

Efficiency in Carbon Dioxide Fixation into Cyclic Carbonates: Operating Bifunctional Polyhydroxylated Pyridinium Organocatalysts in Segmented Flow Conditions

Lorenzo Poletti,^a Caterina Rovegno,^{a,b} Graziano Di Carmine,^a Filippo Vacchi,^b Daniele Ragno,^a Arianna Brandolese,^a Alessandro Massi^{a,*} and Paolo Dambruoso^{b,*}

^a Department of Chemical, Pharmaceutical and Agricultural Sciences, University of Ferrara, Via L. Borsari, 46 – 44121 Ferrara (Italy)

^b Institute for Organic Synthesis and Photoreactivity of the Italian National Research Council, Area della Ricerca di Bologna, Via P. Gobetti, 101 – 40129 – Bologna (Italy)

Table of contents

1. Flow apparatus (Figure S1)	S2
2. ¹ H and ¹³ C NMR spectra of intermediates 2 , 6 , 9 , 13 , 15 and organocatalysts 3 , 5 , 8 , 14 , 16	S3
3. ¹ H and ¹³ C NMR spectra of cyclic carbonates 18a-g	S13

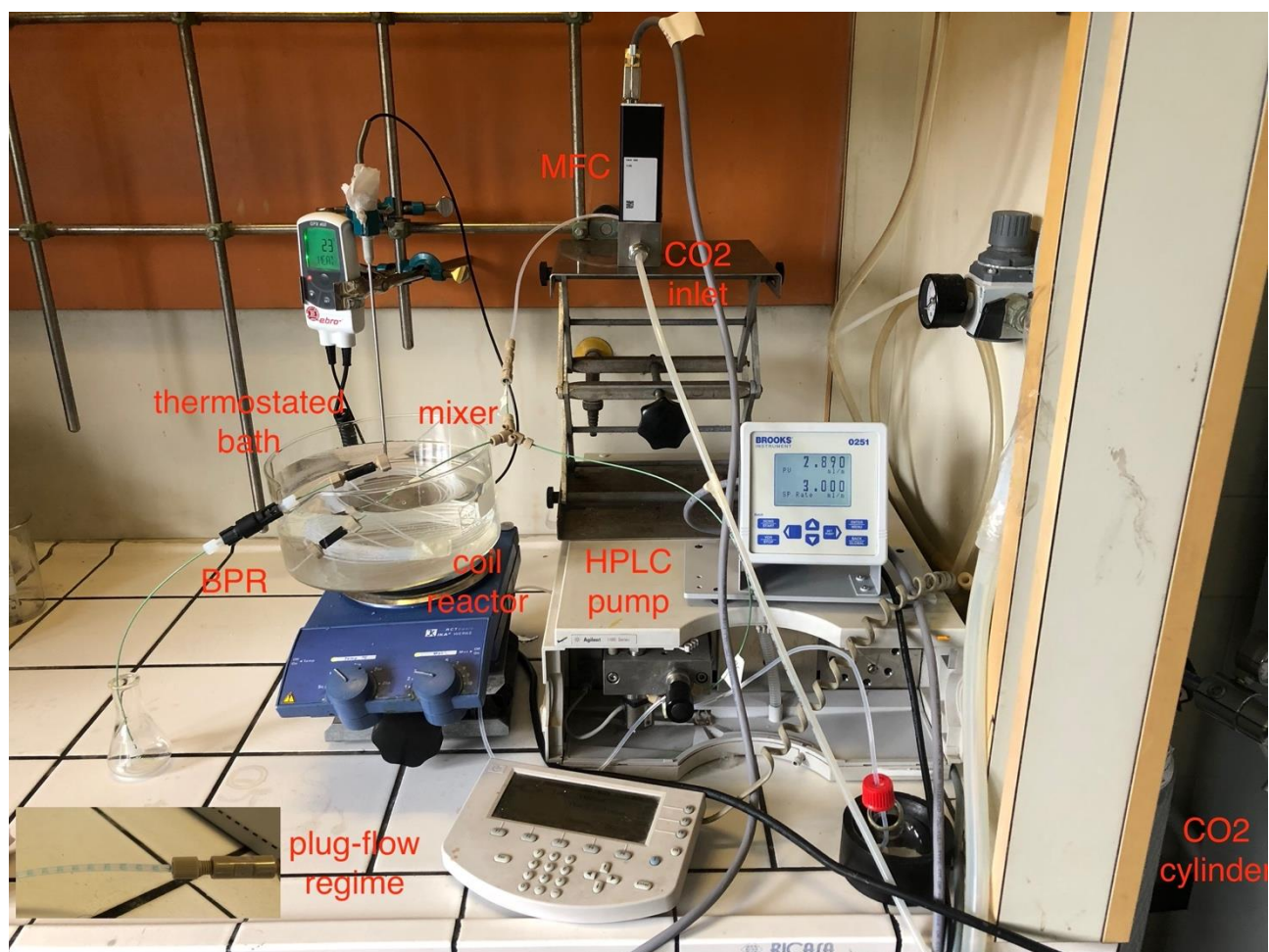


Figure S1. Flow apparatus

The volume of gaseous CO₂ is controlled by the mass flow controller (MFC) and mixed with the liquid phase in a T-mixer. The reactor consists of a 4.42 mL spiral capillary (FEP tubing; 0.75 mm internal diameter; length 10 m) placed inside a thermostated bath. The liquid flow rate is controlled by a HPLC pump while the back-pressure regulator (BPR) maintains a constant pressure of CO₂ (8.5 atm) throughout the system.

Figure S2. ^1H -NMR (500 MHz, CDCl_3), $^{13}\text{C}\{^1\text{H}\}$ -NMR (126 MHz, CDCl_3) of (2).

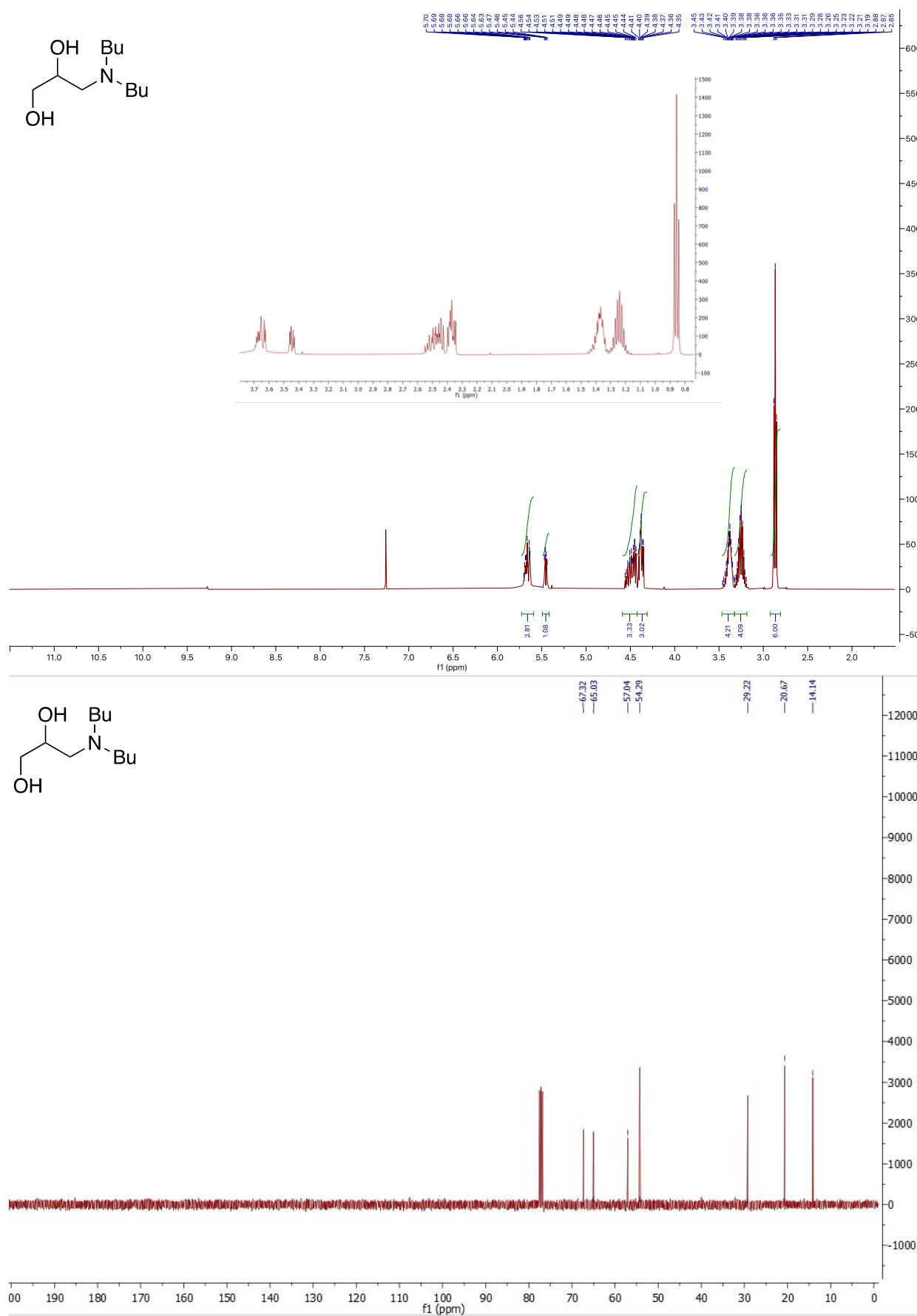


Figure S3. ^1H -NMR (300 MHz, DMSO- d_6), $^{13}\text{C}\{^1\text{H}\}$ -NMR (101 MHz, DMSO- d_6) of (3)

