

Supplementary Materials

Bioactive polyketide and diketopiperazine derivatives from the mangrove-sediment-derived fungus *Aspergillus* sp. SCSIO41407

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Figure S1. ^1H NMR spectrum of **1** (CD_3OD , 500 MHz).

Figure S2. ^1C NMR spectrum of **1** (CD_3OD , 500 MHz).

Figure S3. The DPET spectrum of **1** (CD_3OD).

Figure S4. HSQC spectrum of **1** (CD_3OD).

Figure S5. HMBC spectrum of **1** (CD_3OD).

Figure S6. COSY spectrum of **1** (CD_3OD).

Figure S7. The UV spectrum of **1**.

Figure S8. The IR spectrum of **1**.

Figure S9. HRESIMS spectrum of compound **1**.

Figure S10. ^1H NMR spectrum of **2** ($\text{DMSO}-d_6$, 700MHz).

Figure S11. ^1C NMR spectrum of **2** ($\text{DMSO}-d_6$, 175 MHz).

Figure S12. ^1H NMR spectrum of **3** ($\text{DMSO}-d_6$, 500 MHz).

Figure S13. ^1C NMR spectrum of **3** ($\text{DMSO}-d_6$, 125 MHz).

Figure S14. ^1H NMR spectrum of **4** ($\text{DMSO}-d_6$, 700 MHz).

Figure S15. ^1C NMR spectrum of **4** ($\text{DMSO}-d_6$, 175 MHz).

Figure S16. ^1H NMR spectrum of **5** ($\text{DMSO}-d_6$, 700 MHz).

Figure S17. ^1C NMR spectrum of **5** ($\text{DMSO}-d_6$, 175 MHz).

Figure S18. ^1H NMR spectrum of **6** (CDCl_3 , 700 MHz).

Figure S19. ^1C NMR spectrum of **6** (CDCl_3 , 175 MHz).

Figure S20. ^1H NMR spectrum of **7** (CD_3OD , 700 MHz).

Figure S21. ^1C NMR spectrum of **7** (CD_3OD , 175 MHz).

Figure S22. ^1H NMR spectrum of **8** ($\text{DMSO}-d_6$, 700 MHz).

Figure S23. ^1C NMR spectrum of **8** ($\text{DMSO}-d_6$, 175 MHz).

Figure S24. ^1H NMR spectrum of **9** ($\text{DMSO}-d_6$, 700 MHz).

Figure S25. ^1C NMR spectrum of **9** ($\text{DMSO}-d_6$, 175 MHz).

Figure S26. ^1H NMR spectrum of **10** ($\text{DMSO}-d_6$, 500 MHz).

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Figure S28. ^1H NMR spectrum of **11** ($\text{DMSO}-d_6$, 700 MHz).

Figure S29. ^1C NMR spectrum of **11** ($\text{DMSO}-d_6$, 175 MHz).

Figure S30. ^1H NMR spectrum of **12** ($\text{DMSO}-d_6$, 500 MHz).

Figure S31. ^1C NMR spectrum of **12** ($\text{DMSO}-d_6$, 125 MHz).

Figure S32. ^1H NMR spectrum of **13** ($\text{DMSO}-d_6$, 700 MHz).

Figure S33. ^1C NMR spectrum of **13** ($\text{DMSO}-d_6$, 175 MHz).

Figure S34. ^1H NMR spectrum of **14** ($\text{DMSO}-d_6$, 700 MHz).

Figure S35. ^1C NMR spectrum of **14** ($\text{DMSO}-d_6$, 175 MHz).

Figure S36. ^1H NMR spectrum of **15** ($\text{DMSO}-d_6$, 500 MHz).

Figure S37. ^1C NMR spectrum of **15** ($\text{DMSO}-d_6$, 125 MHz).

Figure S38. Molecular docking of **1**, **10**, **11**, and **12** with NF- κ B p65.

ITS sequence of the strain *Aspergillus* sp. SCSSIO41407.

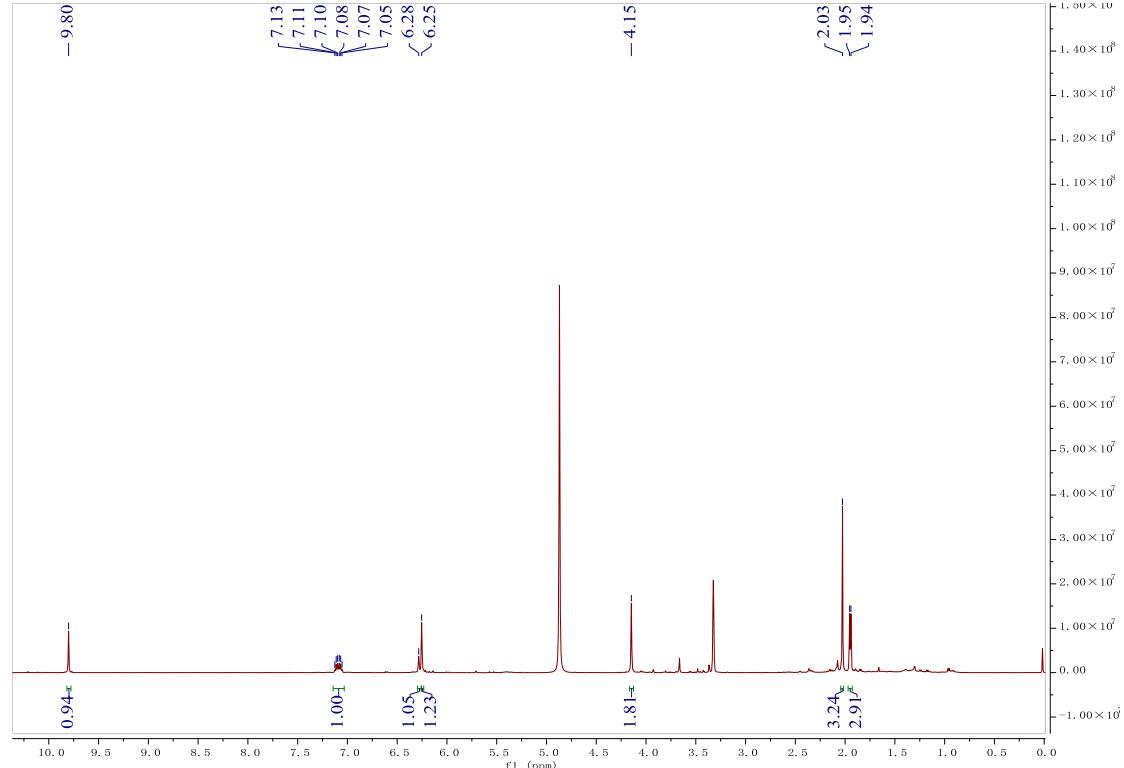


Figure S1. ^1H NMR spectrum of **1** (CD_3OD , 500 MHz).

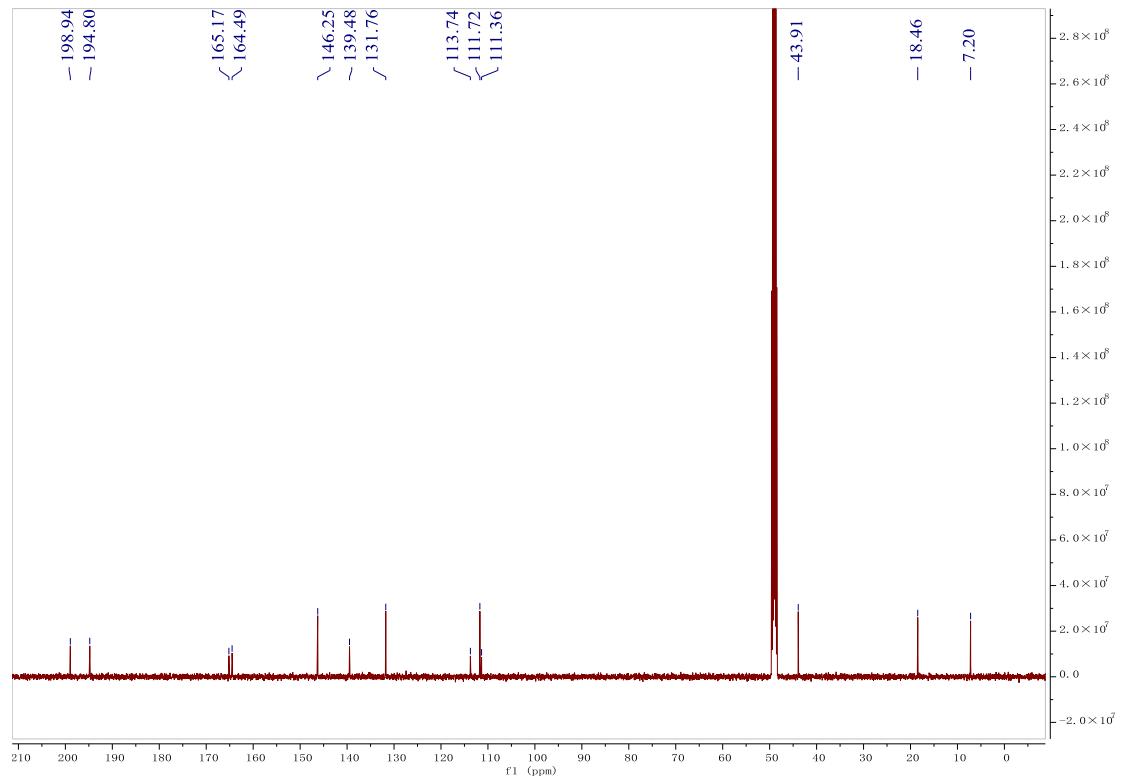


Figure S2. ^{13}C NMR spectrum of **1** (CD_3OD , 125 MHz).

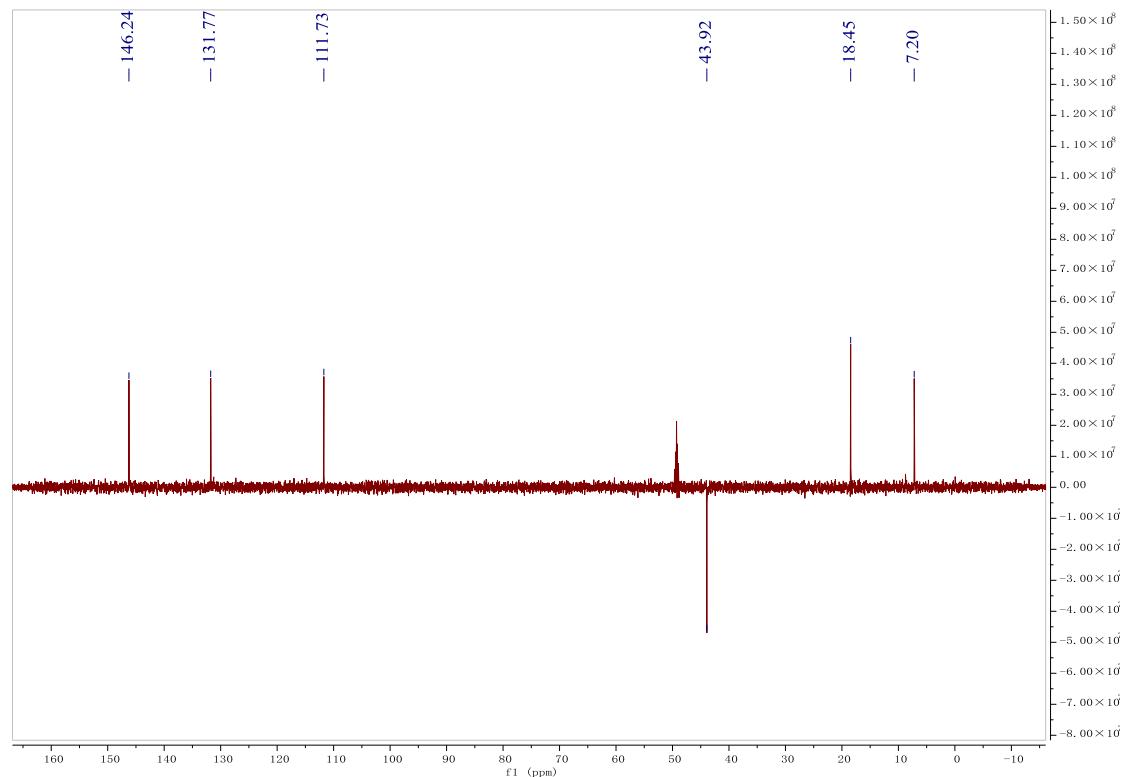


Figure S3. The DPET spectrum of **1** (CD_3OD).

