

# Supplementary Materials

## **Limonin derivatives via hydrogenation: Structural identification and anti-inflammatory activity**

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# 1. Spectrum information of compounds **2-8**

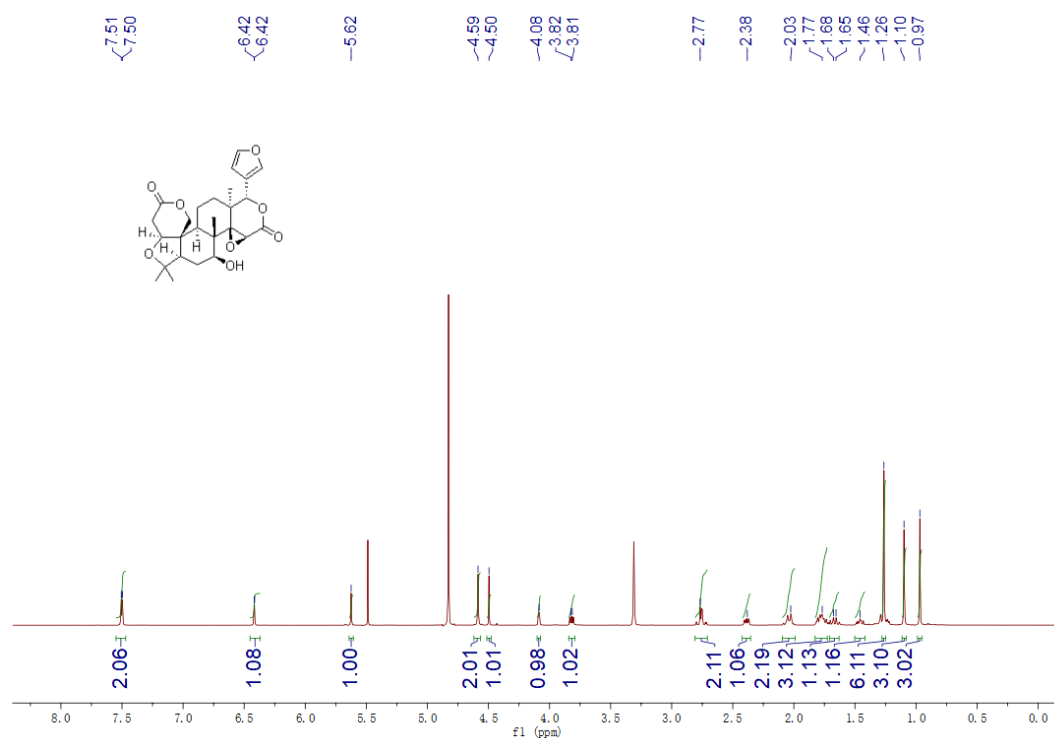


Figure S1:  $^1\text{H}$  NMR spectrum (400 MHz) of **2** in  $\text{CD}_3\text{OD}$

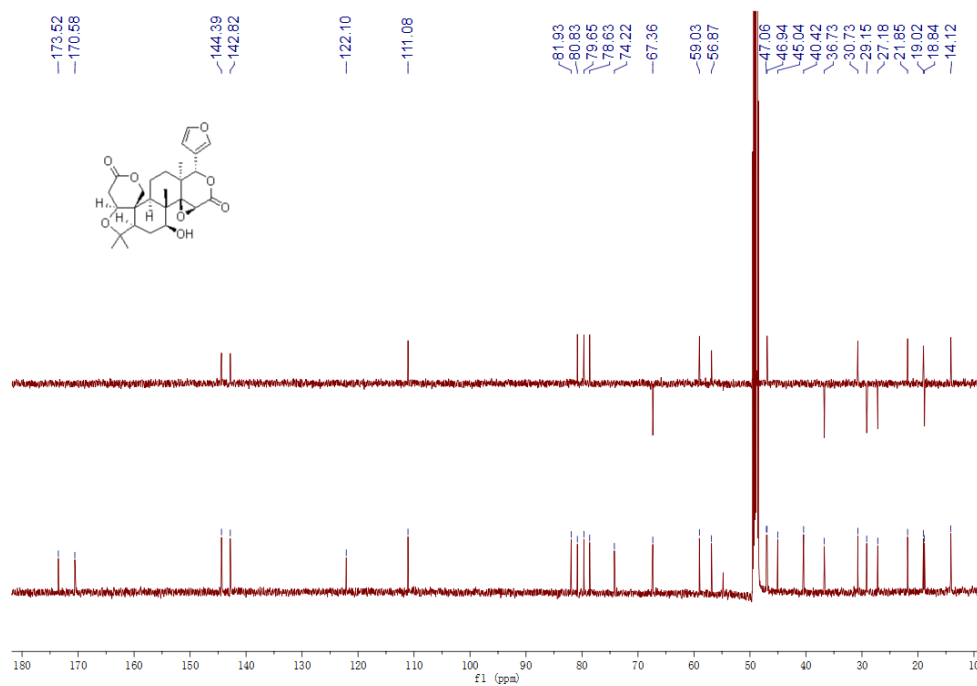
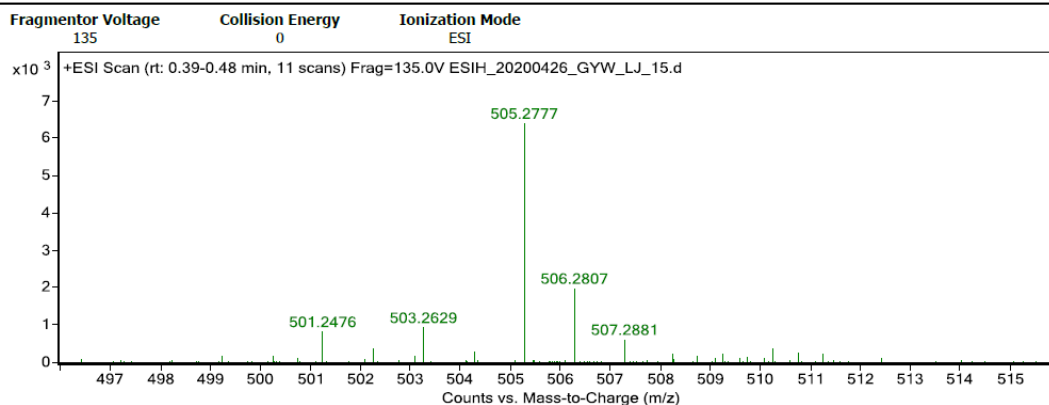


Figure S2:  $^{13}\text{C}$  NMR spectrum (125 MHz) of **2** in  $\text{CD}_3\text{OD}$

## Qualitative Analysis Report

<b>Data Filename</b>	ESI_H_20200426_GYW_LJ_15.d	<b>Sample Name</b>	S0409-1
<b>Sample Type</b>	Sample	<b>Position</b>	P1-A9
<b>Instrument Name</b>	Agilent G6520 Q-TOF	<b>Acq Method</b>	20160322_MS_ESIH_POS_1min.m
<b>Acquired Time</b>	4/26/2020 18:46:11	<b>IRM Calibration Status</b>	Success
<b>DA Method</b>	small molecular data analysis method.m	<b>Comment</b>	ESIH by ZZY

### User Spectra



### Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
505.2777	505.2772	-0.55	-1.08	C <sub>26</sub> H <sub>42</sub> NaO <sub>8</sub>	(M+Na) <sup>+</sup>

--- End Of Report ---

Figure S3: HR-ESI-MS spectrum of compound **3**

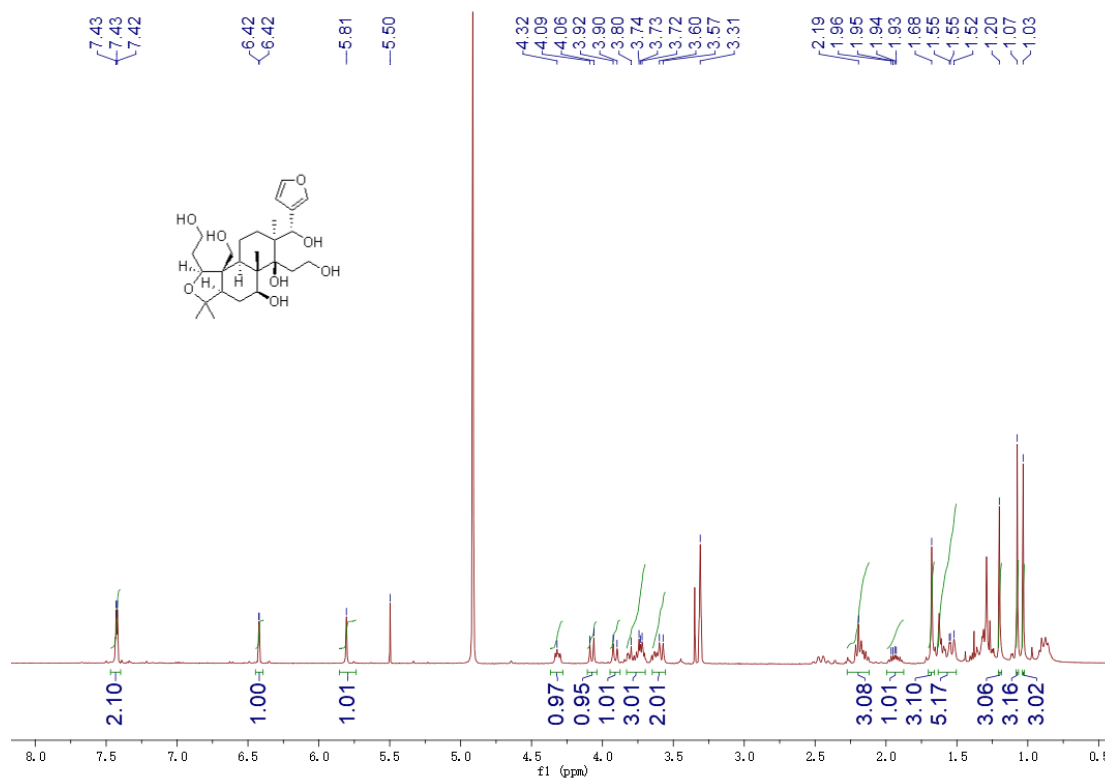


Figure S4: <sup>1</sup>H NMR spectrum (400 MHz) of **3** in CD<sub>3</sub>OD.

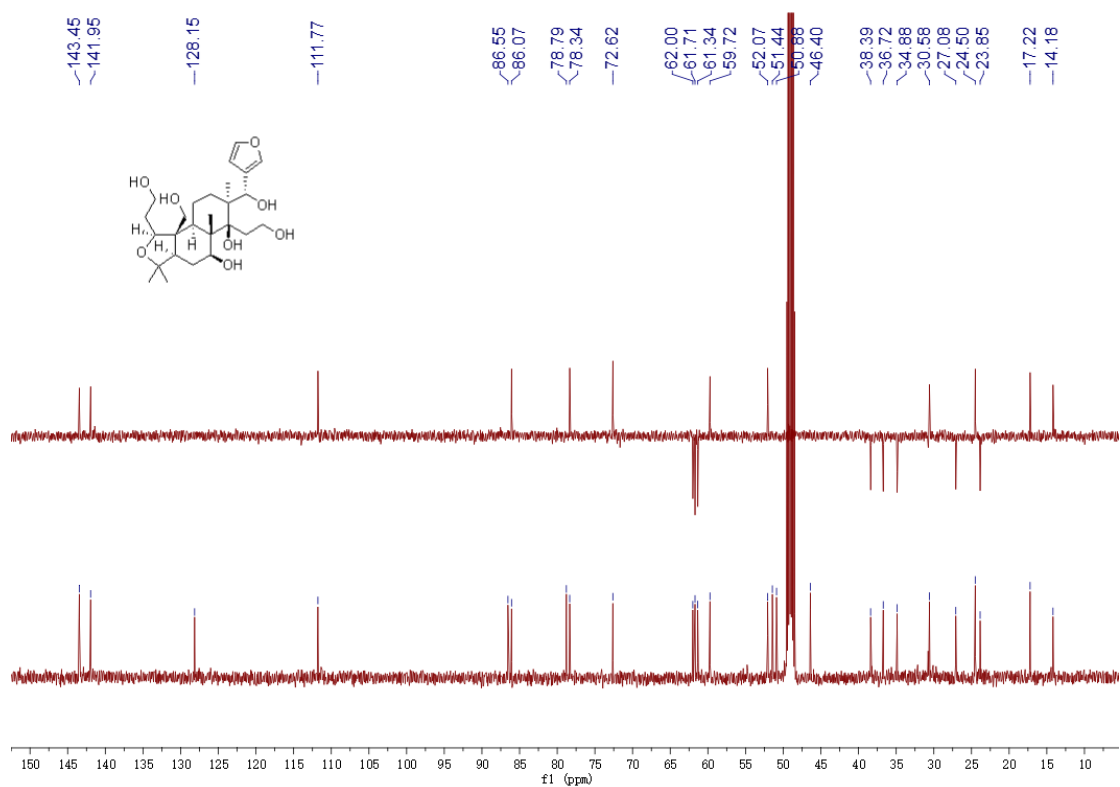


Figure S5:  $^{13}\text{C}$  NMR spectrum (125 MHz) of **3** in  $\text{CD}_3\text{OD}$ .