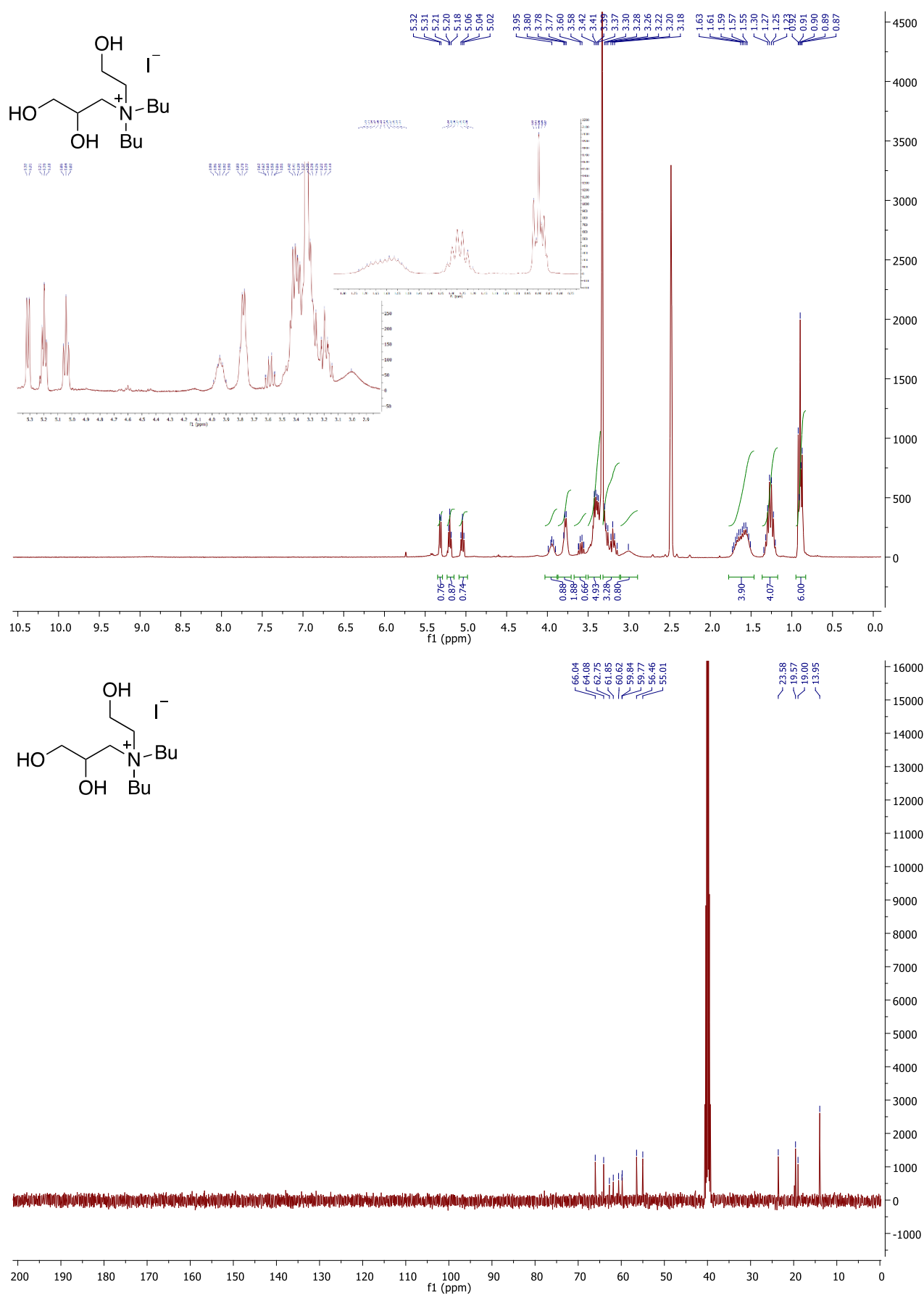


Figure S4. ^1H -NMR (300 MHz, DMSO- d_6), $^{13}\text{C}\{^1\text{H}\}$ -NMR (101 MHz, DMSO- d_6) of (5)

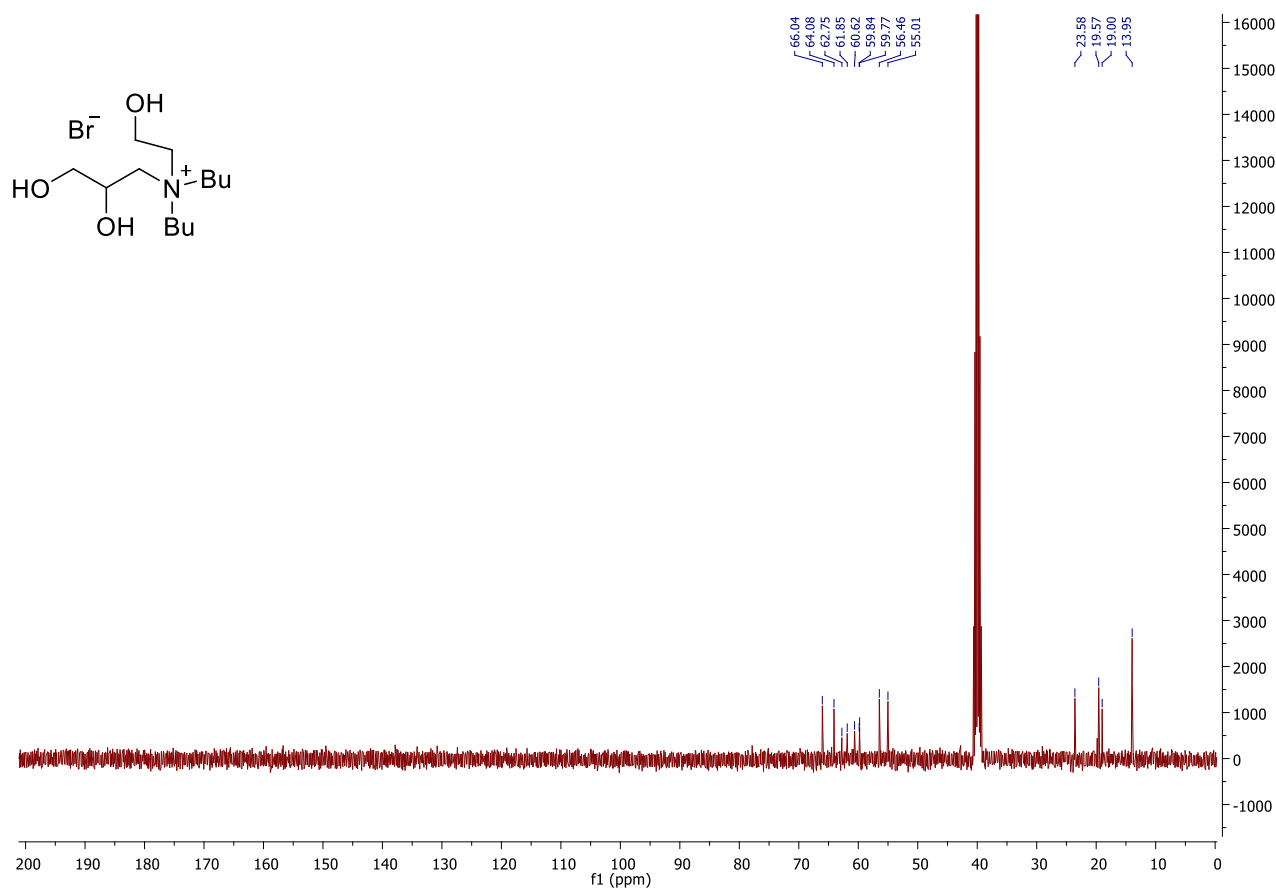
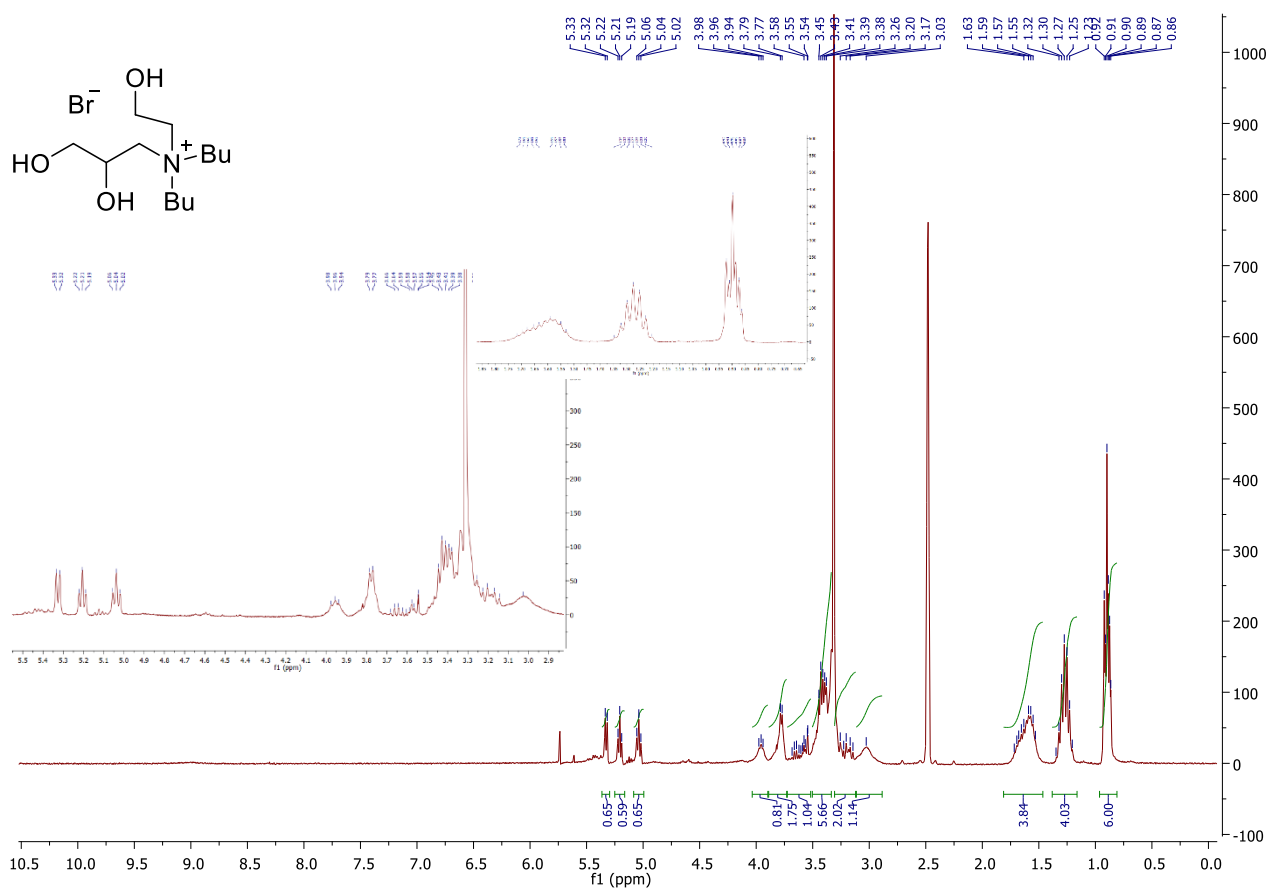


