Supporting Information

Tuning the Selectivity in Iridium-Catalyzed Acceptorless Dehydrogenative Coupling of Primary Alcohols

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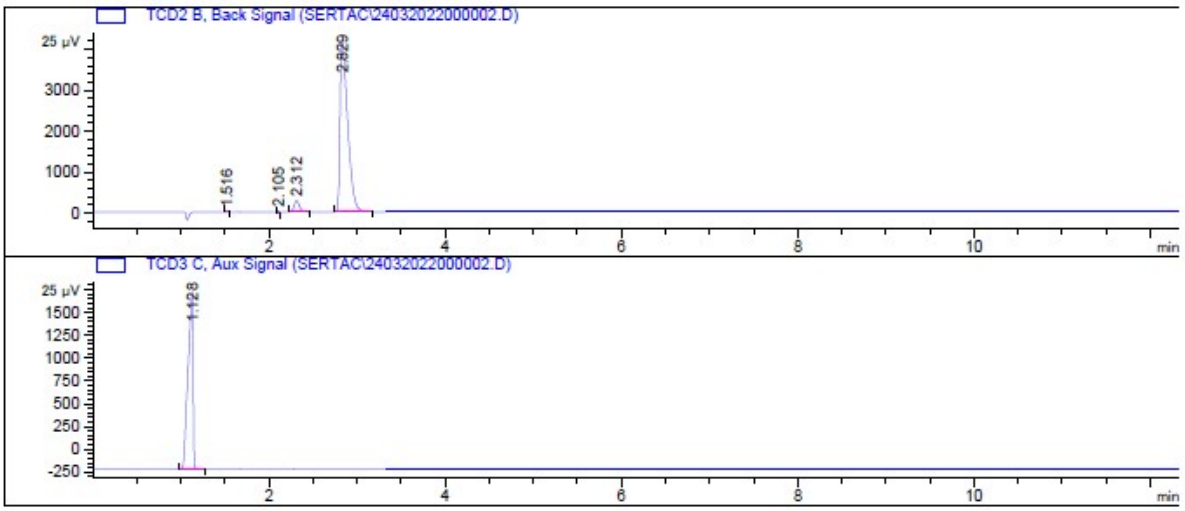

Signal 2: TCD2 B, Back Signal

RetTime [min]	Type	Area [25 µV*s]	Amt/Area	Amount [% mole]	Grp	Name
1.804		-	-	-		CO2
2.629	BB	2.51413e4	2.32397e-3	58.42767		N2
4.335		-	-	-		CO
Totals :				58.42767		

Signal 3: TCD3 C, Aux Signal

RetTime [min]	Type	Area [25 µV*s]	Amt/Area	Amount [% mole]	Grp	Name
1.128	BB	7721.81592	5.57870e-3	43.07771		H2
Totals :				43.07771		

Figure S1. GC traces to confirm H_2 evolution

Traces of ^{1}H and ^{13}C NMR spectra of isolated products

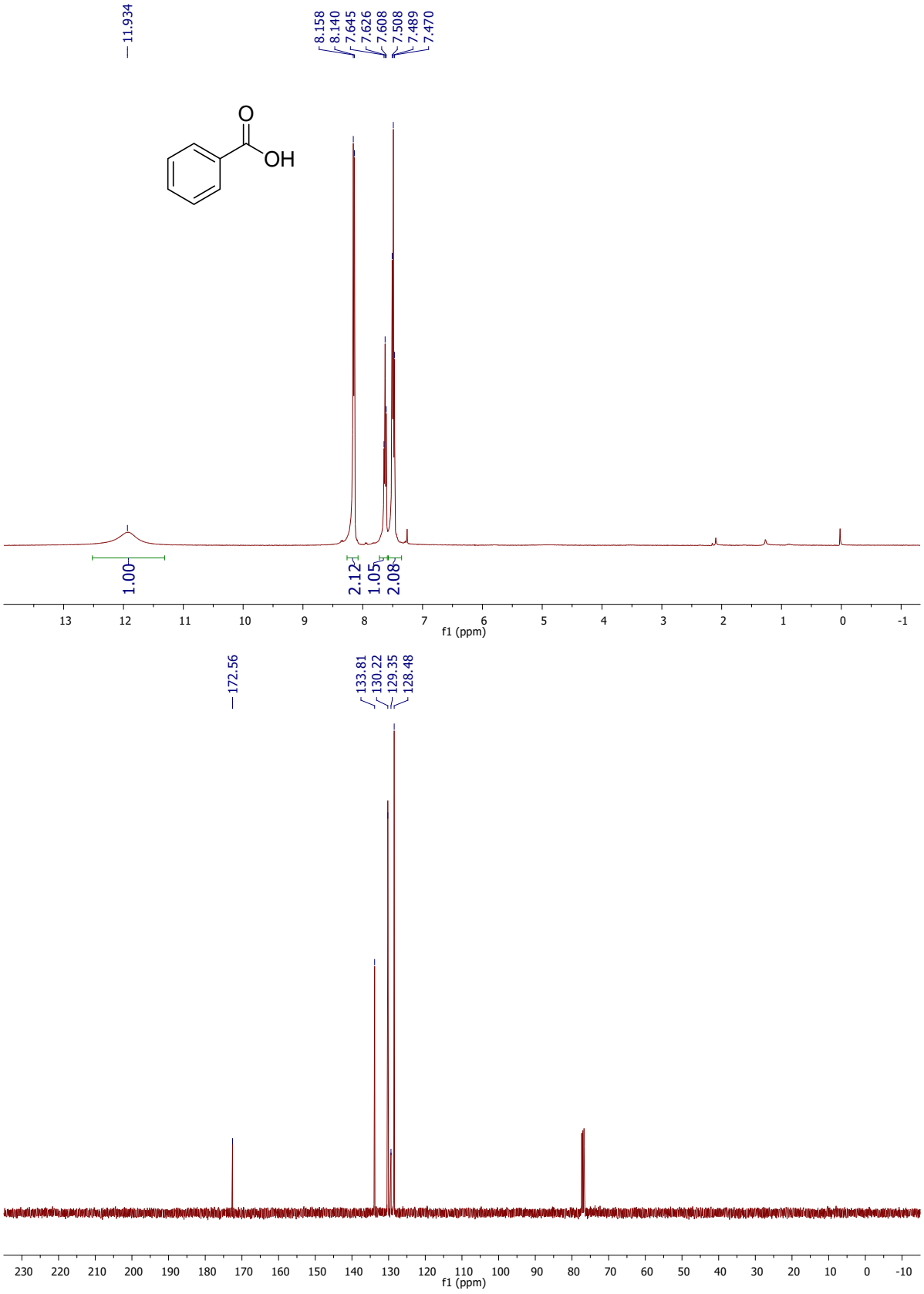

Figure S2. ^{1}H (400 MHz, $CDCl_3$) and $^{13}C\{^{1}H\}$ (100.6 MHz, $CDCl_3$) NMR spectra of **3a**

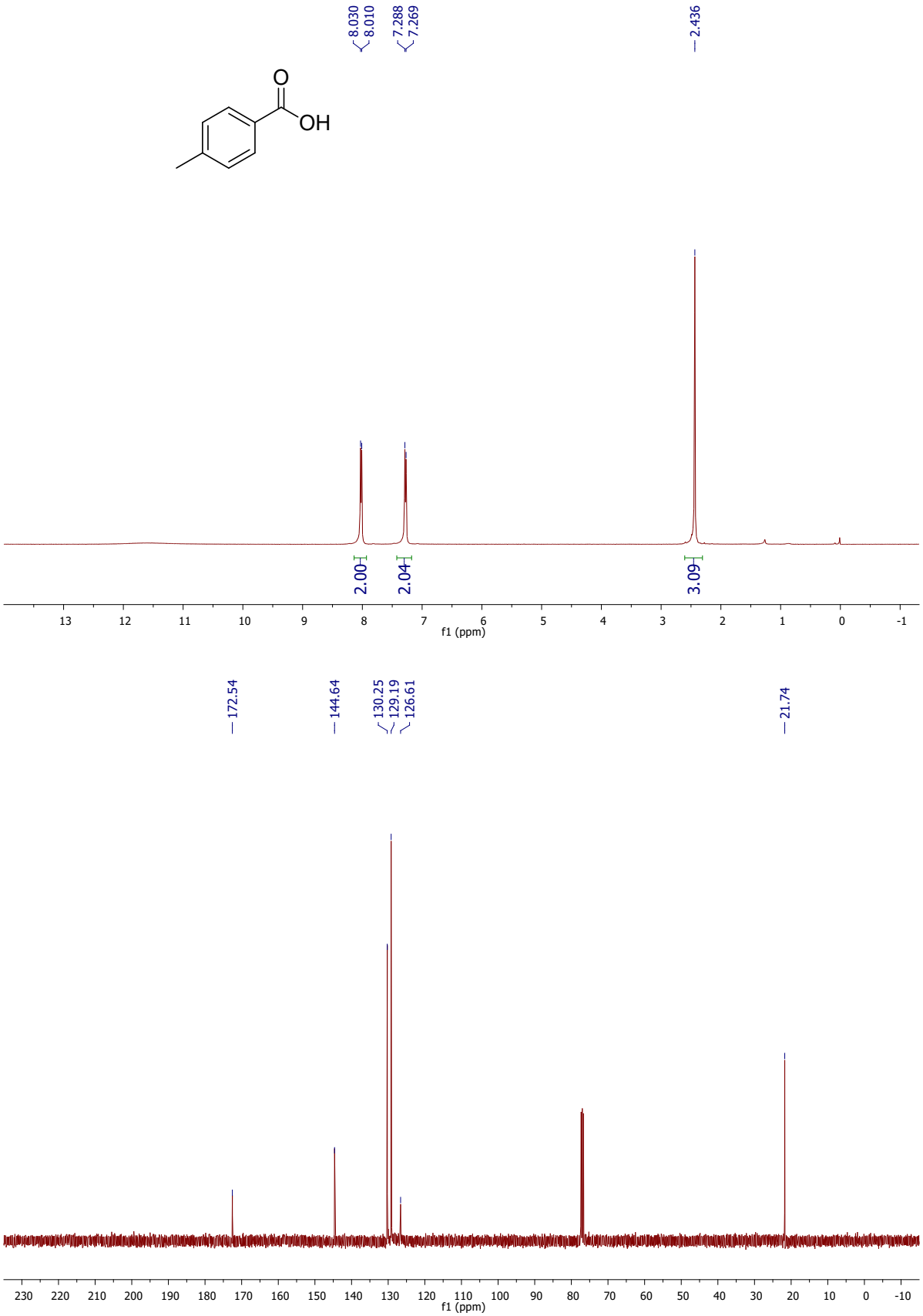

Figure S3. ^{1}H (400 MHz, $CDCl_3$) and $^{13}C\{^{1}H\}$ (100.6 MHz, $CDCl_3$) NMR spectra of **3b**

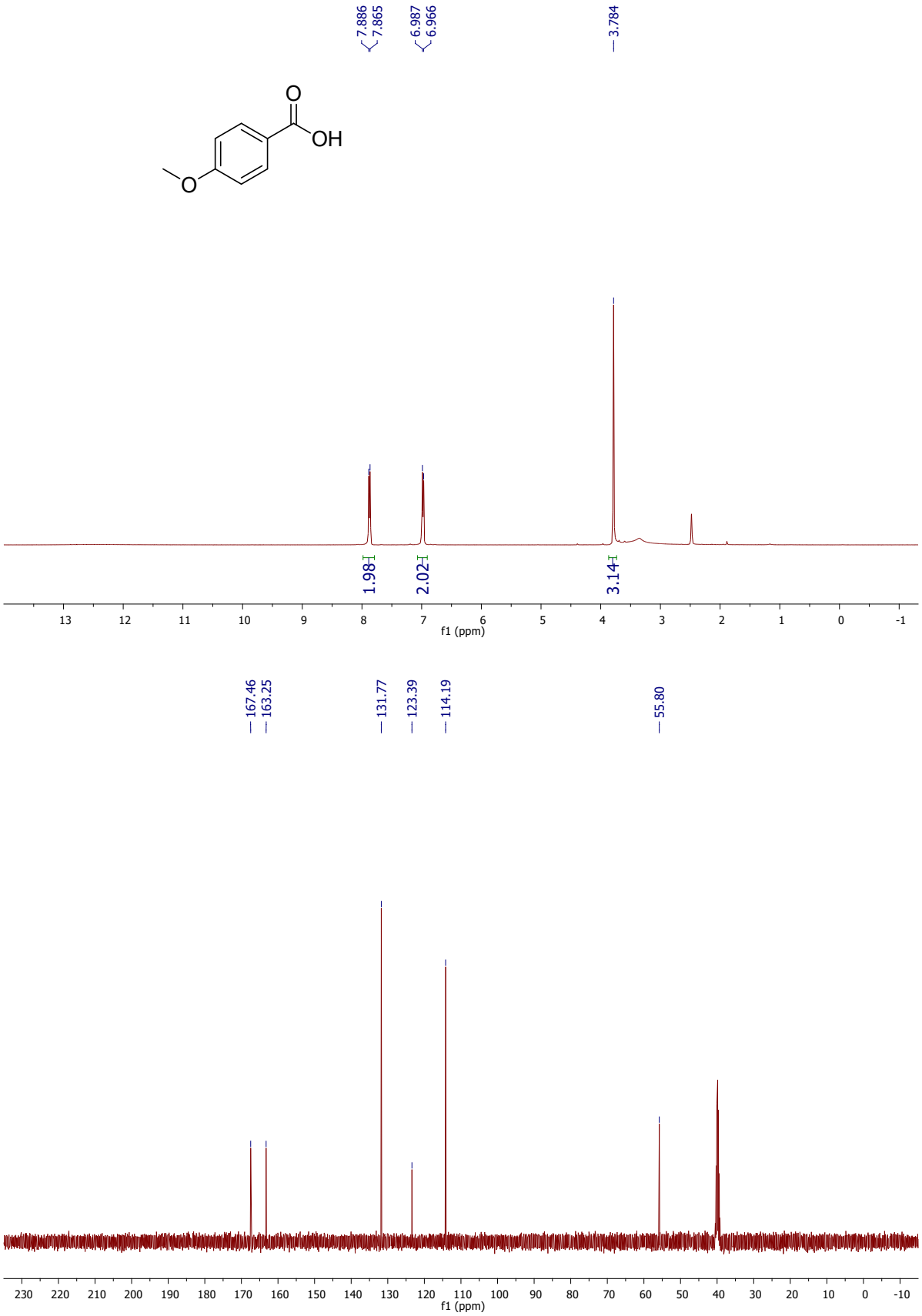

Figure S4. ^{1}H (400 MHz, DMSO-d_6) and $^{13}C\{^{1}H\}$ (100.6 MHz, DMSO-d_6) NMR spectra of **3c**

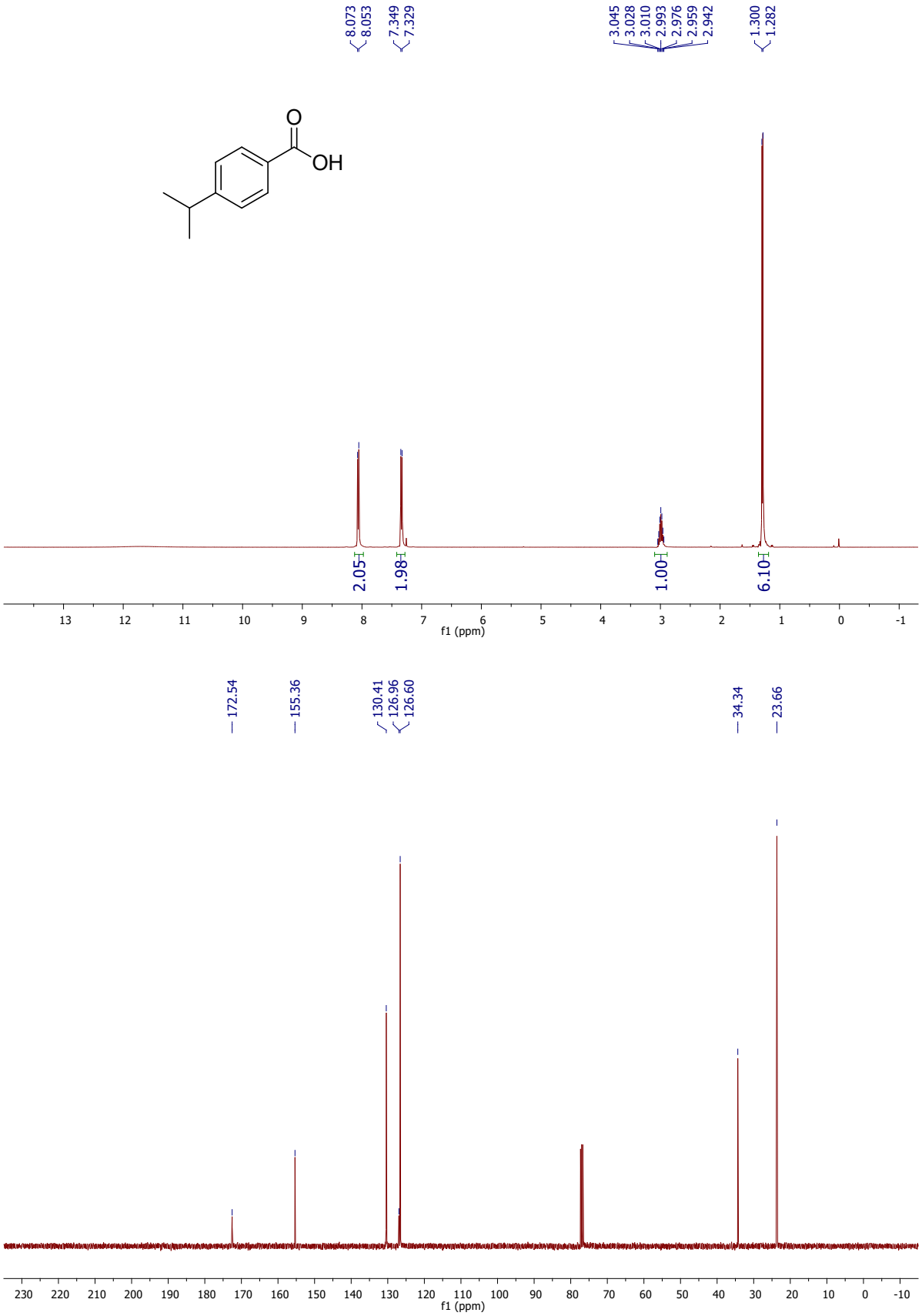

Figure S5. ^{1}H (400 MHz, $CDCl_3$) and $^{13}C\{^{1}H\}$ (100.6 MHz, $CDCl_3$) NMR spectra of **3d**

