

Supporting Information

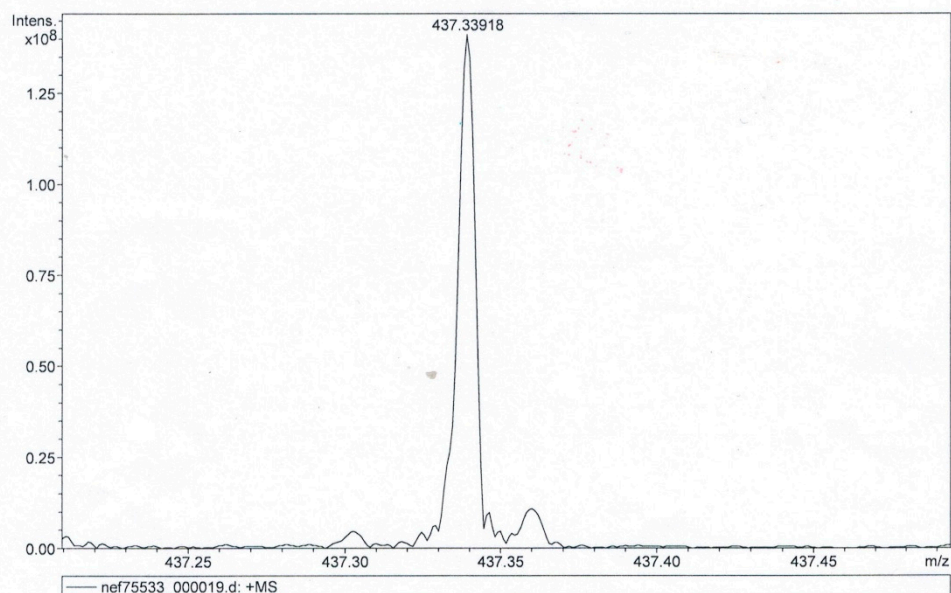
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Mass Spectrum SmartFormula Report

Analysis Info

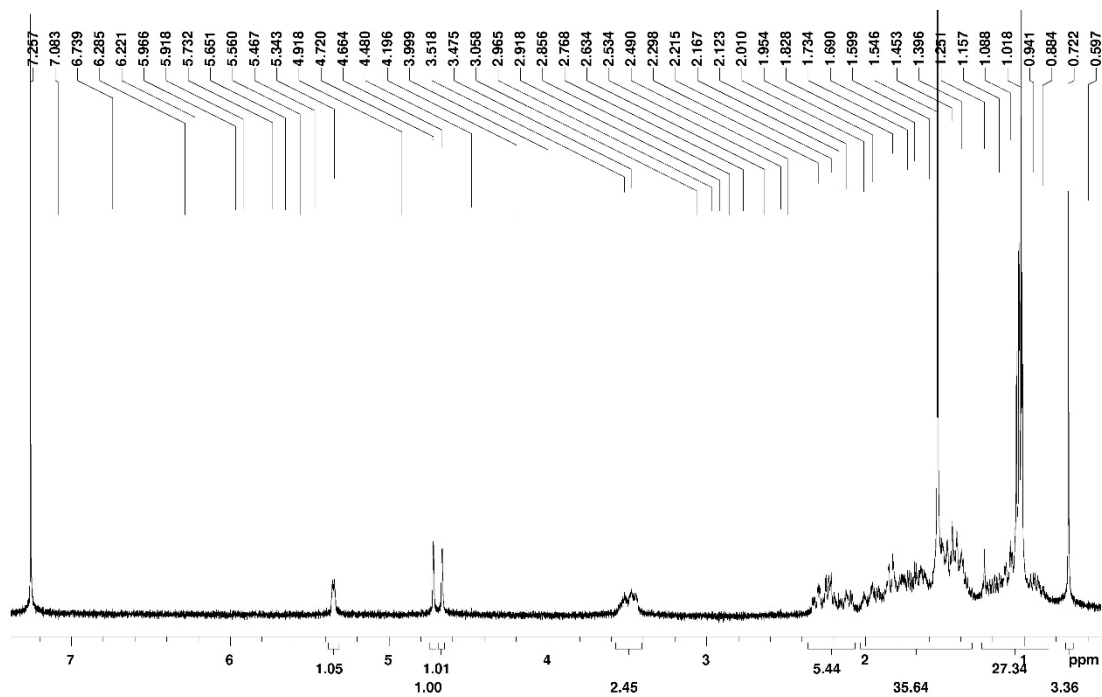
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Method broadband first signal
Sample Name Nef-7-5-5-3-3
Comment ESI Positive

12/6/2016 3:47:07 PM
Operator: YU HSIAO-CHING
Instrument: BRUKER FT-MS solariX

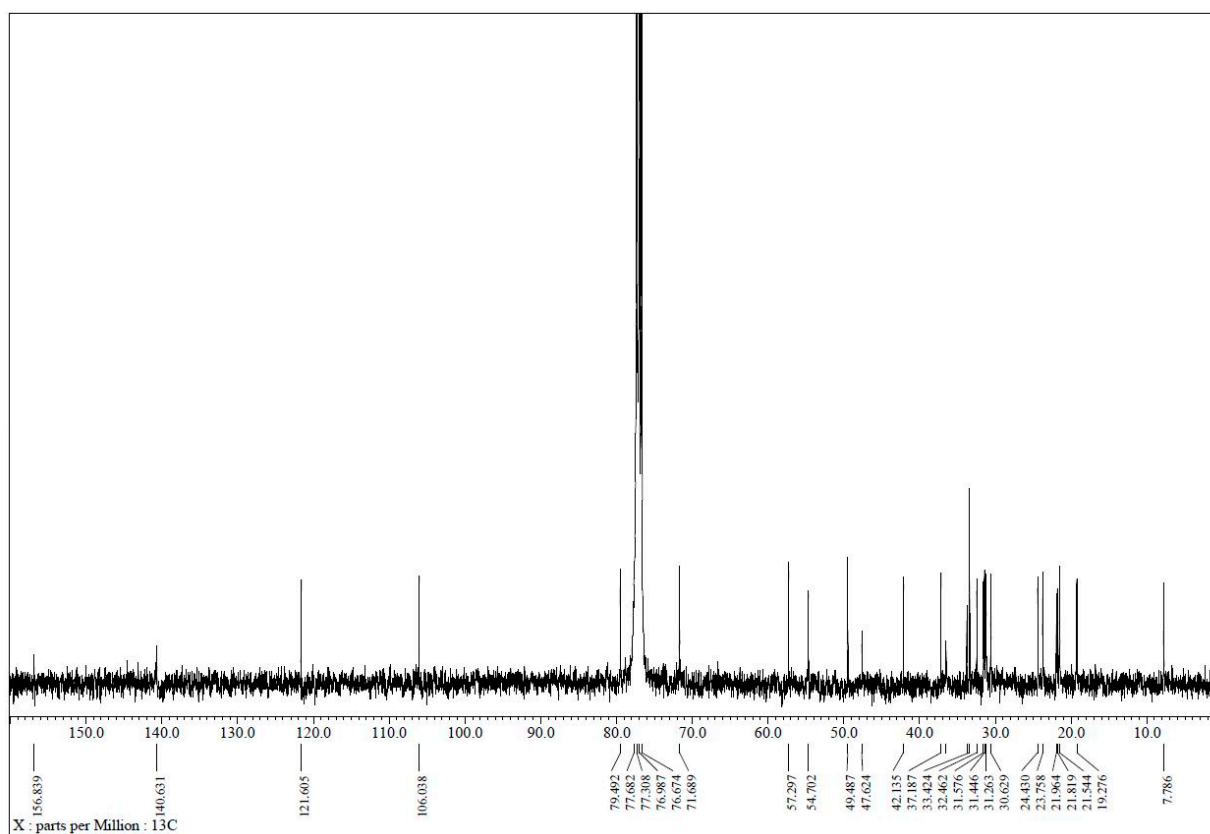


Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻	Conf	N-Rule
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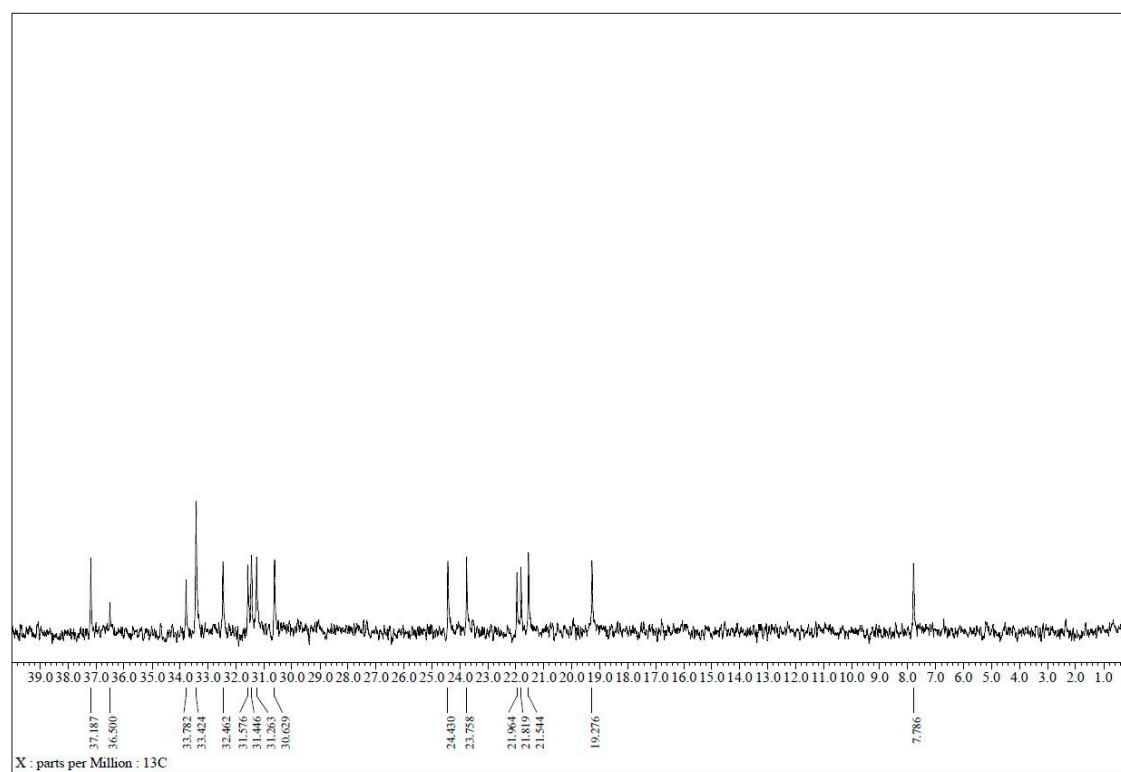
S01. HRESIMS spectrum of compound 1.