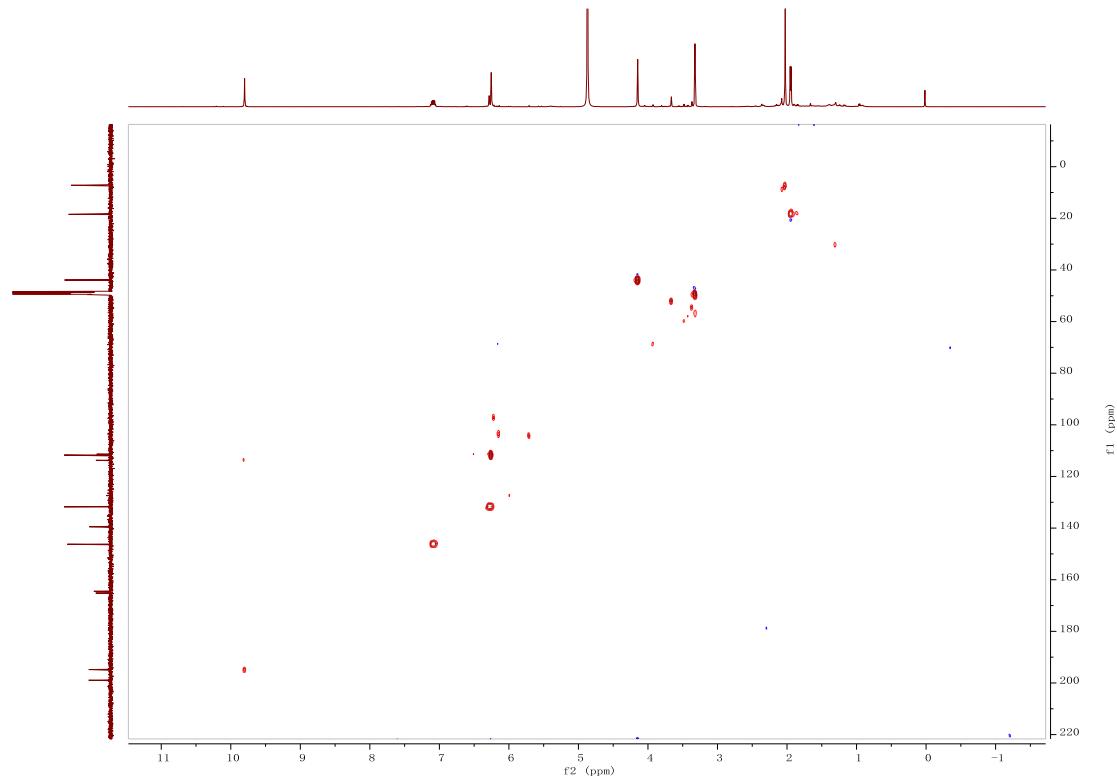


Figure S4. HSQC spectrum of **1** (CD_3OD).

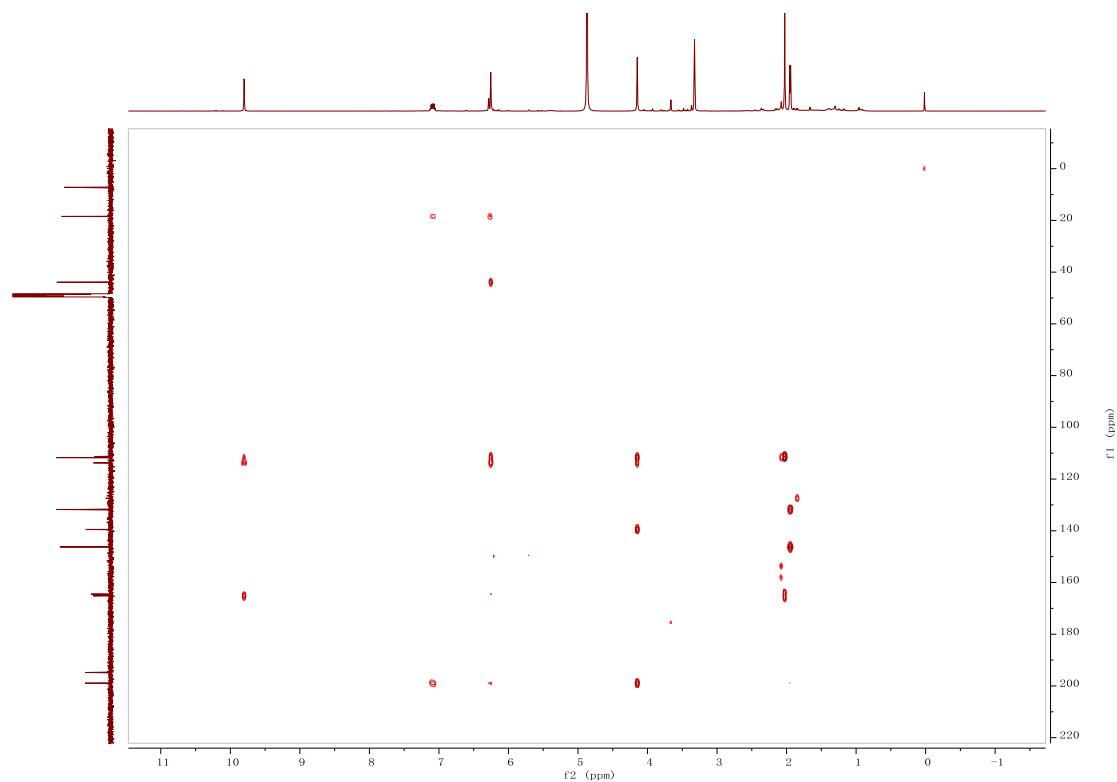


Figure S5. HMBC spectrum of **1** (CD_3OD).

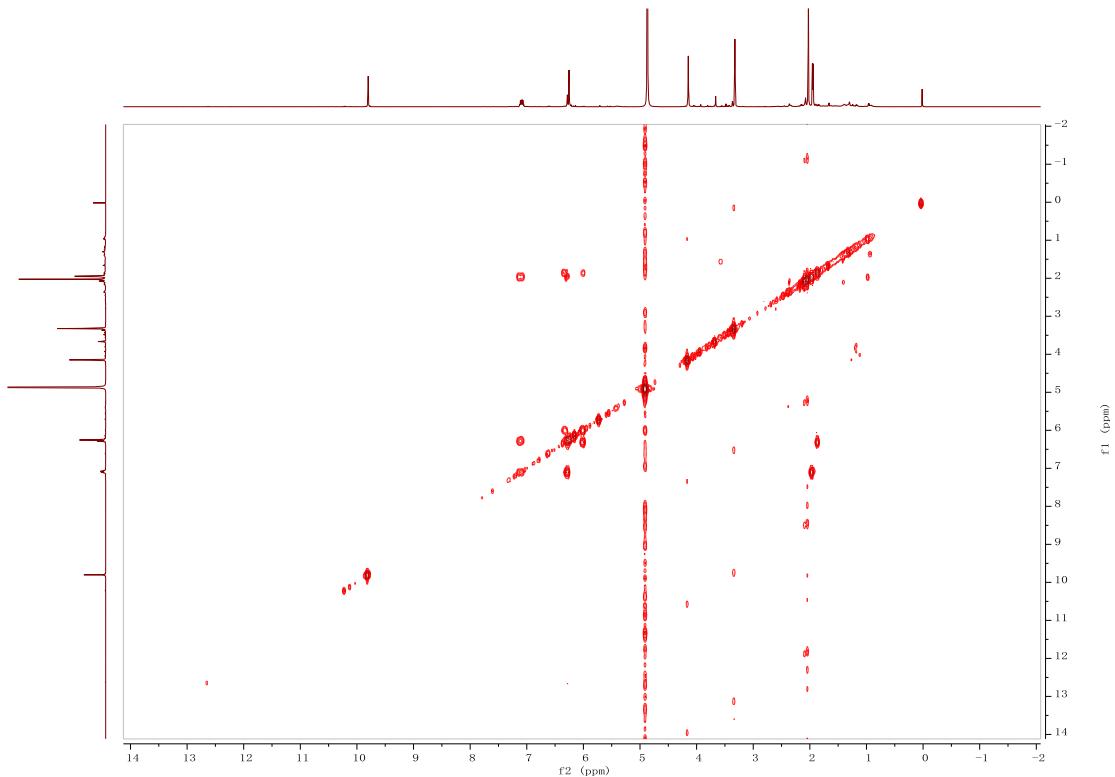


Figure S6. COSY spectrum of **1** (CD_3OD).

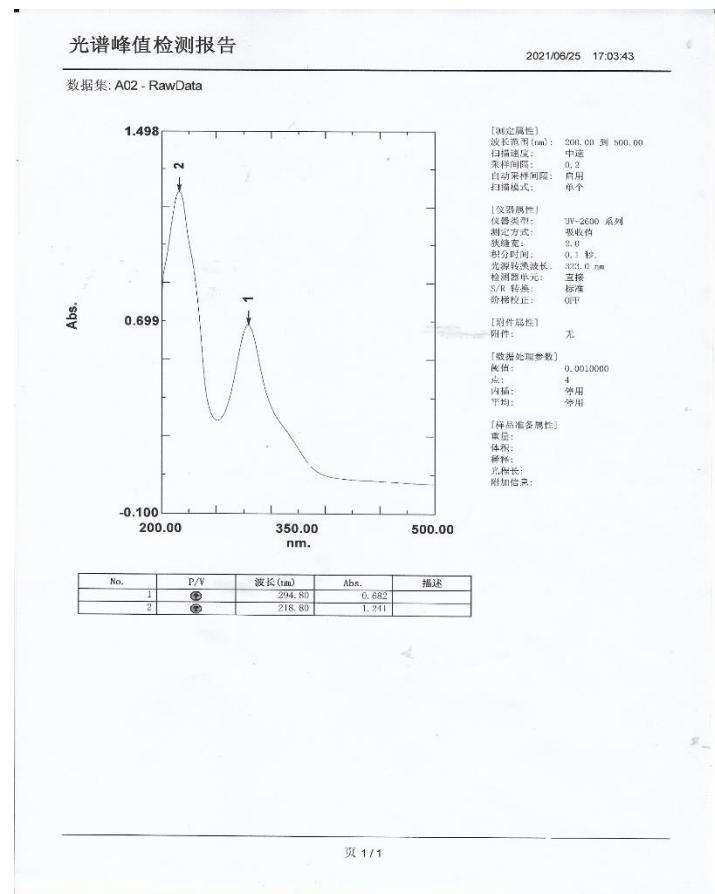


Figure S7. The UV spectrum of **1**.

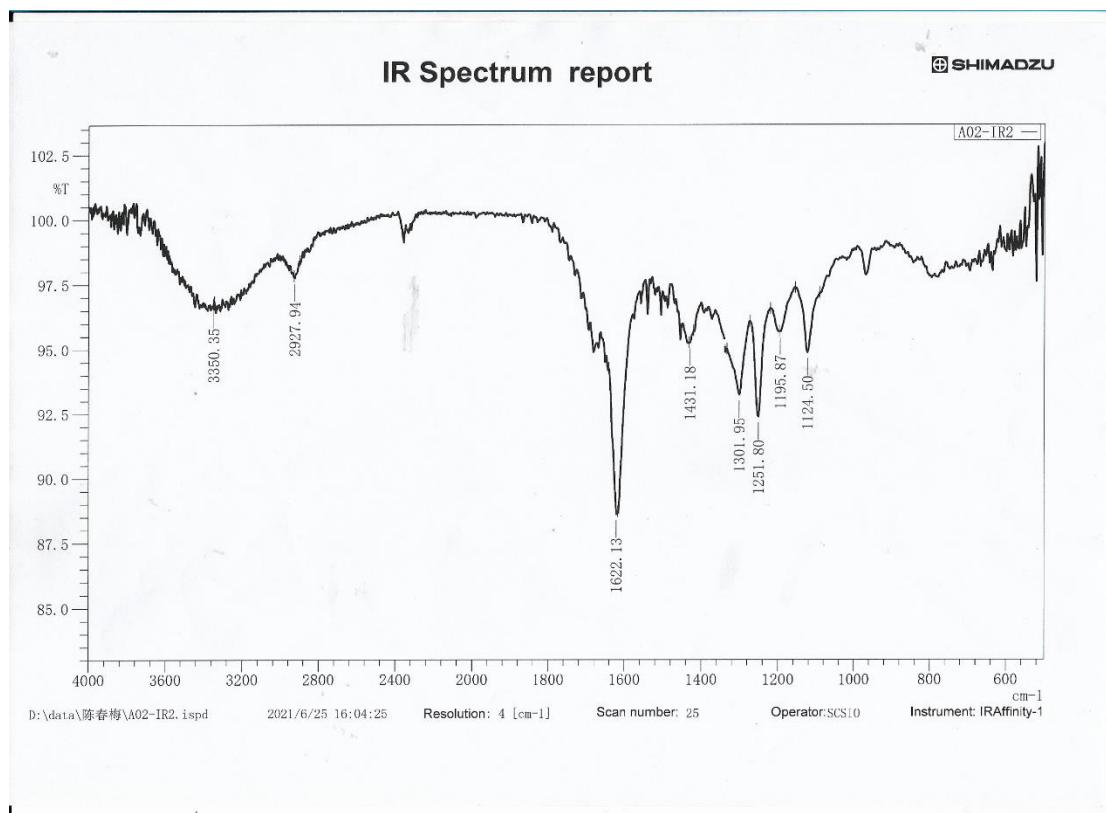


Figure S8. The IR spectrum of **1**.

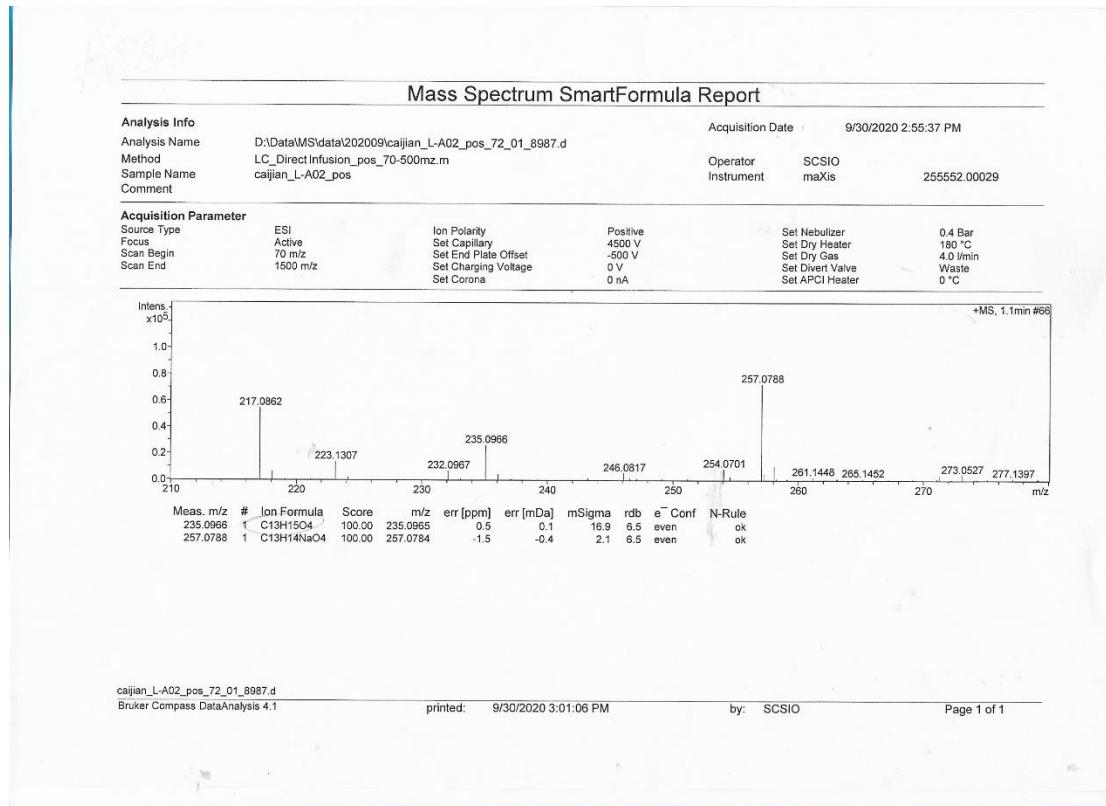


Figure S9. HRESIMS spectrum of compound 1.

