

Supporting Information

New Sesquiterpenoids from the Mangrove-Derived Fungus *Talaromyces* sp. as Modulators of Nuclear Receptors

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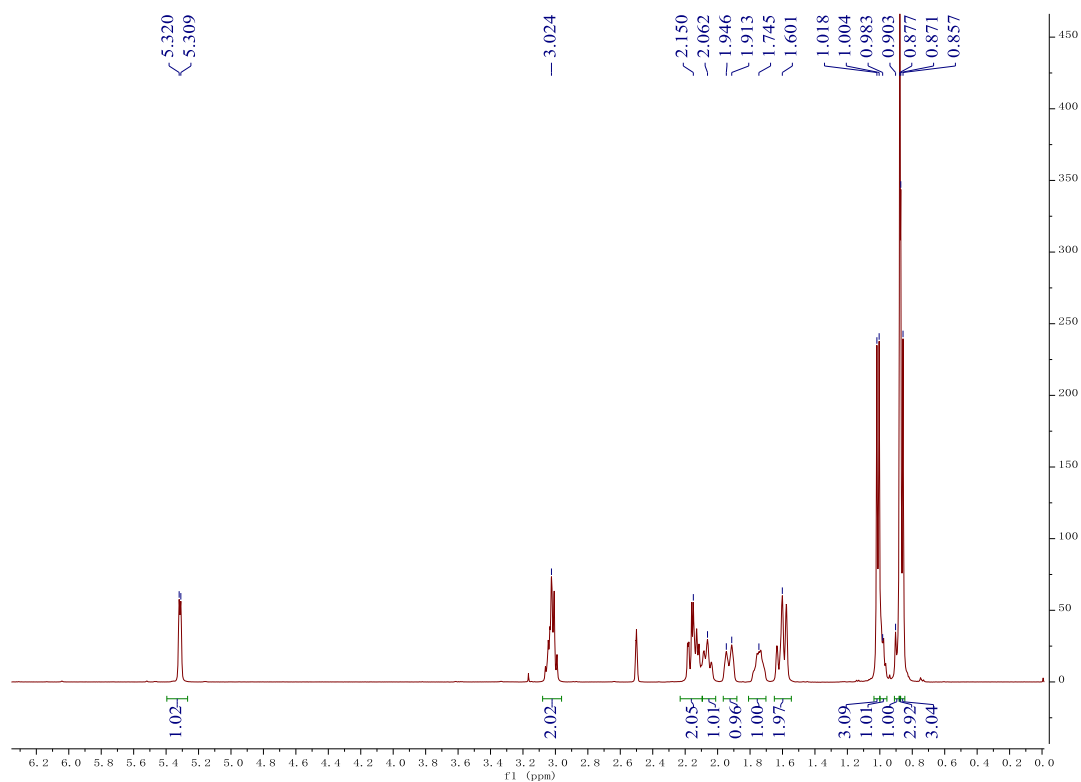


Figure S1. ^1H NMR (500 MHz) spectrum of **1** in $\text{DMSO-}d_6$.

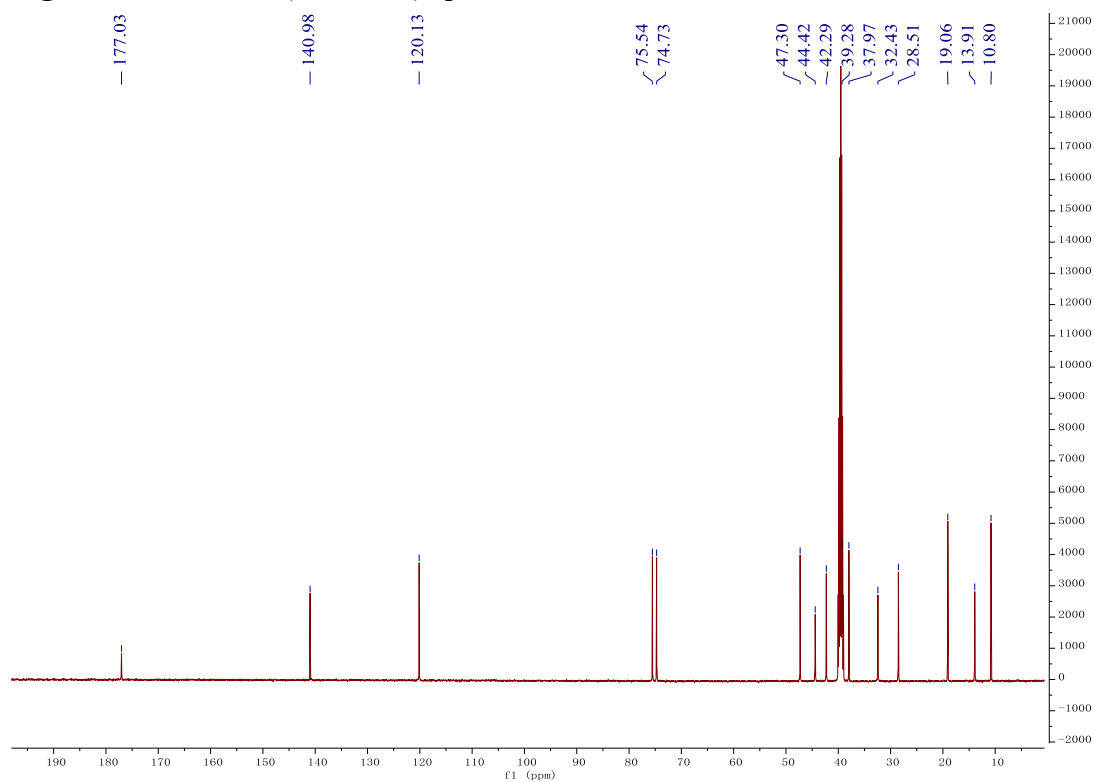


Figure S2. ^{13}C NMR (125 MHz) spectrum of **1** in $\text{DMSO-}d_6$.

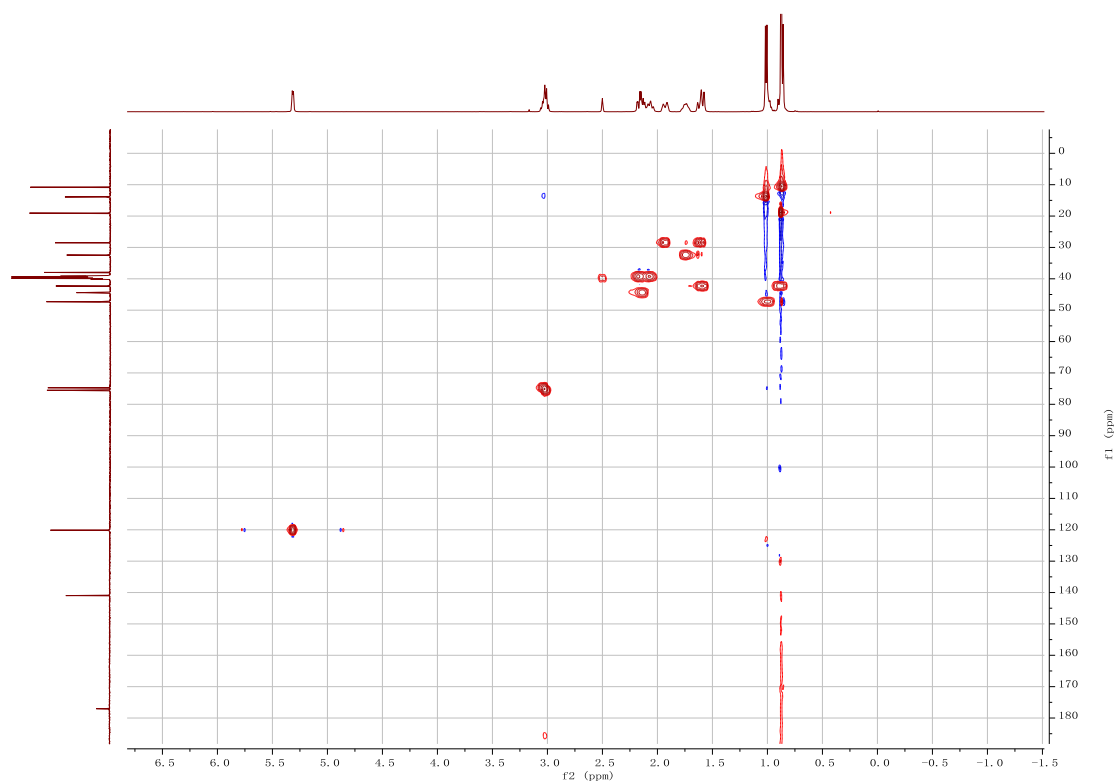


Figure S3. HSQC spectrum of **1** in DMSO- d_6 .



Figure S4. HMBC spectrum of **1** in DMSO- d_6 .

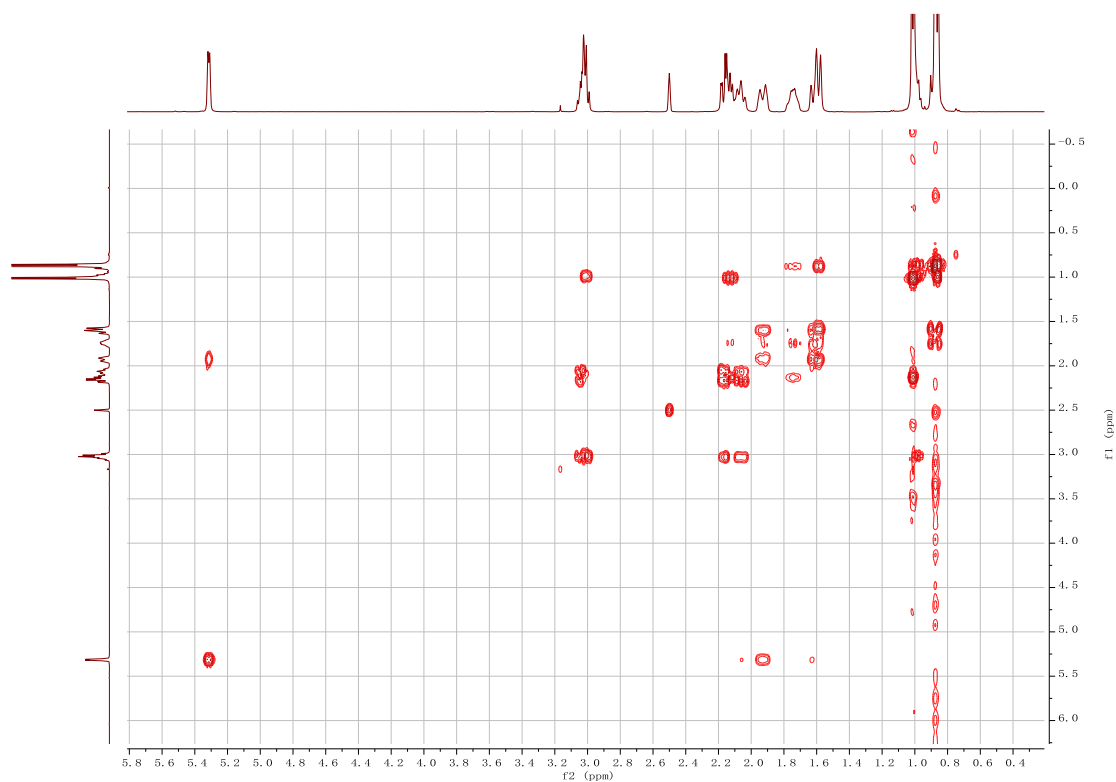


Figure S5. ^1H – ^1H COSY spectrum of **1** in $\text{DMSO-}d_6$.

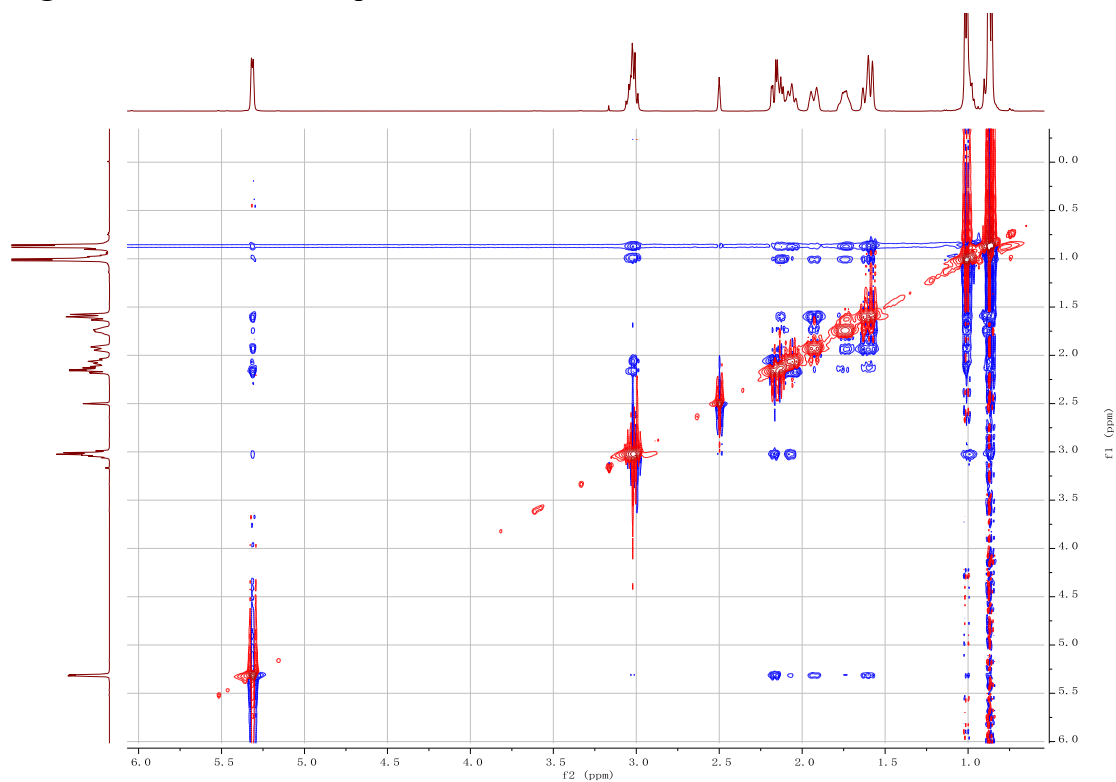


Figure S6. NOESY spectrum of **1** in $\text{DMSO-}d_6$.

