Supplementary Information

Fissisternoids A and B, two Pairs of 2′,5′-Quinodihydrochalcone-Based Meroterpenoid Enantiomers with Unusual Carbon Skeletons from *Fissistigma bracteolatum*

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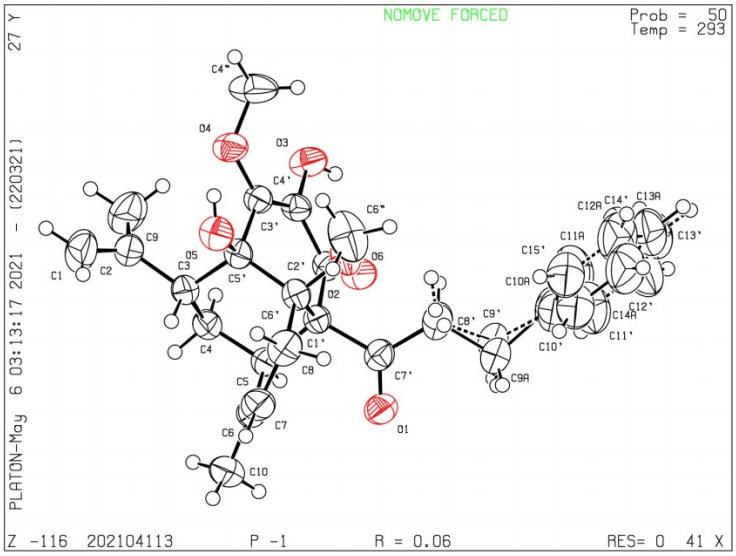
X-Ray Crystallographic analysis of 1.



Crystal data of **1**: $C_{27}H_{32}O_6$, M = 452.53, a = 8.6532(5) Å, b = 9.9783(5) Å, c =14.7.50(7) Å, α = 100.835(4)°, β = 102.254(4)° , γ = 95.682(4)°, Volume = 1205.81(11) Å^3 , T = 293, space group P-1, Z = 2, μ (MuKα) = 0.709 mm^{-1} , 3456 reflections measured, 4294 independent reflections (R_{int} = 0.0247). Final R indexes [all data] R_1 = 0.0588, wR_2 = 0.1722.Crytallographic data for **1** have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication no. CCDC 2107685.

X-ray crystallographic data of 1

Bond precision: C-C = 0.0033 A Wavelength=1.54184

Cell: a = 8.6532(5) b=9.9783(5) c=14.7050(7)

alpha = 100.835(4) beta =102.254(4) gamma = 95.682(4)

Temperature: 293 K

	Calculated	Reported
Volume	1205.81(11)	1205.82(11)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C_{27} H_{32} O_6	C_{27} H_{32} O_6
Sum formula	C_{27} H_{32} O_6	C_{27} H_{32} O_6
Mr	452.53	452.52
Dx,g cm^{-3}	1.246	1.246

Z	2	2
Mu (mm^{-1})	0.709	0.709
F000	484.0 484.0	
F000′	485.51	
h, k, l_{max}	10,11,17	10,11,17
Nref	4299	4294
T_{min}, T_{max}	0.918, 0.945	0.867, 1.000
$T_{min'}$ 0.899		

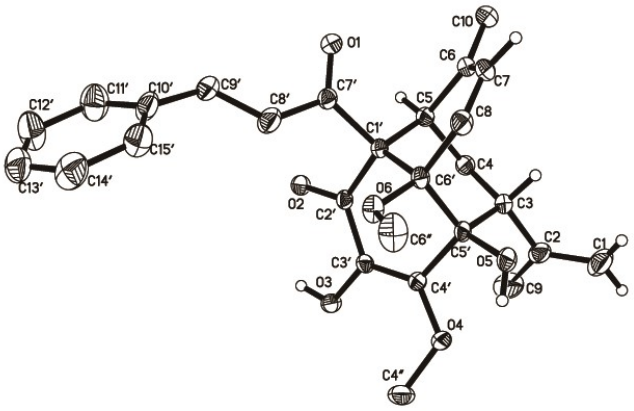
Correction method = # Reported T Limits: T_{min} = 0.867 T_{max} = 1.000

AbsCorr = MULTI-SCAN

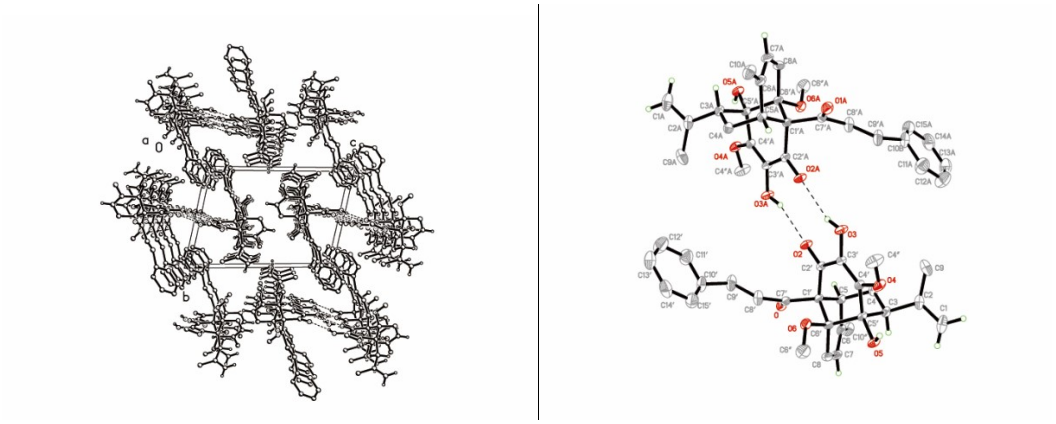
Data completeness = 0.999 Theta(max) = 67.073

R(reflections)= 0.0588 (3456) wR2(reflections)= 0.1722(4294)

S = 1.065 Npar= 302



View of a molecule of **1** with the atom-labelling scheme (Displacement ellipsoids are drawn at the 30% probability level).



View of the pack drawing of **1** (Hydrogen-bonds are shown as dashed lines)

Table S1. Gibbs free energies (ΔG) [a] and Boltzmann distribution (P%)[b] of low-energy conformers of **1**.

Conformers	In MeOH	
	ΔG	P(%)/100
1-1	0.00	0.418
1-2	1.36	0.242
1-3	2.71	0.140
1-4	3.68	0.094
1-5	4.94	0.057
1-6	7.61	0.019

[a] B3LYP/6-31g, in kcal/mol. [b] From ΔG values at 298.15 K.

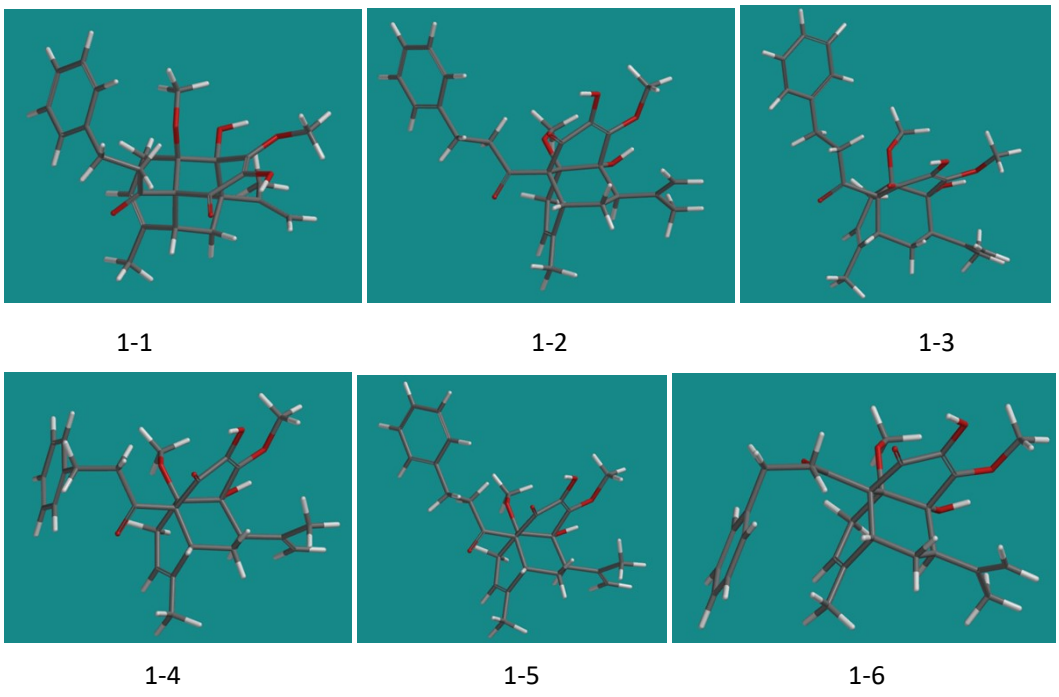


Table S2. Cartesian coordinates for the low-energy reoptimized MMFF conformers of **1** at B3LYP/6-31+G(d,p) level of theory in CH_3OH.

1-1			Standard Orientation		
Center Number	Atomic Number	Atomic Type	(Ångstroms) X	Y	Z
1	6	0	-0.120577	-0.009525	-0.502004
2	6	0	0.596612	1.096983	-1.309054
3	6	0	0.519489	2.480464	-0.720491
4	6	0	-0.011689	2.761079	0.472206
5	6	0	-0.714530	1.676696	1.271825
6	6	0	-0.057103	0.280270	1.035803
7	6	0	-1.645817	-0.137903	-0.880806
8	6	0	-2.216061	1.643428	0.900659
9	6	0	-2.439983	1.187160	-0.551337
10	6	0	-0.847403	-0.779540	1.806725

11	6	0	-2.241665	-1.323326	-0.127500
12	6	0	-1.898504	-1.563653	1.161200
13	8	0	-0.629289	-0.995908	3.005292
14	8	0	-2.449459	-2.529010	1.959540
15	6	0	1.398272	0.293785	1.626837
16	8	0	1.886535	1.343386	1.998657
17	6	0	2.157259	-1.017184	1.809204
18	6	0	3.689810	-0.846733	1.773935
19	6	0	4.246138	-0.584129	0.388602
20	6	0	4.428518	0.723568	-0.084657
21	6	0	4.921783	0.957295	-1.370316
22	6	0	5.243787	-0.113203	-2.206773
23	6	0	5.071461	-1.420076	-1.746210
24	6	0	4.578245	-1.649288	-0.460815
25	1	0	-0.622583	1.902064	2.339407
26	6	0	0.017018	4.135186	1.083484
27	8	0	-1.710515	-0.370965	-2.285022
28	6	0	-3.914248	1.129912	-0.950099
29	6	0	-4.886714	0.737405	-0.118348
30	6	0	-4.232035	1.603090	-2.349531
31	8	0	0.533718	-1.267582	-0.677801
32	6	0	0.811707	-1.776145	-1.979586
33	8	0	-3.130793	-1.992282	-0.893349
34	6	0	-4.020383	-2.972995	-0.334223
35	1	0	0.215947	1.097067	-2.337324
36	1	0	1.656090	0.810703	-1.375716
37	1	0	0.996536	3.269468	-1.301070
38	1	0	-2.647475	2.643400	1.024770
39	1	0	-2.750854	0.994354	1.601541
40	1	0	-1.970696	1.935049	-1.199953
41	1	0	-1.993541	-2.393915	2.820256
42	1	0	1.856788	-1.385587	2.799098
43	1	0	1.817559	-1.752633	1.078693
44	1	0	3.965013	-0.030918	2.449286
45	1	0	4.137799	-1.764014	2.174916
46	1	0	4.175723	1.559608	0.561250
47	1	0	5.060859	1.978878	-1.715574
48	1	0	5.632810	0.068943	-3.205217
49	1	0	5.328542	-2.261766	-2.384698
50	1	0	4.456497	-2.671030	-0.105838
51	1	0	0.439567	4.874082	0.394996
52	1	0	-0.985785	4.477118	1.374538
53	1	0	0.629222	4.124781	1.994784
54	1	0	-2.441509	-0.997340	-2.427474

55	1	0	-5.926585	0.727467	-0.436198
56	1	0	-4.696829	0.415946	0.901451
57	1	0	-3.972758	2.665131	-2.464406
58	1	0	-3.639001	1.060740	-3.093918
59	1	0	-5.294413	1.486866	-2.586746
60	1	0	1.214428	-1.011703	-2.651445
61	1	0	1.576244	-2.544056	-1.832237
62	1	0	-0.075003	-2.219762	-2.440834
63	1	0	-3.461478	-3.801771	0.102015
64	1	0	-4.658340	-2.516109	0.425491
65	1	0	-4.624668	-3.317905	-1.174742

1-2

Center Number	Atomic Number	Atomic Type	Standard Orientation (Ångstroms) X	Y	Z
1	6	0	0.749130	0.368460	0.963926
2	6	0	0.886137	1.633336	1.843558
3	6	0	1.248473	2.896253	1.105345
4	6	0	1.374986	2.983639	-0.221867
5	6	0	1.259752	1.738346	-1.085415
6	6	0	0.242254	0.731623	-0.466774
7	6	0	2.119107	-0.390601	0.785912
8	6	0	2.648033	1.082902	-1.263912
9	6	0	3.190112	0.514333	0.057317
10	6	0	0.173667	-0.526585	-1.331950
11	6	0	1.873181	-1.675348	-0.001097
12	6	0	1.001839	-1.695058	-1.039180
13	8	0	-0.587588	-0.591294	-2.305100
14	8	0	0.772658	-2.765253	-1.859942
15	6	0	-1.193483	1.365654	-0.525832
16	8	0	-1.337821	2.481151	-0.984966
17	6	0	-2.401199	0.567202	-0.048823
18	6	0	-3.673849	0.918426	-0.844257
19	6	0	-4.887906	0.171982	-0.336175
20	6	0	-5.197845	-1.107606	-0.817743
21	6	0	-6.298924	-1.812245	-0.329715
22	6	0	-7.113403	-1.246896	0.653371
23	6	0	-6.817998	0.027272	1.141322
24	6	0	-5.715760	0.727628	0.648994
25	1	0	0.876126	2.022559	-2.070003
26	6	0	1.654227	4.276765	-0.937659
27	8	0	2.597957	-0.704311	2.090921
28	6	0	4.559009	-0.150744	-0.080870
29	6	0	4.930501	-0.853553	-1.157798

30	6	0	5.518258	0.081731	1.063454
31	8	0	-0.245029	-0.510583	1.494300
32	6	0	-0.180330	-0.965017	2.842491
33	8	0	2.644938	-2.684454	0.458933
34	6	0	2.805808	-3.906475	-0.280757
35	1	0	1.605155	1.440244	2.648908
36	1	0	-0.084314	1.786451	2.338011
37	1	0	1.355305	3.789514	1.720041
38	1	0	3.358841	1.824367	-1.646385
39	1	0	2.584838	0.301013	-2.027351
40	1	0	3.322246	1.359506	0.741957
41	1	0	0.096824	-2.425033	-2.488077
42	1	0	-2.199091	-0.504249	-0.081613
43	1	0	-2.544747	0.805353	1.014197
44	1	0	-3.837045	1.999050	-0.791306
45	1	0	-3.497049	0.677889	-1.899229
46	1	0	-4.570484	-1.551512	-1.588097
47	1	0	-6.523918	-2.801281	-0.721144
48	1	0	-7.973842	-1.792396	1.032042
49	1	0	-7.449509	0.479538	1.902060
50	1	0	-5.496166	1.723568	1.028784
51	1	0	1.826629	5.098537	-0.235223
52	1	0	2.532880	4.200038	-1.592716
53	1	0	0.800557	4.540794	-1.575045
54	1	0	3.032690	-1.572388	2.022972
55	1	0	5.921927	-1.295322	-1.223802
56	1	0	4.279192	-1.015473	-2.011718
57	1	0	5.762549	1.150116	1.148431
58	1	0	5.070766	-0.207211	2.020484
59	1	0	6.454656	-0.468654	0.927124
60	1	0	0.061947	-0.161114	3.546306
61	1	0	-1.182450	-1.341407	3.068642
62	1	0	0.548910	-1.769759	2.969523
63	1	0	1.850196	-4.418314	-0.398875
64	1	0	3.239298	-3.700053	-1.261986
65	1	0	3.493509	-4.508960	0.314719