Figure S5. ^1H -NMR (500 MHz, D_2O), $^{13}\text{C}\{^1\text{H}\}$ -NMR (126 MHz, D_2O) of (6)

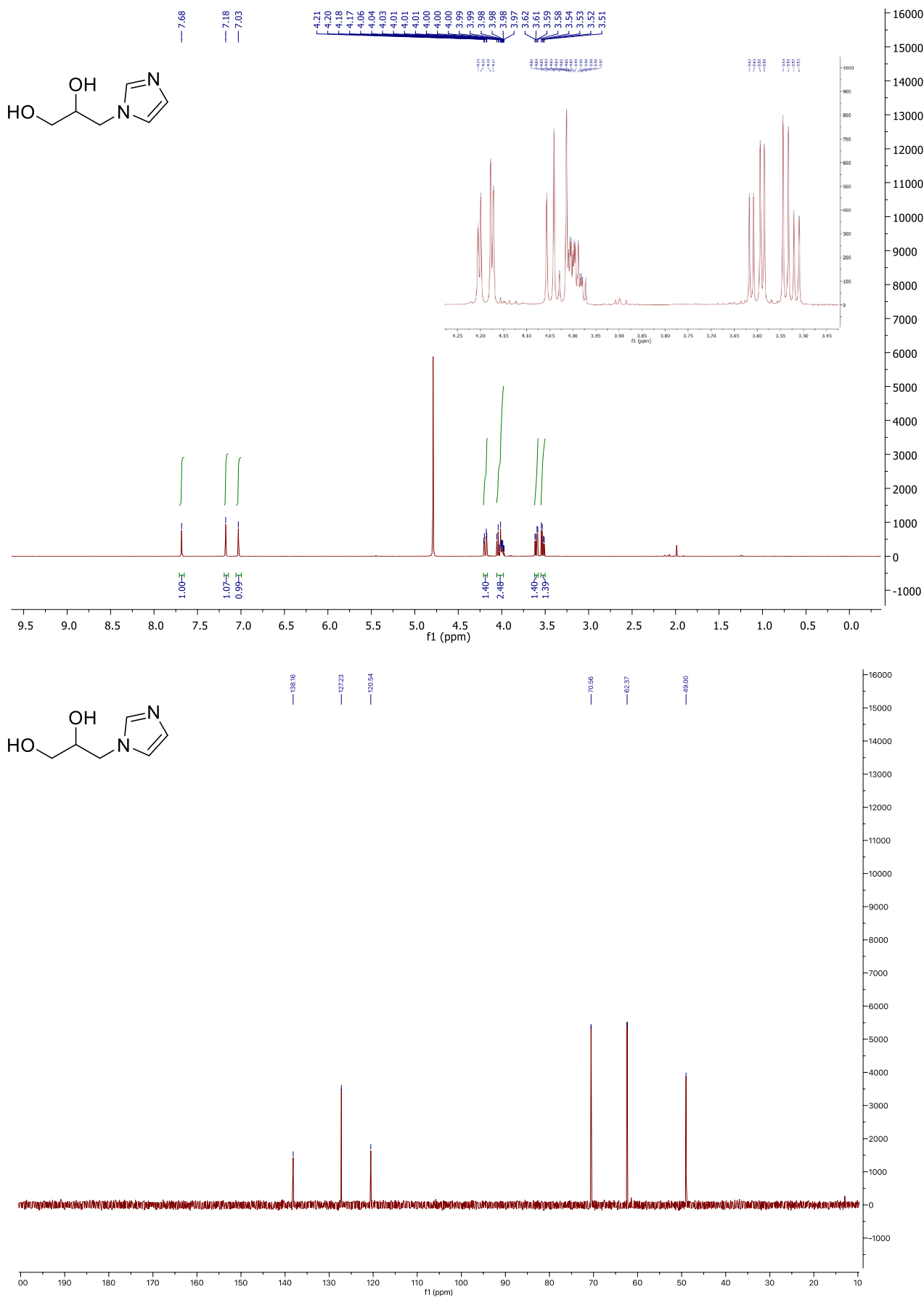


Figure S6. ^1H -NMR (300 MHz, DMSO-d_6), $^{13}\text{C}\{^1\text{H}\}$ -NMR (101 MHz, DMSO-d_6) of (8).

