

Isolation, identification, anti-inflammatory, and *in silico* analysis of new lignans from *Ferula sinkiangensis*

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Contents

MS, UV, IR and NMR Spectra of Compound 1

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

Fig. S2. IR spectrum of **1**

Fig. S3. UV spectrum in MeOH of **1**

Fig. S4. ^1H -NMR spectrum (CD_3OD , 600 MHz) of **1**

Fig. S5. ^{13}C -NMR spectrum (CD_3OD , 150 MHz) of **1**

Fig. S6. ^1H - ^1H COSY spectrum (CD_3OD) of **1**

Fig. S7. HSQC spectrum (CD_3OD) of **1**

Fig. S8. HMBC spectrum (CD_3OD) of **1**

Fig. S9. NOESY spectrum (CD_3OD) of **1**

Fig. S10 The conformers of compounds **1** and **2** with a Boltzmann-population greater than 5% selected for ECD calculations

MS, UV, IR and NMR Spectra of Compound 2

Fig. S11. HRESIMS spectrum of **2**

Fig. S12. IR spectrum of **2**

Fig. S13. UV spectrum in MeOH of **2**

Fig. S14. ^1H -NMR spectrum (CD_3OD , 600 MHz) of **2**

Fig. S15. Comparison of ^1H NMR spectra of compounds **1** and **2** from δ_{H} 2.0 to 6.5 ppm.

Fig. S16. ^{13}C -NMR spectrum (CD_3OD , 150 MHz) of **2**

Fig. S17. ^1H - ^1H COSY spectrum (CD_3OD) of **2**

Fig. S18. HSQC spectrum (CD_3OD) of **2**

Fig. S19. HMBC spectrum (CD_3OD) of **2**

Fig. S20. NOESY spectrum (CD_3OD) of **2**

MS, UV, IR and NMR Spectra of Compound 3

Fig. S21. HRESIMS spectrum of **3**

Fig. S22. IR spectrum of **3**

Fig. S23. UV spectrum in MeOH of **3**

Fig. S24. ^1H -NMR spectrum (CD_3OD , 600 MHz) of **3**

Fig. S25. ^{13}C -NMR spectrum (CD_3OD , 150 MHz) of **3**

Fig. S26. ^1H - ^1H COSY spectrum (CD_3OD) of **3**

Fig. S27. HSQC spectrum (CD_3OD) of **3**

Fig. S28. HMBC spectrum (CD_3OD) of **3**

Fig. S29. NOESY spectrum (CD_3OD) of **3**

MS, UV, IR and NMR Spectra of Compound 1

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T: FTMS + p ESI Full ms [100.00-700.00]

