Supporting Information

Faulknerynes A -C from a Bahamian Sponge *Diplastrella* sp. Stereo-Assignment and Critical Evaluation of two Exciton Coupled CD Methods

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Experimental Section

General Experimental Procedures.

Optical rotations were measured using a digital polarimeter using quartz cells of 1 cm or 5 cm pathlength. UV spectra were measured on a double-beam UV-vis spectrometer in 1 cm matched quartz cells. CD spectra were measured with a spectropolarimeter using spectroscopic grade solvents and a 2 mm quartz cell with 50 nm/min scan rate and 1 nm slit. IR spectra were measured using an FTIR spectrometer equipped with a ZnSe ATR plate. LR ESI mass spectra were obtained on a single quad mass spectrometer coupled to an UHPLC. ^{1}H, ^{13}C, and 2D NMR spectra were recorded at 600 MHz ($\{^{13}C/^{15}N\}^{1}H$, 1.7 mm microcryoprobe, or at 500 MHz ($\{^{13}C\}^{1}H$ 5 mm cryoprobe or $\{^{13}C\}^{1}H$ 5 mm cryoprobe), or a 400 MHz spectrometer ($\{^{13}C\}^{1}H$ 5 mm room temperature probe) in CD_3OD or $CDCl_3$ using solvent signals as internal standards [δ_H CHD_2OH 3.31 ppm; δ_C 49.00 ppm; $CHCl_3$, δ_C 7.24 ppm; δ_C 77.0 ppm). HPLC was carried out using a dual-pump preparative HPLC with a high-dynamic range UV detector operating at 220 nm or a refractive index detector using HPLC grade solvents. TLC was performed on silica gel coated 0.25 mm aluminum backed plates and visualization by vanillin-H_2SO_4-EtOH, phosphomolybdic acid or aqueous ceric ammonium nitrate. Anhydrous solvents were prepared by passage through a commercial alumina cartridges under Ar.

Table S1. NMR data ($CDCl_3$) for faulknerynes B (**4b**) and C (**4c**)

	4b			**4c**		
no.	δ_C, mult.[a]	δ_H, mult. (*J* in Hz)[b]	COSY[b]	δ_C, mult.[a]	δ_H, mult. (*J* in Hz)[b]	COSY[b]
1	66.1, CH	3.72, dd (11.3, 6.7)	H2	66.3, CH	3.69, dd (11.4, 6.3)	H2
	66.1, CH	3.78, br	H2	66.3, CH	3.74, dd (11.4, 3.8)	H2
2	[d]	4.58, m	H1	63.6, CH	4.50, dd (6.2, 3.7)	H1, H7
3	[d]			[d]		
4	[d]			[d]		
5	[d]			[d]		
6	[d]			[d]		
7	[d]	5.50, d (11.0)	H8, H9	18.9, CH_2	2.30, m	H2
8	[d]	6.11, dt (10.9, 7.4)	H7, H9	27.5[c], CH_2	1.57[c], m	
9	30.2, CH_2	2.33, m (7.1)	H7, H8, H10	27.4[c], CH_2	1.55[c], m	
10	27.7, CH_2[c]	1.53, m	H9	29.8, CH_2	2.29, m	H10, H11
11	27.6, CH_2[c]	1.55, m	H12	[d]	5.93, dt (10.8, 7.5)	H10, H12
12	18.9, CH_2	2.28, td (6.8, 1.9)	H11, H15	109.2, CH	5.55, d (10.9)	H10, H11, H15
13	[d]			[d]		
14	[d]			[d]		
15	[d]	6.19, dt (14.0)	H12, H16	117.4, CH	6.34, dd (14.0, 2.2)	H12, H16
16	[d]	6.59, d (14.0)	H15	117.6, CH	6.66, d (14.0)	H15

[a] δ_C are measured by gHSQC exp. in 600 Hz. [b] 600 MHz [c] Peaks may be interchanged within a column. [d] Not detected

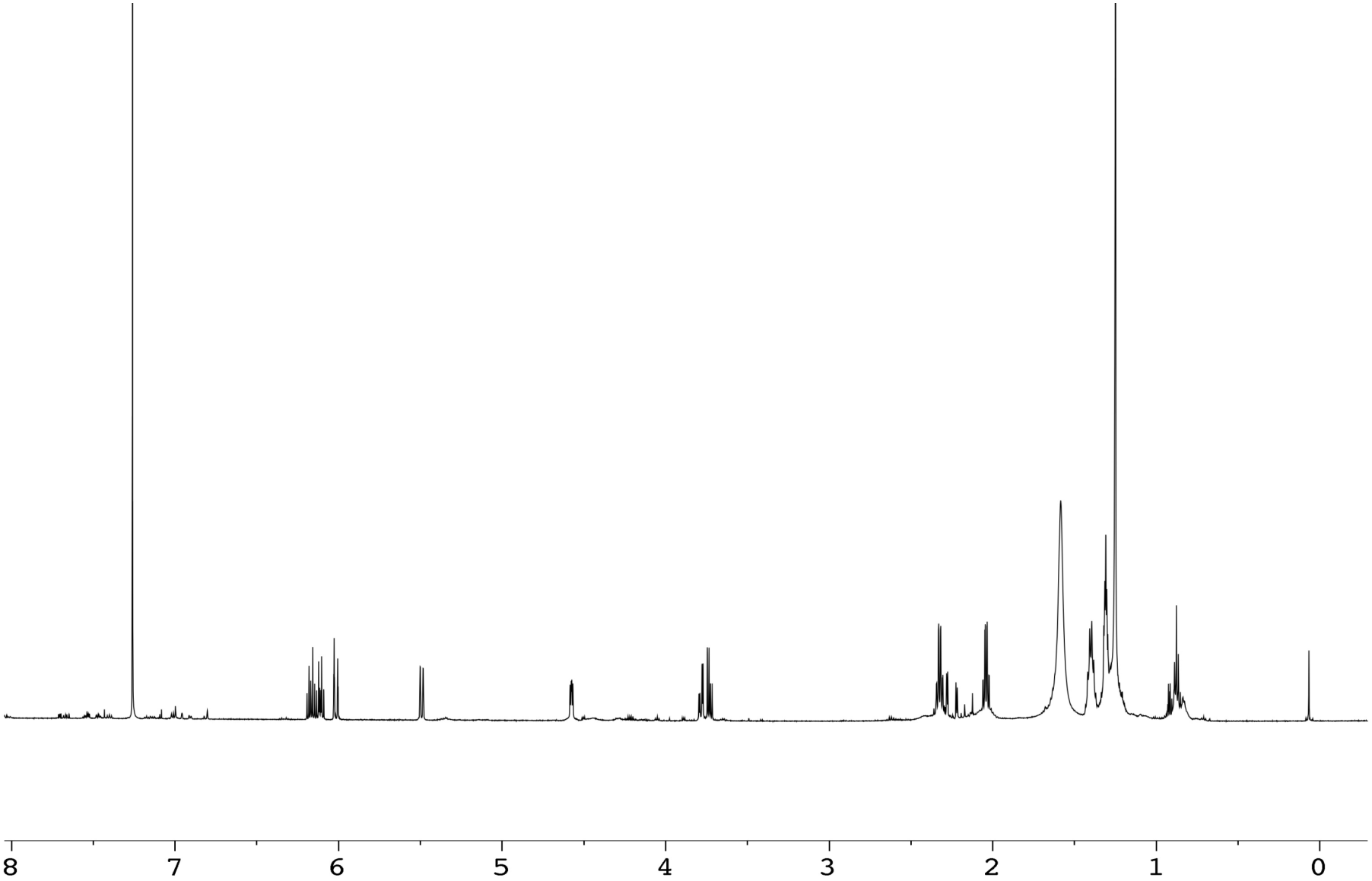

Figure S1. ^{1}H NMR spectrum of **4a** (600 MHz, $CDCl_3$).

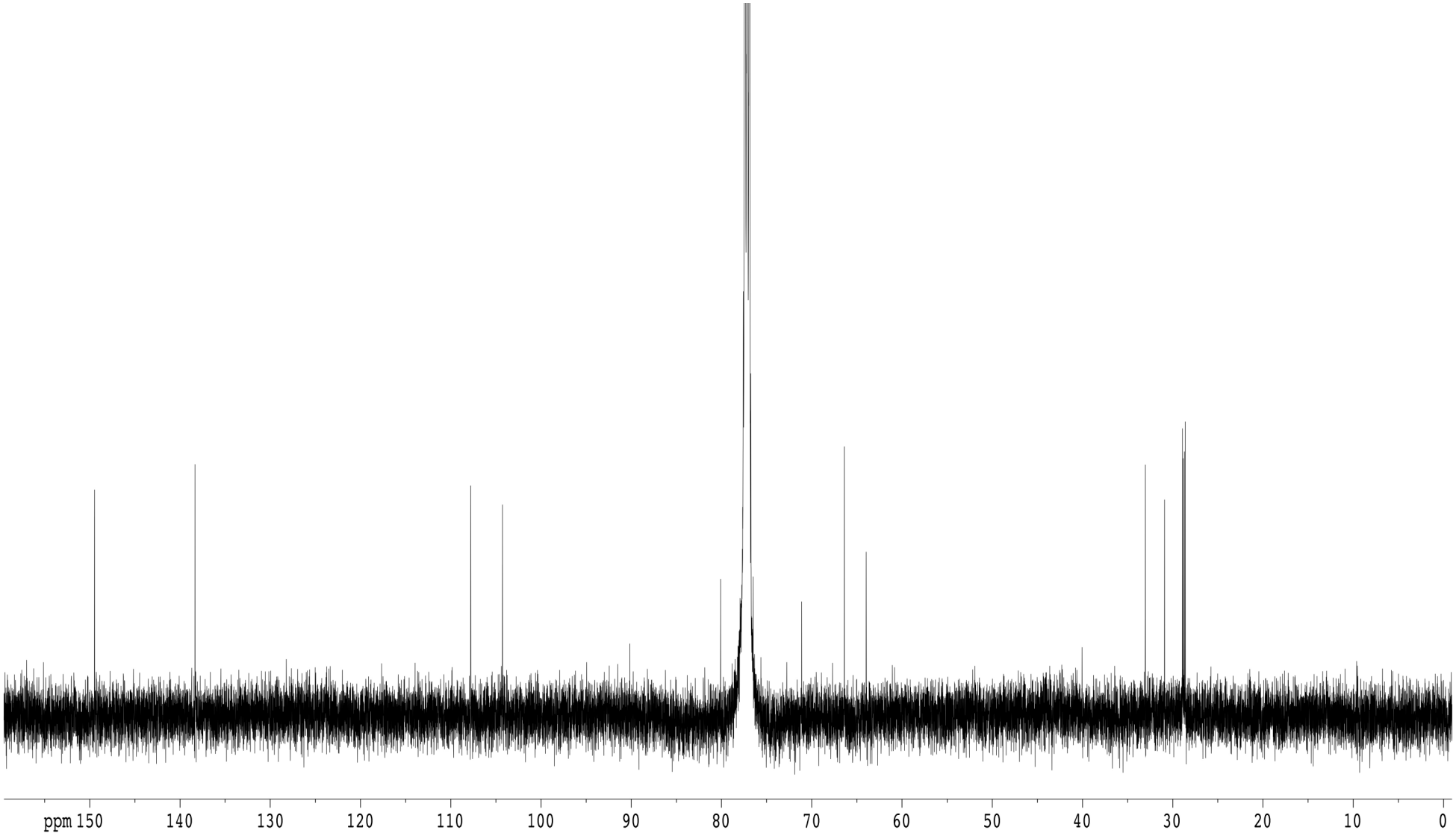

Figure S2. ^{13}C NMR spectrum of **4a** (125 MHz, $CDCl_3$).