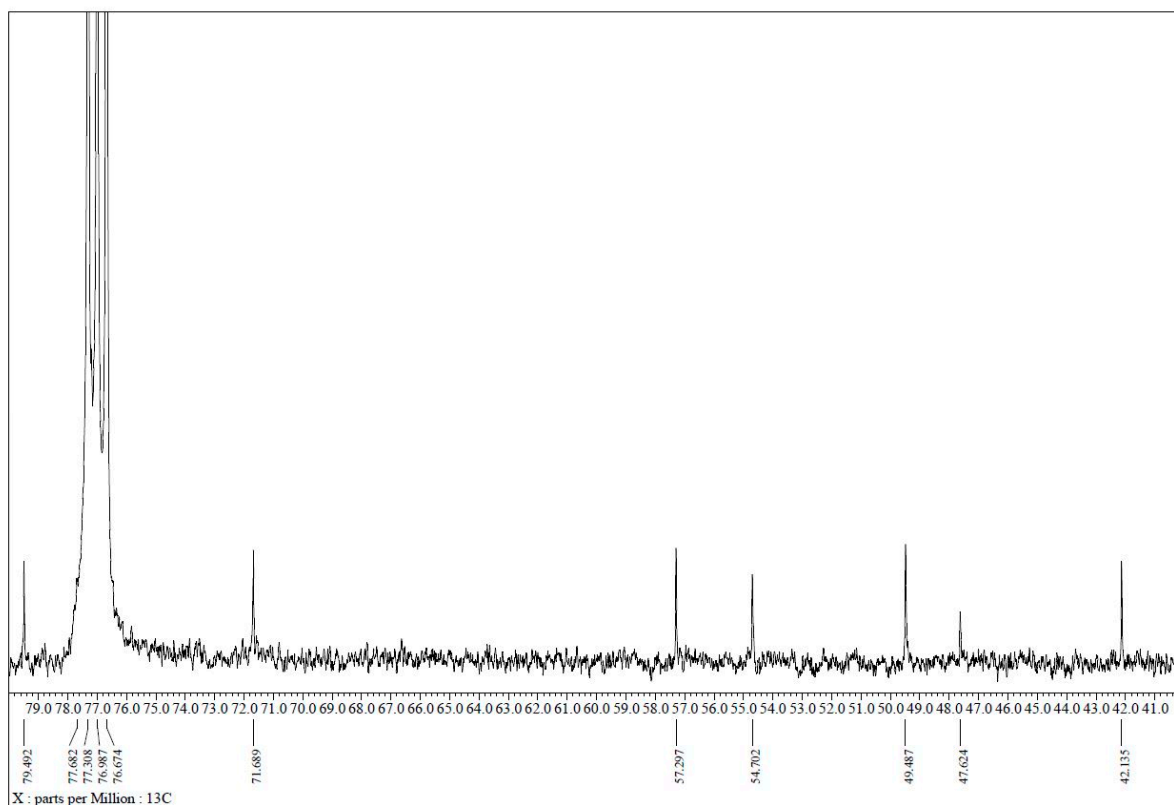
S02. ¹H NMR spectrum (400 MHz) of compound 1 in CDCl₃.



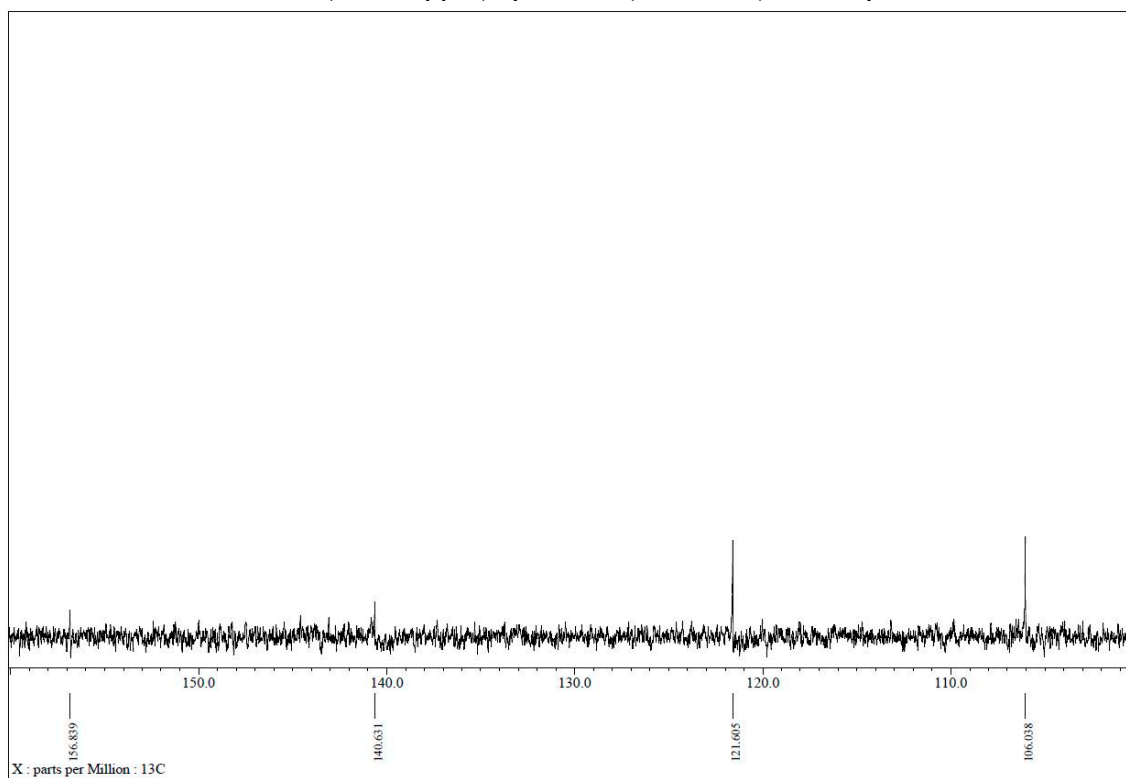
S03. ^{13}C NMR spectrum (100 MHz) of compound **1** in CDCl_3 .



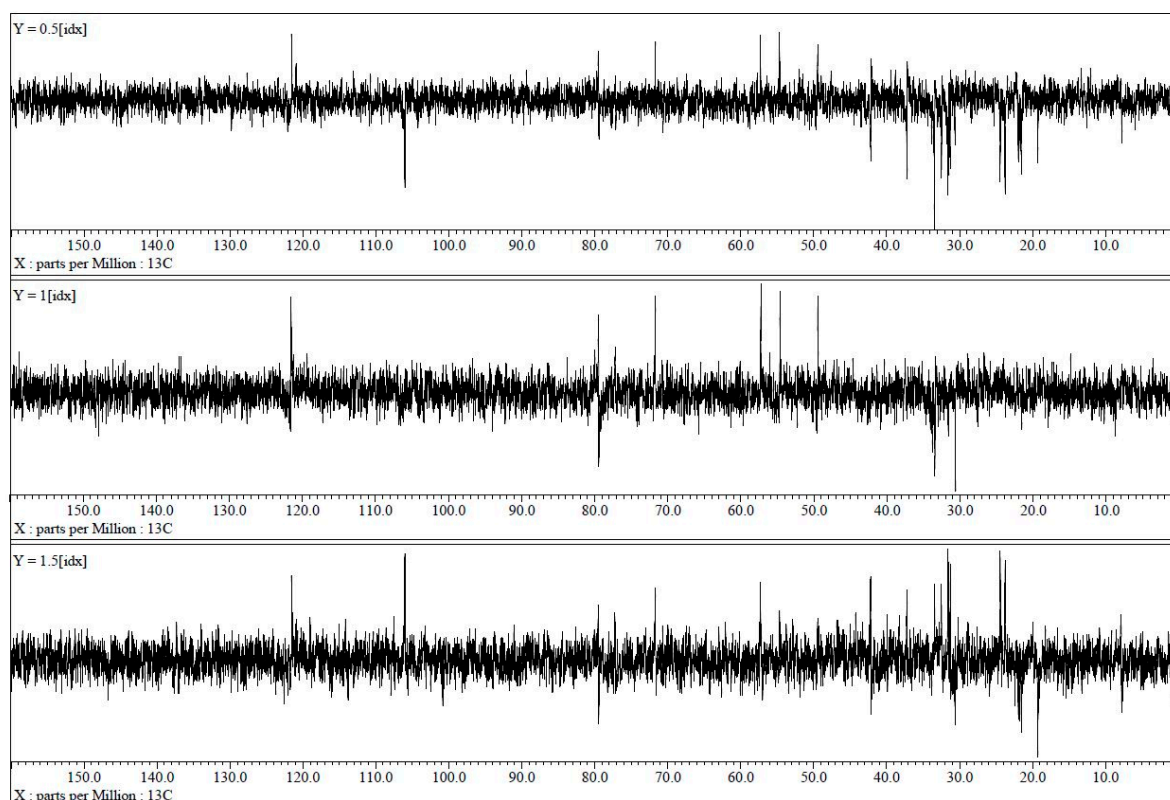
S04. ^{13}C NMR (0–40 ppm) spectrum (100 MHz) of compound **1** in CDCl_3 .