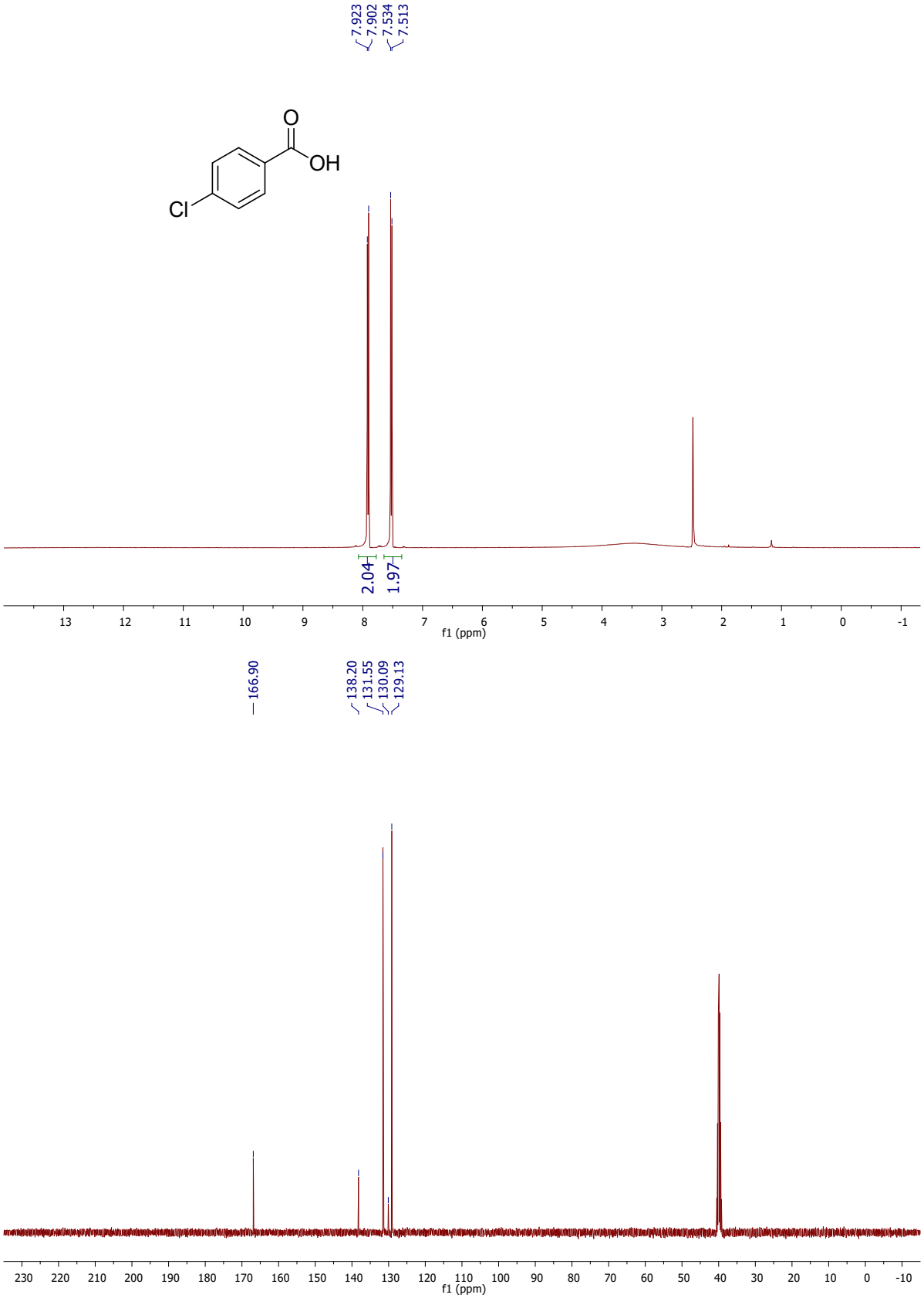

Figure S6. ^{1}H (400 MHz, DMSO-d_6) and $^{13}C\{^{1}H\}$ (100.6 MHz, DMSO-d_6) NMR spectra of **3e**

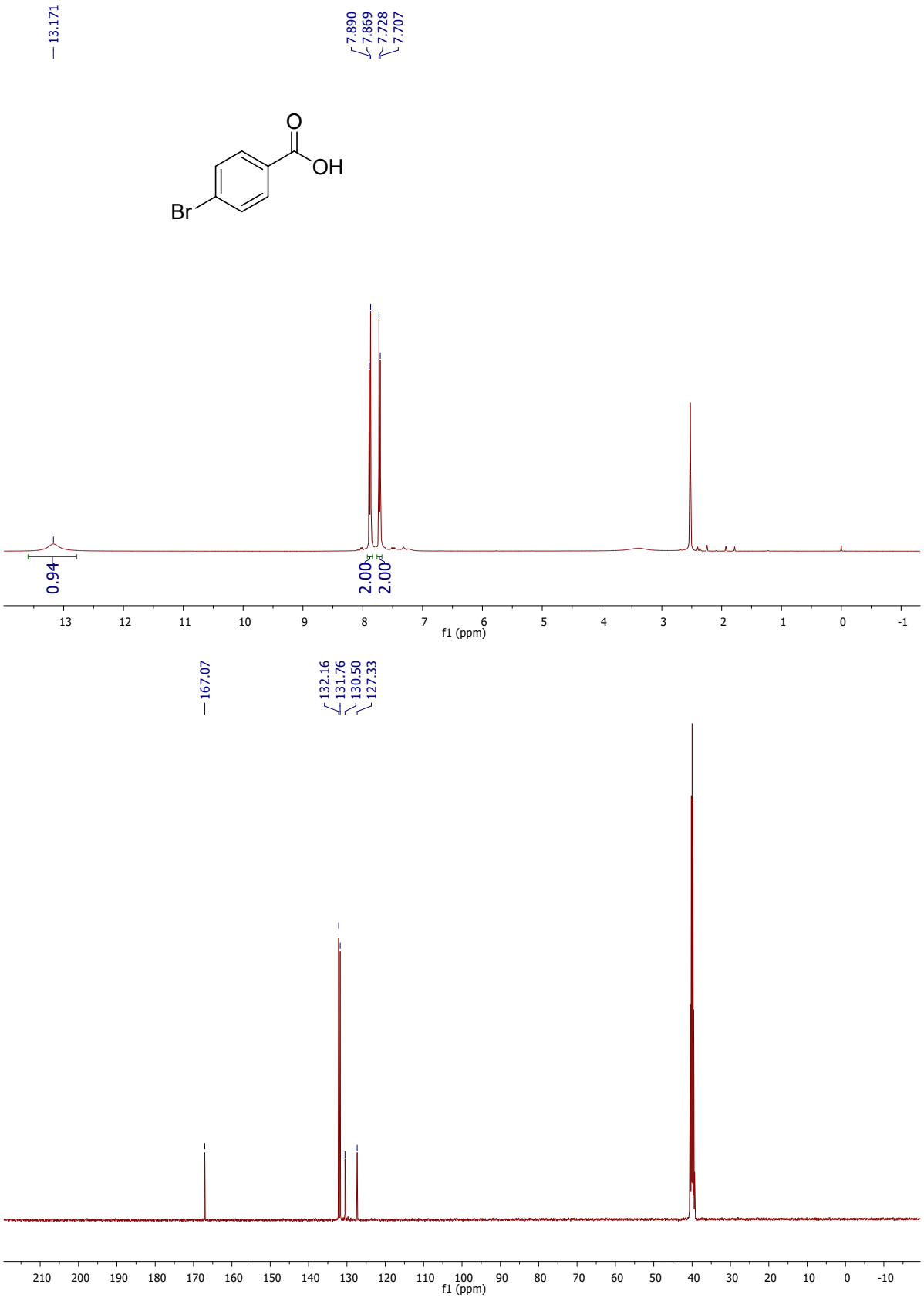

Figure S7. ^{1}H (400 MHz, DMSO-d_6) and $^{13}C\{^{1}H\}$ (100.6 MHz, DMSO-d_6) NMR spectra of **3f**

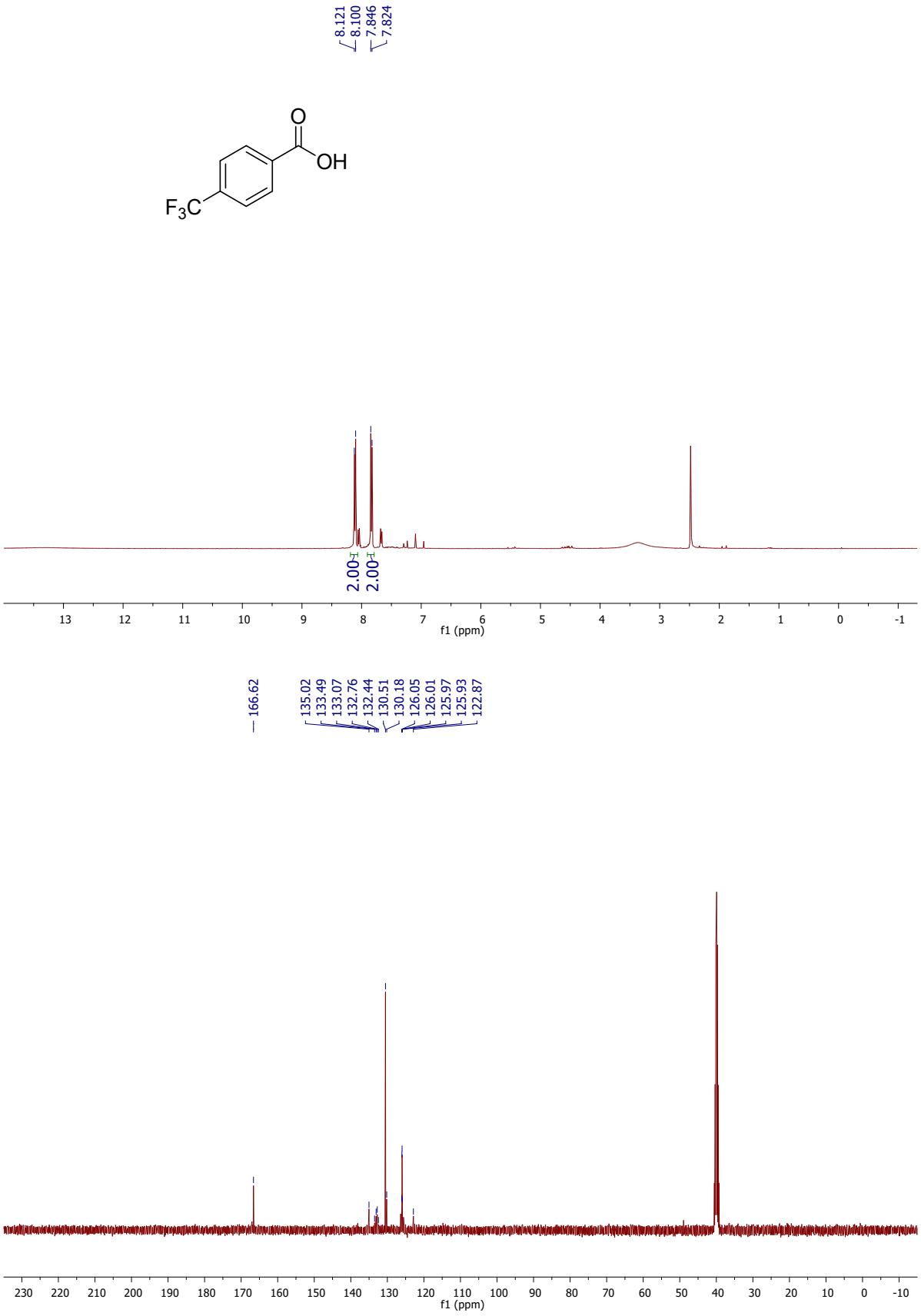

Figure S8. ^{1}H (400 MHz, DMSO-d_6) and $^{13}C\{^{1}H\}$ (100.6 MHz, DMSO-d_6) NMR spectra of **3g**

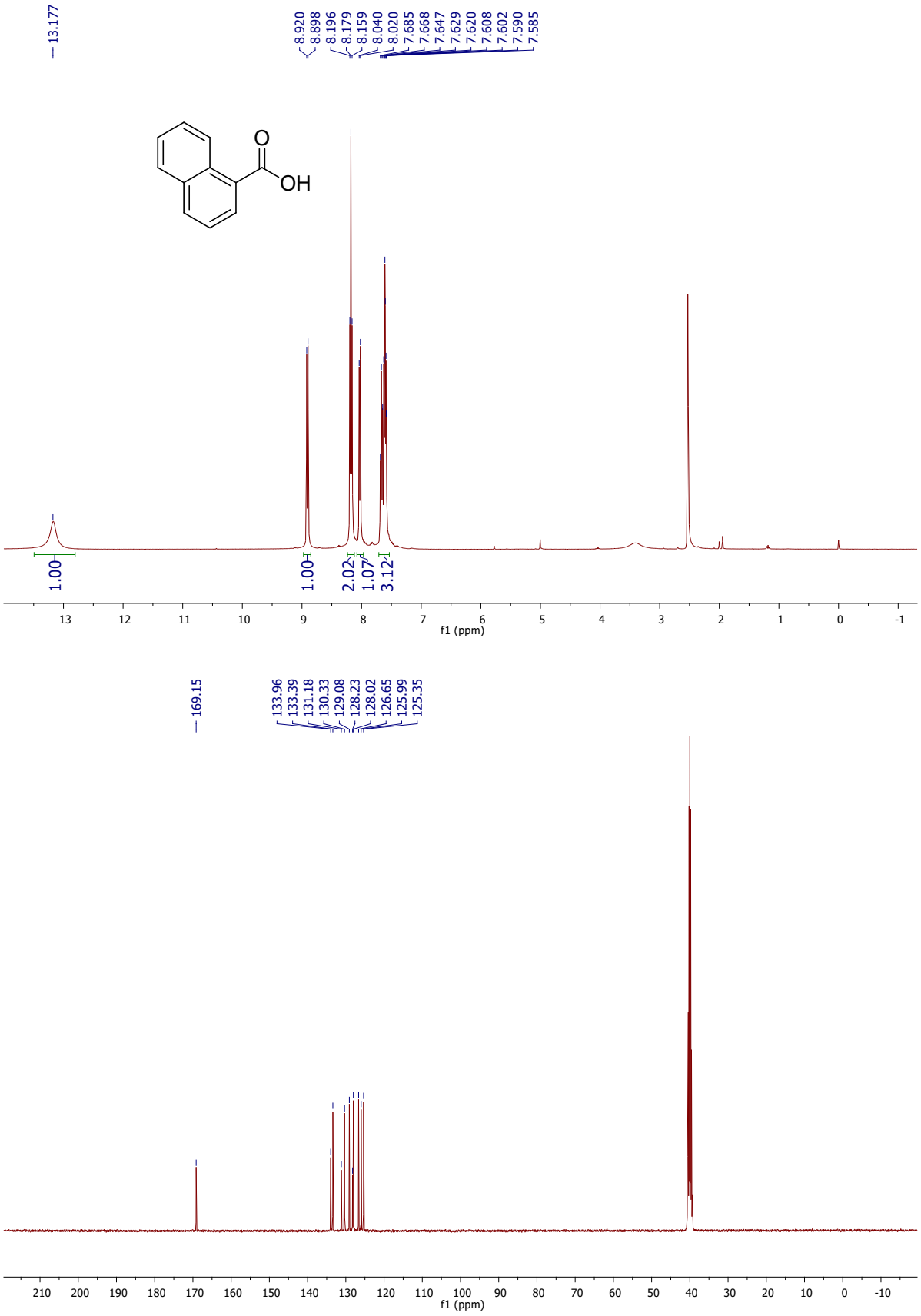

Figure S9. ^{1}H (400 MHz, DMSO-d_6) and $^{13}C\{^{1}H\}$ (100.6 MHz, DMSO-d_6) NMR spectra of **3h**