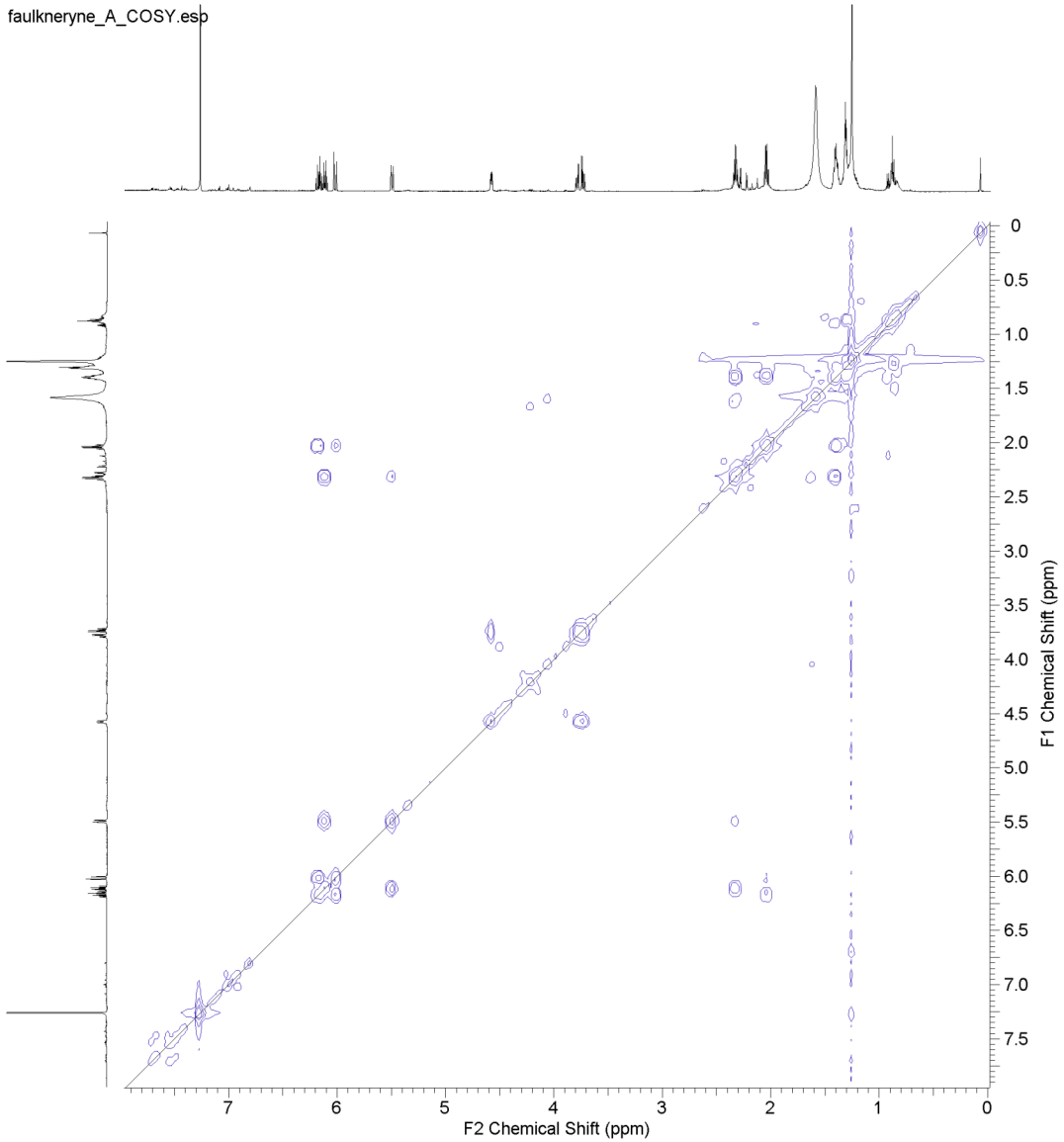

Figure S3. COSY spectrum of **4a** (600 MHz, $CDCl_3$).

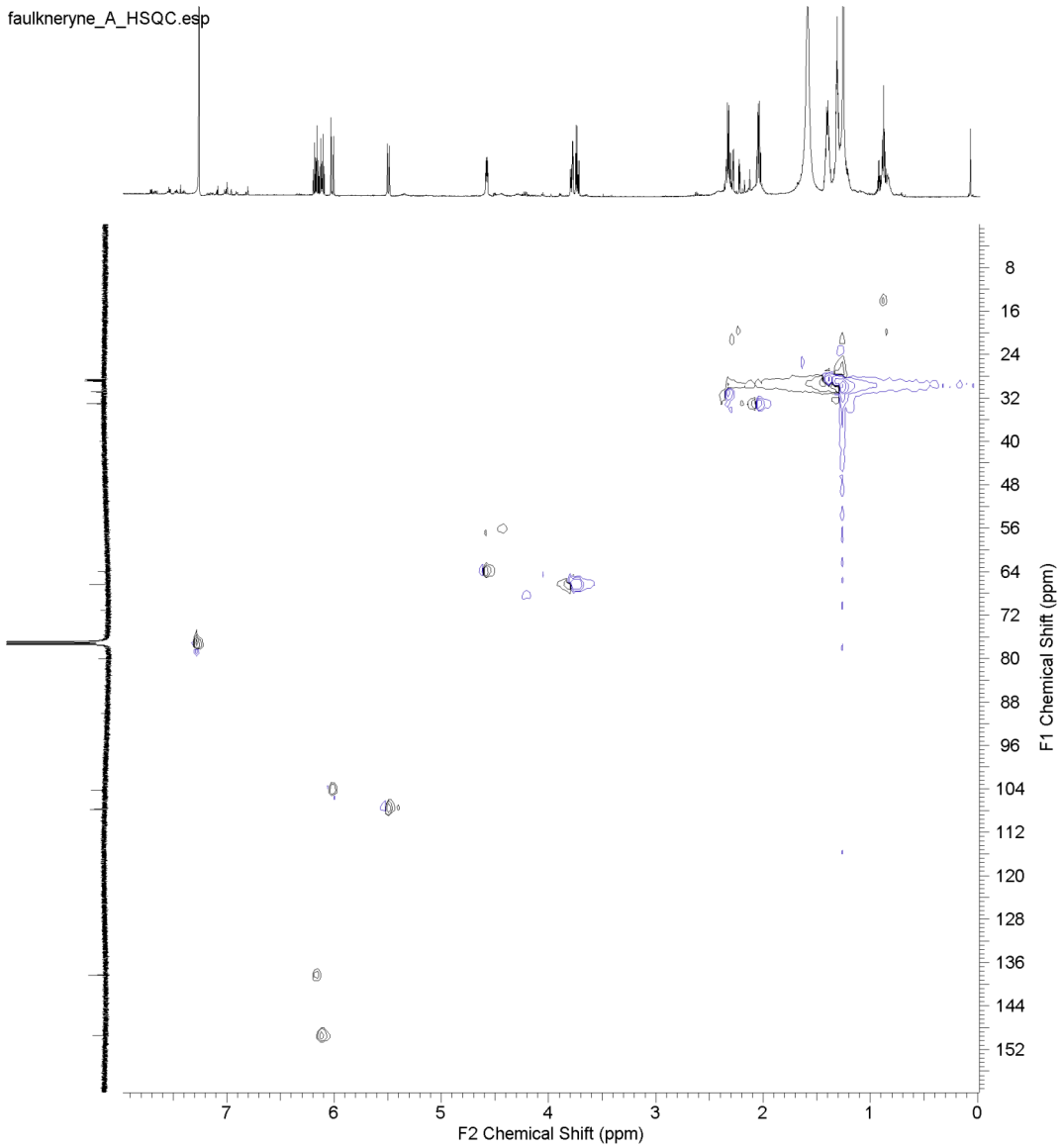

Figure S4. gHSQC spectrum of **4a** (600 MHz, $CDCl_3$).

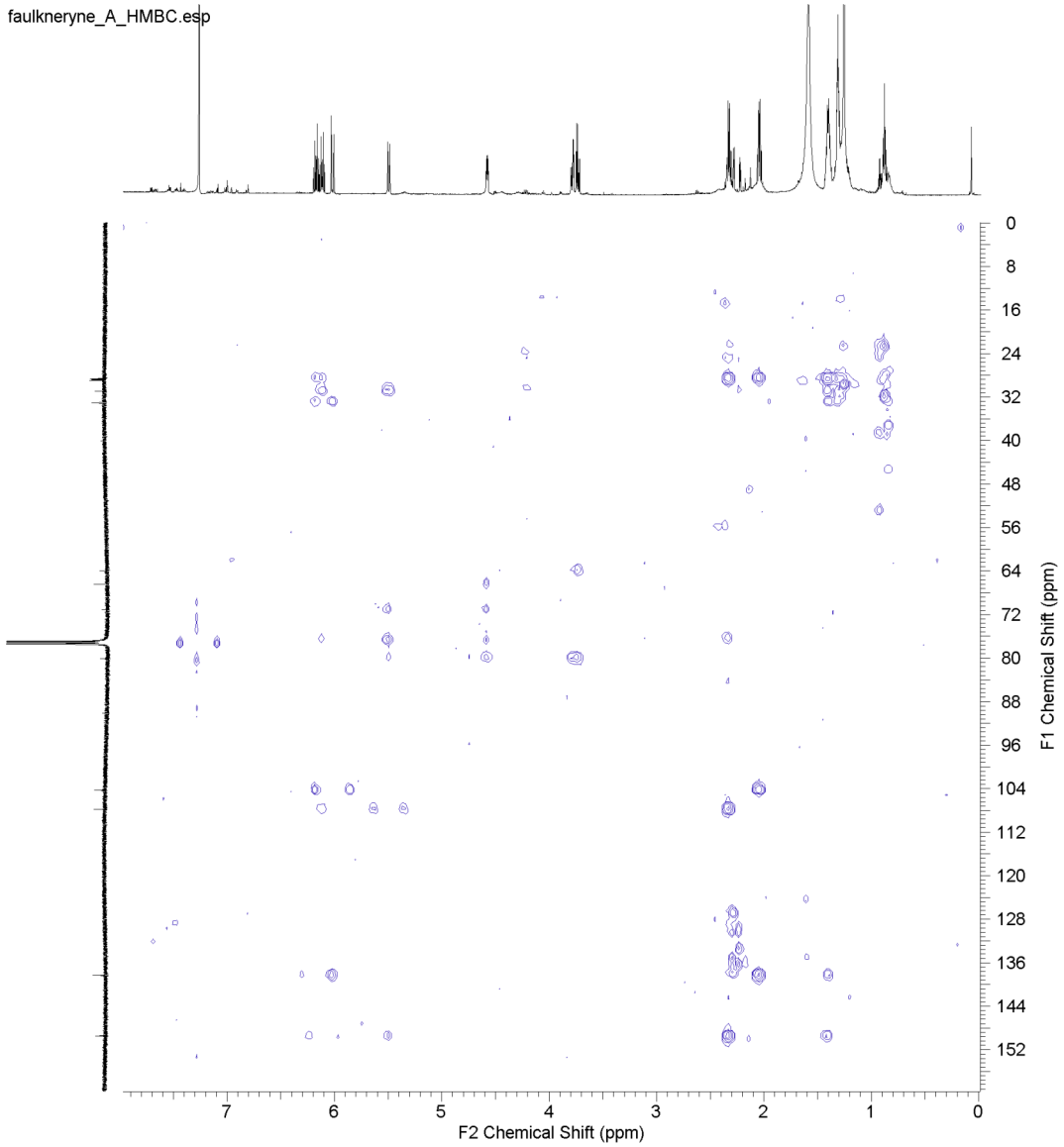

Figure S5. gHMBC spectrum of **4a** (600 MHz, $CDCl_3$, $^{n}J_{CH}$ = 8 Hz)

