Bioactive Indolyl Diketopiperazines from the Marine Derived Endophytic *Aspergillus versicolor* DY180635

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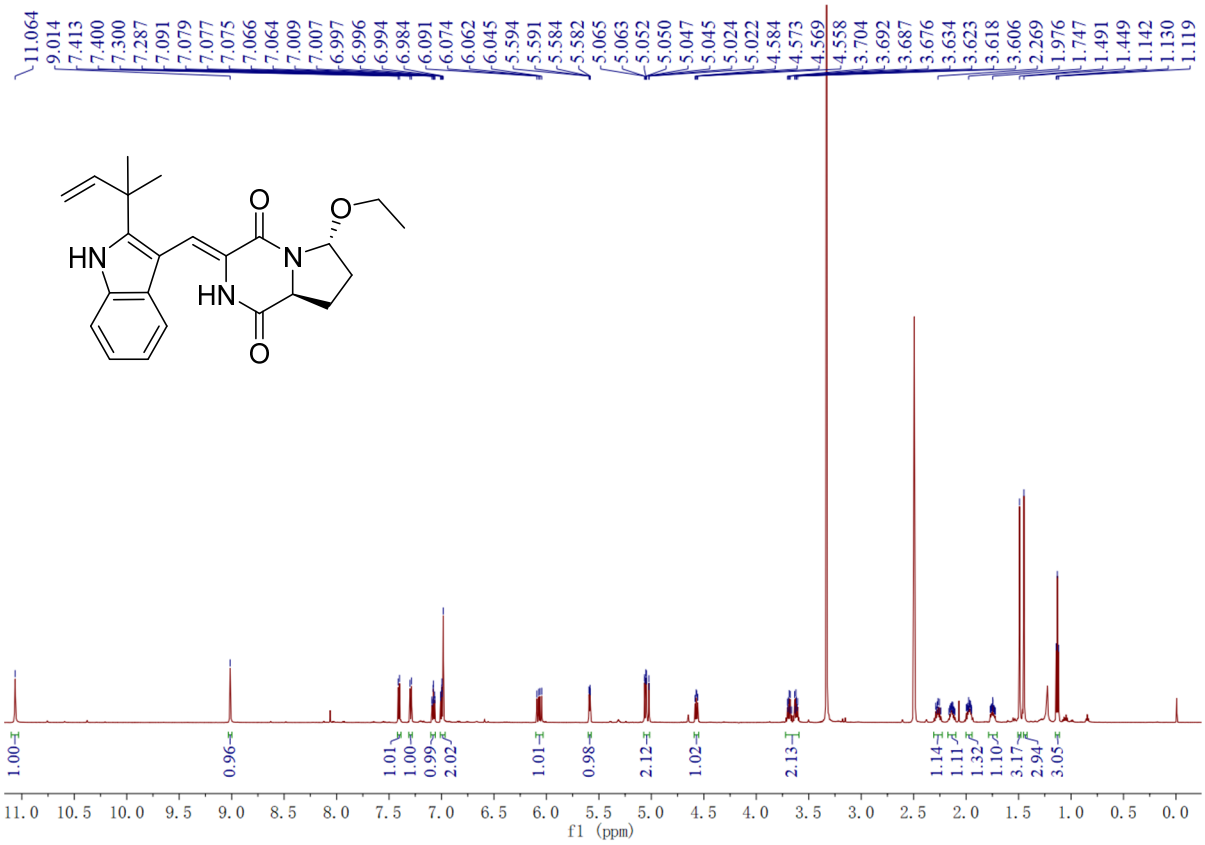


Figure S1. ^{1}H NMR spectra (600 MHz, DMSO-d_6) of **1**.

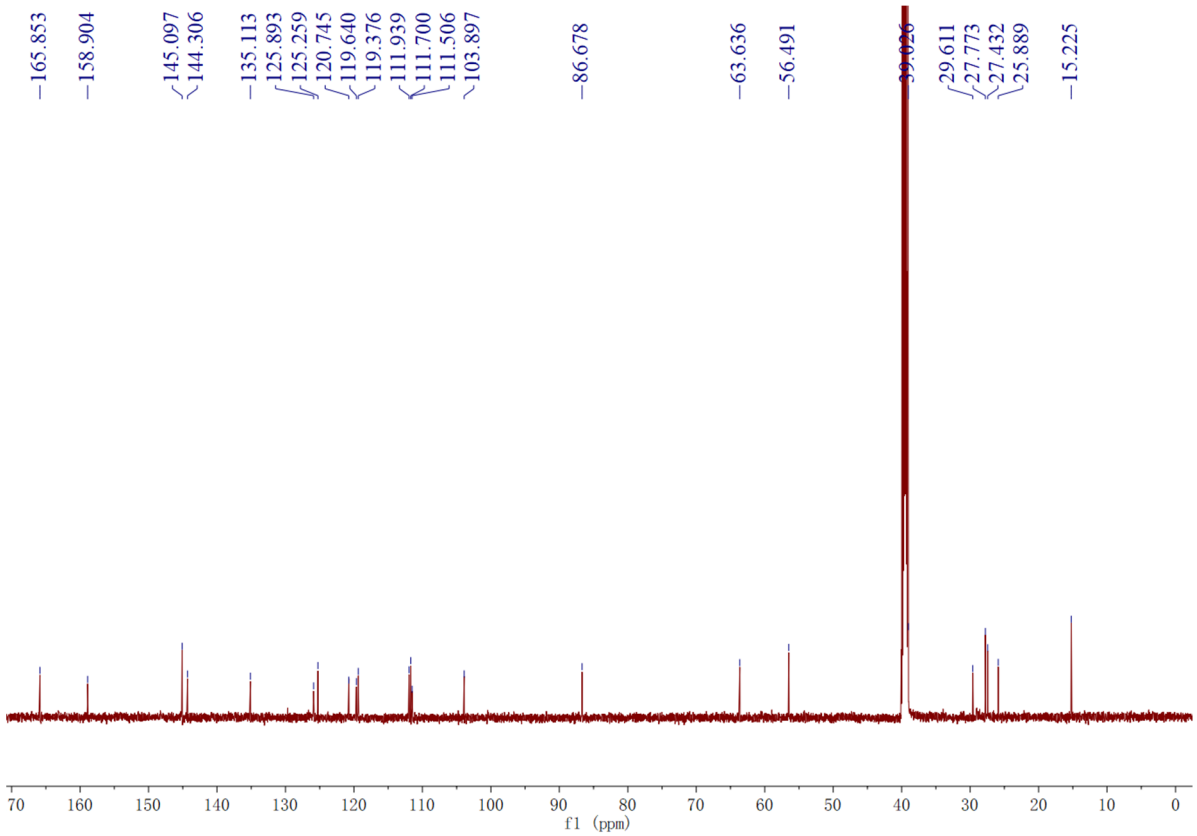


Figure S2. ^{13}C NMR spectra (150 MHz, DMSO-d_6) of **1**.

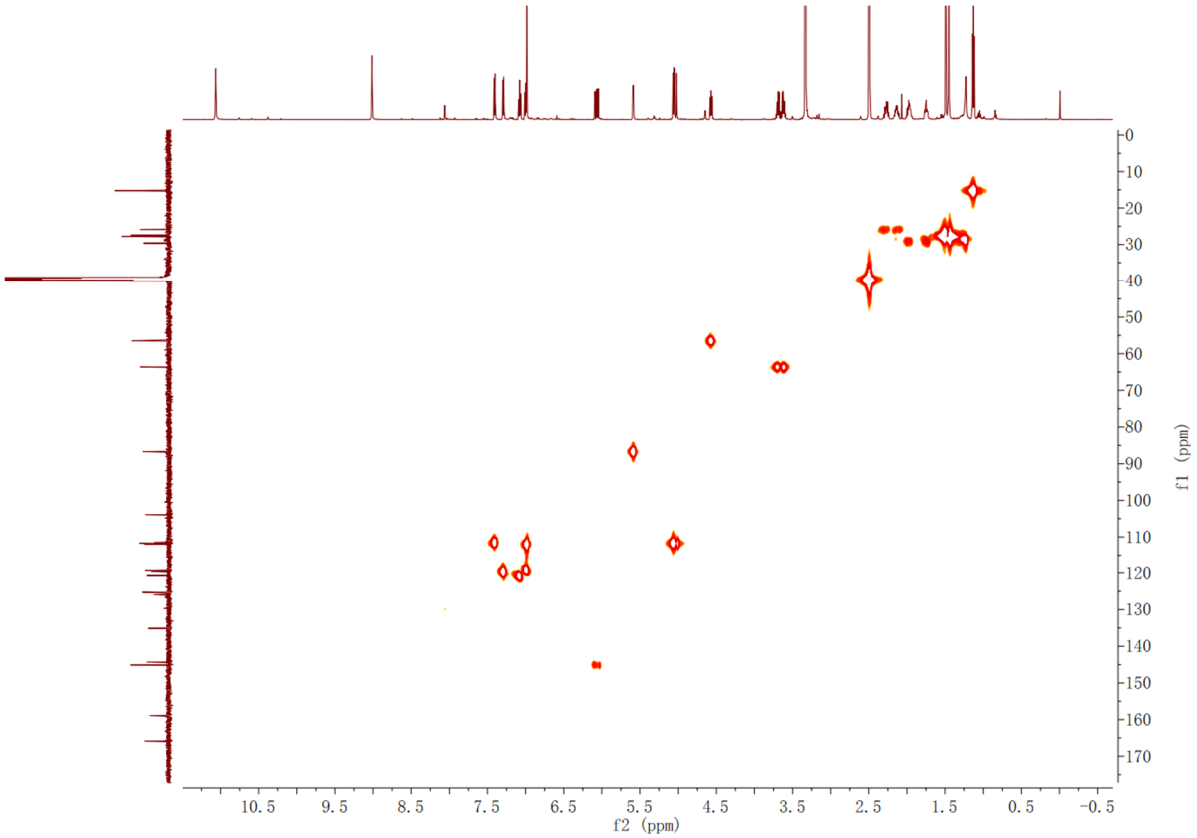
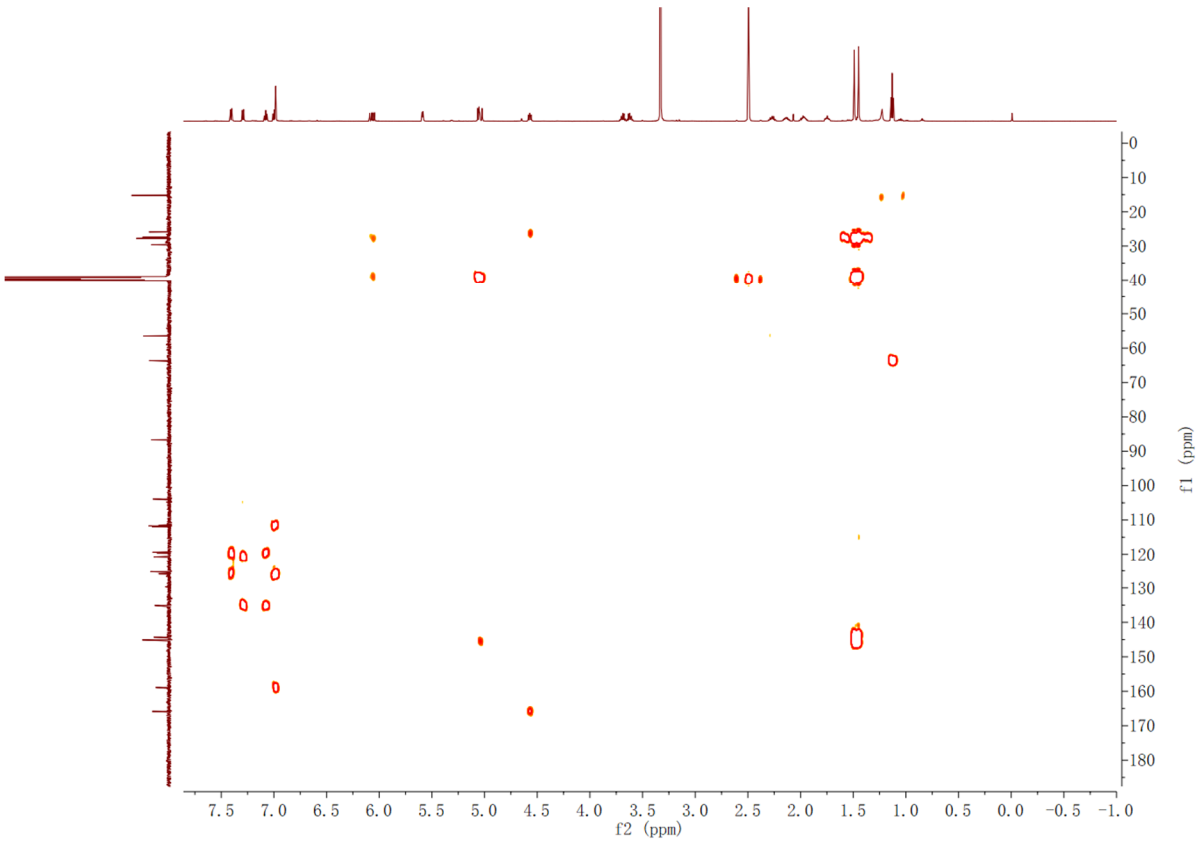


Figure S3. HMQC spectra (DMSO-d_6) of **1**.



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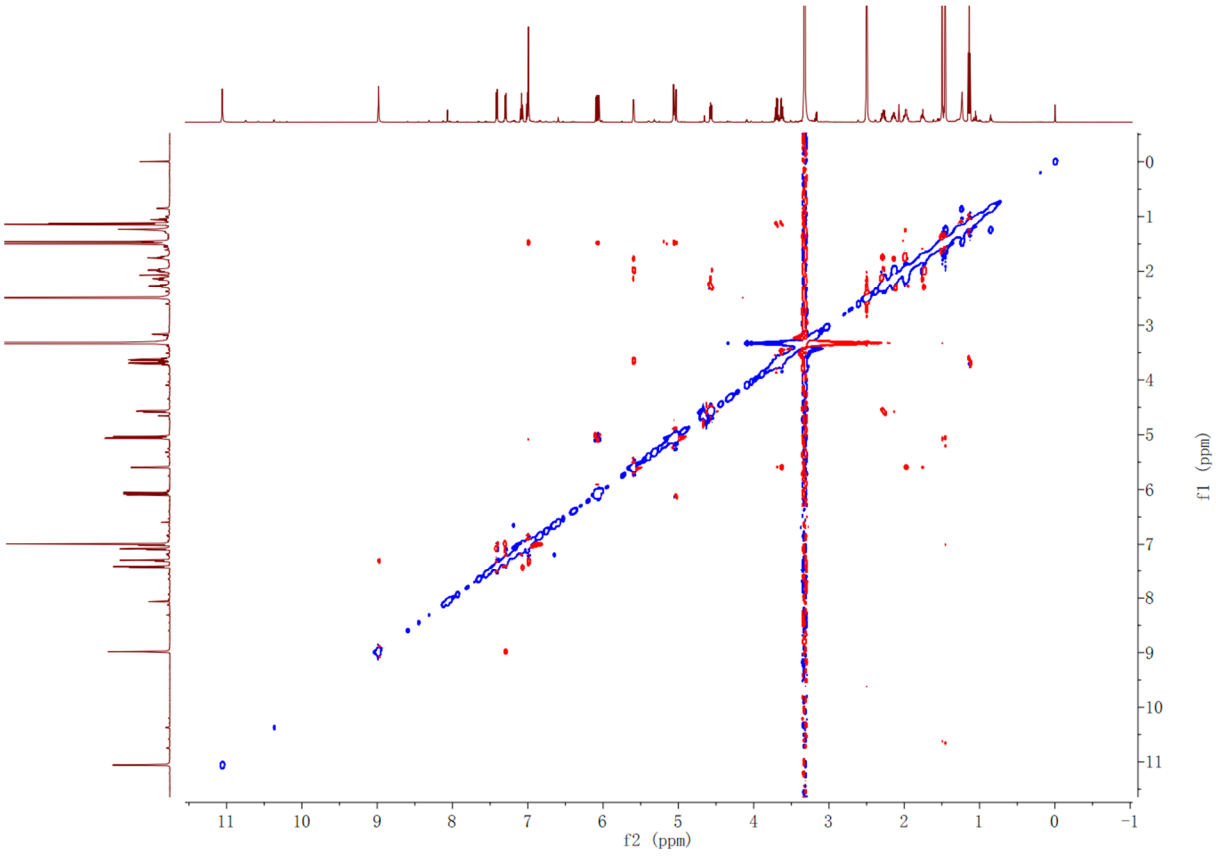


Figure S5. ROESY spectra (DMSO-d_6) of **1**.

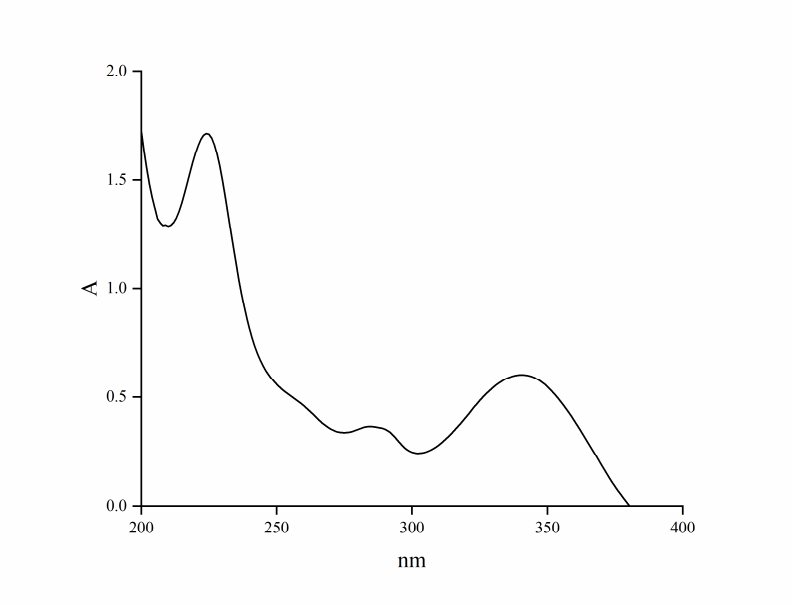


Figure S6. UV spectra (MeOH) of **1**.

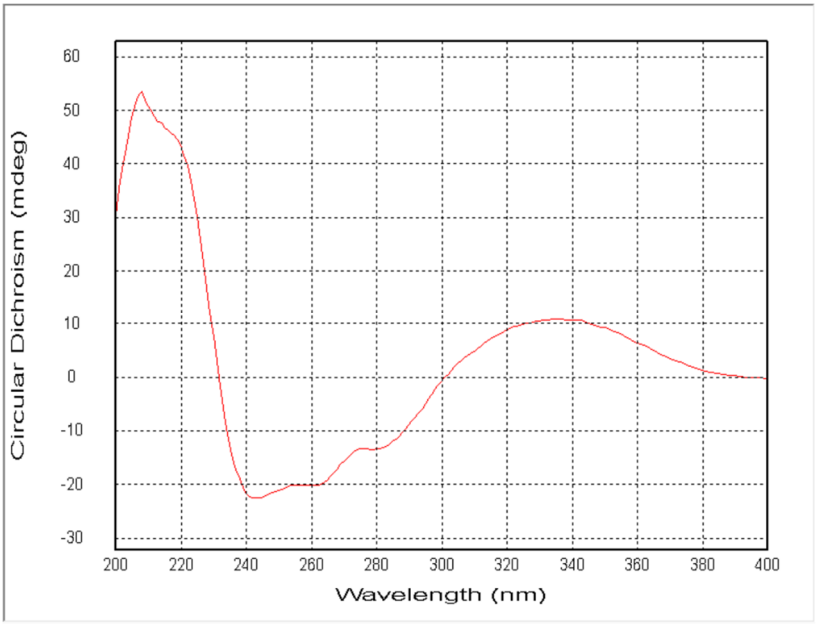


Figure S7. ECD spectra (MeOH) of **1**.

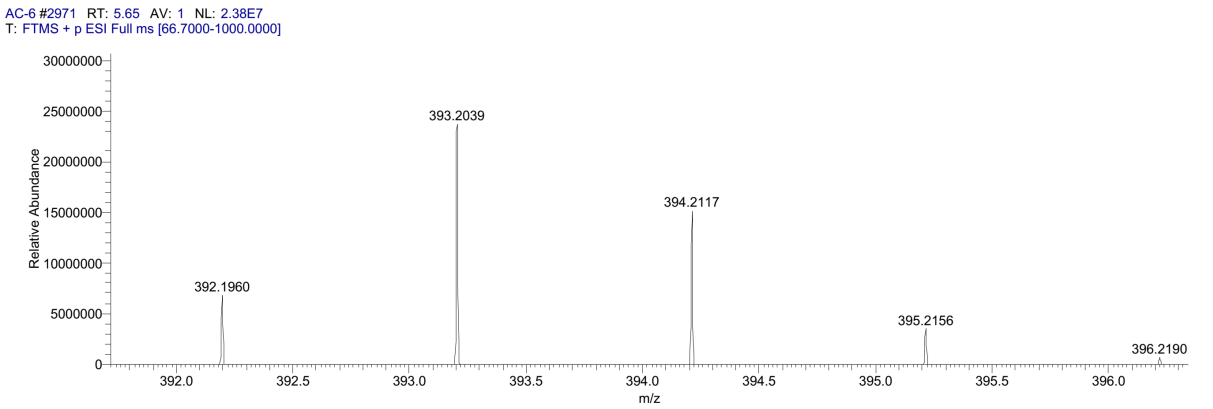


Figure S8. HRESIMS spectra of **1**.

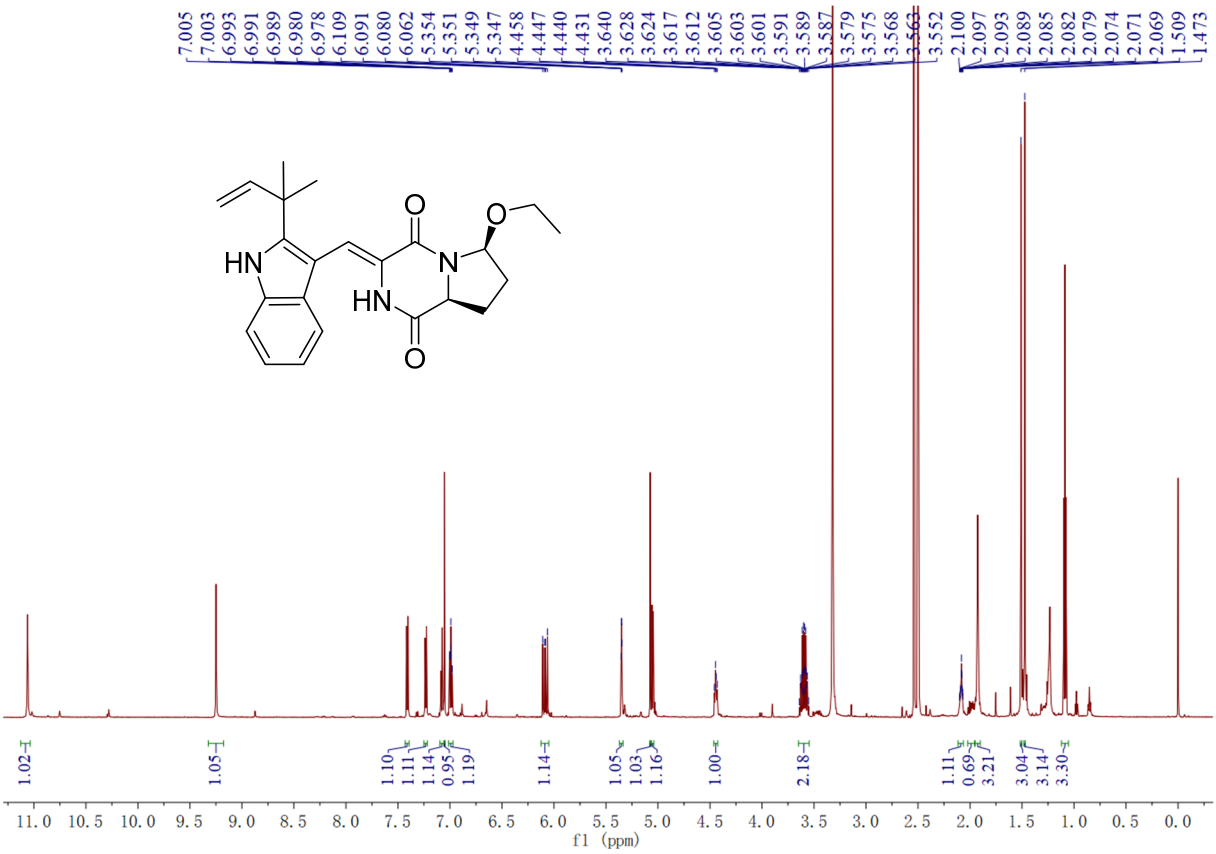
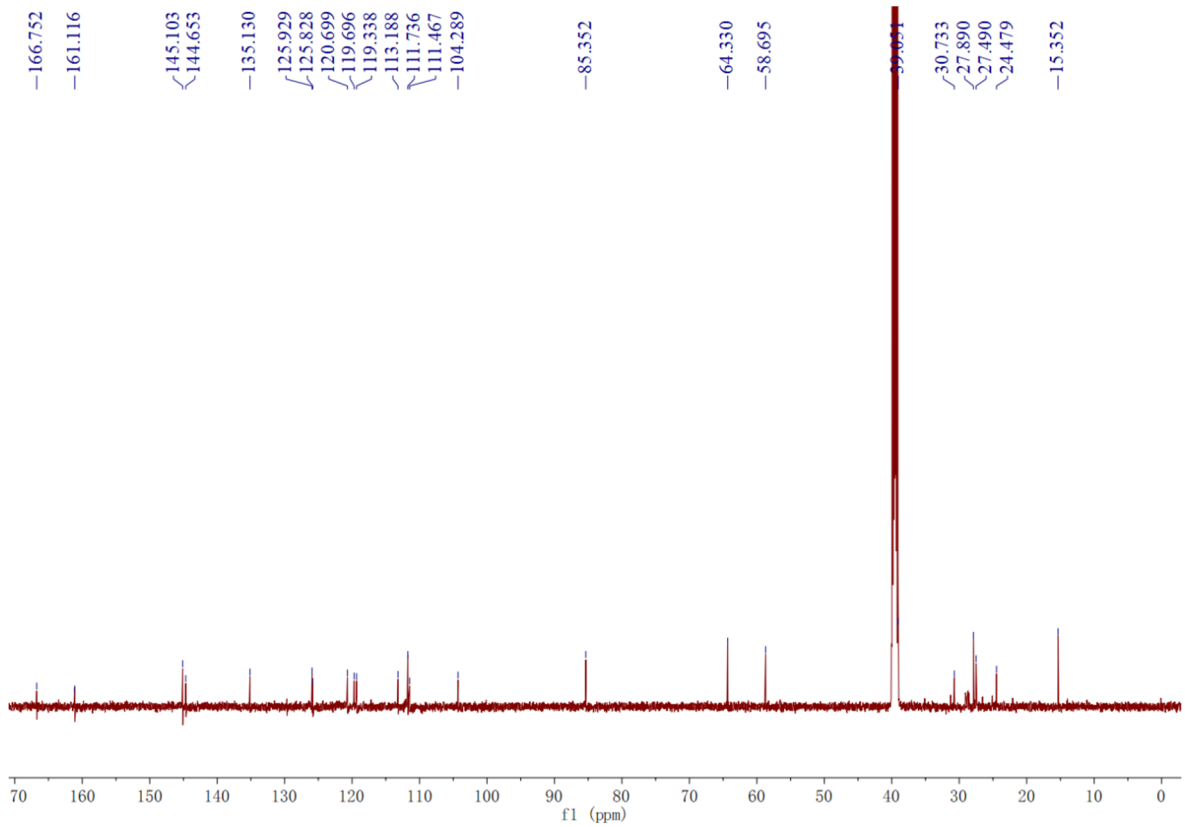


Figure S9. ^{1}H NMR spectra (600 MHz, DMSO-d_6) of **2**.



