

SUPPLEMENTARY MATERIAL

Anti-neuroinflammatory components from *Clausena lenis* Drake

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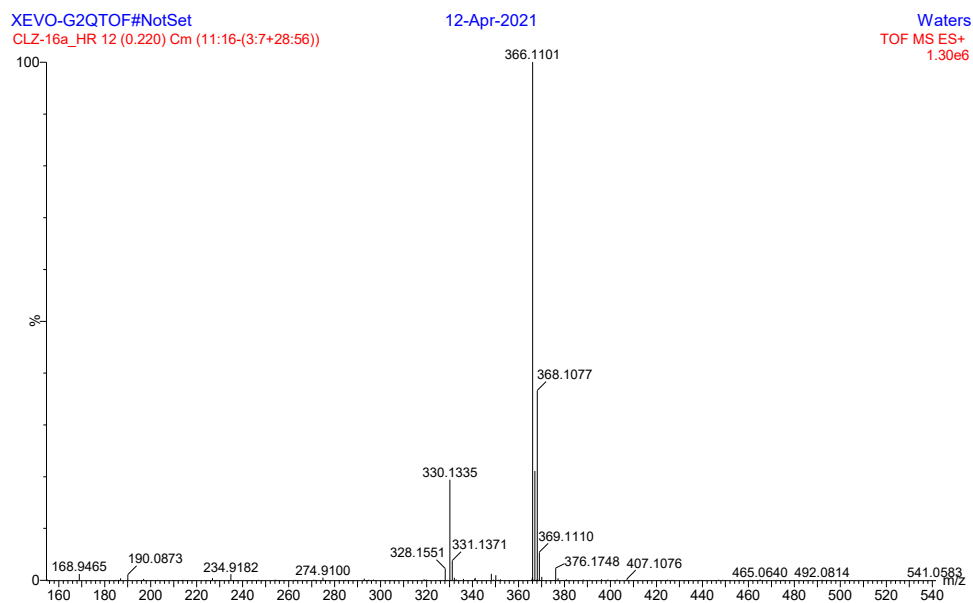
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Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
366.1101	366.1108	-0.7	-1.9	8.5	227.6	0.000	99.98	C ₁₈ H ₂₁ NO ₅ Cl

Figure S1. HR-ESI-MS of **1**.

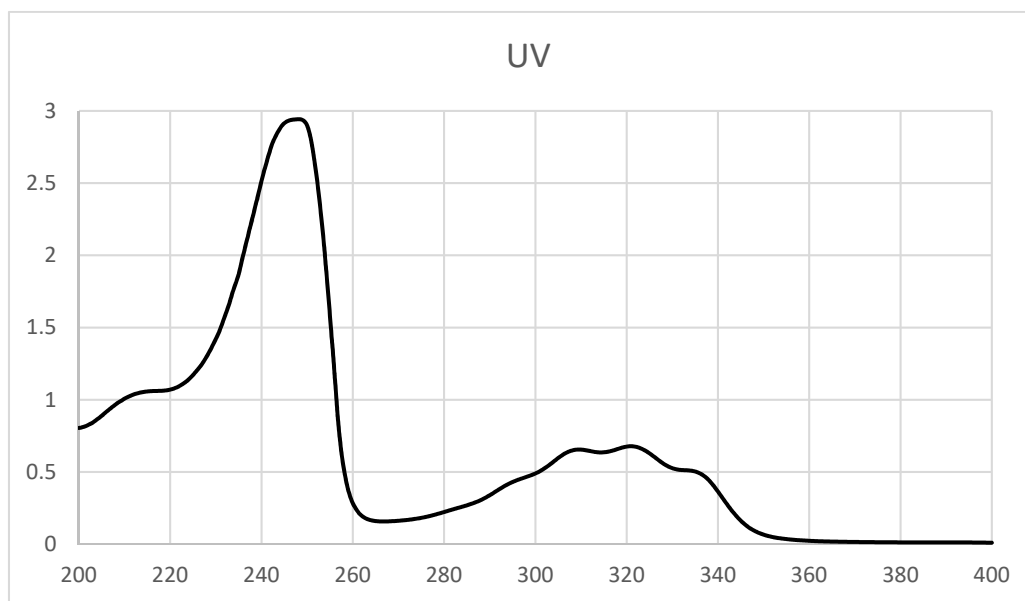


Figure S2. UV spectrum of **1** in MeOH.

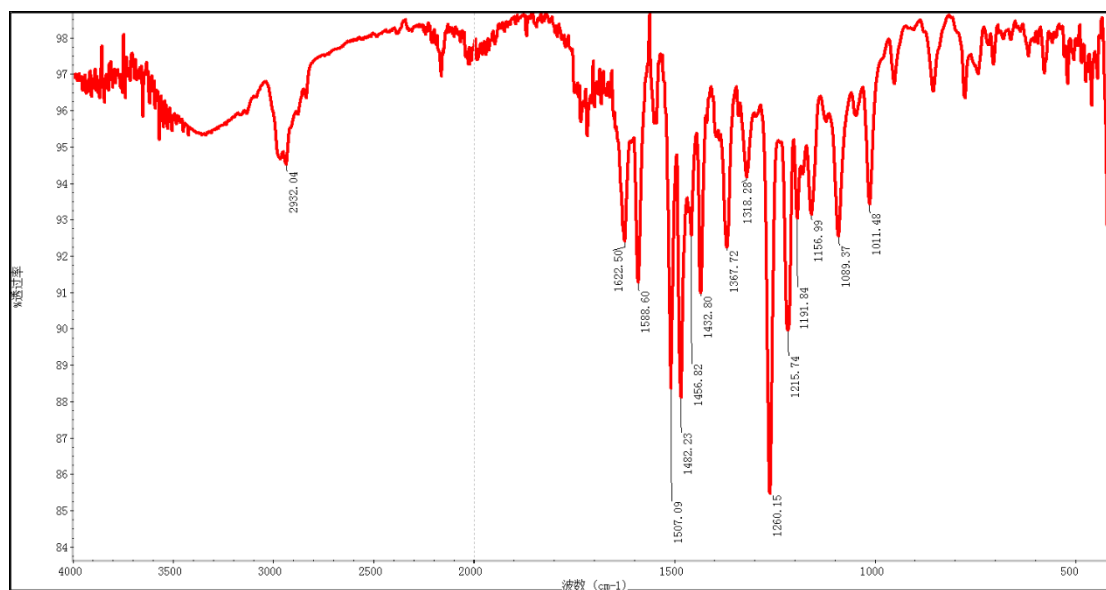


Figure S3. IR spectrum of **1**.

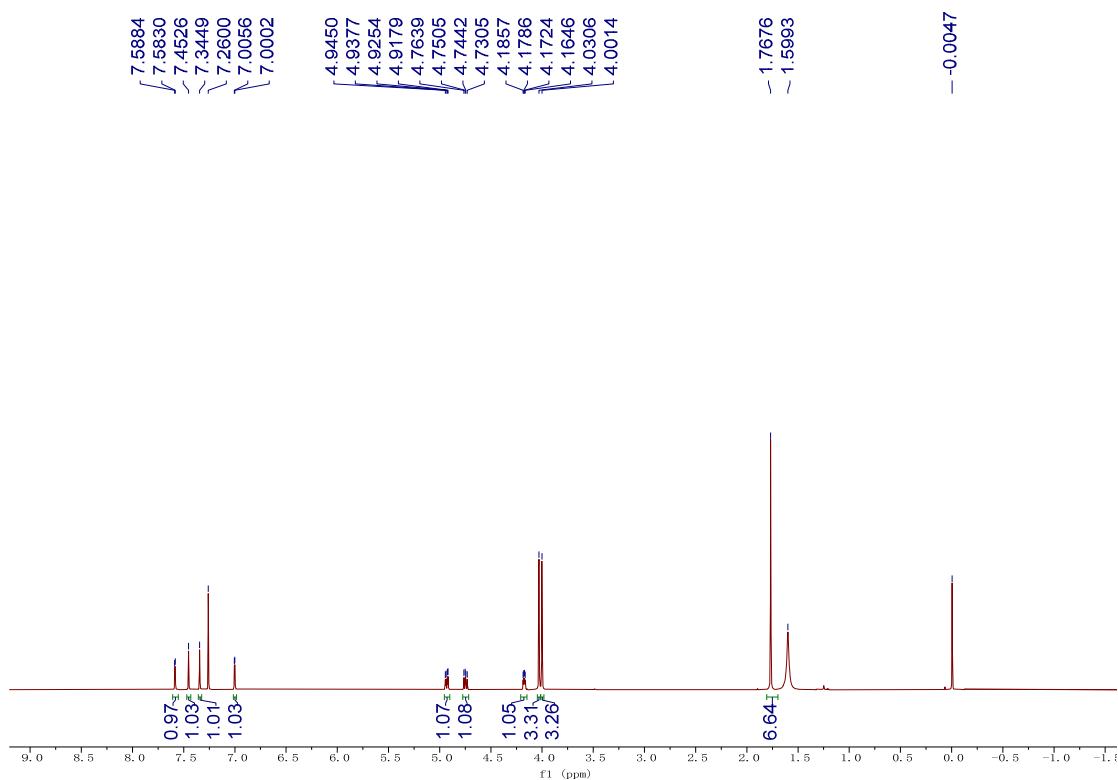


Figure S4. ¹H NMR (500 MHz) spectrum of **1** in CDCl₃.

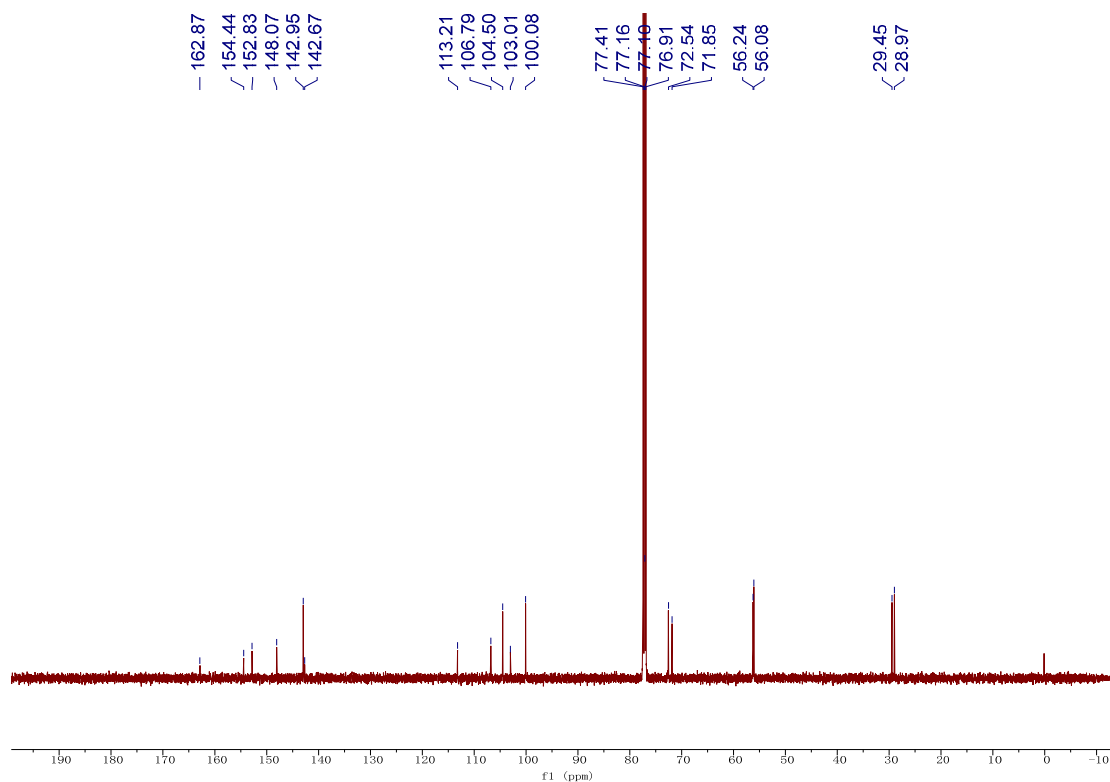


Figure S5. ^{13}C NMR (125 MHz) spectrum of **1** in CDCl_3 .

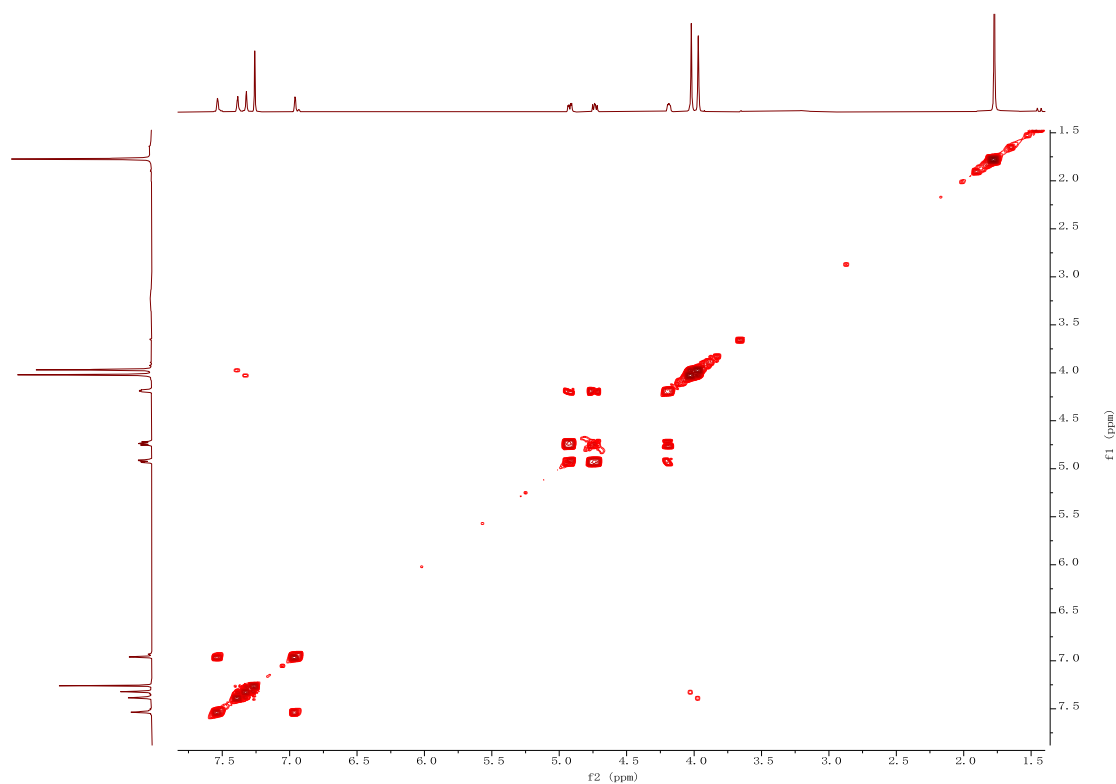


Figure S6. ^1H - ^1H COSY (500 MHz) spectrum of **1** in CDCl_3 .

