

Supplementary Materials: Three New Sesquiterpenoids and One New Sesquiterpoid Derivative from Chinese Eaglewood

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Table S1. Anti-inflammatory activity of the new compounds.

Compound	IC ₅₀ (μM)
1	>100
2	8.1
3	>100
4	>100
Aminoguanidine hydrochloride ^a	11.6

^a positive control.

Table S2. Crystallographic data of Compound (1).

Identification Code	cu_dm15185_0m
Empirical formula	C ₁₅ H ₂₀ O ₃
Formula weight	248.31
Temperature	296.15 K
Wavelength	1.54178 Å
Crystal system	Monoclinic
Space group	C 1 2 1
Unit cell dimensions	a = 17.6380(8) Å, α = 90°; b = 6.6237(4) Å, β = 109.510(4)°; c = 12.0602(7) Å, γ = 90°
Volume	1328.08 (13) Å ³
Z	4
Calculated density	1.242 mg/m ³
Absorption coefficient	0.685 mm ⁻¹
F(000)	536
Crystal size	0.18 × 0.11 × 0.06 mm ³
Theta range for data collection	5.321 to 69.651°
	-19 ≤ h ≤ 21
Limiting indices	-7 ≤ k ≤ 5
	-14 ≤ l ≤ 14
Reflections collected/unique	4997/1923 [R(int) = 0.0514]
Completeness to theta = 67.679°	99.2%
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7533 and 0.4608
Refinement method	Full-matrix least-squares on F ²
Data/restraints/parameters	1923/1/166
Goodness-of-fit on F ²	1.029
Final R indices [I > 2σ(I)]	R ₁ = 0.0478, wR ₂ = 0.1265
R indices (all data)	R ₁ = 0.0504, wR ₂ = 0.1315
Absolute structure parameter	0.1(3)
Largest diff. peak and hole	0.121 and -0.162 e·Å ⁻³

Crystallographic data for have been deposited at the Cambridge Crystallographic Data Centre (deposition No. CCDC 928251). Copies of these data can be obtained free of charge via www.ccdc.cam.ac.uk/conts/retrieving.html or from the Cambridge Crystallographic Data Centre, 12, Union Road, Cambridge CB21EZ, UK. [Fax: +44-1223-336-033; or email: deposit@ccdc.cam.ac.uk].

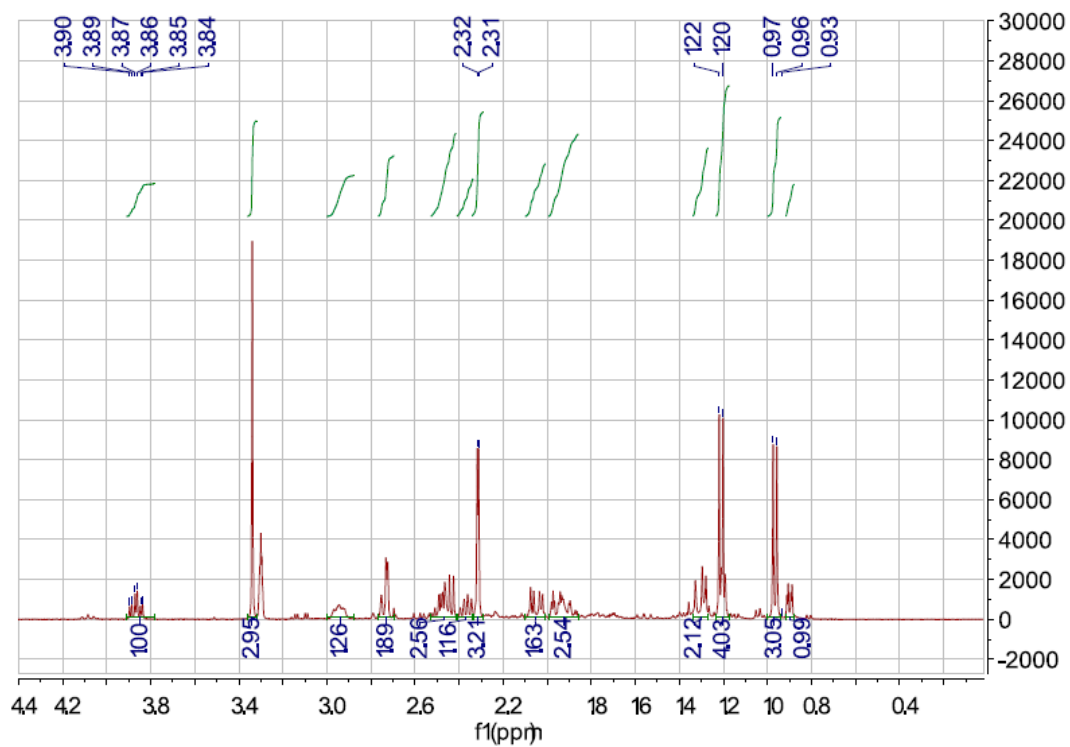


Figure S1. ^1H NMR spectrum of compound (1) (CD_3OD , 400 MHz).

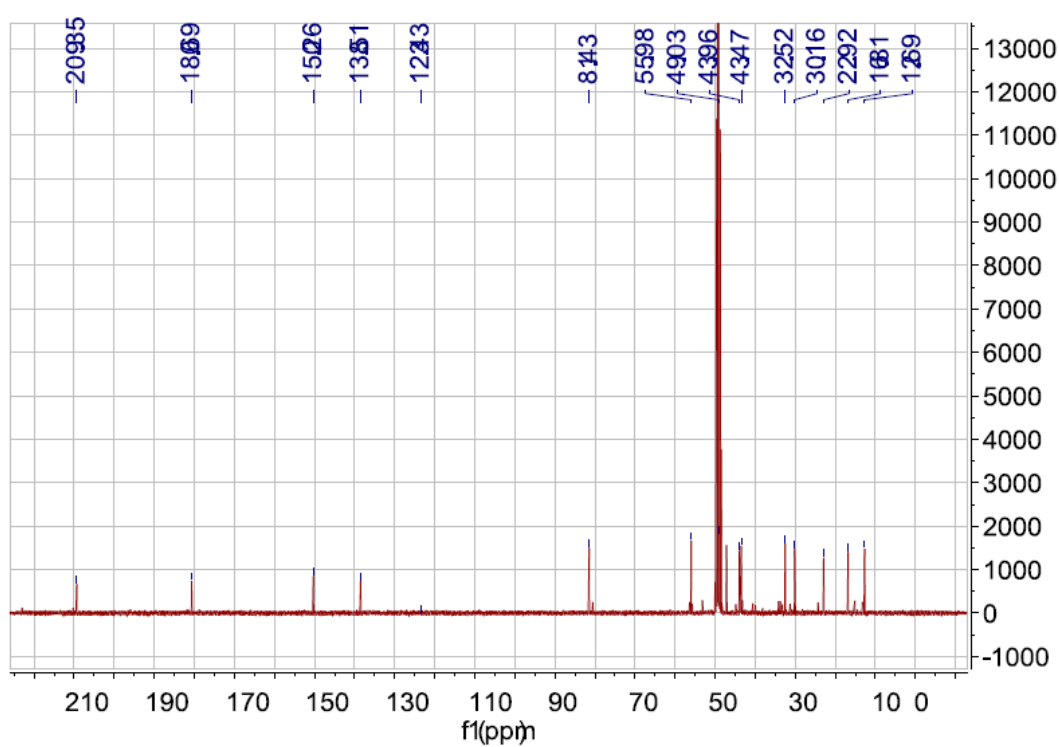


Figure S2. ^{13}C NMR spectrum of compound (1) (CD_3OD , 100 MHz).

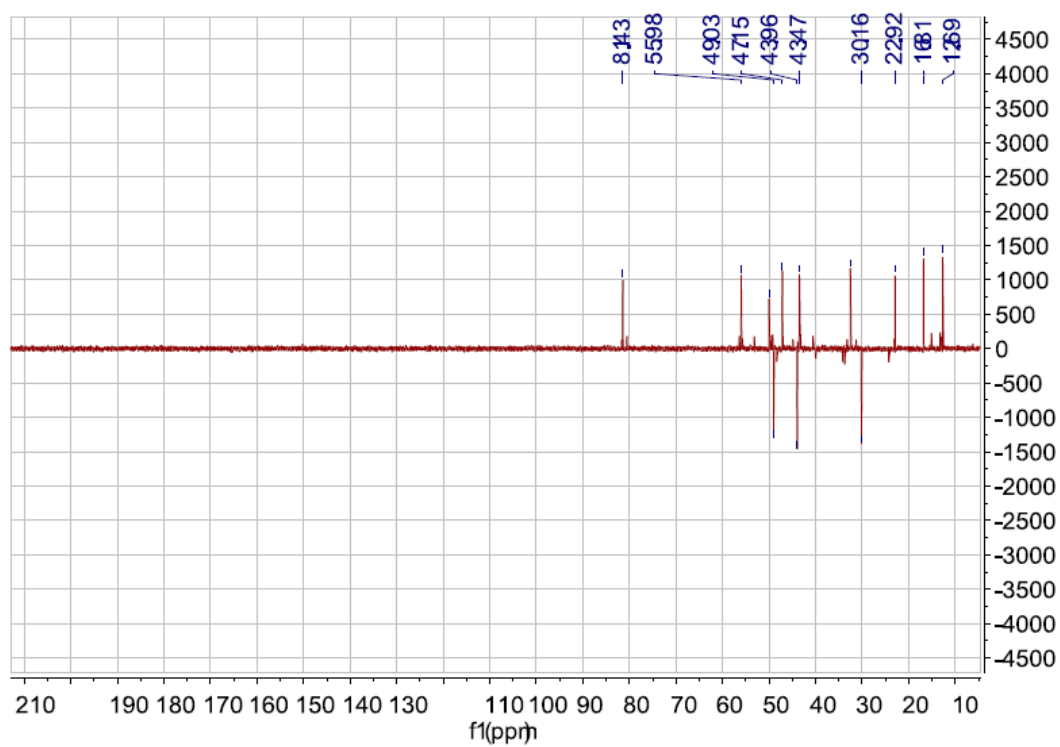


Figure S3. DEPT spectrum of compound (1).

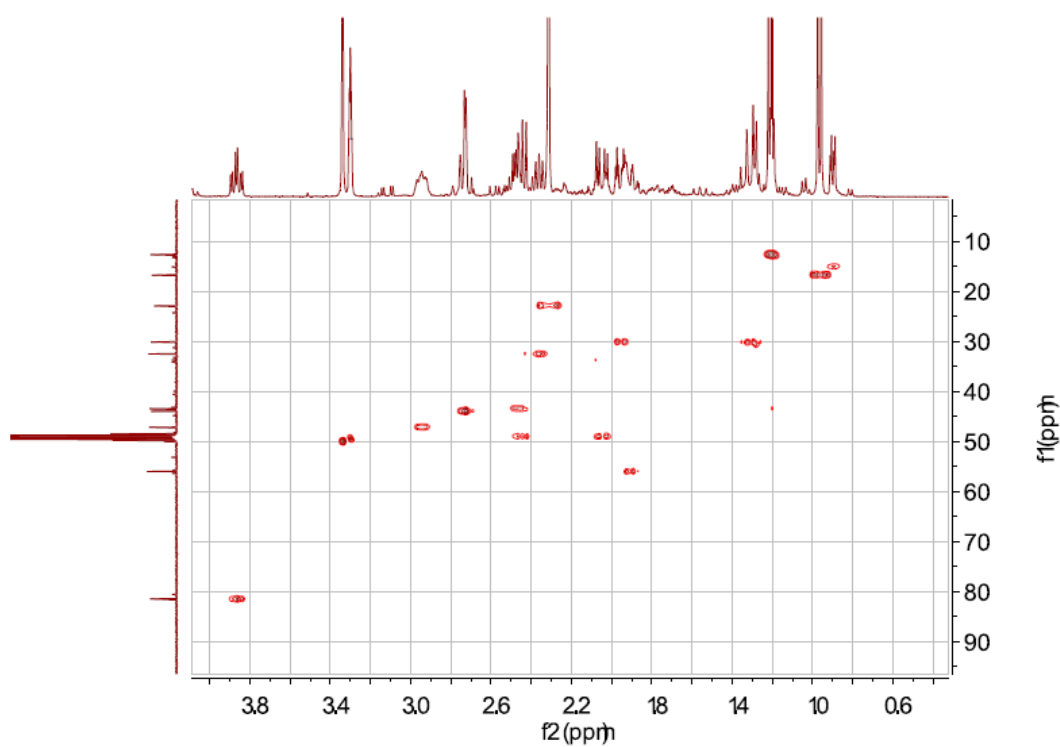


Figure S4. HSQC spectrum of compound (1).