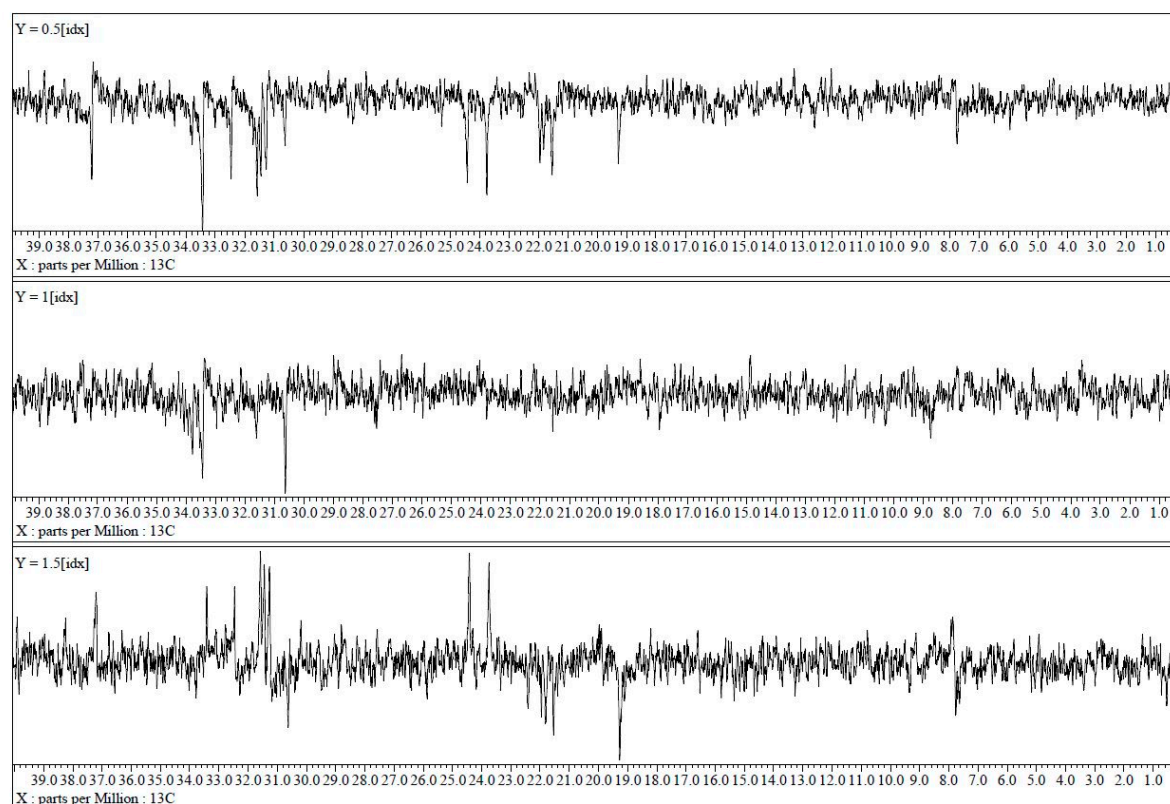
S05. ^{13}C NMR (40–80 ppm) spectrum (100 MHz) of compound **1** in CDCl_3 .



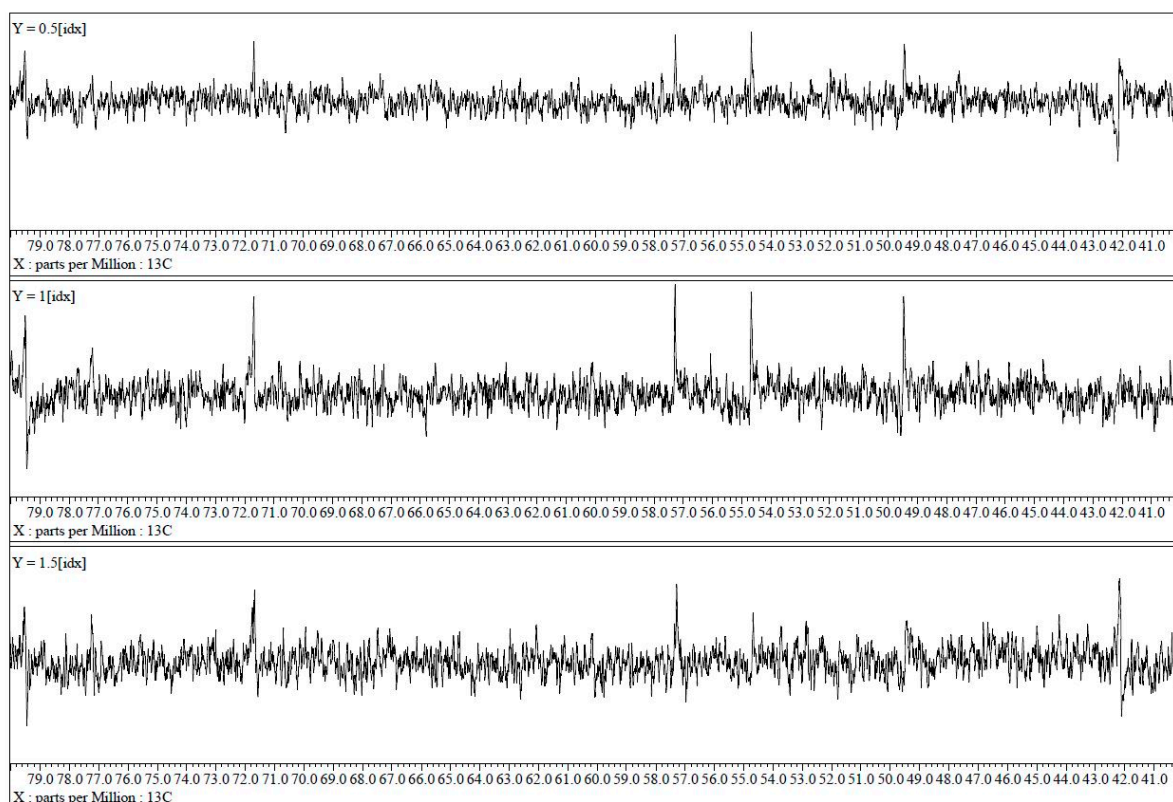
S06. ^{13}C NMR (100–160 ppm) spectrum (100 MHz) of compound **1** in CDCl_3 .



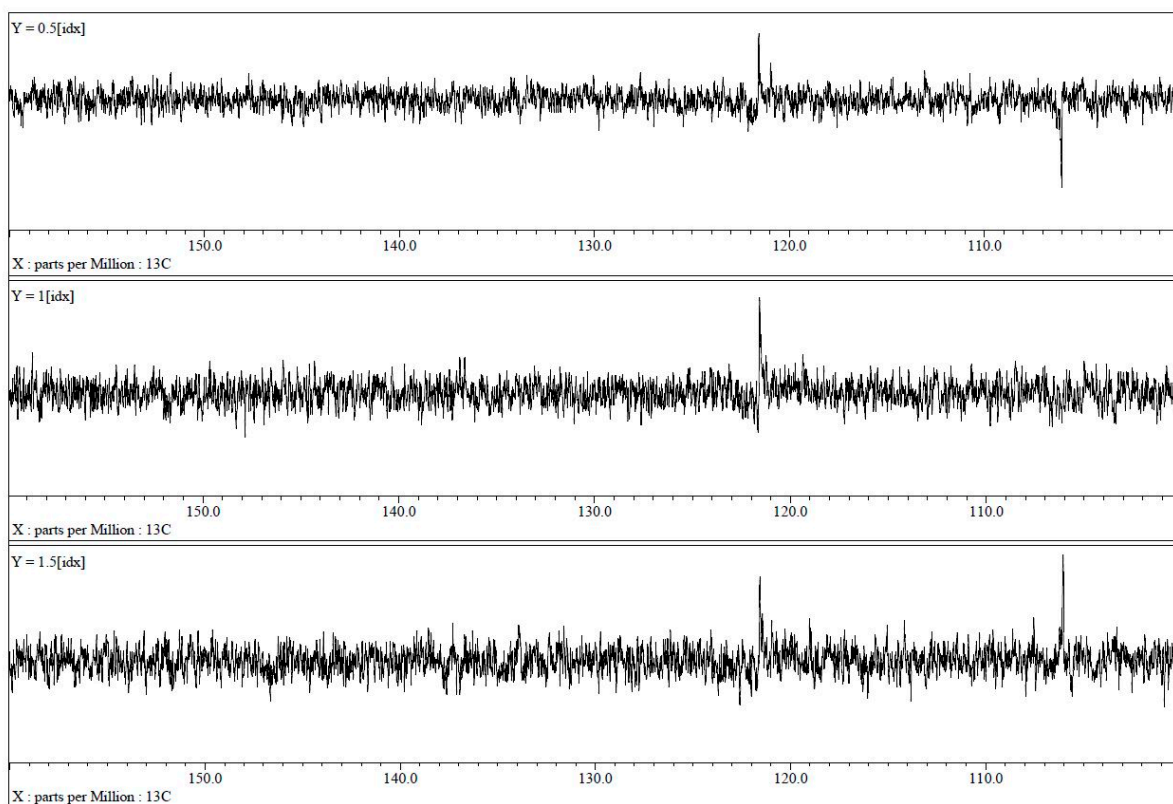
S07. DEPT spectrum of compound **1** in CDCl_3 .



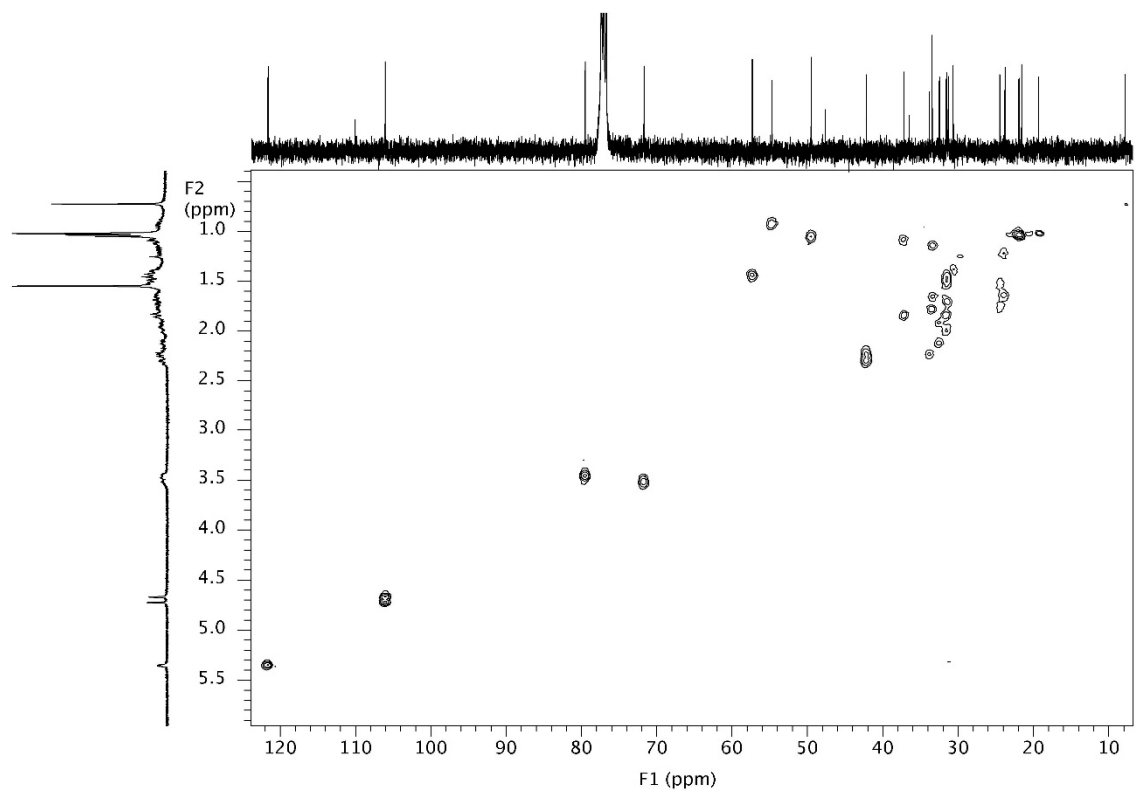
S08. DEPT (0–40 ppm) spectrum of compound **1** in CDCl_3 .