1-3

Center Number	Atomic Number	Atomic Type	Standard Orientation (Ångstroms) X	Y	Z
1	6	0	0.643454	0.272792	0.869418
2	6	0	0.689058	1.437534	1.886350
3	6	0	1.116950	2.768886	1.328767
4	6	0	1.343574	3.001277	0.033467

5	6	0	1.308123	1.860187	-0.968789
6	6	0	0.263856	0.775837	-0.561147
7	6	0	2.032337	-0.459710	0.738490
8	6	0	2.714294	1.229123	-1.101239
9	6	0	3.148390	0.517302	0.191435
10	6	0	0.320584	-0.376423	-1.564843
11	6	0	1.866896	-1.666765	-0.181599
12	6	0	1.107701	-1.579264	-1.300935
13	8	0	-0.298529	-0.317983	-2.633803
14	8	0	0.978824	-2.555504	-2.250543
15	6	0	-1.179676	1.378625	-0.660395
16	8	0	-1.328482	2.574828	-0.813933
17	6	0	-2.399365	0.461828	-0.619747
18	6	0	-3.469813	0.990462	0.360597
19	6	0	-4.758788	0.201344	0.288379
20	6	0	-5.760967	0.549335	-0.628083
21	6	0	-6.939495	-0.191803	-0.719279
22	6	0	-7.137948	-1.298248	0.108992
23	6	0	-6.149496	-1.655372	1.027542
24	6	0	-4.972388	-0.910478	1.113813
25	1	0	1.005465	2.250976	-1.945886
26	6	0	1.670460	4.364747	-0.511262
27	8	0	2.410147	-0.890055	2.043379
28	6	0	4.527835	-0.133558	0.093719
29	6	0	4.972049	-0.753143	-1.006246
30	6	0	5.404757	0.008236	1.315947
31	8	0	-0.391116	-0.650486	1.222461
32	6	0	-0.409524	-1.271519	2.504140
33	8	0	2.592319	-2.718910	0.256803
34	6	0	2.774769	-3.895592	-0.548423
35	1	0	1.325984	1.152461	2.732273
36	1	0	-0.326541	1.543669	2.295165
37	1	0	1.172889	3.587741	2.045182
38	1	0	2.724976	0.537925	-1.949869
39	1	0	3.449105	2.007850	-1.335645
40	1	0	3.220459	1.284645	0.969896
41	1	0	0.384719	-2.143436	-2.917039
42	1	0	-2.808513	0.456428	-1.637800
43	1	0	-2.122280	-0.562102	-0.370098
44	1	0	-3.065303	0.948100	1.379585
45	1	0	-3.654753	2.044833	0.130829
46	1	0	-5.615675	1.413734	-1.272841
47	1	0	-7.705598	0.098179	-1.434003
48	1	0	-8.056863	-1.874661	0.041580

49	1	0	-6.296168	-2.512097	1.680598
50	1	0	-4.207925	-1.191295	1.835837
51	1	0	1.788406	5.101637	0.289645
52	1	0	2.593775	4.359161	-1.106657
53	1	0	0.863266	4.703690	-1.173658
54	1	0	2.859707	-1.745836	1.930807
55	1	0	5.967089	-1.190405	-1.040434
56	1	0	4.377623	-0.849254	-1.910080
57	1	0	5.635403	1.066590	1.503148
58	1	0	4.893265	-0.357269	2.213107
59	1	0	6.351918	-0.528703	1.202105
60	1	0	-0.214472	-0.563839	3.317057
61	1	0	-1.422365	-1.670113	2.617327
62	1	0	0.312139	-2.090095	2.574128
63	1	0	1.816086	-4.366585	-0.769649
64	1	0	3.286162	-3.643276	-1.479778
65	1	0	3.396958	-4.557609	0.055846

1-4

Center Number	Atomic Number	Atomic Type	Standard Orientation (Ångstroms) X	Y	Z
1	6	0	-0.129195	-0.046295	-0.524447
2	6	0	0.638489	1.003370	-1.359822
3	6	0	0.600742	2.410224	-0.824142
4	6	0	0.063286	2.754595	0.349046
5	6	0	-0.687530	1.725881	1.178841
6	6	0	-0.069602	0.300906	1.001519
7	6	0	-1.656761	-0.133016	-0.912156
8	6	0	-2.185624	1.737403	0.789612
9	6	0	-2.400024	1.236903	-0.647700
10	6	0	-0.892307	-0.707139	1.806993
11	6	0	-2.300021	-1.267704	-0.114582
12	6	0	-1.972988	-1.465891	1.187494
13	8	0	-0.686088	-0.882925	3.015050
14	8	0	-2.600601	-2.343830	2.031214
15	6	0	1.379516	0.302582	1.609249
16	8	0	1.876040	1.350106	1.976084
17	6	0	2.118894	-1.015285	1.816407
18	6	0	3.653352	-0.861337	1.816641
19	6	0	4.241570	-0.605917	0.443011
20	6	0	4.464995	0.698895	-0.020340
21	6	0	4.985887	0.926185	-1.296194
22	6	0	5.294539	-0.148139	-2.132719
23	6	0	5.080599	-1.452434	-1.682168

24	6	0	4.560315	-1.675143	-0.406474
25	1	0	-0.599573	1.986877	2.238343
26	6	0	0.132093	4.149449	0.908008
27	8	0	-1.706664	-0.413817	-2.299488
28	6	0	-3.862960	1.197554	-1.080839
29	6	0	-4.192156	1.509589	-2.343262
30	6	0	-4.926818	0.822714	-0.074837
31	8	0	0.473669	-1.336038	-0.648804
32	6	0	0.764982	-1.883575	-1.933723
33	8	0	-3.247530	-1.905859	-0.831160
34	6	0	-3.809215	-3.145732	-0.370261
35	1	0	0.274428	0.975229	-2.393345
36	1	0	1.688870	0.680285	-1.395376
37	1	0	1.113426	3.159880	-1.426033
38	1	0	-2.571198	2.761108	0.872496
39	1	0	-2.757329	1.136407	1.504457
40	1	0	-1.892784	1.936350	-1.317999
41	1	0	-2.125440	-2.213359	2.882113
42	1	0	1.789458	-1.376271	2.799927
43	1	0	1.788148	-1.749225	1.080466
44	1	0	3.922937	-0.048074	2.497183
45	1	0	4.082229	-1.783346	2.227688
46	1	0	4.221853	1.537981	0.625219
47	1	0	5.156342	1.945559	-1.633806
48	1	0	5.704786	0.028727	-3.123597
49	1	0	5.325954	-2.297329	-2.321010
50	1	0	4.405353	-2.695111	-0.059495
51	1	0	0.590262	4.846064	0.198525
52	1	0	-0.861963	4.537624	1.169835
53	1	0	0.730291	4.152602	1.828530
54	1	0	-2.649220	-0.480999	-2.533782
55	1	0	-5.223082	1.478531	-2.688161
56	1	0	-3.447370	1.830472	-3.067361
57	1	0	-4.708094	-0.125512	0.427275
58	1	0	-5.010126	1.584425	0.711112
59	1	0	-5.905173	0.735083	-0.557143
60	1	0	1.353327	-1.197521	-2.553186
61	1	0	1.371387	-2.771156	-1.733873
62	1	0	-0.143969	-2.162803	-2.471167
63	1	0	-3.015381	-3.864452	-0.151341
64	1	0	-4.421036	-2.997992	0.520932
65	1	0	-4.422264	-3.503016	-1.199514

1-5 Standard Orientation

Center Number	Atomic Number	Atomic Type	(Ångstroms) X	Y	Z
1	6	0	0.757642	0.373322	0.989029
2	6	0	0.884928	1.631128	1.880308
3	6	0	1.247874	2.901695	1.155753
4	6	0	1.384388	3.001780	-0.169606
5	6	0	1.280372	1.763236	-1.044872
6	6	0	0.259769	0.748870	-0.440698
7	6	0	2.130978	-0.381184	0.810152
8	6	0	2.675729	1.118840	-1.219690
9	6	0	3.204197	0.541299	0.102510
10	6	0	0.192541	-0.500327	-1.318940
11	6	0	1.890300	-1.659812	0.005751
12	6	0	1.024271	-1.665636	-1.039336
13	8	0	-0.557516	-0.547662	-2.302725
14	8	0	0.838130	-2.710655	-1.904635
15	6	0	-1.175322	1.384146	-0.502168
16	8	0	-1.317732	2.503166	-0.953372
17	6	0	-2.385439	0.580066	-0.041039
18	6	0	-3.651991	0.935875	-0.844206
19	6	0	-4.867540	0.177705	-0.357652
20	6	0	-5.165570	-1.097725	-0.857514
21	6	0	-6.268303	-1.813598	-0.390058
22	6	0	-7.096478	-1.263928	0.590477
23	6	0	-6.813024	0.005866	1.096546
24	6	0	-5.709038	0.717543	0.624740
25	1	0	0.903018	2.054100	-2.029833
26	6	0	1.662174	4.302693	-0.871754
27	8	0	2.592080	-0.696228	2.111909
28	6	0	4.566991	-0.135943	-0.013507
29	6	0	5.447278	-0.037001	0.993669
30	6	0	4.915443	-0.894968	-1.273109
31	8	0	-0.237435	-0.512539	1.505363
32	6	0	-0.169421	-0.979957	2.850408
33	8	0	2.697959	-2.659841	0.414056
34	6	0	2.508206	-4.003530	-0.059908
35	1	0	1.599374	1.431530	2.687590
36	1	0	-0.089740	1.776863	2.368528
37	1	0	1.345923	3.790126	1.778923
38	1	0	3.379617	1.876154	-1.586405
39	1	0	2.628034	0.344868	-1.992859
40	1	0	3.326000	1.374418	0.800579
41	1	0	0.148449	-2.372135	-2.518374
42	1	0	-2.181153	-0.490691	-0.081678

43	1	0	-2.537930	0.808453	1.022858
44	1	0	-3.820651	2.015021	-0.779465
45	1	0	-3.463766	0.709191	-1.900255
46	1	0	-4.527470	-1.529364	-1.626026
47	1	0	-6.483899	-2.799067	-0.795542
48	1	0	-7.958224	-1.818131	0.953221
49	1	0	-7.455213	0.445947	1.855493
50	1	0	-5.498889	1.710036	1.018647
51	1	0	1.826052	5.118688	-0.160631
52	1	0	2.545473	4.236781	-1.521824
53	1	0	0.811241	4.568460	-1.512051
54	1	0	3.427488	-1.183176	1.999434
55	1	0	6.421947	-0.517279	0.948700
56	1	0	5.233961	0.546648	1.885661
57	1	0	4.157192	-1.641599	-1.531327
58	1	0	4.994888	-0.215871	-2.131796
59	1	0	5.876120	-1.407691	-1.165385
60	1	0	-0.011115	-0.165737	3.567459
61	1	0	-1.145225	-1.433905	3.045335
62	1	0	0.620692	-1.722549	2.984803
63	1	0	1.483710	-4.333473	0.129535
64	1	0	2.723561	-4.081974	-1.126670
65	1	0	3.210909	-4.607294	0.516880

	1-6		Standard Orientation		
Center	Atomic	Atomic	(Ångstroms)		
Number	Number	Type	X	Y	Z
1	6	0	1.014150	0.543556	1.146879
2	6	0	1.335704	1.963890	1.670098
3	6	0	1.214589	3.067324	0.650887
4	6	0	0.794550	2.890812	-0.605269
5	6	0	0.498520	1.493999	-1.125696
6	6	0	-0.061707	0.589358	0.015758
7	6	0	2.283322	-0.174763	0.547010
8	6	0	1.768318	0.874622	-1.750433
9	6	0	2.857022	0.609734	-0.699061
10	6	0	-0.308555	-0.819407	-0.526701
11	6	0	1.905991	-1.601888	0.160050
12	6	0	0.702119	-1.870639	-0.399624
13	8	0	-1.368073	-1.108426	-1.091657
14	8	0	0.297855	-3.092597	-0.860875
15	6	0	-1.471228	1.142729	0.442640
16	8	0	-1.917197	2.125119	-0.117003
17	6	0	-2.264052	0.445700	1.542274

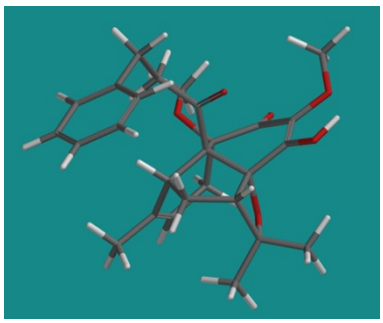
18	6	0	-3.766032	0.796343	1.544394
19	6	0	-4.578686	0.080126	0.483430
20	6	0	-4.775881	0.639438	-0.786566
21	6	0	-5.519627	-0.034306	-1.755945
22	6	0	-6.080865	-1.280836	-1.473683
23	6	0	-5.893151	-1.848585	-0.212503
24	6	0	-5.149942	-1.170800	0.754560
25	1	0	-0.275150	1.558180	-1.896527
26	6	0	0.609026	4.024934	-1.575931
27	8	0	3.276376	-0.195096	1.569174
28	6	0	4.128414	-0.008730	-1.278220
29	6	0	4.124756	-0.897218	-2.279265
30	6	0	5.426340	0.492489	-0.688472
31	8	0	0.431147	-0.254543	2.179901
32	6	0	1.100441	-0.450255	3.421564
33	8	0	2.918515	-2.460957	0.417115
34	6	0	2.929400	-3.791620	-0.125876
35	1	0	2.335818	1.967496	2.120160
36	1	0	0.636014	2.170396	2.493297
37	1	0	1.445993	4.070039	1.008986
38	1	0	2.171126	1.551354	-2.512794
39	1	0	1.500151	-0.047961	-2.274793
40	1	0	3.146183	1.581388	-0.282832
41	1	0	-0.604678	-2.914108	-1.209343
42	1	0	-2.107423	-0.634664	1.494233
43	1	0	-1.809165	0.761167	2.490324
44	1	0	-4.163936	0.535978	2.532857
45	1	0	-3.871289	1.879721	1.430675
46	1	0	-4.335401	1.605896	-1.012733
47	1	0	-5.662337	0.417597	-2.734494
48	1	0	-6.662687	-1.803700	-2.228503
49	1	0	-6.330211	-2.816339	0.021432
50	1	0	-5.015536	-1.616401	1.738719
51	1	0	0.939613	4.978444	-1.151623
52	1	0	1.163488	3.858320	-2.509641
53	1	0	-0.451437	4.115593	-1.844138
54	1	0	3.747207	-1.041946	1.476847
55	1	0	5.054495	-1.298877	-2.675168
56	1	0	3.213244	-1.256028	-2.747994
57	1	0	5.550187	1.565973	-0.890395
58	1	0	5.433757	0.383120	0.401285
59	1	0	6.292137	-0.031603	-1.105699
60	1	0	1.553126	0.469897	3.806061
61	1	0	0.325902	-0.782546	4.119828

62	1	0	1.877646	-1.216415	3.351130
63	1	0	2.082844	-4.370664	0.244790
64	1	0	2.903041	-3.755710	-1.217505
65	1	0	3.870685	-4.227634	0.212538

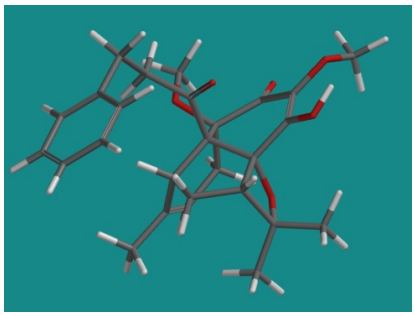
Table S3. Gibbs free energies (ΔG) [a] and Boltzmann distribution (P%)[b] of low-energy conformers of **2**.

Conformers	In MeOH	
	ΔG	P(%)/100
2-1	0.00	0.488
2-2	1.66	0.250
2-3	3.85	0.103
2-4	5.64	0.050
2-5	6.67	0.033

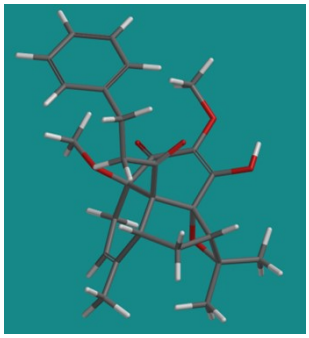
[a] B3LYP/6-31g, in kcal/mol. [b] From ΔG values at 298.15 K.