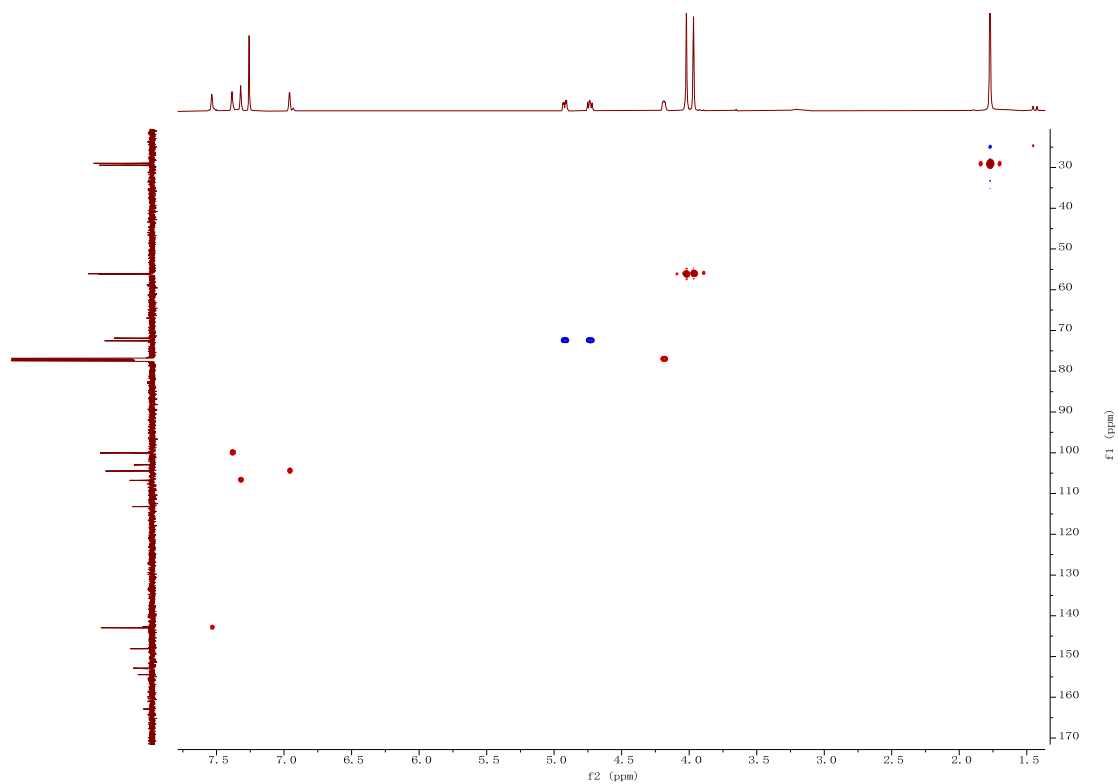


Figure S7. HSQC (500 MHz) spectrum of **1** in CDCl₃.

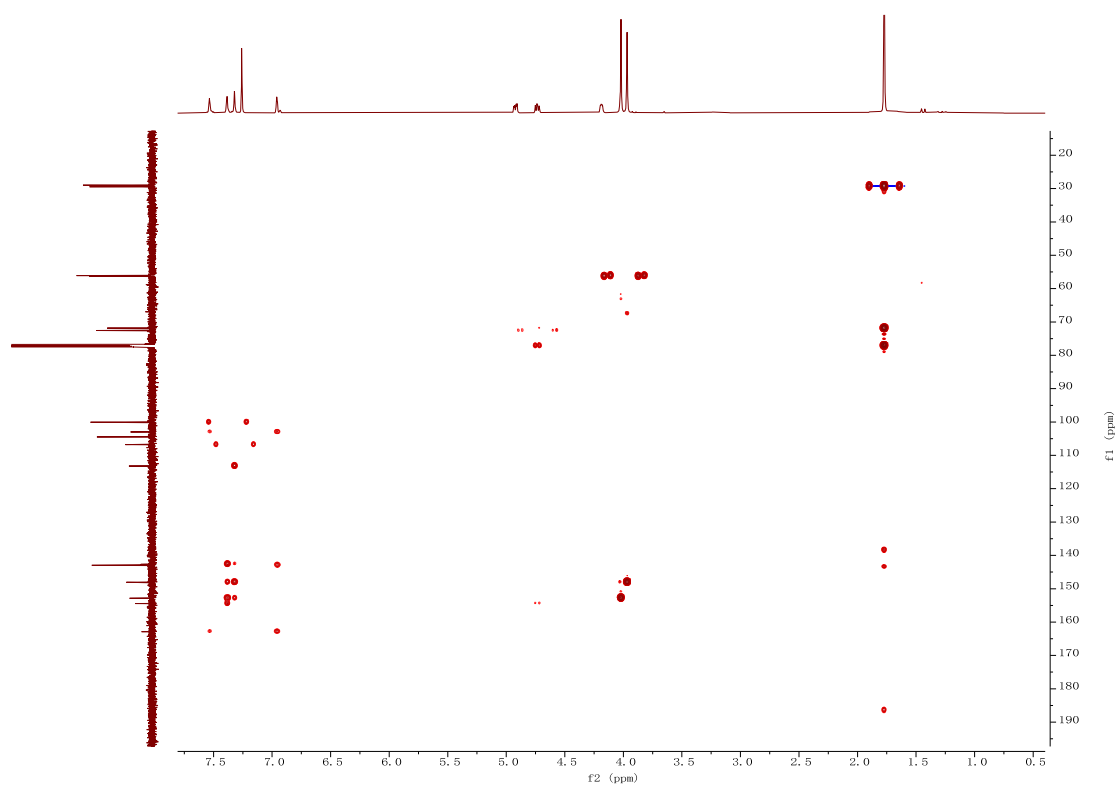


Figure S8. HMBC (500 MHz) spectrum of **1** in CDCl₃.

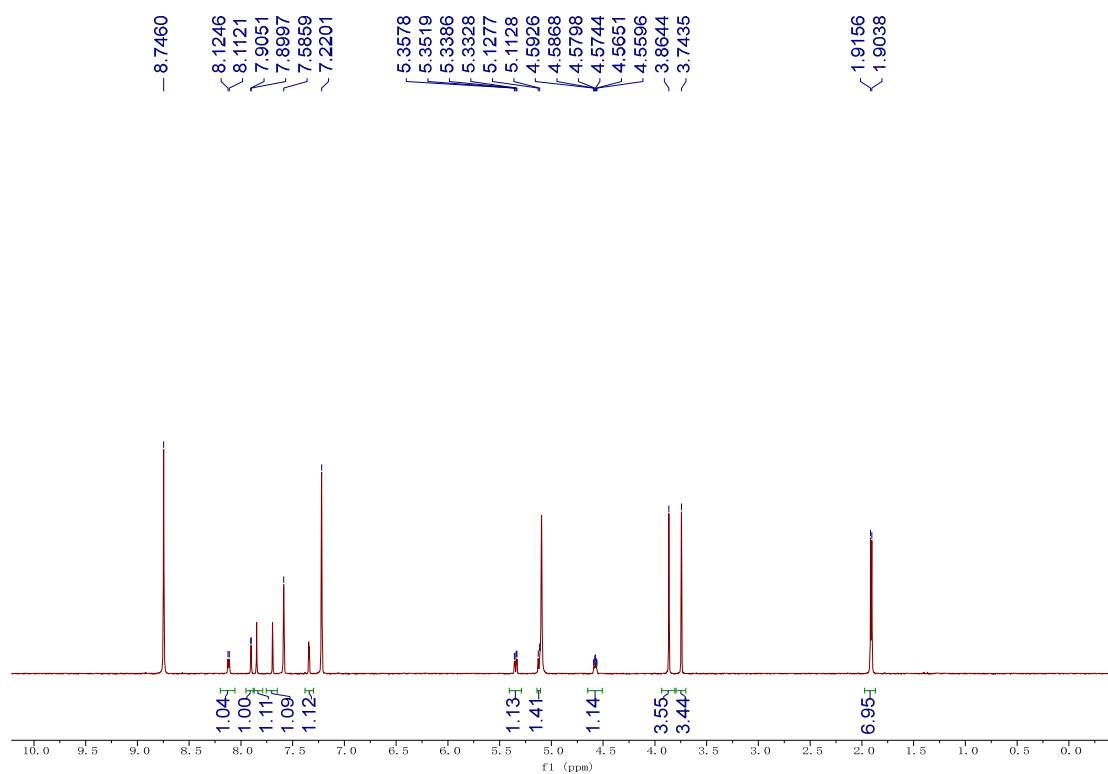


Figure S9. ¹H NMR (500 MHz) spectrum of **1** in C₅D₅N.

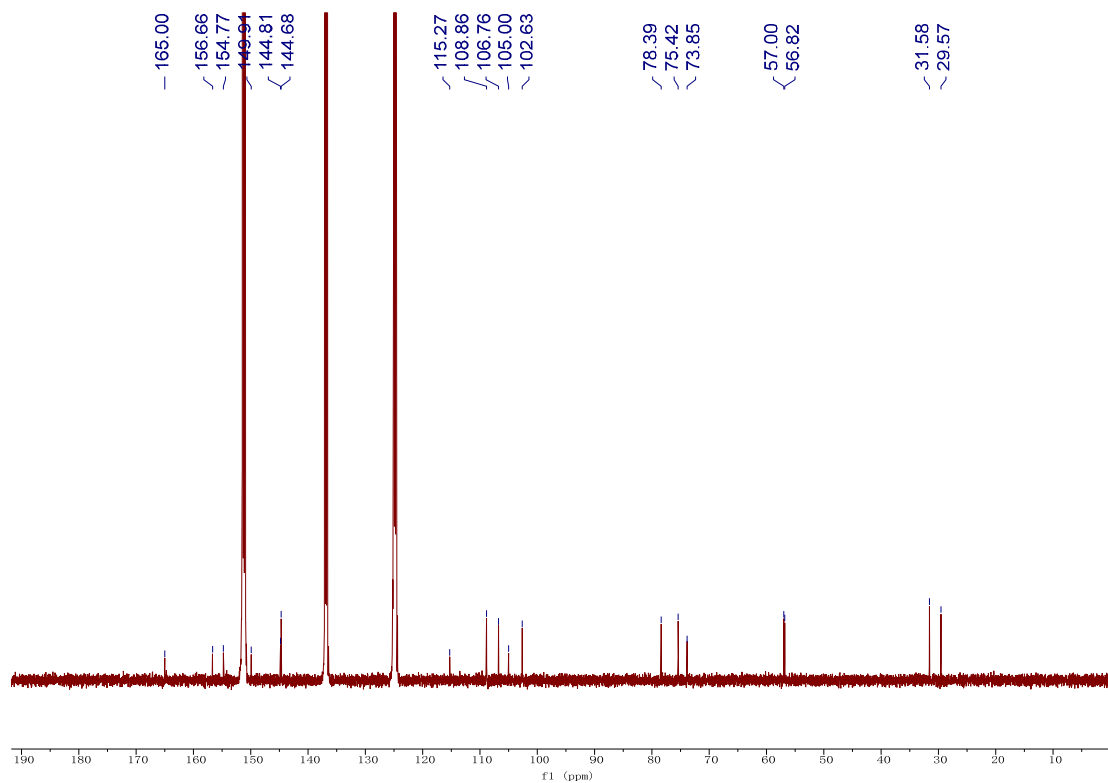


Figure S10. ¹³C NMR (125 MHz) spectrum of **1** in C₅D₅N.

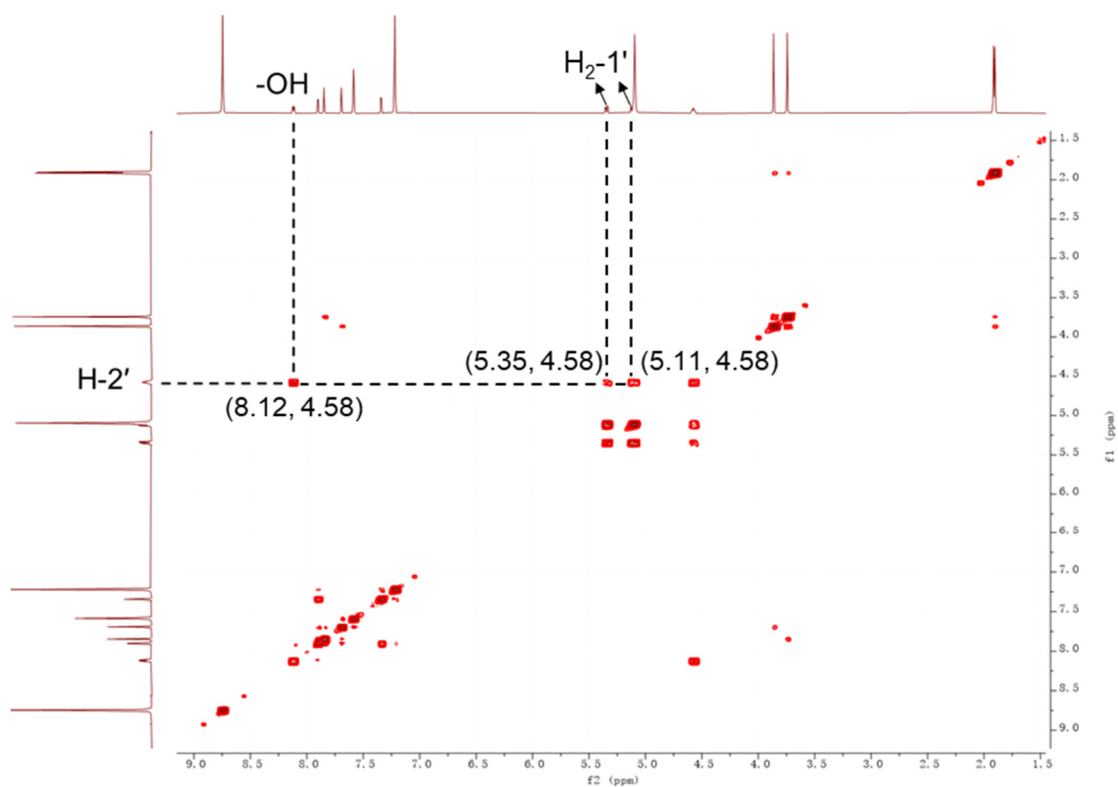


Figure S11. ^1H - ^1H COSY (500 MHz) spectrum of **1** in $\text{C}_5\text{D}_5\text{N}$.

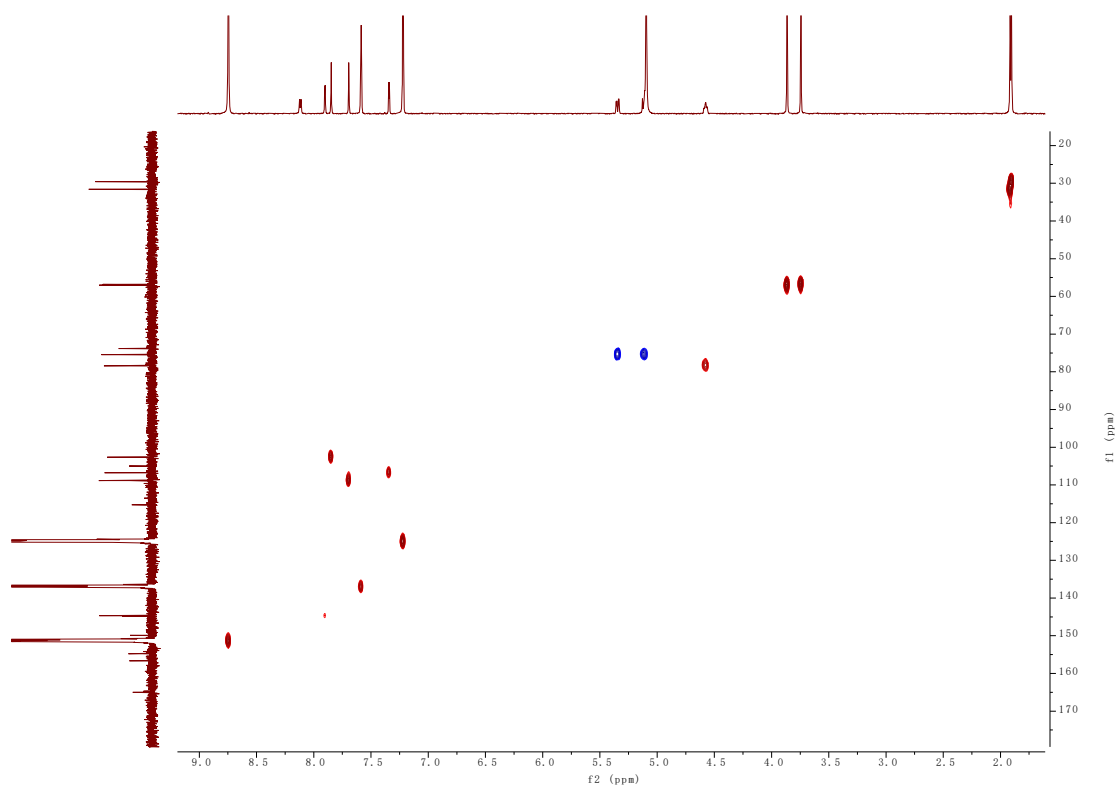


Figure S12. HSQC (500 MHz) spectrum of **1** in $\text{C}_5\text{D}_5\text{N}$.

