

Supporting Information

New antiproliferative germacranolides from *Carpesium divaricatum*

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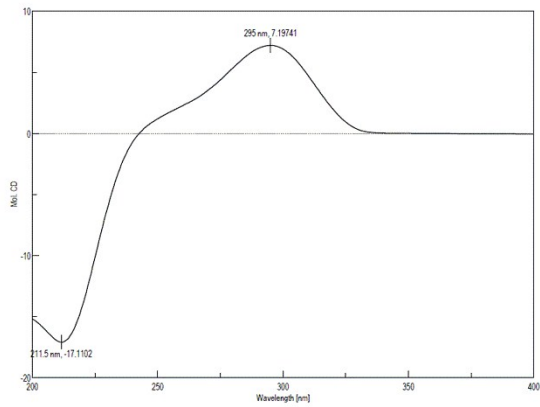
Zhong-Mei Zou, Tel/Fax: 86-10-57833290,

E-mail address: zmzou@implad.ac.cn.

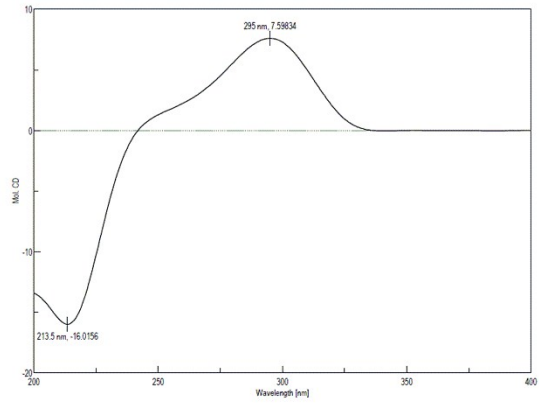
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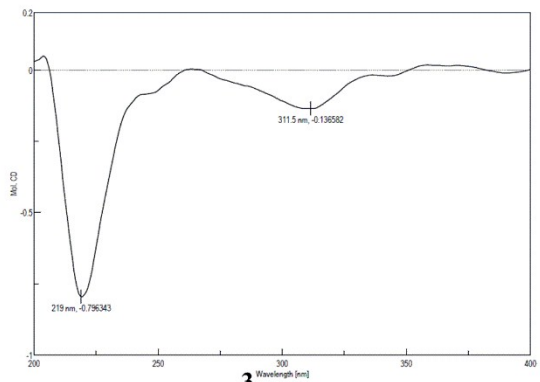


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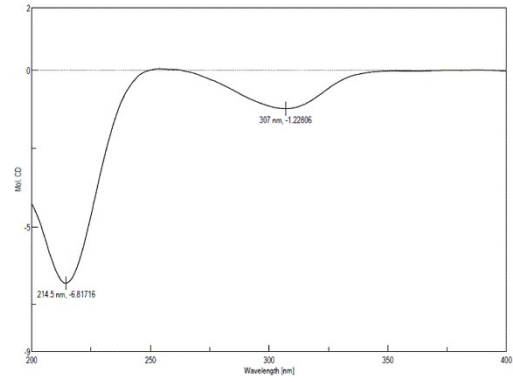


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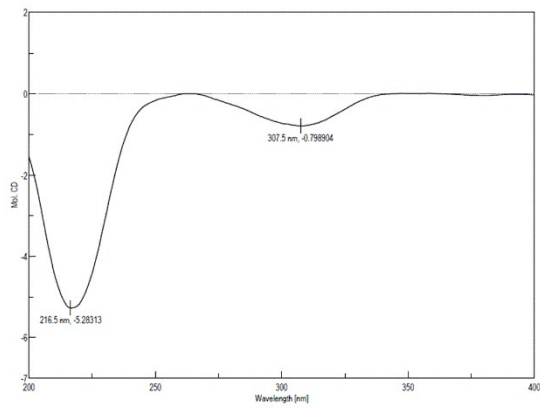
Fig.C1 CD spectra of compounds 1–2