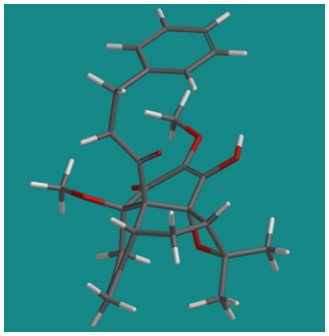
2-1



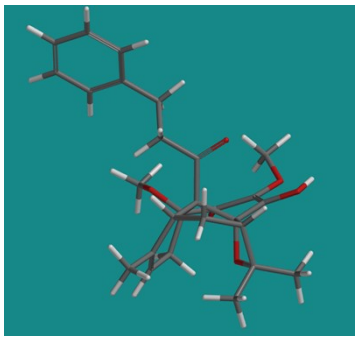
2-2



2-3



2-4



2-5

Table S4. Cartesian coordinates for the low-energy reoptimized MMFF conformers of **2** at B3LYP/6-31+G(d,p) level of theory in CH_3OH.

2-1			Standard Orientation		
Center Number	Atomic Number	Atomic Type	(Ångstroms) X	Y	Z
1	6	0	1.365417	-0.666802	1.301644
2	6	0	0.309864	-0.079190	0.316762
3	6	0	1.064026	0.909415	-0.625342
4	6	0	1.993893	0.165991	-1.511182

5	6	0	2.778239	-0.778464	-0.968920
6	6	0	2.680199	-1.049713	0.517664
7	8	0	3.634113	-1.580434	1.094897
8	8	0	2.000440	0.456555	-2.859702
9	8	0	1.769869	2.000402	0.068654
10	6	0	-0.822584	0.786195	0.915427
11	6	0	-1.217290	1.713797	-0.264407
12	6	0	0.029618	1.925861	-1.136158
13	6	0	1.066623	3.007105	-0.713991
14	6	0	1.952829	3.563029	-1.831655
15	6	0	0.608045	4.156843	0.177442
16	6	0	1.779116	0.374711	2.385338
17	6	0	0.665372	1.261193	2.872352
18	6	0	-0.501946	1.452891	2.234830
19	6	0	-1.595402	2.278761	2.862038
20	1	0	-1.708772	0.183002	1.140556
21	1	0	-0.194622	1.908829	-2.207737
22	6	0	-0.420757	-1.219742	-0.484242
23	8	0	-0.331253	-1.297878	-1.714098
24	6	0	-1.248759	-2.273700	0.251534
25	6	0	-2.482077	-2.718313	-0.536949
26	6	0	-3.549830	-1.653984	-0.613844
27	6	0	-3.751031	-0.937341	-1.800561
28	6	0	-4.726730	0.058150	-1.869300
29	6	0	-5.508438	0.347780	-0.752768
30	6	0	-5.317511	-0.359709	0.432514
31	6	0	-4.344189	-1.357456	0.502231
32	8	0	3.668214	-1.450520	-1.800123
33	6	0	3.888831	-2.816014	-1.458227
34	8	0	0.734272	-1.756689	2.001792
35	6	0	1.570902	-2.715883	2.634684
36	1	0	2.645122	-0.153823	-3.268906
37	1	0	-1.971182	1.201398	-0.872208
38	1	0	-1.673050	2.657317	0.045594
39	1	0	2.401444	2.788311	-2.452912
40	1	0	2.777991	4.153624	-1.417875
41	1	0	1.370790	4.215500	-2.491738
42	1	0	0.117605	3.815253	1.087552
43	1	0	-0.092358	4.806111	-0.358607
44	1	0	1.458614	4.770493	0.495288
45	1	0	2.607309	1.008340	2.048522
46	1	0	2.167394	-0.143018	3.269816
47	1	0	0.850659	1.761281	3.821346
48	1	0	-1.319460	2.634323	3.860642

49	1	0	-1.827769	3.157642	2.255059
50	1	0	-2.506417	1.680407	2.967754
51	1	0	-0.597876	-3.144165	0.393583
52	1	0	-1.554476	-1.917385	1.238044
53	1	0	-2.200947	-3.042158	-1.546728
54	1	0	-2.916184	-3.603315	-0.053844
55	1	0	-3.139188	-1.144198	-2.677208
56	1	0	-4.873441	0.608881	-2.794754
57	1	0	-6.268219	1.122813	-0.807721
58	1	0	-5.929715	-0.136798	1.302430
59	1	0	-4.209653	-1.902983	1.433638
60	1	0	4.657179	-2.900233	-0.684935
61	1	0	2.963593	-3.315907	-1.151140
62	1	0	4.264159	-3.325252	-2.351133
63	1	0	0.935034	-3.347319	3.262117
64	1	0	2.326327	-2.257567	3.276246
65	1	0	2.036289	-3.363355	1.886405

2-2

Center Number	Atomic Number	Atomic Type	Standard Orientation (Ångstroms) X	Y	Z
1	6	0	1.268789	-0.892279	1.225084
2	6	0	0.258546	-0.161995	0.290282
3	6	0	1.069956	0.874861	-0.542945
4	6	0	1.977239	0.175430	-1.485006
5	6	0	2.736384	-0.827226	-1.016912
6	6	0	2.579736	-1.266295	0.426102
7	8	0	3.478480	-1.922738	0.960910
8	8	0	1.999643	0.575436	-2.804872
9	8	0	1.816742	1.860796	0.257720
10	6	0	-0.841251	0.693318	0.960595
11	6	0	-1.177079	1.748214	-0.127175
12	6	0	0.090208	1.982764	-0.963811
13	6	0	1.171027	2.968566	-0.432980
14	6	0	2.096331	3.581932	-1.487185
15	6	0	0.755621	4.050682	0.558402
16	6	0	1.719227	0.021977	2.405458
17	6	0	0.643033	0.911640	2.965648
18	6	0	-0.506464	1.217003	2.340042
19	6	0	-1.568787	2.029739	3.034225
20	1	0	-1.755860	0.110929	1.119072
21	1	0	-0.120864	2.077418	-2.034041
22	6	0	-0.516642	-1.174568	-0.631382
23	8	0	-0.444991	-1.100617	-1.862793

24	6	0	-1.379975	-2.275653	-0.016522
25	6	0	-2.622075	-2.594167	-0.851258
26	6	0	-3.657957	-1.496394	-0.808167
27	6	0	-3.828436	-0.640069	-1.903544
28	6	0	-4.772851	0.386472	-1.859143
29	6	0	-5.553907	0.567687	-0.719537
30	6	0	-5.393390	-0.279001	0.375570
31	6	0	-4.451142	-1.307598	0.331925
32	8	0	3.597241	-1.467546	-1.902014
33	6	0	4.911143	-1.682848	-1.393356
34	8	0	0.568532	-2.001004	1.821406
35	6	0	1.339797	-3.066395	2.359817
36	1	0	2.559585	-0.070929	-3.278557
37	1	0	-1.946929	1.333755	-0.787718
38	1	0	-1.591390	2.678554	0.268852
39	1	0	2.512655	2.846949	-2.175873
40	1	0	2.944912	4.088696	-1.013930
41	1	0	1.554821	4.321943	-2.086635
42	1	0	0.237855	3.649345	1.428207
43	1	0	0.093470	4.780033	0.079806
44	1	0	1.629964	4.590397	0.939548
45	1	0	2.581173	0.642954	2.136675
46	1	0	2.071400	-0.595966	3.239522
47	1	0	0.839208	1.310062	3.959461
48	1	0	-1.290159	2.274120	4.064968
49	1	0	-1.751789	2.972969	2.513002
50	1	0	-2.507940	1.467959	3.073471
51	1	0	-0.756732	-3.175704	0.034920
52	1	0	-1.684201	-2.013612	0.999652
53	1	0	-2.347021	-2.811232	-1.890834
54	1	0	-3.083616	-3.514306	-0.469972
55	1	0	-3.216177	-0.762089	-2.795715
56	1	0	-4.895660	1.045745	-2.714420
57	1	0	-6.289445	1.366925	-0.686435
58	1	0	-6.004916	-0.140434	1.263271
59	1	0	-4.339567	-1.961845	1.193738
60	1	0	4.955365	-2.622208	-0.835223
61	1	0	5.586162	-1.778449	-2.249413
62	1	0	5.260022	-0.841690	-0.784329
63	1	0	1.770558	-3.666540	1.553680
64	1	0	0.661621	-3.714833	2.922274
65	1	0	2.115837	-2.718320	3.044766

2-3 Standard Orientation

Center Number	Atomic Number	Atomic Type	(Ångstroms) X	Y	Z
1	6	0	-0.095924	-0.318916	1.199393
2	6	0	-0.723030	-0.505123	-0.210057
3	6	0	-1.791265	0.616610	-0.393840
4	6	0	-1.148184	1.951220	-0.454864
5	6	0	-0.202125	2.251660	0.449168
6	6	0	0.189203	1.210392	1.477176
7	8	0	0.722181	1.576406	2.529725
8	8	0	-1.522074	2.821638	-1.458341
9	8	0	-2.868461	0.607958	0.613064
10	6	0	-1.525133	-1.804457	-0.463262
11	6	0	-2.485606	-1.390305	-1.609379
12	6	0	-2.794877	0.106973	-1.442884
13	6	0	-3.890347	0.540195	-0.423051
14	6	0	-4.537678	1.907221	-0.660827
15	6	0	-4.976849	-0.461033	-0.043482
16	6	0	-1.065924	-0.782824	2.329308
17	6	0	-1.917618	-1.977589	1.999641
18	6	0	-2.134404	-2.449921	0.761003
19	6	0	-2.912538	-3.723252	0.549523
20	1	0	-0.893187	-2.604276	-0.860739
21	1	0	-2.829279	0.641494	-2.397749
22	6	0	0.412927	-0.444436	-1.305103
23	8	0	0.633547	0.587841	-1.946129
24	6	0	1.221328	-1.700509	-1.646230
25	6	0	2.571712	-1.400051	-2.300957
26	6	0	3.617257	-0.899574	-1.334843
27	6	0	4.354612	-1.801048	-0.555350
28	6	0	5.330607	-1.338555	0.329125
29	6	0	5.575725	0.028186	0.445838
30	6	0	4.845259	0.933227	-0.321551
31	6	0	3.869332	0.472215	-1.206558
32	8	0	0.367689	3.520466	0.403791
33	6	0	1.735337	3.575646	0.798484
34	8	0	1.049041	-1.189643	1.247059
35	6	0	2.048830	-0.903127	2.216008
36	1	0	-0.957089	3.613049	-1.353110
37	1	0	-1.963393	-1.527305	-2.565597
38	1	0	-3.392479	-1.997020	-1.669277
39	1	0	-3.816428	2.705168	-0.832536
40	1	0	-5.140311	2.208907	0.203383
41	1	0	-5.198321	1.869901	-1.533974
42	1	0	-4.573250	-1.406784	0.312417

43	1	0	-5.624318	-0.672714	-0.901051
44	1	0	-5.606378	-0.070448	0.764146
45	1	0	-1.727670	0.029176	2.653052
46	1	0	-0.490798	-1.051730	3.222900
47	1	0	-2.367359	-2.477346	2.855788
48	1	0	-3.240397	-4.166084	1.496207
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50	1	0	-2.288979	-4.464893	0.039398
51	1	0	1.362175	-2.333504	-0.768139
52	1	0	0.622902	-2.264132	-2.372075
53	1	0	2.950482	-2.320496	-2.764930
54	1	0	2.458500	-0.687111	-3.127251
55	1	0	4.175045	-2.870716	-0.635269
56	1	0	5.900188	-2.045640	0.926380
57	1	0	6.336930	0.387767	1.132987
58	1	0	5.037442	1.999138	-0.234170
59	1	0	3.306940	1.189769	-1.801603
60	1	0	2.304612	2.719760	0.422851
61	1	0	2.169575	4.482013	0.365623
62	1	0	1.819002	3.658447	1.885509
63	1	0	1.635053	-0.796584	3.221177
64	1	0	2.608984	-0.008704	1.932194
65	1	0	2.748332	-1.743481	2.231594

2-4

Center	Atomic	Atomic	Standard Orientation (Ångstroms)		
Number	Number	Type	X	Y	Z
1	6	0	-0.902695	-1.490673	0.642674
2	6	0	-1.009259	-0.444915	-0.505312
3	6	0	-1.109779	0.954787	0.148660
4	6	0	0.205243	1.288258	0.748044
5	6	0	0.792781	0.379480	1.546086
6	6	0	0.118064	-0.972916	1.734110
7	8	0	0.387629	-1.663232	2.720811
8	8	0	0.779677	2.505515	0.453507
9	8	0	-2.189677	1.112535	1.131287
10	6	0	-2.274480	-0.541731	-1.396319
11	6	0	-2.512027	0.919741	-1.872583
12	6	0	-1.881954	1.859680	-0.827788
13	6	0	-2.726632	2.260778	0.416099
14	6	0	-2.323413	3.573140	1.092728
15	6	0	-4.247334	2.173012	0.338088
16	6	0	-2.262117	-1.687228	1.383480
17	6	0	-3.464154	-1.695382	0.484165

18	6	0	-3.483585	-1.201826	-0.764576
19	6	0	-4.708992	-1.352139	-1.628501
20	1	0	-2.051808	-1.153246	-2.283225
21	1	0	-1.324362	2.685463	-1.281775
22	6	0	0.204729	-0.444362	-1.520963
23	8	0	0.280362	0.445223	-2.378843
24	6	0	1.267543	-1.534416	-1.503204
25	6	0	2.525262	-1.177365	-2.304106
26	6	0	3.477026	-0.297061	-1.526257
27	6	0	4.478205	-0.867487	-0.727943
28	6	0	5.353319	-0.057036	-0.002478
29	6	0	5.232176	1.329899	-0.061701
30	6	0	4.239376	1.907283	-0.850075
31	6	0	3.366734	1.098243	-1.579367
32	8	0	1.996912	0.734754	2.142823
33	6	0	2.785812	-0.317751	2.683878
34	8	0	-0.603636	-2.756377	0.019504
35	6	0	-0.066091	-3.783174	0.845270
36	1	0	1.644544	2.518624	0.912411
37	1	0	-2.010611	1.069908	-2.836268
38	1	0	-3.561165	1.161523	-2.059092
39	1	0	-1.247869	3.658846	1.252979
40	1	0	-2.801794	3.669601	2.073781
41	1	0	-2.632114	4.428703	0.482111
42	1	0	-4.595986	1.188615	0.024127
43	1	0	-4.641920	2.911572	-0.367729
44	1	0	-4.701907	2.366951	1.316211
45	1	0	-2.415993	-0.946908	2.175770
46	1	0	-2.266426	-2.648788	1.908443
47	1	0	-4.358707	-2.155160	0.899941
48	1	0	-5.474677	-1.971884	-1.149273
49	1	0	-5.163060	-0.381289	-1.844102
50	1	0	-4.447127	-1.833255	-2.576545
51	1	0	1.564255	-1.756362	-0.476905
52	1	0	0.815666	-2.421867	-1.959242
53	1	0	3.051395	-2.105782	-2.562691
54	1	0	2.280450	-0.704801	-3.262973
55	1	0	4.587985	-1.948187	-0.672266
56	1	0	6.132516	-0.508015	0.606419
57	1	0	5.915798	1.960854	0.500050
58	1	0	4.146811	2.988834	-0.906419
59	1	0	2.599807	1.566866	-2.194477
60	1	0	2.876994	-1.157671	1.987941
61	1	0	3.789890	0.078143	2.863651

62	1	0	2.386030	-0.640095	3.649472
63	1	0	-0.046629	-4.704826	0.256381
64	1	0	-0.668410	-3.967338	1.736729
65	1	0	0.965731	-3.549426	1.121201