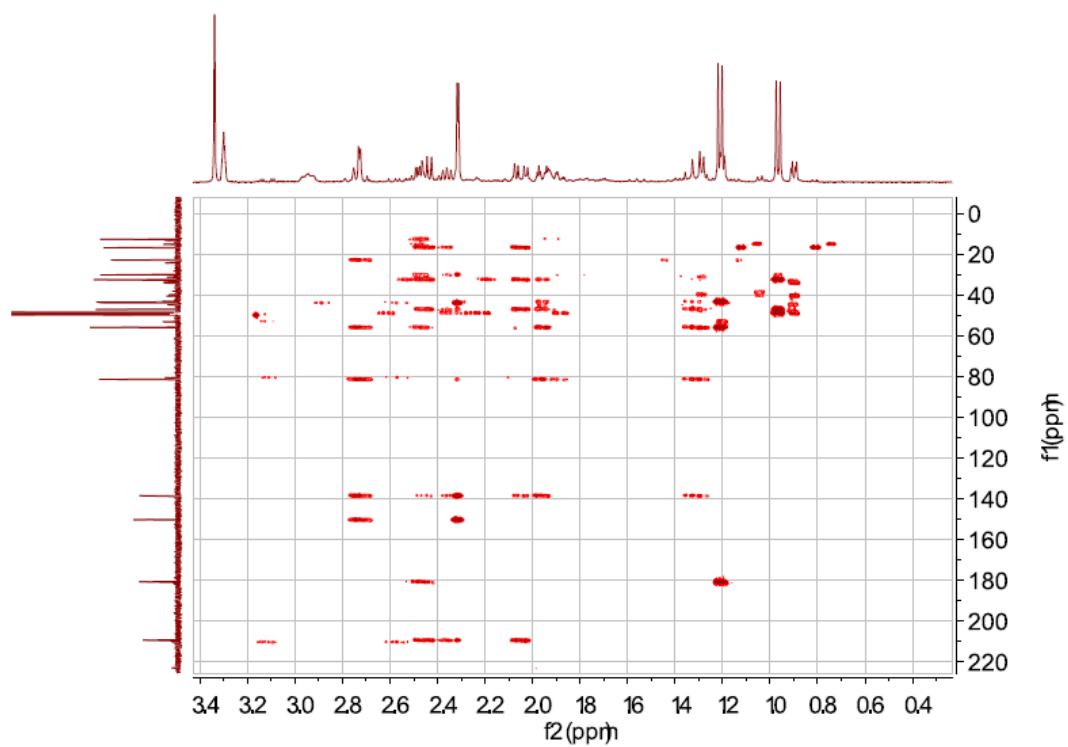


Figure S5. HMBC spectrum of compound (1).

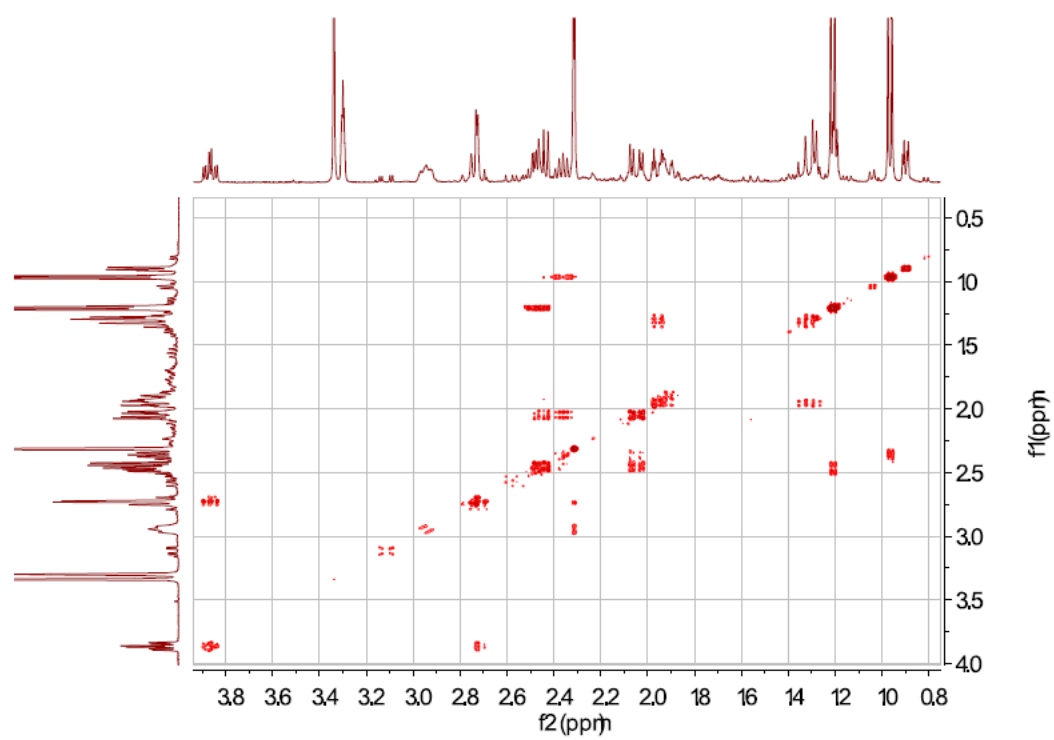


Figure S6. ¹H-¹H COSY spectrum of compound (1).

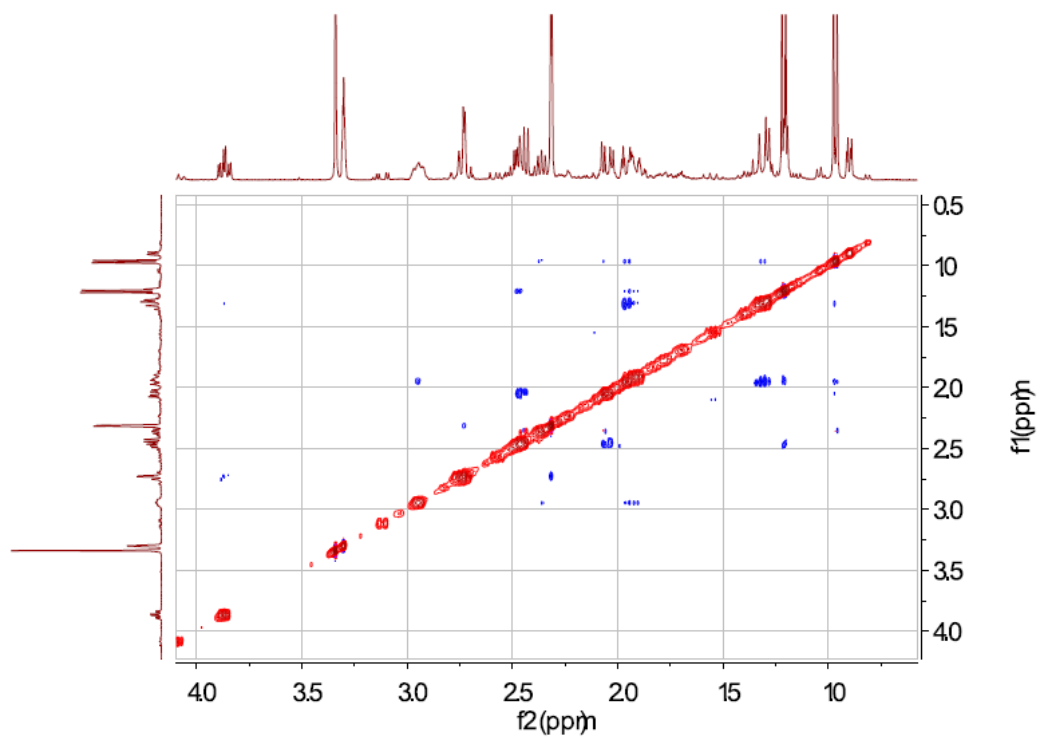


Figure S7. NOESY spectrum of compound (1).

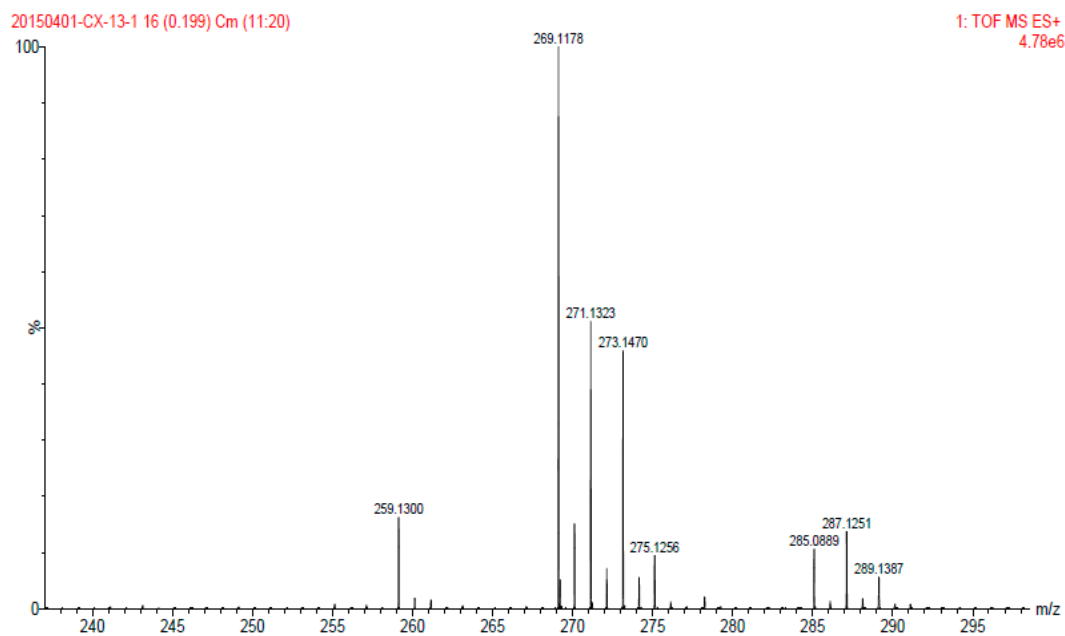


Figure S8. HR-ESIMS spectrum of compound (1).