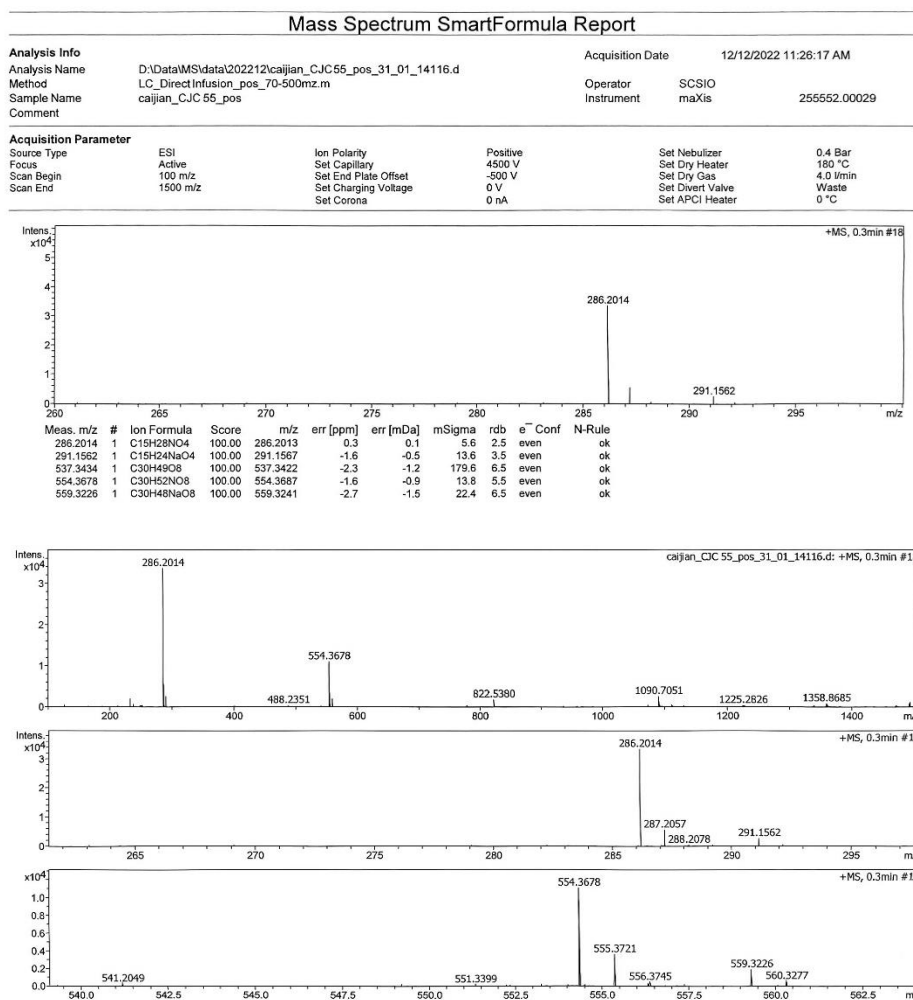


Figure S7. HRESIMS spectrum of **1**.

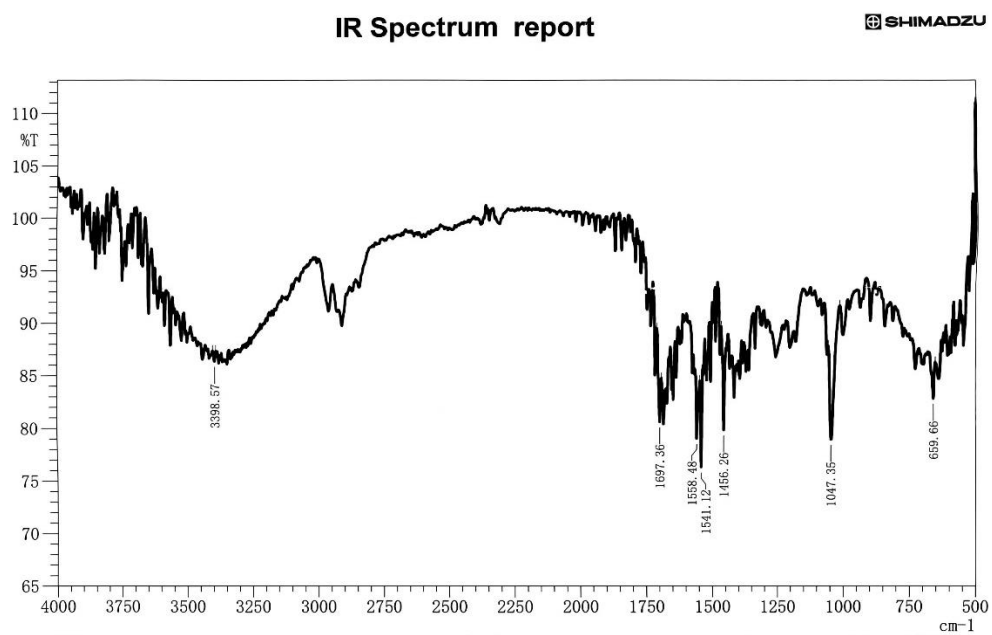


Figure S8. IR spectrum of **1**.

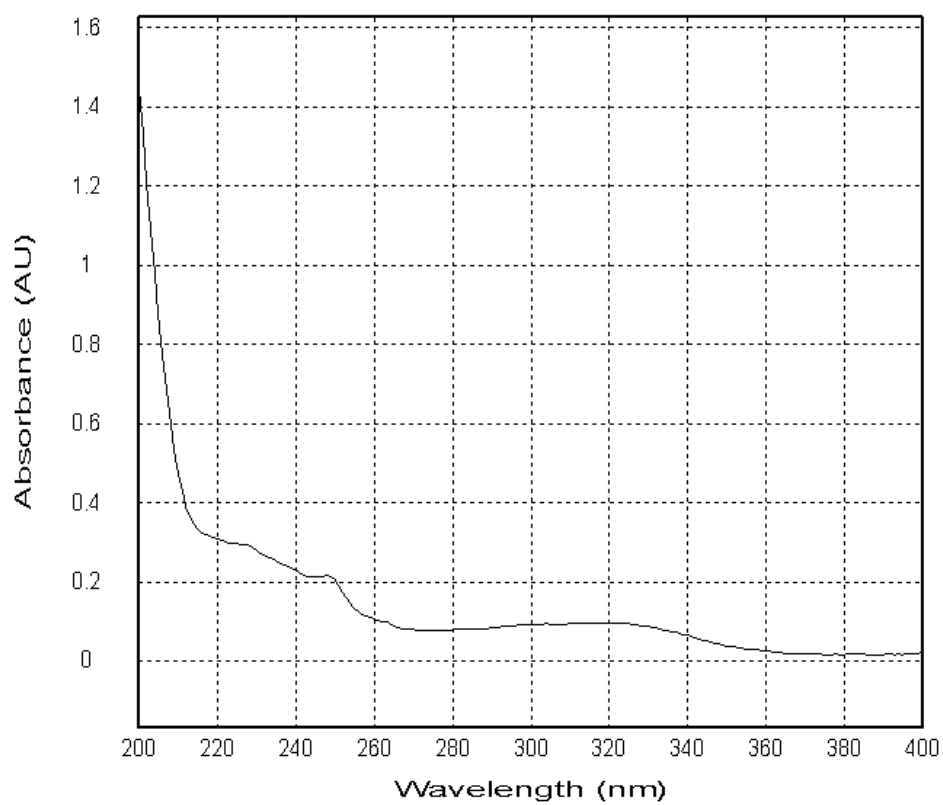


Figure S9. UV spectrum of **1** in MeOH.

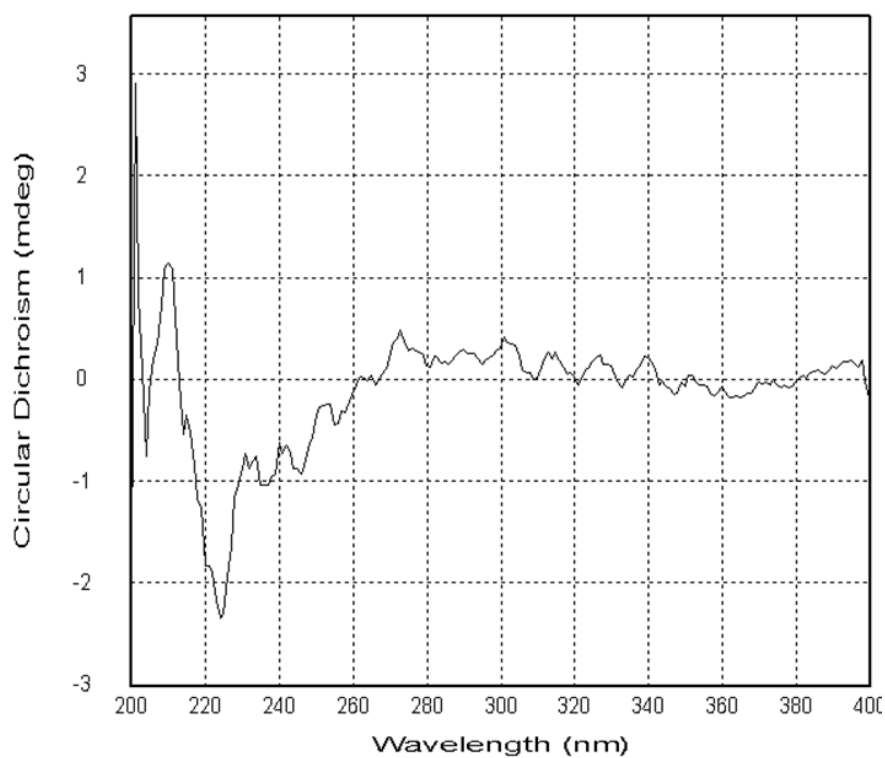


Figure S10. ECD spectrum of **1** in MeOH.

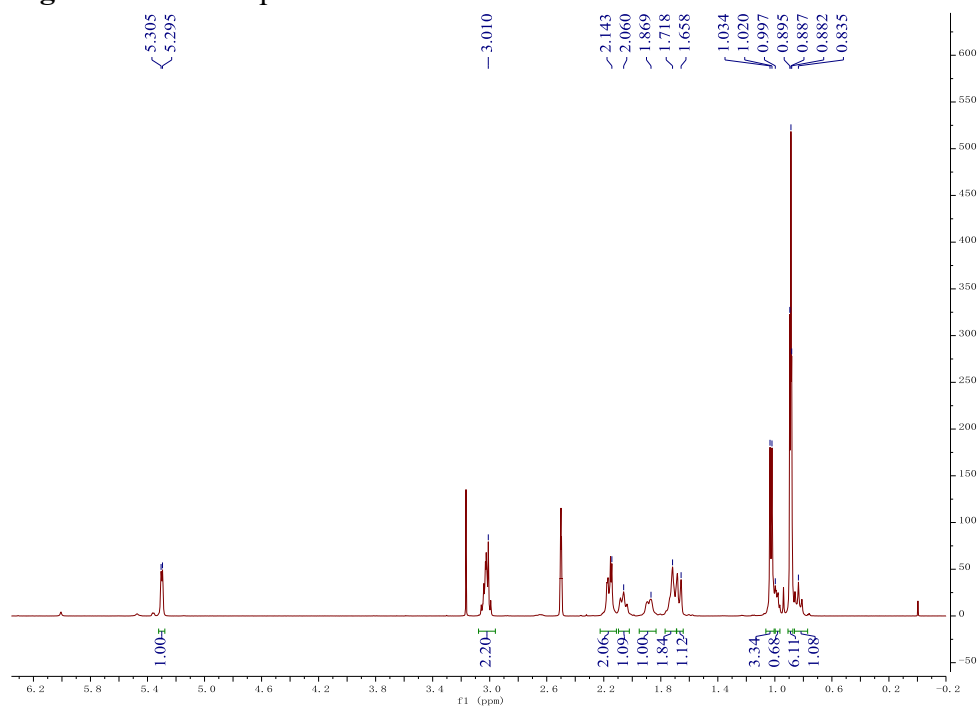


Figure S11. ^1H NMR (500 MHz) spectrum of **2** in $\text{DMSO}-d_6$.

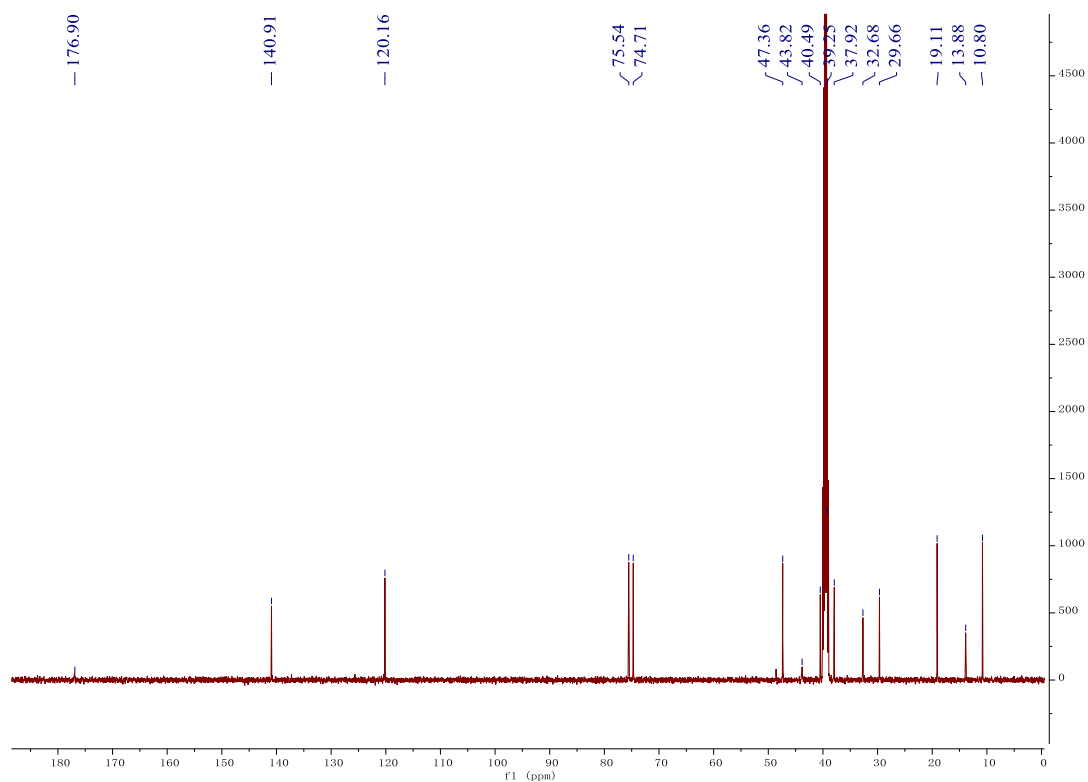


Figure S12. ^{13}C NMR (125 MHz) spectrum of **2** in $\text{DMSO}-d_6$.