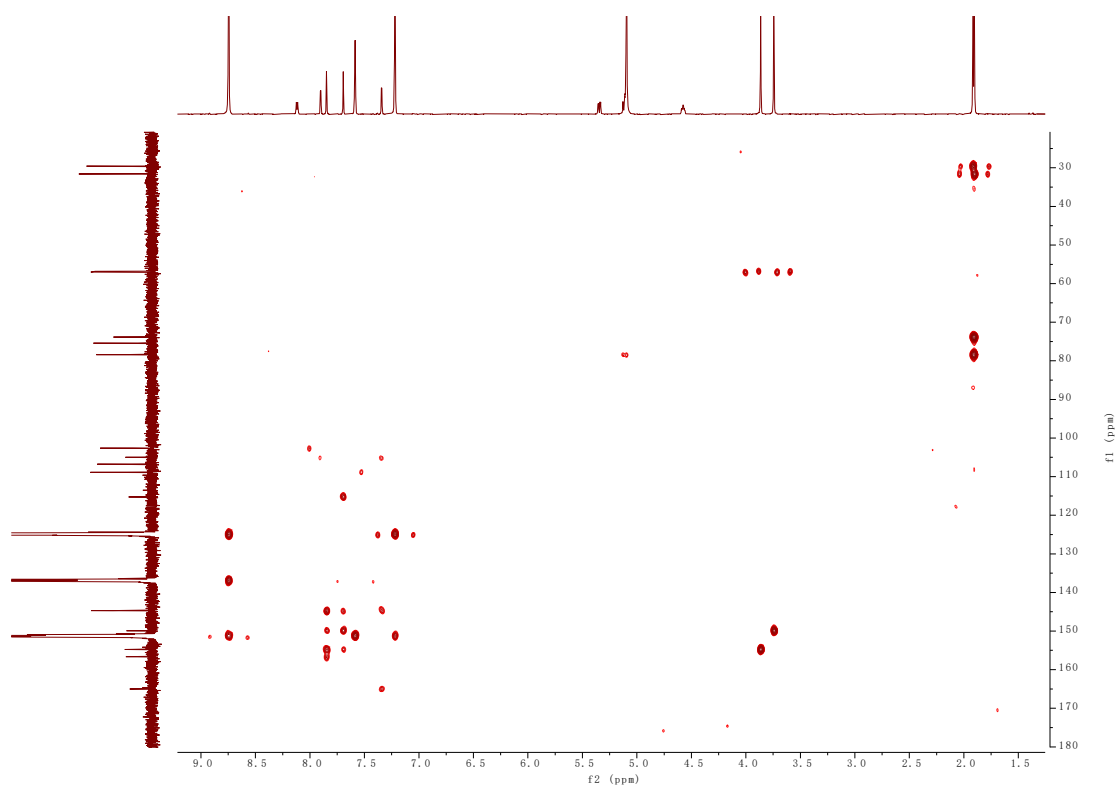


Figure S13. HMBC (500 MHz) spectrum of **1** in C_5D_5N .

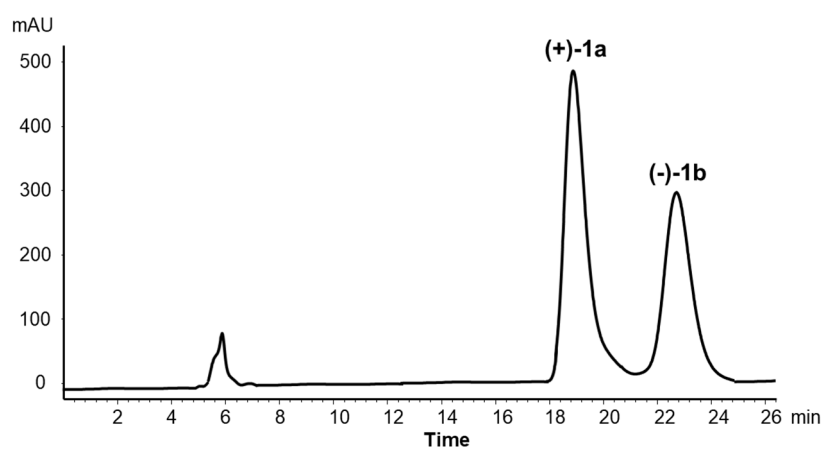


Figure S14. Chiral HPLC separation of racemate **1** (*n*-hexane/isopropanol, 85:15; $T = 30\text{ }^{\circ}C$; flow rate: 3.0 mL/min; wavelength: 254 nm).

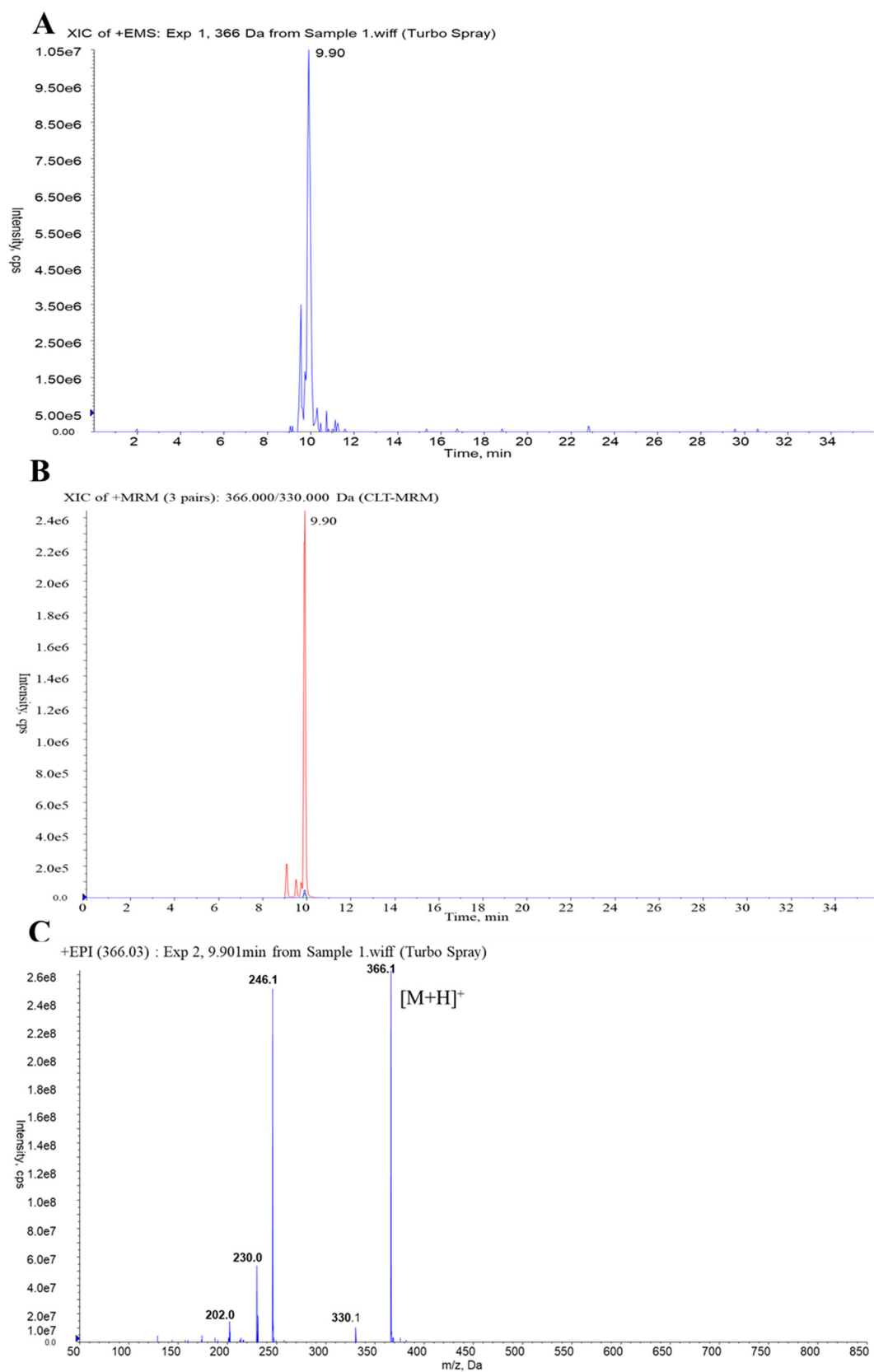


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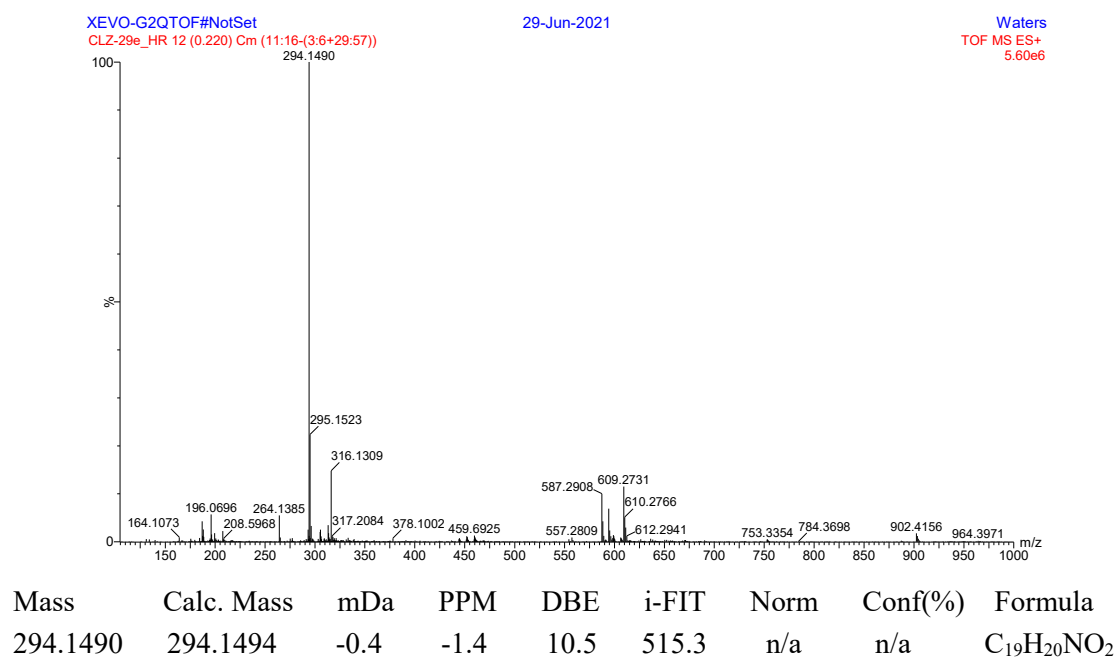


Figure S16. HR-ESI-MS of **2**.

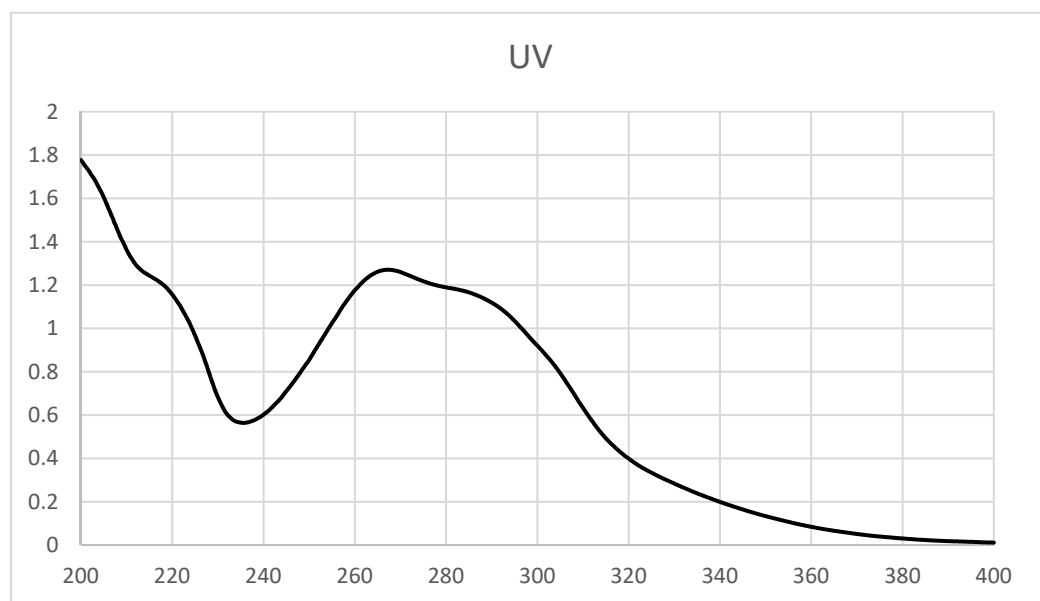


Figure S17. UV spectrum of **2** in MeOH.

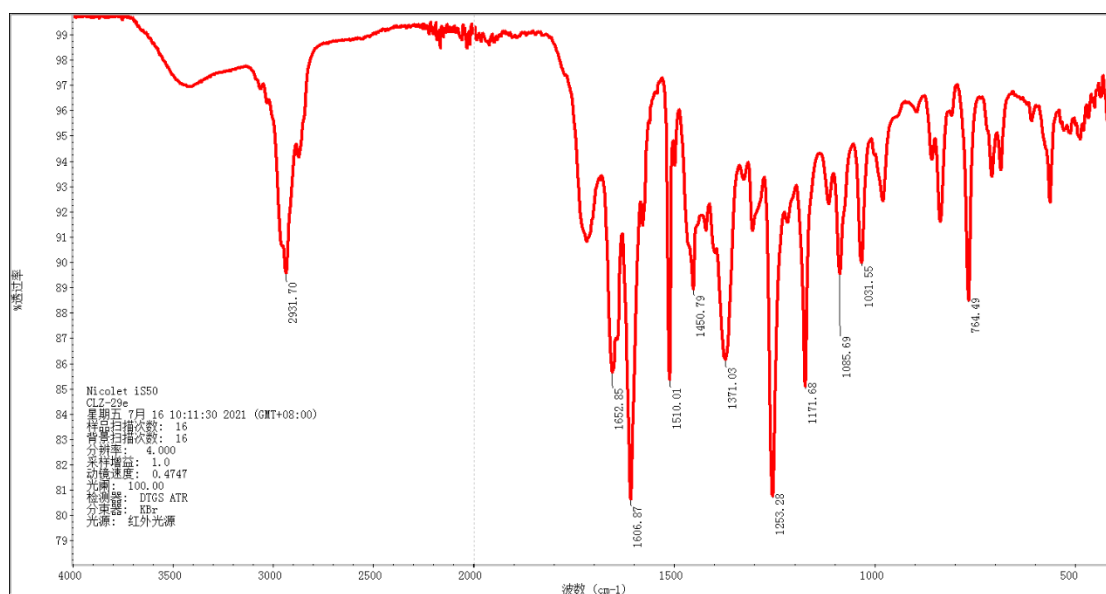


Figure S18. IR spectrum of **2**.

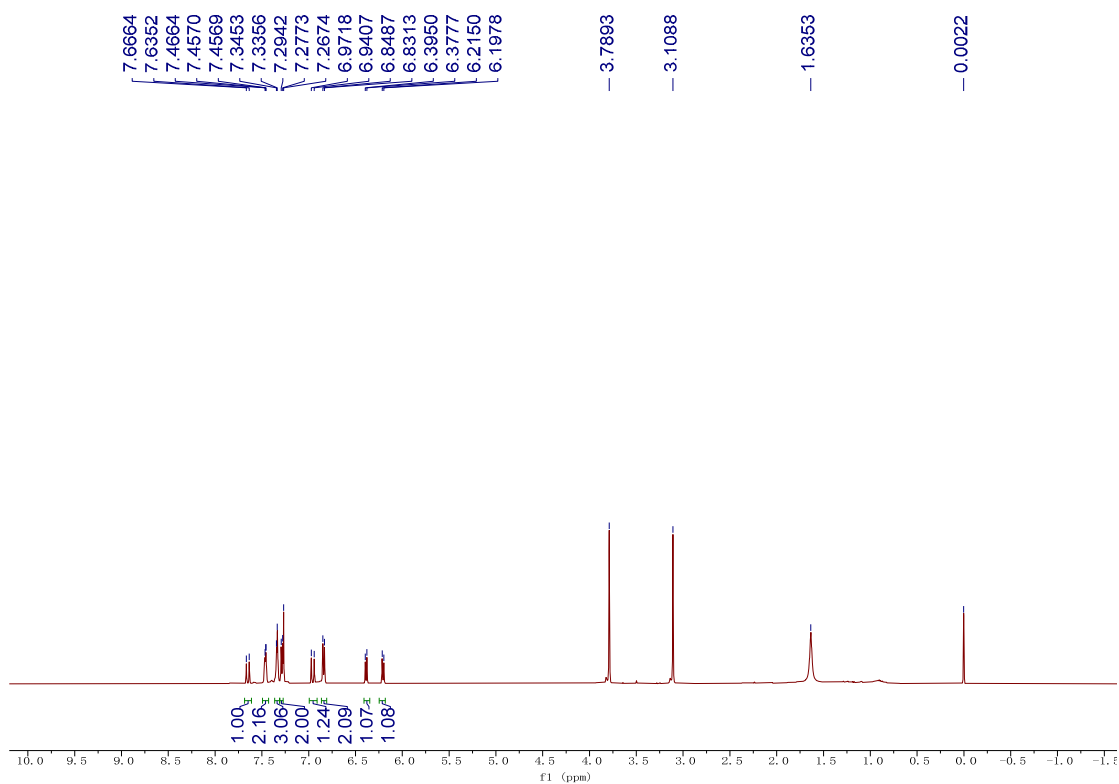


Figure S19. ¹H NMR (500 MHz) spectrum of **2** in CDCl₃.