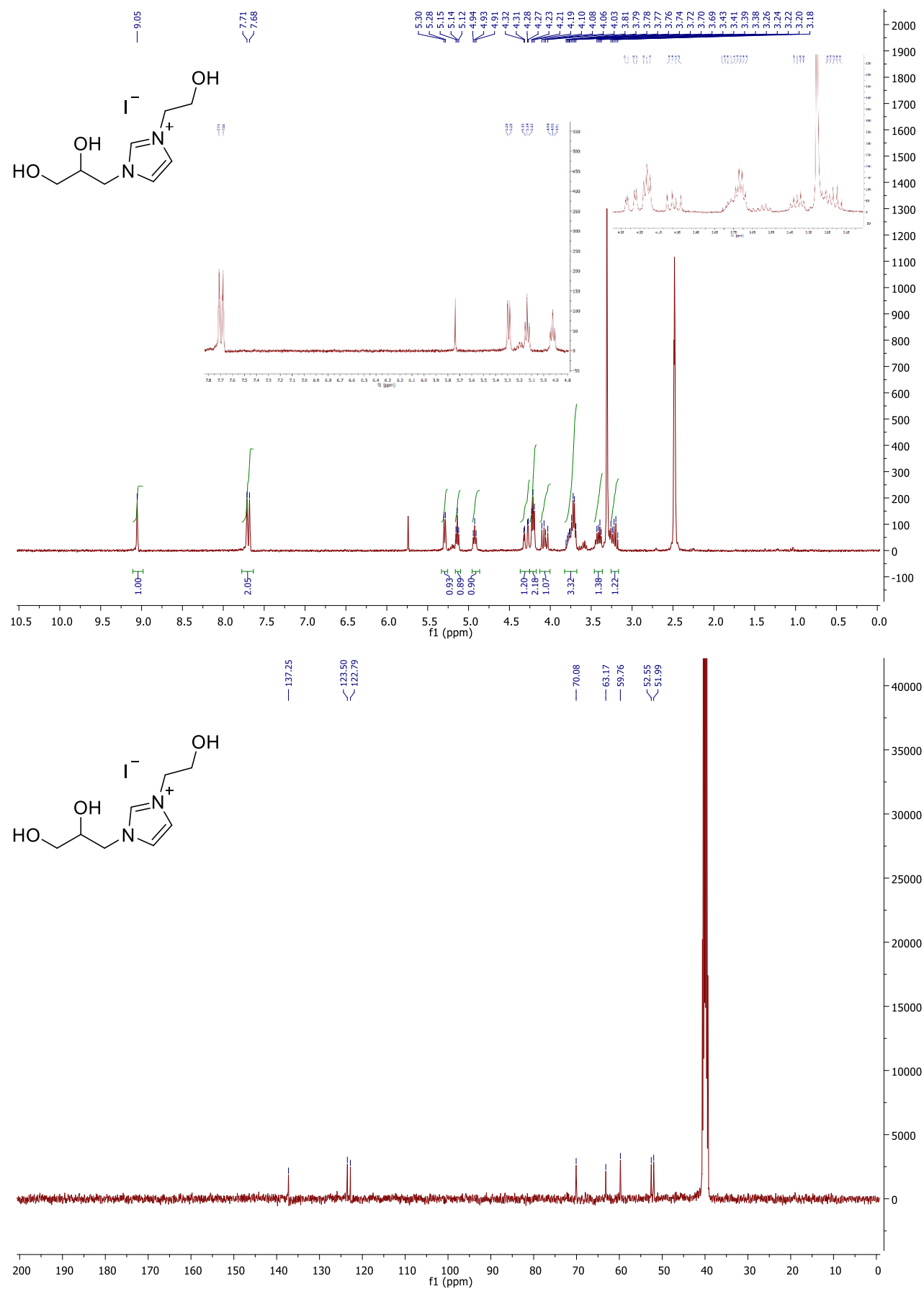


Figure S7. ^1H -NMR (400 MHz, D_2O), $^{13}\text{C}\{^1\text{H}\}$ -NMR (101 MHz, D_2O) of (9).

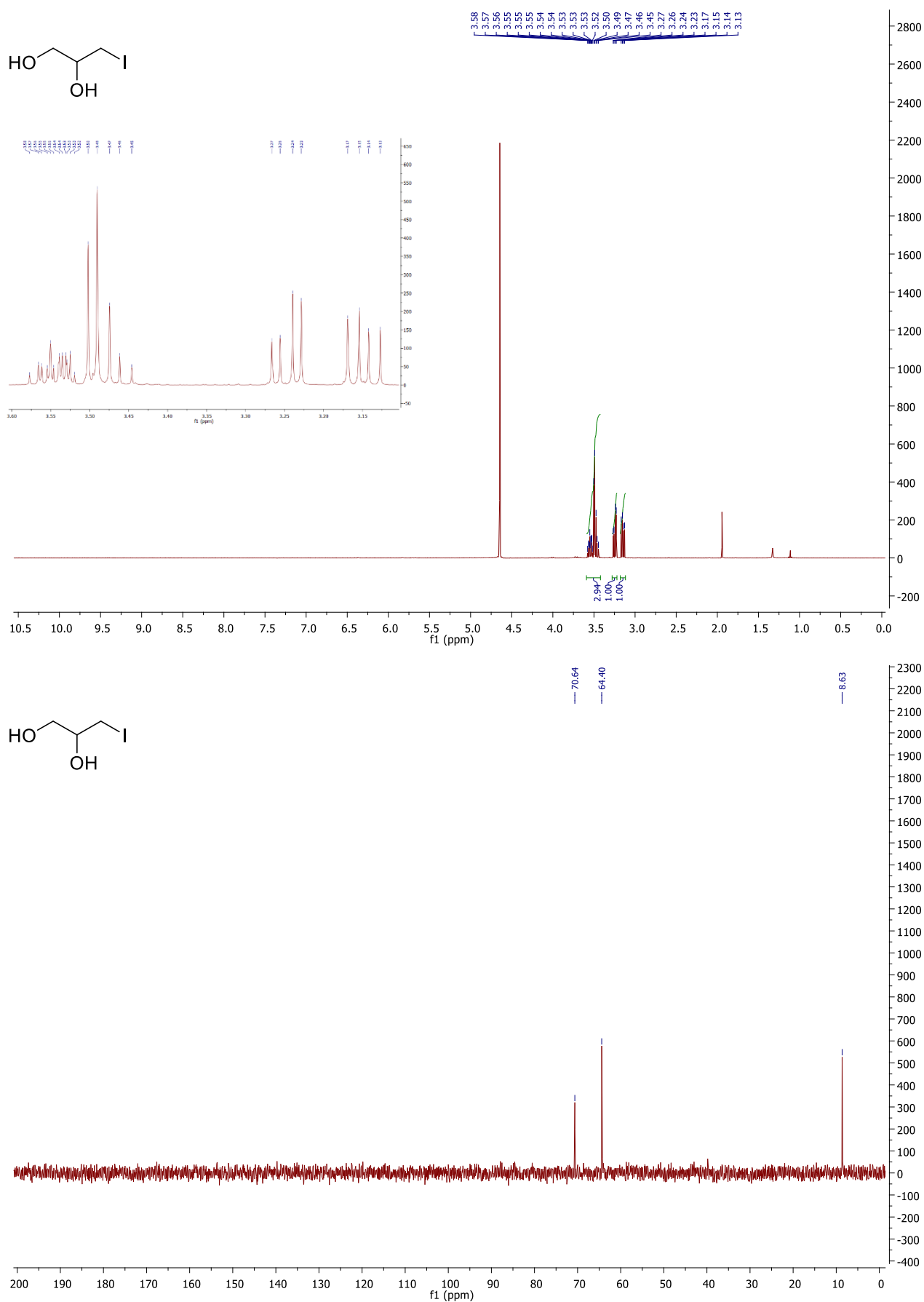


Figure S8. ^1H -NMR (400 MHz, CDCl_3), $^{13}\text{C}\{^1\text{H}\}$ -NMR (101 MHz, CDCl_3) of (13).

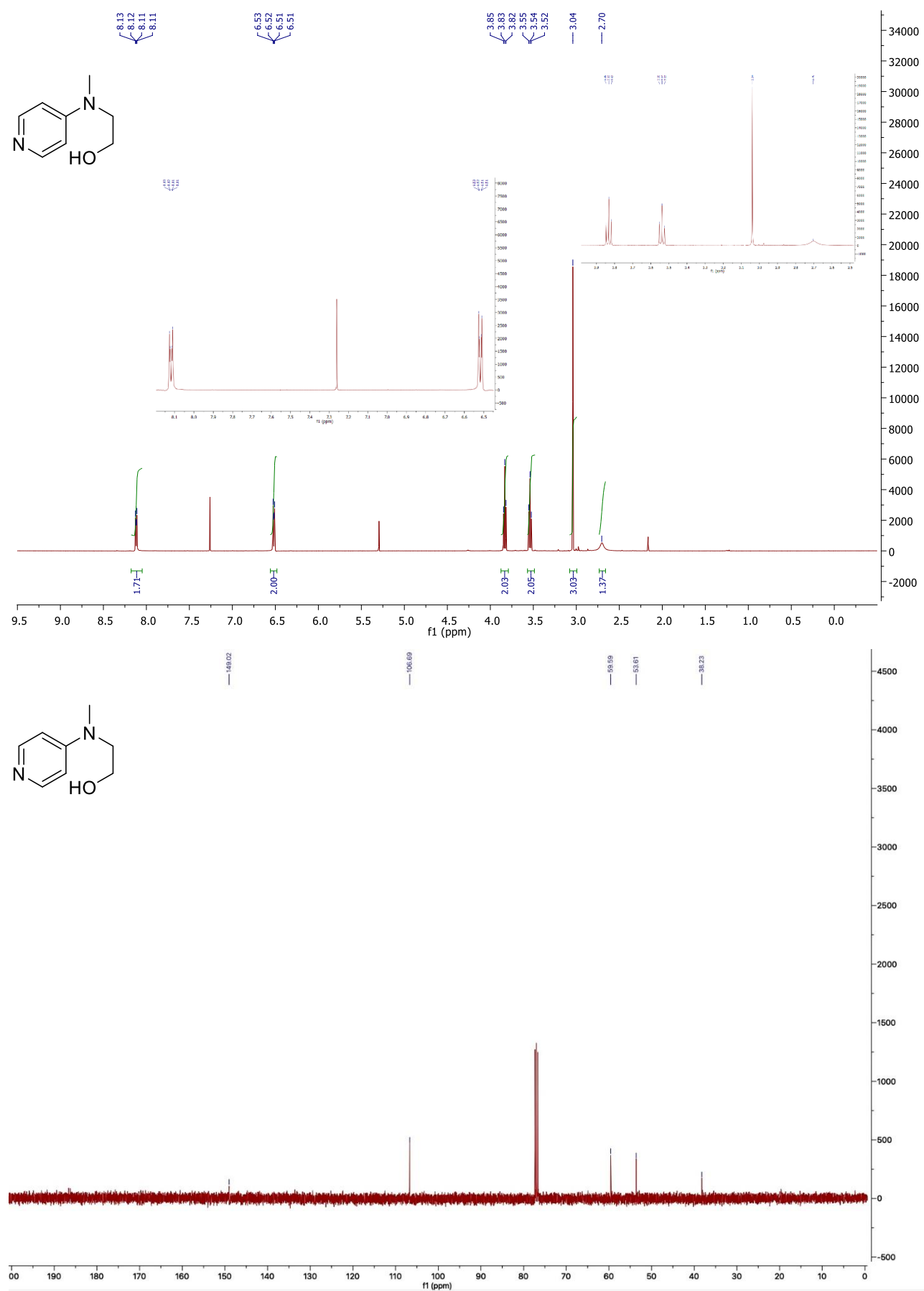


Figure S9. ^1H -NMR (300 MHz, DMSO- d_6), $^{13}\text{C}\{^1\text{H}\}$ -NMR (101 MHz, DMSO- d_6) of (14)

