Supporting Information

Archromones A–F, Unusual Polycyclic Dearomatic Geranylquinol Derivatives from the Roots of *Arnebia euchroma*

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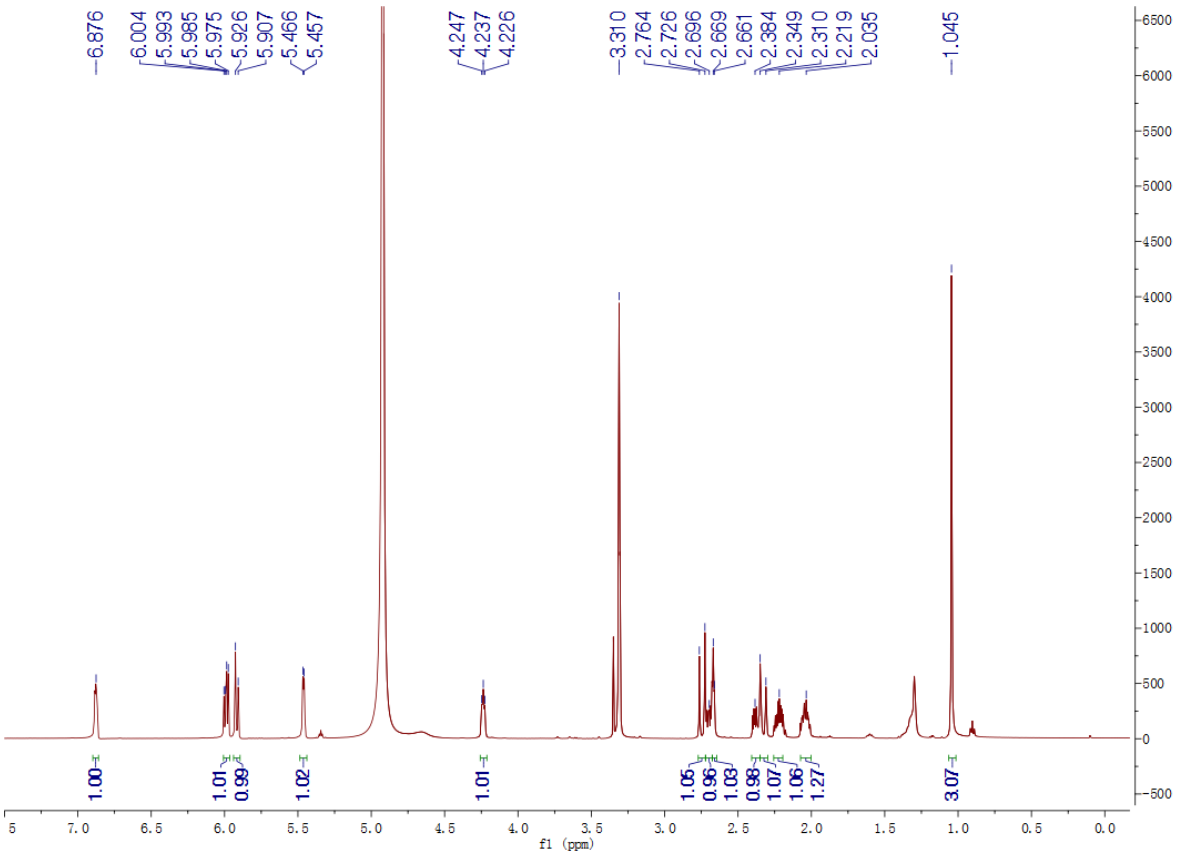


Figure S1. The ^{1}H NMR spectrum of compound **1** in CD_3OD

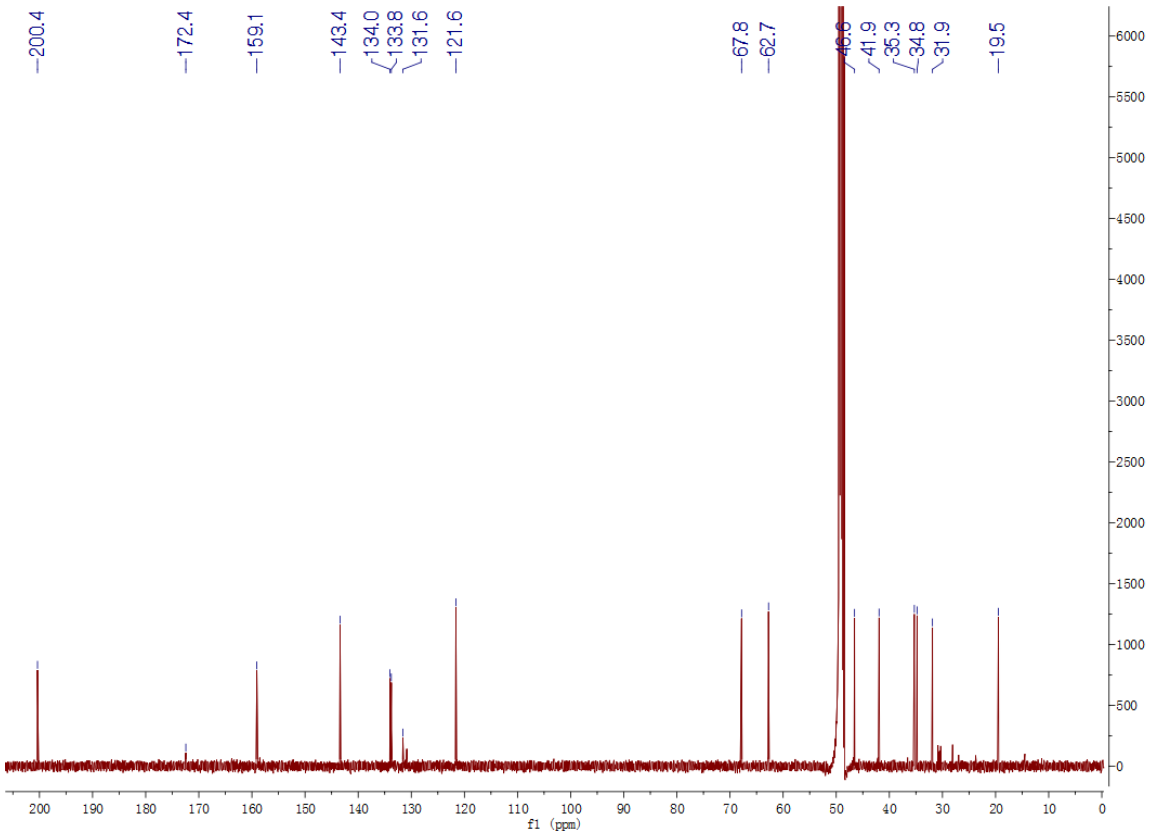


Figure S2. The ^{13}C NMR spectrum of compound **1** in CD_3OD

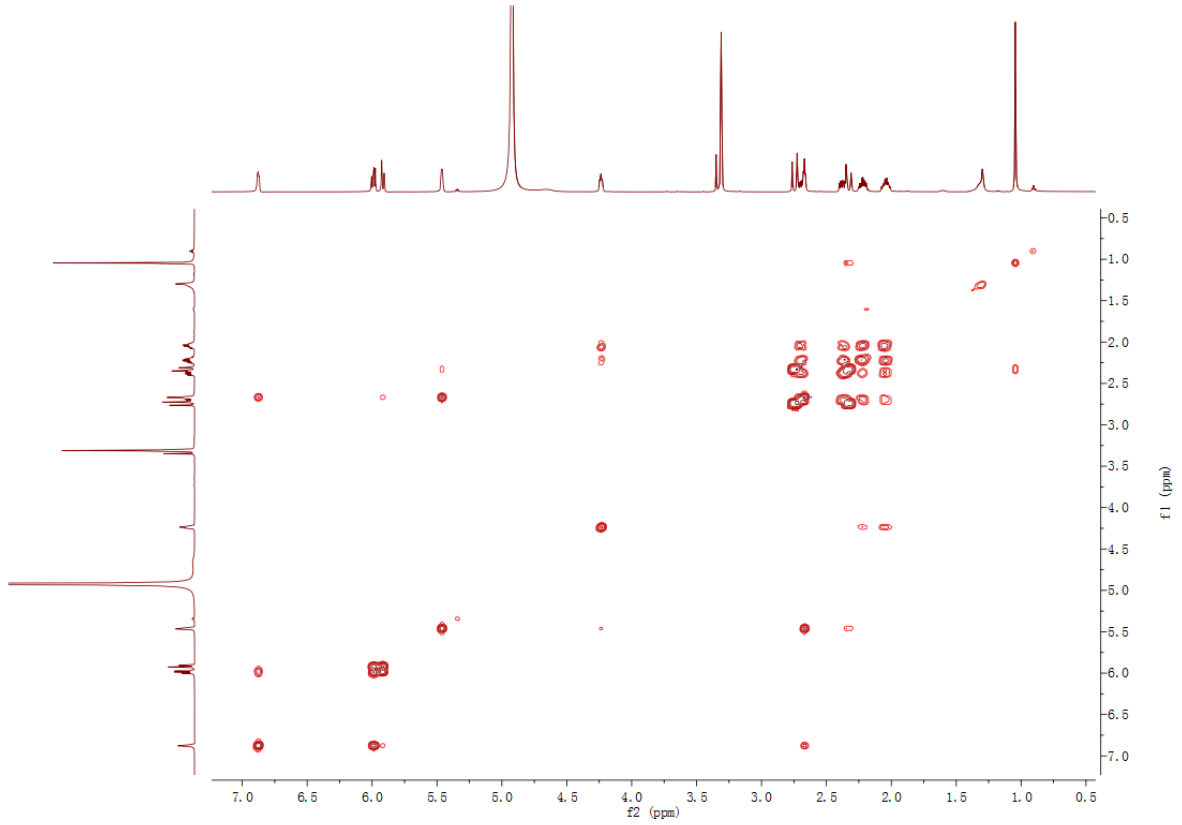


Figure S3. The ^{1}H-^{1}H COSY spectrum of compound **1** in CD_3OD

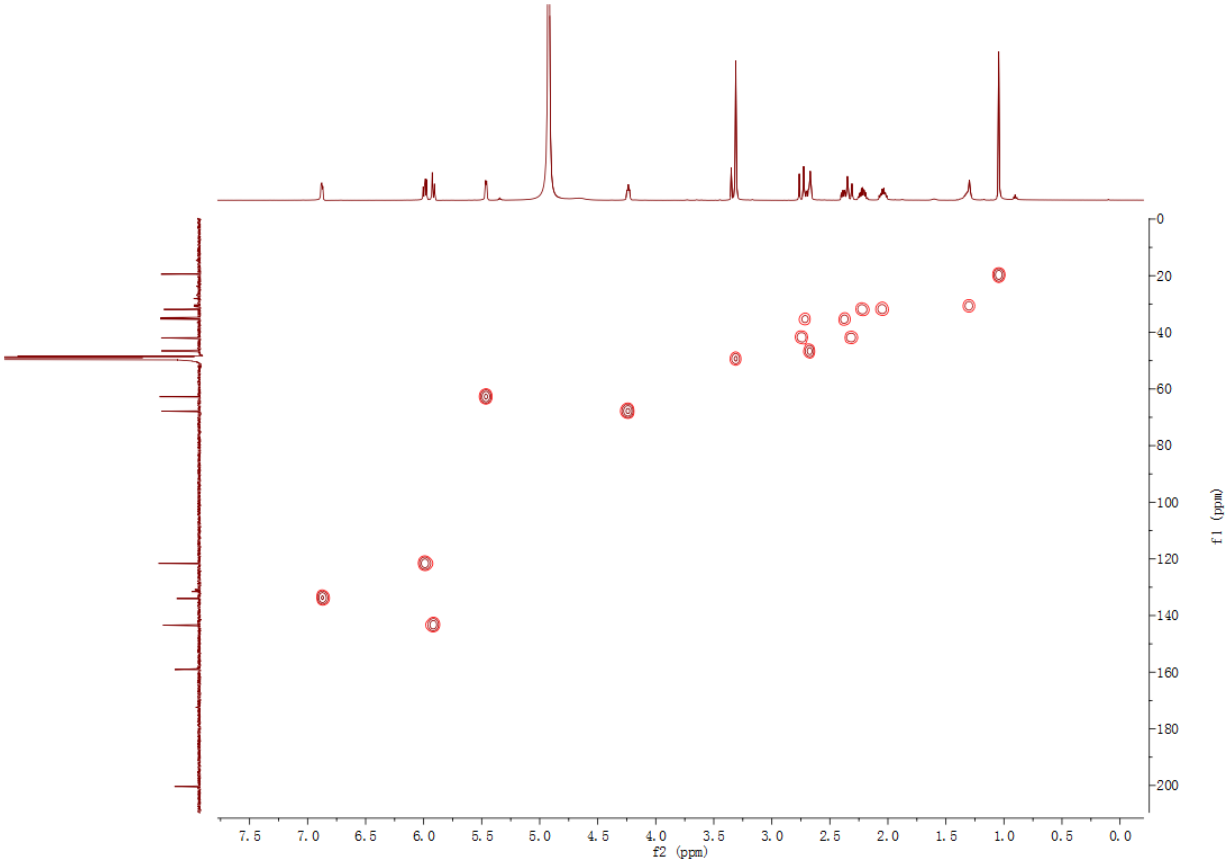


Figure S4. The HSQC spectrum of compound **1** in CD_3OD

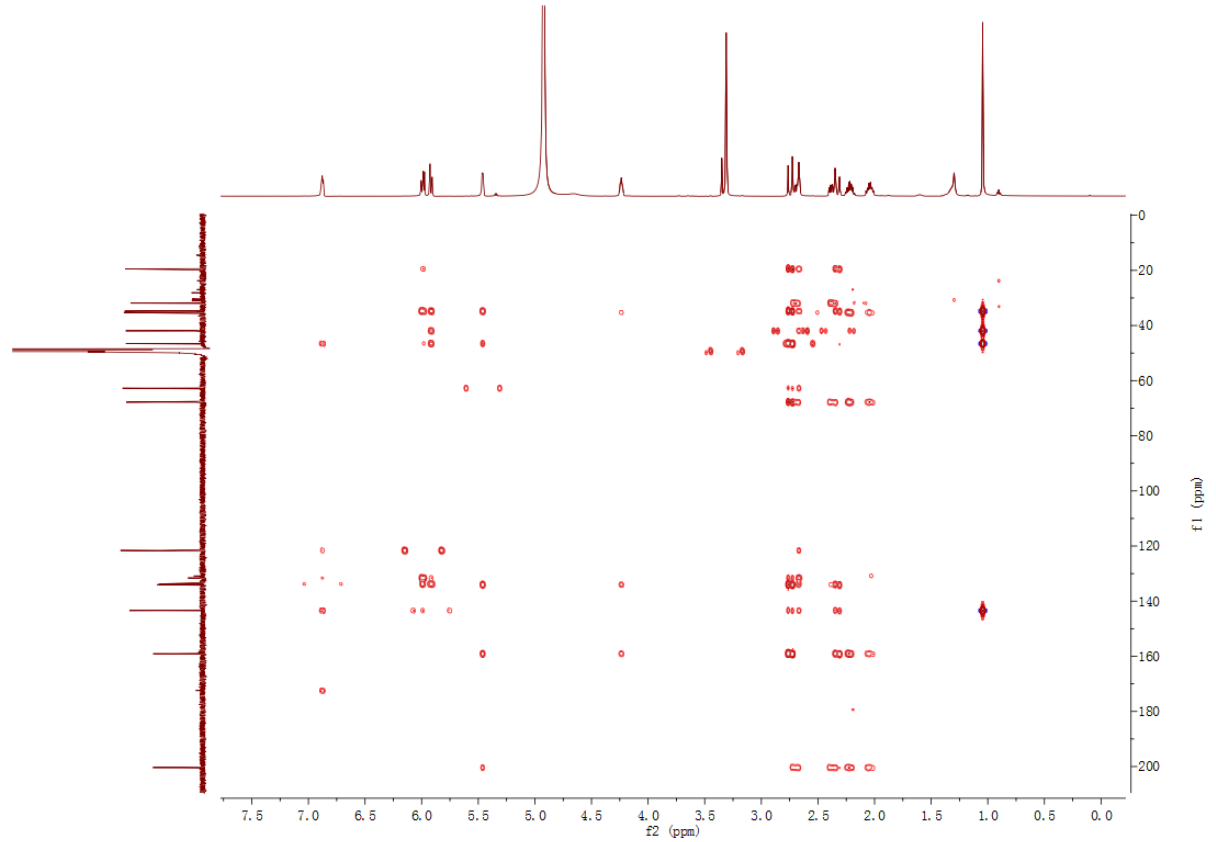


Figure S5. The HMBC spectrum of compound **1** in CD_3OD

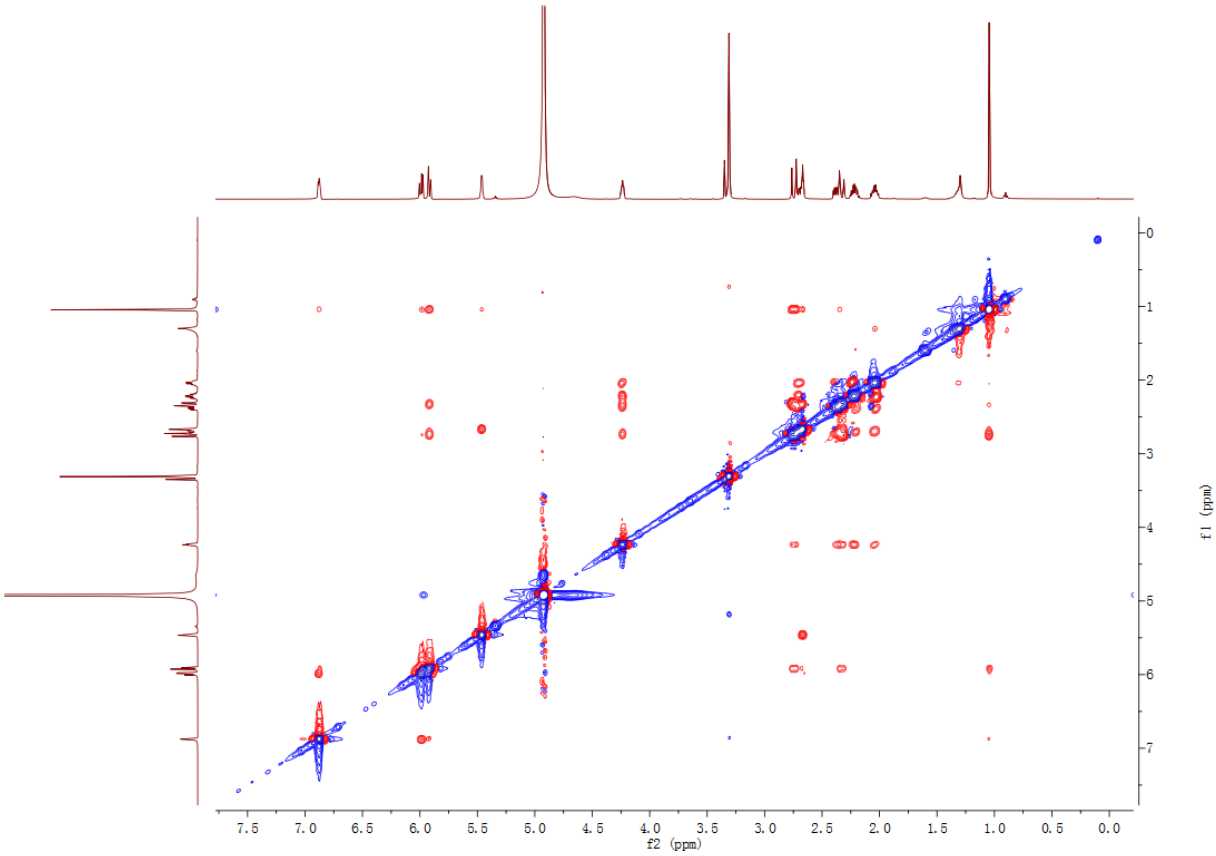


Figure S6. The ROESY spectrum of compound **1** in CD_3OD

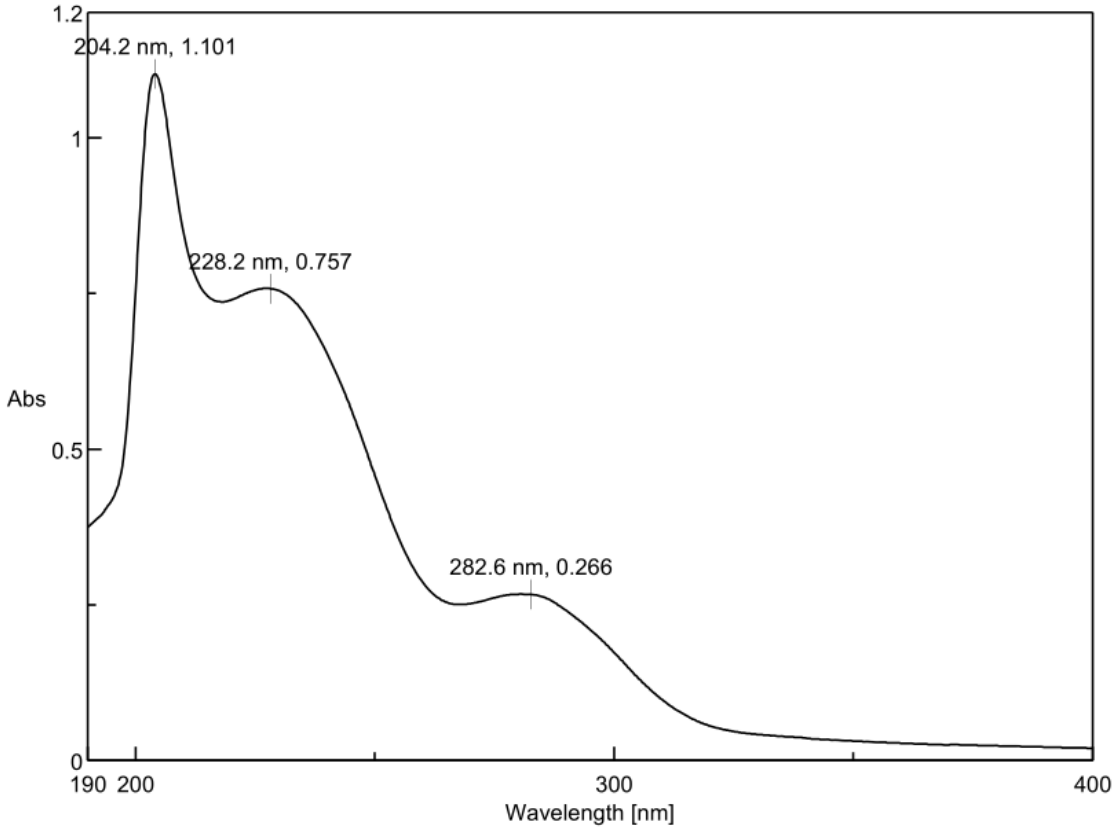


Figure S7. The UV spectrum of compound **1** in H_2O

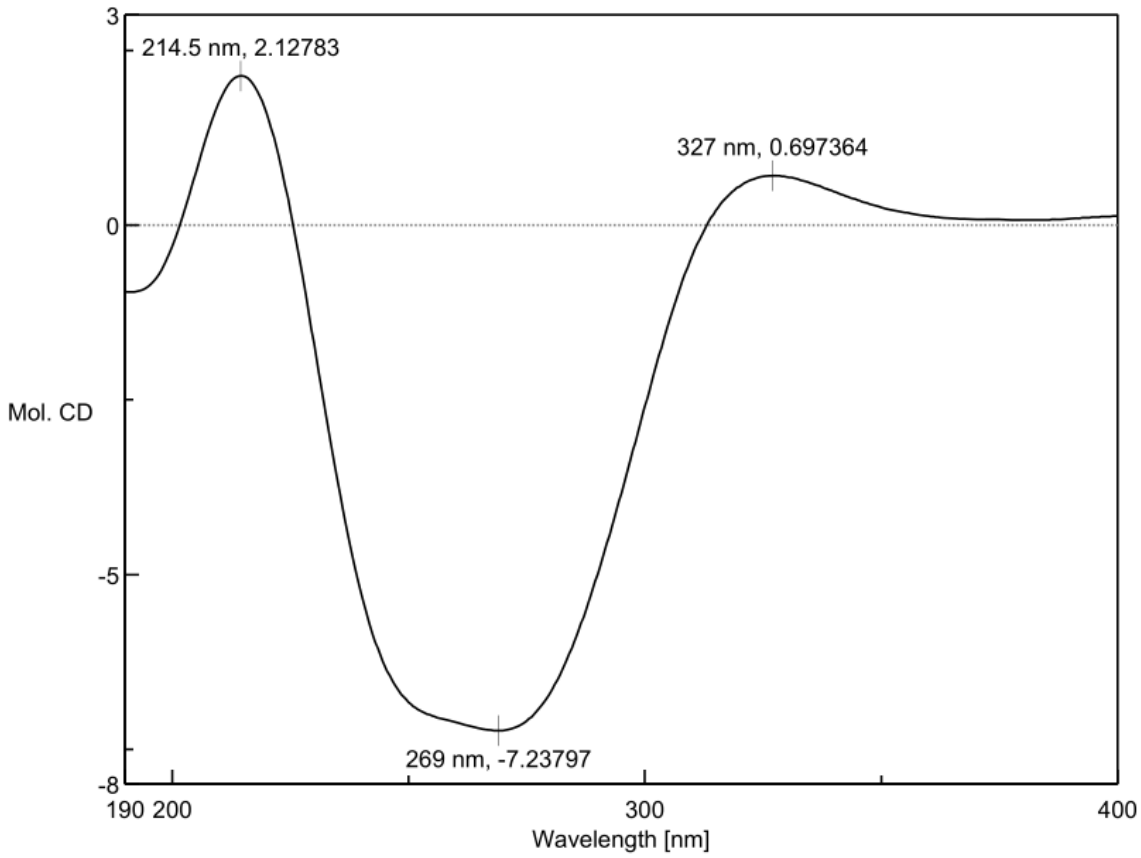


Figure S8. The ECD spectrum of compound **1** in H_2O

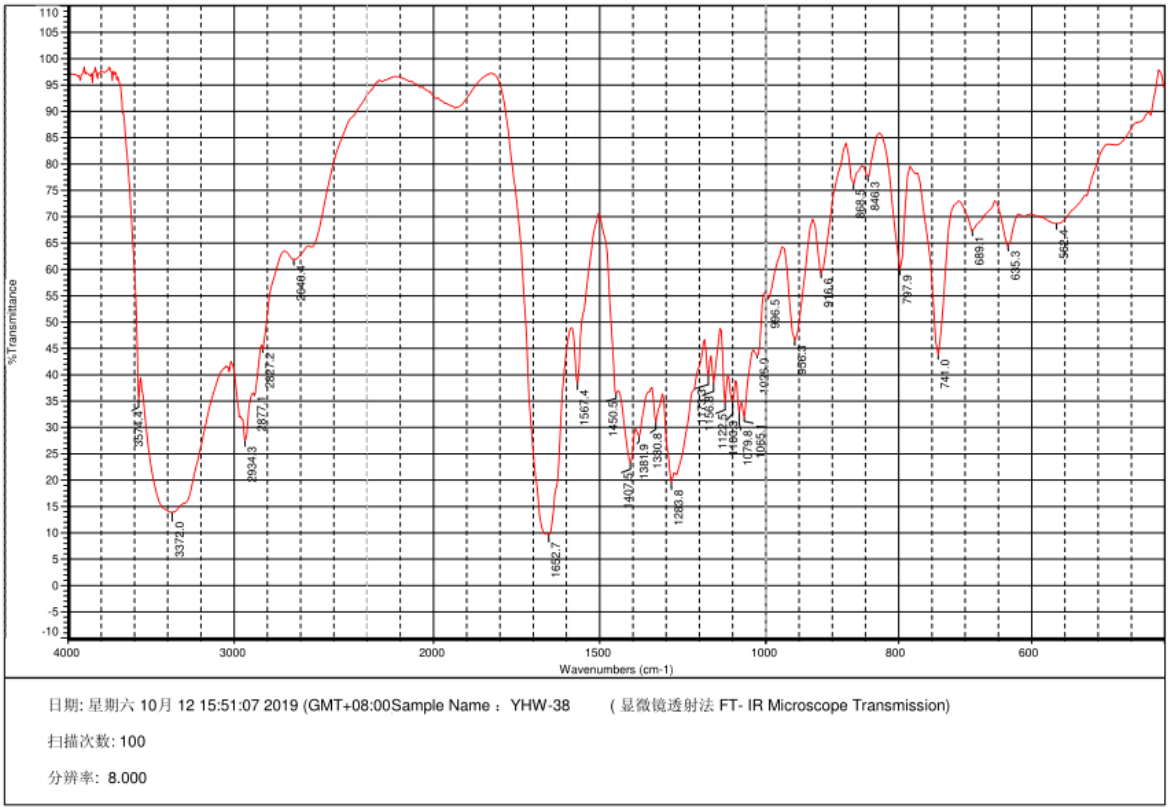
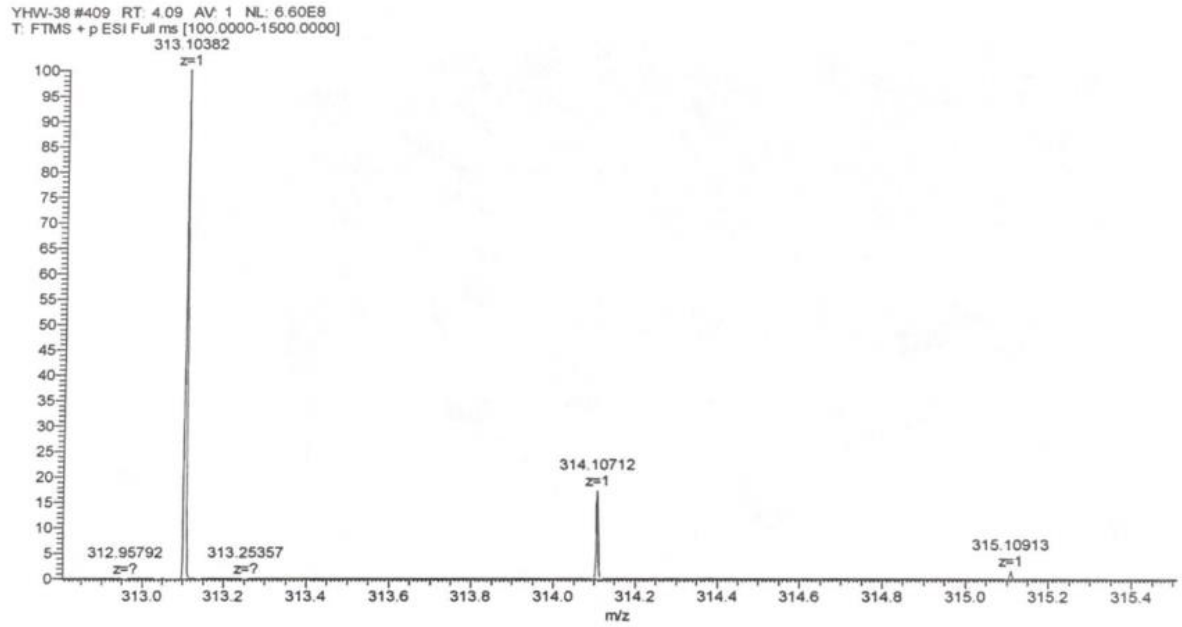


Figure S9. The IR spectrum of compound **1**



m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition	
313.10382	313.10464	-2.63	7.5	C16 H18 O5 Na	M+Na