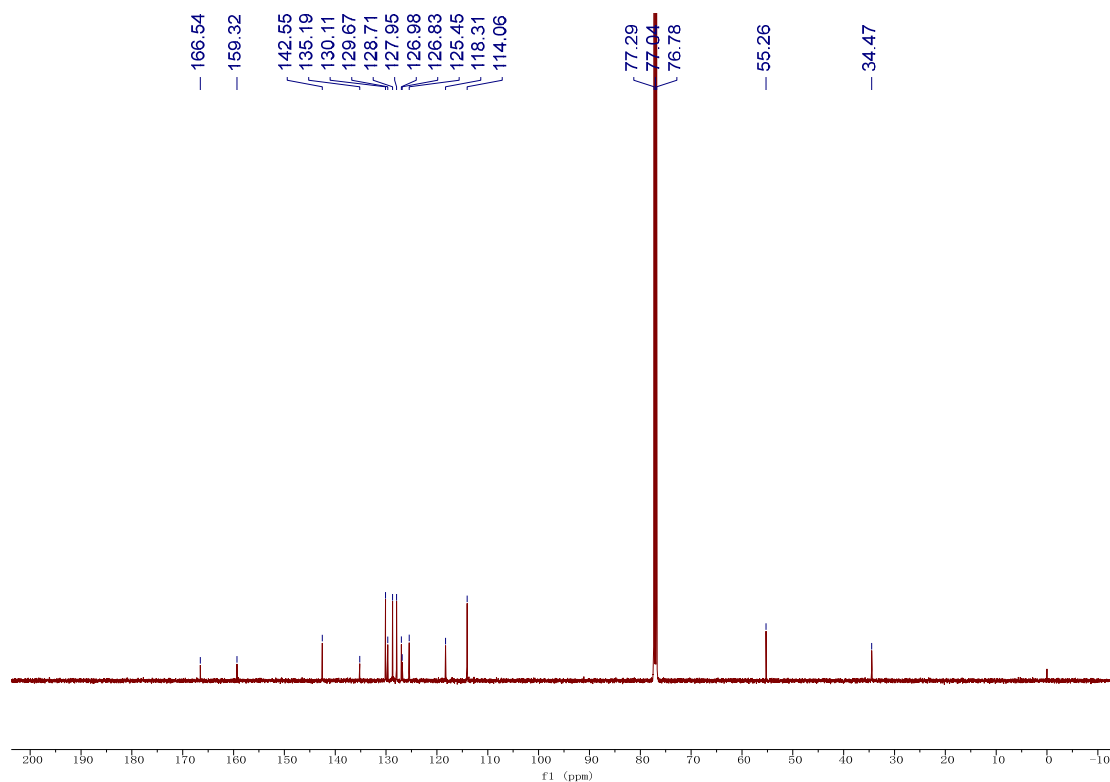


Figure S20. ^{13}C NMR (125 MHz) spectrum of **2** in CDCl_3 .

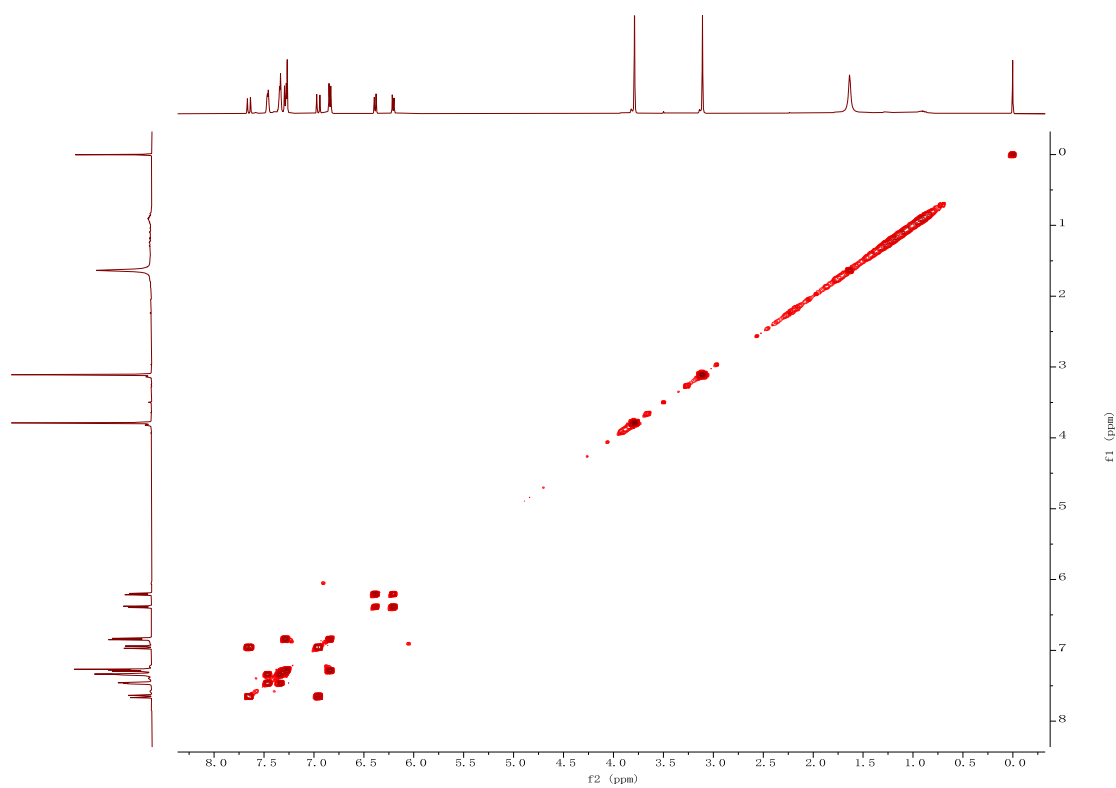


Figure S21. ^1H - ^1H COSY (500 MHz) spectrum of **2** in CDCl_3 .

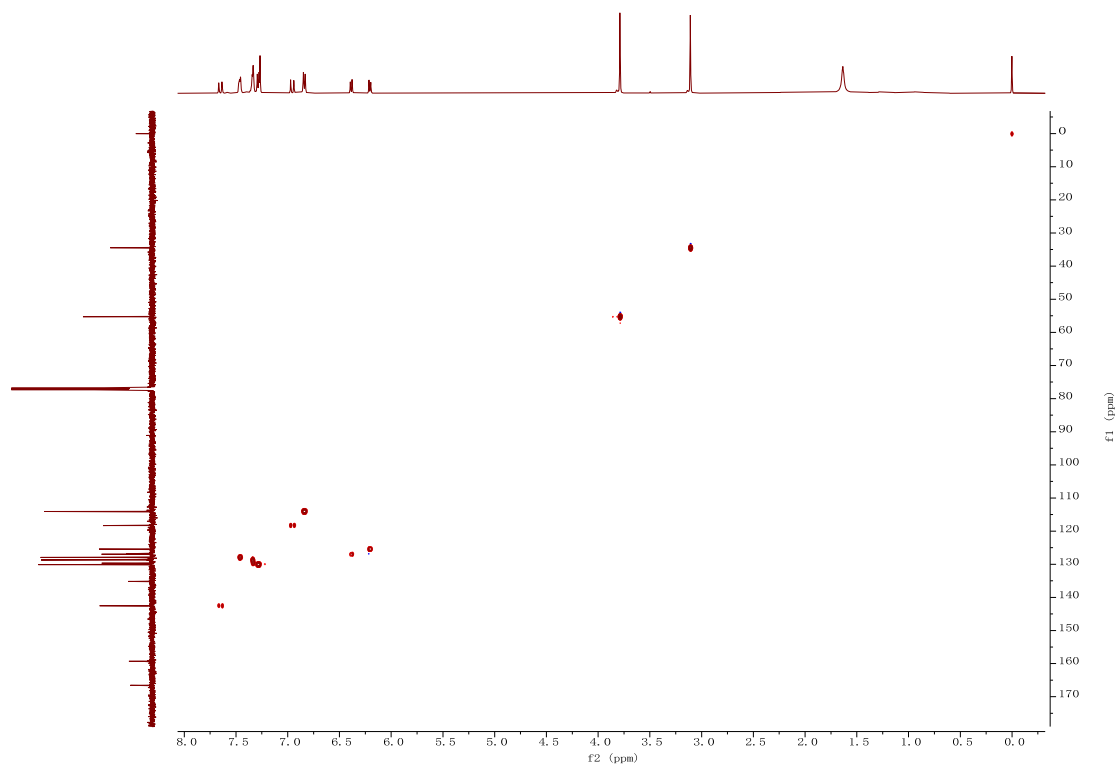


Figure S22. HSQC (500 MHz) spectrum of **2** in CDCl₃.

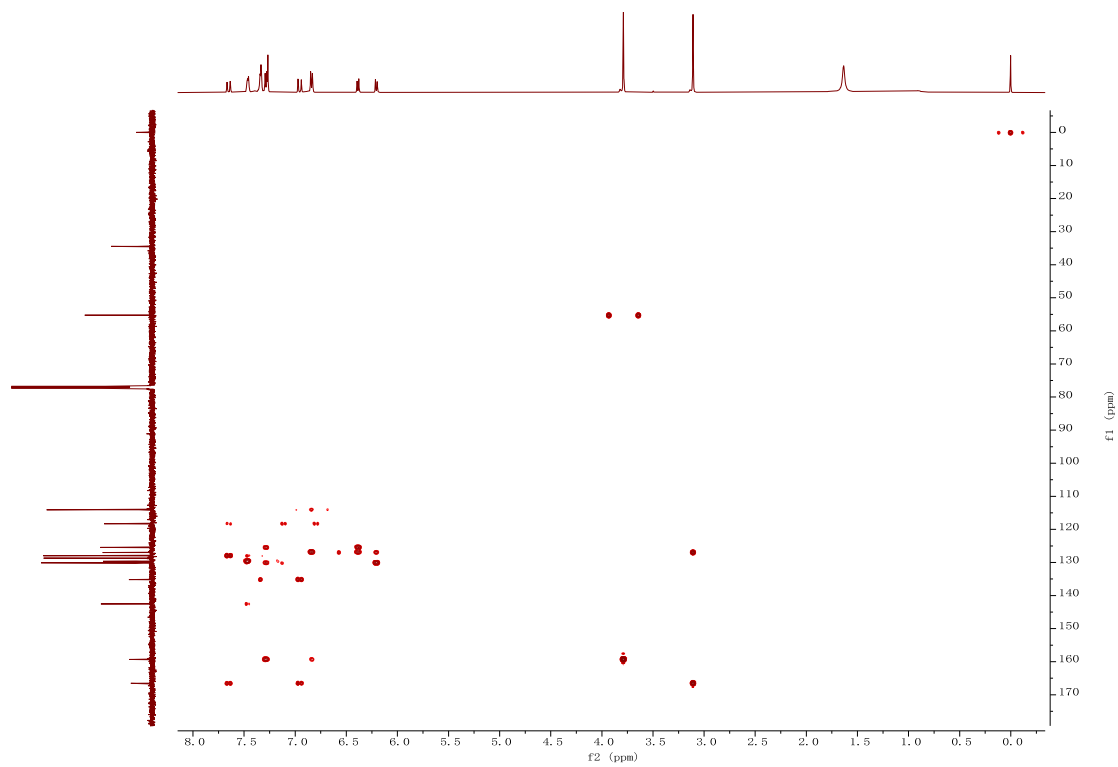


Figure S23. HMBC (500 MHz) spectrum of **2** in CDCl₃.

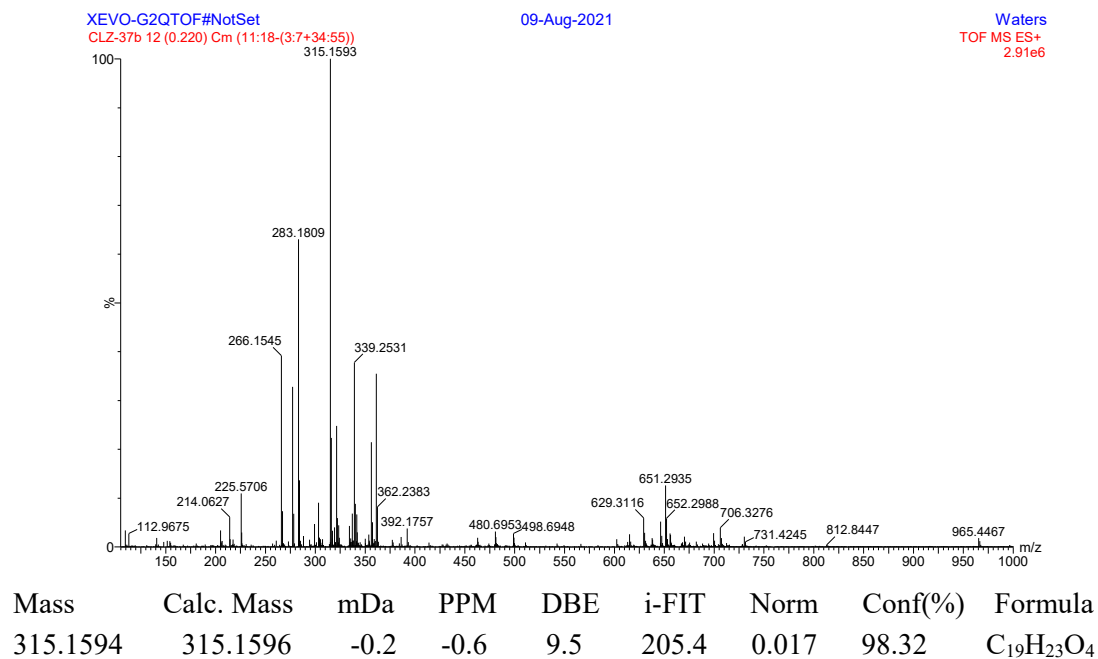


Figure S24. HR-ESI-MS of **3**.

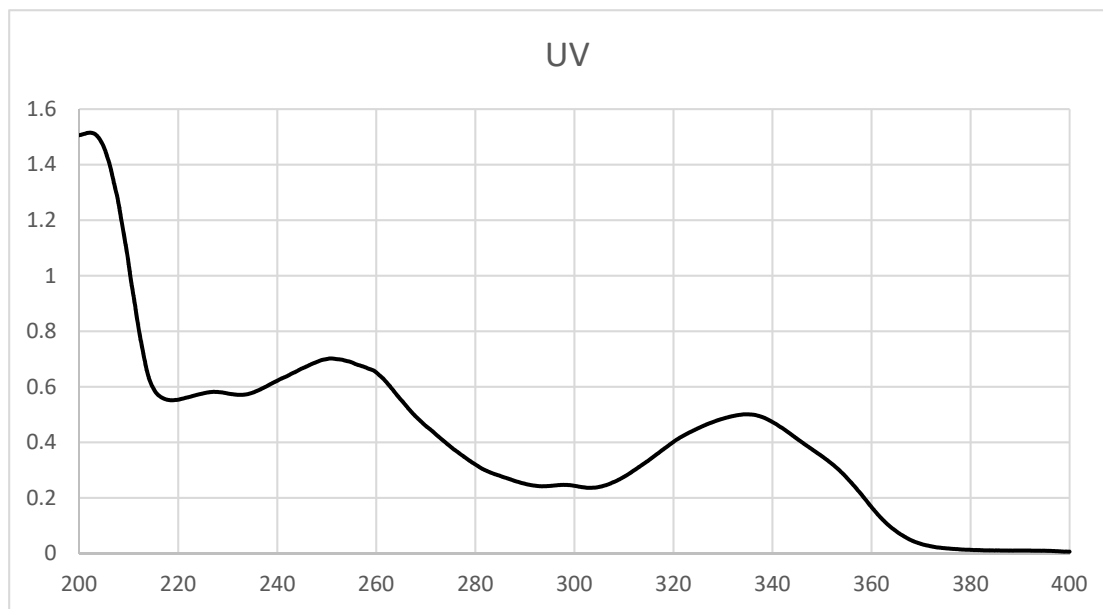


Figure S25. UV spectrum of **3** in MeOH.

