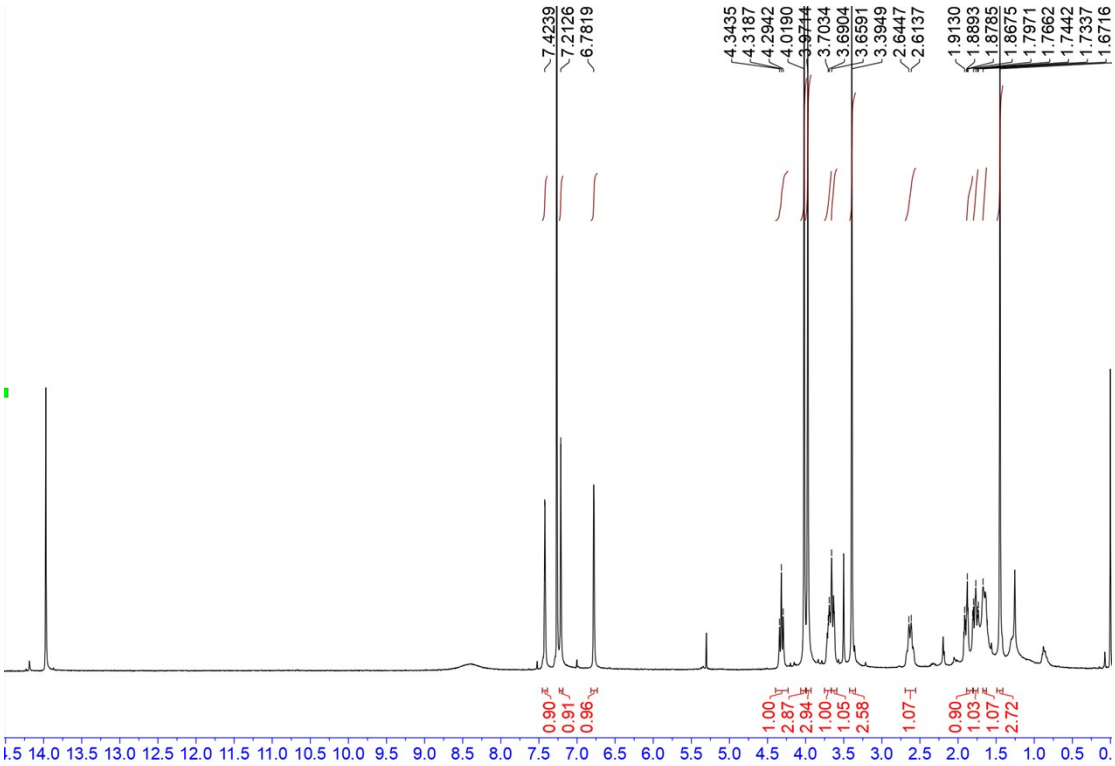


Figure S10. The ^{1}H NMR spectrum of **2** in acetone-d_6 (400 MHz).

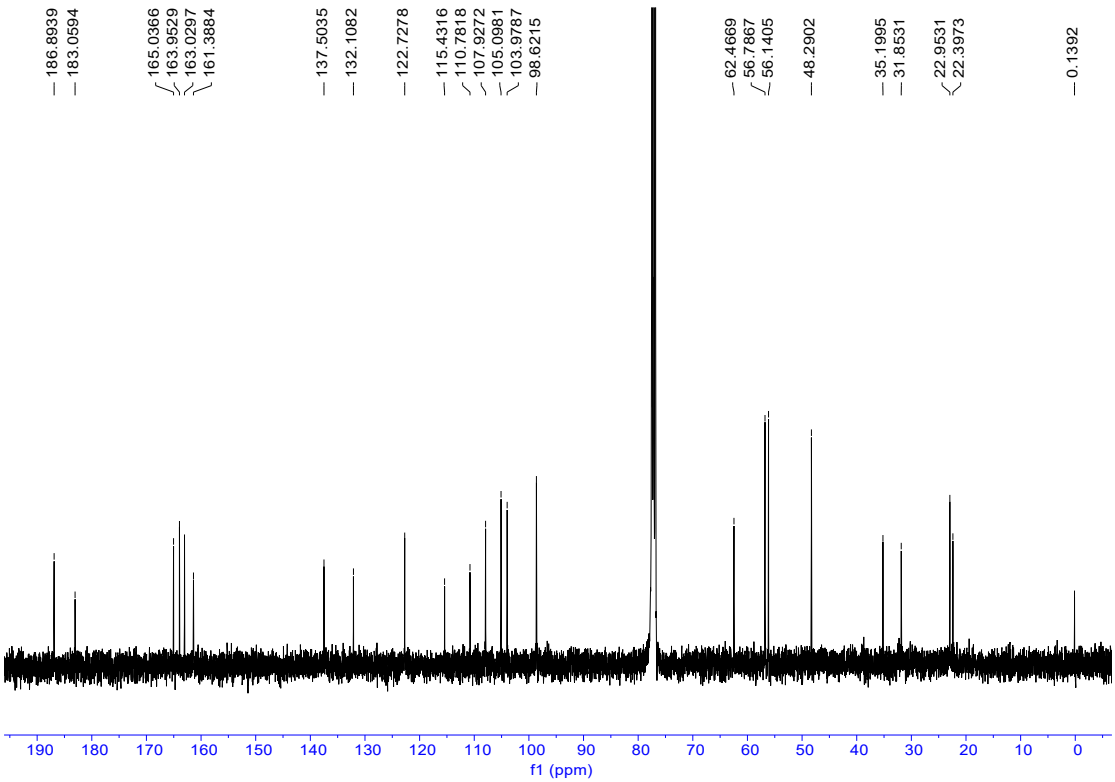


Figure S11. The ^{13}C NMR spectrum of **2** in acetone-d_6 (100 MHz) .

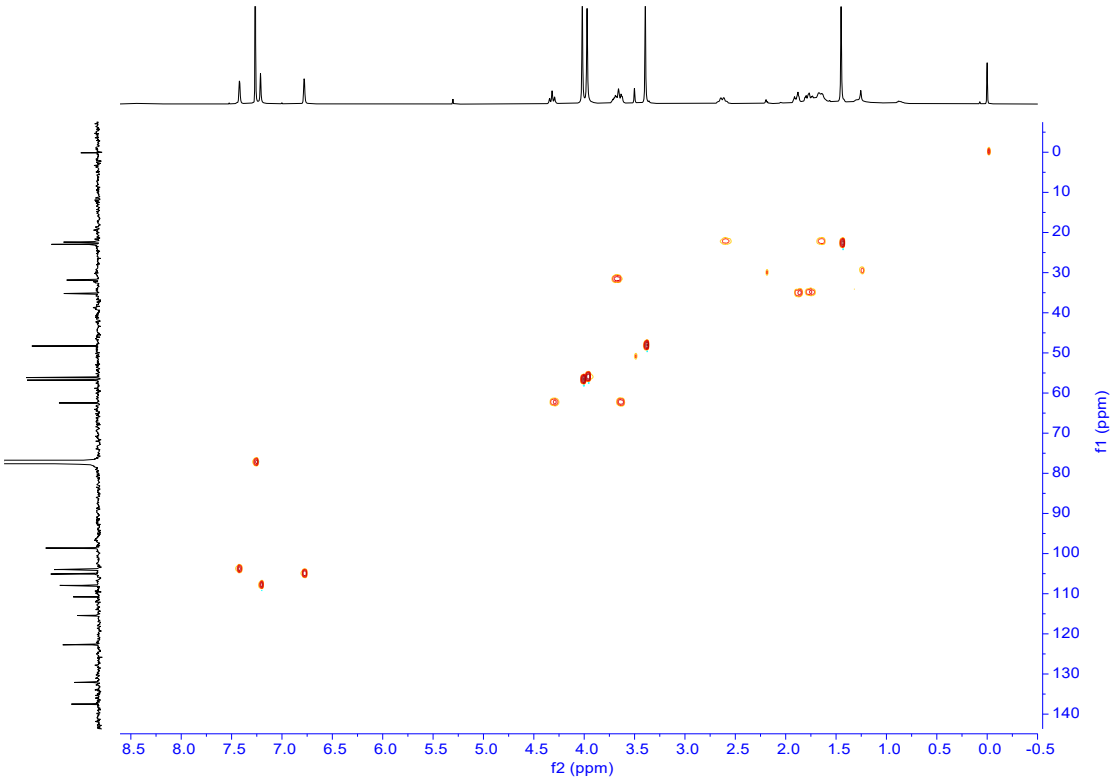


Figure S12. The HSQC spectrum of **2** in acetone-d_6.

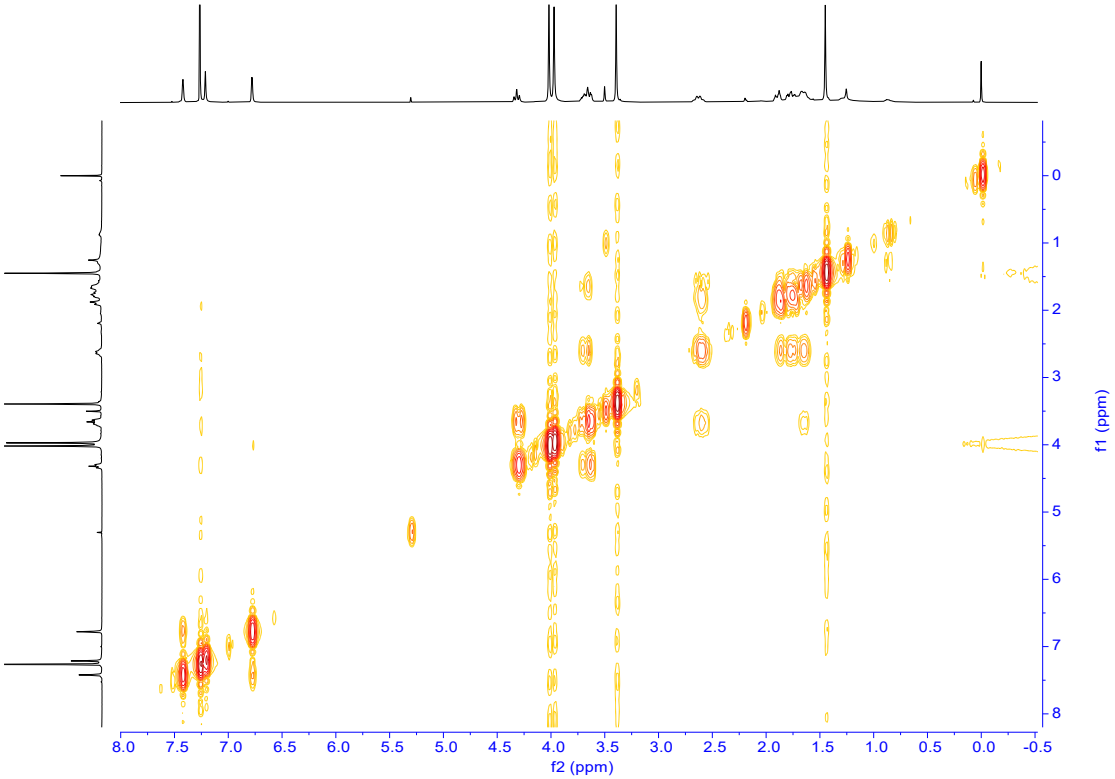


Figure S13. The $^{1}H-^{1}H$ COSY spectrum of **2** in acetone-d_6.

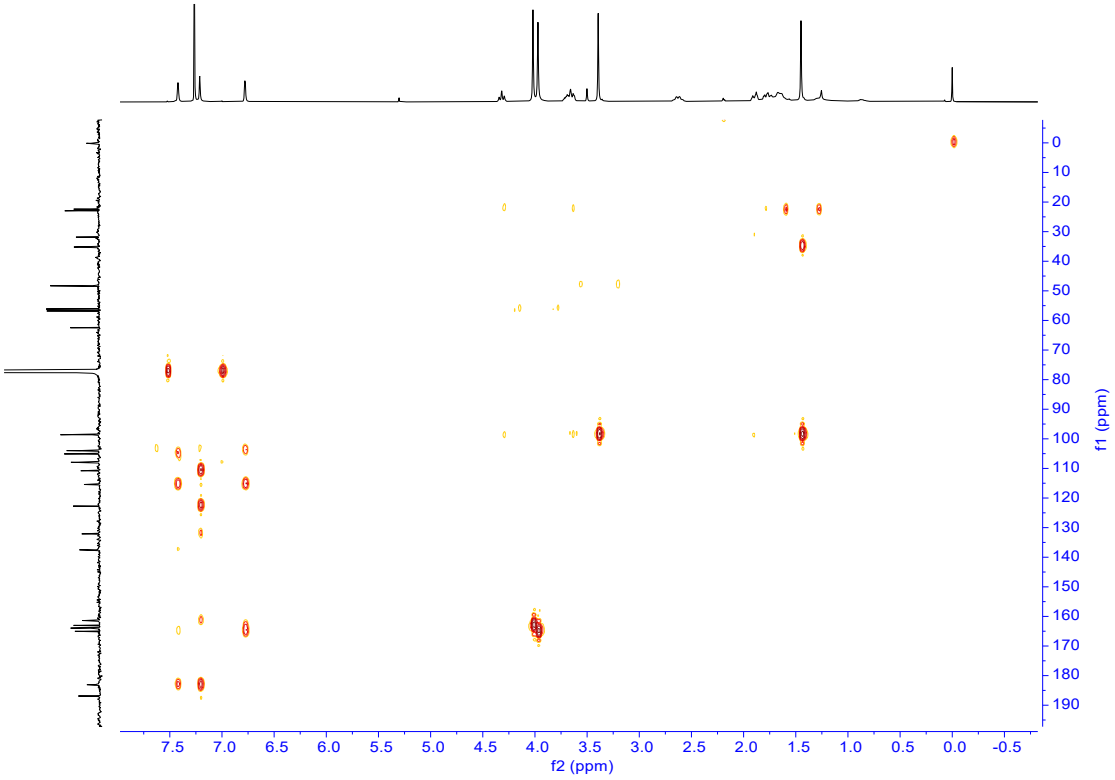


Figure S14. The HMBC spectrum of **2** in acetone-d_6.

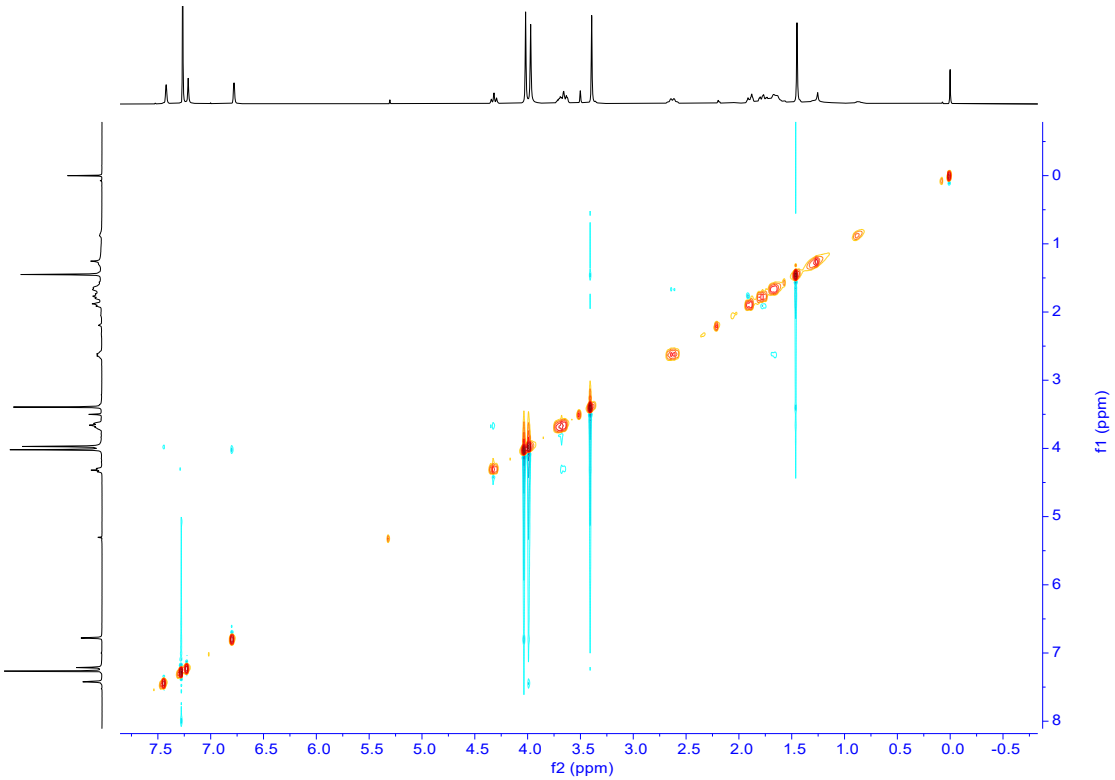


Figure S15. The NOESY spectrum of **2** in acetone-d_6.

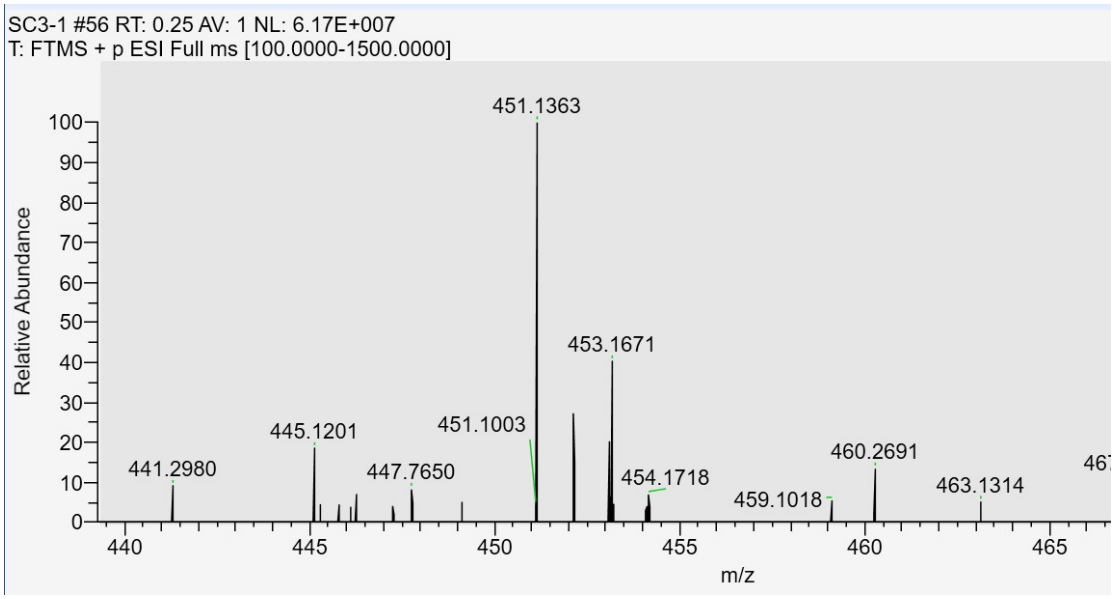


Figure S16. (+)-HRESIMS of compound **2**

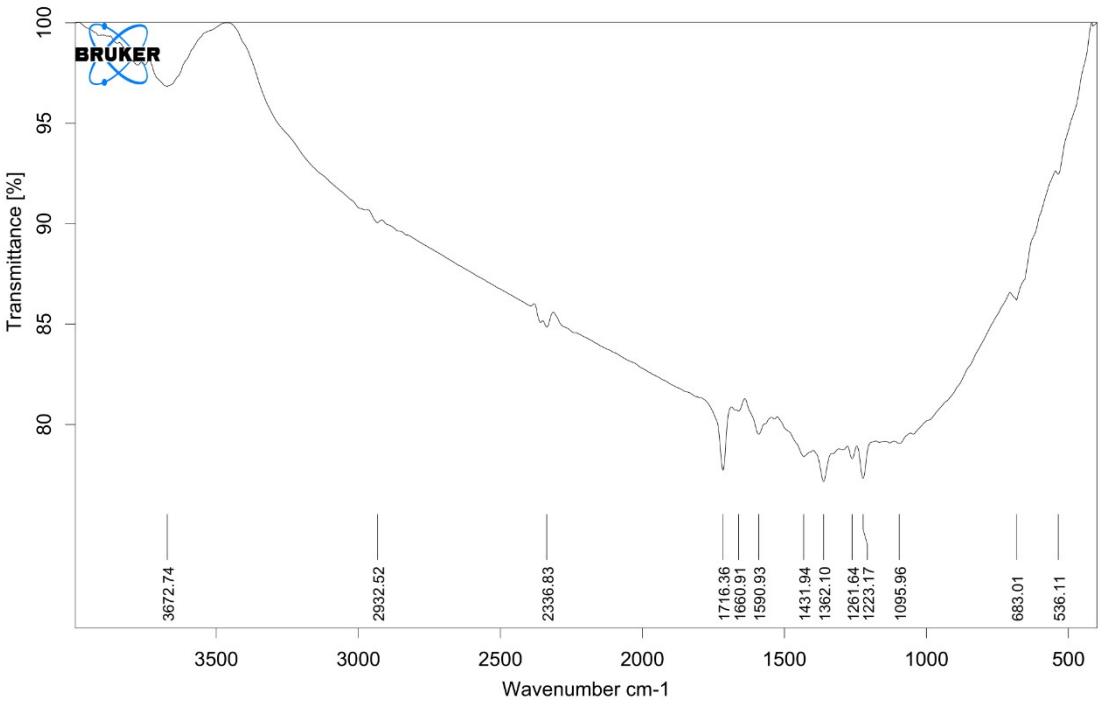


Figure S17. IR spectrum (film on KBr pellet) of compound **2**

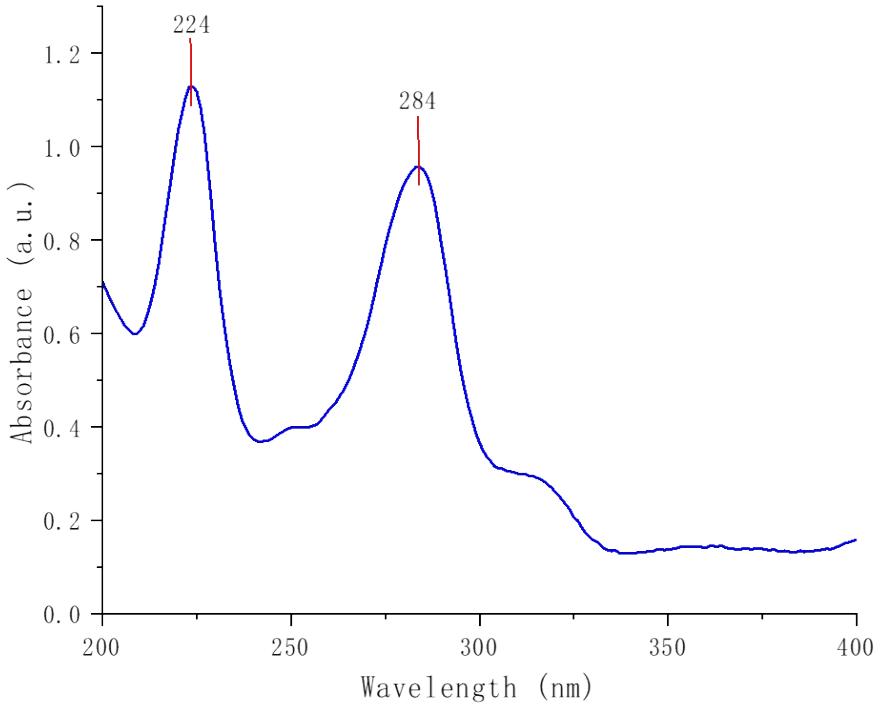


Figure S18. UV spectrum of compound **2** (MeCN)

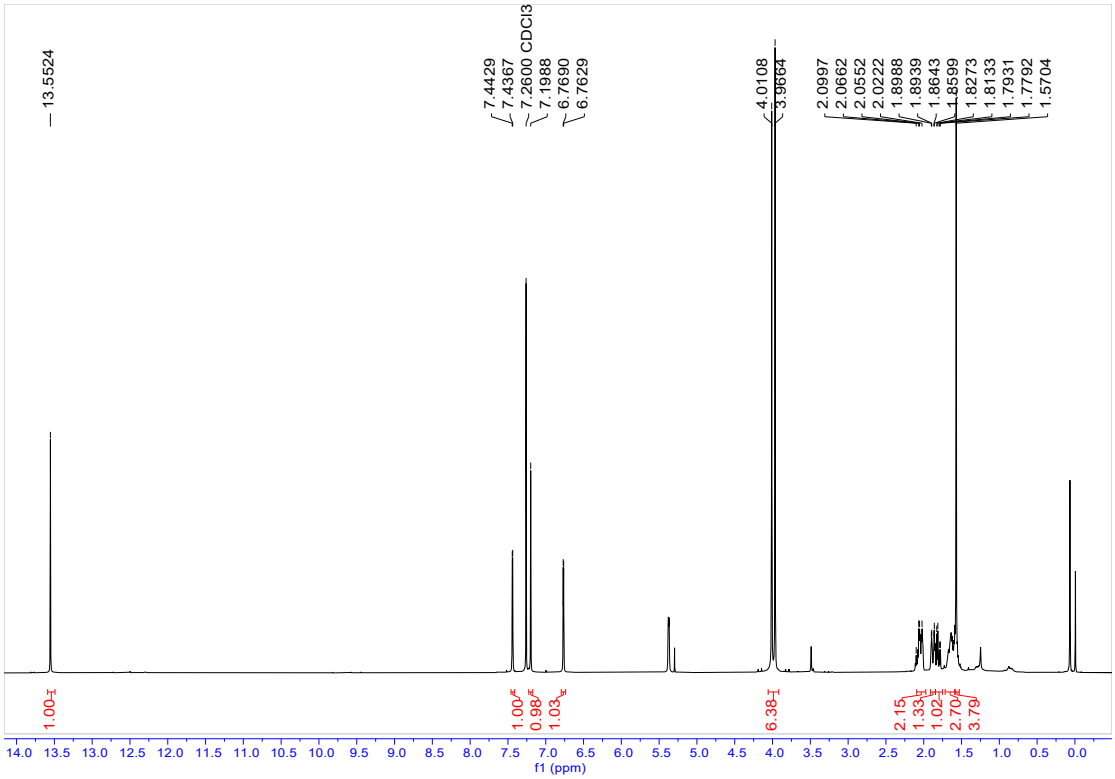


Figure S19. The ^{1}H NMR spectrum of **3** in $CDCl_3$ (400 MHz).

