

# Supplementary Materials: Additional Two New Compounds from the Marine-Derived Fungus *Pseudallescheria ellipsoidea* F42-3

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## List of Supporting Information

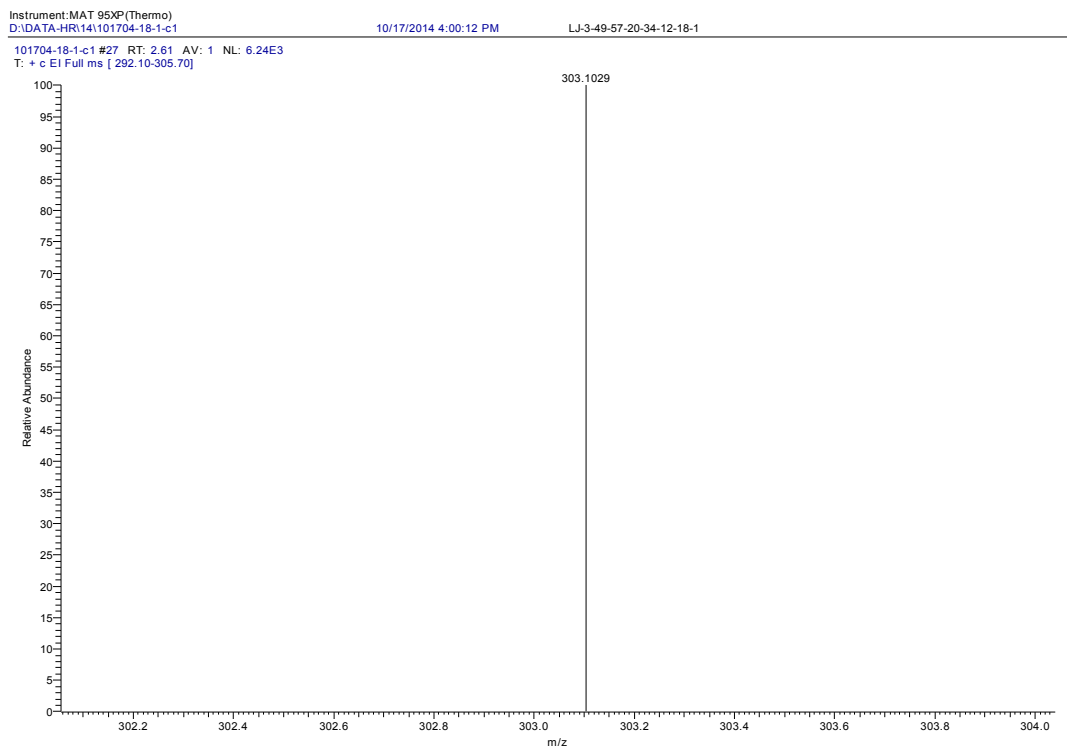
- Figure S1.** HR-EI mass spectrum of compound 1.
- Figure S2.** <sup>1</sup>H-NMR spectrum of compound 1 in acetone-*d*<sub>6</sub> (400 MHz).
- Figure S3.** <sup>13</sup>C-NMR spectrum of compound 1 in acetone-*d*<sub>6</sub> (100 MHz).
- Figure S4.** DEPT 135 spectrum of compound 1 in acetone-*d*<sub>6</sub> (100 MHz).
- Figure S5.** DEPT 90 spectrum of compound 1 in acetone-*d*<sub>6</sub> (100 MHz).
- Figure S6.** HMQC spectrum of compound 1 in acetone-*d*<sub>6</sub>.
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- Figure S14.** DEPT 90 spectrum of compound 2 in DMSO-*d*<sub>6</sub> (100 MHz).
- Figure S15.** HMQC spectrum of compound 2 in DMSO-*d*<sub>6</sub>.
- Figure S16.** <sup>1</sup>H-<sup>1</sup>H COSY spectrum of compound 2 in DMSO-*d*<sub>6</sub>.
- Figure S17.** HMBC spectrum of compound 2 in DMSO-*d*<sub>6</sub>.
- Figure S18.** NOESY spectrum of compound 2 in DMSO-*d*<sub>6</sub>.
- Figure S19.** HR-EI mass spectrum of compound 3.
- Figure S20.** <sup>1</sup>H-NMR spectrum of compound 3 in CD<sub>3</sub>OD (400 MHz).
- Figure S21.** <sup>13</sup>C-NMR spectrum of compound 3 in CD<sub>3</sub>OD (100 MHz).
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- Figure S25.** HMQC spectrum of compound 3 in CD<sub>3</sub>OD.
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- Figure S27.** HMBC spectrum of compound 3 in CD<sub>3</sub>OD.
- Figure S28.** NOESY spectrum of compound 3 in CD<sub>3</sub>OD.
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- Figure S30.** <sup>1</sup>H-NMR spectrum of compound 4 in DMSO-*d*<sub>6</sub> (400 MHz).
- Figure S31.** <sup>13</sup>C-NMR spectrum of compound 4 in DMSO-*d*<sub>6</sub> (100 MHz).
- Figure S32.** DEPT 135 spectrum of compound 4 in DMSO-*d*<sub>6</sub> (100 MHz).
- Figure S33.** DEPT 90 spectrum of compound 4 in DMSO-*d*<sub>6</sub> (100 MHz).
- Figure S34.** HMQC spectrum of compound 4 in DMSO-*d*<sub>6</sub>.
- Figure S35.** <sup>1</sup>H-<sup>1</sup>H COSY spectrum of compound 4 in DMSO-*d*<sub>6</sub>.

**Figure S36.** HMBC spectrum of compound **4** in DMSO-*d*<sub>6</sub>.

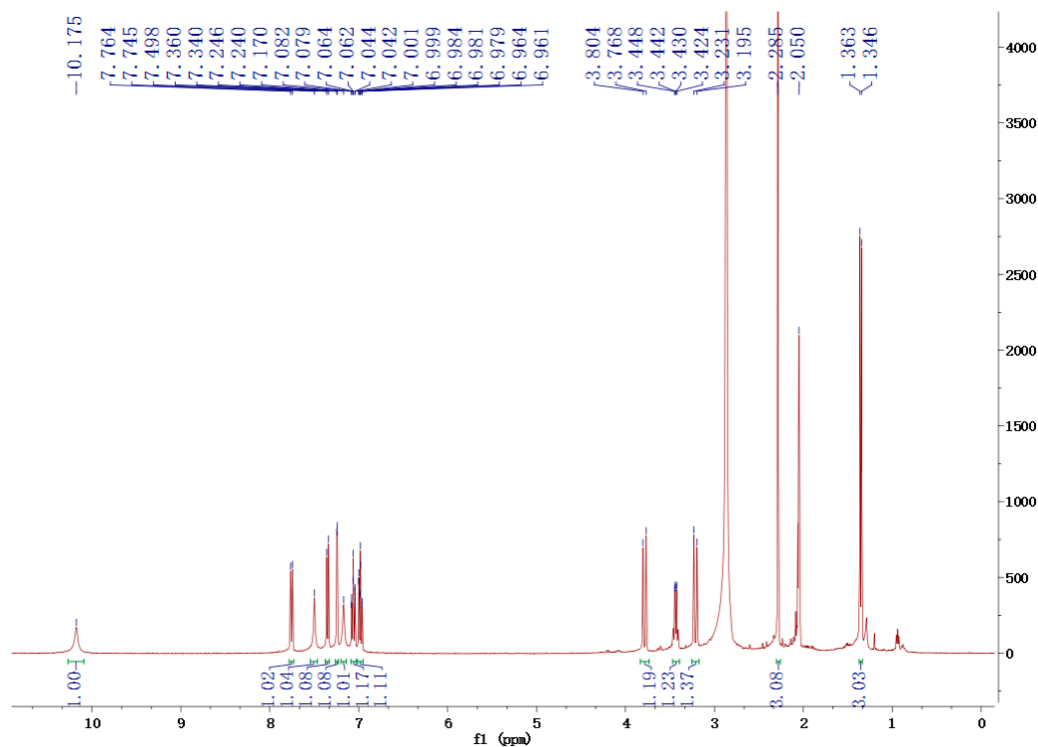
**Figure S37.** NOESY spectrum of compound **4** in DMSO-*d*<sub>6</sub>.

**Figure S38.** Comparison of the experimental ECD spectra of **3** with the calculated ECD spectra for four (3*S*) stereochemical options.

**Figure S39.** Experimental CD spectra of **2**.



**Figure S1.** HR-EI mass spectrum of compound **1**.



**Figure S2.** <sup>1</sup>H-NMR spectrum of compound **1** in acetone-*d*<sub>6</sub> (400 MHz).

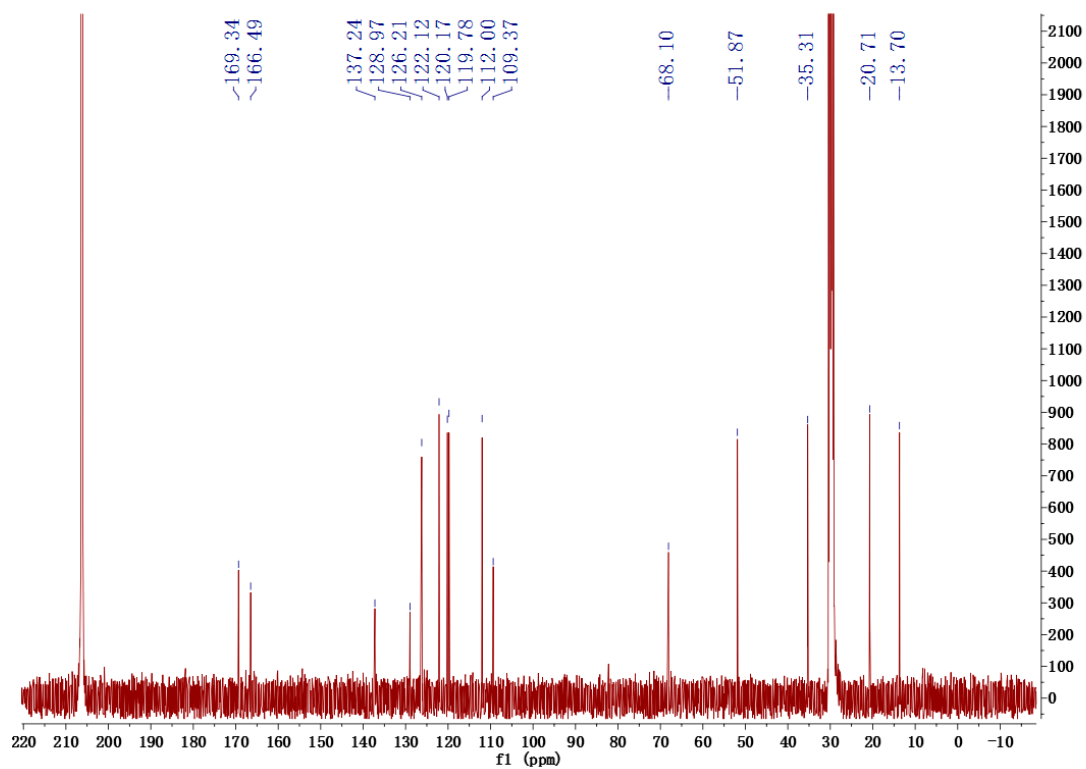


Figure S3. <sup>13</sup>C-NMR spectrum of compound 1 in acetone-*d*<sub>6</sub> (100 MHz).

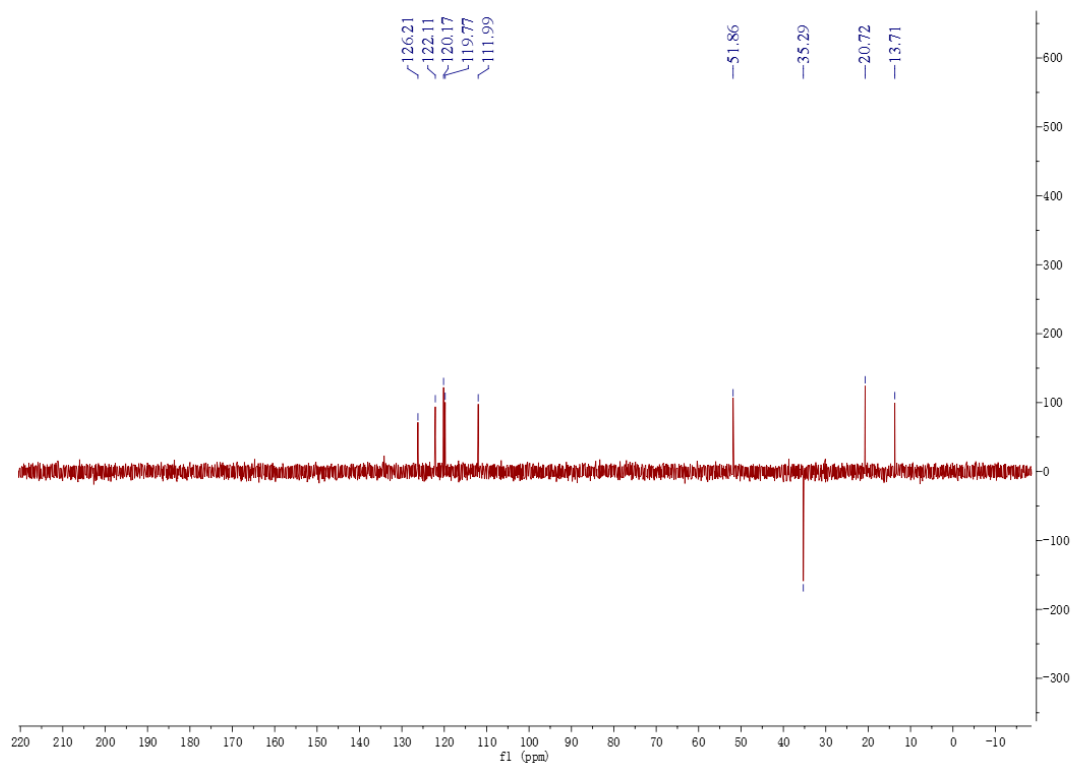


Figure S4. DEPT135 spectrum of compound 1 in acetone-*d*<sub>6</sub> (100 MHz).