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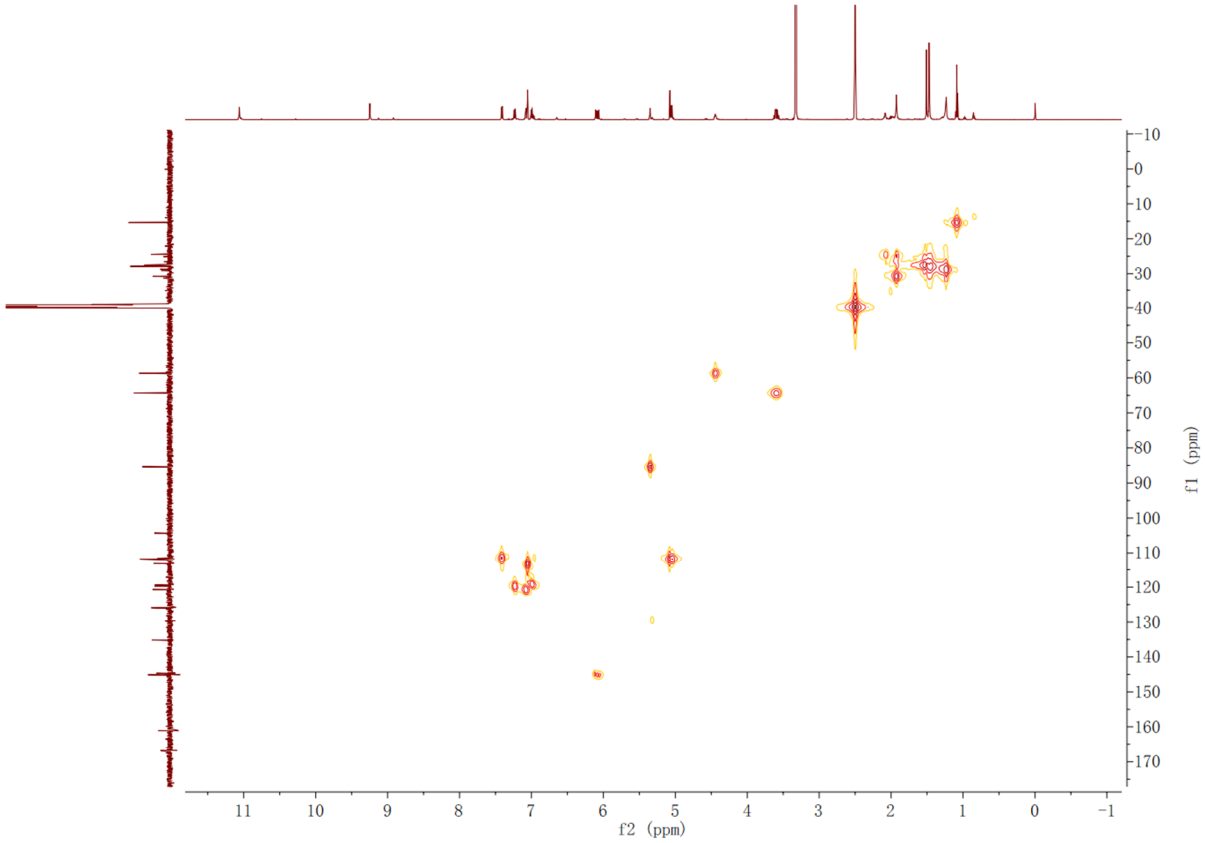

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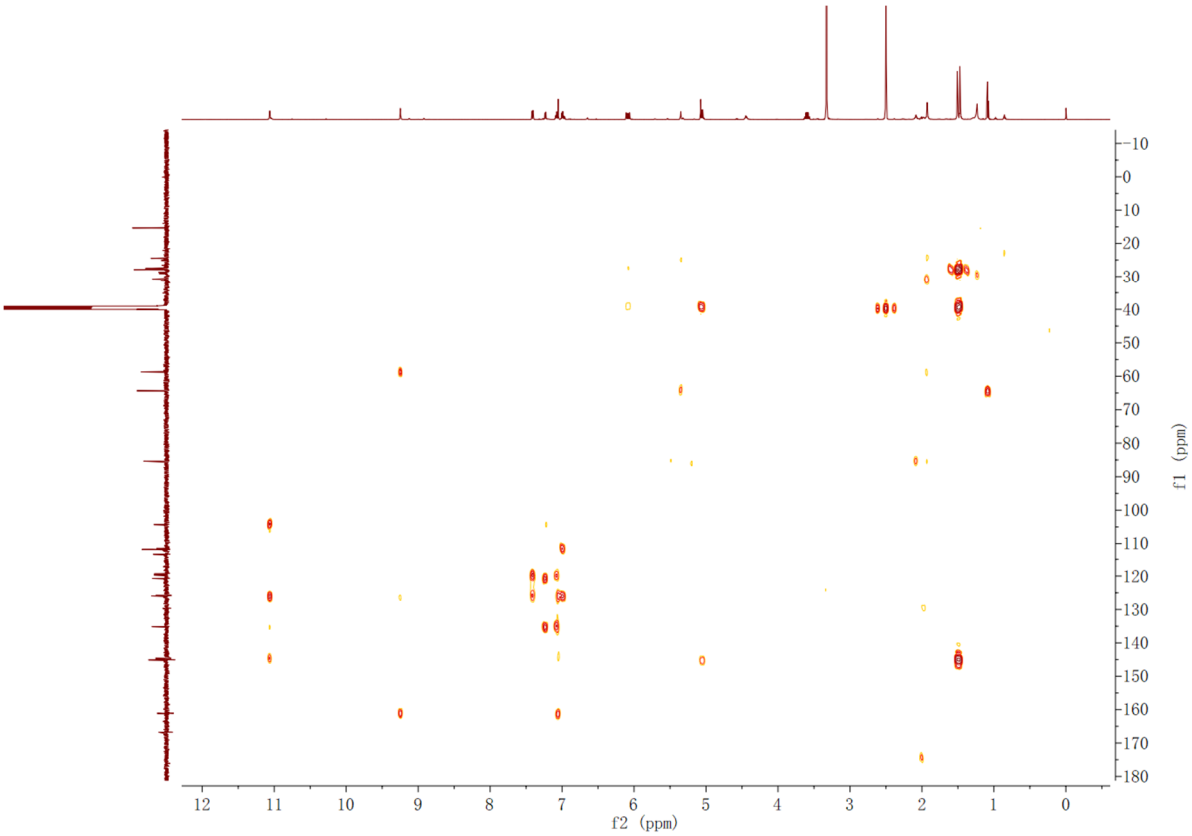

Figure S12. HMBC spectra (DMSO-d_6) of **2**.

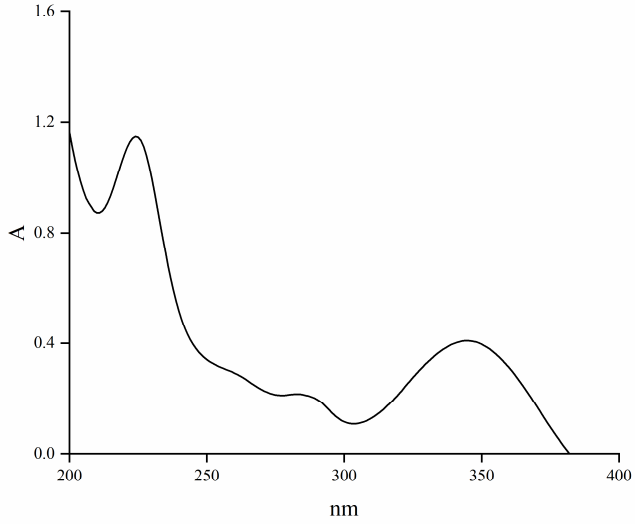

Figure S13. UV spectra (MeOH) of **2**.

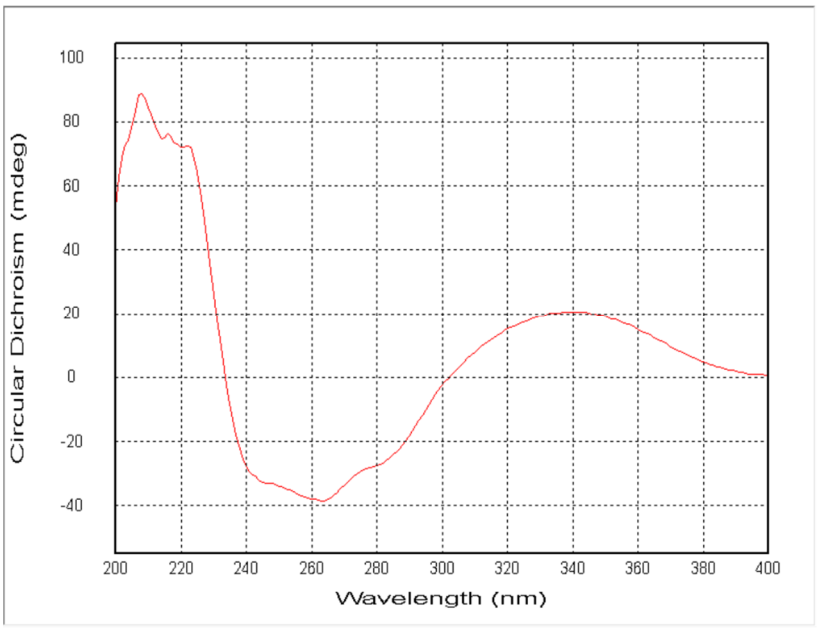

Figure S14. ECD spectra (MeOH) of **2**.

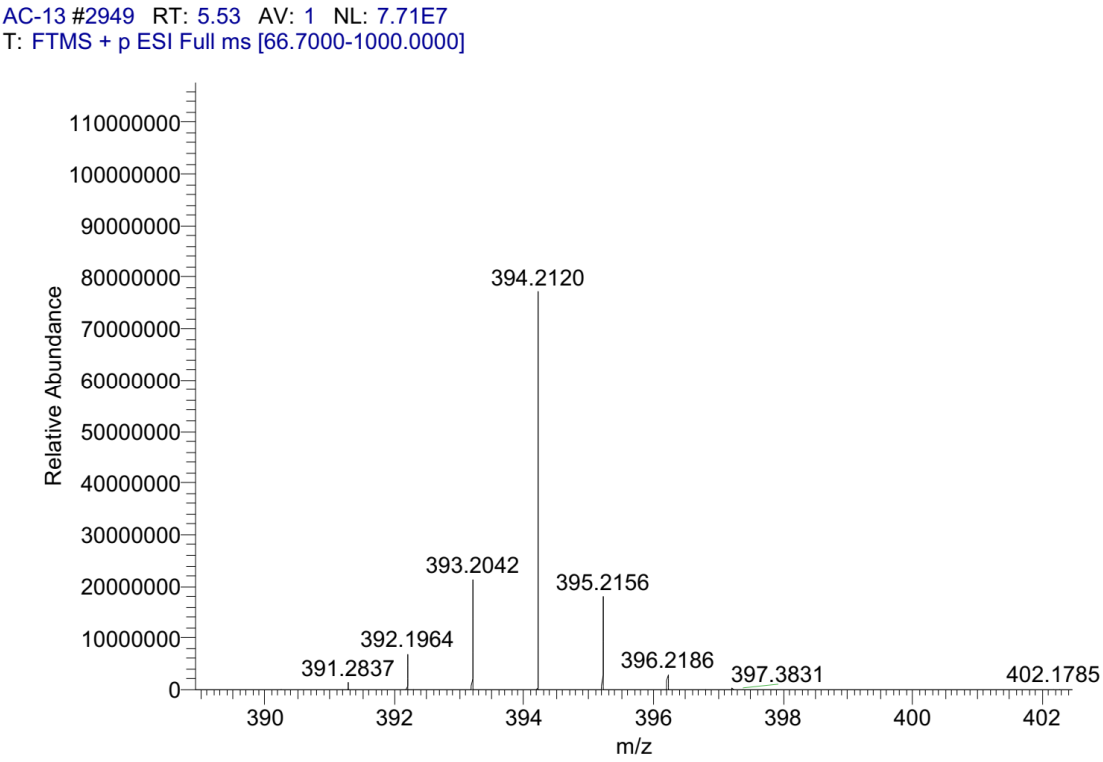

Figure S15. HRESIMS spectra of **2**.

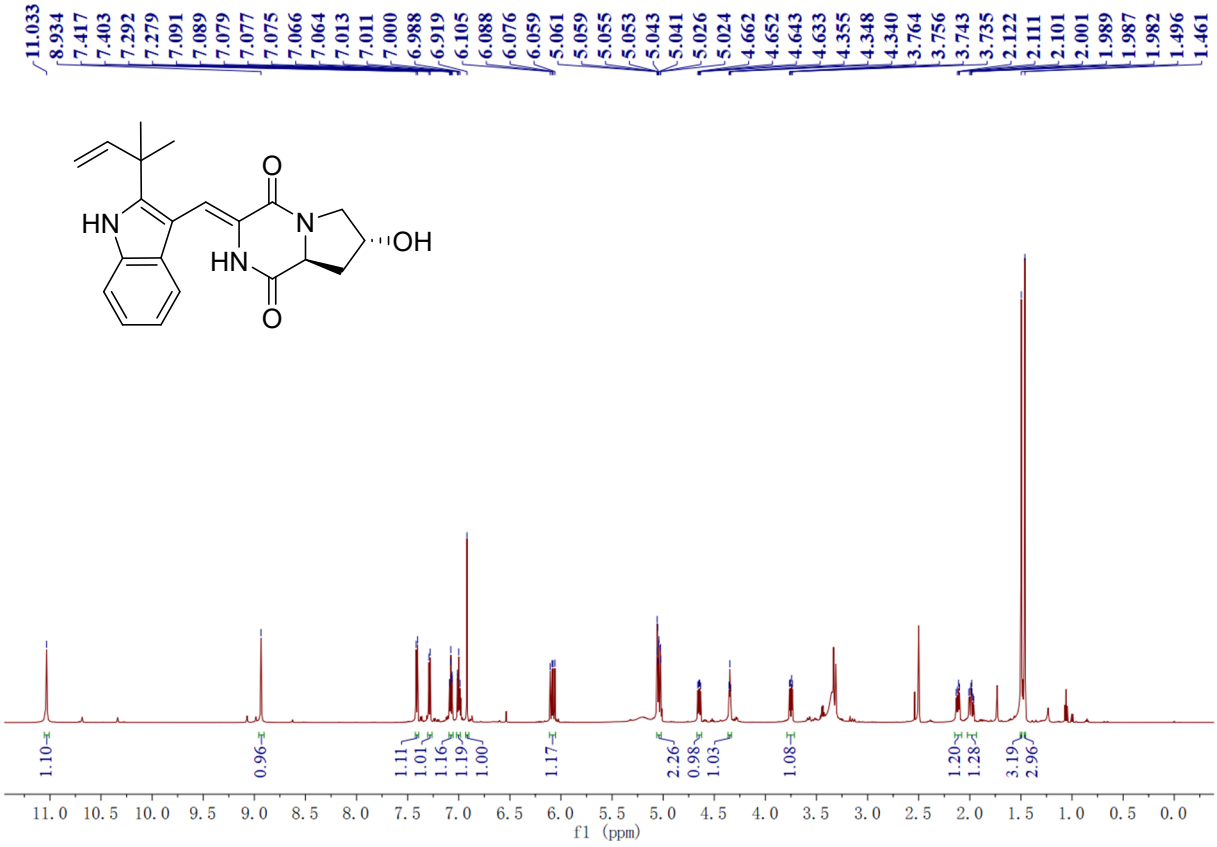

Figure S16. ^{1}H NMR spectra (600 MHz, DMSO-d_6) of **3**.

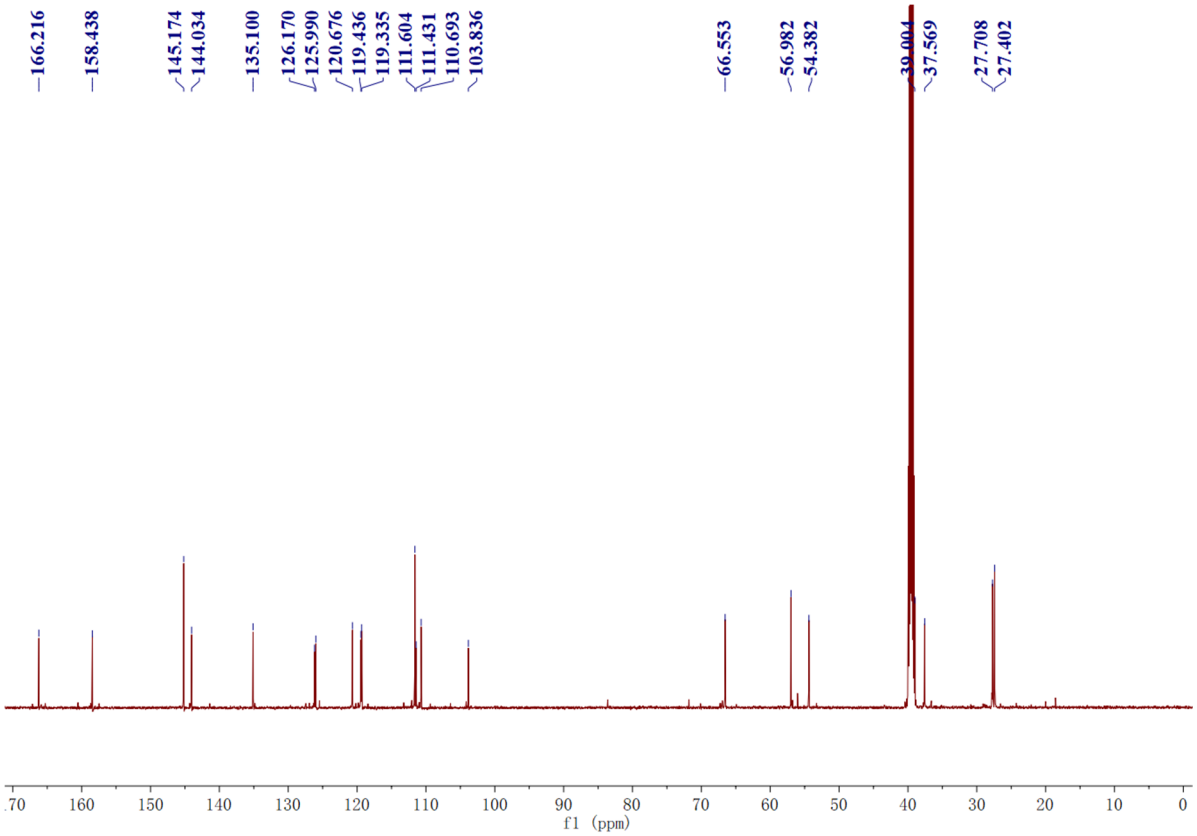

Figure S17. ^{13}C NMR spectra (150 MHz, DMSO-d_6) of **3**.

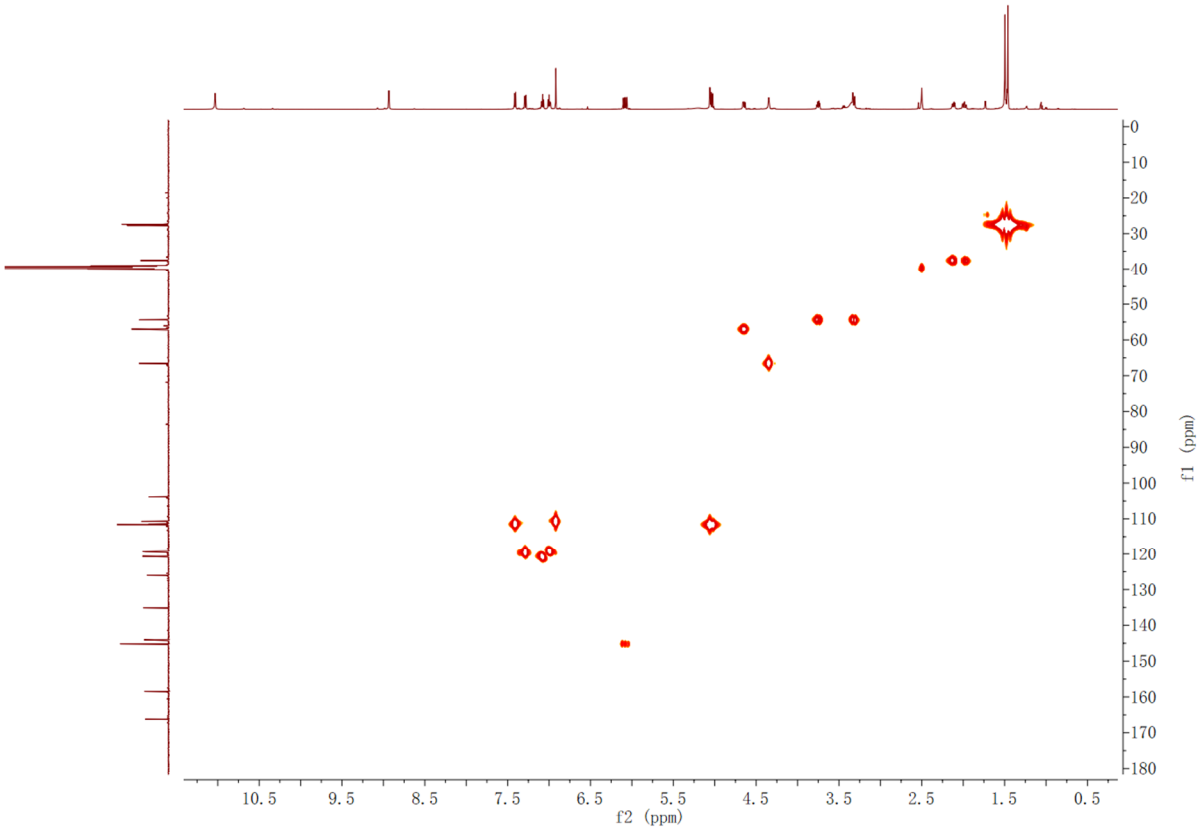

Figure S18. HMQC spectra (DMSO-d_6) of **3**.