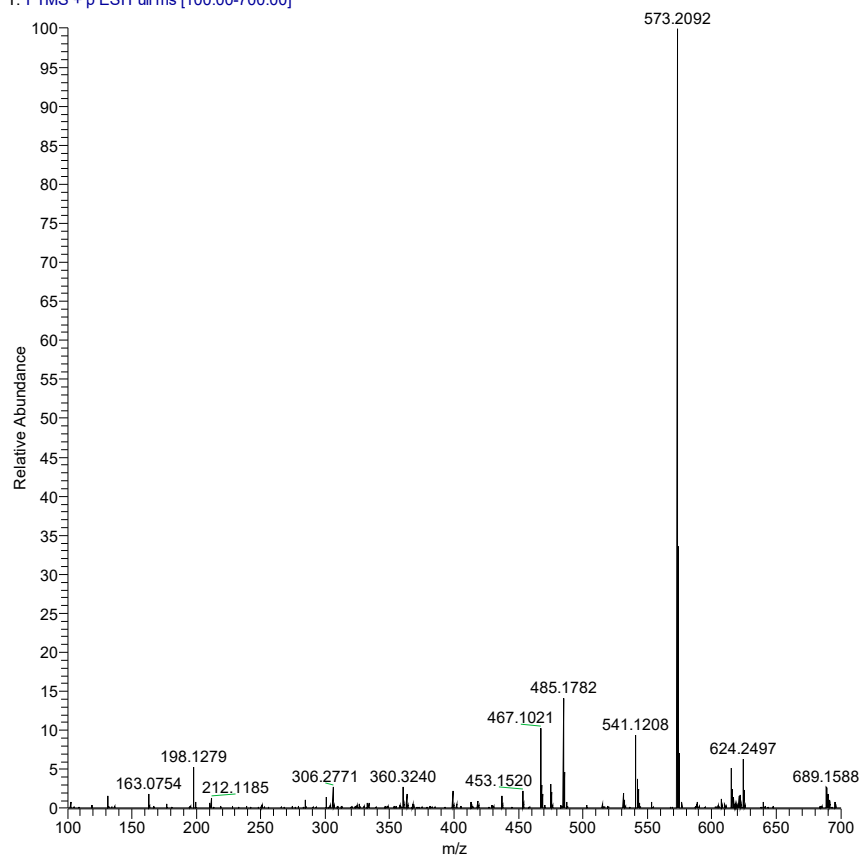


Fig. S1. HRESIMS spectrum of 1

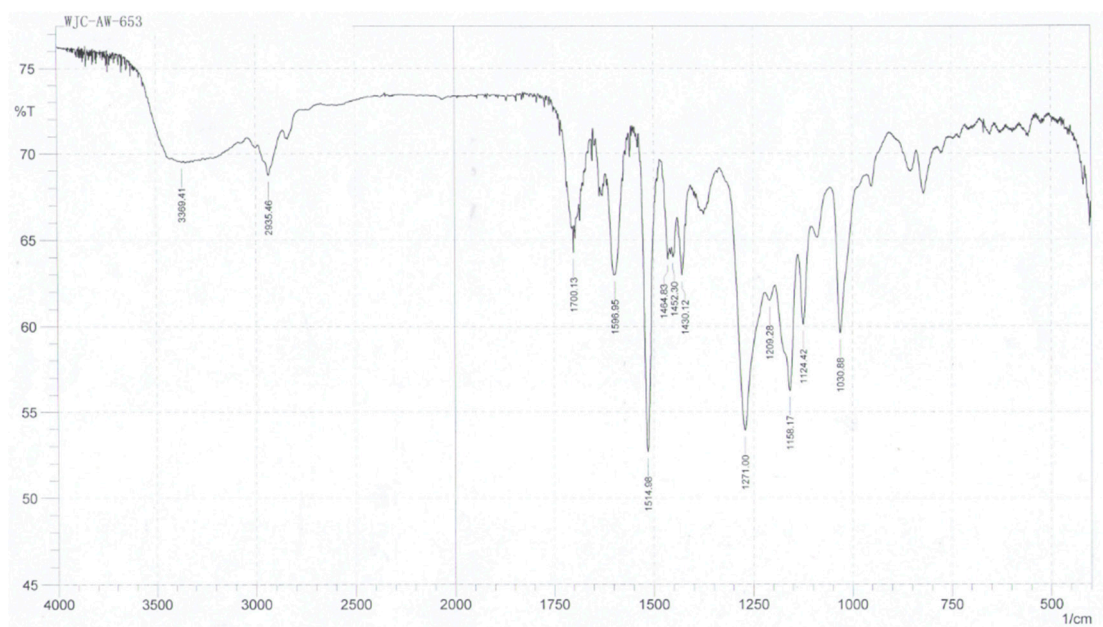


Fig. S2. IR spectrum of 1

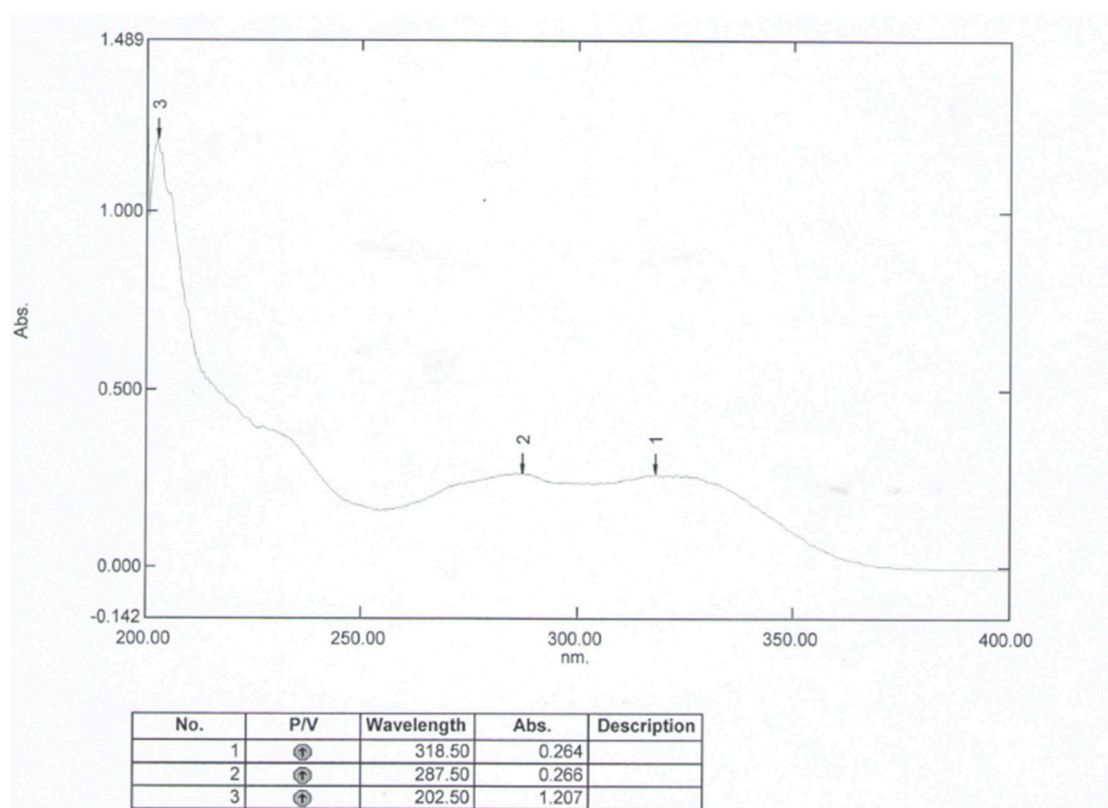


Fig. S3. UV spectrum in MeOH of **1**

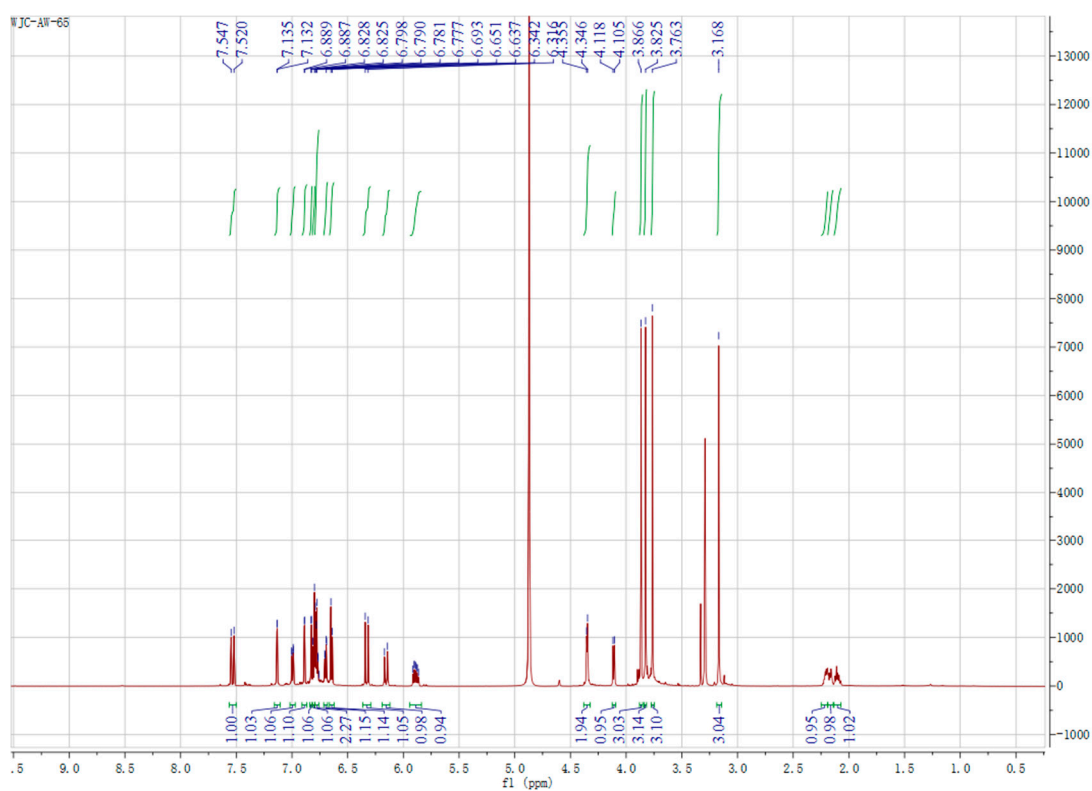


Fig. S4. ^1H -NMR spectrum (CD_3OD , 600 MHz) of **1**

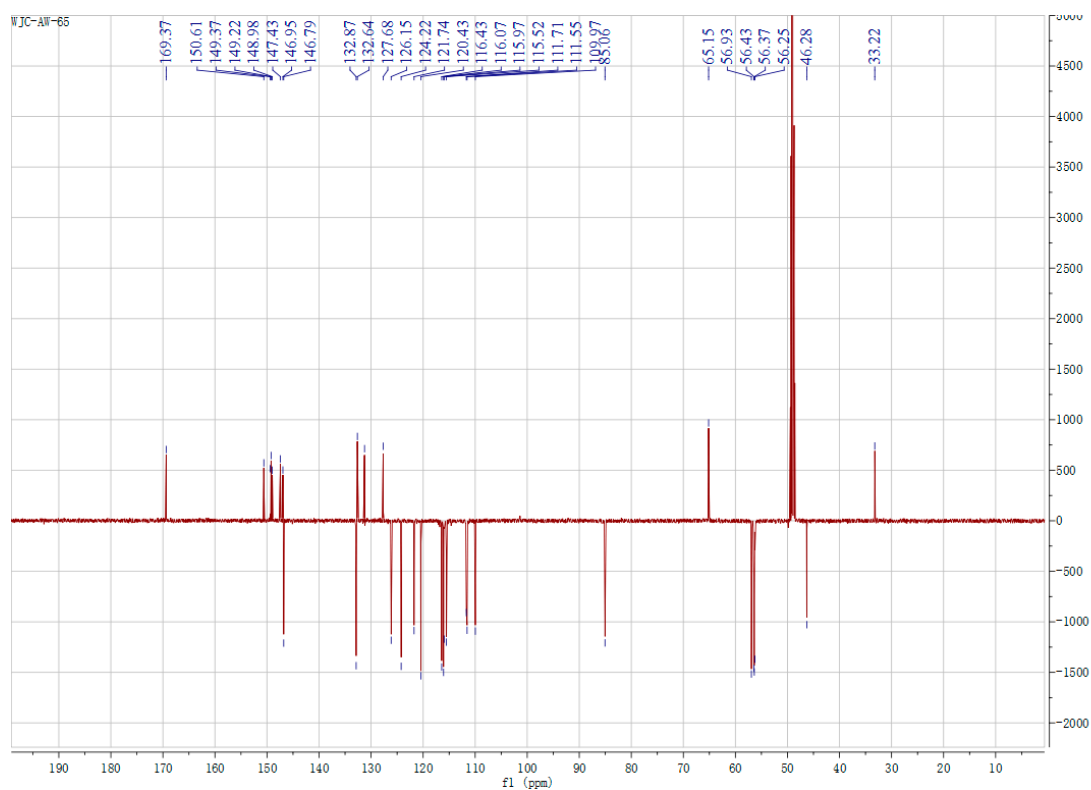


Fig. S5. ¹³C-NMR spectrum (CD₃OD, 150 MHz) of **1**

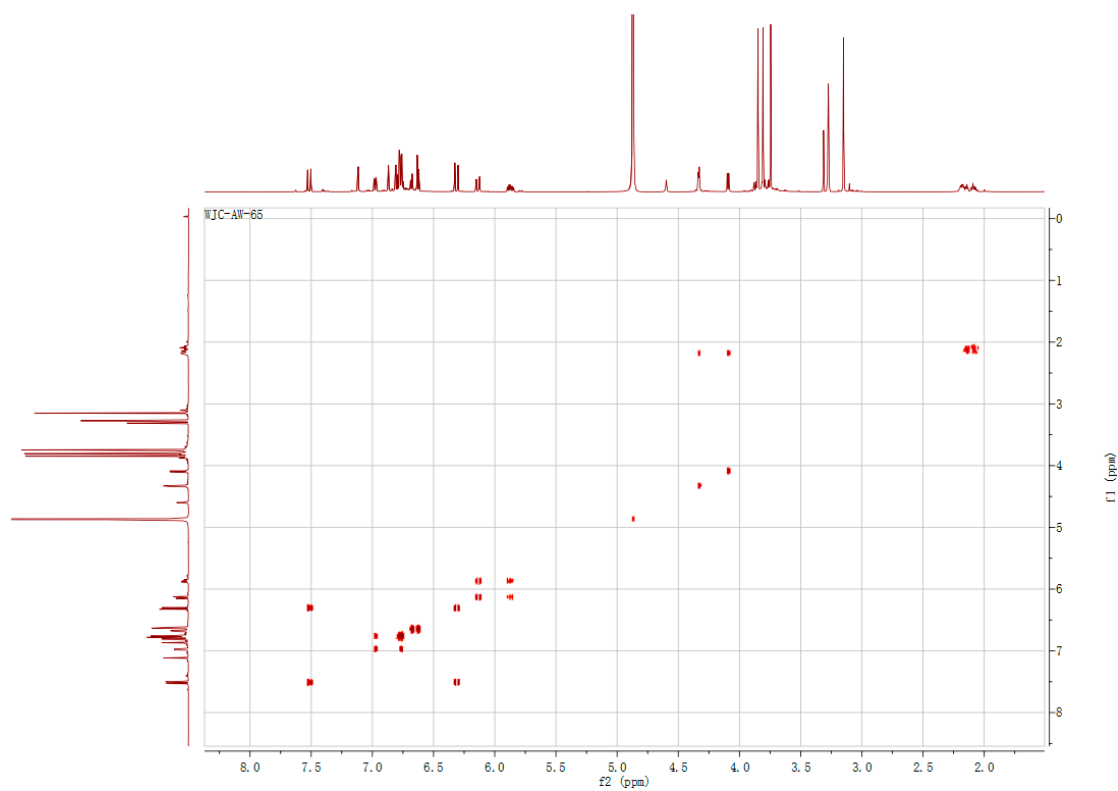


Fig. S6. ¹H-¹H COSY spectrum (CD₃OD) of **1**

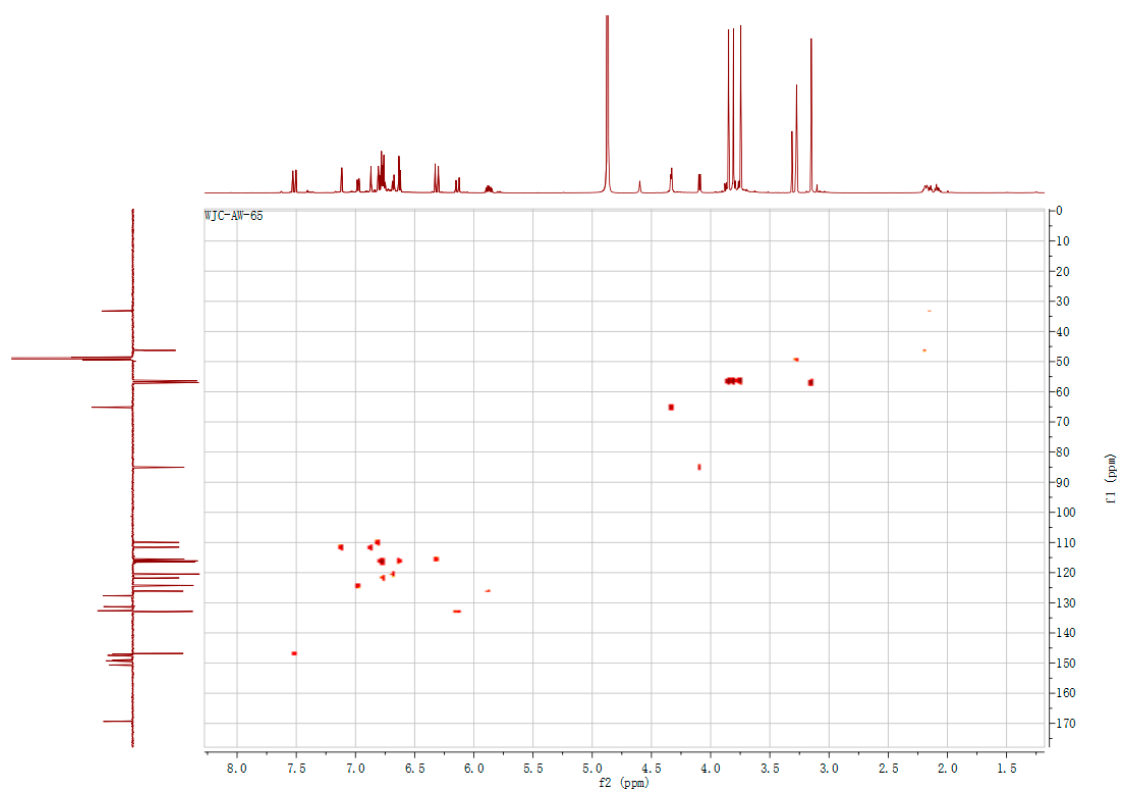