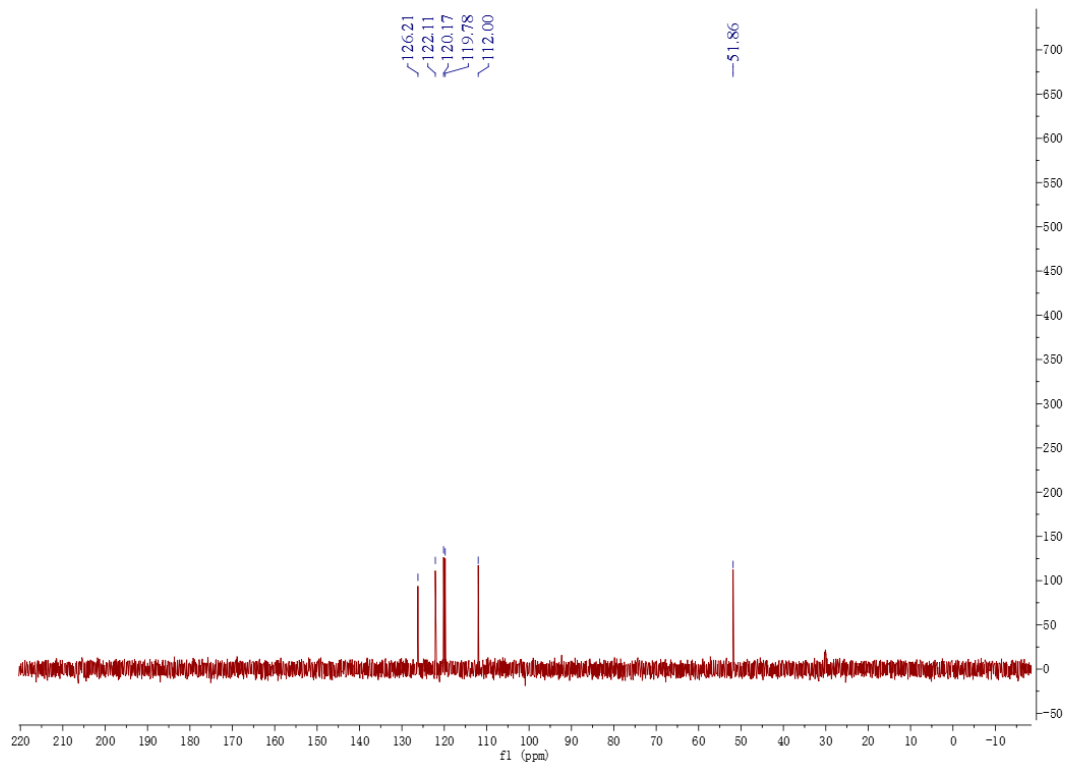


Figure S5. DEPT90 spectrum of compound 1 in acetone-*d*<sub>6</sub> (100 MHz).

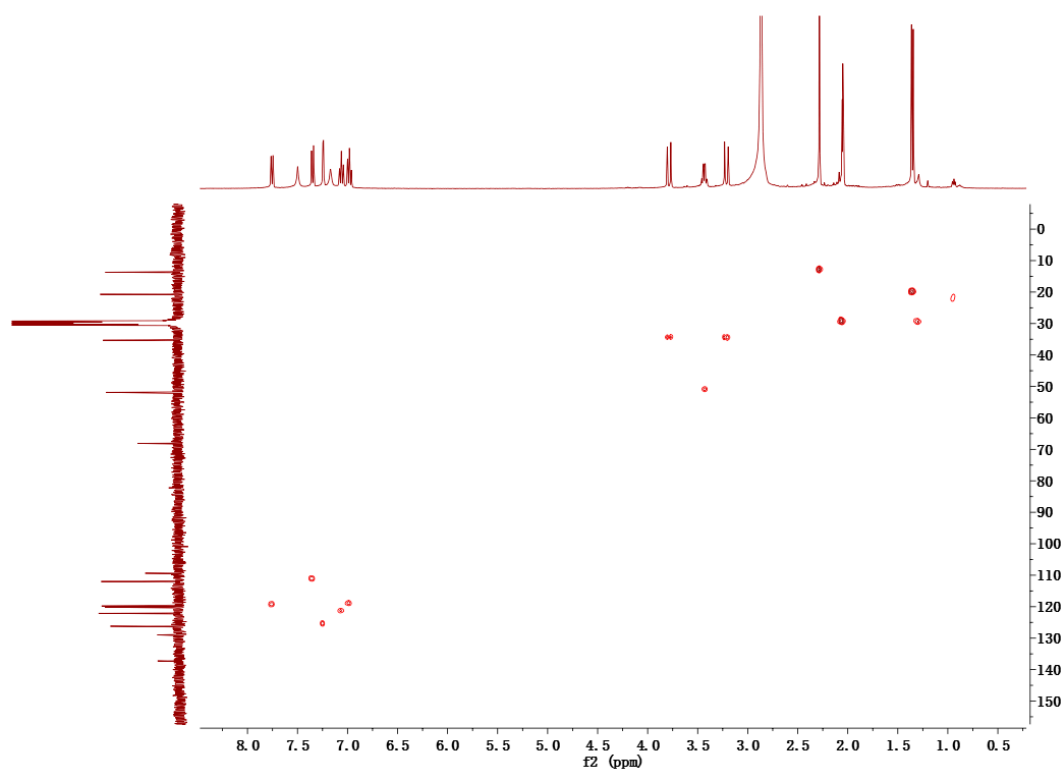


Figure S6. HMQC spectrum of compound 1 in acetone-*d*<sub>6</sub>.

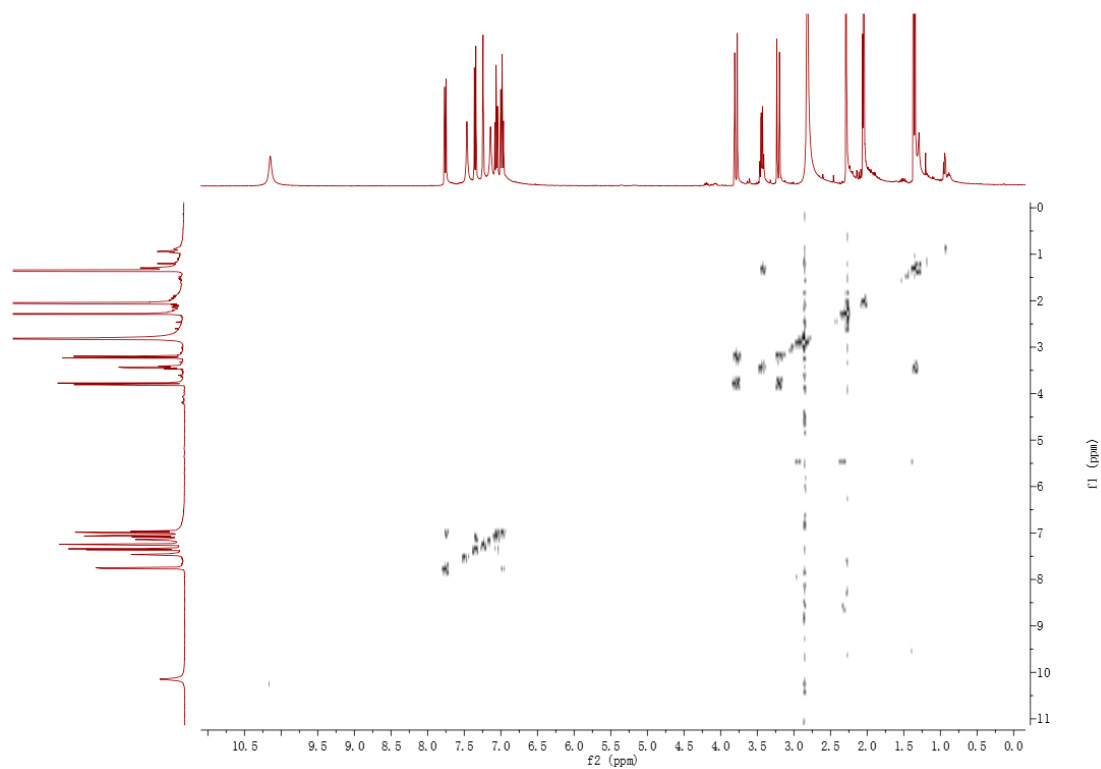


Figure S7. <sup>1</sup>H-<sup>1</sup>H COSY spectrum of compound **1** in acetone-*d*<sub>6</sub>.

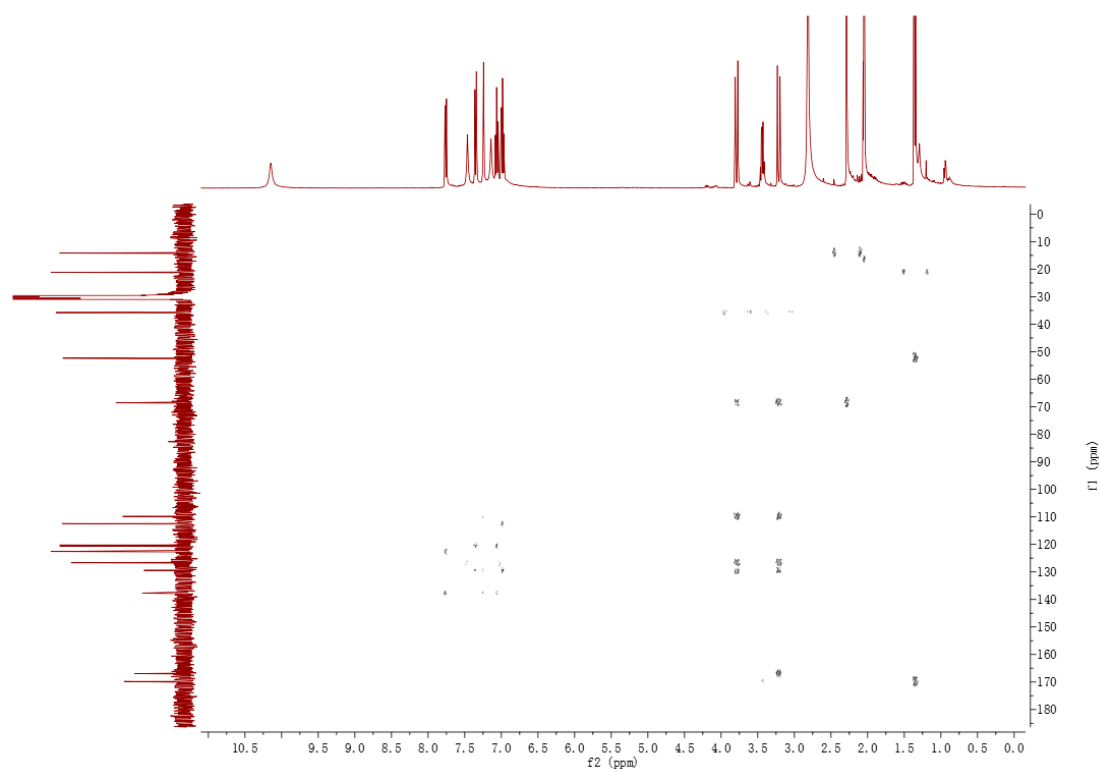


Figure S8. HMBC spectrum of compound **1** in acetone-*d*<sub>6</sub>.