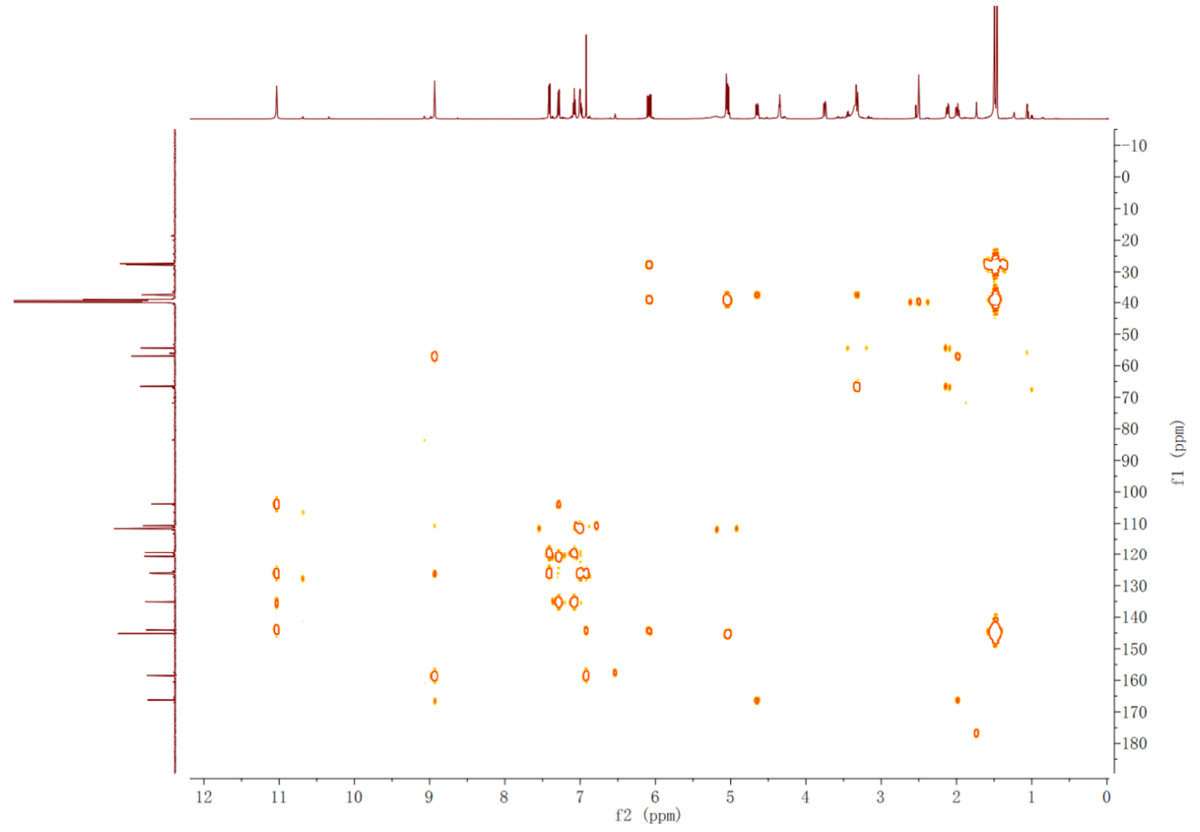

Figure S19. HMBC spectra (DMSO-d_6) of **3**.

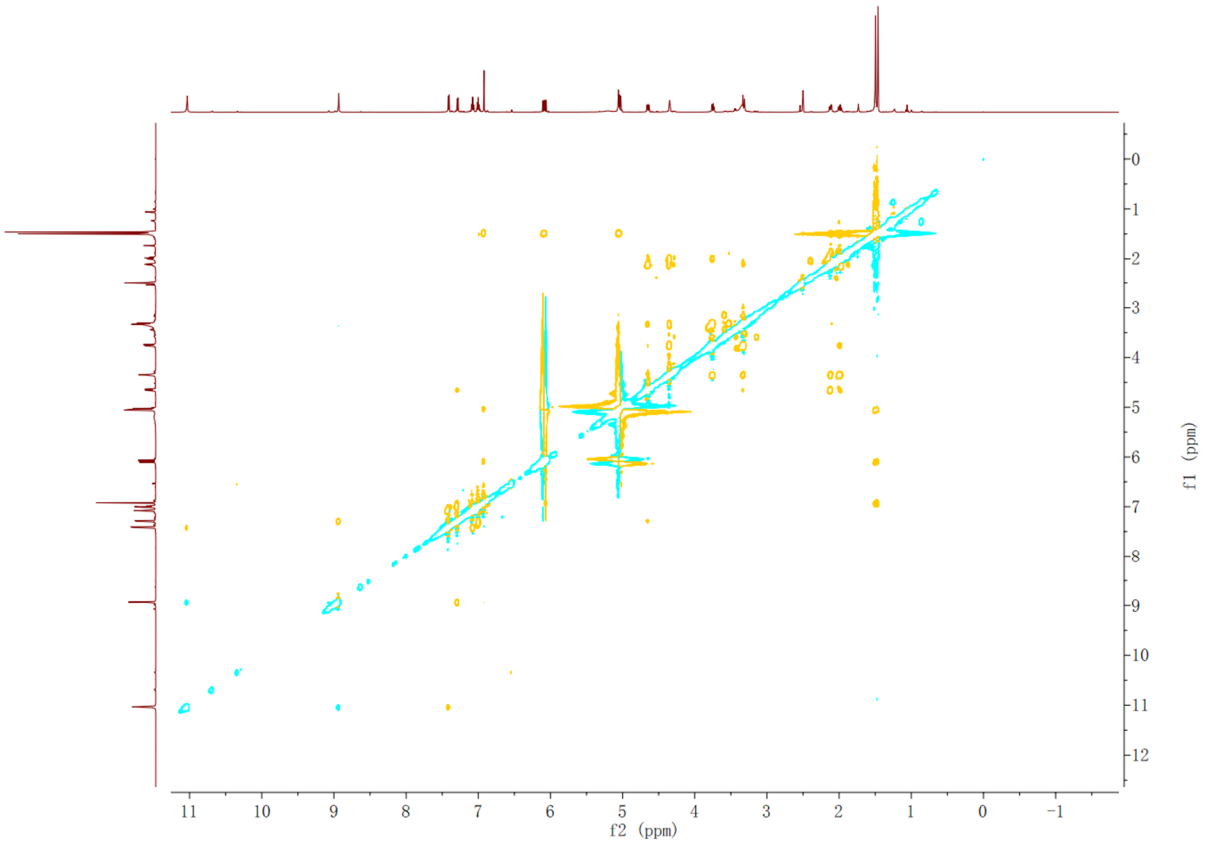

Figure S20. ROESY spectra (DMSO-d_6) of **3**.

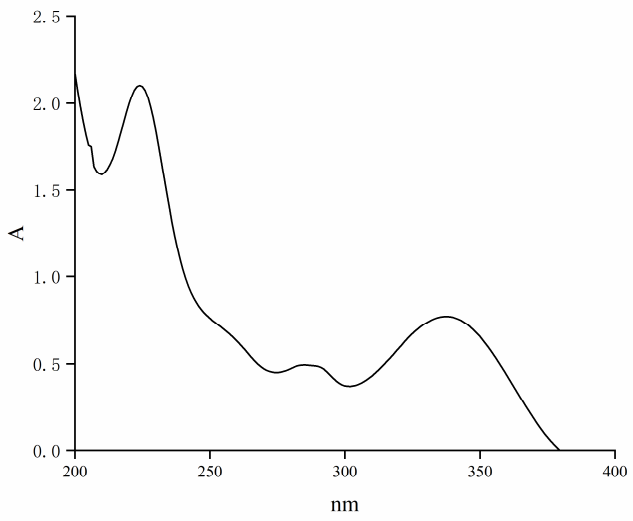

Figure S21. UV spectra (MeOH) of **3**.

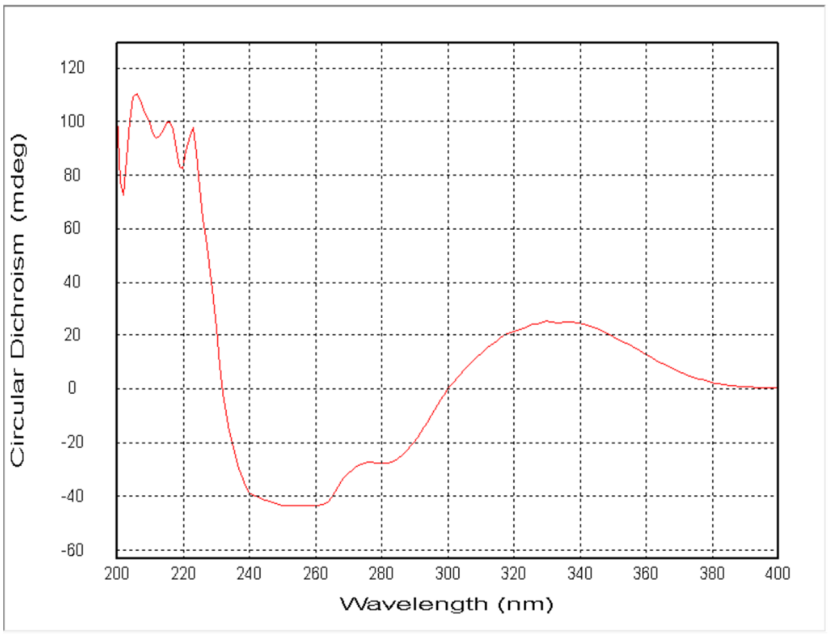

Figure S22. ECD spectra (MeOH) of **3**.

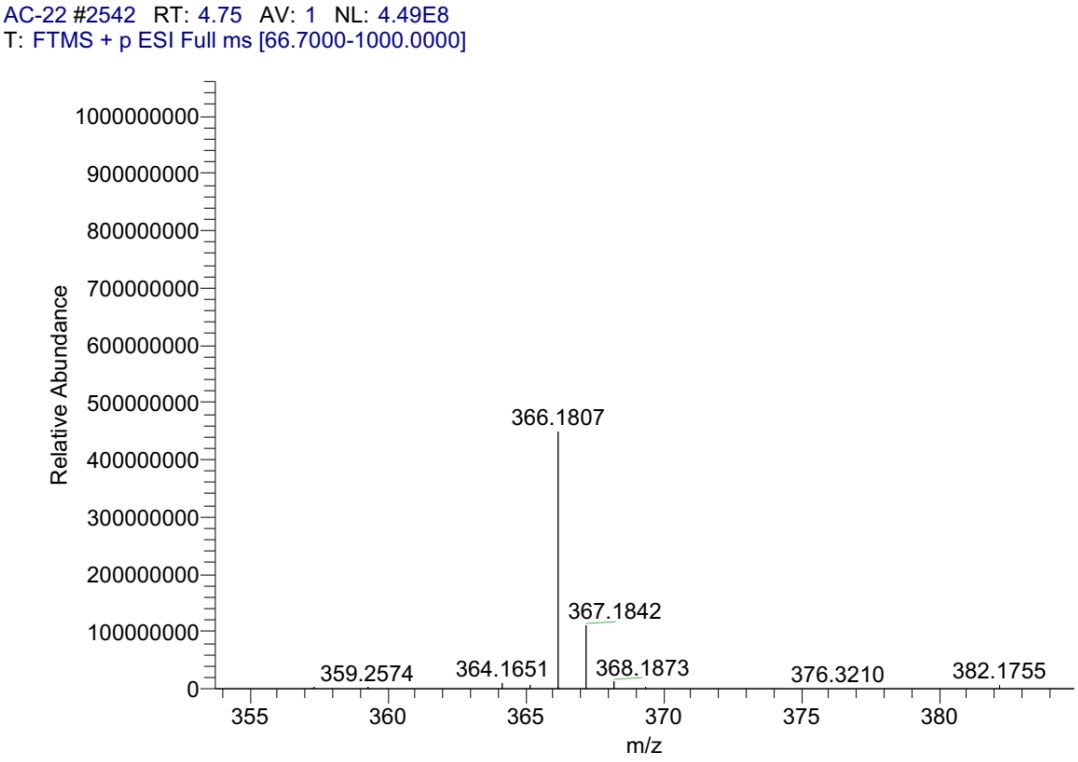

Figure S23. HRESIMS spectra of **3**.

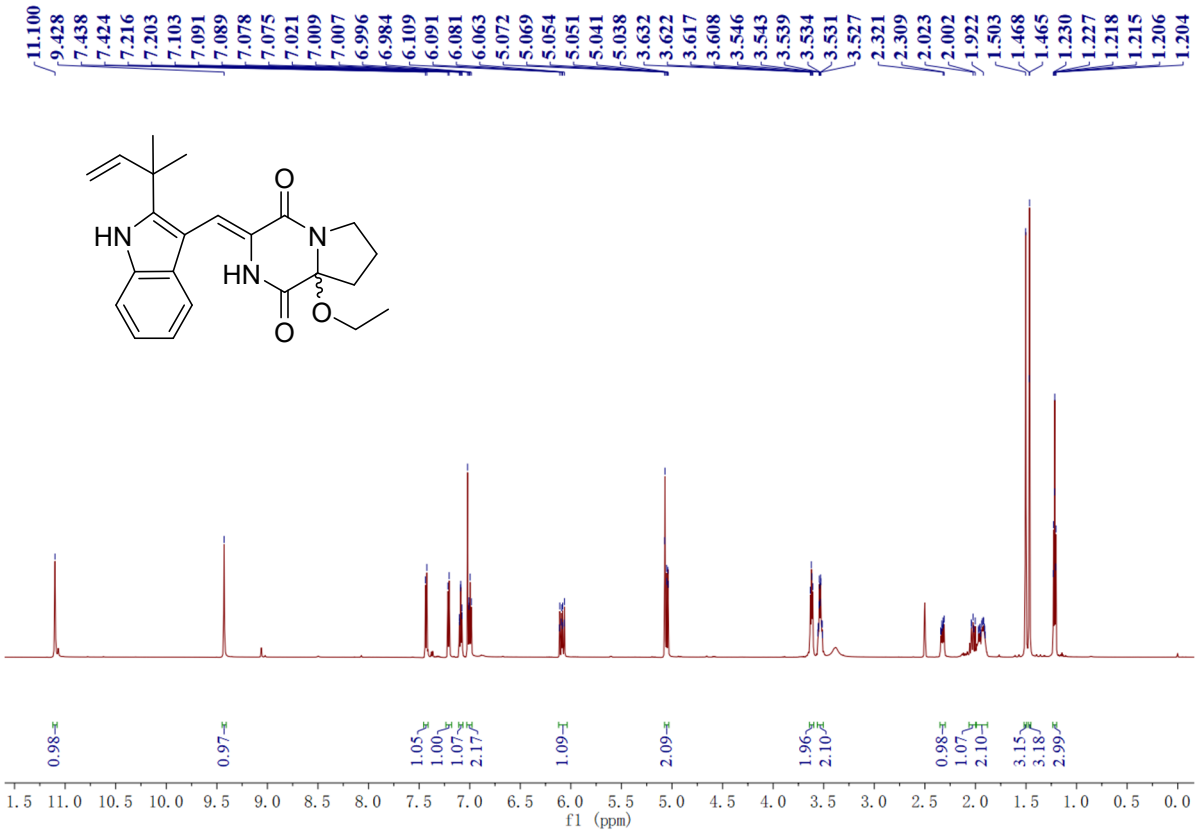

Figure S24. ^{1}H NMR spectra (600 MHz, DMSO-d_6) of **4**.

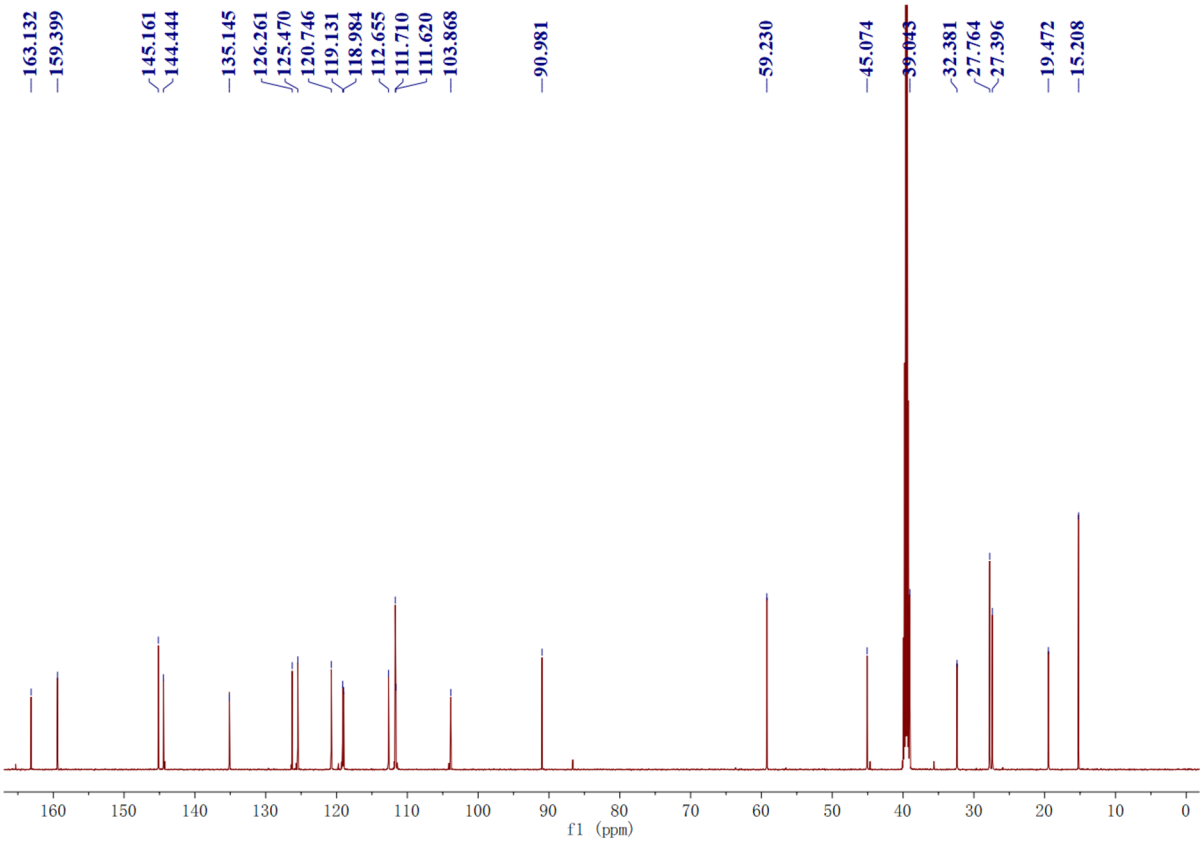

Figure S25. ^{13}C NMR spectra (150 MHz, DMSO-d_6) of **4**.

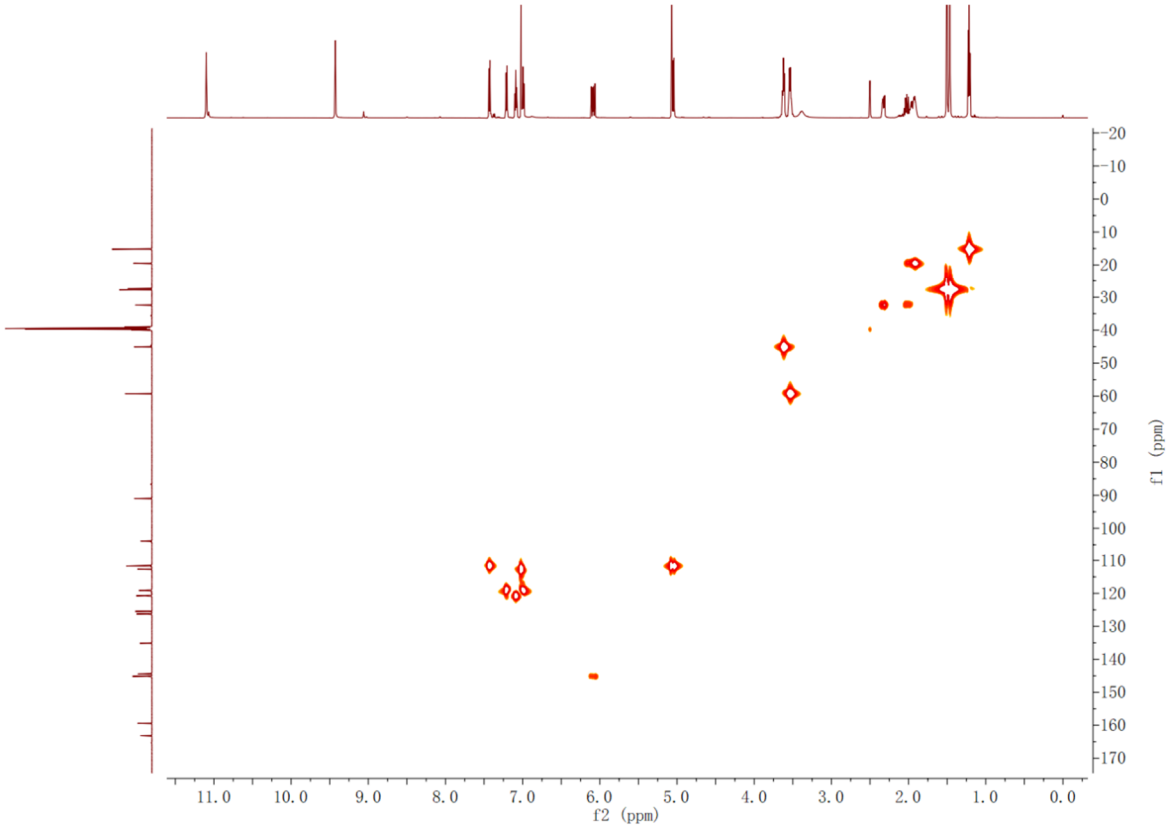

Figure S26. HMQC spectra (DMSO-d_6) of **4**.

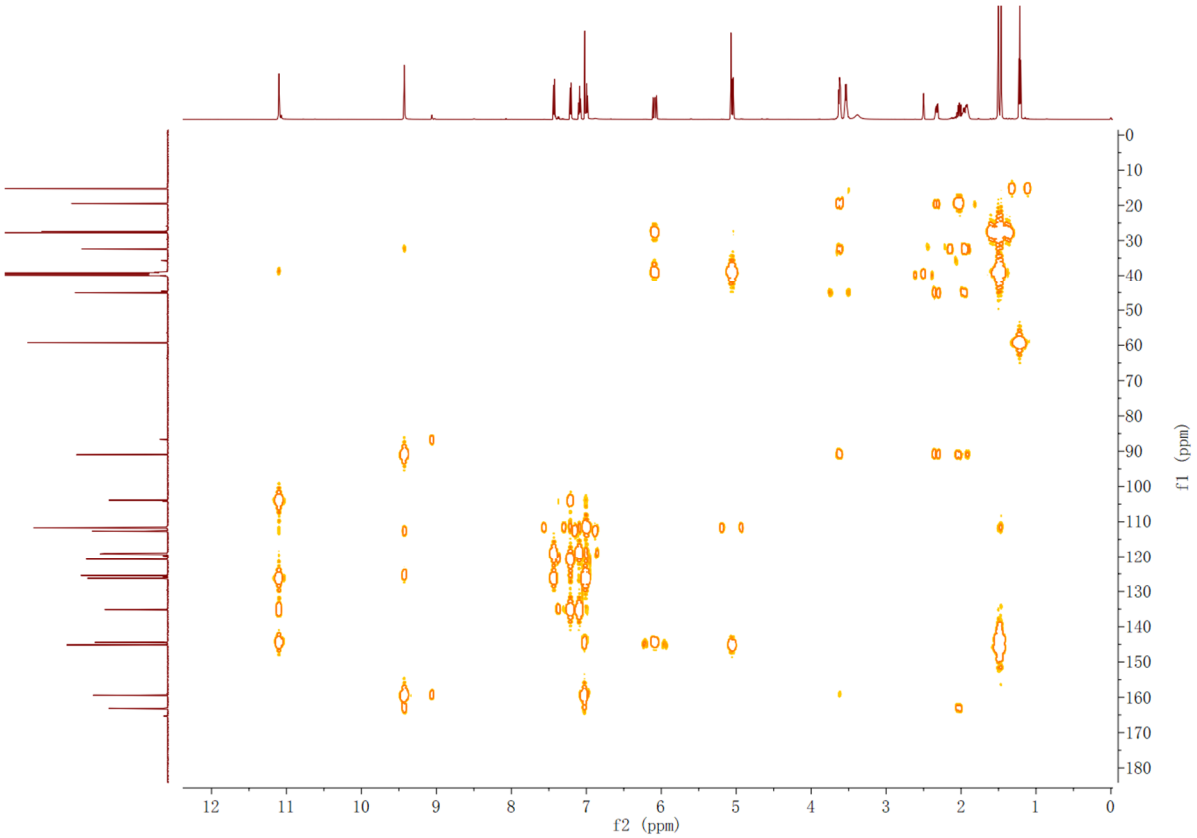

Figure S27. HMBC spectra (DMSO-d_6) of **4**.

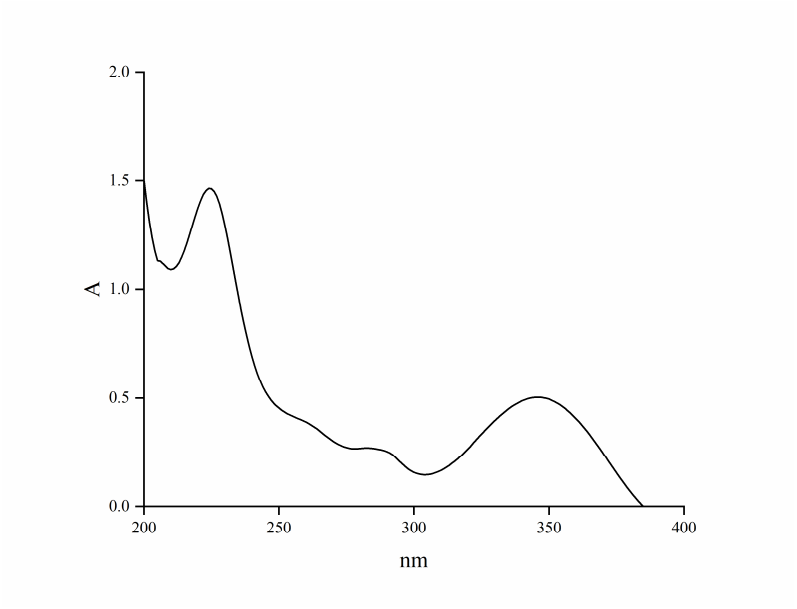

Figure S28. UV spectra (MeOH) of **4**.

