Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Information

Clindanones A and B and Cladosporols F and G, Polyketides from a Deep-sea Derived Fungus *Cladosporium cladosporioides* HDN14-342

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List of Supplementary information

Figure S1. ^{1}H NMR (500 MHz, acetone-d_6) spectrum of **1**.

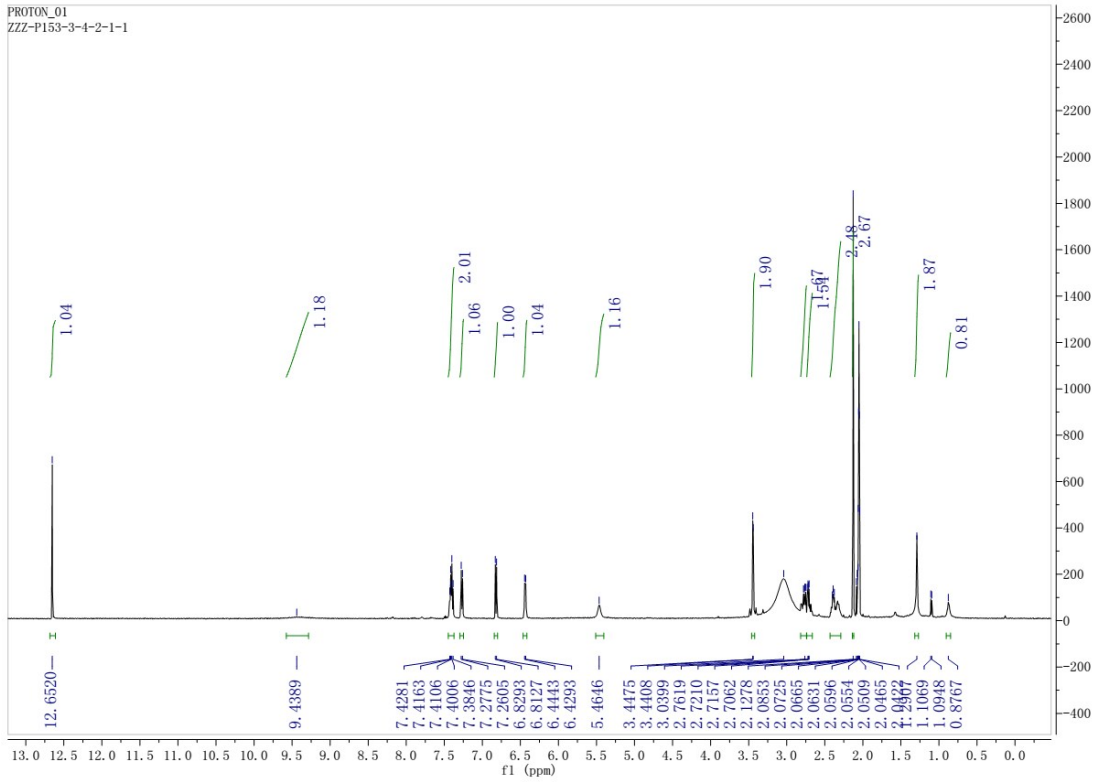


Figure S2. ^{13}C NMR (125 MHz, acetone-d_6) spectrum of **1**.

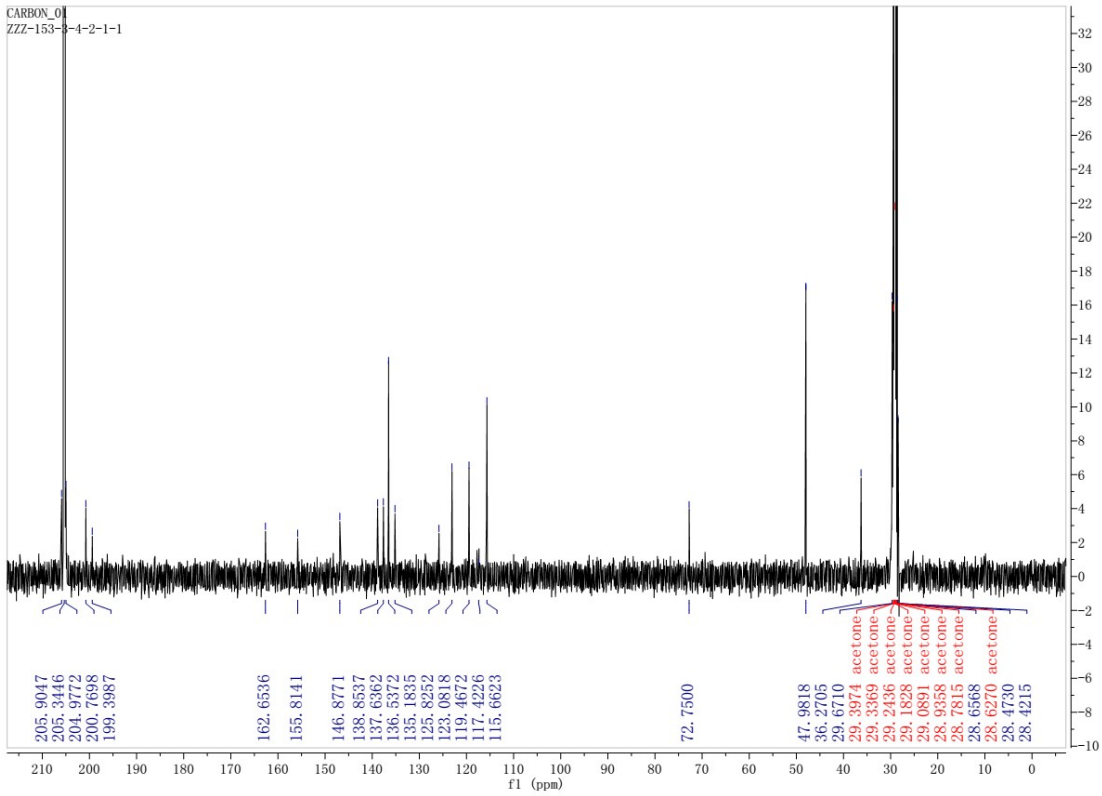


Figure S3. DEPT (125 MHz, acetone-d_6) spectrum of **1**.

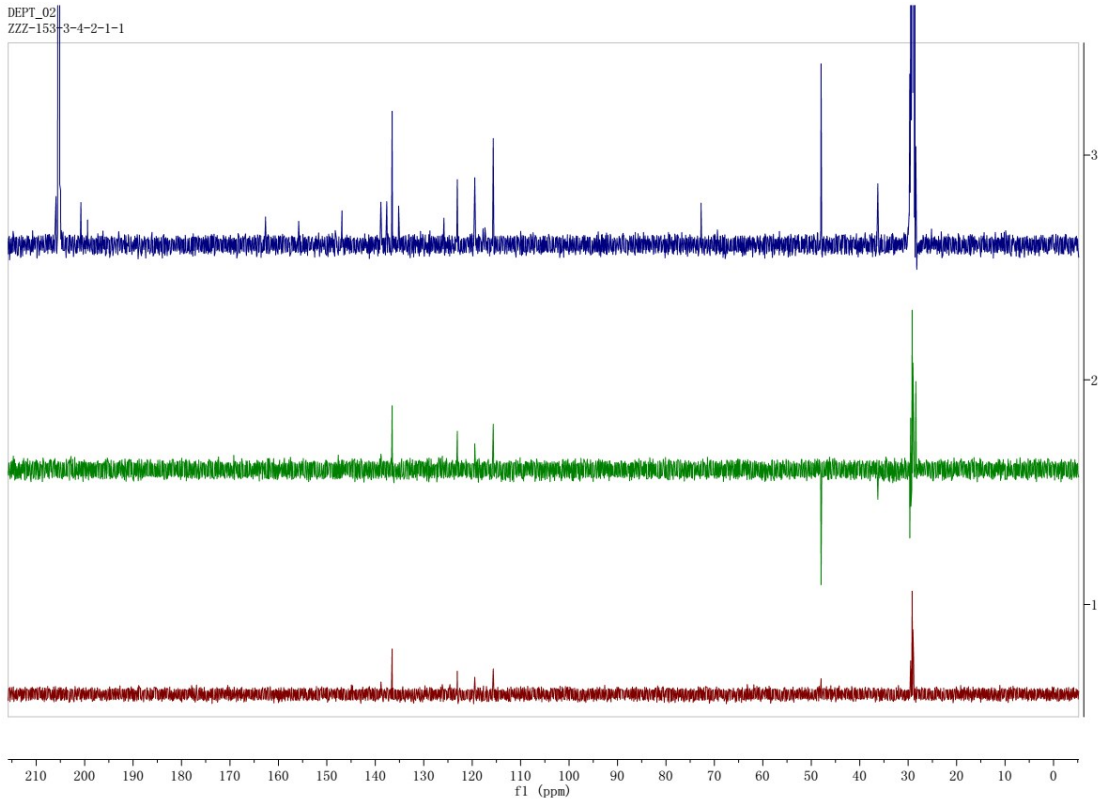


Figure S4. HSQC spectrum of **1** in acetone-d_6.

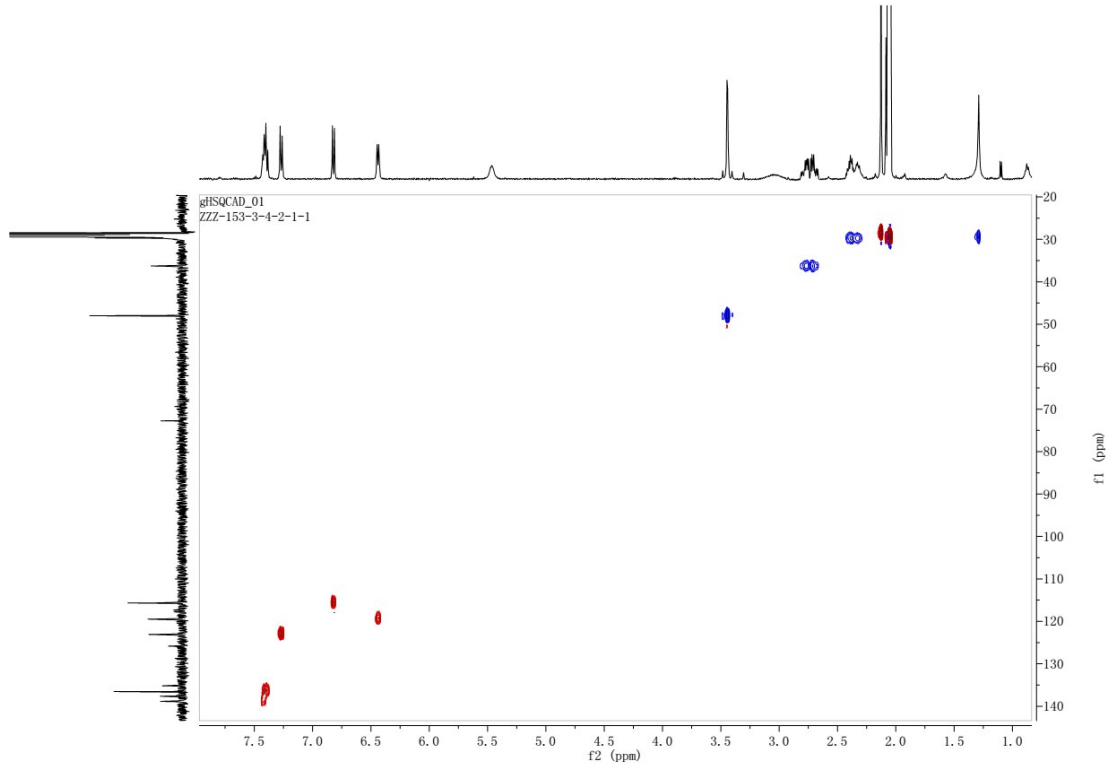


Figure S5. ^{1}H-^{1}H COSY spectrum of **1** in acetone-d_6.

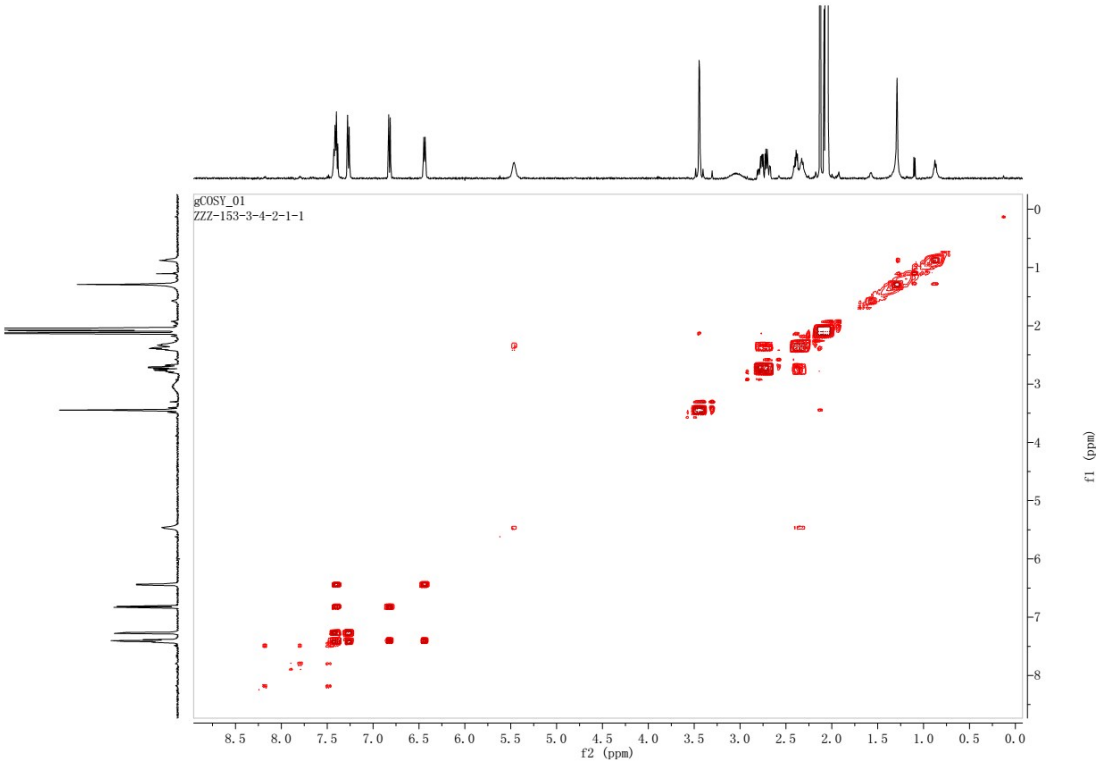


Figure S6. HMBC spectrum of **1** in acetone-d_6.

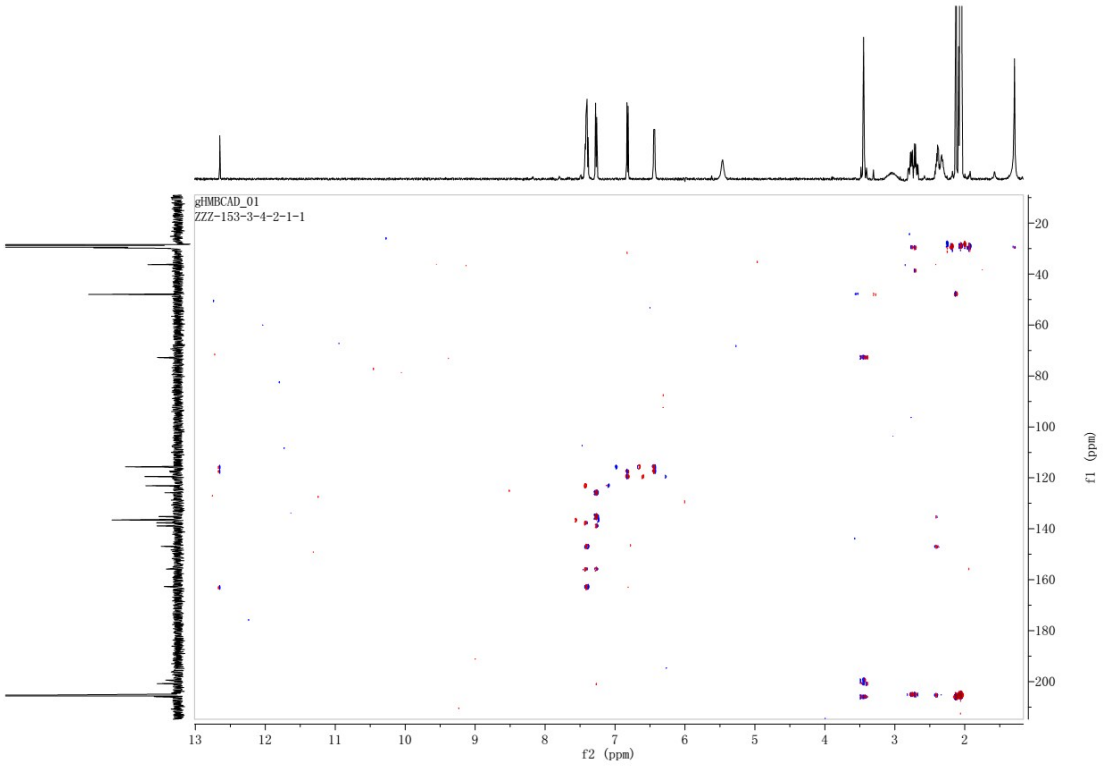


Figure S7. HRESIMS spectrum of **1**.