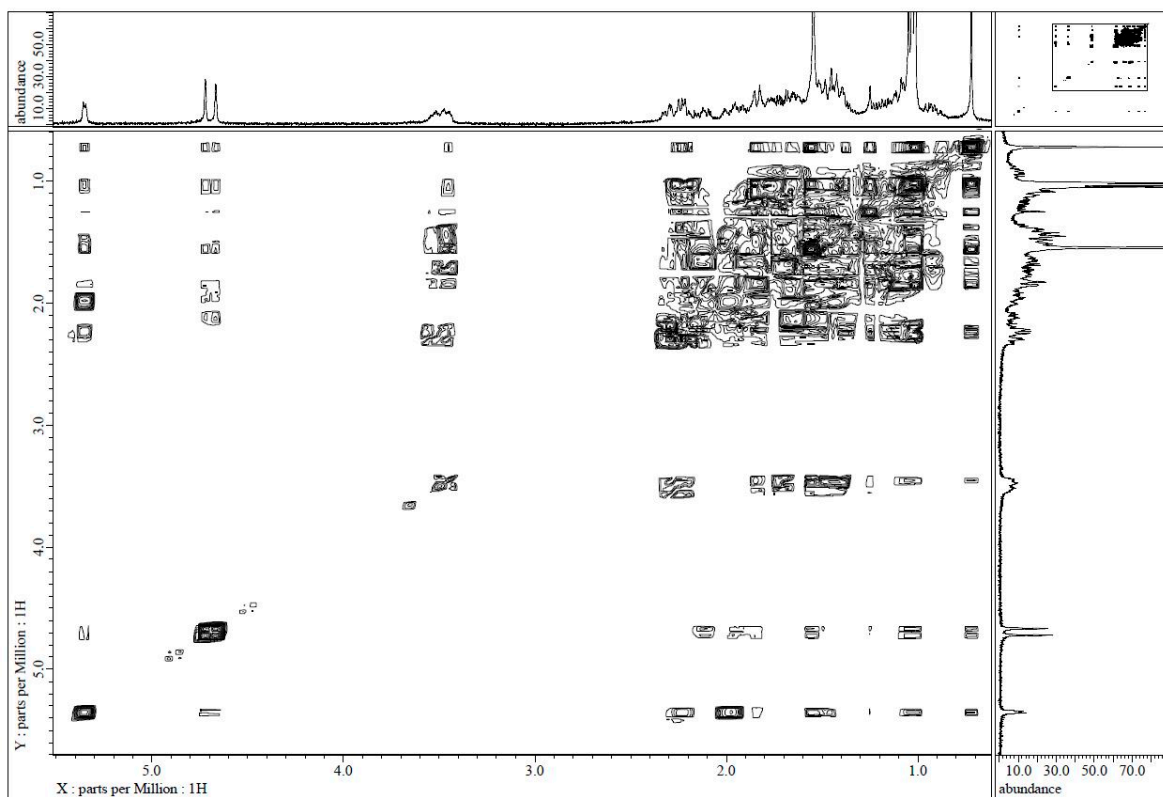
S09. DEPT (40–80 ppm) spectrum of compound **1** in CDCl_3 .



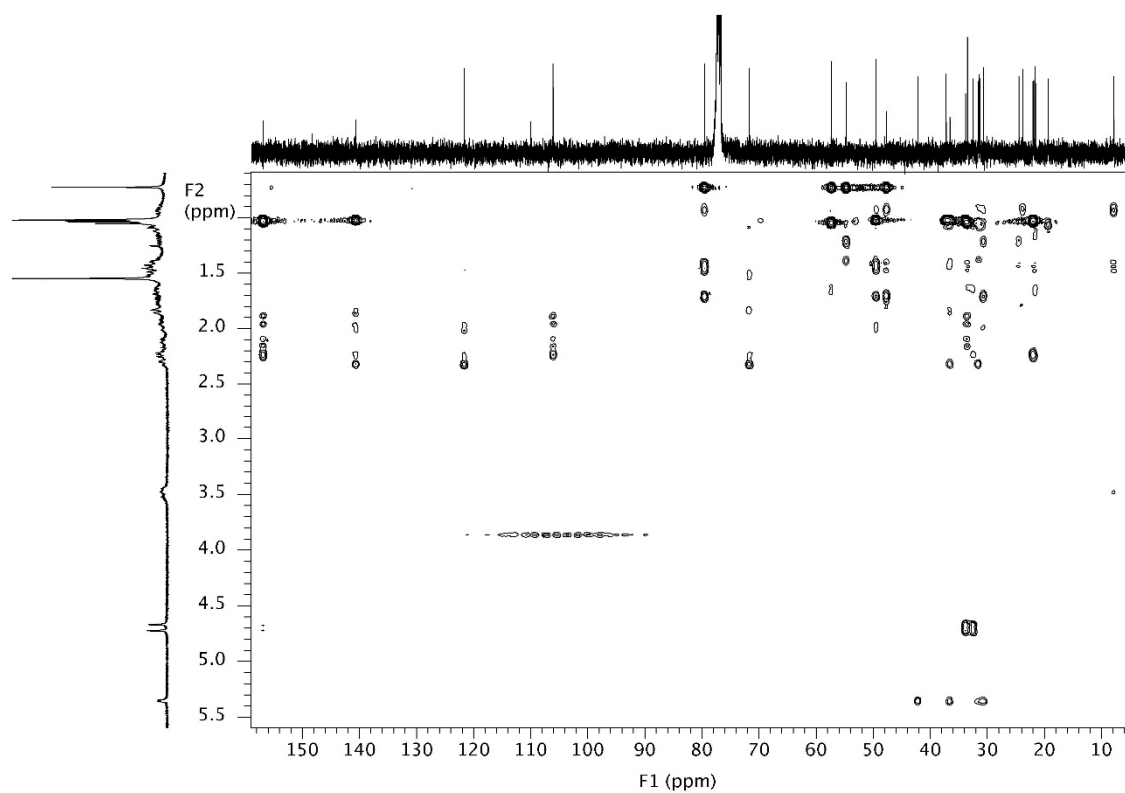
S10. DEPT (100–160 ppm) spectrum of compound **1** in CDCl_3 .



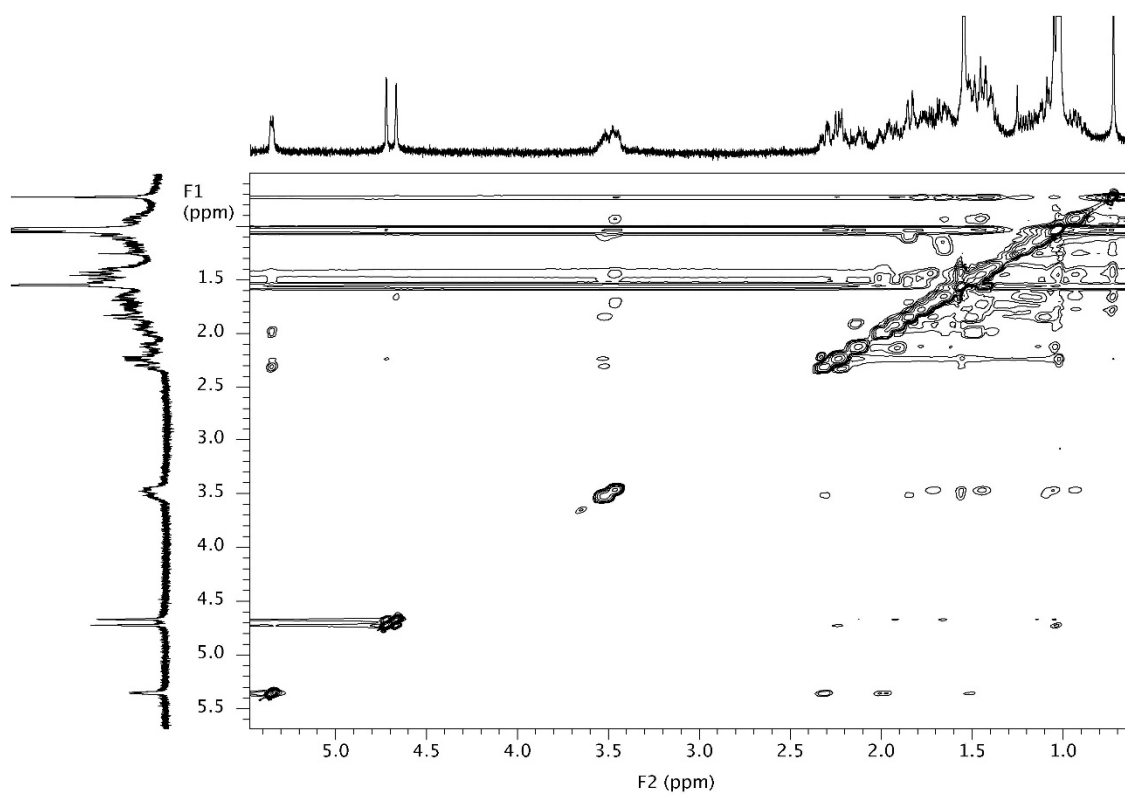
S11. gHSQC spectrum of compound **1** in CDCl₃.