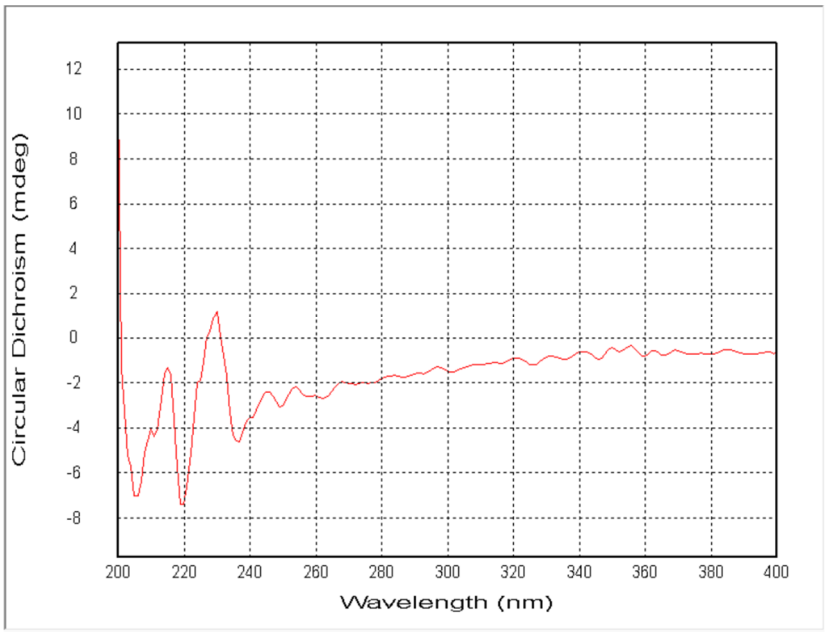

Figure S29. ECD spectra (MeOH) of **4**.

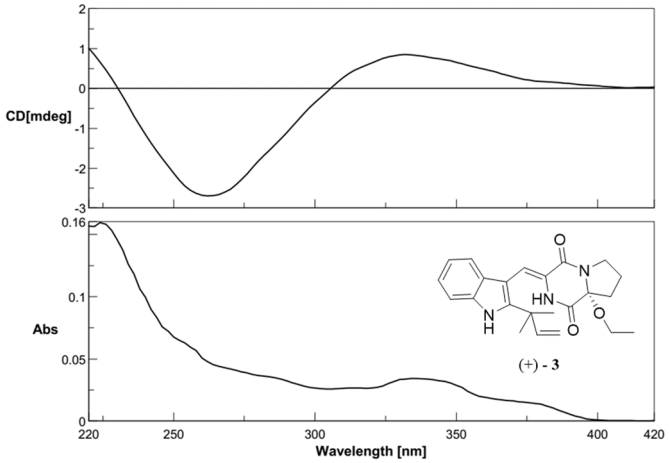

Figure S30. ECD spectra (MeOH) of (+) - **4**.

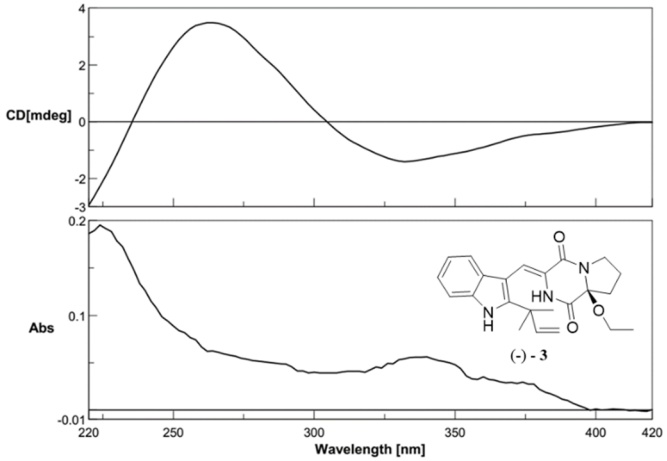

Figure S31. ECD spectra (MeOH) of (-) - **4**.

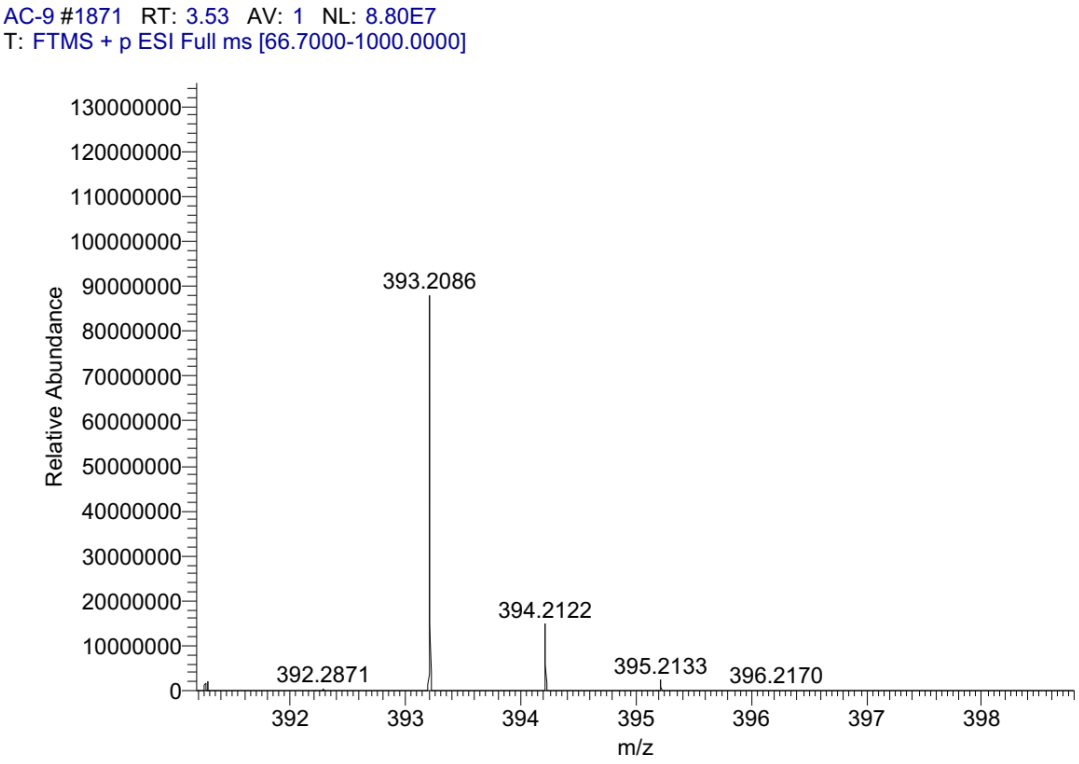

Figure S32. HRESIMS spectra of **4**.

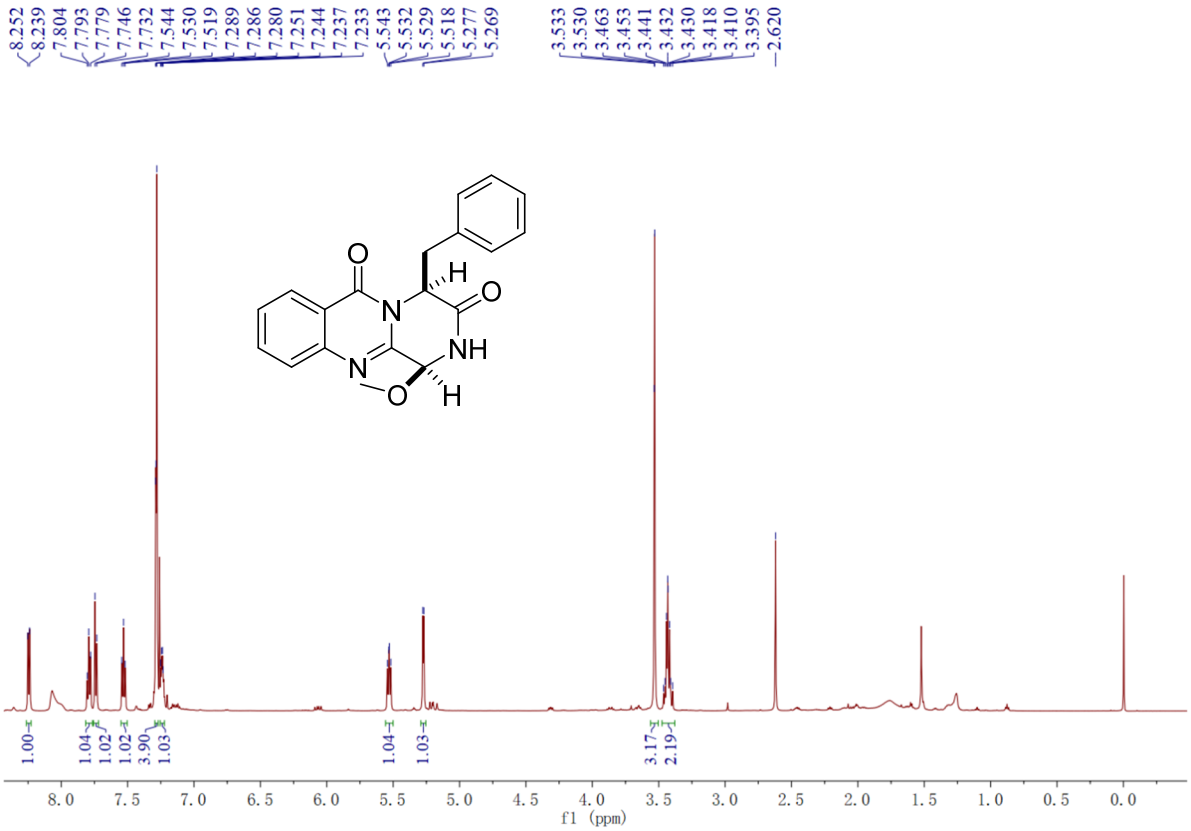

Figure S33. ^{1}H NMR spectra (600 MHz, $CDCl_3$) of **5**.

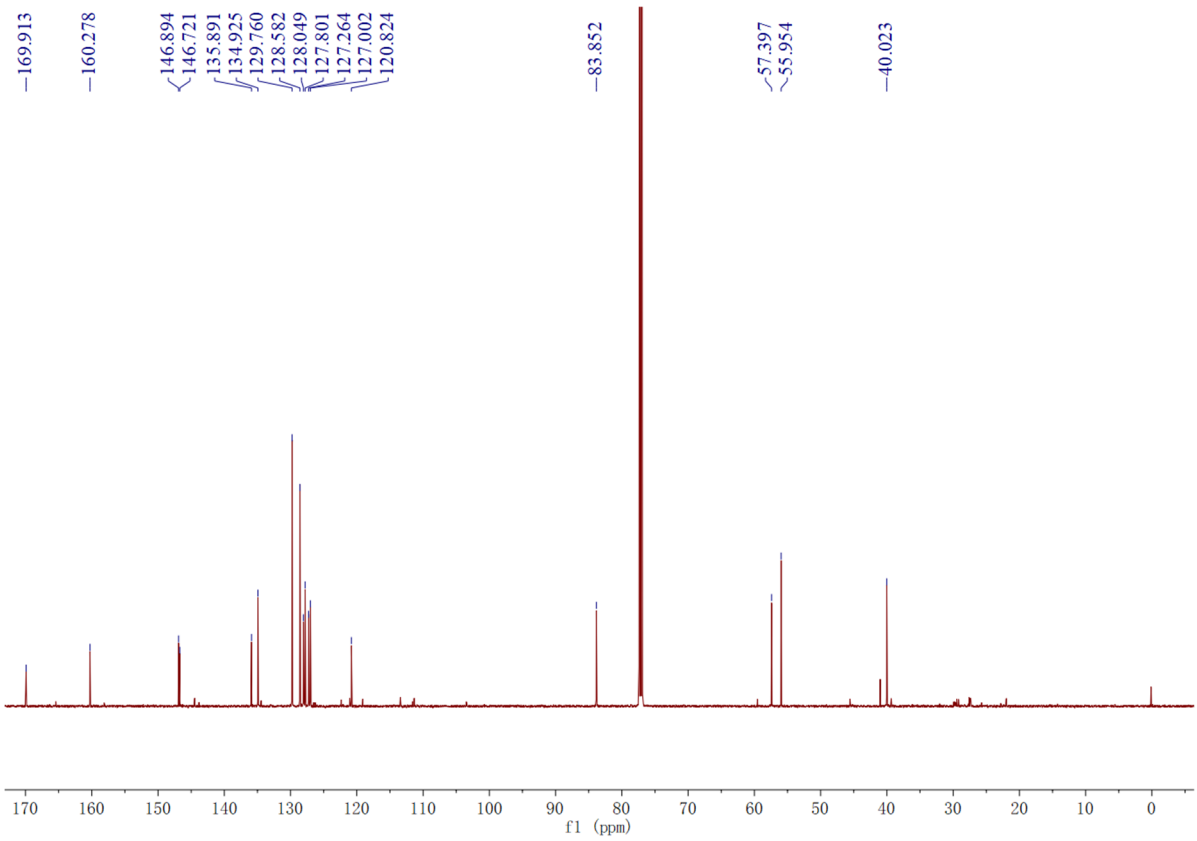

Figure S34. ^{13}C NMR spectra (150 MHz, $CDCl_3$) of **5**.

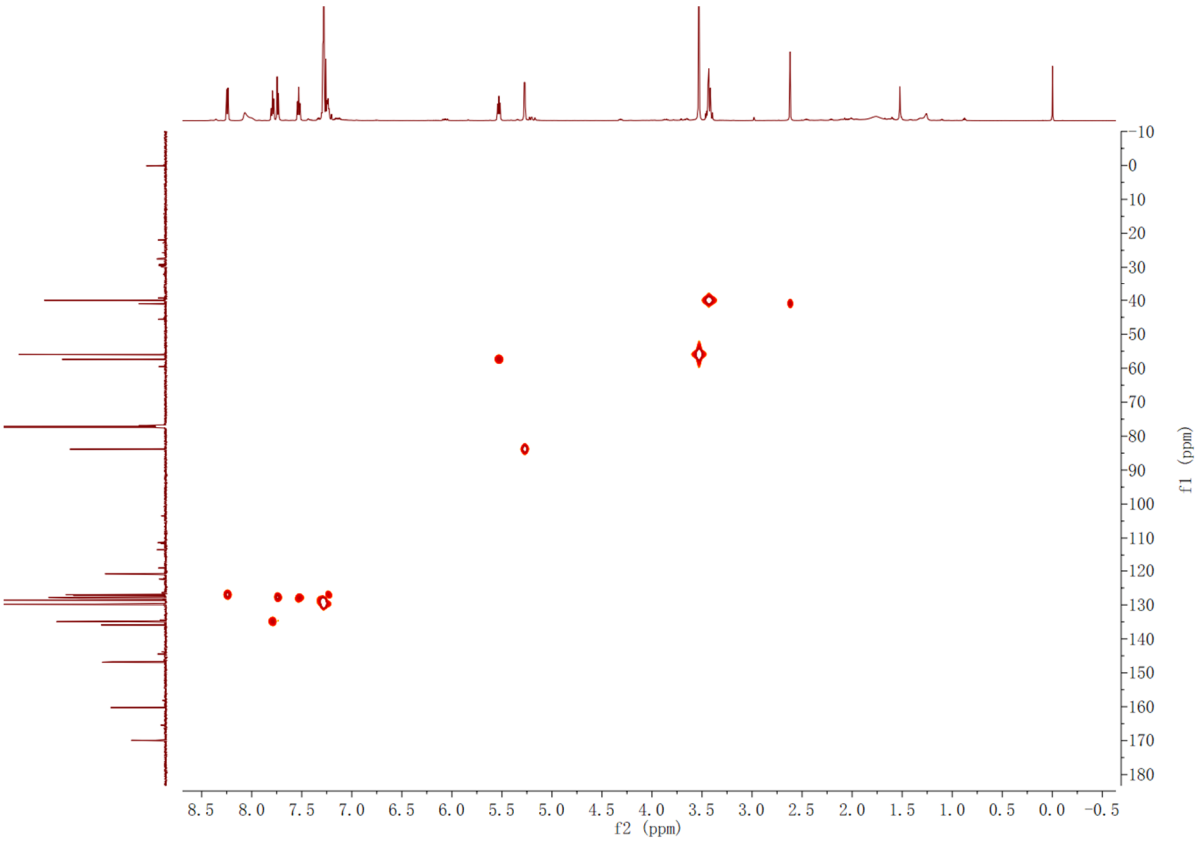

Figure S35. HMQC spectra ($CDCl_3$) of **5**.

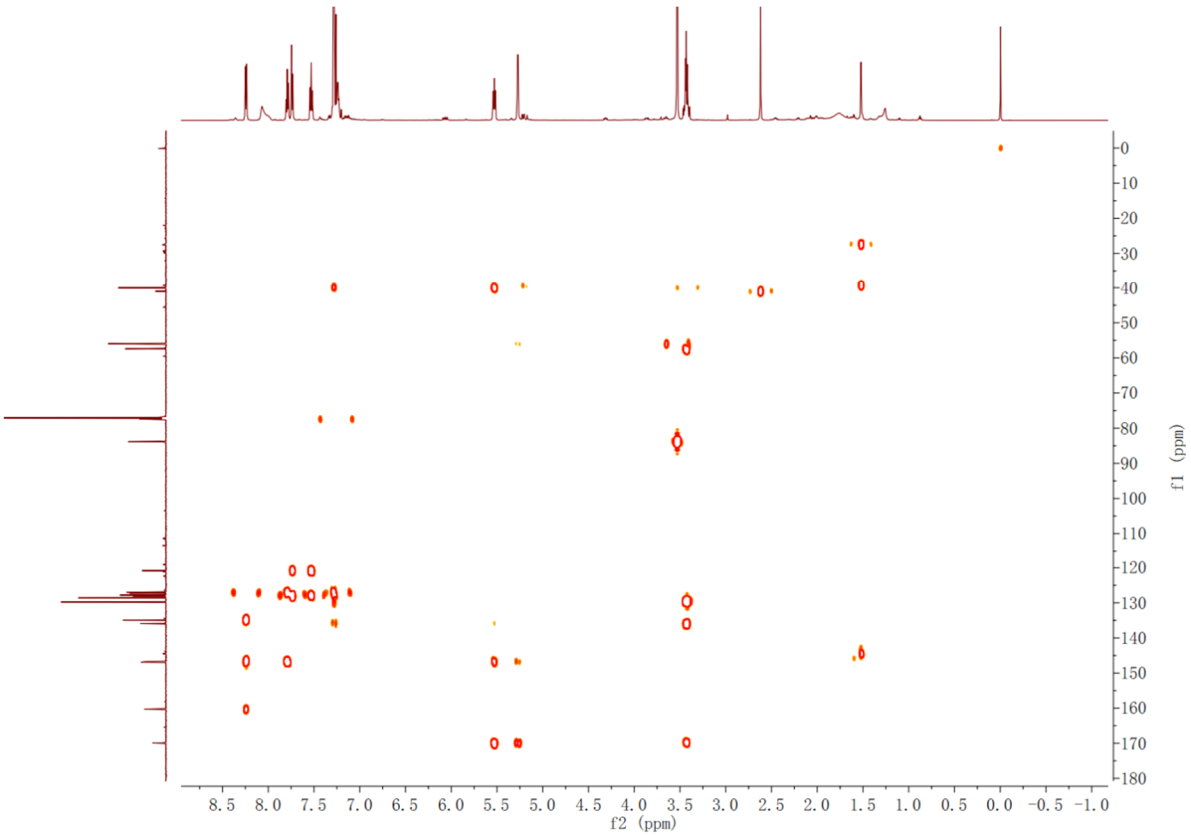

Figure S36. HMBC spectra ($CDCl_3$) of **5**.

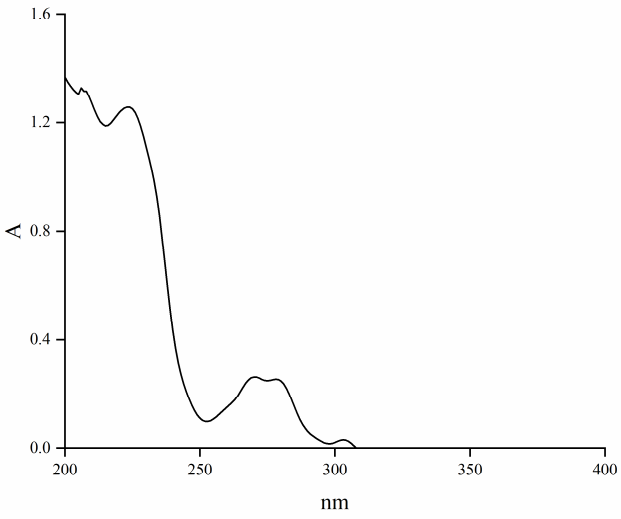

Figure S37. UV spectra (MeOH) of **5**.

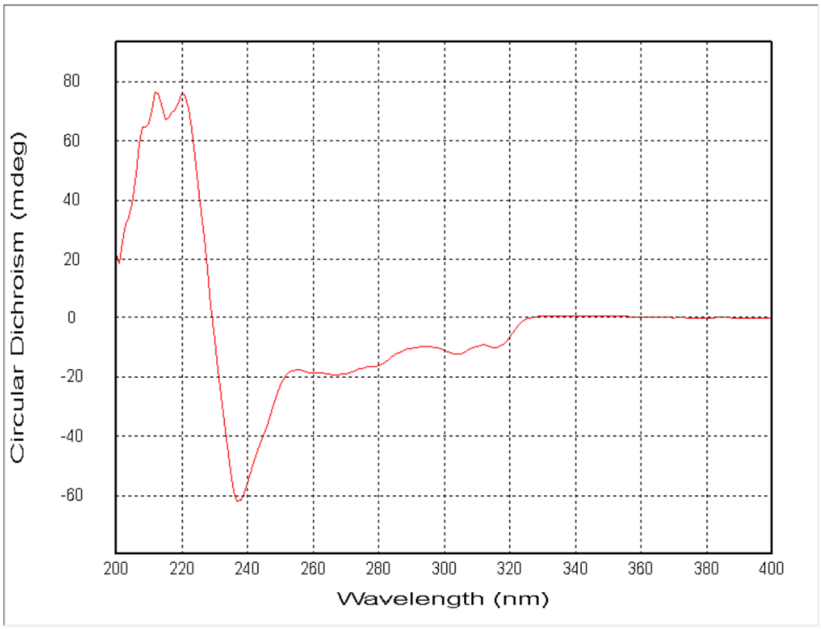

Figure S38. ECD spectra (MeOH) of **5**.

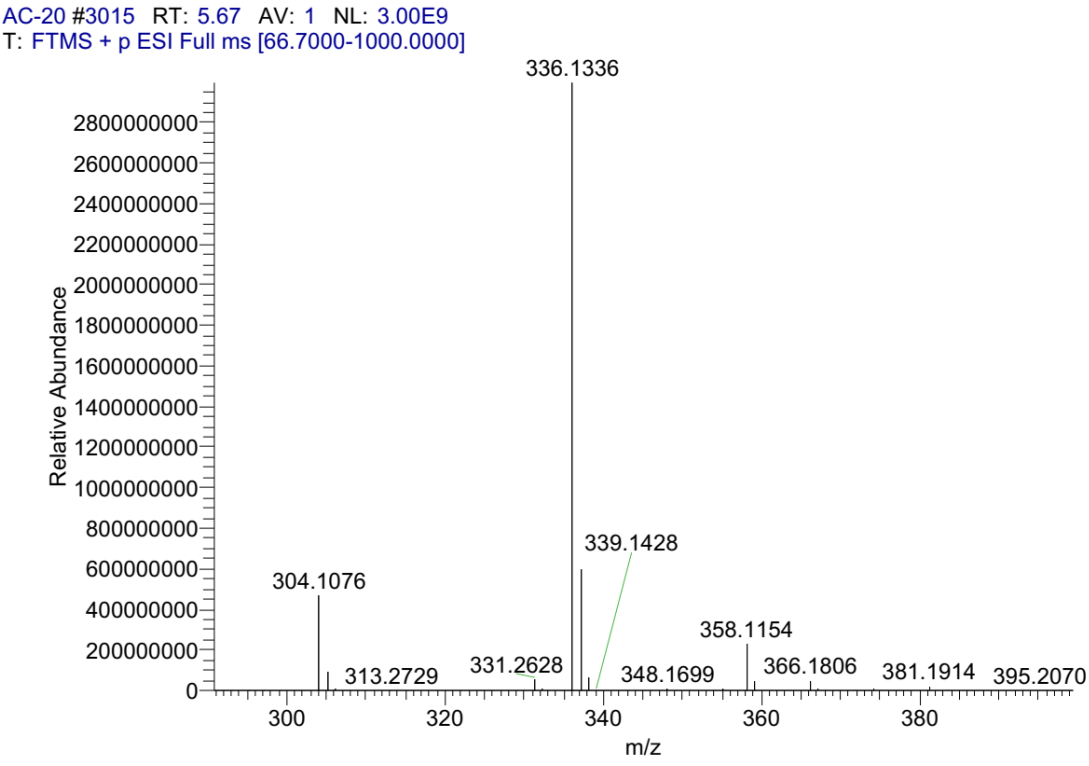

Figure S39. HRESIMS spectra of **5**.