2-5

Center Number	Atomic Number	Atomic Type	Standard Orientation (Ångstroms) X	Y	Z
1	6	0	-0.902695	-1.490673	0.642674
2	6	0	-1.009259	-0.444915	-0.505312
3	6	0	-1.109779	0.954787	0.148660
4	6	0	0.205243	1.288258	0.748044
5	6	0	0.792781	0.379480	1.546086
6	6	0	0.118064	-0.972916	1.734110
7	8	0	0.387629	-1.663232	2.720811
8	8	0	0.779677	2.505515	0.453507
9	8	0	-2.189677	1.112535	1.131287
10	6	0	-2.274480	-0.541731	-1.396319
11	6	0	-2.512027	0.919741	-1.872583
12	6	0	-1.881954	1.859680	-0.827788
13	6	0	-2.726632	2.260778	0.416099
14	6	0	-2.323413	3.573140	1.092728
15	6	0	-4.247334	2.173012	0.338088
16	6	0	-2.262117	-1.687228	1.383480
17	6	0	-3.464154	-1.695382	0.484165
18	6	0	-3.483585	-1.201826	-0.764576
19	6	0	-4.708992	-1.352139	-1.628501
20	1	0	-2.051808	-1.153246	-2.283225
21	1	0	-1.324362	2.685463	-1.281775
22	6	0	0.204729	-0.444362	-1.520963
23	8	0	0.280362	0.445223	-2.378843
24	6	0	1.267543	-1.534416	-1.503204
25	6	0	2.525262	-1.177365	-2.304106
26	6	0	3.477026	-0.297061	-1.526257
27	6	0	4.478205	-0.867487	-0.727943
28	6	0	5.353319	-0.057036	-0.002478
29	6	0	5.232176	1.329899	-0.061701
30	6	0	4.239376	1.907283	-0.850075
31	6	0	3.366734	1.098243	-1.579367
32	8	0	1.996912	0.734754	2.142823
33	6	0	2.785812	-0.317751	2.683878
34	8	0	-0.603636	-2.756377	0.019504
35	6	0	-0.066091	-3.783174	0.845270
36	1	0	1.644544	2.518624	0.912411

37	1	0	-2.010611	1.069908	-2.836268
38	1	0	-3.561165	1.161523	-2.059092
39	1	0	-1.247869	3.658846	1.252979
40	1	0	-2.801794	3.669601	2.073781
41	1	0	-2.632114	4.428703	0.482111
42	1	0	-4.595986	1.188615	0.024127
43	1	0	-4.641920	2.911572	-0.367729
44	1	0	-4.701907	2.366951	1.316211
45	1	0	-2.415993	-0.946908	2.175770
46	1	0	-2.266426	-2.648788	1.908443
47	1	0	-4.358707	-2.155160	0.899941
48	1	0	-5.474677	-1.971884	-1.149273
49	1	0	-5.163060	-0.381289	-1.844102
50	1	0	-4.447127	-1.833255	-2.576545
51	1	0	1.564255	-1.756362	-0.476905
52	1	0	0.815666	-2.421867	-1.959242
53	1	0	3.051395	-2.105782	-2.562691
54	1	0	2.280450	-0.704801	-3.262973
55	1	0	4.587985	-1.948187	-0.672266
56	1	0	6.132516	-0.508015	0.606419
57	1	0	5.915798	1.960854	0.500050
58	1	0	4.146811	2.988834	-0.906419
59	1	0	2.599807	1.566866	-2.194477
60	1	0	2.876994	-1.157671	1.987941
61	1	0	3.789890	0.078143	2.863651
62	1	0	2.386030	-0.640095	3.649472
63	1	0	-0.046629	-4.704826	0.256381
64	1	0	-0.668410	-3.967338	1.736729
65	1	0	0.965731	-3.549426	1.121201

Table S5. The NO product inhibitory effects of compounds **1** and **2** in RAW 264.7 macrophages.

Compd.	Cell viability [a] %	NO Production inhibitory effect[b] (IC_{50} μM)
1	0.94	13.2 ± 0.78
2	0.98	9.8 ± 0.63
L-NMMA [c]	---	26.8 ± 1.98

[a] the cell viability at the concentration of 30 μM; [b] the NO Production inhibitory effect of compounds **1** and **2** at the concentrations from 1.875 to 30 μM; [c] the positive control group.

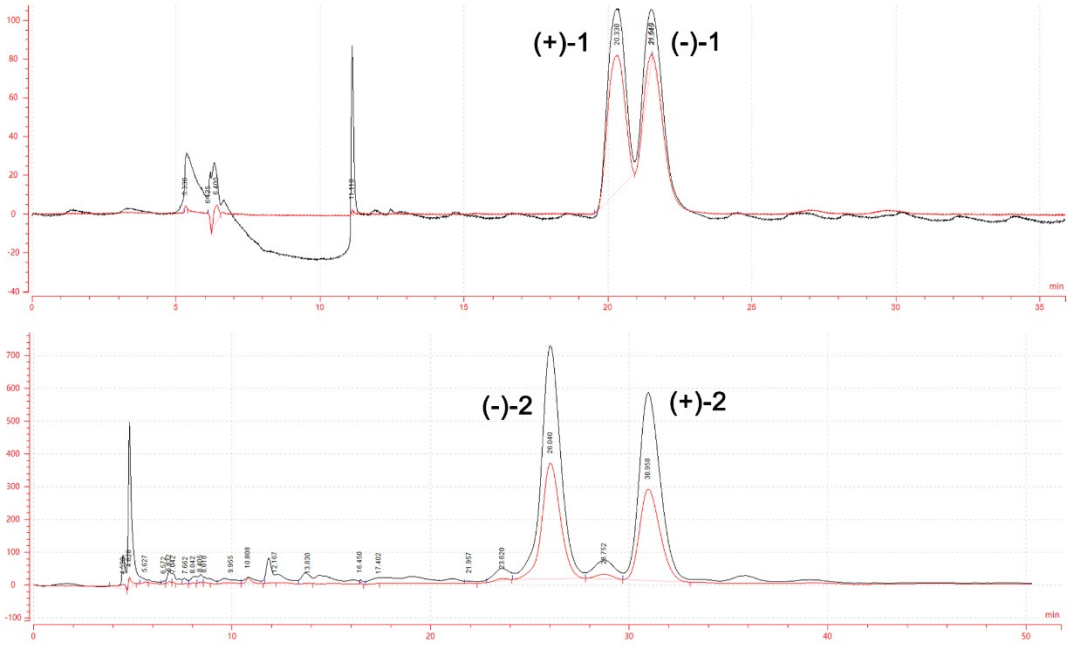

Figure S1. The chiral HPLC resolution of **1** and **2** led to the separation of two pairs of enantiomers (−)-**1** and (+)-**1**, and (−)-**2** and (+)-**2**, respectively. The spectra were obtained by Pre-HPLC with a LC-120 system (Separation, Beijing, China), equipped with a Chiralpak® IC column (10 mm × 250 mm i.d., 5 μm, Daicel, Tokyo, Japan) with flow rate at 3.0 ml/min (v/v: n-hexane: isopropanol = 90:10, **1**; cyclohexane: isopropanol = 80:20, **2**), detected by a binary channel UV detector at 210 and 300 nm.

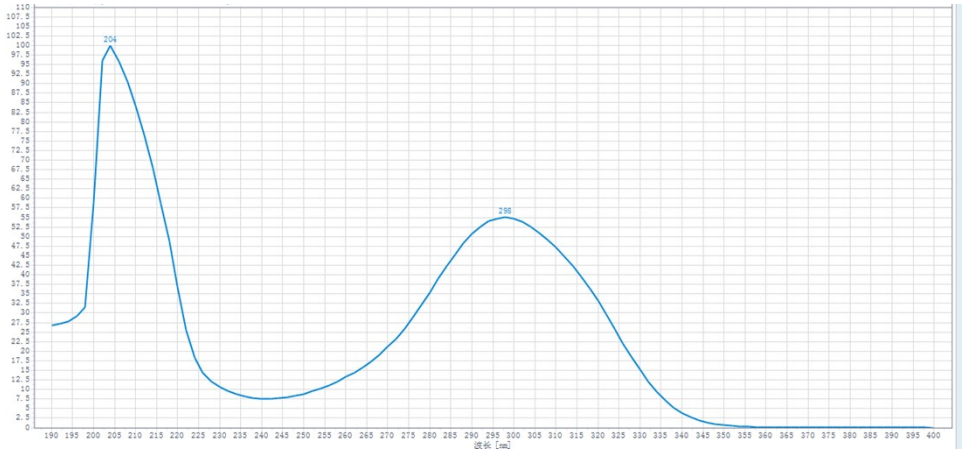

Figure S1-1 UV spectrum of compound **1**

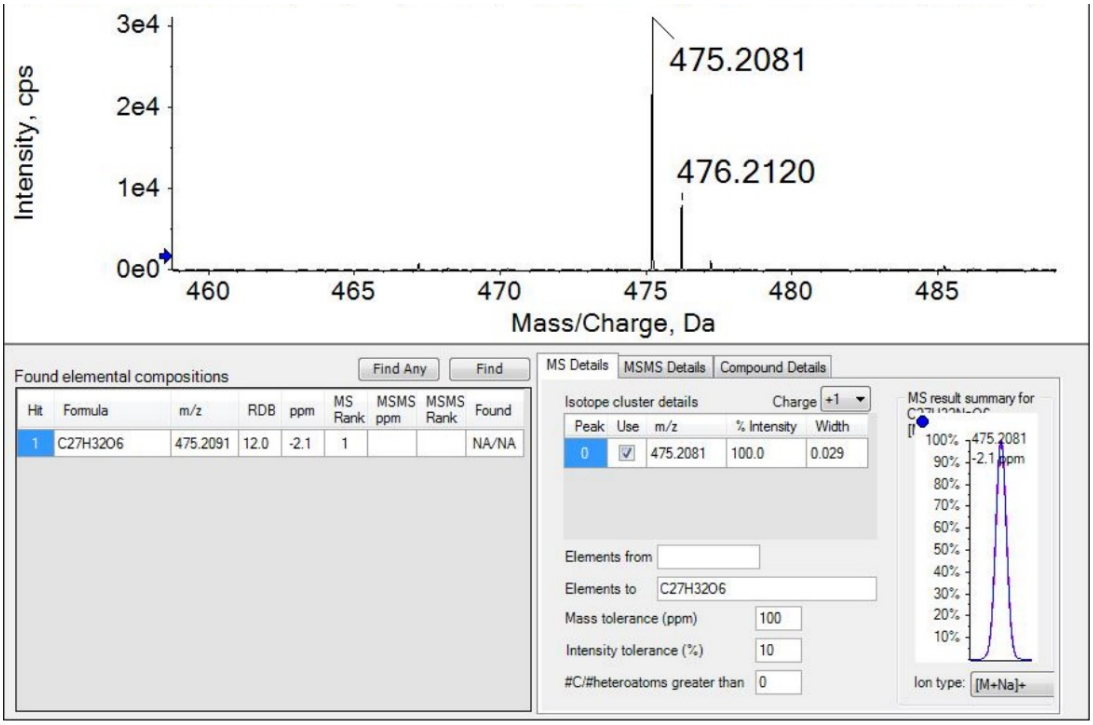

Figure S1-2 HRESIMS of compound **1**

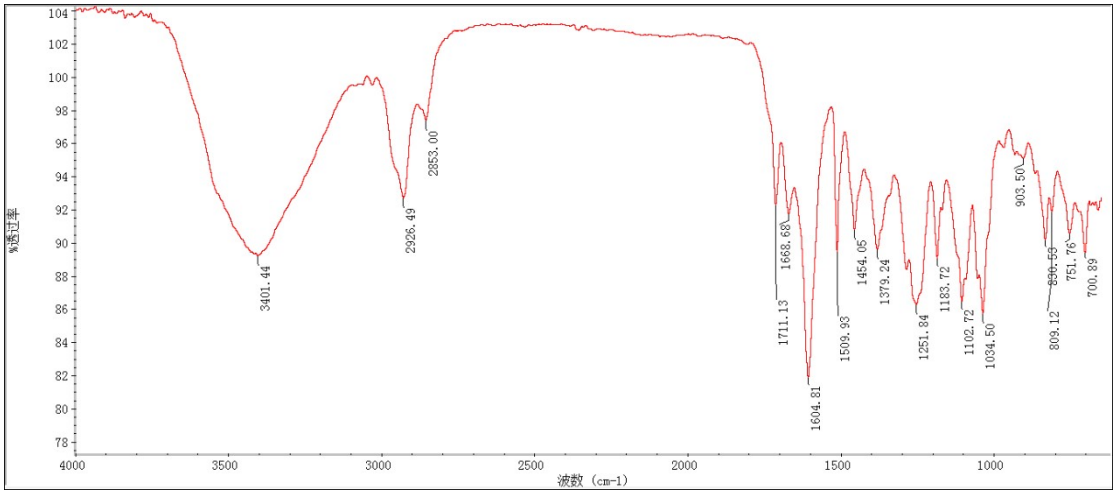

Figure S1-3 IR spectrum of compound **1** (MeOH)

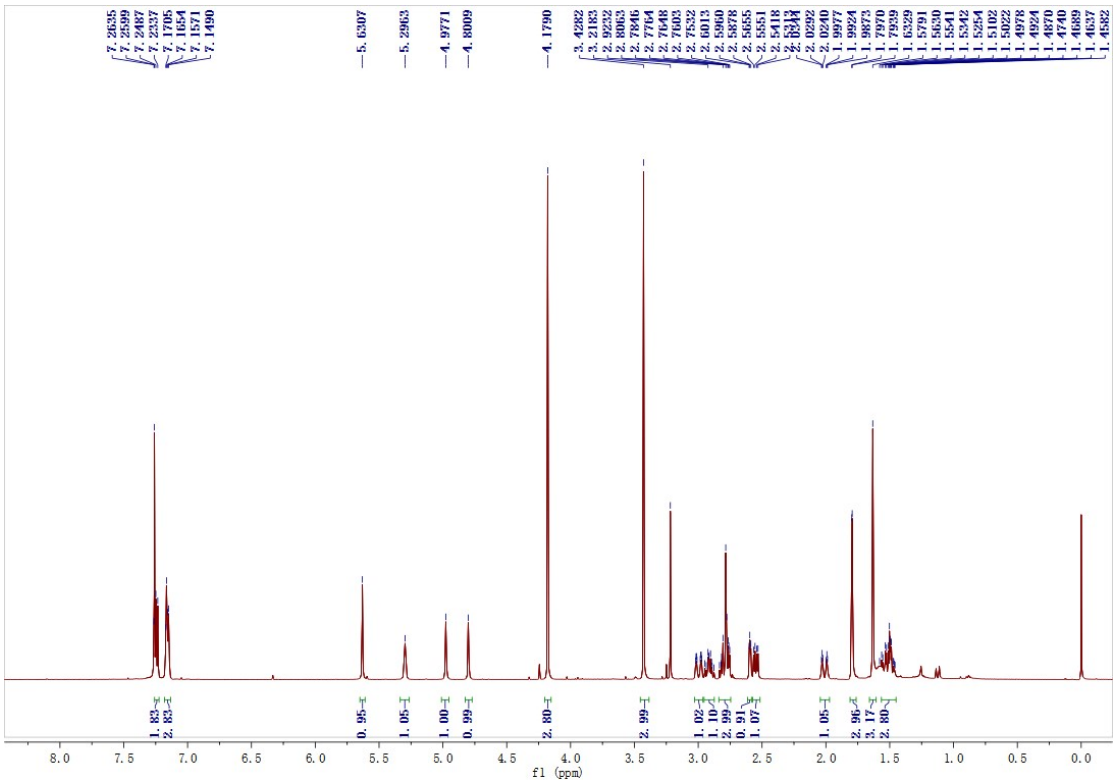

Figure S1-4 ^{1}H NMR spectrum of compound **1** ($CDCl_3$, 500 MHz)

