Supporting Information

Formal Cross-Coupling of Amines and Carboxylic Acids to Form sp^3–sp^2 Carbon–Carbon Bonds

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This document contains general information, experimental procedures, supplementary tables, DFT calculations, additional discussion and compound data and spectra. Machine readable reaction data can be accessed at https://github.com/cernaklab/douthwaite-sp3-sp2-cross-coupling-of-activated-amines-and-acids.

Contents

General Information

All reactions were conducted in oven- or flame-dried glassware under an atmosphere of nitrogen unless stated otherwise. Reactions were set up in an MBraun LABmaster Pro Glove Box (H_2O level <0.1 ppm, O_2 level <0.1 ppm), or using standard Schlenk technique with a glass vacuum manifold connected to an inlet of dry nitrogen gas. Tetrahydrofuran, dichloromethane, toluene, acetonitrile and *N*,*N*-dimethylformamide were purified using an MBraun SPS solvent purification system by purging with nitrogen, and then passing the solvent through a column of activated alumina. *N*-methylpyrrolidinone was purchased as anhydrous and degassed by sparging overnight with nitrogen. Other solvents were purchased as anhydrous and used as received. Reagents were purchased from Sigma Aldrich, Thermo Fischer Scientific, Alfa Aesar, Oakwood Chemical, or TCI Chemical. All chemicals were used as received. Glass 1-dram (Fisherbrand™ parts No. 03-339-21B) or 2-dram vials (Fisherbrand™ parts No. 03-339-21D) were used as reaction vessels, fitted with standard screwcaps (#03-452-225 or #03-452-300) or with Teflon-coated silicone septa (#CG-4910-02), and magnetic stir bars (Fisher Scientific #14-513-93 or #14-513-65; stirbars.com #SBM-0803-MIC or #SBM-1003-MIC).

^{1}H NMR spectra were recorded on a Varian MR-500 MHz, Varian MR-400 MHz or Bruker Avance Neo 500 MHz spectrometer. Chemical shifts are reported in parts per million (ppm) and the spectra are calibrated to the resonance resulting from incomplete deuteration of the solvent ($CDCl_3$: 7.26 ppm; DMSO-d_6: 2.50 ppm; MeOD-d_4: 3.31 ppm; Acetone-d_6: 2.05 ppm; D_2O: 4.79 ppm). ^{13}C NMR spectra were recorded on the same spectrometers with complete proton decoupling. Chemical shifts are reported in ppm with the solvent resonance as the internal standard ($^{13}CDCl_3$: 77.16 ppm, t; DMSO-d_6: 39.52 ppm, sept; MeOD-d_4: 49.00 ppm, sept). Data are reported using the abbreviations: s = singlet, d = doublet, t = triplet, q = quartet, p = pentet, h = hextet, m = multiplet, br = broad. Coupling constant(s) are reported in Hz. ^{19}F NMR spectra were recorded on the same spectrometers as above. ^{13}C and ^{19}F signals are singlets unless otherwise stated. ^{1}H-COSY, HSQC and HMBC were used where appropriate to facilitate structural determination.

High resolution mass spectrometry data (HRMS) were obtained on an Agilent 6230 TOF LC/MS equipped with ESI detector in positive mode and on a Micromass AutoSpec Ultima Magnetic Sector instrument with EI detector in positive mode. Reaction analysis was typically performed by thin-layer chromatography on silica gel or using a Waters I-class ACQUITY UPLC-MS (Waters Corporation, Milford, MA, USA) equipped with in-line photodiode array detector (PDA), evaporative light scattering detector (ELSD) and QDa mass detector (Both ESI positive and negative ionization modes). Typically 0.1 µL sample injections were taken from acetonitrile solutions of reaction mixtures or products (~1 mg/mL). A partial loop injection mode was used with the needle placement at 2.0 mm from bottom of the wells and a 0.2 µL air gap at pre-aspiration and post-aspiration. Column used: Waters Cortecs UPLC C18+ column, 2.1mm × 50 mm with (Waters #186007114) with Waters Cortecs UPLC C18+ VanGuard Pre-column 2.1mm × 5 mm (Waters #186007125), Mobile Phase A: 0.1 % formic acid in Optima LC/MS-grade water, Mobile Phase B: 0.1%

formic acid in Optima LC/MS-grade MeCN. Flow rate: 0.8 mL/min. Column temperature: 45 °C. The PDA sampling rate was 20 points/sec. The QDa detector monitored m/z 150-750 with a scan time of 0.06 seconds and a cone voltage of 30 V. The ELSD had a gain of 750, data rate of 10 pps, time constant “normal” 0.2000 sec, a gas pressure of 40.0 psi, with the nebulizer in cooling mode at 75% power level and the drift tube temperature set to 50 °C. The PDA detector range was between 210 nm – 400 nm with a resolution of 1.2 nm. 2 minute and 8 minute methods were used. The method gradients are below: 2 min method, 0 min: 0.8 mL/min, 95% 0.1% formic acid in water/5% 0.1% formic acid in acetonitrile; 1.5 min: 0.8 mL/min, 0.1% 0.1% formic acid in water/99.9% 0.1% formic acid in acetonitrile; 1.91 min : 0.8 mL/min, 95% 0.1% formic acid in water/5% 0.1% formic acid in acetonitrile. 8 min method, 0 min: 0.8 mL/min, 95% 0.1% formic acid in water/5% 0.1% formic acid in acetonitrile; 7.5 min: 0.8 mL/min, 0.1% 0.1% formic acid in water/99.9% 0.1% formic acid in acetonitrile; 7.91 min: 0.8 mL/min, 95% 0.1% formic acid in water/5% 0.1% formic acid in acetonitrile.

Flash chromatography was performed on silica gel (230 – 400 Mesh, Grade 60) under a positive pressure of nitrogen. Thin Layer Chromatography was performed on 25 µm TLC silica gel 60 F254 glass plates purchased from Fisher Scientific (part number: S07876). Visualization was performed using ultraviolet light (254 and 365 nm) and/or potassium permanganate ($KMnO_4$) stain. Reverse-phase prep-HPLC was performed on a Teledyne ISCO CombiFlash® EZ Prep (RediSep Prep C18, 100 Å, 5 µm, 150 mm × 20 mm (part no. 692203810) using water and acetonitrile eluent.

General Procedures

General Procedure A: Synthesis of *N*-Acyl-Glutarimides

A flame-dried round-bottomed flask was charged under a nitrogen atmosphere with a stirrer bar, carboxylic acid (1.0 equiv.), CH_2Cl_2 (*ca.* 0.67 M) and three drops of DMF. The vessel was cooled to 0 °C and thionyl chloride (2 equiv.) was added dropwise to the stirring reaction. The reaction was then heated to reflux at 60 °C for 2 h, and then cooled to room temperature and the volatiles were removed *in vacuo.* A second flame dried round-bottomed flask was charged under nitrogen with a stirrer bar, glutarimide (1.1 equiv.), DMAP (0.1 equiv.), Et_3N (2.0 equiv.) and CH_2Cl_2 (*ca.* 0.88 M wrt to glutarimide) and cooled to 0 °C. The acyl chloride residue was dissolved in CH_2Cl_2 (*ca*. 0.8 M) and added dropwise to the 0 °C solution. The resulting reaction was allowed to slowly warm to room temperature while stirring overnight (typically 16 h), and then quenched with 1M (HCl) or sat. $NaHCO_3$ solution. The layers were separated, and the organic layer was washed with water (x3) and brine and then dried over Na_2SO_4. The volatiles were then removed *in vacuo* to give a crude residue which was purified as stated below for each specific compound. The yields are unoptimized.

General Procedure B: Synthesis of Alkylpyridinium Salts

A round-bottom flask equipped with a magnetic stir bar was charged with triphenylpyrylium tetrafluoroborate (1.98 g, 5.0 mmol, 1.0 equiv.) and ethanol (5 mL, 1.0 M). Amine (5.5 - 6.0 mmol, 1.1 - 1.2 equiv.) was then added with stirring. The reaction was heated to reflux for 5 hours with stirring. After, the reaction was allowed to cool to room temperature, Et_2O (25 mL) was added and the mixture was stirred rigorously overnight for precipitation. The desired product was collected by filtration and washed with Et_2O (25 mL). If no solid formed with Et_2O addition, the mixture was concentrated *in vacuo* and the residue was purified by chromatography with 1-20% Acetone/DCM to give isolated product. The yields are unoptimized.

General Procedure C: Decarbonylative-Deaminative Coupling of *N*-Acyl-Glutarimides and Alkylpyridinium Salts

A stock solution in NMP was prepared inside a N_2-filled glovebox in a flame-dried 1- or 2-dram vial such that it contained (unless otherwise stated) $NiBr_2$•DME (6.2 mg/mL, 20 mM), 5,5'-dimethyl-2,2'-bipyridine **L4** (3.7 mg/mL, 20 mM) and phthalimide **4** (29.4 mg/mL, 200 mM). The stock solution was stirred at room temperature for 1 h, and then added *via* micropipette to a different flame-dried vial containing *N*-acyl-glutarimide (1 equiv.), alkylpyridinium salt (2 equiv.), manganese powder (3 equiv.) and any additive (if required, as specified). The volume of stock solution added was such so that the reaction concentration of *N*-acyl-glutarimide was 0.1 M. The reaction vial was then sealed with a screw cap, followed by a piece of electrical tape around the joint. The vial was then removed from the glovebox and placed into a preheated 80 °C heating block on a hotplate. The reaction was stirred at this temperature for 18 h and then cooled to room temperature. The reaction was quenched with water and EtOAc was added. The layers were separated and the organic layer washed with water (x3) and brine. The organic layer was then dried over Na_2SO_4 and concentrated to *ca.* 10 mL. The solution was then washed through a plug of silica and celite with more EtOAc and concentrated. The crude residue was purified *via* column chromatography as specified.

CAUTION: this reaction may form highly toxic volatile $Ni(CO)_4$ as a byproduct and therefore appropriate personal protective equipment (laboratory coat, gloves, eye protection) and ventilation (fumehood) should be employed at all stages of handling reaction materials, and the appropriate hazardous waste disposal methods should be followed.

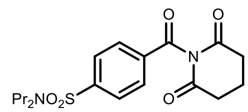
https://www.sigmaaldrich.com/US/en/technical-documents/technical-article/environmental-testing-and-industrial-hygiene/air-testing/nickel-carbonyl

https://www.cdc.gov/niosh/npg/npgd0444.html

Substrate Synthesis

N-Acyl-Glutarimides

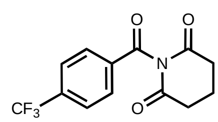
4-(2,6-dioxopiperidine-1-carbonyl)-*N*,*N*-dipropylbenzenesulfonamide (**1**)



Following General Procedure A using probenecid (5.71 g, 20.0 mmol) and purifying v*ia* silica column chromatography (40-65% EtOAc in hexanes) yielded the target compound (5.68 g, 14.9 mmol, 75%) as an off-white solid. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.96 (d, *J* = 8.5 Hz, 2H), 7.90 (d, *J* = 8.5 Hz, 2H), 3.08 (t, *J* = 7.7 Hz, 4H), 2.79 (t, *J* = 6.5 Hz, 4H), 2.16 (p, *J* = 6.5 Hz, 2H), 1.62-1.50 (m, 4H), 0.87 (t, *J* = 7.4 Hz, 6H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 172.1, 170.2, 145.7, 134.7, 130.7, 127.6, 50.2, 32.3, 22.1, 17.4, 11.1.

All data match that previously reported in the literature.[1]

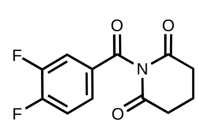
1-(4-(trifluoromethyl)benzoyl)piperidine-2,6-dione (**S2**)



Following General Procedure A using 4-(trifluoromethyl)benzoic acid (1.90 g, 10.0 mmol) and purifying v*ia* silica column chromatography (50% EtOAc in hexanes) yielded the target compound (1.48 g, 5.19 mmol, 52%) as a pale-orange solid.**^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.96 (d, *J* = 8.2 Hz, 2H), 7.75 (d, *J* = 8.2 Hz, 2H), 7.28 (t, *J* = 6.6 Hz, 4H), 2.15 (p, *J* = 6.8 Hz, 2H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 172.1, 170.3, 135.9 (q, $^{2}J_{C-F}$ = 33.1 Hz), 134.8 (q, $^{5}J_{C-F}$ = 0.8 Hz), 130.4, 126.2 (q, $^{3}J_{C-F}$ = 3.8 Hz), 123.3 (q, $^{1}J_{C-F}$ = 273.1 Hz), 32.3, 17.4; **^{19}F NMR (471 MHz, $CDCl_3$)** δ -63.4.

All data match that previously reported in the literature.[1]

1-(3,4-difluorobenzoyl)piperidine-2,6-dione (**S3**)

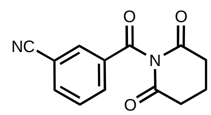


Following modified General Procedure A using 3,4-difluorobenzoic acid (1.30 g, 8.25 mmol, 1.1 equiv.) and glutarimide (848 mg, 7.50 mmol, 1.0 equiv.) and purifying v*ia* silica column chromatography (50-75% EtOAc in hexanes) yielded the target compound (1.47 g, 7.50 mmol, 77%) as an off-white crystalline solid. **^{1}H NMR**

(500 MHz, $CDCl_3$) δ 7.73-7.66 (m, 1H), 7.66-7.59 (m, 1H), 7.32-7.21 (m, 1H), 7.25 (t, *J* = 6.6 Hz 4H), 2.12 (p, *J* = 6.6 Hz, 2H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 172.0, 169.1 (d, $^3J_{C\text{-}F}$ = 2.4 Hz), 154.8 (dd, $^1J_{C\text{-}F}$ = 260.3 Hz, $^2J_{C\text{-}F}$ = 12.9 Hz), 150.6 (dd, $^1J_{C\text{-}F}$ = 252.1 Hz, $^2J_{C\text{-}F}$ = 13.2 Hz), 129.1 (dd, $^3J_{C\text{-}F}$ = 5.3 Hz, $^4J_{C\text{-}F}$ = 3.6 Hz, 127.4 (dd, $^3J_{C\text{-}F}$ = 8.0 Hz, $^4J_{C\text{-}F}$ = 3.6 Hz), 119.4 (dd, $^2J_{C\text{-}F}$ = 18.8 Hz, $^3J_{C\text{-}F}$ = 2.1 Hz), 118.3 (d, $^2J_{C\text{-}F}$ = 18.3 Hz), 32.3, 17.4; **^{19}F NMR (471 MHz, $CDCl_3$)** δ -125.8 - -125.9 (m), -134.8 - -135.0 (m).

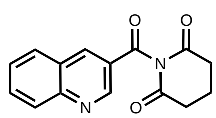
All data match that previously reported in the literature.[2]

3-(2,6-dioxopiperidine-1-carbonyl)benzonitrile (**S4**)



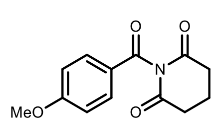
Following General Procedure A using 3-cyanobenzoic acid (1.30 g, 8.25 mmol) and purifying v*ia* silica column chromatography (60-100% EtOAc in hexanes) yielded the target compound (1.33 g, 5.49 mmol, 73%) as an off-white solid. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.12 (dt, *J* = 8.0, 1.3 Hz, 1H), 8.06 (t, *J* = 1.3 Hz, 1H), 7.90 (dt, *J* = 7.8 Hz, 1.2 Hz, 1H), 7.64 (t, *J* = 7.9 Hz, 1H), 2.80 (t, *J* = 6.6 Hz, 4H), 2.17 (t, *J* = 6.6 Hz, 2H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ172.1, 169.6, 137.6, 133.9, 133.5, 133.1, 130.3, 32.3, 17.4.

1-(quinoline-3-carbonyl)piperidine-2,6-dione (**S5**)



Following General Procedure A using quinoline-3-carboxylic acid (866 mg, 5.00 mmol) and purifying v*ia* silica column chromatography (90% EtOAc in hexanes) yielded the target compound (769 mg, 2.87 mmol, 57%) as a pale-yellow solid. The compound shows some decomposition on silica, observed by 2D TLC, and therefore it is advised to rapidly purify the compound when using silica column chromatography. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 9.26 (d, *J* = 2.2 Hz, 1H), 8.64 (d, *J* = 1.9 Hz, 1H), 8.16 (d, *J* = 8.5 Hz, 1H), 7.93 (d, *J* = 8.2 Hz, 1H), 7.88 (td, *J* = 7.2, 1.0 Hz, 1H), 7.64 (t, *J* = 7.6 Hz, 1H), 2.83 (t, *J* = 6.6 Hz, 4H), 2.19 (p, *J* = 6.6 Hz, 2H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 172.0, 169.9, 150.4, 149.5, 139.9, 133.1, 129.7, 129.6, 128.0, 126.7, 124.7, 32.4, 17.5; **HRMS:** m/z: $[M+H]^+$ calc'd for $[C_{15}H_{13}N_2O_3]^+$ expect 269.0921; found 269.0921.

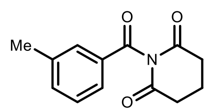
1-(4-methoxybenzoyl)piperidine-2,6-dione (**S6**)



Following General Procedure A using 4-methoxybenzoic acid (761 mg, 5.00 mmol) and purifying v*ia* silica column chromatography (50-100% EtOAc in hexanes) yielded the target compound (957 mg, 3.87 mmol, 77%) as an orange solid. The compound shows some decomposition on silica, observed by 2D TLC, and therefore it is advised to rapidly purify the compound when using silica column chromatography. **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.81 (d, *J* = 8.9 Hz, 2H), 6.93 (d, *J* = 8.9 Hz, 2H), 3.85 (s, 3H), 2.72 (t, *J* = 6.6 Hz, 4H), 2.09 (p, *J* = 6.6 Hz, 2H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 172.1, 169.7, 165.1, 132.7, 124.4, 114.5, 55.7, 32.4, 17.4.

All data match that previously reported in the literature.[3]

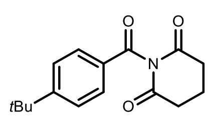
1-(3-methylbenzoyl)piperidine-2,6-dione (**S7**)



Following General Procedure A using 3-methylbenzoic acid (681 mg, 5.00 mmol) and purifying v*ia* silica column chromatography (50% EtOAc in hexanes) yielded the target compound (719 mg, 3.11 mmol, 62%) as a white solid. **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.69 (s, 1H), 7.62 (d, *J* = 7.8 Hz, 1H), 7.44 (d, *J* = 7.5 Hz, 1H), 7.36 (t, *J* = 7.7Hz, 1H), 2.76 (t, *J* = 6.6 Hz, 4H), 2.40 (s, 3H), 2.13 (p, *J* = 6.5 Hz, 2H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 172.1, 171.0, 139.2, 136.0, 131.8, 130.7, 129.1, 127.5, 32.5, 21.4, 17.6.

All data match that previously reported in the literature.[4]

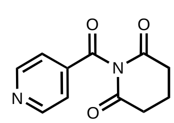
1-(4-(*tert*-butyl)benzoyl)piperidine-2,6-dione (**S8**)



Following General Procedure A using 4-(*tert*-butyl)benzoic acid (1.00 g, 5.61 mmol) and purifying v*ia* silica column chromatography (50% EtOAc in hexanes) yielded the target compound (1.10 g, 5.61 mmol, 72%) as a white solid. **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.79 (d, *J* = 8.6 Hz, 2H), 7.49 (d, *J* = 8.6 Hz, 2H), 2.74 (t, *J* = 6.5 Hz, 4H), 2.11 (p, *J* = 6.5 Hz, 2H), 1.32 (s, 9H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 172.1, 170.5, 159.2, 130.3, 129.1, 126.3, 35.4, 2104, 31.0, 17.6.

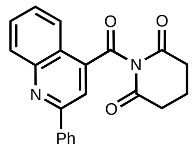
All data match that previously reported in the literature.[5]

1-isonicotinoylpiperidine-2,6-dione (**S9**)



Following General Procedure A using isonicotinic acid (616 mg, 5.00 mmol) and purifying v*ia* silica column chromatography (60-100% EtOAc in hexanes) yielded the target compound (580 mg, 2.66 mmol, 53%) as a white solid. **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.86-8.82 (m, 2H), 7.63-7.61 (m, 2H), 2.78 (t, *J* = 6.6 Hz, 4H), 2.15 (p, *J* = 6.6 Hz, 2H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 171.9, 170.6, 151.3, 138.4, 122.3, 32.3, 17.4; **HRMS:** m/z: $[M+H]^+$ calc'd for $[C_{11}H_{11}N_2O_3]^+$ expect 219.0764; found 219.0770.

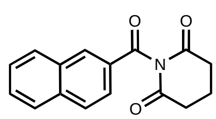
1-(2-phenylquinoline-4-carbonyl)piperidine-2,6-dione (**S10**)



Following modified General Procedure A using cinchophen (5.00 g, 20.1 mmol) at 0.30 M instead of 0.67 M, and purifying v*ia* silica column chromatography (1% MeOH in CH_2Cl_2) yielded the target compound (5.92 g, 2.66 mmol, 53%) as a white solid. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.67 (d, *J* = 8.6 Hz, 1H), 8.25 (d, *J* = 8.5 Hz, 1H), 8.08 (d, *J* = 7.5 Hz, 2H), 7.94 (s, 1H), 7.82 (t, *J* = 7.5 Hz, 1H), 7.70 (t, *J* = 8.0 Hz), 7.58-7.46 (m, 3H), 2.79 (t, *J* = 6.5 Hz, 4H), 2.14 (p, *J* = 6.5 Hz, 2H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 172.2, 170.8, 156.9, 149.4, 138.7, 137.9, 130.6, 130.4, 129.9, 129.1, 128.9, 127.5, 125.1, 123.1, 119.2, 32.6, 17.4.

All data match that previously reported in the literature.[5]

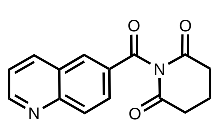
1-(2-naphthoyl)piperidine-2,6-dione (**30**)



Following General Procedure A using 2-napthoic acid (1.47 g, 8.54 mmol) and purifying v*ia* silica column chromatography (60-100% EtOAc in hexanes) yielded the target compound (1.79 g, 6.70 mmol, 78%) as a white solid. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.34 (s, 1H), 7.94 (d, *J* = 8.4 Hz, 1H), 7.92 (s, 2H), 7.88 (d, *J* = 8.2 Hz), 7.64 (t, *J* = 7.5 Hz, 1H), 7.56 (t, *J* = 7.7 Hz, 1H), 2.83 (t, *J* = 6.5 Hz, 4H), 2.20 (q, *J* = 6.5 Hz, 2H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 172.1, 171.0, 136.4, 132.7, 132.5, 129.8, 129.5, 129.2, 129.2, 127.9, 127.2, 124.8, 32.5, 17.6.

All data match that previously reported in the literature.[1]

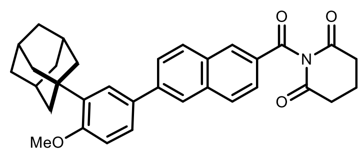
1-(quinoline-6-carbonyl)piperidine-2,6-dione (**S11**)



Following General Procedure A using quinoline-6-carboxylic acid (1.73 g, 10.0 mmol) and purifying v*ia* silica column chromatography (80-90% EtOAc in hexanes) yielded the target compound (1.73 g, 6.45 mmol, 65%) as a white solid. The compound shows some decomposition on silica, observed by 2D TLC, and therefore it is advised to rapidly purify the compound when using silica column chromatography. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 9.02 (dd, *J* = 4.2, 1.6 Hz, 1H), 8.37 (d, *J* = 1.7 Hz, 1H), 8.24 (d, *J* = 8.4 Hz, 1H, 8.17 (d, *J* = 8.9 Hz, 1H), 8.10 (dd, *J* = 8.9, 1.9 Hz, 1H), 7.45 (dd, *J* = 8.3, 4.3 Hz, 1H), 2.81 (t, *J* = 6.6 Hz, 4H), 2.17 (p, *J* = 6.5 Hz, 2H); **^{13}C NMR (126 MHz, $CDCl_3$),** δ172.2, 170.7, 153.5, 150.6, 137.8, 132.5, 130.8, 129.8, 128.4, 127.5, 122.3, 32.4, 17.5.

All data match that previously reported in the literature.[6]

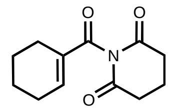
1-(6-(3-(adamantan-1-yl)-4-methoxyphenyl)-2-naphthoyl)piperidine-2,6-dione (**S12**)



A flame-dried round-bottomed flask was charged with and stirrer bar, adapalene (450 mg, 1.09 mmol, 1 equiv.) and CH_2Cl_2 (10 mL) under a nitrogen atmosphere. The resulting solution was cooled to 0 °C and DMF (100 uL) was added, followed by dropwise addition of oxalyl chloride (561 uL, 6.54 mmol, 6.0 equiv.). The reaction was allowed to warm to room temperature, and then stirred for 4 h, after which time the volatiles were removed *in vacuo*. The acyl chloride residue was dissolved in CH_2Cl_2 (10 mL) under nitrogen and cooled to 0 °C. Glutarimide (148 mg, 1.31 mmol, 1.2 equiv.) and DMAP (13.3 mg, 0.11 mmol, 0.10 equiv.) were added, followed by dropwise addition of Et_3N (314 µL, 2.18 mmol, 2.0 equiv.). The reaction was slowly allowed to room temperature, stirred for 16 h, and then quenched with sat. $NaHCO_3$ solution. The layers were separated, and the organic layer washed with water (x3) and brine, dried over Na_2SO_4, filtered and concentrated. The crude residue was purified *via* silica column chromatography. 2 columns were used, 50% EtOAc in Hexanes followed by 1% MeOH in CH_2Cl_2. This afforded the title compound as a pale-yellow solid (127 mg, 0.250 mmol, 23%). **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.34 (s, 1H), 8.01 (s, 1H), 7.99-7.89 (m, 3H), 7.82 (dd, *J* = 8.4, 1.3 Hz, 1H), 7.61 (d, *J* = 2.2 Hz, 1H), 7.55 (dd, *J* = 8.4, 2.2 Hz, 1H, 7.00 (d, *J* = 8.5 Hz, 1H), 3.91 (s, 3H), 2.84 (t, *J* = 6.5 Hz, 4H), 2.26-2.15 (m, 8H), 2.11 (s, br, 3H), 1.81 (s, br, 6H); **^{13}C NMR (126 MHz, $CDCl_3$)** 172.1, 170.8, 159.2, 142.7, 139.1, 136.9, 132.5, 132.1, 131.2, 130.2, 129.2, 128.7, 126.9, 126.0, 125.9, 125.2, 124.8, 112.1, 55.2, 40.6, 37.2, 37.1, 32.5, 29.1, 17.6.

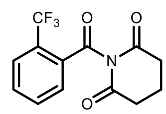
All data match that previously reported in the literature.[7]

1-(cyclohex-1-ene-1-carbonyl)piperidine-2,6-dione (**S13**)



Following modified General Procedure A using 1-cyclohexene-1-carboxylic acid (1.42 g, 11.3 mmol, 1.5 equiv.), glutarimide (848 mg, 7.50 mmol, 1.0 equiv.) and DMAP (229 mg, 1.88 mmol, 0.25 equiv.), and purifying v*ia* silica column chromatography (75% EtOAc in hexanes) yielded the target compound (495 mg, 2.24 mmol, 30%) as a pale yellow solid. **^{1}H NMR (500 MHz, $CDCl_3$)** δ 6.80-6.75 (m, 1H), 2.69 (t, J = 6.5 Hz, 4H), 2.40-2.33 (m, 2H), 2.30-2.23 (m, 2H), 2.06 (p, J = 6.5 Hz, 2H), 1.72-1.66 (m, 2H), 1.66-1.60 (m, 2H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 171.8, 171.0, 146.2, 134.6, 32.4, 26.4, 23.3, 21.5, 21.0, 17.4; **HRMS(EI+):** m/z: $[M]^+$ calc'd for $[C_{12}H_{15}NO_3]^+$ expect 221.1052; found 221.1041.

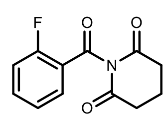
1-(2-(trifluoromethyl)benzoyl)piperidine-2,6-dione (**S14**)



Following General Procedure A using 2-(trifluoromethyl)benzoic acid (951 mg, 5.00 mmol) and purifying v*ia* silica column chromatography (25-75% EtOAc in hexanes) yielded the target compound (691 mg, 2.42 mmol, 49%) as a pale-orange solid. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.83-7.77 (m, 1H), 7.71-7.58 (m, 3H), 2.72 (t, J = 6.5 Hz, 4H), 2.06 (p, J = 6.5 Hz, 2H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 171.8, 168.6, 133.1 (q, J_{C-F} = 1.5 Hz), 132.9, 132.3 (q, J_{C-F} = 0.5 Hz), 130.9, 129.0 (q, $^{2}J_{C-F}$ = 33.1 Hz), 127.6 (q, $^{3}J_{C-F}$ = 5.8 Hz), 123.2 (q, $^{1}J_{C-F}$ = 274.1 Hz), 32.8, 17.0; **^{19}F NMR (471 MHz, $CDCl_3$)** δ -58.9.

All data match that previously reported in the literature.[4]

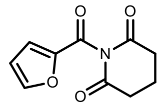
1-(2-fluorobenzoyl)piperidine-2,6-dione (**S15**)



Following General Procedure A using 2-fluorobenzoic acid (701 mg, 5.00 mmol) and purifying v*ia* silica column chromatography (45-60% EtOAc in hexanes) yielded the target compound (780 mg, 3.32 mmol, 66%) as a pale-orange solid. **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.99 (td, J = 7.9, 1.5 Hz, 1H), 7.61-7.50 (m, 1H), 7.23 (t, J = 7.6 Hz, 1H), 7.06 (dd, J = 11.9, 8.4 Hz, 1H), 2.66 (t, J = 6.7 Hz, 4H), 2.01 (q, J = 6.5 Hz, 2H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 171.8, 167.0 (d, $^{3}J_{C-F}$ = 1.9 Hz), 161.7 (d, $^{1}J_{C-F}$ = 258.1 Hz), 136.8 (d, $^{3}J_{C-F}$ = 9.9 Hz), 132.6, 125.0 (d, $^{4}J_{C-F}$ = 3.6 Hz), 120.2 (d, $^{3}J_{C-F}$ = 7.8 Hz), 117.0 (d, $^{2}J_{C-F}$ = 23.5 Hz), 32.2, 17.0; **^{19}F NMR (471 MHz, $CDCl_3$)** δ -113.3.

All data match that previously reported in the literature.[4]

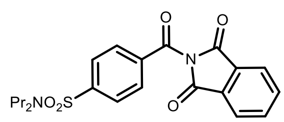
1-(furan-2-carbonyl)piperidine-2,6-dione (**S16**)



Following General Procedure A using furan-2-carboxylic acid (560 mg, 5.00 mmol) and purifying v*ia* silica column chromatography (45-70% EtOAc in hexanes) yielded the target compound (495 mg, 2.39 mmol, 49%) as a beige solid. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.60 (d, *J* = 0.9 Hz, 1H), 7.38 (d, *J* = 3.6 Hz, 1H), 6.60 (dd, *J* = 3.6, 1.6, 1H), 2.74 (t, *J* = 6.6 Hz, 4H), 2.10 (p, *J* = 6.6 Hz, 2H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 171.6, 159.3, 148.2, 147.5, 122.0, 113.6, 32.4, 17.4.

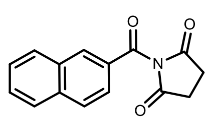
All data match that previously reported in the literature.[2]

4-(1,3-dioxoisoindoline-2-carbonyl)-*N*,*N*-dipropylbenzenesulfonamide (**45**)



Following a modified General Procedure A using probenecid (1.43 g, 5.00 mmol) and phthalimide **4** (736 mg, 5.00 mmol) as substrates, yielded the target compound as an off-white solid (1.90 g, 4.58 mmol, 92%). The compound was found to decompose on silica by 2D TLC, and so was used without further purification. NMR analysis confirmed the compound was pure. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.04-7.98 (m, 2H), 7.97-7.85 (m, 6H), 3.12 (t, *J* = 7.6 Hz, 4H), 1.56 (h, *J* = 7.7 Hz, 4H), 0.88 (t, *J* = 7.3 Hz, 6H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 166.0, 165.2, 145.1, 135.8, 135.7, 131.2, 130.8, 127.1, 124.7, 50.0, 22.0, 11.2; **HRMS:** m/z: $[M+H]^+$ calc'd for $[C_{21}H_{23}N_2O_5S]^+$ expect 415.1322; found 415.1320.

1-(2-naphthoyl)pyrrolidine-2,5-dione (**S17**)

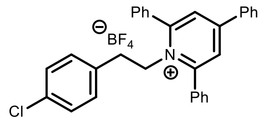


Following a modified General Procedure A using 2-napthoic acid (861 mg, 5.00 mmol) and succinimide (545 mg, 5.50 mmol) as substrates, and purifying v*ia* silica column chromatography (40-100% EtOAc in hexanes) yielded the target compound (1.03 g, 4.07 mmol, 81%) as a white solid. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.35 (s, 1H), 8.00-7.83 (m, 4H), 7.65 (td, *J* = 7.6, 0.9 Hz, 1H), 7.57 (td, *J* = 7.6, 0.9 Hz, 1H), 2.98 (s, 3H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 174.9, 167.9, 136.5, 133.3, 132.3, 129.9, 129.7, 129.0, 128.7, 127.9, 127.3, 124.9, 29.2.

All data match that previously reported in the literature.[8,9]

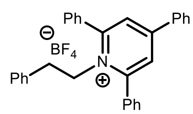
Alkylpyridinium Salts

1-(4-chlorophenethyl)-2,4,6-triphenylpyridin-1-ium tetrafluoroborate (**2**)



Following General Procedure B, using 2-(4-chlorophenyl)ethan-1-amine (2.00 g, 12.9 mmol) affords **2** as a white solid (5.30 g, 9.90 mmol, 93%). **^{1}H NMR (500 MHz, DMSO-d$_6$)** δ 8.50 (s, 2H), 8.28 (d, *J* = 7.5 Hz, 2H), 7.82 (dd, *J* = 7.8, 1.8 Hz, 4H), 7.77-7.69 (m, 6H), 7.67 (dt, *J* = 7.2, 2.0 Hz, 1H), 7.63 (t, *J* = 7.8 Hz, 2H), 7.18 (d, *J* = 8.4 Hz, 2H), 6.42 (d, *J* = 8.4 Hz, 2H), 4.53 (t, *J* = 7.6 Hz, 2H), 2.63 (t, *J* = 7.6 Hz, 2H); **^{13}C NMR (126 MHz, DMSO-d$_6$)** δ 156.6, 154.9, 135.1, 133.6, 133.4, 133.0, 132.4, 131.5, 130.4, 130.1, 129.8, 129.6, 129.2, 129.2, 126.5, 55.9, 34.4; **HRMS:** m/z: [M]$^+$ calc'd for [$C_{31}H_{25}NCl$]$^+$ expect 446.1670; found 446.1676.

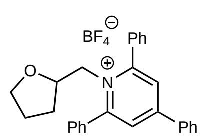
1-phenethyl-2,4,6-triphenylpyridin-1-ium tetrafluoroborate (**S18**)



Following General Procedure B, using 2-phenylethan-1-amine (1.50 g, 12.4 mmol) affords **S18** as a white solid (4.85 g, 9.71 mmol, 93%). **^{1}H NMR (499 MHz, DMSO-d$_6$)** δ 8.50 (s, 2H), 8.27 (d, *J* = 7.5, 2H), 7.87-7.82 (m, 4H), 7.78-7.70 (m, 6H), 7.78-7.60 (m, 3H), 7,19-7.08 (m, 3H), 6.38 (d, *J* = 7.1, 2H), 4.53 (t, *J* = 8.0, 2H), 2.65 (t, *J* = 7.9, 2H); **^{13}C NMR (126 MHz, DMSO-d$_6$)** δ 156.6, 154.9, 136.1, 133.6, 133.4, 132.9, 131.5, 130.1, 129.7, 129.6, 129.2, 129.2, 128.5, 127.6, 126.5, 56.2, 35.2.

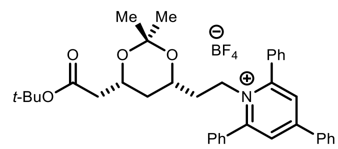
All data match that previously reported in the literature.[10]

2,4,6-triphenyl-1-((tetrahydrofuran-2-yl)methyl)pyridin-1-ium tetrafluoroborate (**S19**)



Following General Procedure B, using (tetrahydrofuran-2-yl)methanamine (1.00 g, 9.89 mmol) affords **S19** as a white solid (3.00 g, 6.00 mmol, 80%). **^{1}H NMR (499 MHz, DMSO-d$_6$)**: δ 8.46 (s, 2H), 8.31-8.25 (m, 2H), 7.96-7.90 (m, 4H), 7.76-7.66 (m, 6H), 7.69-7.59 (m, 3H), 4.70 (dd, *J* = 14.4, 3.3 Hz, 1H), 4.49 (dd, *J* = 14.4, 9.8 Hz, 1H), 3.72-3.60 (m, 1H), 3.42-3.32 (m, 1H), 3.16-3.08 (m, 1H), 1.56-1.43 (m, 2H), 1.22-1.09 (m, 2H); **^{13}C NMR (126 MHz, DMSO-d$_6$)**: δ 156.8, 154.5, 133.4, 133.2, 132.4, 130.7, 129.7, 129.6, 129.1, 128.8, 125.9, 75.5, 67.4, 58.0, 28.4, 24.7; **HRMS:** m/z: [M]$^+$ calc'd for [$C_{28}H_{26}NO$]$^+$ expect 392.2009; found 392.2005.

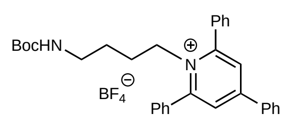
1-(2-((4*R*,6*R*)-6-(2-(*tert*-butoxy)-2-oxoethyl)-2,2-dimethyl-1,3-dioxan-4-yl)ethyl)-2,4,6-triphenylpyridin-1-ium tetrafluoroborate (**S20**)



Following General Procedure B, using *tert*-butyl 2-((4*R*,6*R*)-6-(2-aminoethyl)-2,2-dimethyl-1,3-dioxan-4-yl)acetate (1.00 g, 3.66 mmol) affords **S20** as a white solid (1.60 g, 2.50 mmol, 84%). **^{1}H NMR (499 MHz, $CDCl_3$):** δ 7.83 (s, 2H), 7.80-7.75 (m, 4H), 7.75-7.71 (m, 2H), 7.62-7.57 (m, 6H), 7.56-7.51 (m, 1H), 7.51-7.46 (m, 2H), 4.67-4.58 (m, 1H), 4.50-4.42 (m, 1H), 3.99-3.92 (m, 1H), 3.29-3.22 (m, 1H), 2.23 (dd, *J* = 15.3, 7.2 Hz, 1H), 2.11 (dd, *J* = 15.4, 5.9 Hz, 1H), 1.60-1.50 (m, 2H), 1.39 (s, 9H), 1.13 (s, 3H), 1.11-1.06 (m, 1H), 0.99 (s, 3H), 0.69 (q, *J* = 11.7 Hz, 1H); **^{13}C NMR (126 MHz, $CDCl_3$):** δ 170.1, 156.8, 156.0, 134.2, 132.9, 132.1, 131.2, 129.8, 129.5, 129.3, 128.3, 126.9, 98.6, 80.8, 66.1, 65.7, 51.9, 42.4, 35.9, 35.4, 29.9, 28.2, 19.6.

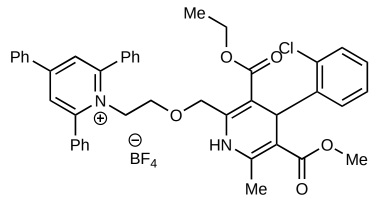
All data match that previously reported in the literature.[11]

1-(4-((*tert*-butoxycarbonyl)amino)butyl)-2,4,6-triphenylpyridin-1-ium tetrafluoroborate (**S21**)



A round-bottom flask equipped with a magnetic stir bar was charged with *tert*-butyl (4-aminobutyl)carbamate hydrochloride (500 mg, 2.22 mmol, 1.2 equiv.). Ethanol (2 ml, 1 M) and triethylamine (0.310 ml, 1.2 equiv.) were added and stirred for 20 min followed by addition of triphenylpyrylium tetrafluoroborate (735 mg, 1.85 mmol, 1.0 equiv.). Reaction was heated to reflux for 5 hours with stirring. After reaction was allowed to cool to room temperature, Et_2O (25 mL) was added, and the mixture was stirred rigorously overnight for precipitation. The desired product was collected by filtration and washed with Et_2O (25 mL) affording **S21** as a white solid (1.00 g, 1.77 mmol, 95%). **^{1}H NMR (499 MHz, DMSO-d_6):** δ 8.47 (s, 2H), 8.27 (dd, *J* = 7.2, 1.9 Hz, 2H), 7.92-7.86 (m, 4H), 7.74-7.69 (m, 6H), 7.67-7.59 (m, 3H), 6.56 (t, *J* = 5.7 Hz, 1H), 4.37 (t, *J* = 7.7 Hz, 2H), 2.47-2.41 (m, 2H), 1.41-1.25 (m, 11H), 0.86-0.76 (m, 2H); **^{13}C NMR (126 MHz, DMSO-d_6):** δ 156.0, 155.3, 154.2, 133.1, 133.0, 132.4, 130.9, 129.6, 129.3, 129.1, 128.7, 126.1, 77.5, 54.3, 38.7, 28.2, 26.4, 26.0; **HRMS:** m/z: $[M]^+$ calc'd for $[C_{32}H_{35}N_2O_2]^+$ expect 479.2693; found 479.2684.

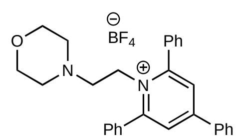
1-(2-((4-(2-chlorophenyl)-3-(ethoxycarbonyl)-5-(methoxycarbonyl)-6-methyl-1,4-dihydropyridin-2-yl)methoxy)ethyl)-2,4,6-triphenylpyridin-1-ium tetrafluoroborate (**S22**)



A round-bottom flask equipped with a magnetic stir bar was charged with triphenylpyrylium tetrafluoroborate (1.59 g, 4.01 mmol, 1.0 equiv.) and 3-ethyl 5-methyl 2-((2-aminoethoxy)methyl)-4-(2-chlorophenyl)-6-methyl-1,4-dihydropyridine-3,5-dicarboxylate besylate (2.50 g, 4.41 mmol, 1.1 equiv.). DCM (8ml, 0.5 M) along with 2 g powdered mol sieves were added. Triethylamine (1.12ml, 2.0 equiv.) was added and stirred for 20 min followed by addition of acetic acid (0.460 mL, 2 equiv.). The reaction was stirred at room temperature for 5 hours. The mixture was concentrated *in vacuo* and the residue was purified by silica column chromatography with 1-20% Acetone/DCM, affording **S22** as a yellow solid (2.90 g, 3.70 mmol, 92%). **^{1}H NMR (499 MHz, $CDCl_3$):** δ 7.81-7.75 (m, 6H), 7.64 (d, *J* = 7.7 Hz, 2H), 7.52-7.47 (m, 6H), 7.44-7.38 (m, 2H), 7.28 (d, *J* = 7.6 Hz, 1H), 7.17 (d, *J* = 7.9 Hz, 1H), 7.06-7.00 (m, 2H), 7.00-6.95 (m, 1H), 5.33 (s, 1H), 4.83-4.75 (m, 2H), 4.19 (d, *J* = 13.4 Hz, 1H), 4.08 (d, *J* = 13.4 Hz, 1H), 3.92-3.82 (m, 2H), 3.56 (s, 3H), 3.44-3.38 (m, 1H), 3.37-3.31 (m, 1H), 2.18 (s, 3H), 1.06 (t, *J* = 7.1 Hz, 3H); **^{13}C NMR (126 MHz, $CDCl_3$):** δ 168.0, 166.7, 157.2, 155.9, 145.8, 145.1, 143.7, 133.9, 133.0, 132.1, 132.1, 131.3, 131.0, 129.7, 129.4, 129.3, 129.1, 128.1, 127.4, 127.0, 126.7, 103.5, 103.0, 67.8, 67.3, 59.8, 53.7, 50.7, 36.9, 18.9, 14.2.

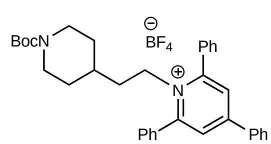
All data match that previously reported in the literature.[12]

1-(2-morpholinoethyl)-2,4,6-triphenylpyridin-1-ium tetrafluoroborate (**S23**)



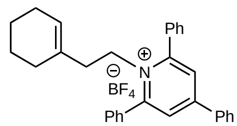
Following General Procedure B, using 2-morpholinoethan-1-amine (1.50 g, 11.5 mmol) affords **S23** as a yellow solid (4.50 g, 8.90 mmol, 92%). **^{1}H NMR (499 MHz, DMSO-d_6)** δ 8.46 (s, 2H), 8.29-8.25 (m, 2H), 7.99-7.94 (m, 4H), 7.76-7.69 (m, 6H), 7.68-7.59 (m, 3H), 4.57 (t, *J* = 6.9 Hz, 2H), 3.32-3.26 (m, 4H), 2.27 (t, *J* = 6.9 Hz, 2H), 1.81-1.76 (m, 4H); **^{13}C NMR (126 MHz, DMSO-d_6)** δ 156.5, 154.3, 133.2, 133.1, 132.4, 131.0, 129.6, 129.6, 129.1, 128.7, 125.9, 65.7, 56.2, 52.5, 51.6; **HRMS:** m/z: $[M]^+$ calc'd for $[C_{29}H_{29}N_2O]^+$ expect 421.2274; found 421.2272.

1-(2-(1-(*tert*-butoxycarbonyl)piperidin-4-yl)ethyl)-2,4,6-triphenylpyridin-1-ium tetrafluoroborate (**S24**)



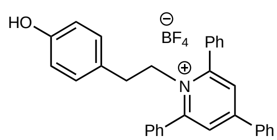
Following General Procedure B, using *tert*-butyl 4-(2-aminoethyl)piperidine-1-carboxylate (1.50 g, 6.57 mmol) affords **S24** as a white solid (2.80 g, 4.60 mmol, 84%). **^{1}H NMR (499 MHz, DMSO-d$_6$)** δ 8.46 (s, 2H), 8.30-8.19 (m, 2H), 7.89 (dd, *J* = 6.6, 2.9 Hz, 4H), 7.78-7.69 (m, 6H), 7.93-7.85 (m, 3H), 4.45-4.33 (m, 2H), 3.71-3.57 (m, 2H), 2.54-2.31 (br, 2H), 1.38-1.29 (m, 11H), 1.00-0.85 (m, 3H), 0.47-0.35 (m, 2H); **^{13}C NMR (126 MHz, DMSO-d$_6$)** δ 155.9, 154.2, 153.7, 133.2, 132.9, 132.3, 130.9, 129.6, 129.2, 129.0, 128.6, 126.1, 78.5, 52.1, 43.1 (br), 35.2, 32.2, 30.4, 28.0; **HRMS:** m/z: [M]$^+$ calc'd for $[C_{35}H_{39}N_2O_2]^+$ expect 519.3006; found 519.2999.

1-(2-(cyclohex-1-en-1-yl)ethyl)-2,4,6-triphenylpyridin-1-ium tetrafluoroborate (**S25**)



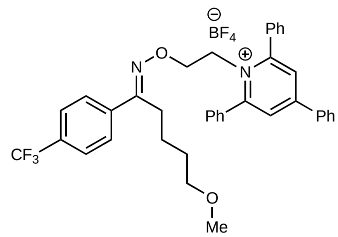
Following General Procedure B, using 2-(cyclohex-1-en-1-yl)ethan-1-amine (1.50 g, 12.0 mmol) affords **S25** as a white solid (4.50 g, 8.90 mmol, 90%). **^{1}H NMR (499 MHz, DMSO-d$_6$)** δ 8.48 (s, 2H), 8.27 (d, *J* = 7.7 Hz, 2H), 7.96-7.87 (m, 4H), 7.79-7.70 (m, 6H), 7.69-7.57 (m, 3H), 4.90-4.82 (m, 1H), 4.43-4.32 (m, 2H), 2.06-1.93 (m, 2H), 1.75-1.66 (m, 2H), 1.33-1.24 (m, 4H), 1.16-1.08 (m, 2H); **^{13}C NMR (126 MHz, DMSO-d$_6$)** δ 156.0, 154.2, 133.2, 132.9, 132.3, 132.0, 131.0, 129.6, 129.3, 129.1, 128.7, 126.0, 124.5, 53.6, 37.1, 26.6, 24.4, 21.9, 21.3; **HRMS:** m/z [M]$^+$ calc'd for $[C_{31}H_{30}]^+$ expect 416.2362; found 416.2371.

1-(4-hydroxyphenethyl)-2,4,6-triphenylpyridin-1-ium tetrafluoroborate (**S26**)



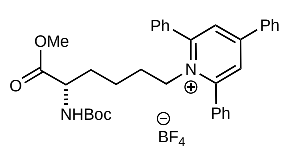
Following General Procedure B, using 4-(2-aminoethyl)phenol (1.50 g, 10.9 mmol) affords **S26** as a green solid (4.40 g, 8.50 mmol, 94%). **^{1}H NMR (499 MHz, DMSO-d$_6$)** δ 9.38 (s, 1H), 8.48 (s, 2H), 8.27 (d, *J* = 7.6 Hz, 2H), 7.89-7.80 (m, 4H), 7.80-7.69 (m, 6H), 7.69-7.59 (m, 3H), 6.51 (d, *J* = 7.9 Hz, 2H), 6.18 (d, *J* = 8.0 Hz, 2H), 4.47 (t, *J* = 7.9 Hz, 2H), 2.53 (t, *J* = 7.8 Hz, 2H); **^{13}C NMR (126 MHz, DMSO-d$_6$)** δ 156.5, 156.1, 154.4, 133.2, 133.0, 132.4, 131.0, 129.6, 129.3, 129.1, 129.1, 128.7, 126.0, 125.5, 115.5, 56.1, 34.0; **HRMS:** m/z: [M]$^+$ calc'd for $[C_{31}H_{26}NO]^+$ expect 428.2009; found 428.2004.

(*E*)-1-(2-(((5-methoxy-1-(4-(trifluoromethyl)phenyl)pentylidene)amino)oxy)ethyl)-2,4,6-triphenylpyridin-1-ium tetrafluoroborate (**S27**)



A round-bottom flask equipped with a magnetic stir bar was charged with (*E*)-5-methoxy-1-(4-(trifluoromethyl)phenyl)pentan-1-one *O*-(2-aminoethyl) oxime maleate (600 mg, 1.38 mmol, 1.2 equiv.). Ethanol (2 ml, 1 M) and triethylamine (0.350 ml, 2 equiv.) were added and stirred for 20 min followed by addition of triphenylpyrylium tetrafluoroborate (497 mg, 1.26 mmol, 1 equiv.). Reaction was heated to reflux for 5 hours with stirring. After reaction was allowed to cool to room temperature, Et_2O (25 mL) was added, and the mixture was stirred rigorously overnight for precipitation. The desired product was collected by filtration and washed with Et_2O (25 mL) to afford **S27** as a white solid (760 mg, 1.09 mmol, 87%). **^{1}H NMR (499 MHz, DMSO-d$_6$)** δ 8.42 (s, 2H), 8.14 (d, *J* = 7.8 Hz, 2H), 7.95-7.89 (m, *J* = 4H), 7.75-7.68 (m, 6H), 7.64 (t, *J* = 7.4 Hz, 1H), 7.61-7.52 (m, 6H), 4.94 (t, *J* = 5.5 Hz, 2H), 4.02 (t, *J* = 5.4 Hz, 2H), 3.16 (t, *J* = 6.2 Hz, 2H), 3.11 (s, 3H), 2.60 (t, *J* = 7.7 Hz, 2H), 1.40-1.32 (m, 2H), 1.30-1.22 (m, 2H); **^{13}C NMR (126 MHz, DMSO-d$_6$)** δ 158.4, 157.1, 154.9, 137.8, 133.2, 132.9, 132.4, 131.2, 129.7, 129.5 (q, $^2J_{C\text{-}F}$ = 31.9 Hz), 129.4, 129.2, 128.6, 126.8, 125.8, 125.3 (q, $^3J_{C\text{-}F}$ = 3.8 Hz), 124.0 (q, $^1J_{C\text{-}F}$ = 272.4 Hz), 71.2, 70.0, 57.7, 54.9, 28.8, 25.0, 22.6; **^{19}F NMR (470 MHz, DMSO-d$_6$)** δ -61.3, -148.3 (minor), -148.3 (major) (d, *J* = 2.3 Hz); **HRMS:** m/z: $[M]^+$ calc'd for $[C_{38}H_{36}F_3N_2O_2]^+$ expect 609.2723; found 609.2731.

(*S*)-1-(5-((*tert*-butoxycarbonyl)amino)-6-methoxy-6-oxohexyl)-2,4,6-triphenylpyridin-1-ium tetrafluoroborate (**S28**)

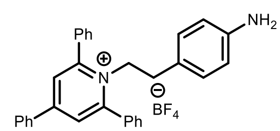


A round-bottom flask equipped with a magnetic stir bar was charged with methyl (*tert*-butoxycarbonyl)-*L*-lysinate hydrochloride (300 mg, 1.01 mmol, 1.2 equiv.). Ethanol (2 ml, 1 M) and triethylamine (0.14 ml, 1.2 equiv.) were added and stirred for 20 min followed by addition of triphenylpyrylium tetrafluoroborate (334 mg, 0.84 mmol, 1.0 equiv.). Reaction was heated to reflux for 5 hours with stirring. The mixture was concentrated in vacuo and purifying v*ia* silica column chromatography (0-10% Acetone/DCM) affords **S28** as a white solid (530 mg, 0.73 mmol, 87%). **^{1}H NMR (500 MHz, CDCl$_3$)** δ 7.80 (s, 2H), 7.79-7.74 (m, 4H), 7.72-7.67 (m, 2H), 7.62-7.55 (m, 6H), 7.55-7.49 (m, 1H), 7.46 (t, *J* = 7.9 Hz, 2H), 4.82 (d, *J* = 8.2 Hz, 1H), 4.37 (t, *J* = 7.9 Hz, 2H), 3.92 (q, *J* = 5.2 Hz, 1H), 3.63 (s, 3H), 1.52-1.43 (m, 2H), 1.38 (s, 9H), 1.30-1.16

(m, 1H), 1.10-1.00 (m, 1H), 0.88-0.70 (m, 2H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 172.6, 156.4, 155.8, 155.3, 134.0, 132.7, 132.1, 131.1, 129.7, 129.4, 129.1, 128.1, 126.7, 79.9, 54.3, 52.8, 52.3, 31.3, 29.1, 28.3, 22.1.

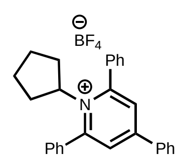
All data match that previously reported in the literature.[13]

1-(4-aminophenethyl)-2,4,6-triphenylpyridin-1-ium tetrafluoroborate (**S29**)



Following General Procedure B, using 4-(2-aminoethyl)aniline (2.42 g, 6.12 mmol) affords **S29** as a yellow solid (2.90 g, 5.60 mmol, 92%). **^{1}H NMR (499 MHz, DMSO-d_6)** δ 8.48 (s, 1H), 8.28 (d, *J* = 7.6 Hz, 2H), 7.90-7.84 (m, 4H), 7.79-7.72 (m, 6H), 7.72-7.62 (m, 3H), 6.34 (d, *J* = 8.0 Hz, 2H), 6.05 (d, *J* = 8.0 Hz, 2H), 4.99 (s, br, 2H), 4.46 (t, *J* = 7.5 Hz, 2H), 2.48 (t, *J* = 7.5 Hz, 2H); **^{13}C NMR (126 MHz, DMSO-d_6)** δ 156.5, 154.7, 148.3, 133.7, 133.5, 132.9, 131.5, 130.1, 129.7, 129.5, 129.2, 129.0, 126.4, 122.6, 114.5, 56.7, 34.6; **HRMS:** m/z: $[M]^+$ calc'd for $[C_{31}H_{27}N_2]^+$ expect 427.2169; found 427.2160.

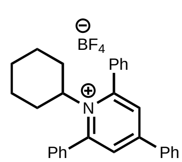
1-cyclopentyl-2,4,6-triphenylpyridin-1-ium tetrafluoroborate (**38**)



Following General Procedure B, using cyclopentylamine (1.12 g, 1.30 mL 13.2 mmol) affords **38** as a white solid (4.40 g, 9.50 mmol, 79%). **^{1}H NMR (500 MHz, DMSO-d_6)** δ 8.37 (s, 2H), 8.24 (d, *J* = 7.4 Hz, 2H), 7.90-7.83 (m, 4H), 7.73-7.68 (m, 6H), 7.68-7.63 (m, 1H), 7.60 (t, *J* = 7.8 Hz, 2H), 4.95 (p, *J* = 8.9 Hz, 1H), 2.26-2.14 (m, 2H), 1.99-1.83 (m, 2H), 1.18-1.05 (m, 2H), 0.84-0.70 (m, 2H); **^{13}C NMR (126 MHz, DMSO-d_6)** δ 158.3, 153.6, 134.7, 133.4, 132.8, 131.2, 130.3, 130.1, 129.2, 129.2, 127.6, 70.8, 34.0, 24.8.

All data match that previously reported in the literature.[14]

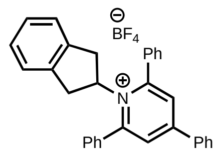
1-cyclohexyl-2,4,6-triphenylpyridin-1-ium tetrafluoroborate (**S30**)



Following General Procedure B, using cyclohexylamine (1.19 g, 1.37 mL, 12.0 mmol) affords **S30** as a white solid (2.09 g, 4.38 mmol, 37%). **^{1}H NMR (500 MHz, DMSO-d_6)** δ 8.40 (s, 2H), 8.24 (d, *J* = 7.7 Hz, 2H), 7.83-7.75 (m, 4H), 7.75-7.67 (m, 6H), 7.65 (d, *J* = 7.0 Hz, 1H), 7.60 (t, *J* = 7.5 Hz, 2H), 4.45 (t, *J* = 12.0 Hz, 1H), 2.11 (d, *J* = 11.4 Hz, 2H), 1.52 (d, *J* = 11.9 Hz, 2H), 1.42-1.23 (m, 3H), 0.61 (q, *J* = 12.9 Hz, 2H), 0.50 (t, *J* = 13.1 Hz, 1H); **^{13}C NMR (126 MHz, DMSO-d_6)** δ 157.5, 153.6, 134.5, 133.3, 132.9, 131.3, 130.1, 129.9, 129.1, 129.1, 127.4, 71.7, 33.6, 26.6, 24.8.

All data match that previously reported in the literature.[10]

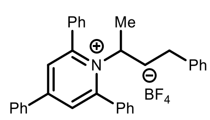
1-(2,3-dihydro-1*H*-inden-2-yl)-2,4,6-triphenylpyridin-1-ium tetrafluoroborate (**S31**)



A round-bottom flask equipped with a magnetic stir bar was charged with triphenylpyrylium tetrafluoroborate (4.68 g, 11.8 mmol, 1.0 equiv.) and 2-aminoindan hydrochloride (2.00 g, 11.8 mmol, 1.0 equiv.). DCM (24 ml, 0.5 M) along with 6.00 g powdered 4Å molecular sieves were added. Triethylamine (3.3 ml, 2 equiv.) was added and stirred for 20 min followed by addition of acetic acid (1.4 mL, 2 equiv.). The reaction was stirred at room temperature overnight. The mixture was filtered over a pad of celite to remove molecular sieves and eluted with additional DCM. The resulting solution was washed with 1 M HCl, sat. NaHCO3 (aq.), sat. NaCl (aq.), which was then dried over Na_2SO_4 and concentrated *in vacuo*. The resulting crude reaction mixture was dissolved in 10 mL DCM and was added dropwise into 100 mL Et_2O at room temperature and stirred vigorously for 2 h. The resulting solid was filtered, washed with cold Et_2O and dried under vacuum to afford **S31** as a pale-yellow solid (5.1 g, 10.0 mmol, 85%). **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.78 (s, 2H), 7.72-7.65 (m, 6H), 7.52-7.47 (m, 1H), 7.45-7.40 (m, 2H), 7.37-7.30 (m, 6H), 6.91 (dt, *J* = 7.3, 3.7 Hz, 2H), 6.74 (dt, *J* = 5.4, 3.4 Hz, 2H), 5.64 (tt, *J* = 10.7, 4.5 Hz, 1H), 3.69 (dd, *J* = 18.5, 4.4 Hz, 2H), 3.37 (dd, *J* = 18.5, 10.7 Hz, 2H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 157.8, 155.2, 139.3, 134.2, 133.5, 132.0, 130.7, 129.7, 129.6, 128.7, 128.3, 128.2, 126.8, 124.1, 67.7, 41.7.

All data match that previously reported in the literature.[13]

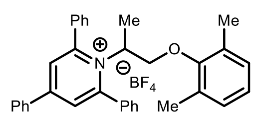
2,4,6-triphenyl-1-(4-phenylbutan-2-yl)pyridin-1-ium tetrafluoroborate (**S32**)



A round-bottom flask equipped with a magnetic stir bar was charged with triphenylpyrylium tetrafluoroborate (4.59 g, 11.6 mmol, 1.0 equiv.) and 4-phenylbutan-2-amine (1.73 g, 11.6 mmol, 1.0 equiv.). DCM (23 ml, 0.5 M) along with 6 g powdered 4Å molecular sieves were added. Triethylamine (3.23 ml, 2.0 equiv.) was added and stirred for 20 min followed by addition of acetic acid (1.33 mL, 2.0 equiv.). The reaction was stirred at room temperature overnight. The mixture was filtered over a pad of celite to remove molecular sieves and eluted with additional DCM. The resulting solution was washed with 1 M HCl, sat. $NaHCO_3$ (aq.), sat. NaCl (aq.), which was then dried over Na_2SO_4 and concentrated in vacuo. The resulting crude reaction mixture was dissolved in 10 mL DCM and was added dropwise into 100 mL Et_2O at room temperature and stirred vigorously for 2 h. The resulting solid was filtered, washed with cold Et_2O and dried under vacuum to afford **S32** as a yellow solid (4.2 g, 8.0 mmol, 69%). **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.71 (d, *J* = 6.8 Hz, 2H), 7.66 (s, 2H), 7.63 (d, *J* = 7.7 Hz, 2H), 7.58-7.42 (m, 7H), 7.37 (t, *J* = 7.7 Hz, 2H), 7.18-7.09 (m, 3H), 6.91-6.83 (m, 2H), 4.94-4.80 (m, 1H), 2.42-2.30 (m, 1H), 2.25-2.07 (m, 2H), 1.79-1.67 (m, 1H), 1.43 (d, *J* = 6.9 Hz, 3H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 157.1, 154.9, 138.9, 133.8, 133.6, 131.8, 130.7, 129.4, 128.6, 128.2, 128.0, 126.3, 65.9, 37.5, 32.3, 21.6 (*3 aromatic carbon signals are not observed due to signal broadening*).

All data match that previously reported in the literature.[13]

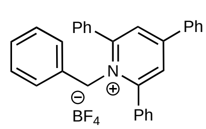
1-(1-(2,6-dimethylphenoxy)propan-2-yl)-2,4,6-triphenylpyridin-1-ium tetrafluoroborate (**S33**)



A round-bottom flask equipped with a magnetic stir bar was charged with triphenylpyrylium tetrafluoroborate (3.96 g, 10.0 mmol, 1.0 equiv.) and mexiletine (2.16 g, 10.0 mmol, 1.0 equiv.). DCM (20 ml, 0.5 M) along with 5.00 g powdered 4Å molecular sieves were added. Triethylamine (2.79 ml, 2.0 equiv.) was added and stirred for 20 min followed by addition of acetic acid (1.14 mL, 2.0 equiv.). Reaction was stirred at room temperature overnight. The mixture was filtered over a pad of celite to remove molecular sieves and eluted with additional DCM. The resulting solution was washed with 1 M HCl, sat. $NaHCO_3$ (aq.), sat. NaCl (aq.), which was then dried over Na_2SO_4 and concentrated in vacuo. The resulting crude reaction mixture was dissolved in 10 mL DCM and was added dropwise into 100 mL Et_2O at room temperature and stirred vigorously for 2 h. The resulting solid was filtered, washed with cold Et_2O and dried under vacuum to afford **S33** as a white solid (3.90 g, 7.00 mmol, 70%). **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.01-7.67 (m, 7H), 7.63-7.51 (m, 7H), 7.48 (t, *J* = 7.8 Hz, 2H), 6.95-6.87 (m, 3H), 5.48 (h, *J* = 7.0 Hz, 1H), 4.12 (dd, *J* = 9.9, 6.7 Hz, 1H), 3.53 (dd, *J* = 9.9, 6.9 Hz, 1H), 1.92 (s, 6H), 1.54 (d, *J* = 7.2 Hz, 3H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 155.9, 154.4, 134.1, 133.7, 132.2, 131.2, 130.1, 129.7, 129.4, 129.3, 129.0, 128.5, 124.6, 73.6, 65.4, 19.4, 16.4

All data match that previously reported in the literature.[15]

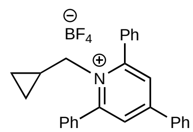
1-benzyl-2,4,6-triphenylpyridin-1-ium tetrafluoroborate (**S34**)



Following General Procedure B, using phenylmethanamine (1.00 g, 9.50 mmol) affords **S34** as a white solid (3.10 g, 6.40 mmol, 84%). **^{1}H NMR (499 MHz, $CDCl_3$):** δ 7.81 (s, 2H), 7.69 (d, *J* = 7.6 Hz, 2H), 7.62 (d, *J* = 7.5 Hz, 4H), 7.49-7.35 (m, 9H), 7.10-7.01 (m, 3H), 6.42 (d, *J* = 7.4 Hz, 2H), 5.71 (s, 2H); **^{13}C NMR (126 MHz, $CDCl_3$):** δ 157.3, 156.1, 133.7, 133.6, 132.7, 132.2, 130.8, 129.6, 129.0, 129.0, 128.8, 128.1, 128.1, 126.4, 126.2, 58.2.

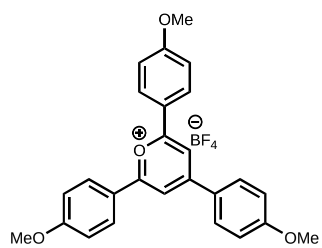
All data match that previously reported in the literature.[14]

1-(cyclopropylmethyl)-2,4,6-triphenylpyridin-1-ium tetrafluoroborate (**S35**)



Following General Procedure B, using cyclopropylmethanamine (1.00 g, 11.7 mmol) affords **S35** as a white solid (4.85 g, 10.8 mmol, 92%). **^{1}H NMR (499 MHz, DMSO-d_6)** δ 8.48 (s, 2H), 8.28 (d, *J* = 7.4 Hz, 2H), 7.98-7.91 (m, 4H), 7.76-7.70 (m, 6H), 7.69-7.59 (m, 3H), 4.43 (d, *J* = 6.7 Hz, 2H), 0.80-0.71 (m, 1H), 0.29-0.21 (m, 2H), - 0.32-- 0.42 (m, 2H); **^{13}C NMR (126 MHz, DMSO-d_6)** δ 156.2, 154.33, 133.4, 133.2, 132.4, 131.0, 129.6, 129.6, 129.1, 128.7, 126.3, 58.8, 10.5, 4.6; **HRMS:** m/z: $[M]^+$ calc'd for $[C_{27}H_{24}N]^+$ expect 362.1903; found 362.1900

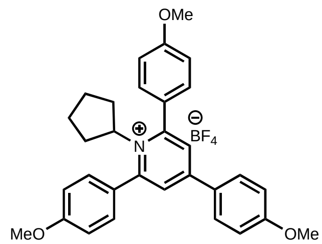
2,4,6-tris(4-methoxyphenyl)pyrylium tetrafluoroborate (**S36**)



A flame-dried round bottom flask equipped with a stirrer bar was charged with toluene (5 mL), *p*-anisaldehyde (6.81 g, 6.08 mL, 50.0 mmol) and 4'-methoxyacetophenone (15.0 g, 13.9 mL, 100 mmol). To the solution was slowly added $BF_3.Et_2O$ (17.0 g, 15.2 mL, 120 mmol), and the resulting reaction refluxed at 100 °C for 2 h. The volatiles were then removed *in vacuo*, and the crude residue redissolved in acetone. Diethyl ether was added slowly with stirring until no more precipitate was visibly seen to form, and the solid was collected *via* suction filtration. The precipitate was then recrystallized from acetone to yield the title compound as a bright orange solid (4.78 g, 9.83 mmol, 20%). **^{1}H NMR (500 MHz, DMSO-d_6)** δ 8.76 (s, 2H), 8.58 (d, *J* = 9.1 Hz, 2H), 8.47 (d, *J* = 9.1 Hz, 4H), 7.27 (d, *J* = 9.1 Hz, 6H), 3.97 (s, 3H), 3.95 (s, 6H); **^{13}C NMR (126 MHz, DMSO-d_6)** δ 168.0, 165.7, 164.9, 162.0, 132.9, 131.0, 124.7, 121.6, 115.7, 115.7, 110.9, 56.5, 56.4

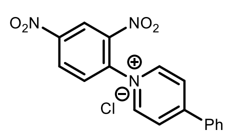
All data match that previously reported in the literature.[10]

1-cyclopentyl-2,4,6-tris(4-methoxyphenyl)pyridin-1-ium tetrafluoroborate (**S37**)



2,4,6-Tris(4-methoxyphenyl)pyrylium tetrafluoroborate **S36** (1.22g, 2.50 mmol) and powdered 4 Å molecular sieves were suspended in CH_2Cl_2 (5 mL) in a round bottom flask equipped with a septum and vent needle. Triethylamine (506 mg, 697 µL, 5.00 mmol) and cyclopentylamine (213 mg, 247 µL, 2.50 mmol) were added sequentially to the reaction. The vent needle was removed and the reaction stirred at room temperature for 20 min. The vent needle was added and acetic acid (286 µL, 5.00 mmol) was added, followed by more CH_2Cl_2 (5 mL). The vent needle was removed and the reaction stirred at room temperature for 19 h. The reaction was then opened to air and filtered through a celite plug washing with a small portion of CH_2Cl_2. The filtrate was collected and washed with 1 M HCl (4 x 20 mL), sat. $NaHCO_3$ (4 x 20 mL) and brine (20 mL), and then dried over Na_2SO_4 and concentrated to give the title compound as a crystalline orange solid which was used without further purification (1.19 g, 2.15 mmol, 86%). **^{1}H NMR (500 MHz, DMSO-d$_6$)** δ 8.24 (d, *J* = 8.9 Hz, 2H), 8.21 (s, 2H), 7.77 (d, *J* = 8.5 Hz, 4H), 7.22 (d, *J* = 8.8 Hz, 4H), 7.12 (d, *J* = 8.9 Hz, 2H), 4.93 (p, *J* = 4.9 Hz, 1H), 3.89 (s, 6H), 3.87 (s, 3H), 2.23-2.10 (m, 2H), 1.96-1.84 (m, 2H), 1.21-1.08 (m, 2H), 0.91-0.78 (m, 2H); **^{13}C NMR (126 MHz, DMSO-d$_6$)** δ 163.3, 161.3, 158.2, 125.6, 132.0, 131.1, 127.1, 126.1, 125.4, 115.5, 114.6, 70.5, 56.2, 56.0, 34.1, 24.9; **HRMS:** m/z: $[M]^+$ calc'd for $[C_{31}H_{32}NO_3]^+$ expect 466.2377; found 466.2377.

1-(2,4-dinitrophenyl)-4-phenylpyridin-1-ium chloride (**S38**)

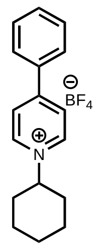


4-phenylpyridine (3.14 g, 20.2 mmol) was dissolved in acetone (20 mL) and 2,4-dinitrochlorobenzene (4.05 g, 20.0 mmol) was added in a single portion. The resulting mixture was heated to reflux at 60 °C for 16 h, and then cooled to room temperature, concentrated, and then filtered, washing the filter cake with hexanes. The filter cake was collected and dried *in vacuo* to yield the title compound as a light brown solid (5.37 g, 75%). **^{1}H NMR (500 MHz, DMSO-d$_6$)** δ 9.55 (d, *J* = 6.1 Hz, 2H), 9.12 (s, 1H), 8.99 (d, *J* = 8.5 Hz, 1H), 8.90 (d, *J* = 6.1 Hz, 2H), 8.55 (d, *J* = 8.4 Hz, 1H), 8.29 (d, *J* = 7.1 Hz, 2H), 7.80-7.64 (m, 3H); **^{13}C NMR**

(126 MHz, DMSO-d$_6$) δ 157.7, 149.4, 146.5, 143.7, 139.1, 133.6, 133.5, 132.7, 130.7, 130.4, 129.2, 124.6, 121.9

All data match that previously reported in the literature.[16]

1-cyclohexyl-4-phenylpyridin-1-ium tetrafluoroborate (**S39**)



1-(2,4-Dinitrophenyl)-4-phenylpyridin-1-ium chloride **S38** (1.79 g, 5.00 mmol) was dissolved in *n*-butanol (10 mL), cyclohexylamine (595 mg, 687 μL, 6.00 mmol) was added dropwise and the resulting mixture heated to reflux at 120 °C for 30 h. The reaction was then cooled to room temperature and added portionwise to Et_2O with stirring, and the resulting suspension stored in the freezer overnight to promote crystallization. The solid was then collected *via* filtration and washed with EtOAc until the filtrate became colorless. The solid was then washed with Et_2O to remove any residue EtOAc, and then dried *in vacuo* to give the chloride salt as a tan solid (1.31 g, 4.78 mmol, 96%). A portion of the chloride salt (660 mg, 2.41 mmol) was dissolved in CH_2Cl_2 inside a separatory funnel. The solution was washed with sat. aq. $NaBF_4$ solution (4 x 40 mL; NB density is greater than CH_2Cl_2), then with brine (2 x 40 mL) and dried over Na_2SO_4, filtered and concentrated to give the title compound as a tan solid (719 mg, 2.21 mmol, 92%). **^{1}H NMR (500 MHz, CDCl$_3$)** δ 8.98 (d, *J* = 7.0 Hz, 2H), 8.23 (d, *J* = 7.0 Hz, 2H), 7.81-7.75 (m, 2H), 7.60-7.49 (m, 3H), 4.68-4.54 (m, 1H), 2.28-2.16 (m, 2H), 2.00-1.85 (m, 4H), 1.72 (d, *J* = 13.2 Hz, 1H), 1.62-1.46 (m, 2H), 1.31 (qt, *J* = 13.2, 3.4 Hz, 1H); **^{13}C NMR (126 MHz, CDCl$_3$)** δ 156.7, 143.0, 133.7, 132.3, 129.9, 127.9, 125.4, 71.4, 33.5, 25.2, 24.4; **^{19}F NMR (471 MHz, CDCl$_3$)** δ -151.4, -151.4

All data match that previously reported in the literature.[17]

Extended Optimization Data

General Procedure for High-Throughput Experimentation in 24- and 96-Well Plates

Stock solutions, or suspensions, were prepared as shown in the heatmap preparation table. In an inert atmosphere glovebox, reagents were weighed and dissolved or suspended in anhydrous solvent to achieve their listed concentrations in the table. Stock solutions of reagents were stirred until either a clear solution or a uniform slurry was achieved. A 24- or 96-well aluminum microvial plate (Analytical Sales & Services cat. no. 25243) was equipped with oven-dried shell vials (Analytical Sales & Services cat. no. 884001) and then moved into the glovebox. Stock solutions were dosed to the appropriate shell vials according to the plate map shown in table using single channel micropipetters. A parylene-coated stir dowel (Analytical Sales & Services cat. no. 13258) was then added to each vial. The microvial plate was sealed, removed from the glove box, and stirred on a tumble stirrer with heating to indicated temperature for planned reaction time in a heating block.

The reactions were quenched by opening the reaction block and adding 100 µL water and 500 µL EtOAc. Reactions were extracted by resealing the plate and either shaking manually or stirring on the tumble stirrer at 1400 rpm for 15 minutes. The plate was then allowed to sit for ~10 min to allow to organic and aqueous phases to separate. From each reaction, a 40 µL aliquot of the quenched reaction mixture was added into a 96-well polypropylene collection plate (Analytical Sales & Services cat. no. 17P687). The solvent was evaporated by blowing nitrogen down on the analytical plate. A solution of caffeine in MeCN (1.2 mg/mL, 100 µL) as internal standard was added, followed by pure MeCN (700 µL) and mixed by pipetting up and down to give a final caffeine internal standard concentration of 0.15 mg/mL. The reactions were then analyzed by UPLCMS. The assay yields were produced by measuring the UV absorbance of desired product relative to the caffeine internal standard.

General Procedure for Singleton Optimization Reactions

Inside a N_2-filled glovebox, a flame-dried 1- or 2-dram vial was charged with a stirrer bar, *N*-acyl glutarimide, pyridinium salt, nickel precatalyst, ligand, Mn and additive (if required). Solvent was added to the vial and then it was sealed with a screw cap, followed by a piece of electrical tape around the joint. The vial was then removed from the glovebox and placed into a preheated heating block on a hotplate. The reaction was stirred for the specified time (typically overnight) and allowed to reach room temperature. For UPLC-MS analysis an aliquot (8.4 µL for a 0.1 M reaction) was removed and added to an internal standard solution of 0.15 mg/mL caffeine in MeCN (992 µL for a 0.1 M reaction). The sample was then analyzed by UPLC-MS, with the yield produced by measuring the UV absorbance or MS TIC(+) of the product relative to the caffeine internal standard. For ^{1}H NMR analysis, the reaction was quenched with water and EtOAc was added. The layers were separated and the organic layer washed with water (x3) and brine. The organic layer was then dried over Na_2SO_4 and concentrated to *ca.* 10 mL. The solution was then washed through a plug of silica and celite with more EtOAc and concentrated. The residue was then dissolved in deuterated solvent (typically $CDCl_3$) with an internal standard (dibromomethane, 1,3,5-trimethoxybenzene or dimethoxyethane), and the ^{1}H NMR spectrum obtained, with yield determined through comparison of peak integrals to the internal standard.

Calibration Curves for UPLC-MS Assay Yield

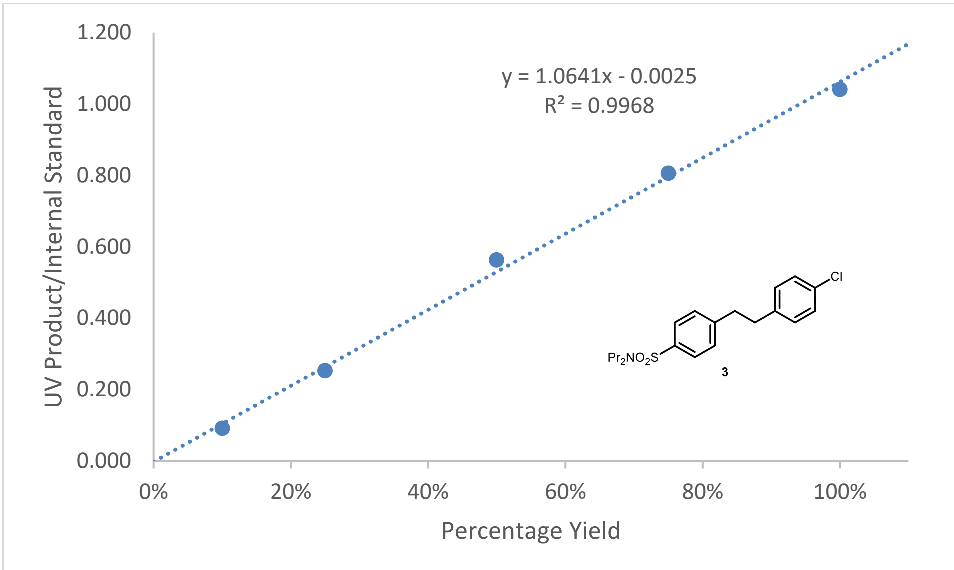


Figure S1: Calibration curve of UV integration of **3** relative to 0.15 mg/mL caffeine internal standard. [**3**]$_{max}$ = 0.84 µM = 100% yield

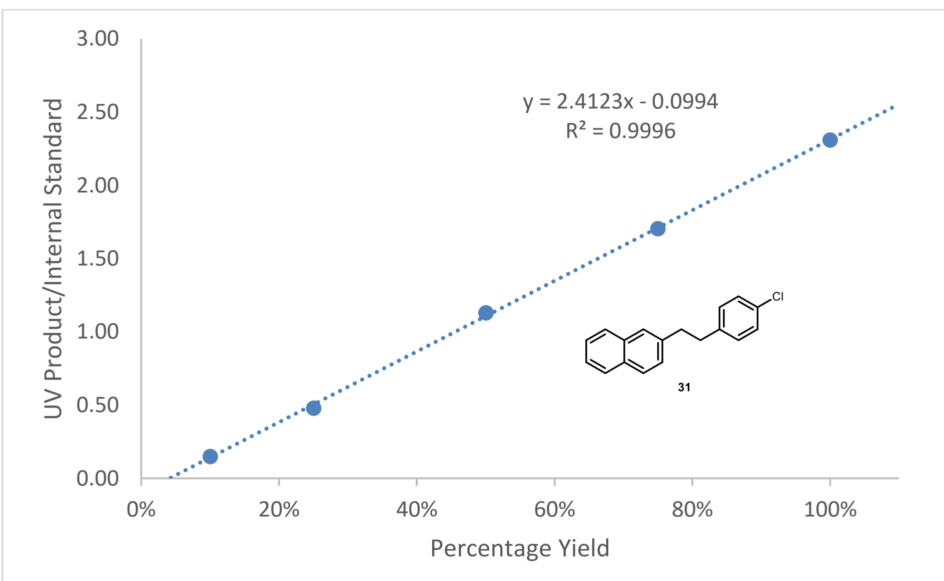


Figure S2: Calibration curve of UV integration of **31** relative to 0.15 mg/mL caffeine internal standard. [**31**]$_{max}$ = 0.84 µM = 100% yield

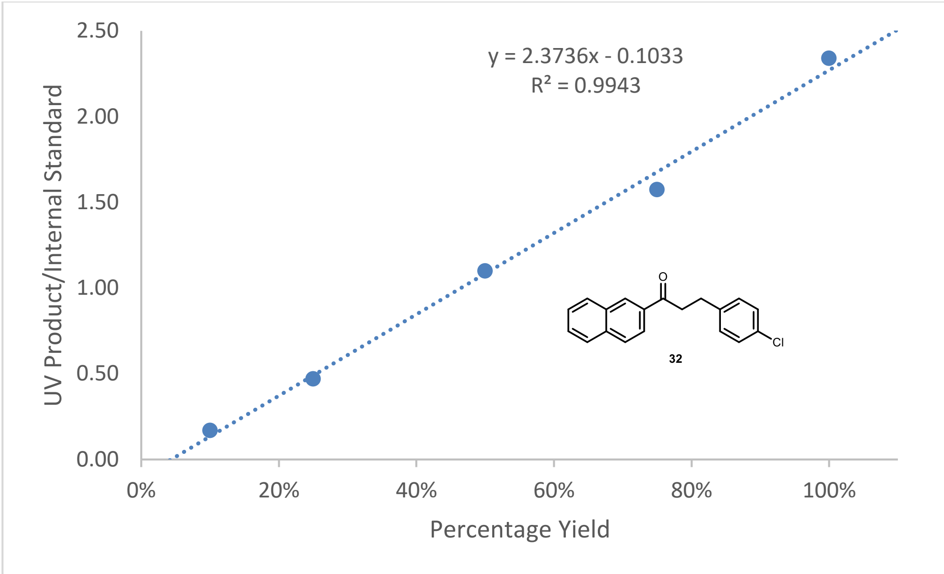


Figure S3: Calibration curve of UV integration of **32** relative to 0.15 mg/mL caffeine internal standard. [**32**]$_{max}$ = 0.84 µM = 100% yield

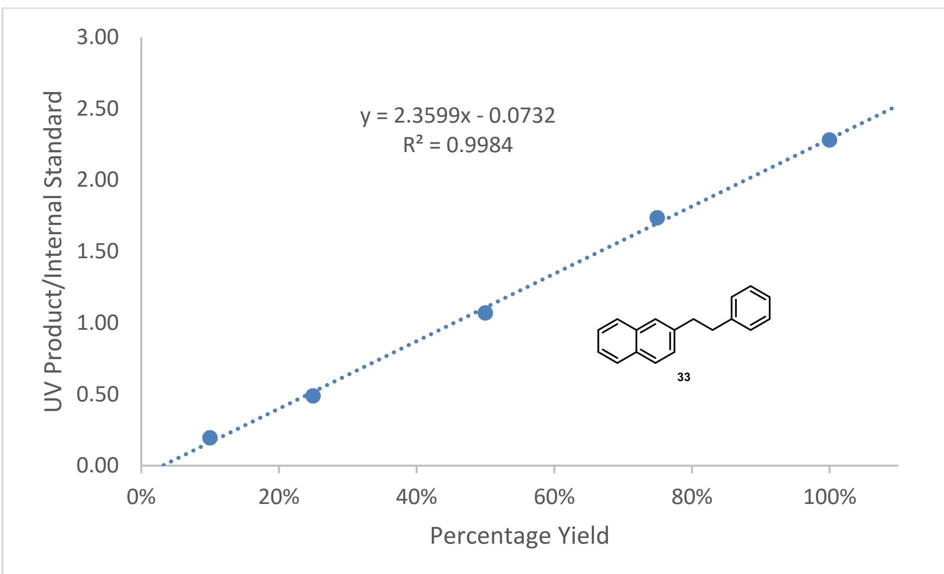


Figure S4: Calibration curve of UV integration of **33** relative to 0.15 mg/mL caffeine internal standard. [**33**]$_{max}$ = 0.84 µM = 100% yield

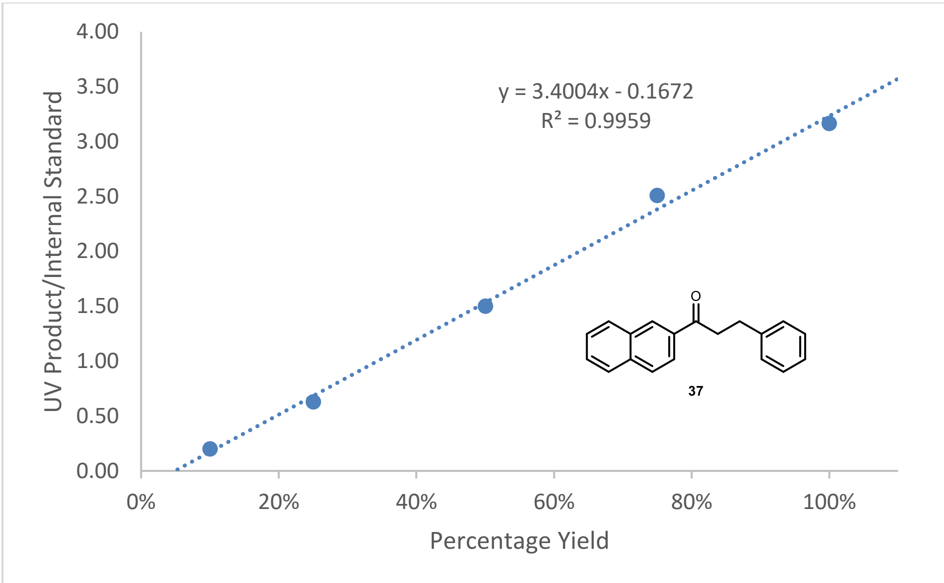


Figure S5: Calibration curve of UV integration of **37** relative to 0.15 mg/mL caffeine internal standard. [**37**]$_{max}$ = 0.84 µM = 100% yield

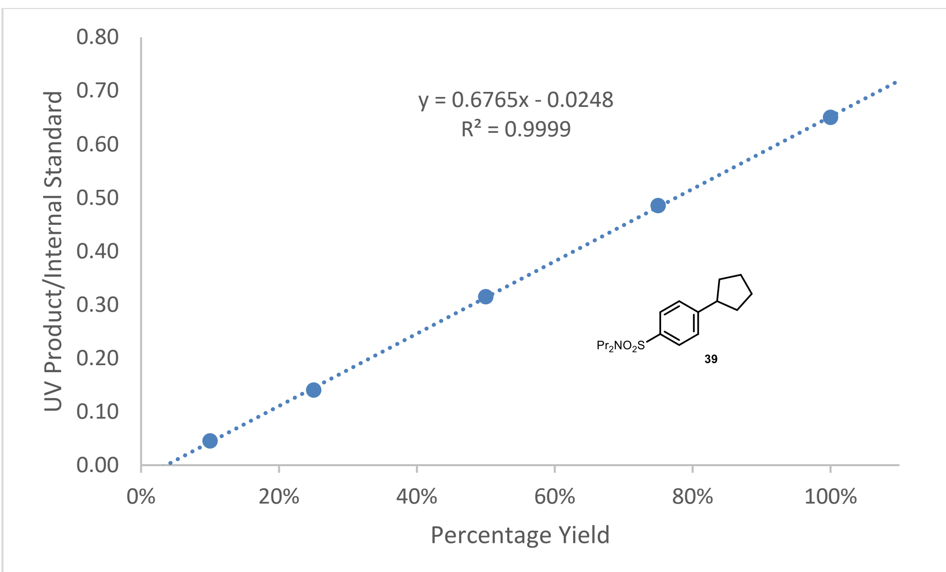


Figure S6: Calibration curve of UV integration of **39** relative to 0.15 mg/mL caffeine internal standard. [**39**]$_{max}$ = 0.84 µM = 100% yield

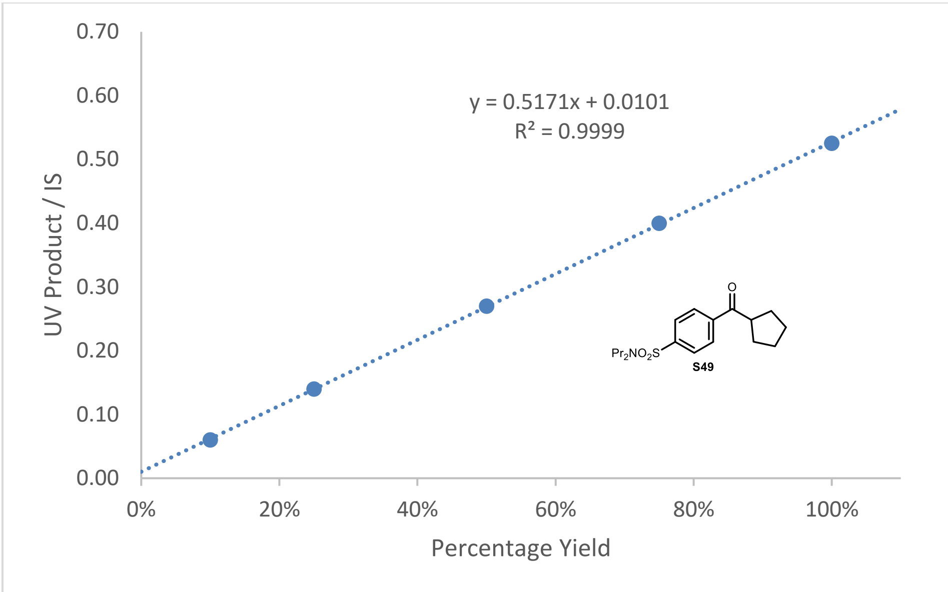
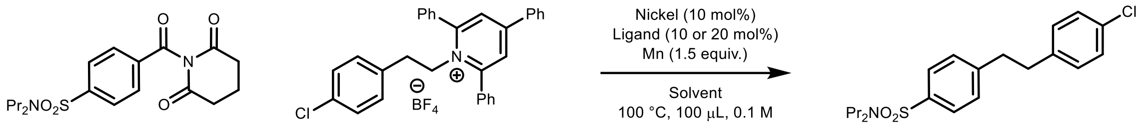


Figure S7: Calibration curve of UV integration of **S49** relative to 0.15 mg/mL caffeine internal standard. [**S49**]$_{max}$ = 0.84 µM = 100% yield

Reaction Optimization

96-Well Screen of 4 Catalysts, 8 Ligands and 3 Solvents



1 **2** 1.2 equiv. **3**

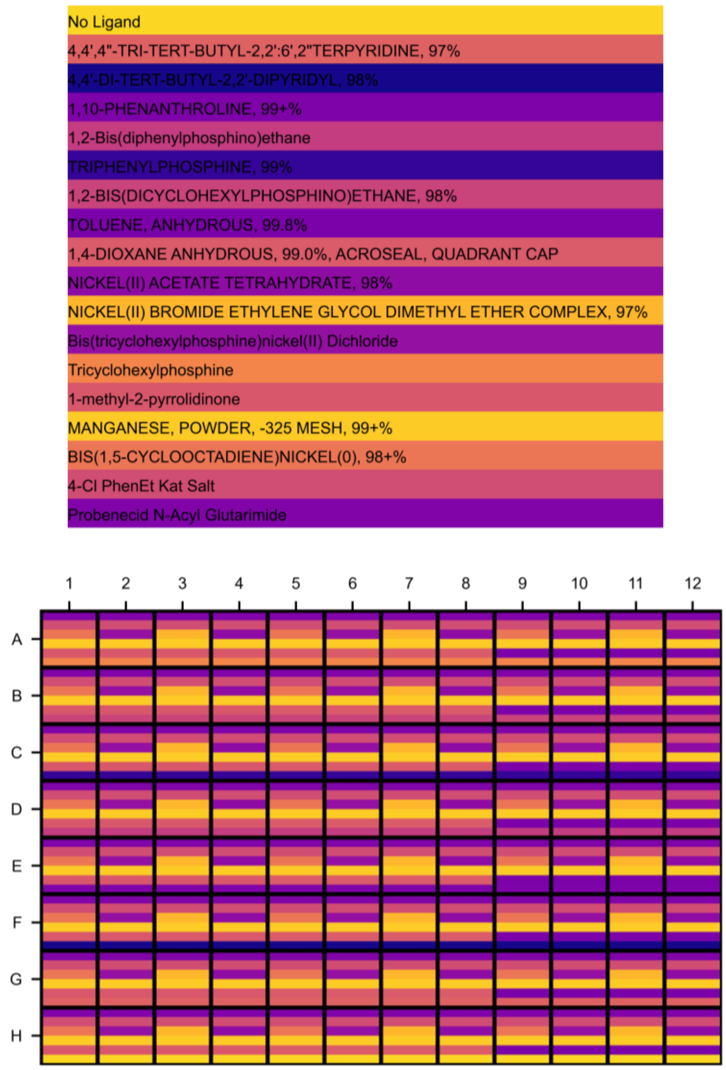


Figure S8: Input heatmap of 96-well screen of 4 catalysts, 8 ligands and 3 solvents

Reagents	Solvent	C_{stock} (M)	V_{dose} (µL)	Wells
$Ni(COD)_2$	NMP	0.01	20	A1-H1
$Ni(COD)_2$	1,4-Dioxane	0.01	20	A5-H5
$Ni(COD)_2$	Toluene	0.01	20	A9-H9
$Ni(PCy_3)_2Cl_2$	NMP	0.01	20	A2-H2
$Ni(PCy_3)_2Cl_2$	1,4-Dioxane	0.01	20	A6-H6
$Ni(PCy_3)_2Cl_2$	Toluene	0.01	20	A10-H10
$NiBr_2$•DME	NMP	0.01	20	A3-H3
$NiBr_2$•DME	1,4-Dioxane	0.01	20	A6-H6
$NiBr_2$•DME	Toluene	0.01	20	A11-H11
$Ni(OAc)_2$•$4H_2O$	NMP	0.01	20	A4-H4
$Ni(OAc)_2$•$4H_2O$	1,4-Dioxane	0.01	20	A8-H8
$Ni(OAc)_2$•$4H_2O$	Toluene	0.01	20	A12-H12
PCy_3	NMP	0.02	20	A1-A4
PCy_3	1,4-Dioxane	0.02	20	A5-A8
PCy_3	Toluene	0.02	20	A9-A12
dcype	NMP	0.01	20	B1-B4
dcype	1,4-Dioxane	0.01	20	B5-B8
dcype	Toluene	0.01	20	B9-B12
PPh_3	NMP	0.02	20	C1-C4
PPh_3	1,4-Dioxane	0.02	20	C5-C8
PPh_3	Toluene	0.02	20	C9-C12
dppe	NMP	0.01	20	D1-D4
dppe	1,4-Dioxane	0.01	20	D5-D8
dppe	Toluene	0.01	20	D9-D12
phenanthroline	NMP	0.01	20	E1-E4
phenanthroline	1,4-Dioxane	0.01	20	E5-E8
phenanthroline	Toluene	0.01	20	E9-E12
dtbpy (**L1**)	NMP	0.01	20	F1-F4
dtbpy (**L1**)	1,4-Dioxane	0.01	20	F5-F8
dtbpy (**L1**)	Toluene	0.01	20	F9-F12
4,4'-di-*tert*-butyl-2,2,:6',2''-terpyridine	NMP	0.01	20	G1-G4
4,4'-di-*tert*-butyl-2,2,:6',2''-terpyridine	1,4-Dioxane	0.01	20	G5-G8
4,4'-di-*tert*-butyl-2,2,:6',2''-terpyridine	Toluene	0.01	20	G9-G12
No ligand	NMP	0	20	H1-H4
No ligand	1,4-Dioxane	0	20	H5-H8
No ligand	Toluene	0	20	H9-H12
Probenecid *N*-Acyl Glutarimide (**1**)	NMP	0.1	20	A-H, 1-4
Probenecid *N*-Acyl Glutarimide (**1**)	1,4-Dioxane	0.1	20	A-H, 5-8

Probenecid *N*-Acyl Glutarimide (**1**)	Toluene	0.1	20	A-H, 9-12
4-Cl PhenEt Kat Salt (**2**)	NMP	0.12	20	A-H, 1-4
4-Cl PhenEt Kat Salt (**2**)	1,4-Dioxane	0.12	20	A-H, 5-8
4-Cl PhenEt Kat Salt (**2**)	Toluene	0.12	20	A-H, 9-12
Mn powder	NMP	0.15	20	A-H, 1-4
Mn powder	1,4-Dioxane	0.15	20	A-H, 5-8
Mn powder	Toluene	0.15	20	A-H, 9-12

Table S1: Reagents, stock solution concentrations, dosing volumes and well locations in the 96-well screen of 4 catalysts, 8 ligands and 3 solvents

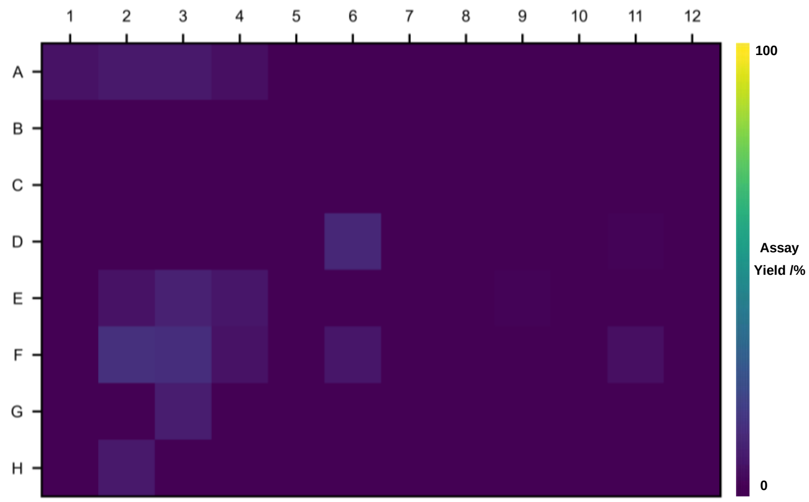
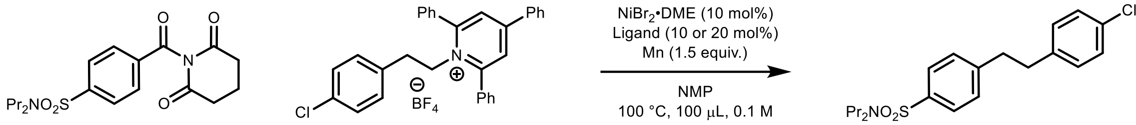


Figure S9: Output heatmap of 96-well screen of 4 catalysts, 8 ligands and 3 solvents

24-Well Screen of 24 Ligands



1 **2** 1.2 equiv. **3**

1,1'-BIS(DIPHENYLPHOSPHINO)FERROCENE, 97%
Tyrannophos
2,6-BIS[(4R)-(+)-ISOPROPYL-2-OXAZOLIN-2-YL]PYRIDINE, 99%
2,2-BIS((4S)-(-)-4-ISOPROPYLOXAZOLINE)PROPANE, 96%
2-Amidinopyridine hydrochloride
(2Z,6Z)-N_2,N_6-Dicyanopyridine-2,6-bis(carboximidamide)
4-DIMETHYLAMINOPYRIDINE, 99+%, REAGENTPLUS
2,4,6-COLLIDINE 99%
PYRIDINE, 99.5%, EXTRA DRY
2-pyridinecarbonitrile
4,7-DIMETHOXY-1,10-PHENANTHROLINE, 97%
3,4,7,8-TETRAMETHYL-1,10-PHENANTHROLINE, 98+%
NEOCUPROINE, 98+%
4,7-DICHLORO-1,10-PHENANTHROLINE, 97%
4,7-DIPHENYL-1,10-PHENANTHROLINE, 97%
1,10-Phenanthroline-5,6-dione
4-4'-DIMETHOXY-2-2'-BIPYRIDINE, 97%
4,4'-Dibromo-2,2'-bipyridine
2,2_-Bipyridyl
4,5-Diazafluoren-9-one
Dimethyl 2,2_-bipyridine-4,4_-dicarboxylate
2,2_-Bipyridine-5,5_-dicarboxylic Acid
5,5_-Bis(trifluoromethyl)-2,2_-bipyridine
4,4'-Bis(trifluoromethyl)-2,2'-bipyridyl
1-methyl-2-pyrrolidinone
MANGANESE, POWDER, -325 MESH, 99+%
NICKEL(II) BROMIDE ETHYLENE GLYCOL DIMETHYL ETHER COMPLEX, 97%
4-Cl Phen Et Kat Salt
Probenecid N-Acyl Glutarimide

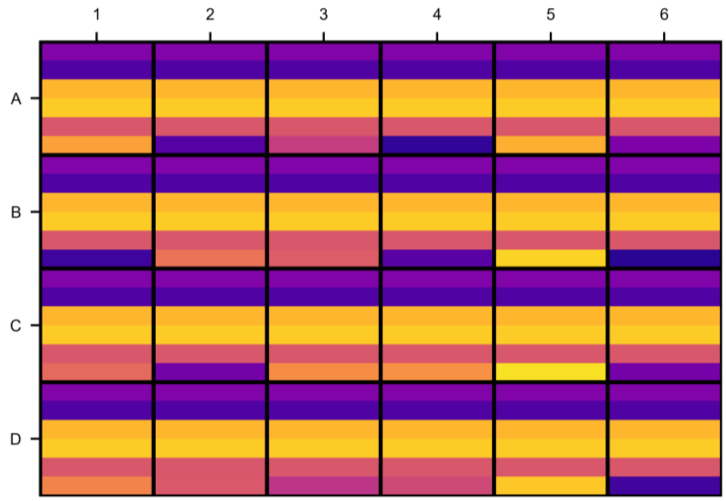


Figure S10: Input heatmap of 24-well screen of 24 ligands

Reagents	Solvent	C_{stock} (M)	V_{dose} (µL)	Wells
$NiBr_2$•DME	NMP	0.01	20	All
4,4'-bis(trifluoromethyl)-2,2'-bipyridine	NMP	0.01	20	A1
5,5'-bis(trifluoromethyl)-2,2'-bipyridine	NMP	0.01	20	A2
[2,2'-bipyridine]-5,5'-dicarboxylic acid	NMP	0.01	20	A3
dimethyl [2,2'-bipyridine]-4,4'-dicarboxylate	NMP	0.01	20	A4
4,5-diazafluoren-9-one	NMP	0.01	20	A5
2,2’-bipyridine	NMP	0.01	20	A6
4,4'-dibromo-2,2'-bipyridine	NMP	0.01	20	B1
4,4’-dimethoxy-2,2’-bipyridine	NMP	0.01	20	B2
1,10-phenanthroline-5,6-dione	NMP	0.01	20	B3
4,7-diphenyl-1,10-phenanthroline	NMP	0.01	20	B4
4,7-dichloro-1,10-phenanthroline	NMP	0.01	20	B5
neocuproine	NMP	0.01	20	B6
tmphen	NMP	0.01	20	C1
4,7-dimethoxy-1,10-phenanthroline	NMP	0.01	20	C2
2-pyridinecarbonitrile	NMP	0.02	20	C3
pyridine	NMP	0.02	20	C4
2,4,6-collidine	NMP	0.02	20	C5
DMAP	NMP	0.02	20	C6

(2*Z*,6*Z*)-N'[2],N'[6]-dicyanopyridine-2,6-bis(carboximidamide)	NMP	0.01	20	D1
pyridine-2-carboxamidine hydrochloride (**L2**)	NMP	0.01	20	D2
(4*S*,4'*S*)-2,2'-(propane-2,2-diyl)bis(4-isopropyl-4,5-dihydrooxazole)	NMP	0.01	20	D3
2,6-bis((*R*)-4-isopropyl-4,5-dihydrooxazol-2-yl)pyridine	NMP	0.01	20	D4
TyrannoPhos	NMP	0.01	20	D5
dppf	NMP	0.01	20	D6
Probenecid *N*-Acyl Glutarimide (**1**)	NMP	0.1	20	All
4-Cl PhenEt Kat Salt (**2**)	NMP	0.12	20	All
Mn powder	NMP	0.15	20	All

Table S2: Reagents, stock solution concentrations, dosing volumes and well locations in the 24-well screen of 24 ligands

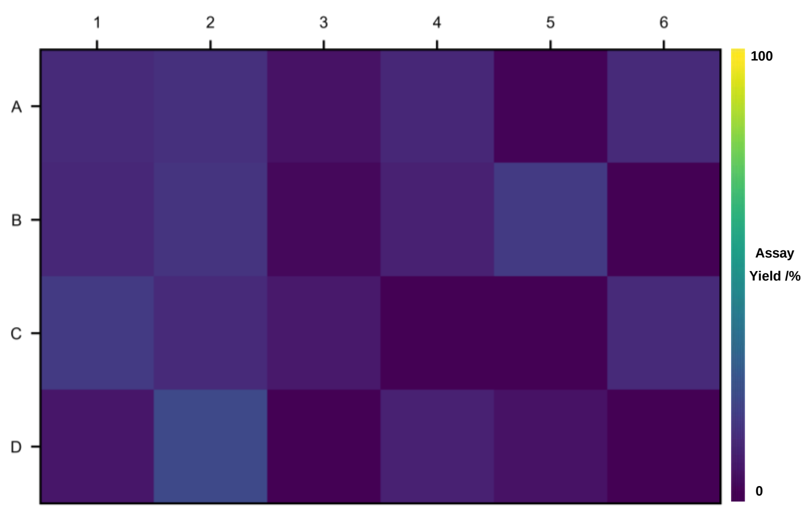
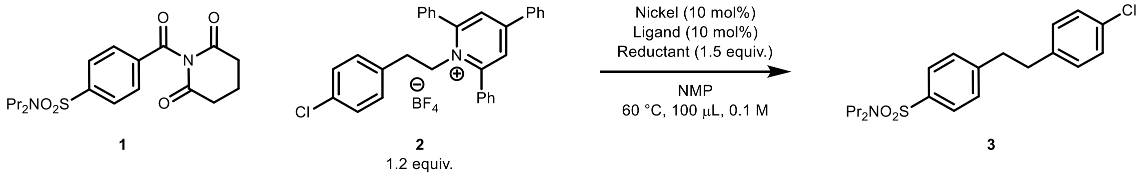


Figure S11: Output heatmap of 24-well screen of 24 ligands

96-Well Screen of 3 Catalysts, 8 Ligands and 4 Reductants



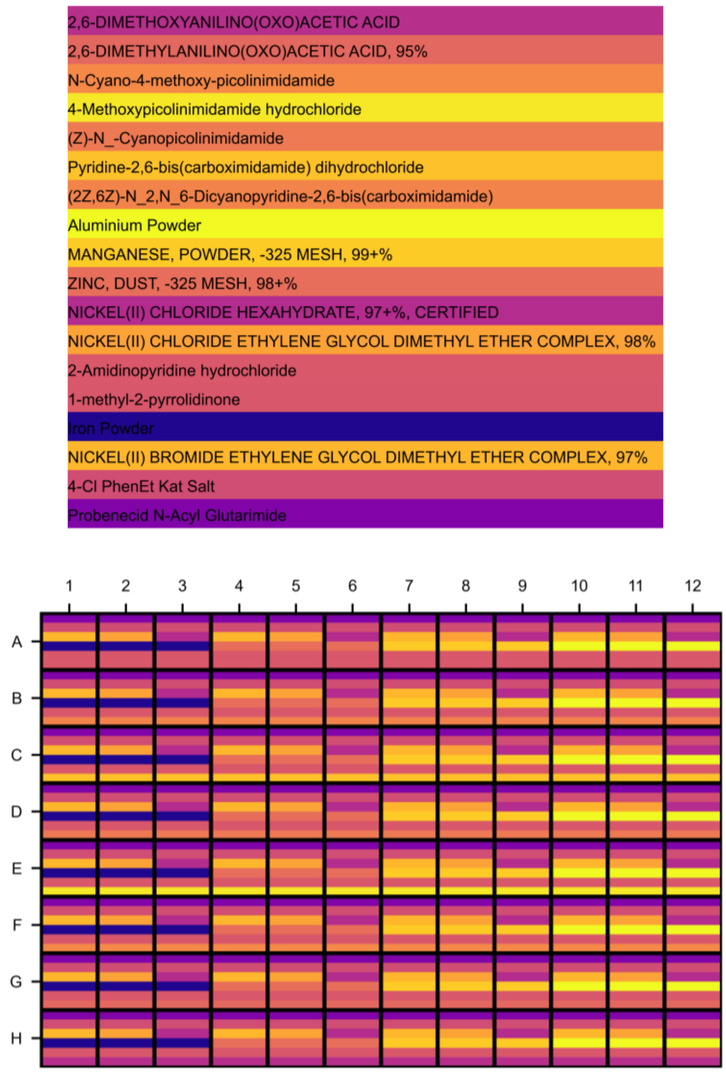


Figure S12: Input heatmap of 96-well screen of 3 catalysts, 8 ligands and 4 reductants

Reagents	Solvent	C_{stock} (M)	V_{dose} (µL)	Wells
$NiBr_2$•DME	NMP	0.01	20	A1-H1, A4-H4, A7-H7, A10-H10
$NiCl_2$•DME	NMP	0.01	20	A2-H2, A5-H5, A8-H8, A11-H11

$NiCl_2 \cdot 6H_2O$	NMP	0.01	20	A3-H3, A6-H6, A9-H9, A12-H12
pyridine-2-carboxamidine hydrochloride (**L2**)	NMP	0.01	20	A1-A12
(2*Z*,6*Z*)-N'^{2},N'^{6}-dicyanopyridine-2,6-bis(carboximidamide)	NMP	0.01	20	B1-B12
Pyridine-2,6-bis(carboximidamide) dihydrochloride	NMP	0.01	20	C1-C12
(*Z*)-*N′*-cyanopicolinimidamide	NMP	0.01	20	D1-D12
4-methoxypicolinimidamide hydrochloride	NMP	0.01	20	E1-E12
N-cyano-4-methoxy-picolinimidamide (**L3**)	NMP	0.01	20	F1-F12
2,6-dimethylanilino(oxo)acetic acid	NMP	0.01	20	G1-G12
2,6-dimethoxyanilino(oxo)acetic acid	NMP	0.01	20	H1-H12
Fe powder	NMP	0.15	20	A-H, 1-3
Zn powder	NMP	0.15	20	A-H, 4-6
Mn Powder	NMP	0.15	20	A-H, 7-9
Al Powder	NMP	0.15	20	A-H, 10-12
Probenecid *N*-Acyl Glutarimide (**1**)	NMP	0.1	20	All
4-Cl PhenEt Kat Salt (**2**)	NMP	0.12	20	All

Table S3: Reagents, stock solution concentrations, dosing volumes and well locations in the 96-well screen of 3 catalysts, 8 ligands and 4 reductants

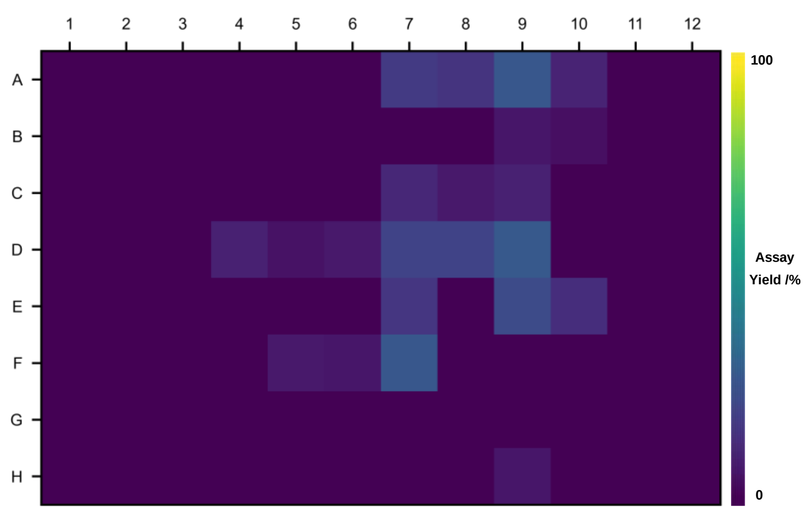
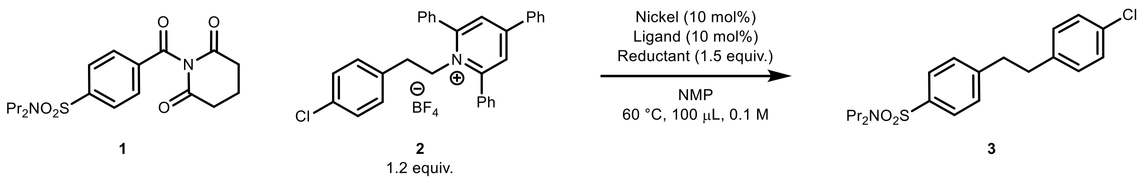


Figure S13: Output heatmap of 96-well screen of 3 catalysts, 8 ligands and 4 reductants

24-Well Screen of 6 Catalysts and 4 Ligands



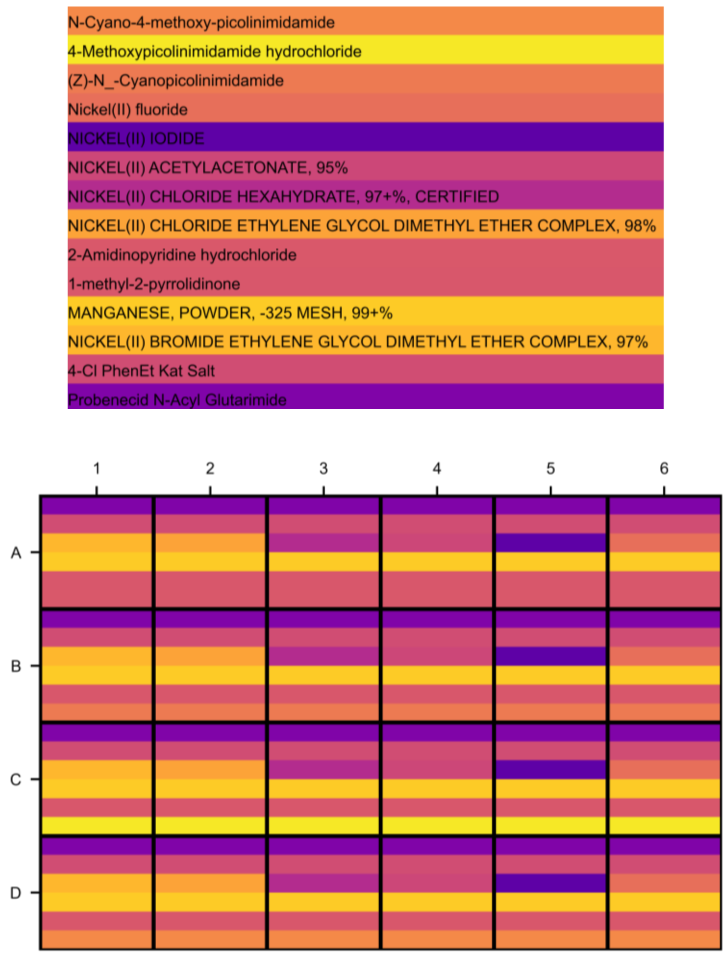


Figure S14: Input heatmap of 24-well screen of 6 catalysts and 4 ligands

Reagents	Solvent	C_{stock} (M)	V_{dose} (μL)	Wells
$NiBr_2$•DME	NMP	0.01	20	A1-D1
$NiCl_2$•DME	NMP	0.01	20	A2-D2
$NiCl_2$•$6H_2O$	NMP	0.01	20	A3-D3
$Ni(acac)_2$	NMP	0.01	20	A4-D4
NiI_2	NMP	0.01	20	A5-D5
NiF_2	NMP	0.01	20	A6-D6
pyridine-2-carboxamidine hydrochloride (**L2**)	NMP	0.01	20	A1-A6

(*Z*)-*N*′-cyanopicolinimidamide	NMP	0.01	20	B1-B6
4-methoxypicolinimidamide hydrochloride	NMP	0.01	20	C1-C6
N-cyano-4-methoxy-picolinimidamide (**L3**)	NMP	0.01	20	D1-D6
Mn Powder	NMP	0.15	20	All
Probenecid *N*-Acyl Glutarimide (**1**)	NMP	0.1	20	All
4-Cl PhenEt Kat Salt (**2**)	NMP	0.12	20	All

Table S4: Reagents, stock solution concentrations, dosing volumes and well locations in the 24-well screen of 6 catalysts and 4 ligands

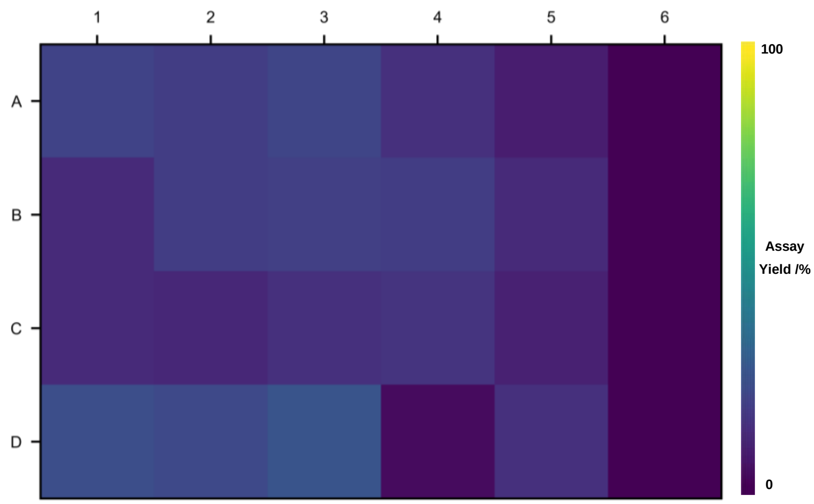
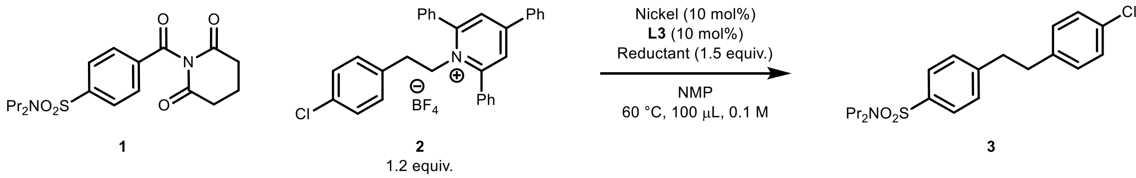


Figure S15: Output heatmap of 24-well screen of 6 catalysts and 4 ligands

24-Well Screen of 4 Catalysts and 6 Water Equivalencies



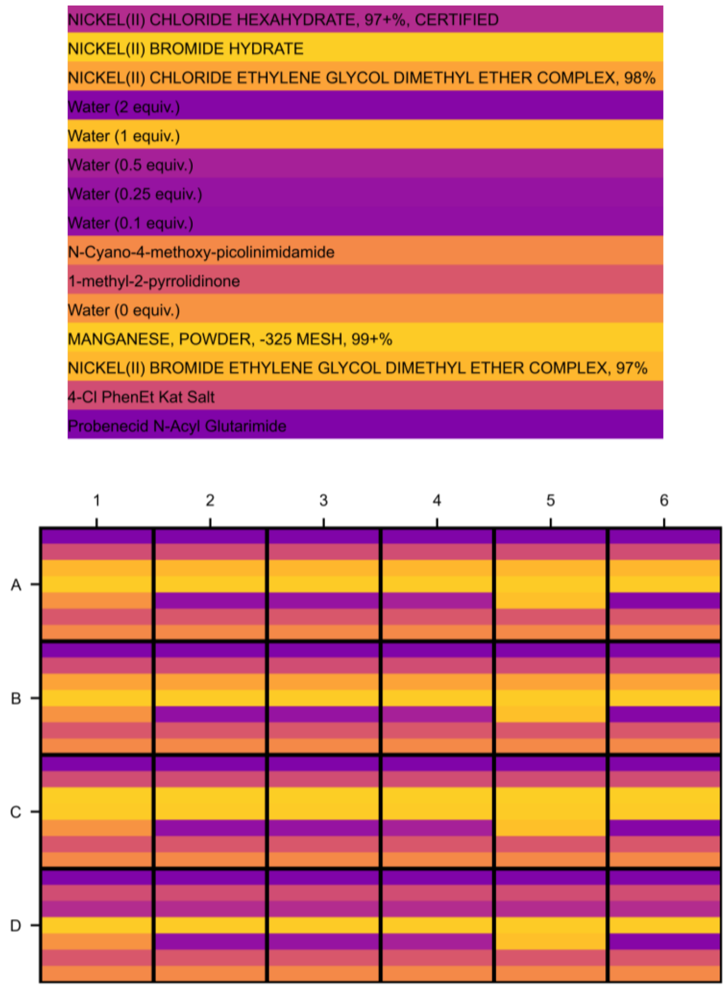


Figure S16: Input heatmap of 24-well screen of 4 catalysts and 6 water equivalencies

Reagents	Solvent	C_{stock} (M)	V_{dose} (μL)	Wells
$NiBr_2$•DME	NMP	0.01	16.6	A1-A6
$NiCl_2$•DME	NMP	0.01	16.6	B1-B6
$NiBr_2$•xH_2O	NMP	0.01	16.6	C1-C6
$NiCl_2$•6H_2O	NMP	0.01	16.6	D1-D6
N-cyano-4-methoxy-picolinimidamide (**L3**)	NMP	0.01	16.6	All
Mn Powder	NMP	0.15	16.6	All

Probenecid *N*-Acyl Glutarimide (**1**)	NMP	0.1	16.6	All
4-Cl PhenEt Kat Salt (**2**)	NMP	0.12	16.6	All
No Water	NMP	0	16.6	A1-D1
Water (0.10 equiv.)	NMP	0.01	16.6	A2-D2
Water (0.25 equiv.)	NMP	0.025	16.6	A3-D3
Water (0.50 equiv.)	NMP	0.05	16.6	A4-D4
Water (1.00 equiv.)	NMP	0.1	16.6	A5-D5
Water (2.00 equiv.)	NMP	0.1	16.6	A6-D6

Table S5: Reagents, stock solution concentrations, dosing volumes and well locations in the 24-well screen of 4 catalysts and 6 water equivalencies

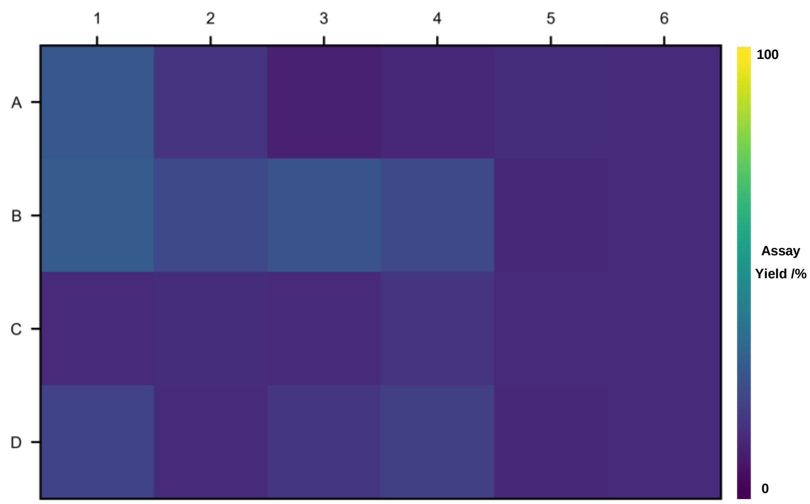
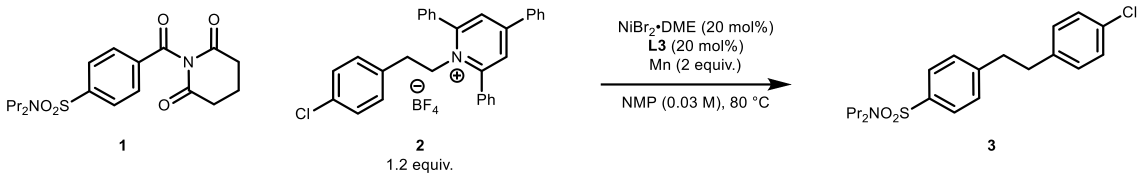


Figure S17: Output heatmap of 24-well screen of 4 catalysts and 6 water equivalencies

Slow Addition Study

Liao *et al*. recently reported that combined slow addition of alkylpyridinium salts and aryl bromides can be beneficial for Ni-catalyzed reductive cross-electrophile coupling.[12] Inspired by these findings we tried an analogous protocol at this stage of our optimization using ligand **L3**. We did not see an improvement in yield compared to the General Singleton protocol.

Slow Addition Procedure



A flame dried 2-dram vial was equipped with a stirrer bar inside a nitrogen-filled glovebox. The vial was charged with $NiBr_2$•DME (6.2 mg, 0.02 mmol), **L3** (3.5 mg, 0.02 mmol), Mn (11.0 mg, 0.20 mmol) and NMP (2 mL). The vial was sealed with a screwcap with a Teflon-coated silicone septum, removed from the glovebox and a N_2 balloon equipped with a needle was added through the septum. The vial was then heated to 80 °C and a solution of **1** (38.0 mg, 0.10 mmol) and **2** (64.1 mg, 0.12 mmol) in NMP (1 mL) was added either over 12 h *via* syringe pump (entry 2) or in 4 portions of 0.25 mL every 3 h (entry 3).