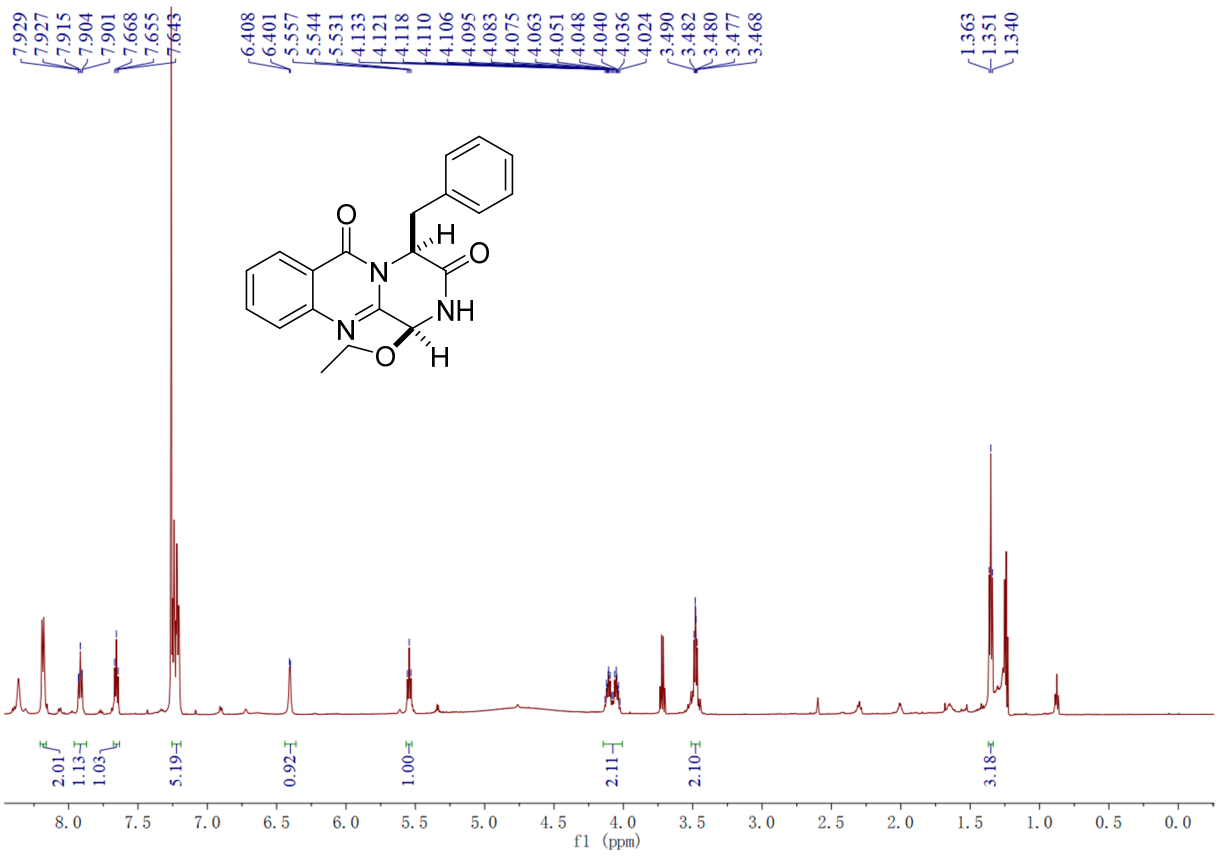

Figure S40. ^{1}H NMR spectra (600 MHz, $CDCl_3$) of **6**.

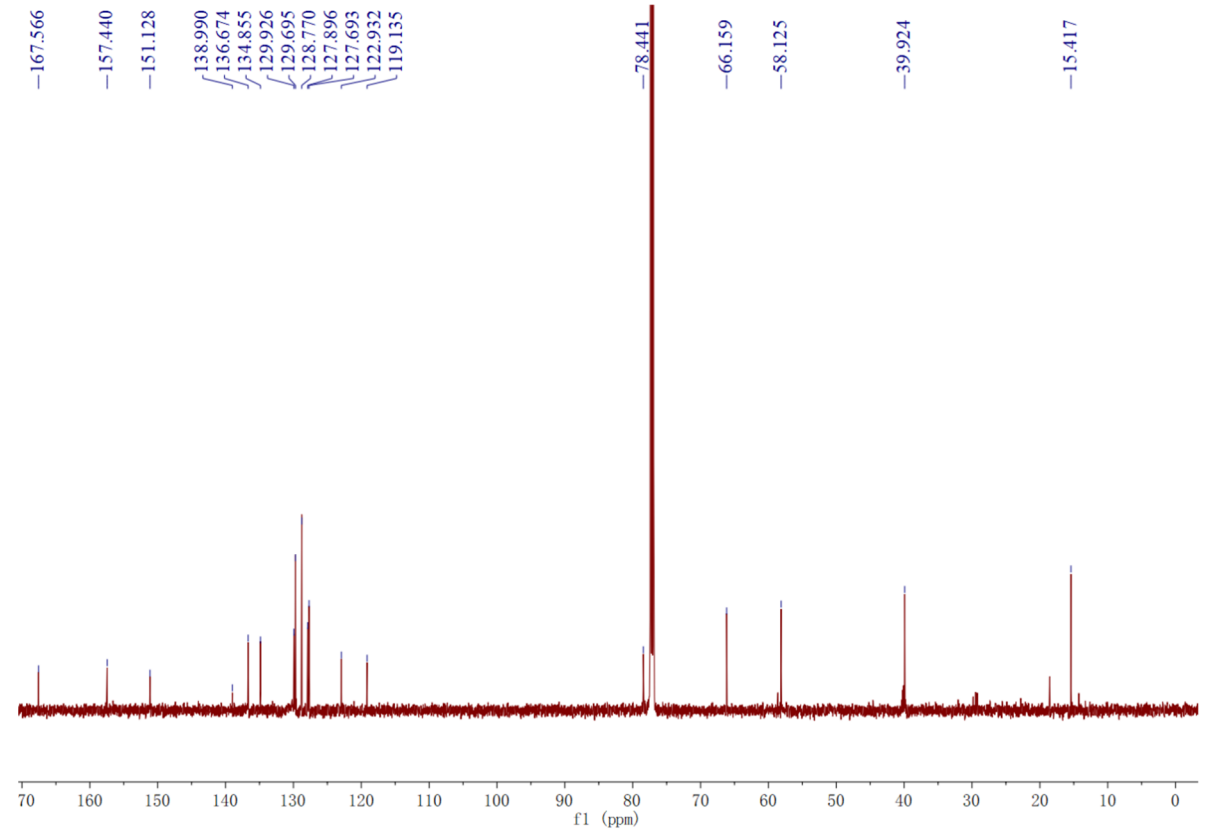

Figure S41. ^{13}C NMR spectra (150 MHz, $CDCl_3$) of **6**.

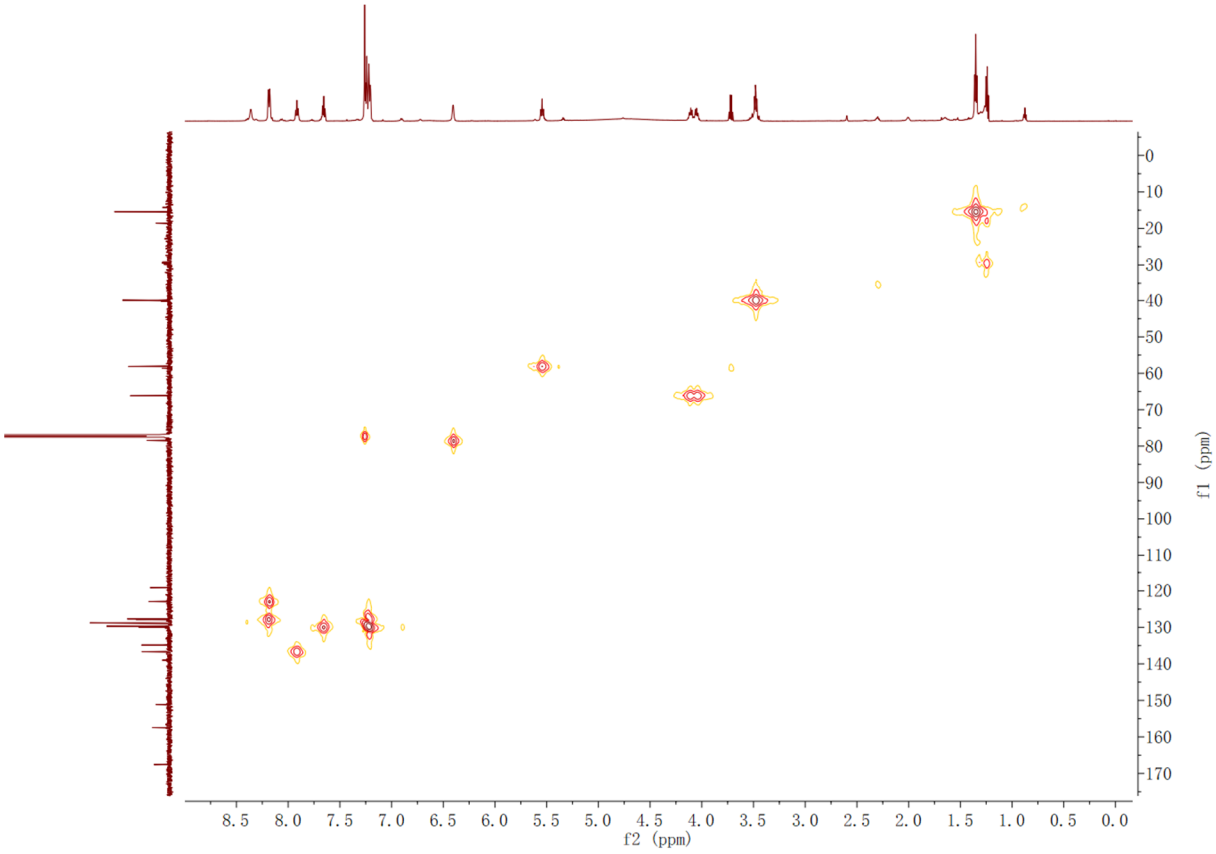

Figure S42. HMQC spectra ($CDCl_3$) of **6**.

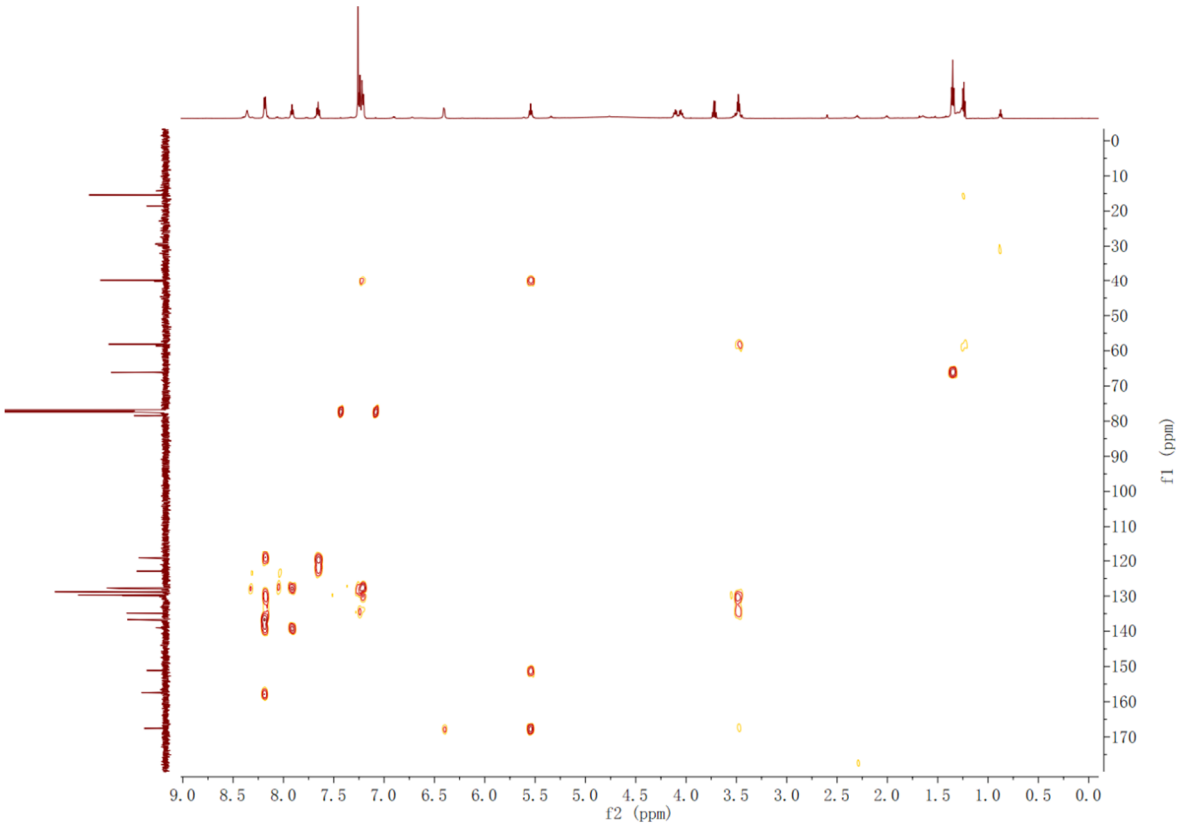

Figure S43. HMBC spectra ($CDCl_3$) of **6**.

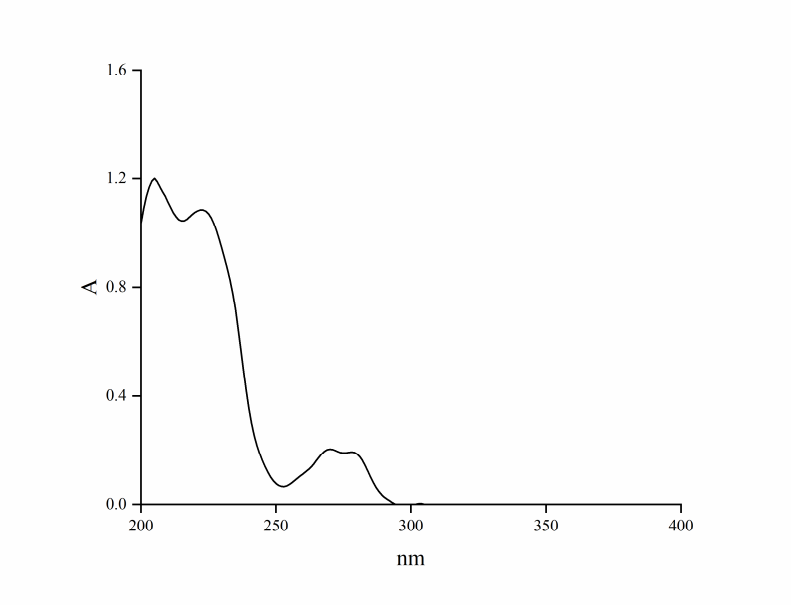

Figure S44. UV spectra (MeOH) of **6**.

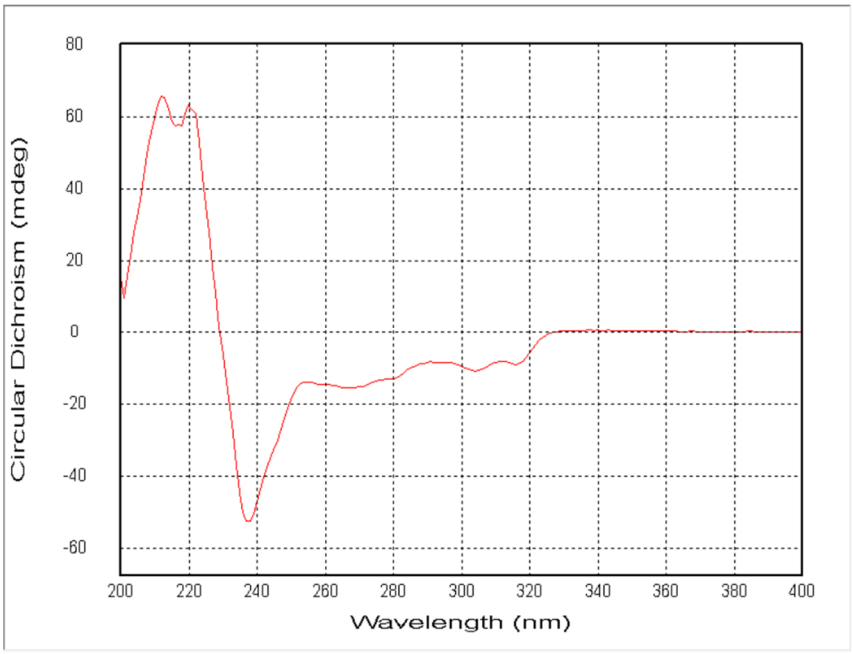

Figure S45. ECD spectra (MeOH) of **6**.

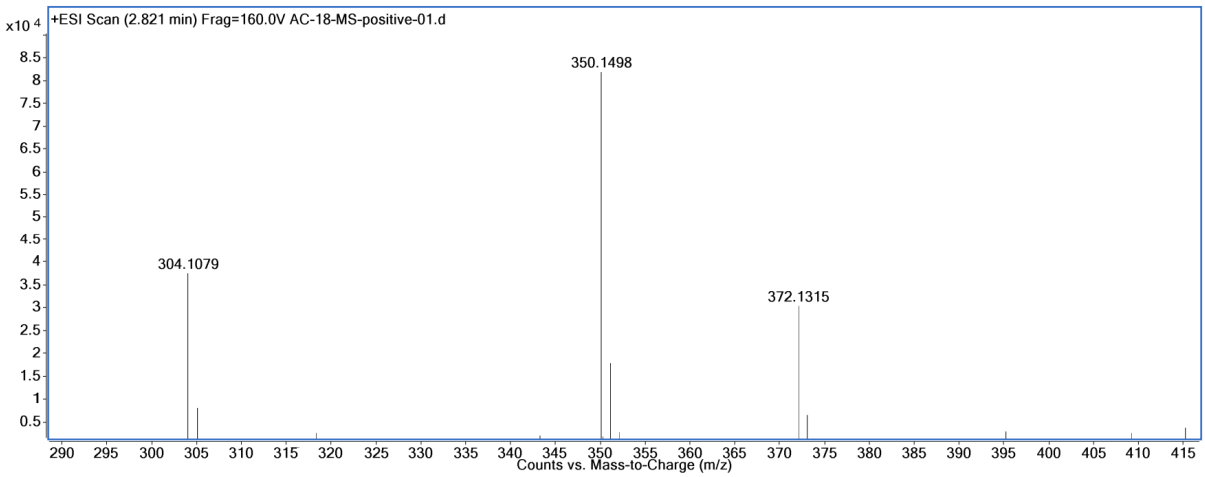

Figure S46. HRESIMS spectra of **6**.

Table S1. Energies of conformers of **1** with Boltzmann distribution over 1% at MMFF.

Label	E (kcal/mol)	rel. E (kcal/mol)	Boltzmann Dist
M0001	51.83	0.00	0.214
M0002	52.03	0.20	0.153
M0003	52.17	0.34	0.121
M0004	52.26	0.43	0.103
M0005	52.26	0.43	0.103
M0006	52.55	0.72	0.064
M0007	52.66	0.83	0.053
M0008	52.84	1.01	0.039
M0009	53.26	1.43	0.019
M0010	53.45	1.62	0.014
M0011	53.53	1.70	0.012
M0012	53.62	1.79	0.010

Table S2. Gibbs free energies[a] and equilibrium populations[b] of low-energy conformers of **1**.

Conformers	In MeOH	
	G	*P* (%)
1-1	-804640.53898995	21.78
1-2	-804640.19950704	12.27
1-3	-804640.14616869	11.22
1-4	-804639.38311653	3.09
1-5	-804639.77217273	5.96
1-6	-804638.47824711	0.67
1-7	-804640.38022992	16.66
1-8	-804639.18419586	2.21
1-9	-804640.14616869	11.22
1-10	-804639.64165065	4.78

1-11	-804639.93281529	7.82
1-12	-804639.21243381	2.32

[a]B3LYP/6-31G(d,p), in kcal/mol. [b]From *G* values at 298.15K.

Table S3. Cartesian coordinates for the low-energy reoptimized MMFF conformers of **1** at B3LYP/6-31+G(d,p) level of theory in gas.

1-1		Standard Orientation (Ångstroms)			
Center number	Atomic number	Atomic Type	X	Y	Z
1.	6.	0.	4.644157	2.411265	0.291423
2.	6.	0.	3.805298	1.304376	0.136323
3.	6.	0.	2.437460	1.419027	-0.224611
4.	6.	0.	1.920899	2.703780	-0.478794
5.	6.	0.	2.749067	3.809151	-0.325865
6.	6.	0.	4.095674	3.667392	0.062220
7.	7.	0.	4.080717	-0.040490	0.258156
8.	6.	0.	2.958320	-0.793353	-0.009286
9.	6.	0.	1.903761	0.069691	-0.309795
10.	6.	0.	3.050259	-2.319121	0.032501
11.	7.	0.	-0.748569	1.274035	0.574396
12.	6.	0.	-0.619346	0.226627	-0.359857
13.	6.	0.	0.562170	-0.334789	-0.702772
14.	6.	0.	-1.885417	2.008200	0.809546
15.	6.	0.	-2.986086	1.720500	-0.199096
16.	7.	0.	-3.019211	0.296191	-0.565213
17.	6.	0.	-1.885587	-0.406431	-0.864255
18.	6.	0.	-4.424297	2.005275	0.229864
19.	6.	0.	-5.216045	1.095870	-0.727859
20.	6.	0.	-4.392165	-0.200003	-0.767762
21.	8.	0.	-1.894723	-1.493102	-1.441591
22.	8.	0.	-1.972394	2.845059	1.693655
23.	6.	0.	4.266252	-2.714397	0.863315
24.	6.	0.	3.136749	-2.857227	-1.413952
25.	6.	0.	5.389763	-3.292762	0.435938
26.	6.	0.	1.819028	-2.937233	0.745144
27.	8.	0.	-4.848424	-1.014020	0.288025
28.	6.	0.	-4.373742	-2.363634	0.307446
29.	6.	0.	-5.212359	-3.130251	1.315772
30.	1.	0.	-2.747981	2.324147	-1.093011
31.	1.	0.	5.686855	2.293109	0.571907
32.	1.	0.	0.892835	2.832783	-0.798148

33.	1.	0.	2.352367	4.802307	-0.513443
34.	1.	0.	4.716626	4.550870	0.174571
35.	1.	0.	4.971867	-0.447905	0.498075
36.	1.	0.	0.048147	1.492708	1.161298
37.	1.	0.	0.449360	-1.214020	-1.328953
38.	1.	0.	-4.570877	1.696487	1.268152
39.	1.	0.	-4.677110	3.063364	0.145518
40.	1.	0.	-6.235420	0.888917	-0.399528
41.	1.	0.	-5.254599	1.538714	-1.729672
42.	1.	0.	-4.438919	-0.747243	-1.717160
43.	1.	0.	4.168073	-2.493994	1.927330
44.	1.	0.	3.222737	-3.948520	-1.414092
45.	1.	0.	2.239245	-2.588618	-1.976476
46.	1.	0.	3.997212	-2.440610	-1.945595
47.	1.	0.	6.183572	-3.551300	1.130550
48.	1.	0.	5.558428	-3.547284	-0.605667
49.	1.	0.	1.719215	-2.546884	1.762639
50.	1.	0.	0.889935	-2.727578	0.213301
51.	1.	0.	1.940453	-4.023286	0.806215
52.	1.	0.	-3.311866	-2.393072	0.578456
53.	1.	0.	-4.460313	-2.802846	-0.696680
54.	1.	0.	-6.268335	-3.120302	1.030116
55.	1.	0.	-4.877152	-4.170592	1.374525
56.	1.	0.	-5.123479	-2.682730	2.310141

1-2		Standard Orientation (Ångstroms)			
Center number	Atom number	Type	X	Y	Z
1.	6.	0.	4.166535	2.896443	0.282706
2.	6.	0.	3.544364	1.645954	0.237308
3.	6.	0.	2.146764	1.477385	0.422249
4.	6.	0.	1.367873	2.614016	0.713528
5.	6.	0.	1.981039	3.860746	0.758128
6.	6.	0.	3.364669	4.003263	0.536758
7.	7.	0.	4.079350	0.390975	0.049545
8.	6.	0.	3.091366	-0.571510	0.100135
9.	6.	0.	1.868599	0.056579	0.320882
10.	6.	0.	3.476396	-2.043886	-0.036671
11.	7.	0.	-0.733788	0.830336	-1.007589
12.	6.	0.	-0.600519	-0.231884	-0.090630
13.	6.	0.	0.567842	-0.587540	0.488500

14.	6.	0.	-1.813357	1.060143	-1.825792
15.	6.	0.	-2.838237	-0.060322	-1.786731
16.	7.	0.	-2.950026	-0.650799	-0.445182
17.	6.	0.	-1.853081	-0.963701	0.308558
18.	6.	0.	-4.283915	0.285660	-2.138614
19.	6.	0.	-5.043558	-0.879017	-1.476329
20.	6.	0.	-4.329027	-1.065663	-0.129340
21.	8.	0.	-1.886938	-1.733717	1.266507
22.	8.	0.	-1.895992	2.027086	-2.565984
23.	6.	0.	4.801146	-2.135056	-0.785931
24.	6.	0.	2.438443	-2.818616	-0.887100
25.	6.	0.	5.979678	-2.535615	-0.306057
26.	6.	0.	3.559168	-2.670820	1.373556
27.	8.	0.	-4.962896	-0.214536	0.796978
28.	6.	0.	-4.586330	-0.367981	2.169017
29.	6.	0.	-5.598503	0.390515	3.010294
30.	1.	0.	-2.470914	-0.824830	-2.494806
31.	1.	0.	5.237750	2.998778	0.134695
32.	1.	0.	0.307007	2.520737	0.924031
33.	1.	0.	1.384338	4.741087	0.976550
34.	1.	0.	3.814156	4.990638	0.577732
35.	1.	0.	5.050649	0.173489	-0.114259
36.	1.	0.	0.028144	1.493083	-1.094241
37.	1.	0.	0.479598	-1.429702	1.169066
38.	1.	0.	-4.562052	1.239436	-1.682431
39.	1.	0.	-4.438601	0.359509	-3.216111
40.	1.	0.	-6.105017	-0.682826	-1.319693
41.	1.	0.	-4.941470	-1.790121	-2.076844
42.	1.	0.	-4.316869	-2.095726	0.247464
43.	1.	0.	4.739881	-1.838972	-1.834177
44.	1.	0.	2.765264	-3.856155	-1.007500
45.	1.	0.	1.453295	-2.821876	-0.418301
46.	1.	0.	2.335351	-2.373572	-1.881429
47.	1.	0.	6.856627	-2.580538	-0.945115
48.	1.	0.	6.116872	-2.849407	0.723967
49.	1.	0.	4.283268	-2.146454	2.003778
50.	1.	0.	2.587170	-2.615231	1.870408
51.	1.	0.	3.850770	-3.724179	1.311545
52.	1.	0.	-3.573612	0.018909	2.333673
53.	1.	0.	-4.568812	-1.434808	2.433022
54.	1.	0.	-6.604464	-0.014659	2.866600
55.	1.	0.	-5.340922	0.315869	4.071467