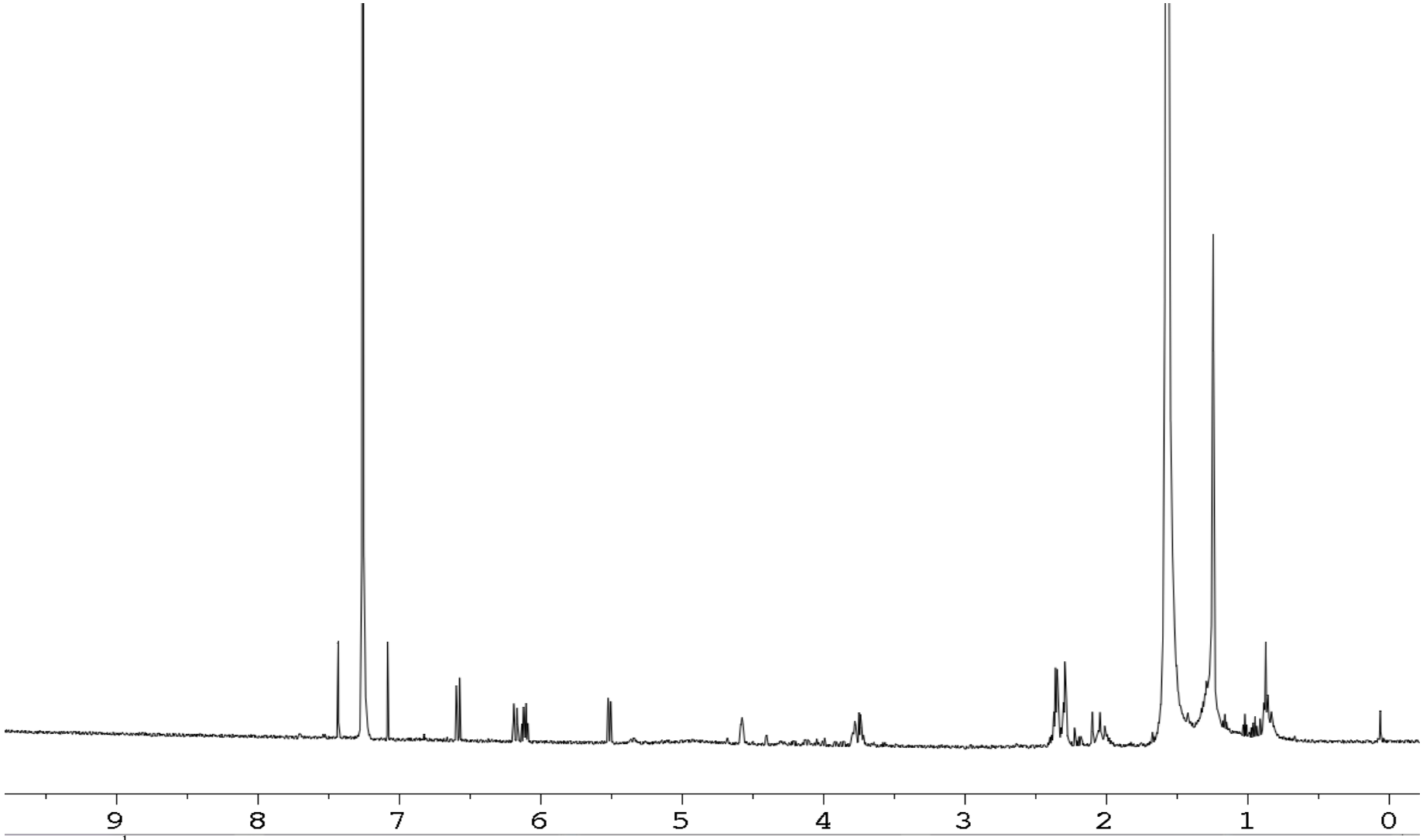

Figure S6. ^{1}H NMR spectrum of **4b** (600 MHz, $CDCl_3$)

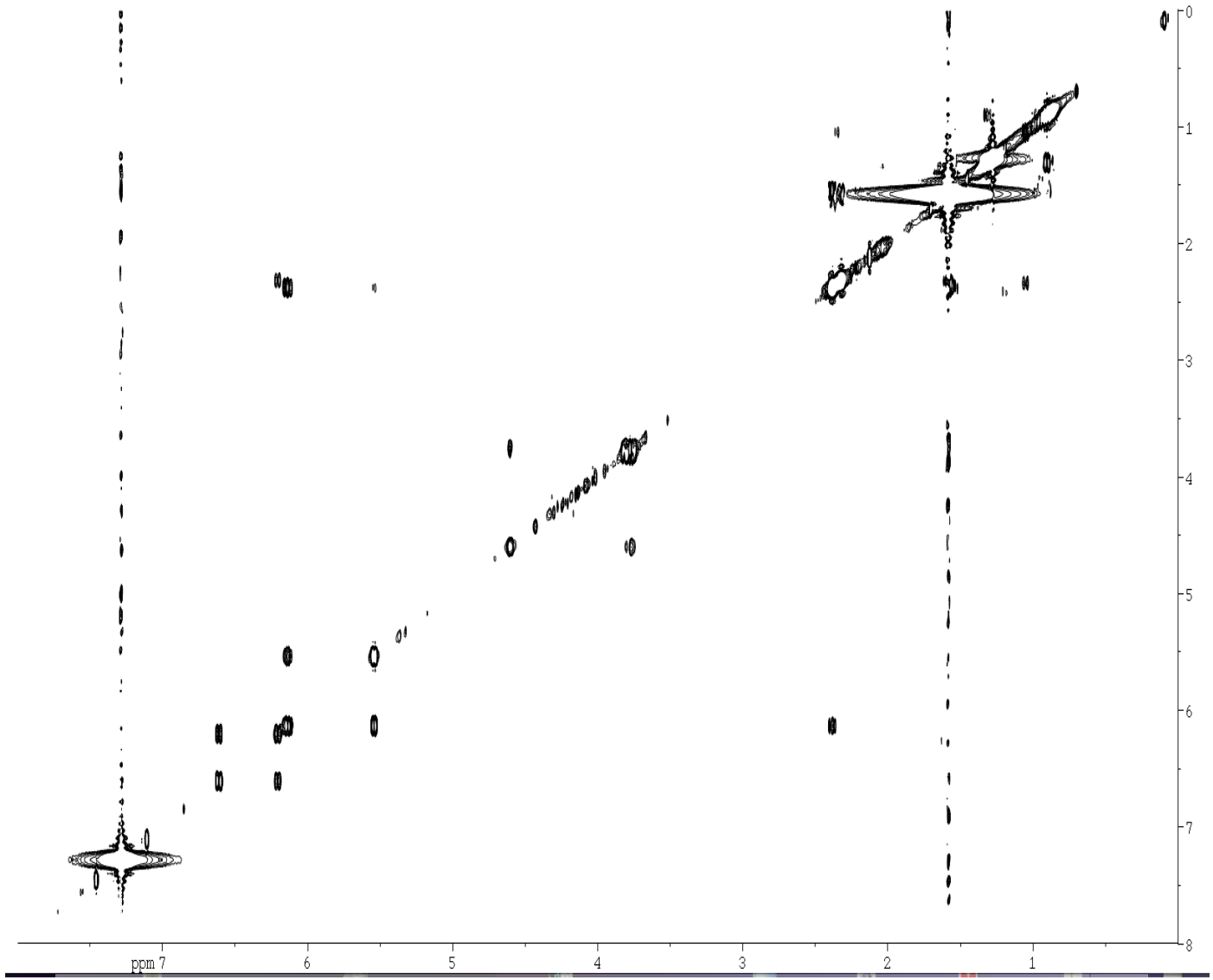

Figure S7. COSY NMR spectrum of **4b** (600 MHz, $CDCl_3$)

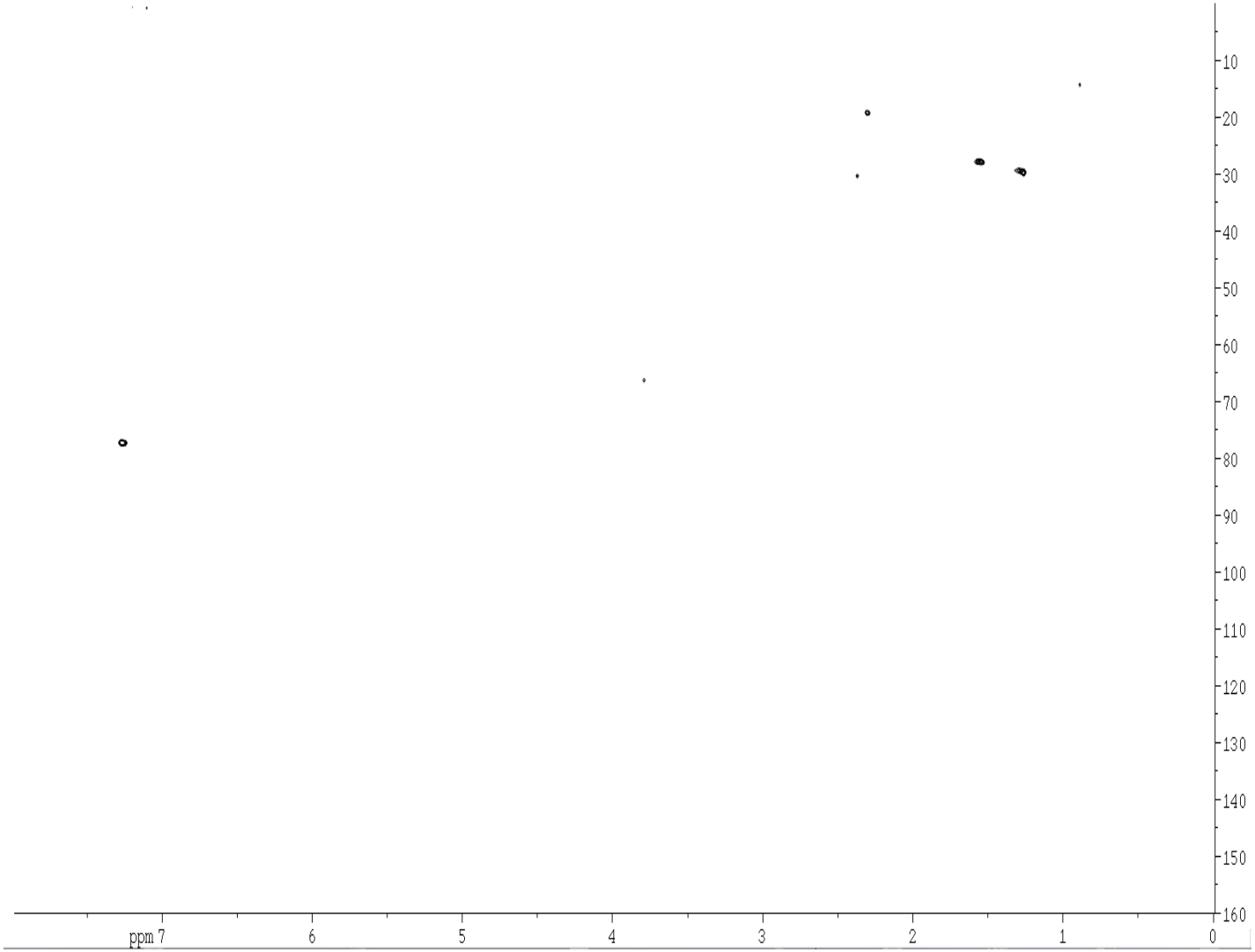

Figure S8. gHSQC spectrum of **4b** (600 MHz, $CDCl_3$)