Fig. S7. HSQC spectrum (CD₃OD) of **1**

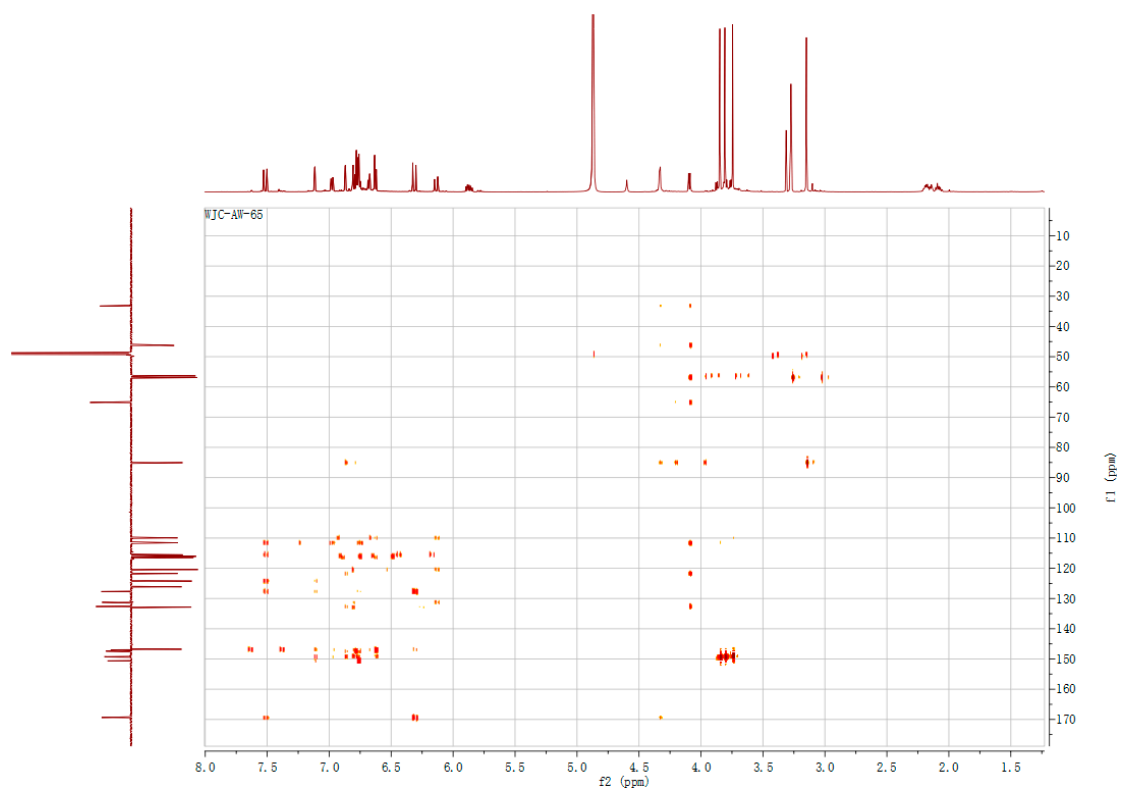


Fig. S8. HMBC spectrum (CD₃OD) of **1**

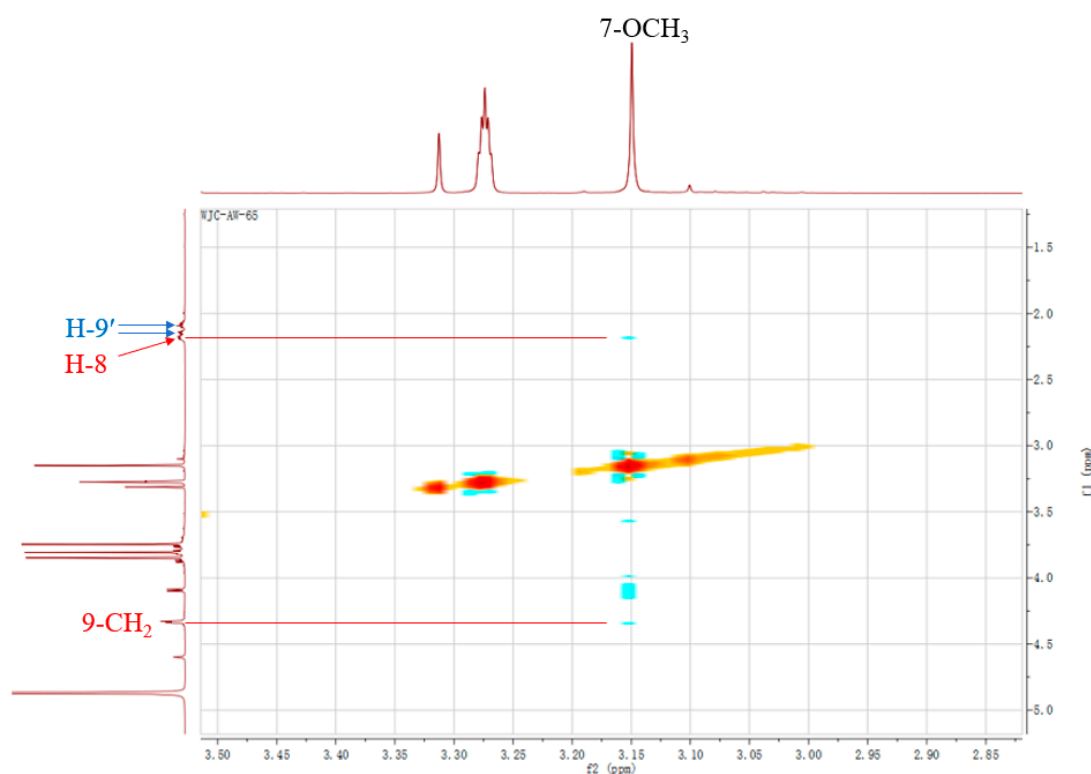
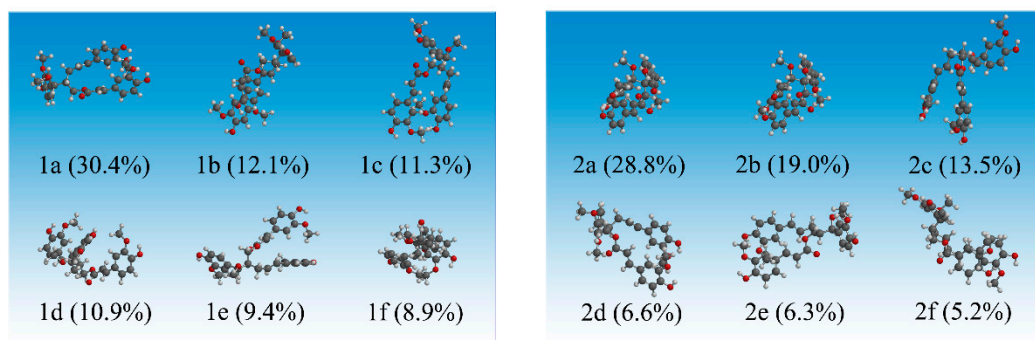


Fig. S9. NOESY spectrum (CD₃OD) of **1**



Compound **1**

Compound **2**

Fig. S10 The conformers of compounds **1** and **2** with a Boltzmann-population greater than 5% selected for ECD calculations

MS, UV, IR and NMR Spectra of Compound 2

AW-66_170629163024 #10 RT: 0.07 AV: 1 NL: 5.01E7
T: FTMS + p ESI Full ms [100.00-700.00]