56.	1.	0.	-5.613683	1.448711	2.732942

1-3		Standard Orientation (Ångstroms)			
Center number	Atom number	Type	X	Y	Z
1.	6.	0.	-4.588818	-2.419101	0.278286
2.	6.	0.	-3.768987	-1.303181	0.086659
3.	6.	0.	-2.415410	-1.406676	-0.324229
4.	6.	0.	-1.888519	-2.686593	-0.579254
5.	6.	0.	-2.695830	-3.800706	-0.385589
6.	6.	0.	-4.031127	-3.670313	0.044503
7.	7.	0.	-4.052126	0.039142	0.205233
8.	6.	0.	-2.951820	0.803495	-0.129599
9.	6.	0.	-1.898140	-0.053625	-0.448332
10.	6.	0.	-3.060284	2.317261	0.053638
11.	7.	0.	0.707536	-1.210254	0.579590
12.	6.	0.	0.618026	-0.223394	-0.422554
13.	6.	0.	-0.545676	0.325596	-0.838533
14.	6.	0.	1.827188	-1.940496	0.895504
15.	6.	0.	2.963676	-1.724911	-0.090787
16.	7.	0.	3.023030	-0.327062	-0.544984
17.	6.	0.	1.907032	0.362845	-0.928576
18.	6.	0.	4.384550	-1.994293	0.400977
19.	6.	0.	5.214991	-1.155055	-0.587708
20.	6.	0.	4.406745	0.142636	-0.735727
21.	8.	0.	1.946279	1.407166	-1.577550
22.	8.	0.	1.874563	-2.725230	1.828998
23.	6.	0.	-4.477264	2.732223	-0.329011
24.	6.	0.	-2.102817	3.104594	-0.871568
25.	6.	0.	-5.420341	3.232723	0.471140
26.	6.	0.	-2.726785	2.656335	1.525316
27.	8.	0.	4.839599	1.017522	0.280639
28.	6.	0.	4.371593	2.367433	0.206191
29.	6.	0.	5.191463	3.191881	1.183910
30.	1.	0.	2.748482	-2.382094	-0.952229
31.	1.	0.	-5.622647	-2.311876	0.593652
32.	1.	0.	-0.868860	-2.802913	-0.929627
33.	1.	0.	-2.292839	-4.791313	-0.573080
34.	1.	0.	-4.636259	-4.560290	0.187956
35.	1.	0.	-4.945982	0.441374	0.444706
36.	1.	0.	-0.114895	-1.397519	1.141328

37.	1.	0.	-0.407564	1.155158	-1.521254
38.	1.	0.	4.503008	-1.620615	1.421404
39.	1.	0.	4.628303	-3.057790	0.392393
40.	1.	0.	6.225964	-0.936410	-0.241457
41.	1.	0.	5.279703	-1.661648	-1.557466
42.	1.	0.	4.488265	0.628239	-1.715768
43.	1.	0.	-4.708618	2.593740	-1.385861
44.	1.	0.	-2.314813	4.173967	-0.779331
45.	1.	0.	-1.056723	2.947990	-0.602277
46.	1.	0.	-2.236109	2.822534	-1.920448
47.	1.	0.	-6.393982	3.511711	0.079345
48.	1.	0.	-5.259953	3.403388	1.531119
49.	1.	0.	-3.391955	2.136564	2.220966
50.	1.	0.	-1.702137	2.350819	1.752020
51.	1.	0.	-2.811699	3.733256	1.703341
52.	1.	0.	3.304192	2.417264	0.451980
53.	1.	0.	4.481860	2.743509	-0.820831
54.	1.	0.	6.253015	3.163471	0.921144
55.	1.	0.	4.857846	4.234349	1.173587
56.	1.	0.	5.081130	2.804617	2.201164

1-4		Standard Orientation (Ångstroms)			
Center number	Atom number	Type	X	Y	Z
1.	6.	0.	-4.937502	-2.077982	0.366335
2.	6.	0.	-4.027202	-1.033271	0.187246
3.	6.	0.	-2.677887	-1.242482	-0.198194
4.	6.	0.	-2.258022	-2.561440	-0.456712
5.	6.	0.	-3.157485	-3.606073	-0.281443
6.	6.	0.	-4.482352	-3.370374	0.134105
7.	7.	0.	-4.212174	0.329096	0.299490
8.	6.	0.	-3.045605	1.003293	0.002894
9.	6.	0.	-2.056042	0.067288	-0.299334
10.	6.	0.	-2.992395	2.529090	0.021564
11.	7.	0.	0.506914	-1.346006	0.541846
12.	6.	0.	0.449137	-0.266091	-0.364054
13.	6.	0.	-0.690151	0.389818	-0.682309
14.	6.	0.	1.588396	-2.164741	0.754228
15.	6.	0.	2.701369	-1.933380	-0.254865
16.	7.	0.	2.837093	-0.505634	-0.581192
17.	6.	0.	1.755048	0.283292	-0.863886

18.	6.	0.	4.117073	-2.335000	0.154174
19.	6.	0.	4.966750	-1.462290	-0.787997
20.	6.	0.	4.240322	-0.108966	-0.788704
21.	8.	0.	1.843089	1.373007	-1.427655
22.	8.	0.	1.619780	-3.024025	1.620909
23.	6.	0.	-1.774046	2.977062	0.820334
24.	6.	0.	-4.234681	3.114397	0.742482
25.	6.	0.	-0.826302	3.830137	0.435834
26.	6.	0.	-2.983911	3.055717	-1.431896
27.	8.	0.	4.766952	0.643994	0.280503
28.	6.	0.	4.375531	2.018110	0.346703
29.	6.	0.	5.268145	2.700361	1.369313
30.	1.	0.	2.413983	-2.493054	-1.162941
31.	1.	0.	-5.963931	-1.886567	0.666238
32.	1.	0.	-1.248925	-2.763610	-0.797149
33.	1.	0.	-2.834496	-4.624810	-0.473046
34.	1.	0.	-5.160458	-4.208150	0.264337
35.	1.	0.	-5.068452	0.770358	0.590475
36.	1.	0.	-0.295454	-1.513175	1.137602
37.	1.	0.	-0.515109	1.291654	-1.257597
38.	1.	0.	4.293451	-2.064281	1.198443
39.	1.	0.	4.290088	-3.406420	0.041186
40.	1.	0.	6.001178	-1.339516	-0.464319
41.	1.	0.	4.965021	-1.881384	-1.800715
42.	1.	0.	4.318881	0.456089	-1.725604
43.	1.	0.	-1.726632	2.555754	1.824516
44.	1.	0.	-4.151864	4.203285	0.778149
45.	1.	0.	-5.163527	2.876704	0.209902
46.	1.	0.	-4.315183	2.753044	1.773033
47.	1.	0.	-0.015693	4.098316	1.105855
48.	1.	0.	-0.799586	4.276655	-0.552830
49.	1.	0.	-2.107487	2.711150	-1.985102
50.	1.	0.	-3.874237	2.706344	-1.962860
51.	1.	0.	-2.988739	4.150265	-1.445957
52.	1.	0.	3.319783	2.103409	0.630091
53.	1.	0.	4.479174	2.483070	-0.644164
54.	1.	0.	6.319009	2.635544	1.072226
55.	1.	0.	4.997694	3.756830	1.464091
56.	1.	0.	5.160993	2.227650	2.350151

1-5	Standard Orientation (Ångstroms)

Center number	Atom number	Type	X	Y	Z
1.	6.	0.	-4.106763	2.925798	-0.137625
2.	6.	0.	-3.505320	1.665401	-0.195062
3.	6.	0.	-2.118707	1.489976	-0.441241
4.	6.	0.	-1.326105	2.631273	-0.669160
5.	6.	0.	-1.917431	3.887592	-0.605833
6.	6.	0.	-3.292366	4.034670	-0.336991
7.	7.	0.	-4.052485	0.408505	-0.073279
8.	6.	0.	-3.085159	-0.564346	-0.246269
9.	6.	0.	-1.859799	0.061433	-0.456452
10.	6.	0.	-3.495205	-2.021273	-0.042476
11.	7.	0.	0.684541	0.712331	1.015864
12.	6.	0.	0.592317	-0.259442	-0.000952
13.	6.	0.	-0.551797	-0.564506	-0.652736
14.	6.	0.	1.733739	0.870660	1.888222
15.	6.	0.	2.768421	-0.236458	1.780859
16.	7.	0.	2.932097	-0.697569	0.394664
17.	6.	0.	1.865497	-0.940988	-0.425265
18.	6.	0.	4.197581	0.084474	2.214054
19.	6.	0.	4.991354	-1.007347	1.472931
20.	6.	0.	4.325105	-1.072550	0.089980
21.	8.	0.	1.939987	-1.613250	-1.451849
22.	8.	0.	1.785139	1.766187	2.715921
23.	6.	0.	-4.904781	-2.193235	-0.597906
24.	6.	0.	-3.414861	-2.348485	1.466627
25.	6.	0.	-6.014582	-2.485537	0.082567
26.	6.	0.	-2.584088	-2.999901	-0.818609
27.	8.	0.	4.982158	-0.135260	-0.730860
28.	6.	0.	4.665257	-0.171713	-2.126001
29.	6.	0.	5.698656	0.671103	-2.853525
30.	1.	0.	2.384150	-1.066430	2.400722
31.	1.	0.	-5.170782	3.034940	0.051473
32.	1.	0.	-0.272045	2.533913	-0.910361
33.	1.	0.	-1.311323	4.772339	-0.774808
34.	1.	0.	-3.725221	5.029416	-0.294167
35.	1.	0.	-5.028500	0.193069	0.063910
36.	1.	0.	-0.080465	1.368025	1.127255
37.	1.	0.	-0.432626	-1.328064	-1.413789
38.	1.	0.	4.481604	1.078703	1.859130
39.	1.	0.	4.314478	0.058173	3.298495
40.	1.	0.	6.055340	-0.789485	1.372104

41.	1.	0.	4.879026	-1.971352	1.982216
42.	1.	0.	4.335930	-2.063350	-0.380451
43.	1.	0.	-4.974801	-2.057890	-1.677901
44.	1.	0.	-3.718740	-3.383177	1.655750
45.	1.	0.	-2.387544	-2.221887	1.817583
46.	1.	0.	-4.053133	-1.686178	2.058580
47.	1.	0.	-6.966868	-2.601513	-0.426344
48.	1.	0.	-6.020088	-2.639580	1.157174
49.	1.	0.	-2.549297	-2.755197	-1.884575
50.	1.	0.	-1.563759	-2.990814	-0.430506
51.	1.	0.	-2.975143	-4.016519	-0.715954
52.	1.	0.	3.653843	0.214483	-2.299520
53.	1.	0.	4.677191	-1.211326	-2.482824
54.	1.	0.	5.683933	1.701120	-2.485026
55.	1.	0.	6.704564	0.268613	-2.702104
56.	1.	0.	5.487152	0.686085	-3.927331

1-6		Standard Orientation (Ångstroms)			
Center number	Atom number	Type	X	Y	Z
1.	6.	0.	4.459124	2.734357	0.264641
2.	6.	0.	3.770656	1.519231	0.228049
3.	6.	0.	2.367636	1.424467	0.420723
4.	6.	0.	1.654130	2.601888	0.718734
5.	6.	0.	2.332839	3.814545	0.755597
6.	6.	0.	3.719575	3.883422	0.520892
7.	7.	0.	4.242392	0.236063	0.049277
8.	6.	0.	3.204997	-0.674378	0.112935
9.	6.	0.	2.016791	0.019946	0.323886
10.	6.	0.	3.463627	-2.173027	-0.010776
11.	7.	0.	-0.569679	0.970238	-0.952060
12.	6.	0.	-0.465600	-0.144801	-0.094272
13.	6.	0.	0.691191	-0.574907	0.457269
14.	6.	0.	-1.643900	1.279319	-1.750005
15.	6.	0.	-2.710855	0.198962	-1.758753
16.	7.	0.	-2.831548	-0.460084	-0.451022
17.	6.	0.	-1.739002	-0.856150	0.271268
18.	6.	0.	-4.145417	0.619655	-2.071990
19.	6.	0.	-4.942631	-0.551534	-1.468528
20.	6.	0.	-4.220958	-0.843232	-0.143732
21.	8.	0.	-1.795409	-1.679358	1.182811

22.	8.	0.	-1.693573	2.283860	-2.442396
23.	6.	0.	2.460696	-2.776946	-0.986466
24.	6.	0.	3.391602	-2.814824	1.393822
25.	6.	0.	1.694905	-3.849216	-0.791278
26.	6.	0.	4.873403	-2.442578	-0.598789
27.	8.	0.	-4.816007	-0.025699	0.837990
28.	6.	0.	-4.422623	-0.262198	2.193099
29.	6.	0.	-5.404587	0.471447	3.090546
30.	1.	0.	-2.381996	-0.538302	-2.513297
31.	1.	0.	5.533359	2.779151	0.109225
32.	1.	0.	0.592830	2.566321	0.943493
33.	1.	0.	1.785649	4.725162	0.979218
34.	1.	0.	4.221407	4.845480	0.554976
35.	1.	0.	5.200513	-0.003075	-0.143878
36.	1.	0.	0.217077	1.605050	-1.021138
37.	1.	0.	0.576439	-1.464854	1.066727
38.	1.	0.	-4.381974	1.554890	-1.557539
39.	1.	0.	-4.308601	0.762352	-3.141316
40.	1.	0.	-5.993783	-0.324175	-1.286435
41.	1.	0.	-4.883389	-1.429291	-2.122284
42.	1.	0.	-4.243005	-1.893187	0.172864
43.	1.	0.	2.423752	-2.271884	-1.951552
44.	1.	0.	3.618601	-3.884523	1.343426
45.	1.	0.	4.122103	-2.345091	2.058843
46.	1.	0.	2.402900	-2.695858	1.843070
47.	1.	0.	1.039664	-4.214911	-1.575665
48.	1.	0.	1.671841	-4.393624	0.147154
49.	1.	0.	4.998532	-1.982870	-1.584724
50.	1.	0.	5.666441	-2.077636	0.065101
51.	1.	0.	5.018262	-3.519433	-0.713350
52.	1.	0.	-3.399216	0.093624	2.362114
53.	1.	0.	-4.424649	-1.341789	2.398914
54.	1.	0.	-5.400232	1.543188	2.870660
55.	1.	0.	-6.421510	0.096589	2.941642
56.	1.	0.	-5.132854	0.334062	4.141902

1-7		Standard Orientation (Ångstroms)			
Center number	Atom number	Type	X	Y	Z
1.	6.	0.	-4.887181	-2.163875	0.352398
2.	6.	0.	-3.992895	-1.098473	0.220733

3.	6.	0.	-2.645215	-1.268204	-0.189149
4.	6.	0.	-2.209961	-2.565682	-0.520646
5.	6.	0.	-3.093203	-3.630700	-0.392106
6.	6.	0.	-4.416983	-3.435611	0.047503
7.	7.	0.	-4.194915	0.253392	0.407820
8.	6.	0.	-3.042151	0.958847	0.132417
9.	6.	0.	-2.043046	0.053439	-0.229887
10.	6.	0.	-2.992602	2.479850	0.262851
11.	7.	0.	0.549759	-1.358935	0.518822
12.	6.	0.	0.468103	-0.225162	-0.317148
13.	6.	0.	-0.685915	0.422336	-0.599500
14.	6.	0.	1.640983	-2.181341	0.656058
15.	6.	0.	2.734328	-1.867792	-0.352528
16.	7.	0.	2.856177	-0.418062	-0.569937
17.	6.	0.	1.764528	0.380430	-0.776990
18.	6.	0.	4.159287	-2.290955	-0.001479
19.	6.	0.	4.987948	-1.339382	-0.884224
20.	6.	0.	4.253961	0.004364	-0.762919
21.	8.	0.	1.836871	1.515663	-1.244941
22.	8.	0.	1.693597	-3.099170	1.459184
23.	6.	0.	-2.707693	3.063290	-1.118257
24.	6.	0.	-1.934006	2.881555	1.312264
25.	6.	0.	-1.701628	3.865941	-1.464981
26.	6.	0.	-4.362833	3.042001	0.716415
27.	8.	0.	4.792666	0.669512	0.357006
28.	6.	0.	4.396696	2.031435	0.542158
29.	6.	0.	5.307408	2.634469	1.598017
30.	1.	0.	2.432227	-2.357461	-1.295532
31.	1.	0.	-5.912892	-2.003216	0.672134
32.	1.	0.	-1.201554	-2.734751	-0.880718
33.	1.	0.	-2.758333	-4.633385	-0.639733
34.	1.	0.	-5.082407	-4.288487	0.139614
35.	1.	0.	-5.058823	0.668434	0.714421
36.	1.	0.	-0.245792	-1.579326	1.106357
37.	1.	0.	-0.545160	1.357460	-1.132393
38.	1.	0.	4.352790	-2.104660	1.058113
39.	1.	0.	4.336369	-3.348507	-0.203738
40.	1.	0.	6.027020	-1.236090	-0.568806
41.	1.	0.	4.971148	-1.675195	-1.927396
42.	1.	0.	4.314790	0.645480	-1.650844
43.	1.	0.	-3.440493	2.781385	-1.874838
44.	1.	0.	-1.901209	3.969942	1.424312

45.	1.	0.	-2.186803	2.447629	2.284335
46.	1.	0.	-0.937021	2.531836	1.037419
47.	1.	0.	-1.609785	4.234802	-2.481842
48.	1.	0.	-0.928635	4.174960	-0.769316
49.	1.	0.	-5.158115	2.813801	-0.001977
50.	1.	0.	-4.650592	2.654312	1.700573
51.	1.	0.	-4.299724	4.129987	0.795168
52.	1.	0.	3.346807	2.086732	0.853813
53.	1.	0.	4.477229	2.575091	-0.409965
54.	1.	0.	5.223340	2.083049	2.539190
55.	1.	0.	6.352004	2.600773	1.274812
56.	1.	0.	5.033814	3.677921	1.783905

1-8		Standard Orientation (Ångstroms)			
Center number	Atom number	Type	X	Y	Z
1.	6.	0.	4.447234	2.710820	0.475628
2.	6.	0.	3.759757	1.506330	0.307429
3.	6.	0.	2.359980	1.385041	0.509477
4.	6.	0.	1.648960	2.518605	0.950184
5.	6.	0.	2.326558	3.720848	1.117049
6.	6.	0.	3.710013	3.820285	0.873622
7.	7.	0.	4.230785	0.254576	-0.028235
8.	6.	0.	3.197529	-0.661709	-0.049340
9.	6.	0.	2.010611	-0.000535	0.259832
10.	6.	0.	3.442264	-2.130048	-0.388807
11.	7.	0.	-0.589810	1.075175	-0.874206
12.	6.	0.	-0.473834	-0.132829	-0.155012
13.	6.	0.	0.690276	-0.615293	0.337027
14.	6.	0.	-1.670185	1.469380	-1.625312
15.	6.	0.	-2.730035	0.390073	-1.756646
16.	7.	0.	-2.840309	-0.417879	-0.534458
17.	6.	0.	-1.742118	-0.888643	0.132769
18.	6.	0.	-4.168747	0.834702	-2.013317
19.	6.	0.	-4.956347	-0.402986	-1.544666
20.	6.	0.	-4.226380	-0.838983	-0.265067
21.	8.	0.	-1.789992	-1.812234	0.942643
22.	8.	0.	-1.729837	2.548511	-2.193346
23.	6.	0.	3.042958	-2.962764	0.825812
24.	6.	0.	4.944911	-2.398424	-0.649557
25.	6.	0.	2.150685	-3.951876	0.869270

26.	6.	0.	2.652669	-2.509429	-1.659694
27.	8.	0.	-4.818809	-0.139499	0.805405
28.	6.	0.	-4.417308	-0.526070	2.123231
29.	6.	0.	-5.399577	0.093317	3.102718
30.	1.	0.	-2.399236	-0.251446	-2.593442
31.	1.	0.	5.519020	2.776477	0.310969
32.	1.	0.	0.590612	2.454921	1.183035
33.	1.	0.	1.781215	4.598227	1.450921
34.	1.	0.	4.211025	4.773359	1.012088
35.	1.	0.	5.190216	0.037846	-0.240400
36.	1.	0.	0.192671	1.719019	-0.870724
37.	1.	0.	0.598246	-1.571123	0.843881
38.	1.	0.	-4.407845	1.703159	-1.393792
39.	1.	0.	-4.338120	1.098312	-3.058416
40.	1.	0.	-6.007963	-0.204702	-1.333636
41.	1.	0.	-4.894604	-1.199965	-2.294554
42.	1.	0.	-4.243000	-1.918023	-0.068756
43.	1.	0.	3.578898	-2.697191	1.737385
44.	1.	0.	5.090150	-3.457313	-0.877033
45.	1.	0.	5.313798	-1.822364	-1.506241
46.	1.	0.	5.561042	-2.166255	0.226242
47.	1.	0.	1.957615	-4.487914	1.793235
48.	1.	0.	1.573961	-4.260413	0.003406
49.	1.	0.	1.580206	-2.351947	-1.528218
50.	1.	0.	2.981803	-1.894866	-2.502840
51.	1.	0.	2.821949	-3.559677	-1.917791
52.	1.	0.	-3.395421	-0.184595	2.327551
53.	1.	0.	-4.411210	-1.622057	2.204659
54.	1.	0.	-5.402356	1.183266	3.007924
55.	1.	0.	-6.414936	-0.268222	2.915220
56.	1.	0.	-5.122537	-0.162720	4.130224

1-9		Standard Orientation (Ångstroms)			
Center number	Atom number	Type	X	Y	Z
1.	6.	0.	-4.588037	-2.419732	0.278799
2.	6.	0.	-3.768507	-1.303628	0.086975
3.	6.	0.	-2.414967	-1.406838	-0.324098
4.	6.	0.	-1.887787	-2.686642	-0.579044
5.	6.	0.	-2.694809	-3.800939	-0.385200
6.	6.	0.	-4.030085	-3.670832	0.045032

7.	7.	0.	-4.051912	0.038637	0.205620
8.	6.	0.	-2.951855	0.803225	-0.129541
9.	6.	0.	-1.898045	-0.053667	-0.448370
10.	6.	0.	-3.060761	2.316985	0.053534
11.	7.	0.	0.707849	-1.209425	0.579839
12.	6.	0.	0.618122	-0.222906	-0.422612
13.	6.	0.	-0.545666	0.325804	-0.838690
14.	6.	0.	1.827440	-1.939936	0.895412
15.	6.	0.	2.963717	-1.724309	-0.091124
16.	7.	0.	3.023103	-0.326358	-0.544973
17.	6.	0.	1.907055	0.363410	-0.928805
18.	6.	0.	4.384723	-1.993994	0.400100
19.	6.	0.	5.214925	-1.154666	-0.588725
20.	6.	0.	4.406814	0.143156	-0.736117
21.	8.	0.	1.946223	1.407612	-1.577921
22.	8.	0.	1.874863	-2.724824	1.828764
23.	6.	0.	-4.477664	2.731507	-0.329881
24.	6.	0.	-2.103021	3.104514	-0.871218
25.	6.	0.	-5.421376	3.231618	0.469767
26.	6.	0.	-2.728152	2.656246	1.525370
27.	8.	0.	4.840222	1.017628	0.280386
28.	6.	0.	4.370893	2.367154	0.207409
29.	6.	0.	5.190292	3.191440	1.185644
30.	1.	0.	2.748150	-2.381256	-0.952654
31.	1.	0.	-5.621845	-2.312725	0.594312
32.	1.	0.	-0.868139	-2.802764	-0.929519
33.	1.	0.	-2.291594	-4.791464	-0.572643
34.	1.	0.	-4.634988	-4.560943	0.188615
35.	1.	0.	-4.945960	0.440670	0.444706
36.	1.	0.	-0.114616	-1.396910	1.141454
37.	1.	0.	-0.407721	1.155184	-1.521670
38.	1.	0.	4.503570	-1.620527	1.420554
39.	1.	0.	4.628341	-3.057521	0.391190
40.	1.	0.	6.226068	-0.936263	-0.242815
41.	1.	0.	5.279170	-1.661066	-1.558611
42.	1.	0.	4.487958	0.629140	-1.716009
43.	1.	0.	-4.708369	2.592978	-1.386867
44.	1.	0.	-2.315221	4.173842	-0.778983
45.	1.	0.	-1.057020	2.948006	-0.601513
46.	1.	0.	-2.235857	2.822504	-1.920169
47.	1.	0.	-6.394900	3.510260	0.077438
48.	1.	0.	-5.261667	3.402222	1.529859

49.	1.	0.	-3.393580	2.136352	2.220676
50.	1.	0.	-1.703550	2.351010	1.752650
51.	1.	0.	-2.813448	3.733159	1.703258
52.	1.	0.	3.303522	2.415725	0.453642
53.	1.	0.	4.480362	2.744289	-0.819317
54.	1.	0.	5.080622	2.803068	2.202545
55.	1.	0.	6.251785	3.164296	0.922522
56.	1.	0.	4.855690	4.233602	1.176427