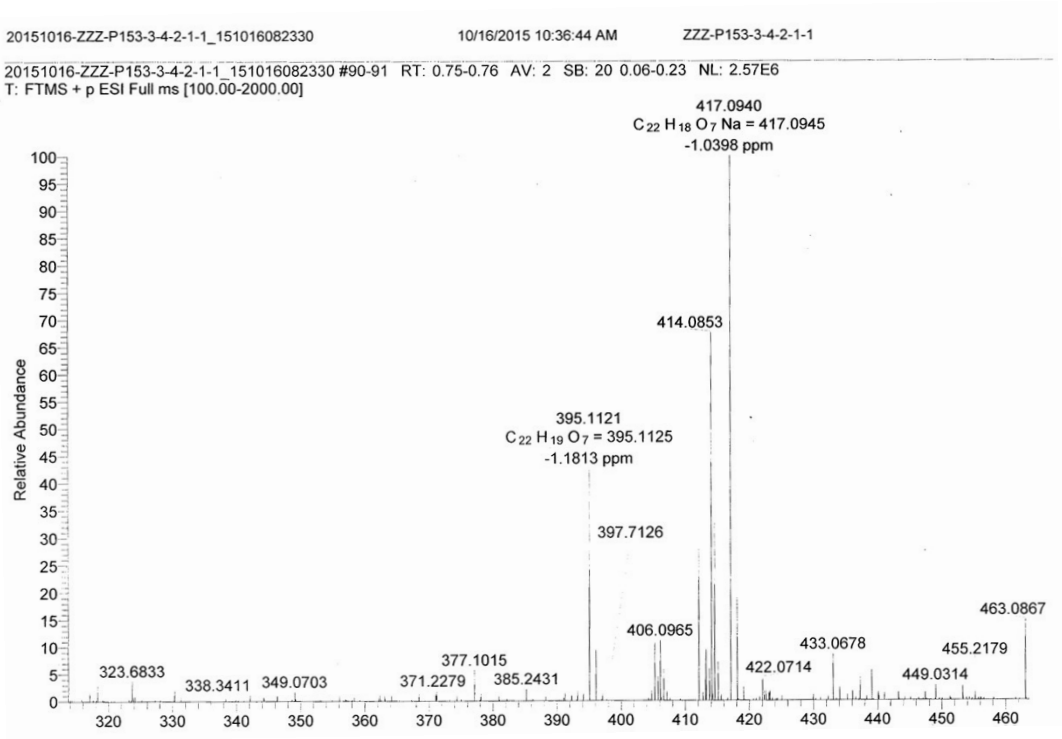


Figure S8. ^{1}H NMR (500 MHz, acetone-d_6) spectrum of **2**.

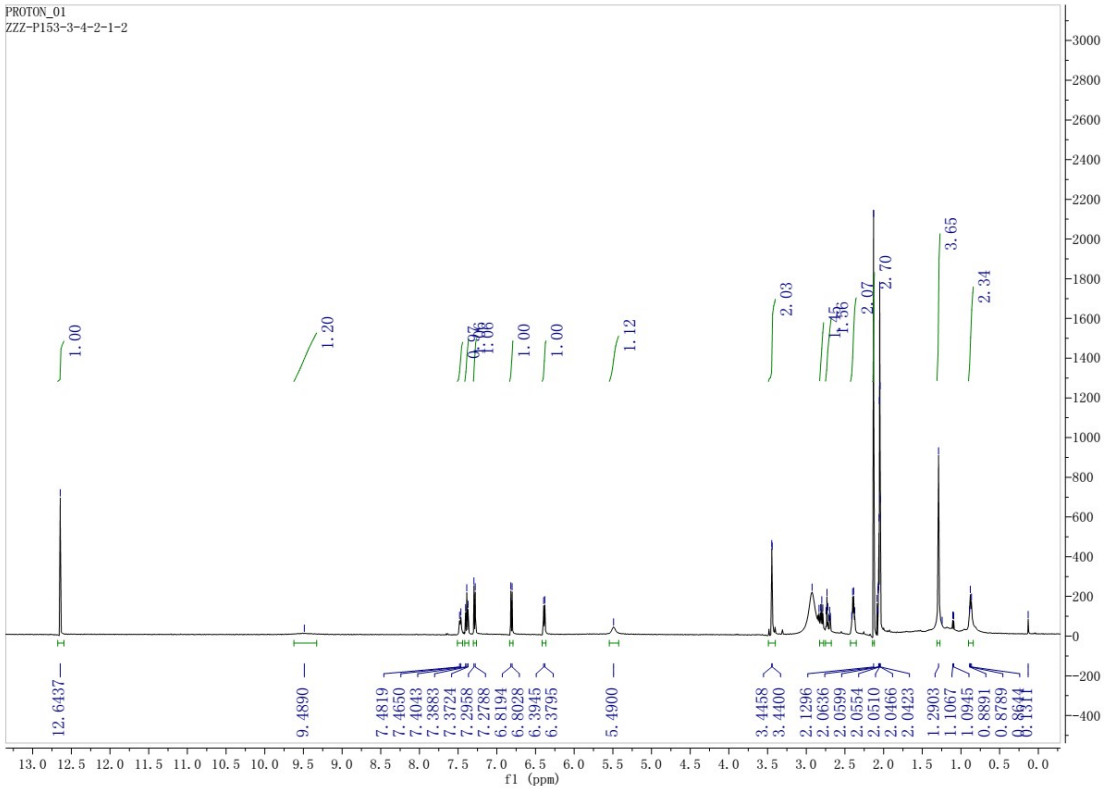


Figure S9. ^{13}C NMR (125 MHz, acetone-d_6) spectrum of **2**.

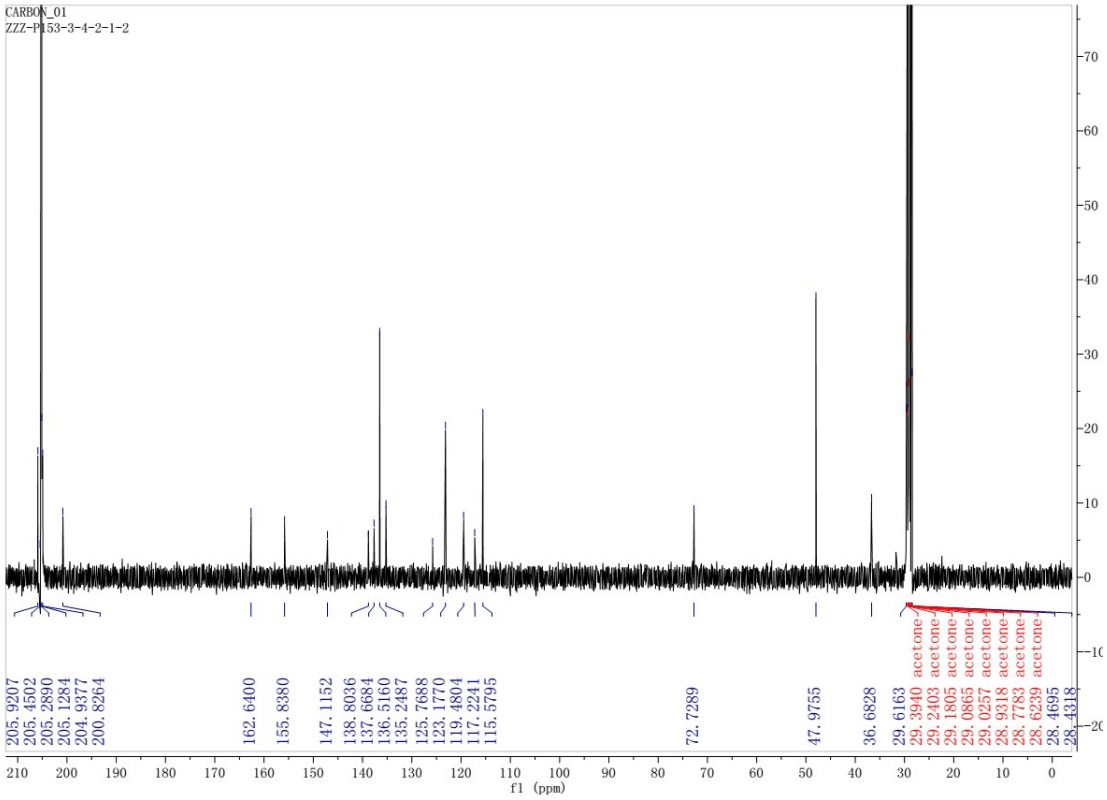


Figure S10. DEPT (125 MHz, acetone-d_6) spectrum of **2**.

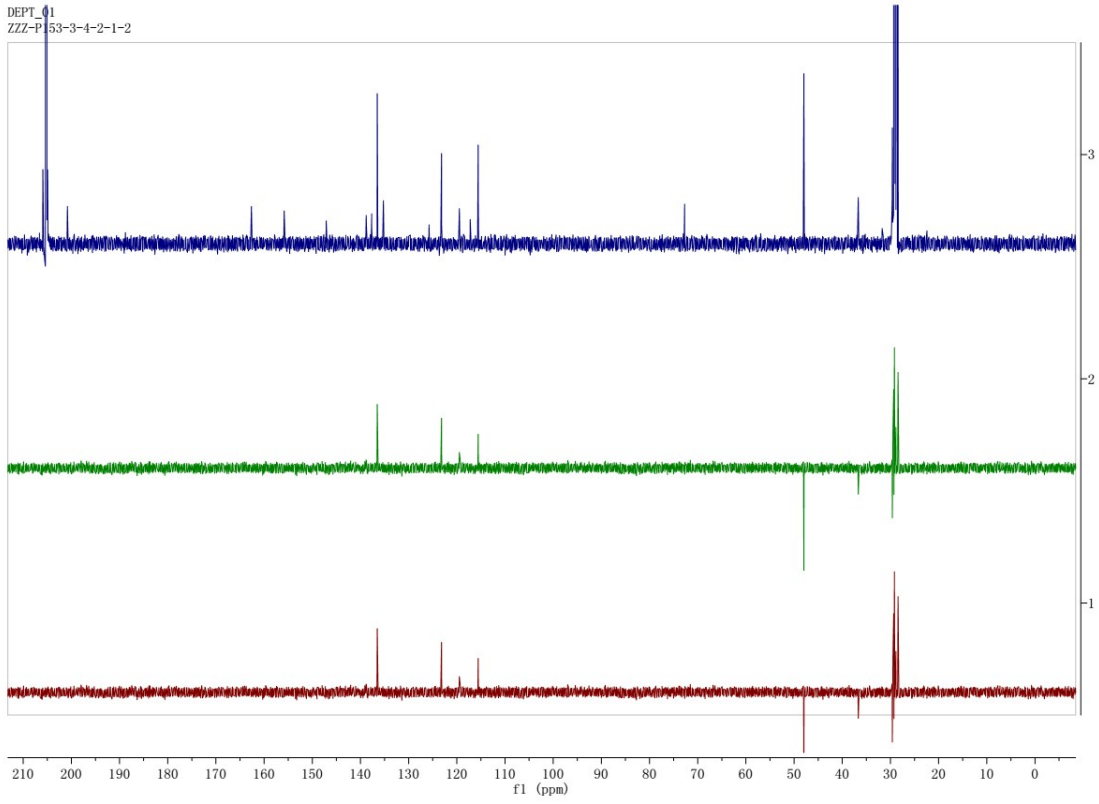


Figure S11. HSQC spectrum of **2** in acetone-d_6.

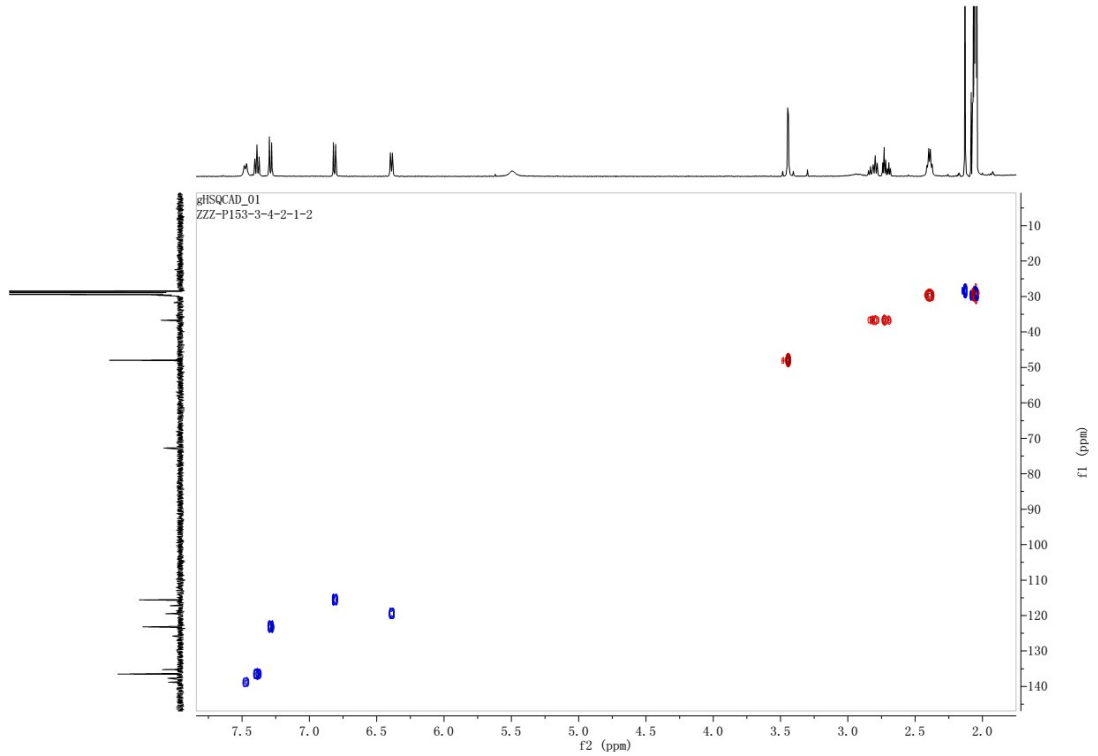


Figure S12. ^{1}H-^{1}H COSY spectrum of **2** in acetone-d_6.

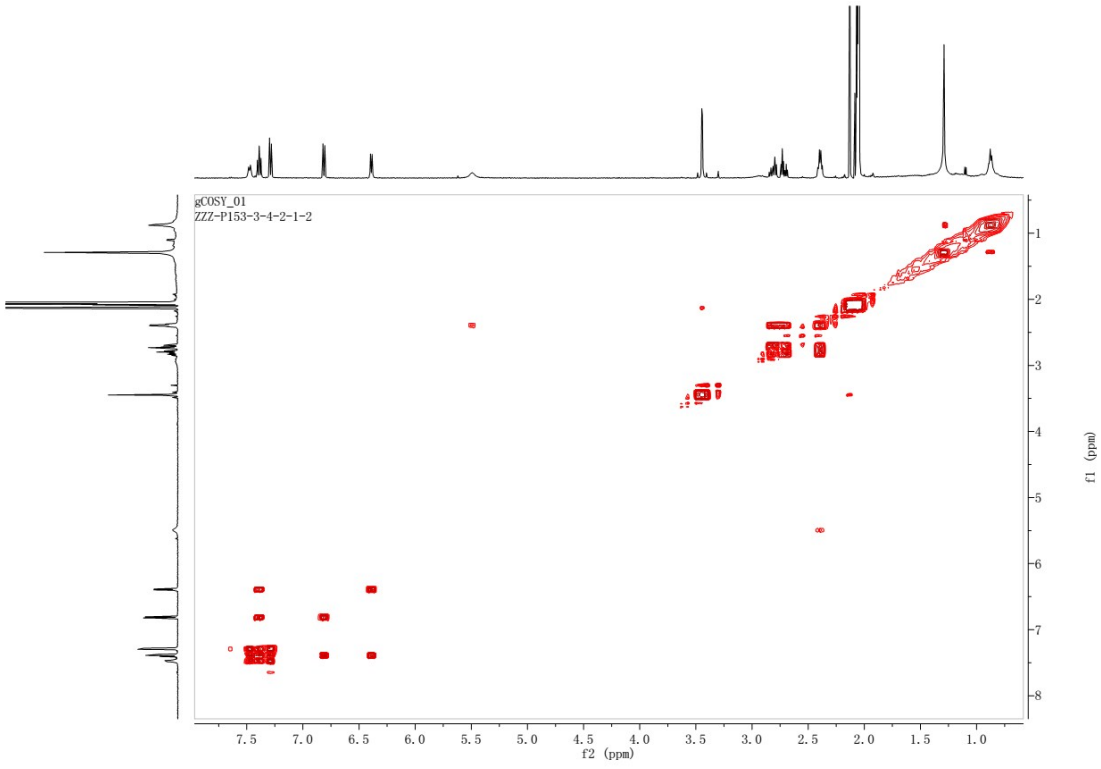


Figure S13. HMBC spectrum of **2** in acetone-d_6.

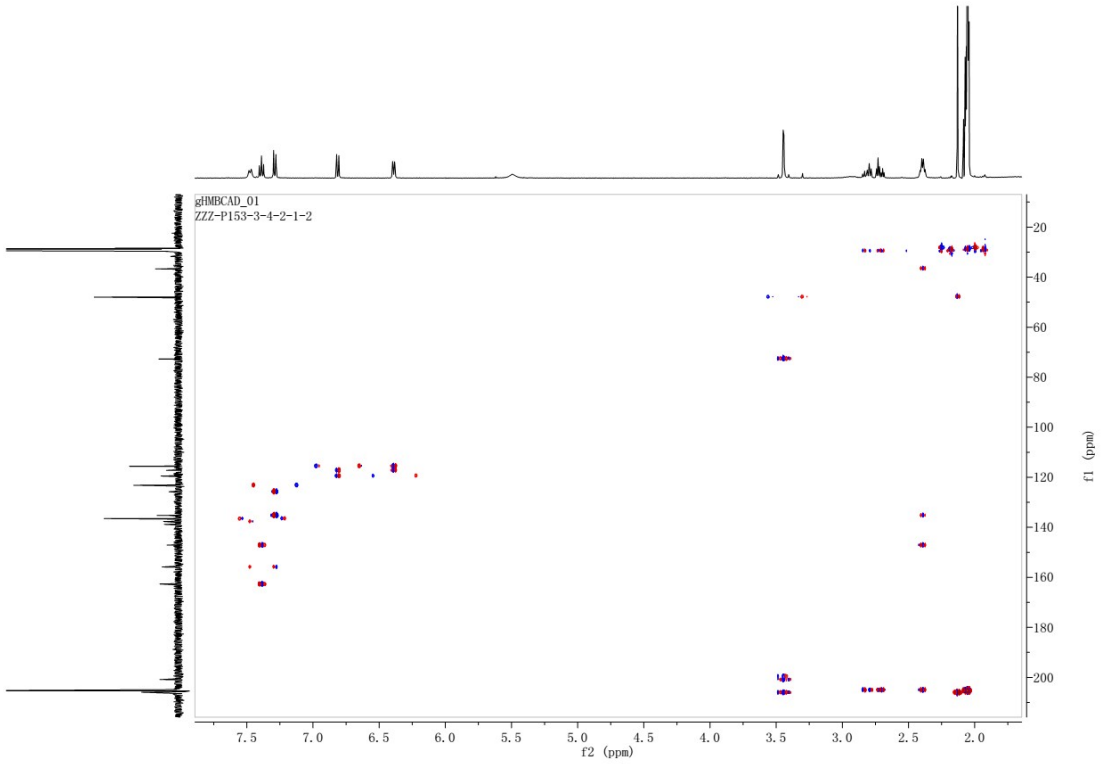


Figure S14. HRESIMS spectrum of **2**.