Entry	3 / %	Procedure
1	31	General Singleton
2	16	Syringe pump over 12 h
3	32	Portion wise over 12 h

Table S6: Comparison of the Slow Addition Procedure with the General Singleton Procedure. Yields are determined by ^{1}H NMR through comparison to an internal standard

Extended Ligand Screen

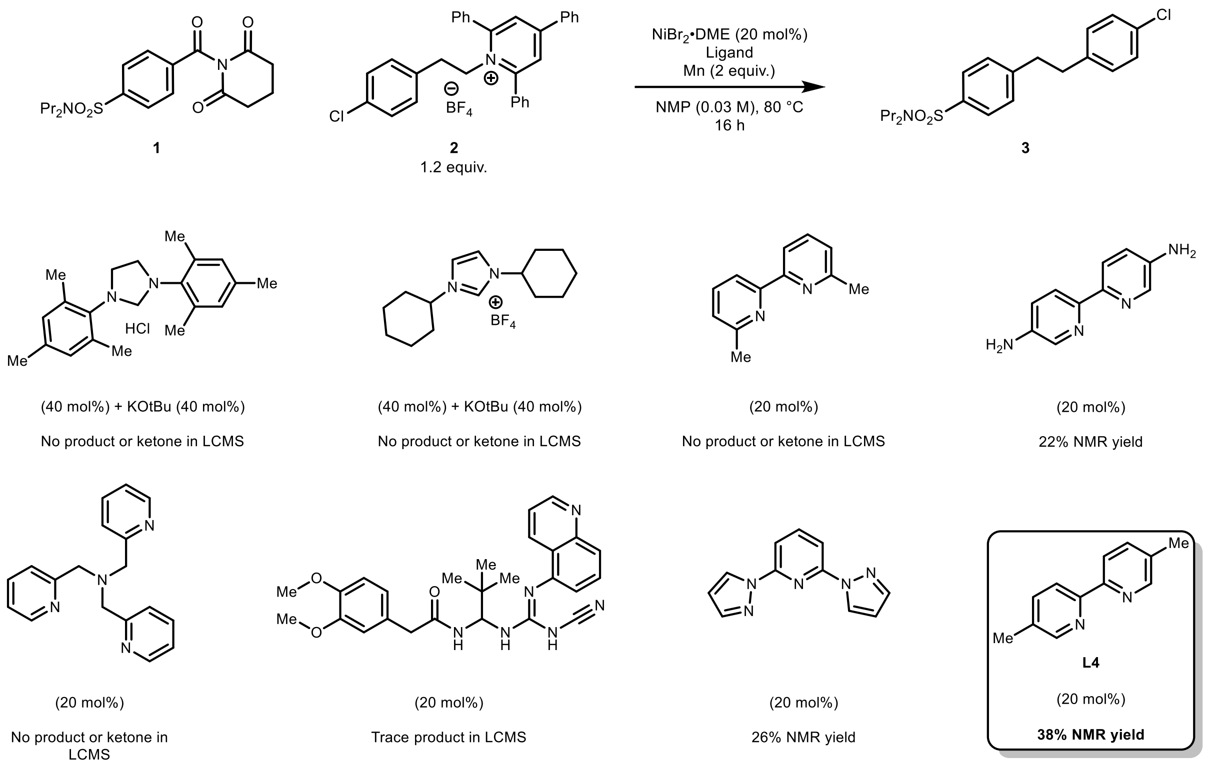
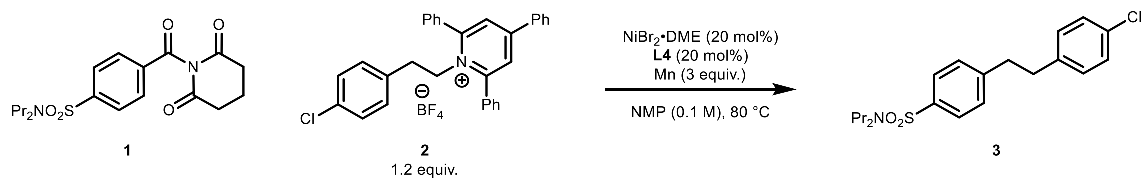


Figure S18: Extended screen of ligands using the General Singleton procedure on 0.1 mmol scale. The screen identified **L4** as a ligand for further optimization

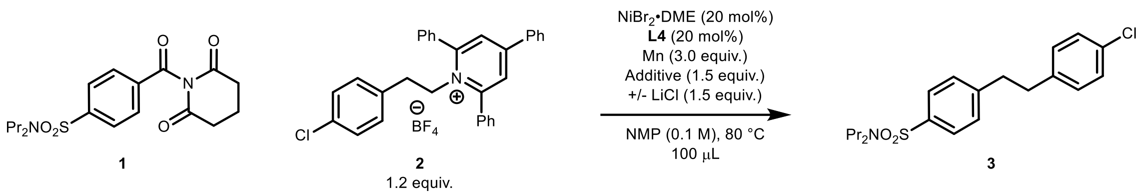
Catalyst and Ligand Ratio



Entry	$NiBr_2$•DME / %	L4 / %	3 / %
1	20	20	38
2	20	40	15
3	20	10	22
4	2	2	Trace

Table S7: Examination of catalyst:ligand ratio using $NiBr_2$•DME and **L4**. Reactions were performed using the General Singleton procedure on 0.1 mmol scale. Yields are determined by ^{1}H NMR through comparison to an internal standard

24-Well Screen of 12 Additives +/- LiCl



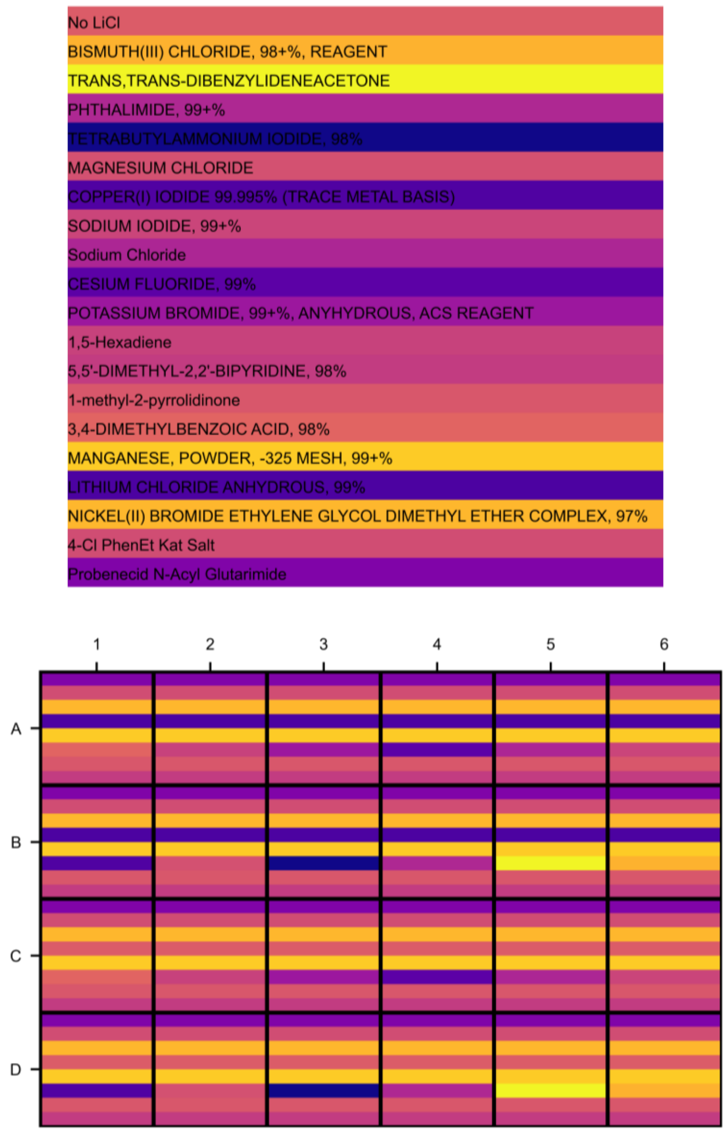


Figure S19: Input heatmap of 24-well screen of 12 additives +/- LiCl

Reagents	Solvent	C_{stock} (M)	V_{dose} (μL)	Wells
$NiBr_2$•DME	NMP	0.02	14.3	All
5,5'-dimethyl-2,2'-bipyridine (**L4**)	NMP	0.02	14.3	All
LiCl	NMP	0.15	14.3	A1-A6, B1-B6
No LiCl	NMP	0	14.3	C1-C6, D1-D6
3,4-dimethylbenzoic acid	NMP	0.15	14.3	A1, C1
1,5-hexadiene	NMP	0.15	14.3	A2, C2
KBr	NMP	0.15	14.3	A3, C3
CsF	NMP	0.15	14.3	A4, C4
NaCl	NMP	0.15	14.3	A5, C5
NaI	NMP	0.15	14.3	A6, C6
CuI	NMP	0.15	14.3	B1, D1
$MgCl_2$	NMP	0.15	14.3	B2, D2
TBAI	NMP	0.15	14.3	B3, D3
Phthalimide	NMP	0.15	14.3	B4, D4
trans,*trans*-dibenzylideneacetone	NMP	0.15	14.3	B5, D5
$BiCl_3$	NMP	0.15	14.3	B6, D6
Mn Powder	NMP	0.15	14.3	All
Probenecid *N*-Acyl Glutarimide (**1**)	NMP	0.1	14.3	All
4-Cl PhenEt Kat Salt (**2**)	NMP	0.12	14.3	All

Table S8: Reagents, stock solution concentrations, dosing volumes and well locations in the 24-well screen of 12 additives +/- LiCl

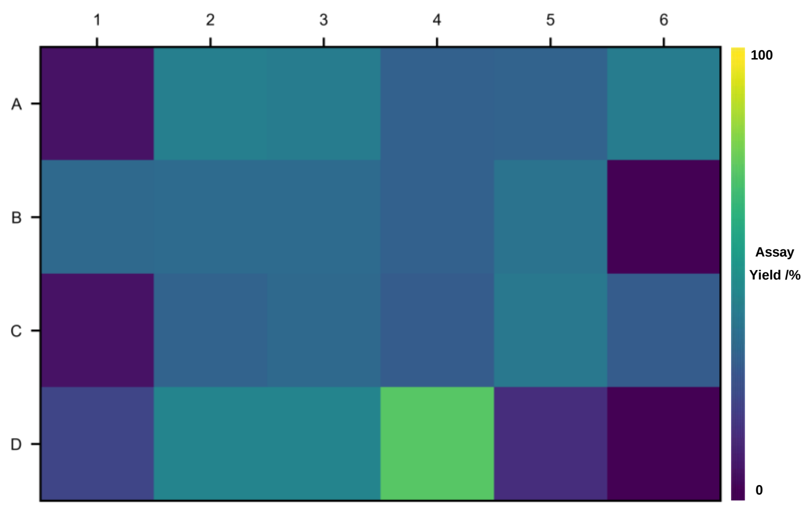


Figure S20: Output heatmap of 24-well screen of 12 additives +/- LiCl

Evaluation of Cyclic Imide and Hydantoin Additives

Cyclic imides such as **4** and the related family of hydantoins have recently been shown to promote reactivity in Ni-catalyzed C(sp^3)-C(sp^2) coupling reactions through the stabilization of Ni(II) oxidative addition complexes, and by preventing the formation of unreactive low-valent Ni-oligomers,[18] which are known to be unreactive towards oxidative addition.[19–21] Intrigued by our result which used cyclic imides to both activate **1** as an *N*-acyl glutarimide and as a beneficial additive in the reaction, we compared the performance of ten cyclic imides and hydantoins **4** and **S40**-**S48** under our optimized conditions (Figure S21). We observed that replacing **4** with glutarimide **S40** lowered the yield, perhaps suggesting that **S40** generated in the reaction can trap the Ni-catalyst off cycle,[21,22] hence why addition of **4** is beneficial. Alternatively, **S40** may be poor at stabilizing Ni. Succinimide **S41**, hexahydrophthalimide **S43** and maleimide **S42** all resulted in a lower yield of **3**, the latter likely due to η^2-binding of the alkene bond to the Ni-center. A slight improvement in yield to 79% was observed with α-methyl-α-phenylsuccinimide **S44**. The hydantoin series **S45**-**S48** resulted in yields that were lower than, or comparable to **4**. Although **S44** did give a small increase in yield compared to **4**, we decided to proceed with the latter due to its significantly lower cost ($0.27/g vs $136/g).[23,24]

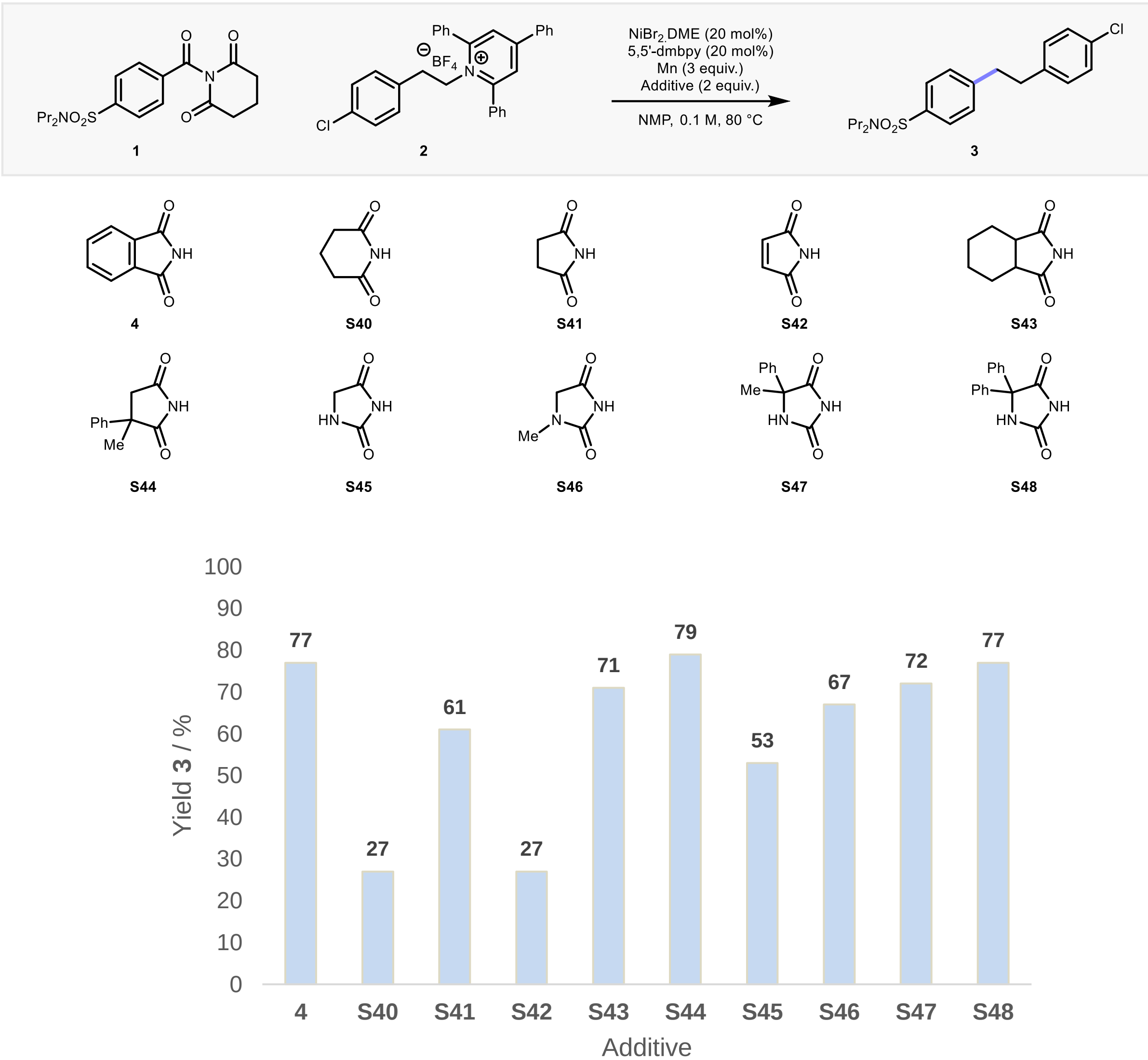
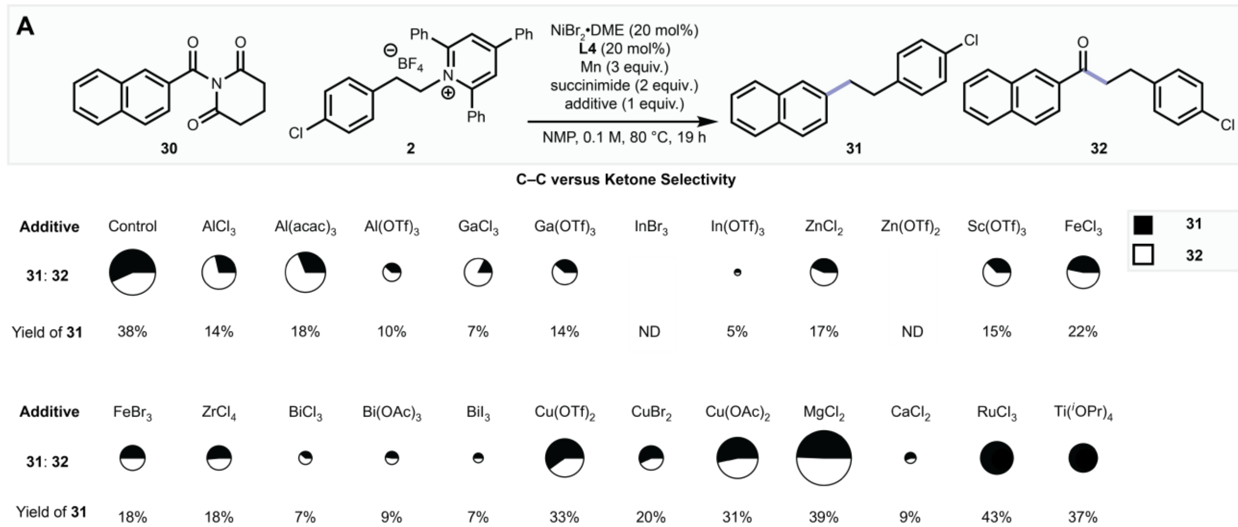


Figure S21: Evaluation of cyclic imide and hydantoin additives in the coupling of **1** and **2** to form **3**. Reactions were performed on 25 µmol scale using a modified General Singleton Procedure in which a $NiBr_2$•DME and **L4** stock solution in NMP was made and dosed to each reaction. The reactions were analyzed by UPLC-MS.

C–C versus Ketone Selectivity Screening

Metal Salt Additive Screen

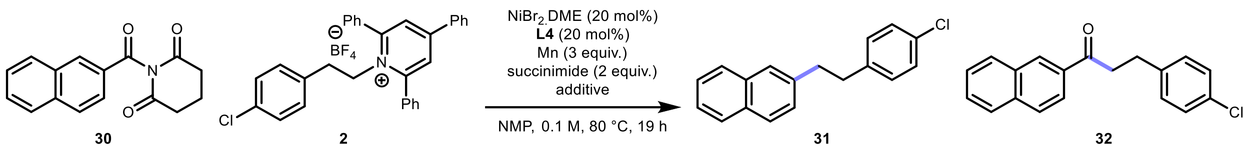


Entry	Additive	31 / %	32 / %	Total Yield / %	Ratio 31:32
1	None (control)	38	29	67	1.3:1
2	$AlCl_3$	14	35	49	1:2.5
3	$Al(acac)_3$	18	40	58	1:2.2
4	$Al(OTf)_3$	10	16	26	1:1.6
5	$GaCl_3$	7	33	40	1:4.4
6	$Ga(OTf)_3$	14	22	36	1:1.6
7	$InBr_3$	ND	ND	-	-
8	$In(OTf)_3$	5	5	10	1:1
9	$ZnCl_2$	17	22	39	1:1.3
10	$Zn(OTf)_2$	ND	ND	-	-
11	$Sc(OTf)_2$	15	25	40	1:1.7
12	$FeCl_3$	22	25	47	1:1.1
13	$FeBr_3$	18	18	36	1:1
14	$ZrCl_4$	18	17	35	1.1:1
15	$BiCl_3$	7	11	18	1:1.6
16	$Bi(OAc)_3$	9	10	19	1:1.1
17	BiI_3	7	7	14	1:1
18	$Cu(OTf)_2$	33	22	55	1.5:1
19	$CuBr_2$	20	15	35	1.3:1
20	$Cu(OAc)_2$	31	27	58	1.1:1
21	$MgCl_2$	39	40	79	1:1
22	$CaCl_2$	9	7	16	1.3:1

23	$RuCl_3$	43	ND	43	>20:1
24	$Ti(iOPr)_4$	37	ND	37	>20:1

Table S9: Effect of metal salts on the reaction between **30** and **2**. Reactions were run on 50 µmol scale using General Procedure C. Yields were determined by UPLC-MS. ND = not detected

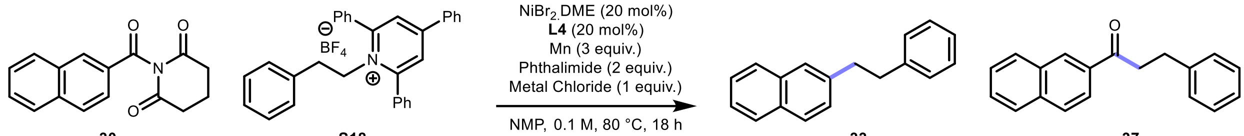
Extended Additive Screen



Entry	Additive	mol%	31 / %	32 / %	Total Yield / %	Ratio 31:32
1	None (control)	-	41	28	69	1.5:1
2	$Ru_2(C_6H_6)_2Cl_4$	100	8	ND	8	>20:1
3	[Ru(*p*-cymene)Cl_2]$_2$	100	28	ND	28	>20:1
4	$[(C_6H_5)_3P]_3RuCl_2$	100	24	ND	24	>20:1
5	$TiCl_4$	100	14	25	39	1:1.8
6	Cp_2TiCl_2	100	12	8	20	1.4:1
7	$Ga(acac)_3$	100	18	62	80	1:3.5
8	Pivalic Acid	100	7	14	21	1:1.9
9	$AlBr_3$	100	11	33	44	1:3.1
10	TMANO	100	13	9	22	1.4:1
11	NMO	100	21	11	32	1.9:1
12	$RuCl_3$	20	45	14	59	3.3:1
13	$RuCl_3$ + TMANO	20 + 100	19	9	28	2.1:1
14	$RuCl_3$ + NMO	20 + 100	8	ND	8	>20:1
15	$GaCl_3$	20	15	58	73	1:3.9
16	$RuCl_3$	200	14	ND	14	>20:1
17	$GaCl_3$	200	5	8	13	1:1.4

Table S10: Extended additive screen. Reactions were run on 50 µmol scale using General Procedure C Yields were determined by UPLC-MS. ND = not detected, TMANO = trimethylamine *N*-oxide, NMO = 4-methylmorpholine *N*-oxide

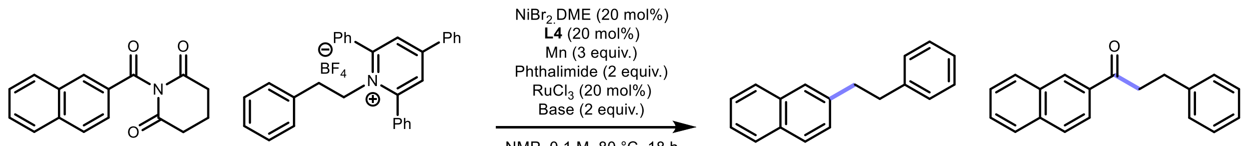
Metal Chloride Screen



Entry	Metal Chloride	33 / %	37 / %	Total Yield / %	Ratio 33:37
1	None (control)	32	14	46	2.3:1
2	$RuCl_3$	48	ND	48	>20:1
3	VCl_3	14	11	25	1.3:1
4	$CrCl_3$	ND	ND	-	-
5	$CoCl_2$	26	10	36	2.6:1
6	$PdCl_2$	32	ND	32	>20:1

Table S11: Extended additive screen. Reactions were run on 50 µmol scale using General Procedure C Yields were determined by UPLC-MS. ND = not detected

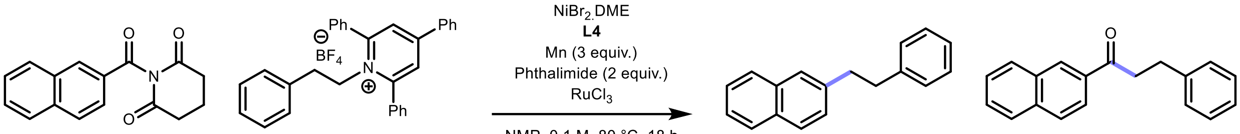
Base Screen



Entry	Base	$RuCl_3$ (Y/N)?	33 / %	37 / %	Total Yield / %	Ratio 33:37
1	None	N	33	20	53	1.7:1
2	None	Y	59	14	73	4.2:1
3	BTMG	N	10	ND	10	>20:1
4	BTMG	Y	11	ND	11	>20:1
5	DIPEA	N	20	11	31	1.8:1
6	DIPEA	Y	53	ND	53	>20:1
7	Cs_2CO_3	N	3	ND	3	>20:1
8	Cs_2CO_3	Y	18	11	29	1.6:1
9	K_3PO_4	N	12	ND	12	>20:1
10	K_3PO_4	Y	9	ND	9	>20:1
11	KO*t*Bu	N	13	6	19	2.0:1
12	KO*t*Bu	Y	12	ND	12	>20:1
13	H^+ sponge	N	34	20	54	1.7:1
14	H^+ sponge	Y	56	12	68	4.8:1

Table S12: Base screen in the presence and absence of $RuCl_3$. Reactions were run on 50 µmol scale using General Procedure C. Yields were determined by UPLC-MS. ND = not detected

$RuCl_3$ Loading Optimization



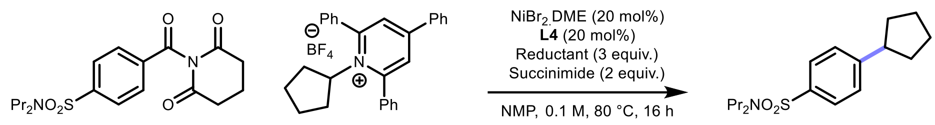
30 S18 33 37

Entry	[Ni] / mol%	L4 / mol%	$RuCl_3$ / mol%	33 / %	37 / %	Total Yield / %	Ratio 33:37
1	20	20	0	59	28	87	2.1:1
2	20	20	10	66	26	92	2.6:1
3	20	20	20	70	23	93	3.1:1
4	20	20	30	63	ND	63	>20:1
5	20	20	40	80	17	97	4.7:1
6	20	20	50	75*	ND	75	>20:1
7	40	40	0	67	31	98	2.2:1
8	40	40	10	72	29	101	2.5:1
9	40	40	20	73	27	100	2.7:1

Table S13: Optimization of $RuCl_3$ and NiBr•DME loadings. Reactions were run on 50 µmol scale using General Procedure C. Yields were determined by UPLC-MS. ND = not detected. *yield from ^{1}H NMR through reference to an internal standard

Secondary and Benzyl Pyridinium Salt Optimization

Initial Yield



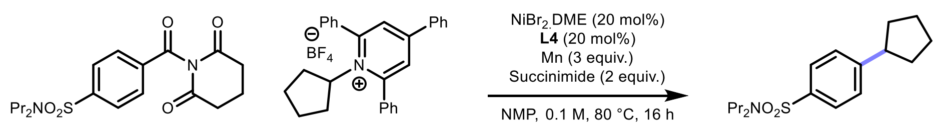
1 38 39

Entry	Reductant	39 / %
1	Mn	18
2	Zn	8

Table S14: Result of coupling secondary pyridinium salt **38** using conditions similar to those used for primary pyridinium salts. Reactions were performed at 50 µmol scale using General Procedure C. Yields were determined by UPLC-MS.

Slow Addition

Liao *et al*. recently reported that combined slow addition of alkylpyridinium salts and aryl bromides can be beneficial for Ni-catalyzed reductive cross-electrophile coupling, in particular for the coupling of secondary pyridinium salts, which saw a 65% increase in yield compared to the standard reaction.[12] Given that our system is analogous to that of Liao *et al*. we attempted a similar method to synthesize **39**, however only a modest 6% increase in yield was observed compared to the result in Table S14 Entry 1.



1 38 39 24%

Slow addition of **1** and **38** over 6 h

Figure S22: Combined slow addition of **1** and **38** to make **39**

A flame dried 2-dram vial was equipped with a stirrer bar inside a nitrogen-filled glovebox. The vial was charged with $NiBr_2$•DME (6.2 mg, 0.02 mmol), **L4** (3.7 mg, 0.02 mmol), Mn (16.5 mg, 0.30 mmol) and NMP (1 mL). The vial was sealed with a screwcap with a Teflon-coated silicone septum, removed from the glovebox and a N_2 balloon equipped with a needle was added through the septum. The vial was then heated to 80 °C and a solution of **1** (38.0 mg, 0.10 mmol) and **2** (92.7 mg, 0.20 mmol) in NMP (1 mL) was added over 6 h *via* syringe pump. The reaction was analyzed by UPLC-MS.

Kinetic Studies

The reactions below were set up using General Procedure C with **L4** as the ligand and succinimide as the additive on a 0.25 mmol scale with respect to **1**. The vial was septum was equipped with a nitrogen balloon and at the specified time intervals an 8.4 uL aliquot was taken from the reaction, added to 992 uL of 0.15 mg/mL caffeine solution in MeCN/Water 50:50, then passed through a syringe filter and analyzed by UPLC-MS.

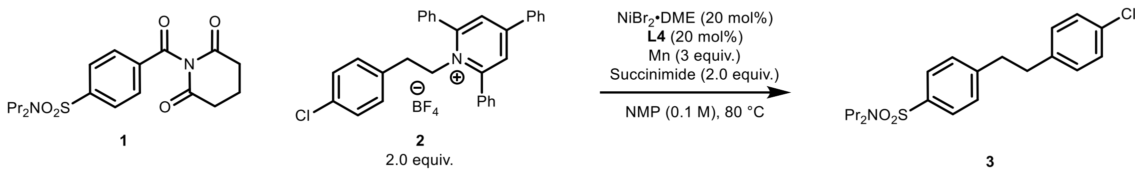


Figure S23: Conditions for 1° alkylpyridinium salt kinetic experiment

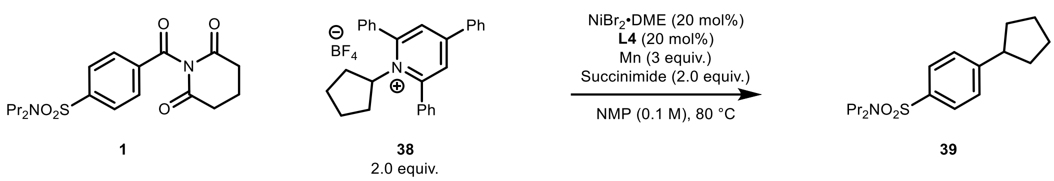


Figure S24: Conditions for 2° alkylpyridinium salt kinetic experiment

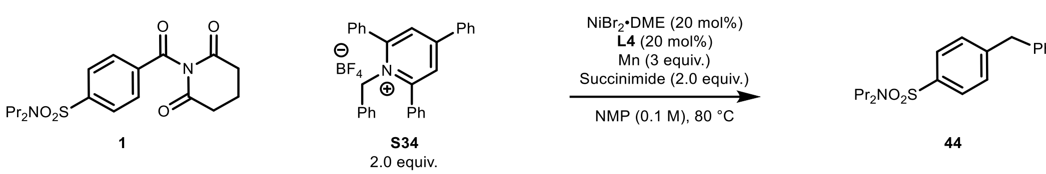


Figure S25: Conditions for benzylpyridinium salt kinetic experiment

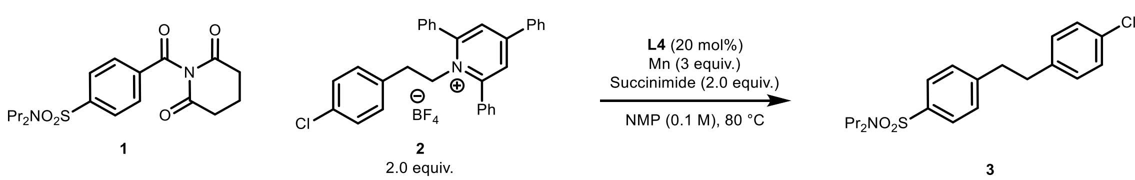


Figure S26: Conditions for 1° alkylpyridinium salt kinetic experiment in the absence of $NiBr_2$•DME

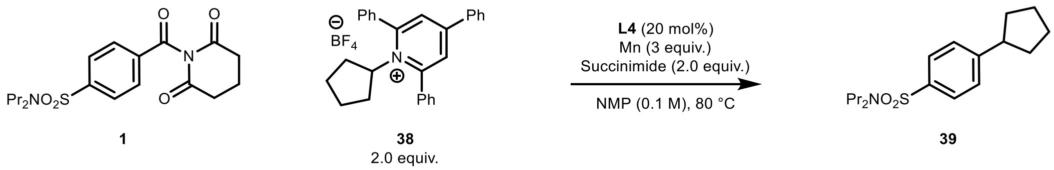


Figure S27: Conditions for 2° alkylpyridinium salt kinetic experiment in the absence of $NiBr_2$•DME

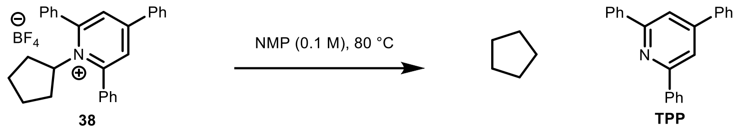


Figure S28: Conditions for 2° alkylpyridinium salt thermal decomposition kinetic experiment

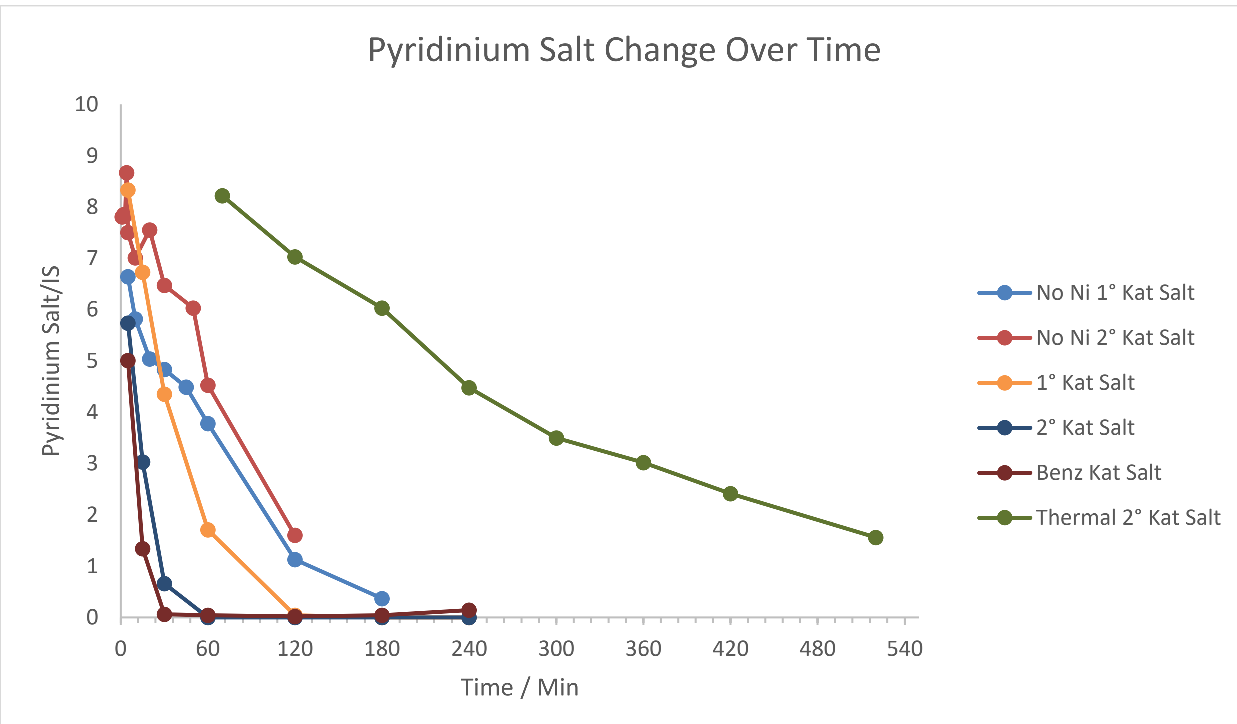


Figure S29: Change in pyridinium (Kat.) salt over time for the experiments shown in Figure S23-Figure S28

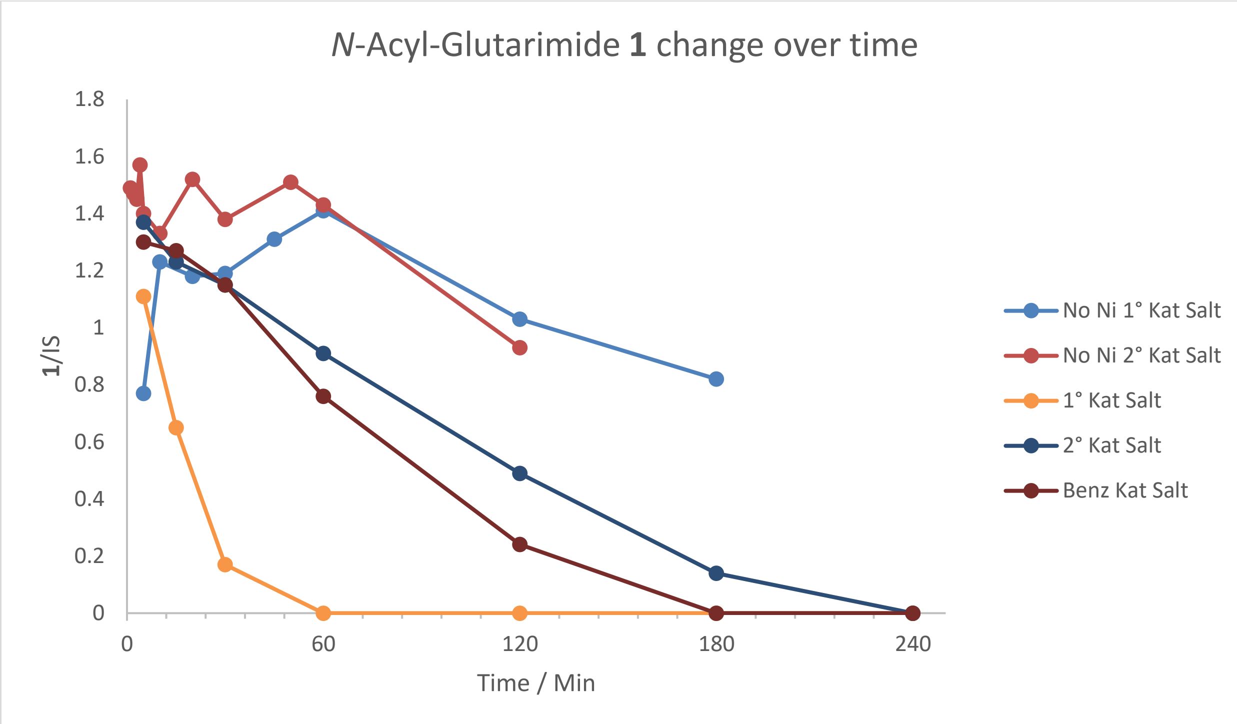
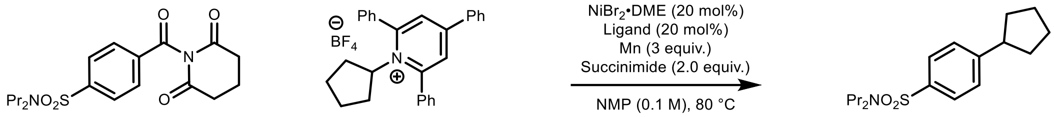


Figure S30: Change in *N*-acyl-glutarimide **1** over time for the experiments shown in Figure S23-Figure S28

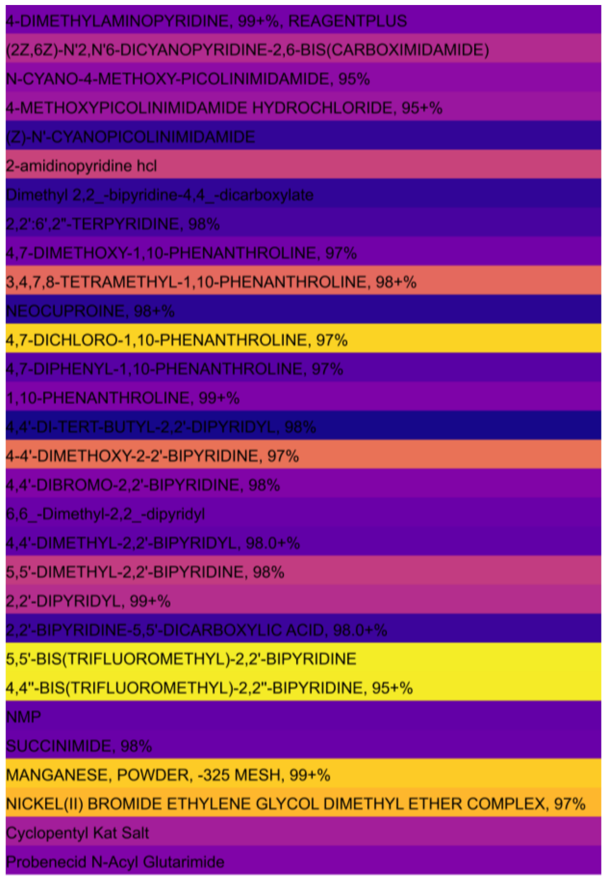
Through monitoring reaction kinetics we were able to draw conclusions which guided our efforts in optimizing the C(sp)^3–C(sp)^2 coupling of secondary and benzyl pyridinium salts with *N*-acyl-glutarimides. The data suggest that the rate of reduction of pyridinium salt is benzyl > secondary > primary. *N*-acyl-glutarimide **1** is consumed fastest in the presence of primary pyridinium salt **2**, and remains present in solution after secondary pyridinium salt **38** and benzylpyridinium salt **S34** have been consumed. Taken together these results suggest that the rate of primary pyridinium salt **2** reduction is comparable to oxidative addition of [Ni] into **1**, leading to productive formation of **3**. However, in the case of **38** and **S34**, pyridinium salt reduction occurs at too high a rate. Remaining **1** is then consumed slowly to decarboxylated and homocoupled products that can be observed by UPLC-MS. We therefore focused our efforts on reducing the rate of pyridinium salt reduction.

In the absence of $NiBr_2$•DME the rate of pyridinium salt reduction was reduced for both **2** and **38**, suggesting that a nickel species plays an active role in the reduction event. Inspired by this finding, we decided to examine a range of ligands, with the hypothesis that those with electron-withdrawing groups would reduce the rate of pyridinium salt reduction by Ni. We found that 5,5'-bis(trifluoromethyl)-2,2'-bipyridine (**L5**) gave an increase in yield relative to 5,5'-dimethyl-2,2'-bipyridine (**L4**), suggesting that our hypothesis was correct.

24-Well Screen of 24 Ligands



1 38 2.0 equiv. 39



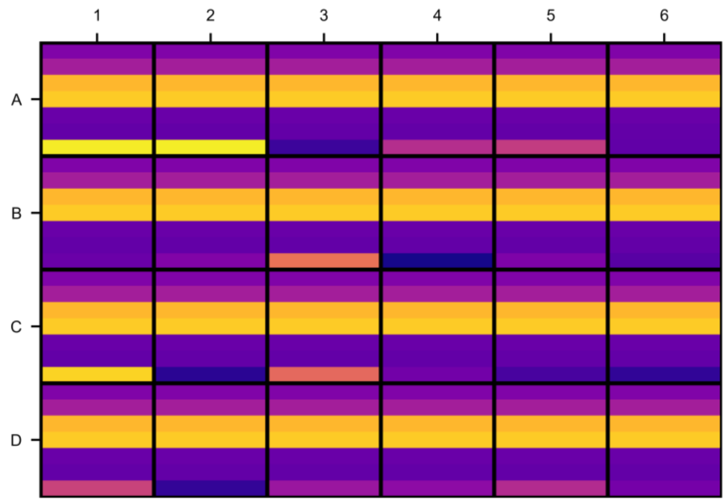


Figure S31: Input heatmap of 24-well screen of 24 ligands to optimize the coupling of secondary alkylpyridinium salts

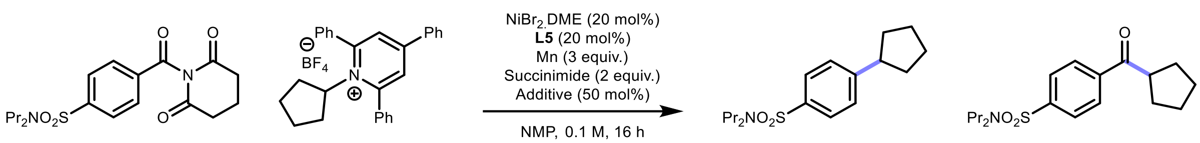
Reagents	Solvent	C_{stock} (M)	V_{dose} (μL)	Wells
$NiBr_2$•DME	NMP	0.02	16.6	All
4,4'-bis(trifluoromethyl)-2,2'-bipyridine	NMP	0.02	16.6	A1
5,5'-bis(trifluoromethyl)-2,2'-bipyridine (**L5**)	NMP	0.02	16.6	A2
[2,2'-bipyridine]-5,5'-dicarboxylic acid	NMP	0.02	16.6	A3
2,2'-bipyridine	NMP	0.02	16.6	A4
5,5'-dimethyl-2,2'-bipyridine (**L4**)	NMP	0.02	16.6	A5
4,4'-dimethyl-2,2'-bipyridine	NMP	0.02	16.6	A6
6,6'-dimethyl-2,2'-bipyridine	NMP	0.02	16.6	B1
4,4-dibromo-2,2'-bipyridine	NMP	0.02	16.6	B2
4,4'-dimethoxy-2,2'-bipyridine	NMP	0.02	16.6	B3
dtbpy (**L1**)	NMP	0.02	16.6	B4
1,10-phenanthroline	NMP	0.02	16.6	B5
4,7-diphenyl-1,10-phenanthroline	NMP	0.02	16.6	B6
4,7-dichloro-1,10-phenanthroline	NMP	0.02	16.6	C1
neocuproine	NMP	0.02	16.6	C2
tmphen	NMP	0.02	16.6	C3
4,7-dimethoxy-1,10-phenanthroline	NMP	0.02	16.6	C4
2,2':6,2"-terpyridine	NMP	0.02	16.6	C5
dimethyl-2,2'-bipyridine-4,4'-dicarboxylate	NMP	0.02	16.6	C6
2-amindinopyridine HCl (**L2**)	NMP	0.02	16.6	D1
(*Z*)-*N*'-cyanopicolinimidamide	NMP	0.02	16.6	D2
4-methoxypicolinamidamide HCl	NMP	0.02	16.6	D3
N-cyano-4-methoxy-picolinimidamide (**L3**)	NMP	0.02	16.6	D4

(2*Z*,6*Z*)-*N*'2,*N*'6-dicyanopyridine-2,6-bis(carboximidamide	NMP	0.02	16.6	D5
DMAP	NMP	0.04	16.6	D6
succinimide	NMP	0.20	16.6	All
Mn powder	NMP	0.30	16.6	All
probenecid *N*-acyl Glutarimide (**1**)	NMP	0.10	16.6	All
Cyclopentyl pyridinium salt (**38**)	NMP	0.20	16.6	All

Table S15: Reagents, stock solution concentrations, dosing volumes and well locations in the 24-well screen of 24 ligands to optimize the coupling of secondary alkylpyridinium salts

Figure S32: Output heatmap of 24-well screen of 24 ligands to optimize the coupling of secondary alkylpyridinium salts

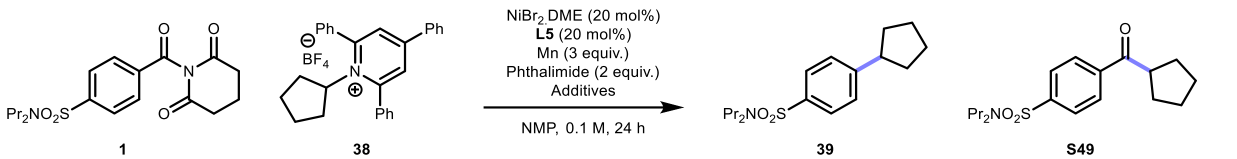
Scale Up Reactions



Entry	T / °C	Additive	39 / %	S49 / %	Total Yield / %	Ratio 39:S49
1	80	-	21	6	27	3.5:1
2	80	$RuCl_3$	15	ND	15	>20:1
3	80	$GaCl_3$	32 (24)	6	38	5.3:1
4	40	-	21	5	25	4.2:1
5	40	$RuCl_3$	14	ND	14	>20:1
6	40	$GaCl_3$	33	11	44	3.0:1

Table S16: Repeat of the conditions identified in Figure S32 on 0.25 mmol scale using General Procedure C at both 80 °C and 40 °C and in the presence of $RuCl_3$ and $GaCl_3$. Yields were determined by UPLC-MS. ND = not detected. Isolated yield in parenthesis.

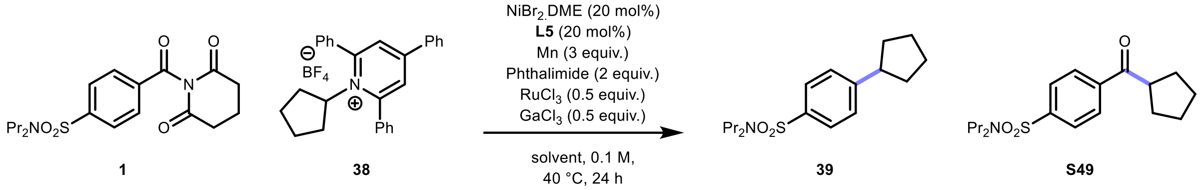
Additive Loading Optimization



Entry	T / °C	$RuCl_3$ / mol%	$GaCl_3$ / mol%	$MgCl_2$ / mol%	39 / %	S49 / %	Total Yield / %	Ratio 39:S49
1	40	0	50	0	24	5	29	4.8:1
2	40	50	50	0	51	10	61	5.1:1
3	40	100	50	0	42	8	50	5.3:1
4	40	50	100	0	39	7	46	5.6:1
5	40	100	100	0	42	7	49	6.0:1
6	80	0	50	0	29	7	36	4.1:1
7	80	50	50	0	26	4	30	6.5:1
8	40	0	0	100	20	3	23	6.7:1
9	80	0	0	100	15	2	17	7.5:1
10	40	0	50	100	35	6	41	5.8:1
11	80	0	50	100	14	3	17	5.7:1
12	40	50	0	100	18	3	21	6.0:1
13	80	50	0	100	14	Trace	14	>20:1
14	40	50	50	100	36	5	41	7.2:1
15	80	50	50	100	17	Trace	17	>20:1

Table S17: Additive loading optimization in the formation of **39** from **1** and **38**. Reactions were run on 100 µmol scale using General Procedure C. Yields were determined by UPLC-MS. ND = not detected.

Solvent Screen



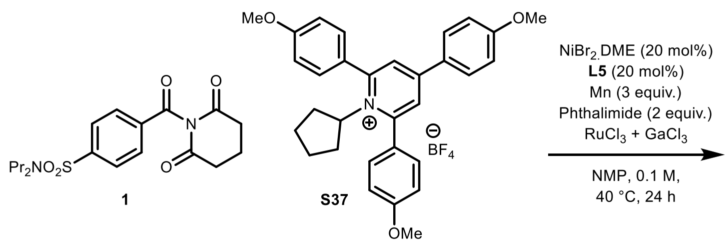
1 **38** **39** **S49**

Entry	Solvent	38 / %	S49 / %	Total Yield / %	Ratio 38:S49
1	NMP	51	10	61	5.1:1
2	DMA	30	8	38	3.8:1
3	DMF	10	Trace	10	10:1
4	DMSO	10	6	16	1.7:1
5	THF	7	4	11	1.8:1
6	Dioxane	ND	ND	-	-
7	Ether	10	9	19	1.1:1
8	Diglyme	ND	ND	-	-
9	CPME	ND	ND	-	-
10	TBME	ND	ND	-	-
11	2-MeTHF	ND	ND	-	-
12	Toluene	ND	ND	-	-
13	Trifluorotoluene	ND	ND	-	-
14	Xylene	ND	ND	-	-
15	Benzene	ND	ND	-	-
16	Fluorobenzene	ND	ND	-	-
17	MeCN	ND	ND	-	-
18	Adiponitrile	ND	ND	-	-
19	Heptane	ND	ND	-	-
20	DCM	ND	ND	-	-

Table S18: Solvent screen for the formation of **39** from **1** and **38**. Reactions were run on 50 µmol scale using General Procedure for Singleton Optimization. Yields were determined by UPLC-MS. ND = not detected.

Pyridinium Salt Derivatization

To try and slow the rate of reduction of pyridinium salt with the aim of increasing yield, we attempted the coupling of pyridinium salts with lower reduction potentials.



Entry	$RuCl_3$ / mol%	$GaCl_3$ / mol%	39 / %	S49 / %	Total Yield / %	Ratio 39:S49
1	0	0	17	ND	17	>20:1
2	50	0	21	ND	21	>20:1
3	50	50	26	ND	26	>20:1

Table S19: Evaluation of derivatized pyridinium salt **S37** in the formation of **39**. Reactions were run on 50 µmol scale using General Procedure C. Yields were determined by UPLC-MS. ND = not detected.

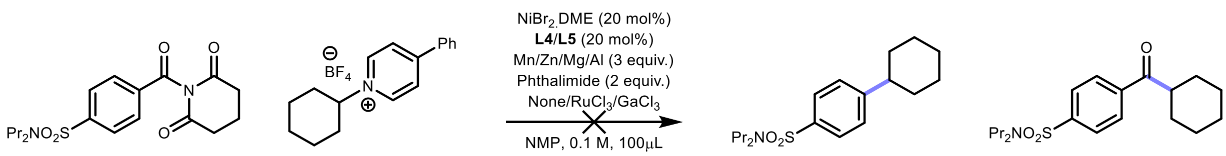
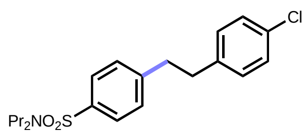


Figure S33: Attempted coupling of **S39** with **1** to produce **36** using all combinations of 2 ligands, 3 reductant and 3 additives with high-throughput experimentation. In each case no **39** or **S49** was detected by UPLC-MS

Decarbonylative-Deaminative Coupling of *N*-Acyl-Glutarimides and Alkylpyridinium Salts

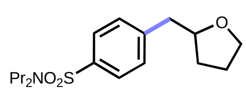
Products

4-(4-chlorophenethyl)-*N*,*N*-dipropylbenzenesulfonamide (**3**)



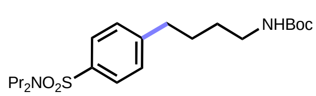
Following General Procedure C, using **1** (95.0 mg, 0.25 mmol) and **2** (267 mg, 0.50 mmol) as the substrates. The crude product was purified via silica gel chromatography (0.2-0.3% EtOAc in toluene) to give the title compound **3** as a white solid (60.0 mg, 0.16 mmol, 63%). **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.69 (d, *J* = 8.3 Hz, 2H), 7.24-7.20 (m, 4H), 7.03 (d, *J* = 8.4 Hz, 2H), 3.06 (t, *J* = 7.8 Hz, 4H), 2.98-2.93 (m, 2H), 2.92-2.87 (m, 2H), 1.54 (h, *J* = 7.6 Hz, 4H), 0.86 (t, *J* = 7.5 Hz, 6H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 145.9, 139.2, 138.0, 131.9, 129.8, 129.1, 128.5, 127.2, 49.9, 37.5, 36.7, 22.0, 11.2; **HRMS:** m/z: $[M+H]^+$ calc'd for $[C_{20}H_{27}NO_2ClS]^+$ expect 380.1446; found 380.1452.

N,*N*-dipropyl-4-((tetrahydrofuran-2-yl)methyl)benzenesulfonamide (**5**)



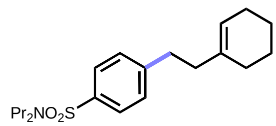
Following General Procedure C, using **1** (95.0 mg, 0.250 mmol) and **S19** (240 mg, 0.500 mmol) as the substrates. The crude product was purified via silica gel chromatography (5-10% EtOAc in Hexane) to give the title compound **5** as a yellow liquid (59.2 mg, 0.182 mmol, 73%). **^{1}H NMR (499 MHz, $CDCl_3$)**: δ 7.70 (d, *J* = 8.1 Hz, 2H), 7.35 (d, *J* = 8.0 Hz, 2H), 4.10-4.04 (m, 1H), 3.89-3.83 (m, 1H), 3.76-3.69 (m, 1H), 3.09-3.02 (m, 4H), 2.92 (dd, *J* = 13.8, 6.9 Hz, 1H), 2.84 (dd, *J* = 13.8, 5.5 Hz, 1H), 1.98-1.89 (m, 1H), 1.90-1.80 (m, 2H), 1.59-1.48 (m, 5H), 0.86 (t, *J* = 7.4 Hz, 6H); **^{13}C NMR (126 MHz, $CDCl_3$)**: δ 144.0, 138.0, 129.9, 127.2, 79.4, 68.1, 50.3, 41.8, 31.2, 25.7, 22.2, 11.3; **HRMS:** m/z: $[M+H]^+$ calc'd for $[C_{17}H_{28}NO_3S]^+$ expect 326.1784; found 326.1785.

N,*N*-dipropyl-4-((tetrahydrofuran-2-yl)methyl)benzenesulfonamide (**6**)



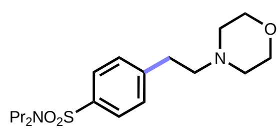
Following General Procedure C, using **1** (95.0 mg, 0.250 mmol) and **S21** (283 mg, 0.500 mmol) as the substrates. The crude product was purified via silica gel chromatography (5-12% EtOAc in Hexane) to give the title compound **6** as a yellow liquid (57.0 mg, 0.138 mmol, 55%). **^{1}H NMR (499 MHz, CDCl$_3$)**: δ 7.69 (d, *J* = 7.9 Hz, 2H), 7.27 (d, *J* = 8.0 Hz, 2H), 4.52 (s, 1H), 3.14 (m, 2H), 3.05 (m, 4H), 2.68 (t, *J* = 7.7 Hz, 2H), 1.69-1.62 (m, 2H), 1.61-1.48 (m, 6H), 1.44 (s, 9H), 0.87 (t, *J* = 7.4 Hz, 6H); **^{13}C NMR (126 MHz, CDCl$_3$)**: δ 156.1, 147.2, 137.7, 129.0, 127.3, 79.3, 50.2, 40.4, 35.5, 29.8, 28.6, 28.3, 22.2, 11.3; **HRMS:** m/z: [M+Na]$^+$ calc'd for $[C_{21}H_{36}N_2O_4SNa]^+$ expect 435.2293; found 435.2282.

4-(2-(cyclohex-1-en-1-yl)ethyl)-*N*,*N*-dipropylbenzenesulfonamide (**7**)



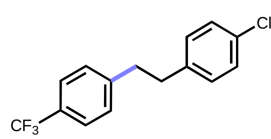
Following General Procedure C, using **1** (95.0 mg, 0.250 mmol) and **S25** (257 mg, 0.500 mmol) as the substrates. The crude product was purified via silica gel chromatography (2-5% EtOAc in Hexane) to give the title compound **7** as a colorless liquid (49.3 mg, 0.141 mmol, 56%). **^{1}H NMR (499 MHz, CDCl$_3$)**: δ 7.69 (d, *J* = 8.2 Hz, 2H), 7.27 (d, *J* = 8.2 Hz, 2H), 5.38-5.32 (m, 1H), 3.09-3.02 (m, 4H), 2.79-2.72 (m, 2H), 2.22 (t, *J* = 8.0 Hz, 2H), 1.98-1.90 (m, 4H), 1.65-1.57 (m, 2H), 1.53 (q, *J* = 7.7 Hz, 6H), 0.86 (t, *J* = 7.4 Hz, 6H); **^{13}C NMR (126 MHz, CDCl$_3$)**: δ 147.5, 137.5, 136.5, 129.1, 127.2, 122.2, 50.1, 39.5, 34.3, 28.5, 25.3, 23.1, 22.6, 22.1, 11.3; **HRMS:** m/z: [M+H]$^+$ calc'd for $[C_{20}H_{32}NO_2S]^+$ expect 350.2148; found 350.2144.

4-(2-morpholinoethyl)-*N*,*N*-dipropylbenzenesulfonamide (**8**)



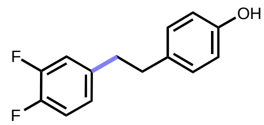
Following General Procedure C, using **1** (95.0 mg, 0.250 mmol) and **S23** (254 mg, 0.500 mmol) as the substrates. The crude product was purified via silica gel chromatography (20-40% EtOAc in Hexane) to give the title compound **8** as a colorless liquid (52.7 mg, 0.149 mmol, 59%). **^{1}H NMR (499 MHz, CDCl$_3$)**: δ 7.70 (d, *J* = 8.1 Hz, 2H), 7.31 (d, *J* = 8.1 Hz, 2H), 3.72 (t, *J* = 4.7 Hz, 4H), 3.09-3.03 (m, 4H), 2.85 (dd, *J* = 9.6, 6.4 Hz, 2H), 2.64-2.57 (m, 2H), 2.50 (t, *J* = 4.7 Hz, 4H), 1.53 (dt, *J* = 15.2, 7.5 Hz, 4H), 0.85 (t, *J* = 7.4 Hz, 6H); **^{13}C NMR (126 MHz, CDCl$_3$)**: δ 145.2, 138.1, 129.4, 127.3, 67.0, 60.2, 53.8, 50.2, 33.2, 22.2, 11.3; **HRMS:** m/z: [M+H]$^+$ calc'd for $[C_{18}H_{31}N_2O_3S]^+$ expect 355.2050; found 355.2037.

1-chloro-4-(4-(trifluoromethyl)phenethyl)benzene (**9**)



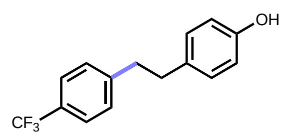
Following General Procedure C, using **S2** (42.8 mg, 0.15 mmol) and **2** (160 mg, 0.3 mmol) as the substrates. The crude product was purified via silica gel chromatography (2-5% EtOAc in Hexane) to give the title compound **9** as a white solid (24.9 mg, 0.15 mmol, 58%). **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.53 (d, J = 8.1 Hz, 2H), 7.26-7.21 (m, 4H), 7.07 (d, J = 8.3 Hz, 2H), 2.99-2.93 (m, 2H), 2.93-2.88 (m, 2H); **^{13}C NMR (126 MHz, $CDCl_3$)** 145.3 (q, $^{5}J_{C-F}$ = 1.2 Hz), 139.4, 131.9, 129.8, 128.8, 128.5, 128.5 (q, $^{2}J_{C-F}$ = 32.4 Hz), 125.3 (q, $^{3}J_{C-F}$ = 3.7 Hz), 124.3 (q, $^{1}J_{C-F}$ = 271.7 Hz), 37.5, 36.8; **^{19}F NMR (471 MHz, $CDCl_3$)** -62.3; **HRMS(EI+):** m/z: $[M]^+$ calc'd for $[C_{15}H_{12}ClF_3]^+$ expect 284.0580; found 284.0568.

4-(3,4-difluorophenethyl)phenol (**10**)



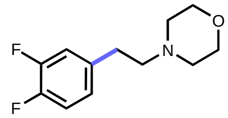
Following General Procedure C, using **S3** (63.3 mg, 0.250 mmol) and **S26** (257 mg, 0.500 mmol) as the substrates. The crude product was purified via silica gel chromatography (2-5% EtOAc in Hexane) to give the title compound **10** as a yellow liquid (26.0 mg, 0.111 mmol, 44%). **^{1}H NMR (499 MHz, $CDCl_3$)**: δ 7.08-6.98 (m, 3H), 6.96-6.89 (m, 1H), 6.85-6.79 (m, 1H), 6.77-6.73 (m, 2H), 4.73 (s, 1H), 2.87-2.78 (m, 4H); **^{13}C NMR (126 MHz, $CDCl_3$)**: δ 153.9, 150.2 (dd, $^{1}J_{C-F}$ = 247.3 Hz, $^{2}J_{C-F}$ = 12.7 Hz), 148.9 (dd, $^{1}J_{C-F}$ = 245.3 Hz, $^{2}J_{C-F}$ = 12.7 Hz), 138.7 (dd, $^{3}J_{C-F}$ = 5.2 Hz, $^{4}J_{C-F}$ = 3.8 Hz), 133.4, 129.7, 124.4 (dd, $^{3}J_{C-F}$ = 5.8 Hz, $^{4}J_{C-F}$ = 3.6 Hz), 117.3 (d, $^{2}J_{C-F}$ = 16.8 Hz), 117.0 (d, $^{2}J_{C-F}$ = 16.8 Hz), 115.4, 37.4 (d, J_{C-F} = 1.3 Hz), 36.9; **^{19}F NMR (470 MHz, $CDCl_3$)** δ -138.5 - -138.6 (m), -142.2 - -142.4 (m); **HRMS(EI+): calculated for** $C_{14}H_{12}F_2O$ $[M^+]$: 234.0856, found 234.0846

4-(4-(trifluoromethyl)phenethyl)phenol (**11**)



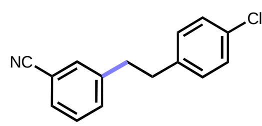
Following General Procedure C, using **S2** (71.3 mg, 0.250 mmol) and **S26** (257 mg, 0.500 mmol) as the substrates. The crude product was purified via silica gel chromatography (2-5% EtOAc in Hexane) to give the title compound **10** as a white solid (31.0 mg, 0.116 mmol, 47%). **^{1}H NMR (500 MHz, $CDCl_3$)**: δ 7.52 (d, J = 8.0 Hz, 2H), 7.25 (d, J = 7.9 Hz, 2H), 7.02 (d, J = 8.5 Hz, 2H), 6.76 (d, J = 8.5 Hz, 2H), 4.65 (s, 1H), 2.94 (dd, J = 8.8, 5.8 Hz, 2H), 2.86 (dd, J = 8.8, 5.8 Hz, 2H); **^{13}C NMR (126 MHz, $CDCl_3$)**: δ 153.9, 145.9, 133.4, 129.6, 128.9, 128.4 (q, $^{2}J_{C-F}$ = 32.4 Hz), 125.6 (q, $^{3}J_{C-F}$ = 3.8 Hz), 124.4 (q, $^{1}J_{C-F}$ = 271.5 Hz), 115.4, 38.0, 36.7; **^{19}F NMR (471 MHz, $CDCl_3$):** δ -62.24; **HRMS(EI+): calculated for** $C_{15}H_{13}F_3O$ $[M^+]$: 266.0918, found 266.0911

4-(3,4-difluorophenethyl)morpholine (**12**)



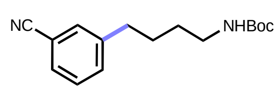
Following General Procedure C, using **S3** (63.3 mg, 0.250 mmol) and **S23** (254 mg, 0.500 mmol) as the substrates. The crude product was purified via silica gel chromatography (20-40% EtOAc in Hexane) to give the title compound **12** as a yellow liquid (21.9 mg, 0.096 mmol, 39%). **^{1}H NMR (499 MHz, $CDCl_3$):** δ 7.11-6.97 (m, 2H), 6.94-6.86 (m, 1H), 3.73 (t, J = 4.7 Hz, 4H), 2.77-2.73 (dd, m, 2H), 2.58-2.54 (m, 2H), 2.50 (t, J = 4.6 Hz, 4H); **^{13}C NMR (126 MHz, $CDCl_3$)**: δ 150.3 (dd, $^1J_{C-F}$ = 248.2 Hz, $^2J_{C-F}$ = 12.7 Hz), 148.6 (dd, $^1J_{C-F}$ = 246.8 Hz, $^2J_{C-F}$ = 12.8 Hz), 137.3 (dd, $^3J_{C-F}$ = 4.5 Hz, $^4J_{C-F}$ = 3.2 Hz), 124.6 (dd, $^3J_{C-F}$ = 6.1 Hz, $^4J_{C-F}$ = 3.6 Hz), 117.5 (d, $^2J_{C-F}$ = 16.9 Hz), 117.2 (d, $^2J_{C-F}$ = 16.9 Hz), 67.1, 60.5, 53.8, 32.6; **^{19}F NMR (470 MHz, $CDCl_3$):** δ -138.2 - -138.5 (m), -141.7 - -142.1 (m); **HRMS: calculated for** $C_{12}H_{16}F_2NO$ [M+H$^+$]: 228.1194, found 228.1202

3-(4-chlorophenethyl)benzonitrile (**13**)



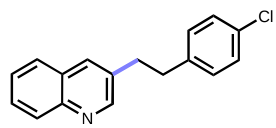
Following General Procedure C, using **S4** (36.3 mg, 0.150 mmol) and **2** (160 mg, 0.300 mmol) as the substrates. The crude product was purified via silica gel chromatography (5% EtOAc in Hexane) to give the title compound **13** as a white solid (23.4 mg, 0.097 mmol, 65%). **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.49 (dt, J = 7.1, 1.6 Hz, 1H), 7.43 (s, br, 1H), 7.40-7.31 (m, 2H), 7.24 (d, J = 8.4 Hz, 2H), 7.04 (d, J = 8.4 Hz, 2H), 2.98-2.85 (m, 4H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 142.5, 139.0, 133.1, 132.1, 132.0, 130.0, 129.8, 129.2, 128.6, 118.9, 112.5, 37.2, 36.7; **HRMS:** m/z: [M]$^+$ calc'd for [$C_{15}H_{12}NCl$]$^+$ expect 241.0658; found 241.0648.

tert-butyl (4-(3-cyanophenyl)butyl)carbamate (**14**)



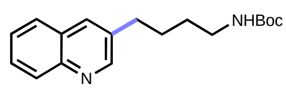
Following General Procedure C, using **S4** (60.5 mg, 0.250 mmol) and **S21** (283 mg, 0.500 mmol) as the substrates. The crude product was purified via silica gel chromatography (10-15% EtOAc in Hexane) to give the title compound **14** as a yellow liquid (41.1 mg, 0.150 mmol, 60%). **^{1}H NMR (499 MHz, $CDCl_3$)**: δ 7.50-7.43 (m, 2H), 7.42-7.34 (m, 2H), 4.53 (s, 1H), 3.20-3.08 (m, 2H), 2.66 (t, J = 7.7 Hz, 2H), 1.70-1.58 (m, 2H), 1.54-1.46 (m, 2H), 1.43 (s, 9H); **^{13}C NMR (126 MHz, $CDCl_3$)**: δ 156.1, 143.7, 133.1, 132.1, 129.8, 129.2, 119.1, 112.5, 40.3, 35.2, 29.8, 28.5, 28.3; **HRMS:** m/z: $[M+Na]^+$ calc'd for $[C_{16}H_{22}N_2O_2Na]^+$ expect 297.1573; found 297.1572.

3-(4-chlorophenethyl)quinoline (**15**)



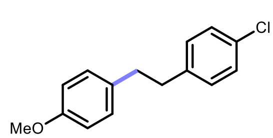
Following General Procedure C, using **S5** (67.0 mg, 0.250 mmol) and **2** (267 mg, 0.500 mmol) as the substrates. The crude product was purified via silica gel chromatography (10-15% EtOAc in Hexane) to give the title compound **15** as a white solid (34.4 mg, 0.128 mmol, 52%). **^{1}H NMR (499 MHz, $CDCl_3$)**: δ 8.73 (d, *J* = 2.2 Hz, 1H), 8.08 (d, *J* = 8.4 Hz, 1H), 7.85 (d, *J* = 2.3 Hz, 1H), 7.75 (dd, *J* = 8.2, 1.4 Hz, 1H), 7.68 (m, 1H), 7.53 (m, 1H), 7.29-7.22 (m, 2H), 7.13-7.07 (m, 2H), 3.10 (d, *J* = 7.1 Hz, 2H), 3.04-2.97 (d, *J* = 7.1 Hz, 2H); **^{13}C NMR (126 MHz, $CDCl_3$)**: δ 152.0, 147.1, 139.3, 134.6, 133.9, 132.2, 130.0, 129.4, 128.9, 128.8, 128.2, 127.5, 126.8, 36.9, 35.1; **HRMS:** m/z: $[M+Na]^+$ calc'd for $[C_{17}H_{15}NCl]^+$ expect 268.0888 found 268.0885.

tert-butyl (4-(quinolin-3-yl)butyl)carbamate (**16**)



Following General Procedure C, using **S5** (40.2 mg, 0.15 mmol) and **S21** (170 mg, 0.30 mmol) as the substrates. The crude product was purified via silica gel chromatography (30% EtOAc in Hexane) to give the title compound **16** as a yellow oil (14 mg, 0.047 mmol, 31%). **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.76 (d, *J* = 2.1 Hz), 8.07 (d, *J* = 8.5 Hz, 1H), 7.91 (d, *J* = 1.3 Hz, 1H), 7.76 (d, *J* = 8.0 Hz, 1H), 7.65 (dd, *J* = 7.0, 1.3 Hz, 1H), 7.52 (dd, *J* = 6.8 Hz, 0.8 Hz, 1H), 4.55 (s, br, 1H), 3.17 (q, *J* = 6.3 Hz, 2H), 2.82 (t, *J* = 7.6 Hz, 2H), 1.79-1.70 (m, 2H), 1.61-1.52 (m, 2H), 1.43 (s, 9H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 156.0, 152.0, 146.9, 134.7, 134.2, 129.2, 128.6, 128.2, 127.3, 126.6, 79.2, 40.2, 32.8, 29.7, 28.4, 28.3; **HRMS:** m/z: $[M+H]^+$ calc'd for $[C_{18}H_{25}N_2O_2]^+$ expect 301.1911; found 301.1903.

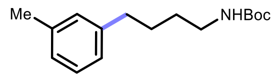
1-chloro-4-(4-methoxyphenethyl)benzene (**17**)



Following General Procedure C, using **S6** (61.8 mg, 0.25 mmol) and **2** (267 mg, 0.50 mmol) as the substrates. The crude product was purified via silica gel chromatography (1% EtOAc in Hexane) to give the title compound **17** as a white solid (5.8 mg, 0.023 mmol, 9%). **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.23 (d, *J* = 8.2 Hz, 2H), 7.06 (t, *J* = 8.0 Hz, 4H), 6.82 (d, *J* = 8.2 Hz, 2H), 3.79 (s, 3H), 2.92-2.76 (m, 4H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 158.0, 140.3, 133.5, 131.7, 130.0, 129.5, 128.5, 113.9, 55.4, 37.6, 37.0

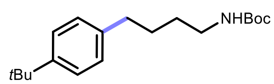
All data match that previously reported in the literature.[25]

tert-butyl (4-(*m*-tolyl)butyl)carbamate (**18**)



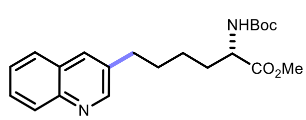
Following General Procedure C, using **S7** (57.8 mg, 0.25 mmol) and **S21** (283 mg, 0.50 mmol) as the substrates. The crude product was purified via silica gel chromatography (4% EtOAc in Hexane) to give the title compound **18** as a white solid (24.6 mg, 0.093 mmol, 37%). **^{1}H NMR (499 MHz, $CDCl_3$)** δ 7.17 (t, *J* = 7.5 Hz, 1H), 7.03-6.93 (m, 3H), 4.52 (s, 1H), 3.14 (q, *J* = 6.1 Hz, 2H), 2.59 (t, *J* = 7.6 Hz, 2H), 2.33 (s, 3H), 1.64 (p, *J* = 7.7 Hz, 2H), 1.51 (p, *J* = 7.4 Hz, 2H), 1.45 (s, 9H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 156.1, 142.3, 138.0, 129.3, 128.3, 126.6, 125.5, 79.2, 40.5, 35.5, 29.8, 28.7, 28.6, 21.5; **HRMS:** m/z: $[M\text{-}t\text{Bu}+H]^+$ calc'd for $[C_{12}H_{18}NO_2]^+$ expect 208.1332; found 208.1334.

tert-butyl (4-(4-(*tert*-butyl)phenyl)butyl)carbamate (**19**)



Following General Procedure C, using **S8** (68.3 mg, 0.25 mmol) and **S21** (283 mg, 0.50 mmol) as the substrates. The crude product was purified via silica gel chromatography (1-5% EtOAc in Hexane) to give the title compound **19** as a white solid (16.5 mg, 0.054 mmol, 22%). **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.30 (d, *J* = 8.0 Hz, 2H), 7.11 (d, *J* = 8.0 Hz, 2H), 4.49 (s, br, 1H), 3.14 (q, *J* = 6.2 Hz, 2H), 2.60 (t, *J* = 7.5 Hz, 2H), 1.64 (p, *J* = 7.9 Hz, 2H), 1.52 (p, *J* = 7.4 Hz, 2H), 1.44 (s, 9H), 1.31 (s, 9H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 156.1, 148.7, 139.3, 128.2, 125.3, 79.2, 40.6, 35.1, 34.5, 31.5, 29.9, 28.7, 28.6; **HRMS:** m/z: $[M\text{-}t\text{Bu}+Na]^+$ calc'd for $[C_{15}H_{23}NO_2Na]^+$ expect 272.1621; found 272.1622.

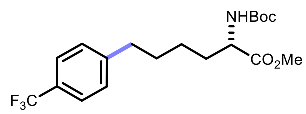
methyl (*S*)-2-((tert-butoxycarbonyl)amino)-6-(quinolin-3-yl)hexanoate (**20**)



Following General Procedure C, using **S5** (26.8 mg, 0.10 mmol) and **S28** (128 mg, 0.20 mmol) as the substrates. The crude product was purified via silica gel chromatography (20% EtOAc in Hexane) to give the title compound **20** as a white solid (15.3 mg, 0.041 mmol, 41%). **^{1}H NMR (400 MHz, $CDCl_3$),** δ Mixture of rotamers, 8.76 (d, *J* = 2.0 Hz, 1H), 8.07(d, *J* = 8.4 Hz, 1H), 7.90 (d, *J* = 1.2 Hz, 1H), 7.76 (d, *J* = 8.2 Hz, 1H), 7.65 (dd, *J* = 7.0, 1.2 Hz, 1H), 7.52 (dd, *J* = 7.0, 0.8 Hz, 1H), 5.01 (d, *J* = 7.6 Hz, 1H, major rot.), 4.72

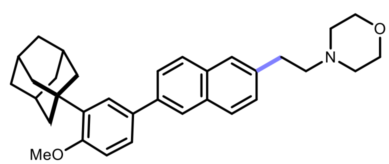
(s, br, 1H, minor rot.), 4.32 (q, J = 5.4 Hz, 1H, major rot.), 4.20-4.06 (br, s, 1H, minor rot.), 3.71 (s, 3H), 2.80 (t, J = 7.7 Hz, 2H), 1.94-1.80 (m, 1H), 1.78-1.61 (m, 3H), 1.52-1.36 (m, 2H), 1.42 (s, 9H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 173.3, 155.4, 152.0, 146.9, 134.7, 134.2, 129.2, 128.6, 128.1, 127.3, 126.6, 79.9, 53.3, 52.3, 33.0, 32.7, 30.6, 28.3, 24.9; **HRMS:** m/z: $[M+Na]^+$ calc'd for $[C_{21}H_{28}N_2O_4Na]^+$ expect 395.1491; found 395.1937.

methyl (*S*)-2-((*tert*-butoxycarbonyl)amino)-6-(4-(trifluoromethyl)phenyl)hexanoate (**21**)



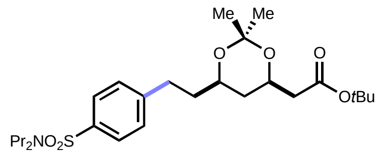
Following General Procedure C, using **S2** (28.5 mg, 0.10 mmol) and **S28** (128 mg, 0.20 mmol) as the substrates. The crude product was purified via silica gel chromatography (15-20% EtOAc in Hexane) to give the title compound **21** as a clear colorless oil (19.1 mg, 0.049 mmol, 49%). **^{1}H NMR (500 MHz, $CDCl_3$)** δ Mixture of rotamers, 7.52 (d, J = 8.0 Hz, 2H), 7.26 (d, J = 8.0 Hz, 2H), 4.99 (d, J = 7.8 Hz, 1H, major rot.), 4.70 (s, br, 1H, minor rot.), 4.30 (q, J = 5.5 Hz, 1H, major rot.), 4.11 (s, br, 1H, minor rot.), 3.72 (s, 3H), 2.66 (t, J = 7.7 Hz, 2H), 1.90-1.75 (m, 1H), 1.72-1.57 (m, 3H), 1.43 (s, 9H), 1.41-1.32 (m, 2H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 173.3, 155.3, 146.3, 128.7, 128.2 (q, $^2J_{C-F}$ = 31.9 Hz), 125.2 (q, $^3J_{C-F}$ = 3.6 Hz), 124.4 (q, $^1J_{C-F}$ = 271.7 Hz), 79.9, 53.2, 52.3, 35.5, 32.7, 30.6, 29.7, 29.4, 28.3, 24.8; **^{19}F NMR (471 MHz, $CDCl_3$)** δ -62.3; **HRMS:** m/z: $[M+Na]^+$ calc'd for $[C_{19}H_{26}NO_4F_3Na]^+$ expect 412.1712; found 412.1725.

4-(2-(6-(3-(adamantan-1-yl)-4-methoxyphenyl)naphthalen-2-yl)ethyl)morpholine (**22**)



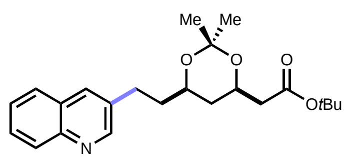
Following General Procedure C, using **S12** (50.7 mg, 0.100 mmol) and **S23** (102 mg, 0.200 mmol) as the substrates. The crude product was purified via silica gel chromatography (1st column: 20-40% EtOAc in Hexane, 2nd column: 15-20% Acetone in Hexane) to give the title compound **22** as a white solid (28.7 mg, 0.060 mmol, 60%). **^{1}H NMR (499 MHz, $CDCl_3$):** δ 7.96 (s, 1H), 7.83 (d, J = 8.6 Hz, 2H), 7.72 (dd, J = 8.5, 1.8 Hz, 1H), 7.66 (s, 1H), 7.60 (d, J = 2.4 Hz, 1H), 7.53 (dd, J = 8.4, 2.3 Hz, 1H), 7.36 (dd, J = 8.4, 1.8 Hz, 1H), 6.99 (d, J = 8.4 Hz, 1H), 3.90 (s, 3H), 3.78 (t, J = 4.6 Hz, 4H), 3.02-2.95 (m, 2H), 2.73-2.68 (m, 2H), 2.57 (t, J = 4.6 Hz, 4H), 2.20 (d, J = 2.9 Hz, 6H), 2.11 (t, J = 3.3 Hz, 3H), 1.82 (d, J = 3.2 Hz, 6H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 158.6, 139.0, 138.6, 137.5, 133.4, 132.6, 132.5, 128.3, 127.9, 127.9, 126.7, 126.0, 126.0, 125.7, 124.9, 112.2, 67.2, 60.9, 55.3, 53.9, 40.8, 37.3, 37.3, 33.6, 29.3; **HRMS:** m/z: $[M+H]^+$ calc'd for $[C_{33}H_{40}NO_2]^+$ expect 482.3054; found 482.3072.

tert-butyl 2-((4*R*,6*R*)-6-(4-(*N*,*N*-dipropylsulfamoyl)phenethyl)-2,2-dimethyl-1,3-dioxan-4-yl)acetate (**23**)



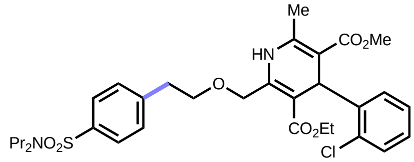
Following General Procedure C, using **1** (95.0 mg, 0.250 mmol) and **S20** (326 mg, 0.500 mmol) as the substrates. The crude product was purified via silica gel chromatography (10-15% EtOAc in Hexane) to give the title compound **23** as a white solid (75.2 mg, 0.151 mmol, 60%). **^{1}H NMR (499 MHz, $CDCl_3$)**: δ 7.74-7.68 (m, 2H), 7.32-7.27 (m, 2H), 4.21 (dtd, *J* = 11.6, 6.6, 2.4 Hz, 1H), 3.82-3.73 (m, 1H), 3.10-3.04 (m, 4H), 2.81 (ddd, *J* = 14.2, 9.2, 5.3 Hz, 1H), 2.72 (ddd, *J* = 13.9, 8.9, 7.5 Hz, 1H), 2.43 (dd, *J* = 15.1, 6.9 Hz, 1H), 2.29 (dd, *J* = 15.1, 6.2 Hz, 1H), 1.82 (dtd, *J* = 13.8, 8.6, 5.3 Hz, 1H), 1.76-1.62 (m, 2H), 1.61-1.49 (m, 5H), 1.40 (d, *J* = 9.4 Hz, 6H), 1.22 (dt, *J* = 12.6, 11.5 Hz, 1H), 0.87 (t, *J* = 7.4 Hz, 5H); **^{13}C NMR (126 MHz, $CDCl_3$)**: δ 170.4, 147.1, 137.8, 129.2, 127.3, 98.9, 67.6, 66.3, 50.2, 42.8, 37.5, 36.6, 31.1, 30.3, 28.2, 22.2, 19.9, 11.3; **HRMS:** m/z: $[M+Na]^+$ calc'd for $[C_{26}H_{43}NO_6SNa]^+$ expect 520.2703; found 520.2706.

tert-butyl 2-((4R,6R)-2,2-dimethyl-6-(2-(quinolin-3-yl)ethyl)-1,3-dioxan-4-yl)acetate (**24**)



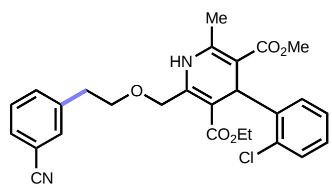
Following General Procedure C, using **S5** (67.0 mg, 0.250 mmol) and **S20** (326 mg, 0.500 mmol) as the substrates. The crude product was purified via silica gel chromatography (15-20% EtOAc in Hexane) to give the title compound **24** as a white solid (47.8 mg, 0.124 mmol, 50%). **^{1}H NMR (499 MHz, $CDCl_3$)**: δ 8.78 (d, *J* = 2.2 Hz, 1H), 8.07 (d, *J* = 2.1 Hz, 1H), 7.92 (dd, *J* = 2.1, 1.0 Hz, 1H), 7.75 (dd, *J* = 8.2, 1.4 Hz, 1H), 7.66 (m, 1H), 7.52 (m, 1H), 4.25-4.16 (m, 1H), 3.88-3.79 (m, 1H), 2.99-2.81 (m, 2H), 2.43 (dd, *J* = 15.1, 7.0 Hz, 1H), 2.29 (dd, *J* = 15.1, 6.2 Hz, 1H), 1.91 (m, 1H), 1.85-1.74 (m, 1H), 1.58-1.52 (m, 1H), 1.43 (s, 9H), 1.41 (s, 3H), 1.29-1.20 (m, 1H); **^{13}C NMR (126 MHz, $CDCl_3$)**: δ 170.3, 152.3, 147.0, 134.7, 134.5, 129.3, 128.7, 128.3, 127.4, 126.7, 98.9, 80.7, 67.6, 66.3, 42.8, 37.6, 36.7, 30.3, 28.6, 28.2, 19.9; **HRMS:** m/z: $[M+H]^+$ calc'd for $[C_{23}H_{32}NO_4]^+$ expect 386.2326; found 386.2320.

3-ethyl 5-methyl 4-(2-chlorophenyl)-2-((4-(*N*,*N*-dipropylsulfamoyl)phenethoxy)methyl)-6-methyl-1,4-dihydropyridine-3,5-dicarboxylate (**25**)



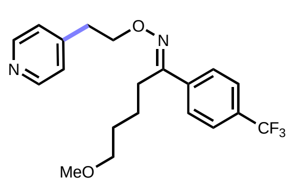
Following General Procedure C, using **1** (38.0 mg, 0.100 mmol) and **S22** (140 mg, 0.200 mmol) as the substrates. The crude product was purified via silica gel chromatography (10-15% EtOAc in Hexane) to give the title compound **25** as a yellow solid (38.7 mg, 0.061 mmol, 61%). **^{1}H NMR (499 MHz, $CDCl_3$)**: δ 7.81-7.75 (m, 2H), 7.41-7.36 (m, 2H), 7.34 (dd, *J* = 7.8, 1.7 Hz, 1H), 7.23 (dd, *J* = 8.0, 1.4 Hz, 1H), 7.13 (td, *J* = 7.5, 1.4 Hz, 1H), 7.04 (td, *J* = 7.6, 1.7 Hz, 1H), 6.80 (s, 1H), 5.39 (s, 1H), 4.77 (d, *J* = 16.1 Hz, 1H), 4.68 (d, *J* = 16.1 Hz, 1H), 4.04 (qt, *J* = 8.1, 4.2 Hz, 2H), 3.88-3.77 (m, 2H), 3.61 (s, 3H), 3.12-3.06 (m, 4H), 3.05-2.99 (m, 2H), 2.20 (s, 3H), 1.63-1.52 (m, 4H), 1.18 (t, *J* = 7.1 Hz, 3H), 0.88 (t, *J* = 7.4 Hz, 6H); **^{13}C NMR (126 MHz, $CDCl_3$)**: δ 168.0, 167.2, 145.7, 145.1, 143.7, 143.6, 138.7, 132.5, 131.6, 129.5, 129.4, 127.5, 127.5, 126.9, 104.1, 101.6, 71.4, 67.9, 59.9, 50.9, 50.3, 37.4, 36.0, 22.3, 19.6, 14.4, 11.3; **HRMS:** m/z: $[M+Na]^+$ calc'd for $[C_{32}H_{41}N_2o_7SClNa]^+$ expect 655.2221; found 655.2195.

3-ethyl 5-methyl 4-(2-chlorophenyl)-2-((3-cyanophenethoxy)methyl)-6-methyl-1,4-dihydropyridine-3,5-dicarboxylate (**26**)



Following General Procedure C, using **S4** (36.3 mg, 0.150 mmol) and **S22** (210 mg, 0.300 mmol) as the substrates. The crude product was purified via silica gel chromatography (10-15% EtOAc in Hexane) to give the title compound **26** as a yellow solid (45.0 mg, 0.091 mmol, 61%). **^{1}H NMR (499 MHz, $CDCl_3$)**: δ 7.57-7.53 (m, 2H), 7.51-7.47 (m, 1H), 7.44 (t, *J* = 8.0 Hz, 1H), 7.32 (dd, *J* = 7.8, 1.7 Hz, 1H), 7.22 (dd, *J* = 7.9, 1.3 Hz, 1H), 7.12 (td, *J* = 7.5, 1.4 Hz, 1H), 7.03 (td, *J* = 7.6, 1.7 Hz, 1H), 6.71 (s, 1H), 5.37 (s, 1H), 4.75 (d, *J* = 16.0 Hz, 1H), 4.67 (d, *J* = 16.1 Hz, 1H), 4.03 (qt, *J* = 7.2, 3.8 Hz, 2H), 3.79 (qt, *J* = 9.6, 6.4 Hz, 2H), 3.59 (s, 3H), 2.99 (t, *J* = 6.4 Hz, 2H), 2.17 (s, 3H), 1.17 (t, *J* = 7.1 Hz, 3H); **^{13}C NMR (126 MHz, $CDCl_3$)**: δ 168.0, 167.2, 145.7, 145.0, 143.6, 140.4, 133.5, 132.5, 132.5, 131.5, 130.5, 129.5, 129.4, 127.5, 126.9, 118.8, 112.9, 104.1, 101.7, 71.3, 67.8, 59.9, 50.9, 37.3, 35.7, 19.5, 14.3; **HRMS:** m/z: $[M+Na]^+$ calc'd for $[C_{27}H_{27}N_2O_5ClNa]^+$ expect 517.1501; found 517.1490.

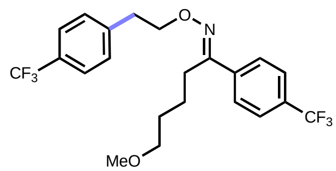
(*E*)-5-methoxy-1-(4-(trifluoromethyl)phenyl)pentan-1-one *O*-(2-(pyridin-4-yl)ethyl) oxime (**27**)



Following General Procedure C, using **S9** (32.7 mg, 0.150 mmol) and **S27** (210 mg, 0.300 mmol) as the substrates. The crude product was purified via silica gel chromatography (10-15% EtOAc in Hexane) to give the title compound **27** as a colorless liquid (44.2 mg, 0.116 mmol, 77%). **^{1}H NMR (500 MHz, MeOD-**

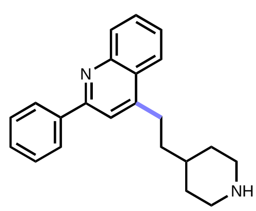
d$_4$): δ 8.49-8.44 (m, 2H), 7.81 (d, *J* = 8.3 Hz, 1H), 7.67 (d, *J* = 8.3 Hz, 2H), 7.40 (d, *J* = 5.2 Hz, 2H), 4.49 (t, *J* = 6.2 Hz, 2H), 3.31 (m, 2H), 3.28 (s, 3H), 3.12 (t, *J* = 6.2 Hz, 2H), 2.74 (t, *J* = 7.4 Hz, 2H), 1.55-1.44 (m, 4H); **^{13}C NMR (126 MHz, MeOD-d$_4$):** δ 158.9, 151.6, 149.7, 140.6, 131.9 (q, $^2J_{C-F}$ = 32.3 Hz), 128.0, 126.4 (q, $^3J_{C-F}$ = 3.8 Hz), 125.6 (q, $^1J_{C-F}$ = 271.3 Hz), 74.5, 73.3, 58.8, 36.1, 30.4, 26.8, 24.1; **^{19}F NMR (471 MHz, MeOD-d$_4$):** δ -64.25; **HRMS:** m/z: $[M+H]^+$ calc'd for $[C_{20}H_{24}F_3N_2O_2]^+$ expect 381.1784; found 381.1795.

(*E*)-5-methoxy-1-(4-(trifluoromethyl)phenyl)pentan-1-one *O*-(4-(trifluoromethyl)phenethyl) oxime (**28**)



Following General Procedure C, using **S2** (42.8 mg, 0.150 mmol) and **S27** (210 mg, 0.300 mmol) as the substrates. The crude product was purified via silica gel chromatography (5-10% EtOAc in Hexane) to give the title compound **28** as a colorless liquid (46.4 mg, 0.104 mmol, 69%). **^{1}H NMR (500 MHz, CDCl$_3$):** δ 7.72 (d, *J* = 8.3 Hz, 2H), 7.61 (d, *J* = 8.2 Hz, 2H), 7.57 (d, *J* = 8.0 Hz, 2H), 7.37 (d, *J* = 8.0 Hz, 2H), 4.44 (t, *J* = 6.6 Hz, 2H), 3.34-3.27 (m, 5H), 3.11 (t, *J* = 6.6 Hz, 2H), 2.76-2.69 (m, 2H), 1.61-1.46 (m, 4H); **^{13}C NMR (126 MHz, CDCl$_3$):** δ 157.6, 143.2, 139.2, 131.0 (q, $^2J_{C-F}$ = 32.4 Hz), 129.5, 128.8 (q, $^2J_{C-F}$ = 32.3 Hz), 126.7, 125.5 (q, $^3J_{C-F}$ = 3.9 Hz), 125.4 (q, $^3J_{C-F}$ = 3.9 Hz), 124.4 (q, $^1J_{C-F}$ = 270.9 Hz), 124.2 (q, $^1J_{C-F}$ = 271.8 Hz), 74.3, 72.4, 58.7, 35.8, 29.7, 26.4, 23.2; **^{19}F NMR (471 MHz, CDCl$_3$):** δ -62.35, -62.74; **HRMS:** m/z: $[M+H]^+$ calc'd for $[C_{22}H_{24}F_6NO_2]^+$ expect 448.1706; found 448.1710.

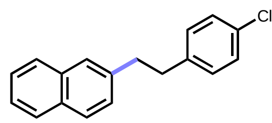
2-phenyl-4-(2-(piperidin-4-yl)ethyl)quinoline (**29**)



Following General Procedure C, using **S10** (2.07 g, 6.01 mmol) and **S24** (7.29 g, 12.0 mmol) as the substrates. The crude product was purified via silica gel chromatography (1st column: 7% EtOAc in Hexane). The crude was a mixture after 1st column, The mixture was concentrated in vacuo. DCM (9ml) and TFA (9ml) were added, and reaction mixture was stirred at room temperature for 1 h after remove the TFA/DCM solvent mixture in vacuo. The crude product was purified via silica gel chromatography (2nd column: 8% Methanol in DCM) to give the title compound **29** as a white solid (908 mg, 2.87 mmol, 48%). **^{1}H NMR (499 MHz, CDCl$_3$):** δ 8.19 (dd, *J* = 8.5, 1.2 Hz, 1H), 8.16-8.12 (m, 2H), 7.95 (dd, *J* = 8.5, 1.4 Hz, 1H), 7.74-7.69

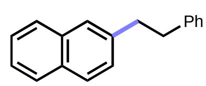
(m, 1H), 7.67 (s, 1H), 7.57-7.50 (m, 3H), 7.50-7.43 (m, 1H), 3.45 (d, J = 12.7, 2H), 3.16-3.10 (m, 2H), 2.89 (td, J = 12.3, 3.0 Hz, 2H), 2.04-1.97 (m, 2H), 1.85-1.80 (m, 2H), 1.72-1.63 (m, 3H); **^{13}C NMR (126 MHz, $CDCl_3$):** δ 157.3, 148.7, 148.2, 139.8, 130.8, 129.5, 129.5, 129.0, 127.6, 126.4, 126.3, 123.1, 118.7, 44.1, 36.4, 34.3, 29.5, 28.8.

2-(4-chlorophenethyl)naphthalene (**31**)



Following General Procedure C, using **30** (66.8 mg, 0.250 mmol) and **2** (268 mg, 0.500 mmol) as the substrates, $RuCl_3$ (26.0 mg, 0.125 mmol) as the additive. The crude product was purified via silica gel chromatography (1st column: 0.5% EtOAc in Hexane, 2nd column: 5% DCM in Hexane) to give the title compound **31** as a white solid (31.8 mg, 0.119 mmol, 48%). **^{1}H NMR (499 MHz, $CDCl_3$)**: δ 7.85-7.79 (m, 1H), 7.79-7.74 (m, 2H), 7.59 (s, 1H), 7.49-7.39 (m, 2H), 7.31 (d, J = 8.6 Hz, 1H), 7.24 (d, J = 8.2 Hz, 2H), 7.12 (d, J = 8.2 Hz, 2H), 3.10-3.03 (m, 2H), 3.03-2.95 (m, 2H); **^{13}C NMR (126 MHz, $CDCl_3$)**: δ 140.2, 138.9, 133.7, 132.2, 131.8, 130.0, 128.6, 128.1, 127.8, 127.6, 127.4, 126.7, 126.1, 125.4, 38.1, 37.2; **HRMS(EI+):** m/z: $[M]^+$ calc'd for $[C_{18}H_{15}Cl]^+$ expect 266.0862; found 266.0850.

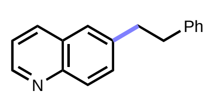
2-phenethylnaphthalene (**33**)



Following General Procedure C, using **30** (66.8 mg, 0.250 mmol) and **S18** (250 mg, 0.500 mmol) as the substrates, $RuCl_3$ (26.0 mg, 0.125 mmol) as the additive. The crude product was purified via silica gel chromatography (0.5% EtOAc in Hexane) to give the title compound **33** as a white solid (37.3 mg, 0.161 mmol, 64%). **^{1}H NMR (499 MHz, $CDCl_3$)**: δ 7.87-7.77 (m, 3H), 7.64 (s, 1H), 7.51-7.41 (m, 2H), 7.39-7.28 (m, 3H), 7.28-7.20 (m, 3H), 3.14-3.00 (m, 4H); **^{13}C NMR (126 MHz, $CDCl_3$)**: δ 141.9, 139.4, 133.8, 132.2, 128.6, 128.5, 128.0, 127.8, 127.6, 127.5, 126.6, 126.1, 126.0, 125.3, 38.2, 38.0.

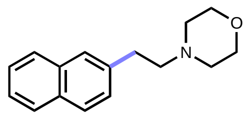
All data match that previously reported in the literature.[26]

6-phenethylquinoline (**34**)



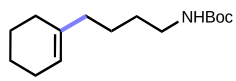
Following General Procedure C, using **S11** (67.0 mg, 0.250 mmol) and **S18** (250 mg, 0.500 mmol) as the substrates, $RuCl_3$ (26.0 mg, 0.125 mmol) as the additive. The crude product was purified via silica gel chromatography (10-15% EtOAc in Hexane) to give the title compound **34** as a colorless liquid (27.0 mg, 0.116 mmol, 47%). **^{1}H NMR (499 MHz, $CDCl_3$)**: δ 8.88 (dd, *J* = 4.3, 1.7 Hz, 1H), 8.11-8.03 (m, 2H), 7.61-7.55 (m, 2H), 7.38 (dd, *J* = 8.2, 4.2 Hz, 1H), 7.33-7.18 (m, 5H), 3.13 (dd, *J* = 9.5, 6.3 Hz, 2H), 3.07-3.00 (m, 2H); **^{13}C NMR (126 MHz, $CDCl_3$)**: δ 149.8, 147.3, 141.4, 140.3, 135.8, 131.1, 129.4, 128.6, 128.5, 128.4, 126.4, 126.2, 121.2, 37.9, 37.8.; **HRMS:** m/z: $[M+H]^+$ calc'd for $[C_{17}H_{16}N]^+$ expect 234.1277; found 234.1281.

4-(2-(naphthalen-2-yl)ethyl)morpholine (**35**)



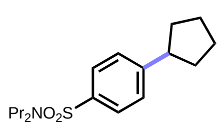
Following General Procedure C, using **30** (66.8 mg, 0.250 mmol) and **S23** (254 mg, 0.500 mmol) as the substrates, $RuCl_3$ (26.0 mg, 0.125 mmol) as the additive. The crude product was purified via silica gel chromatography (1st column: 20-40% EtOAc in Hexane, 2nd column: 10-20% Acetone in Hexane) to give the title compound **35** as a white solid (34.7 mg, 0.144 mmol, 58%). **^{1}H NMR (499 MHz, $CDCl_3$)** δ 7.83-7.73 (m, 3H), 7.64 (s, 1H), 7.47 98-7.39 (m, 2H), 7.34 (d, *J* = 8.3 Hz, 1H), 3.75 (t, *J* = 4.8 Hz, 4H), 2.98-2.93 (m, 2H), 2.70-2.65 (m, 2H), 2.54 (t, *J* = 4.5 Hz, 4H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 137.8, 133.7, 132.2, 128.1, 127.7, 127.5, 127.5, 126.9, 126.1, 125.4, 67.1, 60.9, 53.9, 33.6; **HRMS:** m/z: $[M+H]^+$ calc'd for $[C_{16}H_{20}NO]^+$ expect 242.1539; found 242.1534.

tert-butyl (4-(cyclohex-1-en-1-yl)butyl)carbamate (**36**)



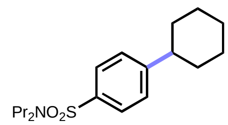
Following General Procedure C, using **S13** (55.3 mg, 0.250 mmol) and **S21** (240 mg, 0.500 mmol) as the substrates, $RuCl_3$ (26.0 mg, 0.125 mmol) as the additive. The crude product was purified via silica gel chromatography (2% EtOAc in Hexane) to give the title compound **36** as a colorless liquid (27.0 mg, 0.107 mmol, 43%). **^{1}H NMR (500 MHz, $CDCl_3$)**: δ 5.40-5.35 (m, 2H), 4.50 (s, 1H), 3.15-3.05 (m, 2H), 2.00-1.85 (m, 6H), 1.63-1.56 (m, 2H), 1.56-1.49 (m, 2H), 1.43 (m, 13H); **^{13}C NMR (126 MHz, $CDCl_3$)**: δ 156.1, 137.6, 121.2, 79.1, 40.7, 37.8, 29.8, 28.6, 28.3, 25.4, 25.0, 23.1, 22.7; **HRMS:** m/z: $[M-Boc+H]^+$ calc'd for $[C_{10}H_{20}NO]^+$ expect 154.1590; found 154.1591.

4-cyclopentyl-*N*,*N*-dipropylbenzenesulfonamide (**39**)



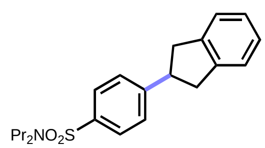
Following a modified version of General Procedure C, using **L5** as the ligand, **1** (95.1 mg, 0.25 mmol) and **38** (232 mg, 0.50 mmol) as the substrates and $RuCl_3$ (25.9 mg, 0.125 mmol) and $GaCl_3$ (22.0 mg, 0.125 mmol) as the additives and stirring at 40 °C. The crude product was purified via silica gel chromatography (2% EtOAc in Hexane) to give the title compound **39** as a white solid (28.9 mg, 0.093 mmol, 37%). **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.70 (d, *J* = 8.3 Hz, 2H), 7.34 (d, *J* = 8.2 Hz, 2H), 3.11-3.00 (m, 5H), 2.13-2.03 (m, 2H), 1.88-1.76 (m, 2H), 1.76-1.66 (m, 2H), 1.64-1.50 (m, 6H), 0.87 (t, *J* = 7.4 Hz, 6H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 151.5, 137.2, 127.6, 127.1, 50.2, 45.8, 34.5, 25.6, 22.2, 11.2; **HRMS:** m/z: $[M+Na]^+$ calc'd for $[C_{17}H_{27}No_2SNa]^+$ expect 332.1660; found 332.1655.

4-cyclohexyl-*N*,*N*-dipropylbenzenesulfonamide (**40**)



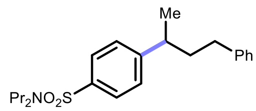
Following a modified version of General Procedure C, using **L5** as the ligand, **1** (95.1 mg, 0.25 mmol) and **S30** (239 mg, 0.50 mmol) as the substrates and $RuCl_3$ (25.9 mg, 0.125 mmol) and $GaCl_3$ (22.0 mg, 0.125 mmol) as the additives and stirring at 40 °C. The crude product was purified via silica gel chromatography (2% EtOAc in Hexane) to give the title compound **40** as a white solid (28.5 mg, 0.088 mmol, 35%). **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.70 (d, *J* = 8.3 Hz, 2H), 7.31 (d, *J* = 8.3 Hz, 2H), 3.06 (t, *J* = 7.6 Hz, 4H), 2.61-2.51 (m 1H), 1.92-1.81 (m, 4H), 1.76 (d, *J* = 12.6 Hz, 1H), 1.56 (h, *J* = 7.6Hz, 4H), 1.47-1.34 (m, 4H), 1.31-1.20 (m, 1H), 0.87 (t, *J* = 7.4 Hz, 6H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 152.7, 137.4, 127.4, 127.2, 50.2, 44.5, 34.2, 26.7, 26.0, 22.2, 11.2; **HRMS:** m/z: $[M+Na]^+$ calc'd for $[C_{18}H_{29}No_2SNa]^+$ expect 346.1817; found 346.1810.

4-(2,3-dihydro-1*H*-inden-2-yl)-*N*,*N*-dipropylbenzenesulfonamide (**41**)



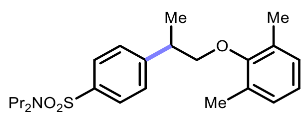
Following a modified version of General Procedure C, using **L5** as the ligand, **1** (95.1 mg, 0.25 mmol) and **S31** (256 mg, 0.50 mmol) as the substrates and $RuCl_3$ (25.9 mg, 0.125 mmol) and $GaCl_3$ (22.0 mg, 0.125 mmol) as the additives and stirring at 40 °C. The crude product was purified via silica gel chromatography (1-2% EtOAc in Hexane) to give the title compound **41** as a yellow solid (24.4 mg, 0.068 mmol, 27%). **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.72 (d, *J* = 8.4 Hz, 2H), 7.39 (d, *J* = 8.4 Hz, 2H), 7.28-7.22 (m, 2H), 7.22-7.17 (m, 2H), 3.74 (p, *J* = 8.4 Hz, 1H), 3.40 (d, *J* = 8.3 Hz, 1H), 3.37 (d, *J* = 8.3 Hz, 1H), 3.12-3.02 (m, 6H), 1.61-1.51 (m, 4H), 0.87 (t, *J* = 7.4 Hz, 6H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 150.4, 142.3, 137.9, 127.6, 127.3, 126.7, 124.4, 50.2, 45.1, 40.7, 22.2, 11.2; **HRMS:** m/z: $[M+Na]^+$ calc'd for $[C_{21}H_{27}No_2SNa]^+$ expect 380.1655; found 380.1648.

4-(4-phenylbutan-2-yl)-*N*,*N*-dipropylbenzenesulfonamide (**42**)



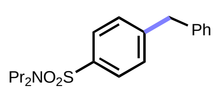
Following a modified version of General Procedure C, using **L5** as the ligand, **1** (95.1 mg, 0.25 mmol) and **S32** (264 mg, 0.50 mmol) as the substrates and $RuCl_3$ (25.9 mg, 0.125 mmol) and $GaCl_3$ (22.0 mg, 0.125 mmol) as the additives and stirring at 40 °C. The crude product was purified via silica gel chromatography (0.2-3% EtOAc in Hexane) to give the title compound **42** as a clear colorless oil (38.7 mg, 0.103 mmol, 41%). **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.74 (d, *J* = 8.3 Hz, 2H), 7.31 (d, *J* = 8.3 Hz, 2H), 7.27 (t, *J* = 7.5 Hz, 2H), 7.18 (t, *J* = 7.3 Hz, 1H), 7.11 (d, *J* = 7.4 Hz, 2H), 3.13-3.05 (m, 4H), 2.79 (h, *J* = 7.1 Hz, 1H), 2.57-2.42 (m, 2H), 1.93 (q, *J* = 7.7 Hz, 2H), 1.56 (h, *J* = 7.7 Hz, 4H), 1.29 (d, *J* = 6.9 Hz, 3H), 0.87 (t, *J* = 7.4 H, 6H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 152.1, 142.0, 137.7, 128.4, 128.3, 127.7, 127.3, 125.9, 50.1, 39.7, 39.4, 33.8, 22.1, 22.1, 11.2; **HRMS:** m/z: $[M+Na]^+$ calc'd for $[C_{22}H_{31}No_2SNa]^+$ expect 396.1968; found 396.1973.

4-(1-(2,6-dimethylphenoxy)propan-2-yl)-*N*,*N*-dipropylbenzenesulfonamide (**43**)



Following a modified version of General Procedure C, using **L5** as the ligand, **1** (95.1 mg, 0.25 mmol) and **S33** (279 mg, 0.50 mmol) as the substrates and $RuCl_3$ (25.9 mg, 0.125 mmol) and $GaCl_3$ (22.0 mg, 0.125 mmol) as the additives and stirring at 40 °C. The crude product was purified via silica gel chromatography (1-2% EtOAc in Hexane) and C-18 reverse-phase HPLC (Water/MeCN) to give the title compound **43** as a white solid (22.1 mg, 0.055 mmol, 22%). **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.77 (d, *J* = 8.3 Hz, 2H), 7.47 (d, *J* = 8.3 Hz, 2H), 6.96 (d, *J* = 7.4 Hz, 2H), 6.89 (dd, *J* = 7.9, 6.9 Hz, 1H), 3.86-3.79 (m, 2H), 3.32 (h, *J* = 6.8 Hz, 1H), 3.13-3.00 (m, 4H), 2.10 (s, 6H), 1.56 (h, *J* = 7.7 Hz, 4H), 1.47 (d, *J* = 7.1 Hz, 3H), 0.88 (t, *J* = 7.4 Hz, 6H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 155.4, 149.1, 138.3, 130.9, 129.0, 128.3, 127.3, 124.1, 76.7, 50.2, 40.8, 22.2, 17.8, 16.2, 11.3; **HRMS:** m/z: $[M+H]^+$ calc'd for $[C_{23}H_{34}No_3SNa]^+$ expect 404.2254; found 404.2262.

4-benzyl-*N*,*N*-dipropylbenzenesulfonamide (**44**)

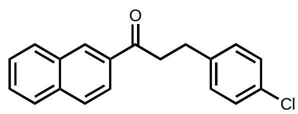


Following a modified version of General Procedure C, using **L5** as the ligand, **1** (95.1 mg, 0.25 mmol) and **S34** (243 mg, 0.50 mmol) as the substrates and $RuCl_3$ (25.9 mg, 0.125 mmol) and $GaCl_3$ (22.0 mg, 0.125 mmol) as the additives and stirring at 40 °C. The crude product was purified via silica gel chromatography (2% EtOAc in Hexane) and C-18 reverse-phase HPLC (Water/MeCN) to give the title compound **44** as a yellow oil (9.0 mg, 0.027 mmol, 11%). **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.71 (d, *J* = 8.3 Hz, 2H), 7.34-7.27 (m, 4H), 7.26-7.21 (m, 1H), 7.17 (d, *J* = 7.8 Hz, 2H), 4.04 (s, 2H), 3.07-3.02 (m, 4H), 1.60-1.50 (m, 4H), 0.86 (t, *J* = 7.4 Hz); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 145.9, 139.7, 137.9, 129.4, 129.0, 128.7, 127.3, 126.6, 50.1, 41.7, 22.1, 11.2; **HRMS:** m/z: $[M+Na]^+$ calc'd for $[C_{19}H_{25}No_2SNa]^+$ expect 354.1498; found 354.1488.

Ketones

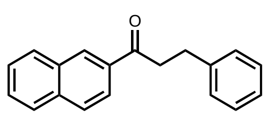
^{1}H NMR and UPLC-MS were used to determine the selectivity between C–C product and ketone. For known ketones, reference to previously reported ^{1}H NMR data was used to assign the correct peak. Below is the synthesis and characterization of novel ketones, and those which needed to be isolated to generate calibration curves for UPLC-MS analysis.

3-(4-chlorophenyl)-1-(naphthalen-2-yl)propan-1-one (**32**)



Following General Procedure C, using **30** (66.8 mg, 0.25 mmol) and **2** (268 mg, 0.50 mmol) as the substrates. The crude product was purified via silica gel chromatography (0.5% EtOAc in Hexane) to give the title compound **32** as a white solid (4.4 mg, 0.015 mmol, 6%). **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.45 (s, 1H), 8.03 (dd, *J* = 8.7, 1.2 Hz), 7.94 (d, *J* = 8.0 Hz, 1H), 7.89 (t, *J* = 8.4 Hz, 2H), 7.61 (t, *J* = 7.2 Hz, 1H), 7.55 (t, *J* = 7.2 Hz, 1H), 7.28 (d, *J* = 8.3 Hz, 2H), 7.22 (d, *J* = 8.3 Hz, 2H), 3.42 (t, *J* = 7.5 Hz, 2H), 3.11 (t, *J* = 7.5 Hz, 2H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 198.8, 139.8, 135.6, 134.1, 132.5, 131.9, 129.9, 129.7, 129.6, 128.7, 128.5 (2 signals), 127.8, 126.9, 123.8, 40.3, 29.5; **HRMS(EI+)** :m/z: $[M]^+$ calc'd for $[C_{19}H_{15}ClO]^+$ expect 294.0811; found 294.0776. ***Target analyte mass overlaps isotope of calibration standard mass which skews measured mass.***

1-(naphthalen-2-yl)-3-phenylpropan-1-one (**37**)

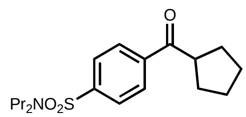


Following General Procedure C, using **30** (400 mg, 1.50 mmol) and **S18** (1.50 g, 3.00 mmol) as the substrates, $GaCl_3$ (264 mg, 1.50 mmol) as the additive. The crude product was purified via silica gel chromatography (0.5% EtOAc in Hexane) to give the title compound **37** as a colorless liquid (85.9 mg, 0.33 mmol, 22%). **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.47 (s, 1H), 8.05 (dd, *J* = 8.6, 1.7 Hz, 1H), 7.94 (d, *J* = 8.1 Hz, 1H), 7.89 (t, *J* = 9.0 Hz, 2H), 7.60 (td, *J* = 7.0, 1.0 Hz, 1H), 7.55 (td, *J* = 7.5, 0.9 Hz, 1H), 7.36-7.28 (m, 4H), 7.23 (tt, *J* = 6.8, 2.0 Hz, 1H), 3.45 (t, *J* = 7.4 Hz, 2H), 3.14 (t, *J* = 8.0 Hz, 2H); **^{13}C NMR**

(126 MHz, $CDCl_3$) δ 199.2, 141.4, 135.6, 134.2, 132.6, 129.7, 129.6, 128.6, 128.6, 128.5, 128.5, 127.8, 126.8, 126.2, 123.9, 40.6, 30.3.

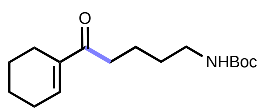
All data match that previously reported in the literature.[27]

4-(cyclopentanecarbonyl)-*N*,*N*-dipropylbenzenesulfonamide (**S49**)



Isolated as a side product in the formation of **39** using General Procedure C. White solid (10.6 mg, 0.034 mmol, 13%). **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.06 (d, *J* = 8.2 Hz, 2H), 7.89 (d, *J* = 8.2 Hz, 2H), 3.70 (p, *J* = 7.9 Hz, 1H), 3.10 (t, *J* = 7.7 Hz, 4H), 2.00-1.85 (m, 4H), 1.79-1.61 (m, 4H), 1.60-1.50 (m, 4H), 0.87 (t, *J* = 7.4 Hz, 6H); **^{13}C NMR (126 MHz, $CDCl_3$)** δ 201.7, 143.8, 139.7, 129.0, 127.2, 50.0, 46.8, 29.9, 26.3, 22.0, 11.2

tert-butyl (4-(cyclohex-1-en-1-yl)butyl)carbamate (**S50**)



Following General Procedure C, using **S13** (22.1 mg, 0.100 mmol) and **S21** (96.0 mg, 0.200 mmol) as the substrates. The crude product was purified via silica gel chromatography (5-10% EtOAc in Hexane) to give the title compound **S50** as a colorless liquid (13.0 mg, 0.046 mmol, 46%). **^{1}H NMR (500 MHz, $CDCl_3$)**: δ 6.91-6.86 (m, 1H), 4.58 (s, 1H), 3.17-3.05 (m, 2H), 2.64 (t, *J* = 7.3 Hz, 2H), 2.29-2.15 (m, 4H), 1.66-1.55 (m, 6H), 1.52-1.38 (m, 11H); **^{13}C NMR (126 MHz, $CDCl_3$):** δ 201.3, 156.1, 140.0, 139.3, 79.2, 40.4, 36.5, 29.8, 28.6, 26.2, 23.3, 22.1, 21.8, 21.7; **HRMS:** m/z: $[M+Na]^+$ calc'd for $[C_{16}H_{27}NO_3Na]^+$ expect 304.1883; found 304.1878.

All data match that previously reported in the literature.[28]

Extended Scope Exploration

Generally, most primary alkylpyridinium salts tried were compatible with the procedure, and choice of *N*-acyl-glutarimide was more crucial for a productive reaction. To illustrate this we performed an extended screen of *N*-acyl-glutarimdies (Figure S34), which we hope can be used in tandem with the results in the manuscript to provide sufficient data for machine learning studies (https://github.com/cernaklab/douthwaite-sp3-sp2-cross-coupling-of-activated-amines-and-acids). An additional substrate was also unsuccessful (Figure S35).

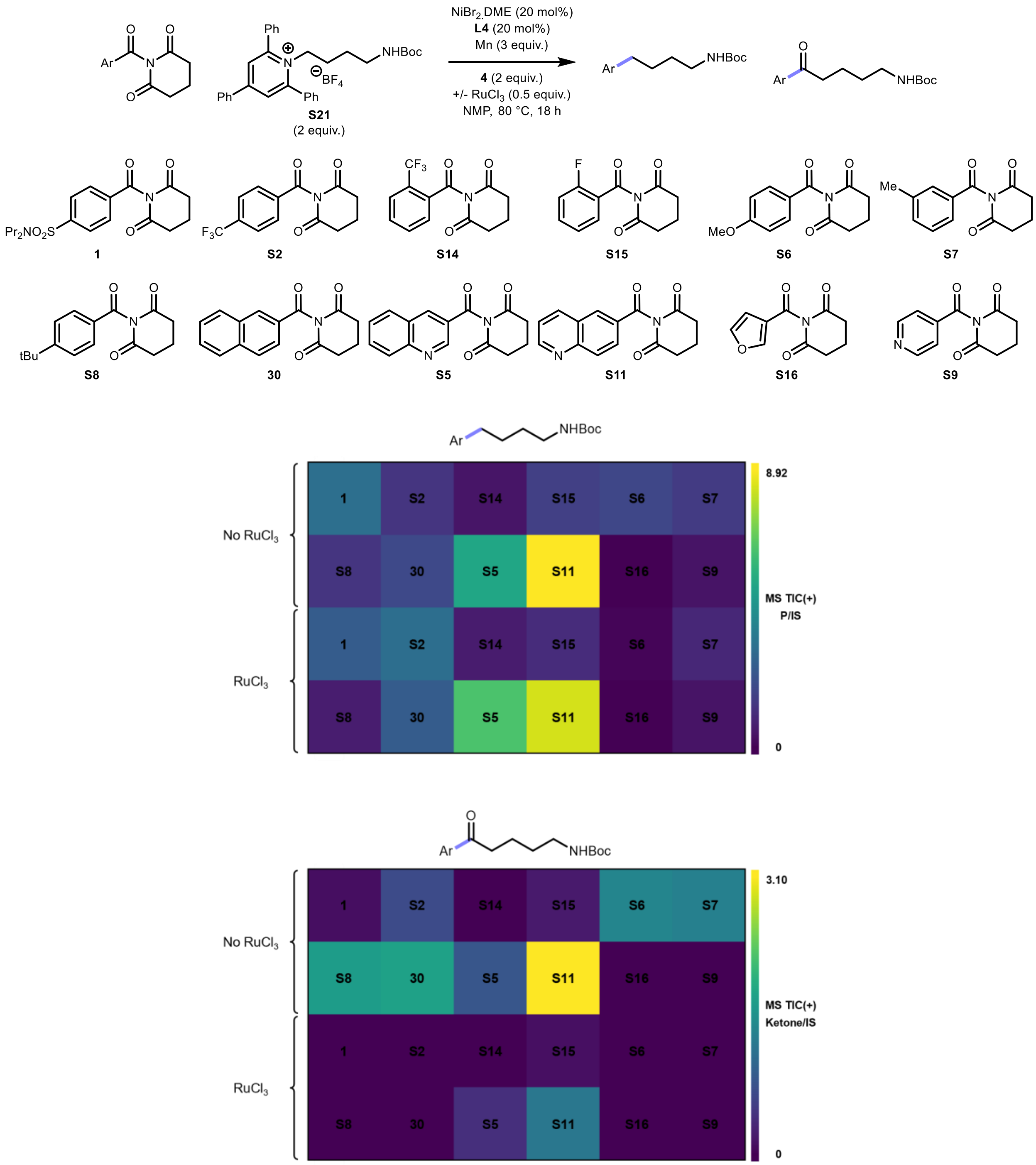
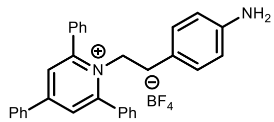


Figure S34: Extended scope exploration of *N*-acyl-glutarimides. Reactions were performed at 50 µmol scale using the General Singleton procedure. Values are MS TIC(+) integrals relative to caffeine internal standard.



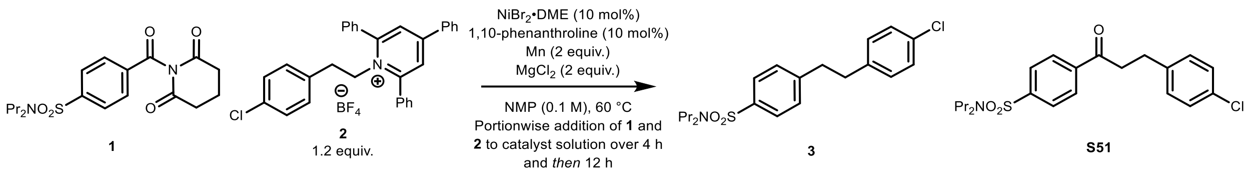
S29

Figure S35: Substrate **S29** failed in all attempted coupling reactions

Mechanistic and Control Experiments

Comparison to Matsuo's Conditions

Coupling of 1 and 2



Entry	T / °C	3 / %	S51 / %
1	60	15	ND
2	100	10	ND
3	150	Trace	ND

Table S20: Application of the procedure reported by Matsuo[27] for ketone synthesis to the reaction between **1** and **2**. Reactions were performed on 0.20 mmol scale, and yield was determined by ^{1}H NMR through comparison to an internal standard. No ketone product was detected by either UPLC-MS or ^{1}H NMR in any of the reactions. ND = not detected

Synthesis of common products 33 and 37

The reaction to form C–C product **33** and ketone **37** is common to both our report and Matsuo's report.[27] A comparison of the conditions is shown in Figure S36.

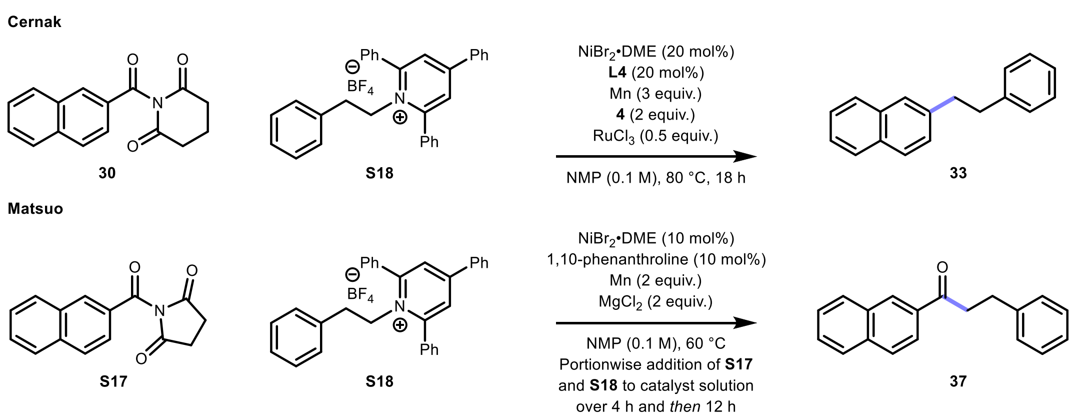


Figure S36: Comparison optimized reaction conditions from Cernak and Matsuo[27] for the selective formations of C–C product **33** and ketone **37**

To try elucidate the origins of this selectivity difference we subjected both **30** and **S17** to our optimized conditions (both with and without 0.5 equiv. $RuCl_3$) and to Matsuo's protocol (Table S21). We found *N*-acyl-glutarimide substrate **30** had greater reactivity than *N*-acyl-succinimide **S17** with our standard protocol, and gave greater selectivity for **33** with the $RuCl_3$ modification. This greater reactivity of **30** is consistent with previous reports comparing activated twisted amides.[29] Rigorously following Matsuo's protocol [27] with either

30 or **S17** gave a significant decline in both yield and selectivity, and we were unable to reproduce the reported yield of 70% for **37**.

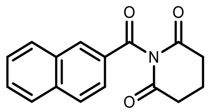
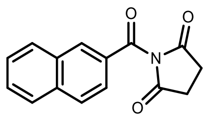
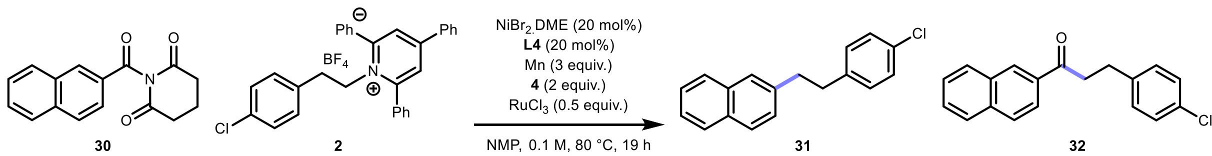
	Cernak		**Cernak + $RuCl_3$**		**Matsuo**	
Substrate	**33**	**37**	**33**	**37**	**33**	**37**
 **30**	59%†	28%†	75%†‡	ND†	10%	16%
 **S17**	38%	21%	54%	12%	20%	12% (70%)*

Table S21: Comparison of Cernak and Matsuo protocols using both *N*-acyl-glutarimide substrate **30** and *N*-acyl succinimide substrate **S17**. Yields were determined by UPLC-MS. ND = not detected. †Value from Table S13, ‡^{1}H NMR yield, *reported isolated yield from Ref. 27

Headspace Volume Evaluation

As the C(sp^3)–C(sp^2) coupling reaction generates CO as a gaseous byproduct, we evaluated the effect of reaction vessel headspace, purging the reaction with N_2 and running the reaction with a CO atmosphere (Table S22). We observed only small changes in yield and no significant difference in selectivity compared to the control reactions, both in the presence and absence of $RuCl_3$. Additionally, performing the reaction under a CO atmosphere gave no observable C–C or ketone products.



Entry	Condition	$RuCl_3$ (N/Y)	31 / %	32 / %	Total Yield / %	Ratio 31:32
1	2-dram vial (control)	N	54	32	86	1.7:1
2	2-dram vial (control)	Y	53	ND	53	>20:1
3	2-dram vial with N_2 atmosphere purge	N	60	30	90	2.0:1
4	2-dram vial with N_2 atmosphere purge	Y	41	ND	41	>20:1
5	20 mL scintillation vial	N	50	26	76	1.9:1
6	20 mL scintillation vial	Y	31	ND	31	>20:1
7	25 mL RBF	N	42	25	67	1.7:1
8	25 mL RBF	Y	49	ND	49	>20:1
9	2-dram vial with CO balloon	N	ND	ND	-	-
10	2-dram vial with CO balloon	Y	ND	ND	-	-

Table S22: Headspace volume evaluation in the formation of **31** from **30** and **2**. Reactions were run on 100 µmol scale using General Procedure for Singleton Optimization. Yields were determined by UPLC-MS. ND = not detected. RBF = round-bottom flask

Investigations into role of $RuCl_3$

Reaction in the Absence of $NiBr_2$•DME

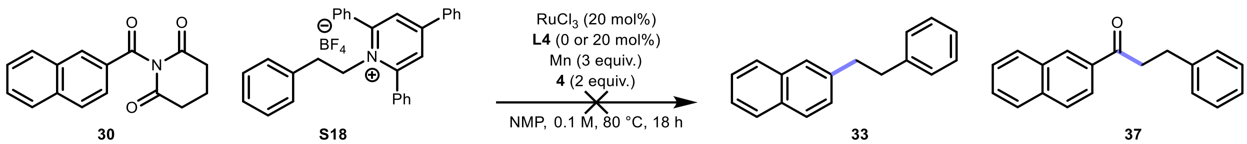


Figure S37: Control reaction in the absence of $NiBr_2$•DME to probe the role of $RuCl_3$. No conversion to **33** or **37** was observed

Following a modified General Singleton procedure without $NiBr_2$•DME using **27** (40.1 mg, 0.15 mmol), **S18** (150 mg, 0.30 mmol), Mn (24.7 mg, 0.45 mmol), **4** (44.1 mg, 0.30 mmol), $RuCl_3$ (6.2 mg, 0.030 mmol) and **L4** (5.5 mg, 0.030 mmol). Products **33** and **37** were not detected by UPLC-MS analysis. An analogous reaction in the absence of **L4** also yielded no **33** or **37**.

