Supporting Information

An indole diketopiperazine alkaloid and a bisabolane sesquiterpenoid with unprecedented skeletons from *Aspergillus fumigatus*

Yaqin Jiang,‡[a] Chunmei Chen,‡[a] Hucheng Zhu,‡[a] Qin Li,[a] Lina Mao,[a] Hong Liao,[a] Yiyang Nan,[a] Zhiping Wang,[b] Hongjian Zhou,[a] Qun Zhou,*[a] Yonghui Zhang*[a]

[a]Hubei Key Laboratory of Natural Medicinal Chemistry and Resource Evaluation, School of Pharmacy, Tongji Medical College, Huazhong University of Science and Technology, Wuhan 430030, People's Republic of China.

[b]Guangdong Provincial Key Laboratory of Advanced Drug Delivery Systems and Guangdong Provincial Engineering Center of Topical Precise Drug Delivery System, School of Pharmacy, Guangdong Pharmaceutical University, Guangzhou, 510006, People's Republic of China.

*Corresponding authors E-mail:

zhangyh@mails.tjmu.edu.cn (Y.Z.), zqtcm@hust.edu.cn(Q. Zhou)

List of Supporting Information

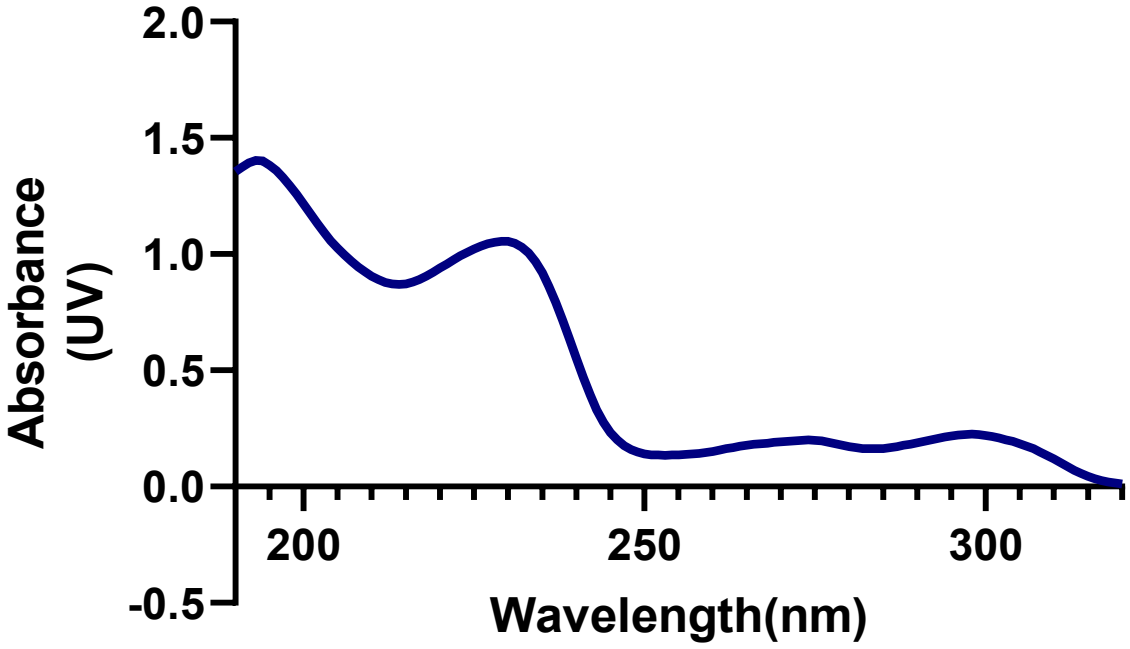


Figure S1. UV spectrum of compound **1** in MeCN.

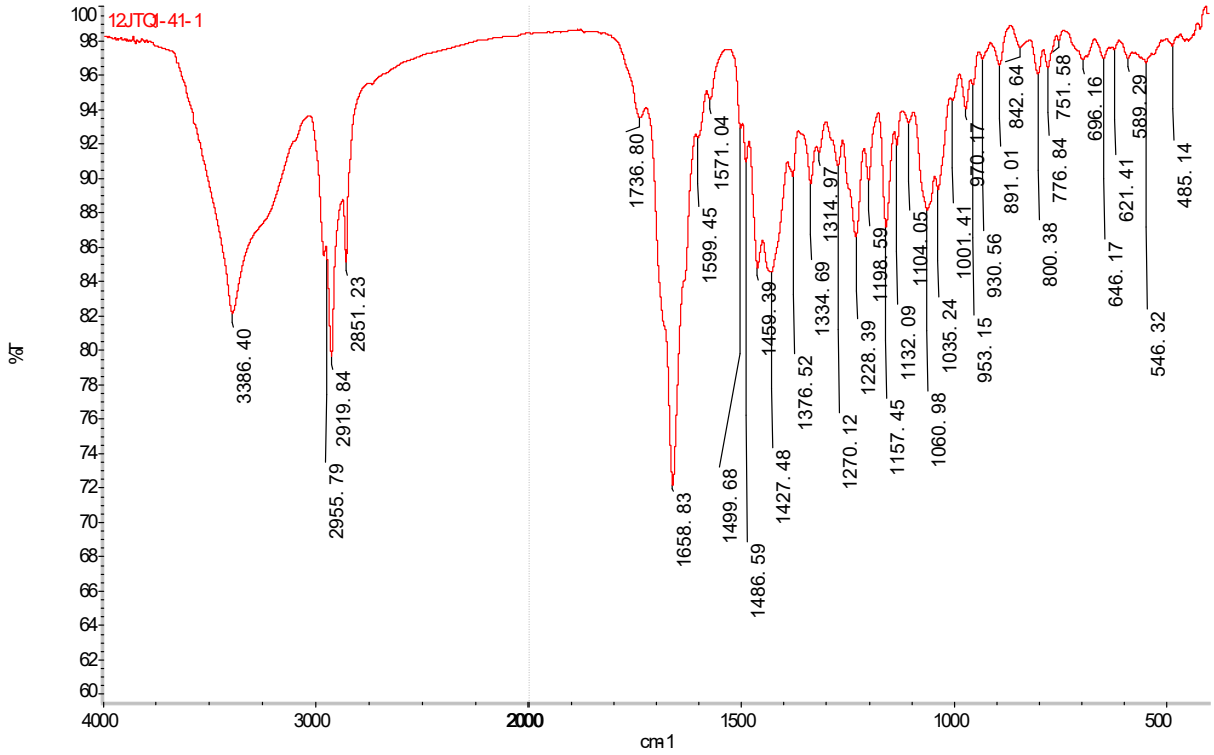


Figure S2. IR spectrum of compound **1**.

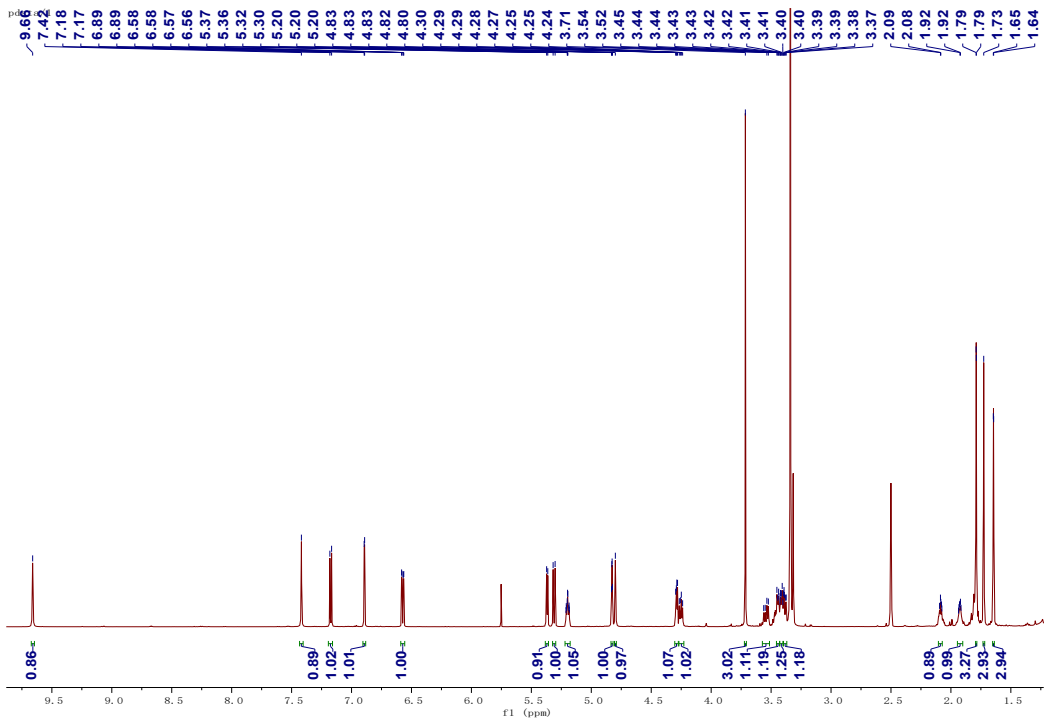


Figure S3. ^{1}H NMR spectrum of compound **1** (600 MHz, DMSO-d_6).

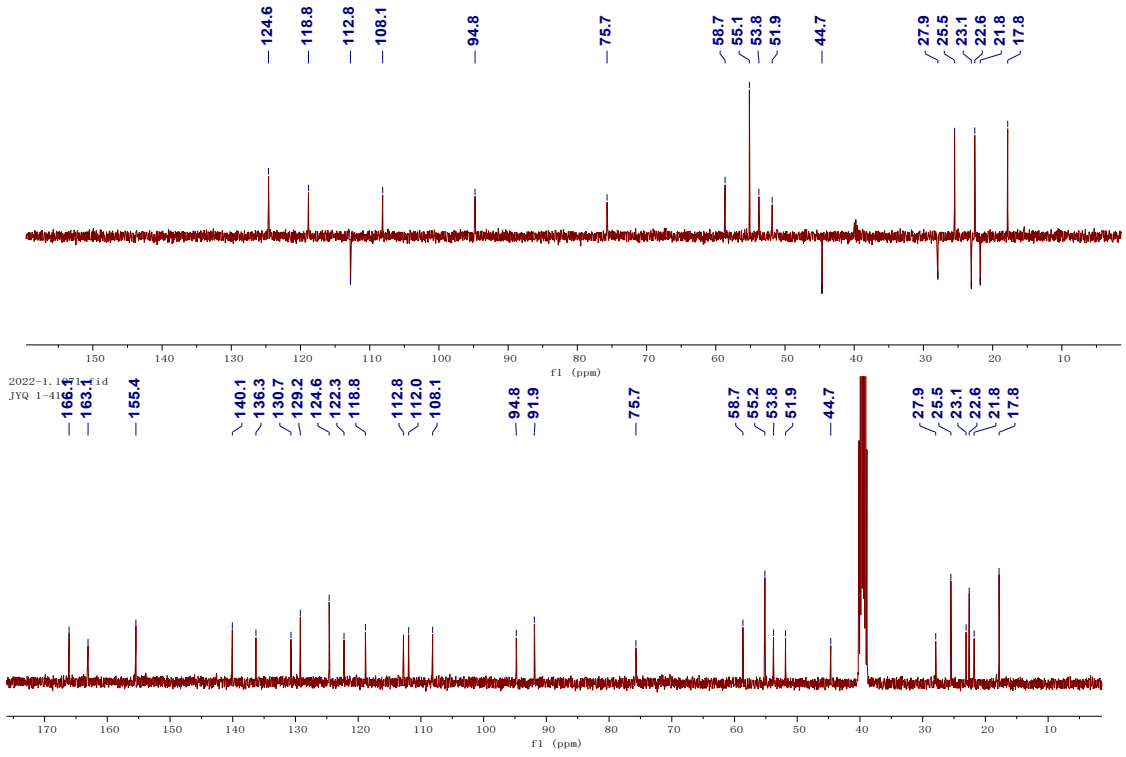


Figure S4. ^{13}C and DEPT NMR spectra of compound **1** (150 MHz, DMSO-d_6).

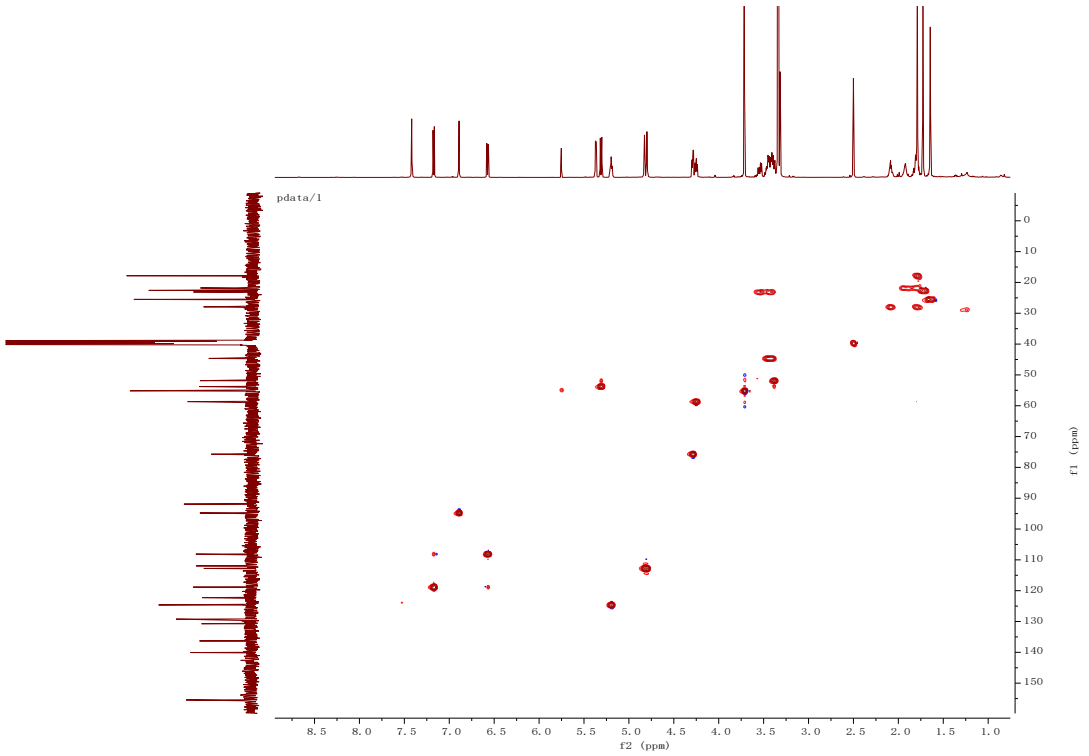


Figure S5. HSQC spectrum of compound **1** (DMSO-d_6).

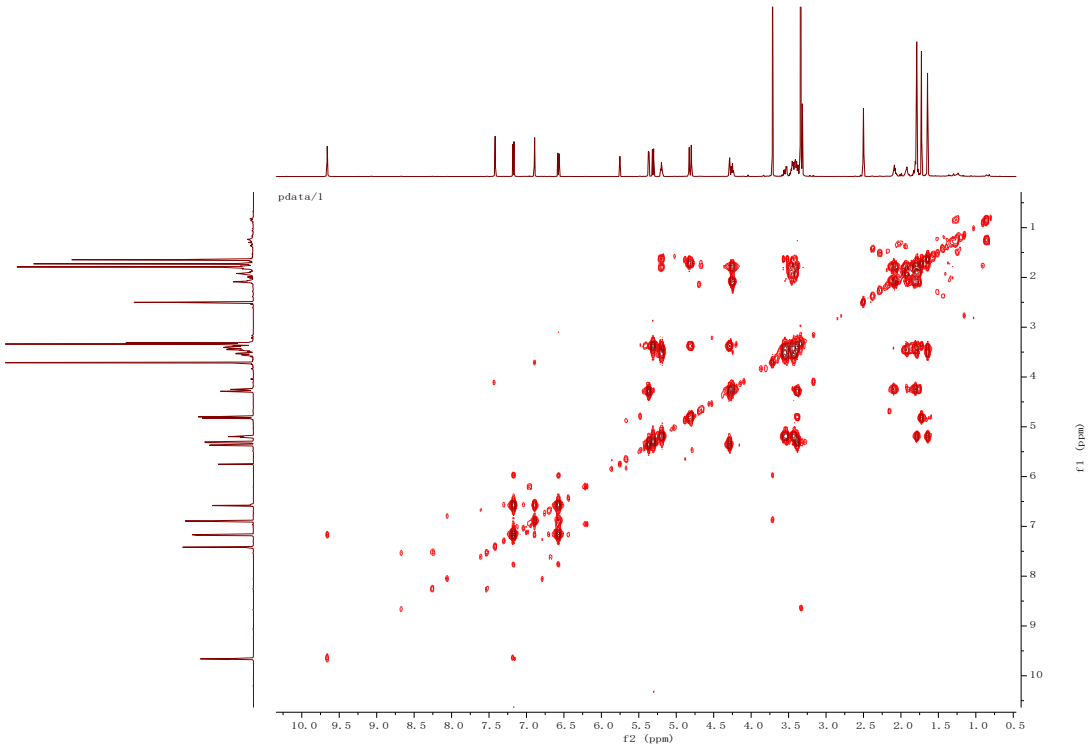


Figure S6. $^{1}H-^{1}H$ COSY spectrum of compound **1** (DMSO-d_6).

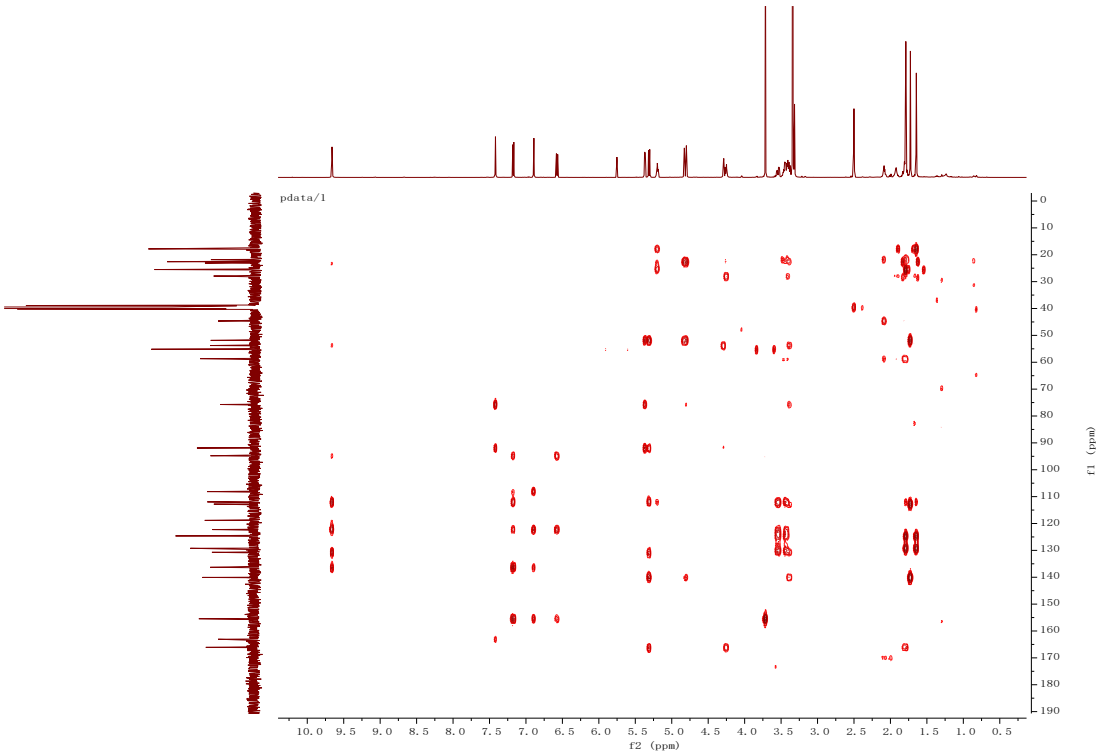


Figure S7. HMBC spectrum of compound **1** (DMSO-d_6).