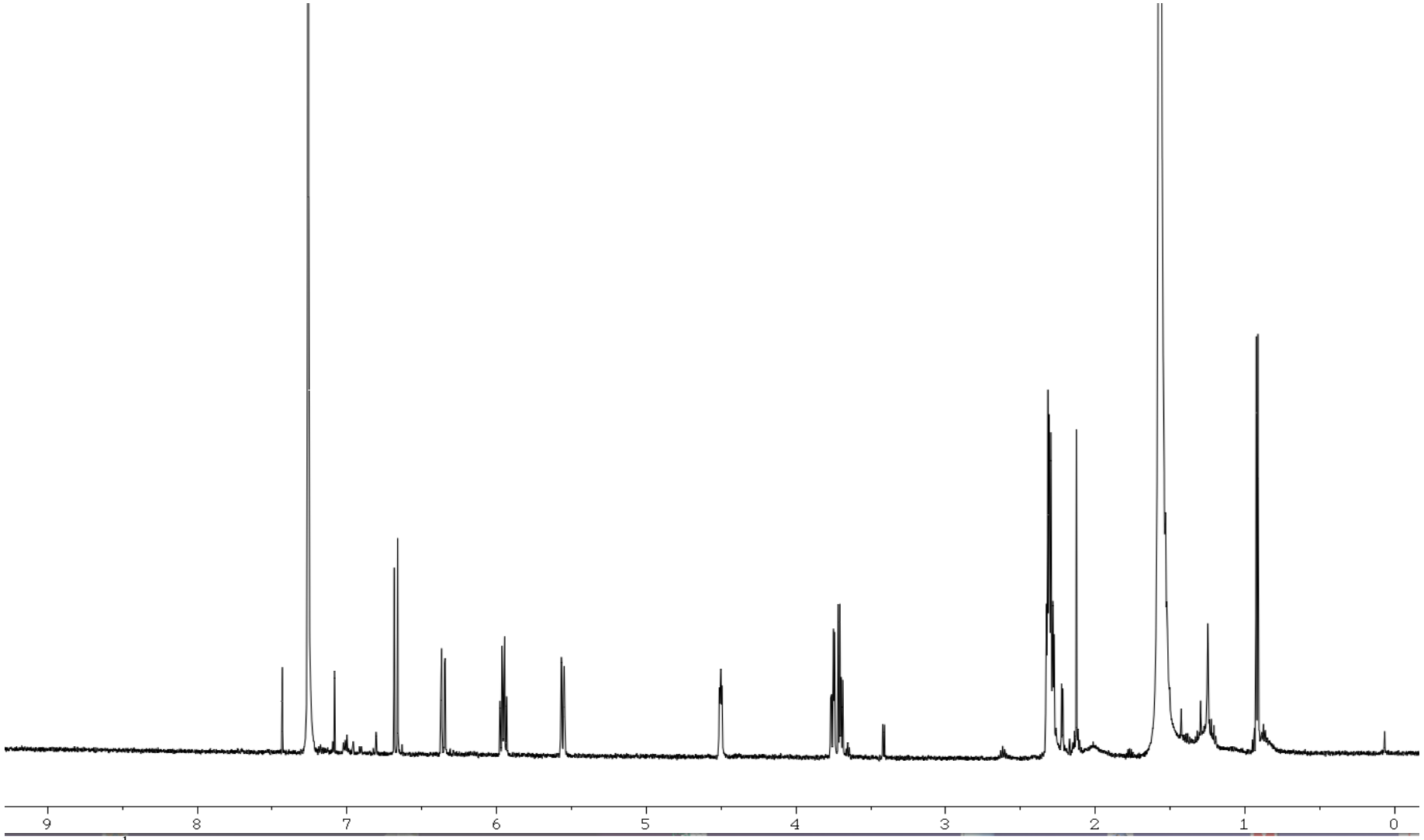

Figure S9. ^{1}H NMR spectrum of faulkneryne C (**4c**, 600 MHz, $CDCl_3$).

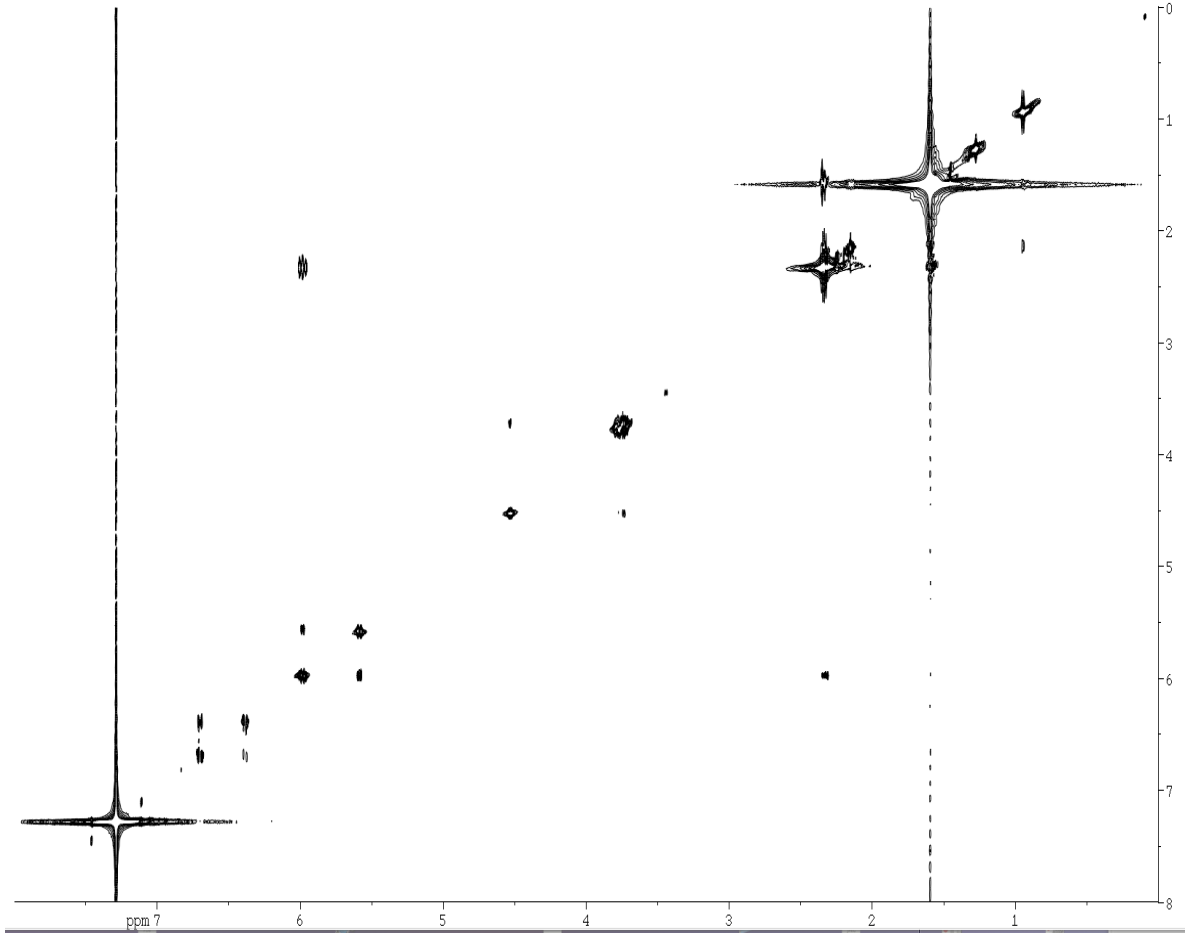

Figure S10. COSY spectrum of faulkneryne C (**4c**, 600 MHz, $CDCl_3$).

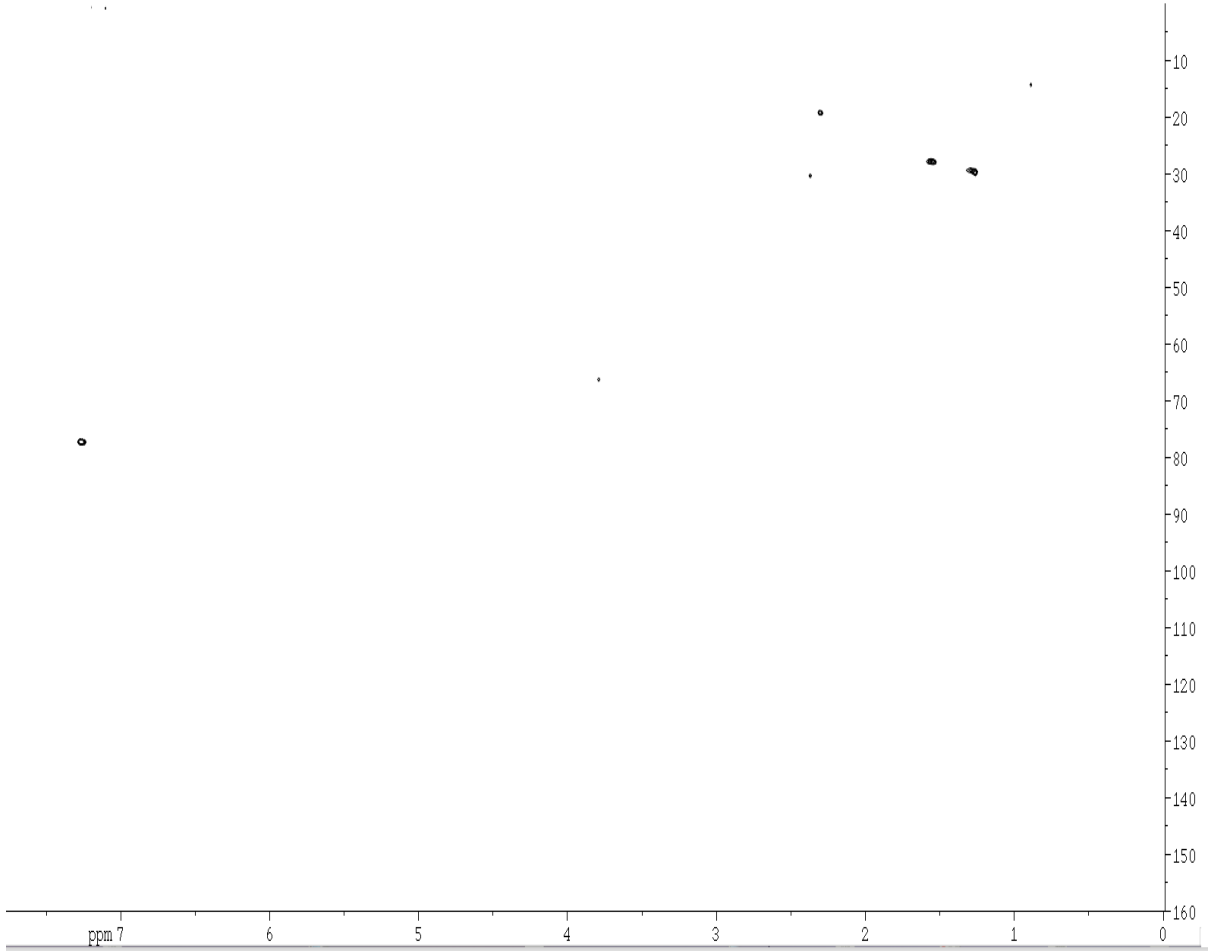

Figure S11. gHSQC spectrum of faulkneryne C (**4c**, 600 MHz, $CDCl_3$).