Spiking of Ketone in $RuCl_3$ Promoted Reaction

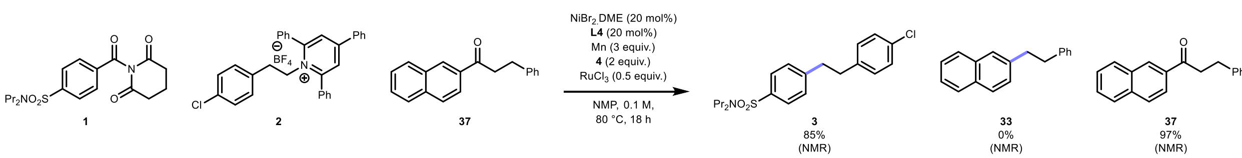


Figure S38: Spiking of ketone **37** into the $RuCl_3$ promoted reaction between **1** and **2.** Yields are determined from crude ^{1}H NMR with reference to an internal standard.

Following General Procedure C, using **1** (19.0 mg, 0.050 mmol) and **2** (53.4 mg, 0.10 mmol) as the substrates and $RuCl_3$ (5.2 mg, 0.025 mmol) and ketone **37** (13.0 mg, 0.050 mmol) as additives. The crude reaction mixture was analyzed by ^{1}H NMR through reference to 0.050 mmol trimethoxybenzene internal standard. No conversion of **37** to **33** was observed and the formation of **3** was unaffected.

Role of Phthalimide - Replacement of 1 with 45

Evaluation in C(sp^3)–C(sp^2) Coupling

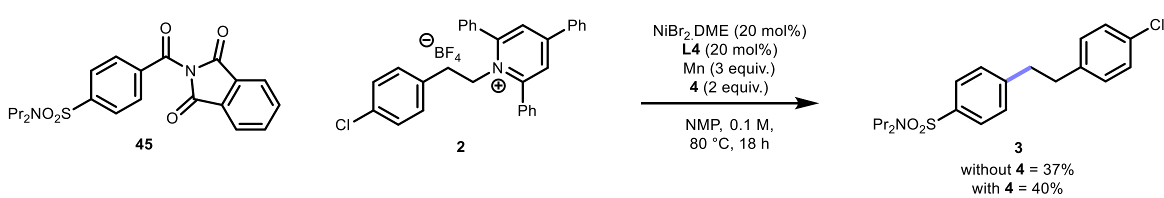


Figure S39: Evaluation of **45** in coupling with **2** both in the presence and absence of additional phthalimide

Following a modified General Procedure C using **45** (41.4 mg, 0.10 mmol) and **3** (107 mg, 0.20 mmol) as the substrates. For the reaction without **4**, **4** was excluded from the stock solution prestir. The yield was determined by [1]H NMR of the crude reaction mixtures through comparison to 0.1 mmol dibromomethane internal standard.

Proof of Radical Mechanism

Radical Ring Opening

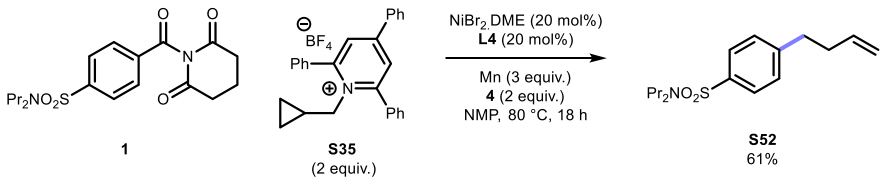


Figure S40: Radical ring opening with substrate **S35**

Following General Procedure C, using **1** (95.0 mg, 0.250 mmol) and **S35** (181 mg, 0.500 mmol) as the substrates. The crude product was purified via silica gel chromatography (2-5% EtOAc in Hexane) to give 4-(but-3-en-1-yl)-*N*,*N*-dipropylbenzenesulfonamide (**S52**) as a colorless liquid (45.1 mg, 0.153 mmol, 61%).**^{1}H NMR (499 MHz, $CDCl_3$)**: δ 7.72-7.68 (d, *J* = 8.1 Hz, 2H), 7.29 (d, *J* = 8.1 Hz, 2H), 5.80 (m, 1H), 5.09-4.87 (m, 2H), 3.08-3.03 (t, J = 7.6 Hz, 4H), 2.76 (t, *J* = 7.6Hz, 2H), 2.41-2.33 (m, 2H), 1.58-1.48 (m, 4H), 0.85 (t, *J* = 7.4 Hz, 6H); **^{13}C NMR (126 MHz, $CDCl_3$)**: δ 146.8, 137.7, 137.3, 129.1, 127.2, 115.7, 50.1, 35.2, 35.1, 22.1, 11.3; **HRMS:** m/z: $[M+H]^+$ calc'd for $[C_{16}H_{26}NO_2S]^+$ expect 296.1679; found 296.1676.

Radical Trapping

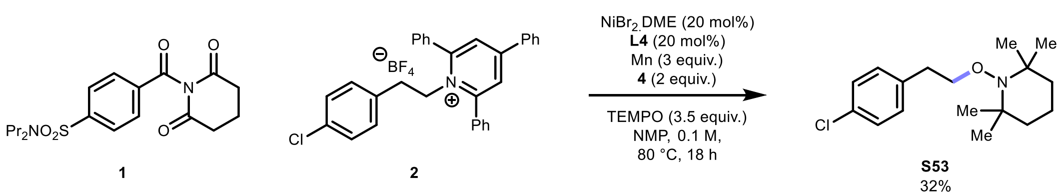
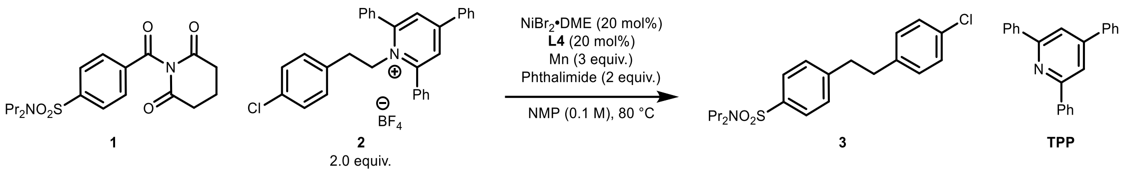


Figure S41: Radical trapping experiment using TEMPO

Following General Procedure C, using **1** (38.0 mg, 0.10 mmol) and **2** (107 mg, 0.20 mmol) as the substrates, and TEMPO (54.7 mg, 0.35 mmol) as the additive. Through comparison to literature data,[30] TEMPO adduct **S53** was observed in 32% yield by [1]H NMR analysis through comparison to 0.1 mmol dibromomethane internal standard. Coupling product **3** was not observed by either UPLC-MS or [1]HNMR analysis.

Rate of TPP Formation in Presence and Absence of 1



The above reaction above was set up using General Procedure **C** on a 0.25 mmol scale with respect to **1**. An identical reaction without **1** was set up in parallel. The vials' septa were equipped with nitrogen balloons, and at the specified time intervals an 8.4 uL aliquot was taken from the reaction, added to 992 uL of 0.15 mg/mL caffeine solution in MeCN/Water 50:50, then passed through a syringe filter and analyzed by UPLC-MS.

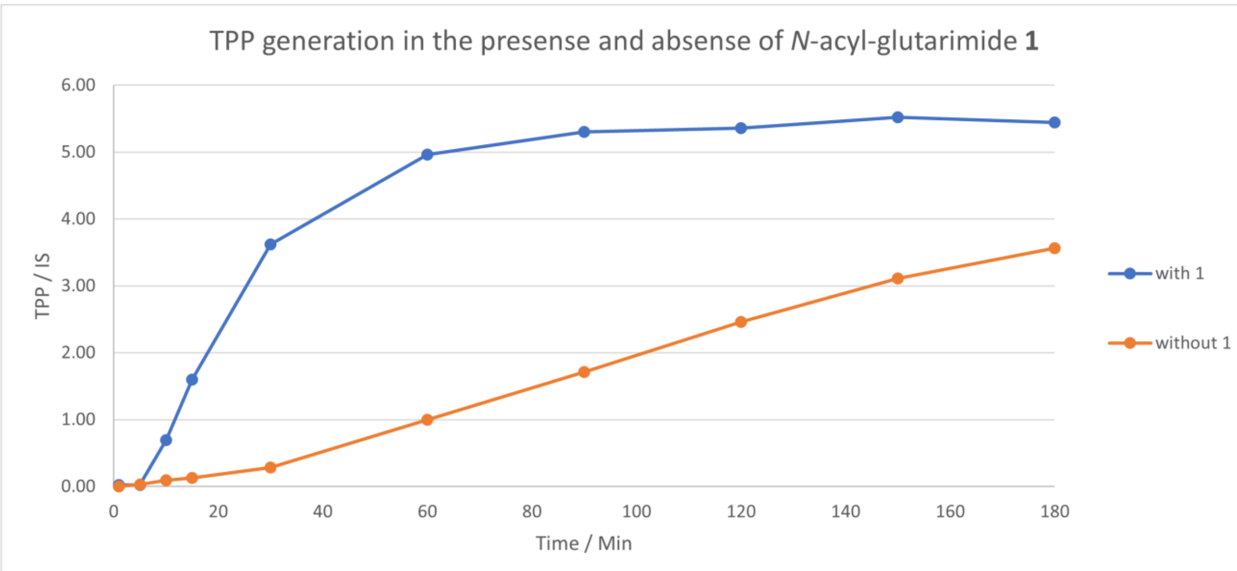


Figure S42: Rate of TPP generation in the presence and absence of substrate **1**. Y-axis values are UPLC-MS UV response of TPP relative to a caffeine internal standard.

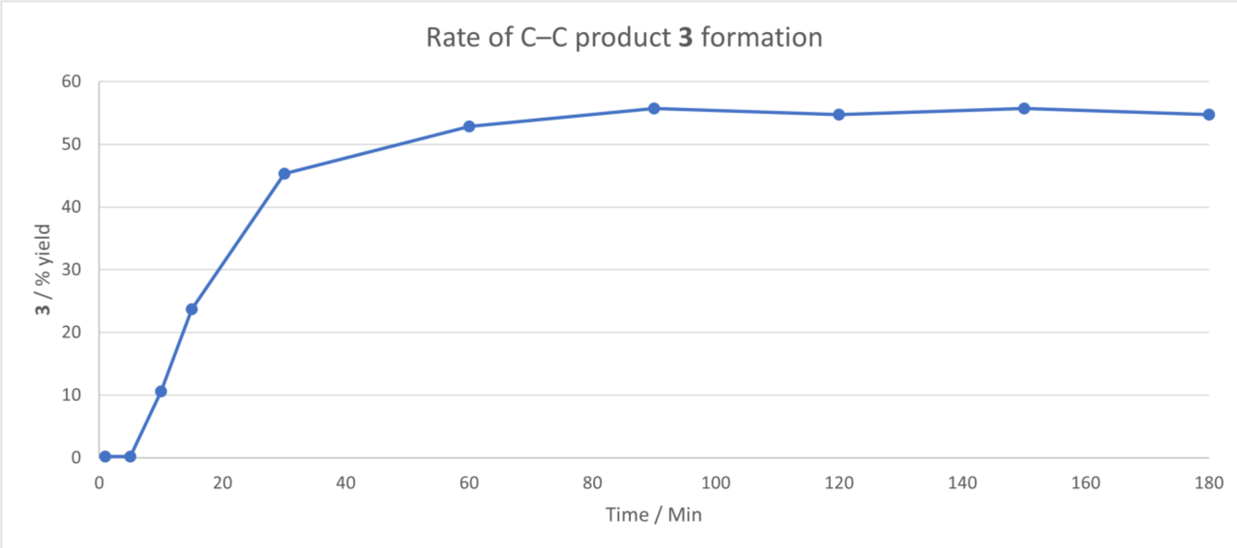


Figure S43: Rate of formation of **3**. Y-axis values are UPLC-MS UV response of TPP relative to a caffeine internal standard.

After an initial induction period of 5 minutes for both reactions, the rate of TPP formation is significantly higher in the presence of **1** (Figure S42). The rate of TPP formation also correlates well to the rate of **3** formation (Figure S43). This suggests that a Ni complex that forms after oxidative addition of **1** is primary reductant of substrate **2** in the catalytic cycle, rather than Mn. Based on previous reports this is likely a Ni(I) species,[31–33] although we cannot confirm a radical rebound or radical chain bimetallic pathway at this time. This supports DFT calculations that for Ni(II)-glutarimide complexes (X = glutarimide, Figure 6C) decarbonylation occurs before radical addition (Figure S47 and Figure S48), assuming radical addition is barrierless. This is in accordance with experimental observations of no ketone being observed for the substrate pair **1** and **2**. However, the possibility of X = phthalimide and decarbonylation happening after radical addition cannot be ruled out at this stage.

Computational Details

Reaction pathways were evaluated using the reaction discovery tools developed in the Zimmerman group, particularly the double-ended Growing String Method (GSM).[34,35] GSM identifies minimum energy reaction paths and transition states without the requirement of prior knowledge of their geometries.[36–38] After obtaining the reaction path from GSM, the transition state geometry was reoptimized to tighter convergence (gradient tolerance < $3x10^{-4}$ a.u.) using an eigenvector-following algorithm.

All geometries (intermediates and transition states) were optimized using the spin-unrestricted B3LYP density functional and the LANL2DZ basis set.[39–44] Frequency calculations were conducted at the same level of theory for all stationary points to obtain free energy corrections at 353K, where vibrational frequencies below $50cm^{-1}$ were adjusted to $50cm^{-1}$.[45–47] Single-point computations were performed using the conductor-like polarizable continuum model (CPCM) for N-methylpyrrolidinone, the ωB97X-D exchange functional, and the polarized, triple-zeta quality cc-pVTZ basis set. Report energies are from these single point energies, plus free energy corrections. For CPCM, the method, radii, van der Waals scale and the dielectric constant were SWIG, UFF, 1.2, and 32.6, respectively. All simulations were performed using Q-CHEM 5.2.[48]

1. Oxidative addition

1-1. Oxidative addition of 1 and 45 to Ni(0) 5,5'-dimethyl-2,2'-bipyridine

Nickel-catalyzed reactions that involve twisted amides are known to initiate with oxidative addition of the carbonyl carbon-imide nitrogen to the catalyst.[49] The phthalimide additive could facilitate this process after undergoing transamidation with glutarimide in **1**. To rule out this possibility the reaction of **45** was tested with and without phthalimide additive. These reactions gave significantly less product compared to substrate **1** (Figure 6A). To provide additional insight, oxidative addition pathways were evaluated using quantum chemical simulations. In particular, oxidative addition of **1** and **45** to Ni(0) at two different positions were specifically examined.

The first oxidative addition pathway starts with the carbonyl of the substrate (**1P** or **1G**) ligated to the metal center. For the glutarimide-derivatized acid complex **1G**, oxidative addition occurs via **TS-1G-3G** (**TS-1** in Figure 6B), which shows a barrier of 27.3 kcal/mol to give Ni(II) complex **3G** (Figure S44, solid black line). In contrast, when the starting complex is **1P**, the activation energy is much higher at 49.8 kcal/mol via **TS-1P-3P** (Figure S44, solid purple line, **TS-45** in Figure 6C). This difference is attributed to both **TS-1G-3G** being much less crowded around Ni and significantly relieved dihedral angle of O=C-N-C at ~2.7°, compared to 43.5° of **TS-1P-3P**.

The second oxidative addition pathway proceeds via a Ni-π complex to the substrate aryl group (Figure S44, dashed lines). The glutarimide-derivatized substrate results in a lower-energy intermediate **2G** compared to the phthalimide-counterpart, **2P** by 4.8 kcal/mol. This can be accounted by the change in dihedral O=C-N-C, which favors planarity (~0°) for the stabilization through amide bond resonance. Between **1G** and **2G**, it is relieved (112.2° to 75.0°), whereas it becomes slightly more strained from 95.0° to 104.0° between **1P** and **2P**. Although the barriers for oxidative addition above these intermediates are similar (20.8 kcal/mol from **2G**, 22.6 kcal/mol from **2P**), the overall activation energy starting from **1G** (29.1 kcal/mol) is significantly lower than **1P** (35.7 kcal/mol) due to the strain in the aryl-ligated Ni complex.

The higher activation barriers of Ni(0) complexes with **45** for both routes is consistent with relative thermodynamics, where the resulting oxidative addition Ni(ii) singlet complex **3P** is less favorable than **3G** by 4 kcal/mol. In all, this suggests the oxidative addition of glutarimide-derivatized substrate **1**'s over phthalimide-derivatized **45**. This is in agreement with the result in Figure 6A, where the yield with **1** is significantly higher than **45**.

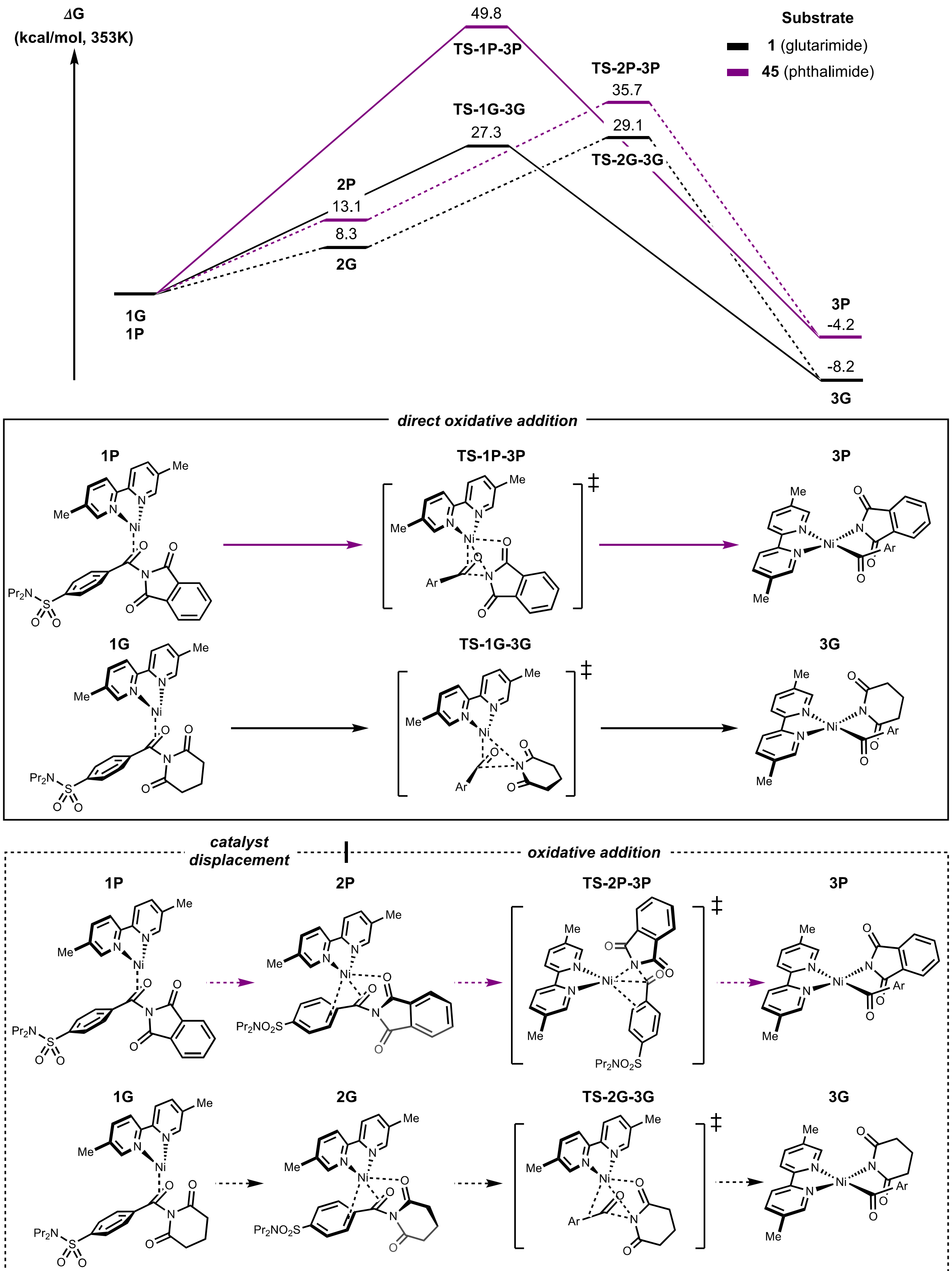


Figure S44: Energy diagram of oxidative addition of **1** and **45** to Ni(0). Values correspond to relative free energies in kcal/mol computed at ωB97X-D/cc-pVTZ/CPCM(NMP)//B3LYP/LANL2DZ level of theory. G and P correspond to glutarimide and phthalimide, respectively.

1-2. Oxidative addition of 1 and 45 to Ni(I)-phthalimide complex

While oxidative addition of Ni(0) seems plausible and is supported by quantum chemical results, the possibility of Ni(I) complexes undergoing oxidative addition remains. Thus, oxidative addition pathways of two Ni(I) complexes were evaluated. Ni(I)-phthalimide was considered first, as two equivalents of phthalimide were added to the reaction. With a Ni(I)-phthalimide complex ligated to each acid-substrate (**4G**, **4P**), the activation barriers of oxidative addition were comparable, showing 40.0 kcal/mol and 39.9 kcal/mol for **TS-4G-5G** and **TS-4P-5P** (Figure S45, black and purple paths), respectively. Comparing the resulting Ni(III) complexes, **5G** is thermodynamically favored by 1.4 kcal/mol over **5P**. In all, the barriers are higher than those for Ni(0) routes (Figure S44) and no significant differences between the substrates is expected. The oxidative addition of **1** or **45** to a Ni(I)-phthalimide complex is therefore less likely to be operative.

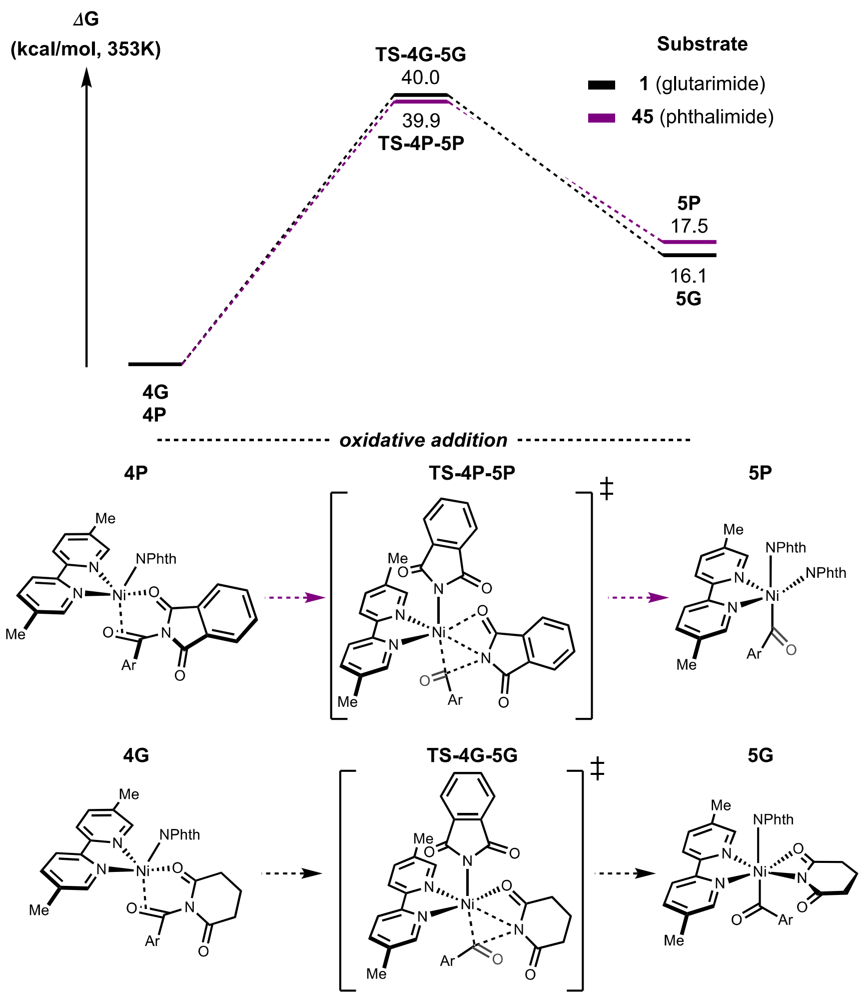


Figure S45: Energy diagram of oxidative addition of **1** and **45** to Ni(I)-phthalimide complex.

1-3. Oxidative addition of 1 and 45 to Ni(I)-alkyl complex

Besides the pathways shown in Sections 1-1 and 1-2, oxidative addition to Ni(I)-alkyl complexes is also possible. Complex **6G** is one such Ni(I) alkyl, which could be formed by Ni(0) capturing a deaminated alkyl radical. Three oxidative addition products, **7G**, **8G** and **9G** can form from **6G**. **9G** is 8.2 kcal/mol above **6G** and ruled out as viable based on thermodynamics (Figure S46). The two thermodynamically more feasible species, **7G** and **8G**, undergo an almost barrierless reductive elimination to generate the ketone product (not shown, **TS-7G-RE** and **TS-8G-RE**). The ketone product is not experimentally observed for this specific substrate pair. Since the Ni(I) alkyl pathways are not consistent with experimental observations, oxidative addition of **1** to Ni(I)-alkyl therefore appears to be unlikely.

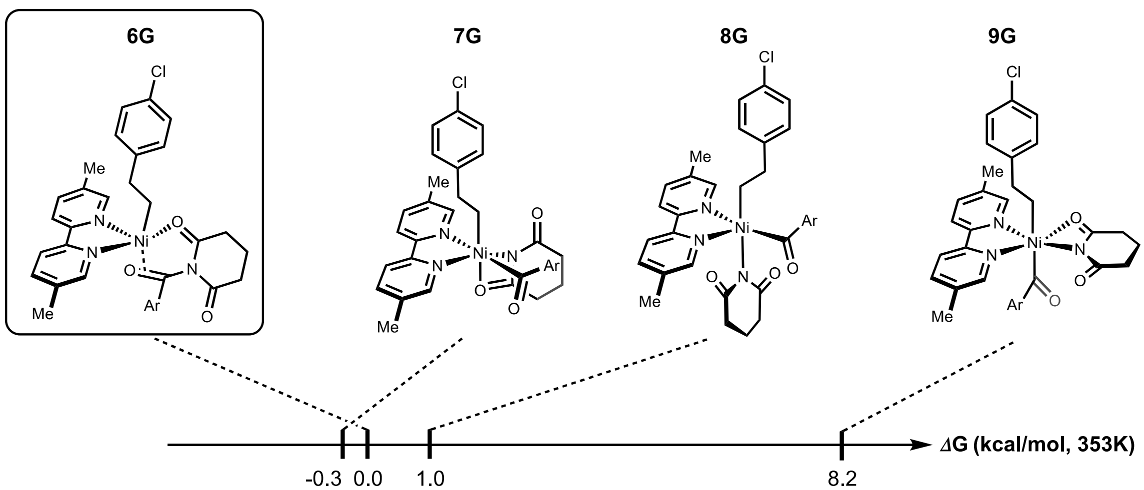


Figure S46: Relative free energies of Ni(I)-alkyl ligated to 1 (**6G**) and its oxidative addition products (**7G, 8G and 9G**).

2. Decarbonylation

For the C–C product to form, decarbonylation must take place. With vacant coordination sites after oxidative addition (**3G**), the phthalimide additive may facilitate decarbonylation after ligand exchange with glutarimide. Therefore, decarbonylation was examined for nickel complexes with either the glutarimide or phthalimide as a ligand. First, nickel complexes after alkyl radical addition where the alkyl and aryl carbonyl are *trans* to each other (Figure S47, **9G** and **9P**) were considered. **9P** undergoes CO displacement through a 21.2 kcal/mol barrier (**TS-9P-10P**) resulting in a hexa-coordinated Ni(III) complex **10P** which is 15.3 kcal/mol uphill. Then, detachment of CO from Ni happens in a barrierless manner, resulting in decarbonylated complex **11P**. In contrast with phthalimide, CO displacement occurs via isomerization of a glutarimide's carbonyl, where the oxygen forms a bond with the displacing CO (**TS-9G-10G** to **10G**). The higher 29.0 kcal/mol barrier of **TS-9G-10G** compared to **TS-9P-10P** (21.2 kcal/mol) can be explained with the weaker binding of glutarimide to Ni due to this tautomerization. In contrast to the barrierless decarbonylation with phthalimide present, **10G** needs to overcome a barrier of 8.7 kcal/mol at **TS-10G-11G** to liberate CO from the bonding of glutarimide to give **11G**.

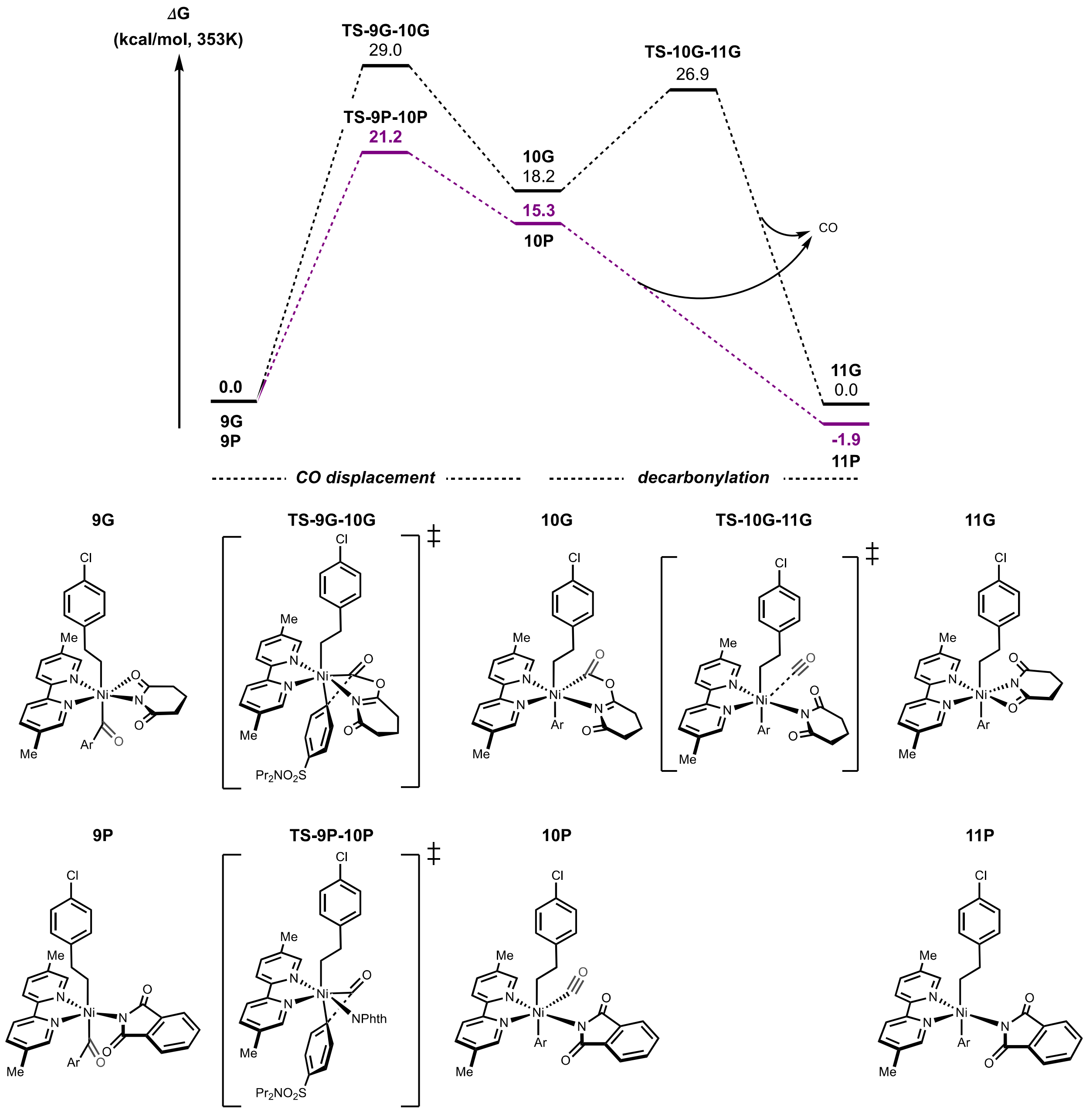


Figure S47: Energy diagram of decarbonylation of **9G** and **9P**.

An alternative point where decarbonylation could happen is before the alkyl radical adds to the oxidative addition product. As d^{8} Ni(II) complexes, these products typically have zero or two unpaired electrons. Therefore, singlet and triplet states of **3G** and **3P** (denoted **3G^{1}**, **3G^{3}**, **3P^{1}** and **3P^{3}**) have been considered as starting points for decarbonylation (Figure S48). For the singlet complexes, glutarimide (**3G^{1}**) and phthalimide (**3P^{1}**) complexes show approximately 23 kcal/mol barriers (**TS-3G^{1}-12G^{1}** and **TS-3P^{1}-12P^{1}**) for the displacement of CO. The resulting complexes **13G^{1}** and **13P^{1}** are relaxed to thermodynamically favored square planar isomers **14G^{1}** and **14P^{1}**, respectively. Similarly, when the decarbonylation happens after an energetically uphill change in spin into the triplet state (**3G^{3}** and **3P^{3}**), an activation energy of 25.2 and 23.4 kcal/mol is required for glutarimide (**TS-3G^{3}-12G^{3}**) and phthalimide (**TS-3P^{3}-12P^{3}**), respectively. Resulting Ni(III) complexes **12G^{3}** and **12P^{3}** can undergo a barrierless decarbonylation to give pyramidal complexes **13G^{3}** and **13P^{3}**. To summarize, the decarbonylation activation energies before alkyl radical addition (~23.0 kcal/mol) are not significantly higher than that of **TS-9P-10P** (21.2 kcal/mol) and therefore, these pathways cannot be ruled out. Future experimental evidence on whether a nickel complex with a phthalimide ligand is generated in the course of the reaction will help specify the operating pathway.

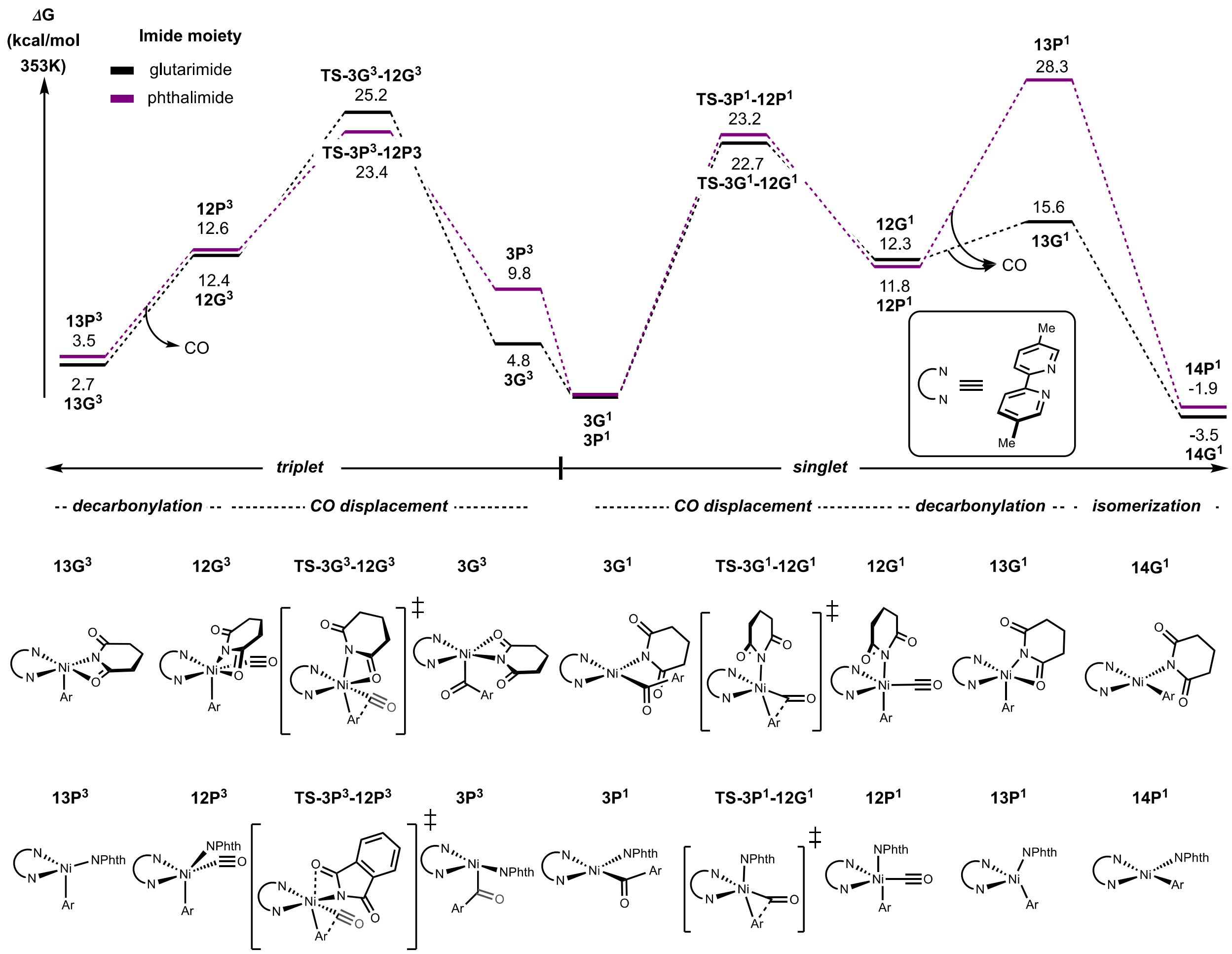


Figure S48. Energy diagram of decarbonylation before alkyl radical adds to the Ni(II) complex. Superscripts **1** and **3** correspond to singlet and triplet spin states, respectively. Phth = phthalimide.

XYZ coordinates for intermediates and transition states

1G

Total free energy (Ha) = -3666.12108

Potential energy (Ha) = -3666.65257

77

C	-1.51648181	-0.71538095	0.22449105
C	-2.88439855	-0.52920993	0.01776642
H	-3.51149805	-1.30782723	-0.40147752
C	-3.44942309	0.69268181	0.36893826
S	-5.28004723	0.89767861	0.18481067
C	-2.69799500	1.73401762	0.91485536
H	-3.16806627	2.67678895	1.17083953
C	-1.33455187	1.53836065	1.11393304
H	-0.71481697	2.32729682	1.52197198
C	-0.72278239	0.30673012	0.78617912
C	0.70151390	0.08720728	1.11814176
O	-5.83547777	-0.47109917	-0.51341351
O	-5.93259666	1.37886865	1.59795638
N	-5.40004225	2.32201841	-0.89883169
C	-4.80333290	2.18874450	-2.23777480
C	-6.41948638	3.33351394	-0.57031733

H	-6.52662471	3.32231735	0.51942864
C	-7.80851151	3.18495124	-1.22260417
H	-5.97744796	4.30033266	-0.85007325
C	-5.56121077	1.34027972	-3.28057694
H	-3.78974148	1.78223916	-2.11732144
H	-4.68073346	3.21796219	-2.60429055
C	-8.55396028	1.90210595	-0.82229650
H	-7.71969912	3.24762079	-2.31567510
H	-8.39655257	4.06343531	-0.91575370
H	-5.71354921	0.33528621	-2.87184739
C	-4.78308388	1.26969185	-4.60465859
H	-6.55644523	1.76598394	-3.45645471
H	-3.78972237	0.82652042	-4.45745219
H	-4.64024272	2.26681623	-5.04155214
H	-5.31496606	0.65693435	-5.34073411
H	-8.00756958	1.00389092	-1.13050703
H	-9.54778324	1.86850276	-1.28416705
H	-8.67907719	1.84656106	0.26521110
O	1.46241719	1.12548442	1.58158908
N	1.43351528	-0.83426798	0.20989733
C	1.85064157	-0.28252283	-1.03188640
C	1.71661662	-2.14424982	0.60611778
O	1.43935408	0.82459676	-1.40272386
C	2.78764548	-1.11183232	-1.89133072

O	1.15600770	-2.66384194	1.59310388
C	2.71280690	-2.94741887	-0.21382862
H	2.14178822	-3.63044612	-0.86069598
H	3.25945196	-3.57744053	0.49429627
C	3.64136483	-2.07354849	-1.06099024
H	3.38765709	-0.40537932	-2.47098647
H	2.17816359	-1.67764560	-2.61276034
H	4.26767057	-2.69455321	-1.71031968
H	4.31729128	-1.50437694	-0.40962993
C	-2.15911043	-4.08621559	4.54393362
C	-1.22726441	-2.97034787	4.94555059
C	-0.94567447	-2.68801774	6.29258822
C	-0.07238160	-1.65156922	6.62345223
C	0.51165448	-0.89387577	5.60378743
C	1.42305158	0.24206350	5.80742607
N	1.80494881	0.85570987	4.65085526
C	2.62626265	1.92577715	4.68200551
C	3.13050851	2.45209188	5.87845571
C	4.06155489	3.63891793	5.87143953
C	2.73969998	1.81878814	7.07212371
C	1.88652398	0.71494778	7.04059242
N	0.23870011	-1.16680069	4.28994504
C	-0.60019858	-2.17726477	3.97480190
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H	-2.36042986	-4.06674368	3.46947523
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H	-1.41052676	-3.27534927	7.07812400
H	0.14225402	-1.43200693	7.66244227
H	2.86583817	2.35823996	3.71738037
H	5.09919794	3.32889068	6.05172532
H	3.79585120	4.35948885	6.65271853
H	4.03521055	4.15808703	4.90895947
H	3.10124935	2.19350036	8.02459626
H	1.58580202	0.23424375	7.96358985
H	-0.73692029	-2.35365702	2.91798320
Ni	1.05222348	0.06345360	3.03681690
H	-1.06405111	-1.66490273	-0.03850176

TS-1G-3G

Total free energy (Ha) = -3666.077584

Potential energy (Ha) = -3666.608631

77

C	-2.90160830	0.75973476	2.12498543
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H	-4.95822904	0.25003772	1.63326405

C	-4.33157719	2.10591445	0.75949573
S	-5.98959357	2.37973607	-0.04403350
C	-3.35137781	3.08190942	0.59821123
H	-3.55506940	3.97729056	0.02273989
C	-2.11835338	2.87837500	1.21590156
H	-1.33016726	3.61707613	1.12687256
C	-1.88169713	1.71072199	1.97144046
C	-0.58274865	1.54791050	2.64585342
O	-6.98378535	1.22543246	0.53848820
O	-6.38947977	3.94990572	0.11318610
N	-5.60443328	2.15288782	-1.78387155
C	-5.14211895	0.81638693	-2.19498331
C	-6.18749269	3.12627805	-2.72594323
H	-6.26082853	4.07496451	-2.18395790
C	-7.55256269	2.78350874	-3.35614000
H	-5.43411414	3.25599566	-3.51570843
C	-6.18776805	-0.31417619	-2.29575240
H	-4.34657577	0.50370670	-1.50404543
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H	-7.46309891	1.88127865	-3.97654944
H	-7.79222205	3.60432734	-4.04887990
H	-6.68038228	-0.42522653	-1.32371330
C	-5.52797552	-1.63661631	-2.71873700

H	-6.96649258	-0.03935526	-3.01675747
H	-4.74936116	-1.93782869	-2.00624373
H	-5.05980847	-1.55385205	-3.70853233
H	-6.26567601	-2.44489387	-2.76651913
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N	0.47415027	0.30033940	1.11881925
C	1.68556671	0.83090856	0.71063304
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H	-0.12540840	-1.93545294	-1.28914486
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C	-1.36970765	-4.15870638	3.55951244
C	-0.47081658	-3.18215555	4.27614443

C	0.30563044	-3.53975861	5.38874899
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C	1.18549164	-1.29531849	5.49224058
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N	2.02583788	0.90892616	5.20306491
C	2.84037615	1.95000602	5.46631379
C	3.76779270	1.93099376	6.51696342
C	4.67643649	3.10738888	6.77076793
C	3.81795731	0.76801634	7.30615573
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C	-0.39092960	-1.85340273	3.82764039
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H	3.02987022	-1.21071435	7.63296038
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Ni	0.60050233	0.88146844	3.87698027
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2G

Total free energy (Ha) = -3666.107797

Potential energy (Ha) = -3666.637331

77

C	0.20812910	-0.79823517	0.41572062
C	-1.19413712	-0.57169496	0.24832635
H	-1.86535995	-1.40439652	0.06772774
C	-1.70280390	0.69249976	0.37334718
S	-3.53490061	0.86809416	0.45884925
C	-0.88388719	1.84524229	0.56589736
H	-1.33390973	2.82832173	0.63139859
C	0.47333307	1.67831223	0.66334230
H	1.13066675	2.53343182	0.77740663
C	1.08612688	0.36741578	0.58651379
C	2.51522012	0.24807397	0.63666484
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N	-3.97169178	1.69253747	-1.07267662

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H	-6.97989592	3.41248236	-1.14416401
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C	-4.13285282	-0.86428558	-4.01356266
H	-5.63326664	0.21904503	-2.88391158
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H	-4.09259865	-0.16306094	-4.85732326
H	-4.80001094	-1.68623315	-4.29584950
H	-6.49487131	0.52829323	-0.14559829
H	-8.06956536	1.33280486	-0.27888333
H	-6.86008499	1.91067486	0.88724561
O	3.33763990	1.12119875	1.00845227
N	3.10025033	-1.06304864	0.16613412
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C	3.23093138	-2.11647929	1.06671771

O	3.35084250	-0.12361320	-1.92400671
C	4.34572290	-2.30642663	-1.61272036
O	2.66244423	-2.07285946	2.18231377
C	4.03879951	-3.32733280	0.64795614
H	3.33204669	-4.09471056	0.29606461
H	4.50522020	-3.72615150	1.55339611
C	5.05974365	-3.00673730	-0.44959416
H	5.03702057	-1.98229215	-2.39520206
H	3.63158994	-2.99776593	-2.08561856
H	5.54848965	-3.92301579	-0.79602462
H	5.84573783	-2.35337944	-0.05017294
C	-4.18821637	-2.52862185	3.68320692
C	-2.88053317	-1.95222662	4.16519618
C	-2.67139429	-1.52316225	5.48418650
C	-1.45569237	-0.93778911	5.84361529
C	-0.45407821	-0.77004316	4.88229831
C	0.82294020	-0.08053086	5.11814236
N	1.54415198	0.18111088	3.98953232
C	2.71711786	0.84391980	4.07200114
C	3.24940020	1.28552715	5.29109084
C	4.56299118	2.02652892	5.33359180
C	2.51473702	1.00332296	6.45568105
C	1.30149950	0.32083310	6.37149011
N	-0.64558466	-1.20294948	3.59529511

C	-1.81828746	-1.78606125	3.26564686
H	-4.08982913	-3.59243248	3.43105432
H	-4.52028069	-2.00351743	2.77940536
H	-4.96743107	-2.43633192	4.44531804
H	-3.46395975	-1.62345564	6.21840158
H	-1.30633526	-0.58157485	6.85568067
H	3.22411170	1.03410931	3.12932524
H	5.33766026	1.43254274	5.83553225
H	4.47094259	2.97146252	5.88224460
H	4.91886211	2.25457886	4.32505940
H	2.89113388	1.31829208	7.42418907
H	0.73897882	0.10021837	7.27075501
H	-1.92578640	-2.09183659	2.23565495
Ni	0.76571993	-0.60492711	2.34833368
H	0.61520626	-1.73063974	0.03312826

TS-2G-3G

Total free energy (Ha) = -3666.074749

Potential energy (Ha) = -3666.597717

77

C -0.571334 -0.586500 0.676057

C -1.914917 -0.236938 0.486526

H -2.693659 -0.984618 0.389022

C -2.240308 1.108935 0.395146

S -4.018235 1.570837 0.116086

C -1.295034 2.130489 0.509092

H -1.597219 3.168445 0.430484

C 0.032328 1.778737 0.728895

H 0.800109 2.537106 0.832920

C 0.412691 0.418662 0.811038

C 1.793154 0.107978 1.290146

O -4.877268 0.186723 0.221733

O -4.398471 2.827193 1.079830

N -3.976250 2.240875 -1.547317

C -3.550283 1.331118 -2.624031

C -4.750529 3.471410 -1.796889

H -4.740596 4.039674 -0.861007

C -6.202698 3.315614 -2.290574

H -4.164558 4.039341 -2.533386

C -4.557733 0.266281 -3.105840

H -2.626438 0.830804 -2.301994

H -3.267194 1.986939 -3.459330

C -7.131767 2.609434 -1.291219

H -6.216113 2.794062 -3.256798

H -6.577328 4.331577 -2.487220

H -4.854091 -0.352235 -2.251352

C -3.948475 -0.606923 -4.216056

H -5.467911 0.753647 -3.474636

H -3.045998 -1.122518 -3.865081

H -3.666966 -0.005961 -5.090672

H -4.660180 -1.369344 -4.551257

H -6.811669 1.579418 -1.099715

H -8.159855 2.578101 -1.670450

H -7.138064 3.131366 -0.327360

O 2.789974 0.860628 1.216108

N 2.225594 -1.686073 0.558556

C 2.214047 -1.851794 -0.829767

C 3.025135 -2.411434 1.393481

O 1.401025 -1.236727 -1.548291

C 3.207628 -2.839365 -1.439931

O 2.836789 -2.336093 2.647623

C 4.115621 -3.314032 0.845304

H 3.751119 -4.351111 0.898977

H 4.970746 -3.249072 1.525329

C 4.486157 -2.951443 -0.598490

H 3.406778 -2.501427 -2.460639

H 2.716916 -3.821760 -1.516976

H 5.166645 -3.699070 -1.020742

H 5.014928 -1.989551 -0.611486

C -2.374100 -4.742961 4.653483

C -1.484598 -3.557221 4.936029

C -1.344046 -3.012562 6.221975

C -0.507614 -1.916142 6.434914

C 0.188715 -1.357334 5.356651

C 1.102998 -0.206845 5.452395

N 1.613680 0.234626 4.264442

C 2.504141 1.249400 4.242675

C 2.919084 1.911805 5.405783

C 3.915235 3.042306 5.333875

C 2.378579 1.473748 6.627192

C 1.478076 0.409254 6.651328

N 0.049053 -1.882731 4.102435

C -0.755407 -2.946326 3.906341

H -1.794061 -5.596495 4.281430

H -3.126690 -4.504328 3.892613

H -2.901490 -5.065760 5.555516

H -1.890916 -3.445389 7.053259

H -0.408976 -1.499037 7.429372

H 2.893649 1.502501 3.260159

H 4.841100 2.788716 5.865306

H 3.516556 3.955602 5.791915

H 4.177728 3.271445 4.297453

H 2.670289 1.956138 7.554871

H 1.079188 0.054938 7.593030

H -0.814297 -3.314937 2.888484

Ni 1.104763 -0.885052 2.732185

H -0.273329 -1.625354 0.612159

3G

Total free energy (Ha) = -3666.134222

Potential energy (Ha) = -3666.662261

77

C	-2.47111789	0.45218083	1.50564384
C	-3.64372052	0.01582017	0.87372162
H	-3.70876163	-0.95453032	0.39533236
C	-4.74480243	0.86307259	0.87425231
S	-6.31356143	0.29378995	0.04560744
C	-4.74575526	2.11962820	1.47804653
H	-5.63966858	2.73297399	1.46965177
C	-3.57123946	2.54565404	2.09599790
H	-3.50648549	3.51722469	2.57433423
C	-2.42960207	1.71691488	2.11312842
C	-1.18993567	2.20404232	2.83572169
O	-6.10653061	-1.27868665	-0.33132908

O	-7.57658036	0.75188445	0.96528917
N	-6.36451201	1.34811497	-1.40643304
C	-5.27121560	1.18275557	-2.37761992
C	-7.65820747	1.97249730	-1.73944502
H	-8.17983471	2.12925326	-0.78911253
C	-8.58357384	1.21714560	-2.71348704
H	-7.41144999	2.96299578	-2.14810688
C	-5.31980095	-0.03585644	-3.32368635
H	-4.32424075	1.15744910	-1.82043301
H	-5.25811602	2.11453691	-2.96088802
C	-9.05800270	-0.14870180	-2.19518819
H	-8.09074014	1.10363561	-3.68833932
H	-9.45444844	1.86708631	-2.88780069
H	-5.40627580	-0.94553801	-2.71971088
C	-4.06002423	-0.09444173	-4.20261208
H	-6.21412267	0.01546722	-3.95573362
H	-3.15349941	-0.17964124	-3.58981301
H	-3.95968886	0.80649538	-4.82214689
H	-4.08856642	-0.95853149	-4.87483524
H	-8.21997488	-0.83794617	-2.04363172
H	-9.75079821	-0.61380404	-2.90572195
H	-9.57195082	-0.04593240	-1.23261641
O	-1.16315705	3.38457359	3.23707076
N	1.14157731	1.73818691	1.70162190

C	1.91309238	2.86386490	1.97127261
C	0.97178197	1.19791081	0.44470800
O	2.14852982	3.19341517	3.15579522
C	2.44918455	3.67794487	0.80325756
O	0.34065310	0.12120088	0.28202063
C	1.54864547	1.93218721	-0.76199618
H	0.74983778	2.57219069	-1.16731611
H	1.77198715	1.18368389	-1.52741093
C	2.77105888	2.79087431	-0.40839054
H	3.32155289	4.23414652	1.15594781
H	1.67934773	4.41630475	0.53164281
H	3.07240058	3.40243020	-1.26610223
H	3.62319160	2.13851405	-0.17043176
C	-3.67253200	0.58261690	7.05754678
C	-2.32653285	0.13195890	6.54701224
C	-1.56151537	-0.83773031	7.21391444
C	-0.32390039	-1.22099220	6.70107917
C	0.14847742	-0.64194020	5.51850671
C	1.43872042	-0.96040337	4.89354635
N	1.69619554	-0.24958346	3.75900021
C	2.84214453	-0.44858306	3.08592665
C	3.81575842	-1.37221471	3.49837242
C	5.08147843	-1.56006530	2.70054294
C	3.55232561	-2.09822396	4.66825966

C	2.36196205	-1.89525240	5.37018156
N	-0.59641076	0.29893973	4.85686994
C	-1.79223356	0.67090473	5.37014686
H	-4.39438034	-0.24333650	7.05534416
H	-4.08405696	1.38496294	6.43893195
H	-3.60215293	0.95356255	8.08673968
H	-1.93102154	-1.28560684	8.13077357
H	0.27028466	-1.96264119	7.21962560
H	2.96700346	0.15491328	2.19711697
H	4.86781749	-1.98985969	1.71404462
H	5.77811409	-2.22917113	3.21361752
H	5.59105399	-0.60411640	2.53471637
H	4.27747302	-2.81982995	5.03056322
H	2.16467817	-2.46021645	6.27272035
H	-2.33592972	1.42564407	4.82238451
Ni	0.24636084	1.01890007	3.24529611
H	-1.57532355	-0.15879766	1.48103551

1P

Total free energy (Ha) = -3779.22929

Potential energy (Ha) = -3779.75315

78

C	-1.58126805	-0.51285166	0.33471241
C	-2.94595234	-0.29993025	0.13132666
H	-3.59193970	-1.07242861	-0.27035084
C	-3.48087939	0.93885477	0.46968288
S	-5.29803846	1.21312702	0.25059487
C	-2.70634827	1.96741552	1.00567999
H	-3.15904599	2.91916152	1.25944461
C	-1.34853424	1.74090124	1.21192107
H	-0.71226629	2.51603561	1.62094958
C	-0.76457847	0.49517906	0.88942957
C	0.65880317	0.24522890	1.21392106
O	-5.94093456	-0.22613554	-0.17621086
O	-5.88187871	1.99769114	1.55311313
N	-5.36138379	2.40416501	-1.09283527
C	-4.82763083	1.95940997	-2.38918233
C	-6.28710178	3.53995555	-0.94443621
H	-6.34689879	3.75226353	0.12818523
C	-7.70900041	3.37845716	-1.51604739
H	-5.78636318	4.39417146	-1.42228251
C	-5.69901226	1.01096280	-3.24011132
H	-3.85604643	1.47951270	-2.20557794
H	-4.61198284	2.88028031	-2.95002749
C	-8.52860732	2.26209059	-0.85027214
H	-7.65965438	3.21915713	-2.60145434

H	-8.21941218	4.34340399	-1.37421840
H	-5.94247490	0.12756347	-2.63962443
C	-4.96845720	0.59995450	-4.52908331
H	-6.64896848	1.49789618	-3.49127400
H	-4.02172315	0.09247809	-4.30343439
H	-4.73624029	1.47177479	-5.15507269
H	-5.57920833	-0.08582358	-5.12658638
H	-8.06307467	1.27998748	-0.98913548
H	-9.54044950	2.21849540	-1.27018998
H	-8.61190553	2.43054740	0.22947663
O	1.43404377	1.27176156	1.69473426
N	1.34002931	-0.68681912	0.32301442
C	1.66820447	-0.35630773	-1.02335931
C	1.93284006	-1.90428778	0.70511601
O	1.28982594	0.65125553	-1.62848273
C	2.52574580	-1.46786655	-1.52050558
O	1.82401452	-2.45897371	1.81163477
C	2.68485070	-2.39552114	-0.48256168
C	-1.96614666	-4.23853179	4.32187638
C	-1.07917105	-3.11681522	4.80057393
C	-0.75257850	-2.95615292	6.15811025
C	0.06898766	-1.90386524	6.56219562
C	0.56146999	-1.00989672	5.60602673
C	1.42601869	0.14677448	5.88576917

N	1.76498473	0.86268674	4.77514739
C	2.54709779	1.95731742	4.87871069
C	3.04702569	2.41123606	6.10595239
C	3.91795091	3.64038088	6.18185093
C	2.69996073	1.67295073	7.25220515
C	1.88990043	0.54185694	7.14594823
N	0.24636870	-1.16576169	4.28329250
C	-0.54595919	-2.18824389	3.89773437
H	-1.53445780	-5.21697142	4.56551702
H	-2.10904549	-4.19669702	3.23858812
H	-2.95593709	-4.19085054	4.79166471
H	-1.14200026	-3.65184633	6.89461651
H	0.32062935	-1.78184517	7.60885039
H	2.76183608	2.46766511	3.94696598
H	4.90963265	3.40129439	6.58533116
H	3.47549606	4.40205469	6.83529692
H	4.05819273	4.08797894	5.19395417
H	3.06250563	1.98628172	8.22626346
H	1.62354764	-0.02090255	8.03245037
H	-0.74412351	-2.25467974	2.83740252
Ni	1.01791792	0.16166852	3.12012595
H	-1.14494433	-1.46882655	0.06465911
C	3.11487269	-1.66246243	-2.76318559
C	3.43722846	-3.55068920	-0.65207948

C	4.04018925	-3.75620823	-1.90465965
H	3.55487956	-4.26329483	0.15685051
C	3.88164943	-2.82625938	-2.94443284
H	2.98572332	-0.93855740	-3.56019832
H	4.63764364	-4.64651250	-2.07197469
H	4.35874084	-3.01010889	-3.90148952

TS-1P-3P

Total free energy (Ha) = -3779.149887

Potential energy (Ha) = -3779.661619

78

C -1.800772 0.663470 1.321360

C -3.069041 1.180847 1.052471

H -3.966301 0.577679 1.123750

C -3.164672 2.512938 0.664297

S -4.845187 3.193774 0.244774

C -2.066064 3.361399 0.572763

H -2.193976 4.400063 0.290813

C -0.804732 2.834476 0.853401

H 0.083441 3.451683 0.782376

C -0.665167 1.479200 1.209423

C 0.696239 0.967877 1.512400

O -5.931061 2.064246 0.699495

O -4.958426 4.705742 0.839046

N -4.737067 3.384068 -1.535446

C -4.485653 2.170957 -2.335529

C -5.317155 4.611558 -2.110667

H -5.219548 5.388857 -1.345407

C -6.776751 4.547034 -2.601597

H -4.655298 4.886518 -2.944090

C -5.644071 1.166916 -2.506026

H -3.618786 1.649035 -1.907696

H -4.166314 2.544761 -3.319819

C -7.801888 4.272119 -1.491499

H -6.870132 3.797892 -3.399631

H -6.992795 5.518306 -3.071720

H -5.985237 0.843718 -1.516413

C -5.197826 -0.045292 -3.340592

H -6.497912 1.658287 -2.987800

H -4.352094 -0.560834 -2.868335

H -4.881985 0.255871 -4.348037

H -6.013362 -0.768520 -3.449486

H -7.638919 3.295827 -1.022152

H -8.822419 4.287478 -1.891556

H -7.734512 5.028005 -0.700215

O 1.759427 1.630257 1.377818

N 0.793445 -0.793966 0.499525

C 0.327541 -0.968016 -0.821909

C 2.001918 -1.442615 0.655642

O -0.729507 -0.508331 -1.287644

C 1.336527 -1.825640 -1.535604

O 2.642487 -1.434944 1.742544

C 2.361493 -2.120303 -0.622106

C -2.125079 -4.320591 4.726379

C -1.096431 -3.268374 5.054438

C -0.546768 -3.137455 6.341620

C 0.406171 -2.153707 6.602182

C 0.808988 -1.281223 5.578478

C 1.788538 -0.185631 5.780145

N 2.110383 0.544708 4.679732

C 2.954637 1.591021 4.775962

C 3.553463 1.976417 5.982783

C 4.495324 3.152181 6.046540

C 3.237946 1.210694 7.118957

C 2.358425 0.133575 7.022761

N 0.280199 -1.412014 4.327695

C -0.633785 -2.375857 4.080250

H -1.721885 -5.329720 4.872725

H -2.456709 -4.241694 3.687083

H -3.009238 -4.227107 5.368059

H -0.862516 -3.806493 7.136197

H 0.827620 -2.069213 7.596056

H 3.151773 2.117190 3.848173

H 5.485014 2.849781 6.409812

H 4.121088 3.926251 6.727888

H 4.625500 3.608376 5.061214

H 3.677131 1.461778 8.079752

H 2.118195 -0.439654 7.909560

H -0.993264 -2.433965 3.058864

Ni 1.165329 -0.110064 2.909135

H -1.679991 -0.381291 1.575714

C 1.364647 -2.310020 -2.834982

C 3.445600 -2.909736 -0.979717

C 3.484485 -3.402860 -2.296361

H 4.233981 -3.132488 -0.269160

C 2.461358 -3.107165 -3.209353

H 0.568931 -2.077086 -3.534228

H 4.319007 -4.020344 -2.612660

H 2.519161 -3.499384 -4.219713

2P

Total free energy (Ha) = -3779.208365

Potential energy (Ha) = -3779.73354

78

C	-0.57486335	0.12487979	0.33049724
C	-1.97988920	0.38181444	0.38680055
H	-2.69080413	-0.42427103	0.23816100
C	-2.43333518	1.63893029	0.68205389
S	-4.23589422	1.84405461	1.00983049
C	-1.56612401	2.75961968	0.84582671
H	-1.97922358	3.73861489	1.05680945
C	-0.21347858	2.56785135	0.72916099
H	0.47543835	3.40101333	0.81465083
C	0.34898679	1.25902225	0.45948502
C	1.77109179	1.13052124	0.28004519
O	-4.86466511	0.32953496	1.09798505
O	-4.44683873	2.85044302	2.27321123
N	-4.84059200	2.73603857	-0.42141009
C	-4.65862151	2.08757375	-1.72785634
C	-5.78452604	3.84086298	-0.18441972
H	-5.54010245	4.25132390	0.80091941
C	-7.28966414	3.51215211	-0.24617491
H	-5.53708735	4.60797692	-0.93192538
C	-5.64794548	0.96898699	-2.11558170

H	-3.63594309	1.68636684	-1.76206028
H	-4.69539121	2.90014527	-2.46742763
C	-7.75583460	2.51627172	0.82701192
H	-7.55047273	3.14190060	-1.24649105
H	-7.82764492	4.46446506	-0.12448510
H	-5.64590769	0.20836081	-1.32659208
C	-5.26900768	0.34162641	-3.46728246
H	-6.66655793	1.37149903	-2.16668122
H	-4.26132411	-0.09218779	-3.43334253
H	-5.28311788	1.08606944	-4.27407683
H	-5.96594709	-0.45825141	-3.74053546
H	-7.24818284	1.55022075	0.72905225
H	-8.83547419	2.34088187	0.75257843
H	-7.53907573	2.89656729	1.83202873
O	2.63572018	2.00456384	0.55748591
N	2.26254254	-0.13280073	-0.30472129
C	2.87291560	-0.19121667	-1.59135890
C	2.38996950	-1.35232493	0.37731154
O	2.90251470	0.72328338	-2.41789714
C	3.41382832	-1.57380531	-1.71309993
O	1.94681262	-1.58229355	1.51998519
C	3.11705176	-2.27257983	-0.53352296
C	-4.44665801	-1.75864591	4.18798618
C	-3.04130756	-1.29078808	4.47152935

C	-2.55524536	-1.06050202	5.76691865
C	-1.25950729	-0.57281826	5.95172087
C	-0.45356169	-0.30655626	4.84027298
C	0.88511871	0.30040689	4.90142195
N	1.38966573	0.68881042	3.69341703
C	2.59154277	1.29961068	3.62376177
C	3.37416637	1.55420159	4.75857579
C	4.70613241	2.25177766	4.63545104
C	2.86486598	1.13643982	5.99993927
C	1.61973031	0.51238785	6.07407907
N	-0.91591720	-0.54838934	3.57333962
C	-2.16470444	-1.03336989	3.40789533
H	-4.46282633	-2.80994749	3.87165200
H	-4.88994207	-1.16420611	3.38027707
H	-5.08059522	-1.66848577	5.07490466
H	-3.19518137	-1.23838295	6.62491228
H	-0.89727576	-0.36764939	6.95185239
H	2.91560536	1.60417393	2.63161243
H	5.51959314	1.62941545	5.02832296
H	4.71487919	3.19280126	5.19917032
H	4.93348257	2.48461789	3.59154335
H	3.44091281	1.30122941	6.90540016
H	1.22997566	0.18938611	7.03183570
H	-2.48954394	-1.18265565	2.38907332

Ni	0.28066513	0.13872484	2.15950891
H	-0.25219965	-0.78198038	-0.17388496
C	4.09176946	-2.17848478	-2.76280419
C	3.49081140	-3.59978188	-0.36363907
C	4.18062790	-4.21984647	-1.41959637
H	3.25682150	-4.13350203	0.55072394
C	4.47649902	-3.52068104	-2.60035653
H	4.31421381	-1.63018073	-3.67142343
H	4.48877412	-5.25550533	-1.32210962
H	5.00981416	-4.02529115	-3.3991412

TS-2P-3P

Total free energy (Ha) = -3779.17242

Potential energy (Ha) = -3779.695486

78

C	-1.20544383	0.23738904	0.53804784
C	-2.49515678	0.78542489	0.60853702
H	-3.37574806	0.15482035	0.65340131
C	-2.63813897	2.16441123	0.58935814
S	-4.34852561	2.87919671	0.67167597
C	-1.54824697	3.03668185	0.51592080

H	-1.70259075	4.10940929	0.49567711
C	-0.27085306	2.49406137	0.48078017
H	0.60563186	3.13023851	0.44240467
C	-0.07168448	1.08834198	0.49820749
C	1.32539099	0.63543357	0.75977899
O	-5.36258122	1.62731201	0.93436738
O	-4.35116627	4.14548035	1.69498838
N	-4.53687356	3.58371997	-0.97032214
C	-4.48833926	2.63521541	-2.09603873
C	-5.14960854	4.92087657	-1.06554300
H	-4.86711692	5.45609536	-0.15291958
C	-6.67785402	5.00142816	-1.25302573
H	-4.64358449	5.41520769	-1.90703016
C	-5.73702115	1.76954129	-2.36395850
H	-3.62466227	1.97389794	-1.93976731
H	-4.25176969	3.24425799	-2.98013726
C	-7.48321857	4.41495903	-0.08363567
H	-6.96760540	4.51852409	-2.19560974
H	-6.92279324	6.06805794	-1.36992864
H	-5.98497481	1.21983437	-1.44945208
C	-5.49343822	0.79507042	-3.52799312
H	-6.59500155	2.41250585	-2.59261626
H	-4.66545062	0.11007053	-3.30529120
H	-5.24275368	1.32987813	-4.45354177

H	-6.38363503	0.18775733	-3.72489743
H	-7.30382173	3.34056234	0.03130161
H	-8.55842867	4.56273098	-0.23787713
H	-7.20284444	4.89346670	0.86169757
O	2.35210830	1.35893772	0.61232026
N	1.55448810	-1.03628404	0.45339385
C	1.18361212	-1.67470392	-0.76954734
C	2.83189679	-1.55021313	0.87057840
O	0.13672821	-1.49250525	-1.41016223
C	2.28244009	-2.61076406	-1.13439929
O	3.41332010	-1.25055180	1.91937320
C	3.27312724	-2.53481283	-0.15063816
C	-2.78612434	-4.08192585	4.43477119
C	-1.79218123	-2.96814050	4.64951383
C	-1.47897550	-2.48723067	5.93356558
C	-0.56187650	-1.44979667	6.08844362
C	0.04628937	-0.88510476	4.95939918
C	1.02605452	0.21264328	4.99431046
N	1.42077998	0.66330116	3.76712267
C	2.36125278	1.62522138	3.66064173
C	2.94491103	2.22714810	4.78344691
C	3.99200071	3.30065763	4.62227042
C	2.52288267	1.78460611	6.04941628
C	1.56963818	0.77160669	6.15675855

N	-0.25547325	-1.34961992	3.70822530
C	-1.14324179	-2.36033371	3.56916967
H	-2.50228804	-4.98286099	4.99178978
H	-2.86009671	-4.35090198	3.37702993
H	-3.78744968	-3.79004783	4.77443286
H	-1.95595611	-2.92244378	6.80606057
H	-0.32908624	-1.07749348	7.07846599
H	2.65197835	1.88206960	2.64371488
H	4.93667942	3.00782454	5.09676515
H	3.67257794	4.24245959	5.08561262
H	4.19467926	3.49617092	3.56588505
H	2.94853496	2.22222669	6.94709382
H	1.26440290	0.41629092	7.13366342
H	-1.33566281	-2.68511142	2.55326072
Ni	0.63731031	-0.30030450	2.27971579
H	-1.10175449	-0.82809591	0.39346901
C	2.40247634	-3.46597433	-2.22365160
C	4.42250647	-3.31484448	-0.21624993
C	4.55771167	-4.17900224	-1.31506886
H	5.18444611	-3.25068844	0.55261085
C	3.56250531	-4.25327367	-2.30437009
H	1.62734854	-3.51668449	-2.98028460
H	5.44389459	-4.79891089	-1.40375402
H	3.69426937	-4.92978309	-3.14253645

3P

Total free energy (Ha) = -3779.235963

Potential energy (Ha) = -3779.760606

78

C	-1.20697928	1.99313345	1.97395840
C	-2.33537573	2.61121311	1.42750272
H	-3.33669505	2.37553281	1.76698639
C	-2.14440641	3.52634710	0.40101915
S	-3.65547574	4.23172544	-0.42494866
C	-0.88683047	3.90824242	-0.06310803
H	-0.79417121	4.65291184	-0.84564246
C	0.23160709	3.30876020	0.51660705
H	1.23452652	3.57537343	0.20221117
C	0.07513288	2.32551639	1.51478125
C	1.28787141	1.65332387	2.09630619
O	-4.90611830	3.95953726	0.58683089
O	-3.33454085	5.74780471	-0.92242797
N	-3.74043184	3.23778368	-1.91513078
C	-3.79754104	1.77430987	-1.75258954
C	-4.15773994	3.92190693	-3.15303678

H	-3.82638817	4.96200986	-3.06186461
C	-5.65608108	3.88070480	-3.51074783
H	-3.56837023	3.46111274	-3.95833436
C	-5.11045075	1.15503093	-1.22883672
H	-2.97709947	1.46842717	-1.09042366
H	-3.55733462	1.36852363	-2.74537702
C	-6.56301021	4.59958851	-2.50071846
H	-5.98060868	2.83903410	-3.63795010
H	-5.75790796	4.35357888	-4.49945501
H	-5.38018660	1.64502838	-0.28683040
C	-4.94862719	-0.36039740	-1.01789506
H	-5.92796067	1.35447057	-1.93296959
H	-4.14464389	-0.57769069	-0.30285100
H	-4.70745818	-0.86762208	-1.96268690
H	-5.87273511	-0.80514952	-0.63246694
H	-6.50926284	4.13883092	-1.50842797
H	-7.60844573	4.57356335	-2.82967637
H	-6.26804742	5.64982927	-2.38892614
O	2.39980953	2.21174867	1.98838793
N	0.67086807	-0.76715429	1.23554460
C	-0.54959582	-0.99467691	0.60209762
C	1.73231217	-1.12414293	0.38585981
O	-1.68603252	-0.82846617	1.10403118
C	-0.25586326	-1.51080633	-0.77675029

O	2.93983032	-1.07956573	0.68419256
C	1.13695421	-1.58803206	-0.90873647
C	-1.21175699	-5.00750226	3.73724997
C	-0.55614856	-3.78756456	4.33381789
C	-0.44003828	-3.60869550	5.72203536
C	0.18485615	-2.47172445	6.23518238
C	0.68824519	-1.51103522	5.35134347
C	1.39696352	-0.28506743	5.74031839
N	1.70357813	0.55395346	4.70246408
C	2.45594060	1.65336314	4.93545226
C	2.90152792	2.01301330	6.21503348
C	3.73350370	3.25490883	6.41470108
C	2.54358373	1.17605629	7.28288895
C	1.80122676	0.02009078	7.04345791
N	0.56327817	-1.67422431	4.00408177
C	-0.03482245	-2.77714087	3.51346560
H	-0.62209978	-5.91176112	3.93391609
H	-1.32084427	-4.90912952	2.65373158
H	-2.20910635	-5.16868862	4.16217059
H	-0.84037813	-4.35657436	6.39927425
H	0.26745906	-2.33511806	7.30648471
H	2.71518799	2.23708666	4.06173174
H	4.69588388	3.01679270	6.88336585
H	3.22242463	3.97508018	7.06536595

H	3.93842134	3.75038621	5.46207286
H	2.85919645	1.41674231	8.29311417
H	1.55637131	-0.64739013	7.86024297
H	-0.09506764	-2.83629028	2.43661840
Ni	1.07227806	-0.03989386	2.95630967
H	-1.32596481	1.22218829	2.72511202
C	-1.10268846	-1.89061355	-1.80960451
C	1.73134557	-2.04127742	-2.07839372
C	0.88321784	-2.42102914	-3.13447537
H	2.81063981	-2.09717456	-2.16995034
C	-0.51177867	-2.34722603	-3.00183614
H	-2.18006899	-1.83274821	-1.69910318
H	1.31233657	-2.77678304	-4.06577919
H	-1.14282092	-2.64766985	-3.83236779

4G

Total free energy (Ha) = -4178.552173

Potential energy (Ha) = -4179.179064

92

C	-2.01989749	-0.11871194	0.72033671
C	-2.70447120	0.96197082	0.16389686

H	-3.78225267	1.05242290	0.23494273
C	-1.96875460	1.95982911	-0.47289243
S	-2.86327219	3.46660639	-1.07432703
C	-0.57899675	1.92512196	-0.57600771
H	-0.04111585	2.72122914	-1.07750257
C	0.09771935	0.84565368	-0.01475515
H	1.17748742	0.78087340	-0.06766536
C	-0.61265407	-0.18149951	0.64365108
C	0.15958230	-1.24762524	1.29782665
O	-4.45538118	3.19813566	-0.84012797
O	-2.18028439	4.78601365	-0.39498591
N	-2.39162246	3.53093493	-2.80283768
C	-2.80302143	2.38903705	-3.63953636
C	-2.06449374	4.85797309	-3.36124270
H	-1.59929715	5.42841176	-2.55070703
C	-3.21133076	5.68111122	-3.97947585
H	-1.29059205	4.66774016	-4.11769189
C	-4.28932427	2.28482157	-4.04003822
H	-2.50753644	1.46763638	-3.11856513
H	-2.17283177	2.45110265	-4.53773167
C	-4.31929110	6.06422541	-2.98637363
H	-3.63894152	5.14481507	-4.83743506
H	-2.75492327	6.59412259	-4.39099273
H	-4.89893909	2.25205307	-3.13080908

C	-4.53638641	1.03373050	-4.89979233
H	-4.59188622	3.18187692	-4.59321464
H	-4.26442565	0.11969649	-4.35681653
H	-3.94428817	1.06098944	-5.82380135
H	-5.59167657	0.95228168	-5.18139841
H	-4.82404577	5.18142969	-2.57887213
H	-5.07629085	6.68970096	-3.47348233
H	-3.90848571	6.62319780	-2.13766588
O	1.42553837	-1.10474644	1.59457026
N	-0.38584703	-2.61449185	1.27357418
C	-0.93138016	-3.13421728	0.06399984
C	-0.23631627	-3.37226298	2.43116647
O	-0.83493892	-2.49973951	-0.99441030
C	-1.64477061	-4.46461630	0.15751225
O	0.34643612	-2.87994721	3.43059782
C	-0.80834882	-4.76398400	2.49233311
H	-1.80029455	-4.64742560	2.95276697
H	-0.19350668	-5.34393927	3.18557282
C	-0.93562330	-5.42941532	1.11828712
H	-1.71646976	-4.86147474	-0.85742130
H	-2.66737858	-4.27178771	0.51521039
H	-1.49658485	-6.36559474	1.20205183
H	0.05746720	-5.68291232	0.72557678
C	4.60186411	-2.93346590	6.47370175

C	3.95093616	-1.68829532	5.92520750
C	4.47823572	-0.40713598	6.16067013
C	3.84778817	0.72204990	5.64083252
C	2.67805373	0.57195665	4.88229565
C	1.90058803	1.69224572	4.31688652
N	0.83664523	1.34429449	3.54343074
C	0.00771389	2.29271003	3.07183429
C	0.19522124	3.66512510	3.30948703
C	-0.78706675	4.68459477	2.79084705
C	1.31878836	4.02226171	4.06858018
C	2.16909986	3.03984468	4.57869479
N	2.17946797	-0.66850265	4.64924294
C	2.78716143	-1.76074199	5.14929880
H	5.61466633	-3.06349169	6.07240616
H	4.02488354	-3.82710516	6.21856227
H	4.68673744	-2.88973976	7.56622780
H	5.38166765	-0.29523839	6.75256685
H	4.26271779	1.70462085	5.82640612
H	-0.39666703	5.70045195	2.90573084
H	-1.73304844	4.63057627	3.34564447
H	-1.03342816	4.53605037	1.73329910
H	1.51579360	5.06915684	4.27641120
H	3.01319293	3.32561029	5.19375745
H	2.31543690	-2.70698803	4.91260923

Ni	0.53121218	-0.74381175	3.42822470
H	-2.55735507	-0.88364129	1.27022272
N	-1.14285272	-0.67782866	4.54220080
C	-1.21124261	-0.01472448	5.77547514
C	-2.33052006	-1.35696476	4.31500216
O	-0.30336246	0.66664865	6.29477231
C	-2.56686282	-0.27315134	6.36727645
O	-2.60325493	-2.07193893	3.31478333
C	-3.25436822	-1.09882593	5.47006986
C	-3.14918067	0.15520670	7.55160976
C	-4.55149357	-1.52284373	5.72395418
C	-4.46384948	-0.26807996	7.82108856
H	-2.60697349	0.79370849	8.24083232
C	-5.15439935	-1.09372523	6.92075001
H	-5.07924605	-2.15971072	5.02202789
H	-4.95285311	0.04839252	8.73704969
H	-6.16870255	-1.40387949	7.15187610
H	-0.84016642	1.94361793	2.49680598

TS-4G-5G

Total free energy (Ha) = -4178.488411

Potential energy (Ha) = -4179.112493

92

C -1.596891 0.356527 0.668089

C -2.016882 1.489881 -0.029974

H -3.049262 1.817537 -0.004160

C -1.071411 2.227296 -0.732028

S -1.607026 3.824244 -1.518762

C 0.272144 1.870357 -0.796228

H 0.980362 2.481287 -1.343564

C 0.681748 0.731939 -0.103048

H 1.722054 0.428467 -0.111119

C -0.246913 -0.021250 0.649008

C 0.325809 -1.084608 1.514699

O -3.065818 4.168553 -0.863349

O -0.386557 4.891577 -1.369738

N -1.697600 3.416515 -3.260192

C -2.684287 2.392535 -3.649988

C -1.153500 4.411175 -4.207133

H -0.309852 4.891576 -3.700384

C -2.115207 5.488104 -4.746163

H -0.745647 3.820685 -5.039159

C -4.171947 2.797986 -3.703654

H -2.570378 1.540934 -2.965388

H -2.353184 2.038246 -4.636422

C -2.704793 6.407494 -3.666112

H -2.921289 5.015410 -5.322771

H -1.539504 6.088290 -5.466651

H -4.468135 3.193503 -2.726099

C -5.050829 1.595246 -4.085773

H -4.314161 3.606086 -4.430776

H -4.947392 0.779697 -3.358891

H -4.778823 1.198878 -5.072563

H -6.108477 1.877720 -4.119878

H -3.313903 5.849280 -2.946269

H -3.340779 7.176778 -4.119066

H -1.911300 6.910458 -3.101609

O 1.433459 -1.602356 1.354702

N -1.080896 -2.590050 1.902115

C -2.079867 -3.002608 1.013455

C -0.516212 -3.433869 2.806700

O -2.629182 -2.210221 0.224245

C -2.525741 -4.460152 1.073436

O 0.262676 -2.922719 3.677511

C -0.827415 -4.907103 2.844261

H -1.573344 -5.029374 3.642121

H 0.074942 -5.442758 3.153653

C -1.396144 -5.403004 1.509972

H -2.927345 -4.712594 0.088746

H -3.354393 -4.510858 1.795006

H -1.768092 -6.428029 1.612304

H -0.607844 -5.421252 0.745437

C 4.854473 -2.063287 5.422118

C 3.833878 -0.999904 5.103221

C 4.095905 0.366899 5.294905

C 3.128114 1.321791 4.984828

C 1.887352 0.904851 4.486093

C 0.779663 1.811599 4.133163

N -0.333927 1.221600 3.615582

C -1.416823 1.967030 3.333463

C -1.452153 3.362200 3.478321

C -2.678742 4.147447 3.085405

C -0.292277 3.971301 3.979243

C 0.817802 3.197613 4.317602

N 1.641592 -0.415939 4.303405

C 2.573751 -1.341418 4.594380

H 5.754238 -1.950042 4.804562

H 4.450564 -3.063481 5.241953

H 5.169509 -2.011467 6.471275

H 5.058000 0.683541 5.685910

H 3.340077 2.372735 5.132978

H -2.585363 5.196606 3.380053

H -3.580421 3.742383 3.559531

H -2.838361 4.123448 1.999203

H -0.262411 5.047790 4.110277

H 1.698531 3.672632 4.730143

H 2.282368 -2.367065 4.409699

Ni -0.206700 -0.877376 3.558773

H -2.316241 -0.249737 1.196993

N -1.482820 -1.071797 5.120509

C -1.341827 -0.371060 6.322075

C -2.523765 -1.992452 5.237764

O -0.486316 0.507303 6.566853

C -2.393619 -0.860170 7.275399

O -2.900847 -2.807028 4.362719

C -3.119914 -1.853598 6.609217

C -2.693119 -0.494186 8.580487

C -4.173154 -2.516516 7.223917

C -3.758920 -1.158086 9.214786

H -2.122156 0.275387 9.089001

C -4.487714 -2.154363 8.546294

H -4.730550 -3.285753 6.700161

H -4.022016 -0.898828 10.235200

H -5.305284 -2.651990 9.058968

H -2.286639 1.431866 2.978259

5G

Total free energy (Ha) = -4178.526496

Potential energy (Ha) = -4179.150539

92

C	-1.51695345	0.75140397	0.64255420
C	-1.88733881	1.81344022	-0.19213377
H	-2.92339202	2.11427946	-0.29674534
C	-0.89266533	2.50670400	-0.86936283
S	-1.37895156	3.97298808	-1.91530925
C	0.45916584	2.18982114	-0.76936645
H	1.20340491	2.77120243	-1.30069137
C	0.82150020	1.11449239	0.04090289
H	1.86187095	0.82382083	0.13159228
C	-0.16393704	0.40332351	0.76053814
C	0.31717078	-0.71329622	1.62813852
O	-2.94863807	4.26758568	-1.58866212
O	-0.26416905	5.13862556	-1.69311449
N	-1.11610842	3.35523167	-3.57692852
C	-1.96753350	2.23209454	-4.00590345
C	-0.42530660	4.25246257	-4.52292527
H	0.27271632	4.85165699	-3.92835527

C	-1.29324193	5.18515389	-5.39003173
H	0.17335303	3.59213920	-5.16591656
C	-3.42980687	2.53382305	-4.39339373
H	-1.96183045	1.48137226	-3.20283542
H	-1.43678747	1.77721353	-4.85430290
C	-2.13870118	6.18653929	-4.58842353
H	-1.93656745	4.59148058	-6.05296748
H	-0.60203916	5.73138144	-6.04921202
H	-3.92040930	3.03896821	-3.55447502
C	-4.18106914	1.24091500	-4.75121937
H	-3.45866645	3.22477557	-5.24416317
H	-4.19505836	0.54095813	-3.90583439
H	-3.71546906	0.72690515	-5.60238551
H	-5.22086553	1.45474215	-5.02064675
H	-2.84752655	5.67663536	-3.92675621
H	-2.71330248	6.83372068	-5.26072665
H	-1.50517809	6.82315544	-3.96056349
O	1.26246367	-1.42414236	1.31838438
N	-1.77075196	-2.13083442	2.51995111
C	-3.10848165	-2.05087343	2.22082917
C	-1.09751863	-3.31137482	2.68372665
O	-3.70165947	-0.94055269	2.16268554
C	-3.85289625	-3.35475814	1.98711973
O	0.05982120	-3.20217722	3.20399190

C	-1.70091025	-4.63285473	2.29603050
H	-1.98316884	-5.12442256	3.23564626
H	-0.92839229	-5.24644851	1.82084403
C	-2.93615904	-4.44338252	1.39870823
H	-4.71070006	-3.14120680	1.34377753
H	-4.23453276	-3.67867910	2.96508414
H	-3.48258102	-5.38776642	1.30340965
H	-2.62120549	-4.15265960	0.38703903
C	4.90249515	-1.35577337	4.77109230
C	3.69023433	-0.47361071	4.60840655
C	3.73490043	0.90995538	4.85123176
C	2.58882181	1.69339727	4.71388305
C	1.38586991	1.08627242	4.33667190
C	0.08767105	1.77524135	4.20792688
N	-0.94627935	0.99562965	3.79811181
C	-2.19464449	1.49394866	3.71413848
C	-2.48800748	2.83329237	4.01094333
C	-3.89446842	3.36209262	3.88587750
C	-1.41606768	3.64971016	4.40808238
C	-0.12831472	3.12437603	4.51004085
N	1.35883476	-0.24489447	4.08355040
C	2.45823606	-1.00791419	4.20859090
H	5.77316944	-0.93984514	4.25104202
H	4.71909760	-2.35797548	4.37337870

H	5.17323350	-1.46260031	5.82920406
H	4.66971578	1.37382779	5.15044081
H	2.63299970	2.75751488	4.90781905
H	-4.21512977	3.86351313	4.80652142
H	-4.60209496	2.55528675	3.67568973
H	-3.97055831	4.09353258	3.07134347
H	-1.59045084	4.69502309	4.64335587
H	0.68846863	3.75437453	4.83923892
H	2.33360151	-2.05790921	3.97001706
Ni	-0.42270342	-1.01165782	3.52120444
H	-2.28082760	0.20489683	1.18694152
N	-1.11854285	-1.47478449	5.40465973
C	-0.74214117	-0.78905529	6.56699935
C	-2.00340049	-2.50128121	5.75809372
O	0.03430590	0.18905564	6.64127091
C	-1.43062589	-1.41771444	7.74108561
O	-2.55502180	-3.32840223	4.99698783
C	-2.20352397	-2.46843793	7.24512379
C	-1.39532804	-1.11719867	9.09591059
C	-2.97481810	-3.26269965	8.08248737
C	-2.17166769	-1.91346312	9.95718781
H	-0.79000775	-0.29911800	9.47146095
C	-2.94927946	-2.97049118	9.45815251
H	-3.57236880	-4.07629523	7.68569060

H	-2.17064966	-1.70985168	11.02352279
H	-3.53888696	-3.56905696	10.14558494
H	-2.95936479	0.79763125	3.38345353

4P

Total free energy (Ha) = -4291.654334

Potential energy (Ha) = -4292.272825

93

C	-2.01055931	-0.00443097	0.58180706
C	-2.65577415	1.10396357	0.03174867
H	-3.73195920	1.22046002	0.08862444
C	-1.88120173	2.09766582	-0.56394653
S	-2.70935472	3.63461693	-1.18238787
C	-0.49037049	2.03470365	-0.63353743
H	0.07468021	2.83385559	-1.09877326
C	0.14861599	0.93431893	-0.07021248
H	1.22871228	0.85443989	-0.08210430
C	-0.60158903	-0.09094633	0.54842355
C	0.13230281	-1.16303280	1.22634695
O	-4.29038949	3.51498731	-0.80159620
O	-1.85217609	4.91820426	-0.64580525

N	-2.40415348	3.55966848	-2.94832588
C	-3.01803441	2.42727501	-3.66495145
C	-1.99081054	4.80854893	-3.61564796
H	-1.40033819	5.37061533	-2.88422229
C	-3.09388877	5.71573373	-4.19337723
H	-1.30738280	4.49504495	-4.41733908
C	-4.53682839	2.47727385	-3.93268971
H	-2.78544594	1.51083678	-3.10472351
H	-2.46745656	2.35544235	-4.61356616
C	-4.05806840	6.28902176	-3.14324035
H	-3.65416045	5.17768036	-4.96933408
H	-2.58087264	6.54171426	-4.70922713
H	-5.05749232	2.61282773	-2.97831245
C	-5.01453850	1.19095693	-4.62613079
H	-4.78031998	3.34675455	-4.55483410
H	-4.80575683	0.30718264	-4.00998250
H	-4.51694180	1.04666179	-5.59423335
H	-6.09418816	1.22164948	-4.80821534
H	-4.61080293	5.49901834	-2.62261696
H	-4.79000946	6.95527644	-3.61428777
H	-3.51447600	6.86100498	-2.38284173
O	1.38180645	-1.02167324	1.60271897
N	-0.39886256	-2.49827162	1.22697695
C	-1.07284568	-3.18979995	0.17661418

C	-0.22853435	-3.32230337	2.34415289
O	-1.34237630	-2.73012291	-0.93603812
C	-1.33817198	-4.55316119	0.71317894
O	0.33098624	-2.94412777	3.39742941
C	-0.82160782	-4.63276979	2.01649062
C	4.57901083	-2.94371612	6.43904737
C	3.91421731	-1.69046083	5.92697777
C	4.40350214	-0.40928567	6.23280982
C	3.76446134	0.72680952	5.73901536
C	2.62370055	0.58384207	4.93675466
C	1.84950615	1.71094712	4.37927686
N	0.80286627	1.37255923	3.57786382
C	-0.00731587	2.32659412	3.08464850
C	0.18314618	3.69738237	3.32927060
C	-0.76884895	4.72638806	2.77309453
C	1.28293051	4.04483538	4.12710410
C	2.11350103	3.05633879	4.65785598
N	2.15786177	-0.65636187	4.64187777
C	2.77463517	-1.75522875	5.11532902
H	5.59320526	-3.05071720	6.03402411
H	4.01246799	-3.83591180	6.15685181
H	4.66364572	-2.93114546	7.53221034
H	5.28421844	-0.30260858	6.85883766
H	4.14952100	1.70927286	5.98083222

H	-0.39753873	5.74035811	2.94977233
H	-1.75360411	4.64728280	3.25159948
H	-0.93017933	4.61291873	1.69475935
H	1.47910950	5.08977696	4.34499831
H	2.94247798	3.33620023	5.29565681
H	2.33008963	-2.70078587	4.82888468
Ni	0.50671476	-0.70817561	3.43370274
H	-2.57822332	-0.76458039	1.10632063
N	-1.15255110	-0.69207520	4.54723115
C	-1.22286017	-0.13814522	5.83023720
C	-2.35741589	-1.30676221	4.23499016
O	-0.30545446	0.47257466	6.41766936
C	-2.59584581	-0.41141656	6.37610539
O	-2.62534532	-1.90624531	3.16358108
C	-3.29163172	-1.13001948	5.39592284
C	-3.18762490	-0.07902965	7.58666321
C	-4.60444970	-1.53673895	5.58905927
C	-4.51820741	-0.48683191	7.79553731
H	-2.64083251	0.47596709	8.34152918
C	-5.21610871	-1.20387856	6.81172851
H	-5.13621112	-2.08975294	4.82210245
H	-5.01369974	-0.24322528	8.73018479
H	-6.24239529	-1.50464385	6.99785677
H	-0.84001168	1.98397553	2.48356720

C	-1.97436818	-5.63391619	0.12056099
C	-0.92864056	-5.79438926	2.76897573
C	-2.08498634	-6.81714529	0.87293689
H	-2.37234109	-5.56302029	-0.88549756
C	-1.57144334	-6.89507426	2.17599897
H	-0.53566105	-5.84652207	3.77797905
H	-2.57700887	-7.68196308	0.44061588
H	-1.67343750	-7.81894427	2.73543002

TS-4P-5P

Total free energy (Ha) = -4291.590720

Potential energy (Ha) = -4292.205375

93

C	-1.89998415	0.32297933	0.82450728
C	-2.44533010	1.38944275	0.10245756
H	-3.50859045	1.59823256	0.11822393
C	-1.58995670	2.20460502	-0.62751891
S	-2.30465509	3.73682708	-1.40858266
C	-0.21493327	1.99209780	-0.69959408
H	0.41859824	2.64775565	-1.28505290
C	0.32005651	0.91086445	-0.00071698

H	1.38412113	0.70644706	-0.03972136
C	-0.51793985	0.08596472	0.78173386
C	0.15816630	-0.94987625	1.60563042
O	-3.92134701	3.63897902	-1.22399611
O	-1.51821762	5.02836144	-0.79351633
N	-1.76131620	3.58157747	-3.11058837
C	-2.32389871	2.43964308	-3.85775655
C	-1.23493556	4.79817553	-3.76093911
H	-0.72646200	5.37136428	-2.97830248
C	-2.22998256	5.71093573	-4.50463838
H	-0.46398003	4.43970667	-4.45743294
C	-3.77679847	2.54596930	-4.36332309
H	-2.23712432	1.55154863	-3.21651188
H	-1.63588262	2.27904987	-4.69980653
C	-3.31155455	6.33118728	-3.60709924
H	-2.69485329	5.16320254	-5.33477414
H	-1.63255272	6.51113393	-4.96677888
H	-4.42808898	2.78337311	-3.51523386
C	-4.22496980	1.23265138	-5.02554853
H	-3.86620839	3.37103357	-5.07927522
H	-4.18521085	0.39707009	-4.31560332
H	-3.58887699	0.97471671	-5.88261314
H	-5.25537633	1.31063597	-5.38816432
H	-3.94014549	5.56456687	-3.14097235

H	-3.96517014	6.99199382	-4.18799289
H	-2.86225257	6.91999674	-2.79937358
O	1.16427109	-1.58105200	1.30284030
N	-1.47558550	-2.34235591	2.13189082
C	-2.40473298	-2.98696226	1.27393937
C	-0.86743341	-3.28918394	2.91482717
O	-3.12863175	-2.44124923	0.42720588
C	-2.34198439	-4.45796559	1.58518722
O	-0.00132908	-2.94907966	3.77599015
C	-1.38819894	-4.64027979	2.59984800
C	4.62371892	-2.36849884	5.53819787
C	3.74369718	-1.22715404	5.09568163
C	4.17347668	0.10723227	5.11884422
C	3.31260262	1.13718543	4.73194037
C	2.01491562	0.82167808	4.31463072
C	0.98683028	1.80816410	3.93185577
N	-0.24148278	1.30010812	3.63158865
C	-1.26878228	2.12867517	3.34926997
C	-1.11973996	3.52207941	3.27279798
C	-2.26972026	4.40840460	2.86919459
C	0.15447953	4.04278733	3.55077004
C	1.20286061	3.19177662	3.89717985
N	1.61403975	-0.47566616	4.27623993
C	2.43308543	-1.46986828	4.65494292

H	4.67150242	-3.15397560	4.77520575
H	4.23299956	-2.82902099	6.45402411
H	5.64402946	-2.02977518	5.74073237
H	5.18038842	0.34250443	5.44866141
H	3.64960371	2.16551983	4.76623193
H	-2.35949614	5.27369839	3.53545722
H	-3.21827634	3.86486336	2.88766413
H	-2.12167221	4.79019502	1.84976721
H	0.32084246	5.11410917	3.50057417
H	2.17698102	3.60250695	4.13171670
H	2.01169488	-2.46474721	4.60708017
Ni	-0.29928280	-0.80851426	3.68266588
H	-2.54280930	-0.31619045	1.41084605
N	-1.38204036	-0.87984635	5.35713010
C	-1.03146892	-1.38199594	6.61193163
C	-2.71004066	-0.48385813	5.35035073
O	0.09608394	-1.79158845	6.95529485
C	-2.25944365	-1.31810020	7.48049536
O	-3.30853748	0.02806059	4.37064565
C	-3.28912376	-0.76701873	6.70467664
C	-2.47026943	-1.69067814	8.80056779
C	-4.56255081	-0.57254256	7.22162928
C	-3.75762697	-1.49977286	9.33580460
H	-1.66817888	-2.11581341	9.39458033

C	-4.78793998	-0.94922412	8.55848325
H	-5.35326746	-0.14650603	6.61328165
H	-3.95840678	-1.78256856	10.36451401
H	-5.77226101	-0.81307420	8.99542562
H	-2.22815301	1.64794056	3.20946885
C	-3.03922111	-5.52931183	1.04791581
C	-1.10288933	-5.89871923	3.11216808
C	-2.75422645	-6.81076267	1.55540690
H	-3.77595316	-5.37971108	0.26639621
C	-1.80275292	-6.99217193	2.57028569
H	-0.37013633	-6.03253996	3.90008245
H	-3.27922312	-7.67322035	1.15765595
H	-1.60503623	-7.99171255	2.94339916

5P

Total free energy (Ha) = -4291.626437

Potential energy (Ha) = -4292.239997

93

C	-1.84080936	0.34491607	0.67065112
C	-2.48884103	1.37851875	-0.01272738
H	-3.56541775	1.49778905	0.02483858

C	-1.71597541	2.29274030	-0.72063528
S	-2.56080576	3.79620849	-1.42206516
C	-0.32944482	2.20997676	-0.81173059
H	0.23562136	2.94269959	-1.37561206
C	0.31007089	1.16676791	-0.14105510
H	1.38888160	1.06679139	-0.18246524
C	-0.44128998	0.25113788	0.62207644
C	0.32297010	-0.71939052	1.45902646
O	-4.15565689	3.60695510	-1.14032357
O	-1.79935116	5.10939361	-0.82175948
N	-2.11588408	3.71711918	-3.15743072
C	-2.64855107	2.56356978	-3.90857134
C	-1.71294111	4.98402358	-3.80238124
H	-1.18681805	5.56670612	-3.03871709
C	-2.81160450	5.84993502	-4.44653665
H	-0.97207530	4.69363932	-4.56016295
C	-4.14613180	2.56456818	-4.27860088
H	-2.42490756	1.65764352	-3.32784782
H	-2.03277123	2.50712039	-4.81699866
C	-3.85571100	6.39195195	-3.45817423
H	-3.30596142	5.29237333	-5.25282726
H	-2.29753800	6.69235200	-4.93358272
H	-4.73528328	2.69256680	-3.36412740
C	-4.53795140	1.25649655	-4.98493285

H	-4.37230729	3.41906151	-4.92716320
H	-4.34314566	0.38678116	-4.34467032
H	-3.97691251	1.11580472	-5.91830485
H	-5.60419181	1.25192214	-5.23471309
H	-4.41409514	5.58528537	-2.97029938
H	-4.57880983	7.03310983	-3.97506177
H	-3.37915709	6.98342060	-2.66821942
O	1.42548178	-1.17064429	1.19308543
N	-0.68908138	-2.69240606	3.18464828
C	-1.17473975	-3.16703823	1.97950696
C	-0.71607181	-3.72374217	4.14198136
O	-1.22966934	-2.49715111	0.91780688
C	-1.59241668	-4.58911229	2.15386044
O	-0.26980448	-3.66528961	5.30206962
C	-1.31974510	-4.93012800	3.48477641
C	4.33066472	-2.92570322	5.68254714
C	3.60253222	-1.70029554	5.19273071
C	4.16075791	-0.41608371	5.28421716
C	3.43647414	0.70021832	4.86655268
C	2.15072191	0.52282579	4.34260274
C	1.24872159	1.61980748	3.94725565
N	0.01318535	1.24037687	3.51866024
C	-0.92782737	2.16311096	3.23415225
C	-0.68115235	3.54185109	3.29382585

C	-1.74522290	4.53566093	2.90324561
C	0.60434425	3.93645845	3.70147615
C	1.56299500	2.98204663	4.04096770
N	1.63062740	-0.72491410	4.22236713
C	2.31679490	-1.80038853	4.64174032
H	5.32965685	-3.00337552	5.23708242
H	3.77829637	-3.83755710	5.43995387
H	4.45676420	-2.89570596	6.77190431
H	5.15661411	-0.28735171	5.69695286
H	3.86529821	1.68983703	4.96352074
H	-1.65478008	5.46254015	3.47862729
H	-2.74819474	4.12981275	3.06815942
H	-1.67042296	4.79793509	1.83866065
H	0.84789493	4.99213607	3.76426140
H	2.54103960	3.29585503	4.38292198
H	1.80726211	-2.75076921	4.56766574
Ni	-0.28928911	-0.78398976	3.47516056
H	-2.41125449	-0.36492804	1.25439300
N	-1.24950211	-0.66167615	5.22888183
C	-1.03824038	-0.77171709	6.60447101
C	-2.58637773	-0.55107773	4.94819518
O	0.05861318	-0.81087042	7.18908608
C	-2.40421561	-0.77757428	7.24898387
O	-3.01853616	-0.39077554	3.76694155

C	-3.35790700	-0.63704069	6.22615121
C	-2.78355937	-0.88002426	8.57841450
C	-4.71748477	-0.59552992	6.50347744
C	-4.16015867	-0.84374939	8.87092071
H	-2.04111475	-0.98756664	9.36188548
C	-5.11154120	-0.70394456	7.85011384
H	-5.44862275	-0.48731352	5.70940079
H	-4.49229581	-0.92589881	9.90116911
H	-6.16681321	-0.67971954	8.10344327
H	-1.89911526	1.77308749	2.95940177
C	-2.14653741	-5.50200823	1.26727610
C	-1.58868216	-6.19929276	3.97639783
C	-2.43003516	-6.78998443	1.75639504
H	-2.35169135	-5.22923368	0.23799361
C	-2.15576111	-7.13267177	3.08931745
H	-1.37113107	-6.45664630	5.00728636
H	-2.86641330	-7.53082891	1.09424004
H	-2.38482954	-8.13396945	3.43997755

6G

Total free energy (Ha) = -4435.849331

Potential energy (Ha) = -4436.505436

94

C	-2.07489733	0.10468615	0.89136131
C	-2.71339449	1.18308227	0.27773577
H	-3.77827051	1.35527562	0.38412956
C	-1.94160372	2.07555510	-0.46308852
S	-2.74949979	3.59813048	-1.13465190
C	-0.56455505	1.92777088	-0.62425643
H	0.00282616	2.63983619	-1.21245157
C	0.06247210	0.85363314	0.00133259
H	1.13167449	0.70514774	-0.08428977
C	-0.67990594	-0.05945857	0.77973917
C	0.06523636	-1.09923290	1.52426472
O	-4.32429859	3.52832498	-0.71279794
O	-1.86653127	4.89489582	-0.67646721
N	-2.47872293	3.44347005	-2.90011592
C	-3.09681324	2.27846016	-3.55735658
C	-2.07997628	4.66196401	-3.63005409
H	-1.47653779	5.25443860	-2.93418176
C	-3.19495021	5.54356871	-4.22404906
H	-1.41247913	4.31358714	-4.43080597
C	-4.62137886	2.30649979	-3.79325142
H	-2.84312189	1.38626952	-2.96791285
H	-2.56645176	2.17437007	-4.51446082

C	-4.13648639	6.16249997	-3.17959915
H	-3.77175247	4.97316523	-4.96423769
H	-2.69214540	6.34553656	-4.78580434
H	-5.12254440	2.47574435	-2.83392385
C	-5.10156044	0.99040356	-4.42697641
H	-4.88593646	3.14887316	-4.44374552
H	-4.87619473	0.13326493	-3.77979399
H	-4.61703399	0.81214400	-5.39589863
H	-6.18406968	1.00630279	-4.59328191
H	-4.68204840	5.39600493	-2.61817684
H	-4.87416237	6.81396481	-3.66227236
H	-3.57569668	6.76059950	-2.45228880
O	1.38792914	-1.06056556	1.60994711
N	-0.53900115	-2.47328731	1.51734942
C	-1.05907584	-3.01505759	0.30503198
C	-0.29585086	-3.25099123	2.64273561
O	-1.02092758	-2.37027326	-0.74984726
C	-1.67814830	-4.39703126	0.38243195
O	0.28692368	-2.74512398	3.63580028
C	-0.77104738	-4.68522772	2.69060189
H	-1.75731166	-4.68416928	3.18024481
H	-0.09149365	-5.22877090	3.35229901
C	-0.87801752	-5.32743194	1.30351324
H	-1.73981234	-4.77383118	-0.64075465

H	-2.70727971	-4.29366934	0.75880418
H	-1.35983770	-6.30762141	1.37397755
H	0.12415996	-5.48937311	0.88680705
C	4.09178321	-2.88545196	6.91794973
C	3.56525122	-1.61139097	6.30581473
C	4.14644096	-0.36028030	6.57667330
C	3.62778552	0.79435011	5.99480436
C	2.52099087	0.70073066	5.13732001
C	1.87962324	1.85584560	4.48227320
N	0.92147924	1.55660766	3.56154108
C	0.24388365	2.55638052	2.96038274
C	0.48420728	3.91659208	3.21312340
C	-0.32441890	4.99260578	2.53267713
C	1.49000226	4.21664948	4.14624248
C	2.18260582	3.19024513	4.78690190
N	1.96409222	-0.51044909	4.87019982
C	2.46876618	-1.62802054	5.43543428
H	5.16320475	-3.00918181	6.72046351
H	3.57339472	-3.76090645	6.51619526
H	3.95866185	-2.88891902	8.00717661
H	5.00622745	-0.29323804	7.23627425
H	4.08768124	1.75356161	6.19730029
H	-0.51580520	2.25751109	2.25221803
H	0.25459953	5.91646031	2.43153757

H	-1.22155705	5.23456860	3.11893896
H	-0.66639898	4.69935627	1.53518784
H	1.72043096	5.25209719	4.37623456
H	2.93780991	3.42918703	5.52560021
H	1.97033773	-2.54994092	5.16407808
Ni	0.47257695	-0.56347569	3.44279490
H	-2.65184899	-0.58650269	1.49466885
C	-1.37161538	-0.33882728	4.22357756
C	-1.33801961	-0.11495681	5.74829943
H	-1.95835204	-1.23684448	3.98119663
H	-1.83325730	0.51577374	3.70995396
H	-0.81882917	-0.95340561	6.23153466
C	-2.72011814	0.02757204	6.36580005
H	-0.74884264	0.78702710	5.96780252
C	-3.35194954	-1.06493615	6.98451729
C	-3.42387443	1.24358677	6.29128354
H	-2.82462361	-2.01226156	7.05675529
C	-4.64477525	-0.95942738	7.51165576
C	-4.71610851	1.37078779	6.81156243
H	-2.95650289	2.10208021	5.81694457
C	-5.30413457	0.26125701	7.41278151
H	-5.25194529	2.31050694	6.75144188
H	-5.12405362	-1.80538870	7.98985543
Cl	-6.99860062	0.41486602	8.09842940

7G

Total free energy (Ha) = -4435.849756

Potential energy (Ha) = -4436.503391

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C	-3.36123049	-1.14614990	2.49252173
C	-4.33042271	-1.78232187	1.70791634
H	-4.58454121	-2.82487982	1.85830893
C	-4.98133983	-1.03611735	0.73223661
S	-6.27097576	-1.86741662	-0.32713538
C	-4.74522161	0.32057421	0.52652999
H	-5.30828974	0.87015509	-0.21915643
C	-3.79132712	0.94786593	1.32751890
H	-3.58634541	2.00633301	1.21664990
C	-3.08153946	0.21627490	2.30230199
C	-2.05996298	0.94887636	3.12889657
O	-6.61786507	-3.28985056	0.38759994
O	-7.44532313	-0.78092082	-0.62877338
N	-5.40902989	-2.09610652	-1.88581120
C	-4.30194565	-3.06529799	-1.88745206
C	-6.11257874	-1.67891271	-3.11313920

H	-6.74174247	-0.82641460	-2.83742712
C	-6.97638705	-2.72883428	-3.83996230
H	-5.32805764	-1.30545641	-3.78662592
C	-4.65638951	-4.56672611	-1.89880770
H	-3.66840665	-2.85484569	-1.01369500
H	-3.69838533	-2.81253424	-2.77089964
C	-8.14460795	-3.26869529	-2.99923075
H	-6.34979509	-3.55697078	-4.19759686
H	-7.37096040	-2.23680581	-4.74208580
H	-5.29128513	-4.78483893	-1.03342623
C	-3.39049153	-5.43773722	-1.86904474
H	-5.24348972	-4.80168376	-2.79426361
H	-2.79932747	-5.25459607	-0.96171949
H	-2.74476632	-5.24175367	-2.73561236
H	-3.64801630	-6.50219938	-1.88240063
H	-7.79053209	-3.81905781	-2.12029525
H	-8.77053817	-3.94713155	-3.59018990
H	-8.77480422	-2.44980645	-2.63595548
O	-2.11003604	2.19005643	3.20111908
N	-0.36372959	-1.68906061	2.57162843
C	0.38237350	-0.97669528	1.69842593
C	-0.65825315	-3.02522612	2.40378278
O	0.61519518	0.24162020	2.02817919
C	0.90331153	-1.55973479	0.40612734

O	-1.25694670	-3.66733177	3.30418254
C	-0.26393648	-3.69295636	1.08804519
H	-1.09477154	-3.55217188	0.37828129
H	-0.17427732	-4.76716924	1.26875783
C	1.02887488	-3.09082815	0.50658997
H	1.85420794	-1.07723374	0.16317801
H	0.19422951	-1.29003604	-0.39150178
H	1.24826778	-3.52274600	-0.47587405
H	1.87367308	-3.34494383	1.16152061
C	1.72444888	-4.24749044	6.54558063
C	1.82866850	-2.77671102	6.22598206
C	2.86380825	-1.97033671	6.72885276
C	2.90962589	-0.61084465	6.42214210
C	1.91563241	-0.05351851	5.60333987
C	1.85103358	1.37215047	5.22487688
N	0.73025586	1.75183560	4.55603851
C	0.58278751	3.03183841	4.16342774
C	1.54439120	4.02213926	4.41874672
C	1.32966115	5.44503605	3.96647506
C	2.70151425	3.62818111	5.10842191
C	2.85882895	2.30286500	5.51269975
N	0.92030765	-0.83666097	5.11179471
C	0.87298061	-2.15209918	5.41230515
H	2.67110754	-4.76635378	6.35427003

H	0.94568280	-4.72619840	5.94520818
H	1.47451419	-4.40583568	7.60256425
H	3.63046205	-2.40579777	7.36262561
H	3.70397072	0.00574892	6.82501129
H	-0.34057970	3.24510607	3.63798922
H	2.17882274	5.80884784	3.37589152
H	1.21254705	6.12260660	4.82200181
H	0.43108247	5.53112517	3.34963908
H	3.47984255	4.35428614	5.32222565
H	3.75920143	2.00125359	6.03314239
H	0.05063796	-2.70934018	4.97388921
Ni	-0.52329149	0.05428966	3.92300438
H	-2.82640342	-1.71384366	3.24283408
C	-1.96067413	-0.07727503	5.38476848
C	-1.80660511	1.08766538	6.37045292
H	-1.66584425	-1.04527658	5.80712646
H	-2.99464015	-0.15949573	5.04198447
H	-0.80799902	1.06380624	6.82304515
C	-2.86121381	1.06231778	7.46577386
H	-1.88308089	2.03324796	5.82082359
C	-2.71773868	0.23459827	8.59337105
C	-4.02090018	1.84911221	7.36085622
H	-1.83039176	-0.38502961	8.69226819
C	-3.69510926	0.19327513	9.59372320

C	-5.01041319	1.82147268	8.35049365
H	-4.15241921	2.49364572	6.49663931
C	-4.82580249	0.99327465	9.45297944
H	-5.90077563	2.43334086	8.26685477
H	-3.57689416	-0.44300987	10.46240363
Cl	-6.10683584	0.95893426	10.76137458

TS-7G-RE

Total free energy (Ha) = -4435.849754

Potential energy (Ha) = -4436.503249

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C	-3.45599128	-1.29421665	2.67616461
C	-4.38485155	-1.91749582	1.83477794
H	-4.67622065	-2.95214623	1.97490866
C	-4.94355126	-1.17350334	0.80136760
S	-6.19571307	-1.99524062	-0.30916698
C	-4.64783059	0.16956038	0.58748886
H	-5.12657419	0.72055780	-0.21366645
C	-3.72879670	0.78299535	1.43942720
H	-3.47647294	1.82973358	1.31854133
C	-3.11733587	0.05433550	2.47991148

C	-2.12828345	0.78475981	3.34853117
O	-6.36128824	-3.52409894	0.23259388
O	-7.49970975	-1.03205952	-0.44427946
N	-5.37504027	-1.91805981	-1.90612719
C	-4.12436520	-2.67862786	-2.04436192
C	-6.19322287	-1.49914483	-3.05962693
H	-6.93199242	-0.78923892	-2.67354912
C	-6.91149485	-2.59777029	-3.86757635
H	-5.50843833	-0.94104372	-3.71365403
C	-4.21779275	-4.21103656	-2.20387225
H	-3.49569420	-2.44973729	-1.17141916
H	-3.61411954	-2.24032912	-2.91413663
C	-7.95400355	-3.39203000	-3.06562607
H	-6.17476710	-3.27967582	-4.31260929
H	-7.40501715	-2.09303452	-4.71191207
H	-4.74328699	-4.62580422	-1.33722434
C	-2.81980987	-4.83579866	-2.33959788
H	-4.81729361	-4.45751471	-3.08778047
H	-2.20907760	-4.64456826	-1.44711904
H	-2.28187889	-4.42893759	-3.20591320
H	-2.88534221	-5.92152222	-2.46699163
H	-7.49984310	-3.93123349	-2.22658293
H	-8.45472321	-4.12812741	-3.70502503
H	-8.71712179	-2.72529317	-2.64896022

O	-2.17134278	2.03338816	3.40319967
N	-0.44010258	-1.80408512	2.72981532
C	0.22135539	-1.21491170	1.70083354
C	-0.79203246	-3.13397084	2.74639149
O	0.53480709	0.01308208	1.87010676
C	0.54292879	-1.95469208	0.42215301
O	-1.30484648	-3.65193159	3.77335999
C	-0.58471744	-3.95329419	1.47788053
H	-1.49954360	-3.85680866	0.87232972
H	-0.50037102	-5.00479564	1.76422351
C	0.63225904	-3.47170004	0.66709224
H	1.46678086	-1.54499217	0.00331716
H	-0.25831691	-1.73478335	-0.30030420
H	0.69626661	-4.00937480	-0.28535395
H	1.55261611	-3.69758493	1.22258711
C	1.86638115	-4.16131943	6.87765855
C	1.94072114	-2.71655309	6.45041259
C	2.97702346	-1.86421264	6.86746709
C	3.00545297	-0.53350329	6.45153332
C	1.99310643	-0.05288107	5.60819207
C	1.90609182	1.33607505	5.11480977
N	0.76134264	1.65539869	4.45237687
C	0.59394006	2.90027797	3.96562777
C	1.55647588	3.91152936	4.10764999

C	1.31139973	5.29392474	3.55672302
C	2.73861006	3.57852960	4.78649997
C	2.91619258	2.29095911	5.29234520
N	0.99496594	-0.87926117	5.20080954
C	0.96350892	-2.16597415	5.60858809
H	2.75396797	-4.71816104	6.55276577
H	0.98741447	-4.65277137	6.45125725
H	1.80766705	-4.25150194	7.96918853
H	3.75876690	-2.24004434	7.52083913
H	3.80011339	0.11943174	6.79112352
H	-0.35140009	3.07204162	3.46620484
H	2.16398188	5.64476948	2.96390268
H	1.15396438	6.02115540	4.36382857
H	0.42424681	5.31199126	2.91757503
H	3.51914517	4.32223684	4.91493678
H	3.83455270	2.03414608	5.80567184
H	0.13288337	-2.75996874	5.23757679
Ni	-0.47366171	-0.06642341	3.93970185
H	-2.99773737	-1.86390602	3.47481877
C	-2.06878289	-0.07325311	5.34314836
C	-1.81432444	1.04827264	6.35321309
H	-1.73995555	-1.06502607	5.67422936
H	-3.13469514	-0.15253944	5.11503447
H	-0.80164554	0.96085445	6.76134510

C	-2.82396247	1.03832689	7.48958674
H	-1.86611525	2.00881325	5.82507937
C	-2.58030854	0.32013798	8.67263253
C	-4.04651139	1.72113952	7.36373257
H	-1.64141202	-0.21377942	8.79135424
C	-3.52447854	0.27852749	9.70507858
C	-5.00363169	1.69018419	8.38385973
H	-4.25221107	2.28467642	6.45812981
C	-4.72262363	0.96628297	9.53884687
H	-5.94356775	2.21898058	8.28227684
H	-3.33119209	-0.27502441	10.61620341
Cl	-5.96604722	0.91961989	10.88265975

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Total free energy (Ha) = -4435.84774

Potential energy (Ha) = -4436.49873

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C	-2.65041767	-7.72347178	-0.03289069
C	-1.24821428	-7.20273210	0.15291717
C	-0.71964862	-6.90441150	1.41587001
C	0.60231619	-6.47329534	1.53771520

C	1.38768008	-6.33148791	0.38707209
C	2.80163006	-5.91244913	0.40326494
N	3.44262486	-5.94788547	-0.79565956
C	4.74059355	-5.58428272	-0.88195751
C	5.48269178	-5.14718303	0.22329059
C	6.92220021	-4.72336062	0.07089702
C	4.82072477	-5.10893628	1.46191160
C	3.48474114	-5.49317781	1.55495461
N	0.86762696	-6.60351979	-0.84053684
C	-0.40230189	-7.03299254	-0.95547817
H	-3.30941156	-7.40562166	0.78137065
H	-2.65449687	-8.82117052	-0.05688691
H	-3.08005715	-7.37912939	-0.97878228
H	-1.33490773	-7.01802285	2.30311943
H	1.01132019	-6.25978274	2.51746679
H	5.18024772	-5.67718089	-1.86655641
H	7.31197625	-4.99390594	-0.91459997
H	7.56019709	-5.19162403	0.82914272
H	7.02742953	-3.63651806	0.18192285
H	5.35011786	-4.77795165	2.35012811
H	2.97999233	-5.45842992	2.51204896
H	-0.72445484	-7.24821734	-1.96538228
Ni	2.24918288	-6.41794039	-2.45013720
C	1.15545550	-6.62243489	-4.05426363

N	2.85772243	-8.35484265	-2.58588240
C	4.10993609	-8.30941329	-3.11418448
C	2.21040043	-9.53250080	-2.23446561
C	4.91008276	-9.57466892	-3.35958252
C	2.95439726	-10.85293801	-2.43938956
H	5.55693272	-9.74509891	-2.48505054
H	5.57074399	-9.39480313	-4.21255995
C	3.98486267	-10.78220358	-3.57519416
H	4.56649653	-11.70923119	-3.62768142
H	3.46476206	-10.67652713	-4.53676776
H	2.20071285	-11.62567512	-2.61308387
H	3.45658107	-11.10525340	-1.49240776
O	4.60410354	-7.16634883	-3.38896594
O	1.06485912	-9.52885399	-1.73610366
O	-0.03238975	-6.95383302	-3.90503033
C	1.69395550	-6.45907456	-5.45267250
C	0.81958694	-6.70384187	-6.53133147
H	-0.19465305	-7.01942609	-6.31552747
C	1.25192889	-6.53434947	-7.84776320
H	0.60148065	-6.71128594	-8.69666066
C	2.56382873	-6.11859372	-8.05679630
S	3.12024276	-5.83163433	-9.80824338
C	3.45401469	-5.86380032	-7.02057407
H	4.46839865	-5.54505394	-7.22643393

C	3.01127846	-6.04154446	-5.70641418
H	3.69861037	-5.89607003	-4.88372358
N	4.56287135	-7.00395948	-9.93696139
C	5.70194681	-6.40844061	-10.67773242
C	4.12816788	-8.36699691	-10.34608216
H	5.64441010	-5.32244937	-10.55407226
H	5.63287630	-6.62832833	-11.75548869
C	7.03103616	-6.93220063	-10.11016569
C	4.10295531	-9.34728534	-9.16449651
H	4.83202629	-8.71786310	-11.11243891
H	3.14120525	-8.31808831	-10.82776697
H	7.06513052	-6.70316898	-9.03812291
C	8.23872797	-6.31114244	-10.83115601
H	7.06940499	-8.02666441	-10.20066591
H	5.09186039	-9.35515970	-8.68879976
C	3.70935004	-10.76495401	-9.60973040
H	3.39687476	-8.98211796	-8.40822655
H	8.24601474	-5.22014653	-10.72019877
H	8.22232436	-6.53782561	-11.90428118
H	9.17959529	-6.69642257	-10.42295243
H	4.42845916	-11.16954161	-10.33334298
H	2.72050305	-10.76947996	-10.08473518
H	3.67333999	-11.45154217	-8.75687397
O	3.73815622	-4.33074832	-9.92323167

O	1.88921038	-6.28923811	-10.77449601
Cl	0.45067287	2.23352957	-2.62102456
C	0.46238430	0.40742276	-2.77450879
C	0.08239514	-0.36328182	-1.68013144
C	0.09164074	-1.75720461	-1.80784404
C	0.47481260	-2.37869261	-3.00885054
C	0.52325503	-3.89312695	-3.12780772
C	1.92632608	-4.44132418	-2.81414634
C	0.84758539	-1.56129933	-4.09092786
C	0.84448335	-0.16625721	-3.98368629
H	-0.21864937	0.11039025	-0.75341011
H	-0.21064500	-2.36882701	-0.96214197
H	0.21282500	-4.18190323	-4.13782601
H	-0.20768450	-4.33736169	-2.44106711
H	2.64845637	-4.17498374	-3.59585719
H	2.27577639	-4.03316247	-1.85970401
H	1.13947359	-2.01950542	-5.03167754
H	1.12791847	0.45734675	-4.82273772

TS-8G-RE

Total free energy (Ha) = -4435.847047

Potential energy (Ha) = -4436.497876

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C	-2.52190429	-8.24259339	-0.85098281
C	-1.20290796	-7.62443681	-0.46561105
C	-0.75540584	-7.56625995	0.85964498
C	0.49537724	-7.01817805	1.15421446
C	1.29279531	-6.52878615	0.11410590
C	2.64255390	-5.96581727	0.31090428
N	3.34265477	-5.70216349	-0.82408581
C	4.59819000	-5.21110756	-0.74862092
C	5.23451604	-4.93095512	0.46802413
C	6.63380848	-4.36894046	0.50311868
C	4.50644626	-5.19296092	1.64139993
C	3.21484658	-5.71116473	1.56688397
N	0.85059129	-6.57237350	-1.17424462
C	-0.35185130	-7.10235196	-1.45477500
H	-3.14993220	-8.42879152	0.02547272
H	-2.36280220	-9.20069049	-1.36202874
H	-3.07851974	-7.59817959	-1.54061899
H	-1.37759947	-7.95476958	1.65984465
H	0.84259299	-6.98948590	2.17963411
H	5.09810067	-5.07365114	-1.69971138
H	7.08087894	-4.35716048	-0.49515598
H	7.28532386	-4.95900406	1.15834124

H	6.63931901	-3.33878155	0.88157190
H	4.95215690	-4.99317389	2.61114685
H	2.66021713	-5.90758203	2.47585184
H	-0.63120354	-7.09120676	-2.49903198
Ni	2.30226573	-6.05520706	-2.63683116
C	1.20097241	-5.67350970	-4.20661877
N	2.97249318	-7.91681462	-3.06742994
C	4.23571147	-7.66038240	-3.49535910
C	2.41972584	-9.18611657	-3.00125517
C	5.17189442	-8.76794704	-3.93090802
C	3.32028191	-10.37139192	-3.35017913
H	5.81758747	-9.02489162	-3.07671968
H	5.82505302	-8.37161558	-4.71404098
C	4.38710812	-10.00675272	-4.39467239
H	5.06551451	-10.85045422	-4.56309422
H	3.90083750	-9.79008412	-5.35524298
H	2.67405252	-11.18666884	-3.68637308
H	3.80723806	-10.70979787	-2.42218922
O	4.60714681	-6.43624150	-3.51101048
O	1.23575626	-9.37067914	-2.64307438
O	-0.04079458	-5.78366010	-4.08822863
C	1.82329648	-5.75020270	-5.57454161
C	1.04757600	-6.29978609	-6.61338650
H	0.03772665	-6.62485571	-6.39322291

C	1.56856885	-6.41270292	-7.90433767
H	0.98568913	-6.81965812	-8.72277271
C	2.86571003	-5.96286554	-8.12877823
S	3.57455722	-6.12299835	-9.83743048
C	3.65147850	-5.38775433	-7.13639929
H	4.64411068	-5.01748713	-7.36305936
C	3.12275157	-5.28981544	-5.84706025
H	3.72876595	-4.88157873	-5.05016559
N	4.72848987	-7.58143423	-9.63864685
C	6.07219557	-7.31688374	-10.20461530
C	4.07278466	-8.86055101	-10.01479753
H	6.23584296	-6.23502947	-10.18673066
H	6.13288146	-7.64273094	-11.25606050
C	7.14548764	-8.02710553	-9.36318254
C	3.67717599	-9.69349649	-8.78683151
H	4.78100398	-9.42286073	-10.63858460
H	3.19244256	-8.65870129	-10.64132743
H	7.06382535	-7.67165910	-8.32852472
C	8.55814791	-7.77128384	-9.91245833
H	6.94609818	-9.10756655	-9.34237609
H	4.56590612	-9.84623637	-8.16042853
C	3.06594458	-11.04661755	-9.18392906
H	2.96255721	-9.12331052	-8.17964792
H	8.79144367	-6.69971068	-9.91895433

H	8.65860583	-8.14068479	-10.94060691
H	9.31456224	-8.27599530	-9.30133432
H	3.77083295	-11.64336034	-9.77698927
H	2.15656261	-10.91316671	-9.78281941
H	2.79746847	-11.63267573	-8.29802338
O	4.50730306	-4.81870466	-10.11803134
O	2.34441898	-6.50419584	-10.83666808
Cl	-0.21212862	2.52337217	-2.83717621
C	0.07411226	0.72430221	-2.64729615
C	0.84307915	0.27371118	-1.57929575
C	1.05542508	-1.10322763	-1.44101332
C	0.50978585	-2.02161214	-2.35308137
C	0.76670563	-3.51286972	-2.21648614
C	1.88434407	-4.00917287	-3.13758134
C	-0.26511662	-1.52393722	-3.41639306
C	-0.48697311	-0.15158558	-3.57274420
H	1.26489712	0.97707199	-0.87149891
H	1.65207504	-1.46602660	-0.60847562
H	-0.14656445	-4.06991380	-2.46383365
H	1.01345585	-3.74709013	-1.17564733
H	1.80866087	-3.54960937	-4.12706003
H	2.89338649	-3.78418033	-2.76733250
H	-0.70446965	-2.21765828	-4.12781889
H	-1.08640632	0.22520591	-4.39258536

9G

Total free energy (Ha) = -4435.836266

Potential energy (Ha) = -4436.489858

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C	0.73143153	2.03470981	0.89488096
C	0.82554961	3.13977461	0.04023840
H	-0.05110053	3.69492130	-0.27299750
C	2.08600264	3.53284934	-0.39227228
S	2.21379079	5.02770701	-1.49620435
C	3.25895900	2.88357623	-0.01369029
H	4.22199441	3.23949364	-0.36115494
C	3.15069222	1.77589749	0.82662927
H	4.03166373	1.22540348	1.13685358
C	1.88836109	1.34841090	1.29125905
C	1.83280208	0.17598812	2.23828082
O	0.72593746	5.69616683	-1.53853330
O	3.48876858	5.92435855	-1.02683091
N	2.69136062	4.29347689	-3.06172947
C	1.74585569	3.33769755	-3.66113351
C	3.73112621	4.99304751	-3.84000071

