Supplementary Information for

An Active Representation Learning Method for Reaction Yield Prediction with Small-scale Data

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1. Supplementary Methods

1.1. General information

Unless otherwise noted, all reactions were performed under a nitrogen atmosphere using flame-dried glassware. All new compounds were fully characterized. ^{1}H NMR (400 MHz) spectra were recorded on a Bruker Avance 400 spectrometer and ^{1}H NMR (500 MHz) spectra were recorded on a Bruker Avance 500 spectrometer in $CDCl_3$ [using $CDCl_3$ (for ^{1}H, δ = 7.26, as the internal standard]. ^{13}C NMR (100 MHz) spectra on a Bruker Avance 400 spectrometer and ^{13}C NMR (125 MHz) spectra were recorded on a Bruker Avance 500 spectrometer in $CDCl_3$ [using $CDCl_3$ (for ^{13}C, δ = 77.0), as internal standard]. The following abbreviations were used to explain the multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, dd = doublet of doublet, ddd = doublet of doublet of doublet, dt = doublet of triplet, m = multiplet, s br = single broad. High-resolution mass spectra were obtained with a Water XEVO G2 Q-Tof (Waters Corporation). Commercially available reagents were purchased from Energy Chemical, J & K Scientific, and Adamas-beta.

1.2. Synthesis of starting materials

Compounds **A2-A3** have been reported in our provious work[1], and their spectroscopic data matched those reported in the literature. Tetrachloromethane (**A1**), alkenes **B1-B6**, initiators **D1-D3** and solvents **E1-E4** were commercially available and were used as received. NHC-BH_2CN (**C1**), DMAP-BH_2CN (**C2**), DMAP-BH_3 (**C3**) and NHC−BH_3 (**C4**) were known compounds and prepared according to the literature procedures[1].

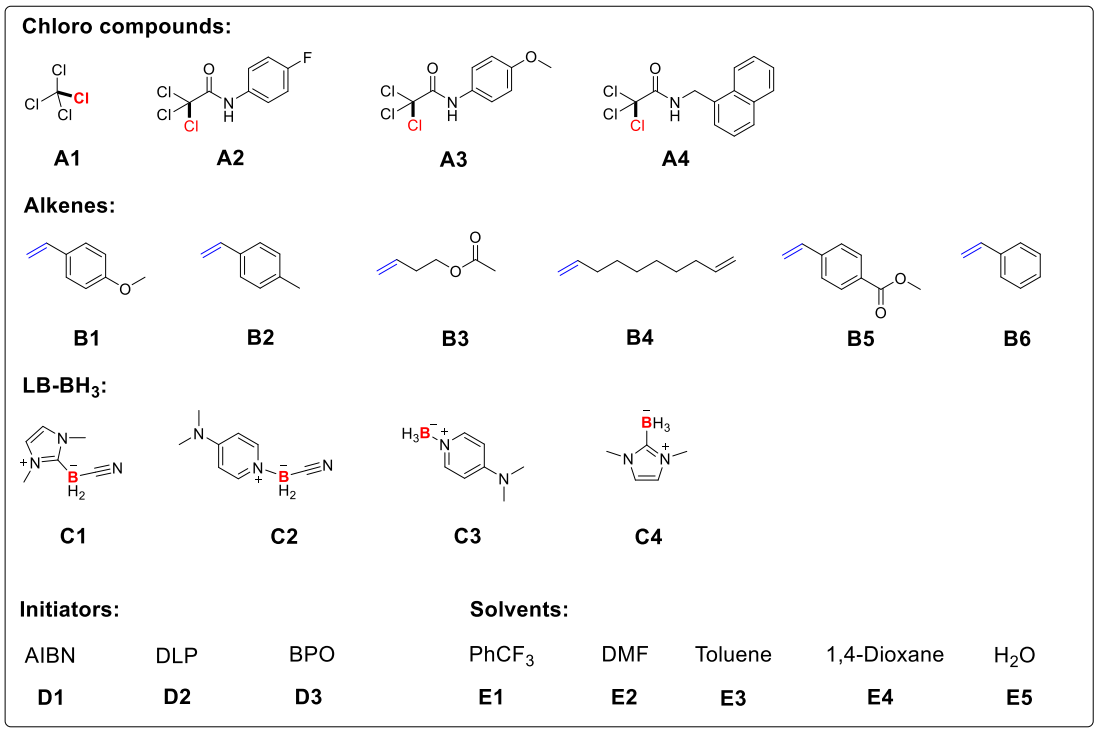
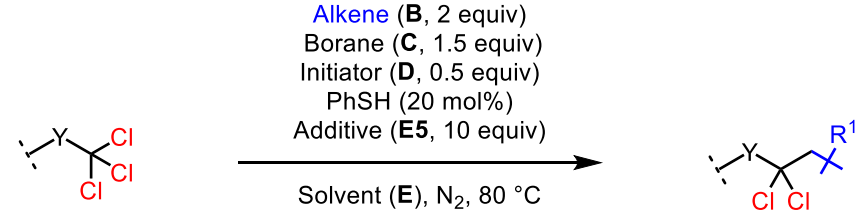


Fig. S1. Components of the reaction space of Lewis base-boryl radicals enabled coupling reaction.

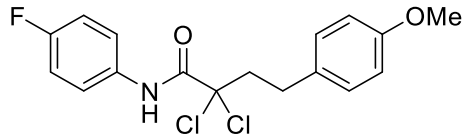
1.3. Dechlorinative coupling reactions of trichloromethyl groups



General Procedure

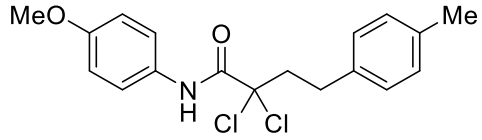
To an N_2 flushed glass tube charged with a magnetic stir bar, substrate (**A**, 0.1 mmol, 1.0 equiv), alkene (**B**, 2.0 equiv), borane (**C**, 1.5 equiv), initiator (**D**, 0.5 equiv), H_2O (10.0 equiv), PhSH (20 mol%), and solvent (**E**, 0.1 M) were added. The reaction mixture was stirred at 80℃ for 2 h. The resulting mixture was cooled down to room temperature then filtered through Na_2SO_4 under reduced pressure. The solvent was evaporated under reduced pressure. The crude mixture was purified by flash column chromatography on silica gel to give pure desired product.

2,2-Dichloro-N-(4-fluorophenyl)-4-(4-methoxyphenyl)butanamide (A)



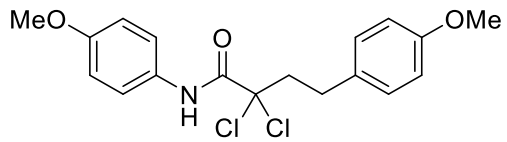
According to the ***general procedure***, the product **A** was prepared and purified by column chromatography on silica gel (petroleum ether : ethyl acetate = 50 : 1). White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.79-2.83 (2H, m), 2.86-2.91 (2H, m), 3.78 (3H, s), 6.82-6.86 (2H, m), 7.05-7.11 (2H, m), 7.13-7.17 (2H, m), 7.51-7.56 (2H, m), 8.46 (1H, s br); ^{13}C NMR (125 MHz, $CDCl_3$), 30.8, 46.6, 55.3, 86.6, 114.0, 115.9 (d, *J* = 22.8 Hz), 122.1 (d, *J* = 8.1 Hz), 129.5, 131.5, 132.5(d, *J* = 3.1 Hz), 158.2, 160.1 (d, *J* = 243.9 Hz), 163.4; ^{19}F NMR (376 MHz, $CDCl_3$) δ -116.1 (m). ESIHRMS: Found: *m*/*z* 378.0434. Calcd for $C_{17}H_{16}Cl_2FNO_2Na$: $(M+Na)^+$ 378.0434.

2,2-Dichloro-N-(4-methoxyphenyl)-4-(p-tolyl)butanamide (B)



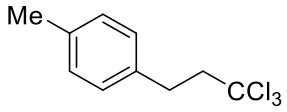
According to the ***general procedure***, the product **B** was prepared and purified by column chromatography on silica gel (petroleum ether : ethyl acetate = 50 : 1). Yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.31 (3H, s), 2.79-2.85 (2H, m), 2.87-2.91 (2H, m), 3.80 (3H, s), 6.88-6.90 (2H, m), 7.08-7.13 (4H, m), 7.44-7.47 (2H, m), 8.44 (1H, s br); ^{13}C NMR (100 MHz, $CDCl_3$) δ 21.0, 31.2, 46.6, 55.5, 86.8, 114.3, 122.1, 128.4, 129.2, 129.5, 135.9, 136.5, 157.3, 163.2. Found: *m*/*z* 374.0685. ESIHRMS: Calcd for $C_{18}H_{19}Cl_2NO_2Na$: $(M+Na)^+$ 374.0685.

2,2-Dichloro-N,4-bis(4-methoxyphenyl)butanamide (C)



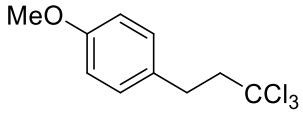
According to the ***general procedure***, the product **C** was prepared and purified by column chromatography on silica gel (petroleum ether : ethyl acetate = 50 : 1). White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.79-2.83 (2H, m), 2.86-2.90 (2H, m), 3.78 (3H, s), 3.81 (3H, s), 6.82-6.86 (2H, m), 6.89-6.93 (2H, m), 7.14-7.17 (2H, m), 7.46-7.50 (2H, m), 8.41 (1H, s br); ^{13}C NMR (100 MHz, $CDCl_3$) δ 30.8, 46.7, 55.2, 55.5, 86.7, 114.0, 114.3, 122.0, 129.5, 129.5, 131.6, 157.3, 158.1, 163.2. ESIHRMS: Found: *m*/*z* 390.0628. Calcd for $C_{18}H_{19}Cl_2NO_3Na$: $(M+Na)^+$ 390.0634.

1-Methyl-4-(3,3,3-trichloropropyl)benzene (D)



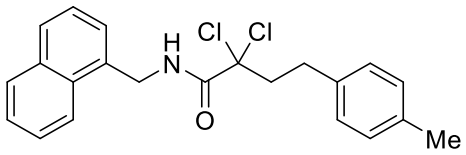
According to the ***general procedure*** with slight modification of the reaction conditions using carbon tetrachloride **A1** (4.0 equiv.), 1-methyl-4-vinylbenzene **B2** (1.0 equiv.), the product **D** was prepared and purified by column chromatography on silica gel (petroleum ether). White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.34 (3H, s), 2.93-2.97 (2H, m), 2.99-3.10 (2H, m), 7.14 (4H, s); ^{13}C NMR (125 MHz, $CDCl_3$) δ 21.0, 32.3, 56.9, 99.3, 128.4, 129.4, 135.7, 136.2. EIHRMS: Found: *m*/*z* 236.9940. Calcd for $C_{10}H_{12}Cl_3$: $(M+H)^+$ 236.9999.

1-Methoxy-4-(3,3,3-trichloropropyl)benzene (E)



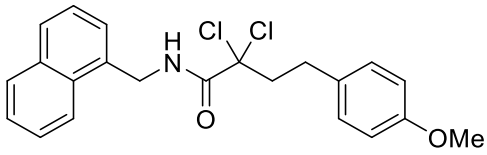
According to the ***general procedure*** with slight modification of the reaction conditions using carbon tetrachloride **A1** (4.0 equiv.), 1-methoxy-4-vinylbenzene **B1** (1.0 equiv.), the product **E** was prepared and purified by column chromatography on silica gel (petroleum ether). White solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 2.89-2.99 (2H, m), 2.99-3.07 (2H, m), 3.80 (3H, s), 6.82-6.89 (2H, m), 7.12-7.18 (2H, m); ^{13}C NMR (125 MHz, $CDCl_3$) δ 31.9, 55.3, 57.0, 99.3, 114.2, 129.5, 130.9, 158.4. ESIHRMS: Found: m/z 252.9886. Calcd for $C_{10}H_{12}Cl_3O$: $(M+H)^+$ 252.9948.

2,2-Dichloro-N-(naphthalen-2-ylmethyl)-4-(p-tolyl)butanamide (F)



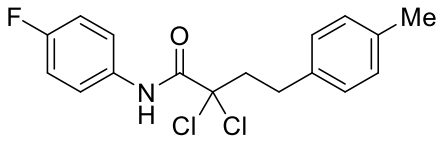
According to the ***general procedure***, the product **F**[1] was prepared and purified by column chromatography on silica gel (petroleum ether : ethyl acetate = 30 : 1). White solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 2.33 (3H, s), 2.77-2.81 (2H, m), 2.83-2.86 (2H, m), 4.99 (2H, d, *J* = 5.5 Hz), 7.07 (1H, s br), 7.09-7.13 (4H, m), 7.45-7.50 (2H, m), 7.52-7.58 (2H, m), 7.87 (1H, d, *J* = 8.0 Hz), 7.91 (1H, dd, *J* = 7.5, 1.5 Hz), 7.99 (1H, d, *J* = 8.0 Hz); ^{13}C NMR (125 MHz, $CDCl_3$) δ 21.0, 31.1, 42.9, 46.8, 86.3, 123.2, 125.4, 126.2, 126.8, 126.9, 128.4, 128.9, 129.1, 129.2, 131.3, 132.2, 133.9, 135.9, 136.6, 165.3. ESIHRMS: Found: m/z 386.1077. Calcd for $C_{22}H_{22}Cl_2NO$: $(M+H)^+$ 386.1073.