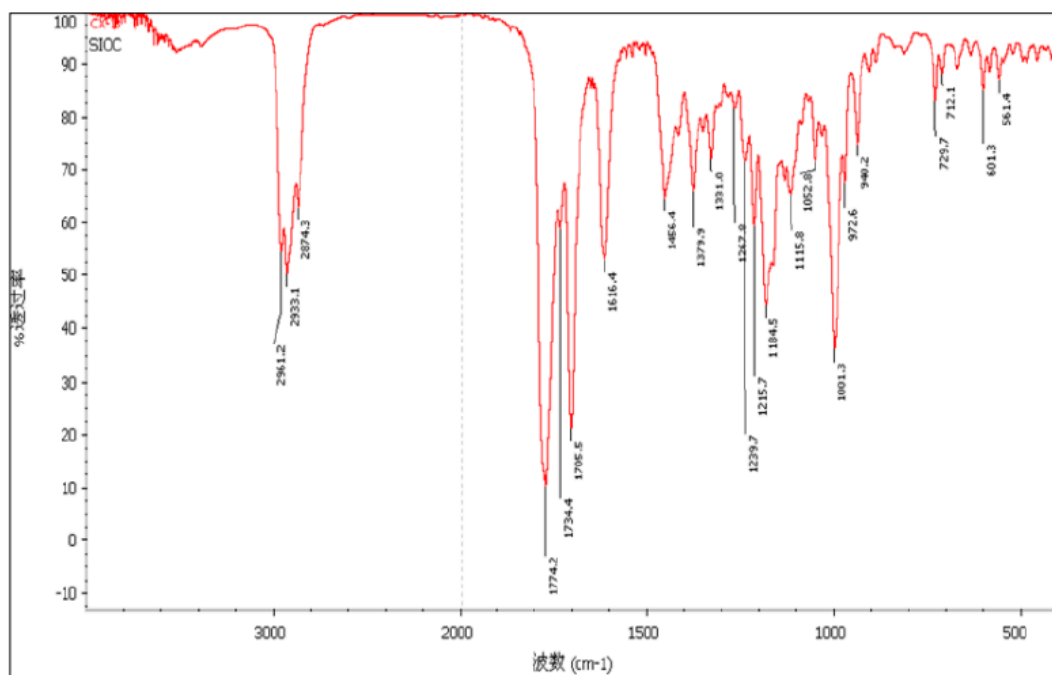
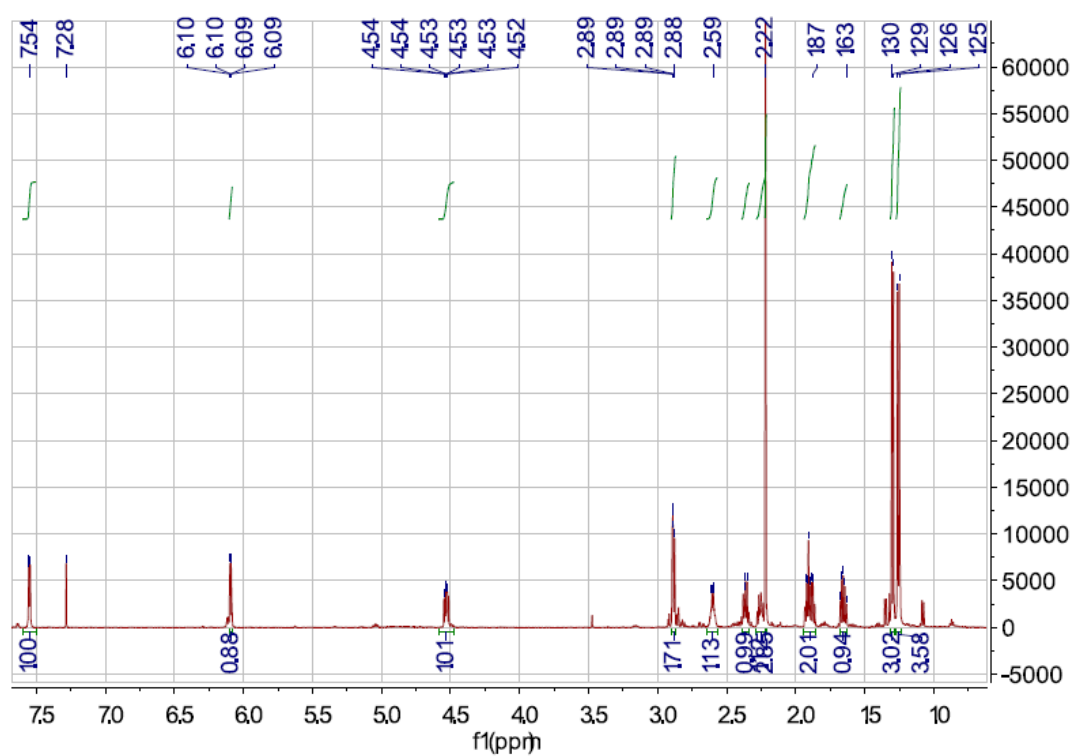


Figure S9. IR of compound (1).

Figure S10. ¹H NMR spectrum of compound (2) (CDCl₃, 600 MHz).

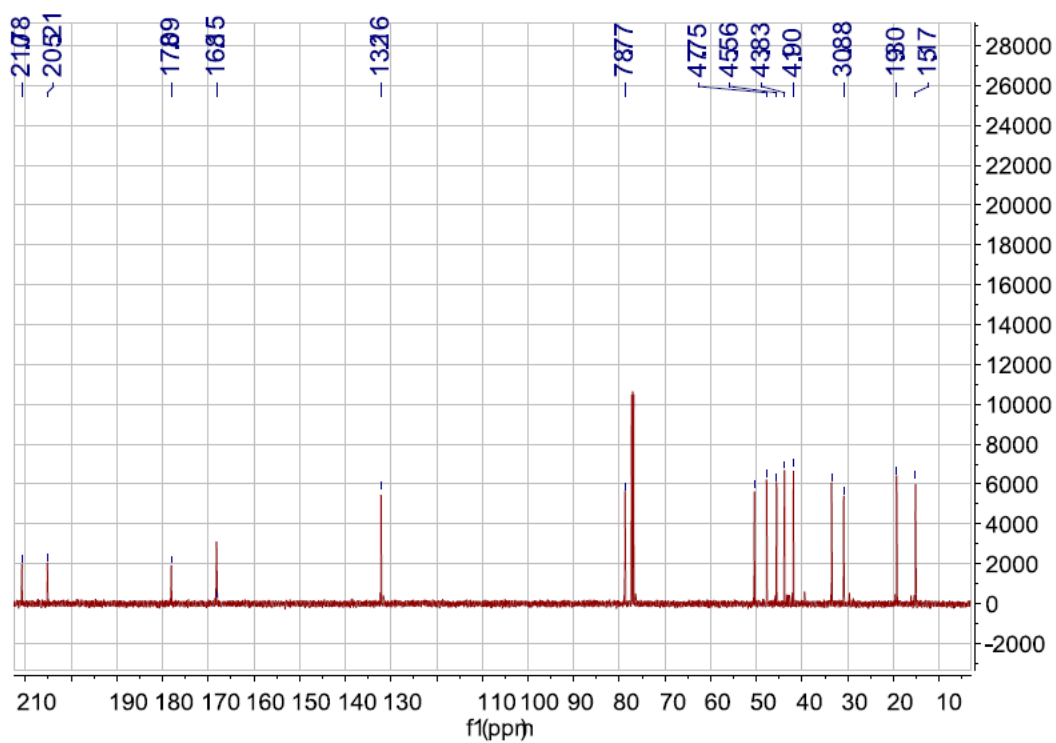


Figure S11. ¹³C NMR spectrum of compound (2) (CDCl₃, 150 MHz).

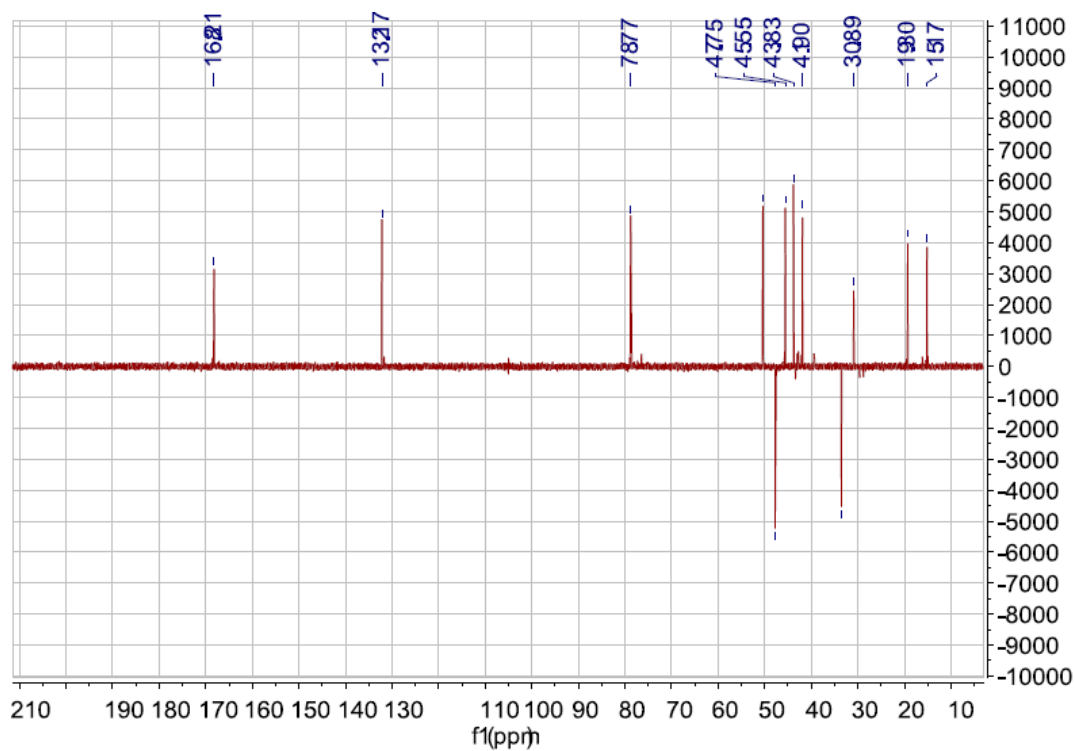


Figure S12. DEPT spectrum of compound (2).

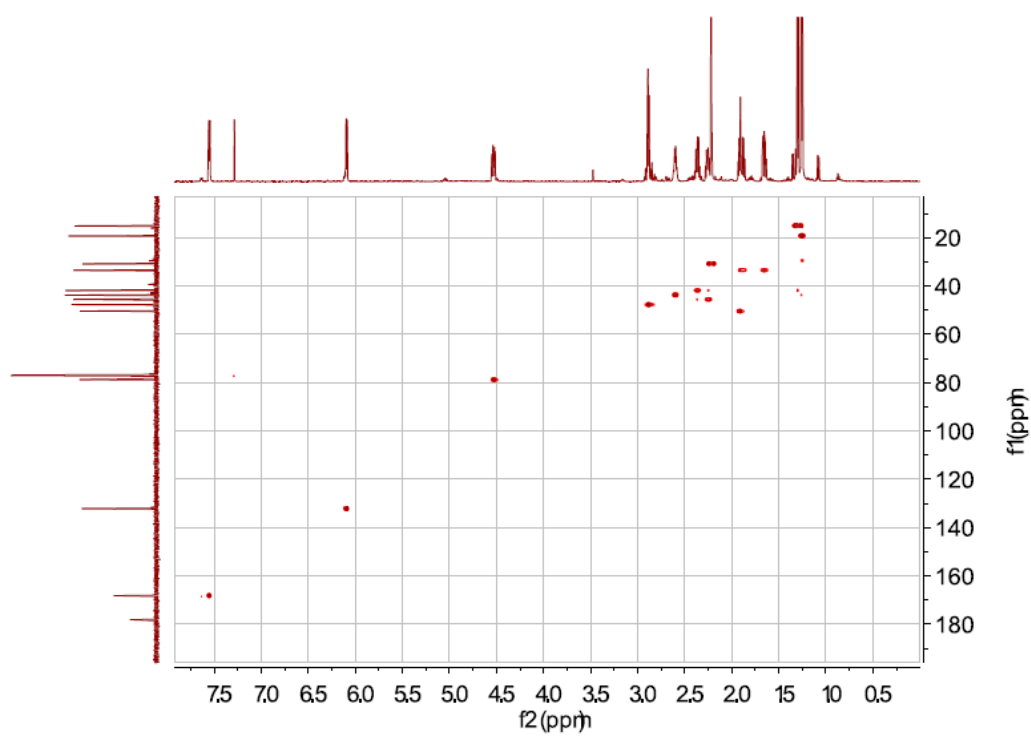


Figure S13. HSQC spectrum of compound (2).