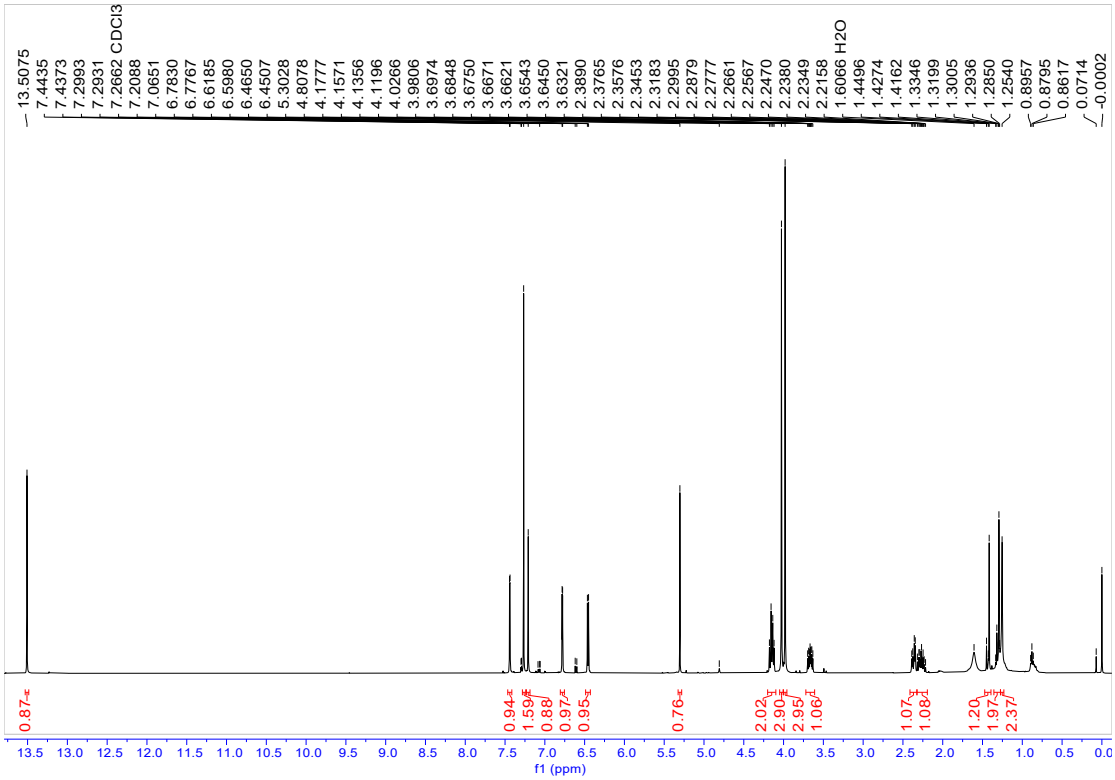


Figure S20. The ^{1}H NMR spectrum of **4** in $CDCl_3$ (400 MHz).

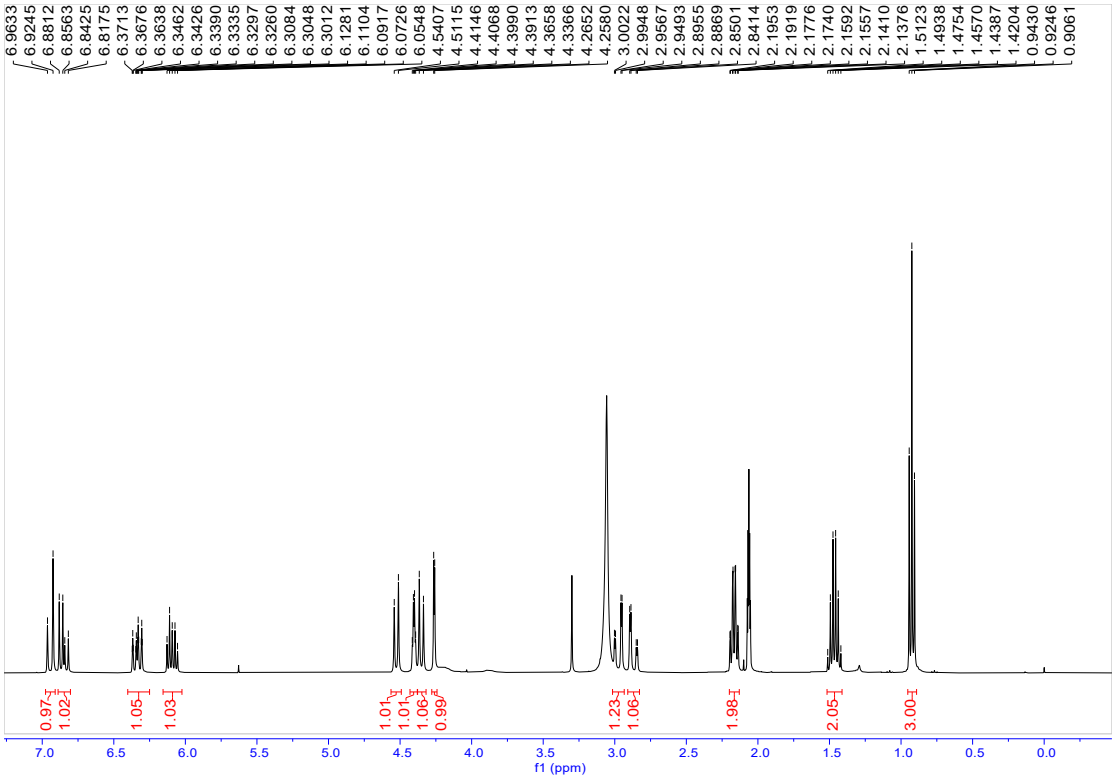


Figure S21. The ^{1}H NMR spectrum of **5** in acetone-d_6 (400 MHz).

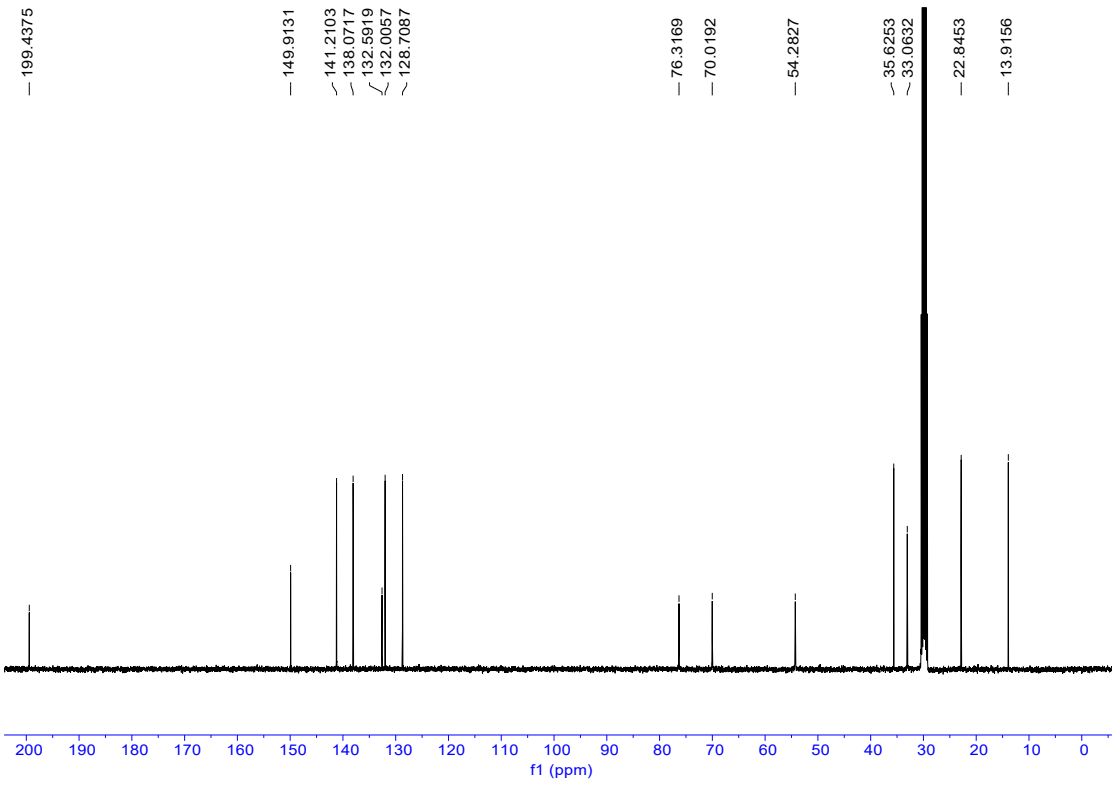


Figure S22. The ^{13}C NMR spectrum of **5** in acetone-d_6 (100 MHz).

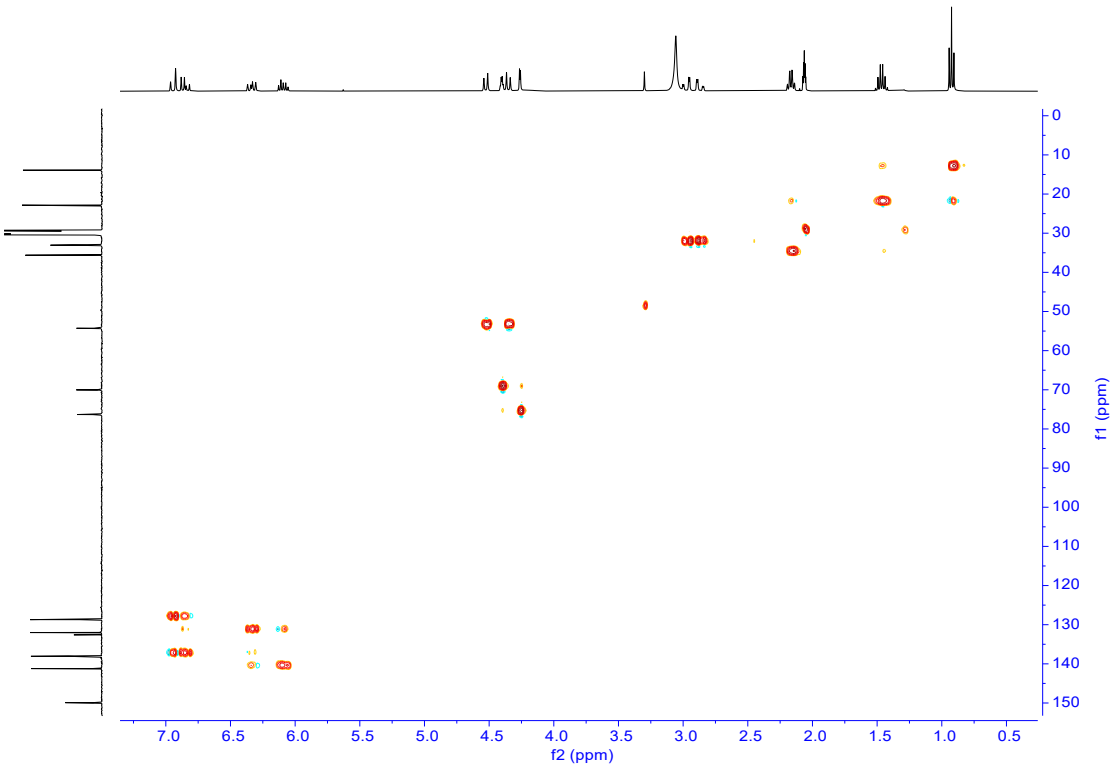


Figure S23. The HSQC spectrum of **5** in acetone-d_6.

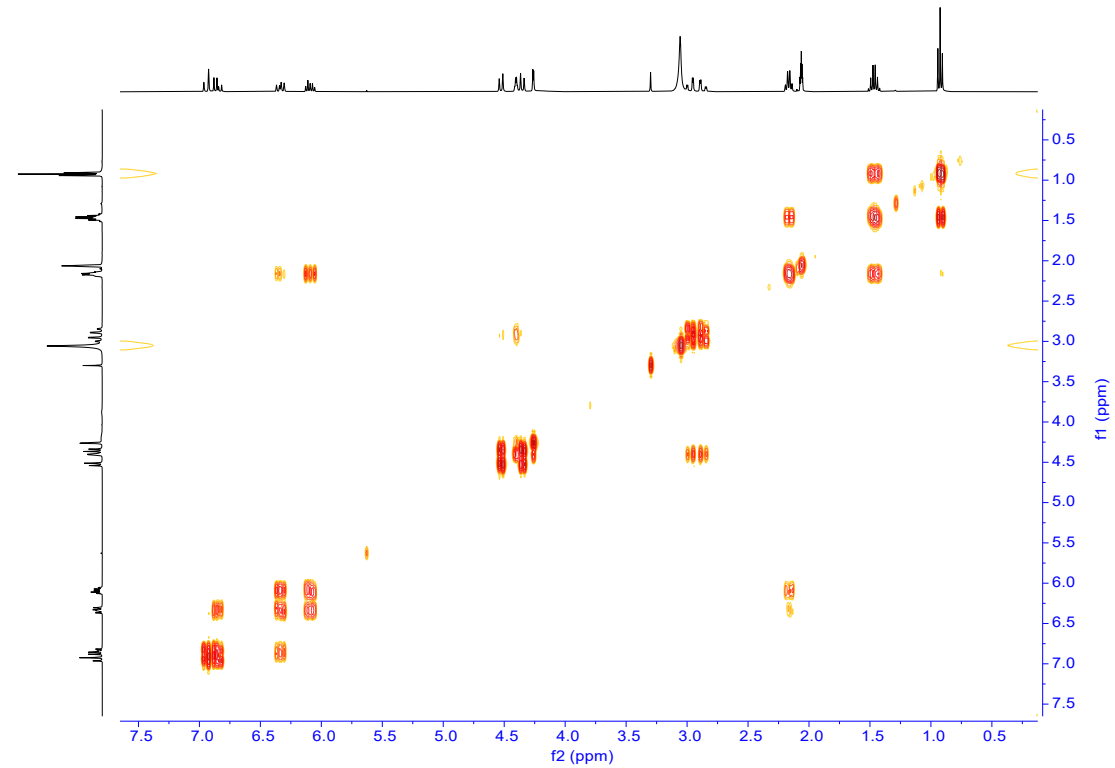


Figure S24. The ^{1}H–^{1}H COSY spectrum of **5** in acetone-d_6.

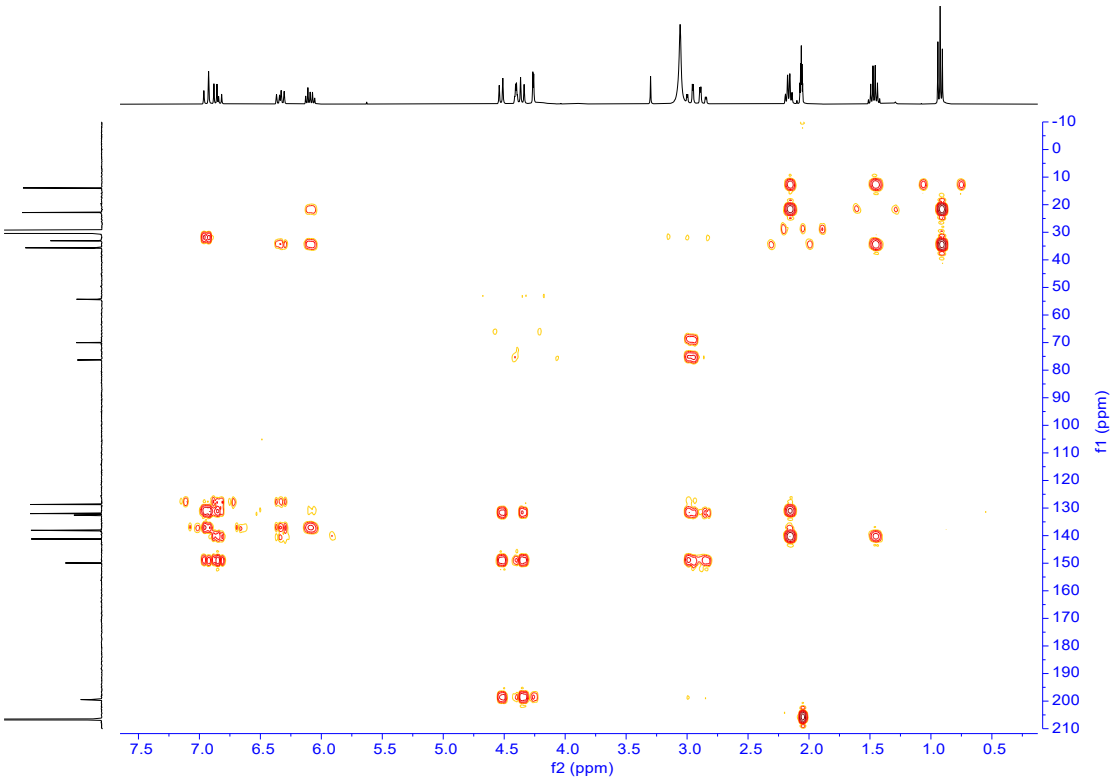


Figure S25. The HMBC spectrum of **5** in acetone-d_6.

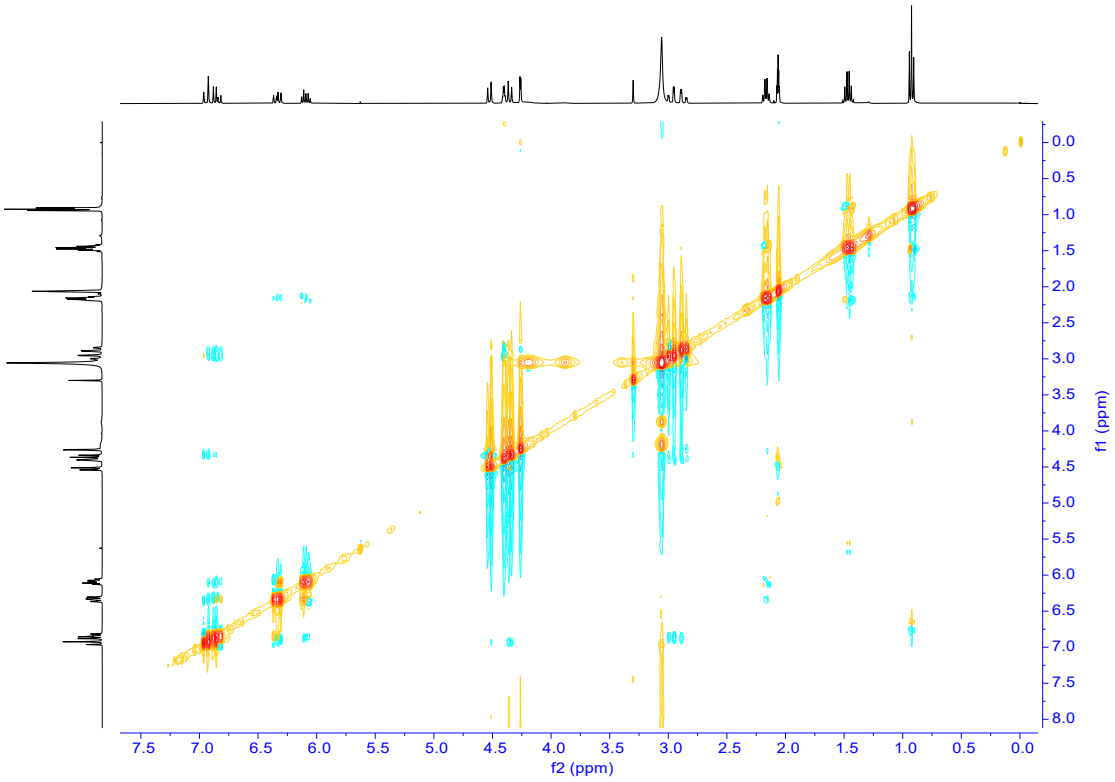


Figure S26. The NOESY spectrum of **5** in acetone-d_6.

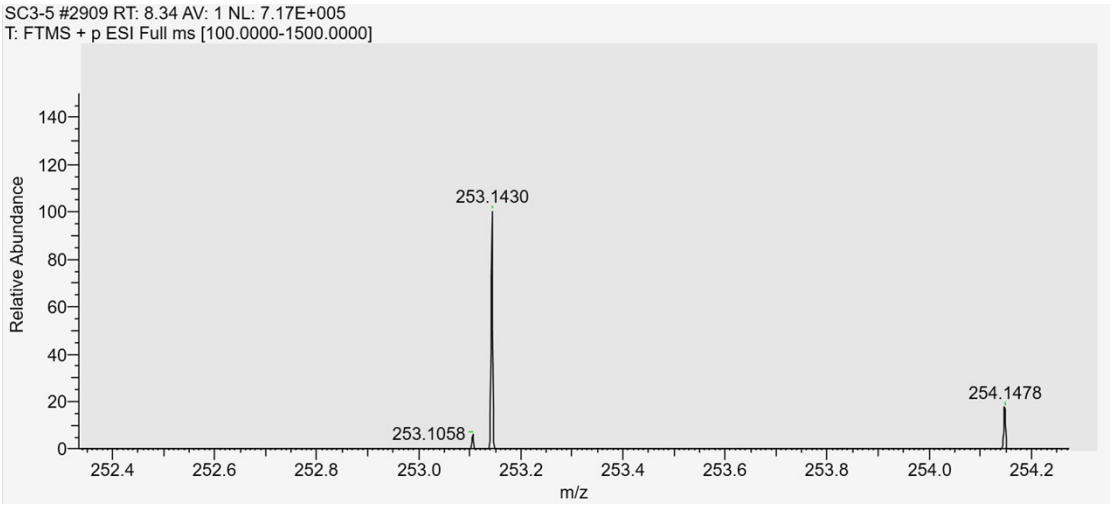


Figure S27. (+)-HRESIMS of compound **5**

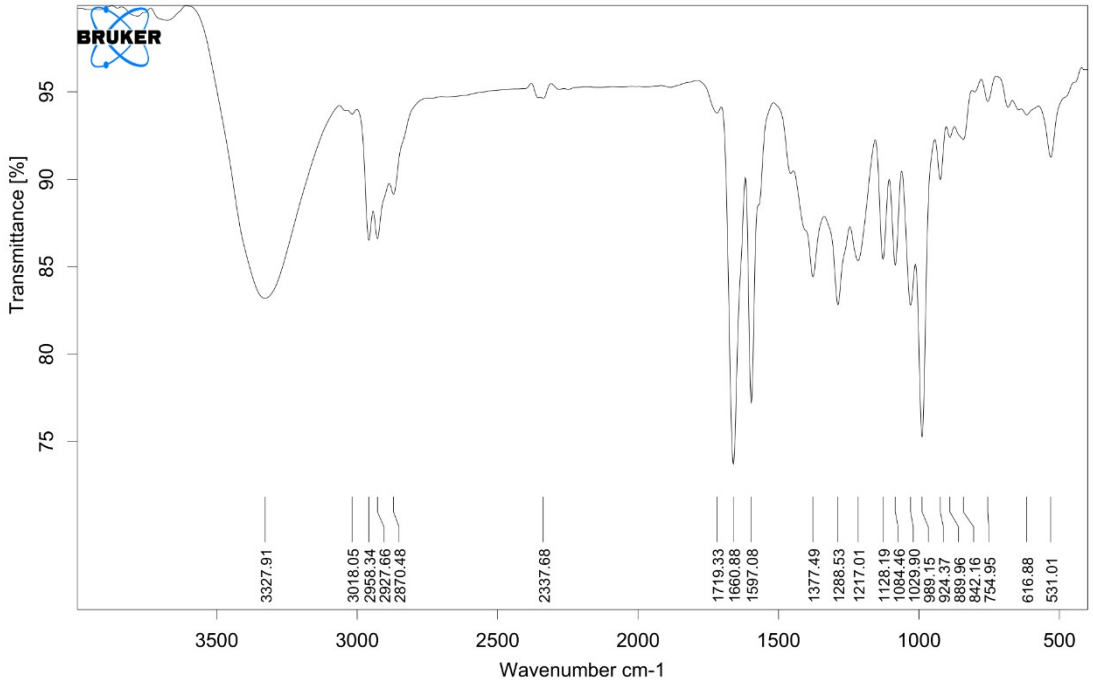


Figure S28. IR spectrum (film on KBr pellet) of compound **5**

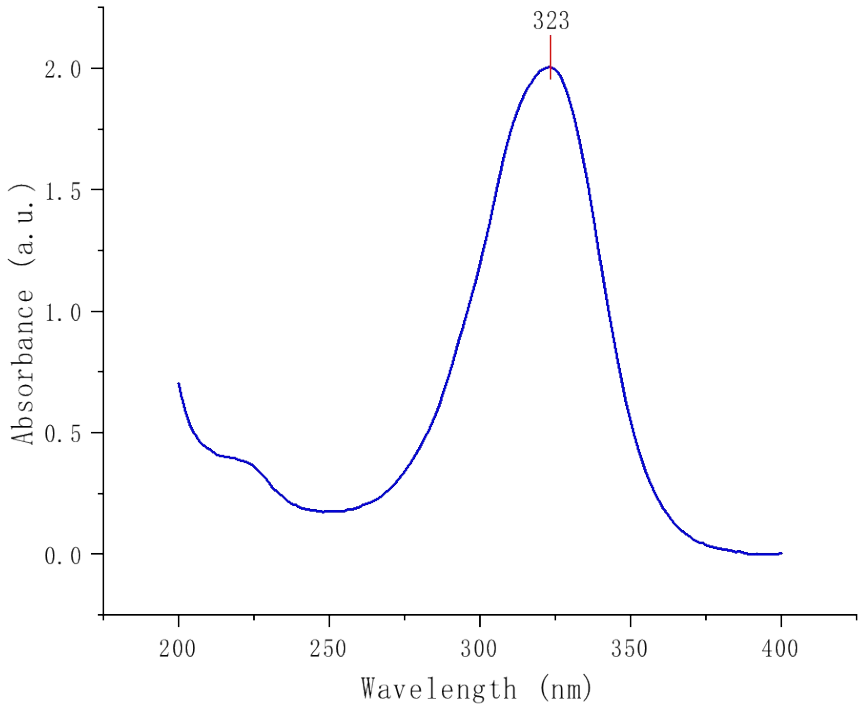


Figure S29. UV spectrum of compound **5** (MeOH)

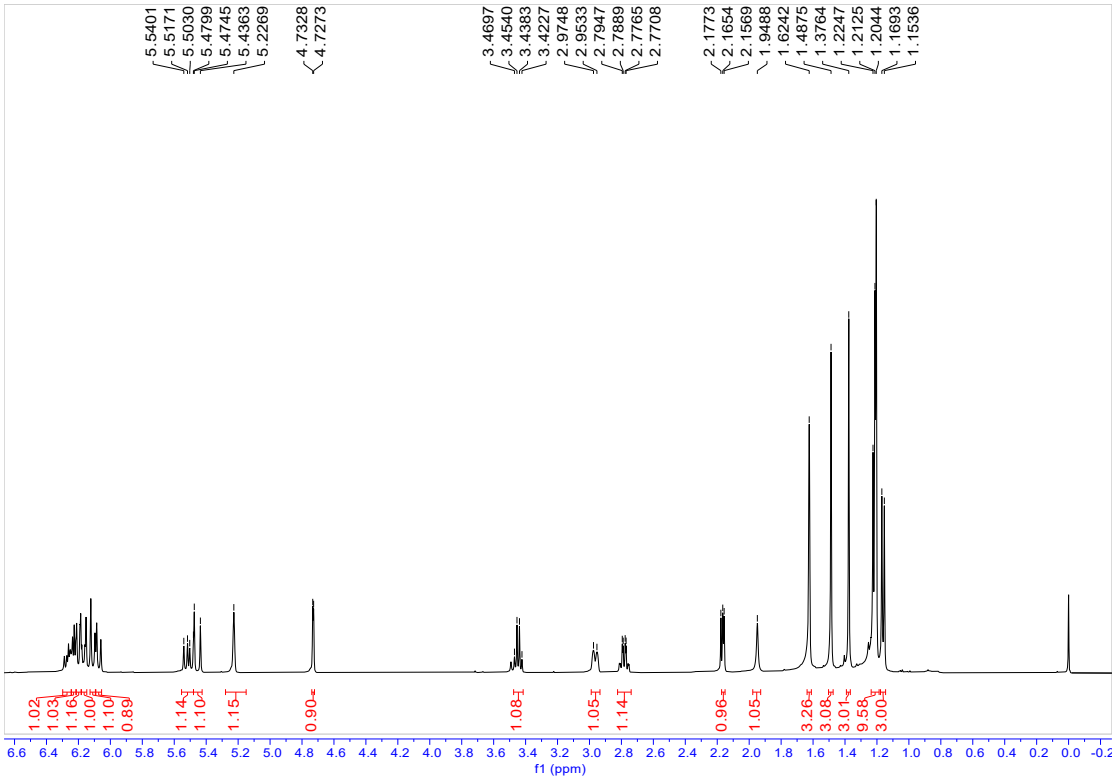


Figure S30. The ^{1}H NMR spectrum of **6** in $CDCl_3$ (400 MHz).