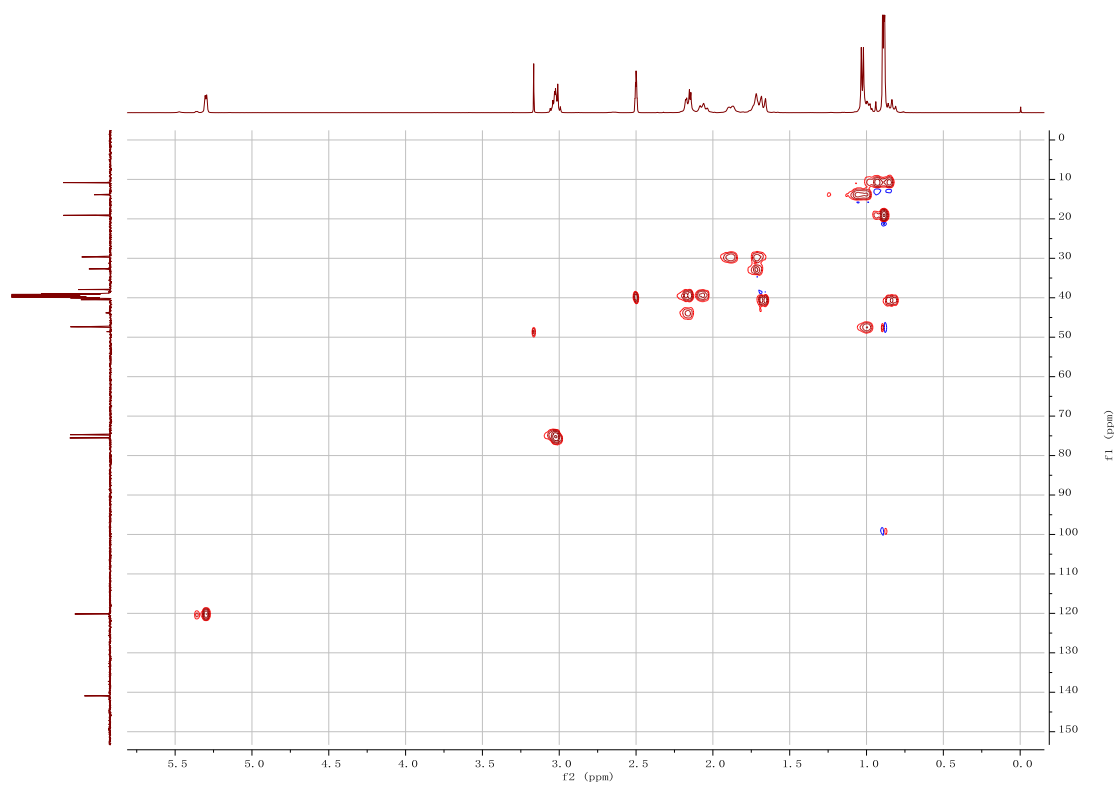


Figure S13. HSQC spectrum of **2** in $\text{DMSO}-d_6$.

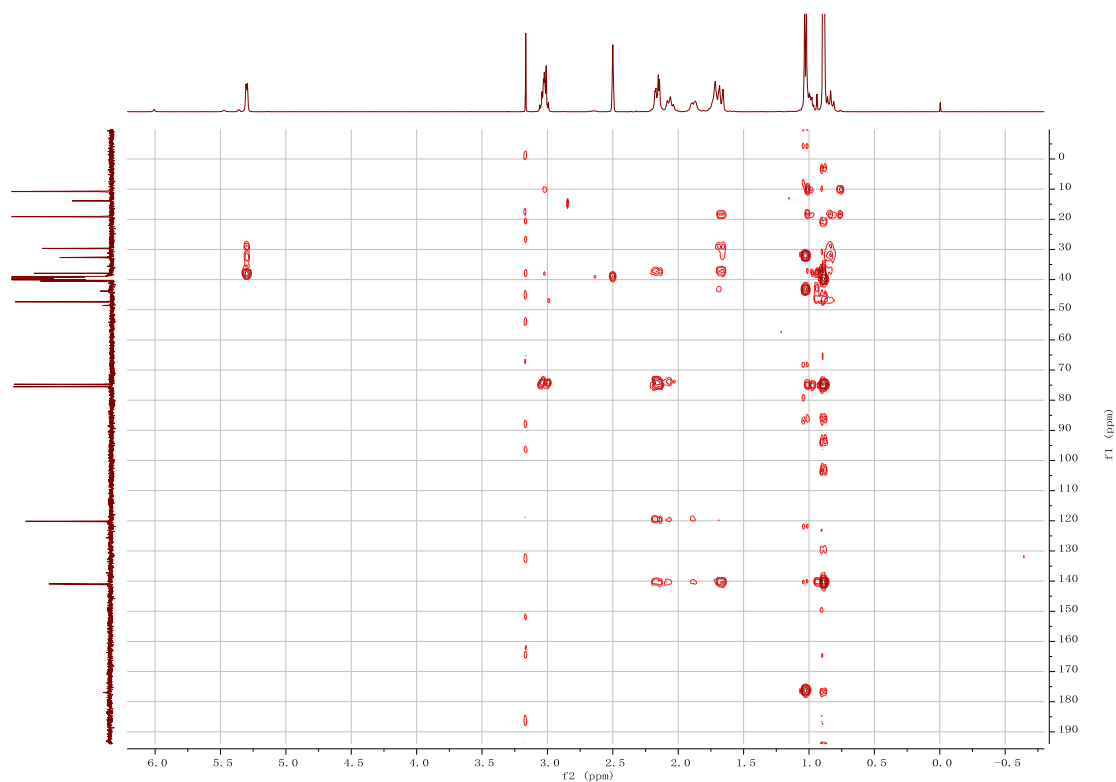


Figure S14. HMBC spectrum of **2** in DMSO- d_6 .

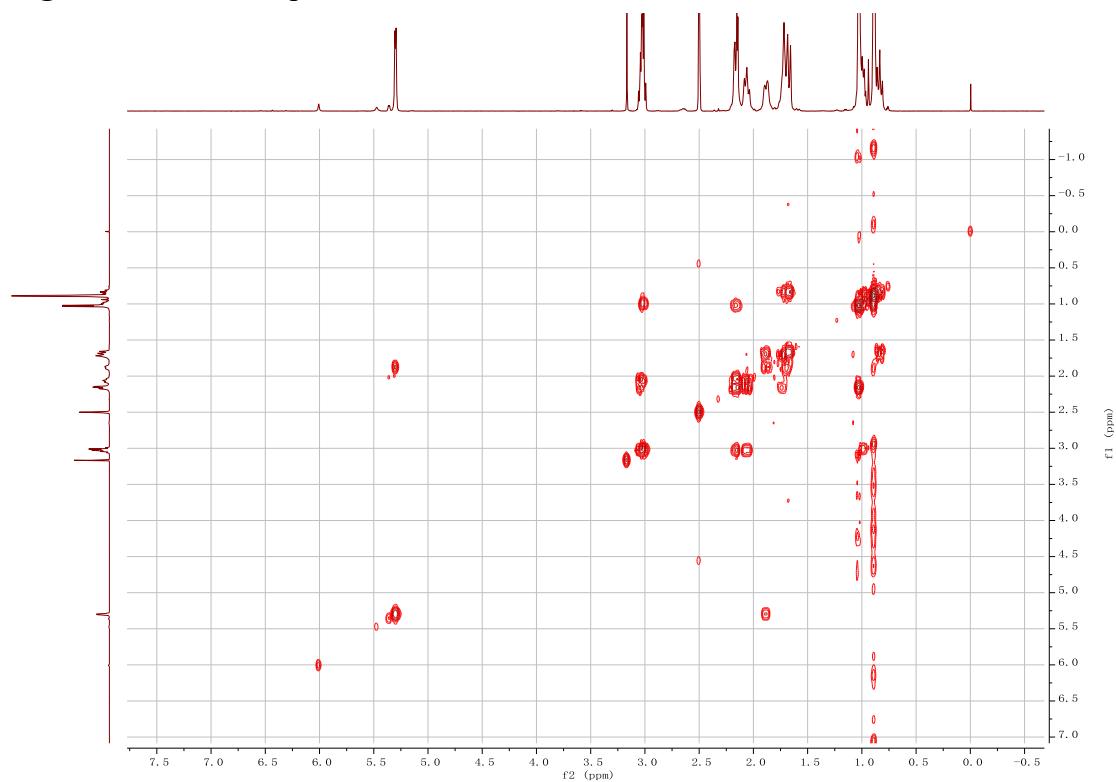


Figure S15. ^1H - ^1H COSY spectrum of **2** in DMSO- d_6 .

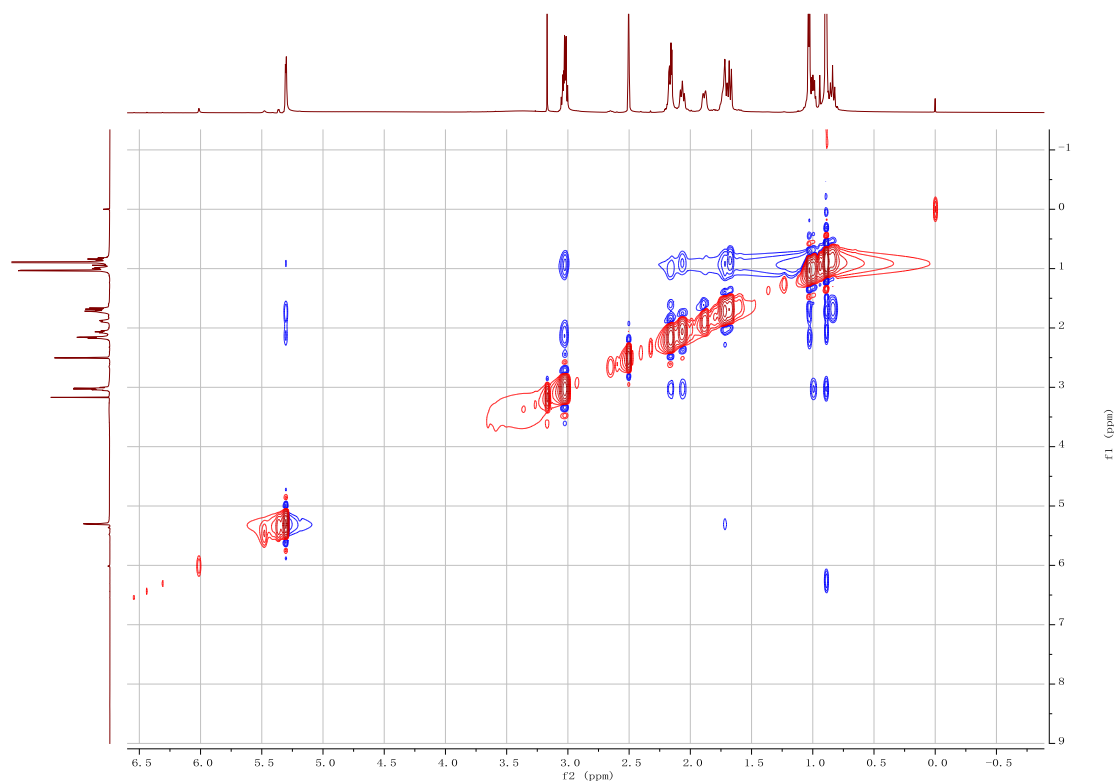


Figure S16. NOESY spectrum of **2** in DMSO-*d*₆.

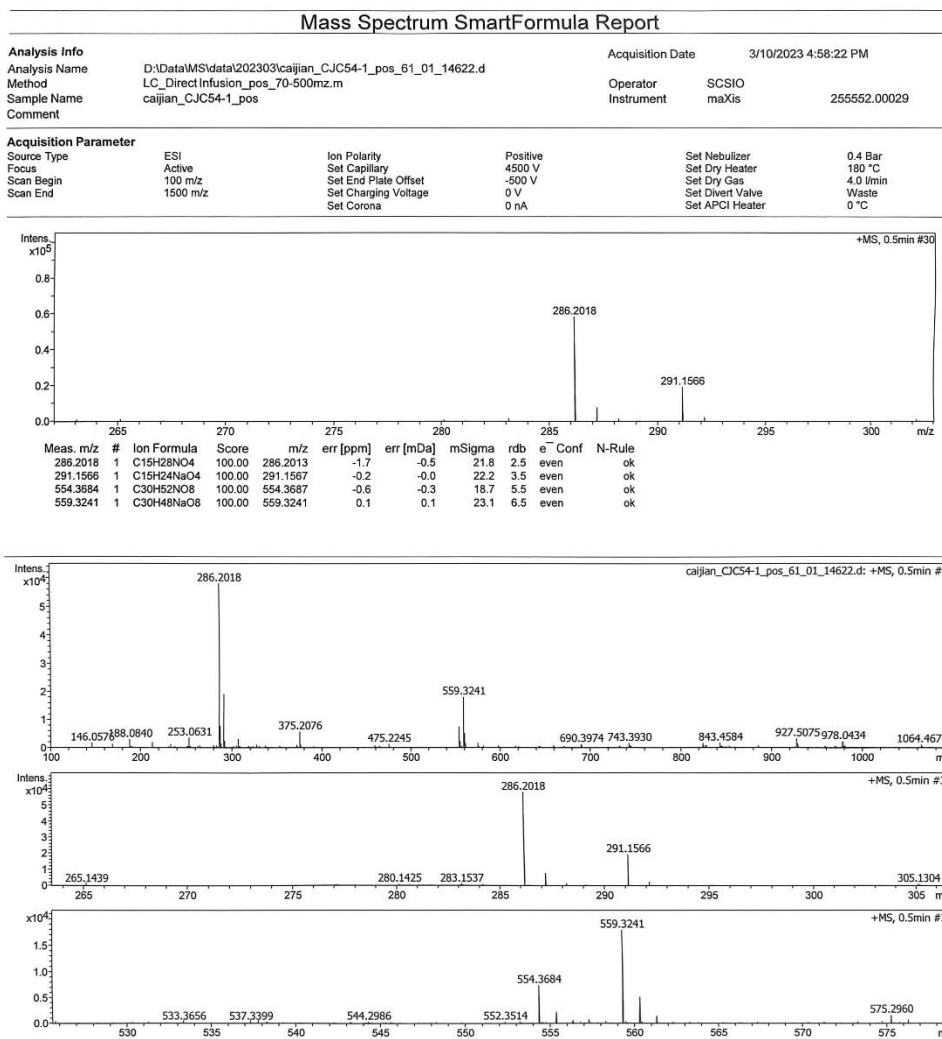


Figure S17. HRESIMS spectrum of **2**.