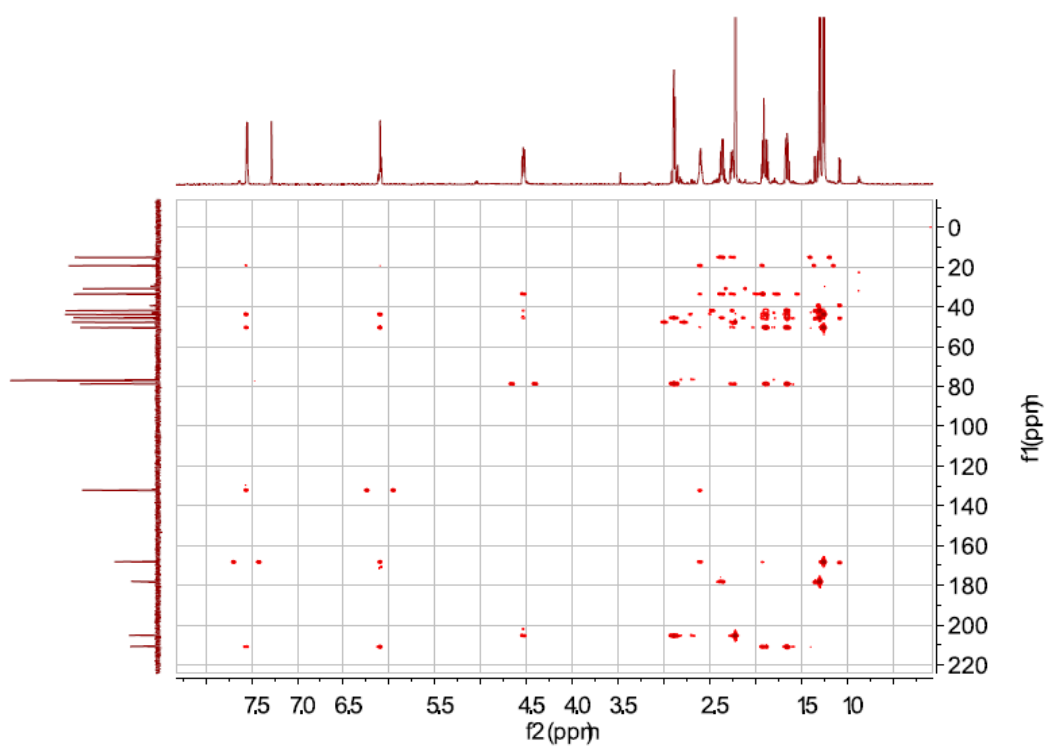


Figure S14. HMBC spectrum of compound (2).

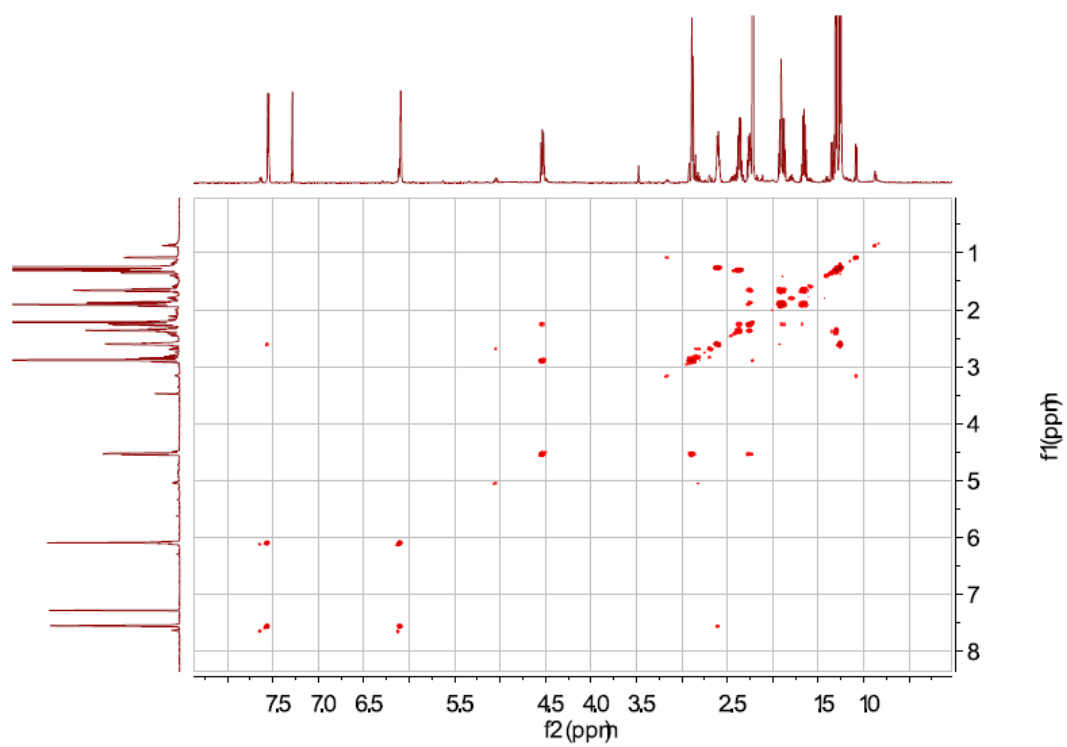


Figure S15. ^1H - ^1H COSY spectrum of compound (2).

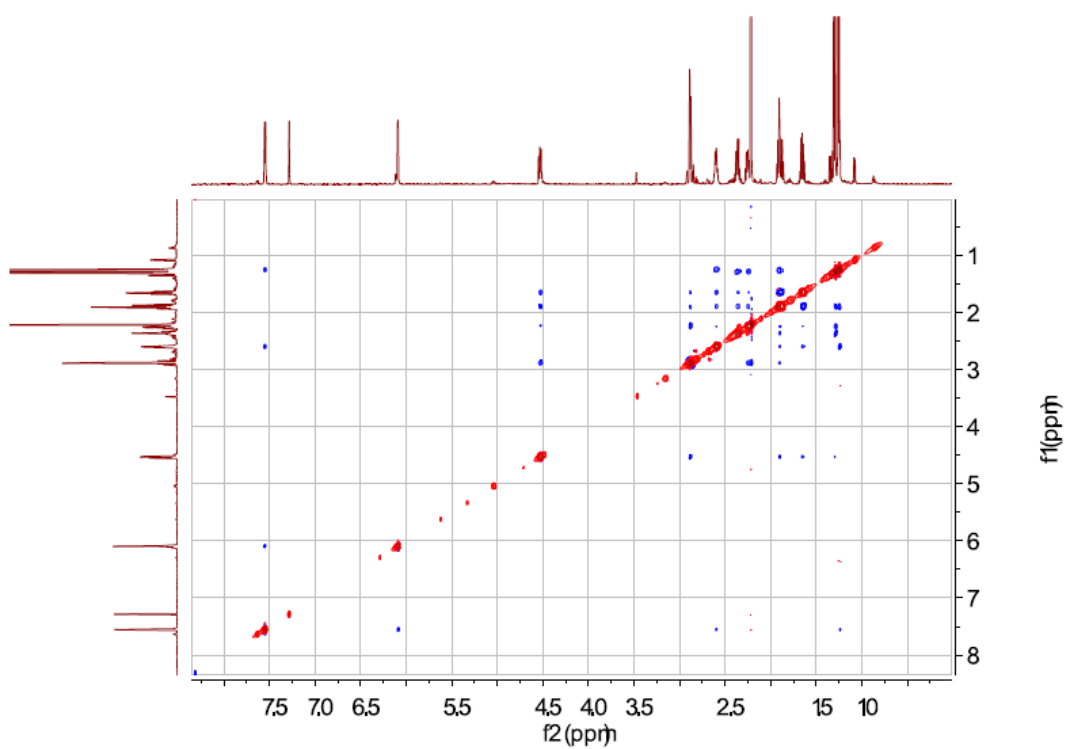


Figure S16. NOESY spectrum of compound (2).

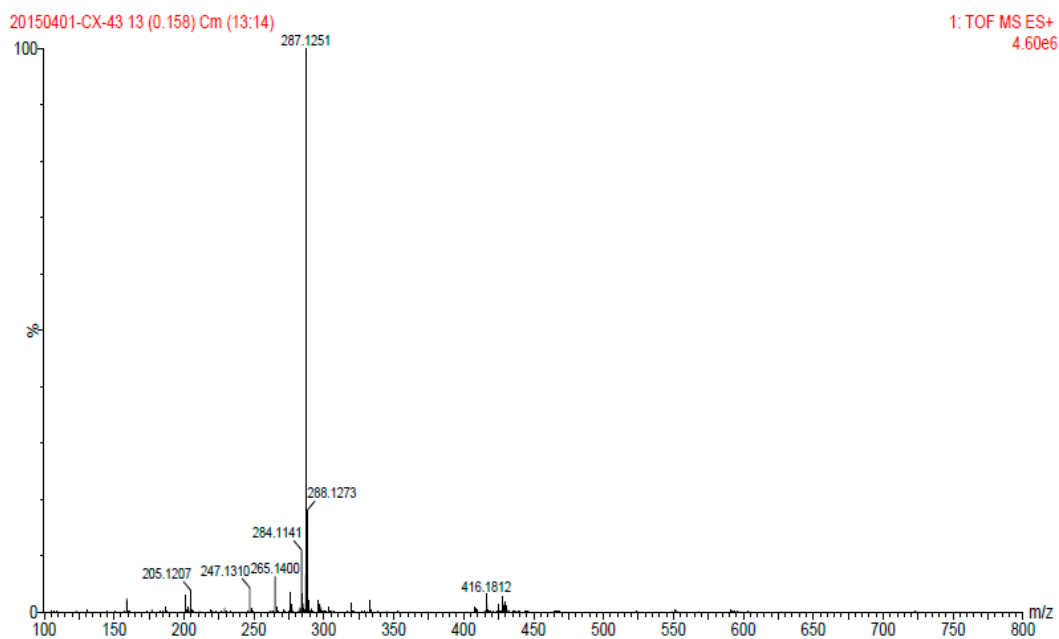


Figure S17. HR-ESIMS spectrum of compound (2).

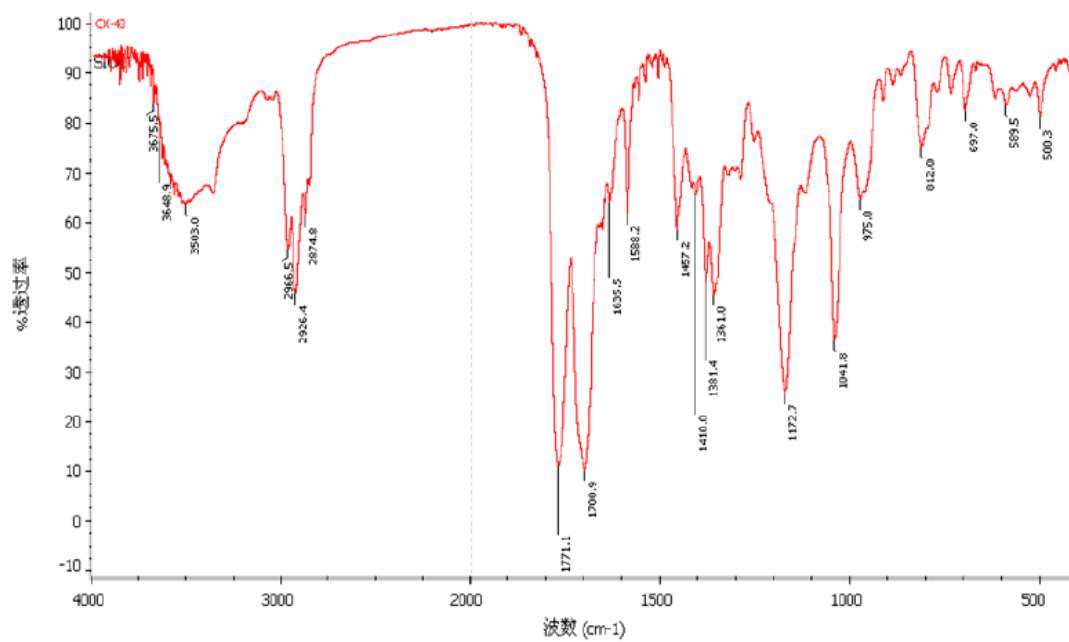


Figure S18. IR of compound (2).