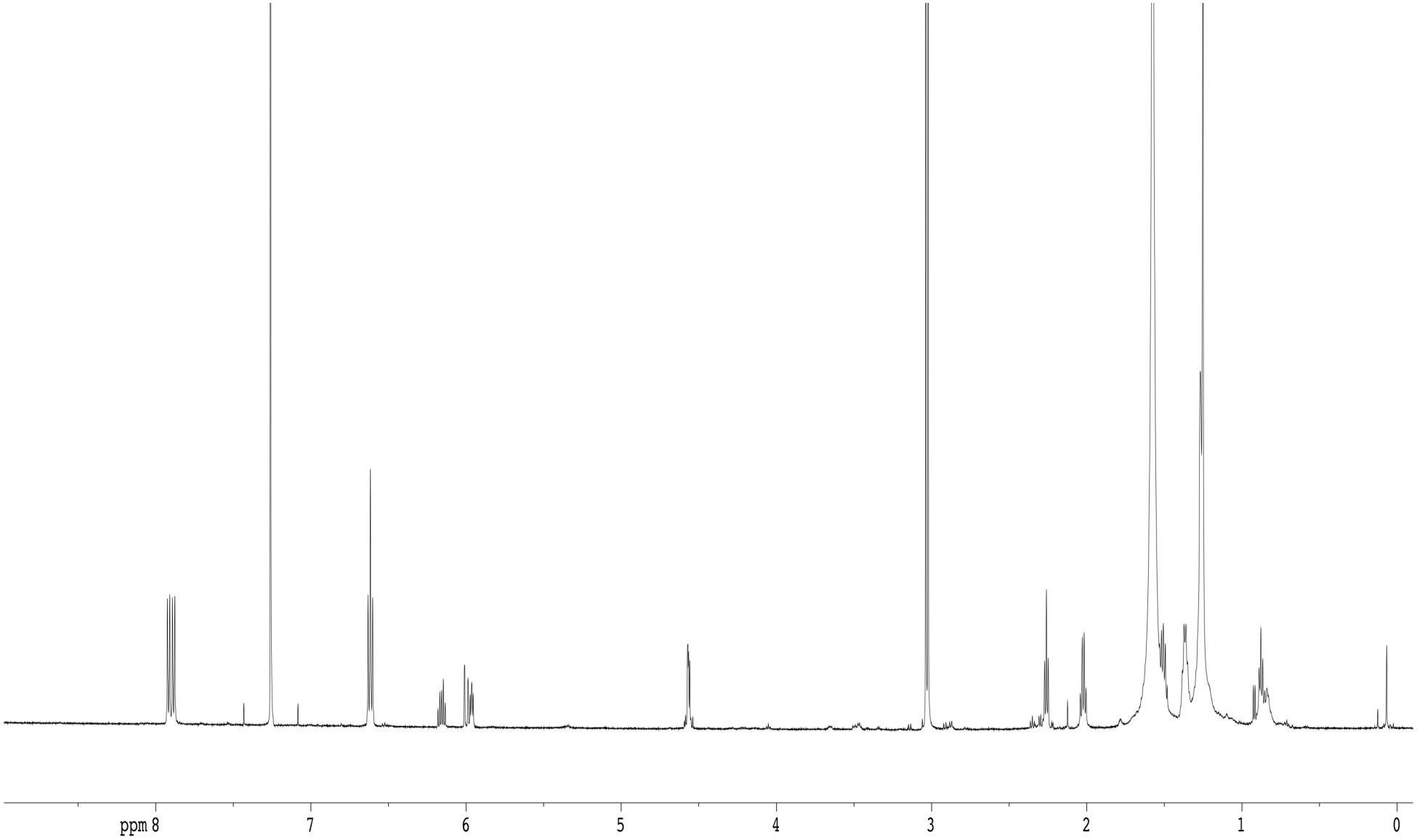

Figure S12. ^{1}H NMR spectrum of **5** (600 MHz, $CDCl_3$)

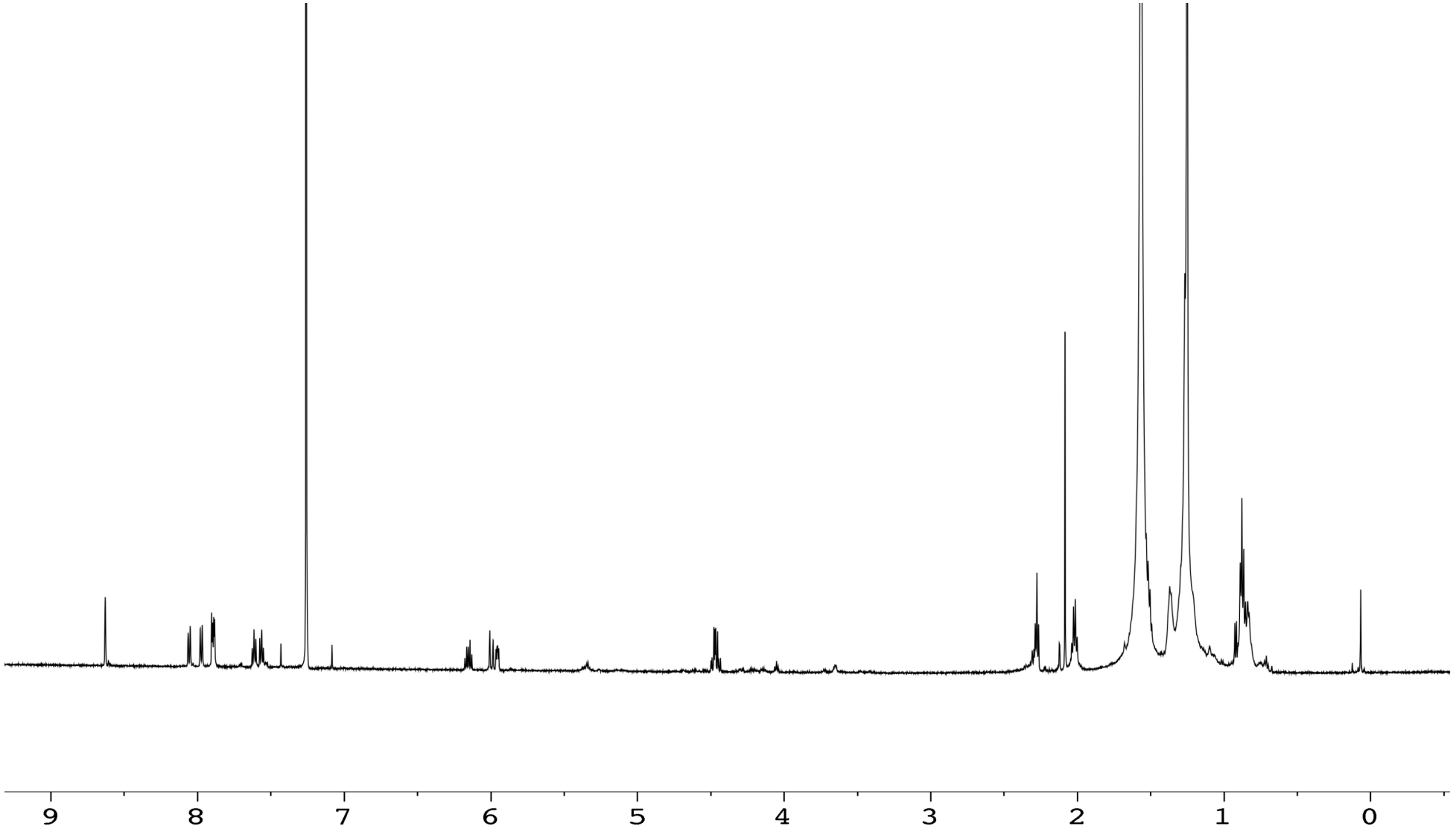

Figure S13. ^{1}H NMR spectrum of **6** (600 MHz, $CDCl_3$)