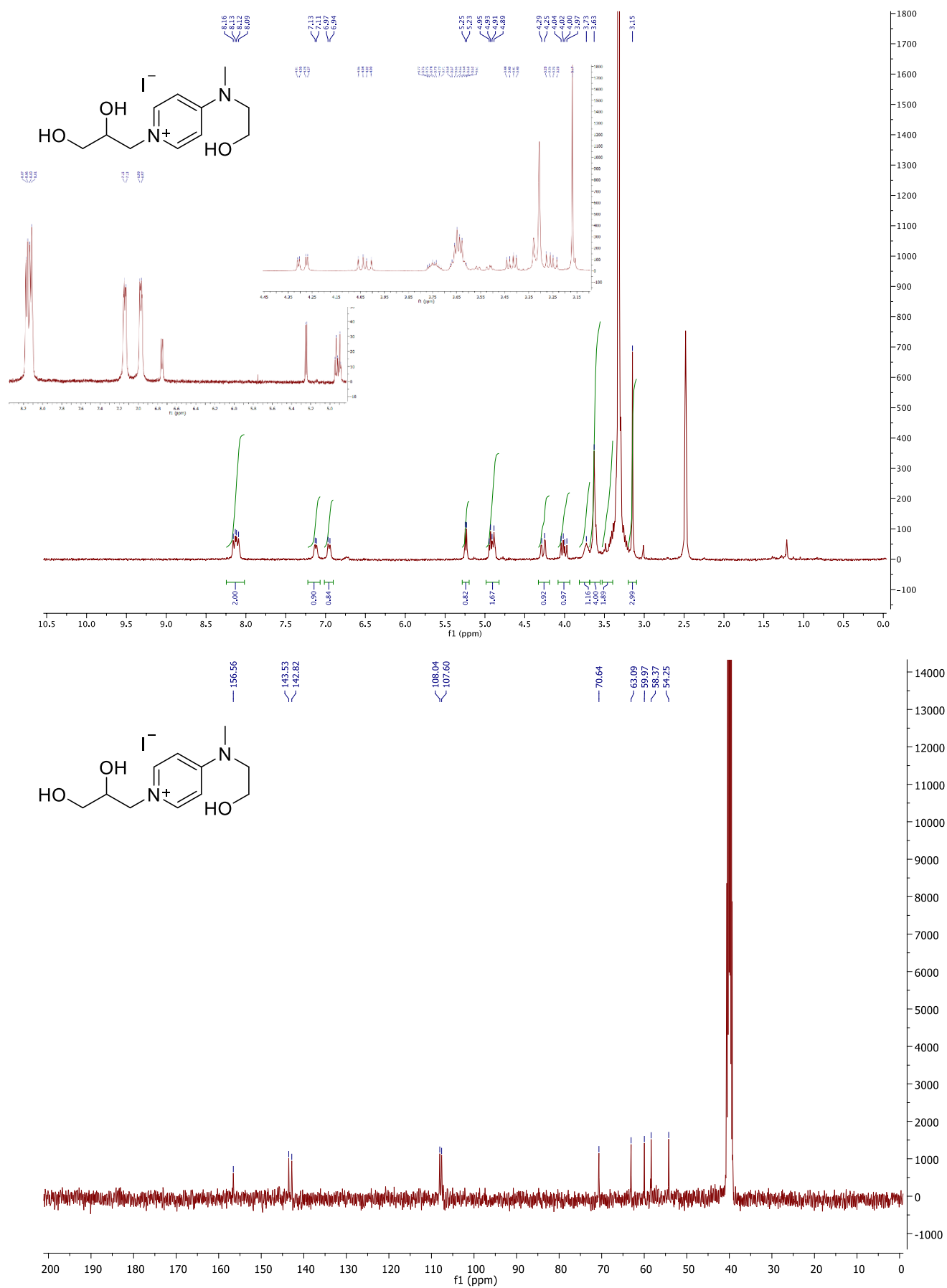


Figure S10. ^1H -NMR (300 MHz, CDCl_3), $^{13}\text{C}\{^1\text{H}\}$ -NMR (101 MHz, CDCl_3) of (15).

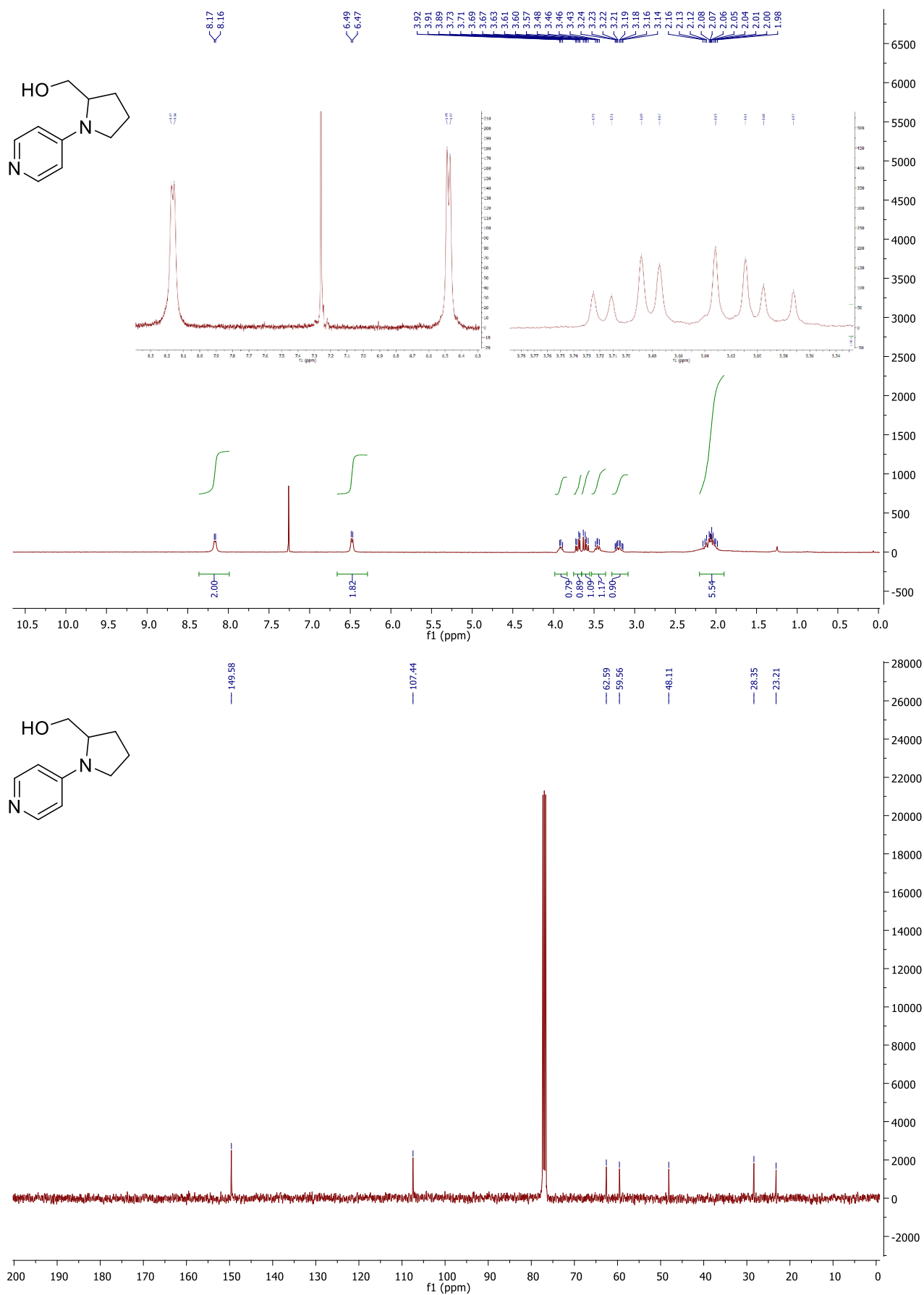


Figure S11. ^1H -NMR (300 MHz, DMSO-d_6), $^{13}\text{C}\{^1\text{H}\}$ -NMR (101 MHz, DMSO-d_6) of (16).