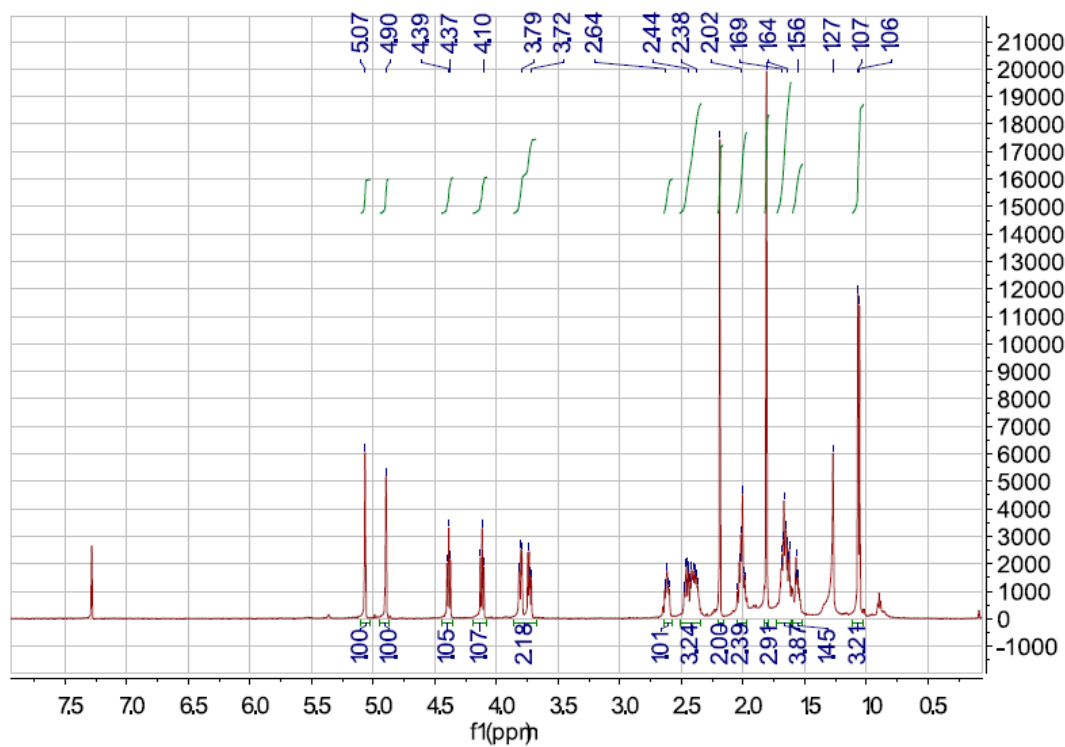


Figure S19. ¹H NMR spectrum of compound (3) (CDCl₃, 600 MHz).

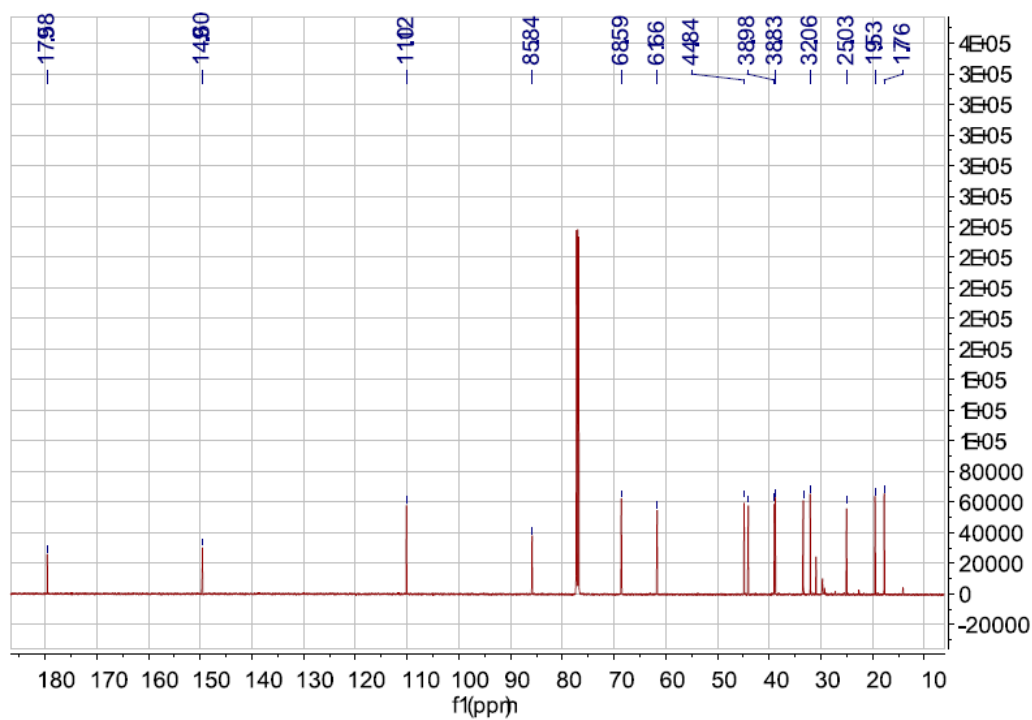


Figure S20. ¹³C NMR spectrum of compound (3) (CDCl₃, 150 MHz).

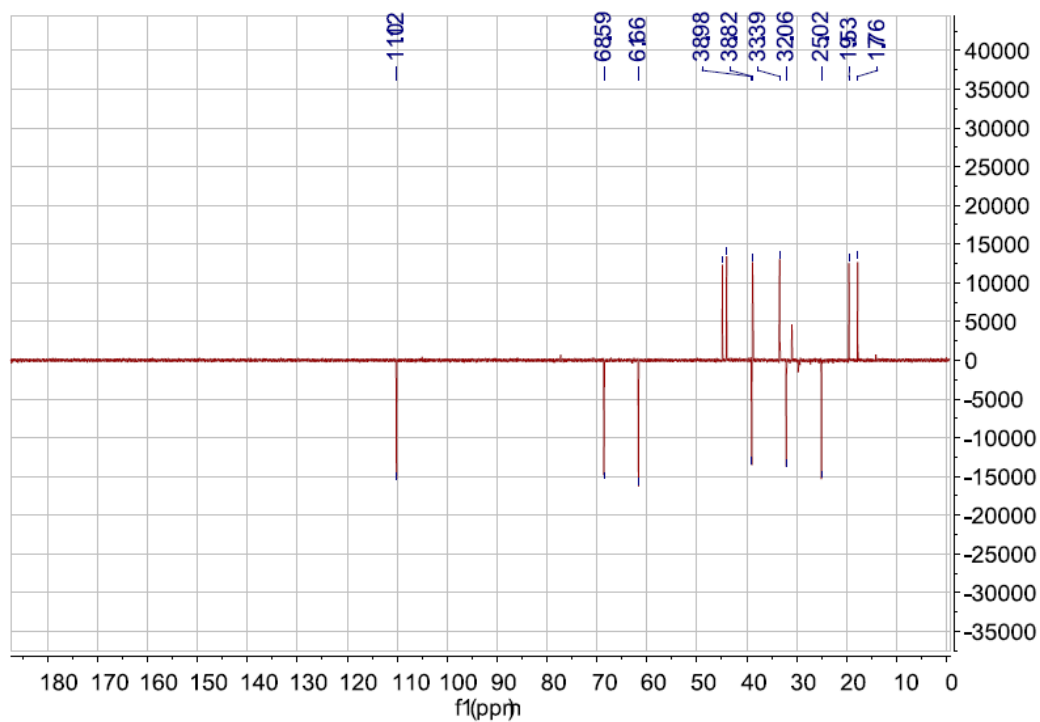


Figure S21. DEPT spectrum of compound (3).

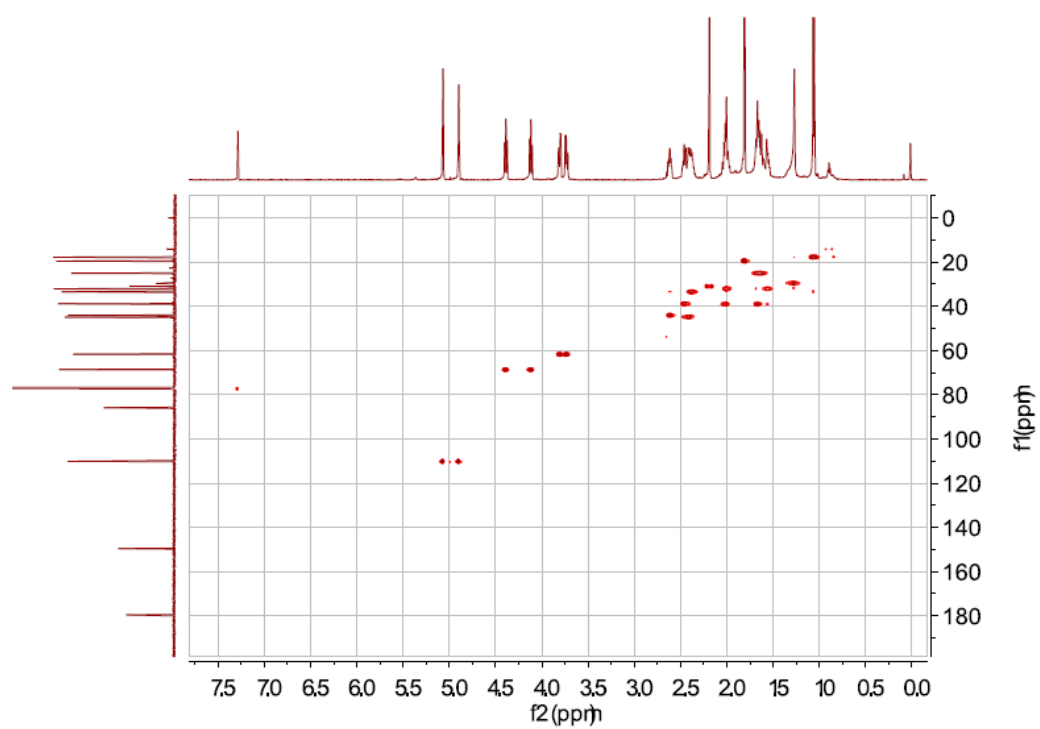


Figure S22. HSQC spectrum of compound (3).

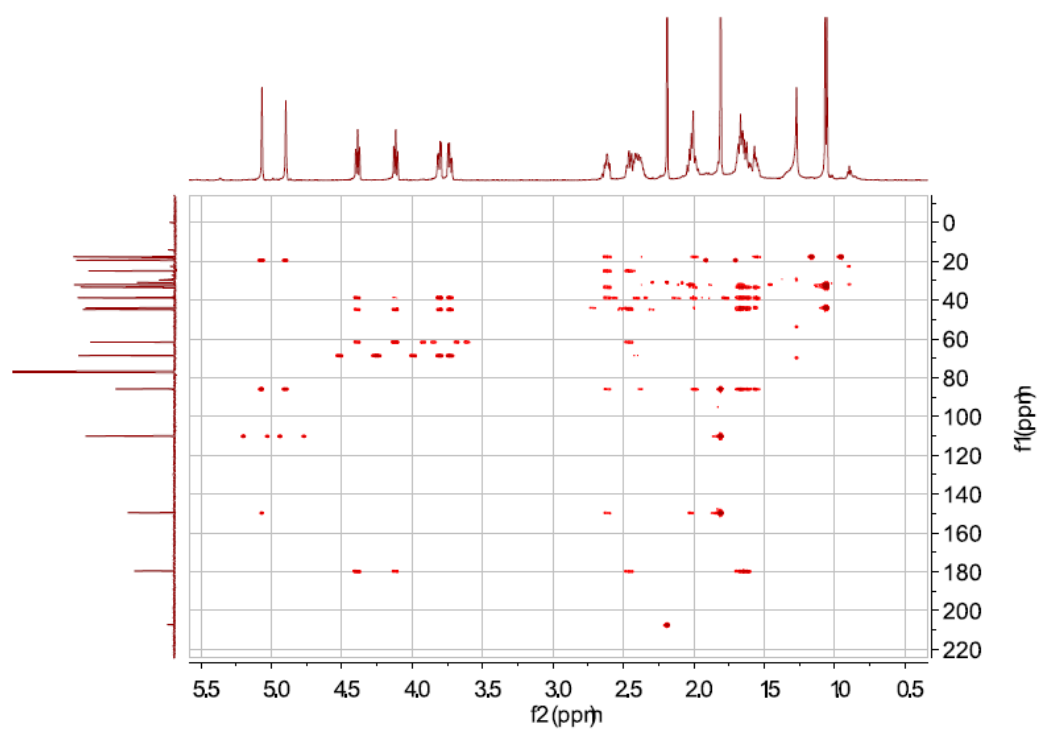


Figure S23. HMBC spectrum of compound (3).