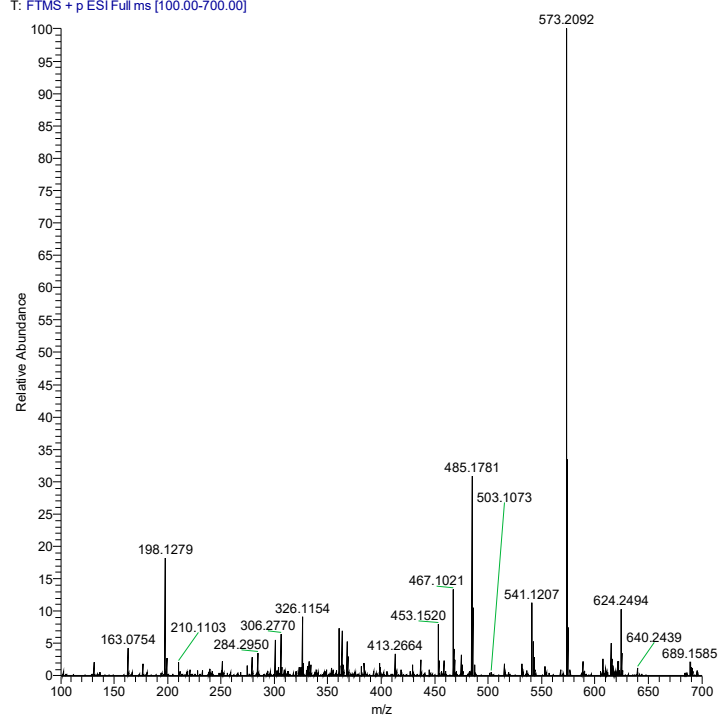


Fig. S11. HRESIMS spectrum of 2

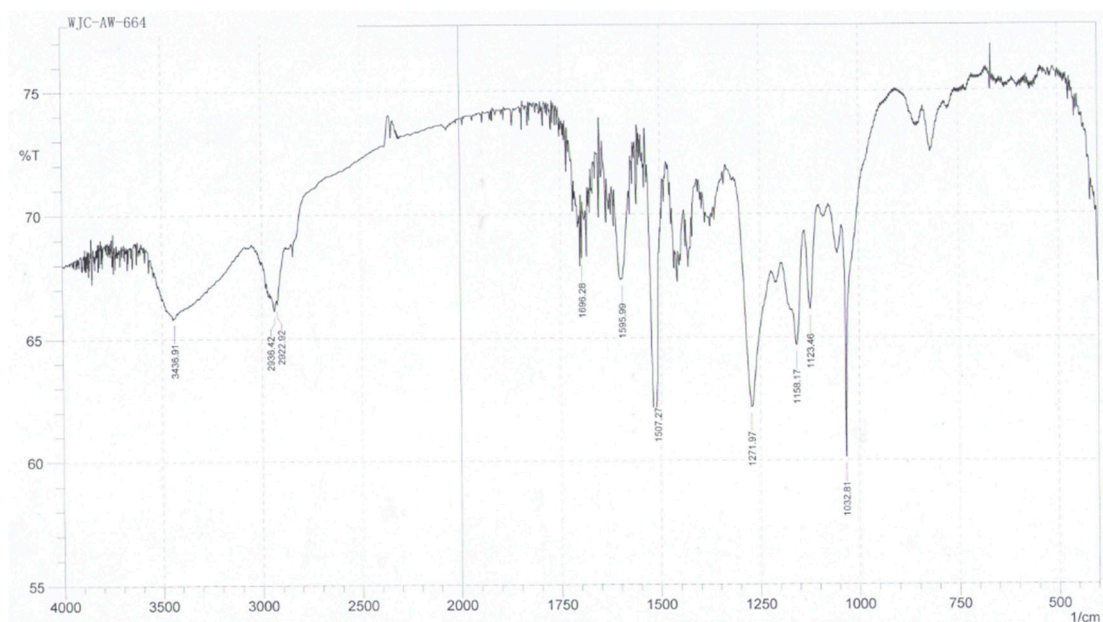


Fig. S12. IR spectrum of 2

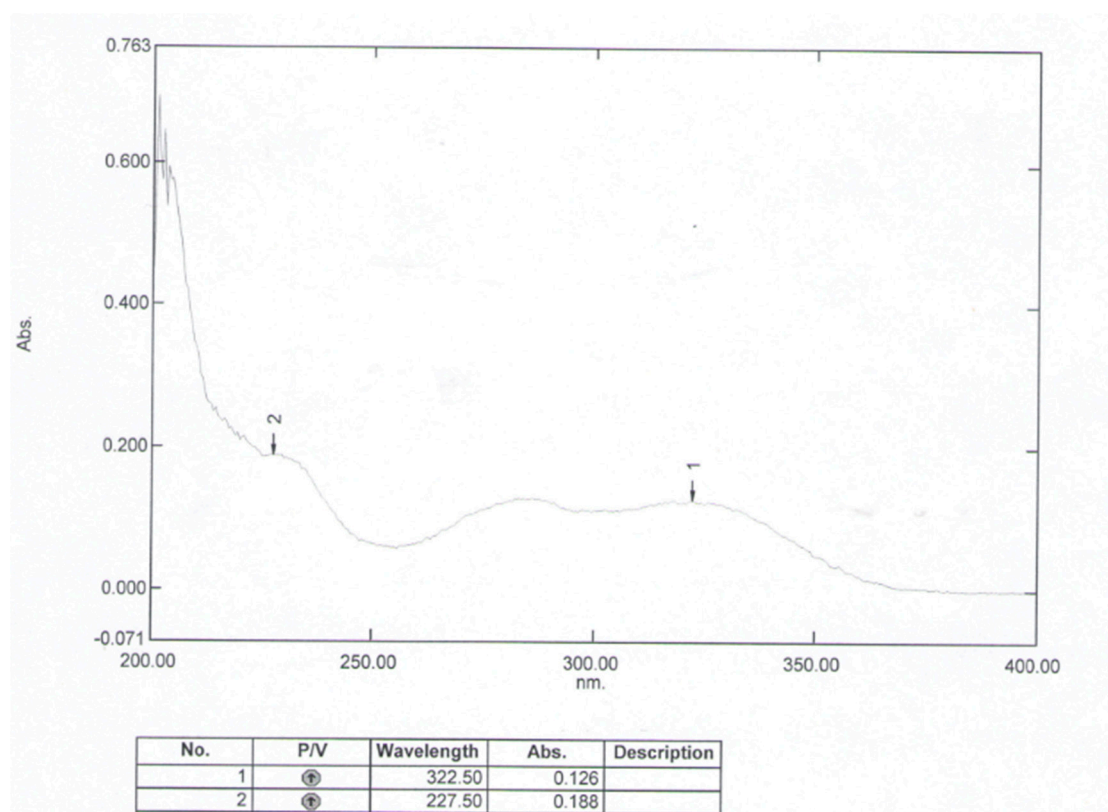


Fig. S13. UV spectrum in MeOH of **2**

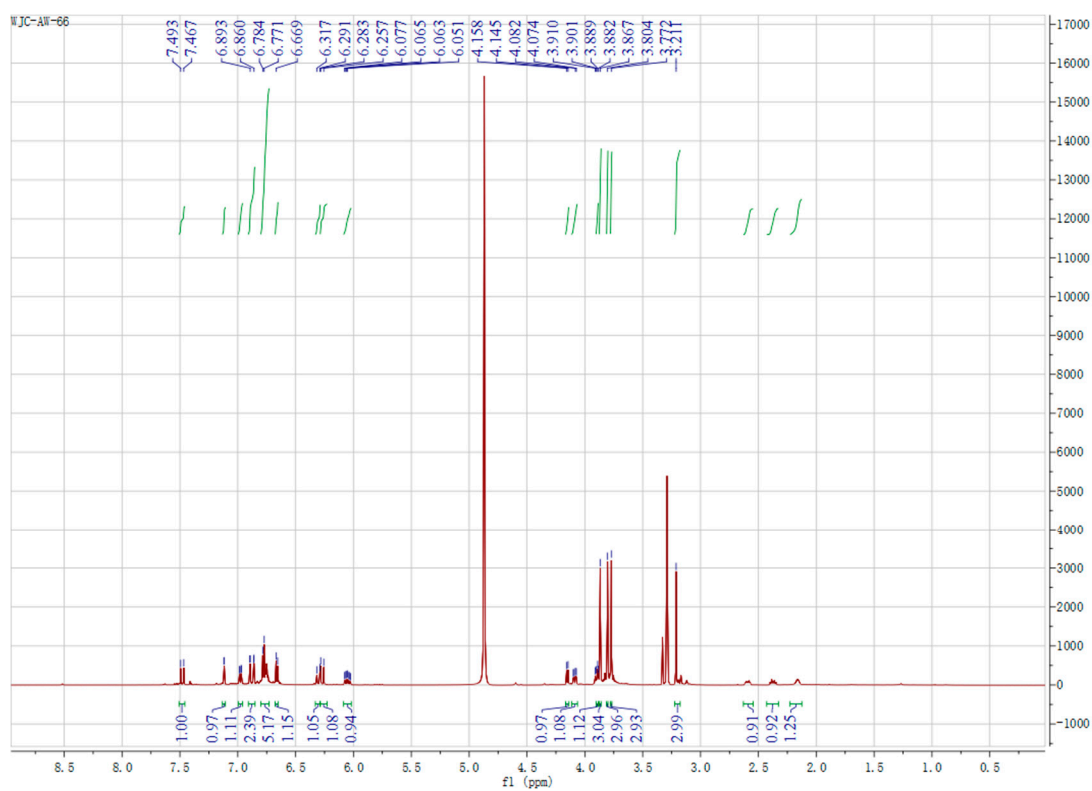


Fig. S14. ^1H -NMR spectrum (CD_3OD , 600 MHz) of **2**

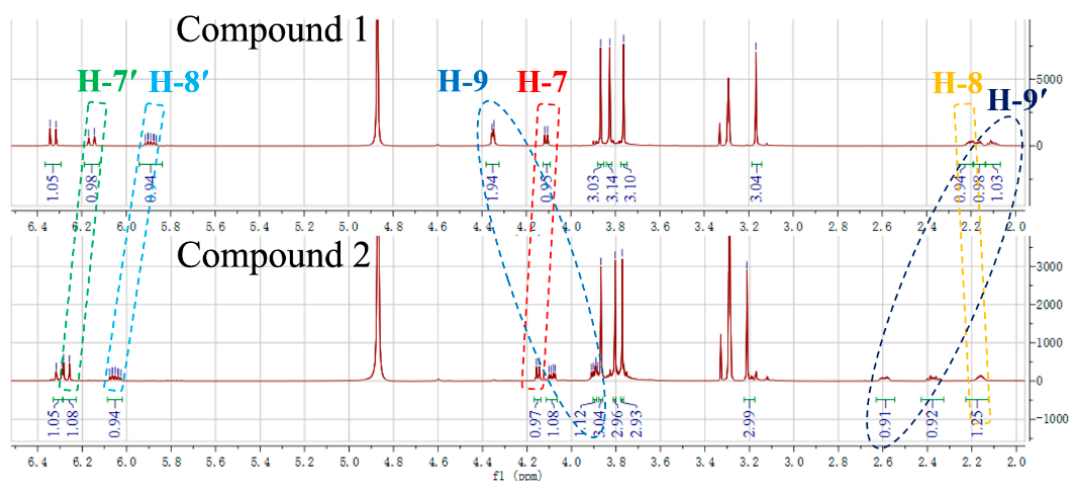


Fig. S15. Comparison of ^1H NMR spectra of compounds **1** and **2** from δ_{H} 2.0 to 6.5 ppm.