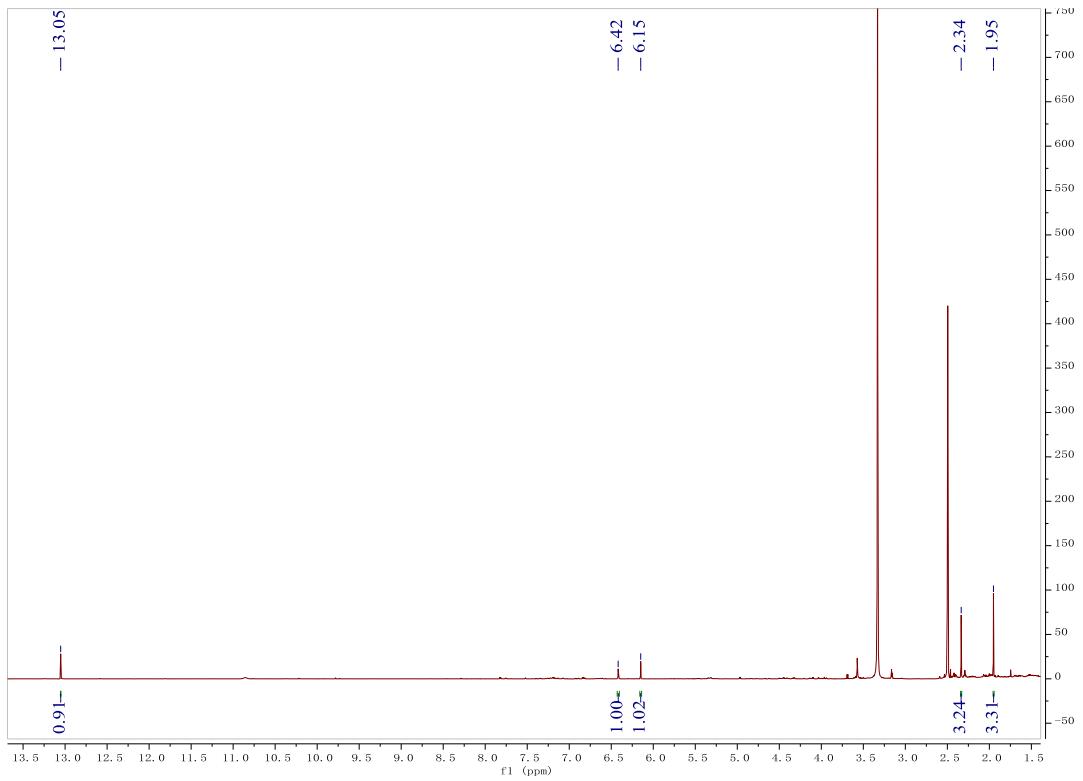


Figure S10. ^1H NMR spectrum of **2** ((DMSO- d_6 , 700 MHz).

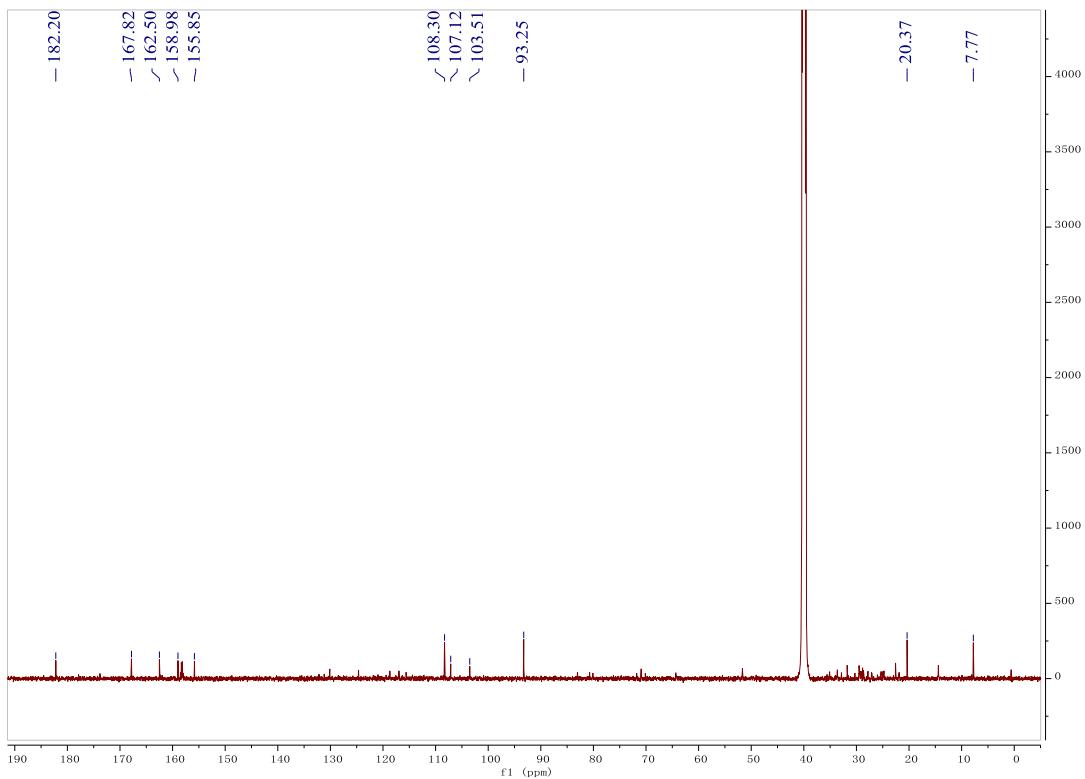


Figure S11. ^{13}C NMR spectrum of **2** ((DMSO- d_6 , 175 MHz).

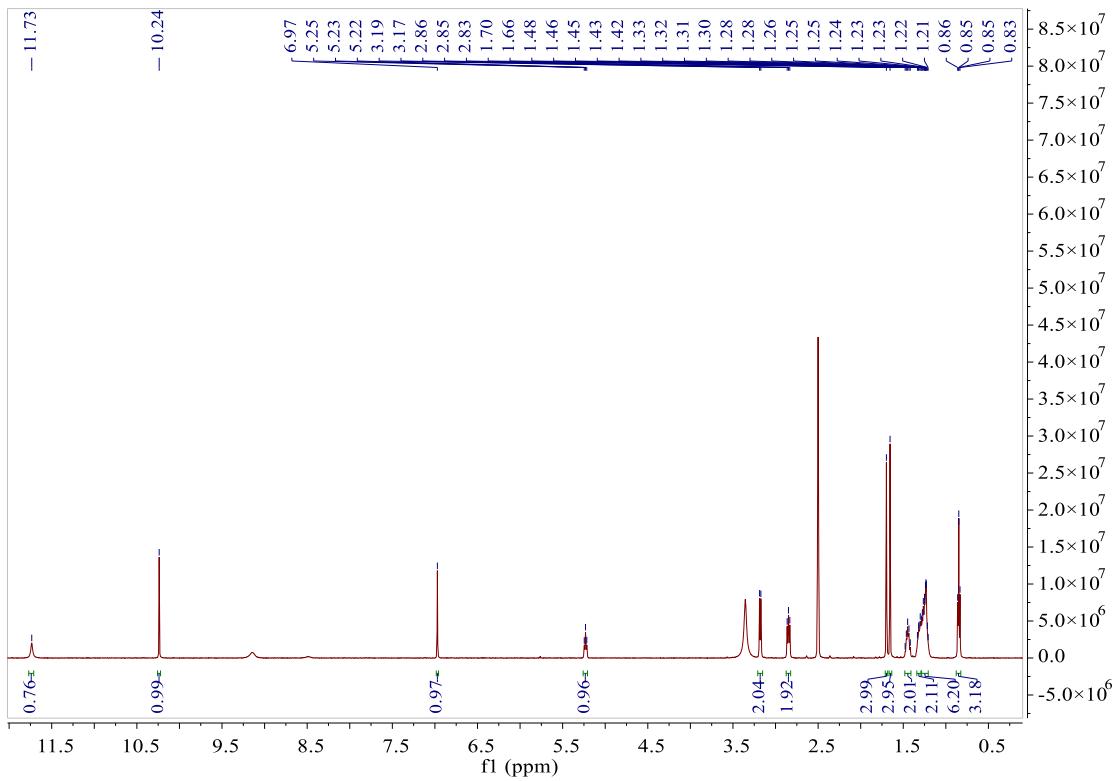


Figure S12. ^1H NMR spectrum of **3** ((DMSO- d_6 , 500 MHz).

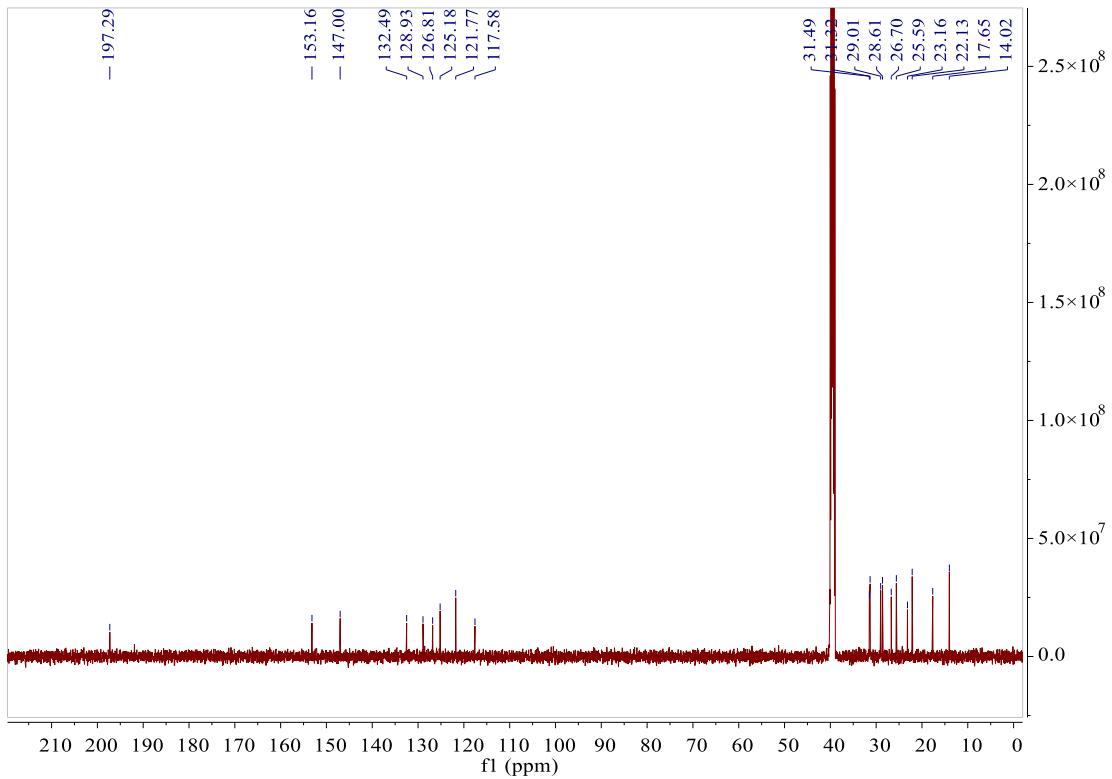


Figure S13. ^{13}C NMR spectrum of **3** ((DMSO- d_6 , 125MHz).