H	4.38402498	5.48653597	-3.11254268
C	3.26525503	6.01544323	-4.89495831
H	4.31978315	4.20099760	-4.32391394
C	0.46787498	3.89510268	-4.32196568
H	1.45428212	2.61897213	-2.88248802
H	2.33565269	2.77203946	-4.39647720
C	2.47109886	7.19750879	-4.31956999
H	2.68085239	5.50739646	-5.67378615
H	4.17293373	6.38825189	-5.39334064
H	-0.06348617	4.51569338	-3.59252166
C	-0.43733477	2.75171877	-4.81045161
H	0.73255106	4.54672628	-5.16290160
H	-0.73576117	2.10148441	-3.97796818
H	0.06978581	2.12601394	-5.55671192
H	-1.35091587	3.14411029	-5.26967623
H	1.55166183	6.86434080	-3.82566519
H	2.19303331	7.90129278	-5.11254732
H	3.06218707	7.74106642	-3.57327703
O	2.78397398	-0.62529454	2.24145919
N	-0.89971448	-0.80414725	2.14955670
C	-1.95487371	-0.29541025	1.43241256
C	-0.50653153	-2.11279128	2.11708548
O	-2.28859705	0.91496906	1.52607253
C	-2.72533379	-1.24660345	0.52304438

O	0.41271392	-2.43326766	2.93534115
C	-1.15439434	-3.10828149	1.18498016
H	-1.89112205	-3.68328957	1.76666443
H	-0.39064816	-3.81939704	0.85537824
C	-1.84386692	-2.39817793	0.00727531
H	-3.14468292	-0.65187051	-0.29293559
H	-3.57536734	-1.64782422	1.09579556
H	-2.44420209	-3.10956910	-0.56930544
H	-1.08176820	-1.99660156	-0.67364462
C	4.56006413	-2.18071005	6.33970945
C	3.65453353	-1.00247114	6.08248440
C	3.84162786	0.23358180	6.72977803
C	2.99112927	1.30670520	6.46718875
C	1.93878510	1.14185470	5.55615508
C	0.96997707	2.17929723	5.16834401
N	0.08409881	1.80739324	4.20134879
C	-0.88116936	2.66136431	3.79554893
C	-1.00521167	3.95687821	4.31493649
C	-2.09369467	4.88109194	3.82849450
C	-0.07749454	4.35028385	5.29718157
C	0.90604692	3.46304073	5.72914130
N	1.76147863	-0.05868502	4.94371410
C	2.58859066	-1.09713106	5.18052579
H	5.60865898	-1.92232904	6.15008874

H	4.30188492	-3.02561907	5.69549507
H	4.48952824	-2.51694806	7.38193821
H	4.65965456	0.35450273	7.43304811
H	3.15008833	2.25986268	6.95665494
H	-1.55616596	2.27773678	3.03602234
H	-1.67544966	5.82136577	3.44981483
H	-2.79030418	5.13588107	4.63702939
H	-2.67090415	4.42056841	3.02221291
H	-0.12992524	5.34694435	5.72431847
H	1.60926890	3.76456962	6.49612699
H	2.38448403	-1.99610356	4.61291606
Ni	0.32231554	-0.16727725	3.60214406
H	-0.24169476	1.70538260	1.23665265
C	-1.16289699	-0.68838827	4.94177378
C	-0.90729853	-0.52237490	6.44499127
H	-1.32272621	-1.73970848	4.68216016
H	-2.01291683	-0.08533157	4.60502275
H	-0.05111025	-1.13930568	6.74545943
C	-2.12006116	-0.91853521	7.27422375
H	-0.64772671	0.51840727	6.67699707
C	-2.34366453	-2.26272017	7.62231720
C	-3.06949940	0.03707073	7.67584757
H	-1.62300439	-3.01880476	7.32385957
C	-3.47688298	-2.64836002	8.34630578

C -4.21019146 -0.32830592 8.40038995

H -2.91672557 1.08181342 7.41982372

C -4.39225869 -1.66951285 8.72278099

H -4.93733813 0.41378868 8.70764159

H -3.64159047 -3.68528475 8.61358062

Cl -5.87991122 -2.16217742 9.67198189

TS-9G-10G

Total free energy (Ha) = -4435.790104

Potential energy (Ha) = -4436.443322

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C -1.19864496 0.81749679 0.72282422

C -2.28078573 0.27107991 0.01637611

H -2.17488678 -0.07433837 -1.00628512

C -3.49884246 0.14368287 0.67155765

S -4.93670976 -0.60083336 -0.24350543

C -3.68434116 0.52387041 1.99768474

H -4.64764080 0.39048544 2.47672585

C -2.59316012 1.05891940 2.68700407

H -2.72896273 1.39480276 3.70853224

C -1.33719929 1.20055946 2.06884273

C	-0.35270580	2.65177944	3.04677058
O	-4.31446444	-1.38281700	-1.53209312
O	-5.85978217	-1.39711893	0.83614559
N	-5.89679157	0.83039492	-0.74316818
C	-5.26809758	1.74261889	-1.70926089
C	-7.34640803	0.79762948	-0.48297472
H	-7.48740177	0.20267832	0.42547387
C	-8.25854443	0.24550557	-1.59717631
H	-7.62639366	1.83395409	-0.24643929
C	-5.26241969	1.32339178	-3.19398640
H	-4.23264172	1.91665376	-1.38408512
H	-5.79015312	2.70280807	-1.58884648
C	-7.99424567	-1.22714838	-1.94730956
H	-8.17813215	0.87031894	-2.49673784
H	-9.29343472	0.35907001	-1.24019945
H	-4.79263173	0.33747385	-3.27826704
C	-4.51171747	2.35136804	-4.05632250
H	-6.29241194	1.21973708	-3.55536192
H	-3.46580859	2.44901000	-3.73737725
H	-4.97343523	3.34543522	-3.99152685
H	-4.51032036	2.05326762	-5.11035683
H	-6.98427070	-1.37262242	-2.34683366
H	-8.70768218	-1.58219673	-2.70003468
H	-8.08630799	-1.86112960	-1.05857505

O	-1.03744206	3.31738909	3.80732365
N	1.67036734	1.98292620	1.17906293
C	1.24987922	3.24230741	1.12147393
C	2.75320000	1.57793531	0.38158901
O	0.22317265	3.63874297	1.83411642
C	1.87165796	4.32075101	0.26162047
O	3.06607325	0.37178685	0.30553584
C	3.53569823	2.59796339	-0.44191545
H	3.17845145	2.51581901	-1.48013091
H	4.58090154	2.27588919	-0.44789231
C	3.36664984	4.03655831	0.05838483
H	1.68545293	5.28452495	0.74161541
H	1.34986043	4.33953831	-0.70703973
H	3.80233521	4.74897791	-0.64944810
H	3.89611593	4.16582294	1.01180984
C	-2.03388051	1.46252313	8.16723580
C	-1.39396369	0.56801524	7.13481901
C	-1.20680650	-0.80746977	7.35334967
C	-0.61987029	-1.59991865	6.36933512
C	-0.21829388	-1.01407621	5.15836699
C	0.42989131	-1.75064421	4.06004504
N	0.91909878	-0.99470314	3.03421879
C	1.54705525	-1.60133262	2.00229679
C	1.71272295	-2.99184288	1.91861882

C	2.41206040	-3.60388340	0.73080805
C	1.19712601	-3.76664644	2.96732578
C	0.55859926	-3.14571280	4.03921749
N	-0.39791901	0.31497964	4.94725730
C	-0.96501242	1.08147499	5.90329245
H	-3.08211563	1.18581198	8.33674252
H	-2.01341783	2.50938288	7.85146596
H	-1.51899429	1.39018771	9.13268205
H	-1.51697700	-1.25457388	8.29280014
H	-0.46653848	-2.65635867	6.54988922
H	1.95882363	-0.94587334	1.24346892
H	1.69692150	-4.11160592	0.07035172
H	3.15306581	-4.34915970	1.04210900
H	2.92501521	-2.83868159	0.14181479
H	1.29469599	-4.84763152	2.94723501
H	0.15578600	-3.74498961	4.84579762
H	-1.08331605	2.12880913	5.65090843
Ni	0.55962609	1.02694696	3.12801585
H	-0.24151883	0.91014416	0.22577024
C	2.19228501	1.57038898	4.18606154
H	3.00374697	1.46802737	3.45568592
H	2.28946165	0.77124088	4.93249894
C	2.21042946	2.94923723	4.86695399
H	2.14124571	3.74243796	4.11205195

C	3.46131306	3.16001469	5.70441275
H	1.32429596	3.05681790	5.50517951
C	3.50553136	2.76173967	7.05220205
C	4.62415656	3.71347891	5.14025741
C	4.66979384	2.90073876	7.81600283
H	2.61706648	2.33796107	7.51213744
C	5.79895504	3.86176533	5.88588872
H	4.61185463	4.03377048	4.10194487
C	5.79907993	3.44806945	7.21450575
H	4.69590537	2.59460062	8.85500019
H	6.69041893	4.29082817	5.44430572
Cl	7.33111680	3.63258888	8.20380400

10G

Total free energy (Ha) = -4435.807209

Potential energy (Ha) = -4436.460973

94

C	-1.08928034	-0.02038936	0.94771242
C	-2.20757115	-0.41824677	0.20181662
H	-2.11602534	-0.95945786	-0.73386045
C	-3.46975453	-0.10941170	0.69666148

S	-4.95181156	-0.68554044	-0.26340372
C	-3.66061840	0.56355494	1.89923175
H	-4.66019037	0.78507620	2.25708929
C	-2.52709309	0.95130392	2.62520940
H	-2.67415736	1.49533527	3.55307926
C	-1.22287604	0.66241355	2.17393630
C	-0.13817539	2.88231532	3.33819572
O	-4.37759140	-1.43409848	-1.59726050
O	-5.97988180	-1.48661678	0.71259497
N	-5.77524735	0.86823181	-0.64698326
C	-5.01745547	1.82624605	-1.46754516
C	-7.24582142	0.89065632	-0.54218495
H	-7.50823891	0.19336984	0.26039732
C	-8.06018479	0.55152956	-1.80600203
H	-7.49979549	1.90226459	-0.19465426
C	-4.86797800	1.52922105	-2.97494641
H	-4.01560439	1.92677242	-1.02660477
H	-5.51722458	2.79430881	-1.31914597
C	-7.84764734	-0.87928849	-2.32483626
H	-7.84179812	1.28052817	-2.59785898
H	-9.11990827	0.69477189	-1.54562996
H	-4.42932438	0.53243070	-3.09282656
C	-3.98936311	2.58799108	-3.66069681
H	-5.85466066	1.50084805	-3.45239783

H	-2.98349518	2.61127427	-3.22112054
H	-4.41927877	3.59358435	-3.56177428
H	-3.87955948	2.37622933	-4.72986872
H	-6.80722315	-1.05413143	-2.62013389
H	-8.48391914	-1.07663890	-3.19566067
H	-8.09002247	-1.61550705	-1.54994880
O	-0.82352649	3.50713468	4.12024024
N	1.40379618	2.07219671	1.11261982
C	1.00320238	3.32633244	1.13101117
C	2.07099968	1.57914501	-0.02830207
O	0.30290235	3.81395028	2.14931678
C	1.24119372	4.35655517	0.04918289
O	2.55820513	0.43179645	-0.02418516
C	2.15309546	2.44307945	-1.27635969
H	1.21566355	2.31737938	-1.84005066
H	2.96042406	2.05122595	-1.89878076
C	2.35127992	3.92317215	-0.91527077
H	1.45286739	5.31473631	0.53285457
H	0.28927928	4.48542558	-0.48776775
H	2.34055194	4.54584142	-1.81508496
H	3.33260157	4.05883392	-0.44233668
C	-2.51443342	1.38707285	8.07549297
C	-1.72132477	0.54095826	7.11119648
C	-1.52885302	-0.83630801	7.31113329

C	-0.78631679	-1.57941381	6.39630264
C	-0.23657606	-0.94301987	5.27284808
C	0.58846633	-1.61960995	4.25982818
N	1.05990334	-0.83516879	3.24812346
C	1.86428688	-1.37005827	2.30426624
C	2.23280303	-2.72281520	2.29461240
C	3.13732541	-3.25339164	1.21029349
C	1.73008033	-3.53498516	3.32153831
C	0.91291564	-2.98212095	4.30553482
N	-0.43227510	0.38611524	5.07344841
C	-1.14600104	1.10620334	5.96451800
H	-3.55511958	1.04607688	8.13978825
H	-2.52493455	2.43550707	7.76464658
H	-2.09361189	1.33953648	9.08724512
H	-1.95783337	-1.32435262	8.18081272
H	-0.63865538	-2.63949685	6.55938434
H	2.20910616	-0.69648477	1.52807690
H	2.73180109	-4.17013127	0.76683169
H	4.13206202	-3.49483258	1.60676187
H	3.26500978	-2.51533556	0.41411843
H	1.97583326	-4.59178920	3.35254524
H	0.52946219	-3.60876097	5.10030644
H	-1.25650341	2.15861007	5.73276331
Ni	0.45428099	1.08883548	3.23479325

H	-0.10444956	-0.26377949	0.56242497
C	2.17766832	1.62144690	4.21651103
H	2.89306070	1.61429736	3.38609274
H	2.35553156	0.74576636	4.85009662
C	2.28662836	2.90843407	5.05285081
H	2.18981210	3.78858811	4.40565653
C	3.60629714	2.98209614	5.80378640
H	1.45926524	2.95947230	5.77162955
C	3.71596794	2.51269331	7.12418720
C	4.76283373	3.48288115	5.17992243
C	4.93828984	2.53446258	7.80597954
H	2.83402376	2.12827403	7.62903835
C	5.99401570	3.51382972	5.84354667
H	4.70033514	3.85621952	4.16156700
C	6.05808101	3.03454138	7.14874727
H	5.01518401	2.17554389	8.82538683
H	6.88028608	3.90421029	5.35810423
Cl	7.66473184	3.06698207	8.02953332

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Total free energy (Ha) = -4435.793363

Potential energy (Ha) = -4436.444507

94

C	-1.08994716	0.01183682	0.66160020
C	-2.22586165	-0.41079266	-0.04560199
H	-2.15482374	-0.84091274	-1.03887780
C	-3.46994258	-0.27543889	0.55880878
S	-4.97812861	-0.85647056	-0.35563054
C	-3.62477341	0.24500764	1.83818061
H	-4.60822635	0.32499969	2.28902171
C	-2.47483158	0.65968689	2.52258544
H	-2.61101533	1.06881236	3.52032183
C	-1.18303964	0.56193722	1.95826887
C	-0.87386049	3.16514914	3.09864317
O	-4.46123373	-1.48333626	-1.77194335
O	-5.90617216	-1.76907813	0.62407718
N	-5.88953840	0.67733206	-0.57388948
C	-5.21869145	1.74019338	-1.34037029
C	-7.35175817	0.62070152	-0.39802853
H	-7.54303448	-0.14452173	0.36174011
C	-8.21338703	0.33613005	-1.64445890
H	-7.63271259	1.59163182	0.03424951
C	-5.11592250	1.57627850	-2.87218342
H	-4.20716171	1.86485379	-0.92957701
H	-5.76529410	2.66242336	-1.09609299

C	-7.97976268	-1.05091626	-2.26408667
H	-8.05345471	1.12053646	-2.39629924
H	-9.26407877	0.42681176	-1.32913178
H	-4.60157847	0.63447767	-3.09241521
C	-4.36145679	2.75920420	-3.50116088
H	-6.11845423	1.49888923	-3.30940458
H	-3.34741833	2.84484799	-3.08955545
H	-4.87746293	3.71040097	-3.31504872
H	-4.27059640	2.63608498	-4.58586673
H	-6.95037390	-1.16871510	-2.62064997
H	-8.65322534	-1.21725794	-3.11308725
H	-8.15744659	-1.84168484	-1.52610445
O	-1.46873714	4.01523665	2.57937924
N	1.54605078	2.19746341	1.53141111
C	1.79423079	3.52813833	1.82327454
C	1.98261247	1.66266740	0.32746597
O	1.40362743	4.03917561	2.91082688
C	2.52096080	4.44970844	0.84675050
O	1.93892128	0.42789000	0.09861755
C	2.51640646	2.57637737	-0.76810655
H	1.65821879	3.00048106	-1.31189833
H	3.06896372	1.94642867	-1.46830581
C	3.36844180	3.70708688	-0.18381873
H	3.10432429	5.15271999	1.44830115

H	1.74532390	5.04356492	0.33902507
H	3.71204222	4.38685846	-0.97111186
H	4.26556920	3.28822790	0.29185667
C	-2.35114377	1.81063940	7.69448497
C	-1.63581731	0.84757476	6.78065693
C	-1.58168091	-0.53167384	7.04653906
C	-0.90089345	-1.38034434	6.17984690
C	-0.27452897	-0.85875989	5.03642733
C	0.47993485	-1.66950361	4.07242680
N	1.03307231	-0.98837105	3.03090130
C	1.75375492	-1.65428029	2.10399439
C	1.96793482	-3.03994278	2.16011319
C	2.78983569	-3.72968288	1.10055281
C	1.39030659	-3.74104701	3.22903296
C	0.64460274	-3.05673939	4.18609888
N	-0.33745069	0.47431025	4.77267510
C	-0.99128214	1.29671068	5.62406224
H	-3.41341304	1.55442819	7.78693354
H	-2.28564420	2.83723296	7.32293656
H	-1.92255351	1.79244304	8.70377251
H	-2.06867518	-0.93448822	7.92885353
H	-0.85820777	-2.44099445	6.38930289
H	2.12048850	-1.04878275	1.28491475
H	2.30466245	-4.65046656	0.75804142

H	3.78063051	-4.00586585	1.48488483
H	2.93898687	-3.08076401	0.23328367
H	1.51662531	-4.81624533	3.30803439
H	0.19255846	-3.60123745	5.00532537
H	-0.99045045	2.34554280	5.36317678
Ni	0.53037438	1.07857486	3.03459252
H	-0.11968234	-0.09979146	0.19398240
C	2.25370169	1.37655466	4.25242276
H	2.95206732	1.69666932	3.48054447
H	2.49637382	0.36923236	4.59874379
C	2.10869412	2.38640073	5.39459298
H	1.53274089	3.24689059	5.04816429
C	3.47272450	2.87070044	5.86647801
H	1.57532218	1.93130577	6.23684040
C	4.20989313	2.15914348	6.82824390
C	4.03660861	4.03587549	5.31546410
C	5.47679415	2.59169895	7.23721009
H	3.79066040	1.25889574	7.26941056
C	5.30173334	4.48243279	5.71262042
H	3.47256203	4.59452318	4.57466804
C	5.99977109	3.74892393	6.66788308
H	6.04045651	2.04304090	7.98202463
H	5.73165486	5.38340932	5.29174360
Cl	7.65585390	4.32713511	7.19608623

11G

Total free energy (Ha) = -4322.509538

Potential energy (Ha) = -4323.157644

92

C	-1.00747235	-0.64225052	0.82408781
C	-2.19208578	-0.92731635	0.12843953
H	-2.20538241	-1.55799589	-0.75394839
C	-3.37670705	-0.37282240	0.59896721
S	-4.95505627	-0.76308172	-0.29645978
C	-3.42994958	0.43642228	1.73028811
H	-4.37361185	0.84843509	2.07188998
C	-2.23287818	0.70937720	2.40454512
H	-2.27071295	1.36619079	3.26800499
C	-1.00101857	0.17584286	1.97029746
O	-4.56403086	-1.73920444	-1.54667318
O	-6.09714072	-1.25099073	0.75656066
N	-5.48166468	0.87059711	-0.83579939
C	-4.54593465	1.62040547	-1.68767602
C	-6.92658614	1.15730384	-0.78941891
H	-7.32796789	0.57992156	0.05028594

C	-7.75512556	0.86790076	-2.05634258
H	-7.00747009	2.22148969	-0.52508232
C	-4.37955343	1.17280885	-3.15546674
H	-3.56137199	1.60165854	-1.19926509
H	-4.89068545	2.66386933	-1.64882797
C	-7.81690421	-0.61937081	-2.43763981
H	-7.37335513	1.46099979	-2.89836621
H	-8.77210692	1.24028283	-1.85995677
H	-4.09460542	0.11518086	-3.17268930
C	-3.32025028	2.02471903	-3.87375123
H	-5.33780695	1.25049472	-3.68316803
H	-2.34083778	1.93362094	-3.38598102
H	-3.59398446	3.08820782	-3.87751272
H	-3.20148373	1.70829923	-4.91571458
H	-6.82209220	-1.02600818	-2.65045844
H	-8.44204486	-0.76875380	-3.32581805
H	-8.23939121	-1.21342922	-1.61886946
N	0.57469897	2.47820117	2.12553861
C	-0.07984634	3.64272357	2.45893507
C	1.19293197	2.25152547	0.93513975
O	-0.65194566	3.78204471	3.56729808
C	-0.12538046	4.75197579	1.41262464
O	1.68420907	1.08334999	0.77911295
C	1.24333617	3.30759631	-0.14184170

H	0.42488347	3.09865823	-0.84779635
H	2.17794323	3.19492994	-0.69930871
C	1.08100672	4.71534320	0.45807863
H	-0.20071694	5.70506919	1.94282660
H	-1.05888941	4.62841763	0.84220281
H	0.95927498	5.45683965	-0.33881827
H	1.99203616	4.98641441	1.00823264
C	-1.90287861	2.14224578	7.57096805
C	-1.24709595	1.05189627	6.76112330
C	-1.16523882	-0.27299066	7.22198249
C	-0.53324352	-1.24875310	6.45097578
C	0.01648199	-0.89486817	5.21217461
C	0.71126326	-1.82323277	4.30565970
N	1.17509179	-1.26484436	3.15580062
C	1.85318098	-1.99878784	2.25046478
C	2.10091907	-3.36451340	2.43005120
C	2.86879410	-4.15750320	1.40274095
C	1.60894795	-3.95407962	3.60942162
C	0.92042665	-3.18805391	4.54785559
N	-0.07129396	0.38837496	4.76619012
C	-0.68146455	1.33532606	5.50825896
H	-2.78766000	1.77052314	8.09845954
H	-2.20849452	2.97787191	6.93505131
H	-1.21297095	2.53982445	8.32721656

H	-1.60031546	-0.54017425	8.17979050
H	-0.47545030	-2.26932735	6.80892075
H	2.19532781	-1.46160339	1.37335368
H	2.33849918	-5.07872075	1.13631642
H	3.85651852	-4.44698838	1.78344354
H	3.02222663	-3.57952927	0.48702911
H	1.76800092	-5.01241144	3.79008165
H	0.54864911	-3.64855882	5.45472119
H	-0.72170668	2.32525688	5.05974286
Ni	0.74689673	0.65054936	2.89114186
H	-0.08000622	-1.05792124	0.44312601
C	2.55916521	1.07249553	3.74866697
H	3.22613876	0.95043648	2.88763734
H	2.73634810	0.26845522	4.47053286
C	2.71105189	2.44607158	4.41552584
H	2.60822295	3.23827879	3.66716190
C	4.05676340	2.57636986	5.11427278
H	1.91162733	2.60260235	5.14998632
C	4.19458921	2.25856389	6.47648432
C	5.20547529	2.97019238	4.40510094
C	5.43651359	2.32499428	7.11847890
H	3.31876511	1.95757237	7.04460741
C	6.45618965	3.04344430	5.02822081
H	5.12226047	3.22241514	3.35177561

C	6.54779263	2.71581327	6.37788914
H	5.53514663	2.08237304	8.16972969
H	7.33697666	3.34961585	4.47687035
Cl	8.18032046	2.80390147	7.20562000

9P

Total free energy (Ha) = -4548.935243

Potential energy (Ha) = -4549.581036

95

C	0.86091187	2.54283839	1.08789712
C	1.19492643	3.67143724	0.32986646
H	0.50208776	4.49306633	0.19045304
C	2.46006808	3.73122048	-0.24075021
S	2.92451289	5.25502886	-1.20749076
C	3.41132522	2.72355673	-0.09586473
H	4.39255509	2.82230490	-0.54571783
C	3.06114863	1.59530791	0.64474620
H	3.75815765	0.77433503	0.77005023
C	1.78788324	1.50152139	1.24655463
C	1.47627646	0.28735894	2.06980352
O	1.70595850	6.32051666	-0.99939951

O	4.44570381	5.67836619	-0.81241214
N	3.01612397	4.61193560	-2.88255564
C	1.76737383	4.07515684	-3.45136497
C	4.14353757	5.07449792	-3.71469146
H	4.97699123	5.26000012	-3.02917223
C	3.91788058	6.31682387	-4.59867475
H	4.41733985	4.21315742	-4.34009220
C	0.68139430	5.07944824	-3.89295359
H	1.33151432	3.38270973	-2.71779227
H	2.08256417	3.45933288	-4.30528761
C	3.62932913	7.60282768	-3.80818489
H	3.11293535	6.12352890	-5.31975694
H	4.83395288	6.44878391	-5.19395501
H	0.42503255	5.71585929	-3.03935522
C	-0.56581733	4.34550448	-4.41147660
H	1.07730284	5.73897956	-4.67382579
H	-0.99594167	3.69841907	-3.63616463
H	-0.32911229	3.71376273	-5.27776076
H	-1.34114536	5.05537865	-4.71889552
H	2.69750387	7.52836001	-3.23626083
H	3.54213151	8.46239485	-4.48269929
H	4.43459208	7.80941986	-3.09384824
O	2.10115980	-0.76995174	1.86970048
N	-1.29891432	-0.06560303	2.18608364

C	-2.23336095	0.79314782	1.63365027
C	-1.49865914	-1.36869560	1.72076863
O	-2.33029115	2.02594778	1.85560794
C	-3.09908349	-0.01244858	0.71086427
O	-0.82634648	-2.35092572	2.09971008
C	-2.64206985	-1.33884224	0.75702950
C	4.02189588	-3.06571839	5.58319618
C	3.33556939	-1.72307184	5.58864299
C	3.76513495	-0.67019150	6.41923826
C	3.11551727	0.56214302	6.38967736
C	2.02095302	0.74460073	5.53324564
C	1.24932823	1.98622107	5.38505960
N	0.25969082	1.93991714	4.44758316
C	-0.54022195	3.01034995	4.24677794
C	-0.38267966	4.20884060	4.95539765
C	-1.28584471	5.38606841	4.68595128
C	0.64980430	4.26466779	5.90979483
C	1.46251148	3.15499706	6.12974841
N	1.60510352	-0.28196821	4.74278175
C	2.23949215	-1.47409114	4.75628543
H	5.09776980	-2.95913790	5.40162966
H	3.61278673	-3.71563489	4.80490740
H	3.90289169	-3.57842636	6.54602692
H	4.61329051	-0.81664617	7.08034397

H	3.46065130	1.37365199	7.01804107
H	-1.31119206	2.88401217	3.49185327
H	-0.71015347	6.25561242	4.34595979
H	-1.82854161	5.68749506	5.59022355
H	-2.02268609	5.14947603	3.91373157
H	0.81366263	5.17414587	6.47942702
H	2.24947068	3.19790222	6.87299657
H	1.86606136	-2.21613287	4.06175567
Ni	0.09097808	0.08933452	3.55043631
H	-0.12547904	2.46627228	1.52768835
C	-1.32786659	-0.50163632	4.92131667
C	-0.96940593	-0.60745785	6.40806110
H	-1.60422580	-1.47563297	4.50159741
H	-2.13245110	0.21920609	4.74611047
H	-0.18910259	-1.36653559	6.55046729
C	-2.17684417	-0.97430371	7.25893832
H	-0.55927668	0.34253565	6.77570438
C	-2.63150752	-2.30405263	7.32178893
C	-2.88754034	0.00532505	7.97257969
H	-2.09922566	-3.07766884	6.77560104
C	-3.75873600	-2.65166400	8.07295187
C	-4.01827193	-0.32242869	8.73044085
H	-2.55379277	1.03867913	7.93926327
C	-4.43307042	-1.64956436	8.76581024

H	-4.55935424	0.43722907	9.28165352
H	-4.10311720	-3.67777852	8.11941866
Cl	-5.90784321	-2.09441563	9.75768565
C	-4.17046655	0.35719952	-0.08882135
C	-3.24137192	-2.33809668	0.00425885
C	-4.78604835	-0.64882637	-0.85712545
H	-4.51911387	1.38381642	-0.11694120
C	-4.32870659	-1.97380733	-0.81217443
H	-2.88272560	-3.36076630	0.04518850
H	-5.62835307	-0.39677129	-1.49341949
H	-4.82208970	-2.72899399	-1.41548277

TS-9P-10P

Total free energy (Ha) = -4548.90147

Potential energy (Ha) = -4549.546401

95

C	-1.22608814	0.73276395	0.66700783
C	-2.26937813	0.26095768	-0.14293204
H	-2.14515432	0.12602390	-1.21169879
C	-3.48353724	-0.04609406	0.45806918
S	-4.88763475	-0.64021523	-0.60969309

C	-3.69985802	0.07112387	1.82725777
H	-4.65813147	-0.19691630	2.25809313
C	-2.64579352	0.53312889	2.62206809
H	-2.80905733	0.64815609	3.68746941
C	-1.40192817	0.86278689	2.05326624
C	-0.50385586	2.28366088	3.16289863
O	-4.23811778	-1.04304625	-2.05105148
O	-5.74848442	-1.73737332	0.23199093
N	-5.92726840	0.82016795	-0.70407803
C	-5.34540906	2.00844645	-1.35127480
C	-7.38142863	0.62045892	-0.55748935
H	-7.51165157	-0.23930436	0.10760206
C	-8.20559655	0.40476048	-1.84266999
H	-7.74638545	1.50909502	-0.02364332
C	-5.22344563	2.00651696	-2.88987064
H	-4.35101857	2.18007661	-0.91707436
H	-5.97135650	2.84998121	-1.02203230
C	-7.82773215	-0.86520589	-2.62103532
H	-8.12546990	1.28730720	-2.49092980
H	-9.26024328	0.34797137	-1.53362418
H	-4.63524965	1.13396058	-3.19427756
C	-4.56312408	3.30196488	-3.38929482
H	-6.21486209	1.89402074	-3.34414083
H	-3.56065345	3.42656813	-2.96024335

H	-5.15367096	4.18596789	-3.11533723
H	-4.45986614	3.29528772	-4.47970773
H	-6.79758017	-0.82111275	-2.99159964
H	-8.48990938	-1.00603722	-3.48310571
H	-7.90459017	-1.75252420	-1.98180939
O	-1.18600628	3.15308050	3.59413813
N	1.75032496	1.39589820	1.51333731
C	1.49655897	2.68604926	1.05965674
C	3.03841914	1.03031091	1.09555818
O	0.44903656	3.33860191	1.30196171
C	2.66325513	3.17699274	0.26242783
O	3.61737804	-0.05122382	1.34691719
C	3.61878513	2.15482090	0.28742449
C	-2.20211532	1.08221092	8.18385303
C	-1.56387305	0.20529736	7.13606280
C	-1.39602553	-1.17830563	7.32202379
C	-0.80749744	-1.95380009	6.32613452
C	-0.38670436	-1.34526350	5.13263117
C	0.24904385	-2.06772131	4.01707841
N	0.78109349	-1.29451860	3.02597245
C	1.36248876	-1.88284501	1.96278667
C	1.46514426	-3.27555712	1.81766142
C	2.13289006	-3.85910356	0.59865793
C	0.92317599	-4.06699832	2.83763368

C	0.31064609	-3.46339491	3.93694711
N	-0.54348773	-0.00919435	4.95443162
C	-1.10813130	0.73998595	5.92440183
H	-3.24797216	0.79863664	8.35501843
H	-2.18753958	2.13408095	7.88451867
H	-1.68114642	0.99784448	9.14494002
H	-1.72008303	-1.64324968	8.24777822
H	-0.66555584	-3.01550969	6.48344950
H	1.80017855	-1.21874046	1.23534319
H	1.44712525	-3.87238905	-0.25868273
H	2.45969624	-4.88806579	0.77610729
H	3.00549607	-3.26368308	0.31143544
H	0.97580130	-5.14899158	2.77312637
H	-0.12393966	-4.07808125	4.71498472
H	-1.19884413	1.79997918	5.71760746
Ni	0.51348269	0.73611982	3.15651230
H	-0.27614848	0.98042269	0.21464423
C	2.88952023	4.36801234	-0.41309031
C	4.83865694	2.28577341	-0.36104131
C	4.12236198	4.51251346	-1.07612188
H	2.14388569	5.15551434	-0.42727331
C	5.08149520	3.48851715	-1.05037680
H	5.57438989	1.48903983	-0.33530800
H	4.33611648	5.42967740	-1.61559519

H	6.02393203	3.62777209	-1.57040749
C	2.08118253	1.16164180	4.36218483
H	2.86716900	0.63081910	3.81858109
H	1.86017901	0.64420790	5.30073748
C	2.42729006	2.63619422	4.60073433
H	2.55315351	3.14980542	3.64168766
C	3.70114191	2.77577316	5.42258021
H	1.60506446	3.14050625	5.12223727
C	3.65025953	3.05490483	6.79851544
C	4.96199369	2.58568526	4.82794729
C	4.81677309	3.14140446	7.56819718
H	2.68763074	3.21312809	7.27683661
C	6.13838313	2.66753358	5.57969866
H	5.02707850	2.36874641	3.76559961
C	6.04232973	2.94290969	6.94124563
H	4.77079183	3.36124292	8.62804200
H	7.10635582	2.52129148	5.11585286
Cl	7.57700975	3.04961711	7.93648645

10P

Total free energy (Ha) = -4548.910891

Potential energy (Ha) = -4549.554807

95

C	-1.07945108	-0.05007853	0.94726202
C	-2.17822810	-0.36812415	0.13707903
H	-2.05826229	-0.78614980	-0.85653397
C	-3.45369890	-0.14476108	0.64286204
S	-4.91874625	-0.57840227	-0.41404634
C	-3.67705313	0.36178764	1.91787572
H	-4.68717640	0.51029134	2.28393467
C	-2.56301043	0.66514059	2.71167742
H	-2.74096910	1.06500321	3.70518018
C	-1.24776161	0.46445448	2.24700179
C	-0.24471236	2.56440681	3.73128931
O	-4.33344755	-1.34282748	-1.73289555
O	-6.04836497	-1.30922227	0.50404638
N	-5.59763801	1.03847472	-0.80692441
C	-4.72707905	1.94959461	-1.56651786
C	-7.06257741	1.18736591	-0.75087086
H	-7.41376917	0.51476642	0.03871951
C	-7.86026177	0.92257715	-2.04292429
H	-7.23902945	2.21682075	-0.40799383
C	-4.53523613	1.67616042	-3.07287892
H	-3.74275688	1.95489839	-1.07729559
H	-5.15176627	2.95217343	-1.41405247

C	-7.74835161	-0.51831952	-2.56585972
H	-7.55838338	1.63442794	-2.82285023
H	-8.91266488	1.15017421	-1.81464448
H	-4.18028250	0.64766512	-3.19858924
C	-3.53811503	2.66955568	-3.69142696
H	-5.49785174	1.74639960	-3.59392117
H	-2.55528756	2.59738328	-3.20824279
H	-3.88535285	3.70598727	-3.58632089
H	-3.39824707	2.47211714	-4.75986539
H	-6.71854533	-0.77055777	-2.84214306
H	-8.37972161	-0.66176691	-3.45060177
H	-8.06215415	-1.23706309	-1.80024727
O	-0.89682174	3.30567904	4.37313166
N	1.49293874	1.66991506	1.64391126
C	1.15268552	2.98260715	1.44587704
C	2.43174926	1.32243780	0.65048894
O	0.35574546	3.65333209	2.17773802
C	1.86201596	3.54547263	0.26141906
O	2.98071963	0.20973751	0.50832935
C	2.66637600	2.51275016	-0.23105497
C	-2.64183342	0.93655153	8.20933934
C	-1.89850605	0.10636496	7.19322095
C	-1.80875368	-1.29218976	7.29222516
C	-1.10545824	-2.01409758	6.33245541

C	-0.49129342	-1.33936813	5.26477754
C	0.29428923	-2.01026272	4.21814869
N	0.88291386	-1.20379819	3.28964891
C	1.65926968	-1.74901163	2.32857499
C	1.87555214	-3.12993979	2.21313803
C	2.74547472	-3.67161500	1.10672746
C	1.25028984	-3.96103591	3.15305808
C	0.46587666	-3.39996476	4.15800556
N	-0.58365832	0.01136810	5.16191152
C	-1.26206792	0.70700248	6.09981920
H	-3.68488346	0.61114807	8.30155173
H	-2.64441783	1.99444723	7.93178256
H	-2.18541566	0.85200071	9.20335609
H	-2.28592359	-1.81114273	8.11751704
H	-1.03490441	-3.09059765	6.41769332
H	2.13306328	-1.05898668	1.63894145
H	2.15707827	-4.27132978	0.40082271
H	3.53739712	-4.31835773	1.50286120
H	3.21687558	-2.85985562	0.54656507
H	1.37880916	-5.03769554	3.10361262
H	-0.01081903	-4.04252647	4.88656792
H	-1.30352253	1.77963551	5.96739768
Ni	0.43100925	0.78762142	3.37363805
H	-0.08363282	-0.21632997	0.55125702

C	1.83517652	4.79797583	-0.33373700
C	3.47627489	2.69080008	-1.34226398
C	2.65223045	4.99150288	-1.46403082
H	1.20880350	5.59311578	0.05478433
C	3.45906185	3.95649216	-1.95928607
H	4.09678447	1.88515745	-1.71911396
H	2.65805076	5.95613101	-1.96075572
H	4.07819672	4.13481510	-2.83248729
C	2.15279119	1.06033778	4.48027116
H	2.86797281	0.60364225	3.79095066
H	2.00970801	0.41975441	5.35600343
C	2.58356656	2.47965020	4.88033080
H	2.62909193	3.12105663	3.99309230
C	3.94439304	2.46340811	5.56034196
H	1.84569793	2.92458466	5.55926668
C	4.05309825	2.31795683	6.95420793
C	5.12723411	2.54168873	4.80443857
C	5.30139537	2.24813472	7.58294741
H	3.15140835	2.26280132	7.55772692
C	6.38471461	2.47387099	5.41426146
H	5.06573579	2.65886185	3.72628423
C	6.44716273	2.32528732	6.79664853
H	5.38008279	2.13980055	8.65803911
H	7.29263140	2.53837180	4.82705017

Cl	8.08748670	2.23477349	7.60660751

11P

Total free energy (Ha) = -4435.607502

Potential energy (Ha) = -4436.24756

93

C	-1.16412970	-0.59331668	1.04301318
C	-2.34419403	-0.75804316	0.30416433
H	-2.38438730	-1.37368527	-0.58779040
C	-3.49047958	-0.10869003	0.74848673
S	-5.06852263	-0.33753213	-0.20195259
C	-3.51077673	0.68289601	1.89188755
H	-4.42727949	1.16743354	2.21110033
C	-2.32058412	0.82445134	2.61809237
H	-2.33710476	1.45383396	3.50306570
C	-1.13036587	0.18790289	2.21363011
O	-4.77425227	-1.47424434	-1.33791005
O	-6.30229500	-0.55007113	0.83995785
N	-5.32485001	1.29078539	-0.91847539
C	-4.26833876	1.79056739	-1.81347788
C	-6.70578504	1.80614687	-0.94152163

H	-7.20180739	1.40413103	-0.05162213
C	-7.56227052	1.50532233	-2.18811542
H	-6.61515451	2.89318473	-0.80446099
C	-4.17160198	1.18587139	-3.22964171
H	-3.30505867	1.65286954	-1.30233229
H	-4.43066152	2.87623206	-1.87527714
C	-7.84739823	0.01080923	-2.40334640
H	-7.08720536	1.93369669	-3.08067142
H	-8.51112662	2.04768830	-2.05836517
H	-4.07387947	0.09858791	-3.14095767
C	-2.97658436	1.77279553	-3.99871256
H	-5.09849628	1.37601818	-3.78412435
H	-2.03184059	1.56893113	-3.47853315
H	-3.06639286	2.86148335	-4.11063663
H	-2.90338880	1.33973758	-5.00232590
H	-6.92281440	-0.55917786	-2.54383152
H	-8.47900683	-0.14315767	-3.28608378
H	-8.36201670	-0.41690644	-1.53502957
N	1.27770301	1.50917737	1.74970594
C	0.80195007	2.80874419	1.82143504
C	1.98189857	1.30333417	0.57267314
O	0.12217603	3.23054207	2.78954573
C	1.24390158	3.53196666	0.59088101
O	2.51671809	0.23394478	0.20173376

C	1.97262851	2.60739169	-0.17668518
C	-2.25083852	1.16037649	7.80437378
C	-1.52529717	0.20873755	6.88693024
C	-1.47111766	-1.17451490	7.14041145
C	-0.78940605	-2.02360924	6.27196788
C	-0.15776968	-1.49452726	5.13738203
C	0.60125613	-2.27464387	4.14825642
N	1.11041006	-1.54949151	3.11570370
C	1.85046888	-2.13817595	2.15413676
C	2.11684015	-3.51587521	2.16168214
C	2.93197519	-4.14632332	1.06087460
C	1.58626604	-4.27132518	3.22158096
C	0.83026117	-3.65508937	4.21810438
N	-0.22234097	-0.15603617	4.89200254
C	-0.87706129	0.66994544	5.73678826
H	-3.31086392	0.89359212	7.89112869
H	-2.19406076	2.18920166	7.43784534
H	-1.82543450	1.14007886	8.81497887
H	-1.96562427	-1.58205981	8.01627492
H	-0.75312543	-3.08704727	6.47186016
H	2.22686718	-1.47726568	1.37598833
H	2.29471484	-4.73398941	0.38741384
H	3.69241106	-4.82384780	1.46515818
H	3.43718340	-3.38625364	0.45876885

H	1.76914504	-5.34024632	3.26776770
H	0.42998598	-4.24146534	5.03594722
H	-0.87732102	1.72033313	5.46953354
Ni	0.61417577	0.43865208	3.22106087
H	-0.26118357	-1.07514908	0.68111102
C	1.05125298	4.83711834	0.16224306
C	2.53003040	2.96121711	-1.39589199
C	1.61279550	5.20585537	-1.07499408
H	0.48633525	5.54493817	0.75900203
C	2.33990327	4.28368386	-1.84093381
H	3.09035603	2.24239172	-1.98382324
H	1.48033921	6.21829695	-1.44244205
H	2.76144279	4.59420938	-2.79150966
C	2.36529189	0.74295531	4.23013737
H	3.12414830	0.62238826	3.45208400
H	2.45007195	-0.07049310	4.95955867
C	2.44298004	2.11705413	4.91173012
H	2.33552031	2.91411279	4.17044976
C	3.75693906	2.28565920	5.66157657
H	1.61360815	2.23850873	5.62136232
C	3.86993001	1.91737658	7.01310424
C	4.90189402	2.77143014	5.00594197
C	5.08607224	2.02461495	7.69729013
H	2.99612974	1.54460083	7.54056080

C	6.12699196	2.88592622	5.67225112
H	4.83524386	3.06485870	3.96231497
C	6.19575163	2.50660029	7.00962040
H	5.16642773	1.74374009	8.74059137
H	7.00505483	3.26384455	5.16274790
Cl	7.79404970	2.64809049	7.89339296

TS-3G¹-12G¹

Total free energy (Ha) = -3666.098077

Potential energy (Ha) = -3666.6239

77

C	-1.55486169	0.53919501	0.17357136
C	-2.46558614	-0.36492876	-0.38819224
H	-2.25985447	-0.88084818	-1.31962687
C	-3.65416791	-0.60664747	0.29284088
S	-4.86619980	-1.82109274	-0.43347313
C	-3.97280199	-0.01067409	1.51065997
H	-4.90147922	-0.25468883	2.01393931
C	-3.05088756	0.88088648	2.06774347
H	-3.26837381	1.35431597	3.01927669
C	-1.83554801	1.14784566	1.41044701

C	-1.02566516	2.79280680	1.69580391
O	-4.07748402	-2.59518425	-1.63274746
O	-5.53042826	-2.66974064	0.78720683
N	-6.16760341	-0.75038281	-1.04617005
C	-5.79168100	0.20925379	-2.09819376
C	-7.55989188	-1.16995300	-0.79780900
H	-7.55784251	-1.70511353	0.15750031
C	-8.24807243	-2.03755006	-1.87018025
H	-8.12202576	-0.23683808	-0.65139593
C	-5.60495911	-0.32665927	-3.53277926
H	-4.86530826	0.70822218	-1.78147468
H	-6.57547625	0.97992995	-2.07919930
C	-7.58880502	-3.40925679	-2.08328578
H	-8.30105183	-1.48962015	-2.82005907
H	-9.28868534	-2.17686042	-1.54055549
H	-4.86407541	-1.13362202	-3.51388916
C	-5.15359851	0.79509540	-4.48297728
H	-6.54318555	-0.76413157	-3.89346914
H	-4.20318710	1.23386856	-4.15353804
H	-5.89495565	1.60335862	-4.53133745
H	-5.00928128	0.41409628	-5.49956502
H	-6.55943267	-3.31227540	-2.44575910
H	-8.14931195	-3.99985157	-2.81716304
H	-7.55212793	-3.97492991	-1.14531946

O	-1.49322014	3.81272994	1.29378103
N	1.66880347	2.41797458	2.36197361
C	2.03440077	3.38876615	3.28036208
C	2.41320176	2.10082607	1.25086443
O	1.25899469	3.73622235	4.20183363
C	3.39476229	4.06660297	3.13591582
O	1.97115231	1.29549697	0.38216412
C	3.77837954	2.74644522	1.04968874
H	3.64508395	3.61016249	0.38007418
H	4.40494275	2.02777926	0.51343687
C	4.40511406	3.20108858	2.37345608
H	3.73826870	4.32425989	4.14183157
H	3.23701482	5.01649665	2.60206993
H	5.33268530	3.75603657	2.19271101
H	4.67041951	2.32285931	2.97799946
C	-1.96007632	3.23350178	7.61845888
C	-1.44551794	2.11352252	6.74961546
C	-1.18542477	0.83158893	7.26246013
C	-0.67406942	-0.16654997	6.43394994
C	-0.44159884	0.11939646	5.07986744
C	0.13591152	-0.84098147	4.11852600
N	0.47192640	-0.33656719	2.89712591
C	1.03618903	-1.13898425	1.96715624
C	1.28052584	-2.50229481	2.18561749

C	1.87983610	-3.35997817	1.09921857
C	0.92351440	-3.02375708	3.43846303
C	0.35664897	-2.19481717	4.40548867
N	-0.71233897	1.35049023	4.57911140
C	-1.18286703	2.31882058	5.38712828
H	-2.82341255	2.91602061	8.21477243
H	-2.26215033	4.09497752	7.01595043
H	-1.18713012	3.57703503	8.31784473
H	-1.36942100	0.62070815	8.31156664
H	-0.44988205	-1.14410778	6.84298005
H	1.31082714	-0.64607345	1.04190121
H	1.09753590	-3.89887652	0.54838938
H	2.56343303	-4.10909646	1.51265593
H	2.43182101	-2.75367989	0.37500217
H	1.08890300	-4.07433881	3.65610793
H	0.08105865	-2.60280772	5.36982202
H	-1.31741927	3.29148926	4.93223742
Ni	-0.08646400	1.55851977	2.46664777
H	-0.61803525	0.75961978	-0.32882686

12G[1]

Total free energy (Ha) = -3666.114683

Potential energy (Ha) = -3666.639426

77

C	-1.43881537	-0.28020403	0.16135298
C	-2.49794646	-1.07369966	-0.29946619
H	-2.41450074	-1.67975154	-1.19471322
C	-3.67823742	-1.08189528	0.43623534
S	-5.09914064	-2.11967138	-0.15776931
C	-3.83859429	-0.35341396	1.61010469
H	-4.76892120	-0.40503471	2.16518808
C	-2.76612313	0.42809186	2.05858401
H	-2.88535550	1.00287988	2.96998307
C	-1.54946259	0.46597896	1.35024209
C	-0.65385972	2.77031280	1.03319091
O	-4.50069220	-3.14358256	-1.27883280
O	-5.88892213	-2.70607940	1.14030305
N	-6.20304929	-0.89613305	-0.88021588
C	-5.69938392	-0.17091952	-2.05850488
C	-7.63857523	-1.02805417	-0.57121625
H	-7.70081674	-1.44551802	0.43939856
C	-8.50530872	-1.87091983	-1.52783218
H	-8.02384462	0.00034869	-0.52559869
C	-5.68034582	-0.91146200	-3.41306477
H	-4.68152588	0.17573107	-1.83037535

H	-6.32129109	0.73308353	-2.13037870
C	-8.10285201	-3.35165748	-1.60348793
H	-8.50136386	-1.42313139	-2.53041662
H	-9.54070979	-1.79013757	-1.16373008
H	-5.12520495	-1.84798178	-3.29213480
C	-5.03429422	-0.04387277	-4.50531548
H	-6.70129551	-1.18083462	-3.70840623
H	-4.00462085	0.22608574	-4.23753015
H	-5.59282804	0.88798186	-4.66459286
H	-4.99973572	-0.57820840	-5.46075943
H	-7.08727632	-3.47764119	-1.99460010
H	-8.78664947	-3.90645059	-2.25623886
H	-8.12636642	-3.81343583	-0.60996502
O	-1.08501558	3.65446937	0.41081230
N	1.67523468	2.51040385	2.24010917
C	1.60650261	3.65863400	3.00922768
C	2.80503178	2.15924671	1.52684674
O	0.50329151	4.10348365	3.41397688
C	2.88864890	4.42229425	3.32807055
O	2.76185802	1.26763737	0.64054471
C	4.11928754	2.88423970	1.79920387
H	4.25663105	3.63994895	1.01110194
H	4.92304032	2.15248400	1.67423622
C	4.14055167	3.55148818	3.17926625

H	2.77942248	4.83353364	4.33606834
H	2.94133723	5.28153806	2.64237048
H	5.04878414	4.15153093	3.30627373
H	4.15313592	2.78189663	3.96334537
C	-2.35729108	2.97044908	7.09157206
C	-1.62742309	1.93005209	6.27893360
C	-1.36150747	0.64369345	6.77783815
C	-0.66903375	-0.28292527	5.99976340
C	-0.25244584	0.08074987	4.70887397
C	0.50387829	-0.81302535	3.80728681
N	0.79119831	-0.33484959	2.56204271
C	1.49492477	-1.09655026	1.69615746
C	1.94896775	-2.38724479	2.00475389
C	2.71199526	-3.18935650	0.98006488
C	1.65276381	-2.87933919	3.28240913
C	0.93666850	-2.09168325	4.18289903
N	-0.52295436	1.31312136	4.21984692
C	-1.17766479	2.21282296	4.97964130
H	-3.35234930	2.61959420	7.39201374
H	-2.48549776	3.89552588	6.52231298
H	-1.80920638	3.21647986	8.00967520
H	-1.69144443	0.37023886	7.77522908
H	-0.46725148	-1.26991922	6.39643164
H	1.73373928	-0.62627357	0.75297472

H	2.03513511	-3.61110201	0.22556745
H	3.24865543	-4.02220489	1.44430906
H	3.43947222	-2.56510516	0.45038542
H	1.98499172	-3.87046588	3.57439011
H	0.72142976	-2.47235830	5.17284680
H	-1.30373752	3.19046609	4.53244632
Ni	0.02617186	1.43711981	1.97169458
H	-0.51780487	-0.25256750	-0.41313556

13G[1]

Total free energy (Ha) = -3552.778455

Potential energy (Ha) = -3553.301116

75

C	-1.29522482	-0.16856857	0.52778450
C	-2.27001424	-0.96014686	-0.09228681
H	-2.09231419	-1.44507504	-1.04617014
C	-3.48795507	-1.13203324	0.55867231
S	-4.78346414	-2.19847966	-0.22962064
C	-3.76535751	-0.56148554	1.79644159
H	-4.72127804	-0.73487973	2.27862920
C	-2.76851482	0.21110916	2.40562724

H	-2.98257714	0.64610824	3.37705670
C	-1.51557965	0.42258809	1.79096177
O	-4.05383049	-3.03378774	-1.42785319
O	-5.58835477	-3.00386223	0.93618374
N	-5.95888265	-0.99726766	-0.86814400
C	-5.46072859	-0.04455721	-1.87143697
C	-7.38972954	-1.29720648	-0.68912527
H	-7.47259619	-1.86659707	0.24270795
C	-8.10719588	-2.05838057	-1.82229046
H	-7.87707040	-0.32516488	-0.52626710
C	-5.23604534	-0.56255797	-3.30803672
H	-4.52018882	0.38333098	-1.49672493
H	-6.19114503	0.77738237	-1.87723969
C	-7.55429560	-3.47017751	-2.07399254
H	-8.07795837	-1.46893310	-2.74871382
H	-9.16818220	-2.12296135	-1.53653557
H	-4.53447717	-1.40309110	-3.27280570
C	-4.69746355	0.55305930	-4.21857840
H	-6.17626485	-0.95303095	-3.71538877
H	-3.74440138	0.94695673	-3.84238218
H	-5.40207376	1.39270894	-4.28273563
H	-4.52607470	0.18330891	-5.23541596
H	-6.50659713	-3.44358204	-2.39345647
H	-8.13273271	-3.98290580	-2.85159206

H	-7.59773862	-4.07353577	-1.16005404
N	1.39763695	2.77725344	2.75837756
C	2.17073575	3.47285126	3.67403716
C	1.57516484	2.82856906	1.42703157
O	1.95380257	3.40572070	4.90043144
C	3.27420667	4.36844558	3.10496344
O	0.71900607	2.09715785	0.77771258
C	2.64819196	3.63781450	0.75925050
H	2.21425431	4.59886619	0.44355255
H	2.96895965	3.12177354	-0.15069610
C	3.80851212	3.87014027	1.74816512
H	4.06703350	4.43356207	3.85511585
H	2.85781231	5.38173834	2.99459996
H	4.52486644	4.58714335	1.33344635
H	4.34965924	2.92616615	1.89643334
C	-1.98189835	3.09003029	7.21244474
C	-1.36442940	1.95179043	6.43972041
C	-1.03667541	0.72882913	7.04787712
C	-0.45308194	-0.28809332	6.29765787
C	-0.19990452	-0.09844600	4.93038538
C	0.43819976	-1.13694387	4.09469414
N	1.15795604	-0.70181337	3.03220080
C	1.74934341	-1.60478889	2.22809011
C	1.66520949	-2.99250164	2.42092565

C	2.32949767	-3.95635965	1.47025585
C	0.91857144	-3.43309929	3.52617551
C	0.30224378	-2.50704222	4.36749239
N	-0.53012334	1.08454085	4.34317626
C	-1.08394542	2.07684607	5.07680298
H	-2.97869217	2.82494280	7.58655563
H	-2.08408463	3.98346714	6.59012440
H	-1.36588865	3.35659949	8.07902379
H	-1.22213169	0.58366224	8.10745092
H	-0.16442197	-1.21872666	6.76974346
H	2.30822223	-1.19765663	1.39158226
H	1.58353327	-4.51897171	0.89499369
H	2.94791084	-4.68674269	2.00514872
H	2.97117830	-3.43089708	0.75649036
H	0.80692398	-4.49597739	3.71691466
H	-0.30250108	-2.84782104	5.19978891
H	-1.29579322	2.99551757	4.54663418
Ni	-0.07521674	1.45001437	2.51460264
H	-0.35157173	-0.00509190	0.01822790

14G[1]

Total free energy (Ha) = -3552.808982

Potential energy (Ha) = -3553.331387

75

C	-4.84992042	-0.28371337	3.88577110
C	-3.55372985	0.12146667	4.54204986
C	-3.50317126	0.69361486	5.82002774
C	-2.27392095	1.05711454	6.37266549
C	-1.09942103	0.84723490	5.64628190
C	0.24765121	1.17996441	6.12390022
N	1.24191794	0.87236804	5.24525983
C	2.52425750	1.13058534	5.56634642
C	2.90189469	1.71157299	6.78429598
C	4.35299915	1.97314895	7.10054804
C	1.87494108	2.02838786	7.68844064
C	0.54580038	1.76287661	7.36094104
N	-1.14120631	0.29025885	4.39353408
C	-2.33551491	-0.06063856	3.86915991
H	-5.67905665	-0.26533695	4.59872029
H	-4.78493288	-1.29302953	3.46498901
H	-5.10335030	0.39274218	3.05970643
H	-4.41874381	0.85123229	6.38048428
H	-2.23348023	1.49693171	7.36126071
H	3.25442133	0.85766358	4.81759703
H	4.98880081	1.78463378	6.23100601

H	4.70350339	1.32809148	7.91602338
H	4.51132168	3.01157044	7.41375373
H	2.11562213	2.48201685	8.64467546
H	-0.24374708	2.01001555	8.05960128
H	-2.30772253	-0.50056128	2.88326191
Ni	0.60894593	0.08015161	3.53977988
N	2.34728405	-0.12139693	2.77492737
C	2.82653910	0.91710161	1.99903290
C	2.97679376	-1.34081966	2.93480911
C	4.14693241	0.73280239	1.25862769
C	4.30226266	-1.58096123	2.22118228
H	4.95482607	1.14357001	1.88449399
H	4.10210987	1.35169041	0.35810898
C	4.42826142	-0.74257630	0.94073914
H	5.42440979	-0.85919483	0.49885882
H	3.70349144	-1.09989158	0.19703747
H	4.37540729	-2.65437467	2.02479906
H	5.11841982	-1.33067405	2.91715374
O	2.19587434	2.00088120	1.92862030
O	2.47533365	-2.22326033	3.67488873
C	-0.08732860	-0.62783592	1.91304435
C	-0.28767505	-2.01568880	1.74128177
H	0.03209444	-2.70474282	2.51649493
C	-0.88869418	-2.52391107	0.58160206

H	-1.08025454	-3.58529733	0.46483162
C	-1.27591982	-1.62603850	-0.41132402
S	-2.07351703	-2.29138165	-1.95418106
C	-1.08463944	-0.25106133	-0.29437101
H	-1.42710081	0.41232899	-1.08112709
C	-0.48019896	0.24047702	0.87163871
H	-0.30734373	1.30785623	0.96695442
O	-2.84191478	-1.04896812	-2.66456432
O	-2.84462734	-3.66668465	-1.55736842
N	-0.75794669	-2.78351165	-3.09956295
C	-0.15675230	-4.10302991	-2.84696648
C	0.07289959	-1.67347432	-3.60942207
H	-0.86426400	-4.67183348	-2.23510724
H	0.78802598	-4.00673082	-2.28317540
C	0.09121691	-4.86368665	-4.16129099
C	-0.44743584	-1.09290272	-4.93193856
H	1.08656116	-2.07634175	-3.74183784
H	0.15922959	-0.87144685	-2.85924448
H	-0.86868380	-4.96879581	-4.68005591
C	0.72596825	-6.24044173	-3.90987265
H	0.74360150	-4.26913694	-4.81581654
H	-0.49424544	-1.89881028	-5.67574796
C	0.43712096	0.05590670	-5.44092574
H	-1.47394592	-0.74819459	-4.76940954

H	0.07597331	-6.86654771	-3.28646629
H	1.69179252	-6.14661907	-3.39687200
H	0.89894037	-6.77198185	-4.85212867
H	1.46817880	-0.27715396	-5.62063804
H	0.47386323	0.87857896	-4.71525692
H	0.05082600	0.46228934	-6.38221976

3G[3]

Total free energy (Ha) = -3666.126587

Potential energy (Ha) = -3666.652781

77

C	-2.17576273	0.52181907	1.22632855
C	-3.00866901	-0.03130513	0.24534366
H	-2.60670132	-0.47361860	-0.65887241
C	-4.38011023	-0.02551768	0.46958410
S	-5.49864668	-0.77286946	-0.81995503
C	-4.96467568	0.49170667	1.62415754
H	-6.03887431	0.44267125	1.76182242
C	-4.12353270	1.04267355	2.59008037
H	-4.52233271	1.46475462	3.50614712
C	-2.72638272	1.06105931	2.39969550

C	-1.83505962	1.63242823	3.47854324
O	-4.56202465	-1.71242104	-1.76797885
O	-6.79347448	-1.40576193	-0.06263902
N	-6.10633061	0.67282576	-1.69755629
C	-5.11021164	1.45712456	-2.44453190
C	-7.55282451	0.73322864	-1.97479752
H	-8.04970221	0.20563106	-1.15395813
C	-8.04701212	0.16494731	-3.31929085
H	-7.82320090	1.79566681	-1.89501114
C	-4.60371894	0.89369102	-3.78885260
H	-4.24869593	1.62304036	-1.78257065
H	-5.57248794	2.44296454	-2.59700605
C	-7.81017538	-1.34394954	-3.48559669
H	-7.58944244	0.71679943	-4.15091841
H	-9.12595555	0.37582165	-3.37122571
H	-4.20745726	-0.11325406	-3.61969507
C	-3.51904092	1.80218447	-4.39090969
H	-5.43817626	0.79565129	-4.49353313
H	-2.65553640	1.88633641	-3.71868778
H	-3.89901552	2.81592968	-4.57473044
H	-3.15766385	1.40429963	-5.34542433
H	-6.74228993	-1.59025997	-3.48345282
H	-8.23525026	-1.70381843	-4.42981769
H	-8.27358271	-1.90304445	-2.66476839

O	-2.37325248	2.27856817	4.40649845
N	0.99913824	2.23622519	1.89361325
C	1.19846150	3.47603577	2.43014076
C	1.29011273	1.91340408	0.58950118
O	0.86276112	3.61226979	3.65378665
C	1.76267111	4.61382681	1.61457279
O	1.05356955	0.76379775	0.13260475
C	1.87264859	2.99431913	-0.31747799
H	1.03635408	3.44970983	-0.87064578
H	2.50629353	2.49971675	-1.05878176
C	2.63478267	4.07634686	0.46506956
H	2.31478369	5.28024240	2.28337780
H	0.91836346	5.19412479	1.21162564
H	2.93388819	4.89244382	-0.20145270
H	3.55736430	3.64773324	0.87938481
C	-0.56226637	2.67441942	8.89077656
C	-0.27642540	1.60334942	7.86886659
C	-0.18598381	0.24452867	8.21661655
C	0.07602236	-0.72059981	7.24330894
C	0.25515001	-0.32136458	5.91274555
C	0.51731687	-1.23351751	4.78198506
N	0.55798731	-0.64274794	3.55323143
C	0.80429754	-1.37871852	2.44818168
C	1.01102754	-2.76565298	2.49901044

C	1.25453879	-3.55299278	1.23599497
C	0.96667824	-3.37580875	3.76344420
C	0.72344029	-2.61306300	4.90643464
N	0.17103603	0.99520548	5.58242425
C	-0.09157340	1.92781221	6.51815342
H	-1.47042390	2.44729999	9.46136493
H	-0.70214439	3.64788257	8.41254528
H	0.26069480	2.76942712	9.61068293
H	-0.32958096	-0.05981926	9.24889900
H	0.12654415	-1.76660334	7.51998621
H	0.84729283	-0.82364808	1.51412525
H	0.33352673	-4.04471373	0.89628208
H	2.00565959	-4.33513111	1.39075365
H	1.59653681	-2.90374392	0.42508831
H	1.12884787	-4.44547105	3.85398238
H	0.70330100	-3.08777695	5.87977387
H	-0.16699029	2.94553268	6.15697473
Ni	0.18178659	1.40785510	3.58377156
H	-1.10348197	0.54013723	1.06639821

TS-3G^3-12G^3

Total free energy (Ha) = -3666.094071

Potential energy (Ha) = -3666.617475

77

C	-2.28282843	1.52773602	1.50464343
C	-3.31558663	0.73223129	0.98799127
H	-3.38578191	0.48593480	-0.06589545
C	-4.25743400	0.22540984	1.87779849
S	-5.54337751	-0.94681865	1.22018906
C	-4.23000776	0.48247358	3.24673922
H	-4.98476249	0.05958892	3.90096399
C	-3.19258059	1.28103683	3.74266192
H	-3.15212468	1.49342102	4.80799175
C	-2.19848919	1.78428268	2.88415837
C	-1.14930197	3.36428721	3.45814633
O	-5.21583920	-1.15010084	-0.36705321
O	-5.61037750	-2.25766732	2.18626258
N	-7.07426895	-0.05657552	1.51498664
C	-7.22411486	1.24454359	0.83952417
C	-8.22574145	-0.85236715	1.98191970
H	-7.81330180	-1.66283962	2.59233916
C	-9.17265122	-1.44205990	0.91829585
H	-8.78603071	-0.18616726	2.65295279
C	-7.48150107	1.24615779	-0.68199745
H	-6.32291930	1.83765401	1.04847725

H	-8.04988824	1.74520027	1.36453201
C	-8.51157598	-2.47620267	-0.00721057
H	-9.62317627	-0.63519225	0.32540177
H	-10.00221719	-1.91597246	1.46461845
H	-6.67159076	0.69965030	-1.17760554
C	-7.57376268	2.68178926	-1.22420386
H	-8.40945917	0.70672084	-0.90589463
H	-6.64463561	3.23753632	-1.04365687
H	-8.39243105	3.23854705	-0.74942661
H	-7.75489735	2.68164369	-2.30454227
H	-7.68367934	-2.04038414	-0.57703112
H	-9.23857191	-2.87929330	-0.72192696
H	-8.10237477	-3.31200770	0.57201938
O	-1.84289068	4.33884724	3.48244168
N	1.98606497	2.26607909	3.44803833
C	3.02589343	2.68113359	4.26077668
C	2.04431746	2.22016799	2.10114154
O	2.90670983	2.72720480	5.50475640
C	4.31888988	3.12334076	3.57315359
O	0.94900792	1.88643037	1.50849127
C	3.29941286	2.55502636	1.33201367
H	3.21035046	3.59094664	0.97084563
H	3.34649216	1.91664694	0.44427437
C	4.54208190	2.40656794	2.22950815

H	5.14314799	2.95309467	4.27096682
H	4.25582247	4.21038978	3.41051648
H	5.42814436	2.80631225	1.72453123
H	4.73230111	1.34046499	2.41352089
C	0.01579492	3.03105661	8.96447293
C	-0.07832927	1.94869990	7.91995329
C	-0.06518113	0.58478197	8.24814085
C	-0.09392681	-0.38490815	7.24423737
C	-0.14901932	0.01531320	5.90414831
C	-0.13255812	-0.90975332	4.75281856
N	0.04625805	-0.32413168	3.53943219
C	0.08358232	-1.06972561	2.41848036
C	-0.07349893	-2.46304066	2.43100020
C	-0.07360314	-3.25709933	1.14956248
C	-0.26153435	-3.06991959	3.68414322
C	-0.28883606	-2.29895859	4.84633724
N	-0.19003365	1.33877532	5.59016473
C	-0.14507388	2.27158129	6.55659917
H	-0.41940267	2.71009073	9.91610427
H	-0.49797184	3.94238979	8.64303276
H	1.06458686	3.29711726	9.14975174
H	-0.01765933	0.27996388	9.28897715
H	-0.05572498	-1.43514400	7.50621713
H	0.23408016	-0.51625000	1.49888770

H	-1.08898273	-3.58622261	0.89453826
H	0.55052250	-4.15395374	1.23266783
H	0.29836910	-2.66008403	0.31193954
H	-0.39686247	-4.14502575	3.74815659
H	-0.44828294	-2.77429190	5.80640457
H	-0.15068086	3.30076218	6.22050295
Ni	-0.02081562	1.77018571	3.55785874
H	-1.52024541	1.91709820	0.83622711

12G[3]

Total free energy (Ha) = -3666.11453

Potential energy (Ha) = -3666.635776

77

C	-2.29222603	0.57816607	1.41190025
C	-3.47820791	-0.00643339	0.94363025
H	-3.65044139	-0.20004733	-0.10981329
C	-4.44985946	-0.35073823	1.87761020
S	-6.02591505	-1.13561915	1.28767683
C	-4.28713255	-0.15129840	3.24502415
H	-5.06437415	-0.44950635	3.94067436
C	-3.09244152	0.43117052	3.68580030

H	-2.96459828	0.58925521	4.75421468
C	-2.06712425	0.80094699	2.78794109
C	-1.17286131	3.29432705	3.21370100
O	-5.83777792	-1.45909143	-0.30134117
O	-6.44190229	-2.33456714	2.30995016
N	-7.23332379	0.16505275	1.57246396
C	-7.03101342	1.42549097	0.84291981
C	-8.52853652	-0.23223997	2.14962487
H	-8.32712437	-1.08961778	2.80055143
C	-9.67173353	-0.58576117	1.17628295
H	-8.83336864	0.60529792	2.79399285
C	-7.42222502	1.46684686	-0.64908312
H	-5.97221251	1.70361034	0.93742906
H	-7.59936198	2.18240970	1.40292188
C	-9.37699837	-1.79942508	0.28133056
H	-9.92672196	0.28869424	0.56249615
H	-10.55849838	-0.79167603	1.79548636
H	-6.86893104	0.68403155	-1.17923402
C	-7.12063710	2.84614631	-1.25836681
H	-8.48773081	1.23546360	-0.76193418
H	-6.05553245	3.09555104	-1.16691300
H	-7.69031162	3.64018084	-0.75746038
H	-7.37754886	2.87240359	-2.32297075
H	-8.51771636	-1.62004795	-0.37439591

H	-10.24109699	-2.03593822	-0.35052543
H	-9.14323000	-2.68212394	0.88760448
O	-1.90207904	4.06192617	2.73355725
N	1.70246340	2.29859822	3.32265032
C	2.63920084	2.86100941	4.17140072
C	1.83246603	2.24070939	1.98050970
O	2.45115415	2.92081216	5.40653931
C	3.90131291	3.45146877	3.54090636
O	0.83185314	1.74198809	1.34129112
C	3.06403815	2.74652829	1.26669326
H	2.85314799	3.76385896	0.90318101
H	3.23517185	2.12653847	0.38105151
C	4.27506055	2.76157953	2.21701193
H	4.70422768	3.38557663	4.28030154
H	3.71863776	4.52302192	3.36381244
H	5.12484795	3.26747902	1.74573729
H	4.59124424	1.72920601	2.41974070
C	-0.76122319	2.90161316	8.76603649
C	-0.49166991	1.80617250	7.76588311
C	-0.14491643	0.50437575	8.16324890
C	0.14187530	-0.46925906	7.20818342
C	0.07121198	-0.14252349	5.84664361
C	0.40099664	-1.07896878	4.75451627
N	0.45487825	-0.53306250	3.51225285

C	0.76035249	-1.29150214	2.44226246
C	1.02864402	-2.66367479	2.54075674
C	1.33267104	-3.48551690	1.31336274
C	0.97130320	-3.23321394	3.82446164
C	0.65780250	-2.44581632	4.93213878
N	-0.29088051	1.11071172	5.46342423
C	-0.55044186	2.05223045	6.38859276
H	-1.50653269	2.59480238	9.50925331
H	-1.12704521	3.80784297	8.27502058
H	0.15392589	3.16747414	9.30957586
H	-0.08529223	0.25907454	9.21917053
H	0.43279400	-1.46404046	7.52169784
H	0.78064188	-0.77057558	1.49217113
H	0.44629086	-4.04528462	0.98790934
H	2.12784887	-4.21376746	1.50533418
H	1.64471350	-2.85319648	0.47709857
H	1.16756519	-4.29304961	3.95400963
H	0.60461166	-2.89424408	5.91626501
H	-0.79761570	3.03582647	6.01009950
Ni	-0.21415760	1.43945871	3.39065120
H	-1.52832070	0.86019230	0.69205660

13G[3]

Total free energy (Ha) = -3552.799077

Potential energy (Ha) = -3553.320028

75

C	-1.82299319	-0.14615253	1.61654095
C	-3.11983673	-0.43282564	1.16421347
H	-3.32829130	-0.66957518	0.12616421
C	-4.15300703	-0.42743229	2.09567140
S	-5.87522693	-0.82564557	1.53411263
C	-3.94705461	-0.16273364	3.44630970
H	-4.77670580	-0.19063688	4.14474074
C	-2.64150909	0.11361906	3.87135681
H	-2.48212024	0.31924628	4.92676992
C	-1.54913244	0.12818122	2.97539902
O	-5.77025057	-1.40976134	0.01375380
O	-6.61507858	-1.70860243	2.68624981
N	-6.69014926	0.77760812	1.56909947
C	-6.17573922	1.79686338	0.64378448
C	-8.02959421	0.84320600	2.17573734
H	-8.04884879	0.08772436	2.96856902
C	-9.24764757	0.64509918	1.25090245
H	-8.08648214	1.82903129	2.65958888
C	-6.56864857	1.67960532	-0.84448532

H	-5.07937907	1.80074869	0.72234171
H	-6.51684904	2.76084594	1.04855050
C	-9.30082708	-0.73039765	0.56767376
H	-9.28186884	1.44386635	0.49737184
H	-10.14277308	0.78017283	1.87725568
H	-6.25349800	0.69710522	-1.21191632
C	-5.92187581	2.79933161	-1.67596815
H	-7.65936147	1.72313825	-0.94496806
H	-4.82723261	2.76663989	-1.59834773
H	-6.24968400	3.79167086	-1.33848194
H	-6.18255764	2.70474554	-2.73578783
H	-8.44400192	-0.88465754	-0.09749189
H	-10.21476443	-0.83285138	-0.02938193
H	-9.28204305	-1.53628786	1.30981958
N	0.80575348	2.40467734	3.06681386
C	0.64026801	3.68755248	3.54956082
C	1.26192154	2.11892743	1.81913336
O	0.21686057	3.90182509	4.71025866
C	0.95831427	4.85006709	2.61228600
O	1.30344175	0.87283514	1.51440937
C	1.66794437	3.19492293	0.84286781
H	0.81715957	3.37320807	0.16744848
H	2.48612386	2.81348768	0.22465579
C	2.04285617	4.49291909	1.58073735

H	1.24356734	5.70614753	3.22970146
H	0.02610571	5.12631267	2.09560301
H	2.17589931	5.31271595	0.86669605
H	3.00442026	4.35684704	2.09377780
C	-0.56672856	2.23586615	8.75561719
C	-0.22488447	1.08727241	7.83958105
C	-0.07534015	-0.22613180	8.31499041
C	0.24683950	-1.26306879	7.43841272
C	0.41355348	-0.98240519	6.07635013
C	0.76170631	-1.98685451	5.05108012
N	0.91076672	-1.50103298	3.78955385
C	1.23630339	-2.31966944	2.76990770
C	1.42996951	-3.69655699	2.94203360
C	1.76974733	-4.58598279	1.77281776
C	1.27329903	-4.20384620	4.24409572
C	0.94056174	-3.35461625	5.29936939
N	0.25942426	0.29049501	5.61774338
C	-0.04348590	1.29830814	6.46350452
H	-1.54561824	2.08851575	9.22881800
H	-0.59855657	3.18035965	8.20608643
H	0.17211313	2.33612409	9.55988139
H	-0.20763027	-0.43673860	9.37188647
H	0.36460238	-2.27176205	7.81471951
H	1.33528379	-1.84463289	1.80066315

H	0.90947876	-5.20440617	1.48656644
H	2.59536937	-5.26544131	2.01265196
H	2.05849895	-3.99764758	0.89717174
H	1.41064769	-5.26463882	4.42904892
H	0.81914696	-3.75550933	6.29789959
H	-0.12093086	2.28468867	6.00995882
Ni	0.35440385	0.46177122	3.54651760
H	-1.01222026	-0.13555301	0.89246003

TS-3P[1]-12P[1]

Total free energy (Ha) = -3779.201784

Potential energy (Ha) = -3779.721471

78

C	-3.72834671	3.88264709	3.77037916
C	-2.80632875	2.74009884	4.11360696
C	-2.94986279	1.99564982	5.29619229
C	-2.04737217	0.97735800	5.60283504
C	-1.00573085	0.69205502	4.70801235
C	0.05119929	-0.31051867	4.95281213
N	1.08909356	-0.30668926	4.06877662
C	2.13403425	-1.14495363	4.24162312

C	2.19837403	-2.06897737	5.29368885
C	3.37317032	-3.00463471	5.42761850
C	1.11968000	-2.08992944	6.19191404
C	0.05096237	-1.20953643	6.02758584
N	-0.88549628	1.39060421	3.54907296
C	-1.74395698	2.38871660	3.26849523
H	-3.52743602	4.75287470	4.40817843
H	-4.77978140	3.60765668	3.91222352
H	-3.59638709	4.20080652	2.73226455
H	-3.75797462	2.22392300	5.98438784
H	-2.14807854	0.43012049	6.53211898
H	2.94112377	-1.03343799	3.52695046
H	4.22875658	-2.65067802	4.84535390
H	3.11852302	-4.00918329	5.06514028
H	3.68868058	-3.10359205	6.47197777
H	1.11845633	-2.79015078	7.02147281
H	-0.77553883	-1.22862868	6.72683714
H	-1.55572197	2.93421884	2.35222714
Ni	0.92893728	0.87006160	2.45790529
C	0.70454908	1.24974553	0.78173744
N	2.27681053	2.17023278	2.92825390
C	2.10288944	3.51879395	3.24296796
C	3.62428096	1.84438800	2.89384741
C	3.47085599	4.10241693	3.46533258

C	4.40211614	3.07589210	3.25092161
O	1.01436574	4.12402861	3.32026123
O	4.09609258	0.71457032	2.61266160
O	0.56445124	1.77628300	-0.27809528
C	0.42162649	-0.56154080	1.04327341
C	1.52424440	-1.38571298	0.74032507
H	2.53026168	-0.98085307	0.80042989
C	1.32669336	-2.72459794	0.38907973
H	2.16456990	-3.37730268	0.17292828
C	0.01950350	-3.19854879	0.31999788
S	-0.25558934	-4.99947690	-0.07460752
C	-1.09399240	-2.40938038	0.59037165
H	-2.08545926	-2.84452522	0.52945674
C	-0.88442718	-1.07142729	0.94730496
H	-1.73534556	-0.43455452	1.16499342
O	-1.86947648	-5.23126303	-0.07496091
O	0.69200393	-5.90667904	0.88784652
N	0.47667155	-5.12469830	-1.71699196
C	1.26645864	-6.35235770	-1.96114872
C	-0.26728234	-4.44183982	-2.79387672
H	2.04957963	-6.39316735	-1.19741731
H	1.75701278	-6.17412696	-2.92767353
C	0.51810905	-7.69885404	-1.97536228
C	-1.48718285	-5.16318634	-3.40165930

H	0.47569610	-4.22938236	-3.57515036
H	-0.58477397	-3.46652047	-2.40138985
H	0.02895109	-7.83858261	-1.00387034
C	1.48686272	-8.86434953	-2.23470562
H	-0.27024949	-7.69145373	-2.73661755
H	-1.16288483	-6.08039650	-3.90913391
C	-2.21888114	-4.25546858	-4.40437330
H	-2.16194009	-5.45786295	-2.59034709
H	2.26195965	-8.91116650	-1.45990888
H	1.98820051	-8.76129908	-3.20591559
H	0.95647725	-9.82257022	-2.23345926
H	-1.55104301	-3.92954556	-5.21260891
H	-2.60978441	-3.35629466	-3.91180319
H	-3.06540954	-4.77765806	-4.86307919
C	3.87394748	5.38297476	3.81556807
C	5.76616159	3.29627871	3.38008551
C	5.25495374	5.61846216	3.94999109
H	3.14689211	6.17140058	3.97785525
C	6.18630011	4.59151832	3.73557599
H	6.47987512	2.49726240	3.21035598
H	5.60624666	6.60881000	4.22237046
H	7.24587276	4.80055570	3.84476672

12P[1]

Total free energy (Ha) = -3779.219904

Potential energy (Ha) = -3779.738123

78

C	-3.67058850	2.70161957	3.08522695
C	-2.53659106	1.84135282	3.58363152
C	-2.67419328	0.99836662	4.69856813
C	-1.59913611	0.22215379	5.13075955
C	-0.38570247	0.28325017	4.42884568
C	0.83350977	-0.45293724	4.81943453
N	1.91035232	-0.31453873	3.99780871
C	3.08450120	-0.90169308	4.31408573
C	3.25609756	-1.69170504	5.45887109
C	4.58702111	-2.33614387	5.75455552
C	2.14100660	-1.85432507	6.29418076
C	0.93463940	-1.23081674	5.98063897
N	-0.25936463	1.07648454	3.33774475
C	-1.29103039	1.84411512	2.93656503
H	-4.20277720	3.18210770	3.91357724
H	-4.40496846	2.10484976	2.52828601
H	-3.30579017	3.48668706	2.41643695
H	-3.61853456	0.95789442	5.23269633

H	-1.71139339	-0.41786158	5.99698197
H	3.91114348	-0.67978759	3.65380565
H	5.39742853	-1.82824048	5.22353617
H	4.59414920	-3.38943169	5.44409989
H	4.81354331	-2.31026106	6.82573503
H	2.21924628	-2.45580925	7.19445463
H	0.08433723	-1.34357219	6.64082502
H	-1.08399100	2.50217865	2.10214566
Ni	1.66266360	0.66428082	2.23828244
C	1.98532349	1.07845850	0.55716685
N	2.53261505	2.31185771	2.81121607
C	1.96250164	3.58114346	2.69443922
C	3.83244610	2.41191176	3.30570577
C	2.94683424	4.57201141	3.23977635
C	4.09226022	3.85685139	3.61297657
O	0.84692583	3.84281145	2.19550607
O	4.64140546	1.46821647	3.44690109
O	2.22034469	1.37171332	-0.54608898
C	0.97644919	-0.99792410	1.46311095
C	1.80210586	-2.13778596	1.38714108
H	2.84865244	-2.07406200	1.66820118
C	1.29201402	-3.37490057	0.97574005
H	1.91758414	-4.26006118	0.94502667
C	-0.04912617	-3.44300159	0.60981702

S	-0.78896633	-5.08792525	0.16897409
C	-0.89126890	-2.33784827	0.63121079
H	-1.92923448	-2.45039036	0.33782245
C	-0.36341169	-1.10896447	1.04927205
H	-1.01333887	-0.24162448	1.06683411
O	-2.36949880	-4.82310003	-0.14069607
O	-0.37659136	-6.19020417	1.29306647
N	0.15199303	-5.54928485	-1.30019509
C	0.40528071	-6.99845451	-1.43825454
C	0.01676209	-4.65464706	-2.46595905
H	0.79598786	-7.34287688	-0.47555739
H	1.21854633	-7.07658509	-2.17299377
C	-0.77906150	-7.89681422	-1.84419101
C	-1.28593662	-4.70794212	-3.29061885
H	0.87900790	-4.88775862	-3.10677568
H	0.17241268	-3.62788385	-2.10759549
H	-1.60275982	-7.74009122	-1.13653117
C	-0.37061945	-9.37930578	-1.84626255
H	-1.15285219	-7.61391841	-2.83539199
H	-1.40859982	-5.70487245	-3.73016105
C	-1.26831822	-3.65102774	-4.40778730
H	-2.13785309	-4.54605521	-2.62111626
H	-0.02436481	-9.69196341	-0.85354421
H	0.44116548	-9.56978591	-2.56053535

H	-1.21463361	-10.02025954	-2.12306967
H	-0.42424913	-3.80638075	-5.09221385
H	-1.17980442	-2.63852354	-3.99375569
H	-2.18929810	-3.68987324	-4.99915103
C	2.87080835	5.94953841	3.38969582
C	5.20191975	4.49465784	4.14960681
C	3.98772700	6.60685524	3.93733746
H	1.98213137	6.49557800	3.09216327
C	5.13506398	5.89078095	4.31121774
H	6.08683919	3.93406469	4.43081601
H	3.96417749	7.68375887	4.07068039
H	5.98353850	6.42346832	4.72885827

13P[1]

Total free energy (Ha) = -3665.862741

Potential energy (Ha) = -3666.374443

76

C	-3.55587732	3.00376101	3.00227402
C	-2.54294989	2.11228230	3.67562801
C	-2.74934616	1.58014474	4.95845985
C	-1.78228043	0.76550290	5.54564974

C	-0.60673446	0.46111028	4.84252008
C	0.49257324	-0.35602567	5.41337644
N	1.63478071	-0.43355499	4.68429119
C	2.70825665	-1.09251382	5.16012266
C	2.70062804	-1.75975381	6.39448969
C	3.91843225	-2.50509682	6.87931334
C	1.51157313	-1.70644219	7.13912675
C	0.40993675	-0.99971230	6.65738576
N	-0.42164720	0.96517121	3.59263990
C	-1.34343923	1.77615396	3.03211522
H	-3.95871216	3.74681122	3.69928898
H	-4.40387901	2.42054564	2.62004957
H	-3.11174494	3.53764330	2.15734959
H	-3.65813846	1.81676742	5.50325780
H	-1.93854837	0.38547044	6.54685890
H	3.59699093	-1.04099489	4.54393447
H	4.80517824	-2.23196001	6.30021192
H	3.78131558	-3.59019751	6.78450964
H	4.12308256	-2.29320200	7.93475112
H	1.45050687	-2.21094743	8.09845868
H	-0.49833746	-0.95993561	7.24549688
H	-1.07701358	2.19550300	2.07127963
Ni	1.30870032	0.35061076	2.71920165
N	2.38443018	1.93654419	2.68888627

C	1.99100261	3.20973499	2.26625404
C	3.71637741	1.96695848	3.11404323
C	3.15655278	4.13428500	2.45074410
C	4.21264053	3.37361371	2.97167469
O	0.86759562	3.51446037	1.80996071
O	4.37054835	0.98238885	3.52223606
C	0.60652658	-1.30469909	2.13687093
C	1.63809364	-2.22014320	1.82821110
H	2.67092115	-1.98364143	2.08019571
C	1.36612820	-3.44279024	1.20329142
H	2.15607615	-4.14767228	0.96851244
C	0.03860841	-3.74180066	0.91050062
S	-0.35505779	-5.37779764	0.12719646
C	-1.01493784	-2.88841721	1.22049669
H	-2.03157126	-3.18744528	0.98889886
C	-0.72033575	-1.66419416	1.83685050
H	-1.53851511	-0.99159546	2.07294928
O	-1.98100183	-5.49364735	0.06037600
O	0.50693951	-6.55233473	0.85131184
N	0.39094976	-5.19430746	-1.50787366
C	0.98955470	-6.42656708	-2.06401637
C	-0.21990095	-4.16393400	-2.36819447
H	1.74653041	-6.77169113	-1.35240894
H	1.51513567	-6.09566563	-2.97009120

C	0.04306535	-7.59888867	-2.38879866
C	-1.49517246	-4.53333112	-3.15213242
H	0.57259851	-3.84752423	-3.06149566
H	-0.43116684	-3.29570905	-1.73044288
H	-0.48008690	-7.89422228	-1.47155558
C	0.82337108	-8.80065896	-2.94641971
H	-0.72235420	-7.28472403	-3.10754022
H	-1.27003470	-5.32385731	-3.87907651
C	-2.06319954	-3.30962340	-3.89017698
H	-2.23643177	-4.93501727	-2.45210161
H	1.56402699	-9.16024812	-2.22139282
H	1.35739496	-8.53832684	-3.86922741
H	0.15096185	-9.63425895	-3.17650747
H	-1.33123077	-2.88900820	-4.59224333
H	-2.34289879	-2.51622005	-3.18537608
H	-2.95803498	-3.57639210	-4.46291355
C	3.29775858	5.49206846	2.19809979
C	5.44506455	3.94570203	3.25773410
C	4.54044612	6.08323853	2.48862348
H	2.47634969	6.07222624	1.79156880
C	5.59781064	5.32182849	3.01060196
H	6.25781646	3.34942018	3.65828896
H	4.68590755	7.14328535	2.30615348
H	6.54665736	5.80331008	3.22488338

14P[1]

Total free energy (Ha) = -3665.910948

Potential energy (Ha) = -3666.426408

76

C	-4.5788320200	-1.7508422400	4.2568794600
C	-3.3843427000	-1.0458254900	4.8491714800
C	-3.3852383900	-0.5434995300	6.1596609600
C	-2.2500981000	0.0906073500	6.6642653100
C	-1.1142397100	0.2214155100	5.8596046800
C	0.1361261700	0.8684923500	6.2767938300
N	1.1088129100	0.8626675400	5.3225577000
C	2.3060003600	1.4249786800	5.5771008700
C	2.6148812000	2.0312966700	6.8027361300
C	3.9744825100	2.6359443500	7.0456689200
C	1.6095752300	2.0401457200	7.7830697100
C	0.3683627100	1.4584201300	7.5238517700
N	-1.1057391300	-0.2695727500	4.5804903600
C	-2.2122329700	-0.8790646000	4.0988168700
H	-5.5082661900	-1.2154963300	4.4798714200
H	-4.6801235300	-2.7653344300	4.6638518200

H	-4.4904618900	-1.8404482000	3.1705235300
H	-4.2682383900	-0.6480573700	6.7821932800
H	-2.2495801900	0.4802536400	7.6746600000
H	3.0209272600	1.3781591700	4.7672681300
H	4.5477039900	2.7069960000	6.1173243900
H	4.5566735900	2.0281340800	7.7499963100
H	3.8922574300	3.6420745700	7.4719152800
H	1.7969500900	2.5042684100	8.7458927700
H	-0.4040240600	1.4719581700	8.2829655100
H	-2.1467943900	-1.2363145800	3.0818985300
Ni	0.5837390000	-0.0285295200	3.6222073500
N	2.2672278900	0.2033983200	2.7891125900
C	2.6120771100	1.2496826100	1.9336752600
C	3.2554579600	-0.7855796300	2.7787879500
C	3.9523901100	0.9249197200	1.3441623700
C	4.3459289600	-0.3178884300	1.8605678400
O	1.9333901900	2.2774745700	1.7206182300
O	3.2242104500	-1.8489938600	3.4313699500
C	0.0139109900	-0.9202540200	2.0408916900
C	0.2325739800	-2.3073075500	1.8844355600
H	0.7903364800	-2.8556847200	2.6366166900
C	-0.2424143800	-2.9906608400	0.7580095600
H	-0.0860997000	-4.0573622900	0.6400855100
C	-0.9233997000	-2.2635914700	-0.2149730100

S	-1.6185689300	-3.1682806300	-1.6775853200
C	-1.1499793600	-0.8946830800	-0.1136280200
H	-1.6916035400	-0.3796342000	-0.8999216400
C	-0.6682971700	-0.2244831000	1.0208319700
H	-0.8268992400	0.8453000500	1.1094819300
O	-2.4462387200	-2.0817470400	-2.5709996800
O	-2.3756210600	-4.5216412500	-1.1802420900
N	-0.1239993000	-3.7513381500	-2.5025762100
C	-0.2455311500	-5.0713838400	-3.1509412400
C	0.7888654900	-2.7043253700	-2.9940403800
H	-0.6618794200	-5.7550841000	-2.4040911400
H	0.7878506400	-5.3883361200	-3.3480841000
C	-1.0941161400	-5.1649646800	-4.4346915600
C	0.4170646500	-1.9691168400	-4.2983525400
H	1.7674888200	-3.1940055600	-3.0986591500
H	0.9020353100	-1.9674099200	-2.1879294800
H	-2.1041919700	-4.7951938100	-4.2187898300
C	-1.1701636800	-6.6147522800	-4.9406128200
H	-0.6783632900	-4.5193870900	-5.2174601400
H	0.3953055400	-2.6806895800	-5.1329796100
C	1.4212765800	-0.8463209200	-4.6038428300
H	-0.5953848200	-1.5628281300	-4.1963442300
H	-1.6145307400	-7.2717775200	-4.1831800700
H	-0.1731459800	-7.0066302500	-5.1801364500

H	-1.7825874700	-6.6863292100	-5.8458476600
H	2.4401807000	-1.2390985800	-4.7182188800
H	1.4418149500	-0.1019189600	-3.7976091900
H	1.1596408900	-0.3243497100	-5.5308222500
C	4.7541381600	1.6271544300	0.4551638800
C	5.5550895800	-0.8996580900	1.5056628600
C	5.9814044500	1.0463091300	0.0870480400
H	4.4410809600	2.5866057600	0.0579709600
C	6.3759549000	-0.1970623200	0.6044441400
H	5.8492868100	-1.8627952400	1.9087515600
H	6.6332523000	1.5653165500	-0.6085636200
H	7.3275863700	-0.6225538600	0.3021817200

3P[3]

Total free energy (Ha) = -3779.223041

Potential energy (Ha) = -3779.743268

78

C	-2.13154611	0.55690003	1.19631827
C	-2.98121041	0.00451187	0.22997809
H	-2.59449155	-0.46972248	-0.66458641
C	-4.35186578	0.05449217	0.45431594

S	-5.49112062	-0.70335225	-0.81166548
C	-4.92136925	0.62143277	1.59271493
H	-5.99646639	0.60859558	1.73080517
C	-4.06523347	1.17686108	2.54282576
H	-4.45424901	1.63939313	3.44333821
C	-2.66825450	1.14457515	2.35337141
C	-1.76328221	1.71074693	3.41209107
O	-4.57007647	-1.66925001	-1.74840806
O	-6.78312210	-1.30995590	-0.02841921
N	-6.09234549	0.73383765	-1.70465770
C	-5.09399103	1.50118680	-2.46684703
C	-7.54013770	0.80239727	-1.97494669
H	-8.03751850	0.29469207	-1.14199668
C	-8.04730753	0.21548894	-3.30641913
H	-7.79904730	1.86880312	-1.91259336
C	-4.60058622	0.91752787	-3.80738425
H	-4.22732440	1.66845699	-1.81207394
H	-5.54915418	2.48873685	-2.62825477
C	-7.82477544	-1.29788841	-3.44889969
H	-7.58987117	0.74915892	-4.14982879
H	-9.12460597	0.43522969	-3.35539777
H	-4.21210030	-0.09103984	-3.62957767
C	-3.51161437	1.80959918	-4.42610163
H	-5.44013821	0.81894681	-4.50600626

H	-2.64355523	1.89456516	-3.76003790
H	-3.88390537	2.82430031	-4.61949503
H	-3.15957296	1.39753164	-5.37808678
H	-6.75900181	-1.55311538	-3.45312214
H	-8.26209242	-1.66992017	-4.38267363
H	-8.28481435	-1.83914484	-2.61432453
O	-2.23946777	2.48551000	4.27302745
N	1.17983445	2.19565420	2.11770602
C	1.64924787	3.47652573	2.41647808
C	1.46448043	1.88043424	0.79865126
O	1.51884742	4.01557127	3.53793057
C	2.29799302	4.03261341	1.18785454
O	1.16300196	0.80853564	0.21591427
C	2.18435614	3.04962182	0.19146487
C	-0.73389859	2.56064694	8.91425239
C	-0.38926614	1.50869208	7.89063950
C	-0.23966486	0.15361705	8.23319515
C	0.06745075	-0.79428479	7.25671827
C	0.23712885	-0.38304471	5.92864646
C	0.54478424	-1.27966948	4.79773329
N	0.59670560	-0.67816062	3.57443610
C	0.87659715	-1.39875245	2.46742657
C	1.10994156	-2.78161421	2.51055372
C	1.39128094	-3.55332700	1.24594194

C	1.05653770	-3.40292571	3.76922571
C	0.77728079	-2.65552733	4.91402833
N	0.09938655	0.93154103	5.60237032
C	-0.21093916	1.84692217	6.54287737
H	-1.69376589	2.34290638	9.39800052
H	-0.80920484	3.54966906	8.45398953
H	0.02597913	2.61327211	9.70352139
H	-0.37153558	-0.16090954	9.26386962
H	0.16439371	-1.83789793	7.52949535
H	0.92542830	-0.83565068	1.53871888
H	0.49383909	-4.08435021	0.90238924
H	2.17557045	-4.30216220	1.40103315
H	1.70740783	-2.88734615	0.43826214
H	1.23889808	-4.46970681	3.85399817
H	0.74754244	-3.13996325	5.88218519
H	-0.33793599	2.86222902	6.18966682
Ni	0.21333675	1.34879405	3.61704364
H	-1.05878977	0.54543208	1.03435836
C	2.92009033	5.24777582	0.93782744
C	2.68739946	3.25214625	-1.08582130
C	3.43348520	5.46330022	-0.35460058
H	3.00427093	6.00272405	1.71202073
C	3.31889344	4.48168100	-1.35026170
H	2.59427751	2.48844110	-1.85045175

H	3.92516472	6.40282063	-0.58598579
H	3.72311533	4.67498799	-2.33880525

TS-3P^3-12P^3

Total free energy (Ha) = -3779.19471

Potential energy (Ha) = -3779.70954

78

C	-1.65334880	1.41269805	0.30203320
C	-2.53033118	0.59448070	-0.42749265
H	-2.33271554	0.32404210	-1.45896090
C	-3.66705106	0.10979993	0.21068623
S	-4.83505725	-0.98335284	-0.74052305
C	-3.96903989	0.38226499	1.54224493
H	-4.85636213	-0.03876768	2.00208836
C	-3.08279179	1.19273911	2.25929789
H	-3.29963773	1.42270956	3.29905195
C	-1.92306196	1.70607921	1.65035824
C	-1.21616016	3.27440559	2.48094115
O	-4.05808447	-1.44014621	-2.09992128
O	-5.42443348	-2.11300016	0.27515102
N	-6.20521089	0.12590308	-1.07475787

C	-5.91615659	1.30091210	-1.91302456
C	-7.56578268	-0.39906576	-0.86555060
H	-7.49543051	-1.13287789	-0.05586950
C	-8.27948230	-1.03912144	-2.07331701
H	-8.15453701	0.45048152	-0.49173205
C	-5.76614825	1.07997210	-3.43277385
H	-5.00144701	1.77407049	-1.52988978
H	-6.73294986	2.00885977	-1.71252856
C	-7.58280667	-2.29669598	-2.61666992
H	-8.40412020	-0.29735371	-2.87334726
H	-9.29496443	-1.29749510	-1.73656634
H	-4.98152490	0.33495871	-3.60348611
C	-5.42458949	2.39585172	-4.15056618
H	-6.69433033	0.66369401	-3.84193317
H	-4.47948468	2.81516448	-3.78249014
H	-6.20582935	3.15190791	-3.99720510
H	-5.31984264	2.23891230	-5.22952480
H	-6.58940127	-2.06892856	-3.01896751
H	-8.17378193	-2.75309268	-3.41929969
H	-7.44928994	-3.04113895	-1.82328022
O	-1.84048221	4.25402992	2.18010499
N	1.46680729	2.29262459	1.57021671
C	2.35335728	2.76946307	2.50665256
C	1.97608154	2.49807925	0.28942897

O	2.08543468	2.69082462	3.74271263
C	3.54889044	3.33882383	1.82303534
O	1.43101746	2.17005362	-0.78545800
C	3.31691915	3.17298476	0.44604742
C	-2.06068611	2.78825942	8.00174614
C	-1.51532536	1.77448798	7.02778942
C	-1.27953004	0.43820587	7.39291416
C	-0.76157524	-0.46690315	6.46691051
C	-0.47991378	-0.03522975	5.16395433
C	0.08506244	-0.89176919	4.10129305
N	0.42759443	-0.24269559	2.95802955
C	0.93469580	-0.92078908	1.91249594
C	1.13353194	-2.30981115	1.93638921
C	1.66430775	-3.03679739	0.72730219
C	0.79164049	-2.98031827	3.12202263
C	0.26613627	-2.27628223	4.20662430
N	-0.71727280	1.25565660	4.80887281
C	-1.21185282	2.13003067	5.70639535
H	-3.03318581	2.47547631	8.40054769
H	-2.19106083	3.76448010	7.52616872
H	-1.38499192	2.92014721	8.85543892
H	-1.49435820	0.10774495	8.40450681
H	-0.57059311	-1.49090189	6.76310513
H	1.17712876	-0.32546914	1.04003489

H	0.84882042	-3.51820892	0.17204002
H	2.37595966	-3.82001680	1.00980439
H	2.16692601	-2.35045397	0.03969223
H	0.92969484	-4.05457898	3.19310107
H	-0.00785407	-2.80515653	5.11112577
H	-1.35929861	3.14127611	5.34516533
Ni	-0.03004640	1.79931542	2.90312306
H	-0.75431976	1.78865776	-0.17972596
C	4.70640885	3.94086405	2.29577547
C	4.23857553	3.60130493	-0.49691709
C	5.64656519	4.38097169	1.34505938
H	4.87842288	4.06967625	3.35890381
C	5.41683610	4.21335903	-0.02804762
H	4.05211748	3.47107710	-1.55749498
H	6.56236151	4.85830159	1.67874008
H	6.15836526	4.56337186	-0.73926720

12P[3]

Total free energy (Ha) = -3779.211941

Potential energy (Ha) = -3779.730096

78

C	-1.49967560	0.43066108	0.48732777
C	-2.52525995	-0.12985268	-0.28874322
H	-2.36697778	-0.42178304	-1.32142312
C	-3.76714504	-0.32908134	0.30617103
S	-5.13554545	-1.07355620	-0.70609605
C	-4.02548202	-0.01975542	1.63764106
H	-5.00070248	-0.21945136	2.06851833
C	-2.98391814	0.53172084	2.39577999
H	-3.17953370	0.77210278	3.43846481
C	-1.70793044	0.76778746	1.84124411
C	-1.10784904	3.28608459	2.85727751
O	-4.45331868	-1.68124405	-2.05787398
O	-6.03707949	-2.03910713	0.24752139
N	-6.17956935	0.34268627	-1.06630733
C	-5.55964312	1.44860067	-1.81147797
C	-7.63719172	0.14988626	-0.97470311
H	-7.80376331	-0.58849528	-0.18289579
C	-8.38287996	-0.28617286	-2.25272008
H	-8.03764717	1.10990646	-0.61804887
C	-5.37729779	1.28059318	-3.33502180
H	-4.57943061	1.65041831	-1.35810880
H	-6.18226833	2.33047981	-1.60084393
C	-7.97075672	-1.66887857	-2.77957172
H	-8.25145478	0.47166853	-3.03611598

H	-9.45586425	-0.28887497	-2.00715402
H	-4.80091077	0.36789381	-3.52236921
C	-4.66357914	2.50005732	-3.94158728
H	-6.35343283	1.14405117	-3.81586083
H	-3.66855568	2.63625297	-3.49901792
H	-5.23218240	3.42411663	-3.77255430
H	-4.53315316	2.38231688	-5.02284820
H	-6.91064958	-1.69644522	-3.05380898
H	-8.55729697	-1.93709862	-3.66621106
H	-8.12943963	-2.44097711	-2.01803567
O	-1.65279187	4.17799766	2.35612849
N	1.35300976	2.31311047	1.86530758
C	1.87895959	3.51353592	2.35715988
C	2.01056267	1.97526144	0.68504689
O	1.49381836	4.08393256	3.40400642
C	2.94605264	3.98471432	1.41915609
O	1.80873608	0.94806060	-0.00690691
C	3.01999760	3.04245462	0.38508301
C	-2.38369642	2.43440440	8.00683796
C	-1.67790119	1.45796029	7.10033995
C	-1.33386657	0.16152050	7.51999716
C	-0.67598332	-0.70756318	6.65220852
C	-0.36384279	-0.28605981	5.35162878
C	0.33350672	-1.12009807	4.35454228

N	0.66078816	-0.49266763	3.19199940
C	1.27843073	-1.17090555	2.20382899
C	1.61391722	-2.52966512	2.31753894
C	2.27406317	-3.25137173	1.17035284
C	1.28547223	-3.17469703	3.51936177
C	0.64246612	-2.47321361	4.54017762
N	-0.70331460	0.96646860	4.94142694
C	-1.33105851	1.80747703	5.78971782
H	-3.35956738	2.04771138	8.32471813
H	-2.55075275	3.39224050	7.50577867
H	-1.79896875	2.62942325	8.91383006
H	-1.57479164	-0.16397274	8.52723795
H	-0.40401229	-1.69983870	6.98920917
H	1.49048377	-0.60403132	1.30204903
H	1.53264306	-3.80608072	0.58032057
H	3.01864823	-3.97275202	1.52353883
H	2.76813559	-2.54808817	0.49401797
H	1.52506159	-4.22484485	3.65372231
H	0.37692717	-2.98155797	5.45868390
H	-1.55388314	2.79387192	5.40134942
Ni	-0.14112076	1.43348107	2.95798534
H	-0.52542926	0.58616619	0.03225621
C	3.76343209	5.10672095	1.43751103
C	3.91238412	3.18783762	-0.66760524

C	4.67197050	5.26574741	0.37492271
H	3.69932789	5.83233493	2.24109986
C	4.74480549	4.32200762	-0.66118342
H	3.96047094	2.45431836	-1.46510801
H	5.32571837	6.13184938	0.35384658
H	5.45339344	4.47185706	-1.46949029

13P[3]

Total free energy (Ha) = -3666.895587

Potential energy (Ha) = -3666.410592

76

C	-1.32832115	0.08388901	0.55907076
C	-2.41089316	-0.32237706	-0.23428654
H	-2.28526129	-0.62883901	-1.26716991
C	-3.67549318	-0.34026341	0.34539892
S	-5.12078004	-0.90360547	-0.67707991
C	-3.90251329	0.00724741	1.67314016
H	-4.90140235	-0.04779981	2.09237693
C	-2.80181964	0.39963023	2.44620793
H	-2.97684224	0.66288127	3.48664467
C	-1.49554019	0.44934742	1.91271045

O	-4.51266944	-1.54375625	-2.04988245
O	-6.11860594	-1.79534388	0.25227835
N	-6.00838637	0.62937814	-0.98486268
C	-5.28599935	1.67241714	-1.72974527
C	-7.47779978	0.58640752	-0.88666122
H	-7.71598617	-0.16009573	-0.12148929
C	-8.27286553	0.27739096	-2.17092363
H	-7.77513687	1.56862974	-0.49211304
C	-5.11887379	1.49188360	-3.25384327
H	-4.29164745	1.78250615	-1.27498386
H	-5.82534521	2.60714364	-1.51847536
C	-8.00664572	-1.12047398	-2.75134879
H	-8.07428622	1.04784474	-2.92776803
H	-9.33870904	0.37244841	-1.91262541
H	-4.61455435	0.53784053	-3.44219920
C	-4.31512033	2.65374165	-3.86037809
H	-6.10256420	1.43066748	-3.73476957
H	-3.31466158	2.71948082	-3.41371675
H	-4.81615676	3.61713234	-3.69711268
H	-4.18852150	2.52305669	-4.94065361
H	-6.96055560	-1.24202971	-3.05328902
H	-8.63587704	-1.30483156	-3.63020504
H	-8.21926108	-1.89760231	-2.00828352
N	1.41824260	1.91100394	1.78971813

C	1.32311095	3.28095421	2.00955059
C	2.29995540	1.65023252	0.74837915
O	0.57948095	3.78067130	2.88942025
C	2.22693936	3.97542720	1.04214330
O	2.58896962	0.51879540	0.29553997
C	2.83023408	2.97145776	0.26569878
C	-2.34210368	2.42521911	7.68649936
C	-1.62146961	1.36018280	6.89897833
C	-1.40929915	0.06839009	7.41418378
C	-0.72458859	-0.88832095	6.66578488
C	-0.25396553	-0.55692059	5.38752807
C	0.50452182	-1.46939897	4.50832734
N	0.91794278	-0.92913465	3.32854875
C	1.63466191	-1.65458457	2.44735799
C	1.97550241	-2.99558713	2.68943478
C	2.75157781	-3.78524199	1.66598138
C	1.54835266	-3.55826297	3.90275584
C	0.81553962	-2.79840932	4.81685396
N	-0.47658098	0.68856770	4.88484707
C	-1.12948014	1.61814235	5.61321739
H	-3.34373903	2.09103416	7.98211720
H	-2.45321251	3.34363116	7.10349983
H	-1.79742287	2.67579933	8.60502541
H	-1.77810968	-0.18381848	8.40339641

H	-0.55806383	-1.87710814	7.07416184
H	1.94507765	-1.13179751	1.54556221
H	2.07461669	-4.36938650	1.02877974
H	3.44202898	-4.48845326	2.14334876
H	3.32729318	-3.12518192	1.01095798
H	1.79102439	-4.59064224	4.13423401
H	0.49420882	-3.24121579	5.75157199
H	-1.24573727	2.58898138	5.14399517
Ni	0.15034747	0.93865313	2.94832186
H	-0.33831061	0.10792654	0.11051742
C	2.51222810	5.31847981	0.83816895
C	3.73675461	3.28178352	-0.73768623
C	3.43039084	5.64284662	-0.17744108
H	2.04171904	6.08781935	1.44075101
C	4.03273857	4.64066401	-0.95253597
H	4.19758548	2.50199878	-1.33433945
H	3.67630811	6.68300928	-0.36569396
H	4.73656593	4.91912969	-1.73045170

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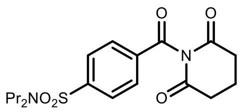
NMR Spectra

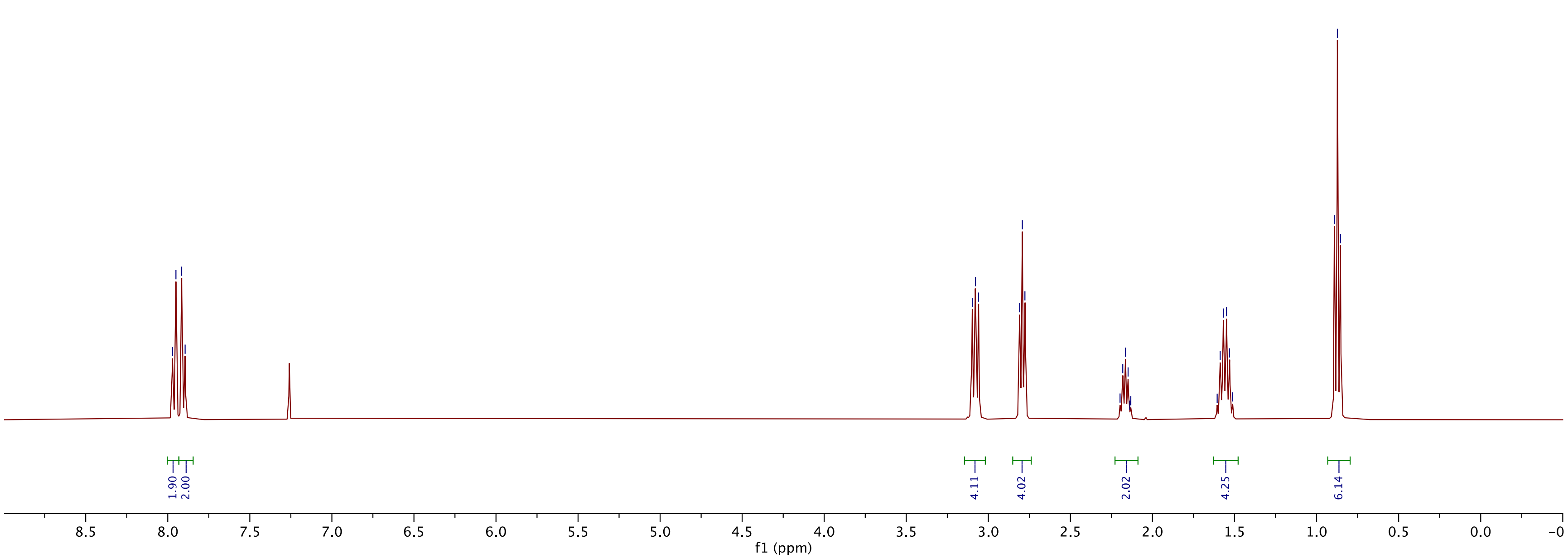
Starting Materials

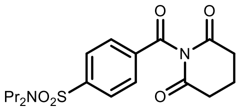


1

^{1}H NMR

(400 MHz, $CDCl_3$)

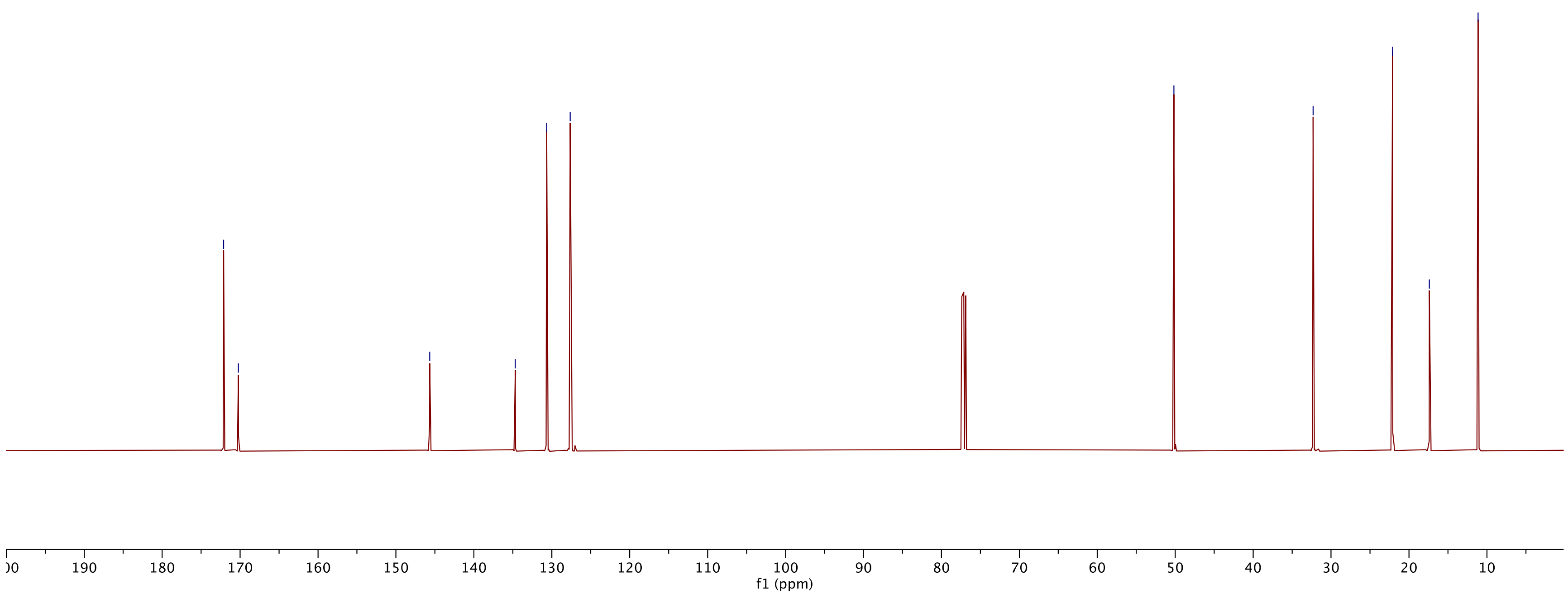


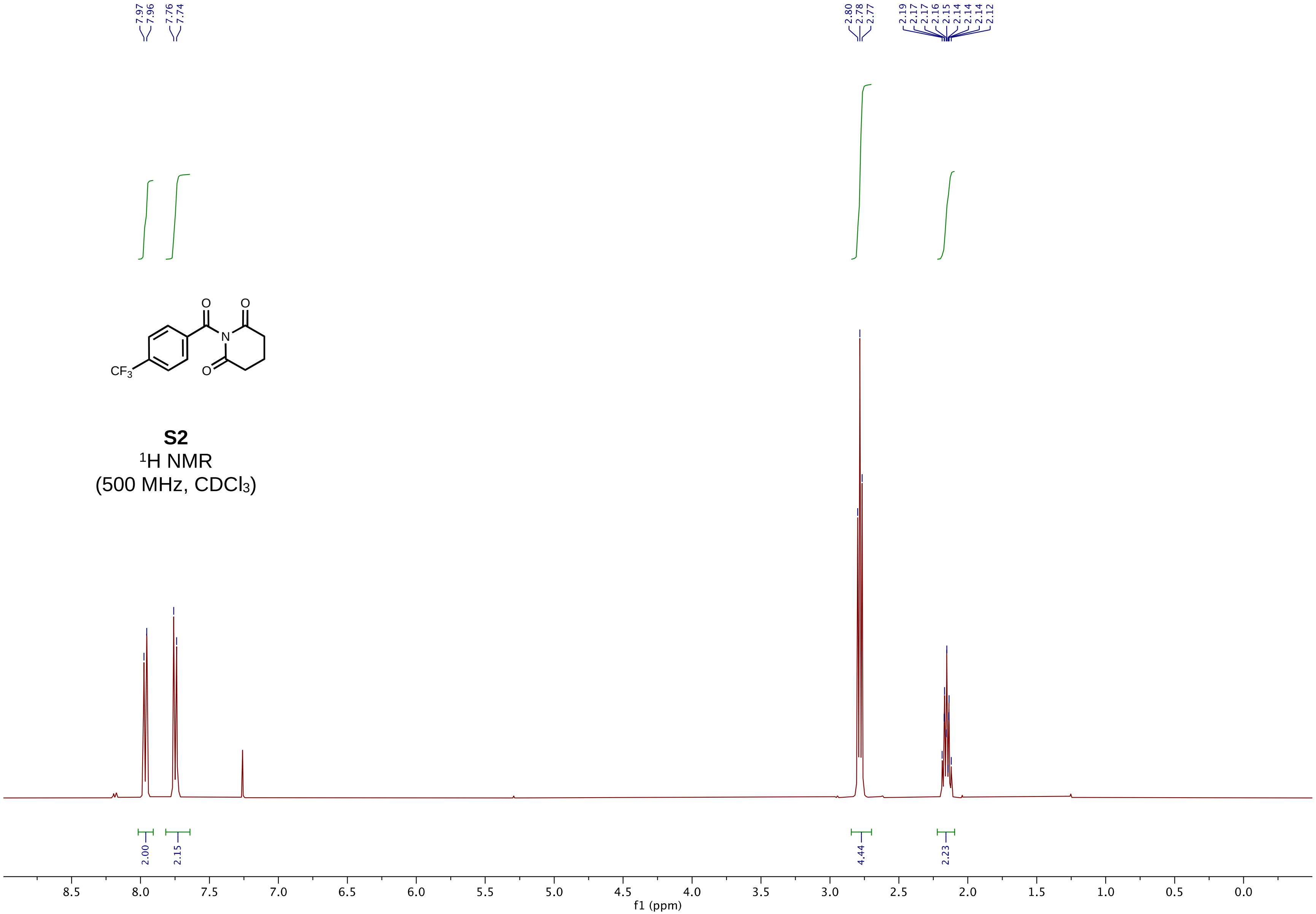


1

^{13}C NMR

(126 MHz, $CDCl_3$)





S2

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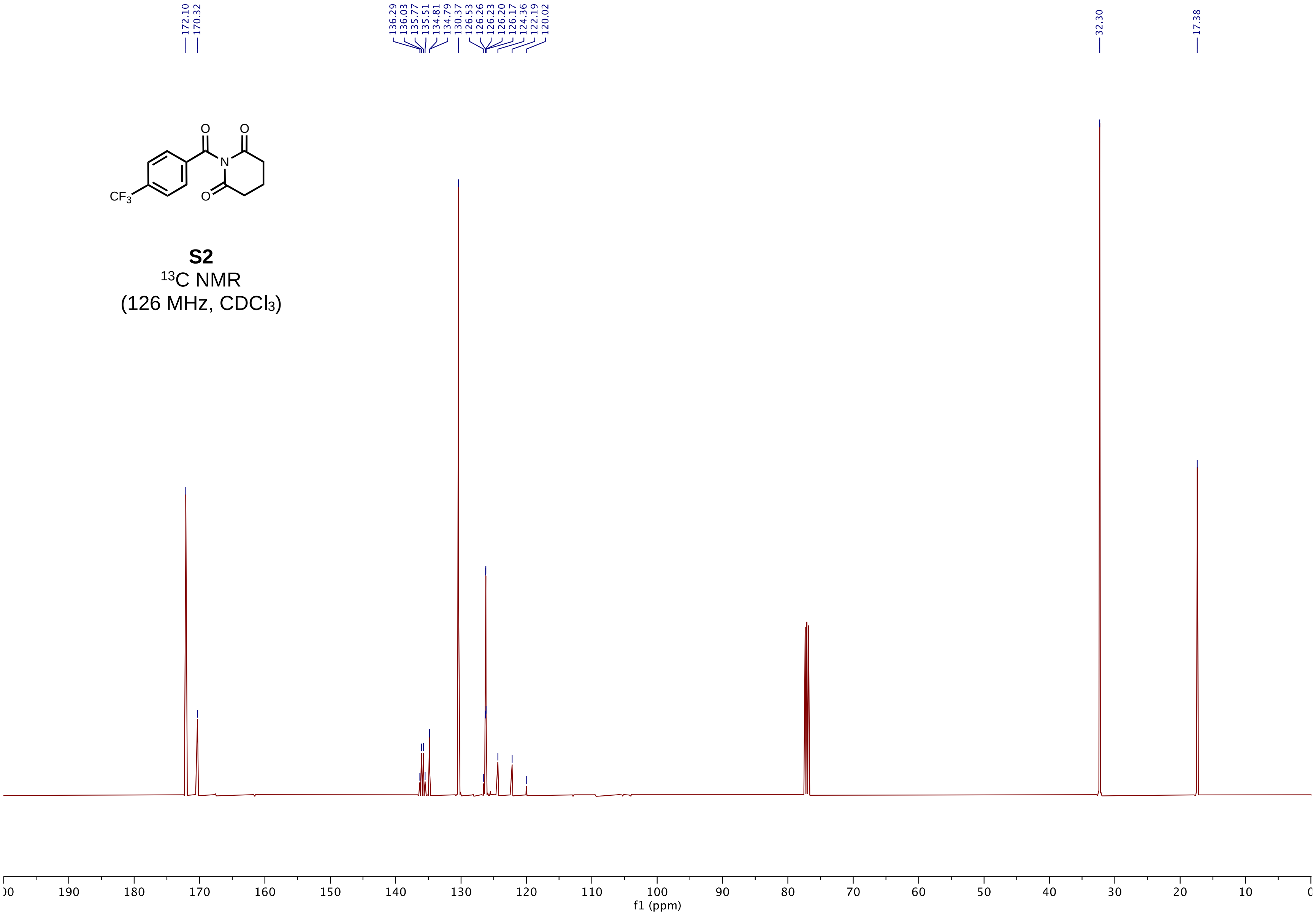
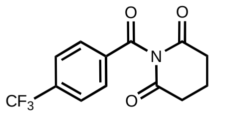
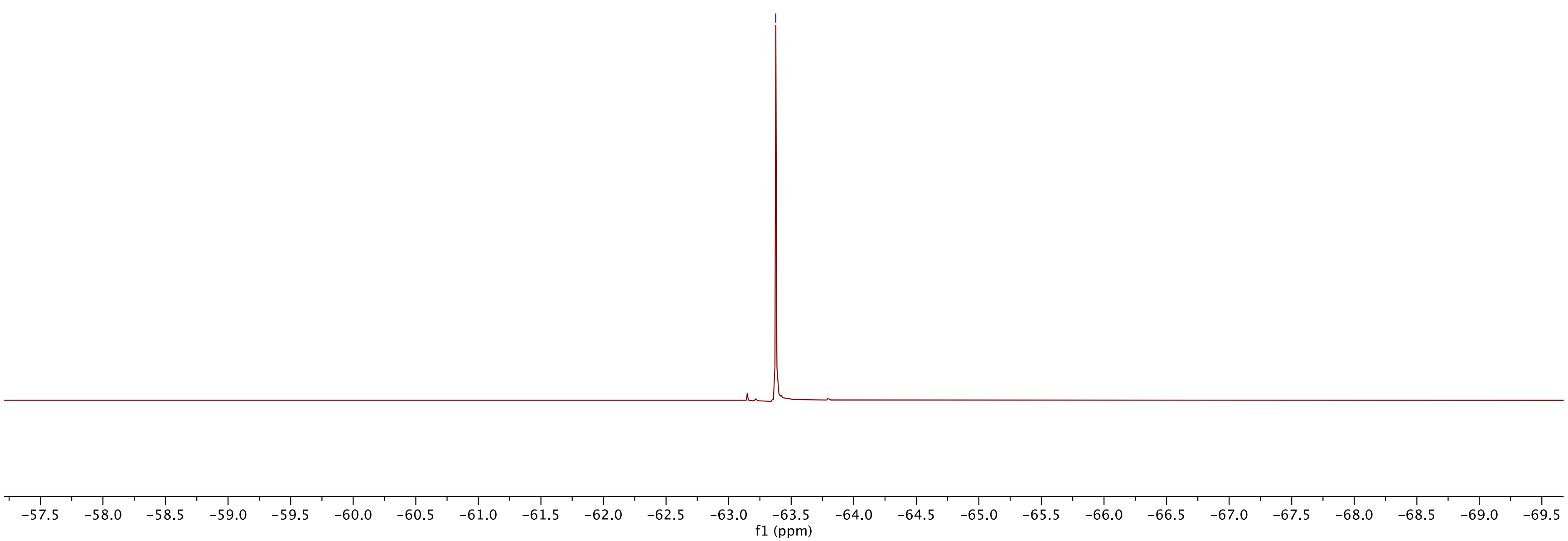


172.10
170.32
136.29
136.03
135.77
135.51
134.81
134.79
130.37
126.53
126.26
126.23
126.20
126.17
124.36
122.19
120.02
32.30
17.38
CF3
O
N
S2
13C NMR
(126 MHz, CDCl3)
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)



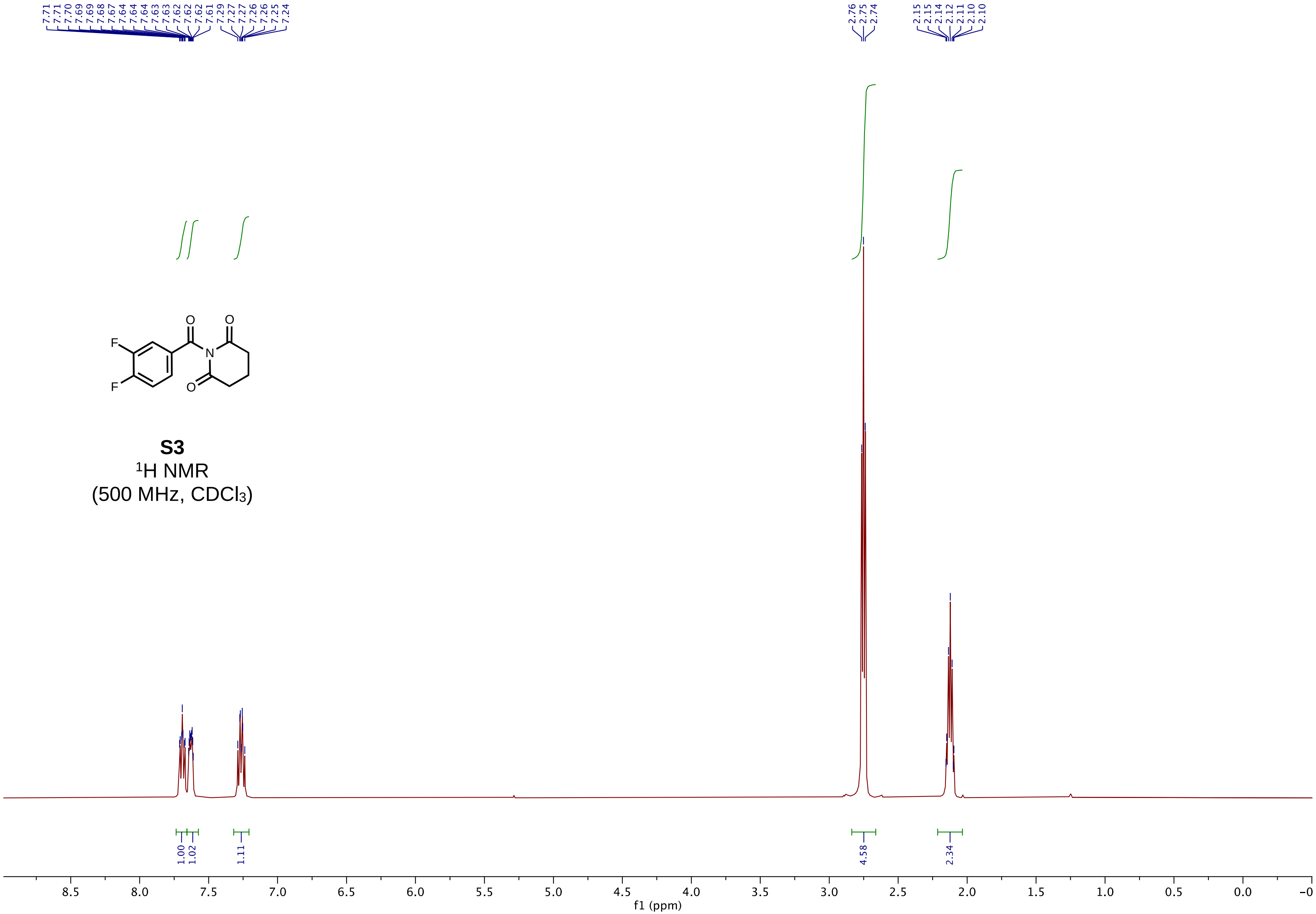
S2
^{19}F NMR
(471 MHz, $CDCl_3$)