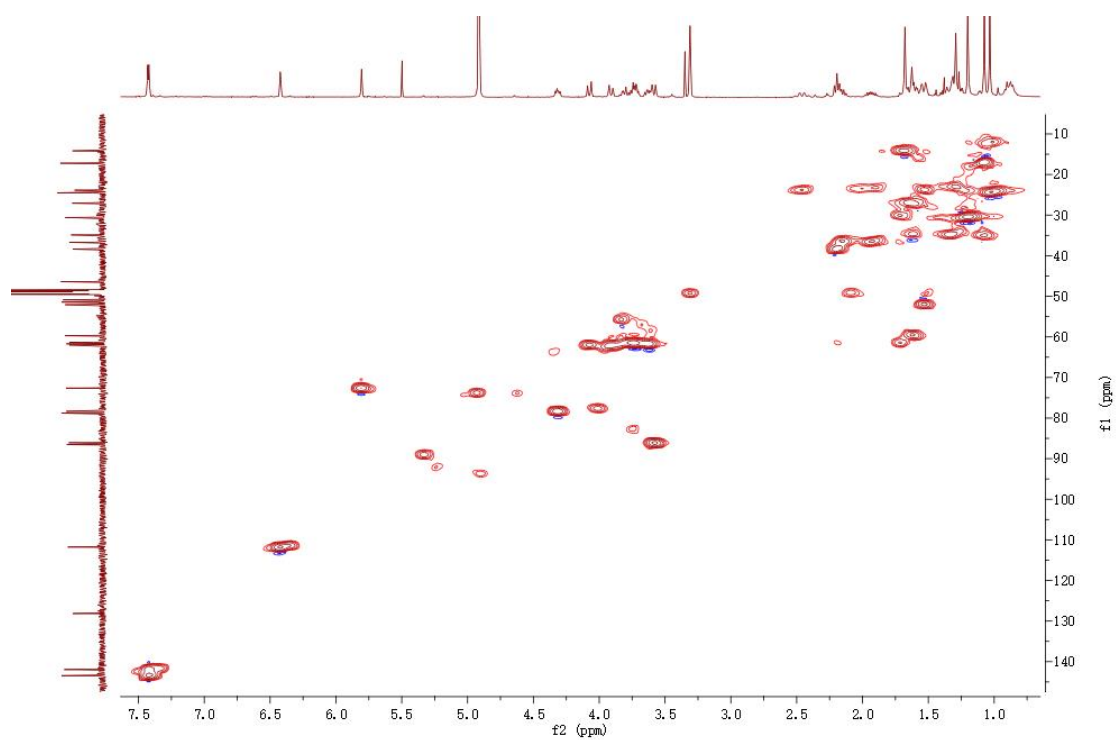


Figure S6: HSQC spectrum (500 MHz) of **3** in  $\text{CD}_3\text{OD}$ .

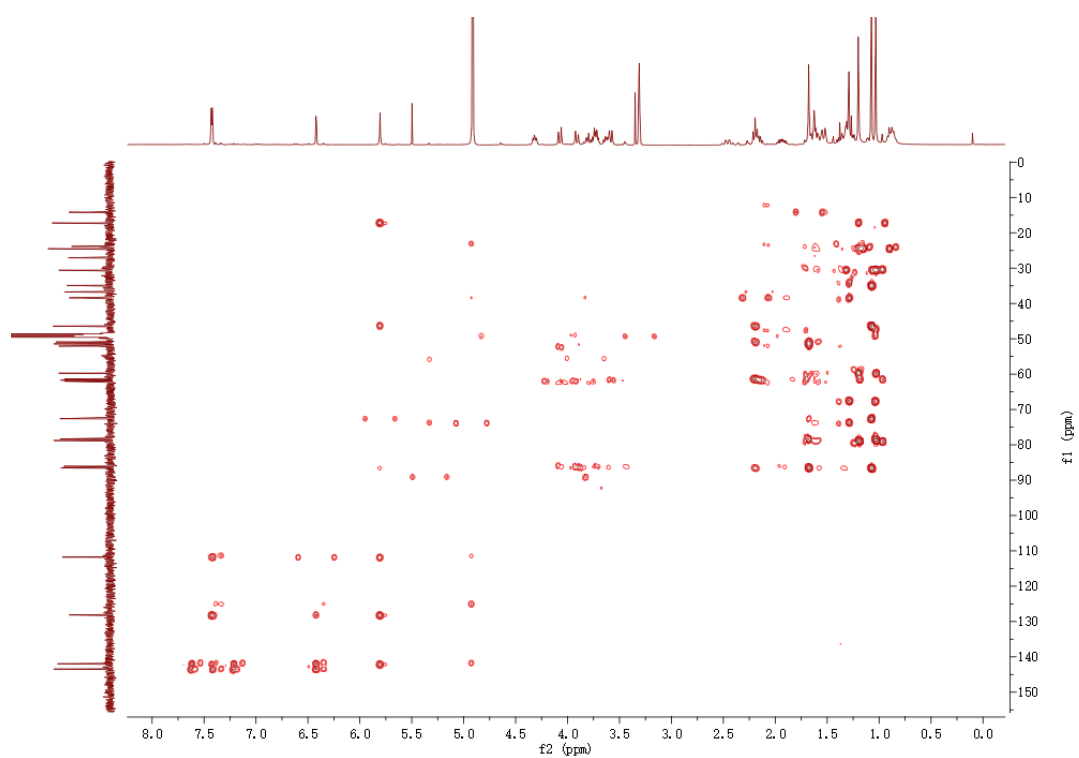


Figure S7: HMBC spectrum (500 MHz) of **3** in CD<sub>3</sub>OD.

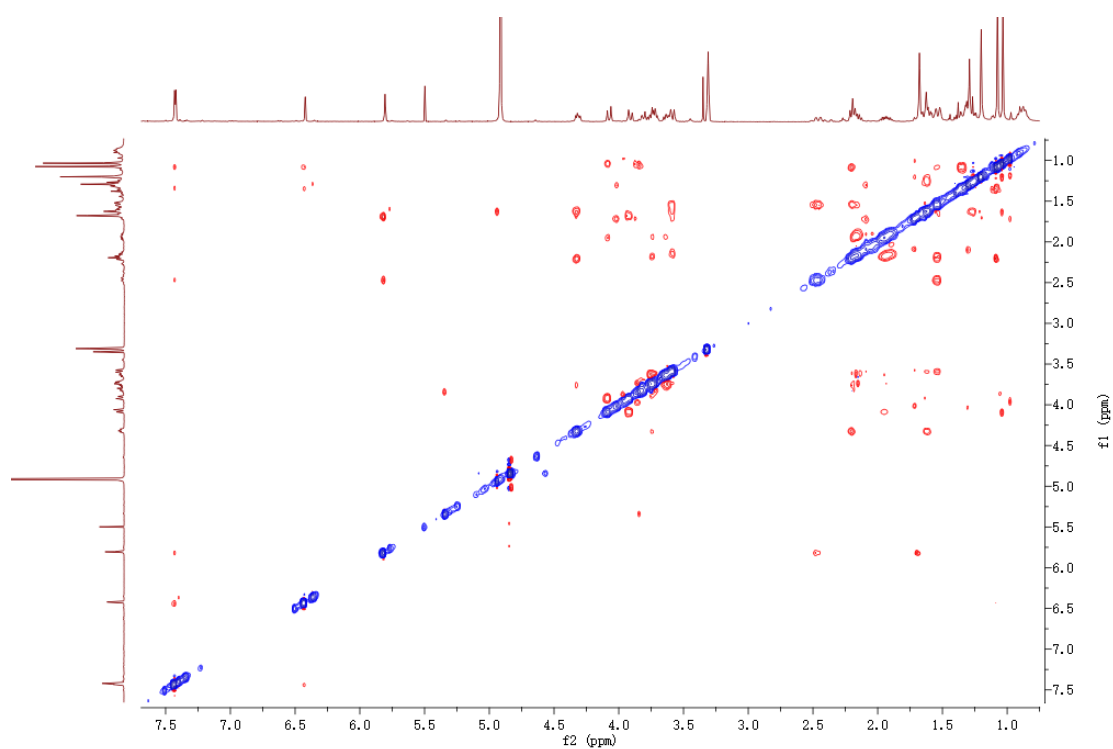


Figure S8: NOESY spectrum (500 MHz) of **3** in CD<sub>3</sub>OD.

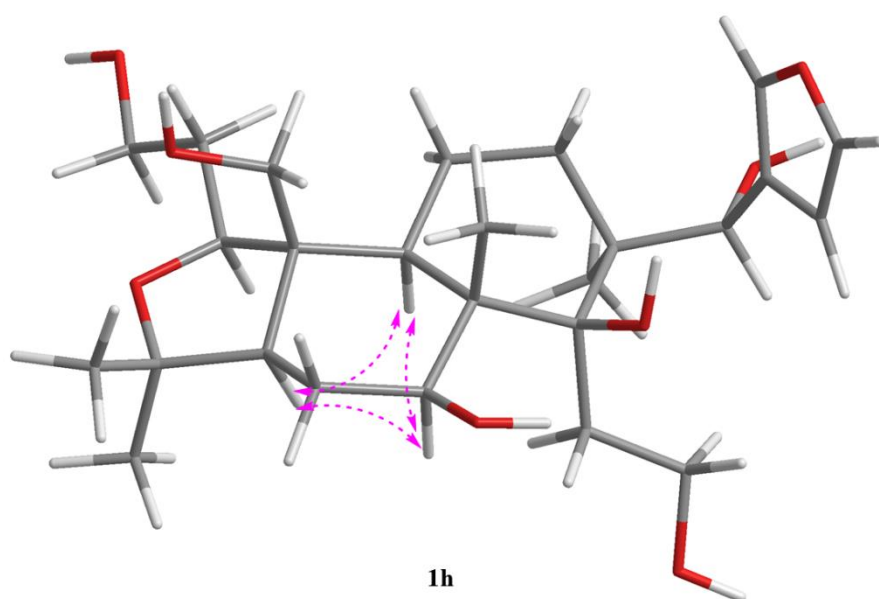


Figure S9: Key NOE correlations for compound **3**

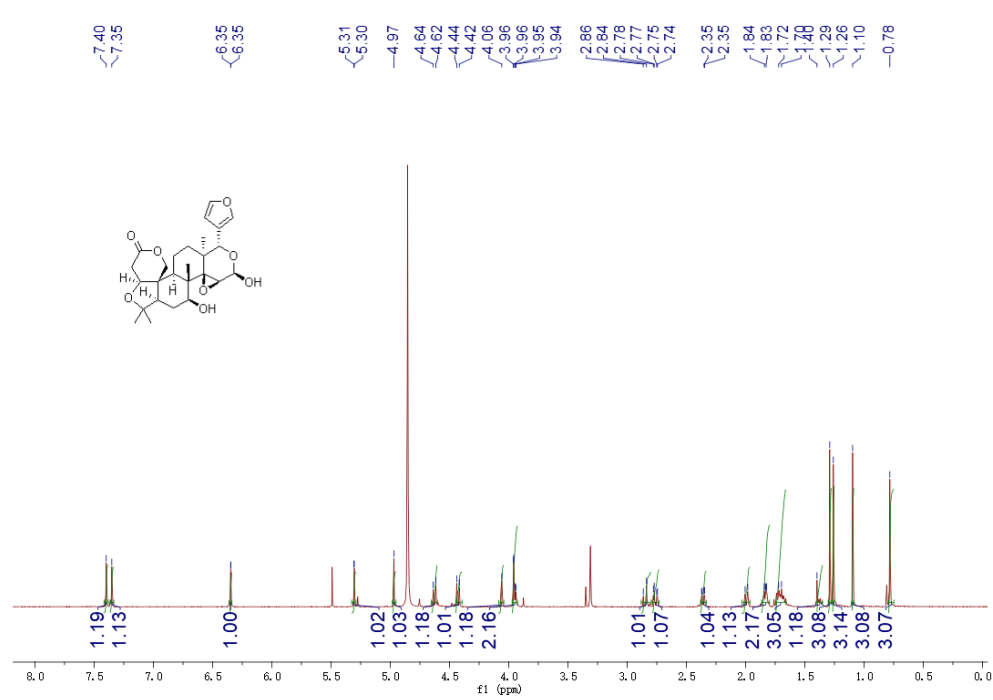


Figure S10:  $^1\text{H}$  NMR spectrum (400 MHz) of **4** in  $\text{CD}_3\text{OD}$