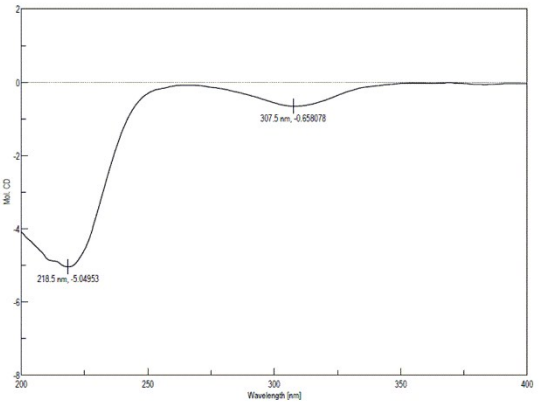
3



4



5



6

Fig.C2 CD spectra of compounds 3–6

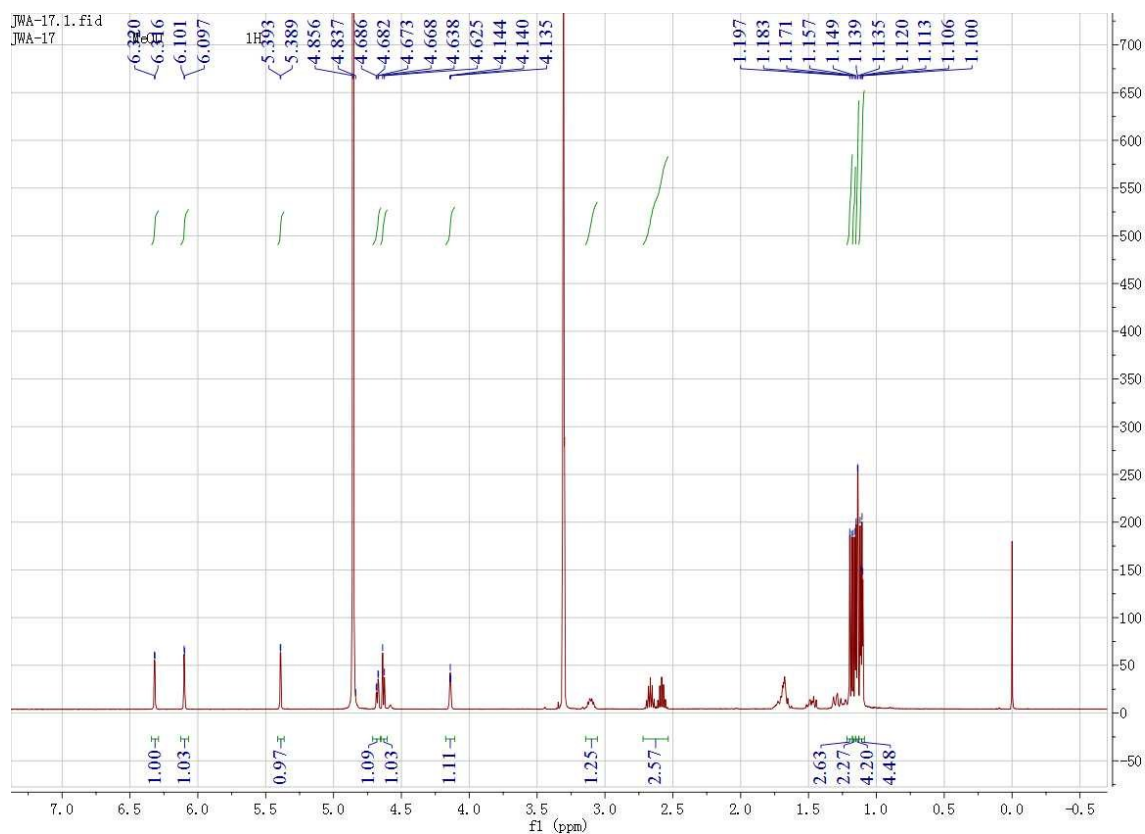


Fig. S1.1 ^1H NMR spectrum (500 MHz) of compound **1** in CD_3OD

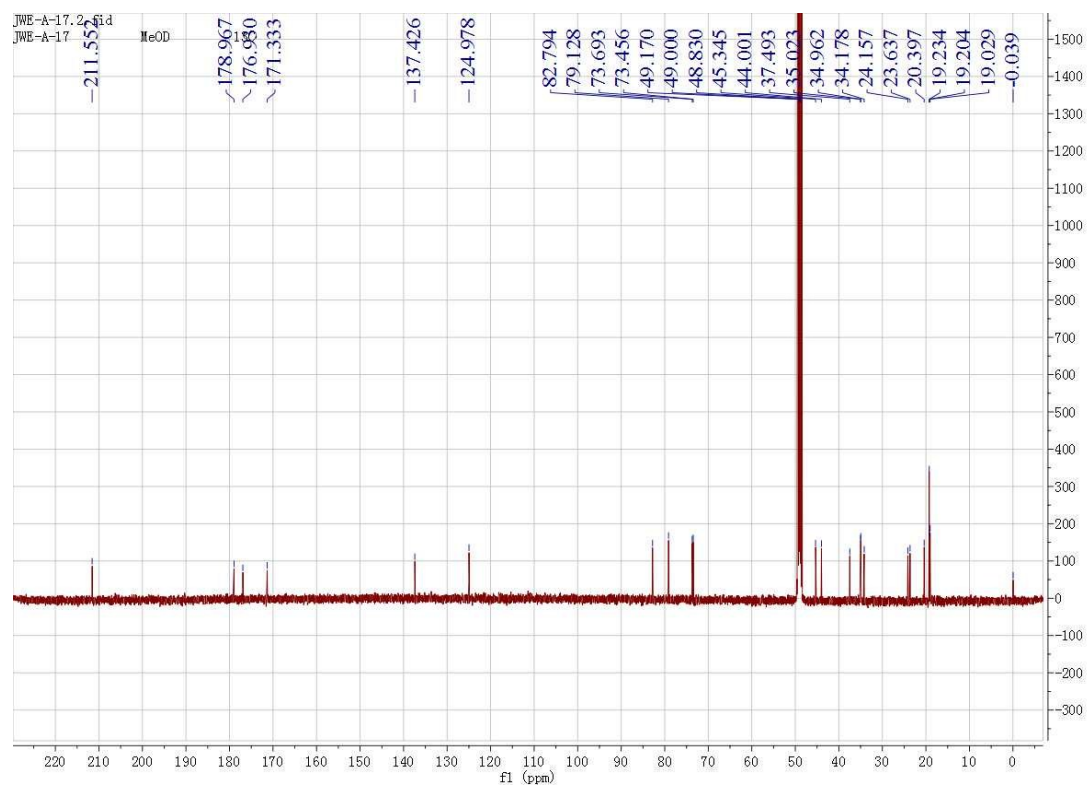


Fig. S1.2 ^{13}C NMR spectrum (125 MHz) of compound **1** in CD_3OD

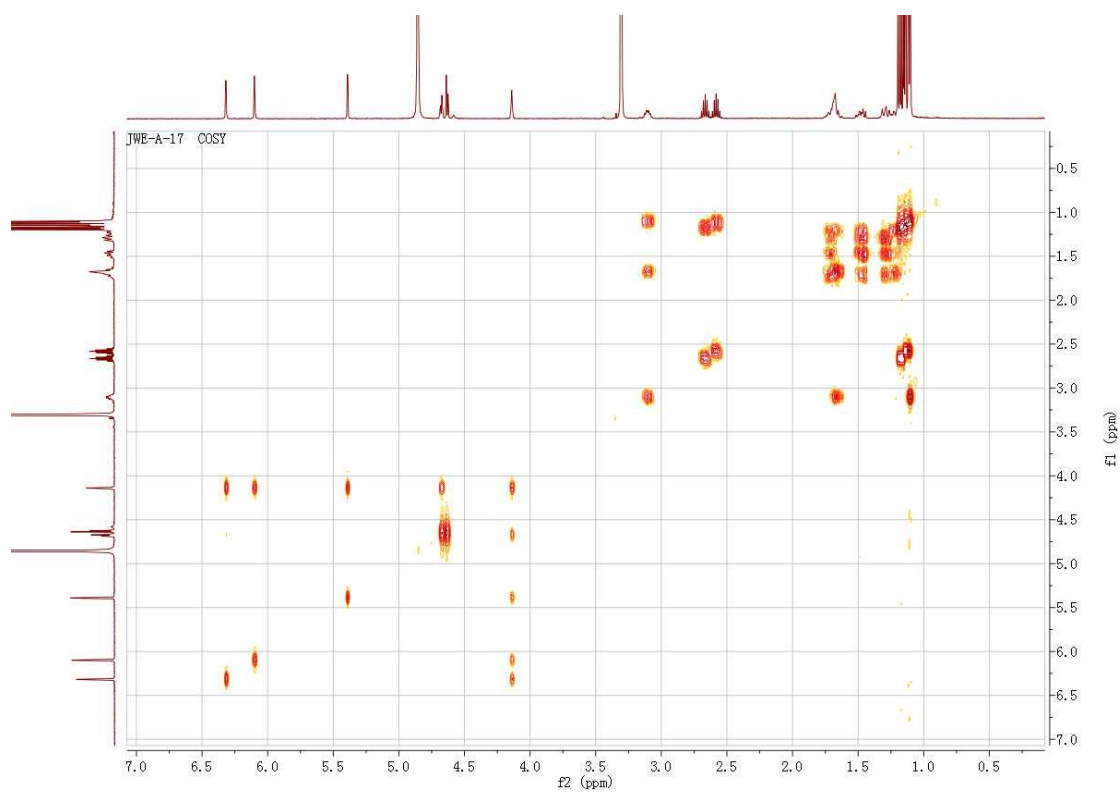


Fig. S1.3 ^1H - ^1H COSY spectrum (500 MHz) of compound **1** in CD_3OD

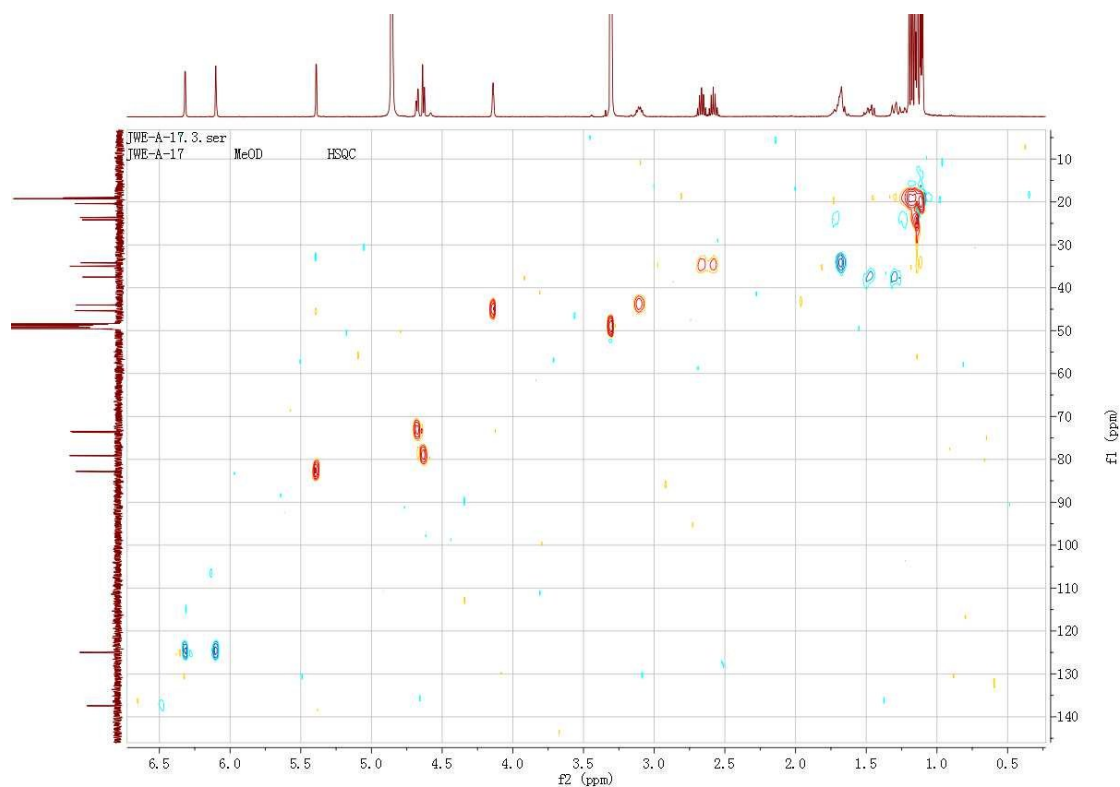


Fig. S1.4 HSQC spectrum (500 MHz) of compound **1** in CD_3OD

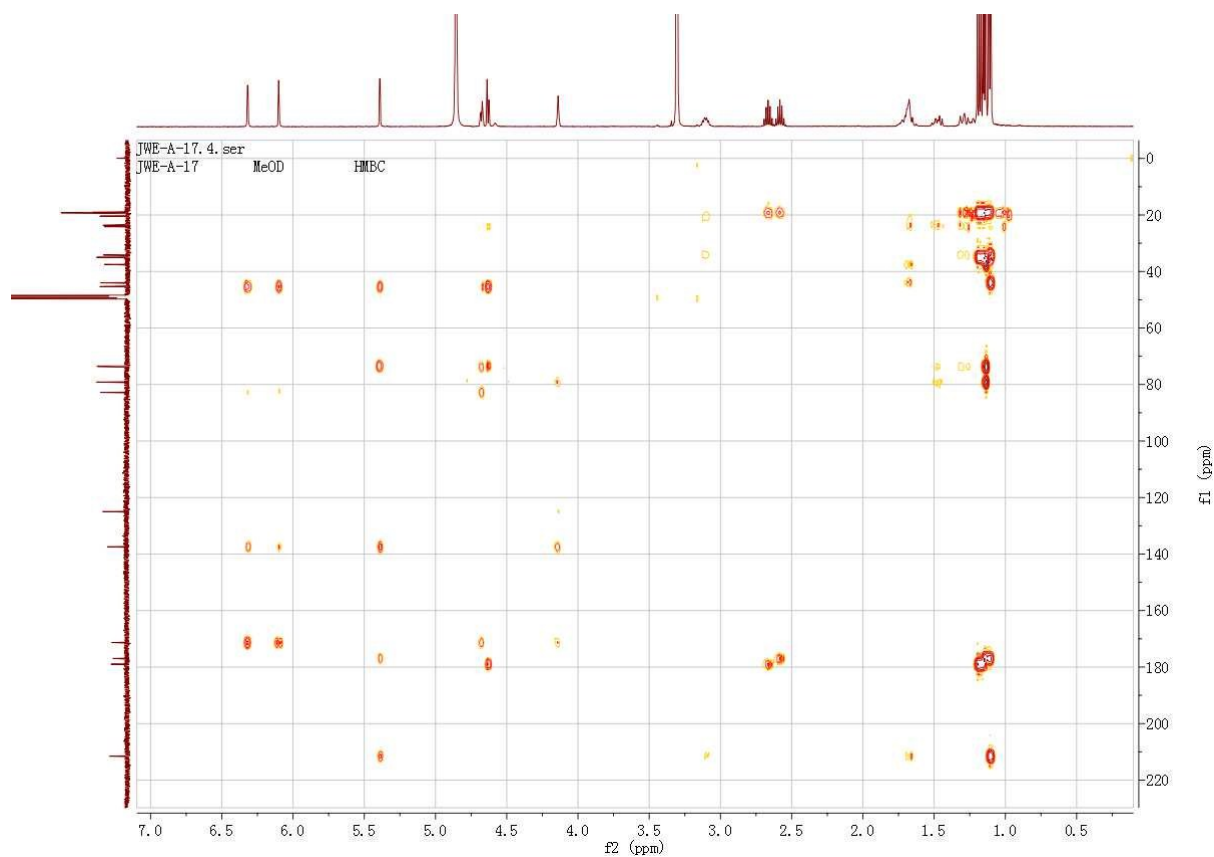


Fig. S1.5 HMBC spectrum (500 MHz) of compound **1** in CD₃OD

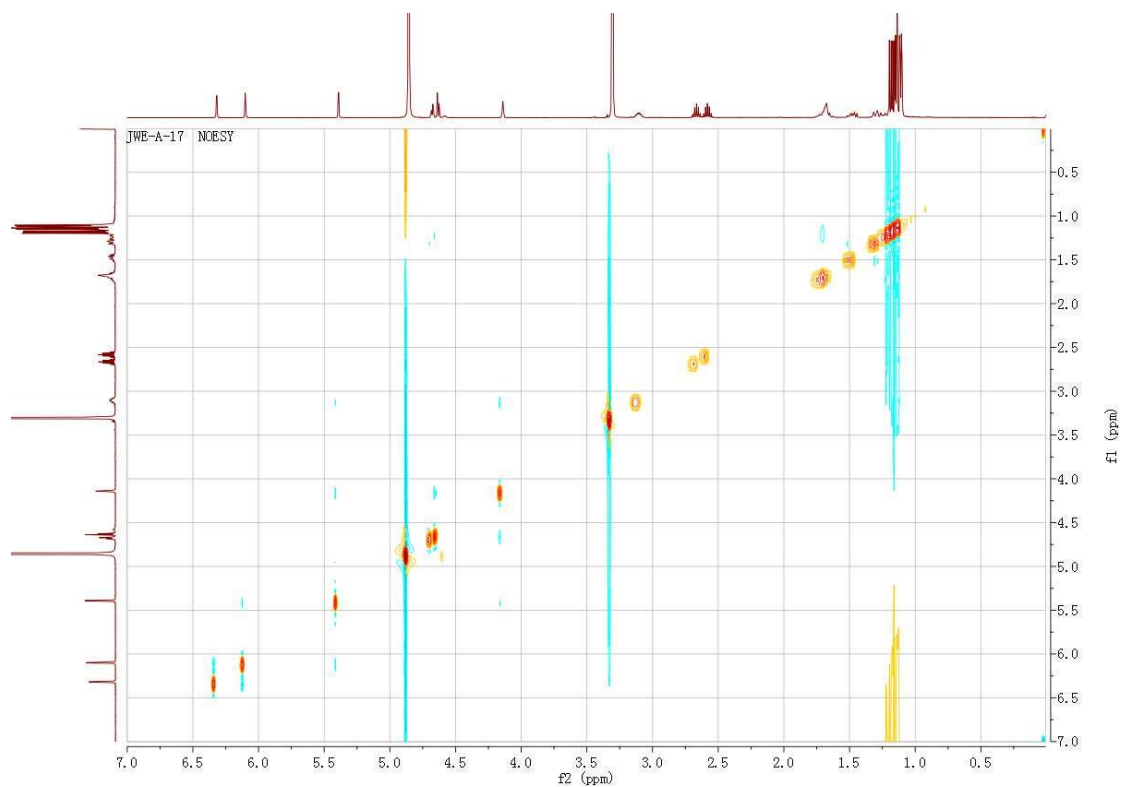


Fig. S1.6 ROESY spectrum (500 MHz) of compound **1** in CD₃OD

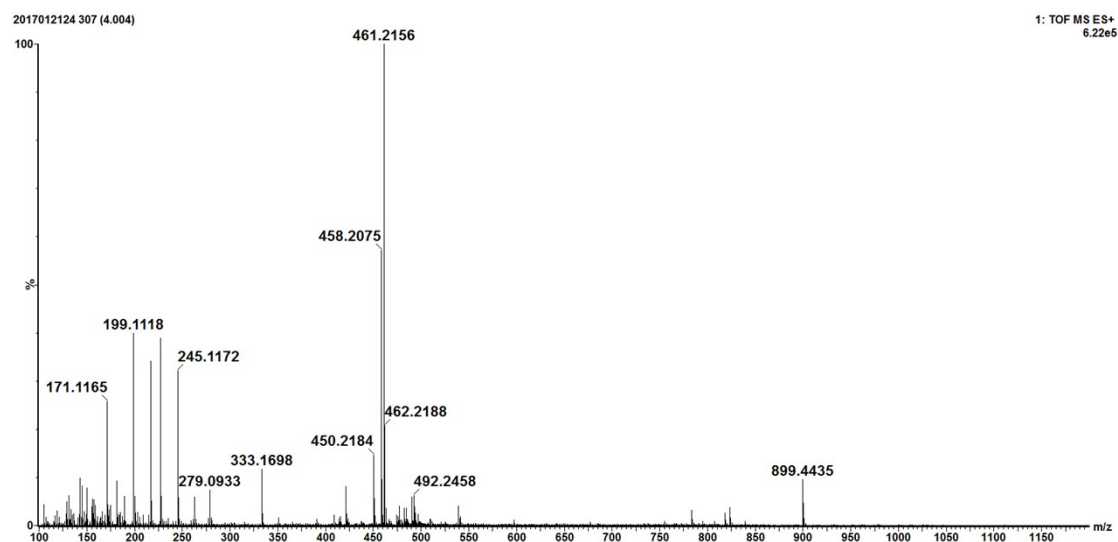


Fig. S1.7 HRESIMS spectrum of compound **1**

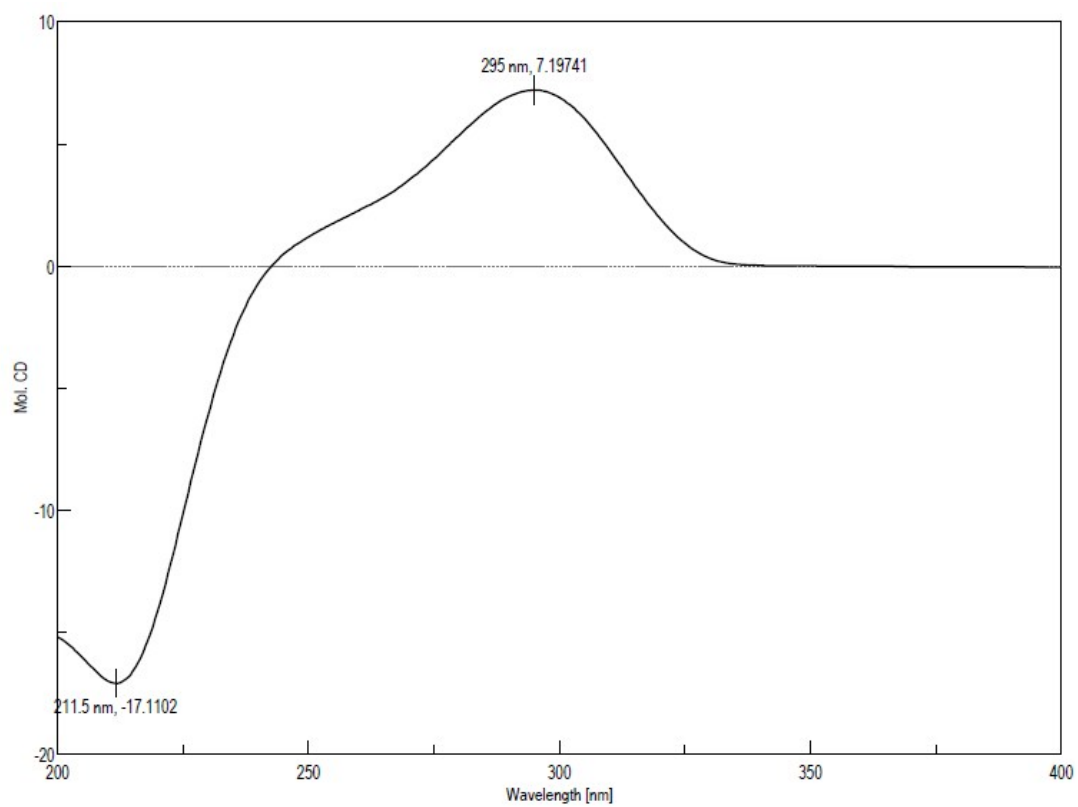


Fig. S1.8 CD spectrum of compound **1**

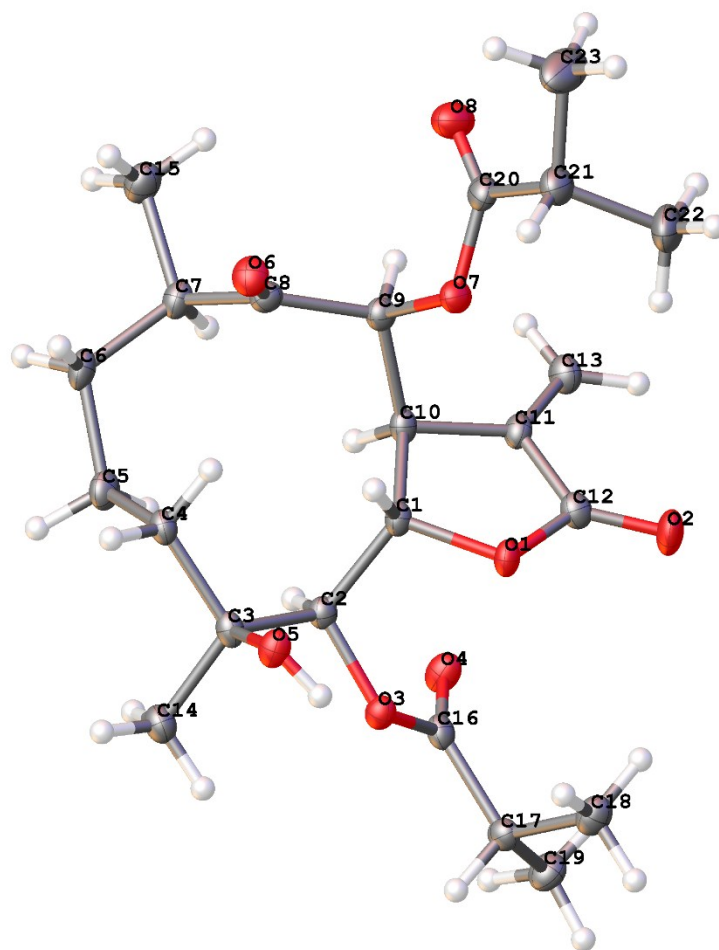


Fig. S1.9 X-ray ORTEP drawing of 1

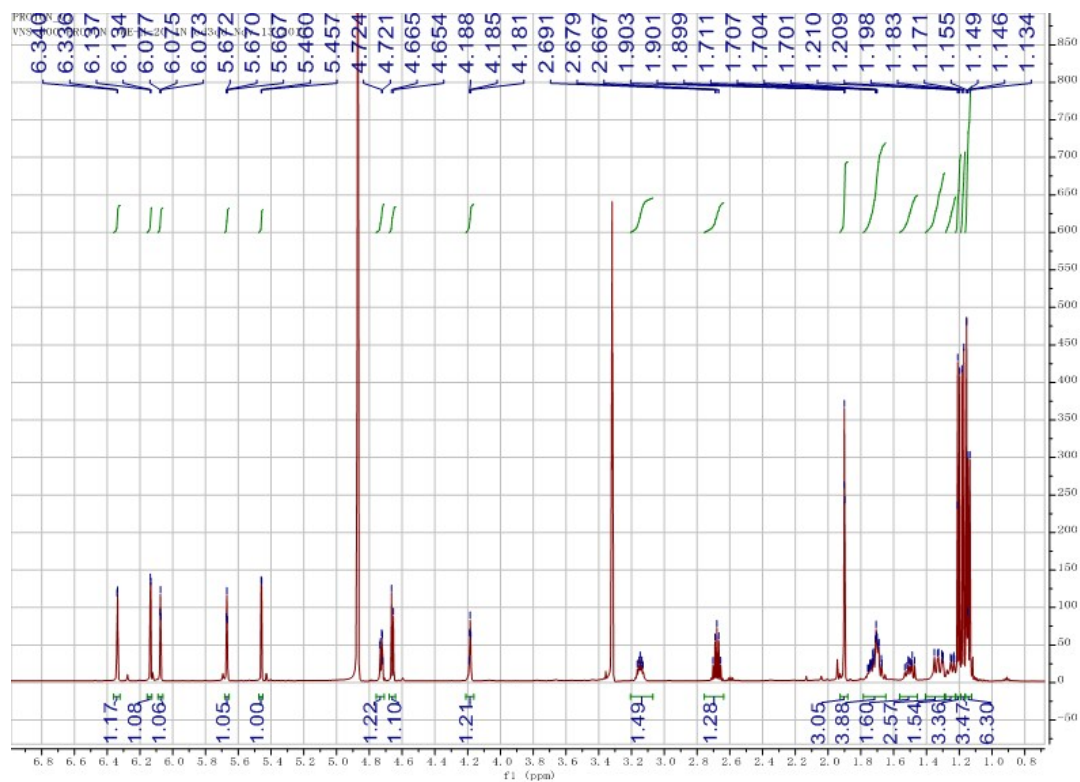


Fig. S2.1 ¹H NMR spectrum (600 MHz) of compound **2** in CD₃OD

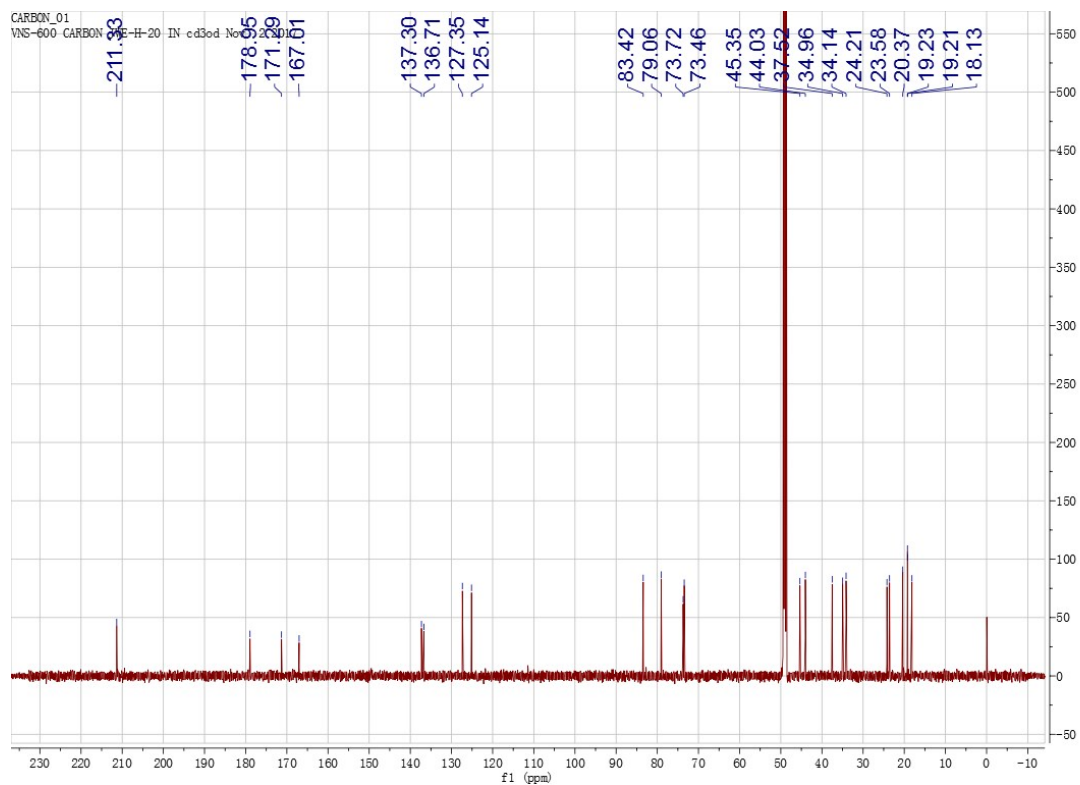


Fig. S2.2 ¹³C NMR spectrum (150 MHz) of compound **2** in CD₃OD

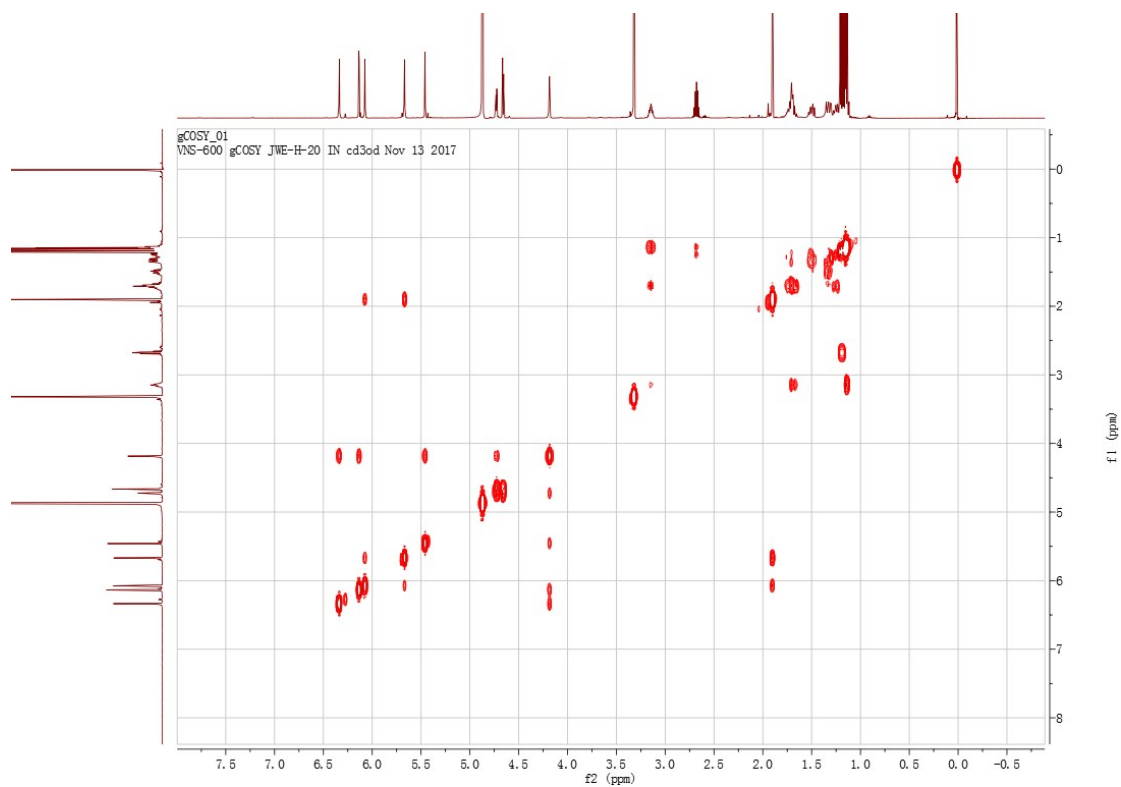


Fig. S2.3 ^1H - ^1H COSY spectrum (600 MHz) of compound **2** in CD_3OD

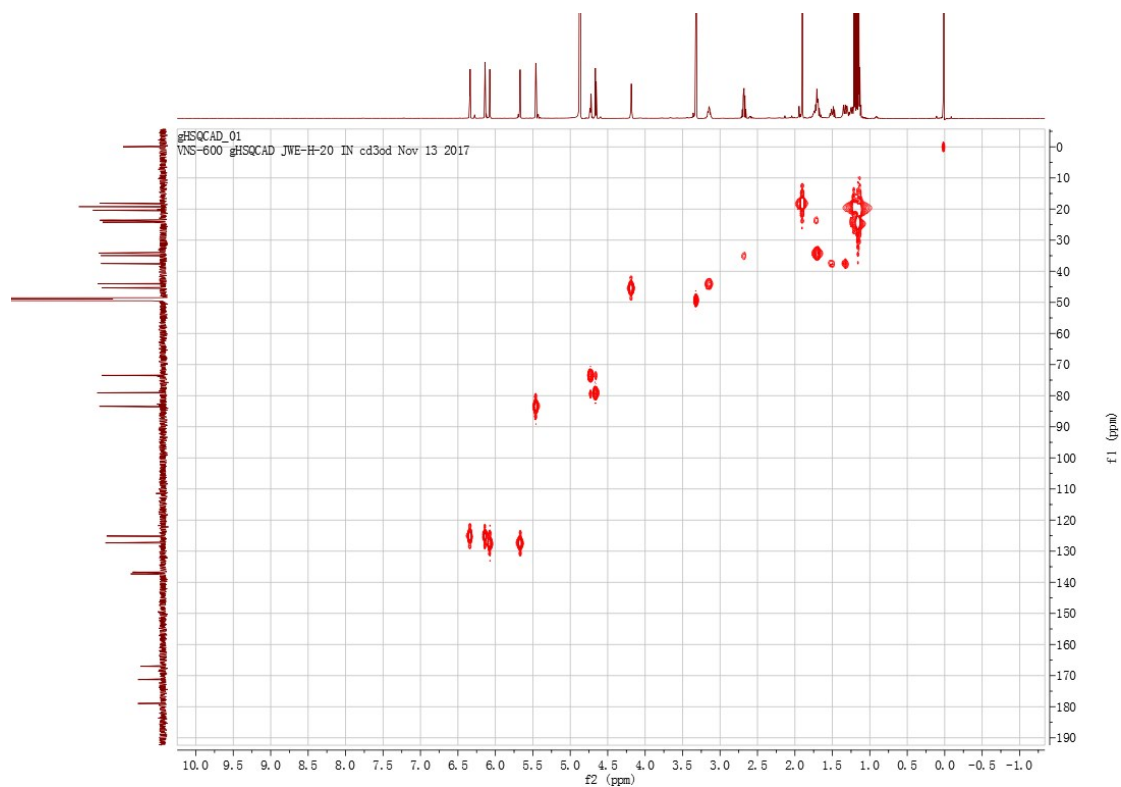


Fig. S2.4 HSQC spectrum (600 MHz) of compound **2** in CD_3OD

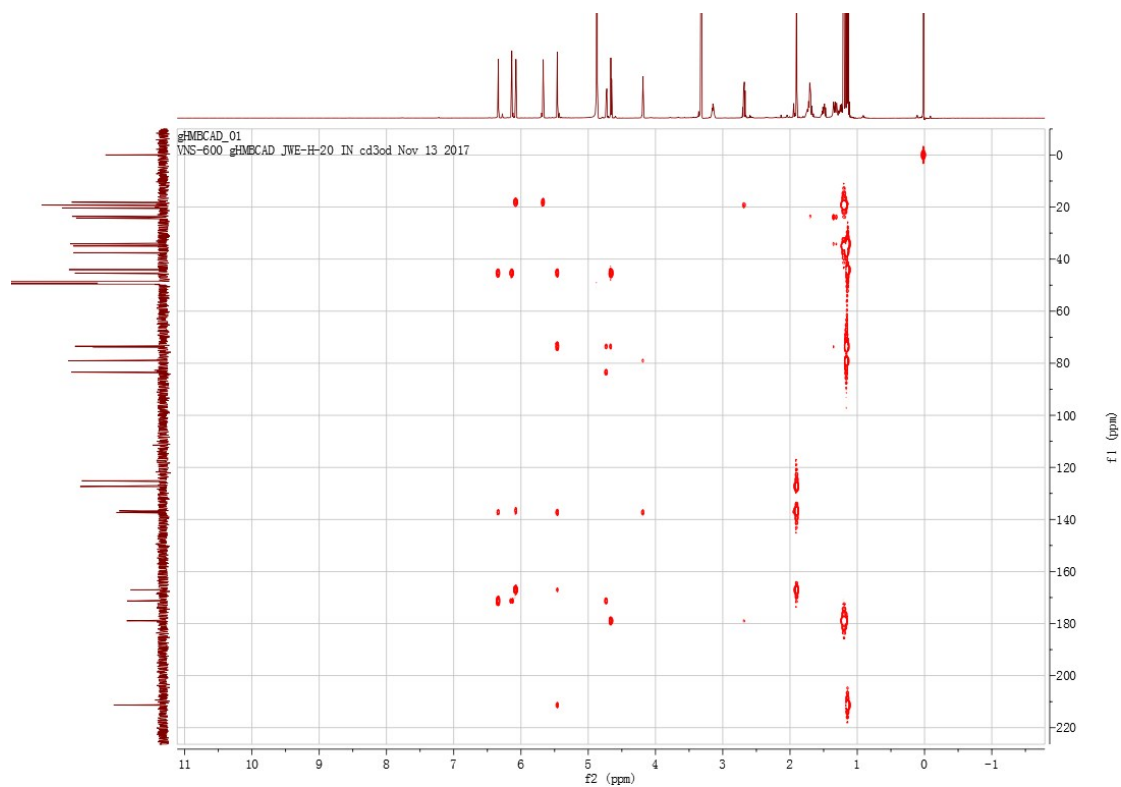


Fig. S2.5 HMBC spectrum (600 MHz) of compound **2** in CD₃OD

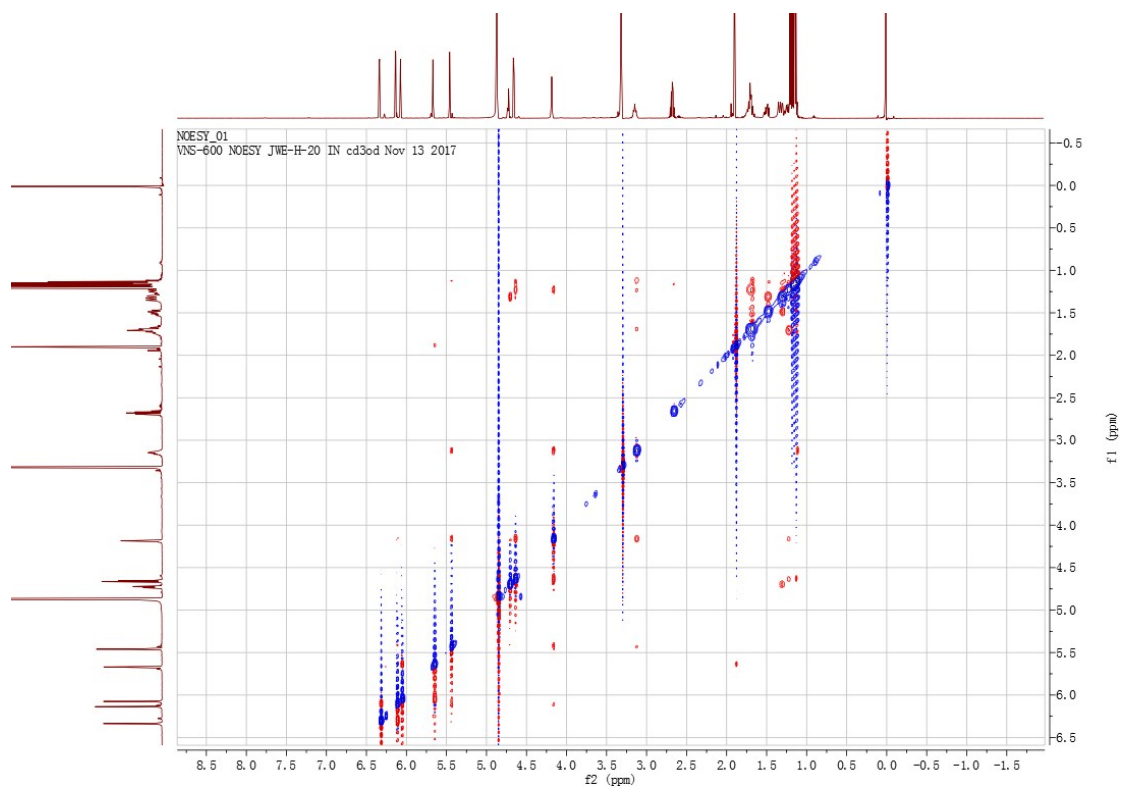
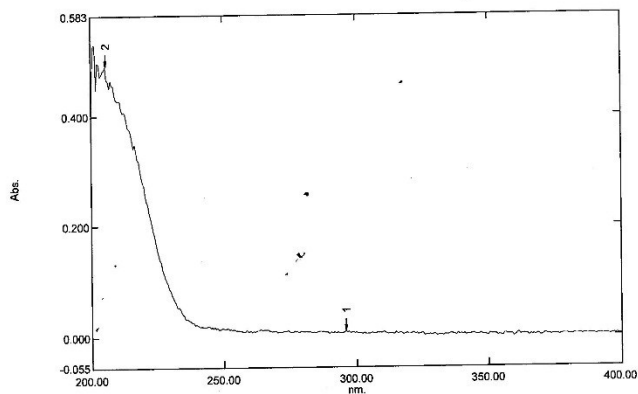