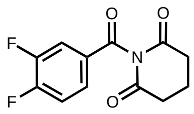


S3

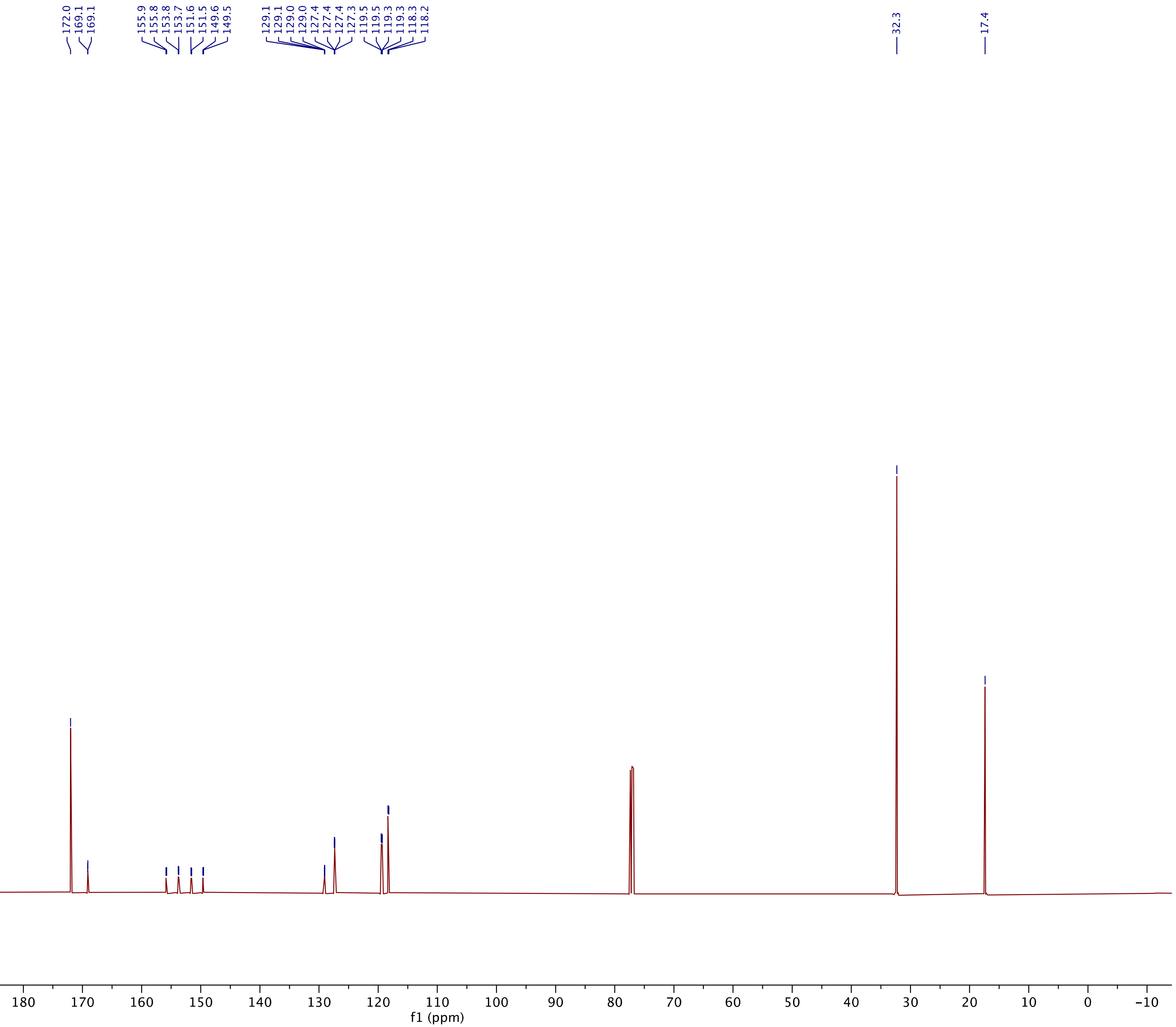
^{1}H NMR

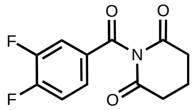
(500 MHz, $CDCl_3$)



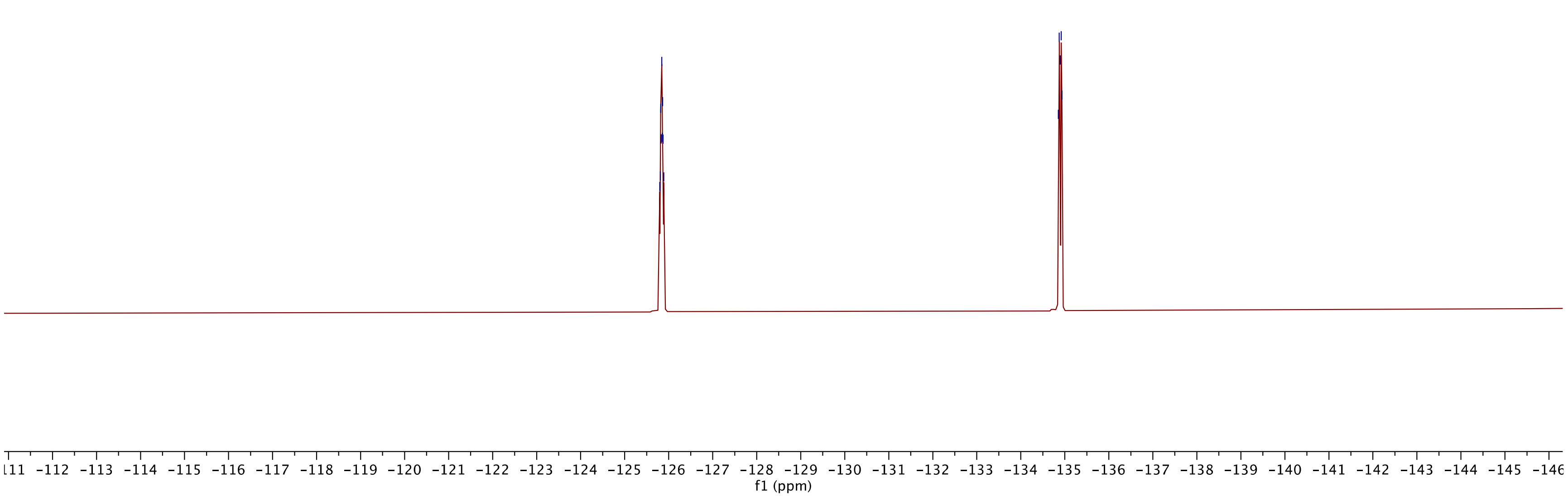


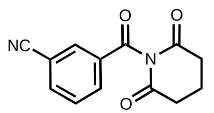
S3
^{13}C NMR
(126 MHz, $CDCl_3$)





S3
^{19}F NMR
(471 MHz, $CDCl_3$)





S4
^{1}H NMR
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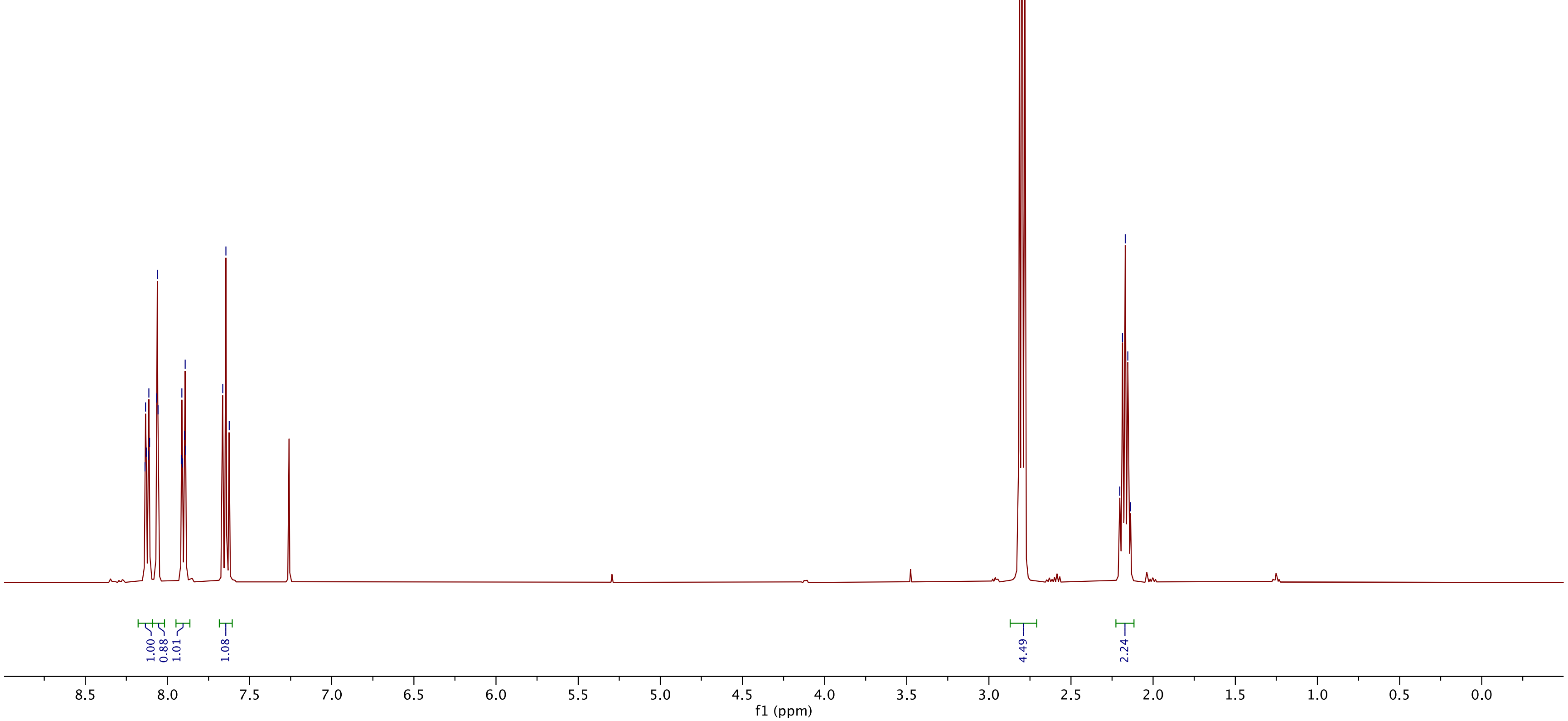
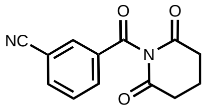
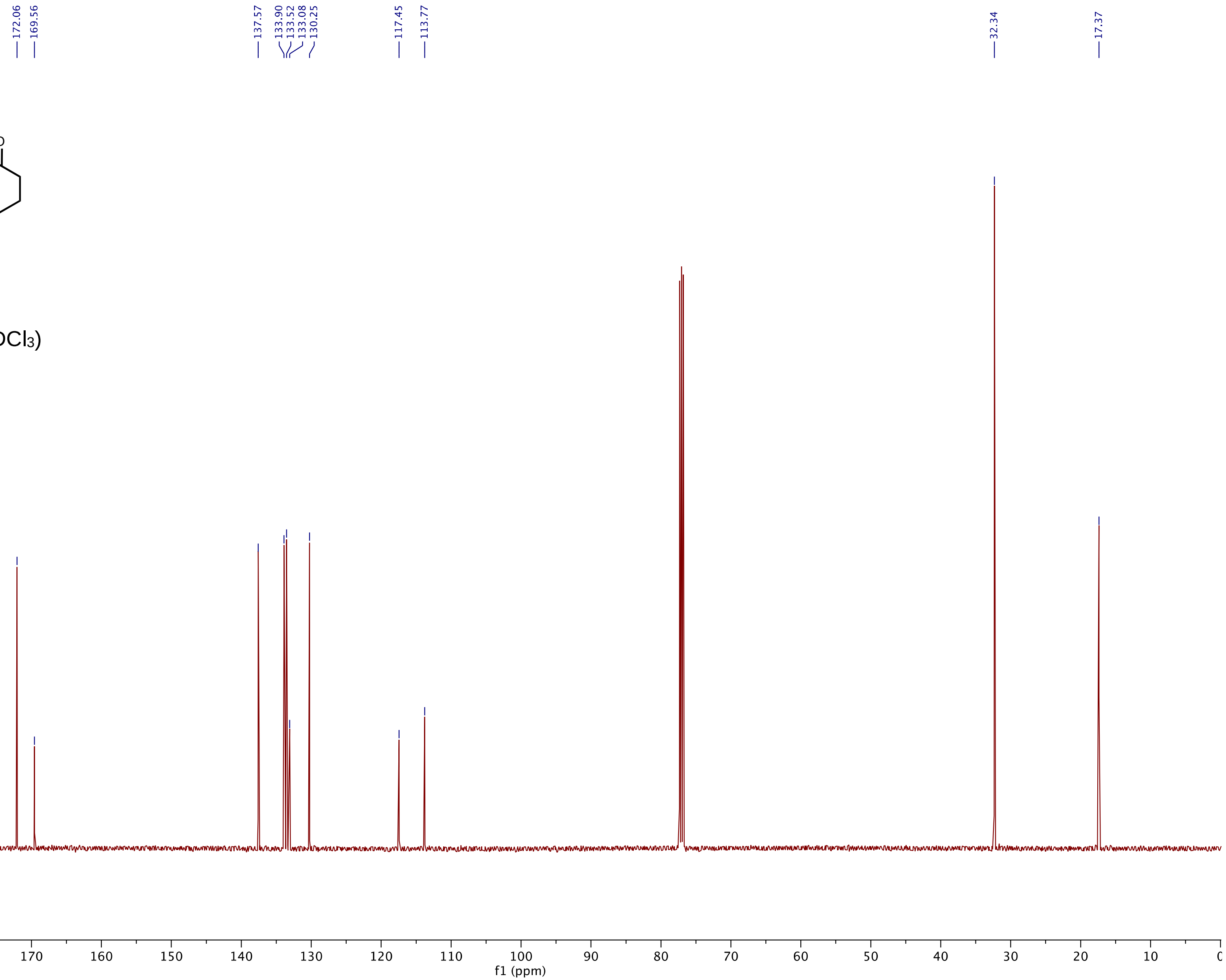


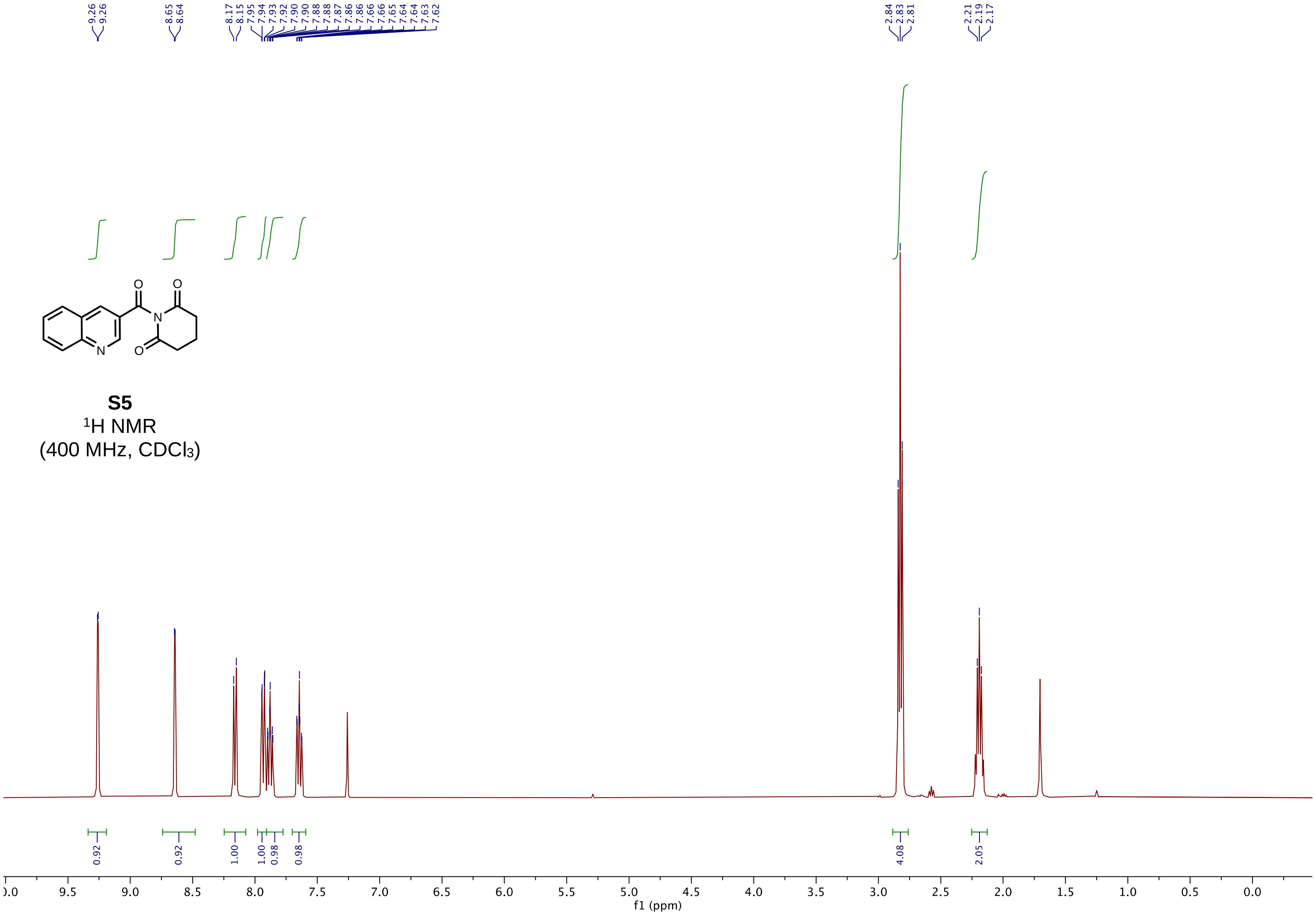


S4

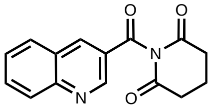
^{13}C NMR

(126 MHz, $CDCl_3$)

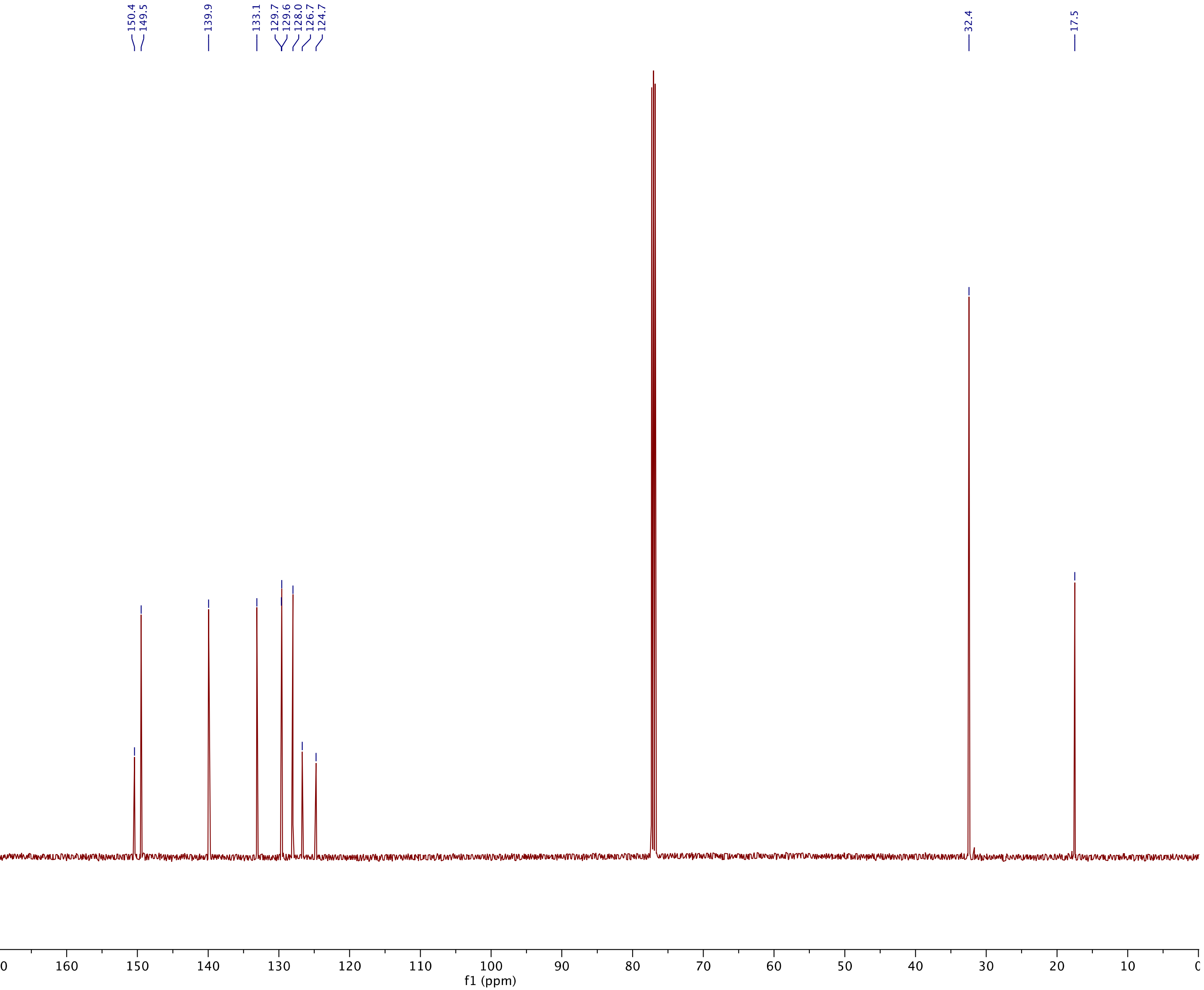


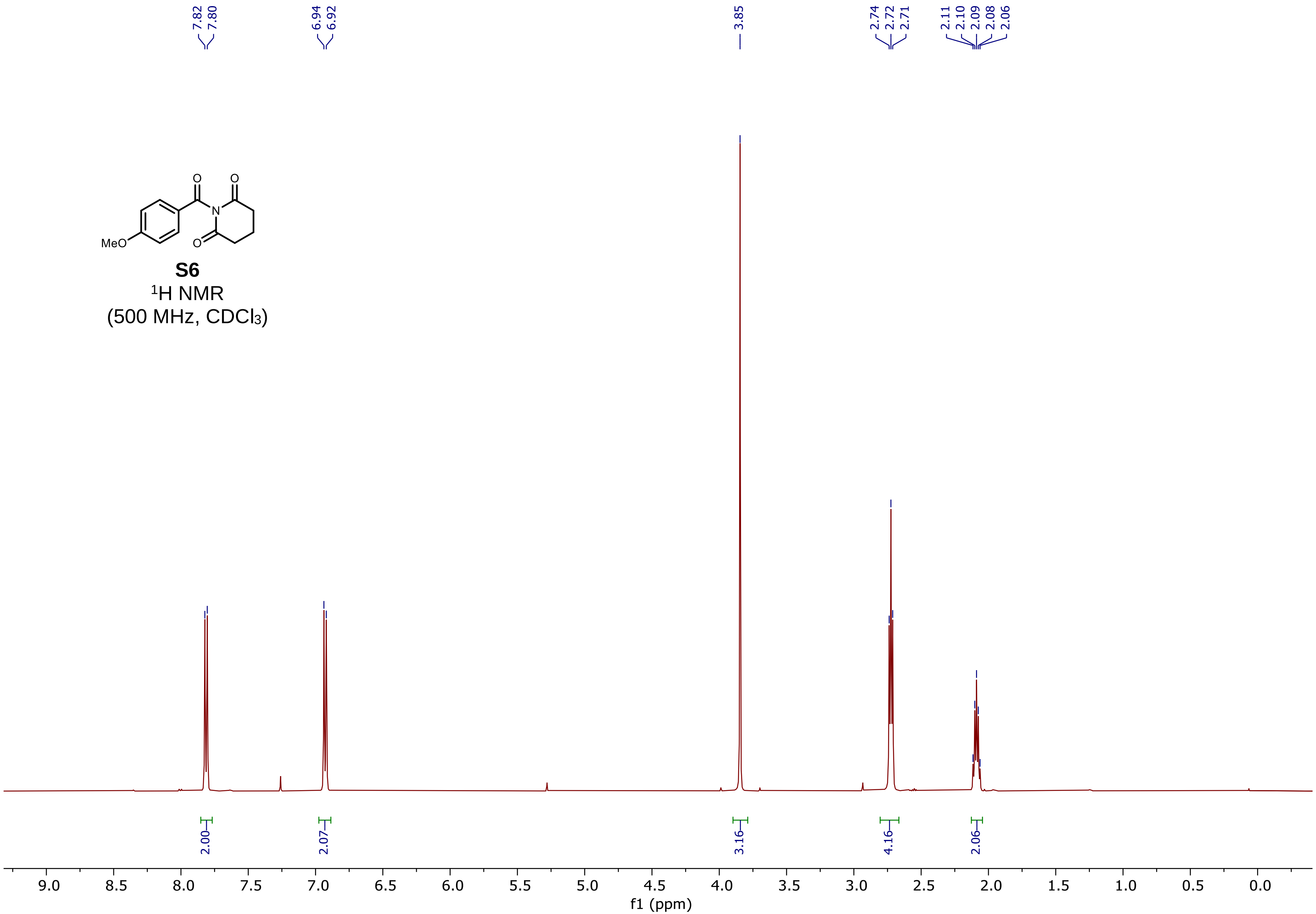


S5
^{1}H NMR
(400 MHz, $CDCl_3$)

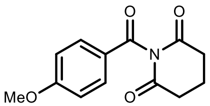


S5
^{13}C NMR
(126 MHz, $CDCl_3$)





7.82
7.80
6.94
6.92
3.85
2.74
2.72
2.71
2.11
2.10
2.09
2.08
2.06
MeO
O
N
S6
1H NMR
(500 MHz, CDCl3)
2.00
2.07
3.16
4.16
2.06
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)



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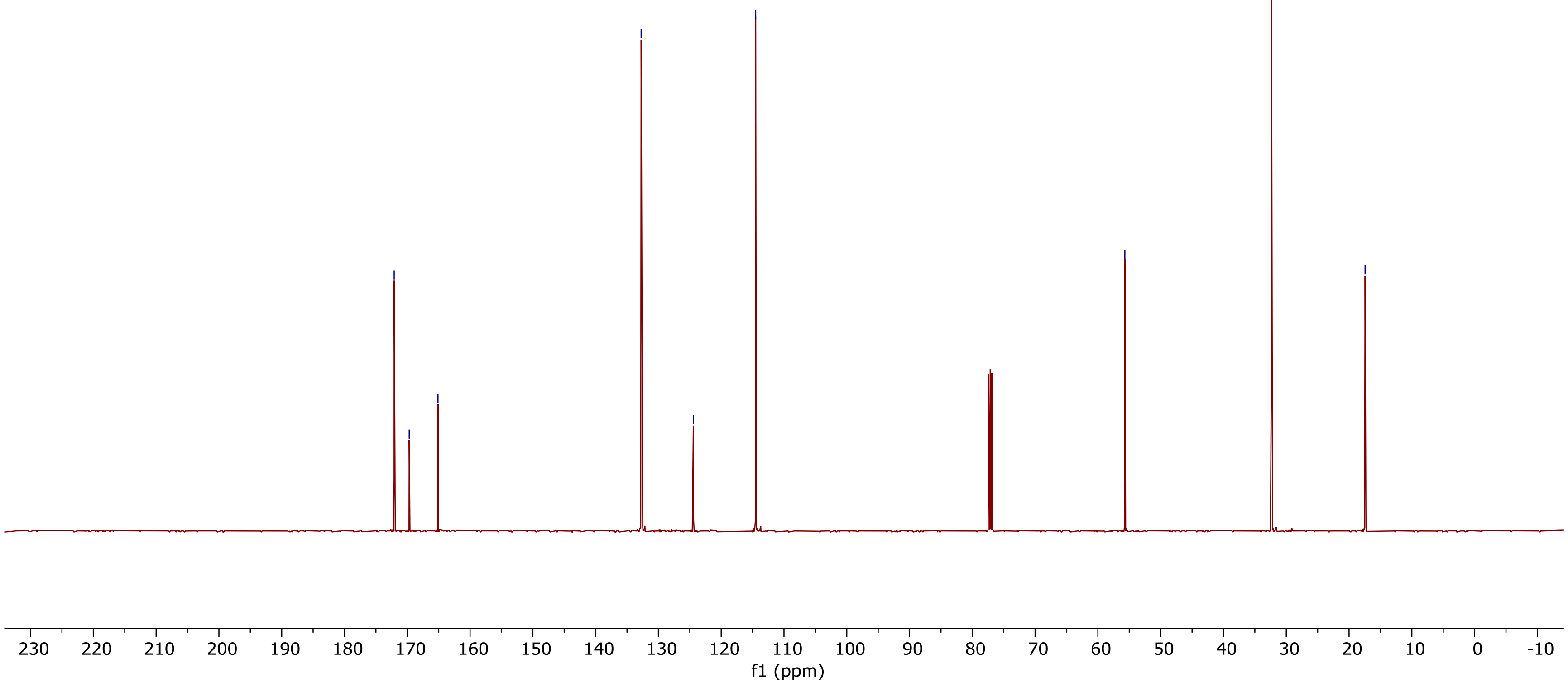
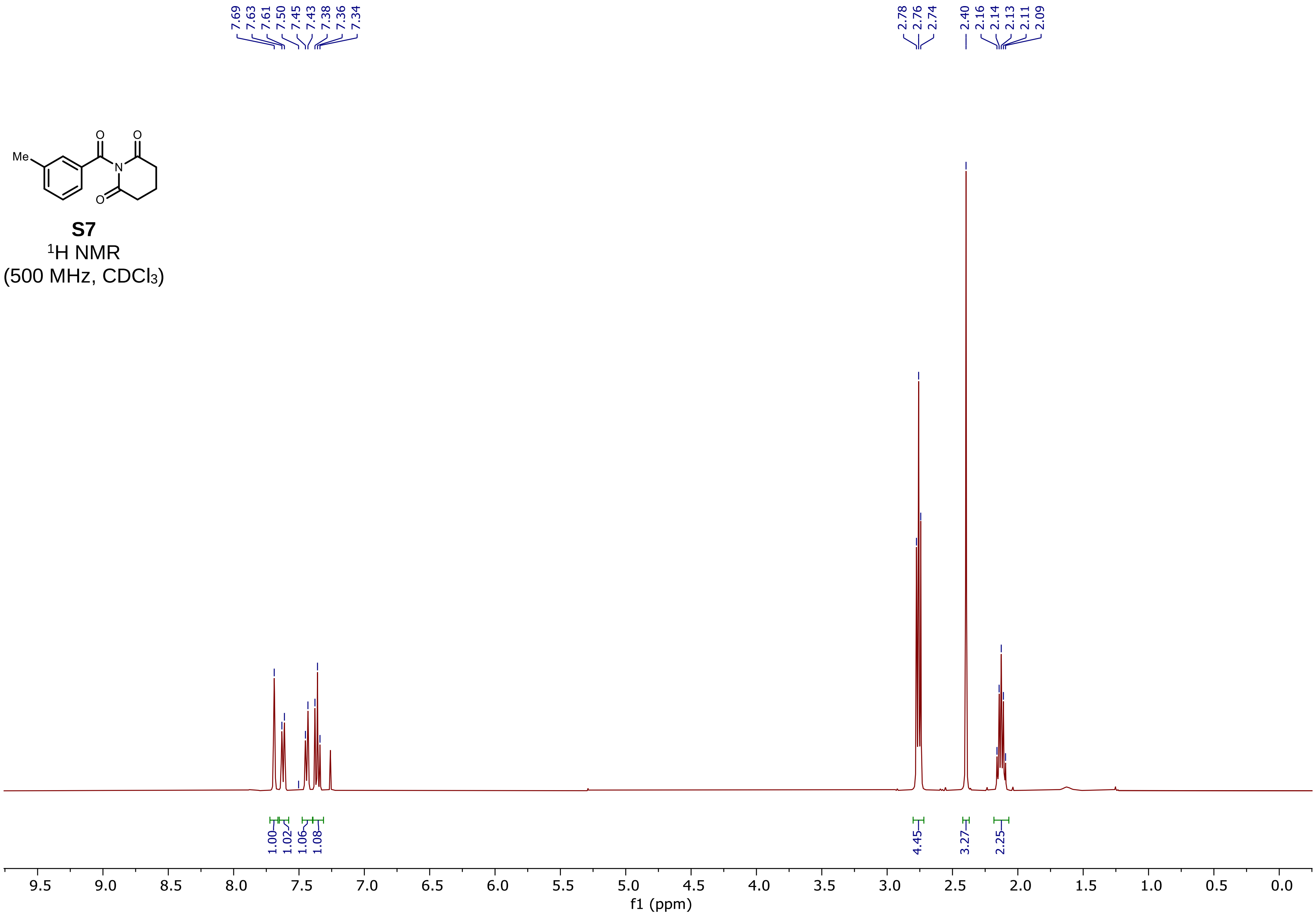
(126 MHz, $CDCl_3$)





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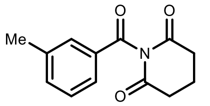
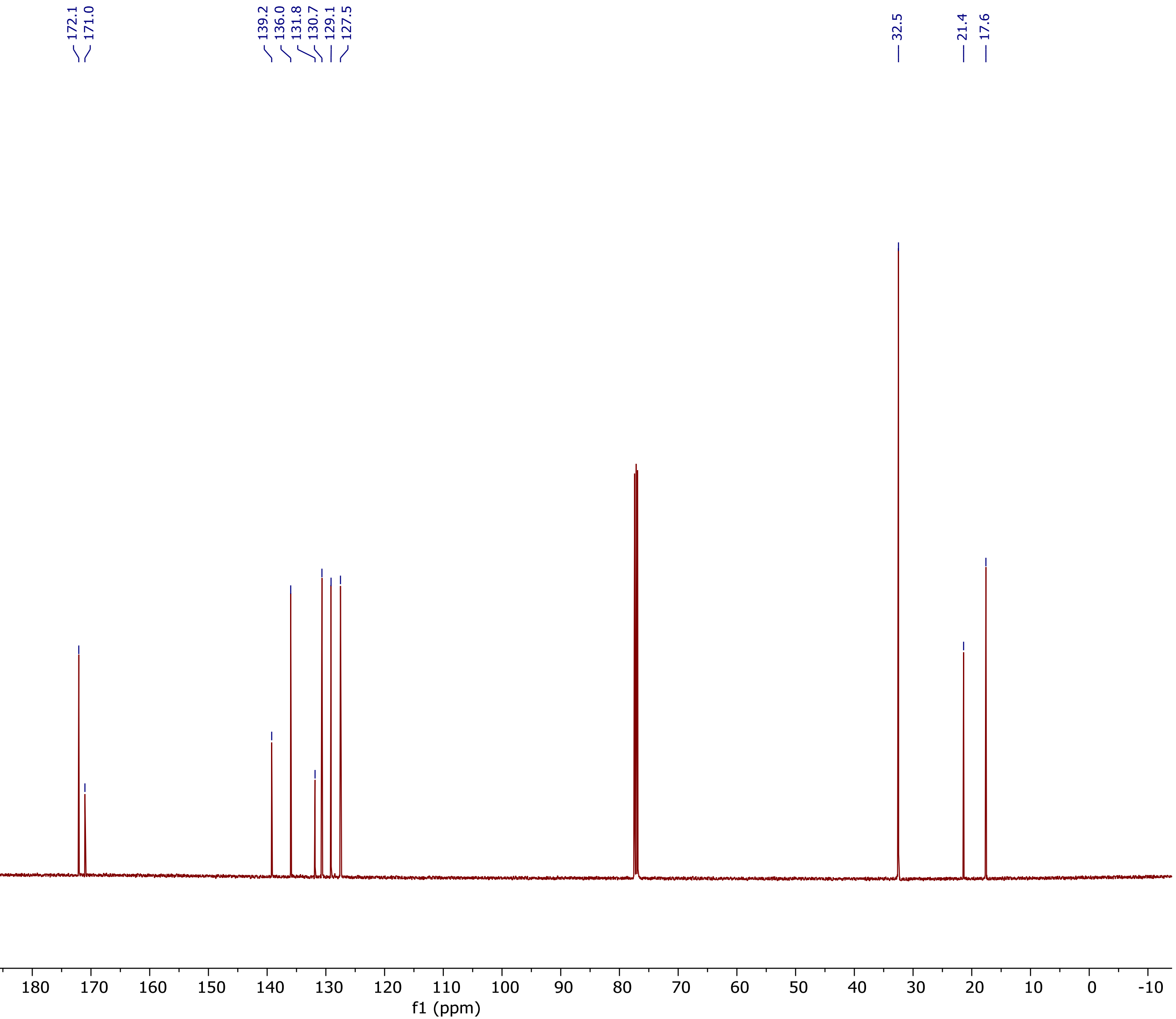
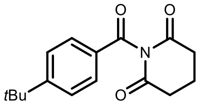


S7

^{13}C NMR

(126 MHz, $CDCl_3$)





S8
^{1}H NMR
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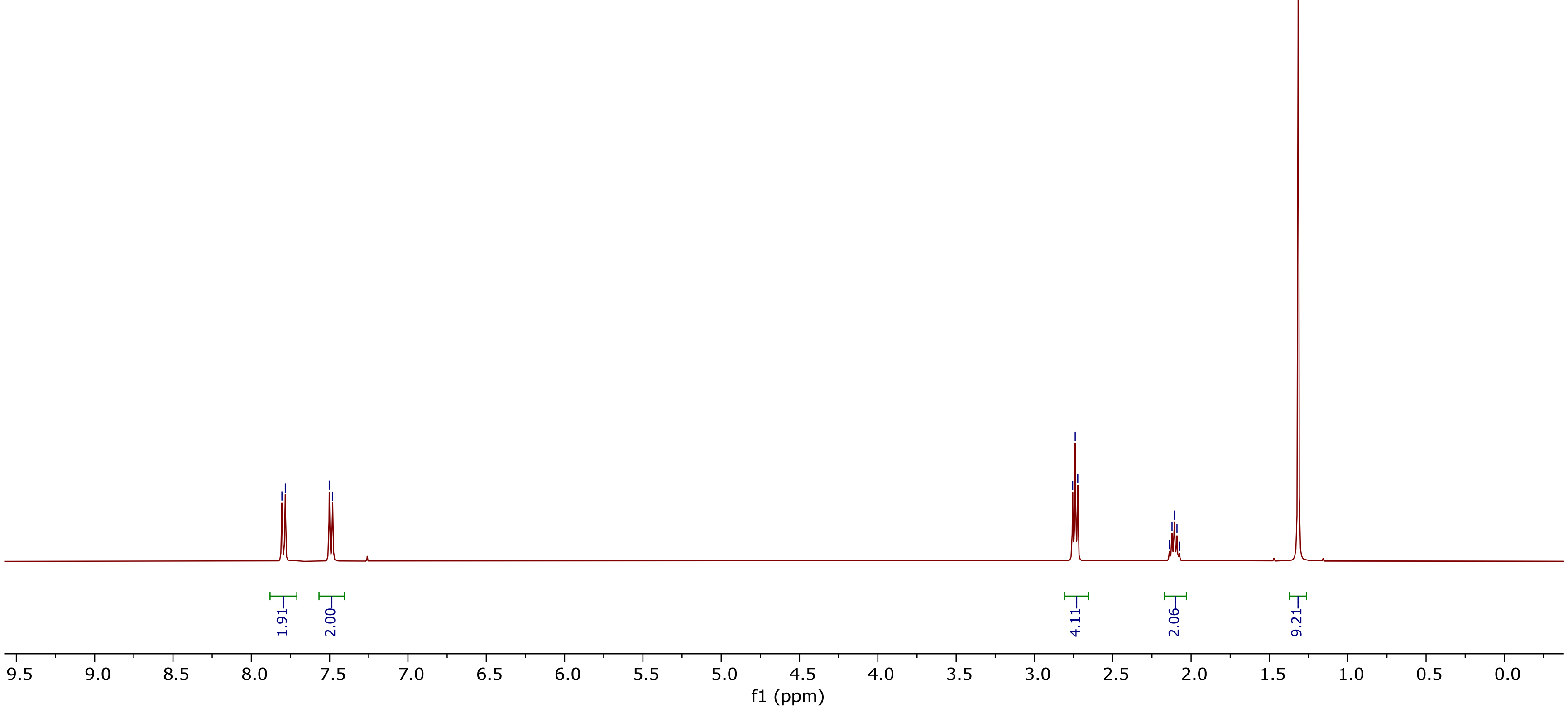
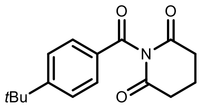
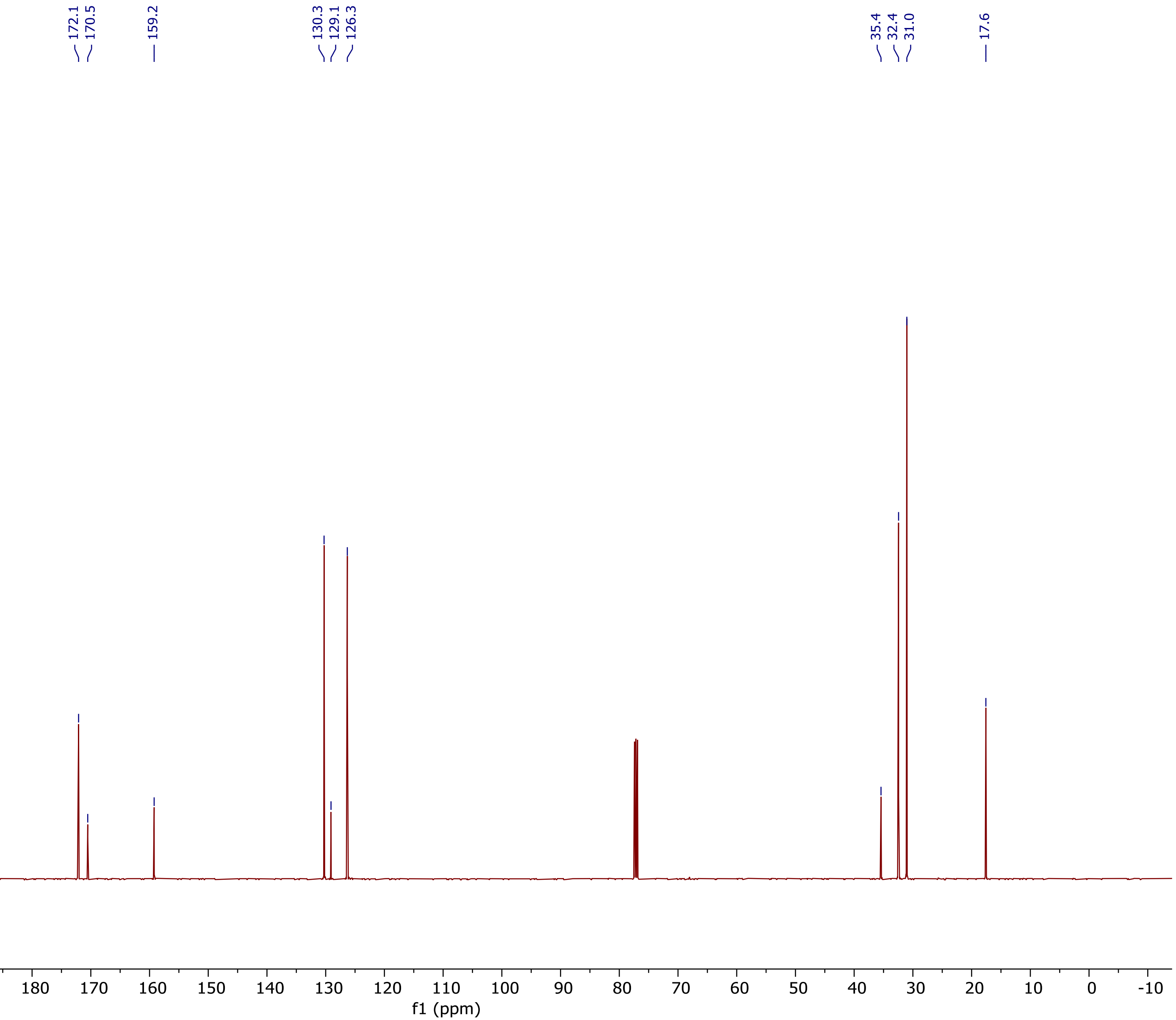
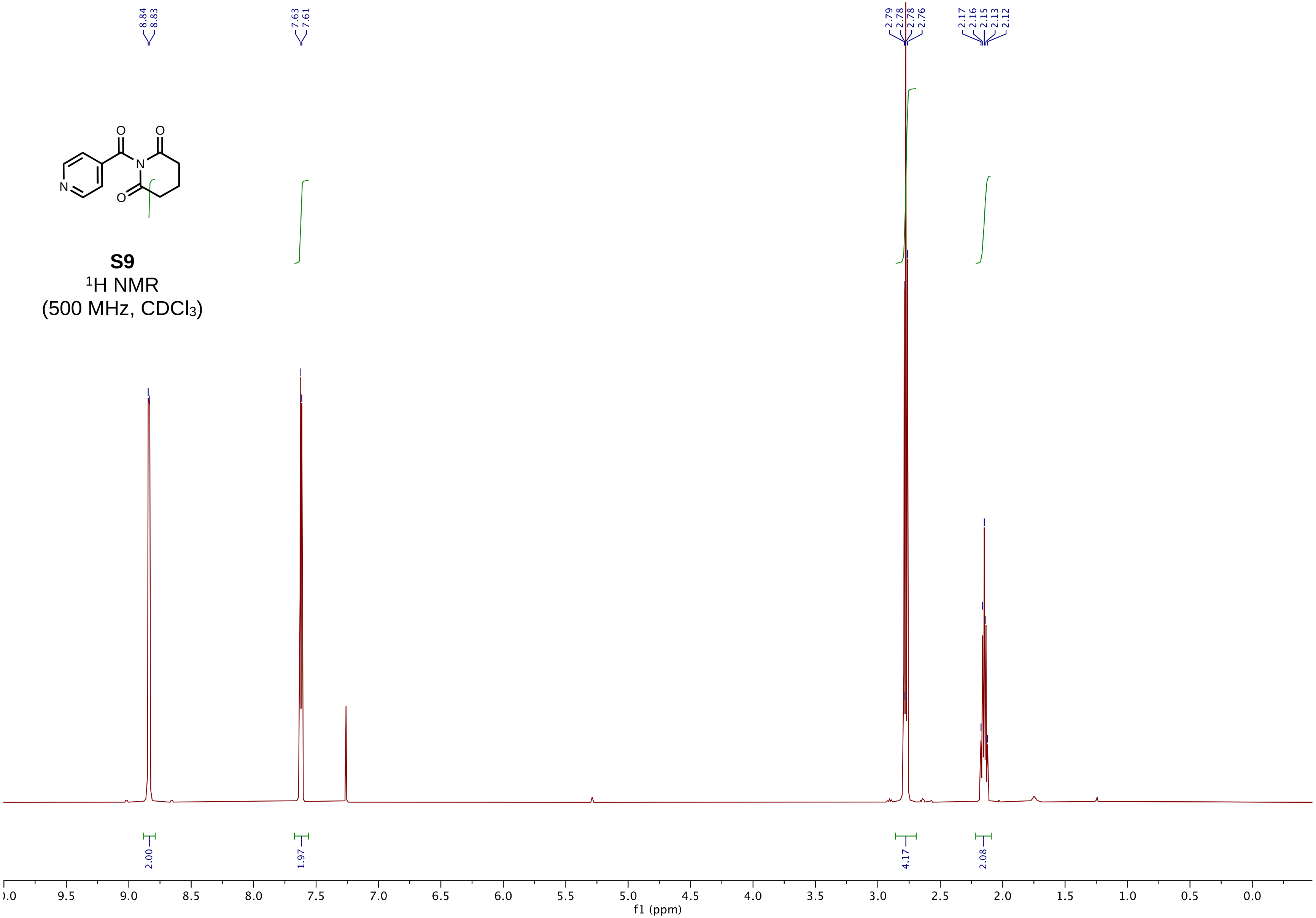




S8
^{13}C NMR
(126 MHz, $CDCl_3$)

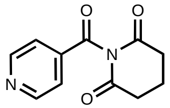




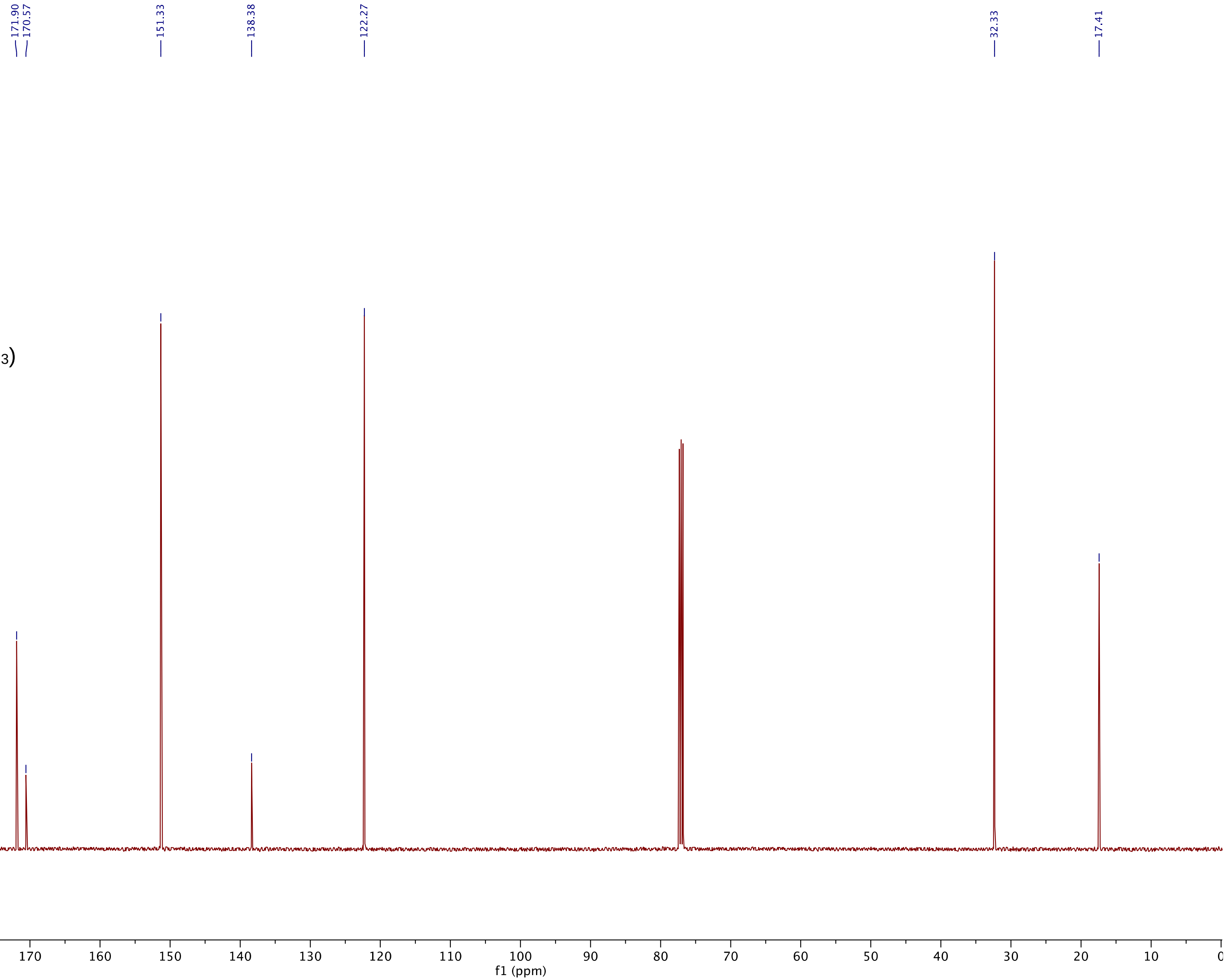
S9

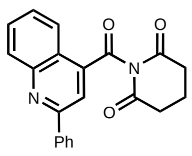
^{1}H NMR

(500 MHz, $CDCl_3$)

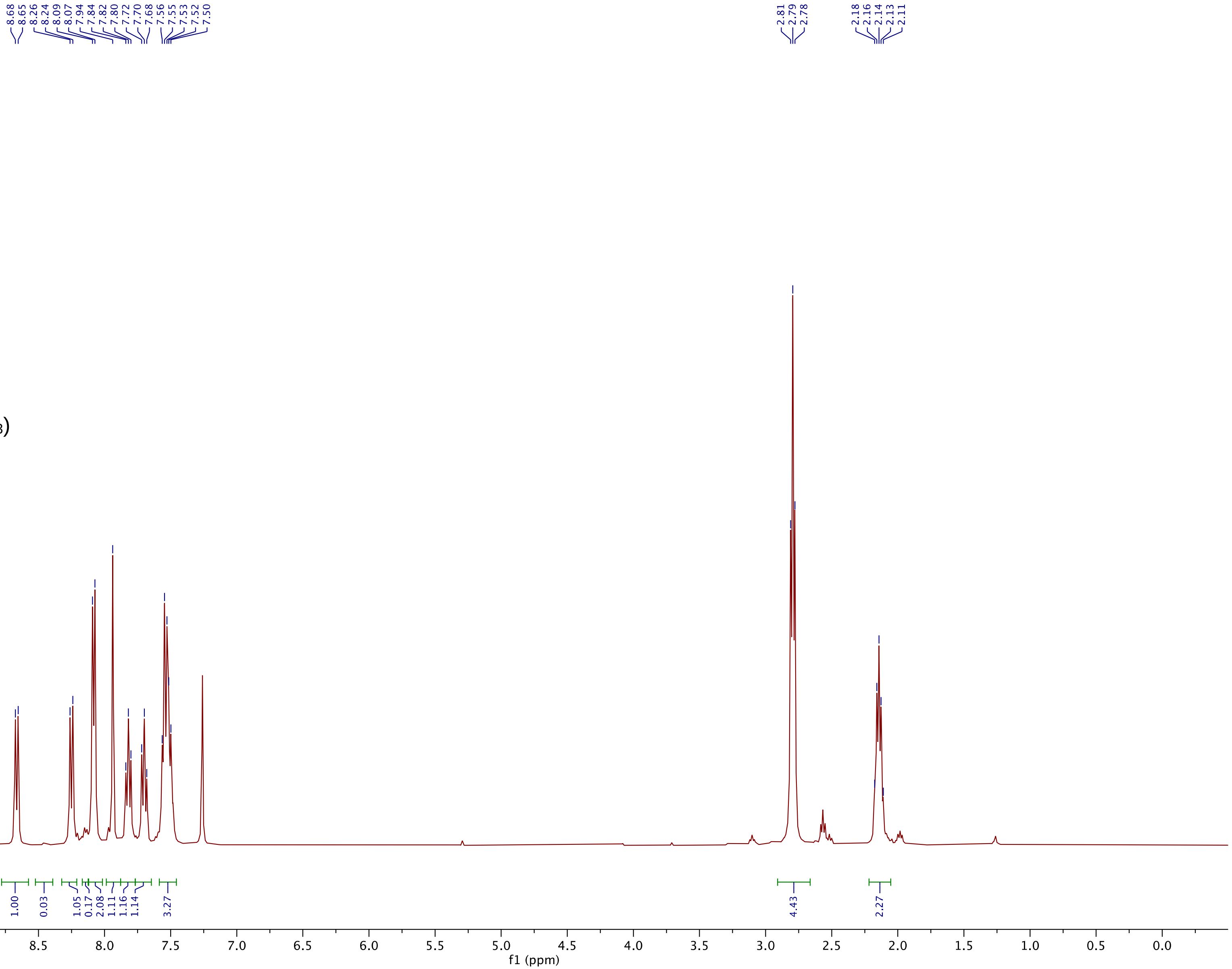


S9
^{13}C NMR
(126 MHz, $CDCl_3$)

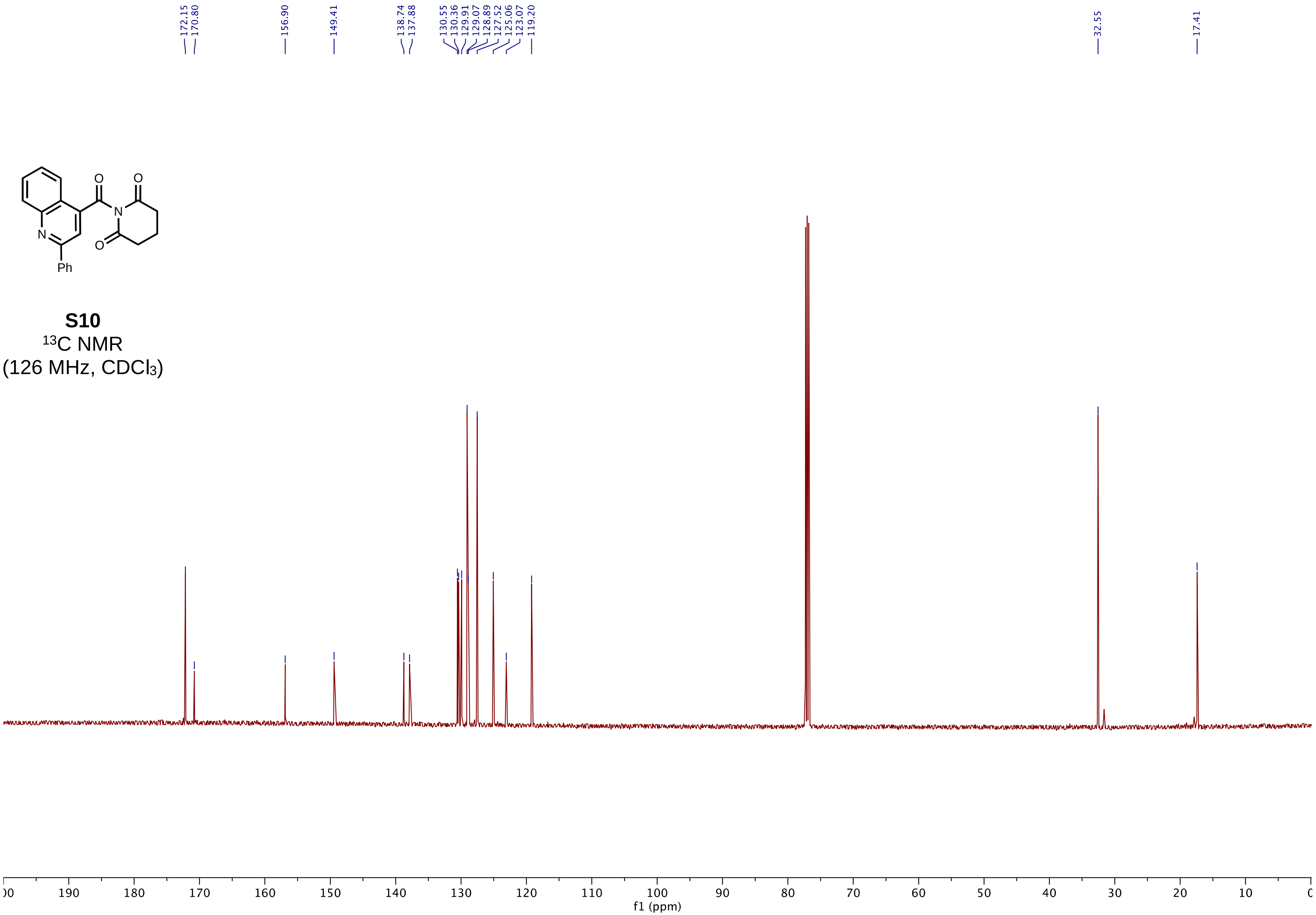


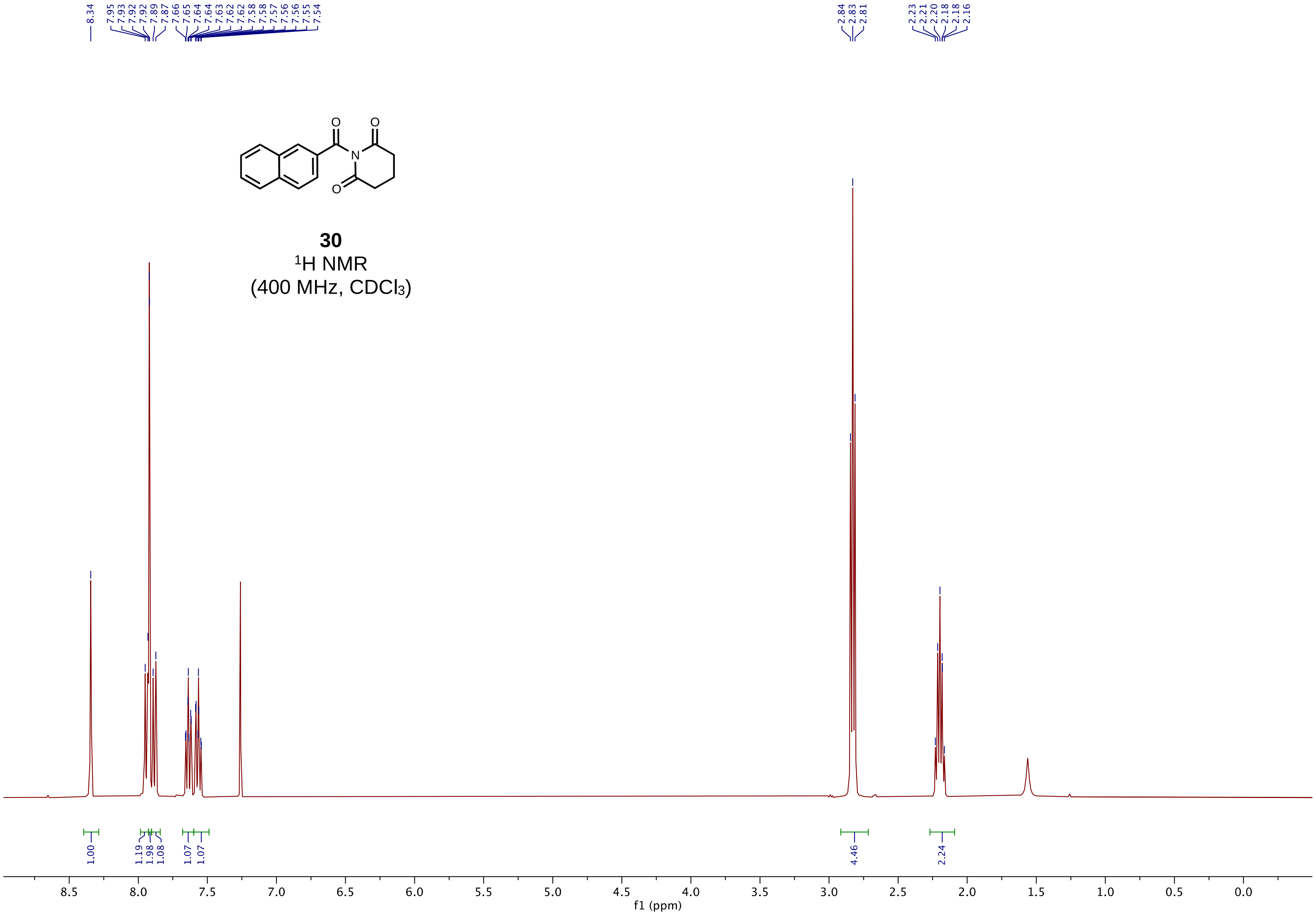


S10
^{1}H NMR
(400 MHz, $CDCl_3$)



S10
^{13}C NMR
(126 MHz, $CDCl_3$)

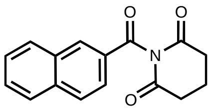




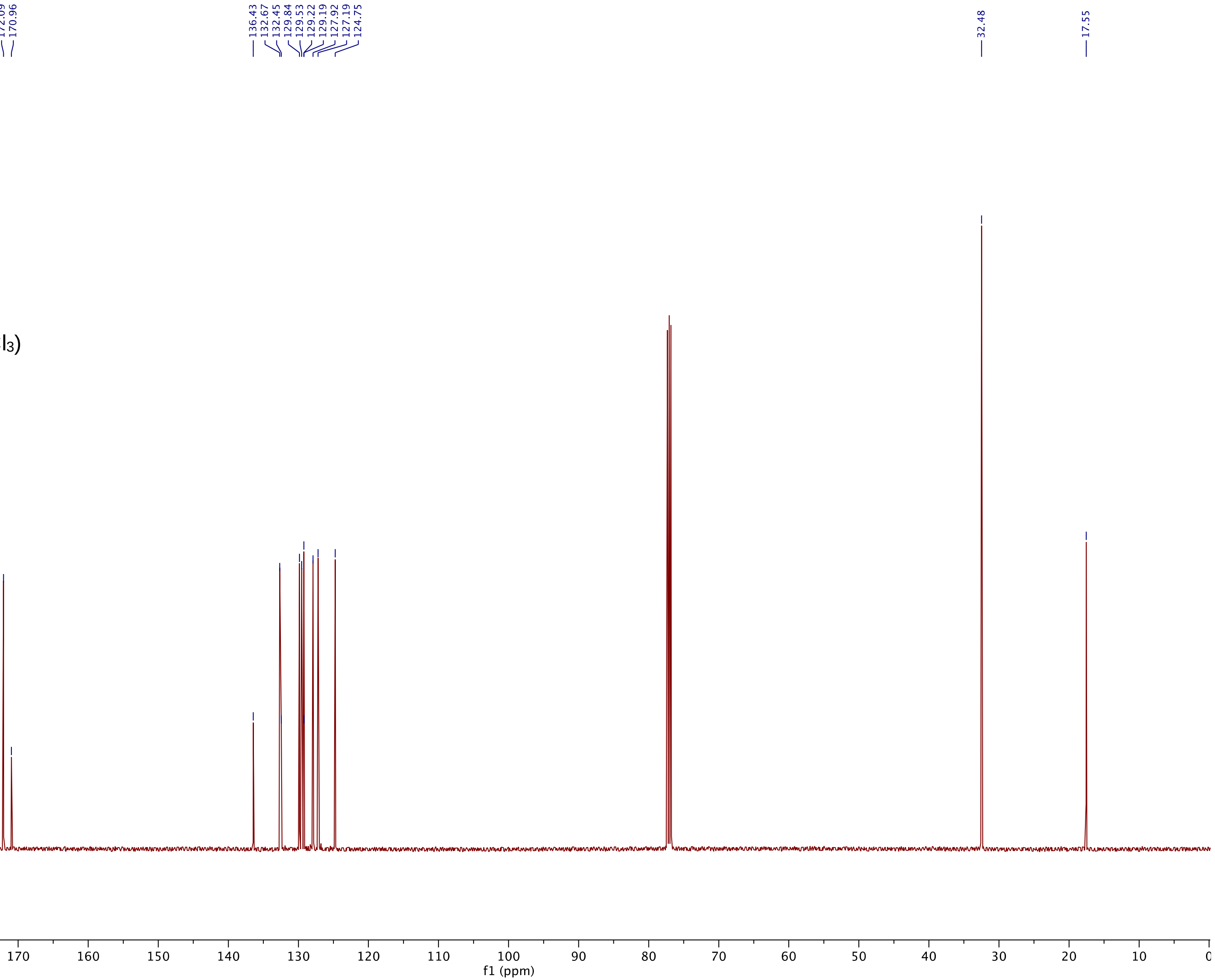
30

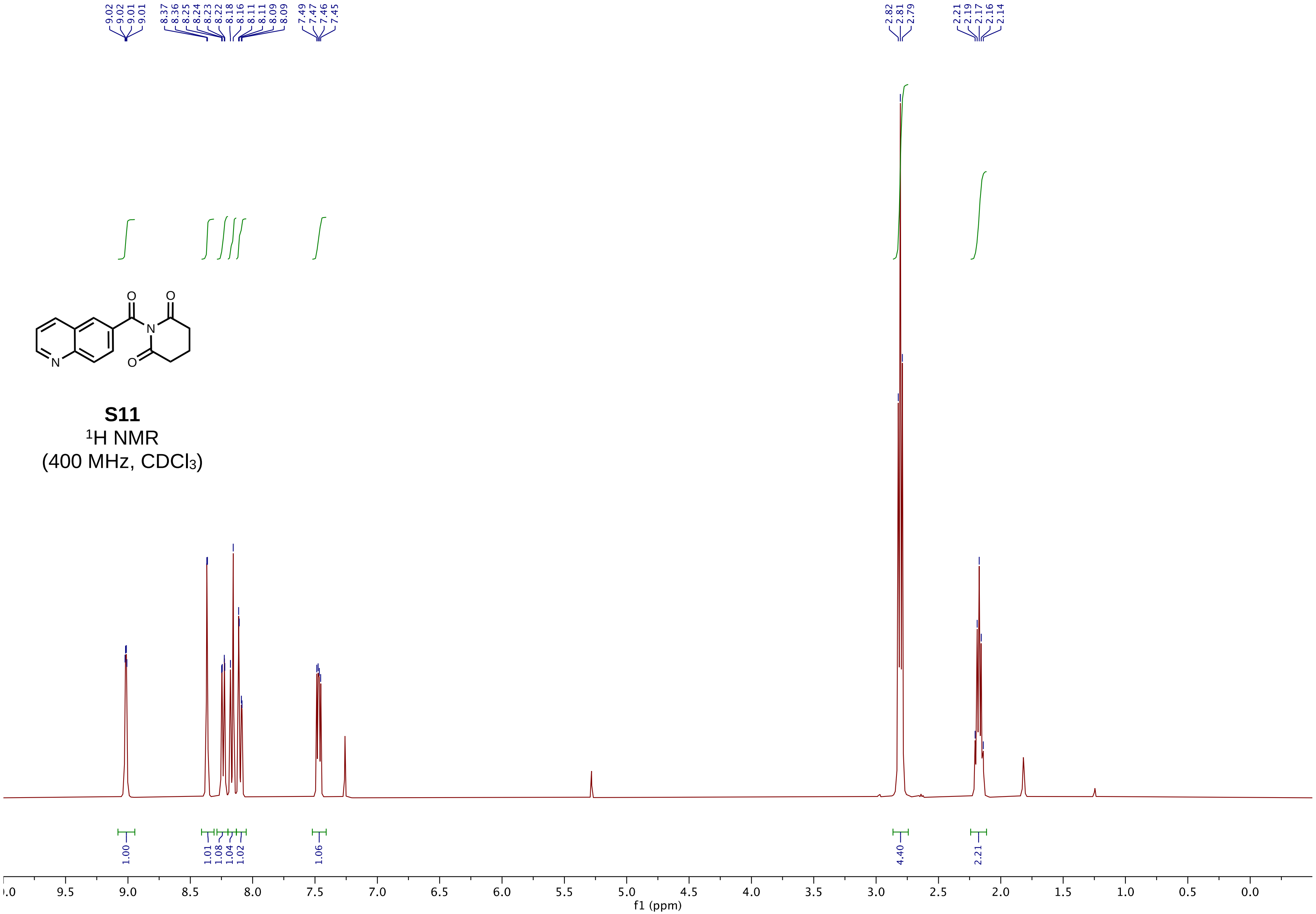
^{1}H NMR

(400 MHz, $CDCl_3$)



30
^{13}C NMR
(126 MHz, $CDCl_3$)

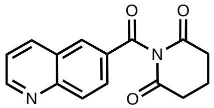




S11

^{1}H NMR

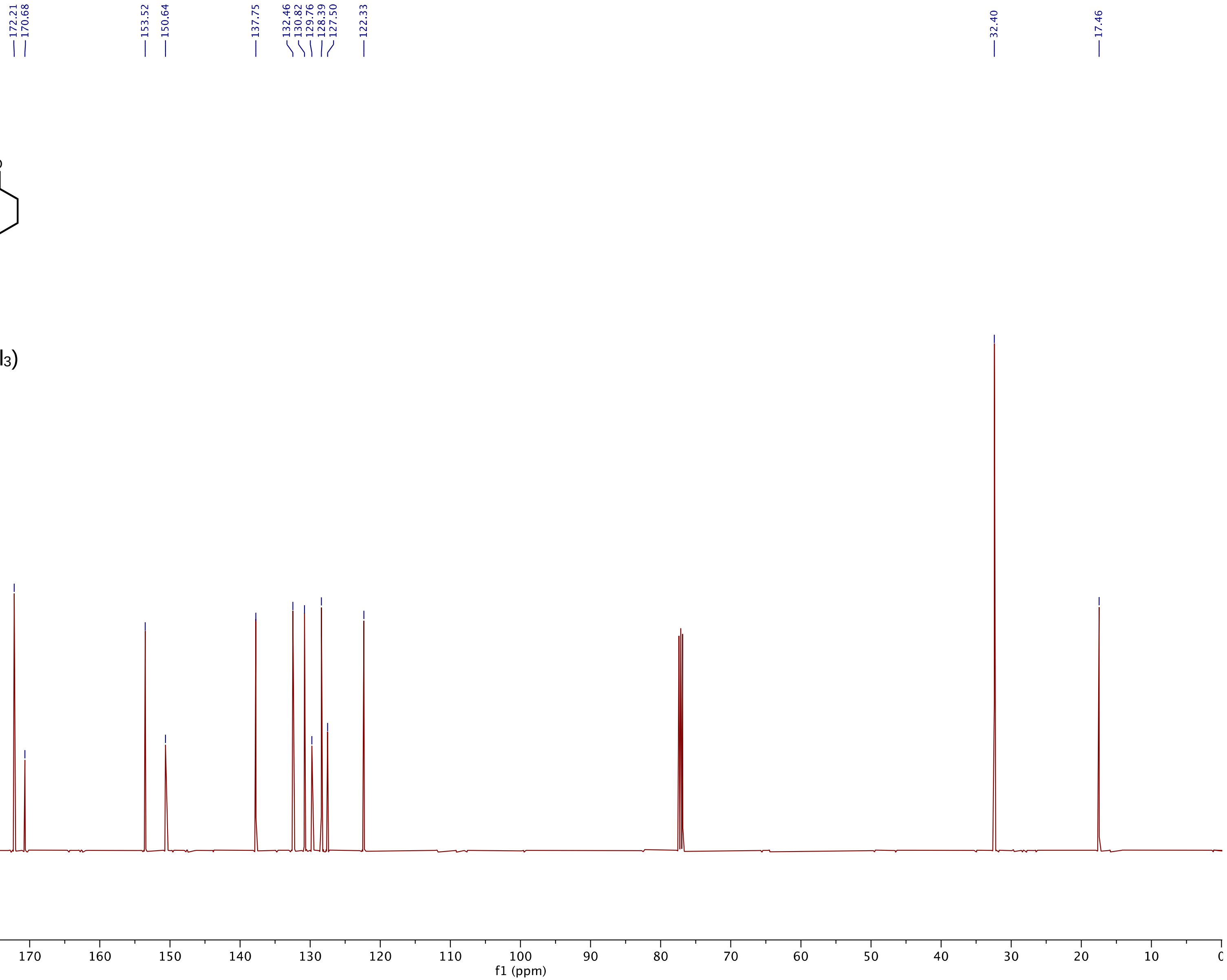
(400 MHz, $CDCl_3$)

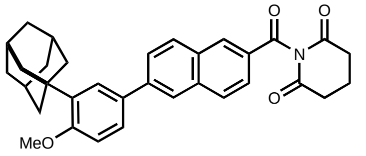


S11

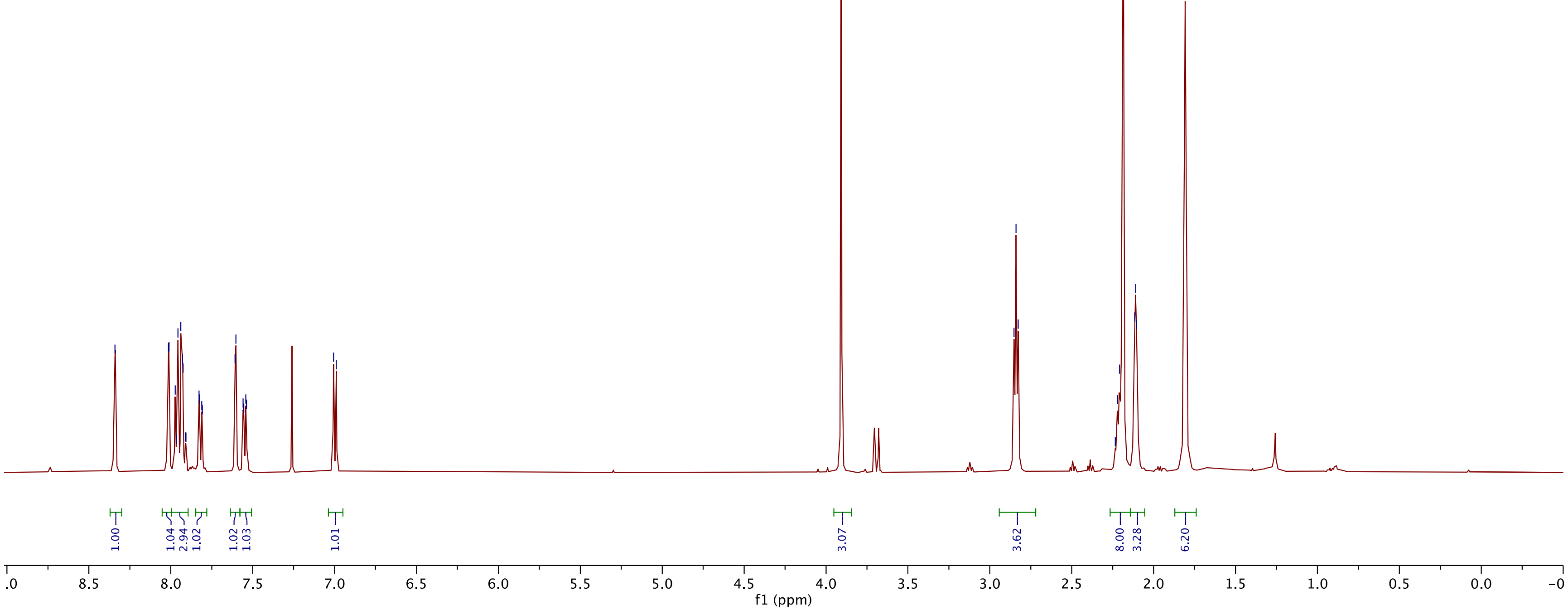
^{13}C NMR

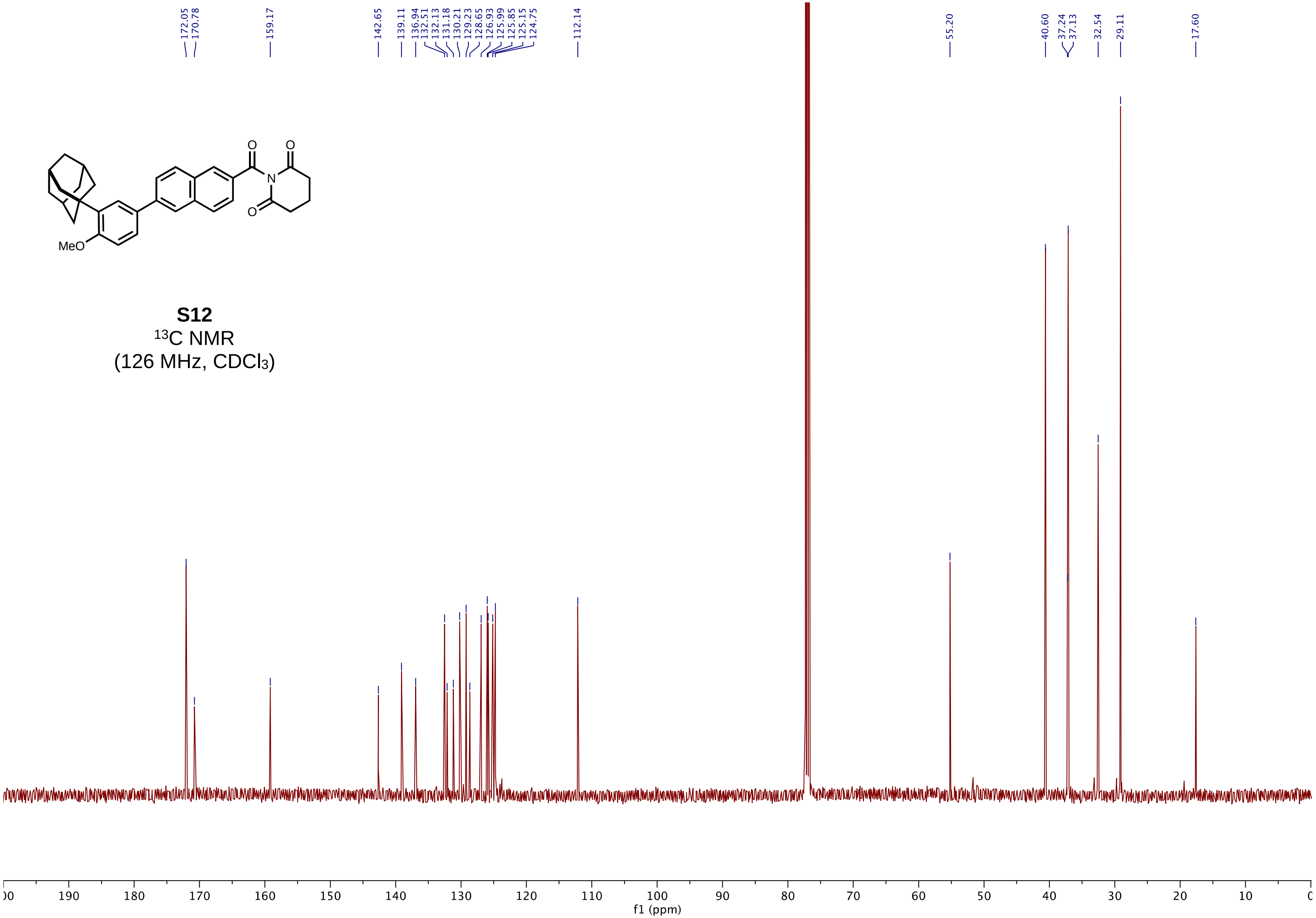
(126 MHz, $CDCl_3$)





S12
[1]H NMR
(500 MHz, $CDCl_3$)

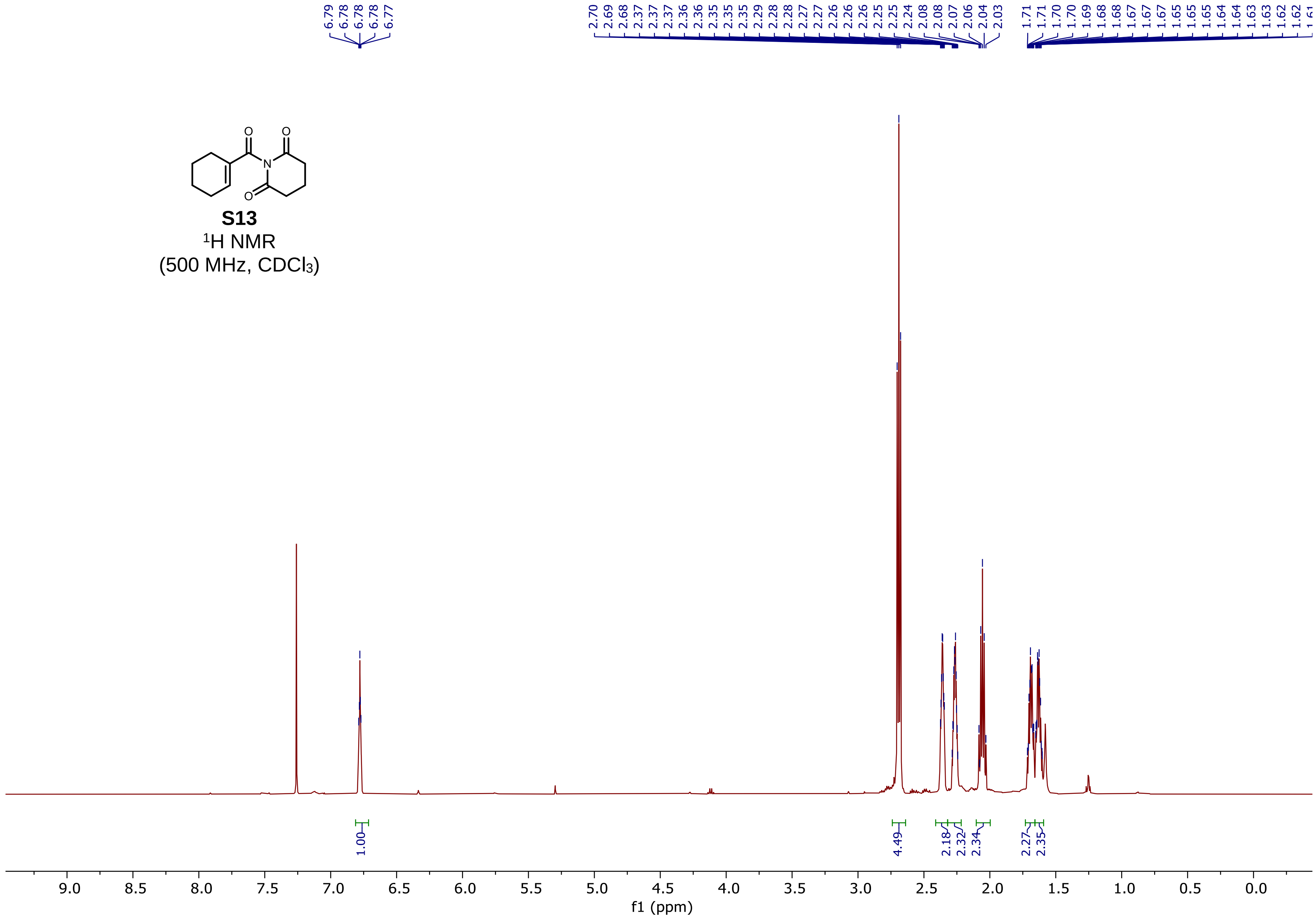


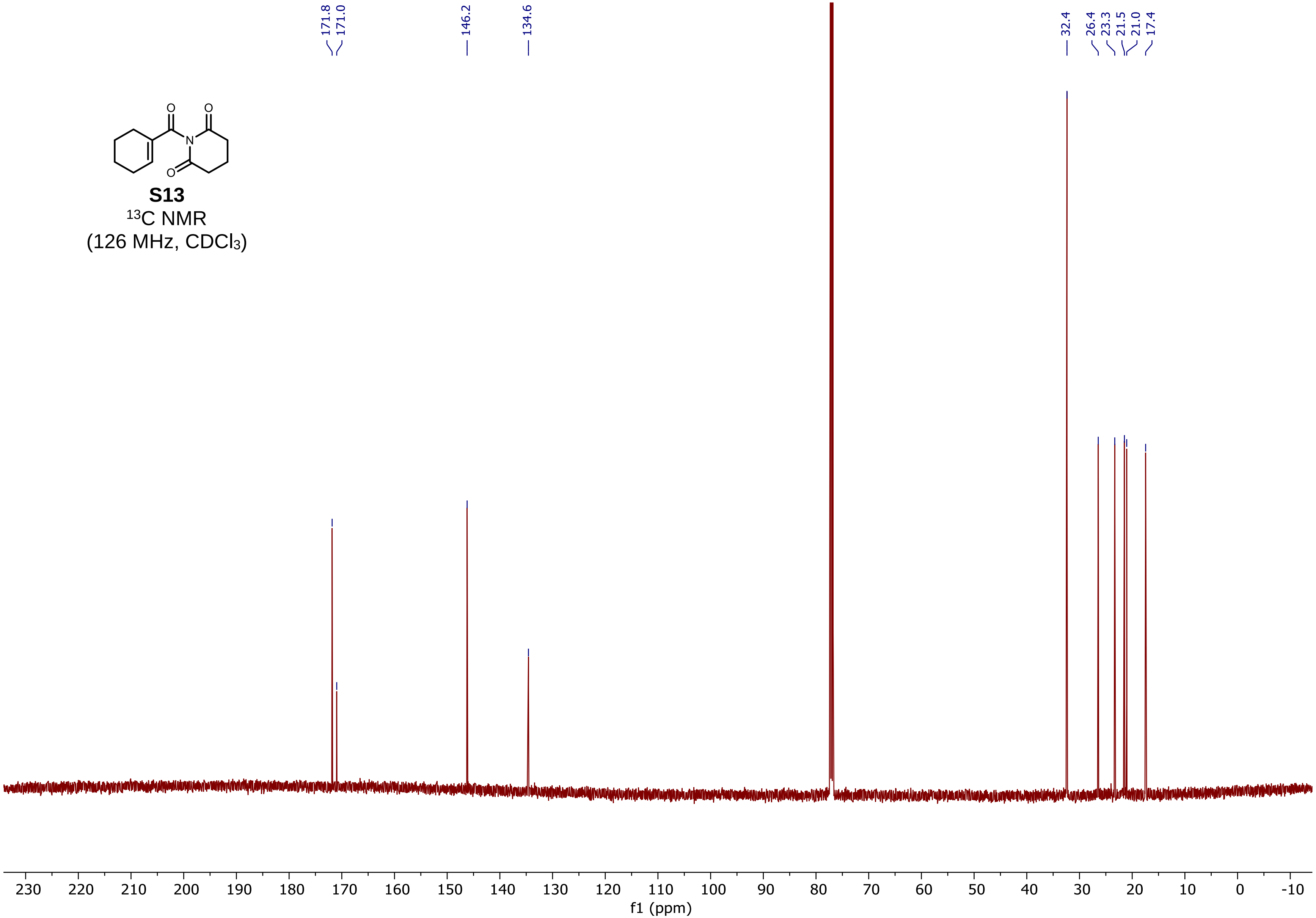


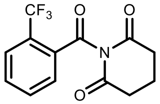
S12

^{13}C NMR

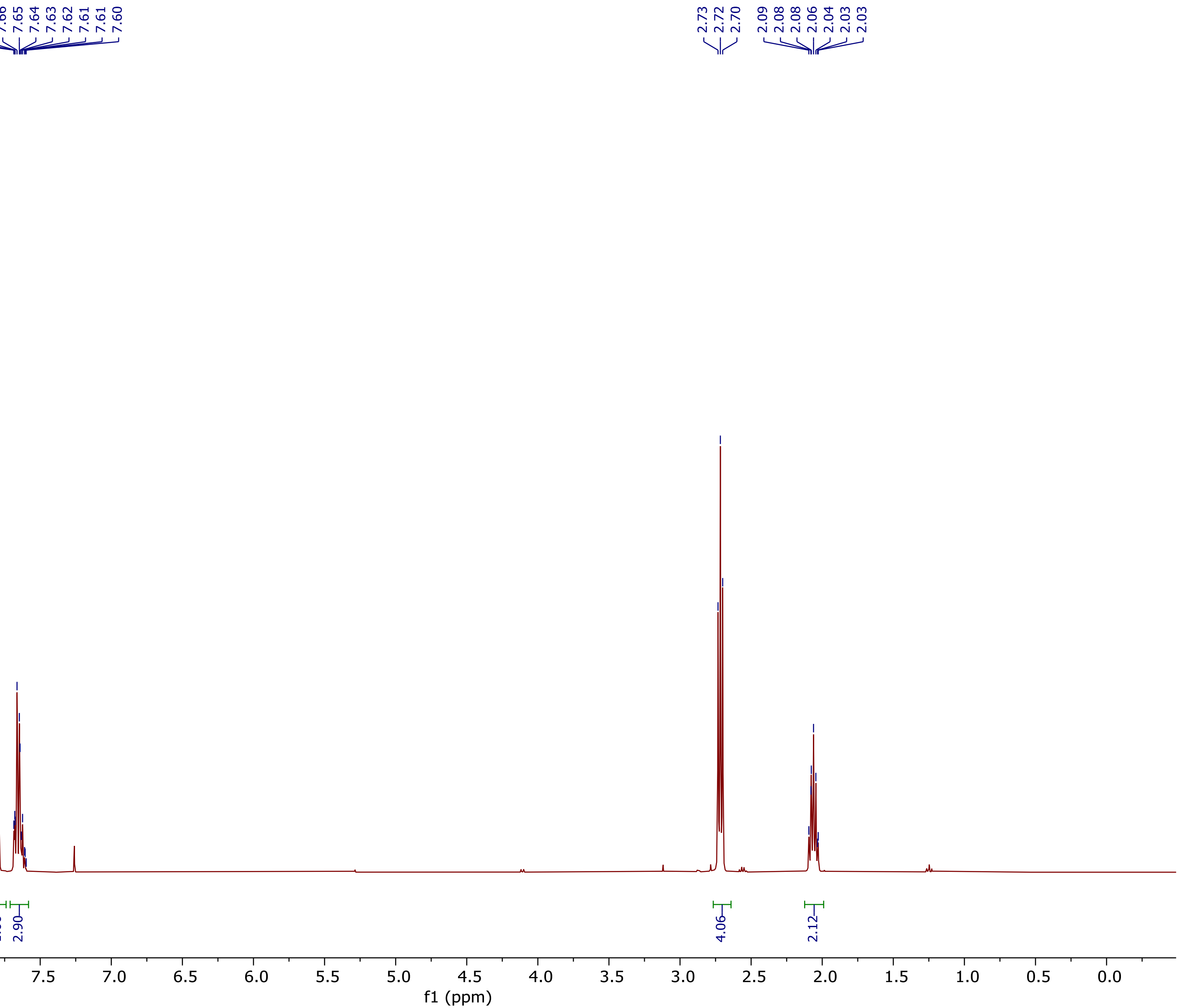
(126 MHz, $CDCl_3$)

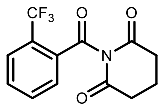

S13
1H NMR
(500 MHz, CDCl3)
f1 (ppm)


S13
13C NMR
(126 MHz, CDCl3)
171.8
171.0
146.2
134.6
32.4
26.4
23.3
21.5
21.0
17.4
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

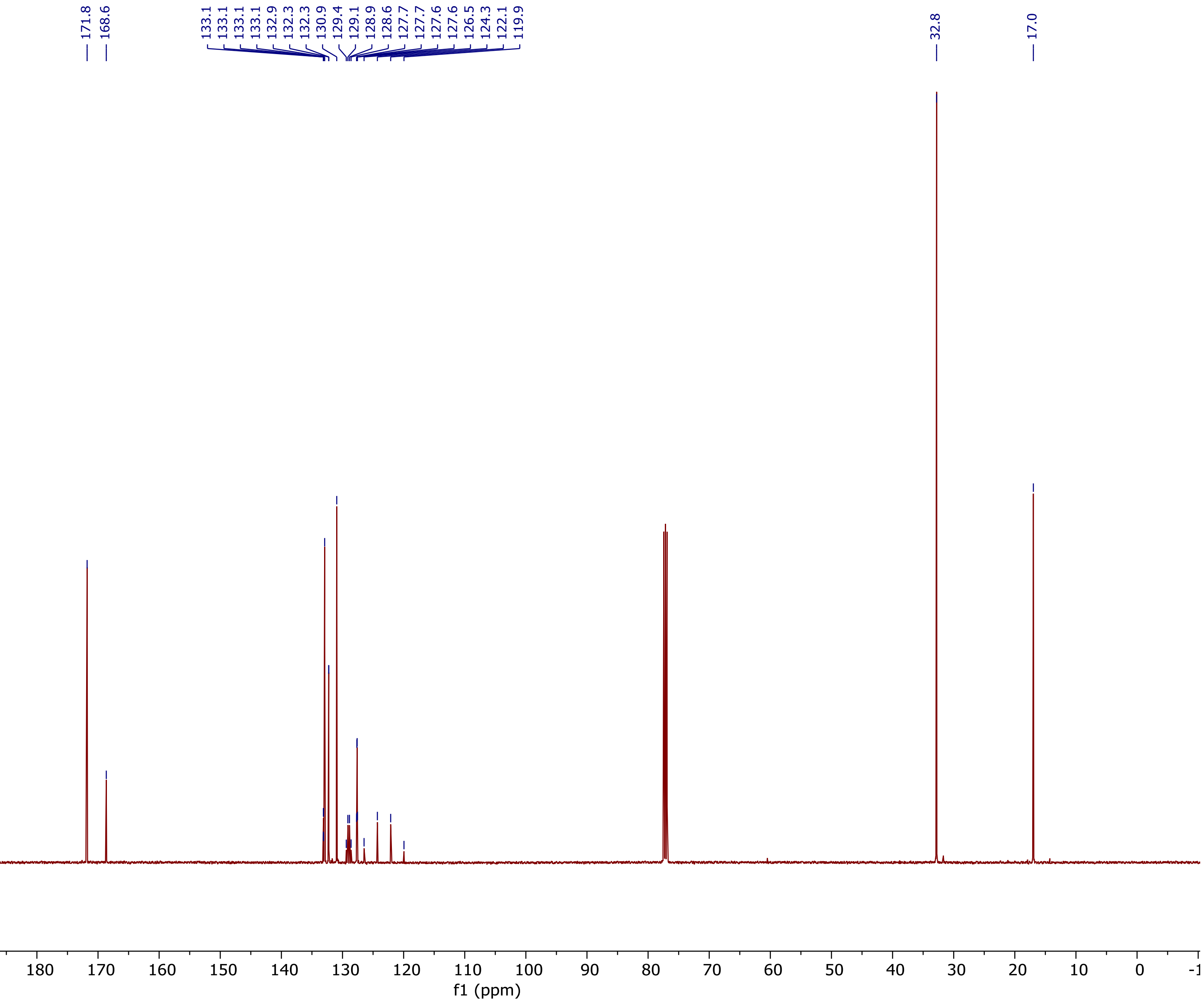


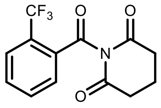
S14
^1H NMR
(400 MHz, $CDCl_3$)



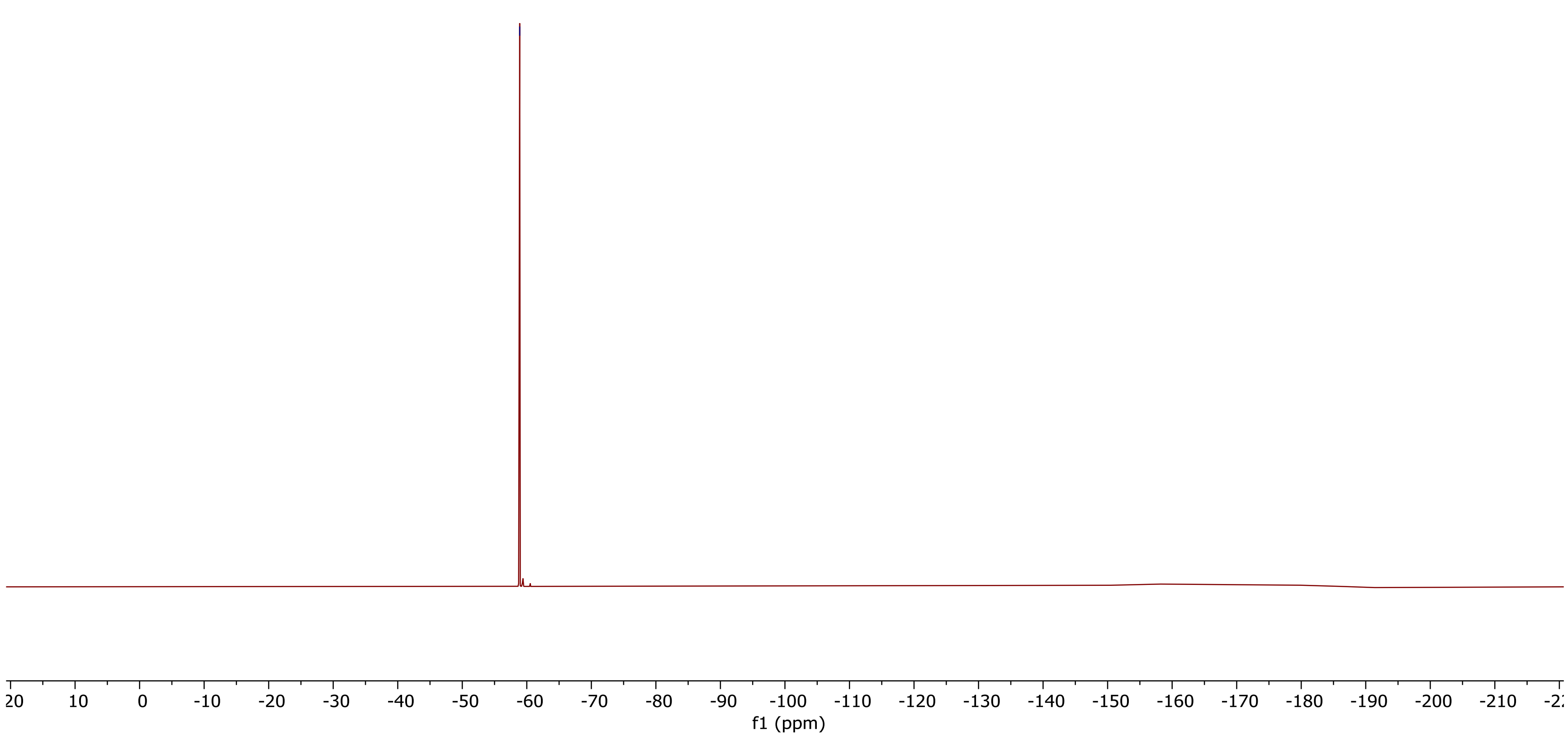


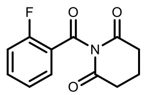
S14
^{13}C NMR
(126 MHz, $CDCl_3$)





S14
^{19}F NMR
(471 MHz, $CDCl_3$)

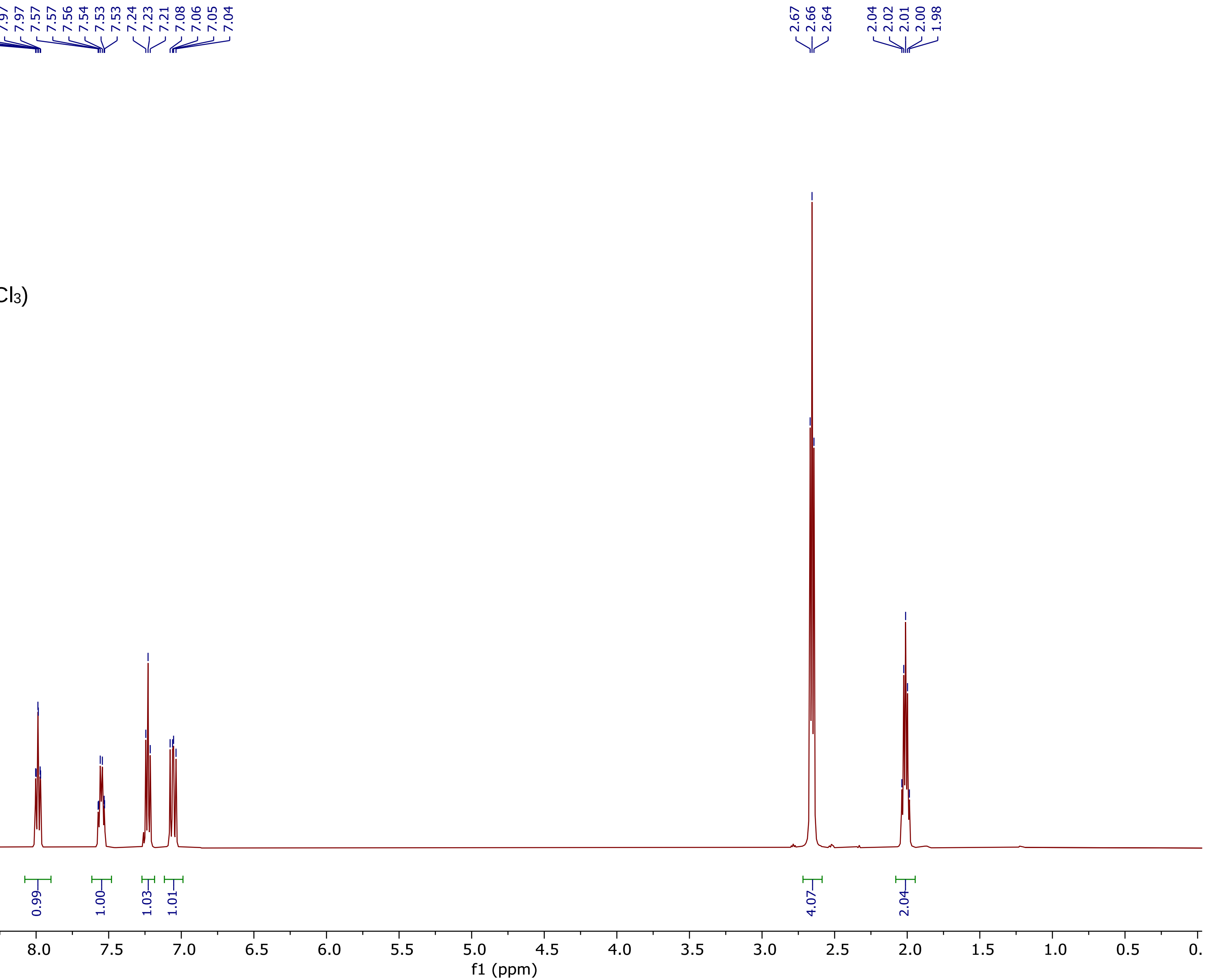


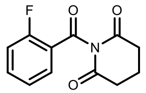


S15

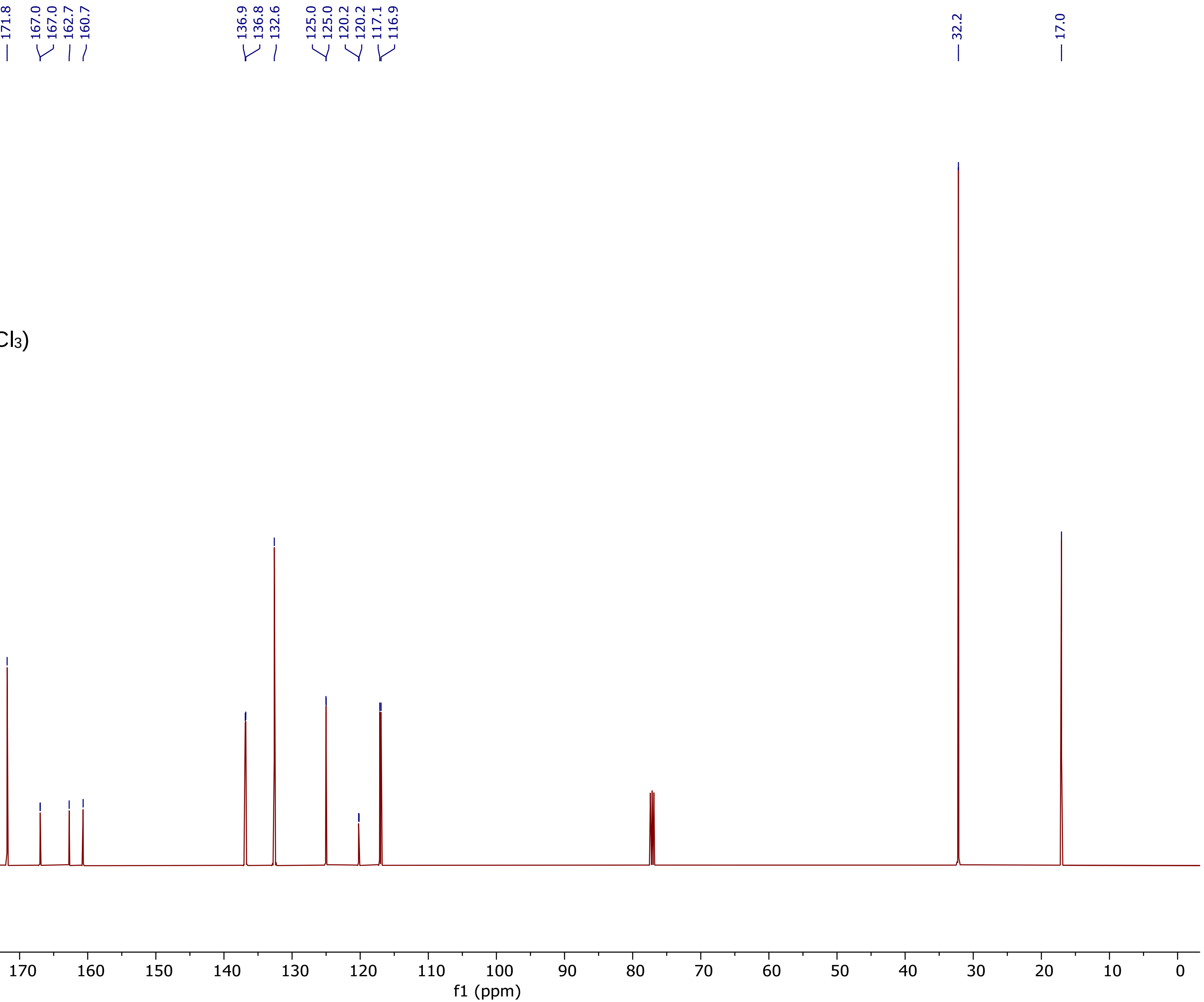
^{1}H NMR

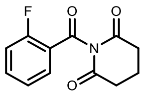
(500 MHz, $CDCl_3$)



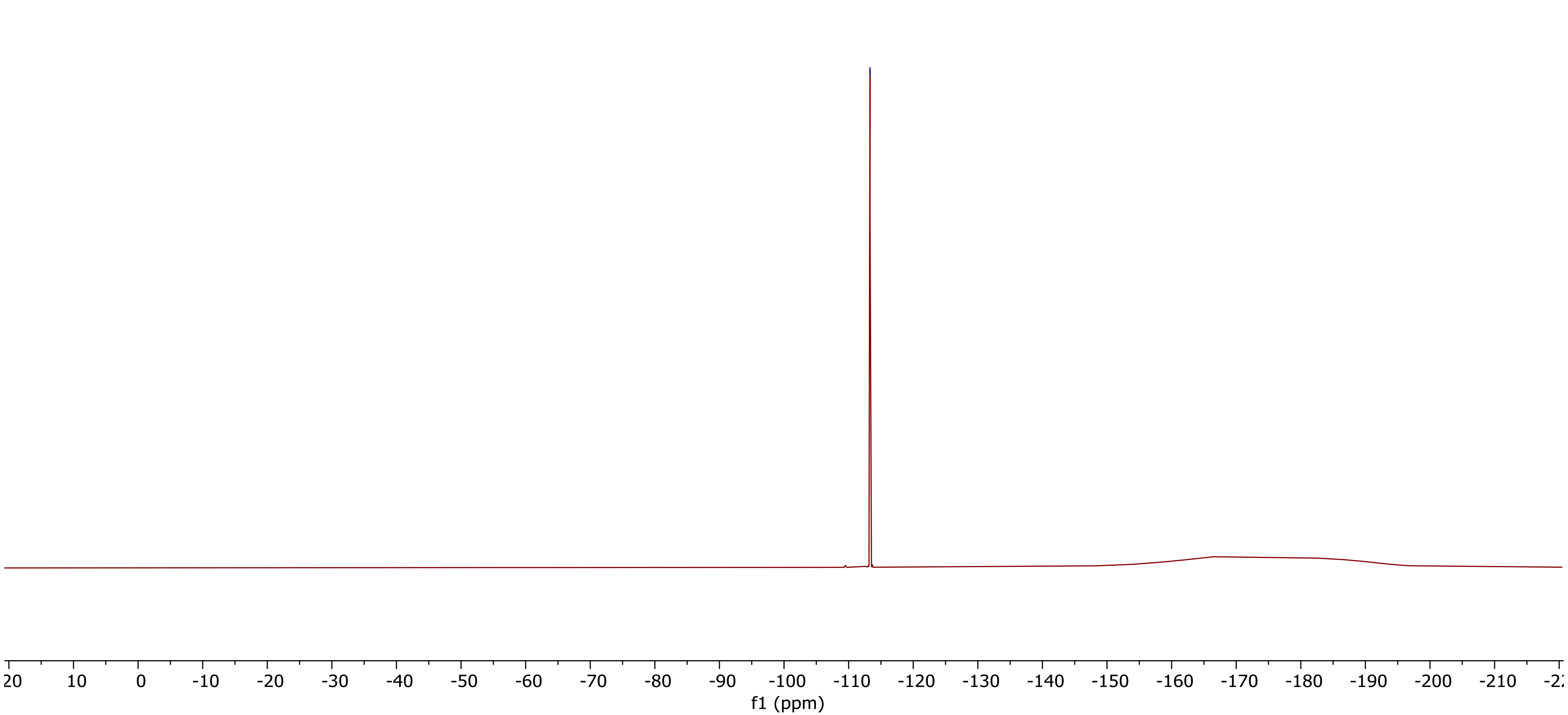


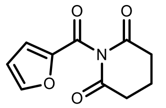
S15
^{13}C NMR
(126 MHz, $CDCl_3$)



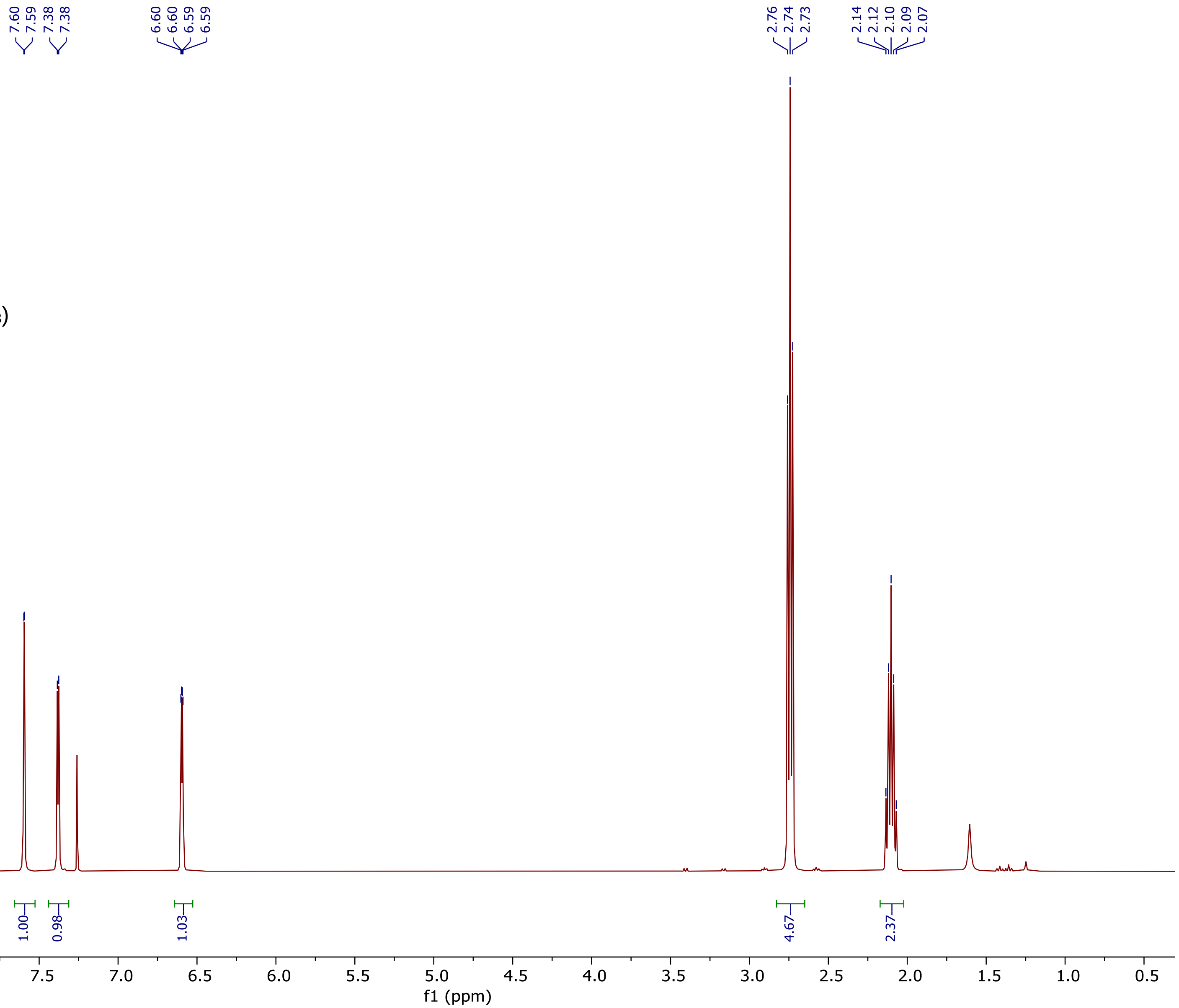


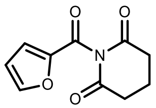
S15
^{19}F NMR
(471 MHz, $CDCl_3$)



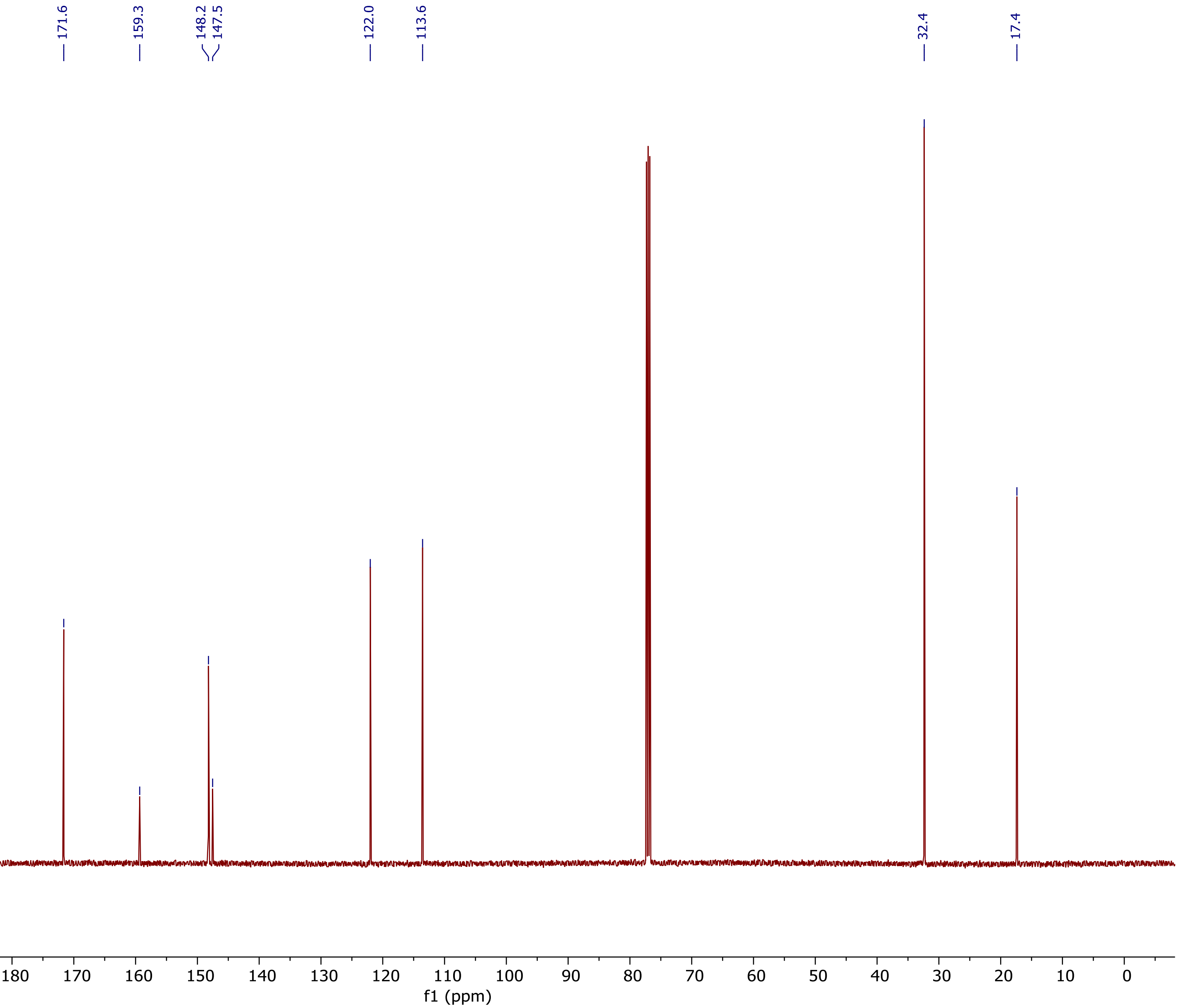


S16
^{1}H NMR
(400 MHz, $CDCl_3$)





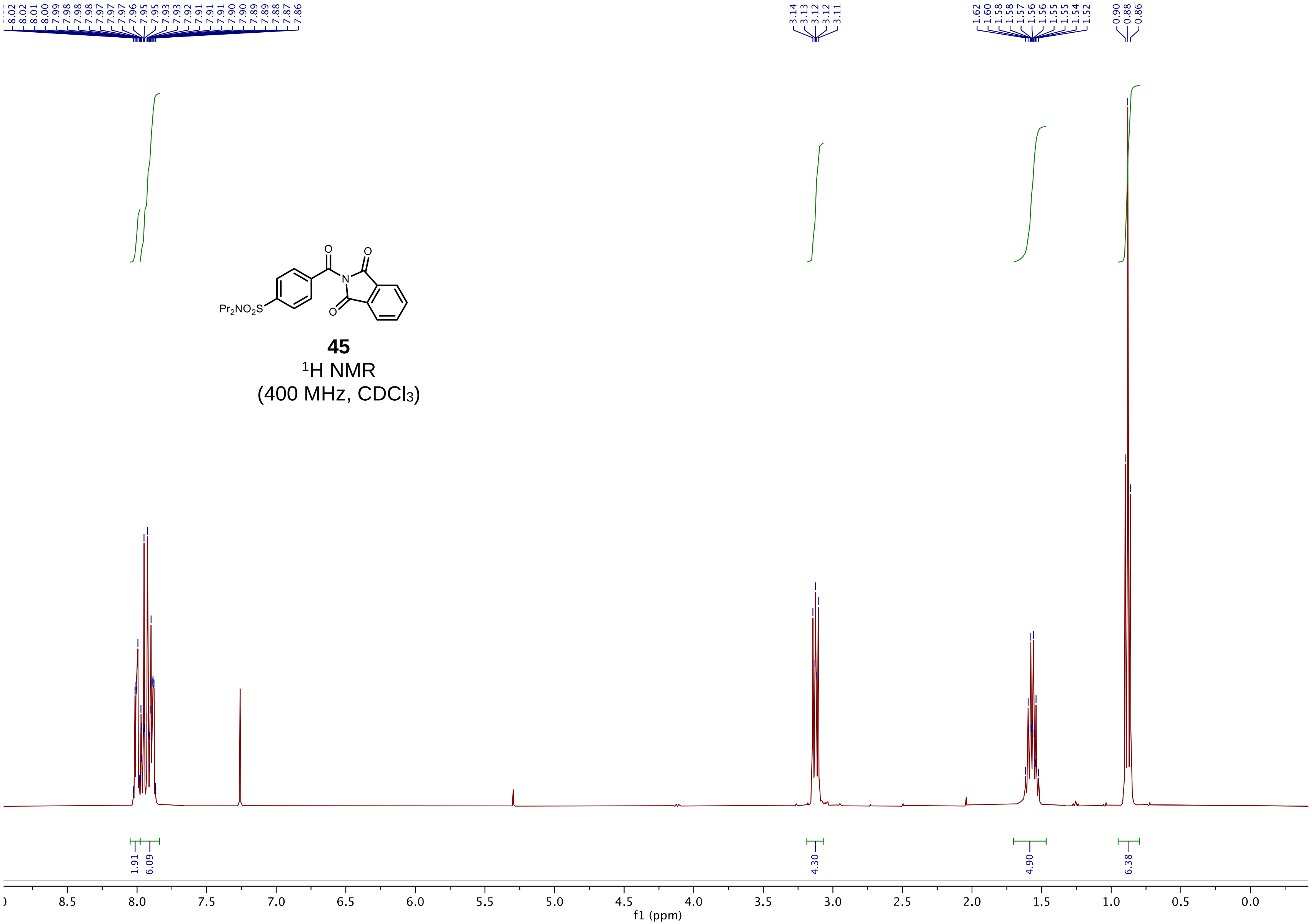
S16
^{13}C NMR
(126 MHz, $CDCl_3$)

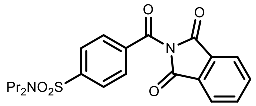


45

^{1}H NMR

(400 MHz, $CDCl_3$)

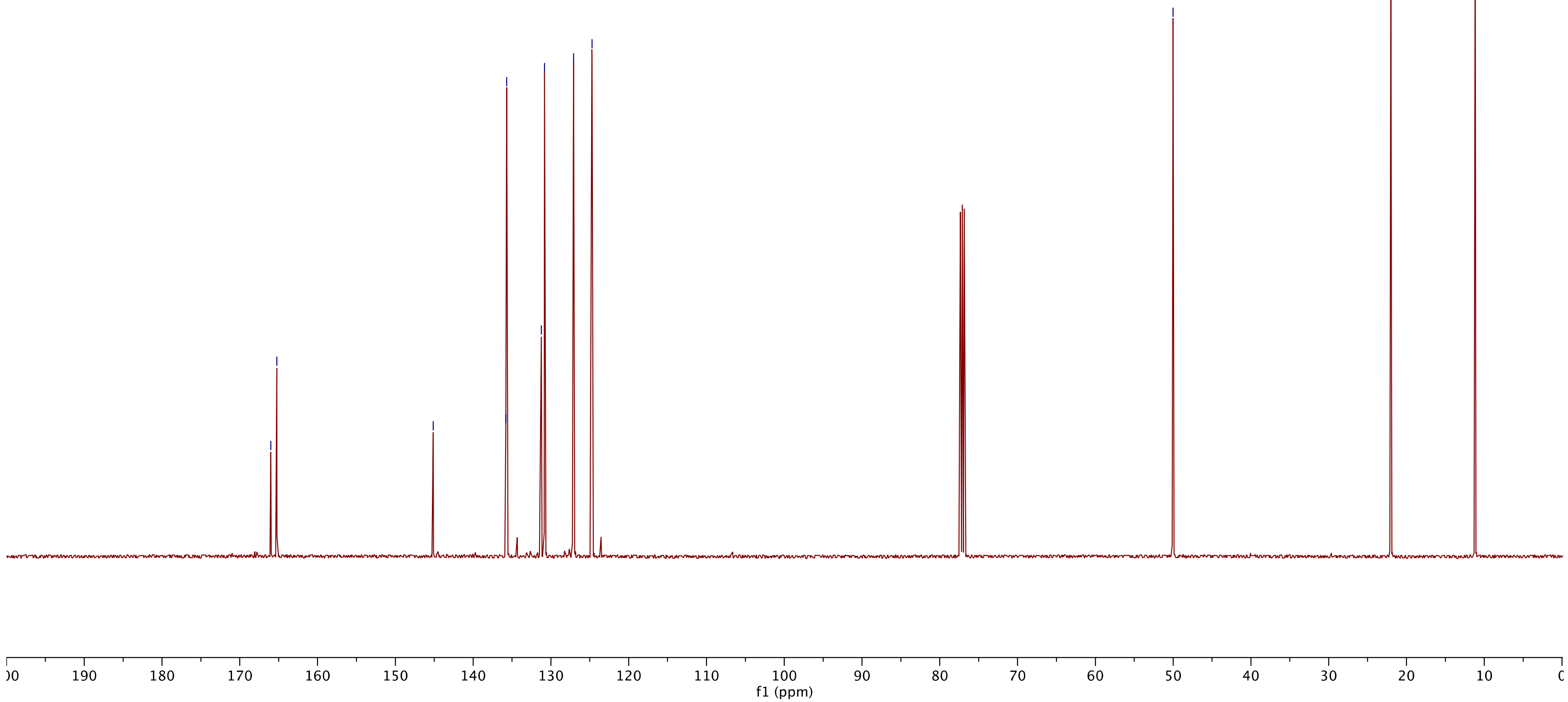


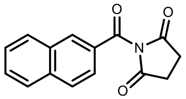


45

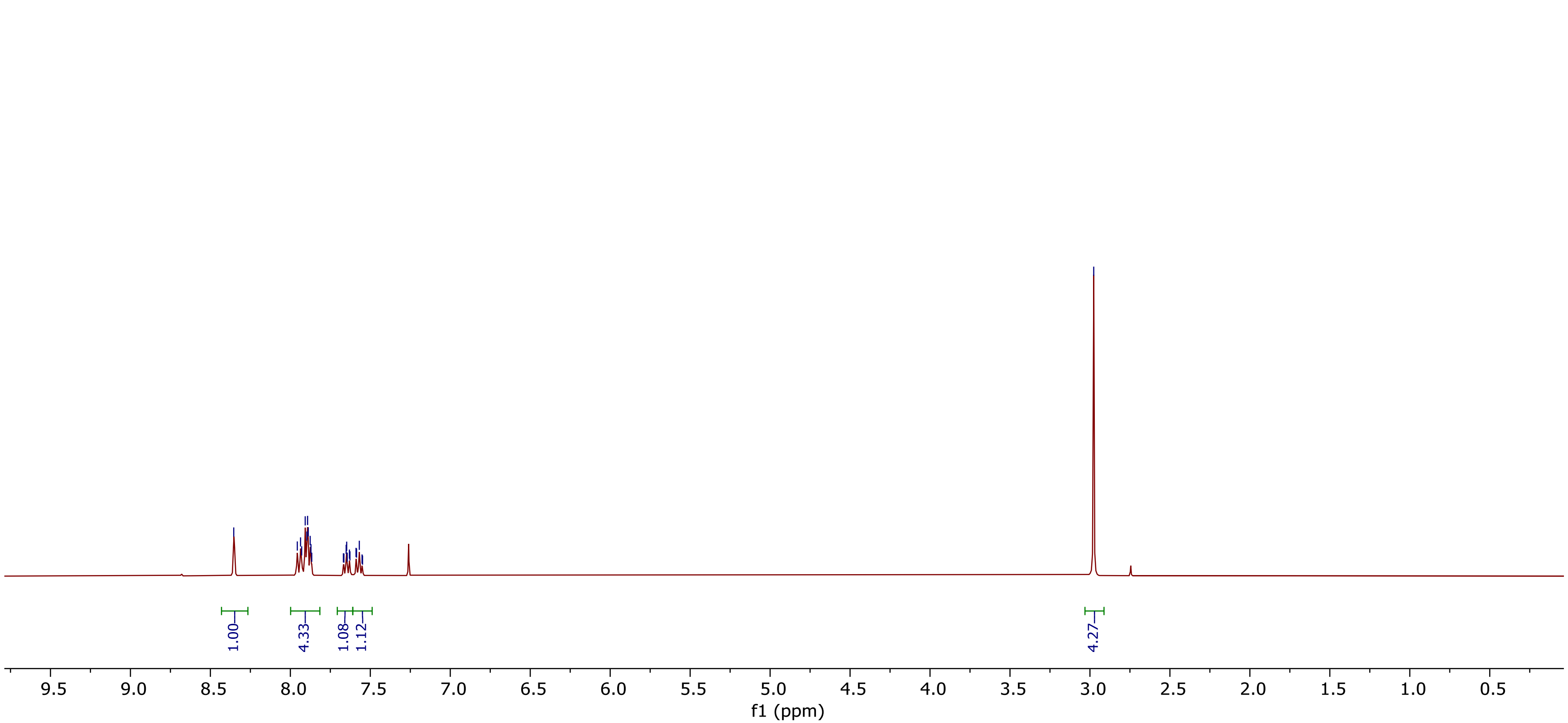
^{13}C NMR

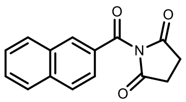
(126 MHz, $CDCl_3$)