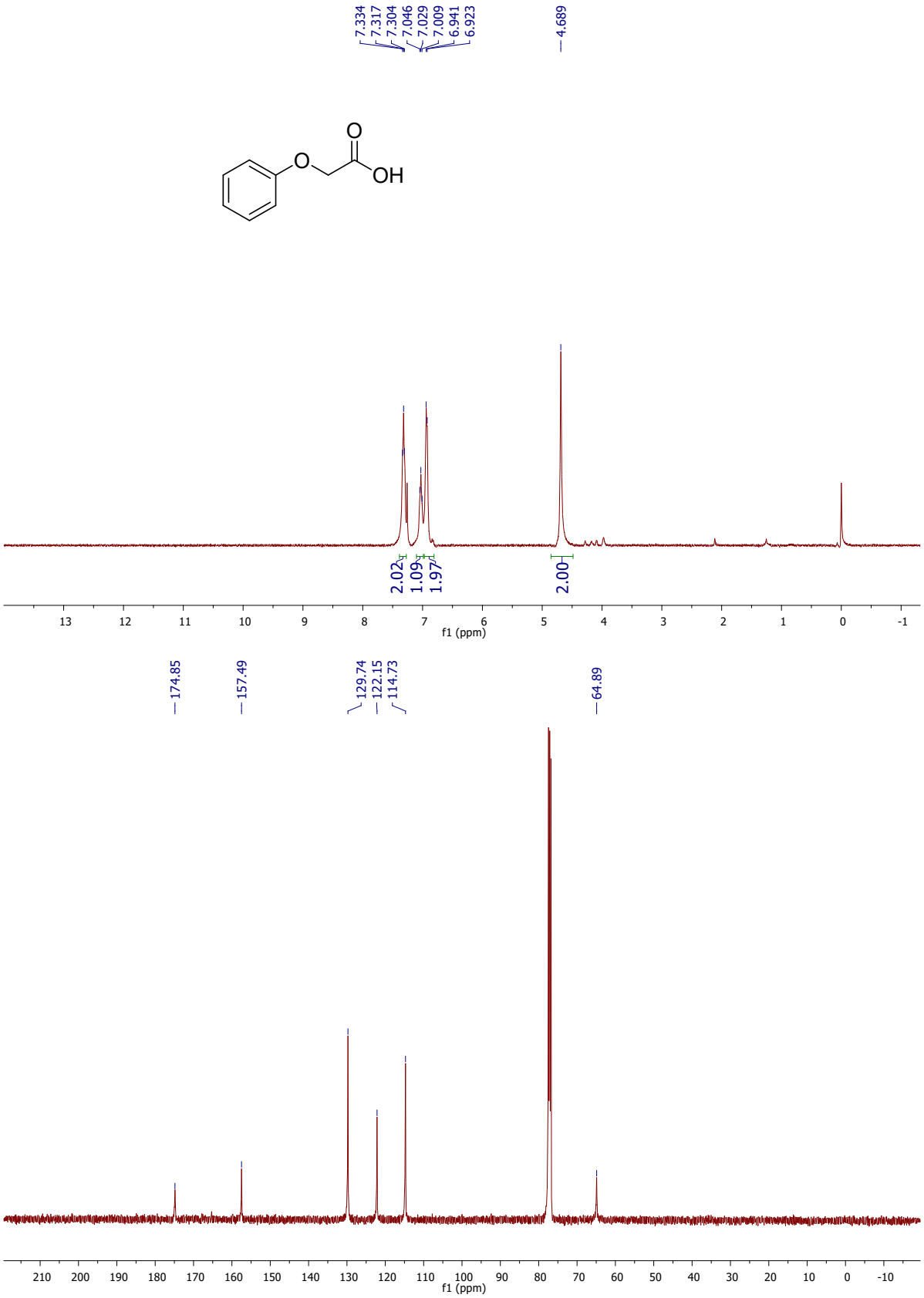

Figure S10. ^{1}H (400 MHz, $CDCl_3$) and $^{13}C\{^{1}H\}$ (100.6 MHz, $CDCl_3$) NMR spectra of **3i**

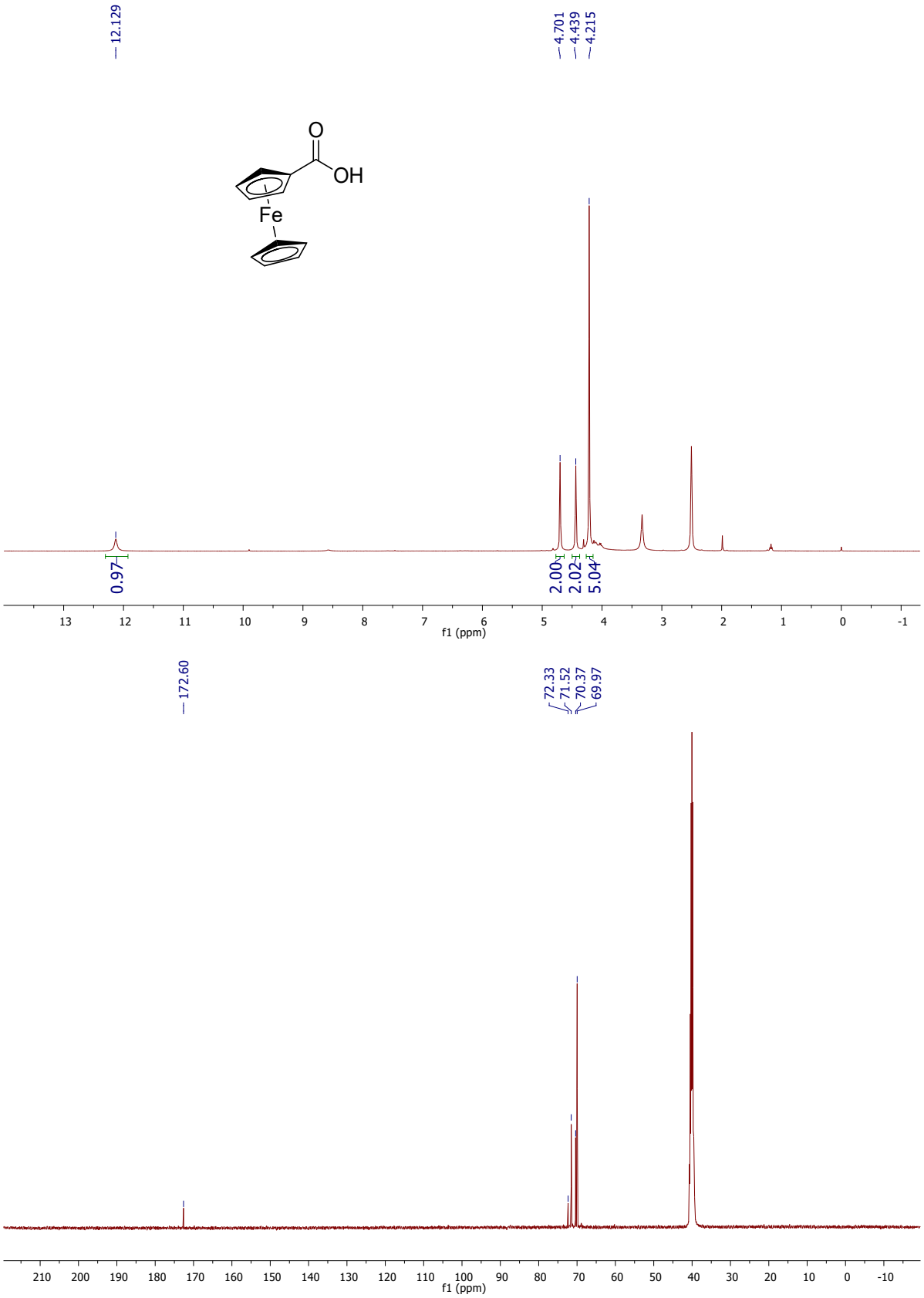

Figure S11. ^{1}H (400 MHz, DMSO-d_6) and $^{13}C\{^{1}H\}$ (100.6 MHz, DMSO-d_6) NMR spectra of **3j**

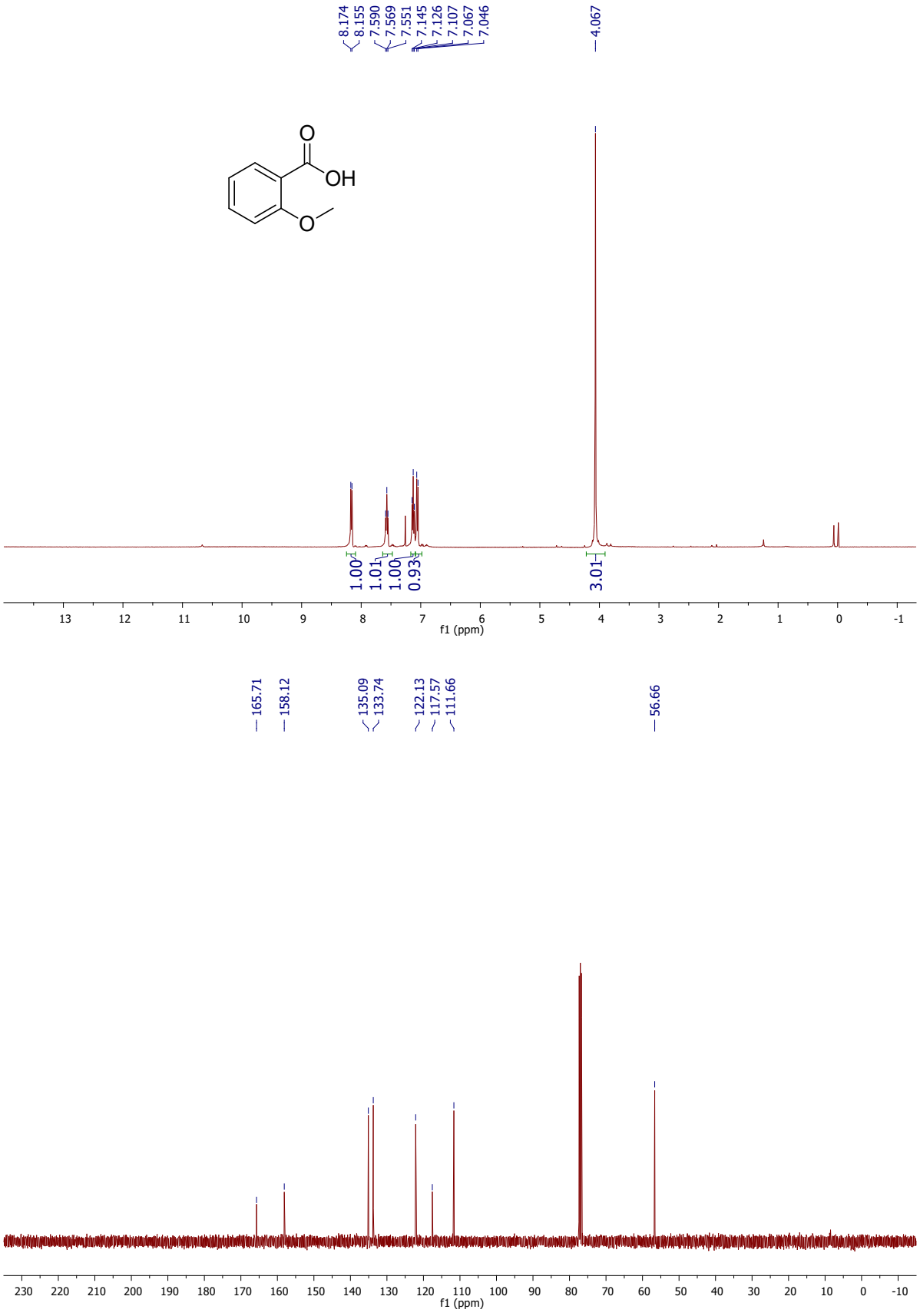

Figure S12. ^{1}H (400 MHz, $CDCl_3$) and $^{13}C\{^{1}H\}$ (100.6 MHz, $CDCl_3$) NMR spectra of **3k**

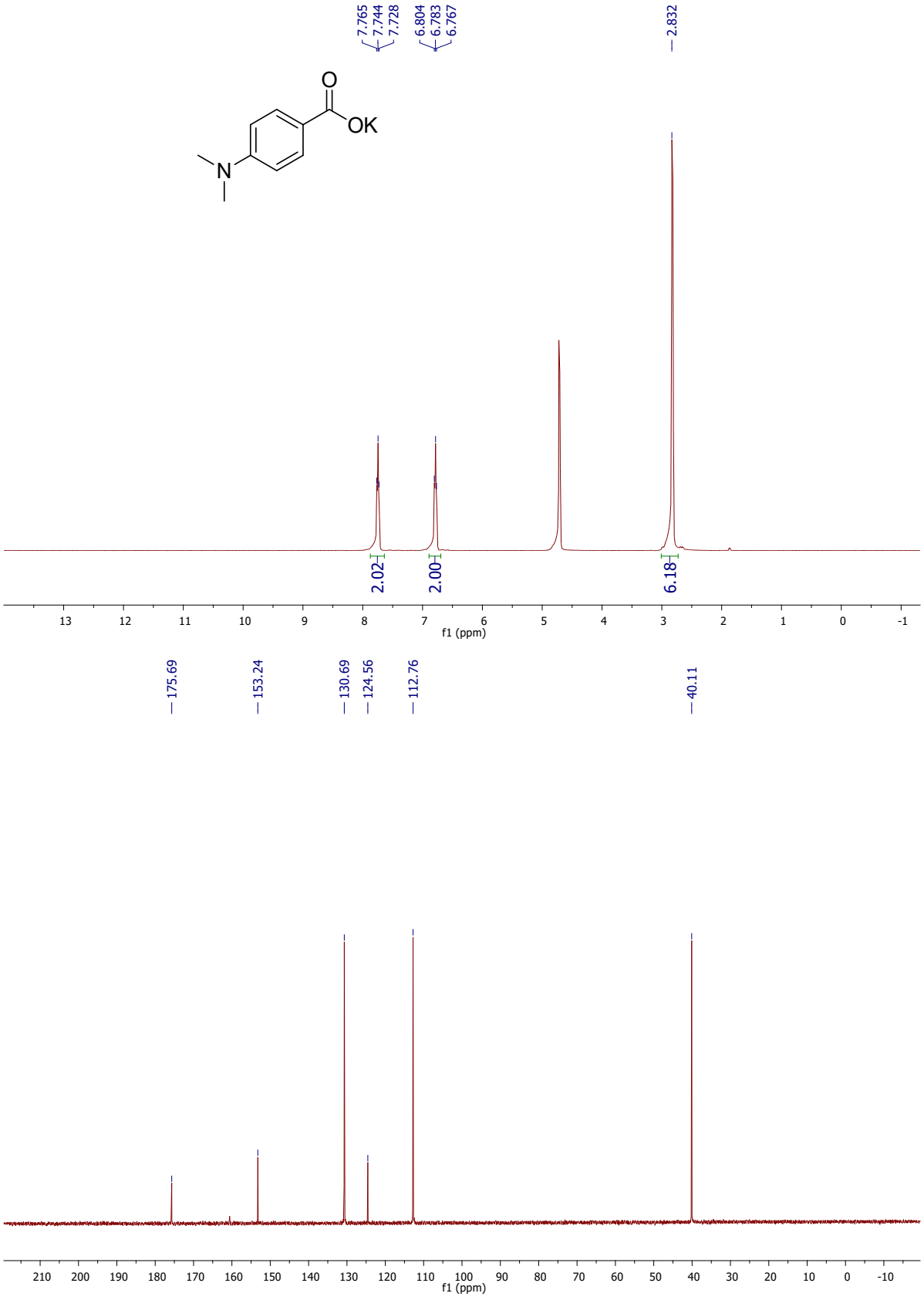

Figure S13. ^{1}H (400 MHz, D_2O) and $^{13}C\{^{1}H\}$ (100.6 MHz, D_2O) NMR spectra of **3l**