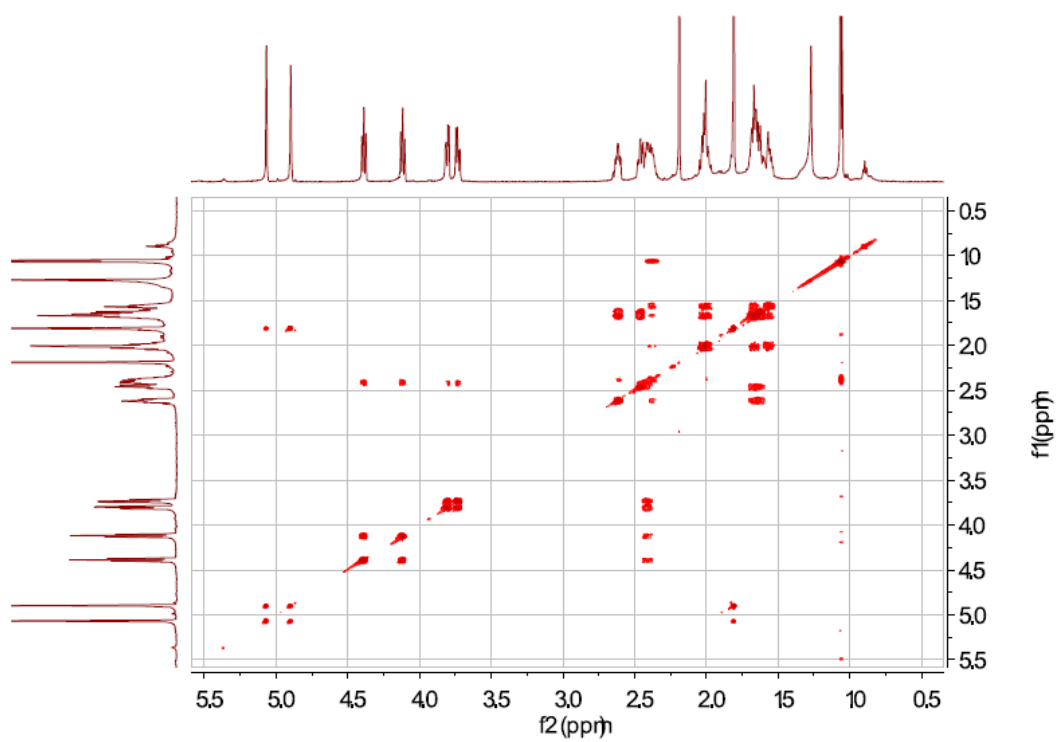


Figure S24. ¹H-¹H COSY spectrum of compound (3).

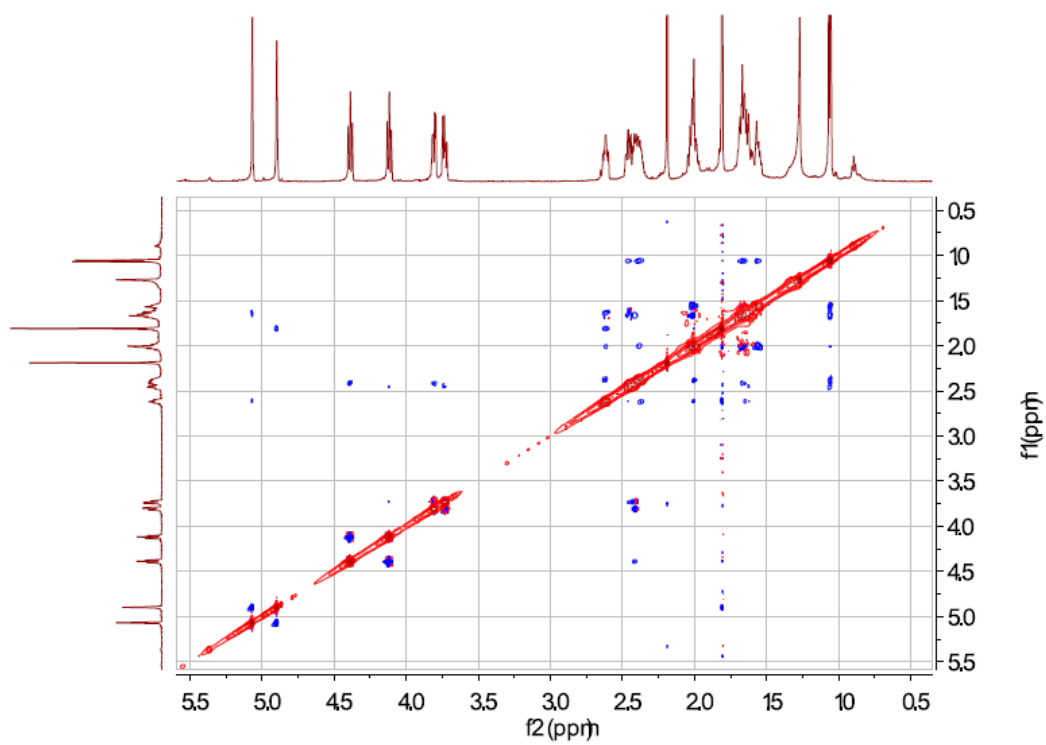


Figure S25. NOESY spectrum of compound (3).

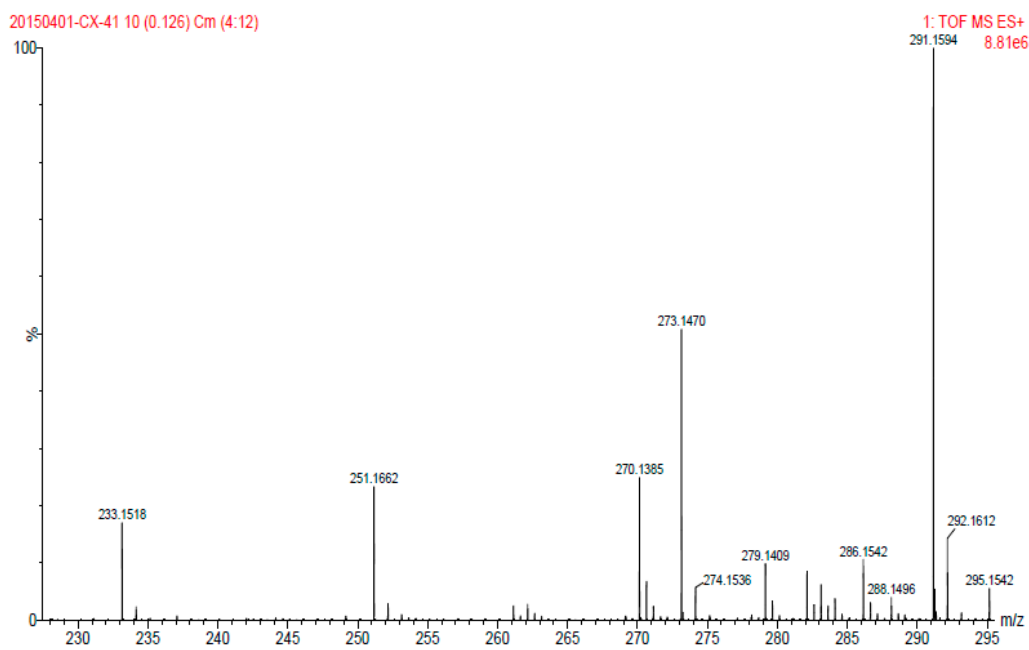


Figure S26. HR-ESIMS spectrum of compound (3).

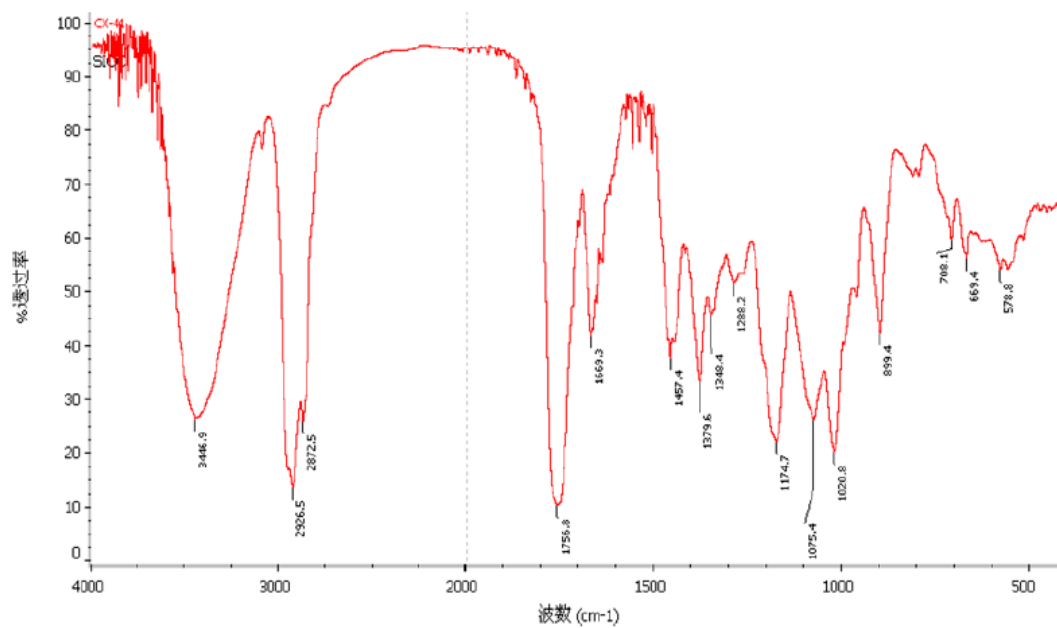
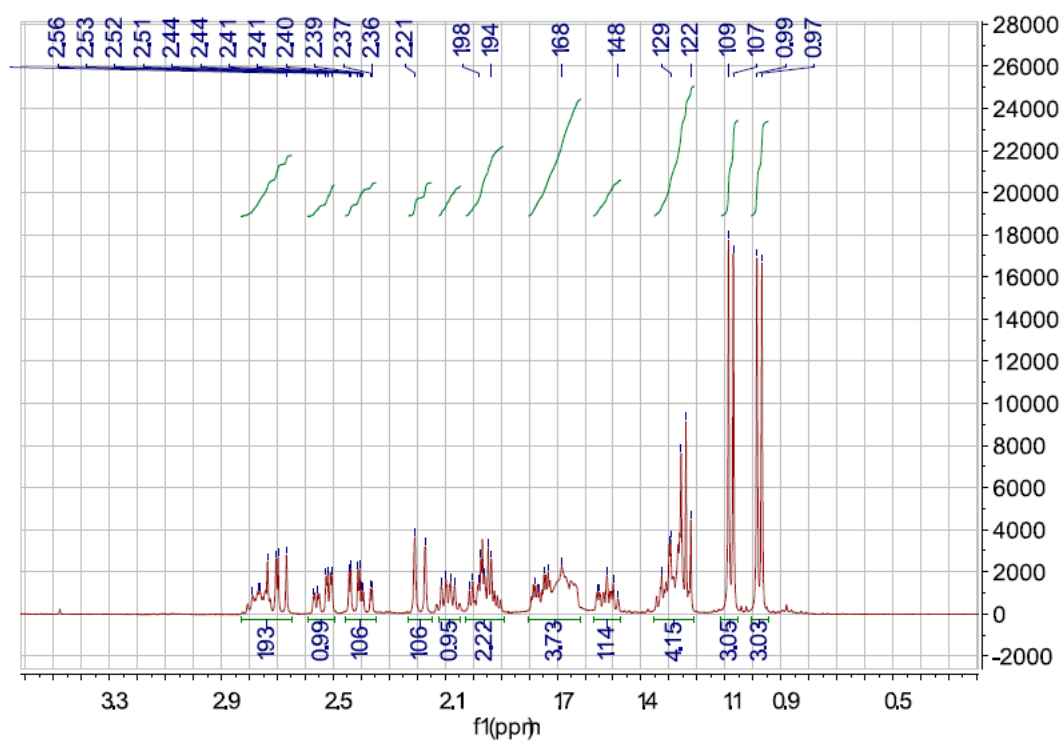


Figure S27. IR of compound (3).

Figure S28. ¹H NMR spectrum of compound (4) (CDCl₃, 400 MHz).