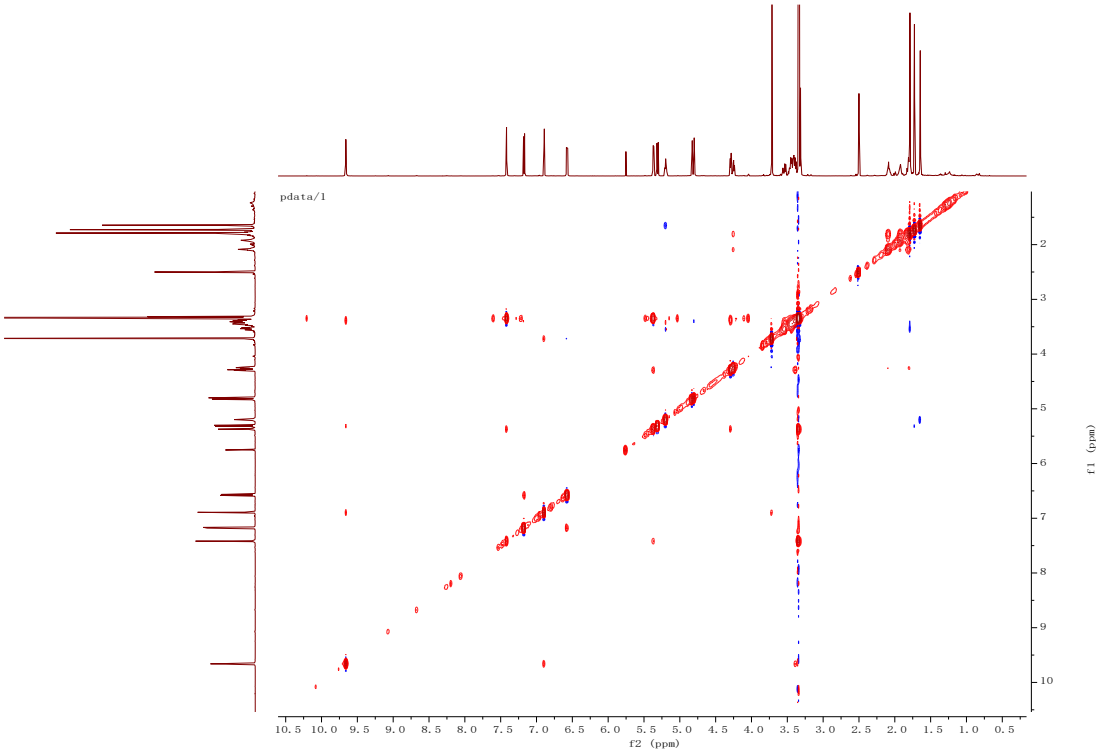


Figure S8. NOESY spectrum of compound **1** (DMSO-d_6).

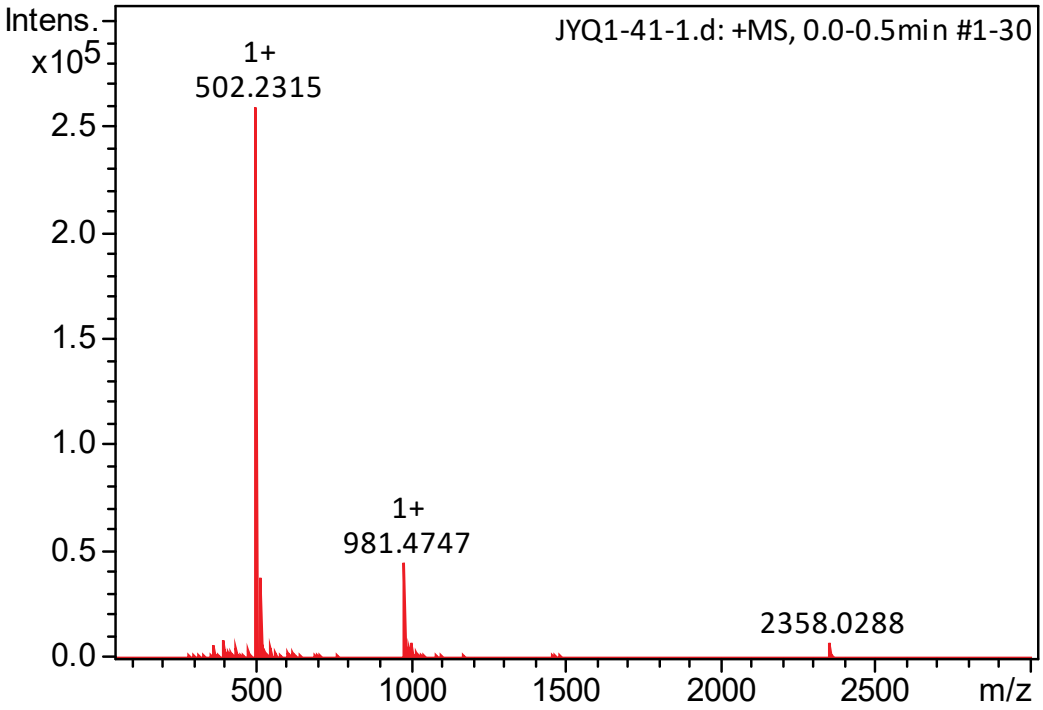


Figure S9. HRESIMS spectrum of compound **1**.

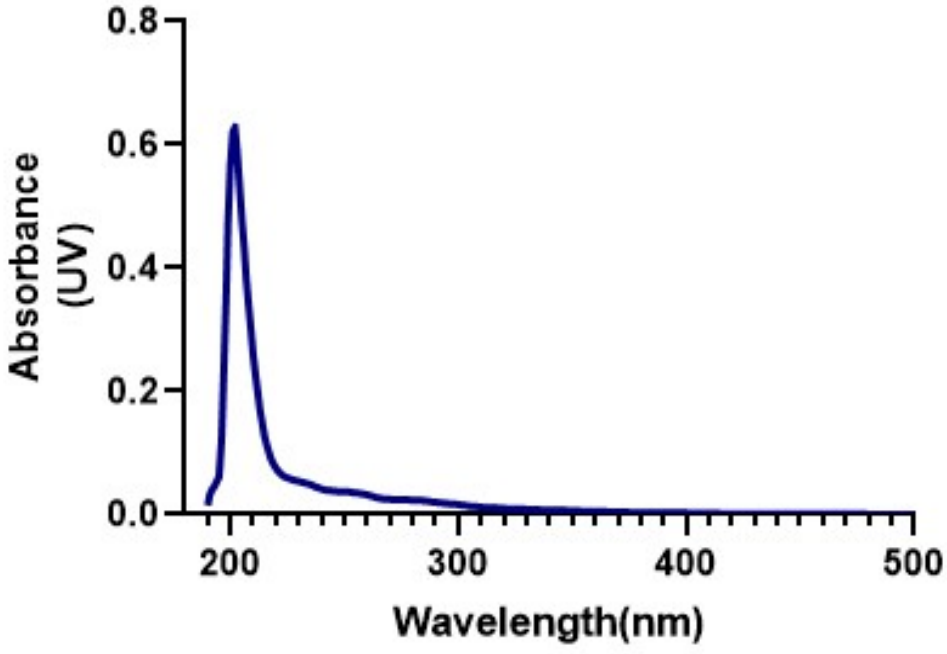


Figure S10. UV spectrum of compound **2** in MeOH.

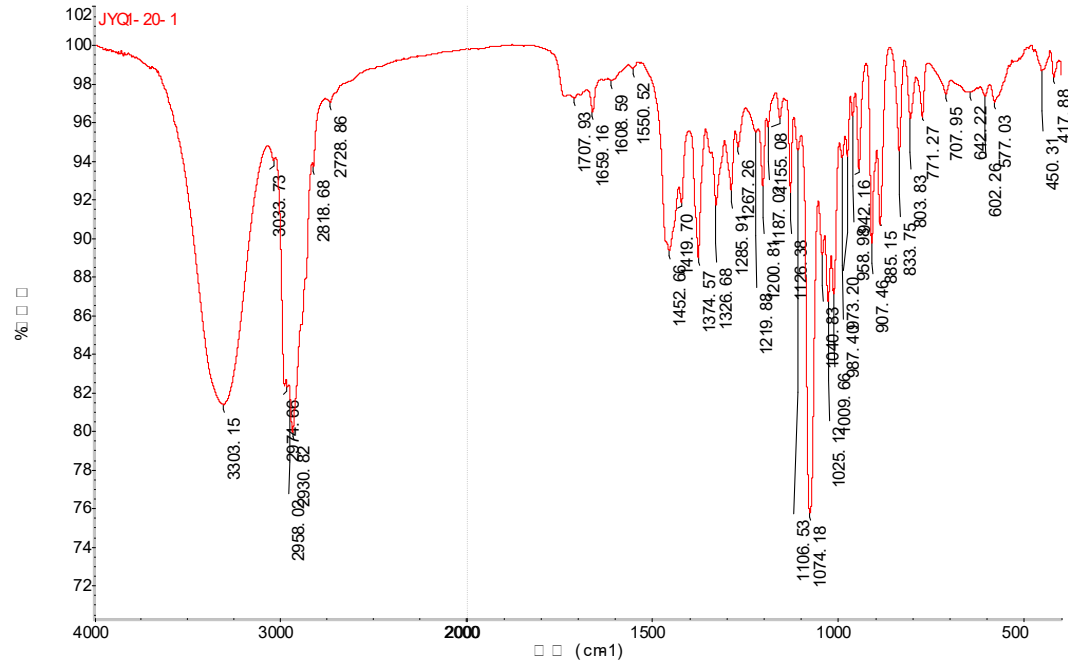


Figure S11. IR spectrum of compound **2**.

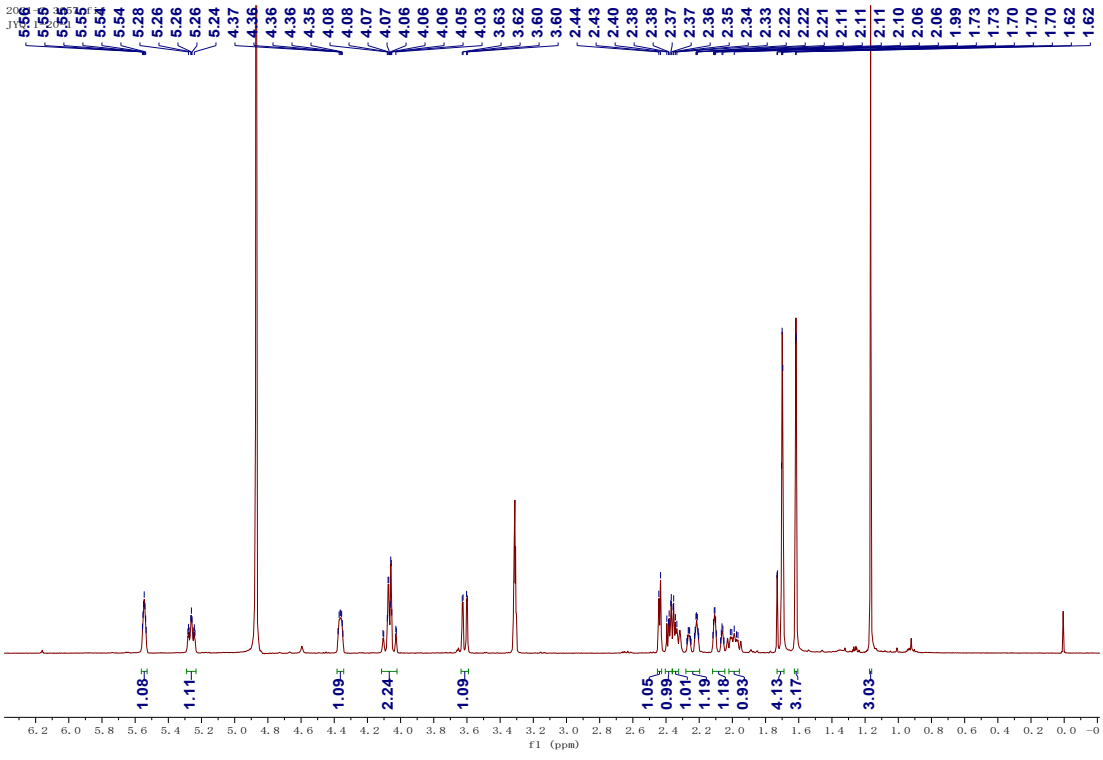


Figure S12. ^{1}H NMR spectrum of compound **2** (400 MHz, CD_3OD).

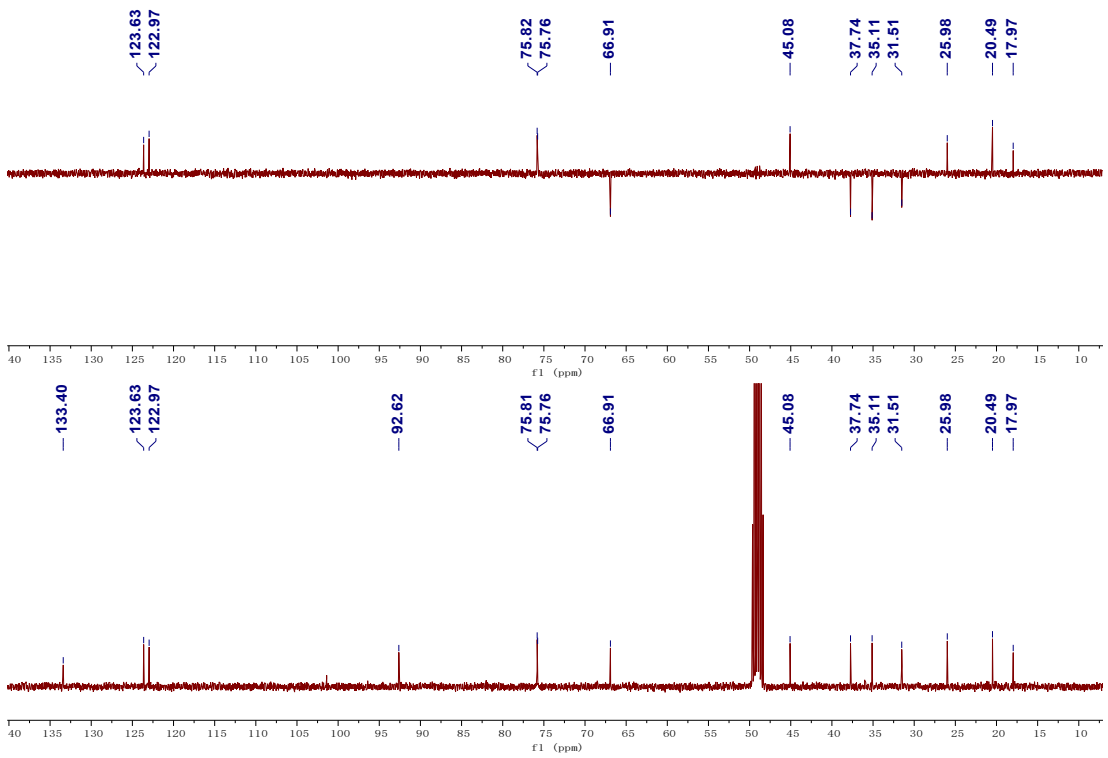


Figure S13. ^{13}C and DEPT NMR spectra of compound **2** (100 MHz, CD_3OD).

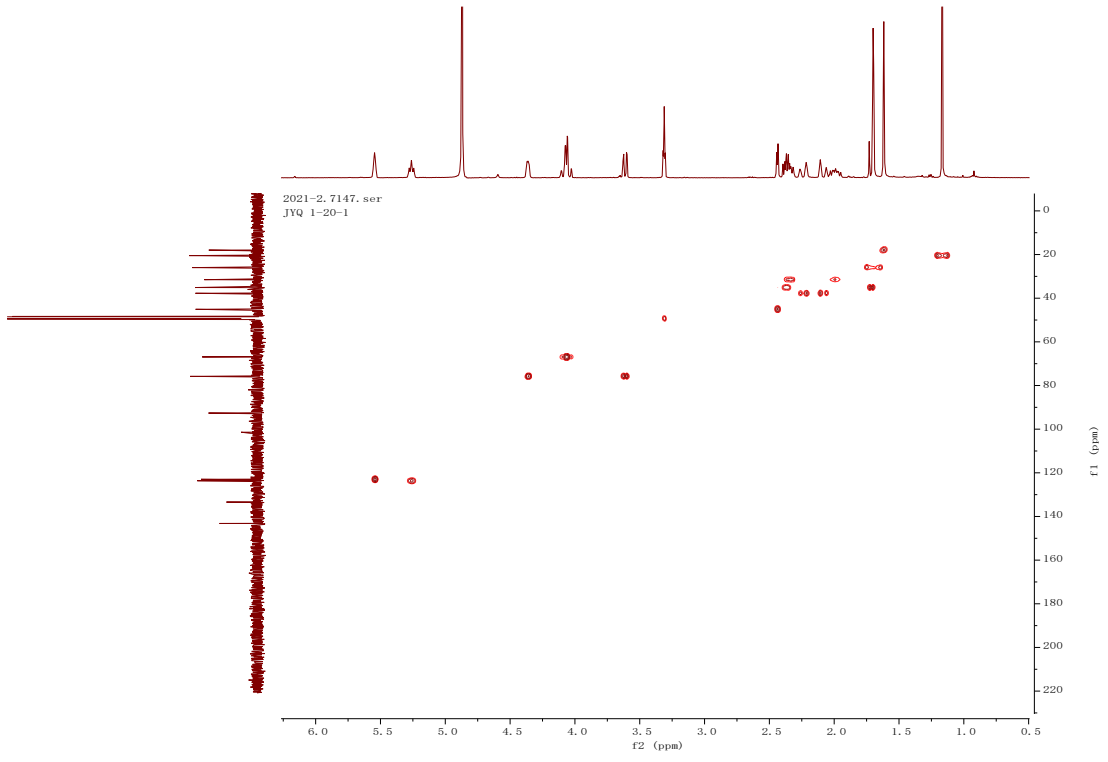


Figure S14. HSQC spectrum of compound **2** (CD_3OD).