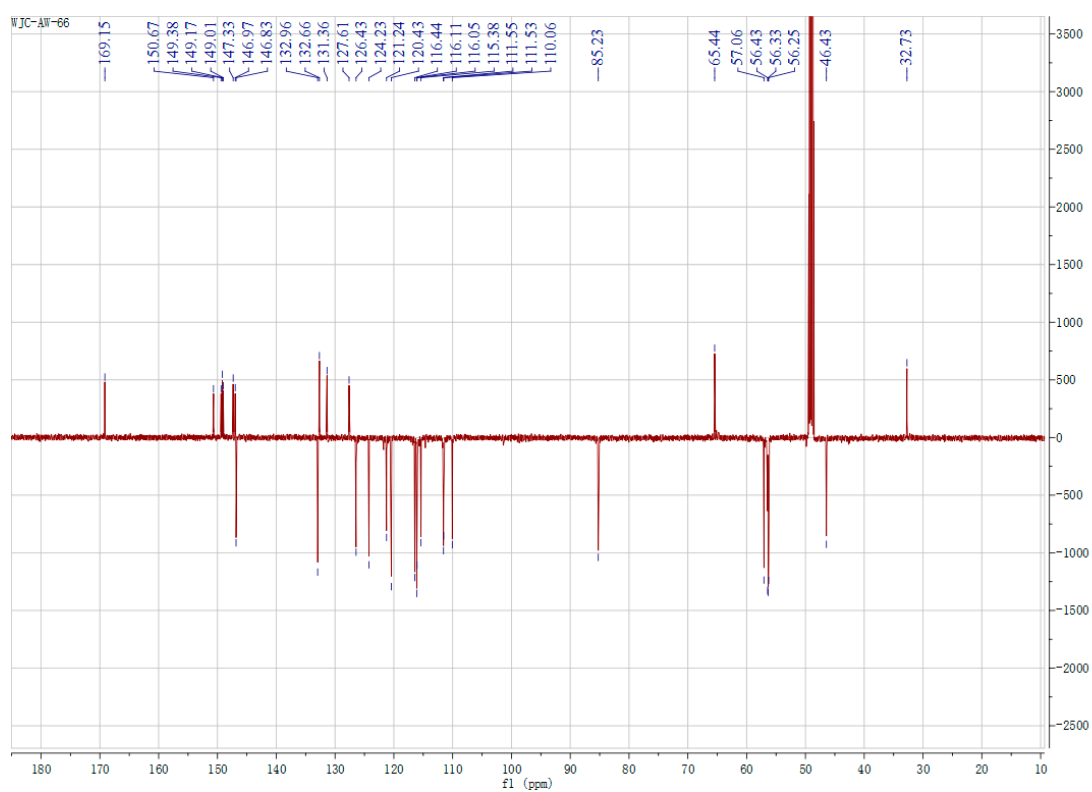


Fig. S16. ^{13}C -NMR spectrum (CD_3OD , 150 MHz) of **2**

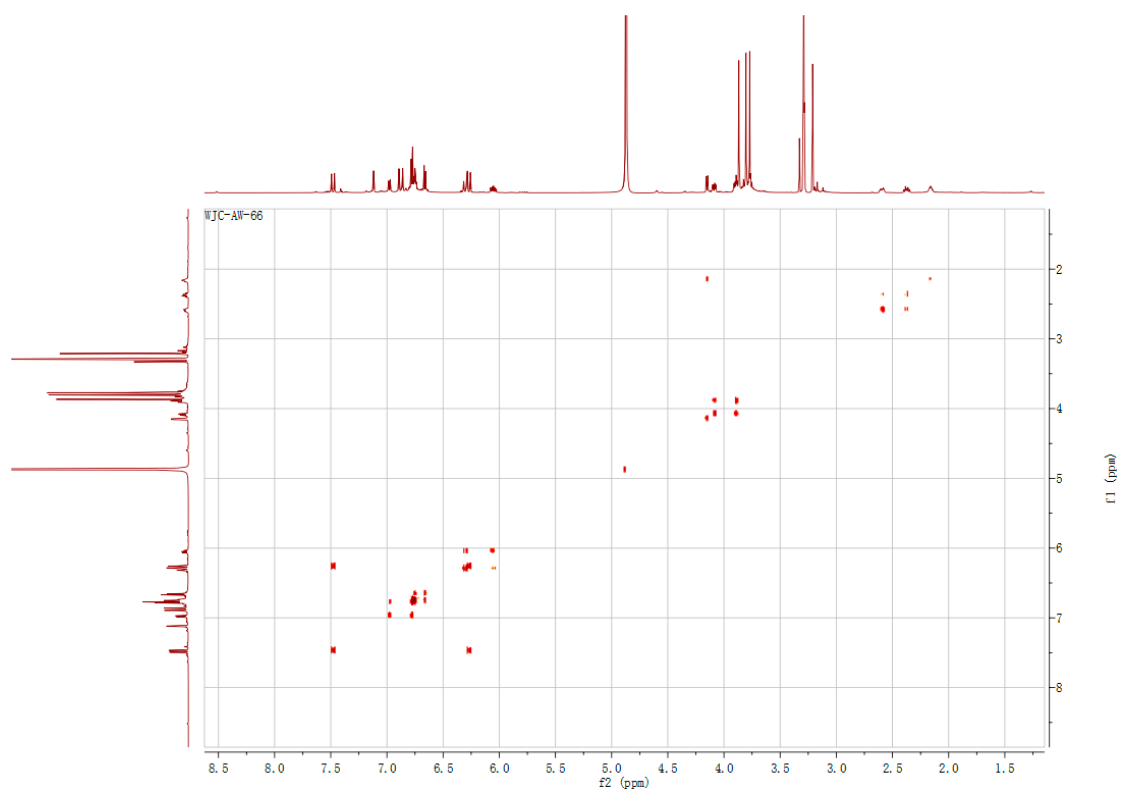


Fig. S17. ^1H - ^1H COSY spectrum (CD_3OD) of **2**

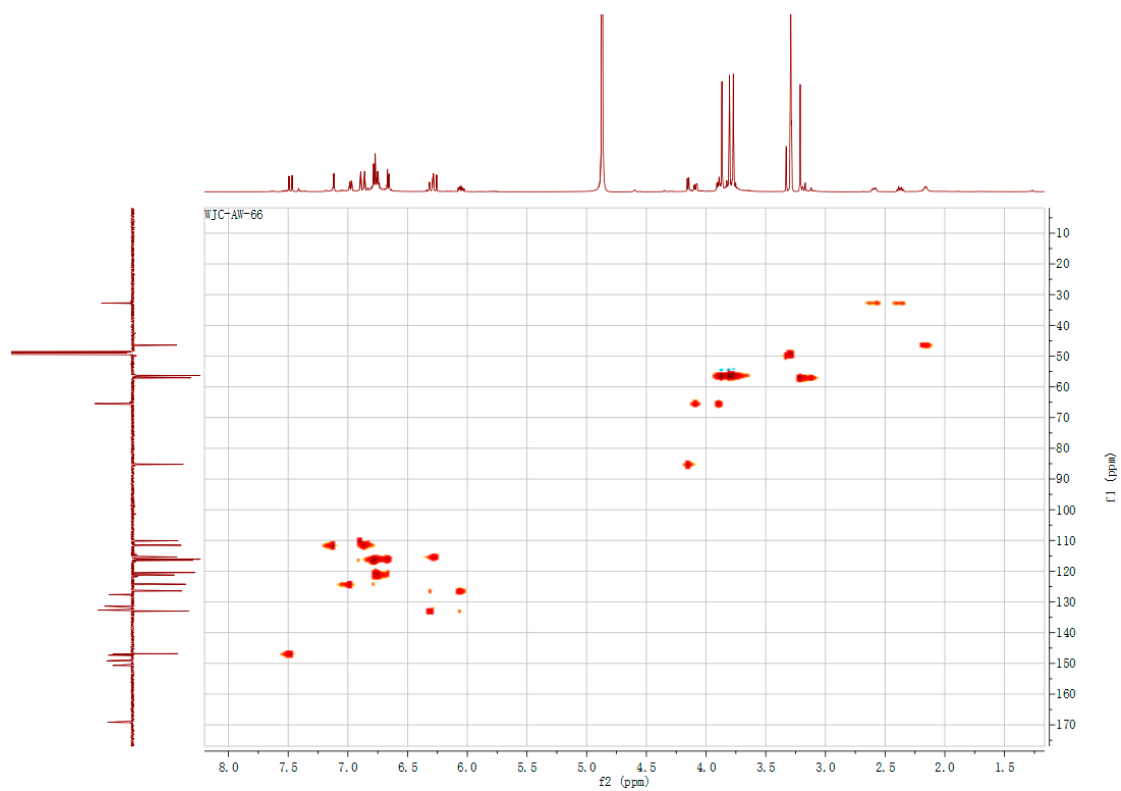


Fig. S18. HSQC spectrum (CD_3OD) of **2**

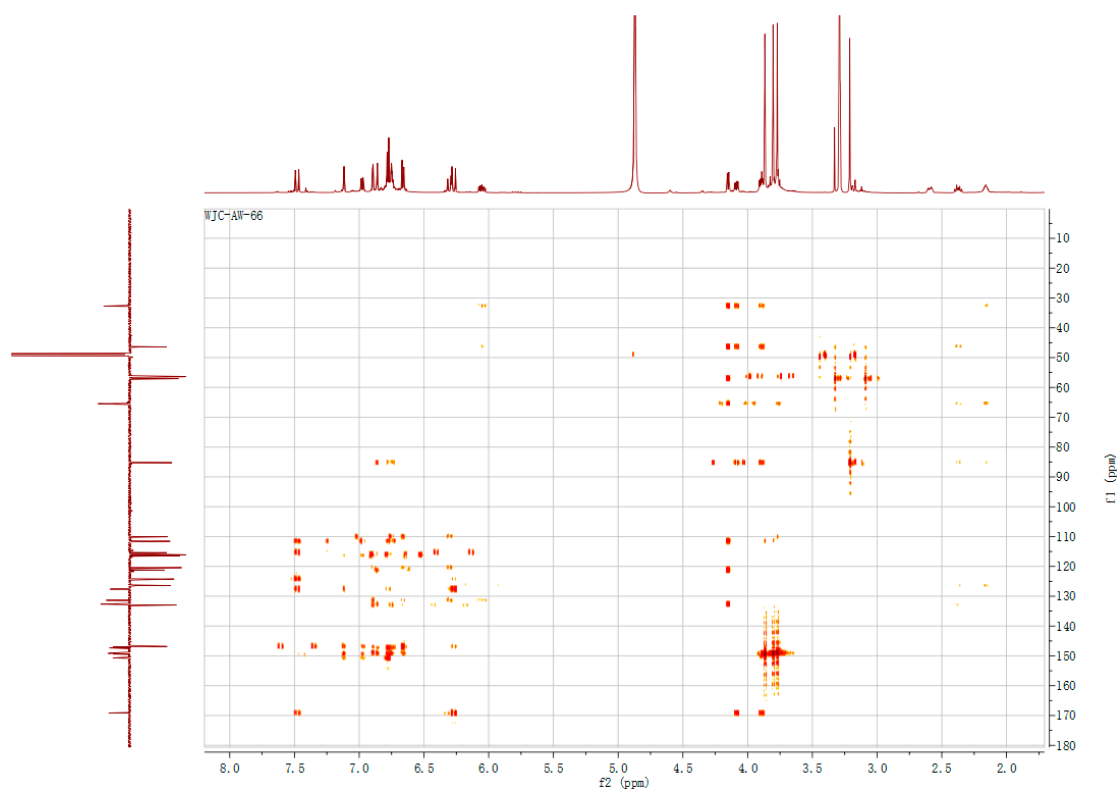