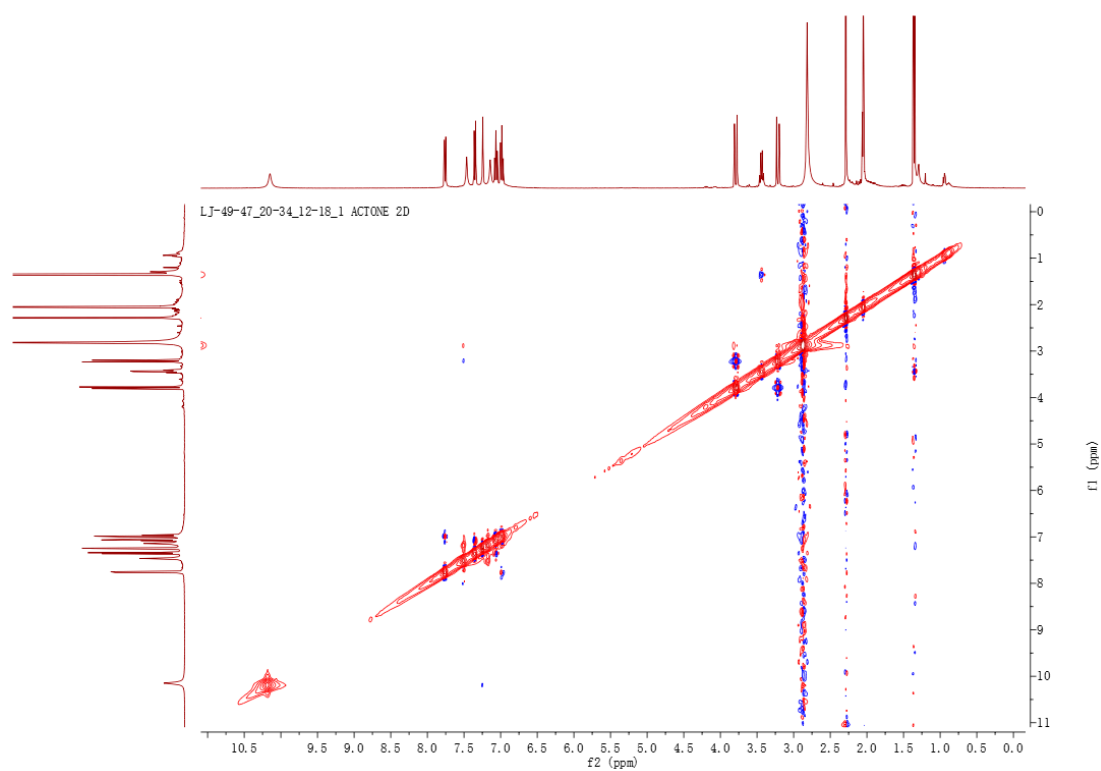
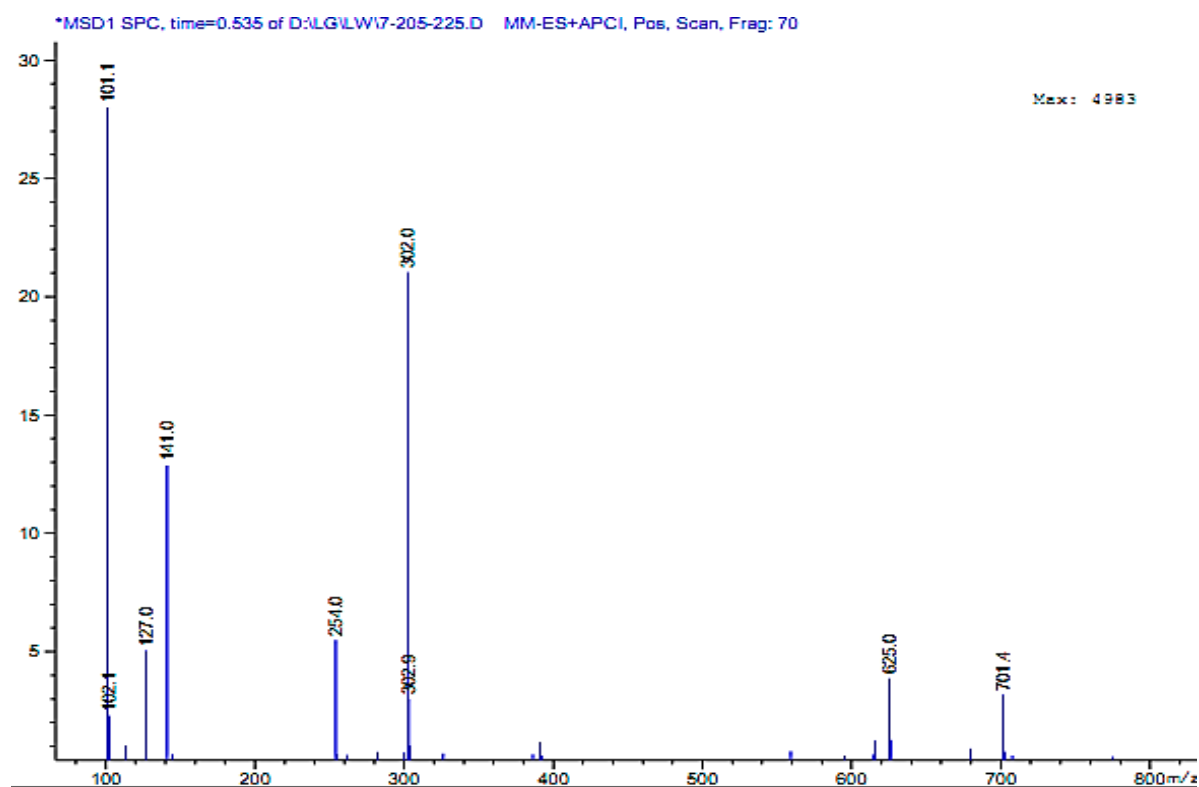
Figure S9. NOESY spectrum of compound 1 in acetone-*d*<sub>6</sub>.

Figure S10. LR-ESI mass spectrum of compound 2.

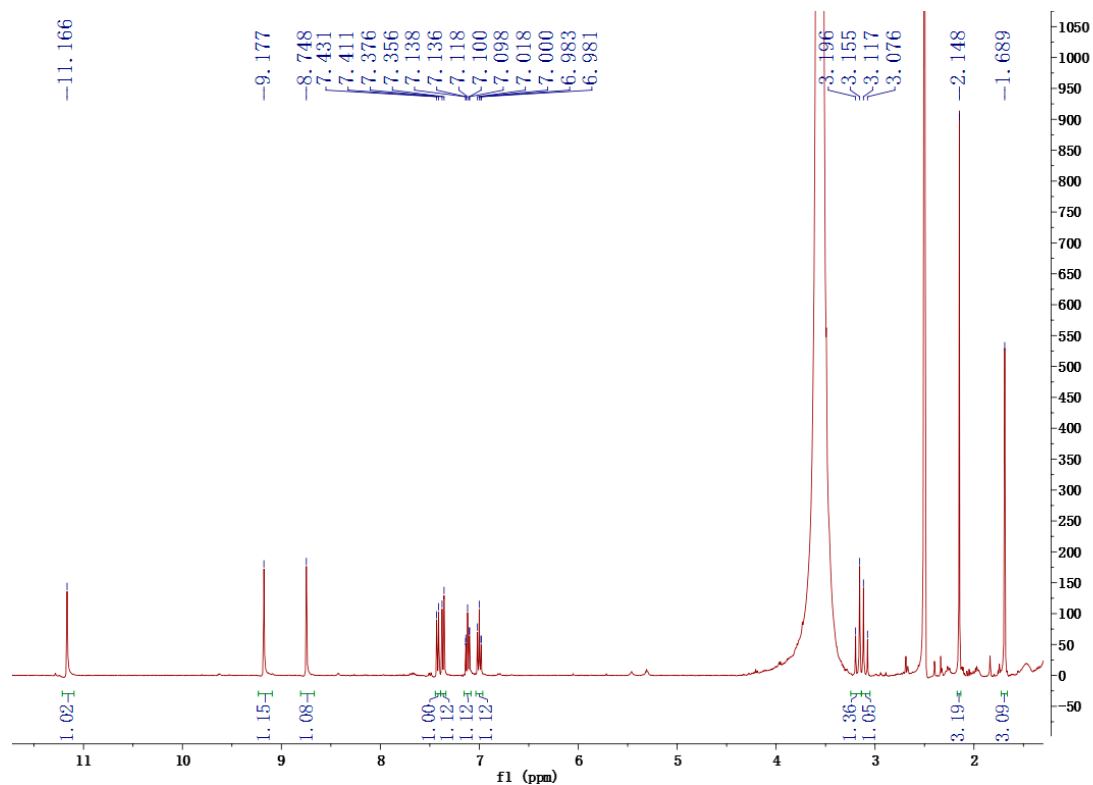


Figure S11.  $^1\text{H-NMR}$  spectrum of compound 2 in  $\text{DMSO-}d_6$  (400 MHz).

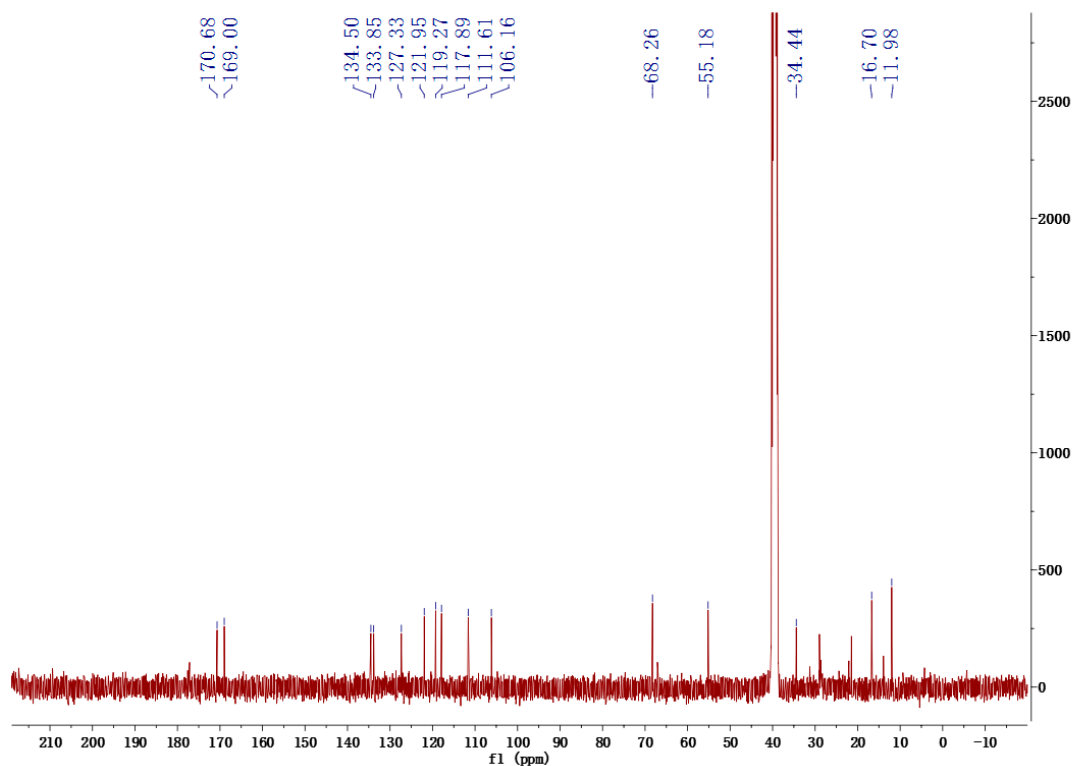


Figure S12.  $^{13}\text{C-NMR}$  spectrum of compound 2 in  $\text{DMSO-}d_6$  (100 MHz).

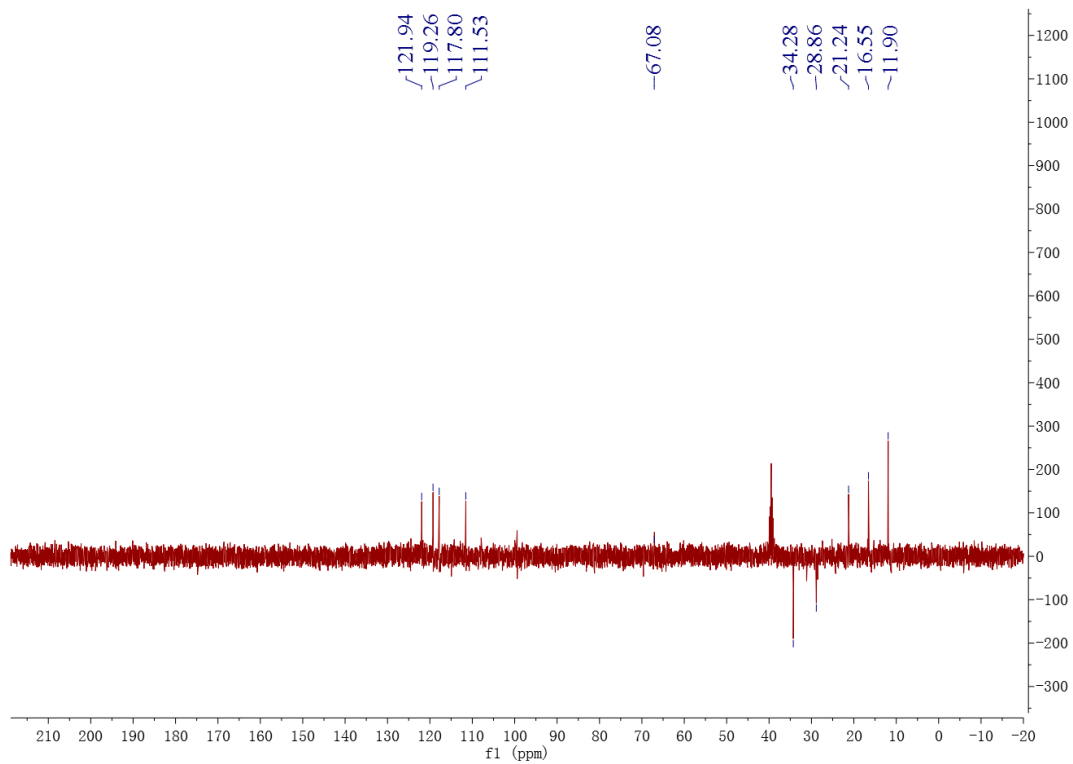


Figure S13. DEPT135 spectrum of compound 2 in DMSO-*d*<sub>6</sub> (100 MHz).

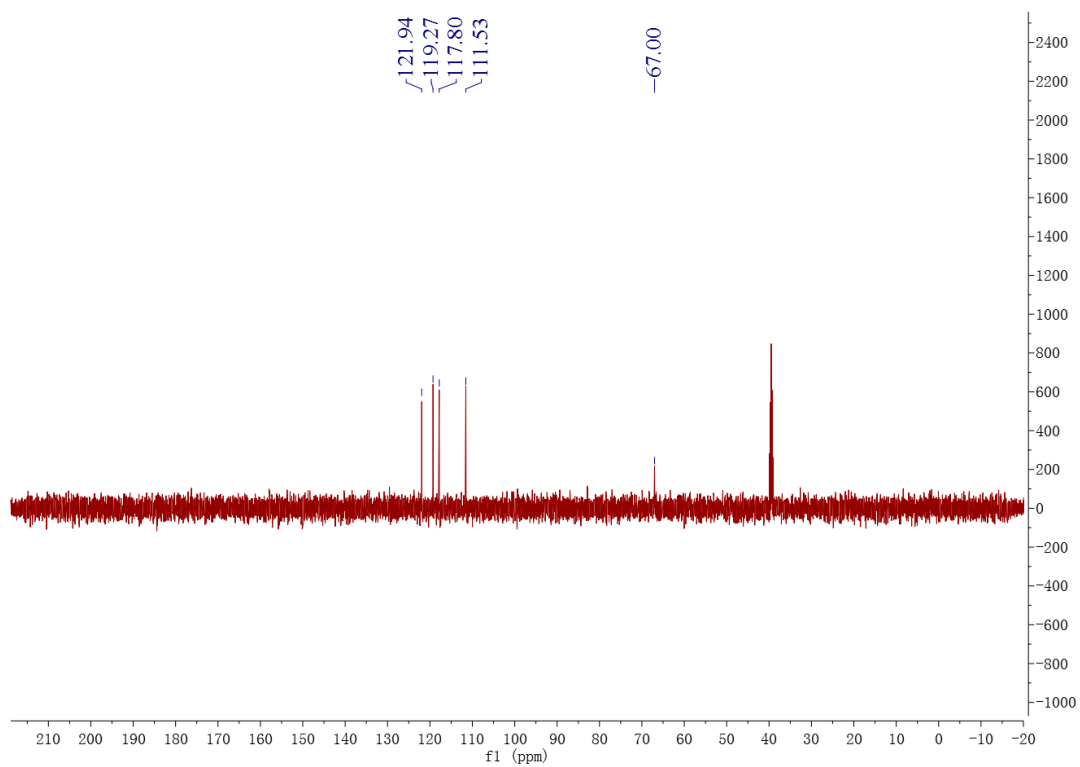


Figure S14. DEPT90 spectrum of compound 2 in DMSO-*d*<sub>6</sub> (100 MHz).