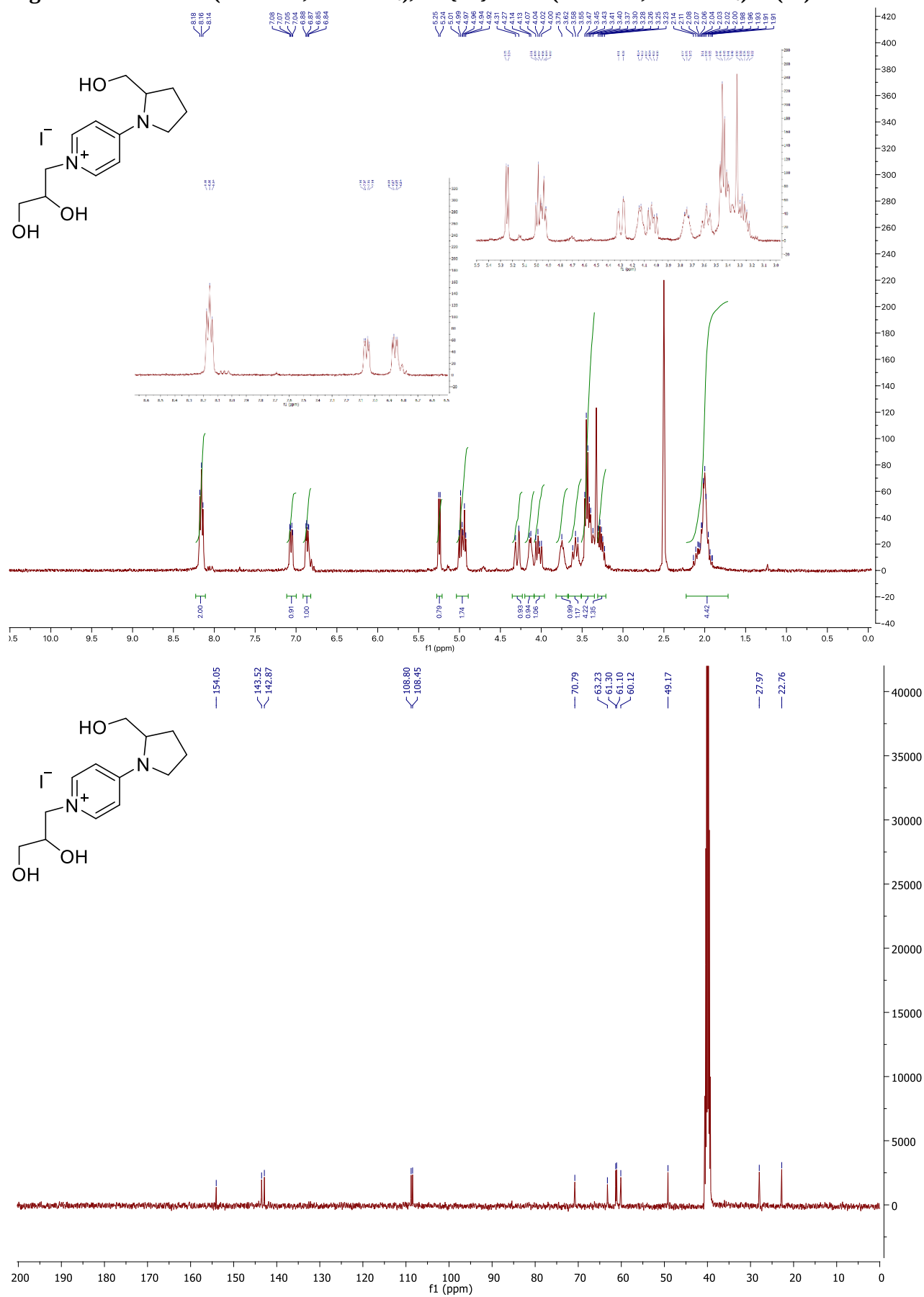


Figure S12. ^1H -NMR (500 MHz, CDCl_3), $^{13}\text{C}\{^1\text{H}\}$ -NMR (126 MHz, CDCl_3) of (18a).

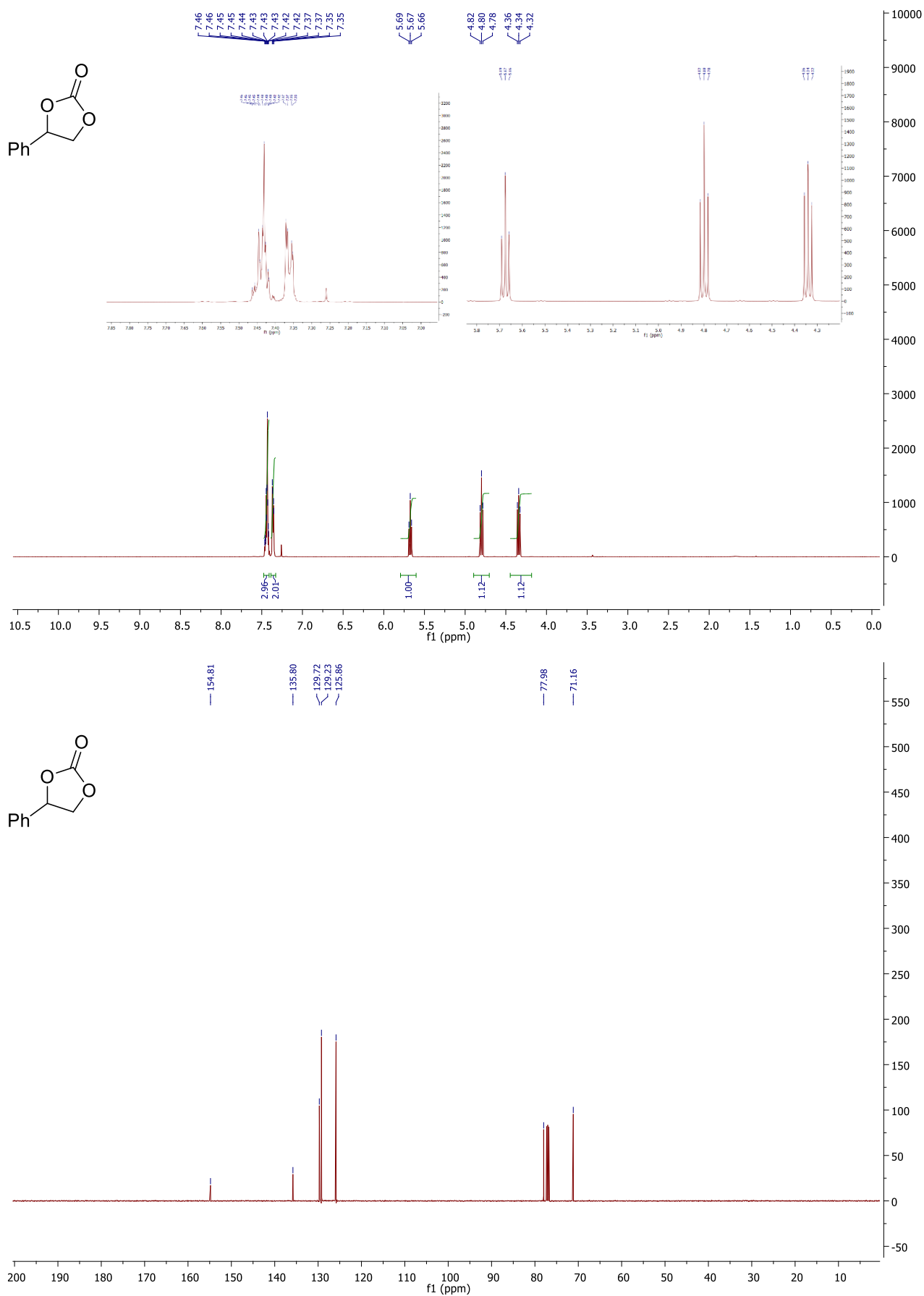


Figure S13. ^1H -NMR (300 MHz, CDCl_3), $^{13}\text{C}\{^1\text{H}\}$ -NMR (101 MHz, CDCl_3) of (18b).