Fig. S2.6 NOESY spectrum (600 MHz) of compound **2** in CD₃OD

Data Set: Storage 004614 - RawData - D:\2018\JCB-H-20.spc



No.	P/V	Wavelength	Abs.	Description
1	●	296.00	0.009	
2	●	205.50	0.490	

样品溶于 1.20ml MeOH
旋光: -0.002°
UV: 吸取 0.5ml → 3.0ml

Measurement Properties
Wavelength Range (nm.): 200.00 to 400.00
Scan Speed: Medium
Sampling Interval: 0.5
Auto Sampling Interval: Disabled
Scan Mode: Single

Sample Preparation Properties
Weight:
Volume:

Fig. S2.7 UV spectrum of compound 2

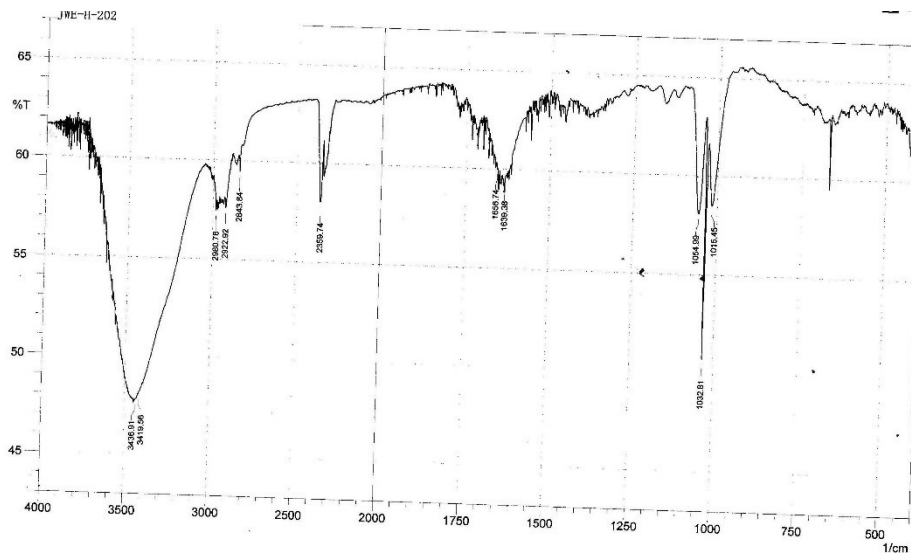


Fig. S2.8 IR spectrum of compound 2

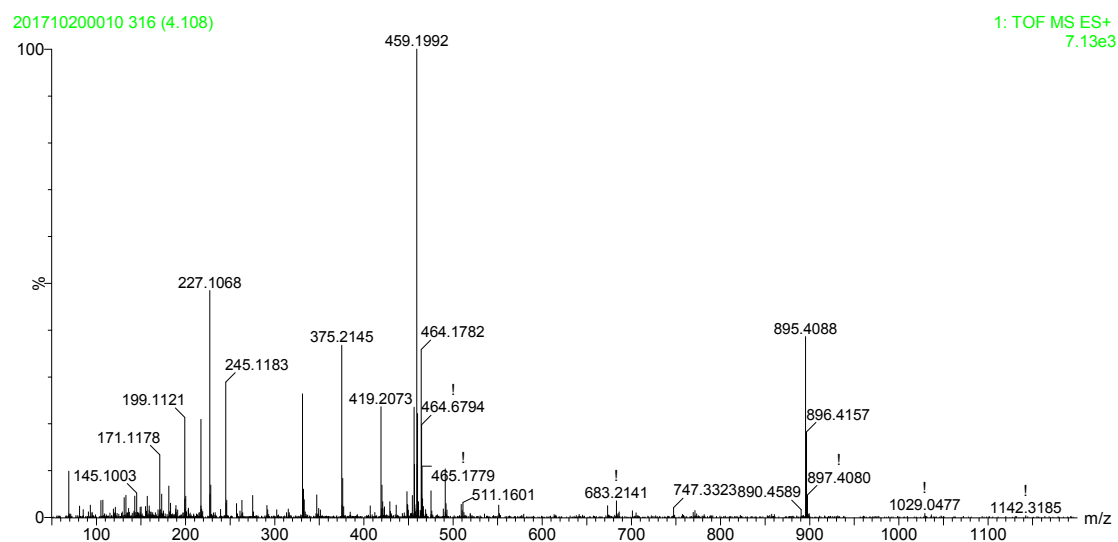


Fig. S2.9 HRESIMS spectrum of compound **2**

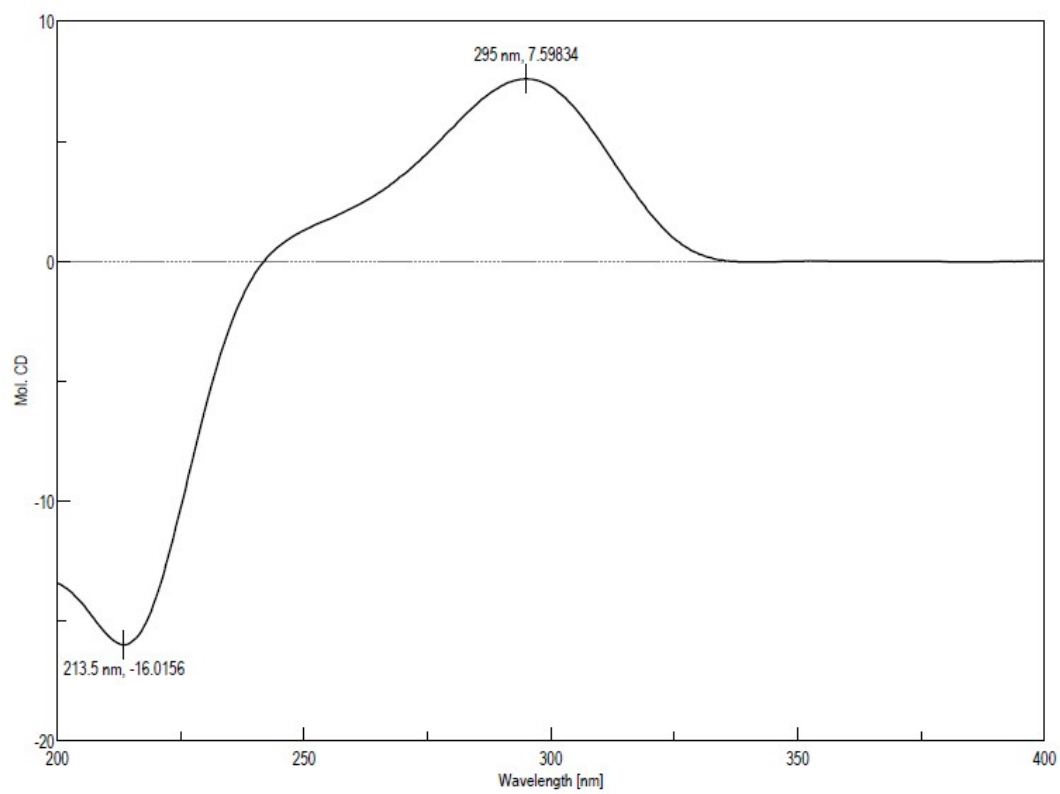


Fig. S2.10 CD spectrum of compound **2**

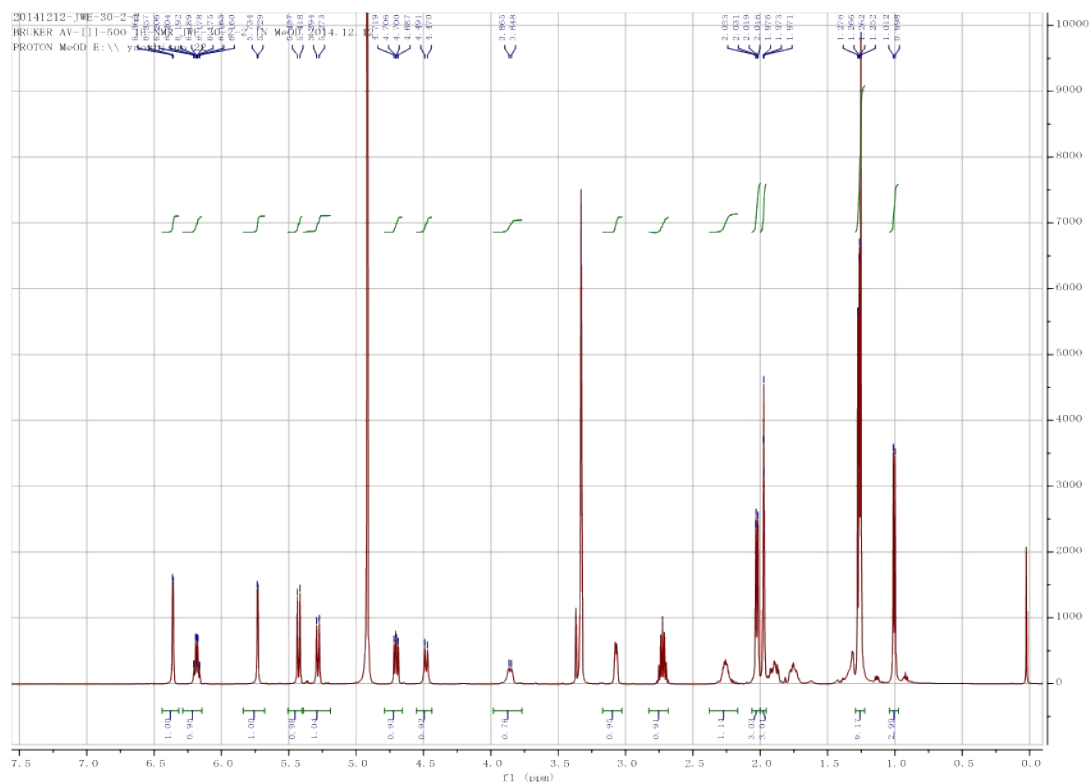


Fig. S3.1 ^1H NMR spectrum (600 MHz) of compound **3** in CD_3OD

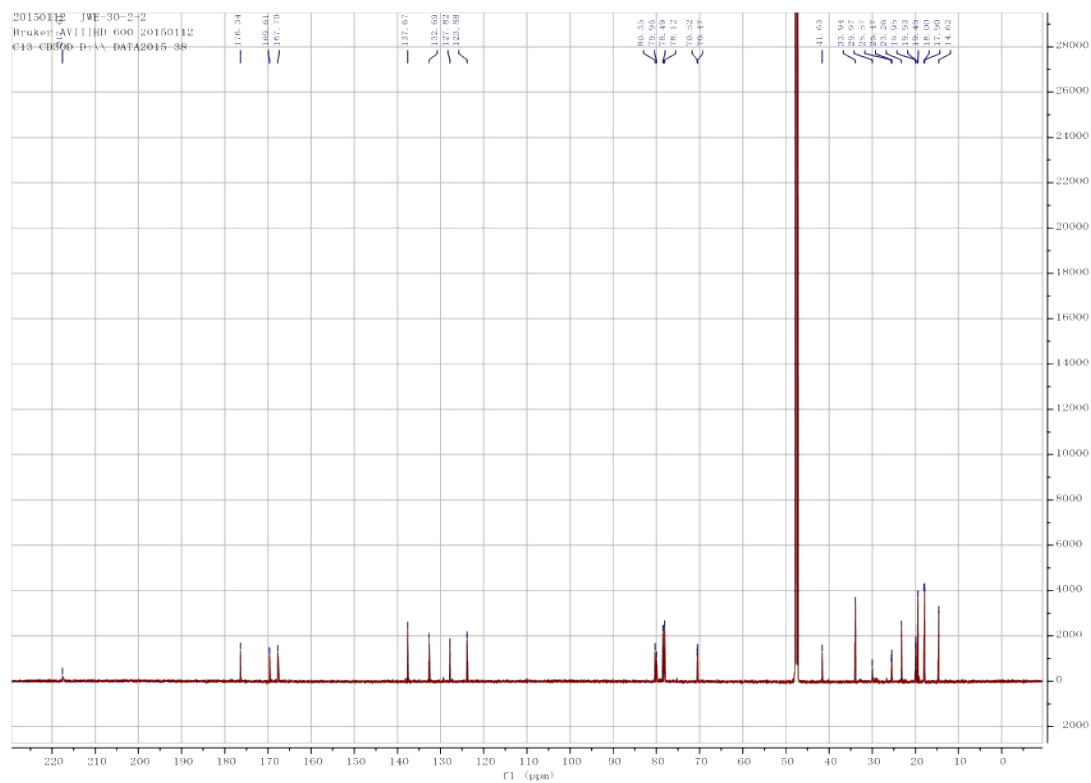


Fig. S3.2 ^{13}C NMR spectrum (150 MHz) of compound **3** in CD_3OD

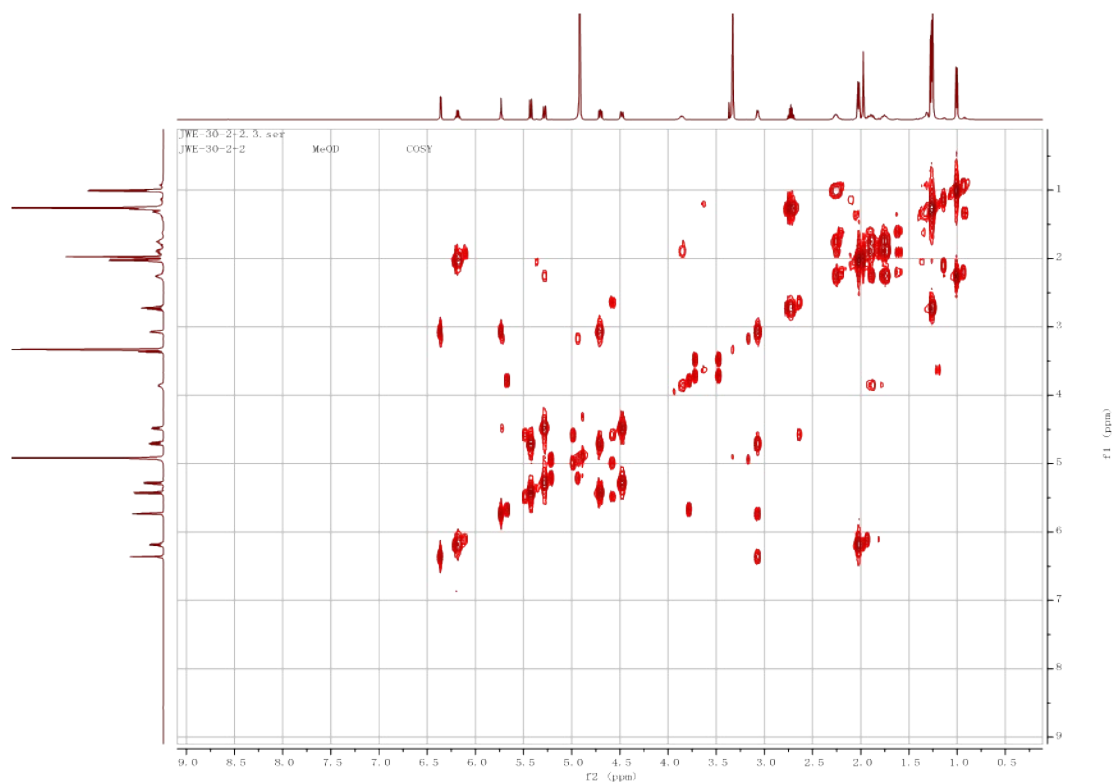


Fig. S3.3 ^1H - ^1H COSY spectrum (600 MHz) of compound **3** in CD_3OD

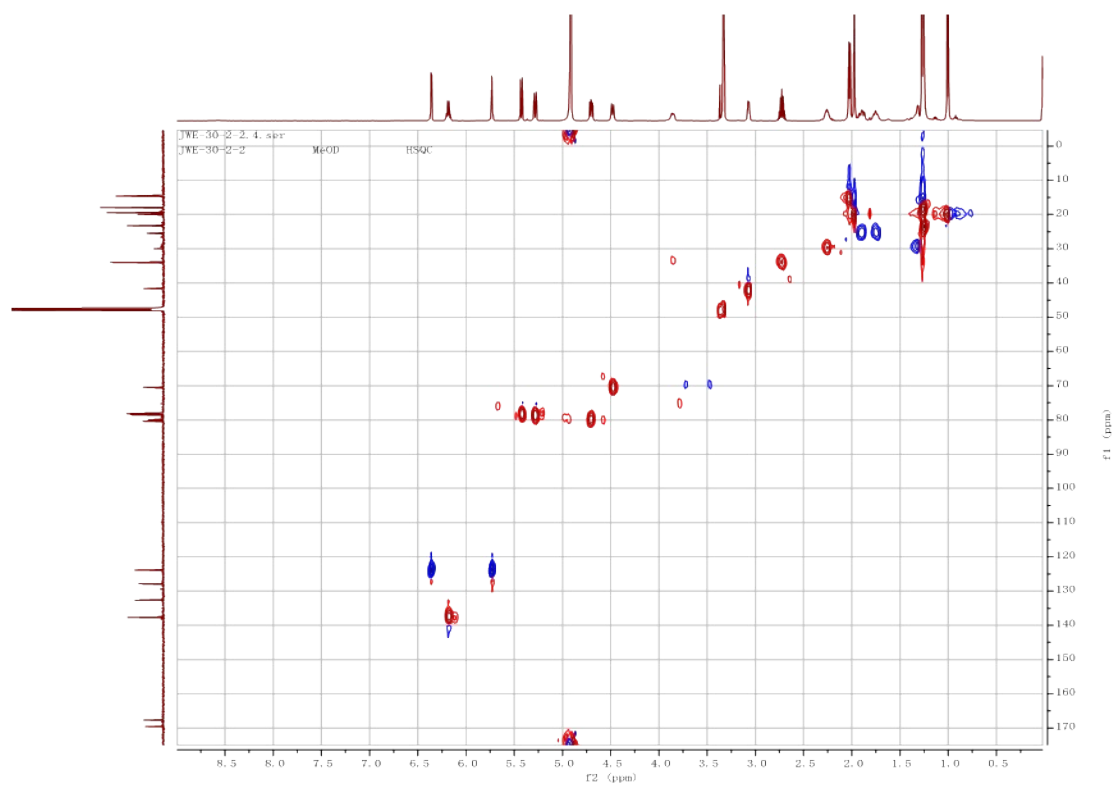


Fig. S3.4 HSQC spectrum (600 MHz) of compound **3** in CD_3OD

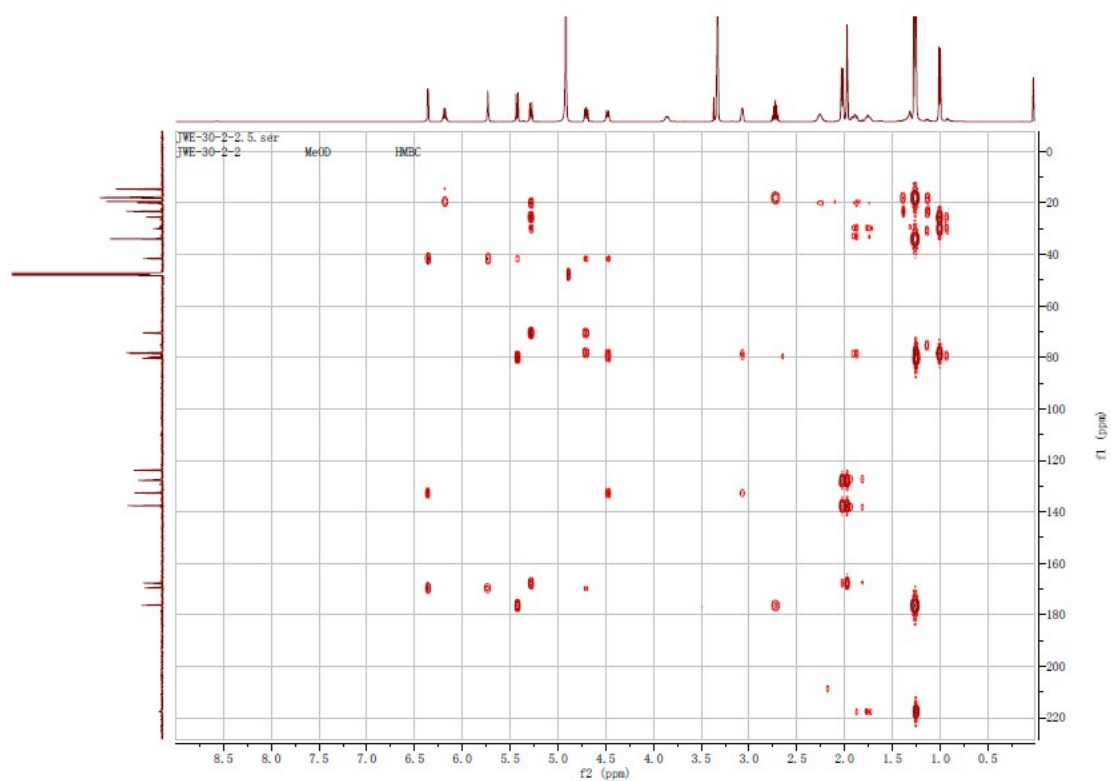


Fig. S3.5 HMBC spectrum (600 MHz) of compound **3** in CD₃OD

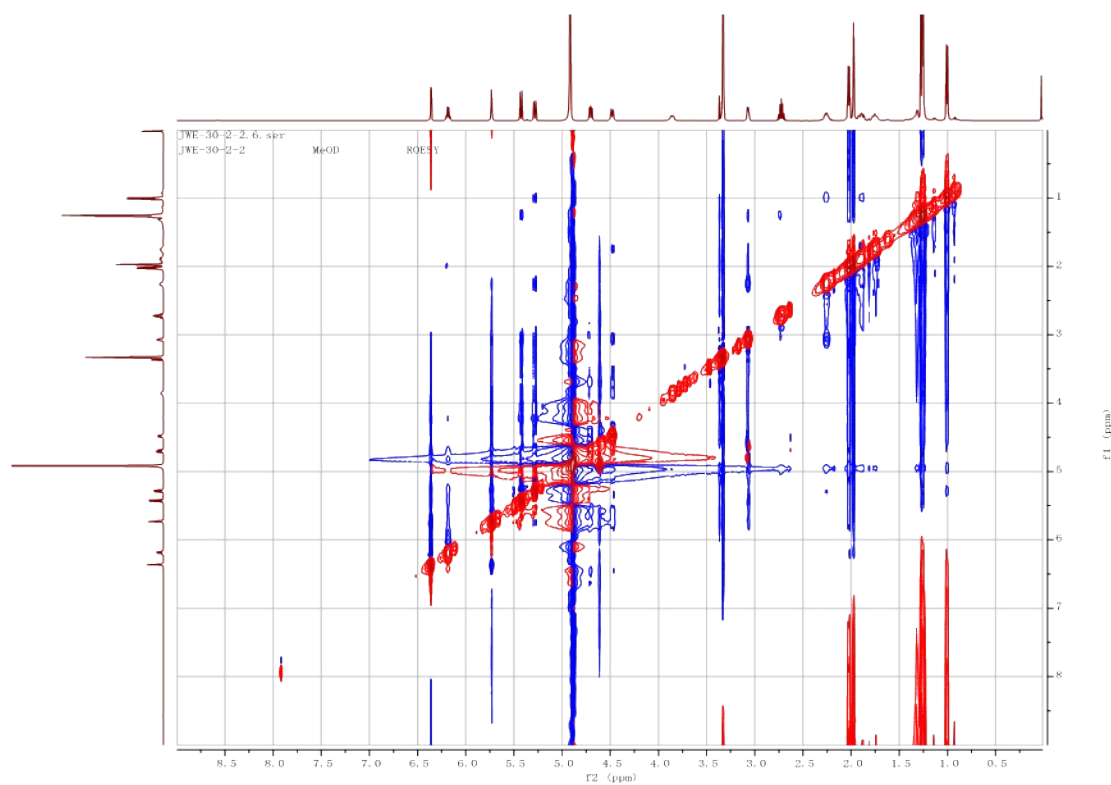
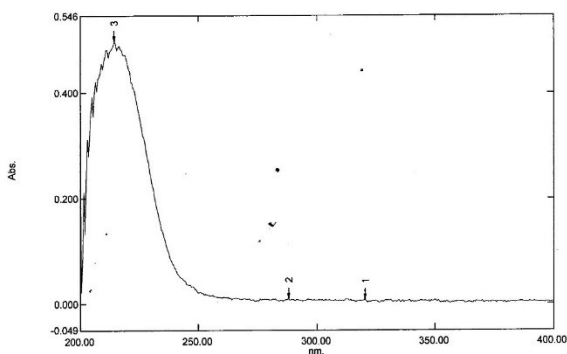


Fig. S3.6 ROESY spectrum (600 MHz) of compound **3** in CD₃OD

1.5mg

Data Set: Storage 012536 - RawData - D:\2018\34-4.spc



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2	●	288.50	0.008	
3	●	214.50	0.496	

样品溶于2.0ml MeOH
旋光: -0.015°
UV: 吸取0.5ml → 3ml.

