

## Two New Prenylated Tryptophan Analogues Isolated from the Coral-derived Fungus *Tritirachium* sp. SCSIO 41037

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Abstract: Two new prenylated tryptophan analogues, tritianamides A (**1**) and B (**2**), together with ten known nitrogen-containing compounds (**3–12**), were isolated from the ethyl acetate extract of coral-derived fungus *Tritirachium* sp. SCSIO 41037. The compounds were purified by extraction, silica gel column chromatography and semi-preparative HPLC. Their structures were identified using NMR and HR-ESI-MS data. The absolute configurations of compounds **1** and **2** were determined by the calculated ECD. In bioassay, all compounds were screened for enzyme inhibitory activity against acetylcholinesterase (AChE) in both virtual screening and in vitro assays. The results revealed that compounds **3** and **5** exhibited moderate inhibitory effects, with IC<sub>50</sub> values of 0.32 and 0.46 mM, respectively. We also propose a biosynthetic pathway of tritianamides A (**1**) and B (**2**) originating from tryptophan.

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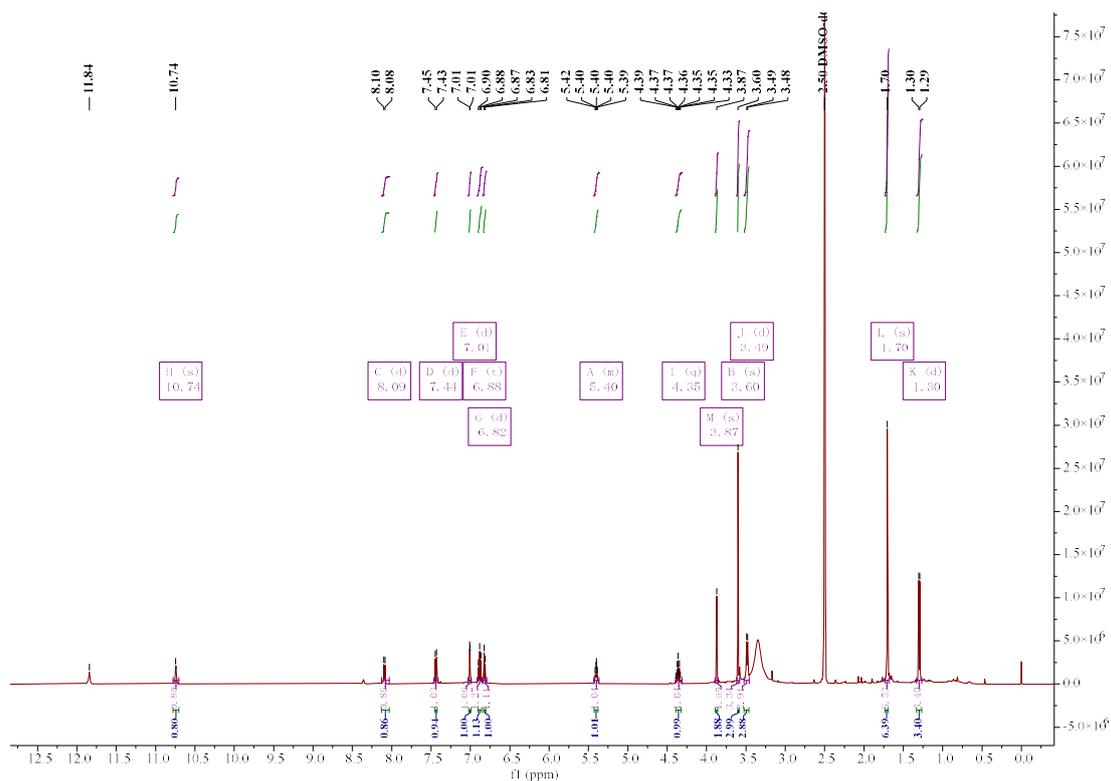


Figure S1. <sup>1</sup>H NMR of compound 1 (in DMSO-d<sub>6</sub>)