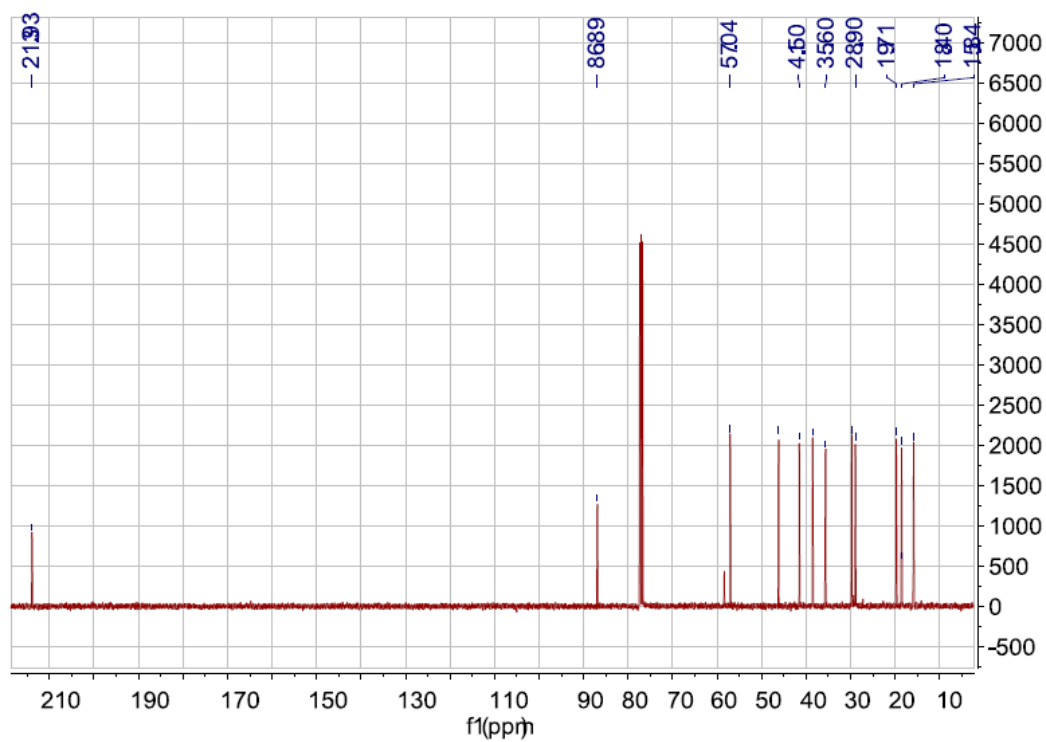


Figure S29. ^{13}C NMR spectrum of compound (4) (CDCl_3 , 100 MHz).

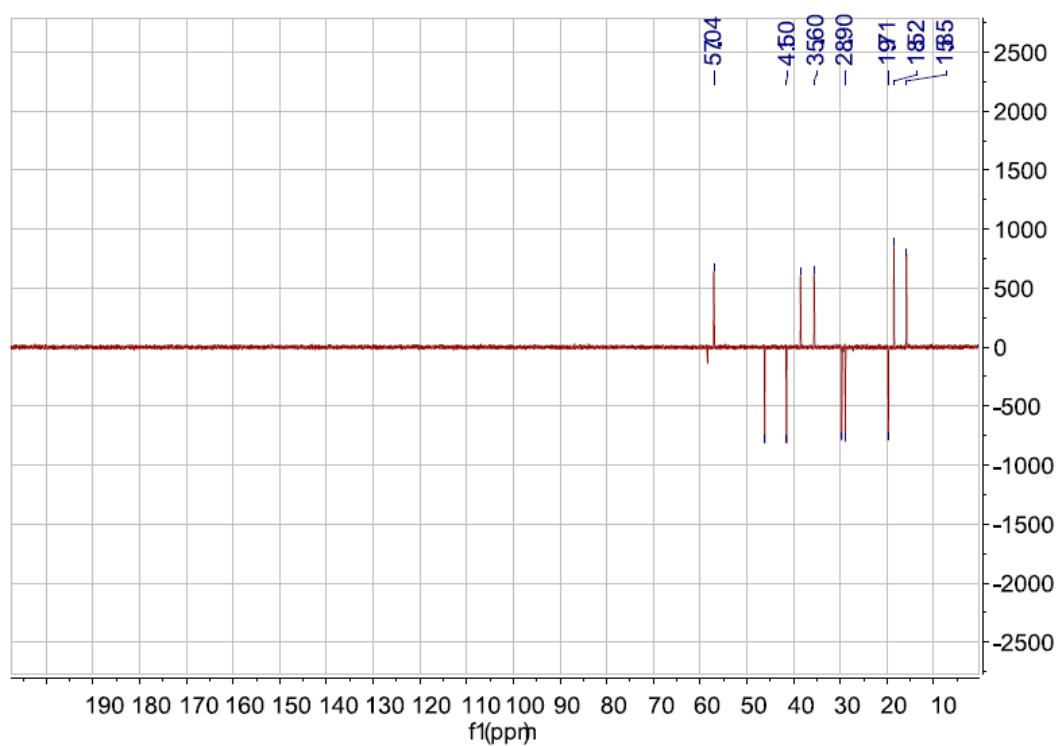


Figure S30. DEPT spectrum of compound (4).

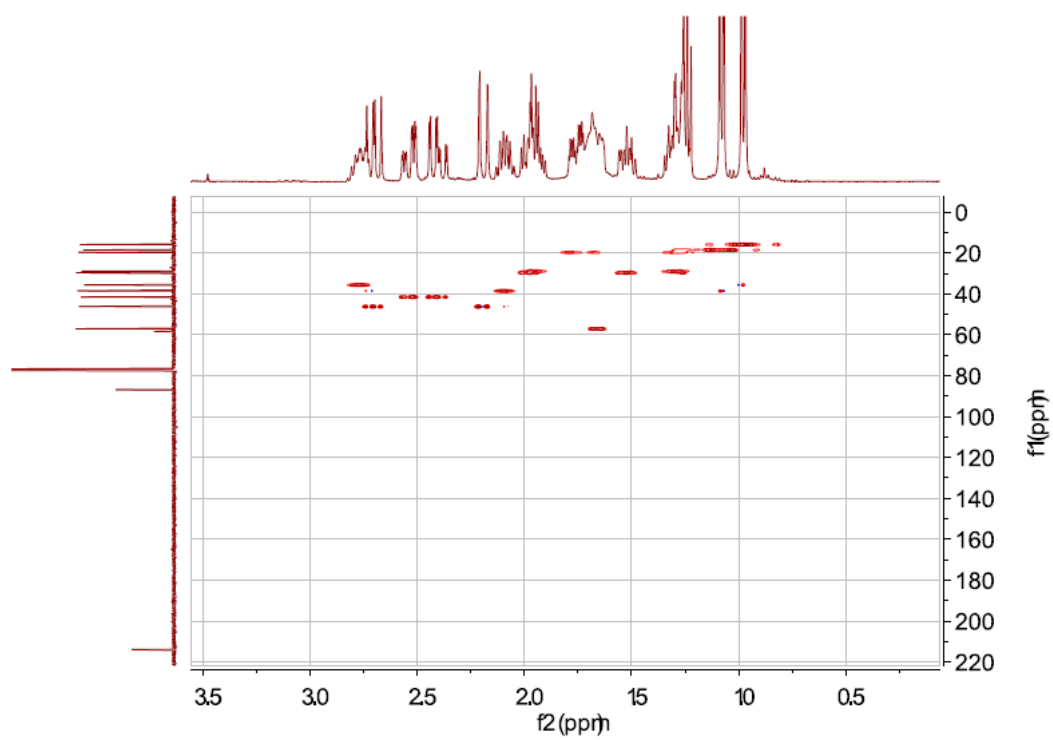


Figure S31. HSQC spectrum of compound (4).

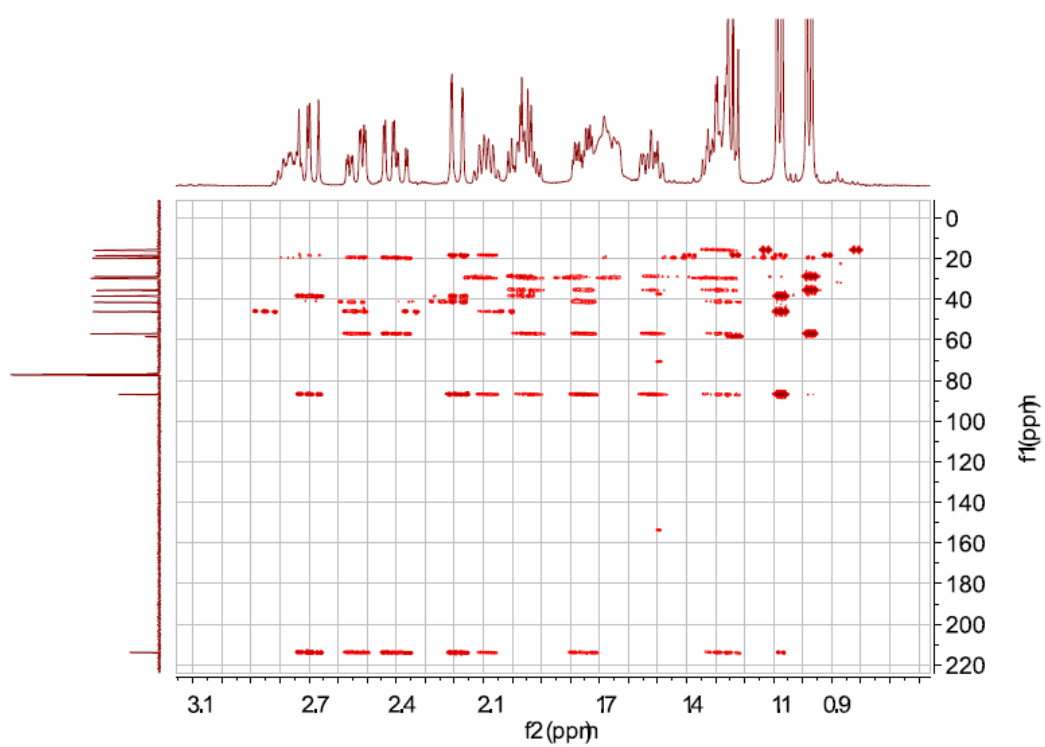


Figure S32. HMBC spectrum of compound (4).

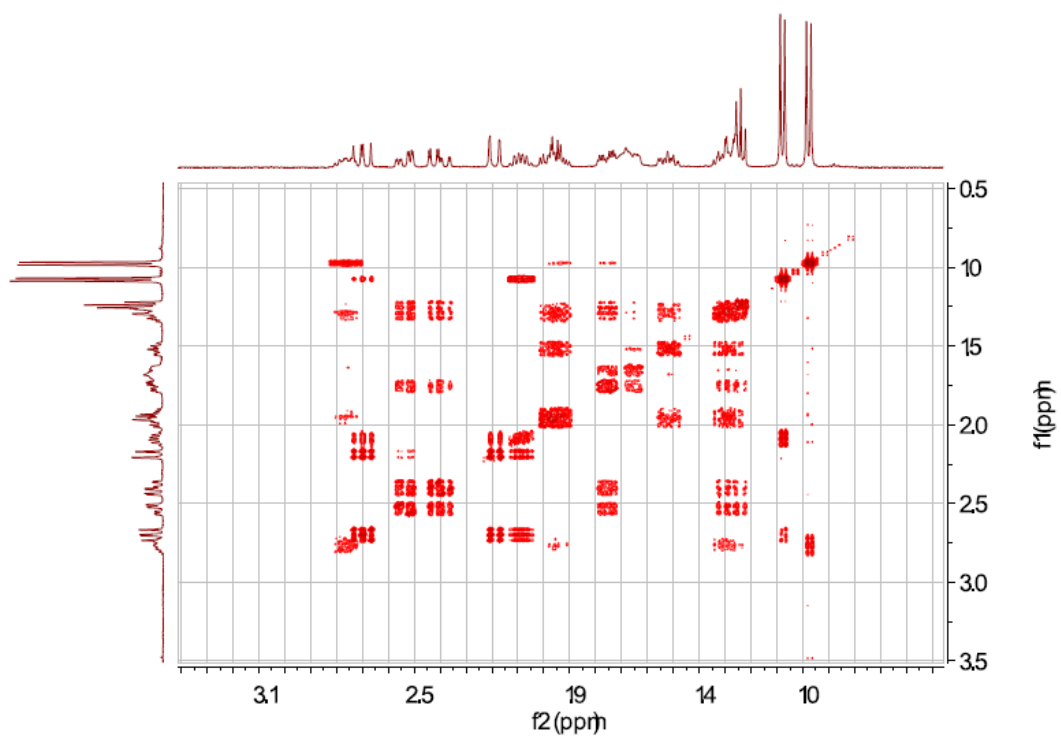


Figure S33. ^1H - ^1H COSY spectrum of compound (4).