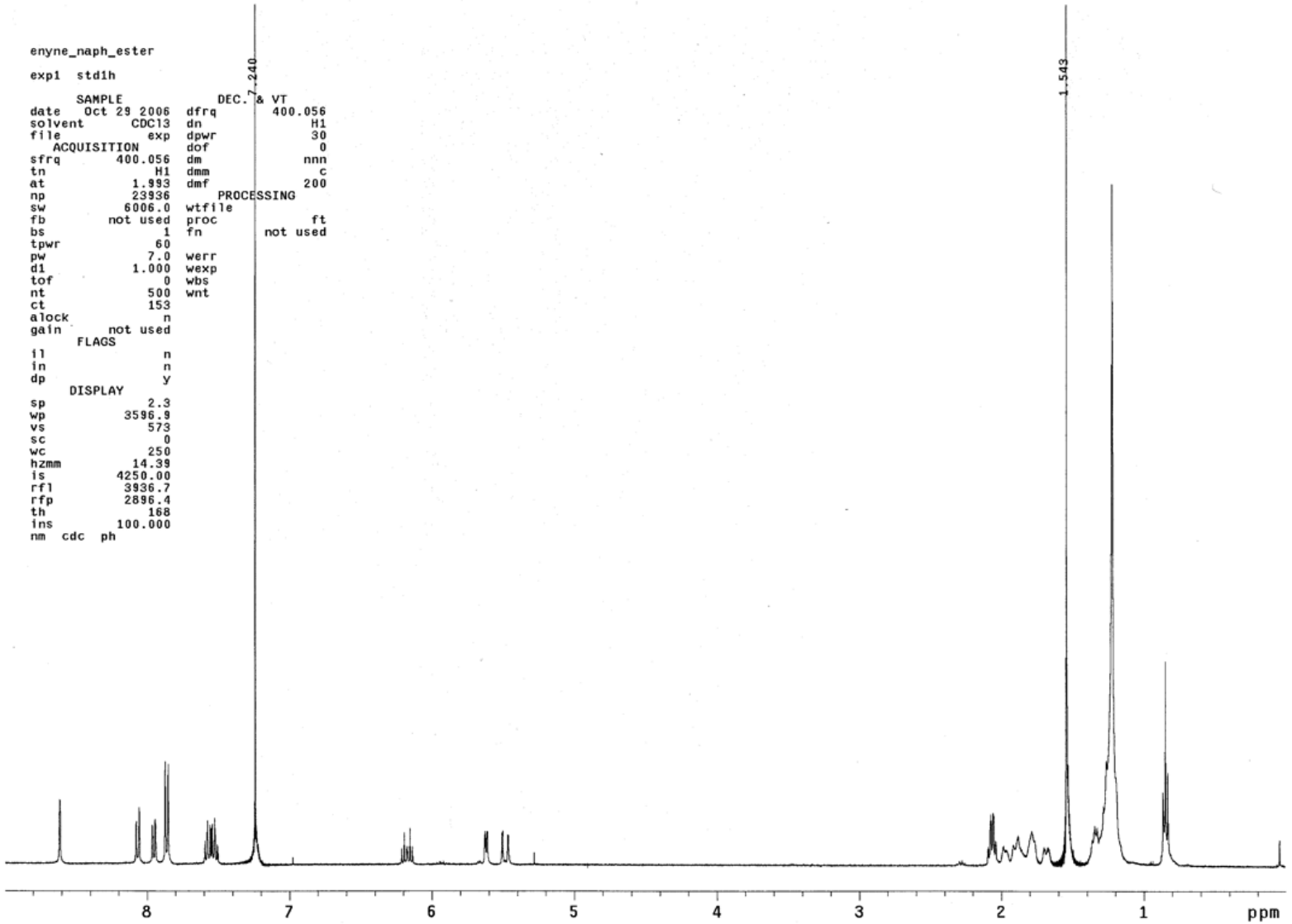

Figure S14. ^{1}H NMR spectrum of **7** (400 MHz, $CDCl_3$)

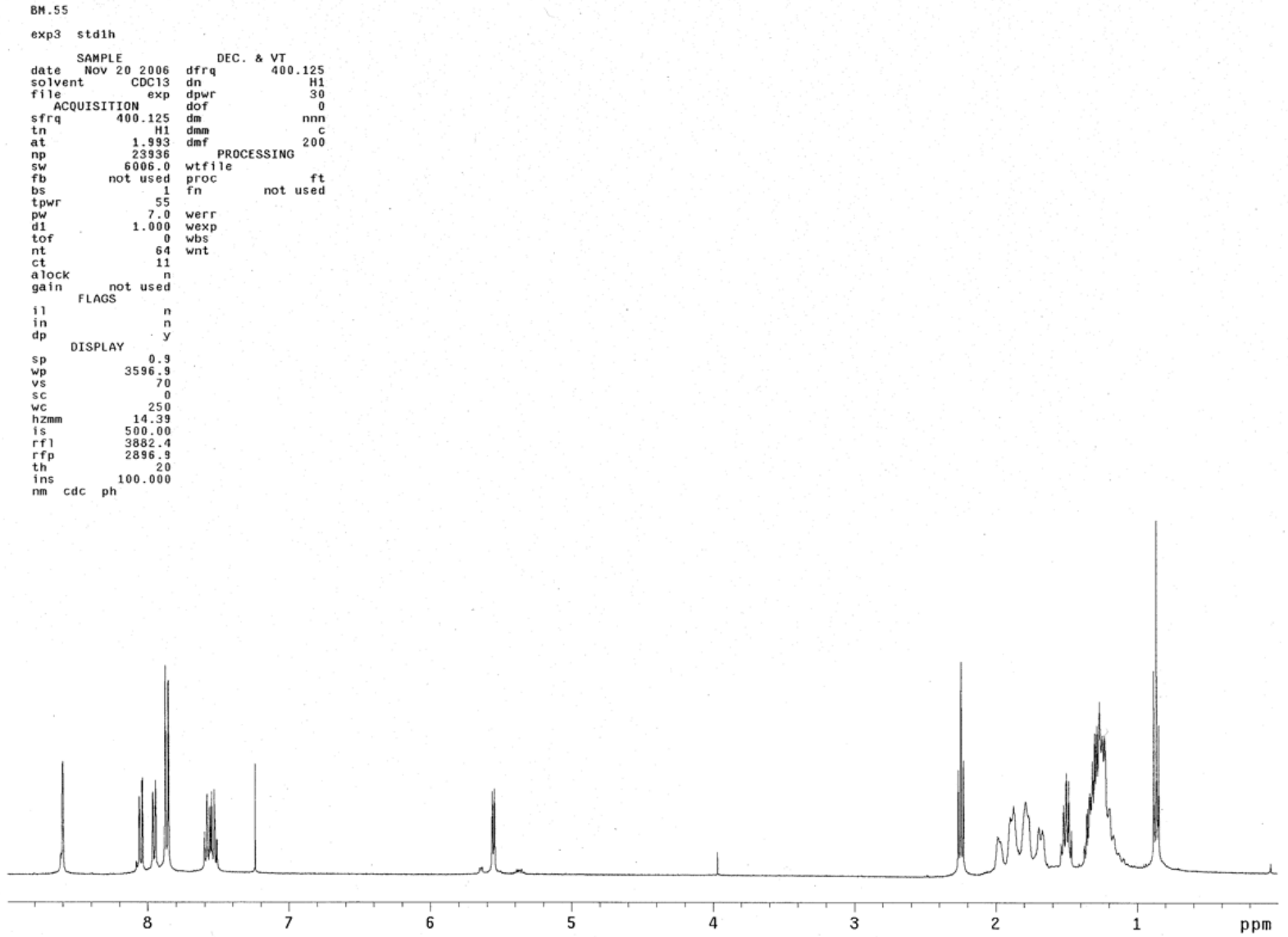

Figure S15. ^{1}H NMR spectrum of **8** (400 MHz, $CDCl_3$)

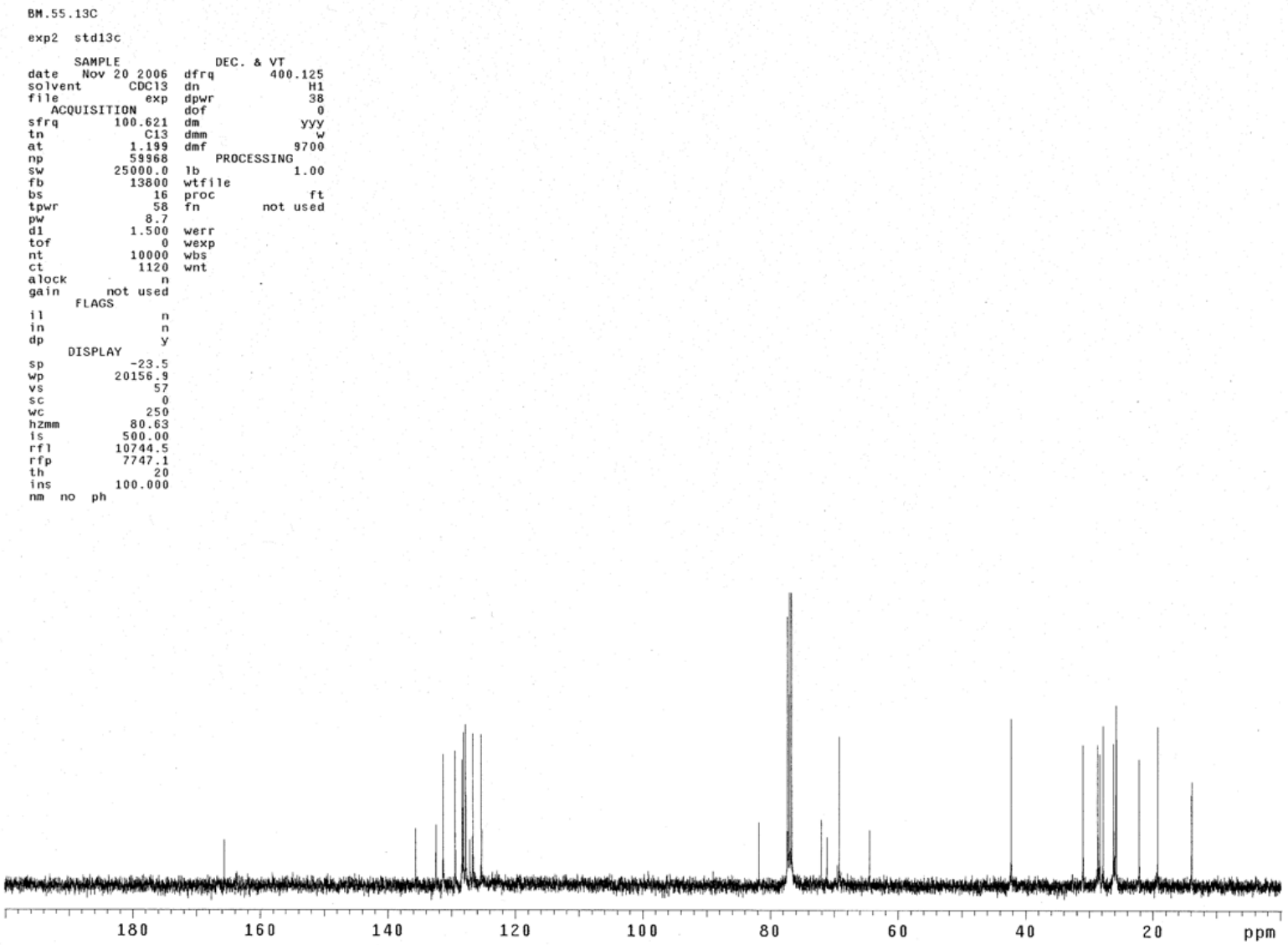

Figure S16. ^{13}C NMR spectrum of **8** (400 MHz, $CDCl_3$)