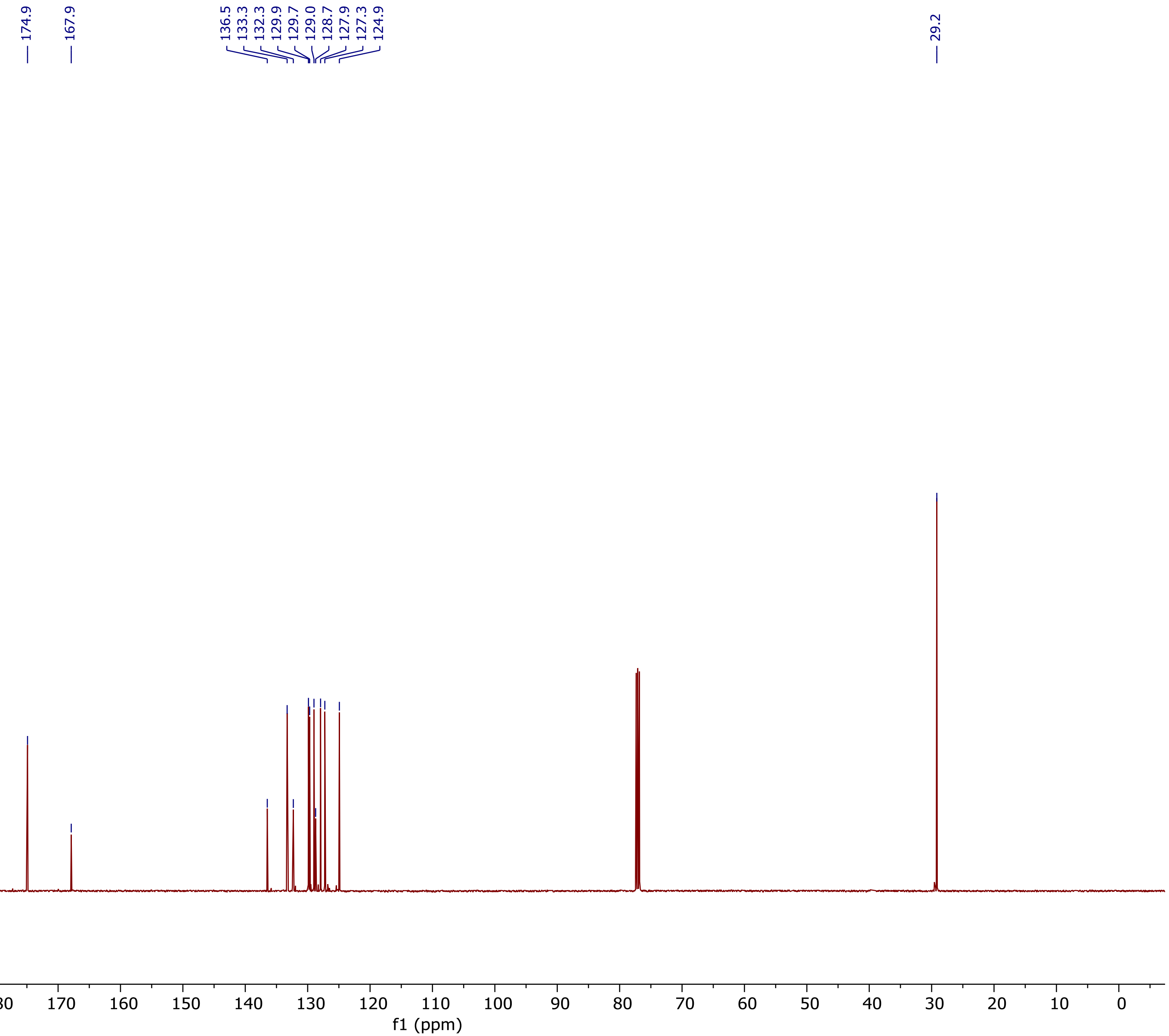


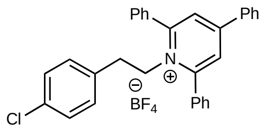
S17
^{1}H NMR
(400 MHz, $CDCl_3$)



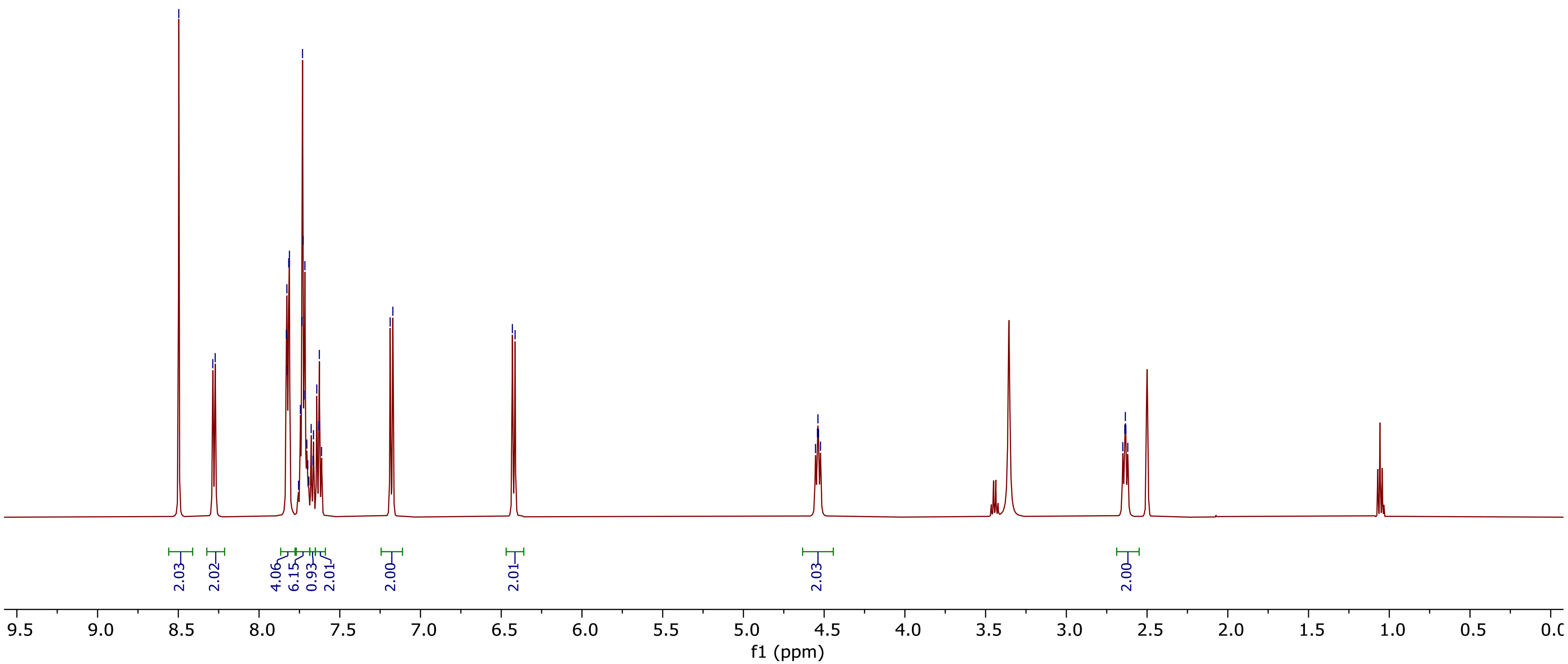


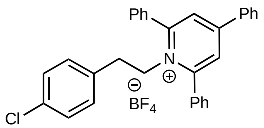
S17
^{13}C NMR
(126 MHz, $CDCl_3$)



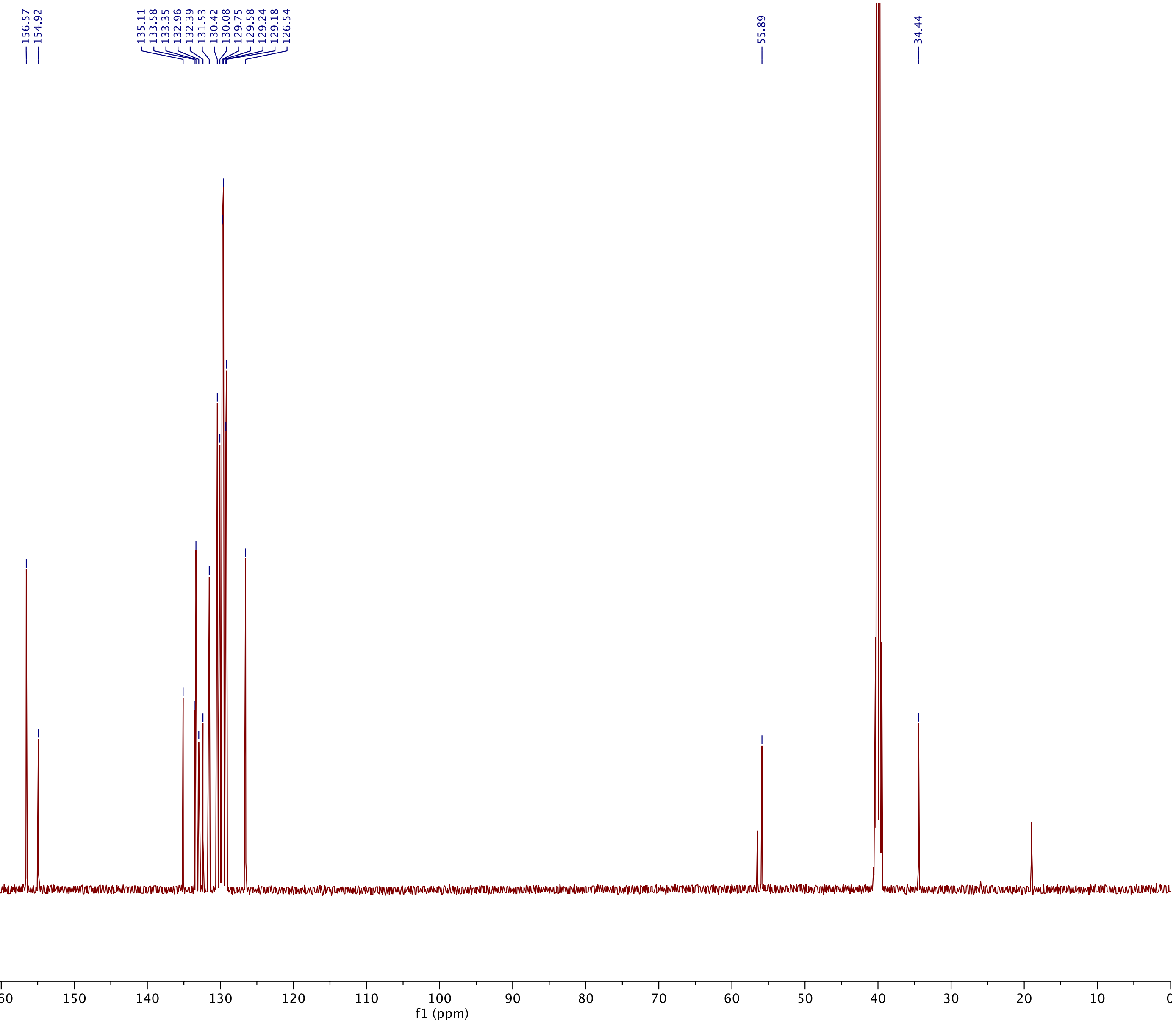


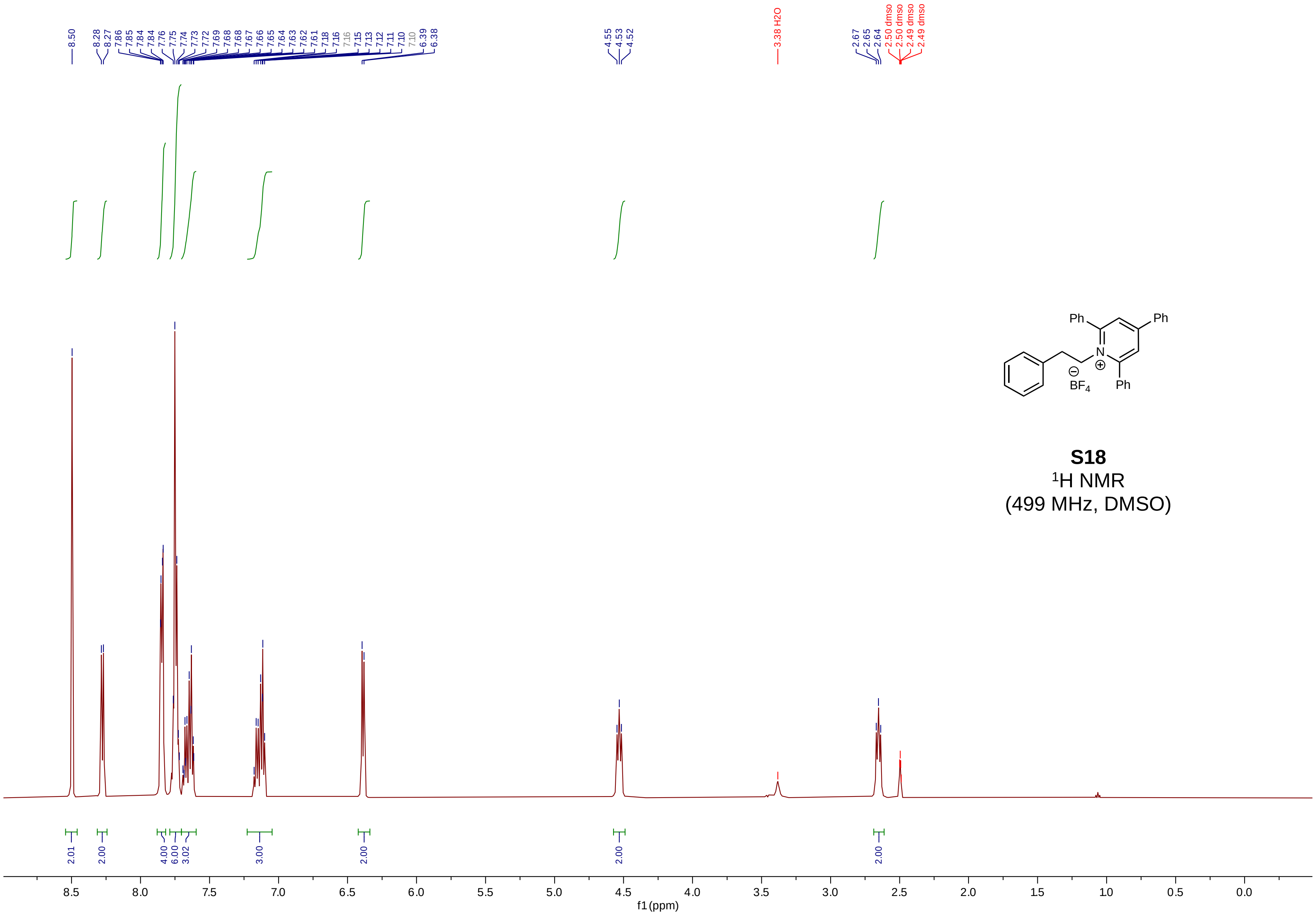
2
^{1}H NMR
(500 MHz, DMSO)





2
^{13}C NMR
(126 MHz, DMSO)

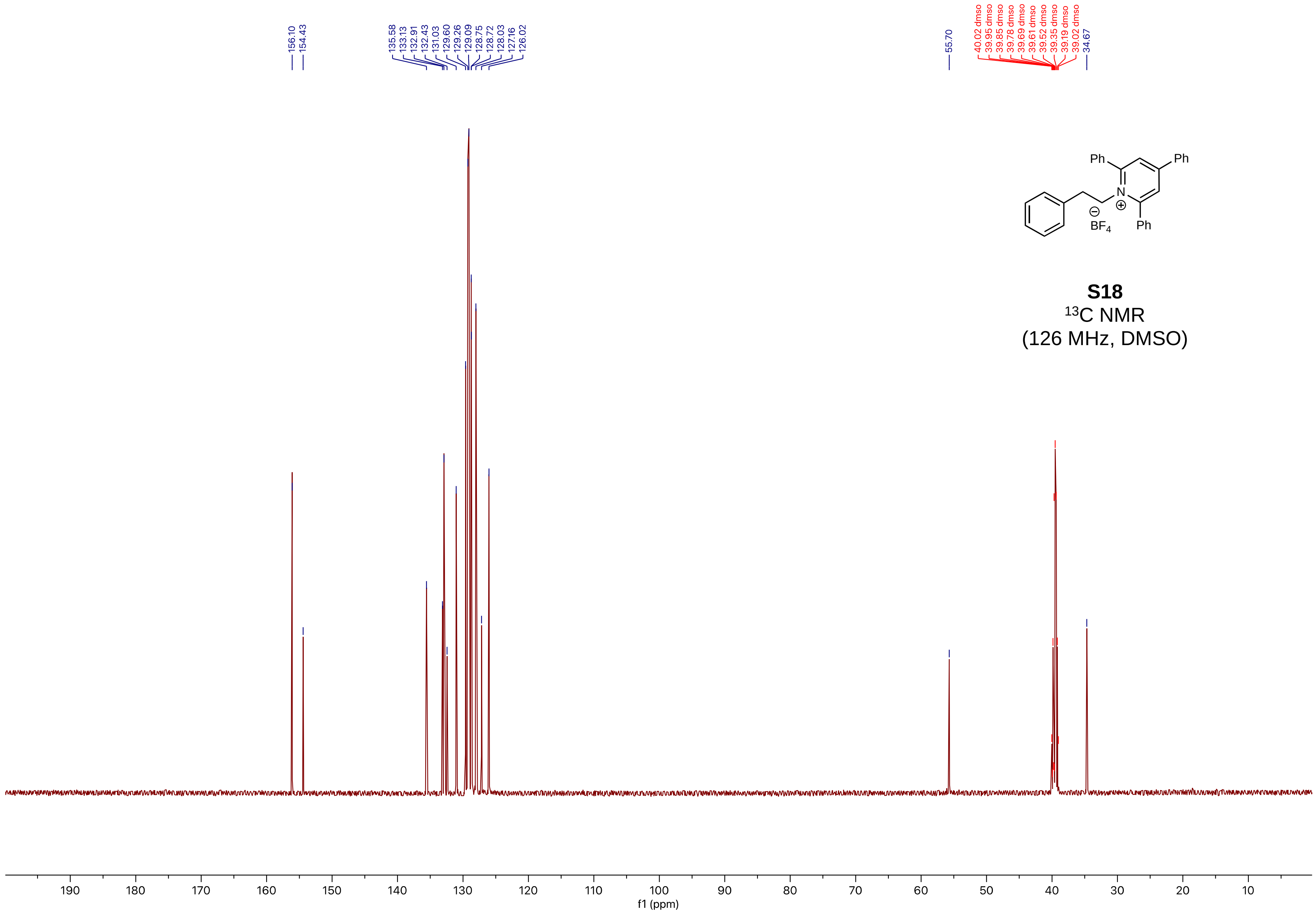




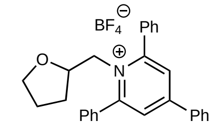
S18

^{1}H NMR

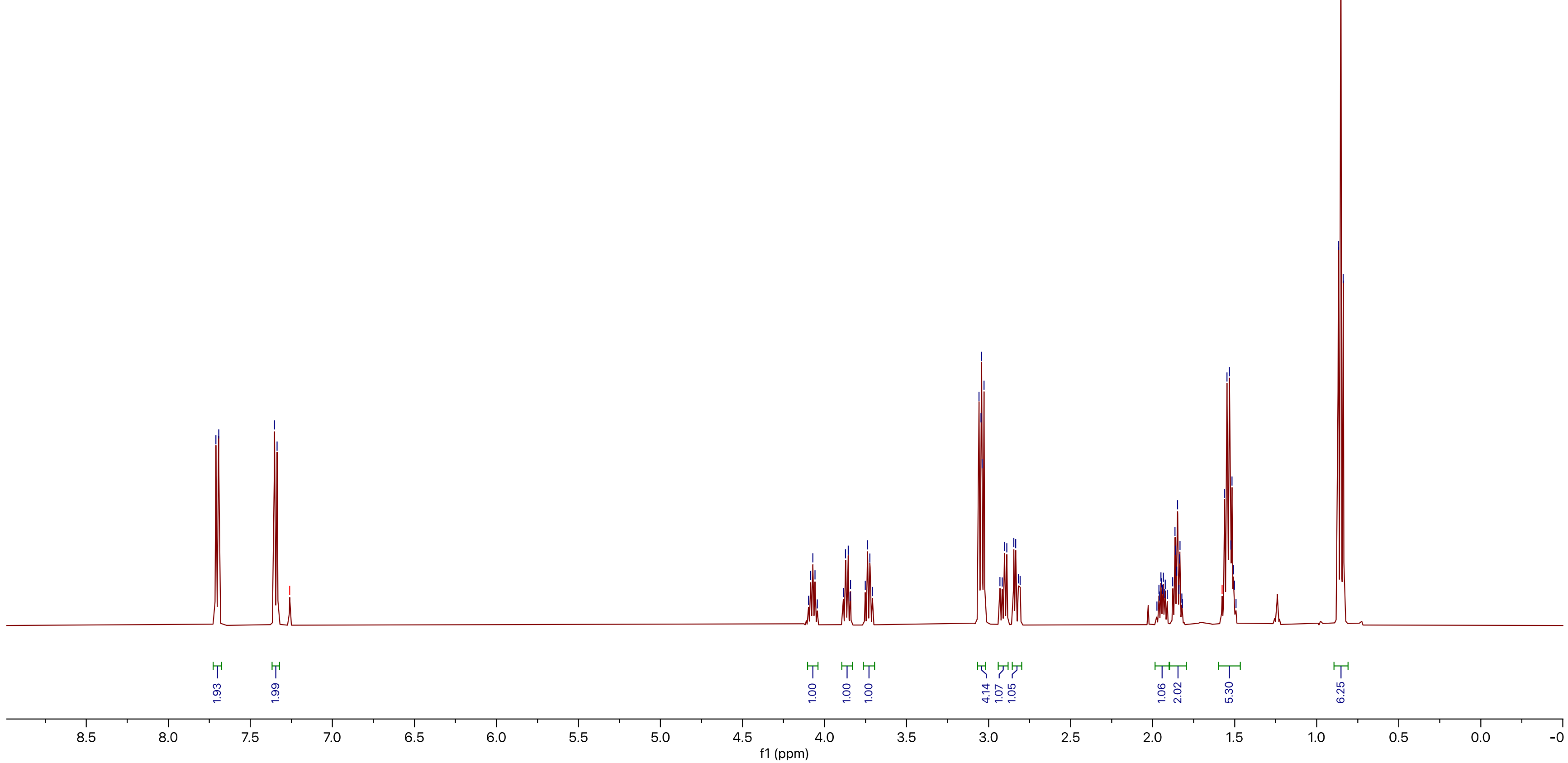
(499 MHz, DMSO)

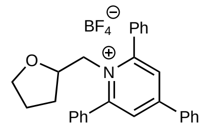


S18
^{13}C NMR
(126 MHz, DMSO)

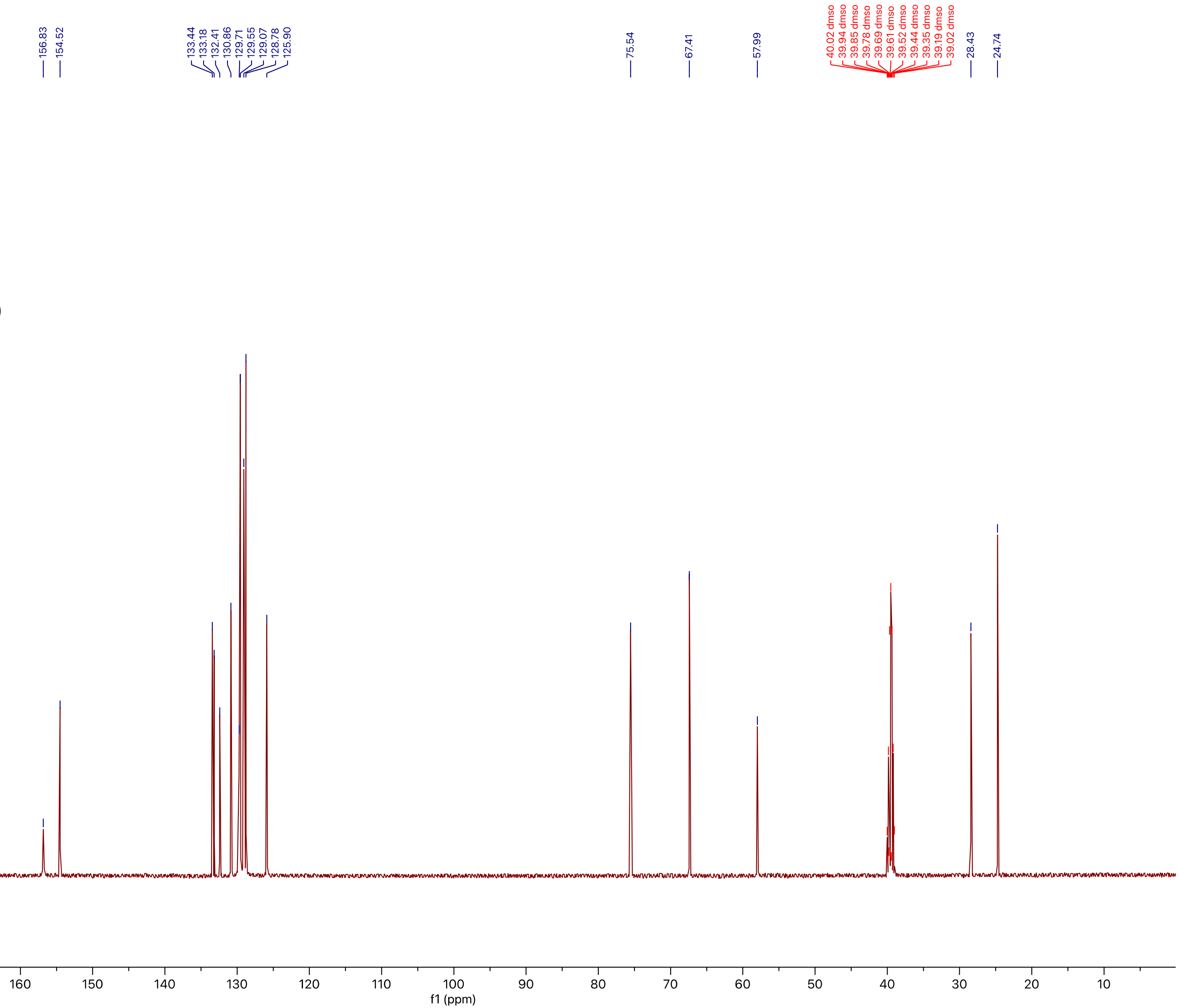


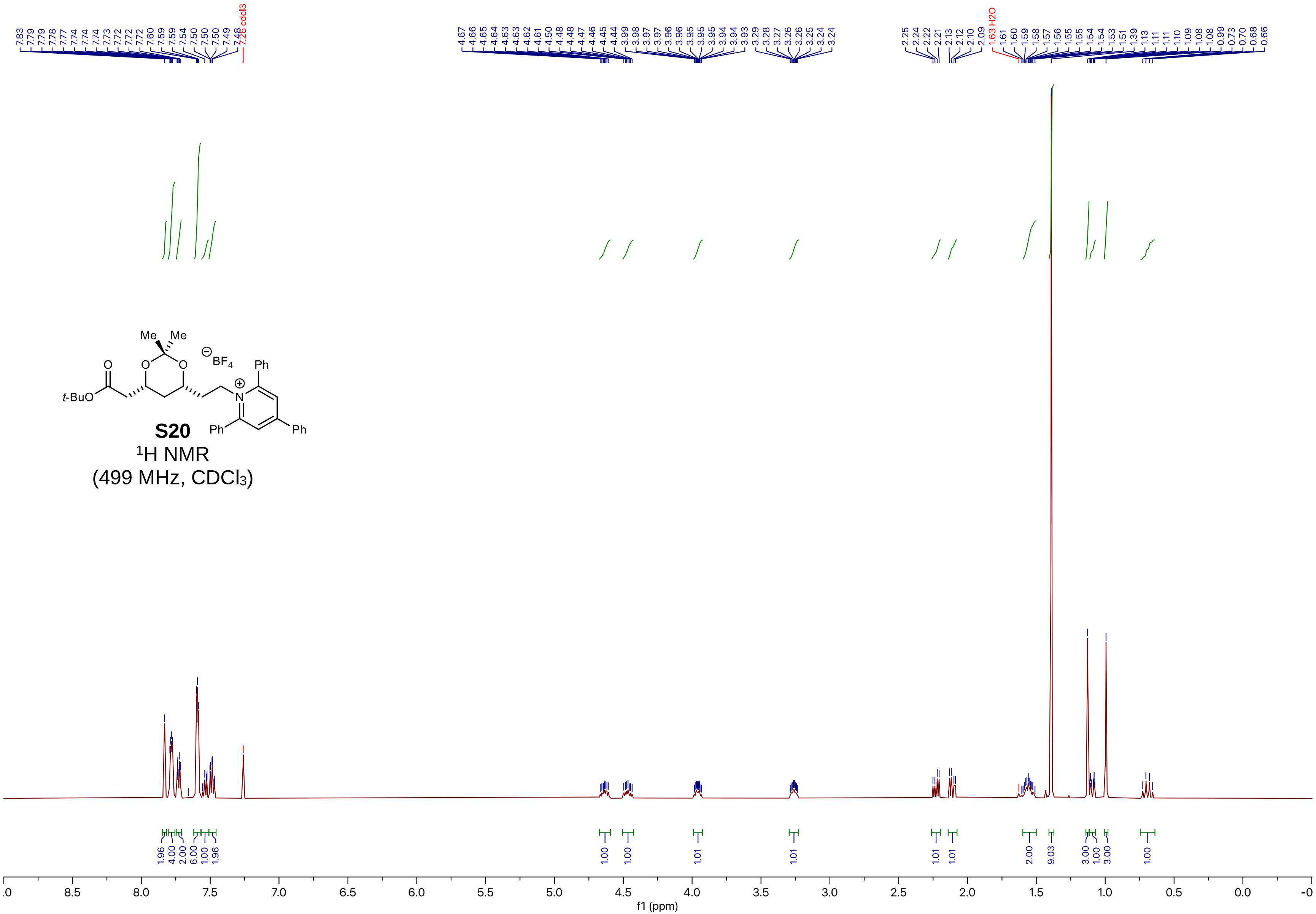
S19
^{1}H NMR
(499 MHz, DMSO)



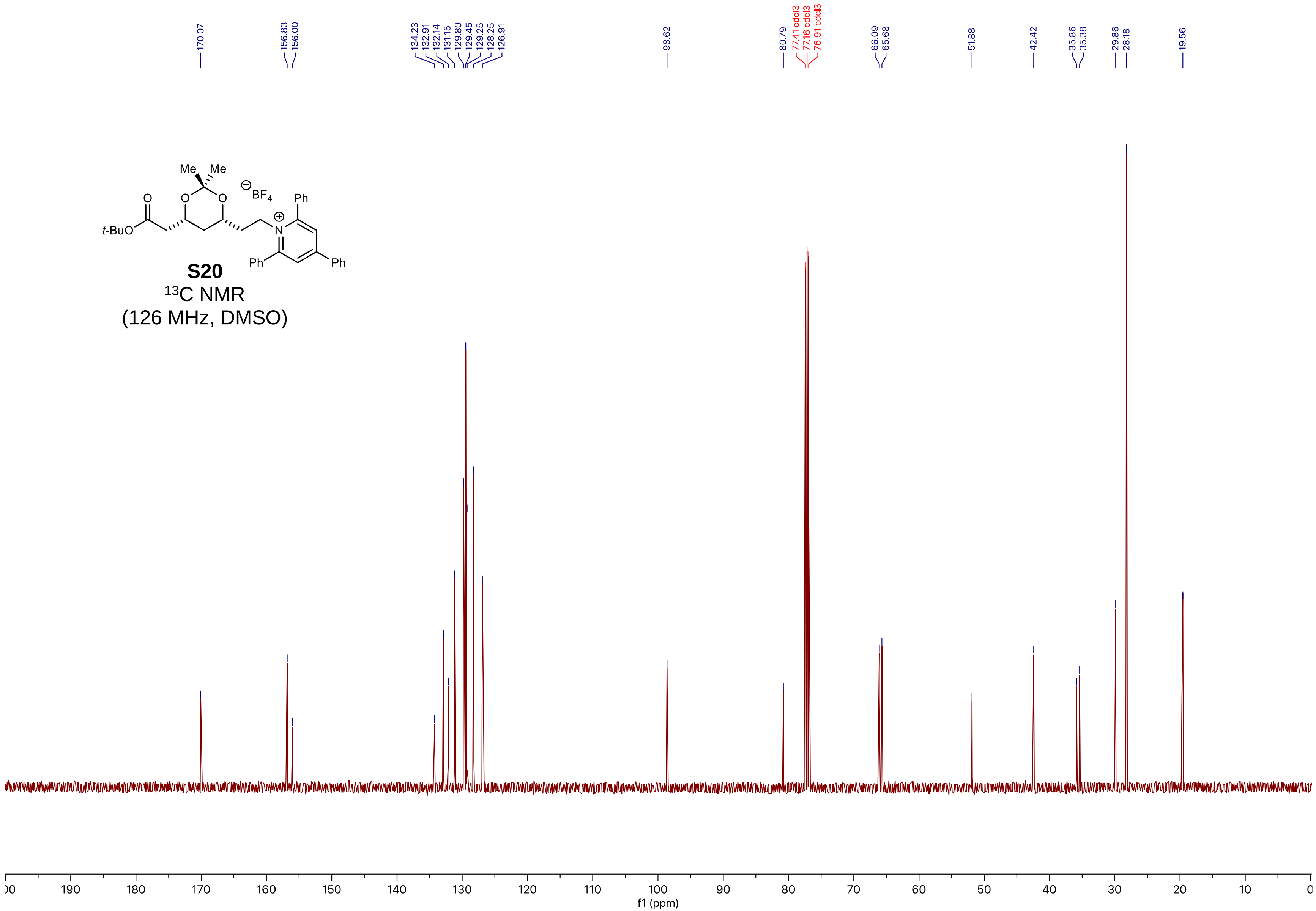


S19
^{13}C NMR
(126 MHz, DMSO)

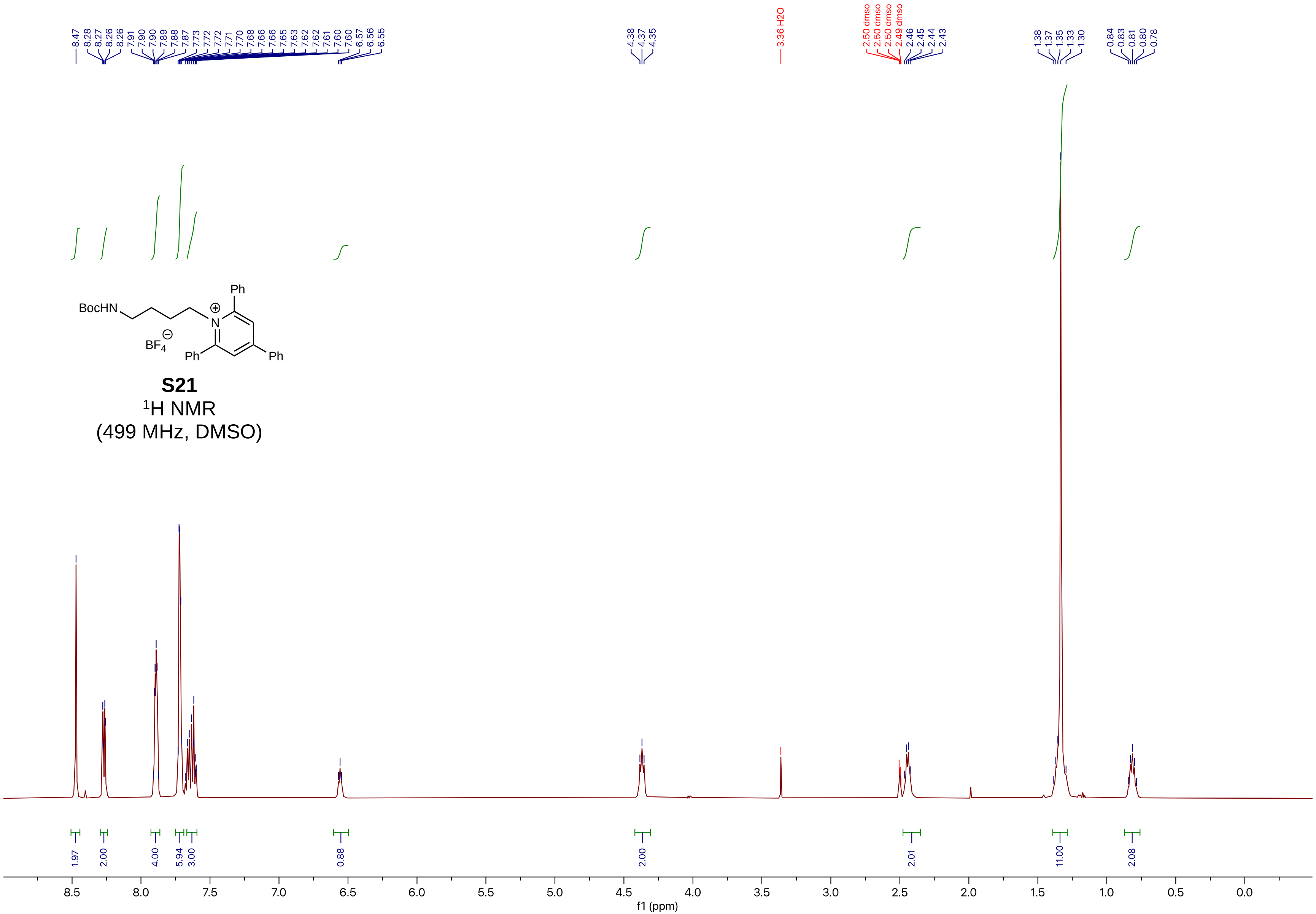




S20
^{1}H NMR
(499 MHz, $CDCl_3$)



170.07
156.83
156.00
134.23
132.91
132.14
131.15
129.80
129.45
129.25
128.25
126.91
98.62
80.79
77.41 cdcl3
77.16 cdcl3
76.91 cdcl3
66.09
65.68
51.88
42.42
35.86
35.38
29.86
28.18
19.56
Me
Me
O
O
O
t-BuO
BF4
Ph
N
Ph
Ph
S20
13C NMR
(126 MHz, DMSO)
f1 (ppm)



S21

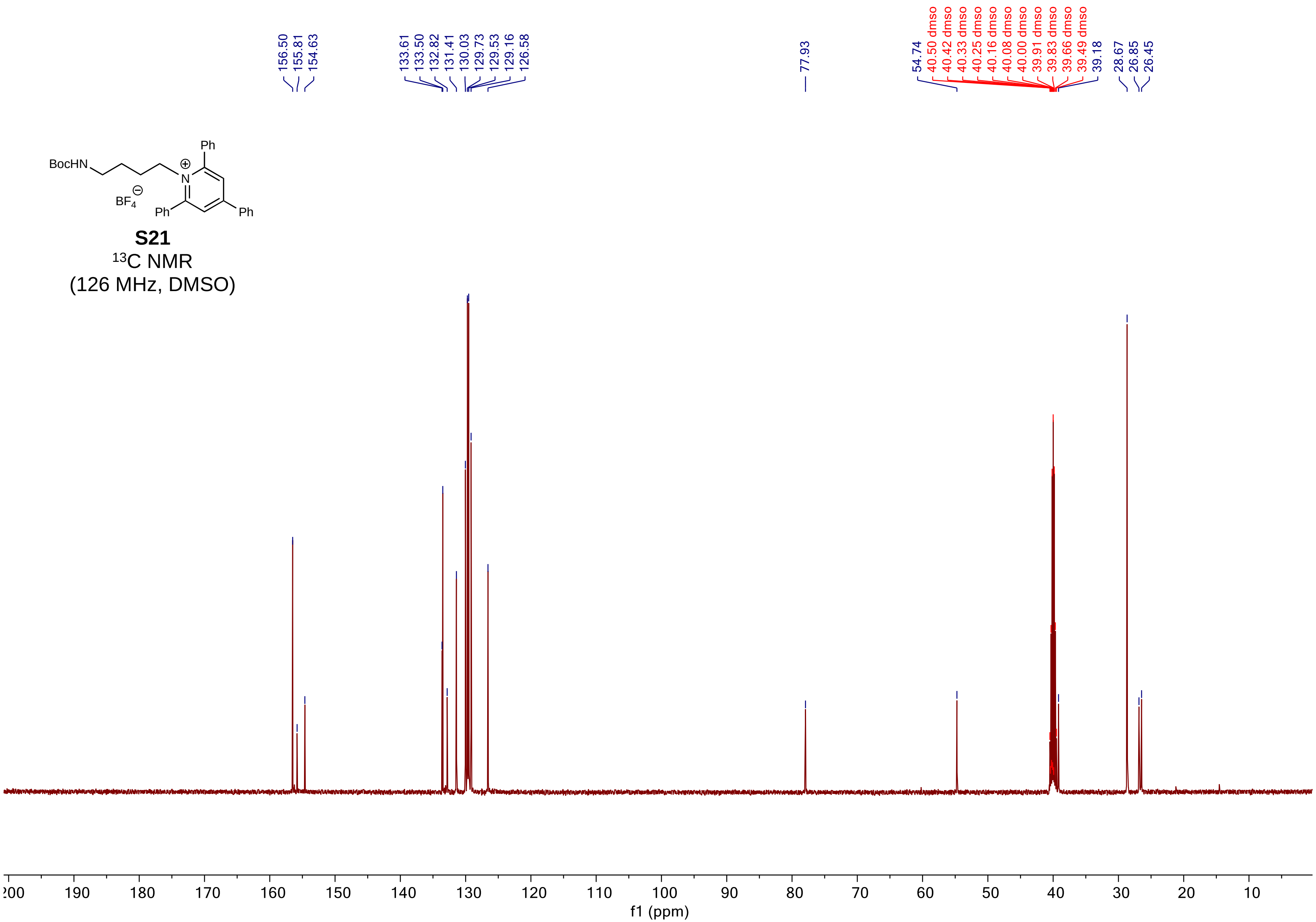
^{1}H NMR

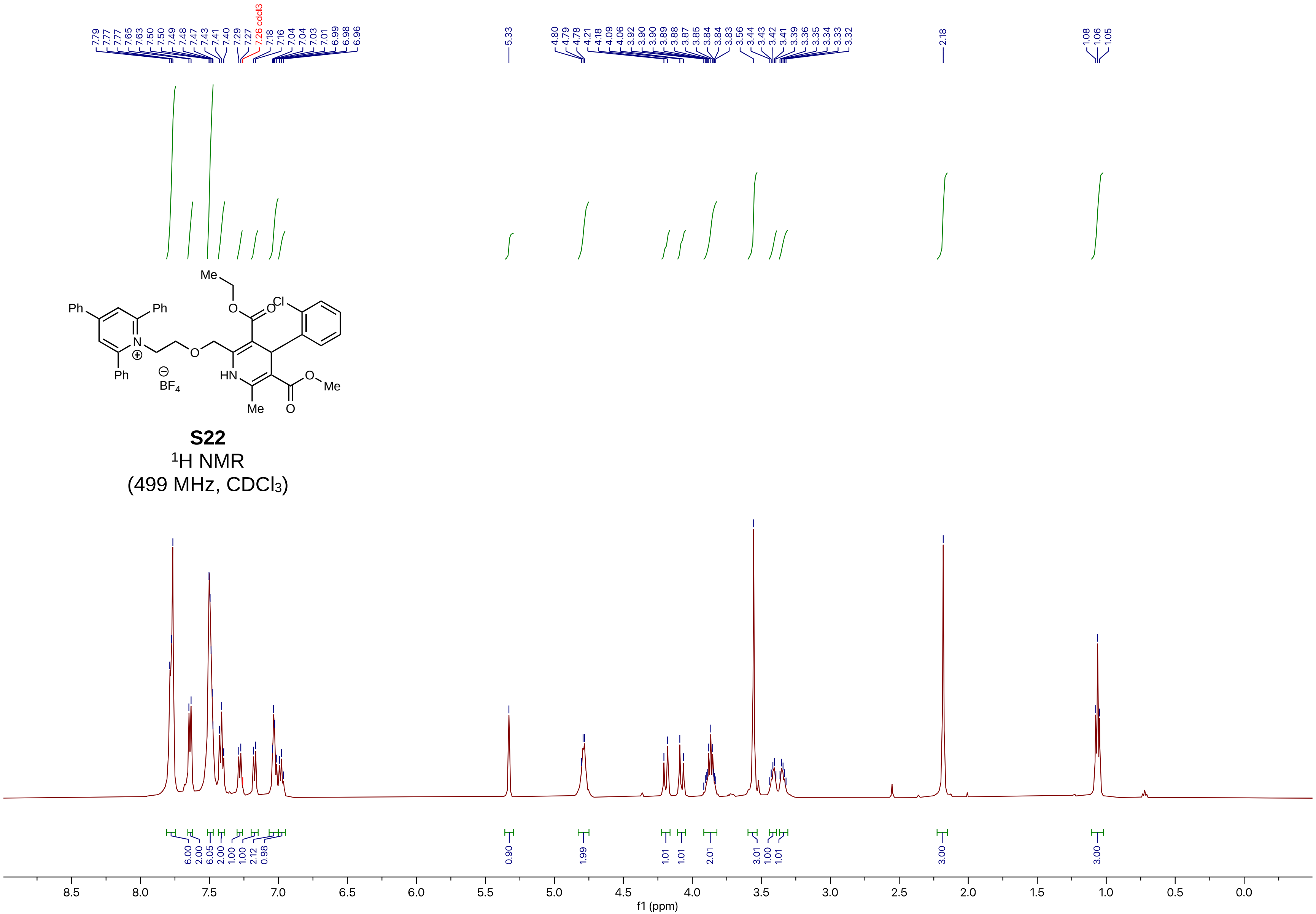
(499 MHz, DMSO)

S21

^{13}C NMR

(126 MHz, DMSO)

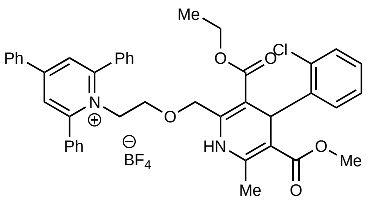




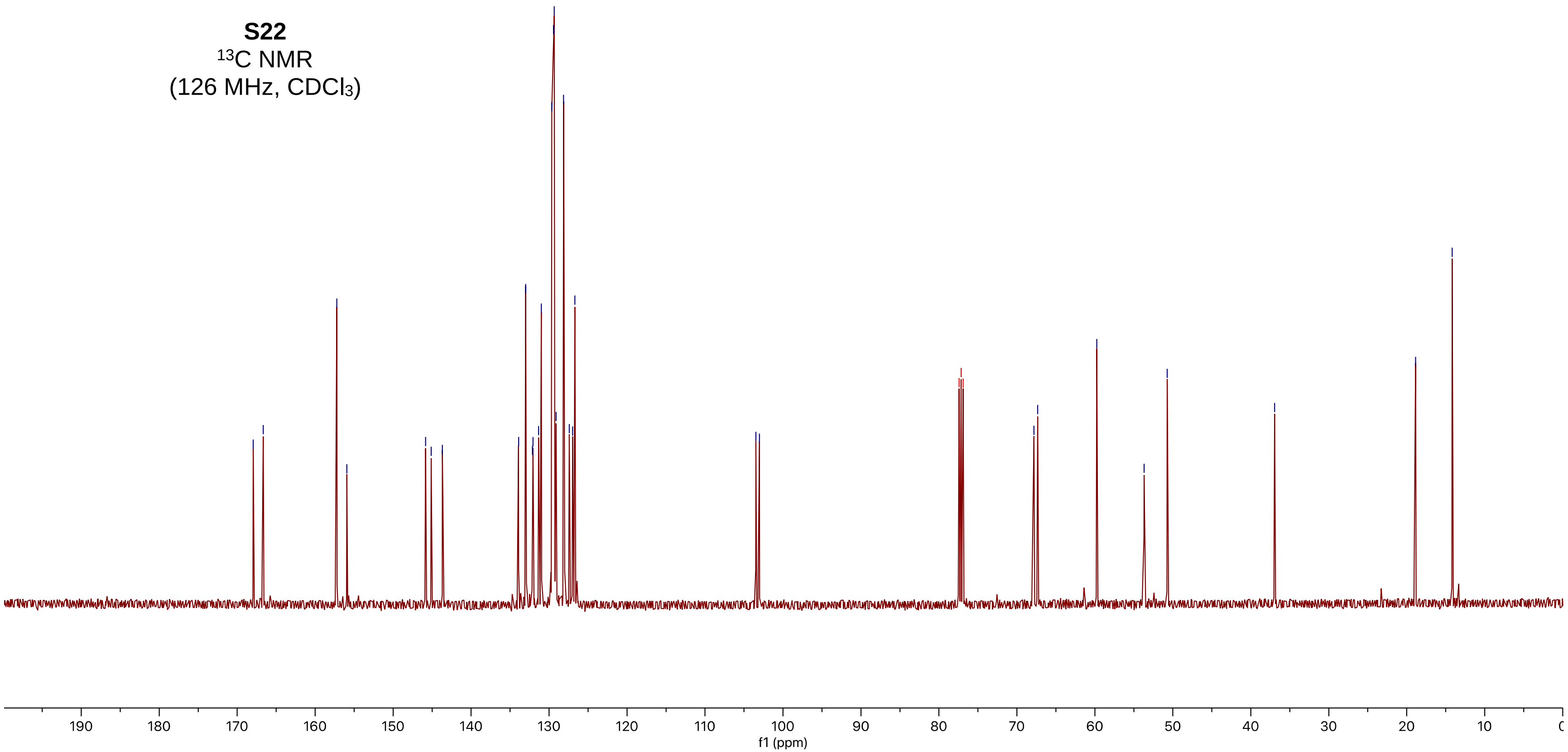
S22

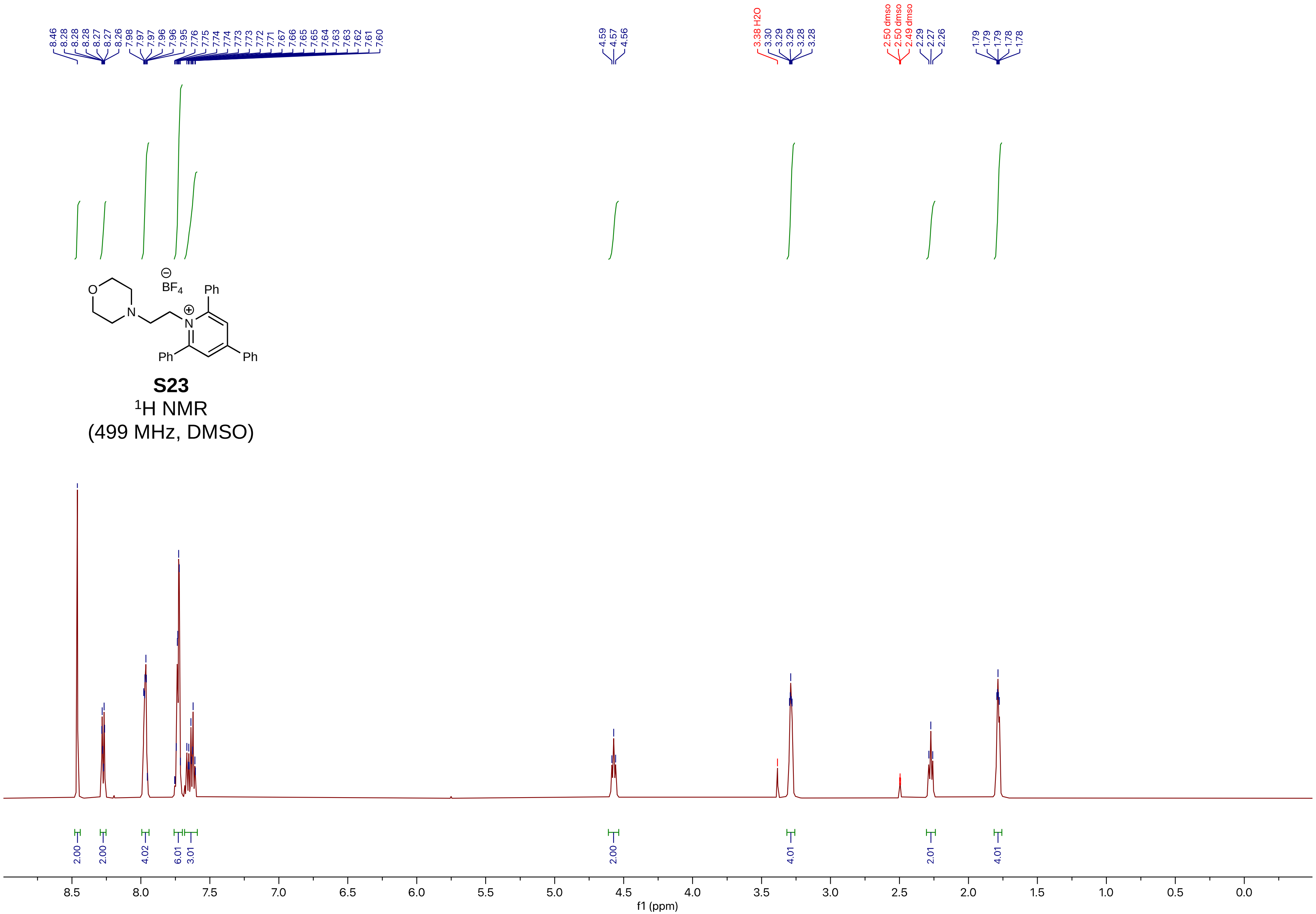
^{1}H NMR

(499 MHz, $CDCl_3$)



S22
^{13}C NMR
(126 MHz, $CDCl_3$)

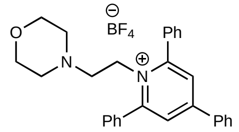




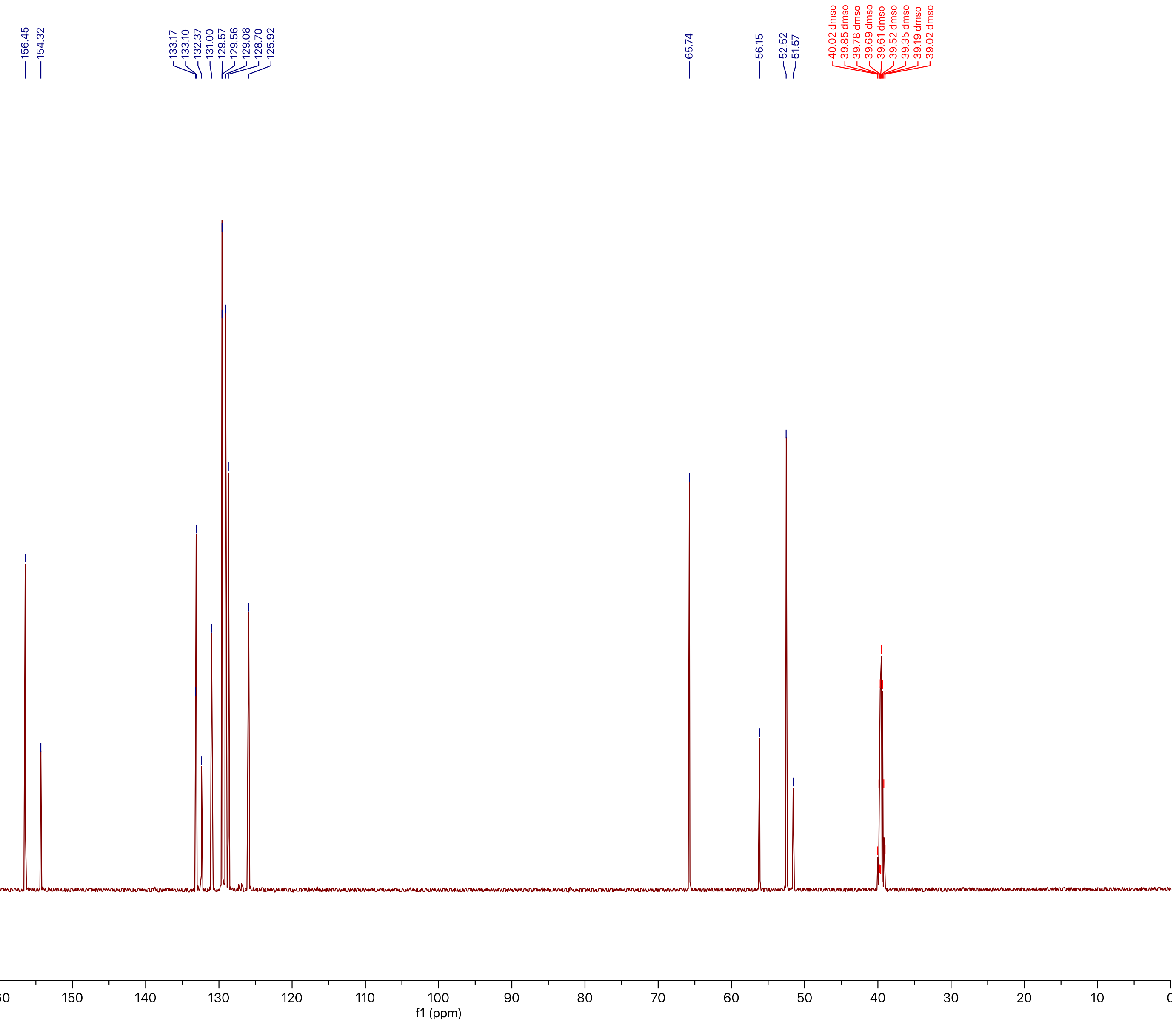
S23

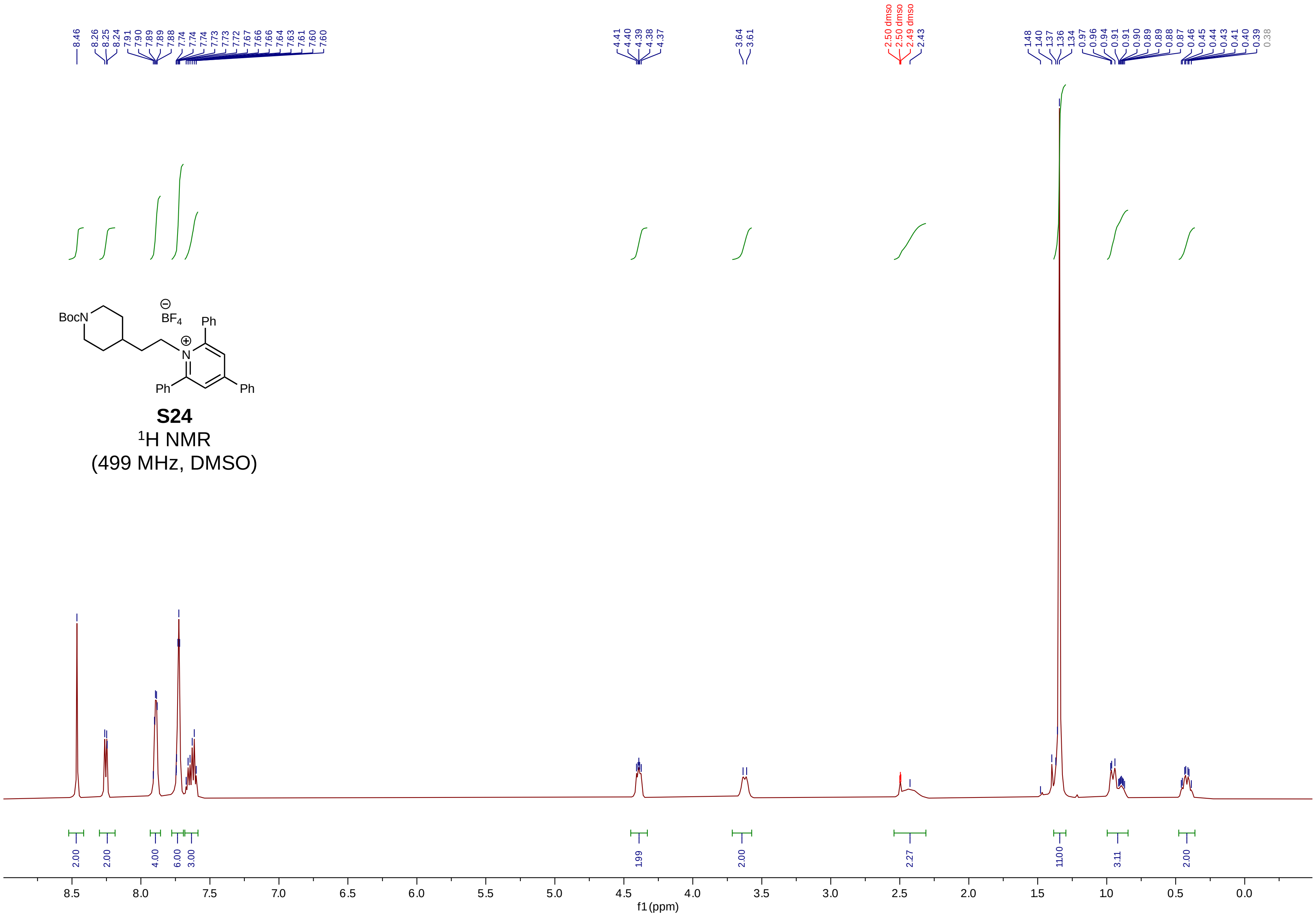
^{1}H NMR

(499 MHz, DMSO)



S23
^{13}C NMR
(126 MHz, DMSO)

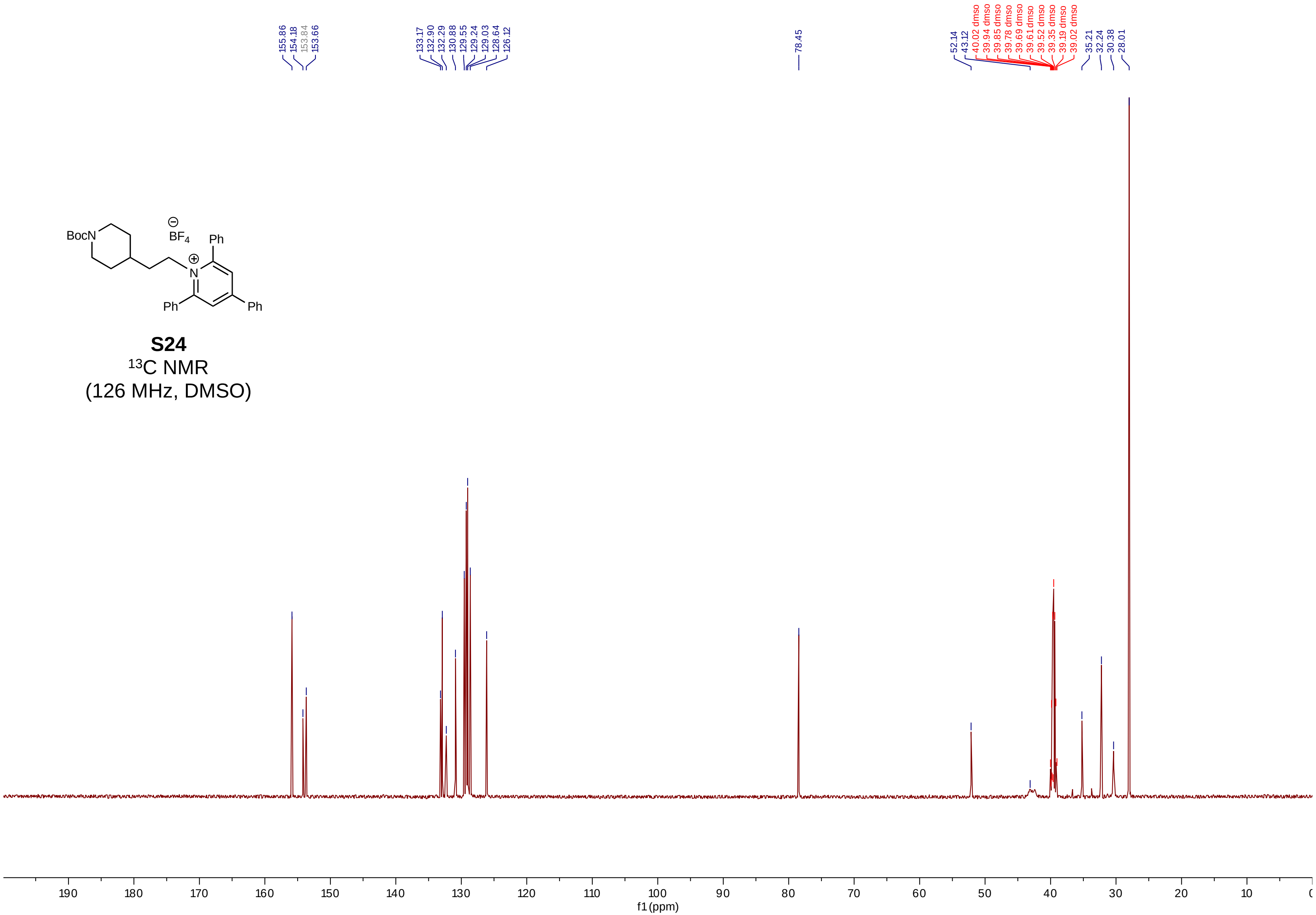




S24

^{1}H NMR

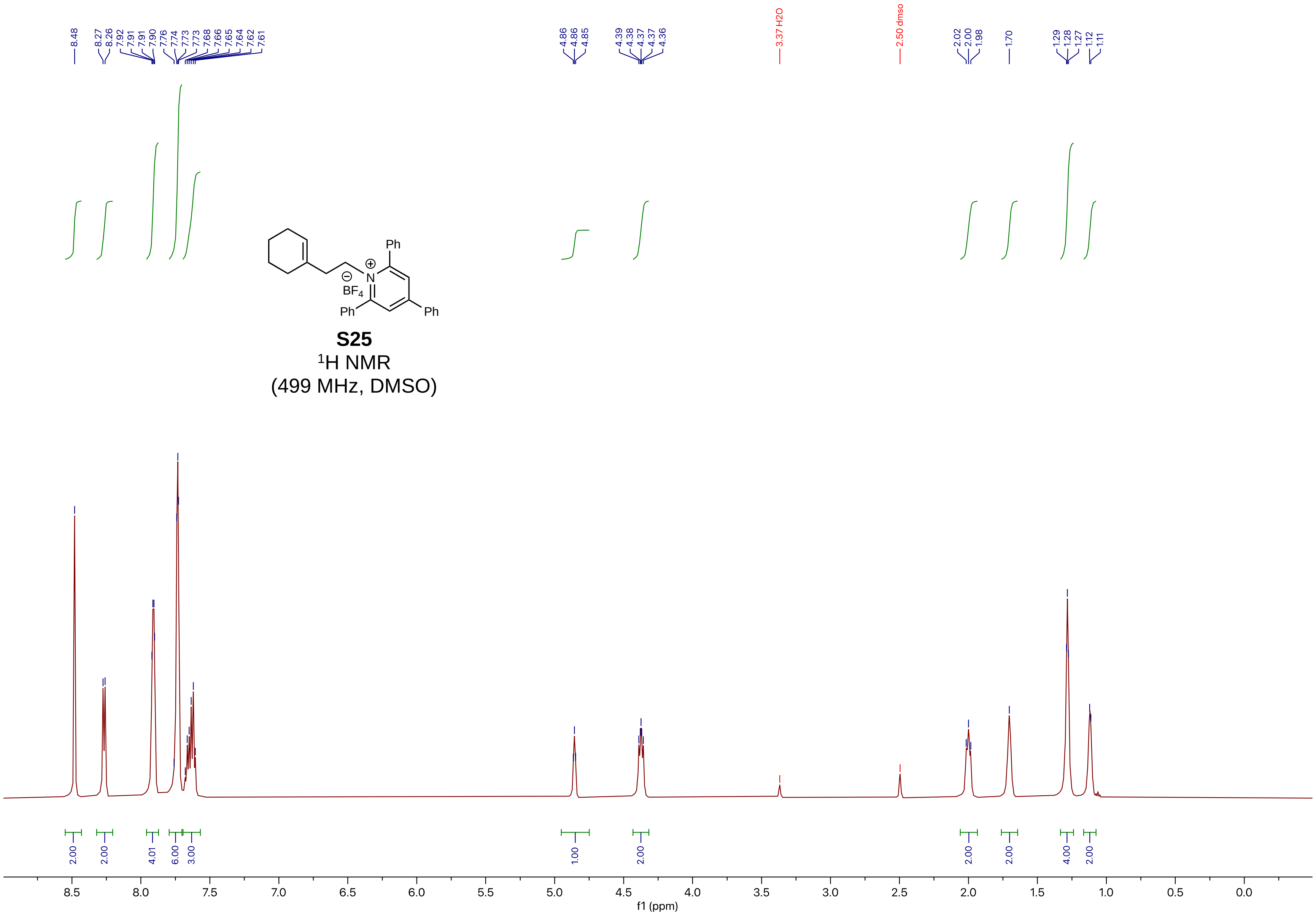
(499 MHz, DMSO)



S24

^{13}C NMR

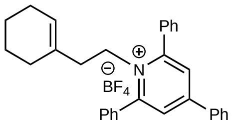
(126 MHz, DMSO)



S25

^{1}H NMR

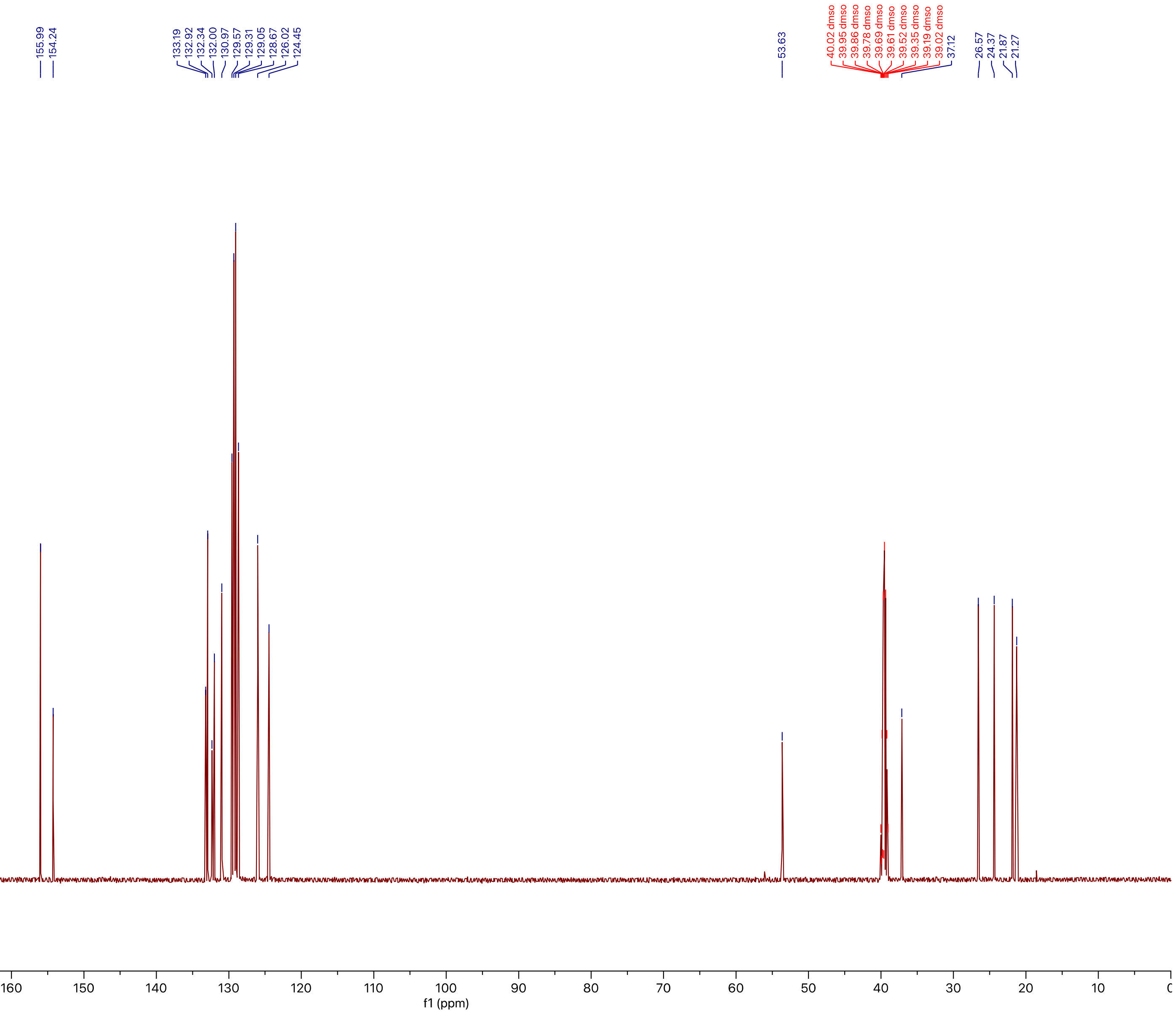
(499 MHz, DMSO)

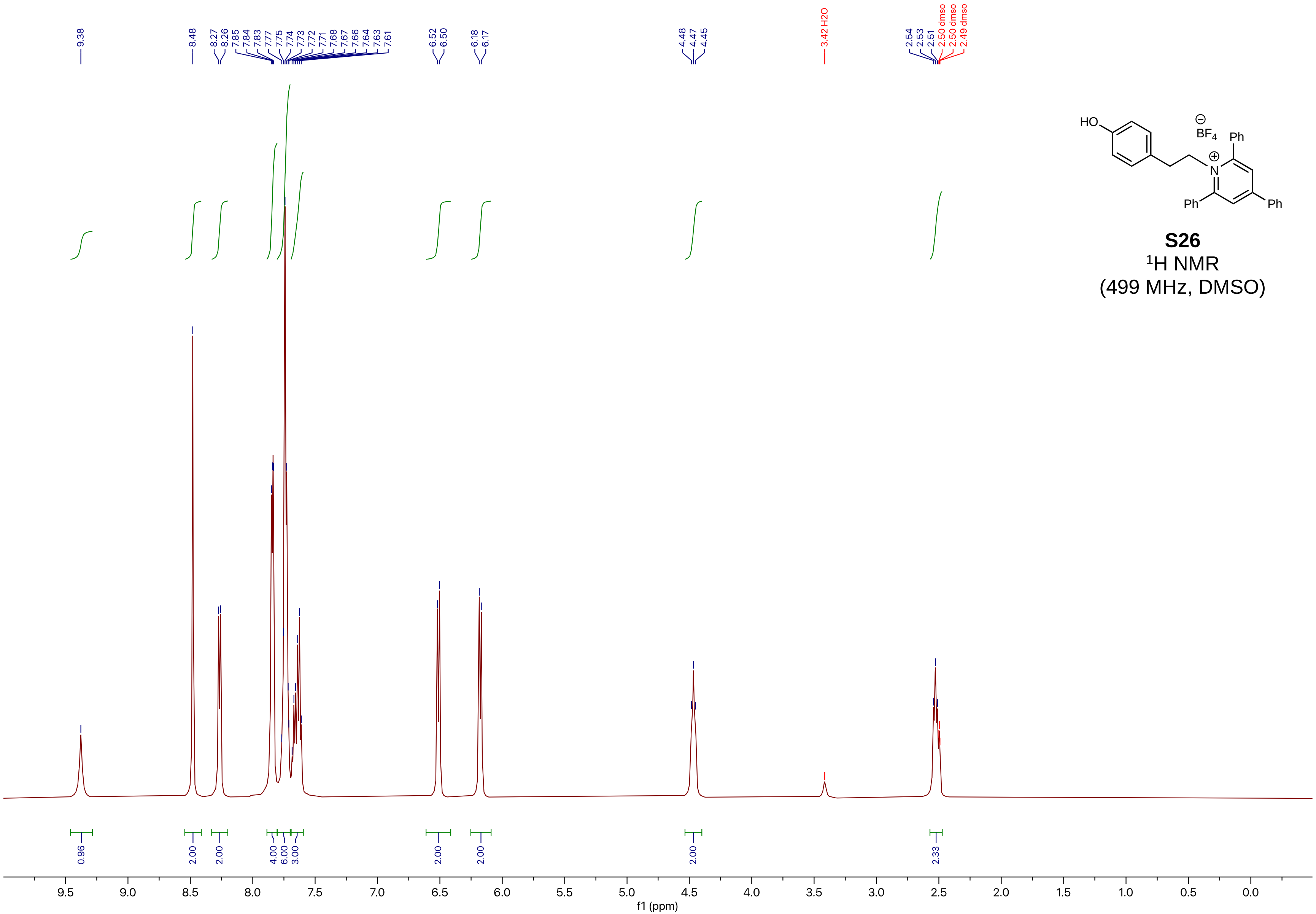


S25

^{13}C NMR

(126 MHz, DMSO)

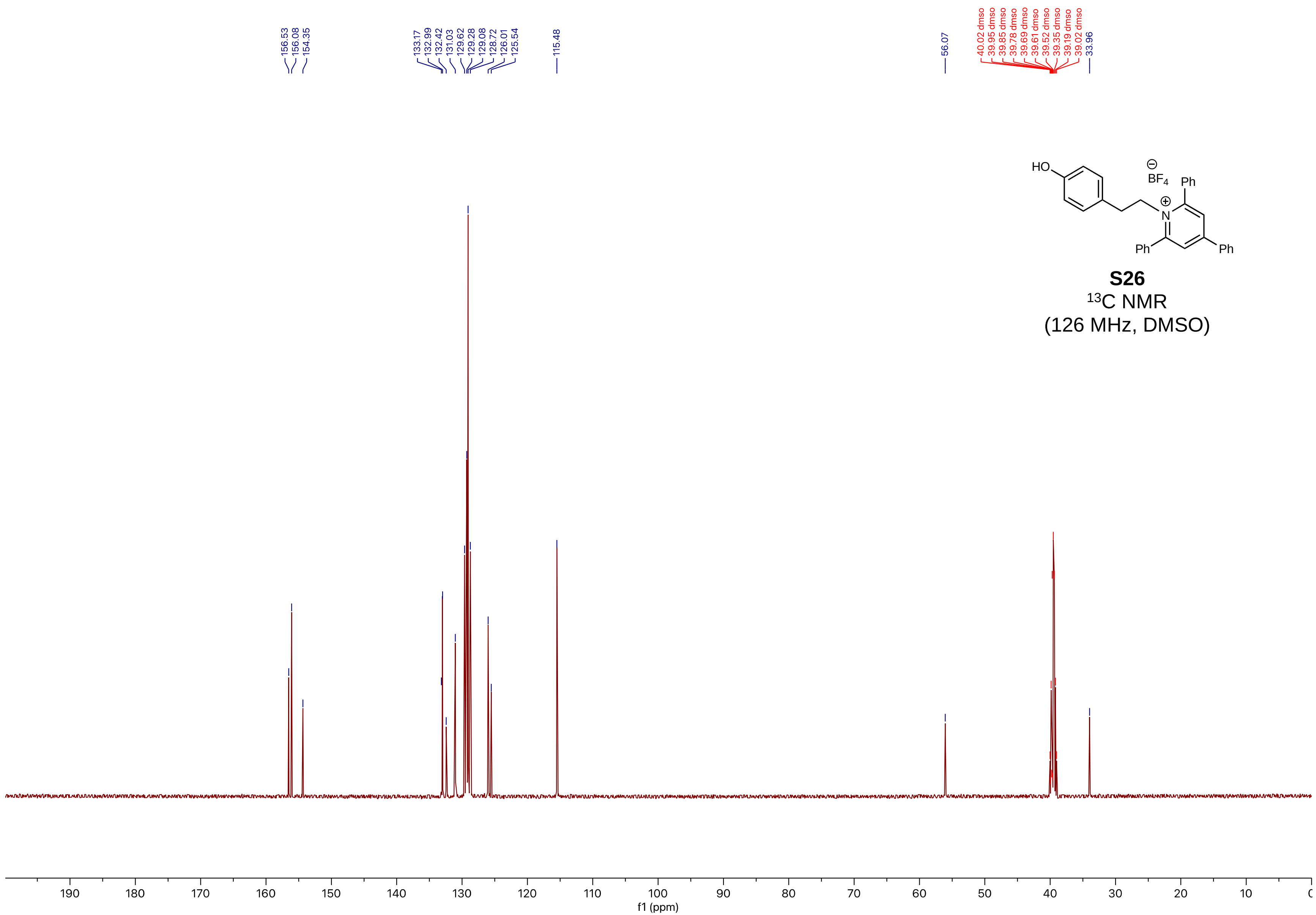




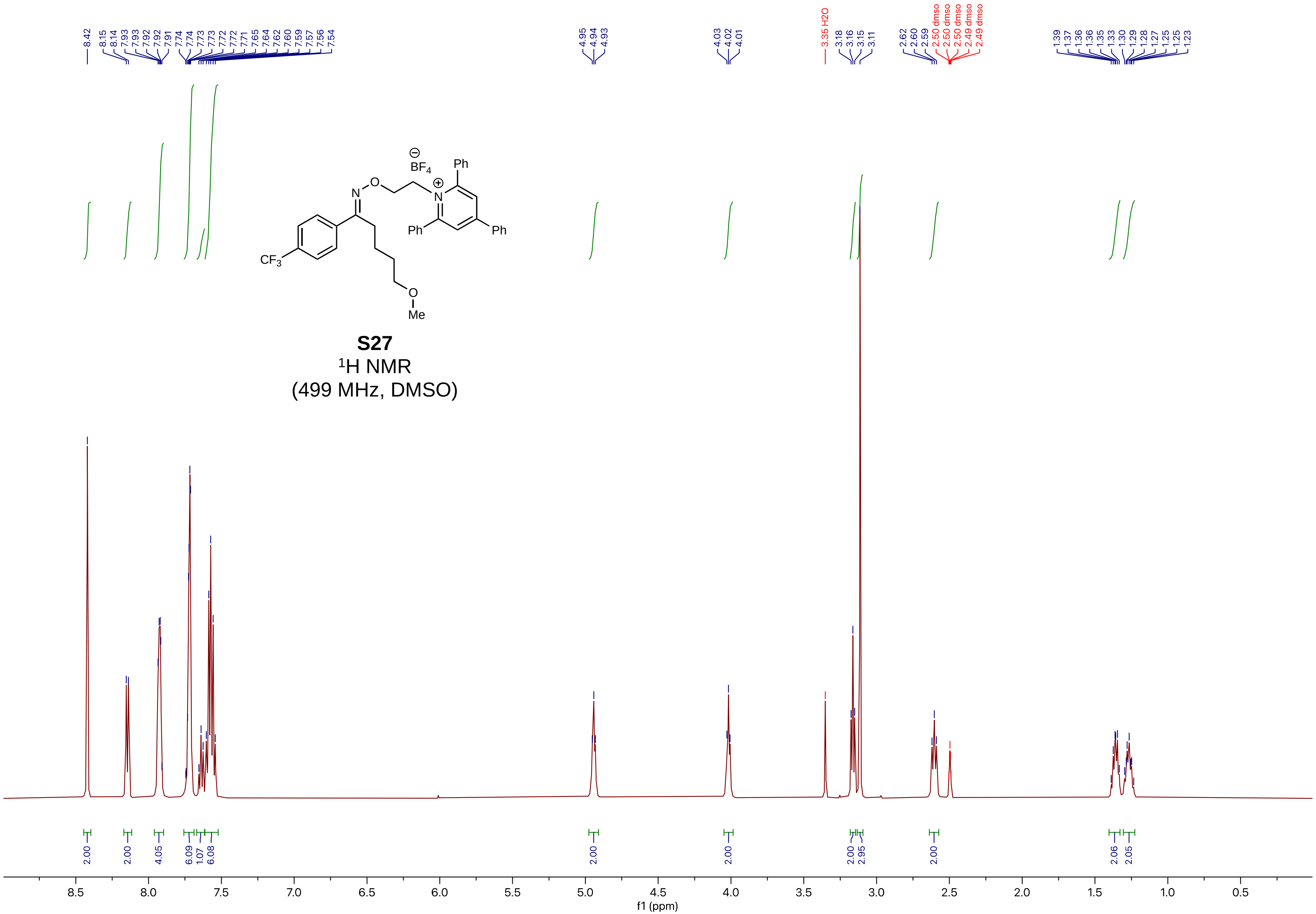
S26

^{1}H NMR

(499 MHz, DMSO)



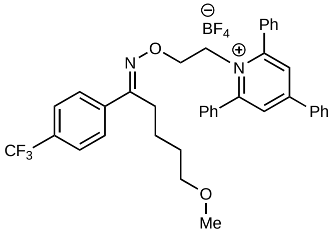
S26
^{13}C NMR
(126 MHz, DMSO)



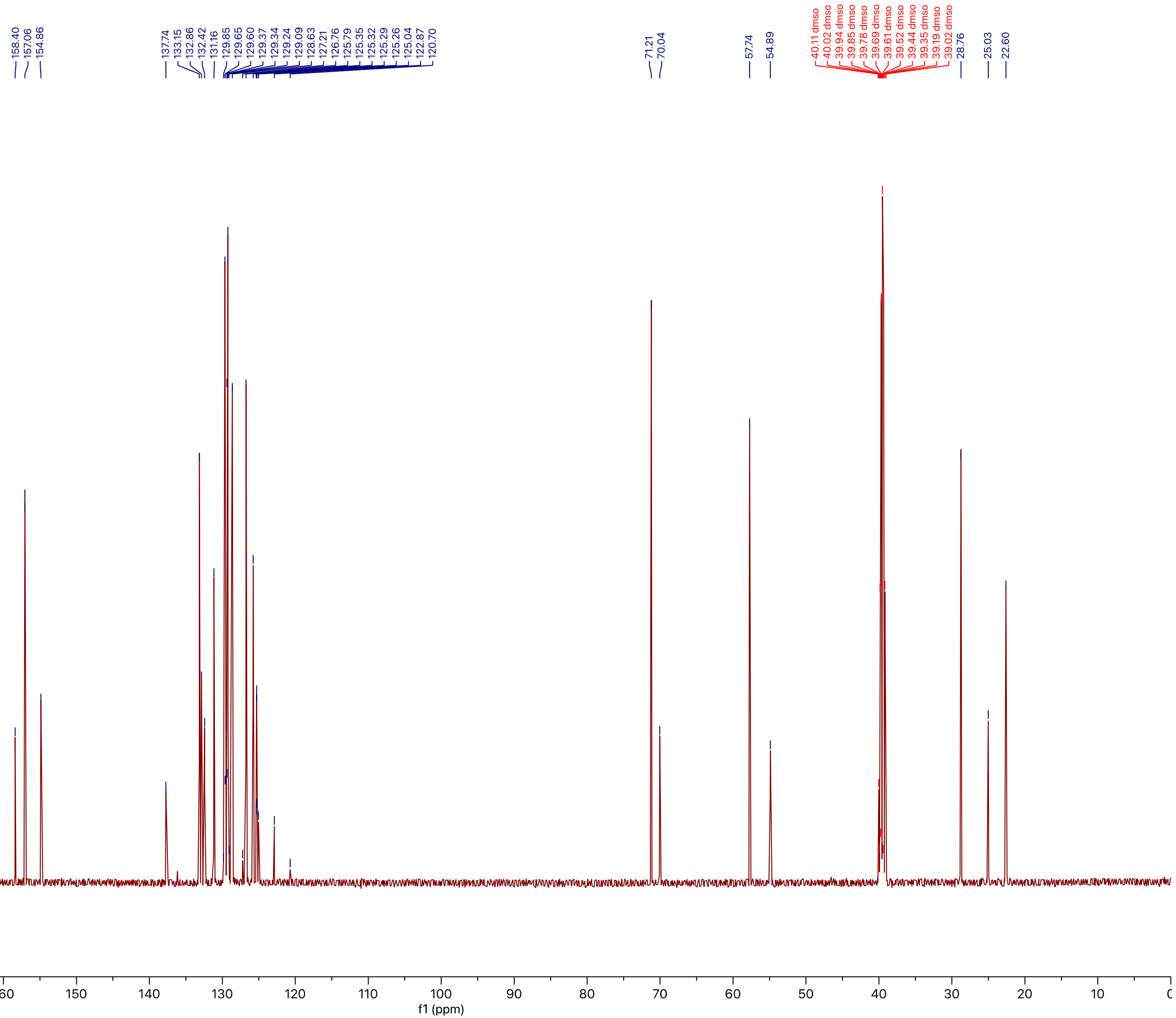
S27

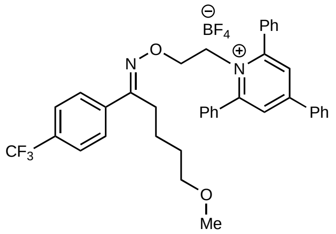
^{1}H NMR

(499 MHz, DMSO)

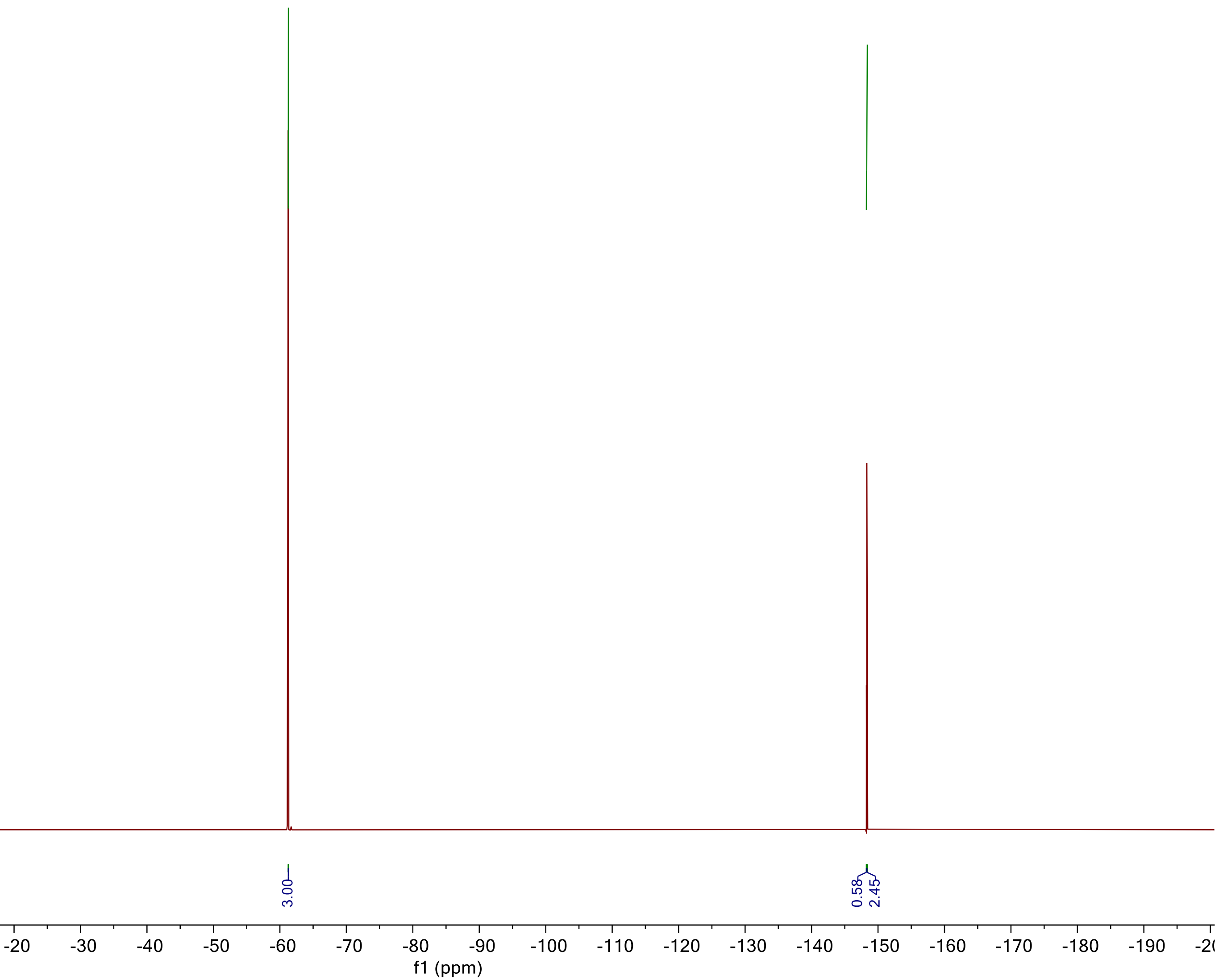


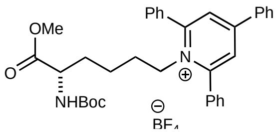
S27
^{13}C NMR
(126 MHz, DMSO)





S27
^{19}F NMR
(470 MHz, DMSO)

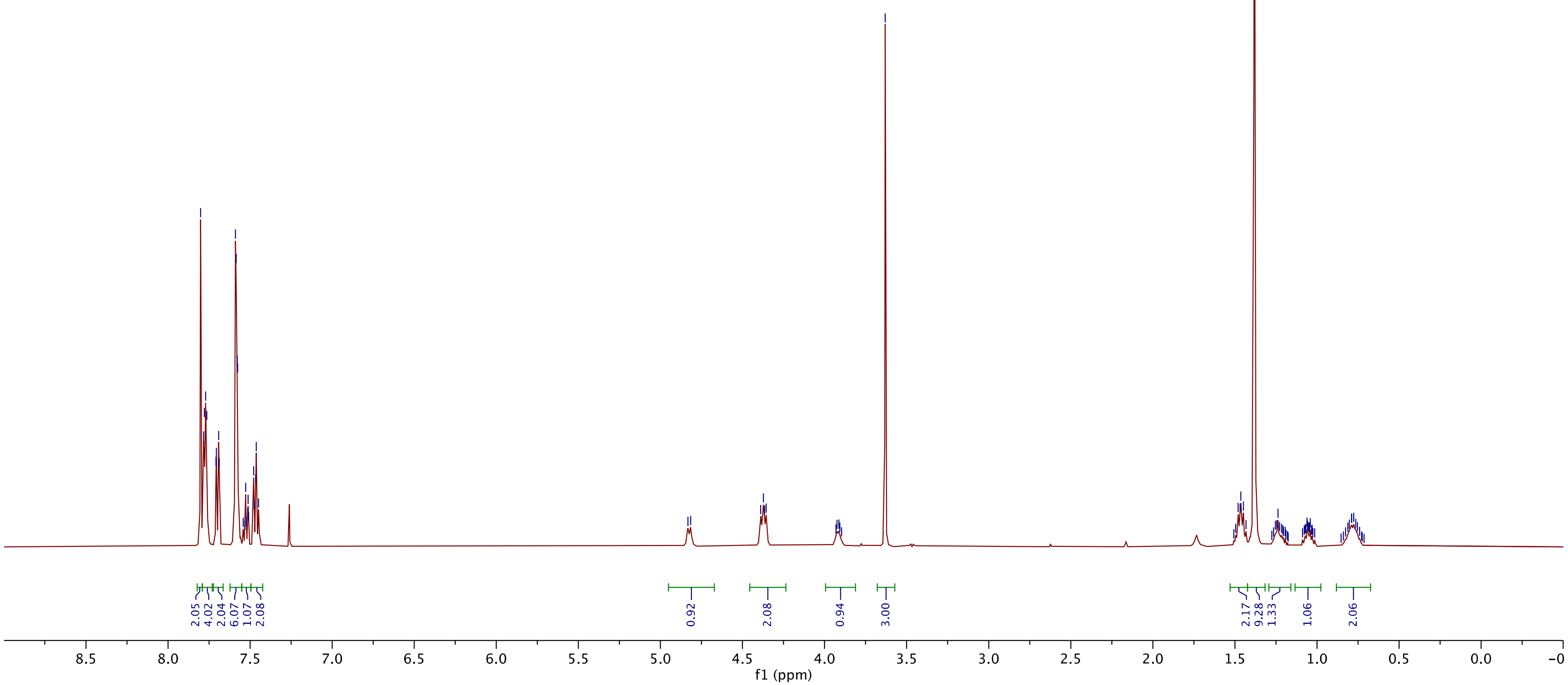


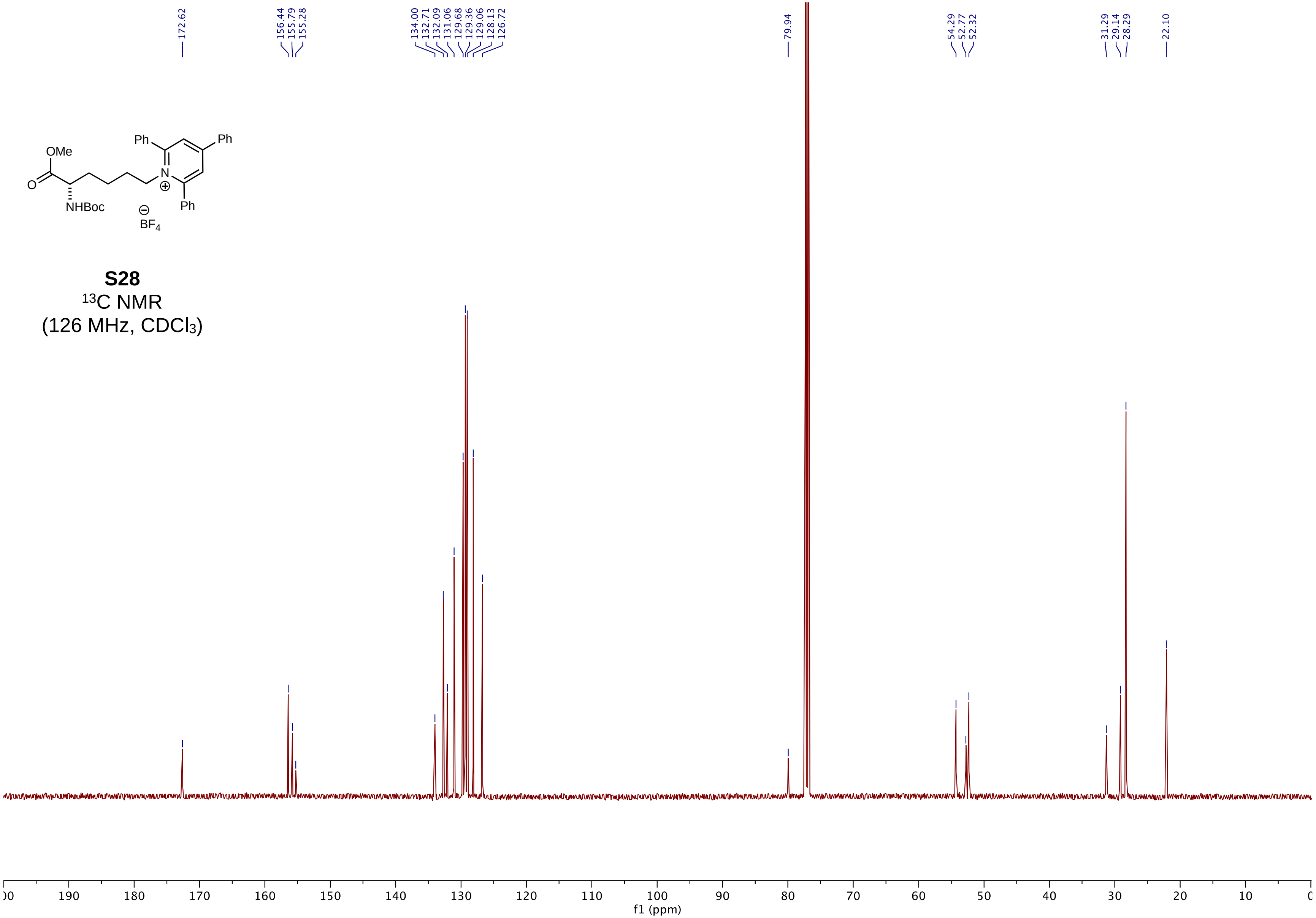


S28

^{1}H NMR

(500 MHz, $CDCl_3$)

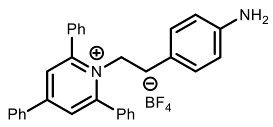




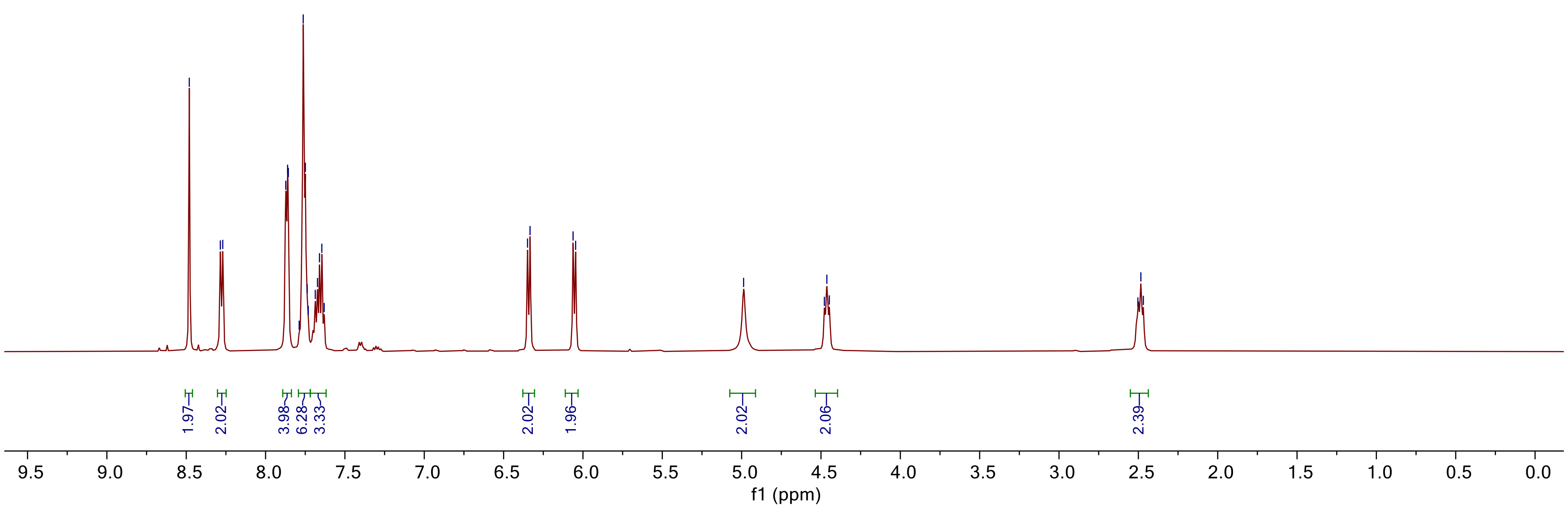
S28

^{13}C NMR

(126 MHz, $CDCl_3$)



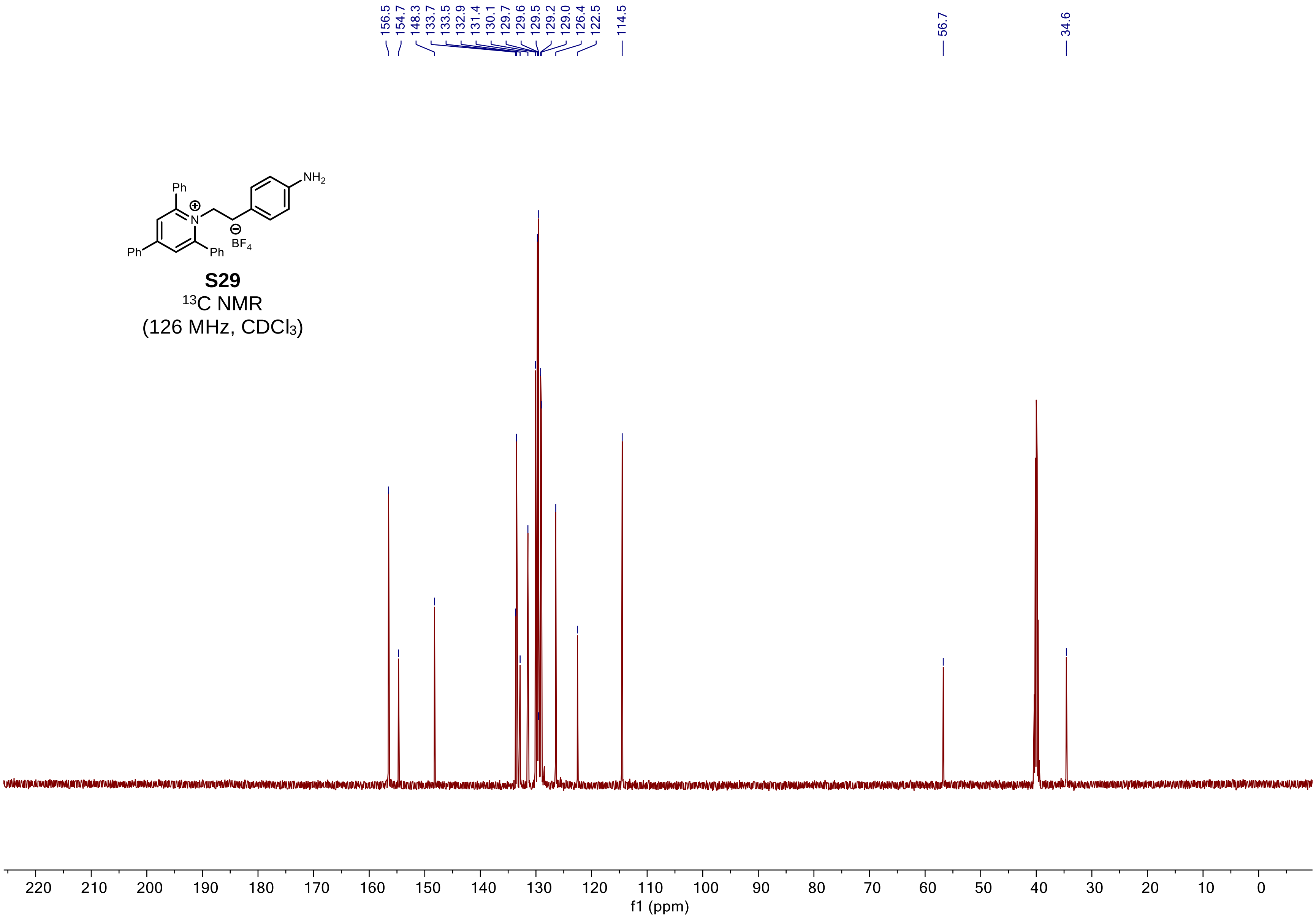
S29
^{1}H NMR
(499 MHz, $CDCl_3$)

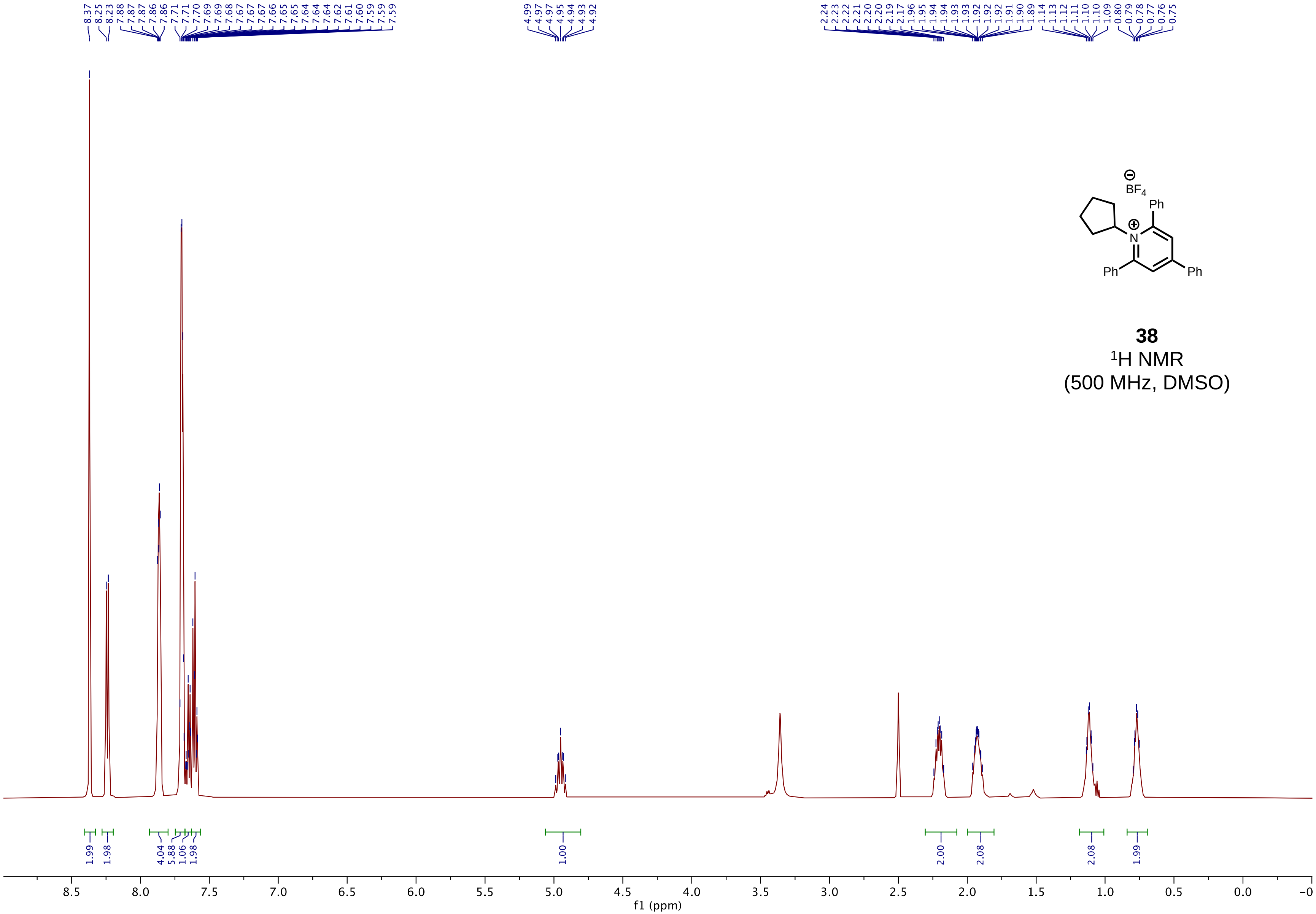


S29

^{13}C NMR

(126 MHz, $CDCl_3$)

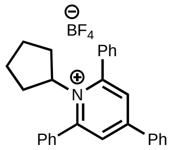




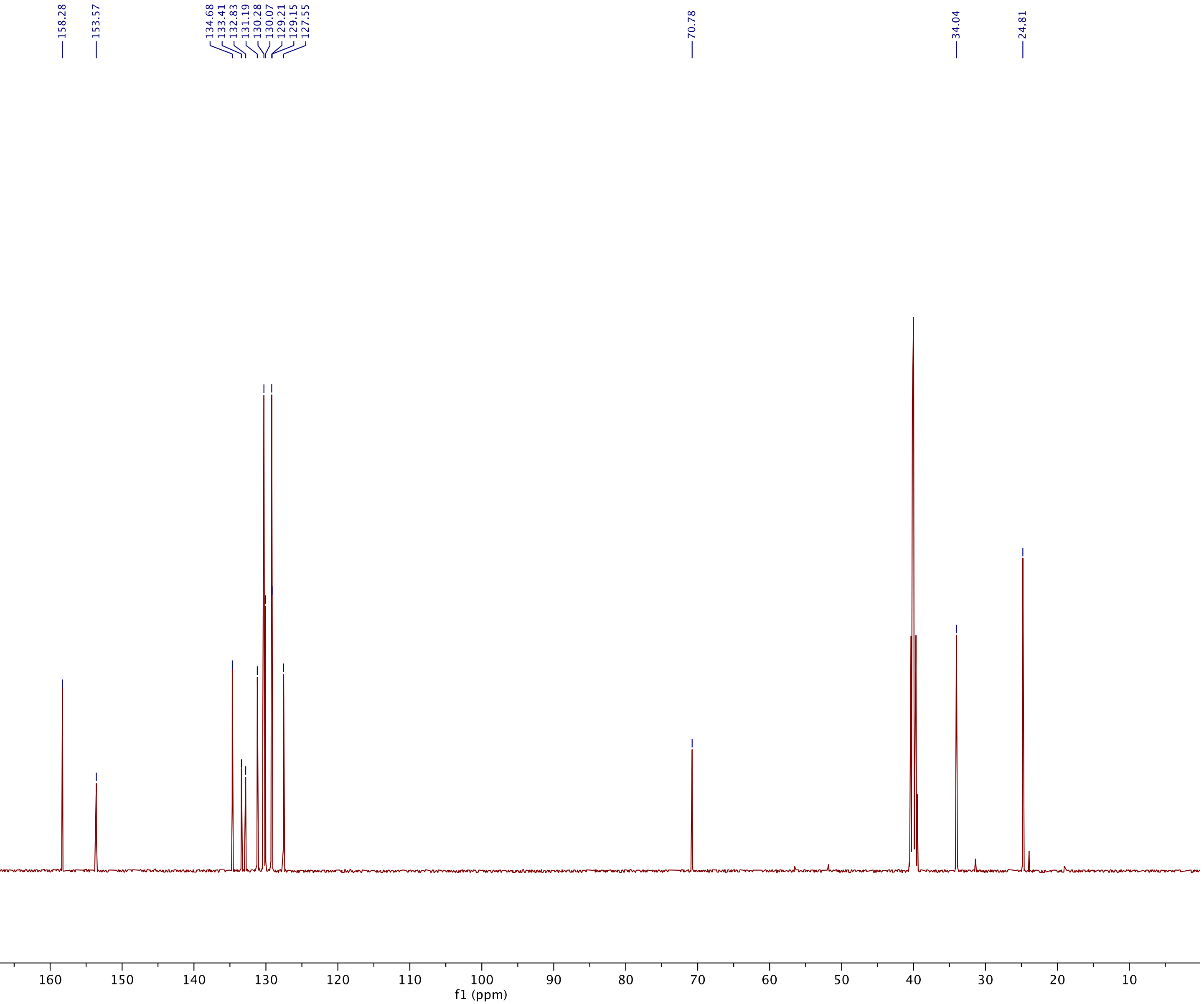
38

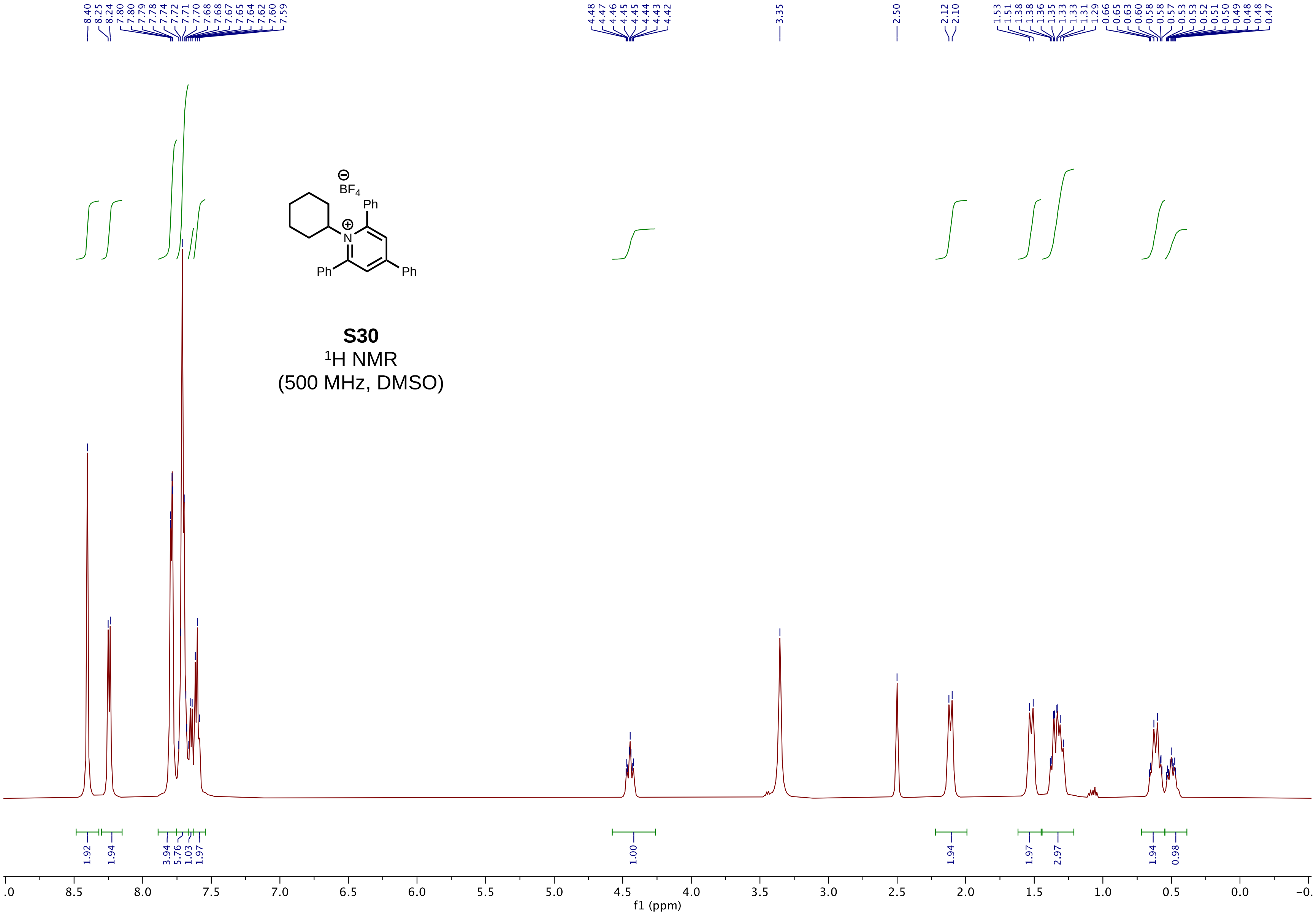
^{1}H NMR

(500 MHz, DMSO)

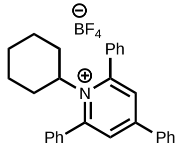


38
^{13}C NMR
(126 MHz, DMSO)

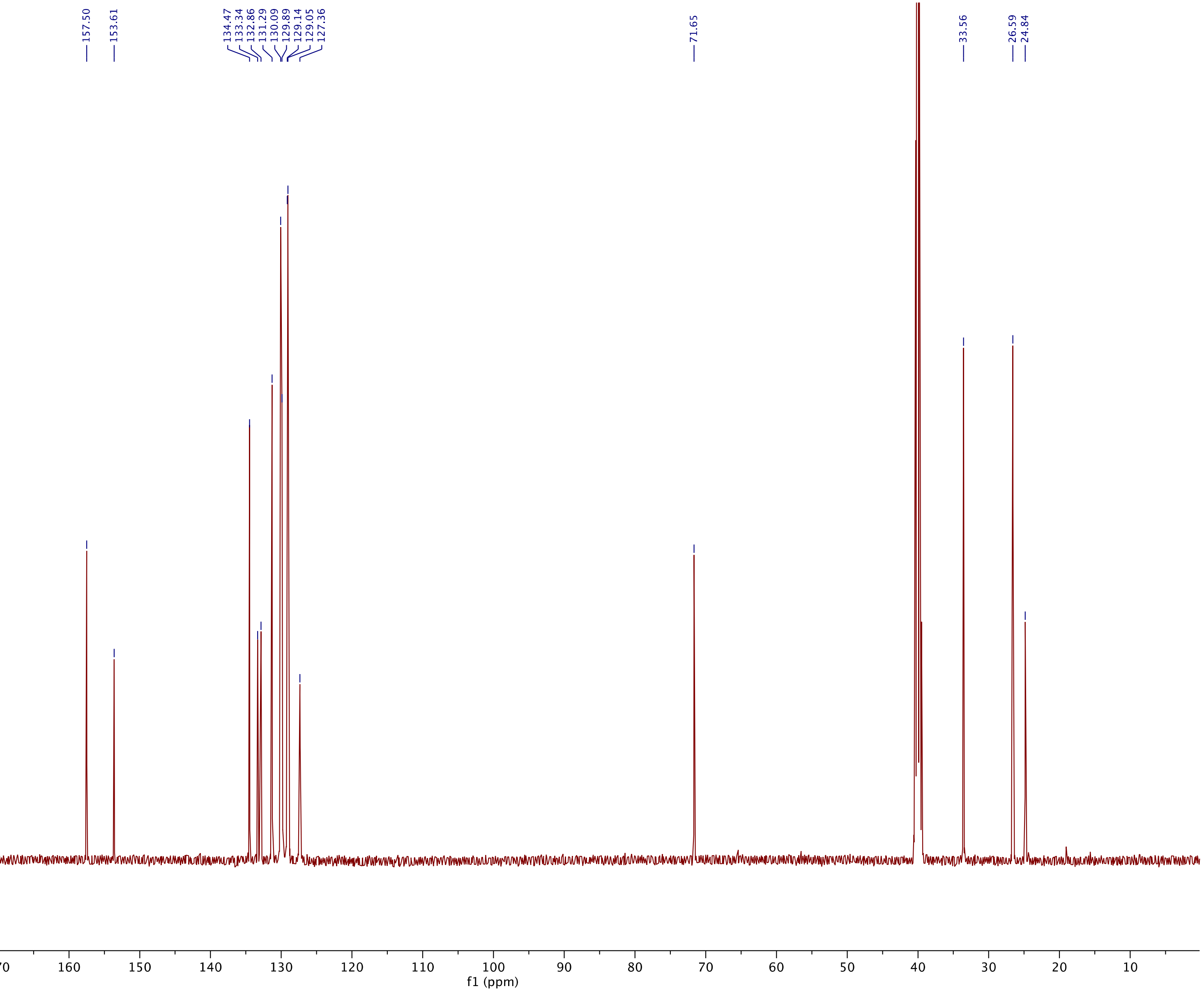


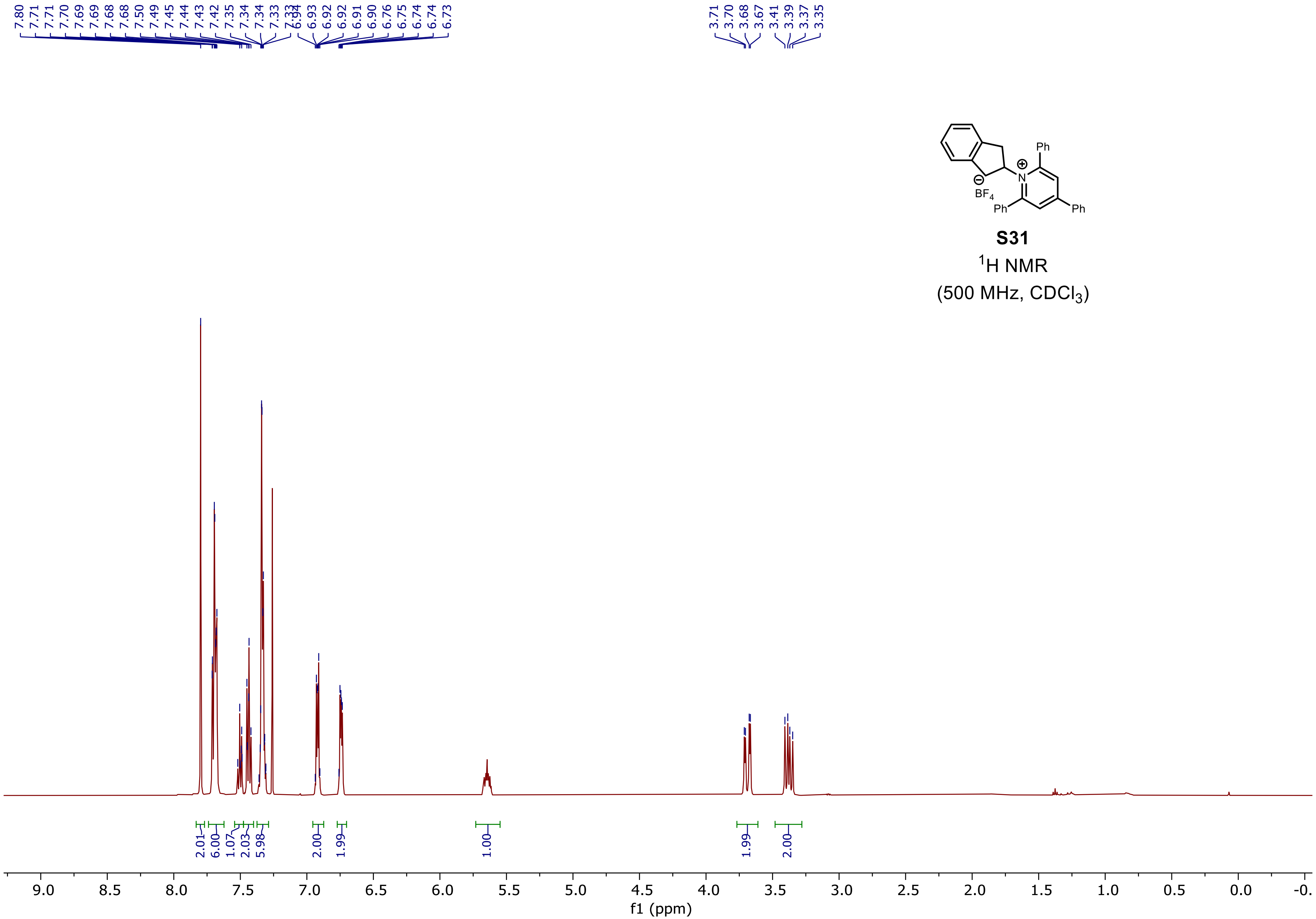


8.40
8.25
8.24
7.80
7.79
7.78
7.74
7.72
7.71
7.70
7.68
7.68
7.67
7.65
7.64
7.62
7.60
7.59
4.48
4.47
4.46
4.45
4.45
4.44
4.43
4.42
3.35
2.50
2.12
2.10
1.53
1.51
1.38
1.38
1.36
1.35
1.33
1.33
1.31
1.29
0.66
0.65
0.63
0.60
0.58
0.58
0.57
0.53
0.53
0.52
0.51
0.50
0.49
0.48
0.48
0.47
BF4
Ph
N
Ph
Ph
S30
1H NMR
(500 MHz, DMSO)
1.92
1.94
3.94
5.76
1.03
1.97
1.00
1.94
1.97
2.97
1.94
0.98
f1 (ppm)



S30
^{13}C NMR
(126 MHz, DMSO)