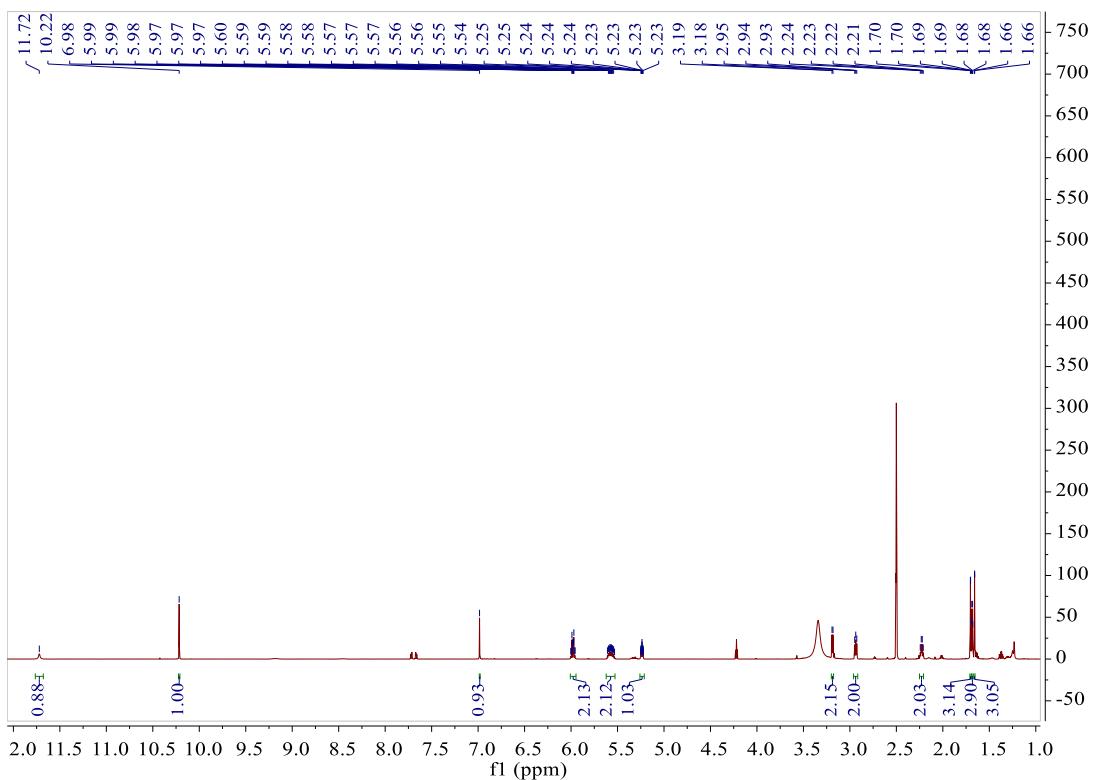


Figure S14. ^1H NMR spectrum of **4** (DMSO- d_6 , 700 MHz).

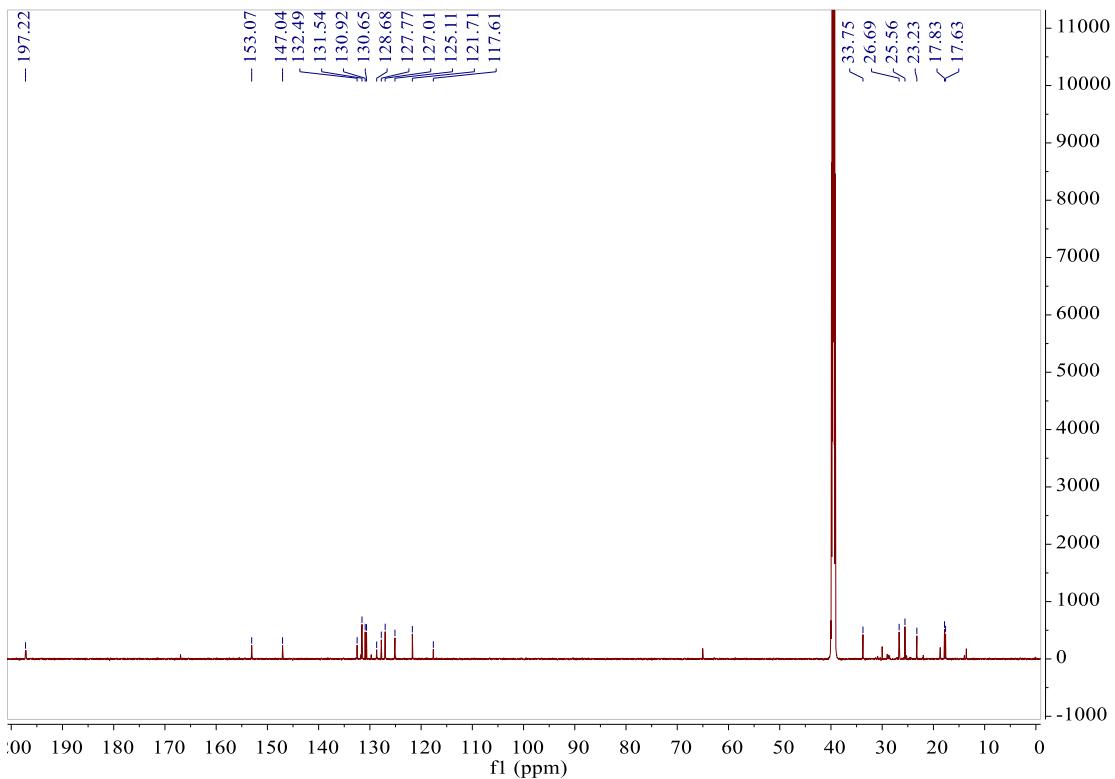


Figure S15. ^{13}C NMR spectrum of **4** (DMSO- d_6 , 175 MHz).

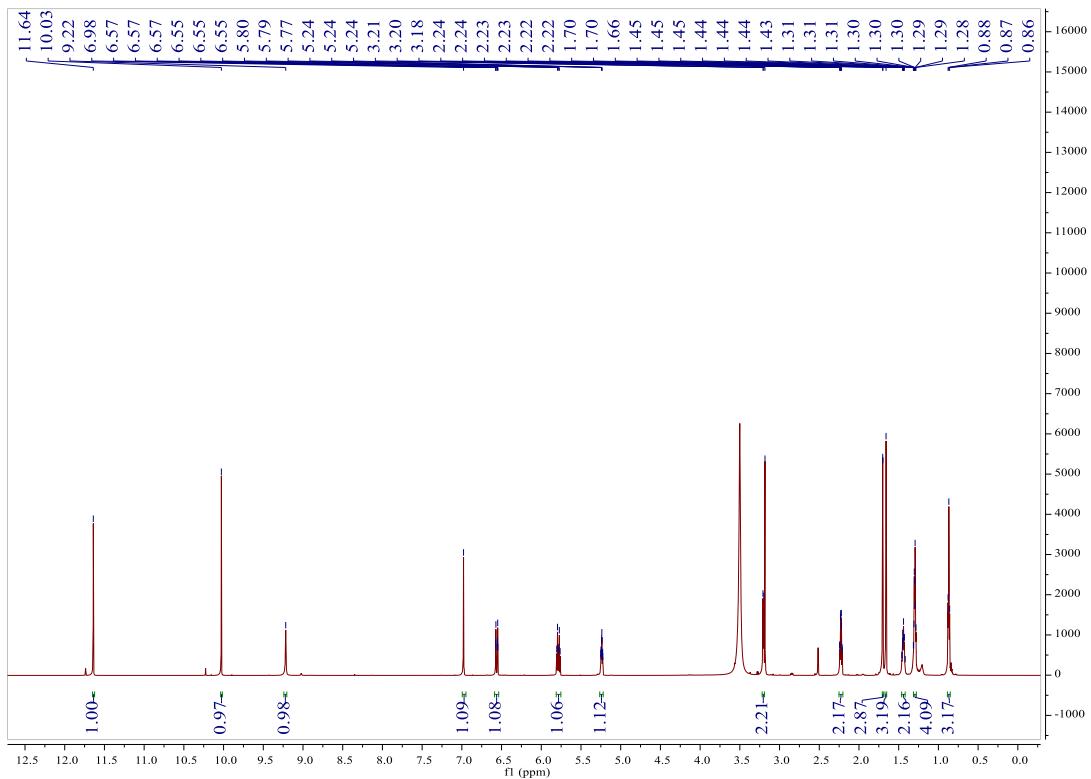


Figure S16. ^1H NMR spectrum of **5** (DMSO- d_6 , 700 MHz).

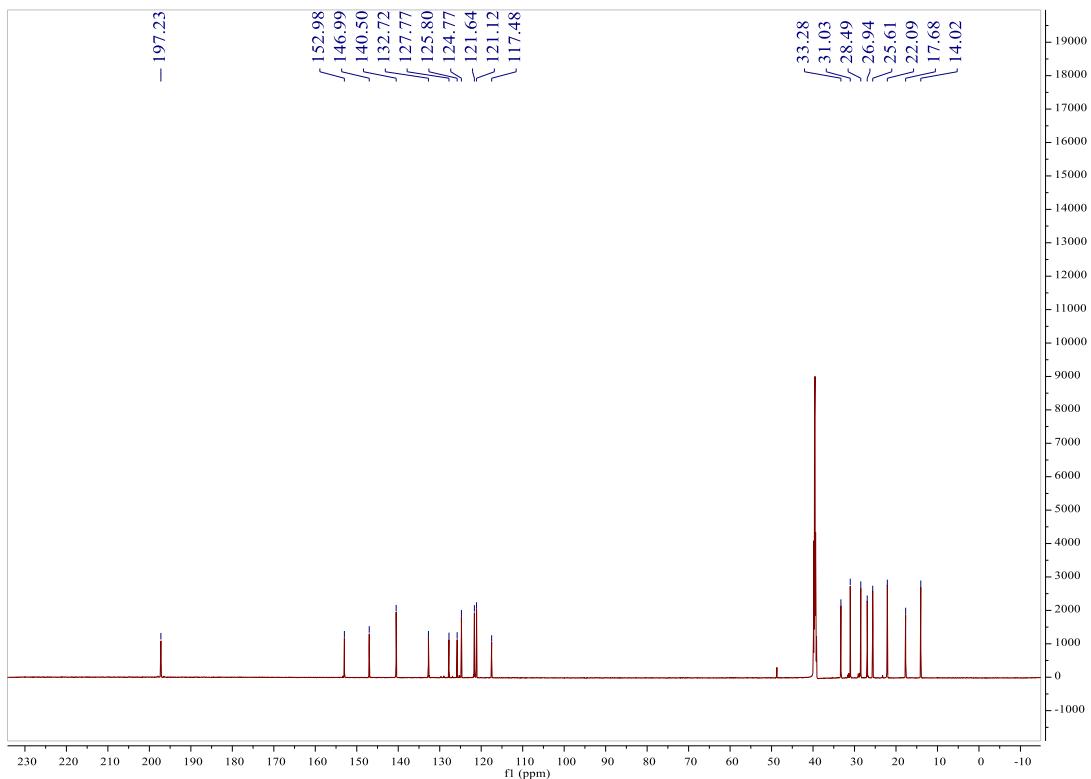


Figure S17. ^{13}C NMR spectrum of **5** (DMSO- d_6 , 175 MHz).

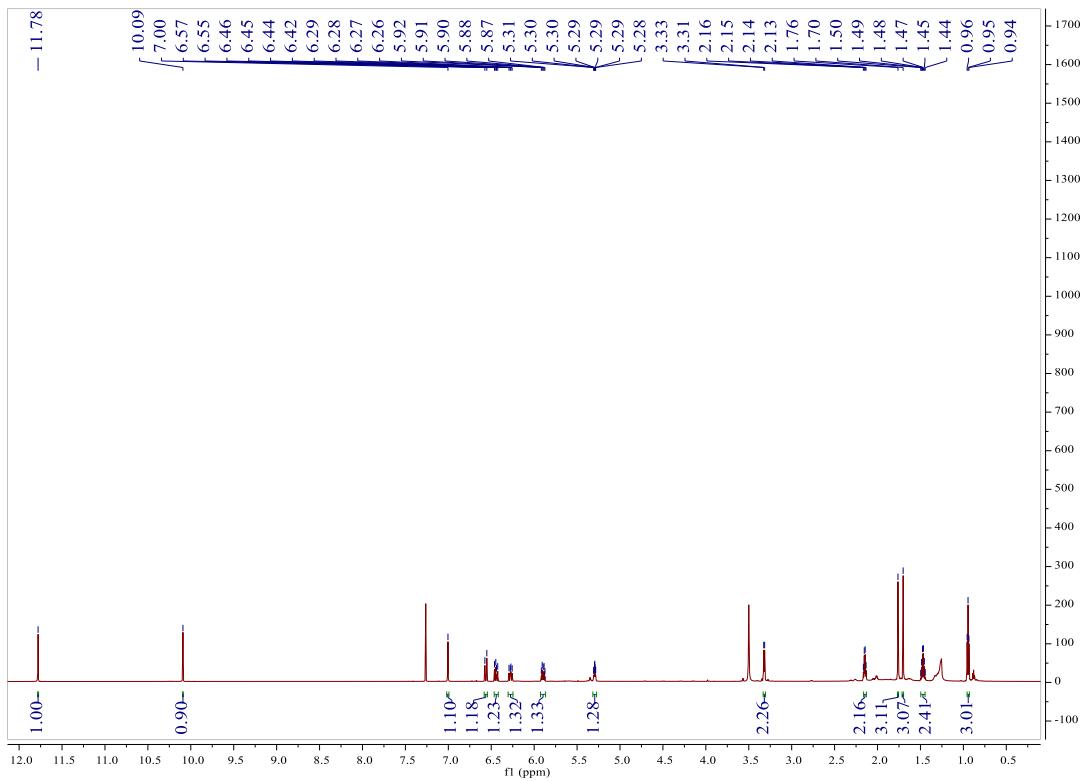


Figure S18. ^1H NMR spectrum of **6** (CDCl_3 , 700 MHz).