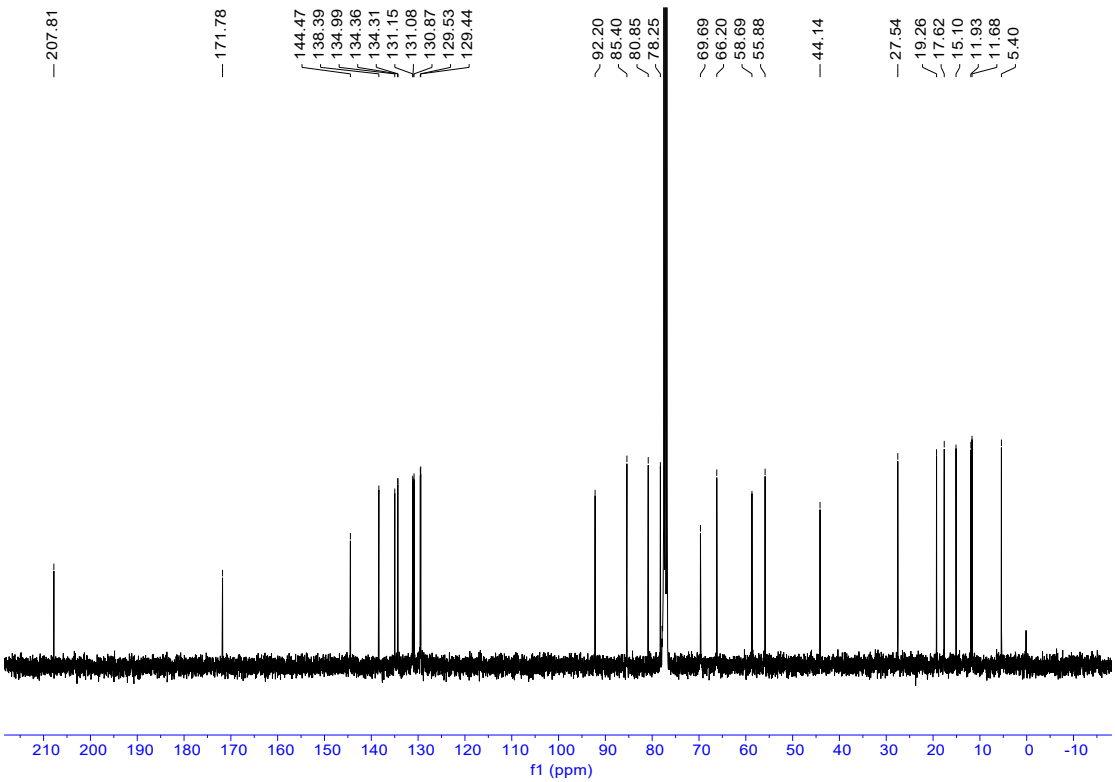


Figure S31. The ^{13}C NMR spectrum of **6** in $CDCl_3$ (100 MHz).

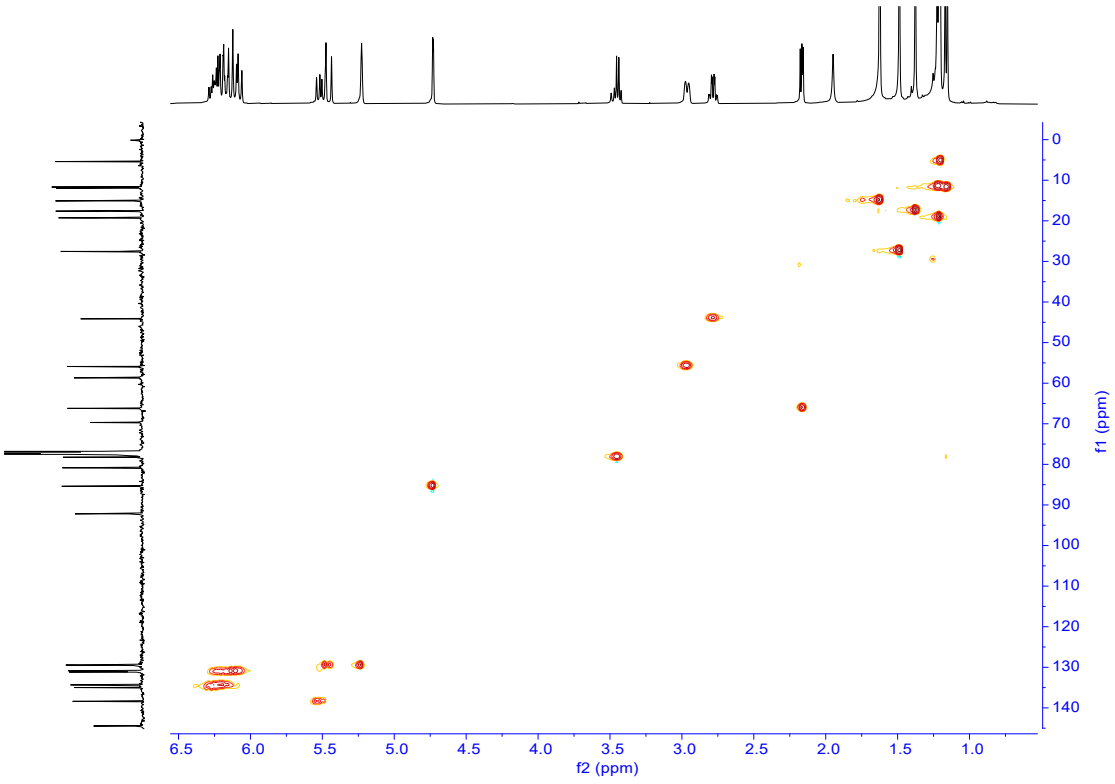


Figure S32. The HSQC spectrum of **6** in $CDCl_3$.

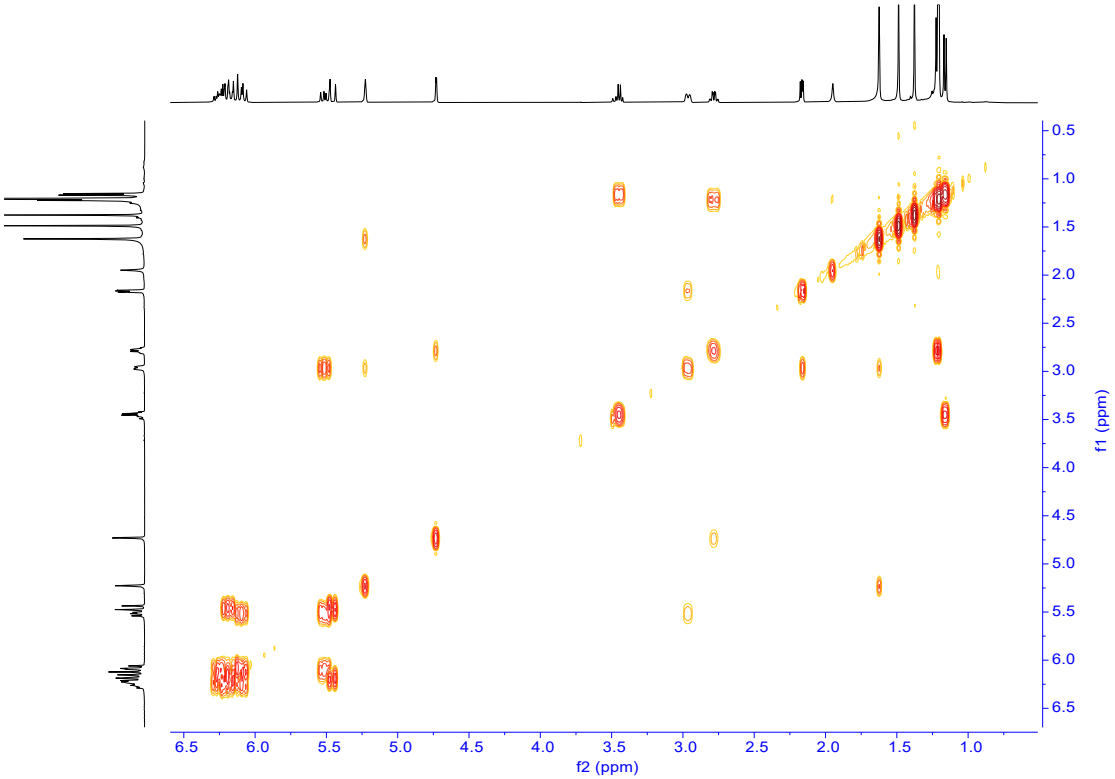


Figure S33. The $^{1}H-^{1}H$ COSY spectrum of **6** in $CDCl_3$.

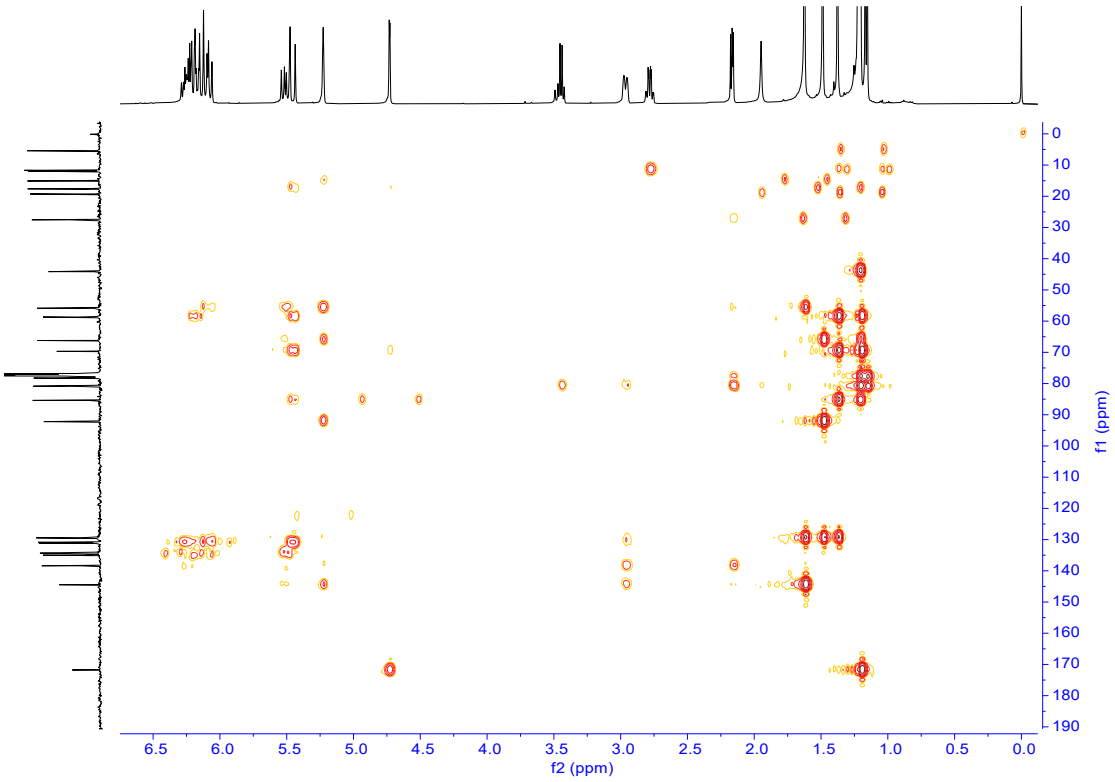


Figure S34. The HMBC spectrum of **6** in $CDCl_3$.

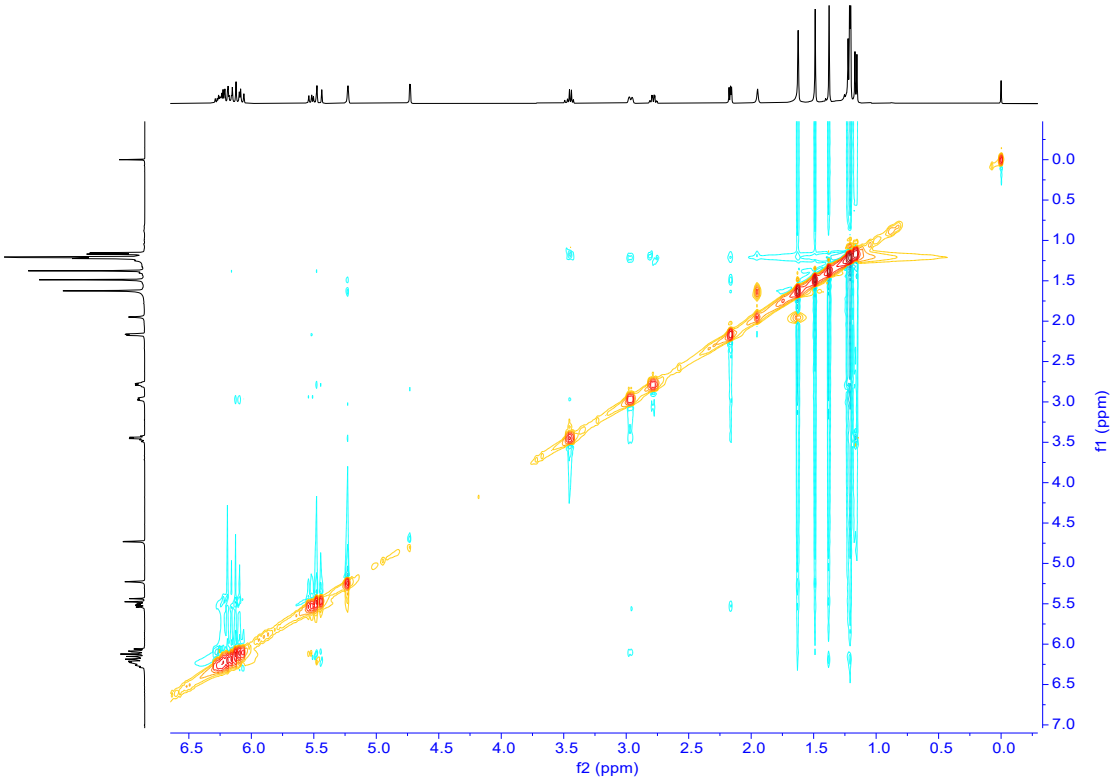


Figure S35. The NOESY spectrum of **6** in $CDCl_3$.

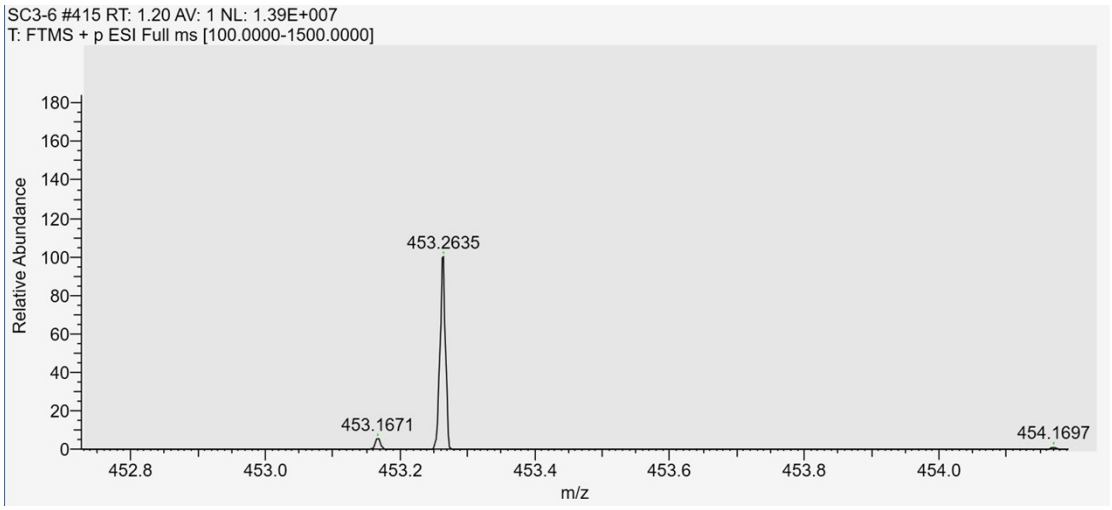


Figure S36. (+)-HRESIMS of compound **6**

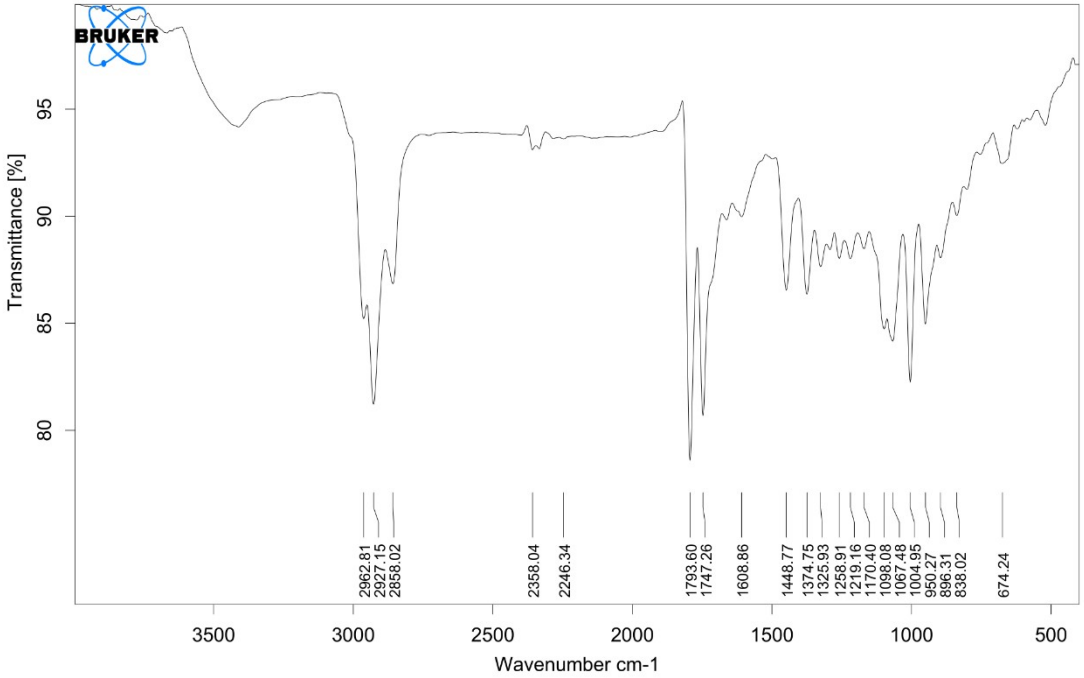


Figure S37. IR spectrum (film on KBr pellet) of compound **6**

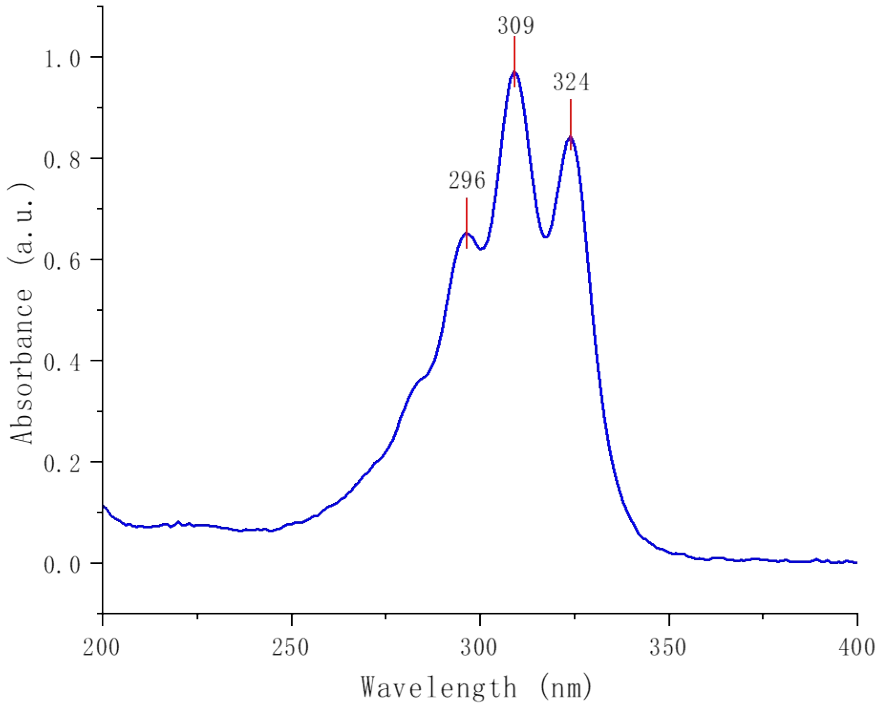


Figure S38. UV spectrum of compound **6** (MeCN)

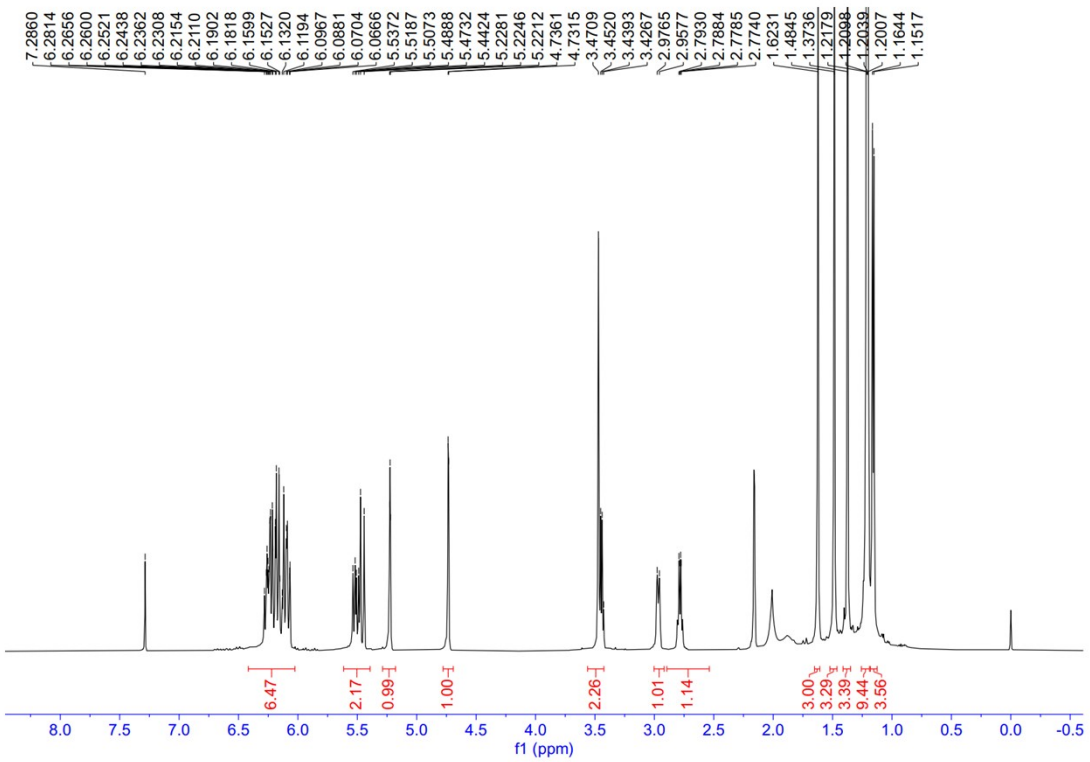


Figure S39. The ^{1}H NMR spectrum of **7** in $CDCl_3$ (400 MHz).

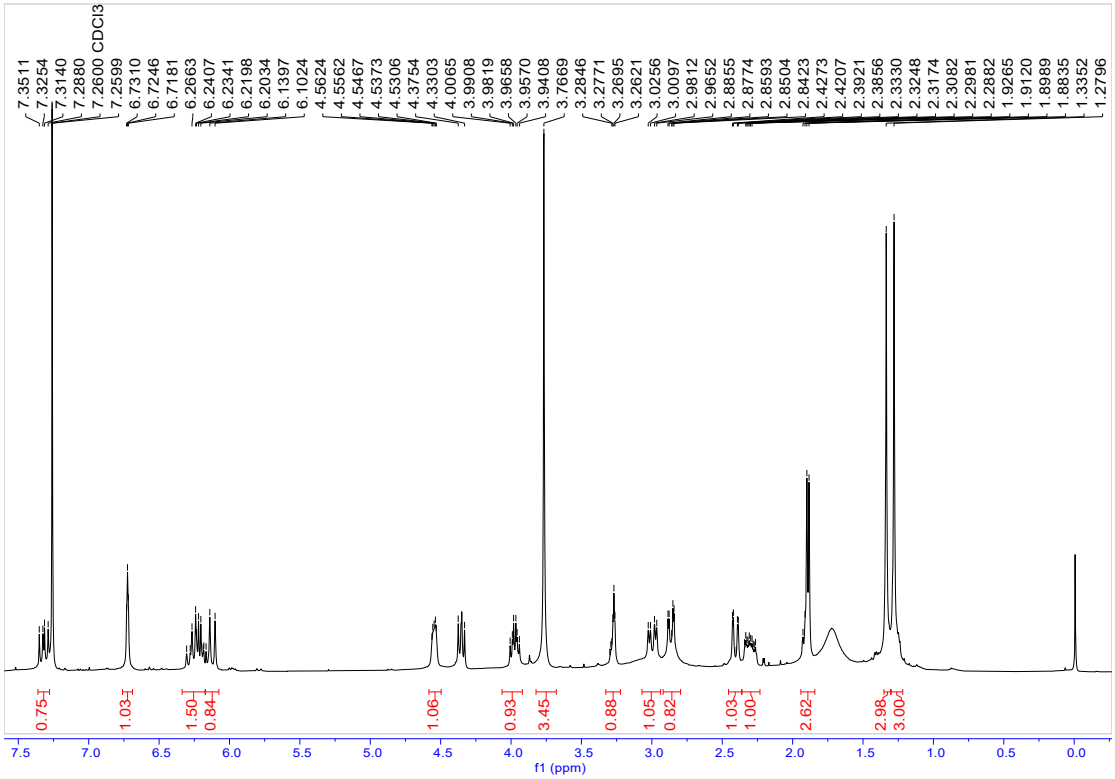
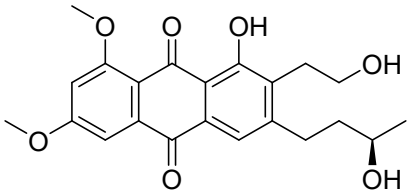
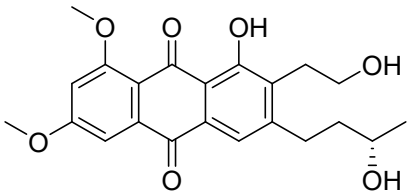


Figure S40. The ^{1}H NMR spectrum of **8** in $CDCl_3$ (400 MHz).