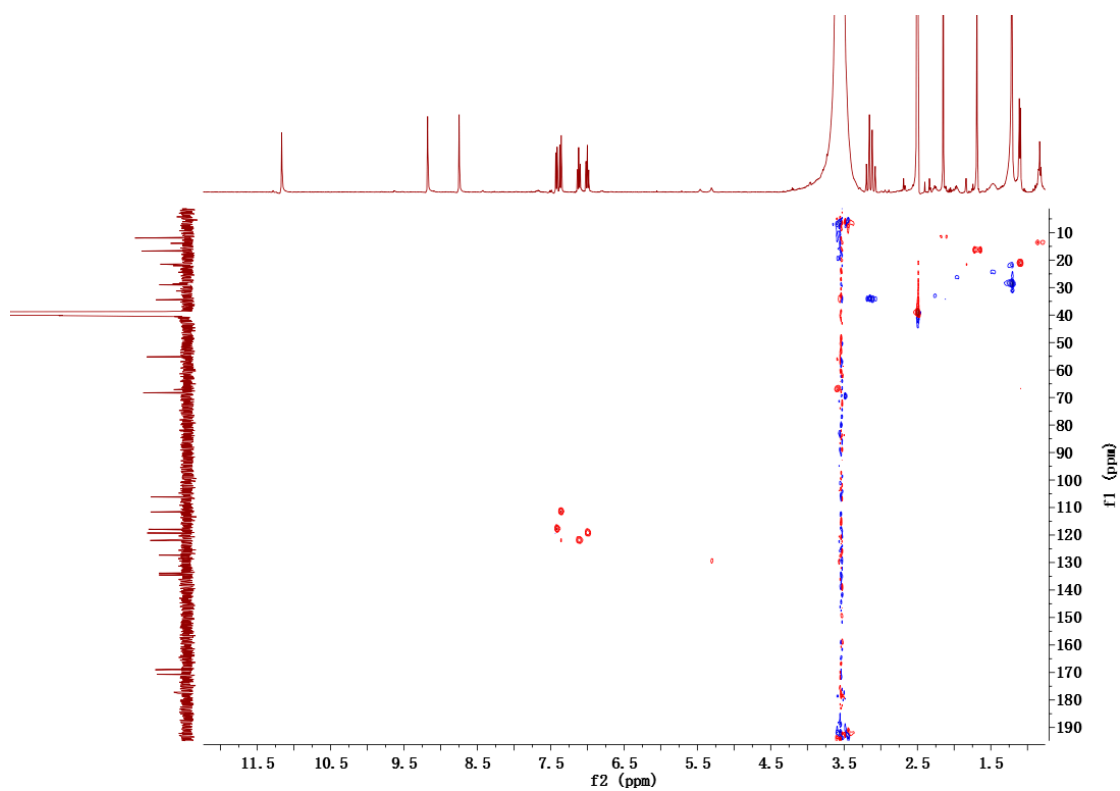


Figure S15. HMQC spectrum of compound 2 in DMSO- $d_6$ .

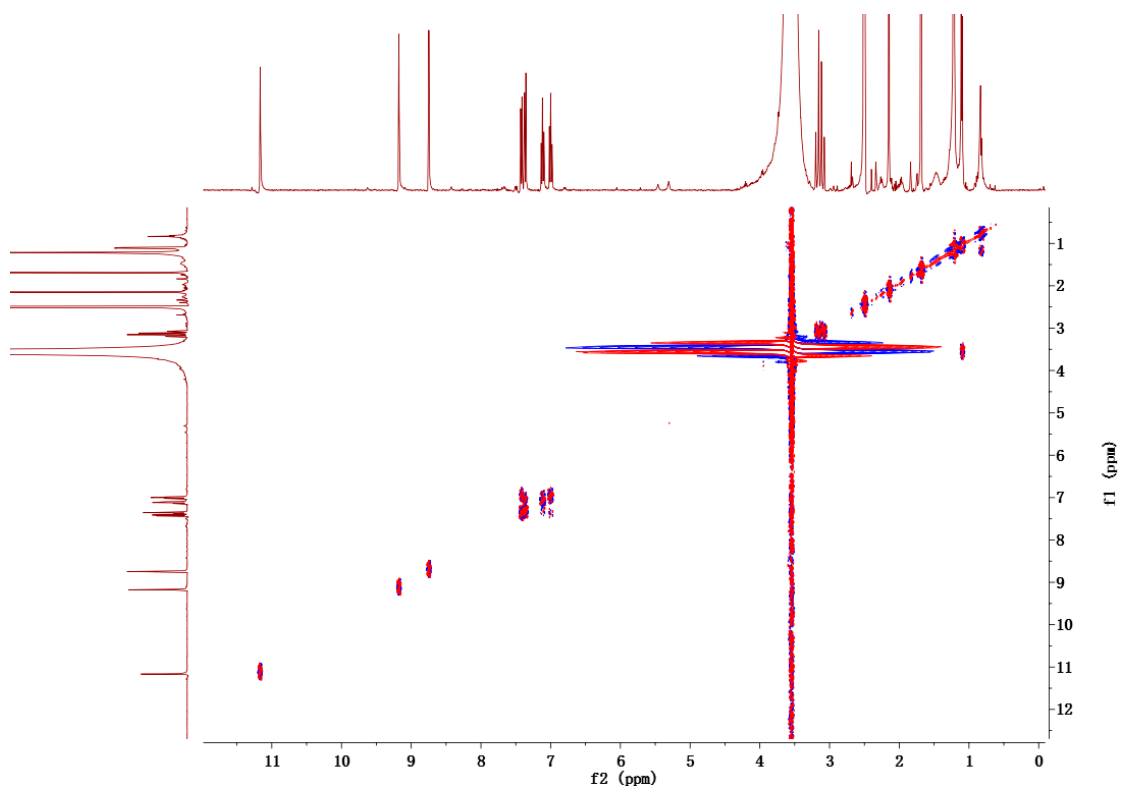


Figure S16.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound 2 in DMSO- $d_6$ .

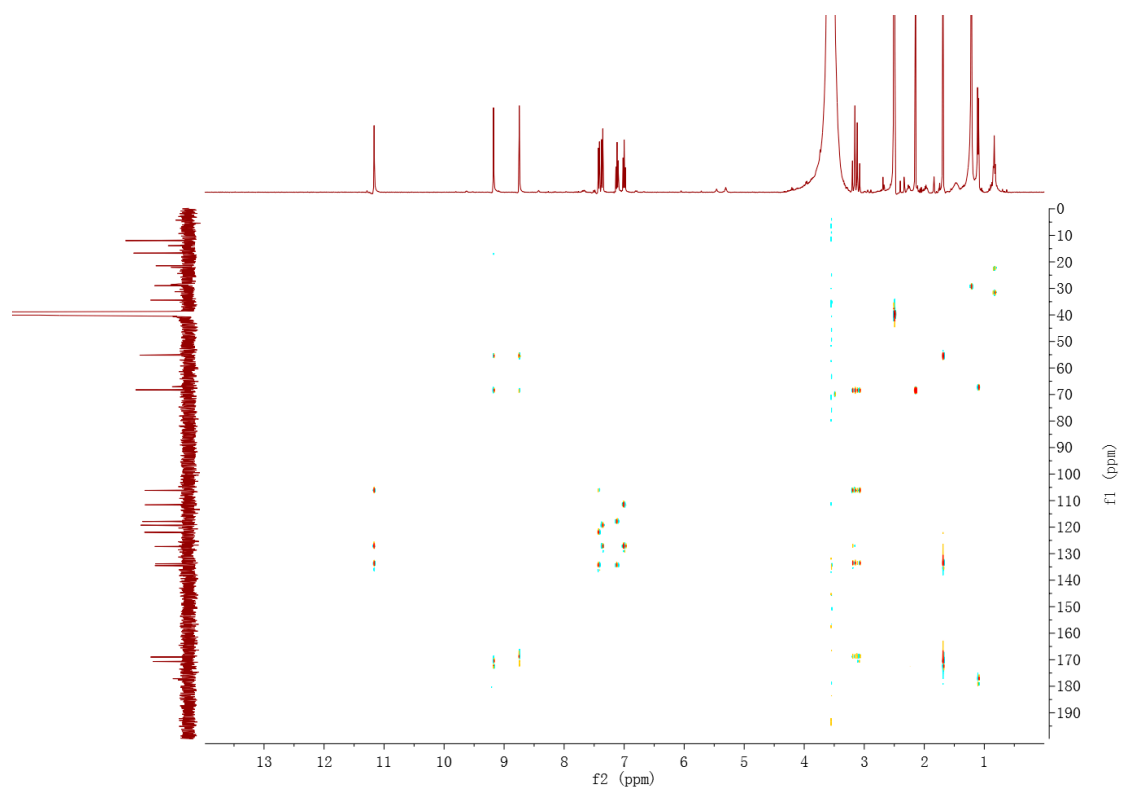


Figure S17. HMBC spectrum of compound 2 in DMSO-*d*<sub>6</sub>.

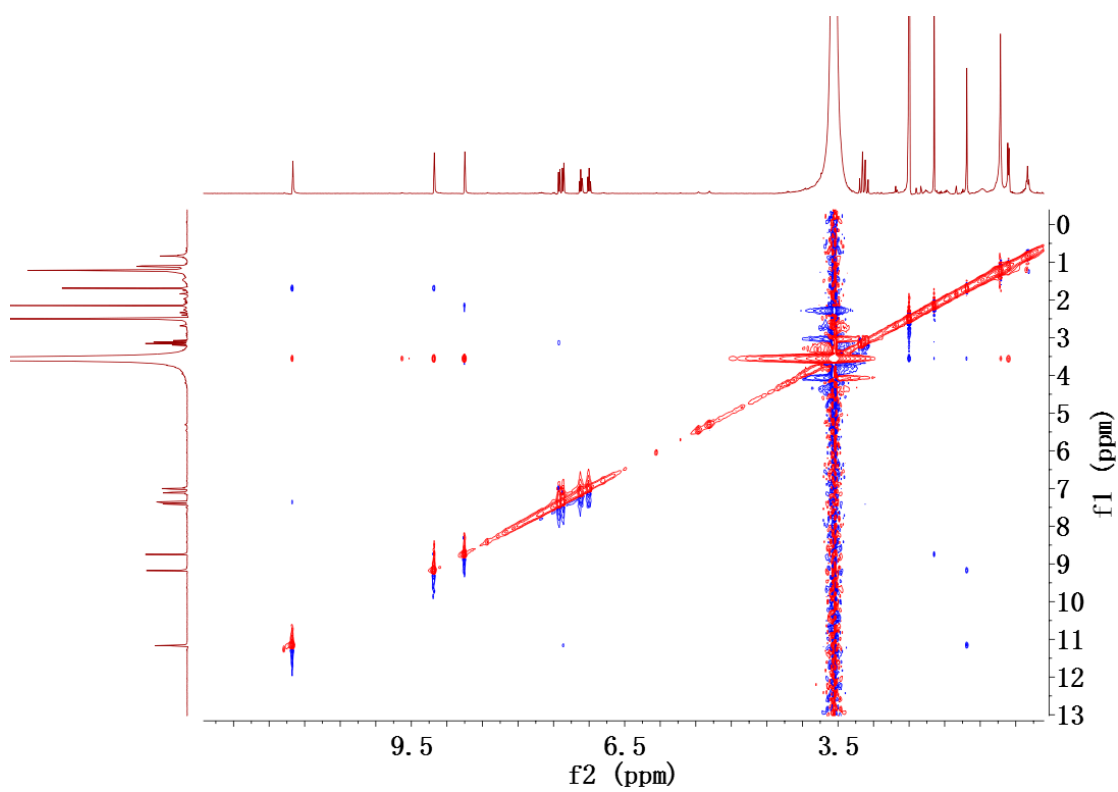


Figure S18. NOESY spectrum of compound 2 in DMSO-*d*<sub>6</sub>.