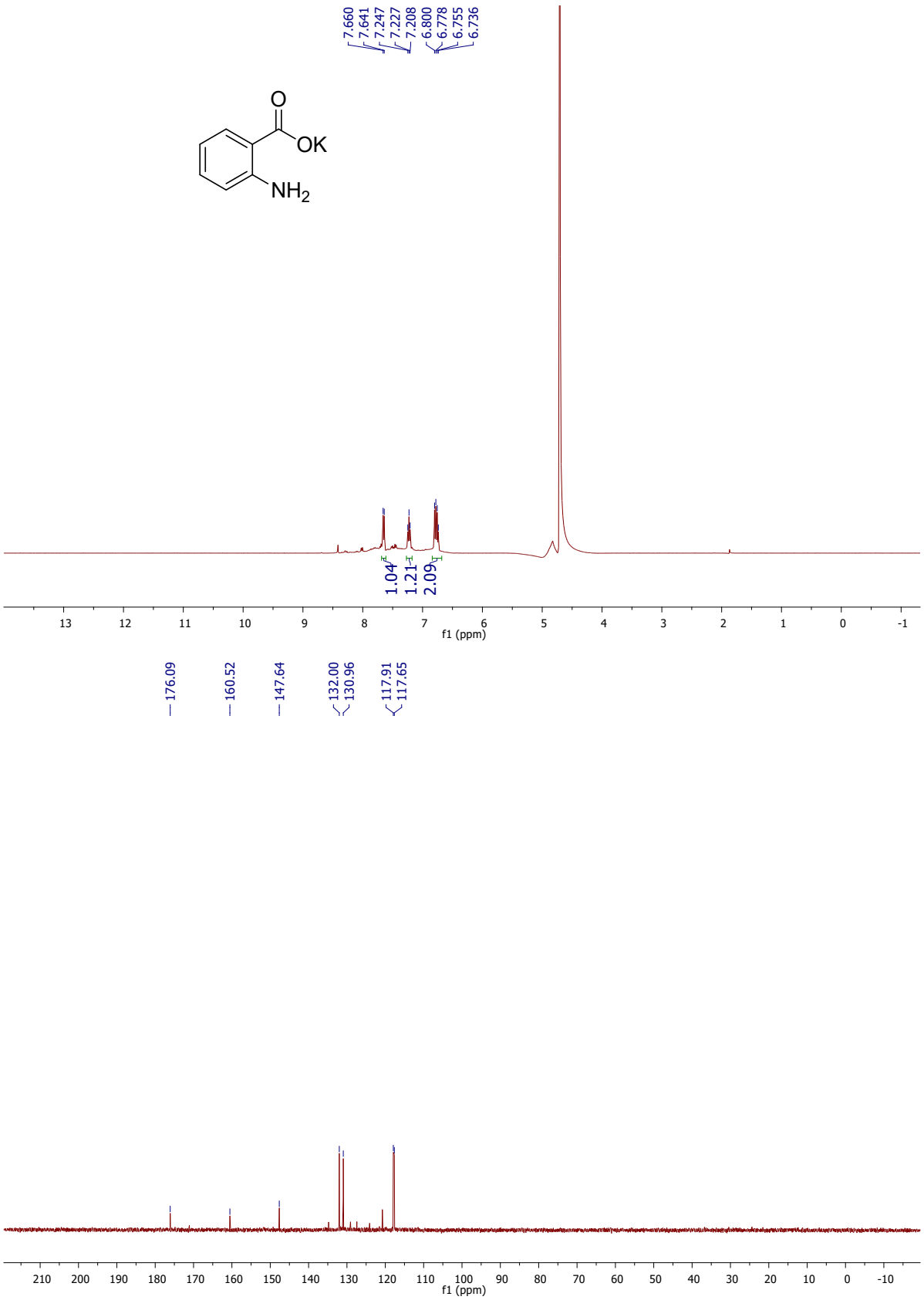

Figure S14. ^{1}H (400 MHz, D_2O) and $^{13}C\{^{1}H\}$ (100.6 MHz, D_2O) NMR spectra of **3m**

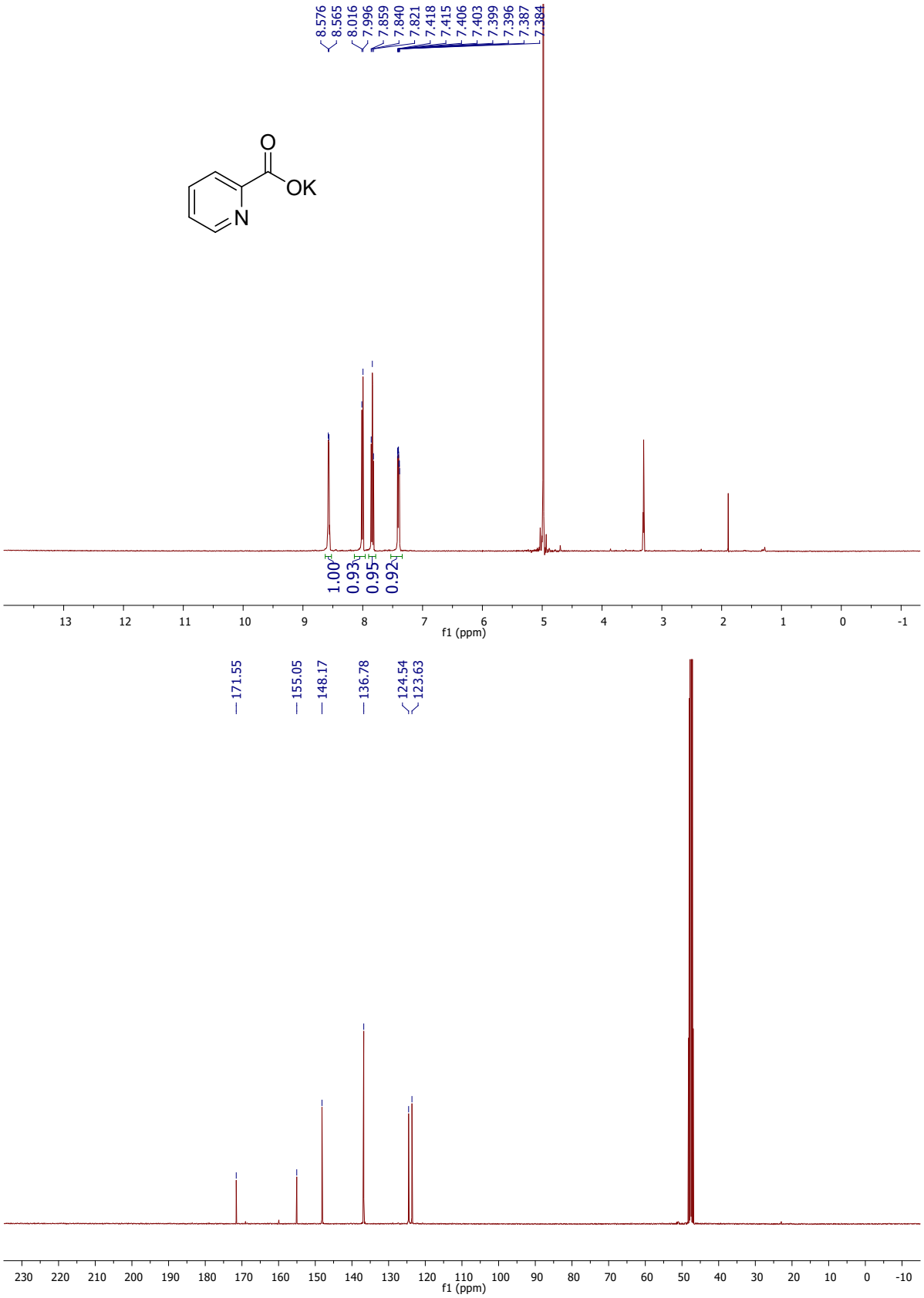

Figure S15. ^{1}H (400 MHz, CD_3OD) and $^{13}C\{^{1}H\}$ (100.6 MHz, CD_3OD) NMR spectra of **3n**

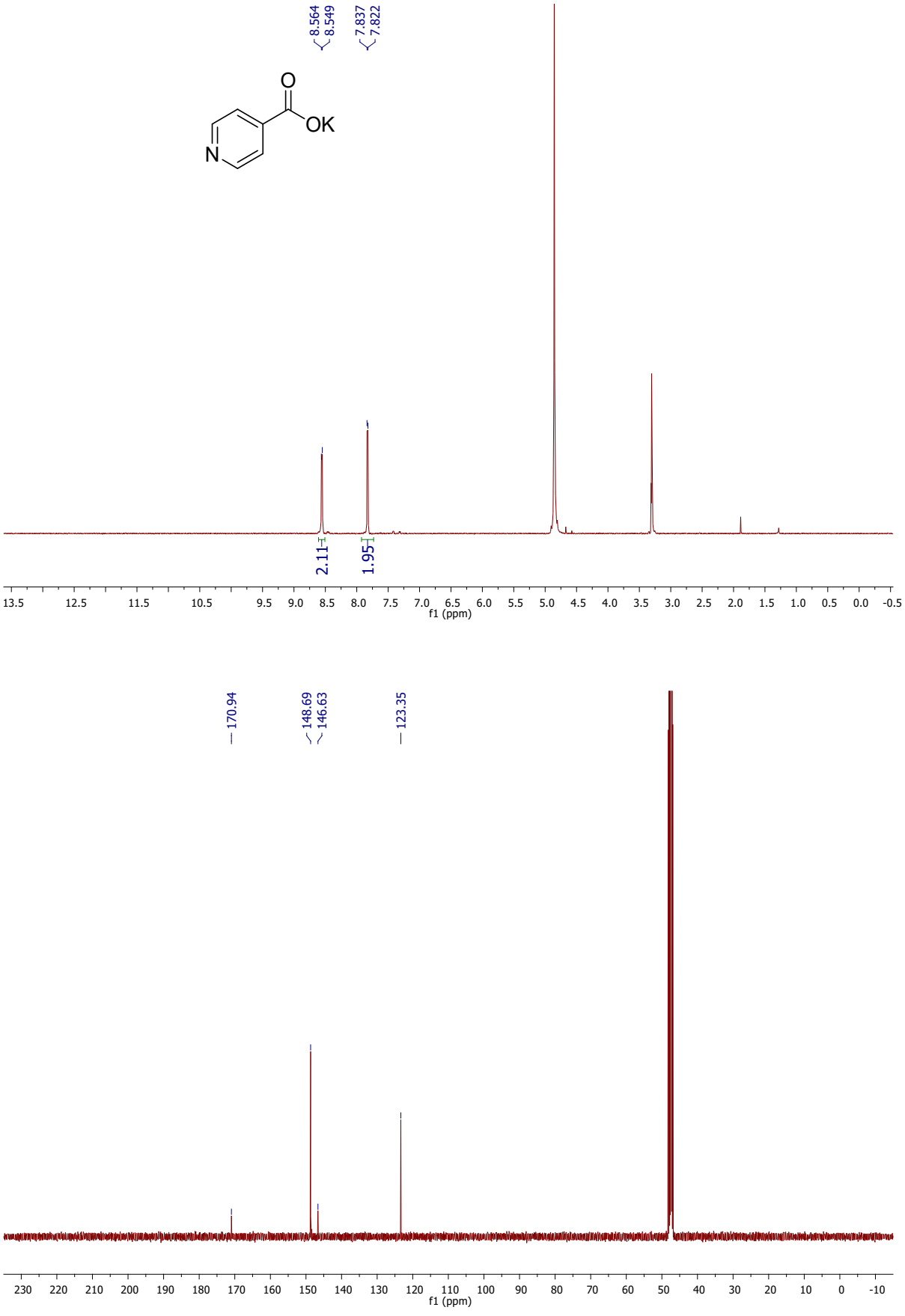

Figure S16. ^{1}H (400 MHz, CD_3OD) and $^{13}C\{^{1}H\}$ (100.6 MHz, CD_3OD) NMR spectra of **3o**

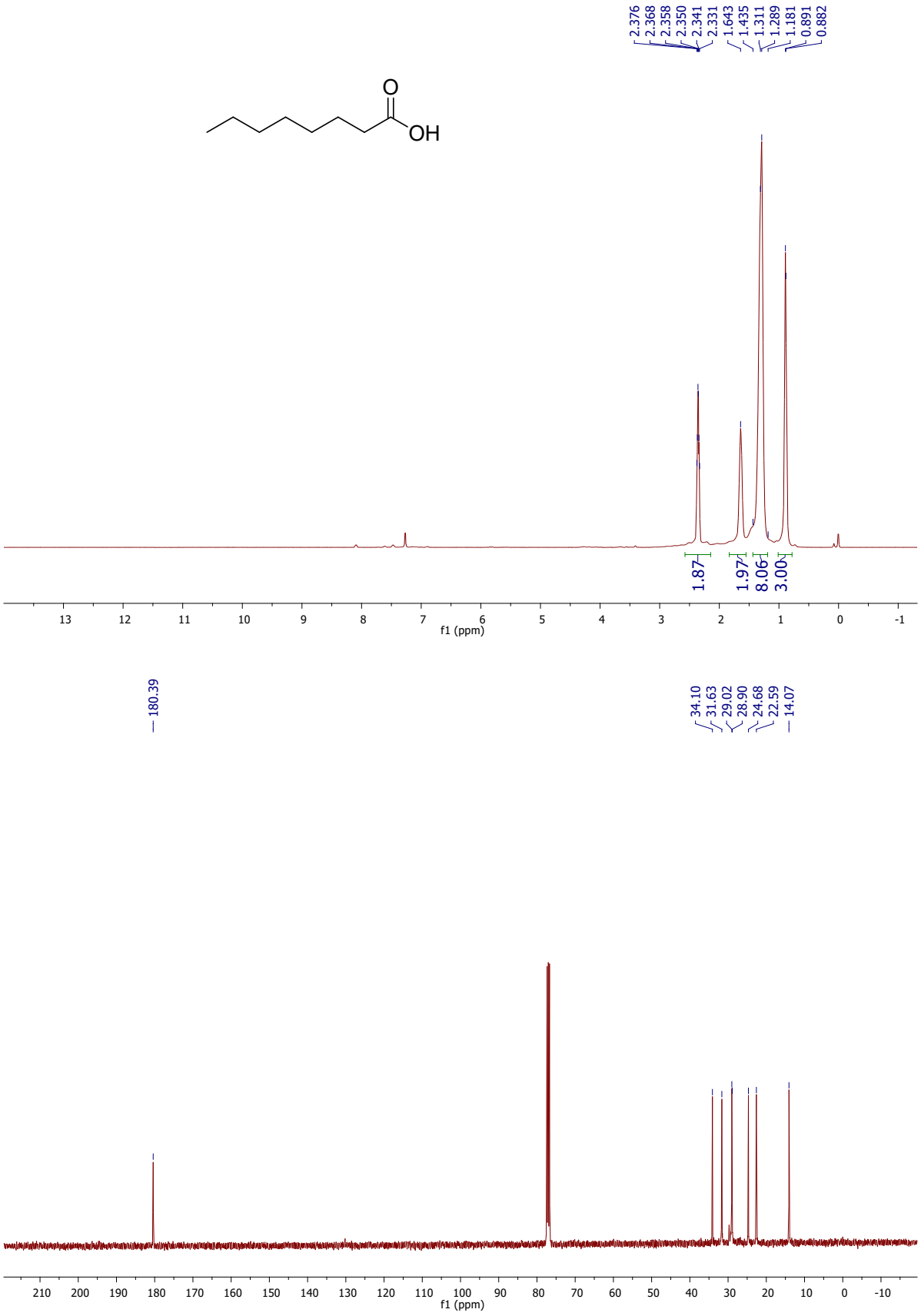

Figure S17. ^{1}H (400 MHz, $CDCl_3$) and $^{13}C\{^{1}H\}$ (100.6 MHz, $CDCl_3$) NMR spectra of **3p**

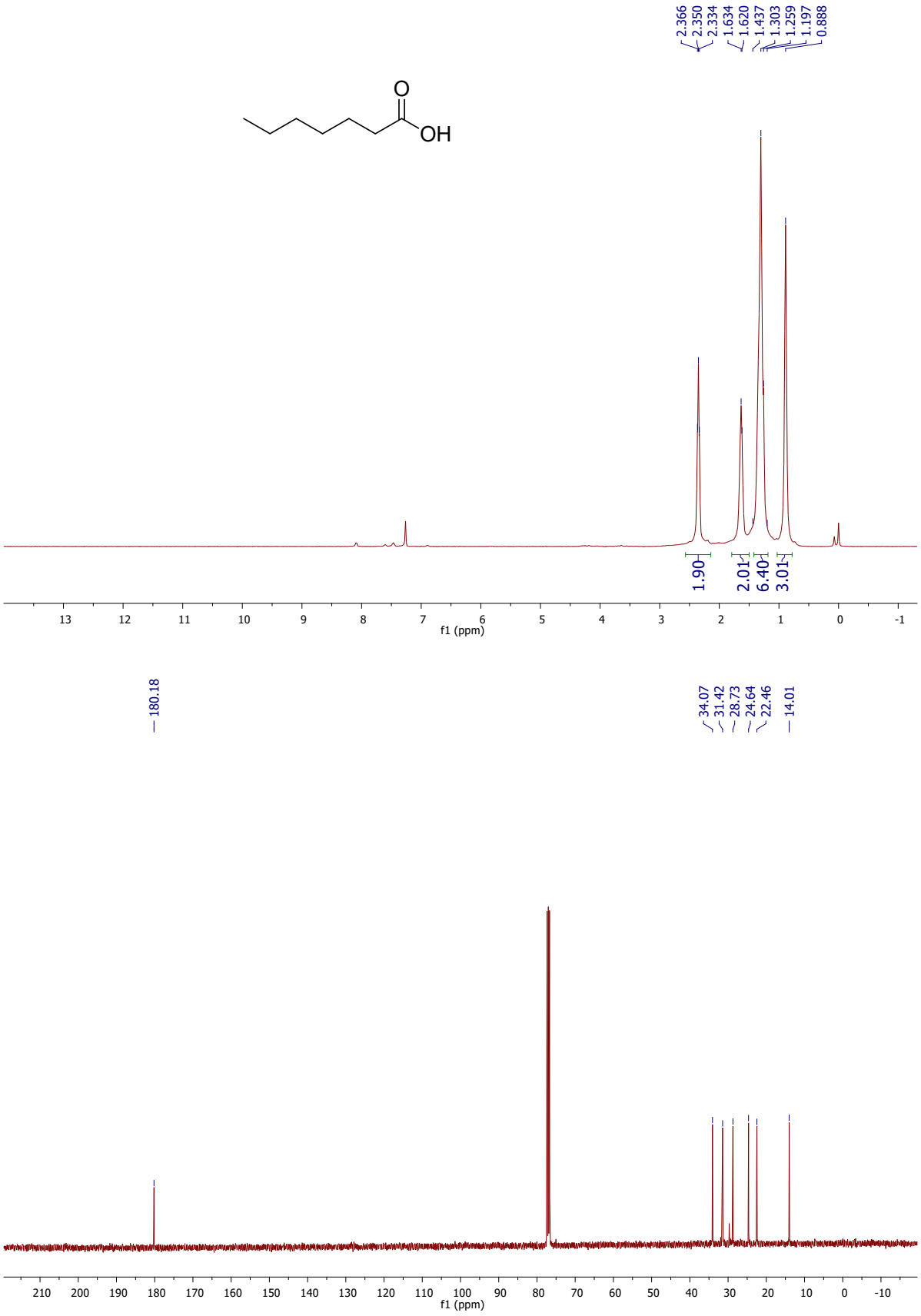

Figure S18. ^{1}H (400 MHz, $CDCl_3$) and $^{13}C\{^{1}H\}$ (100.6 MHz, $CDCl_3$) NMR spectra of **3q**