1A



1B

Table S1. Conformational analysis of the B3LYP/6-31G(d) optimized conformers of cpd-**1A** in the gas phase (T=298.15 K)

Conformer	**E[a] (Hartree)**	**C[b] (Hartree)**	**G[c] (kcal/mol)**	**ΔG[d] (kcal/mol)**	**Population[e]**
cpd-**1A**-1	-1379.251174	0.367908	-865249.249635	0.0	48.36%
cpd-**1A**-2	-1379.249315	0.367499	-865248.339766	0.909869	10.40%
cpd-**1A**-3	-1379.249211	0.367584	-865248.221106	1.028529	8.51%
cpd-**1A**-4	-1379.247336	0.365731	-865248.206893	1.042742	8.31%
cpd-**1A**-5	-1379.24923	0.367627	-865248.205795	1.04384	8.29%
cpd-**1A**-6	-1379.249282	0.367872	-865248.085064	1.164571	6.76%
cpd-**1A**-7	-1379.247778	0.366687	-865247.884609	1.365026	4.82%
cpd-**1A**-8	-1379.250101	0.369067	-865247.849048	1.400586	4.54%

[a]Electronic energy obtained at M062X/6-311+G(2d,p) level of theory; [b]Thermal correction to Gibbs free energy obtained at B3LYP/6-31G(d) level of theory; [c]Gibbs free energy (E + C); [d]The relative Gibbs free energy; [e]The Boltzmann distribution of each conformer.

Table S2. Atomic coordinates (Å) of cpd-**1A**-1 obtained at the B3LYP/6-31G(d) level of theory in the gas phase.

C	1.206474	-1.748635	-0.503142	O	-1.349177	-2.720047	0.137015
C	2.483213	-1.221347	-0.832276	O	4.968556	-1.291066	0.972324
C	2.618557	0.159314	-1.038317	H	-5.801040	-0.497385	0.588700
C	1.476600	0.978397	-0.972053	H	-3.129507	2.718907	-0.406366
C	0.228115	0.459750	-0.662033	H	1.538470	2.042678	-1.168033
C	-3.332981	1.676261	-0.204380	H	4.768967	0.101694	-1.167084
C	-4.605754	1.194092	0.101618	H	3.977984	1.045876	-2.426835
C	-4.797640	-0.168728	0.354868	H	5.120264	2.591519	-1.024949
C	-3.728267	-1.064165	0.305131	H	3.423765	2.808781	-0.660333
C	-2.416768	-0.595790	-0.007742	H	5.502064	1.307644	0.996993
C	-1.248694	-1.495949	-0.076984	H	-5.569771	-2.420814	1.778845
C	0.064758	-0.917519	-0.412632	H	-5.886080	-2.698737	0.037739
C	-0.930268	1.376580	-0.588343	H	-5.051924	-3.946866	1.006945
C	-2.263798	0.785325	-0.255810	H	-4.910720	3.828725	0.648270
C	-5.180145	-2.874210	0.858954	H	-5.221174	3.543283	-1.090434
C	-5.587357	3.356947	-0.073968	H	-6.589337	3.772964	0.036748
C	3.957984	0.805763	-1.354599	H	0.170673	-3.254483	-0.065447

C	4.254560	2.096823	-0.567717	H	2.716317	1.305602	1.264241
C	4.576064	1.886584	0.916709	H	3.804983	3.794538	1.606862
C	4.732560	3.210872	1.659006	H	4.964636	3.028625	2.712256
C	3.631100	-2.198882	-0.897492	H	5.537647	3.813522	1.222749
C	4.297427	-2.431557	0.474175	H	3.252747	-3.160250	-1.258048
O	-0.811731	2.582717	-0.786998	H	4.393269	-1.859353	-1.603877
O	1.130909	-3.067979	-0.276648	H	3.540727	-2.799433	1.182688
O	3.600362	1.060995	1.583024	H	5.055748	-3.214934	0.365806
O	-3.885629	-2.380666	0.544970	H	4.304719	-0.635804	1.268862
O	-5.719273	1.961564	0.178296	-	-	-	-

Table S3. Atomic coordinates (Å) of cpd-**1A**-2 obtained at the B3LYP/6-31G(d) level of theory in the gas phase.

C	1.249109	1.572550	-0.596172	O	-1.256512	2.666306	0.041428
C	2.500952	0.985311	-0.914363	O	4.798704	1.372777	1.211491
C	2.559783	-0.393468	-1.153719	H	-5.783913	0.638959	0.633117
C	1.391173	-1.164801	-1.049329	H	-3.264472	-2.706508	-0.332520
C	0.174488	-0.596021	-0.709569	H	1.421530	-2.233691	-1.230864
C	-3.421889	-1.652213	-0.150786	H	3.562924	-2.068318	-1.984469
C	-4.667300	-1.111303	0.166876	H	4.378778	-0.548784	-2.297331
C	-4.799140	0.263919	0.389850	H	5.611405	-2.047514	-0.745981
C	-3.695351	1.113010	0.298116	H	5.294920	-0.462470	-0.035491
C	-2.410374	0.583974	-0.027644	H	3.534141	-2.874657	0.539856
C	-1.207206	1.433483	-0.142053	H	-5.456652	2.577355	1.766787
C	0.074211	0.792854	-0.481882	H	-4.891471	4.062694	0.949794
C	-1.016608	-1.461131	-0.592487	H	-5.789746	2.825548	0.024715
C	-2.318358	-0.807372	-0.244528	H	-5.068259	-3.718932	0.778574
C	-5.063755	2.992588	0.830216	H	-6.754923	-3.607890	0.197208
C	-5.739373	-3.234942	0.059117	H	-5.400226	-3.457581	-0.959489
C	3.840103	-1.111790	-1.526014	H	0.278767	3.132947	-0.198193
C	4.819511	-1.390552	-0.365904	H	2.974241	-1.459598	2.294581
C	4.196049	-2.054805	0.860990	H	4.795001	-3.018907	2.717811
C	5.256565	-2.594473	1.817198	H	5.847895	-3.384937	1.341955
C	3.697264	1.904073	-0.959417	H	5.930969	-1.787937	2.124361
C	4.175873	2.377472	0.432642	H	4.537359	1.427655	-1.471619
O	-0.957074	-2.675520	-0.769041	H	3.427463	2.801468	-1.529002
O	1.229045	2.902234	-0.410242	H	4.933707	3.154868	0.286994
O	3.394996	-1.054889	1.520974	H	3.331365	2.834575	0.964562
O	-3.795502	2.440869	0.508802	H	4.146863	0.675595	1.423312
O	-5.810161	-1.830792	0.283400	-	-	-	-

Table S4. Atomic coordinates (Å) of cpd-**1A**-3 obtained at the B3LYP/6-31G(d) level of theory in the gas phase.

C	-1.220555	1.720249	-0.487209	O	1.368638	2.609021	0.137064
C	-2.515717	1.235490	-0.808006	O	-4.972978	1.347746	1.031935
C	-2.693318	-0.137175	-1.035142	H	5.746550	0.293038	0.519770
C	-1.574562	-0.989180	-0.998797	H	3.028531	-2.875952	-0.506690
C	-0.307694	-0.512292	-0.696175	H	-1.669170	-2.047796	-1.211724
C	3.220514	-1.831831	-0.294002	H	-4.842592	-0.016447	-1.130864
C	4.512997	-1.393783	0.010163	H	-4.097654	-0.963569	-2.416417
C	4.748895	-0.044661	0.284288	H	-5.260922	-2.499137	-1.021141
C	3.693324	0.879996	0.256000	H	-3.565952	-2.766681	-0.683311
C	2.372199	0.457147	-0.051901	H	-5.579462	-1.233300	1.023774
C	1.231004	1.391178	-0.094840	H	5.896767	2.469649	0.001139
C	-0.101689	0.855401	-0.424968	H	5.096695	3.718036	0.996404
C	0.823183	-1.466009	-0.653325	H	5.585170	2.170004	1.740743
C	2.177241	-0.920595	-0.323054	H	7.401178	-2.879397	0.262586
C	5.199309	2.645321	0.829977	H	7.191944	-1.240734	-0.416331
C	6.810917	-1.963983	0.315646	H	6.887652	-1.537869	1.323907
C	-4.055098	-0.740479	-1.341184	H	-0.136020	3.187870	-0.038250
C	-4.376088	-2.034544	-0.568934	H	-2.791629	-1.316271	1.253878
C	-4.671863	-1.837539	0.922556	H	-5.070313	-2.994615	2.706242
C	-4.857641	-3.167718	1.647354	H	-5.686118	-3.739419	1.213237
C	-3.635718	2.246646	-0.842368	H	-3.948829	-3.777992	1.573988
C	-4.277153	2.476674	0.541363	H	-3.234155	3.202372	-1.192783
O	0.664981	-2.662748	-0.873773	H	-4.416346	1.940580	-1.543903
O	-1.104113	3.033077	-0.239831	H	-3.501175	2.812887	1.244813
O	-3.663946	-1.050609	1.587827	H	-5.014900	3.282177	0.455091
O	3.892856	2.187234	0.517062	H	-4.323584	0.669069	1.307235
O	5.475740	-2.347019	0.016462	-	-	-	-

Table S5. Atomic coordinates (Å) of cpd-**1A**-4 obtained at the B3LYP/6-31G(d) level of theory in the gas phase.

C	1.290898	1.367188	0.040155	O	-1.205877	2.473728	0.674754
C	2.539736	0.775345	-0.274756	O	2.926890	3.190395	-1.881105
C	2.563999	-0.549927	-0.725101	H	-5.846963	0.626826	0.590151
C	1.364063	-1.274561	-0.817921	H	-3.396888	-2.654304	-0.716320
C	0.147415	-0.701545	-0.484508	H	1.367149	-2.303105	-1.164112
C	-3.524433	-1.635103	-0.378221	H	3.668455	-1.814705	-2.035220
C	-4.768751	-1.084955	-0.069685	H	4.650175	-0.556070	-1.301731
C	-4.861950	0.242750	0.362443	H	3.493716	-2.969650	0.194007
C	-3.720429	1.035061	0.491288	H	5.136848	-2.868174	-0.428719
C	-2.435791	0.495097	0.181396	H	3.962208	-0.969266	1.656670
C	-1.195309	1.284753	0.296234	H	-4.841064	3.907787	1.513781

C	0.084518	0.639090	-0.047758	H	-5.711024	2.879820	0.339293
C	-1.085601	-1.507788	-0.601502	H	-5.534128	2.347163	2.040255
C	-2.383266	-0.847483	-0.251120	H	-6.952120	-3.442331	-0.585374
C	-5.048223	2.880207	1.213538	H	-5.505788	-3.189216	-1.604637
C	-5.914300	-3.107239	-0.590574	H	-5.322703	-3.729962	0.090801
C	3.844218	-1.264971	-1.103106	H	0.340864	2.889038	0.621532
C	4.306960	-2.266861	-0.027341	H	6.595382	-1.223723	0.702194
C	4.766129	-1.609795	1.277611	H	4.275460	-3.266259	2.602768
C	5.134945	-2.637221	2.345216	H	5.937140	-3.298181	1.989494
C	3.772690	1.637656	-0.149255	H	5.483275	-2.133105	3.251623
C	4.049646	2.459060	-1.421652	H	3.628738	2.330639	0.686516
O	-1.060948	-2.678665	-0.970441	H	4.653486	1.036112	0.089289
O	1.300662	2.657354	0.435906	H	4.909275	3.121559	-1.225166
O	5.851709	-0.702109	1.046223	H	4.335211	1.789586	-2.242695
O	-3.781774	2.316035	0.904971	H	2.424108	3.476956	-1.099910
O	-5.944885	-1.751737	-0.154906	-	-	-	-

Table S6. Atomic coordinates (Å) of cpd-**1A**-5 obtained at the B3LYP/6-31G(d) level of theory in the gas phase.

C	-1.039196	1.451961	-0.544365	O	1.481088	2.595923	-0.095697
C	-2.300517	0.840696	-0.768626	O	-4.306900	1.401924	1.431524
C	-2.367139	-0.558120	-0.878390	H	6.032975	0.631213	0.520894
C	-1.192503	-1.318137	-0.743193	H	3.498036	-2.786714	-0.083897
C	0.034588	-0.719325	-0.506650	H	-1.227996	-2.399203	-0.825778
C	3.656084	-1.720619	0.004678	H	-4.381236	-0.683915	-1.637218
C	4.909469	-1.153246	0.236102	H	-3.460971	-2.176272	-1.728046
C	5.042517	0.235897	0.341037	H	-4.088506	-2.822815	0.419163
C	3.933010	1.073089	0.215998	H	-3.892066	-1.213144	1.072559
C	2.640308	0.516758	-0.022929	H	-6.284778	-2.118969	-0.586339
C	1.432707	1.351604	-0.168229	H	5.730262	2.652089	1.507409
C	0.140201	0.683340	-0.404407	H	6.010394	2.764327	-0.258140
C	1.237441	-1.570400	-0.368832	H	5.134118	4.067827	0.594163
C	2.546827	-0.888394	-0.121245	H	5.616221	-3.589483	-0.706947
C	5.308444	2.992238	0.553513	H	7.007407	-3.634295	0.414572
C	5.986106	-3.277571	0.276829	H	5.340755	-3.696897	1.057612
C	-3.663912	-1.303864	-1.097872	H	-0.057005	3.039287	-0.320991
C	-4.319877	-1.768150	0.228606	H	-5.668433	0.351464	0.625568
C	-5.840968	-1.555091	0.245141	H	-6.033740	-1.483001	2.406061
C	-6.462601	-2.032528	1.558278	H	-7.541856	-1.853196	1.549439
C	-3.499124	1.757941	-0.883670	H	-6.285257	-3.102339	1.722104
C	-3.918528	2.381611	0.456990	H	-3.253058	2.582239	-1.563361
O	1.175289	-2.793317	-0.451234	H	-4.359740	1.227554	-1.291746
O	-1.015912	2.792430	-0.474172	H	-3.114659	3.008529	0.856182

O	-6.171148	-0.195451	-0.014306	H	-4.803516	3.005684	0.308806
O	4.033393	2.413269	0.314234	H	-3.522651	0.860187	1.616407
O	6.057350	-1.858316	0.374520	-	-	-	-

Table S7. Atomic coordinates (Å) of cpd-**1A**-6 obtained at the B3LYP/6-31G(d) level of theory in the gas phase.

C	-1.189810	-1.776315	-0.460780	O	1.371557	-2.741265	0.161100
C	-2.469095	-1.250888	-0.782414	O	-5.186594	-1.477579	0.862136
C	-2.607865	0.129274	-0.984860	H	5.820546	-0.507521	0.583623
C	-1.469163	0.950303	-0.933209	H	3.138109	2.698041	-0.417359
C	-0.216873	0.434036	-0.639143	H	-1.540170	2.016477	-1.112842
C	3.344930	1.657007	-0.210464	H	-4.102202	0.858394	-2.346205
C	4.619828	1.178841	0.091687	H	-4.748202	0.084122	-0.908993
C	4.815495	-0.182057	0.352413	H	-3.544569	2.893965	-1.086441
C	3.747416	-1.079369	0.312897	H	-5.213940	2.446961	-0.804460
C	2.433673	-0.615193	0.003278	H	-2.870025	1.938463	1.092402
C	1.266645	-1.517914	-0.056322	H	5.908234	-2.711657	0.050376
C	-0.049605	-0.942807	-0.384747	H	5.595915	-2.421285	1.790007
C	0.939858	1.351973	-0.579581	H	5.079455	-3.954326	1.031098
C	2.276769	0.764133	-0.251137	H	4.922925	3.817508	0.618766
C	5.204599	-2.882460	0.874628	H	6.598697	3.760728	-0.000527
C	5.597021	3.341809	-0.103332	H	5.225365	3.520564	-1.119225
C	-3.963740	0.754729	-1.260488	H	-0.148628	-3.280182	-0.029968
C	-4.177256	2.134493	-0.611348	H	-5.582396	1.260919	1.427938
C	-3.919922	2.176184	0.899901	H	-4.060286	3.533642	2.580418
C	-4.245196	3.540006	1.502260	H	-3.630970	4.324792	1.046912
C	-3.608094	-2.236930	-0.892060	H	-5.298906	3.799704	1.334127
C	-4.331420	-2.523900	0.439309	H	-4.350098	-1.894065	-1.619102
O	0.821437	2.556723	-0.787984	H	-3.201621	-3.184041	-1.259994
O	-1.110852	-3.096276	-0.233690	H	-4.975059	-3.399310	0.300681
O	-4.632622	1.137324	1.593263	H	-3.588705	-2.779273	1.209265
O	3.908381	-2.394404	0.560550	H	-4.656490	-0.718530	1.174176
O	5.732924	1.948752	0.157926	-	-	-	-

Table S8. Atomic coordinates (Å) of cpd-**1A**-7 obtained at the B3LYP/6-31G(d) level of theory in the gas phase.

C	0.928907	-1.701760	-0.463384	O	-1.657352	-2.652251	0.063044
C	2.221900	-1.185379	-0.738076	O	4.622180	-1.423752	1.118246
C	2.384650	0.199478	-0.868012	H	-6.074030	-0.368087	0.541555
C	1.265291	1.043022	-0.768634	H	-3.319648	2.842729	-0.218487
C	0.000075	0.536719	-0.519930	H	1.373373	2.116622	-0.882342
C	-3.548132	1.795183	-0.077546	H	4.493524	0.118185	-1.329954
C	-4.836054	1.322961	0.173683	H	3.681643	1.569769	-1.884953

C	-5.059434	-0.047447	0.348257	H	3.652006	2.539850	0.312228
C	-4.006199	-0.959850	0.272890	H	3.950497	0.986604	1.096038
C	-2.679286	-0.501628	0.014530	H	6.012249	2.233991	-0.764022
C	-1.526704	-1.420109	-0.080645	H	-5.401769	-3.848390	0.787801
C	-0.196053	-0.851249	-0.354392	H	-5.907805	-2.355221	1.628712
C	-1.142482	1.469770	-0.426270	H	-6.188323	-2.533219	-0.131298
C	-2.494643	0.887239	-0.153812	H	-6.768166	3.941556	0.203526
C	-5.505064	-2.766814	0.694771	H	-5.103403	3.930042	0.854355
C	-5.772197	3.510997	0.093247	H	-5.378512	3.743434	-0.903297
C	3.734597	0.852303	-1.055887	H	-0.147505	-3.206759	-0.134938
C	4.196451	1.592343	0.217194	H	6.434275	0.407916	1.315533
C	5.705457	1.857649	0.219412	H	5.664669	3.832762	1.124717
C	6.125944	2.854172	1.294767	H	5.808560	2.506629	2.287357
C	3.346851	-2.184415	-0.860486	H	7.213544	2.977802	1.300949
C	4.014242	-2.535346	0.480155	H	2.949779	-3.111890	-1.284357
O	-1.002113	2.681812	-0.565124	H	4.112006	-1.820875	-1.555099
O	0.821873	-3.031320	-0.312881	H	3.260075	-2.912800	1.176219
O	6.439066	0.621983	0.366919	H	4.744711	-3.342540	0.309150
O	-4.194574	-2.284582	0.436977	H	5.253546	-1.010883	0.501396
O	-5.937080	2.107578	0.267598	-	-	-	-

Table S9. Atomic coordinates (Å) of cpd-**1A**-8 obtained at the B3LYP/6-31G(d) level of theory in the gas phase.

C	-1.320447	1.554137	-0.559050	O	1.188439	2.690076	-0.016906
C	-2.574282	0.946632	-0.831847	O	-4.898372	1.441591	1.284702
C	-2.627329	-0.443547	-1.023029	H	5.752684	0.729655	0.516686
C	-1.445540	-1.198882	-0.916803	H	3.245750	-2.671657	-0.270543
C	-0.226060	-0.605656	-0.621532	H	-1.461930	-2.270994	-1.078503
C	3.395194	-1.610286	-0.127390	H	-4.406105	-0.686244	-2.199732
C	4.643444	-1.046306	0.138706	H	-3.629781	-2.180362	-1.722780
C	4.765865	0.336758	0.313101	H	-5.391052	-0.354331	-0.004218
C	3.650877	1.171560	0.224818	H	-5.747164	-1.981474	-0.582186
C	2.363243	0.618752	-0.047515	H	-5.289074	-1.931052	1.792996
C	1.150851	1.452031	-0.155888	H	5.432376	2.701238	1.597264
C	-0.135828	0.788035	-0.441424	H	5.717073	2.897515	-0.160376
C	0.978870	-1.456576	-0.510601	H	4.828429	4.153425	0.748821
C	2.280846	-0.780410	-0.217694	H	5.089831	-3.626041	0.830531
C	5.011159	3.082288	0.658753	H	5.372295	-3.425225	-0.924854
C	5.735442	-3.162246	0.075582	H	6.758763	-3.518119	0.199592
C	-3.908210	-1.185334	-1.359321	H	-0.355878	3.135290	-0.236314
C	-4.942871	-1.326636	-0.221156	H	-2.685726	-1.005796	1.268440
C	-4.431612	-1.894467	1.112401	H	-3.546261	-3.648536	2.017091
C	-3.823916	-3.292274	1.020456	H	-4.540083	-3.998290	0.584944

C	-3.772649	1.859872	-0.901502	H	-2.922946	-3.301313	0.397381
C	-4.242213	2.394640	0.474662	H	-3.504207	2.732318	-1.508948
O	0.921786	-2.674721	-0.651704	H	-4.615119	1.364150	-1.390210
O	-1.307836	2.887696	-0.421043	H	-3.386420	2.848161	0.991969
O	-3.518560	-0.988882	1.768387	H	-4.974369	3.188927	0.293610
O	3.741104	2.505608	0.388307	H	-4.267081	0.740060	1.548932
O	5.795564	-1.749344	0.246760	-	-	-	-

Table S10. Key transitions, oscillator strengths, and rotatory strengths in the ECD spectrum of conformer cpd-**1A**-1 at the CAM-B3LYP/Def2SVP level of theory in MeOH with IEFPCM solvent model.

Num[a]	***Transition***[b]	***CI-coeff***[b]	***ΔE (eV)***[d]	***λ (nm)***[e]	***f***[f]	R_{vel}[g]	R_{len}[h]
1	105->107	0.22621	3.2711	379.03	0.3129	14.5534	15.2431
	106->107	0.6459					
2	100->107	-0.31382	3.4078	363.82	0.0005	2.5158	3.4309
	102->107	0.58216					
3	105->107	0.64172	3.6239	342.13	0.0263	-18.0873	-18.9084
	106->107	-0.22862					
4	100->107	0.55822	3.7520	330.45	0.0006	1.744	1.4189
	102->107	0.29972					
	102->108	-0.25205					
5	104->107	0.66186	3.9186	316.40	0.0602	-9.4841	-9.2127
6	103->107	0.6704	4.4771	276.93	0.2526	11.4118	12.8778
7	106->108	0.6283	5.0809	244.02	0.2586	-26.3797	-28.218
8	105->108	0.6043	5.2237	237.35	0.3838	7.4807	11.6734
9	101->107	0.62492	5.4012	229.55	0.0132	3.4708	2.7389
10	103->108	0.30185	5.5045	225.24	0.0197	1.4771	1.566
	104->108	-0.32214					
	106->109	0.40261					
11	103->108	0.23383	5.5885	221.86	0.1532	16.7489	17.2636
	104->108	0.48594					
	105->109	0.22978					
	106->109	0.23617					
12	99->107	0.57549	5.7608	215.22	0.0324	15.272	16.278
13	99->107	-0.24287	5.7942	213.98	0.0061	-2.4444	-2.8078
	102->108	0.55427					
14	97->107	0.56352	5.9509	208.35	0.3095	-15.4672	-21.025
	105->109	-0.30527					
15	103->108	-0.30719	6.0641	204.46	0.1873	-22.9817	-25.1486
	105->109	-0.29835					
	106->109	0.35942					
16	95->107	0.26036	6.1330	202.16	0.0158	-2.8346	-3.0066
	98->107	0.37082					

	100->108	-0.29273					
17	103->108	-0.36709	6.2136	199.54	0.2987	-40.2533	-45.2581
	105->109	0.42081					
	106->109	0.25056					
18	98->107	0.33791	6.3204	196.17	0.0684	16.9305	19.6422
	100->108	0.34913					
19	93->107	0.25363	6.4337	192.71	0.0237	8.5962	9.2468
	100->108	0.24748					
	102->109	-0.25931					
	104->109	0.28948					
20	102->109	0.44458	6.4908	191.01	0.0051	0.8973	2.0762
	104->109	0.25058					
21	93->107	0.32394	6.5673	188.79	0.0100	12.3751	11.7348
	94->107	-0.22902					
	104->109	-0.2343					
22	93->107	0.27451	6.6431	186.64	0.0048	-7.2344	-7.5223
	103->109	0.2909					
	105->110	-0.22466					
23	94->107	-0.26296	6.7159	184.61	0.0082	-8.4293	-7.3216
	103->109	0.38863					
24	104->109	0.29853	6.8044	182.21	0.3791	28.2323	27.7406
	106->110	0.46477					
25	95->107	0.23424	6.8499	181.00	0.0852	-21.1878	-23.1124
	102->109	0.23359					
	106->110	-0.231					
26	91->107	0.28566	6.8764	180.31	0.0690	30.512	33.4431
	92->107	0.22558					
	96->107	0.27354					
27	101->108	0.5981	6.9042	179.58	0.0493	22.5347	25.3029
28	92->107	-0.31225	6.9172	179.24	0.0737	19.0991	14.1603
	96->107	-0.24095					
	103->109	0.23992					
	105->110	0.34761					
29	94->107	0.23241	6.9467	178.48	0.0070	7.6493	12.1678
	95->107	0.23018					
	105->110	0.36008					
30	91->107	0.23426	7.0817	175.08	0.0018	-1.1592	-2.2361
	100->109	0.39669					
	102->110	0.32583					
31	92->107	-0.26976	7.1790	172.70	0.0014	6.0185	5.725
	95->107	-0.27133					
	96->107	0.24867					
	100->109	0.36166					

32	100->109	-0.27945	7.2128	171.89	0.0017	-4.5843	-3.3784
	102->110	0.45379					
33	104->110	0.5161	7.2427	171.18	0.0940	-38.3385	-42.7018
34	89->107	0.38315	7.2982	169.88	0.0104	-9.4468	-11.8005
	99->108	0.36587					
35	89->107	0.34448	7.3218	169.33	0.1095	43.7309	49.4117
	97->108	-0.24147					
	99->108	-0.28138					
	103->110	0.2845					
36	99->108	0.25931	7.4074	167.38	0.0373	-3.1809	-2.9737
	103->110	0.41793					

[a]Number of the excited states; [b]Only transitions with contribution over 10.0% were listed; [c]Configuration-interaction coefficient; [d]Excitation energy; [e]Wavelength; [f]Oscillator strength; [g]Rotatory strength in velocity form (10^{-40} cgs); [h]Rotatory strength in length form (10^{-40} cgs).

Table S11. Key transitions, oscillator strengths, and rotatory strengths in the ECD spectrum of conformer cpd-**1A**-2 at the CAM-B3LYP/Def2SVP level of theory in MeOH with IEFPCM solvent model.