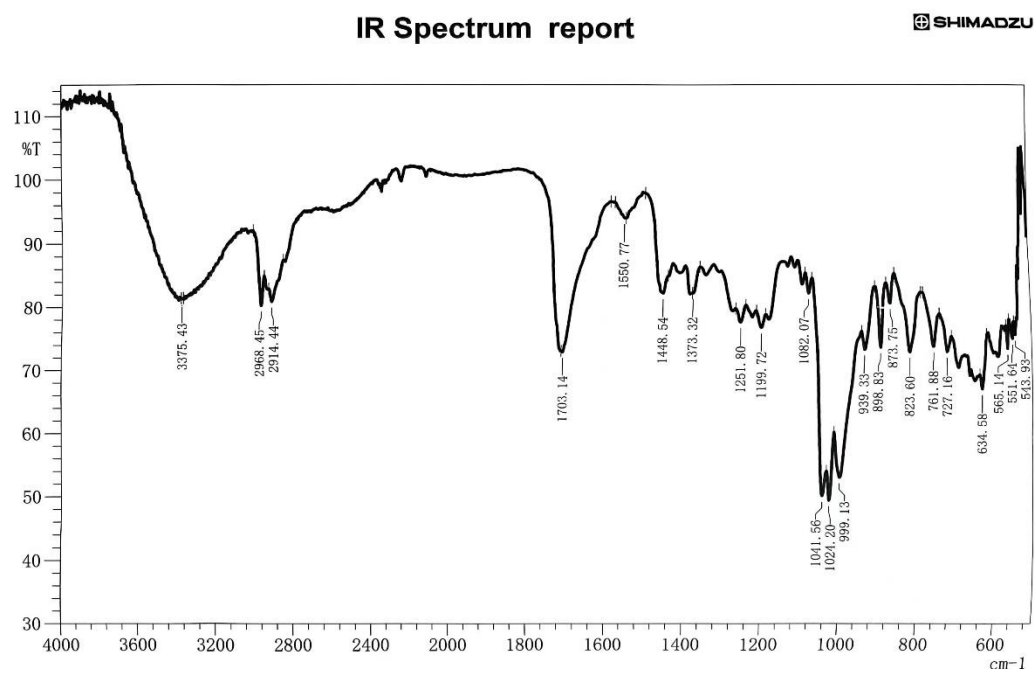


Figure S18. IR spectrum of **2**.

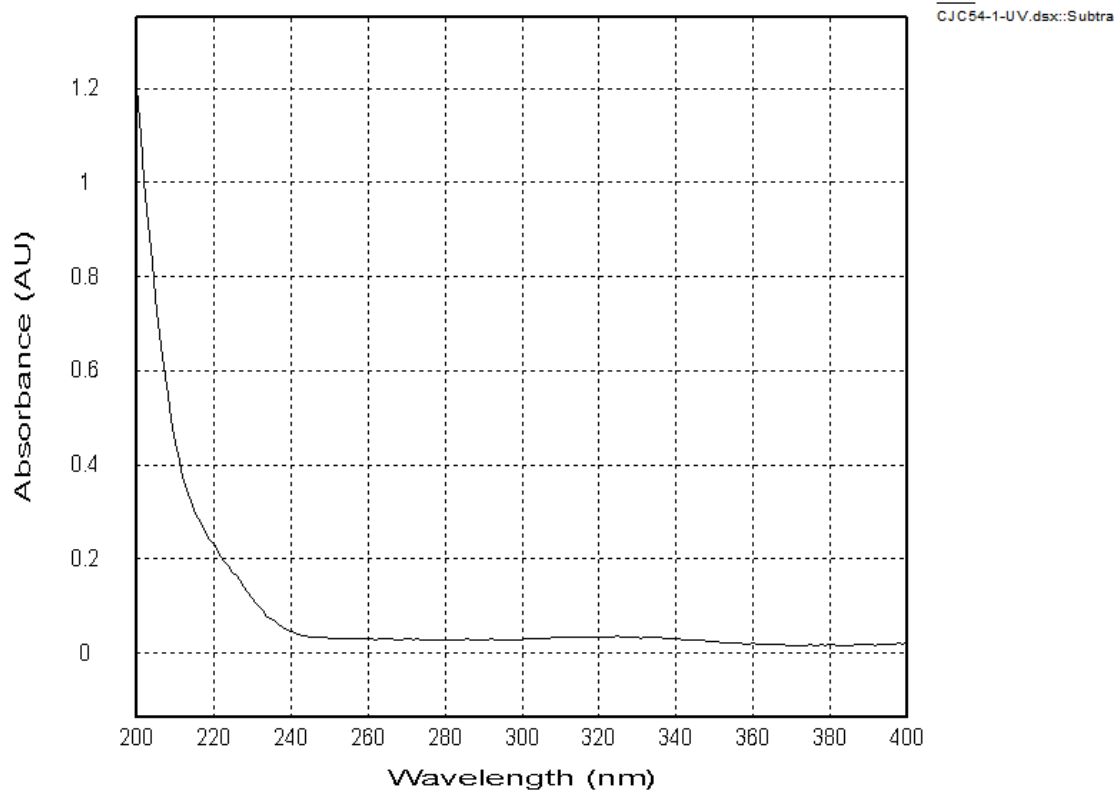


Figure S19. UV spectrum of **2** in MeOH.

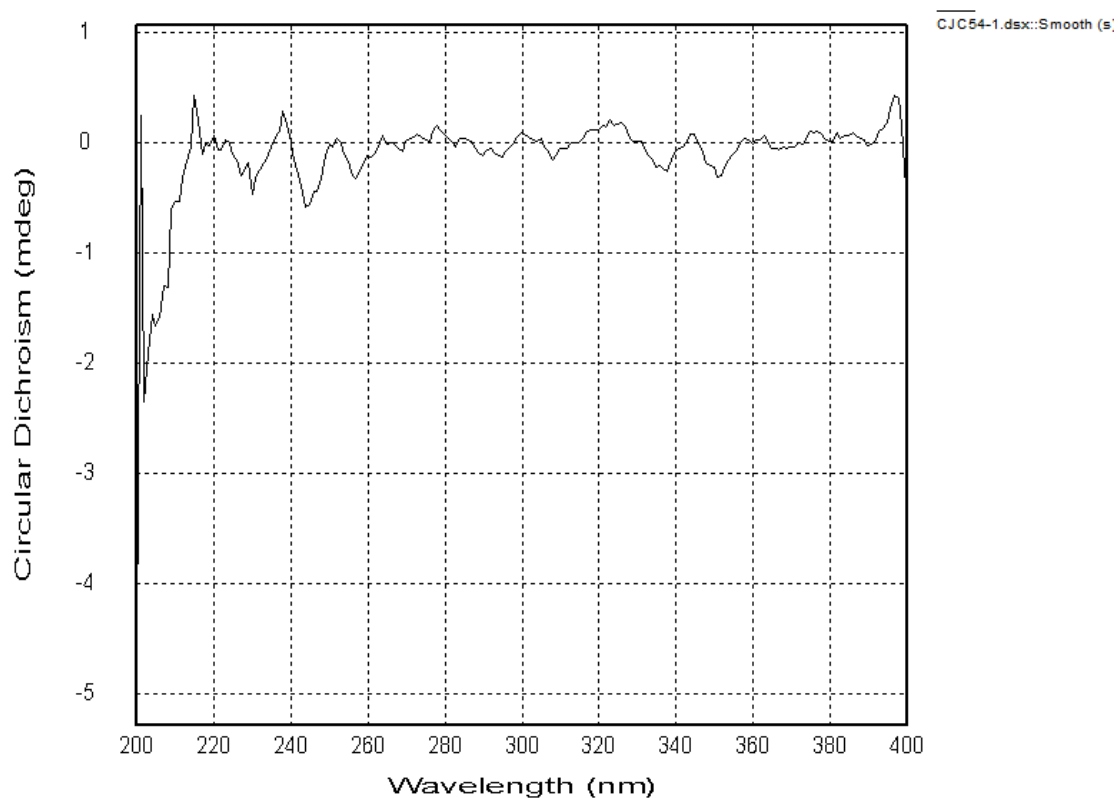


Figure S20. ECD spectrum of **2** in MeOH.

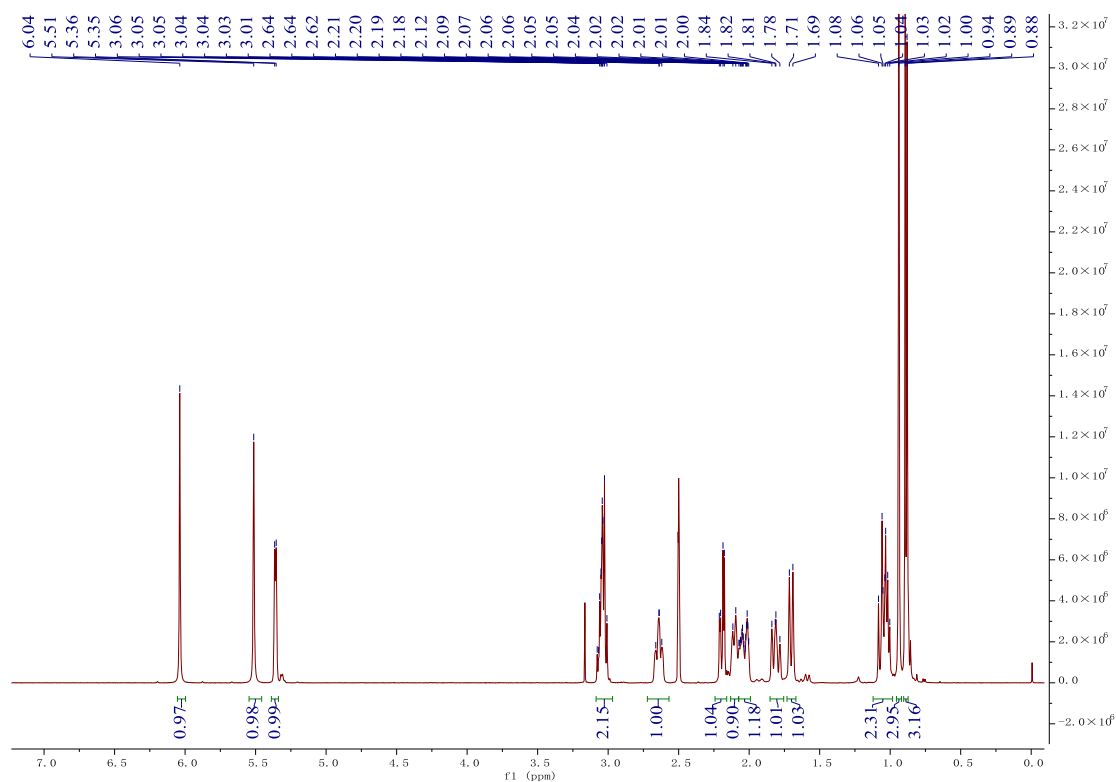


Figure S21. ^1H NMR (500 MHz) spectrum of **3** in $\text{DMSO}-d_6$.

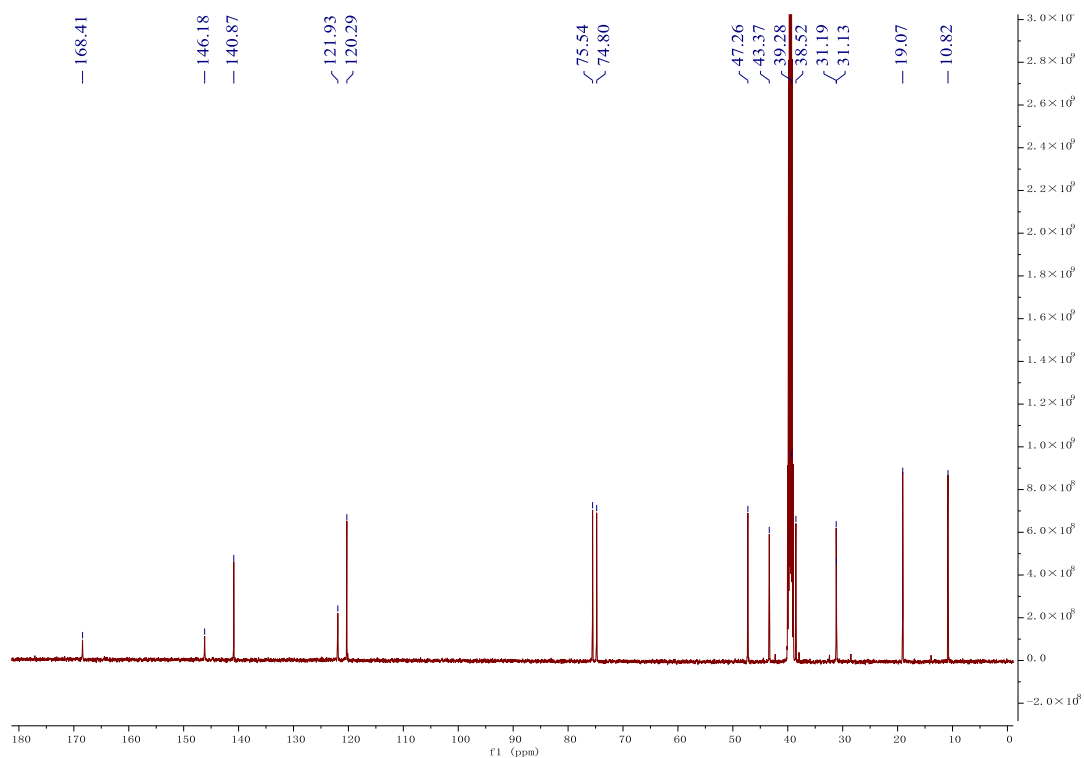


Figure S22. ^{13}C NMR (125 MHz) spectrum of **3** in $\text{DMSO-}d_6$.

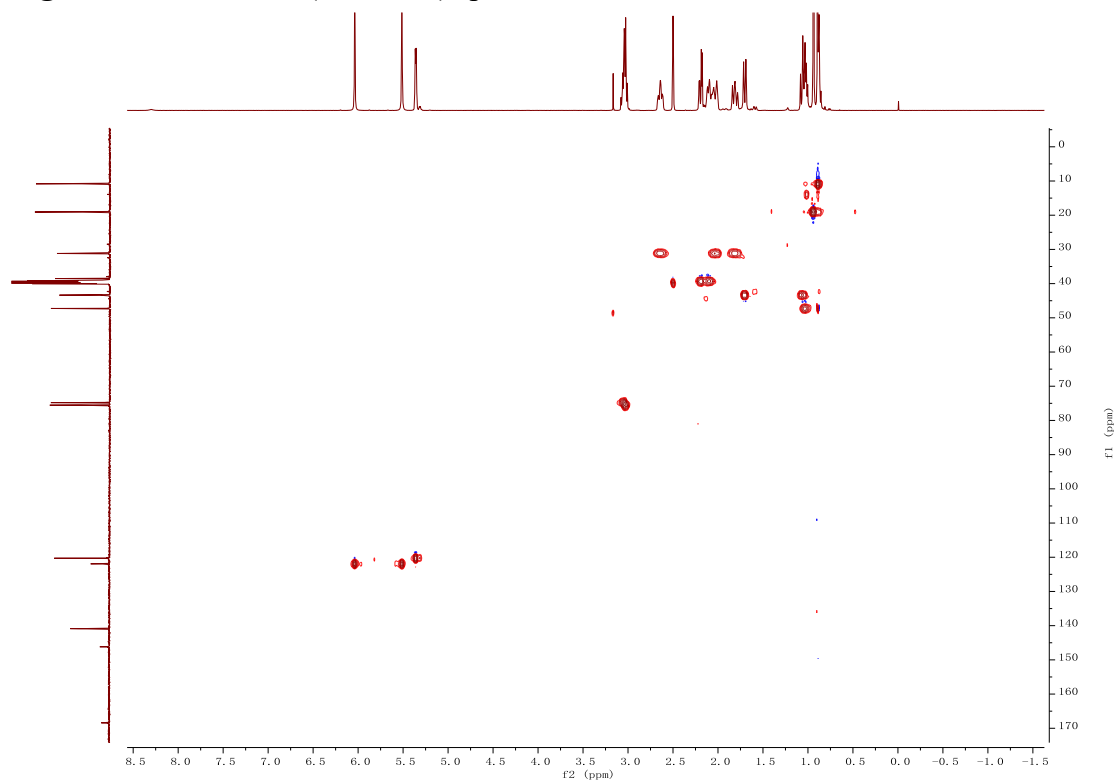


Figure S23. HSQC spectrum of **3** in $\text{DMSO-}d_6$.