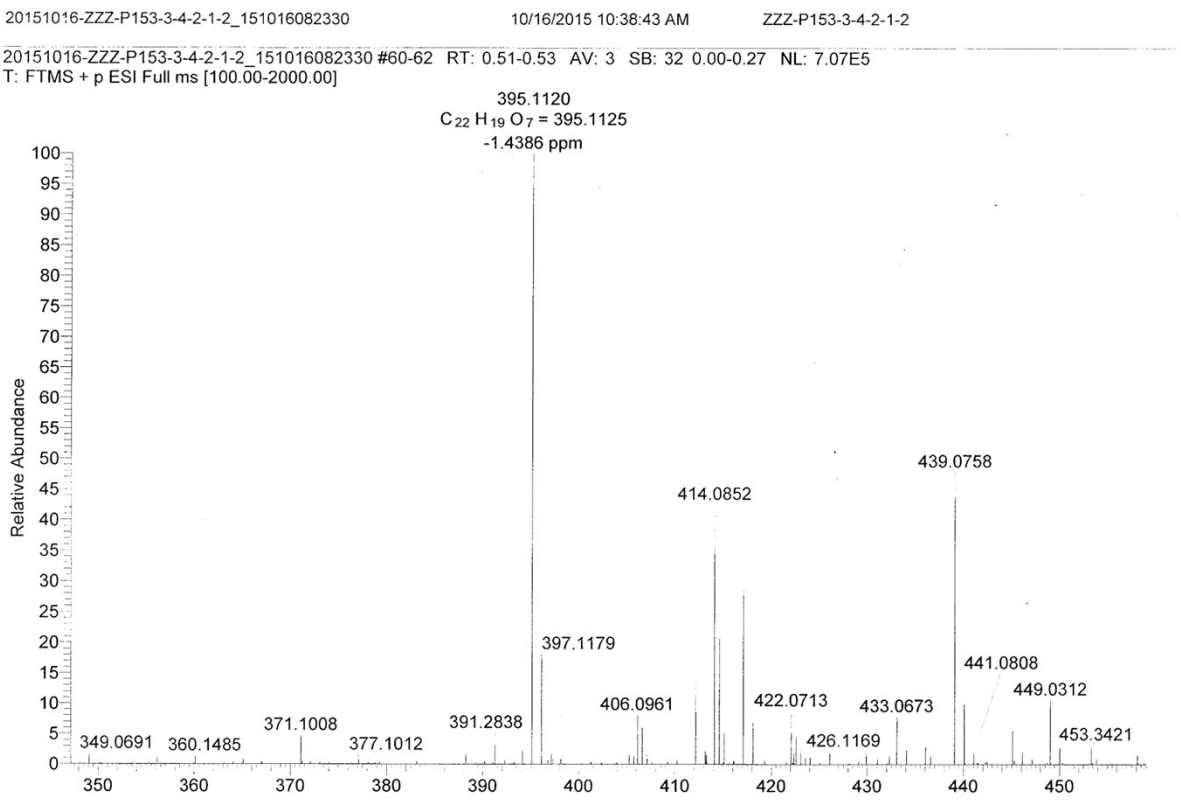


Figure S15. ^{1}H NMR (500 MHz, DMSO-d_6) spectrum of **3**.

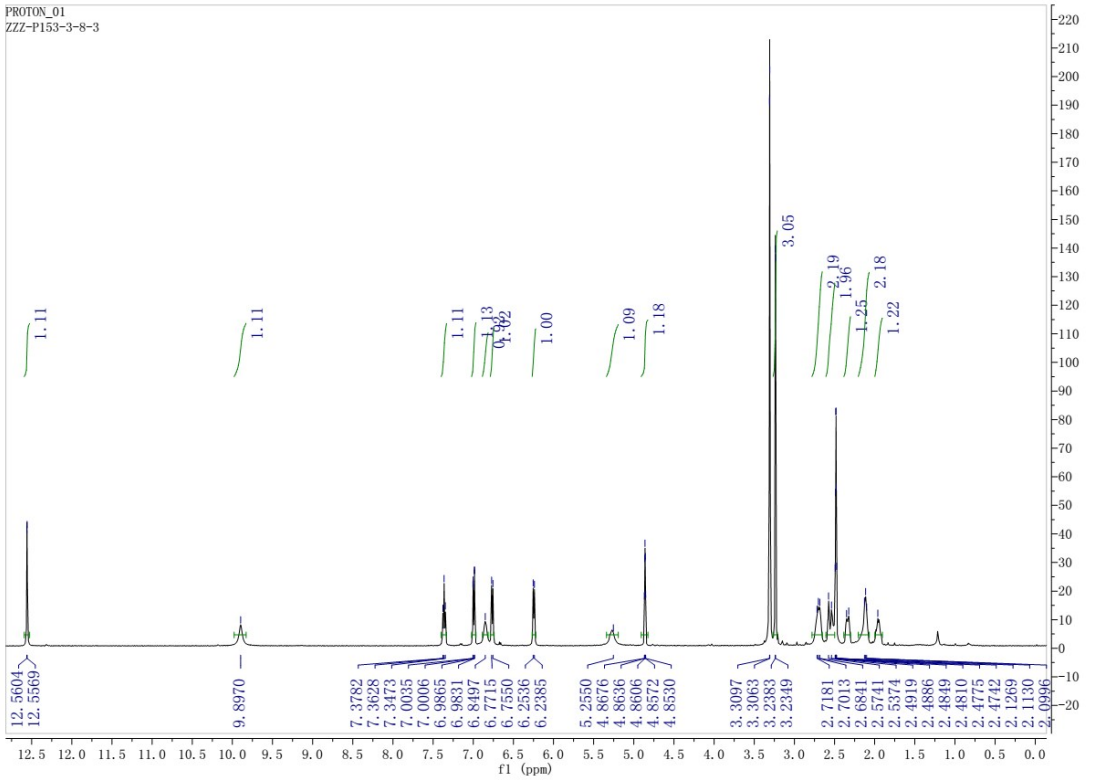


Figure S16. ^{13}C NMR (125 MHz, DMSO-d_6) spectrum of **3**.

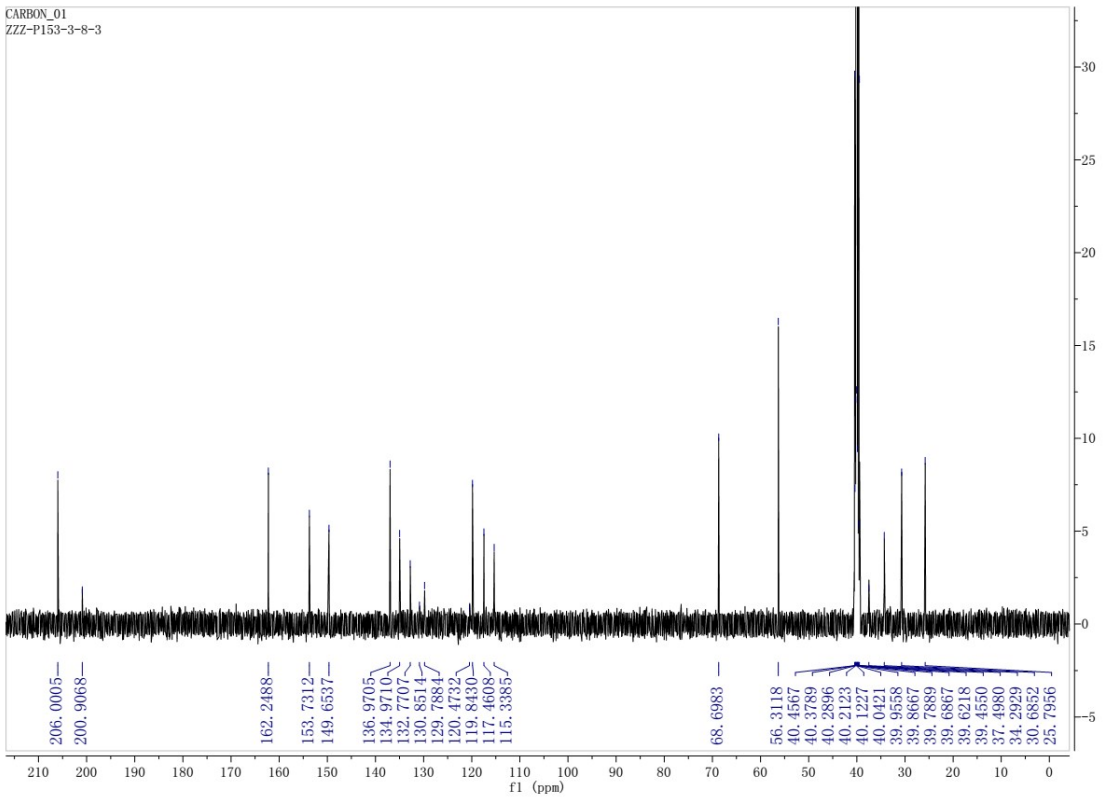


Figure S17. DEPT (125 MHz, DMSO-d_6) spectrum of **3**.

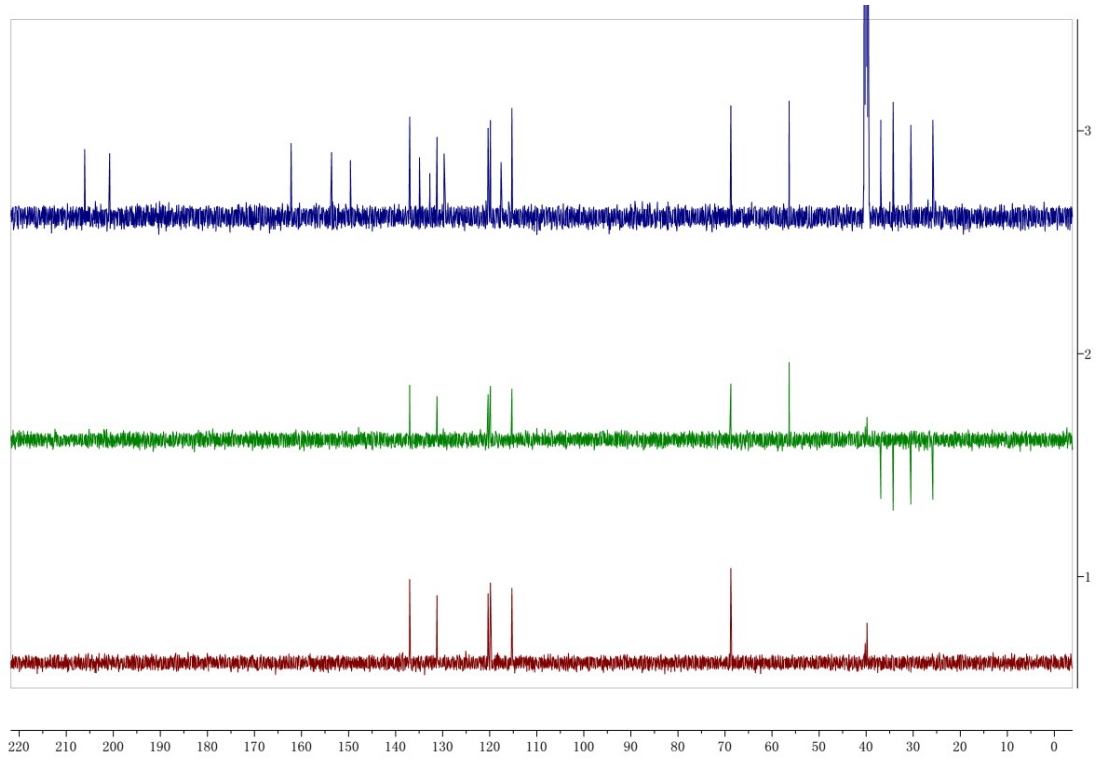


Figure S18. HSQC spectrum of **3** in DMSO-d_6.

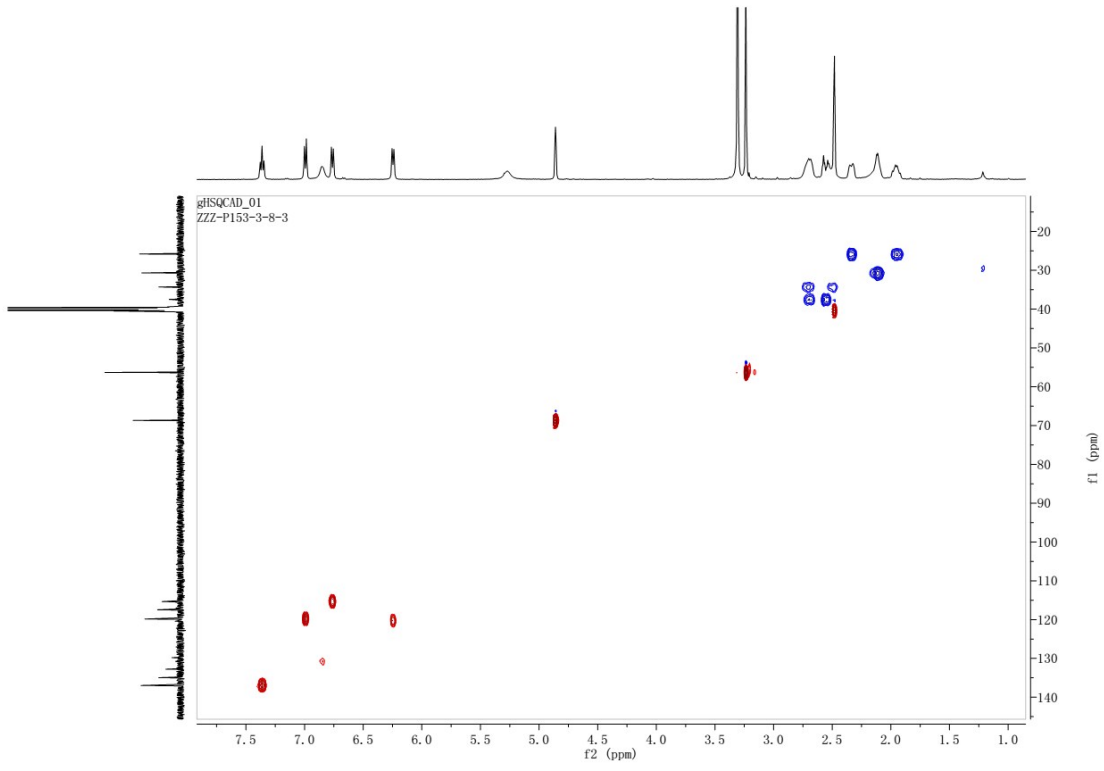


Figure S19. ^{1}H-^{1}H COSY spectrum of **3** in DMSO-d_6.

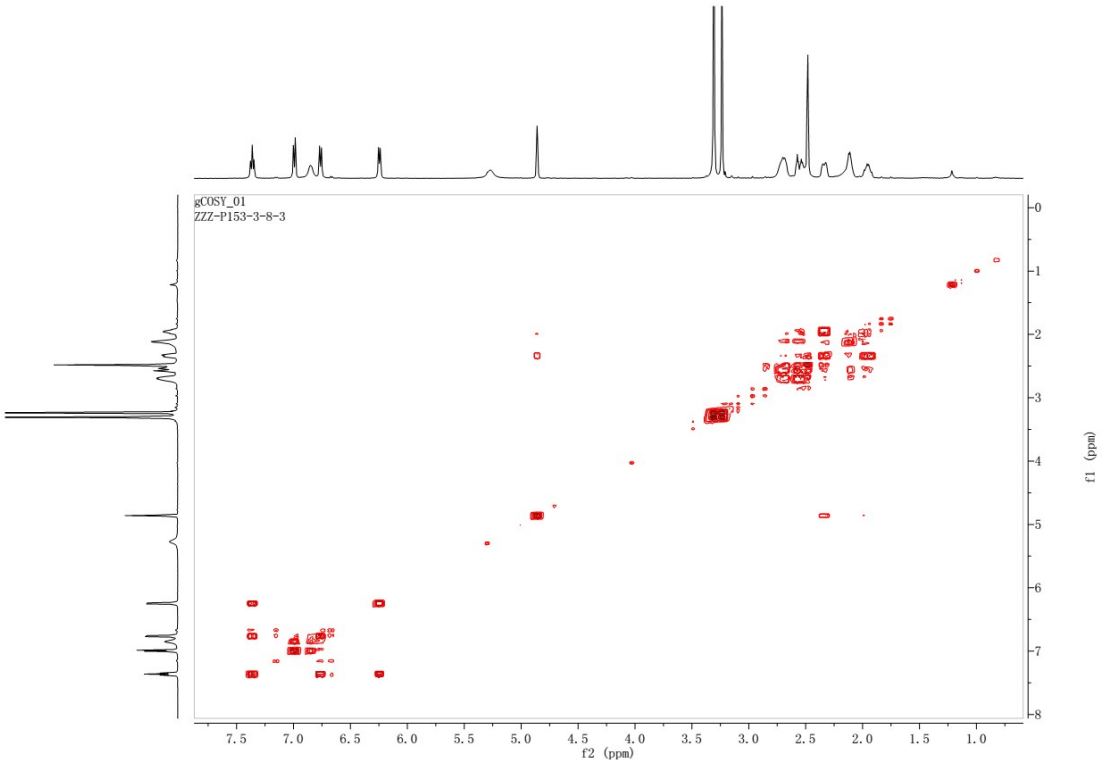


Figure S20. HMBC spectrum of **3** in DMSO-d_6.