1-10		Standard Orientation (Ångstroms)			
Center number	Atom number	Type	X	Y	Z
1.	6.	0.	-4.769690	-2.296893	-0.006026
2.	6.	0.	-3.891289	-1.210373	-0.036278
3.	6.	0.	-2.515839	-1.341468	-0.361420
4.	6.	0.	-2.031482	-2.616489	-0.710265
5.	6.	0.	-2.899330	-3.701406	-0.682019
6.	6.	0.	-4.253666	-3.546751	-0.326874
7.	7.	0.	-4.127449	0.128003	0.191575
8.	6.	0.	-2.972192	0.861108	0.026318
9.	6.	0.	-1.936410	-0.009815	-0.312163
10.	6.	0.	-3.017914	2.380719	0.190636
11.	7.	0.	0.629142	-1.367024	0.584299
12.	6.	0.	0.578620	-0.248006	-0.269316
13.	6.	0.	-0.567226	0.377052	-0.621383
14.	6.	0.	1.735639	-2.132935	0.851239
15.	6.	0.	2.926208	-1.809623	-0.037994
16.	7.	0.	2.985650	-0.387186	-0.398935
17.	6.	0.	1.885638	0.372294	-0.668621
18.	6.	0.	4.310592	-2.075351	0.556401
19.	6.	0.	5.198234	-1.158382	-0.302195
20.	6.	0.	4.366499	0.126758	-0.467289
21.	8.	0.	1.950914	1.501762	-1.156283
22.	8.	0.	1.741539	-3.033780	1.675381
23.	6.	0.	-4.243691	2.746312	1.020975
24.	6.	0.	-3.050350	3.035477	-1.209188
25.	6.	0.	-5.339742	3.387895	0.612813
26.	6.	0.	-1.788143	2.900012	0.980050
27.	8.	0.	4.641428	1.006058	0.599416
28.	6.	0.	4.682753	2.405984	0.276936
29.	6.	0.	6.066749	2.837760	-0.195966

30.	1.	0.	2.799525	-2.419027	-0.950443
31.	1.	0.	-5.817482	-2.167433	0.249387
32.	1.	0.	-0.997371	-2.752321	-1.006966
33.	1.	0.	-2.528404	-4.687816	-0.943455
34.	1.	0.	-4.906138	-4.414417	-0.313117
35.	1.	0.	-5.012117	0.544591	0.439561
36.	1.	0.	-0.209624	-1.614155	1.096947
37.	1.	0.	-0.400394	1.293724	-1.177580
38.	1.	0.	4.328049	-1.763258	1.604271
39.	1.	0.	4.584192	-3.130304	0.507497
40.	1.	0.	6.163533	-0.928846	0.150742
41.	1.	0.	5.373723	-1.613041	-1.284398
42.	1.	0.	4.519654	0.629302	-1.428367
43.	1.	0.	-4.179217	2.441859	2.066671
44.	1.	0.	-3.103909	4.125385	-1.122517
45.	1.	0.	-2.146515	2.783955	-1.769625
46.	1.	0.	-3.908492	2.690296	-1.793158
47.	1.	0.	-6.144347	3.615147	1.305951
48.	1.	0.	-5.473769	3.726543	-0.409706
49.	1.	0.	-1.723434	2.421480	1.962072
50.	1.	0.	-0.851966	2.710468	0.453127
51.	1.	0.	-1.882024	3.979886	1.131972
52.	1.	0.	4.423583	2.922186	1.207040
53.	1.	0.	3.909840	2.638146	-0.462125
54.	1.	0.	6.825721	2.586862	0.551306
55.	1.	0.	6.339786	2.348582	-1.137213
56.	1.	0.	6.091326	3.920072	-0.364793

1-11		Standard Orientation (Ångstroms)			
Center number	Atom number	Type	X	Y	Z
1.	6.	0.	-4.827941	2.154402	-0.425334
2.	6.	0.	-3.942167	1.082638	-0.286048
3.	6.	0.	-2.596855	1.243045	0.135264
4.	6.	0.	-2.155132	2.537696	0.469771
5.	6.	0.	-3.029678	3.608747	0.333180
6.	6.	0.	-4.351268	3.422789	-0.117304
7.	7.	0.	-4.151877	-0.267402	-0.473251
8.	6.	0.	-3.007518	-0.981946	-0.186967
9.	6.	0.	-2.004708	-0.082944	0.181446
10.	6.	0.	-2.968557	-2.495704	-0.340745

11.	7.	0.	0.605018	1.308665	-0.541675
12.	6.	0.	0.506974	0.180134	0.298928
13.	6.	0.	-0.654080	-0.459552	0.569715
14.	6.	0.	1.703065	2.123563	-0.671541
15.	6.	0.	2.783355	1.809742	0.350805
16.	7.	0.	2.893043	0.361019	0.580231
17.	6.	0.	1.794336	-0.429574	0.779212
18.	6.	0.	4.214897	2.220734	0.011935
19.	6.	0.	5.027666	1.270006	0.910216
20.	6.	0.	4.286012	-0.069664	0.790474
21.	8.	0.	1.853513	-1.561822	1.255554
22.	8.	0.	1.769732	3.036238	-1.479341
23.	6.	0.	-2.750771	-3.207026	0.992497
24.	6.	0.	-1.831215	-2.893864	-1.319070
25.	6.	0.	-2.853462	-2.693562	2.217071
26.	6.	0.	-4.300206	-3.034982	-0.923506
27.	8.	0.	4.831210	-0.745865	-0.319455
28.	6.	0.	4.429182	-2.107009	-0.498809
29.	6.	0.	5.346611	-2.722655	-1.541450
30.	1.	0.	2.474576	2.308566	1.286829
31.	1.	0.	-5.852156	2.000716	-0.753142
32.	1.	0.	-1.148666	2.699979	0.838315
33.	1.	0.	-2.689815	4.609198	0.583037
34.	1.	0.	-5.009813	4.280340	-0.215182
35.	1.	0.	-5.017110	-0.677284	-0.782797
36.	1.	0.	-0.182496	1.530827	-1.139318
37.	1.	0.	-0.525421	-1.390941	1.112236
38.	1.	0.	4.418400	2.025411	-1.044152
39.	1.	0.	4.397003	3.278510	0.208469
40.	1.	0.	6.069292	1.157585	0.606576
41.	1.	0.	5.002073	1.613359	1.950756
42.	1.	0.	4.333358	-0.705061	1.683289
43.	1.	0.	-2.525587	-4.268698	0.883188
44.	1.	0.	-1.813217	-3.981326	-1.450039
45.	1.	0.	-1.991557	-2.434858	-2.299621
46.	1.	0.	-0.853486	-2.579416	-0.950420
47.	1.	0.	-2.708312	-3.314636	3.095523
48.	1.	0.	-3.069300	-1.643183	2.387491
49.	1.	0.	-5.149043	-2.813981	-0.267981
50.	1.	0.	-4.495024	-2.627840	-1.922466
51.	1.	0.	-4.245174	-4.122831	-1.019667
52.	1.	0.	3.382112	-2.158662	-0.820206

53.	1.	0.	4.497409	-2.644236	0.457879
54.	1.	0.	5.274698	-2.177661	-2.487372
55.	1.	0.	6.388240	-2.692484	-1.208462
56.	1.	0.	5.068832	-3.765857	-1.722403

1-12		Standard Orientation (Ångstroms)			
Center number	Atom number	Type	X	Y	Z
1.	6.	0.	-4.387672	2.626624	-0.751606
2.	6.	0.	-3.685214	1.445670	-0.497304
3.	6.	0.	-2.277335	1.342075	-0.649179
4.	6.	0.	-1.571173	2.464273	-1.124571
5.	6.	0.	-2.264399	3.642257	-1.377410
6.	6.	0.	-3.657136	3.726923	-1.185305
7.	7.	0.	-4.139897	0.206354	-0.104856
8.	6.	0.	-3.091158	-0.684062	0.004741
9.	6.	0.	-1.908653	-0.021312	-0.313515
10.	6.	0.	-3.378049	-2.137315	0.380626
11.	7.	0.	0.628253	1.134889	0.849813
12.	6.	0.	0.571212	-0.075625	0.132693
13.	6.	0.	-0.568548	-0.600273	-0.369903
14.	6.	0.	1.700822	1.609358	1.561576
15.	6.	0.	2.845586	0.619254	1.692229
16.	7.	0.	2.943452	-0.296900	0.550367
17.	6.	0.	1.868525	-0.784239	-0.133544
18.	6.	0.	4.254239	1.209751	1.784561
19.	6.	0.	5.118933	0.004551	1.376945
20.	6.	0.	4.337184	-0.652258	0.223684
21.	8.	0.	1.951897	-1.707415	-0.943705
22.	8.	0.	1.703147	2.698981	2.112994
23.	6.	0.	-4.721462	-2.203253	1.098449
24.	6.	0.	-2.321044	-2.675351	1.378045
25.	6.	0.	-5.850034	-2.762811	0.659351
26.	6.	0.	-3.361097	-2.997365	-0.903436
27.	8.	0.	4.732393	-0.083772	-1.003711
28.	6.	0.	4.848112	-0.987157	-2.115530
29.	6.	0.	6.228019	-1.632684	-2.180853
30.	1.	0.	2.636708	0.044493	2.612233
31.	1.	0.	-5.465136	2.679836	-0.624588
32.	1.	0.	-0.503811	2.409370	-1.314522
33.	1.	0.	-1.723909	4.511871	-1.738519

34.	1.	0.	-4.169961	4.661413	-1.391228
35.	1.	0.	-5.098357	-0.047004	0.081184
36.	1.	0.	-0.187670	1.736407	0.845425
37.	1.	0.	-0.423261	-1.543103	-0.889183
38.	1.	0.	4.361287	2.026099	1.064626
39.	1.	0.	4.473538	1.597570	2.780283
40.	1.	0.	6.123386	0.272740	1.047061
41.	1.	0.	5.203720	-0.698922	2.213735
42.	1.	0.	4.438994	-1.742396	0.190625
43.	1.	0.	-4.721670	-1.738007	2.085296
44.	1.	0.	-2.576090	-3.700291	1.664979
45.	1.	0.	-1.320621	-2.679896	0.942606
46.	1.	0.	-2.289426	-2.062738	2.284239
47.	1.	0.	-6.746057	-2.768478	1.273016
48.	1.	0.	-5.925054	-3.248647	-0.308443
49.	1.	0.	-4.093594	-2.641781	-1.633774
50.	1.	0.	-2.376383	-2.954703	-1.375616
51.	1.	0.	-3.582008	-4.043950	-0.670293
52.	1.	0.	4.676004	-0.371611	-3.004346
53.	1.	0.	4.050479	-1.734832	-2.067727
54.	1.	0.	6.415193	-2.269114	-1.308994
55.	1.	0.	6.312936	-2.260391	-3.074885
56.	1.	0.	7.010693	-0.868870	-2.219541

Table S4. Energies of conformers of **4b** with Boltzmann distribution over 1% at MMFF.

Label	E (kcal/mol)	rel. E (kcal/mol)	Boltzmann Dist
M0001	89.86	0.00	0.245
M0002	90.21	0.35	0.136
M0003	90.21	0.35	0.135
M0004	90.25	0.39	0.127
M0005	90.57	0.70	0.075
M0006	90.61	0.75	0.069
M0007	90.83	0.97	0.048
M0008	90.90	1.04	0.042
M0009	91.66	1.79	0.012
M0010	91.68	1.82	0.011
M0011	91.75	1.89	0.010

Table S5. Gibbs free energies[a] and equilibrium populations[b] of low-energy conformers of **4b**.

Conformers	In MeOH	
	G	*P* (%)

4b-1	-804640.44611847	24.39
4b-2	-804639.2620071	3.30
4b-3	-804640.39466265	22.36
4b-4	-804639.30969786	3.58
4b-5	-804638.16637464	0.52
4b-6	-804638.93507439	1.90
4b-7	-804639.94034541	10.38
4b-8	-804639.26702718	3.33
4b-9	-804638.92001415	1.85
4b-10	-804639.35236854	3.84
4b-11	-804640.44988353	24.55

[a]B3LYP/6-31G(d,p), in kcal/mol. [b]From *G* values at 298.15K.

Table S6 Cartesian coordinates for the low-energy reoptimized MMFF conformers of **4b** at B3LYP/6-31+G(d,p) level of theory in gas.

4b-1		Standard Orientation (Ångstroms)			
Center number	Atomic number	Atomic Type	X	Y	Z
1.	6.	0.	3.391808	3.286226	0.208876
2.	6.	0.	3.050587	1.935357	0.098611
3.	6.	0.	1.725155	1.495758	-0.154510
4.	6.	0.	0.723707	2.465921	-0.349546
5.	6.	0.	1.056765	3.810687	-0.241802
6.	6.	0.	2.374858	4.218819	0.042581
7.	7.	0.	3.842269	0.809781	0.171997
8.	6.	0.	3.089363	-0.328728	-0.022081
9.	6.	0.	1.760946	0.044715	-0.221910
10.	6.	0.	3.780648	-1.692157	-0.030678
11.	7.	0.	-1.030545	0.133642	0.940125
12.	6.	0.	-0.615578	-0.776495	-0.048232
13.	6.	0.	0.649054	-0.848001	-0.518715
14.	6.	0.	-2.320059	0.350003	1.342105
15.	6.	0.	-3.369775	-0.320914	0.450743
16.	7.	0.	-2.891543	-1.586151	-0.058903
17.	6.	0.	-1.612700	-1.802434	-0.492481
18.	6.	0.	-4.670572	-0.725095	1.154748
19.	6.	0.	-5.229455	-1.809232	0.213846
20.	6.	0.	-3.978012	-2.541408	-0.314519
21.	8.	0.	-1.300157	-2.795729	-1.144250
22.	8.	0.	-2.616327	1.078557	2.279977
23.	6.	0.	5.104946	-1.574114	0.715651

24.	6.	0.	3.976974	-2.142480	-1.496249
25.	6.	0.	6.335060	-1.654775	0.205853
26.	6.	0.	2.943767	-2.752638	0.730418
27.	8.	0.	-3.591119	0.519951	-0.697576
28.	6.	0.	-4.130967	1.829748	-0.476521
29.	6.	0.	-4.112304	2.552432	-1.813379
30.	1.	0.	4.414124	3.595178	0.407070
31.	1.	0.	-0.291135	2.169861	-0.592381
32.	1.	0.	0.287800	4.563873	-0.384953
33.	1.	0.	2.602093	5.277523	0.122053
34.	1.	0.	4.837506	0.789032	0.335636
35.	1.	0.	-0.320337	0.659046	1.437218
36.	1.	0.	0.814232	-1.690173	-1.183370
37.	1.	0.	-4.423416	-1.136169	2.138291
38.	1.	0.	-5.345836	0.116356	1.311571
39.	1.	0.	-5.921863	-2.487197	0.718166
40.	1.	0.	-5.763974	-1.338273	-0.615536
41.	1.	0.	-3.772477	-3.472825	0.224411
42.	1.	0.	-4.035587	-2.784474	-1.379066
43.	1.	0.	4.997272	-1.415556	1.789735
44.	1.	0.	3.009885	-2.247398	-1.994054
45.	1.	0.	4.564348	-1.414844	-2.063789
46.	1.	0.	4.487476	-3.110008	-1.537441
47.	1.	0.	6.521903	-1.817274	-0.851016
48.	1.	0.	7.210168	-1.578247	0.844462
49.	1.	0.	2.757452	-2.437823	1.761790
50.	1.	0.	1.978211	-2.930319	0.254614
51.	1.	0.	3.491448	-3.699913	0.755605
52.	1.	0.	-5.159530	1.761401	-0.094783
53.	1.	0.	-3.541017	2.371900	0.272566
54.	1.	0.	-3.089284	2.643765	-2.189252
55.	1.	0.	-4.534648	3.556514	-1.706173
56.	1.	0.	-4.700533	2.005752	-2.555974

4b-2		Standard Orientation (Ångstroms)			
Center number	Atom number	Type	X	Y	Z
1.	6.	0.	-4.105989	2.778042	0.599653
2.	6.	0.	-3.449362	1.584867	0.286658
3.	6.	0.	-2.147325	1.550444	-0.278641
4.	6.	0.	-1.516838	2.773273	-0.580158

5.	6.	0.	-2.164369	3.963388	-0.269576
6.	6.	0.	-3.442341	3.967625	0.322399
7.	7.	0.	-3.869764	0.279222	0.408474
8.	6.	0.	-2.899232	-0.589090	-0.048256
9.	6.	0.	-1.802697	0.154172	-0.477729
10.	6.	0.	-3.177408	-2.091698	-0.046574
11.	7.	0.	1.038804	0.941452	0.191577
12.	6.	0.	0.693051	0.003105	-0.796619
13.	6.	0.	-0.576528	-0.363769	-1.078291
14.	6.	0.	2.303087	1.220453	0.633752
15.	6.	0.	3.385599	0.270835	0.116734
16.	7.	0.	3.067238	-0.242650	-1.194550
17.	6.	0.	1.809033	-0.582223	-1.608625
18.	6.	0.	4.766549	0.896593	-0.109547
19.	6.	0.	5.427136	-0.112460	-1.069051
20.	6.	0.	4.267214	-0.624420	-1.951536
21.	8.	0.	1.612481	-1.262729	-2.611806
22.	8.	0.	2.541861	2.100349	1.451689
23.	6.	0.	-4.280205	-2.385059	0.964357
24.	6.	0.	-1.932836	-2.889294	0.419257
25.	6.	0.	-5.522144	-2.803045	0.714429
26.	6.	0.	-3.566663	-2.530379	-1.476575
27.	8.	0.	3.424030	-0.870330	0.996360
28.	6.	0.	3.877875	-0.668210	2.342505
29.	6.	0.	3.519553	-1.918418	3.129171
30.	1.	0.	-5.101476	2.776076	1.034296
31.	1.	0.	-0.547536	2.792279	-1.068183
32.	1.	0.	-1.680007	4.908592	-0.494973
33.	1.	0.	-3.921880	4.913706	0.554030
34.	1.	0.	-4.758318	-0.031190	0.771301
35.	1.	0.	0.298651	1.479672	0.627858
36.	1.	0.	-0.647776	-1.113871	-1.860664
37.	1.	0.	4.634291	1.873302	-0.585220
38.	1.	0.	5.317942	1.055363	0.817444
39.	1.	0.	6.228390	0.335485	-1.661217
40.	1.	0.	5.854864	-0.940620	-0.497822
41.	1.	0.	4.235890	-0.144770	-2.935530
42.	1.	0.	4.295809	-1.705350	-2.114741
43.	1.	0.	-3.982199	-2.234198	2.003007
44.	1.	0.	-1.086065	-2.747706	-0.253869
45.	1.	0.	-1.619505	-2.578419	1.420535
46.	1.	0.	-2.172557	-3.956746	0.450547

47.	1.	0.	-5.889751	-2.980155	-0.291437
48.	1.	0.	-6.217702	-3.002215	1.524375
49.	1.	0.	-4.441526	-1.983285	-1.839605
50.	1.	0.	-2.744822	-2.337754	-2.170799
51.	1.	0.	-3.790218	-3.601655	-1.503321
52.	1.	0.	4.966016	-0.510165	2.355387
53.	1.	0.	3.408399	0.220638	2.779190
54.	1.	0.	3.876304	-1.831567	4.160357
55.	1.	0.	3.976939	-2.803470	2.677438
56.	1.	0.	2.435961	-2.064850	3.146764

4b-3		Standard Orientation (Ångstroms)			
Center number	Atom number	Type	X	Y	Z
1.	6.	0.	3.308144	3.291775	0.200467
2.	6.	0.	3.000406	1.936475	0.048572
3.	6.	0.	1.698270	1.479003	-0.277967
4.	6.	0.	0.682620	2.430538	-0.488044
5.	6.	0.	0.981254	3.778704	-0.334114
6.	6.	0.	2.278577	4.206169	0.012361
7.	7.	0.	3.806775	0.823693	0.136267
8.	6.	0.	3.088555	-0.324538	-0.138187
9.	6.	0.	1.763272	0.030833	-0.383163
10.	6.	0.	3.806721	-1.664563	0.013708
11.	7.	0.	-0.966444	0.062426	0.875564
12.	6.	0.	-0.599719	-0.796903	-0.174777
13.	6.	0.	0.645041	-0.852619	-0.697419
14.	6.	0.	-2.234550	0.262957	1.346676
15.	6.	0.	-3.330648	-0.358046	0.476555
16.	7.	0.	-2.883575	-1.586450	-0.139538
17.	6.	0.	-1.625992	-1.785479	-0.638197
18.	6.	0.	-4.589368	-0.811920	1.225196
19.	6.	0.	-5.204343	-1.828627	0.245073
20.	6.	0.	-3.986746	-2.520042	-0.404253
21.	8.	0.	-1.351340	-2.739689	-1.361075
22.	8.	0.	-2.482466	0.948650	2.330201
23.	6.	0.	5.239157	-1.483622	-0.477719
24.	6.	0.	3.173594	-2.778738	-0.851752
25.	6.	0.	6.358923	-1.554222	0.244352
26.	6.	0.	3.746226	-2.089555	1.499495
27.	8.	0.	-3.613586	0.556454	-0.600664

28.	6.	0.	-4.193013	1.825796	-0.267749
29.	6.	0.	-4.170982	2.673852	-1.528852
30.	1.	0.	4.313512	3.617569	0.451236
31.	1.	0.	-0.315755	2.115964	-0.773657
32.	1.	0.	0.202524	4.519553	-0.488238
33.	1.	0.	2.479335	5.267128	0.126234
34.	1.	0.	4.800448	0.819589	0.311249
35.	1.	0.	-0.233420	0.572958	1.354722
36.	1.	0.	0.778950	-1.650999	-1.417719
37.	1.	0.	-4.284914	-1.291315	2.160679
38.	1.	0.	-5.252319	0.014342	1.482684
39.	1.	0.	-5.867511	-2.541558	0.740381
40.	1.	0.	-5.785646	-1.302377	-0.516921
41.	1.	0.	-3.755132	-3.488247	0.052717
42.	1.	0.	-4.104650	-2.684411	-1.478857
43.	1.	0.	5.318070	-1.277273	-1.545765
44.	1.	0.	2.170137	-3.036243	-0.507561
45.	1.	0.	3.112942	-2.484537	-1.903940
46.	1.	0.	3.791726	-3.679086	-0.786848
47.	1.	0.	6.356917	-1.761161	1.309992
48.	1.	0.	7.331857	-1.424827	-0.220373
49.	1.	0.	4.194689	-1.337134	2.154749
50.	1.	0.	2.704979	-2.220420	1.805250
51.	1.	0.	4.270608	-3.038493	1.651597
52.	1.	0.	-5.226903	1.693072	0.081695
53.	1.	0.	-3.632159	2.307739	0.541856
54.	1.	0.	-3.144253	2.835397	-1.869427
55.	1.	0.	-4.630937	3.648279	-1.336543
56.	1.	0.	-4.723650	2.182094	-2.334520

4b-4		Standard Orientation (Ångstroms)			
Center number	Atom number	Type	X	Y	Z
1.	6.	0.	-4.093065	2.688700	0.747880
2.	6.	0.	-3.429973	1.534025	0.322639
3.	6.	0.	-2.154945	1.569401	-0.299679
4.	6.	0.	-1.550135	2.820946	-0.524099
5.	6.	0.	-2.201623	3.971921	-0.096861
6.	6.	0.	-3.457624	3.907220	0.537897
7.	7.	0.	-3.818431	0.214391	0.364792
8.	6.	0.	-2.860069	-0.595859	-0.215933

9.	6.	0.	-1.795443	0.201256	-0.626395
10.	6.	0.	-3.076726	-2.106914	-0.166873
11.	7.	0.	0.991660	0.942692	0.227134
12.	6.	0.	0.704085	0.123341	-0.879033
13.	6.	0.	-0.545491	-0.224699	-1.256362
14.	6.	0.	2.229518	1.163000	0.766210
15.	6.	0.	3.336099	0.269086	0.202122
16.	7.	0.	3.096954	-0.065884	-1.181937
17.	6.	0.	1.864779	-0.347481	-1.704095
18.	6.	0.	4.734313	0.894710	0.144904
19.	6.	0.	5.444533	0.005239	-0.893504
20.	6.	0.	4.339656	-0.359553	-1.909422
21.	8.	0.	1.725151	-0.892313	-2.795371
22.	8.	0.	2.424730	1.944794	1.688441
23.	6.	0.	-4.567560	-2.372487	-0.347117
24.	6.	0.	-2.544708	-2.636948	1.184770
25.	6.	0.	-5.412006	-2.892243	0.545613
26.	6.	0.	-2.347712	-2.841003	-1.315863
27.	8.	0.	3.307463	-0.975865	0.928147
28.	6.	0.	3.667675	-0.952752	2.316729
29.	6.	0.	3.226392	-2.277231	2.917831
30.	1.	0.	-5.069505	2.636421	1.220798
31.	1.	0.	-0.597274	2.889943	-1.039709
32.	1.	0.	-1.738994	4.940201	-0.261805
33.	1.	0.	-3.941555	4.824127	0.860153
34.	1.	0.	-4.697727	-0.138397	0.711467
35.	1.	0.	0.227965	1.439611	0.672132
36.	1.	0.	-0.575902	-0.862853	-2.132663
37.	1.	0.	4.641471	1.926268	-0.208534
38.	1.	0.	5.226899	0.923442	1.117146
39.	1.	0.	6.291042	0.506983	-1.367869
40.	1.	0.	5.818907	-0.900646	-0.409375
41.	1.	0.	4.376440	0.253086	-2.816537
42.	1.	0.	4.368446	-1.407633	-2.219955
43.	1.	0.	-4.950999	-2.097064	-1.330337
44.	1.	0.	-1.472920	-2.437353	1.263578
45.	1.	0.	-3.038200	-2.152352	2.032289
46.	1.	0.	-2.700380	-3.717744	1.264620
47.	1.	0.	-5.100009	-3.194213	1.540578
48.	1.	0.	-6.456950	-3.053419	0.297690
49.	1.	0.	-2.635999	-2.441685	-2.293023
50.	1.	0.	-1.263539	-2.761645	-1.217510