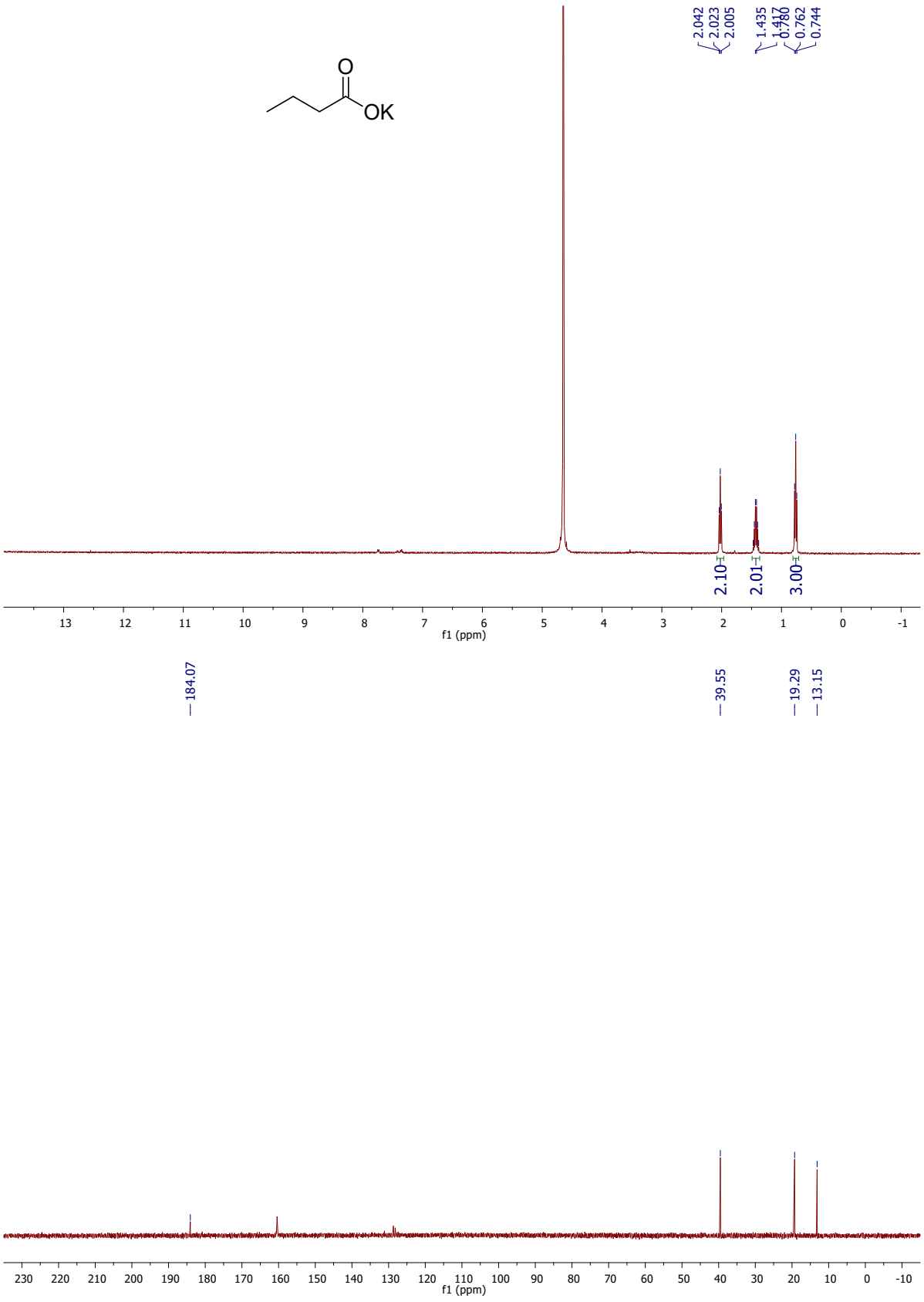

Figure S19. ^{1}H (400 MHz, D_2O) and $^{13}C\{^{1}H\}$ (100.6 MHz, D_2O) NMR spectra of **3r**

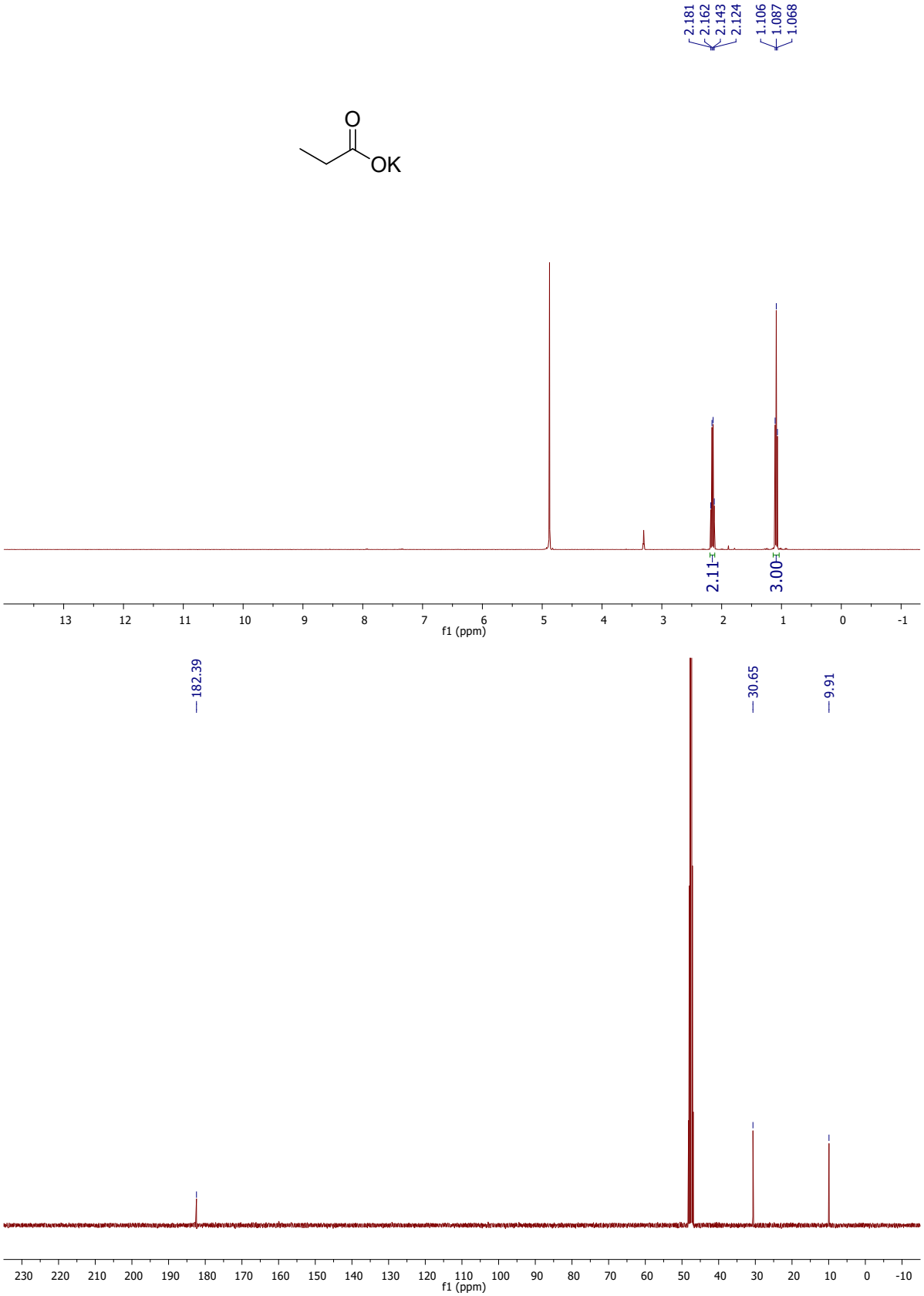

Figure S20. ^{1}H (400 MHz, CD_3OD) and $^{13}C\{^{1}H\}$ (100.6 MHz, CD_3OD) NMR spectra of **3s**

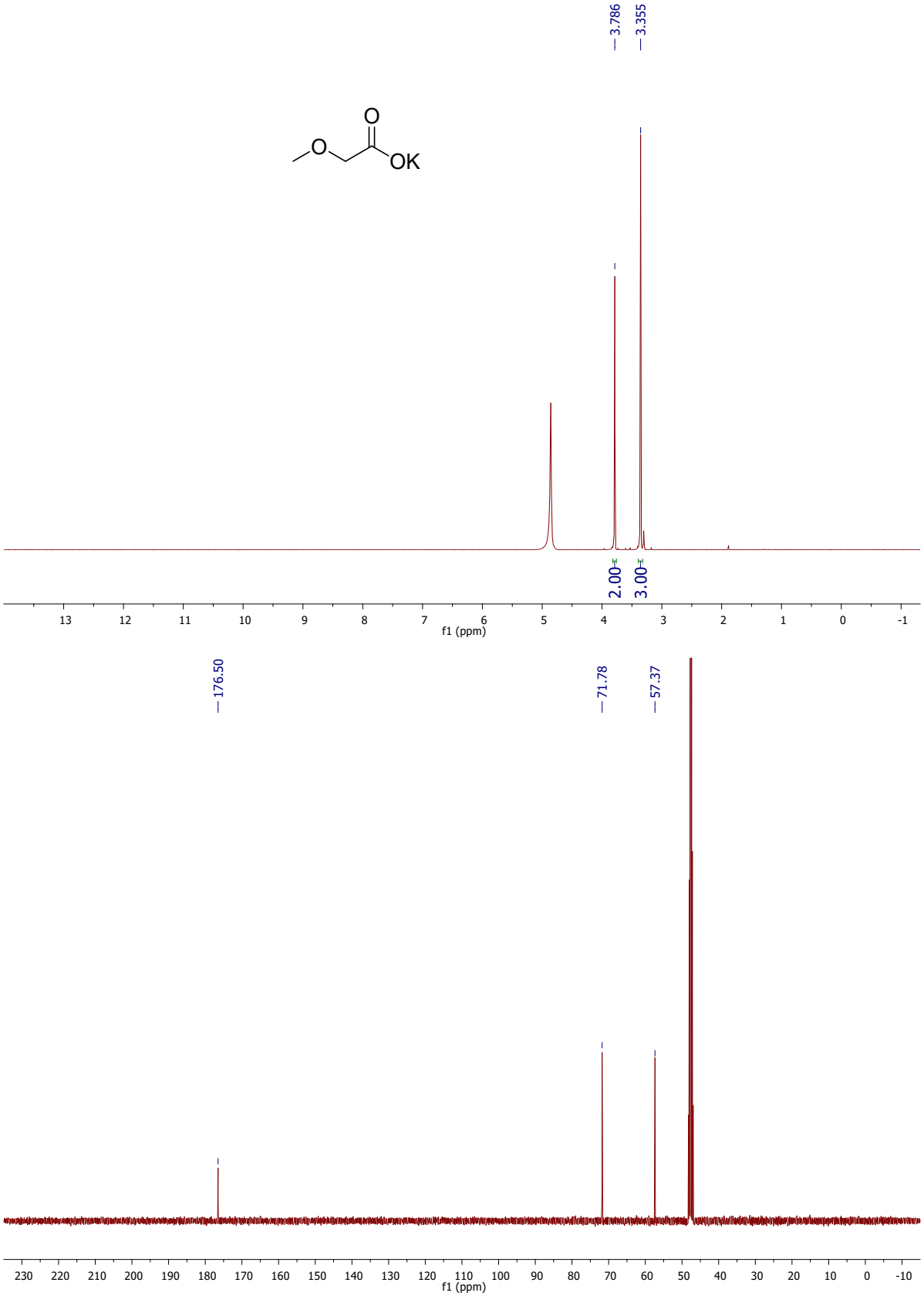

Figure S21. ^{1}H (400 MHz, CD_3OD) and $^{13}C\{^{1}H\}$ (100.6 MHz, CD_3OD) NMR spectra of **3t**

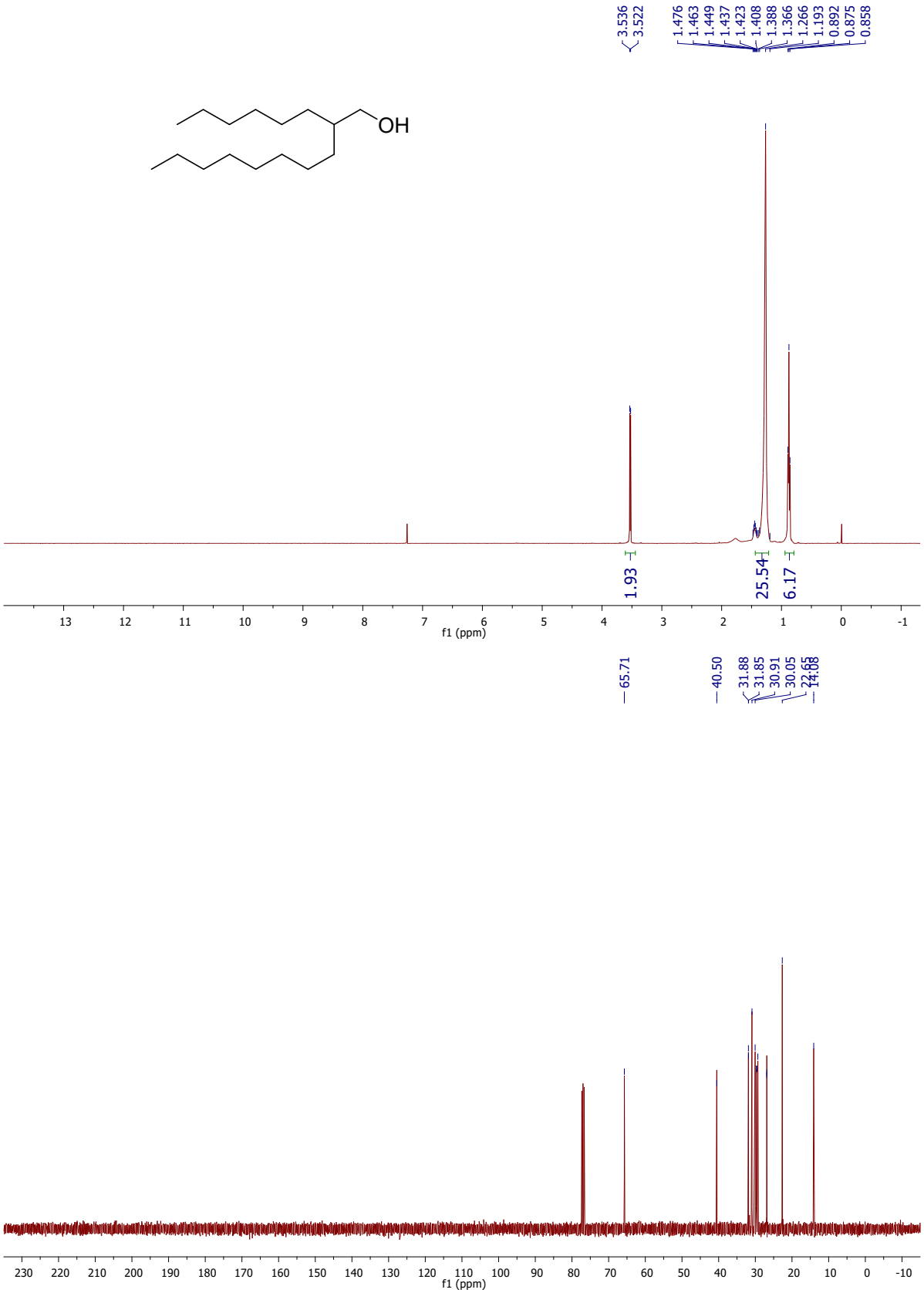

Figure S22. ^{1}H (400 MHz, $CDCl_3$) and $^{13}C\{^{1}H\}$ (100.6 MHz, $CDCl_3$) NMR spectra of **4a**