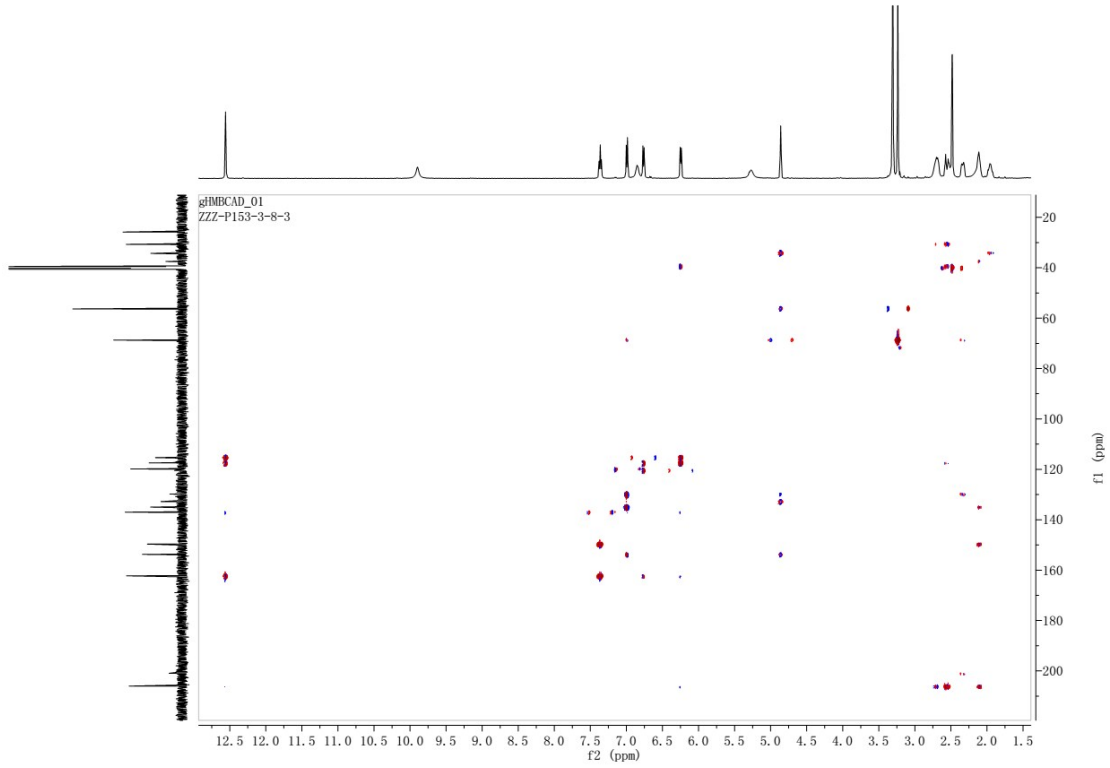


Figure S21. HRESIMS spectrum of **3**.

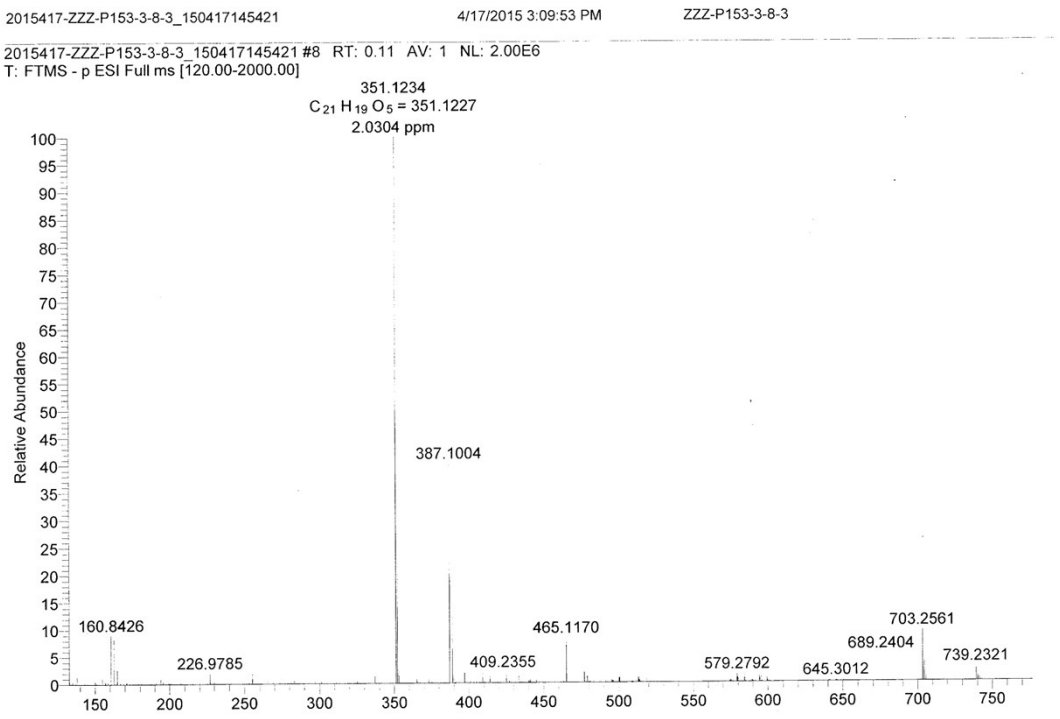


Figure S22. ^{1}H NMR (500 MHz, CD_3OD) spectrum of **4**.

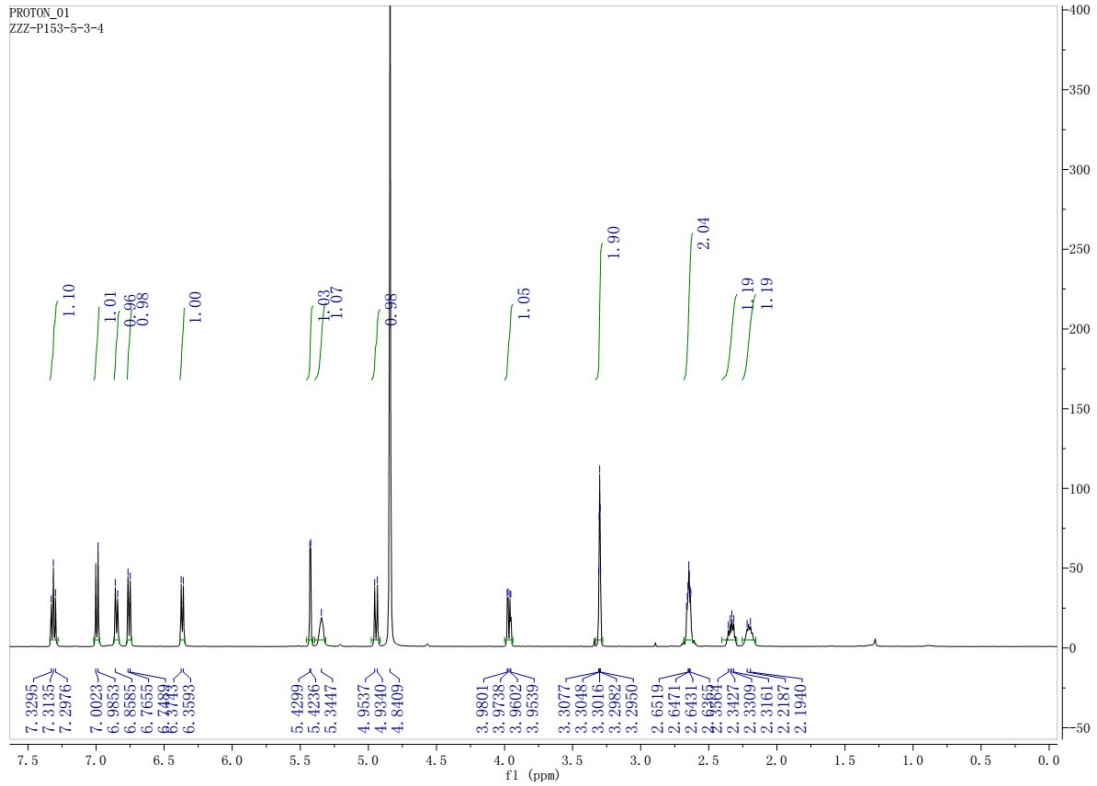


Figure S23. ^{13}C NMR (125 MHz, CD_3OD) spectrum of **4**.

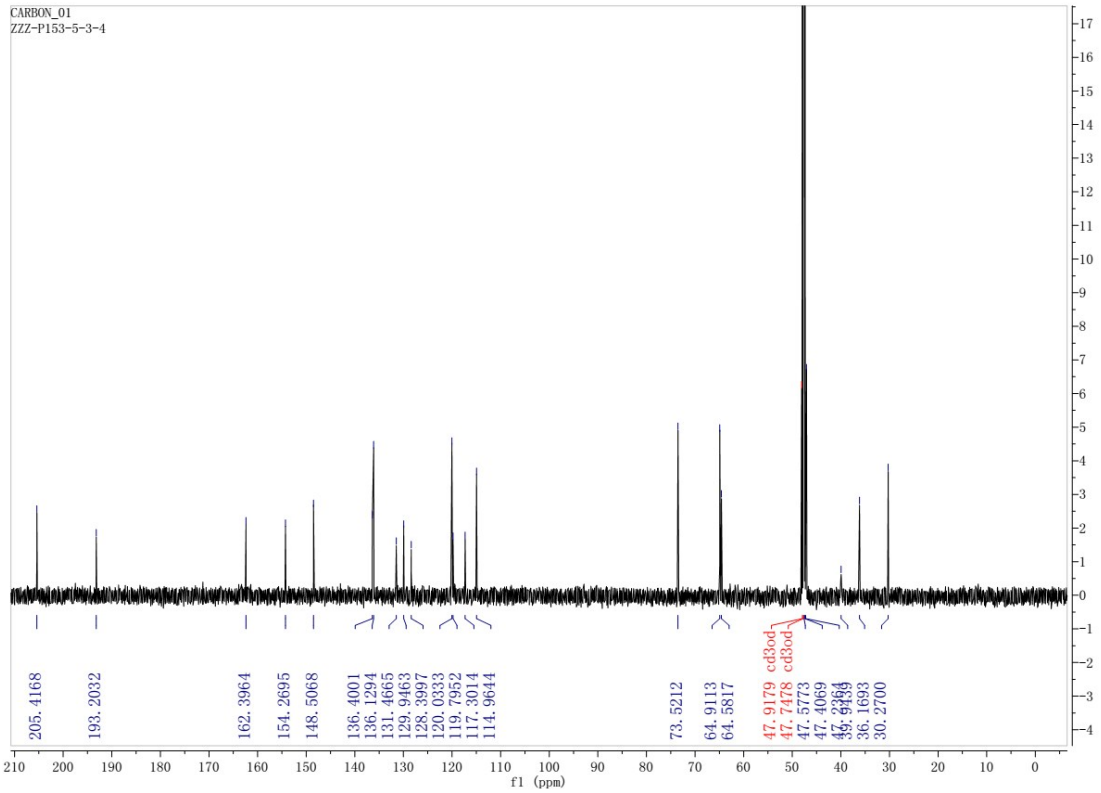


Figure S24. DEPT (125 MHz, CD_3OD) spectrum of **4**.

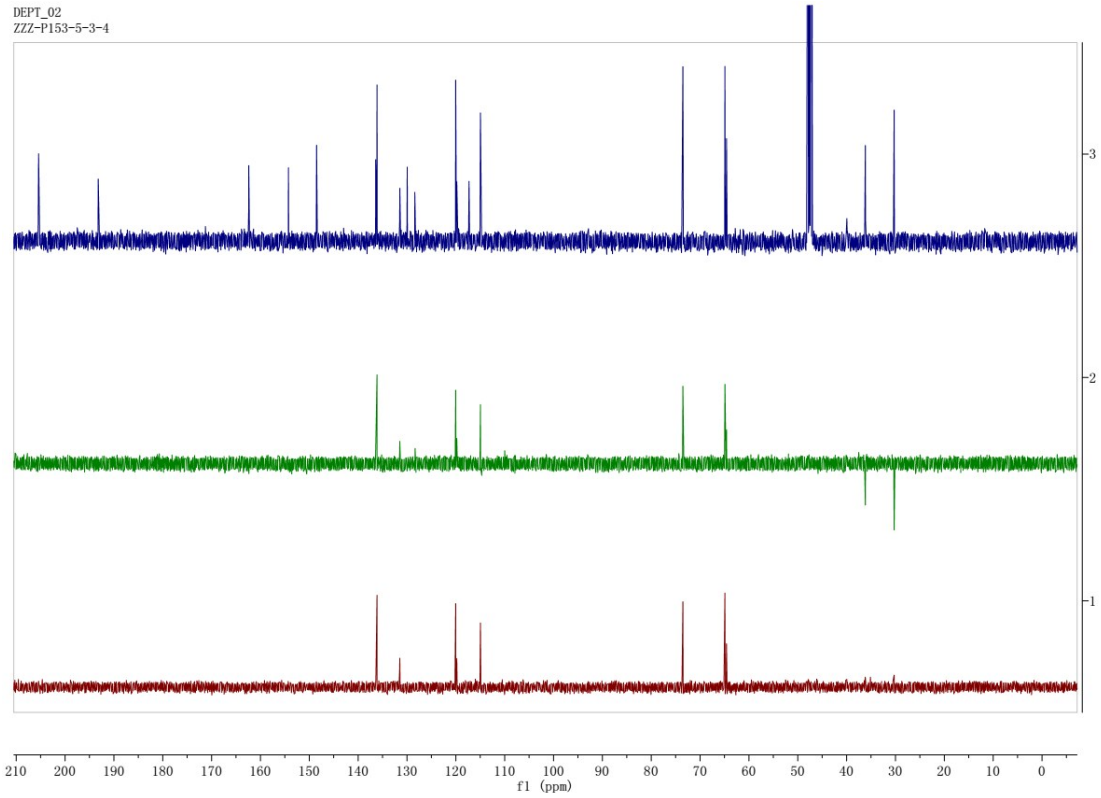


Figure S25. HSQC spectrum of **4** in CD_3OD.

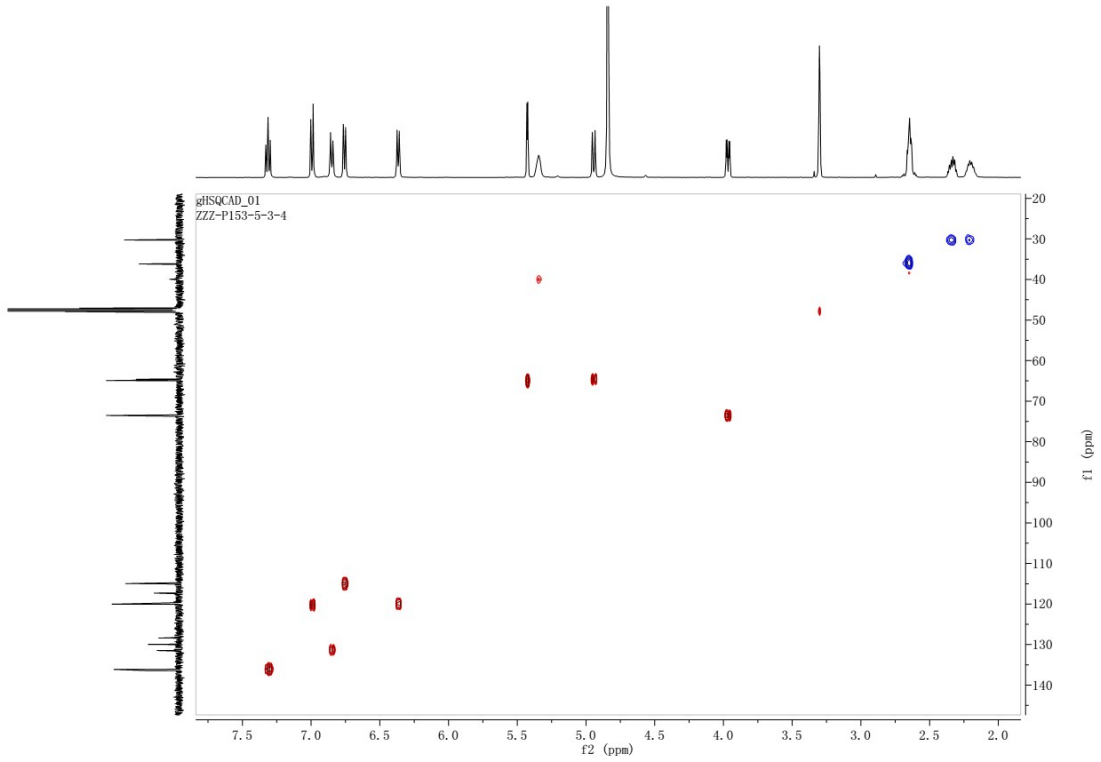


Figure S26. ^1H-^1H COSY spectrum of **4** in CD_3OD.

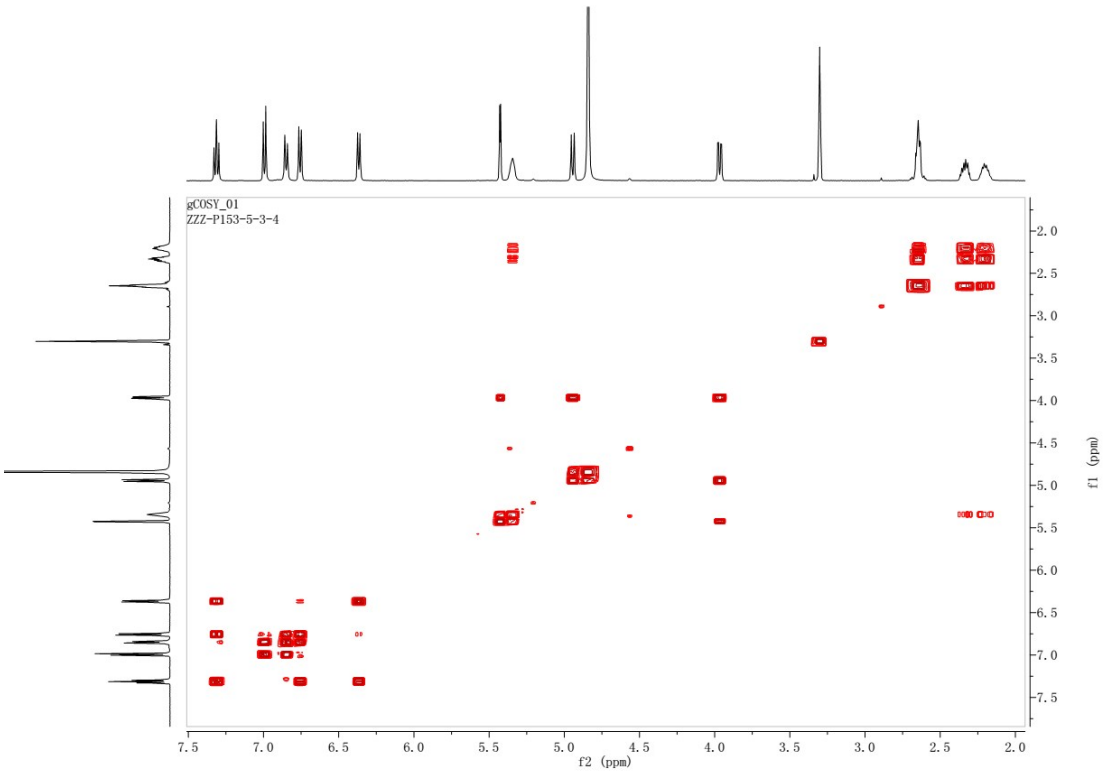


Figure S27. HMBC spectrum of **4** in CD_3OD.