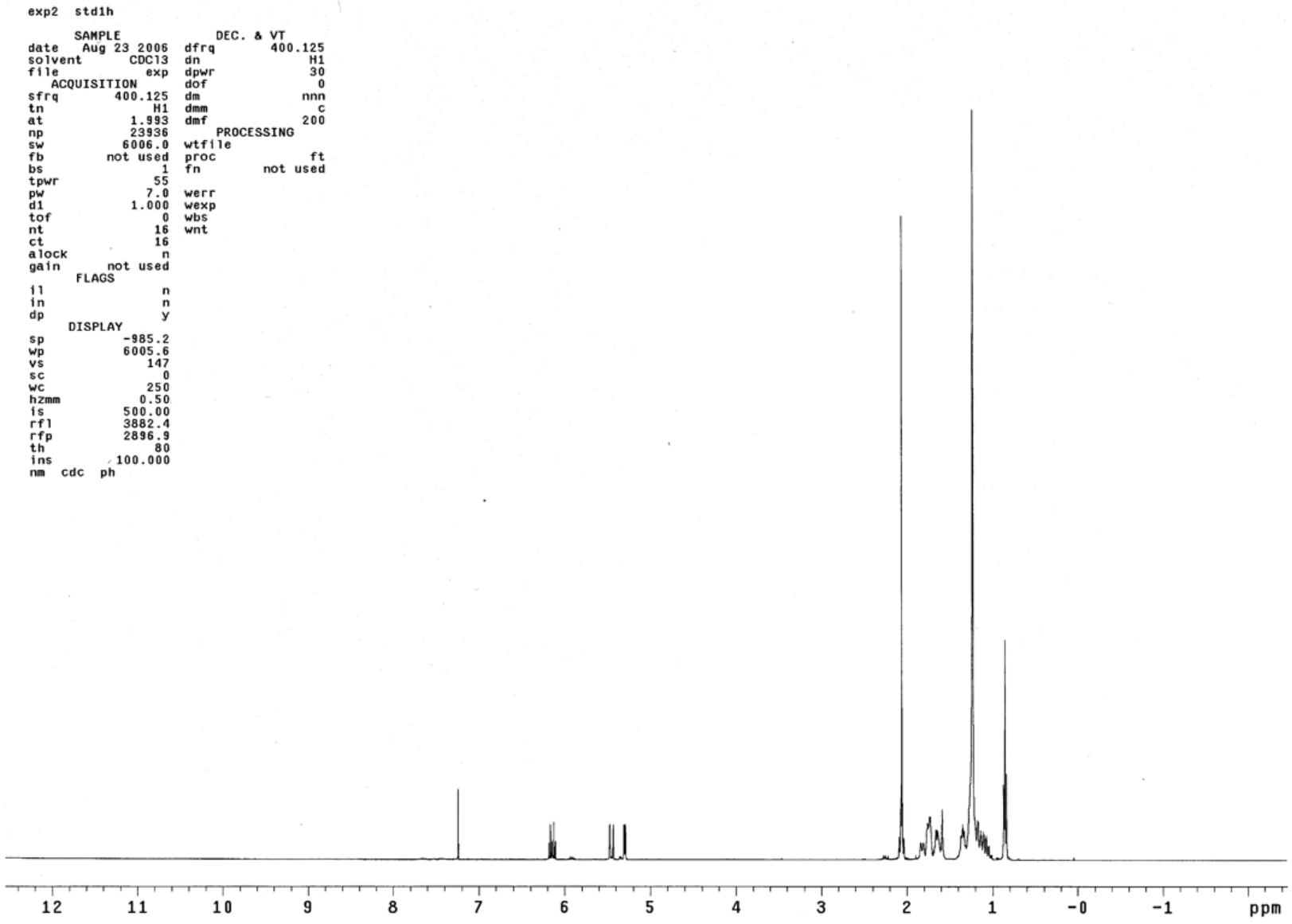

Figure S17. ^{1}H NMR spectrum of **13** (400 MHz, $CDCl_3$)

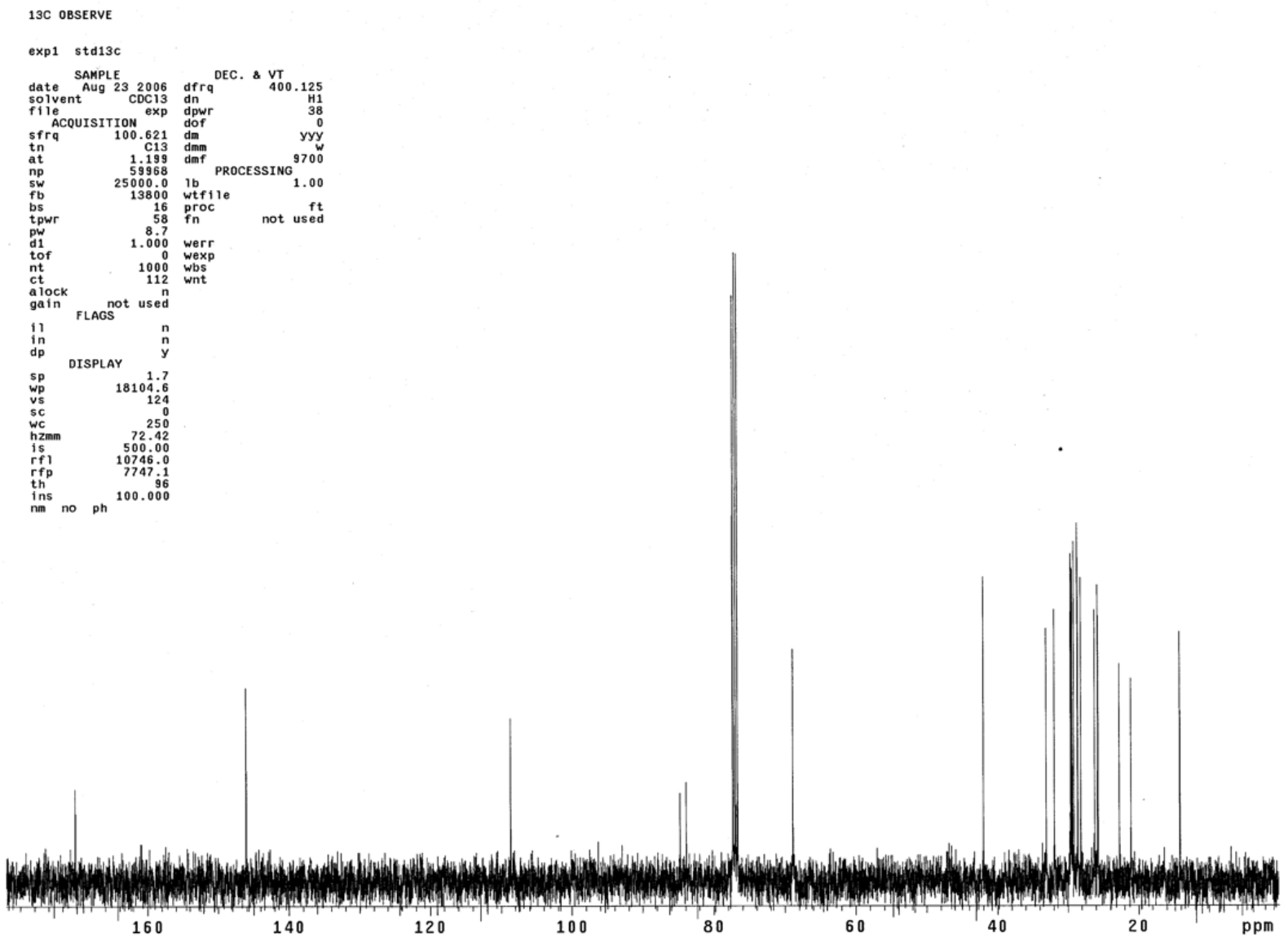

Figure S18. ^{13}C NMR spectrum of **13** (400 MHz, $CDCl_3$)

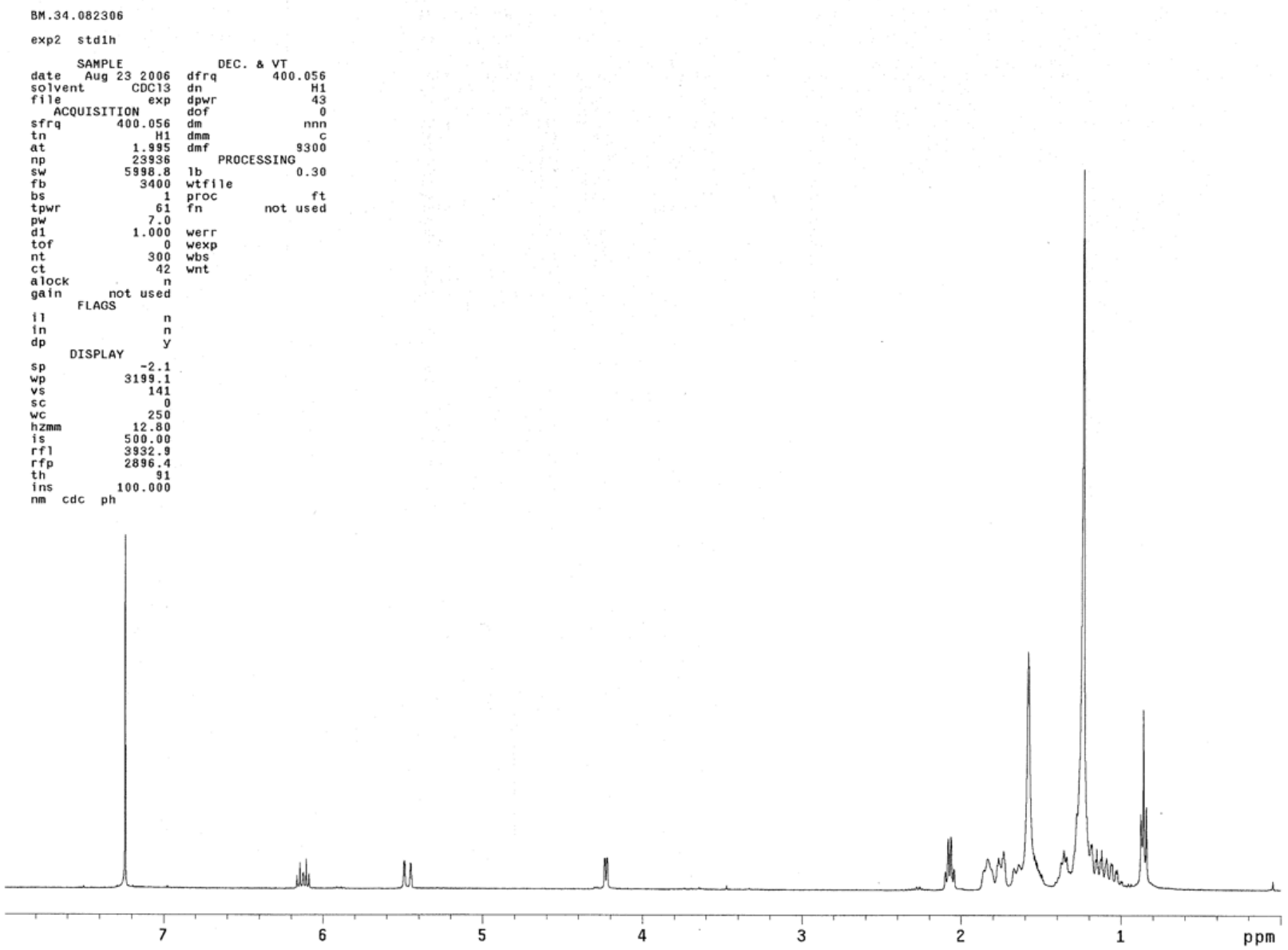

Figure S19. ^{1}H NMR spectrum of **14** (400 MHz, $CDCl_3$)