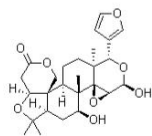


Figure S11:  $^{13}\text{C}$  NMR spectrum (125 MHz) of **4** in  $\text{CD}_3\text{OD}$

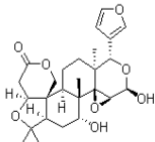


Figure S12:  $^1\text{H}$  NMR spectrum (400 MHz) of **5** in  $\text{CD}_3\text{OD}$ .

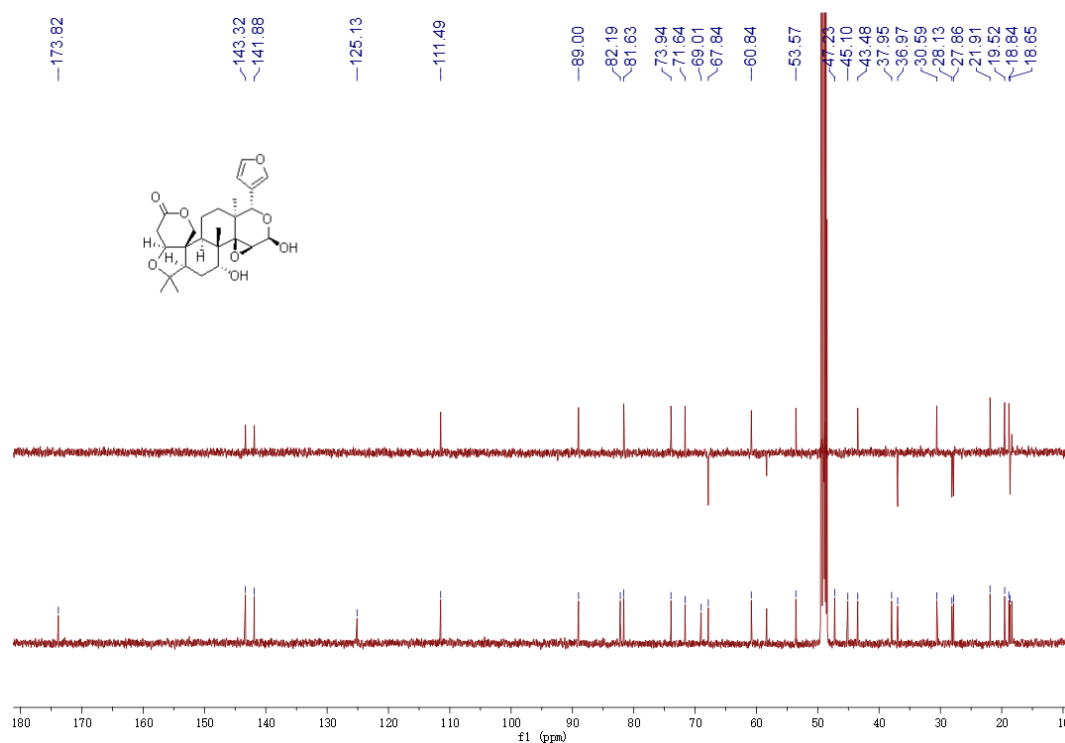


Figure S13:  $^{13}\text{C}$  NMR spectrum (125 MHz) of 5 in  $\text{CD}_3\text{OD}$ .

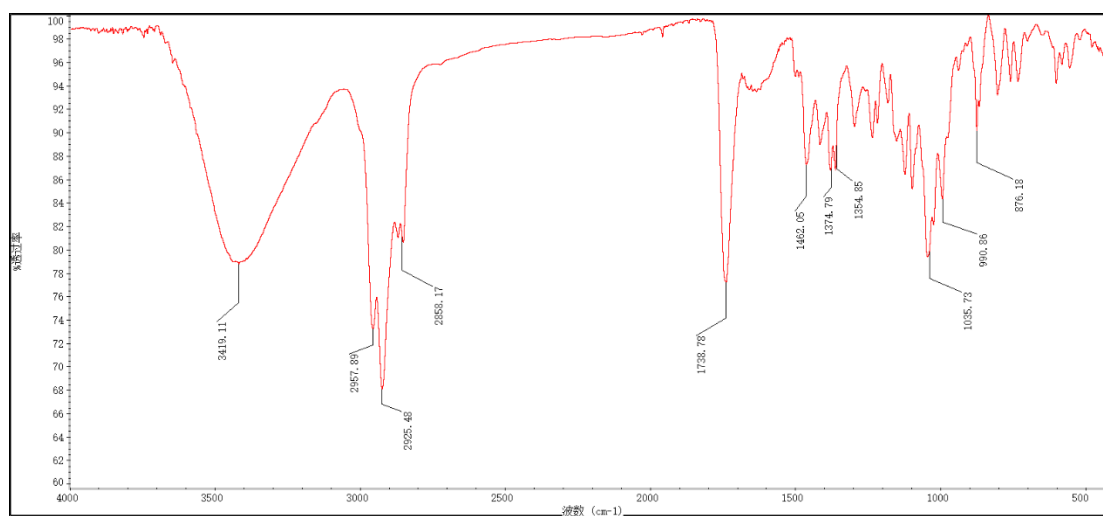


Figure S14: IR spectrum of compound 4



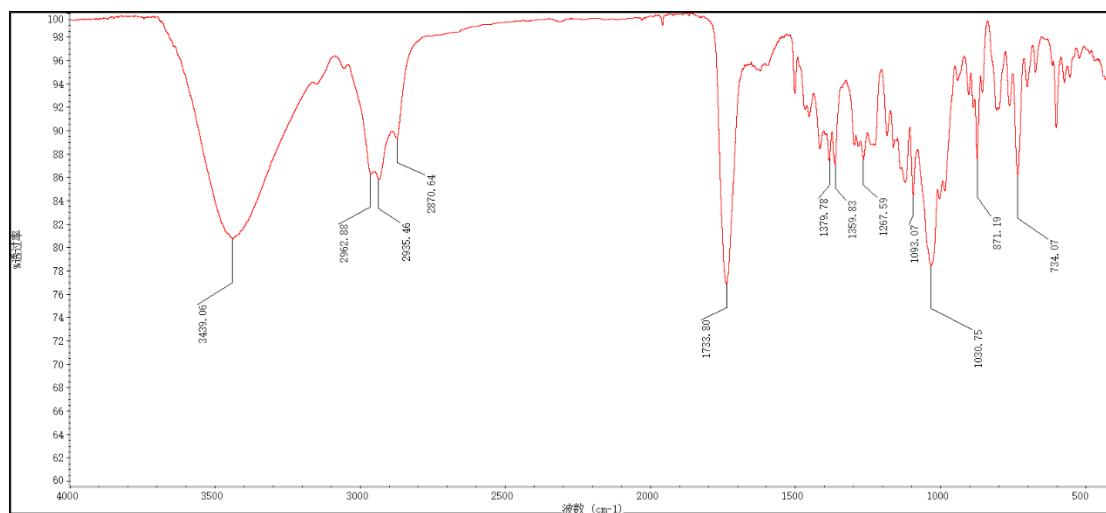


Figure S15: IR spectrum of compound **5**

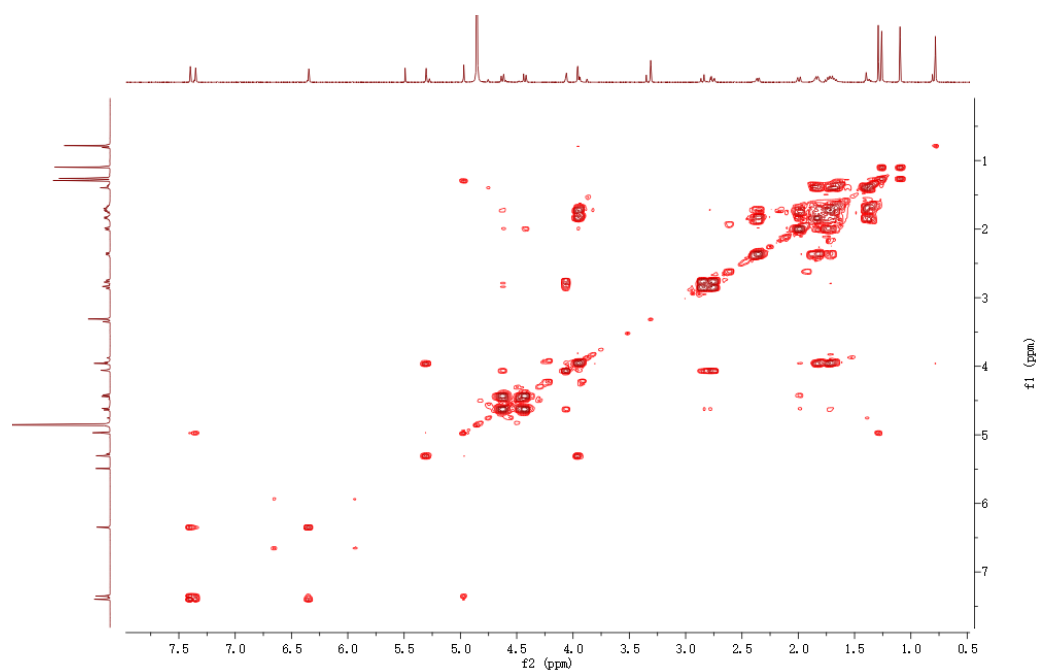


Figure S16:  $^1\text{H}$ - $^1\text{H}$  COSY spectrum (500 MHz) of **4** in  $\text{CD}_3\text{OD}$

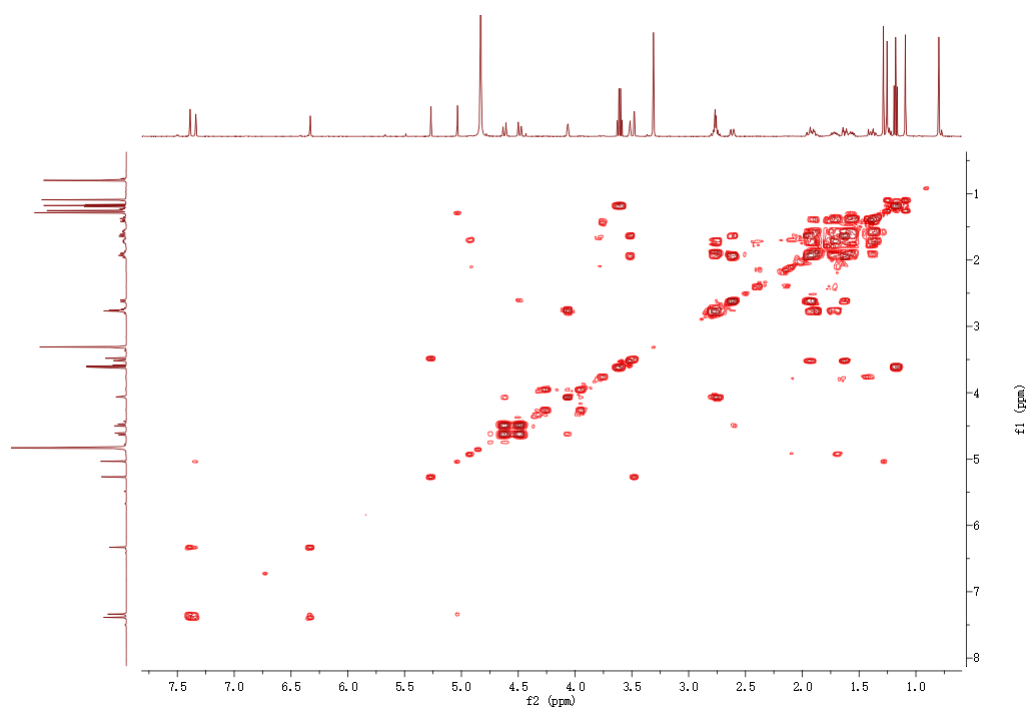


Figure S17:  $^1\text{H}$ – $^1\text{H}$  COSY spectrum (500 MHz) of **5** in  $\text{CD}_3\text{OD}$ .