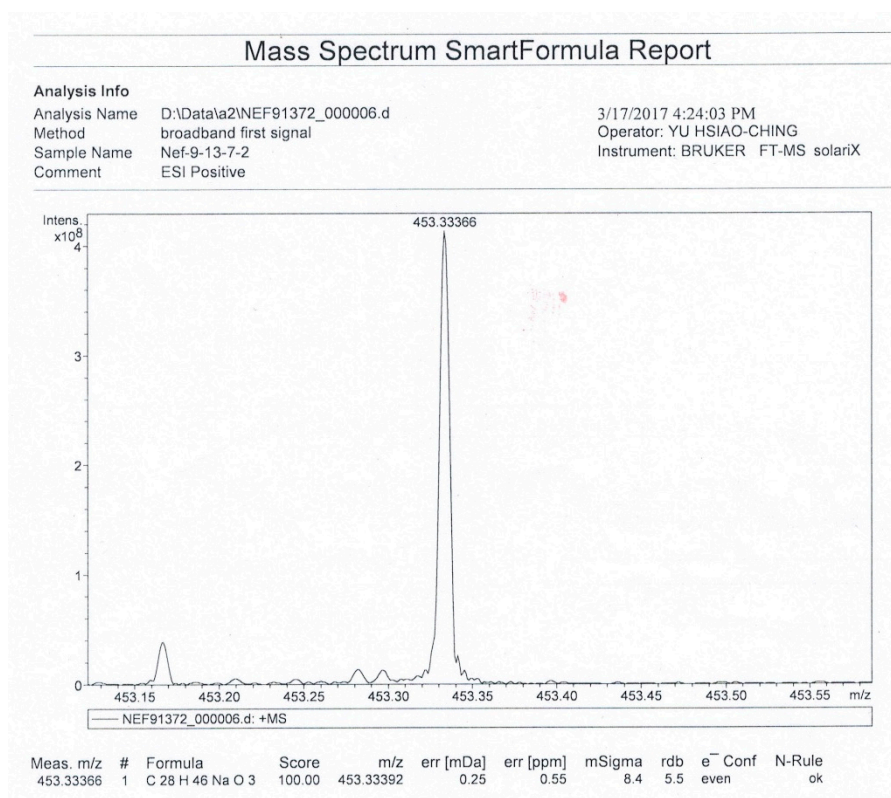
S12. ¹H–¹H COSY spectrum of compound **1** in CDCl₃.



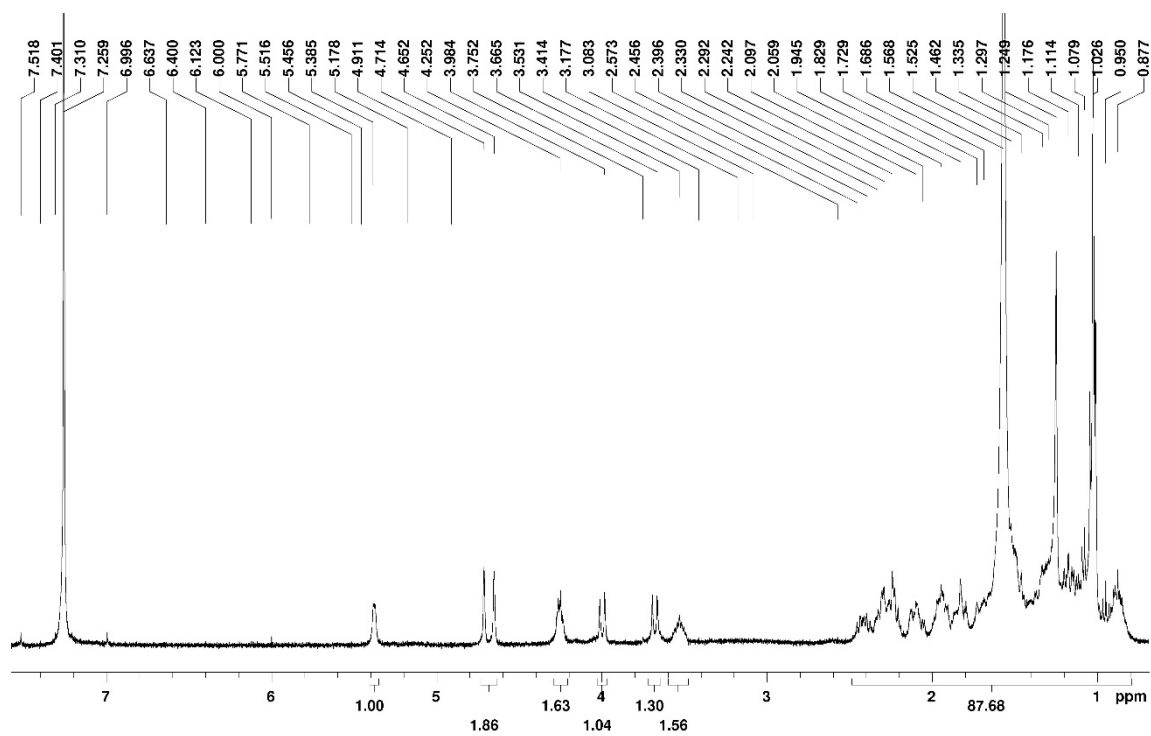
S13. gHMBC spectrum of compound **1** in CDCl_3 .



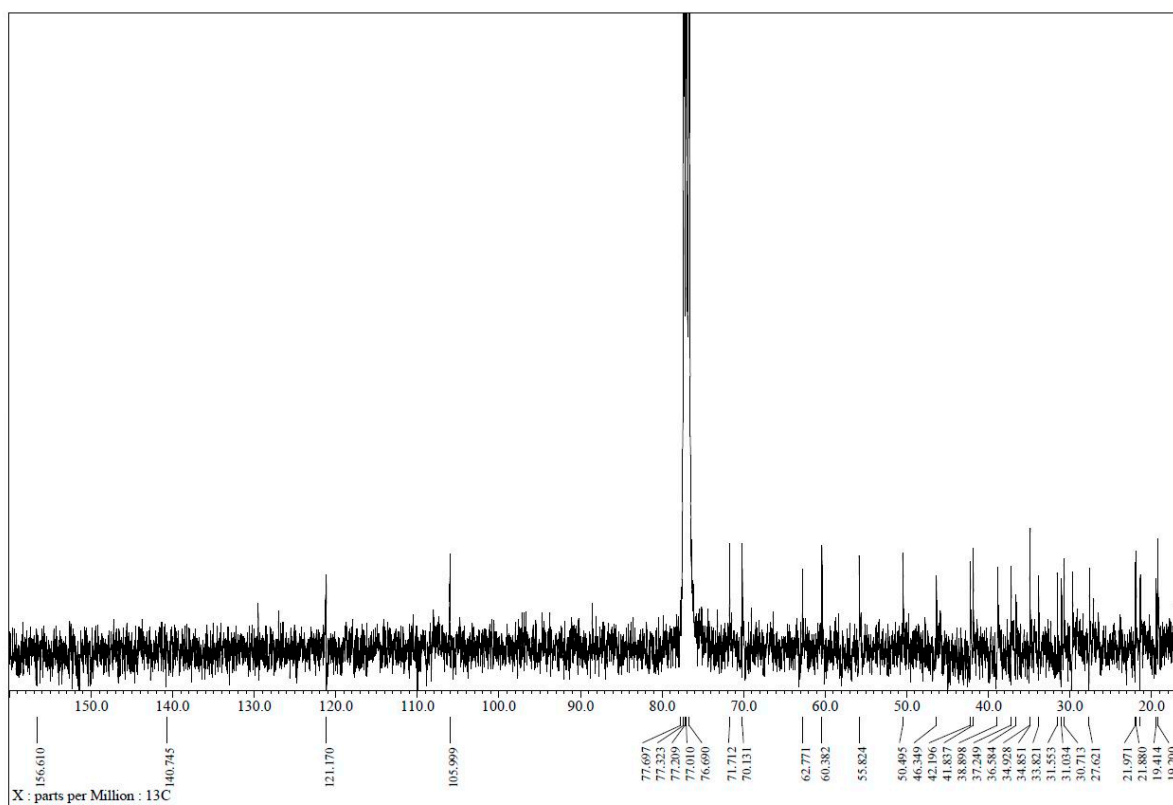
S14. NOESY spectrum of compound **1** in CDCl_3 .



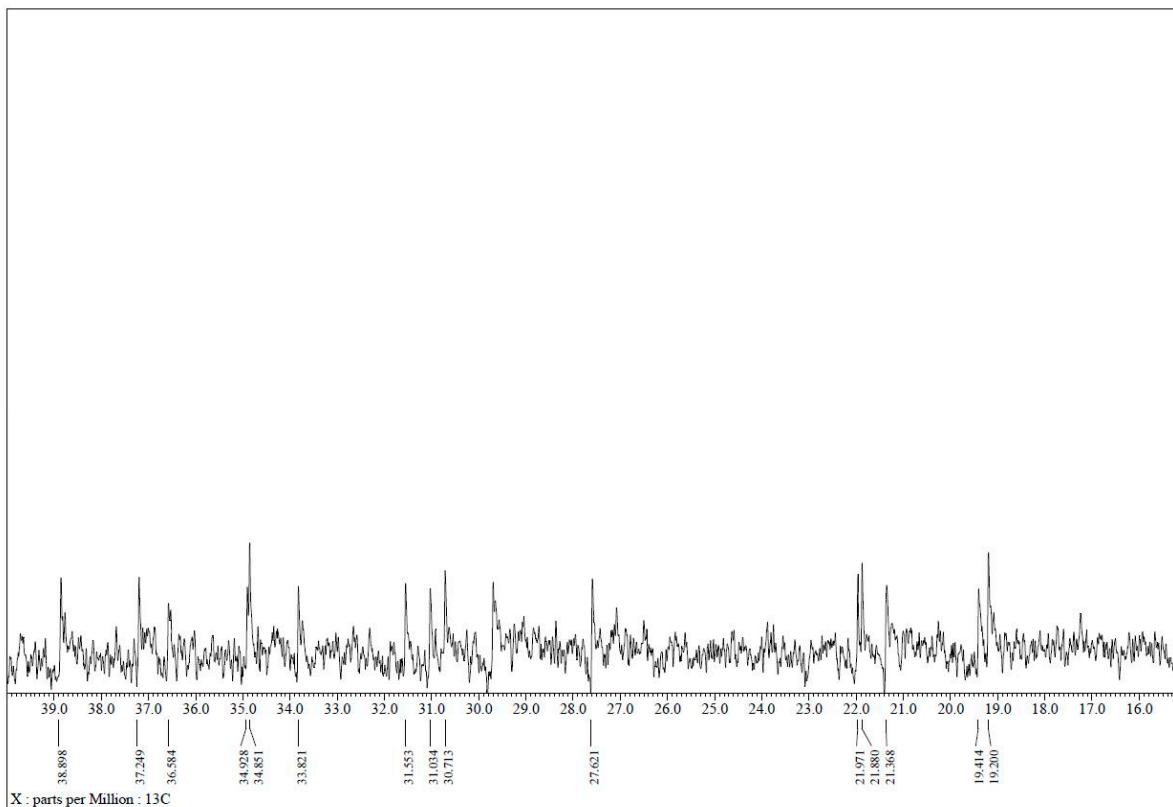
S15. HRESIMS spectrum of compound **2**.