2,2-Dichloro-4-(4-methoxyphenyl)-N-(naphthalen-2-ylmethyl)butanamide (G)



According to the ***general procedure***, the product **G** was prepared and purified by column chromatography on silica gel (petroleum ether : ethyl acetate = 30 : 1). White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.75-2.79 (2H, m), 2.80-2.85 (2H, m), 3.80 (3H, s), 4.98 (2H, d, *J* = 5.2 Hz), 6.83-6.86 (2H, m), 7.07 (1H, s br), 7.12-7.15 (2H, m), 7.44-7.59 (2H, m), 7.51-7.60 (2H, m), 7.85-7.87 (1H, m), 7.90-7.92 (1H, m), 7.97-7.99 (1H, m); ^{13}C NMR (125 MHz, $CDCl_3$) δ 30.7, 43.0, 46.9, 55.3, 86.5, 114.0, 123.2, 125.4, 126.2, 126.8, 126.9, 128.9, 129.2, 129.5, 131.3, 131.7, 132.2, 134.0, 158.2, 165.4. ESIHRMS: Found: m/z 424.0840. Calcd for $C_{22}H_{21}Cl_2NO_2Na$: $(M+Na)^+$ 424.0841.

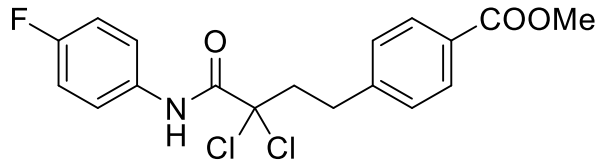
2,2-Dichloro-N-(4-fluorophenyl)-4-(p-tolyl)butanamide (H)



According to the ***general procedure***, the product **H** was prepared and purified by column chromatography on silica gel (petroleum ether : ethyl acetate = 50 : 1). White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.33 (3H, s), 2.81-2.86 (2H, m), 2.89-2.94 (2H, m), 7.05-7.15 (6H, m), 7.51-7.57 (2H, m), 8.47 (1H, s br); ^{13}C NMR (100 MHz, $CDCl_3$) δ 21.0, 31.2,

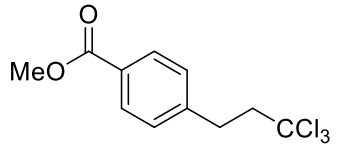
46.5, 86.6, 116.0 (d, J = 22.6 Hz), 122.2 (d, J = 8.0 Hz), 128.4, 129.3, 132.6 (d, J = 2.8 Hz), 136.0, 136.4, δ 161.1 (d, J = 244.0 Hz), 163.5. ^{19}F NMR (376 MHz, $CDCl_3$) δ -116.1 (m). ESIHRMS: Found: m/z 340.0669. Calcd for $C_{17}H_{17}Cl_2FNO$: $(M+H)^+$ 340.0666.

Methyl 4-(3,3-dichloro-4-((4-fluorophenyl)amino)-4-oxobutyl)benzoate (I)



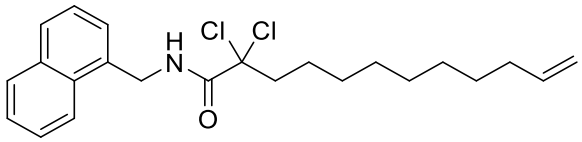
According to the ***general procedure***, the product **I** was prepared and purified by column chromatography on silica gel (petroleum ether : ethyl acetate = 50 : 1). Yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 2.84-2.86 (2H, m), 2.99-3.02 (2H, m), 3.91 (3H, s), 7.07-7.10 (2H, m), 7.30-7.32 (2H, m), 7.51-7.55 (2H, m), 7.96-7.98 (2H, m), 8.45 (1H, s br); ^{13}C NMR (125 MHz, $CDCl_3$) δ 31.7, 45.7, 52.1, 86.2, δ 116.0 (d, J = 22.8 Hz) , δ 122.1 (d, J = 8.1 Hz), 128.6, 130.0, δ 132.4 (d, J = 3.1 Hz), 144.9, δ 160.1 (d, J = 244.0 Hz), 163.3, 166.9. ^{19}F NMR (376 MHz, $CDCl_3$) δ -116.0 (m). ESIHRMS: Found: m/z 406.0392. Calcd for $C_{18}H_{16}Cl_2FNO_3Na$: $(M+Na)^+$ 406.0383.

Methyl-4-(3,3,3-trichloropropyl)benzoate (J)



According to the ***general procedure*** with slight modification of the reaction conditions using carbon tetrachloride **A1** (4.0 equiv.), methyl 4-vinylbenzoate **B5** (1.0 equiv.), the product **J** was prepared and purified by column chromatography on silica gel (petroleum ether : ethyl acetate = 100 : 1). White solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 2.97-3.00 (2H, m), 3.14-3.17 (2H, m), 3.92 (3H, s), 7.31-7.32 (2H, m), 7.99-8.01 (2H, m); ^{13}C NMR (125 MHz, $CDCl_3$) δ 32.8, 52.1, 56.1, 99.0, 128.6, 128.7, 130.1, 144.2, 166.9. EIHRMS: Found: m/z 280.9828. Calcd for $C_{11}H_{12}Cl_3O_2$: $(M+H)^+$ 280.9898.

2,2-Dichloro-N-(naphthalen-2-ylmethyl)dodec-11-enamide (K)



According to the ***general procedure*** with slight modification of the reaction conditions using 2,2,2-trichloro-*N*-(naphthalen-2-ylmethyl)acetamide **A4** (1.0 equiv.), deca-1,9-diene **B4** (8.0 equiv.), the product **K** was prepared and purified by column chromatography on silica gel (petroleum ether : ethyl acetate = 50 : 1). Colorless oil.^{1}H NMR (500 MHz, $CDCl_3$) δ 1.25-1.39 (10H, m), 1.49-1.56 (2H, m), 2.01-2.07 (2H, m), 2.47-2.51 (2H, m), 4.92-5.03 (4H, m), 5.82 (1H, ddt, *J* = 16.9, 10.2, 6.7 Hz), 7.06 (1H, t, *J* = 5.1 Hz, br), 7.44-7.49 (2H, m), 7.51-7.58 (2H, m), 7.85-7.87 (1H, m), 7.89-7.91 (1H, m), 7.95-7.97 (1H, m); ^{13}C NMR (125 MHz, $CDCl_3$) δ 25.2, 28.8, 28.9, 29.0, 29.2, 29.3, 33.8, 42.9, 45.0, 87.4, 114.2, 123.2, 125.4, 126.2, 126.7, 126.8, 128.9, 129.1, 131.3, 132.2, 133.9, 139.2, 165.5. ESIHRMS: Found: m/z 428.1516. Calcd for $C_{23}H_{29}Cl_2NONa$: $(M+Na)^+$ 428.1518.