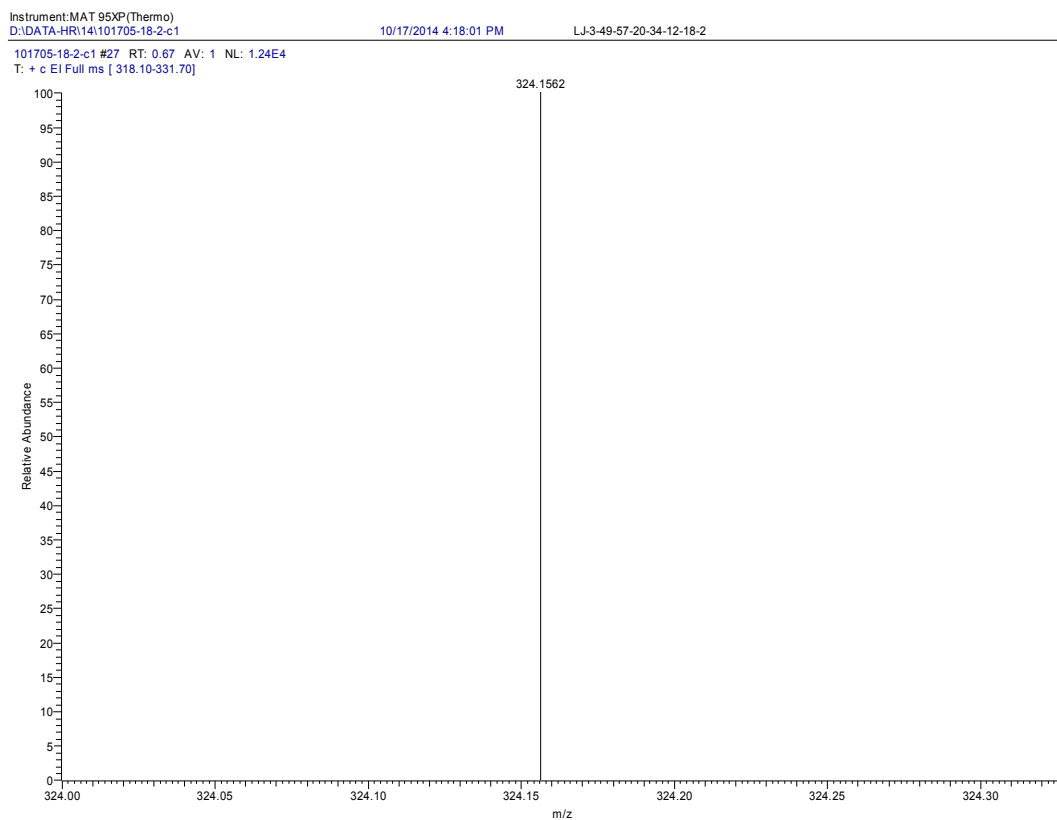


Figure S19. HREI Mass spectrum of compound 3.

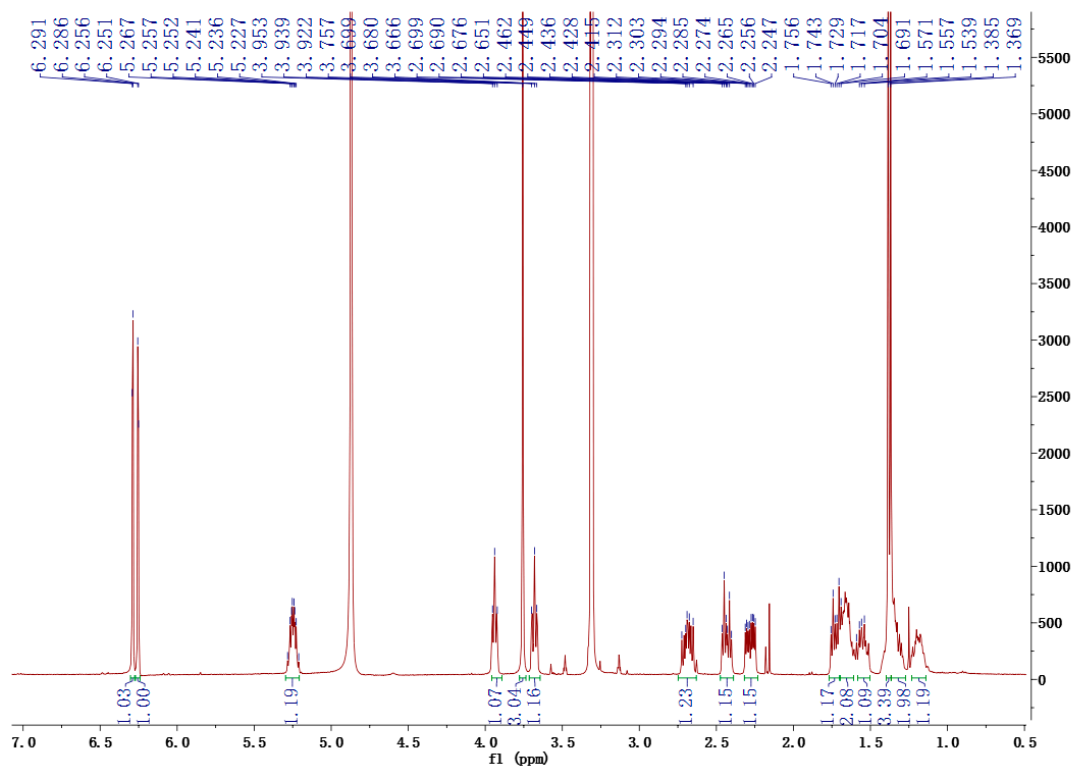


Figure S20.  $^1\text{H-NMR}$  spectrum of compound 3 in  $\text{CD}_3\text{OD}$  (400 MHz).

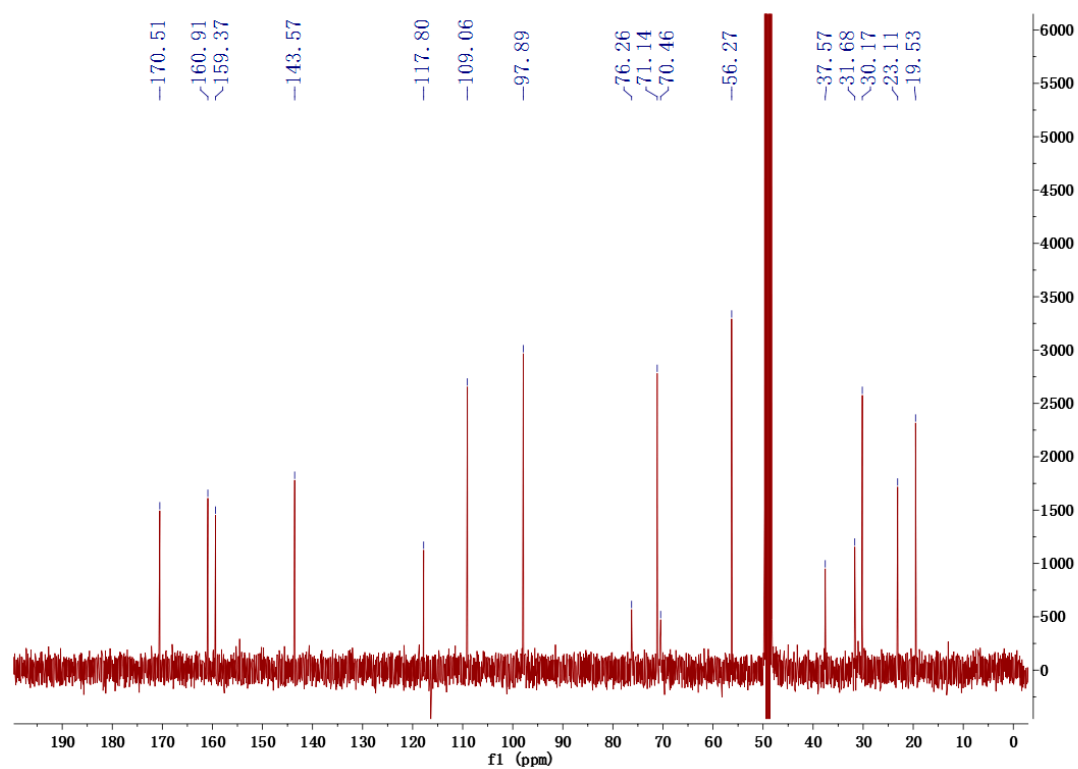


Figure S21.  $^{13}\text{C}$ -NMR spectrum of compound 3 in  $\text{CD}_3\text{OD}$  (100 MHz).

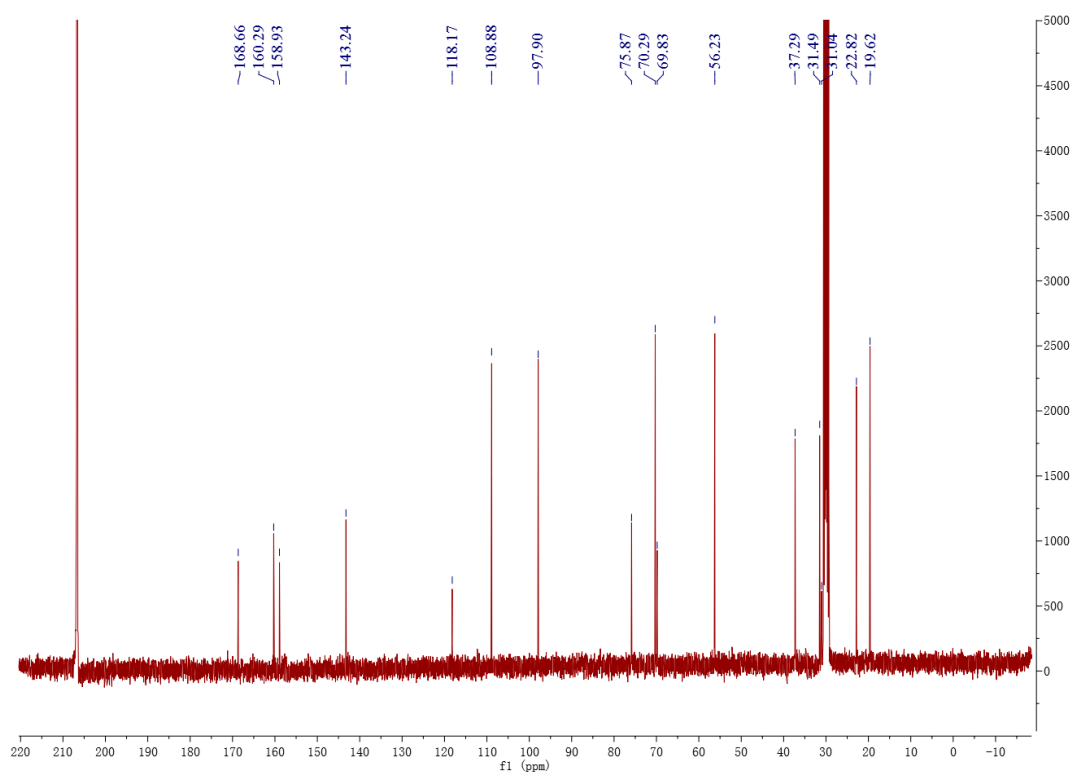


Figure S22.  $^{13}\text{C}$ -NMR spectrum of compound 3 in acetone- $d_6$  (100 MHz).

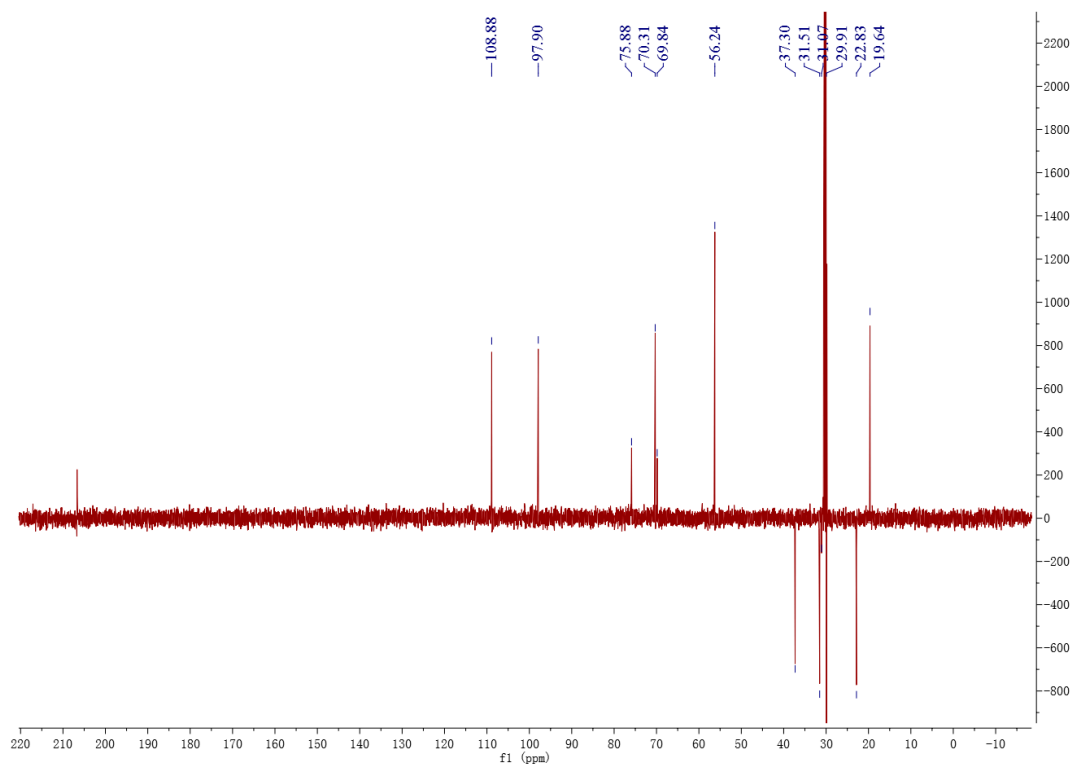


Figure S23. DEPT135 spectrum of compound 3 in acetone- $d_6$  (100 MHz).