Figure S10. The HR-ESI-MS data of compound **1**

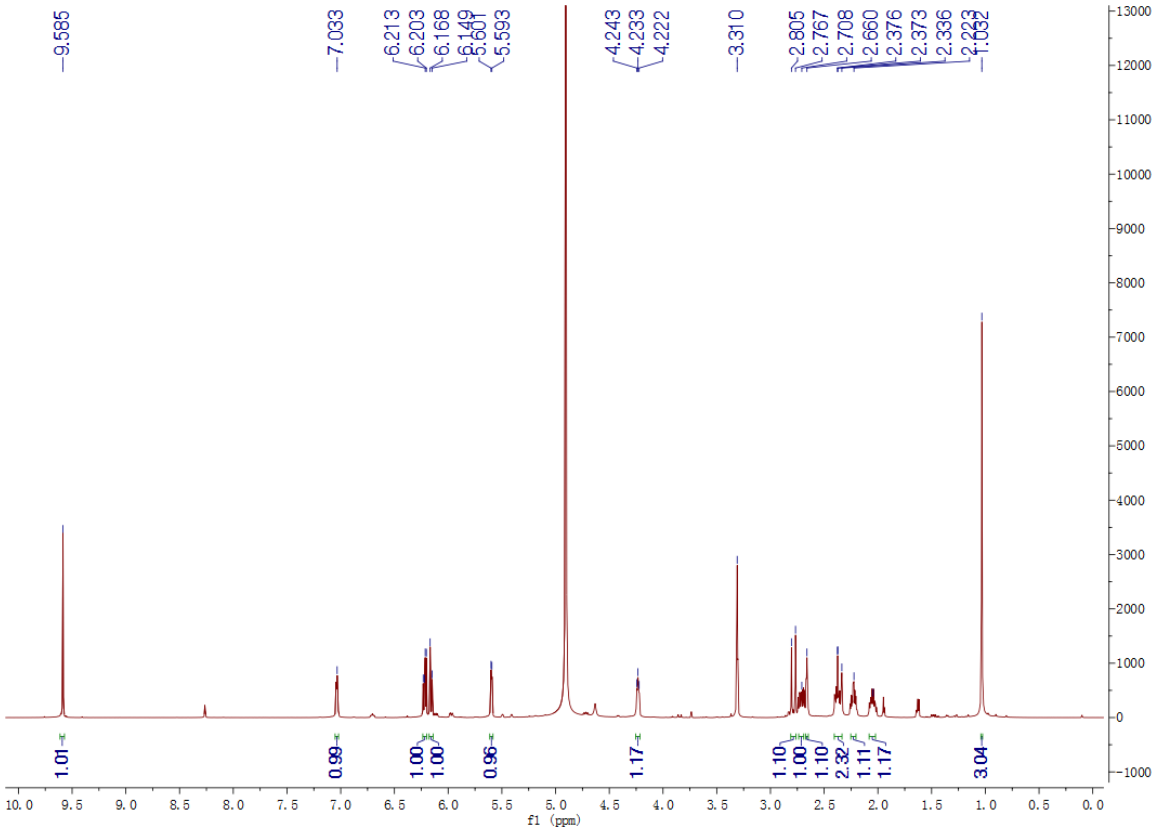


Figure S11. The ^{1}H NMR spectrum of compound **2** in CD_3OD

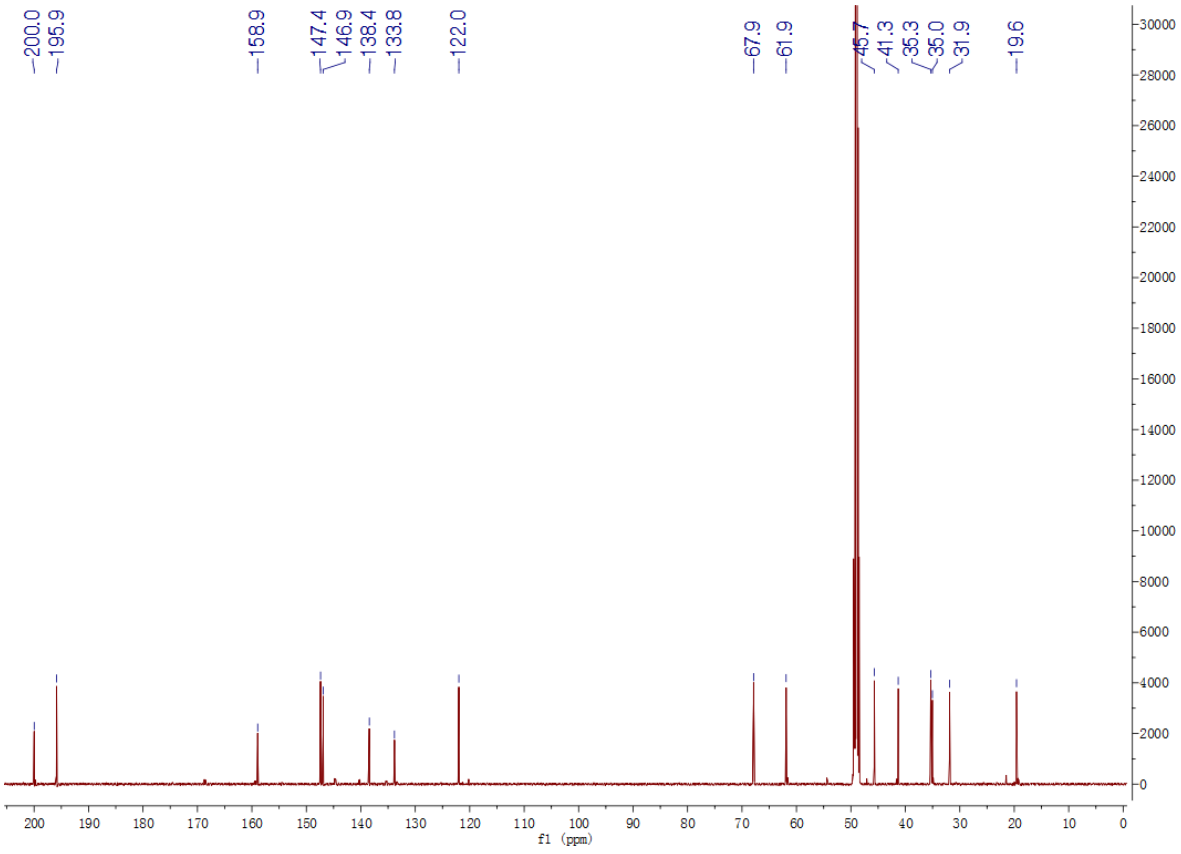


Figure S12. The ^{13}C NMR spectrum of compound **2** in CD_3OD

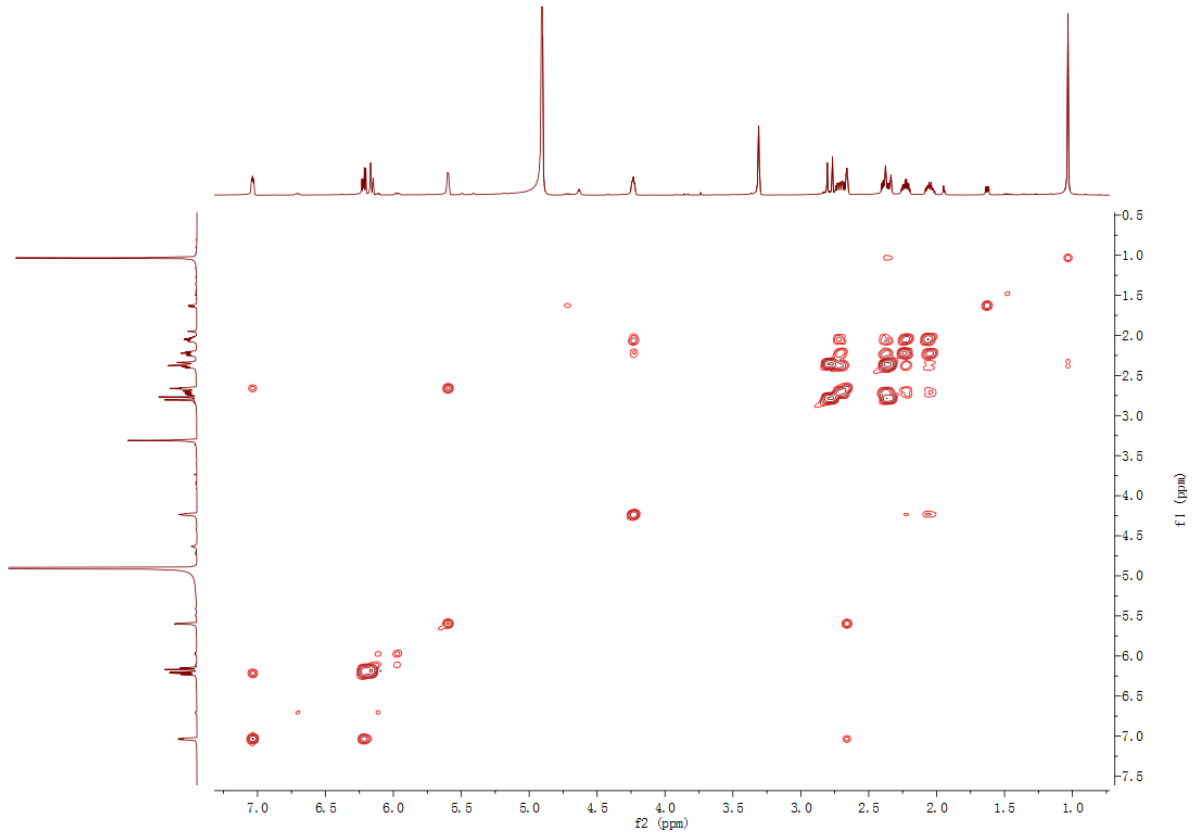


Figure S13. The ^{1}H-^{1}H COSY spectrum of compound **2** in CD_3OD

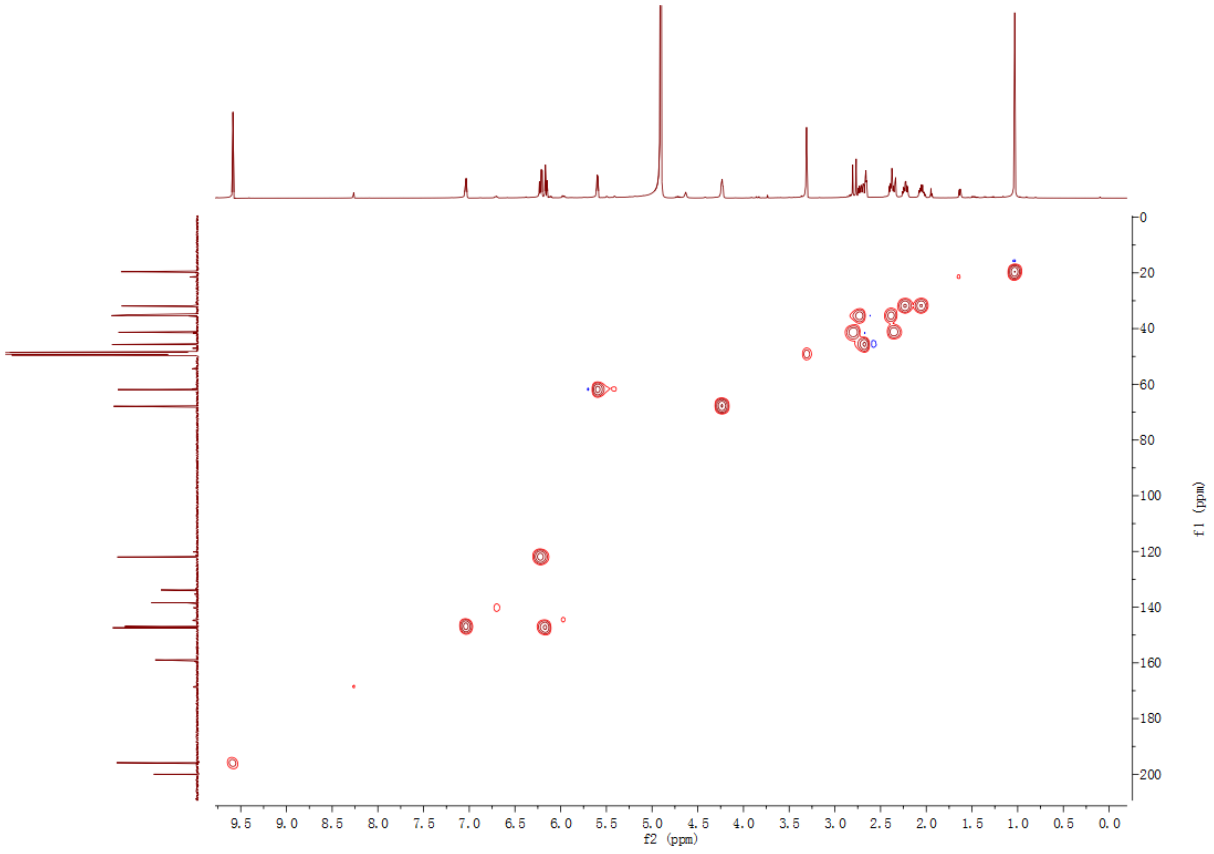


Figure S14. The HSQC spectrum of compound **2** in CD_3OD

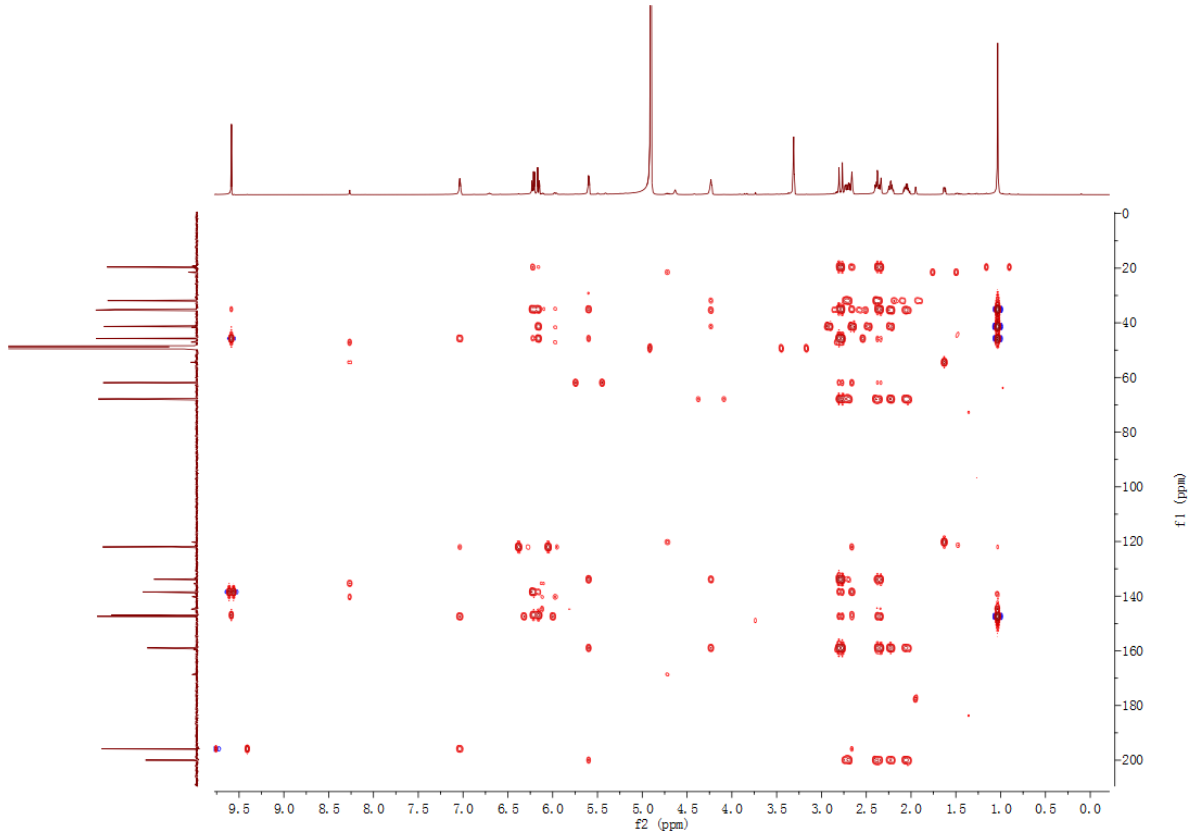


Figure S15. The HMBC spectrum of compound **2** in CD_3OD

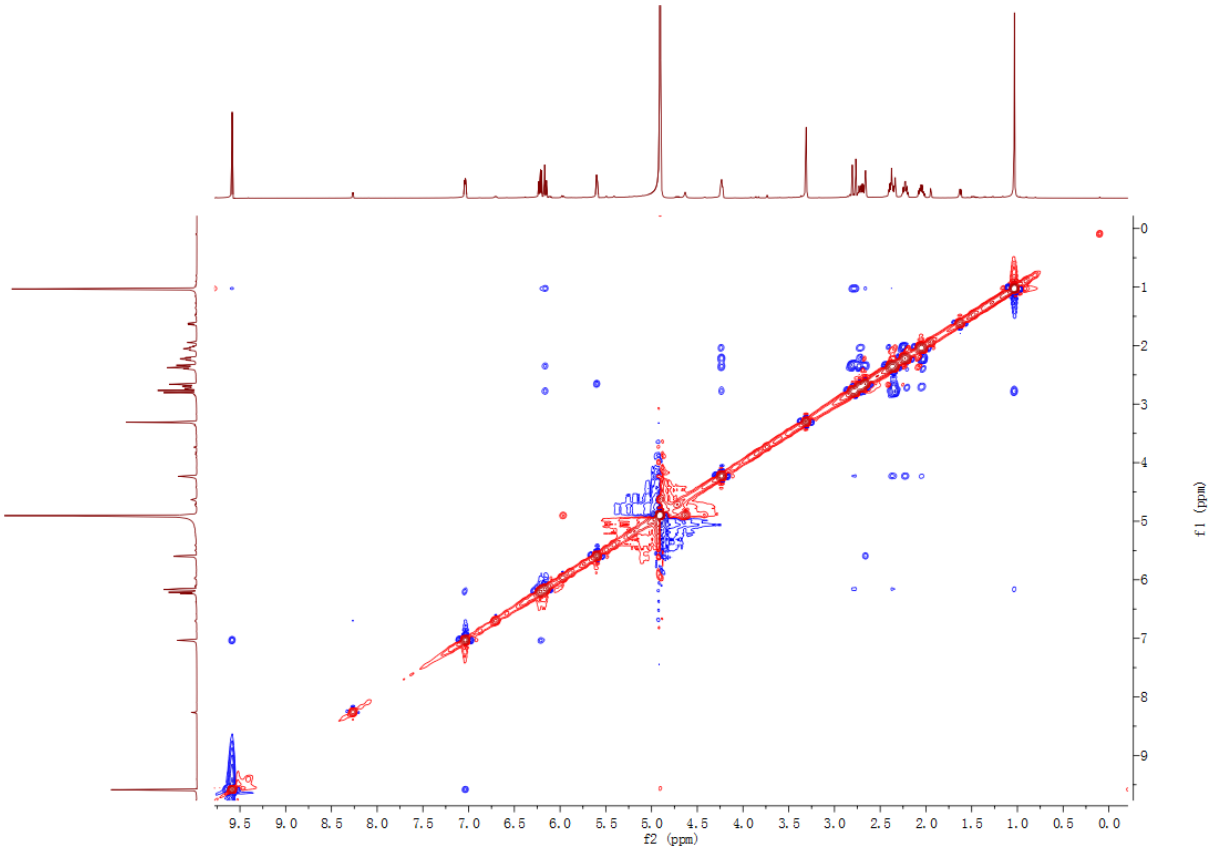


Figure S16. The ROESY spectrum of compound **2** in CD_3OD

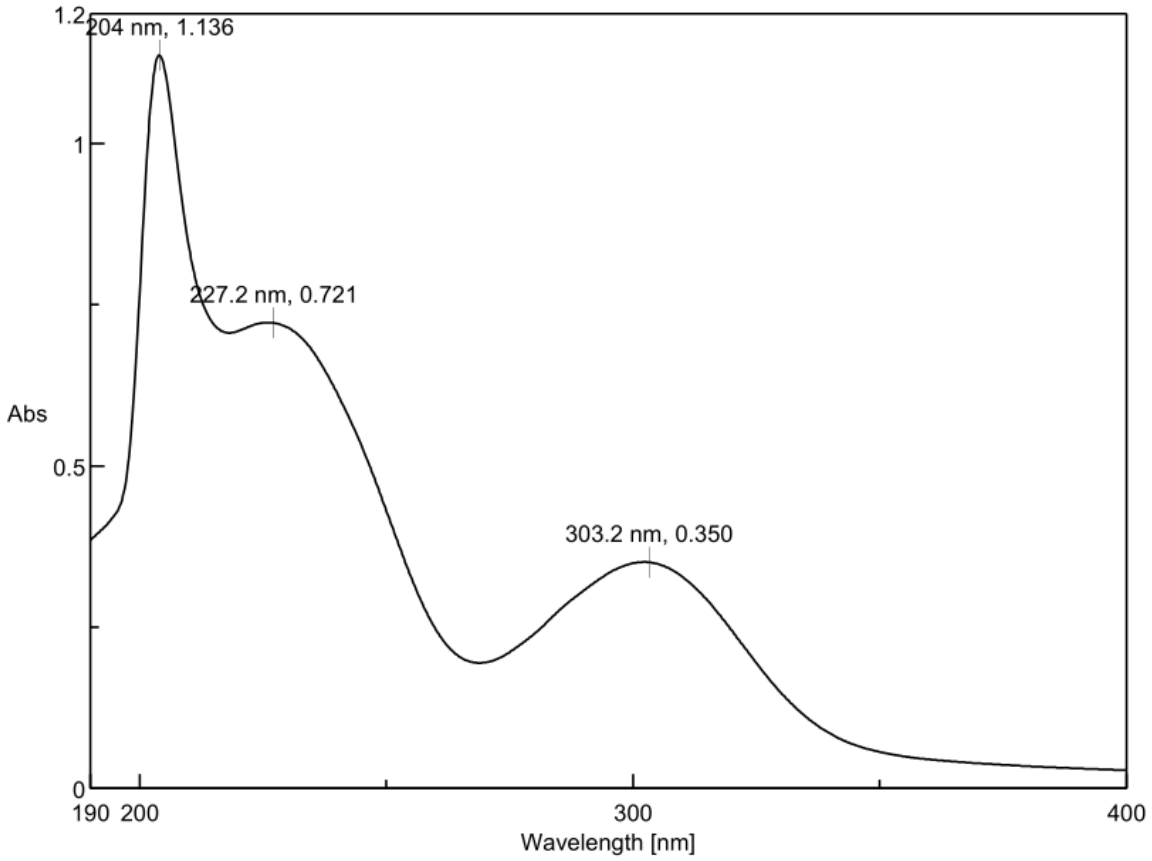


Figure S17. The UV spectrum of compound **2** in H_2O

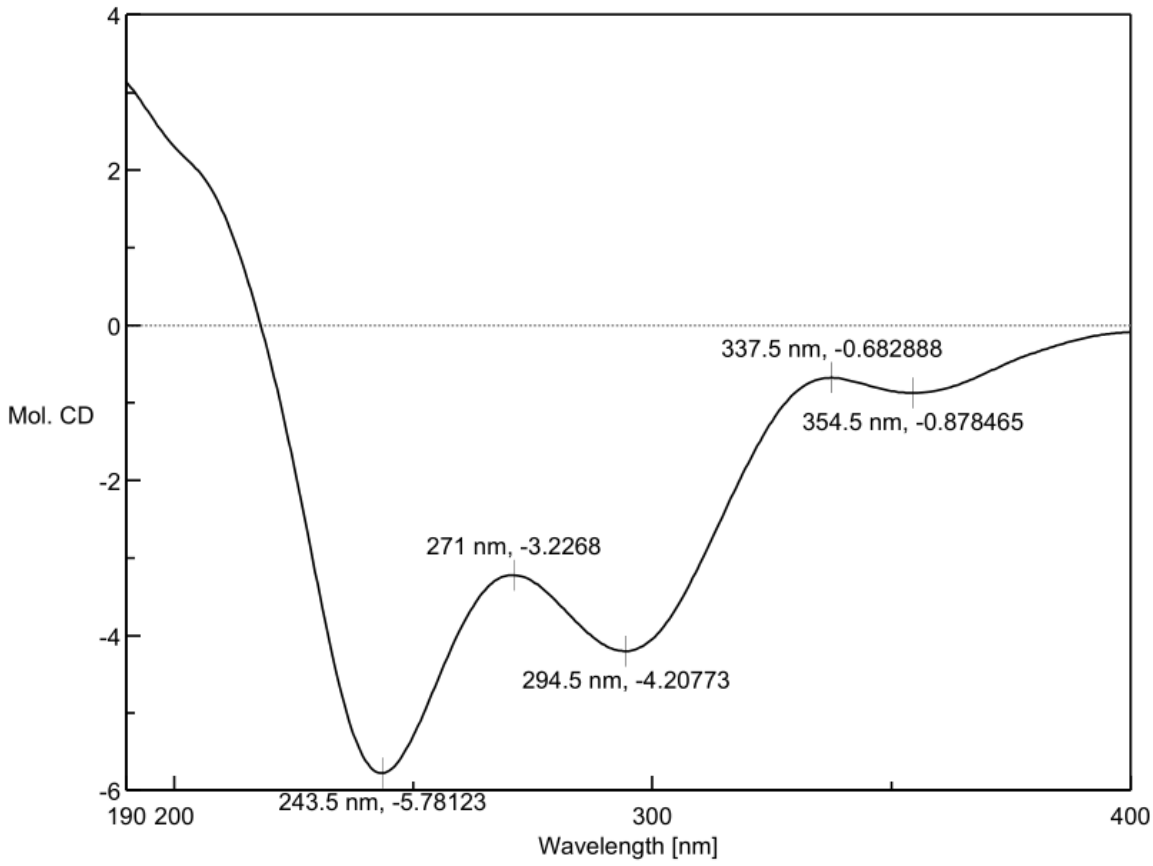


Figure S18. The ECD spectrum of compound **2** in H_2O

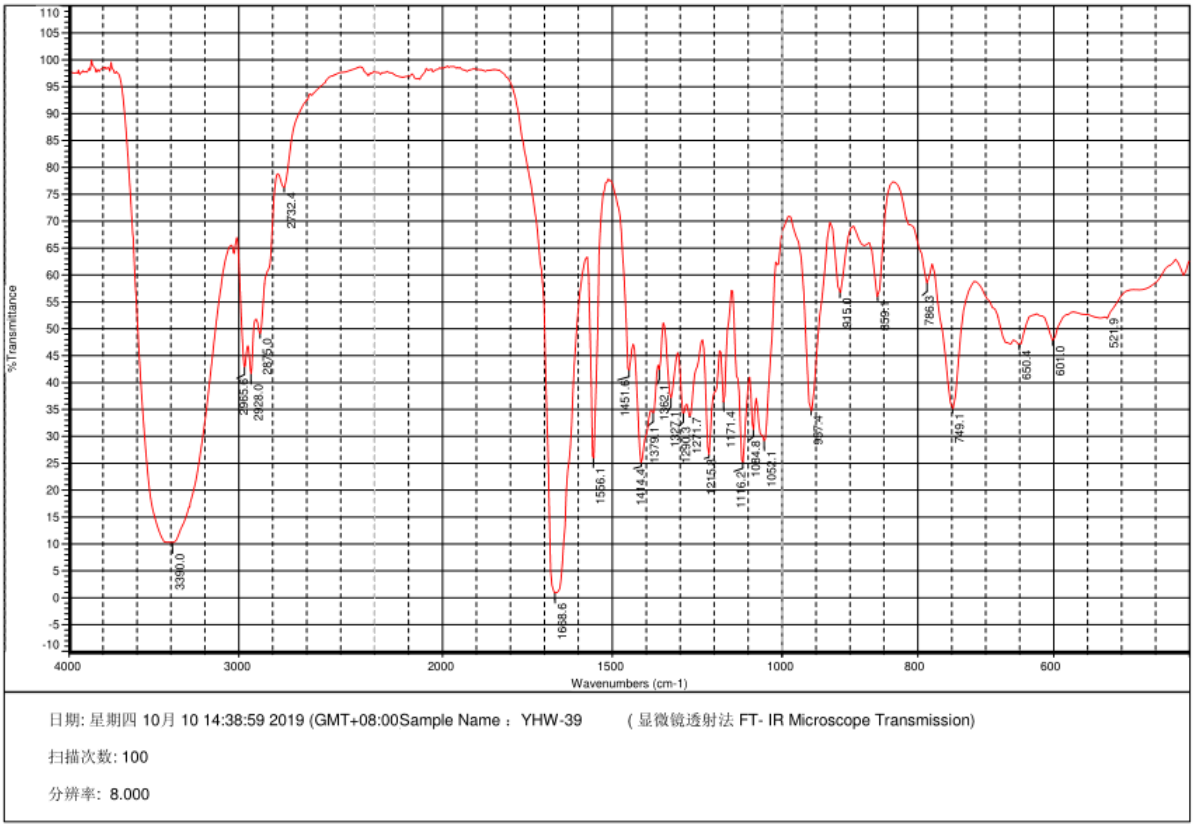
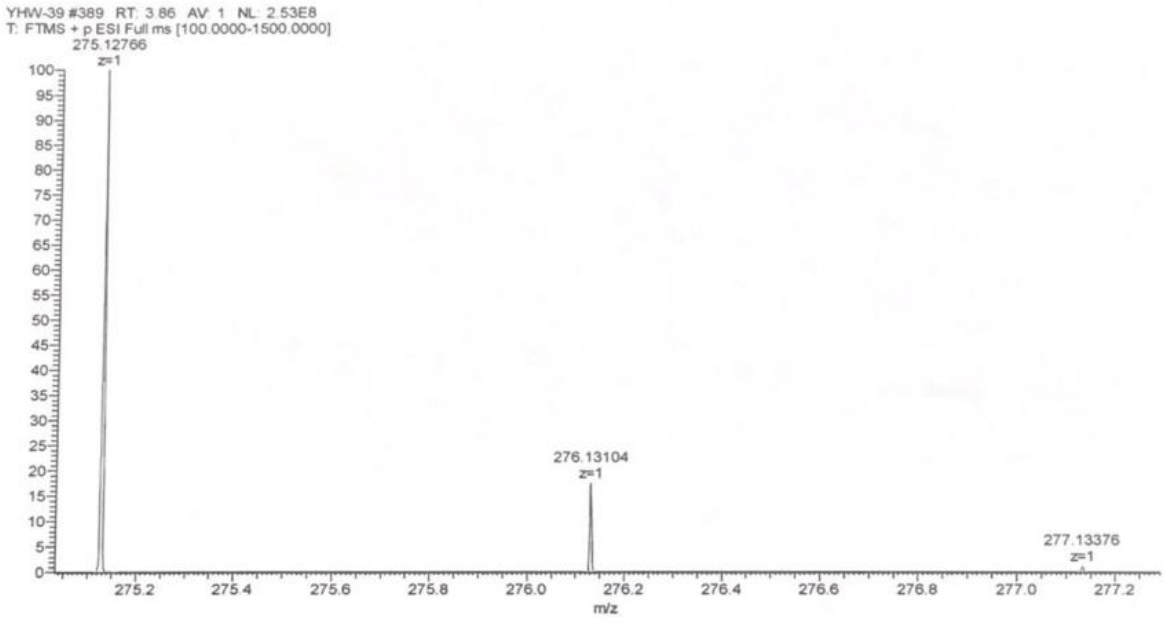


Figure S19. The IR spectrum of compound **2**



m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition	
275.12766	275.12779	-0.46	7.5	C16 H19 O4	M+H