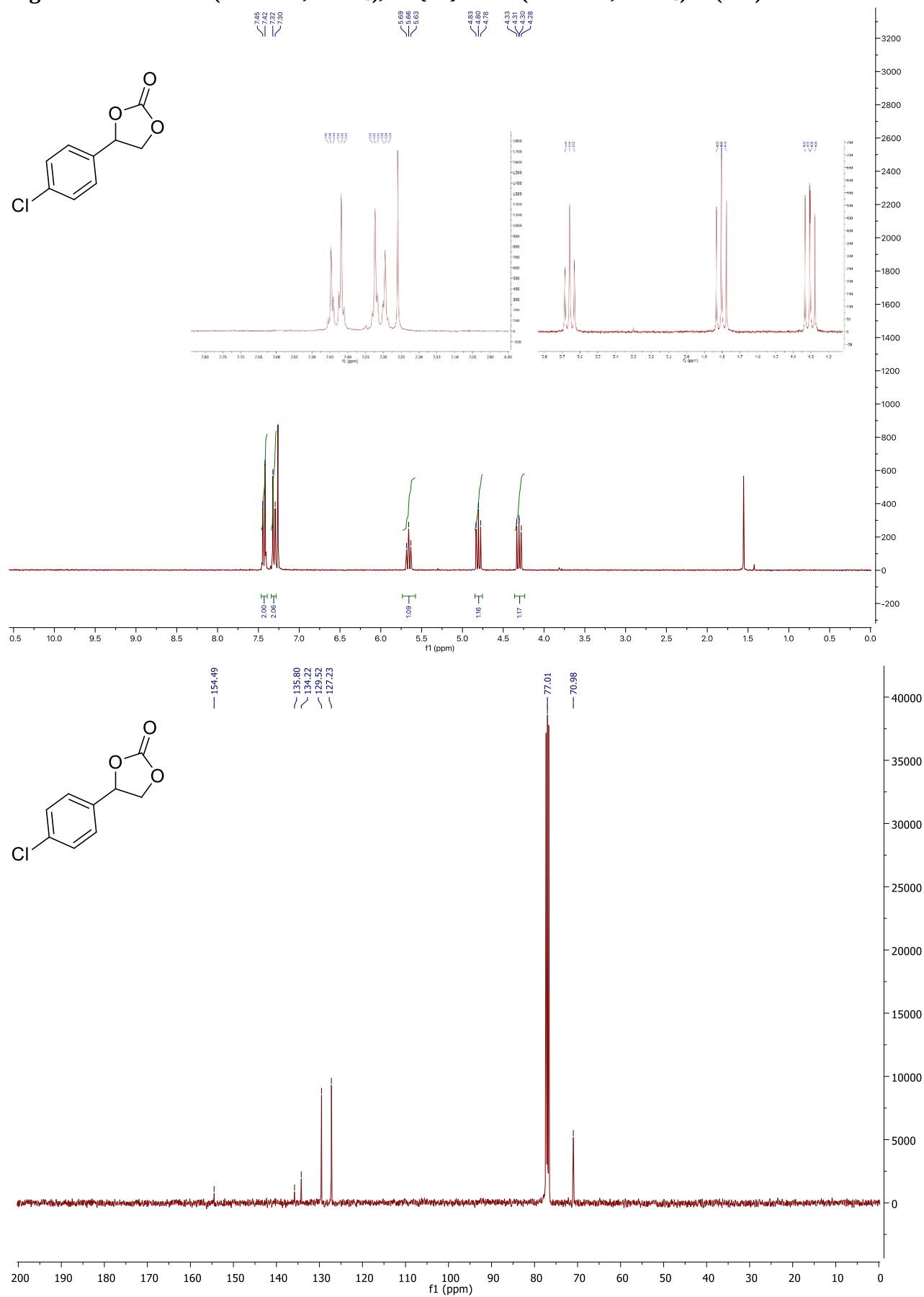


Figure S14. ^1H -NMR (400 MHz, CDCl_3), $^{13}\text{C}\{^1\text{H}\}$ -NMR (101 MHz, CDCl_3) of (18c).

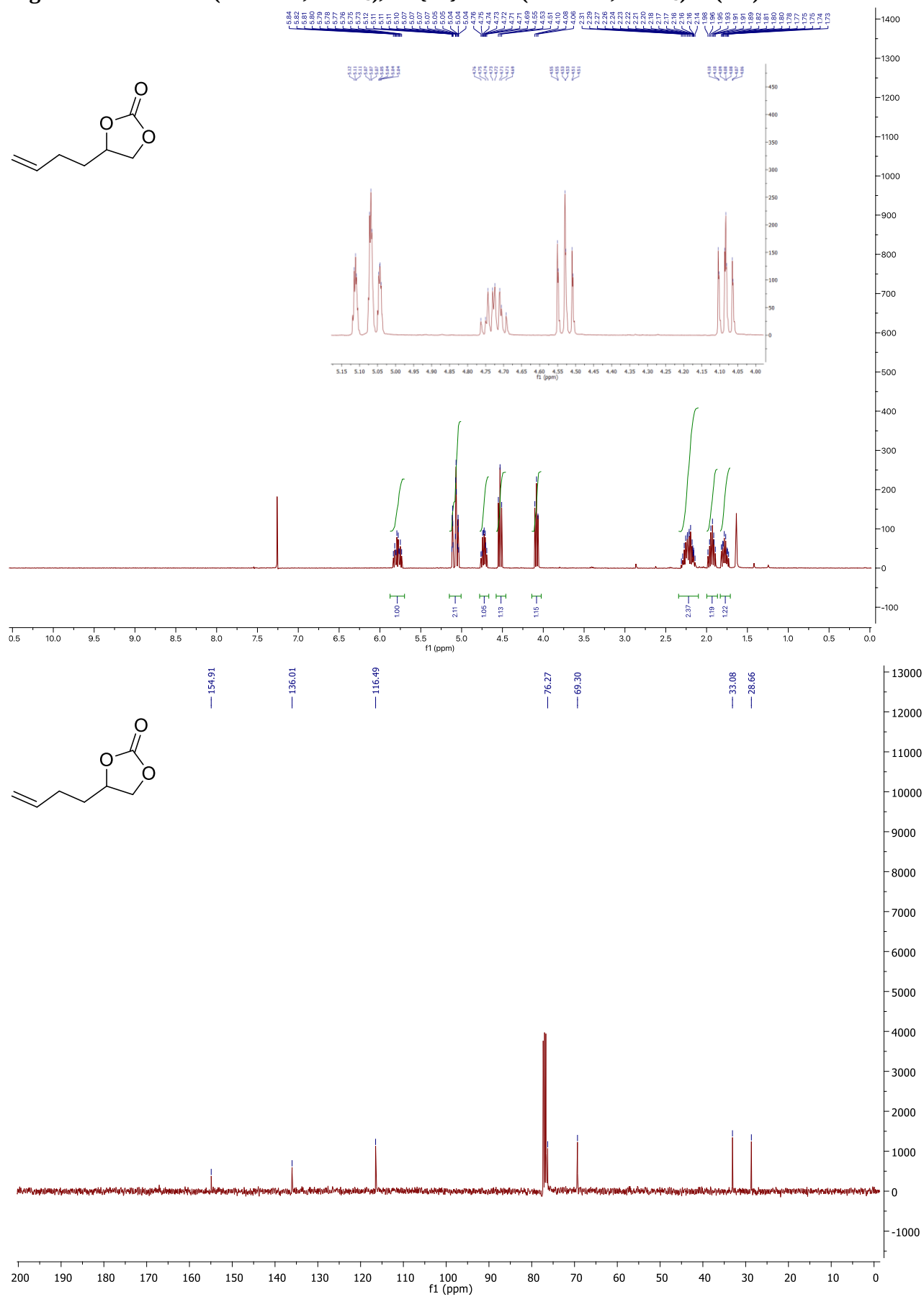


Figure S15. ^1H -NMR (400 MHz, CDCl_3), $^{13}\text{C}\{^1\text{H}\}$ -NMR (101 MHz, CDCl_3) of (18d).

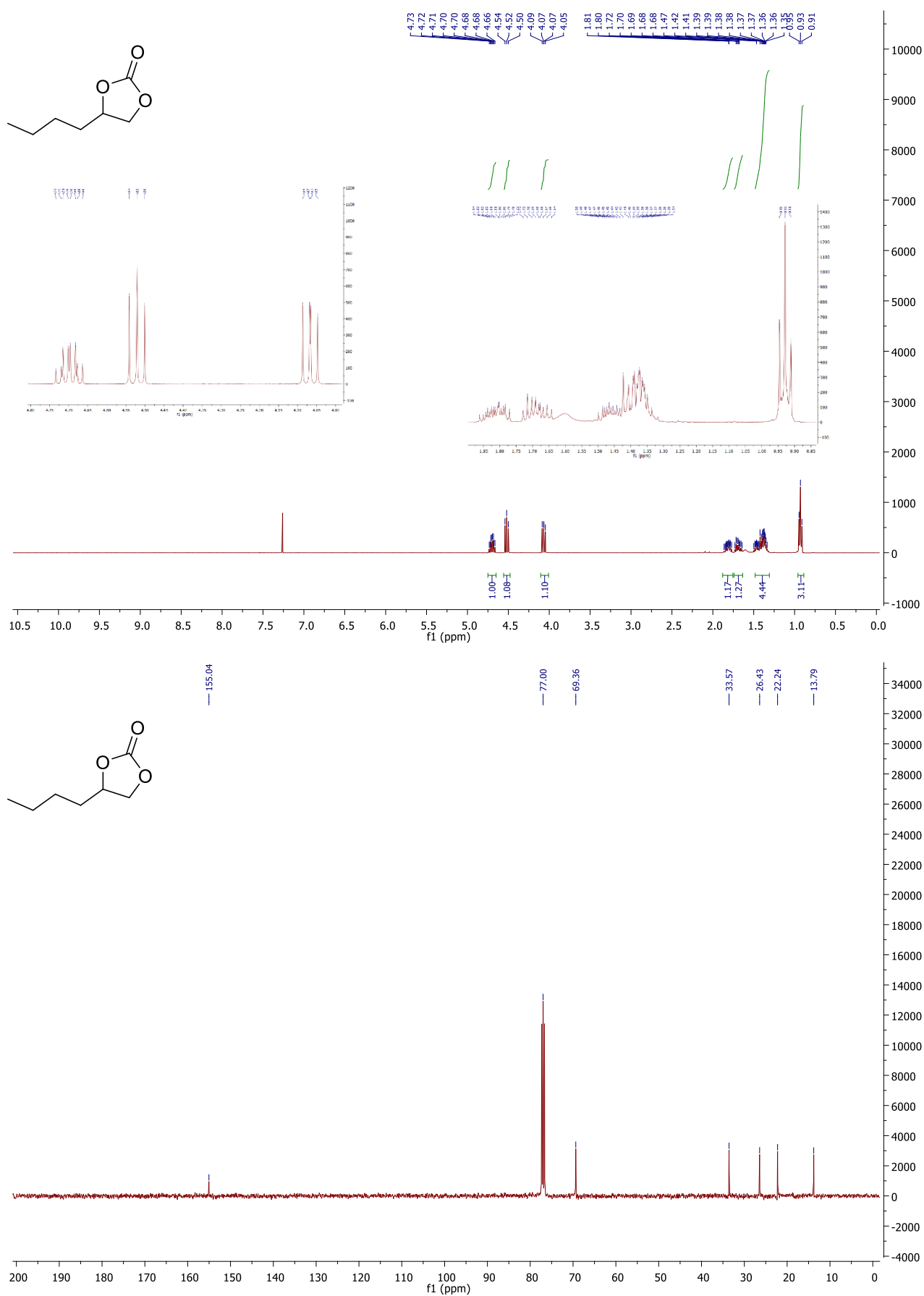


Figure S16. ^1H -NMR (400 MHz, CDCl_3), $^{13}\text{C}\{^1\text{H}\}$ -NMR (101 MHz, CDCl_3) of (18e).