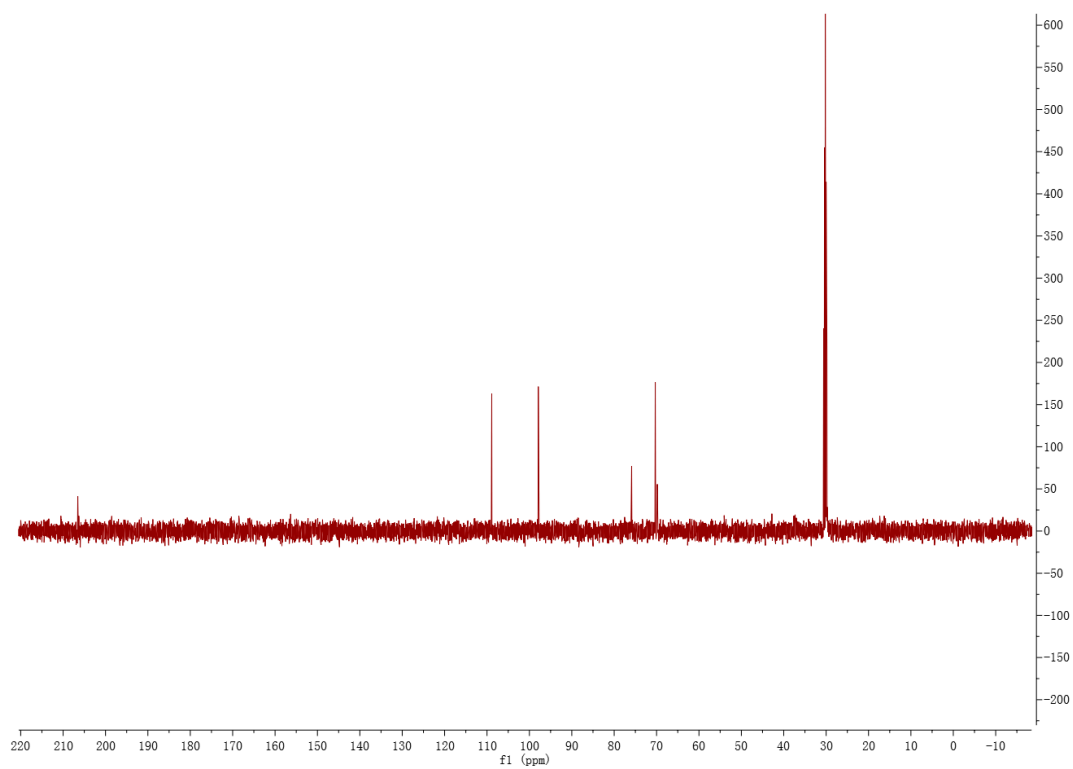


Figure S24. DEPT90 spectrum of compound 6 in acetone- $d_6$  (100 MHz).

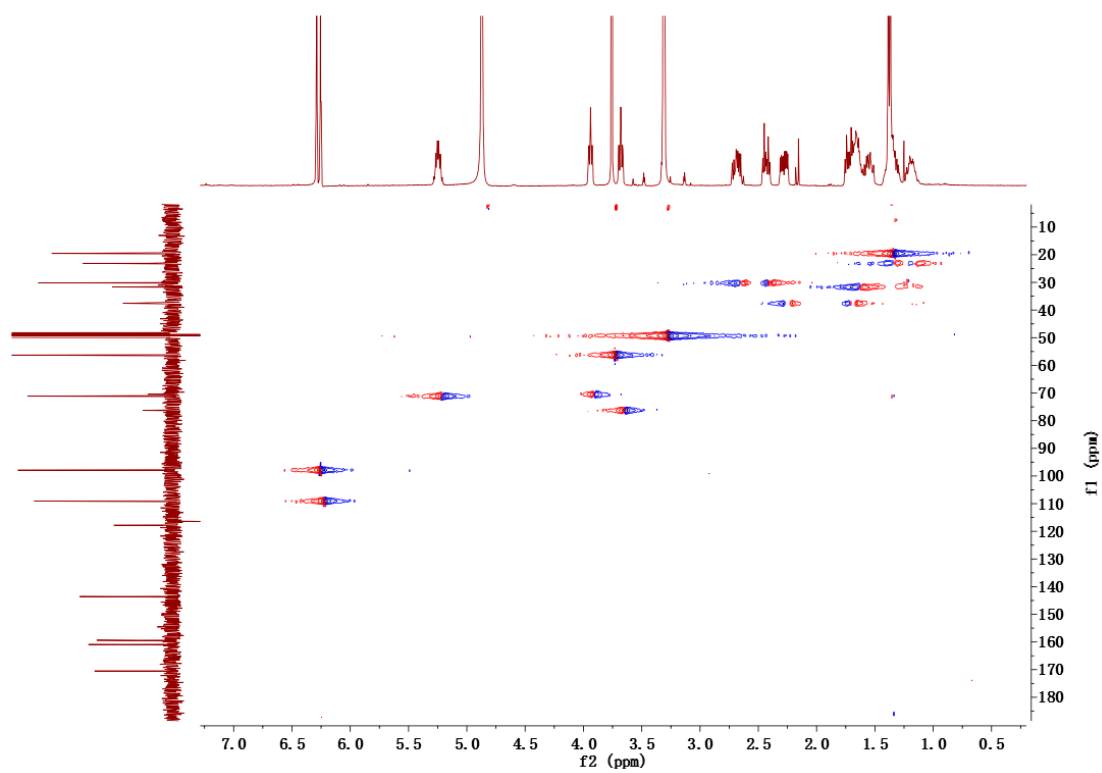


Figure S25. HMQC spectrum of compound 3 in CD<sub>3</sub>OD.

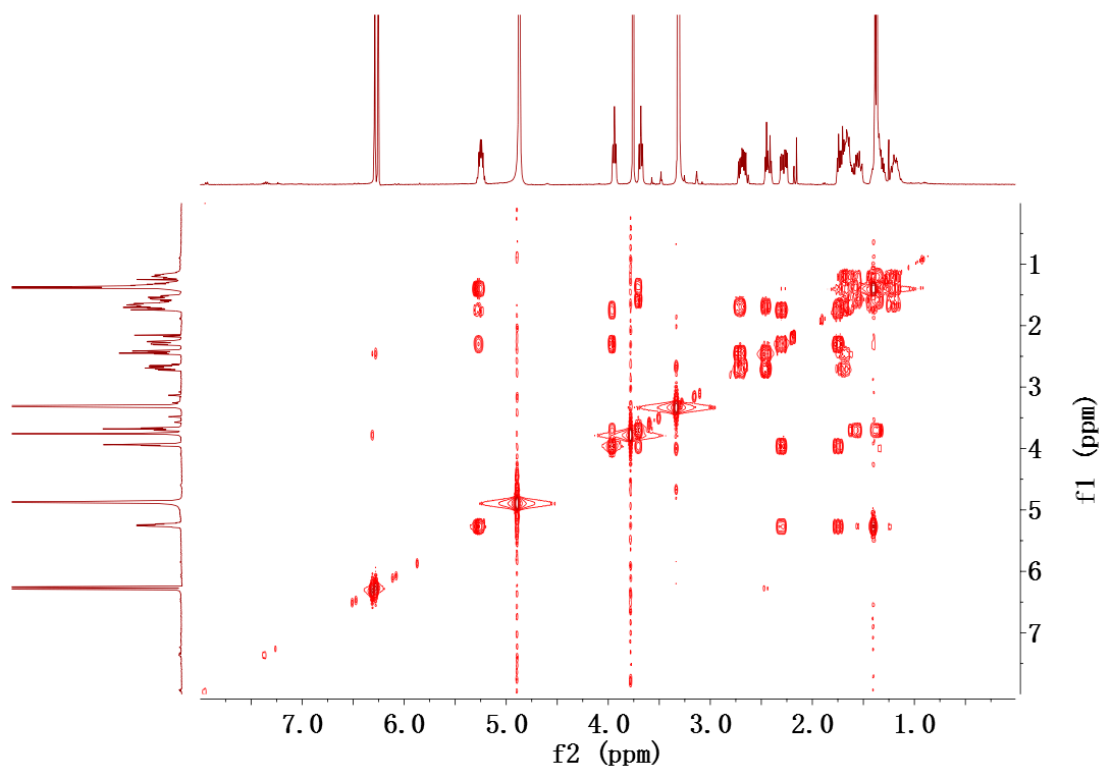


Figure S26. <sup>1</sup>H-<sup>1</sup>H COSY spectrum of compound 3 in CD<sub>3</sub>OD.

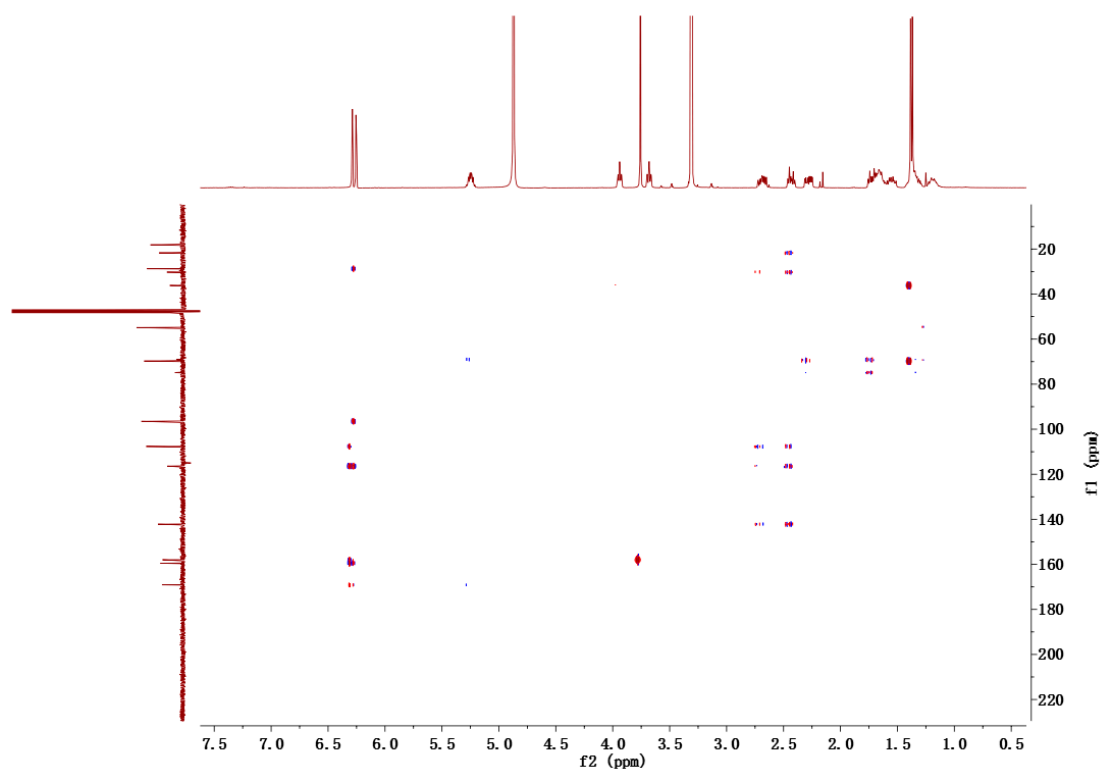


Figure S27. HMBC spectrum of compound 3 in CD<sub>3</sub>OD.

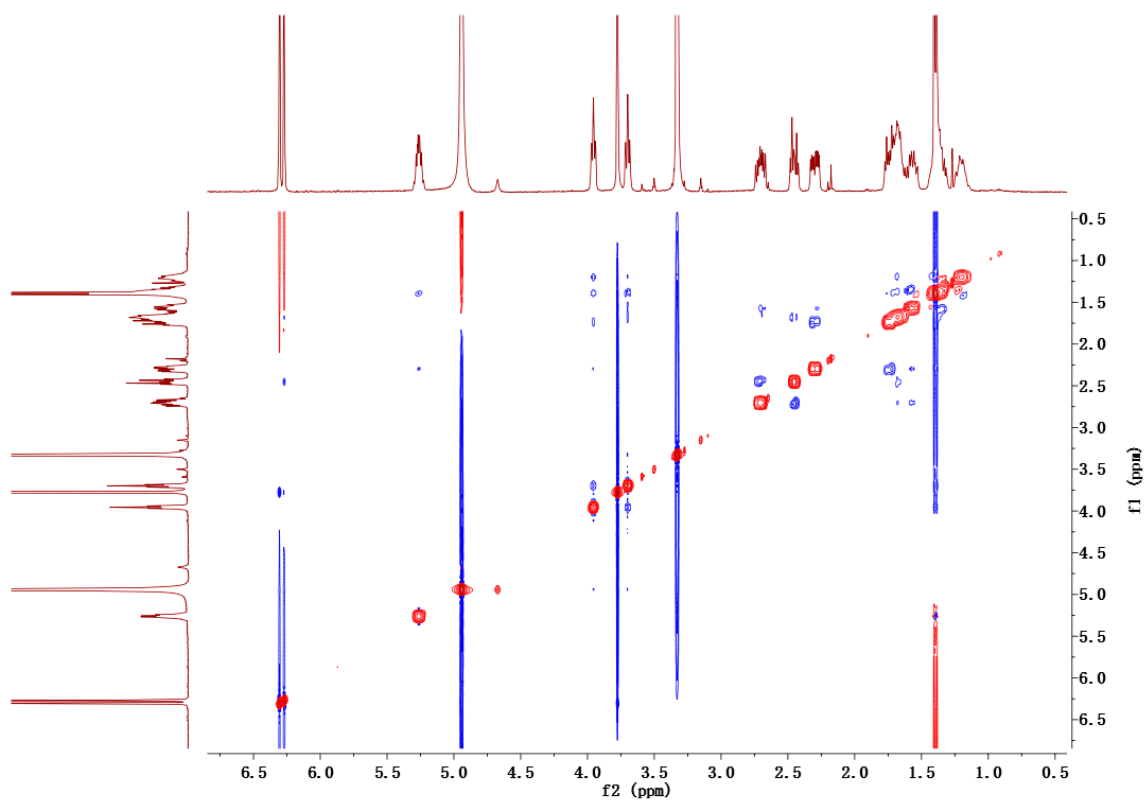


Figure S28. NOESY spectrum of compound 3 in CD<sub>3</sub>OD.