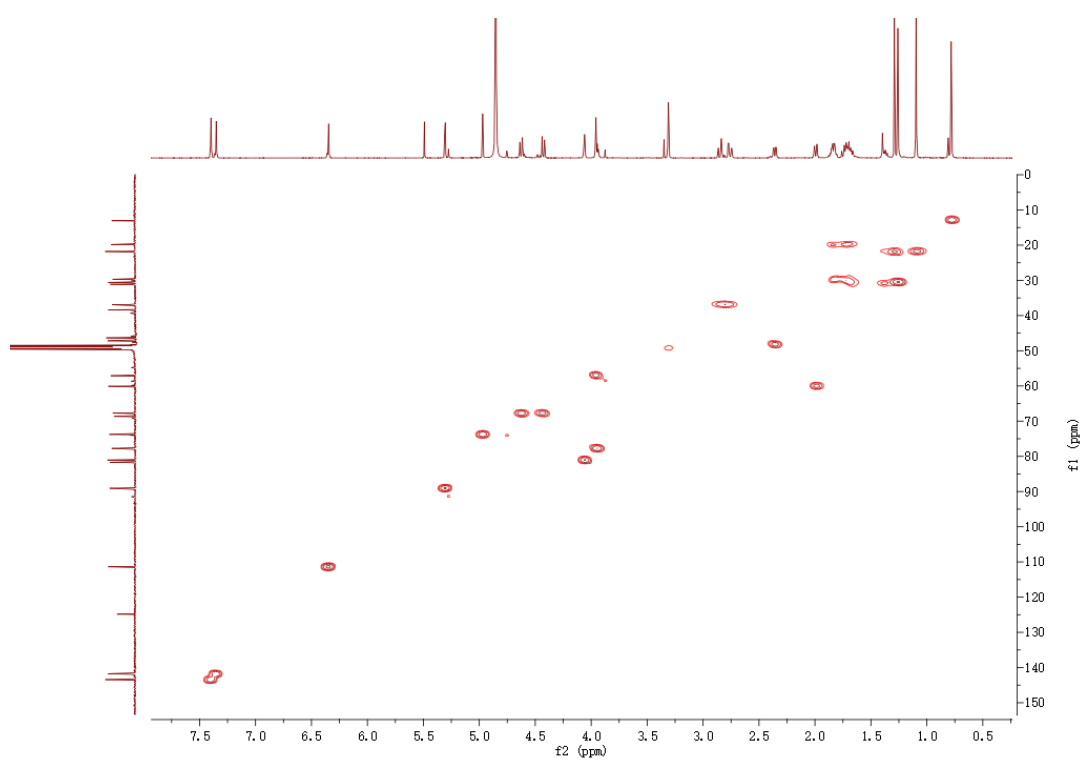


Figure S18: HSQC spectrum (500 MHz) of **4** in  $\text{CD}_3\text{OD}$

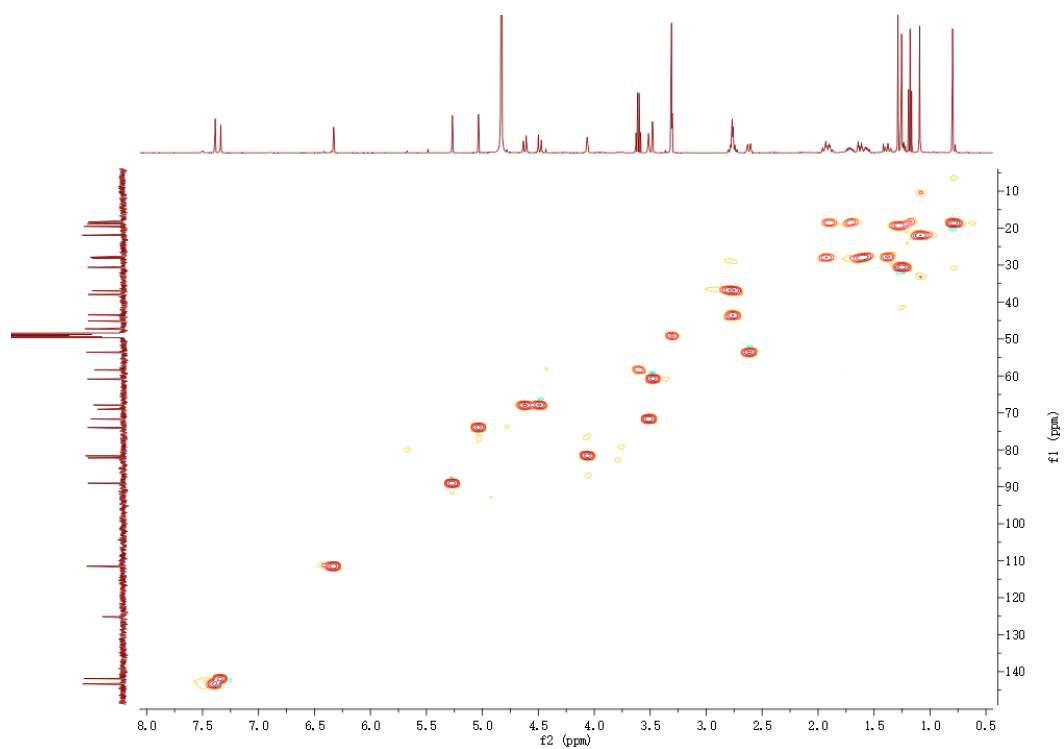


Figure S19: HSQC spectrum (500 MHz) of **5** in CD<sub>3</sub>OD.

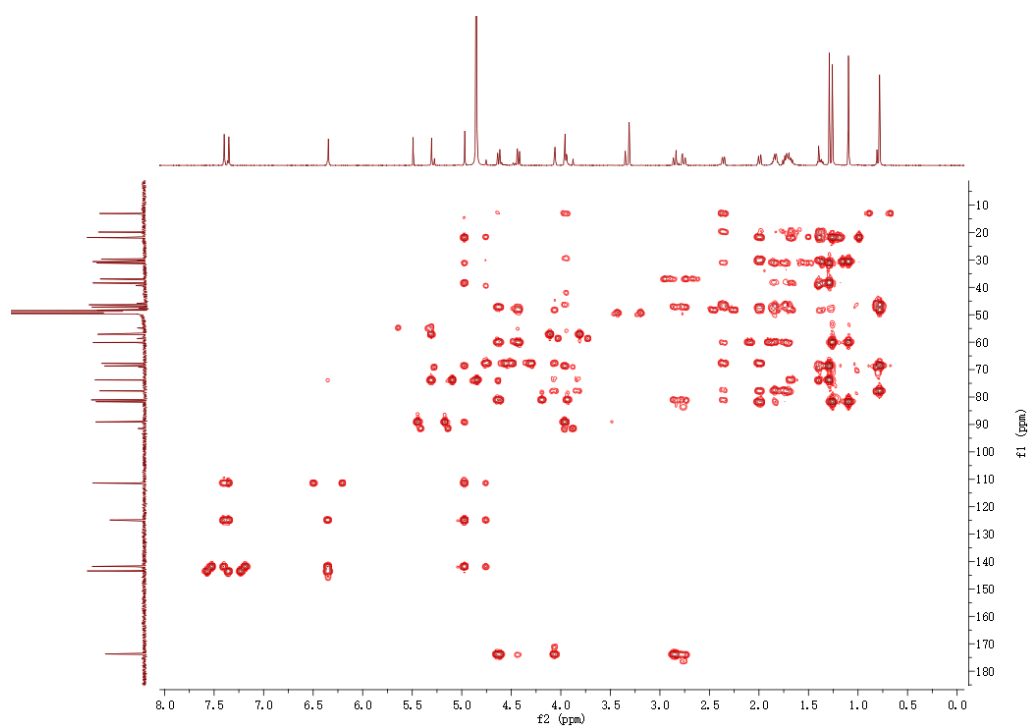


Figure S20: HMBC spectrum (500 MHz) of **4** in CD<sub>3</sub>OD

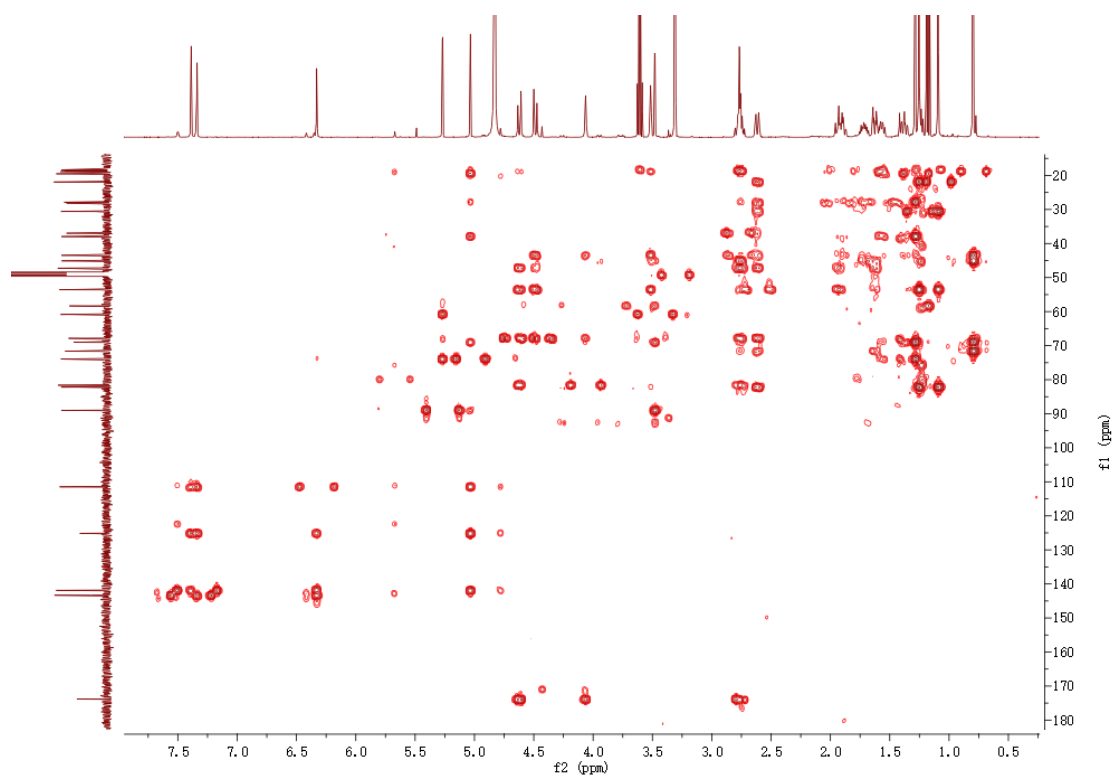


Figure S21: HMBC spectrum (500 MHz) of **5** in CD<sub>3</sub>OD.