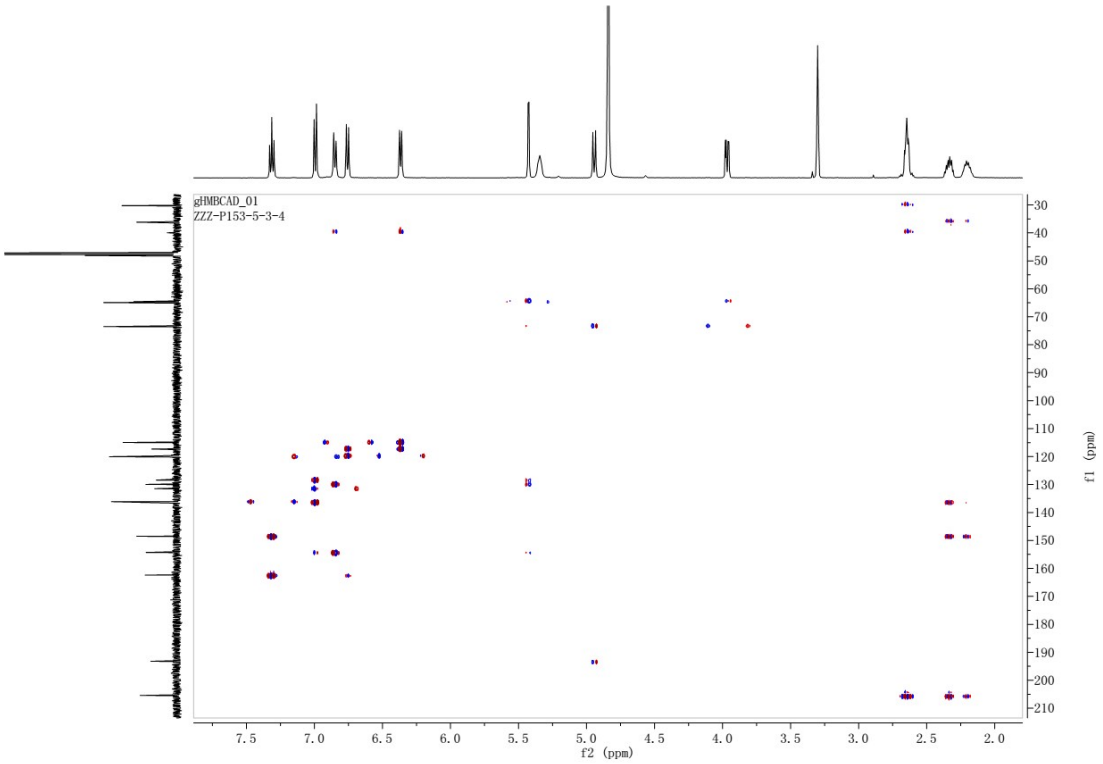


Figure S28. HRESIMS spectrum of **4**.

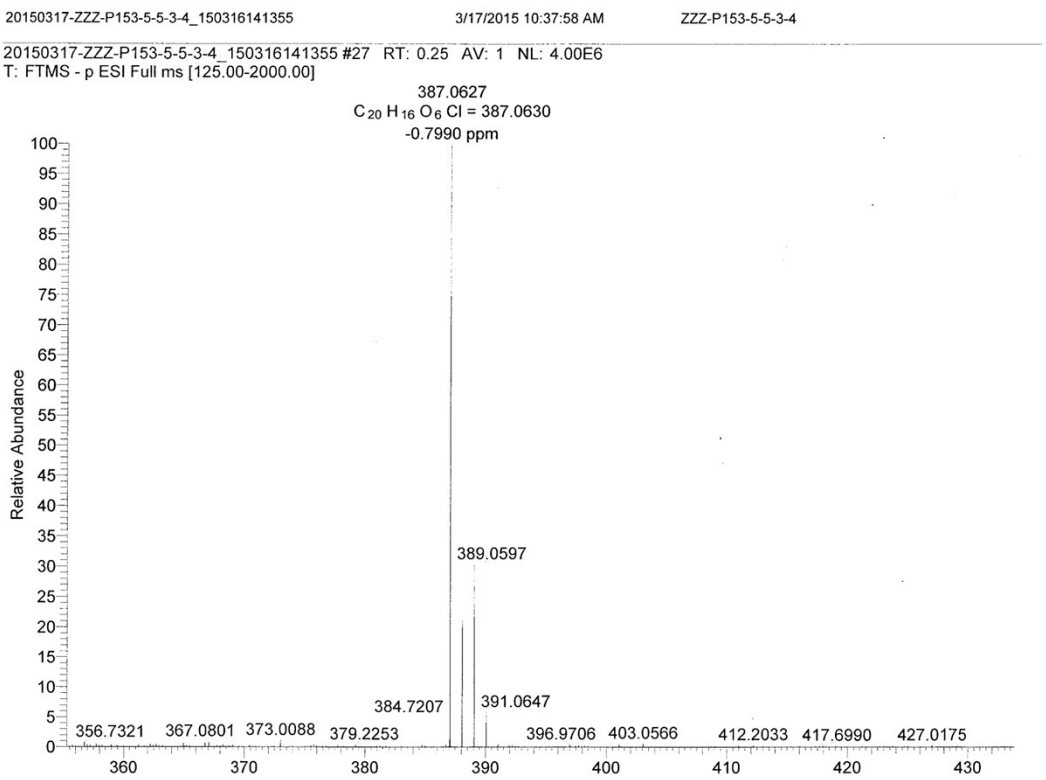


Figure S29. ^{1}H NMR (500 MHz, DMSO-d_6) spectrum of **4**.

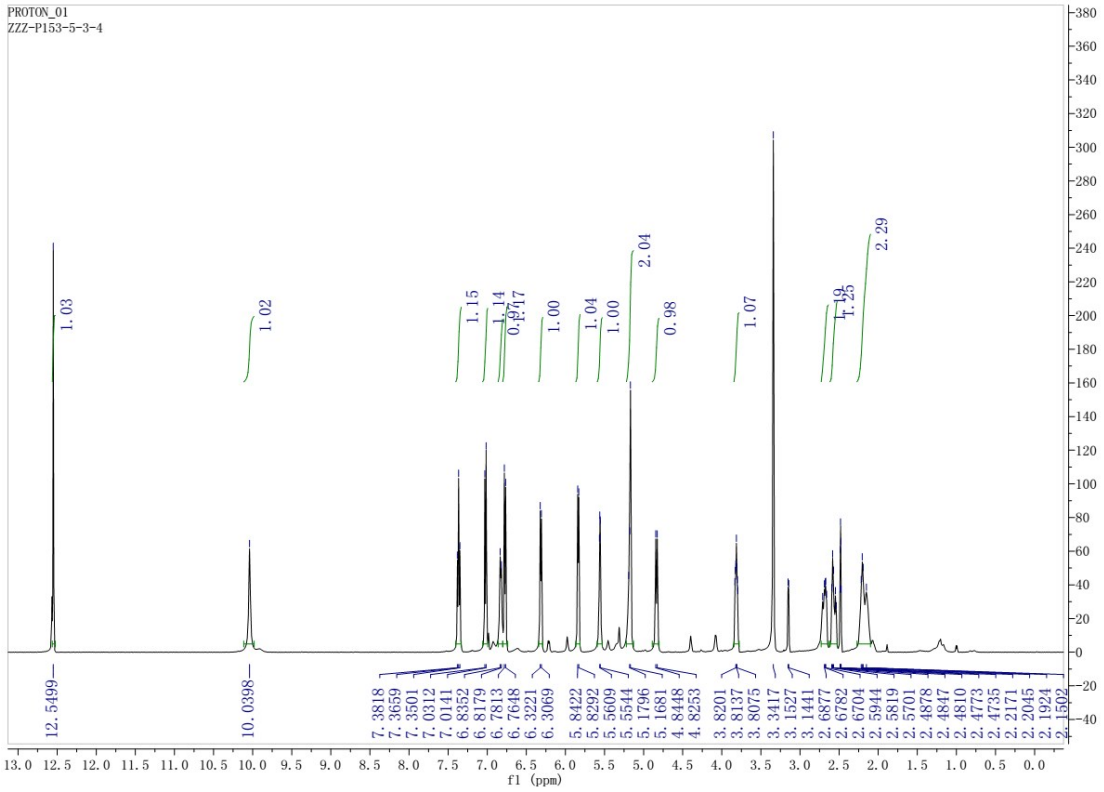


Figure S30. ^{13}C NMR (125 MHz, DMSO-d_6) spectrum of **4**.

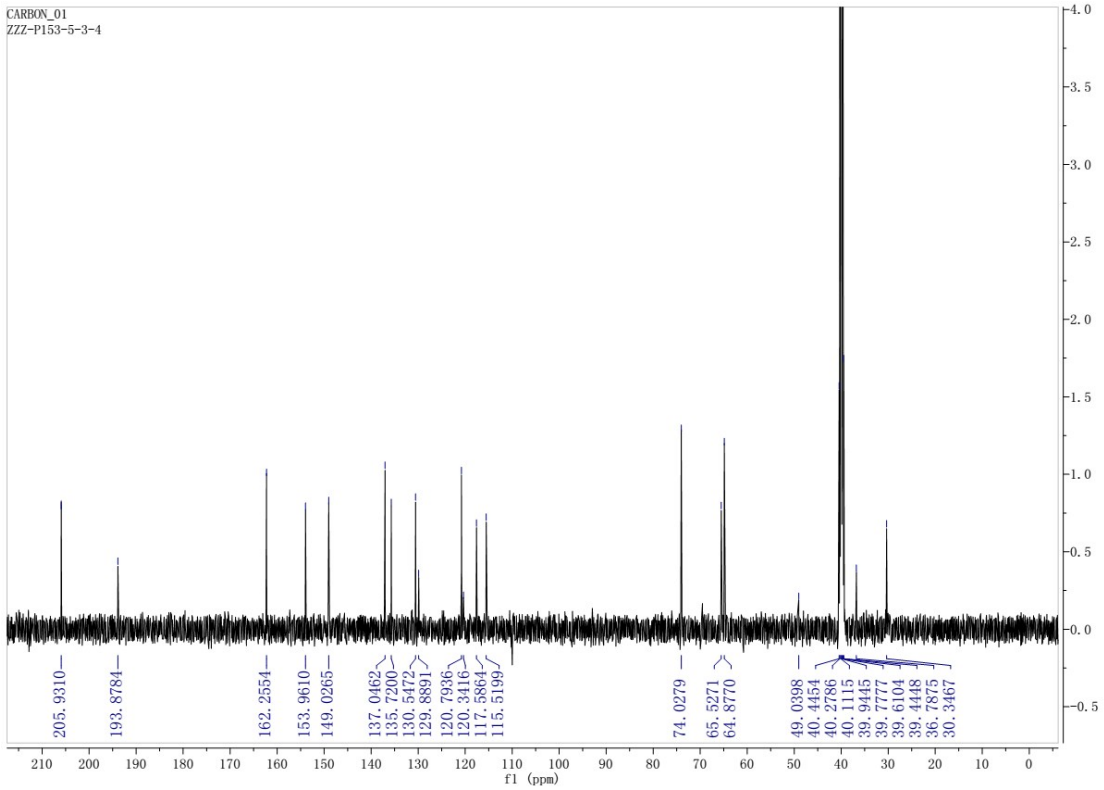


Figure S31. DEPT (125 MHz, DMSO-d_6) spectrum of **4**.

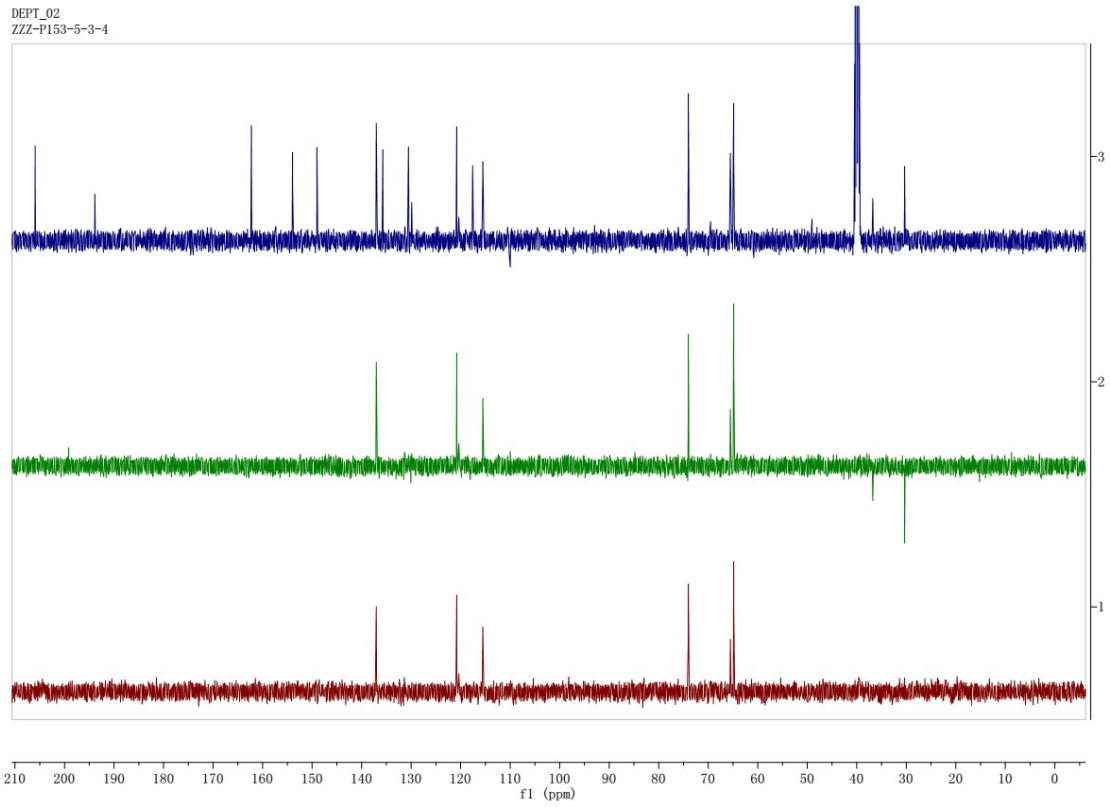


Figure S32. HSQC spectrum of **4** in DMSO-d_6.

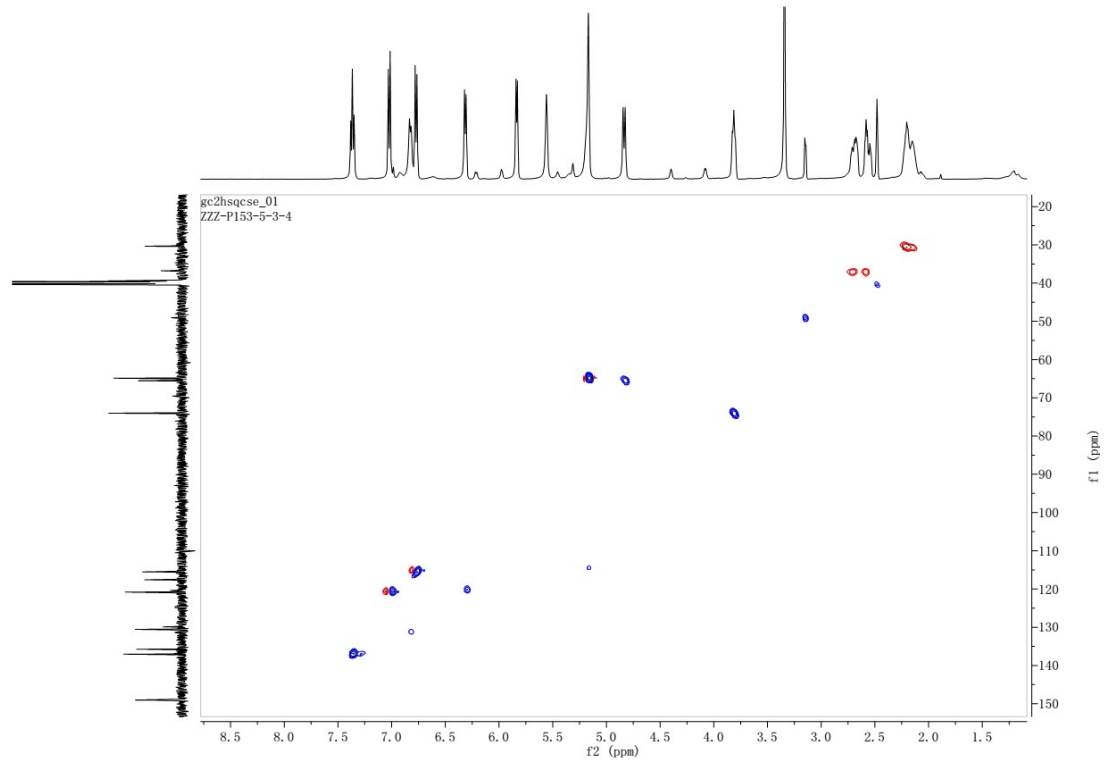


Figure S33. ^{1}H-^{1}H COSY spectrum of **4** in DMSO-d_6.