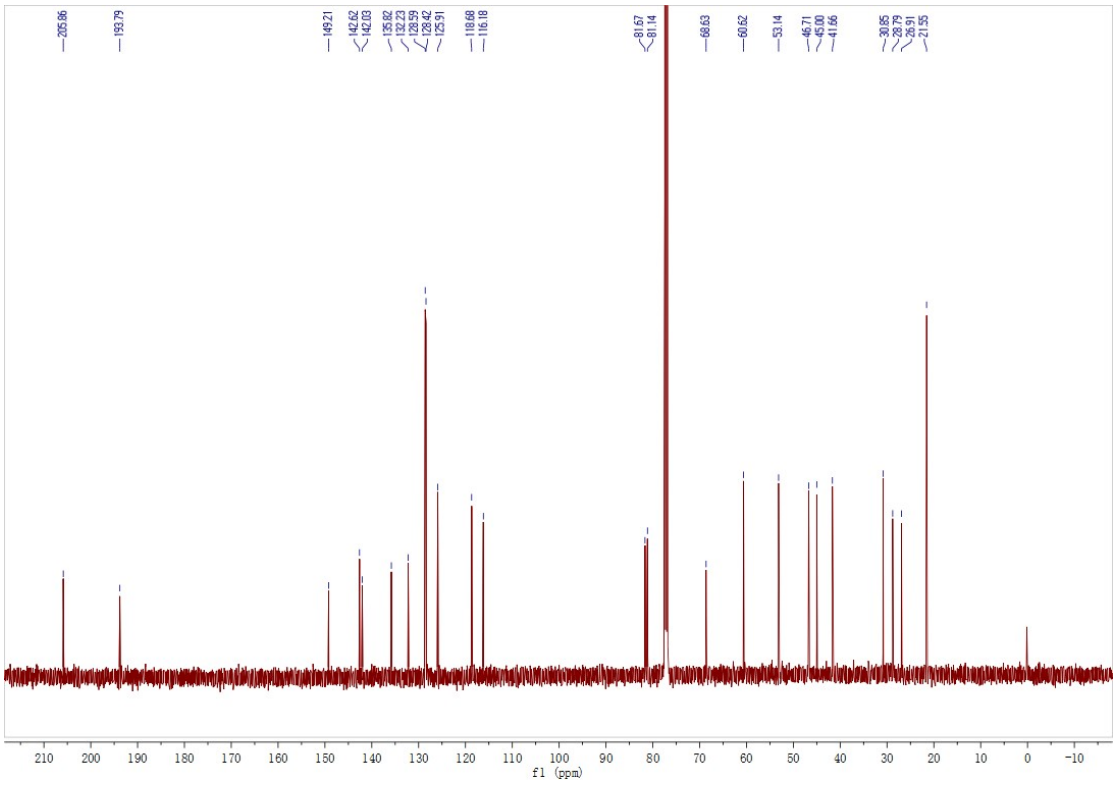

Figure S1-5 ^{13}C NMR spectrum of compound **1** ($CDCl_3$, 125 MHz)

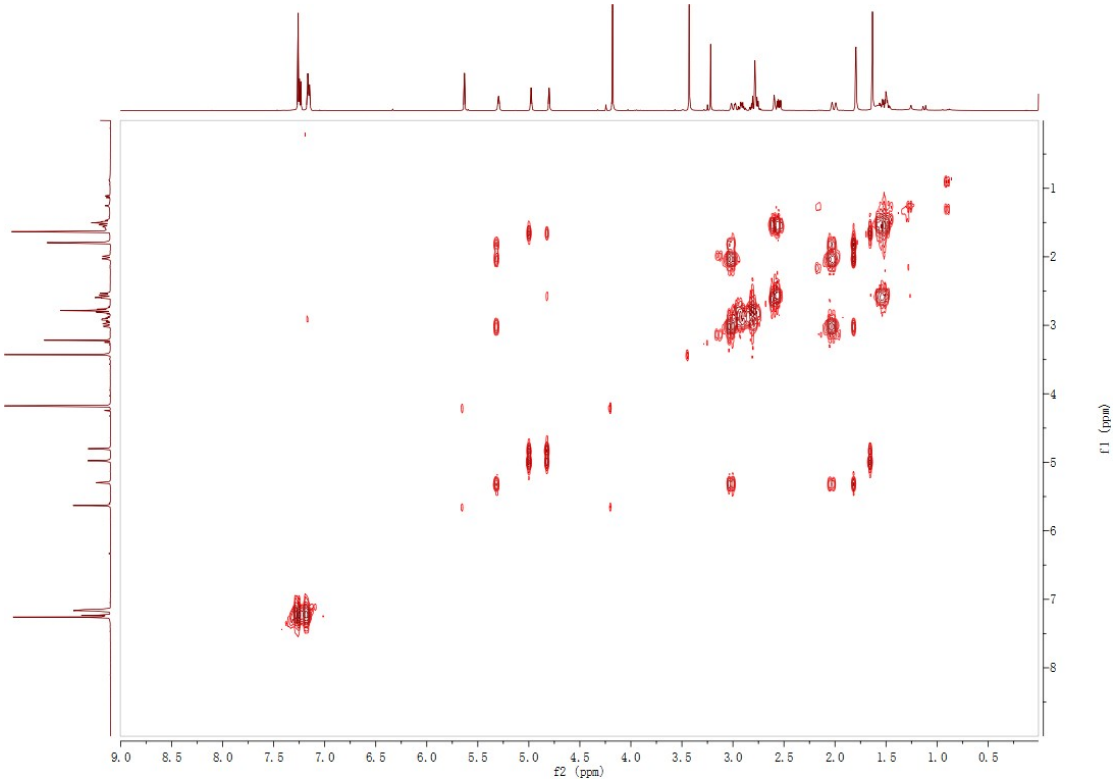

Figure S1-6 ^{1}H-^{1}H COSY spectrum of compound **1** ($CDCl_3$, 500 MHz)

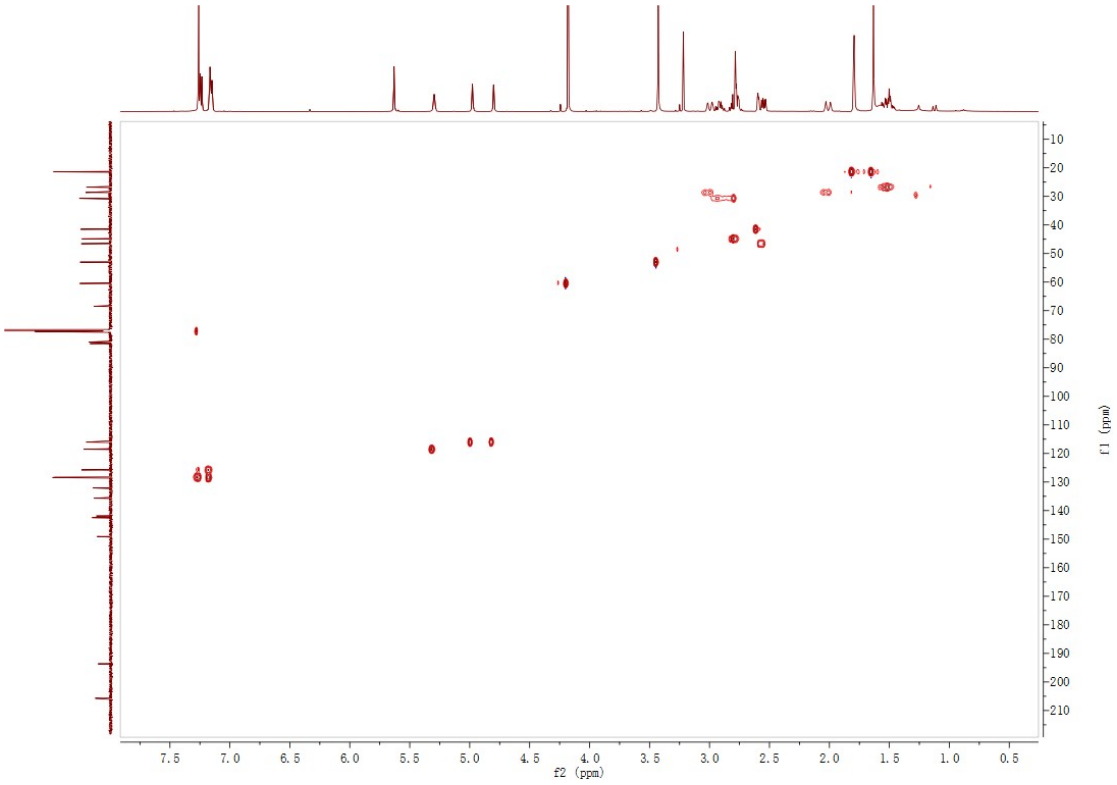

Figure S1-7 HSQC spectrum of compound **1** ($CDCl_3$, 500 MHz)

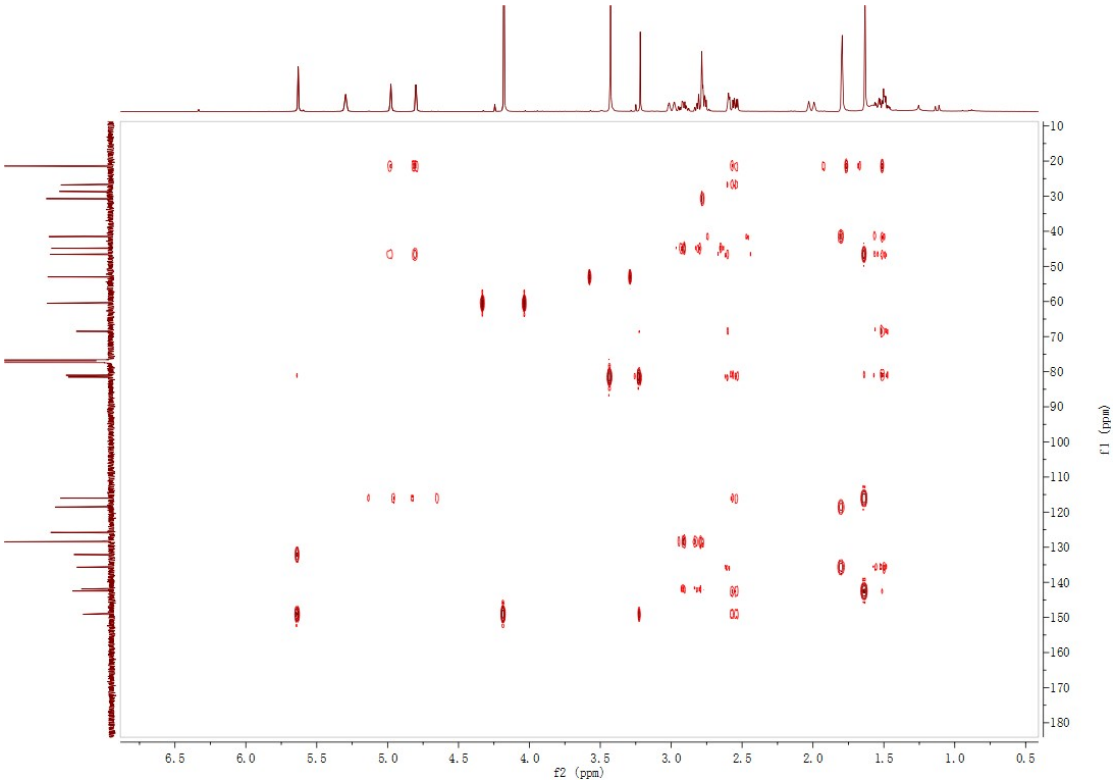

Figure S1-8 HMBC spectrum of compound **1** ($CDCl_3$, 500 MHz)

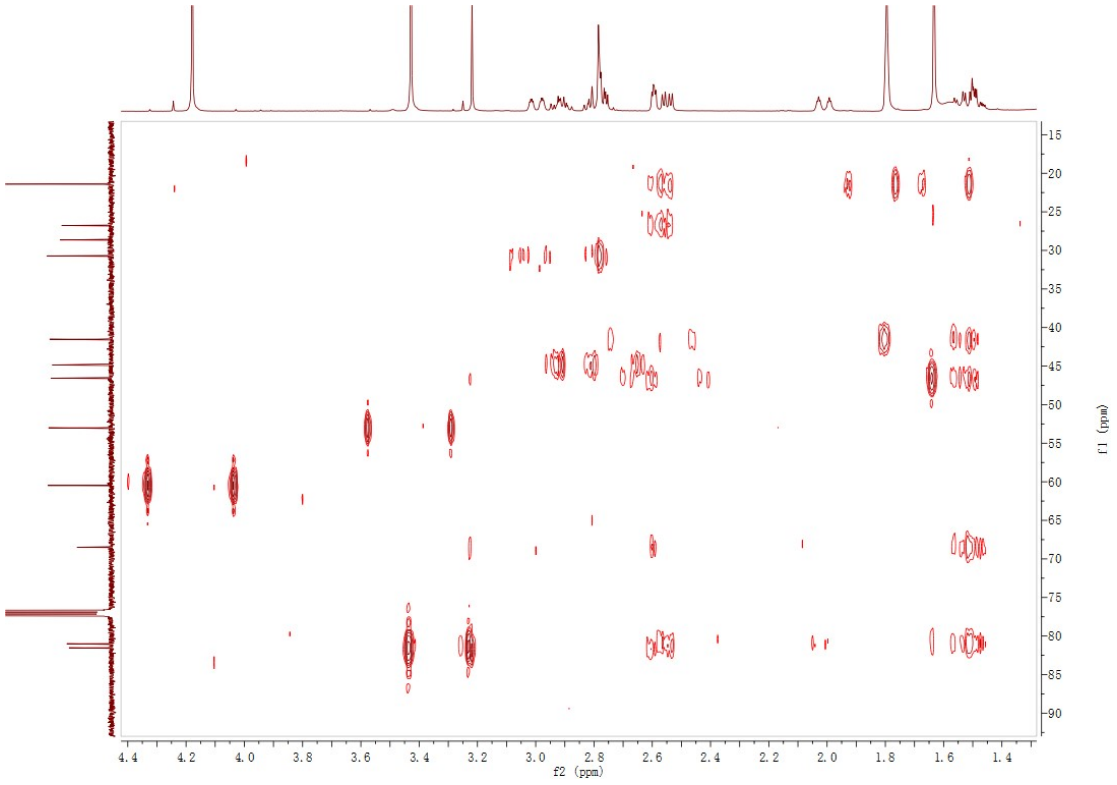

Figure S1-8-1 The expansion HMBC spectrum of compound **1** ($CDCl_3$, 500 MHz)

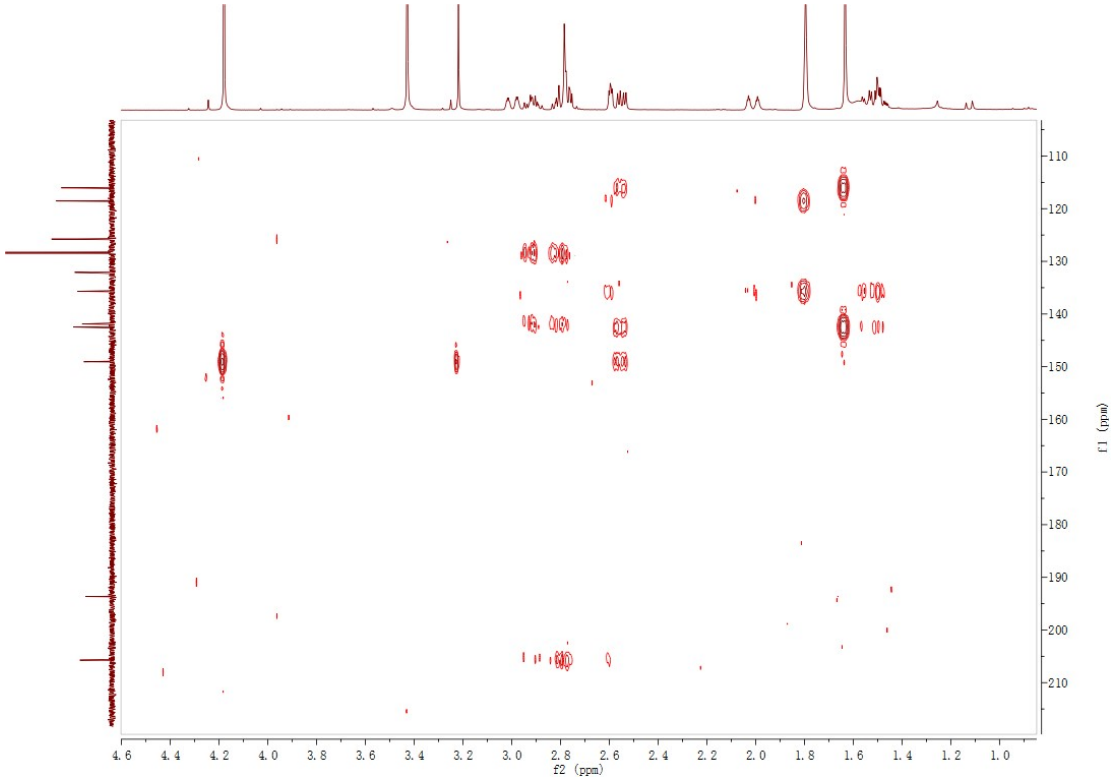

Figure S1-8-3 The expansion HMBC spectrum of compound **1** ($CDCl_3$, 500 MHz)