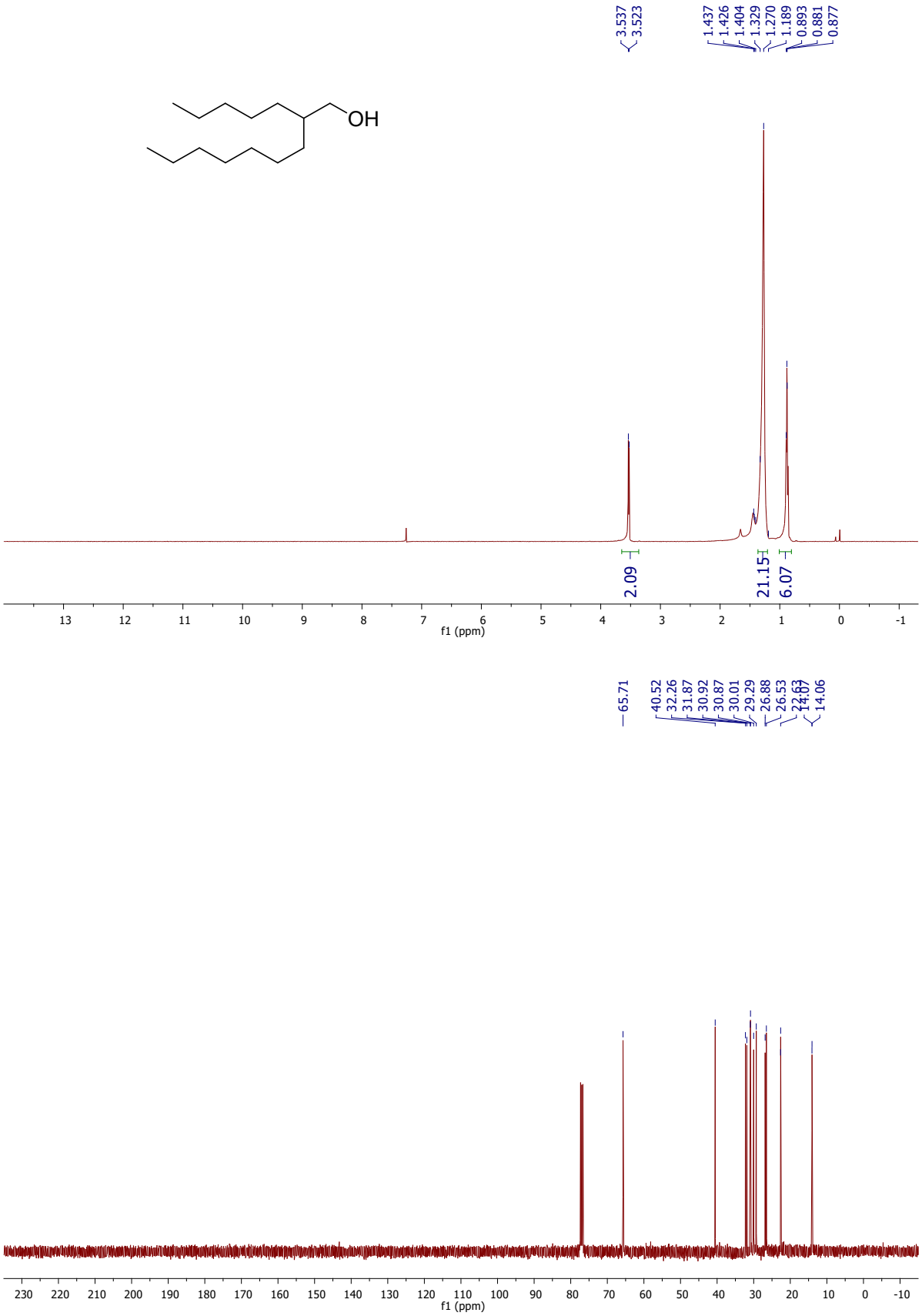

Figure S23. ^{1}H (400 MHz, $CDCl_3$) and $^{13}C\{^{1}H\}$ (100.6 MHz, $CDCl_3$) NMR spectra of **4b**

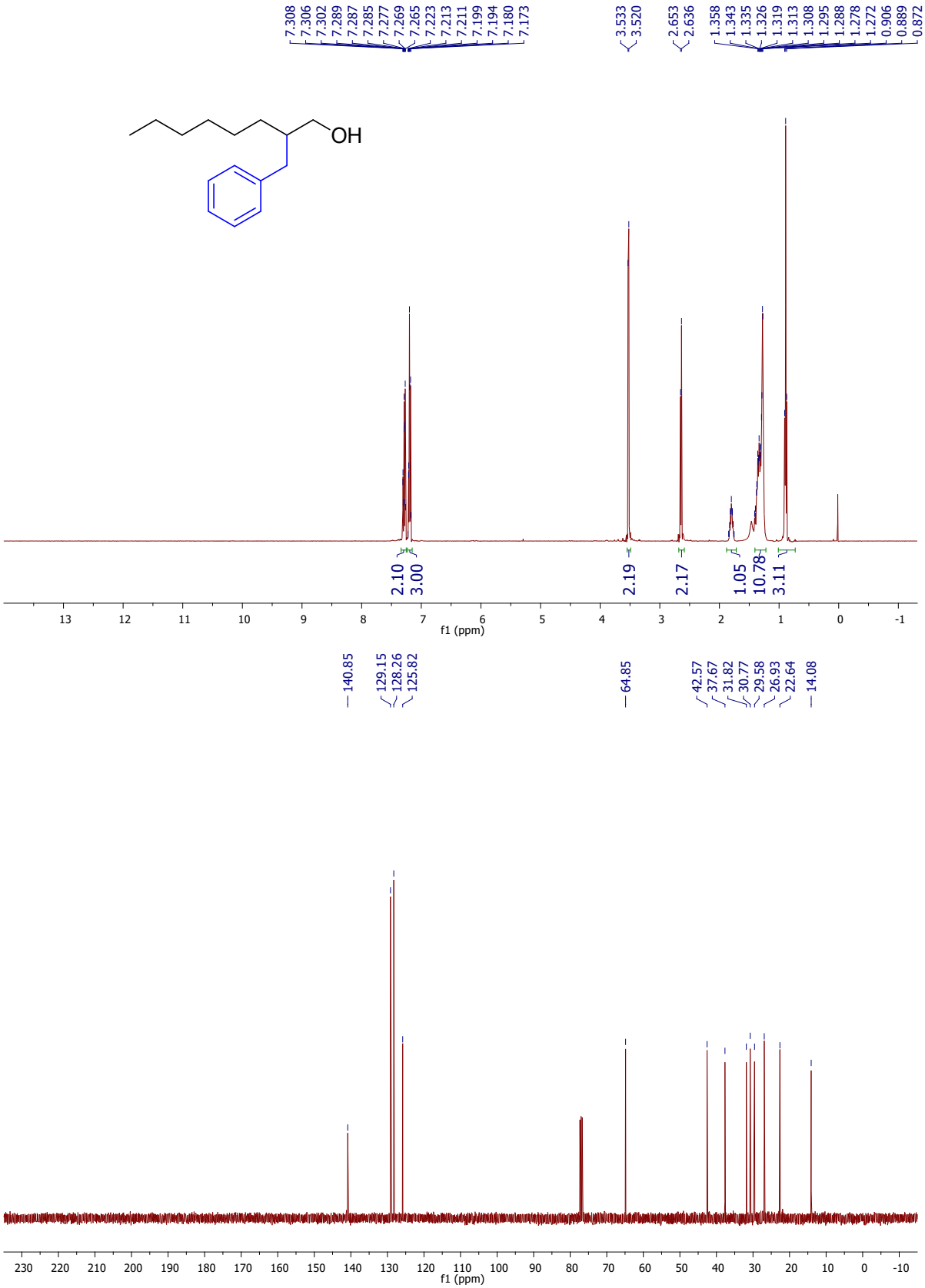

Figure S24. ^{1}H (400 MHz, $CDCl_3$) and $^{13}C\{^{1}H\}$ (100.6 MHz, $CDCl_3$) NMR spectra of **5a**

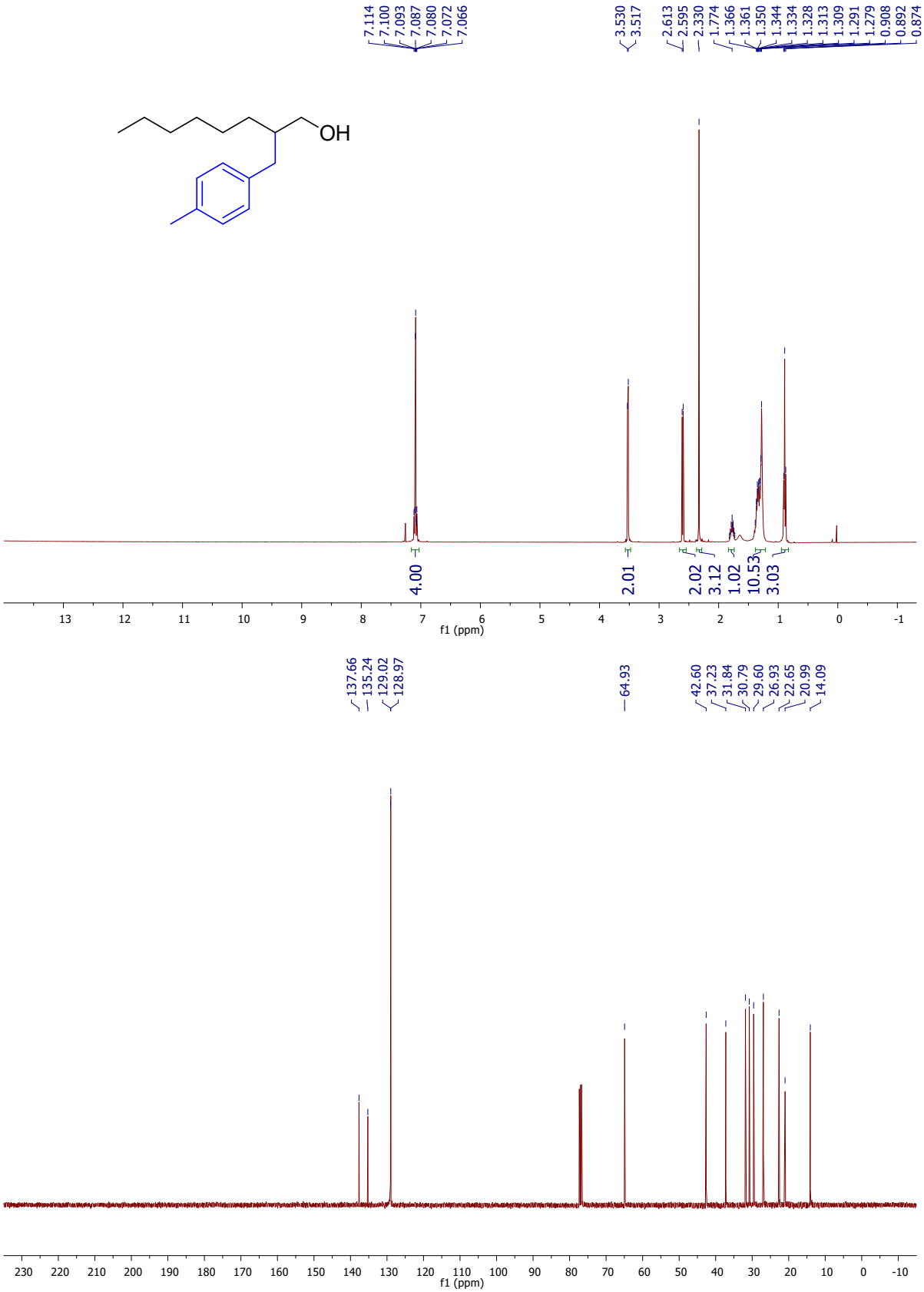

Figure S25. ^{1}H (400 MHz, $CDCl_3$) and $^{13}C\{^{1}H\}$ (100.6 MHz, $CDCl_3$) NMR spectra of **5b**

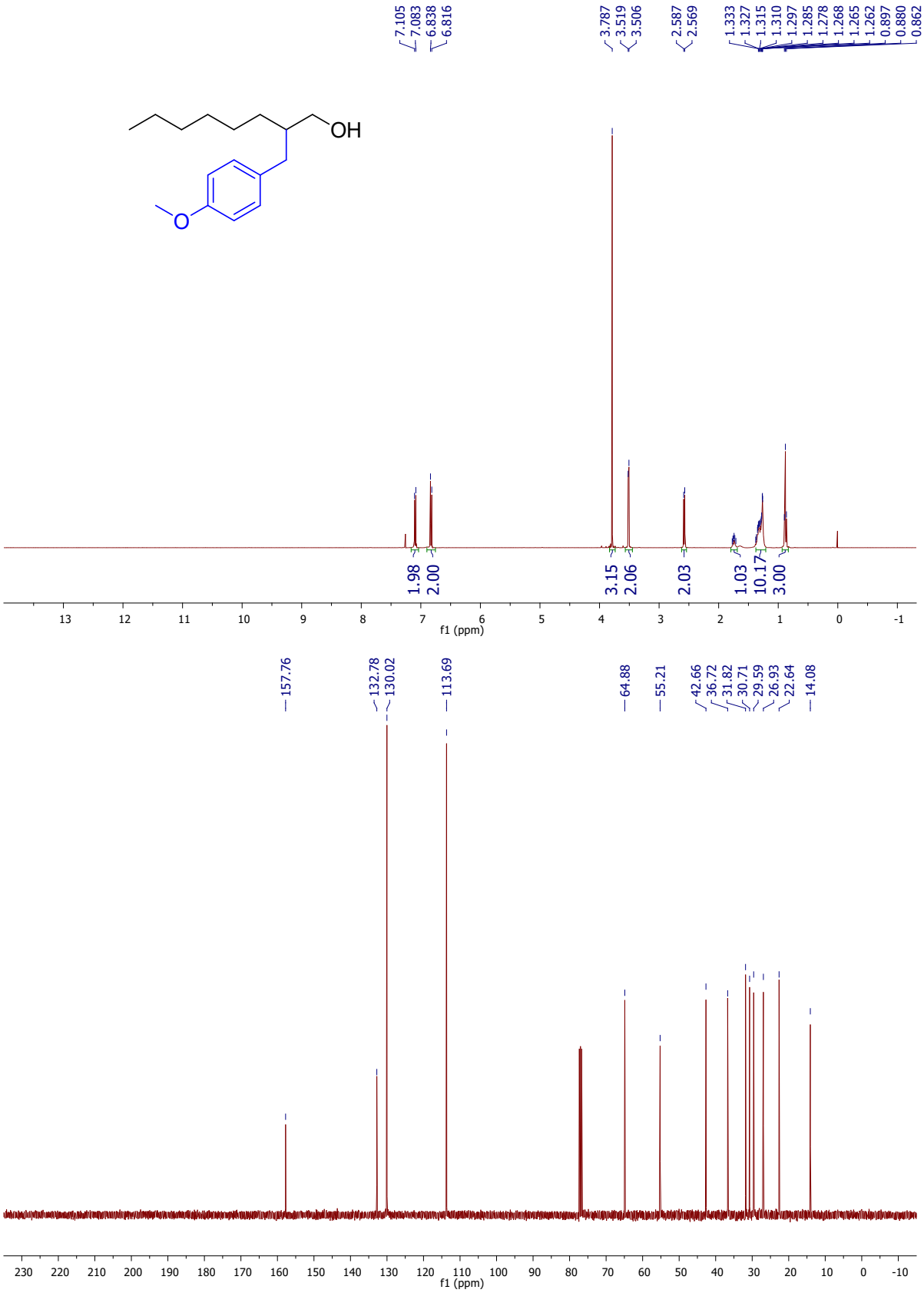

Figure S26. ^{1}H (400 MHz, $CDCl_3$) and $^{13}C\{^{1}H\}$ (100.6 MHz, $CDCl_3$) NMR spectra of **5c**