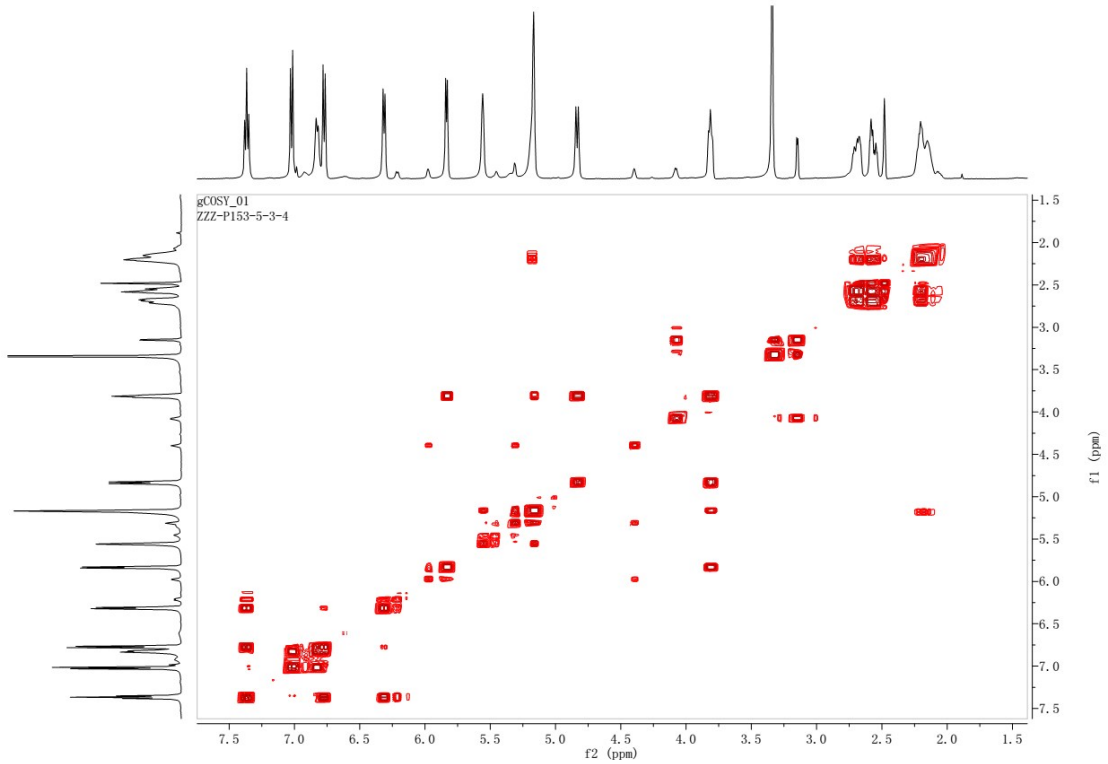


Figure S34. HMBC spectrum of **4** in DMSO-d_6.

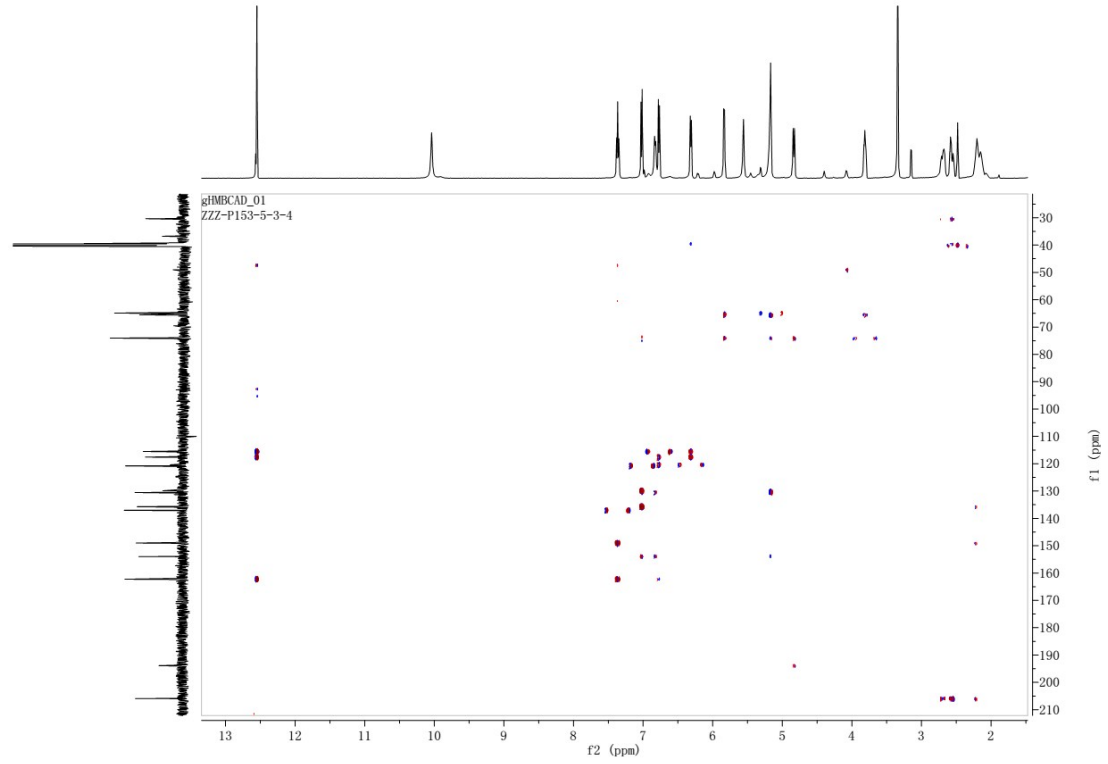


Figure S35. ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of **5**.

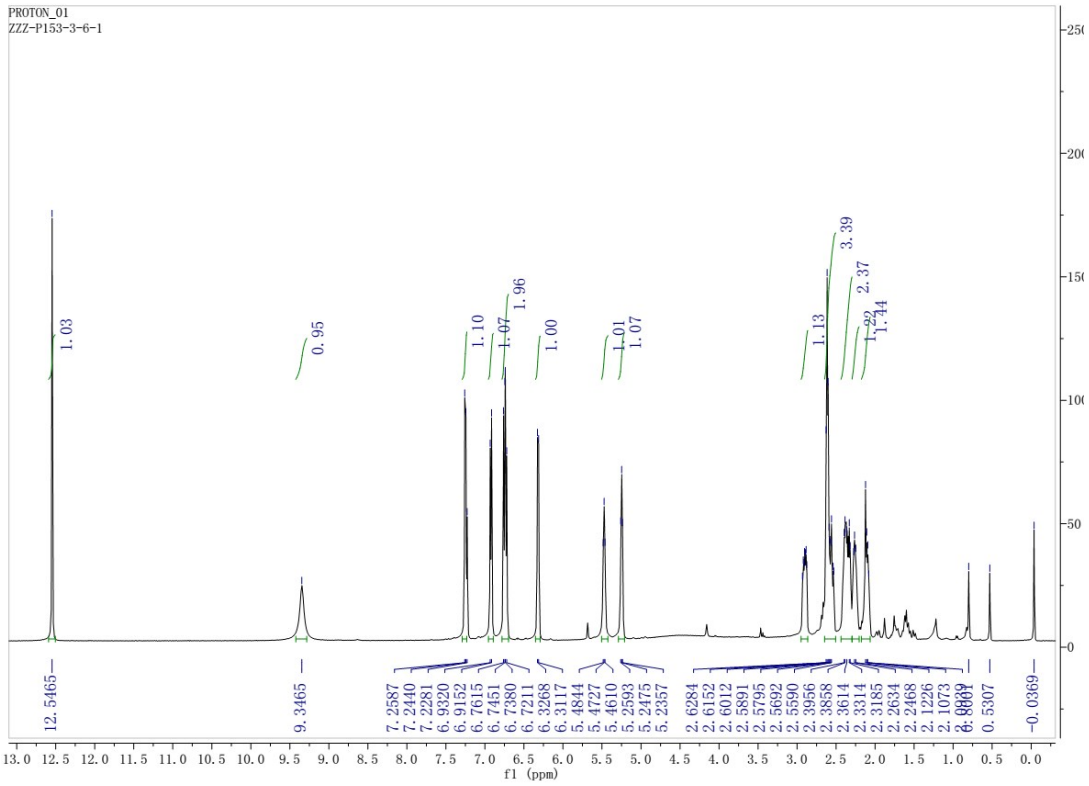


Figure S36. ^{13}C NMR (125 MHz, $CDCl_3$) spectrum of **5**.

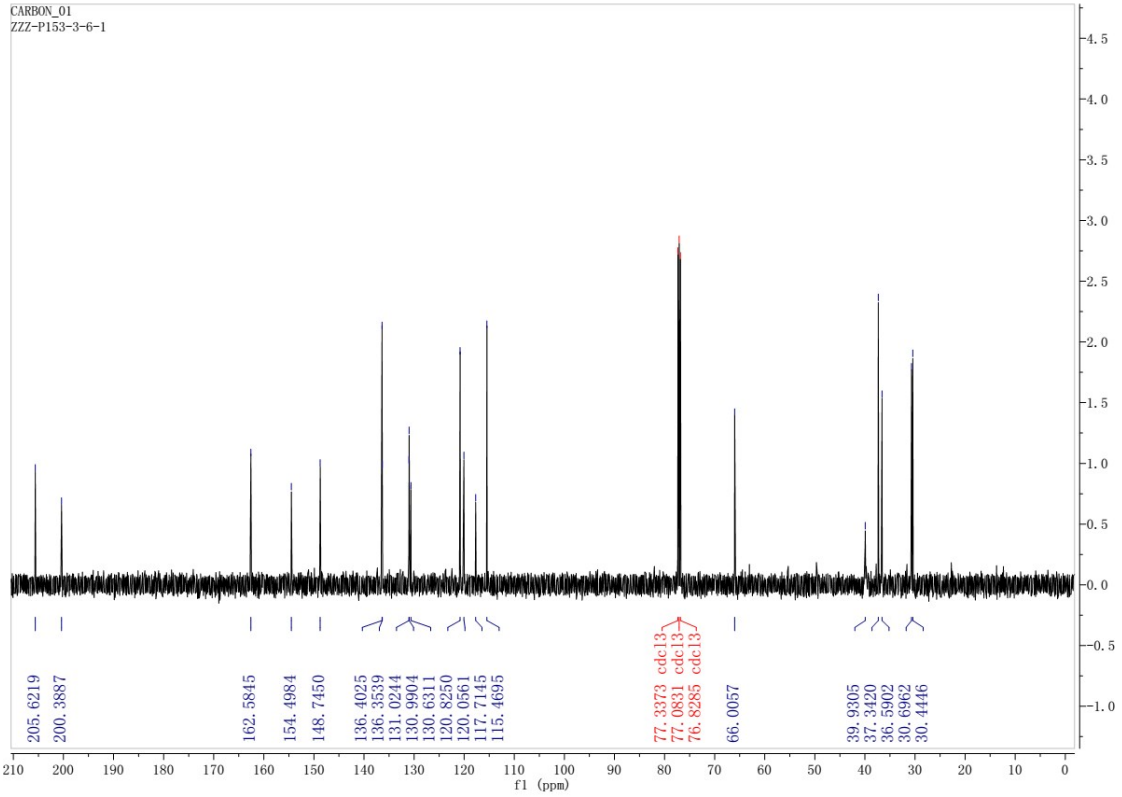


Figure S37. DEPT (125 MHz, $CDCl_3$) spectrum of **5**.

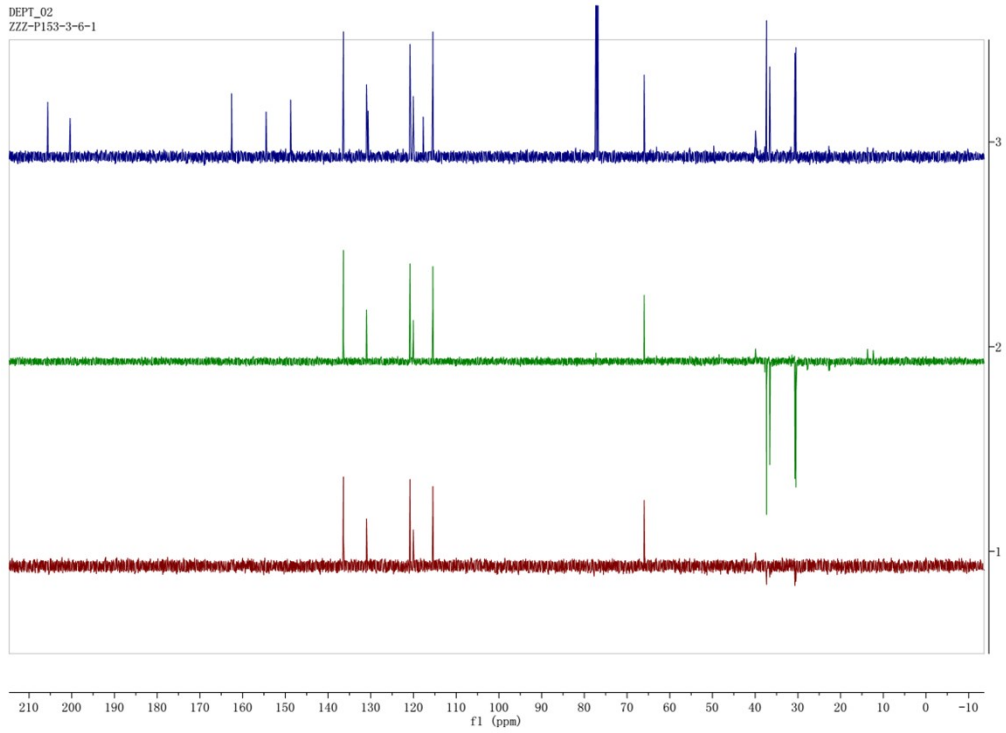


Figure S38. Major dimerized patterns of 1-tetralone dimmers.

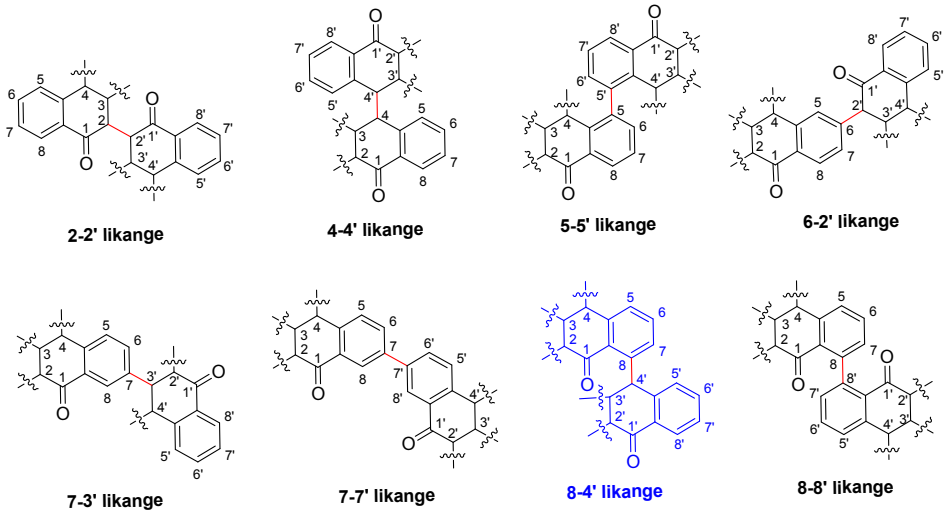


Figure S39. HPLC of HDN14-342 crude extract.

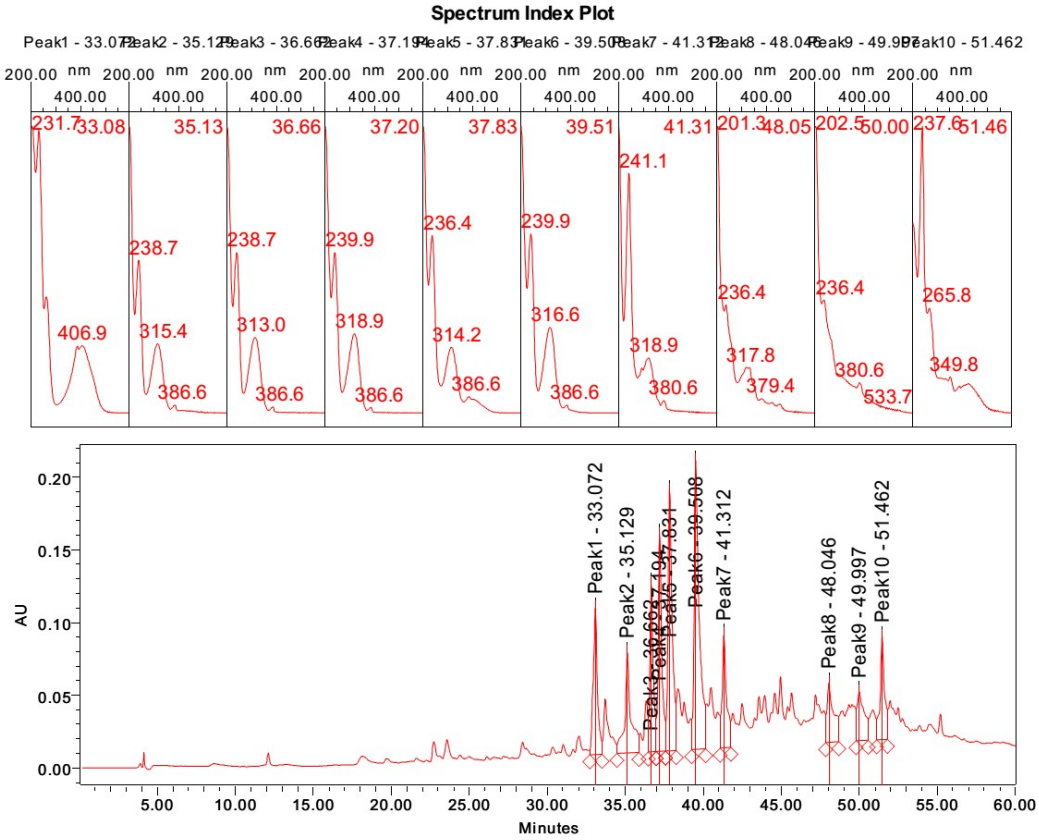


Figure S40. ^{1}H NMR (500 MHz, DMSO-d_6) spectrum of the mixture of **1** and **2**.