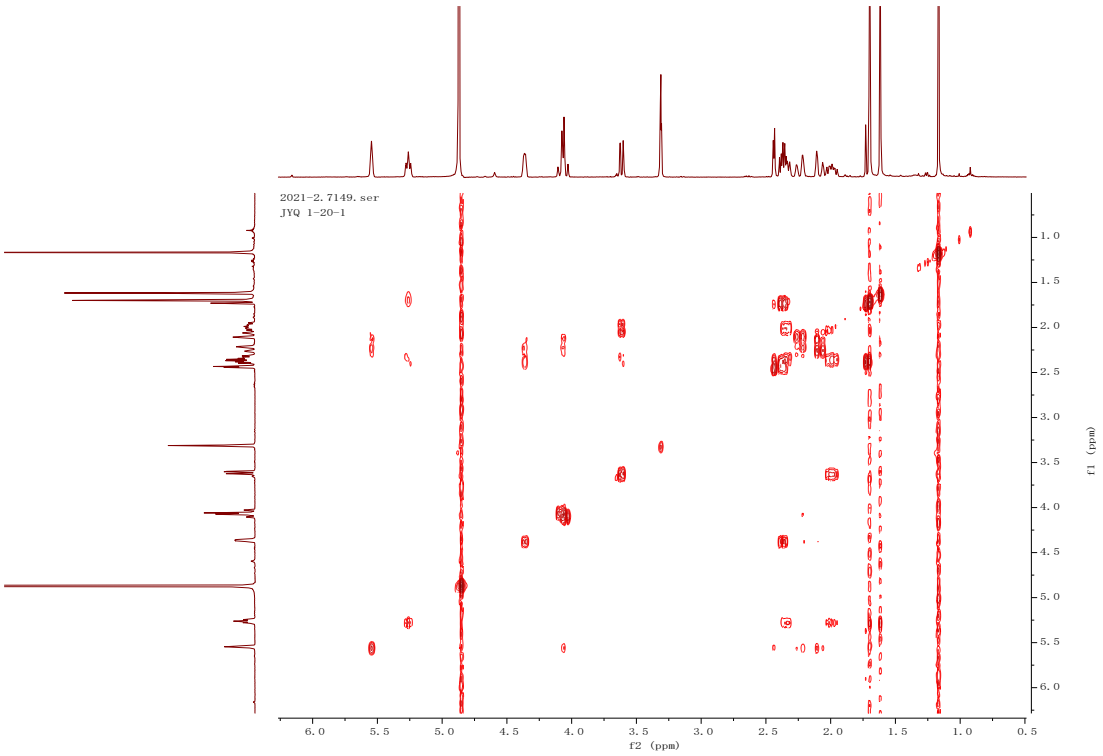


Figure S15. $^{1}H-^{1}H$ COSY spectrum of compound **2** (CD_3OD).

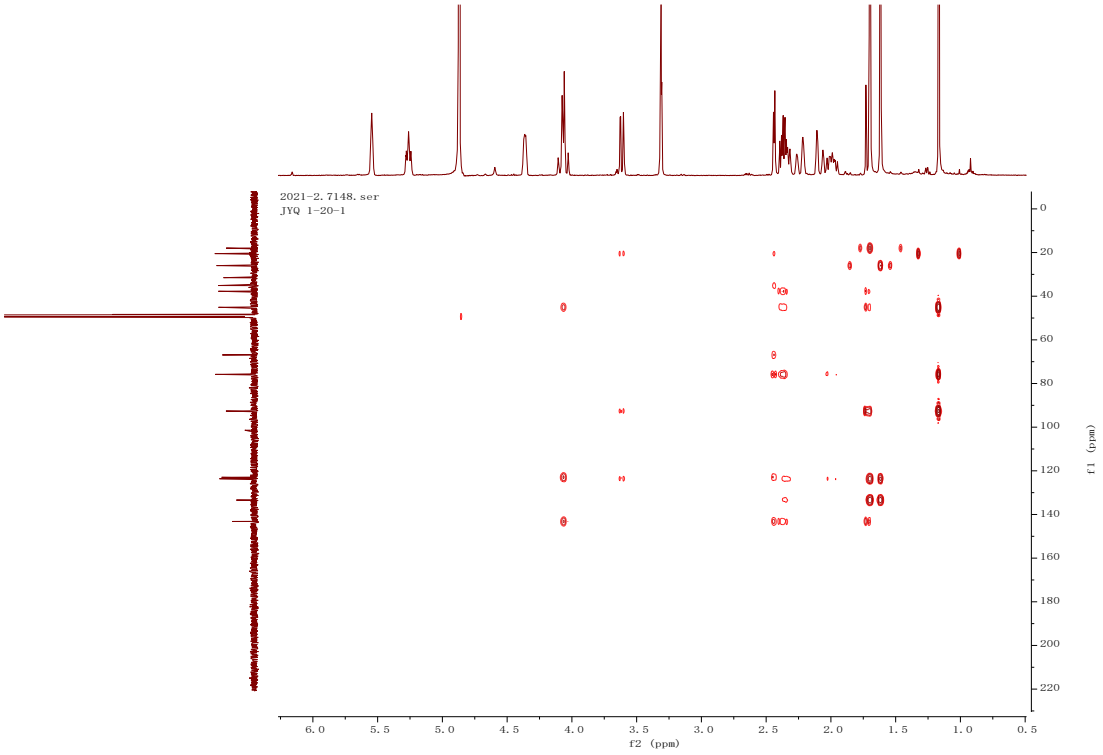


Figure S16. HMBC spectrum of compound **2** (CD_3OD).

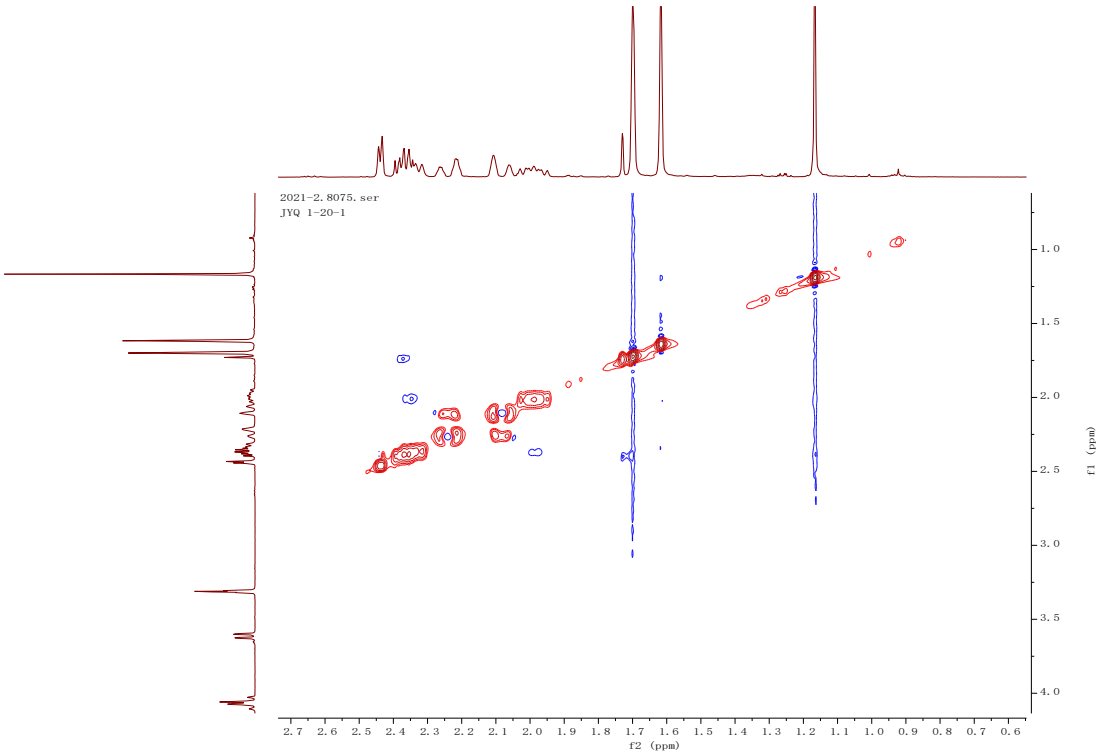


Figure S17. NOESY spectrum of compound **2** (CD_3OD).

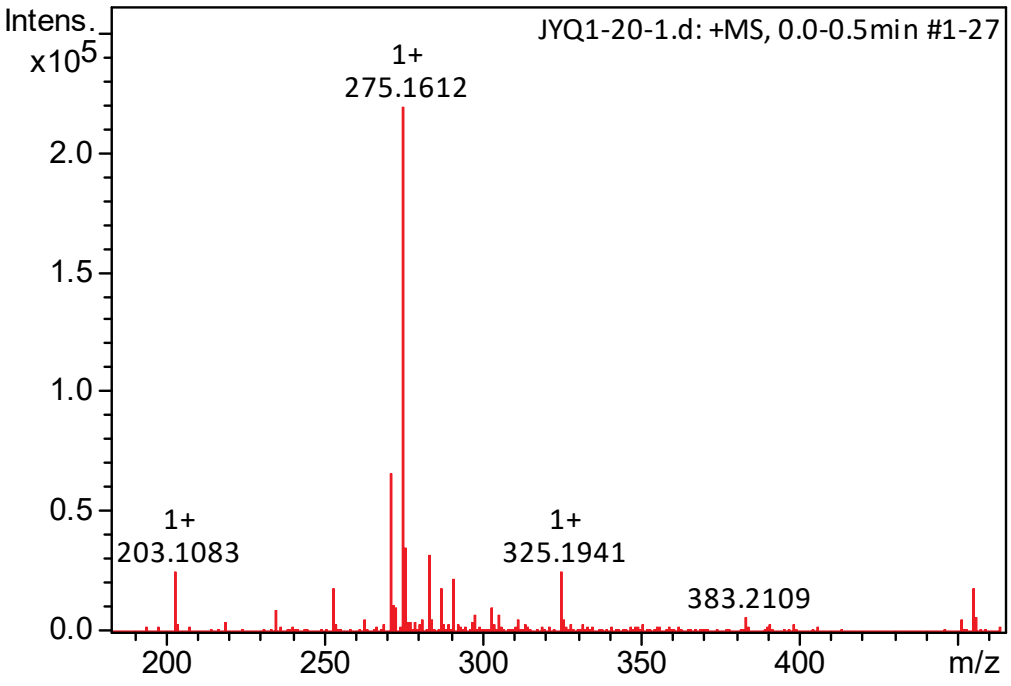
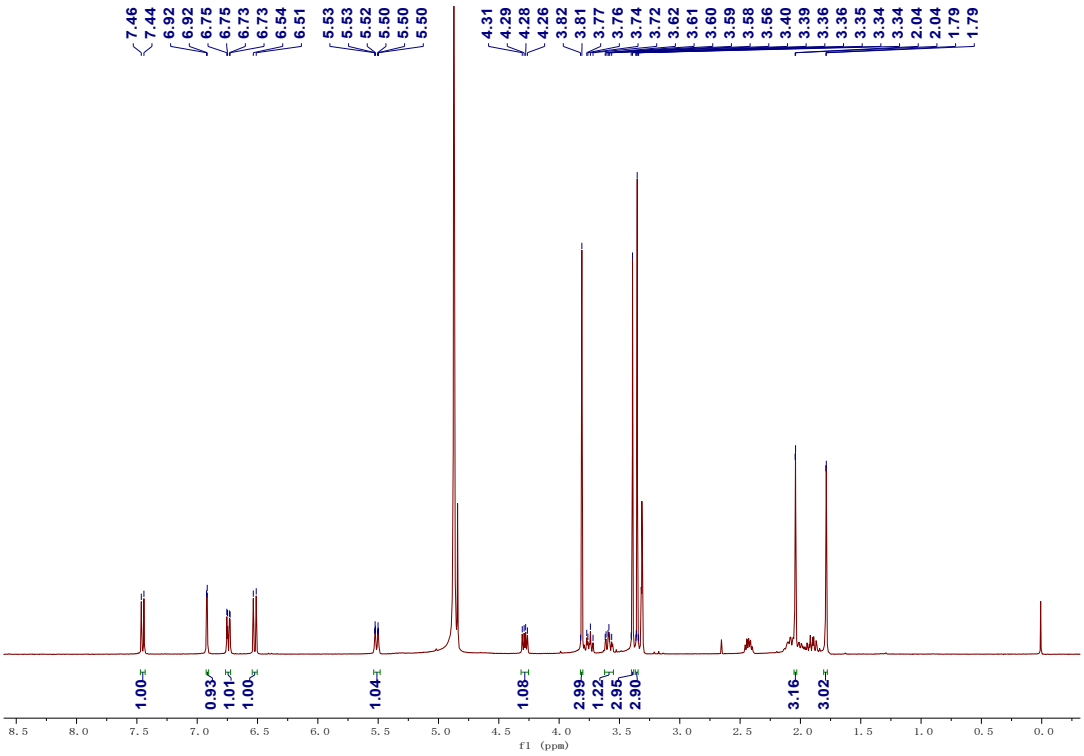
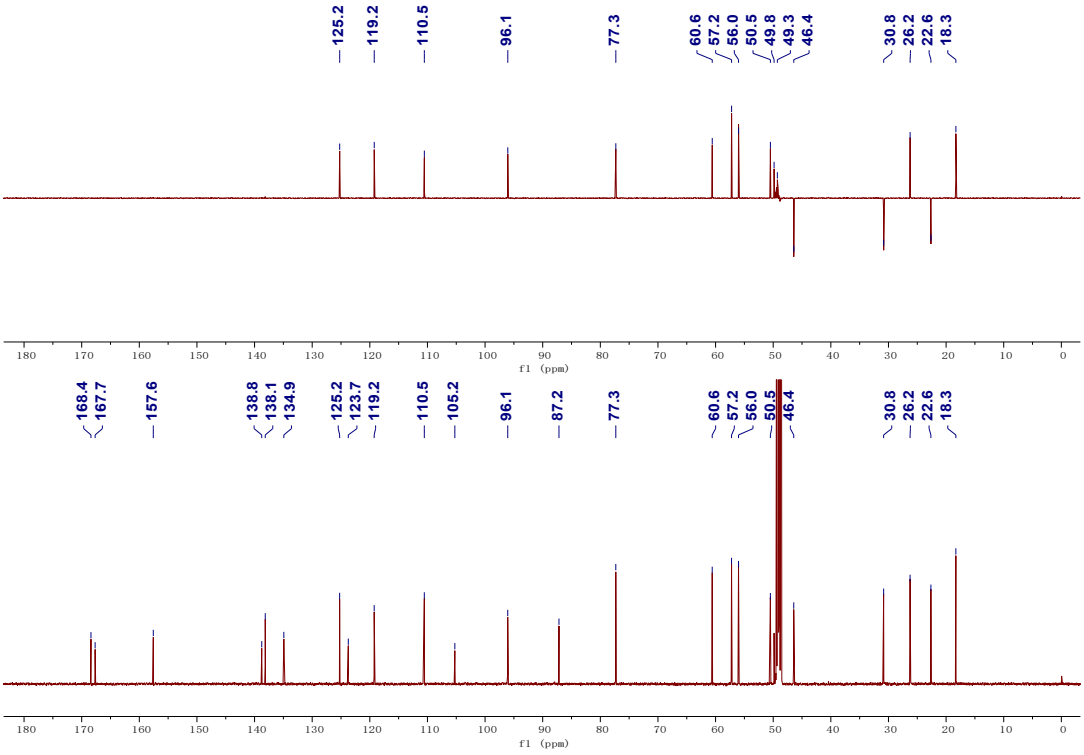


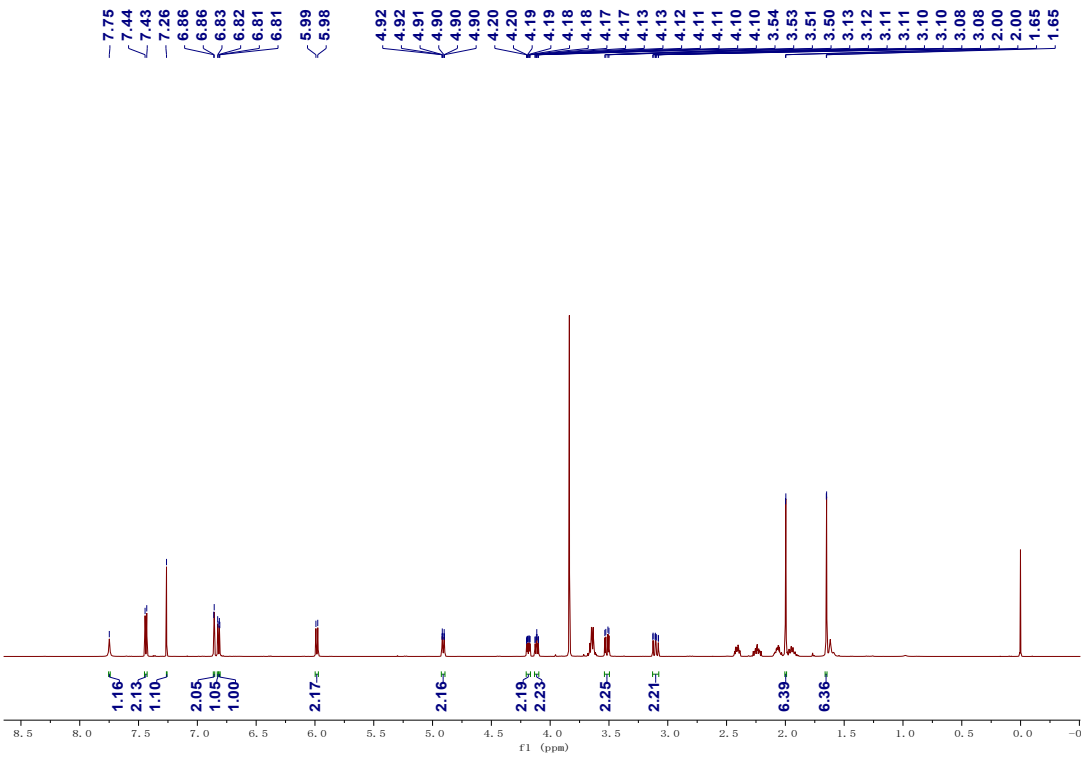
Figure S18. HRESIMS spectrum of compound **2**.



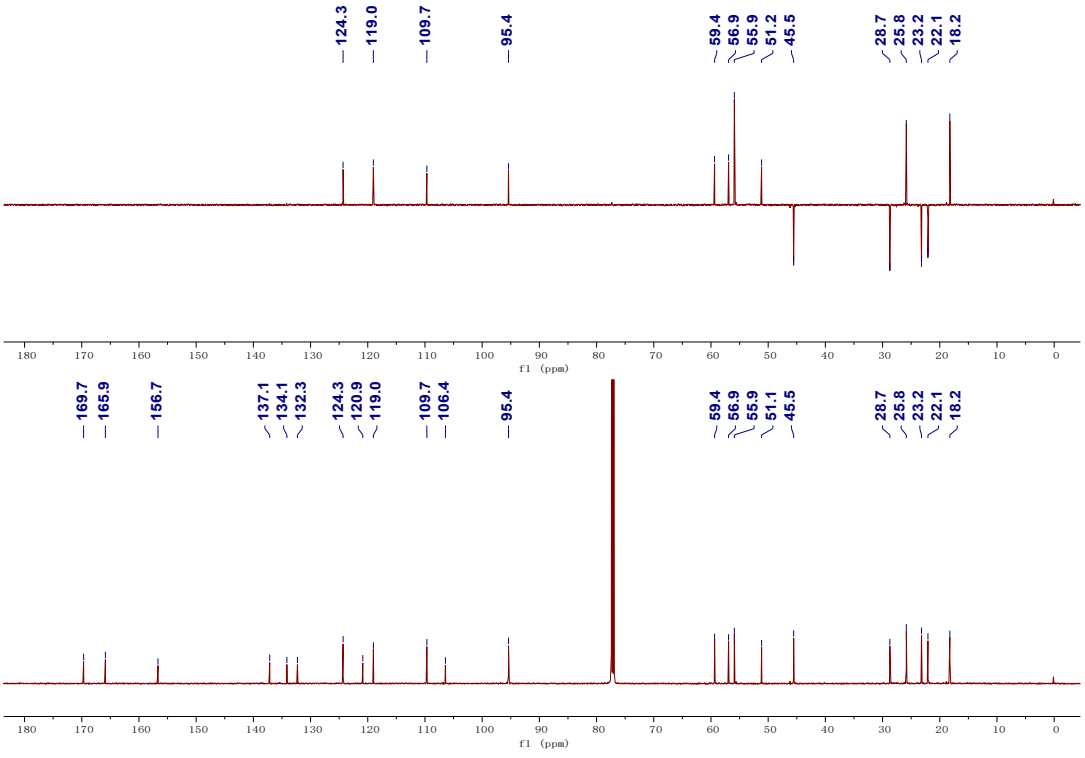
^{1}H NMR spectrum of compound **3** (600 MHz, CD_3OD).