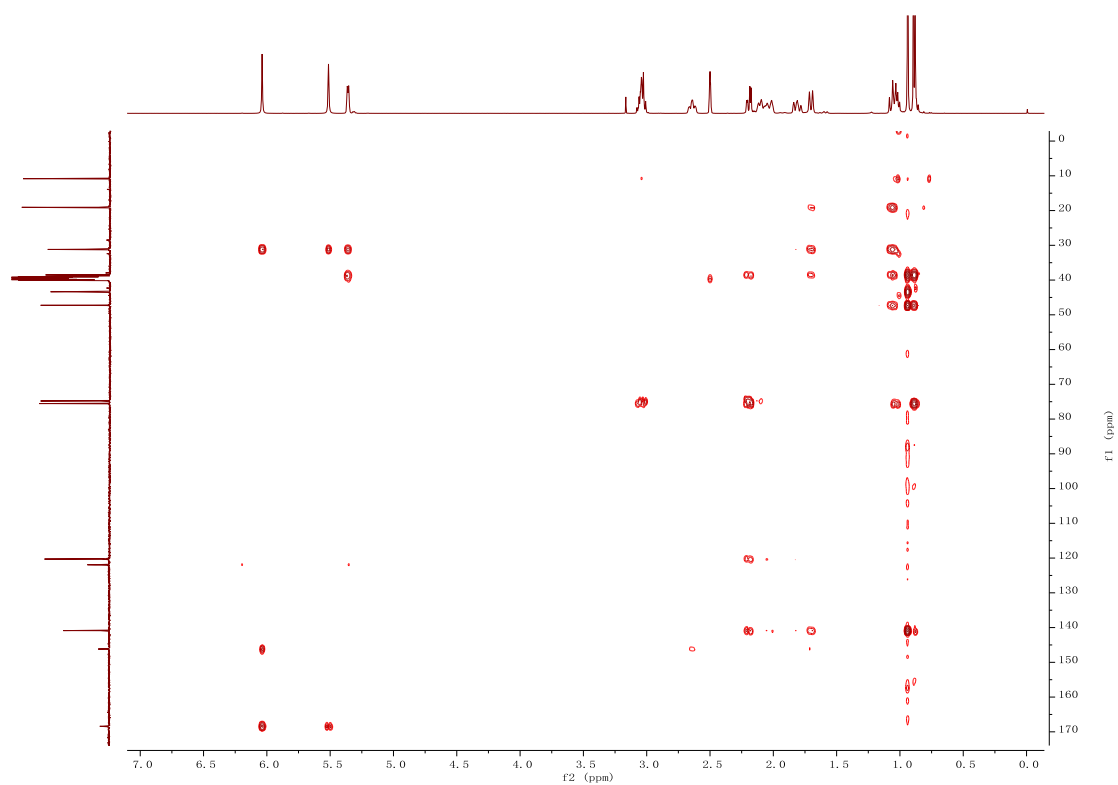


Figure S24. HMBC spectrum of **3** in DMSO-*d*₆.

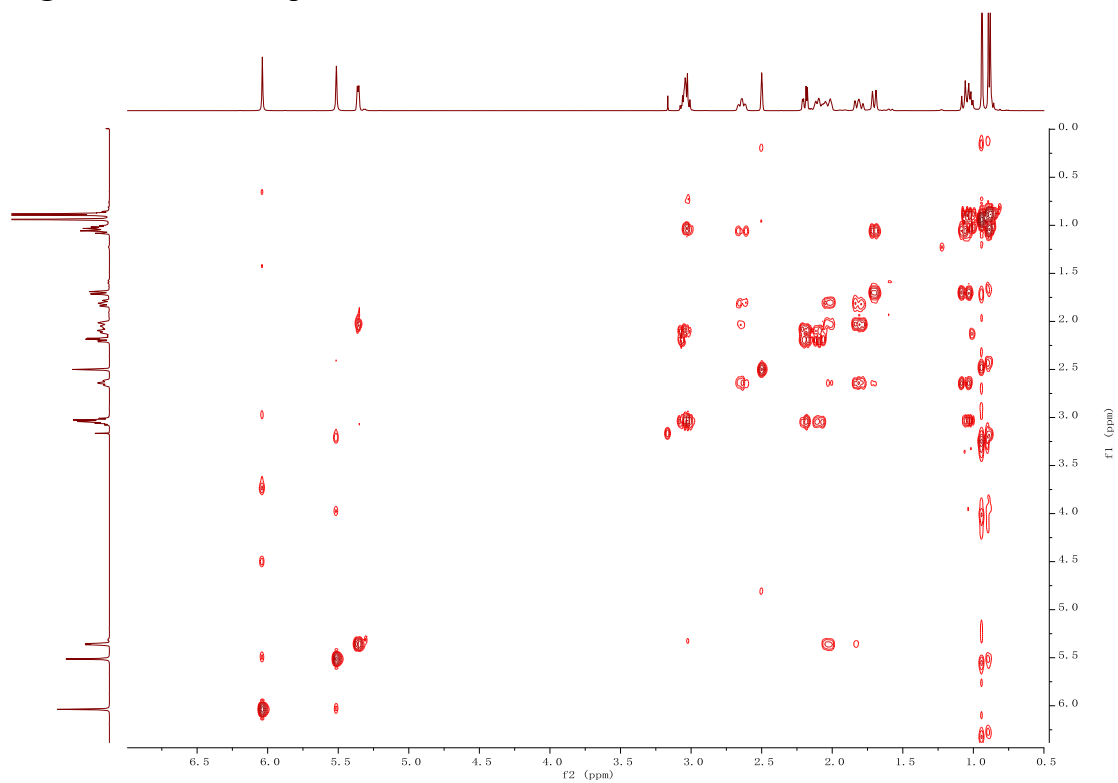


Figure S25. ^1H - ^1H COSY spectrum of **3** in DMSO-*d*₆.

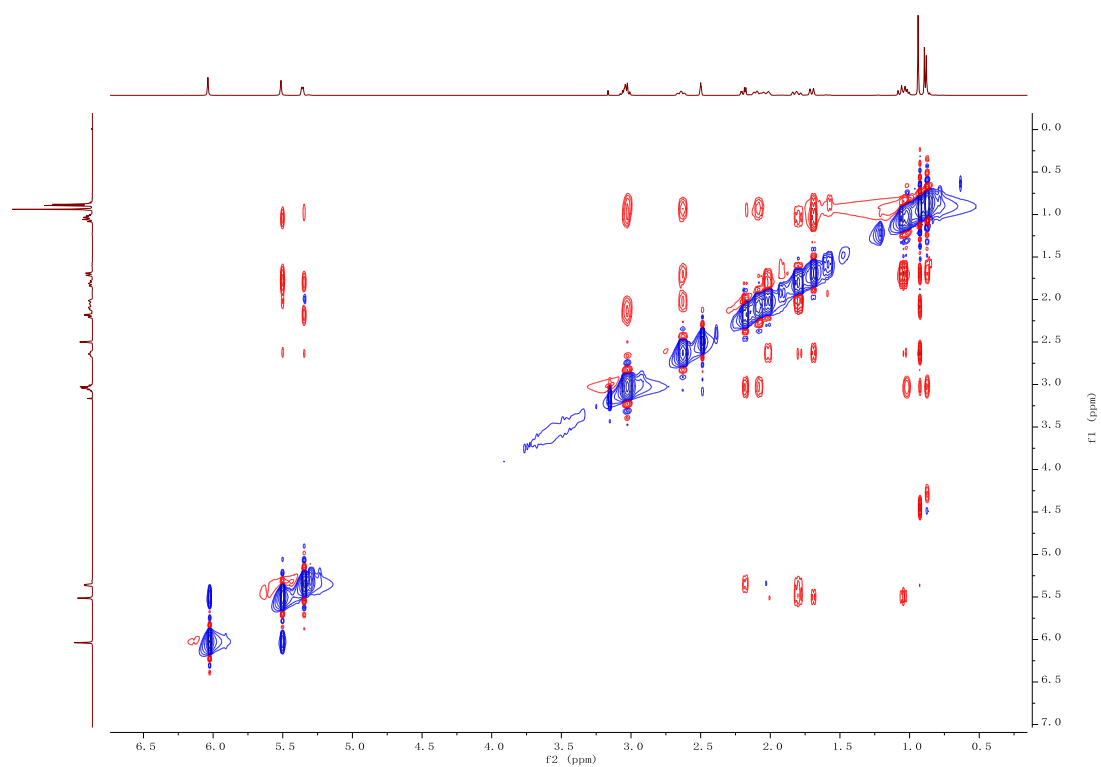


Figure S26. NOESY spectrum of **3** in DMSO-*d*₆.

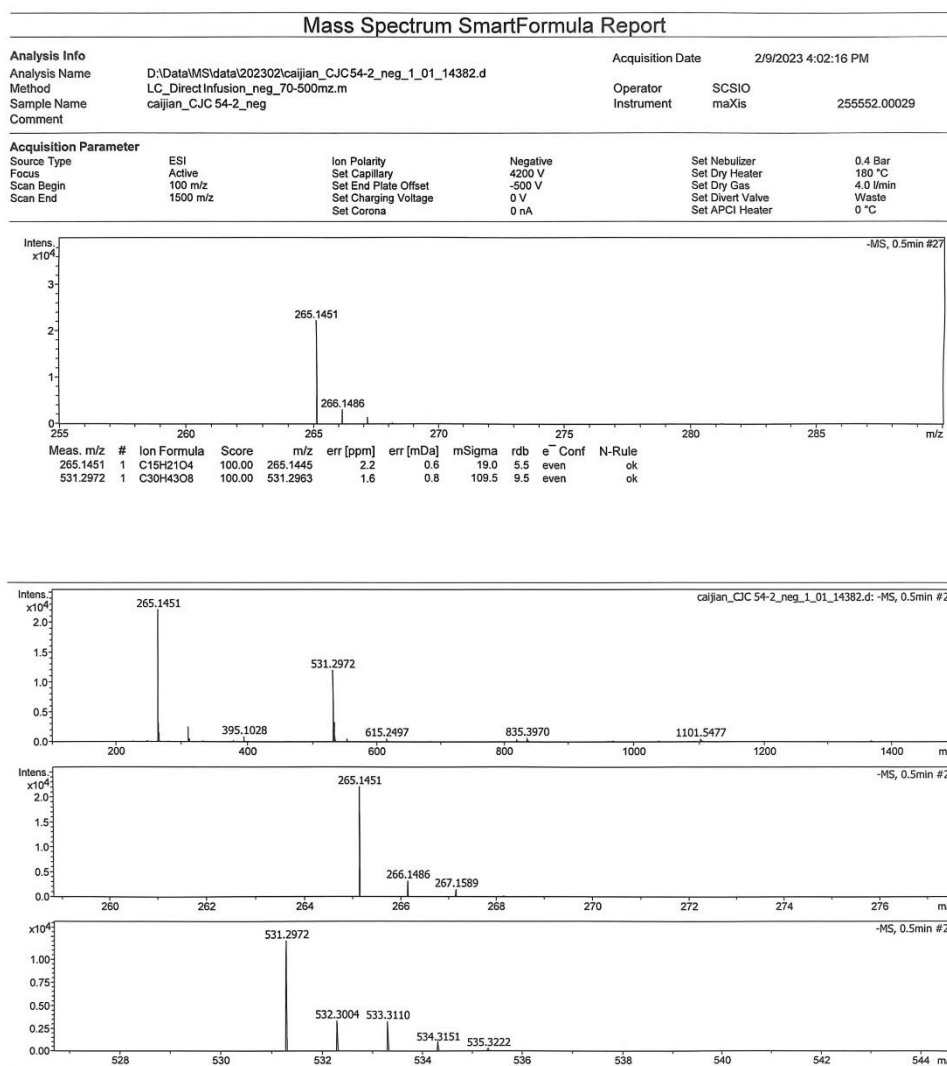


Figure S27. HRESIMS spectrum of **3**.

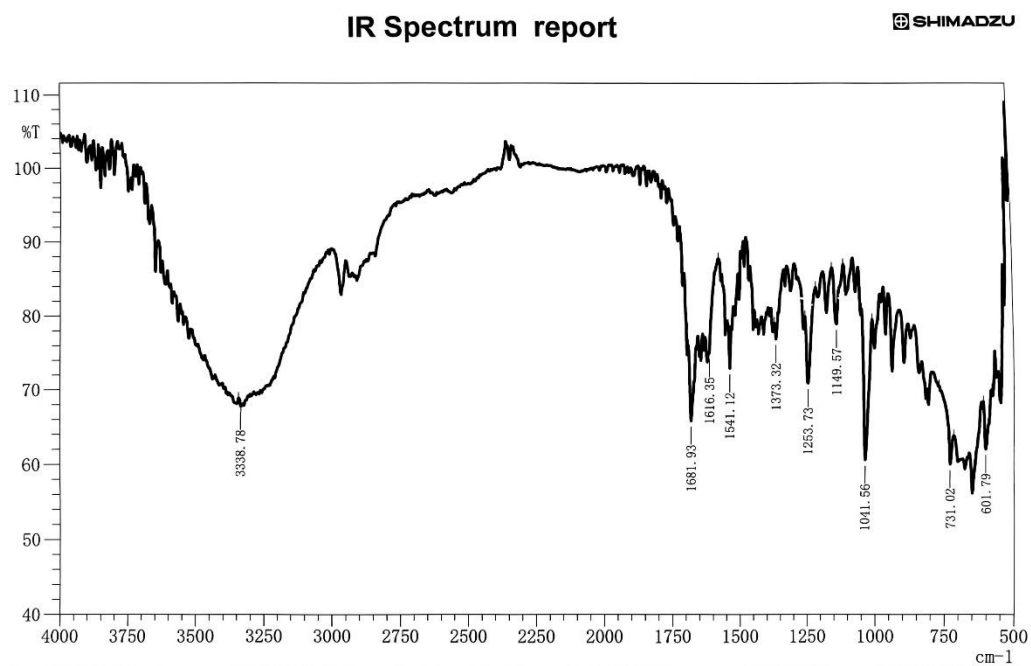


Figure S28. IR spectrum of **3**.