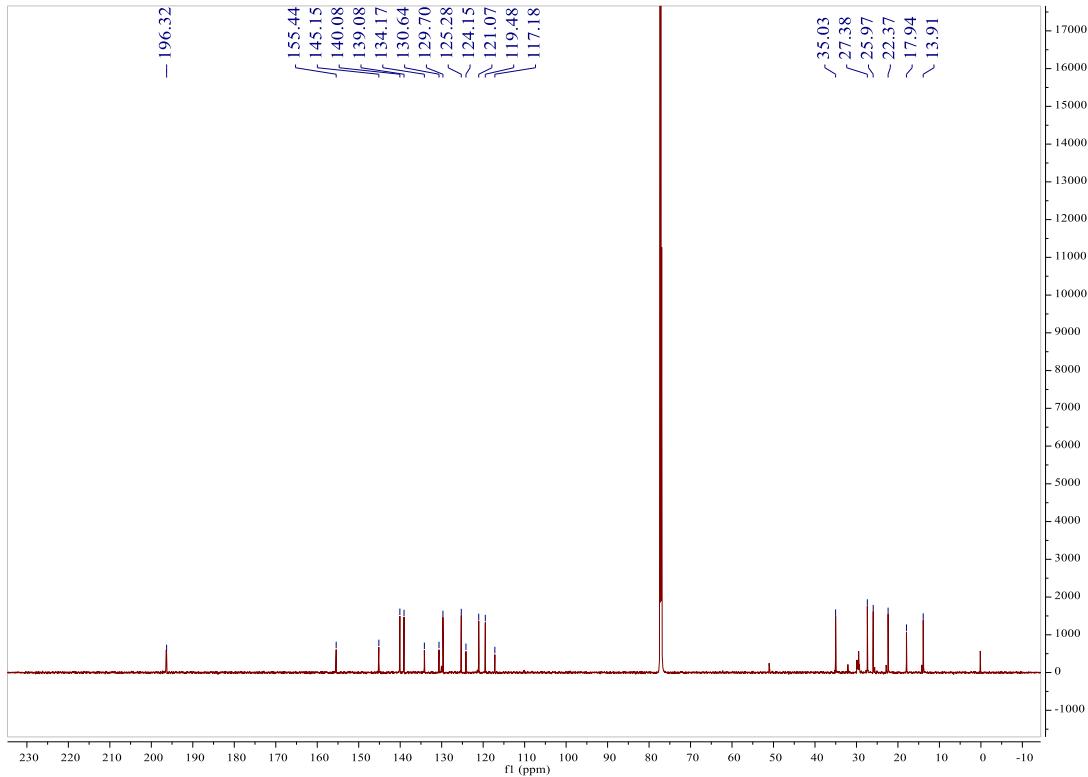


Figure S19. ^{13}C NMR spectrum of **6** CDCl_3 , 175 MHz).

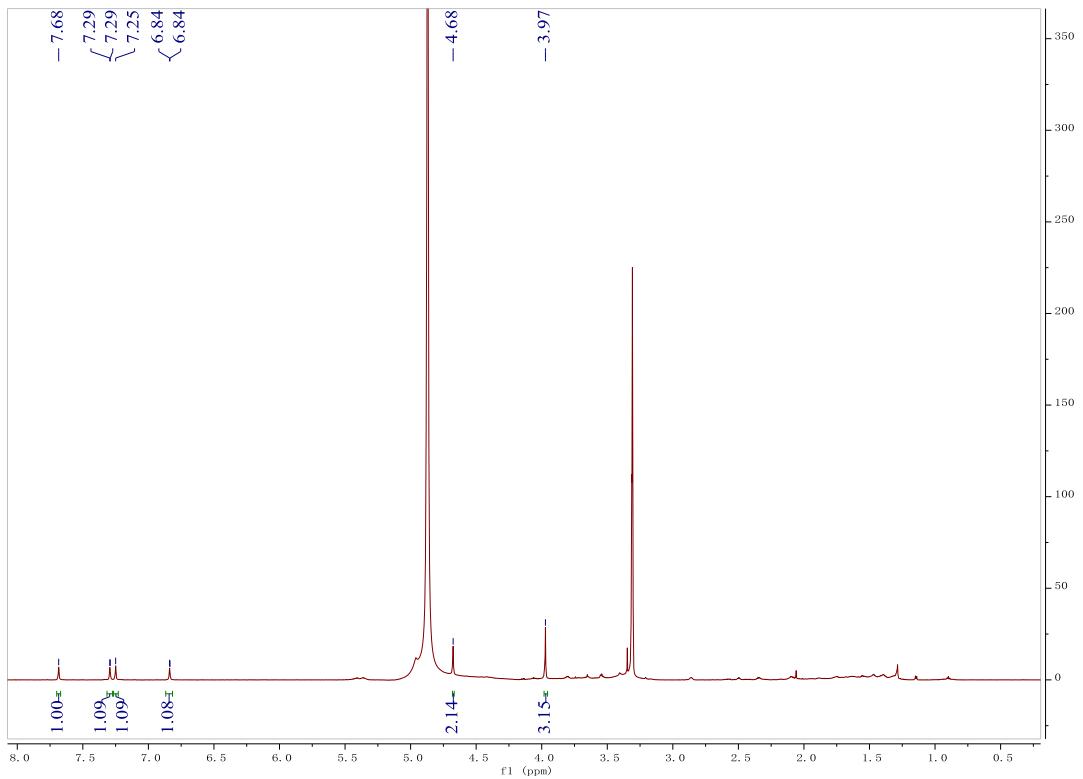


Figure S20. ^1H NMR spectrum of **7** (CD_3OD , 700 MHz).

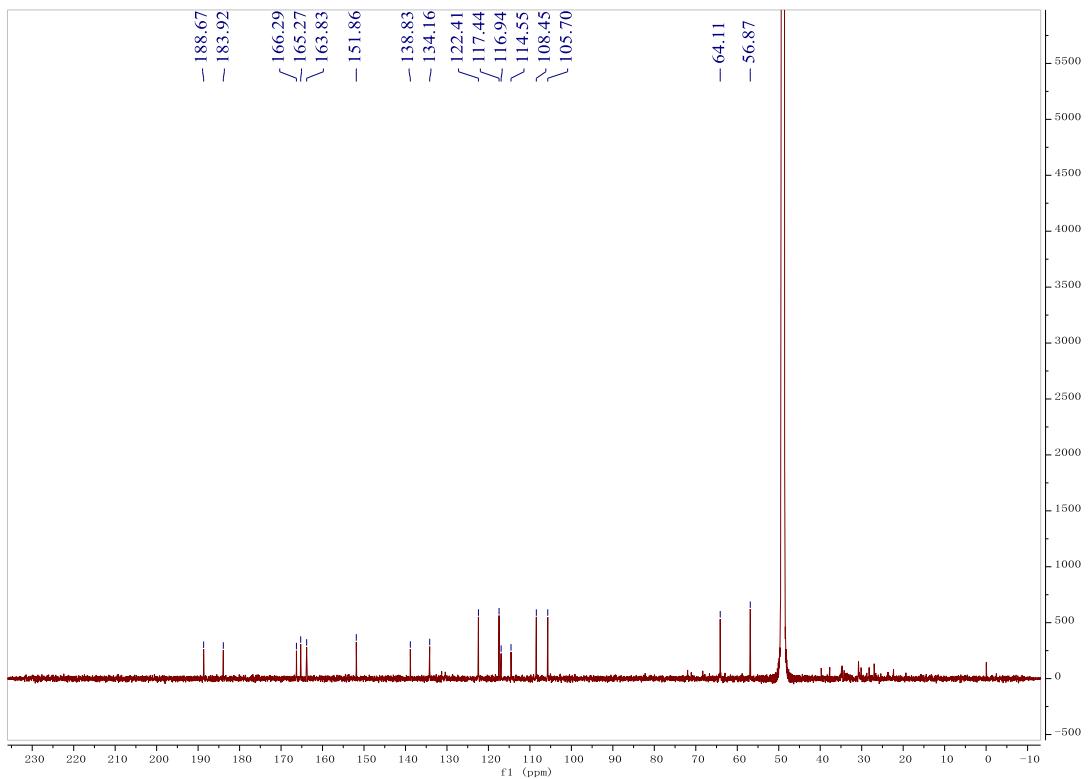


Figure S21. ^{13}C NMR spectrum of **7** (CD_3OD , 175 MHz).

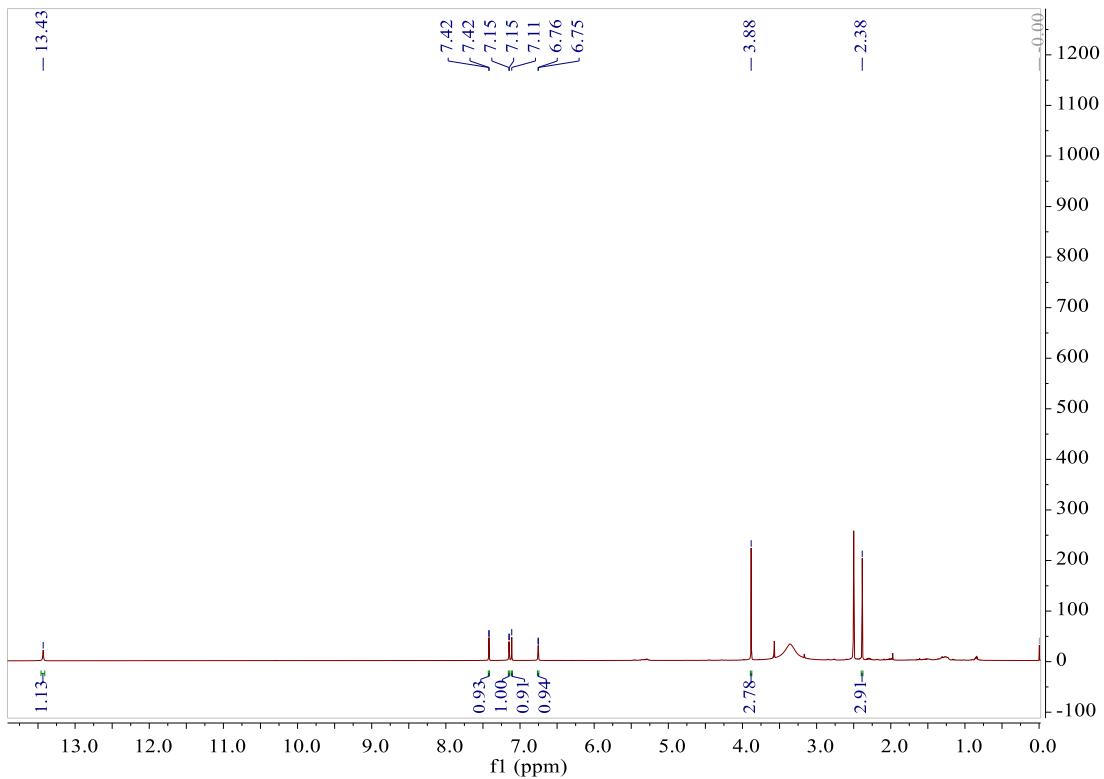


Figure S22. ^1H NMR spectrum of **8** (DMSO- d_6 , 700 MHz).

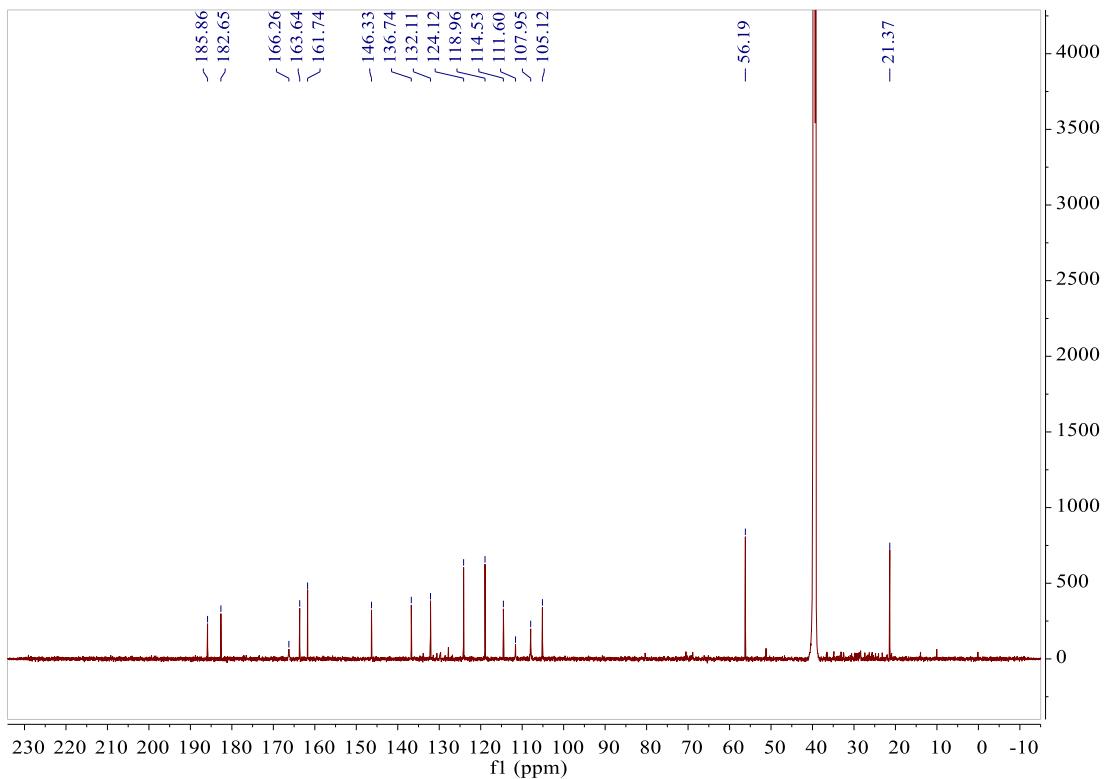


Figure S23. ^{13}C NMR spectrum of **8** (DMSO- d_6 , 175 MHz).