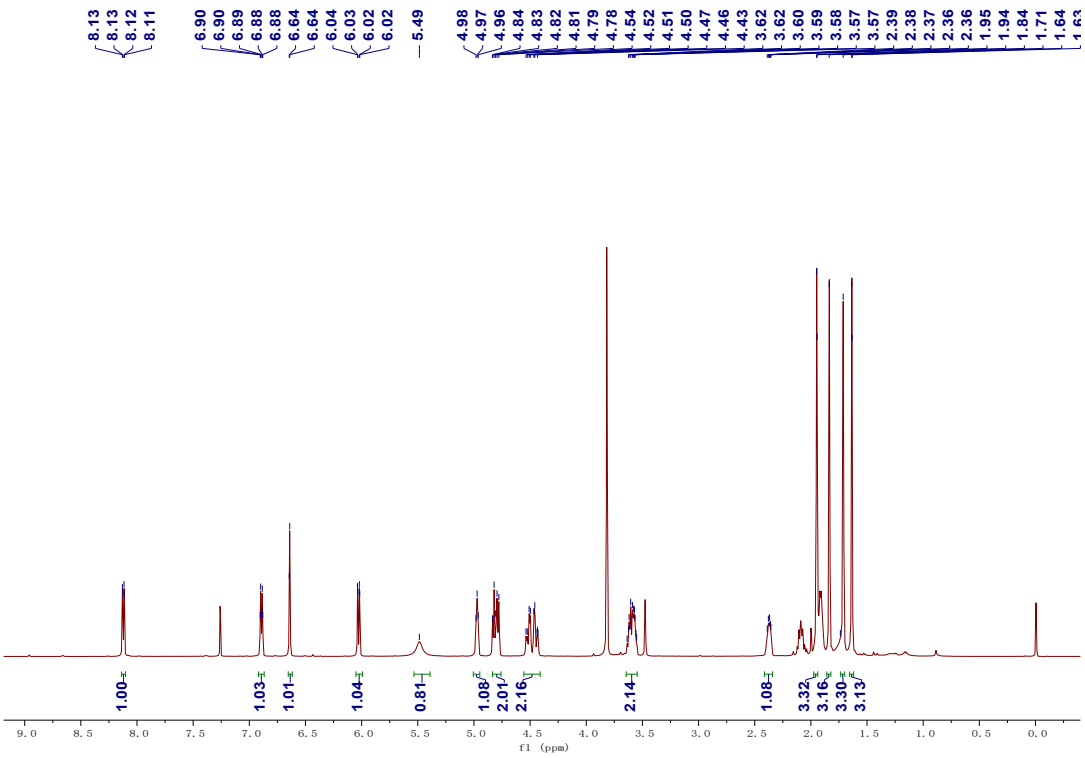
^{13}C and DEPT NMR spectra of compound **3** (150 MHz, CD_3OD).



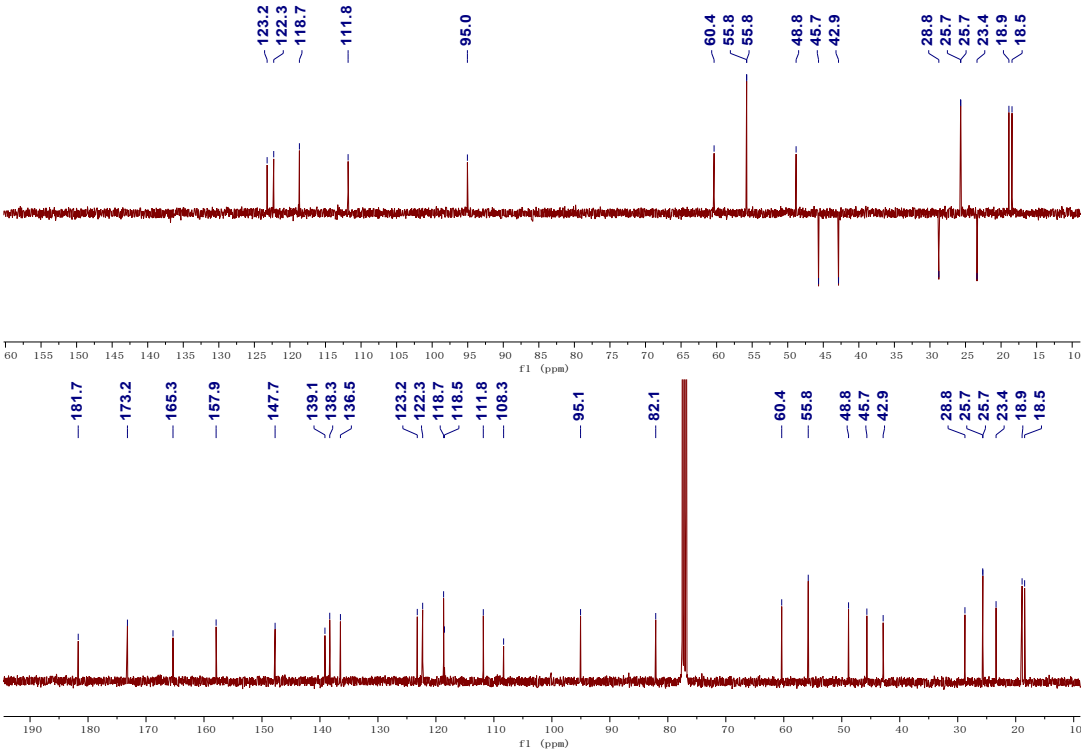
^{1}H NMR spectrum of compound **4** (600 MHz, $CDCl_3$).



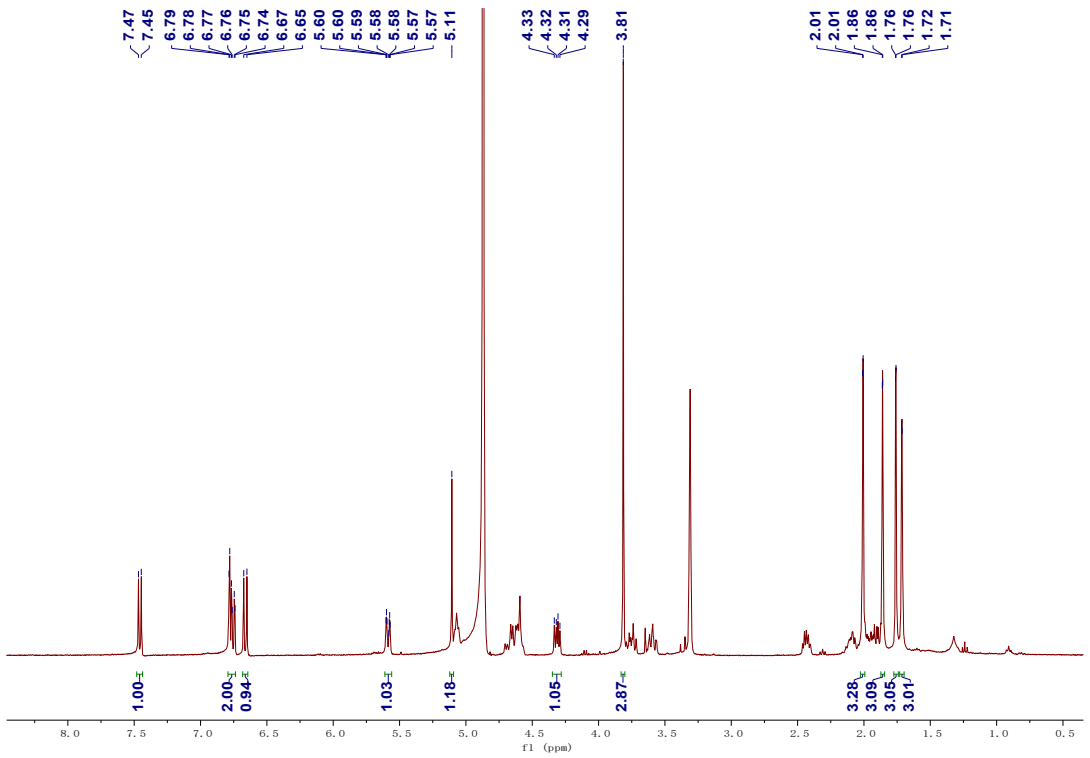
^{13}C and DEPT NMR spectra of compound **4** (150 MHz, $CDCl_3$).



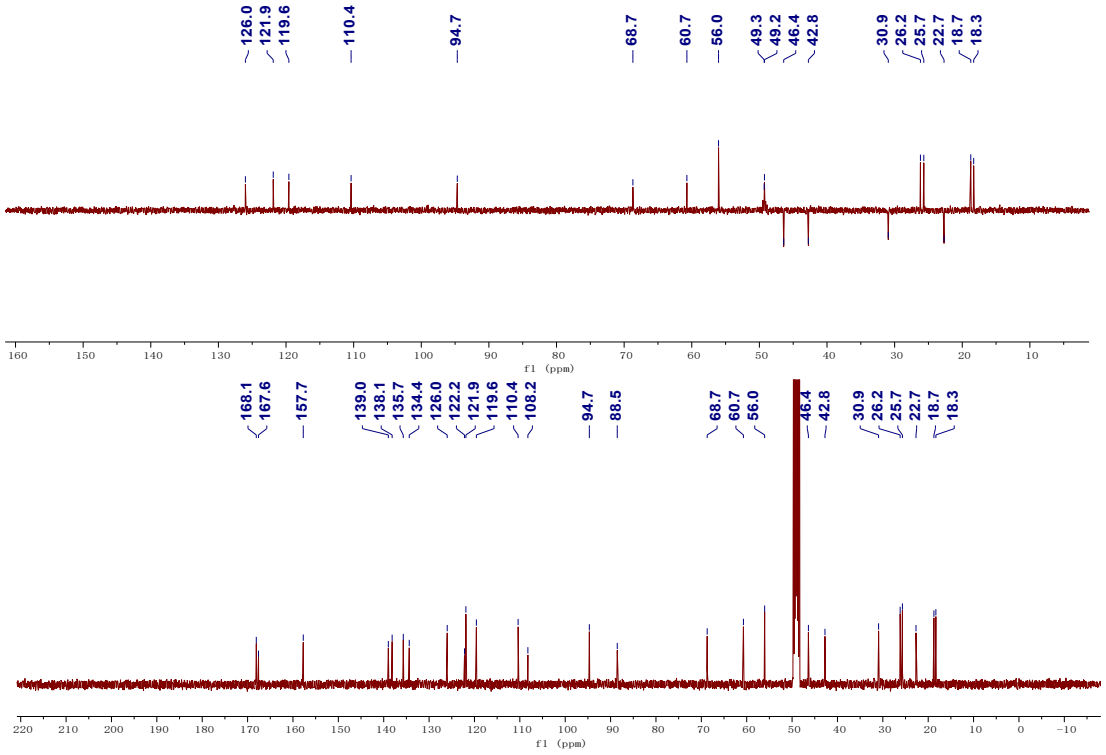
^{1}H NMR spectrum of compound **5** (400 MHz, $CDCl_3$).



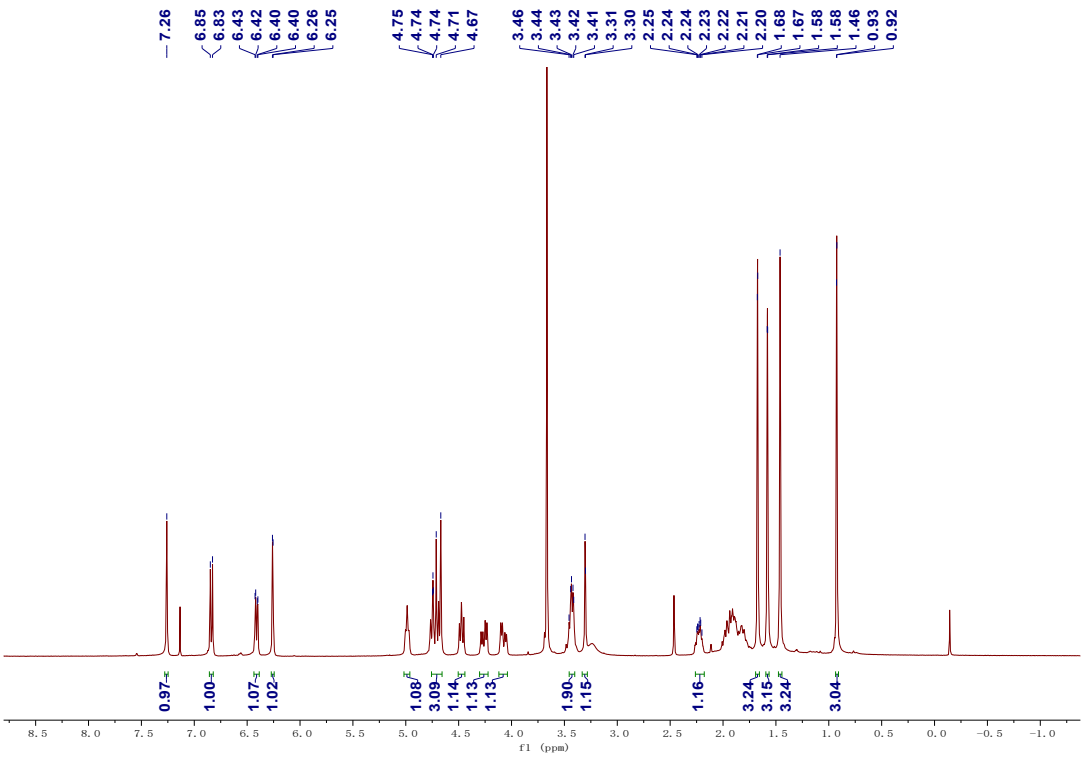
^{13}C and DEPT NMR spectra of compound **5** (100 MHz, $CDCl_3$).



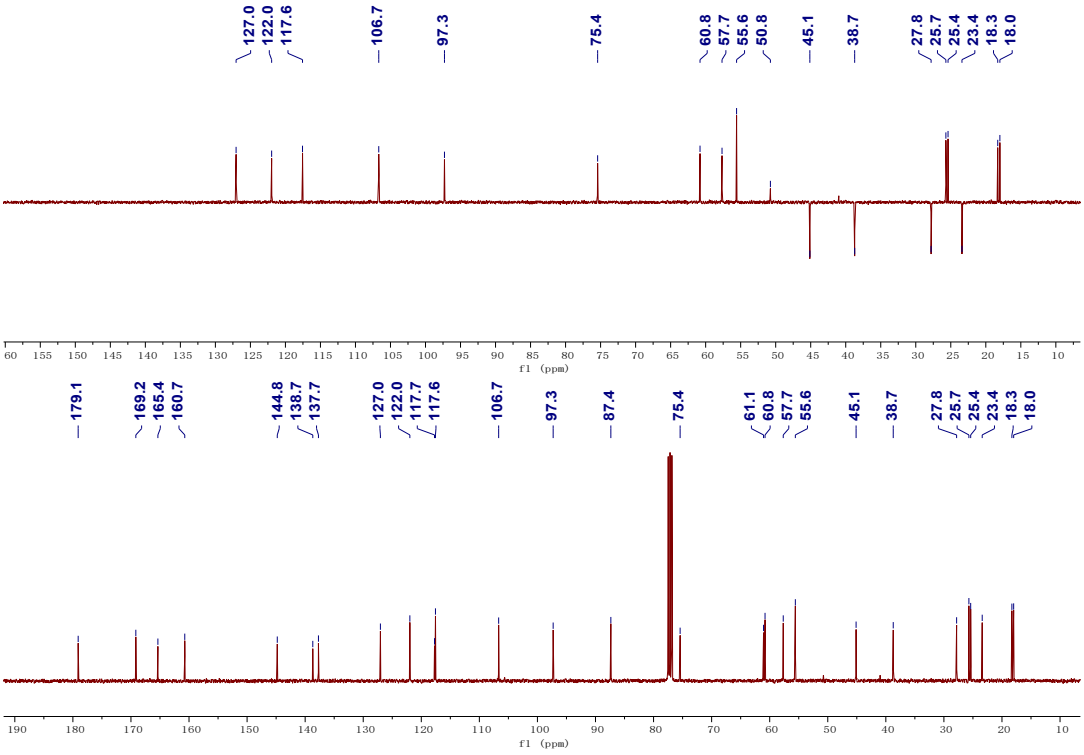
^{1}H NMR spectrum of compound **6** (400 MHz, CD_3OD).



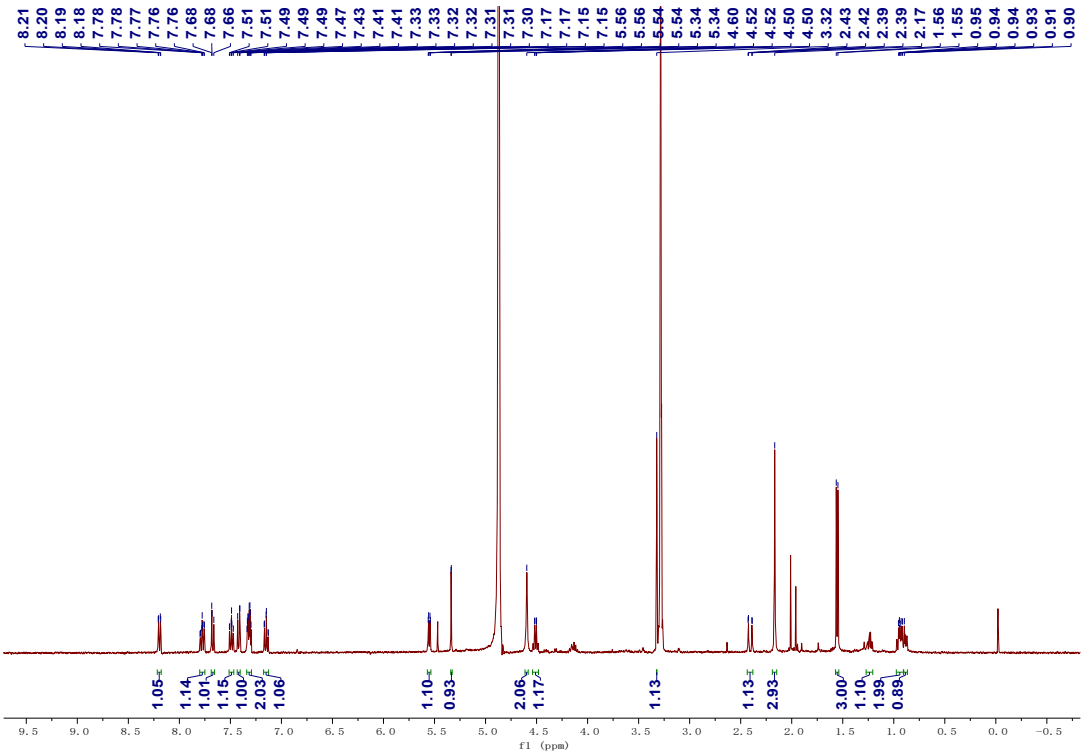
^{13}C and DEPT NMR spectra of compound **6** (100 MHz, CD_3OD).