Num[a]	***Transition***[b]	***CI-coeff***[b]	***ΔE (eV)***[d]	***λ (nm)***[e]	***f***[f]	R_{vel}[g]	R_{len}[h]
1	105->107	0.26308	3.2631	379.96	0.3314	-13.0571	-13.567
	106->107	0.63364					
2	100->107	-0.30068	3.4097	363.63	0.0003	-0.3489	-0.848
	102->107	0.57013					
3	105->107	0.6267	3.5989	344.50	0.0170	18.6701	19.3401
	106->107	-0.26912					
4	100->107	0.56362	3.7539	330.28	0.0001	0.923	0.963
	102->107	0.28855					
	102->108	-0.24554					
5	104->107	0.66288	3.9307	315.43	0.0585	8.2358	8.2811
6	103->107	0.67589	4.4944	275.87	0.2620	-3.3656	-3.7697
7	106->108	0.62515	5.0941	243.39	0.2269	25.6335	26.7317
8	105->108	0.59134	5.2445	236.41	0.4141	6.5656	2.6981
9	101->107	0.64309	5.3837	230.29	0.0075	-11.9284	-11.2517
10	103->108	0.29553	5.5079	225.10	0.0089	-1.5039	-1.2128
	104->108	-0.27088					
	106->109	0.45865					
11	104->108	0.50894	5.6146	220.82	0.1496	-19.4908	-19.2244
	105->109	0.24181					
12	99->107	0.62857	5.6777	218.37	0.0549	-14.186	-15.0421
13	102->108	0.56821	5.8150	213.21	0.0026	-3.4821	-3.3795
14	97->107	0.51863	5.9661	207.81	0.3905	16.9542	24.4437
	105->109	-0.33244					
15	97->107	-0.31331	6.0650	204.43	0.1354	19.8757	20.8804

	103->108	-0.29854					
	105->109	-0.22449					
	106->109	0.3355					
16	98->107	0.40551	6.1187	202.63	0.0083	-1.0022	-1.2839
	100->108	-0.28933					
17	103->108	-0.36877	6.2362	198.81	0.2096	42.4618	44.8903
	105->109	0.43237					
18	95->107	0.30064	6.3324	195.79	0.1778	-22.4939	-23.4108
	98->107	-0.23796					
	104->109	-0.29033					
19	100->108	0.3645	6.4035	193.62	0.0179	-5.6631	-7.0639
20	94->107	-0.2803	6.5075	190.53	0.0033	0.0085	-0.4568
	102->109	0.37596					
21	102->109	-0.27533	6.5625	188.93	0.0118	-6.5374	-6.3731
	104->109	0.36426					
	106->110	-0.2288					
22	93->107	0.30697	6.6495	186.46	0.0079	-9.7519	-10.4984
	95->107	-0.24286					
	100->108	-0.26267					
	102->109	-0.25104					
23	103->109	0.5197	6.7318	184.18	0.0053	3.7071	3.3237
	105->110	-0.24713					
24	104->109	0.25795	6.8230	181.71	0.2919	-10.7924	-8.8776
	106->110	0.46967					
25	91->107	0.3375	6.8803	180.20	0.0008	2.7942	2.6924
	94->107	0.32215					
	100->109	-0.25165					
26	92->107	-0.33477	6.8922	179.89	0.0823	6.4275	7.0449
	96->107	0.40135					
27	93->107	0.33729	6.9098	179.43	0.0845	2.564	4.5297
	95->107	0.30212					
	96->107	-0.29508					
28	101->108	0.56175	6.9686	177.92	0.1061	-2.8026	-3.4663
	105->110	0.22763					
29	101->108	-0.22804	6.9780	177.68	0.0561	-24.8191	-27.2245
	103->109	0.27972					
	105->110	0.47887					
30	91->107	-0.33254	7.0640	175.52	0.0022	7.4719	8.6849
	94->107	0.39529					
31	91->107	0.33041	7.1321	173.84	0.0020	3.4754	3.7179
	100->109	0.47792					
	102->110	0.22795					
32	99->108	0.24934	7.2309	171.46	0.0045	3.9177	3.6093

	100->109	-0.28965					
	102->110	0.42348					
33	104->110	0.4606	7.2892	170.09	0.0377	43.4536	47.9988
34	89->107	0.32396	7.3318	169.10	0.0072	8.0142	9.4977
	90->107	0.32203					
	99->108	0.36975					
35	89->107	0.23321	7.3531	168.62	0.1299	-19.3994	-20.2727
	90->107	0.23281					
	99->108	-0.32063					
	104->110	0.33513					
36	85->107	0.26586	7.4104	167.31	0.0050	-8.0072	-9.2087
	88->107	0.25028					
	90->107	-0.25549					
	92->107	0.22532					

[a]Number of the excited states; [b]Only transitions with contribution over 10.0% were listed; [c]Configuration-interaction coefficient; [d]Excitation energy; [e]Wavelength; [f]Oscillator strength; [g]Rotatory strength in velocity form (10^{-40} cgs); [h]Rotatory strength in length form (10^{-40} cgs).

Table S12. Key transitions, oscillator strengths, and rotatory strengths in the ECD spectrum of conformer cpd-**1A**-3 at the CAM-B3LYP/Def2SVP level of theory in MeOH with IEFPCM solvent model.

Num[a]	***Transition***[b]	***CI-coeff***[b]	***ΔE (eV)***[d]	***λ (nm)***[e]	***f***[f]	R_{vel}[g]	R_{len}[h]
1	106->107	0.67395	3.2857	377.34	0.3590	12.2934	13.7014
2	100->107	-0.33002	3.4311	361.36	0.0004	1.0202	1.9189
	102->107	0.57091					
3	105->107	0.67332	3.6628	338.50	0.0176	-13.7738	-14.5158
4	100->107	0.54241	3.7726	328.64	0.0005	1.7778	1.4435
	102->107	0.3152					
	102->108	-0.26378					
5	103->107	-0.22899	4.0067	309.45	0.0596	-9.5107	-8.9642
	104->107	0.61182					
6	103->107	0.62692	4.5985	269.62	0.2126	9.0257	10.4997
7	106->108	0.63666	4.9959	248.17	0.3535	-28.6263	-29.9136
8	105->108	0.61606	5.1815	239.28	0.2853	8.4151	10.6098
9	101->107	0.54713	5.4339	228.17	0.0187	-5.6166	-7.5886
	104->108	-0.24979					
10	101->107	0.33371	5.4914	225.78	0.0816	8.5567	9.1245
	104->108	0.41164					
	106->109	0.29866					
11	103->108	0.39529	5.5821	222.11	0.1445	14.2666	14.6794
	104->108	-0.30183					
	106->109	0.3409					
12	102->108	0.5814	5.7438	215.86	0.0010	3.4324	3.4917

13	99->107	0.61533	5.8144	213.24	0.0338	6.2687	7.3171
14	97->107	0.53889	6.0050	206.47	0.4132	-30.849	-34.0096
	105->109	-0.35109					
15	97->107	0.2777	6.0765	204.04	0.1048	-8.3842	-10.5989
	104->108	0.27033					
	105->109	0.33446					
	106->109	-0.31583					
16	98->107	-0.29843	6.1379	202.00	0.0056	-0.0095	-0.3755
	100->108	0.38374					
17	103->108	0.40403	6.2171	199.42	0.2713	-27.7682	-30.1032
	105->109	-0.36472					
	106->109	-0.30666					
18	98->107	0.39173	6.3280	195.93	0.0778	21.9496	24.9457
	100->108	0.33308					
19	100->108	0.22399	6.4495	192.24	0.0346	-12.4355	-12.7762
	104->109	0.31207					
	106->110	-0.30909					
20	102->109	0.45398	6.5232	190.07	0.0047	6.6088	6.7218
21	92->107	0.27138	6.5986	187.89	0.0251	-4.54	-5.3037
	94->107	0.27466					
	105->110	-0.26273					
	106->110	-0.27085					
22	92->107	0.29884	6.6736	185.78	0.0225	10.4575	10.6753
	98->107	0.24765					
	105->110	0.3231					
23	94->107	-0.28636	6.7595	183.42	0.0325	-1.3037	-2.142
	96->107	0.28974					
	102->109	0.27162					
24	104->109	0.40874	6.7918	182.55	0.3872	24.1454	23.6434
	105->110	-0.30213					
	106->110	0.36847					
25	93->107	0.41372	6.8369	181.34	0.0007	-0.7716	-0.9668
	95->107	-0.26277					
	102->110	-0.22459					
26	101->108	0.59985	6.8810	180.18	0.0805	36.8988	40.8347
27	93->107	0.26439	6.9398	178.66	0.0152	7.9597	8.2418
	94->107	0.28784					
	95->107	0.32866					
	98->107	-0.25586					
28	91->107	0.3707	6.9649	178.01	0.0024	-5.8004	-6.0009
	96->107	0.28475					
29	103->109	0.59158	6.9994	177.14	0.1367	14.6648	16.1065
	105->110	-0.24451					

30	100->109	-0.32616	7.0684	175.41	0.0006	-2.7071	-3.6776
	102->110	0.40941					
31	96->107	0.23416	7.2002	172.19	0.0029	-4.5244	-5.1044
	99->108	0.2503					
	100->109	0.23259					
	104->110	-0.24989					
32	100->109	0.39436	7.2123	171.91	0.0037	-5.6284	-4.342
	102->110	0.3454					
33	100->109	0.23998	7.2292	171.50	0.0363	-7.5056	-12.1617
	104->110	0.44201					
34	89->107	-0.25704	7.3292	169.16	0.0261	-15.2511	-15.3503
	97->108	0.43574					
	99->108	0.29329					
35	97->108	-0.28847	7.3332	169.07	0.0652	27.3431	29.8849
	99->108	0.38992					
	103->110	-0.23215					
	104->110	0.25104					
36	89->107	0.47393	7.4480	166.47	0.0327	-6.6289	-4.7828
	103->110	0.38914					

[a]Number of the excited states; [b]Only transitions with contribution over 10.0% were listed; [c]Configuration-interaction coefficient; [d]Excitation energy; [e]Wavelength; [f]Oscillator strength; [g]Rotatory strength in velocity form (10^{-40} cgs); [h]Rotatory strength in length form (10^{-40} cgs).

Table S13. Key transitions, oscillator strengths, and rotatory strengths in the ECD spectrum of conformer cpd-**1A**-4 at the CAM-B3LYP/Def2SVP level of theory in MeOH with IEFPCM solvent model.

Num[a]	***Transition***[b]	***CI-coeff***[b]	***ΔE (eV)***[d]	***λ (nm)***[e]	***f***[f]	R_{vel}[g]	R_{len}[h]
1	106->107	0.66029	3.3089	374.70	0.3301	-15.5495	-15.815
2	99->107	-0.30167	3.4190	362.64	0.0000	-1.6151	-1.4186
	101->107	0.26056					
	102->107	0.52983					
3	105->107	0.65536	3.6479	339.88	0.0288	-8.9223	-8.2562
4	99->107	0.55935	3.7724	328.66	0.0003	0.9853	0.6071
	102->107	0.27515					
	102->108	-0.22683					
5	104->107	0.65311	3.9434	314.41	0.0488	-6.9165	-7.1485
6	103->107	0.65347	4.5478	272.63	0.2667	43.4548	45.3461
7	106->108	0.62743	5.1113	242.57	0.3326	-21.874	-22.8647
8	105->108	0.59669	5.2532	236.01	0.3014	13.5993	12.9435
9	101->107	0.59008	5.2972	234.06	0.0113	-10.0692	-11.1071
	102->107	-0.29265					
10	103->108	0.38485	5.5410	223.76	0.0353	-9.5005	-9.5647
	106->109	0.41906					

11	104->108	0.54374	5.5989	221.45	0.1766	-10.0675	-10.0479
	106->109	0.23792					
12	100->107	0.65221	5.8291	212.70	0.0171	-7.4457	-7.4602
13	102->108	0.54084	5.8384	212.36	0.0012	1.7435	1.3858
14	97->107	0.55137	5.9636	207.90	0.2744	-1.4326	-0.457
	105->109	-0.26928					
15	103->108	0.29277	6.1152	202.75	0.2943	7.6255	7.6771
	105->109	0.43135					
	106->109	-0.26448					
16	99->108	0.44587	6.1868	200.40	0.0280	2.2753	1.217
17	103->108	0.37065	6.2258	199.15	0.1459	39.9052	40.6881
	105->109	-0.30135					
	106->109	-0.34006					
18	96->107	0.34759	6.2891	197.14	0.2014	-38.596	-40.5494
	97->107	0.25789					
19	95->107	0.31234	6.4626	191.85	0.0077	-0.3683	-0.7012
	102->109	0.32047					
20	91->107	0.28012	6.4995	190.76	0.0018	2.3202	3.2224
	98->107	0.3148					
	102->109	0.31678					
21	104->109	0.4249	6.5702	188.71	0.0084	3.5665	2.9686
	106->110	-0.30622					
22	93->107	0.39503	6.6821	185.55	0.0001	-0.1642	0.0395
	95->107	0.24148					
	99->108	-0.26784					
23	98->107	-0.23212	6.7481	183.73	0.0091	-4.3995	-5.9702
	103->109	0.38729					
	105->110	-0.27776					
24	101->108	0.53725	6.7694	183.15	0.0019	-8.8649	-9.5032
25	98->107	0.40758	6.7931	182.51	0.0095	8.8628	10.1785
	102->109	-0.28419					
26	91->107	-0.35381	6.8922	179.89	0.0256	-11.01	-11.2861
	92->107	0.38236					
	99->109	-0.22421					
27	104->109	0.3609	6.8988	179.72	0.5892	103.0818	105.4043
	106->110	0.49793					
28	103->109	0.39886	6.9470	178.47	0.0083	-57.2024	-55.3764
	105->110	0.46428					
29	93->107	-0.30691	7.0144	176.76	0.0064	-8.223	-5.6972
	94->107	0.43754					
30	92->107	0.35318	7.0645	175.50	0.0140	-2.7275	-4.7385
	95->107	0.25076					
	96->107	-0.25658					

31	99->109	0.46691	7.1333	173.81	0.0026	-7.0051	-7.2853
	102->110	0.28728					
32	99->109	0.26078	7.2683	170.58	0.0337	-8.3159	-4.3516
	102->110	-0.33093					
	104->110	0.3733					
33	90->107	-0.29913	7.2732	170.47	0.0317	13.4214	10.99
	99->109	-0.22705					
	102->110	0.30302					
	104->110	0.35067					
34	90->107	0.52142	7.3178	169.43	0.1424	15.2071	14.3738
	97->108	-0.27802					
	104->110	0.29251					
35	100->108	0.61866	7.3564	168.54	0.0007	-5.0725	-4.7369
36	85->107	0.42911	7.4623	166.15	0.0013	-5.1565	-4.7934

[a]Number of the excited states; [b]Only transitions with contribution over 10.0% were listed; [c]Configuration-interaction coefficient; [d]Excitation energy; [e]Wavelength; [f]Oscillator strength; [g]Rotatory strength in velocity form (10^{-40} cgs); [h]Rotatory strength in length form (10^{-40} cgs).

Table S14. Key transitions, oscillator strengths, and rotatory strengths in the ECD spectrum of conformer cpd-**1A**-5 at the CAM-B3LYP/Def2SVP level of theory in MeOH with IEFPCM solvent model.

Num[a]	***Transition***[b]	***CI-coeff***[b]	***ΔE (eV)***[d]	***λ (nm)***[e]	***f***[f]	R_{vel}[g]	R_{len}[h]
1	106->107	0.67027	3.2768	378.37	0.3321	14.7987	15.4596
2	100->107	-0.31305	3.4044	364.18	0.0000	-2.0992	-1.85
	102->107	0.56662					
3	105->107	0.66757	3.6574	339.00	0.0195	-15.408	-15.9573
4	100->107	0.55831	3.7524	330.41	0.0000	-0.5717	-0.6335
	102->107	0.28713					
	102->108	-0.24587					
5	104->107	0.65543	3.9461	314.19	0.0559	-6.1893	-6.9366
6	103->107	0.63193	4.5517	272.39	0.2648	-3.4328	-2.6567
7	106->108	0.63636	5.1077	242.74	0.3408	-19.5776	-19.8578
8	105->108	0.61101	5.2832	234.68	0.2766	3.7171	6.6566
9	103->108	0.33355	5.5253	224.39	0.0057	2.2727	1.8366
	106->109	0.46742					
10	101->107	0.5512	5.5569	223.12	0.0091	0.8639	1.1071
11	104->108	0.55664	5.5962	221.55	0.2047	36.1839	36.7388
	105->109	0.24311					
12	102->108	0.56751	5.7989	213.81	0.0009	-0.1068	-0.4392
13	99->107	0.61626	5.9430	208.62	0.0104	-13.1229	-14.0038
14	97->107	0.58604	5.9569	208.14	0.2854	0.7057	-2.7082
	105->109	-0.25921					
15	103->108	0.29451	6.1143	202.78	0.3883	-0.467	-1.9157

	105->109	0.42311					
	106->109	-0.24809					
16	100->108	0.41276	6.1864	200.41	0.0126	9.0214	9.3255
17	103->108	0.38288	6.2287	199.05	0.2038	-64.9352	-67.5261
	105->109	-0.32554					
	106->109	-0.34315					
18	95->107	0.33792	6.3698	194.64	0.1301	28.7022	31.4044
	96->107	-0.30909					
	104->109	0.26011					
19	92->107	-0.22977	6.4335	192.72	0.0009	-1.5937	-1.5302
	100->108	-0.31445					
	102->109	0.36037					
20	89->107	-0.26732	6.5352	189.72	0.0008	-1.215	-0.8532
	93->107	0.22569					
	102->109	0.37563					
21	104->109	0.42304	6.5797	188.43	0.0132	9.7245	9.2093
	106->110	-0.26817					
22	93->107	0.28585	6.6253	187.14	0.0009	1.6096	1.2545
	98->107	0.37647					
	100->108	-0.27656					
23	103->109	0.45292	6.7722	183.08	0.0197	-0.5846	-0.7262
	105->110	-0.23247					
24	93->107	-0.35018	6.8123	182.00	0.0047	-3.5143	-3.8957
	98->107	0.43498					
25	92->107	0.36515	6.8597	180.74	0.0121	12.0195	12.8489
	94->107	0.25195					
26	104->109	0.35932	6.8954	179.81	0.5820	-27.6806	-30.9284
	106->110	0.50503					
27	103->109	0.33322	6.9580	178.19	0.0027	16.116	17.0206
	105->110	0.53179					
28	91->107	-0.37604	7.0172	176.69	0.0005	-1.4366	-2.2209
	94->107	0.39282					
29	100->109	0.41024	7.0781	175.17	0.0007	2.3816	3.1846
	102->110	0.30619					
30	100->109	-0.36044	7.1278	173.94	0.0034	-2.4161	-3.2658
	101->108	0.38701					
31	95->107	0.2497	7.1863	172.53	0.0013	0.9648	1.4581
	96->107	0.26229					
32	90->107	0.39331	7.2645	170.67	0.0146	1.9743	1.4355
	104->110	-0.36175					
33	100->109	-0.24561	7.2736	170.46	0.0019	3.5702	5.6405
	101->108	-0.32186					
	102->110	0.41991					

34	90->107	0.23723	7.3149	169.50	0.1963	-43.2587	-46.5912
	97->108	-0.24566					
	104->110	0.44592					
35	89->107	0.3598	7.3530	168.62	0.0144	11.5157	12.9627
	91->107	0.23857					
36	99->108	0.49098	7.4804	165.75	0.0053	-12.8755	-9.907
	103->110	0.24365					

[a]Number of the excited states; [b]Only transitions with contribution over 10.0% were listed; [c]Configuration-interaction coefficient; [d]Excitation energy; [e]Wavelength; [f]Oscillator strength; [g]Rotatory strength in velocity form (10^{-40} cgs); [h]Rotatory strength in length form (10^{-40} cgs).

Table S15. Key transitions, oscillator strengths, and rotatory strengths in the ECD spectrum of conformer cpd-**1A**-6 at the CAM-B3LYP/Def2SVP level of theory in MeOH with IEFPCM solvent model.

Num[a]	***Transition***[b]	***CI-coeff***[b]	***ΔE (eV)***[d]	***λ (nm)***[e]	***f***[f]	R_{vel}[g]	R_{len}[h]
1	105->107	0.24701	3.2768	378.37	0.3271	-11.209	-11.7417
	106->107	0.63778					
2	100->107	-0.30272	3.4129	363.28	0.0009	-4.1488	-4.959
	102->107	0.58852					
3	105->107	0.63426	3.6143	343.03	0.0189	15.7171	16.3194
	106->107	-0.25373					
4	100->107	0.56417	3.7535	330.32	0.0003	-1.1955	-1.1144
	102->107	0.29052					
	102->108	-0.25238					
5	104->107	0.66297	3.9375	314.88	0.0570	9.2272	8.9304
6	103->107	0.66682	4.5135	274.69	0.2597	-10.0858	-10.9418
7	106->108	0.62527	5.1012	243.05	0.2320	17.7324	18.8736
8	105->108	0.59648	5.2396	236.63	0.3929	1.2587	-2.6328
9	101->107	0.59393	5.4818	226.17	0.0048	-6.2289	-5.266
10	101->107	0.23676	5.5259	224.37	0.0147	3.5317	3.4878
	103->108	0.31426					
	106->109	0.44344					
11	104->108	0.53749	5.6068	221.13	0.1764	-14.4905	-14.8985
	105->109	0.25702					
12	102->108	0.56437	5.8027	213.67	0.0009	-3.0986	-3.0909
13	99->107	0.61053	5.9159	209.58	0.0162	-2.3007	-2.021
14	97->107	0.54943	5.9597	208.04	0.3516	13.3938	18.6802
	105->109	-0.30827					
15	97->107	-0.24394	6.0781	203.98	0.2078	15.3022	16.9814
	103->108	-0.31978					
	105->109	-0.28678					
	106->109	0.33834					
16	98->107	-0.25678	6.1803	200.61	0.0038	5.6132	6.0828

	99->107	0.22649					
	100->108	0.36624					
17	103->108	-0.37411	6.2279	199.08	0.2212	27.652	30.9655
	105->109	0.42083					
	106->109	0.24099					
18	95->107	0.30649	6.3305	195.85	0.1411	-17.3132	-20.3494
	98->107	0.27957					
	104->109	0.25227					
19	93->107	0.29633	6.4016	193.68	0.0136	-5.926	-5.617
	98->107	0.23104					
	100->108	0.33928					
20	96->107	0.22629	6.4819	191.28	0.0054	-5.0364	-5.9518
	102->109	0.46602					
21	95->107	-0.29741	6.5747	188.58	0.0145	-12.8472	-12.3586
	104->109	0.39422					
22	93->107	0.33948	6.6488	186.47	0.0000	0.6111	0.7786
	100->108	-0.27614					
23	103->109	0.48181	6.7282	184.28	0.0103	15.2459	13.8455
	105->110	-0.24384					
24	93->107	0.22754	6.8255	181.65	0.0664	-18.3441	-17.7849
	95->107	0.28231					
	96->107	-0.27487					
	102->109	0.30804					
25	104->109	0.28223	6.8525	180.93	0.4527	10.173	12.9634
	106->110	0.51551					
26	92->107	0.45666	6.8884	179.99	0.0119	1.3828	1.0836
	94->107	-0.23164					
27	91->107	0.35078	6.9235	179.08	0.0256	-25.0207	-25.5384
	98->107	-0.29438					
	100->109	0.23009					
28	103->109	0.26661	6.9541	178.29	0.0764	-4.4175	-5.9303
	105->110	0.51245					
29	101->108	0.60424	7.0384	176.15	0.0376	-18.8745	-20.2958
30	91->107	-0.29108	7.1005	174.61	0.0031	-2.4413	-1.8134
	100->109	0.43283					
	102->110	0.28403					
31	92->107	-0.22631	7.2121	171.91	0.0008	-5.3323	-5.1925
	94->107	-0.29367					
	100->109	0.38797					
	102->110	-0.24477					
32	94->107	-0.3192	7.2570	170.85	0.0020	1.1168	-0.0355
	102->110	0.4366					
33	90->107	-0.37826	7.2867	170.15	0.0464	8.5633	9.0289

	104->110	0.46645					
34	90->107	0.45999	7.3307	169.13	0.1429	7.0661	8.5187
	97->108	-0.27347					
	104->110	0.33294					
35	103->110	0.53948	7.4403	166.64	0.0483	-1.3503	-4.4417
36	85->107	0.43748	7.4682	166.02	0.0003	-0.7405	-0.5459
	93->107	0.22478					

[a]Number of the excited states; [b]Only transitions with contribution over 10.0% were listed; [c]Configuration-interaction coefficient; [d]Excitation energy; [e]Wavelength; [f]Oscillator strength; [g]Rotatory strength in velocity form (10^{-40} cgs); [h]Rotatory strength in length form (10^{-40} cgs).

Table S16. Key transitions, oscillator strengths, and rotatory strengths in the ECD spectrum of conformer cpd-**1A**-7 at the CAM-B3LYP/Def2SVP level of theory in MeOH with IEFPCM solvent model.

Num[a]	***Transition***[b]	***CI-coeff***[b]	***ΔE (eV)***[d]	***λ (nm)***[e]	***f***[f]	R_{vel}[g]	R_{len}[h]
1	106->107	0.65704	3.2803	377.97	0.3314	13.8785	14.2309
2	100->107	-0.301	3.4144	363.12	0.0002	0.7669	1.4373
	102->107	0.58464					
3	105->107	0.6515	3.6414	340.48	0.0178	-11.789	-12.2509
4	100->107	0.56106	3.7573	329.98	0.0003	1.0622	0.7817
	102->107	0.29519					
	102->108	-0.25213					
5	104->107	0.65917	3.9502	313.87	0.0580	-5.4545	-5.7888
6	103->107	0.66256	4.5467	272.69	0.2691	-4.2654	-3.2631
7	106->108	0.63706	5.1049	242.87	0.2916	-15.5994	-16.1012
8	105->108	0.6048	5.2657	235.46	0.3491	-4.4177	-1.4561
9	103->108	0.35149	5.5312	224.15	0.0124	5.1963	4.639
	106->109	0.44871					
10	101->107	0.64531	5.5752	222.39	0.0050	-1.6807	-1.6911
11	104->108	0.54945	5.6118	220.94	0.1748	21.3514	21.4743
	105->109	0.24375					
12	102->108	0.58411	5.8084	213.46	0.0006	-1.0181	-1.2408
13	98->107	0.50394	5.9632	207.92	0.2991	19.2568	17.349
14	98->107	-0.24228	6.0126	206.21	0.0415	-20.3	-23.0191
	99->107	0.48921					
	105->109	0.23099					
15	103->108	0.34356	6.1156	202.73	0.3243	-0.5571	-1.0961
	105->109	0.32706					
	106->109	-0.322					
16	100->108	0.3381	6.2324	198.94	0.0671	-88.4622	-90.5444
	103->108	-0.24279					
	105->109	0.26157					
17	100->108	-0.29822	6.2581	198.12	0.2019	64.2289	66.5402

	103->108	-0.27032					
	105->109	0.30679					
18	95->107	0.32595	6.3884	194.08	0.0765	-5.5218	-5.7858
	99->107	0.26637					
	104->109	0.23323					
19	92->107	0.31266	6.4603	191.92	0.0003	0.8052	0.7321
	102->109	-0.30058					
20	102->109	0.43696	6.5420	189.52	0.0027	1.4562	2.289
21	95->107	-0.24992	6.6030	187.77	0.0099	6.6821	5.3423
	104->109	0.36644					
	106->110	-0.22836					
22	92->107	0.24926	6.6980	185.11	0.0008	-1.0366	-1.065
	93->107	0.4145					
	96->107	-0.23056					
	100->108	-0.27297					
23	103->109	0.43445	6.7697	183.15	0.0343	0.3464	0.7074
	105->110	-0.26783					
24	91->107	0.23494	6.8727	180.40	0.0330	16.1686	16.9869
	94->107	0.31643					
25	103->109	-0.2753	6.8929	179.87	0.5072	-32.2524	-33.9266
	104->109	0.3144					
	106->110	0.46907					
26	103->109	0.31597	6.9600	178.14	0.0709	13.6488	13.2114
	105->110	0.50552					
27	90->107	-0.27921	7.0260	176.47	0.0240	28.4157	27.8402
	96->107	-0.23527					
	97->107	0.30822					
28	91->107	0.42249	7.0670	175.44	0.0006	1.571	1.0846
	94->107	-0.22572					
	101->108	0.27389					
29	92->107	0.2483	7.0846	175.01	0.0006	-0.2311	0.176
	101->108	0.26525					
	102->110	0.24165					
30	101->108	0.4784	7.1175	174.20	0.0080	4.2614	5.0041
31	96->107	-0.24368	7.1508	173.38	0.0021	-6.212	-6.0848
	97->107	-0.30149					
	100->109	0.36377					
	102->110	0.22367					
32	100->109	-0.34508	7.2581	170.82	0.0015	-4.3759	-3.4574
	102->110	0.47258					
33	89->107	-0.41454	7.2948	169.96	0.0448	-12.8025	-13.8428
	104->110	0.46341					
34	89->107	0.46349	7.3389	168.94	0.1604	-13.9365	-15.6084

	98->108	-0.28374					
	104->110	0.35549					
35	92->107	-0.24867	7.4286	166.90	0.0031	-4.208	-3.9783
	93->107	0.29844					
	94->107	0.27213					
	96->107	0.28958					
36	103->110	0.54847	7.4646	166.10	0.0449	15.1745	17.4105

[a]Number of the excited states; [b]Only transitions with contribution over 10.0% were listed; [c]Configuration-interaction coefficient; [d]Excitation energy; [e]Wavelength; [f]Oscillator strength; [g]Rotatory strength in velocity form (10^{-40} cgs); [h]Rotatory strength in length form (10^{-40} cgs).