Figure S20. The HR-ESI-MS data of compound **2**

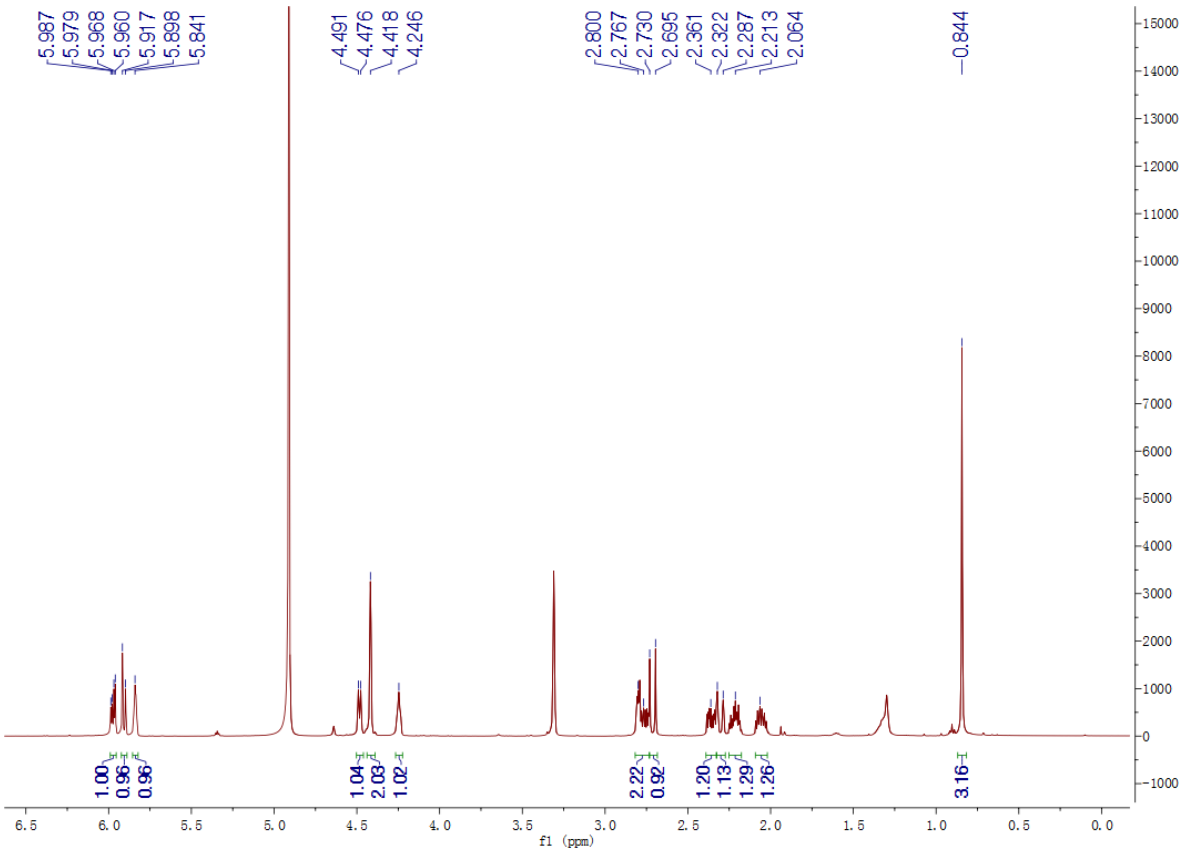


Figure S21. The ^{1}H NMR spectrum of compound **3** in CD_3OD

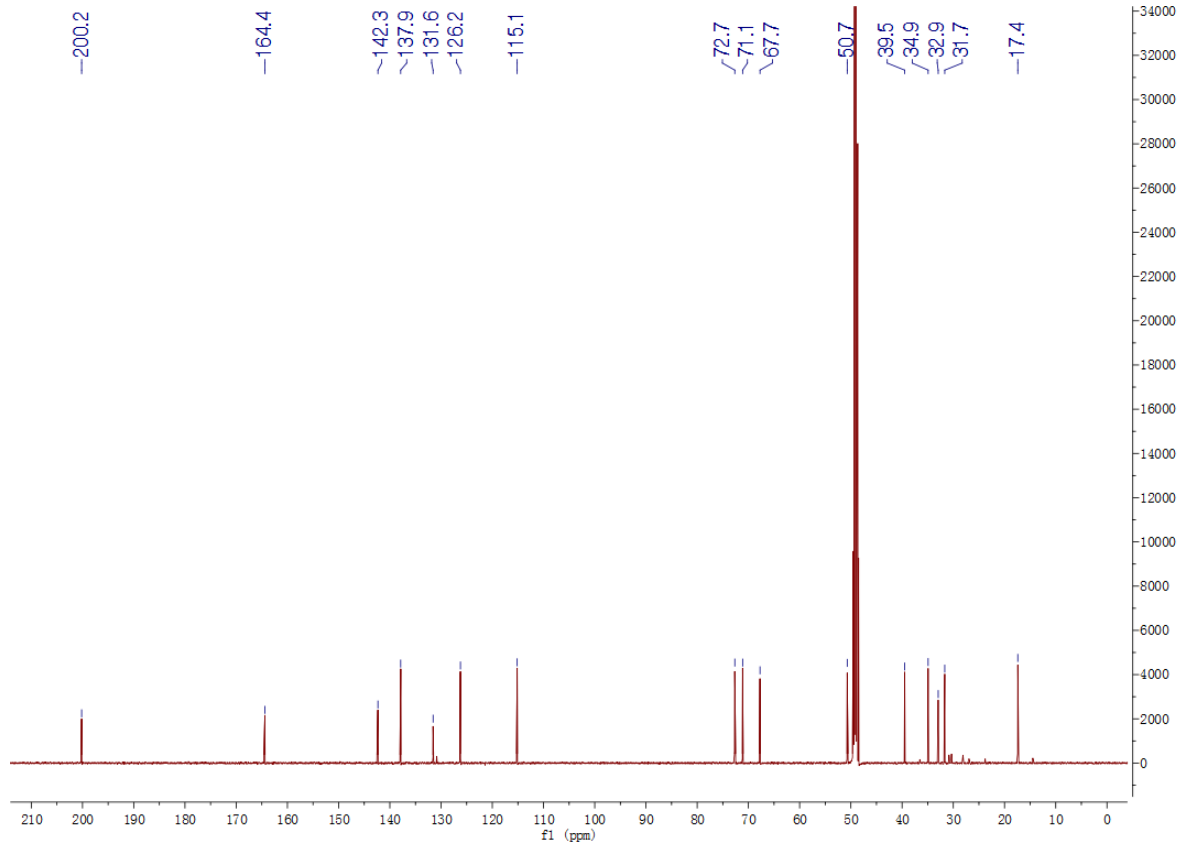


Figure S22. The ^{13}C NMR spectrum of compound **3** in CD_3OD

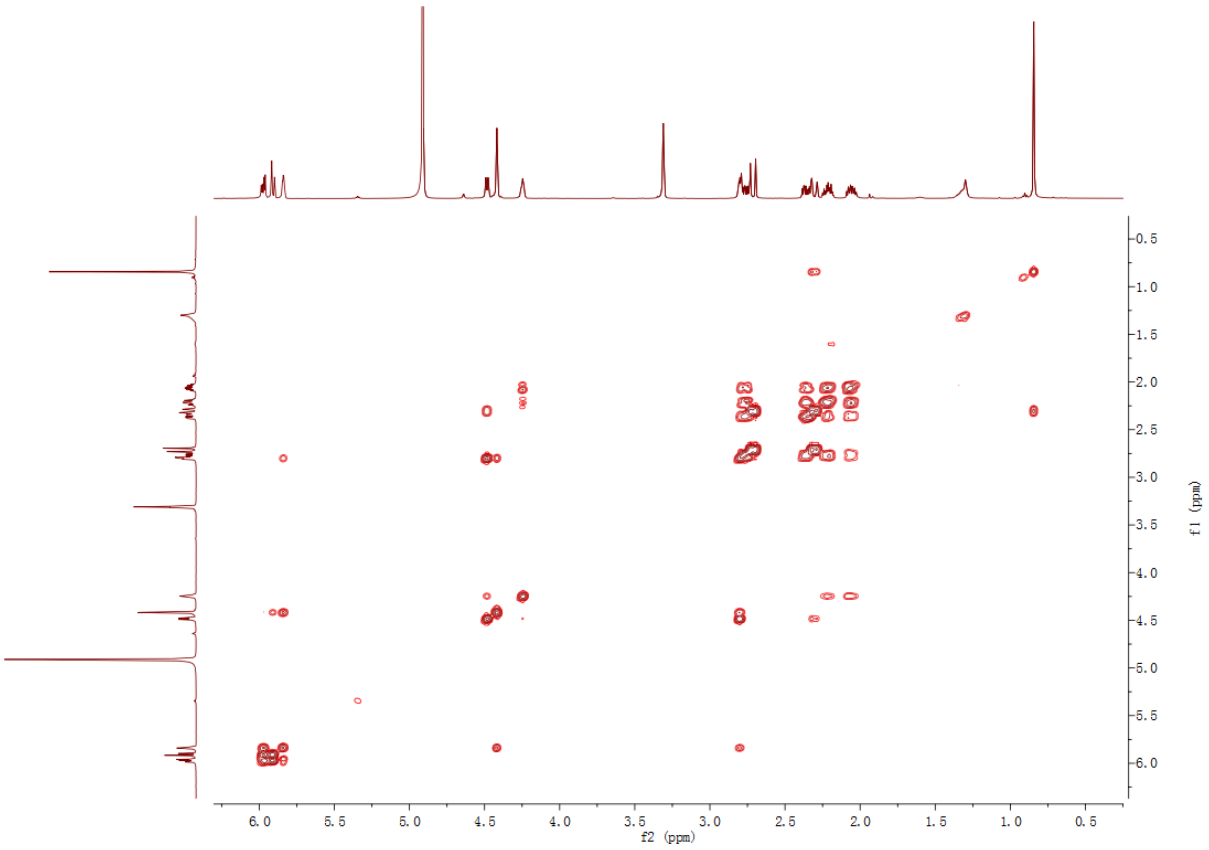


Figure S23. The ^{1}H-^{1}H COSY spectrum of compound **3** in CD_3OD

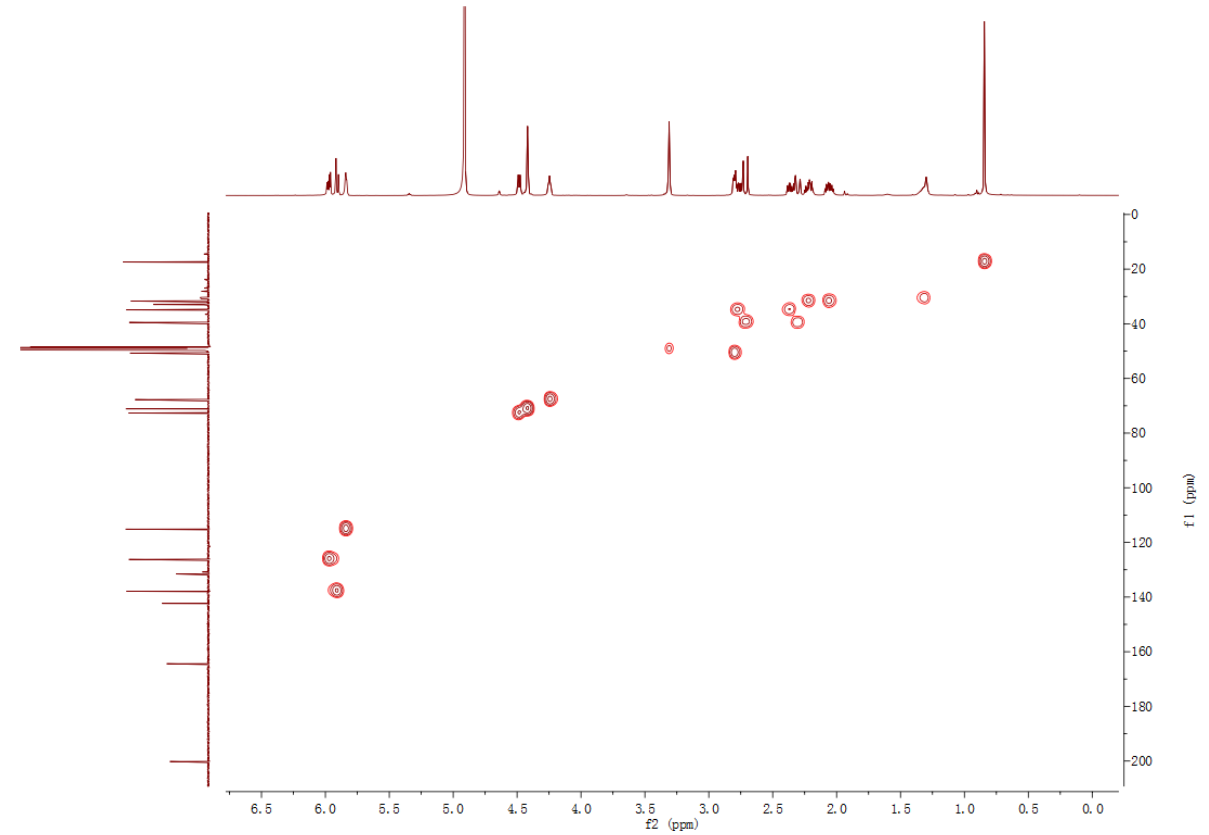


Figure S24. The HSQC spectrum of compound **3** in CD_3OD

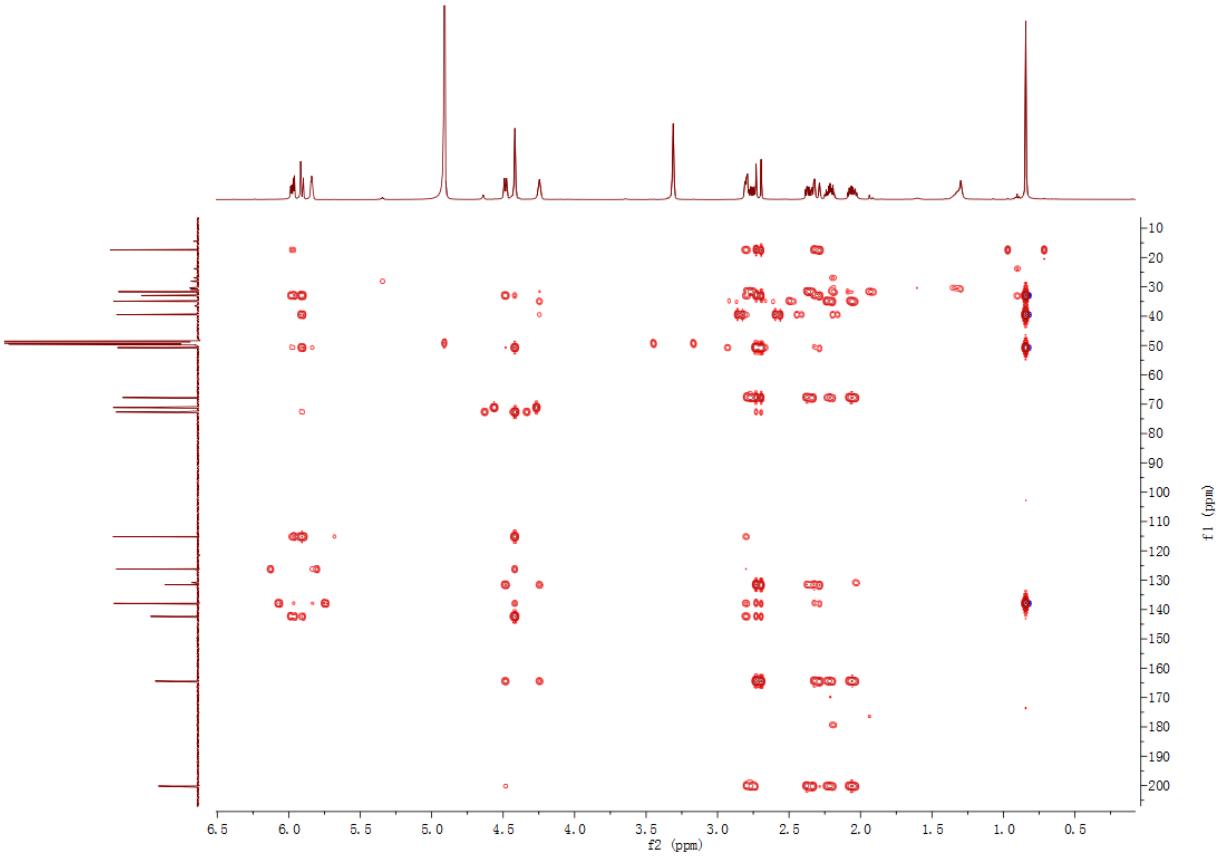


Figure S25. The HMBC spectrum of compound **3** in CD_3OD

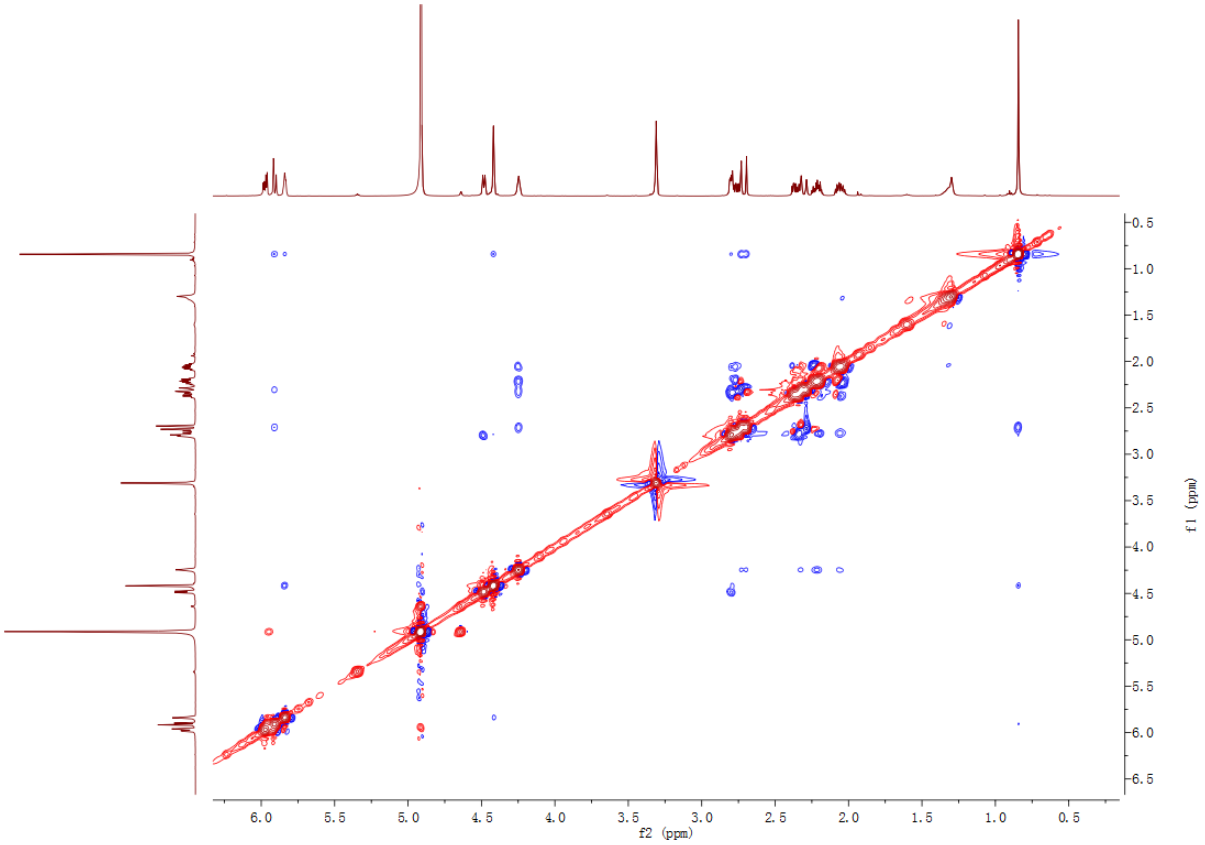


Figure S26. The ROESY spectrum of compound **3** in CD_3OD

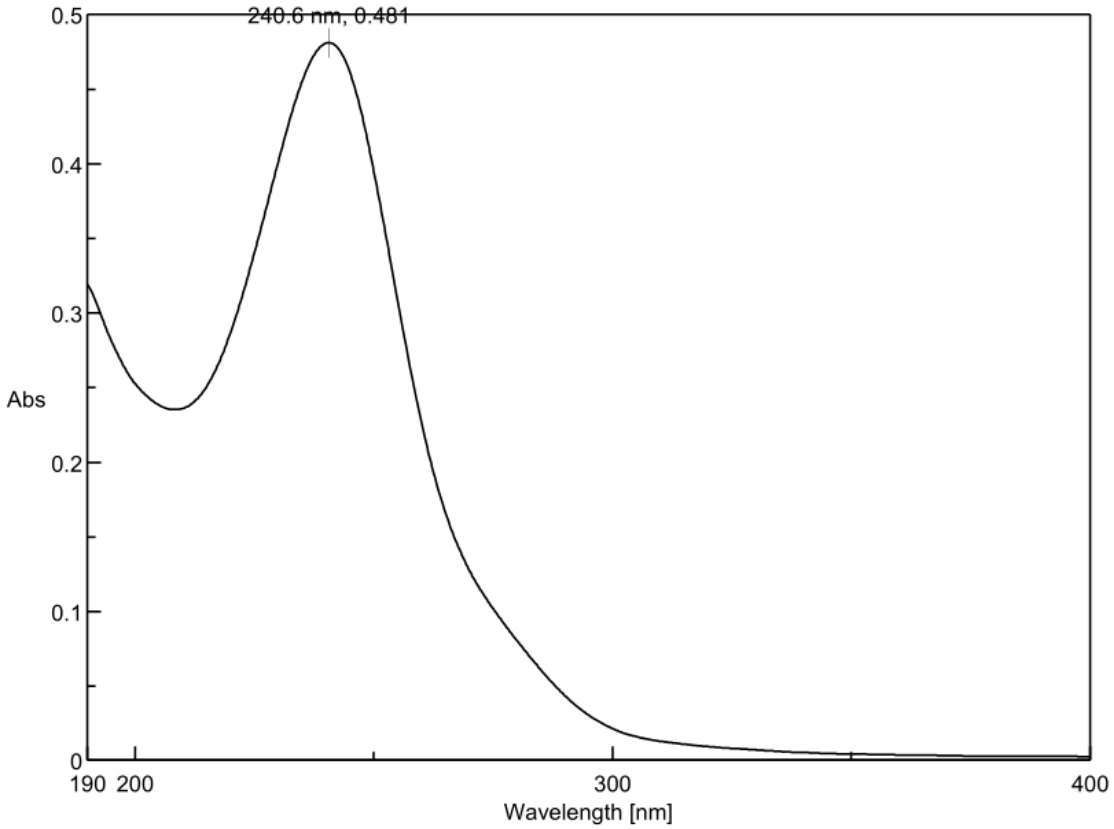


Figure S27. The UV spectrum of compound **3** in H_2O

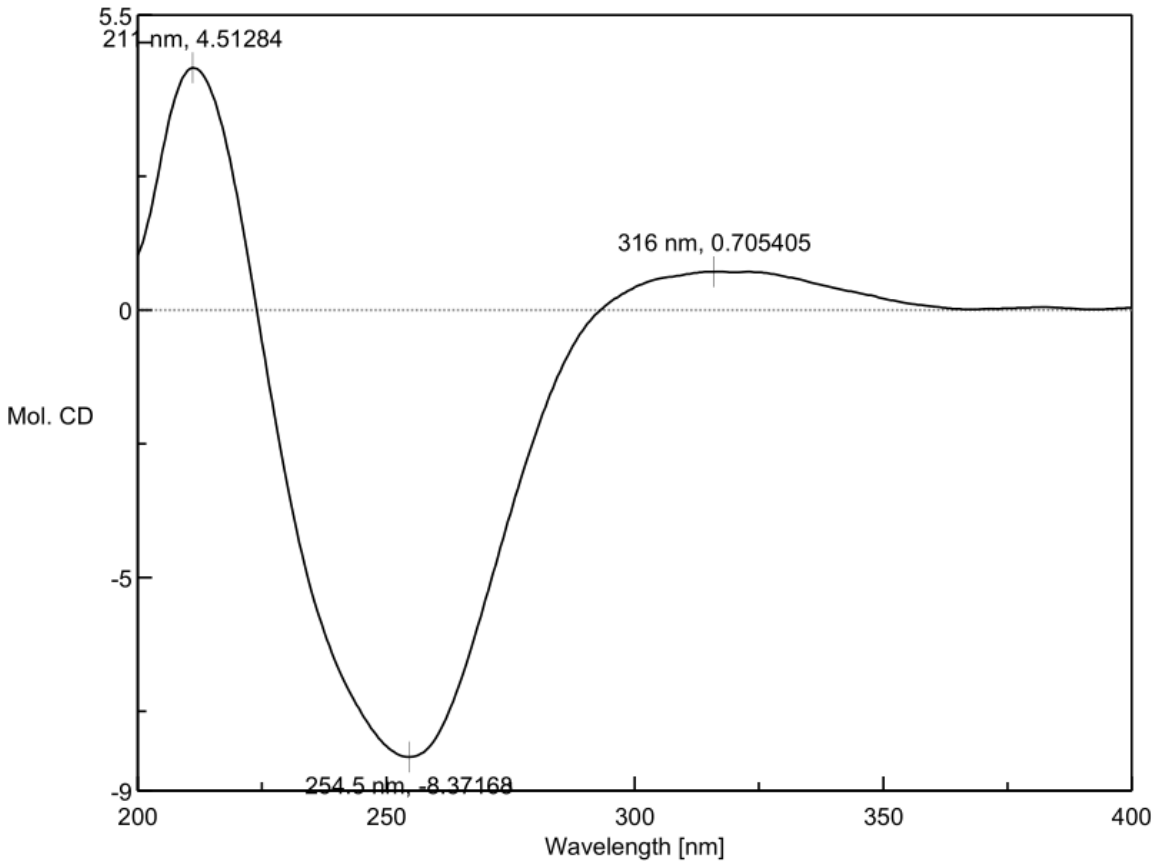


Figure S28. The ECD spectrum of compound **3** in MeOH

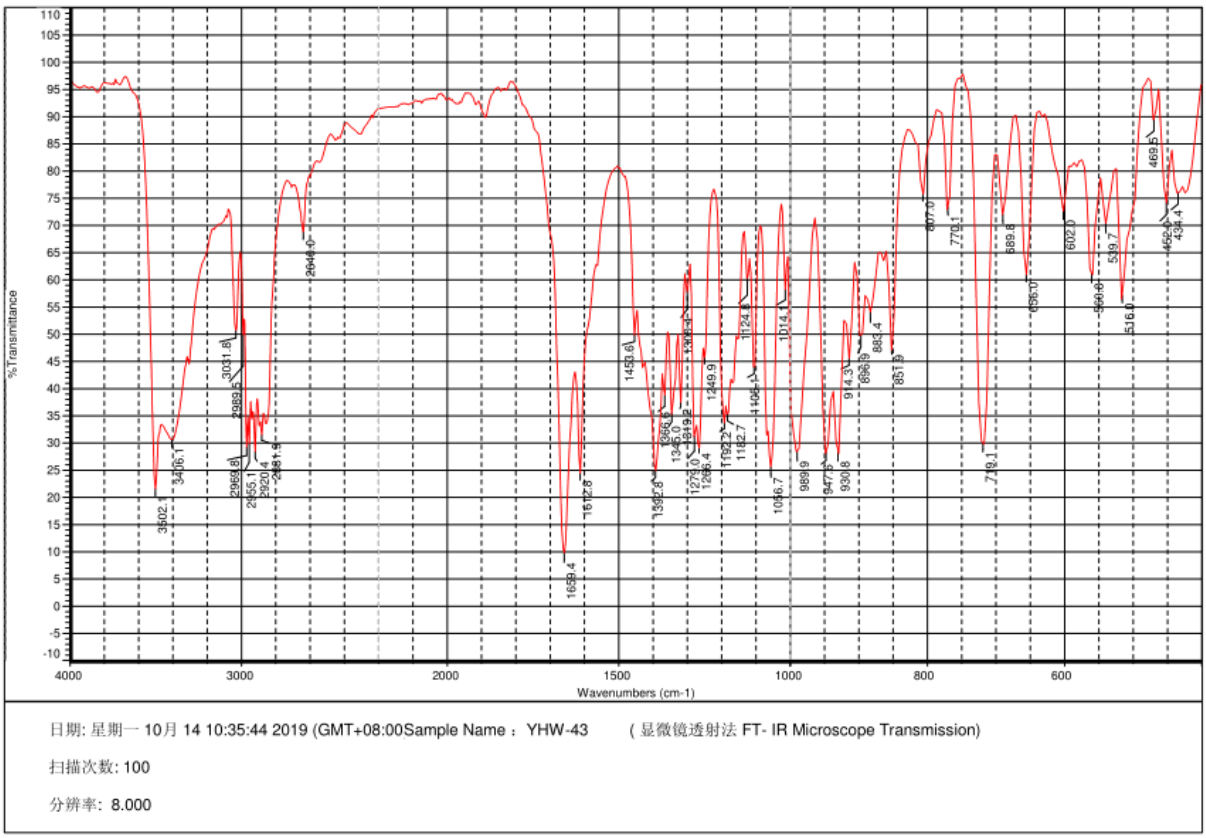
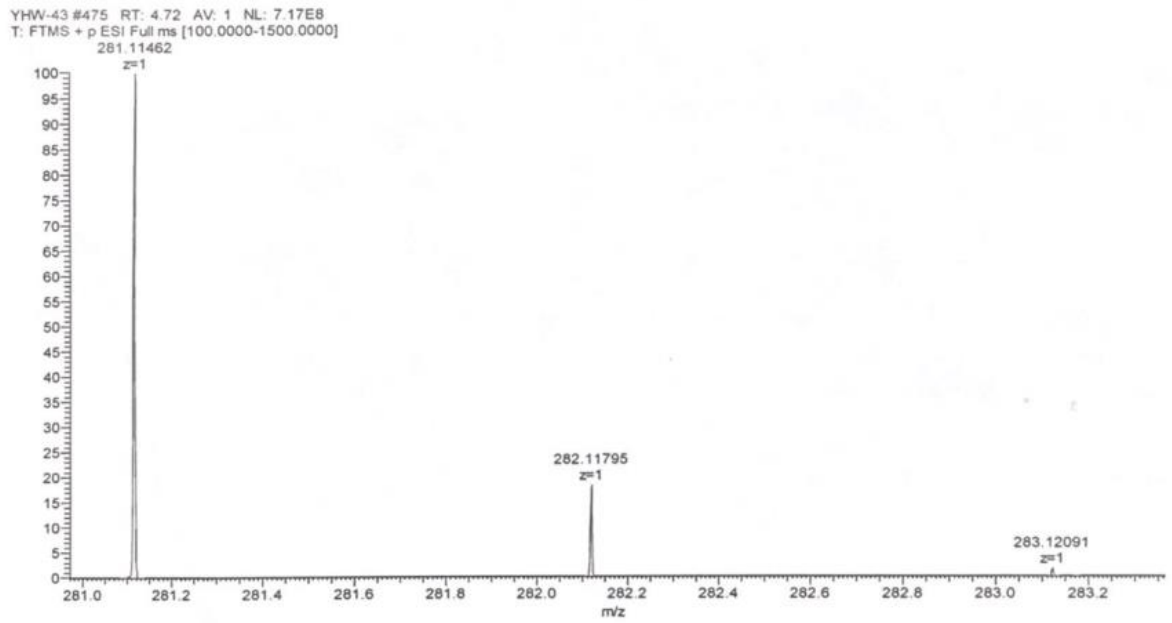


Figure S29. The IR spectrum of compound **3**



m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition	
281.11462	281.11482	-0.7	7.5	C16 H18 O3 Na	M+Na