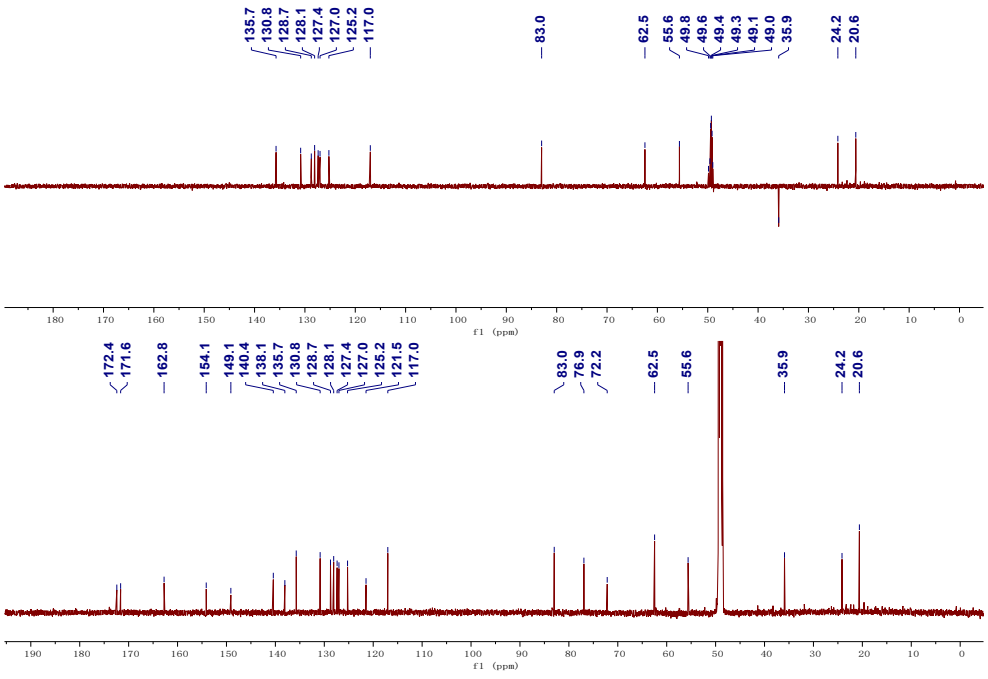
^{1}H NMR spectrum of compound **7** (400 MHz, $CDCl_3$).



^{13}C and DEPT NMR spectra of compound **7** (100 MHz, $CDCl_3$).



^{1}H NMR spectrum of compound **8** (400 MHz, CD_3OD).



^{13}C and DEPT NMR spectra of compound **8** (100 MHz, CD_3OD).

Figure S19. ^{1}H NMR, ^{13}C and DEPT NMR spectra of compounds **3**–**8**

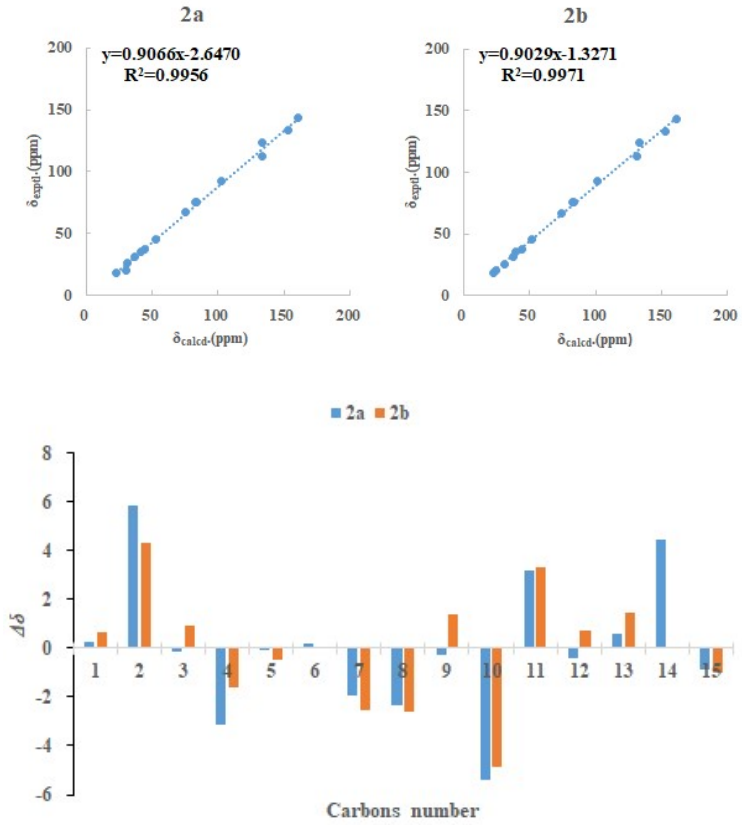
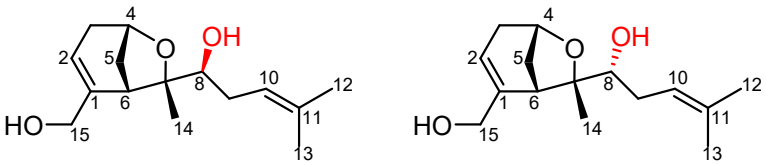


Figure S20. Linear correlation plots (A) and the relative errors (B) between the experimental and calculated ^{13}C NMR chemical shifts of **2a** and **2b**.

NMR calculation for compound 2



2a-DP4+ 0.05% **2b-DP4+ 99.95%**

Table S1. Gibbs free energies[a] and equilibrium populations[b] of low-energy conformers of **2**a.

Conformers	ΔG(a.u.)	P(%)/100	G(a.u.)
2a-1	0.00322	2.22	-811.344912
2a-2	0.00195	8.49	-811.346178
2a-3	0.00243	5.14	-811.345703
2a-4	0.00264	4.07	-811.345484
2a-5	0.00198	8.24	-811.346149

2a-6	0.0	67.1	-811.348129
2a-7	0.00809	0.01	-811.340039
2a-8	0.00266	4.02	-811.345472
2a-9	0.00431	0.7	-811.34382

[a]wB97M-V/def2-TZVP, in a.u.

[b]From ΔG values at 298.15K.

Table S2. Cartesian coordinates for the low-energy reoptimized random reseach conformers of **2a** at B3LYP-D3(BJ)/6-31G* level of theory in methanol.

2a-1		Standard Orientation (A.U.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-9.165582	-2.548781	0.624846
1	6	0	-6.651709	-3.504394	1.666015
2	6	0	-4.399039	-1.602802	1.44356
3	8	0	-5.072555	0.28546	3.302118
4	6	0	-6.937671	-0.703654	5.026653
5	6	0	-9.543956	0.355834	4.346209
6	6	0	10.487693	-0.808523	1.921225
7	6	0	10.065047	-3.585453	-1.871726
8	8	0	-8.384135	-3.027465	-3.863852
9	6	0	-6.928866	-3.560578	4.565169
10	6	0	-1.899078	-2.898702	2.153598
11	6	0	-4.057171	-0.225429	-1.115762
12	6	0	-1.727035	1.533149	-1.196276
13	6	0	-1.430731	2.800878	-3.720199
14	6	0	-2.333174	5.069443	-4.417526
15	6	0	-1.958804	6.052912	-7.063553
16	6	0	-3.81963	6.788475	-2.704929
17	8	0	-6.240966	1.185828	-1.774869
18	1	0	-6.160484	-5.337571	0.821445
19	1	0	-6.378178	-0.154427	6.953326
20	1	0	-9.408295	2.433039	4.165536
21	1	0	10.890006	0.008684	5.908687
22	1	0	12.304556	-0.150783	1.176928
23	1	0	10.197322	-5.667984	-1.762453
24	1	0	12.000171	-2.873727	-2.250767
25	1	0	-7.92561	-1.253159	-3.650248
26	1	0	-5.342822	-4.49573	5.518187
27	1	0	-8.689815	-4.473726	5.178235

28	1	0	-2.124349	-4.232276	3.724892
29	1	0	-1.135973	-3.953244	0.529466
30	1	0	-0.504144	-1.477913	2.73536
31	1	0	-3.866628	-1.693834	-2.579657
32	1	0	-1.921373	2.911589	0.350962
33	1	0	-0.012352	0.427163	-0.804228
34	1	0	-0.432681	1.689374	-5.158954
35	1	0	-3.796234	6.429431	-7.981924
36	1	0	-0.92611	7.868175	-7.053568
37	1	0	-0.90584	4.711057	-8.252472
38	1	0	-5.801675	6.89869	-3.349345
39	1	0	-3.838798	6.154444	-0.729948
40	1	0	-3.061347	8.731783	-2.762032
41	1	0	-6.890283	1.894318	-0.213822

2a-2		Standard Orientation (A.U.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-8.721166	-3.093172	0.130622
1	6	0	-6.522535	-3.630873	1.896593
2	6	0	-4.513789	-1.463224	1.869286
3	8	0	-5.799283	0.506431	3.264515
4	6	0	-7.916404	-0.529113	4.65069
5	6	0	10.384469	0.043519	3.25428
6	6	0	10.523207	-1.447172	0.827561
7	6	0	-8.656664	-4.211086	-2.509329
8	8	0	-9.312254	-2.459388	-4.390724
9	6	0	-7.477076	-3.386686	4.627918
10	6	0	-2.100681	-2.286393	3.248738
11	6	0	-3.824883	-0.343371	-0.764583
12	6	0	-1.568157	1.512015	-0.693199
13	6	0	-0.961458	2.569351	-3.257662
14	6	0	-1.840759	4.721831	-4.277834
15	6	0	-1.124989	5.497211	-6.922233
16	6	0	-3.62181	6.503175	-2.953846
17	8	0	-5.927558	0.888066	-1.873348
18	1	0	-5.647956	-5.470357	1.47547
19	1	0	-7.899236	0.321775	6.548246
20	1	0	10.480717	2.091872	2.849998
21	1	0	12.017143	-0.360561	4.497491

22	1	0	12.046365	-1.013953	-0.502699
23	1	0	-6.749826	-5.032237	-2.831951
24	1	0	-9.994607	-5.808934	-2.65623
25	1	0	-8.260678	-0.985039	-4.0457
26	1	0	-6.06921	-3.971173	6.03418
27	1	0	-9.222358	-4.462563	4.95453
28	1	0	-1.016957	-0.625687	3.857715
29	1	0	-2.523489	-3.410672	4.939391
30	1	0	-0.90008	-3.441703	2.000735
31	1	0	-3.33681	-1.934544	-2.021739
32	1	0	-2.029999	3.014156	0.672348
33	1	0	0.113319	0.532496	0.035474
34	1	0	0.27853	1.393278	-4.432921
35	1	0	-0.180475	7.359722	-6.929511
36	1	0	0.144935	4.11932	-7.823278
37	1	0	-2.82306	5.696158	-8.121353
38	1	0	-5.493964	6.456878	-3.874841
39	1	0	-3.900286	6.042287	-0.95061
40	1	0	-2.937101	8.469913	-3.084729
41	1	0	-6.802455	1.701777	-0.479148

2a-3		Standard Orientation (A.U.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-8.232748	-3.795671	-0.213832
1	6	0	-7.047691	-2.213163	1.87917
2	6	0	-6.475763	0.547298	1.047254
3	8	0	-8.966423	1.722894	1.104596
4	6	0	10.747167	0.095611	2.338479
5	6	0	12.263599	-1.396565	0.368954
6	6	0	10.668348	-3.429925	-0.827693
7	6	0	-6.614755	-5.66108	-1.644912
8	8	0	-4.583816	-6.489318	-0.110734
9	6	0	-9.105357	-1.723755	3.874461
10	6	0	-4.780453	1.951024	2.921056
11	6	0	-5.573633	0.863668	-1.708035
12	6	0	-2.921671	-0.160901	-2.338312
13	6	0	-0.66789	1.203845	-1.253431
14	6	0	0.475454	3.267478	-2.194522
15	6	0	2.749641	4.394642	-0.900963

16	6	0	-0.365967	4.640485	-4.53914
17	8	0	-5.708971	3.44158	-2.397356
18	1	0	-5.362183	-3.161391	2.618703
19	1	0	-12.00334	1.286871	3.493002
20	1	0	12.951504	-0.066836	-1.086352
21	1	0	13.969251	-2.227619	1.24891
22	1	0	11.551267	-4.605564	-2.288192
23	1	0	-7.809033	-7.261001	-2.274194
24	1	0	-5.884079	-4.733671	-3.377424
25	1	0	-3.431311	-7.449466	-1.146937
26	1	0	-8.34036	-0.818642	5.578003
27	1	0	10.110666	-3.453885	4.43038
28	1	0	-4.375291	3.849613	2.187421
29	1	0	-5.721802	2.141921	4.761266
30	1	0	-2.976257	0.965866	3.200614
31	1	0	-6.926248	-0.22717	-2.866699
32	1	0	-2.853143	-2.148478	-1.727695
33	1	0	-2.793255	-0.176458	-4.417903
34	1	0	0.137811	0.39321	0.47323
35	1	0	4.392431	4.455267	-2.189516
36	1	0	2.378136	6.370074	-0.334488
37	1	0	3.295504	3.325343	0.797182
38	1	0	-2.017052	3.775584	-5.441099
39	1	0	-0.90012	6.600126	-4.062414
40	1	0	1.198137	4.764348	-5.917809
41	1	0	-7.355927	4.009579	-1.828213

2a-4		Standard Orientation (A.U.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-9.184493	-2.770902	0.405478
1	6	0	-6.352401	-3.309735	0.47958
2	6	0	-4.63646	-0.929453	0.833058
3	8	0	-5.12865	-0.266132	3.44104
4	6	0	-6.24814	-2.372161	4.759816
5	6	0	-9.091026	-1.922369	5.063164
6	6	0	10.413053	-2.187696	2.551734
7	6	0	10.508222	-2.865733	-2.114313
8	8	0	-9.586048	-1.021143	-3.807393
9	6	0	-5.831524	-4.643907	3.016045

10	6	0	-1.844666	-1.619716	0.462263
11	6	0	-5.260271	1.416495	-0.794829
12	6	0	-3.372691	3.639699	-0.497957
13	6	0	-1.070913	3.553802	-2.177247
14	6	0	-1.056205	3.956992	-4.687347
15	6	0	1.350087	3.797044	-6.200945
16	6	0	-3.390721	4.577945	-6.197388
17	8	0	-7.741275	2.319471	-0.297949
18	1	0	-5.771494	-4.402103	-1.189222
19	1	0	-5.308617	-2.539452	6.608239
20	1	0	-9.39663	-0.015078	5.859782
21	1	0	-9.885182	-3.255856	6.465002
22	1	0	12.450873	-1.826349	2.490107
23	1	0	10.187204	-4.722785	-3.015906
24	1	0	12.574567	-2.686322	-1.810722
25	1	0	-9.435769	0.530018	-2.820658
26	1	0	-3.903236	-5.390632	3.162292
27	1	0	-7.163935	-6.191791	3.389063
28	1	0	-0.636849	-0.199822	1.370678
29	1	0	-1.379917	-3.457687	1.301403
30	1	0	-1.368522	-1.685835	-1.55984
31	1	0	-5.270553	0.798113	-2.779323
32	1	0	-4.496044	5.336255	-0.930337
33	1	0	-2.823725	3.800786	1.502816
34	1	0	0.737577	3.110536	-1.274428
35	1	0	1.192975	2.356706	-7.705024
36	1	0	1.749051	5.606491	-7.164001
37	1	0	2.988136	3.318245	-5.013194
38	1	0	-3.075002	6.276277	-7.368265
39	1	0	-3.848034	3.029812	-7.521604
40	1	0	-5.06707	4.911427	-5.020232
41	1	0	-8.015757	2.108707	1.503016

2a-5		Standard Orientation (A.U.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-8.923009	-0.616025	0.938653
1	6	0	-7.323471	-3.00119	1.162959
2	6	0	-4.402273	-2.588805	1.101791
3	8	0	-3.84024	-1.656785	3.593892

4	6	0	-6.013609	-1.896483	5.192709
5	6	0	-7.490931	0.600767	5.277801
6	6	0	-8.980959	1.010084	2.88632
7	6	0	10.485464	-0.250736	-1.415399
8	8	0	-9.070642	0.302089	-3.60994
9	6	0	-7.606833	-3.939071	3.910153
10	6	0	-3.034024	-5.114458	0.674056
11	6	0	-3.283655	-0.695902	-0.82657
12	6	0	-3.687779	2.144878	-0.410387
13	6	0	-2.016393	3.618872	-2.175891
14	6	0	-2.707038	4.929355	-4.248352
15	6	0	-0.762857	6.312976	-5.807261
16	6	0	-5.396408	5.23992	-5.142802
17	8	0	-4.153484	-1.446674	-3.274896
18	1	0	-7.898287	-4.405191	-0.255195
19	1	0	-5.34038	-2.417604	7.090919
20	1	0	-6.144794	2.16575	5.588824
21	1	0	-8.776397	0.612682	6.927482
22	1	0	10.167566	2.703161	2.769815
23	1	0	11.639861	-1.983685	-1.705637
24	1	0	11.822018	1.321003	-1.129669
25	1	0	-7.487362	-0.652705	-3.587199
26	1	0	-6.793912	-5.825991	4.202096
27	1	0	-9.584671	-3.958981	4.54197
28	1	0	-3.167803	-5.662857	-1.325587
29	1	0	-1.027953	-4.894519	1.174514
30	1	0	-3.817478	-6.640097	1.842853
31	1	0	-1.216481	-1.012552	-0.739159
32	1	0	-5.679282	2.629154	-0.677733
33	1	0	-3.188935	2.563798	1.564575
34	1	0	0.008976	3.559217	-1.724092
35	1	0	1.161288	6.083101	-5.053837
36	1	0	-0.779016	5.648102	-7.785925
37	1	0	-1.195565	8.354613	-5.877071
38	1	0	-6.070106	7.174604	-4.733229
39	1	0	-5.497432	5.022508	-7.214918
40	1	0	-6.727821	3.886246	-4.307256
41	1	0	-3.390734	-0.286527	-4.475097

2a-6	Standard Orientation (A.U.)

Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-9.196285	-2.467155	0.188795
1	6	0	-6.793036	-3.527475	1.377842
2	6	0	-4.471252	-1.697516	1.352145
3	8	0	-5.208553	0.171674	3.205345
4	6	0	-7.220358	-0.787275	4.773136
5	6	0	-9.735376	0.375922	3.93767
6	6	0	10.546183	-0.706649	1.427817
7	6	0	-9.955289	-3.433318	-2.381074
8	8	0	-8.108472	-2.931116	-4.23655
9	6	0	-7.271784	-3.633056	4.24937
10	6	0	-2.068601	-3.092572	2.20072
11	6	0	-3.906841	-0.278118	-1.143369
12	6	0	-1.539802	1.426763	-0.999559
13	6	0	-1.048205	2.793026	-3.440812
14	6	0	-1.879927	5.099427	-4.101179
15	6	0	-1.307814	6.193332	-6.667356
16	6	0	-3.473765	6.758828	-2.426073
17	8	0	-6.00185	1.192131	-1.943534
18	1	0	-6.303187	-5.358305	0.527572
19	1	0	-6.779357	-0.296594	6.745893
20	1	0	-9.515804	2.449981	3.812229
21	1	0	11.198956	0.04579	5.394642
22	1	0	12.284288	0.028162	0.575301
23	1	0	10.186134	-5.509021	-2.310755
24	1	0	11.824037	-2.631542	-2.890477
25	1	0	-7.600388	-1.177131	-3.972953
26	1	0	-5.785574	-4.638977	5.287434
27	1	0	-9.099037	-4.499038	4.720218
28	1	0	-2.448571	-4.4456	3.724512
29	1	0	-1.231812	-4.14295	0.610506
30	1	0	-0.668918	-1.73492	2.908554
31	1	0	-3.632981	-1.721432	-2.619113
32	1	0	-1.805696	2.747211	0.587104
33	1	0	0.11972	0.263095	-0.54226
34	1	0	0.042164	1.732318	-4.850413
35	1	0	-0.175568	4.896523	-7.833187
36	1	0	-3.071405	6.622288	-7.700565
37	1	0	-0.271158	7.998723	-6.501964
38	1	0	-3.654407	6.032099	-0.491526

39	1	0	-2.689577	8.690351	-2.330994
40	1	0	-5.398059	6.931007	-3.215685
41	1	0	-6.748124	1.90941	-0.431298

2a-7		Standard Orientation (A.U.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-8.154204	-3.48369	0.257564
1	6	0	-5.502976	-3.145309	1.304478
2	6	0	-4.673929	-0.308696	1.334818
3	8	0	-6.148597	0.682955	3.414002
4	6	0	-7.120661	-1.354989	4.954769
5	6	0	-9.905313	-1.825767	4.325501
6	6	0	10.161188	-2.936539	1.711709
7	6	0	-8.454927	-4.138139	-2.518056
8	8	0	10.288432	-2.65478	-3.73575
9	6	0	-5.583043	-3.670766	4.158458
10	6	0	-1.843984	-0.074022	1.895877
11	6	0	-5.364592	1.274183	-1.045696
12	6	0	-4.141048	3.93699	-1.153623
13	6	0	-1.493562	4.072209	-2.198241
14	6	0	-0.851898	3.829836	-4.646672
15	6	0	1.86445	3.982779	-5.486671
16	6	0	-2.734812	3.390875	-6.739344
17	8	0	-8.019895	1.560524	-1.272241
18	1	0	-4.128082	-4.316014	0.272868
19	1	0	-6.870307	-0.808762	6.945738
20	1	0	10.946025	-0.017143	4.44502
21	1	0	10.764606	-3.065999	5.773849
22	1	0	12.056792	-3.103764	0.901493
23	1	0	-6.575484	-3.974145	-3.44298
24	1	0	-9.025011	-6.135616	-2.740627
25	1	0	-9.895875	-0.922507	-3.241408
26	1	0	-3.701949	-3.695693	5.031269
27	1	0	-6.543619	-5.455748	4.607862
28	1	0	-1.247561	-1.391295	3.382833
29	1	0	-0.7217	-0.46248	0.190017
30	1	0	-1.400205	1.843291	2.550211
31	1	0	-4.734504	0.204495	-2.717788
32	1	0	-5.42859	5.04457	-2.353844

33	1	0	-4.232555	4.795625	0.740518
34	1	0	0.038101	4.388778	-0.843559
35	1	0	2.138814	5.542794	-6.847398
36	1	0	3.158256	4.281851	-3.886836
37	1	0	2.442403	2.236015	-6.474589
38	1	0	-4.708833	3.472481	-6.103369
39	1	0	-2.486393	4.804423	-8.254449
40	1	0	-2.429274	1.525788	-7.627197
41	1	0	-8.638748	1.741237	0.447869

2a-8		Standard Orientation (A.U.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-9.226381	-2.792575	0.522521
1	6	0	-6.38134	-3.256333	0.596684
2	6	0	-4.724676	-0.82459	0.876395
3	8	0	-5.223198	-0.101227	3.466341
4	6	0	-6.282255	-2.197647	4.848856
5	6	0	-9.133997	-1.812572	5.15463
6	6	0	-10.46004	-2.182427	2.658375
7	6	0	10.558305	-2.989121	-1.986996
8	8	0	-9.693164	-1.165521	-3.732191
9	6	0	-5.815594	-4.506168	3.166426
10	6	0	-1.917654	-1.456648	0.51186
11	6	0	-5.411111	1.45983	-0.813386
12	6	0	-3.579553	3.737152	-0.580264
13	6	0	-1.273999	3.665552	-2.255083
14	6	0	-1.264167	4.01667	-4.772963
15	6	0	1.148665	3.883179	-6.279325
16	6	0	-3.609662	4.551104	-6.298975
17	8	0	-7.912404	2.314756	-0.33319
18	1	0	-5.780008	-4.378985	-1.044595
19	1	0	-5.330021	-2.28937	6.696128
20	1	0	-9.48587	0.107822	5.898629
21	1	0	-9.886717	-3.12754	6.596264
22	1	0	12.506728	-1.875057	2.597792
23	1	0	-10.19066	-4.859744	-2.84151
24	1	0	12.627319	-2.856642	-1.677839
25	1	0	-9.574777	0.413353	-2.7858
26	1	0	-3.868812	-5.200588	3.323528

27	1	0	-7.107416	-6.075447	3.589697
28	1	0	-0.741524	0.015626	1.377268
29	1	0	-1.405477	-3.260127	1.396969
30	1	0	-1.44827	-1.564966	-1.510061
31	1	0	-5.410727	0.787256	-2.780337
32	1	0	-4.745716	5.391236	-1.060804
33	1	0	-3.036753	3.968096	1.415465
34	1	0	0.542657	3.283137	-1.340996
35	1	0	1.027374	2.411977	-7.756523
36	1	0	1.507966	5.683622	-7.274402
37	1	0	2.794468	3.464033	-5.079768
38	1	0	-4.027192	2.964658	-7.590577
39	1	0	-5.295473	4.868194	-5.130706
40	1	0	-3.331818	6.231797	-7.504267
41	1	0	-8.17234	2.157502	1.475493

2a-9		Standard Orientation (A.U.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-8.42391	-3.719656	0.666075
1	6	0	-5.657785	-3.156932	1.192105
2	6	0	-4.947097	-0.356509	0.569123
3	8	0	-6.127196	0.990135	2.640202
4	6	0	-6.758976	-0.73474	4.665358
5	6	0	-9.585318	-1.349915	4.590566
6	6	0	10.199166	-2.935952	2.302175
7	6	0	-9.129745	-4.893448	-1.854387
8	8	0	11.149939	-3.649306	-3.044257
9	6	0	-5.271376	-3.140788	4.069363
10	6	0	-2.076765	0.007213	0.625767
11	6	0	-6.064689	0.751186	-1.919686
12	6	0	-4.981953	3.352266	-2.701897
13	6	0	-2.60512	3.271095	-4.249358
14	6	0	-0.479919	4.633073	-3.965902
15	6	0	1.70796	4.329356	-5.763921
16	6	0	-0.051095	6.52722	-1.884233
17	8	0	-8.732757	0.962402	-1.753854
18	1	0	-4.413382	-4.486164	0.187409
19	1	0	-6.223998	0.178103	6.455595
20	1	0	10.669657	0.43635	4.541778

21	1	0	-10.15561	-2.304269	6.362145
22	1	0	12.190083	-3.279906	1.859347
23	1	0	-7.413699	-4.940285	-3.066382
24	1	0	-9.695365	-6.887697	-1.594514
25	1	0	-10.74165	-1.854928	-2.924517
26	1	0	-3.277987	-2.98519	4.619911
27	1	0	-6.078568	-4.820758	4.984252
28	1	0	-1.215983	-0.984167	2.231466
29	1	0	-1.207092	-0.706843	-1.121438
30	1	0	-1.602081	2.016294	0.800419
31	1	0	-5.669165	-0.61066	-3.44932
32	1	0	-6.493417	4.19682	-3.86539
33	1	0	-4.800152	4.558636	-1.01881
34	1	0	-2.673872	1.951656	-5.85067
35	1	0	2.169918	6.140005	-6.695674
36	1	0	3.433732	3.739208	-4.745992
37	1	0	1.314423	2.922875	-7.243817
38	1	0	1.624847	6.005593	-0.753169
39	1	0	0.345055	8.415953	-2.67932
40	1	0	-1.666263	6.710114	-0.594909
41	1	0	-9.071637	1.433798	-0.010826

Table S3. Gibbs free energies*a* and equilibrium populations*b* of low-energy conformers of **2b**.

Conformers	ΔG(a.u.)	P(%)/100	G(a.u.)
2b-1	0.00297	1.58	-811.351
2b-2	0.00134	8.89	-811.352633
2b-3	0.00215	3.76	-811.35182
2b-4	0.00041	23.73	-811.35356
2b-5	0.00321	1.22	-811.350758
2b-6	0.0	36.72	-811.353972
2b-7	0.00439	0.35	-811.349583
2b-8	0.00583	0.08	-811.348138
2b-9	0.00041	23.68	-811.353558

[a]wB97M-V/def2-TZVP, in a.u.

[b]From ΔG values at 298.15K.

Table S4. Cartesian coordinates for the low-energy reoptimized random reseach conformers of **2b** at B3LYP-D3(BJ)/6-31G* level of theory in methanol.

2b-1		Standard Orientation (A.U.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-6.14889	-4.16875	-1.093238
1	6	0	-7.832317	-3.103384	0.988068
2	6	0	-6.968482	-0.441926	1.95706
3	8	0	-7.924583	1.252877	0.05872
4	6	0	-9.47709	-0.07534	-1.709909
5	6	0	-7.90221	-0.881048	-4.009971
6	6	0	-6.228104	-3.101855	-3.396521
7	6	0	-4.444153	-6.375193	-0.489134
8	8	0	-2.310106	-5.733347	0.981693
9	6	0	10.377008	-2.391599	-0.233966
10	6	0	-8.178199	0.204955	4.504189
11	6	0	-4.073642	-0.124362	2.065643
12	6	0	-3.130661	2.61013	2.340293
13	6	0	-3.429041	4.164153	-0.027922
14	6	0	-1.966118	4.010232	-2.097839
15	6	0	-2.530762	5.563109	-4.416677
16	8	0	-3.234793	-1.660083	4.13856
17	6	0	0.257546	2.246806	-2.343233
18	1	0	-8.008794	-4.446891	2.562504
19	1	0	11.009654	1.209694	-2.282495
20	1	0	-6.755474	0.752499	-4.6213
21	1	0	-9.156523	-1.352175	-5.61593
22	1	0	-5.048186	-3.866326	-4.917165
23	1	0	-5.589181	-7.864736	0.454356
24	1	0	-3.726625	-7.198429	-2.262099
25	1	0	-2.855179	-4.722223	2.422189
26	1	0	11.812957	-1.870136	1.172793
27	1	0	-11.13605	-3.901121	-1.441353
28	1	0	10.223311	-0.15125	4.46204
29	1	0	-7.321932	-0.915284	6.026539
30	1	0	-7.906919	2.221539	4.927872
31	1	0	-3.278332	-0.8843	0.300642
32	1	0	-4.072076	3.531803	3.949574
33	1	0	-1.106979	2.483483	2.848375
34	1	0	-5.056065	5.435024	-0.082334

35	1	0	-2.88736	4.329925	-6.065499
36	1	0	-4.197001	6.777009	-4.148506
37	1	0	-0.910482	6.775671	-4.931909
38	1	0	-1.457166	-1.326997	4.404262
39	1	0	-0.188191	0.678005	-3.647626
40	1	0	1.908271	3.236637	-3.147826
41	1	0	0.836284	1.400113	-0.537581

2b-2		Standard Orientation (A.U.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-7.071529	-4.078423	-0.69176
1	6	0	-7.759884	-2.911406	1.838681
2	6	0	-6.617875	-0.201965	2.213402
3	8	0	-8.378792	1.424368	0.903905
4	6	0	10.458289	-0.020723	-0.042236
5	6	0	-9.92538	-0.923711	-2.751735
6	6	0	-8.073544	-3.092326	-2.804915
7	6	0	-5.361877	-6.374349	-0.693558
8	8	0	-3.627187	-6.445262	1.310379
9	6	0	-10.59547	-2.265143	1.769587
10	6	0	-6.52362	0.500055	5.013419
11	6	0	-4.055109	0.237067	0.911158
12	6	0	-3.124167	2.980579	1.058671
13	6	0	-0.712391	3.369832	-0.416452
14	6	0	-0.519815	3.511898	-2.950135
15	6	0	1.99991	3.837289	-4.233694
16	8	0	-2.236091	-1.447068	1.990555
17	6	0	-2.762617	3.380497	-4.702209
18	1	0	-7.195909	-4.166911	3.38762
19	1	0	12.135448	1.209711	0.000594
20	1	0	-9.205649	0.698461	-3.852679
21	1	0	11.713368	-1.495171	-3.675526
22	1	0	-7.598814	-3.906836	-4.65031
23	1	0	-6.551612	-8.084384	-0.499832
24	1	0	-4.4334	-6.525639	-2.570947
25	1	0	-2.911283	-4.756408	1.525215
26	1	0	11.319987	-1.674735	3.62573
27	1	0	11.755334	-3.837704	1.065131
28	1	0	-8.266047	-0.073784	5.988289

29	1	0	-4.907842	-0.436308	5.926026
30	1	0	-6.326704	2.555757	5.23714
31	1	0	-4.322087	-0.238454	-1.09646
32	1	0	-4.659239	4.190775	0.350864
33	1	0	-2.806795	3.492941	3.048298
34	1	0	1.039737	3.515241	0.682186
35	1	0	3.569007	3.897006	-2.871092
36	1	0	2.360344	2.28097	-5.577989
37	1	0	2.041154	5.598978	-5.353359
38	1	0	-0.610303	-1.013572	1.268133
39	1	0	-4.580919	3.376739	-3.702661
40	1	0	-2.746754	4.993144	-6.02585
41	1	0	-2.676321	1.656418	-5.876091

2b-3		Standard Orientation (A.U.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-6.647948	-4.601236	-0.60097
1	6	0	-8.199065	-2.892637	1.104936
2	6	0	-6.931234	-0.248366	1.568968
3	8	0	-7.662715	1.206625	-0.612475
4	6	0	-9.267884	-0.255314	-2.2205
5	6	0	-7.692916	-1.704415	-4.185625
6	6	0	-6.405791	-3.982205	-3.050268
7	6	0	-5.553927	-6.997327	0.52285
8	8	0	-4.991906	-6.83341	3.109922
9	6	0	10.558433	-2.073392	-0.386725
10	6	0	-7.986695	0.99118	3.955671
11	6	0	-4.012294	-0.301894	1.605969
12	6	0	-2.712765	2.283228	1.896861
13	6	0	-3.052068	4.046802	-0.303723
14	6	0	-1.454876	4.381	-2.250626
15	6	0	-2.083708	6.1941	-4.355832
16	8	0	-3.288898	-1.916338	3.658292
17	6	0	1.025543	3.017304	-2.566456
18	1	0	-8.599946	-3.841978	2.902424
19	1	0	10.567292	1.070083	-3.159657
20	1	0	-6.295477	-0.380542	-4.994522
21	1	0	-8.913263	-2.302393	-5.77595
22	1	0	-5.295857	-5.190421	-4.316384

23	1	0	-6.968685	-8.525803	0.326941
24	1	0	-3.899461	-7.59028	-0.626238
25	1	0	-4.18528	-5.203296	3.419105
26	1	0	-11.93533	-1.065303	0.799189
27	1	0	11.508962	-3.670406	-1.314297
28	1	0	-7.134968	0.135153	5.646522
29	1	0	-7.583915	3.029522	3.953011
30	1	0	10.048807	0.761822	4.058248
31	1	0	-3.386277	-1.131319	-0.198512
32	1	0	-3.37951	3.182297	3.652725
33	1	0	-0.683171	1.889628	2.182767
34	1	0	-4.832741	5.09242	-0.335323
35	1	0	-0.618829	7.671123	-4.541711
36	1	0	-2.157209	5.206136	-6.194515
37	1	0	-3.915459	7.128211	-4.051538
38	1	0	-1.496402	-1.717234	3.948698
39	1	0	2.596928	4.375667	-2.774146
40	1	0	1.48286	1.747818	-0.988566
41	1	0	1.009617	1.871048	-4.311255

2b-4		Standard Orientation (A.U.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-6.250223	-4.066192	0.50482
1	6	0	-7.822038	-2.42378	2.25791
2	6	0	-7.365886	0.459695	1.802143
3	8	0	-8.850961	0.970381	-0.429807
4	6	0	10.387666	-1.170695	-1.058231
5	6	0	-9.066341	-2.797767	-3.063282
6	6	0	-6.87045	-4.232362	-1.949901
7	6	0	-4.002151	-5.400314	1.638952
8	8	0	-2.385423	-6.559522	-0.133201
9	6	0	10.599324	-2.635575	1.42511
10	6	0	-8.317679	2.053701	4.017837
11	6	0	-4.615364	1.124327	1.143619
12	6	0	-4.247621	3.86665	0.261893
13	6	0	-1.590721	4.330451	-0.666496
14	6	0	-0.639342	3.567316	-2.900032
15	6	0	2.069278	4.073818	-3.615408
16	8	0	-3.107951	0.565523	3.298474

17	6	0	-2.169672	2.182756	-4.86572
18	1	0	-7.494862	-2.925162	4.247065
19	1	0	12.204416	-0.449649	-1.771782
20	1	0	-8.4224	-1.547288	-4.606919
21	1	0	-10.43514	-4.122113	-3.92843
22	1	0	-5.756216	-5.455133	-3.190662
23	1	0	-2.989509	-4.026088	2.851141
24	1	0	-4.672214	-6.919316	2.907436
25	1	0	-1.750258	-5.242698	-1.22928
26	1	0	11.894416	-1.694471	2.747855
27	1	0	11.213163	-4.60307	1.168194
28	1	0	-8.521285	4.036792	3.432651
29	1	0	10.175313	1.403446	4.681963
30	1	0	-6.965371	1.953255	5.591309
31	1	0	-4.072802	-0.111005	-0.445012
32	1	0	-5.652697	4.23837	-1.224742
33	1	0	-4.669219	5.152154	1.840955
34	1	0	-0.31557	5.342868	0.616673
35	1	0	2.177205	5.236343	-5.346543
36	1	0	3.104654	5.059642	-2.105754
37	1	0	3.07647	2.295497	-4.04411
38	1	0	-1.388689	1.032931	2.890416
39	1	0	-2.053162	3.16318	-6.70428
40	1	0	-1.401004	0.266786	-5.180227
41	1	0	-4.17198	1.986627	-4.358171

2b-5		Standard Orientation (A.U.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-5.910396	-4.092365	0.243289
1	6	0	-8.083142	-2.570999	1.362991
2	6	0	-7.567772	0.343363	1.394024
3	8	0	-8.161755	1.121856	-1.140148
4	6	0	-9.174779	-0.949858	-2.552447
5	6	0	-7.055333	-2.314832	-3.991979
6	6	0	-5.495276	-3.948736	-2.258232
7	6	0	-4.238913	-5.651536	1.966385
8	8	0	-2.235624	-4.296145	3.090125
9	6	0	10.296162	-2.676913	-0.52492
10	6	0	-9.350517	1.716251	3.217824