LJ-3-29-35-20-24-19-26 #5-13 RT: 0.12-0.34 AV: 9 SB: 3 0.01-0.06 NL: 1.27E6  
T: + c ESI Full ms [50.00-2000.00]

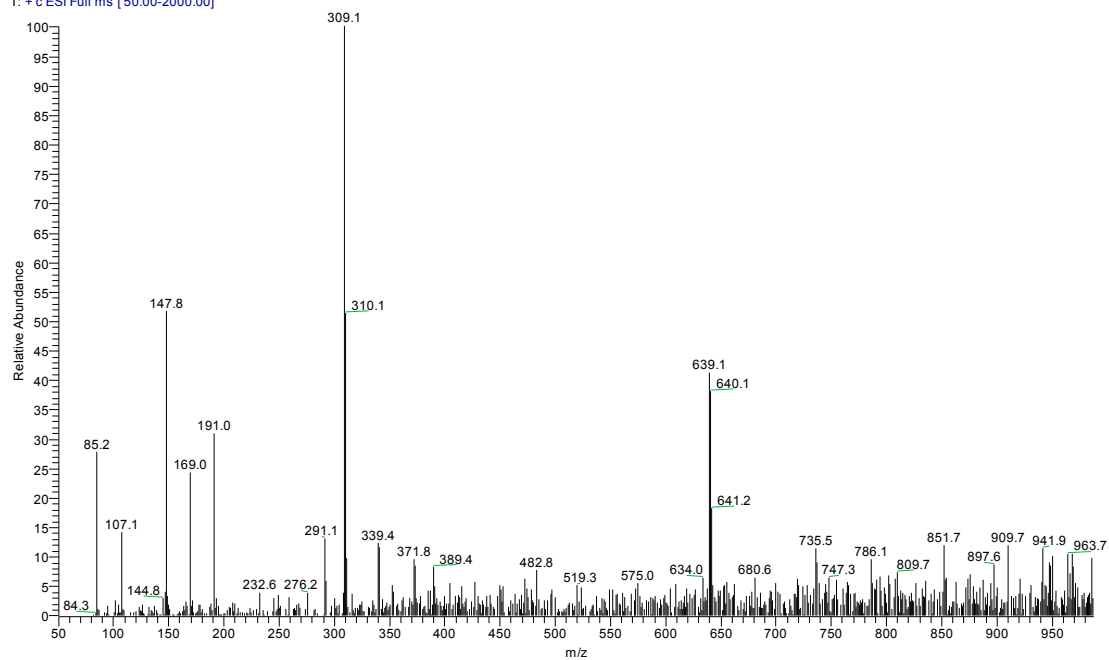


Figure S29. LR-ESI mass spectrum of compound 4.

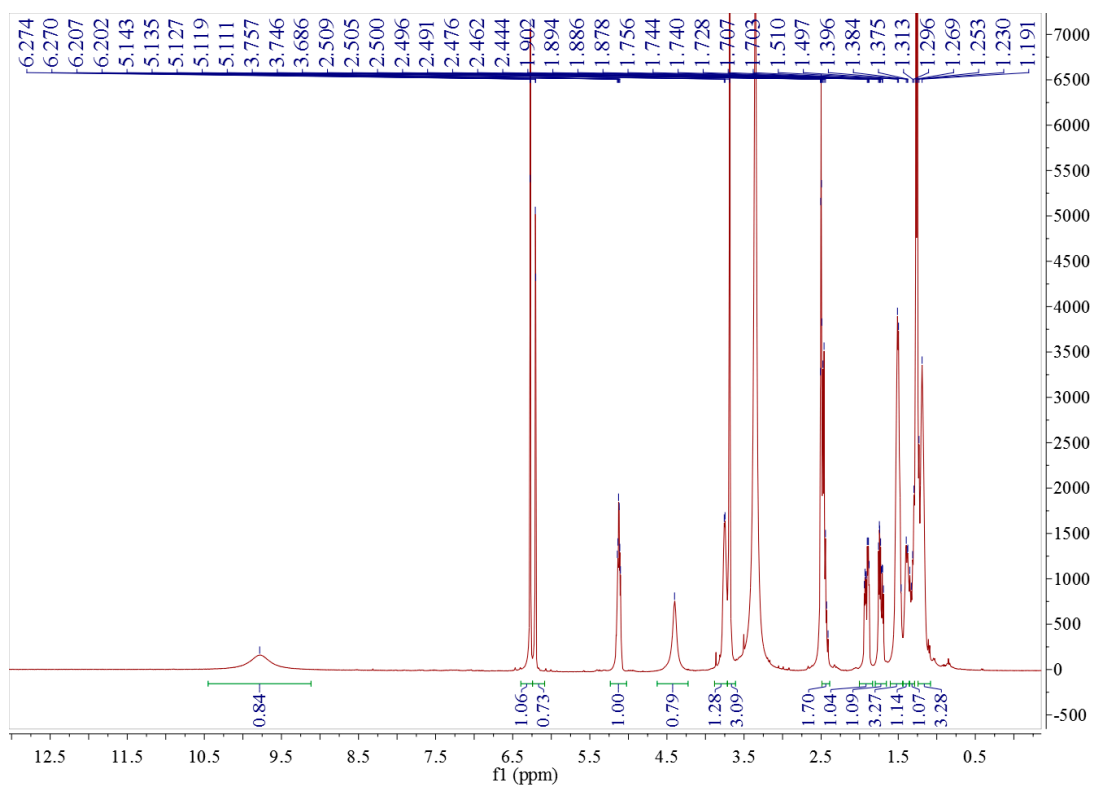


Figure S30. <sup>1</sup>H-NMR spectrum of compound 4 in DMSO-*d*<sub>6</sub> (400 MHz).



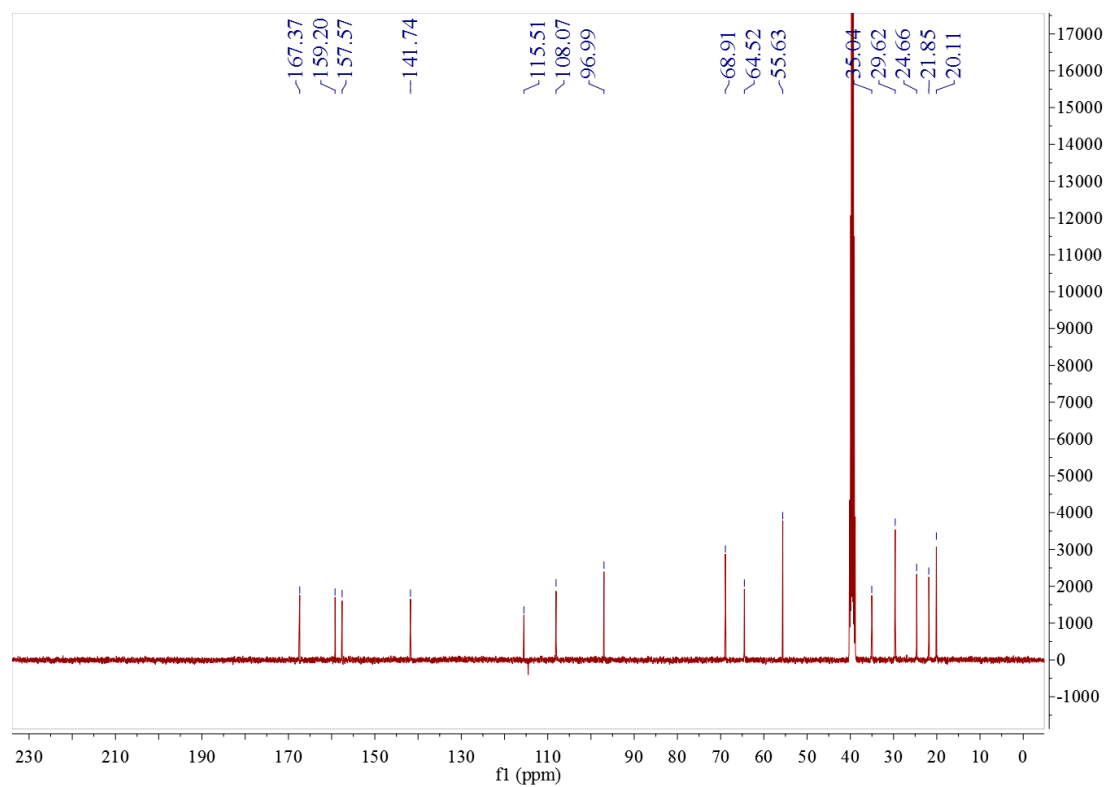


Figure S31. <sup>13</sup>C-NMR spectrum of compound 4 in DMSO-*d*<sub>6</sub> (100 MHz).

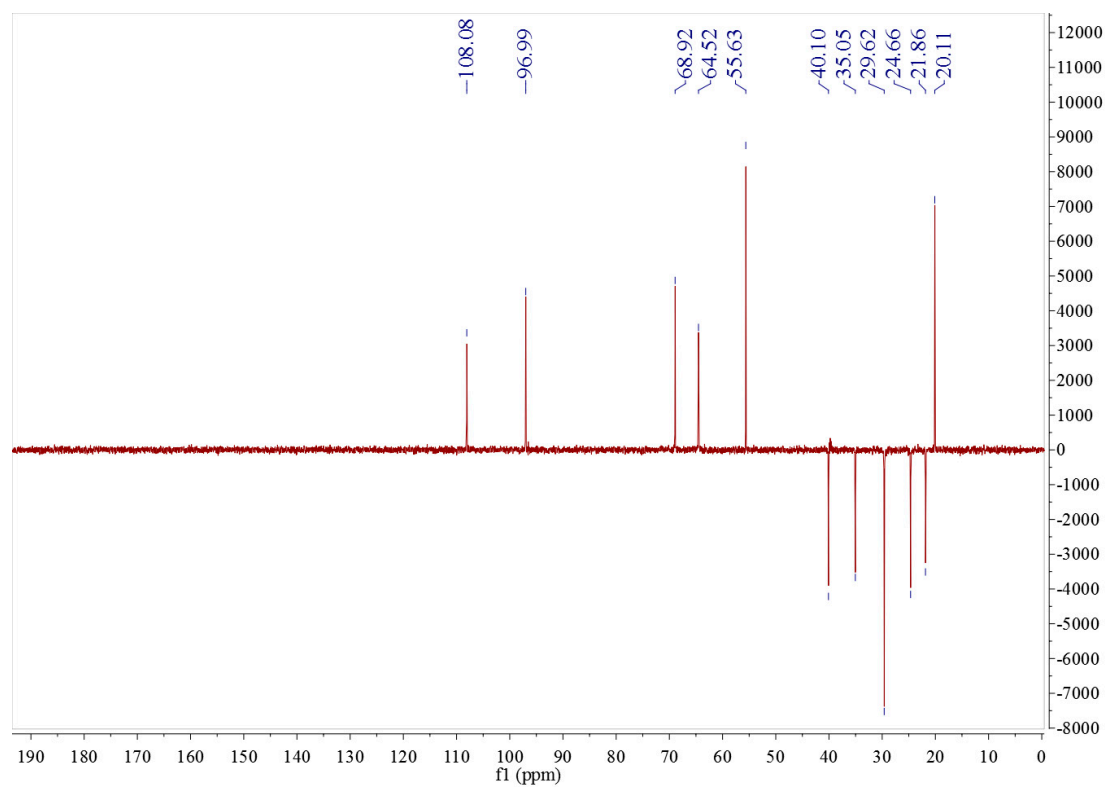


Figure S32. DEPT135 spectrum of compound 4 in DMSO-*d*<sub>6</sub>.

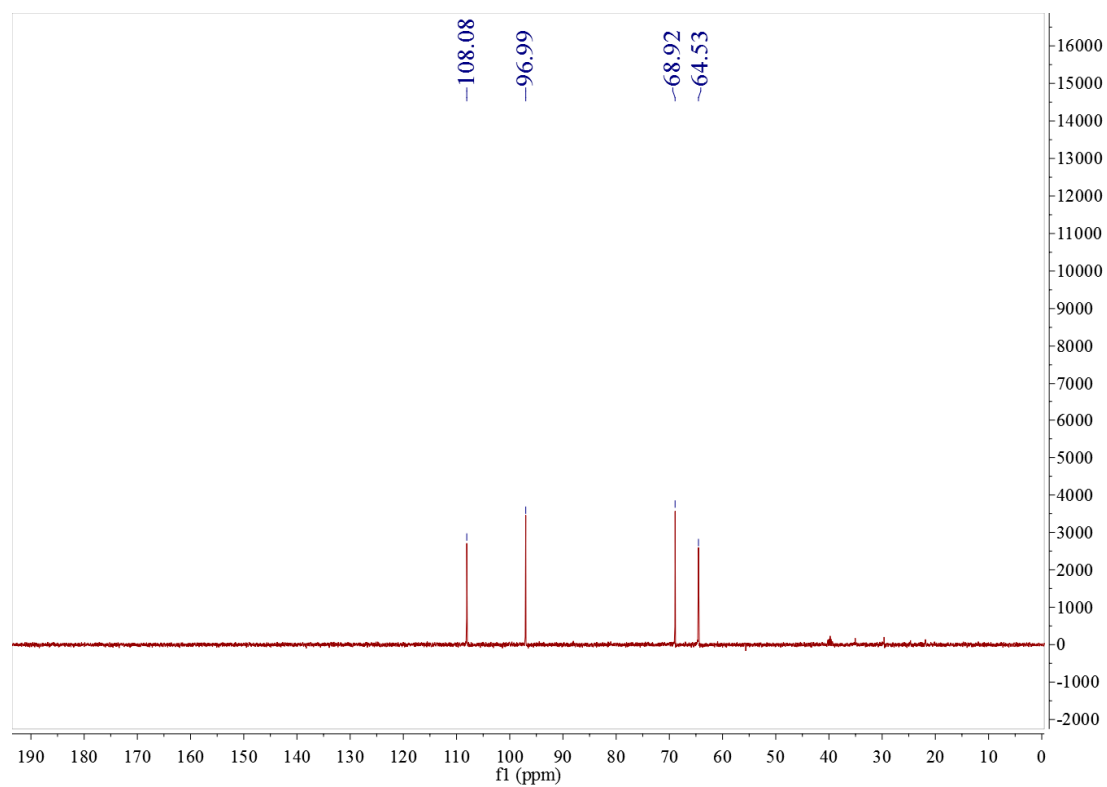


Figure S33. DEPT90 spectrum of compound 4 in DMSO- $d_6$ .