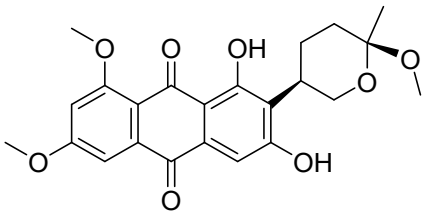
Table S17. Key transitions, oscillator strengths, and rotatory strengths in the ECD spectrum of conformer cpd-**1A**-8 at the CAM-B3LYP/Def2SVP level of theory in MeOH with IEFPCM solvent model.

Num[a]	***Transition***[b]	***CI-coeff***[b]	***ΔE (eV)***[d]	***λ (nm)***[e]	***f***[f]	R_{vel}[g]	R_{len}[h]
1	105->107	0.23689	3.2705	379.10	0.3308	15.3055	16.303
	106->107	0.6398					
2	100->107	-0.28918	3.3941	365.29	0.0002	1.3427	1.7434
	102->107	0.56844					
3	105->107	0.63841	3.6096	343.49	0.0271	-23.2848	-24.1342
	106->107	-0.2394					
4	100->107	0.56559	3.7381	331.68	0.0001	0.2931	0.1365
	102->107	0.28748					
	102->108	-0.24278					
5	104->107	0.66237	3.9129	316.86	0.0504	-9.7042	-10.1315
6	103->107	0.65968	4.4874	276.29	0.2514	11.8287	12.8751
7	106->108	0.60511	5.1017	243.03	0.2641	-43.3996	-46.058
8	105->108	0.59291	5.2310	237.02	0.3360	24.9611	29.3531
9	101->107	0.62133	5.3346	232.41	0.0162	3.5531	2.5336
10	103->108	0.35417	5.5175	224.71	0.0066	-0.3828	-0.4489
	106->109	0.48286					
11	104->108	0.55841	5.5751	222.39	0.1583	16.951	17.2029
	105->109	0.26318					
12	99->107	0.6257	5.6279	220.30	0.0224	12.8017	13.6124
13	102->108	0.57532	5.7990	213.80	0.0013	-1.7948	-2.1026
14	97->107	0.5575	5.9216	209.38	0.3420	-10.2535	-15.7881
	105->109	-0.28851					
15	103->108	0.25492	6.0507	204.91	0.2150	-13.9267	-18.2996
	105->109	0.38314					
	106->109	-0.26799					
16	98->107	0.38021	6.1266	202.37	0.1009	-8.9038	-7.6103
	100->108	-0.23956					
17	103->108	0.38323	6.1923	200.22	0.2145	-67.1457	-73.4851

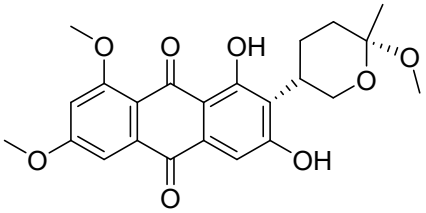
	105->109	-0.34371					
	106->109	-0.2887					
18	96->107	-0.26655	6.2656	197.88	0.0991	33.272	38.0929
	98->107	0.23211					
	100->108	0.34246					
19	96->107	0.23217	6.3991	193.75	0.0138	14.4211	14.5481
	100->108	0.27327					
	102->109	-0.24946					
20	102->109	0.43986	6.4770	191.42	0.0096	2.1828	4.0182
	104->109	-0.25967					
21	104->109	0.36509	6.5281	189.92	0.0132	13.1111	11.9909
22	93->107	0.38465	6.6481	186.49	0.0003	-3.0396	-2.8697
	100->108	-0.24278					
	103->109	-0.23465					
23	96->107	-0.25205	6.6894	185.34	0.0016	-6.1151	-4.8921
	103->109	0.45436					
24	95->107	-0.30747	6.7855	182.72	0.0740	11.1782	11.0438
	96->107	0.31815					
	98->107	0.24165					
	106->110	-0.25351					
25	92->107	-0.28678	6.8268	181.61	0.1554	35.2143	35.1495
	94->107	0.2551					
	106->110	0.30559					
26	106->110	0.32776	6.8329	181.45	0.1518	-16.4599	-18.8449
27	101->108	0.4953	6.8883	179.99	0.2541	9.1375	9.2684
	105->110	0.27353					
	106->110	0.22578					
28	101->108	-0.25455	6.9029	179.61	0.0041	25.1948	23.1718
	103->109	0.30509					
	105->110	0.43021					
29	92->107	0.30307	6.9593	178.16	0.0028	5.6301	7.8658
	93->107	-0.23856					
	94->107	0.32701					
30	100->109	0.4635	7.0694	175.38	0.0008	-4.6387	-5.0618
	102->110	0.30358					
31	89->107	-0.24558	7.1202	174.13	0.0048	12.188	11.7319
	93->107	0.22698					
	94->107	0.22681					
	95->107	0.27394					
32	99->108	0.40036	7.1597	173.17	0.0005	-1.4184	-0.6049
	100->109	0.30109					
33	90->107	-0.36256	7.2432	171.17	0.0433	-15.5393	-15.8987
	104->110	0.45835					

34	90->107	0.31382	7.2875	170.13	0.0826	-19.6616	-19.4677
	99->108	-0.2658					
	102->110	-0.24011					
	104->110	0.26474					
35	90->107	0.23284	7.3016	169.80	0.0906	4.5722	3.1013
	99->108	0.31503					
	102->110	0.28345					
	104->110	0.22649					
36	89->107	0.42873	7.3411	168.89	0.0063	-11.4503	-11.6149
	90->107	-0.26733					
	95->107	0.23047					

[a]Number of the excited states; [b]Only transitions with contribution over 10.0% were listed; [c]Configuration-interaction coefficient; [d]Excitation energy; [e]Wavelength;[f]Oscillator strength; [g]Rotatory strength in velocity form (10^{-40} cgs); [h]Rotatory strength in length form (10^{-40} cgs).



2A



2B

Table S18. Experimental and calculated ^{13}C-NMR chemical shifts of cpd-**2A**

No.	***δ*exptl.**	**cpd-1A-*δ*calcd.**
1	161.4	159.9
2	122.7	121.9
3	163.0	156.9
4	107.9	107.8
4a	132.1	130.5
5	104.0	102.3
6	165.0	161.1
7	105.1	102.4
8	164.0	159.6
8a	115.4	115.2
9	186.9	182.4
9a	110.8	108.2
10	183.1	180.4
10a	137.5	135.6
11	56.8	54.8
12	56.1	55.1
1’	23.0	22.4
2’	98.6	99.6
3'	35.2	34.7

4’	22.4	24.1
5’	31.9	33.1
6'	62.5	62.9
7’	48.3	48.3

Table S19. Experimental and calculated ^{1}H-NMR chemical shifts of cpd-**2A**

No.	***δ*exptl.**	**cpd-1A-*δ*calcd.**
4	7.21	7.46
5	7.42	7.53
7	6.77	6.82
11	4.01	3.83
12	3.97	3.91
1’	1.45	1.27
3’	1.74	1.57
3’	1.86	1.71
4’	1.65	1.69
4’	2.62	2.24
5’	3.65	3.65
6’	3.63	3.71
6’	4.31	3.91
7’	3.39	3.44

Table S20. Conformational analysis of the B3LYP/6-31G(d) optimized conformers of cpd-**2A** in the gas phase (T=298.15 K)

Conformer	**E[a] (Hartree)**	**C[b] (Hartree)**	**G[c] (kcal/mol)**	**ΔG[d] (kcal/mol)**	**Population[e]**
cpd-**2A**-1	-1492.576002	0.379385	-936353.377067	0.0	49.63%
cpd-**2A**-2	-1492.573872	0.378384	-936352.668707	0.70836	15.00%
cpd-**2A**-3	-1492.571371	0.376043	-936352.568169	0.808898	12.66%
cpd-**2A**-4	-1492.571342	0.376246	-936352.422916	0.954151	9.91%
cpd-**2A**-5	-1492.573894	0.379327	-936352.090993	1.286074	5.65%
cpd-**2A**-6	-1492.572434	0.378288	-936351.826377	1.550691	3.62%
cpd-**2A**-7	-1492.571535	0.377411	-936351.812841	1.564226	3.53%

[a]Electronic energy obtained at M062X/6-311+G(2d,p) level of theory; [b]Thermal correction to Gibbs free energy obtained at B3LYP/6-31G(d) level of theory; [c]Gibbs free energy (E + C); [d]The relative Gibbs free energy; [e]The Boltzmann distribution of each conformer.

Table S21. Atomic coordinates (Å) of cpd-**2A**-1 obtained at the B3LYP/6-31G(d) level of theory in the gas phase.

C	0.647787	1.055151	0.054083	O	-2.057001	-2.904300	0.139333
C	1.836910	0.298107	0.127099	O	2.800414	1.938416	0.262974
C	1.734560	-1.103161	0.191040	O	0.768799	2.389576	-0.008637
C	0.480509	-1.734952	0.179627	H	-6.549960	1.093077	-0.125498

C	-0.675969	-0.979709	0.108143	H	-4.388112	-2.616338	0.062624
C	-4.427959	-1.536516	0.021369	H	0.421332	-2.815322	0.226834
C	-5.622370	-0.819665	-0.035926	H	3.664465	-1.474845	0.295710
C	-5.599607	0.578601	-0.083917	H	3.001981	2.070599	0.077284
C	-4.390826	1.276206	-0.078677	H	-0.169696	2.742236	-0.052427
C	-3.154849	0.565505	-0.024809	H	3.717507	-0.419888	-1.470659
C	-1.843171	1.248109	-0.024044	H	3.602995	1.257914	-1.984366
C	-0.627345	0.430598	0.046627	H	3.749115	-0.279044	1.826885
C	-1.981233	-1.680481	0.094978	H	3.562398	1.410634	2.210640
C	-3.219647	-0.842571	0.027141	H	5.987414	0.516177	2.165189
C	-5.560767	3.352906	-0.163996	H	5.718563	1.963411	1.180638
C	-6.942633	-2.801401	-0.005101	H	7.982574	-0.197390	0.645929
C	7.457794	0.317812	-0.163742	H	7.765774	-0.105062	-1.123080
C	5.953279	0.197504	0.026907	H	7.741282	1.373471	-0.155481
C	5.458720	0.904581	1.288218	H	6.975309	-2.365469	-0.756108
C	3.949272	0.726335	1.448596	H	5.284640	-2.933436	-0.808595
C	3.179441	0.995636	0.125717	H	5.804319	-1.590368	-1.864959
C	3.939911	0.610133	-1.171972	H	-5.267674	4.403053	-0.186992
C	5.931546	-2.056837	-0.882420	H	-6.141515	3.114818	-1.064042
O	5.356655	0.785117	-1.113382	H	-6.173891	3.162523	0.725829
O	-1.756844	2.493015	-0.082363	H	-8.008053	-3.033669	-0.027483
O	-6.856395	-1.381064	-0.049070	H	-6.448281	-3.256604	-0.871506
O	5.528739	-1.171537	0.164087	H	-6.498543	-3.198469	0.915412
O	-4.343625	2.623439	-0.121869	-	-	-	-

Table S22. Atomic coordinates (Å) of cpd-**2A**-2 obtained at the B3LYP/6-31G(d) level of theory in the gas phase.

C	0.662902	1.085988	-0.397492	O	-1.958845	-2.919205	-0.207925
C	1.873560	0.362899	-0.543662	O	2.846686	-1.881968	-0.620944
C	1.798619	-1.043825	-0.526443	O	0.753954	2.425954	-0.377666
C	0.549909	-1.691553	-0.417177	H	-6.495357	0.995126	0.360906
C	-0.617552	-0.967477	-0.297834	H	-4.281495	-2.673345	0.034889
C	-4.340206	-1.594064	0.067207	H	0.519547	-2.774150	-0.419624
C	-5.540547	-0.899894	0.209486	H	3.717157	-1.411386	-0.590504
C	-5.541273	0.498913	0.246867	H	2.812733	2.117411	-1.218811
C	-4.350731	1.219405	0.140179	H	-0.190576	2.757471	-0.278463
C	-3.109178	0.532465	-0.009193	H	3.960997	0.155035	-2.393427
C	-1.816142	1.240396	-0.132793	H	4.989625	1.440512	-1.735206
C	-0.595429	0.444855	-0.277075	H	2.821188	2.041444	1.314334
C	-1.903389	-1.693890	-0.185020	H	4.316369	2.554328	0.551195
C	-3.149924	-0.877377	-0.038776	H	3.722958	-0.256460	1.652585
C	-5.549811	3.272869	0.323524	H	4.834396	0.912477	2.362764
C	-6.820540	-2.906464	0.285052	H	7.430606	0.513421	-0.351293

C	6.723379	0.916745	0.377881	H	6.408604	1.903991	0.031015
C	5.529737	-0.023036	0.556800	H	7.232265	1.041680	1.338287
C	4.407011	0.565615	1.416040	H	6.898547	-2.966356	1.035516
C	3.655368	1.690573	0.701645	H	6.766841	-2.097569	-0.516280
C	3.127290	1.221762	-0.674225	H	7.909323	-1.530483	0.740442
C	4.293920	0.634698	-1.469429	H	-5.276985	4.328757	0.321682
C	6.925997	-1.983687	0.560644	H	-6.235139	3.069780	-0.509025
O	5.004647	-0.387330	-0.753486	H	-6.044664	3.024016	1.270847
O	-1.753708	2.489321	-0.117076	H	-7.876695	-3.159315	0.386228
O	-6.758977	-1.484662	0.320250	H	-6.437720	-3.297525	-0.665144
O	5.877528	-1.231844	1.165900	H	-6.254874	-3.349750	1.113192
O	-4.326971	2.567910	0.174281	-	-	-	-

Table S23. Atomic coordinates (Å) of cpd-**2A**-3 obtained at the B3LYP/6-31G(d) level of theory in the gas phase.

C	0.645724	0.762559	0.105322	O	-2.378996	-2.958336	0.109027
C	1.772497	-0.091741	0.158311	O	2.615018	-2.304871	0.225119
C	1.534865	-1.472178	0.182781	O	0.871418	2.082216	0.079261
C	0.238439	-2.001074	0.161684	H	-6.528937	1.398547	-0.157108
C	-0.853103	-1.150376	0.109291	H	-4.684487	-2.478996	0.007022
C	-4.633963	-1.399112	-0.017547	H	0.064374	-3.073114	0.181465
C	-5.764586	-0.585047	-0.080437	H	2.301096	-3.222444	0.248695
C	-5.624997	0.806810	-0.108790	H	3.040737	1.594346	0.148133
C	-4.362723	1.402451	-0.075737	H	-0.032036	2.513880	0.043413
C	-3.190532	0.591254	-0.012482	H	4.108615	-0.958063	-1.123040
C	-1.827755	1.164232	0.021399	H	3.466058	0.465216	-1.979264
C	-0.680030	0.247155	0.080033	H	4.099724	-0.919808	1.519768
C	-2.209468	-1.742582	0.081231	H	3.444990	0.508437	2.332097
C	-3.373271	-0.807324	0.015324	H	5.988519	0.528989	2.187836
C	-5.355148	3.569434	-0.168014	H	5.239486	1.922461	1.392088
C	-7.243835	-2.451454	-0.095330	H	8.057322	1.089940	0.626609
C	7.333780	1.316671	-0.162232	H	7.786490	1.107213	-1.135054
C	6.068428	0.488496	0.038051	H	7.089688	2.381759	-0.128443
C	5.352012	0.832540	1.349879	H	8.054589	-1.249168	-1.032773
C	3.977082	0.162475	1.438412	H	6.857363	-2.562563	-0.915682
C	3.160552	0.508351	0.176790	H	6.522672	-1.141567	-1.944504
C	3.973243	0.126478	-1.071860	H	-5.932193	3.382625	-1.082224
C	6.980572	-1.480285	-1.008123	H	-6.001719	3.427822	0.706941
O	5.243025	0.783467	-1.082305	H	-4.974842	4.591310	-0.179050
O	-1.639083	2.397362	-0.000398	H	-6.777650	-2.934366	-0.962301
O	-7.039564	-1.042568	-0.118222	H	-6.846498	-2.895527	0.825042
O	6.341223	-0.906432	0.120646	H	-8.324404	-2.593881	-0.133890
O	-4.203746	2.740482	-0.102320	-	-	-	-

Table S24. Atomic coordinates (Å) of cpd-**2A**-4 obtained at the B3LYP/6-31G(d) level of theory in the gas phase.

C	-0.905617	-0.106068	0.095043	O	2.908630	-3.005557	-0.135174
C	-1.799468	-1.200706	0.063851	O	-2.103877	-3.544250	-0.043511
C	-1.244553	-2.485429	-0.012492	O	-1.430959	1.124544	0.163529
C	0.139513	-2.695491	-0.054625	H	5.919143	2.208149	0.034307
C	1.000481	-1.611411	-0.022374	H	5.038363	-1.993768	-0.141966
C	4.734893	-0.957456	-0.085272	H	0.560518	-3.695049	-0.113185
C	5.642462	0.101126	-0.058866	H	-1.585564	-4.362255	-0.097287
C	5.179596	1.419322	0.016263	H	-3.751096	-2.015447	0.053001
C	3.812641	1.698535	0.064883	H	-0.652696	1.756235	0.178204
C	2.863944	0.632878	0.038611	H	-3.415319	0.772194	-1.117241
C	1.404780	0.866410	0.086131	H	-3.585335	-0.746084	-2.032656
C	0.503956	-0.295029	0.053644	H	-3.367064	0.636013	1.511609
C	2.458180	-1.865257	-0.070016	H	-3.500411	-0.954231	2.274617
C	3.370224	-0.681722	-0.036922	H	-5.713508	0.306462	2.222620
C	4.268376	4.037858	0.163157	H	-5.783180	-1.248352	1.377514
C	7.520478	-1.358620	-0.183785	H	-7.630529	0.819064	-1.044808
C	-7.325137	0.371285	-0.095431	H	-7.643829	-0.674494	-0.098899
C	-5.811598	0.452059	0.078142	H	-7.824098	0.895229	0.725367
C	-5.334513	-0.247717	1.357438	H	-6.684280	2.983946	-0.889916
C	-3.807596	-0.357593	1.407650	H	-4.989868	3.522716	-0.778142
C	-3.300868	-1.020217	0.110401	H	-5.423236	2.164462	-1.853269
C	-3.837811	-0.235759	-1.099012	H	4.879779	4.064475	-0.747436
C	-5.637353	2.649913	-0.894237	H	3.658375	4.939923	0.219569
O	-5.266675	-0.177312	-1.076133	H	4.923783	3.982725	1.041268
O	0.932825	2.019692	0.152131	H	8.604211	-1.239427	-0.210383
O	6.989457	-0.039983	-0.101635	H	7.237180	-1.956240	0.690748
O	-5.351284	1.792155	0.199040	H	7.183262	-1.866270	-1.095212
O	3.343797	2.960033	0.136563	-	-	-	-

Table S25. Atomic coordinates (Å) of cpd-**2A**-5 obtained at the B3LYP/6-31G(d) level of theory in the gas phase.

C	0.661780	0.996499	0.059095	O	-1.924135	-3.041498	0.152293
C	1.871940	0.274130	0.130657	O	2.899796	-1.933741	0.265845
C	1.810067	-1.129693	0.195586	O	0.744301	2.333982	-0.004933
C	0.574904	-1.797141	0.187010	H	-6.516028	0.870888	-0.117114
C	-0.603158	-1.075888	0.116741	H	-4.310770	-2.814182	0.077314
C	-4.336296	-1.732582	0.035017	H	0.546489	-2.878722	0.235209
C	-5.554983	-1.051333	-0.022923	H	3.750139	-1.445486	0.295539
C	-5.574880	0.344203	-0.074453	H	2.985464	2.079278	0.076361
C	-4.374345	1.071580	-0.071245	H	-0.204359	2.659253	-0.047480
C	-3.124283	0.399672	-0.016332	H	3.767488	-0.391163	-1.471581

C	-1.833433	1.118796	-0.016423	H	3.602942	1.282067	-1.986514
C	-0.595350	0.335554	0.053847	H	3.805991	-0.246104	1.825561
C	-1.886848	-1.816972	0.106613	H	3.570954	1.437737	2.208625
C	-3.149983	-1.015726	0.038724	H	6.021146	0.615878	2.156040
C	-5.599736	3.121456	-0.162618	H	5.705830	2.052963	1.170048
C	-7.937258	-1.190389	-0.082335	H	8.031796	-0.039939	0.631855
C	7.489224	0.457195	-0.177431	H	7.806429	0.040849	-1.136637
C	5.989451	0.292879	0.018366	H	7.741550	1.520791	-0.173077
C	5.478293	0.987021	1.280257	H	7.084791	-2.238960	-0.764277
C	3.975322	0.764398	1.445894	H	5.411795	-2.857940	-0.809550
C	3.193925	1.009894	0.125240	H	5.886941	-1.501948	-1.870327
C	3.961161	0.645169	-1.174630	H	-6.208934	2.922978	0.728592
C	6.031680	-1.962382	-0.887364	H	-5.330043	4.177780	-0.189309
O	5.372470	0.861034	-1.120994	H	-6.175991	2.869817	-1.062333
O	-1.781806	2.366225	-0.074842	H	-8.673172	-1.995262	-0.072667
O	-6.668459	-1.825399	-0.024017	H	-8.098461	-0.538455	0.785628
O	5.606060	-1.087608	0.158890	H	-8.049513	-0.604745	-1.003653
O	-4.367681	2.420077	-0.118496	-	-	-	-

Table S26. Atomic coordinates (Å) of cpd-**2A**-6 obtained at the B3LYP/6-31G(d) level of theory in the gas phase.

C	0.729662	1.090361	-0.428908	O	-1.924934	-2.895907	-0.311549
C	1.931476	0.360130	-0.610047	O	2.884460	-1.882695	-0.790551
C	1.839611	-1.043600	-0.643386	O	0.834549	2.427790	-0.374960
C	0.589557	-1.685437	-0.534687	H	-6.417680	1.041173	0.429952
C	-0.568834	-0.954051	-0.372416	H	-4.242713	-2.636599	-0.025911
C	-4.290682	-1.558057	0.035639	H	0.548090	-2.767033	-0.572723
C	-5.482472	-0.857345	0.215165	H	3.751985	-1.410899	-0.742311
C	-5.469934	0.539981	0.288396	H	2.894932	2.102394	-1.282058
C	-4.274752	1.252781	0.181650	H	-0.104854	2.766250	-0.254521
C	-3.041788	0.559001	-0.004078	H	4.047375	0.122892	-2.429804
C	-1.744788	1.258651	-0.126776	H	5.069714	1.409270	-1.769248
C	-0.532344	0.456329	-0.310024	H	2.864774	2.031522	1.254572
C	-1.859441	-1.672106	-0.257844	H	4.369961	2.539468	0.508528
C	-3.095817	-0.849340	-0.070321	H	3.742498	-0.249124	1.610559
C	-5.451865	3.311848	0.434488	H	4.867371	0.901182	2.326978
C	-6.779320	-2.854242	0.260775	H	7.232818	1.121812	1.324134
C	6.764430	0.947434	0.351966	H	7.499761	0.495198	-0.317740
C	5.597900	-0.020718	0.528210	H	6.450656	1.910395	-0.056195
C	4.451201	0.552098	1.376088	H	5.273025	-2.814399	0.188121
C	3.705724	1.678146	0.652957	H	5.986982	-3.034816	1.805224
C	3.194718	1.206538	-0.728616	H	4.424118	-2.203294	1.630095
C	4.369936	0.607906	-1.504810	H	-5.934753	3.043655	1.382607

C	5.408215	-2.357469	1.173654	H	-5.168755	4.364783	0.454989
O	5.077643	-0.411447	-0.775468	H	-6.151072	3.136166	-0.392651
O	-1.669340	2.505572	-0.077566	H	-6.415674	-3.224539	-0.705077
O	-6.703813	-1.434185	0.330538	H	-6.204682	-3.323136	1.068341
O	6.178096	-1.162932	1.093814	H	-7.836032	-3.099873	0.372867
O	-4.237934	2.599368	0.249344	-	-	-	-

Table S27. Atomic coordinates (Å) of cpd-**2A**-7 obtained at the B3LYP/6-31G(d) level of theory in the gas phase.

C	0.597399	1.149440	-0.105828	O	-1.980926	-2.894433	-0.048802
C	1.812761	0.430746	-0.146190	O	2.845742	-1.768795	-0.180130
C	1.755845	-0.974564	-0.148420	O	0.670379	2.489857	-0.093543
C	0.519703	-1.644480	-0.109439	H	-6.597722	0.964536	0.085825
C	-0.660831	-0.926829	-0.074834	H	-4.319352	-2.678063	0.003982
C	-4.393749	-1.599294	0.012810	H	0.497688	-2.727263	-0.112648
C	-5.610194	-0.919407	0.046388	H	3.677169	-1.260059	-0.329457
C	-5.631423	0.479644	0.058406	H	2.860189	2.258123	-0.237456
C	-4.445295	1.214799	0.035455	H	-0.281399	2.809826	-0.063984
C	-3.187462	0.542438	-0.001621	H	3.533957	0.530607	-2.174548
C	-1.897666	1.265835	-0.032066	H	4.680287	1.729188	-1.557694
C	-0.657797	0.486151	-0.073015	H	3.674790	0.021760	1.630970
C	-1.943116	-1.668060	-0.044970	H	3.483428	1.738255	1.957245
C	-3.207876	-0.867824	-0.010415	H	5.910236	1.095721	1.982950
C	-5.681302	3.253818	0.083949	H	5.610085	2.162168	0.610131
C	-6.867736	-2.941634	0.055946	H	7.997934	0.618373	0.198636
C	7.230126	0.429708	-0.558542	H	7.566488	-0.373092	-1.218929
C	5.907966	0.070047	0.111274	H	7.109641	1.333753	-1.163424
C	5.375018	1.178385	1.032971	H	5.856401	-2.483963	-0.625181
C	3.866387	1.019956	1.226903	H	7.489826	-2.266316	0.071989
C	3.117052	1.202926	-0.124372	H	6.215383	-3.077836	1.015593
C	4.075259	0.856092	-1.283382	H	-6.248934	3.012682	0.991610
C	6.415317	-2.282930	0.294621	H	-5.422625	4.313259	0.086940
O	4.944092	-0.231129	-0.937755	H	-6.293501	3.028430	-0.798405
O	-1.852953	2.515022	-0.024439	H	-6.364951	-3.362789	0.934645
O	-6.826367	-1.518742	0.069811	H	-7.925494	-3.206867	0.077092
O	5.987210	-1.076397	0.919702	H	-6.405372	-3.343995	-0.853257
O	-4.441489	2.563838	0.046854	-	-	-	-

Table S28. Key transitions, oscillator strengths, and rotatory strengths in the ECD spectrum of conformer cpd-**2A**-1 at the Cam-B3LYP/Def2SVP level of theory in acetonitrile with IEFPCM solvent model.