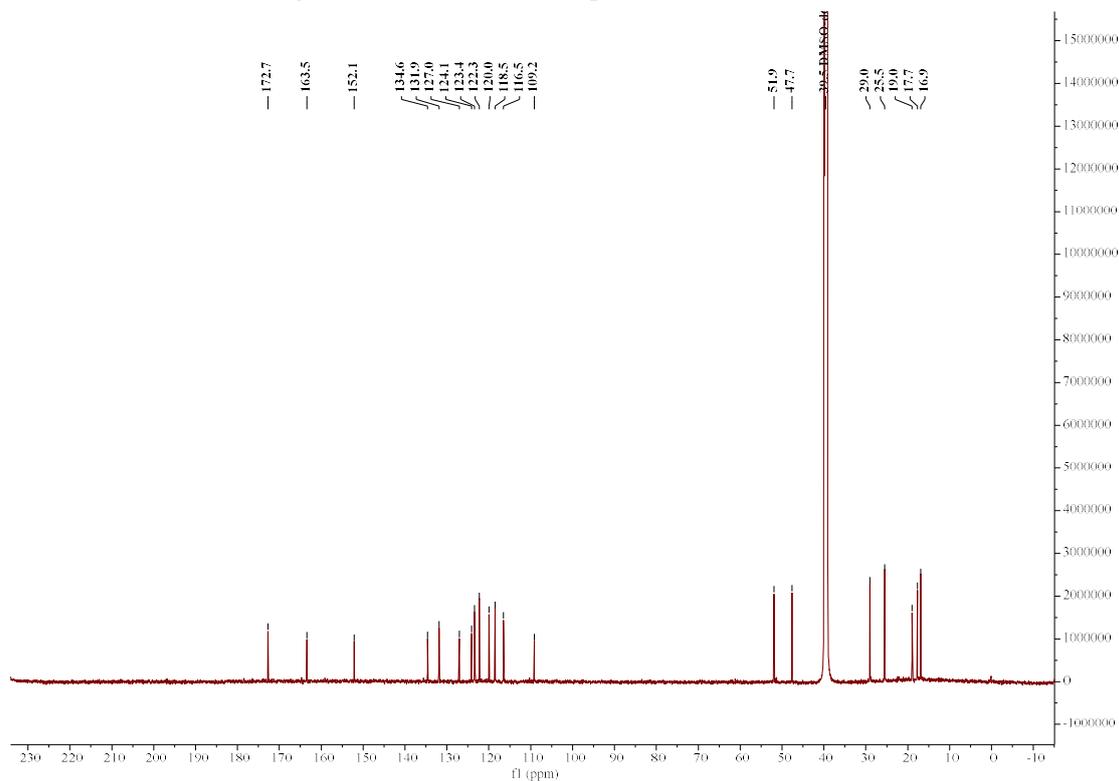


Figure S2. <sup>13</sup>C NMR of compound 1 (in DMSO-d<sub>6</sub>)

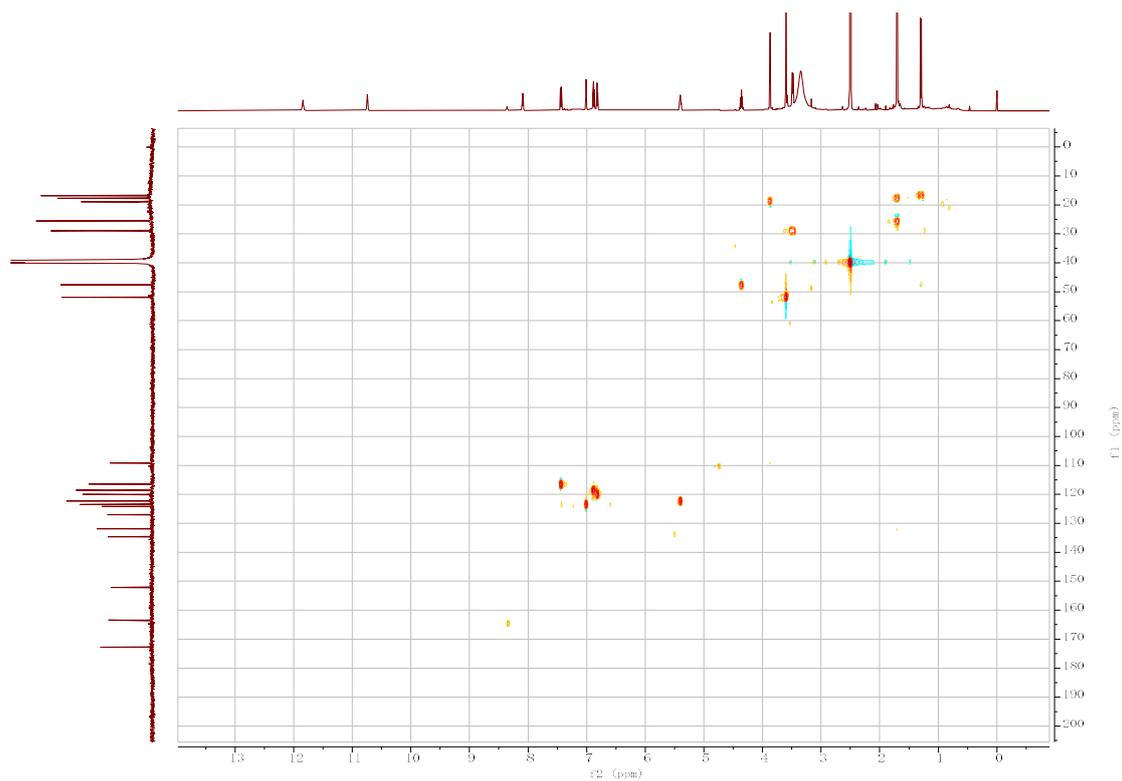


Figure S3.  $^1\text{H}$ - $^{13}\text{C}$  HSQC spectrum of compound **1** (DMSO- $d_6$ )