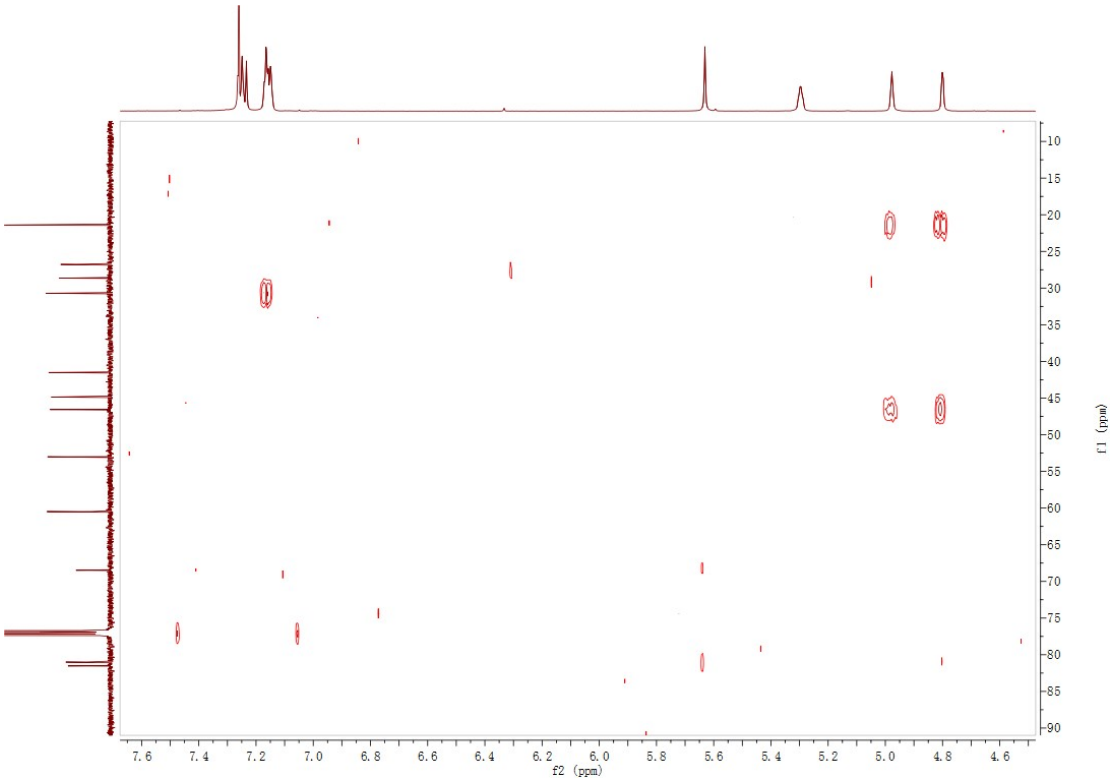

Figure S1-8-3 The expansion HMBC spectrum of compound **1** ($CDCl_3$, 500 MHz)

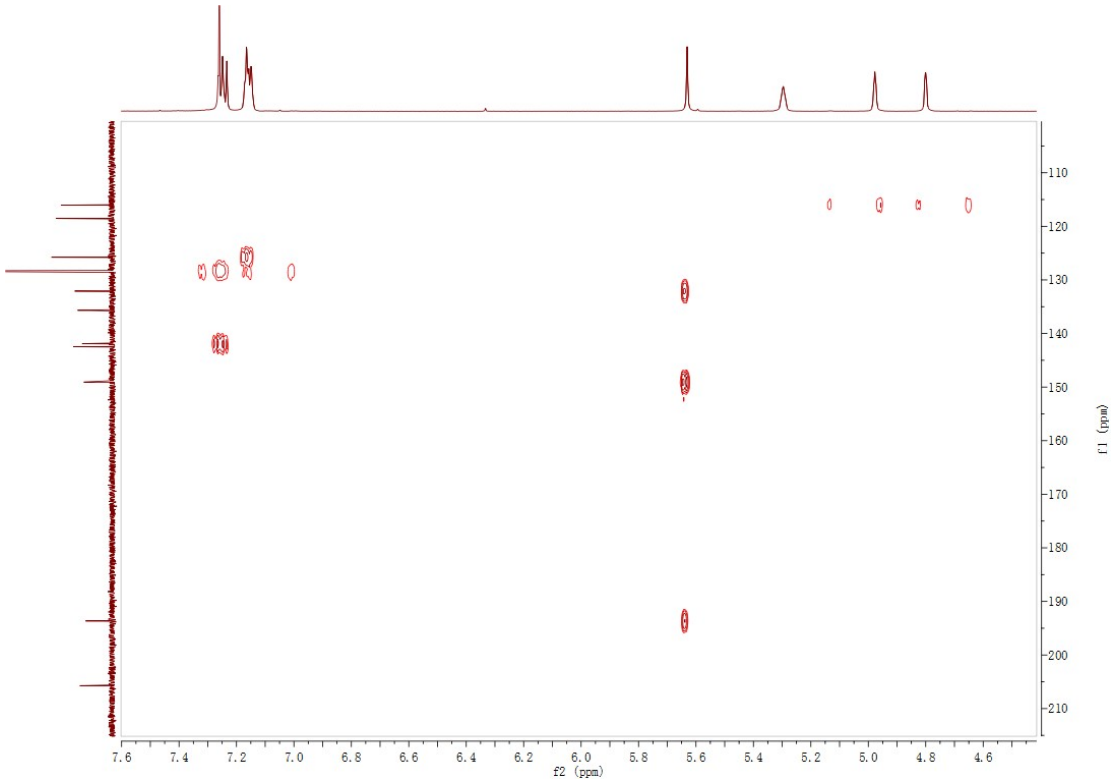

Figure S1-8-4 The expansion HMBC spectrum of compound **1** ($CDCl_3$, 500 MHz)

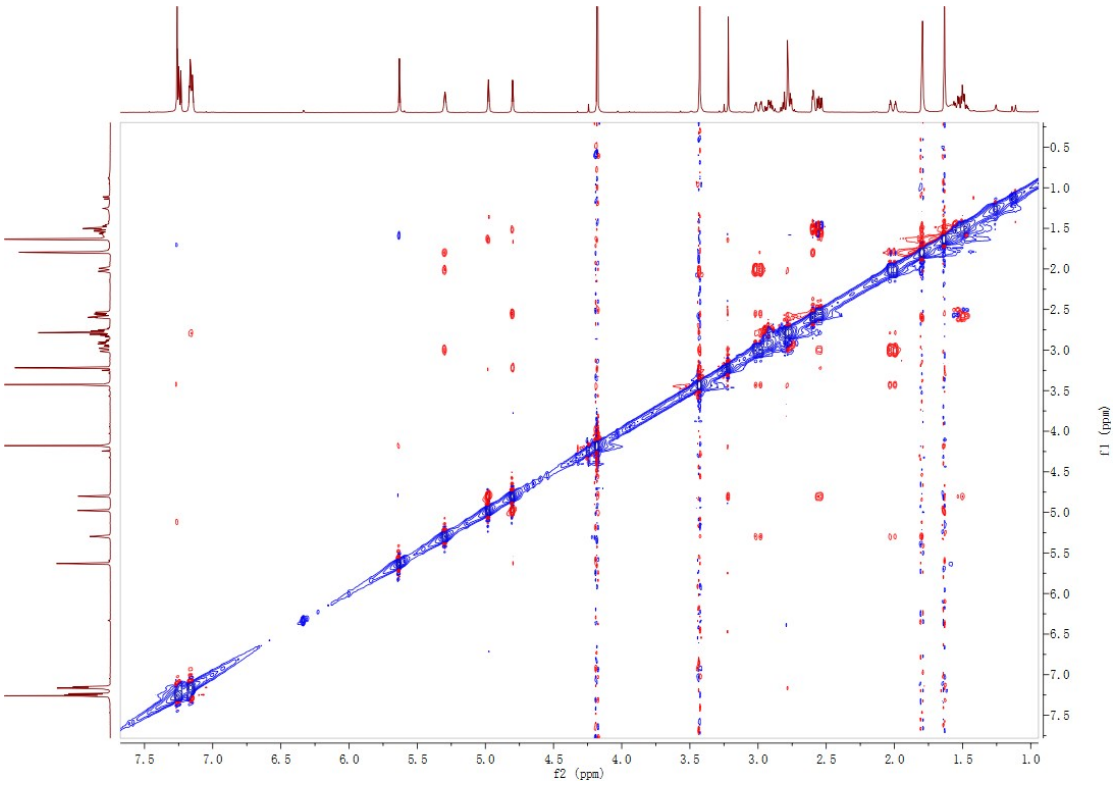

Figure S1-9 ROESY spectrum of compound **1** ($CDCl_3$, 500 MHz)

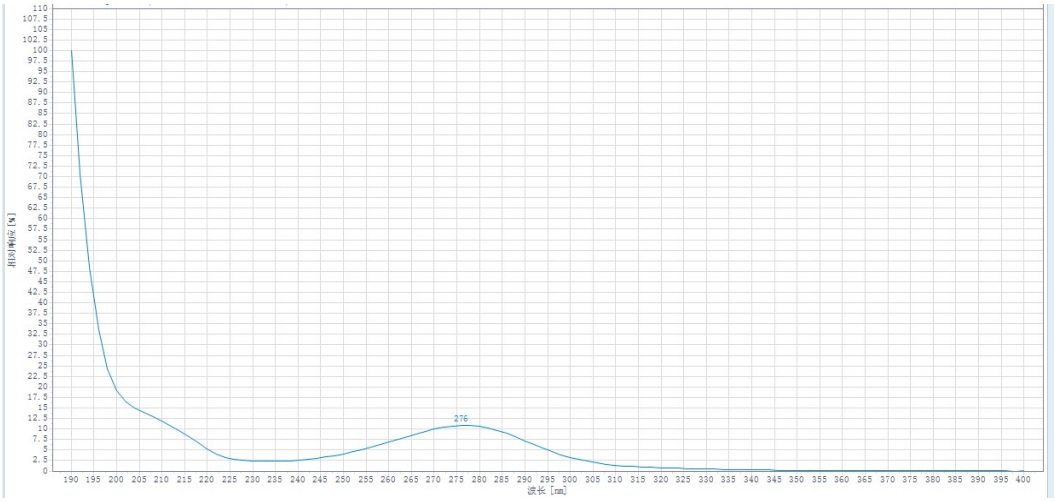

Figure S2-1 UV spectrum of compound **2**

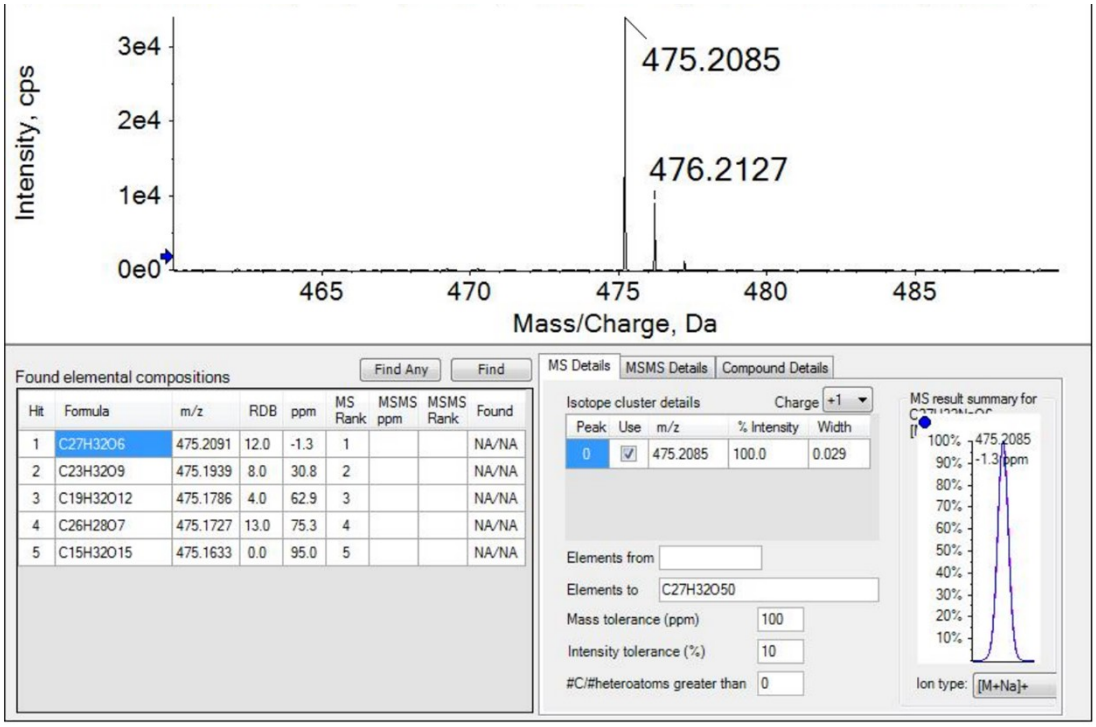

Figure S2-2 HRESIMS of compound **2**

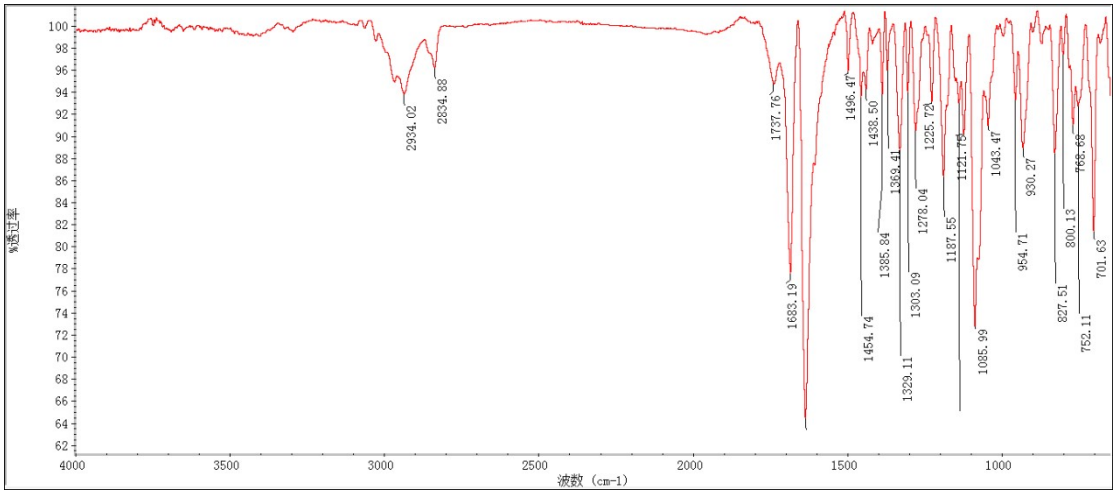

Figure S2-3 IR spectrum of compound **2** (MeOH)

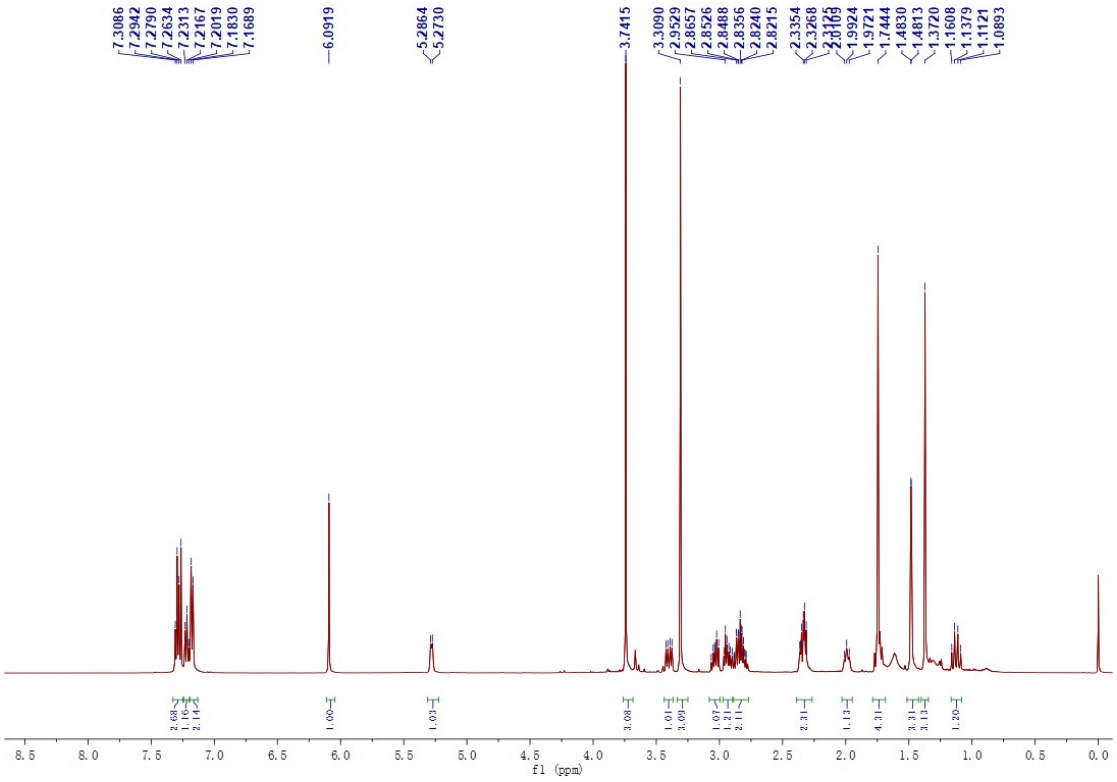

Figure S2-4 ^{1}H NMR spectrum of compound **2** ($CDCl_3$, 500 MHz)