11	6	0	-4.776424	1.005936	1.935028
12	6	0	-3.985846	3.740134	1.357643
13	6	0	-3.81295	4.306784	-1.429376
14	6	0	-1.952496	3.537295	-2.976675
15	6	0	-2.039544	4.088013	-5.7685
16	8	0	-4.158947	0.309556	4.474363
17	6	0	0.290994	2.004114	-2.121166
18	1	0	-8.567222	-3.26641	3.259132
19	1	0	10.578495	-0.17145	-3.875578
20	1	0	-5.853953	-0.869388	-4.900197
21	1	0	-7.857515	-3.469299	-5.540118
22	1	0	-3.956538	-5.048747	-3.101692
23	1	0	-5.443155	-6.580197	3.415899
24	1	0	-3.360004	-7.173922	0.849965
25	1	0	-2.918746	-2.901419	4.077976
26	1	0	12.046264	-1.875322	0.257002
27	1	0	10.683152	-4.603101	-1.197394
28	1	0	-9.209088	3.773777	2.957373
29	1	0	-11.32411	1.181028	2.859979
30	1	0	-8.92438	1.251633	5.201151
31	1	0	-3.592491	-0.234134	0.774904
32	1	0	-5.283039	5.083176	2.284062
33	1	0	-2.129745	3.987898	2.270979
34	1	0	-5.406135	5.327529	-2.258626
35	1	0	-2.05366	2.314171	-6.87317
36	1	0	-3.725924	5.185904	-6.291477
37	1	0	-0.34907	5.146812	-6.386552
38	1	0	-4.96325	1.45832	5.642563
39	1	0	2.066498	2.804314	-2.869724
40	1	0	0.46483	1.873621	-0.056745
41	1	0	0.166225	0.052172	-2.853353

2b-6		Standard Orientation (A.U.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-7.19793	-4.337134	-0.039658
1	6	0	-8.272085	-2.266398	1.630669
2	6	0	-7.489228	0.436148	0.725273
3	8	0	-9.203913	0.92881	-1.335067
4	6	0	11.067237	-1.026878	-1.500483

5	6	0	10.240431	-3.048895	-3.411538
6	6	0	-8.139386	-4.669805	-2.372041
7	6	0	-5.047837	-5.883527	1.010289
8	8	0	-4.245464	-7.887277	-0.54355
9	6	0	11.140264	-2.144757	1.163968
10	6	0	-7.872961	2.394245	2.817994
11	6	0	-4.792385	0.57222	-0.356501
12	6	0	-4.120979	3.151893	-1.520792
13	6	0	-1.486641	3.122293	-2.58305
14	6	0	0.64171	3.930419	-1.439277
15	6	0	3.174882	3.723294	-2.727003
16	8	0	-3.102655	-0.058384	1.632721
17	6	0	0.71467	5.146834	1.138695
18	1	0	-7.750562	-2.560496	3.618947
19	1	0	12.853781	-0.140186	-2.093577
20	1	0	-9.622309	-2.085054	-5.157038
21	1	0	11.876456	-4.234385	-3.955153
22	1	0	-7.330396	-6.130947	-3.591319
23	1	0	-3.414273	-4.621506	1.292625
24	1	0	-5.582354	-6.550194	2.931
25	1	0	-5.668042	-9.010993	-0.772059
26	1	0	12.102712	-0.866454	2.488327
27	1	0	12.049382	-4.010417	1.251384
28	1	0	-6.31221	2.284492	4.184666
29	1	0	-7.930342	4.304977	2.004942
30	1	0	-9.66643	2.089163	3.82078
31	1	0	-4.680769	-0.853014	-1.87764
32	1	0	-5.509216	3.541869	-3.01941
33	1	0	-4.325609	4.636459	-0.082895
34	1	0	-1.284843	2.25511	-4.456093
35	1	0	4.510839	2.60218	-1.579725
36	1	0	3.029003	2.840974	-4.603636
37	1	0	4.04348	5.607883	-2.95956
38	1	0	-1.409787	0.227478	0.994847
39	1	0	-1.121571	5.139132	2.100382
40	1	0	2.080319	4.16307	2.372427
41	1	0	1.378826	7.121039	0.995044

2b-7		Standard Orientation (A.U.)			
Center	Atomic	Atomic	X	Y	Z

number	number	Type			
0	6	0	-8.106402	-4.200343	-0.271989
1	6	0	-7.453496	-2.714502	2.107587
2	6	0	-6.470579	0.019224	1.558272
3	8	0	-8.751759	1.410284	1.030454
4	6	0	10.929636	-0.099987	1.594214
5	6	0	11.890453	-1.403639	-0.811553
6	6	0	10.198104	-3.565759	-1.566134
7	6	0	-6.367101	-6.288817	-1.186192
8	8	0	-4.489276	-5.48968	-2.901894
9	6	0	-9.948617	-2.074547	3.463439
10	6	0	-5.165974	1.153065	3.878558
11	6	0	-4.795496	0.170303	-0.82097
12	6	0	-4.099067	2.879527	-1.679336
13	6	0	-1.807187	3.974419	-0.394637
14	6	0	0.618242	3.712347	-1.137846
15	6	0	2.740881	4.915152	0.334126
16	8	0	-2.602884	-1.356906	-0.490308
17	6	0	1.437483	2.302153	-3.476147
18	1	0	-6.104801	-3.765457	3.286121
19	1	0	-12.38312	1.163655	2.381593
20	1	0	11.980995	0.017055	-2.338858
21	1	0	13.849968	-2.080913	-0.533313
22	1	0	10.709647	-4.637969	-3.262669
23	1	0	-5.527649	-7.251709	0.479818
24	1	0	-7.50853	-7.711589	-2.192408
25	1	0	-3.383948	-4.293131	-2.043646
26	1	0	-9.643057	-1.246084	5.343127
27	1	0	11.200667	-3.720267	3.653756
28	1	0	-3.239923	0.400984	4.091815
29	1	0	-5.06826	3.218667	3.700834
30	1	0	-6.217436	0.729731	5.618886
31	1	0	-5.875648	-0.711686	-2.355412
32	1	0	-3.792896	2.819652	-3.734786
33	1	0	-5.766476	4.075334	-1.352866
34	1	0	-2.142212	5.063029	1.33266
35	1	0	3.785541	6.275534	-0.855991
36	1	0	2.051923	5.919975	2.018322
37	1	0	4.13277	3.485597	0.946508
38	1	0	-1.246536	-0.283436	0.120916
39	1	0	2.397062	3.599968	-4.799911

40	1	0	2.833032	0.828352	-2.992667
41	1	0	-0.127138	1.379812	-4.474348

2b-8		Standard Orientation (A.U.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-7.464709	-3.649798	-1.399568
1	6	0	-7.695367	-3.197858	1.439567
2	6	0	-6.696385	-0.547531	2.291826
3	8	0	-8.716036	1.133459	1.573781
4	6	0	10.903693	-0.279025	0.831236
5	6	0	10.974895	-0.539781	-2.055474
6	6	0	-9.029381	-2.407317	-2.968655
7	6	0	-5.465467	-5.437549	-2.39107
8	8	0	-3.024185	-4.365497	-2.581677
9	6	0	10.522257	-2.872368	2.050517
10	6	0	-6.274194	-0.427177	5.149643
11	6	0	-4.335172	0.300324	0.836295
12	6	0	-3.607159	3.086875	1.17208
13	6	0	-1.041181	3.666181	0.045342
14	6	0	-0.323119	3.299132	-2.372192
15	6	0	2.339384	3.855517	-3.212986
16	8	0	-2.307654	-1.341094	1.566395
17	6	0	-2.064835	2.302612	-4.404168
18	1	0	-6.777482	-4.722686	2.510337
19	1	0	-12.57954	0.741484	1.523709
20	1	0	10.629744	1.339905	-2.895982
21	1	0	12.884353	-1.115013	-2.686814
22	1	0	-8.904082	-2.744085	-5.00834
23	1	0	-5.432911	-7.15581	-1.184663
24	1	0	-5.993907	-6.052593	-4.30855
25	1	0	-2.56378	-3.663406	-0.935339
26	1	0	10.887876	-2.807365	4.093306
27	1	0	11.702735	-4.358572	1.207631
28	1	0	-4.526296	-1.427237	5.656316
29	1	0	-6.113935	1.552628	5.75974
30	1	0	-7.862037	-1.271365	6.187674
31	1	0	-4.74783	-0.005391	-1.172204
32	1	0	-5.117725	4.224775	0.297888
33	1	0	-3.583584	3.583173	3.190195

34	1	0	0.382436	4.413166	1.351591
35	1	0	3.212619	2.164882	-4.071715
36	1	0	2.353031	5.332349	-4.688395
37	1	0	3.545413	4.488665	-1.642258
38	1	0	-0.756461	-0.490627	1.071509
39	1	0	-2.036012	0.215557	-4.461875
40	1	0	-4.038706	2.879055	-4.097722
41	1	0	-1.476991	2.985972	-6.280307

2b-9		Standard Orientation (A.U.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-7.452302	-4.522198	0.741281
1	6	0	-7.878734	-2.055161	2.171093
2	6	0	-6.049653	0.140838	1.398219
3	8	0	-7.076371	0.964021	-0.989762
4	6	0	-9.49127	-0.148384	-1.427459
5	6	0	-9.195521	-2.468113	-3.146355
6	6	0	-8.091907	-4.663697	-1.715342
7	6	0	-6.414702	-6.788969	2.113097
8	8	0	-3.761891	-6.631072	2.62284
9	6	0	10.395467	-0.9578	1.198922
10	6	0	-6.142946	2.304891	3.314745
11	6	0	-3.280717	-0.714847	0.99398
12	6	0	-1.453477	1.377861	0.151595
13	6	0	-2.084335	2.650072	-2.298153
14	6	0	-2.304909	5.13585	-2.76081
15	6	0	-2.986404	6.08317	-5.359448
16	8	0	-2.296653	-1.701893	3.270816
17	6	0	-1.975661	7.183875	-0.80982
18	1	0	-7.833454	-2.373483	4.22208
19	1	0	-10.70667	1.280166	-2.329808
20	1	0	-7.968681	-1.945151	-4.7516
21	1	0	11.037006	-3.01728	-3.972019
22	1	0	-7.868838	-6.45845	-2.727859
23	1	0	-7.313681	-6.978857	3.981631
24	1	0	-6.831719	-8.526733	1.034002
25	1	0	-2.881736	-6.673829	1.019374
26	1	0	11.026212	0.675292	2.312899
27	1	0	11.924286	-2.363489	1.148067

28	1	0	-8.082434	2.713318	3.936255
29	1	0	-4.991206	1.819154	4.974345
30	1	0	-5.388225	4.031956	2.445495
31	1	0	-3.327361	-2.169185	-0.51008
32	1	0	-1.252191	2.73739	1.708275
33	1	0	0.401938	0.430166	-0.003573
34	1	0	-2.412478	1.362488	-3.888894
35	1	0	-4.784256	7.146543	-5.311523
36	1	0	-1.541833	7.402398	-6.091687
37	1	0	-3.197298	4.526776	-6.722107
38	1	0	-2.826441	-3.4607	3.424114
39	1	0	-1.425062	6.462562	1.055984
40	1	0	-0.522822	8.555469	-1.415524
41	1	0	-3.746805	8.267813	-0.583848

Table S5. DP4+ analysis of compound **2.**

Default parameters	2a	2b
sDP4+ (H data)		
sDP4+ (C data)	13.39%	86.61%
sDP4+ (all data)	13.39%	86.61%
uDP4+ (H data)		
uDP4+ (C data)	0.35%	99.65%
uDP4+ (all data)	0.35%	99.65%
DP4+(H data)		
DP4+(C data)	0.05%	99.95%
DP4+(all data)	0.05%	99.95%

ECD calculation of compound 2.

In general, conformational analyses were carried out via random searching in the Sybyl-X 2.0 using the MMFF94S force field with an energy cutoff of 5 kcal/mol.[1] The results showed five lowest energy conformer for both compounds. Subsequently, geometry optimizations and frequency analyses were implemented at the B3LYP-D3(BJ)/6-31G* level in PCM methanol using ORCA5.0.1[2] All conformers used for property calculations in this work were characterized to be stable point on potential energy surface (PES) with no imaginary frequencies. The excitation energies, oscillator strengths, and rotational strengths (velocity) of the first 60 excited states were calculated using the TD-DFT methodology at the PBE0/def2-TZVP level in PCM methanol using ORCA5.0.1.[2] The ECD spectra were simulated by the overlapping Gaussian function (half the bandwidth at 1/e peak height, sigma = 0.30 for all).[3] Gibbs free energies for conformers were determined by using thermal correction at B3LYP-D3(BJ)/6-31G* level and electronic energies evaluated at the wB97M-V/def2-TZVP level in PCM methanol using ORCA5.0.1[2] To get the final spectra, the simulated spectra of the conformers were averaged according to the boltzmann distribution theory and their relative Gibbs free energy (ΔG). By comparing the experiment spectra with the calculated model molecules, the absolute configuration of the only chiral center was determined to be .

[1].Sybyl Software, version X 2.0; Tripos Associates Inc.: St. Louis, MO, 2013.
[2]. Neese, F. (2012) The ORCA program system, Wiley Interdiscip. Rev.: Comput. Mol. Sci., 2, 73-78.
[3]. Stephens, P. J.; Harada, N. ECD cotton effect approximated by the Gaussian curve and other methods. Chirality2010, 22, 229–233.

Table S6. Gibbs free energies[a] and equilibrium populations[b] of low-energy conformers of **2**.

Conformers	ΔG(a.u.)	P(%)/100	G(a.u.)
2-1	0.0	51.74	-811.354315
2-2	0.00146	11.01	-811.352854
2-3	0.00109	16.34	-811.353227
2-4	0.00201	6.15	-811.352304

2-5	0.00118	14.77	-811.353131

[a]wB97M-V/def2-TZVP, in a.u.

[b]From ΔG values at 298.15K.

Table S7. Cartesian coordinates for the low-energy reoptimized random reseach conformers of **2** at B3LYP-D3(BJ)/6-31G* level of theory in methanol.

2-1		Standard Orientation (A.U.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-3.451424	-4.28097	-1.985013
1	6	0	-2.512605	-3.343563	0.565469
2	6	0	-0.391181	-1.287087	0.434259
3	8	0	-1.778295	1.008931	-0.157312
4	6	0	-4.445459	0.538799	-0.051916
5	6	0	-5.4307	-0.072289	-2.708532
6	6	0	-4.790825	-2.727535	-3.464158
7	6	0	-3.190635	-7.016274	-2.650718
8	8	0	-0.567926	-7.673001	-3.014321
9	6	0	-4.683563	-1.753264	1.682842
10	6	0	0.918873	-0.986963	2.987479
11	6	0	1.577757	-1.72723	-1.675801
12	6	0	3.676157	0.271714	-1.815274
13	6	0	2.805963	2.922791	-2.259316
14	6	0	3.440756	5.003983	-0.976811
15	6	0	2.358828	7.535105	-1.687191
16	8	0	2.852501	-4.062765	-1.266044
17	6	0	5.189832	5.077081	1.260169
18	1	0	-1.924079	-4.922217	1.766336
19	1	0	-5.354327	2.247376	0.688951
20	1	0	-4.615895	1.297243	-4.039541
21	1	0	-7.494868	0.183711	-2.799735
22	1	0	-5.544027	-3.421121	-5.250875
23	1	0	-3.9794	-8.164962	-1.101839
24	1	0	-4.263386	-7.426877	-4.381303
25	1	0	-0.378273	-9.475903	-2.851873
26	1	0	-4.340451	-1.220465	3.649045
27	1	0	-6.51447	-2.703838	1.543967
28	1	0	-0.426752	-1.050963	4.554122
29	1	0	2.31556	-2.491322	3.242799
30	1	0	1.876038	0.843105	3.053061

31	1	0	0.545023	-1.746035	-3.486043
32	1	0	4.842464	0.100006	-0.117074
33	1	0	4.886107	-0.330944	-3.394186
34	1	0	1.49252	3.152226	-3.830843
35	1	0	1.09807	7.39686	-3.318331
36	1	0	1.282861	8.339492	-0.104492
37	1	0	3.860301	8.89629	-2.135476
38	1	0	1.750436	-5.423946	-1.817902
39	1	0	6.776621	6.364052	0.897684
40	1	0	4.200095	5.822019	2.92626
41	1	0	5.974377	3.233615	1.750209

2-2		Standard Orientation (A.U.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-2.518234	-3.927905	-2.07401
1	6	0	-2.478698	-3.482238	0.757192
2	6	0	-0.645994	-1.310653	1.544258
3	8	0	-2.082731	0.962404	1.035246
4	6	0	-4.621068	0.304778	0.295034
5	6	0	-4.801105	0.154102	-2.592316
6	6	0	-3.638661	-2.240026	-3.582876
7	6	0	-1.290353	-6.266351	-3.077924
8	8	0	-2.477097	-8.427393	-1.924815
9	6	0	-5.033001	-2.29392	1.469768
10	6	0	-0.044836	-1.417117	4.368539
11	6	0	1.784375	-1.214601	-0.064455
12	6	0	3.51496	1.076415	0.392477
13	6	0	2.452761	3.559427	-0.488676
14	6	0	2.549921	4.450532	-2.850994
15	6	0	1.357547	6.938511	-3.528464
16	8	0	3.178887	-3.525761	0.24947
17	6	0	3.753674	3.081614	-5.029248
18	1	0	-2.062501	-5.238828	1.759315
19	1	0	-5.873095	1.78028	1.033739
20	1	0	-3.841166	1.815985	-3.389901
21	1	0	-6.789381	0.275035	-3.195127
22	1	0	-3.731344	-2.585367	-5.611069
23	1	0	-1.493602	-6.334827	-5.147627
24	1	0	0.73427	-6.229389	-2.604423

25	1	0	-1.323588	-9.828409	-2.047434
26	1	0	-5.300243	-2.150025	3.514329
27	1	0	-6.624993	-3.32199	0.646455
28	1	0	-1.765163	-1.68498	5.478507
29	1	0	1.230932	-2.988009	4.807523
30	1	0	0.823804	0.353665	4.98641
31	1	0	1.207583	-1.184665	-2.052917
32	1	0	3.996759	1.195281	2.408543
33	1	0	5.283096	0.65155	-0.601538
34	1	0	1.454094	4.673884	0.919484
35	1	0	-0.103764	6.684967	-4.98106
36	1	0	0.485705	7.839858	-1.88671
37	1	0	2.760476	8.243863	-4.324868
38	1	0	4.1255	-3.404132	1.801758
39	1	0	2.31759	2.59057	-6.445708
40	1	0	5.132863	4.299314	-5.987513
41	1	0	4.705179	1.337351	-4.471849

2-3		Standard Orientation (A.U.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-2.517784	-4.109378	-2.057611
1	6	0	-2.509243	-3.547448	0.75233
2	6	0	-0.681838	-1.344546	1.46435
3	8	0	-2.122352	0.908322	0.868211
4	6	0	-4.647049	0.218721	0.120789
5	6	0	-4.791593	-0.046519	-2.761787
6	6	0	-3.617897	-2.477051	-3.645116
7	6	0	-1.376158	-6.545612	-2.940389
8	8	0	-2.682985	-8.690519	-1.899461
9	6	0	-5.068364	-2.329389	1.398117
10	6	0	-0.090819	-1.346535	4.291482
11	6	0	1.753332	-1.303423	-0.14029
12	6	0	3.530327	0.951579	0.315237
13	6	0	2.493551	3.464307	-0.505889
14	6	0	2.593758	4.411911	-2.845931
15	6	0	1.424391	6.927333	-3.457424
16	8	0	3.097982	-3.639332	0.182517
17	6	0	3.78119	3.088229	-5.060013
18	1	0	-2.096341	-5.259744	1.832133