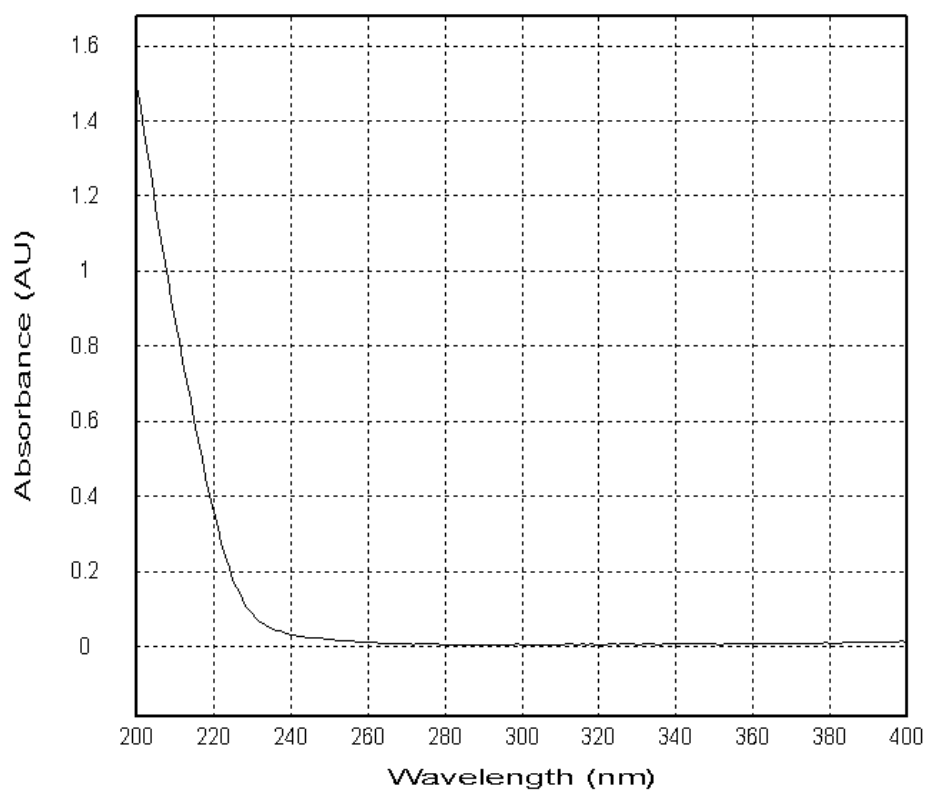


Figure S29. UV spectrum of **3** in MeOH.

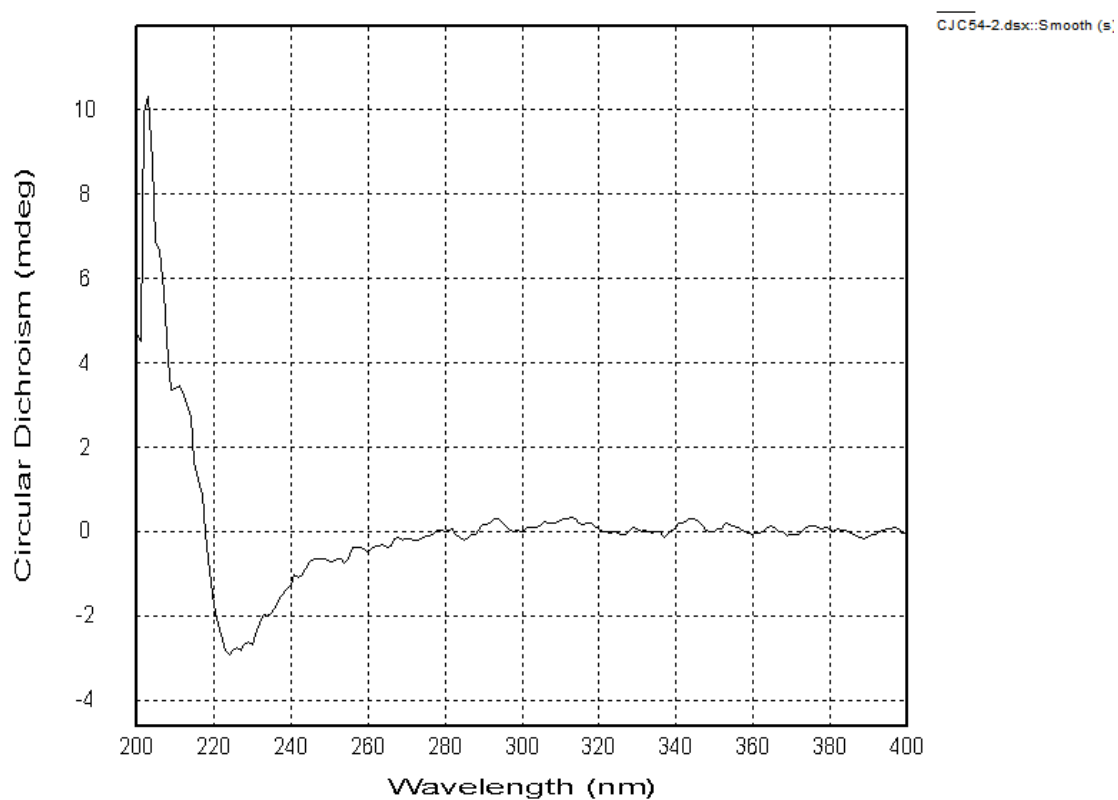


Figure S30. ECD spectrum of **3** in MeOH.

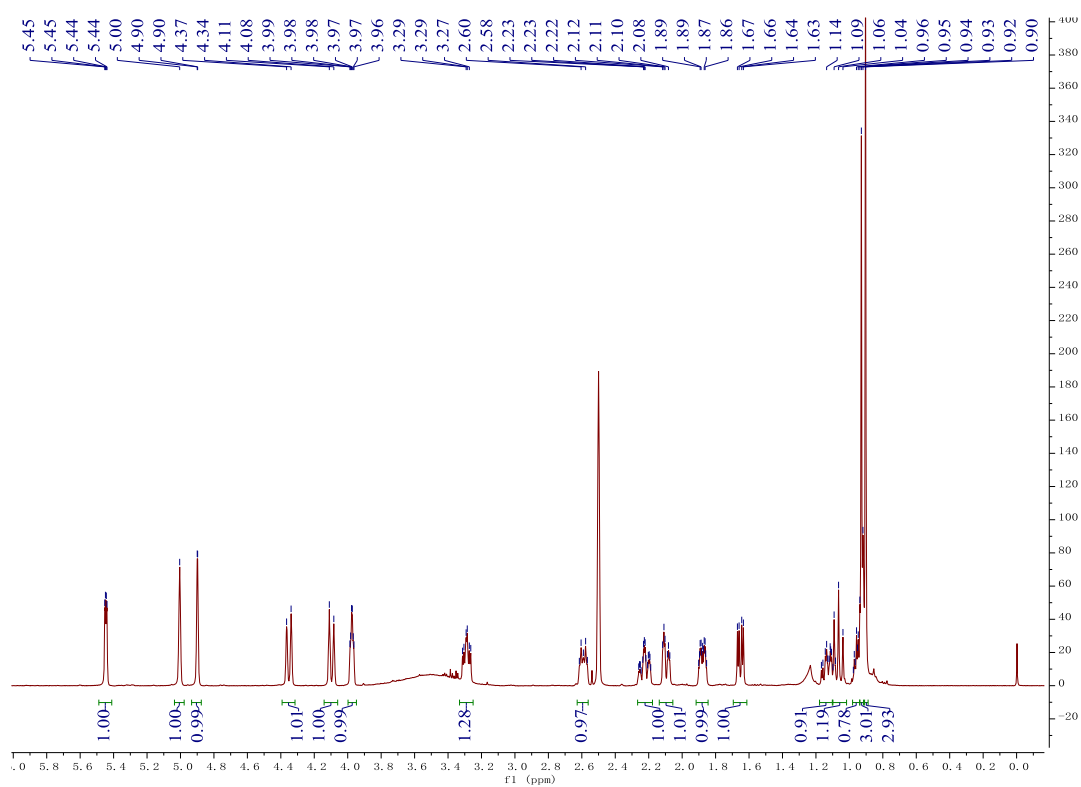


Figure S31. ^1H NMR (500 MHz) spectrum of **4** in $\text{DMSO}-d_6$.

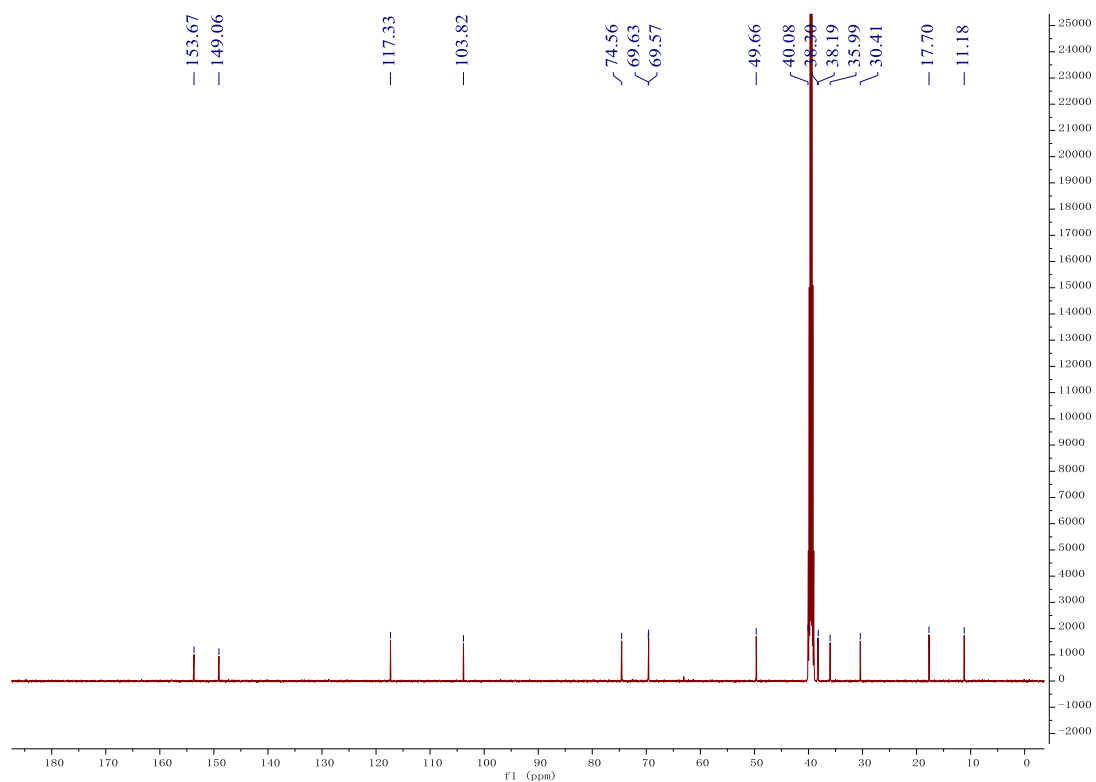


Figure S32. ^{13}C NMR (125 MHz) spectrum of **4** in $\text{DMSO-}d_6$.

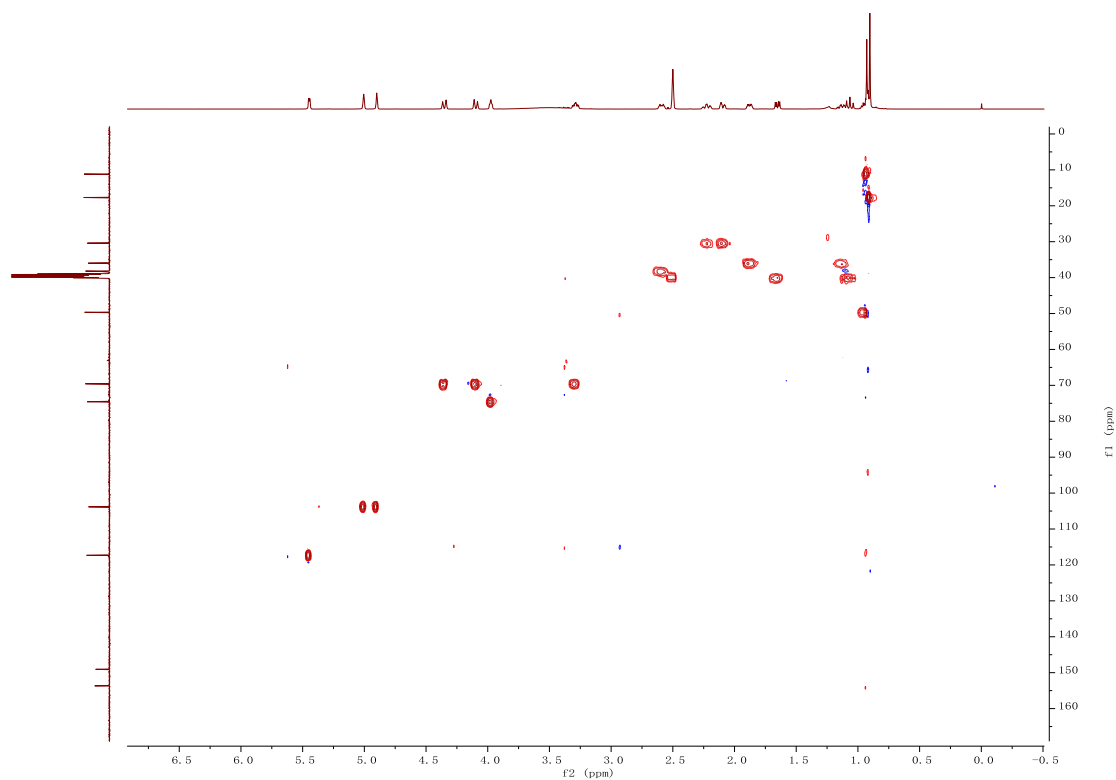


Figure S33. HSQC spectrum of **4** in $\text{DMSO-}d_6$.