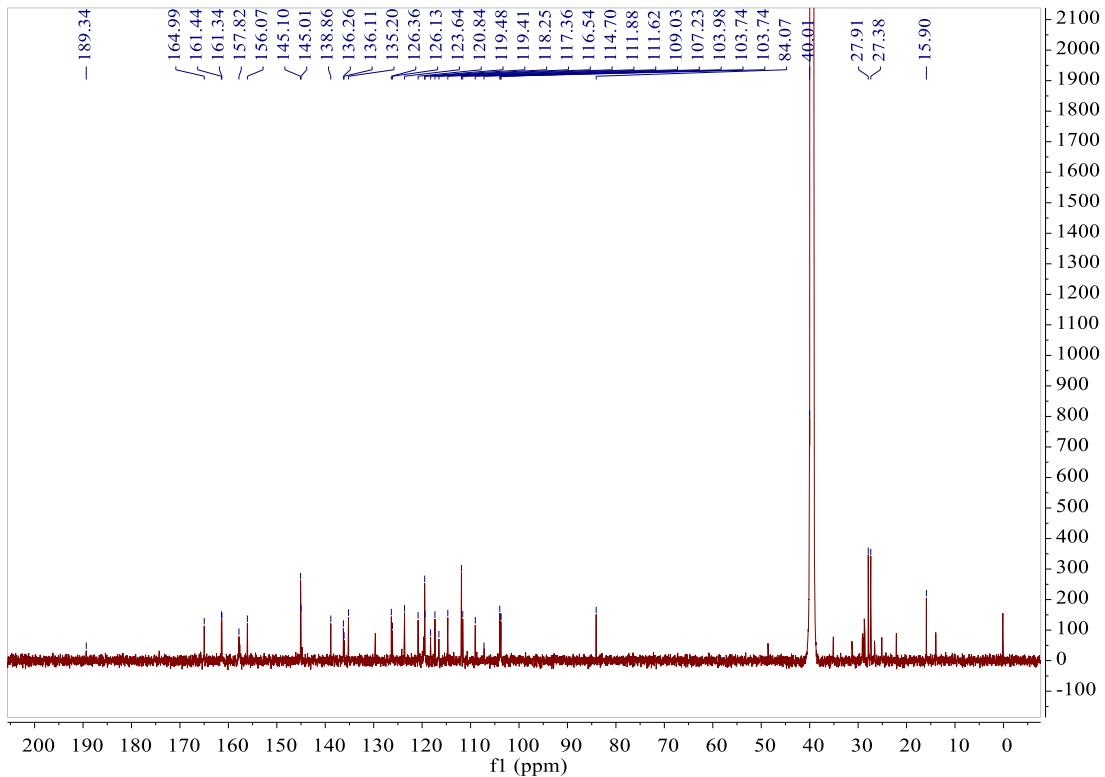
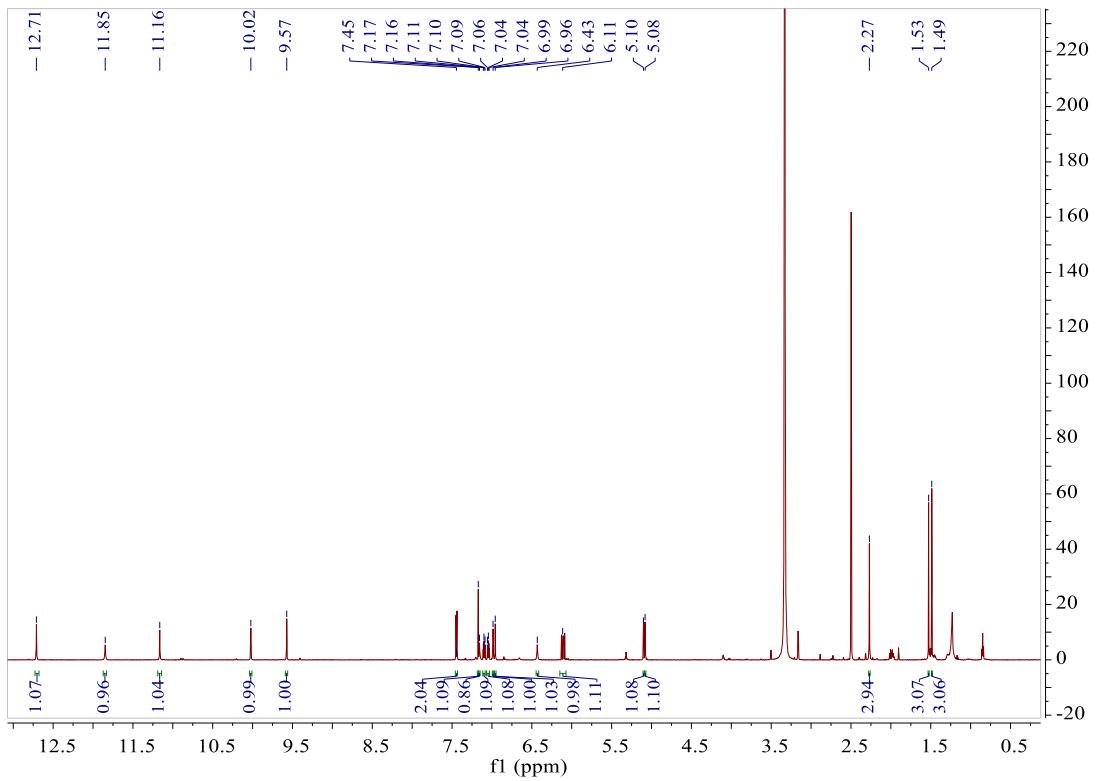


Figure S25. ^{13}C NMR spectrum of **9** (DMSO- d_6 , 175 MHz).

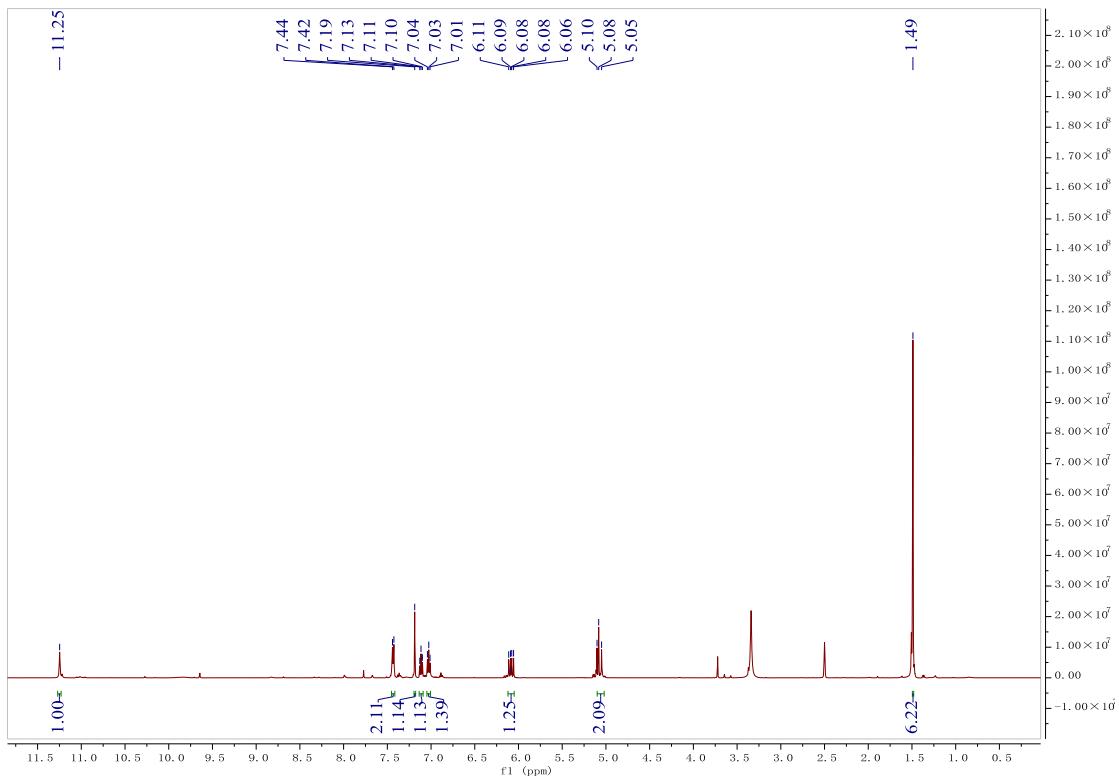


Figure S26. ^1H NMR spectrum of **10** (DMSO- d_6 , 500 MHz).

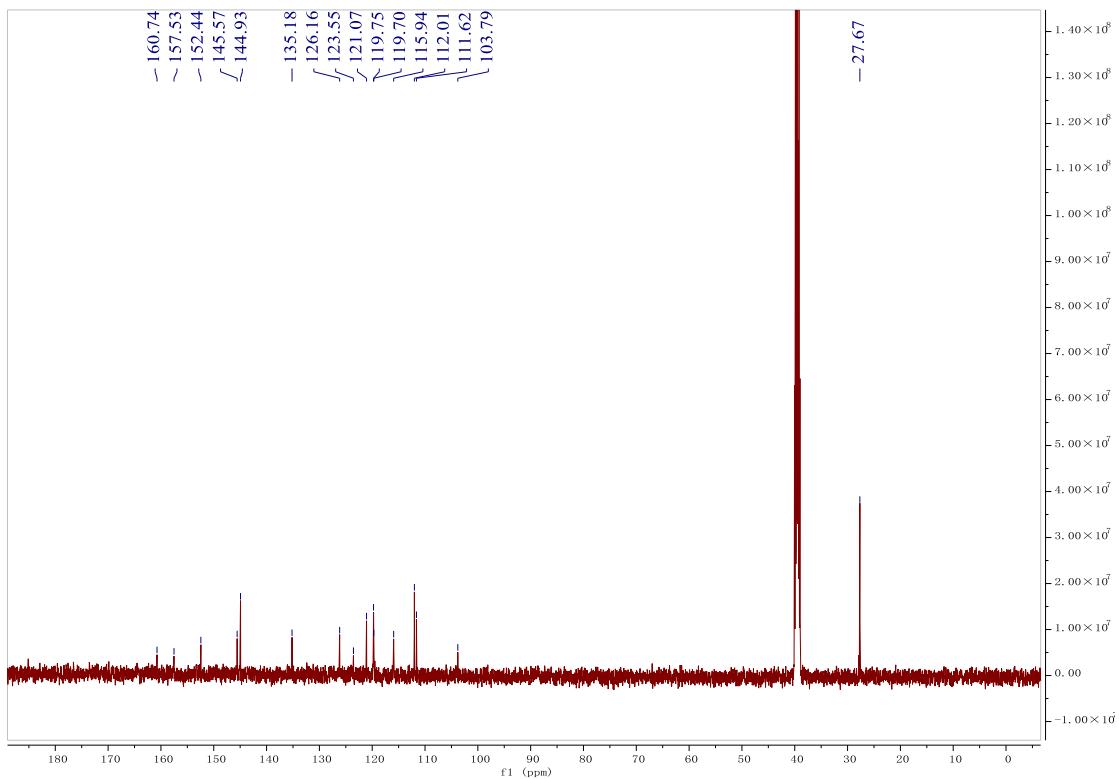


Figure S27. ^{13}C NMR spectrum of **10** (DMSO- d_6 , 125 MHz).

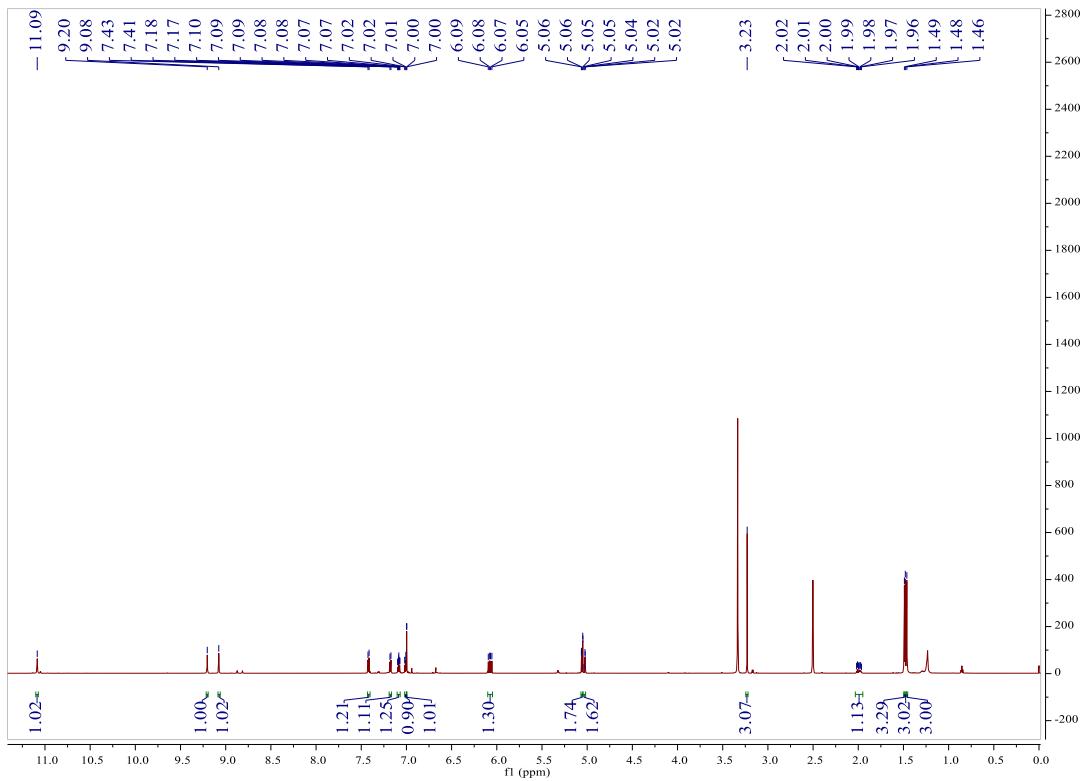


Figure S28. ^1H NMR spectrum of **11** (DMSO- d_6 , 700 MHz).