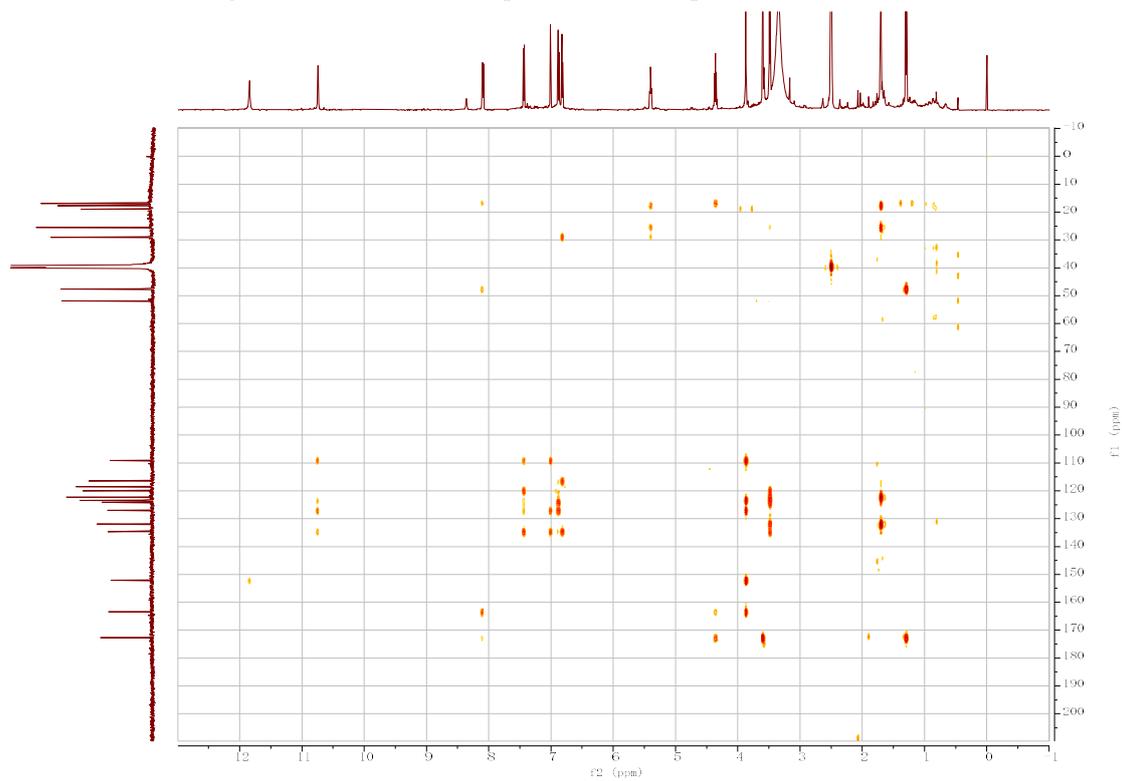
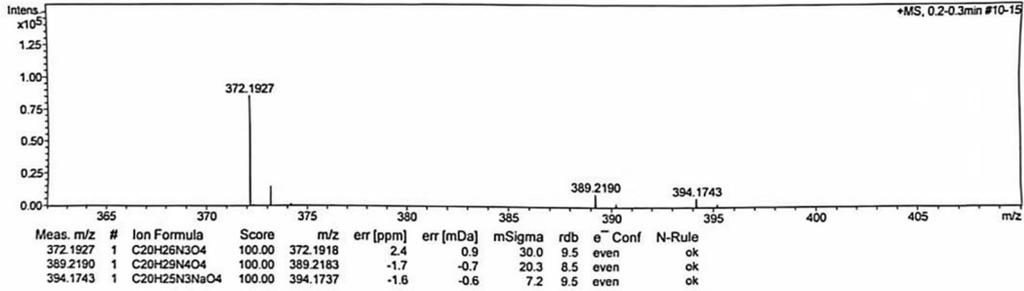


Figure S4.  $^1\text{H}$ - $^{13}\text{C}$  HMBC spectrum of compound **1** (DMSO- $d_6$ )

# Mass Spectrum SmartFormula Report

Analysis Info  
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Method LC\_DirectInfusion\_pos\_70-500mz.m  
Sample Name chenying\_LUF81\_pos  
Acquisition Date 2/26/2024 2:58:14 PM  
Operator SCSIO  
Instrument maXis  
255552.00029  
Comment

Acquisition Parameter  
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Focus Active Set Capillary 4500 V Set Dry Heater 180 °C  
Scan Begin 70 m/z Set End Plate Offset -500 V Set Dry Gas 4.0 l/min  
Scan End 1500 m/z Set Charging Voltage 0 V Set Divert Valve Waste  
Set Corona 0 nA Set APCI Heater 0 °C



chenying\_LUF81\_pos\_45\_01\_16794.d  
Bruker Compass DataAnalysis 4.1

printed: 2/26/2024 3:01:57 PM

by: SCSIO

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Figure S5. HRESIMS spectrum of compound 1