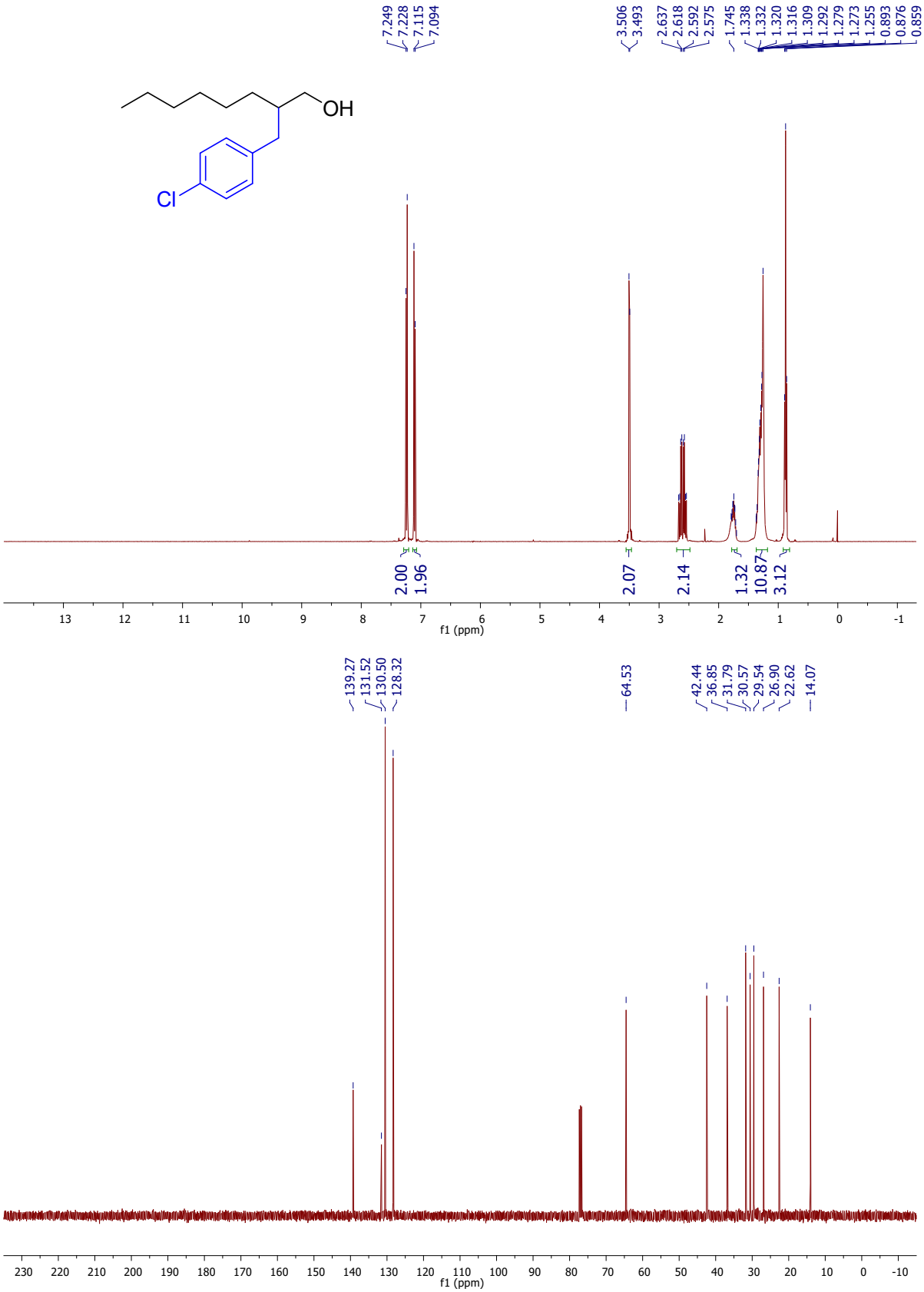

Figure S27. ^{1}H (400 MHz, $CDCl_3$) and $^{13}C\{^{1}H\}$ (100.6 MHz, $CDCl_3$) NMR spectra of **5d**

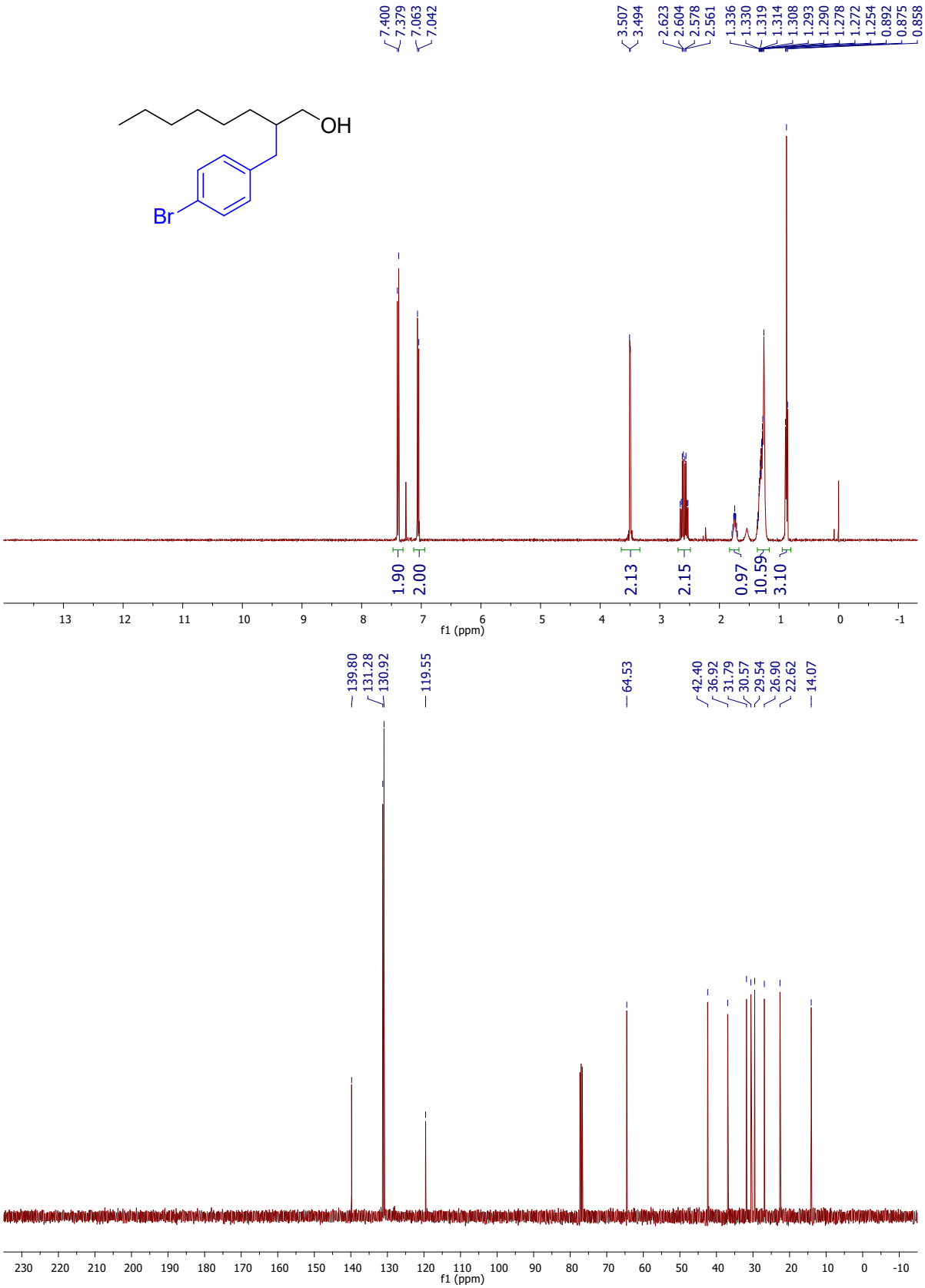

Figure S28. ^{1}H (400 MHz, $CDCl_3$) and $^{13}C\{^{1}H\}$ (100.6 MHz, $CDCl_3$) NMR spectra of **5e**

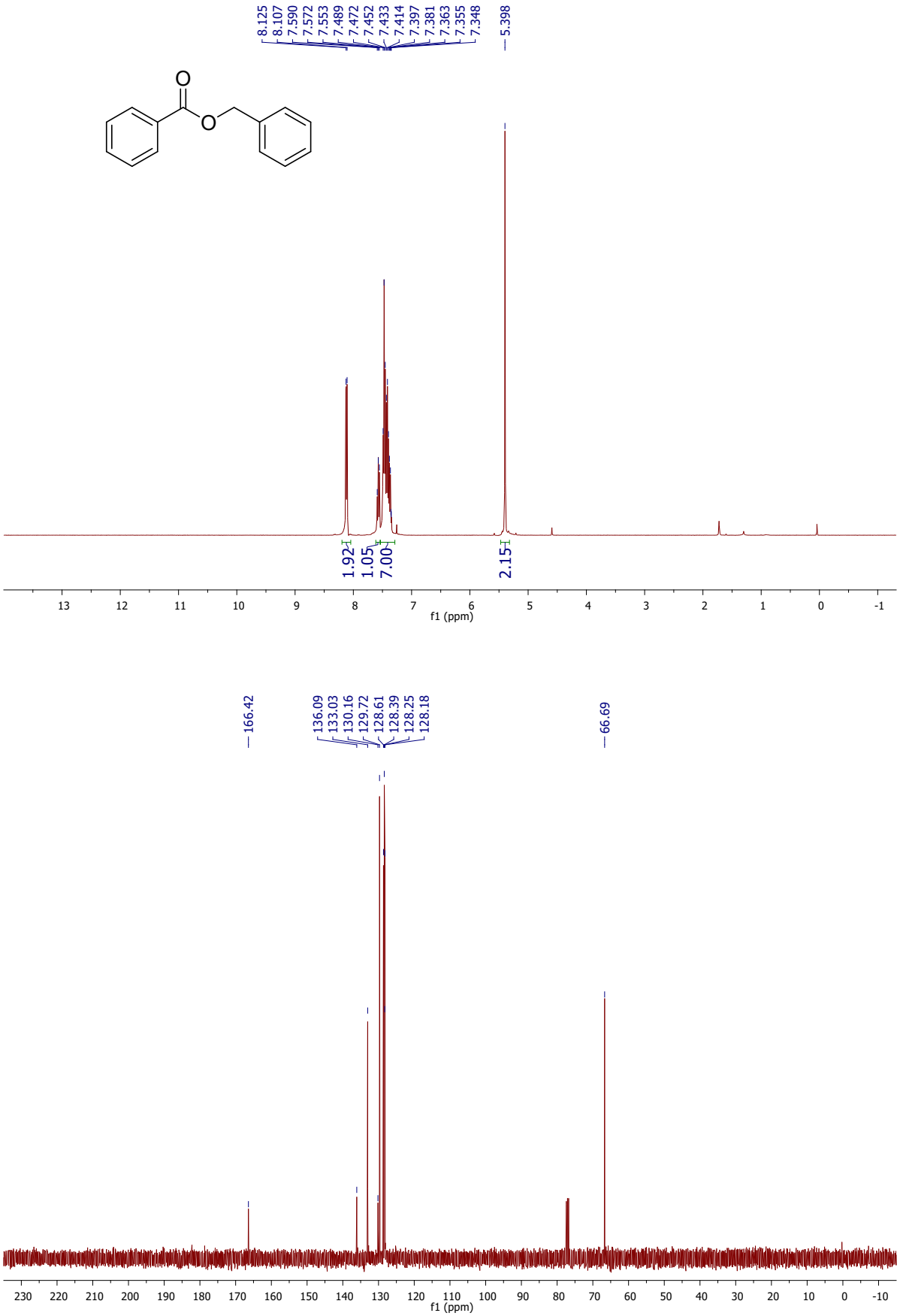

Figure S29. ^{1}H (400 MHz, $CDCl_3$) and $^{13}C\{^{1}H\}$ (100.6 MHz, $CDCl_3$) NMR spectra of **6a**

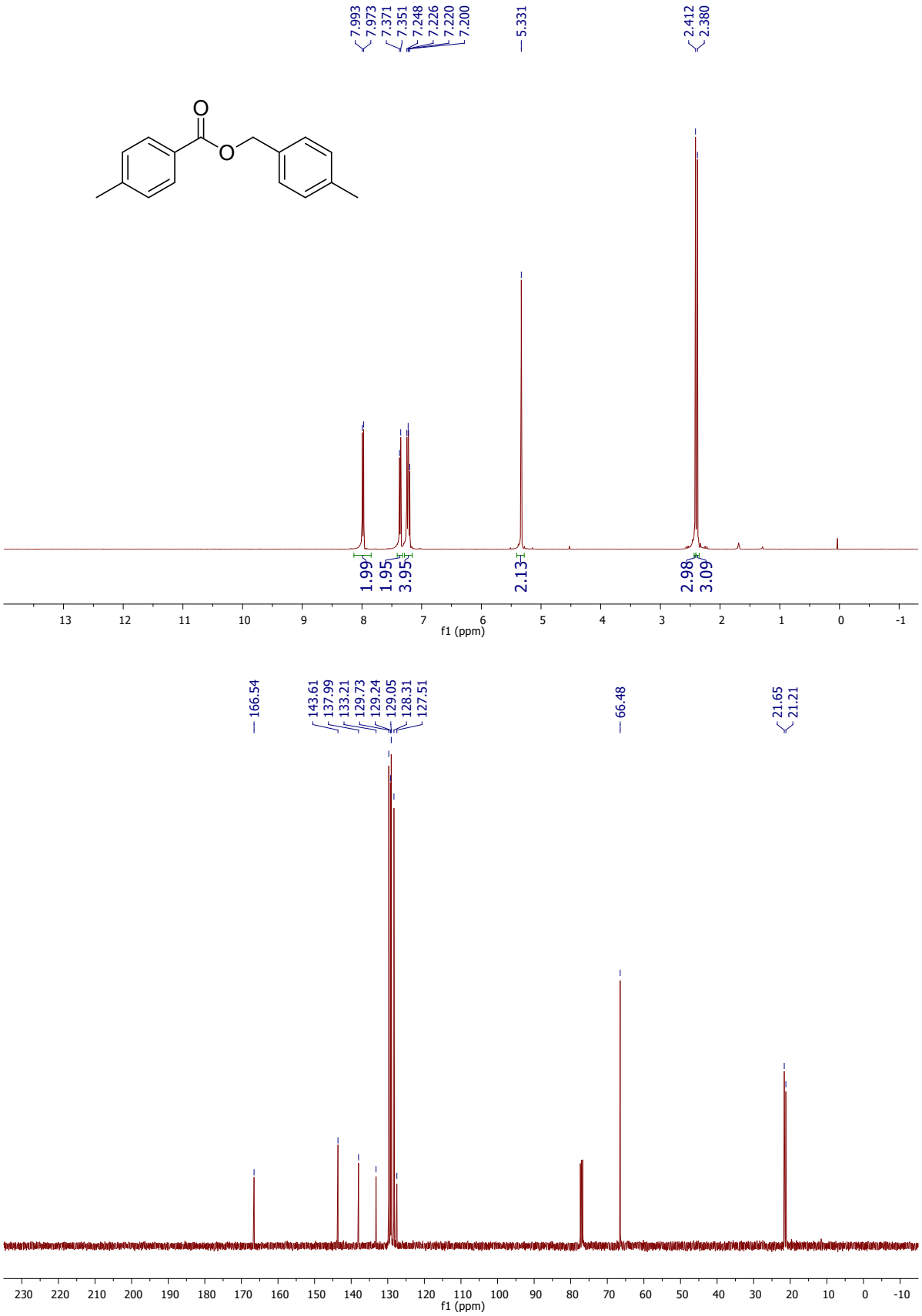

Figure S30. ^{1}H (400 MHz, $CDCl_3$) and $^{13}C\{^{1}H\}$ (100.6 MHz, $CDCl_3$) NMR spectra of **6b**

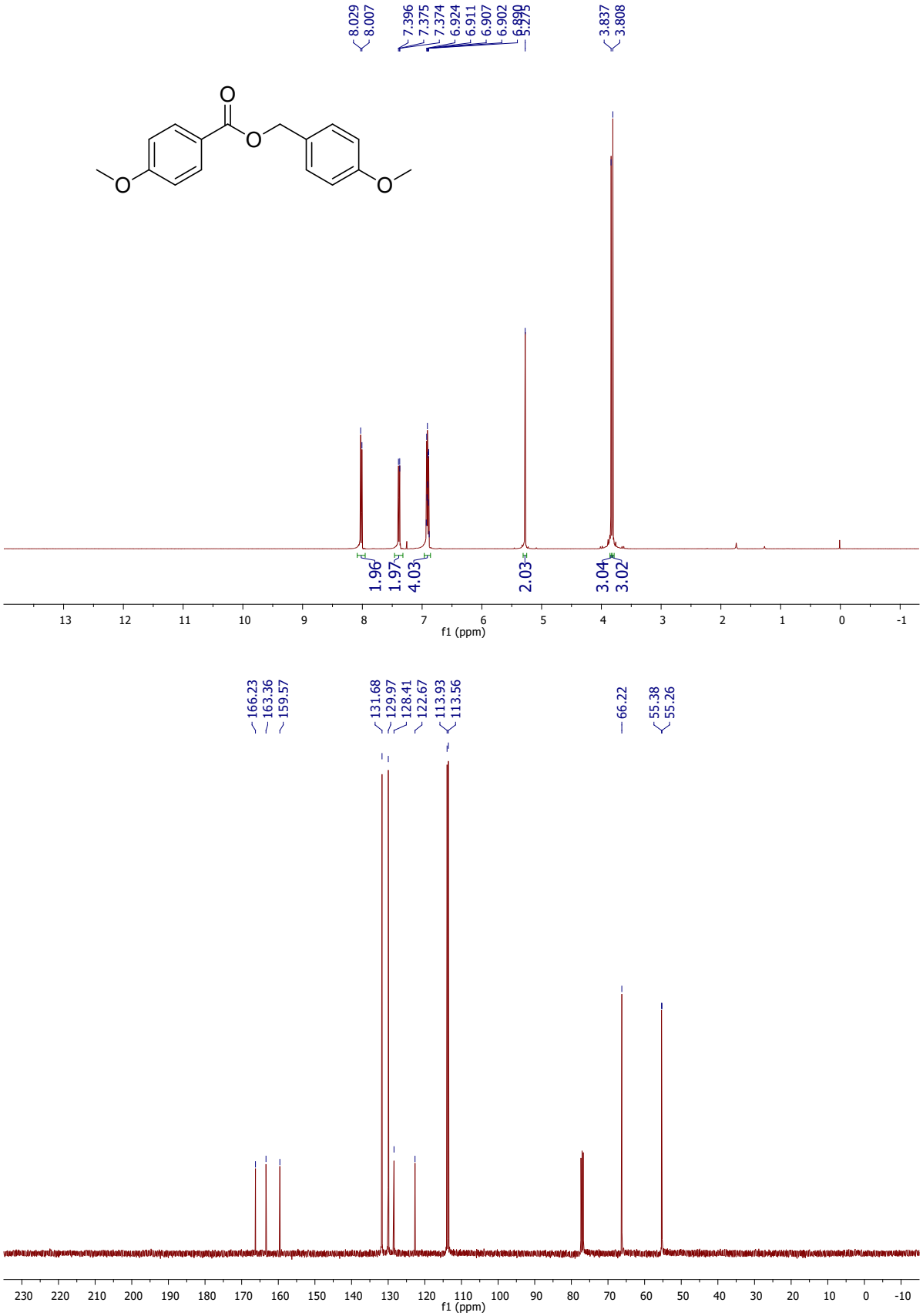

Figure S31. ^{1}H (400 MHz, $CDCl_3$) and $^{13}C\{^{1}H\}$ (100.6 MHz, $CDCl_3$) NMR spectra of **6c**