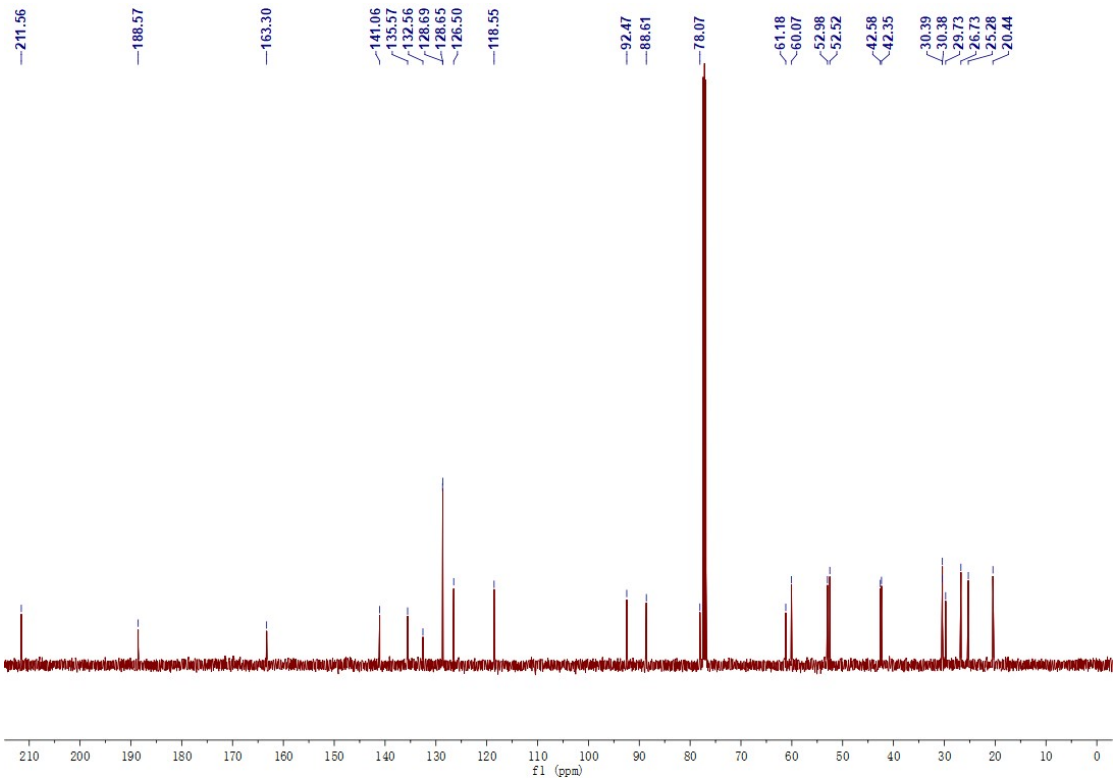

Figure S2-5 ^{13}C NMR spectrum of compound **2** ($CDCl_3$, 125 MHz)

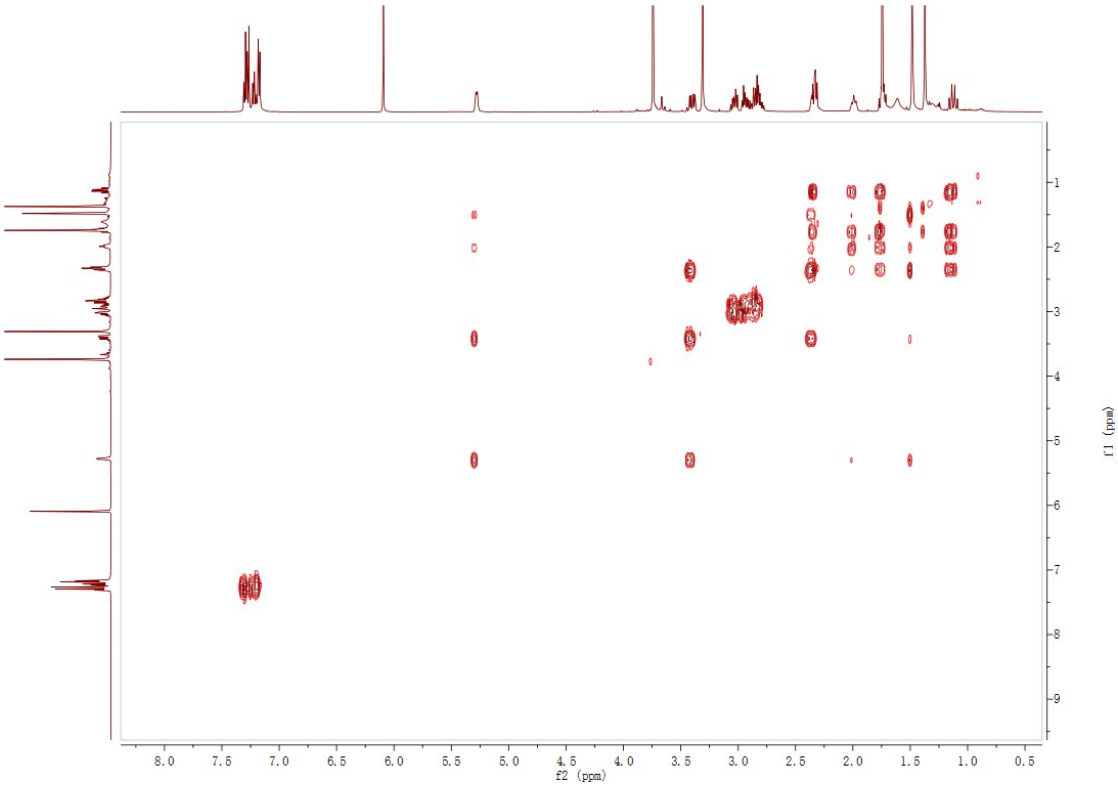

Figure S2-6 ^{1}H-^{1}H COSY spectrum of compound **2** ($CDCl_3$, 500 MHz)

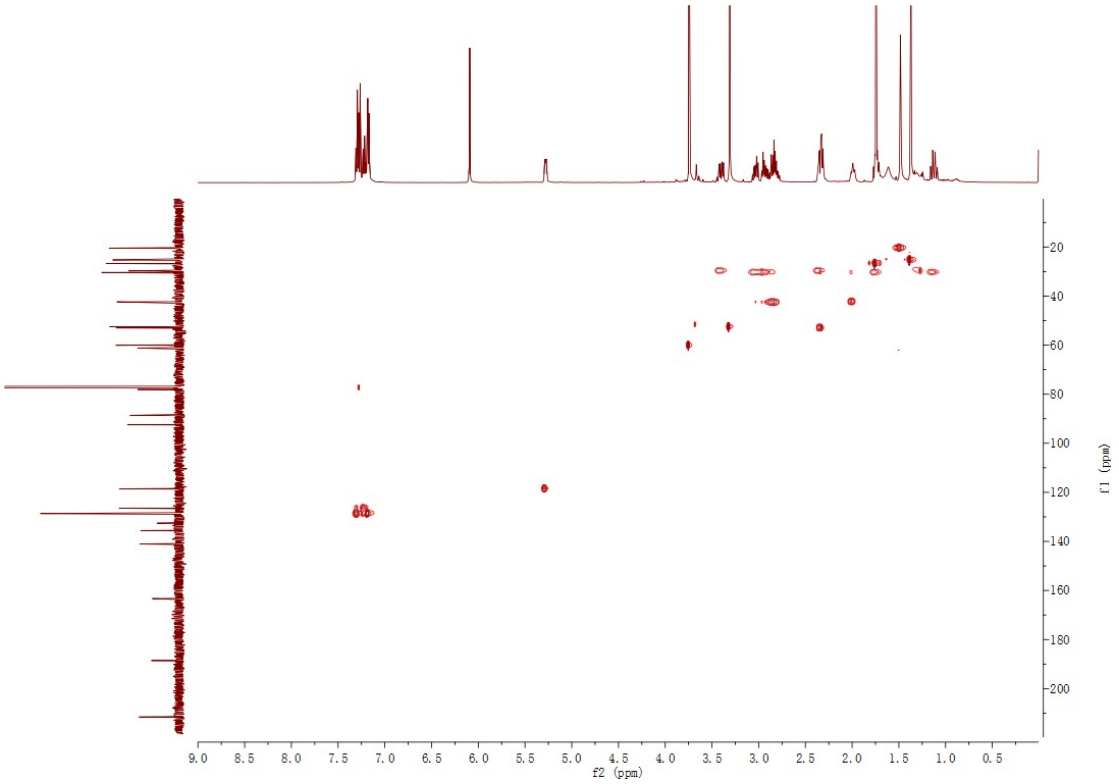

Figure S2-7 HSQC spectrum of compound **2** ($CDCl_3$, 500 MHz)

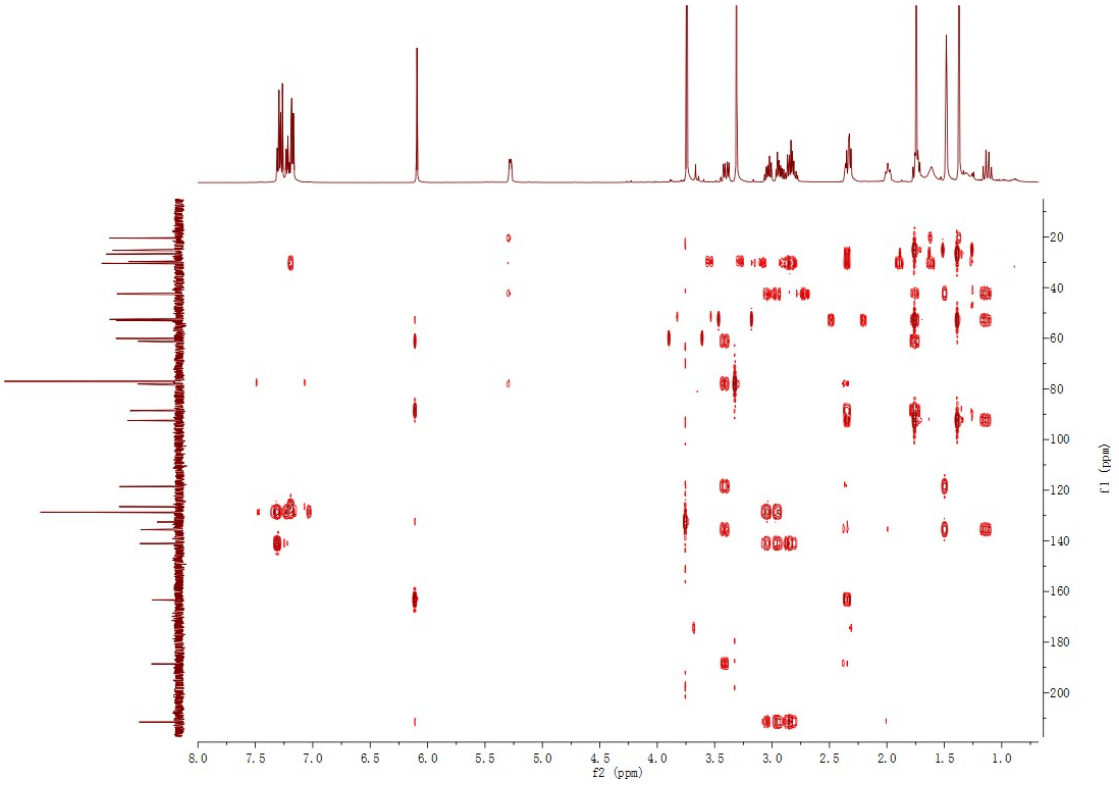

Figure S2-8 HMBC spectrum of compound **2** ($CDCl_3$, 500 MHz)

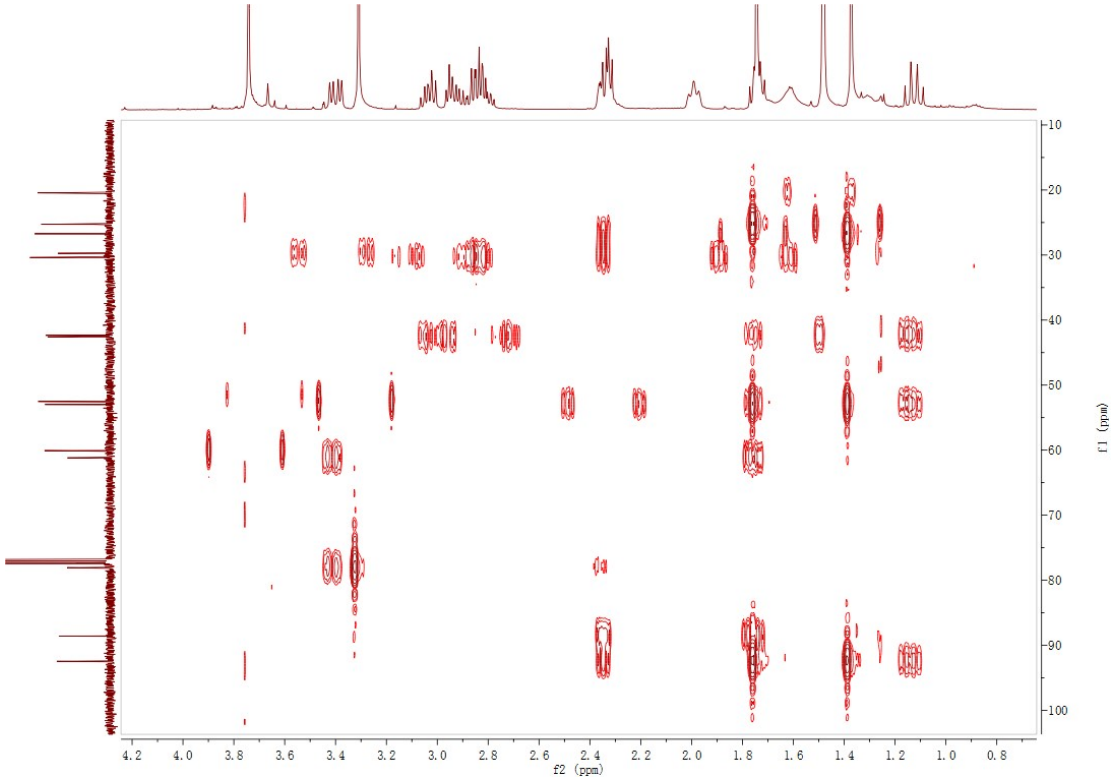

Figure S2-8-1 The expansion HMBC spectrum of compound **2** ($CDCl_3$, 500 MHz)