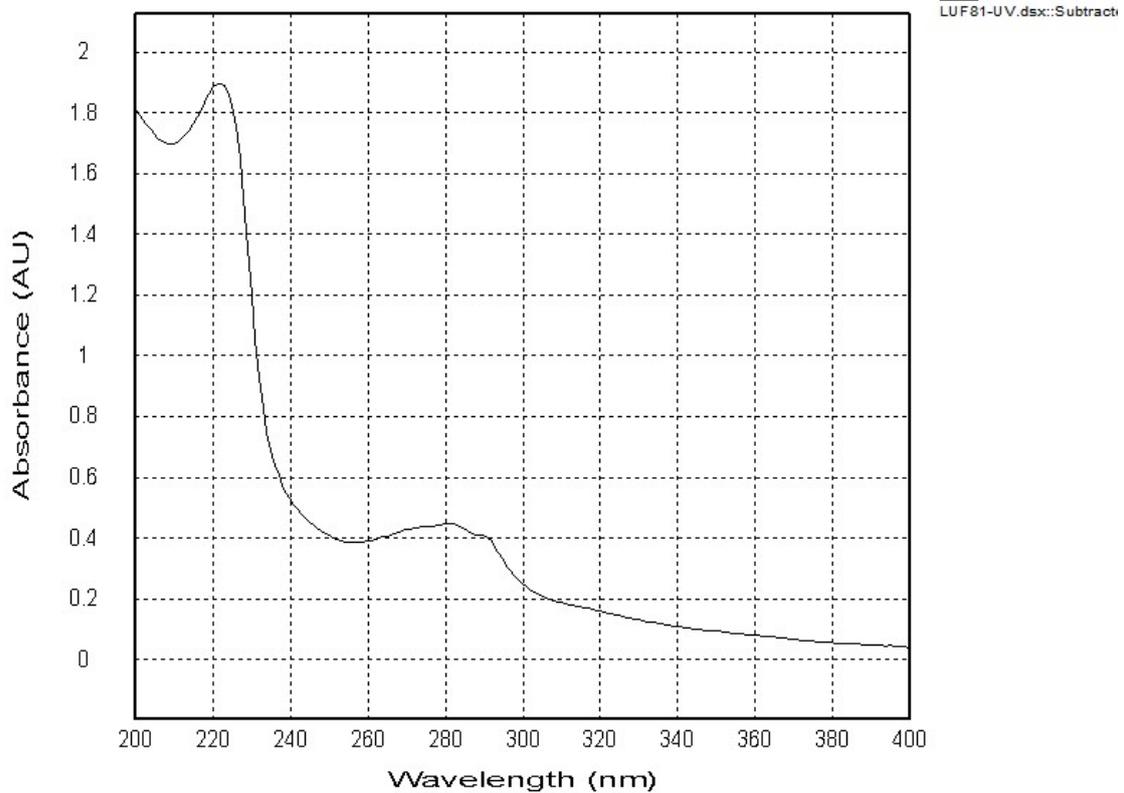


Figure S6. UV of compound 1

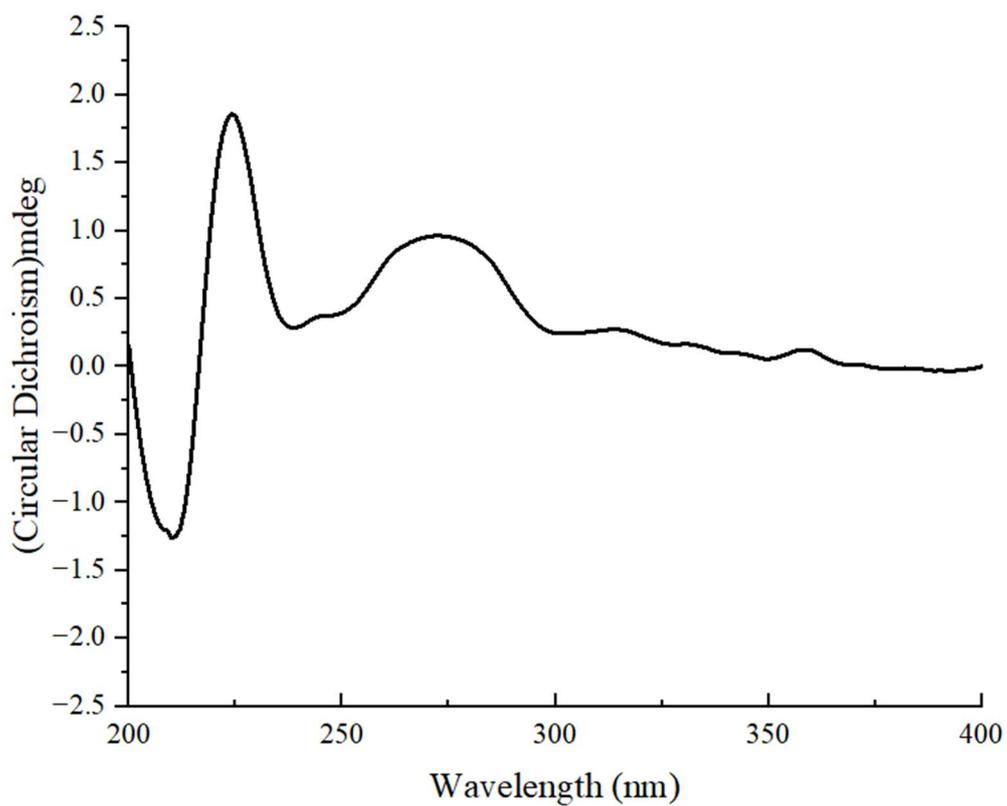