Fig. S19. HMBC spectrum (CD₃OD) of **2**

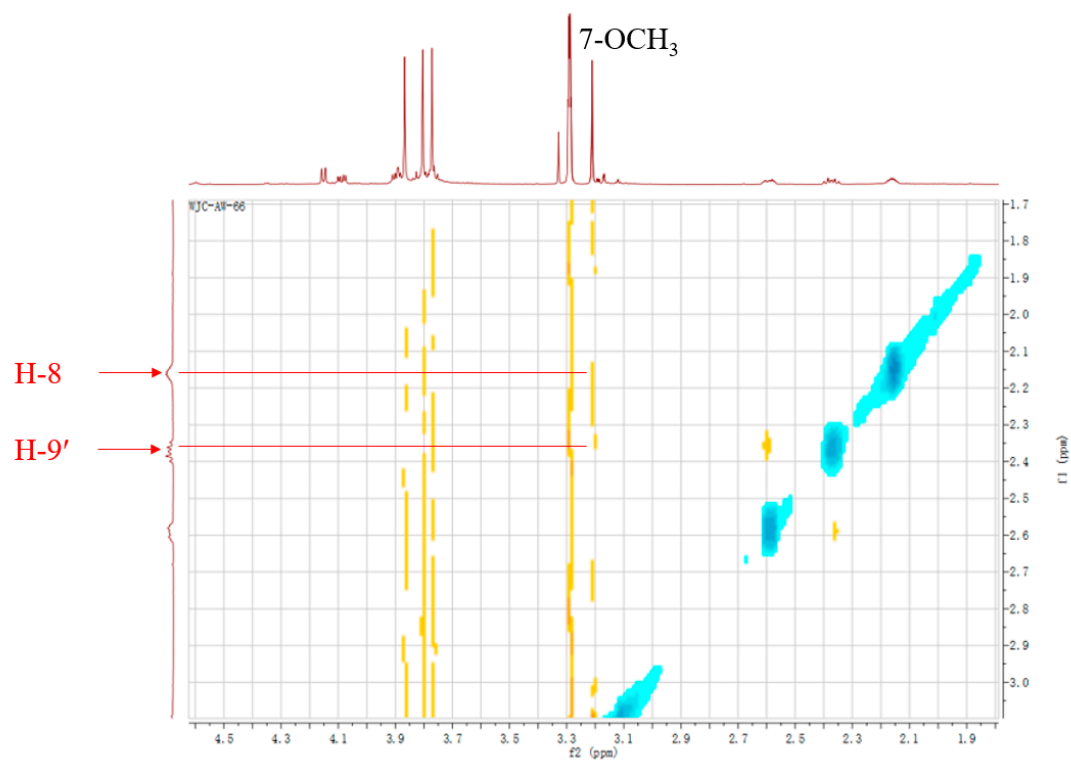


Fig. S20. NOESY spectrum (CD₃OD) of **2**

MS, UV, IR and NMR Spectra of Compound 3

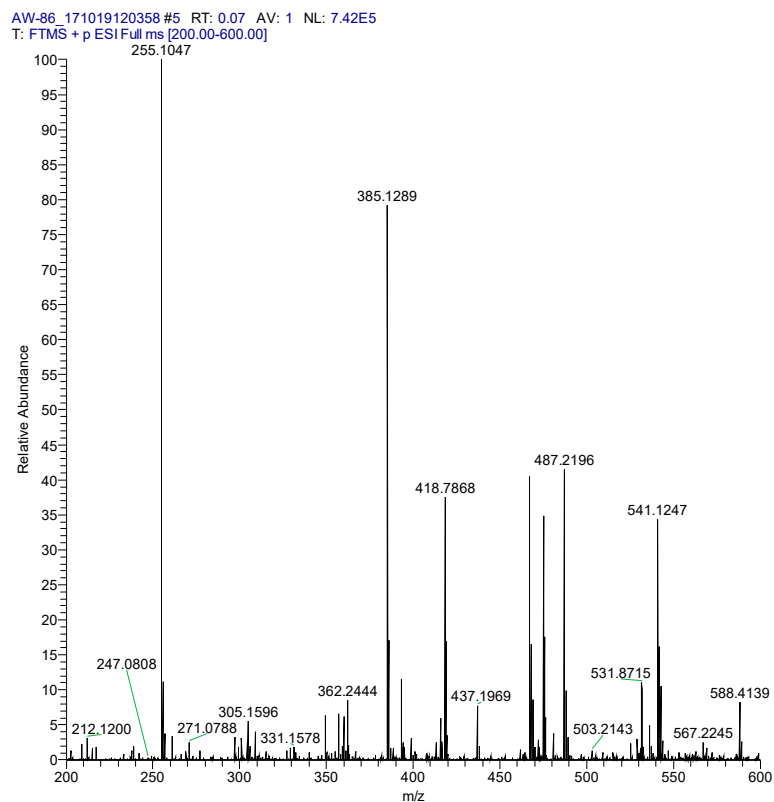


Fig. S21. HRESIMS spectrum of **3**

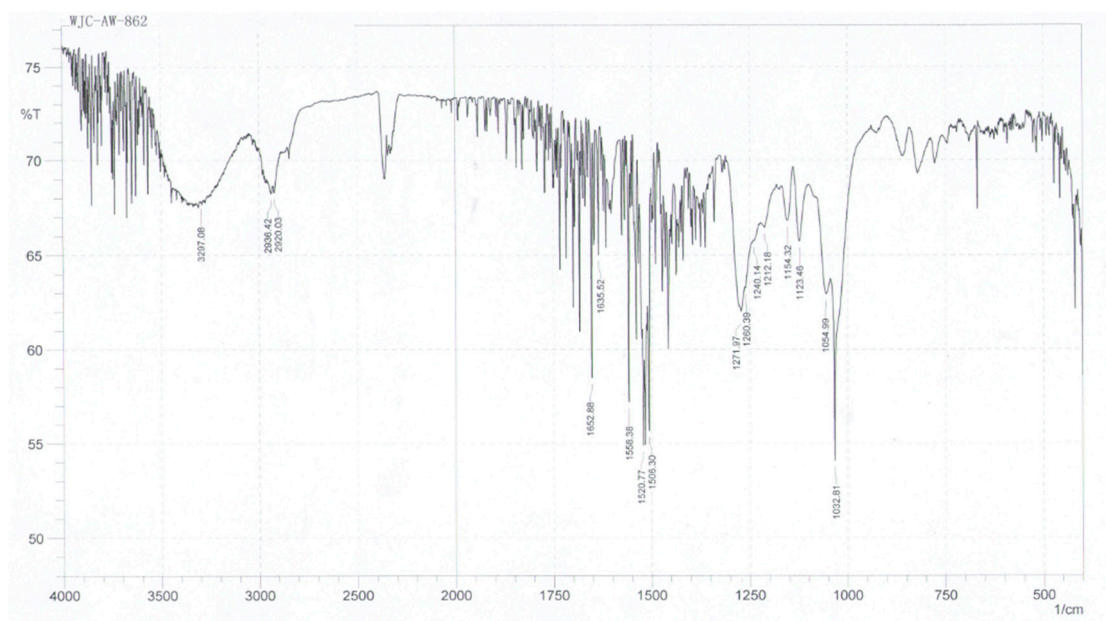


Fig. S22. IR spectrum of **3**