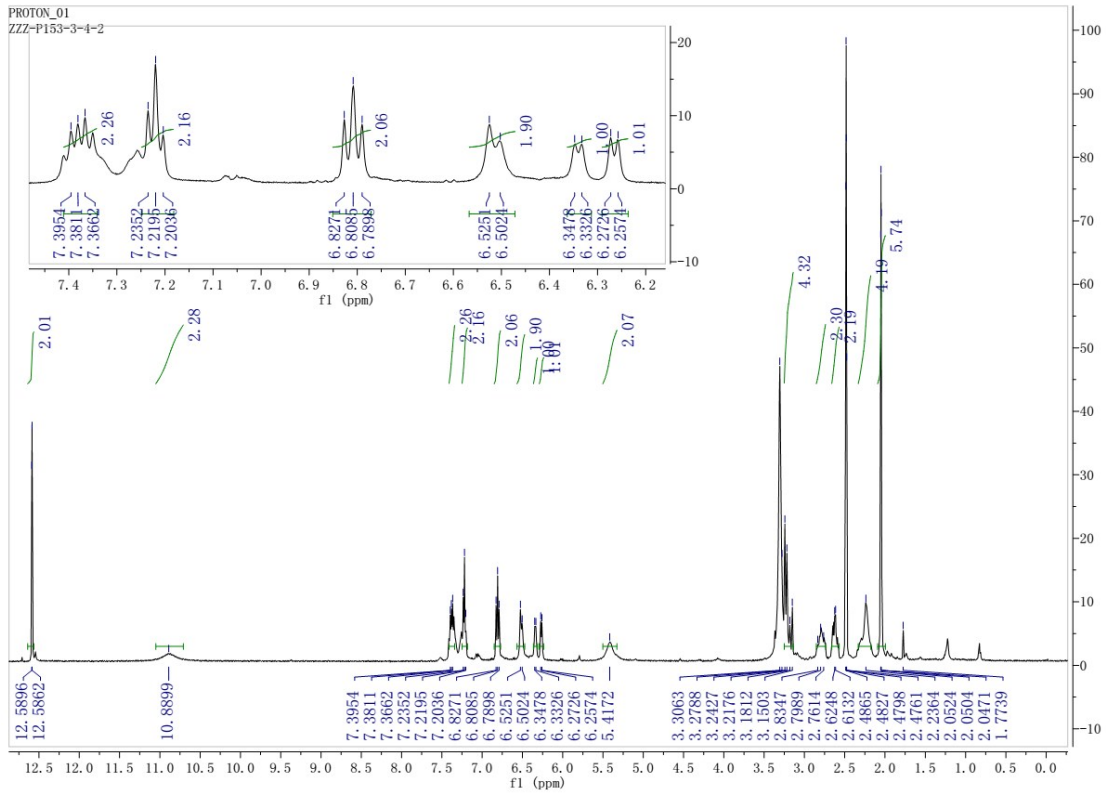


Figure S41. ^{13}C NMR (125 MHz, DMSO-d_6) spectrum of the mixture of **1** and **2**.

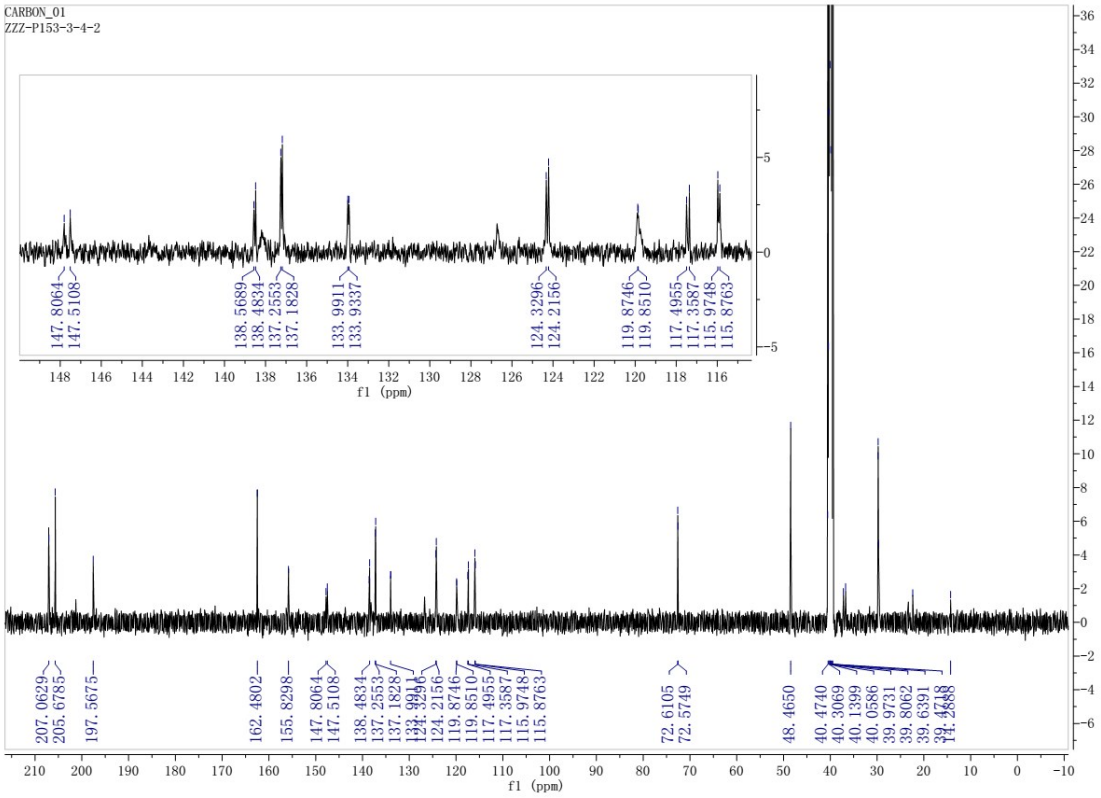
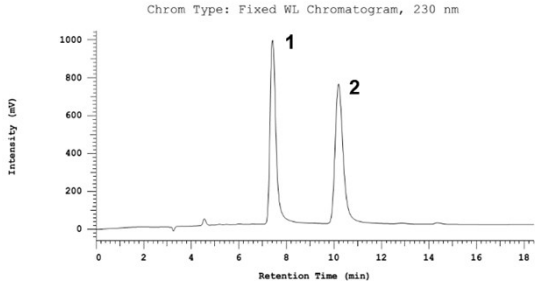


Figure S42. Chiral HPLC separation chromatogram of **1**/**2** on chiral Daicel Chiralpack IC column (250×4.6 mm, 5μm).



Chrom Type: Fixed WL Chromatogram, 230 nm
Peak Quantitation: AREA
Calculation Method: AREA%

No.	RT	Area	Area %	BC
1	7.420	16769557	49.053	BB
2	10.193	17416879	50.947	BB
		34186436	100.000	

Figure S43. The structures of two reported synthetic tetralone and 1,3-indanone dimers.

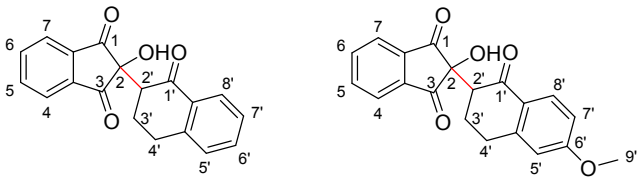


Figure S44. ECD calculation of **1**.

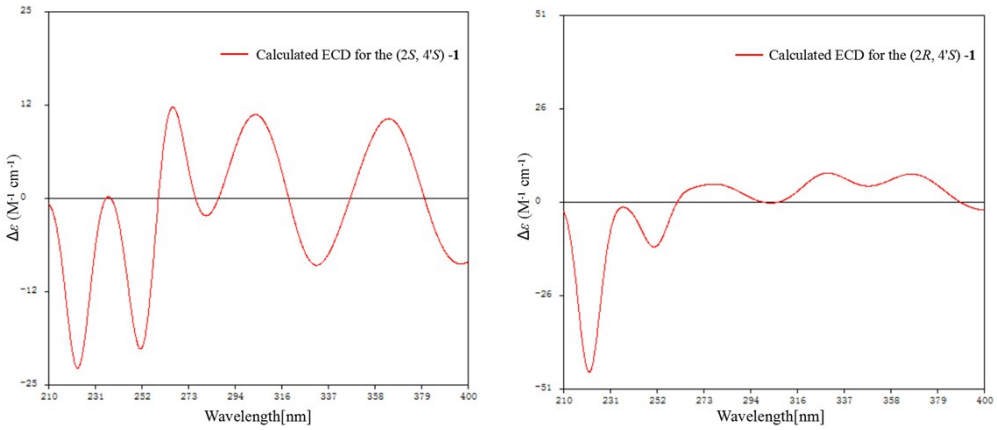
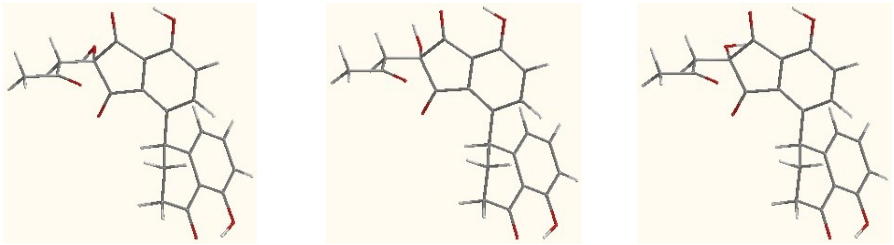


Figure S44-1. B3LYP/6-31+G(d) calculated spectra of (2*S*, 4'*S*)-**1** and (2*R*, 4'*S*)-**1** (σ = 0.18 eV).



Conf. A 50.5% Conf. B 30.2% Conf. C 14.1%

Figure S44-2. DFT-optimized structures for low-energy conformers of (2*S*, 4'*S*)-**1** at B3LYP/6-31+g (d) level in methanol (CPCM) (Conformer populations were calculated using the Gibbs free energy and Boltzmann population at 298 K estimated thereof).

Table S1. Cartesian coordinates of the low-energy reoptimized conformers of (2*S*, 4'*S*)-**1** calculated at B3LYP/6-31+G(d) level of theory with PCM solvent model for MeOH.

Conformer A		Standard Orientation (Ångstroms)		
I	Atom	X	Y	Z
1	C	2.10426	1.32441	-0.36324
2	C	1.07293	0.41461	-0.03863
3	C	-0.20635	0.54934	-0.58225
4	C	-0.39201	1.64142	-1.46187
5	C	0.61902	2.54167	-1.79482
6	C	1.90138	2.3914	-1.2442
7	C	3.34873	1.00344	0.31279
8	C	3.09397	-0.18821	1.25555
9	C	1.63371	-0.59294	0.9015
10	C	-1.33529	-0.43308	-0.31039
11	C	-1.67252	-1.23078	-1.58891

12	C	-2.79307	-2.23435	-1.31461
13	C	-4.02582	-1.58057	-0.74041
14	C	-3.86842	-0.3664	0.06703
15	C	-2.58514	0.21383	0.29024
16	C	-5.01685	0.22953	0.66773
17	C	-4.88629	1.36383	1.47885
18	C	-3.62485	1.90227	1.6955
19	C	-2.48293	1.33683	1.10823
20	O	2.88948	3.25487	-1.56295
21	O	-6.25602	-0.27328	0.48646
22	O	-5.14637	-2.0945	-0.93993
23	O	1.07765	-1.55799	1.4023
24	C	4.1148	-1.32173	1.15292
25	O	3.09533	0.37002	2.5753
26	O	4.41434	1.60579	0.1821
27	C	4.21547	-1.96927	-0.21718
28	C	5.23246	-3.07107	-0.38011
29	O	3.49486	-1.60048	-1.13759
30	H	-1.37307	1.79565	-1.90307
31	H	0.42359	3.36228	-2.47846
32	H	-0.96684	-1.15497	0.42831
33	H	-1.97675	-0.54593	-2.39072
34	H	-0.77767	-1.75671	-1.93784
35	H	-2.45315	-2.98269	-0.58161
36	H	-3.08407	-2.78284	-2.21607
37	H	-5.77589	1.79612	1.92654
38	H	-3.51992	2.77953	2.32851
39	H	-1.51319	1.7865	1.29399
40	H	3.70635	2.97955	-1.08918
41	H	-6.15902	-1.07633	-0.09572
42	H	5.10029	-0.93517	1.44312
43	H	3.8646	-2.10025	1.88703
44	H	2.79058	-0.3131	3.19951
45	H	6.23858	-2.68561	-0.17356
46	H	5.19488	-3.4748	-1.39406
47	H	5.0433	-3.87169	0.34539

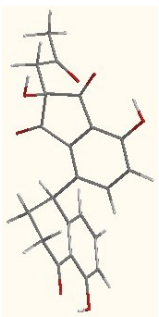
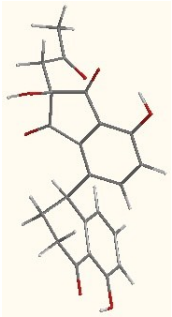
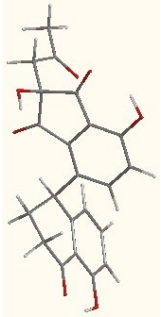
Conformer B		Standard Orientation (Ångstroms)		
I	Atom	X	Y	Z
1	C	2.10183	1.32489	-0.37282
2	C	1.07403	0.41453	-0.03922

3	C	-0.20846	0.54646	-0.57643
4	C	-0.39967	1.63533	-1.45886
5	C	0.60818	2.53599	-1.80033
6	C	1.89302	2.38958	-1.25485
7	C	3.34943	1.00167	0.29505
8	C	3.09917	-0.18109	1.24947
9	C	1.63819	-0.59277	0.90088
10	C	-1.33602	-0.43507	-0.29553
11	C	-1.66842	-1.24626	-1.56678
12	C	-2.78912	-2.24793	-1.28616
13	C	-4.02458	-1.58883	-0.7241
14	C	-3.87065	-0.3672	0.07274
15	C	-2.58842	0.21544	0.29567
16	C	-5.02148	0.23335	0.66422
17	C	-4.89431	1.37429	1.46648
18	C	-3.63376	1.91467	1.68367
19	C	-2.4896	1.34491	1.10512
20	O	2.87865	3.25381	-1.58036
21	O	-6.25988	-0.27133	0.4825
22	O	-5.14422	-2.10453	-0.92399
23	O	1.09046	-1.57198	1.37702
24	C	4.11436	-1.31978	1.15852
25	O	3.02454	0.32375	2.5892
26	O	4.4144	1.61056	0.17108
27	C	4.20903	-1.98121	-0.20556
28	C	5.21875	-3.09092	-0.35915
29	O	3.48853	-1.61758	-1.12804
30	H	-1.38332	1.78684	-1.89524
31	H	0.40803	3.35368	-2.48612
32	H	-0.96743	-1.14883	0.45084
33	H	-1.97044	-0.56965	-2.37644
34	H	-0.77196	-1.77491	-1.90735
35	H	-2.45148	-2.98771	-0.54347
36	H	-3.07593	-2.80659	-2.1827
37	H	-5.78572	1.80998	1.9072
38	H	-3.53137	2.79692	2.31014
39	H	-1.5206	1.79612	1.29103
40	H	3.69731	2.98332	-1.10733
41	H	-6.16046	-1.07917	-0.09252
42	H	5.10925	-0.94518	1.43641
43	H	3.85411	-2.08028	1.90612
44	H	3.88989	0.69985	2.83093
45	H	5.03186	-3.87869	0.38073

46	H	6.2285	-2.70716	-0.16734
47	H	5.17103	-3.51036	-1.36627

Conformer C		Standard Orientation (Ångstroms)		
I	Atom	X	Y	Z
1	C	2.10815	1.31875	-0.36627
2	C	1.07448	0.41324	-0.03232
3	C	-0.20286	0.54331	-0.58209
4	C	-0.3852	1.62606	-1.47386
5	C	0.62754	2.52113	-1.81588
6	C	1.90862	2.37469	-1.26185
7	C	3.35449	0.9992	0.30805
8	C	3.09699	-0.18207	1.26657
9	C	1.63151	-0.58927	0.91869
10	C	-1.33397	-0.43485	-0.30362
11	C	-1.67095	-1.24168	-1.5764
12	C	-2.7933	-2.2415	-1.29568
13	C	-4.02569	-1.5815	-0.72792
14	C	-3.86726	-0.36146	0.07051
15	C	-2.58339	0.21859	0.29055
16	C	-5.0154	0.24063	0.66558
17	C	-4.88398	1.38077	1.46838
18	C	-3.622	1.91908	1.68208
19	C	-2.4804	1.34771	1.09996
20	O	2.90001	3.23052	-1.58986
21	O	-6.25509	-0.26169	0.48682
22	O	-5.14684	-2.09504	-0.92486
23	O	1.07137	-1.55504	1.41054
24	C	4.10318	-1.32398	1.15635
25	O	3.17556	0.25476	2.62837
26	O	4.41924	1.60492	0.17236
27	C	4.18657	-1.97349	-0.21169
28	C	5.1988	-3.07917	-0.37951
29	O	3.45944	-1.6063	-1.12761
30	H	-1.36557	1.77741	-1.91762
31	H	0.43415	3.33417	-2.50907
32	H	-0.96733	-1.15155	0.44089
33	H	-1.9734	-0.5626	-2.38377
34	H	-0.77652	-1.77158	-1.92034
35	H	-2.4553	-2.9846	-0.55649
36	H	-3.08405	-2.79652	-2.19322

37	H	-5.77338	1.8176	1.91203
38	H	-3.51646	2.8009	2.30864
39	H	-1.51011	1.7973	1.28314
40	H	3.71515	2.9575	-1.11102
41	H	-6.15868	-1.0692	-0.08932
42	H	5.0951	-0.94847	1.43922
43	H	3.84326	-2.09022	1.89841
44	H	2.57243	1.00368	2.78104
45	H	6.20948	-2.68904	-0.20612
46	H	5.13651	-3.5002	-1.38513
47	H	5.02958	-3.86666	0.36479

Conf. A 52.8% Conf. B 32.6% Conf. C 14.6%

Figure S44-3. DFT-optimized structures for low-energy conformers of (2*R*, 4'*S*)-**1** at B3LYP/6-31+g (d) level in methanol (CPCM) (Conformer populations were calculated using the Gibbs free energy and Boltzmann population at 298 K estimated thereof).

Table S2. Cartesian coordinates of the low-energy reoptimized conformers of (2*R*, 4'*S*)-**1** calculated at B3LYP/6-31+G(d) level of theory with PCM solvent model for MeOH.