Figure S7. CD spectrum of compound 1

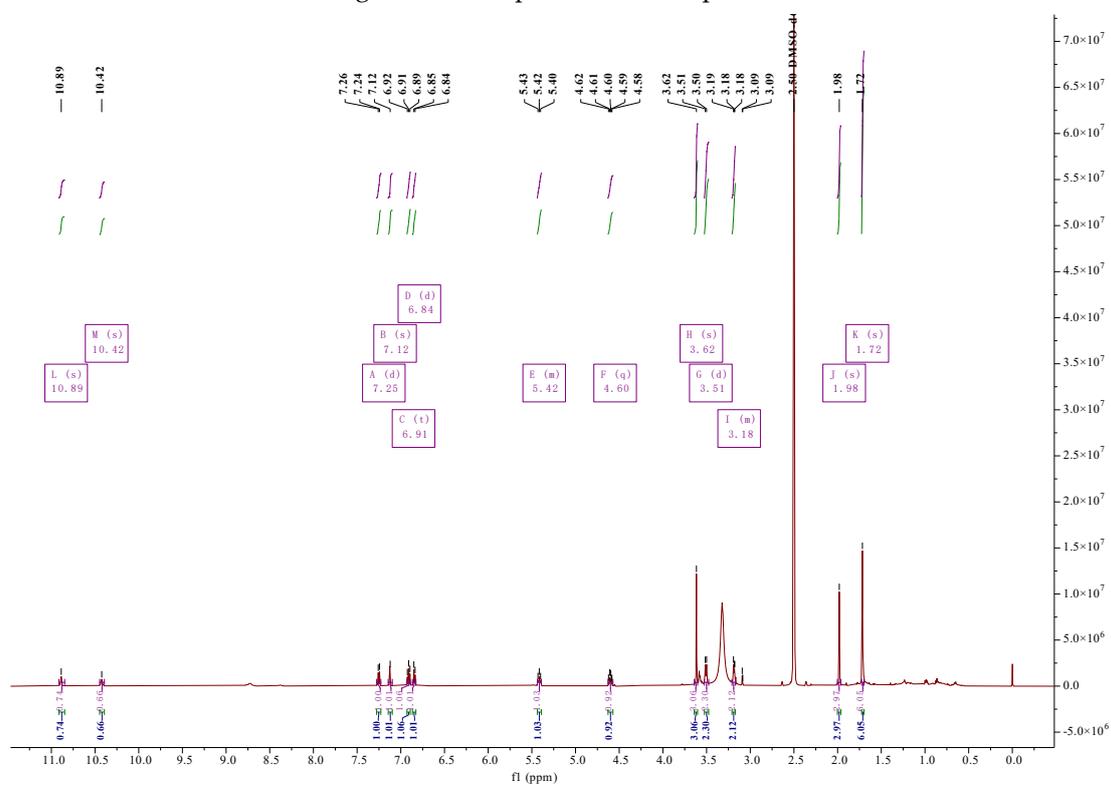


Figure S8. <sup>1</sup>H NMR of compound 2 (in DMSO-*d*<sub>6</sub>)