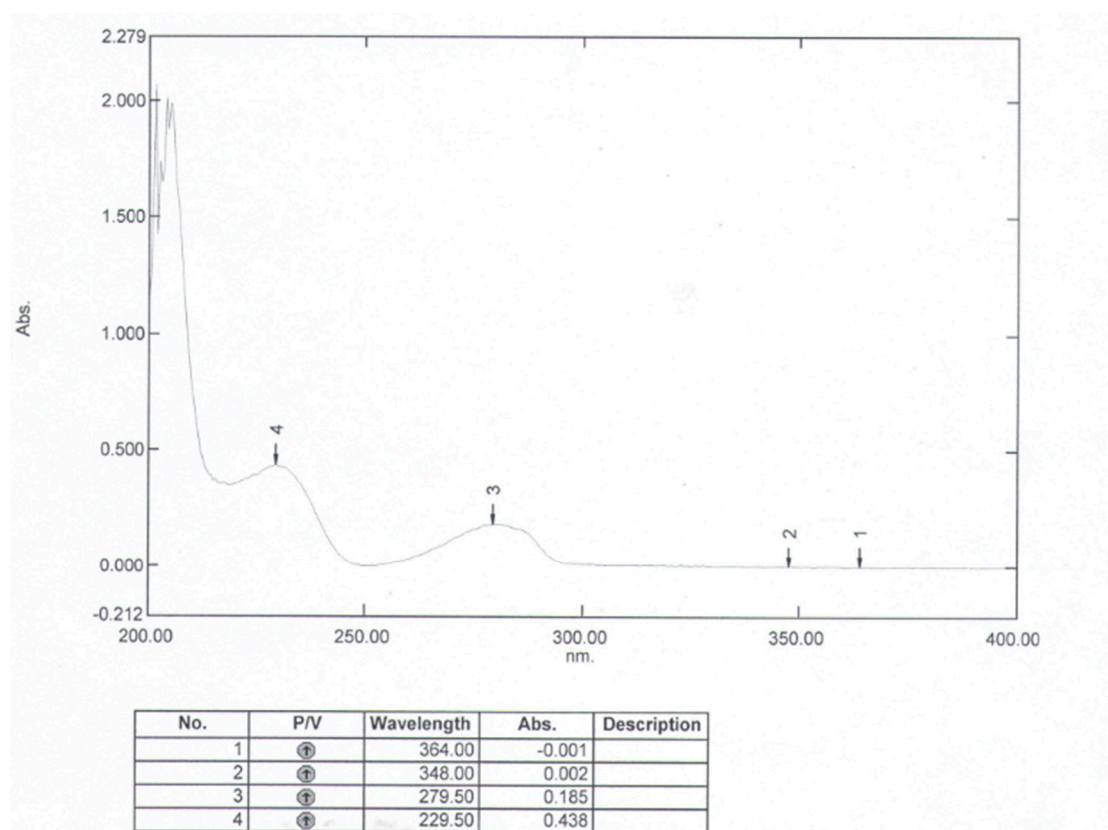


Fig. S23. UV spectrum in MeOH of **3**

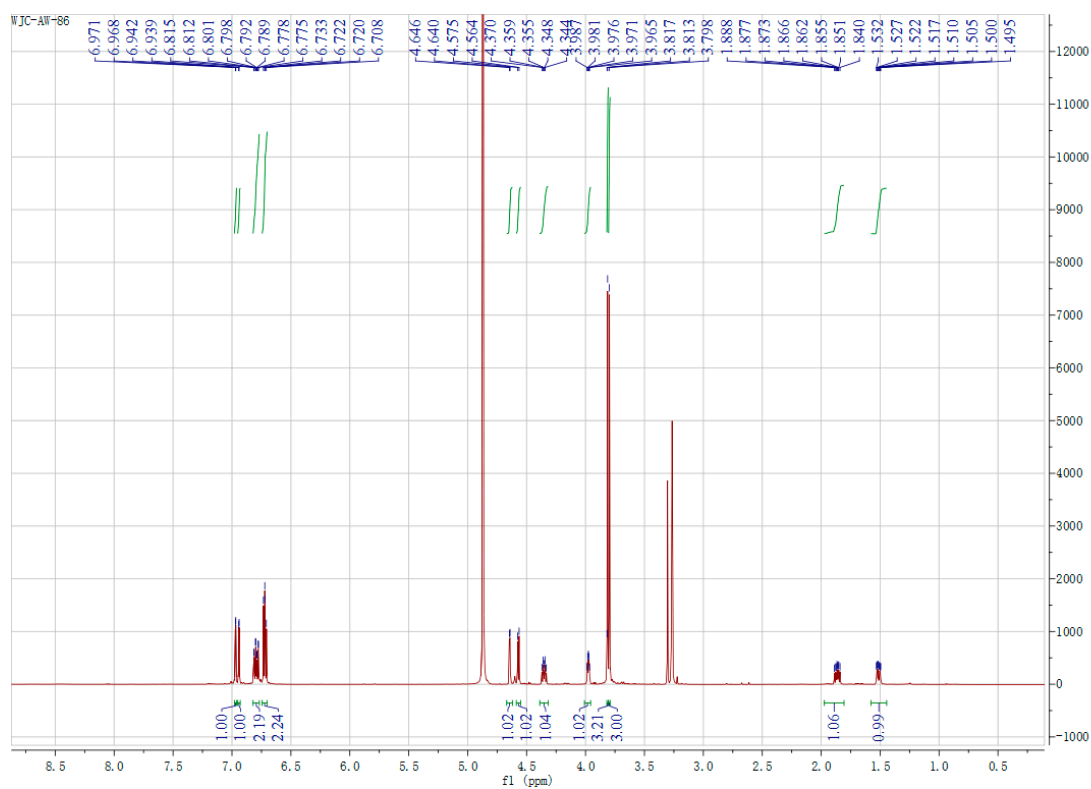


Fig. S24. ^1H -NMR spectrum (CD_3OD , 600 MHz) of **3**

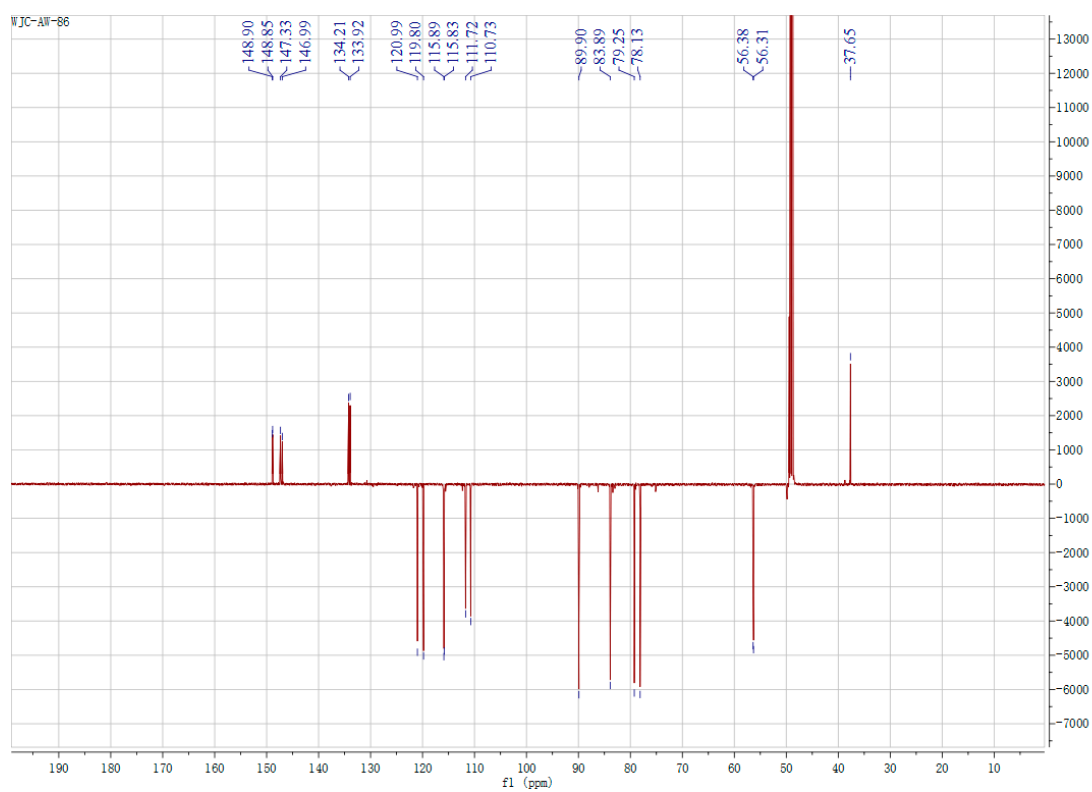


Fig. S25. ¹³C-NMR spectrum (CD₃OD, 150 MHz) of **3**

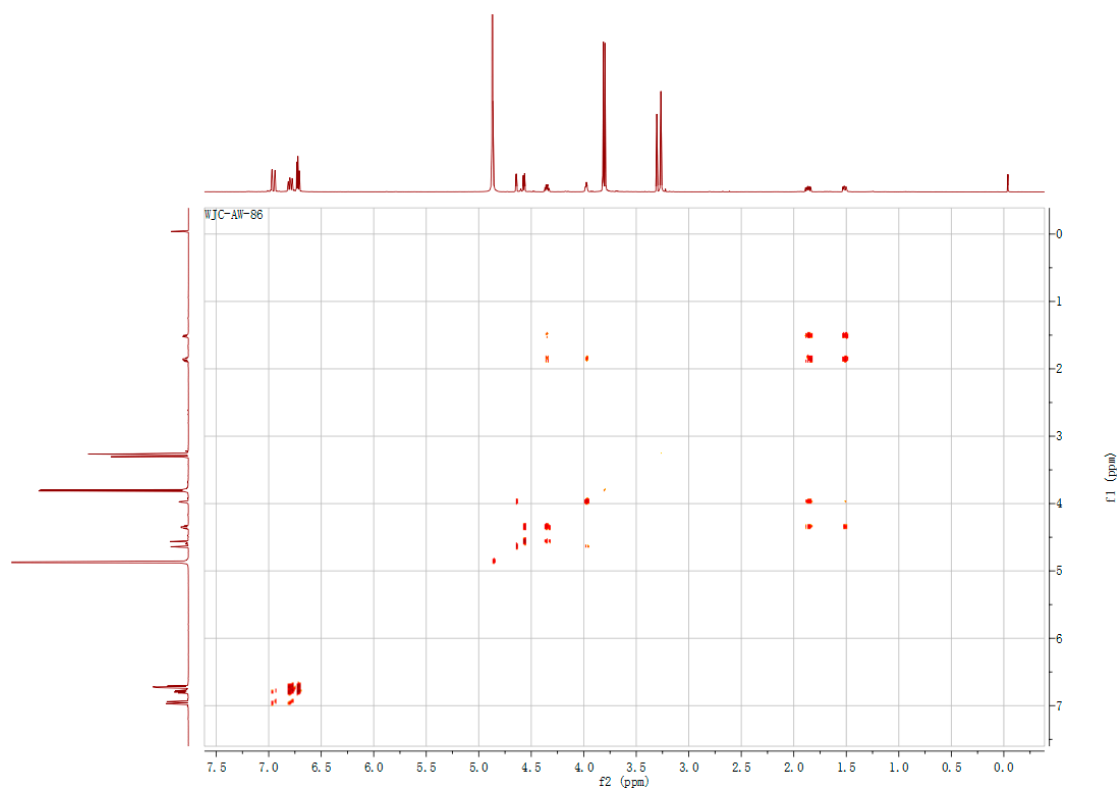