Figure S30. The HR-ESI-MS data of compound **3**

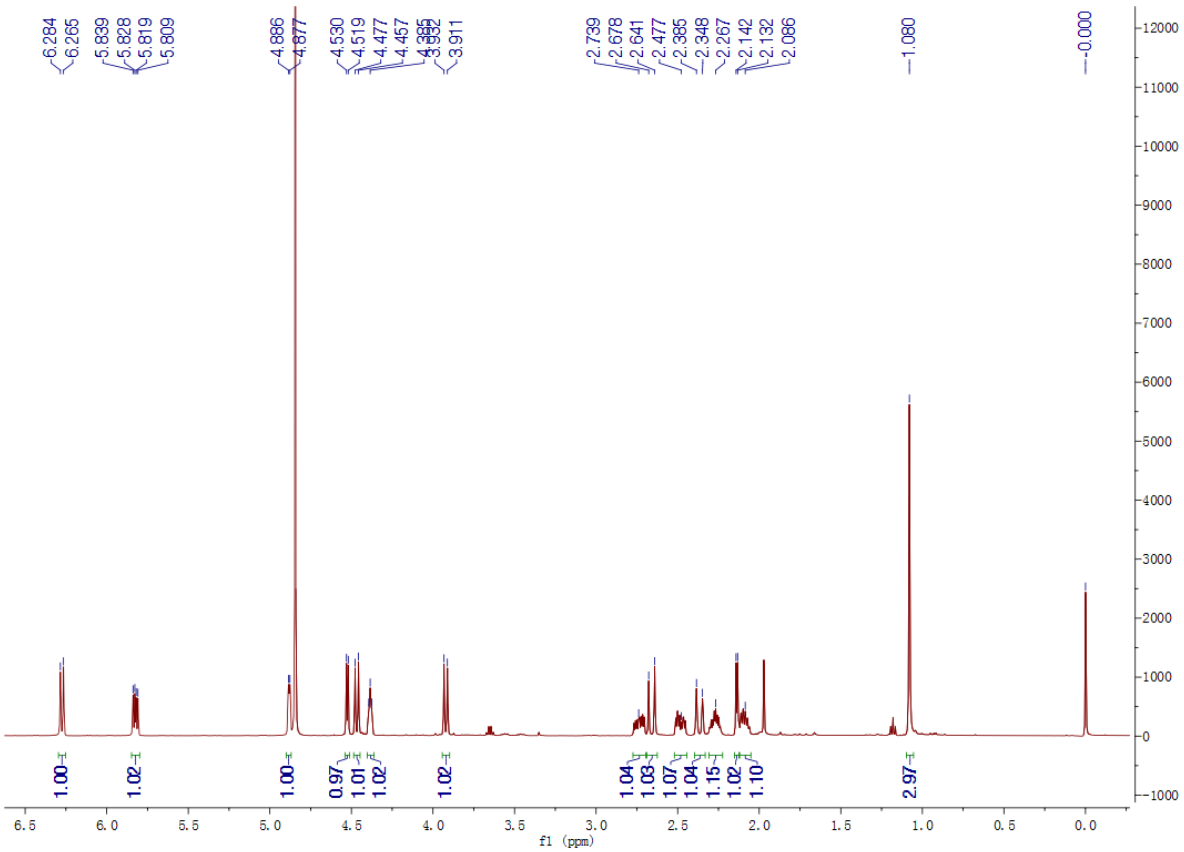


Figure S31. The ^{1}H NMR spectrum of compound **4** in D_2O

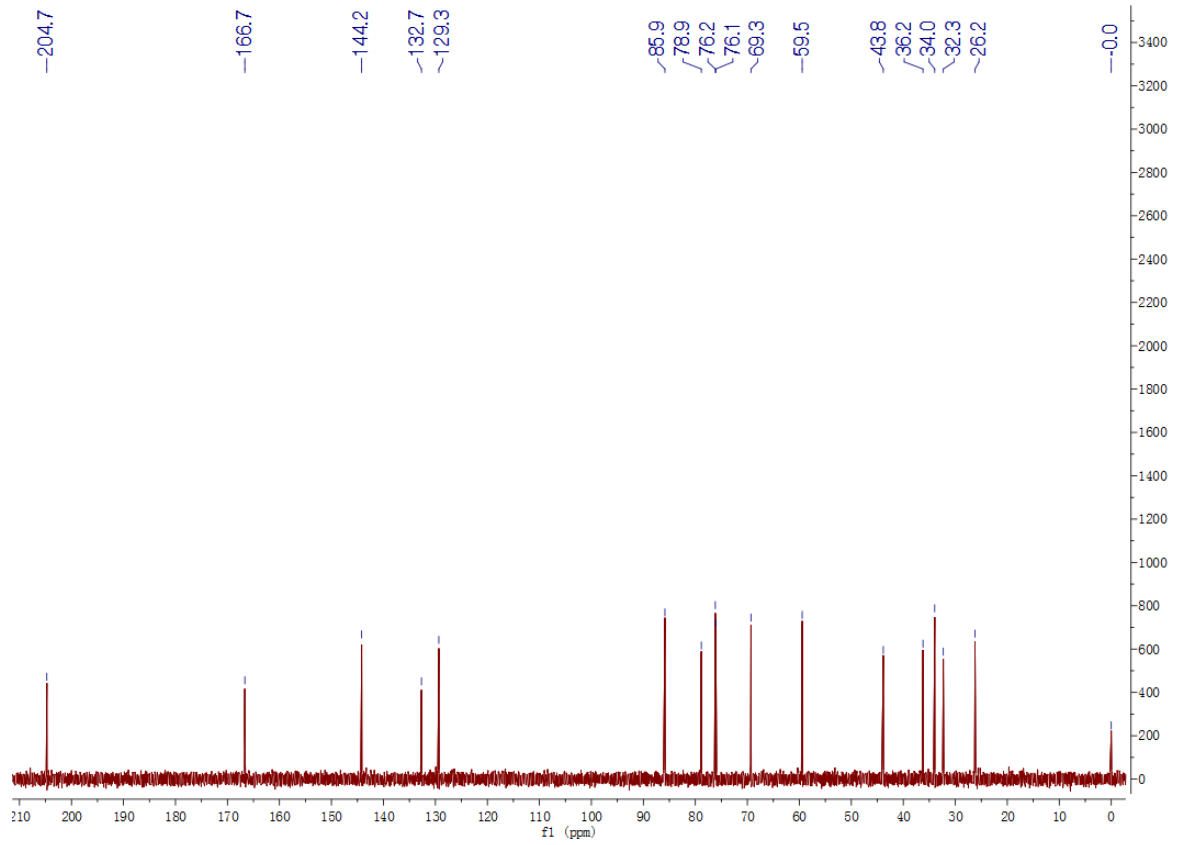


Figure S32. The ^{13}C NMR spectrum of compound **4** in D_2O

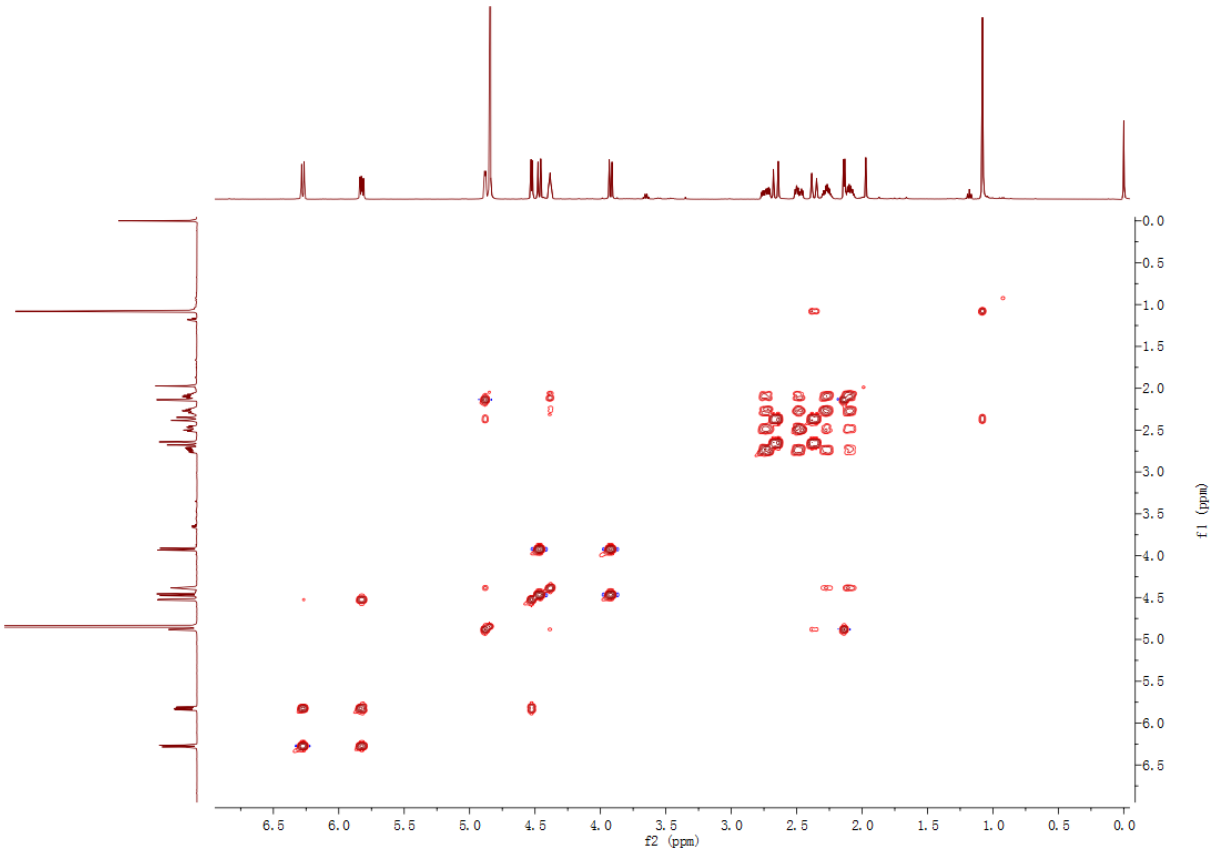


Figure S33. The ^{1}H-^{1}H COSY spectrum of compound **4** in D_2O

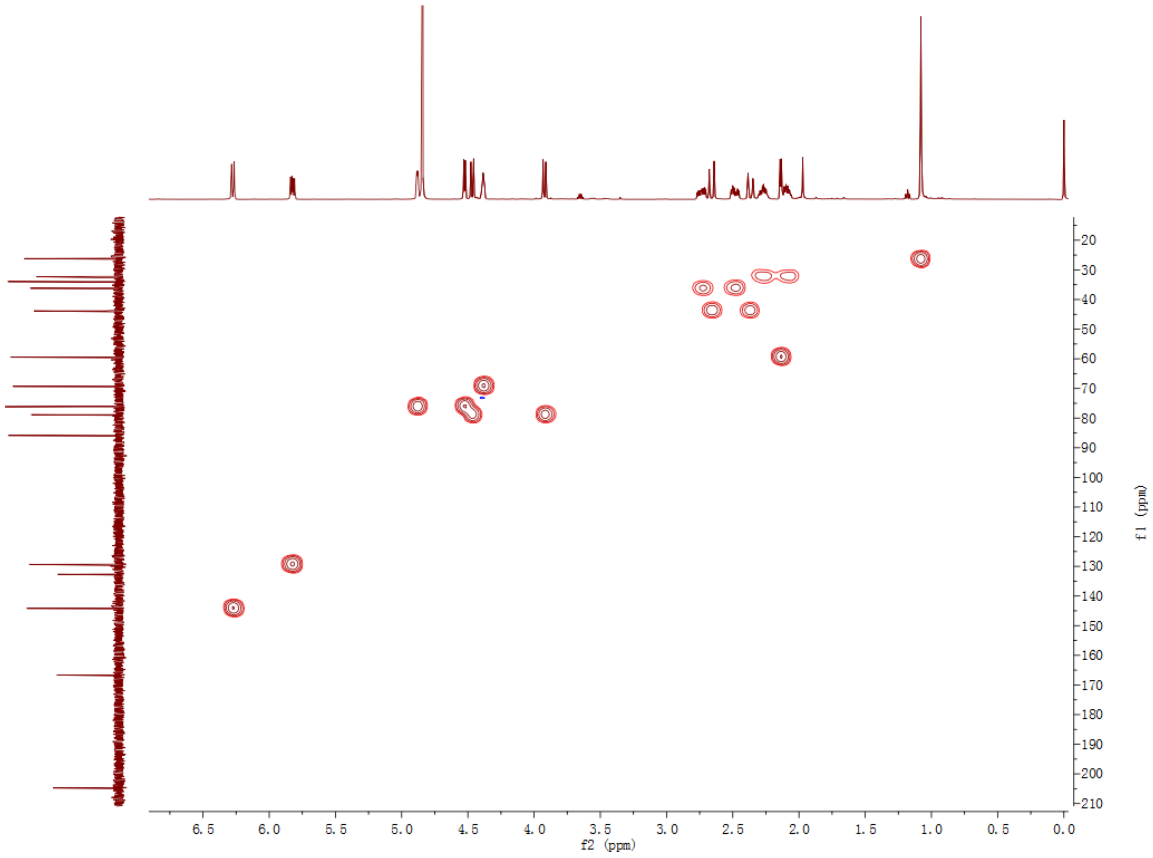


Figure S34. The HSQC spectrum of compound **4** in D_2O

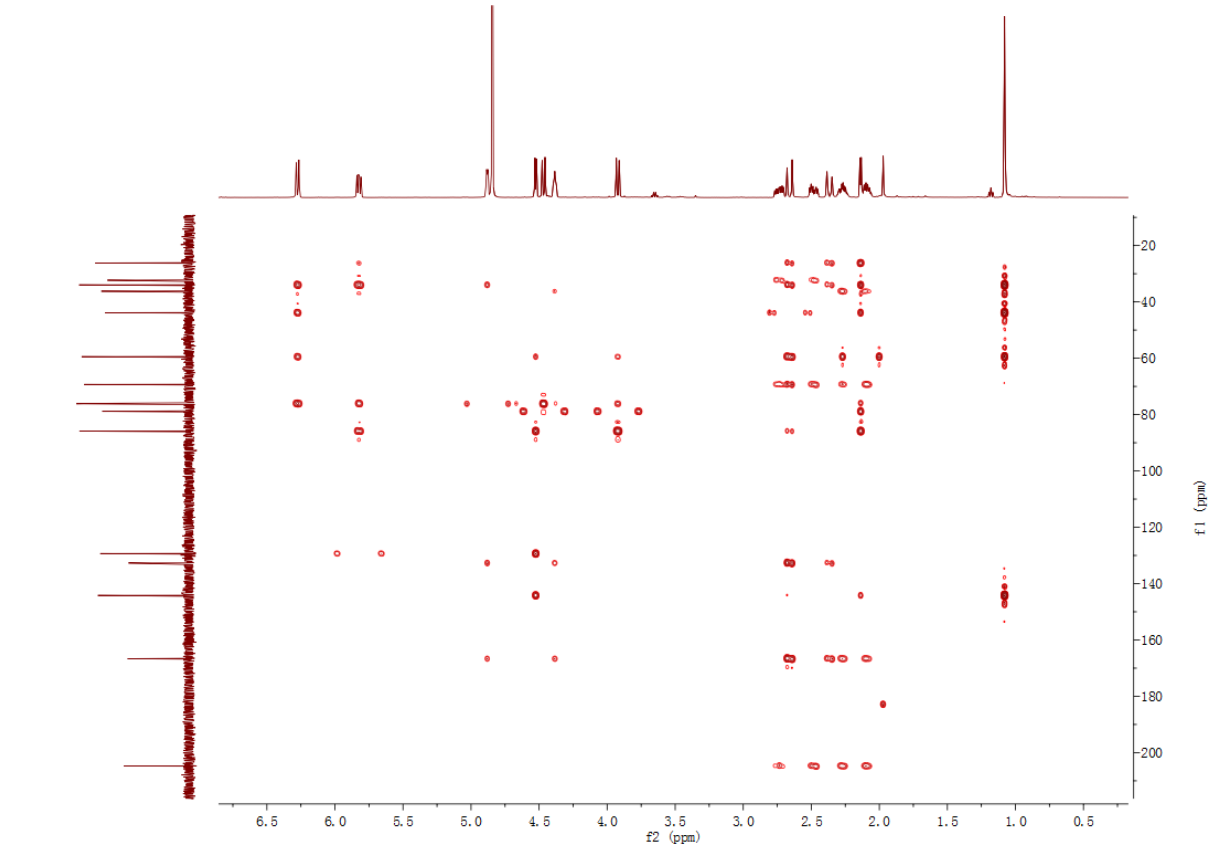


Figure S35. The HMBC spectrum of compound **4** in D_2O

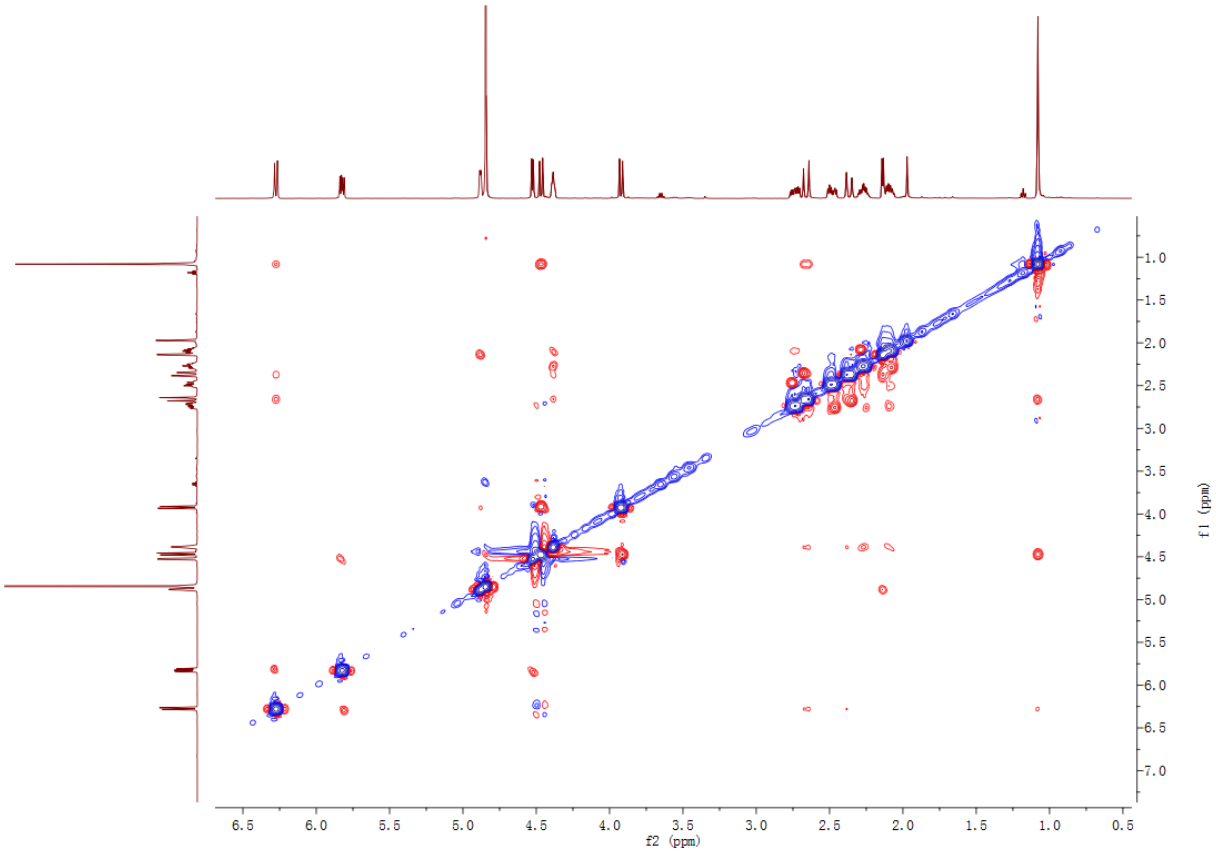


Figure S36. The ROESY spectrum of compound **4** in D_2O

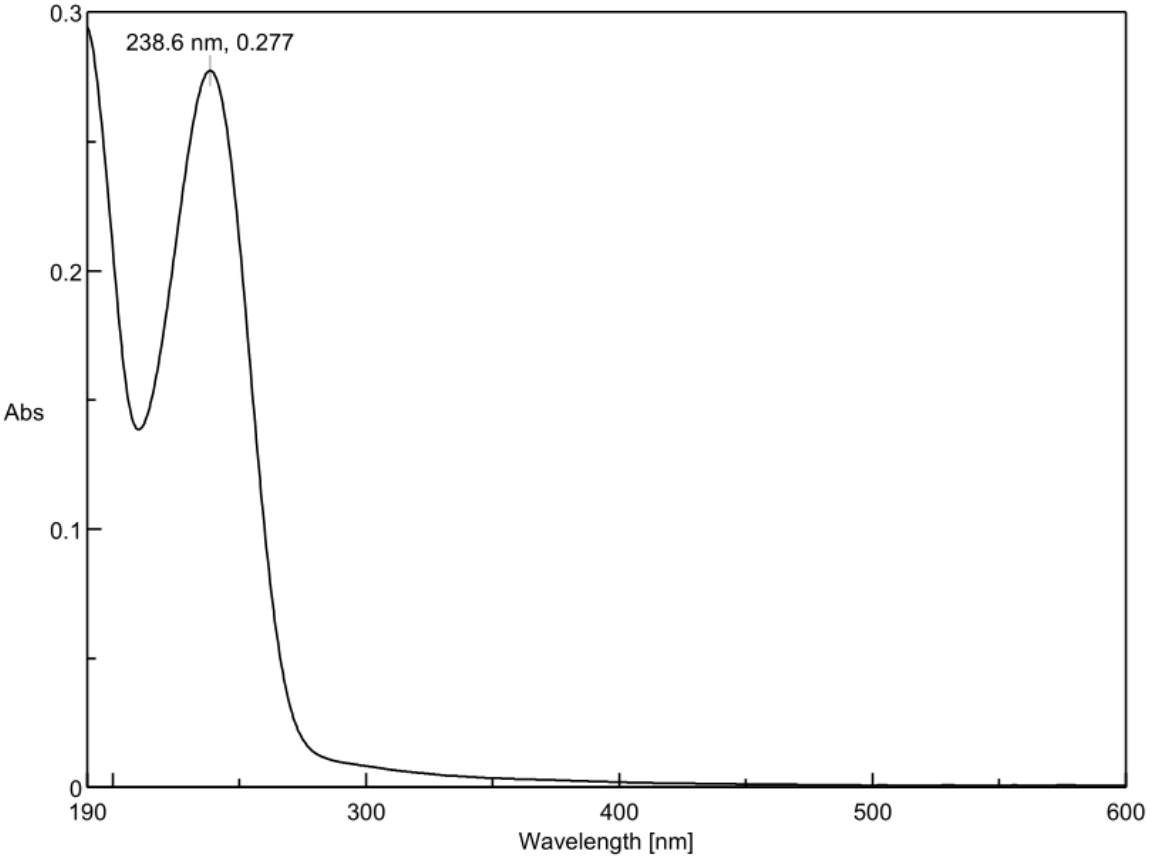


Figure S37. The UV spectrum of compound **4** in H_2O

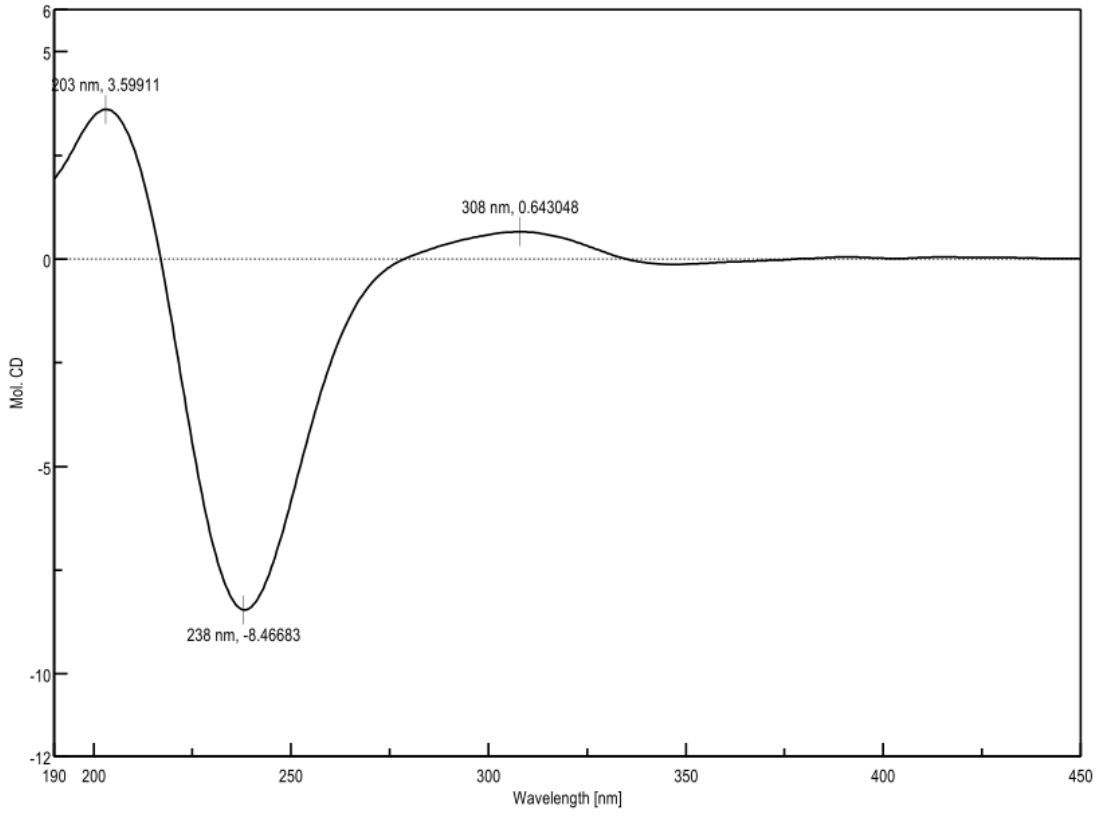


Figure S38. The ECD spectrum of compound **4** in H_2O

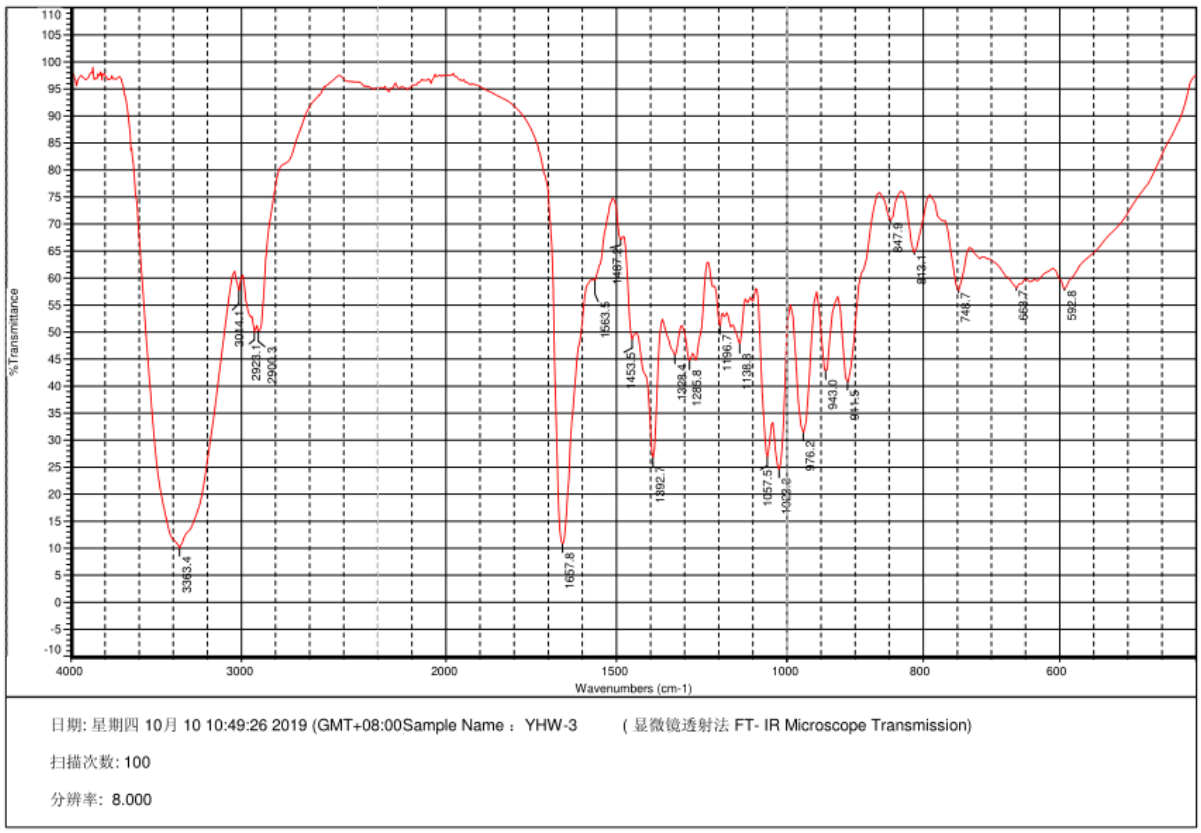
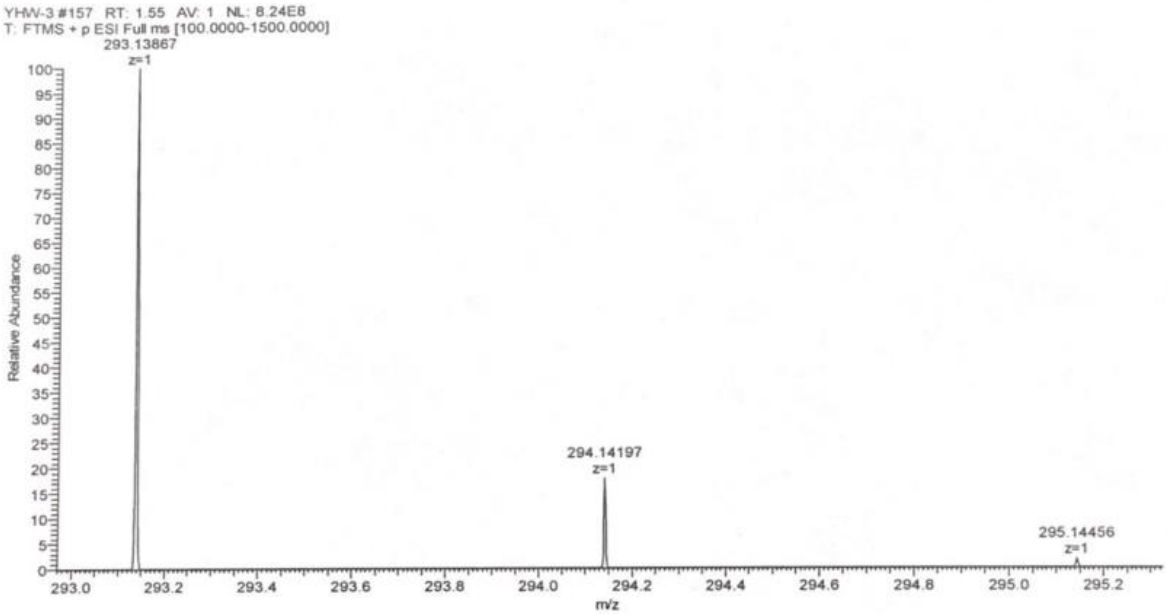


Figure S39. The IR spectrum of compound **4**



m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition	
293.13867	293.13835	1.09	6.5	C16 H21 O5	M+H