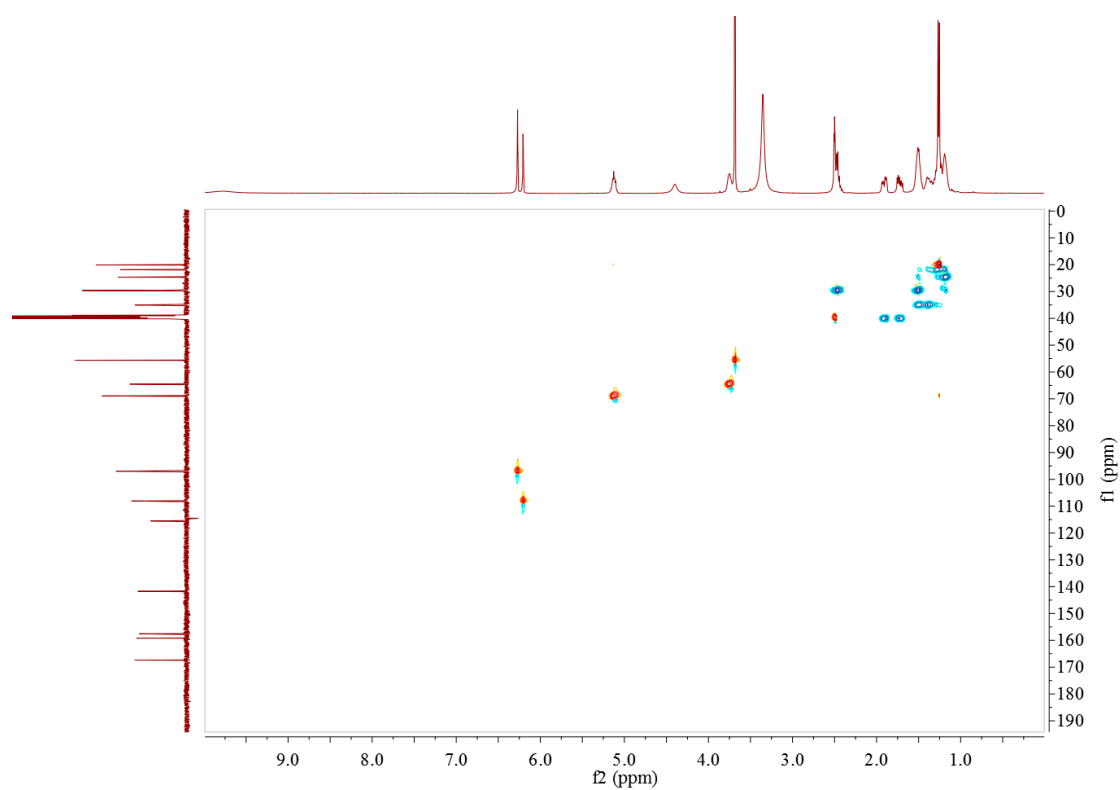


Figure S34. HMQC spectrum of compound 4 in DMSO- $d_6$ .

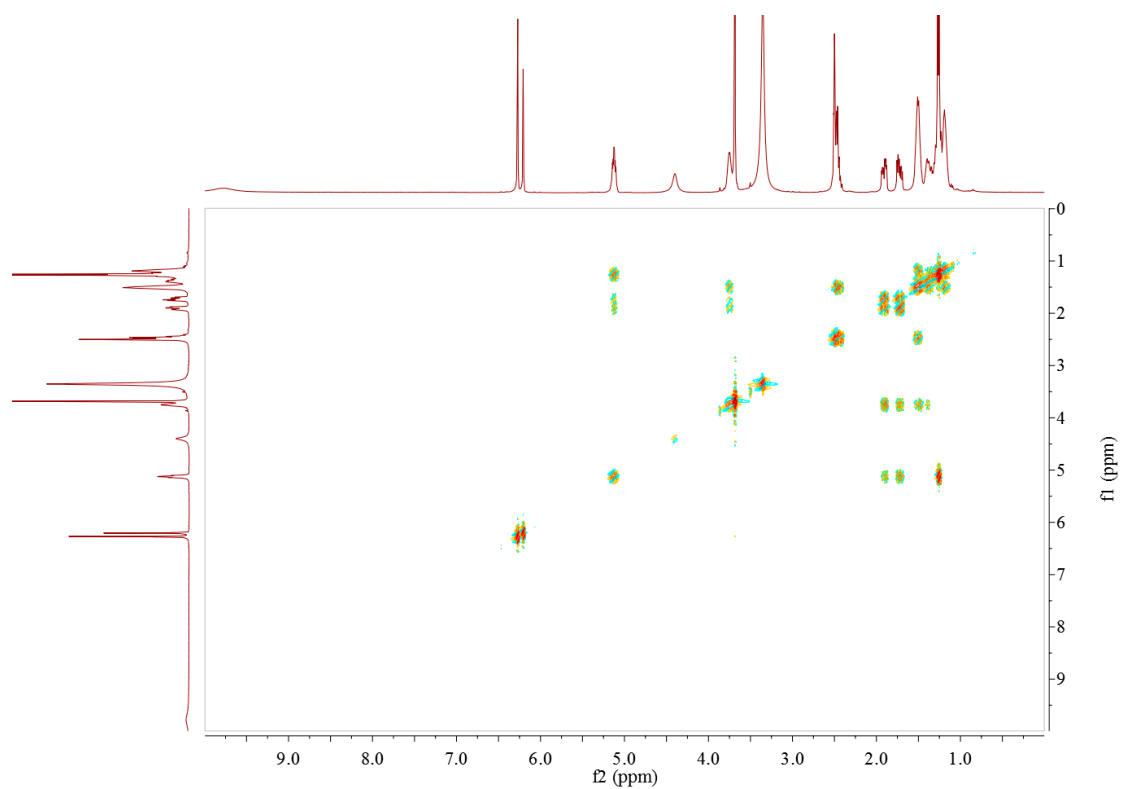


Figure S35.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound 4 in  $\text{DMSO-}d_6$ .

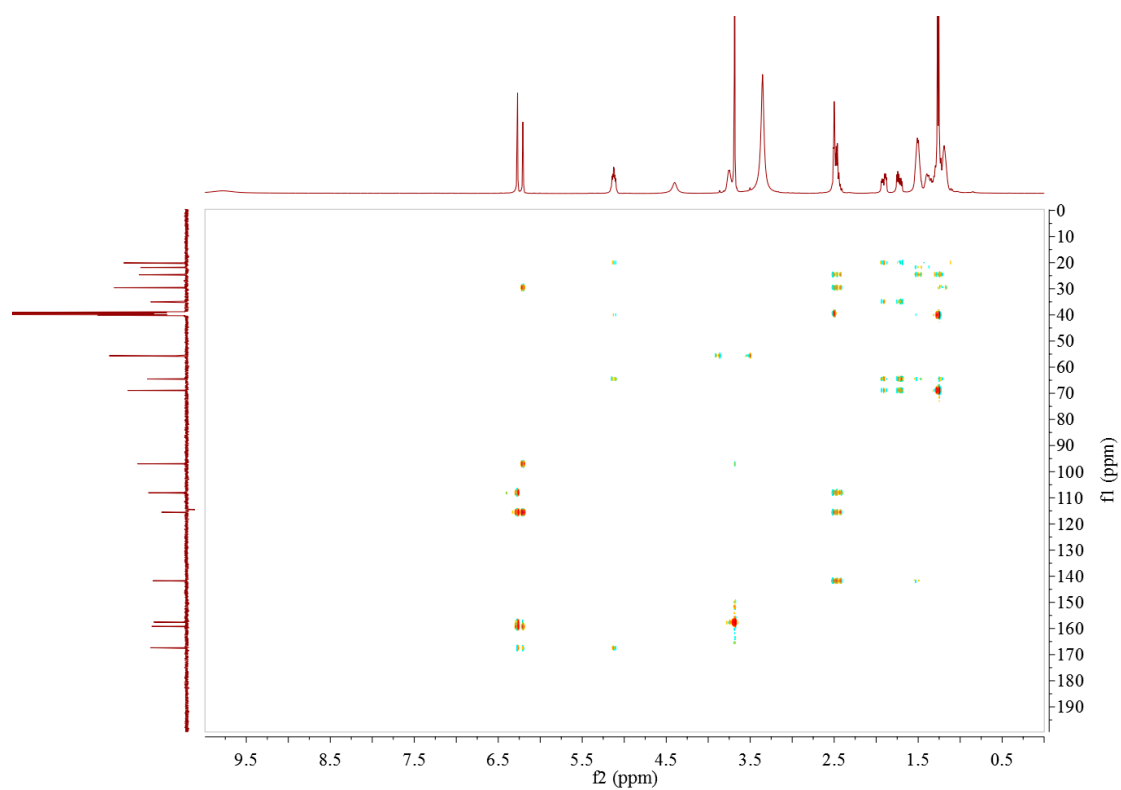


Figure S36. HMBC spectrum of compound 4 in  $\text{DMSO-}d_6$ .

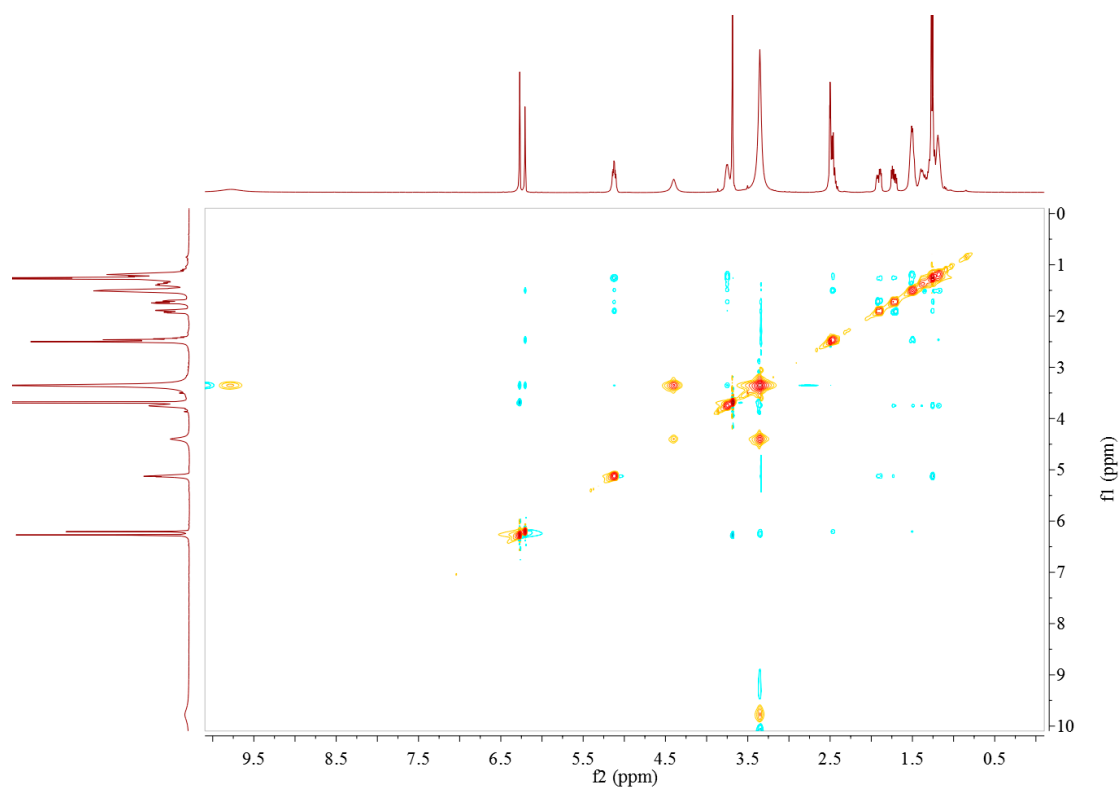


Figure S37. NOESY spectrum of compound 4 in DMSO-*d*<sub>6</sub>.

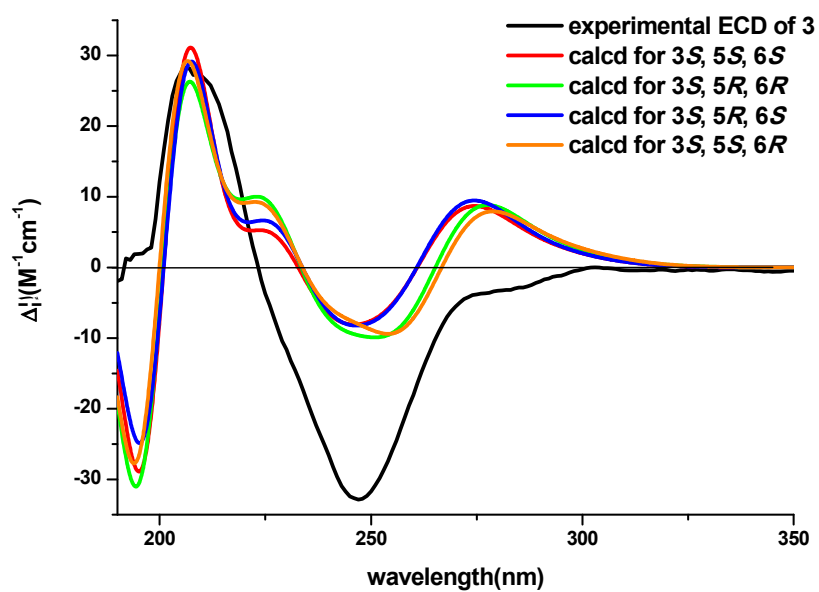


Figure S38. Comparison of the experimental ECD spectra of 3 with the calculated ECD spectra for four (3*S*) stereochemical options.



Figure S39. Experimental CD spectra of 2.