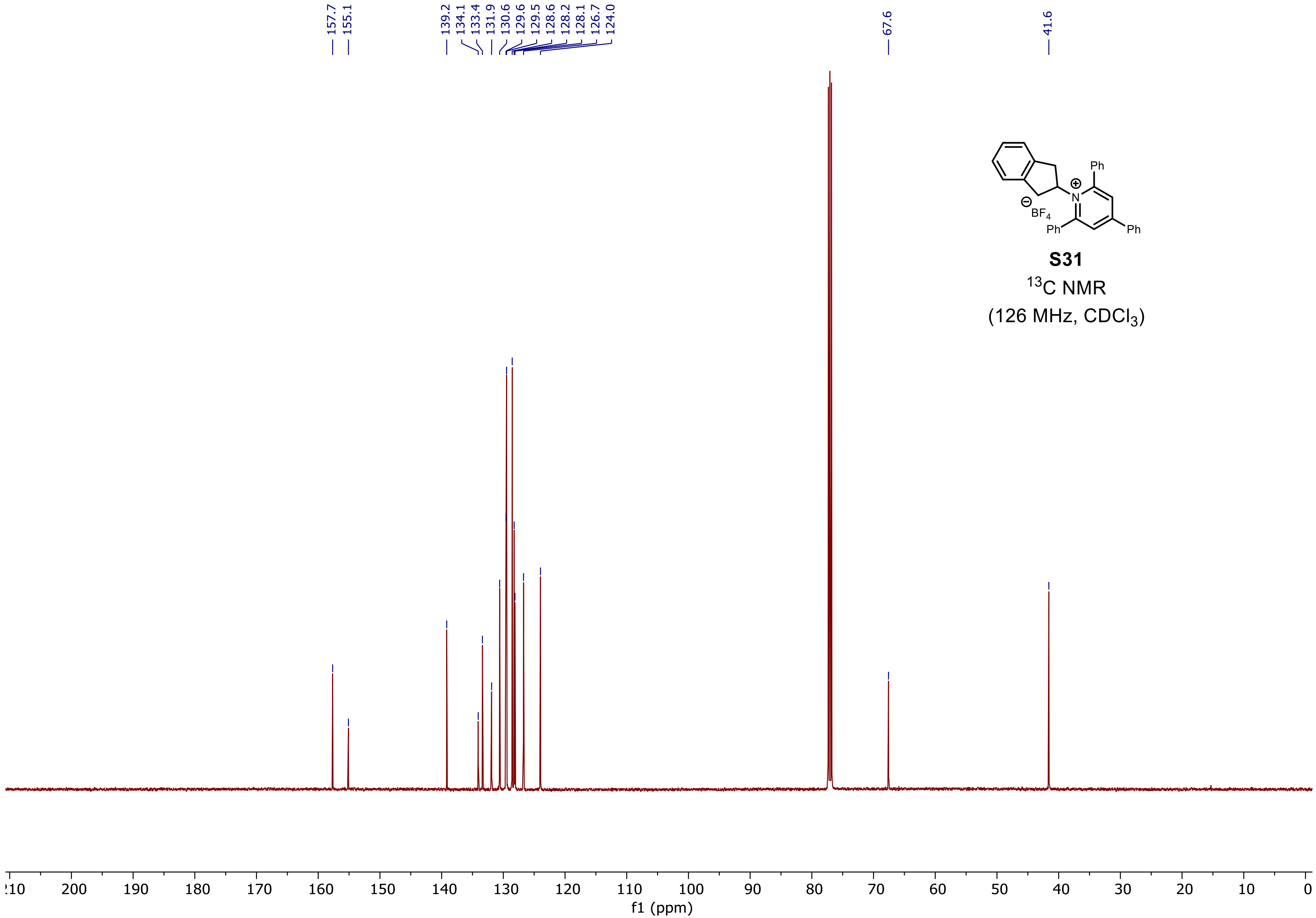




S31

^{1}H NMR

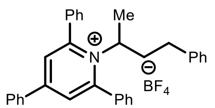
(500 MHz, $CDCl_3$)



S31

^{13}C NMR

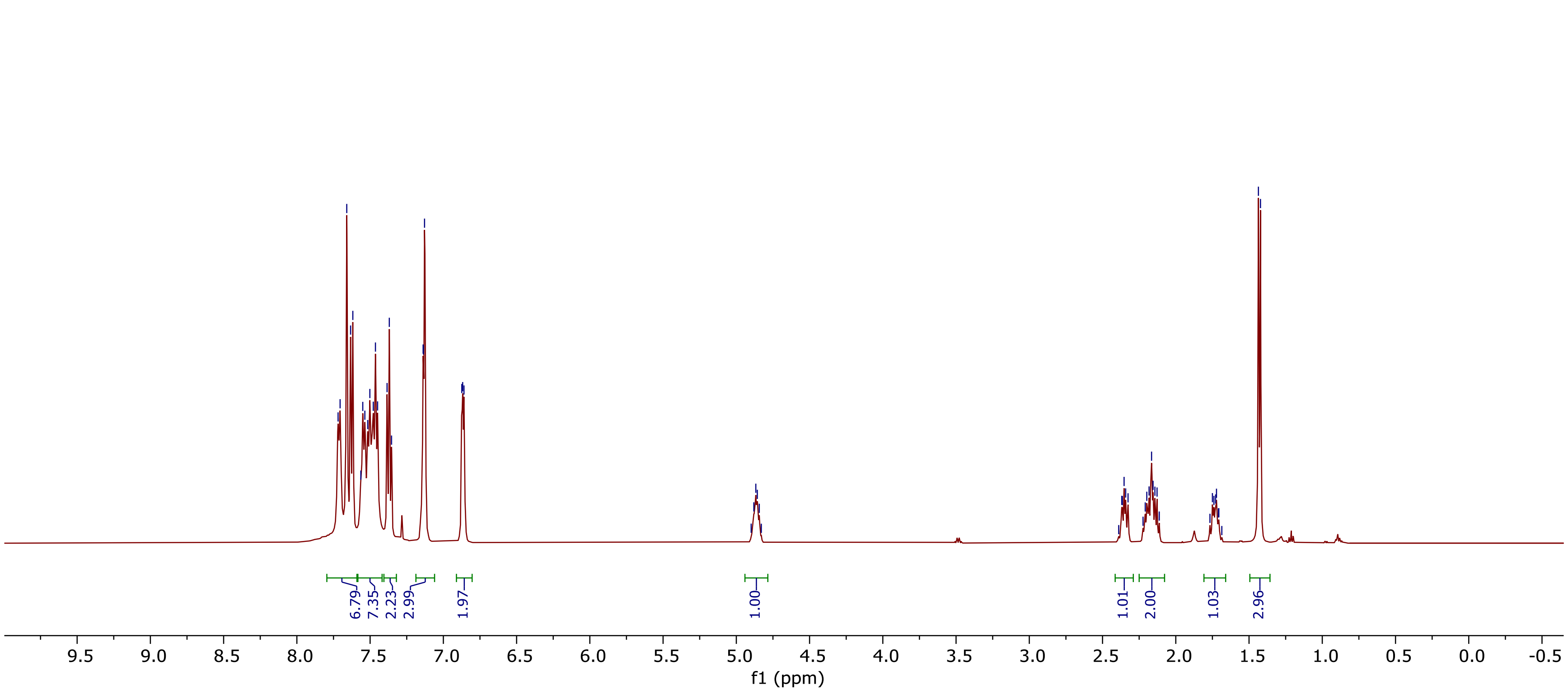
(126 MHz, $CDCl_3$)

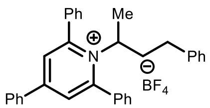


S32

^{1}H NMR

(500 MHz, $CDCl_3$)

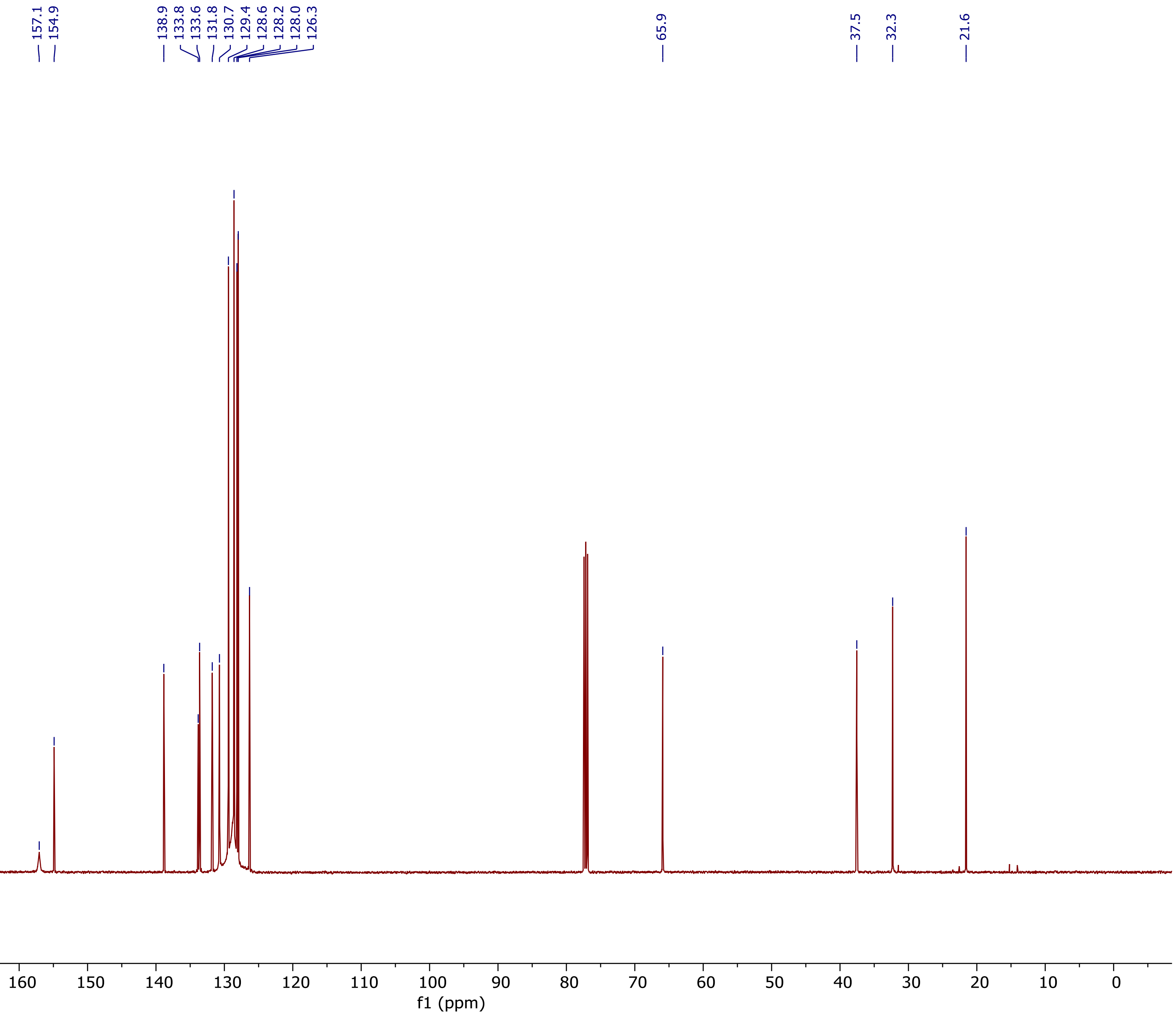


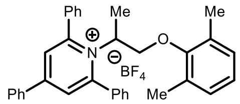


S32

^{13}C NMR

(126 MHz, $CDCl_3$)

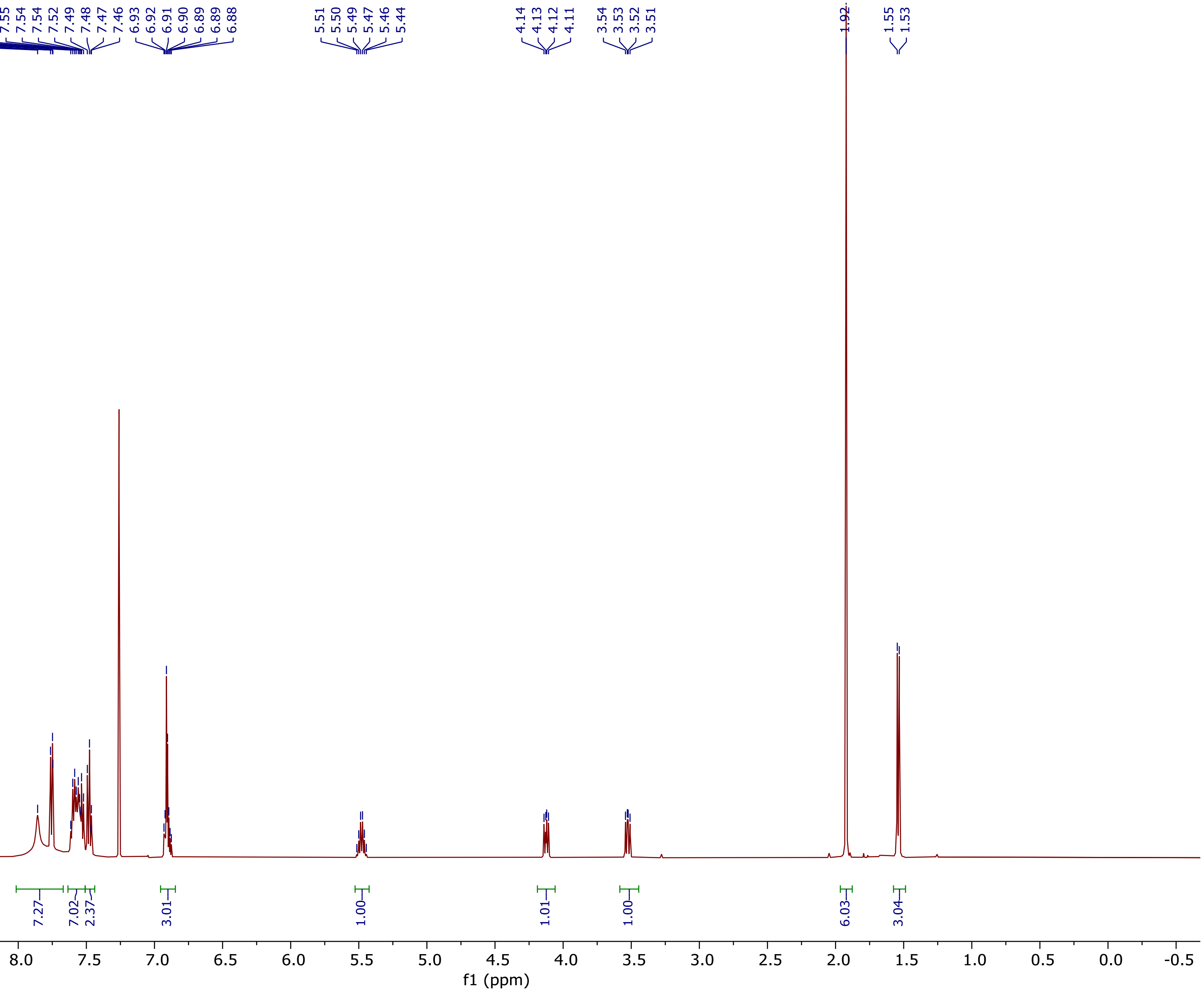


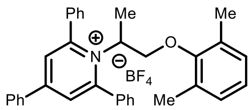


S33

^{1}H NMR

(500 MHz, $CDCl_3$)

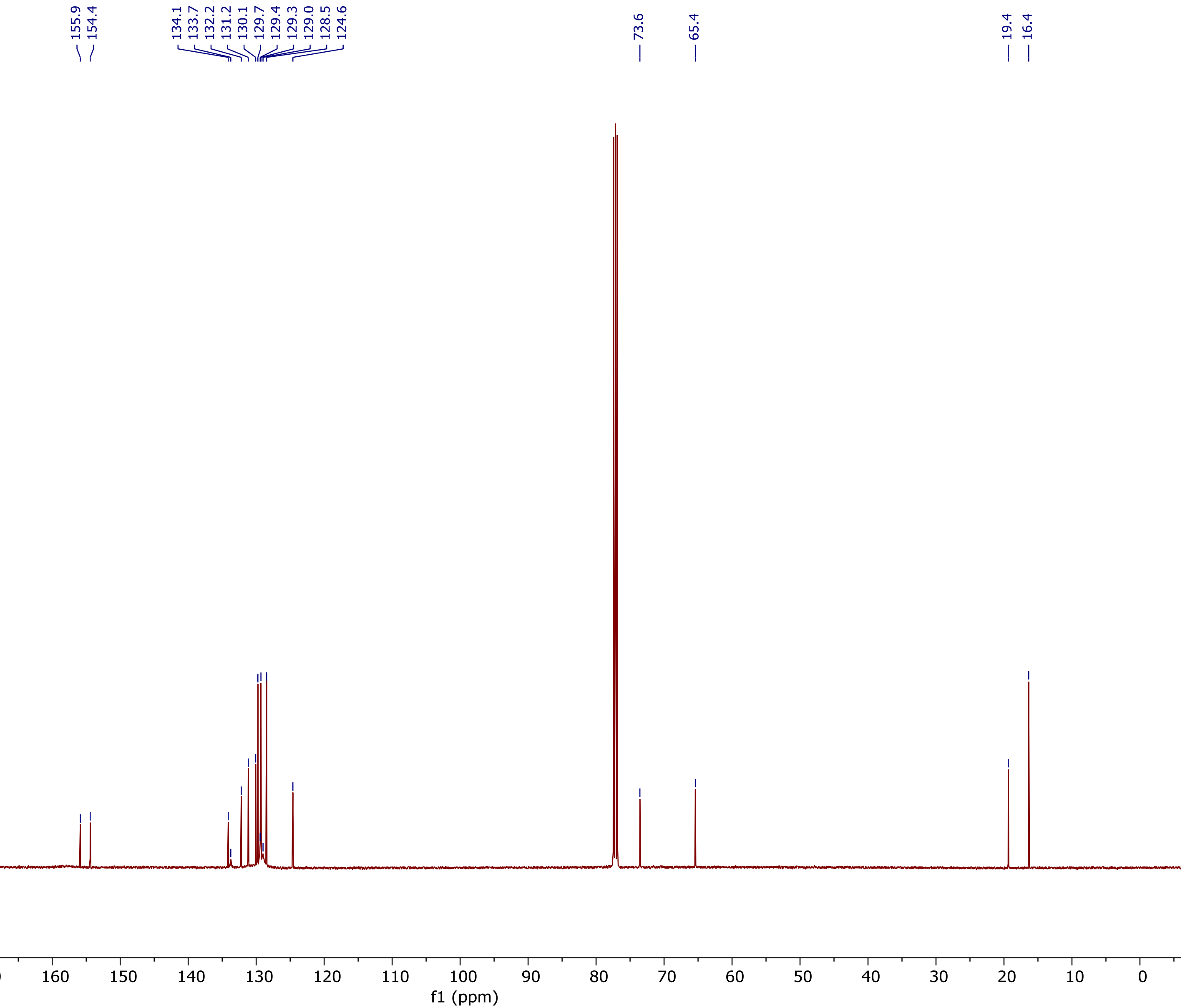


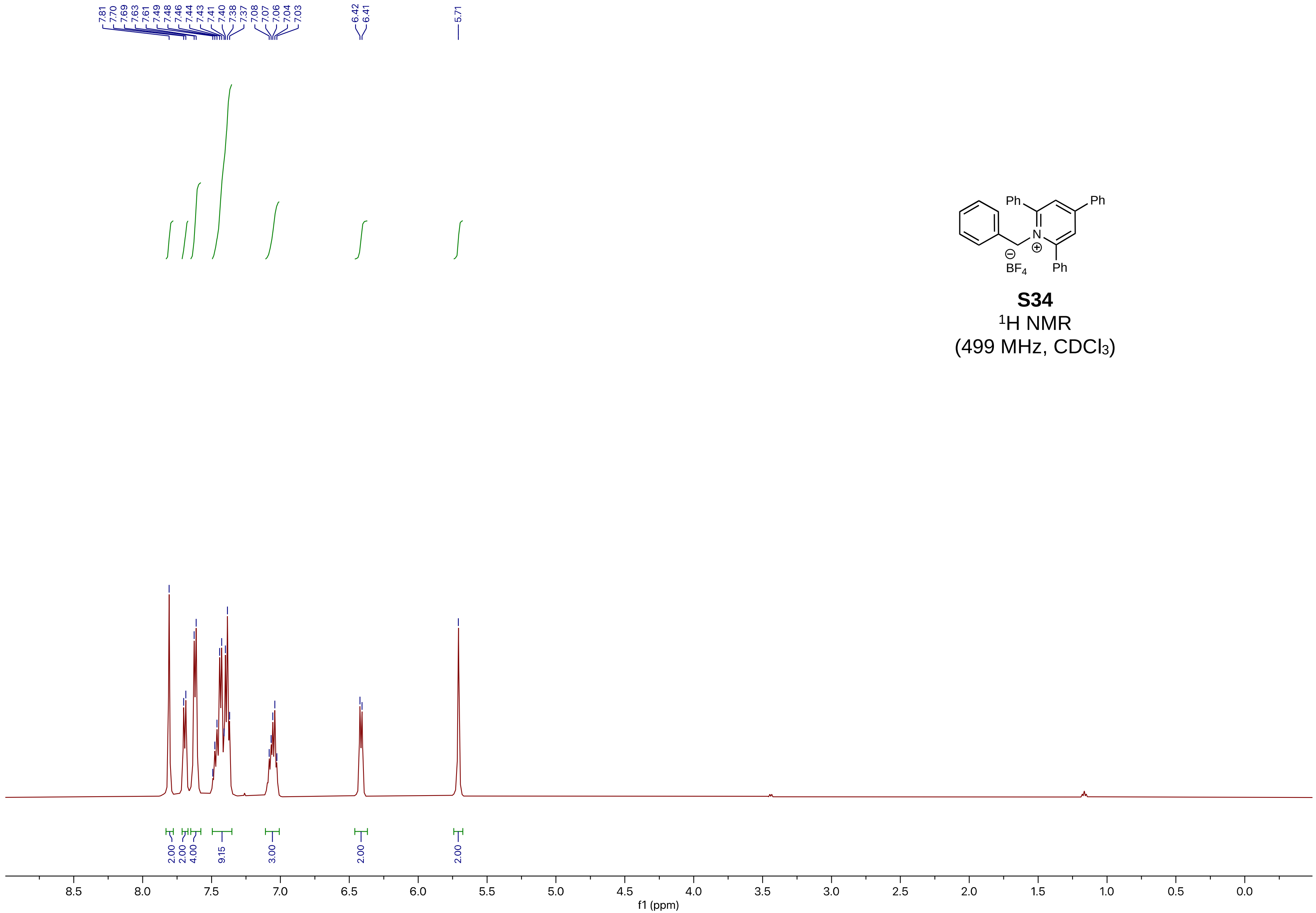


S33

^{13}C NMR

($126\ MHz$, $CDCl_3$)





S34

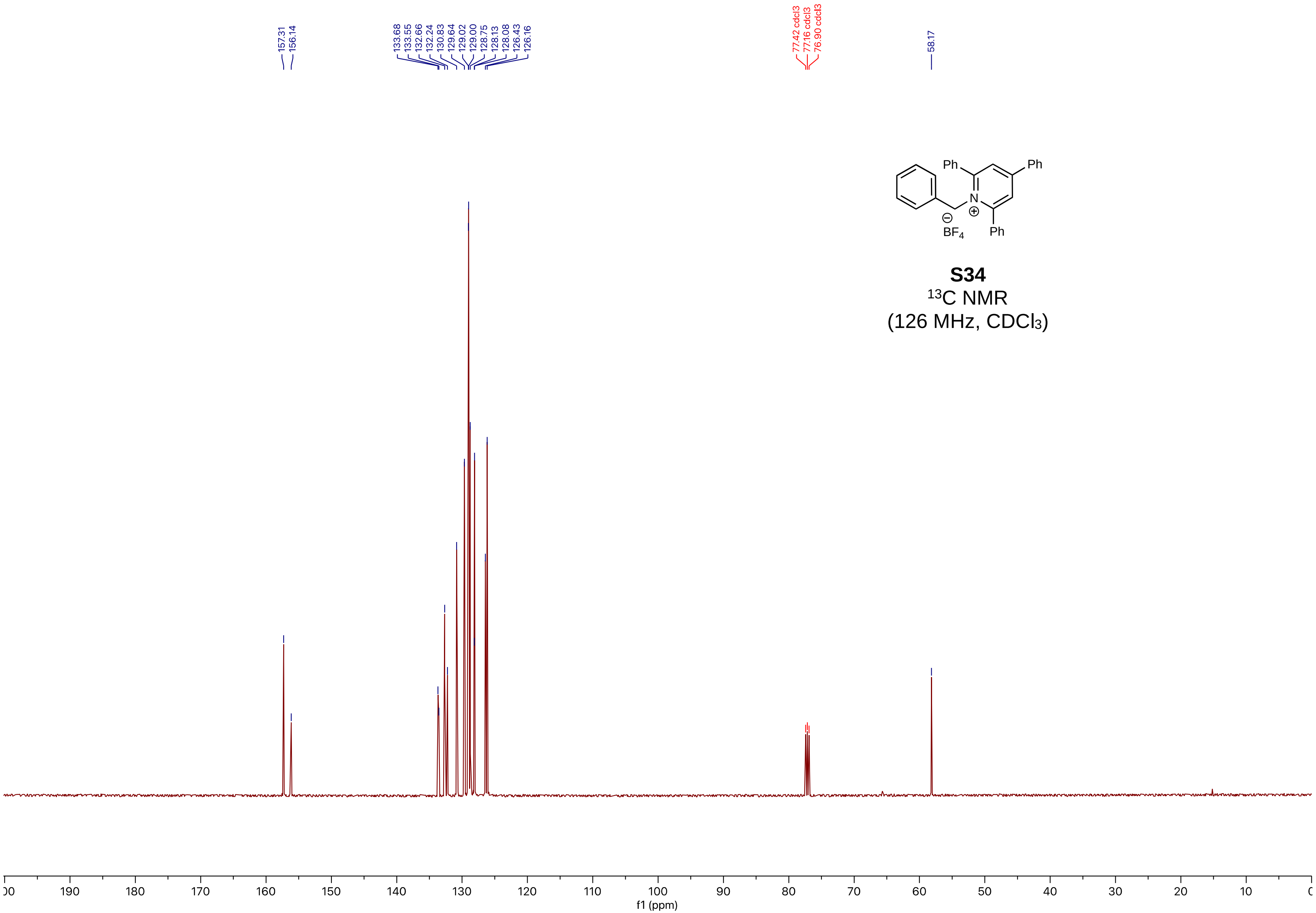
^{1}H NMR

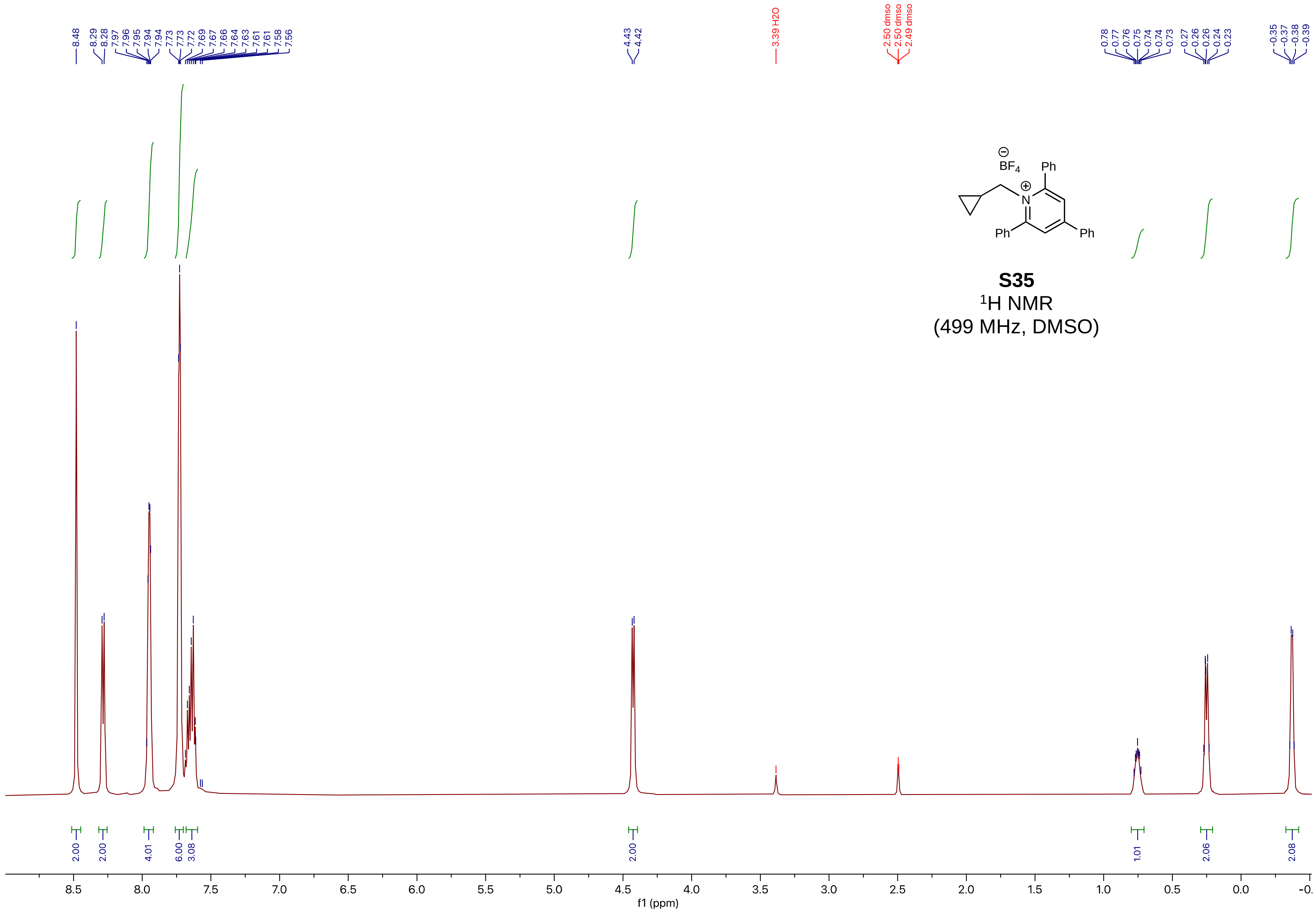
(499 MHz, $CDCl_3$)

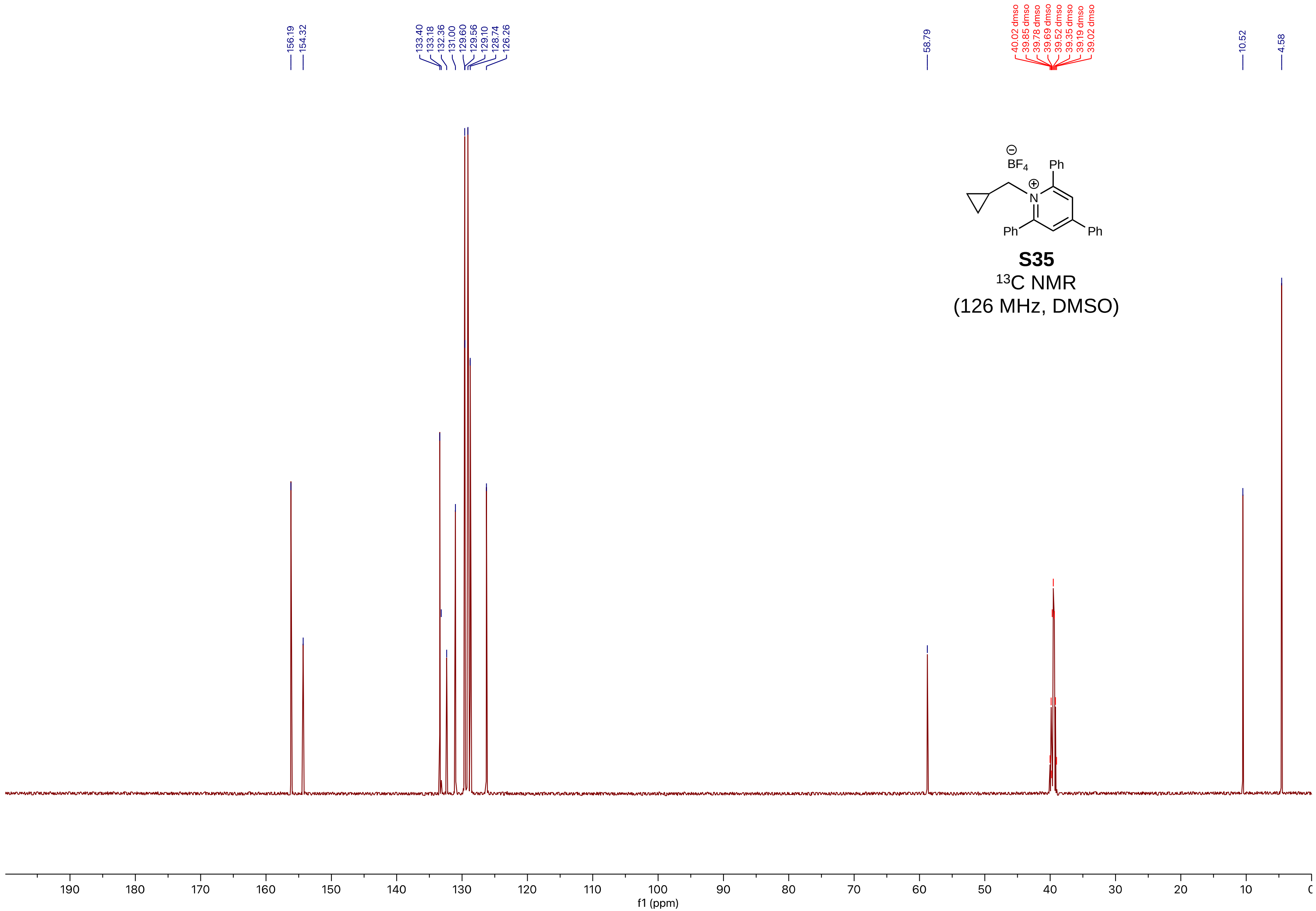
S34

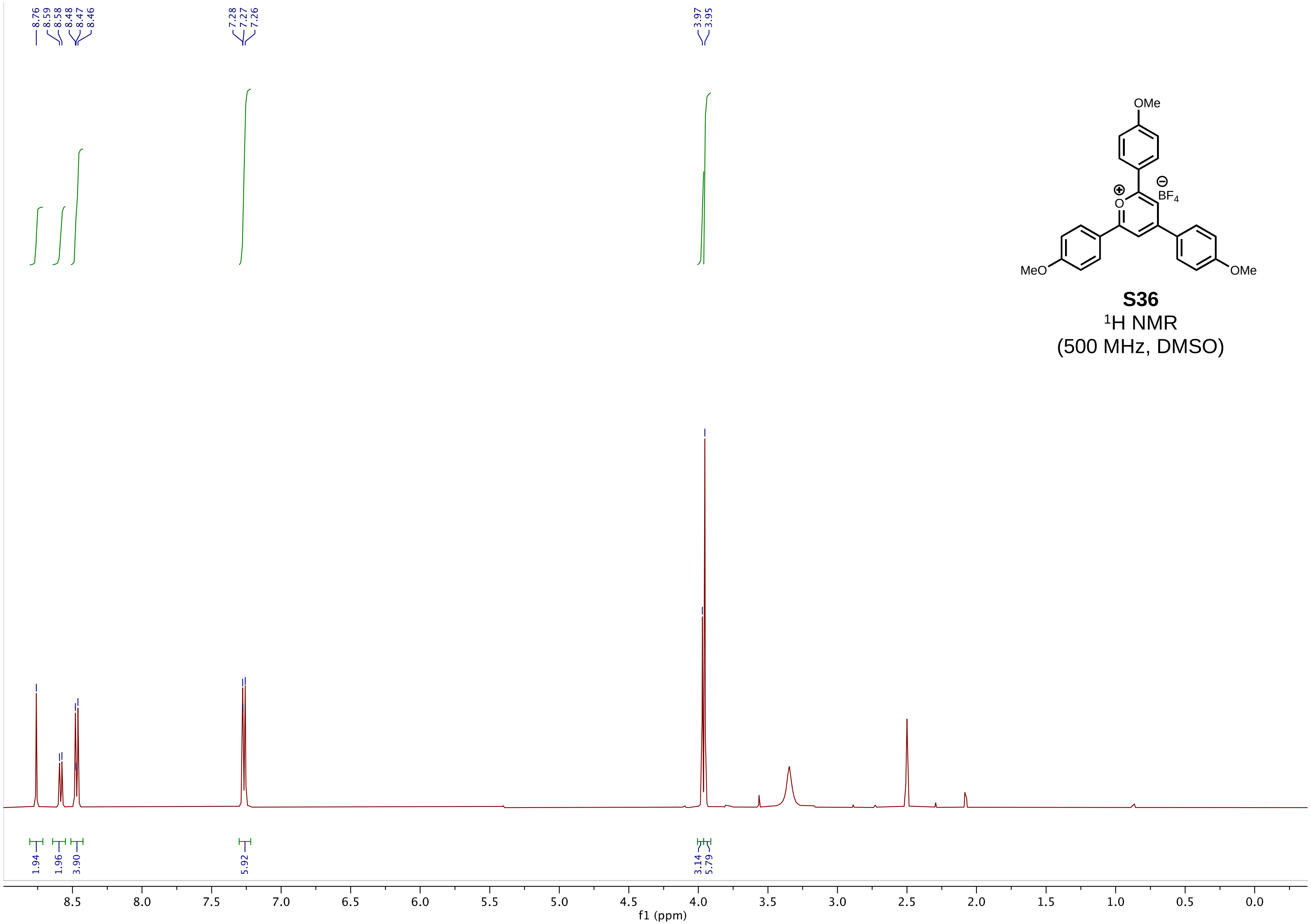
^{13}C NMR

(126 MHz, $CDCl_3$)

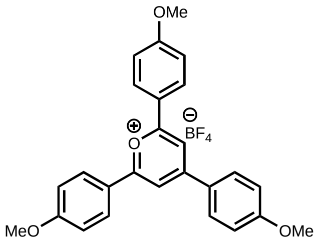



S35
¹H NMR
(499 MHz, DMSO)
f1 (ppm)

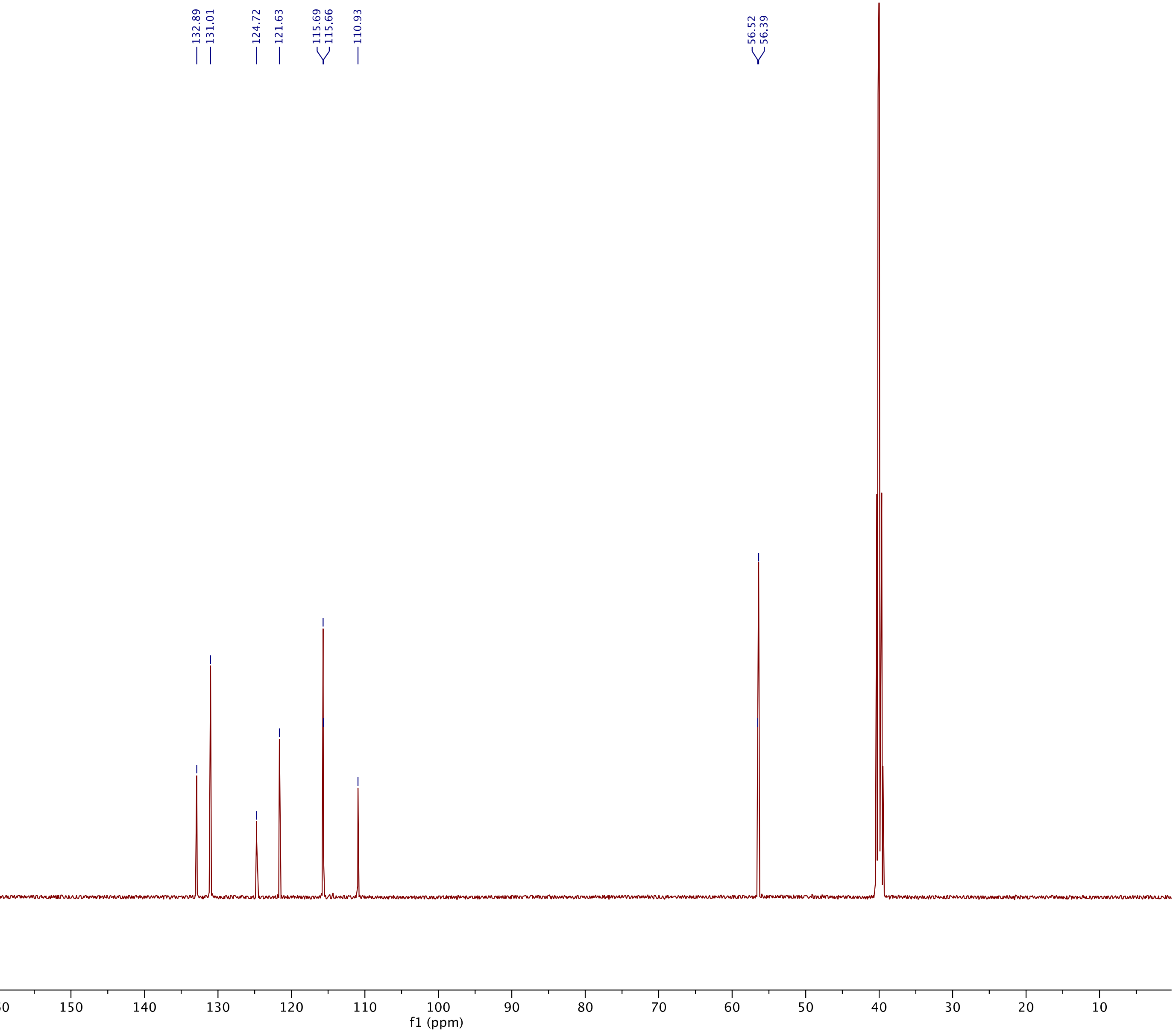

156.19
154.32
133.40
133.18
132.36
131.00
129.60
129.56
129.10
128.74
126.26
58.79
40.02 dmso
39.85 dmso
39.78 dmso
39.69 dmso
39.52 dmso
39.35 dmso
39.19 dmso
39.02 dmso
10.52
4.58
BF4
Ph
N
Ph
Ph
S35
13C NMR
(126 MHz, DMSO)
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

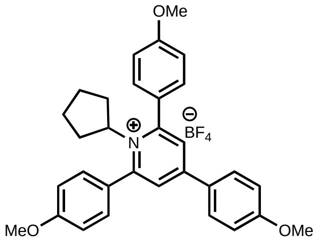


S36
^{1}H NMR
(500 MHz, DMSO)

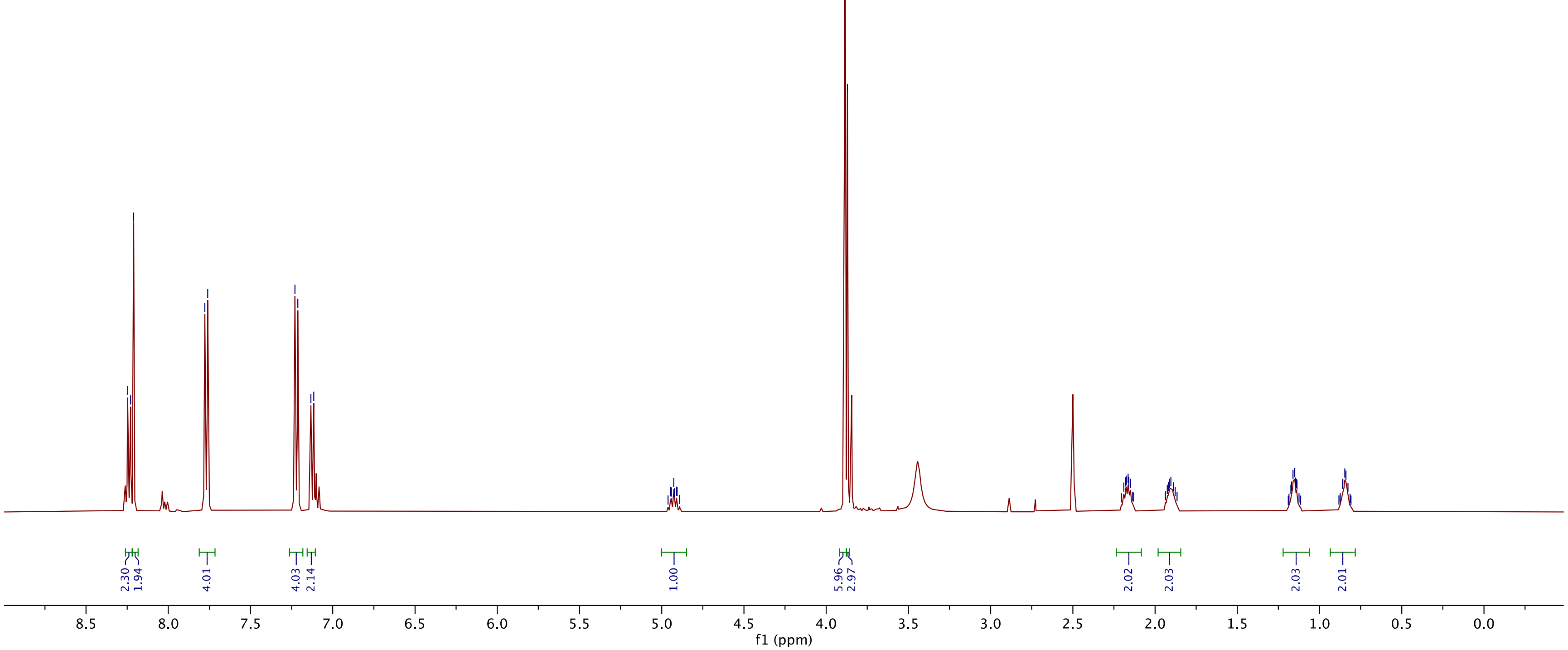


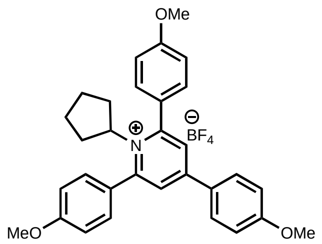
S36
^{13}C NMR
(126 MHz, DMSO)



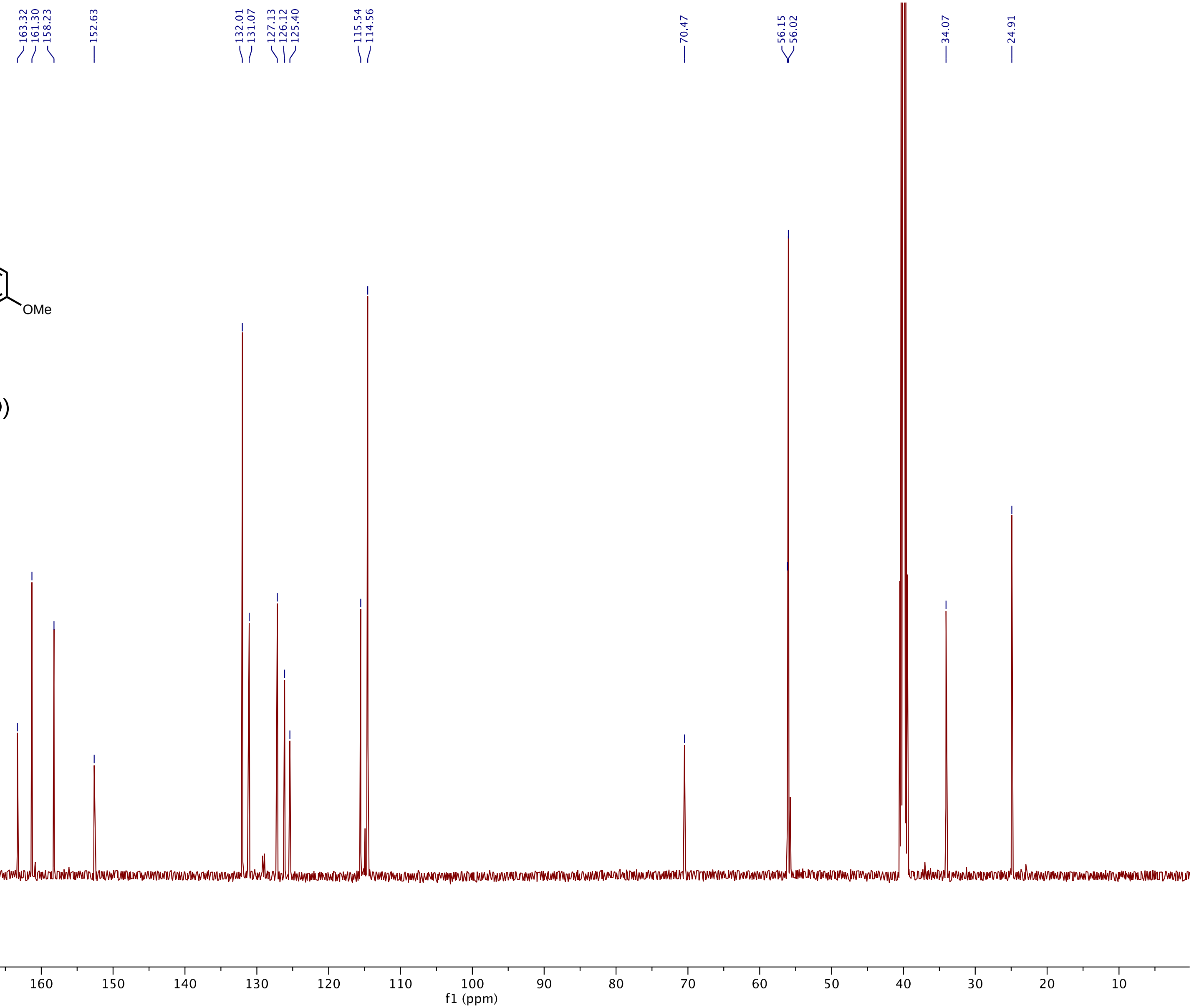


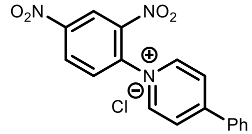
S37
^{1}H NMR
(500 MHz, DMSO)



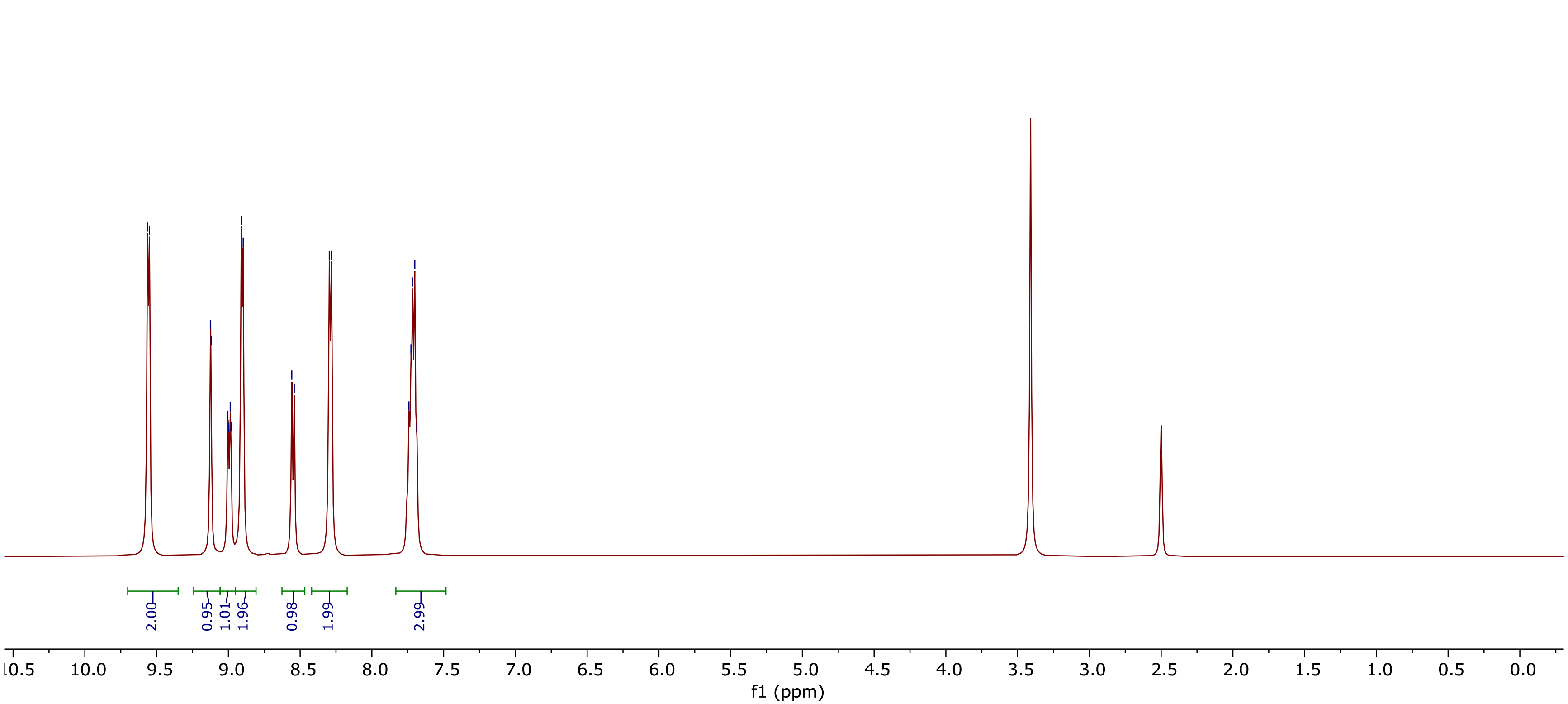


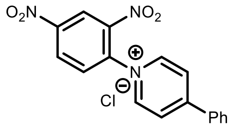
S37
^{13}C NMR
(126 MHz, DMSO)





S38
^1H NMR
(500 MHz, DMSO-d_6)

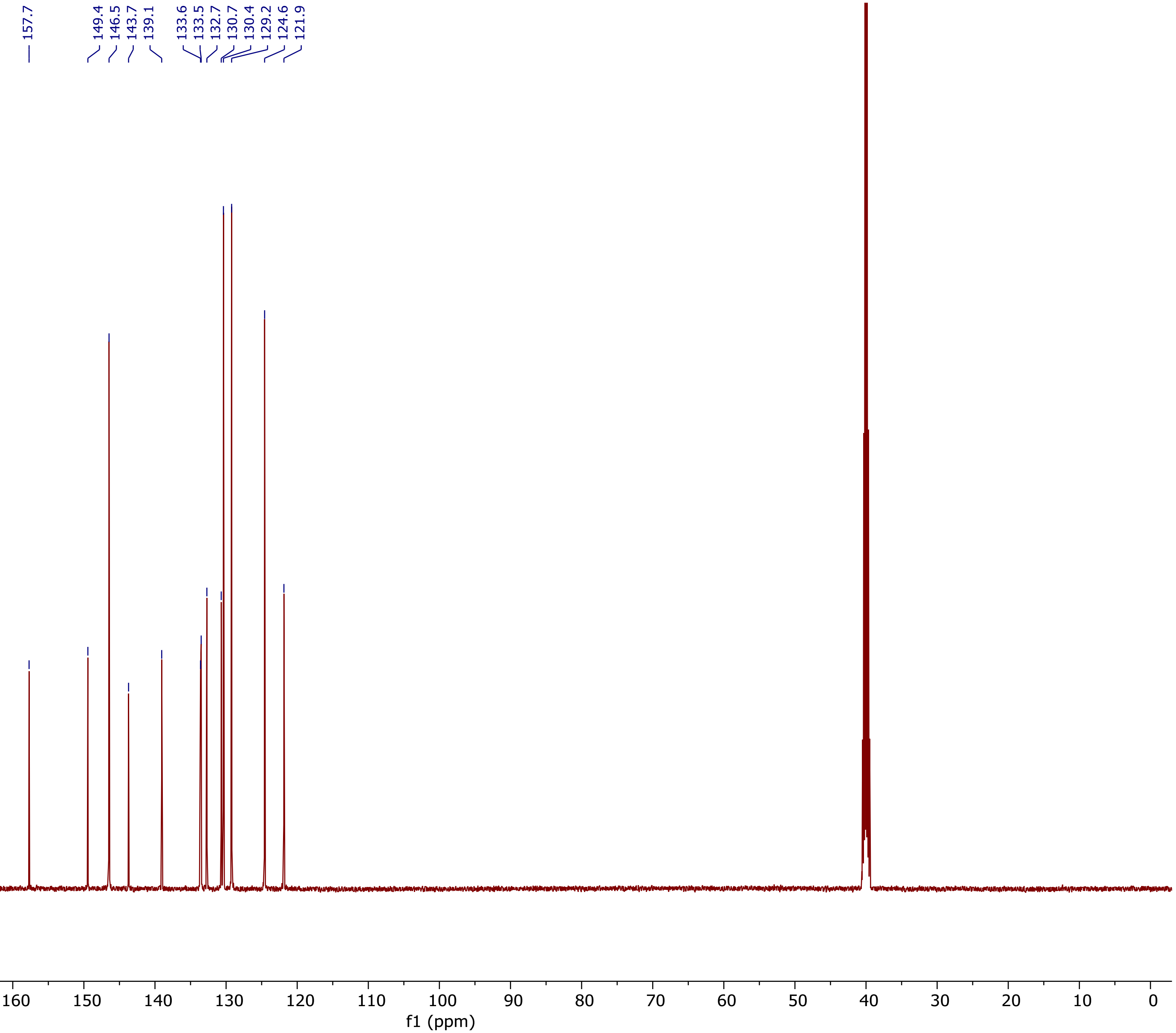


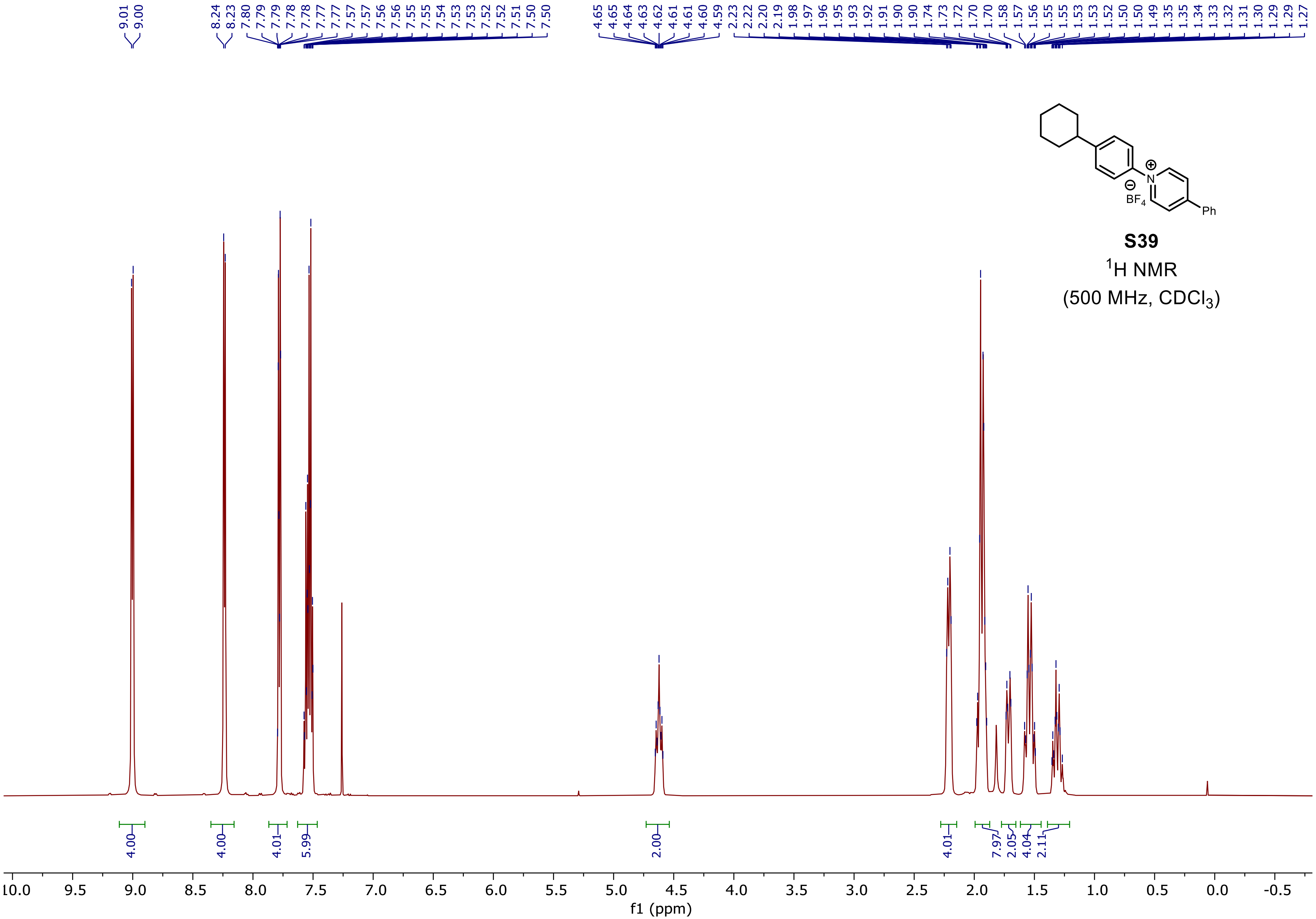


S38

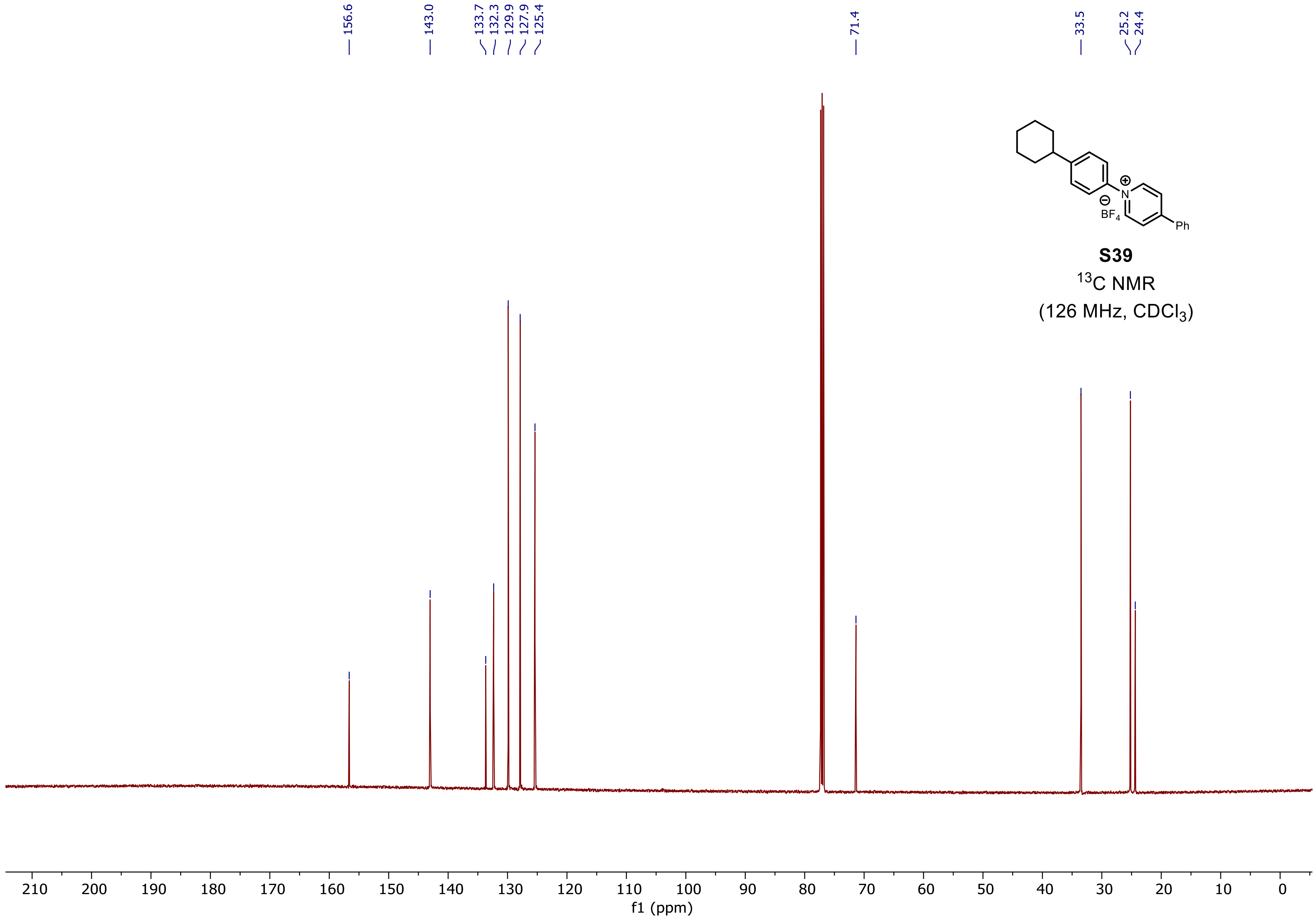
^{13}C NMR

(126 MHz, DMSO-d_6)



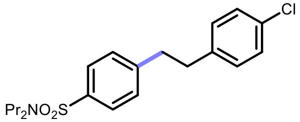


9.01
9.00
8.24
8.23
7.80 7.79 7.79 7.78 7.78 7.77 7.77 7.57 7.57 7.56 7.55 7.55 7.54 7.53 7.53 7.52 7.52 7.51 7.50 7.50
4.65 4.65 4.64 4.63 4.62 4.61 4.61 4.60 4.59
2.23 2.22 2.20 2.19 1.98 1.97 1.96 1.95 1.93 1.92 1.91 1.90 1.90 1.74 1.73 1.72 1.70 1.70 1.58 1.57 1.56 1.55 1.55 1.53 1.53 1.52 1.50 1.50 1.49 1.35 1.35 1.34 1.33 1.32 1.31 1.30 1.29 1.29 1.27
N
BF4
Ph
S39
1H NMR
(500 MHz, CDCl3)
4.00
4.00
4.01
5.99
2.00
4.01
7.97
2.05
4.04
2.11
f1 (ppm)



156.6
143.0
133.7
132.3
129.9
127.9
125.4
71.4
33.5
25.2
24.4
BF4
Ph
S39
13C NMR
(126 MHz, CDCl3)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

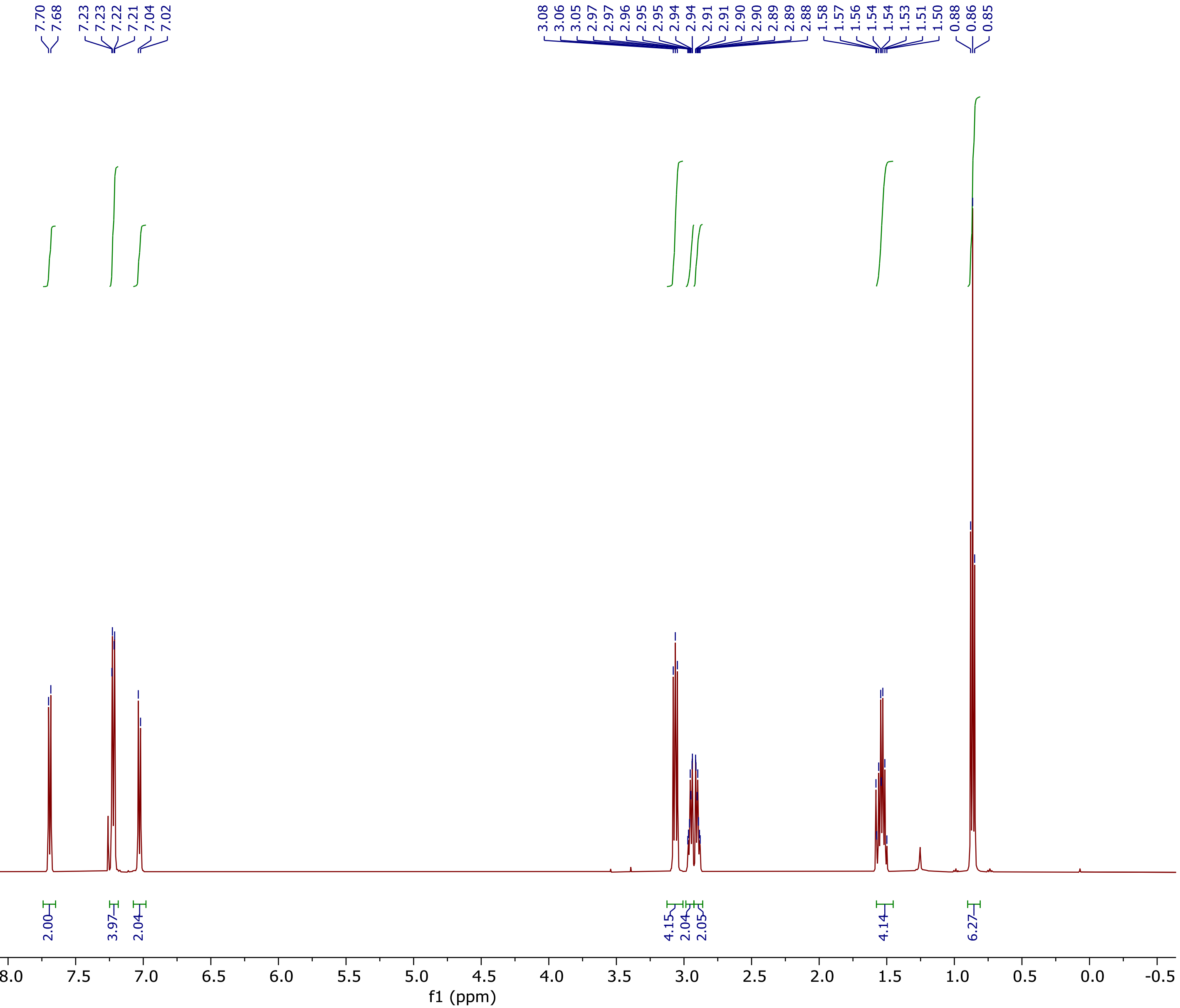
Products

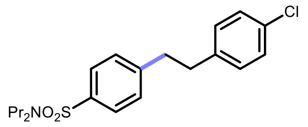


3

^{1}H NMR

(500 MHz, $CDCl_3$)

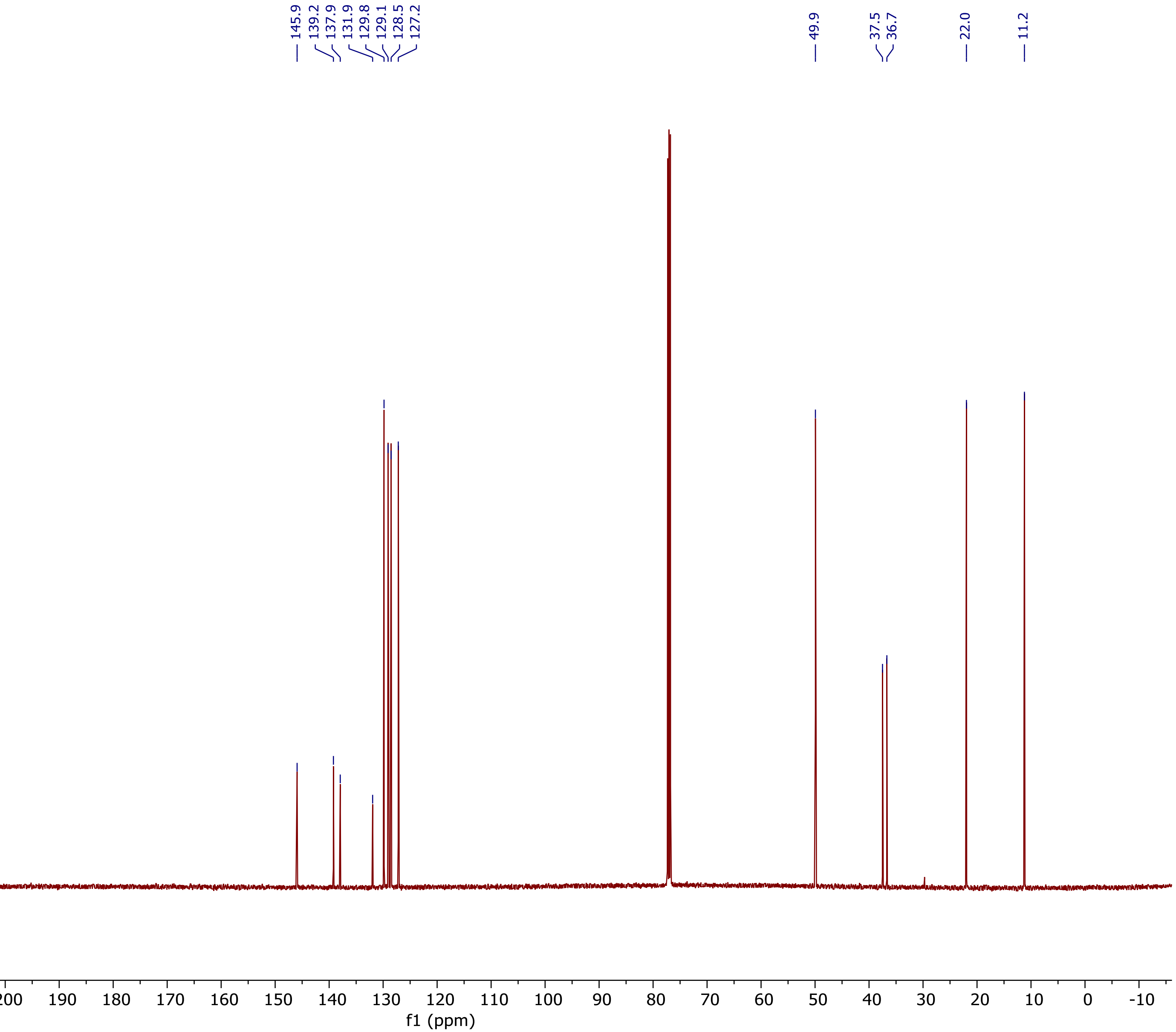


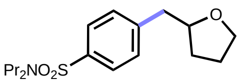


3

^{13}C NMR

(126 MHz, $CDCl_3$)

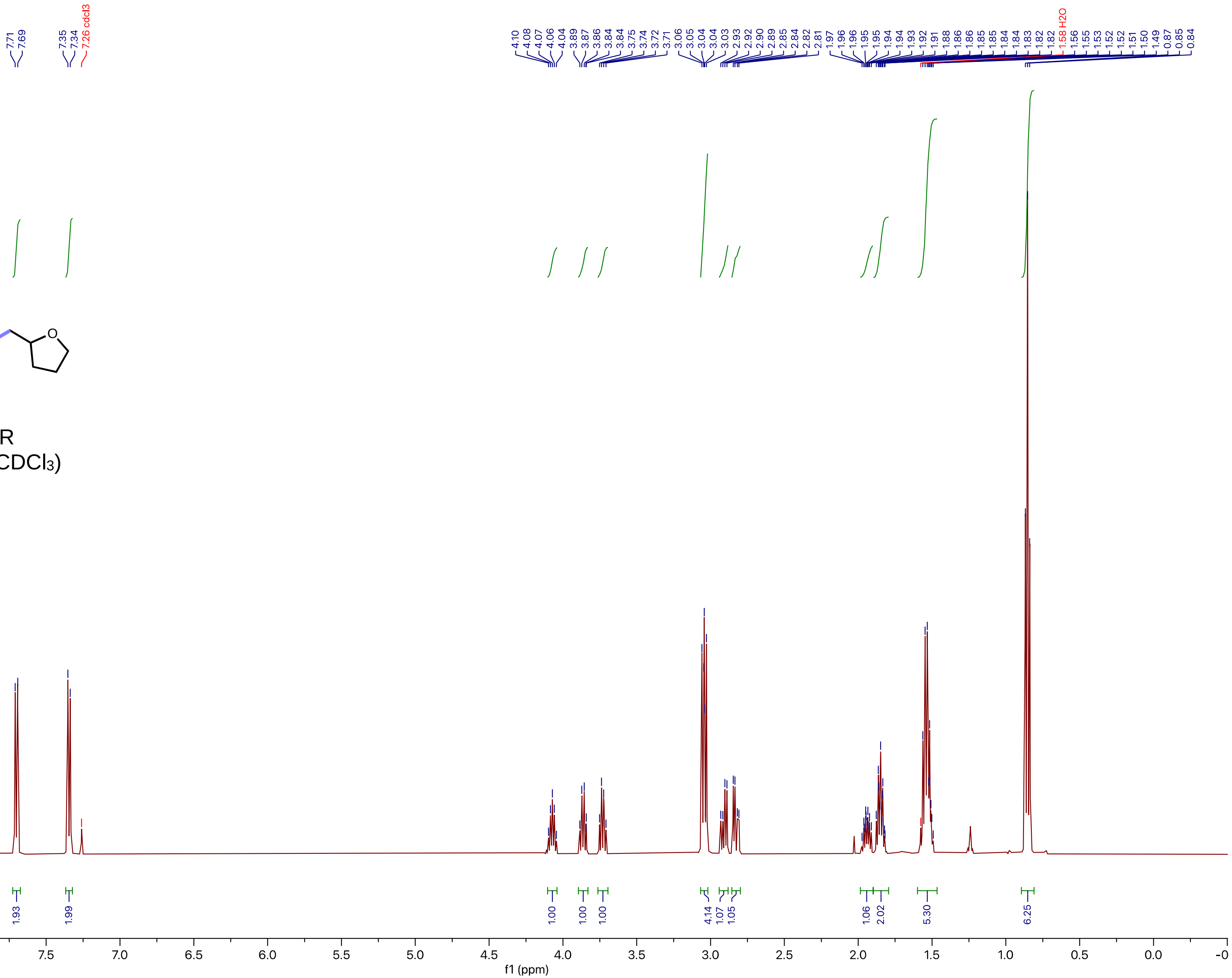


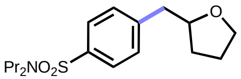


5

^{1}H NMR

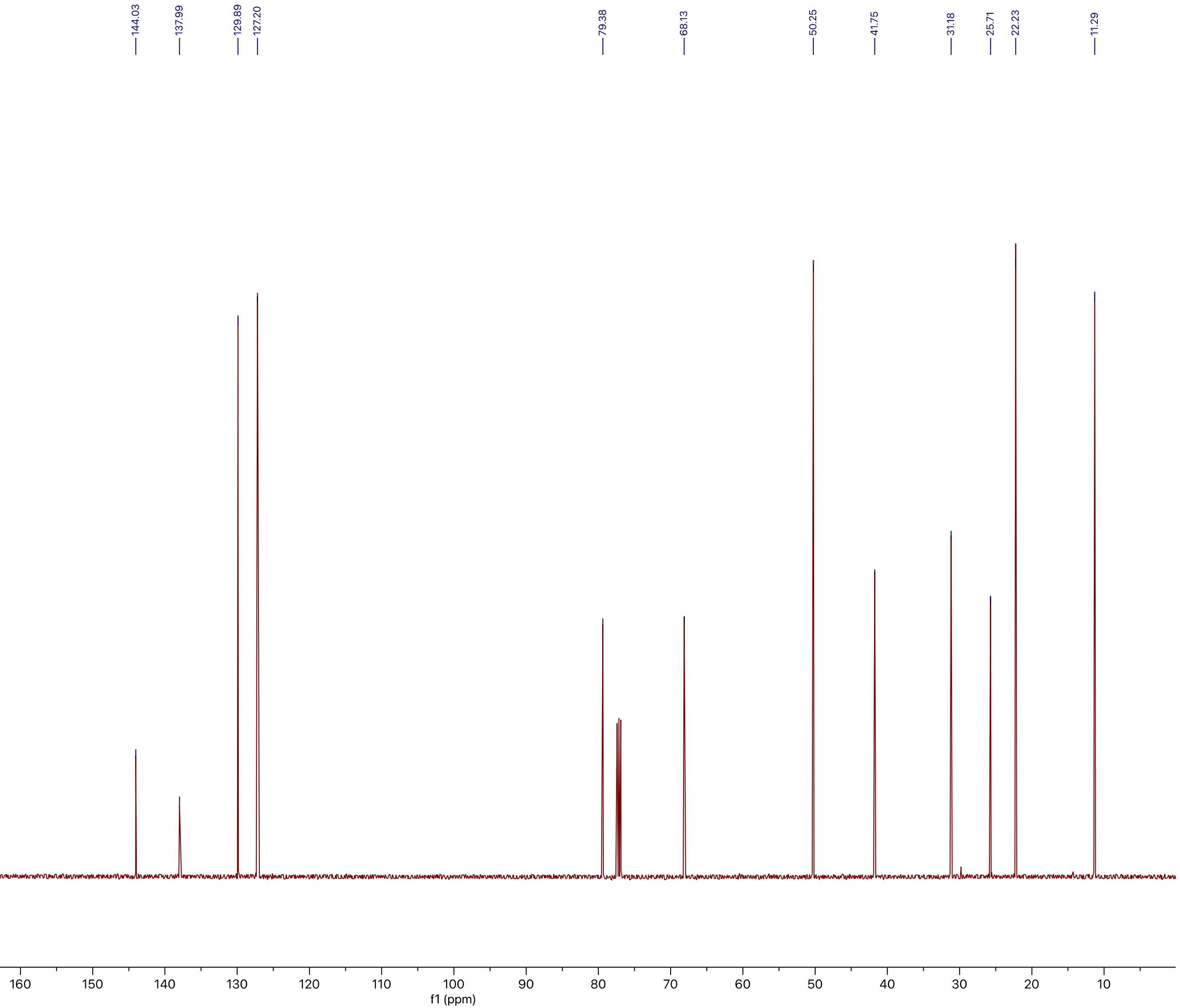
(499 MHz, $CDCl_3$)

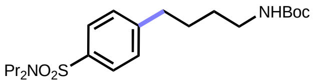




5

^{13}C NMR
(126 MHz, $CDCl_3$)

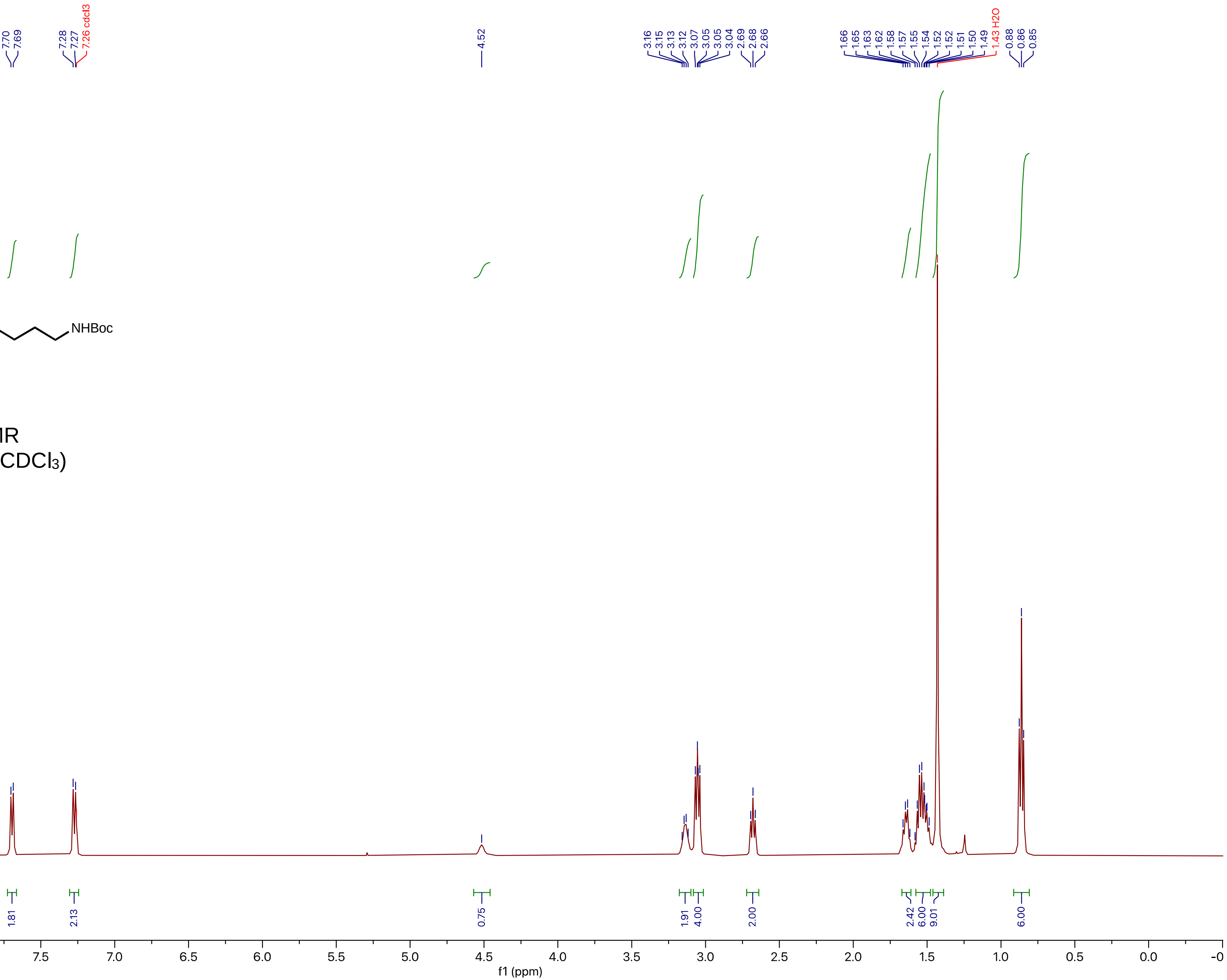


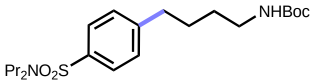


6

^{1}H NMR

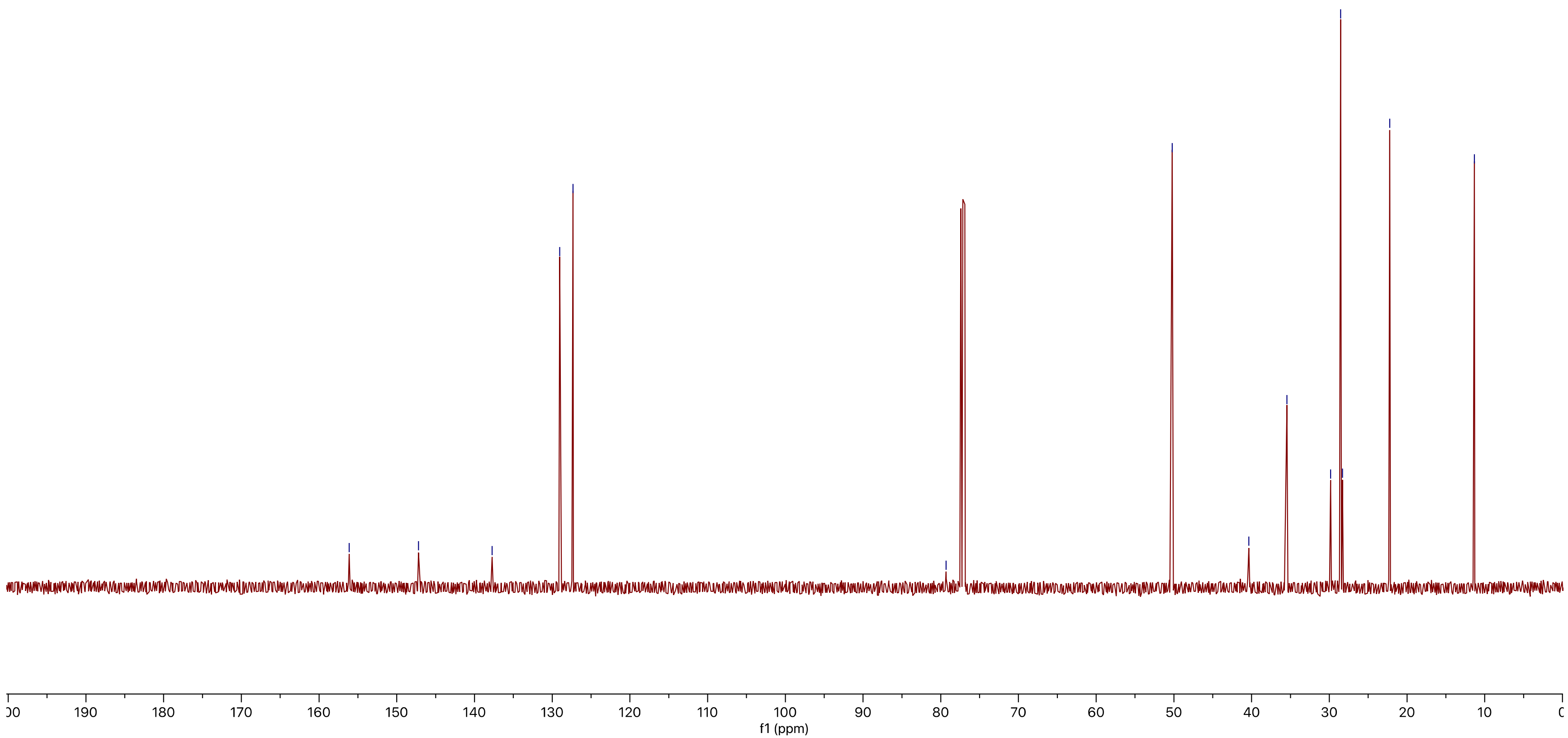
(499 MHz, $CDCl_3$)

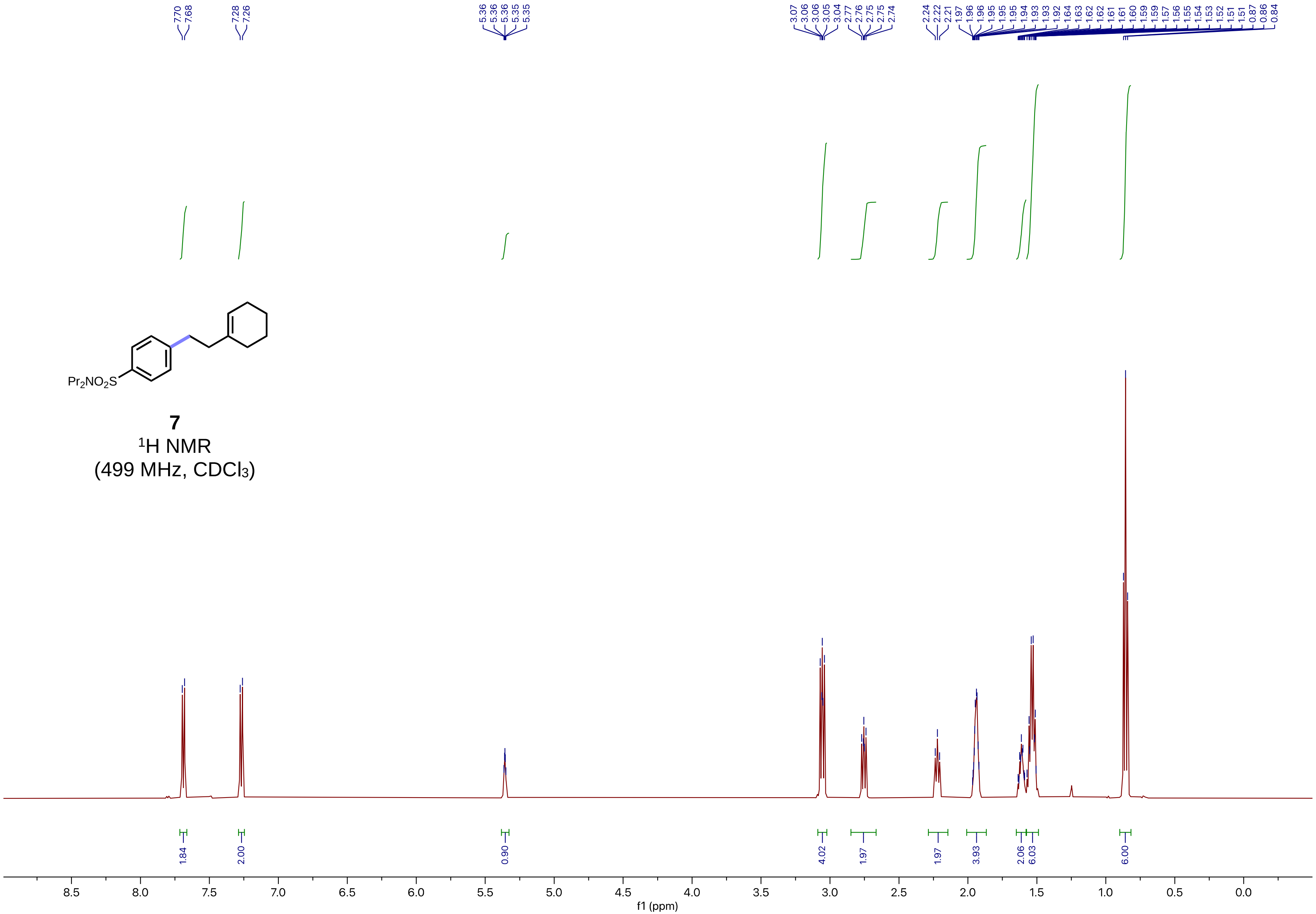




6

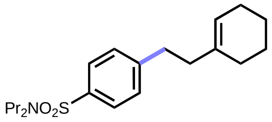
^{13}C NMR
(126 MHz, $CDCl_3$)





7

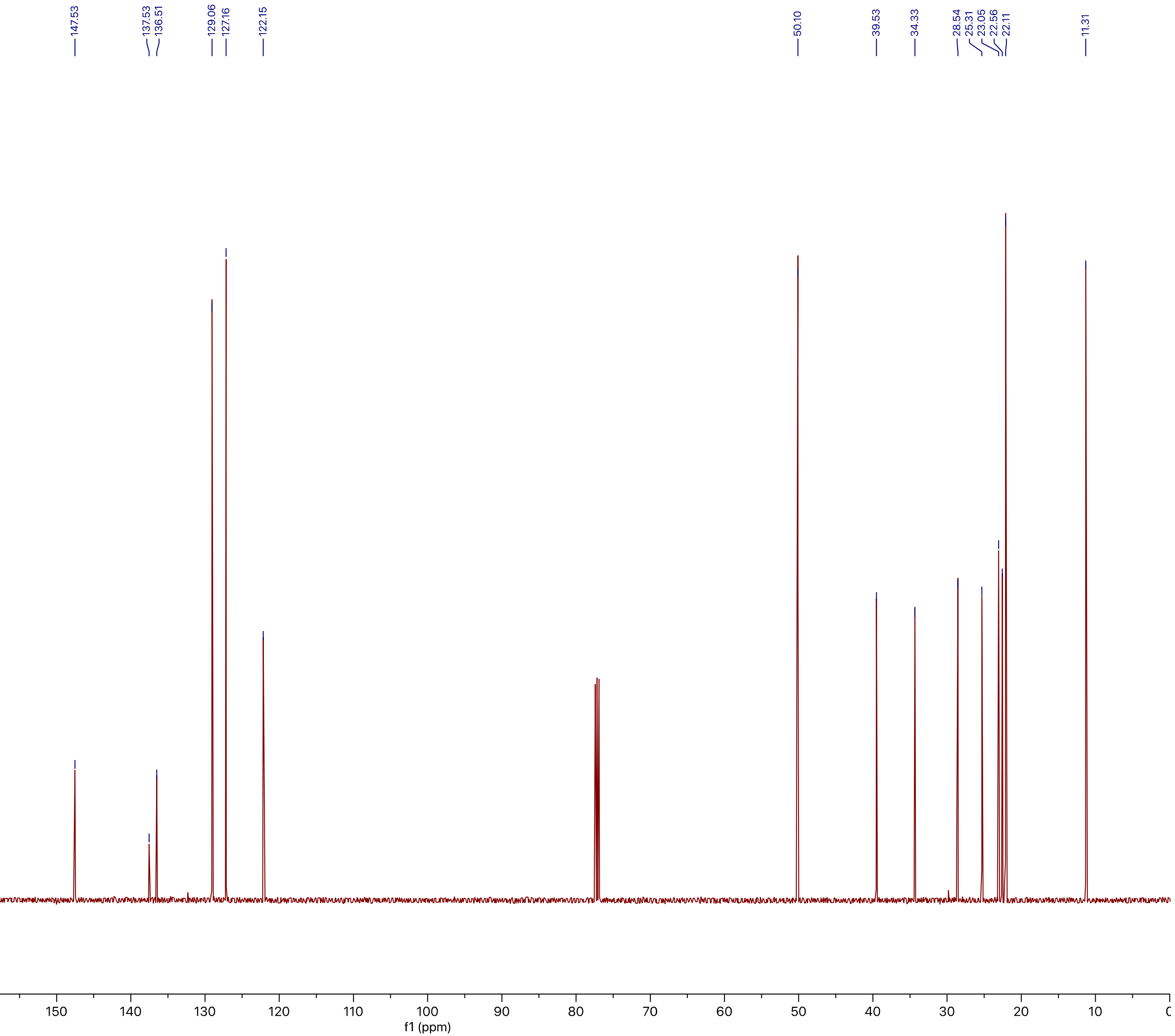
^{1}H NMR
(499 MHz, $CDCl_3$)

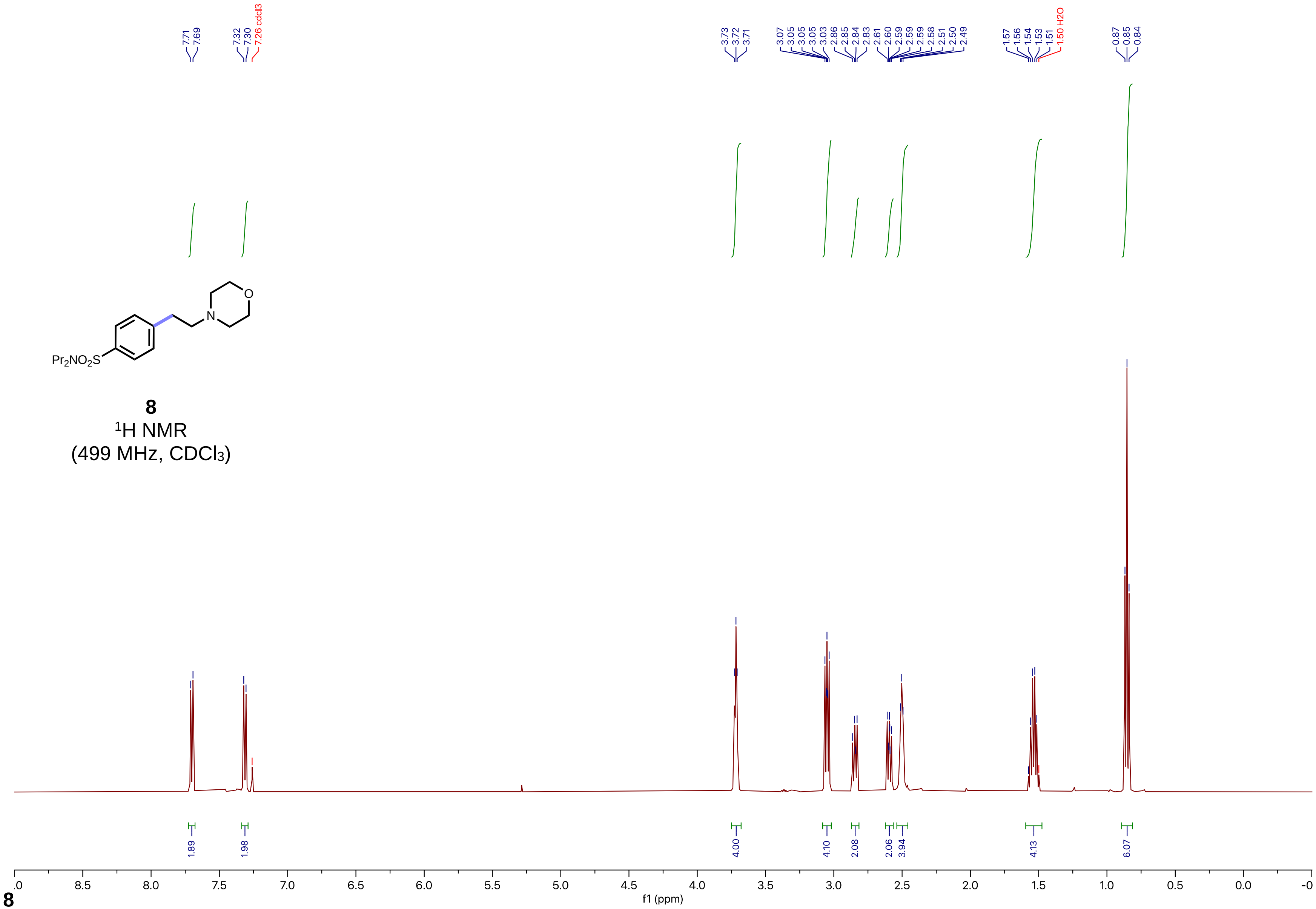


7

^{13}C NMR

(126 MHz, $CDCl_3$)



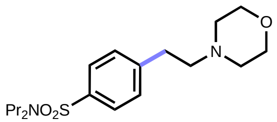


8

^{1}H NMR

(499 MHz, $CDCl_3$)

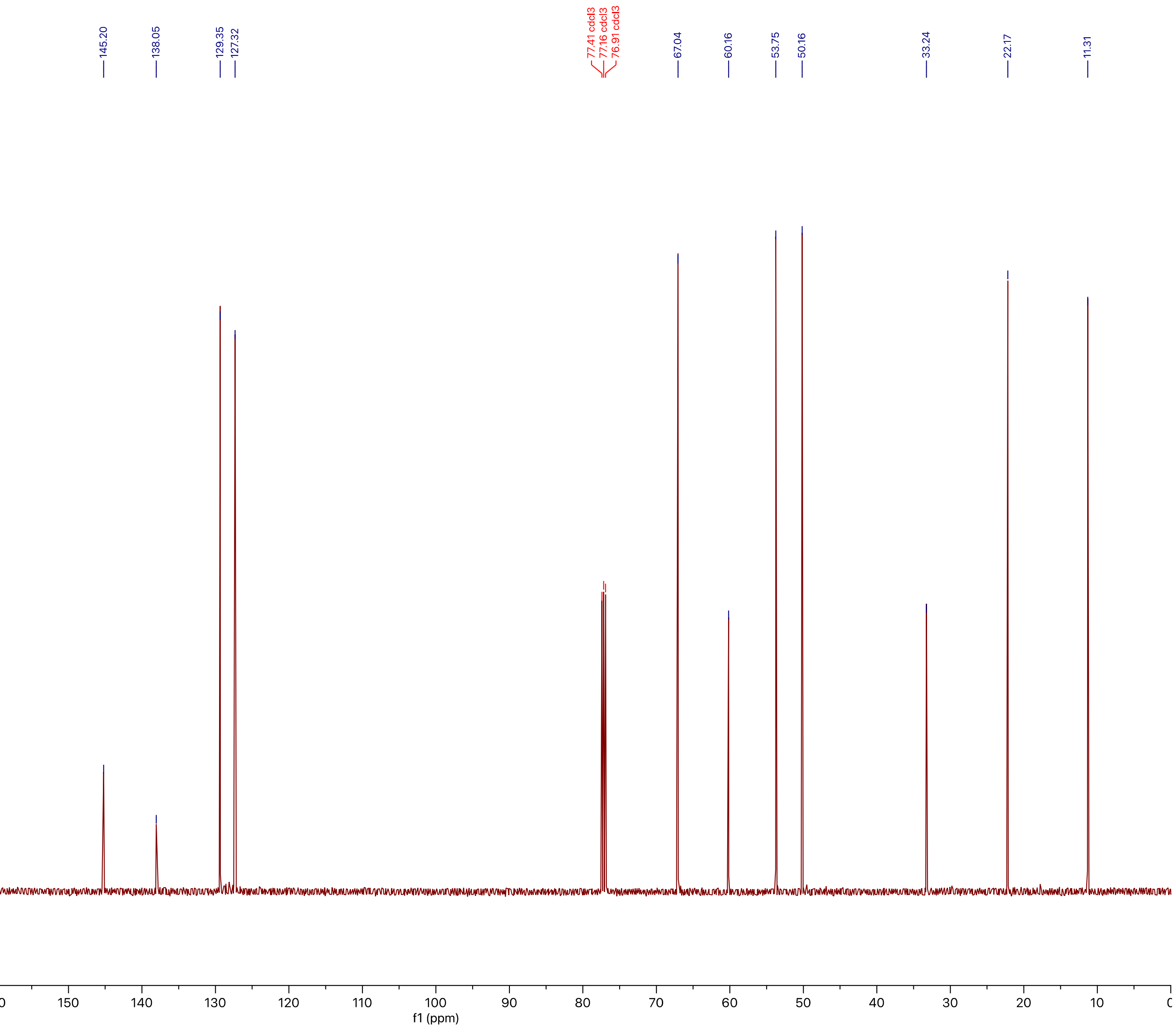
8

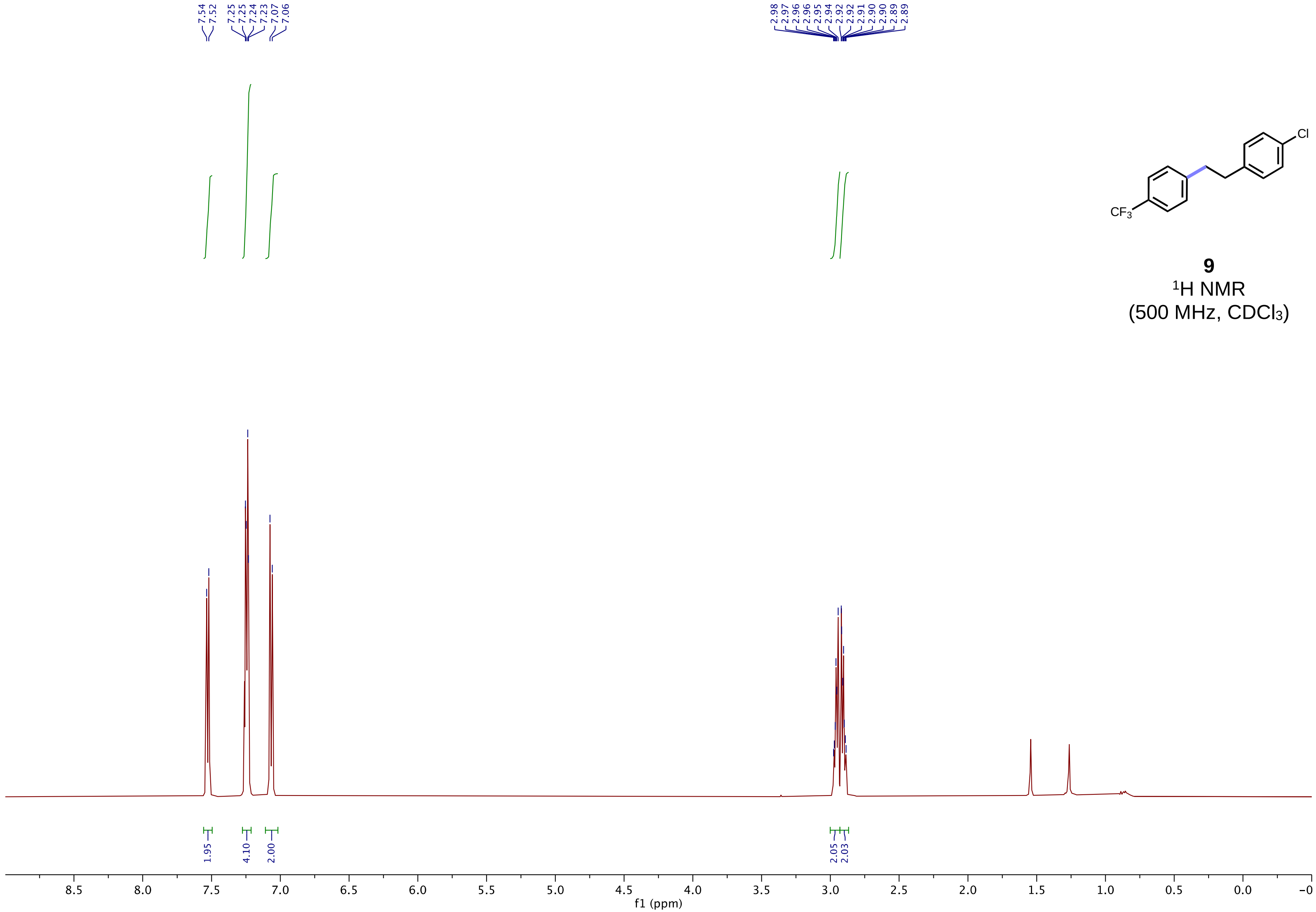


8

^{13}C NMR

(126 MHz, $CDCl_3$)

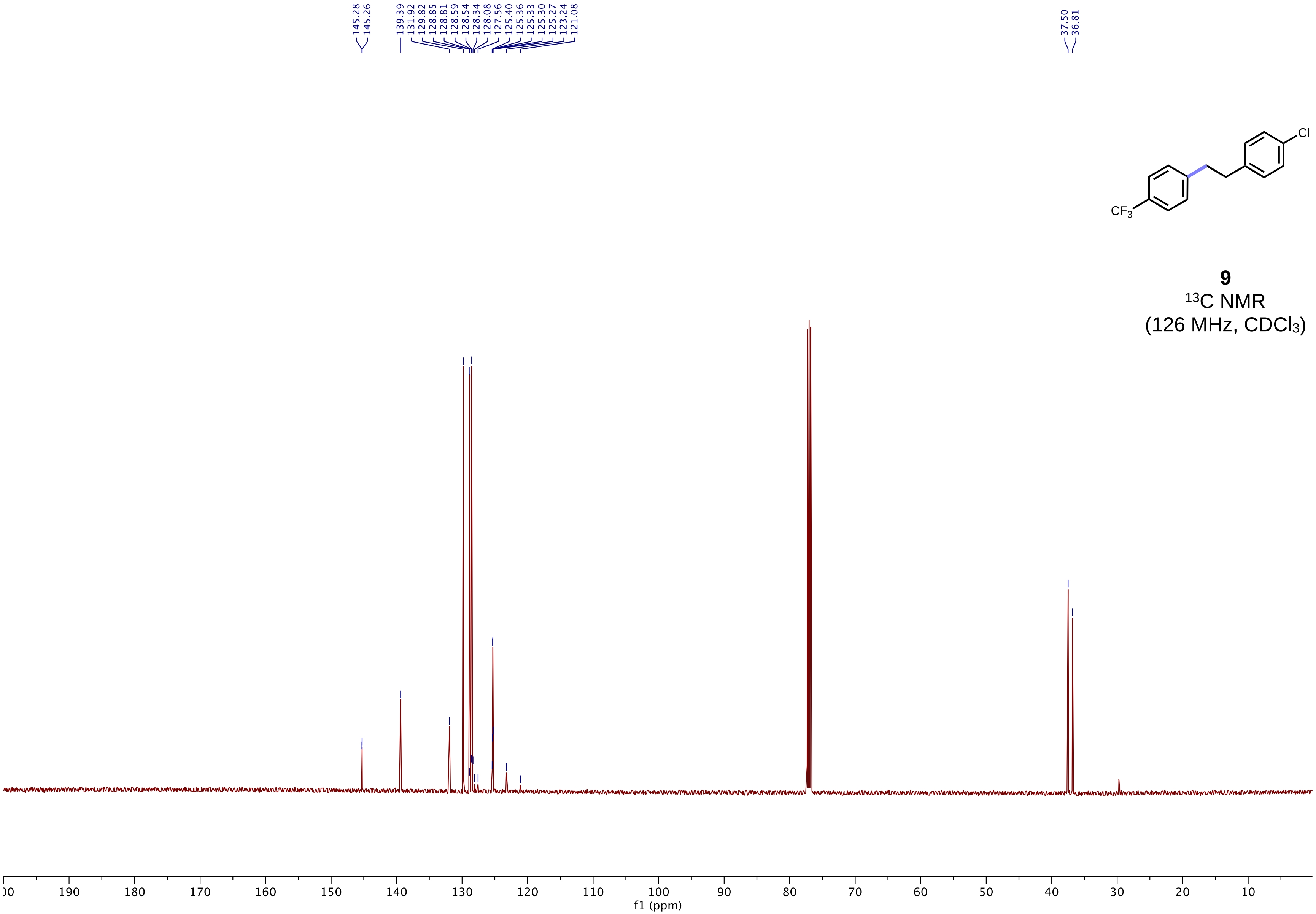




9

^{1}H NMR

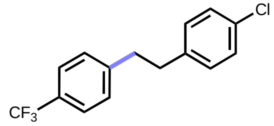
(500 MHz, $CDCl_3$)



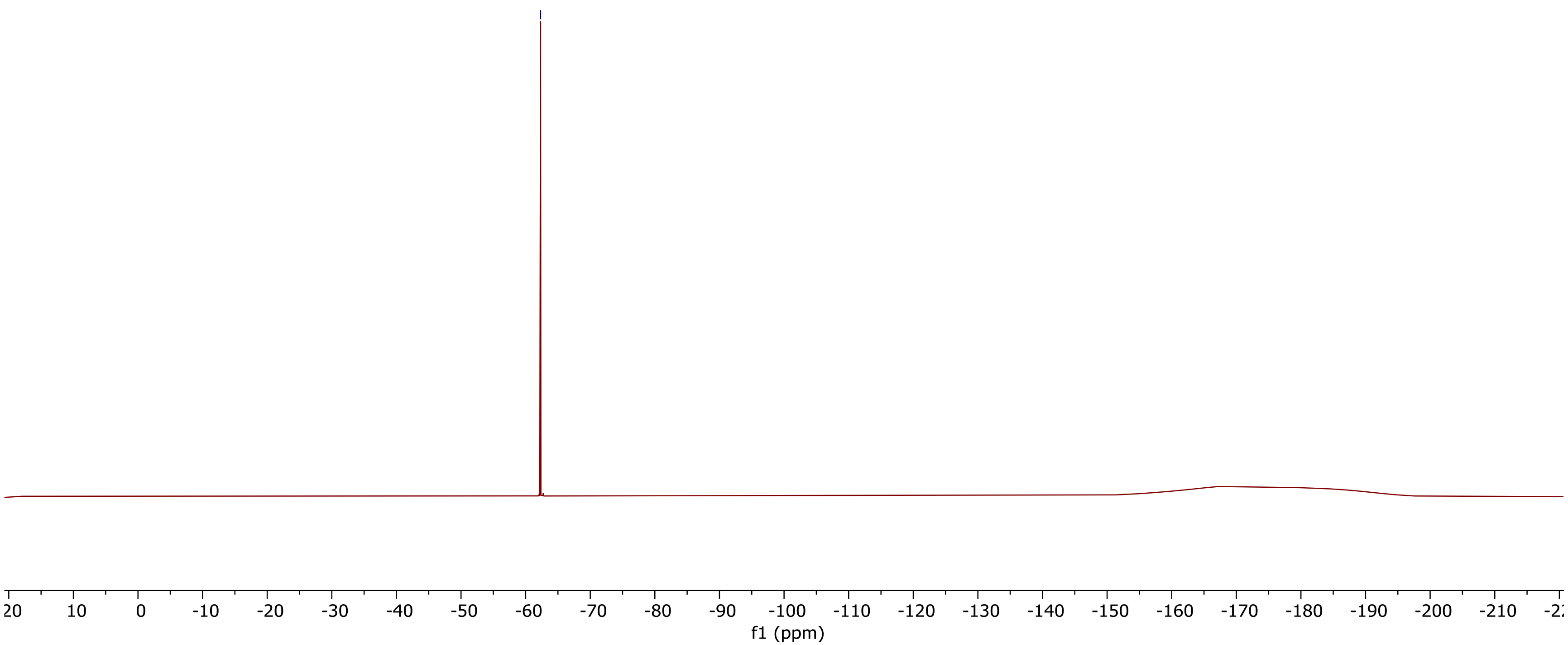
9

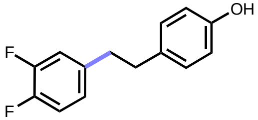
^{13}C NMR

(126 MHz, $CDCl_3$)

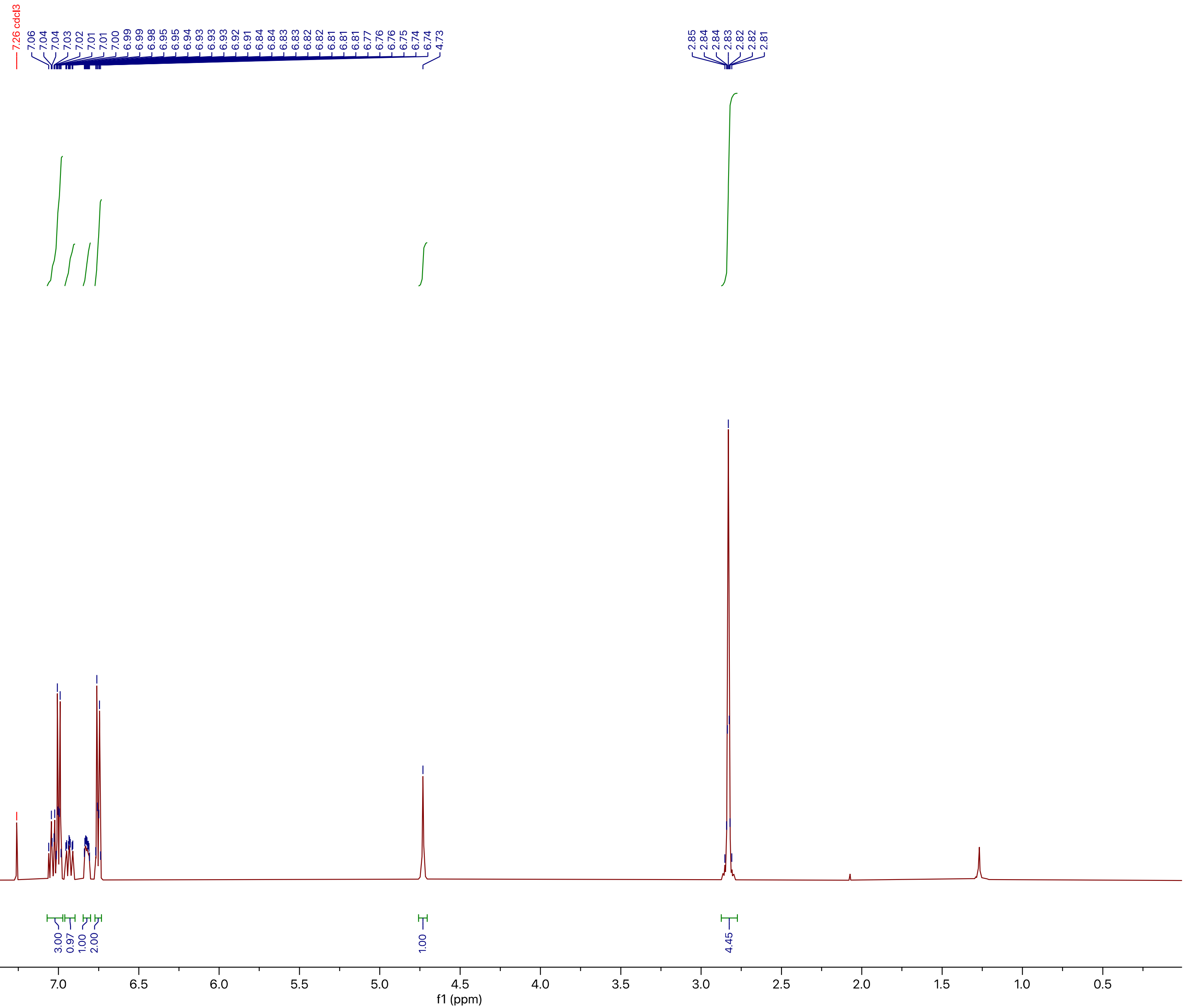


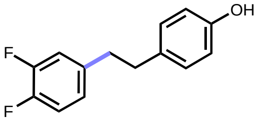
9
^{19}F NMR
(471 MHz, $CDCl_3$)



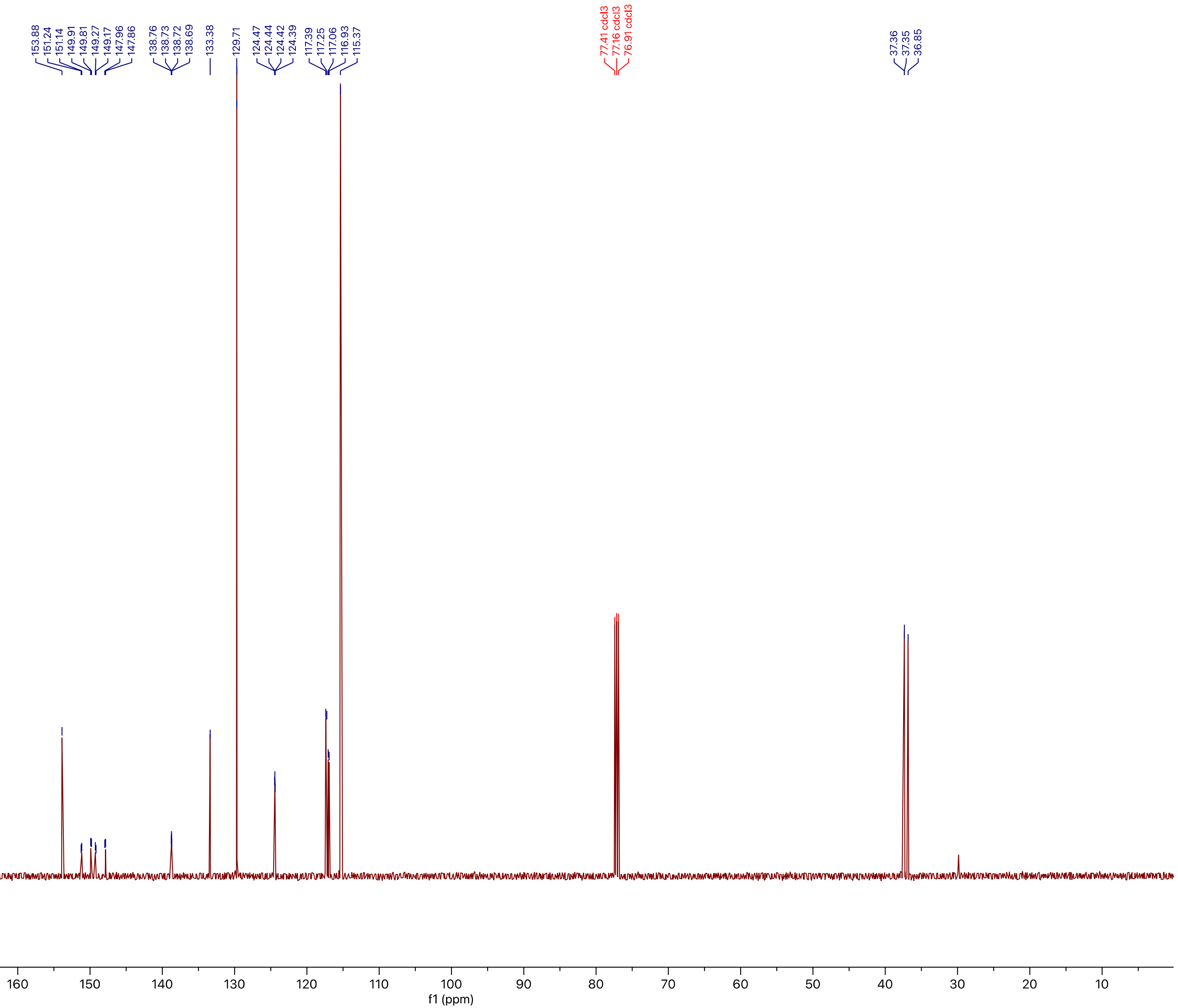


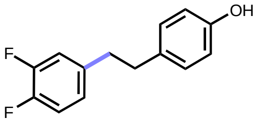
10
^{1}H NMR
(499 MHz, $CDCl_3$)



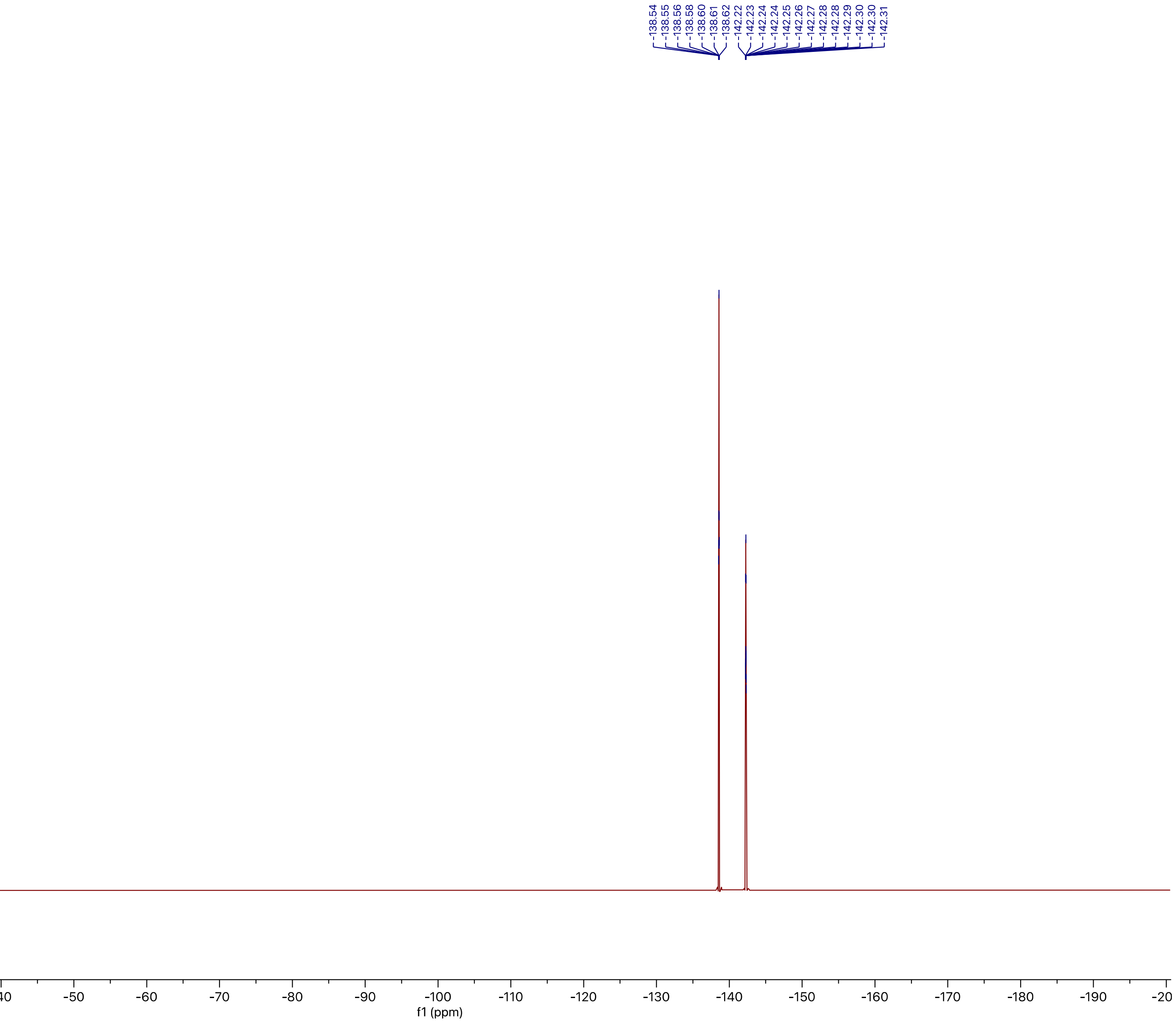


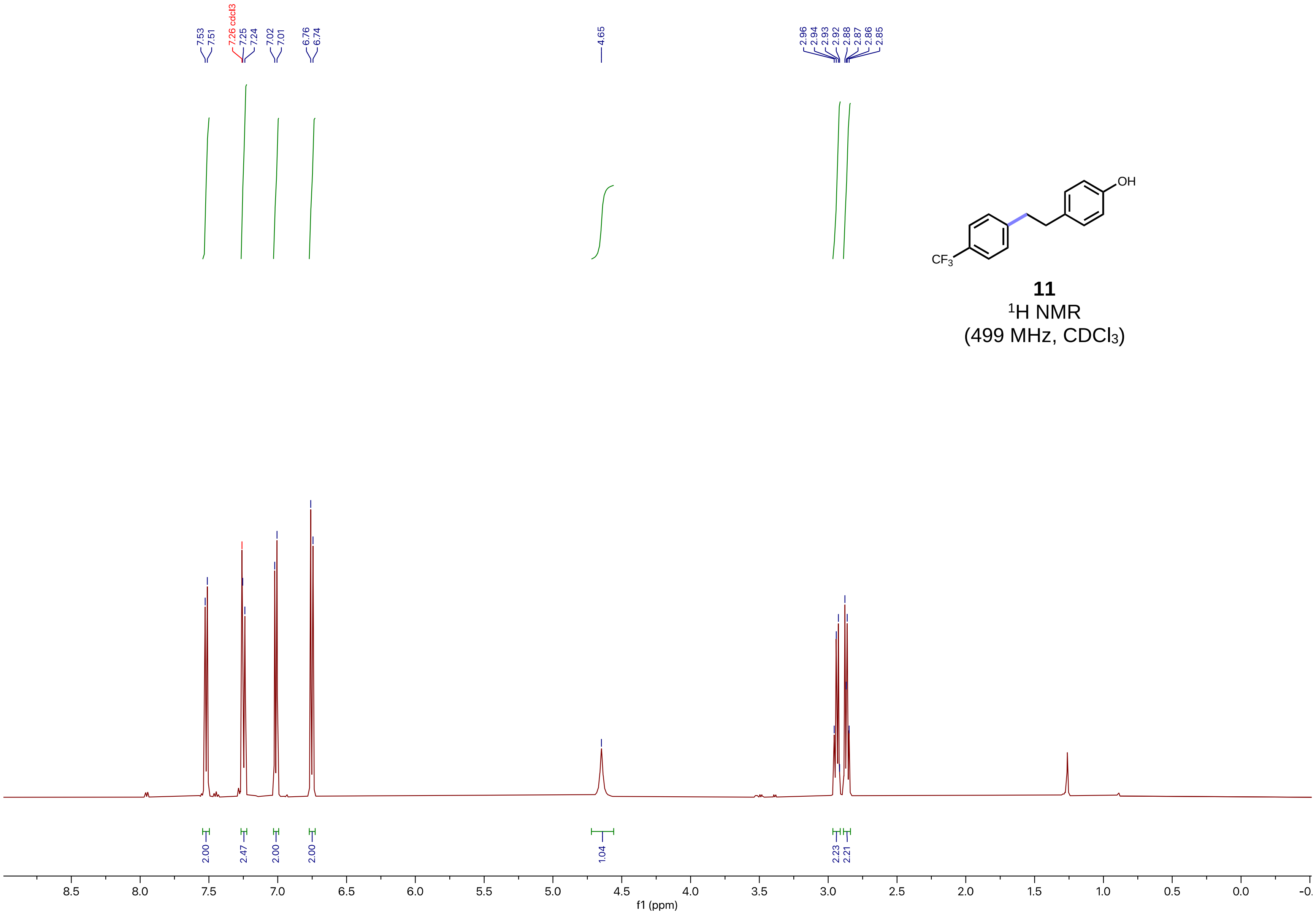
10
^{13}C NMR
(126 MHz, $CDCl_3$)