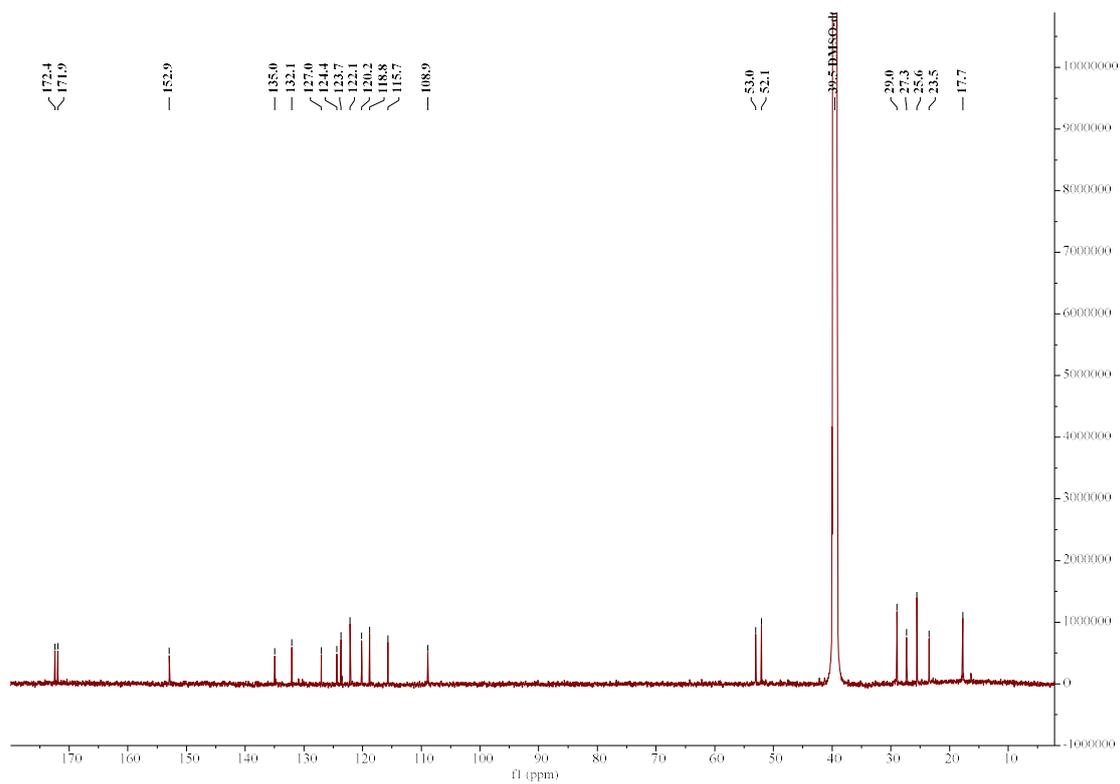


Figure S9.  $^{13}\text{C}$  NMR of compound 2 (in DMSO- $d_6$ )

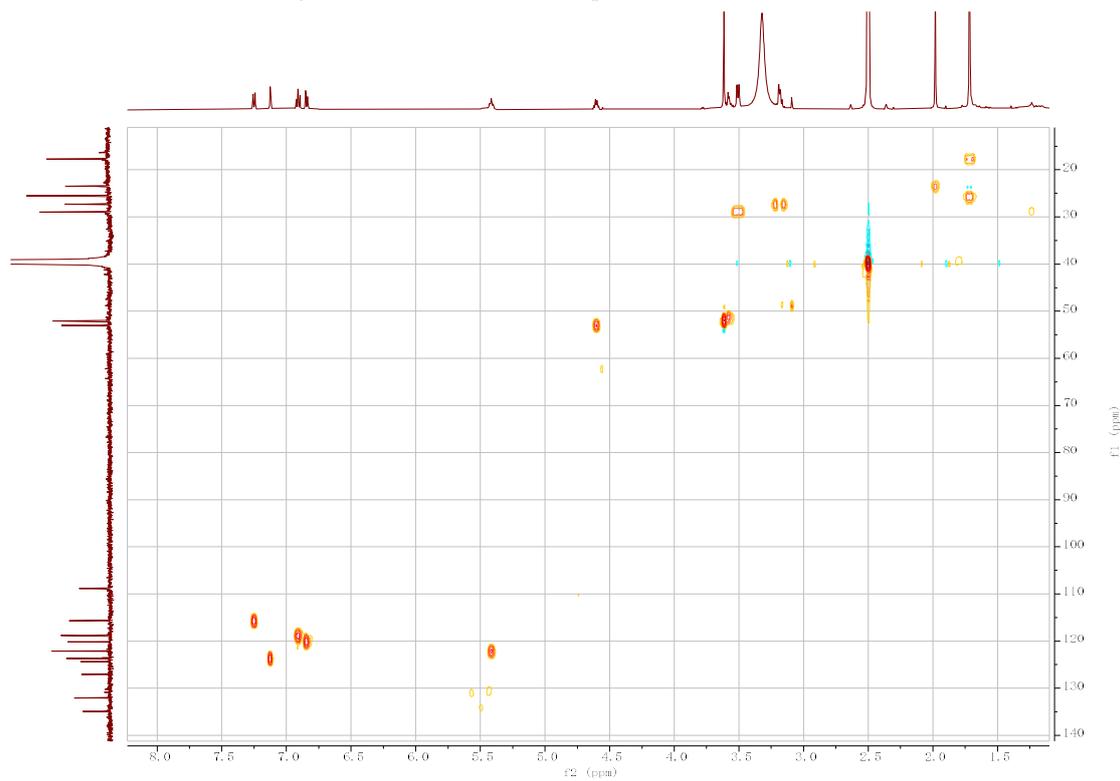


Figure S10.  $^1\text{H}$ - $^{13}\text{C}$  HSQC spectrum of compound 2 (DMSO- $d_6$ )