19	1	0	-5.91071	1.720265	0.783294
20	1	0	-3.819108	1.582615	-3.609705
21	1	0	-6.771375	0.05662	-3.395734
22	1	0	-3.672401	-2.893047	-5.662451
23	1	0	-1.365006	-6.618719	-5.020234
24	1	0	0.571944	-6.715376	-2.264329
25	1	0	-4.431484	-8.534034	-2.389857
26	1	0	-5.349245	-2.098321	3.43292
27	1	0	-6.661049	-3.384826	0.609688
28	1	0	-1.808022	-1.615572	5.406408
29	1	0	1.219096	-2.872256	4.786222
30	1	0	0.738088	0.462091	4.85074
31	1	0	1.180182	-1.269021	-2.129831
32	1	0	4.050176	1.028607	2.324372
33	1	0	5.273401	0.5107	-0.714633
34	1	0	1.507909	4.556196	0.929511
35	1	0	-0.04389	6.724395	-4.910866
36	1	0	0.566775	7.796089	-1.790872
37	1	0	2.837058	8.238478	-4.226484
38	1	0	4.050953	-3.534539	1.732115
39	1	0	2.343806	2.667787	-6.497617
40	1	0	5.186964	4.30874	-5.975266
41	1	0	4.698031	1.310101	-4.554352

2-4		Standard Orientation (A.U.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-3.377501	-3.937529	-1.289954
1	6	0	-2.221069	-3.350178	1.273618
2	6	0	0.120366	-1.553566	1.156339
3	8	0	-0.985854	0.935526	0.918266
4	6	0	-3.692498	0.766984	1.13501
5	6	0	-4.886151	0.521646	-1.493436
6	6	0	-4.612568	-2.109955	-2.523325
7	6	0	-3.200687	-6.588438	-2.291252
8	8	0	-0.722413	-7.290973	-3.107354
9	6	0	-4.109772	-1.633193	2.673871
10	6	0	1.648148	-1.68008	3.605132
11	6	0	1.816889	-1.957978	-1.173682
12	6	0	3.697982	0.203817	-1.699194

13	6	0	2.640115	2.18186	-3.43286
14	6	0	2.128026	4.59972	-2.917177
15	6	0	1.041145	6.311899	-4.908758
16	8	0	3.112687	-4.323632	-0.721204
17	6	0	2.487337	5.831298	-0.389174
18	1	0	-1.767166	-5.089935	2.299602
19	1	0	-4.337385	2.495107	2.077907
20	1	0	-3.96968	1.897683	-2.752265
21	1	0	-6.900194	1.040759	-1.419084
22	1	0	-5.499861	-2.52566	-4.334427
23	1	0	-3.871154	-7.913014	-0.821265
24	1	0	-4.437764	-6.801407	-3.937478
25	1	0	0.49094	-6.682032	-1.870196
26	1	0	-3.598073	-1.339066	4.654503
27	1	0	-6.045278	-2.349256	2.568886
28	1	0	3.020554	-0.1373	3.674621
29	1	0	0.407558	-1.476477	5.243115
30	1	0	2.663757	-3.471874	3.747738
31	1	0	0.585036	-2.164233	-2.835285
32	1	0	4.408038	1.007818	0.064781
33	1	0	5.346564	-0.65379	-2.6365
34	1	0	2.233082	1.513097	-5.342151
35	1	0	2.263553	7.959218	-5.218827
36	1	0	0.793815	5.337637	-6.714027
37	1	0	-0.802736	7.052684	-4.308245
38	1	0	4.195098	-4.635014	-2.155041
39	1	0	0.65656	6.47609	0.341751
40	1	0	3.306325	4.578231	1.026559
41	1	0	3.692647	7.51077	-0.564108

2-5		Standard Orientation (A.U.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-2.282561	-4.472228	-1.50266
1	6	0	-2.083165	-3.785	1.272448
2	6	0	-0.504111	-1.338551	1.765732
3	8	0	-2.271744	0.68284	1.251239
4	6	0	-4.735545	-0.35229	0.732051
5	6	0	-5.077463	-0.744856	-2.117629
6	6	0	-3.696549	-3.051935	-3.037325

7	6	0	-0.909107	-6.814369	-2.335656
8	8	0	-0.945045	-7.264329	-4.986419
9	6	0	-4.716097	-2.88112	2.113436
10	6	0	0.350379	-1.182005	4.518289
11	6	0	1.741761	-1.028524	-0.056694
12	6	0	3.246587	1.445633	0.213422
13	6	0	1.814436	3.774932	-0.550173
14	6	0	1.534448	4.643713	-2.905846
15	6	0	-0.014184	6.964048	-3.439717
16	8	0	3.348676	-3.169554	0.409903
17	6	0	2.632764	3.401256	-5.211877
18	1	0	-1.342151	-5.368042	2.381121
19	1	0	-6.125129	0.999165	1.461615
20	1	0	-4.396117	0.962248	-3.087545
21	1	0	-7.101004	-0.909846	-2.575797
22	1	0	-3.926855	-3.595959	-5.007336
23	1	0	1.036414	-6.740067	-1.597898
24	1	0	-1.813112	-8.474267	-1.471984
25	1	0	-0.109077	-5.857015	-5.787461
26	1	0	-4.848263	-2.606604	4.158246
27	1	0	-6.216219	-4.162392	1.497206
28	1	0	-1.180975	-1.718283	5.796535
29	1	0	1.96357	-2.432466	4.844453
30	1	0	0.897273	0.756543	4.980644
31	1	0	0.977831	-1.101957	-1.991314
32	1	0	3.936213	1.61892	2.1583
33	1	0	4.937465	1.24091	-0.977215
34	1	0	0.856958	4.783404	0.962876
35	1	0	-1.584983	6.523506	-4.723427
36	1	0	-0.80257	7.770237	-1.70894
37	1	0	1.125786	8.420468	-4.380859
38	1	0	4.860265	-2.963593	-0.58446
39	1	0	1.113279	2.680723	-6.429308
40	1	0	3.698592	4.77042	-6.348559
41	1	0	3.884087	1.820249	-4.768668

Table S8. Gibbs free energies[a] and equilibrium populations[b] of low-energy conformers of **2**.

Conformers	ΔG(a.u.)	P(%)/100	G(a.u.)
2-1	0.00158	7.63	-811.348233

2-2	0.00011	36.29	-811.349705
2-3	0.0	40.86	-811.349817
2-4	0.00253	2.8	-811.347285
2-5	0.00113	12.42	-811.348692

[a]wB97M-V/def2-TZVP, in a.u.

[b]From ΔG values at 298.15K.

Table S9. Cartesian coordinates for the low-energy reoptimized random reseach conformers of **2** at B3LYP-D3(BJ)/6-31G* level of theory in methanol.

2-1		Standard Orientation (A.U.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	5.065989	-4.105995	-0.440487
1	6	0	6.643684	-2.476978	1.325827
2	6	0	7.784537	-0.04562	0.108788
3	8	0	5.558636	1.534427	-0.223694
4	6	0	3.508504	0.586924	1.332182
5	6	0	1.640961	-0.858679	-0.32947
6	6	0	2.755854	-3.345931	-1.140468
7	6	0	6.141349	-6.599001	-1.268143
8	8	0	8.500121	-6.331596	-2.540964
9	6	0	4.762827	-1.246181	3.175857
10	6	0	9.660317	1.210746	1.922552
11	6	0	9.07209	-0.303325	-2.497578
12	6	0	10.093256	2.225926	-3.556925
13	6	0	12.758865	2.841132	-2.820087
14	6	0	13.685071	5.021921	-1.940757
15	6	0	16.455848	5.311139	-1.376717
16	8	0	7.44361	-1.418635	-4.34966
17	6	0	12.13607	7.341518	-1.408825
18	1	0	8.120278	-3.606358	2.235013
19	1	0	2.609463	2.215857	2.24167
20	1	0	1.153695	0.30786	-1.979077
21	1	0	-0.141617	-1.164699	0.700691
22	1	0	1.621428	-4.552816	-2.363976
23	1	0	6.522979	-7.78394	0.394926
24	1	0	4.747691	-7.603316	-2.44687
25	1	0	8.243656	-4.978641	-3.757753
26	1	0	5.679434	-0.258388	4.737646
27	1	0	3.425701	-2.61746	3.951947
28	1	0	8.991897	1.171965	3.872527

29	1	0	11.493146	0.252256	1.847796
30	1	0	9.956547	3.179014	1.385828
31	1	0	10.652062	-1.631686	-2.264936
32	1	0	10.040403	1.985135	-5.617864
33	1	0	8.765884	3.747735	-3.111342
34	1	0	14.100027	1.299682	-3.116411
35	1	0	17.278467	6.863148	-2.481046
36	1	0	16.754157	5.78648	0.621521
37	1	0	17.511272	3.58601	-1.798961
38	1	0	5.744863	-0.857196	-3.970065
39	1	0	12.415082	7.957958	0.5532
40	1	0	12.756316	8.915458	-2.609772
41	1	0	10.114928	7.068988	-1.717157

2-2		Standard Orientation (A.U.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	7.055117	-3.990425	1.068385
1	6	0	7.593779	-1.472262	2.340946
2	6	0	7.384144	0.825859	0.516944
3	8	0	4.652166	1.154338	0.265792
4	6	0	3.359838	-0.377551	2.116584
5	6	0	2.492512	-2.850623	0.897702
6	6	0	4.68523	-4.598375	0.442598
7	6	0	9.263684	-5.731919	0.642468
8	8	0	8.616306	-8.200618	-0.18
9	6	0	5.364153	-0.916047	4.121728
10	6	0	8.489751	3.235945	1.656176
11	6	0	8.352848	0.340607	-2.186887
12	6	0	11.25178	0.212659	-2.482426
13	6	0	12.660338	2.682183	-2.556448
14	6	0	13.098735	4.099271	-4.602416
15	6	0	14.560006	6.528354	-4.403607
16	8	0	7.432204	2.238647	-3.85888
17	6	0	12.187272	3.483666	-7.215823
18	1	0	9.426242	-1.498085	3.3048
19	1	0	1.745681	0.71743	2.814932
20	1	0	1.534758	-2.410756	-0.891375
21	1	0	1.07228	-3.780419	2.102803
22	1	0	4.305878	-6.399231	-0.474594

23	1	0	10.502754	-4.960521	-0.834074
24	1	0	10.409952	-5.798566	2.388407
25	1	0	7.535771	-8.935777	1.090923
26	1	0	5.710213	0.732986	5.315578
27	1	0	4.884724	-2.532982	5.316839
28	1	0	8.439375	4.750781	0.252392
29	1	0	7.397635	3.834596	3.302426
30	1	0	10.452481	2.950744	2.239057
31	1	0	7.5825	-1.508734	-2.753771
32	1	0	12.001528	-0.944419	-0.93262
33	1	0	11.623128	-0.848143	-4.221852
34	1	0	13.415593	3.364405	-0.768809
35	1	0	13.409159	8.127923	-5.053515
36	1	0	15.164682	6.909618	-2.464677
37	1	0	16.243374	6.480753	-5.615668
38	1	0	5.626262	2.300488	-3.593131
39	1	0	11.263369	1.646536	-7.34105
40	1	0	10.802357	4.900591	-7.826247
41	1	0	13.760409	3.549807	-8.566785

2-3		Standard Orientation (A.U.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	6.632905	-4.192691	-0.041029
1	6	0	7.543192	-2.127427	1.734342
2	6	0	7.430771	0.553801	0.535779
3	8	0	4.727096	1.13758	0.617678
4	6	0	3.438527	-0.663789	2.209388
5	6	0	2.206488	-2.695953	0.56138
6	6	0	4.160841	-4.453817	-0.507809
7	6	0	8.542508	-5.976098	-1.14079
8	8	0	9.984167	-7.239742	0.777634
9	6	0	5.533218	-1.83489	3.8137
10	6	0	8.838072	2.521783	2.108843
11	6	0	8.152823	0.675422	-2.283986
12	6	0	10.994766	0.416338	-2.879751
13	6	0	12.636867	2.691533	-2.419591
14	6	0	13.056442	4.595666	-4.02722
15	6	0	14.769737	6.74805	-3.314219
16	8	0	7.286877	2.983669	-3.365411

17	6	0	11.887545	4.824927	-6.600369
18	1	0	9.426014	-2.575847	2.460086
19	1	0	2.016202	0.3699	3.30523
20	1	0	1.152599	-1.767819	-0.968479
21	1	0	0.805496	-3.769204	1.665255
22	1	0	3.512856	-5.980906	-1.729243
23	1	0	7.594558	-7.342305	-2.391698
24	1	0	9.947014	-4.960237	-2.276879
25	1	0	8.795769	-8.108154	1.85299
26	1	0	6.143747	-0.563518	5.321584
27	1	0	4.981413	-3.647987	4.639503
28	1	0	10.789634	1.935258	2.453495
29	1	0	8.867277	4.325124	1.101212
30	1	0	7.910337	2.809679	3.930208
31	1	0	7.178712	-0.921536	-3.200383
32	1	0	11.733459	-1.180868	-1.783073
33	1	0	11.127171	-0.139273	-4.871246
34	1	0	13.600942	2.771826	-0.604185
35	1	0	13.744897	8.551064	-3.384831
36	1	0	15.54856	6.518061	-1.413967
37	1	0	16.347436	6.913872	-4.651615
38	1	0	5.528052	3.124114	-2.892715
39	1	0	10.809194	3.158862	-7.154246
40	1	0	10.576503	6.430781	-6.635062
41	1	0	13.347065	5.199852	-8.026296

2-4		Standard Orientation (A.U.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	5.679124	-4.080508	-1.317633
1	6	0	7.253921	-2.830523	0.730437
2	6	0	8.115862	-0.097506	0.063246
3	8	0	5.769377	1.322814	0.299497
4	6	0	3.926846	-0.156574	1.694304
5	6	0	2.031801	-1.340527	-0.138461
6	6	0	3.249333	-3.445673	-1.614441
7	6	0	6.930757	-6.044936	-2.921219
8	8	0	7.86664	-8.128021	-1.449645
9	6	0	5.459456	-2.256089	2.943375
10	6	0	10.072294	0.845112	1.973507

11	6	0	9.131921	0.34074	-2.644506
12	6	0	10.08127	3.072175	-3.11827
13	6	0	12.806092	3.52516	-2.491261
14	6	0	13.833503	5.425649	-1.179947
15	6	0	16.646444	5.588889	-0.805209
16	8	0	7.31288	-0.29327	-4.516441
17	6	0	12.368258	7.523194	0.05121
18	1	0	8.859313	-4.03011	1.24462
19	1	0	2.987521	1.119244	3.028061
20	1	0	1.31986	0.130269	-1.423839
21	1	0	0.371845	-2.033843	0.908523
22	1	0	2.121378	-4.383633	-3.059699
23	1	0	5.630091	-6.69857	-4.406541
24	1	0	8.594334	-5.238681	-3.855426
25	1	0	6.440845	-8.83063	-0.558282
26	1	0	6.437627	-1.596312	4.635575
27	1	0	4.293119	-3.887466	3.443199
28	1	0	10.194796	2.902419	1.913283
29	1	0	9.59605	0.288195	3.901273
30	1	0	11.944659	0.087718	1.52332
31	1	0	10.722987	-0.971069	-2.921145
32	1	0	9.839666	3.351783	-5.160723
33	1	0	8.808665	4.412298	-2.188631
34	1	0	14.100038	2.124558	-3.283928
35	1	0	17.124461	5.540942	1.214244
36	1	0	17.638607	4.038424	-1.743356
37	1	0	17.391075	7.37874	-1.544459
38	1	0	5.705723	0.299348	-3.877427
39	1	0	12.947033	9.358791	-0.722913
40	1	0	10.326853	7.352095	-0.188912
41	1	0	12.77895	7.591025	2.084787

2-5		Standard Orientation (A.U.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	6.659035	-4.251171	-1.138329
1	6	0	7.671242	-2.528249	0.930366
2	6	0	7.135504	0.346003	0.558431
3	8	0	4.477153	0.585026	1.293497
4	6	0	3.604443	-1.750005	2.380413

5	6	0	2.283495	-3.339358	0.351919
6	6	0	4.162992	-4.593415	-1.363089
7	6	0	8.483892	-5.794476	-2.668211
8	8	0	10.243341	-4.334084	-4.116624
9	6	0	6.020631	-3.04839	3.276978
10	6	0	8.714325	1.966004	2.344598
11	6	0	7.242108	1.321857	-2.189208
12	6	0	9.898498	1.668074	-3.305618
13	6	0	11.290545	4.006437	-2.514199
14	6	0	13.685565	4.162679	-1.721276
15	6	0	14.840787	6.678501	-1.072294
16	8	0	5.959922	3.685145	-2.38539
17	6	0	15.433256	1.952453	-1.355007
18	1	0	9.689606	-2.862218	1.236626
19	1	0	2.292732	-1.271997	3.911084
20	1	0	0.994376	-2.111942	-0.717707
21	1	0	1.091209	-4.793632	1.244211
22	1	0	3.439022	-5.907171	-2.774498
23	1	0	9.668225	-6.923767	-1.39171
24	1	0	7.434558	-7.116821	-3.8848
25	1	0	9.277201	-3.309838	-5.275056
26	1	0	6.761235	-2.150616	4.982977
27	1	0	5.769423	-5.069794	3.628919
28	1	0	10.731971	1.725259	1.970939
29	1	0	8.251467	3.959384	2.061248
30	1	0	8.32727	1.482609	4.314388
31	1	0	6.240756	-0.097324	-3.343129
32	1	0	10.988534	-0.045212	-2.93489
33	1	0	9.639761	1.764823	-5.369435
34	1	0	10.21458	5.751492	-2.683092
35	1	0	16.533125	7.037412	-2.218366
36	1	0	13.51199	8.231516	-1.37235
37	1	0	15.453017	6.718281	0.911009
38	1	0	4.349366	3.451523	-1.556143
39	1	0	14.563335	0.128272	-1.771353
40	1	0	17.107329	2.145353	-2.565416
41	1	0	16.132114	1.905185	0.59945

Table S10. IC_{50} (48h, μM) of compounds **1**–**8** against human tumor cell lines.

Compounds	1	2	3	4	5	6	7	8
A549	14.6	>40	>40	>40	>40	>40	>40	>40
HL60	>40	>40	>40	>40	>40	>40	>40	>40
HepG2	>40	>40	>40	>40	>40	>40	>40	>40
MCF7	>40	>40	>40	>40	>40	>40	>40	>40

Table S11. Immunosuppressive effects of compounds **1**–**8** on murine lymphocyte proliferation induced by ConA (5 μg/mL) or LPS (10 μg/mL).

Compounds	IC_{50}(μM)	
	T cells	B cells
1	>40	>40
2	>40	>40
3	>40	>40
4	>40	>40
5	>40	>40
6	>40	>40
7	>40	>40
8	>40	16.6
Cyclosporin A	0.04	