Num[a]	*Transition*[b]	*CI-coeff*[b]	*ΔE (eV)*[d]	*λ (nm)*[e]	*ff*	R_{vel}[g]	R_{len}[h]
1	113->114	0.69009	3.1972	387.78	0.2464	0.1533	0.0886
2	107->114	-0.38691	3.4328	361.18	0.0000	0.115	0.0391
	109->114	0.5429					
3	112->114	0.67634	3.7014	334.97	0.0404	-0.1762	-0.1142
4	107->114	0.51783	3.7904	327.10	0.0001	0.8285	0.7204
	109->114	0.36981					
	109->115	-0.25398					
5	111->114	0.64568	3.8696	320.41	0.1159	-2.3148	-2.0513
6	110->114	0.65214	4.4101	281.13	0.2445	0.0042	-0.0713
7	113->115	0.65529	5.0411	245.95	0.5738	-0.7519	-0.6883
8	112->115	0.61605	5.3891	230.07	0.1838	0.645	0.787
9	111->115	0.45564	5.4658	226.84	0.0209	1.4881	1.2096
	113->116	-0.36757					
10	110->115	0.39169	5.6065	221.14	0.1523	1.1987	1.1277
	111->115	-0.386					
	113->116	-0.26815					
11	108->114	0.66494	5.7091	217.17	0.0177	0.496	0.2119
12	109->115	0.6028	5.8429	212.20	0.0001	-0.873	-0.8875
13	103->114	-0.24398	5.9618	207.96	0.2276	1.6511	1.2716
	104->114	0.54233					
14	102->114	-0.22805	6.0980	203.32	0.1554	-4.0765	-4.411
	103->114	-0.25306					
	112->116	0.46276					
15	102->114	0.25336	6.1097	202.93	0.1971	0.5705	1.1538
	103->114	0.27139					
	110->115	0.25255					
	111->116	-0.23783					
	113->116	0.32247					
16	101->114	-0.231	6.2553	198.21	0.0047	13.2371	13.4465
	105->114	-0.29112					
	106->114	0.33082					
	107->115	0.23686					
17	104->114	-0.24556	6.2773	197.51	0.4862	-14.4928	-15.2441
	110->115	0.36515					
	111->116	0.27575					
	112->116	-0.32535					
	113->116	0.2559					
18	106->114	0.5704	6.4250	192.97	0.0002	-0.1567	-0.4615
	107->115	-0.3133					

19	100->114	0.24183	6.4569	192.02	0.0011	-2.8876	-2.8077
	105->114	0.26716					
	107->115	0.34497					
20	111->116	0.45656	6.4894	191.06	0.0132	2.4624	2.6967
	112->116	0.23751					
	113->117	-0.24559					
21	109->116	0.59104	6.6752	185.74	0.0004	-0.3985	-0.2493
22	91->114	-0.22676	6.7218	184.45	0.0021	2.6215	3.2785
	100->114	0.46231					
	107->115	-0.22705					
23	110->116	0.53224	6.7239	184.39	0.0175	-3.7743	-4.4064
	113->117	0.23712					
24	101->114	-0.27145	6.8452	181.13	0.0045	1.1627	1.2576
	105->114	0.46406					
25	113->117	0.52711	6.8642	180.62	0.3546	1.9486	2.2215
26	99->114	0.52015	6.9149	179.30	0.0002	1.5507	1.5343
	107->116	-0.26229					
27	110->116	0.27764	7.0260	176.46	0.0538	-2.1116	-2.5338
	111->117	-0.2922					
	112->117	0.49433					
28	101->114	-0.28711	7.1126	174.32	0.0010	-7.9423	-7.2347
	102->114	0.36026					
	103->114	-0.33626					
29	99->114	0.22932	7.1765	172.76	0.0001	1.5022	1.7189
	107->116	0.5529					
30	111->117	0.50002	7.2277	171.54	0.1793	-13.2003	-15.0165
	112->117	0.3042					
31	101->114	0.24805	7.3053	169.72	0.0062	6.9589	8.4522
	109->117	0.45804					
32	97->114	0.48428	7.3217	169.34	0.0112	-7.4722	-8.6239
	108->115	-0.32292					
33	97->114	0.32998	7.3255	169.25	0.0361	15.1401	15.0374
	108->115	0.53228					
34	94->114	0.23009	7.3582	168.50	0.0014	3.8215	4.2951
	101->114	-0.24886					
	107->116	-0.22791					
	109->117	0.27662					
35	104->115	-0.28511	7.4128	167.26	0.1638	0.0396	0.886
	110->117	0.55883					
36	91->114	0.32543	7.5712	163.76	0.0003	0.5778	0.5837
	94->114	0.30998					

[a]Number of the excited states; [b]Only transitions with contribution over 10.0% were listed; [c]Configuration-interaction coefficient; [d]Excitation energy; [e]Wavelength; [f]Oscillator strength;

[g]Rotatory strength in velocity form (10^{-40} cgs); [h]Rotatory strength in length form (10^{-40} cgs).

Table S29. Key transitions, oscillator strengths, and rotatory strengths in the ECD spectrum of conformer cpd-**2A**-2 at the Cam-B3LYP/Def2SVP level of theory in acetonitrile with IEFPCM solvent model.

Num[a]	*Transition*[b]	*CI-coeff*[b]	*ΔE (eV)*[d]	*λ (nm)*[e]	*ff*	R_{vel}[g]	R_{len}[h]
1	113->114	0.69184	3.1731	390.74	0.2313	-8.266	-7.3609
2	106->114	-0.39103	3.4417	360.24	0.0000	-0.0895	-0.303
	109->114	0.53422					
3	112->114	0.67157	3.7249	332.85	0.0331	14.4921	13.7247
4	106->114	0.49016	3.8123	325.22	0.0009	4.1956	4.5168
	109->114	0.37394					
	109->115	-0.25379					
5	111->114	0.63619	3.8697	320.40	0.1298	3.0605	2.6131
6	110->114	0.64805	4.4069	281.34	0.2445	-10.0501	-11.2888
7	113->115	0.65948	4.9690	249.51	0.5805	17.7697	19.4948
8	112->115	0.61192	5.3728	230.76	0.1774	5.0166	4.8278
9	111->115	0.50004	5.4348	228.13	0.0363	-7.1735	-7.9242
	113->116	-0.32057					
10	110->115	0.42073	5.6120	220.93	0.1590	-9.8616	-10.0033
	111->115	-0.35101					
	113->116	-0.27947					
11	108->114	0.61442	5.7893	214.16	0.0112	-4.4817	-4.522
12	109->115	0.56761	5.8325	212.57	0.0015	-4.506	-4.5492
13	103->114	-0.34477	5.9696	207.69	0.2225	-0.8787	0.4958
	104->114	-0.25847					
	105->114	0.43412					
14	103->114	0.35442	6.0777	204.00	0.0479	-1.2951	-2.3985
	105->114	0.35776					
	113->116	0.25251					
15	112->116	0.40539	6.1041	203.12	0.2473	35.3262	37.3501
	113->116	0.32843					
16	107->114	0.65273	6.2761	197.55	0.0120	7.4128	7.7204
17	105->114	0.23651	6.2976	196.88	0.4533	-43.5937	-42.5835
	110->115	-0.33438					
	111->116	-0.29311					
	112->116	0.35871					
18	102->114	0.28089	6.3331	195.77	0.0293	31.0085	32.4997
	106->115	0.37616					
19	106->115	0.27051	6.4756	191.46	0.0025	4.2965	3.7238
	111->116	0.28301					
20	102->114	0.23093	6.4852	191.18	0.0064	-7.6577	-8.173
	111->116	0.33561					

	113->117	-0.22707					
21	99->114	0.25049	6.7183	184.55	0.0006	-0.2912	0.0359
	109->116	0.54816					
22	110->116	0.46291	6.7366	184.05	0.0673	2.9845	1.0015
	113->117	0.36138					
23	99->114	0.41048	6.7460	183.79	0.0027	-3.8745	-4.0914
	106->115	-0.30947					
24	110->116	-0.33512	6.8385	181.30	0.2500	-16.3048	-17.7074
	112->117	0.23013					
	113->117	0.42152					
25	98->114	0.50017	6.9318	178.86	0.0007	-3.0587	-3.0549
	106->116	-0.25487					
26	103->114	-0.26703	6.9701	177.88	0.0013	-0.504	-0.6467
	104->114	0.51678					
27	110->116	0.31859	7.0369	176.19	0.0742	0.1041	0.3514
	111->117	-0.32113					
	112->117	0.46105					
28	106->116	0.31348	7.1949	172.32	0.1294	-27.2982	-24.8794
	111->117	0.39799					
	112->117	0.26691					
29	106->116	0.42899	7.2041	172.10	0.0668	21.2717	21.7415
	111->117	-0.28303					
30	94->114	-0.24955	7.2879	170.12	0.0087	18.9322	20.4321
	109->117	0.48435					
31	97->114	0.41778	7.3079	169.66	0.0265	5.224	5.6
	100->114	-0.32609					
32	94->114	-0.24838	7.3449	168.80	0.0074	-2.0272	-1.8363
	97->114	0.36023					
	108->115	-0.29311					
33	108->115	0.43142	7.3606	168.44	0.0046	12.0495	10.7576
	109->117	-0.28435					
34	105->115	-0.25151	7.4038	167.46	0.1662	-2.617	-4.4694
	110->117	0.55446					
35	97->114	0.28375	7.4493	166.44	0.0080	-3.3161	-2.7185
	100->114	0.46056					
36	92->114	0.25713	7.5591	164.02	0.0001	-0.2813	-0.1524
	101->114	0.35893					

[a]Number of the excited states; [b]Only transitions with contribution over 10.0% were listed; [c]Configuration-interaction coefficient; [d]Excitation energy; [e]Wavelength; [f]Oscillator strength; [g]Rotatory strength in velocity form (10^{-40} cgs); [h]Rotatory strength in length form (10^{-40} cgs).

Table S30. Key transitions, oscillator strengths, and rotatory strengths in the ECD spectrum of conformer cpd-**2A**-3 at the Cam-B3LYP/Def2SVP level of theory in acetonitrile with IEFPCM solvent model.

Num[a]	*Transition*[b]	*CI-coeff*[b]	*ΔE (eV)*[d]	*λ (nm)*[e]	*f*[f]	R_{vel}[g]	R_{len}[h]
1	113->114	0.68516	3.2031	387.08	0.2317	1.4278	1.355
2	106->114	-0.38031	3.4266	361.82	0.0000	-0.2134	-0.2535
	108->114	0.28704					
	109->114	0.46869					
3	112->114	0.65977	3.6588	338.87	0.0660	-1.9687	-1.9415
4	106->114	0.52566	3.7766	328.29	0.0000	-0.1598	-0.176
	109->114	0.31552					
5	111->114	0.6444	3.8443	322.52	0.1094	-0.5799	-0.3944
6	110->114	0.65056	4.3854	282.72	0.2506	1.543	1.8793
7	113->115	0.6425	5.0718	244.46	0.5719	-0.9323	-0.9093
8	112->115	0.59512	5.3661	231.05	0.1747	-1.3468	-1.3678
9	111->115	0.46803	5.4740	226.50	0.0171	2.5334	2.5865
	113->116	-0.32624					
10	107->114	0.44485	5.5545	223.22	0.0096	4.3839	4.3783
	108->114	-0.38531					
	109->114	0.24651					
11	110->115	-0.37721	5.5929	221.68	0.1393	0.0427	0.0609
	111->115	0.37952					
	113->116	0.28503					
12	108->115	0.29133	5.8276	212.76	0.0001	-1.4353	-1.4835
	109->115	0.51425					
13	107->114	0.48416	5.9047	209.98	0.0003	-0.0627	-0.0386
	108->114	0.4212					
	109->114	-0.22674					
14	104->114	0.5652	5.9401	208.73	0.2212	1.0139	0.4761
15	101->114	0.29317	6.0794	203.94	0.1395	-1.7096	-1.949
	112->116	0.47771					
16	101->114	0.37336	6.1326	202.17	0.1771	-3.3495	-3.0275
	110->115	-0.2497					
	111->116	0.24844					
	113->116	-0.30461					
17	105->114	0.56398	6.1417	201.87	0.0045	0.791	0.9251
18	104->114	-0.24366	6.2648	197.90	0.5052	1.5117	1.0526
	110->115	0.37095					
	111->116	0.31449					
	112->116	-0.25331					
	113->116	0.275					
19	105->114	0.23552	6.4133	193.32	0.0002	0.4567	0.1461
	106->115	0.47568					

20	101->114	-0.23703	6.4819	191.28	0.0317	-1.2164	-0.9494
	111->116	0.43153					
	112->116	0.30199					
21	99->114	0.24573	6.5314	189.83	0.0004	1.0266	1.1326
	102->114	0.26765					
	105->114	-0.24276					
	109->116	-0.26613					
22	99->114	0.30245	6.6697	185.89	0.0001	-0.6131	-0.5437
	108->116	0.24911					
	109->116	0.43055					
23	110->116	0.56289	6.7101	184.77	0.0158	-2.0191	-1.9824
24	99->114	-0.35549	6.7503	183.67	0.0001	0.9623	1.159
	102->114	0.23864					
	106->115	0.35679					
25	113->117	0.54664	6.8810	180.18	0.3843	-8.4138	-8.4348
26	98->114	0.54916	6.8978	179.74	0.0025	5.2995	5.4793
27	102->114	-0.32828	6.9641	178.03	0.0312	6.9914	7.5836
	103->114	0.49168					
28	110->116	0.25438	7.0114	176.83	0.0136	-5.6025	-6.8943
	111->117	-0.31866					
	112->117	0.47689					
29	106->116	0.51986	7.1411	173.62	0.0004	3.3158	3.8386
30	107->115	0.4509	7.1659	173.02	0.0023	-2.7709	-2.9217
	108->115	-0.37147					
31	111->117	0.48767	7.1995	172.21	0.1737	4.9065	5.5405
	112->117	0.3021					
32	93->114	0.33507	7.2354	171.36	0.0006	-2.6156	-2.7069
	106->116	-0.23124					
	109->117	-0.23712					
33	97->114	0.62134	7.2982	169.88	0.0383	-0.8909	-1.3305
34	106->116	-0.28469	7.3186	169.41	0.0005	0.5601	0.3412
	108->117	0.25227					
	109->117	0.41712					
35	104->115	-0.27904	7.4056	167.42	0.1707	1.6052	2.4807
	110->117	0.56123					
36	90->114	0.44666	7.5386	164.46	0.0001	-0.9286	-0.8431

[a]Number of the excited states; [b]Only transitions with contribution over 10.0% were listed; [c]Configuration-interaction coefficient; [d]Excitation energy; [e]Wavelength; [f]Oscillator strength; [g]Rotatory strength in velocity form (10^{-40} cgs); [h]Rotatory strength in length form (10^{-40} cgs).

Table S31. Key transitions, oscillator strengths, and rotatory strengths in the ECD spectrum of conformer cpd-**2A**-4 at the Cam-B3LYP/Def2SVP level of theory in acetonitrile with IEFPCM solvent model.

Num[a]	*Transition*[b]	*CI-coeff*[b]	*ΔE (eV)*[d]	*λ (nm)*[e]	*ff*	R_{vel}[g]	R_{len}[h]
1	113->114	0.68563	3.2036	387.01	0.2218	-0.253	-0.215
2	106->114	-0.38343	3.4220	362.32	0.0000	1.3941	1.4099
	109->114	0.51815					
3	112->114	0.65731	3.6654	338.26	0.0646	0.5488	0.3829
4	106->114	0.51625	3.7733	328.58	0.0000	0.0642	0.1842
	109->114	0.34221					
	109->115	-0.2375					
5	111->114	0.64525	3.8421	322.70	0.1112	-1.429	-1.4677
6	110->114	0.65089	4.3840	282.81	0.2734	-1.219	-1.4685
7	113->115	0.64225	5.0543	245.30	0.5717	1.601	1.7433
8	112->115	0.6012	5.3462	231.91	0.1537	-1.711	-1.7512
9	111->115	0.48274	5.4608	227.05	0.0230	-3.3371	-3.3592
	113->116	-0.2931					
10	107->114	-0.41588	5.5357	223.97	0.0118	2.0431	2.1003
	108->114	0.43973					
11	110->115	0.38851	5.5910	221.76	0.1287	0.2237	0.23
	111->115	-0.35942					
	113->116	-0.30787					
12	109->115	0.53808	5.7885	214.19	0.0000	0.0059	0.0993
13	107->114	0.48798	5.8643	211.42	0.0000	-0.1074	-0.0726
	108->114	0.45163					
14	104->114	0.56571	5.9404	208.71	0.2013	1.0495	1.4291
15	101->114	0.27604	6.0837	203.80	0.1043	-5.5972	-5.6963
	112->116	0.46879					
16	101->114	0.30542	6.1355	202.08	0.0479	-7.4321	-7.8976
	105->114	0.48782					
17	101->114	-0.23474	6.1414	201.88	0.1009	13.857	14.7165
	105->114	0.32408					
	113->116	0.26524					
18	104->114	-0.24064	6.2665	197.85	0.5208	-2.1693	-1.8571
	110->115	0.3628					
	111->116	0.33568					
	112->116	-0.25461					
	113->116	0.26708					
19	105->114	0.22406	6.4048	193.58	0.0002	-0.8631	-1.1497
	106->115	0.46713					
20	111->116	0.41825	6.4875	191.11	0.0475	2.2459	2.0708
	112->116	0.31428					
	113->117	-0.23242					

21	102->114	0.31077	6.5396	189.59	0.0015	-2.9654	-2.771
	109->116	0.28841					
22	99->114	0.31011	6.6624	186.10	0.0002	-1.077	-0.9539
	109->116	0.45654					
23	110->116	0.5476	6.7140	184.66	0.0216	0.9435	0.0468
	113->117	0.2326					
24	99->114	0.36081	6.7428	183.88	0.0024	5.1018	5.1754
	102->114	0.28673					
	106->115	-0.35381					
25	98->114	-0.22453	6.8776	180.27	0.3273	-23.9275	-25.3339
	113->117	0.47446					
26	98->114	0.4067	6.8840	180.11	0.0949	22.8914	24.5564
	113->117	0.26997					
27	98->114	0.29847	6.9828	177.56	0.0055	-8.7178	-7.5933
	103->114	0.48737					
28	110->116	0.2712	7.0013	177.09	0.0208	7.1104	5.4367
	111->117	-0.30564					
	112->117	0.47782					
29	107->115	0.44401	7.0928	174.80	0.0065	9.9599	10.263
	108->115	-0.40598					
30	102->114	0.23989	7.1300	173.89	0.0004	0.8777	0.885
	106->116	0.46653					
31	111->117	0.4886	7.1812	172.65	0.1743	-3.698	-2.3452
	112->117	0.30756					
32	109->117	0.43358	7.2228	171.66	0.0081	-6.9357	-8.8245
33	97->114	0.23733	7.2736	170.46	0.0104	-1.1795	0.1581
	106->116	0.37681					
	109->117	-0.26817					
34	97->114	0.5609	7.3002	169.84	0.0196	3.9448	3.98
35	104->115	-0.27596	7.3914	167.74	0.1789	-0.808	-1.3437
	110->117	0.55925					
36	93->114	0.26482	7.5068	165.16	0.0003	1.4738	1.5009
	107->115	0.24255					
	108->115	0.23525					

[a]Number of the excited states; [b]Only transitions with contribution over 10.0% were listed; [c]Configuration-interaction coefficient; [d]Excitation energy; [e]Wavelength; [f]Oscillator strength; [g]Rotatory strength in velocity form (10^{-40} cgs); [h]Rotatory strength in length form (10^{-40} cgs).

Table S32. Key transitions, oscillator strengths, and rotatory strengths in the ECD spectrum of conformer cpd-**2A**-5 at the Cam-B3LYP/Def2SVP level of theory in acetonitrile with IEFPCM solvent model.

Num[a]	*Transition*[b]	*CI-coeff*[b]	*ΔE (eV)*[d]	*λ (nm)*[e]	*ff*[f]	R_{vel}[g]	R_{len}[h]
1	113->114	0.69192	3.2216	384.85	0.2961	0.4057	0.4132
2	107->114	-0.40325	3.4545	358.91	0.0000	-0.0884	-0.1652
	109->114	0.52797					
3	112->114	0.68462	3.7379	331.70	0.0184	-0.1086	-0.0795
4	107->114	0.5006	3.8142	325.06	0.0000	0.5266	0.4384
	109->114	0.38449					
	109->115	-0.26566					
5	111->114	0.63561	3.9282	315.63	0.1292	-1.9239	-1.5545
6	110->114	0.6268	4.5527	272.33	0.2033	-0.207	-0.3565
	111->114	0.24672					
7	113->115	0.65342	4.9682	249.56	0.6004	-2.2382	-2.2415
8	112->115	0.63333	5.3263	232.78	0.1280	1.3891	1.4442
9	111->115	0.47863	5.4328	228.22	0.1081	1.792	1.4015
	113->116	-0.34731					
10	110->115	0.43265	5.5970	221.52	0.1580	0.7241	0.7123
	111->115	-0.27776					
	113->116	-0.34416					
11	108->114	0.65981	5.7571	215.36	0.0140	3.303	2.8776
12	109->115	0.59579	5.7942	213.98	0.0004	-2.3849	-2.3799
13	103->114	-0.23899	6.0160	206.09	0.2523	1.1179	1.3572
	104->114	0.56084					
14	111->115	0.28749	6.1128	202.83	0.2954	-2.3248	-2.3715
	112->116	0.43019					
	113->116	0.32852					
15	102->114	0.30312	6.1460	201.73	0.0005	-2.1137	-1.9649
	103->114	0.38245					
	104->114	0.23375					
	112->116	-0.26652					
16	105->114	-0.258	6.2723	197.67	0.0114	22.1896	22.9535
	106->114	0.25515					
	107->115	0.34578					
17	104->114	-0.24655	6.2862	197.23	0.4750	-22.2107	-23.2081
	110->115	0.37774					
	112->116	-0.31873					
	113->116	0.27685					
18	106->114	0.46216	6.4361	192.64	0.0013	0.6448	0.3356
	107->115	-0.42989					
19	105->114	0.23229	6.4943	190.91	0.0015	0.8193	1.0938
	106->114	0.37487					

	111->116	-0.26309					
20	111->116	0.36104	6.5052	190.59	0.0008	-1.2037	-1.1518
	113->117	0.29587					
21	100->114	-0.24989	6.6986	185.09	0.0005	-1.4313	-1.2785
	109->116	0.57245					
22	110->116	-0.24351	6.7355	184.08	0.2035	-0.6462	-0.8783
	111->116	-0.32072					
	113->117	0.46954					
23	91->114	-0.27261	6.8230	181.71	0.0007	0.7336	0.8261
	98->114	0.39191					
	105->114	-0.32609					
24	112->117	0.50479	6.8621	180.68	0.1280	2.7457	3.1874
25	100->114	0.44583	6.8757	180.32	0.0007	-2.5552	-2.5706
	101->114	0.2573					
	109->116	0.25661					
26	98->114	0.29831	6.9211	179.14	0.0009	0.3787	0.2176
	105->114	0.3743					
27	110->116	0.58511	7.0577	175.67	0.1303	-0.1008	-0.3481
	112->117	-0.2713					
28	101->114	0.23491	7.1451	173.52	0.0630	9.4002	10.5845
	102->114	-0.25407					
	103->114	0.23874					
	111->117	0.39855					
29	100->114	0.2606	7.1672	172.99	0.0293	18.0968	15.6662
	107->116	0.45121					
	109->117	-0.30486					
30	102->114	0.27941	7.1716	172.88	0.1065	-43.9384	-43.786
	111->117	0.35766					
31	107->116	0.34555	7.2879	170.12	0.0010	2.0244	2.5952
	109->117	0.50044					
32	108->115	0.62764	7.2991	169.86	0.0100	2.1882	1.7238
33	97->114	-0.35874	7.3741	168.14	0.0757	7.3566	8.3771
	104->115	0.51397					
34	94->114	0.34677	7.4128	167.26	0.0020	7.1443	6.5344
	101->114	-0.25984					
35	97->114	0.49636	7.4897	165.54	0.0136	-0.7448	-0.2752
	110->117	0.3798					
36	91->114	0.2569	7.6379	162.33	0.0009	0.7794	0.7461
	94->114	0.2474					

[a]Number of the excited states; [b]Only transitions with contribution over 10.0% were listed; [c]Configuration-interaction coefficient; [d]Excitation energy; [e]Wavelength; [f]Oscillator strength; [g]Rotatory strength in velocity form (10^{-40} cgs); [h]Rotatory strength in length form (10^{-40} cgs).

Table S33. Key transitions, oscillator strengths, and rotatory strengths in the ECD spectrum of conformer cpd-**2A**-6 at the Cam-B3LYP/Def2SVP level of theory in acetonitrile with IEFPCM solvent model.