Measurement Properties
Wavelength Range (nm.): 200.00 to 400.00
Scan Speed: Medium
Sampling Interval: 0.5
Auto Sampling Interval: Disabled
Scan Mode: Single

Sample Preparation Properties
Weight:
Volume:

Fig. S3.7 UV spectrum of compound 3

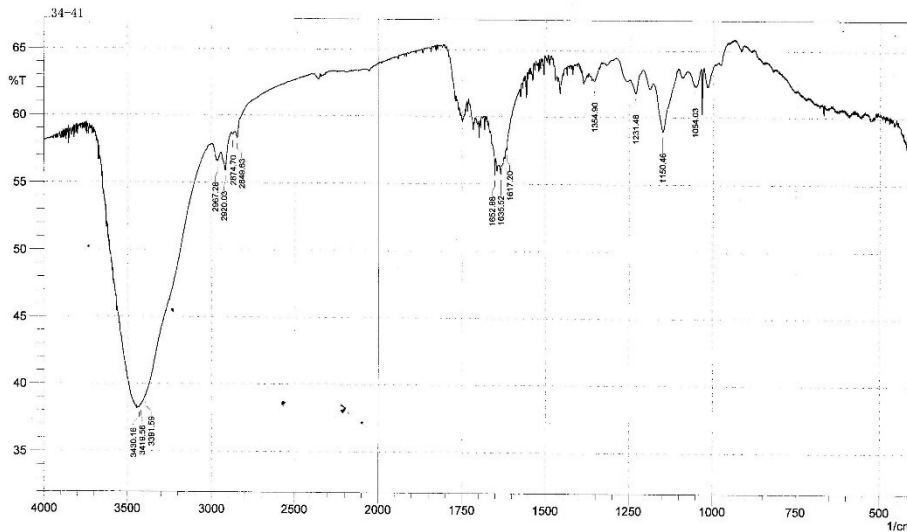


Fig. S3.8 IR spectrum of compound 3

ZT_JWE_34_4

20141102_037 501 (6.512) Cm (500:503)