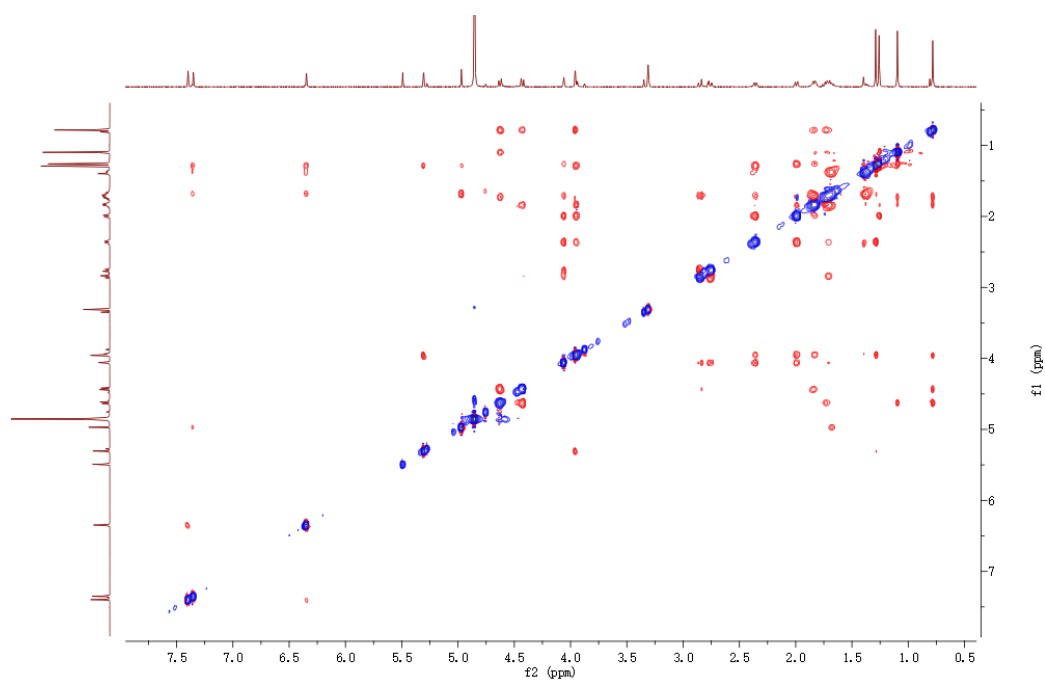


Figure S22: NOESY spectrum (500 MHz) of **4** in CD<sub>3</sub>OD

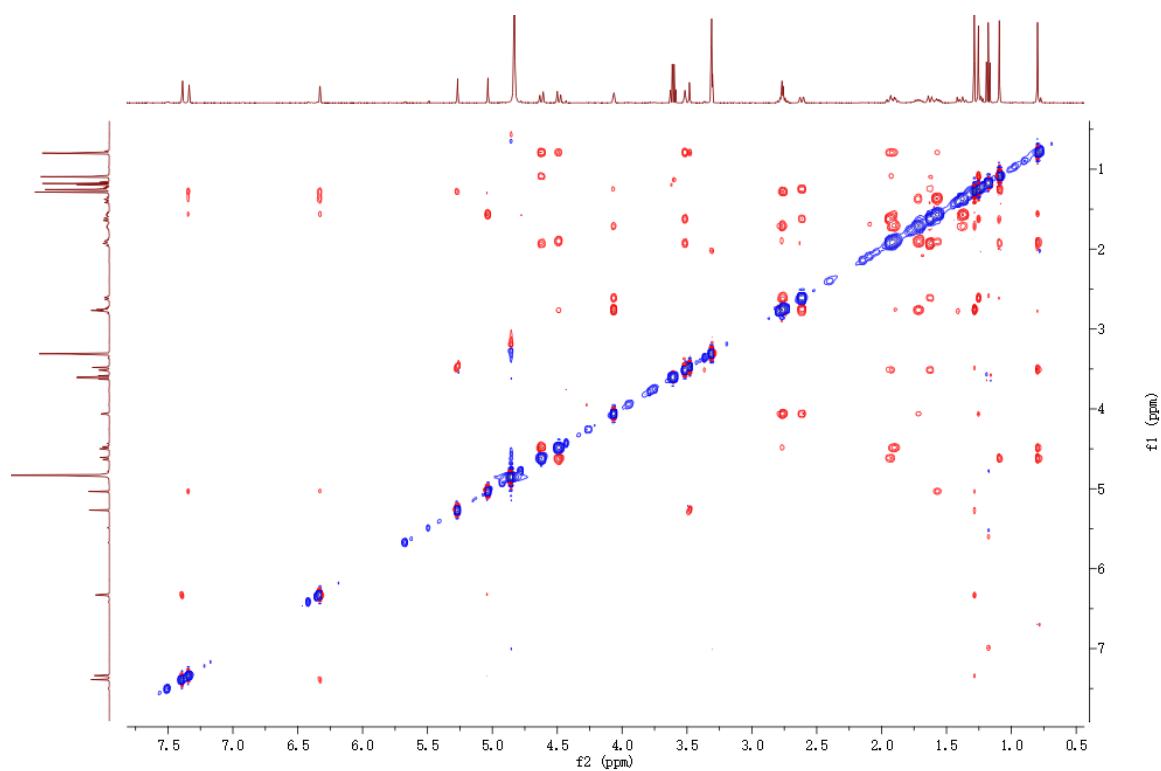


Figure S23: NOESY spectrum (500 MHz) of **5** in CD<sub>3</sub>OD..

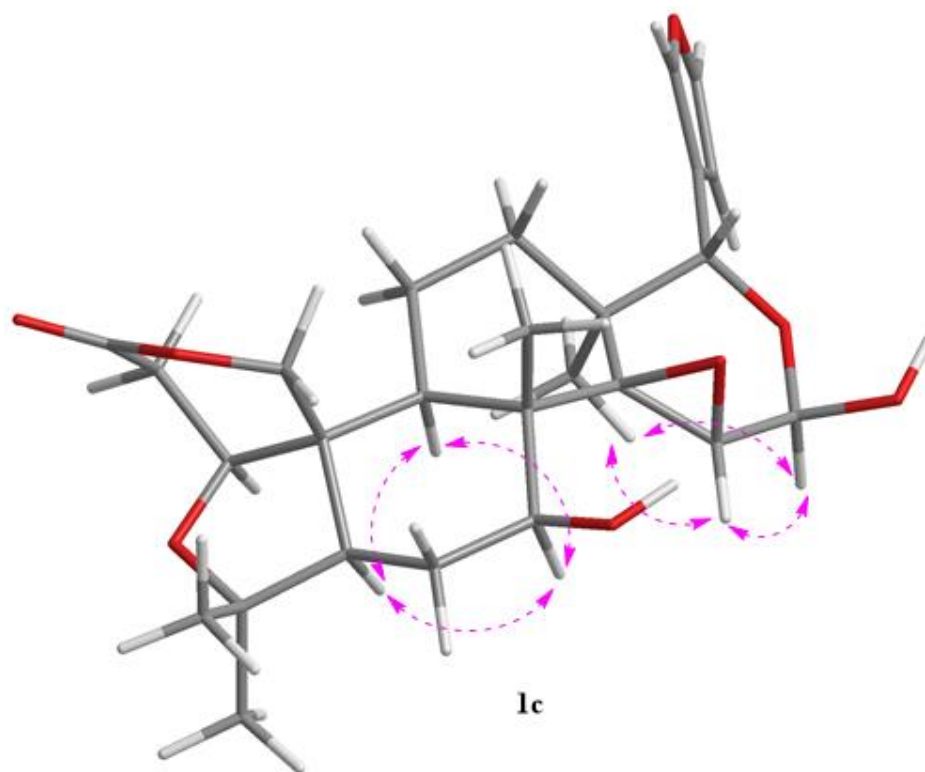


Figure S24: Key NOE correlations for compound **4**

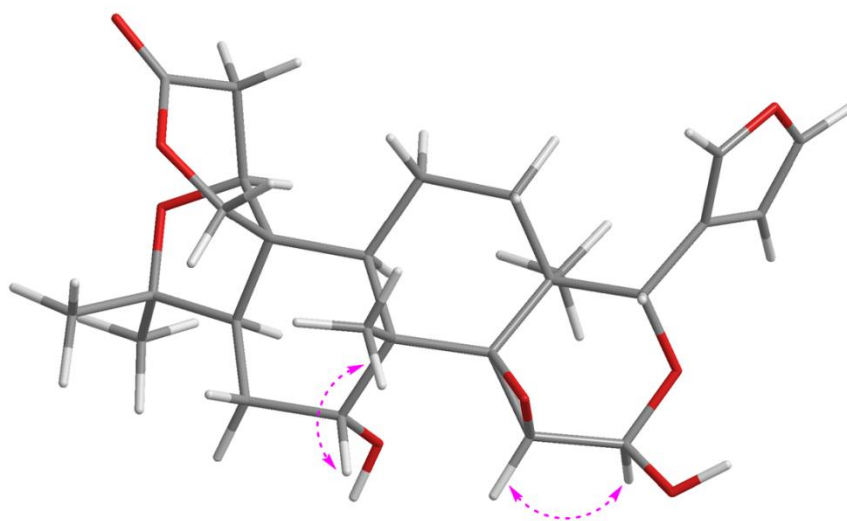


Figure S25: Key NOE correlations for compound **5**

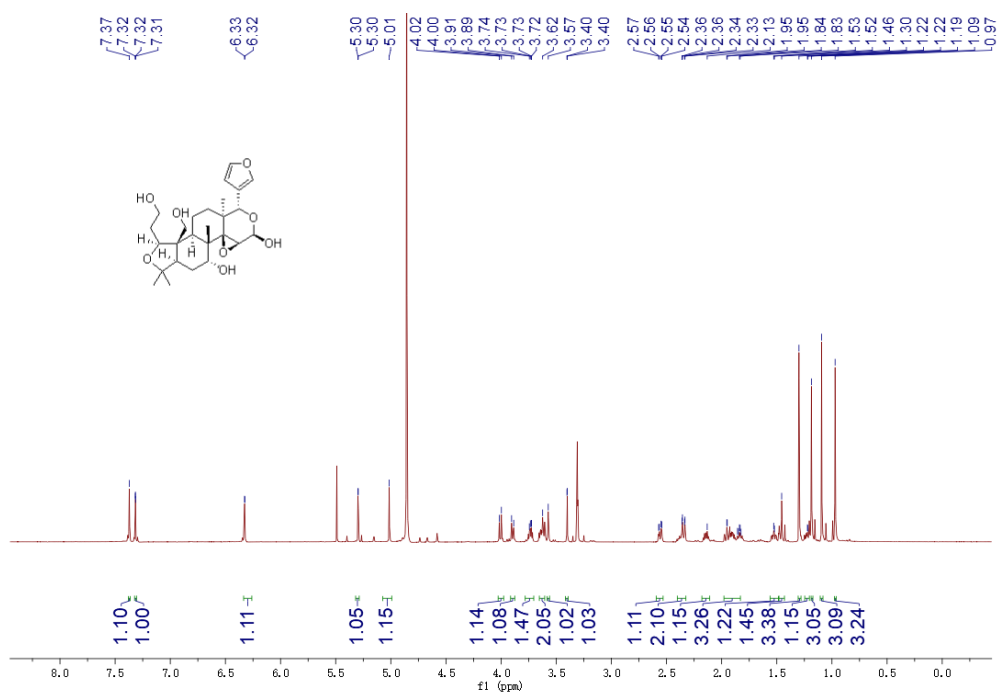


Figure S26:  $^1\text{H}$  NMR spectrum (400 MHz) of **6** in  $\text{CD}_3\text{OD}$ .