2. Supplementary Figures

^{1}H, ^{13}C, and ^{19}F NMR Spectra

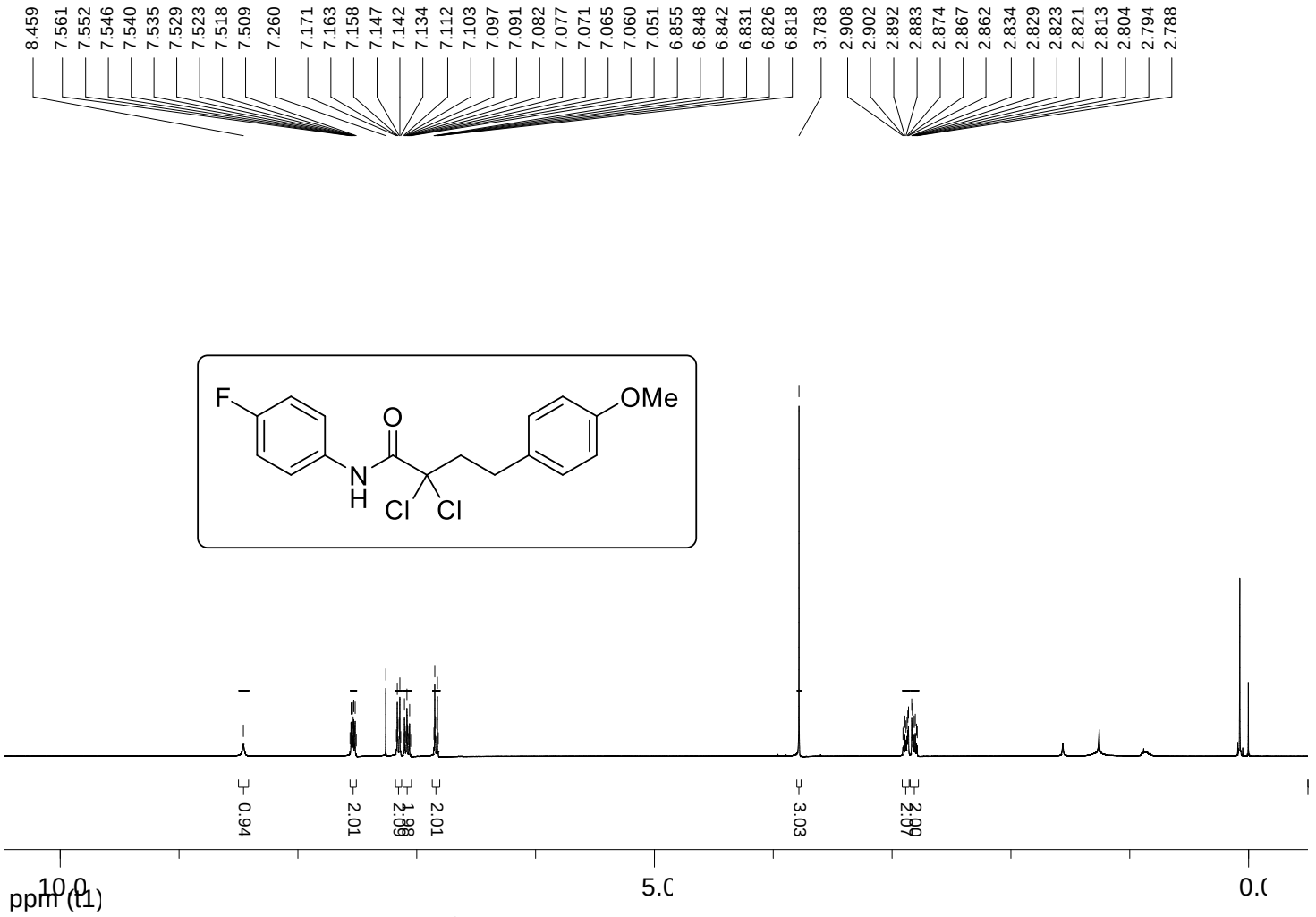


Fig. S1. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of A

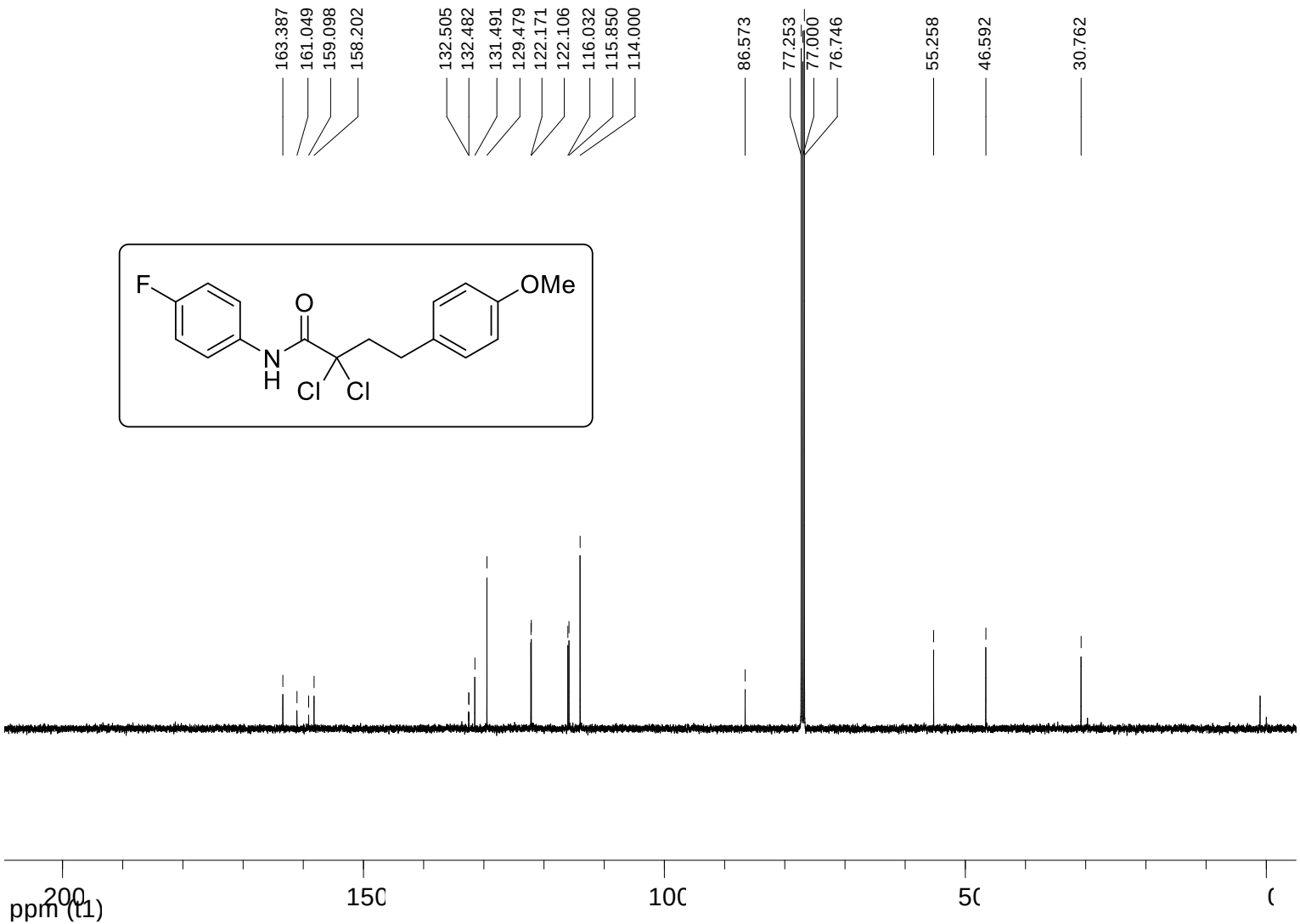


Fig. S2. ^{13}C NMR (125 MHz, $CDCl_3$) spectrum of A

5

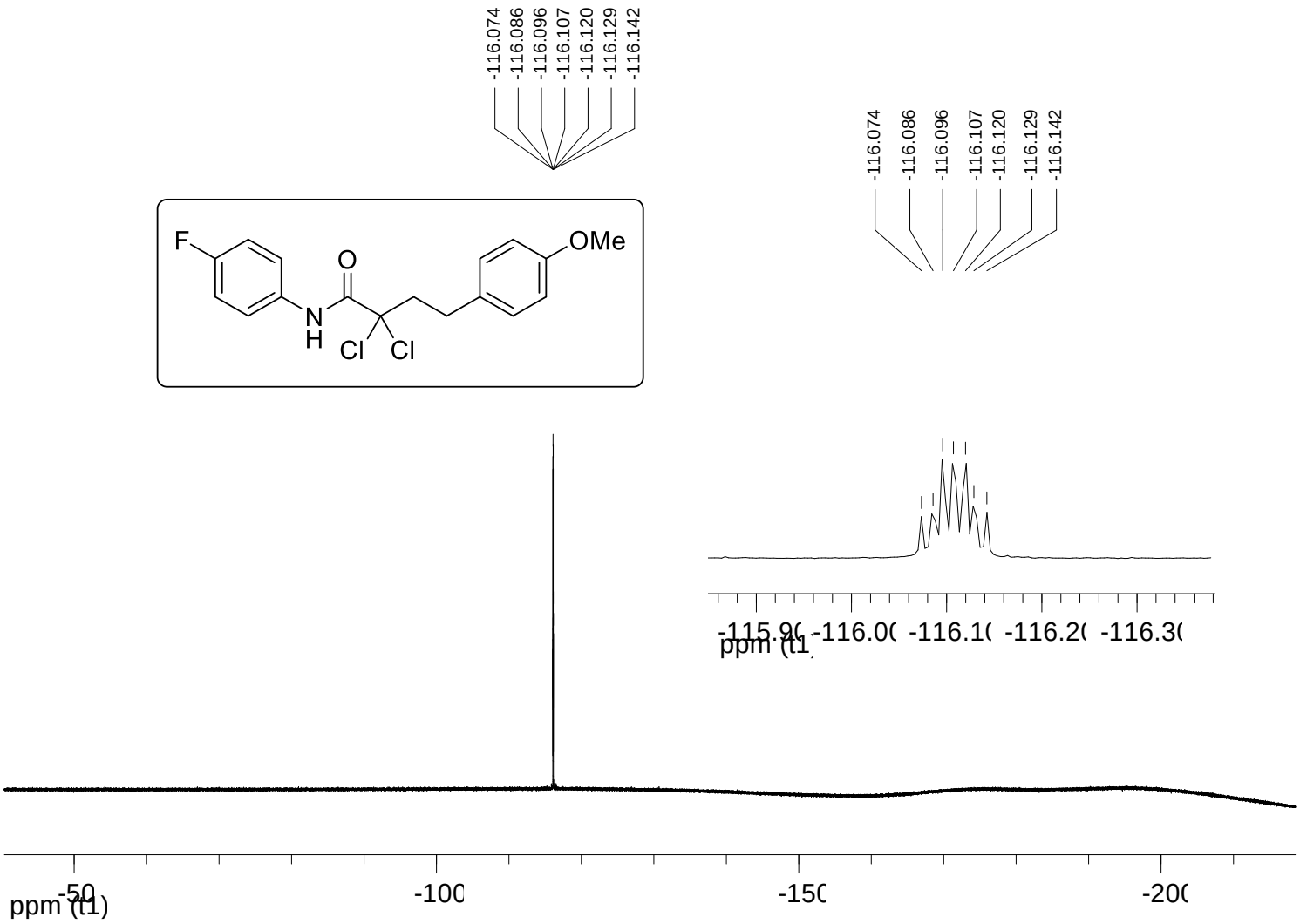


Fig. S3. ^{19}F NMR (376 MHz, $CDCl_3$) spectrum of A

5

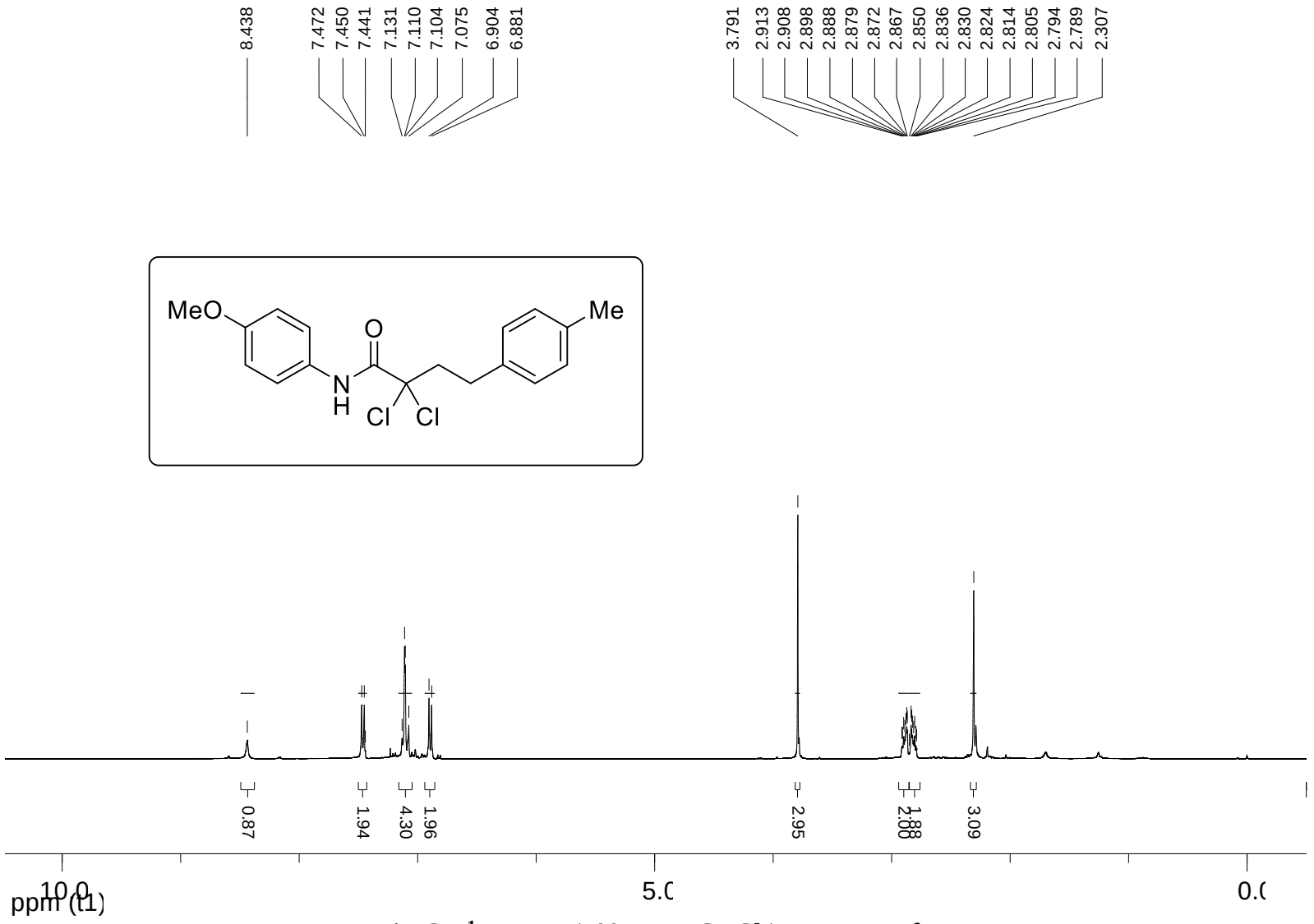


Fig. S4. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of B

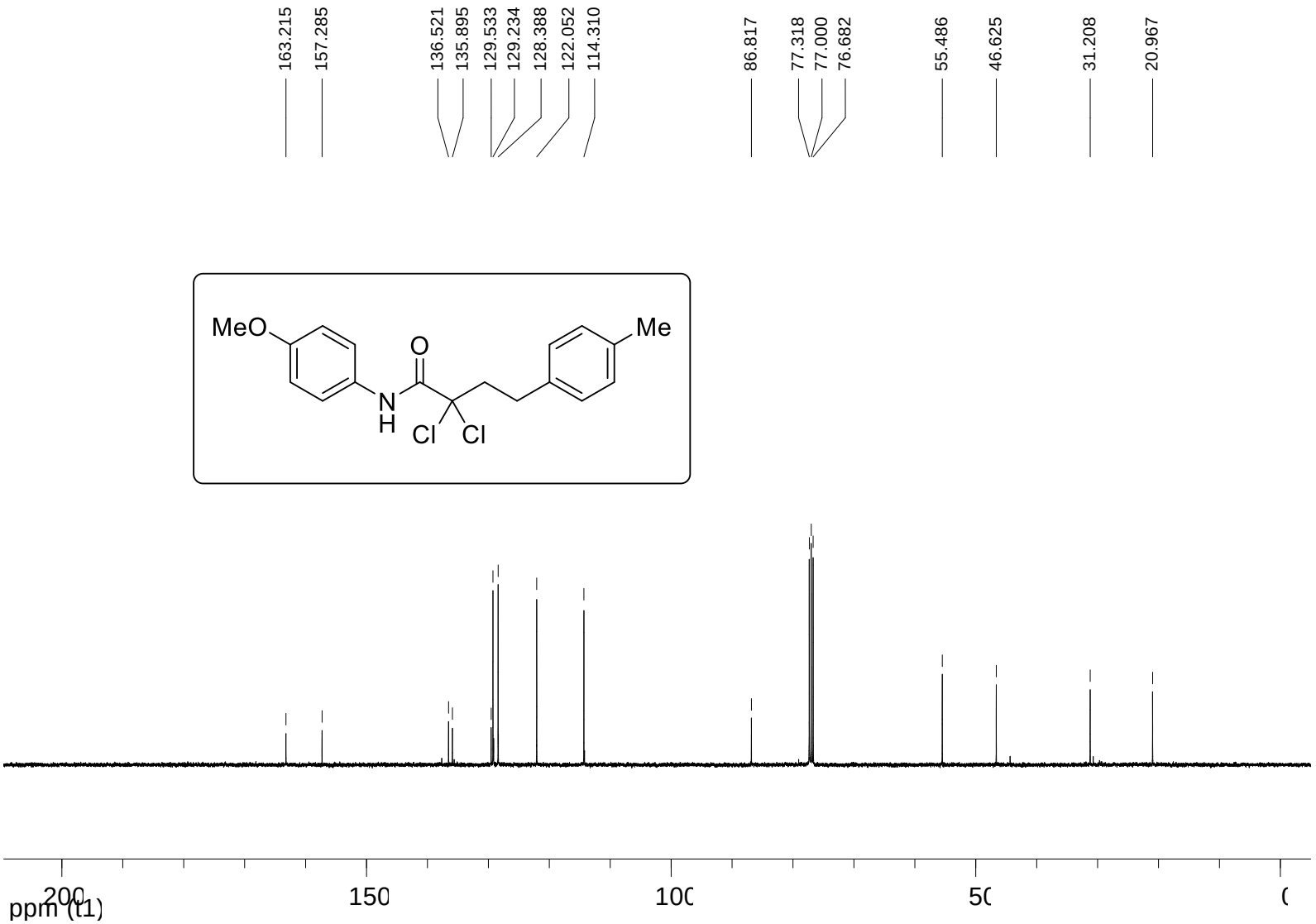


Fig. S5. ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of B

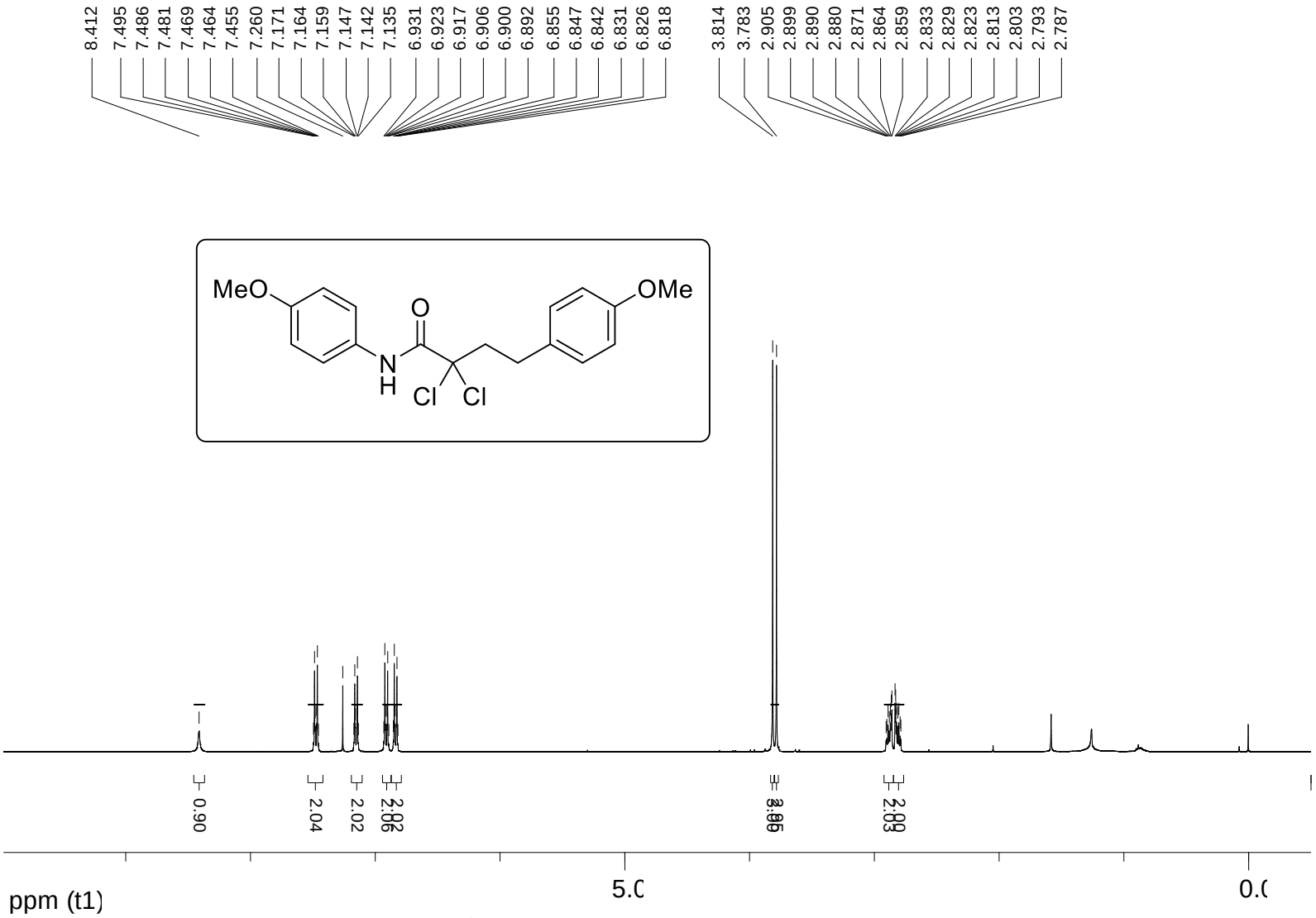


Fig. S6. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of C

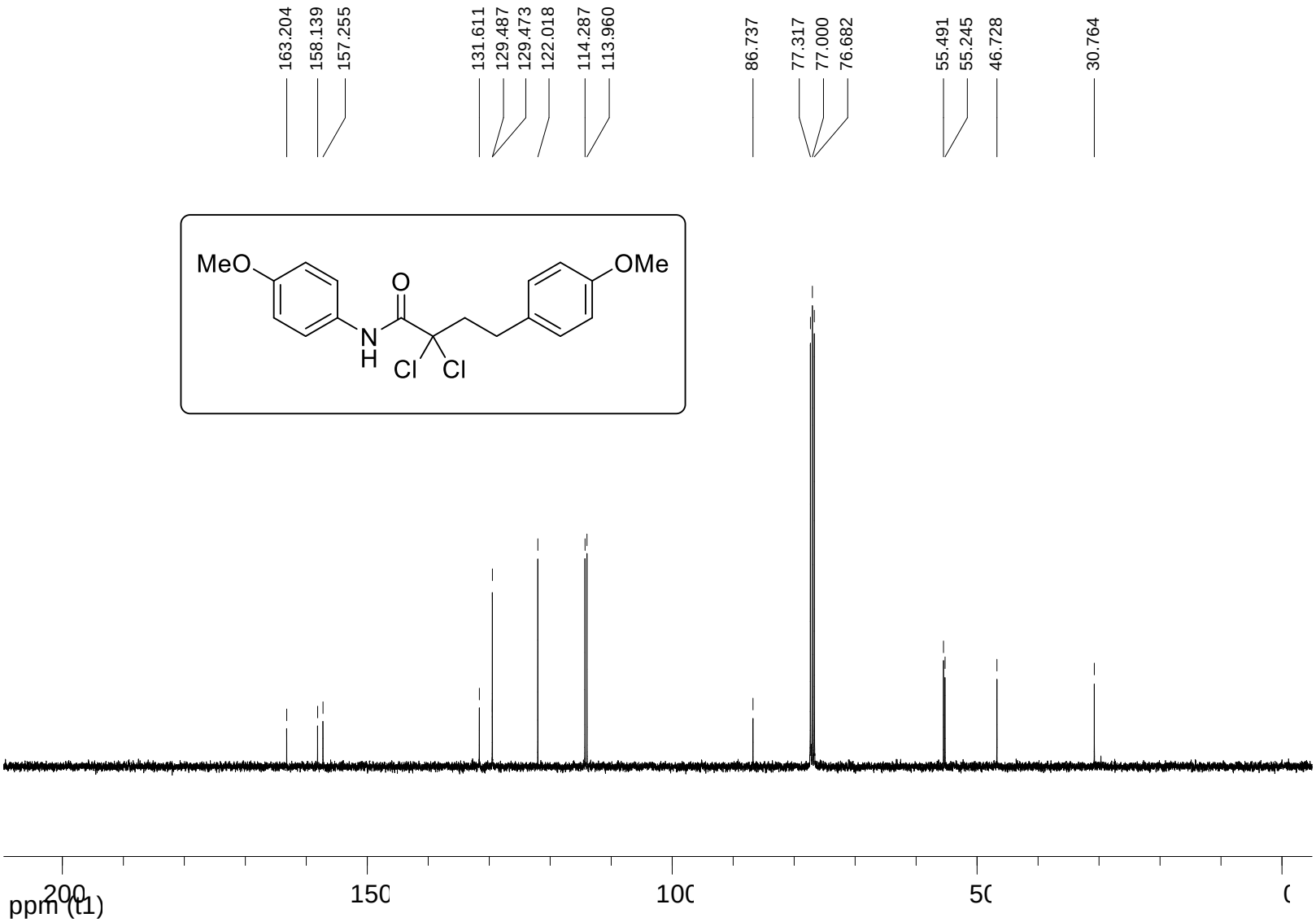