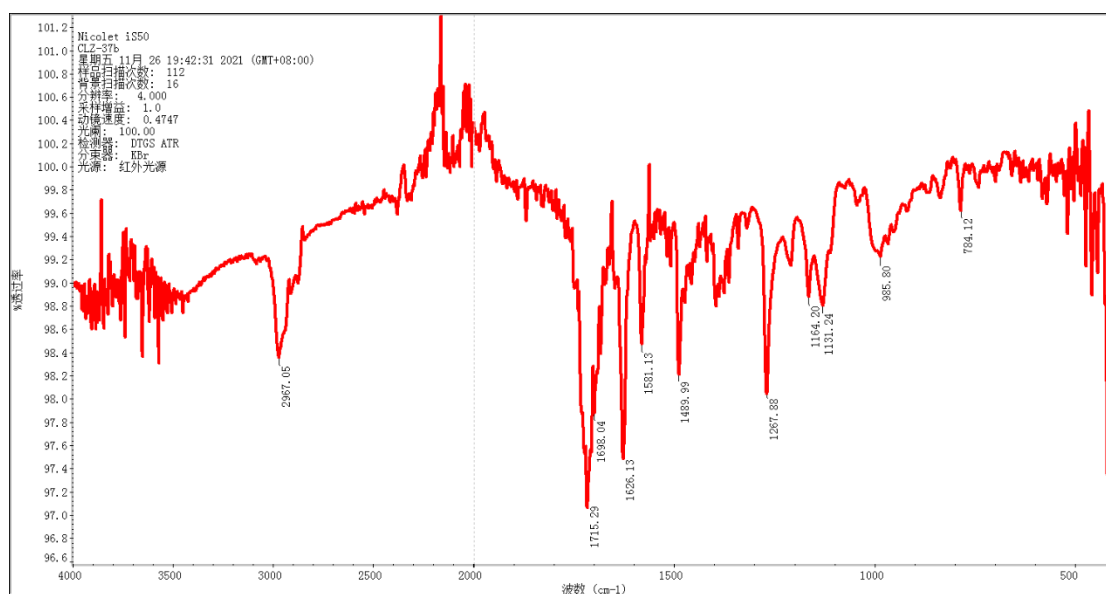


Figure S26. IR spectrum of **3**.

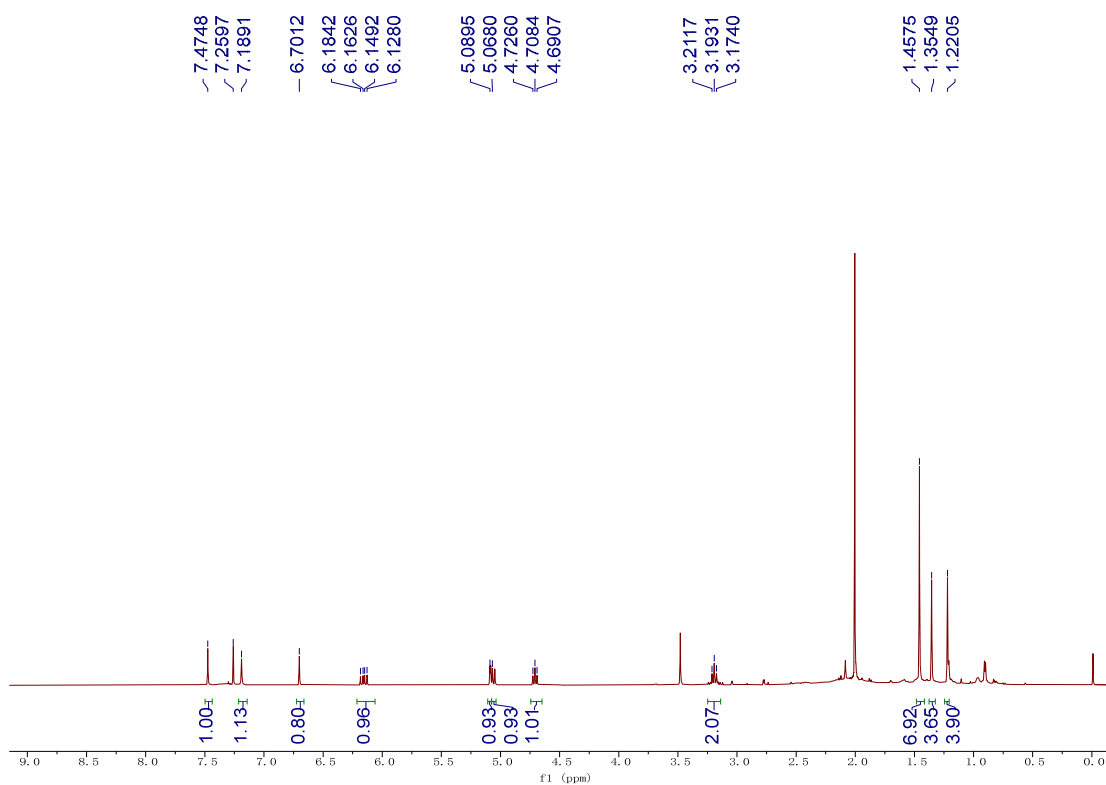


Figure S27. ^1H NMR (500 MHz) spectrum of **3** in CDCl_3 .

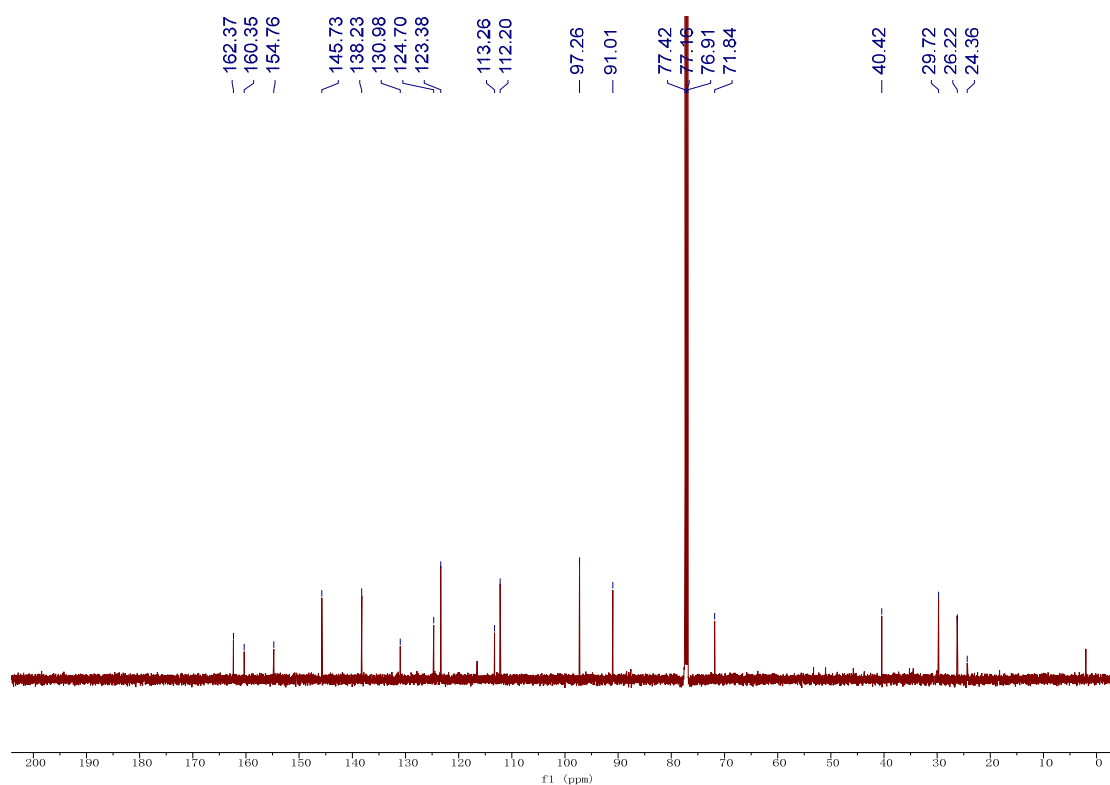


Figure S28. ^{13}C NMR (125 MHz) spectrum of **3** in CDCl_3 .

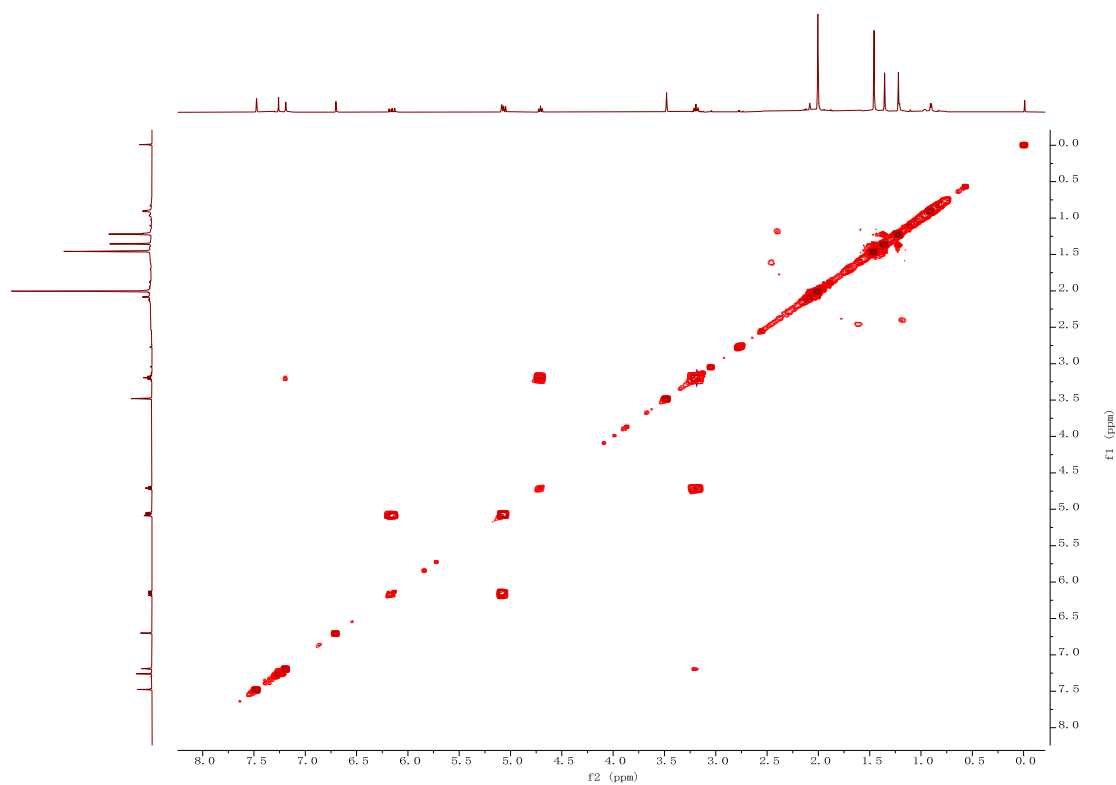


Figure S29. ^1H - ^1H COSY (500 MHz) spectrum of **3** in CDCl_3 .

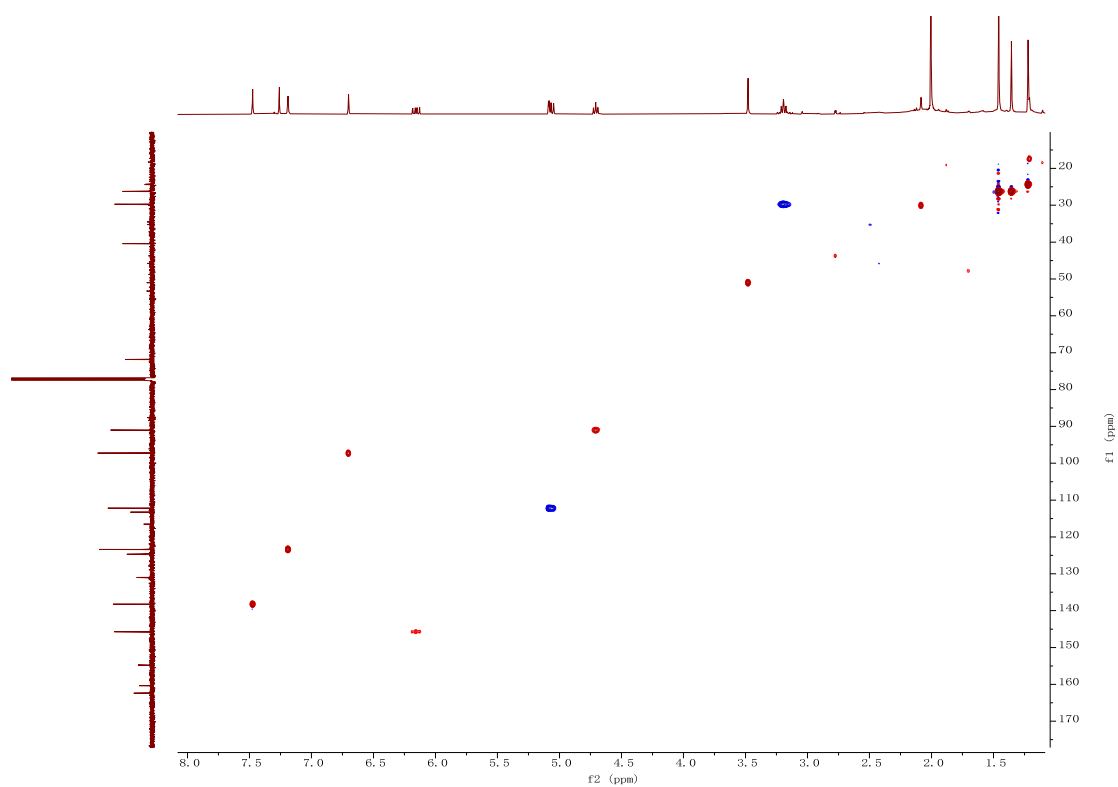


Figure S30. HSQC (500 MHz) spectrum of **3** in CDCl₃.