Figure S40. The HR-ESI-MS data of compound **4**

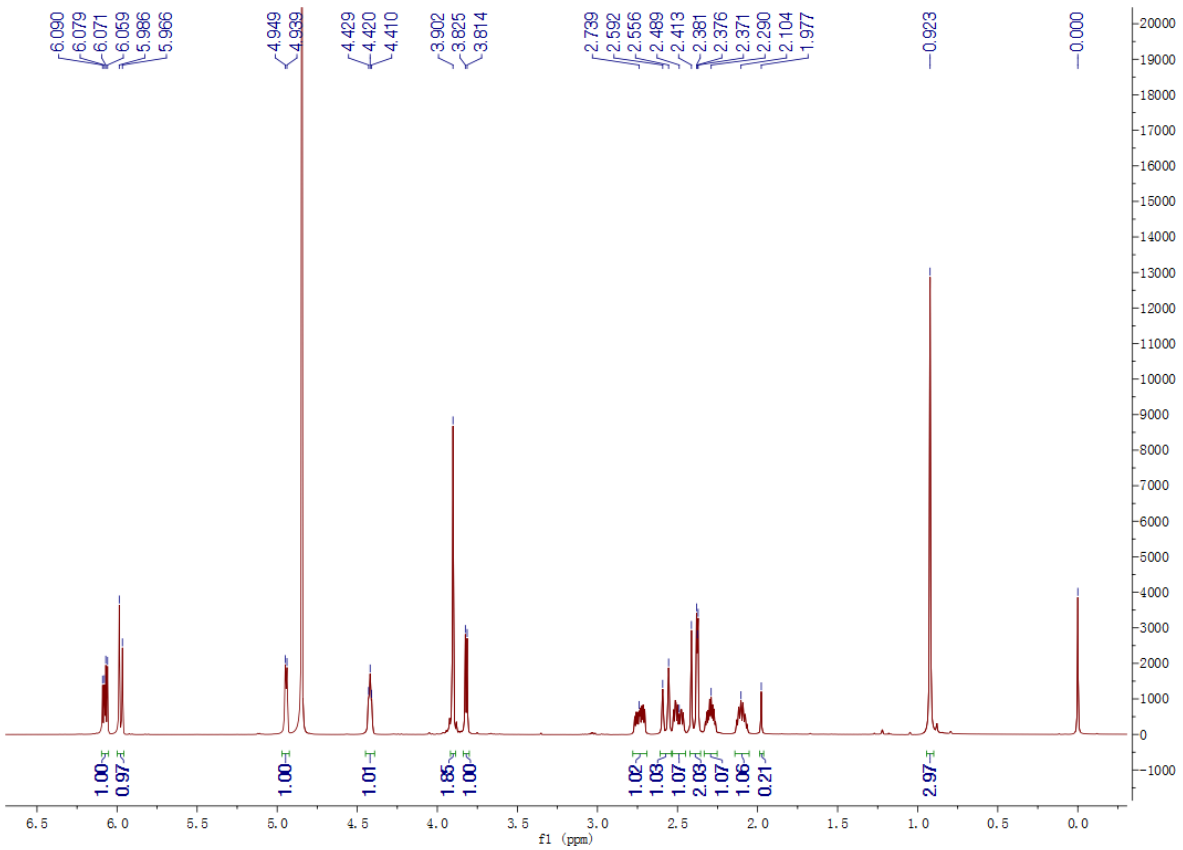


Figure S41. The ^{1}H NMR spectrum of compound **5** in D_2O

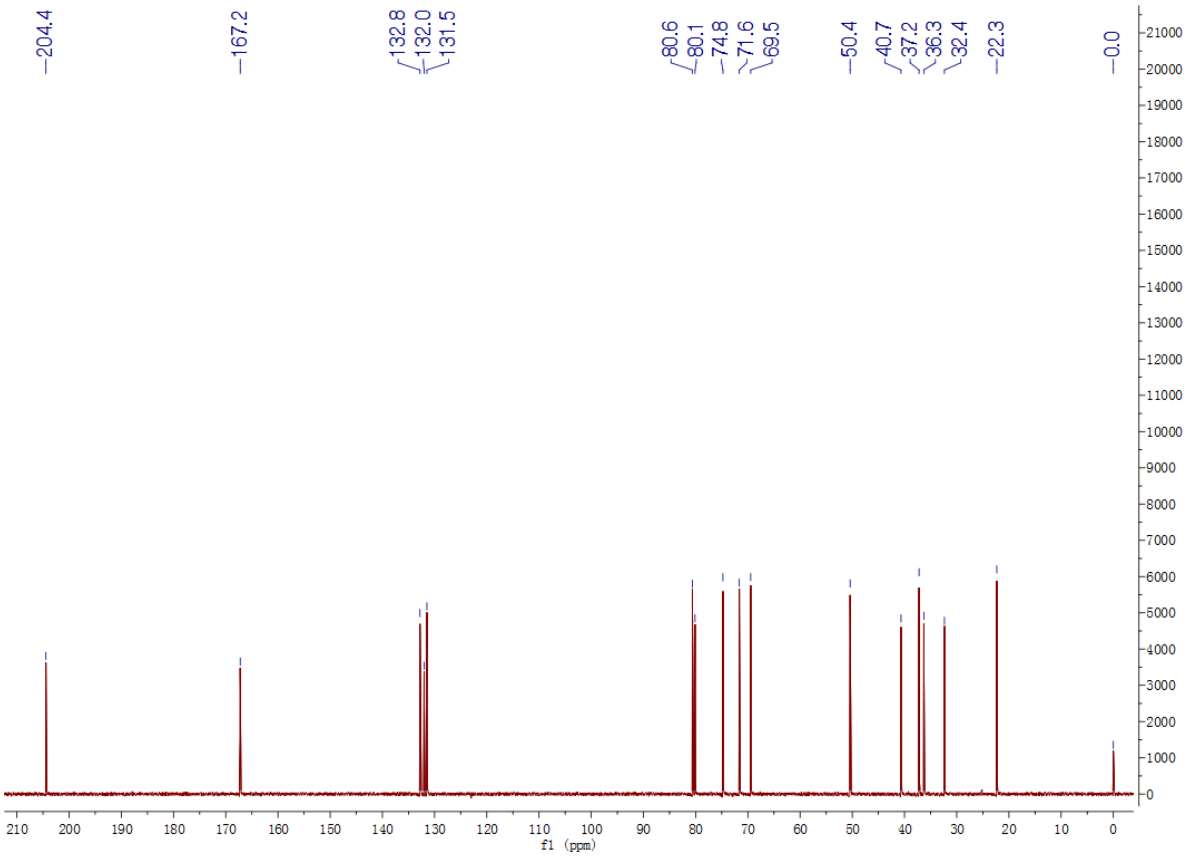


Figure S42. The ^{13}C NMR spectrum of compound **5** in D_2O

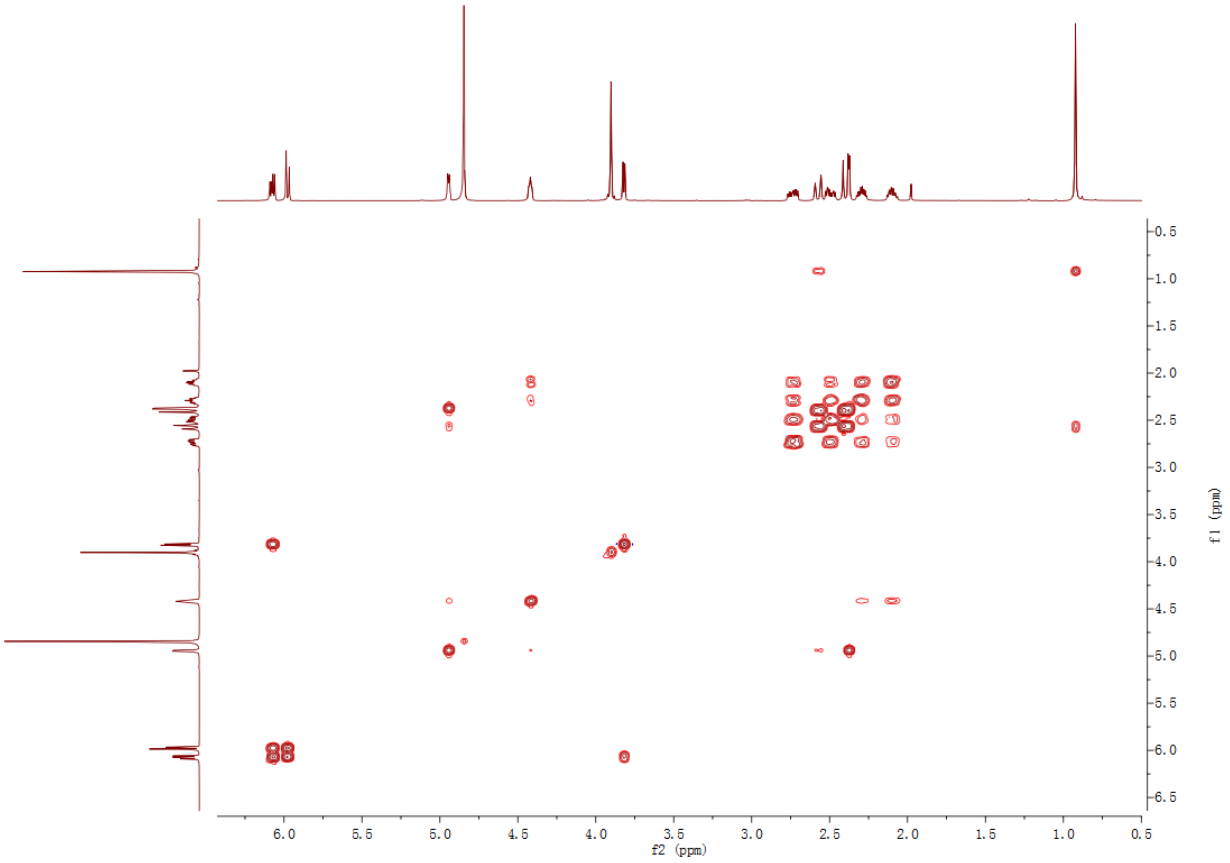


Figure S43. The ^{1}H-^{1}H COSY spectrum of compound **5** in D_2O

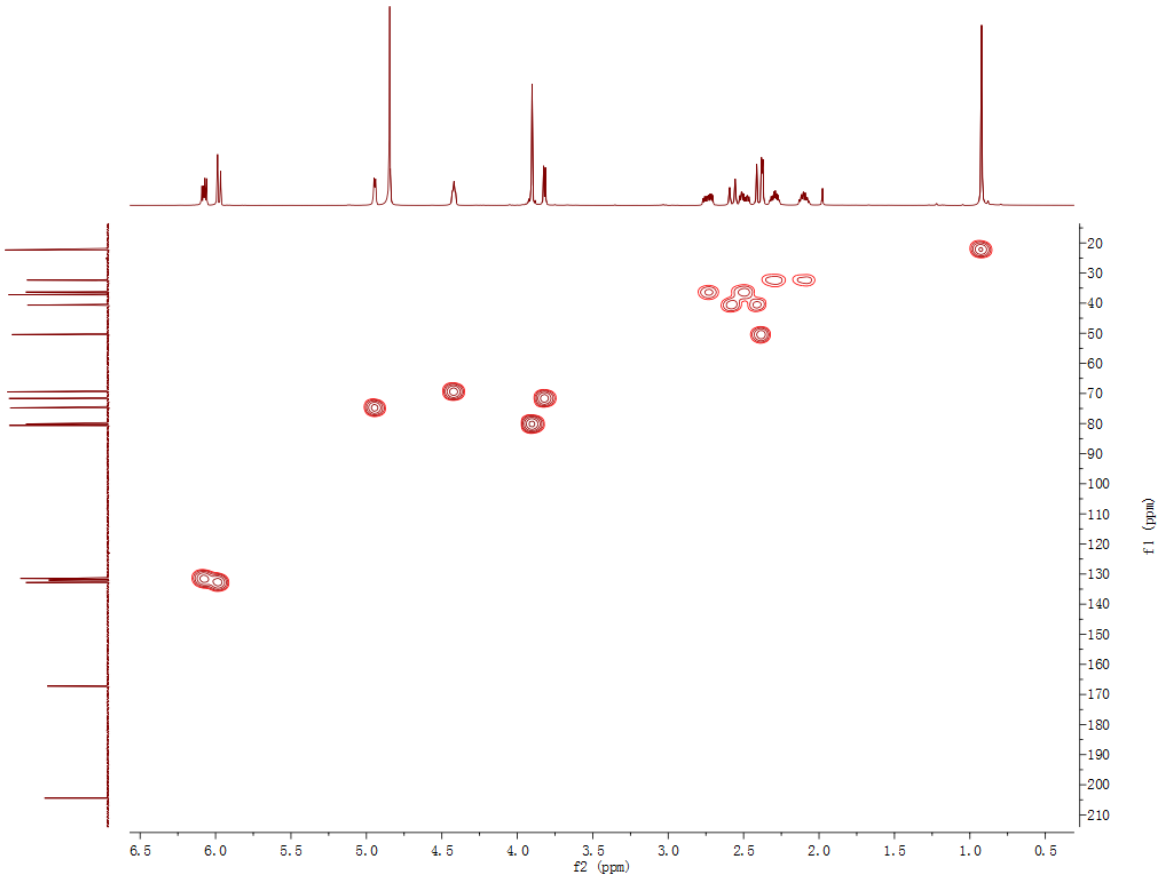


Figure S44. The HSQC spectrum of compound **5** in D_2O

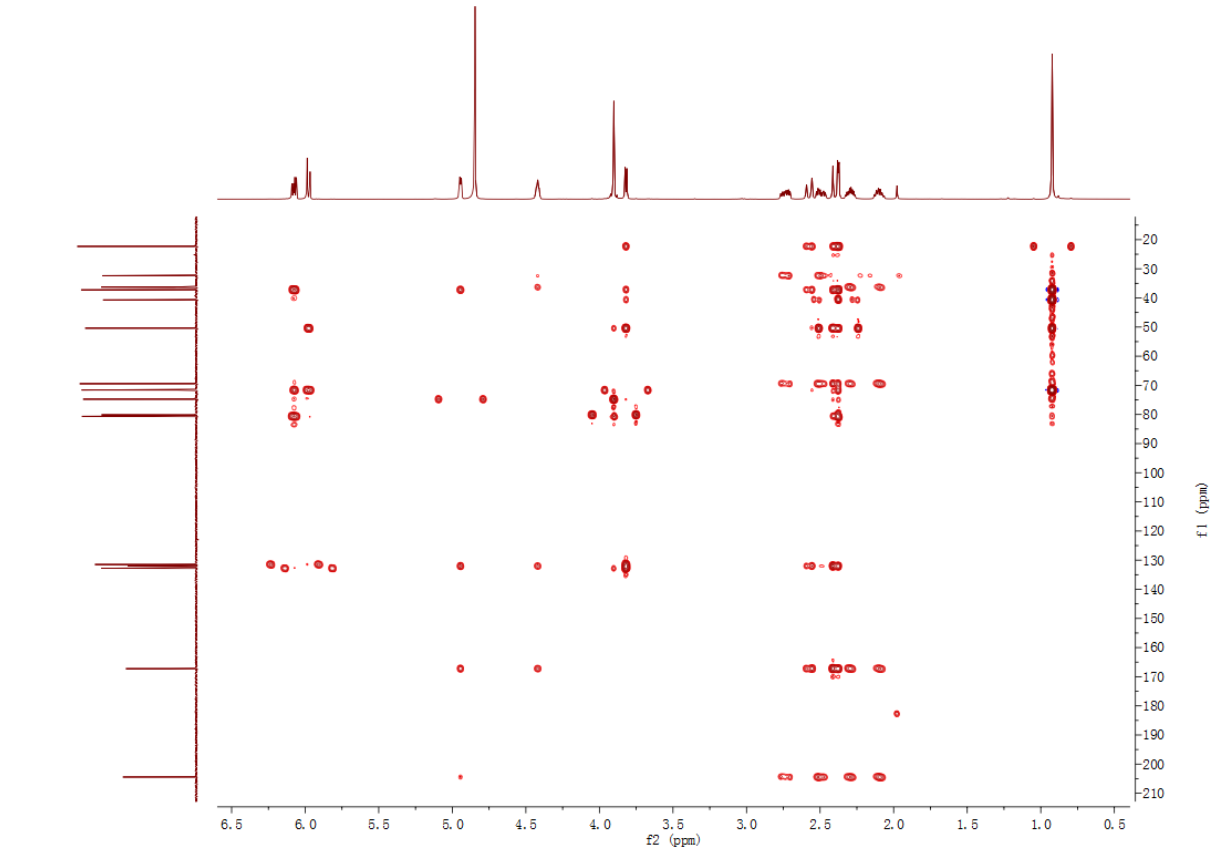


Figure S45. The HMBC spectrum of compound **5** in D_2O

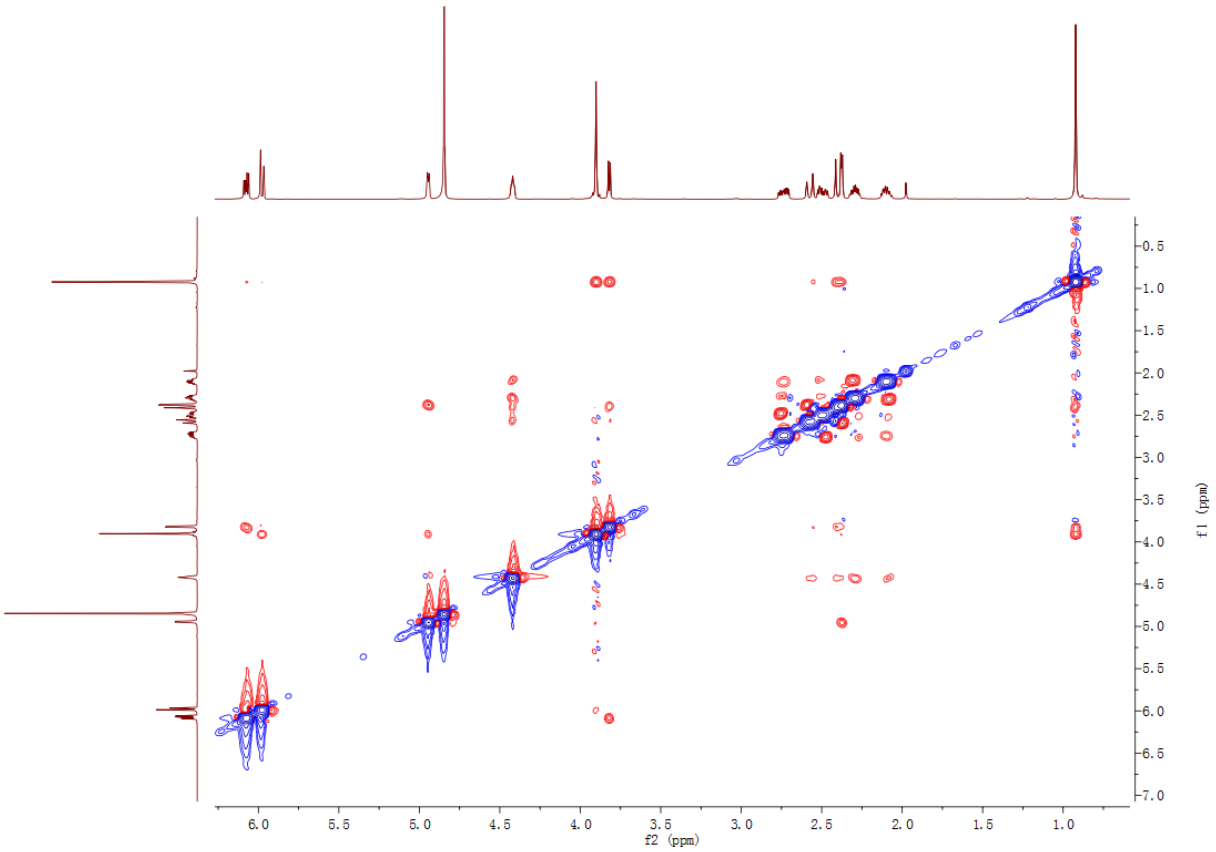


Figure S46. The ROESY spectrum of compound **5** in D_2O

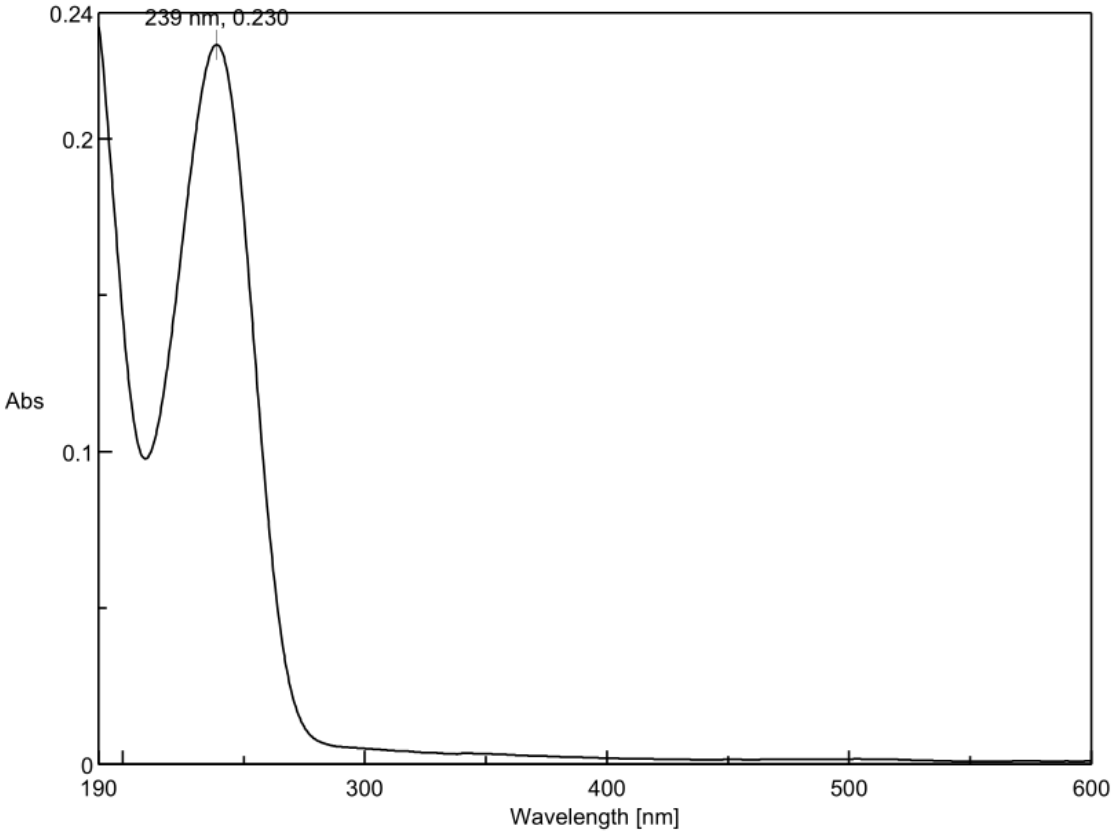


Figure S47. The UV spectrum of compound **5** in H_2O

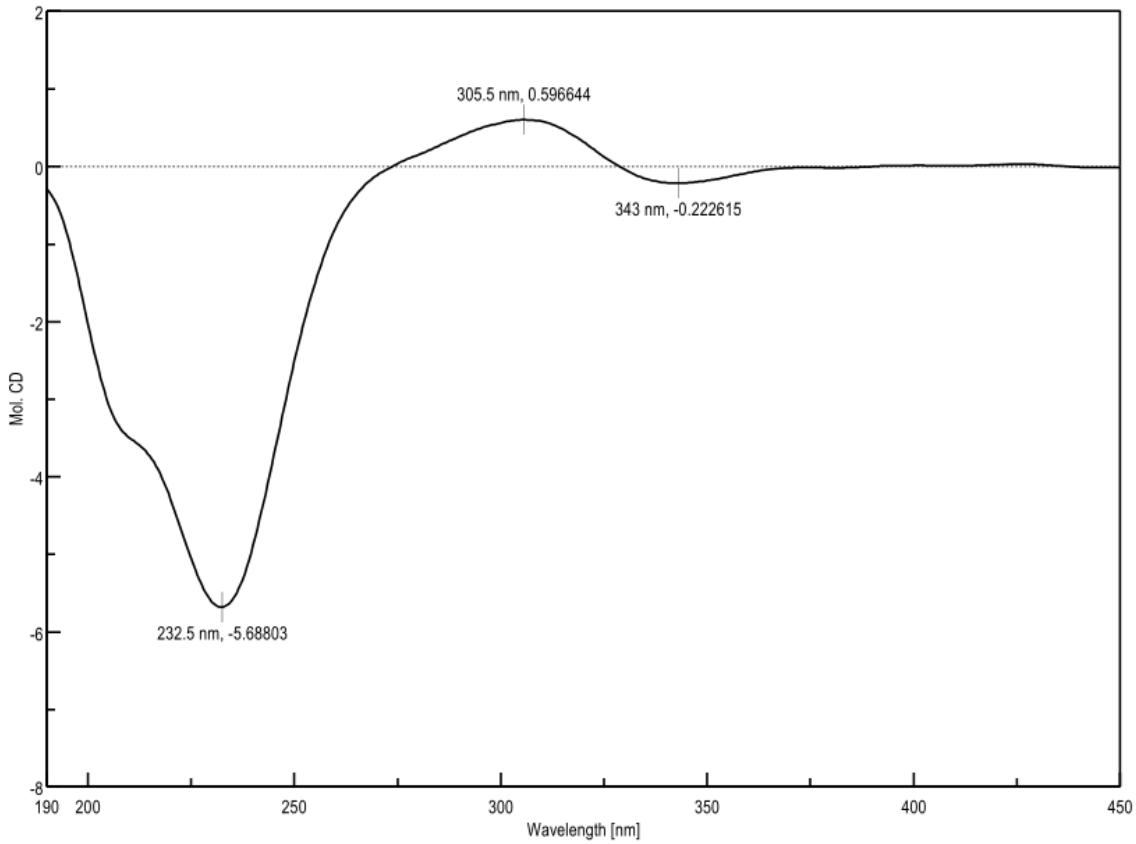


Figure S48. The ECD spectrum of compound **5** in H_2O

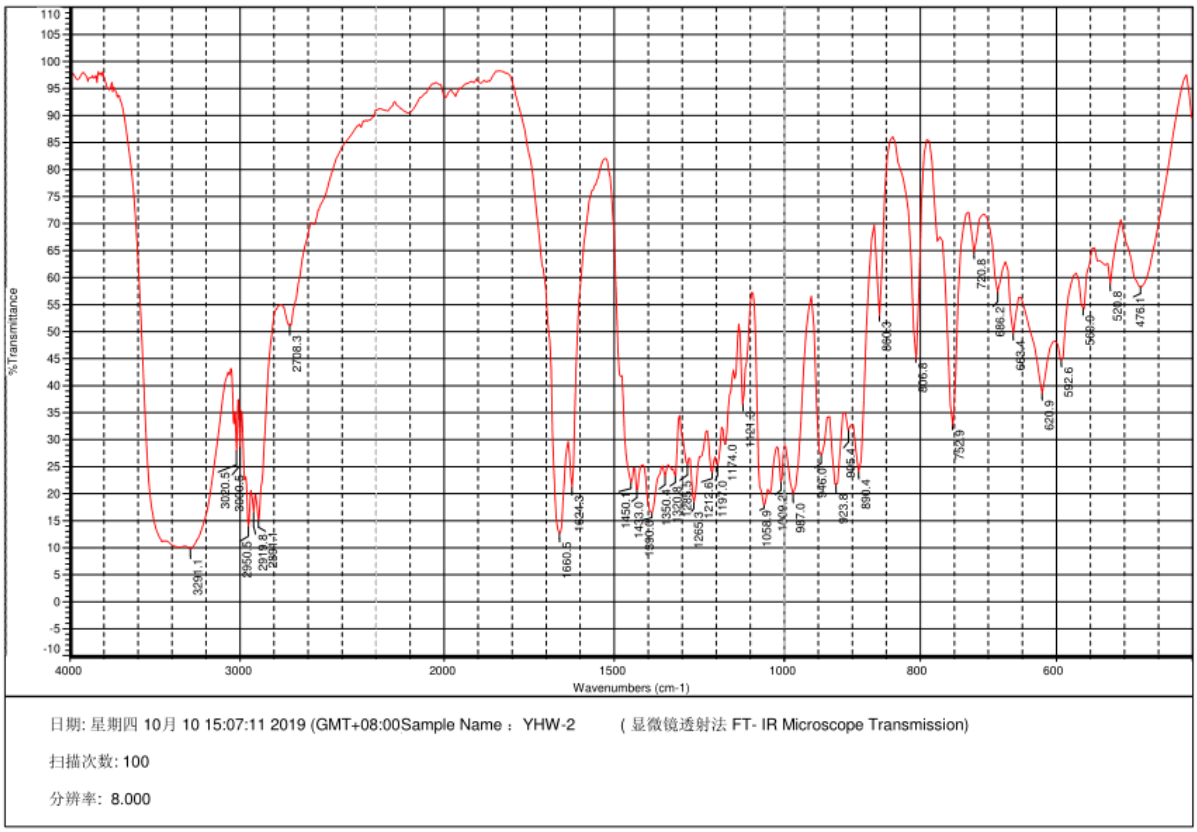
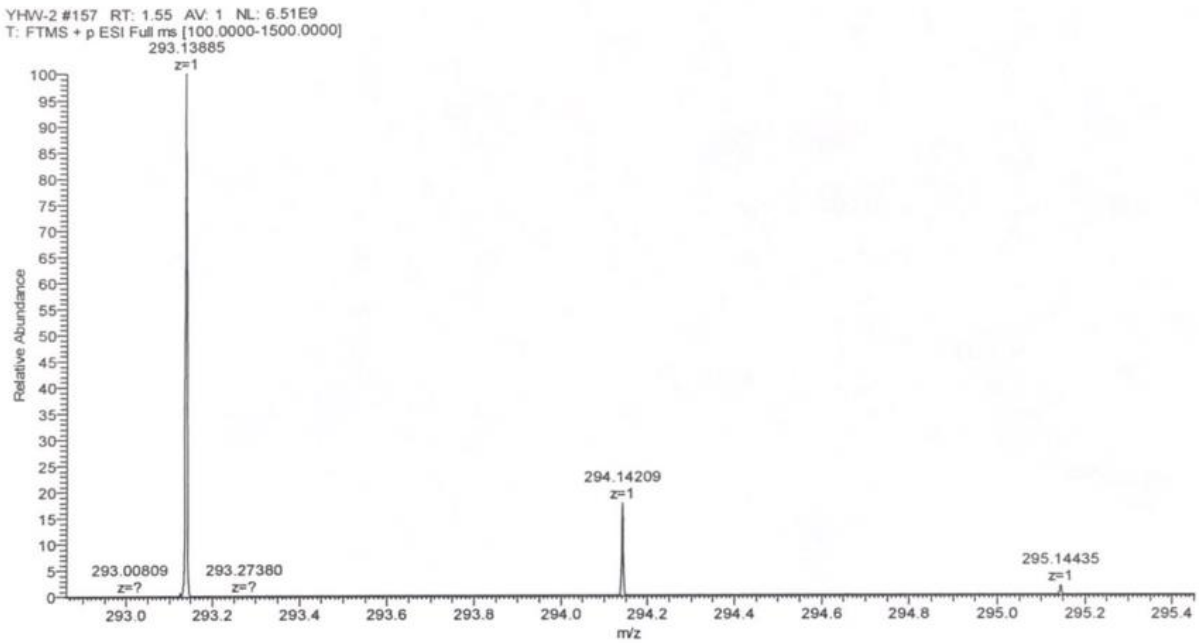


Figure S49. The IR spectrum of compound **5**



m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition	
293.13885	293.13835	1.7	6.5	C16 H21 O5	M+H