Fig. S7. ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of C

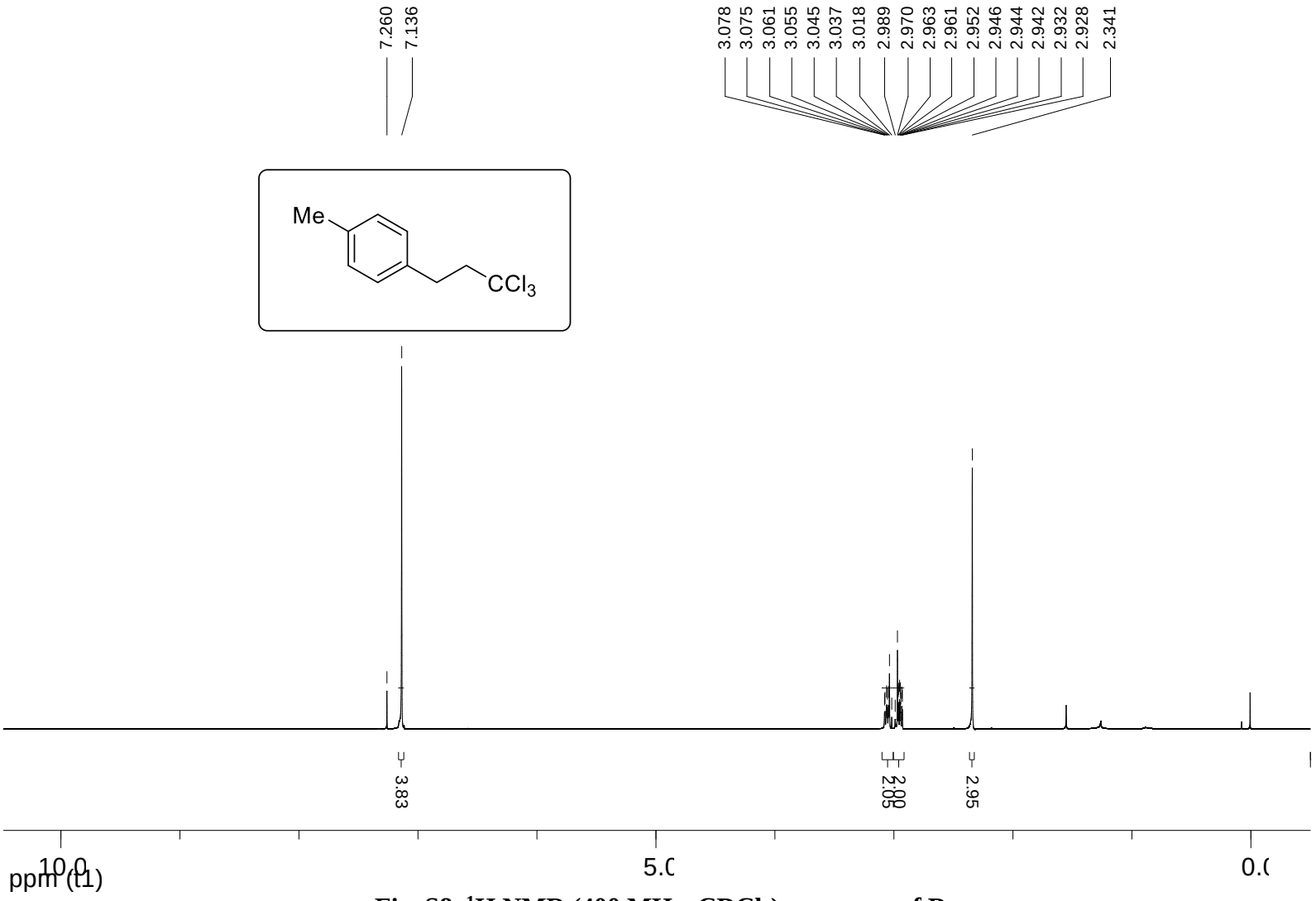


Fig. S8. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of D

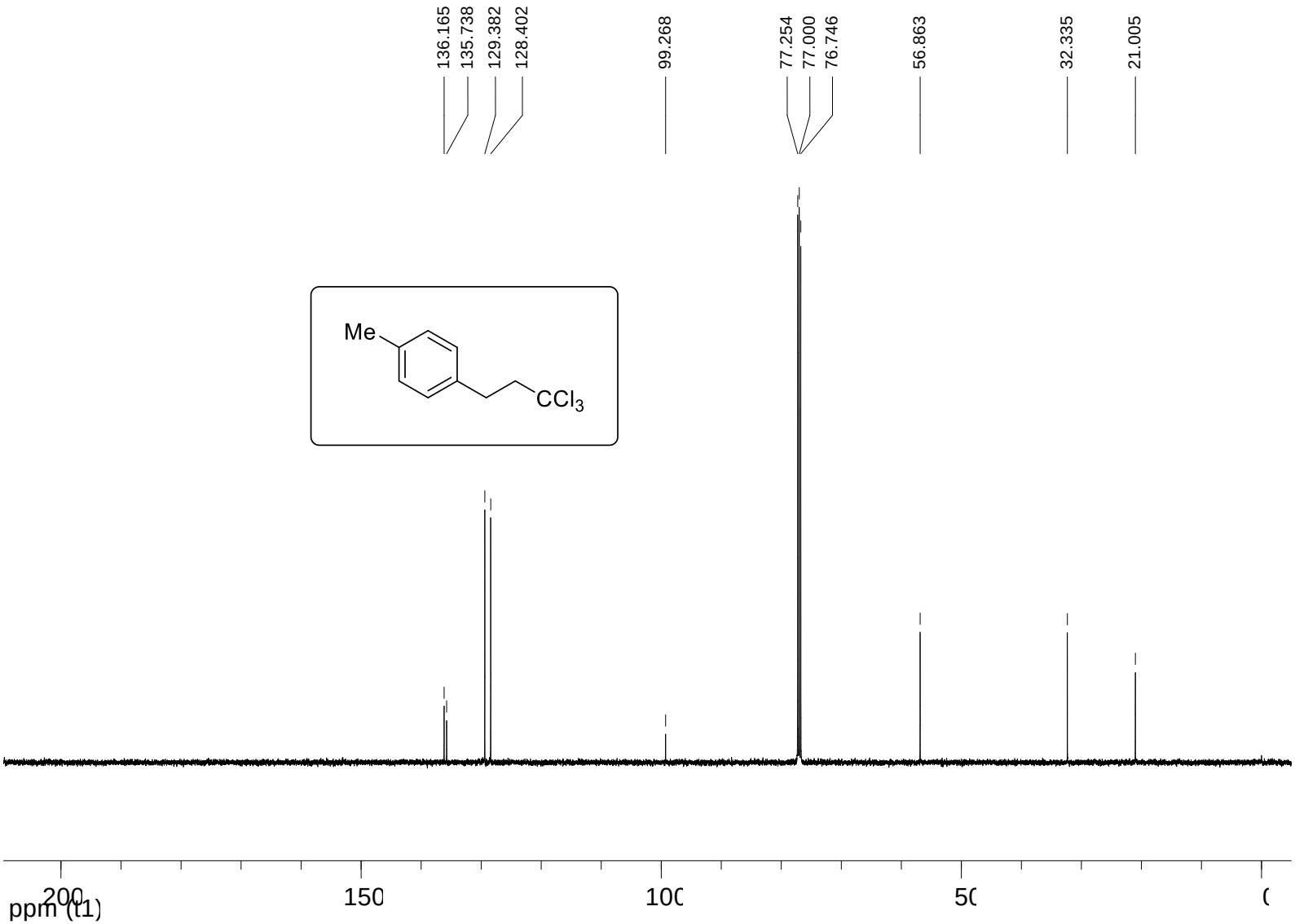


Fig. S9. ^{13}C NMR (125 MHz, $CDCl_3$) spectrum of D

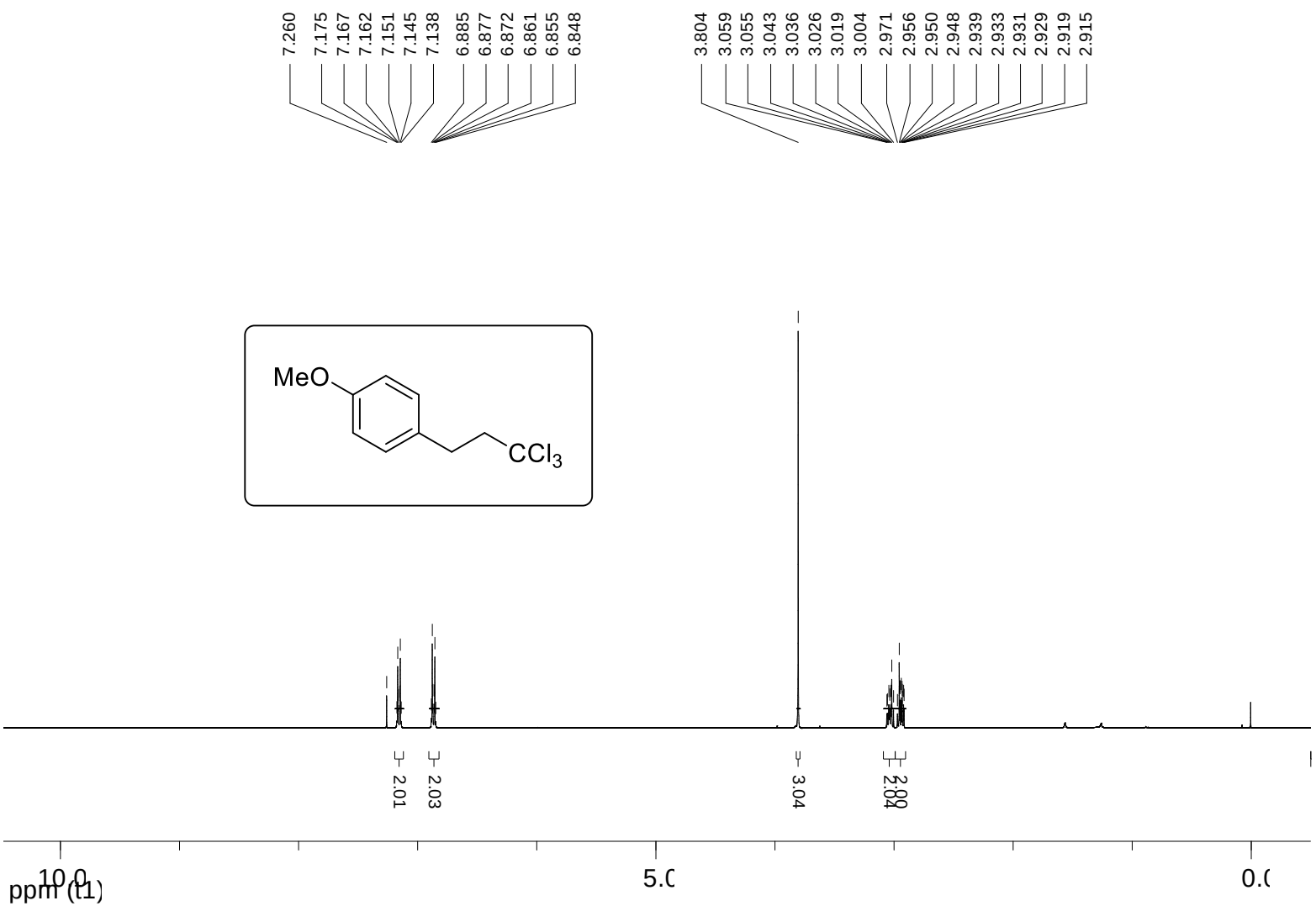


Fig. S10. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of E

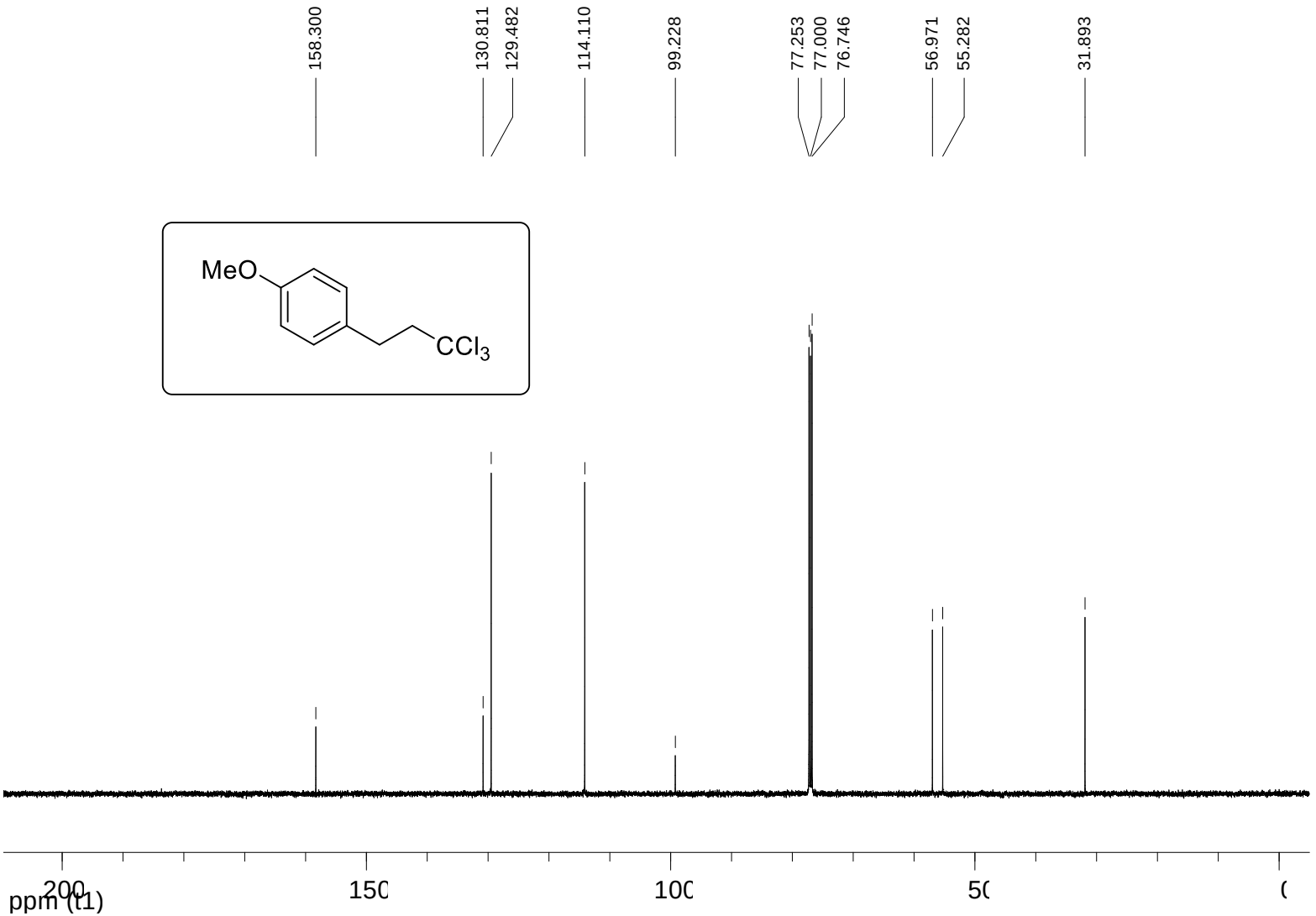


Fig. S11. ^{13}C NMR (125 MHz, $CDCl_3$) spectrum of E

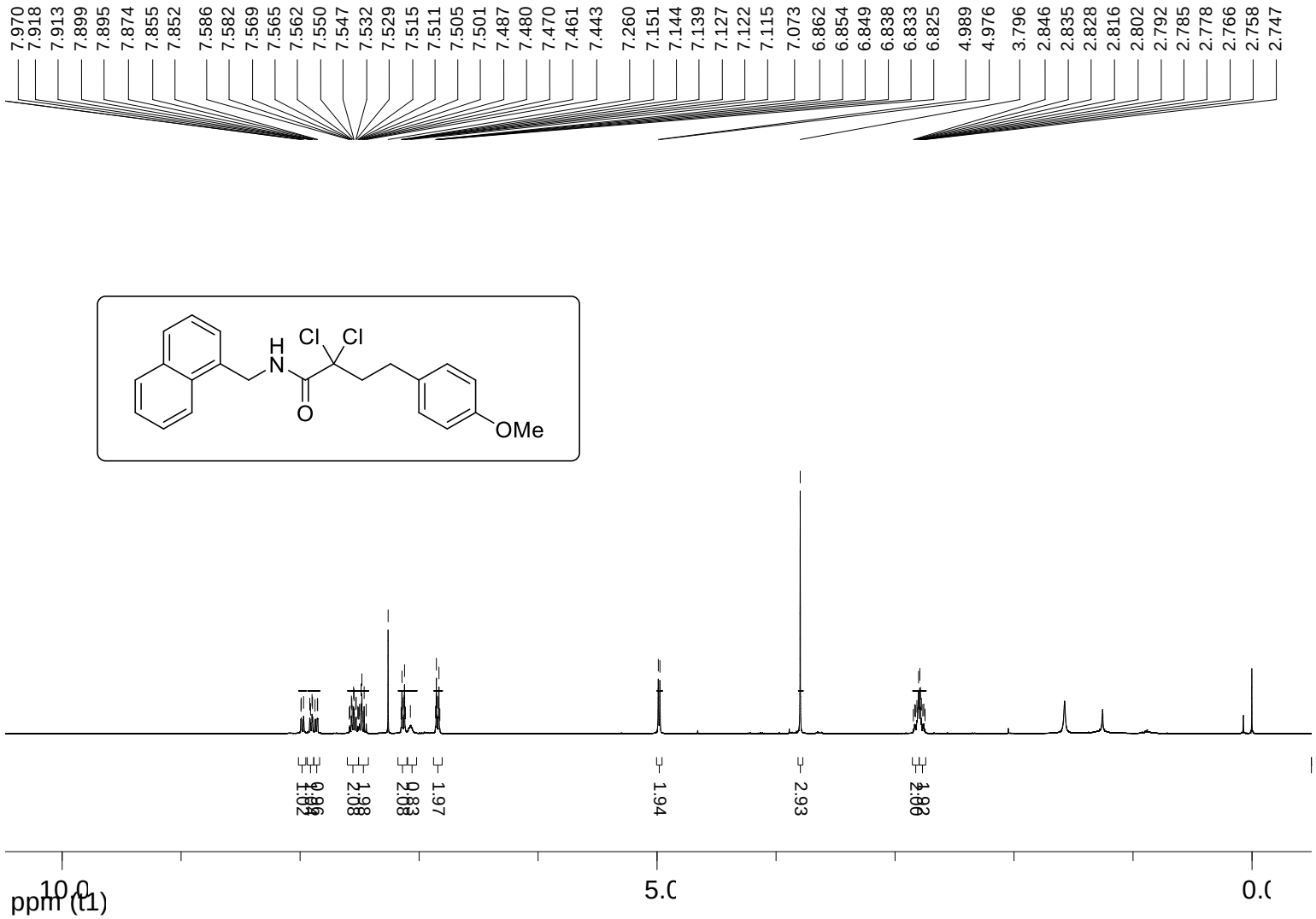


Fig. S12. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of G

5

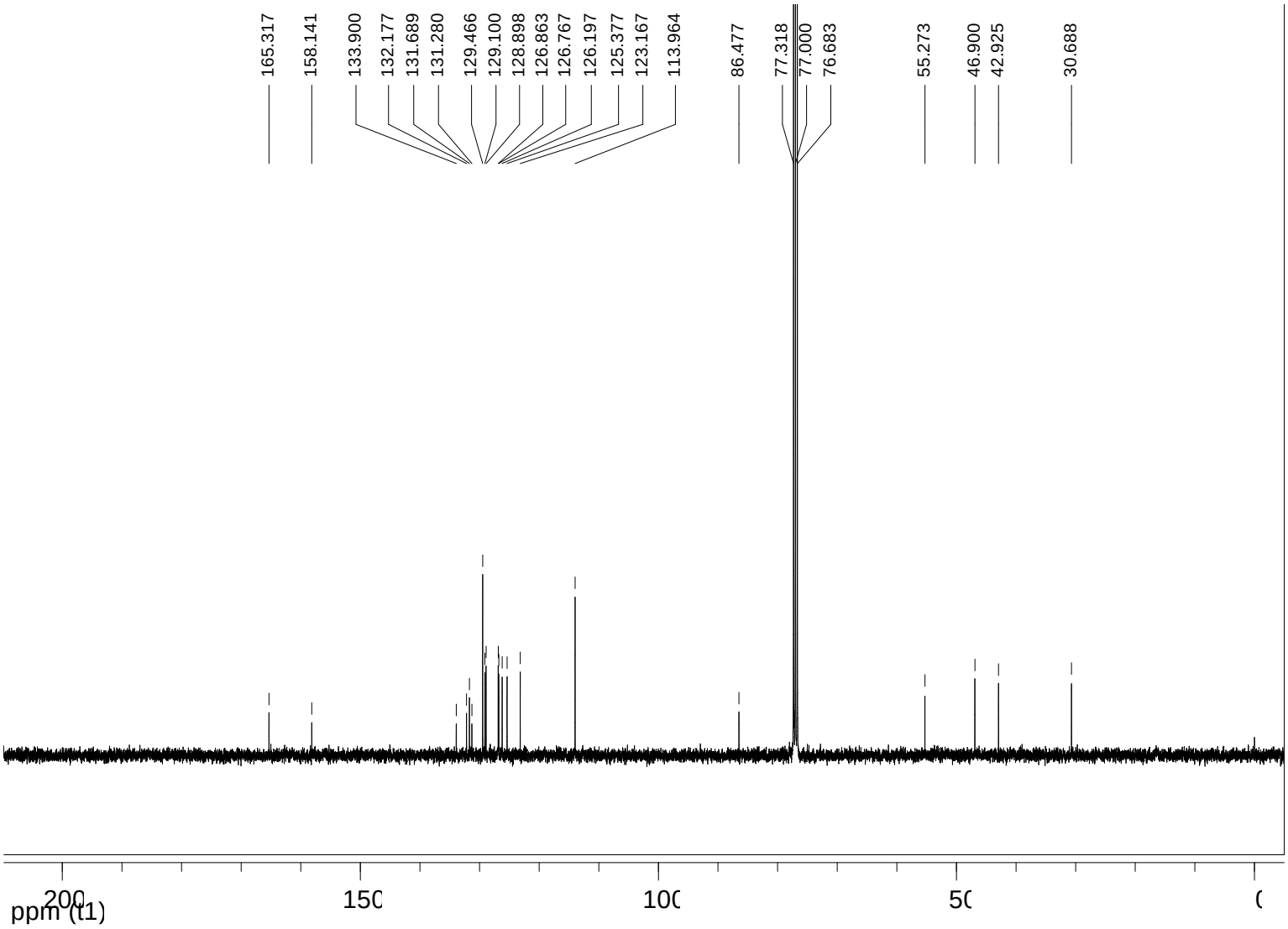


Fig. S13. ^{13}C NMR (125 MHz, $CDCl_3$) spectrum of G

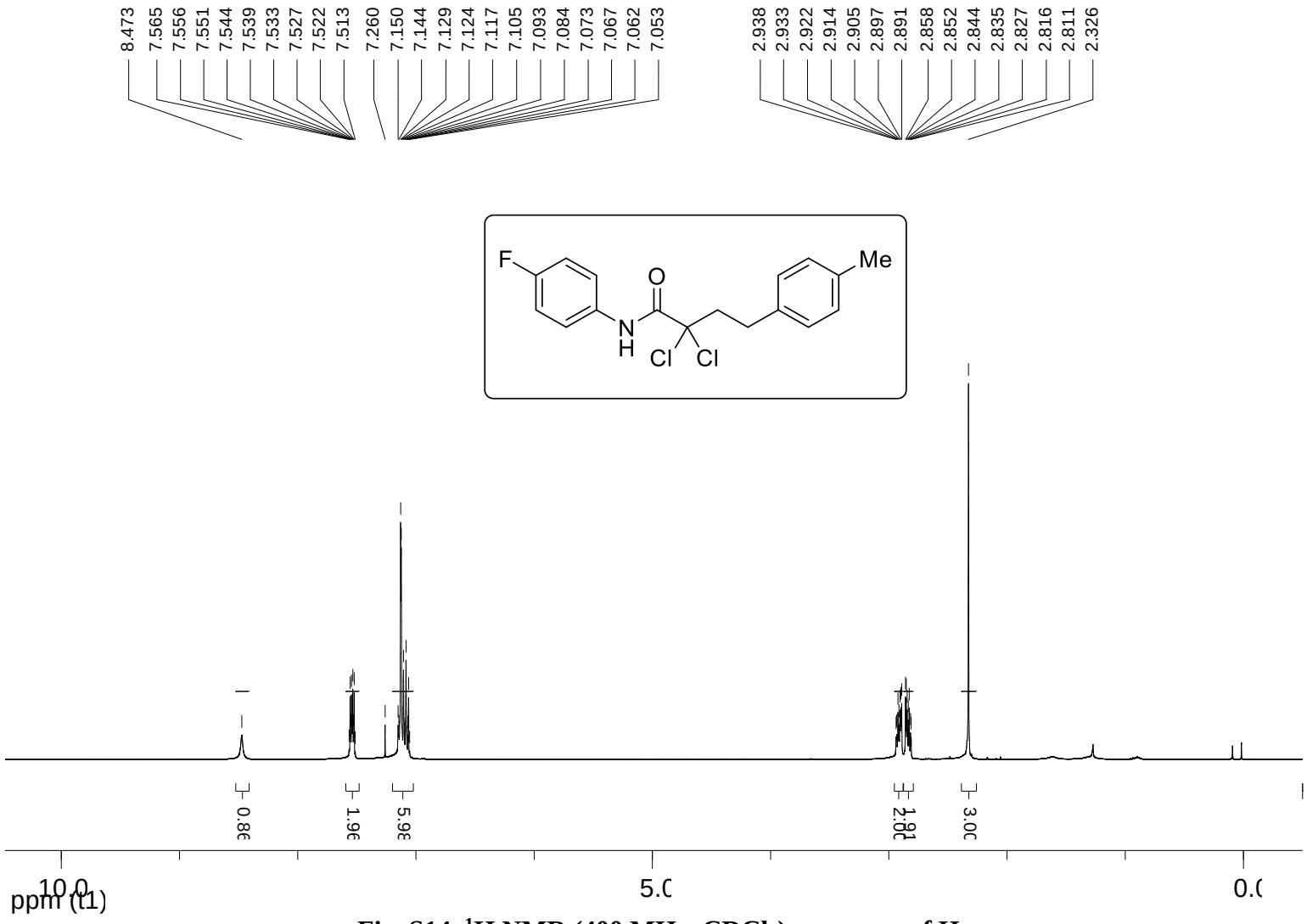