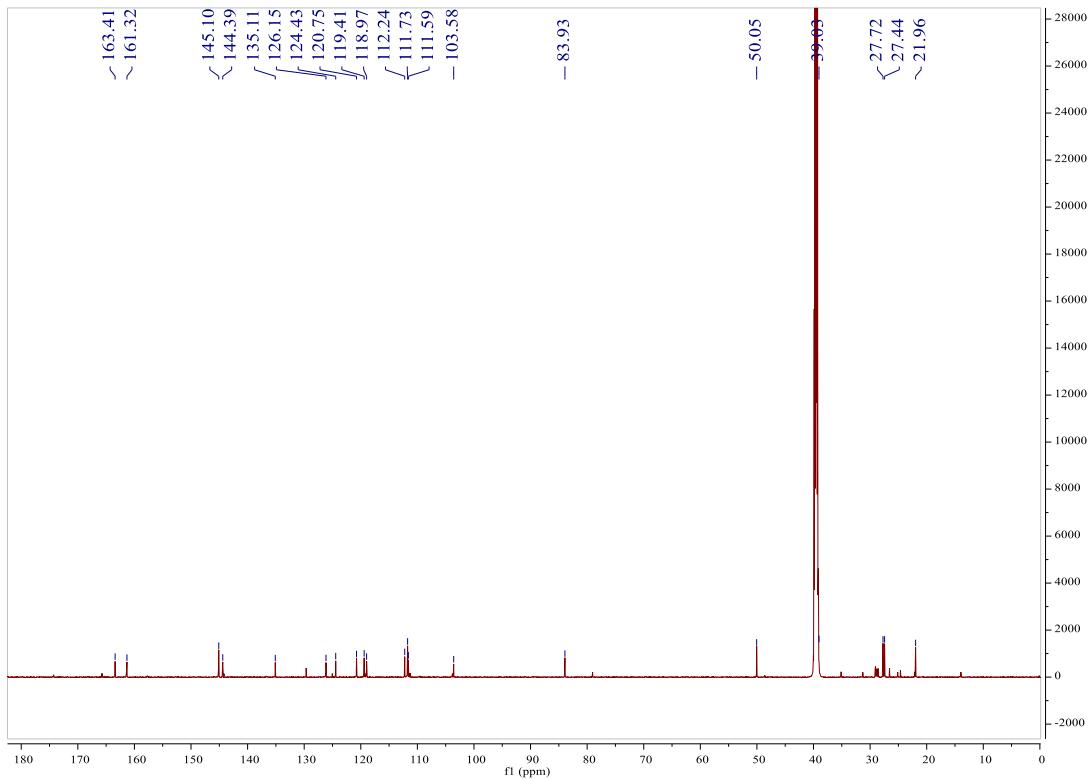


Figure S29. ^{13}C NMR spectrum of **11** (DMSO- d_6 , 175 MHz).

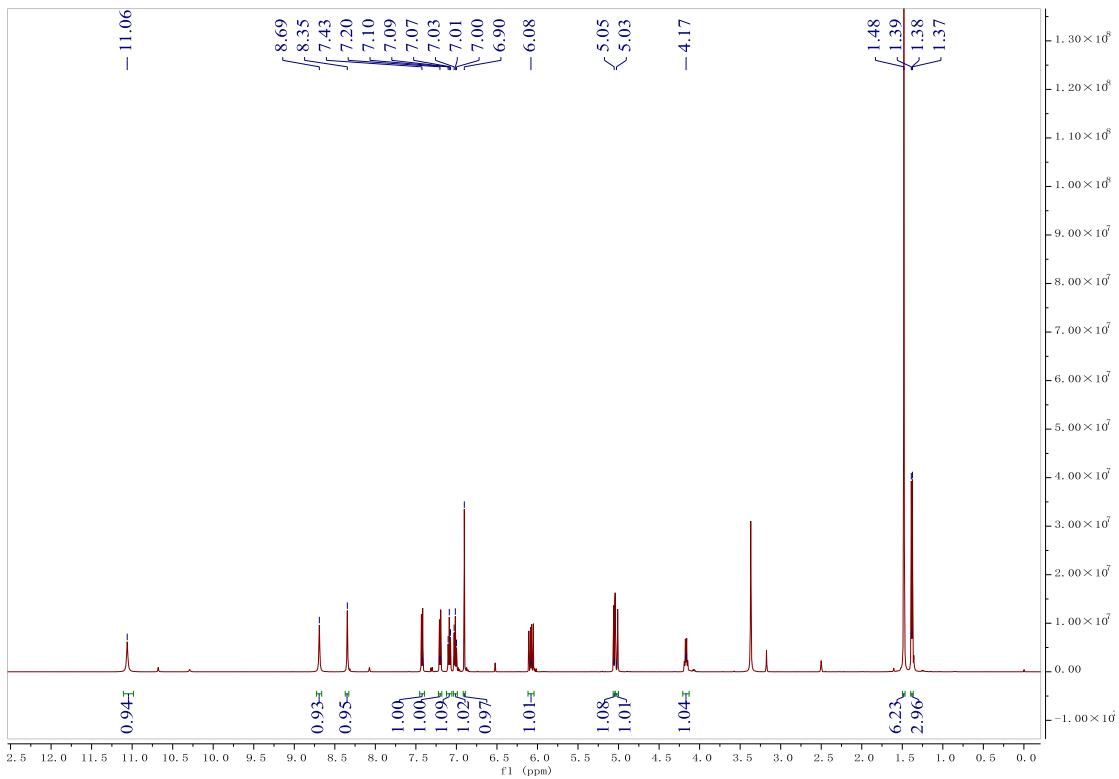


Figure S30. ^1H NMR spectrum of **12** (DMSO- d_6 , 500 MHz).

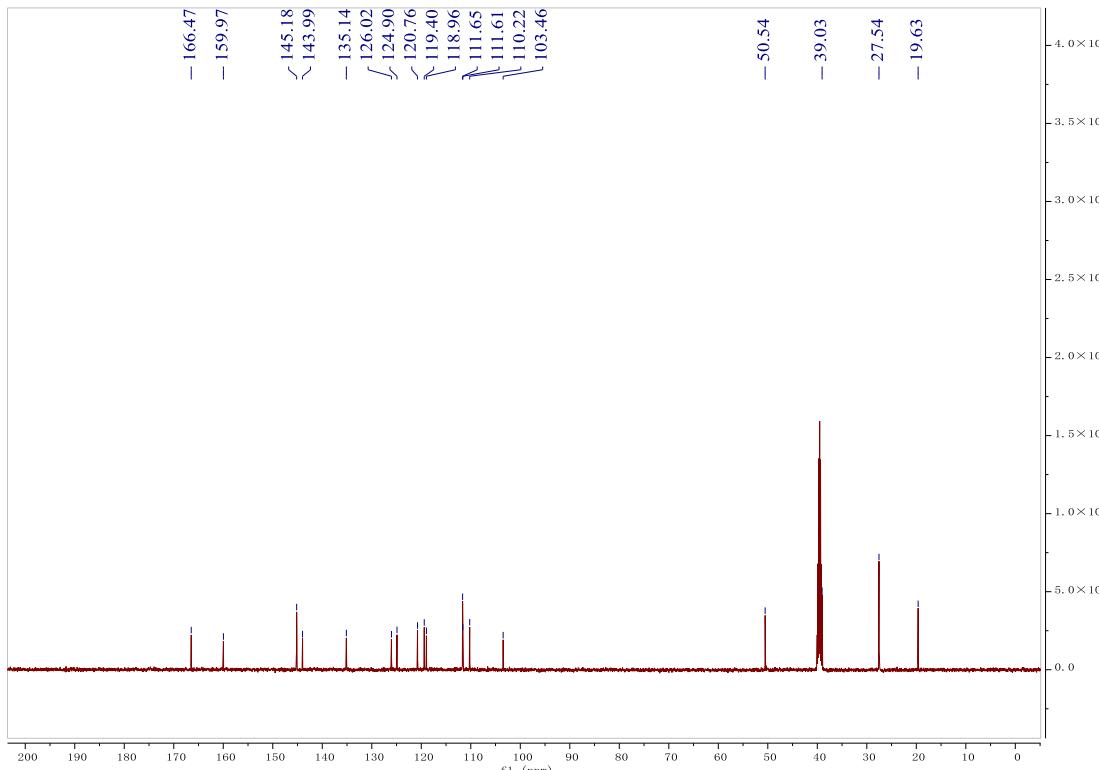


Figure S31. ^{13}C NMR spectrum of **12** (DMSO- d_6 , 125 MHz).

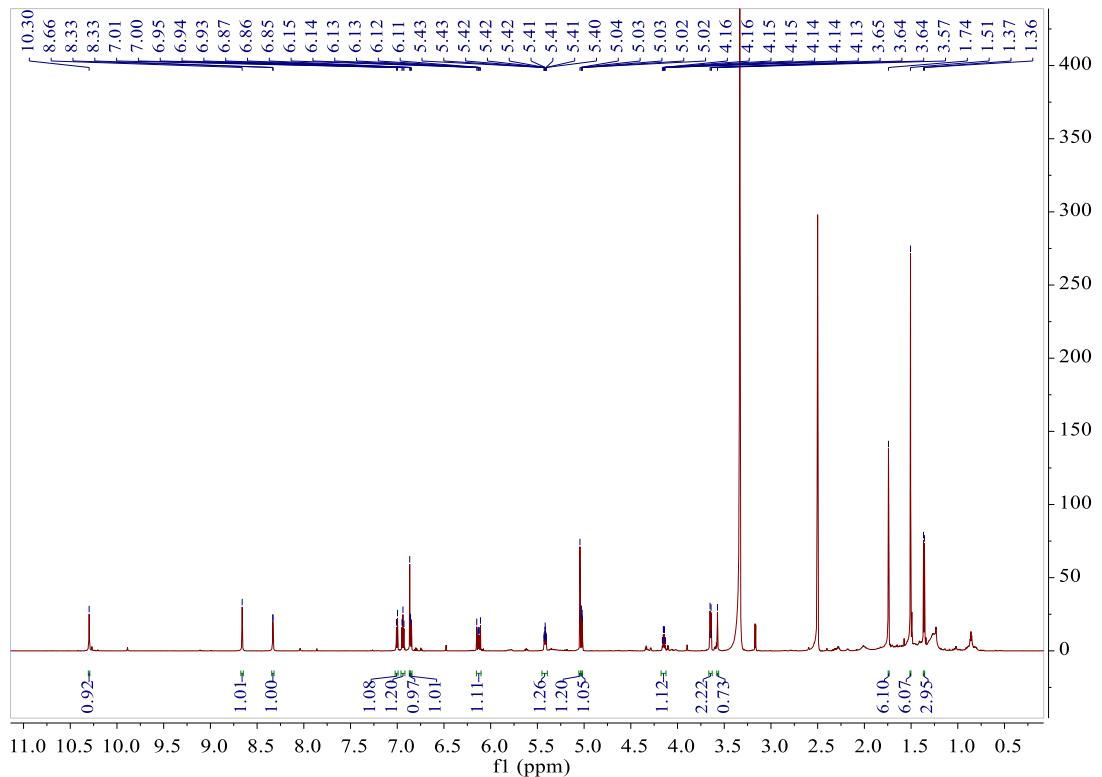


Figure S32. ^1H NMR spectrum of **13** (DMSO- d_6 , 700 MHz).

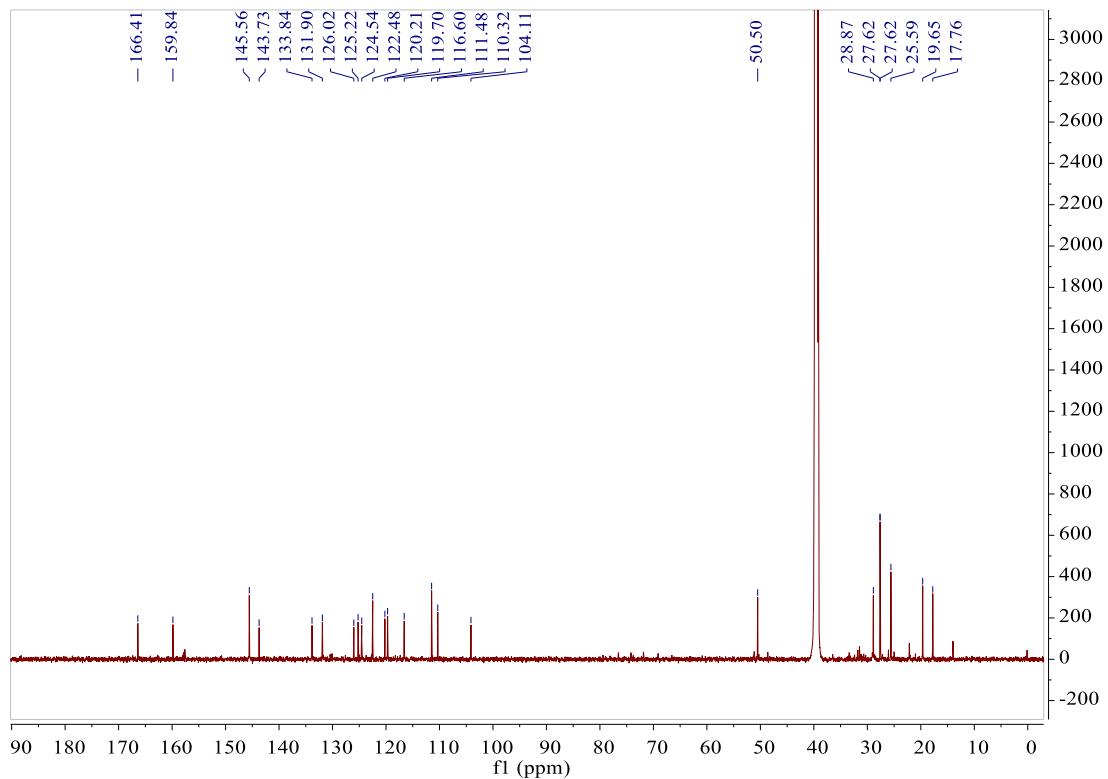


Figure S33. ^{13}C NMR spectrum of **13** (DMSO- d_6 , 175 MHz).