Conformer A		Standard Orientation (Ångstroms)		
I	Atom	X	Y	Z
1	C	1.88582	-1.28271	-0.54823
2	C	1.04007	-0.40728	0.16523
3	C	-0.34053	-0.37637	-0.07028
4	C	-0.81121	-1.27245	-1.05501
5	C	0.01587	-2.14786	-1.76236
6	C	1.39563	-2.1633	-1.5184
7	C	3.27816	-1.12061	-0.16512
8	C	3.35096	-0.10457	0.99014
9	C	1.88169	0.40099	1.08611
10	C	-1.26716	0.55895	0.70937

11	C	-1.62681	-0.01155	2.10171
12	C	-2.63669	-1.15647	1.99899
13	C	-3.86868	-0.78114	1.20851
14	C	-3.76308	0.26929	0.18929
15	C	-2.52709	0.92697	-0.06328
16	C	-4.9151	0.64369	-0.56399
17	C	-4.82865	1.64791	-1.53675
18	C	-3.61082	2.27865	-1.76268
19	C	-2.46643	1.92434	-1.03292
20	O	2.20724	-2.99552	-2.20763
21	O	-6.11322	0.05369	-0.37135
22	O	-4.94528	-1.37491	1.42382
23	O	1.53025	1.29716	1.83396
24	C	4.39046	1.00373	0.82622
25	O	3.57011	-0.82243	2.21151
26	O	4.23313	-1.73986	-0.63781
27	C	4.20722	1.87737	-0.40281
28	C	5.18632	3.00954	-0.58847
29	O	3.29566	1.66246	-1.19348
30	H	-1.87037	-1.28227	-1.29353
31	H	-0.40326	-2.81402	-2.51038
32	H	-0.70712	1.4833	0.87682
33	H	-0.72252	-0.34987	2.61621
34	H	-2.05356	0.7999	2.70436
35	H	-2.18406	-2.02586	1.49841
36	H	-2.96053	-1.50283	2.98579
37	H	-5.7199	1.91561	-2.09604
38	H	-3.54666	3.06176	-2.51355
39	H	-1.52509	2.43291	-1.22263
40	H	3.13166	-2.84735	-1.90771
41	H	-5.98704	-0.63081	0.34104
42	H	5.39443	0.55807	0.79074
43	H	4.36954	1.63688	1.72257
44	H	4.43831	-1.26115	2.16369
45	H	4.99838	3.52244	-1.53409
46	H	5.08896	3.72224	0.24041
47	H	6.21604	2.63351	-0.56597

Conformer B		Standard Orientation (Ångstroms)		
I	Atom	X	Y	Z

1	C	1.89149	-1.2604	-0.56875
2	C	1.03922	-0.41087	0.16808
3	C	-0.33923	-0.37157	-0.0765
4	C	-0.80132	-1.22781	-1.10013
5	C	0.03196	-2.076	-1.83281
6	C	1.4094	-2.10308	-1.57639
7	C	3.28143	-1.11788	-0.16888
8	C	3.34899	-0.12393	1.00645
9	C	1.87616	0.36318	1.12038
10	C	-1.27119	0.53296	0.7323
11	C	-1.63796	-0.09111	2.09965
12	C	-2.64491	-1.23295	1.94698
13	C	-3.87299	-0.8298	1.16414
14	C	-3.7635	0.25951	0.18695
15	C	-2.52747	0.92925	-0.0322
16	C	-4.91194	0.6614	-0.55742
17	C	-4.82229	1.70406	-1.48864
18	C	-3.60464	2.34572	-1.68224
19	C	-2.46347	1.9645	-0.96094
20	O	2.22651	-2.90977	-2.28838
21	O	-6.10981	0.06167	-0.39563
22	O	-4.94953	-1.43351	1.34985
23	O	1.51885	1.20395	1.93088
24	C	4.38266	0.99223	0.84581
25	O	3.64838	-0.91929	2.15978
26	O	4.2362	-1.71413	-0.66626
27	C	4.19451	1.87679	-0.37473
28	C	5.25479	2.91822	-0.63227
29	O	3.22288	1.73532	-1.10831
30	H	-1.85795	-1.2263	-1.34988
31	H	-0.3804	-2.7121	-2.61018
32	H	-0.71298	1.45072	0.93847
33	H	-0.73594	-0.44733	2.6059
34	H	-2.06974	0.69601	2.73034
35	H	-2.18764	-2.08143	1.41571
36	H	-2.9737	-1.61776	2.91776
37	H	-5.71104	1.99226	-2.04167
38	H	-3.53803	3.15859	-2.40056
39	H	-1.52214	2.48185	-1.12503
40	H	3.14854	-2.77125	-1.97584
41	H	-5.98635	-0.65031	0.28973
42	H	5.38382	0.54361	0.82022
43	H	4.35851	1.63389	1.73815

44	H	3.54362	-0.36381	2.95329
45	H	4.95119	3.57437	-1.45081
46	H	5.44623	3.50862	0.27124
47	H	6.1979	2.42194	-0.89535

Conformer C		Standard Orientation (Ångstroms)		
I	Atom	X	Y	Z
1	C	1.89804	-1.26938	-0.56591
2	C	1.04603	-0.42362	0.17738
3	C	-0.33259	-0.38246	-0.06834
4	C	-0.79531	-1.23501	-1.0946
5	C	0.03726	-2.08007	-1.83196
6	C	1.41498	-2.10645	-1.57808
7	C	3.29118	-1.11805	-0.17757
8	C	3.36127	-0.12715	1.0035
9	C	1.88271	0.35424	1.12952
10	C	-1.26456	0.52148	0.74118
11	C	-1.63624	-0.10463	2.10618
12	C	-2.64609	-1.24321	1.9487
13	C	-3.87144	-0.83446	1.16429
14	C	-3.7566	0.25673	0.18994
15	C	-2.518	0.92287	-0.02534
16	C	-4.90226	0.66381	-0.55599
17	C	-4.80741	1.70819	-1.48472
18	C	-3.5873	2.34635	-1.67447
19	C	-2.44882	1.95991	-0.95176
20	O	2.23305	-2.90639	-2.2963
21	O	-6.1023	0.06748	-0.39782
22	O	-4.95012	-1.43545	1.34635
23	O	1.51933	1.2049	1.92522
24	C	4.37144	1.00405	0.82751
25	O	3.76725	-0.79979	2.20039
26	O	4.24332	-1.71748	-0.67931
27	C	4.14683	1.89276	-0.38099
28	C	5.12355	3.02515	-0.58055
29	O	3.2117	1.69162	-1.14728
30	H	-1.85231	-1.23319	-1.34282
31	H	-0.376	-2.71311	-2.61136
32	H	-0.70444	1.43708	0.95106
33	H	-0.73645	-0.46436	2.614

34	H	-2.06727	0.68228	2.73761
35	H	-2.19028	-2.09173	1.41619
36	H	-2.97806	-1.6294	2.91784
37	H	-5.69411	2.0005	-2.03889
38	H	-3.51665	3.1606	-2.39084
39	H	-1.50555	2.47469	-1.11278
40	H	3.15531	-2.76582	-1.98431
41	H	-5.98233	-0.6464	0.28619
42	H	5.37753	0.56863	0.76952
43	H	4.35863	1.62394	1.73347
44	H	3.17422	-1.5483	2.38895
45	H	4.88457	3.57507	-1.4932
46	H	5.08733	3.70576	0.27934
47	H	6.14817	2.63823	-0.63743

Figure S45. ECD calculation of **5**.

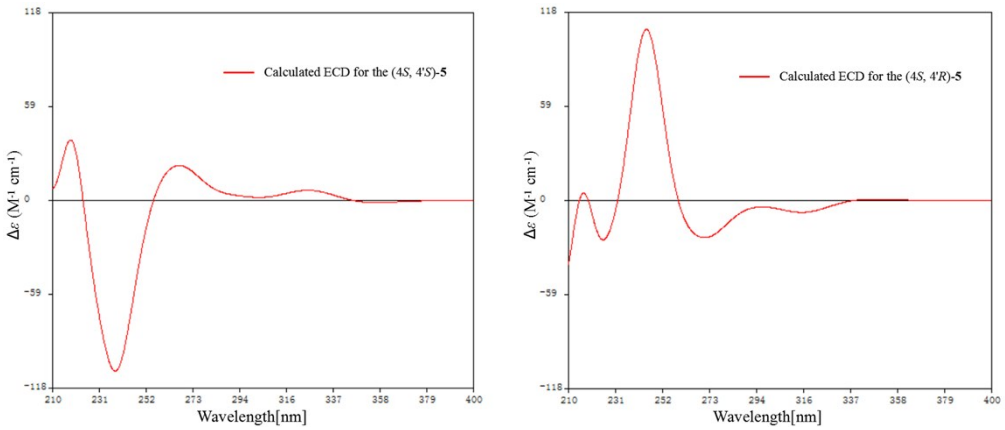
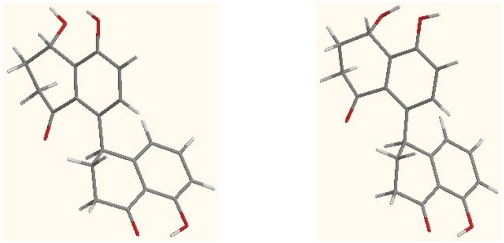


Figure S45-1. B3LYP/6-31+G(d) calculated spectra of (4*S*, 4'*S*)-**5** and (4*S*, 4'*R*)-**5** (σ = 0.20 eV).



Conf. A 60.7% Conf. B 35.0%

Figure S45-2. DFT-optimized structures for low-energy conformers of (4*S*, 4'*S*)-**5** at B3LYP/6-31+g (d) level in methanol (CPCM) (Conformer populations were calculated using the Gibbs free energy and Boltzmann population at 298 K estimated thereof).

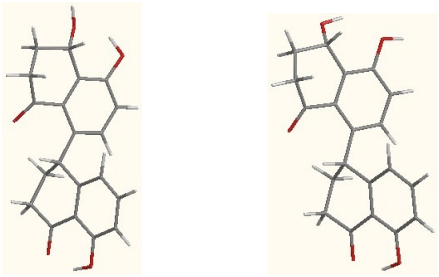
Table S3. Cartesian coordinates of the low-energy reoptimized conformers of (4*S*, 4'*S*)-**5** calculated at B3LYP/6-31+G(d) level of theory with PCM solvent model for MeOH.

Conformer A		Standard Orientation (Ångstroms)		
I	Atom	X	Y	Z
1	C	-2.97307	-0.27906	-0.35994
2	C	-1.78621	0.43587	-0.04718
3	C	-0.53072	-0.01961	-0.52573
4	C	-0.51189	-1.17643	-1.31992
5	C	-1.66262	-1.89865	-1.60945
6	C	-2.8908	-1.46586	-1.10603
7	C	-4.36348	0.19316	0.03061

8	C	-4.39216	1.52095	0.7886
9	C	-3.17024	1.67914	1.70081
10	C	-1.9262	1.63767	0.83912
11	C	0.80226	0.67109	-0.24413
12	C	1.30365	1.38581	-1.5168
13	C	2.64773	2.06915	-1.26431
14	C	3.68912	1.11148	-0.74124
15	C	3.25162	-0.02179	0.08025
16	C	1.86909	-0.2569	0.34029
17	C	4.22957	-0.8785	0.6691
18	C	3.84124	-1.92513	1.51334
19	C	2.49035	-2.12063	1.77389
20	C	1.5127	-1.29992	1.19423
21	O	-4.94681	-0.89485	0.80383
22	O	-3.99989	-2.21862	-1.3813
23	O	-1.11166	2.55902	0.86187
24	O	4.89679	1.31705	-0.98664
25	O	5.55068	-0.70812	0.44626
26	H	0.43933	-1.54317	-1.69605
27	H	-1.62108	-2.8052	-2.20631
28	H	-4.96097	0.29688	-0.88622
29	H	-4.41147	2.34193	0.0606
30	H	-5.32197	1.59065	1.36421
32	H	-3.19109	2.62711	2.24447
32	H	-3.13698	0.85906	2.43085
33	H	0.63299	1.45382	0.49997
34	H	0.56099	2.12704	-1.8301
35	H	1.40433	0.66397	-2.33772
36	H	3.04343	2.54934	-2.16499
37	H	2.52785	2.85953	-0.50654
38	H	4.60522	-2.55909	1.95293
39	H	2.18549	-2.92807	2.43475
40	H	0.46597	-1.48801	1.40899
41	H	-5.89012	-0.70263	0.94269
42	H	-4.66608	-2.03294	-0.68375
43	H	5.64161	0.08294	-0.153

Conformer B		Standard Orientation (Ångstroms)		
I	Atom	X	Y	Z
1	C	2.98524	-0.28103	0.36256

2	C	1.80019	0.43726	0.05663
3	C	0.54102	-0.01878	0.53079
4	C	0.51871	-1.17028	1.32886
5	C	1.67372	-1.87656	1.64887
6	C	2.8991	-1.43776	1.14973
7	C	4.37296	0.11224	-0.13341
8	C	4.42295	1.50088	-0.75717
9	C	3.19358	1.76204	-1.63645
10	C	1.94503	1.67014	-0.78766
11	C	-0.79183	0.66899	0.2391
12	C	-1.29686	1.39715	1.50236
13	C	-2.63878	2.07988	1.23785
14	C	-3.67944	1.1187	0.72008
15	C	-3.24048	-0.02375	-0.08793
16	C	-1.85726	-0.26429	-0.33961
17	C	-4.21776	-0.88379	-0.67307
18	C	-3.82807	-1.93922	-1.50568
19	C	-2.47654	-2.1399	-1.75864
20	C	-1.49956	-1.31586	-1.18252
21	O	4.82744	-0.83153	-1.13111
22	O	4.07368	-2.11287	1.38341
23	O	1.12192	2.5846	-0.77875
24	O	-4.88785	1.32898	0.95782
25	O	-5.53944	-0.7082	-0.45799
26	H	-0.43302	-1.54065	1.69957
27	H	1.61891	-2.7676	2.27011
28	H	5.06861	0.07388	0.71348
29	H	4.46717	2.25061	0.04284
30	H	5.34576	1.59404	-1.33878
32	H	3.22693	2.75147	-2.1004
32	H	3.14015	1.00816	-2.43395
33	H	-0.62052	1.44368	-0.51271
34	H	-0.55425	2.14042	1.81045
35	H	-1.40167	0.68338	2.32988
36	H	-3.03741	2.56962	2.13209
37	H	-2.51468	2.86269	0.4729
38	H	-4.59154	-2.57551	-1.94275
39	H	-2.17064	-2.95381	-2.41104
40	H	-0.45246	-1.50775	-1.39192
41	H	4.90293	-1.69726	-0.69384
42	H	3.91554	-2.88875	1.94596
43	H	-5.63128	0.08914	0.13289



Conf. A 91.5% Conf. B 6.5%

Figure S45-3. DFT-optimized structures for low-energy conformers of (4*S*, 4'*R*)-**5** at B3LYP/6-31+g (d) level in methanol (CPCM) (Conformer populations were calculated using the Gibbs free energy and Boltzmann population at 298 K estimated thereof).

Table S4. Cartesian coordinates of the low-energy reoptimized conformers of (4*S*, 4'*R*)-**5** calculated at B3LYP/6-31+G(d) level of theory with PCM solvent model for MeOH.

Conformer A		Standard Orientation (Ångstroms)		
I	Atom	X	Y	Z
1	C	2.96658	-0.40155	-0.13409
2	C	1.78085	0.36322	0.06879
3	C	0.53233	-0.09294	-0.42809
4	C	0.51377	-1.29447	-1.15061
5	C	1.66537	-2.03066	-1.38767
6	C	2.89089	-1.59697	-0.87468
7	C	4.29866	-0.01561	0.49776
8	C	4.36255	1.42633	0.98228
9	C	3.09043	1.7672	1.76755
10	C	1.90148	1.64365	0.84114
11	C	-0.79697	0.63644	-0.23716
12	C	-1.23839	1.28642	-1.56511
13	C	-2.57696	2.0066	-1.40052
14	C	-3.65491	1.09731	-0.86568
15	C	-3.26934	0.00381	0.03226
16	C	-1.90205	-0.23991	0.35729
17	C	-4.28473	-0.80083	0.63119
18	C	-3.94815	-1.80409	1.54722
19	C	-2.61185	-2.00747	1.86963
20	C	-1.59787	-1.23815	1.28201
21	O	5.35062	-0.26514	-0.47131

22	O	3.97547	-2.39408	-1.10753
23	O	1.10932	2.57652	0.71503
24	O	-4.84881	1.30983	-1.16655
25	O	-5.5933	-0.62035	0.34978
26	H	-0.432	-1.66838	-1.53334
27	H	1.63345	-2.95206	-1.96211
28	H	4.46597	-0.68956	1.35305
29	H	4.45868	2.09072	0.11436
30	H	5.25046	1.56946	1.60837
32	H	2.97117	1.06836	2.60822
32	H	3.12045	2.78341	2.16879
33	H	-0.64461	1.45658	0.46874
34	H	-1.32374	0.5208	-2.34721
35	H	-0.47053	1.99541	-1.89143
36	H	-2.46866	2.83447	-0.68197
37	H	-2.93053	2.44431	-2.33957
38	H	-4.74004	-2.3985	1.9926
39	H	-2.34733	-2.78074	2.58638
40	H	-0.56354	-1.43112	1.54646
41	H	6.2071	-0.22858	-0.01258
42	H	4.78411	-1.85641	-0.93975
43	H	-5.64692	0.13748	-0.29527

Conformer B		Standard Orientation (Ångstroms)		
I	Atom	X	Y	Z
1	C	-2.97405	0.40285	-0.108
2	C	-1.78594	-0.35005	0.09212
3	C	-0.53992	0.11352	-0.40873
4	C	-0.52702	1.31986	-1.11992
5	C	-1.68016	2.06944	-1.32554
6	C	-2.89112	1.61809	-0.80419
7	C	-4.34638	-0.02275	0.41941
8	C	-4.36542	-1.42462	1.01613
9	C	-3.09143	-1.69559	1.82544
10	C	-1.90525	-1.61364	0.89116
11	C	0.78723	-0.62332	-0.23451
12	C	1.20949	-1.26973	-1.57064
13	C	2.54122	-2.0056	-1.421
14	C	3.6334	-1.11159	-0.88926
15	C	3.26719	-0.01729	0.01596

16	C	1.90533	0.24052	0.35286
17	C	4.29612	0.77414	0.60918
18	C	3.9778	1.77878	1.53036
19	C	2.64653	1.99616	1.86379
20	C	1.61939	1.23948	1.28241
21	O	-5.34972	-0.01344	-0.60943
22	O	-4.05396	2.34312	-0.94237
23	O	-1.11849	-2.55328	0.78514
24	O	4.82254	-1.33689	-1.19932
25	O	5.60025	0.57975	0.31728
26	H	0.4139	1.69834	-1.50933
27	H	-1.63618	3.00522	-1.8784
28	H	-4.63426	0.70155	1.19796
29	H	-4.44307	-2.15072	0.19662
30	H	-5.25549	-1.54527	1.6421
32	H	-2.98218	-0.9454	2.62174
32	H	-3.10933	-2.68642	2.2868
33	H	0.63451	-1.44655	0.4681
34	H	1.29669	-0.50017	-2.34868
35	H	0.43119	-1.96824	-1.89495
36	H	2.42935	-2.83675	-0.70685
37	H	2.88247	-2.44127	-2.36553
38	H	4.77972	2.36301	1.97125
39	H	2.39627	2.7703	2.58469
40	H	0.58953	1.44268	1.55648
41	H	-5.40473	0.896	-0.9532
42	H	-3.89581	3.15484	-1.45188
43	H	5.64039	-0.17738	-0.32965

Figure S46. ECD calculated spectra of four absolute configurations of **1**