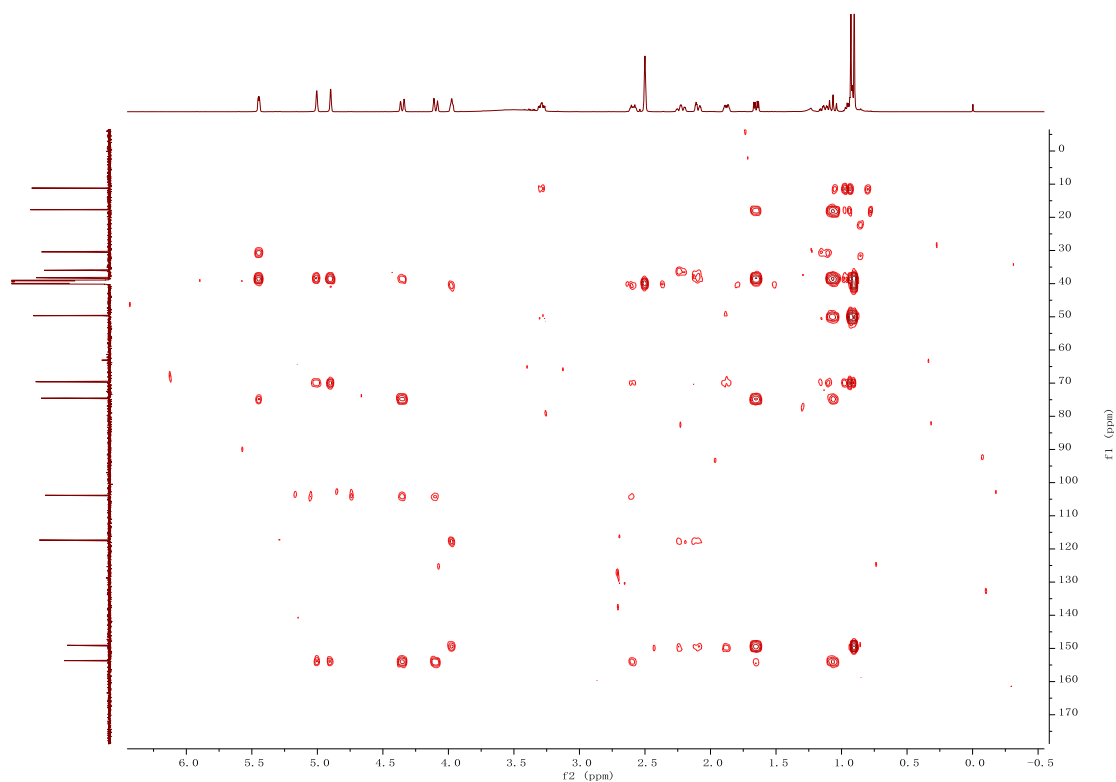


Figure S34. HMBC spectrum of **4** in DMSO- d_6 .

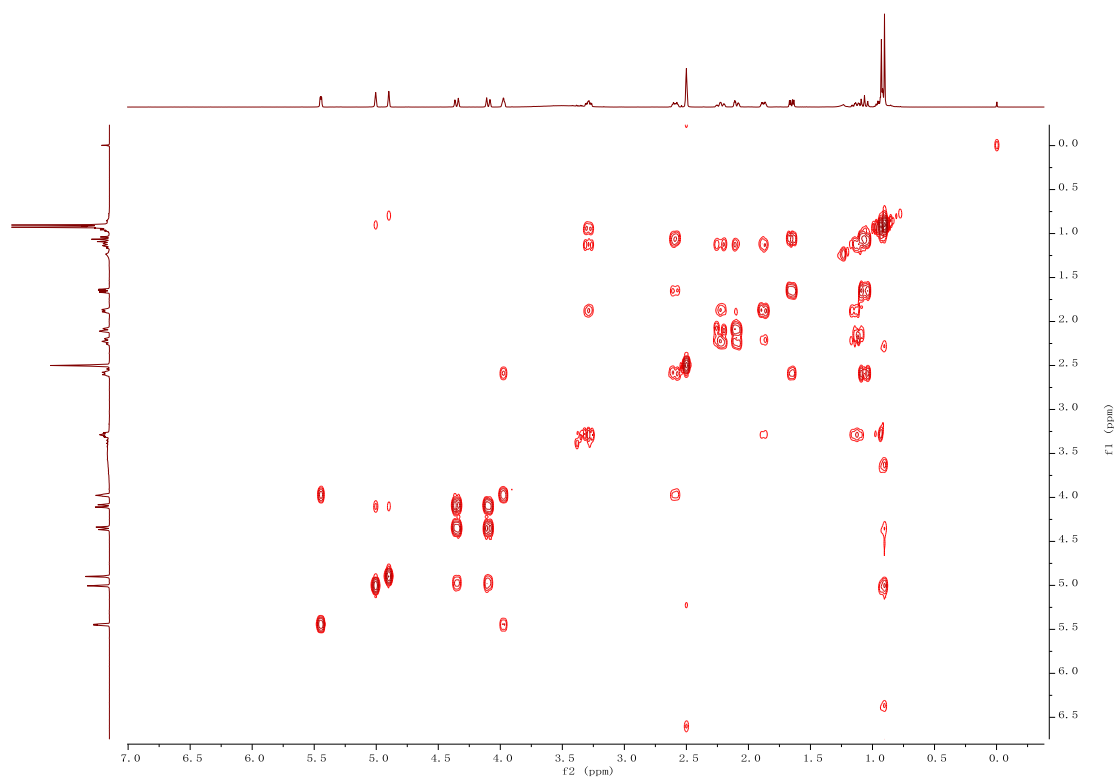


Figure S35. ^1H - ^1H COSY spectrum of **4** in DMSO- d_6 .

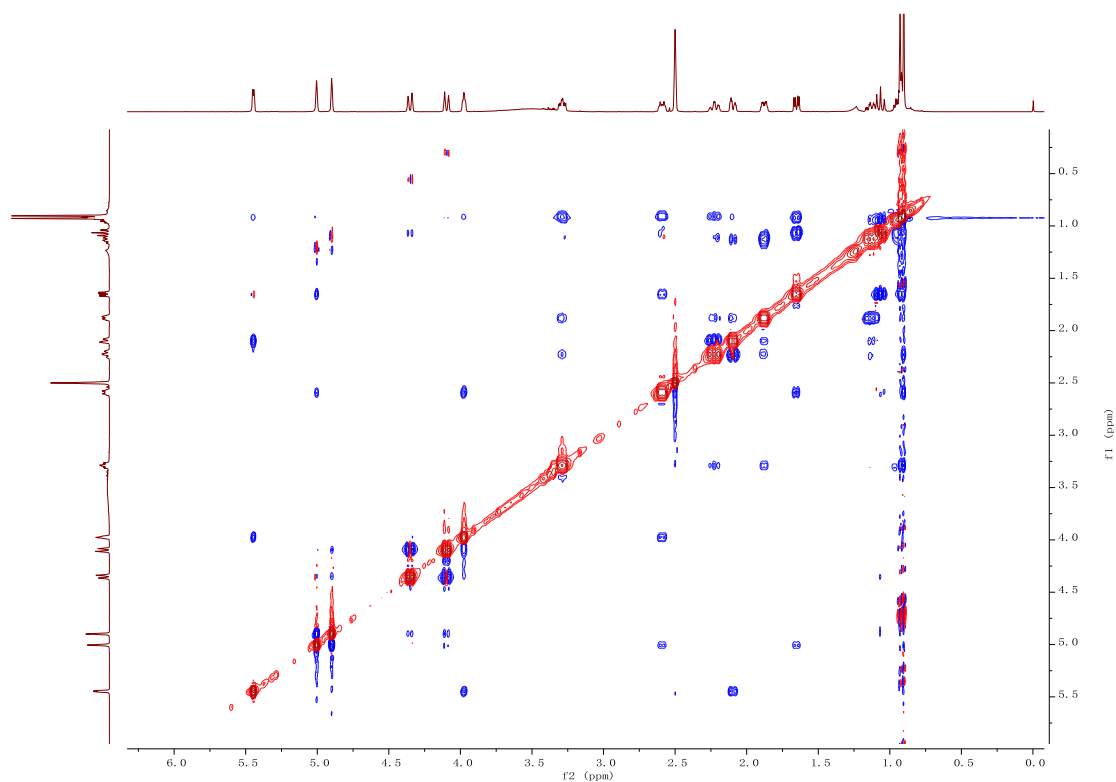


Figure S36. NOESY spectrum of **4** in DMSO- d_6 .

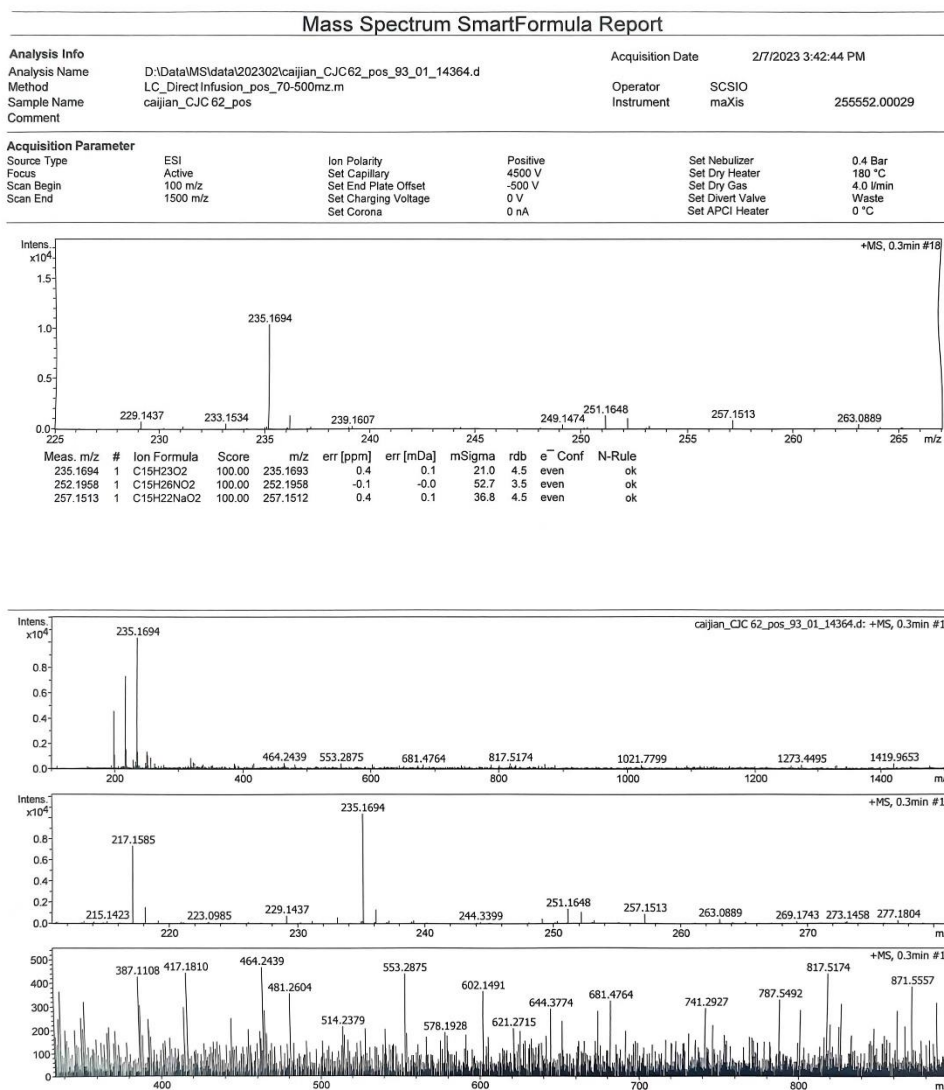


Figure S37. HRESIMS spectrum of **4**.

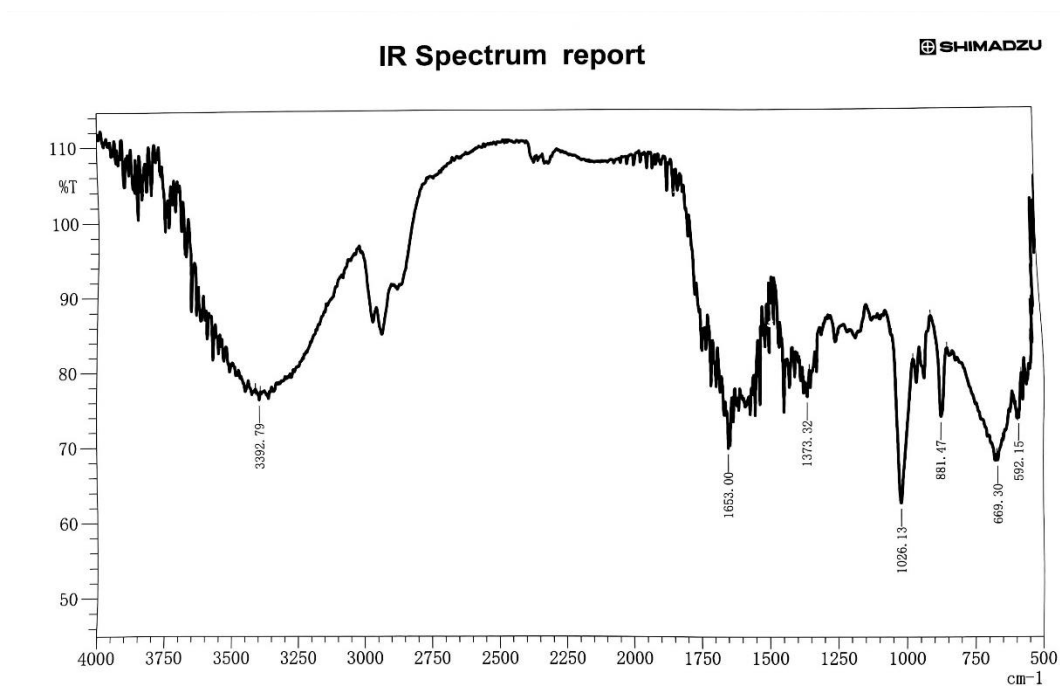


Figure S38. IR spectrum of **4**.