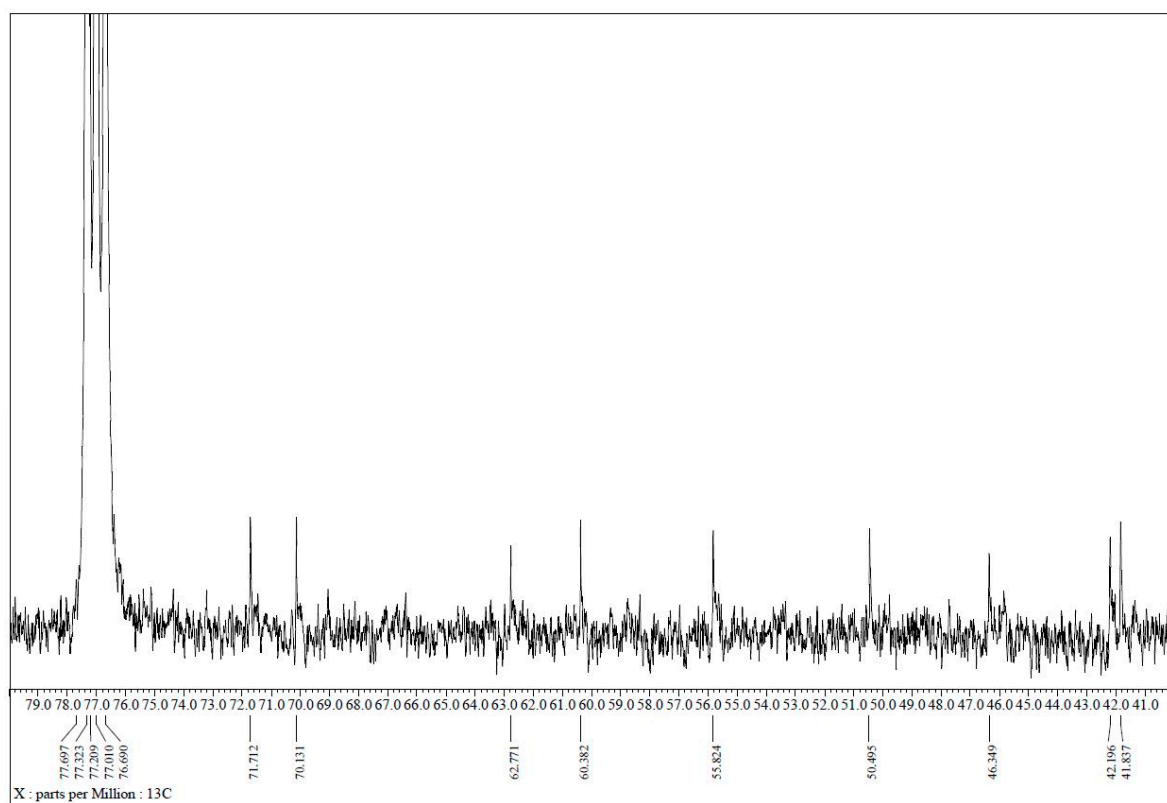
S16. ¹H NMR spectrum (400 MHz) of compound **2** in CDCl₃.



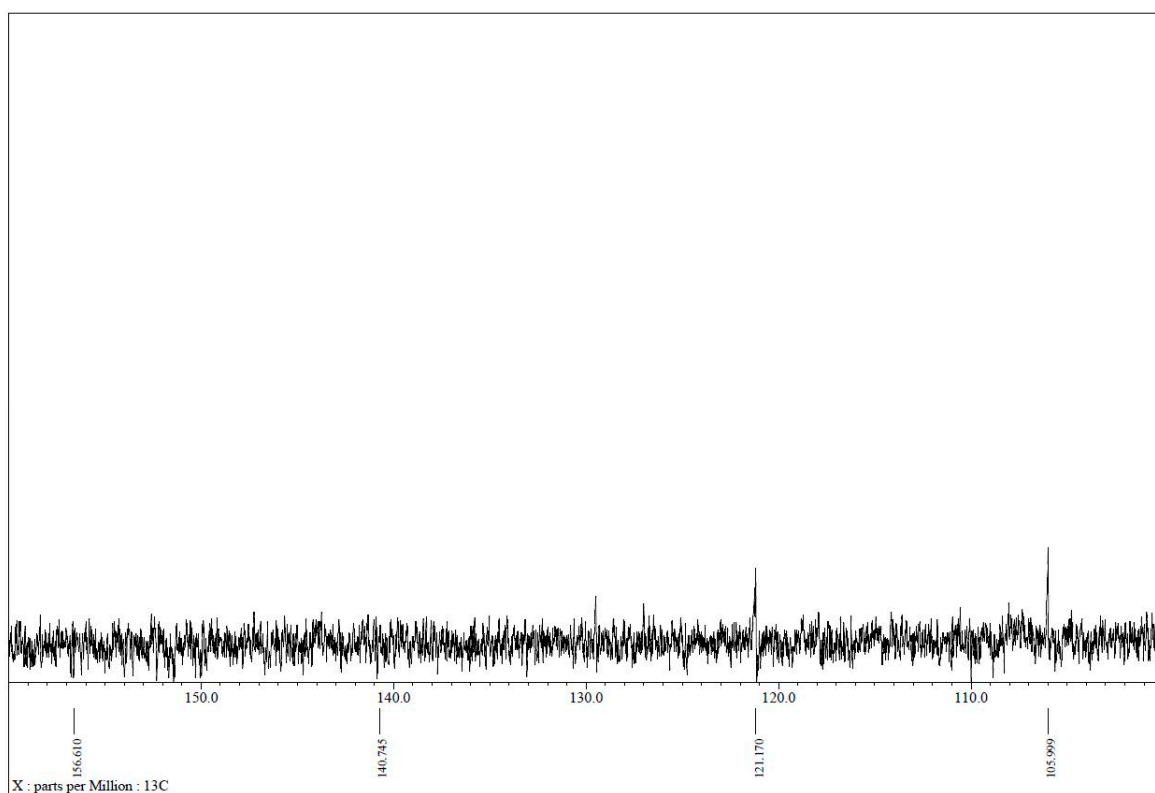
S17. ^{13}C NMR spectrum (100 MHz) of compound **2** in CDCl_3 .



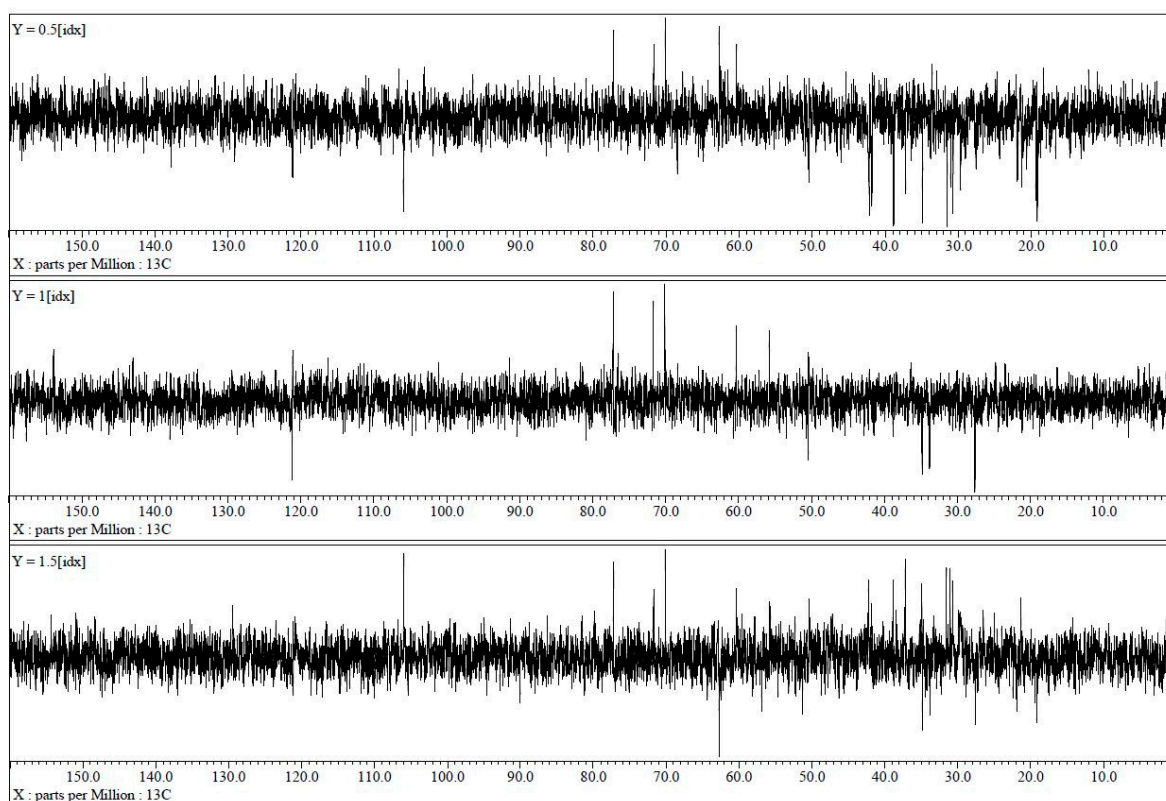
S18. ^{13}C NMR (15–40 ppm) spectrum (100 MHz) of compound **2** in CDCl_3 .