Fig. S14. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of H

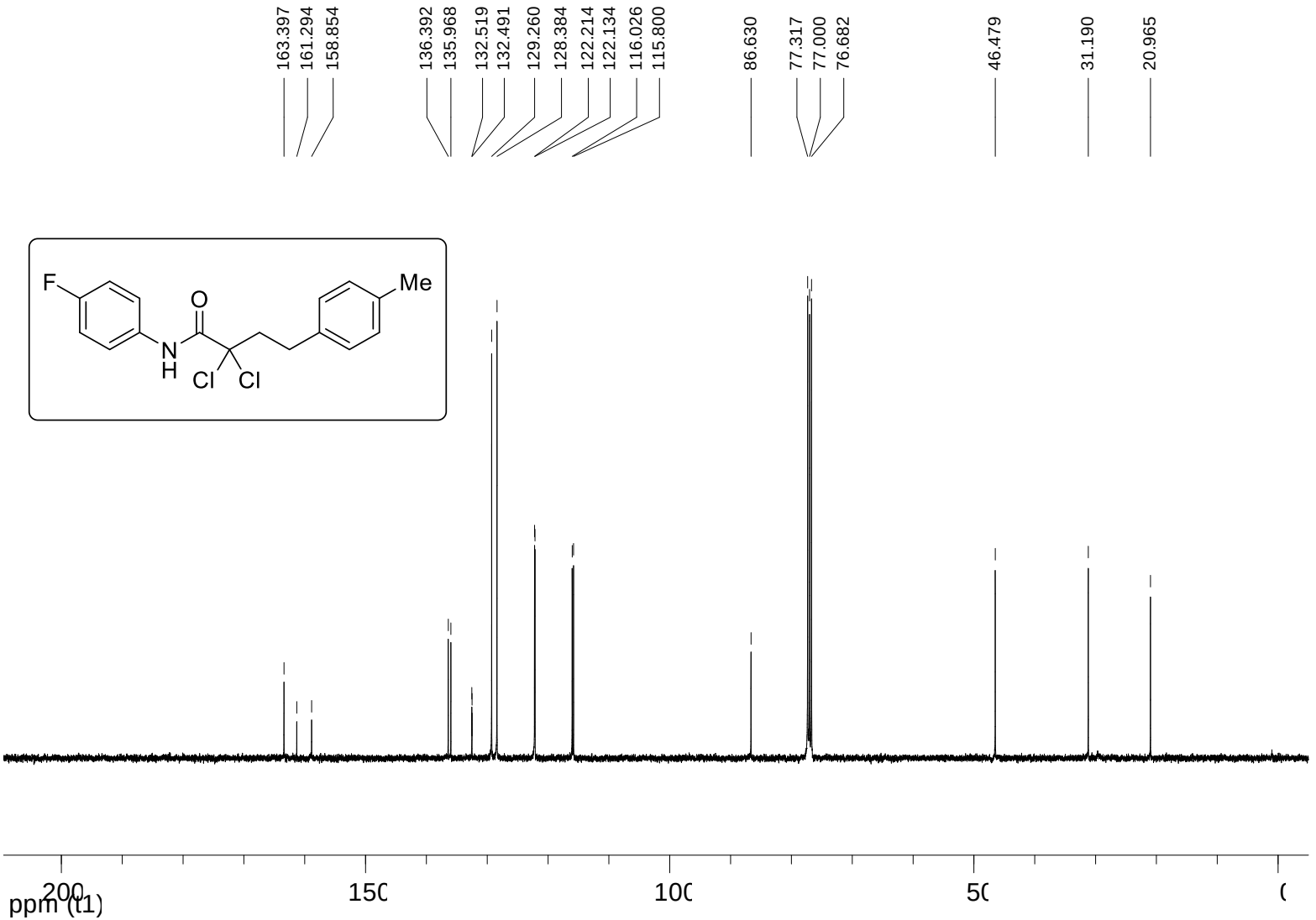


Fig. S15. ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of H

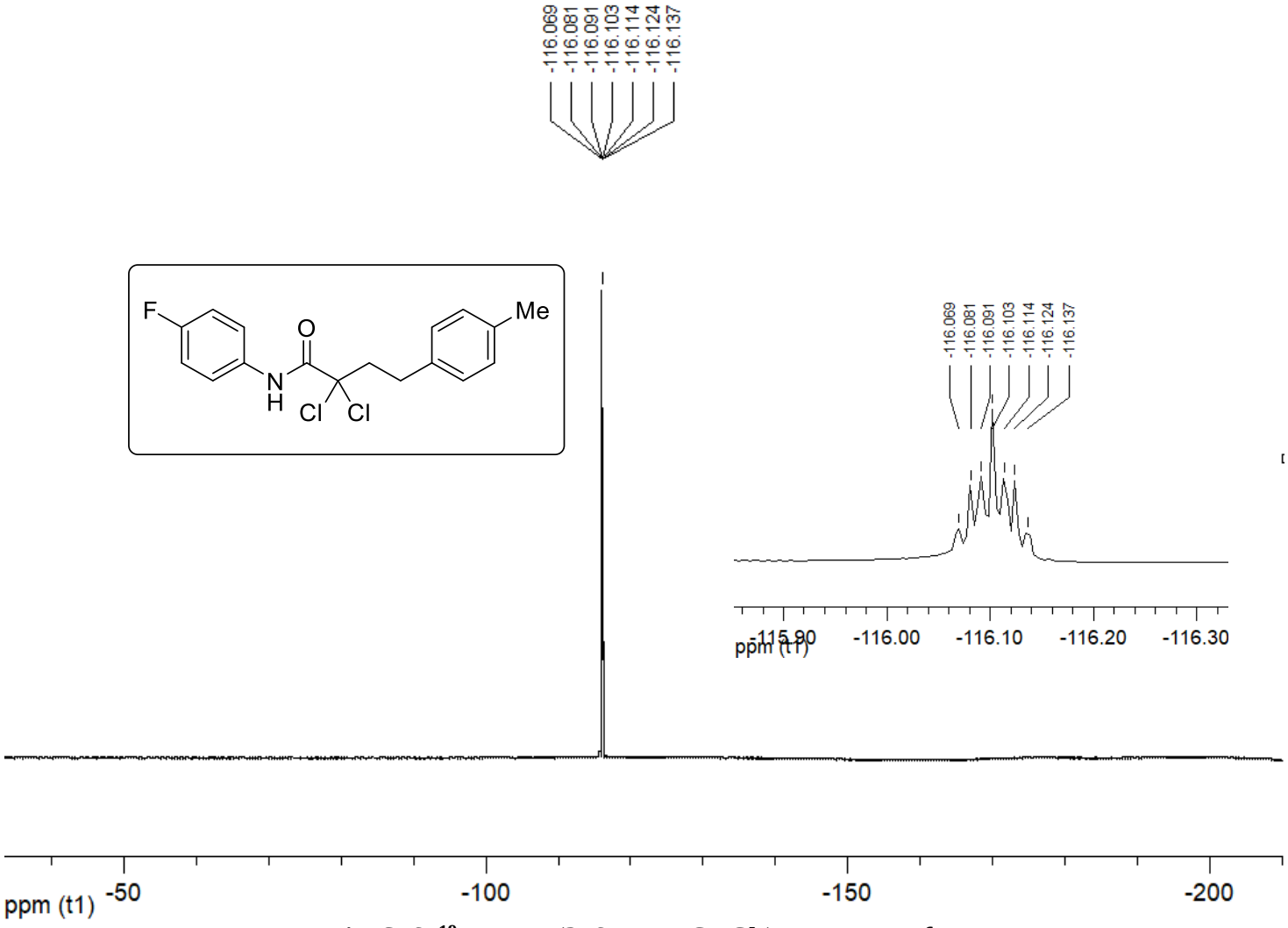


Fig. S16. ^{19}F NMR (376 MHz, $CDCl_3$) spectrum of H

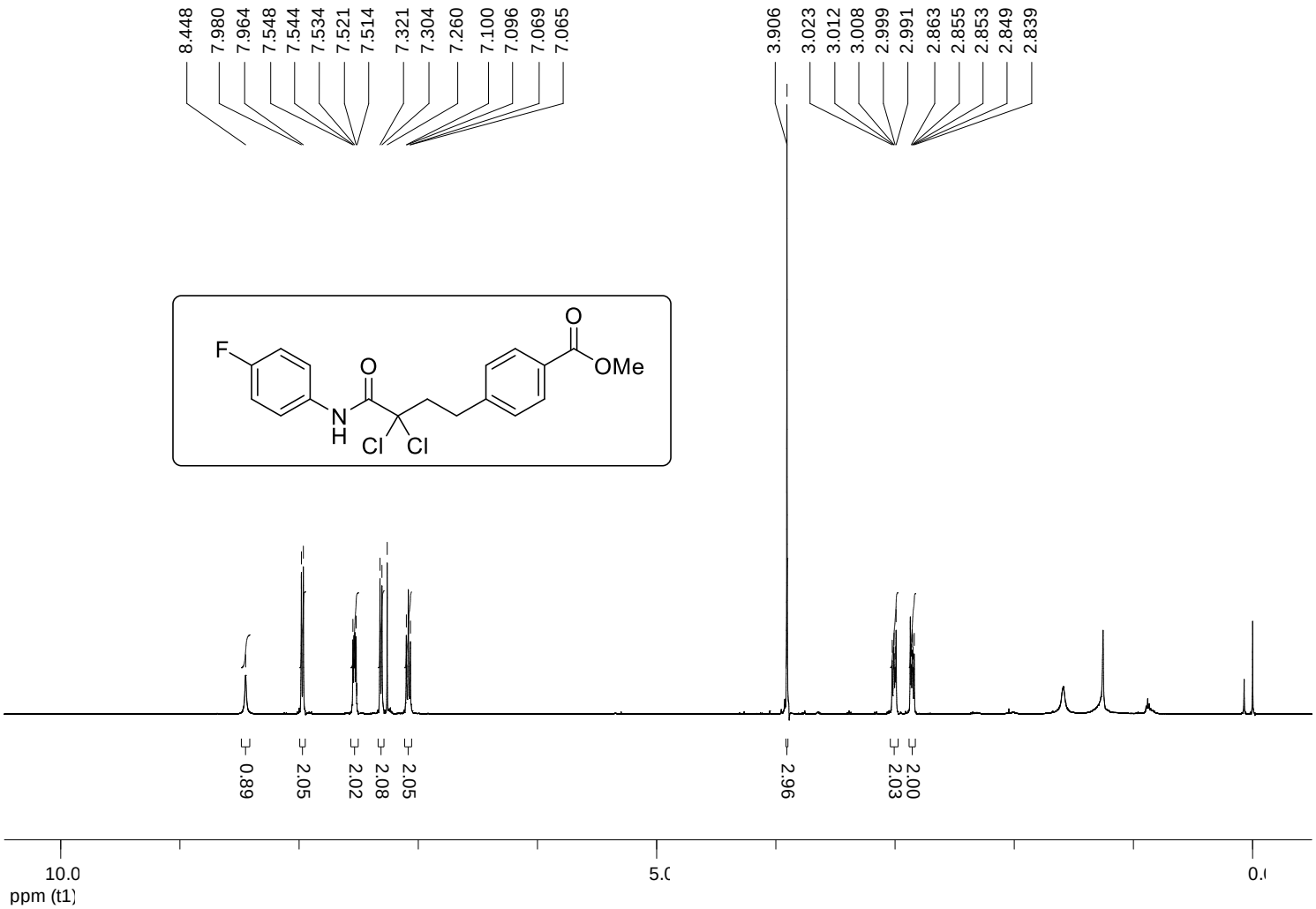


Fig. S17. ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of I

5

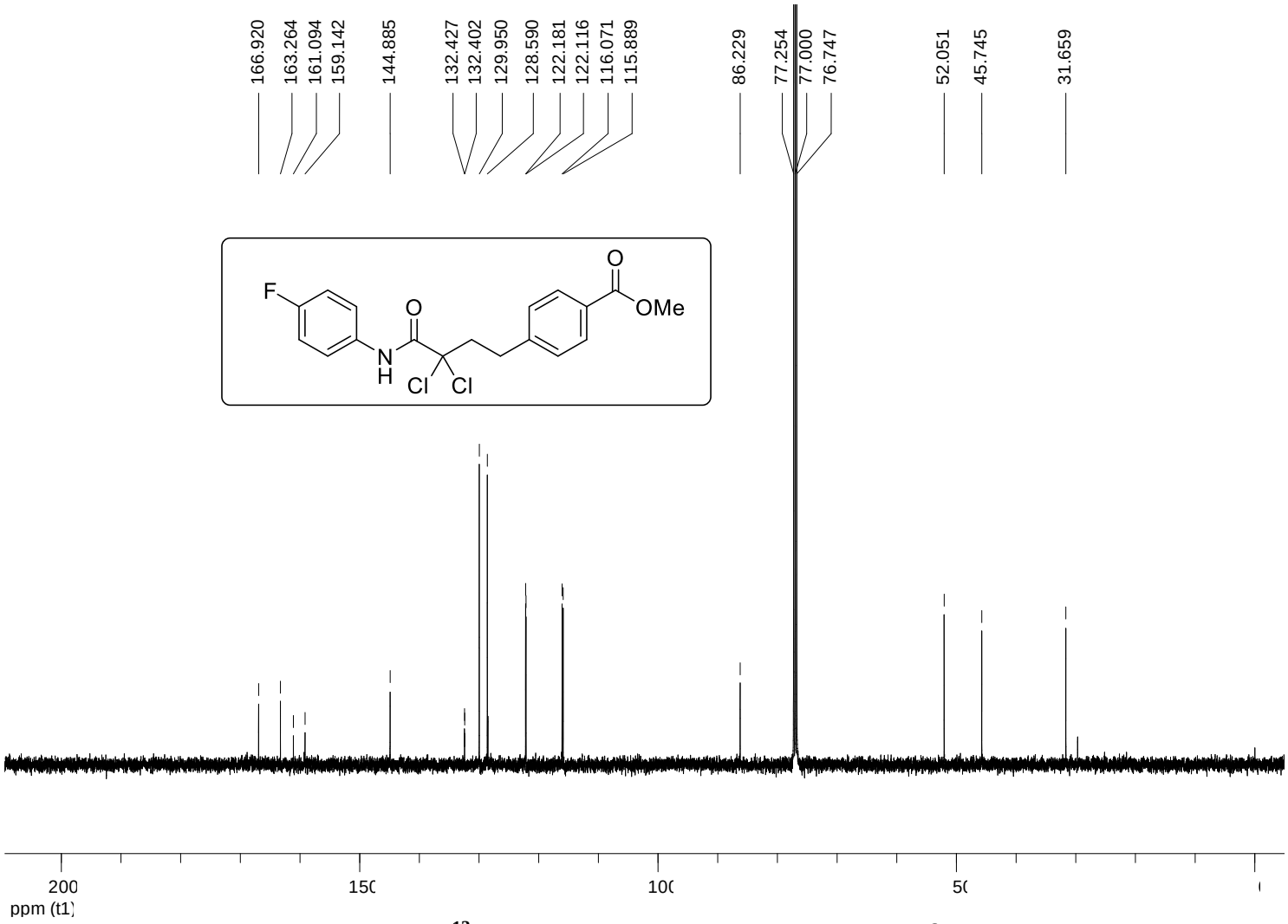


Fig. S18. ^{13}C NMR (125 MHz, $CDCl_3$) spectrum of I

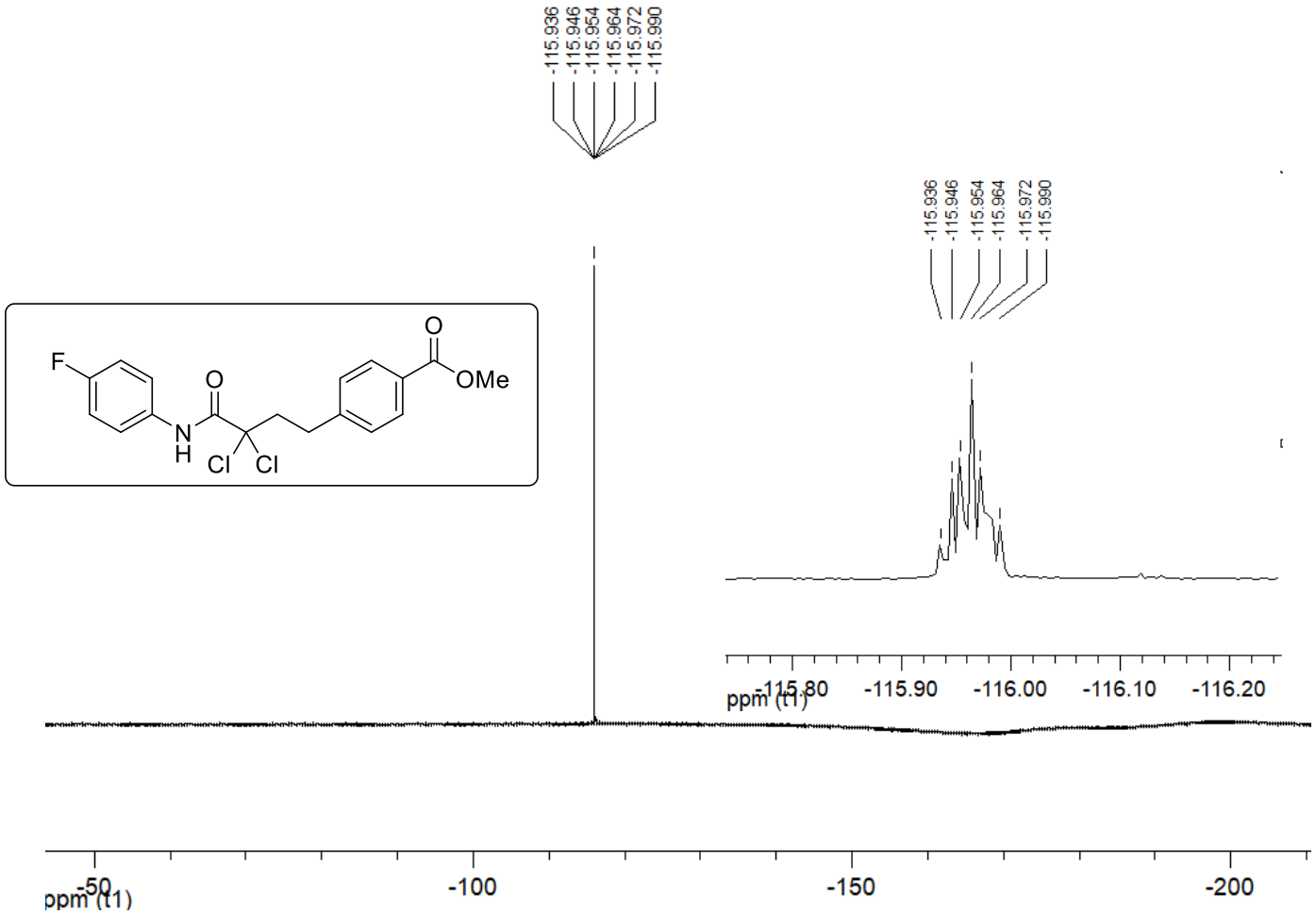


Fig. S19. ^{19}F NMR (376 MHz, $CDCl_3$) spectrum of I

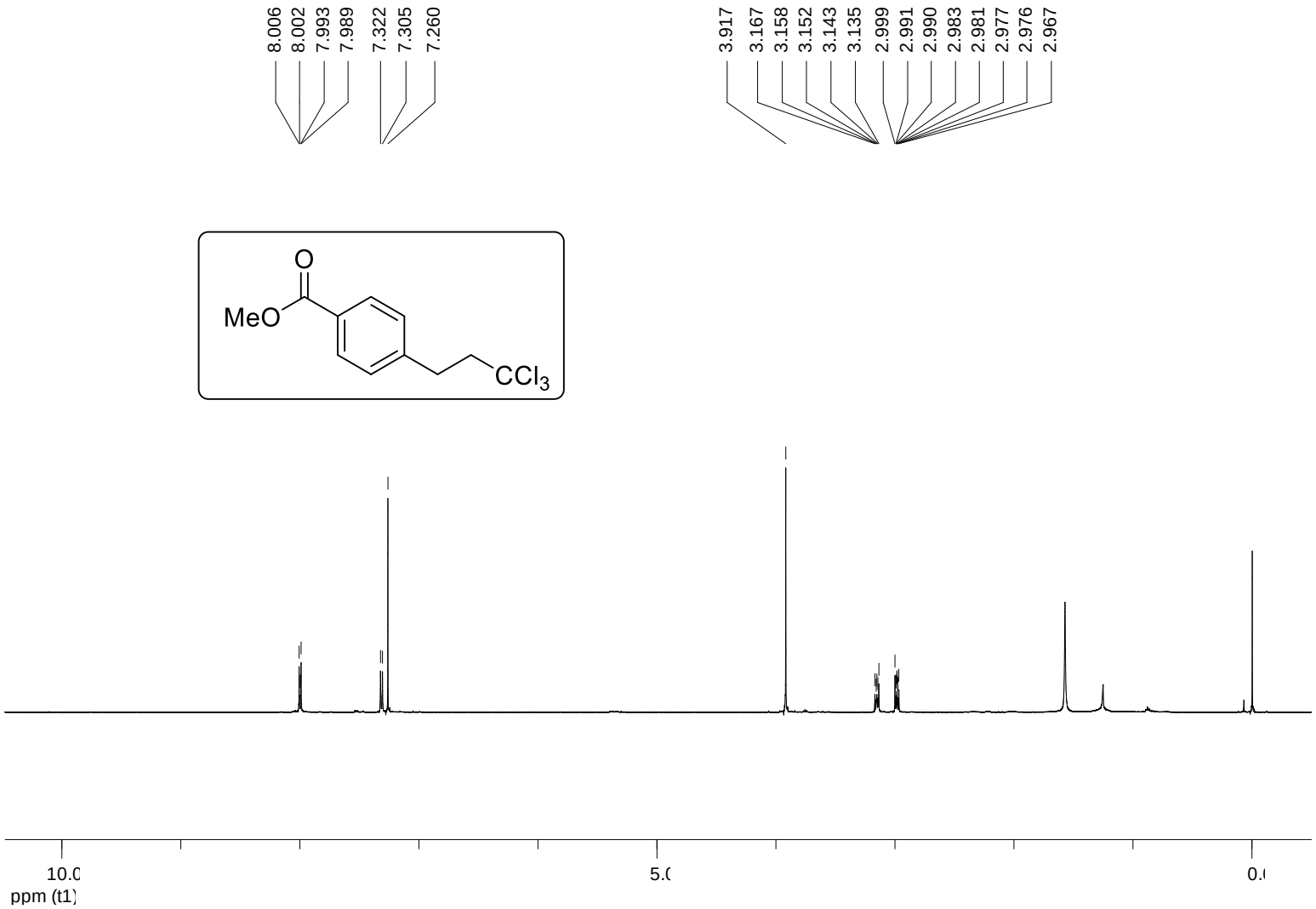


Fig. S20. ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of J

5

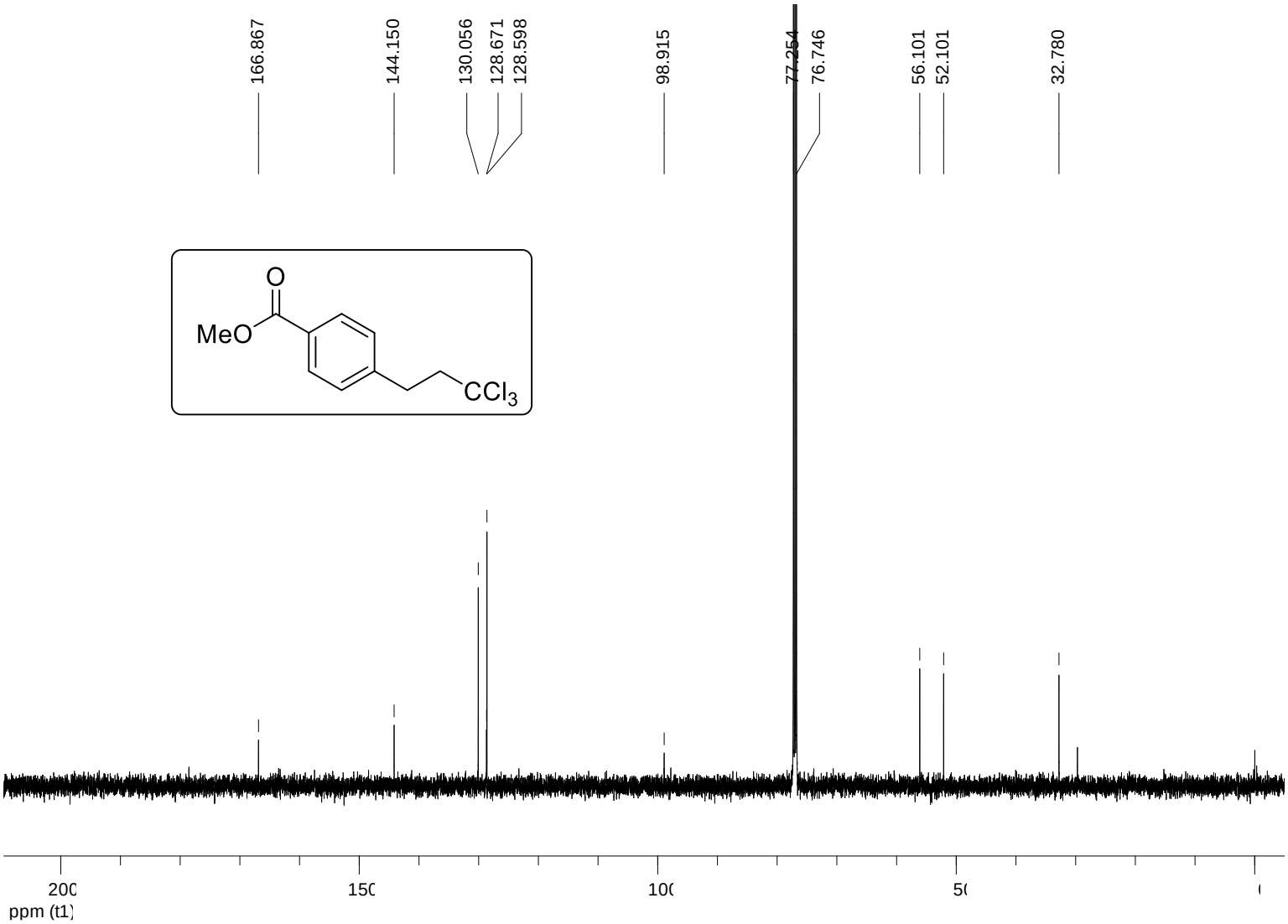