1: TOF MS ES+
8.88e5

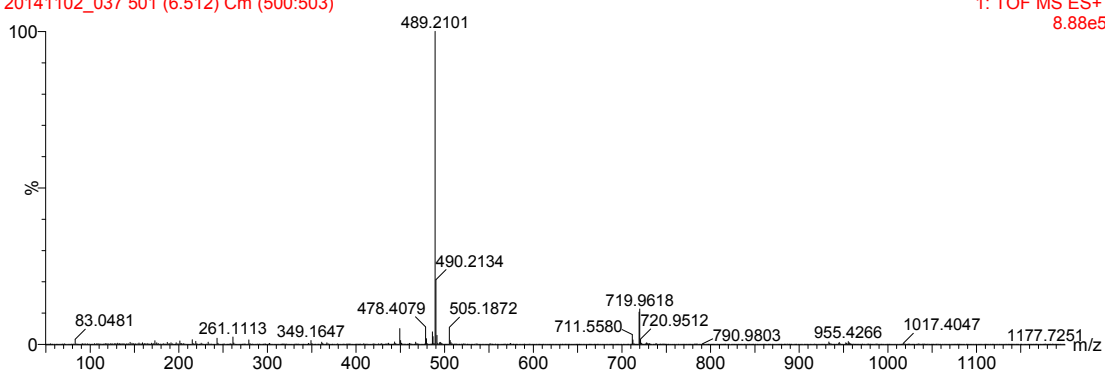


Fig. S3.9 HRESIMS spectrum of compound **3**

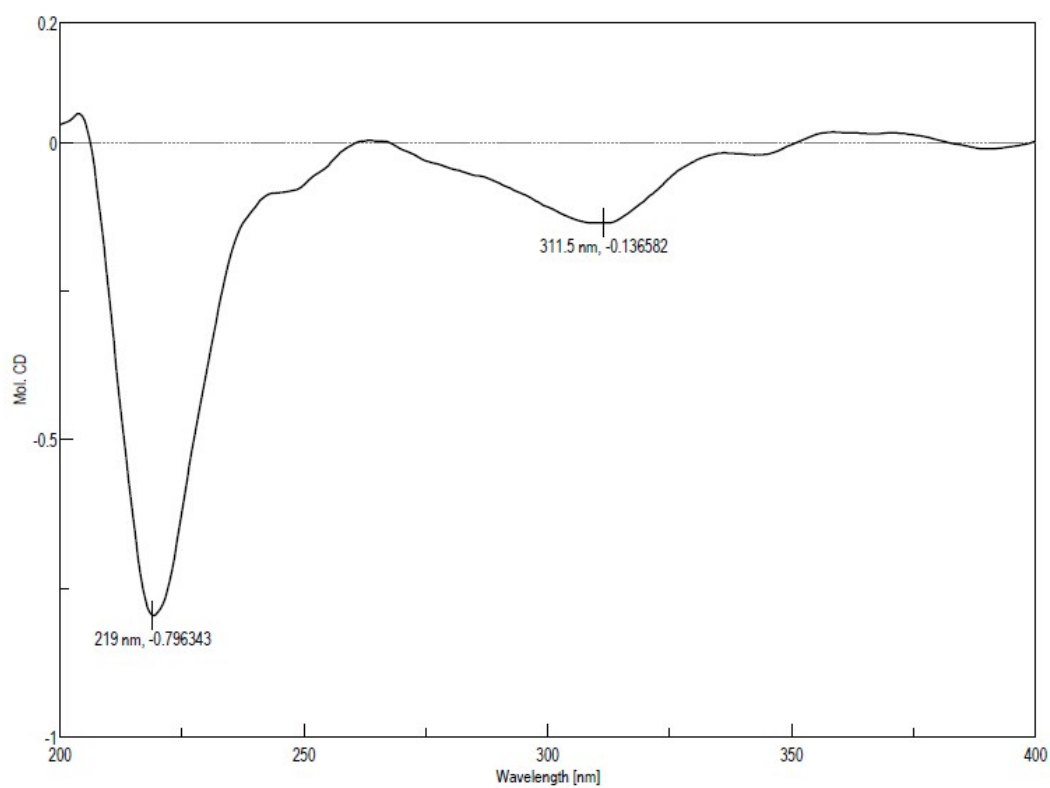


Fig. S3.10 CD spectrum of compound **3**

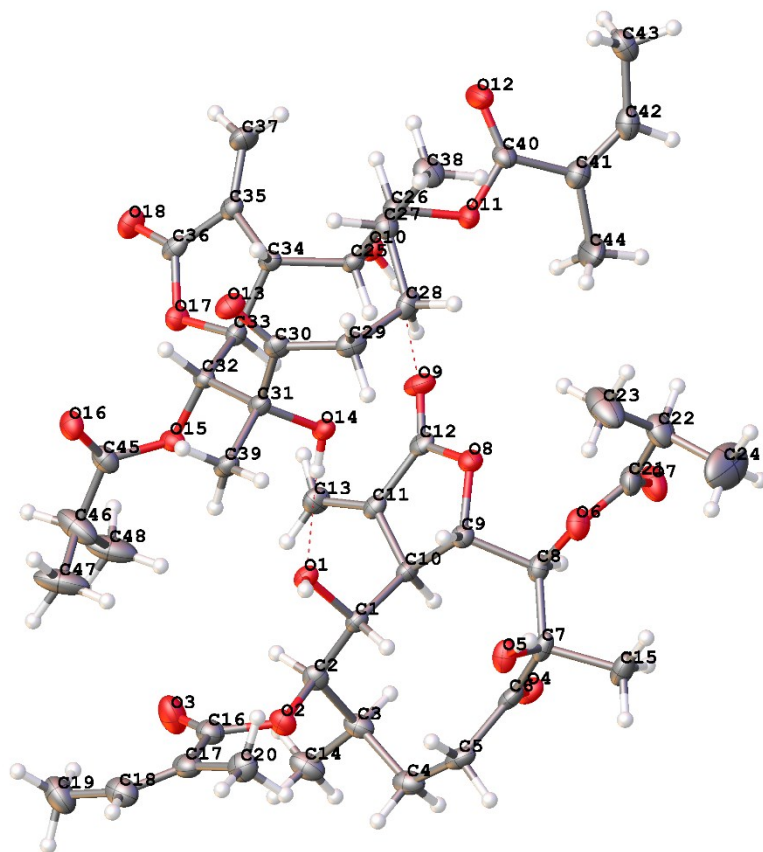


Fig. S3.11 X-ray ORTEP drawing of **3**

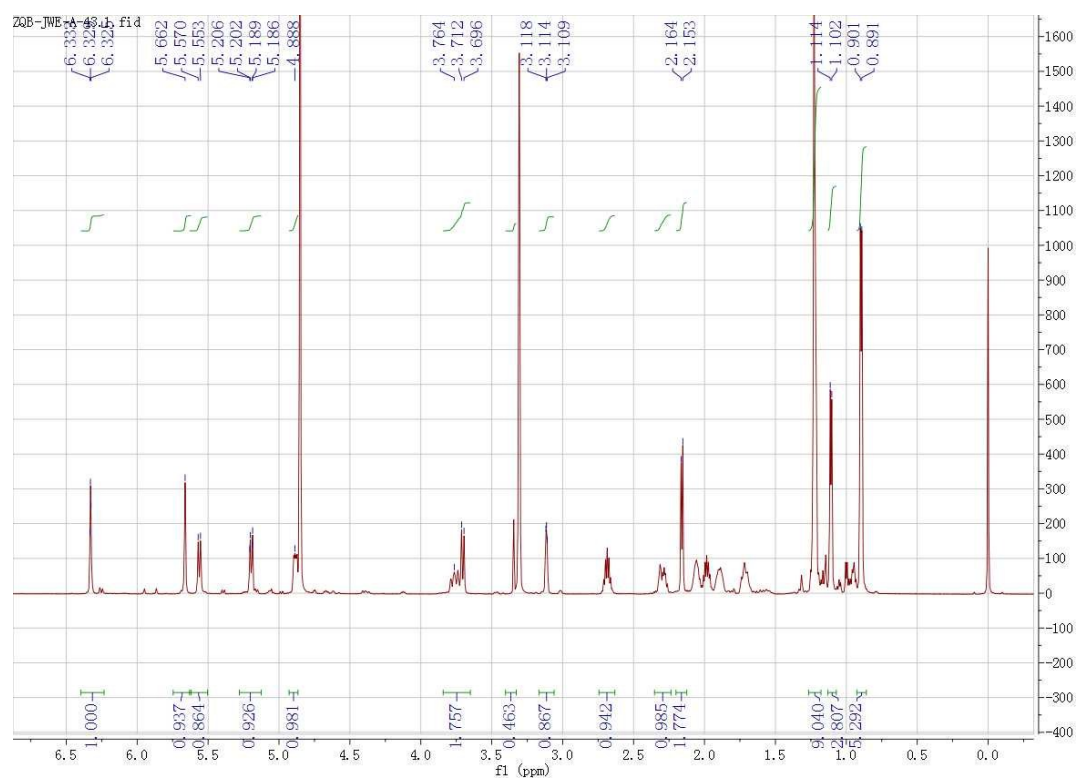


Fig. S4.1 ^1H NMR spectrum (500 MHz) of compound **4** in CD_3OD

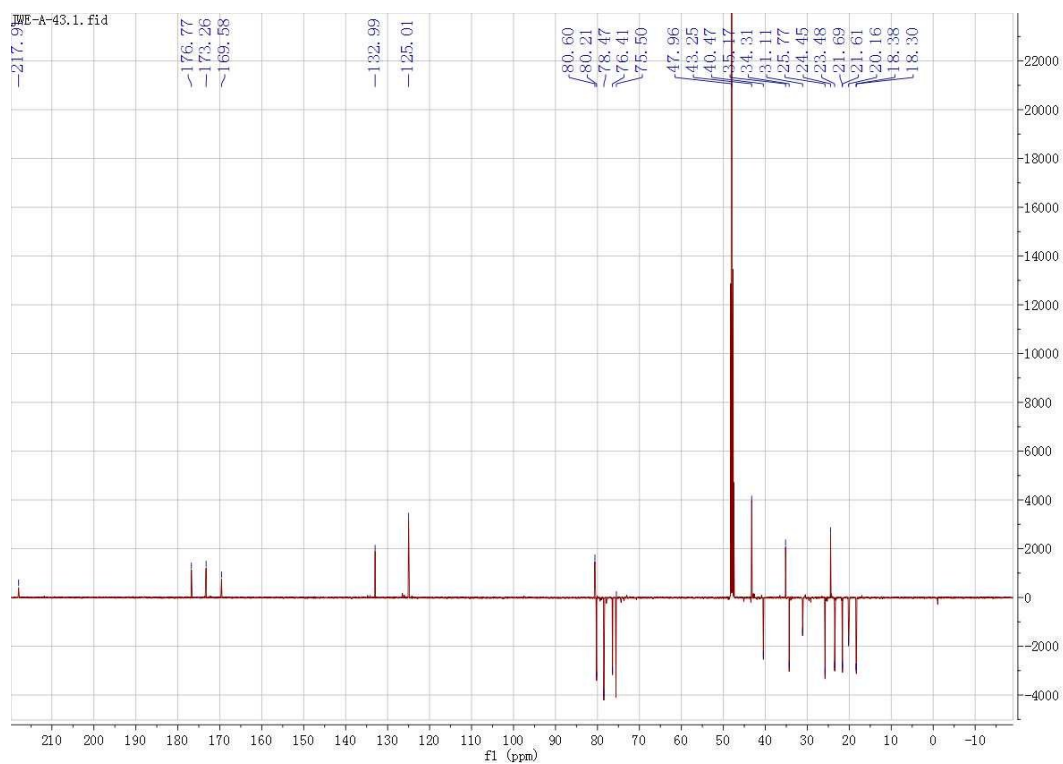


Fig. S4.2 ¹³C NMR spectrum (125 MHz) of compound 4 in CD₃OD

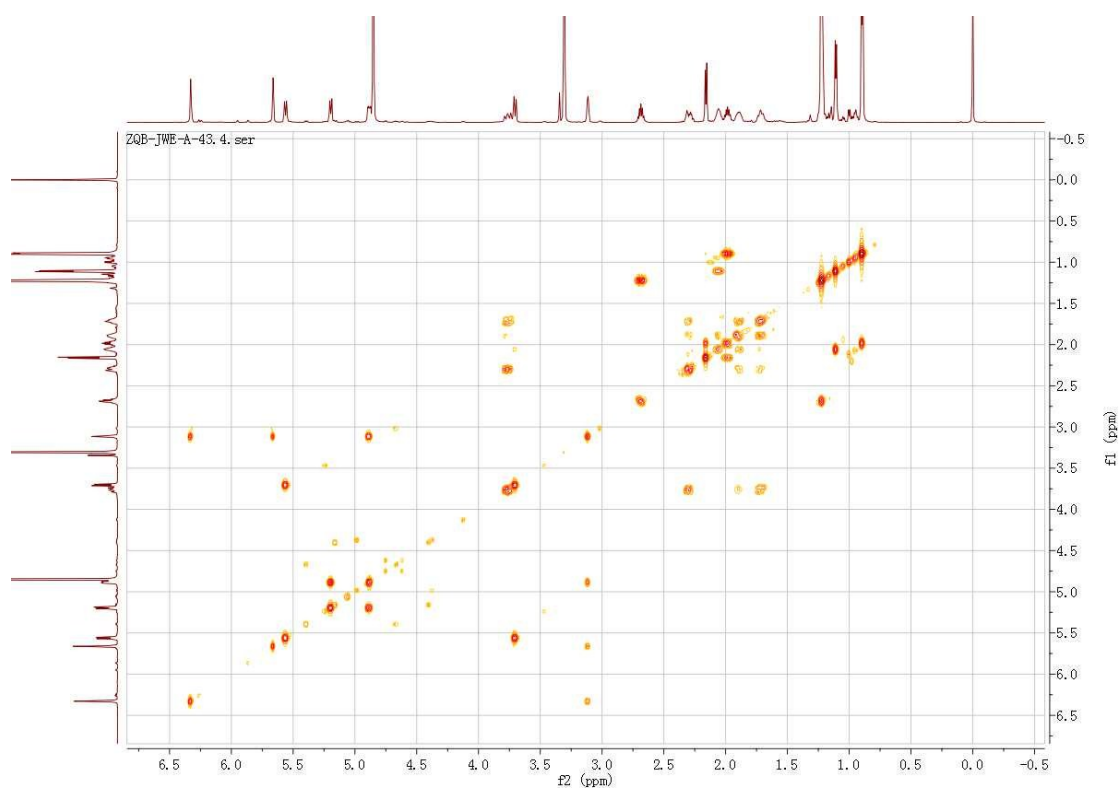


Fig. S4.3 ¹H-¹H COSY spectrum (500 MHz) of compound 4 in CD₃OD

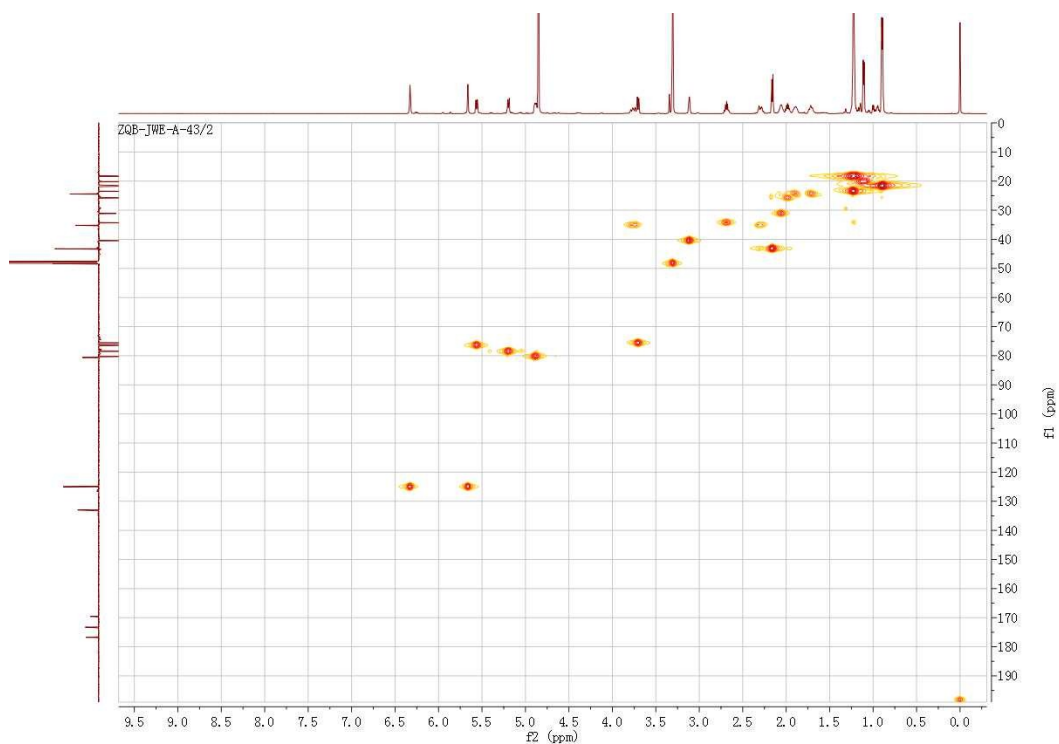


Fig. S4.4 HSQC spectrum (500 MHz) of compound **4** in CD₃OD

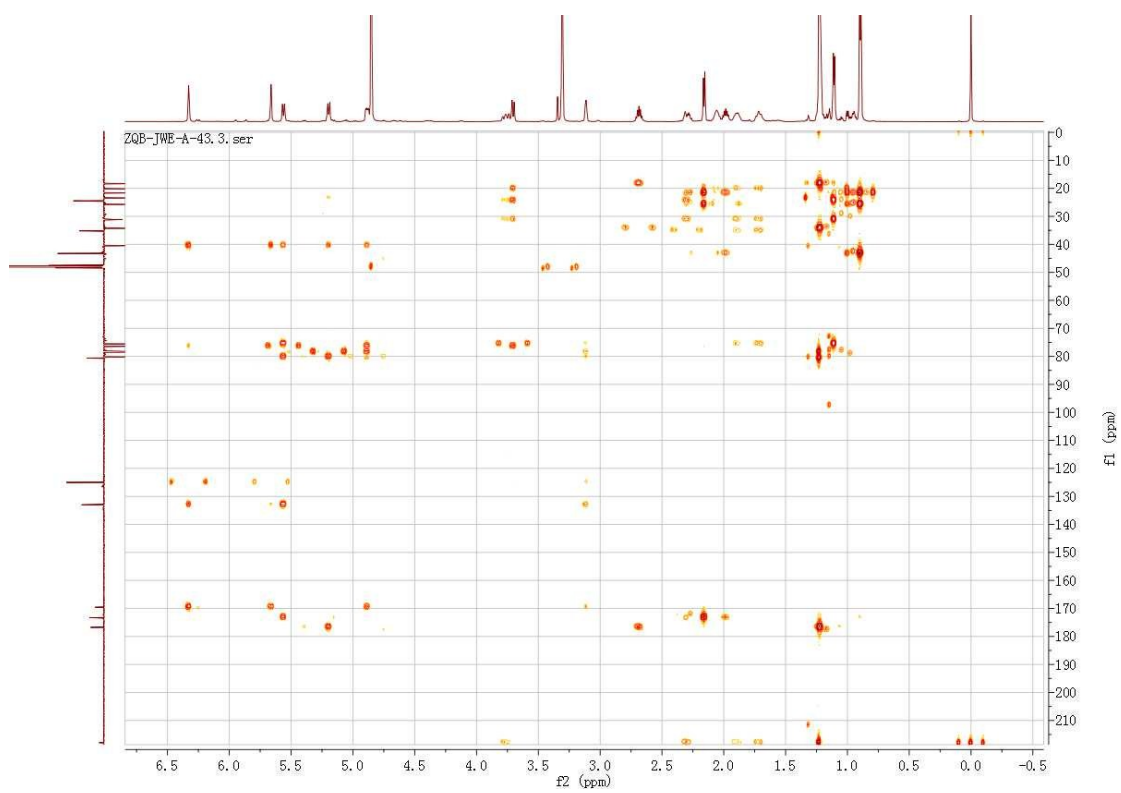


Fig. S4.5 HMBC spectrum (500 MHz) of compound **4** in CD₃OD

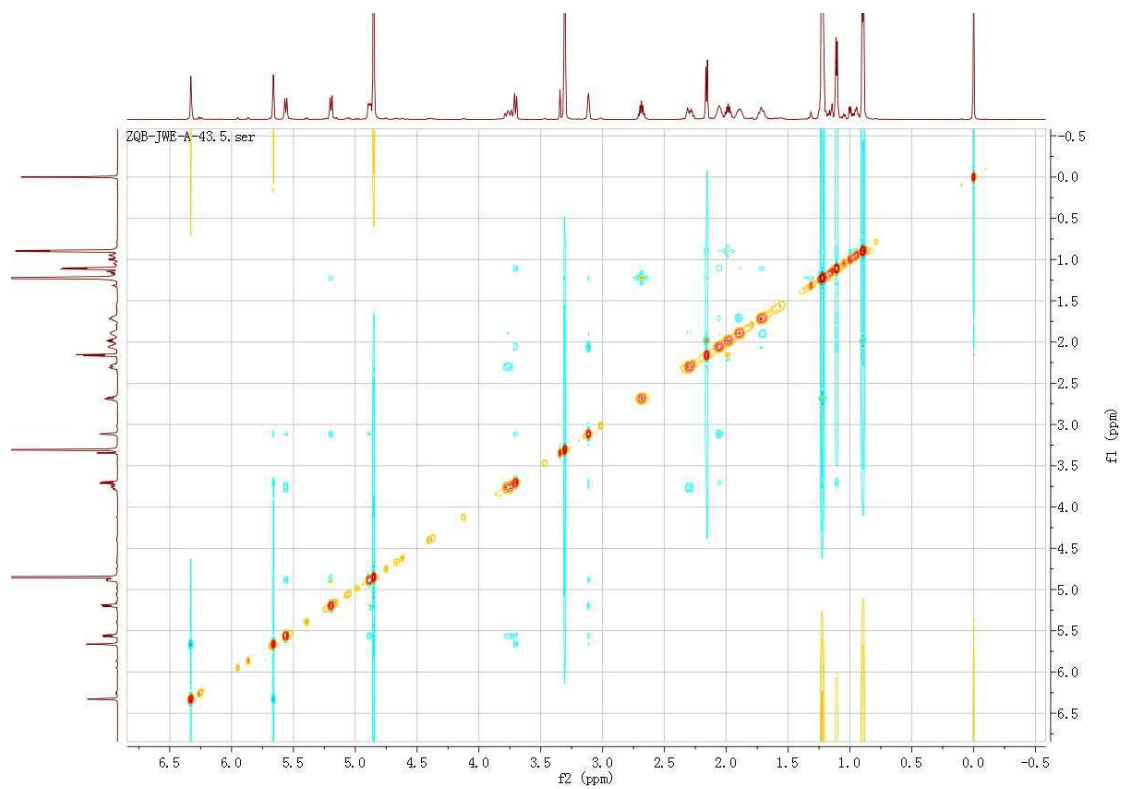


Fig. S4.6 ROESY spectrum (500 MHz) of compound **4** in CD₃OD

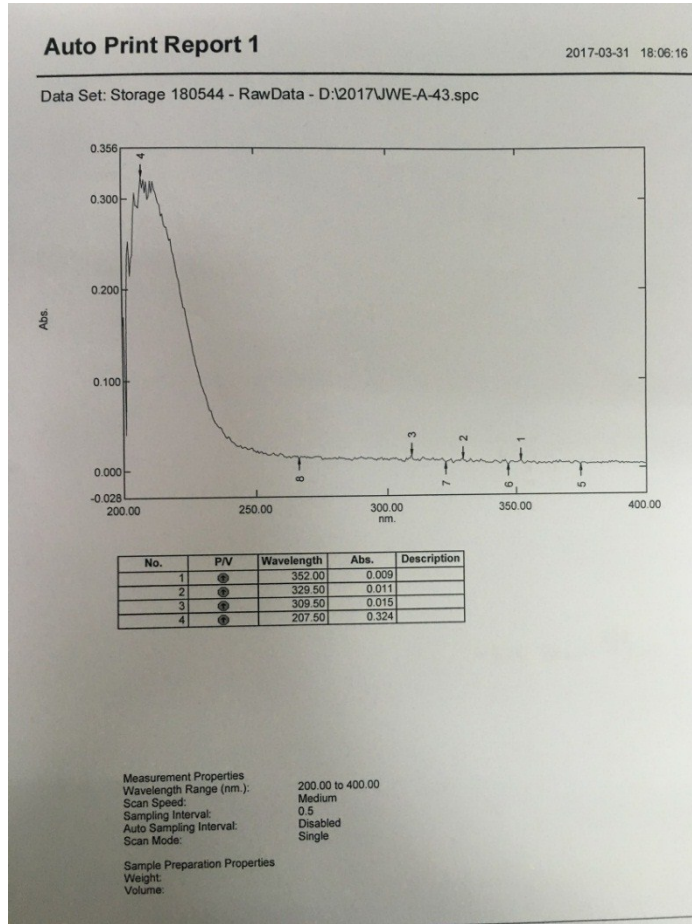


Fig. S4.7 UV spectrum of compound 4

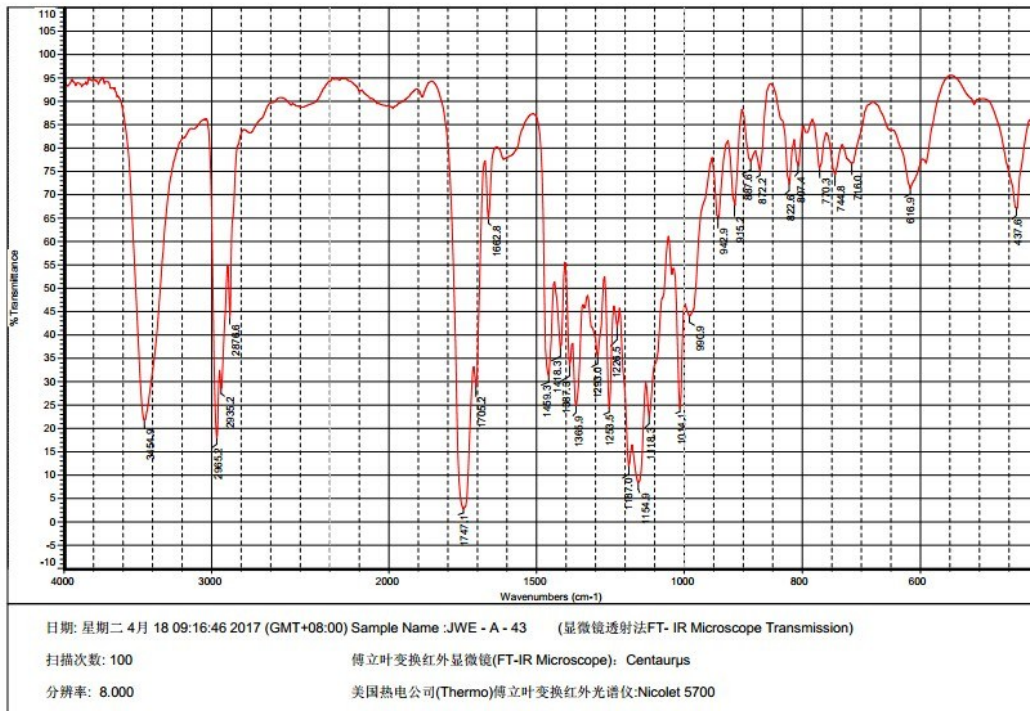