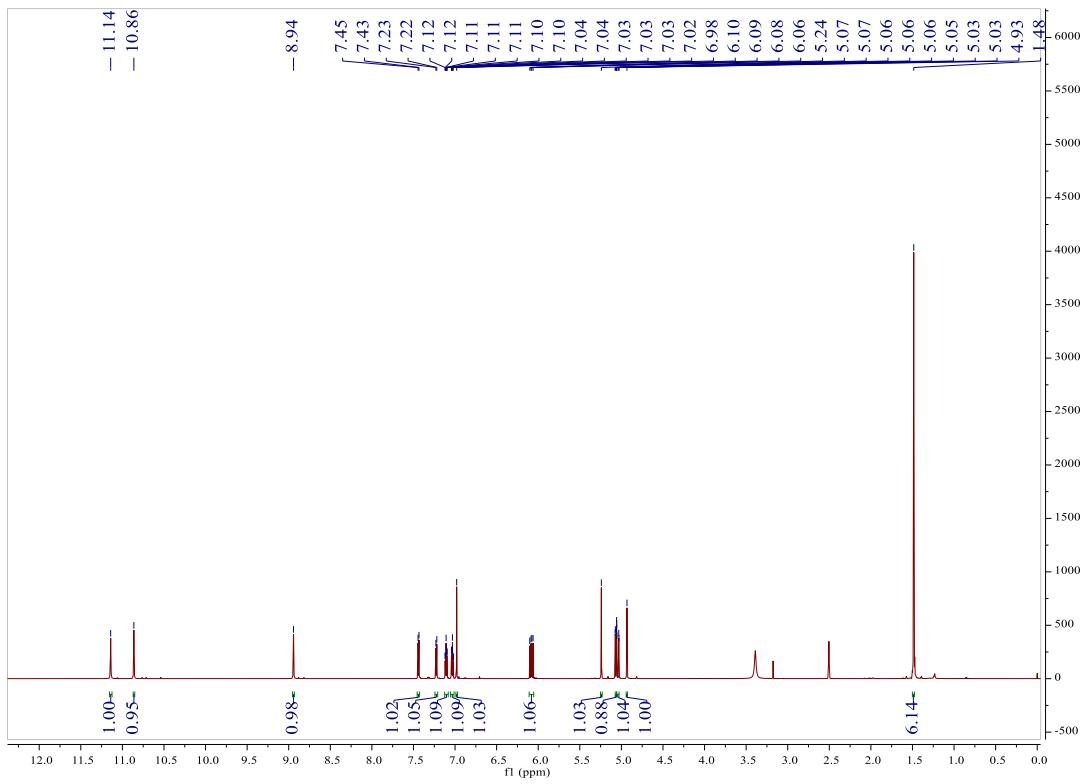


Figure S34. ^1H NMR spectrum of **14** (DMSO- d_6 , 700 MHz).

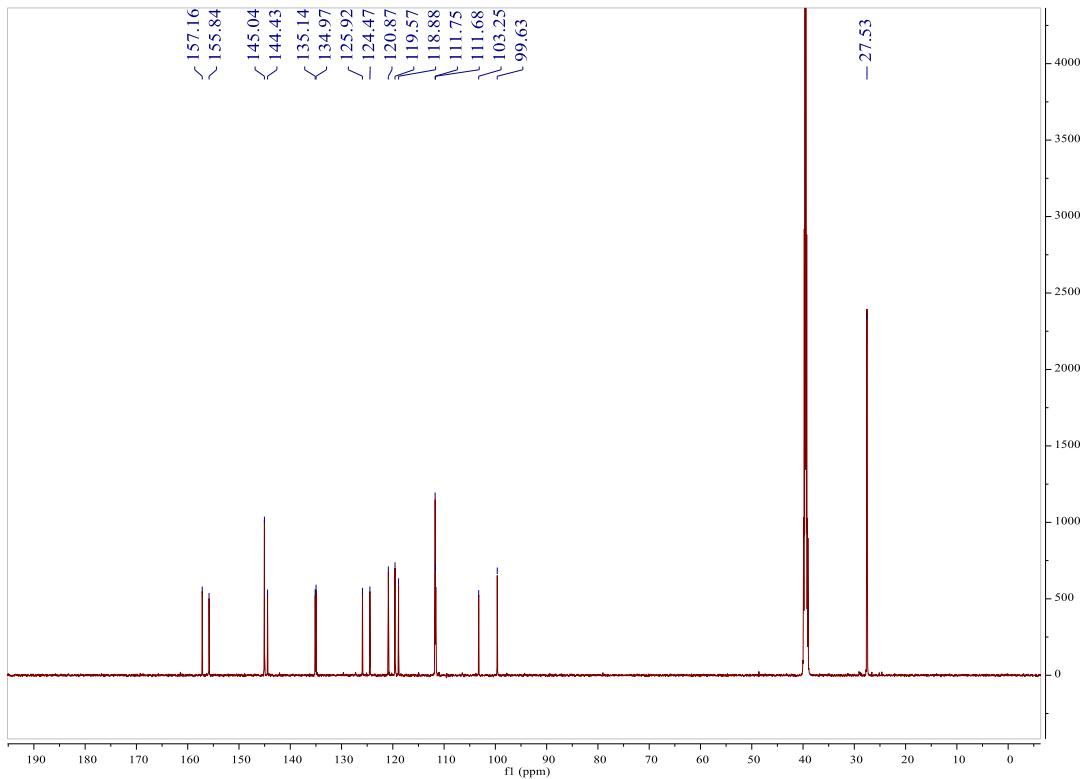
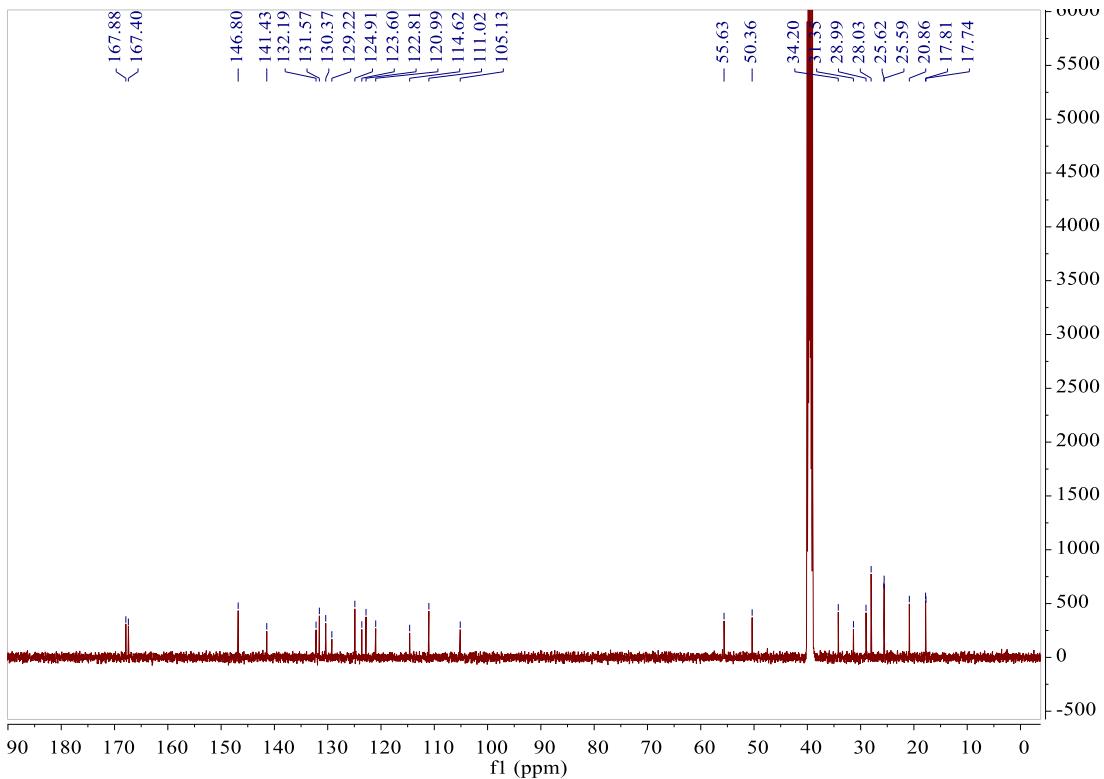
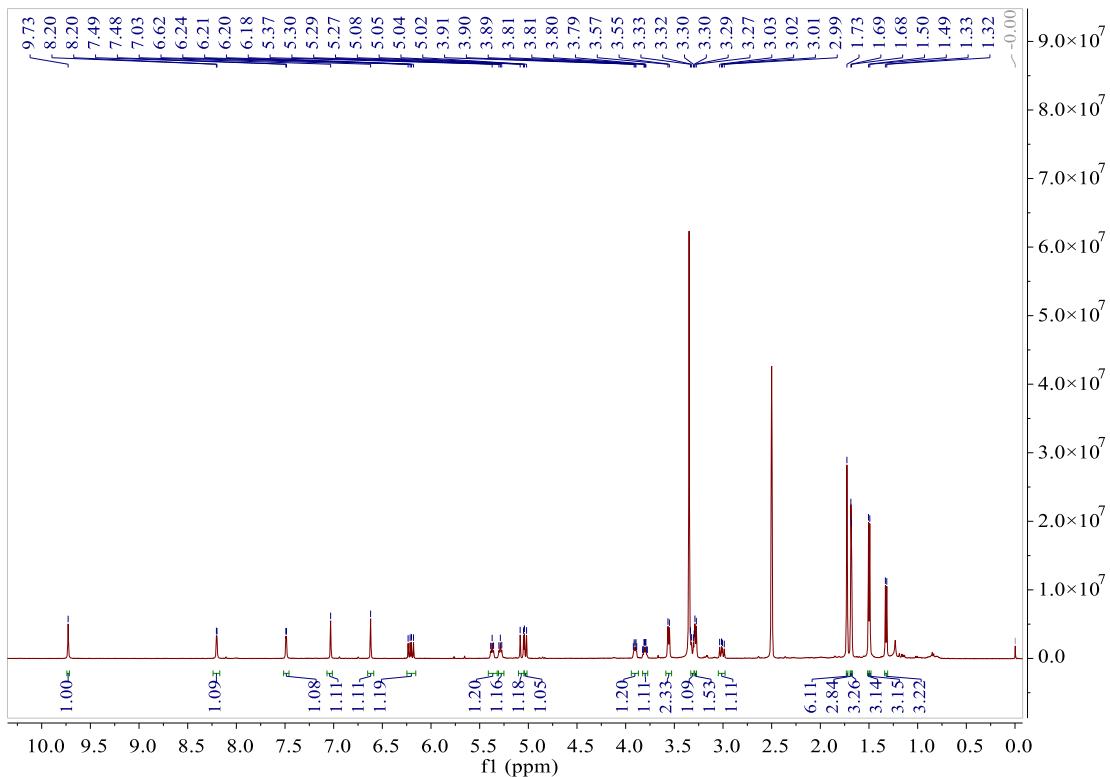


Figure S35. ^{13}C NMR spectrum of **14** (DMSO- d_6 , 175 MHz).



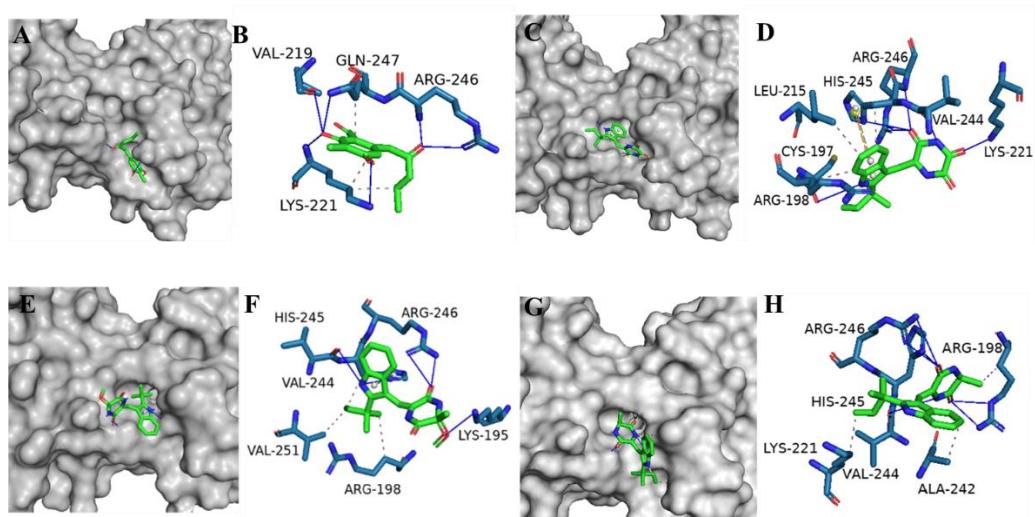


Figure S38. Molecular docking of **1**, **10**, **11**, and **12** with NF- κ B p65. Binding sites of **1** (A), **10** (C), **11** (E), and **12** (G) with NF- κ B p65. 3D diagram of the binding interactions of **1** (B), **10** (D), **11** (F), and **12** (H) with the active site residues of the NF- κ B p65 receptor. Blue solid line: hydrogen bond; grey dotted line: hydrophobic interaction; green dotted line: π - π stacking interaction; orange dotted line: π -cation interaction.

ITS sequence of the strain *Aspergillus* sp. SCSIO41407.

GTACCCCTGTTGCTTCGGCGTGGGCCACGGCCCGCCGGAGACTAACATTGAACGGCTGTCT
 GAAGTTGCAGTCTGAGTTTAGTTAAACAATCGTAAACACTTCAACAACGGATCTC
 TTGGTCCGGCATCGATGAAGAACGCAGCGAAATGCGATAATTAAATGTGAATTGCAGAA
 TTCAGTGAATCATCGAGTCTTGACCGCACATTGCGCCCCCTGGTATTCCGGGGGGCAT
 GCCTGTCCGAGCGTCATTGCTGCCCTCAAGCACGGCTTGTGTGGCTTCCGTCCCT
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 TTAACCAGGTTGACCTCGGATCAGGTAGGGATAACCGCT