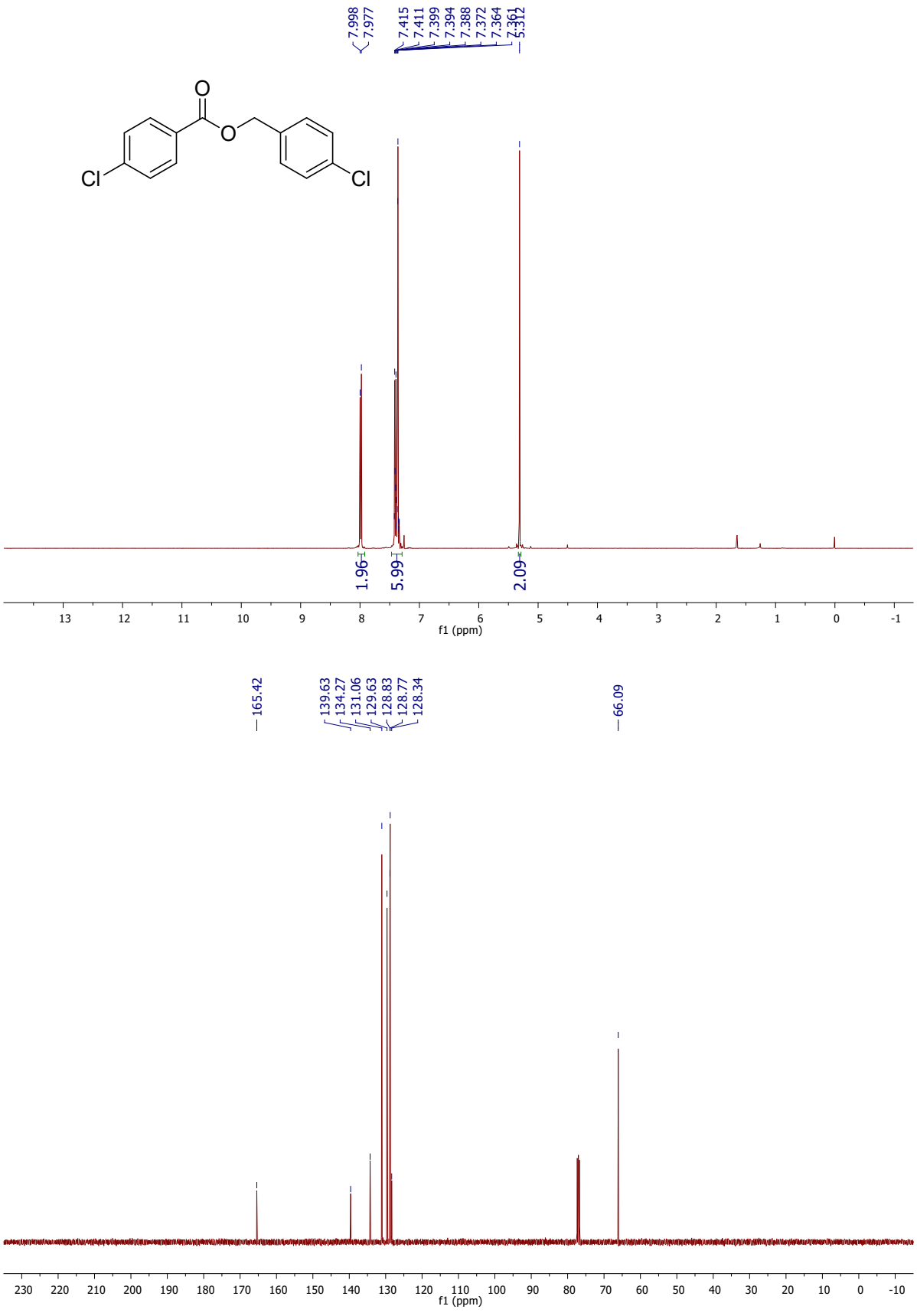

Figure S32. ^{1}H (400 MHz, $CDCl_3$) and $^{13}C\{^{1}H\}$ (100.6 MHz, $CDCl_3$) NMR spectra of **6d**

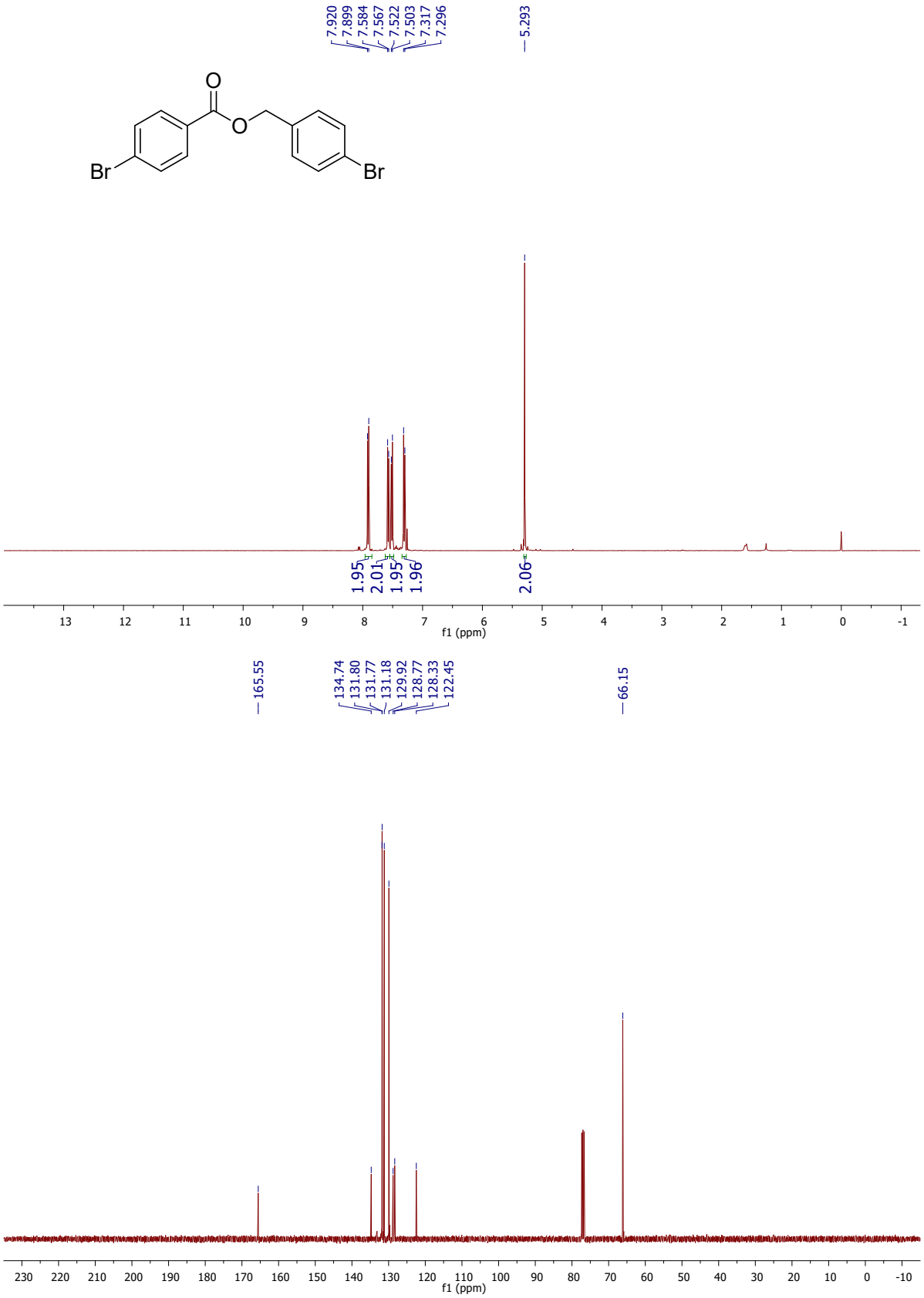

Figure S33. ^{1}H (400 MHz, $CDCl_3$) and $^{13}C\{^{1}H\}$ (100.6 MHz, $CDCl_3$) NMR spectra of **6e**

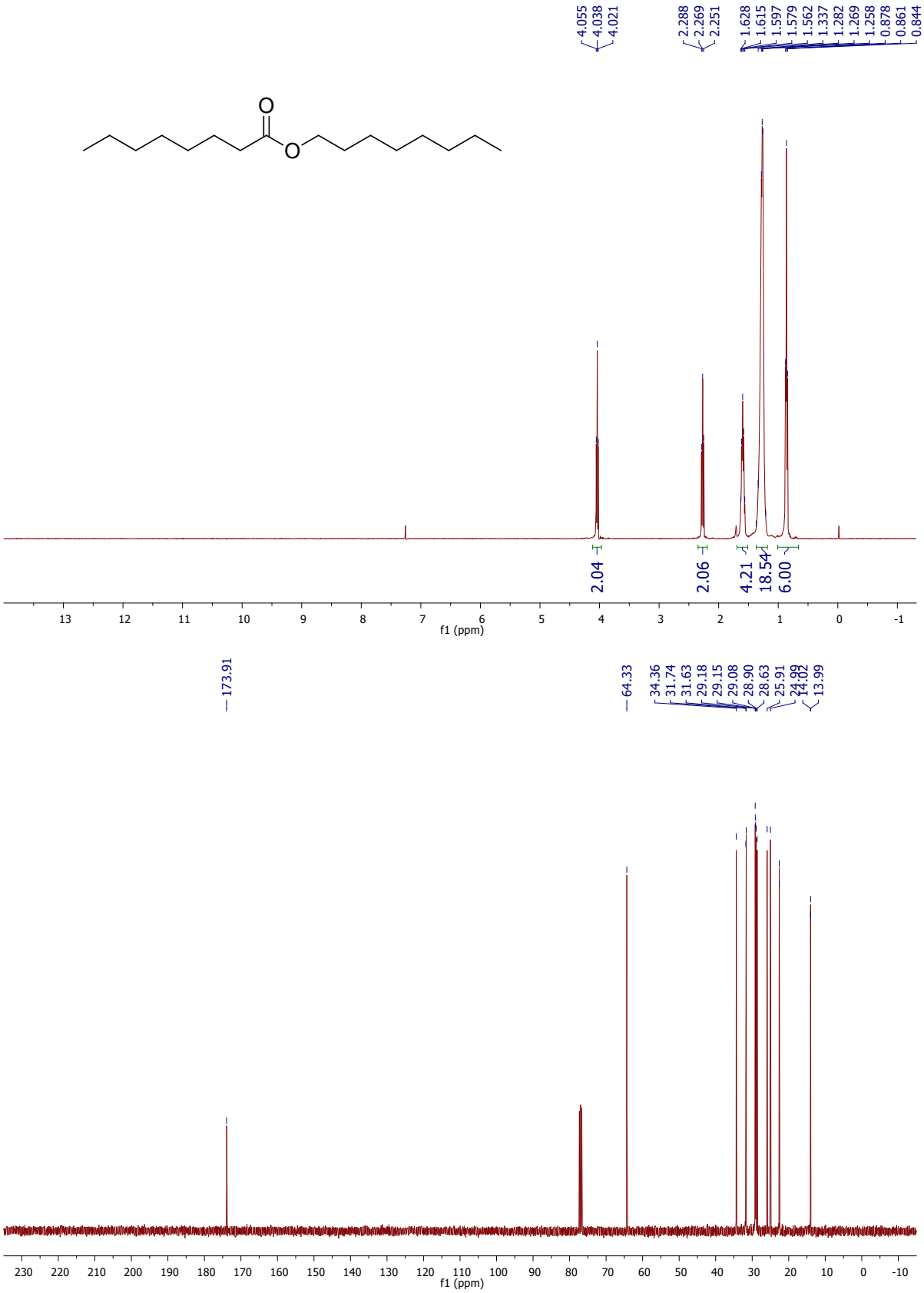

Figure S34. ^{1}H (400 MHz, $CDCl_3$) and $^{13}C\{^{1}H\}$ (100.6 MHz, $CDCl_3$) NMR spectra of **6f**

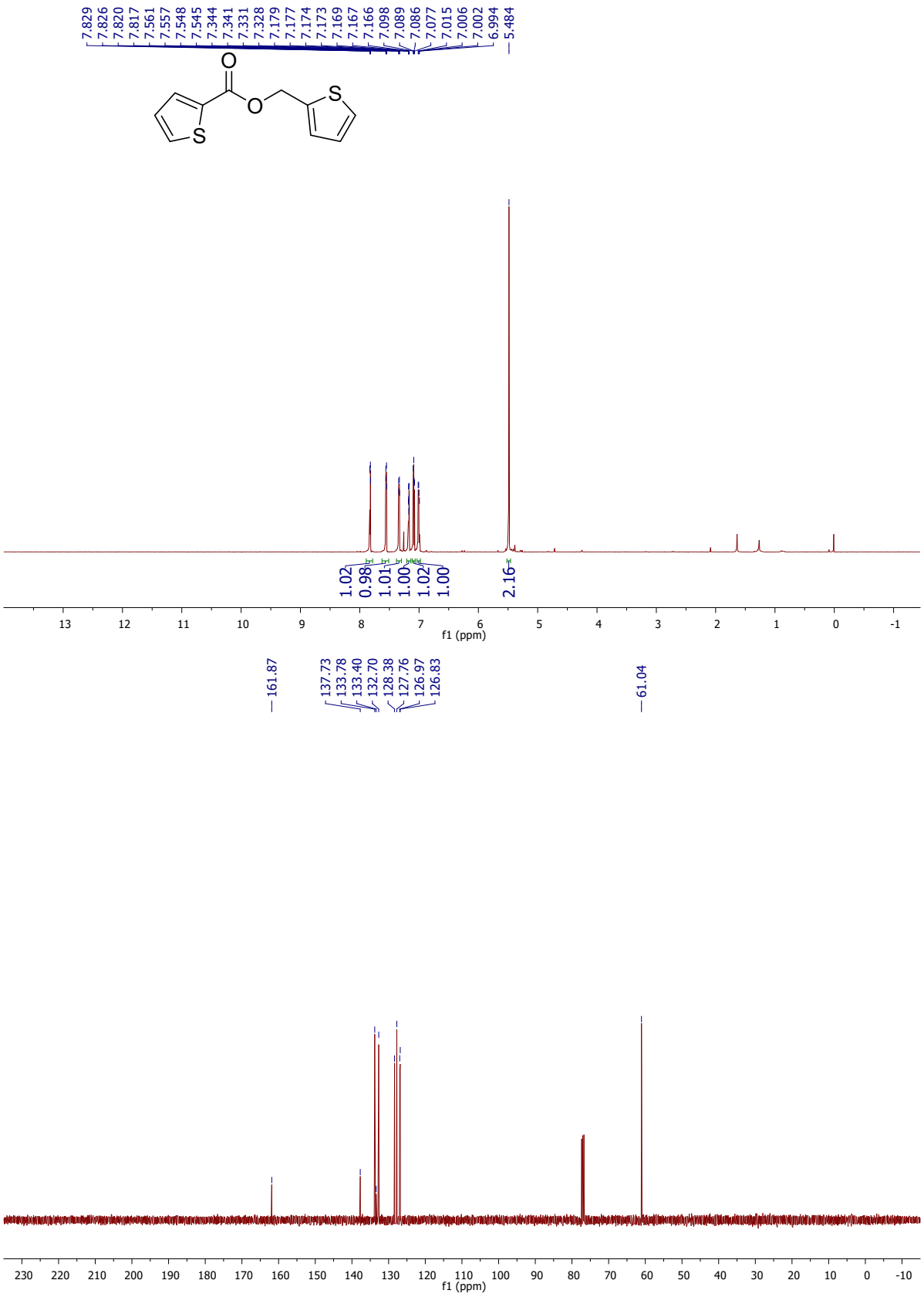

Figure S35. ^{1}H (400 MHz, $CDCl_3$) and $^{13}C\{^{1}H\}$ (100.6 MHz, $CDCl_3$) NMR spectra of **6g**