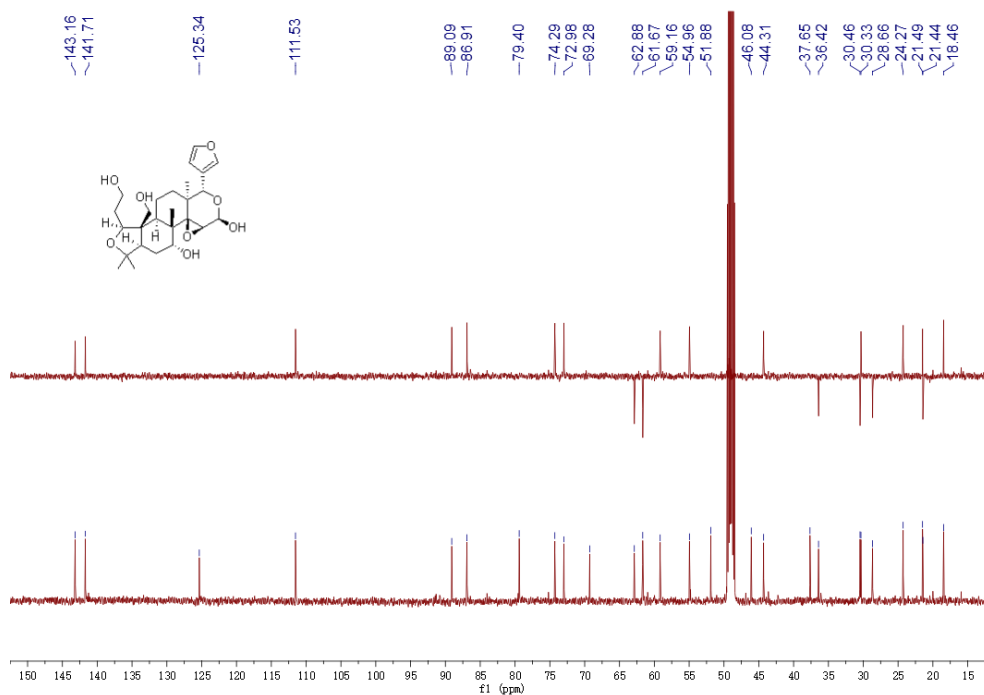


Figure S27: <sup>13</sup>C NMR spectrum (125 MHz) of 6 in CD<sub>3</sub>OD.

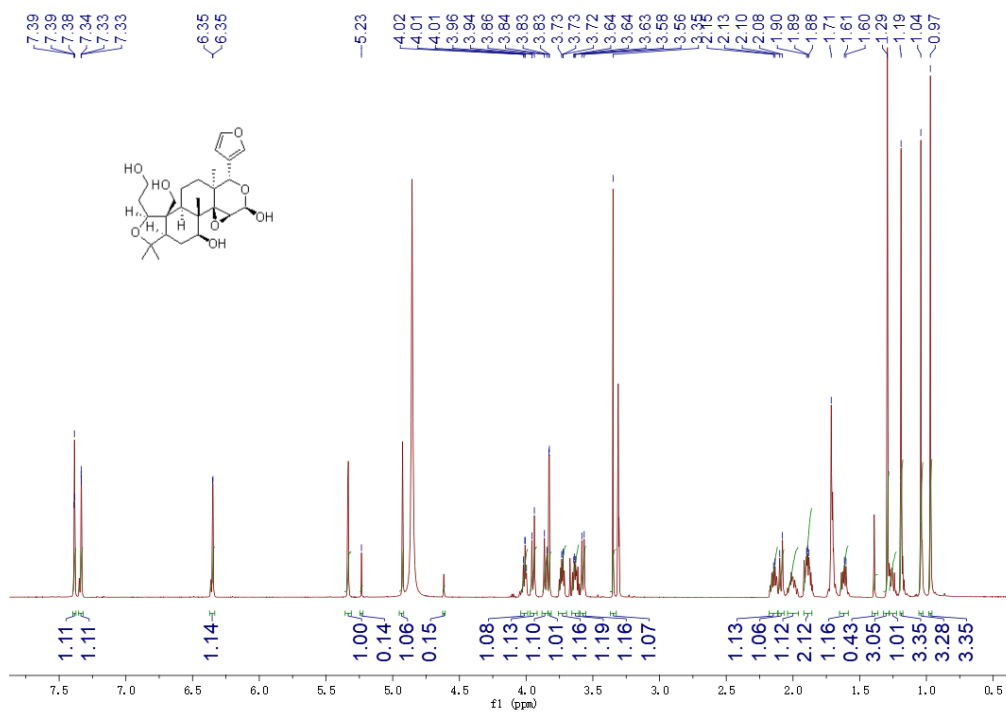


Figure S28: <sup>1</sup>H NMR spectrum (400 MHz) of 7 in CD<sub>3</sub>OD.

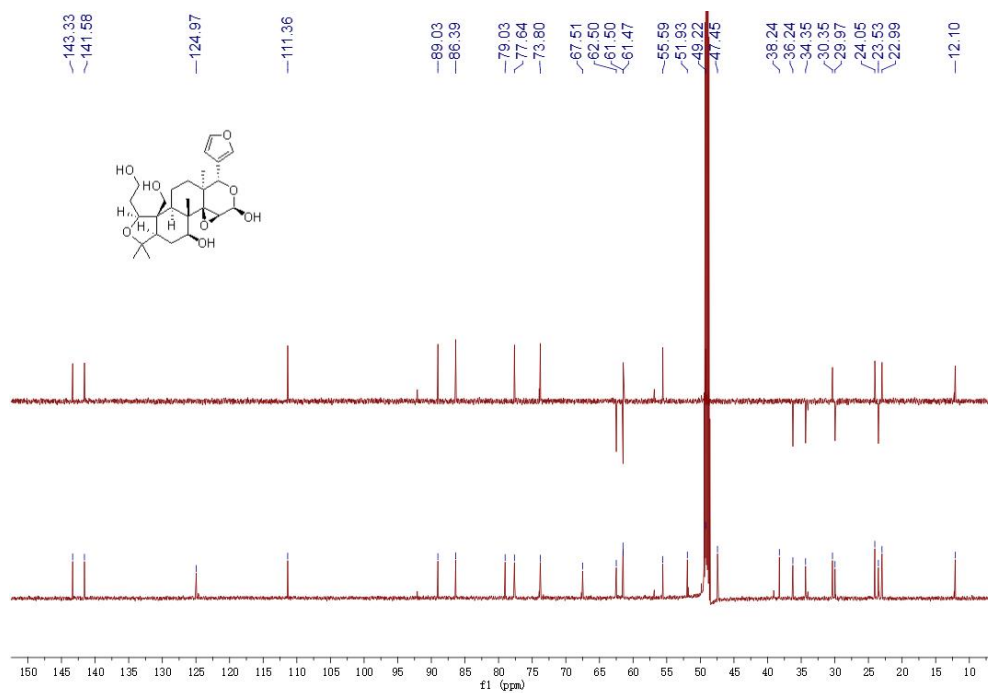


Figure S29: <sup>13</sup>C NMR spectrum (125 MHz) of 7 in CD<sub>3</sub>OD.

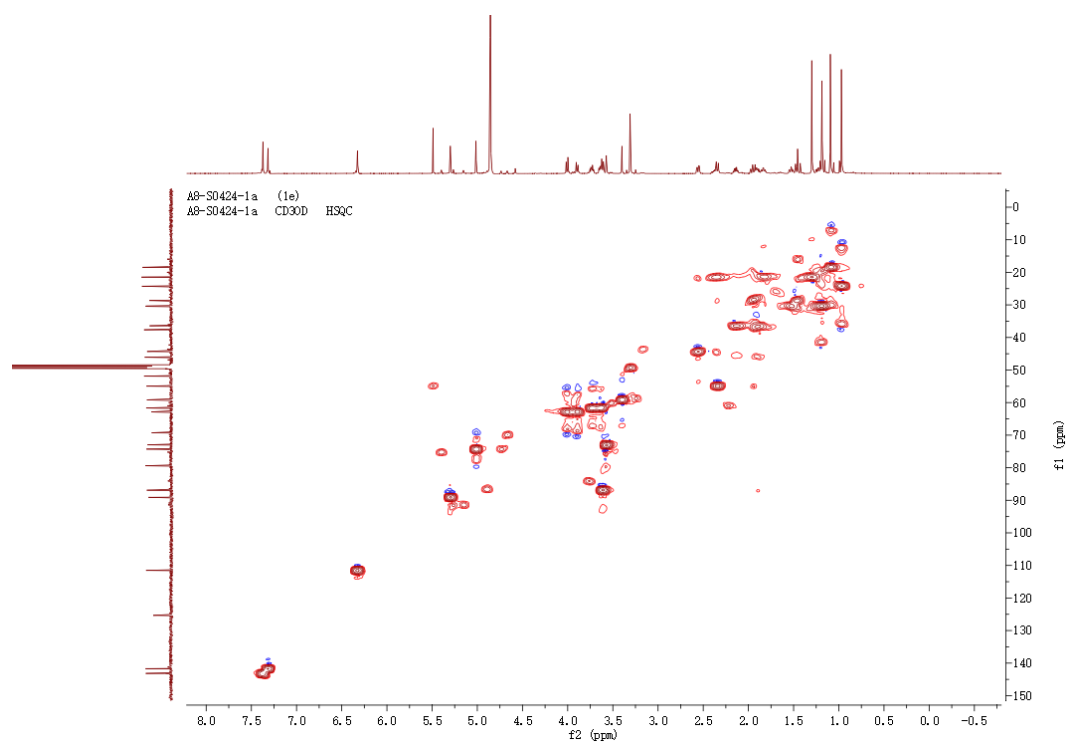


Figure S30: HSQC spectrum (500 MHz) of 6 in CD<sub>3</sub>OD.



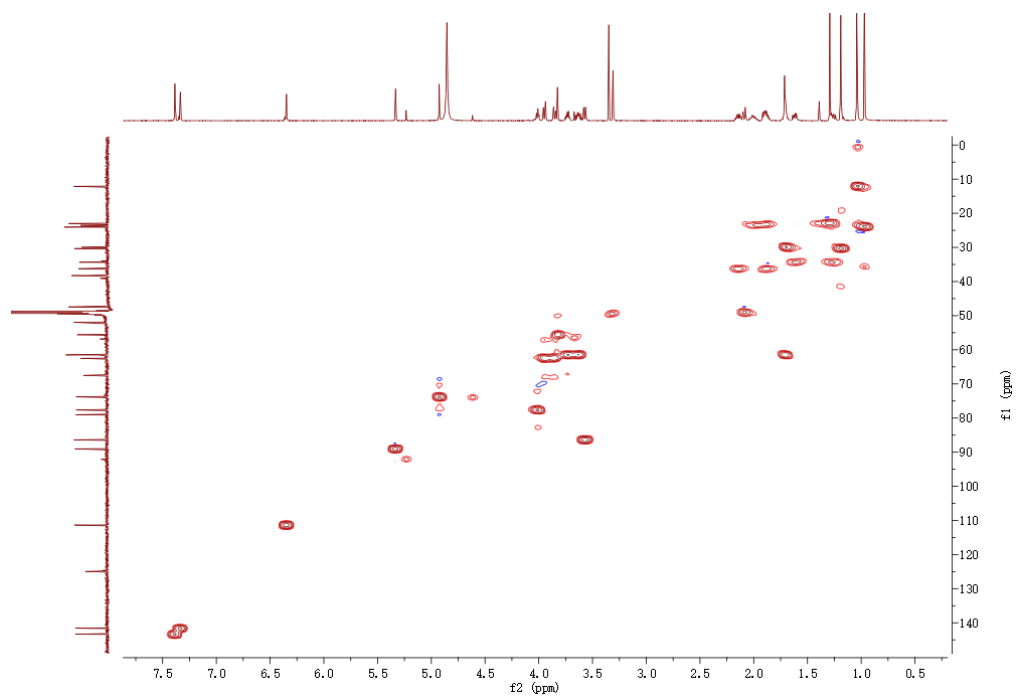


Figure S31: HSQC spectrum (500 MHz) of **7** in CD<sub>3</sub>OD.