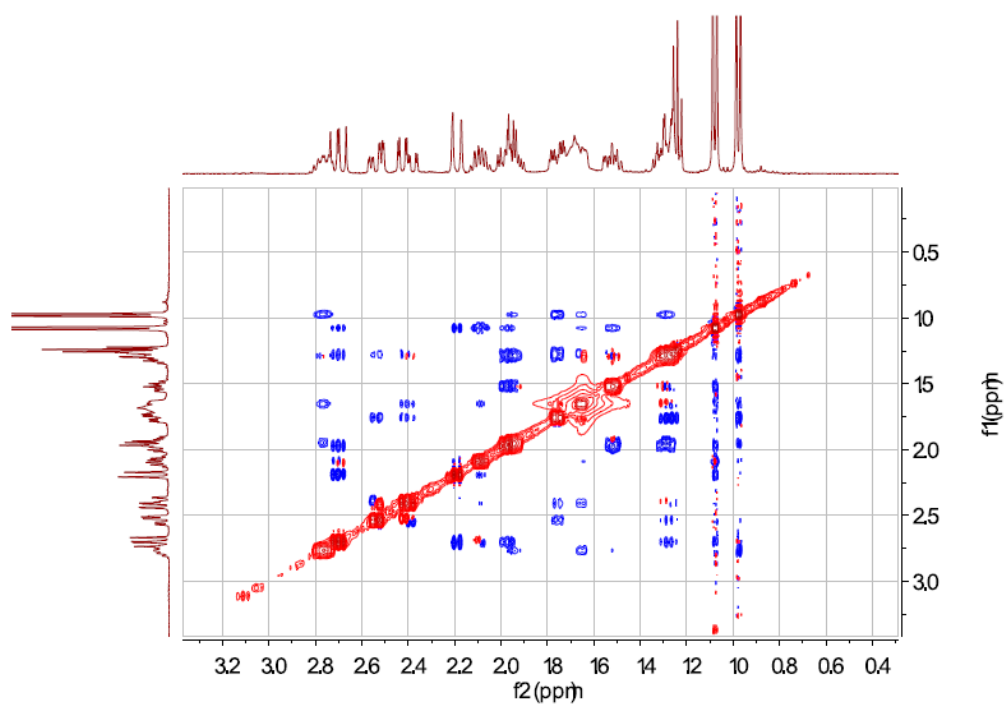


Figure S34. NOESY spectrum of compound (4) (CDCl_3 , 400 MHz).

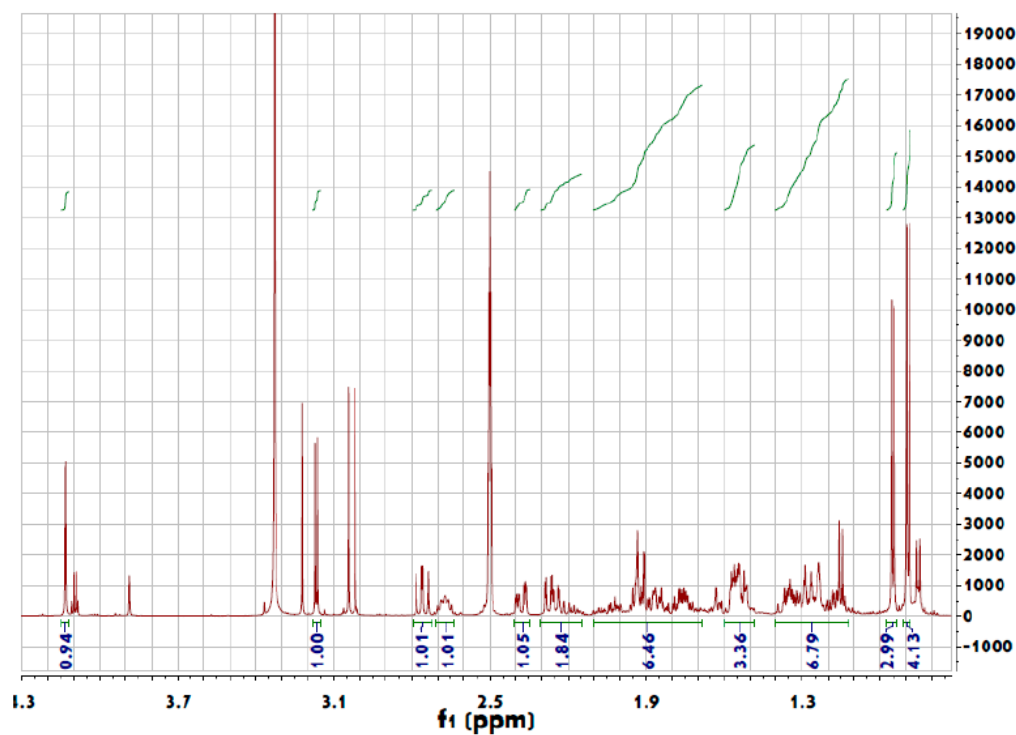


Figure S35. ^1H NMR spectrum of compound (4) (DMSO-d_6 , 400 MHz).

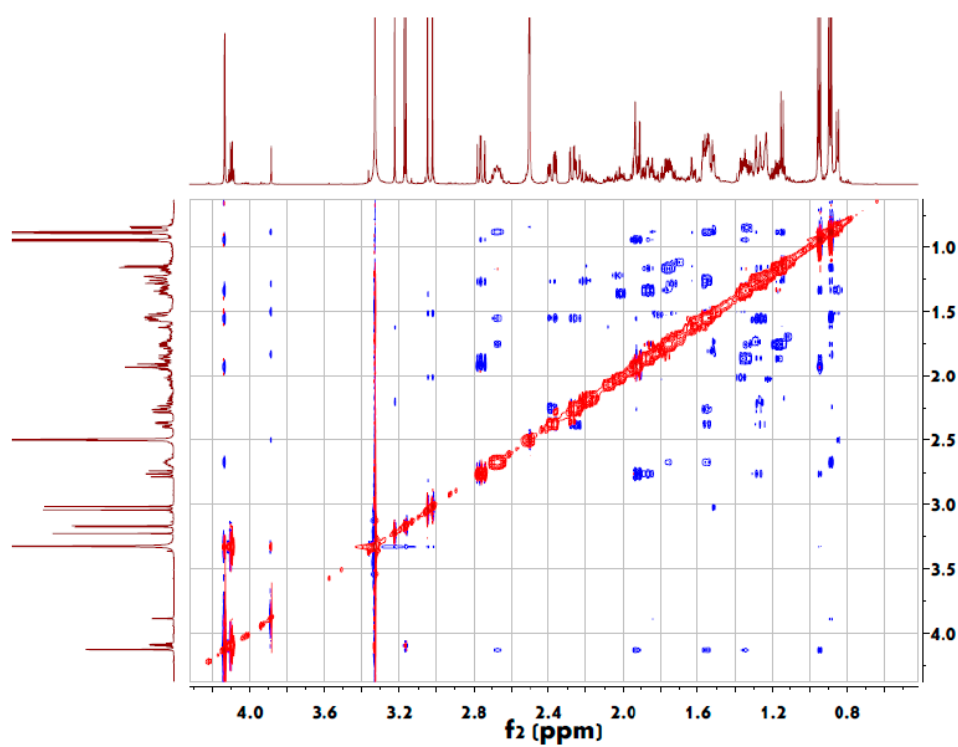


Figure S36. NOESY spectrum of compound (4) (DMSO-d_6).

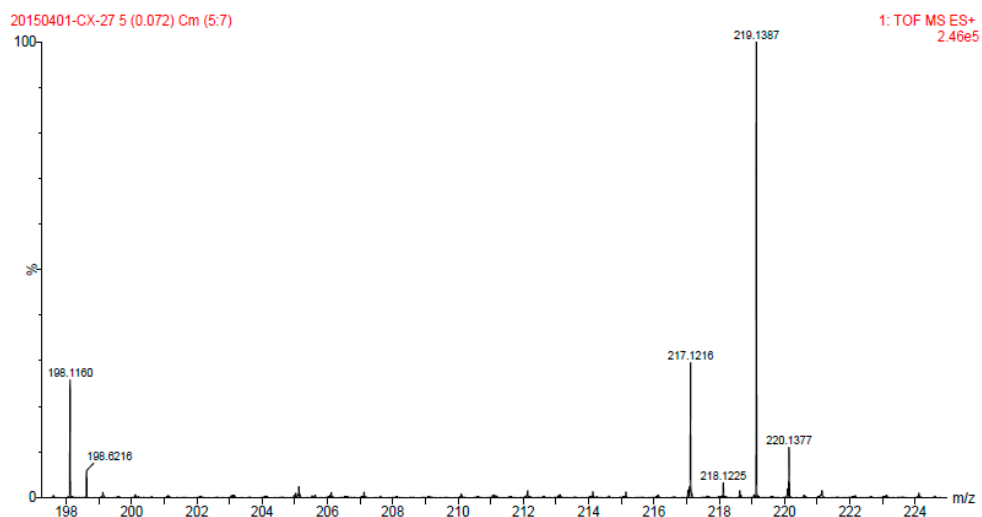


Figure S37. HR-ESIMS spectrum of compound (4).

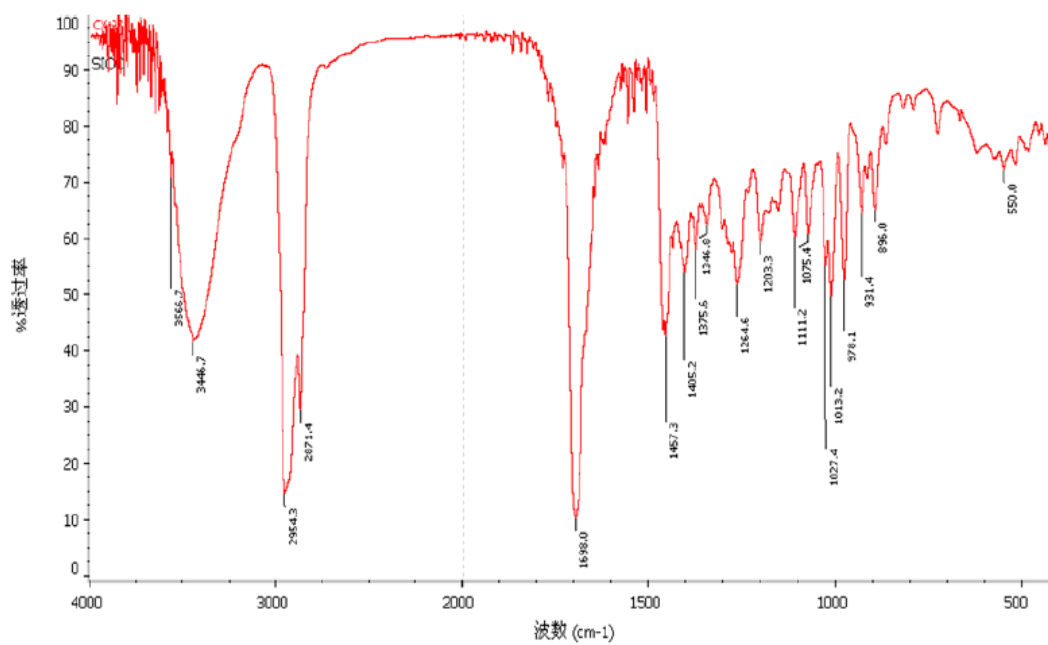


Figure S38. IR of compound (4).