Num[a]	*Transition*[b]	*CI-coeff*[b]	*ΔE (eV)*[d]	*λ (nm)*[e]	*ff*	R_{vel}[g]	R_{len}[h]
1	113->114	0.69182	3.1824	389.59	0.2355	-9.9098	-9.0812
2	107->114	-0.39499	3.4402	360.40	0.0000	-0.261	-0.4439
	109->114	0.50401					
3	112->114	0.67554	3.7290	332.48	0.0293	14.7091	14.1185
4	107->114	0.50042	3.8090	325.50	0.0007	3.6101	3.8638
	109->114	0.36268					
	109->115	-0.24283					
5	111->114	0.63971	3.8737	320.07	0.1270	6.2448	5.7699
6	110->114	0.64996	4.4109	281.09	0.2470	-11.4374	-12.6787
	111->114	0.22478					
7	113->115	0.65893	4.9802	248.96	0.5767	17.1617	19.0148
8	112->115	0.62245	5.3759	230.63	0.1803	4.8207	4.3462
9	111->115	0.4863	5.4375	228.02	0.0266	-9.7232	-10.3108
	113->116	-0.33697					
10	110->115	0.40972	5.6072	221.12	0.1477	-9.4614	-9.5414
	111->115	-0.35092					
	113->116	-0.28116					
11	108->114	0.62261	5.6386	219.88	0.0197	-6.4105	-6.6308
12	109->115	0.57446	5.8259	212.81	0.0001	-0.7791	-0.5036
13	103->114	0.29756	5.9657	207.83	0.2201	-7.3826	-6.1186
	104->114	-0.23837					
	105->114	0.46356					
14	102->114	-0.244	6.0870	203.69	0.0318	-5.5878	-7.0996
	103->114	0.34948					
	105->114	-0.34724					
15	110->115	0.24505	6.1112	202.88	0.2755	43.1595	45.7222
	112->116	0.40007					
	113->116	0.35528					
16	106->114	-0.25644	6.2895	197.13	0.3278	-65.9307	-65.4779
	110->115	-0.29464					
	111->116	-0.22806					
	112->116	0.33844					
17	106->114	0.44714	6.2994	196.82	0.1586	54.0403	56.0833
18	106->114	0.40721	6.3524	195.18	0.0033	5.8025	6.5181
	107->115	-0.36721					
19	101->114	-0.22532	6.4799	191.34	0.0009	1.3565	1.0488
	104->114	0.22416					
	107->115	0.29564					
20	111->116	0.42029	6.4960	190.86	0.0092	-5.0887	-5.9136

	113->117	-0.28851					
21	100->114	0.2643	6.7134	184.68	0.0003	-0.3493	-0.1105
	109->116	0.52241					
22	110->116	0.49292	6.7387	183.99	0.0474	6.112	4.3466
	113->117	0.31041					
23	100->114	0.43431	6.7491	183.70	0.0044	-5.5909	-5.833
	107->115	-0.31286					
24	110->116	-0.28846	6.8454	181.12	0.2805	-25.5499	-27.6201
	112->117	0.23176					
	113->117	0.45495					
25	98->114	-0.24728	6.9284	178.95	0.0012	-3.4135	-3.4913
	99->114	0.47948					
	107->116	-0.23418					
26	110->116	0.31642	7.0292	176.38	0.0760	4.2269	4.7013
	111->117	-0.2916					
	112->117	0.48147					
27	101->114	0.26657	7.0765	175.21	0.0011	-1.33	-1.0774
	104->114	0.4939					
28	107->116	-0.26716	7.2030	172.13	0.0548	-12.0682	-12.8244
	108->115	0.33286					
	111->117	0.30901					
29	107->116	0.43929	7.2111	171.94	0.0625	-11.63	-9.6221
	111->117	0.27139					
30	108->115	0.4398	7.2201	171.72	0.0635	27.2538	29.5662
	111->117	-0.28605					
31	95->114	-0.25977	7.2841	170.21	0.0223	23.7035	26.2083
	109->117	0.31349					
32	97->114	0.38187	7.3129	169.54	0.0295	4.8423	2.9569
	98->114	-0.27266					
	109->117	0.28287					
33	97->114	-0.28618	7.3481	168.73	0.0011	-4.9786	-4.0193
	109->117	0.2913					
34	102->114	-0.28157	7.3880	167.82	0.0439	-5.7402	-7.2216
	110->117	0.35107					
35	97->114	0.26009	7.4005	167.53	0.1265	-3.6951	-4.133
	105->115	-0.26363					
	110->117	0.42932					
36	91->114	0.28005	7.5853	163.45	0.0008	-2.1679	-2.3107
	95->114	0.29139					
	98->114	0.2662					
	99->114	0.24162					

[a]Number of the excited states; [b]Only transitions with contribution over 10.0% were listed; [c]Configuration-interaction coefficient; [d]Excitation energy; [e]Wavelength; [f]Oscillator strength;

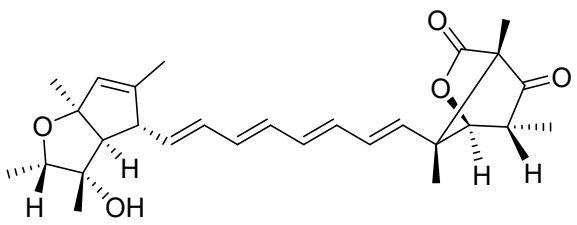
[g]Rotatory strength in velocity form (10^{-40} cgs); [h]Rotatory strength in length form (10^{-40} cgs).

Table S34. Key transitions, oscillator strengths, and rotatory strengths in the ECD spectrum of conformer cpd-**2A**-7 at the Cam-B3LYP/Def2SVP level of theory in acetonitrile with IEFPCM solvent model.

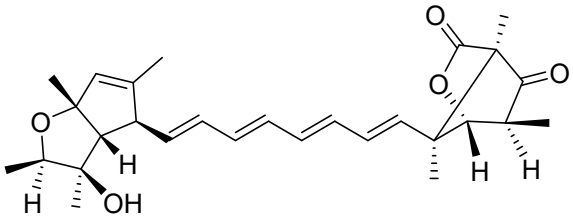
Num[a]	*Transition*[b]	*CI-coeff*[b]	*ΔE (eV)*[d]	*λ (nm)*[e]	*ff*	R_{vel}[g]	R_{len}[h]
1	113->114	0.69132	3.1789	390.03	0.2337	-0.0188	-0.0345
2	106->114	-0.38914	3.4363	360.81	0.0000	1.5446	1.5377
	109->114	0.5384					
3	112->114	0.673	3.6984	335.23	0.0463	5.9038	5.0939
4	106->114	0.50514	3.7992	326.34	0.0001	0.083	0.3215
	109->114	0.3753					
	109->115	-0.2534					
5	111->114	0.64619	3.8599	321.21	0.1205	-0.357	-1.0087
6	110->114	0.64969	4.4002	281.77	0.2409	-7.9834	-7.6262
7	113->115	0.65808	5.0169	247.13	0.5854	4.0853	3.9655
8	112->115	0.60299	5.3844	230.27	0.1810	-1.947	-2.0101
	113->116	-0.22437					
9	111->115	0.49163	5.4564	227.23	0.0312	-2.5151	-2.1639
	113->116	-0.3316					
10	110->115	0.41001	5.6145	220.83	0.1528	-2.5765	-2.5282
	111->115	-0.36359					
	113->116	-0.2725					
11	108->114	0.59406	5.8249	212.85	0.0088	2.9402	2.7989
12	109->115	0.56161	5.8503	211.93	0.0004	-2.6912	-2.6135
13	103->114	0.37345	5.9637	207.90	0.2397	6.5866	7.3612
	104->114	0.49895					
14	103->114	0.42251	6.0689	204.29	0.0069	-0.9745	0.248
	104->114	-0.31318					
	112->116	0.26243					
15	110->115	0.25082	6.0963	203.38	0.3079	12.8315	12.7954
	112->116	0.36222					
	113->116	0.36147					
16	107->114	0.60973	6.1623	201.20	0.0007	-0.0127	-0.0869
17	110->115	0.3454	6.2864	197.22	0.4683	29.5039	31.1921
	111->116	0.27655					
	112->116	-0.33828					
	113->116	0.24467					
18	100->114	-0.24779	6.3243	196.04	0.0346	-34.2501	-35.7062
	105->114	-0.2475					
	106->115	0.32547					
	107->114	0.22931					
19	106->115	-0.26565	6.4630	191.84	0.0068	-10.6663	-10.8209

	111->116	0.36336					
20	106->115	0.28147	6.4709	191.60	0.0046	10.1509	10.0541
	111->116	0.27042					
21	109->116	0.59086	6.6982	185.10	0.0001	-0.9139	-0.3608
22	110->116	0.50953	6.7295	184.24	0.0363	-0.1941	-1.7899
	113->117	0.32416					
23	99->114	0.46096	6.7387	183.99	0.0016	3.7862	3.9429
	106->115	-0.30017					
24	110->116	-0.28858	6.8477	181.06	0.3066	-17.4794	-17.0995
	113->117	0.48213					
25	98->114	0.54203	6.9262	179.01	0.0006	2.1057	2.1489
	106->116	-0.23373					
26	100->114	-0.225	6.9520	178.34	0.0004	0.3749	0.3447
	102->114	0.25772					
	105->114	0.45088					
27	110->116	0.28777	7.0388	176.14	0.0490	3.3752	2.0991
	111->117	-0.32502					
	112->117	0.47096					
28	111->117	0.45693	7.1891	172.46	0.1719	20.1855	21.0438
	112->117	0.30528					
29	106->116	0.49602	7.2007	172.18	0.0358	-17.0014	-16.4189
30	94->114	-0.27495	7.2666	170.62	0.0110	-14.5442	-15.6538
	102->114	-0.24974					
	109->117	0.30859					
31	97->114	0.48586	7.3196	169.39	0.0339	9.59	11.8741
	109->117	-0.23859					
32	97->114	0.3231	7.3389	168.94	0.0010	-0.6182	-1.779
	109->117	0.4084					
33	99->114	0.22872	7.3768	168.07	0.0008	1.4388	1.8014
	101->114	0.29137					
34	104->115	-0.29439	7.4253	166.98	0.1661	-3.4149	-3.996
	110->117	0.55182					
35	108->115	0.56547	7.4475	166.48	0.0090	14.3825	14.4971
36	92->114	0.35382	7.6135	162.85	0.0005	1.4631	1.3741
	94->114	0.26551					

[a]Number of the excited states; [b]Only transitions with contribution over 10.0% were listed; [c]Configuration-interaction coefficient; [d]Excitation energy; [e]Wavelength; [f]Oscillator strength; [g]Rotatory strength in velocity form (10^{-40} cgs); [h]Rotatory strength in length form (10^{-40} cgs).



6A



6B

Table S35. Experimental and calculated ^{13}C-NMR chemical shifts of cpd-**6A**

No.	*δ*exptl.	cpd-6A-*δ*calcd.
1	171.8	168.1
2	69.7	73.9
3	207.8	207.5
4	44.1	47.5
5	85.4	84.3
6	58.7	62.8
7	131.2	129.2
8	134.3	132.0
9	131.1	129.6
10	134.4	133.0
11	130.9	129.4
12	135.0	132.4
13	129.5	128.1
14	138.4	139.0
15	55.9	58.2
16	144.5	144.4
17	129.4	126.5
18	92.2	92.2
19	66.2	68.8
20	80.8	80.0
21	78.2	75.8
22	5.4	7.1
23	11.7	14.6
24	17.6	17.8
25	15.1	16.5
26	27.5	29.2
27	19.3	18.8
28	11.9	13.4

Table 36. Experimental and calculated ^{1}H-NMR chemical shifts of cpd-**6A**

No.	*δ*exptl.	cpd-6A-*δ*calcd.
4	2.79	2.35

5	4.73	4.65
7	5.46	5.93
8	6.2	6.56
9	6.16	6.43
10	6.07	6.63
11	6.28	6.49
12	6.24	6.53
13	6.1	6.3
14	5.53	5.8
15	2.96	2.91
17	5.23	5.38
19	2.16	1.98
21	3.45	3.44
22	1.2	0.85
23	1.22	1.08
24	1.38	0.92
25	1.63	1.4
26	1.49	1.39
27	1.21	0.95
28	1.16	1.0

Table S37. Conformational analysis of the B3LYP/6-31G(d) optimized conformers of cpd-**6A** in the gas phase (T=298.15 K)

Conformer	**E[a] (Hartree)**	**C[b] (Hartree)**	**G[c] (kcal/mol)**	**ΔG[d] (kcal/mol)**	**Population[e]**
cpd-**6A**-1	-1464.554406	0.509547	-918688.149248	0.0	49.83%
cpd-**6A**-2	-1464.552302	0.50833	-918687.592286	0.556963	19.45%
cpd-**6A**-3	-1464.553824	0.510036	-918687.476744	0.672504	16.00%
cpd-**6A**-4	-1464.552767	0.509523	-918687.135472	1.013776	8.99%
cpd-**6A**-5	-1464.553284	0.510468	-918686.86731	1.281939	5.72%

[a]Electronic energy obtained at M062X/6-311+G(2d,p) level of theory; [b]Thermal correction to Gibbs free energy obtained at B3LYP/6-31G(d) level of theory; [c]Gibbs free energy (E + C); [d]The relative Gibbs free energy; [e]The Boltzmann distribution of each conformer.

Table S38. Atomic coordinates (Å) of cpd-**6A**-1 obtained at the B3LYP/6-31G(d) level of theory in the gas phase.

C	7.064932	1.239154	-1.005685	H	-5.027079	0.081934	-1.327848
C	6.960141	0.874080	0.483207	H	-1.361271	-1.074742	1.251326
C	8.360370	0.292466	0.787332	H	-0.175705	0.176668	-1.293457
C	8.491433	-1.006131	-0.032405	H	1.098680	-0.997028	1.287557
C	7.117963	-1.014175	-0.722662	H	2.310511	0.213872	-1.265135
C	6.124025	-0.464479	0.349974	H	3.537751	-0.956182	1.335379
C	4.757664	-0.223837	-0.233238	H	4.739609	0.223922	-1.224775

C	3.574028	-0.504110	0.346207	H	6.832106	-1.929243	-1.239477
C	2.296852	-0.244122	-0.275951	H	5.627948	-2.254051	1.479727
C	1.104215	-0.537887	0.297958	H	7.043063	-1.398057	2.116814
C	-0.176232	-0.290230	-0.307970	H	5.437169	-0.743184	2.381965
C	-1.362930	-0.605263	0.266906	H	8.563475	-1.846791	0.666932
C	-2.651826	-0.368522	-0.339021	H	7.129516	2.868171	1.248246
C	-3.828188	-0.703254	0.223184	H	5.462584	2.265530	1.154200
C	-5.176675	-0.489620	-0.402779	H	6.556248	1.685886	2.435065
C	-5.859927	-1.810859	-0.741181	H	9.801515	-1.981050	-1.466296
C	-7.016459	-1.951461	-0.088803	H	9.653898	-0.230864	-1.703774
C	-7.365639	-0.772869	0.780095	H	10.619827	-0.861934	-0.354576
C	-6.173534	0.221376	0.560202	H	-7.684373	-2.804436	-0.176028
C	-6.884813	1.493651	0.030474	H	-5.679073	0.480811	1.499315
C	-8.088978	0.862731	-0.699892	H	-7.726678	0.336021	-1.597676
C	6.494937	1.989087	1.385870	H	-5.828721	-3.673416	-1.825931
C	9.715731	-1.019363	-0.949764	H	-5.097514	-2.302616	-2.687052
C	6.063901	-1.264634	1.653012	H	-4.224938	-3.057804	-1.360565
C	-5.226936	-2.768602	-1.700520	H	-10.084338	1.213069	-1.428827
C	-7.662011	-1.141205	2.227175	H	-9.540413	2.385250	-0.205719
C	-6.047475	2.455327	-0.794148	H	-8.915545	2.476713	-1.863226
C	-9.228330	1.791221	-1.068538	H	-8.558321	-1.767671	2.285983
O	7.087247	2.322474	-1.521455	H	-6.822226	-1.695437	2.658630
O	7.138617	0.063321	-1.709012	H	-7.828860	-0.242211	2.830469
O	-8.546591	-0.093054	0.266254	H	-5.141000	2.740086	-0.250757
O	9.182243	0.771279	1.531715	H	-5.755846	2.020968	-1.754623
O	-7.364776	2.239657	1.156252	H	-6.626352	3.363127	-0.987739
H	-3.831840	-1.190729	1.199740	H	-8.081616	1.701559	1.535552
H	-2.653549	0.113634	-1.317685	-	-	-	-

Table S39. Atomic coordinates (Å) of cpd-**6A**-2 obtained at the B3LYP/6-31G(d) level of theory in the gas phase.

C	-5.998013	-1.479423	0.344298	H	5.729592	0.853223	-1.872357
C	-6.773665	-0.321849	0.993699	H	1.116433	0.044399	-1.914182
C	-8.152594	-0.394033	0.297422	H	0.380150	1.435605	0.725543
C	-7.920690	-0.044749	-1.186527	H	-1.318417	0.141986	-1.534766
C	-6.398361	0.171671	-1.162917	H	-2.072185	1.512469	1.111217
C	-6.119255	0.872613	0.190001	H	-3.735510	0.221490	-1.174228
C	-4.663175	1.070605	0.522237	H	-4.488019	1.564477	1.478199
C	-3.594870	0.735029	-0.225725	H	-5.955280	0.613596	-2.054921
C	-2.229637	1.002555	0.160383	H	-6.600656	2.617835	1.379603
C	-1.153170	0.656774	-0.587556	H	-6.507262	2.941723	-0.354119
C	0.212136	0.919024	-0.220150	H	-7.932462	2.134745	0.334343

C	1.284362	0.563982	-0.970084	H	-8.430129	0.902589	-1.397661
C	2.655473	0.824666	-0.601514	H	-7.278416	-1.250963	2.855553
C	3.720102	0.462517	-1.342027	H	-5.778970	-0.308486	2.905506
C	5.164401	0.666145	-0.949964	H	-7.359767	0.516542	2.889902
C	5.376954	1.814376	0.021792	H	-7.906699	-2.057373	-2.014801
C	5.802216	1.379804	1.210787	H	-9.505355	-1.287277	-1.960196
C	6.025657	-0.108895	1.264413	H	-8.319104	-0.793248	-3.187514
C	5.724044	-0.586736	-0.199188	H	6.022856	2.010793	2.067778
C	7.088695	-1.169361	-0.658902	H	4.995213	-1.398914	-0.221949
C	8.070687	-0.351668	0.205260	H	8.090906	0.686528	-0.163160
C	-6.794965	-0.336625	2.502274	H	4.079069	3.355123	-0.732340
C	-8.441802	-1.113925	-2.147690	H	5.291243	3.928187	0.436055
C	-6.843625	2.213686	0.391995	H	5.759837	3.517830	-1.226704
C	5.112212	3.230262	-0.387291	H	10.038867	-0.319660	1.077622
C	5.244264	-0.813717	2.363351	H	9.475896	-1.942013	0.610680
C	7.373805	-1.156822	-2.150178	H	10.005239	-0.793837	-0.632924
C	9.483157	-0.887111	0.325276	H	5.558878	-0.454875	3.349081
O	-5.624691	-2.509152	0.832984	H	4.172778	-0.623189	2.246655
O	-5.794145	-1.144957	-0.969996	H	5.409790	-1.895788	2.321625
O	7.433899	-0.392791	1.489414	H	6.565509	-1.647156	-2.702498
O	-9.203996	-0.666993	0.825690	H	7.491353	-0.138448	-2.532207
O	7.143173	-2.541925	-0.249744	H	8.298209	-1.707665	-2.347245
H	3.551167	-0.070822	-2.278061	H	7.174352	-2.520521	0.722798
H	2.820917	1.344877	0.342016	-	-	-	-

Table S40. Atomic coordinates (Å) of cpd-**6A**-3 obtained at the B3LYP/6-31G(d) level of theory in the gas phase.

C	6.400914	-1.285359	-0.358491	H	-4.959315	0.154258	-1.333635
C	7.098417	-0.002217	-0.838136	H	-1.079881	-0.762325	1.016093
C	8.382881	0.037229	0.022170	H	-0.184230	0.881076	-1.421906
C	7.933791	0.249808	1.481897	H	1.355995	-0.356542	0.978638
C	6.410038	0.289347	1.277616	H	2.262529	1.273347	-1.464721
C	6.210398	1.048191	-0.058125	H	3.775134	0.032525	0.949618
C	4.791916	1.098856	-0.563383	H	4.674708	1.633664	-1.506191
C	3.689941	0.590112	0.019629	H	5.812882	0.612036	2.129981
C	2.361256	0.720856	-0.529875	H	7.856958	2.520021	0.101888
C	1.250580	0.199152	0.046155	H	6.609235	2.919911	-1.074125
C	-0.077728	0.323711	-0.490535	H	6.270497	3.102840	0.649470
C	-1.185841	-0.203332	0.085768	H	8.292166	1.232797	1.808723
C	-2.519876	-0.076123	-0.451415	H	7.939996	-0.727382	-2.668376
C	-3.623707	-0.594617	0.118196	H	6.346563	0.023202	-2.857809
C	-5.015228	-0.469602	-0.431958	H	7.791464	1.034546	-2.594964
C	-5.614672	-1.820904	-0.805921	H	8.074764	-1.804960	2.187193

C	-6.735309	-2.071471	-0.124459	H	9.557674	-0.848739	2.381601
C	-7.130610	-0.963601	0.814535	H	8.179058	-0.587917	3.471966
C	-6.014326	0.117125	0.610800	H	-7.345891	-2.964268	-0.230983
C	-6.823515	1.367461	0.182807	H	-5.498094	0.353415	1.544302
C	-8.008566	0.700363	-0.547007	H	-7.644224	0.250074	-1.484645
C	7.301641	0.092718	-2.330066	H	-3.922280	-2.924377	-1.534292
C	8.465943	-0.816489	2.440204	H	-5.496094	-3.623525	-1.982520
C	6.781310	2.475418	-0.088943	H	-4.884916	-2.166912	-2.795318
C	-4.951684	-2.687079	-1.829891	H	-8.974124	2.321325	-1.585960
C	-7.351719	-1.423397	2.249001	H	-10.045179	0.959963	-1.196322
C	-6.077774	2.431337	-0.603679	H	-9.538368	2.091542	0.079775
C	-9.216807	1.571090	-0.826025	H	-7.546461	-0.568317	2.905333
O	6.219964	-2.314205	-0.947867	H	-8.207834	-2.103999	2.304363
O	6.000424	-1.071102	0.935565	H	-6.466004	-1.948763	2.620610
O	-8.370432	-0.336785	0.375022	H	-6.717927	3.310872	-0.718824
O	9.515400	-0.072593	-0.383147	H	-5.172119	2.737734	-0.070704
O	-7.312579	2.011954	1.366438	H	-5.793196	2.078777	-1.599103
H	-3.529809	-1.160479	1.046772	H	-7.983081	1.407985	1.731076
H	-2.622785	0.486923	-1.380306	-	-	-	-

Table S41. Atomic coordinates (Å) of cpd-**6A**-4 obtained at the B3LYP/6-31G(d) level of theory in the gas phase.

C	-5.967324	-0.313759	1.299225	H	4.976371	0.295698	-1.355506
C	-6.631482	0.695206	0.345183	H	1.004700	0.970618	0.920542
C	-8.130218	0.310758	0.471618	H	0.197436	-0.009789	-1.878213
C	-8.286689	-1.097699	-0.131974	H	-1.447662	0.808257	0.630586
C	-6.824326	-1.367593	-0.518840	H	-2.254217	-0.209250	-2.155674
C	-6.287582	0.011380	-1.023353	H	-3.866052	0.635604	0.358465
C	-4.829351	-0.056287	-1.397032	H	-4.657815	-0.424122	-2.410225
C	-3.751430	0.269079	-0.658604	H	-6.632408	-2.235316	-1.148594
C	-2.393350	0.150822	-1.135835	H	-6.974621	-0.049174	-3.090684
C	-1.302524	0.455010	-0.390818	H	-8.113599	0.779160	-2.013825
C	0.053741	0.337983	-0.854501	H	-6.610424	1.571230	-2.485589
C	1.145547	0.627023	-0.104670	H	-8.902229	-1.013880	-1.035227
C	2.505518	0.506135	-0.574118	H	-6.496134	2.376133	1.666364
C	3.596967	0.772275	0.167270	H	-5.300343	2.399609	0.355869
C	5.012926	0.644921	-0.315166	H	-7.001273	2.788103	0.020832
C	5.769564	1.967670	-0.273899	H	-9.087259	-3.063886	0.331385
C	6.867716	1.887906	0.481621	H	-8.318511	-2.257006	1.709923
C	7.084263	0.527262	1.087684	H	-9.912378	-1.716167	1.144906
C	5.863857	-0.310595	0.575401	H	7.575010	2.696841	0.644772
C	6.545640	-1.504546	-0.138207	H	5.262865	-0.703420	1.398953
C	7.834071	-0.825282	-0.648035	H	7.571303	-0.111272	-1.445562

C	-6.333602	2.152146	0.608951	H	5.918314	4.022506	-0.909320
C	-8.938567	-2.097538	0.824368	H	5.194859	2.927284	-2.106966
C	-7.053512	0.607702	-2.216713	H	4.253949	3.426109	-0.708721
C	5.265555	3.153639	-1.034249	H	8.658288	-2.237377	-2.049993
C	7.281484	0.552819	2.597347	H	9.857249	-1.159526	-1.305804
C	5.725390	-2.236288	-1.186507	H	9.164605	-2.505791	-0.371423
C	8.947992	-1.738502	-1.119132	H	6.445761	1.068092	3.081805
O	-5.447520	-0.118504	2.364770	H	7.338822	-0.464222	2.999996
O	-6.088056	-1.550518	0.726881	H	8.208008	1.078072	2.852283
O	8.265521	-0.107800	0.516696	H	6.267575	-3.129289	-1.510841
O	-8.997520	0.997956	0.954524	H	4.765202	-2.554460	-0.768471
O	6.896691	-2.480696	0.850906	H	5.532646	-1.611762	-2.063459
H	3.473671	1.107655	1.198550	H	7.614198	-2.076256	1.369222
H	2.639504	0.167599	-1.602668	-	-	-	-

Table S42. Atomic coordinates (Å) of cpd-**6A**-5 obtained at the B3LYP/6-31G(d) level of theory in the gas phase.

C	6.887832	0.806275	-1.284888	H	-5.897866	1.265823	1.592059
C	6.924172	0.704355	0.247598	H	-1.424971	-0.009317	2.145469
C	8.277801	0.002442	0.506876	H	-0.398004	0.670232	-0.670757
C	8.163039	-1.418209	-0.080063	H	1.018167	-0.269102	1.932334
C	6.723844	-1.358961	-0.617003	H	2.059442	0.389945	-0.884229
C	5.934744	-0.518030	0.436971	H	3.439619	-0.535400	1.737875
C	4.543423	-0.198222	-0.038724	H	4.457893	0.098476	-1.082057
C	3.411384	-0.240766	0.690767	H	6.277175	-2.300411	-0.933708
C	2.107915	0.086045	0.161590	H	5.465047	-0.376645	2.543199
C	0.963242	0.036357	0.886474	H	5.392246	-2.025979	1.905391
C	-0.340396	0.360456	0.373249	H	6.952940	-1.255901	2.241355
C	-1.482491	0.301514	1.101553	H	8.225676	-2.135937	0.745635
C	-2.792177	0.621916	0.586032	H	5.684015	2.372311	0.802370
C	-3.926872	0.553366	1.307789	H	6.840448	1.864793	2.058192
C	-5.315302	0.818851	0.776048	H	7.409486	2.755224	0.637337
C	-5.339409	1.737183	-0.433877	H	10.239288	-1.599186	-0.638267
C	-5.749269	1.094422	-1.530463	H	9.177169	-2.778262	-1.438205
C	-6.142271	-0.337931	-1.278859	H	9.186615	-1.088900	-1.974016
C	-5.982492	-0.503764	0.273175	H	-5.847317	1.536966	-2.518238
C	-7.430419	-0.820534	0.736680	H	-5.360519	-1.362988	0.530713
C	-8.257855	-0.124348	-0.363504	H	-8.175049	0.966786	-0.235039
C	6.697000	2.001744	0.982440	H	-4.985230	3.686083	-1.284769
C	9.257503	-1.740117	-1.099424	H	-5.577167	3.704960	0.389175
C	5.945272	-1.082023	1.859242	H	-3.905794	3.261432	0.063061
C	-4.929156	3.172649	-0.320301	H	-10.155763	-0.086086	-1.379184
C	-5.386249	-1.345914	-2.131684	H	-9.818784	-1.610606	-0.525799

C	-7.797527	-0.440934	2.159951	H	-10.275507	-0.162482	0.390317
C	-9.715145	-0.523659	-0.478492	H	-5.680115	-2.368775	-1.871807
O	6.966996	1.779433	-1.982744	H	-5.598144	-1.185908	-3.194166
O	6.745685	-0.467479	-1.774292	H	-4.308481	-1.243448	-1.970140
O	-7.558668	-0.521870	-1.550516	H	-8.788538	-0.839855	2.395590
O	9.232348	0.484682	1.068271	H	-7.084197	-0.869530	2.871522
O	-7.624677	-2.237593	0.635981	H	-7.820995	0.643986	2.297666
H	-3.868821	0.228481	2.347155	H	-7.600466	-2.434774	-0.316890
H	-2.847829	0.931630	-0.457652	-	-	-	-