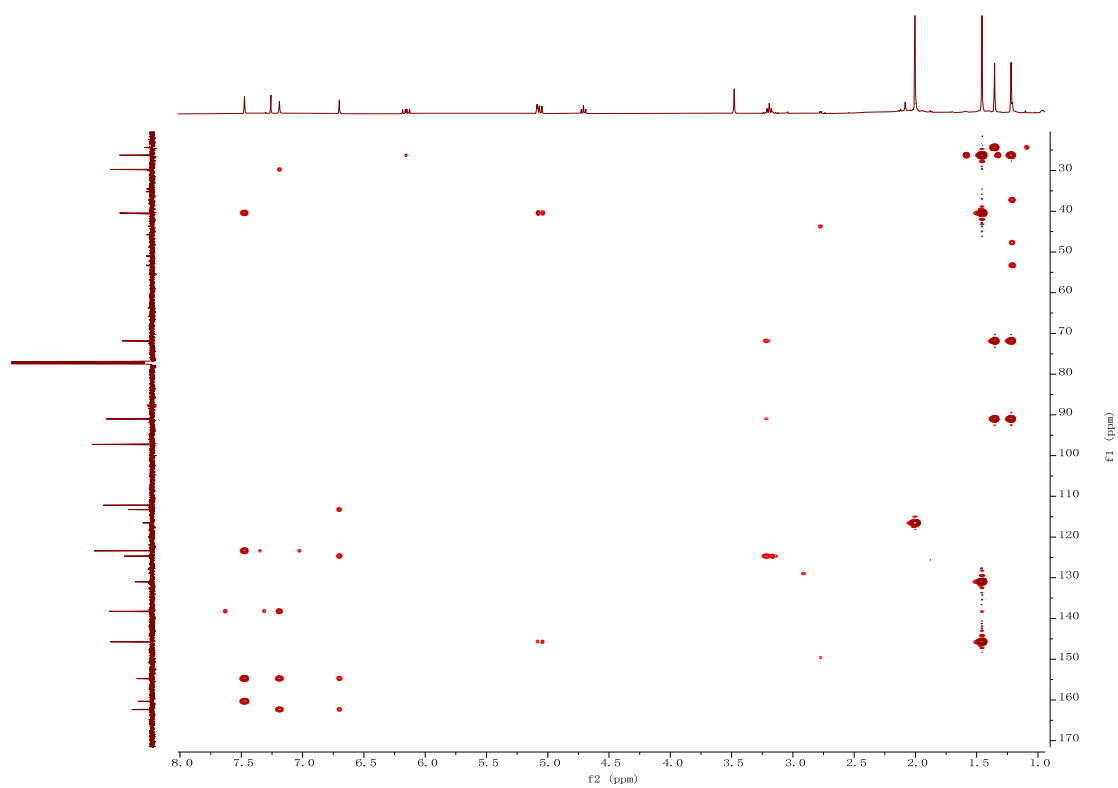


Figure S31. HMBC (500 MHz) spectrum of **3** in CDCl₃.

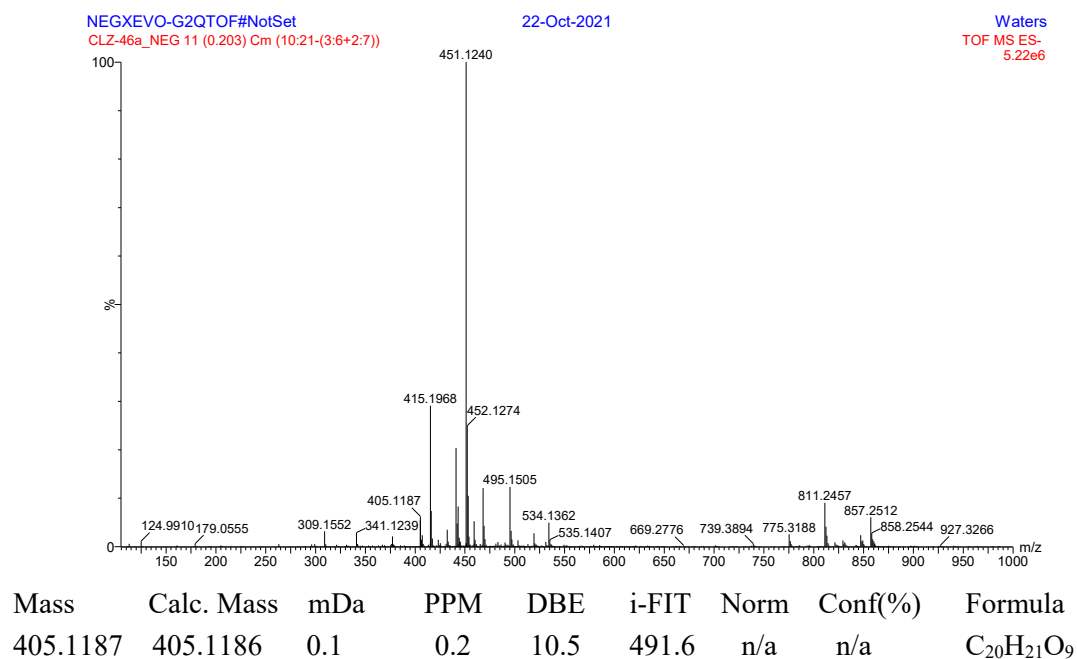


Figure S32. HR-ESI-MS of **4**.

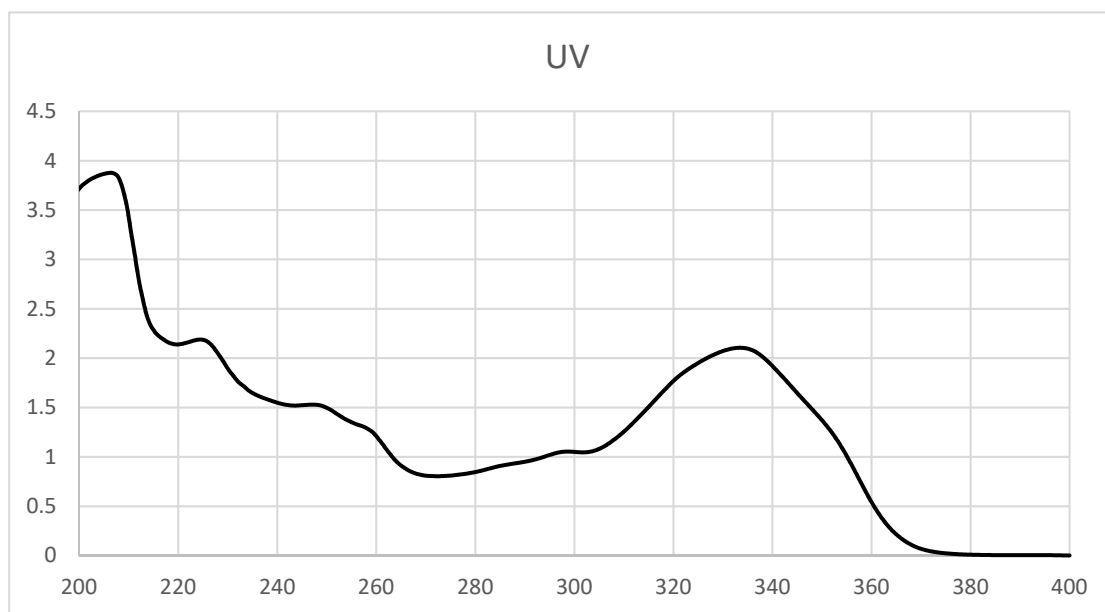


Figure S33. UV spectrum of **4** in MeOH.

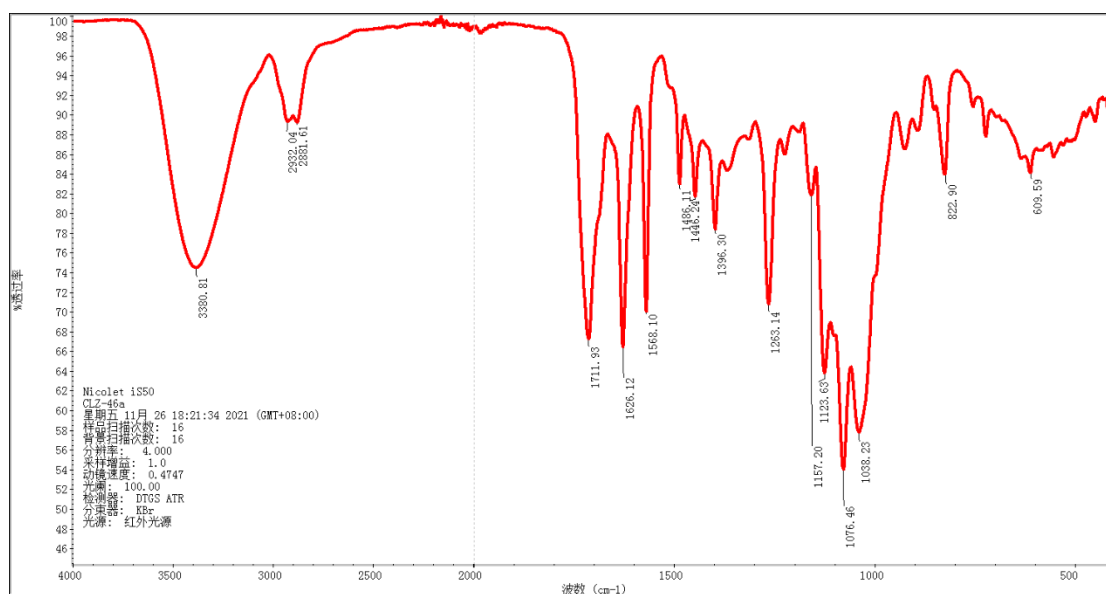


Figure S34. IR spectrum of 4.

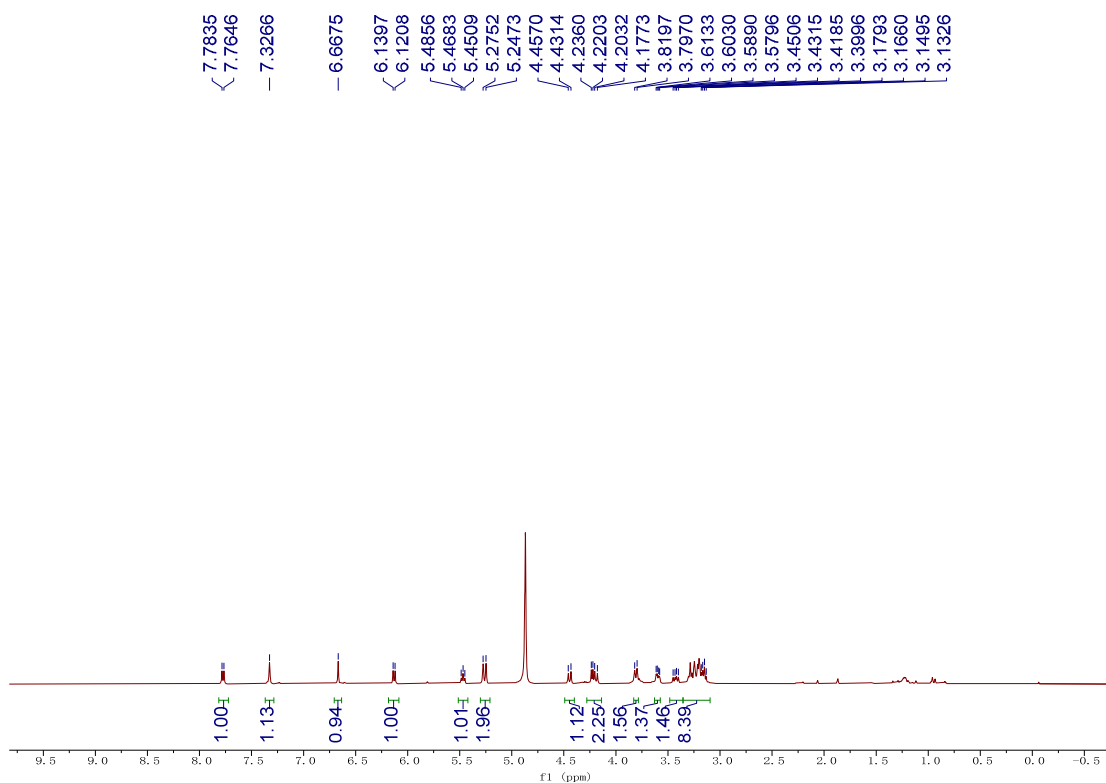


Figure S35. ¹H NMR (500 MHz) spectrum of 4 in MeOD.

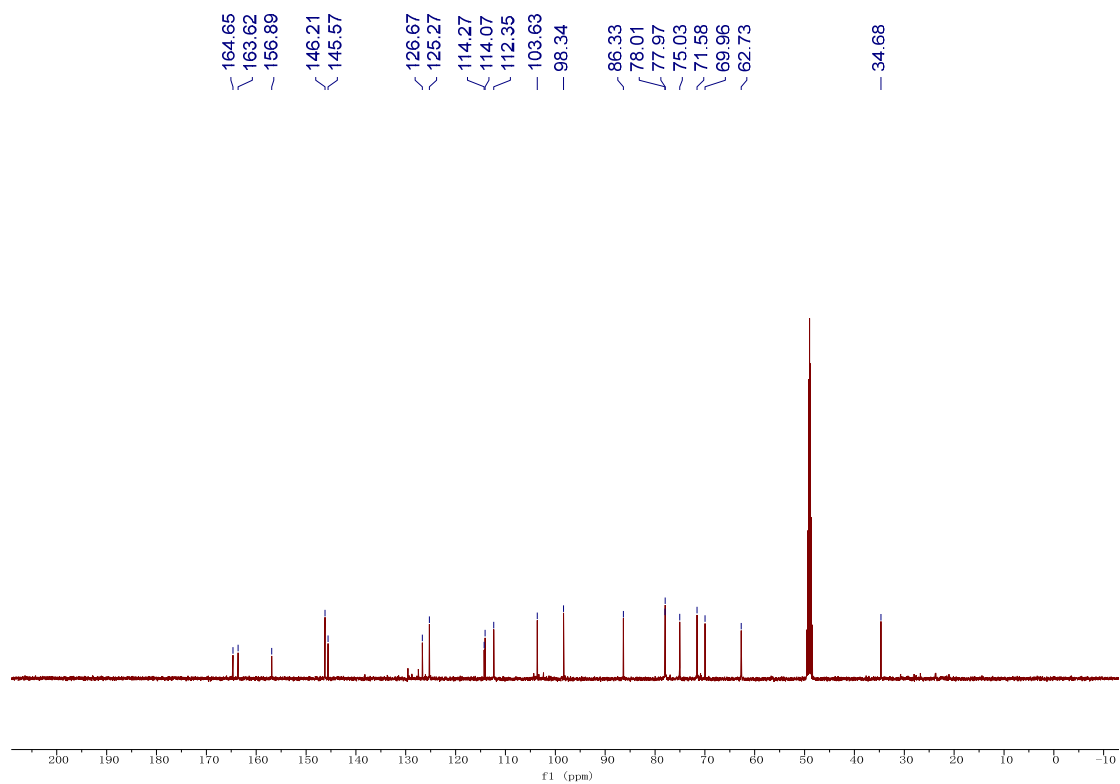


Figure S36. ^{13}C NMR (125 MHz) spectrum of **4** in MeOD.

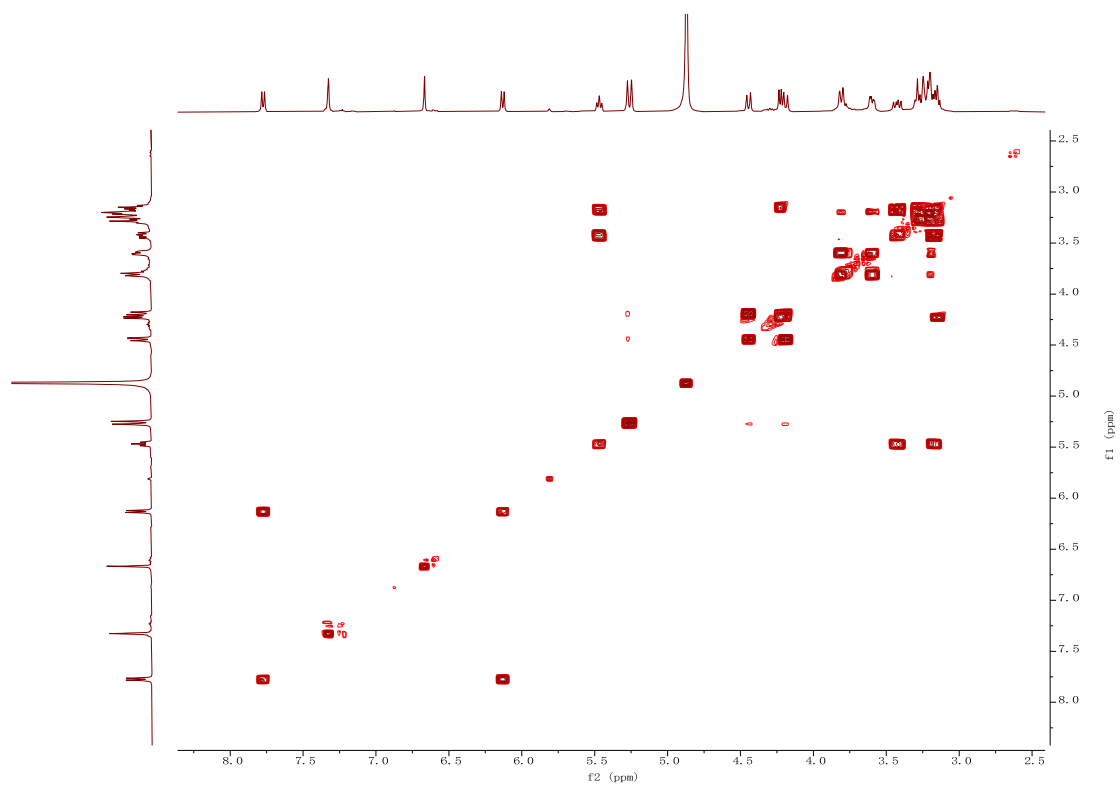


Figure S37. ^1H - ^1H COSY (500 MHz) spectrum of **4** in MeOD.