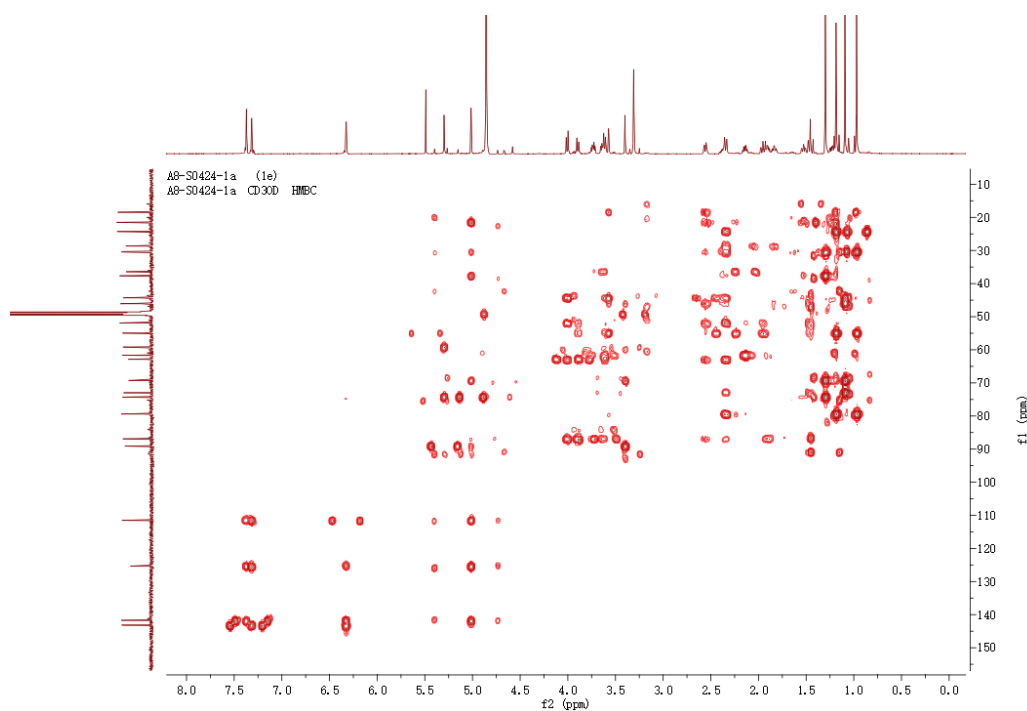


Figure S32: HMBC spectrum (500 MHz) of **6** in CD<sub>3</sub>OD.

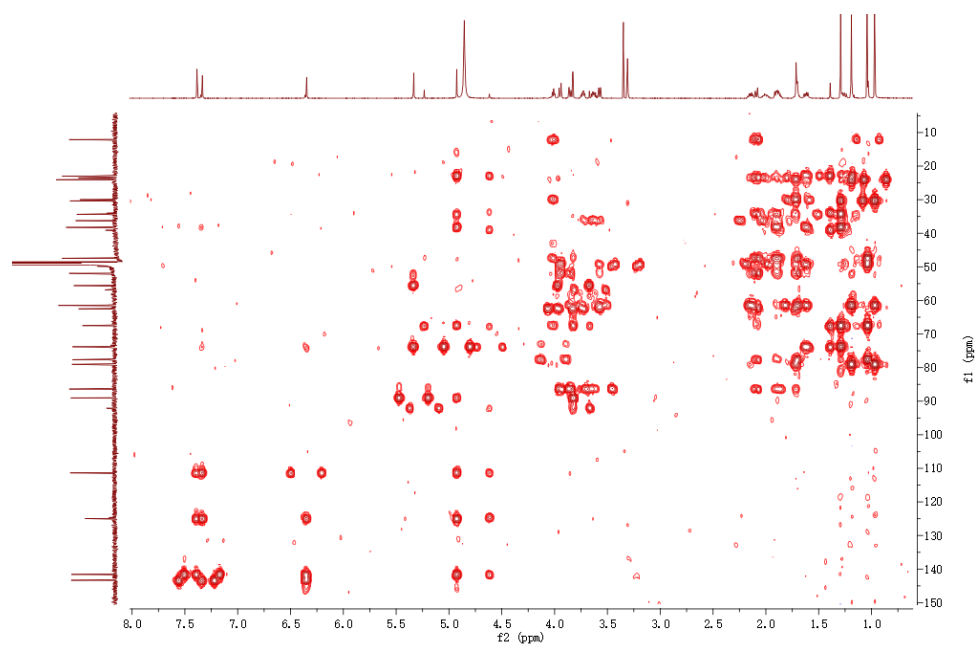


Figure S33: HMBC spectrum (500 MHz) of **7** in CD<sub>3</sub>OD.

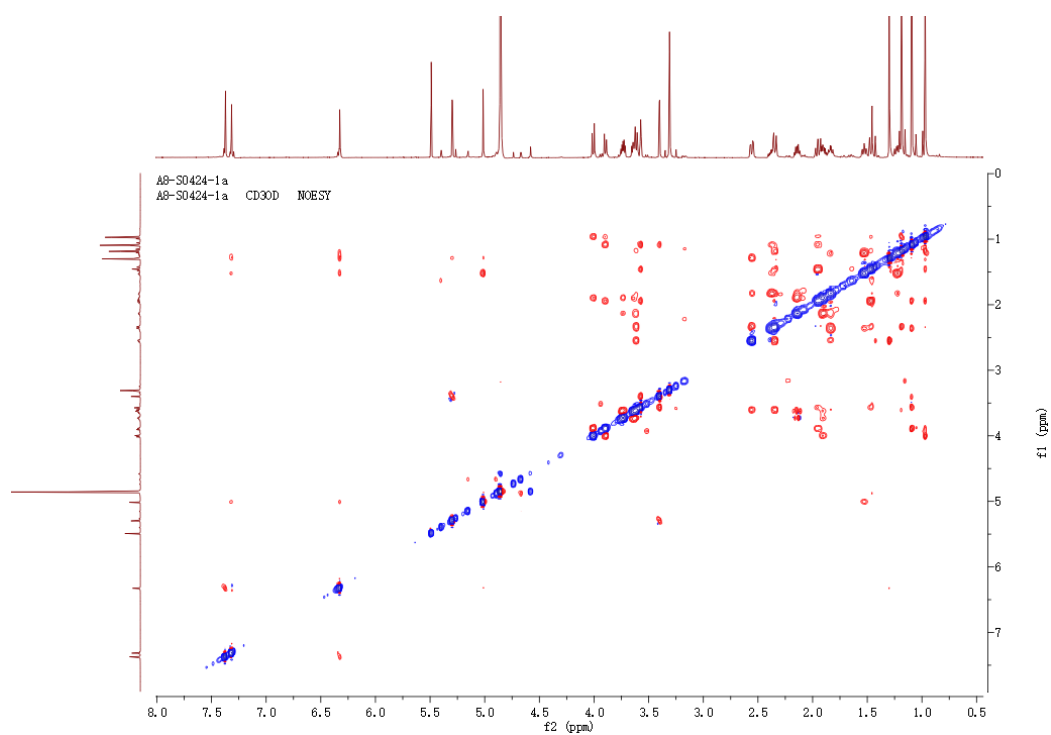


Figure S32: NOESY spectrum (500 MHz) of **6** in CD<sub>3</sub>OD.

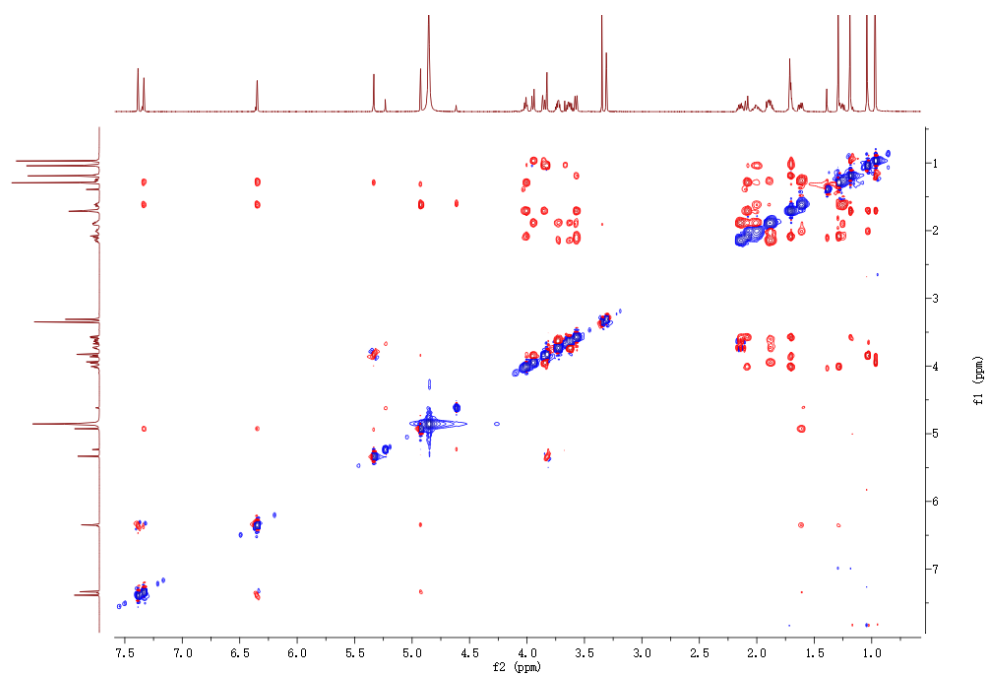


Figure S33: NOESY spectrum (500 MHz) of **7** in CD<sub>3</sub>OD..

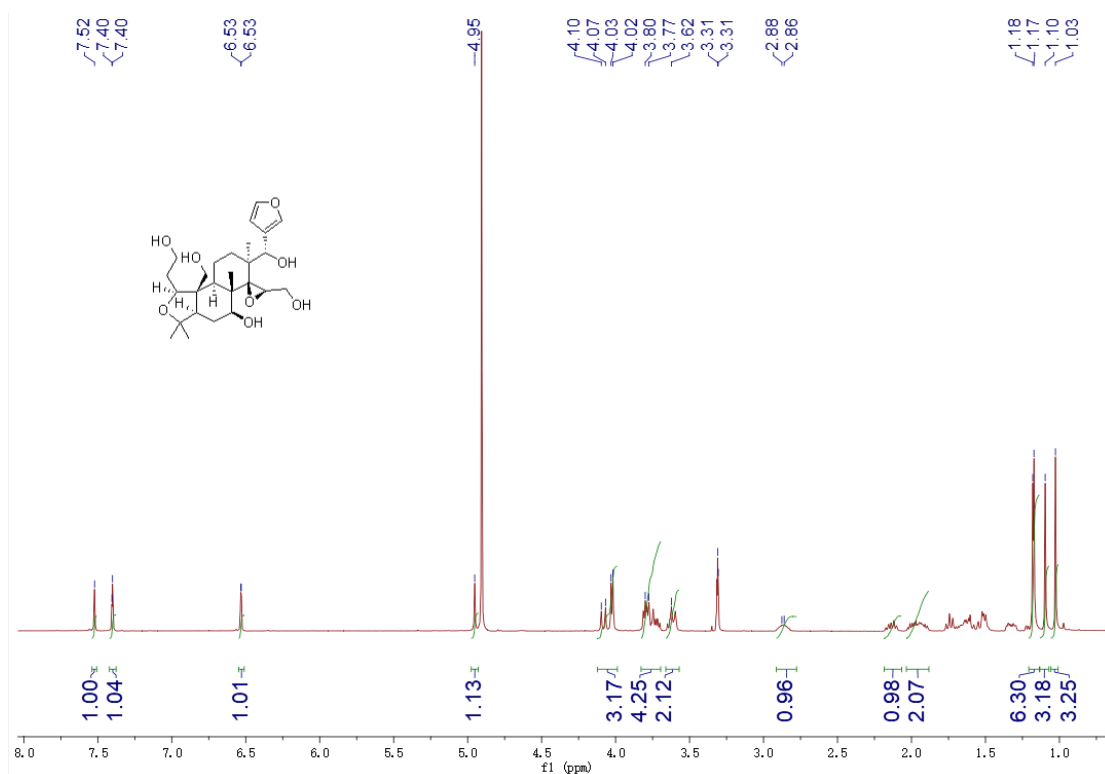


Figure S34: <sup>1</sup>H NMR spectrum (400 MHz) of **8** in CD<sub>3</sub>OD.