Fig. S21. ^{13}C NMR (125 MHz, $CDCl_3$) spectrum of J

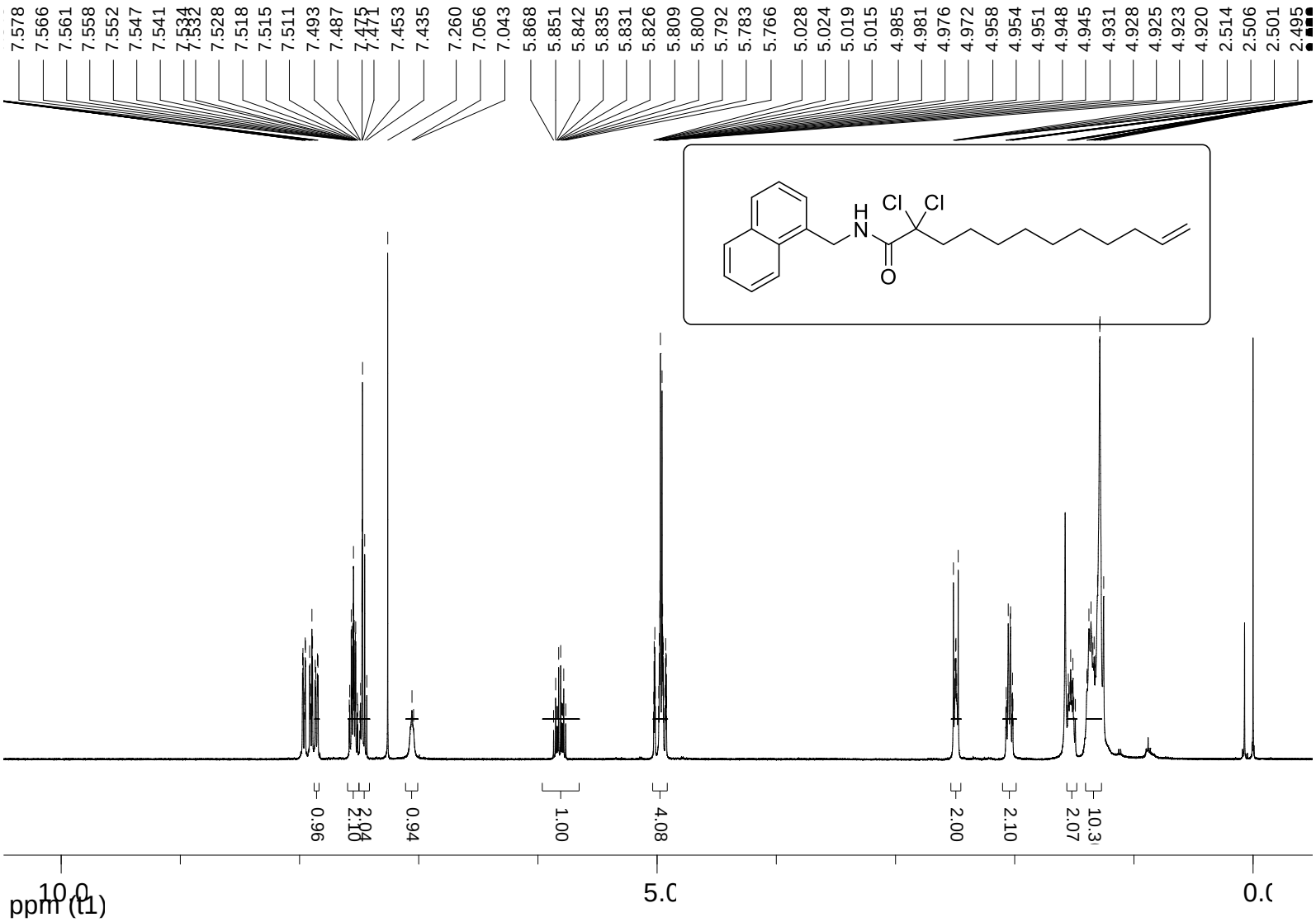


Fig. S22. ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of K

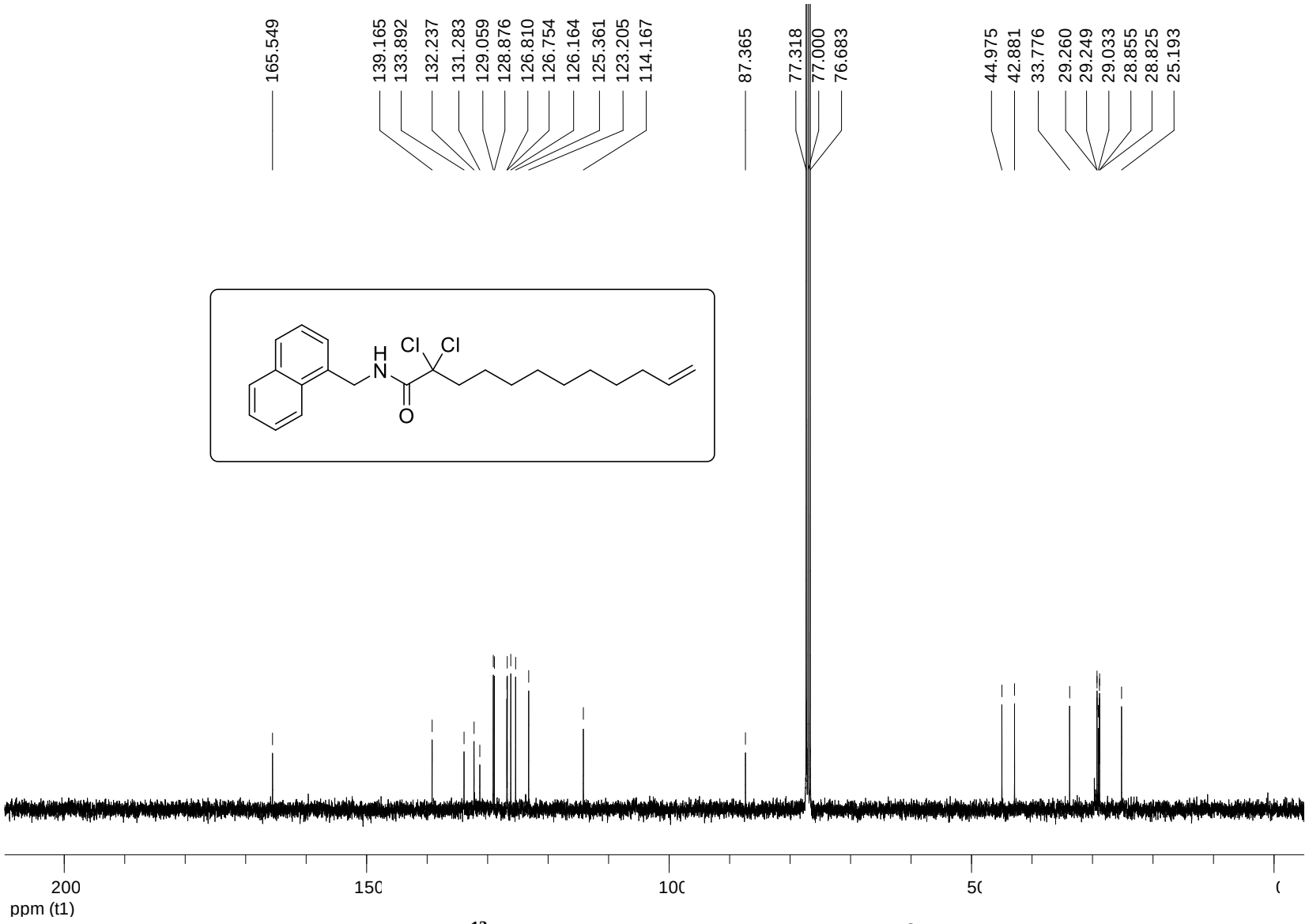


Fig. S23. ^{13}C NMR (125 MHz, $CDCl_3$) spectrum of K

3. Supplementary Tables

Table S1. Performance on the Buchwald–Hartwig coupling HTE Dataset (the best results are in bold).

Split Mode	Measure	RS-coreset	YieldBERT	YieldBERT-DA	Uncertainty-Aware
2.5/97.5	R^2 ↑	**0.656±0.033**	0.436±0.034	0.604±0.031·	0.628±0.062
	MAE(%) ↓	11.976±0.718	15.979±0.817	12.243±0.631	**11.747±1.005**
	RMSE(%) ↓	**15.971±0.805**	20.463±0.623	17.151±0.677	16.586±1.364
5/95	R^2 ↑	**0.773±0.021**	0.622±0.042	0.733±0.027	0.734±0.019
	MAE(%) ↓	**9.534±0.420**	12.117±0.789	9.651±0.338	9.677±0.408