Figure S50. The HR-ESI-MS data of compound **5**

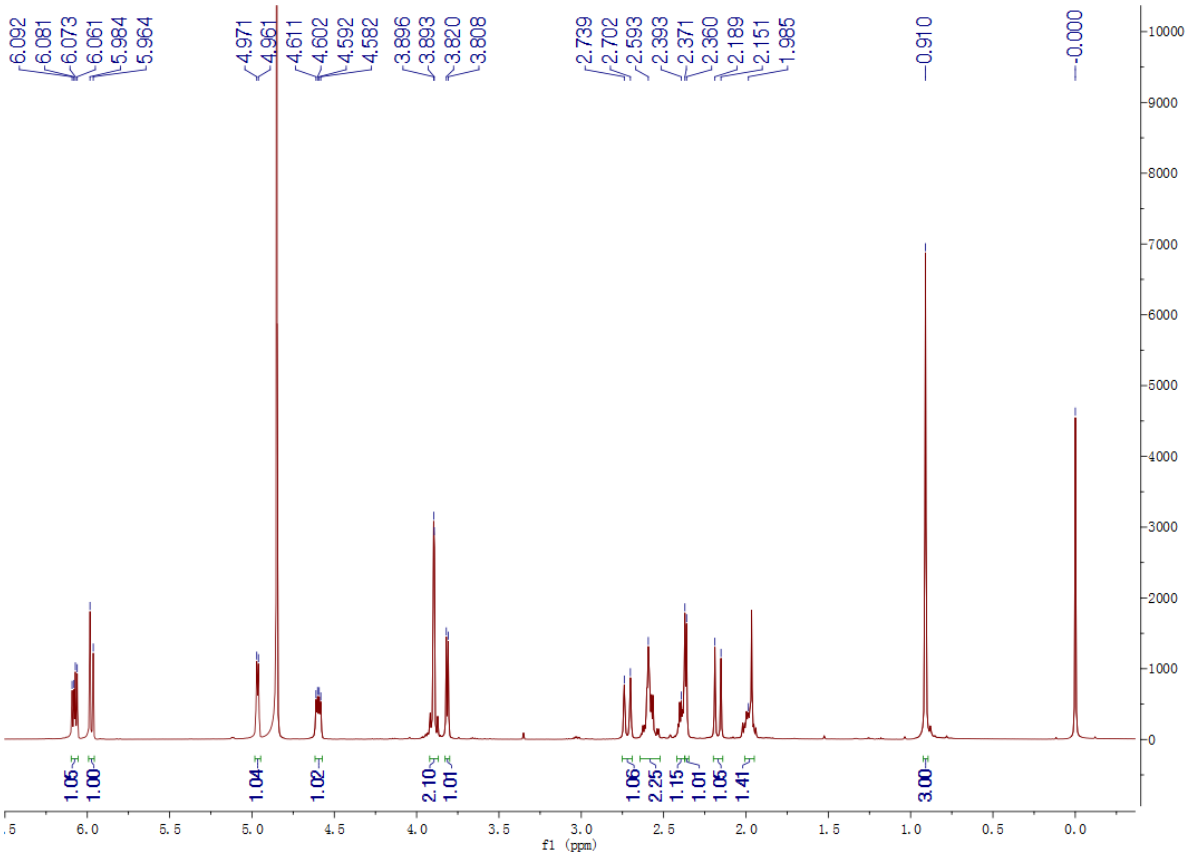


Figure S51. The ^{1}H NMR spectrum of compound **6** in D_2O

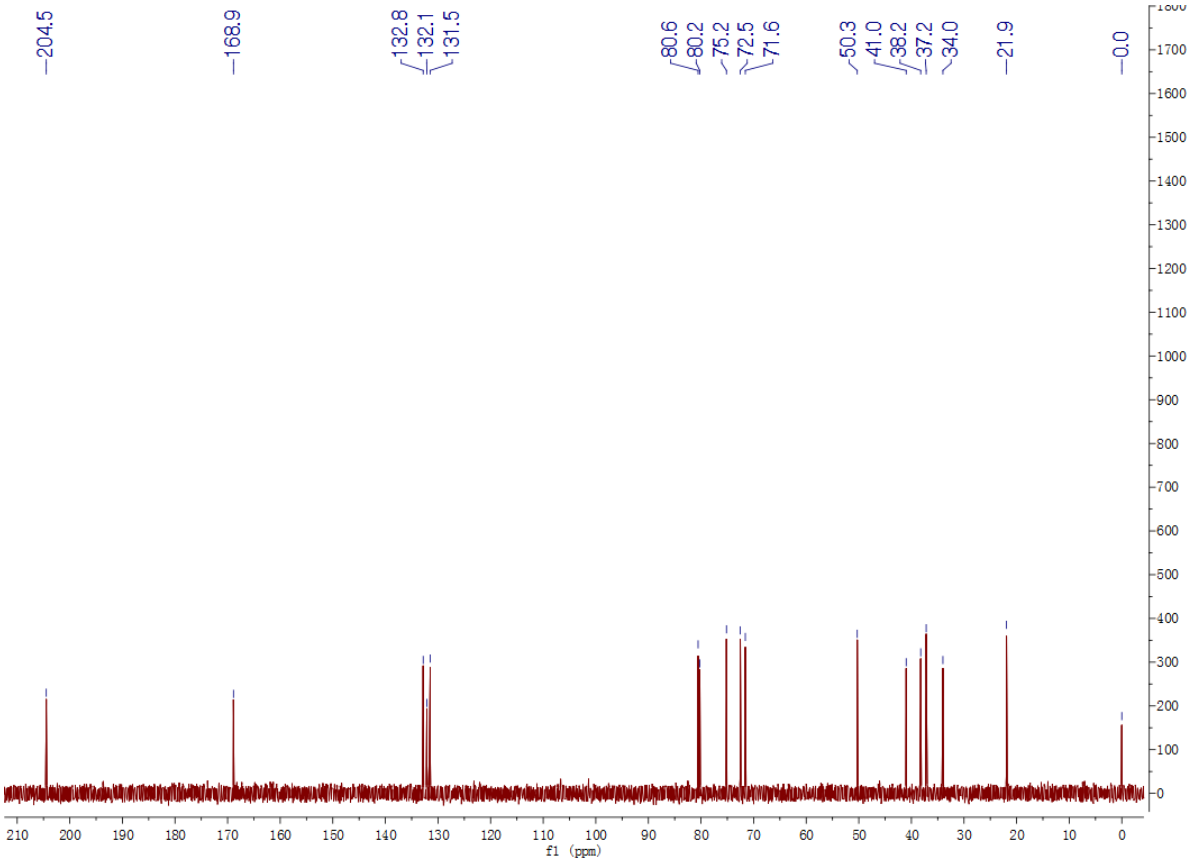


Figure S52. The ^{13}C NMR spectrum of compound **6** in D_2O

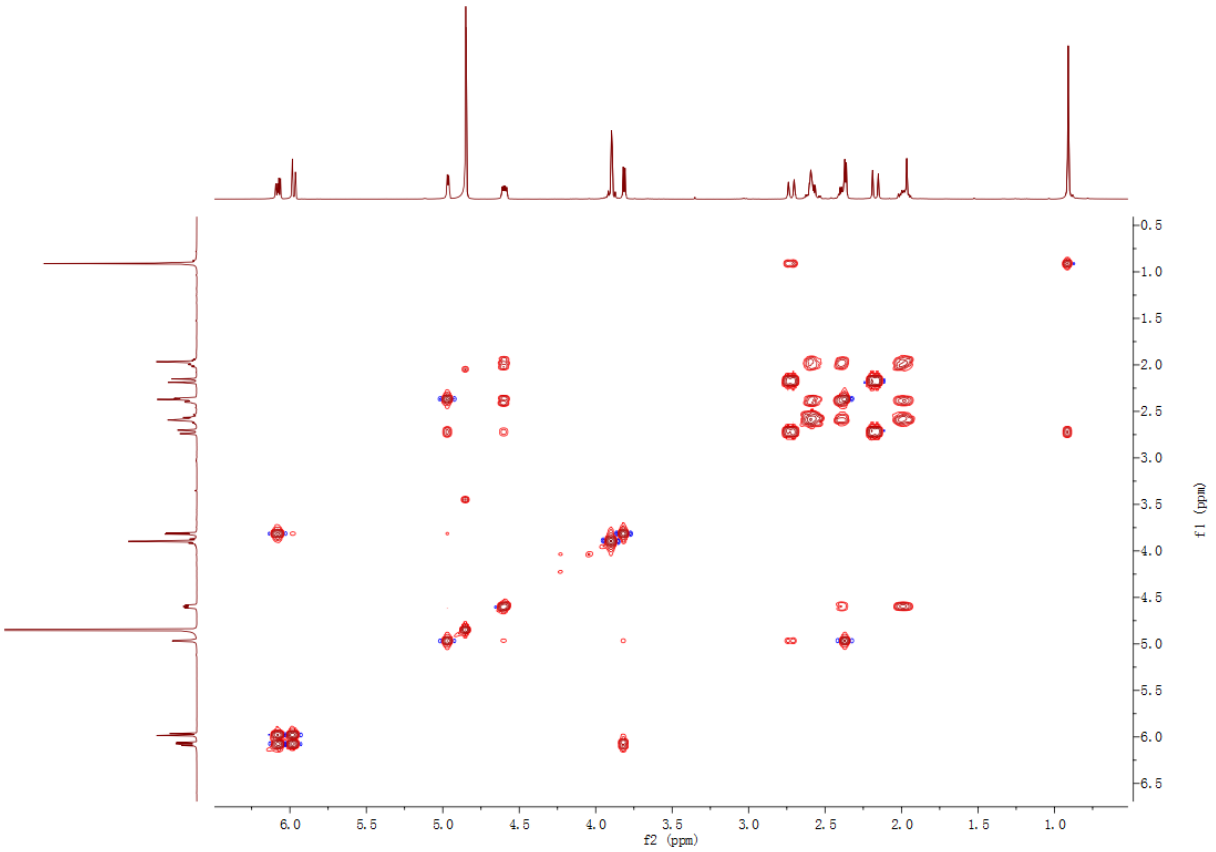


Figure S53. The ^{1}H-^{1}H COSY spectrum of compound **6** in D_2O

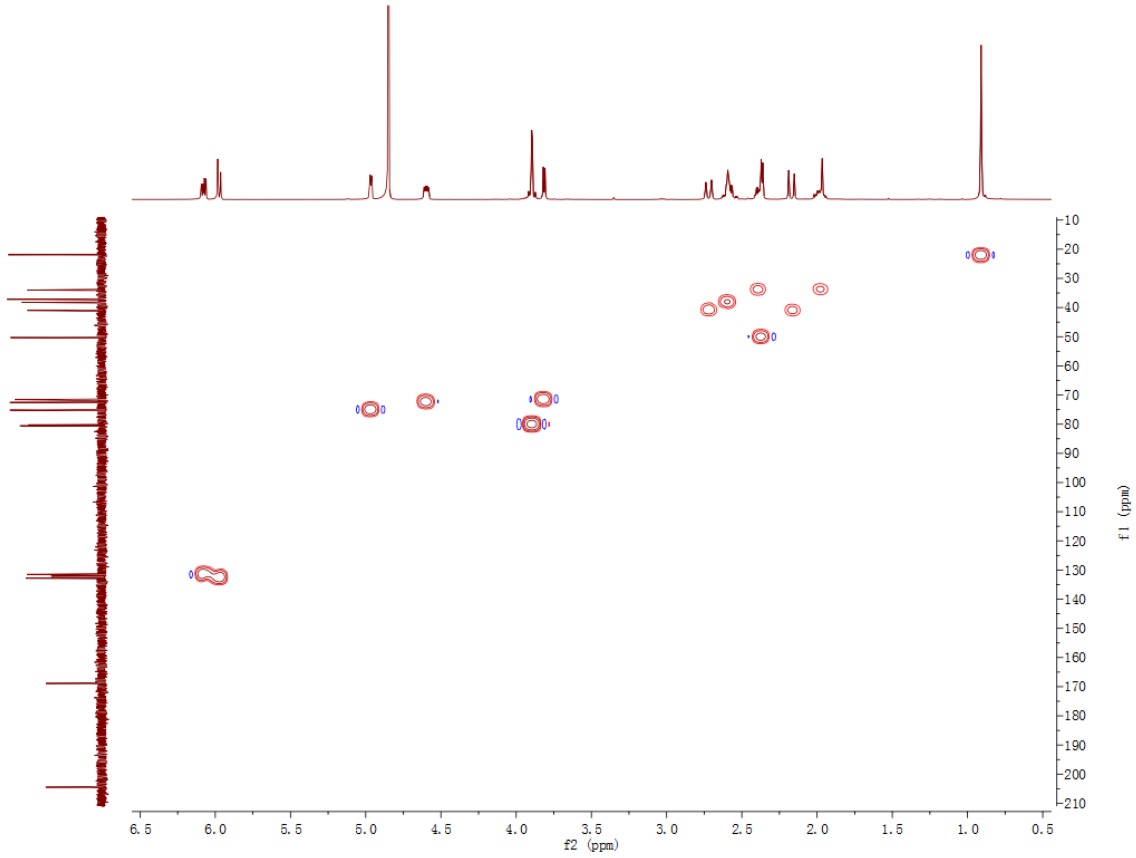


Figure S54. The HSQC spectrum of compound **6** in D_2O

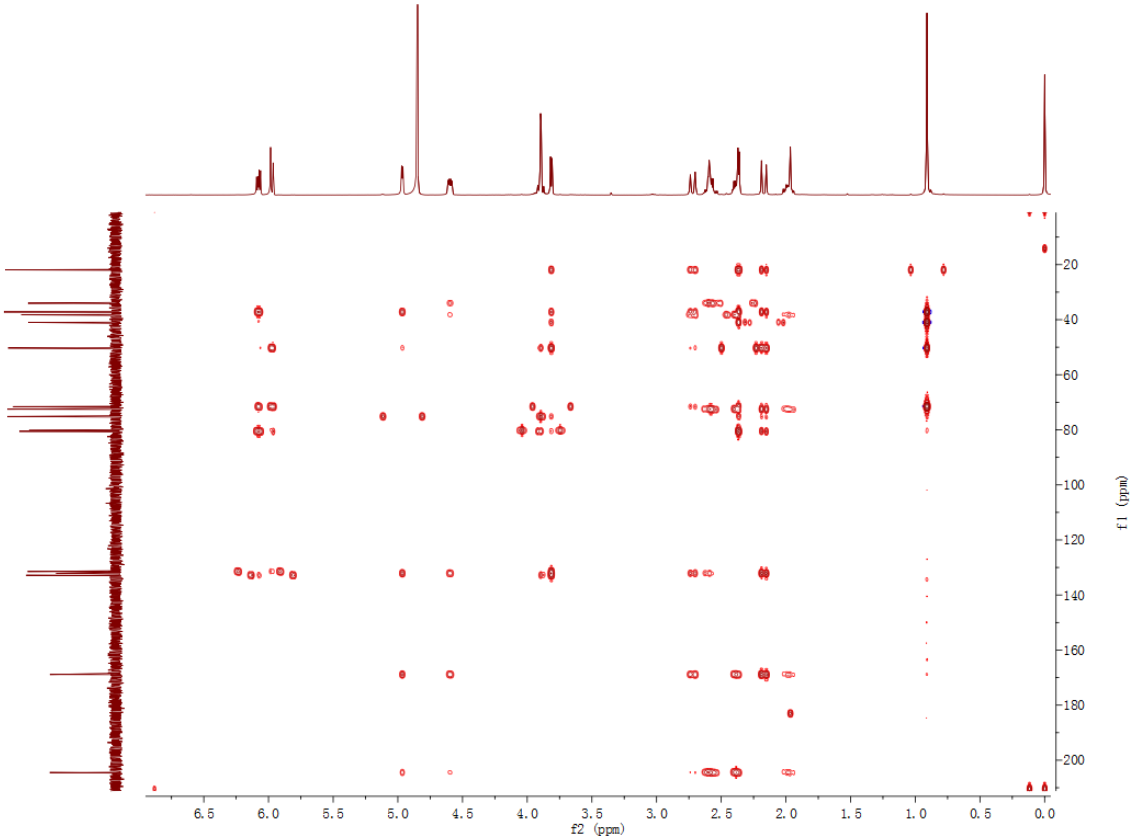


Figure S55. The HMBC spectrum of compound **6** in D_2O

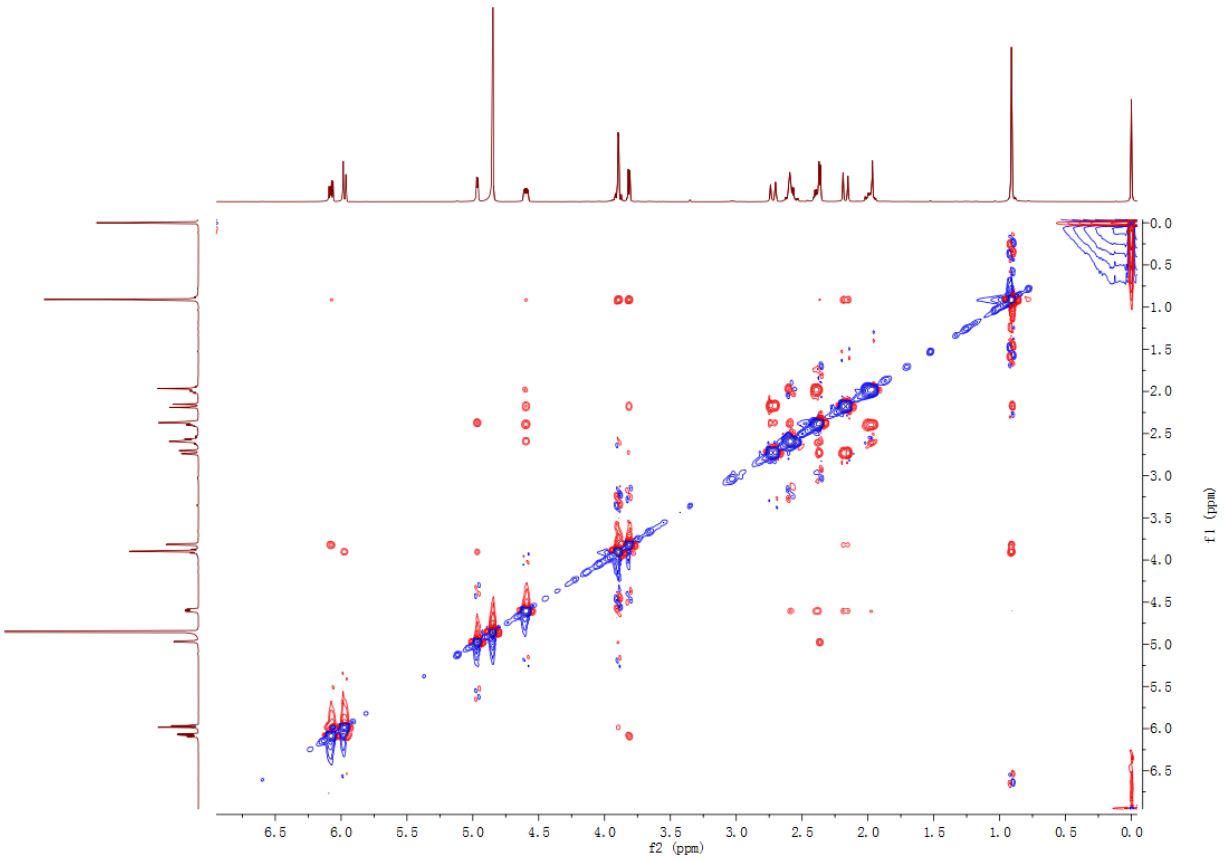


Figure S56. The ROESY spectrum of compound **6** in D_2O

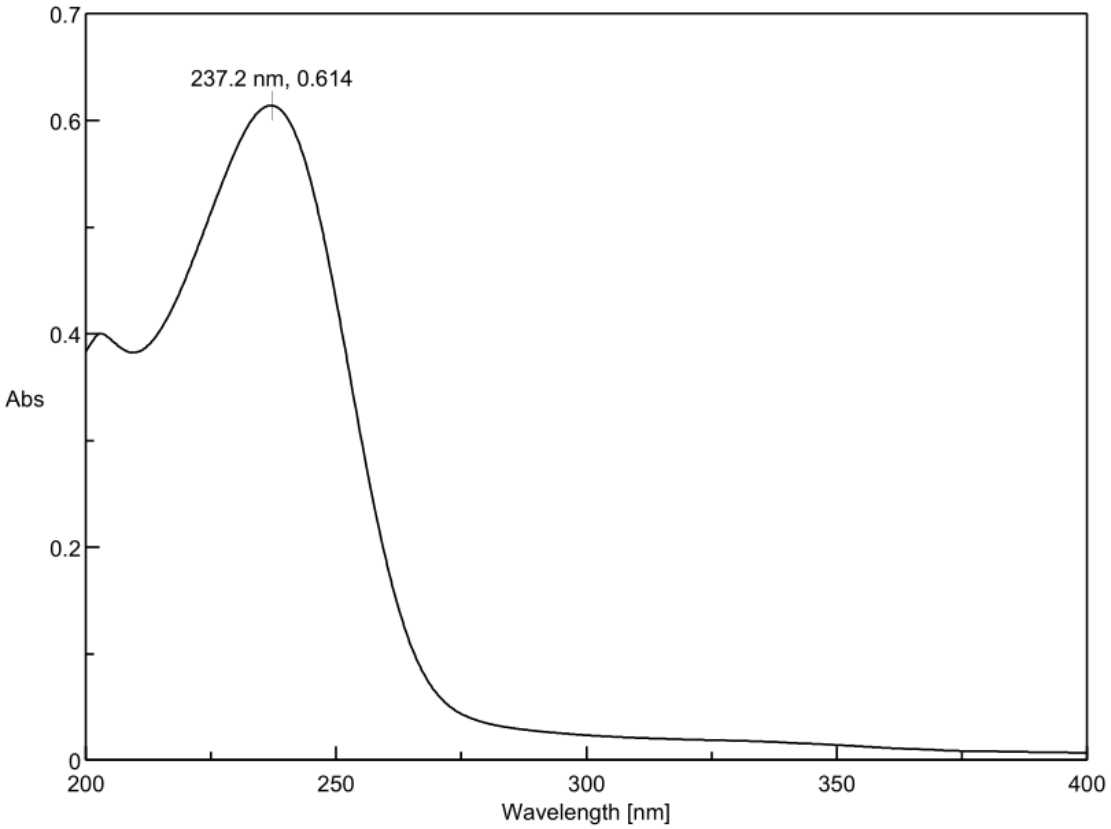


Figure S57. The UV spectrum of compound **6** in H_2O

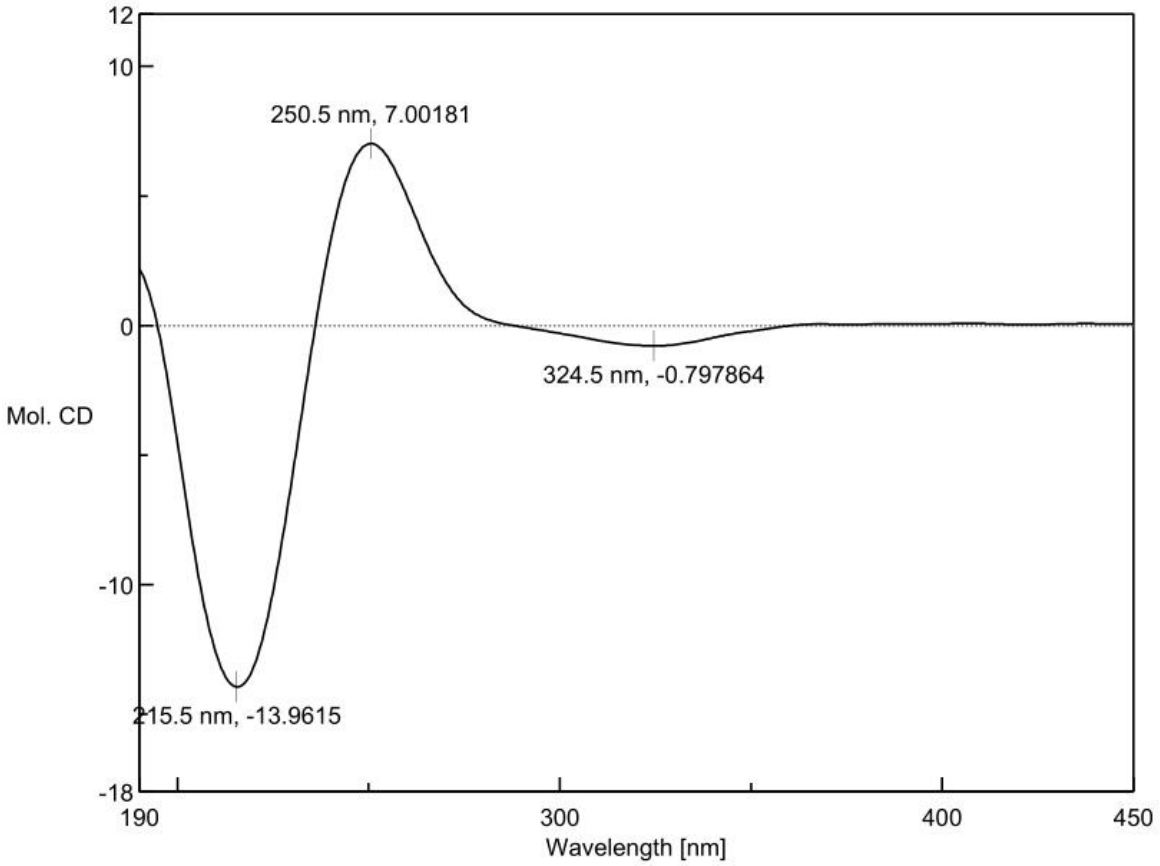


Figure S58. The ECD spectrum of compound **6** in H_2O

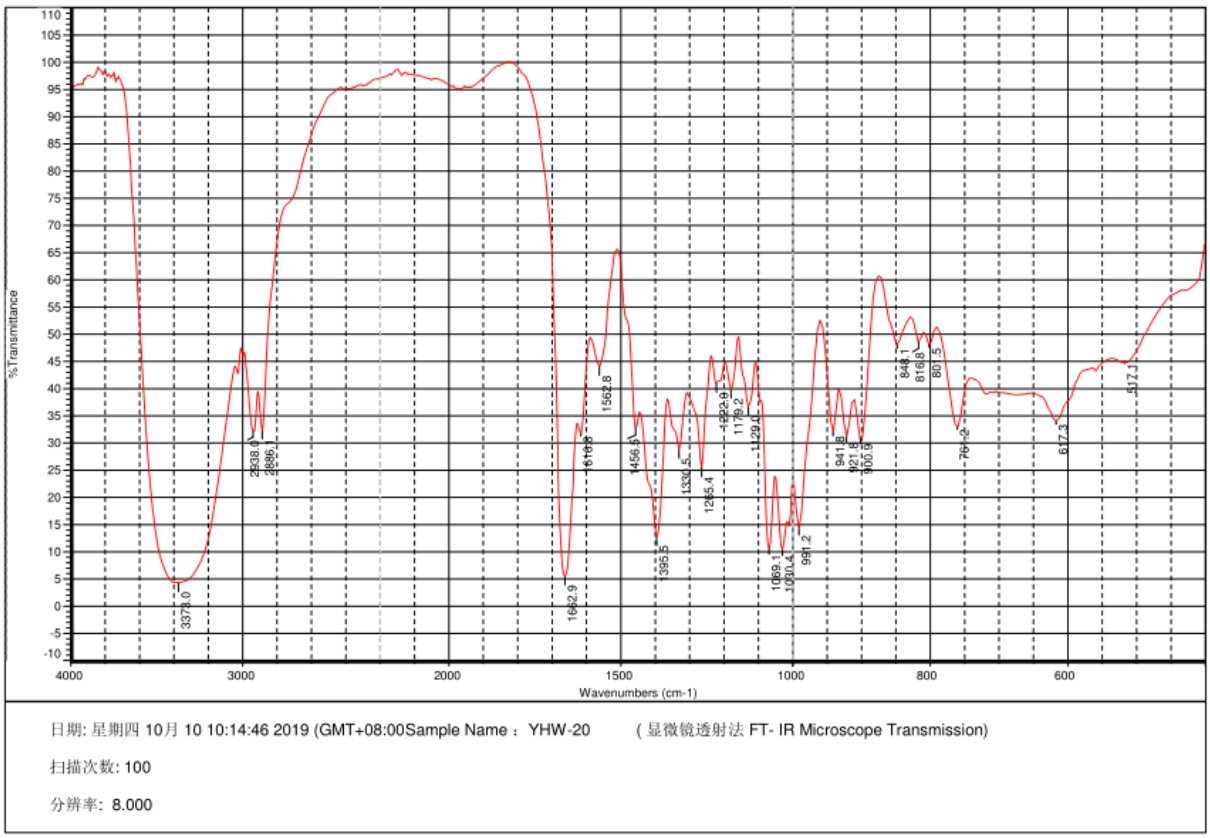
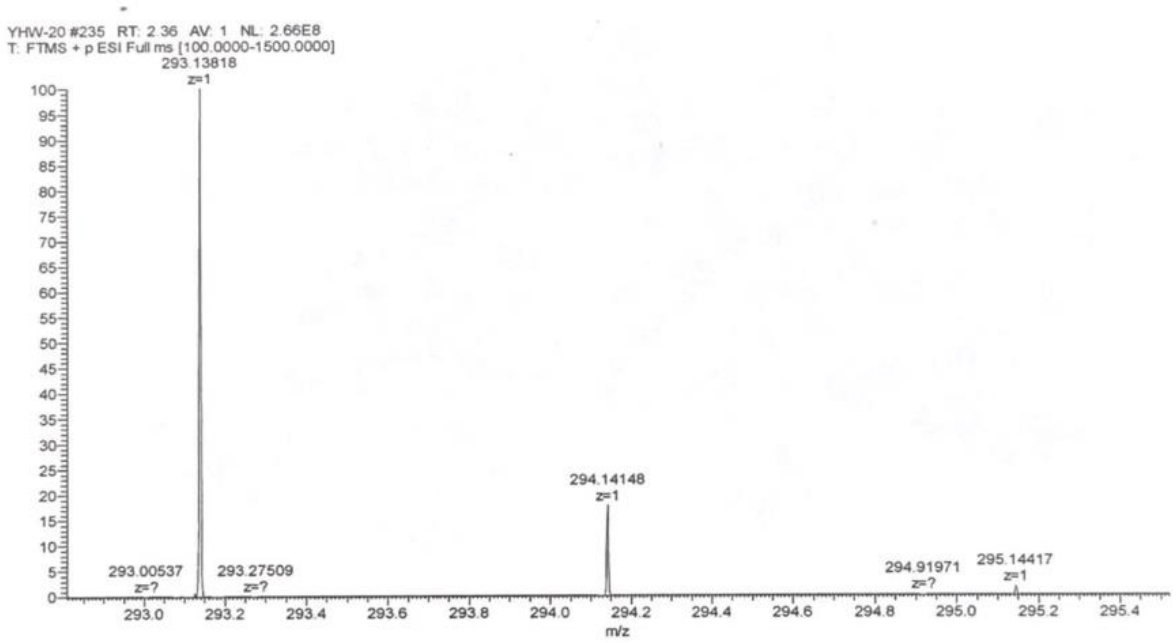


Figure S59. The IR spectrum of compound **6**



m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition	
293.13818	293.13835	-0.58	6.5	C16 H21 O5	M+H