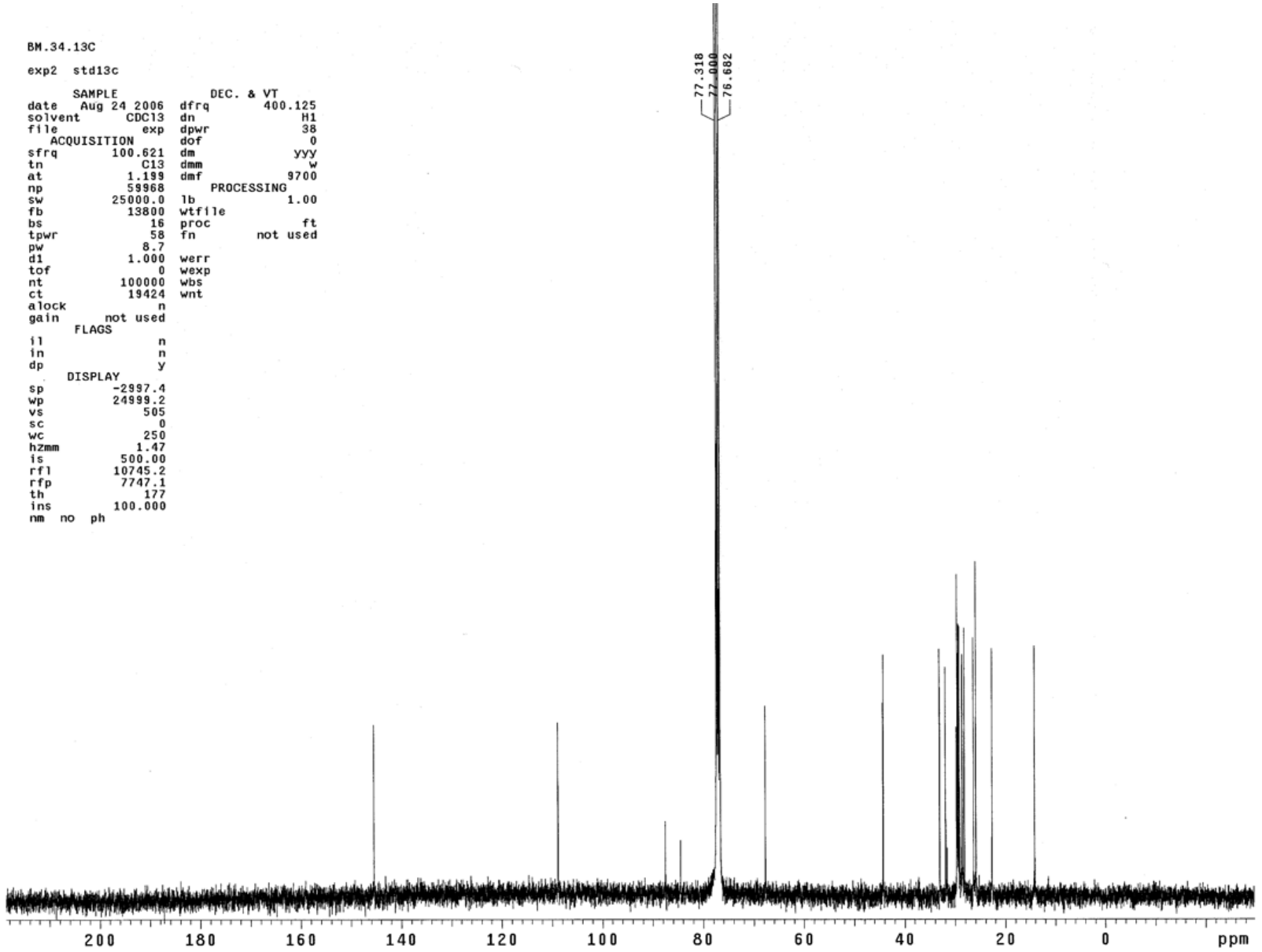

Figure S20. ^{13}C NMR spectrum of **14** (400 MHz, $CDCl_3$)

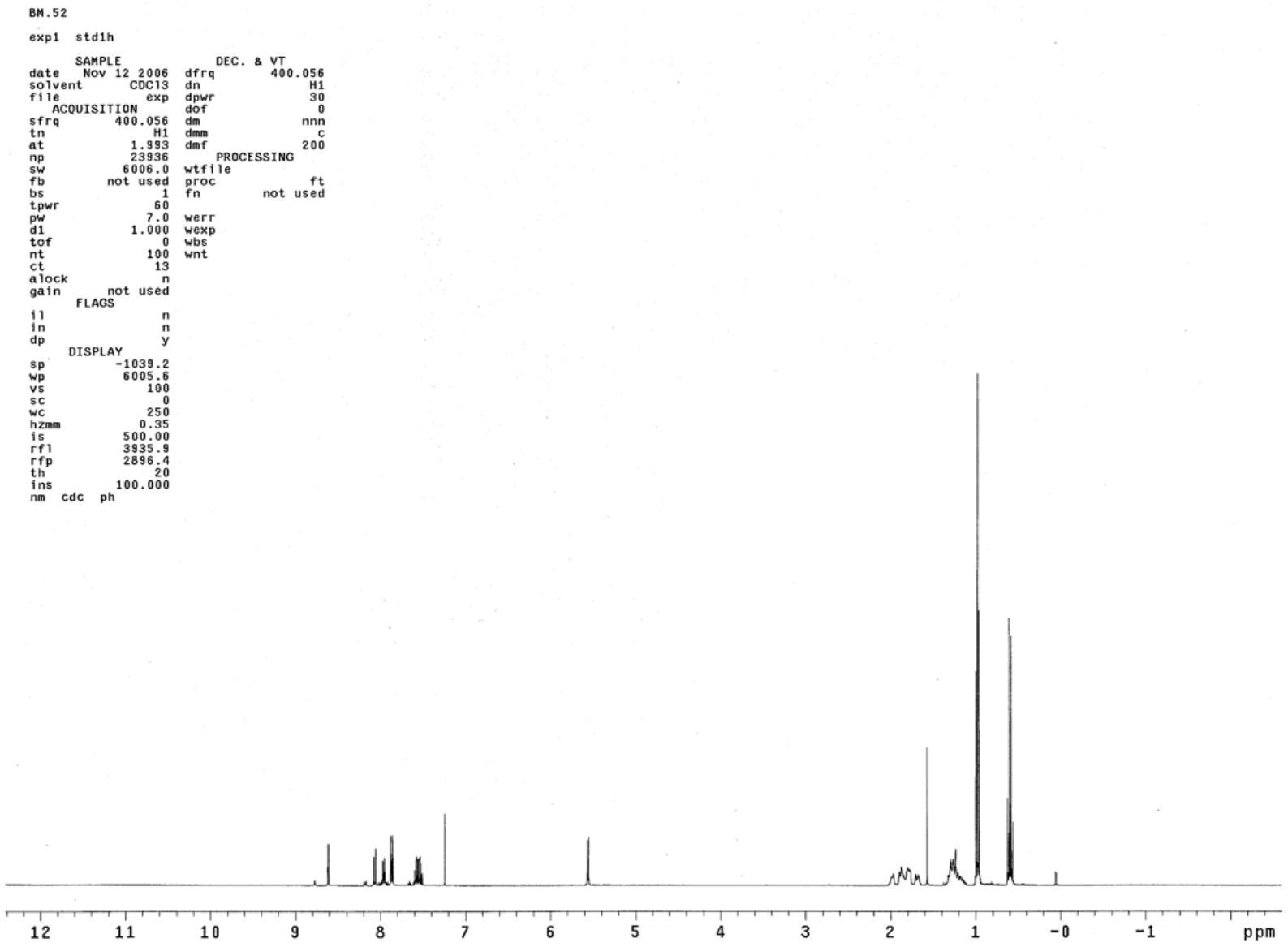

Figure S21. ^{1}H NMR spectrum of **15** (400 MHz, $CDCl_3$)

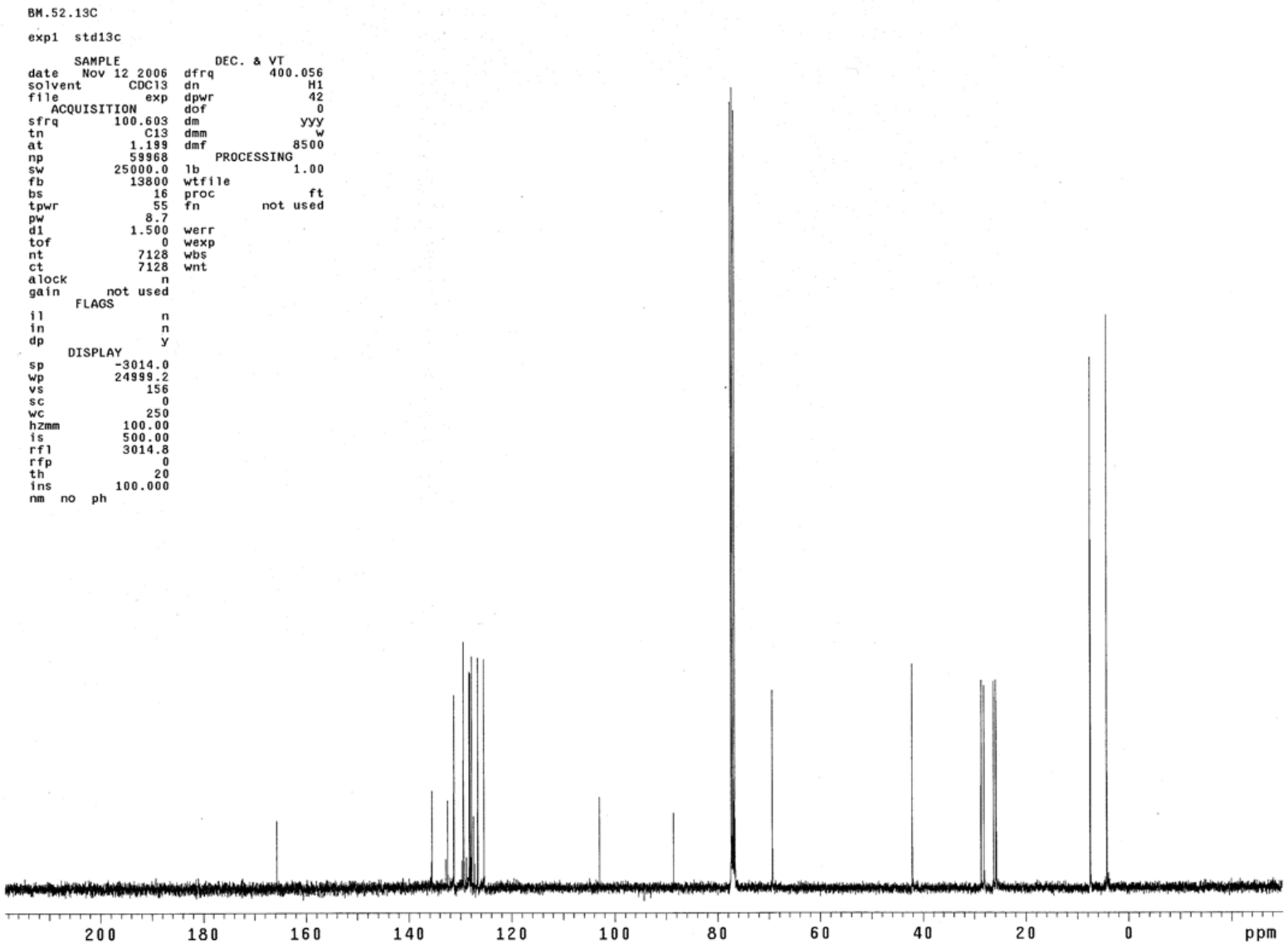

Figure S22. ^{13}C NMR spectrum of **15** (400 MHz, $CDCl_3$)