Fig. S4.8 IR spectrum of compound 4

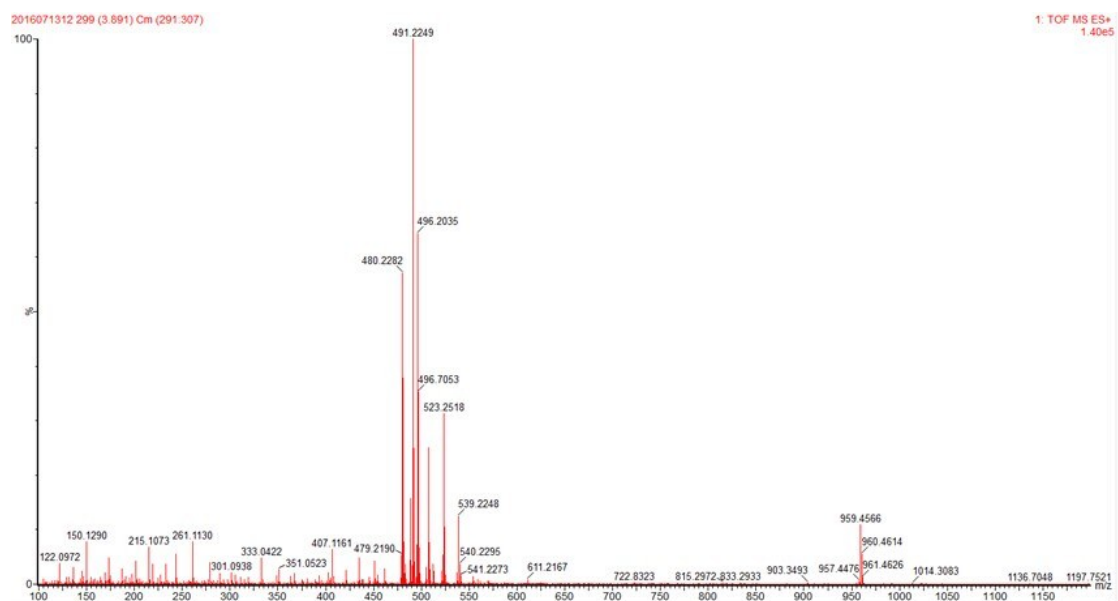


Fig. S4.9 HRESIMS spectrum of compound 4

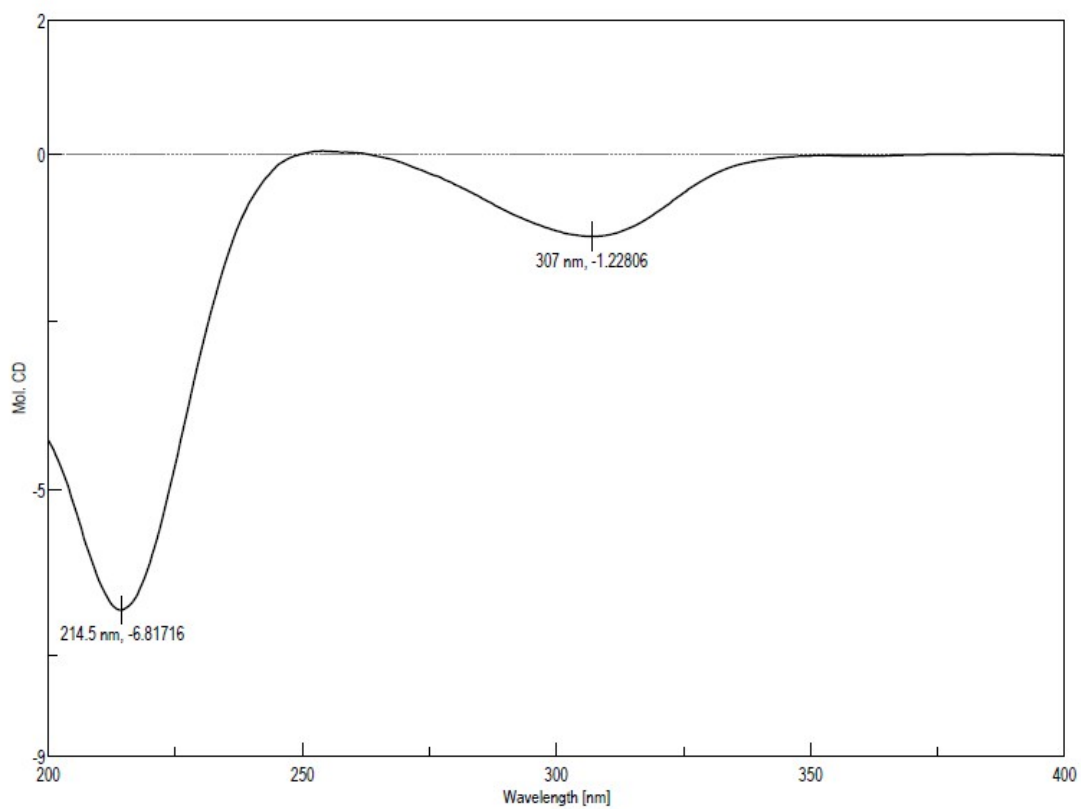


Fig. S4.10 CD spectrum of compound 4

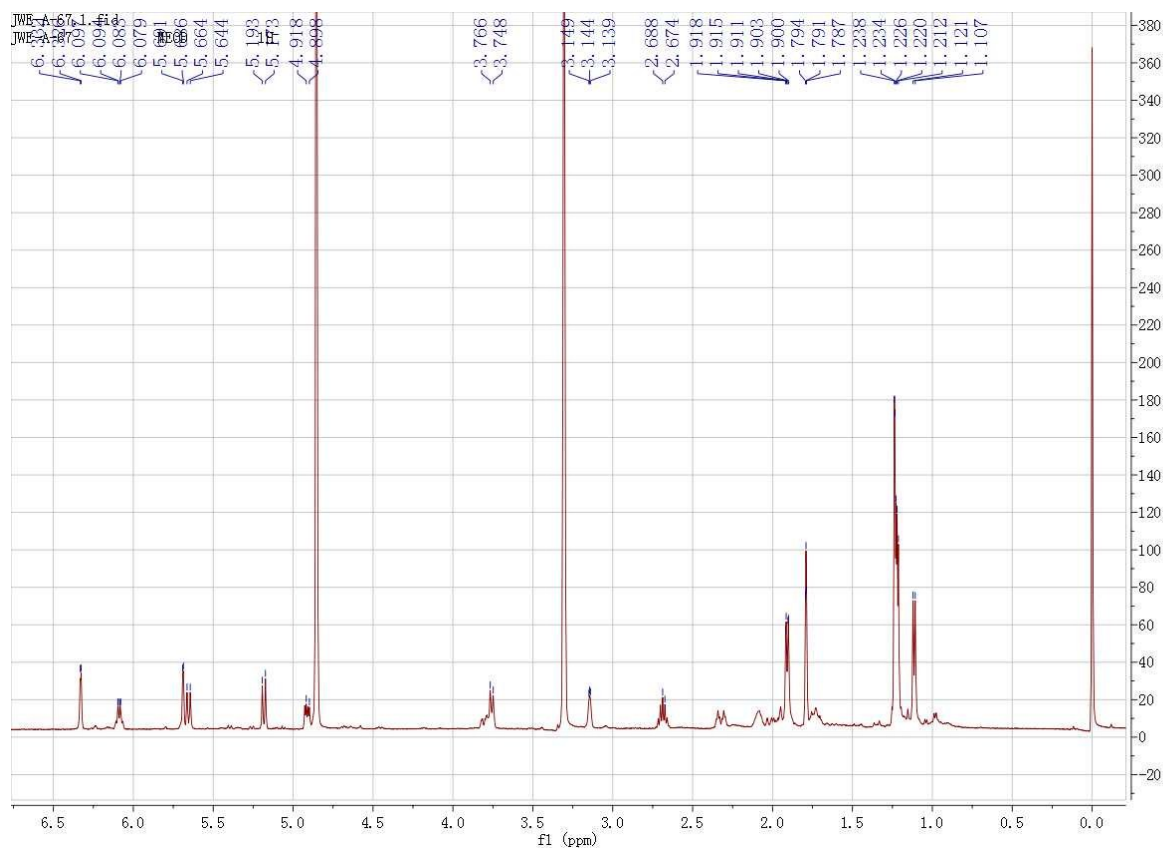


Fig. S5.1 ^1H NMR spectrum (500 MHz) of compound **5** in CD_3OD

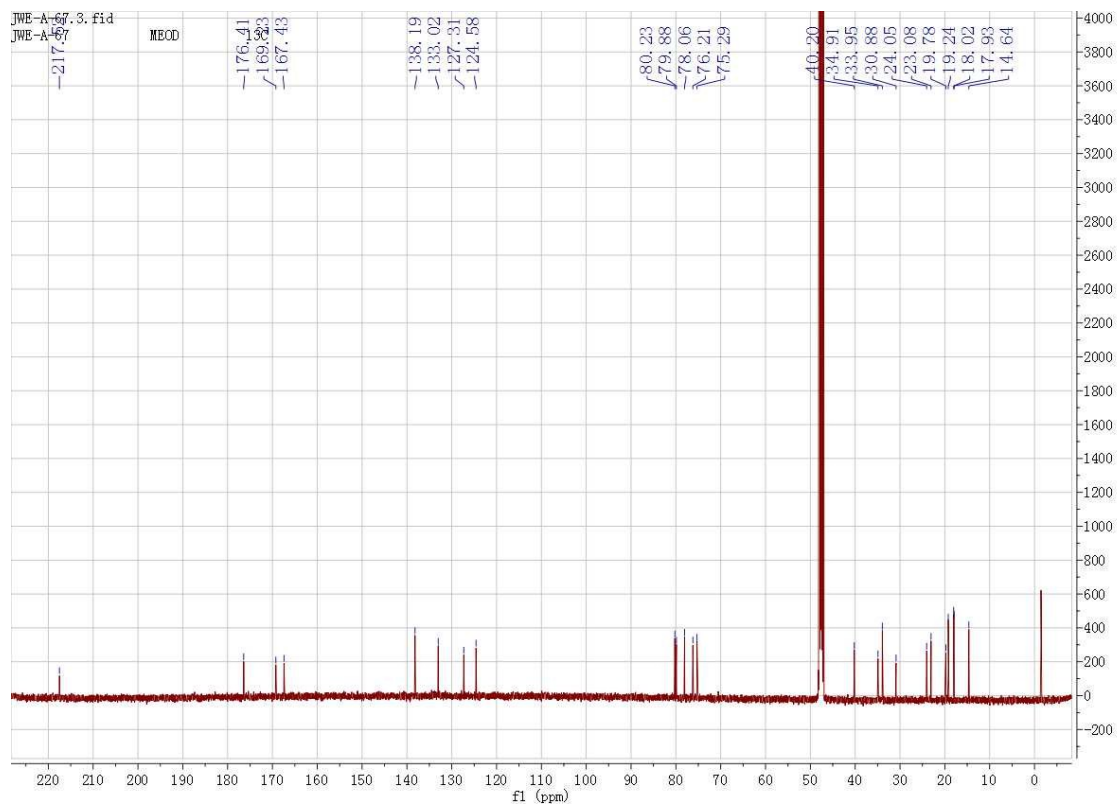


Fig. S5.2 ^{13}C NMR spectrum (500 MHz) of compound **5** in CD_3OD

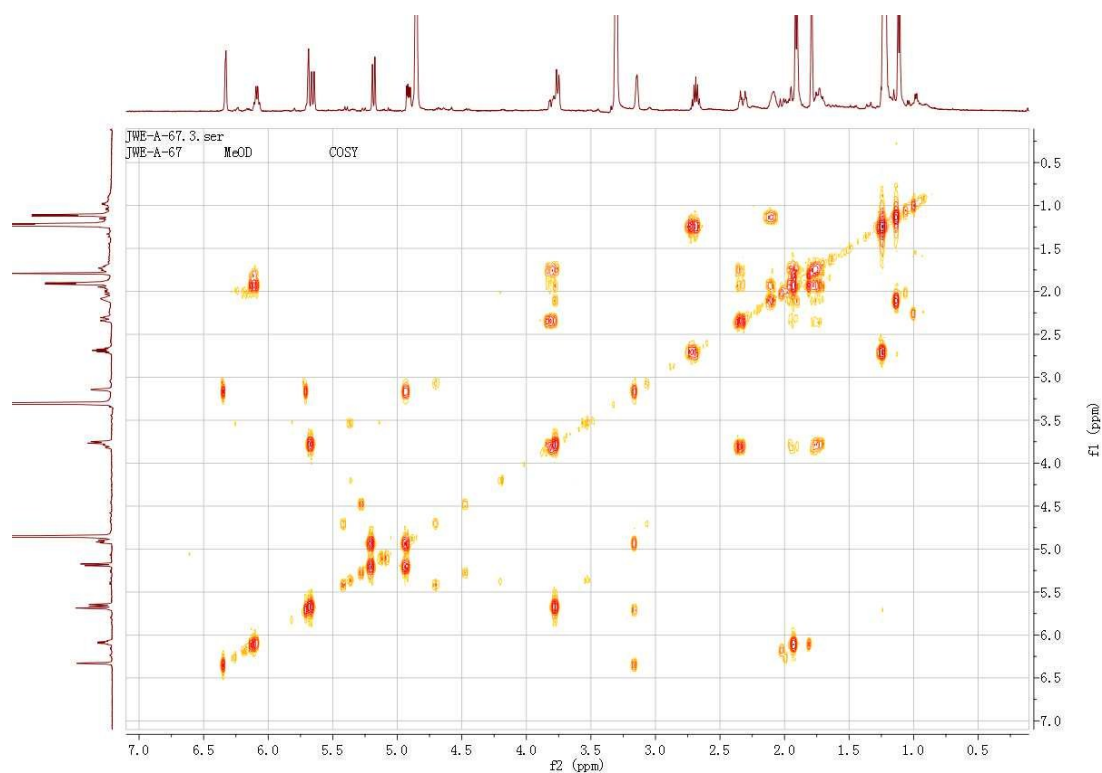


Fig. S5.3 ^1H - ^1H COSY spectrum (500 MHz) of compound **5** in CD_3OD

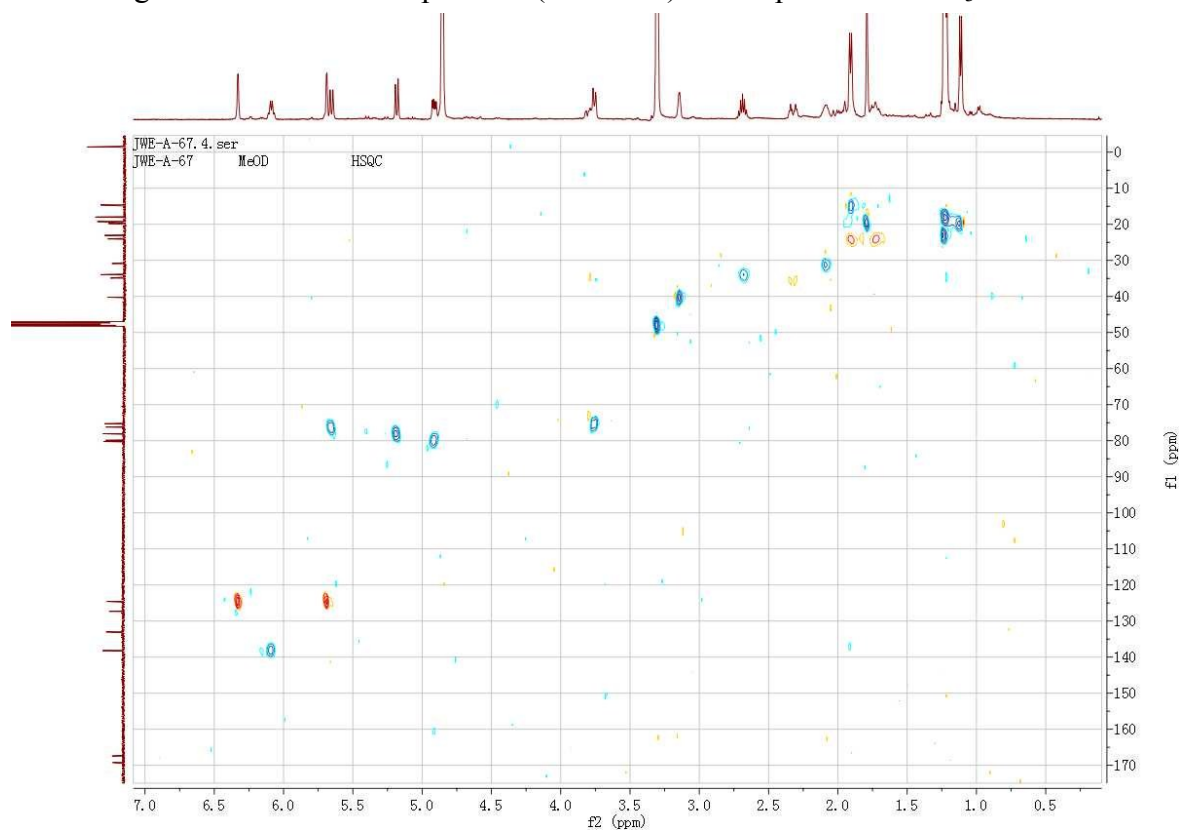


Fig. S5.4 HSQC spectrum (500 MHz) of compound **5** in CD_3OD

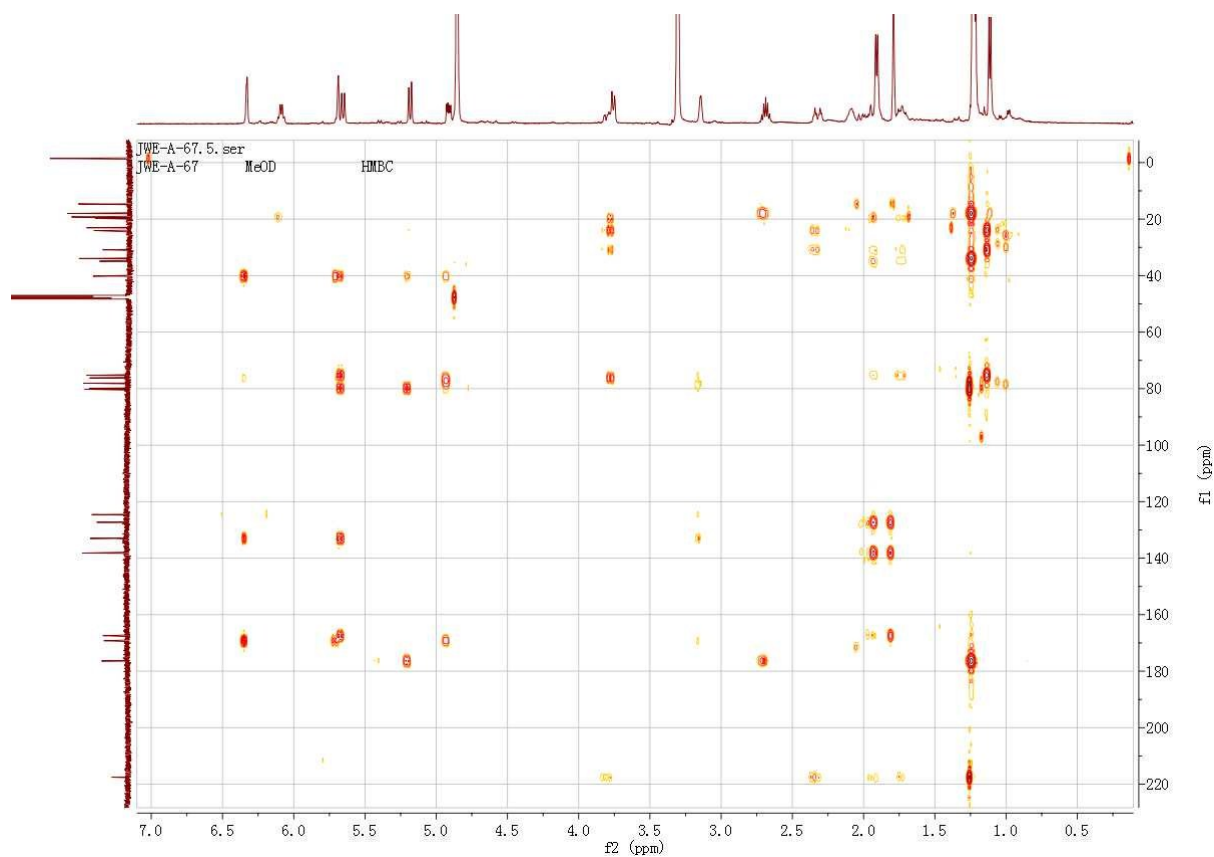


Fig. S5.5 HMBC spectrum (500 MHz) of compound **5** in CD₃OD

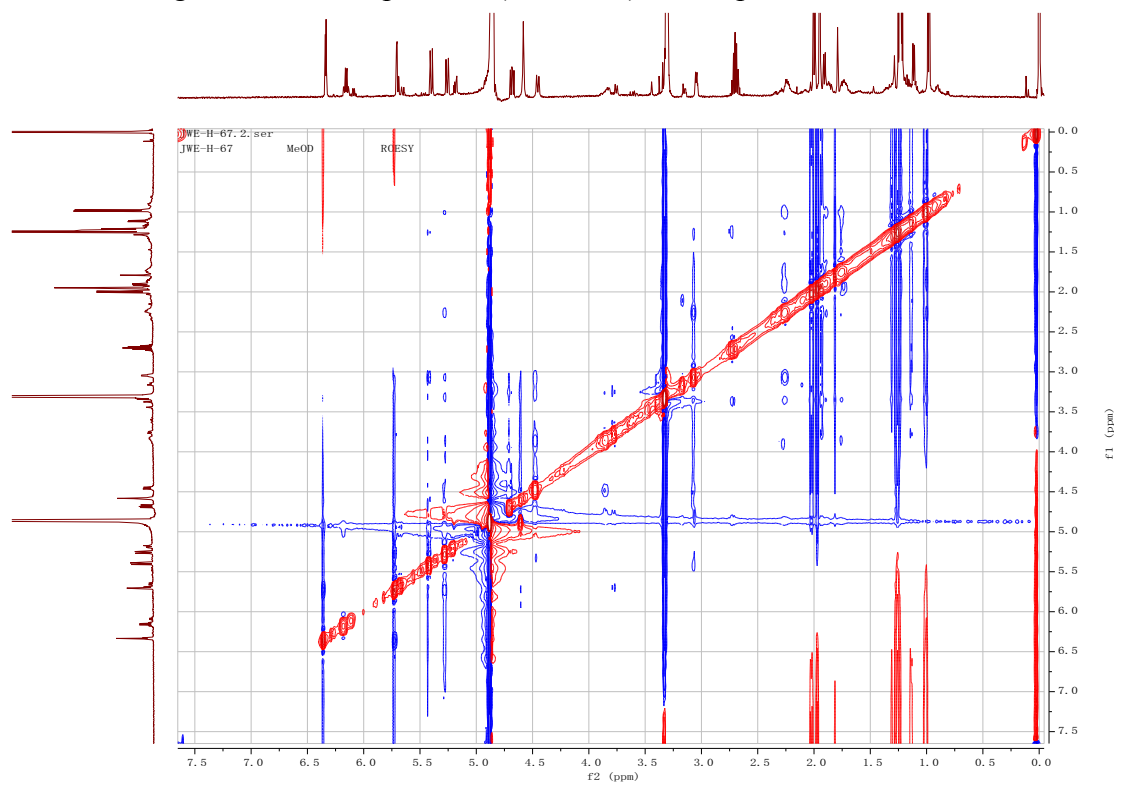


Fig. S5.6 ROESY spectrum (500 MHz) of compound **5** in CD₃OD

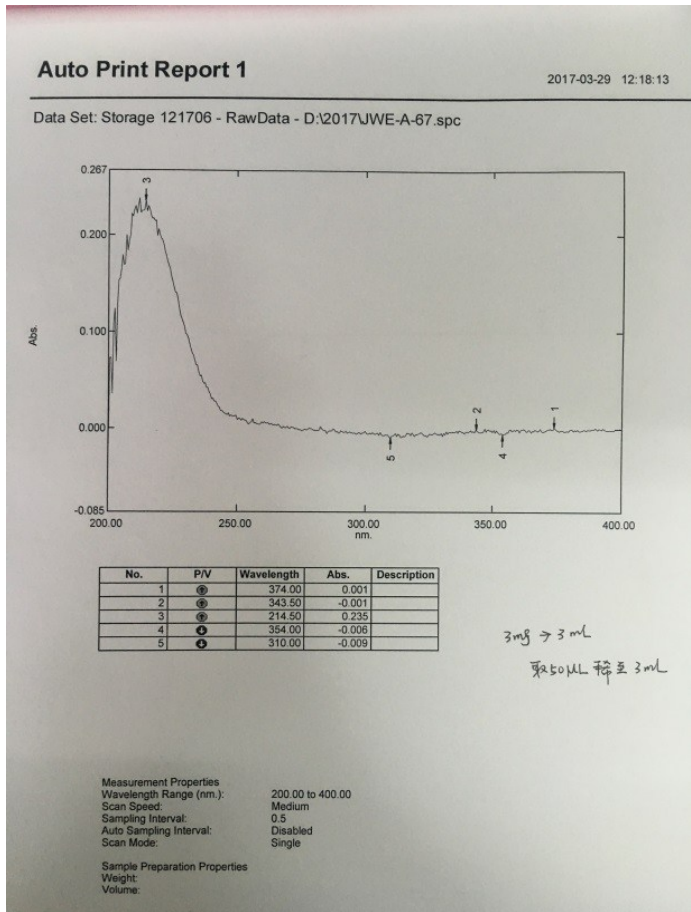


Fig. S5.7 UV spectrum of compound 5

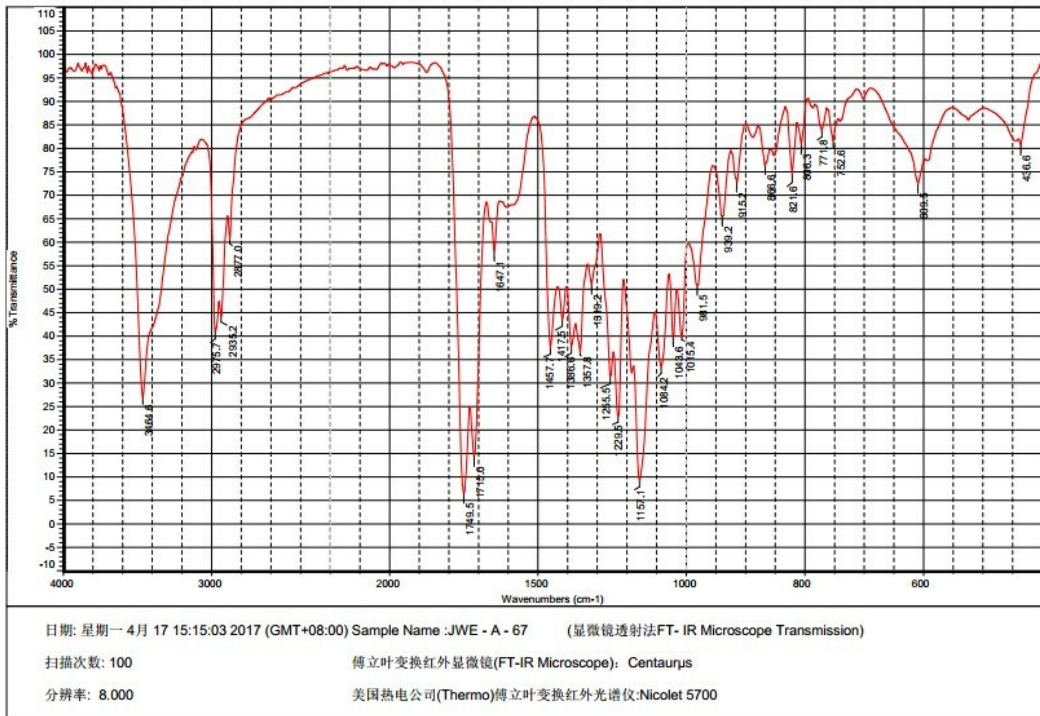


Fig. S5.8 IR spectrum of compound 5

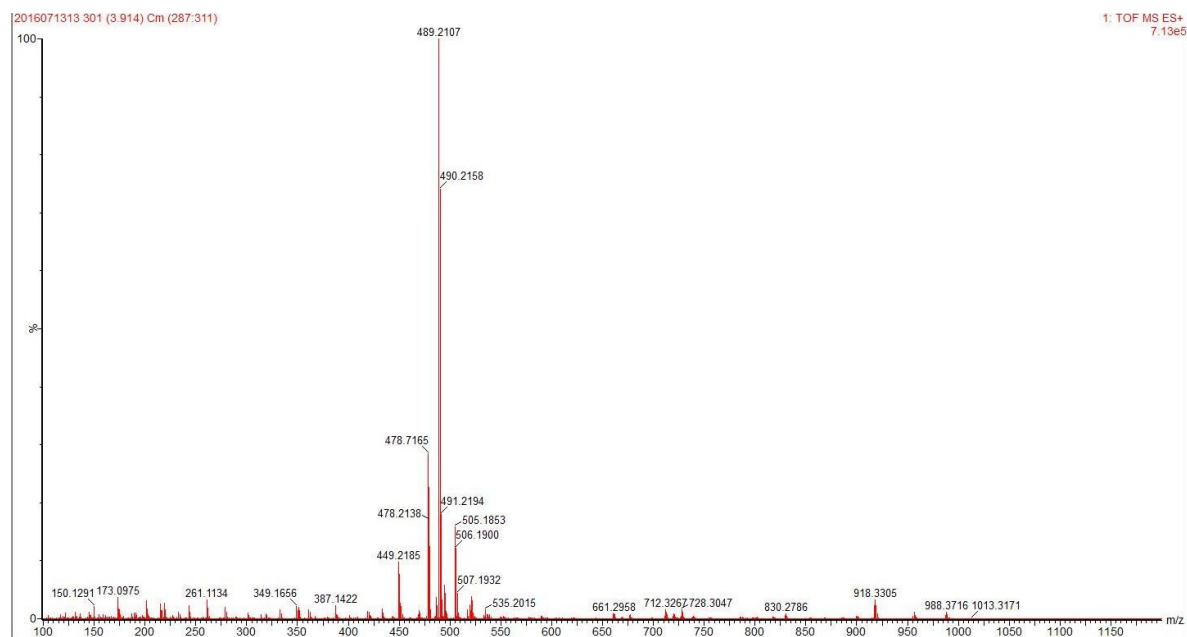