51.	1.	0.	-2.611383	-3.902562	-1.291094
52.	1.	0.	4.755312	-0.831306	2.422917
53.	1.	0.	3.188254	-0.109439	2.826936
54.	1.	0.	3.513289	-2.328391	3.972930
55.	1.	0.	3.692558	-3.114780	2.390782
56.	1.	0.	2.140913	-2.389955	2.846574

4b-5		Standard Orientation (Ångstroms)			
Center number	Atom number	Type	X	Y	Z
1.	6.	0.	-4.387187	2.587074	0.574551
2.	6.	0.	-3.668100	1.420344	0.303546
3.	6.	0.	-2.385633	1.431435	-0.304826
4.	6.	0.	-1.845037	2.671035	-0.699030
5.	6.	0.	-2.554822	3.835882	-0.431281
6.	6.	0.	-3.809091	3.797101	0.207802
7.	7.	0.	-4.007790	0.099976	0.508242
8.	6.	0.	-2.999837	-0.734115	0.063380
9.	6.	0.	-1.962606	0.049546	-0.435099
10.	6.	0.	-3.141339	-2.251527	0.138558
11.	7.	0.	0.845282	1.074872	0.083104
12.	6.	0.	0.533913	0.018658	-0.792874
13.	6.	0.	-0.715875	-0.447919	-1.006819
14.	6.	0.	2.098434	1.455004	0.477413
15.	6.	0.	3.218514	0.504574	0.049810
16.	7.	0.	2.913479	-0.153887	-1.197865
17.	6.	0.	1.668202	-0.592162	-1.557896
18.	6.	0.	4.569711	1.162198	-0.254534
19.	6.	0.	5.265767	0.089572	-1.114800
20.	6.	0.	4.122611	-0.554596	-1.929567
21.	8.	0.	1.497345	-1.378136	-2.485808
22.	8.	0.	2.303691	2.426804	1.194836
23.	6.	0.	-1.861106	-2.844725	0.714478
24.	6.	0.	-3.472697	-2.798510	-1.269063
25.	6.	0.	-1.136728	-3.841086	0.208025
26.	6.	0.	-4.290148	-2.651686	1.100802
27.	8.	0.	3.314437	-0.536975	1.042128
28.	6.	0.	3.746770	-0.174355	2.360711
29.	6.	0.	3.482987	-1.368792	3.262990
30.	1.	0.	-5.365799	2.550168	1.044799
31.	1.	0.	-0.898063	2.720931	-1.227009

32.	1.	0.	-2.139268	4.793750	-0.728820
33.	1.	0.	-4.338950	4.724010	0.404512
34.	1.	0.	-4.852077	-0.214016	0.956663
35.	1.	0.	0.086057	1.618600	0.477315
36.	1.	0.	-0.751372	-1.293398	-1.685042
37.	1.	0.	4.391974	2.078876	-0.825345
38.	1.	0.	5.120741	1.437086	0.645122
39.	1.	0.	6.044810	0.507452	-1.756595
40.	1.	0.	5.730139	-0.659100	-0.467428
41.	1.	0.	4.062792	-0.173750	-2.954728
42.	1.	0.	4.197468	-1.643986	-1.988928
43.	1.	0.	-1.556292	-2.401398	1.662231
44.	1.	0.	-4.391068	-2.337936	-1.644810
45.	1.	0.	-2.674112	-2.587148	-1.983926
46.	1.	0.	-3.625921	-3.881961	-1.237103
47.	1.	0.	-1.372237	-4.319320	-0.737184
48.	1.	0.	-0.253220	-4.203550	0.723802
49.	1.	0.	-4.128935	-2.262284	2.111418
50.	1.	0.	-5.264692	-2.302760	0.738174
51.	1.	0.	-4.342057	-3.741012	1.168364
52.	1.	0.	4.819279	0.068110	2.355616
53.	1.	0.	3.209379	0.713029	2.714479
54.	1.	0.	2.413914	-1.596632	3.297000
55.	1.	0.	3.826796	-1.157501	4.280499
56.	1.	0.	4.009922	-2.254242	2.895658

4b-6		Standard Orientation (Ångstroms)			
Center number	Atom number	Type	X	Y	Z
1.	6.	0.	3.547886	3.334506	0.268222
2.	6.	0.	3.195144	1.989576	0.129369
3.	6.	0.	1.867050	1.564595	-0.131999
4.	6.	0.	0.874874	2.547795	-0.310401
5.	6.	0.	1.218711	3.887401	-0.175096
6.	6.	0.	2.539035	4.279079	0.120695
7.	7.	0.	3.982448	0.857776	0.174493
8.	6.	0.	3.220561	-0.272383	-0.044259
9.	6.	0.	1.893478	0.114930	-0.224873
10.	6.	0.	3.860690	-1.657458	-0.085120
11.	7.	0.	-0.907824	0.240757	0.924586
12.	6.	0.	-0.487952	-0.693263	-0.040990

13.	6.	0.	0.779908	-0.781092	-0.500908
14.	6.	0.	-2.197729	0.466943	1.318018
15.	6.	0.	-3.244629	-0.220561	0.436875
16.	7.	0.	-2.766211	-1.497667	-0.039952
17.	6.	0.	-1.486239	-1.723621	-0.470242
18.	6.	0.	-4.550622	-0.605247	1.141831
19.	6.	0.	-5.107216	-1.707294	0.220378
20.	6.	0.	-3.854763	-2.452149	-0.288290
21.	8.	0.	-1.179747	-2.725741	-1.110628
22.	8.	0.	-2.495842	1.213001	2.242007
23.	6.	0.	3.041988	-2.613828	0.774206
24.	6.	0.	5.287164	-1.623891	0.522979
25.	6.	0.	2.558384	-3.802557	0.417948
26.	6.	0.	3.971104	-2.120668	-1.556093
27.	8.	0.	-3.458113	0.594846	-0.731960
28.	6.	0.	-3.998052	1.909213	-0.542570
29.	6.	0.	-3.957003	2.608842	-1.891191
30.	1.	0.	4.572636	3.630981	0.473501
31.	1.	0.	-0.141587	2.266105	-0.562324
32.	1.	0.	0.456212	4.649364	-0.305515
33.	1.	0.	2.774893	5.333919	0.222779
34.	1.	0.	4.968436	0.851261	0.375236
35.	1.	0.	-0.199420	0.766582	1.423389
36.	1.	0.	0.953370	-1.654145	-1.119563
37.	1.	0.	-4.310276	-0.996149	2.135187
38.	1.	0.	-5.223993	0.241514	1.276824
39.	1.	0.	-5.803143	-2.373755	0.735174
40.	1.	0.	-5.637438	-1.252083	-0.620479
41.	1.	0.	-3.656776	-3.376357	0.265686
42.	1.	0.	-3.906638	-2.711184	-1.349429
43.	1.	0.	2.884962	-2.265842	1.795151
44.	1.	0.	5.964901	-0.991671	-0.063471
45.	1.	0.	5.279769	-1.268734	1.558732
46.	1.	0.	5.704563	-2.633687	0.520621
47.	1.	0.	2.663223	-4.204913	-0.584342
48.	1.	0.	2.010307	-4.415228	1.126544
49.	1.	0.	2.990596	-2.204422	-2.030151
50.	1.	0.	4.562584	-1.403112	-2.132231
51.	1.	0.	4.466167	-3.095041	-1.617759
52.	1.	0.	-5.032743	1.849768	-0.176052
53.	1.	0.	-3.418853	2.463306	0.206261
54.	1.	0.	-4.379472	3.615197	-1.808238

55.	1.	0.	-4.534200	2.050058	-2.633451
56.	1.	0.	-2.927973	2.692146	-2.252264

4b-7		Standard Orientation (Ångstroms)			
Center number	Atom number	Type	X	Y	Z
1.	6.	0.	-3.552046	3.339143	-0.187012
2.	6.	0.	-3.192222	1.990525	-0.121661
3.	6.	0.	-1.867018	1.559223	0.144612
4.	6.	0.	-0.885691	2.536221	0.400561
5.	6.	0.	-1.236481	3.879268	0.337208
6.	6.	0.	-2.553603	4.279475	0.038171
7.	7.	0.	-3.969563	0.858399	-0.253835
8.	6.	0.	-3.204994	-0.277614	-0.082258
9.	6.	0.	-1.884967	0.107291	0.153753
10.	6.	0.	-3.819670	-1.672572	-0.173324
11.	7.	0.	0.933238	0.301621	-0.941505
12.	6.	0.	0.497207	-0.694467	-0.047440
13.	6.	0.	-0.776244	-0.803967	0.393454
14.	6.	0.	2.229454	0.548112	-1.301623
15.	6.	0.	3.261838	-0.203265	-0.455359
16.	7.	0.	2.772040	-1.509083	-0.076762
17.	6.	0.	1.484750	-1.761234	0.313948
18.	6.	0.	4.576777	-0.542857	-1.167588
19.	6.	0.	5.113955	-1.713081	-0.321951
20.	6.	0.	3.850765	-2.489462	0.104024
21.	8.	0.	1.162582	-2.811510	0.863107
22.	8.	0.	2.542955	1.353993	-2.168103
23.	6.	0.	-3.676970	-2.335657	1.193604
24.	6.	0.	-3.136353	-2.474584	-1.301616
25.	6.	0.	-3.064871	-3.485808	1.474855
26.	6.	0.	-5.334770	-1.593148	-0.484675
27.	8.	0.	3.464308	0.525699	0.770690
28.	6.	0.	3.973834	1.862139	0.679296
29.	6.	0.	3.996456	2.429763	2.088965
30.	1.	0.	-4.574339	3.641065	-0.396521
31.	1.	0.	0.127611	2.246107	0.655961
32.	1.	0.	-0.482365	4.636972	0.527458
33.	1.	0.	-2.795239	5.337020	-0.005825
34.	1.	0.	-4.954097	0.857755	-0.461881
35.	1.	0.	0.233642	0.866080	-1.409730

36.	1.	0.	-0.971423	-1.706304	0.964371
37.	1.	0.	4.350535	-0.857195	-2.191042
38.	1.	0.	5.256127	0.307723	-1.228890
39.	1.	0.	5.818961	-2.341063	-0.871595
40.	1.	0.	5.627371	-1.323516	0.561173
41.	1.	0.	3.655736	-3.361345	-0.530186
42.	1.	0.	3.885405	-2.838729	1.139606
43.	1.	0.	-4.152378	-1.780947	2.003102
44.	1.	0.	-3.277008	-1.966615	-2.260424
45.	1.	0.	-2.063124	-2.580641	-1.132035
46.	1.	0.	-3.575482	-3.474231	-1.379097
47.	1.	0.	-2.558211	-4.082396	0.723411
48.	1.	0.	-3.038497	-3.867558	2.490764
49.	1.	0.	-5.888239	-1.061409	0.297475
50.	1.	0.	-5.522120	-1.103917	-1.447652
51.	1.	0.	-5.746375	-2.603805	-0.541980
52.	1.	0.	4.986548	1.860046	0.252512
53.	1.	0.	3.345552	2.473461	0.019532
54.	1.	0.	2.988424	2.452040	2.512704
55.	1.	0.	4.392551	3.450069	2.079027
56.	1.	0.	4.626850	1.818671	2.741265

4b-8		Standard Orientation (Ångstroms)			
Center number	Atom number	Type	X	Y	Z
1.	6.	0.	-4.323363	2.682265	0.435678
2.	6.	0.	-3.616388	1.489834	0.262062
3.	6.	0.	-2.347890	1.433904	-0.372762
4.	6.	0.	-1.808167	2.626788	-0.892471
5.	6.	0.	-2.505388	3.816999	-0.720810
6.	6.	0.	-3.746467	3.847778	-0.055857
7.	7.	0.	-3.957884	0.197323	0.599817
8.	6.	0.	-2.966758	-0.682825	0.210277
9.	6.	0.	-1.936654	0.043106	-0.383852
10.	6.	0.	-3.087226	-2.183030	0.465669
11.	7.	0.	0.884025	1.077393	0.008429
12.	6.	0.	0.553710	-0.051590	-0.763851
13.	6.	0.	-0.704561	-0.518763	-0.925689
14.	6.	0.	2.144443	1.470403	0.366323
15.	6.	0.	3.244903	0.462053	0.030113
16.	7.	0.	2.928920	-0.294586	-1.157705

17.	6.	0.	1.676051	-0.744146	-1.476021
18.	6.	0.	4.612081	1.059588	-0.322587
19.	6.	0.	5.285666	-0.099242	-1.082542
20.	6.	0.	4.130918	-0.783084	-1.846863
21.	8.	0.	1.490699	-1.608011	-2.328499
22.	8.	0.	2.368511	2.501248	0.989017
23.	6.	0.	-3.093024	-2.887801	-0.887625
24.	6.	0.	-4.428225	-2.523484	1.161262
25.	6.	0.	-2.250826	-3.829571	-1.312127
26.	6.	0.	-1.933903	-2.650684	1.378539
27.	8.	0.	3.312477	-0.492009	1.109257
28.	6.	0.	3.736603	-0.024468	2.397133
29.	6.	0.	3.467470	-1.142990	3.390471
30.	1.	0.	-5.291768	2.697656	0.927761
31.	1.	0.	-0.872013	2.618776	-1.441771
32.	1.	0.	-2.090623	4.739701	-1.114923
33.	1.	0.	-4.266924	4.793073	0.063082
34.	1.	0.	-4.802025	-0.068941	1.078371
35.	1.	0.	0.134473	1.667863	0.350584
36.	1.	0.	-0.770055	-1.421516	-1.525378
37.	1.	0.	4.457148	1.927204	-0.971392
38.	1.	0.	5.166314	1.399164	0.552663
39.	1.	0.	6.077949	0.242407	-1.752626
40.	1.	0.	5.727777	-0.800464	-0.369752
41.	1.	0.	4.084234	-0.488040	-2.900594
42.	1.	0.	4.180054	-1.875057	-1.814359
43.	1.	0.	-3.898267	-2.565565	-1.548403
44.	1.	0.	-4.507637	-2.036768	2.140337
45.	1.	0.	-5.291969	-2.236939	0.550918
46.	1.	0.	-4.488926	-3.602439	1.323313
47.	1.	0.	-1.419963	-4.188351	-0.713249
48.	1.	0.	-2.361084	-4.271956	-2.297290
49.	1.	0.	-0.958221	-2.447137	0.932936
50.	1.	0.	-1.980307	-2.127566	2.338339
51.	1.	0.	-2.010807	-3.725210	1.572773
52.	1.	0.	4.808882	0.218504	2.379731
53.	1.	0.	3.196802	0.888008	2.675517
54.	1.	0.	2.398534	-1.369780	3.434481
55.	1.	0.	3.802795	-0.849612	4.390294
56.	1.	0.	3.998679	-2.053989	3.099823

4b-9	Standard Orientation

		(Ångstroms)			
Center number	Atom number	Type	X	Y	Z
1.	6.	0.	3.374659	3.271324	0.315809
2.	6.	0.	3.030243	1.925023	0.166425
3.	6.	0.	1.705431	1.496901	-0.108147
4.	6.	0.	0.708440	2.474856	-0.285111
5.	6.	0.	1.044730	3.815172	-0.138940
6.	6.	0.	2.361761	4.211233	0.166847
7.	7.	0.	3.817971	0.795190	0.214793
8.	6.	0.	3.063130	-0.335015	-0.016243
9.	6.	0.	1.737254	0.048308	-0.215058
10.	6.	0.	3.749514	-1.700389	-0.056962
11.	7.	0.	-1.069406	0.114520	0.920791
12.	6.	0.	-0.644399	-0.768557	-0.088660
13.	6.	0.	0.625764	-0.832336	-0.545146
14.	6.	0.	-2.365480	0.334626	1.300318
15.	6.	0.	-3.394053	-0.280122	0.336467
16.	7.	0.	-2.920705	-1.558741	-0.147283
17.	6.	0.	-1.636689	-1.785035	-0.564219
18.	6.	0.	-4.771964	-0.601457	0.966605
19.	6.	0.	-4.937306	-2.132991	0.839545
20.	6.	0.	-4.013052	-2.511930	-0.326196
21.	8.	0.	-1.314539	-2.777357	-1.212040
22.	8.	0.	-2.672217	1.020790	2.265536
23.	6.	0.	5.071812	-1.606537	0.696339
24.	6.	0.	3.949267	-2.115003	-1.532633
25.	6.	0.	6.303170	-1.678168	0.188226
26.	6.	0.	2.906159	-2.776376	0.674868
27.	8.	0.	-3.492293	0.582454	-0.810573
28.	6.	0.	-3.917640	1.930549	-0.579277
29.	6.	0.	-4.041592	2.601233	-1.937105
30.	1.	0.	4.396344	3.571640	0.529924
31.	1.	0.	-0.304715	2.187462	-0.544525
32.	1.	0.	0.279369	4.574545	-0.268126
33.	1.	0.	2.591555	5.266688	0.276480
34.	1.	0.	4.812083	0.766892	0.384066
35.	1.	0.	-0.362838	0.603298	1.458513
36.	1.	0.	0.797111	-1.660275	-1.225876
37.	1.	0.	-4.825026	-0.241180	1.995133
38.	1.	0.	-5.539728	-0.084223	0.385488
39.	1.	0.	-4.594486	-2.630142	1.752594

40.	1.	0.	-5.975348	-2.428649	0.666607
41.	1.	0.	-3.619866	-3.528827	-0.288291
42.	1.	0.	-4.500057	-2.368172	-1.299763
43.	1.	0.	4.961223	-1.475900	1.773873
44.	1.	0.	2.983813	-2.203711	-2.036671
45.	1.	0.	4.541725	-1.375961	-2.079752
46.	1.	0.	4.456117	-3.083243	-1.595748
47.	1.	0.	6.492508	-1.813521	-0.872003
48.	1.	0.	7.176672	-1.621710	0.831104
49.	1.	0.	2.718780	-2.487216	1.713553
50.	1.	0.	1.940984	-2.937912	0.192570
51.	1.	0.	3.449939	-3.726216	0.677292
52.	1.	0.	-4.881372	1.945993	-0.051047
53.	1.	0.	-3.195046	2.461470	0.054595
54.	1.	0.	-4.356448	3.642628	-1.817437
55.	1.	0.	-4.778418	2.083920	-2.558127
56.	1.	0.	-3.082441	2.586582	-2.462442

4b-10		Standard Orientation (Ångstroms)			
Center number	Atom number	Type	X	Y	Z
1.	6.	0.	-3.572590	3.225146	-0.269759
2.	6.	0.	-3.197472	1.881062	-0.193709
3.	6.	0.	-1.869304	1.466793	0.084225
4.	6.	0.	-0.900951	2.456773	0.340596
5.	6.	0.	-1.266926	3.795110	0.266056
6.	6.	0.	-2.586666	4.178232	-0.044253
7.	7.	0.	-3.960148	0.739560	-0.323122
8.	6.	0.	-3.185391	-0.387256	-0.137396
9.	6.	0.	-1.870896	0.014622	0.102190
10.	6.	0.	-3.785283	-1.780897	-0.251674
11.	7.	0.	0.954825	0.238814	-0.964238
12.	6.	0.	0.525606	-0.751871	-0.061818
13.	6.	0.	-0.751359	-0.878466	0.364112
14.	6.	0.	2.251226	0.510053	-1.305456
15.	6.	0.	3.287136	-0.210490	-0.438050
16.	7.	0.	2.817536	-1.517674	-0.040657
17.	6.	0.	1.529755	-1.790855	0.333721
18.	6.	0.	4.614000	-0.539780	-1.131936
19.	6.	0.	5.166562	-1.679639	-0.255410
20.	6.	0.	3.914365	-2.469733	0.179621

21.	8.	0.	1.221301	-2.836940	0.897978
22.	8.	0.	2.560323	1.316527	-2.173492
23.	6.	0.	-3.741547	-2.538731	1.073090
24.	6.	0.	-3.015748	-2.595400	-1.325653
25.	6.	0.	-3.485159	-2.049513	2.285007
26.	6.	0.	-5.272684	-1.719226	-0.683940
27.	8.	0.	3.458423	0.546652	0.776213
28.	6.	0.	4.024082	1.860353	0.671092
29.	6.	0.	3.862895	2.529051	2.026463
30.	1.	0.	-4.596959	3.513688	-0.487750
31.	1.	0.	0.114027	2.180295	0.604442
32.	1.	0.	-0.522912	4.562741	0.456269
33.	1.	0.	-2.840063	5.232634	-0.096627
34.	1.	0.	-4.945024	0.726092	-0.528879
35.	1.	0.	0.251554	0.787173	-1.445860
36.	1.	0.	-0.936604	-1.774599	0.947987
37.	1.	0.	4.400329	-0.883742	-2.148530
38.	1.	0.	5.276688	0.322271	-1.210637
39.	1.	0.	5.886702	-2.306902	-0.785896
40.	1.	0.	5.667282	-1.261211	0.621935
41.	1.	0.	3.743604	-3.363310	-0.430695
42.	1.	0.	3.945252	-2.788252	1.225228
43.	1.	0.	-3.991949	-3.595775	0.973874
44.	1.	0.	-3.082099	-2.102402	-2.300657
45.	1.	0.	-1.960670	-2.704683	-1.069137
46.	1.	0.	-3.450112	-3.596613	-1.419480
47.	1.	0.	-3.222914	-1.008158	2.445256
48.	1.	0.	-3.516508	-2.688992	3.161701
49.	1.	0.	-5.886290	-1.183382	0.047849
50.	1.	0.	-5.385358	-1.249312	-1.667821
51.	1.	0.	-5.675895	-2.732963	-0.758428
52.	1.	0.	5.088491	1.796660	0.403832
53.	1.	0.	3.522441	2.437189	-0.115308
54.	1.	0.	2.805218	2.621679	2.289050
55.	1.	0.	4.306476	3.529570	2.009391
56.	1.	0.	4.357532	1.943469	2.806720

4b-11		Standard Orientation (Ångstroms)			
Center number	Atom number	Type	X	Y	Z
1.	6.	0.	3.391682	3.286367	0.208648

2.	6.	0.	3.050543	1.935472	0.098451
3.	6.	0.	1.725175	1.495795	-0.154828
4.	6.	0.	0.723683	2.465876	-0.350024
5.	6.	0.	1.056657	3.810668	-0.242337
6.	6.	0.	2.374699	4.218892	0.042160
7.	7.	0.	3.842270	0.809927	0.172031
8.	6.	0.	3.089444	-0.328620	-0.022080
9.	6.	0.	1.761043	0.044745	-0.222124
10.	6.	0.	3.780747	-1.692043	-0.030463
11.	7.	0.	-1.030376	0.133559	0.939731
12.	6.	0.	-0.615452	-0.776502	-0.048713
13.	6.	0.	0.649198	-0.847987	-0.519152
14.	6.	0.	-2.319816	0.349551	1.342147
15.	6.	0.	-3.369691	-0.321113	0.450775
16.	7.	0.	-2.891465	-1.586070	-0.059562
17.	6.	0.	-1.612614	-1.802301	-0.493151
18.	6.	0.	-4.670220	-0.725768	1.155013
19.	6.	0.	-5.229256	-1.809621	0.213870
20.	6.	0.	-3.977875	-2.541365	-0.315252
21.	8.	0.	-1.300119	-2.795464	-1.145142
22.	8.	0.	-2.615935	1.077687	2.280386
23.	6.	0.	5.104946	-1.573914	0.716032
24.	6.	0.	3.977282	-2.142531	-1.495950
25.	6.	0.	6.335139	-1.654683	0.206441
26.	6.	0.	2.943744	-2.752430	0.730632
27.	8.	0.	-3.591475	0.520218	-0.697113
28.	6.	0.	-4.131326	1.829896	-0.475327
29.	6.	0.	-4.113561	2.553006	-1.811963
30.	1.	0.	4.413955	3.595392	0.406947
31.	1.	0.	-0.291119	2.169726	-0.592914
32.	1.	0.	0.287666	4.563805	-0.385610
33.	1.	0.	2.601870	5.277614	0.121567
34.	1.	0.	4.837484	0.789249	0.335812
35.	1.	0.	-0.320100	0.658702	1.437009
36.	1.	0.	0.814415	-1.690046	-1.183941
37.	1.	0.	-4.422693	-1.137196	2.138315
38.	1.	0.	-5.345568	0.115510	1.312400
39.	1.	0.	-5.921351	-2.487907	0.718186
40.	1.	0.	-5.764170	-1.338424	-0.615122
41.	1.	0.	-3.772006	-3.473009	0.223155
42.	1.	0.	-4.035792	-2.783935	-1.379894
43.	1.	0.	4.997122	-1.415243	1.790085

44.	1.	0.	3.010268	-2.247569	-1.993874
45.	1.	0.	4.564692	-1.414933	-2.063501
46.	1.	0.	4.487843	-3.110036	-1.536948
47.	1.	0.	6.522155	-1.817345	-0.850372
48.	1.	0.	7.210141	-1.578111	0.845191
49.	1.	0.	2.757385	-2.437542	1.761972
50.	1.	0.	1.978210	-2.930035	0.254752
51.	1.	0.	3.491352	-3.699743	0.755900
52.	1.	0.	-5.159647	1.761337	-0.092981
53.	1.	0.	-3.540968	2.371864	0.273575
54.	1.	0.	-3.090781	2.644687	-2.188400
55.	1.	0.	-4.536067	3.556961	-1.704200
56.	1.	0.	-4.702104	2.006425	-2.554384