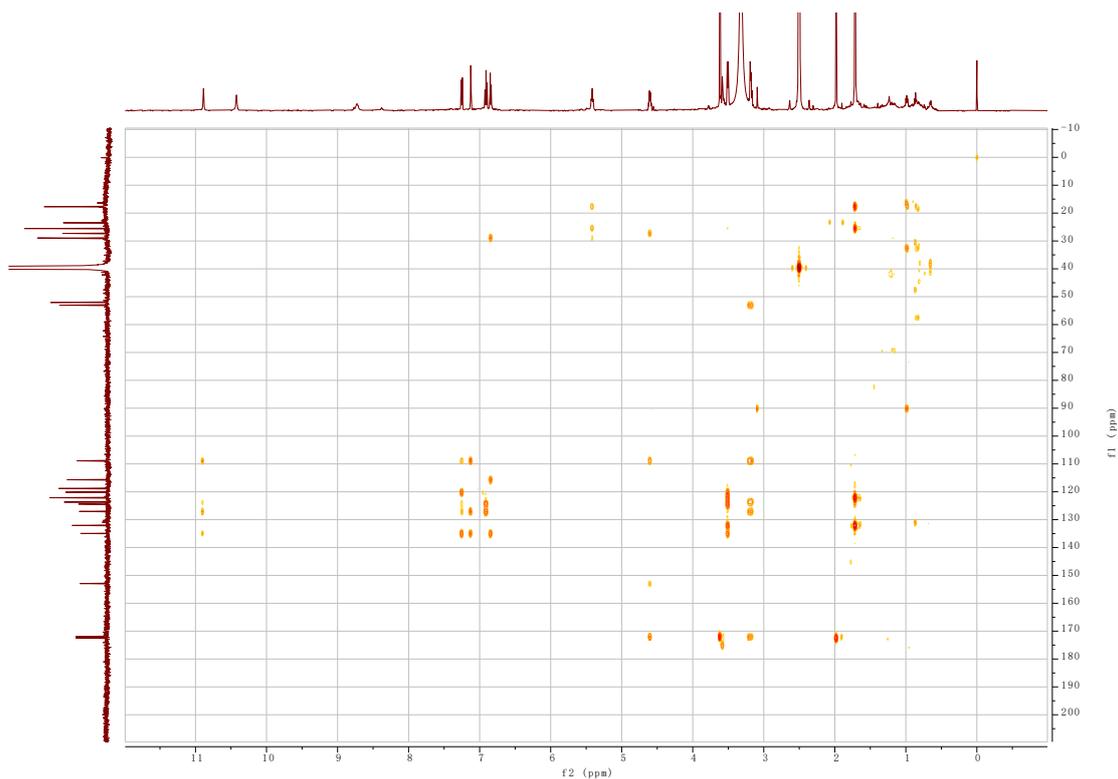


Figure S11.  $^1\text{H}$ - $^{13}\text{C}$  HMBC spectrum of compound 2 (DMSO- $d_6$ )