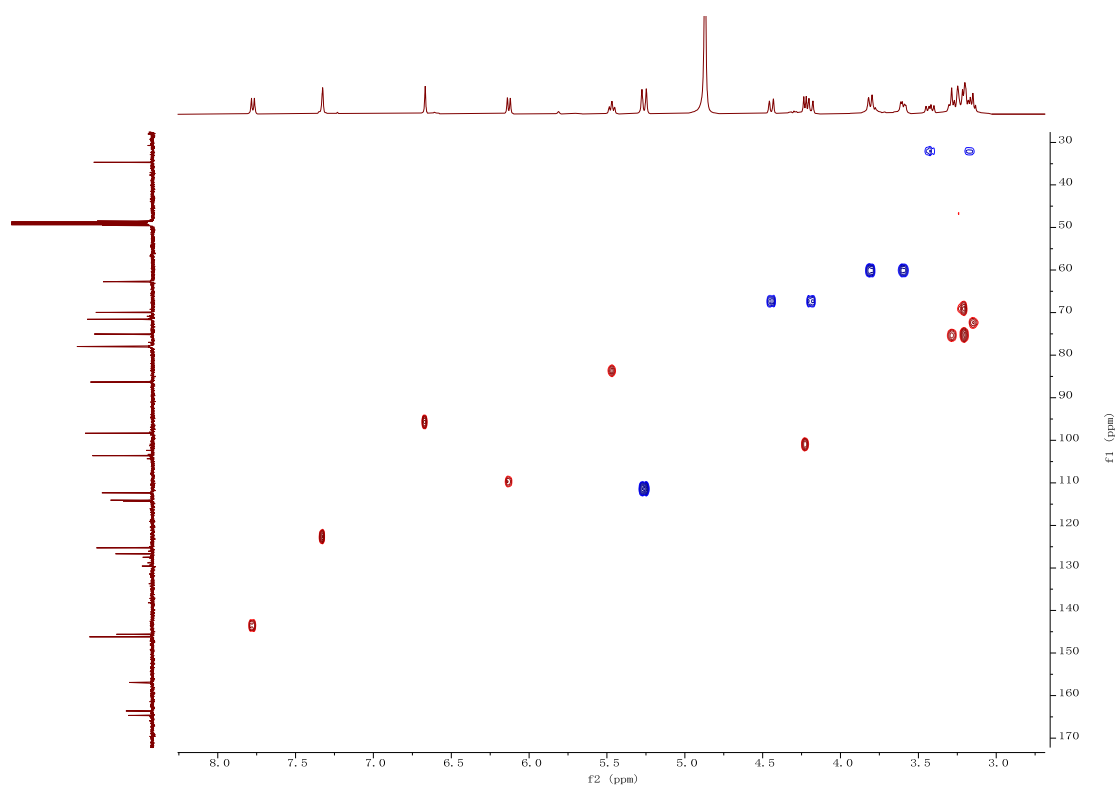


Figure S38. HSQC (500 MHz) spectrum of **4** in MeOD.

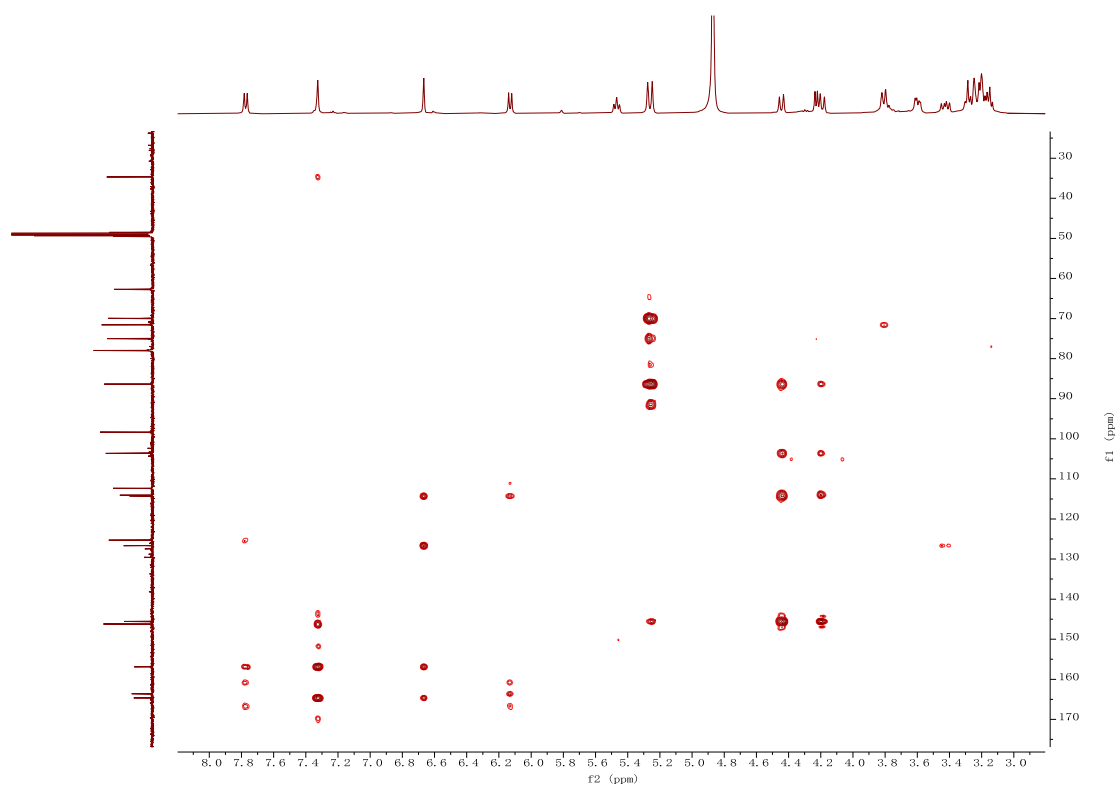


Figure S39. HMBC (500 MHz) spectrum of **4** in MeOD.

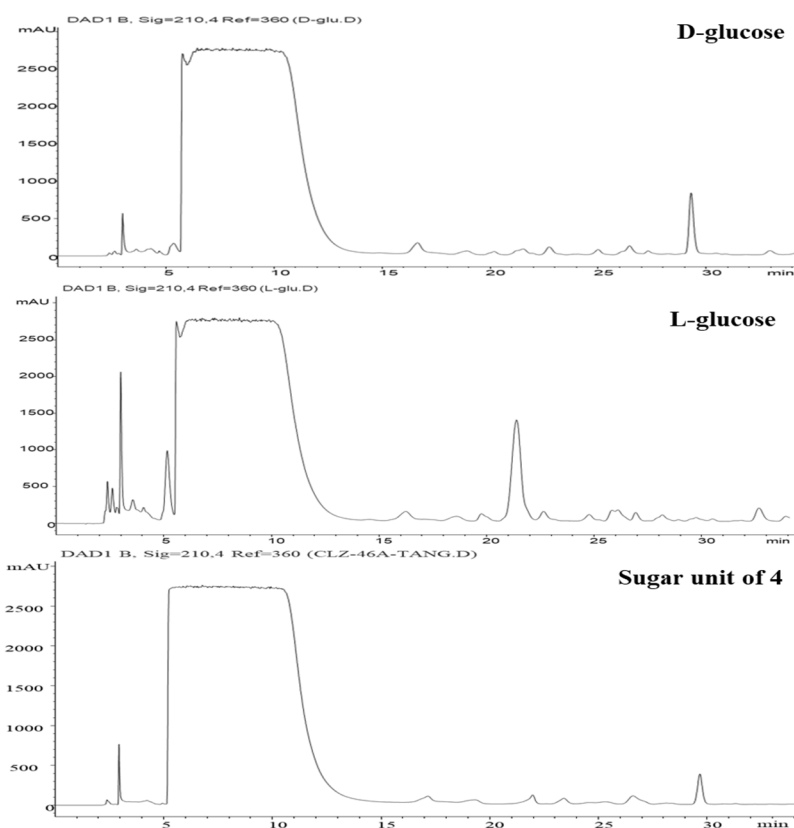


Figure S40. HPLC-UV (210 nm) chromatograms of the derivatives of D-glucose, L-glucose, and the sugar units of claulenoside A (**4**).

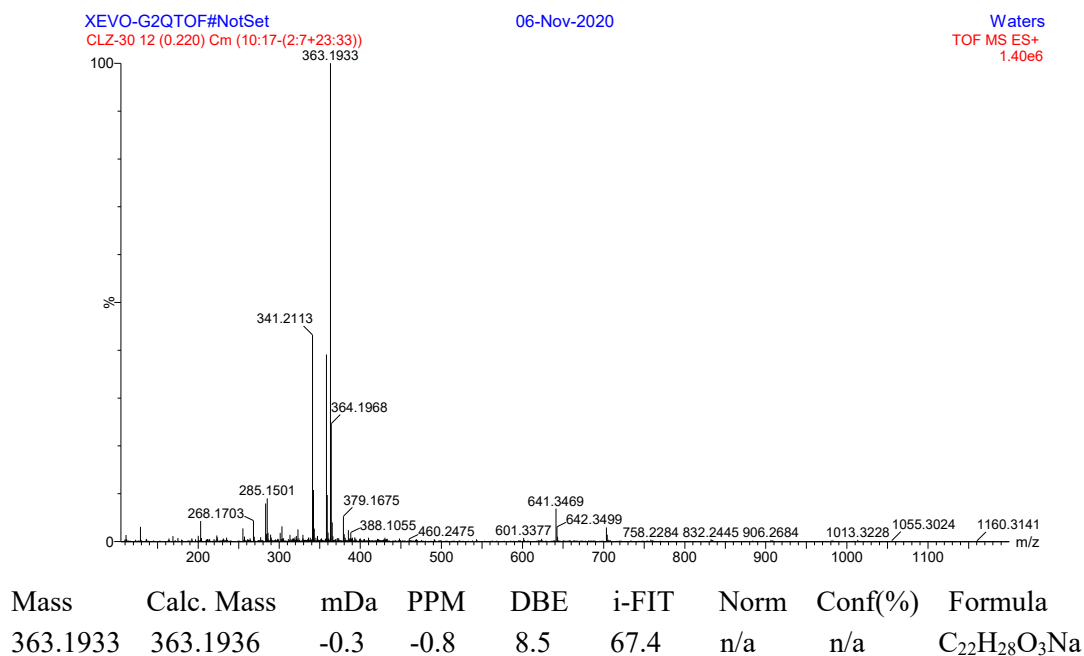


Figure S41. HR-ESI-MS of **5**.

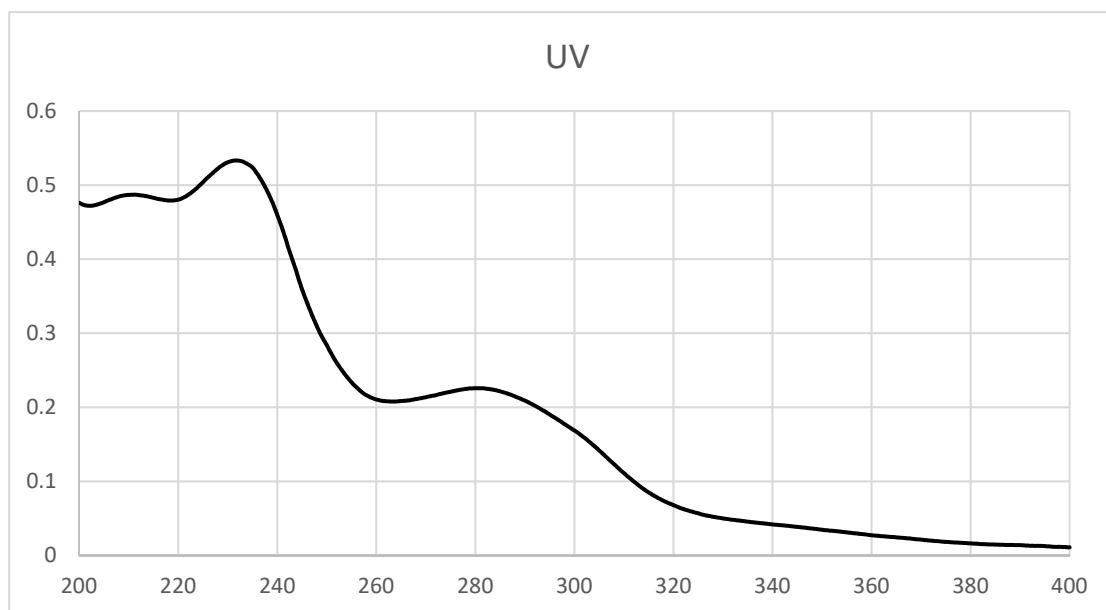


Figure S42. UV spectrum of **5** in MeOH.



Figure S43. IR spectrum of **5**.

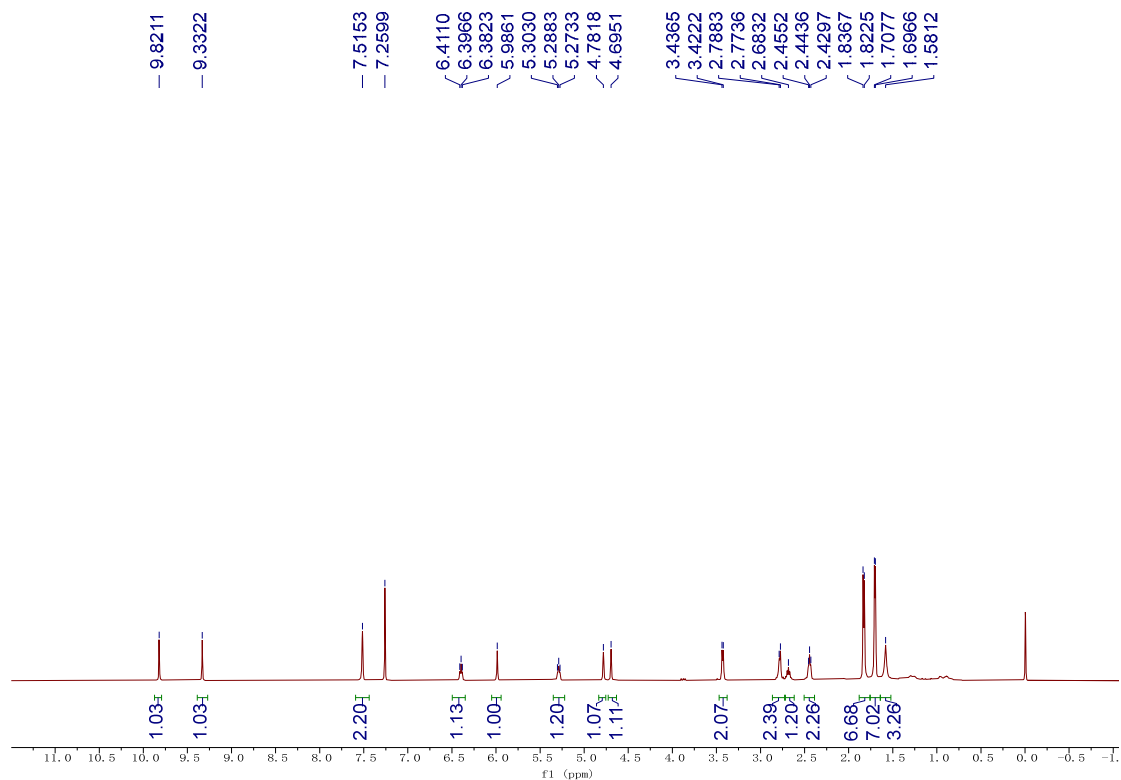


Figure S44. ¹H NMR (500 MHz) spectrum of **5** in CDCl₃.