Figure S60. The HR-ESI-MS data of compound **6**

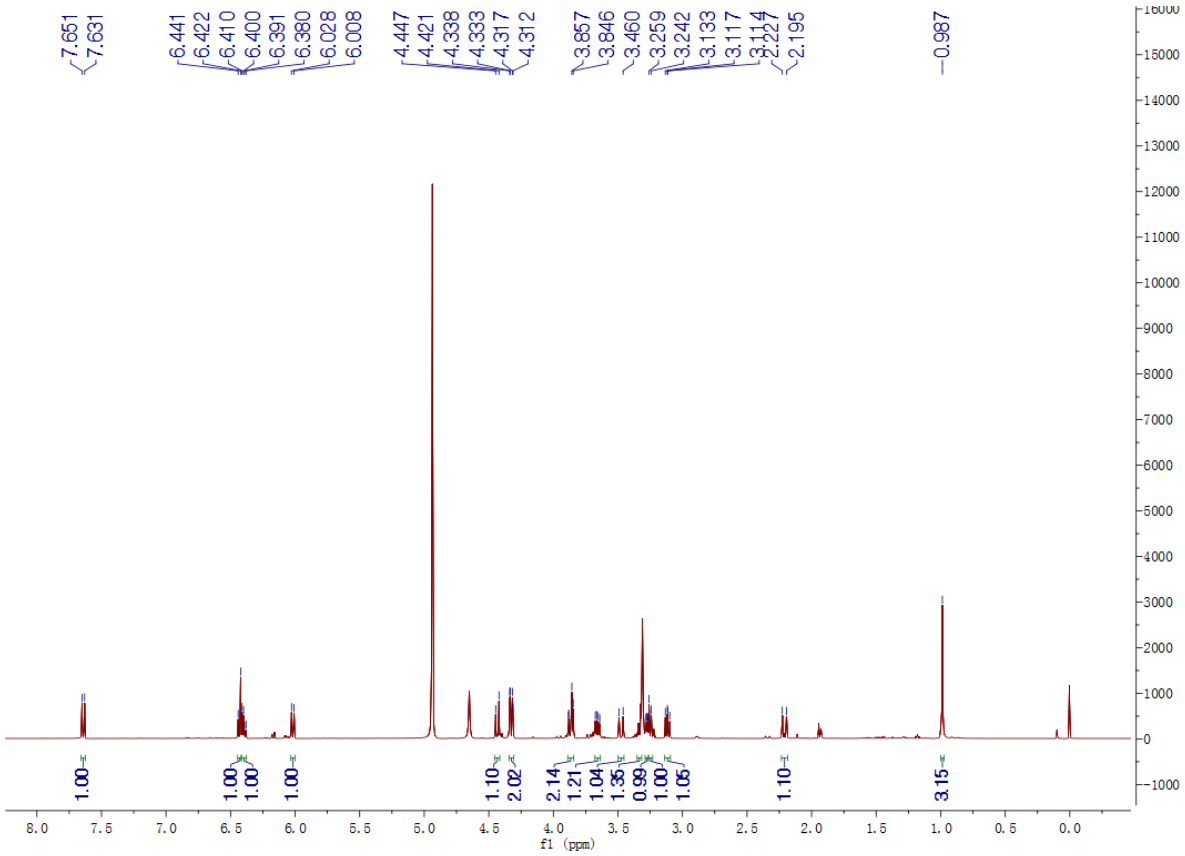


Figure S61. The ^{1}H NMR spectrum of compound **7** in CD_3OD

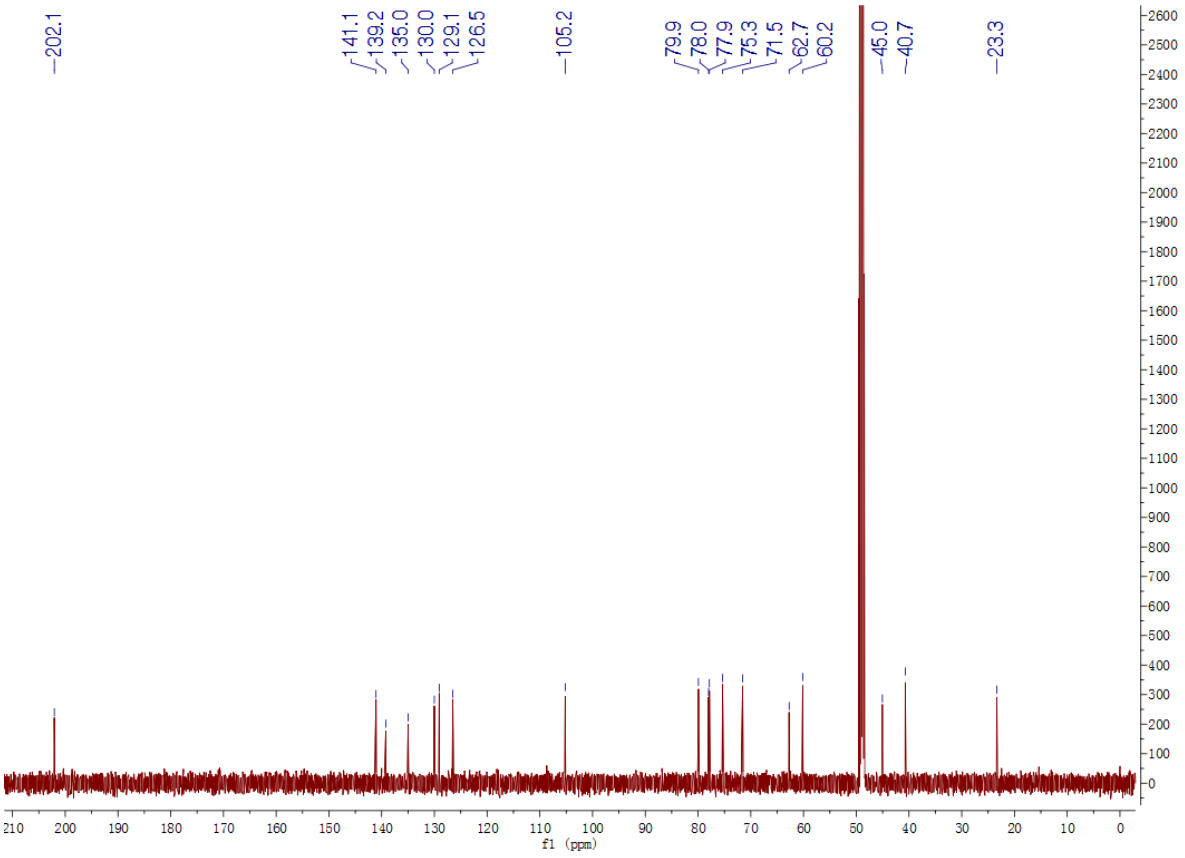


Figure S62. The ^{13}C NMR spectrum of compound **7** in CD_3OD

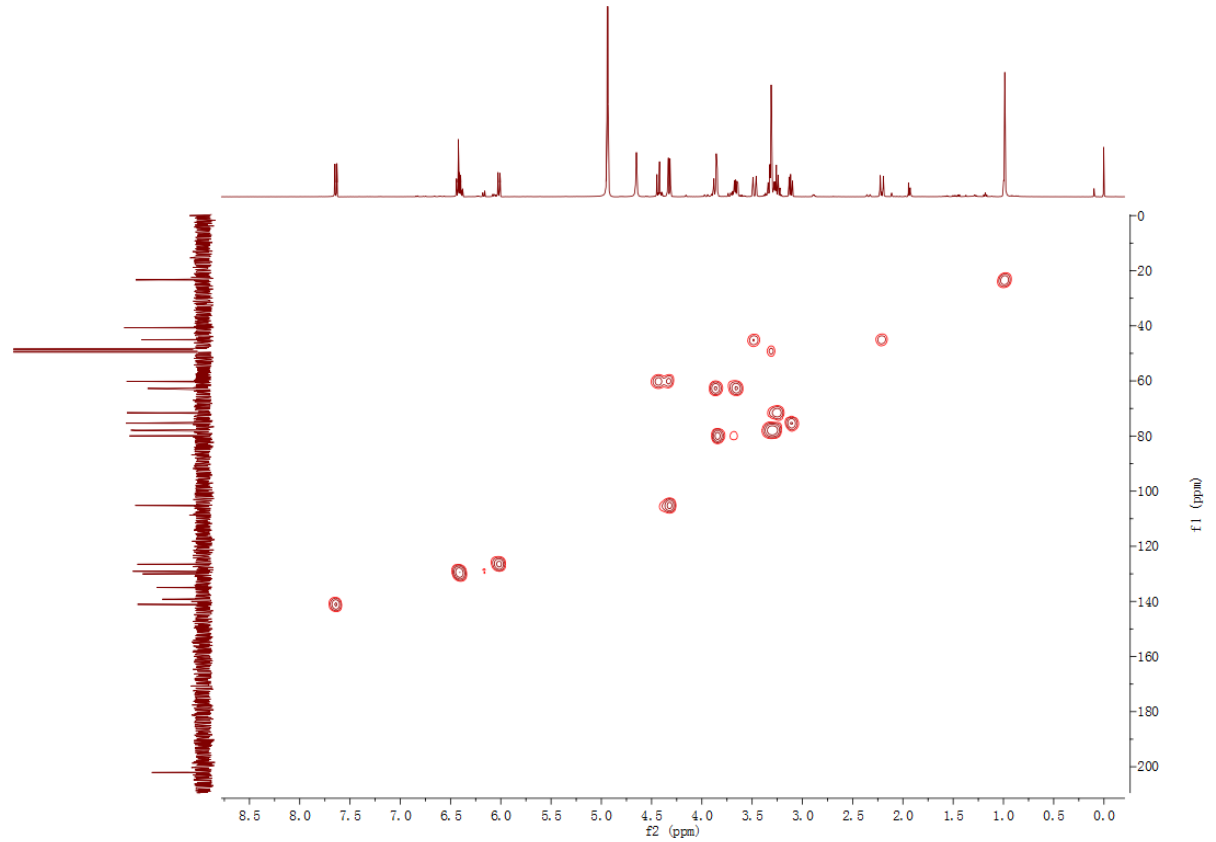


Figure S63. The HSQC spectrum of compound **7** in CD_3OD

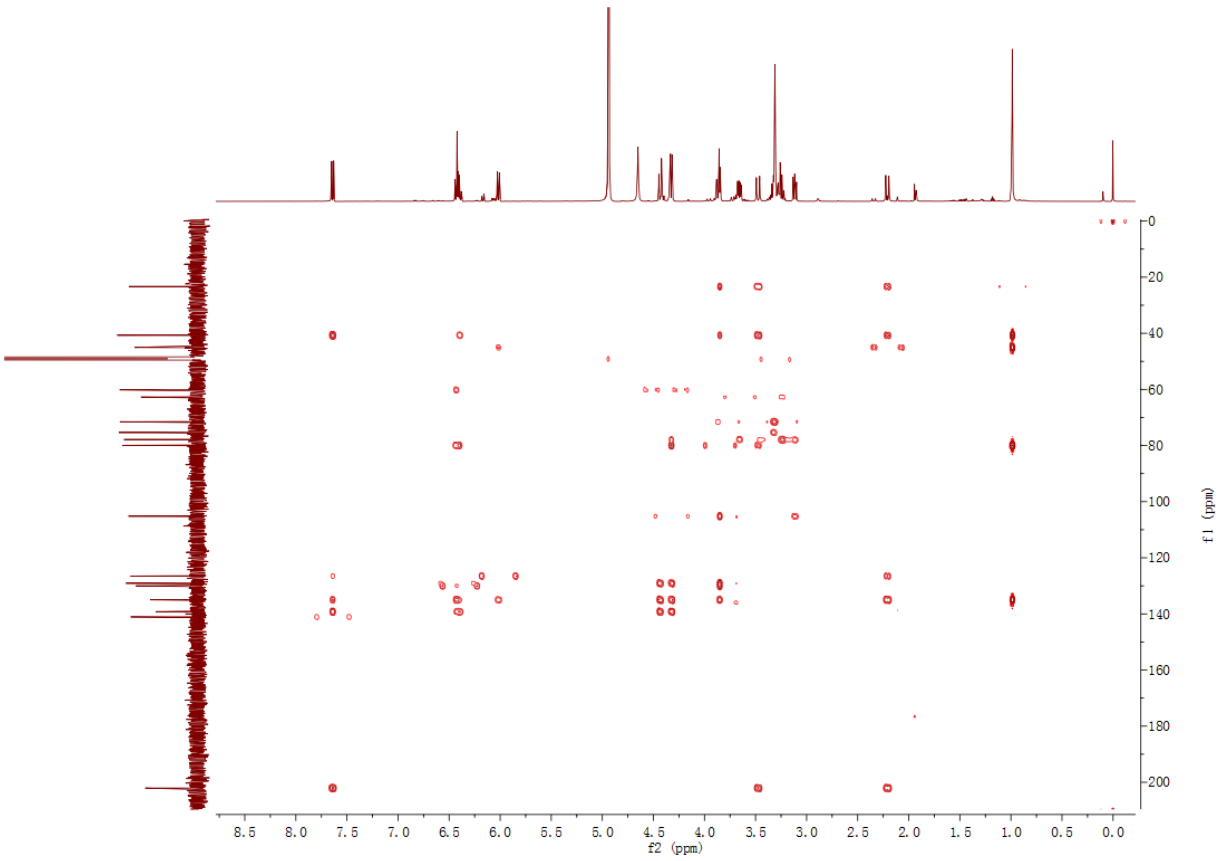


Figure S64. The HMBC spectrum of compound **7** in CD_3OD

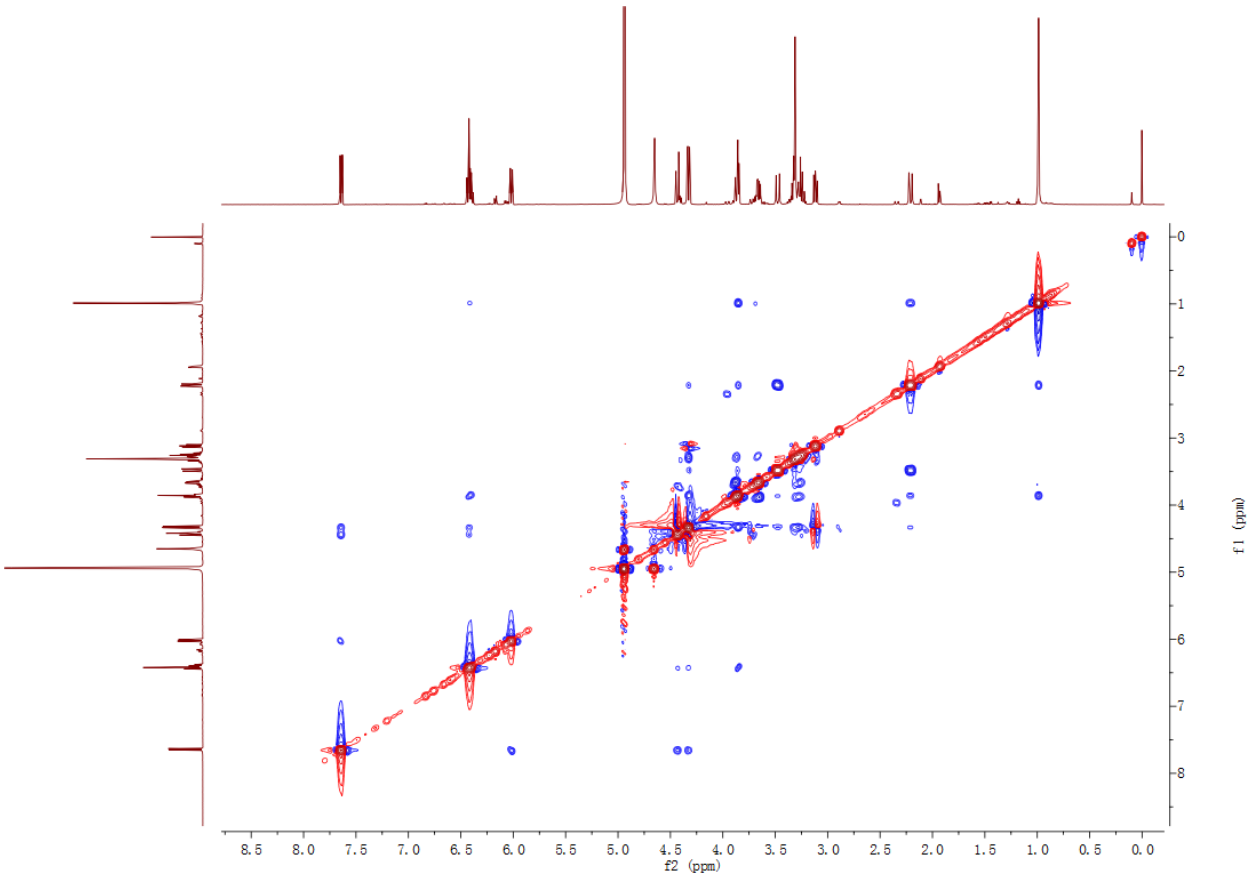


Figure S65. The ROESY spectrum of compound **7** in CD_3OD

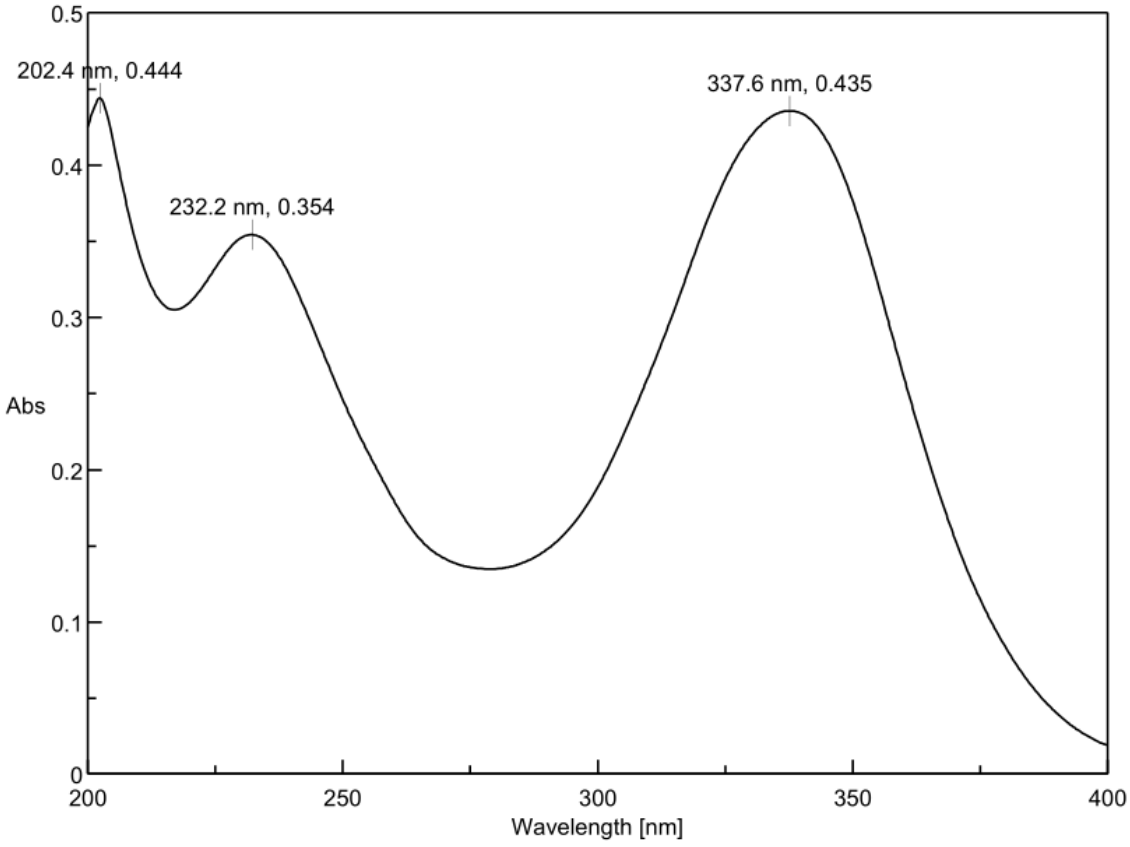


Figure S66. The UV spectrum of compound **7** in MeOH

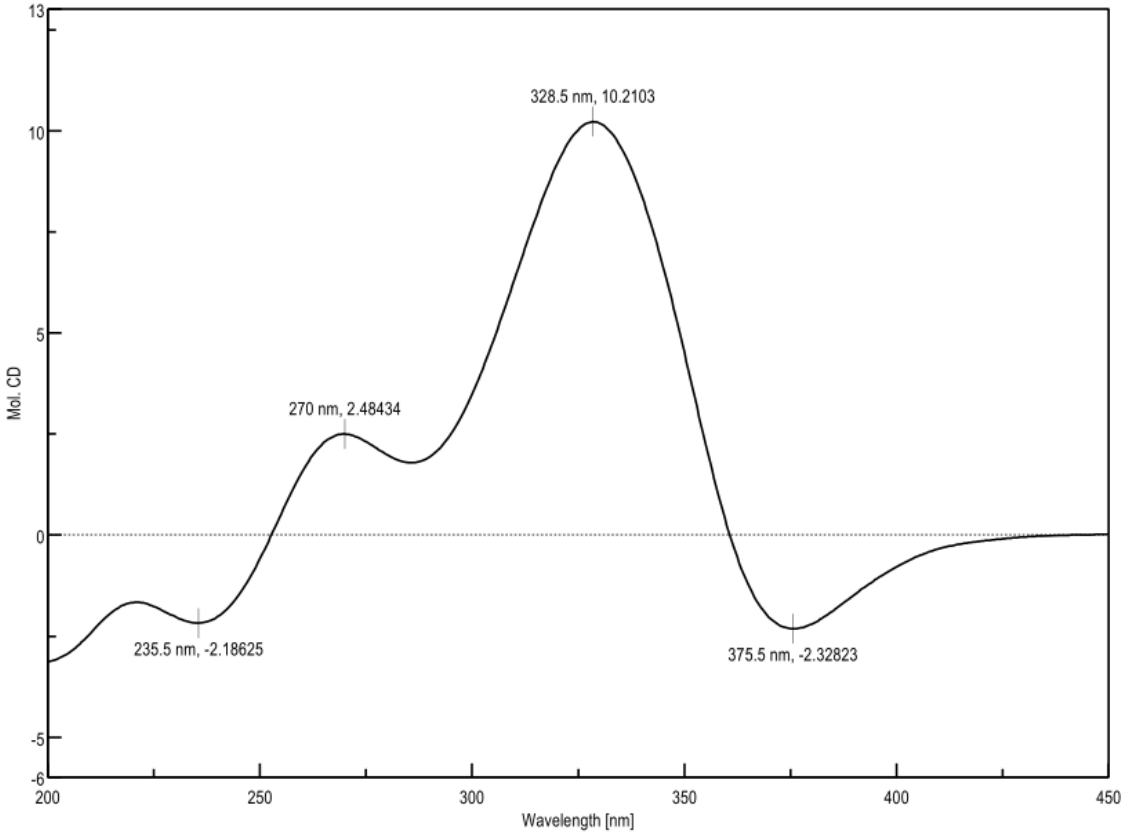


Figure S67. The ECD spectrum of compound **7** in MeOH

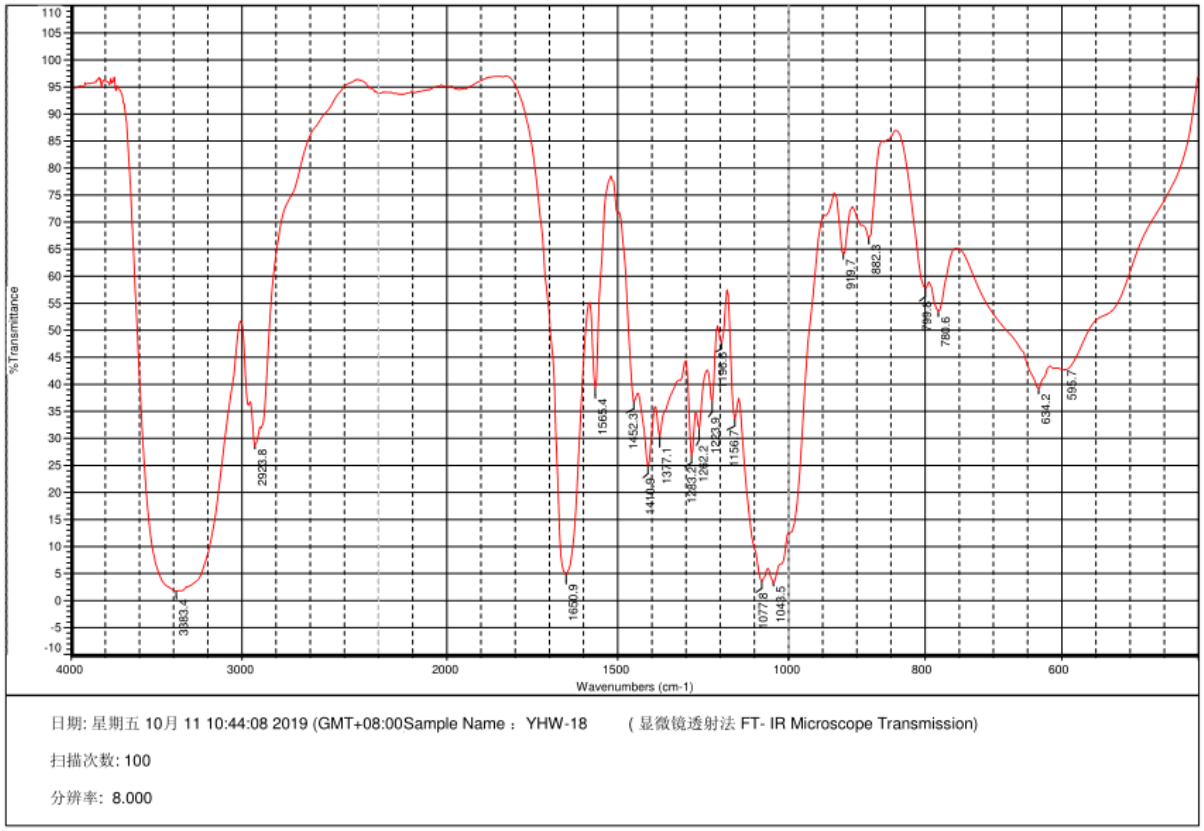
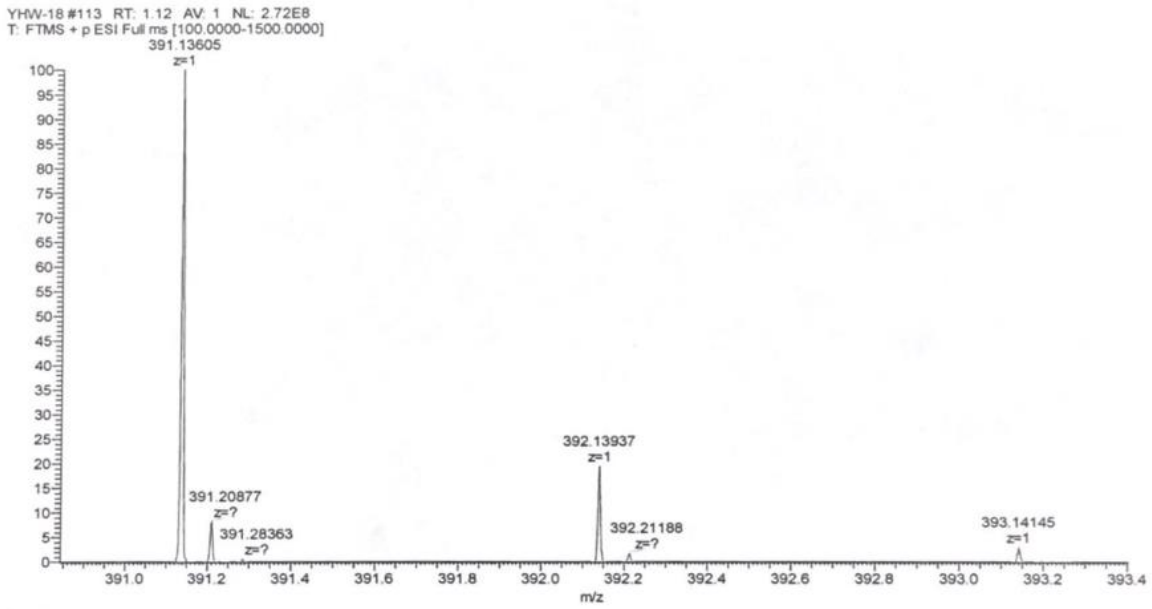


Figure S68. The IR spectrum of compound **7**



m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition	
391.13605	391.13634	-0.74	6.5	C18 H24 O8 Na	M+Na