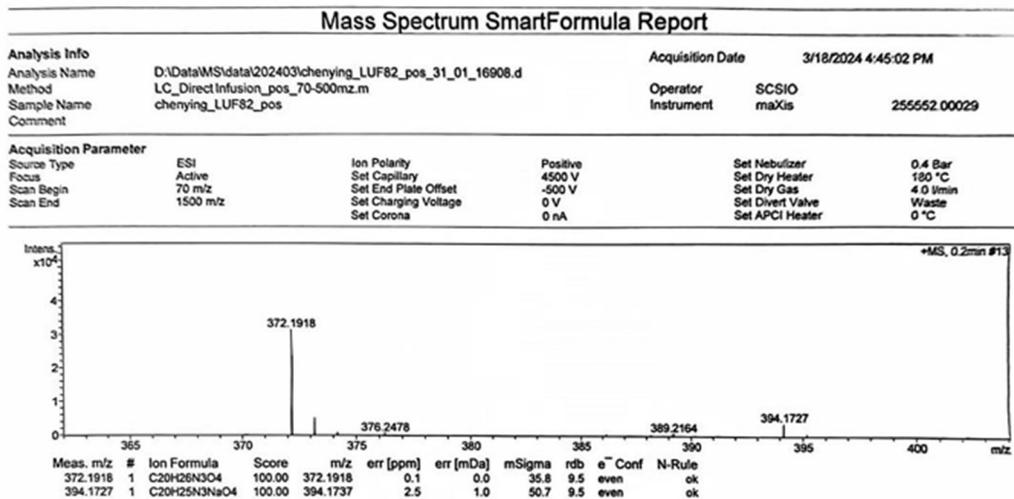


Figure S12. HRESIMS spectrum of compound 2

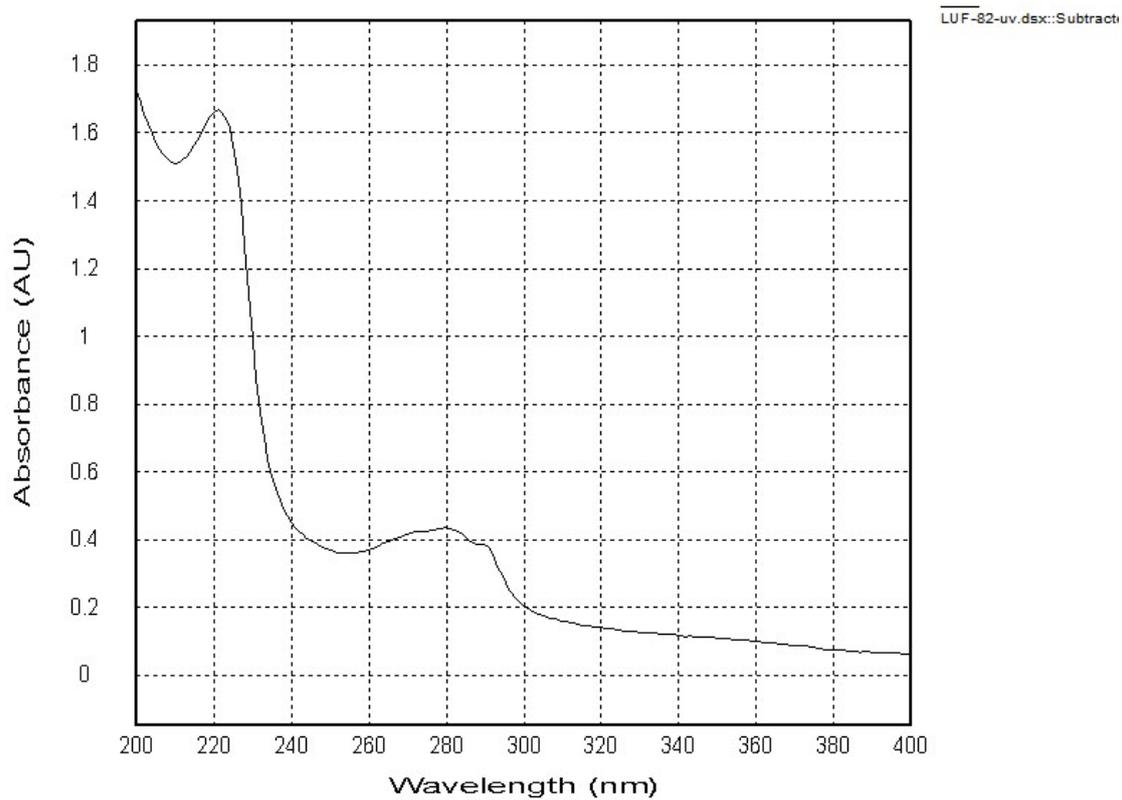


Figure S13. UV spectrum of compound 2

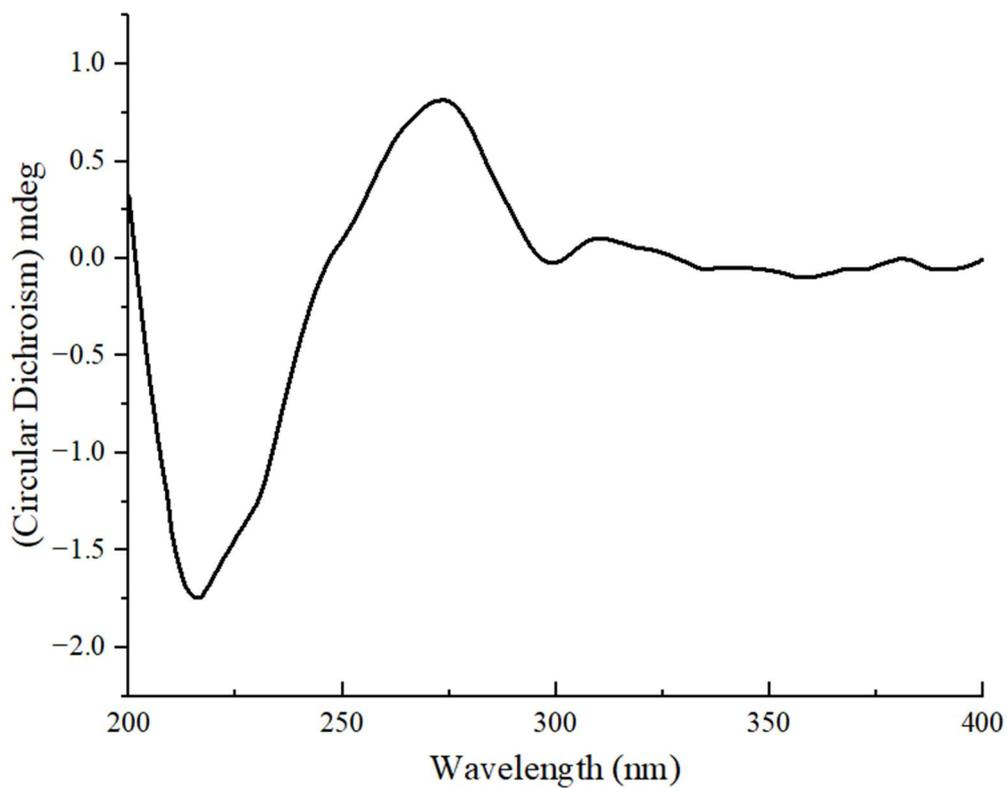


Figure S14. CD spectrum of compound 2