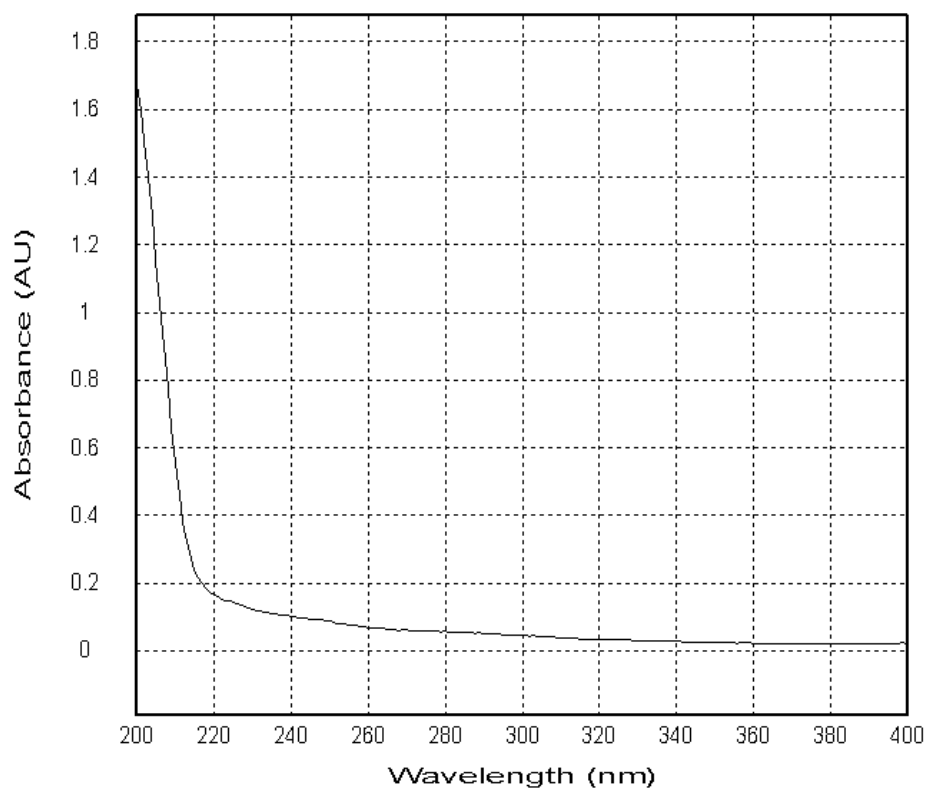


Figure S39. UV spectrum of **4** in MeOH.

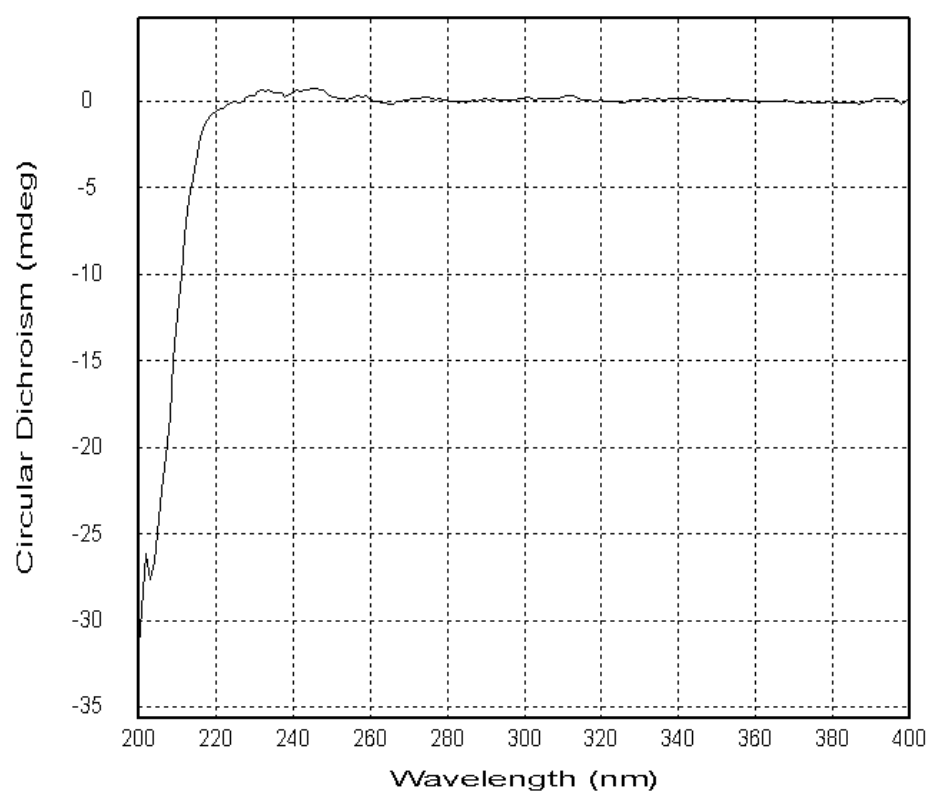
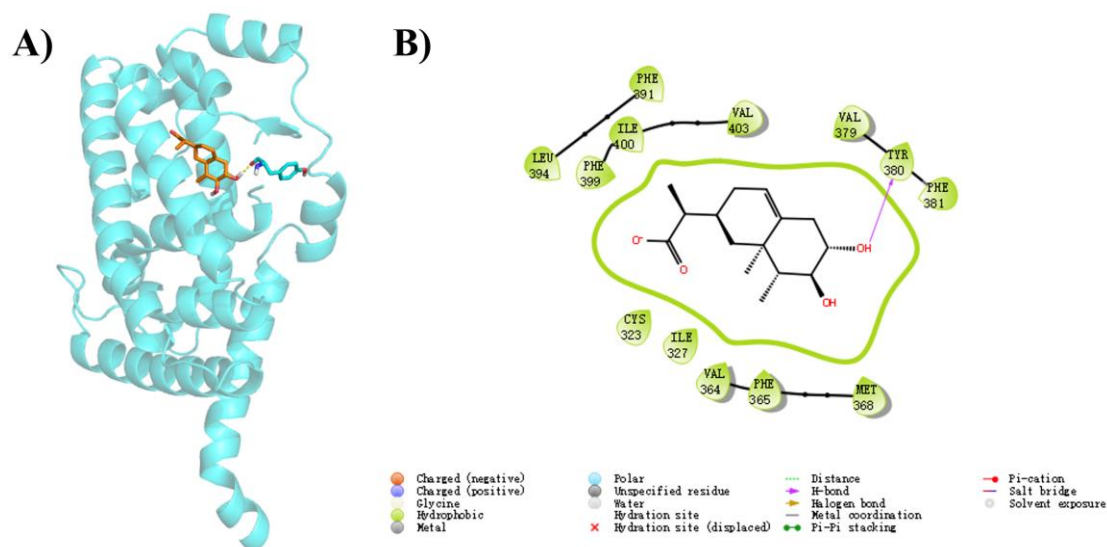


Figure S40. ECD spectrum of **4** in MeOH.

Table S1. Primers of RT-qPCR

Primer	Sequence (5'→3')
H- <i>RORα</i> -F	CACGACGACCTCAGTAACTACA
H- <i>RORα</i> -R	TGGTGAACGAACAGTAGGGAA
H- <i>BMAL1</i> -F	AAATCGCTTTGAGGTGAC
H- <i>BMAL1</i> -R	CTTTCGTTTTCGCGTTGC
H- <i>CLOCK</i> -F	TGCGAGGAACAATAGACCCAA
H- <i>CLOCK</i> -R	ATGGCCTATGTGTGCGTTGTA
H- <i>LXRα</i> -F	GCTGCAAGTGGAATTCATCAACC
H- <i>LXRα</i> -R	ATATGTGTGCTGCAGCCTCTCCA
H- <i>ABCA1</i> -F	ACCCACCCTATGAACAACATGA
H- <i>ABCA1</i> -R	GAGTCGGGTAACGGAAACAGG
H- <i>PPARα</i> -F	TTCGCAATCCATCGGCGAG
H- <i>PPARα</i> -R	CCACAGGATAAGTCACCGAGG
H- <i>ACOX1</i> -F	ACTCGCAGCCAGCGTTATG
H- <i>ACOX1</i> -R	AGGGTCAGCGATGCCAAAC
H- <i>CPT1α</i> -F	ATCAATCGGACTCTGGAAACGG
H- <i>CPT1α</i> -R	TCAGGGAGTAGCGCATGGT
H- <i>GAPDH</i> -F	GCTCTCTGCTCCTCCTGTTC
H- <i>GAPDH</i> -R	ACGACCAAATCCGTTGACTC
H- <i>FXR</i> -F	GGCTCGGGGATACTGGATACA
H- <i>FXR</i> -R	CTGGCATGAAGCGTTGTCC
H- <i>CYP7A1</i> -F	CAACGTATCATGAGACCTCCAGTC
H- <i>CYP7A1</i> -R	CAGCTTCAAACATCACTCGGTAG

**Figure S41.** The docking result of **1** with RORα. A) 3D and B) 2D binding mode of **1** with RORα (PDB code: 1N83) predicted by *in silico* molecular docking.

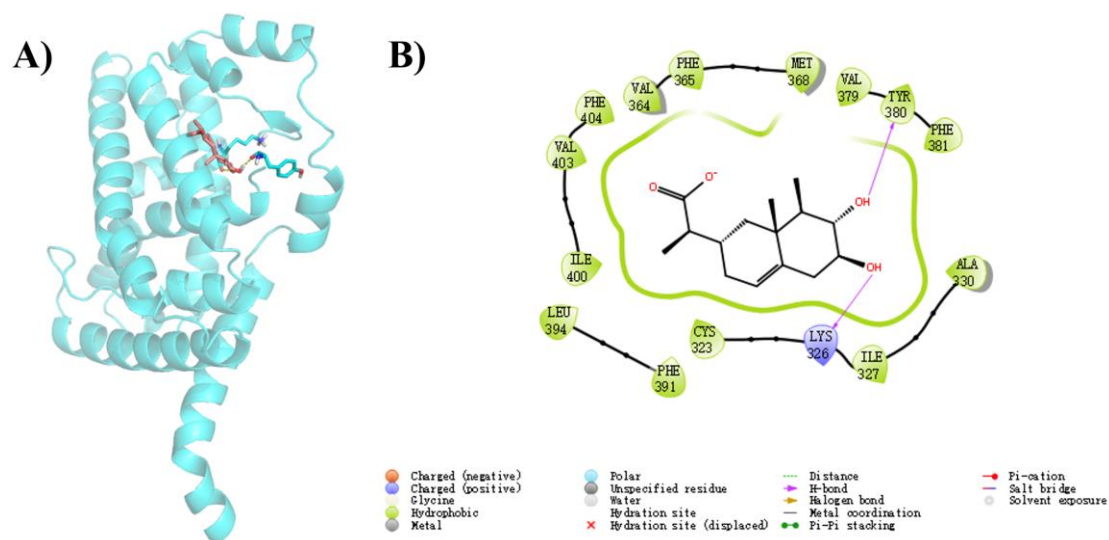


Figure S42. The docking result of **2** with ROR α . A) 3D and B) 2D binding mode of **2** with ROR α (PDB code:1N83) predicted by *in silico* molecular docking.

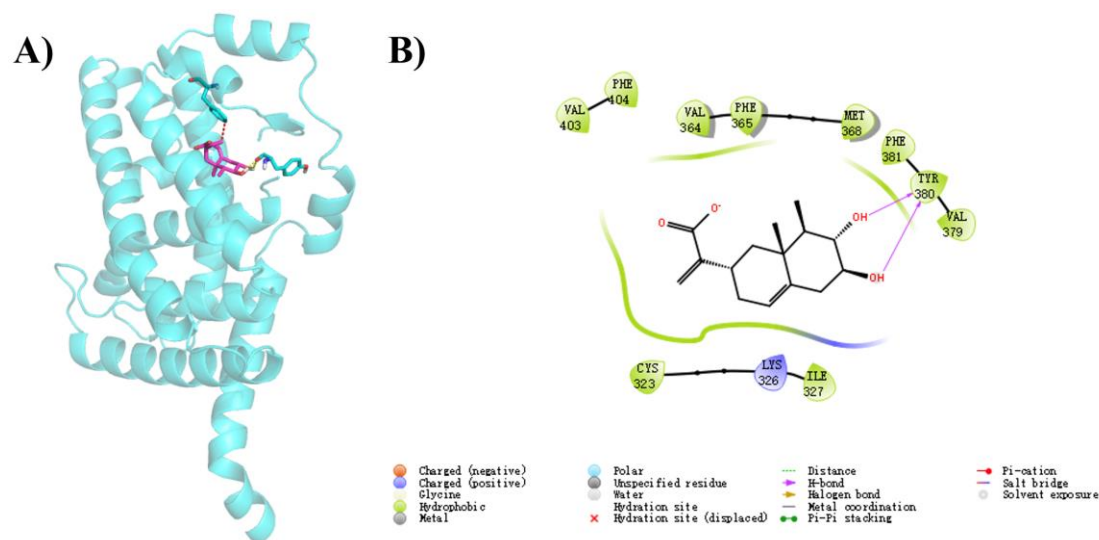
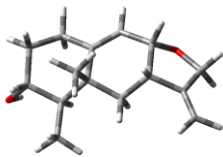
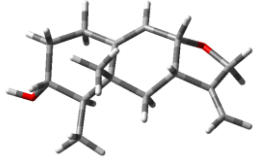
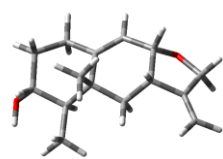
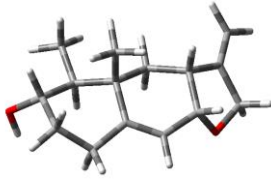
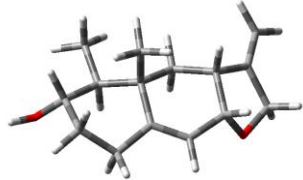
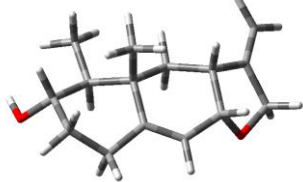


Figure S43. The docking result of **3** with ROR α . A) 3D (Yellow bond:H-bond; Red bond:bad contact) and B) 2D binding mode of **3** with ROR α (PDB code:1N83) predicted by *in silico* molecular docking.

Table S2. Energies of **4** at B3LYP/6–311g (d, p) level.

Configuration	Conformer	E (Hartree)	E (kcal/mol)	Populat ion
3 <i>R</i> , 4 <i>R</i> , 5 <i>R</i> , 7 <i>S</i> , 8 <i>S</i>	 1	-735.220313554	-461358.098958271	28.15%
3 <i>R</i> , 4 <i>R</i> , 5 <i>R</i> , 7 <i>S</i> , 8 <i>S</i>	 2	-735.220802572	-461358.405821956	47.26%
3 <i>R</i> , 4 <i>R</i> , 5 <i>R</i> , 7 <i>S</i> , 8 <i>S</i>	 3	-735.220185619	-461358.018677779	24.59%
3 <i>S</i> , 4 <i>S</i> , 5 <i>S</i> , 7 <i>R</i> , 8 <i>R</i>	 1	-735.220313555	-461358.098958898	28.16%
3 <i>S</i> , 4 <i>S</i> , 5 <i>S</i> , 7 <i>R</i> , 8 <i>R</i>	 2	-735.220802527	-461358.405793718	47.26%
3 <i>S</i> , 4 <i>S</i> , 5 <i>S</i> , 7 <i>R</i> , 8 <i>R</i>	 3	-735.220185592	-461358.018660836	24.59%