Figure S69. The HR-ESI-MS data of compound **7**

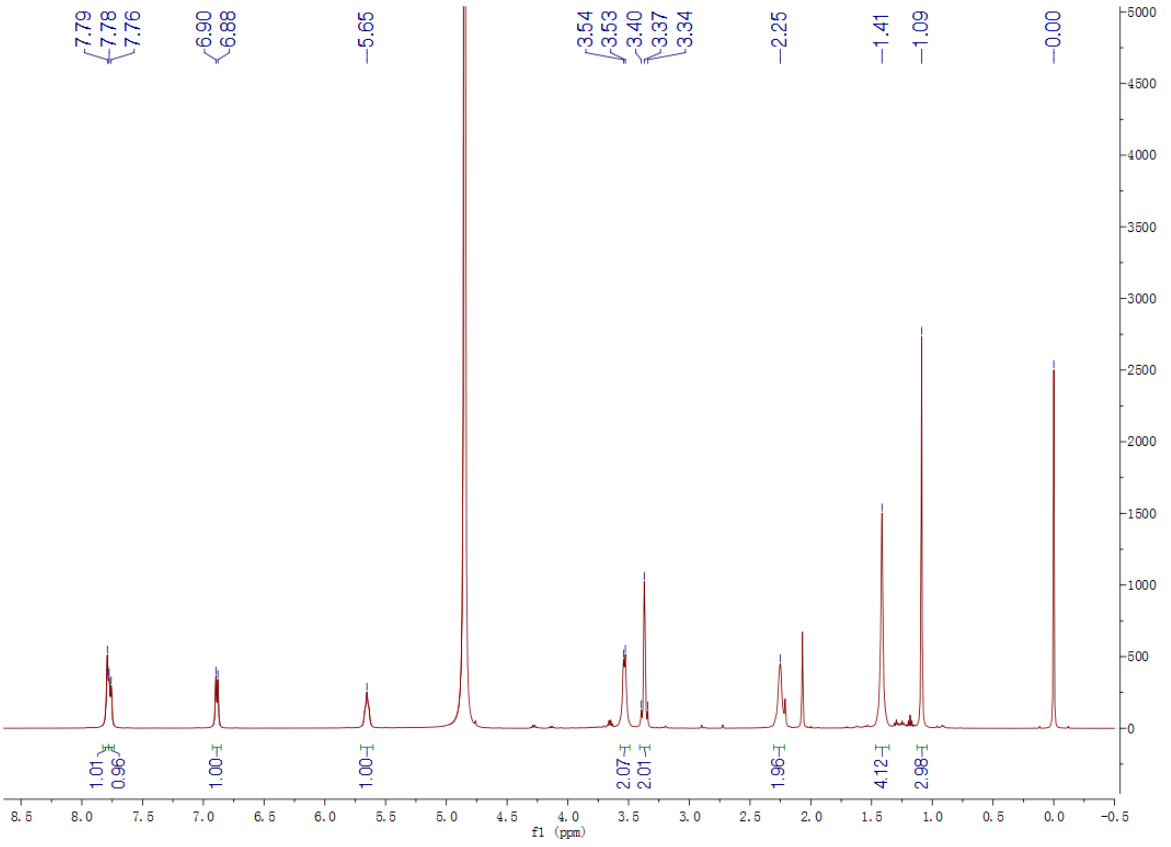


Figure S70. The ^{1}H NMR spectrum of compound **8** in D_2O

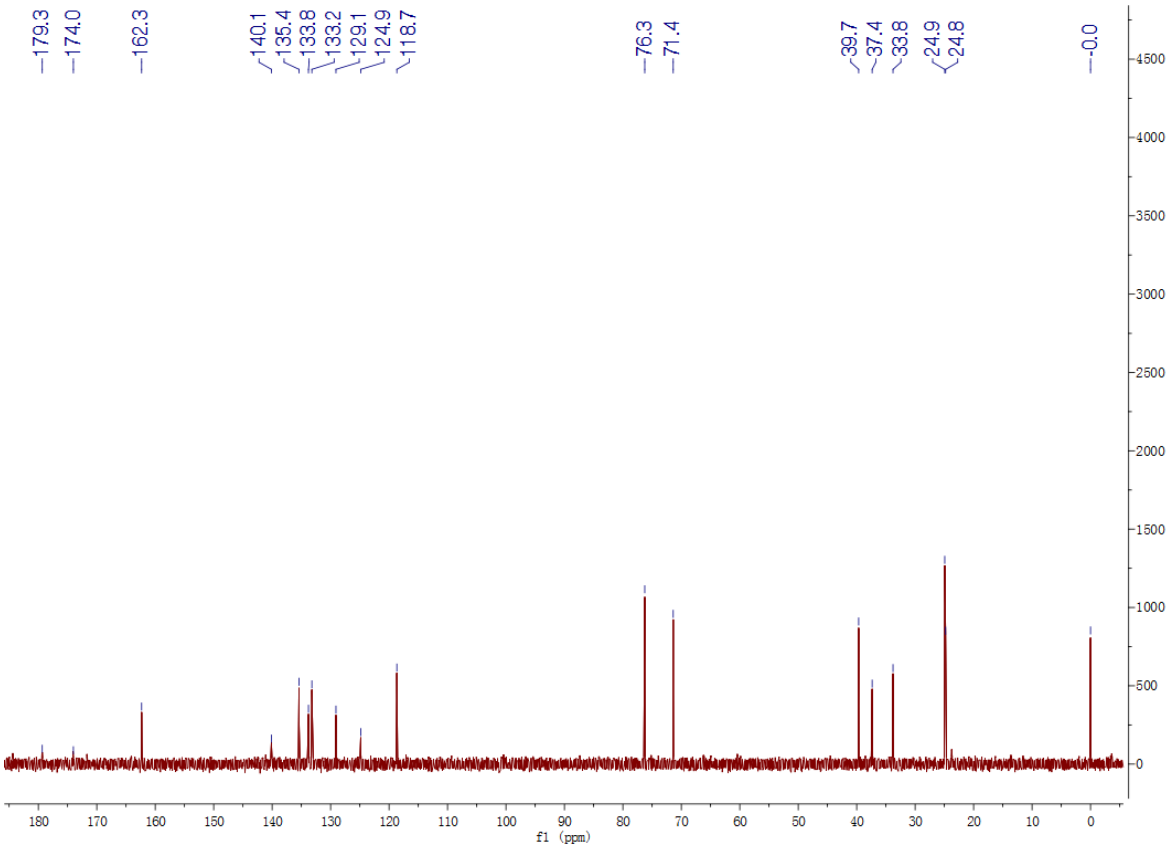


Figure S71. The ^{13}C NMR spectrum of compound **8** in D_2O

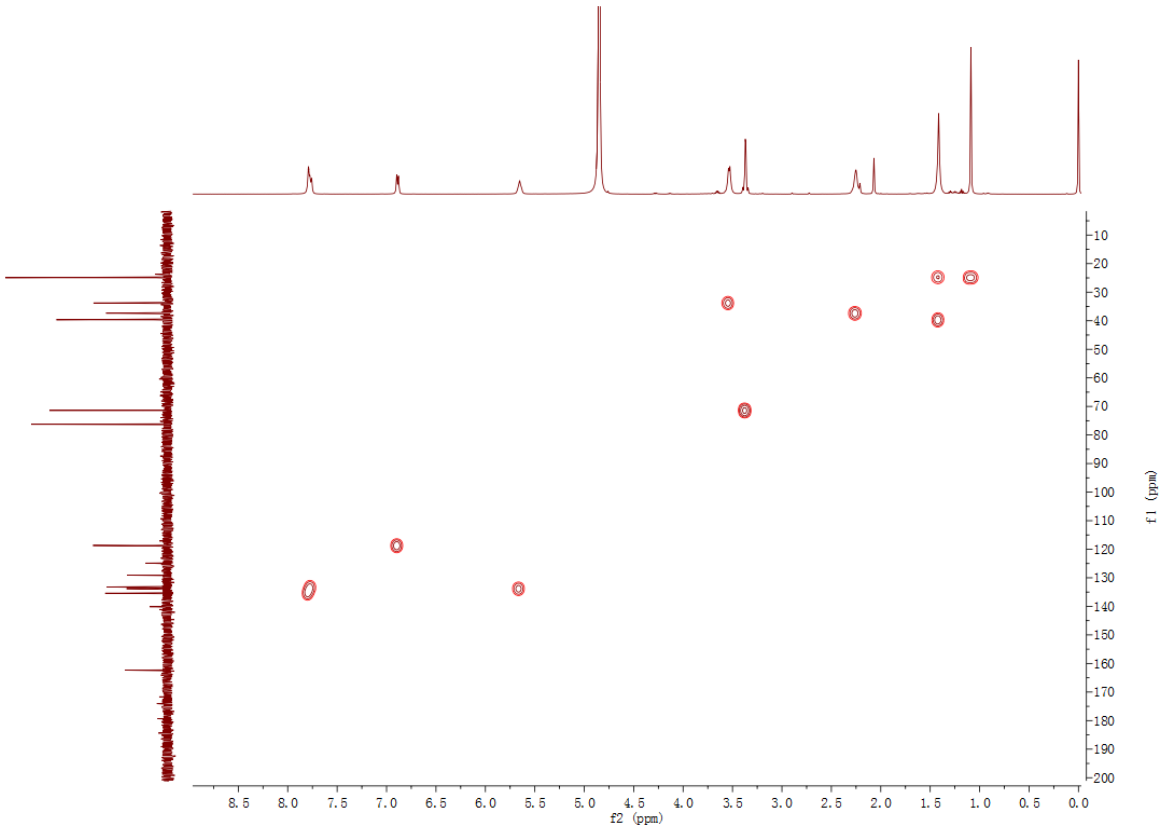


Figure S72. The HSQC spectrum of compound **8** in D_2O

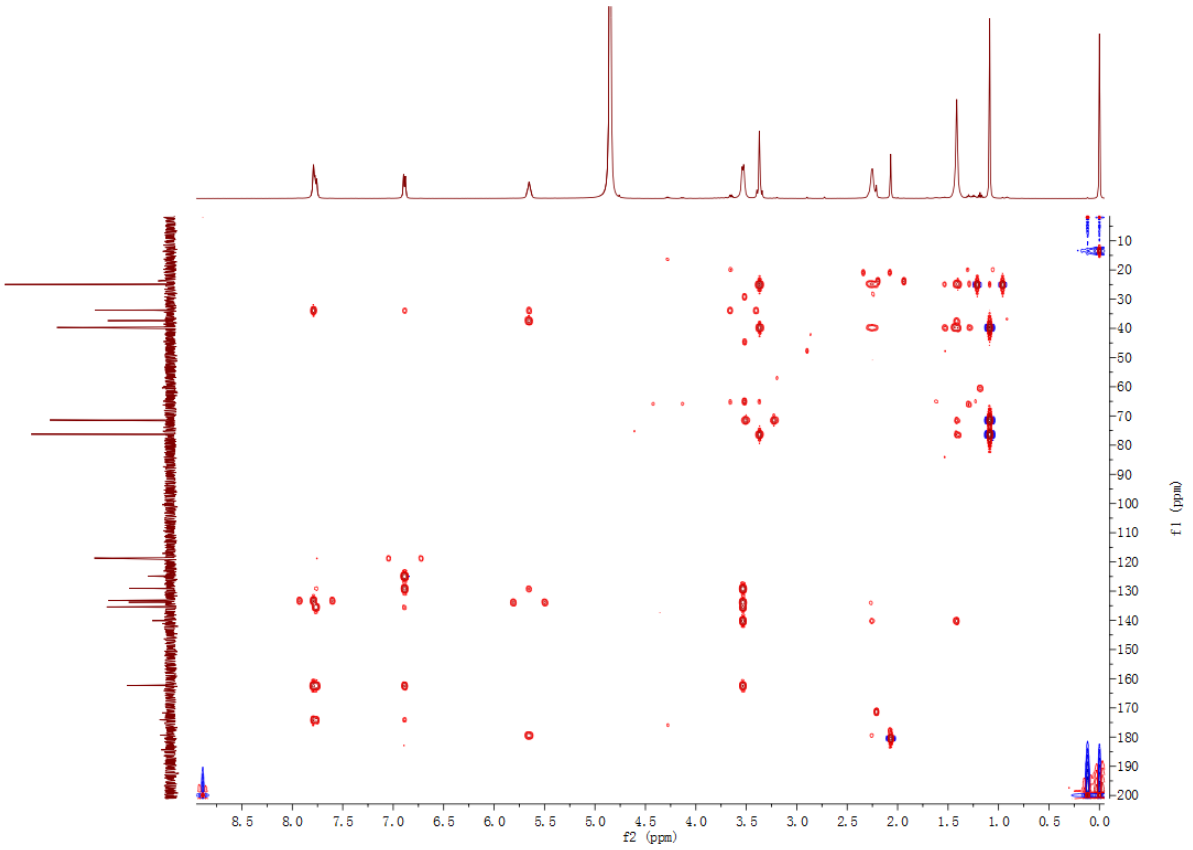


Figure S73. The HMBC spectrum of compound **8** in D_2O

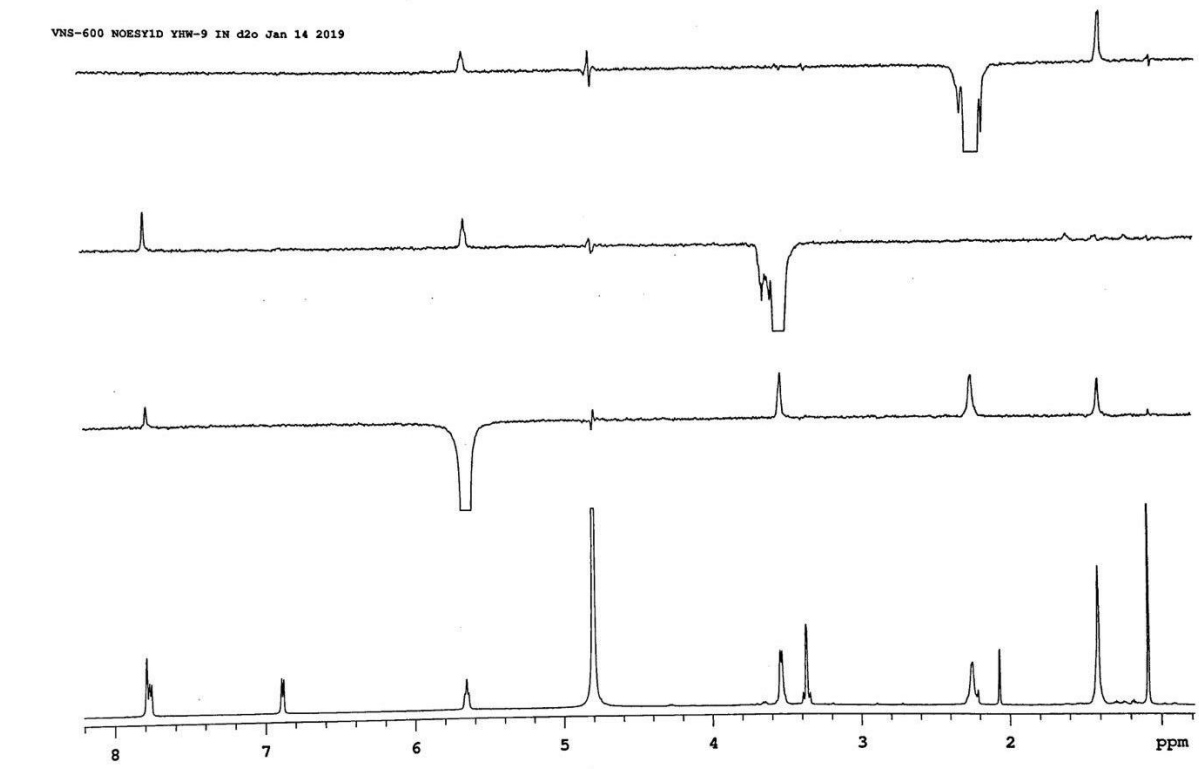


Figure S74. The 1D-NOESY spectrum of compound **8** in D_2O

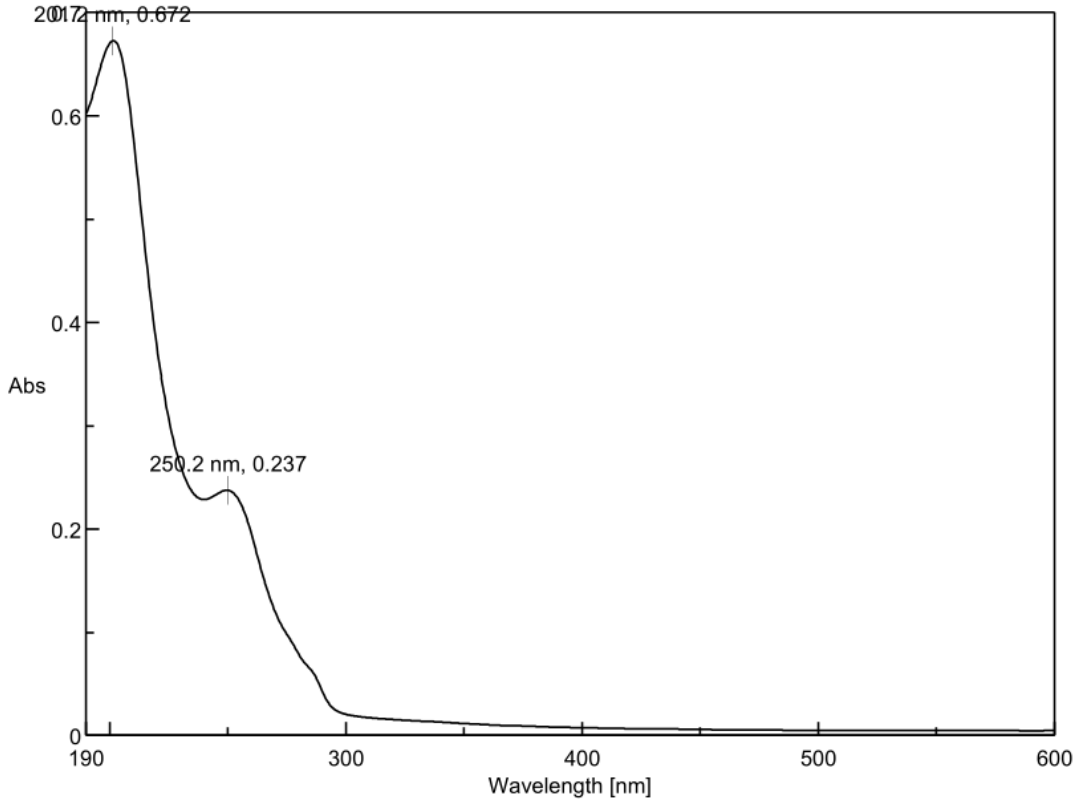


Figure S75. The UV spectrum of compound **8** in H_2O

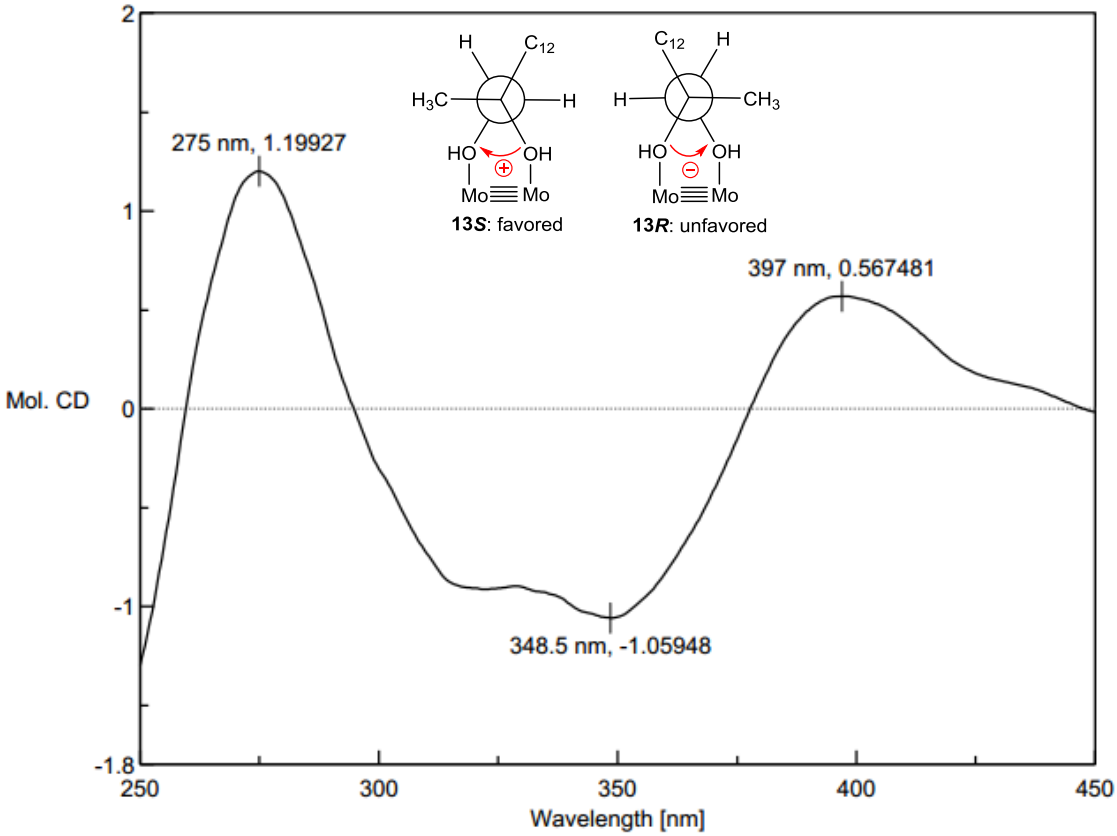


Figure S76. The $[Mo_2(OAc)_4]$ induced ECD spectrum of compound **8** in DMSO

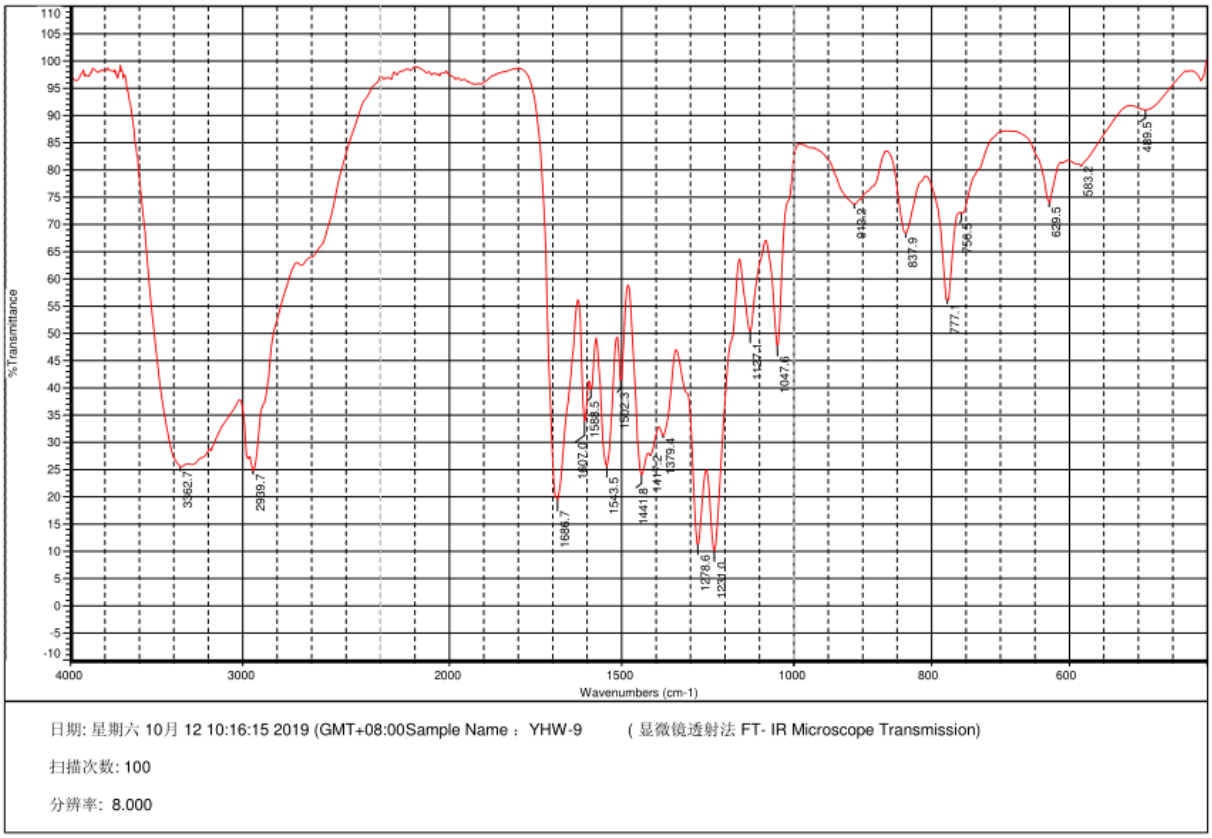
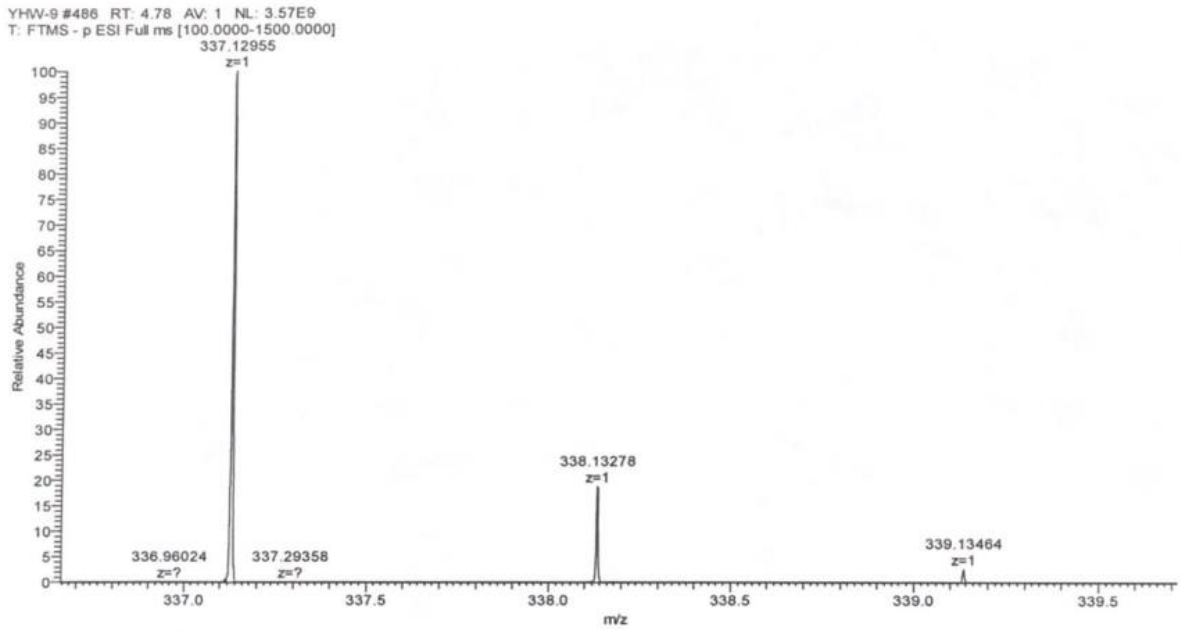


Figure S77. The IR spectrum of compound **8**



m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition	
337.12955	337.12928	0.81	7.5	C17 H21 O7	M-H

Figure S78. The HR-ESI-MS data of compound **8**

Table S1. The cytotoxic activities of 1–8.

comp	IC_{50} (μM)					
	PC9	BGC823	HCT116	HepG2	HeLa	U87-MG
1	>50	>50	>50	>50	>50	>50
2	13.75	17.96	19.82	23.70	25.89	29.29
3	>50	>50	>50	>50	>50	>50
4	>50	>50	>50	>50	>50	>50
5	>50	>50	>50	>50	>50	>50
6	>50	>50	>50	>50	>50	>50
7	>50	>50	>50	>50	>50	>50
8	>50	>50	>50	>50	>50	>50
Paclitaxel	0.0000245	0.000271	0.000109	0.00270	0.0000017	0.000793

General Experimental Procedures. The optical rotations were recorded on a JASCO P-2000 spectrometers (JASCO, Easton, MD, USA) at 20℃. UV and ECD spectra were measured on JASCO V-650 and JASCO J-815 spectrometers (JASCO, Easton, MD, USA), respectively. IR spectra were acquired on a Nicolet 5700 spectrometer utilizing an FT-IR microscope transmission method (Thermo Scientific, Waltham, MA, USA). 1D and 2D NMR spectra were obtained on a Bruker AVIII-500 spectrometer (Bruker-Biospin, Billerica, MA, USA). HRESIMS were conducted with an Agilent 6520 HPLC-Q-TOF mass spectrometer (Agilent Technologies, Waldbronn, Germany) with TMS as an internal standard. The reversed-phase semi-preparative HPLC was performed using a Shimadzu LC-10AT instrument equipped with a YMC-Pack ODS-A-HG column (250 mm × 10 mm, 5 μm; YMC Corp., Kyoto, Japan). Macroporous resin (Diaion HP-20, Mitsubishi Chemical Corp., Tokyo, Japan), RP-C_{18} (50 μm, YMC Corp., Kyoto, Japan) and Sephadex LH-20 (Pharmacia Fine Chemicals, Uppsala, Sweden) were employed for column chromatography. The HPLC-DAD experiments were performed using an Agilent 1260 system with an Apollo C_{18} column (250 × 4.6 mm, 5 μm, Alltech Corp., KY, US

Determination of the Absolute Configuration of Sugar. After enzymatic hydrolysis of compound **7**, the obtained monosaccharide residue was dissolved in anhydrous pyridine (1 mL), and L-cysteine methyl ester hydrochloride (2 mg) was added. Next, the mixture was heated in a water bath (60 ℃) for 1 h. After the reaction solution was dried under vacuum, N-trimethylsilylimidazole (0.5 mL) was added, and the solution was heated in a water bath (60 ℃) for 1 h and then extracted three times with H_2O/*n*-hexane. Then, the *n*-hexane layer was analyzed using GC under following conditions: capillary column, HP-5 (30 m × 0.32 mm, Dikma); injection temperature, 300 ℃; detector temperature (FID), 300 ℃; start temperature, 200 ℃, raised to 280 ℃ at a rate of 10 ℃ min^{-1}, and the final temperature maintained for 30 min; and N_2 was used as the carrier gas. The absolute configuration of the sugar isolated from the hydrolysate of **7** was determined by comparing the retention time of its trimethylsilyl-L-cysteine derivative with that of authentic sugar prepared by a similar procedure.

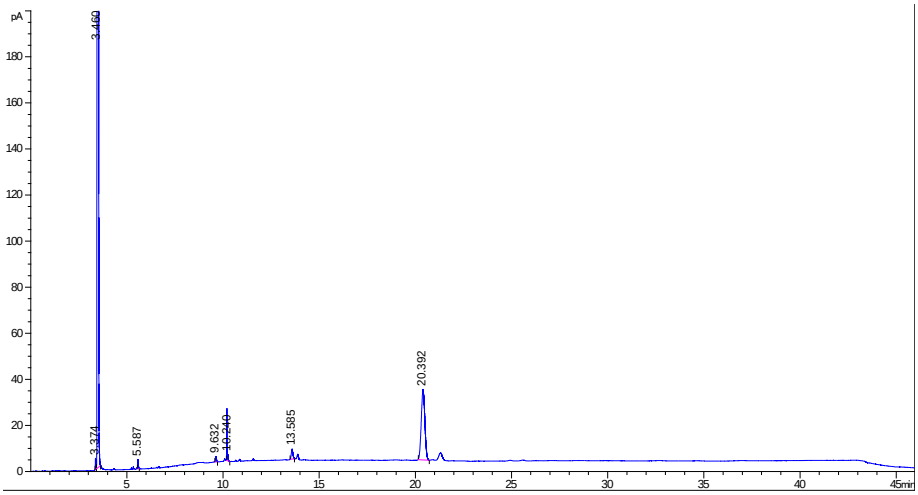


Figure S79. The Gas Chromatographic separation of D-Glu

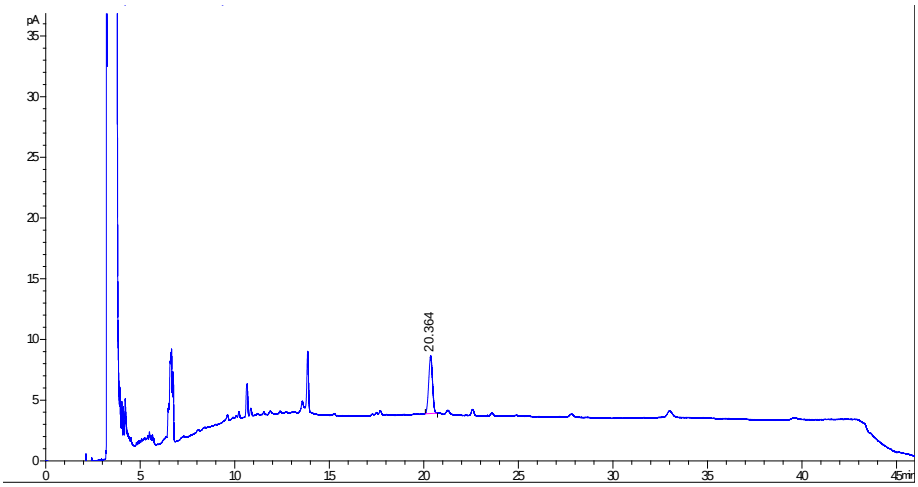
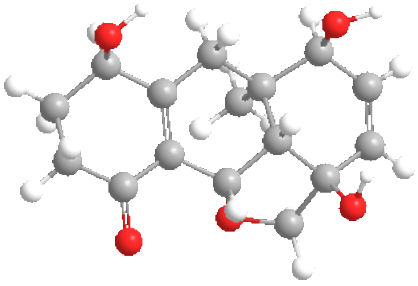


Figure S80. The Gas Chromatographic analysis of sugar moiety of compound **7**

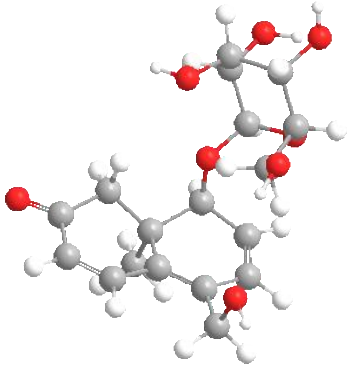
X-ray Crystallographic Analyses of 1, 3, 4 and 5. Single-crystal X-ray diffraction data collection of compounds **1**, **3**, **4** and **5** were measured on a Rigaku Oxford Diffraction XtaLAB Synergy four-circle diffractometer equipped with a microfocus Cu *K*α X−ray source (1.54184 Å, PhotonJet-R 1200W) and a HyPix-6000HE area detector. The sample crystal was cooled to 100K using a cold nitrogen stream (Cobra by Oxford Cryosystems). Date reduction, cell refinement and experimental absorption correction were performed in CrysAlisPro[1]. Structure solution, refinement, and data output were performed with the OLEX2 program package[2] using SHELXL-2014[3] for the refinement. Multi-scan method was used for the absorption correction. Structures were solved by direct methods and refined against F^2 by full-matrix least-squares. All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were generated geometrically at idealized position and constrained to ride on their parent. Crystallographic data for these compounds have been deposited at the Cambridge Crystallographic Data Centre with codes of 2015764 (**1**), 2015765 (**3**), 2015767 (**4**), 2015768 (**5**). Copies of these data can be obtained free of charge via the Internet at www.ccdc.cam.ac.uk/conts/retrieving.html or from the Cambridge Crystallographic Data Centre, 12 Union Road, 54 Cambridge CB2 1EZ, U.K. [Tel: (+44) 1223-336-408; fax: (+44) 1223-336-033; e-mail: deposit@ccdc.cam.ac.uk].

1. Agilent Technologies, CrysAlisPro, Version 1.171.37.35. Yarnton, Oxfordshire, United Kindom, **2014**.
2. Dolomanov, O. V.; Bourhis, L. J.; Gildea, R. J.; Howard, J. A. K.; Puschmann, H. *J. Appl. Cryst.* **2009**, *42*, 339−341.
3. Sheldrick, G. M. *Acta Crystallogr. C*, **2015**, *71*, 3−8.

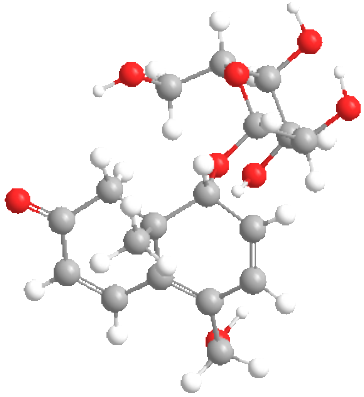
ECD Calculations. Systematic conformation searching of compound **6** was conducted in the Discovery Studio (version 16.1.0.15350) using the MMFF94 force field and only one conformer was obtained due to the rigidity of **6**. The conformational analyses of compound **7** was performed in the Discovery Studio via MMFF94s molecular mechanics force field, generating 21 conformers for 9*S*,10*R*-**7** and 19 conformers for 9*R*,10*S*-**7** because of the existence of a glucose moiety. Therefore, all the obtained conformers were further optimized by Spartan'14 software through MMFF94s molecular force field, giving one stable conformer for 9*S*,10*R*-**7** and two stable conformers for 9*R*,10*S*-**7**. These conformers were further optimized at the B3LYP/6-31+G (d, p) level in water for **6** and in methanol for **7** by the Gaussian 09 program (Gaussian Inc., Wallingford, CT, USA). The energies, oscillator strengths, and rotational strengths (velocity) of the first 50 electronic excitations were calculated using the time-dependent density functional theory at the B3LYP/6-31+g* level in water for **6** and in methanol for **7**, respectively. Finally, the calculated ECD spectra were acquired through overlapping Gaussian function with the half-bandwidth of 0.35 eV for **6** and 0.25 eV for **7**, respectively. Good match of the calculated and experimental ECD spectra allowed their configurations assigned. The calculated preferential conformations are as follows:



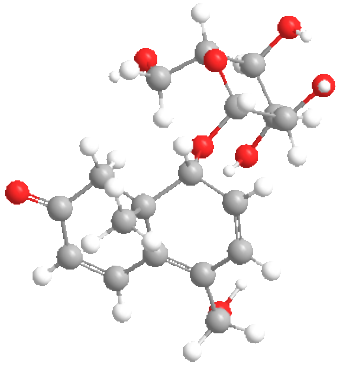
1*R*,6*S*,7*S*,8*R*,11*S*,12*R*-**6** (100%)



9*S*,10*R*-**7** (100%)



9*R*,10*S*-**7**-C1 (93.6%)



9*R*,10*S*-**7**-C2 (6.3%)

Table S2. Cartesian coordinates of the low-energy conformer of 1*R*,6*S*,7*S*,8*R*,11*S*,12*R*-**6**

Conformer of 1*R*,6*S*,7*S*,8*R*,11*S*,12*R*-**6**						Conformer of 1*R*,6*S*,7*S*,8*R*,11*S*,12*R*-**6**				
Number	Atom	X	Y	Z		Number	Atom	X	Y	Z
1	C	-3.9967	0.5421	-0.0343		22	O	2.6032	-2.5457	0.3248
2	C	-3.9683	-0.9857	0.1901		23	H	1.1537	-0.8715	1.3768
3	C	-2.6402	-1.5264	-0.1876		24	H	-3.9246	0.7427	-1.1093
4	C	-1.4524	-0.8091	-0.0208		25	H	-4.9451	0.9559	0.3245
5	C	-1.5076	0.5457	0.4485		26	H	-4.7728	-1.4249	-0.4010
6	C	-2.8096	1.2184	0.6887		27	H	-4.1654	-1.2020	1.2476
7	C	-0.1264	-1.4775	-0.2496		28	H	-2.7629	2.2551	0.3393
8	C	1.0864	-0.7046	0.2879		29	H	-0.4330	2.3838	0.5630
9	C	0.9941	0.8425	0.0269		30	H	-0.1259	1.2564	1.8725
10	C	-0.2778	1.3253	0.7914		31	H	4.3291	-0.9172	-0.8874
11	C	2.2847	-1.3611	-0.4266		32	H	4.3990	1.2646	-0.0439
12	C	3.4952	-0.5213	-0.5015		33	H	2.3727	2.5193	0.2639
13	C	3.5328	0.7680	-0.0277		34	H	1.8272	-2.8623	-1.9944
14	C	2.3604	1.4484	0.5316		35	H	1.9365	-1.2108	-2.6115
15	O	-2.6102	-2.7432	-0.5904		36	H	-2.2598	1.6677	2.4998
16	O	0.1768	-1.6713	-1.6390		37	H	-0.0701	0.8514	-1.9315
17	C	1.6104	-1.8171	-1.7637		38	H	1.6807	0.9958	-2.0812
18	O	-3.0397	1.2230	2.0970		39	H	0.7334	2.3595	-1.5321
19	C	0.8226	1.2757	-1.4743		40	H	3.3985	1.5369	2.1909
20	O	2.4545	1.3785	1.9610		41	H	2.7868	-2.2407	1.2438
21	H	-0.1511	-2.4624	0.2359						

Table S3. Cartesian coordinates of the low-energy conformers of 9*S*,10*R*-**7** and 9*R*,10*S*-**7**

Conformer of 9*S*,10*R*-**7**				
Number	Atom	X	Y	Z
1	C	-3.3077	0.4315	2.3872
2	C	-3.1515	-0.9970	2.0556
3	C	-1.8530	-1.4277	1.4279
4	C	-0.6347	-0.7090	2.0515
5	C	-0.8708	0.8178	2.1660
6	C	-2.2470	1.2465	2.3887
7	C	0.6477	-1.0428	1.1937
8	C	1.7610	-0.0740	1.4663
9	C	1.5256	1.1734	1.8931
10	C	0.1716	1.6839	2.0839
11	O	-4.0942	-1.7672	2.2187
12	C	0.0946	3.1874	2.2174
13	O	-0.0265	3.7623	0.9211
14	O	0.3154	-1.0165	-0.1994
15	C	-0.4134	-1.2539	3.4899
16	C	1.3114	-1.5247	-1.0792
17	O	2.1869	-0.5008	-1.5542
18	C	1.5933	0.4588	-2.4488
19	C	0.9165	-0.2140	-3.6588
20	C	-0.0398	-1.3415	-3.2439
21	C	0.6465	-2.2888	-2.2442
22	C	0.6995	1.4729	-1.7209
23	O	1.9524	-0.7976	-4.4811
24	O	-1.2629	-0.8066	-2.7435
25	O	1.6309	-3.0790	-2.9333

Conformer of 9*S*,10*R*-**7**				
Number	Atom	X	Y	Z
26	O	0.3438	2.5557	-2.5801
27	H	-4.3129	0.7787	2.5898
28	H	-1.7525	-2.5141	1.5421
29	H	-1.9593	-1.2151	0.3571
30	H	-2.4411	2.2969	2.5806
31	H	0.9750	-2.0590	1.4505
32	H	2.7796	-0.3982	1.2765
33	H	2.3631	1.8491	2.0476
34	H	-0.7491	3.5188	2.8279
35	H	0.9955	3.5905	2.6951
36	H	0.0085	4.7258	1.0435
37	H	-0.2592	-2.3391	3.4771
38	H	-1.2717	-1.0554	4.1416
39	H	0.4647	-0.8045	3.9673
40	H	1.9480	-2.2414	-0.5454
41	H	2.4451	1.0269	-2.8459
42	H	0.3975	0.5375	-4.2646
43	H	-0.2930	-1.9190	-4.1424
44	H	-0.0967	-2.9819	-1.8334
45	H	1.2458	1.8898	-0.8709
46	H	-0.2231	1.0315	-1.3409
47	H	1.5927	-0.8444	-5.3861
48	H	-1.8271	-1.5513	-2.4711
49	H	2.2466	-2.4364	-3.3520
50	H	-0.1700	3.1649	-2.0175

Conformer of 9*R*,10*S*-**7**-C1				
1	C	-3.2355	0.8256	-2.2853
2	C	-3.1202	-0.5524	-1.9230
3	C	-1.8389	-1.0521	-1.3377
4	C	-0.5884	-0.4050	-2.0219
5	C	-0.7714	1.1010	-2.1689
6	C	-2.1056	1.6314	-2.3646
7	C	0.7101	-0.7620	-1.1990
8	C	1.8756	0.0839	-1.5966
9	C	1.6755	1.3865	-2.0572
10	C	0.3598	1.9442	-2.1755
11	O	-4.0978	-1.2962	-2.0230
12	C	0.2915	3.4255	-2.3242

Conformer of 9*R*,10*S*-**7**-C2				
1	C	-3.2634	0.7801	-2.2854
2	C	-3.1481	-0.5978	-1.9231
3	C	-1.8668	-1.0977	-1.3375
4	C	-0.6163	-0.4504	-2.0221
5	C	-0.7993	1.0555	-2.1690
6	C	-2.1335	1.5859	-2.3647
7	C	0.6822	-0.8075	-1.1992
8	C	1.8478	0.0383	-1.5967
9	C	1.6476	1.3410	-2.0573
10	C	0.3319	1.8987	-2.1756
11	O	-4.1256	-1.3417	-2.0232
12	C	0.2636	3.3799	-2.3243

13	O	-0.2962	4.0014	-1.1601
14	O	0.4850	-0.5795	0.2107
15	C	-0.4441	-1.0259	-3.4533
16	C	1.4962	-1.1730	1.0472
17	O	0.9217	-2.1522	1.9167
18	C	0.0909	-1.6714	2.9914
19	C	0.7586	-0.5291	3.8041
20	C	1.3520	0.5719	2.8882
21	C	2.2613	-0.0690	1.8129
22	C	-1.3381	-1.3332	2.5082
23	O	1.8236	-1.0915	4.5740
24	O	0.3239	1.4034	2.3297
25	O	3.4436	-0.6182	2.4081
26	O	-1.8337	-2.3891	1.6930
27	H	-4.1789	1.2340	-2.4684
28	H	-1.7769	-2.1466	-1.4107
29	H	-1.8695	-0.7993	-0.2774
30	H	-2.2453	2.6368	-2.5711
31	H	0.9504	-1.8212	-1.3783
32	H	2.8444	-0.2753	-1.5053
33	H	2.5006	1.9473	-2.3147
34	H	1.2826	3.8641	-2.4534
35	H	-0.3003	3.7159	-3.2021
36	H	0.2263	3.6718	-0.3962
37	H	0.4254	-0.6247	-3.9719
38	H	-1.3227	-0.8179	-4.0647
39	H	-0.3290	-2.1112	-3.3931
40	H	2.2224	-1.7290	0.4521
41	H	0.0000	-2.5173	3.6689
42	H	0.0330	-0.0928	4.4951
43	H	1.9710	1.2208	3.5058
44	H	2.5753	0.7074	1.1169
45	H	-1.3233	-0.4131	1.9359
46	H	-2.0207	-1.2017	3.3493
47	H	1.5117	-1.9677	4.8766
48	H	0.2195	1.1640	1.3818
49	H	3.1315	-1.2133	3.1265
50	H	-2.7266	-2.1066	1.4037

13	O	-0.3241	3.9560	-1.1603
14	O	0.4566	-0.6256	0.2112
15	C	-0.4720	-1.0714	-3.4534
16	C	1.4675	-1.2184	1.0474
17	O	0.8913	-2.1981	1.9150
18	C	0.0648	-1.7154	2.9904
19	C	0.7333	-0.5738	3.8020
20	C	1.3235	0.5267	2.8877
21	C	2.2342	-0.1135	1.8098
22	C	-1.3682	-1.3817	2.5127
23	O	1.7949	-1.1383	4.5790
24	O	0.2961	1.3577	2.3290
25	O	3.4186	-0.6622	2.4021
26	O	-2.2269	-1.2261	3.6359
27	H	-4.2068	1.1885	-2.4685
28	H	-1.8048	-2.1921	-1.4108
29	H	-1.8975	-0.8460	-0.2763
30	H	-2.2732	2.5913	-2.5712
31	H	0.9225	-1.8667	-1.3785
32	H	2.8165	-0.3207	-1.5055
33	H	2.4727	1.9018	-2.3149
34	H	1.2547	3.8186	-2.4535
35	H	-0.3282	3.6703	-3.2022
36	H	0.1984	3.6263	-0.3963
37	H	0.3975	-0.6702	-3.9720
38	H	-1.3507	-0.8634	-4.0648
39	H	-0.3569	-2.1567	-3.3932
40	H	2.1938	-1.7748	0.4516
41	H	-0.0262	-2.5625	3.6701
42	H	0.0056	-0.1384	4.4953
43	H	1.9430	1.1754	3.5058
44	H	2.5470	0.6623	1.1168
45	H	-1.7366	-2.1961	1.8910
46	H	-1.3965	-0.4642	1.9304
47	H	2.5594	-1.2110	3.9707
48	H	0.1914	1.1185	1.3820
49	H	3.8819	-1.1459	1.6957
50	H	-3.1169	-1.0421	3.2686