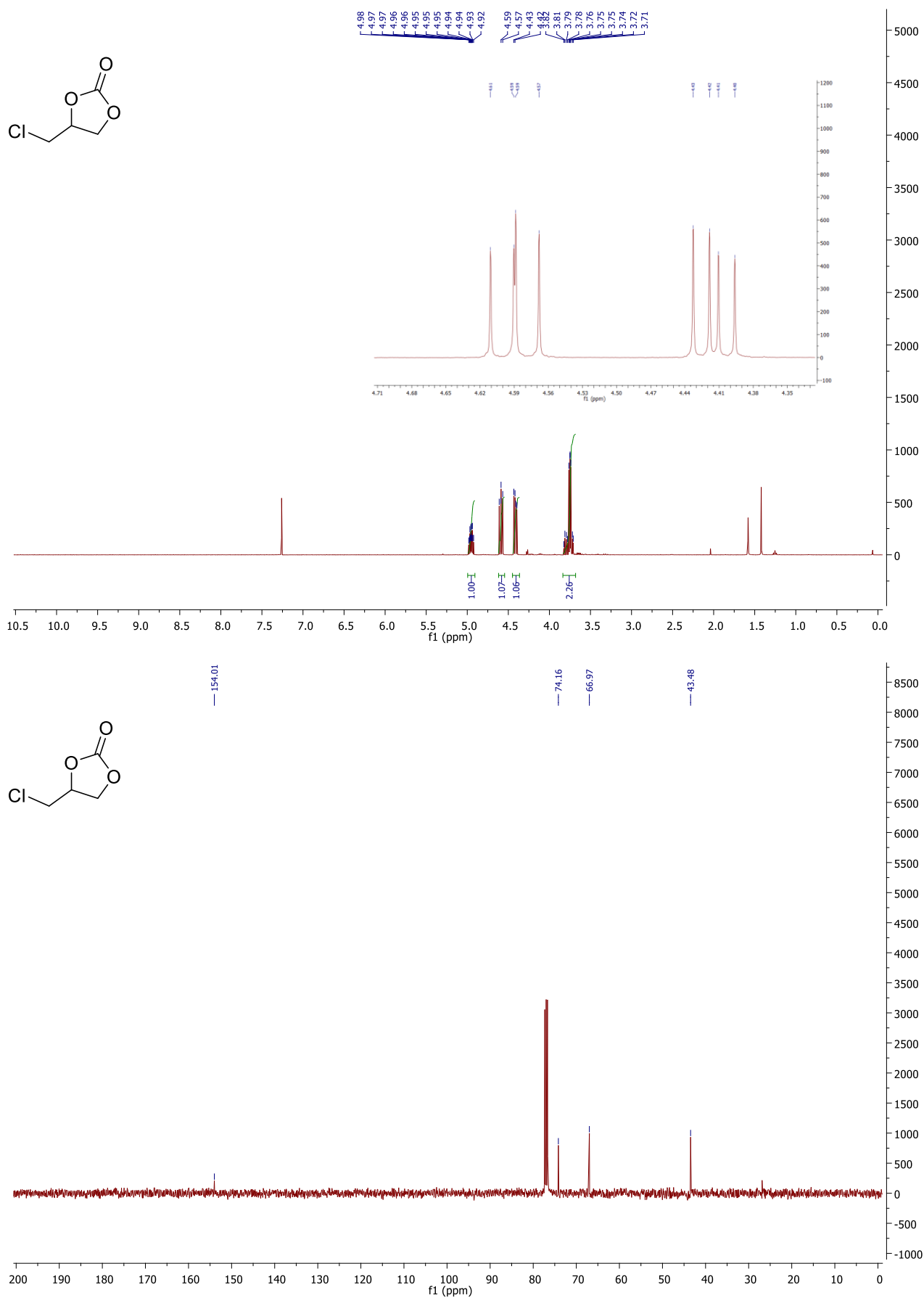


Figure S17. ^1H -NMR (300 MHz, CDCl_3), $^{13}\text{C}\{^1\text{H}\}$ -NMR (101 MHz, CDCl_3) of (18f).

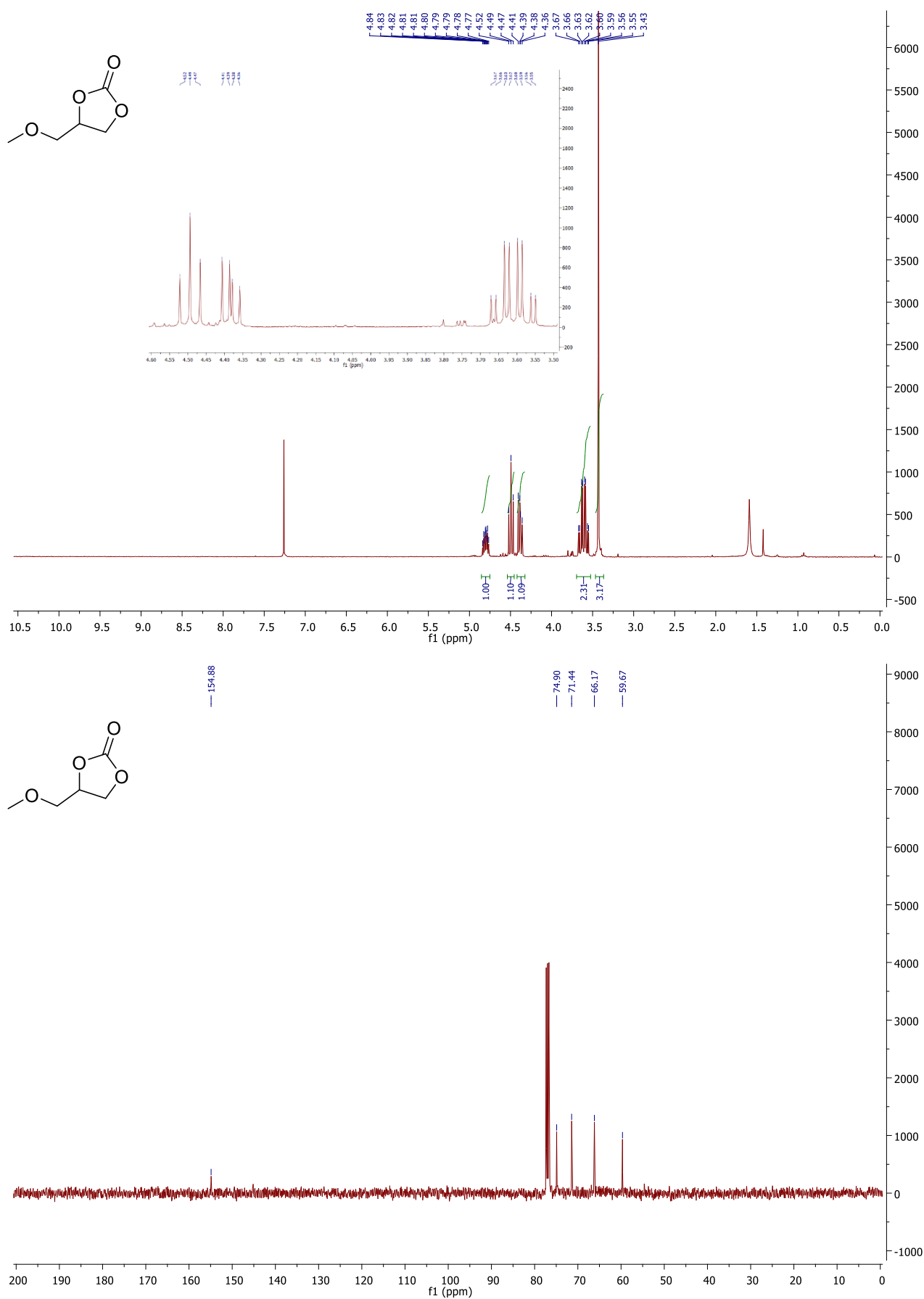


Figure S18. ^1H -NMR (300 MHz, CDCl_3), $^{13}\text{C}\{^1\text{H}\}$ -NMR (101 MHz, CDCl_3) of (18g).