Fig. S26. ¹H-¹H COSY spectrum (CD₃OD) of **3**

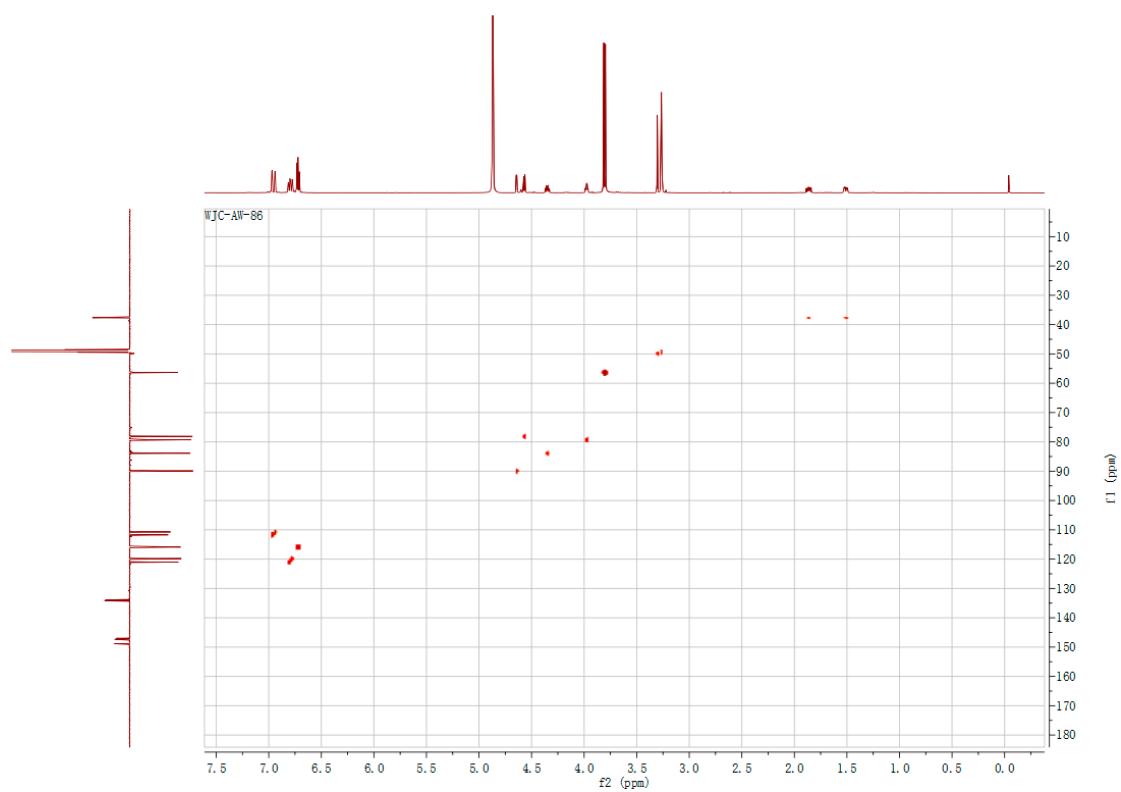


Fig. S27. HSQC spectrum (CD₃OD) of **3**

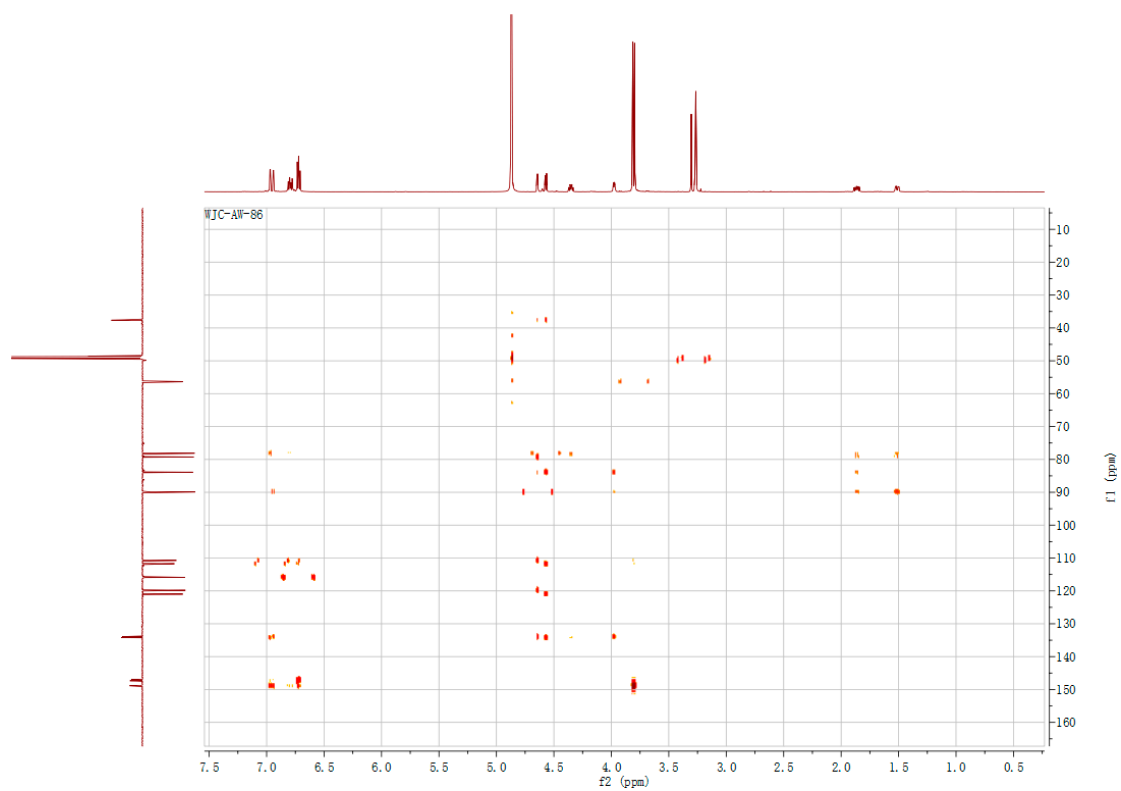


Fig. S28. HMBC spectrum (CD₃OD) of **3**

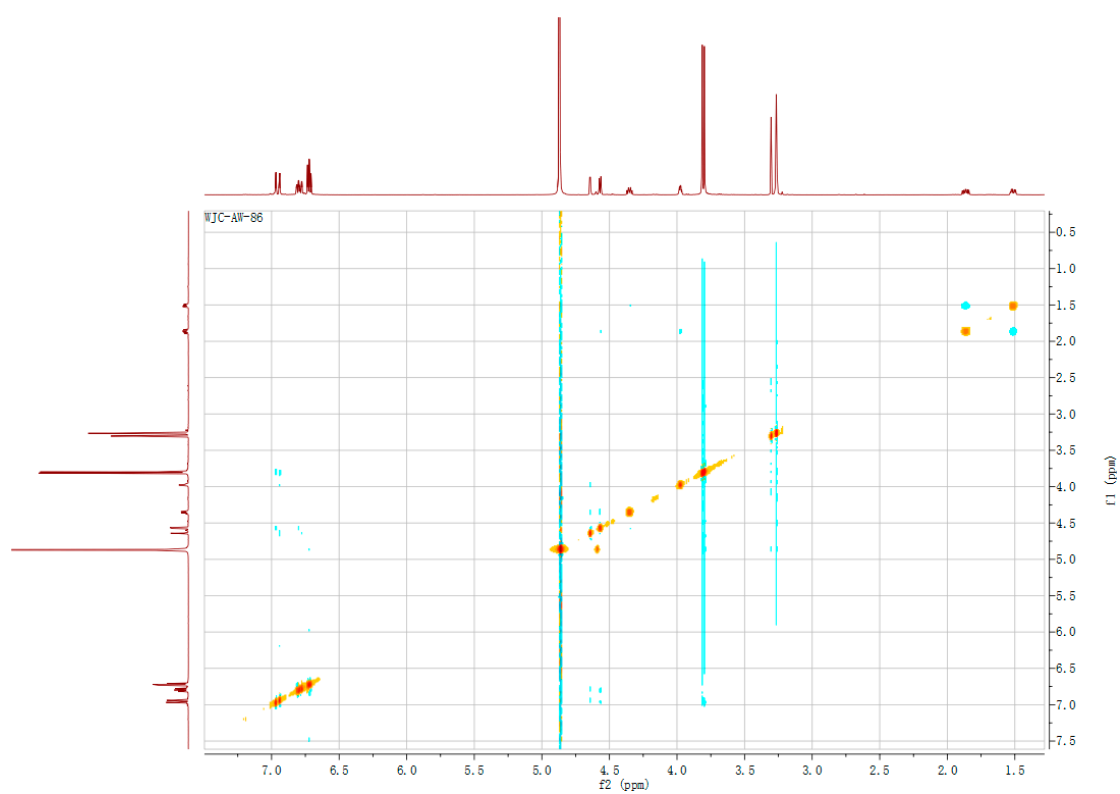


Fig. S29. NOESY spectrum (CD_3OD) of **3**