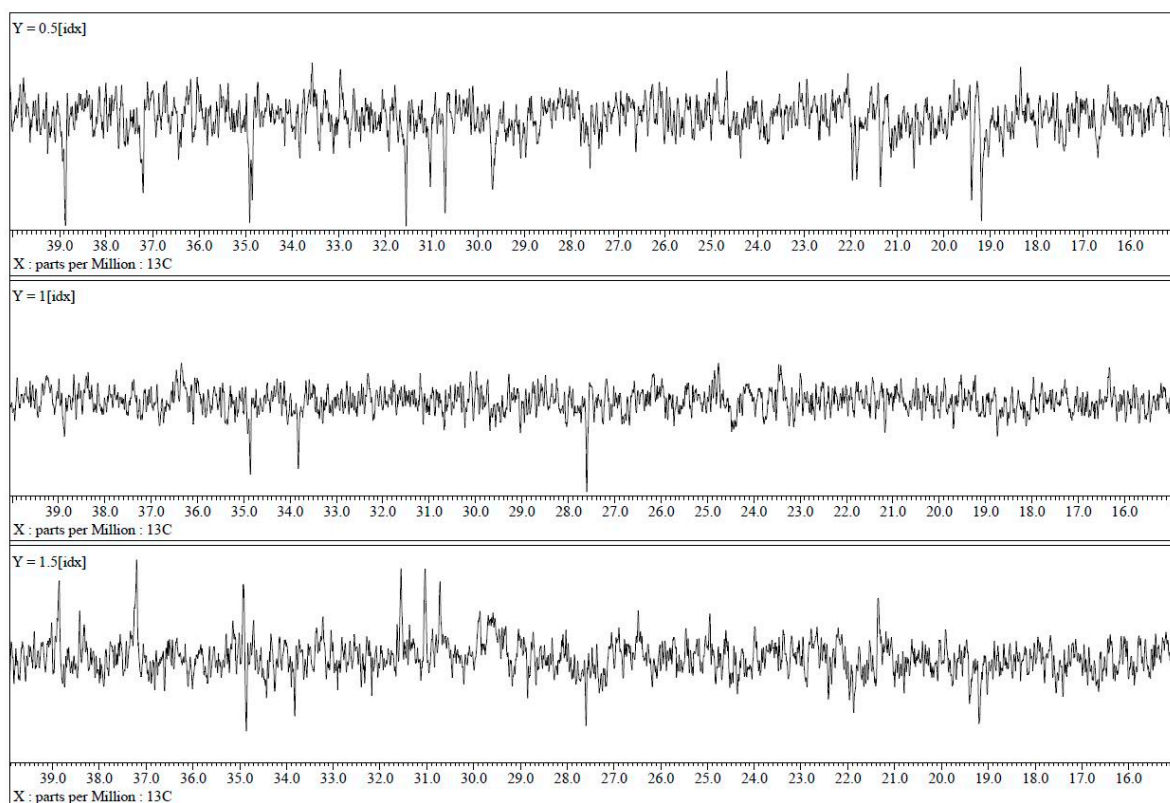
S19. ^{13}C NMR (40–80 ppm) spectrum (100 MHz) of compound **2** in CDCl_3 .



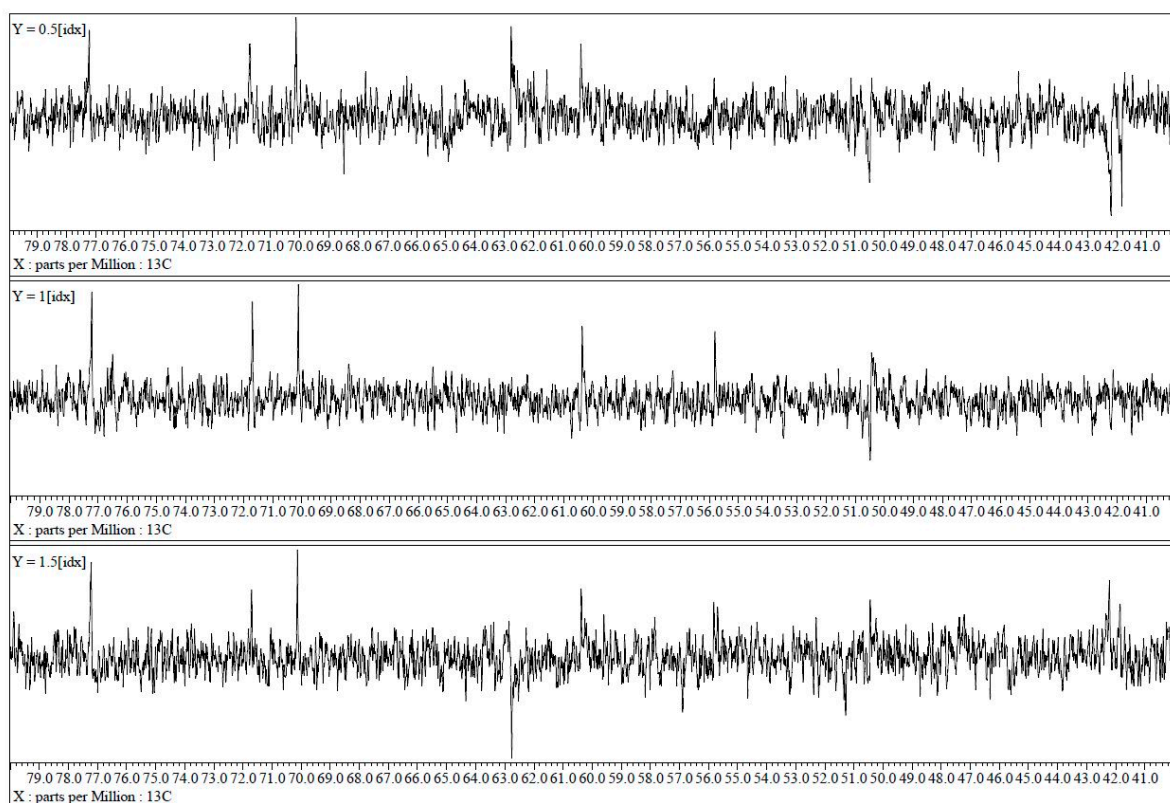
S20. ^{13}C NMR (100–160 ppm) spectrum (100 MHz) of compound **2** in CDCl_3 .



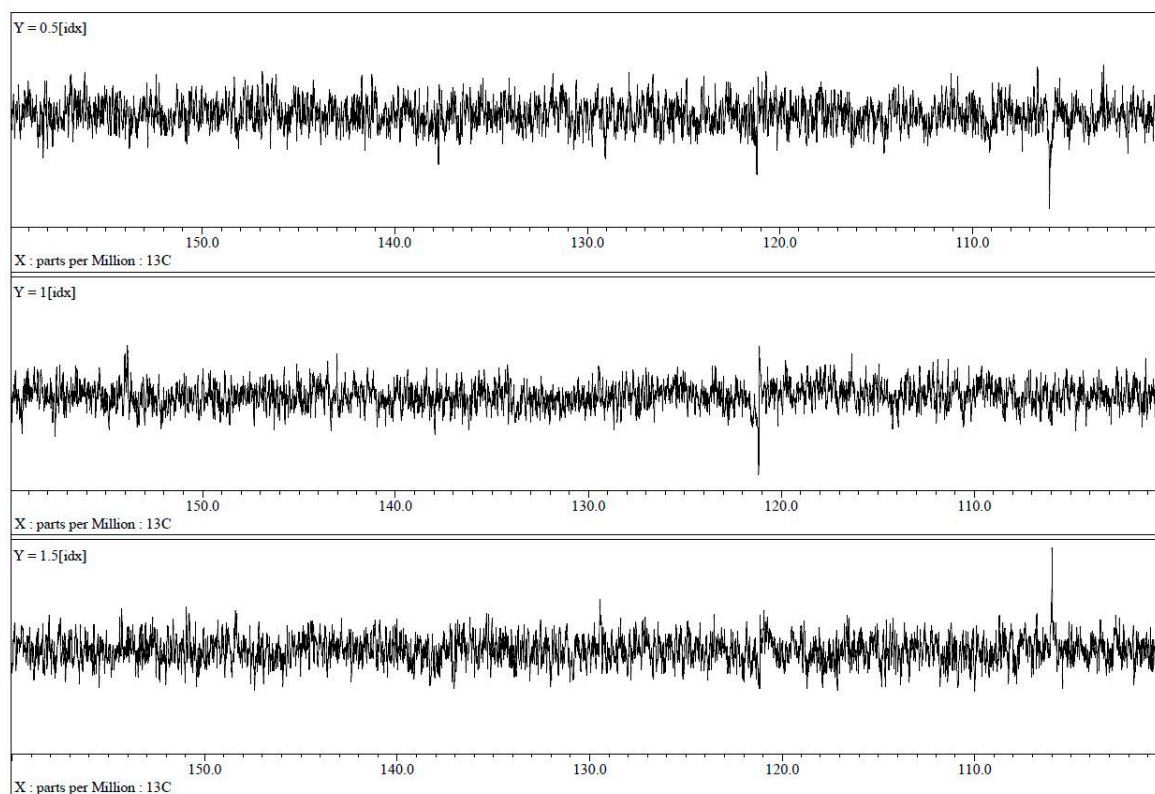
S21. DEPT spectrum of compound **2** in CDCl_3 .



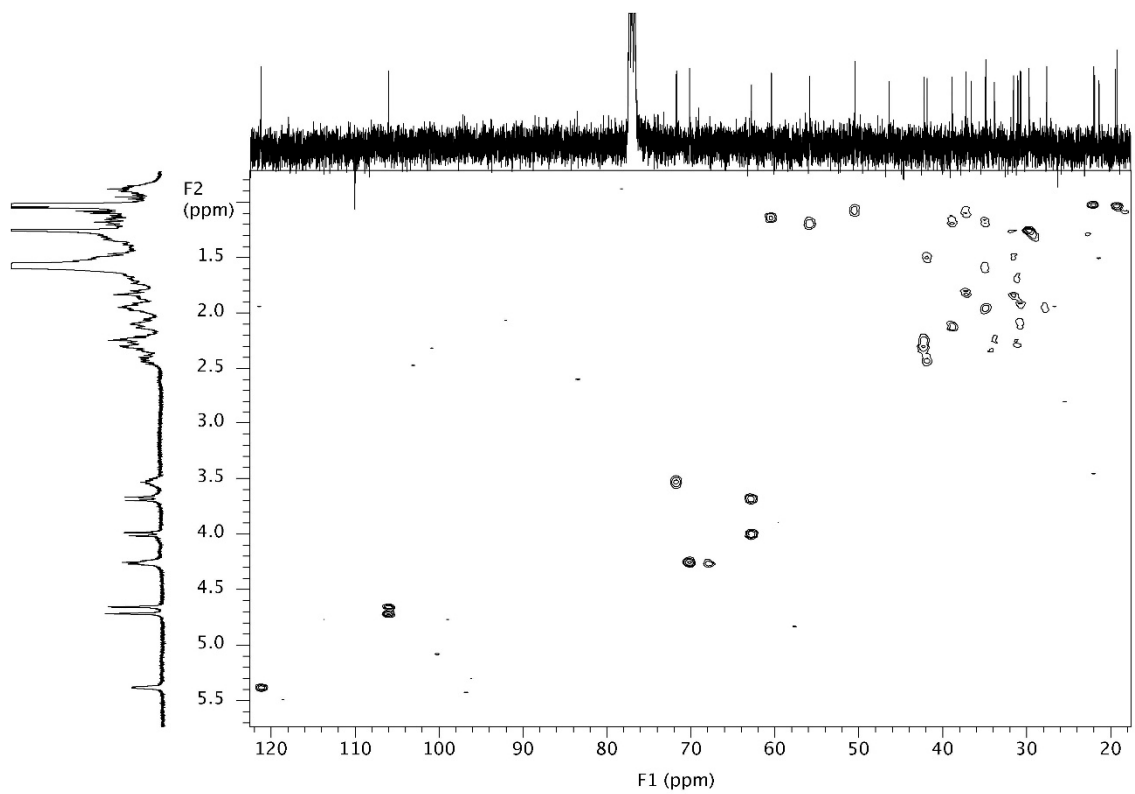
S22. DEPT (15–40 ppm) spectrum of compound **2** in CDCl_3 .