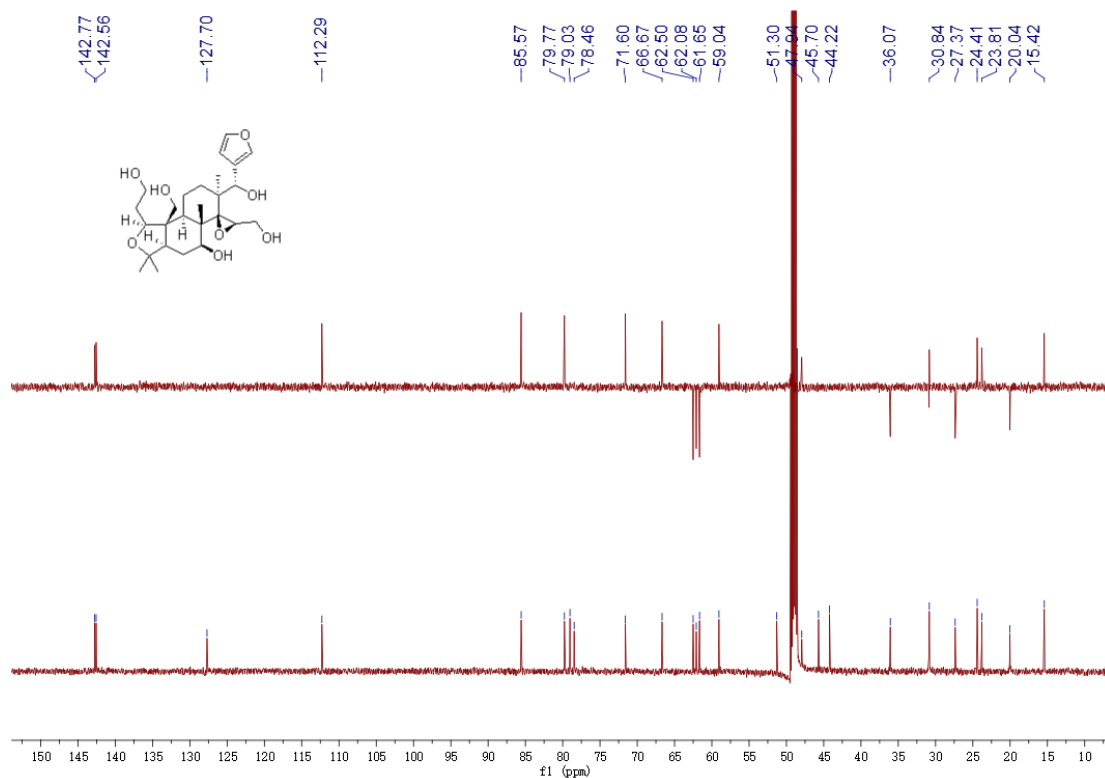


Figure S35:  $^{13}\text{C}$  NMR spectrum (125 MHz) of **8** in  $\text{CD}_3\text{OD}$ .

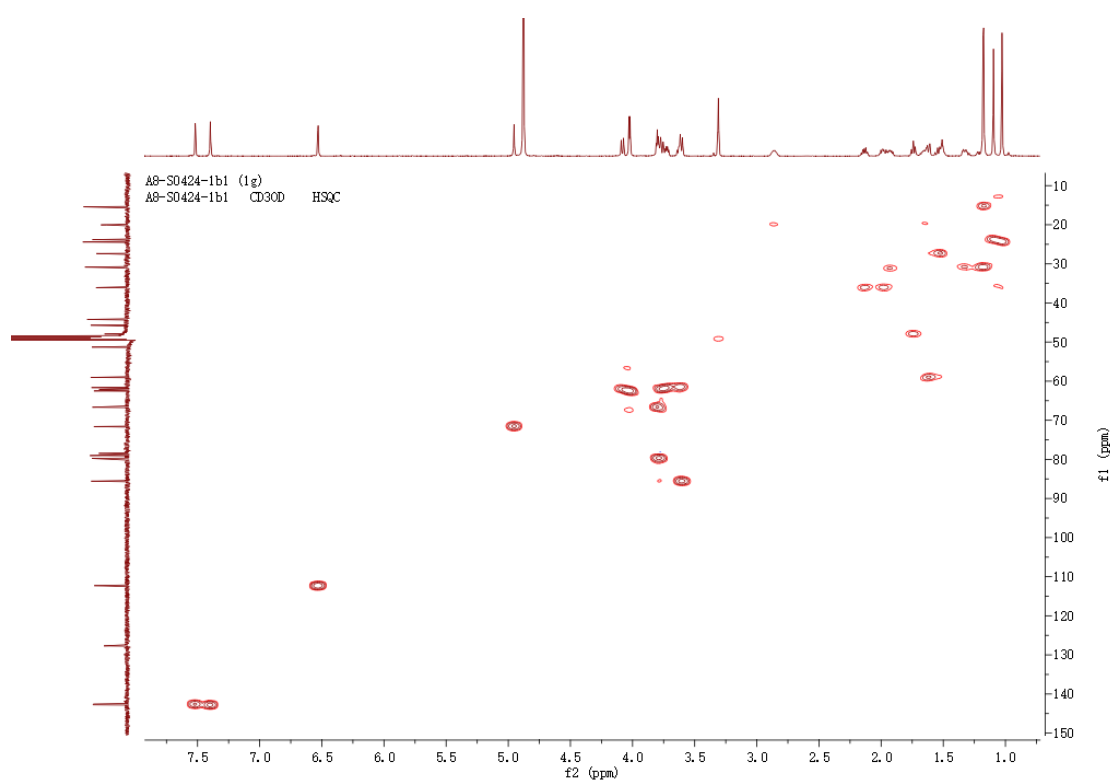


Figure S36: HSQC spectrum (500 MHz) of **8** in  $\text{CD}_3\text{OD}$ .

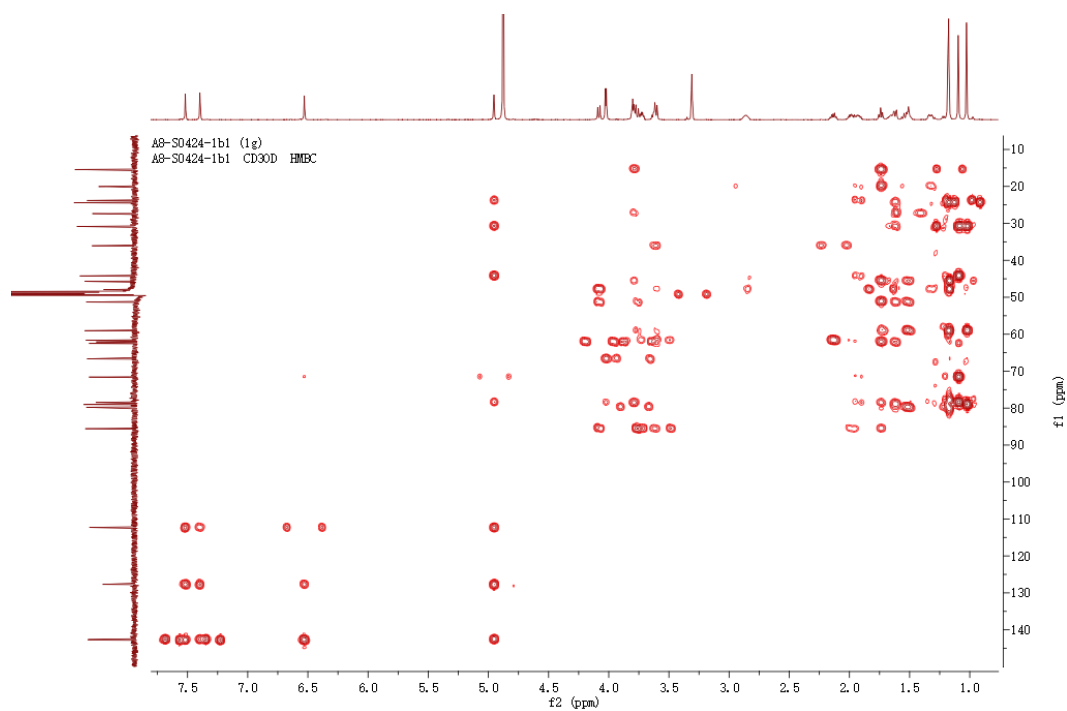


Figure S37: HMBC spectrum (500 MHz) of **8** in CD<sub>3</sub>OD.

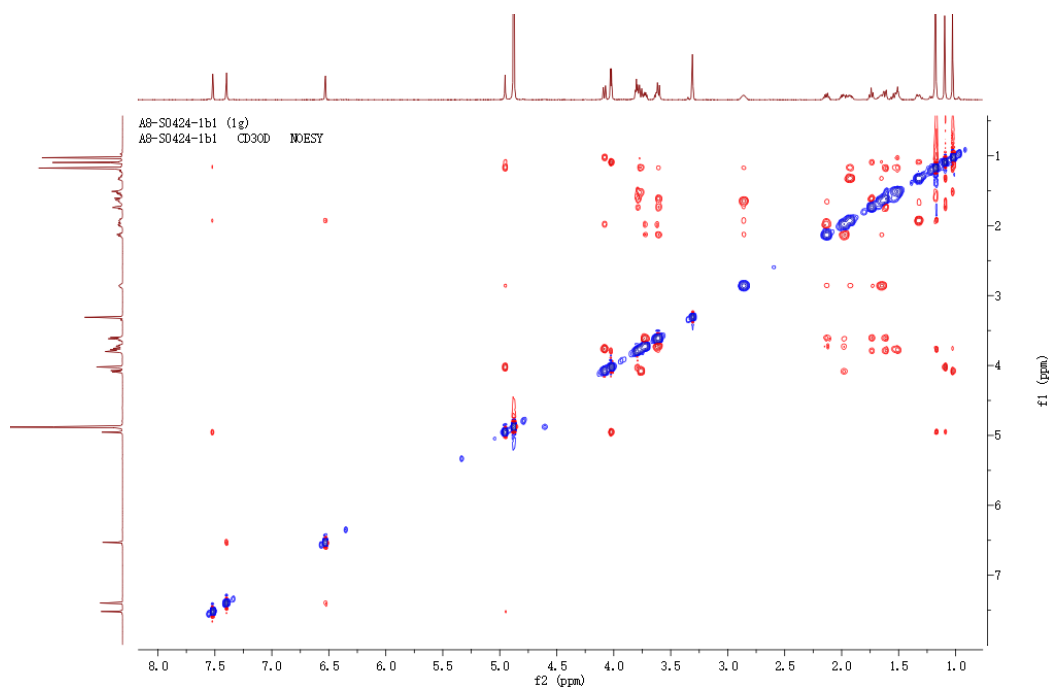


Figure S38: NOESY spectrum (500 MHz) of **8** in CD<sub>3</sub>OD.

## 2. Information of reagents used in the cell experiments

**Table S1 reagents used in the cell experiments**

Reagents	Company	Supplier
Dulbeccos Modified Eagle Medium(high sugar)	/	Gibco
Fetal bovine serum (FBS)	10 %	Gibco
Trypsin	0.25 %	Gibco
MTT	0.5 mg/ml	Sigma-Aldrich
DMSO	100%	Sinopharm
D-Hanks	/	Sinopharm
LPS	100 ng/ml	Sigma-Aldrich
Griess reagent (modified)	/	Sigma-Aldrich
Cell Counting Kit-8(CCK-8)	/	Adamas Life
Mouse TNF- $\alpha$ ELISA	/	Adamas Life