	RMSE(%) ↓	**12.989±0.599**	16.740±0.950	14.073±0.687	14.041±0.492

Table S2. Performance on the Suzuki-Miyaura Cross Coupling HTE Dataset (the best results are in bold).

Split Mode	Measure	RS-corest	YieldBERT	YieldBERT-DA	Uncertainty-Aware	DeepReac+
2.5/97.5	R^2 ↑	**0.470±0.047**	0.330±0.047	0.282±0.047	0.375±0.072	0.125±0.141
	MAE(%) ↓	**15.357±0.616**	17.666±0.496	17.587±0.690	16.705±1.090	18.568±1.668
	RMSE(%) ↓	**20.427±0.902**	22.967±0.804	23.780±0.793	22.156±1.273	24.589±2.200
5/95	R^2 ↑	**0.604±0.019**	0.430±0.040	0.491±0.034	0.567±0.014	0.379±0.063
	MAE(%) ↓	**12.885±0.279**	15.695±0.618	14.294±0.507	13.364±0.223	14.960±0.497
	RMSE(%) ↓	**17.666±0.423**	21.181±0.724	20.016±0.661	18.463±0.308	20.090±0.816

Table S3. Performance on the B-H Dataset Provided by Denmark's Group.

Product Group	Reported result		Our model	
	MAE(%)	R^2	MAE(%)	R^2
a	26.7	0.124	**17.186**	**0.691**
b	14.364	0.777	**12.550**	**0.841**
c	**25.182**	0.257	25.920	**0.455**
d	**9.083**	**0.560**	15.351	-
e	**30.889**	**0.192**	37.436	-
f	**4.222**	**0.781**	6.545	0.510
g	**12.458**	**0.715**	17.007	0.506
h	**14**	-	22.010	-
i	30.958	-	**20.154**	**0.512**
j	**19.875**	-	20.655	-
k	20.375	0.380	**15.214**	**0.620**
l	56.5	-	**7.365**	-
m	30.625	-	**28.580**	-
Average	20.241	0.381	**18.611**	**0.506**

4. Supplementary References

1. Zhao, Q. et al. Boryl Radicals Enabled a Three-Step Sequence to Assemble All-Carbon Quaternary Centers from Activated Trichloromethyl Groups. *J. Am. Chem. Soc.* (2022).