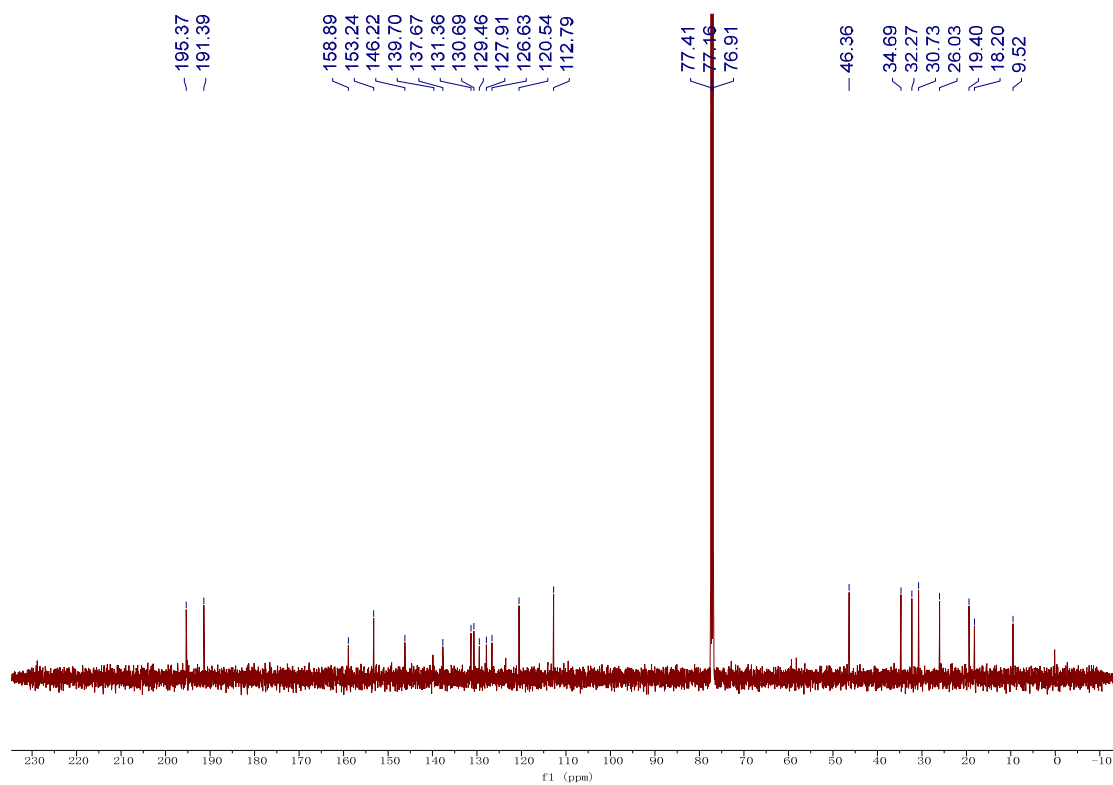


Figure S45. ¹³C NMR (125 MHz) spectrum of **5** in CDCl₃.

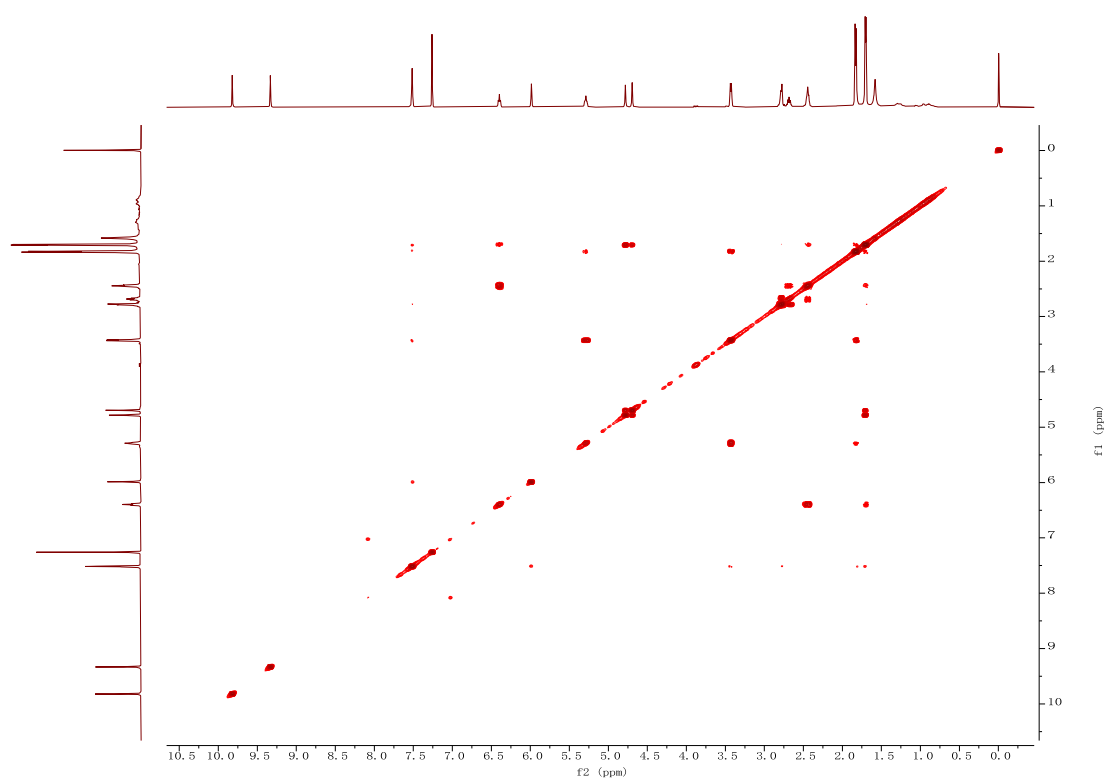


Figure S46. ^1H - ^1H COSY (500 MHz) spectrum of **5** in CDCl_3 .

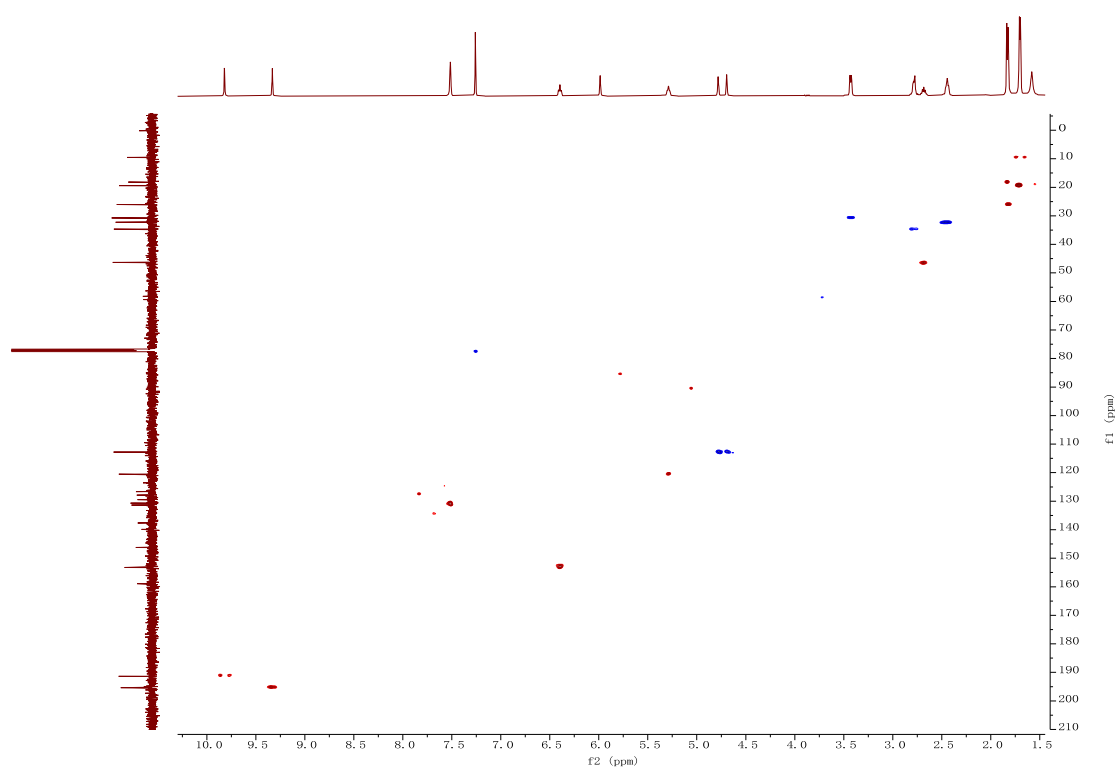


Figure S47. HSQC (500 MHz) spectrum of **5** in CDCl_3 .

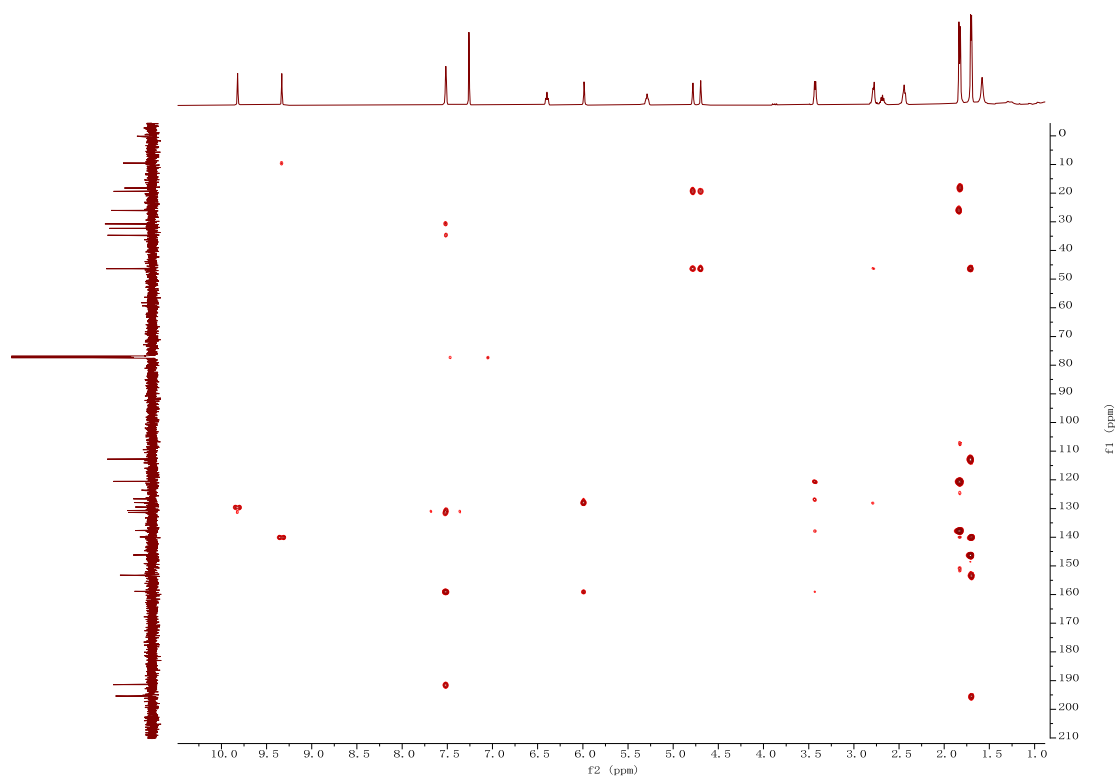


Figure S48. HMBC (500 MHz) spectrum of **5** in CDCl_3 .

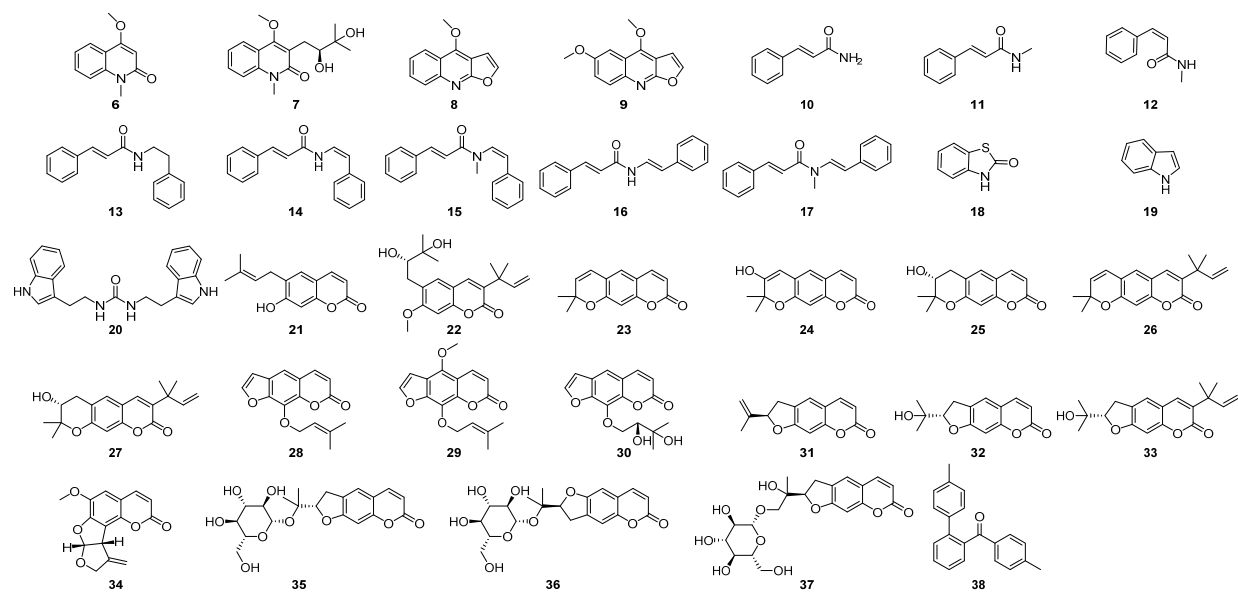


Figure S49. Chemical structures of compounds **6**–**38**.

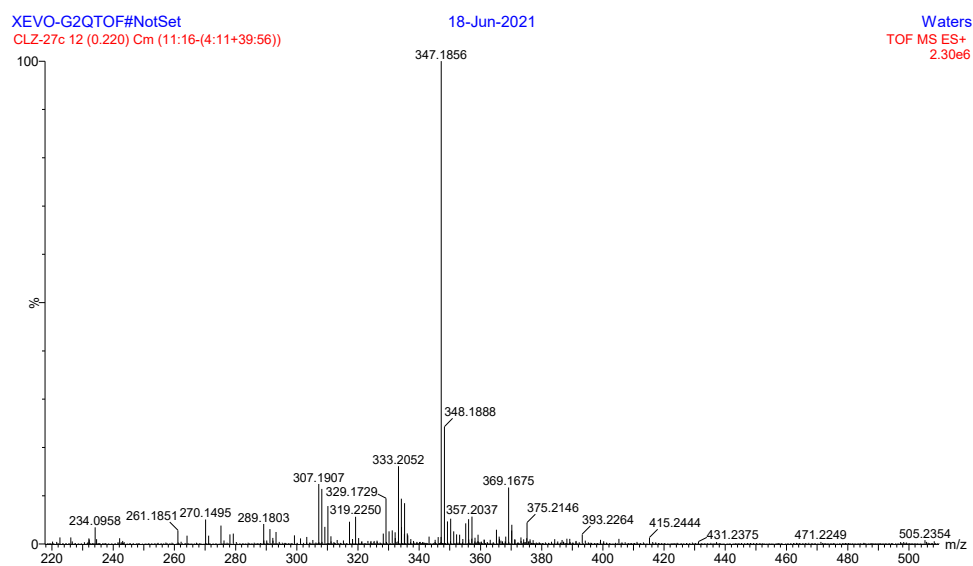


Figure S50. ESI-MS of **22**.

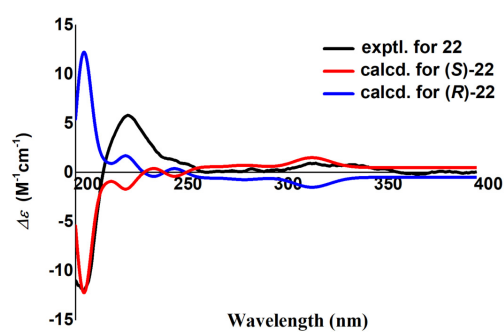


Figure S51. Experimental and calculated ECD spectra of **22**.