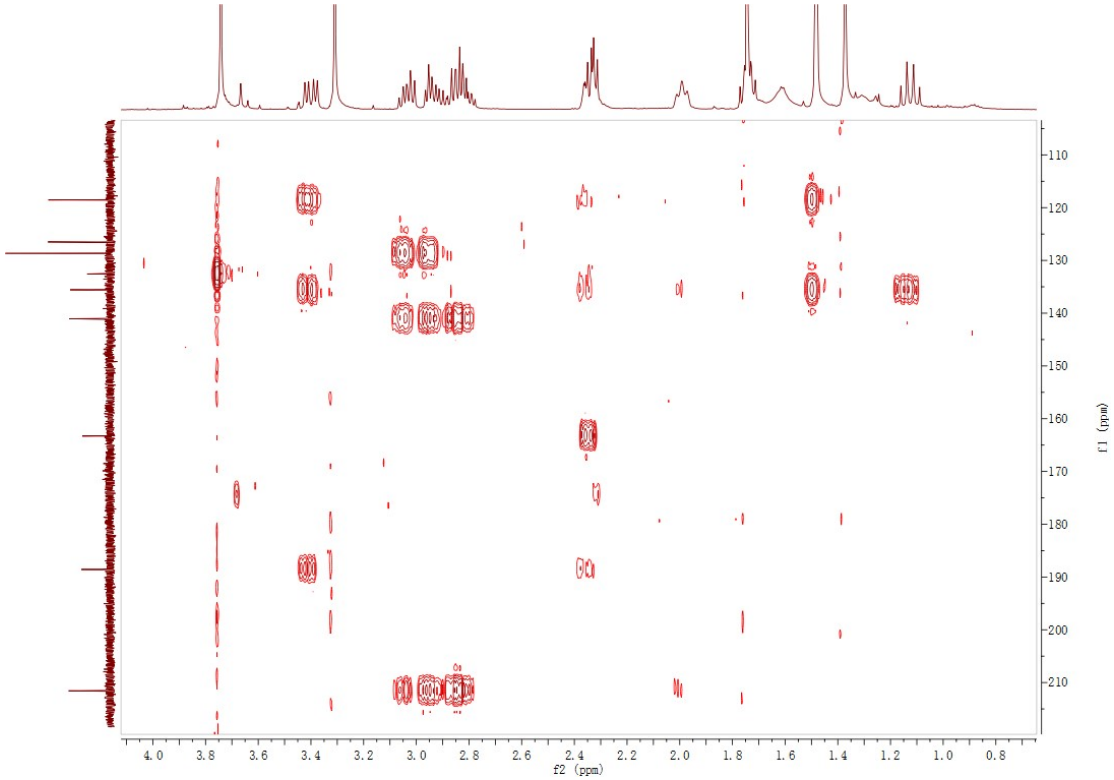

Figure S2-8-2 The expansion HMBC spectrum of compound **2** ($CDCl_3$, 500 MHz)

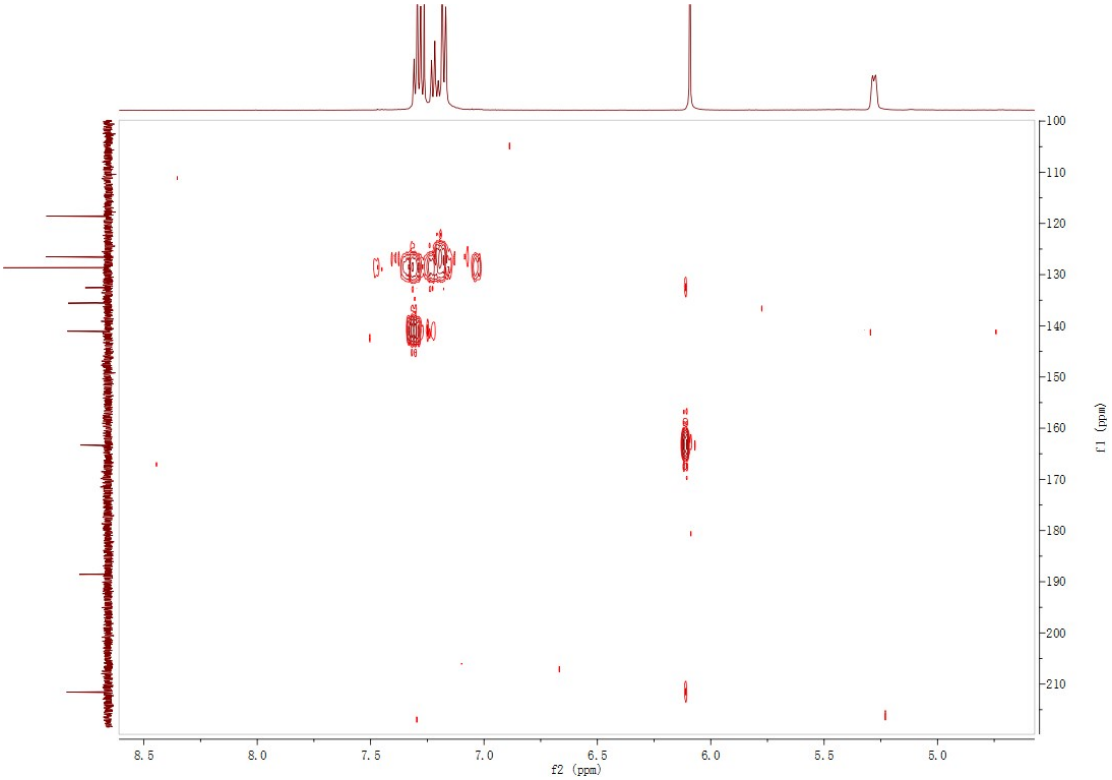

Figure S2-8-3 The expansion HMBC spectrum of compound **2** ($CDCl_3$, 500 MHz)

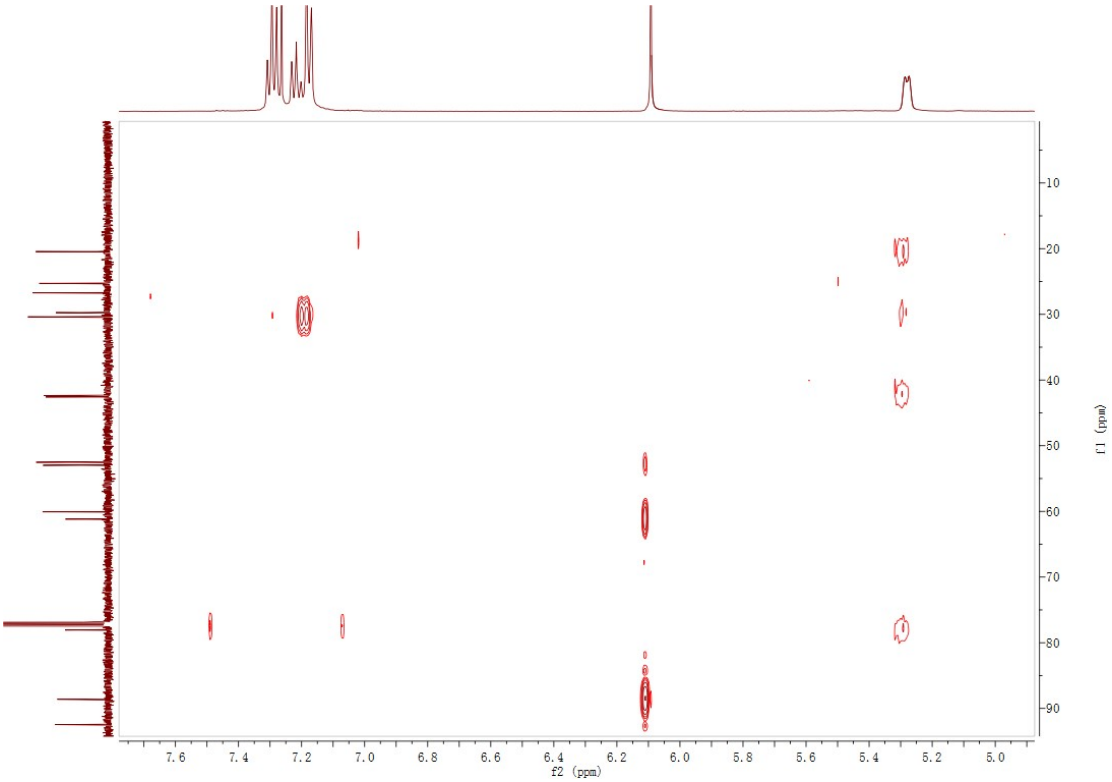

Figure S2-8-4 The expansion HMBC spectrum of compound **2** ($CDCl_3$, 500 MHz)

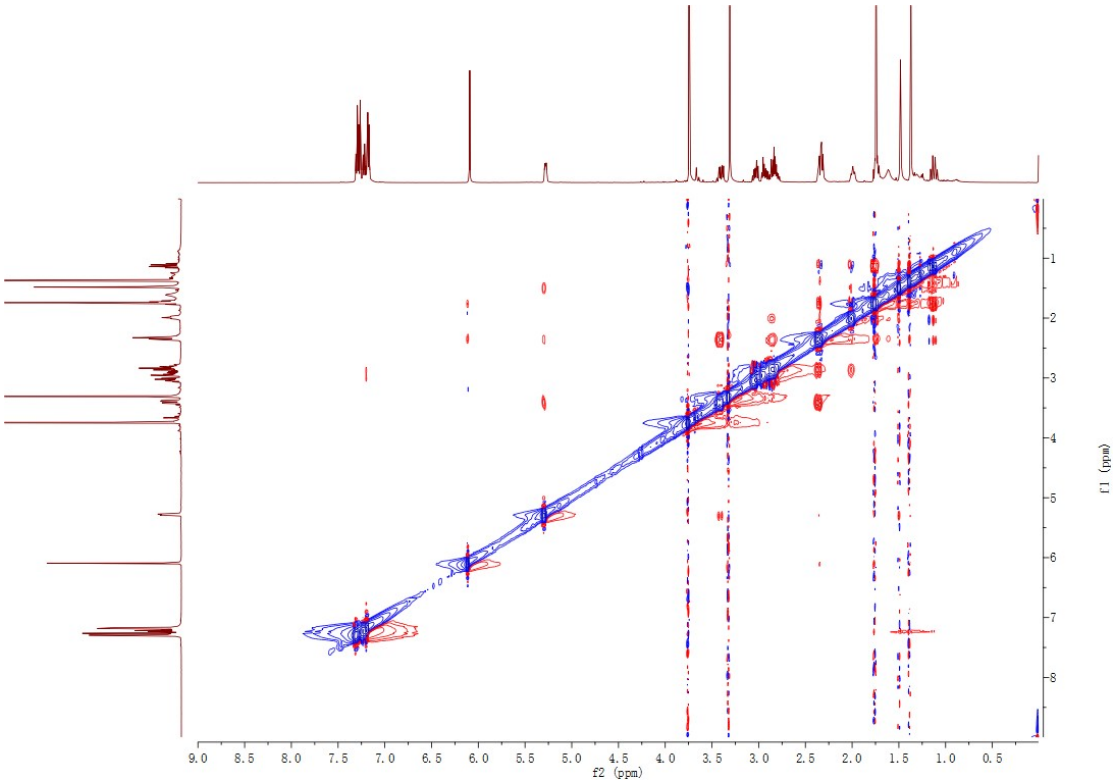

Figure S2-9 ROESY spectrum of compound **2** ($CDCl_3$, 500 MHz)

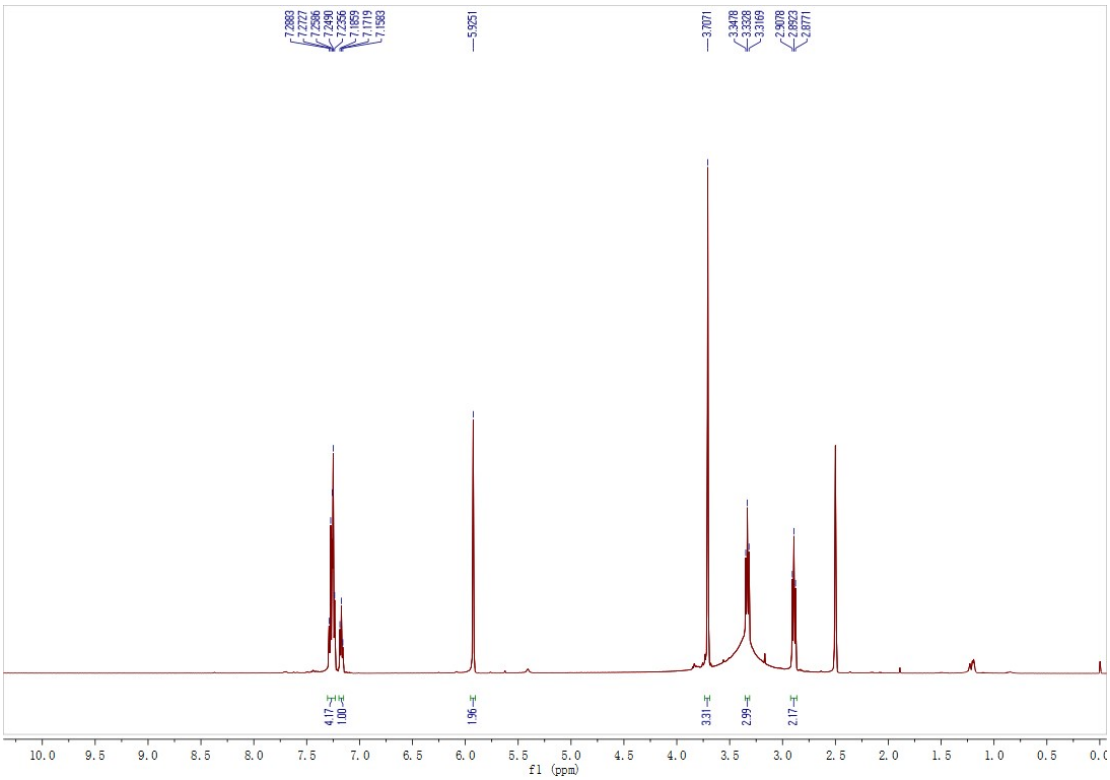

Figure S3-1 ^1H NMR spectrum of compound **3** ($CDCl_3$, 500 MHz)

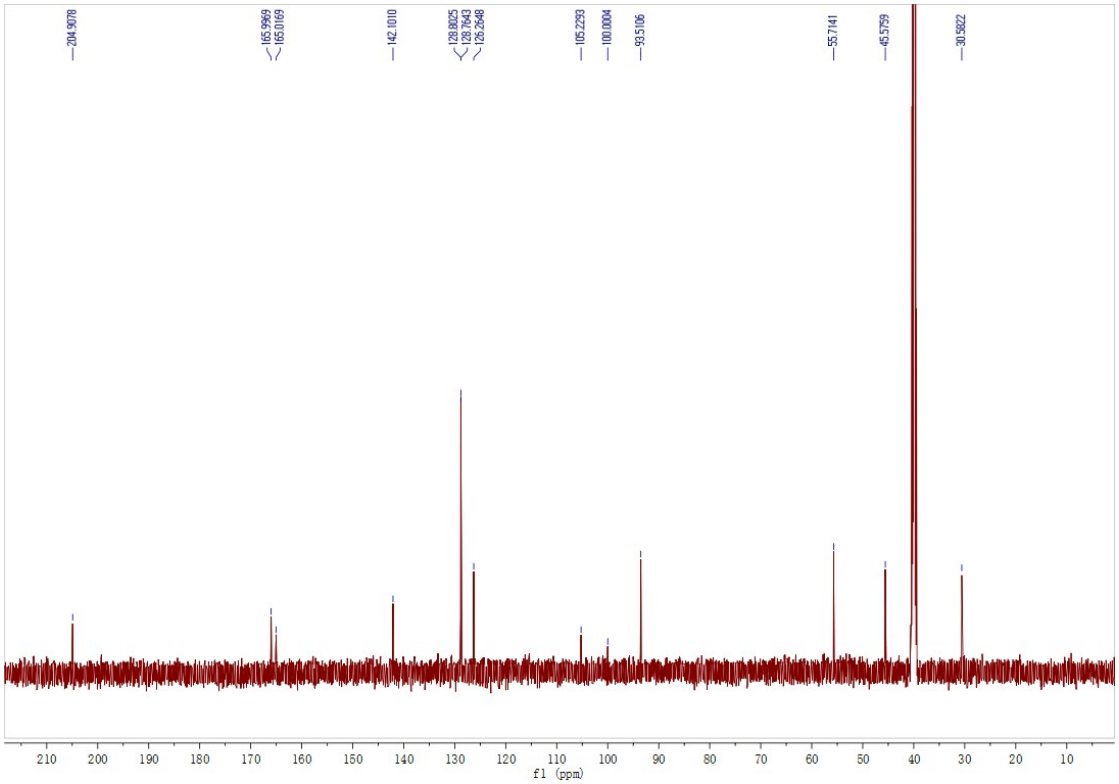

Figure S3-2 ^{13}C NMR spectrum of compound **3** ($CDCl_3$, 125 MHz)