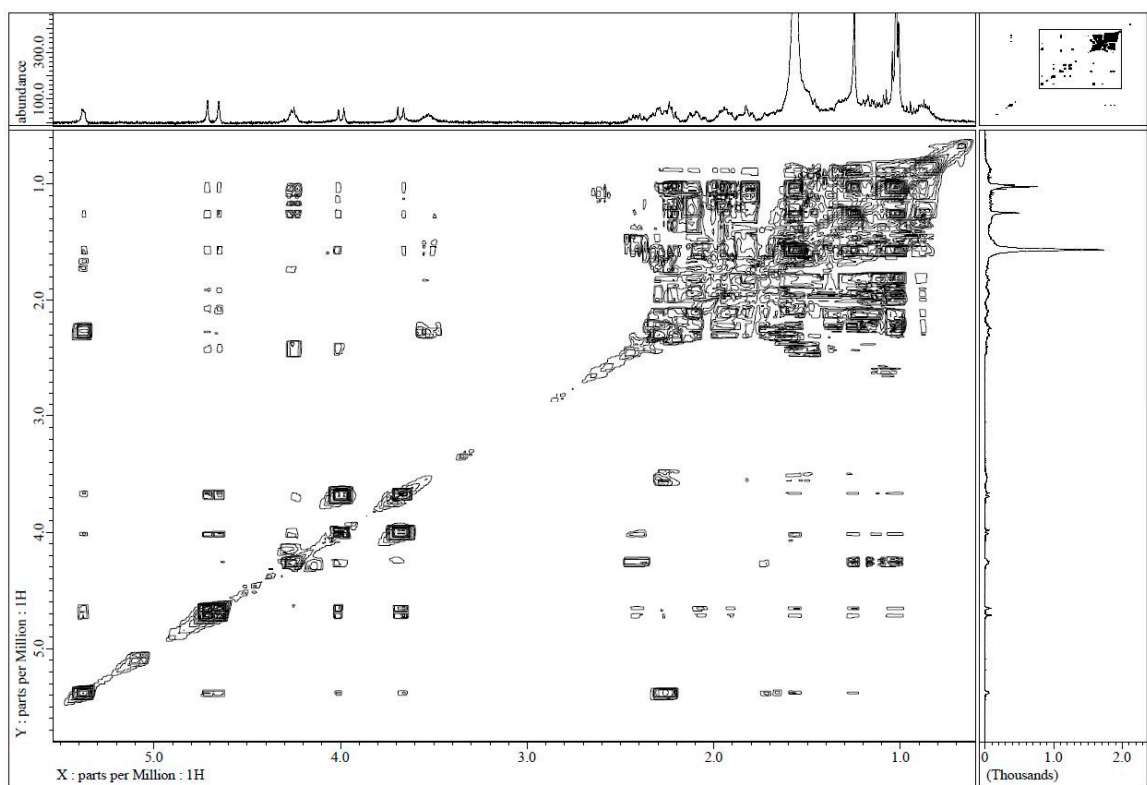
S23. DEPT (40–80 ppm) spectrum of compound **2** in CDCl₃.



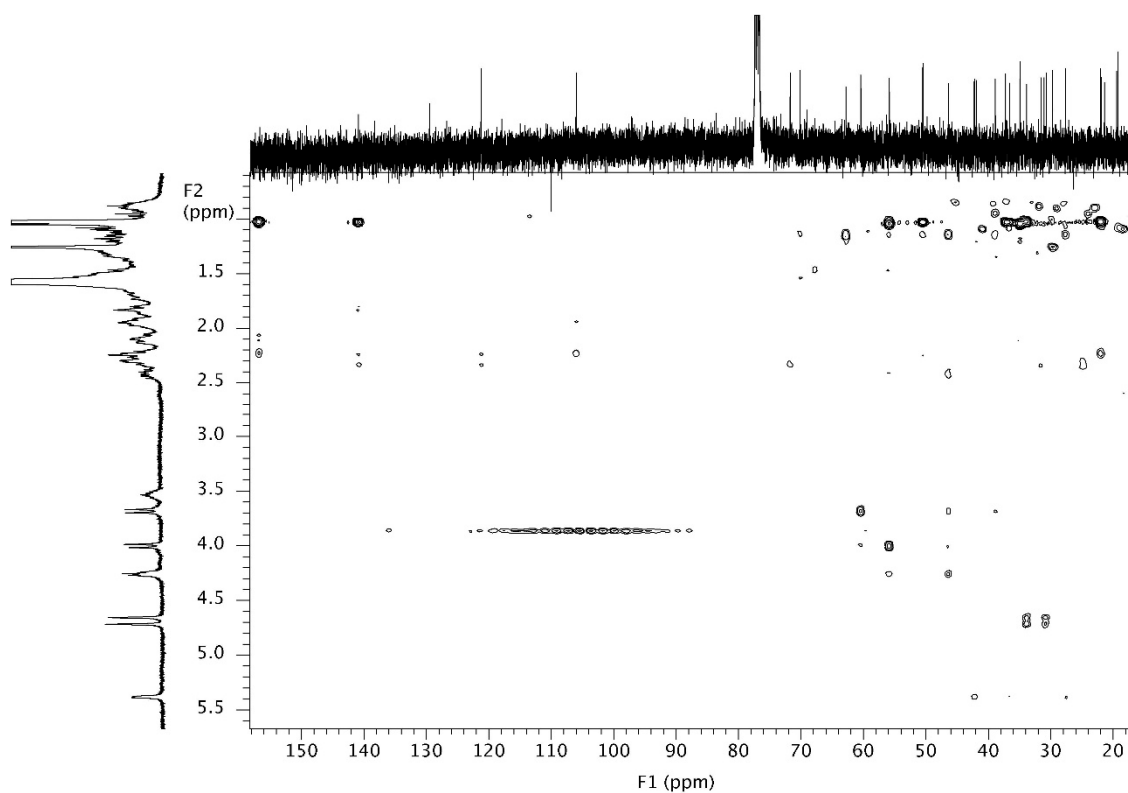
S24. DEPT (100–160 ppm) spectrum of compound **2** in CDCl₃.



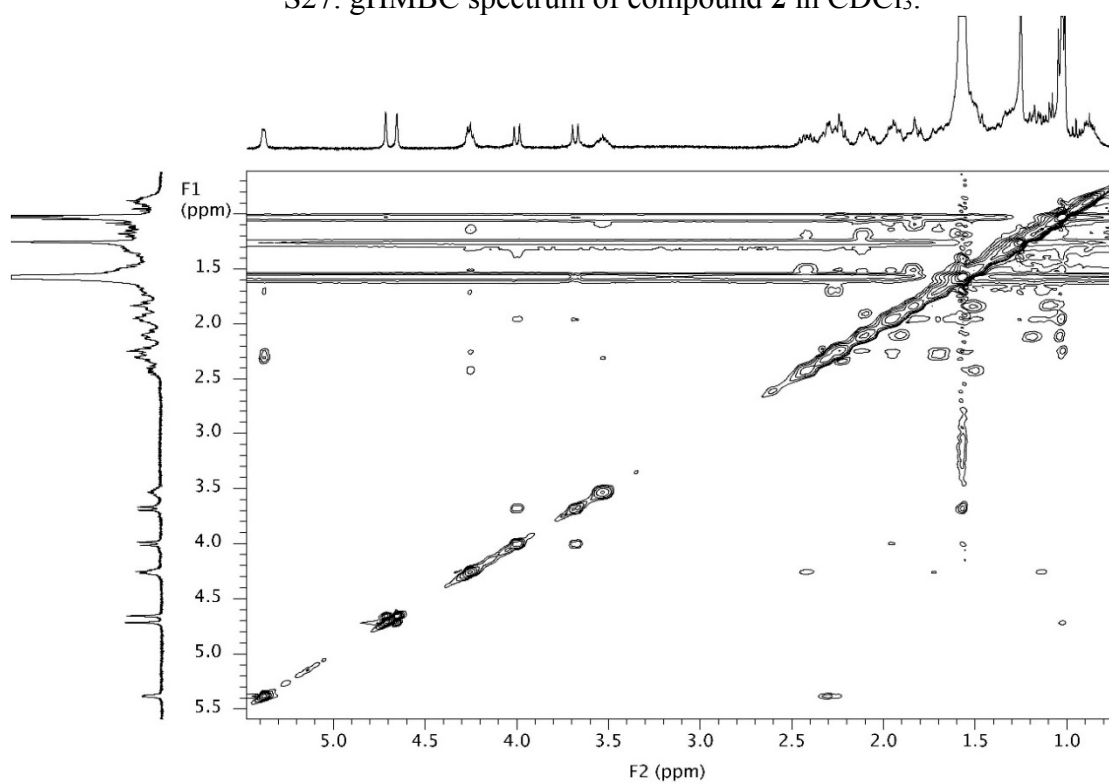
S25. gHSQC spectrum of compound **2** in CDCl₃.



S26. ¹H–¹H COSY spectrum of compound **2** in CDCl₃.



S27. gHMBC spectrum of compound **2** in CDCl_3 .



S28. NOESY spectrum of compound **2** in CDCl_3 .