Fig. S5.9 HRESIMS spectrum of compound **5**

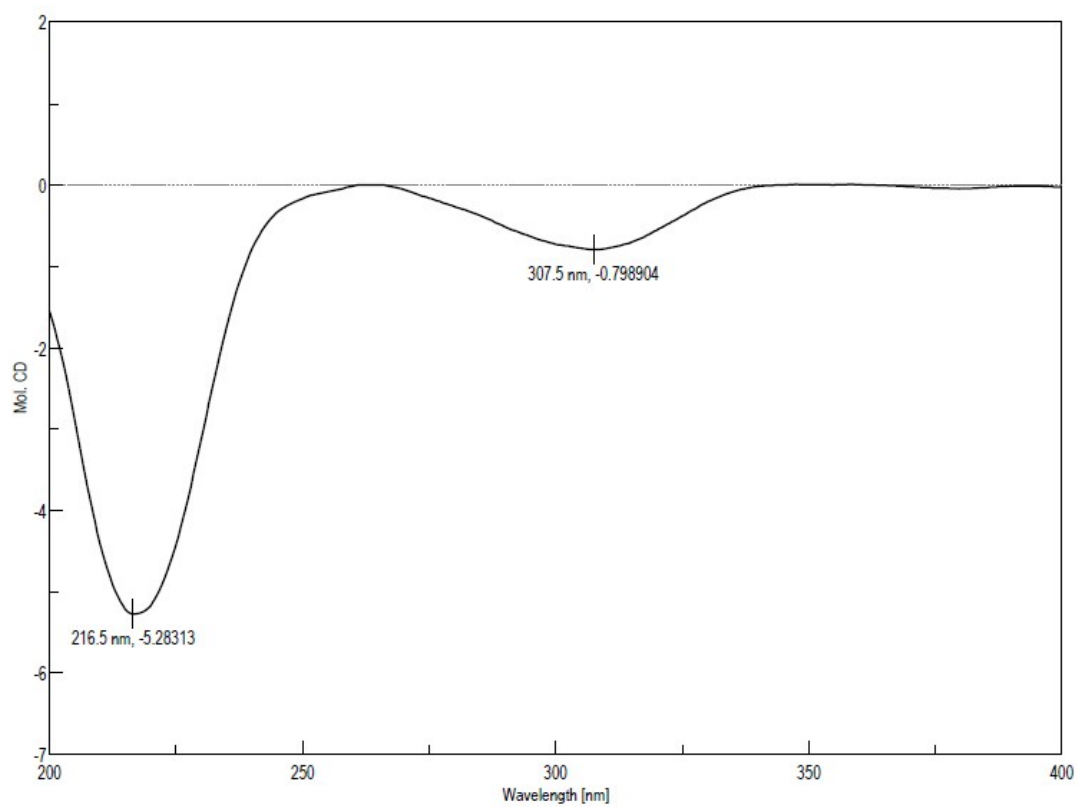


Fig. S5.10 CD spectrum of compound **5**

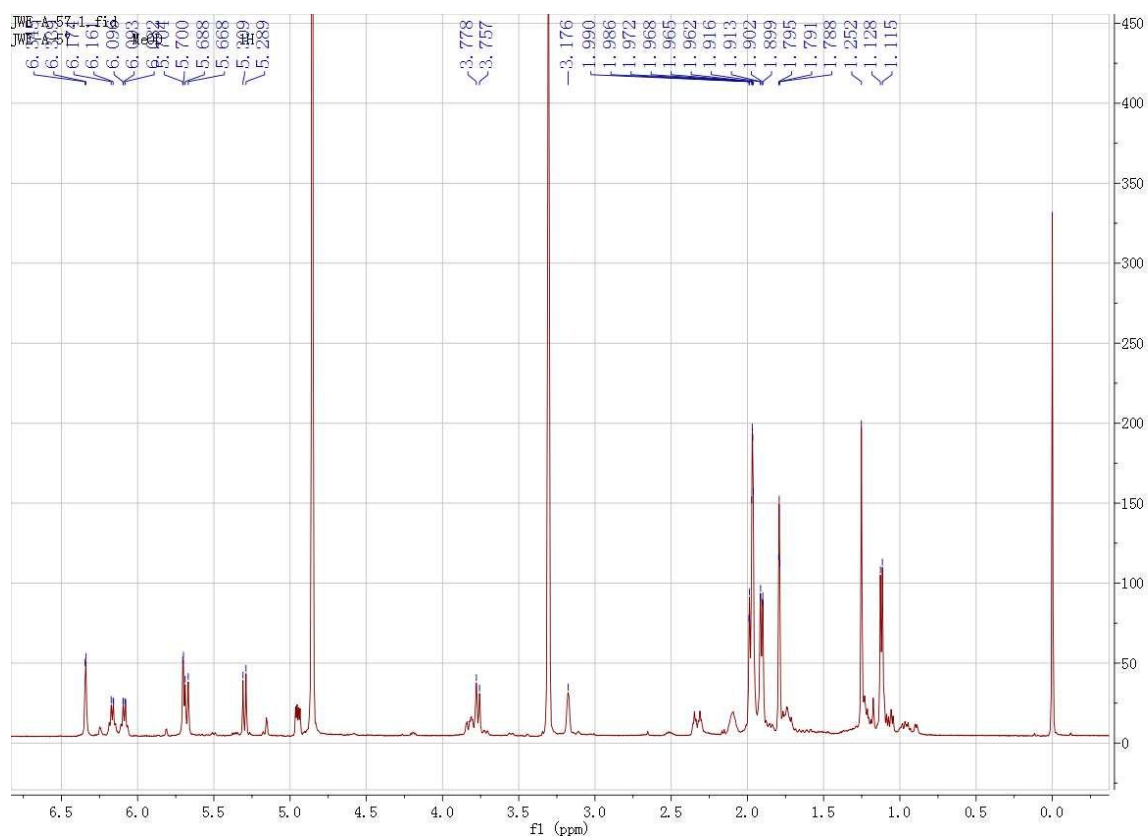


Fig. S6.1 ^1H NMR spectrum (500 MHz) of compound **6** in CD_3OD

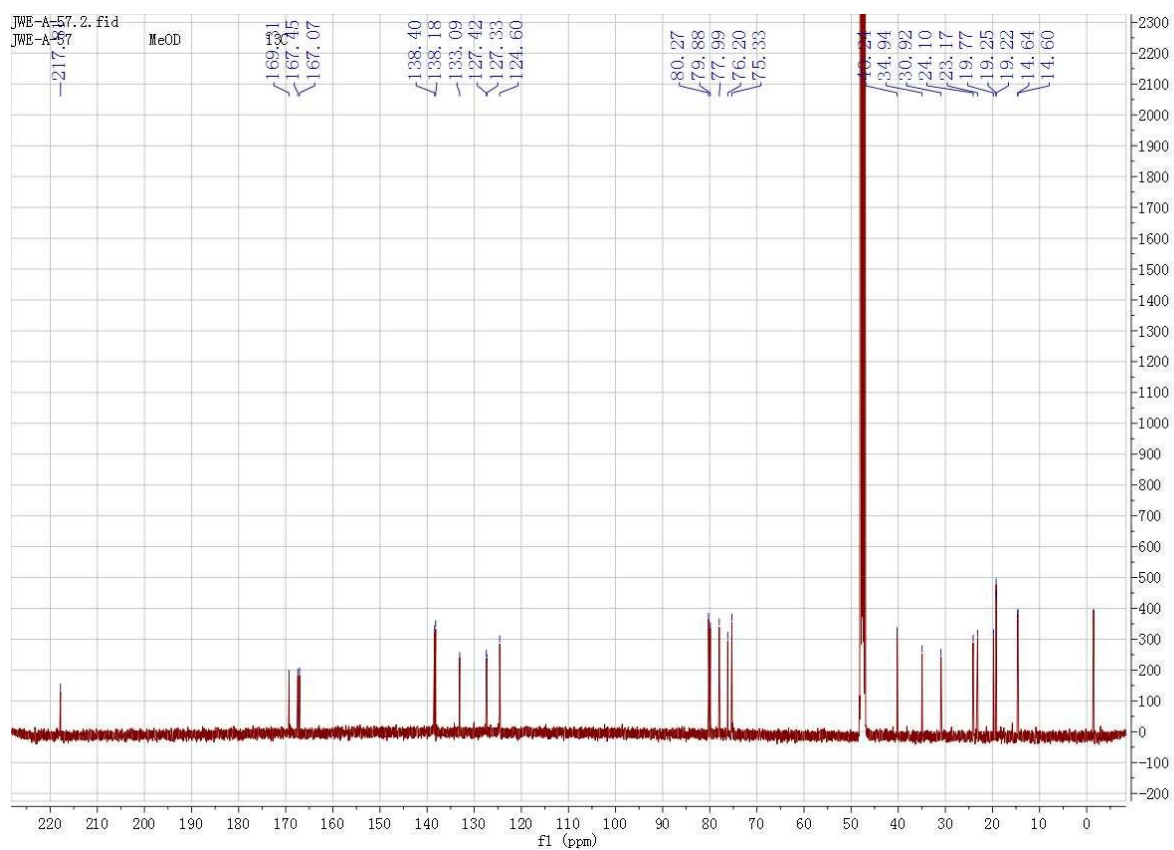


Fig. S6.2 ^{13}C NMR spectrum (125 MHz) of compound **6** in CD_3OD

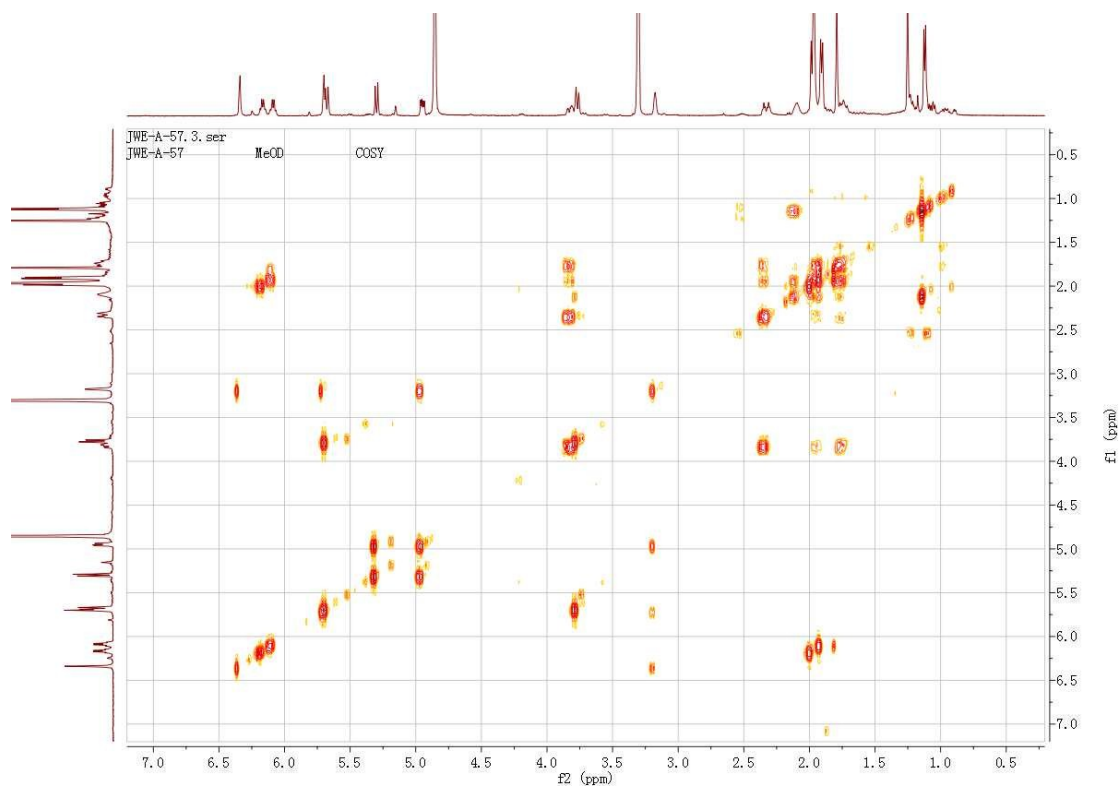


Fig. S6.3 ^1H - ^1H COSY spectrum (500 MHz) of compound **6** in CD_3OD

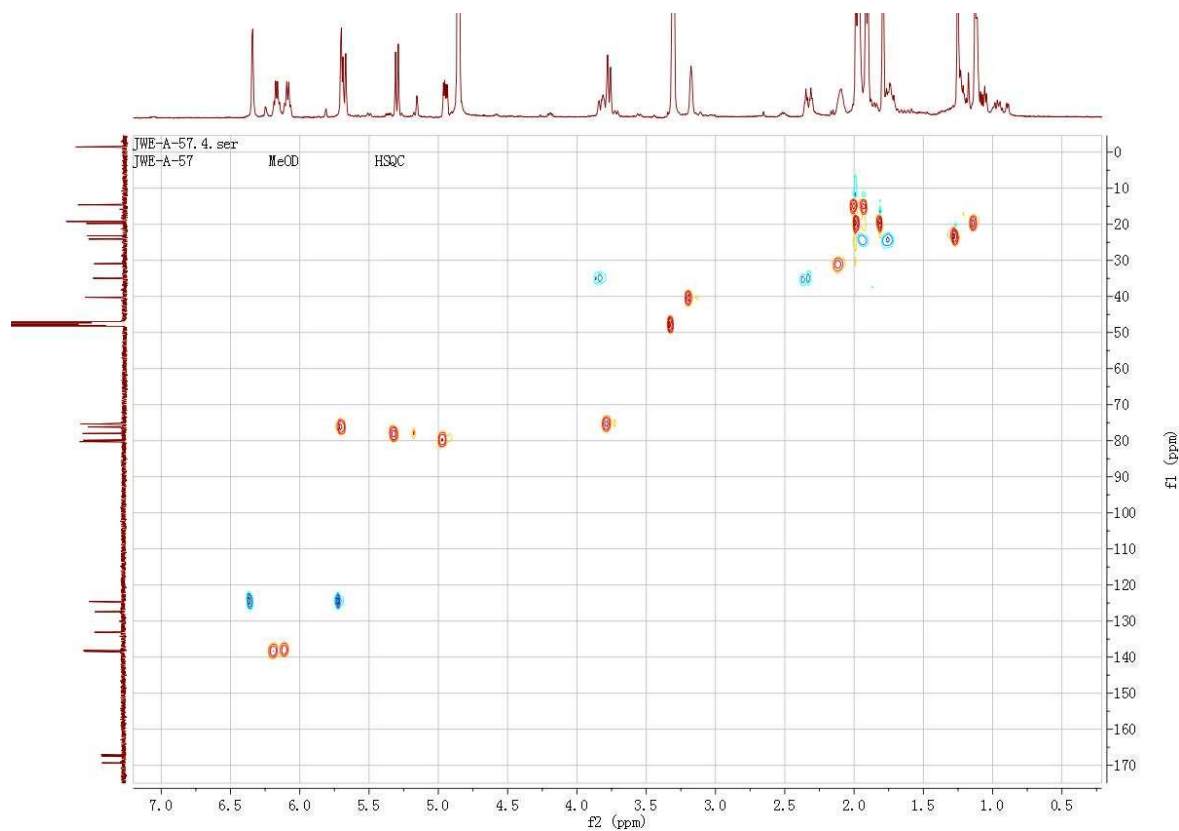


Fig. S6.4 HSQC spectrum (500 MHz) of compound **6** in CD_3OD

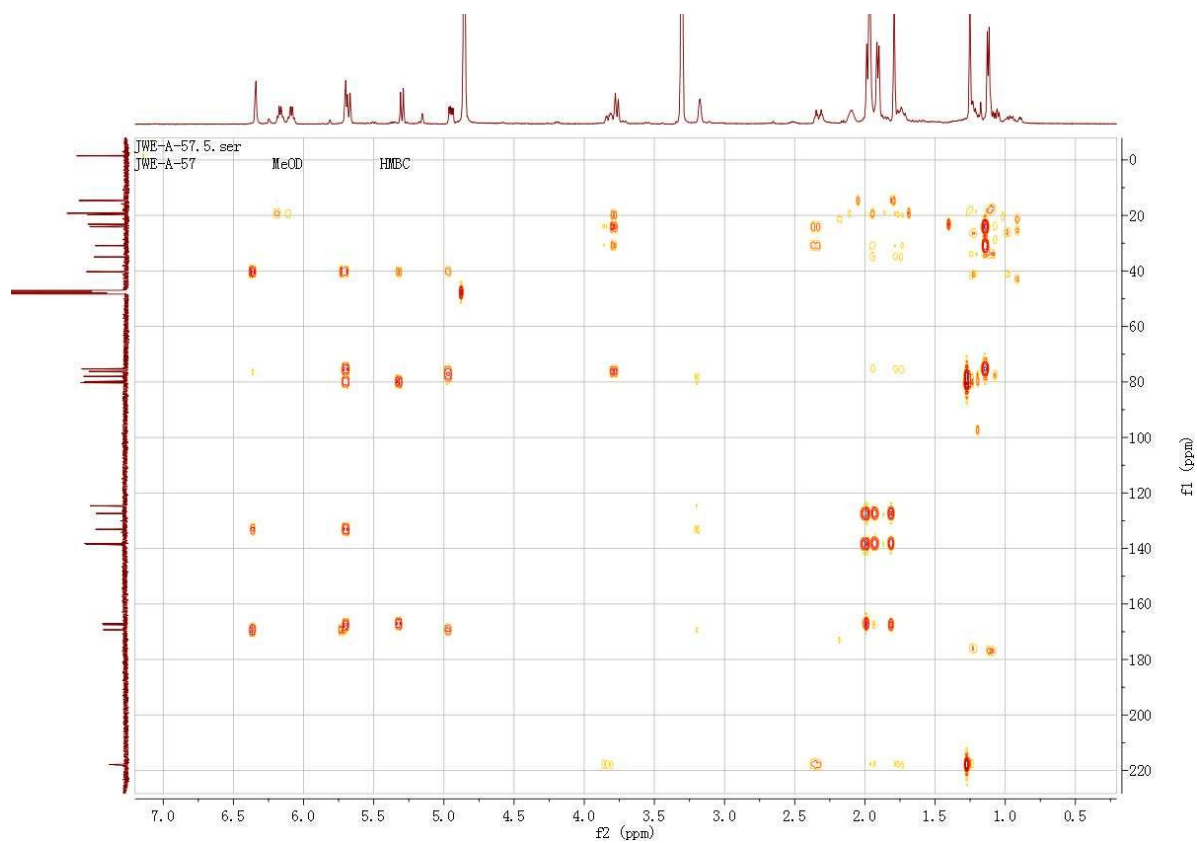


Fig. S6.5 HMBC spectrum (500 MHz) of compound **6** in CD₃OD

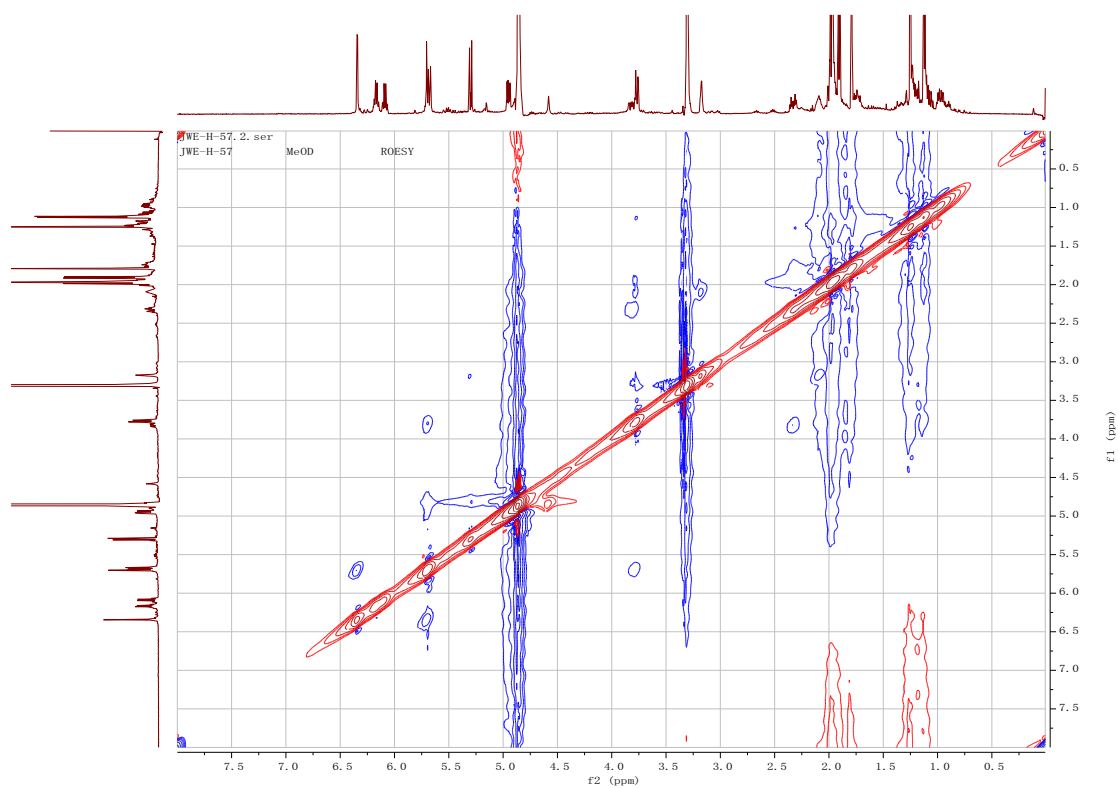


Fig. S6.6 ROESY spectrum (500 MHz) of compound **6** in CD₃OD

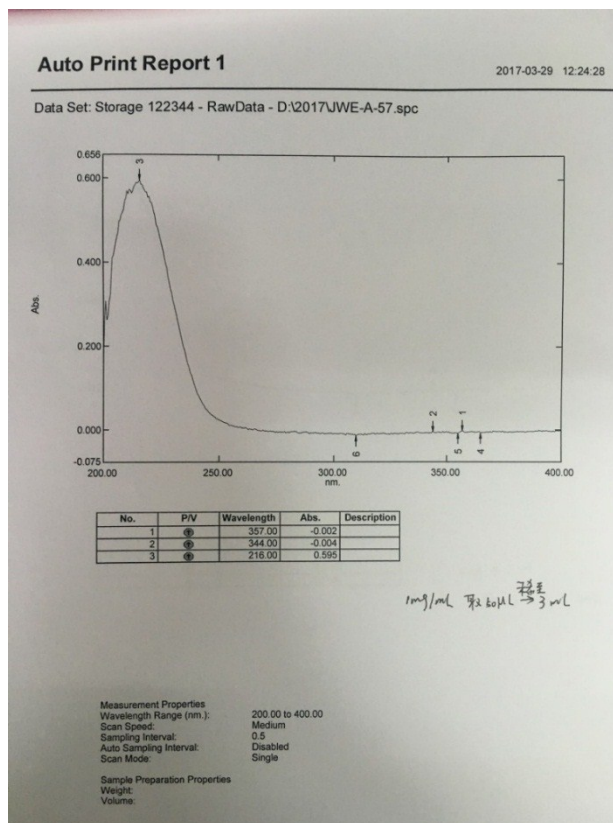


Fig. S6.7 UV spectrum of compound 6

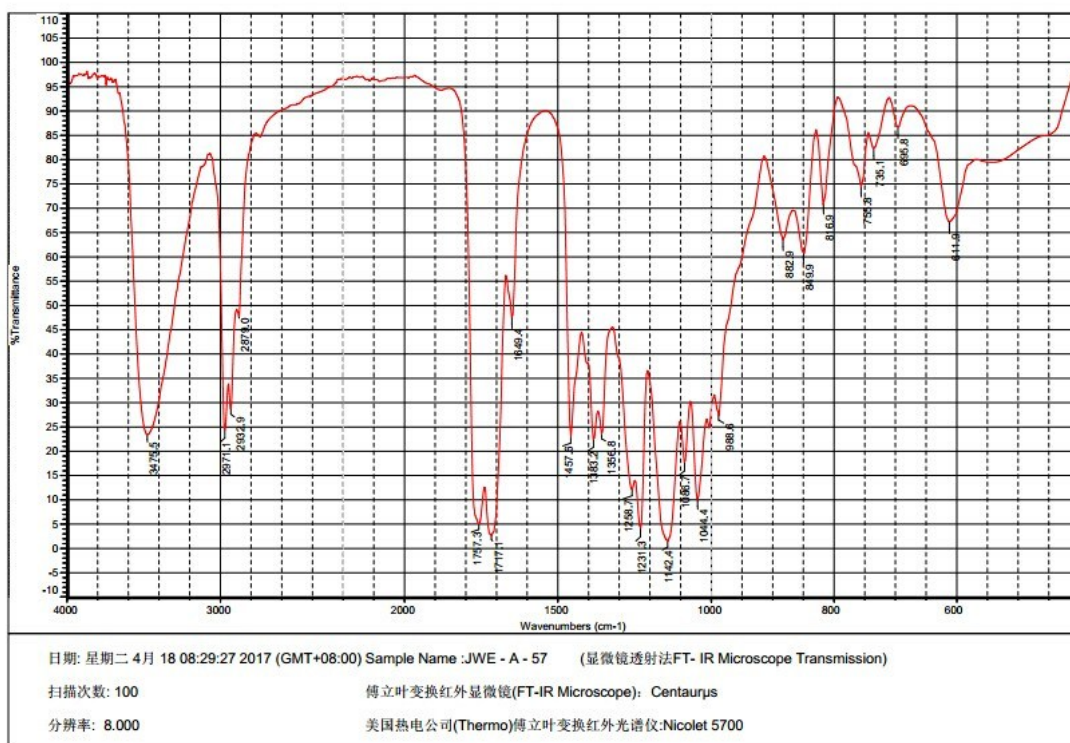


Fig. S6.8 IR spectrum of compound 6

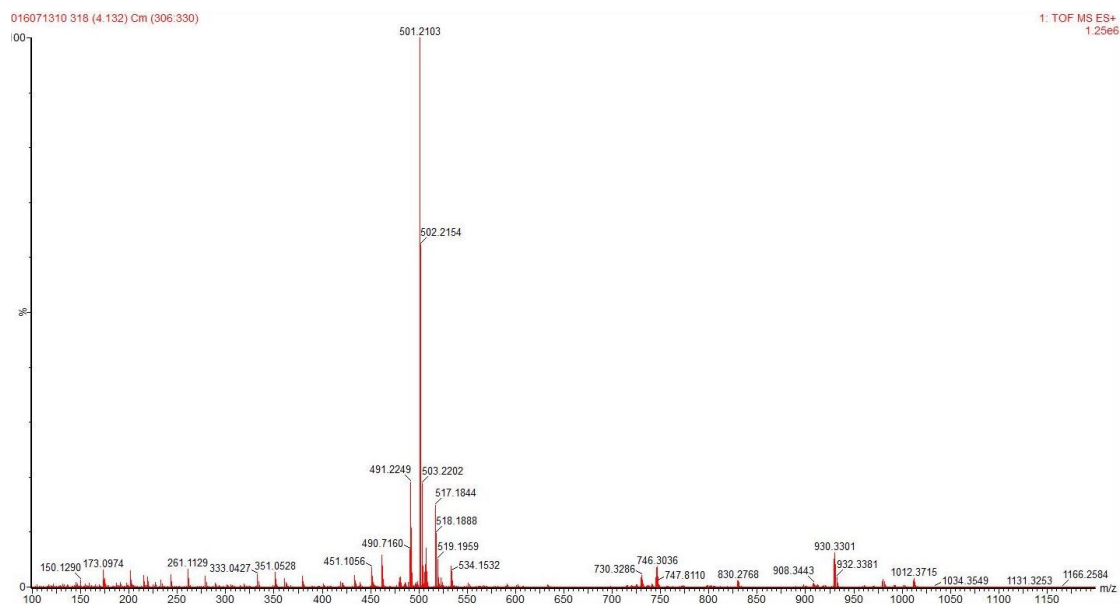


Fig. S6.9 HRESIMS spectrum of compound **6**

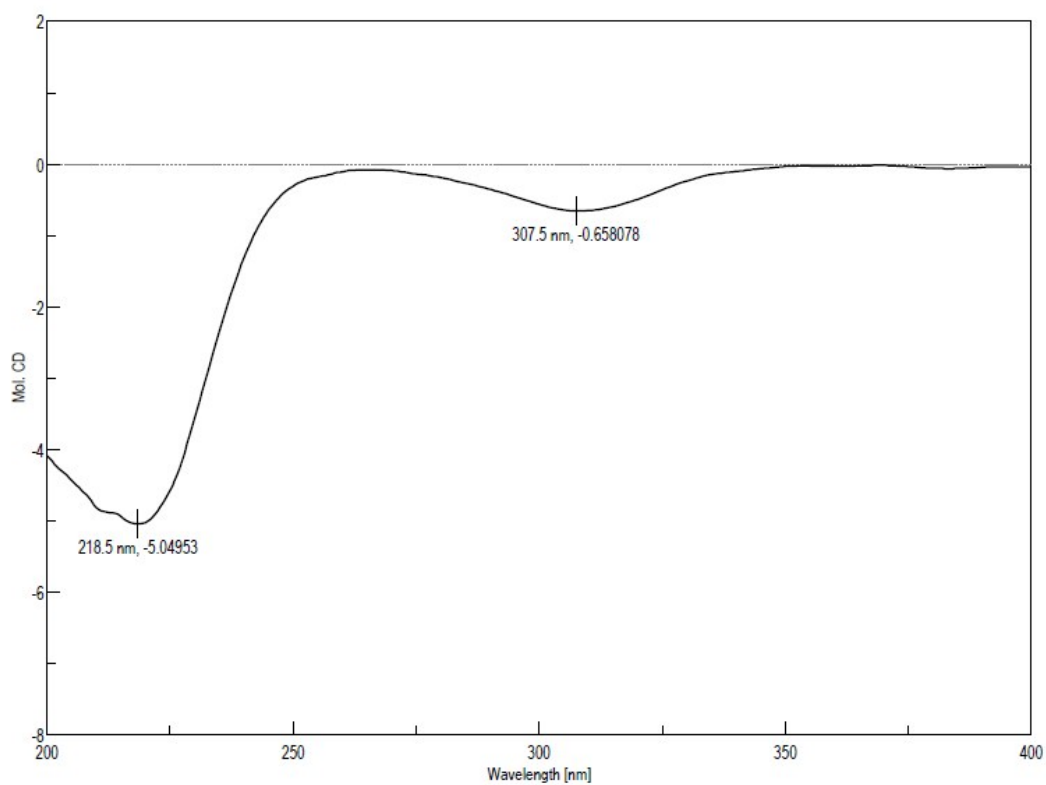


Fig. S6.10 CD spectrum of compound **6**

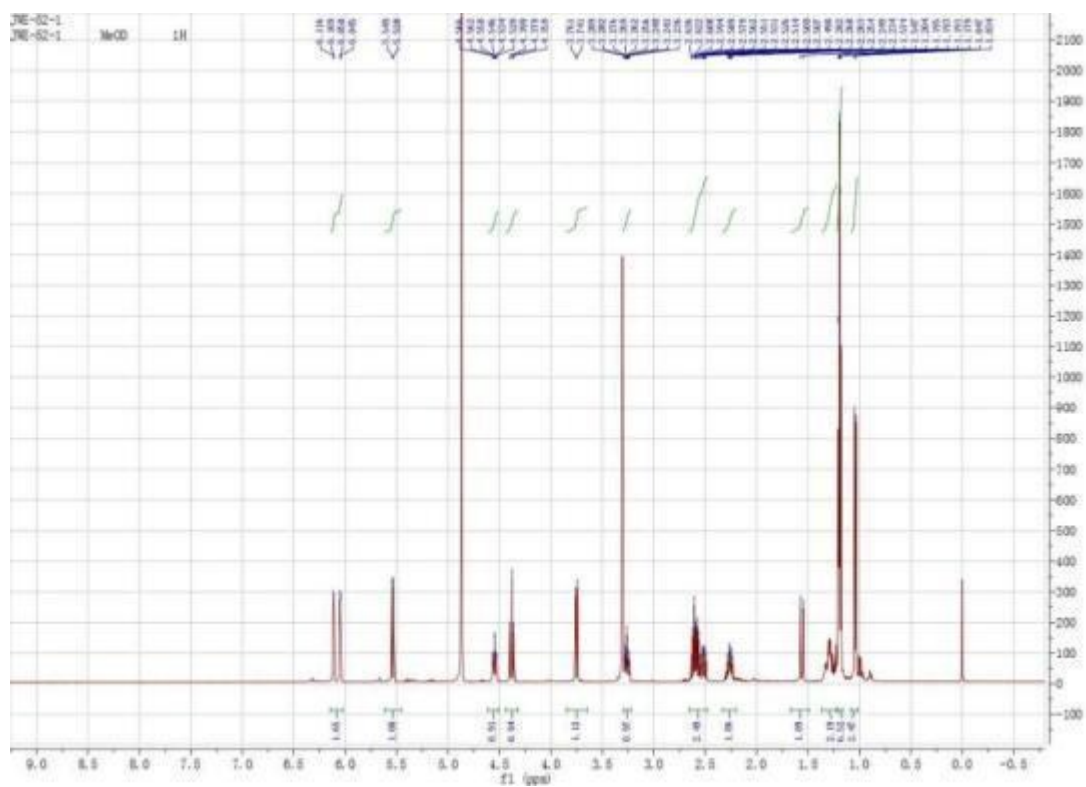


Fig. S7.1 ^1H NMR spectrum (500 MHz) of compound **7** in CD_3OD

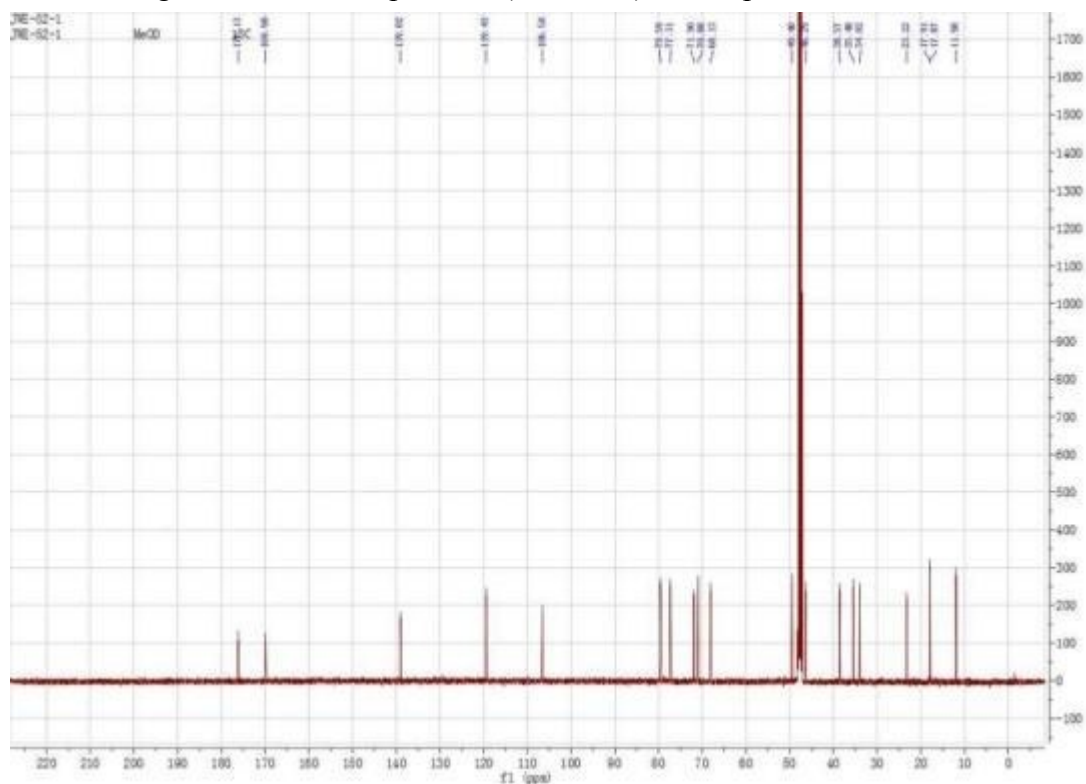


Fig. S7.2 ^{13}C NMR spectrum (125 MHz) of compound **7** in CD_3OD

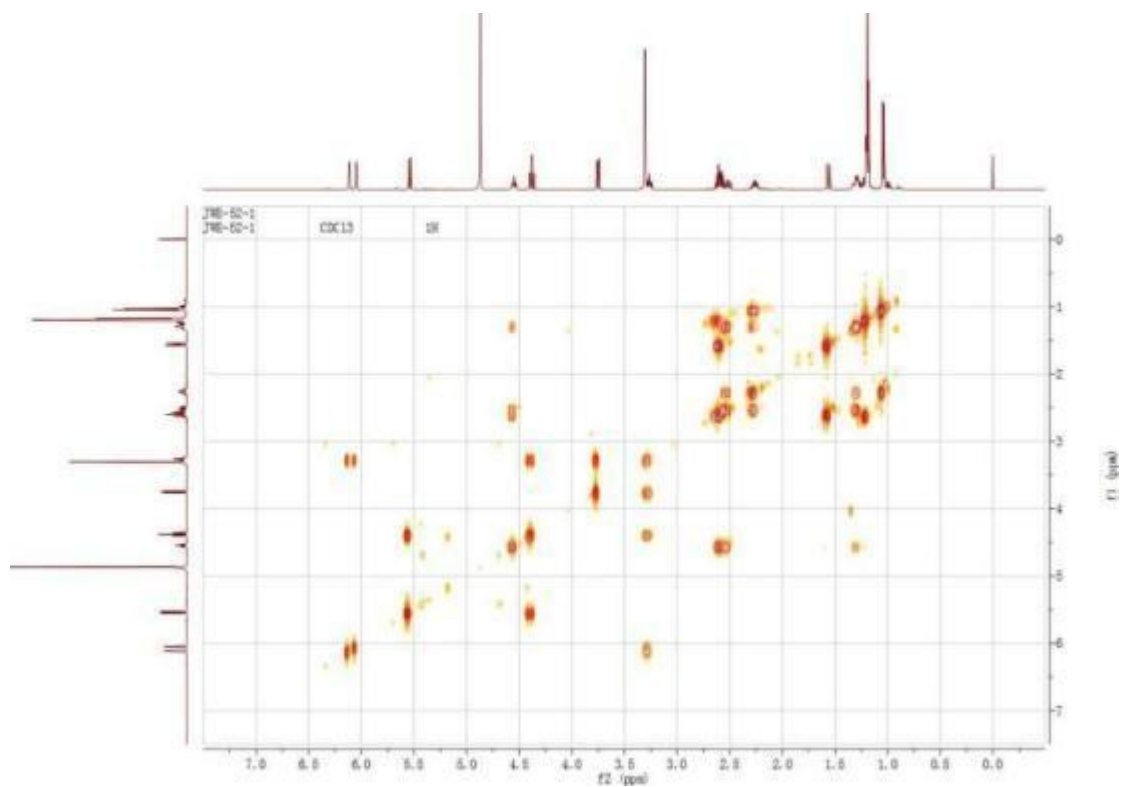


Fig. S7.3 ^1H - ^1H COSY spectrum (500 MHz) of compound **7** in CDCl_3

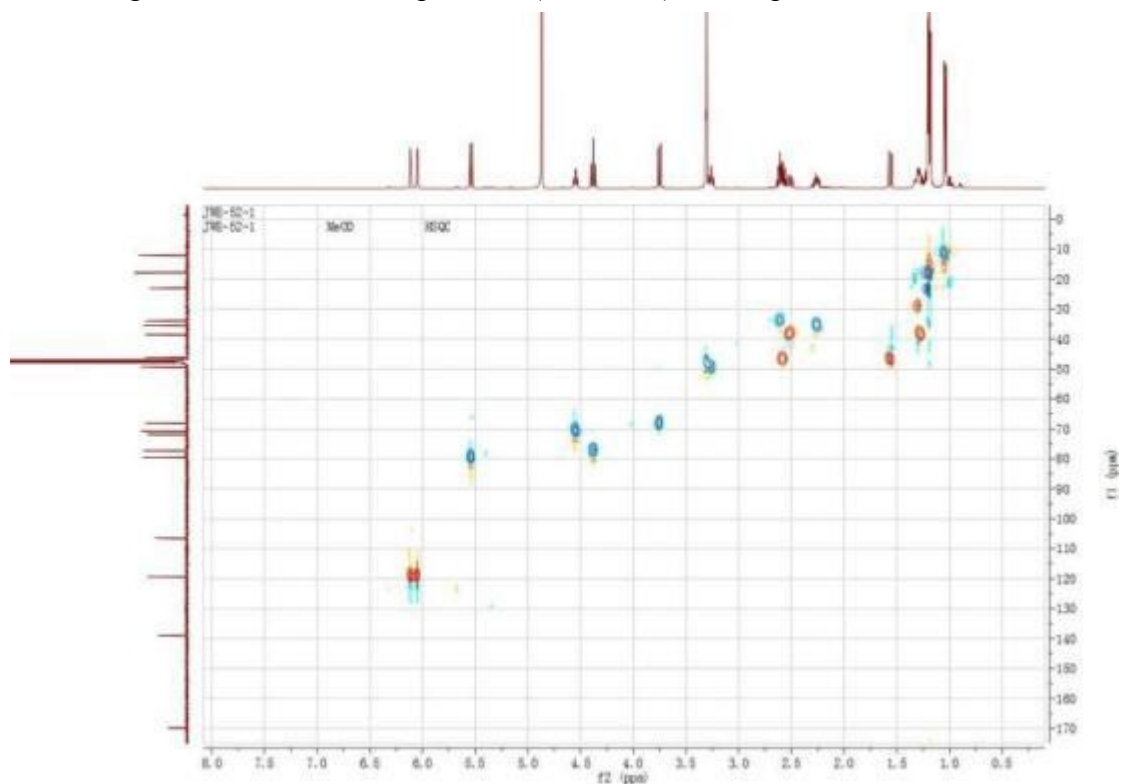


Fig. S7.4 HSQC spectrum (500 MHz) of compound **7** in CD_3OD

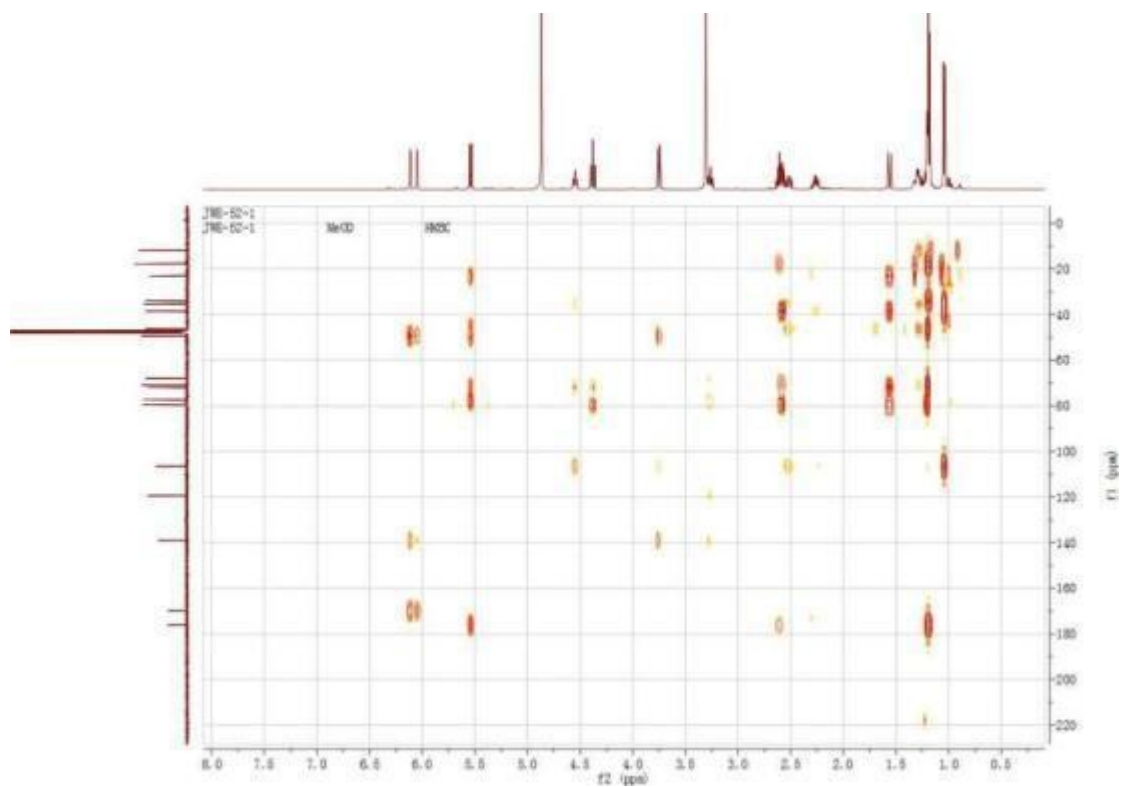


Fig. S7.5 HMBC spectrum (500 MHz) of compound **7** in CD₃OD

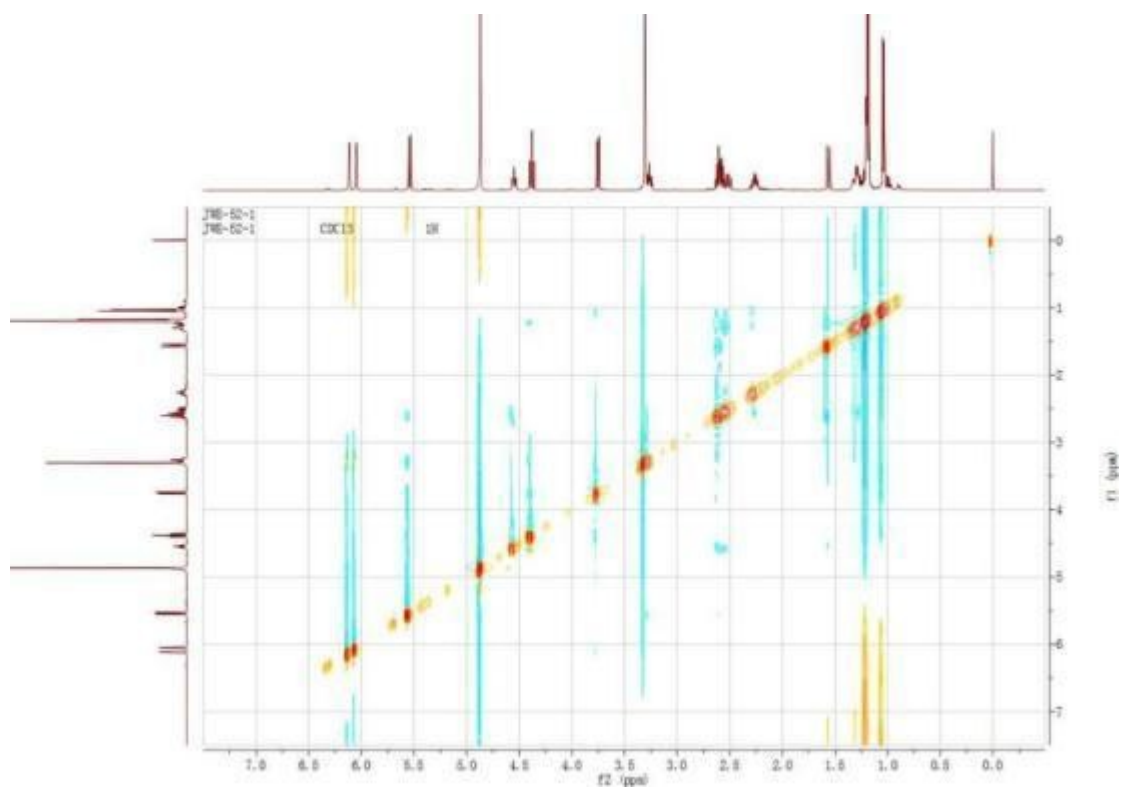


Fig. S7.6 ROESY spectrum (500 MHz) of compound **7** in CD₃OD

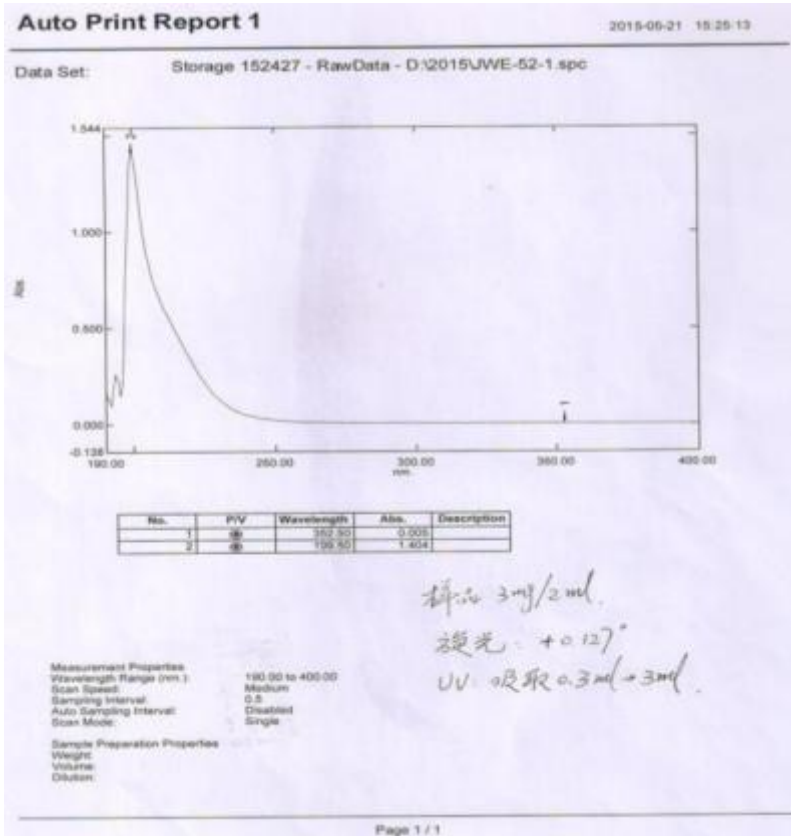


Fig. S7.7 UV spectrum of compound 7

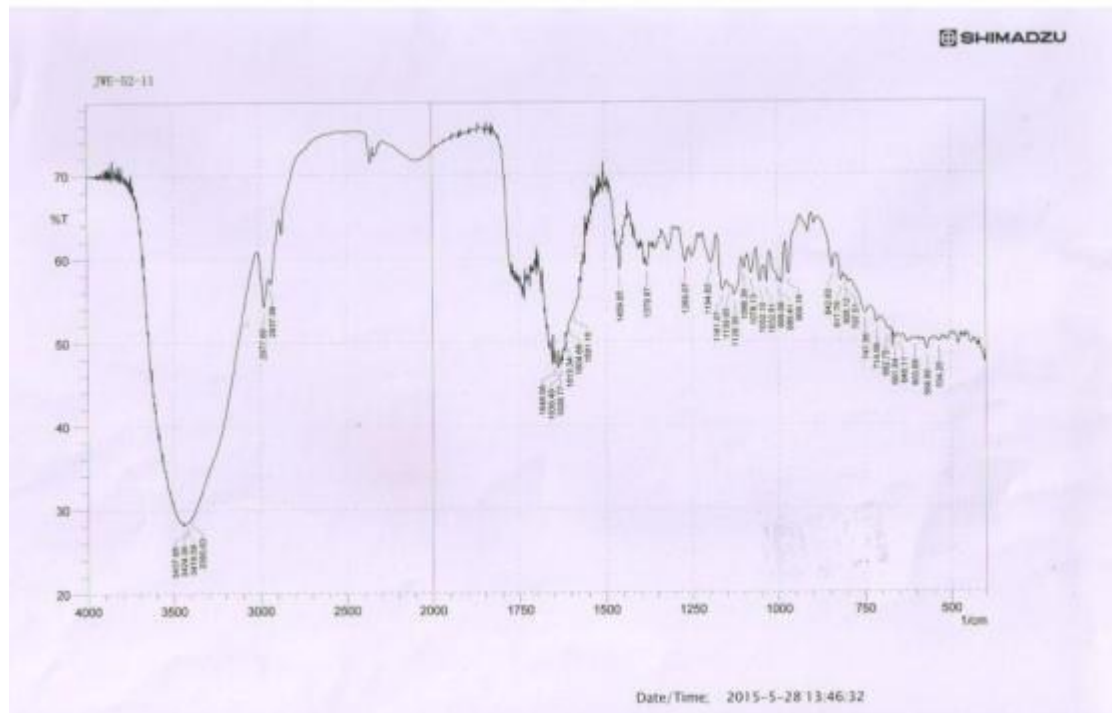


Fig. S7.8 IR spectrum of compound 7

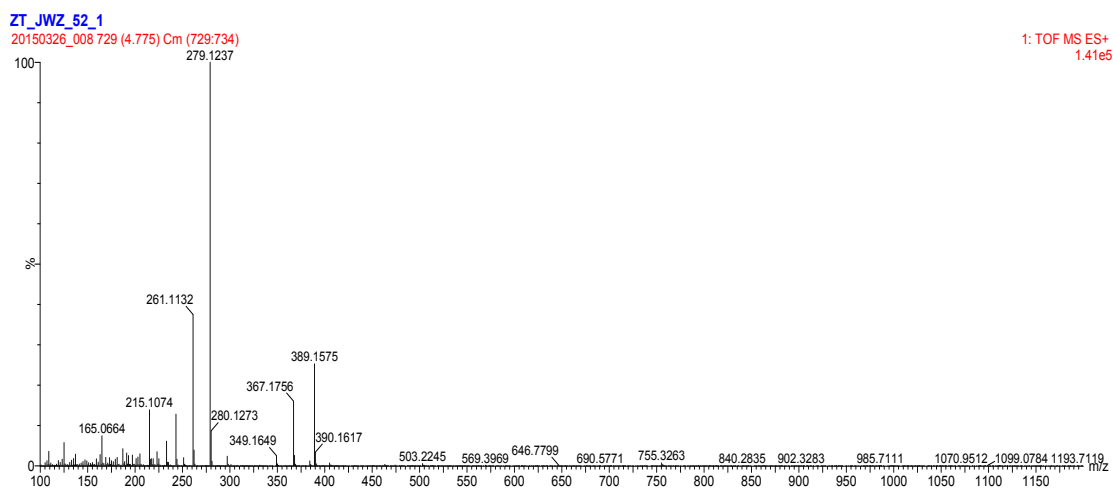


Fig. S7.9 HRMS spectrum of compound 7

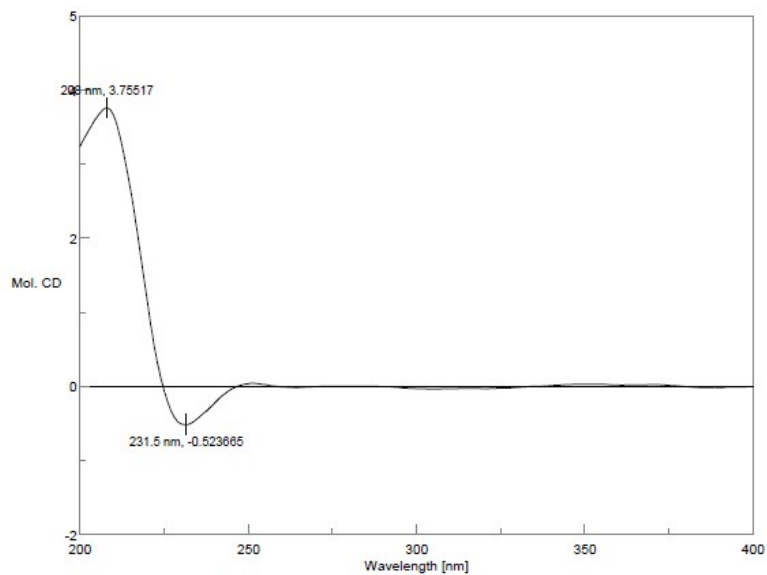


Fig. S7.10 CD spectrum of compound 7