10
^{19}F NMR
(470 MHz, $CDCl_3$)



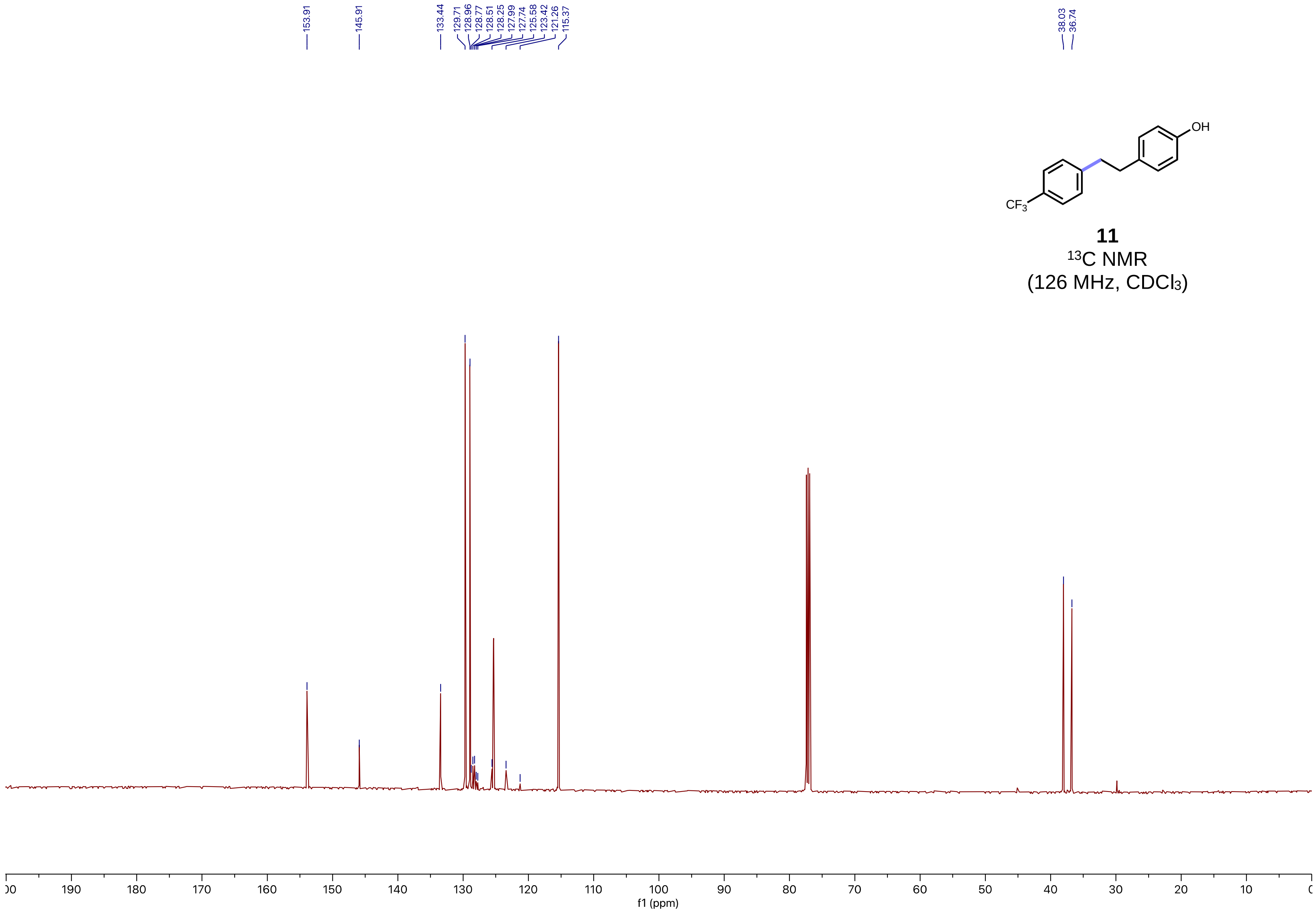


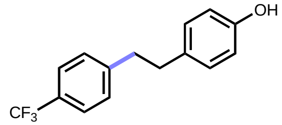
11

^{1}H NMR

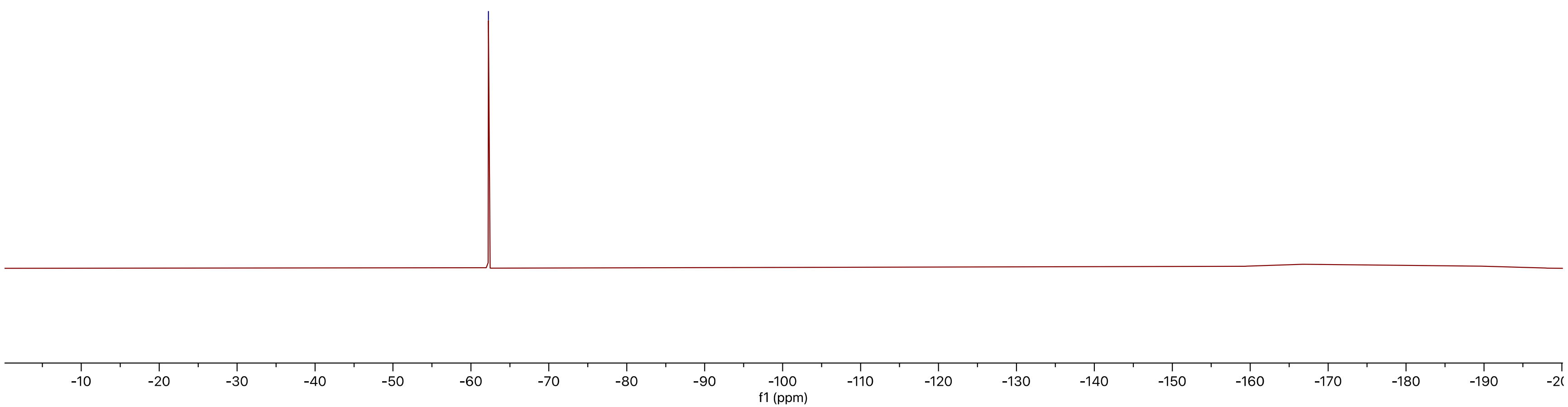
(499 MHz, $CDCl_3$)

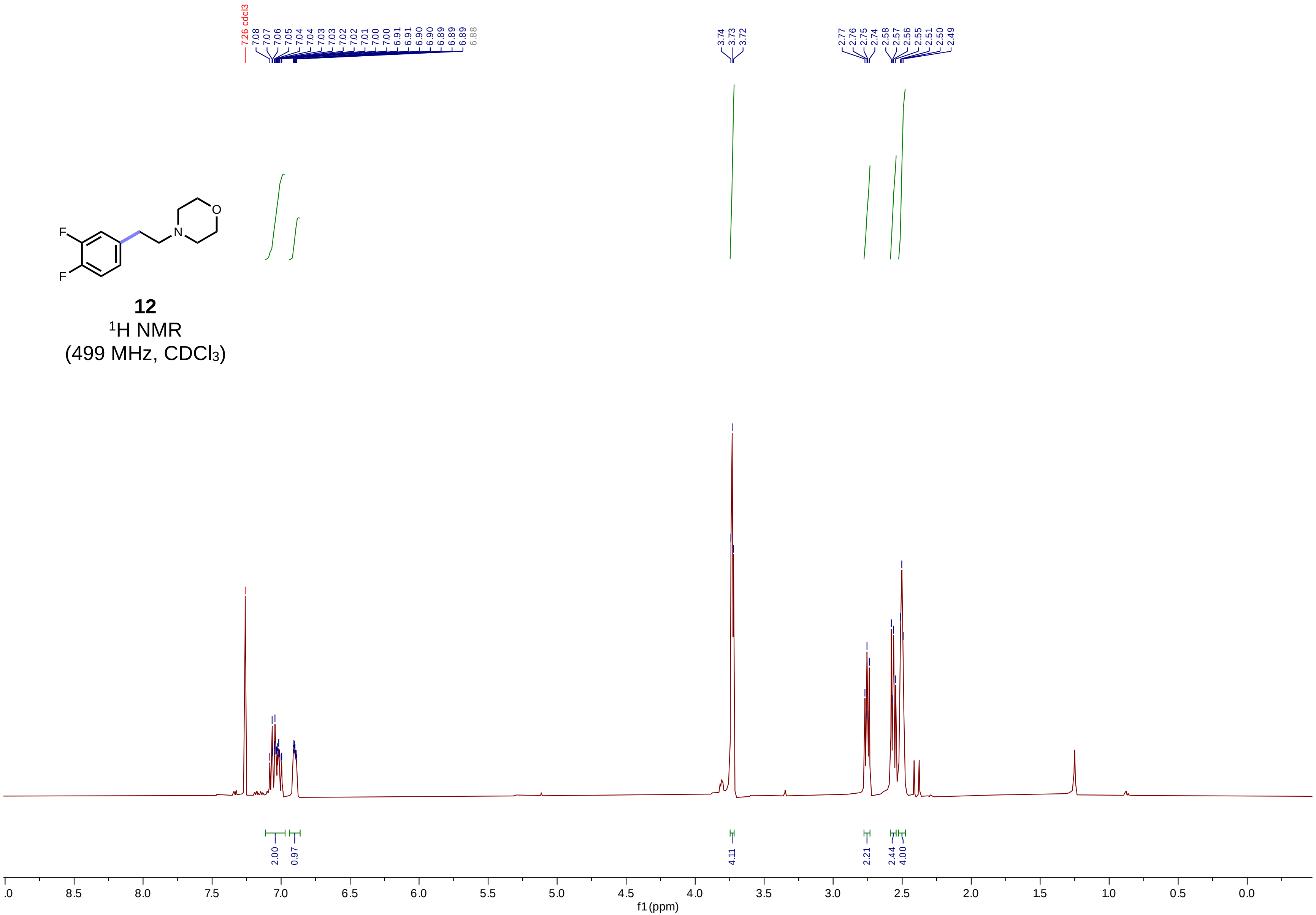
11
^{13}C NMR
(126 MHz, $CDCl_3$)





11
^{19}F NMR
(471 MHz, $CDCl_3$)

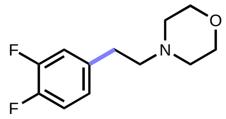




12

^{1}H NMR

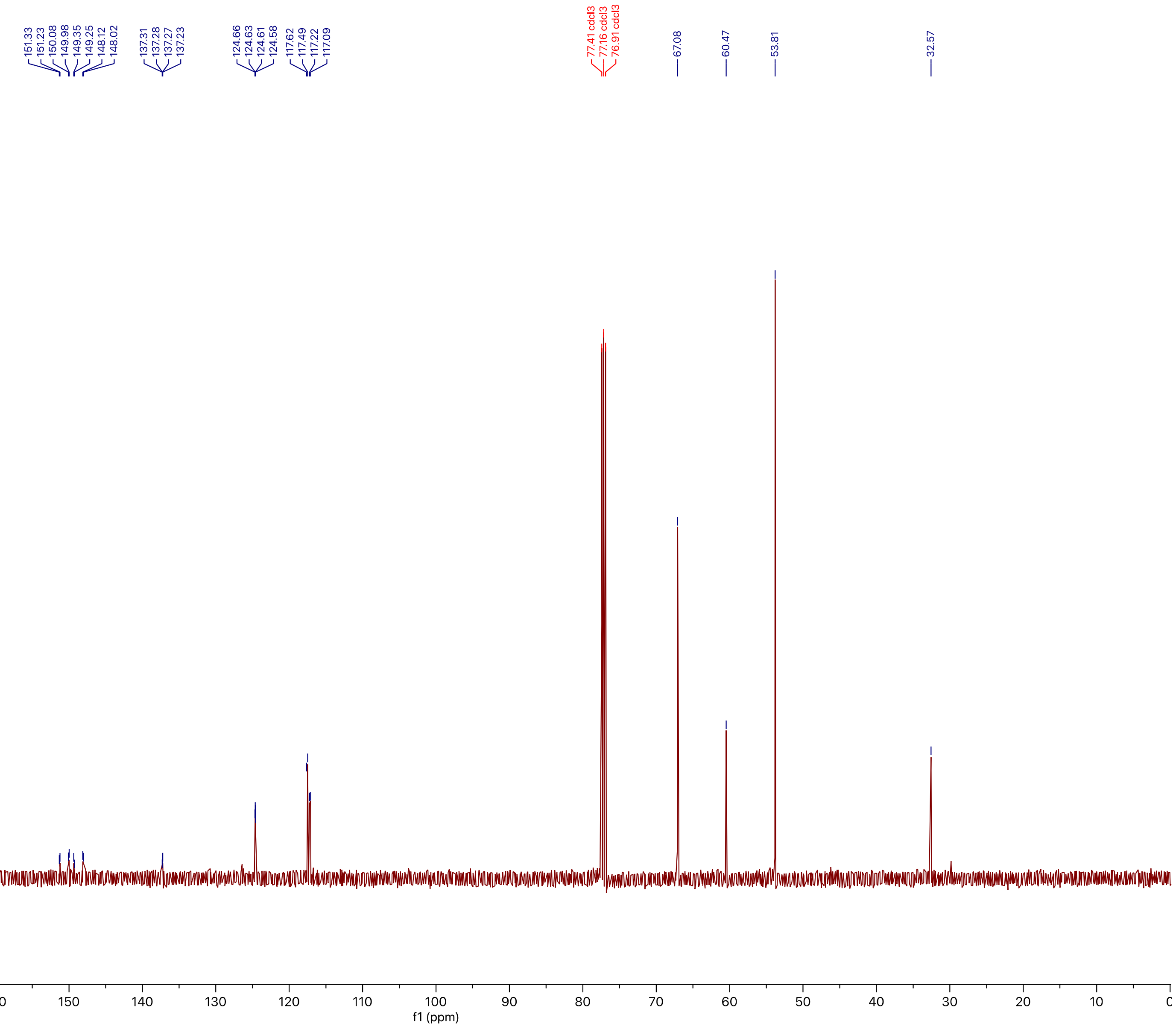
(499 MHz, $CDCl_3$)

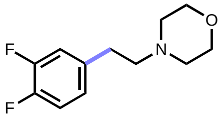


12

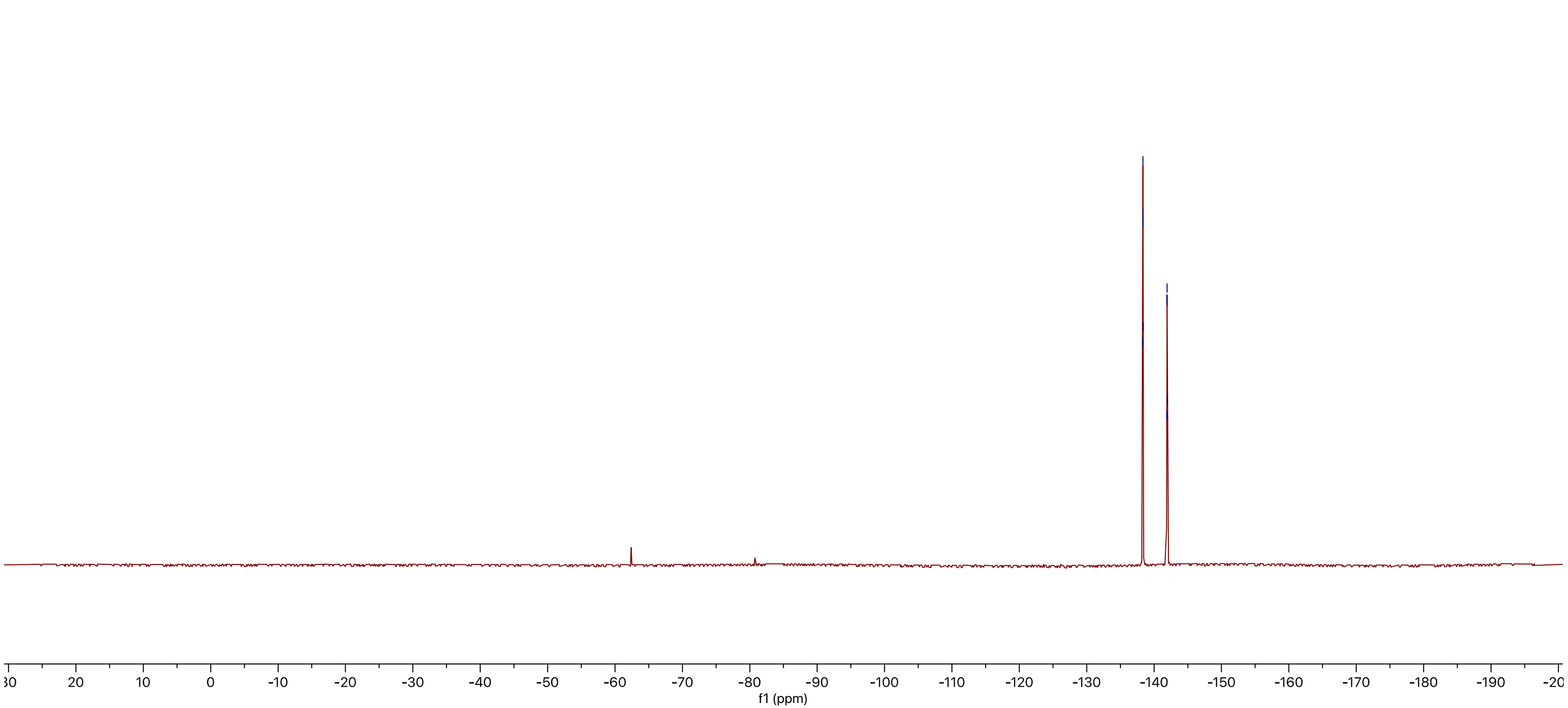
^{13}C NMR

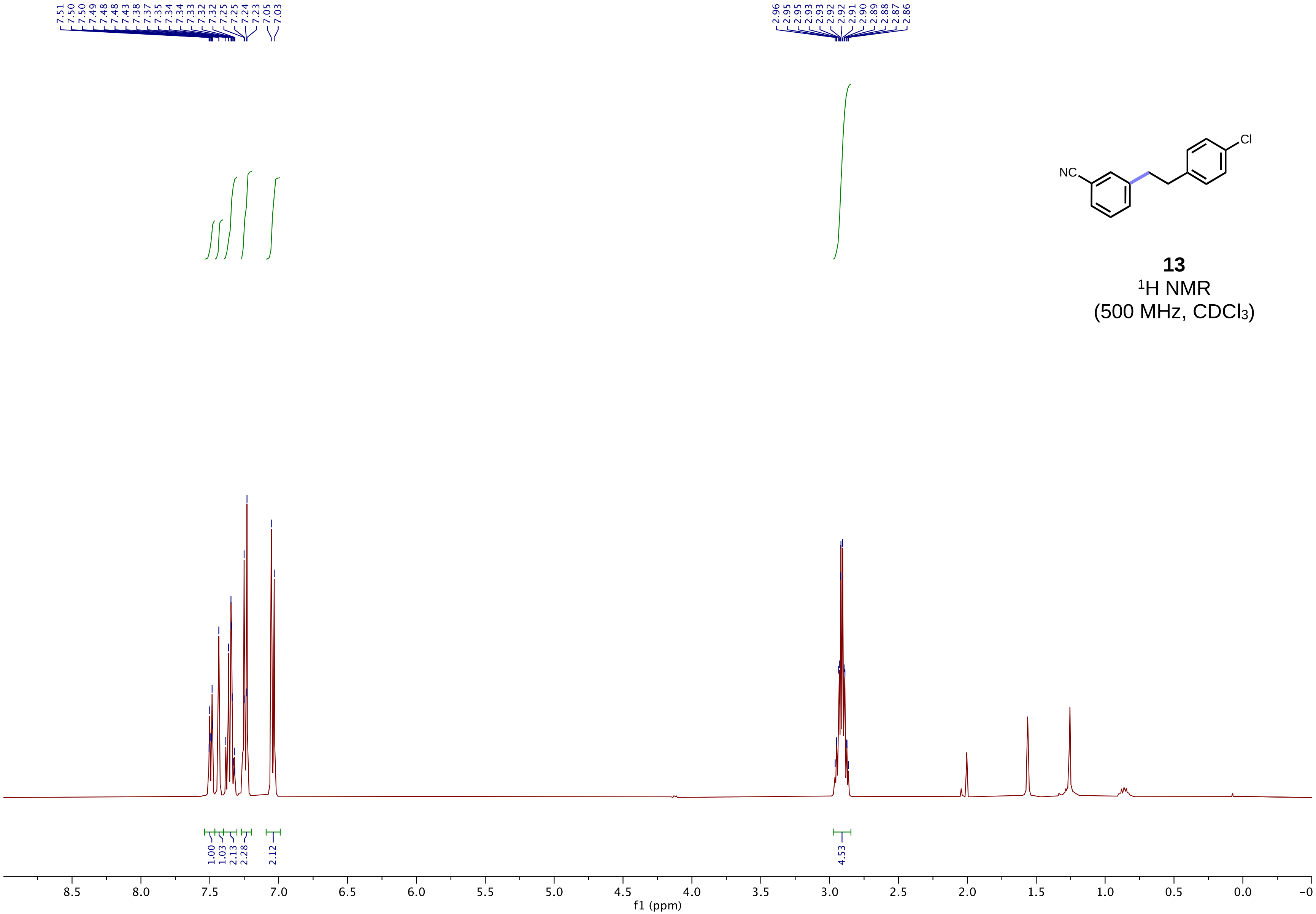
(126 MHz, $CDCl_3$)





12
^{19}F NMR
(470 MHz, $CDCl_3$)

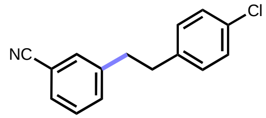




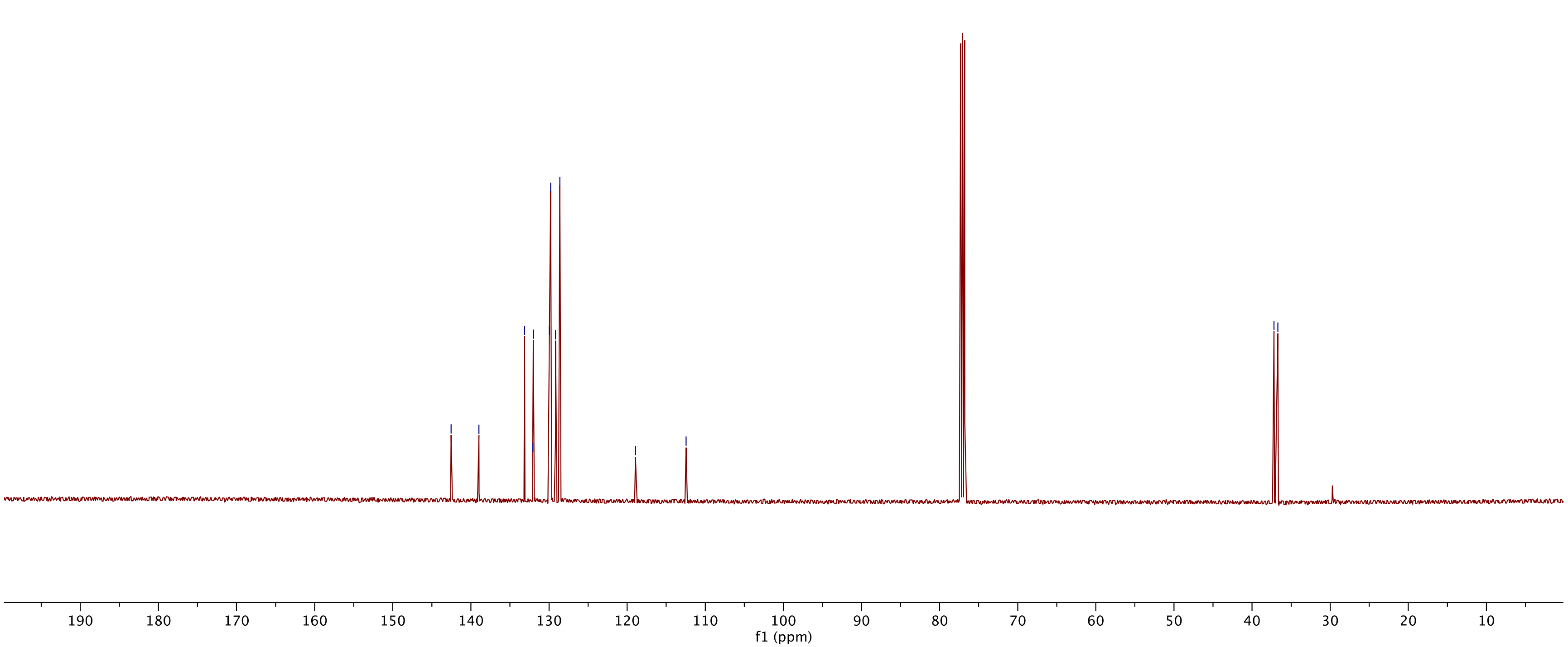
13

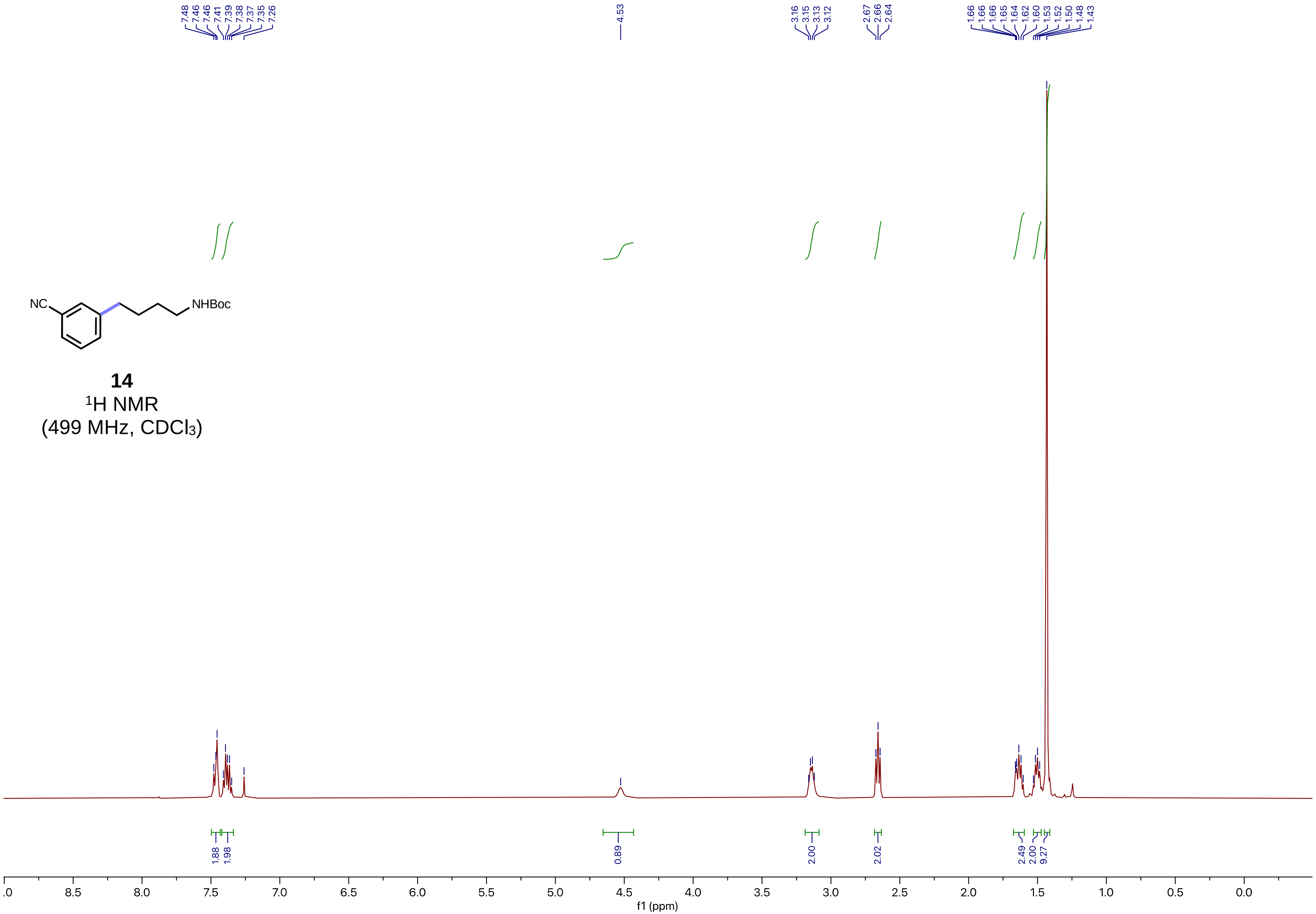
^{1}H NMR

(500 MHz, $CDCl_3$)

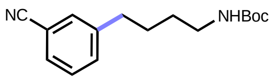


13
^{13}C NMR
(126 MHz, $CDCl_3$)





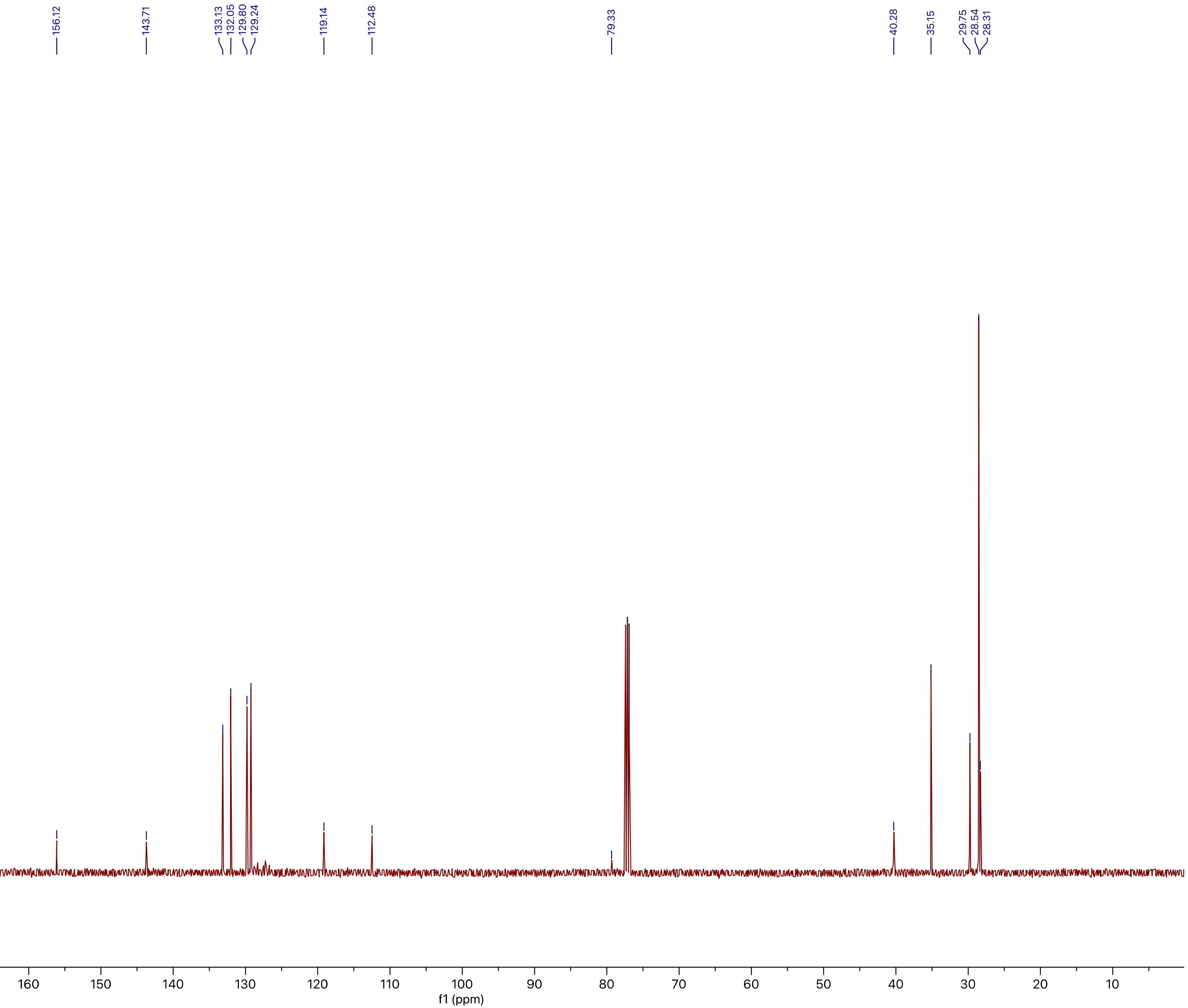
14
^{1}H NMR
(499 MHz, $CDCl_3$)

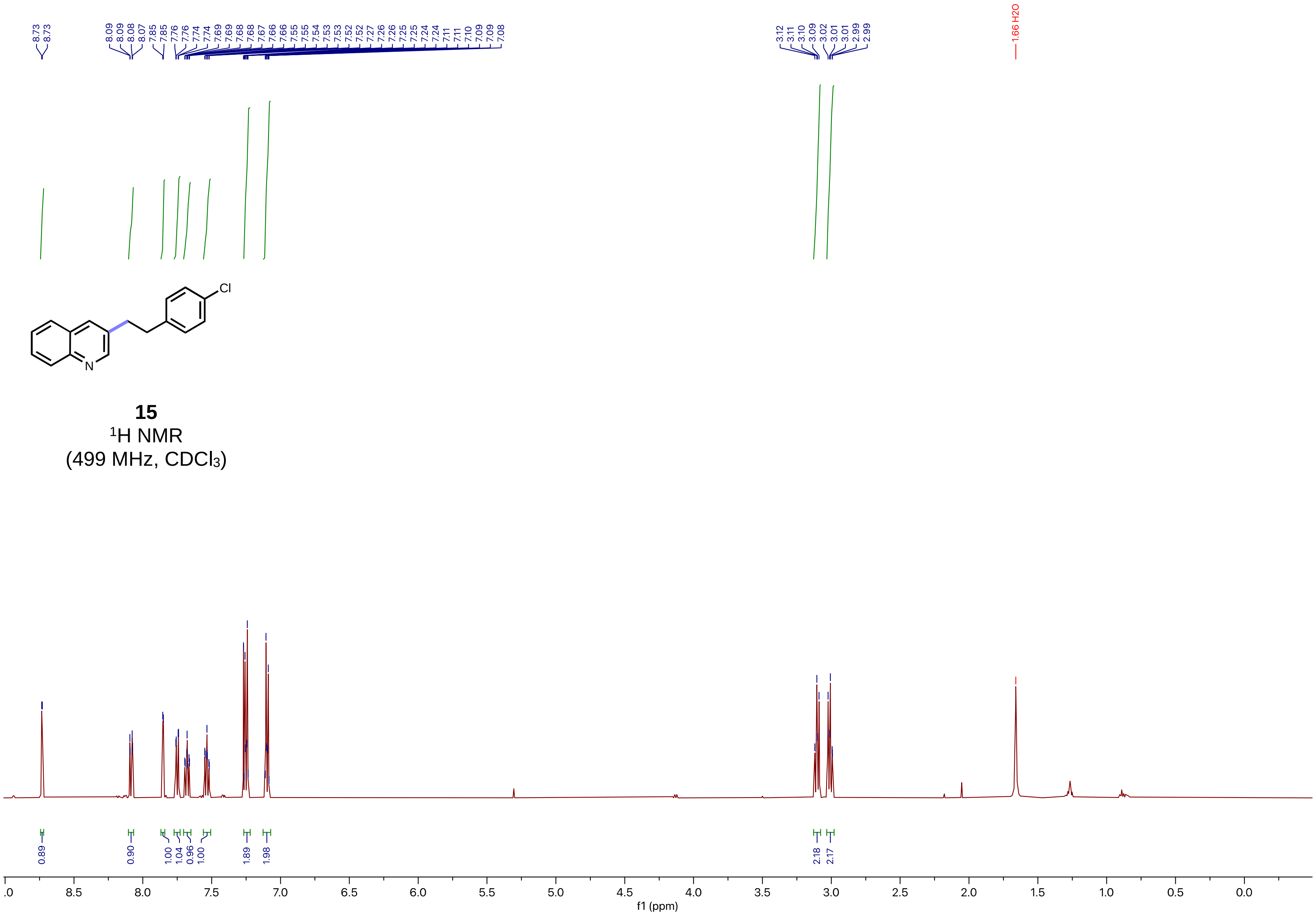


14

^{13}C NMR

(126 MHz, $CDCl_3$)

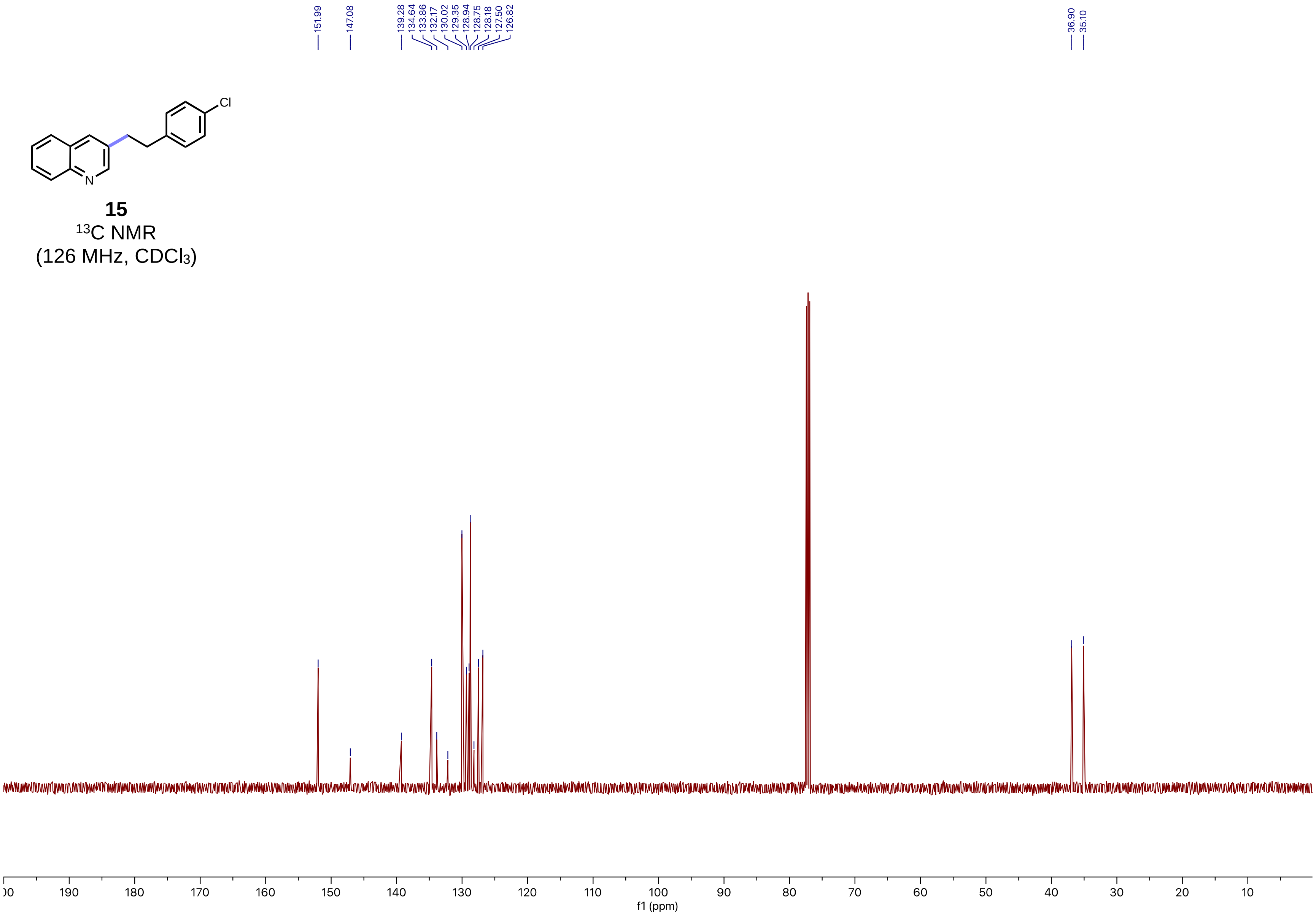




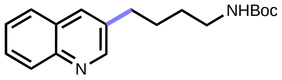
15

^{1}H NMR

(499 MHz, $CDCl_3$)



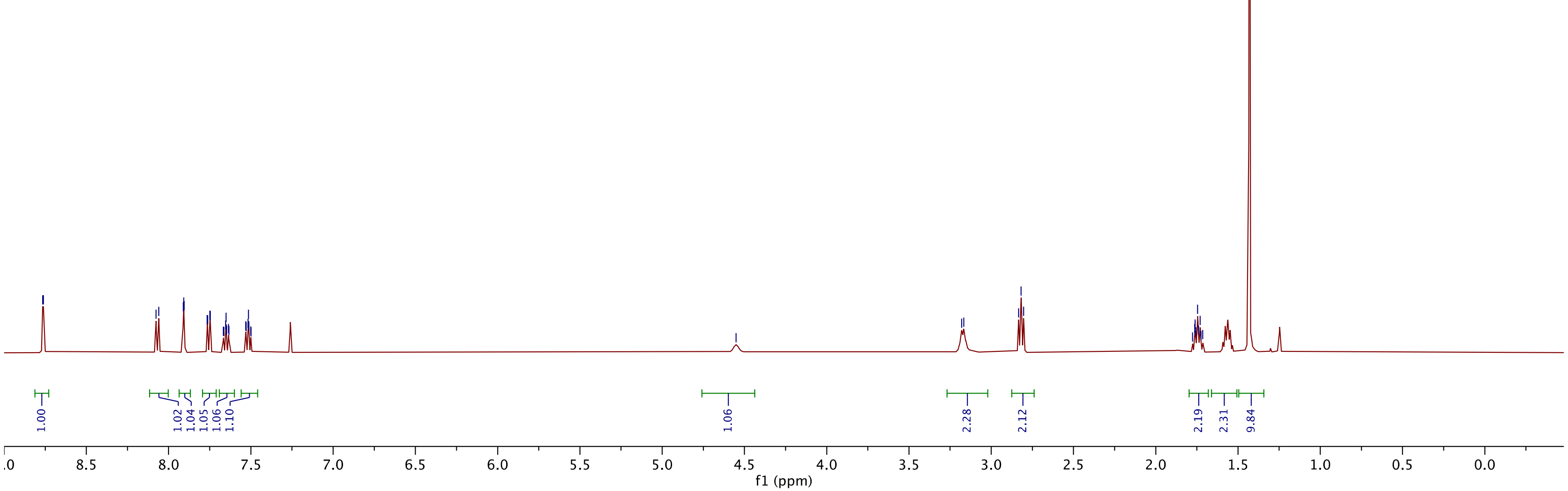
151.99
147.08
139.28
134.64
133.86
132.17
130.02
129.35
128.94
128.75
128.18
127.50
126.82
36.90
35.10
Cl
N
15
^{13}C NMR
(126 MHz, CDCl$_3$)
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

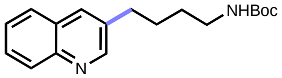


16

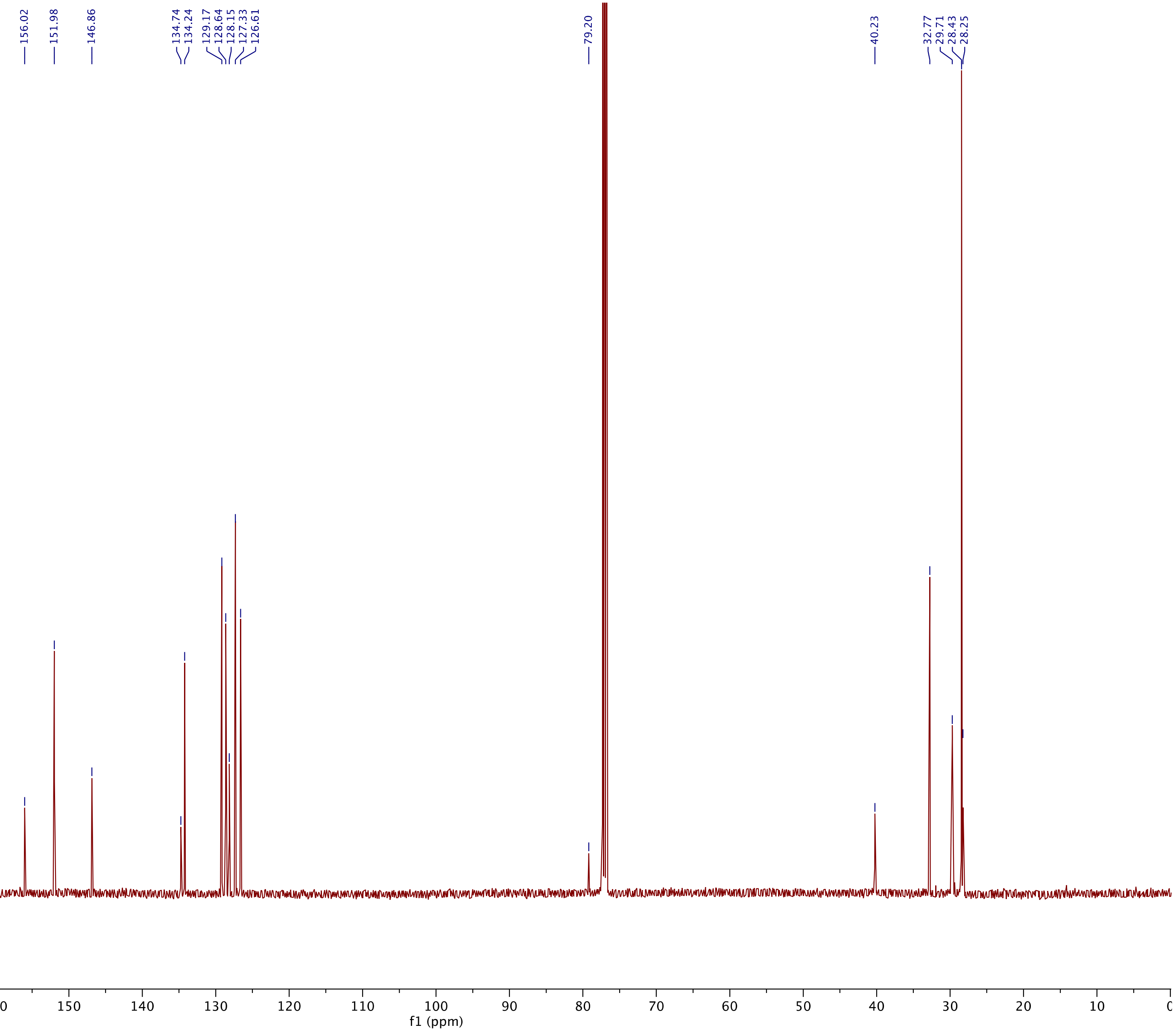
^{1}H NMR

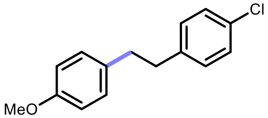
(500 MHz, $CDCl_3$)





16
^{13}C NMR
(126 MHz, $CDCl_3$)

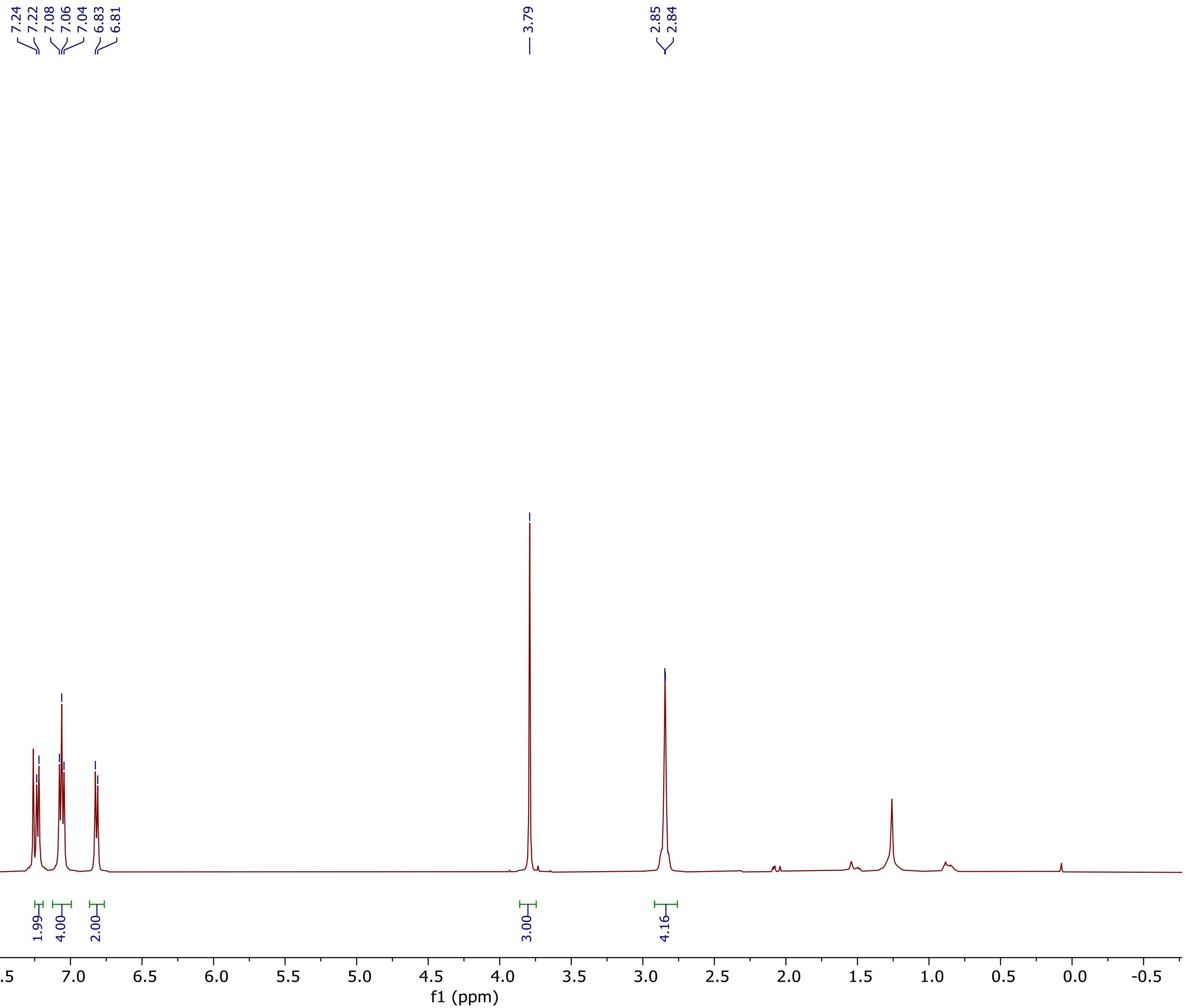


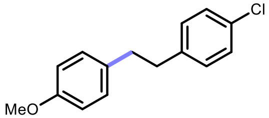


17

^{1}H NMR

(500 MHz, $CDCl_3$)

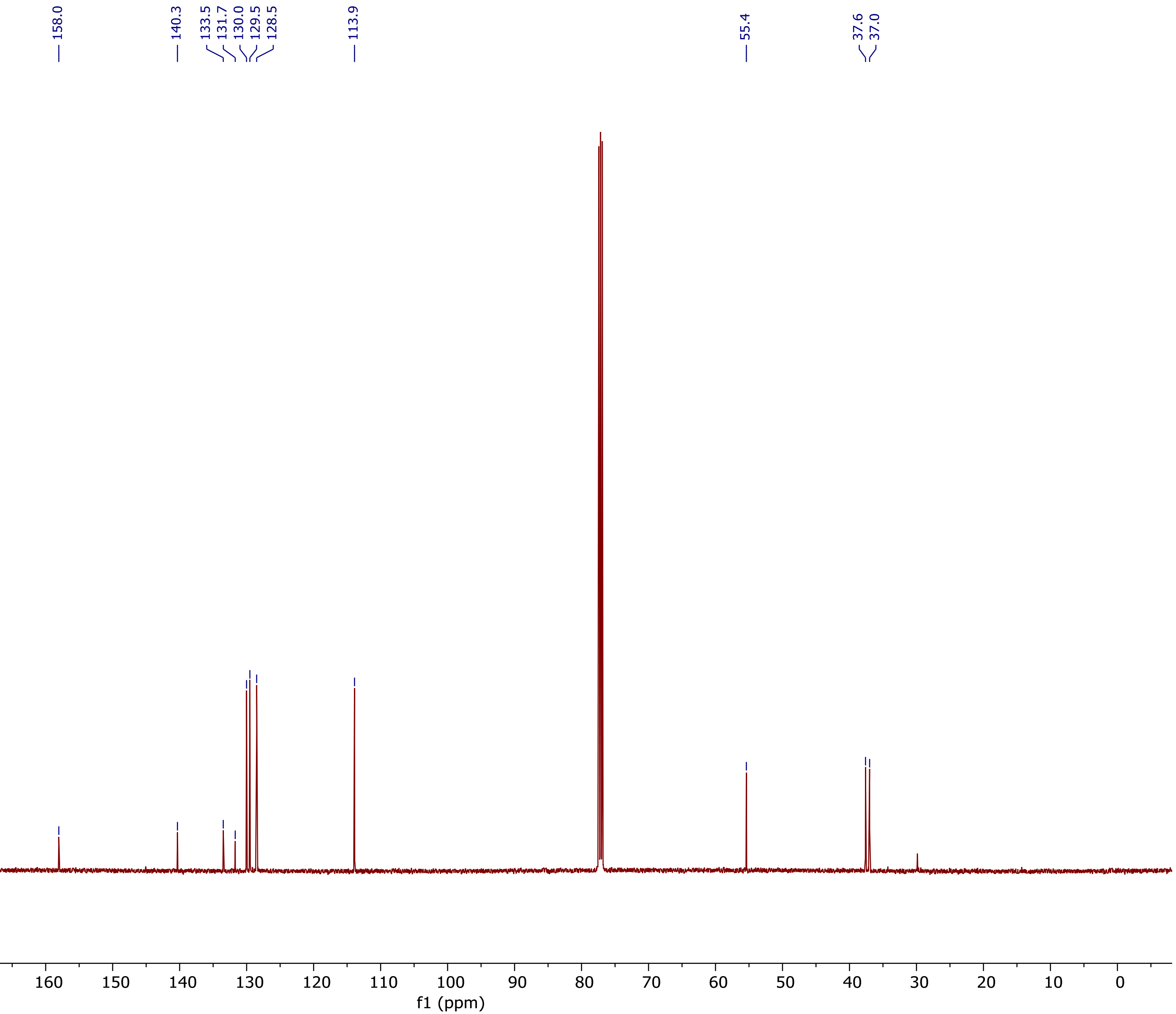


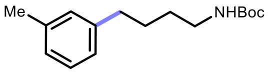


17

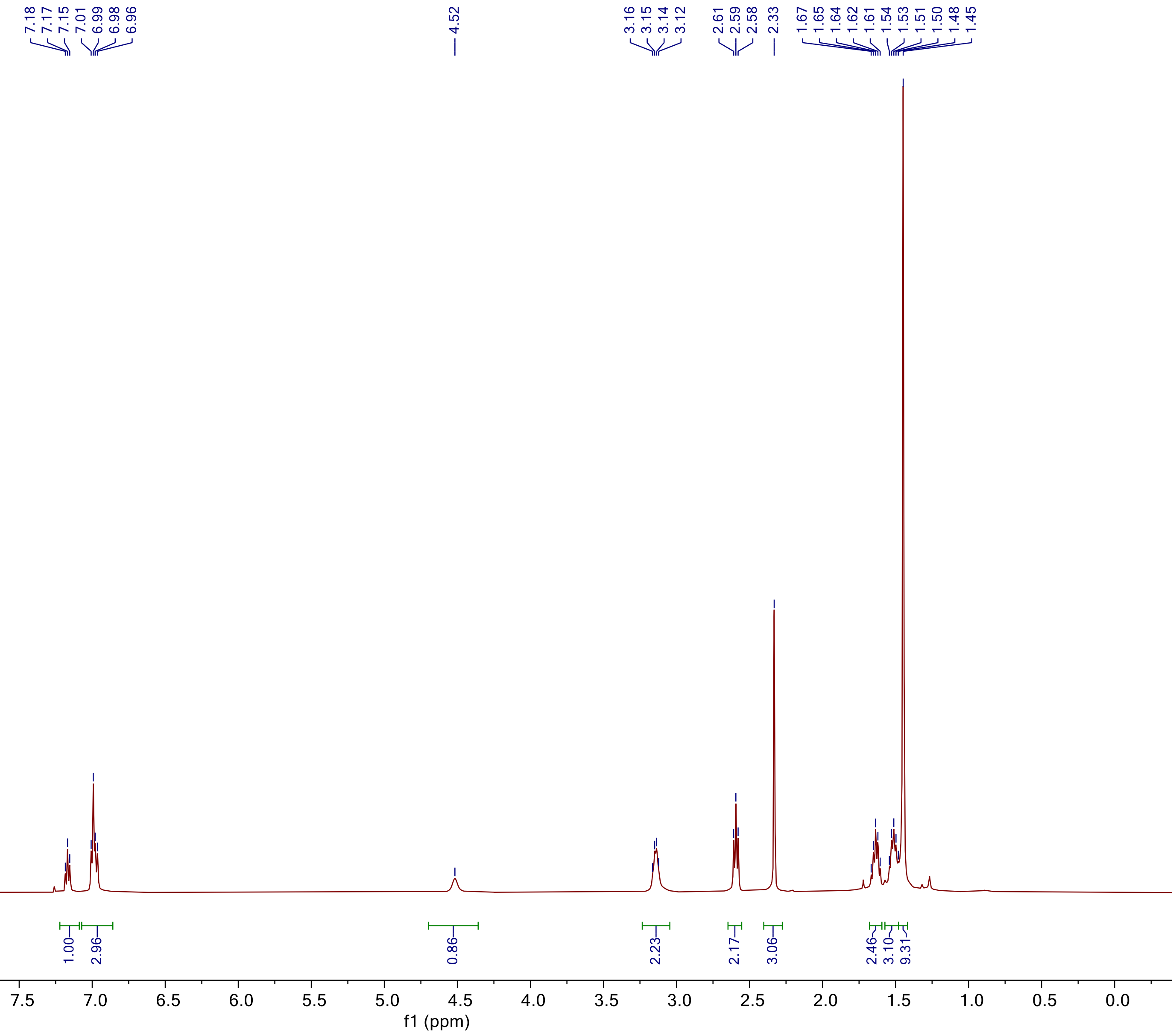
^{13}C NMR

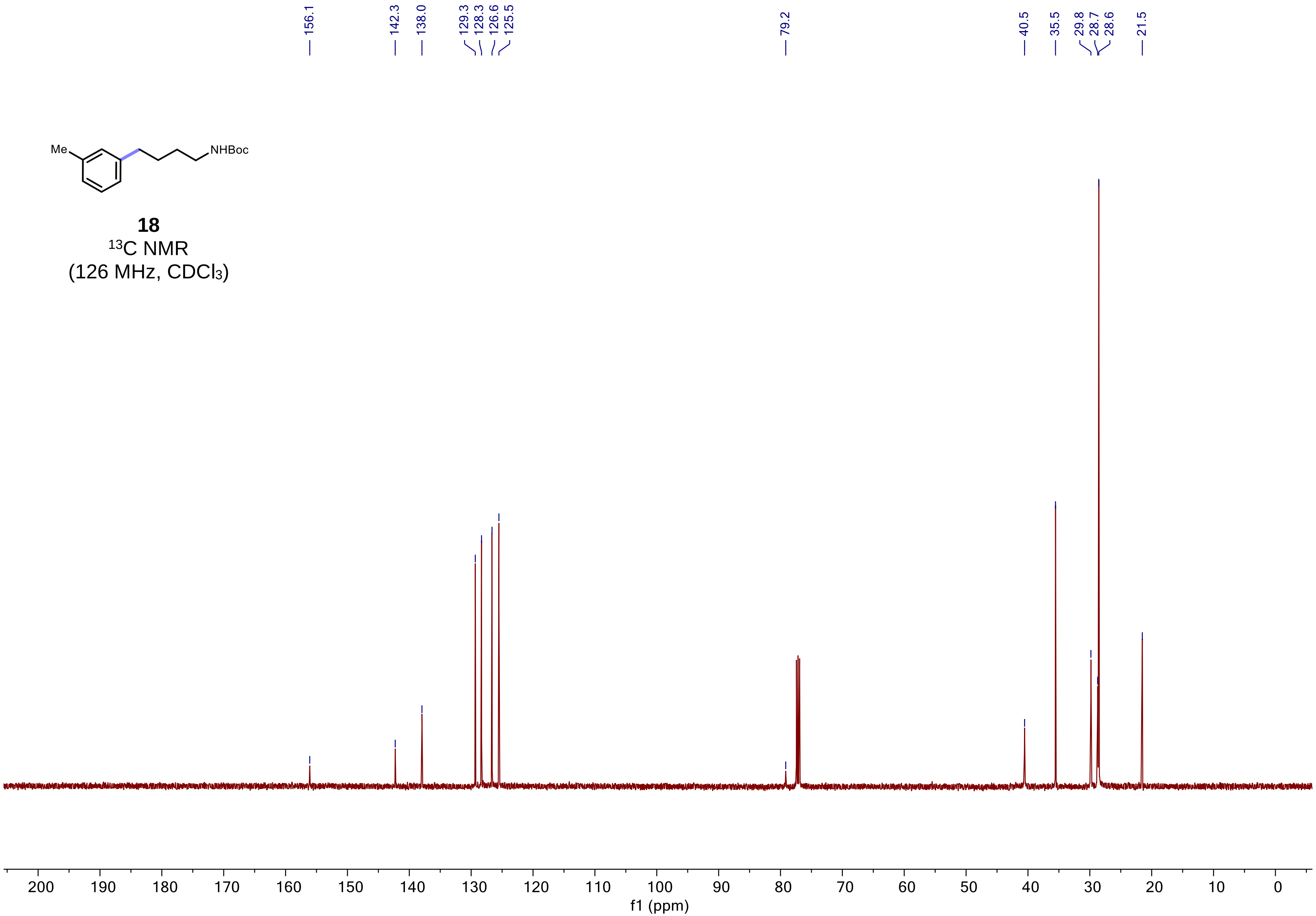
(126 MHz, $CDCl_3$)





18
^{1}H NMR
(499 MHz, $CDCl_3$)

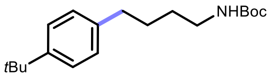




18

^{13}C NMR

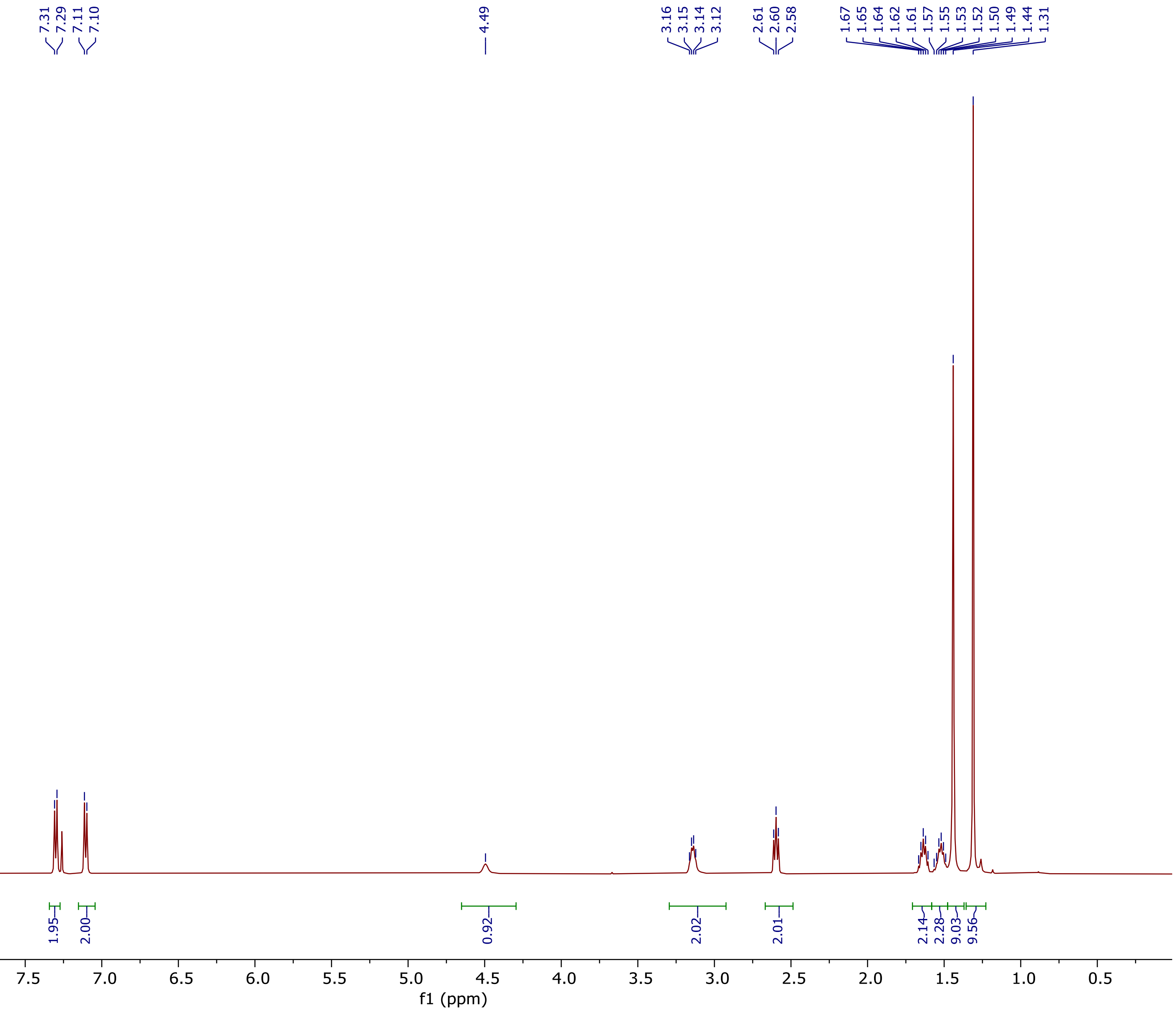
(126 MHz, $CDCl_3$)

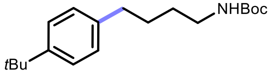


19

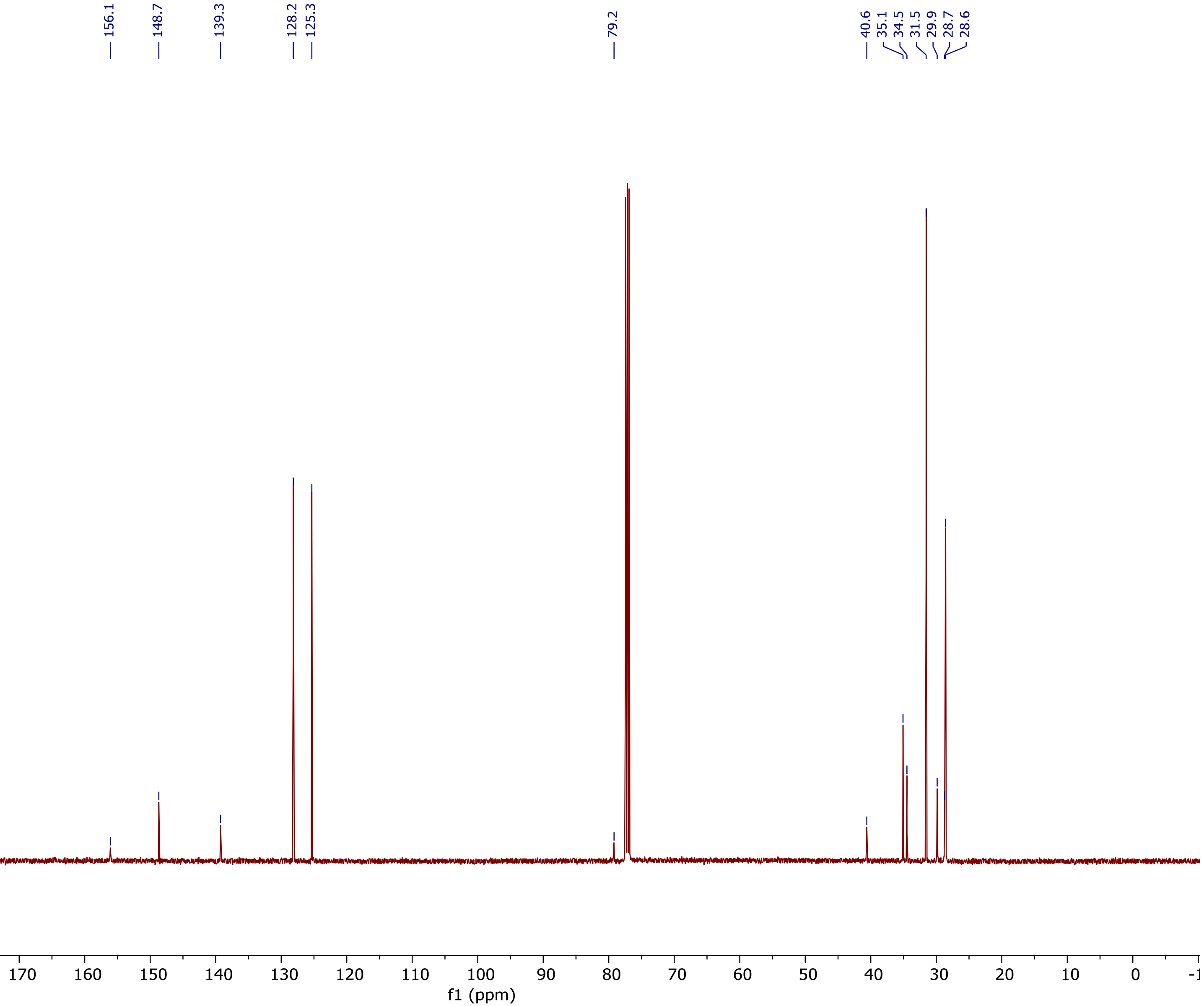
^{1}H NMR

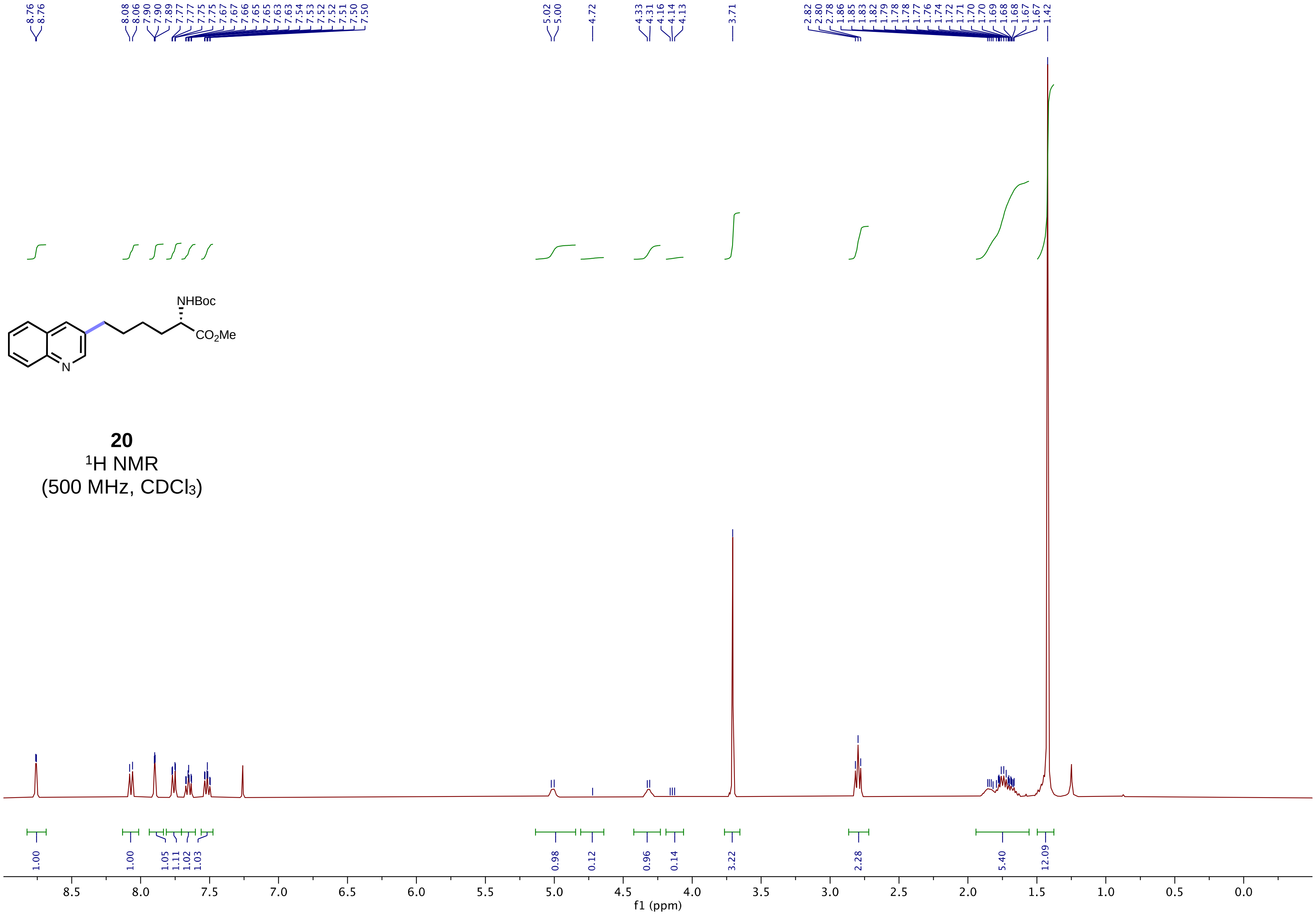
(500 MHz, $CDCl_3$)





19
^{13}C NMR
(126 MHz, $CDCl_3$)

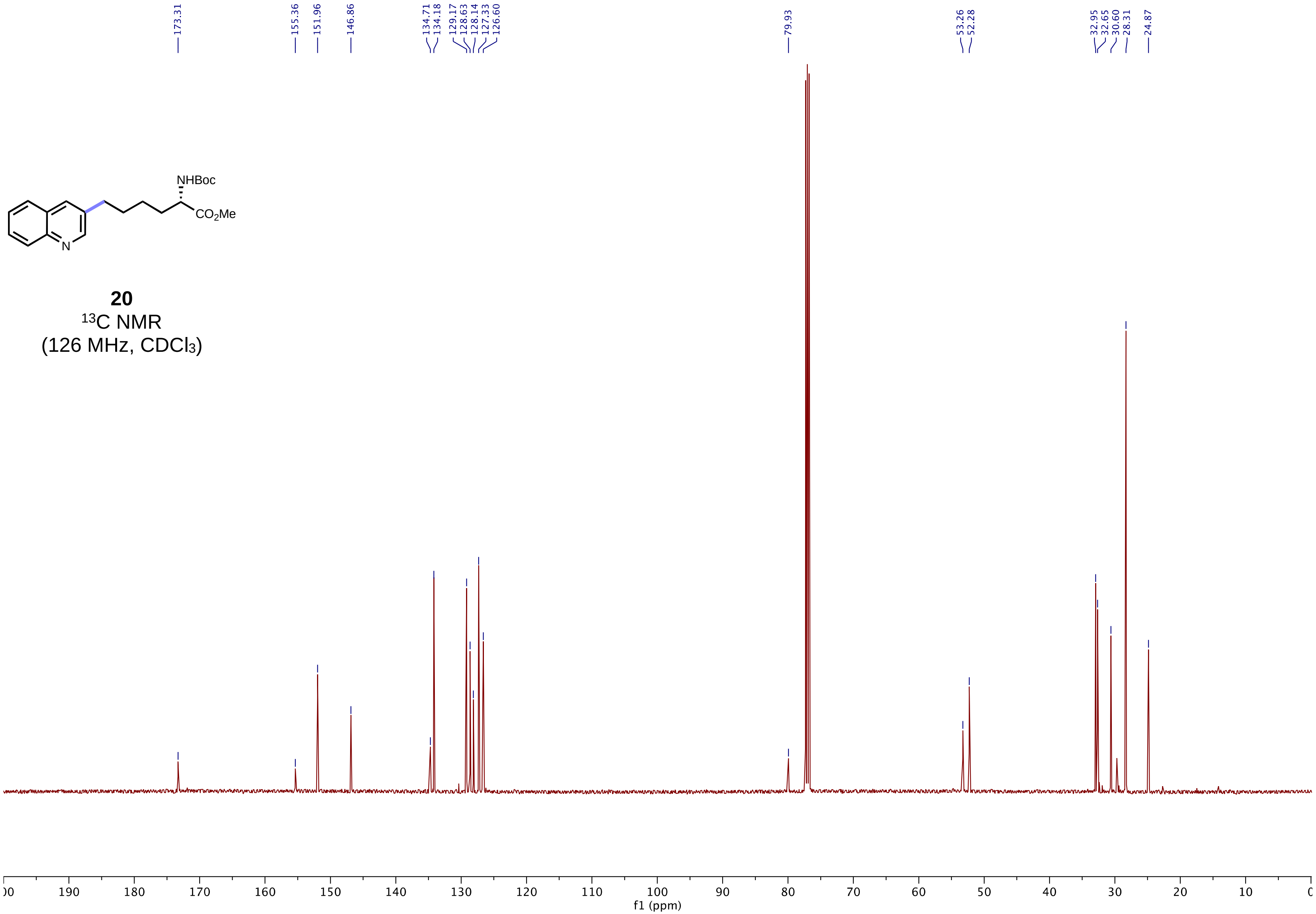




20

^{1}H NMR

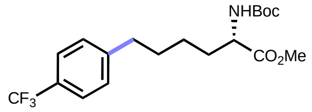
(500 MHz, $CDCl_3$)



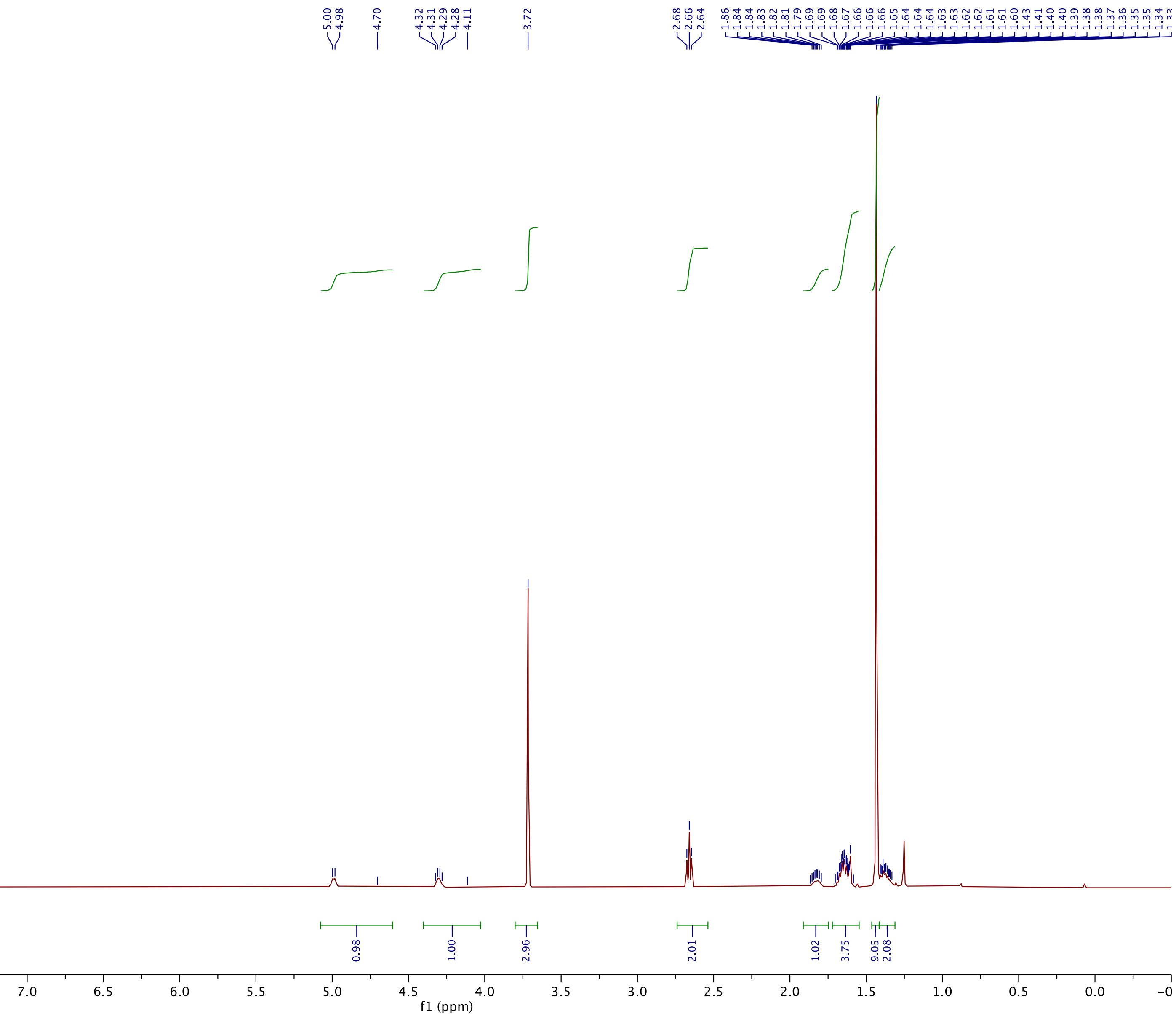
20

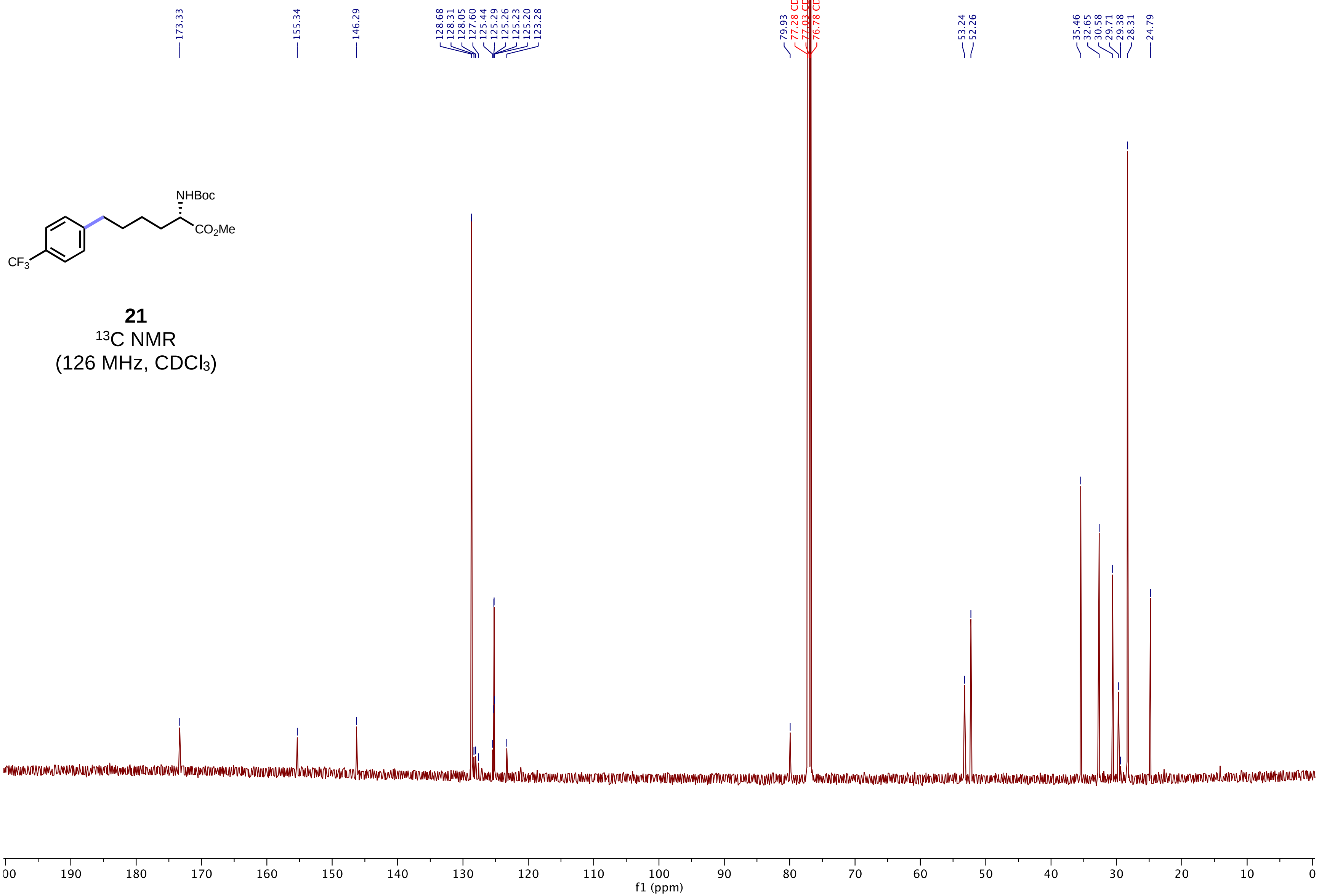
^{13}C NMR

(126 MHz, $CDCl_3$)



21
^1H NMR
(500 MHz, $CDCl_3$)

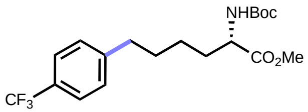




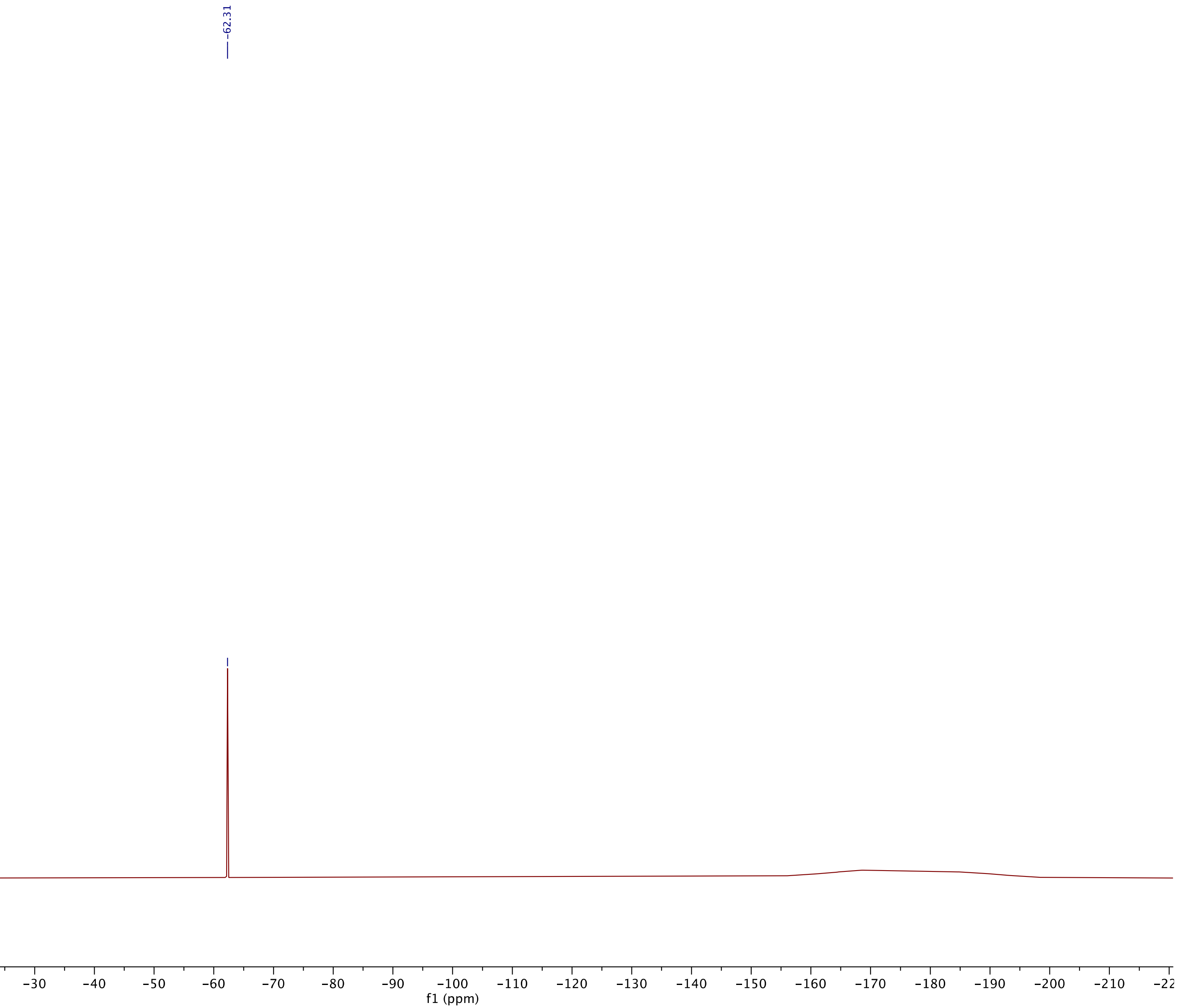
21

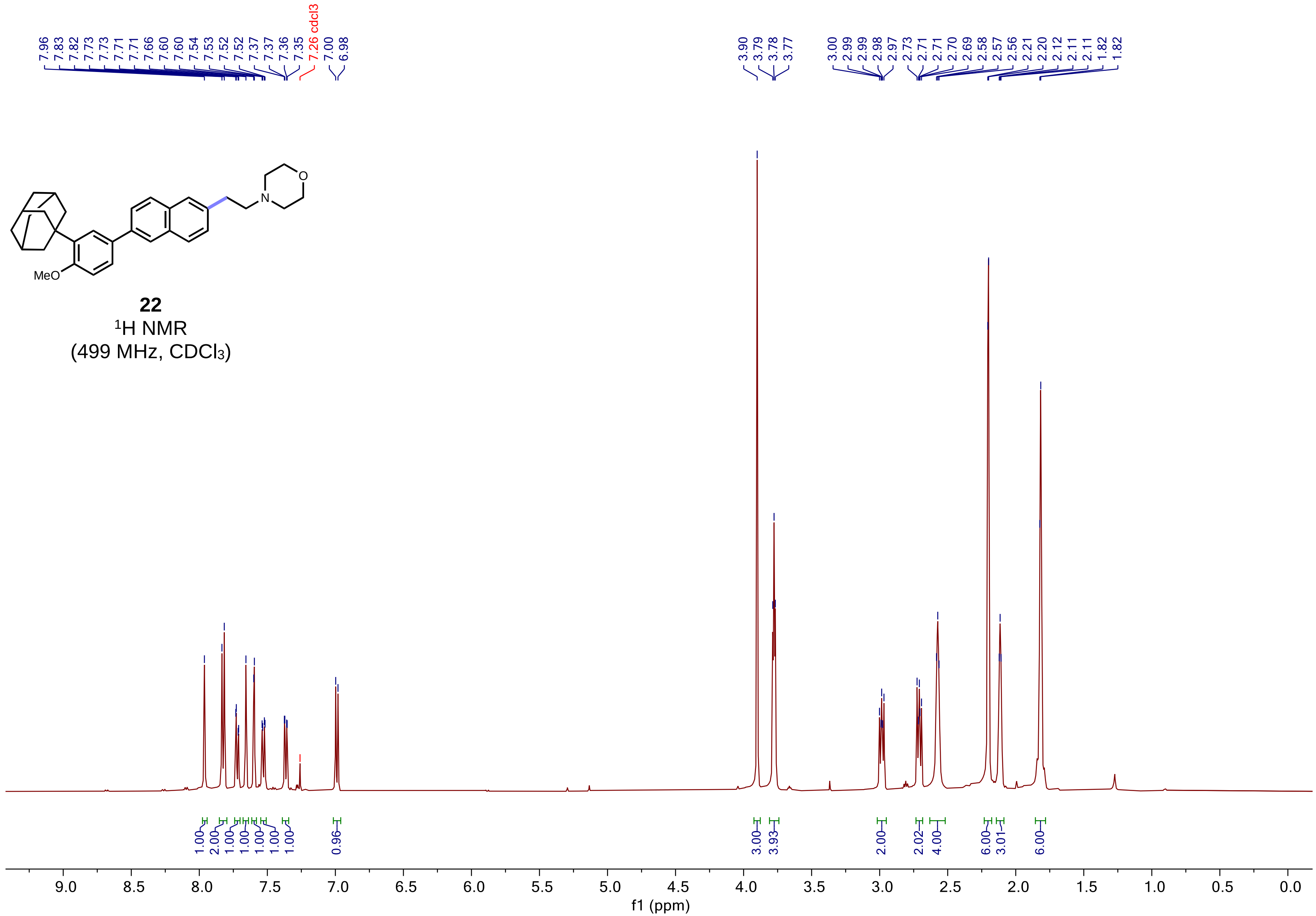
^{13}C NMR

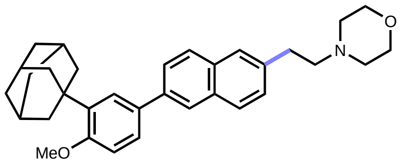
(126 MHz, $CDCl_3$)



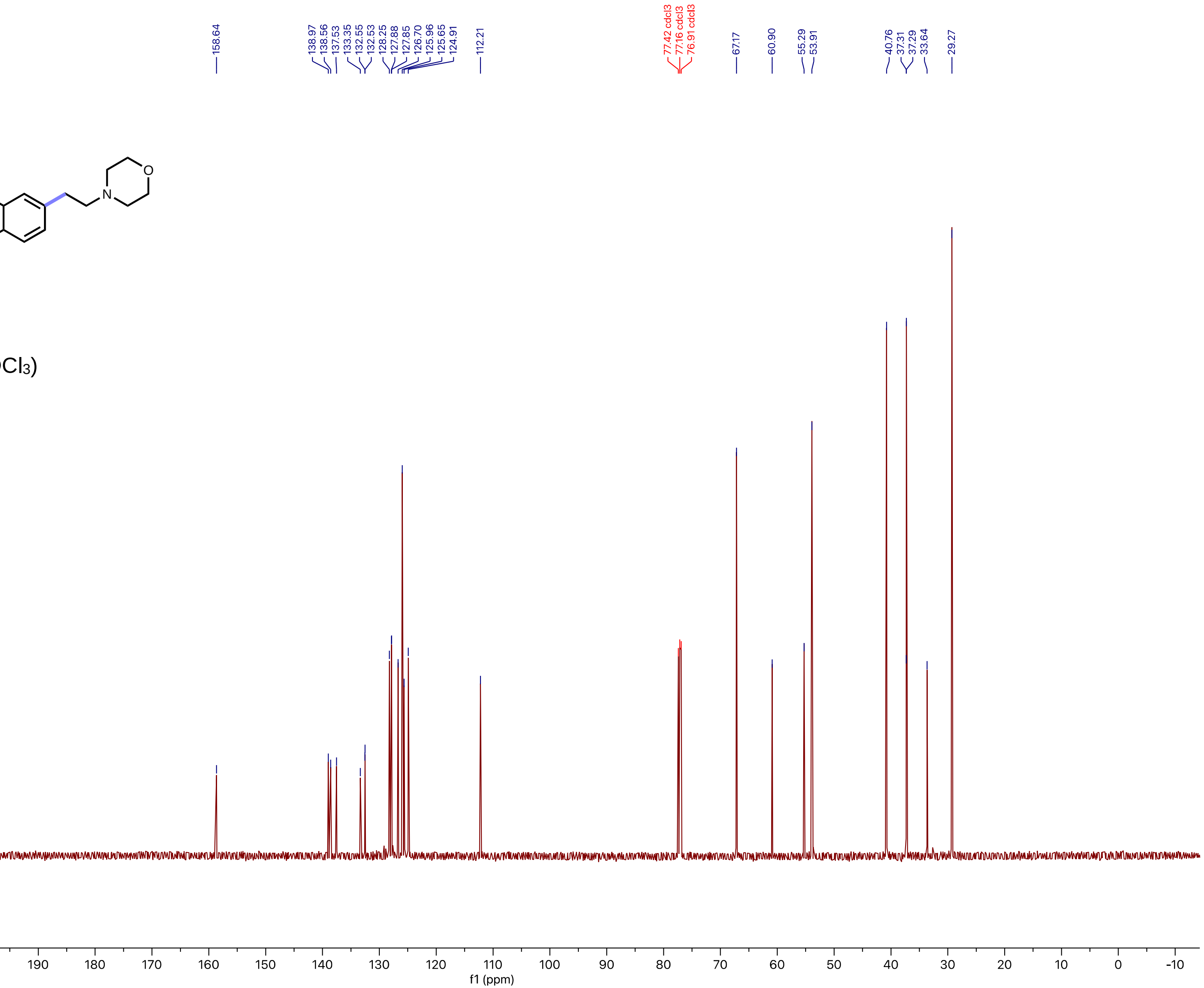
21
^{19}F NMR
(471 MHz, $CDCl_3$)

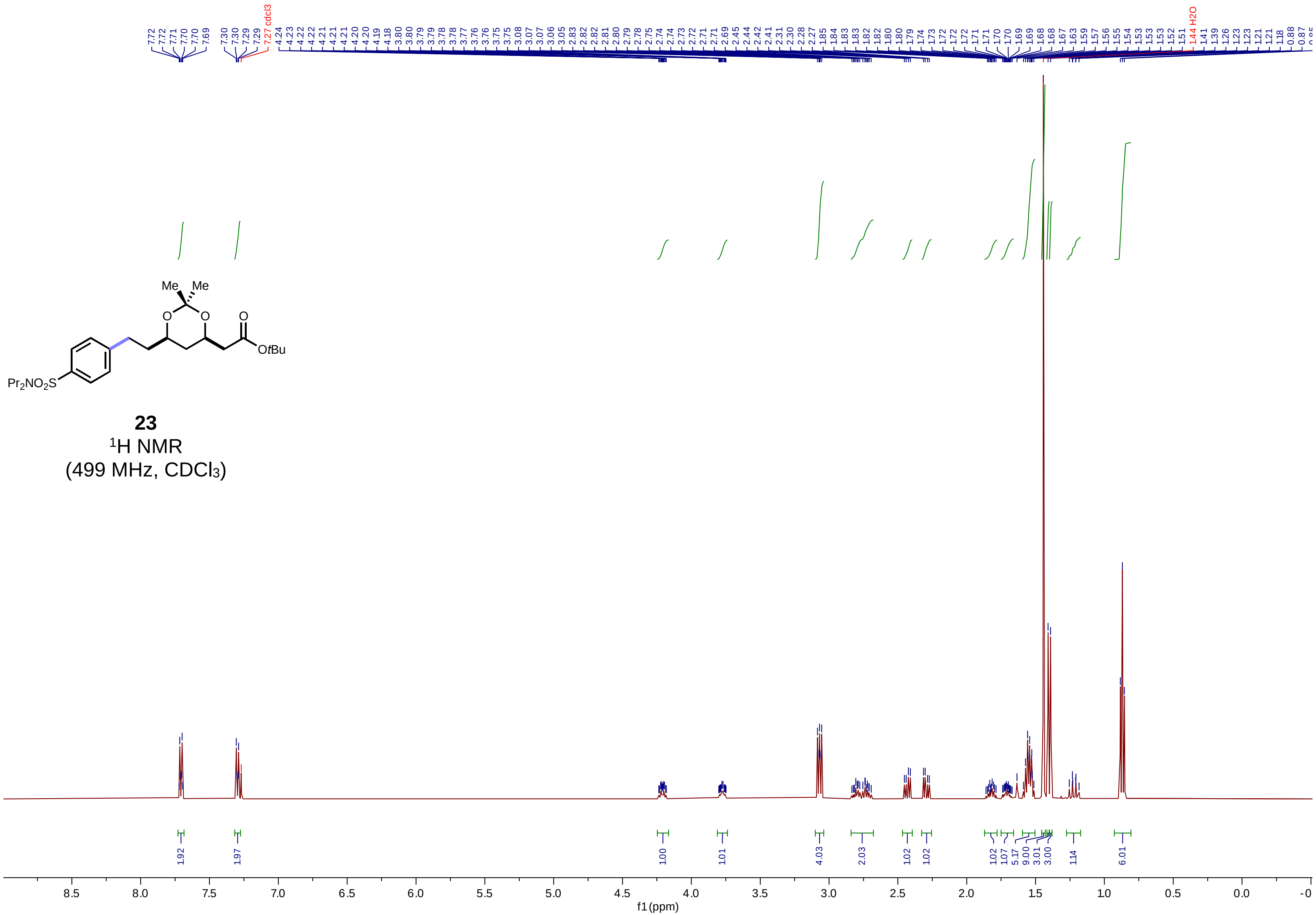



7.96
7.83
7.82
7.73
7.73
7.71
7.71
7.66
7.60
7.60
7.54
7.53
7.52
7.52
7.37
7.37
7.36
7.35
7.26 cdcl3
7.00
6.98
3.90
3.79
3.78
3.77
3.00
2.99
2.99
2.98
2.97
2.73
2.71
2.71
2.70
2.69
2.58
2.57
2.56
2.21
2.20
2.12
2.11
2.11
1.82
1.82
O
N
MeO
22
^{1}H NMR
(499 MHz, $CDCl_3$)
1.00
2.00
1.00
1.00
1.00
1.00
1.00
0.96
3.00
3.93
2.00
2.02
4.00
6.00
3.01
6.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

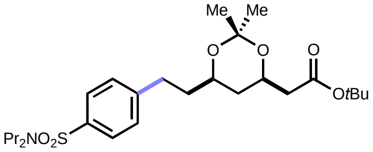


22
^{13}C NMR
(126 MHz, $CDCl_3$)





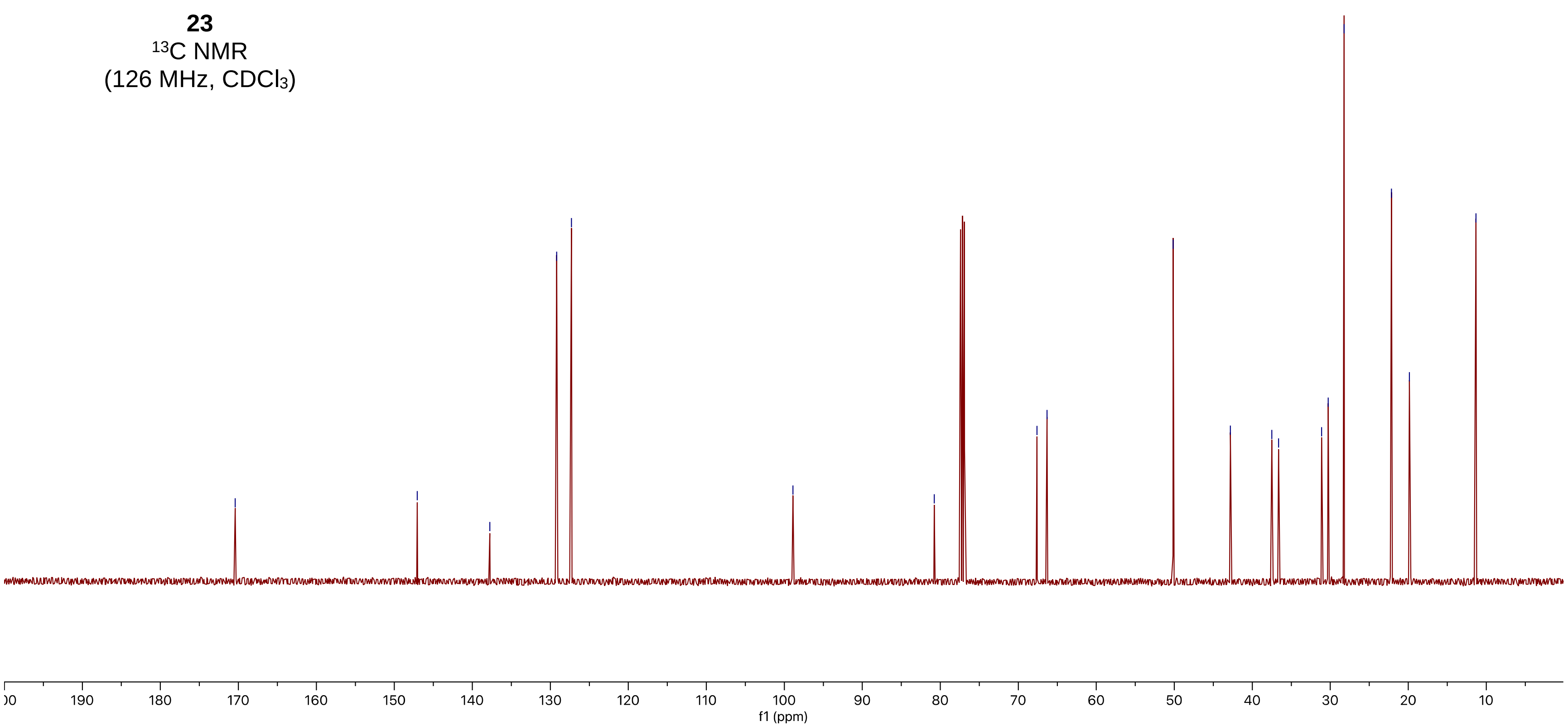
23
^{1}H NMR
(499 MHz, $CDCl_3$)

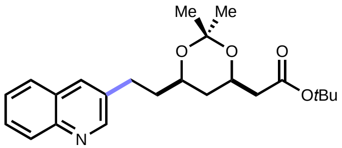


23

^{13}C NMR

(126 MHz, $CDCl_3$)

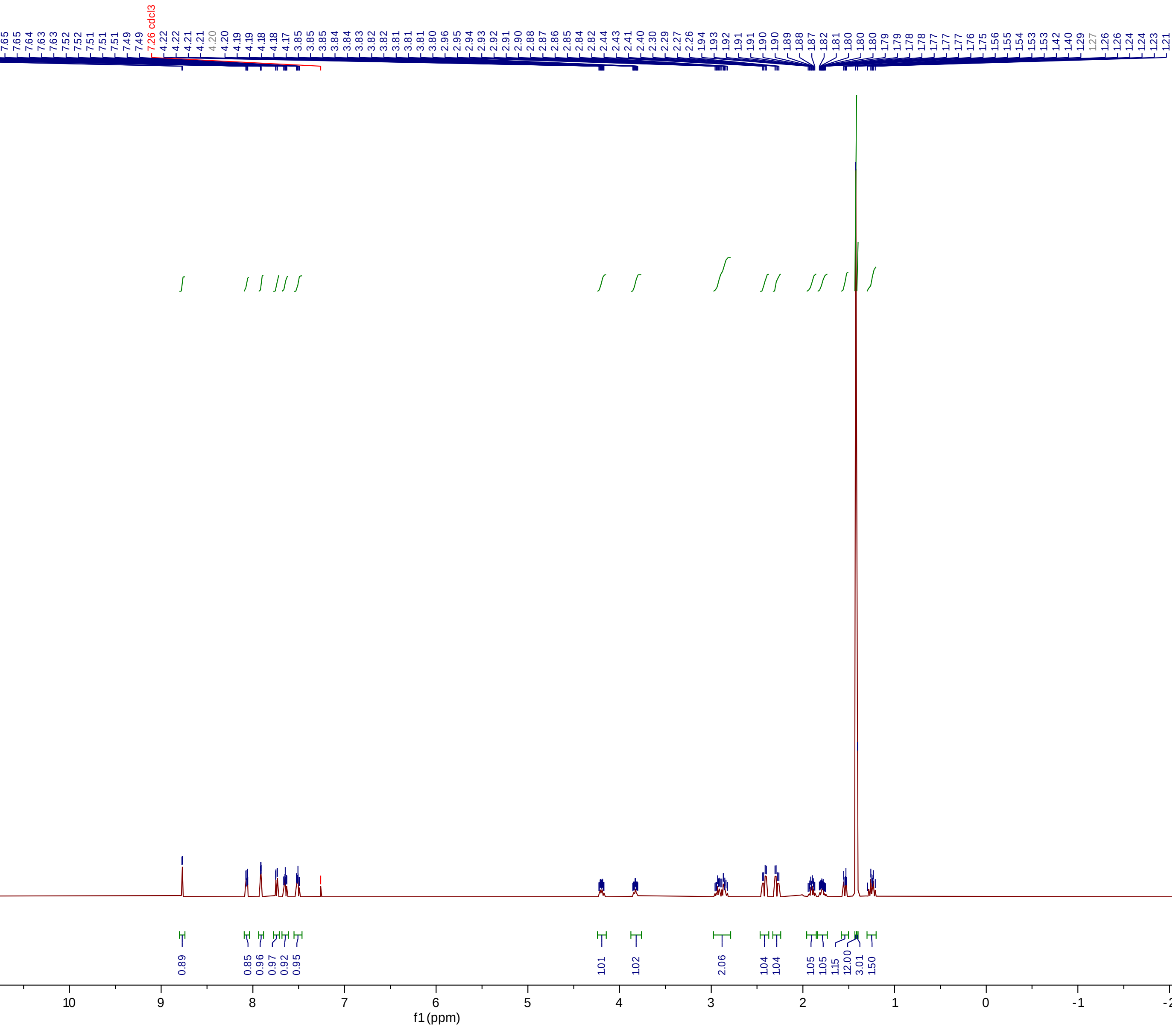


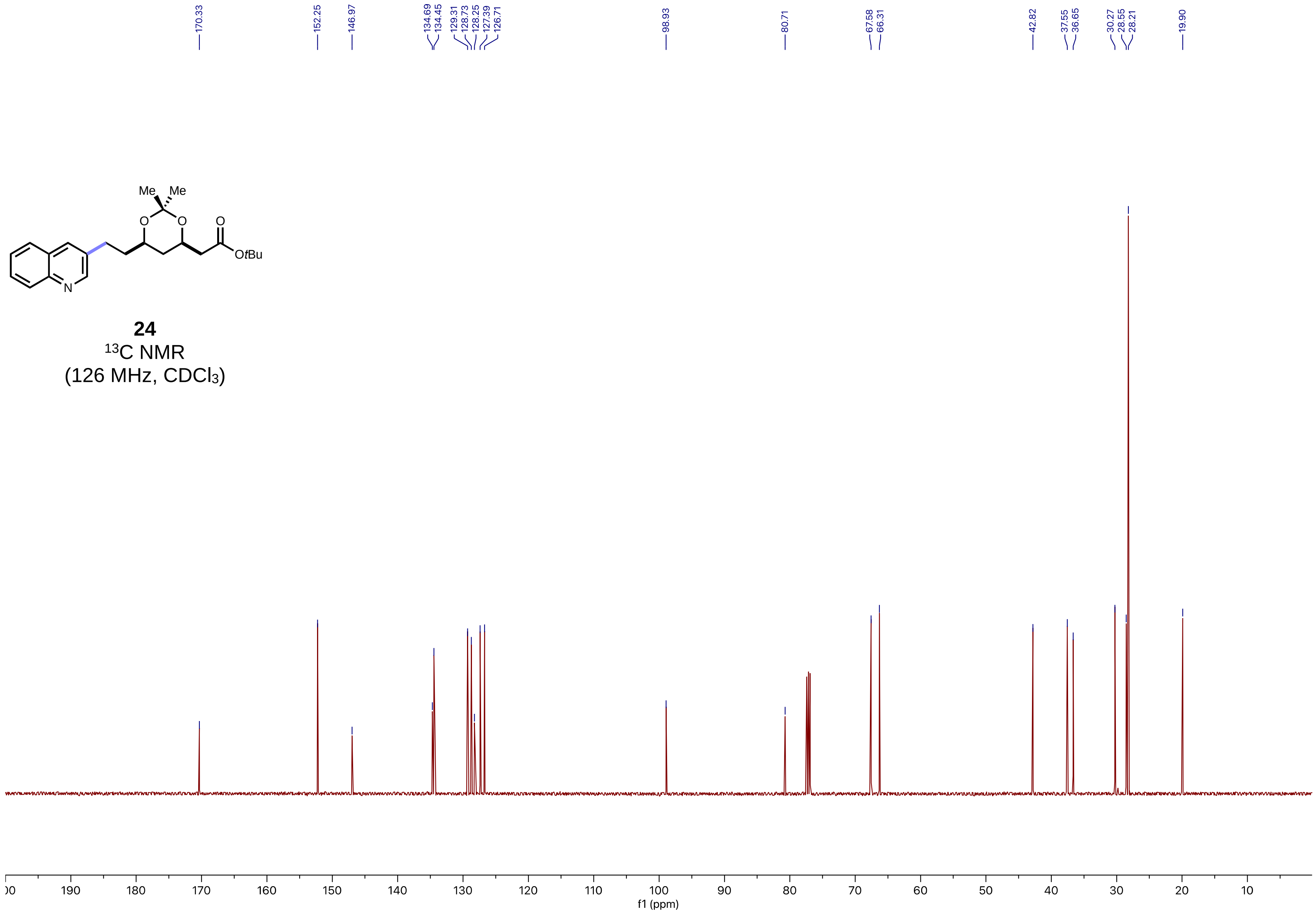


24

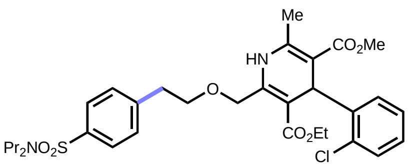
^1H NMR

(499 MHz, $CDCl_3$)





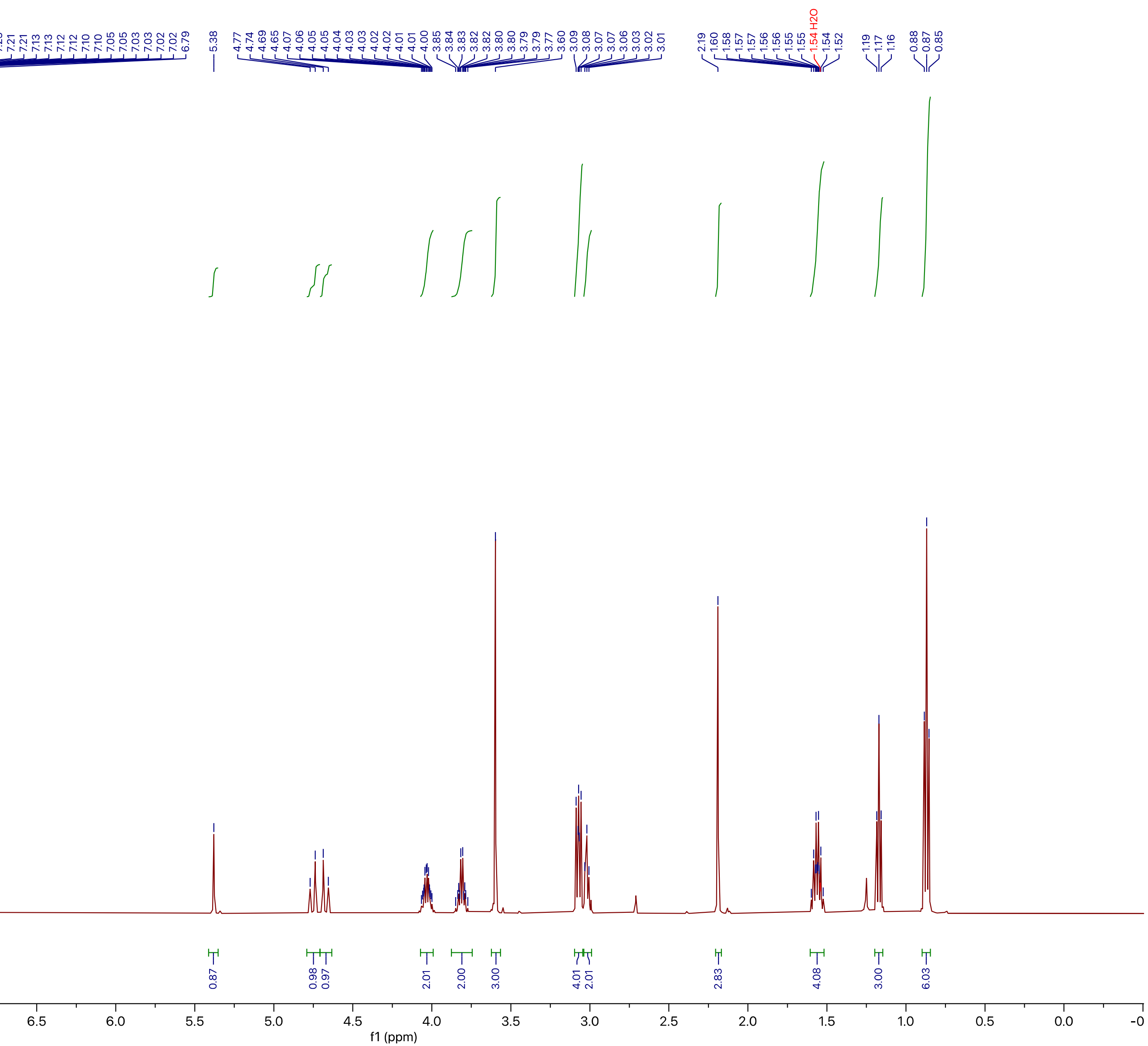
24
^{13}C NMR
(126 MHz, $CDCl_3$)

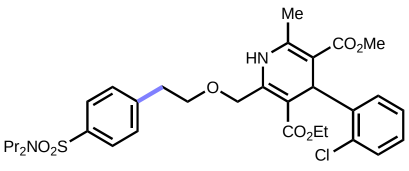


25

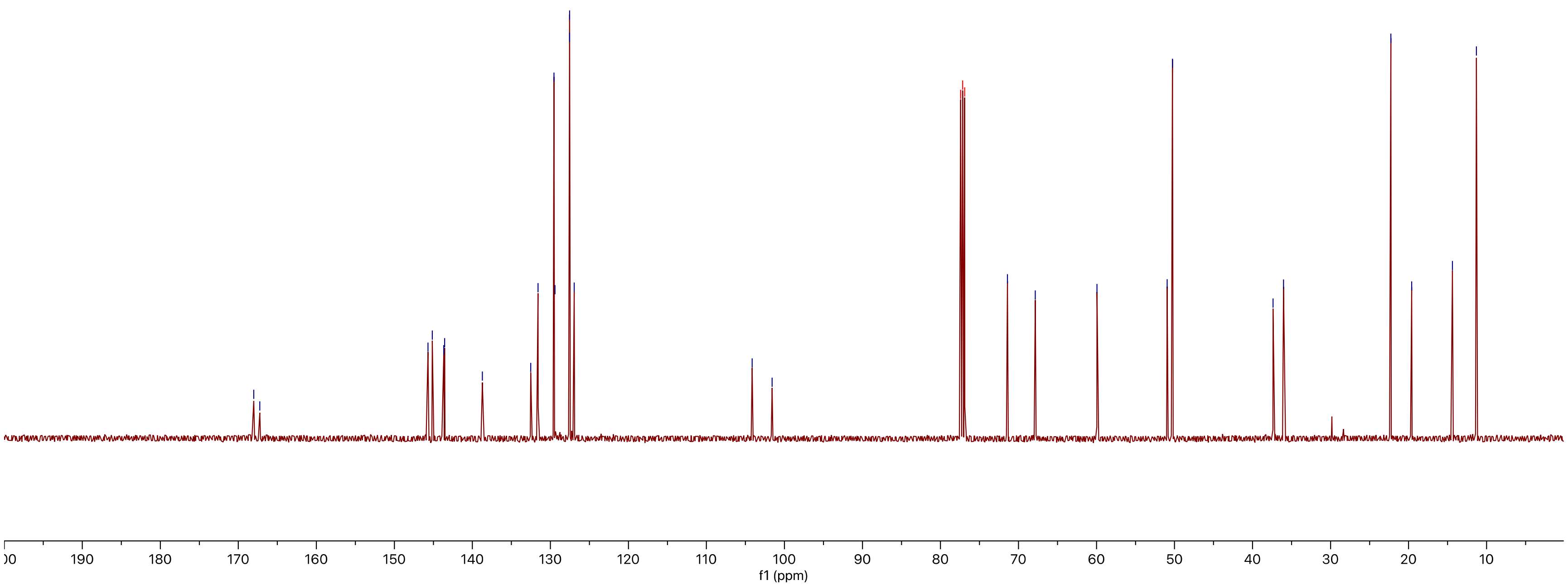
^{1}H NMR

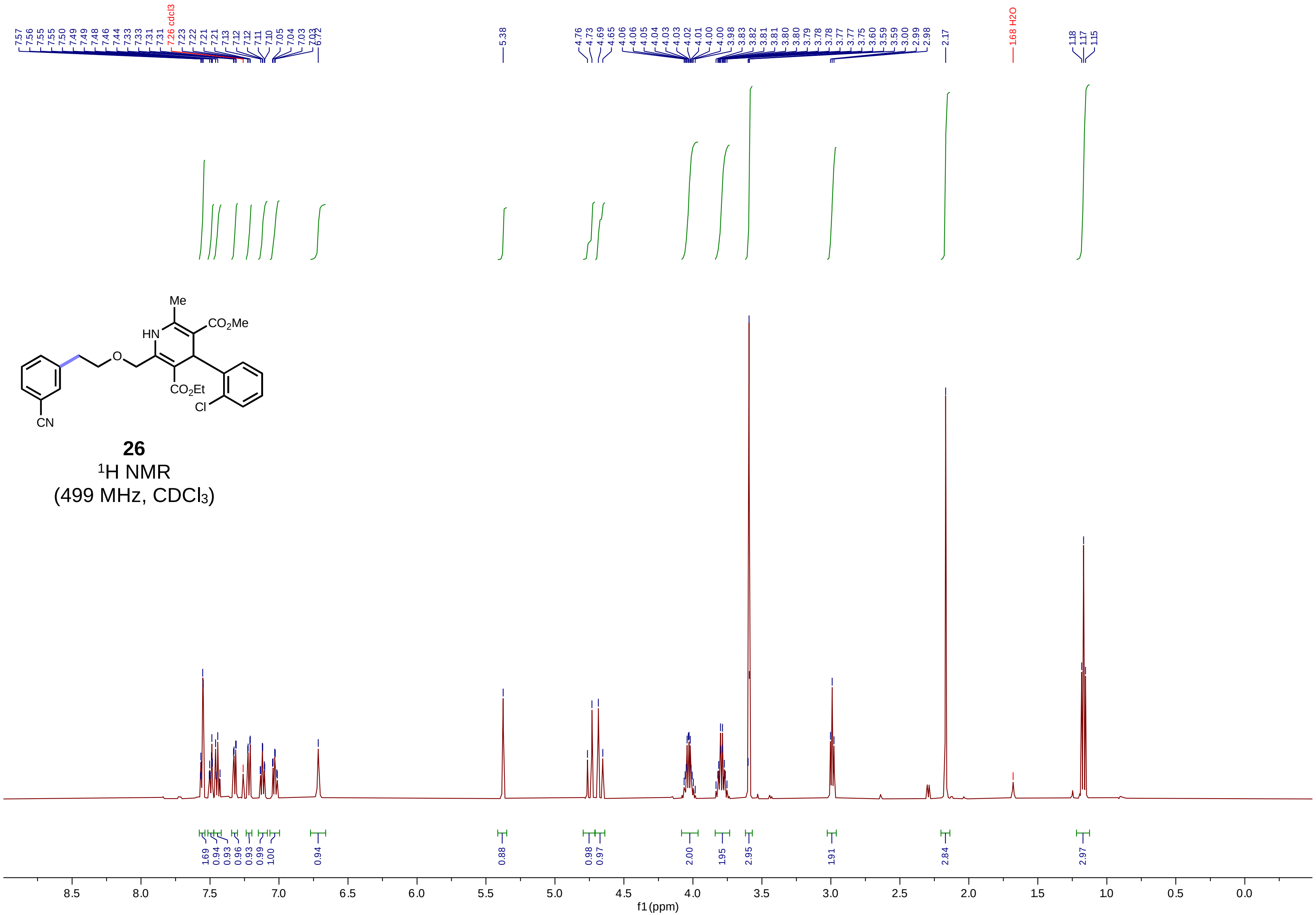
(499 MHz, $CDCl_3$)





25
^{13}C NMR
(126 MHz, $CDCl_3$)

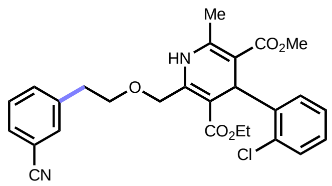




26

^{1}H NMR

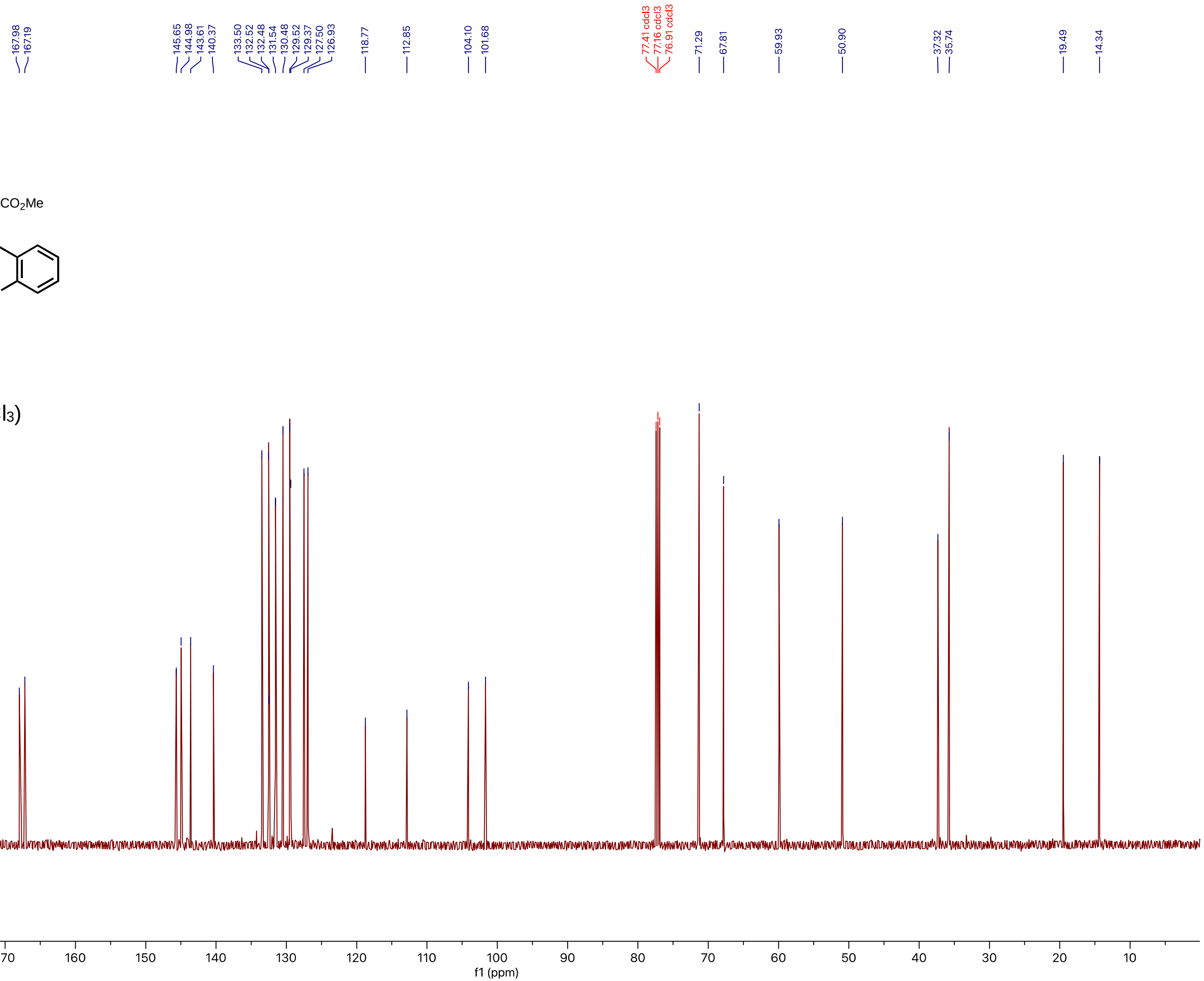
(499 MHz, $CDCl_3$)

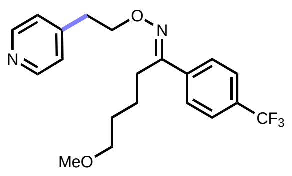


26

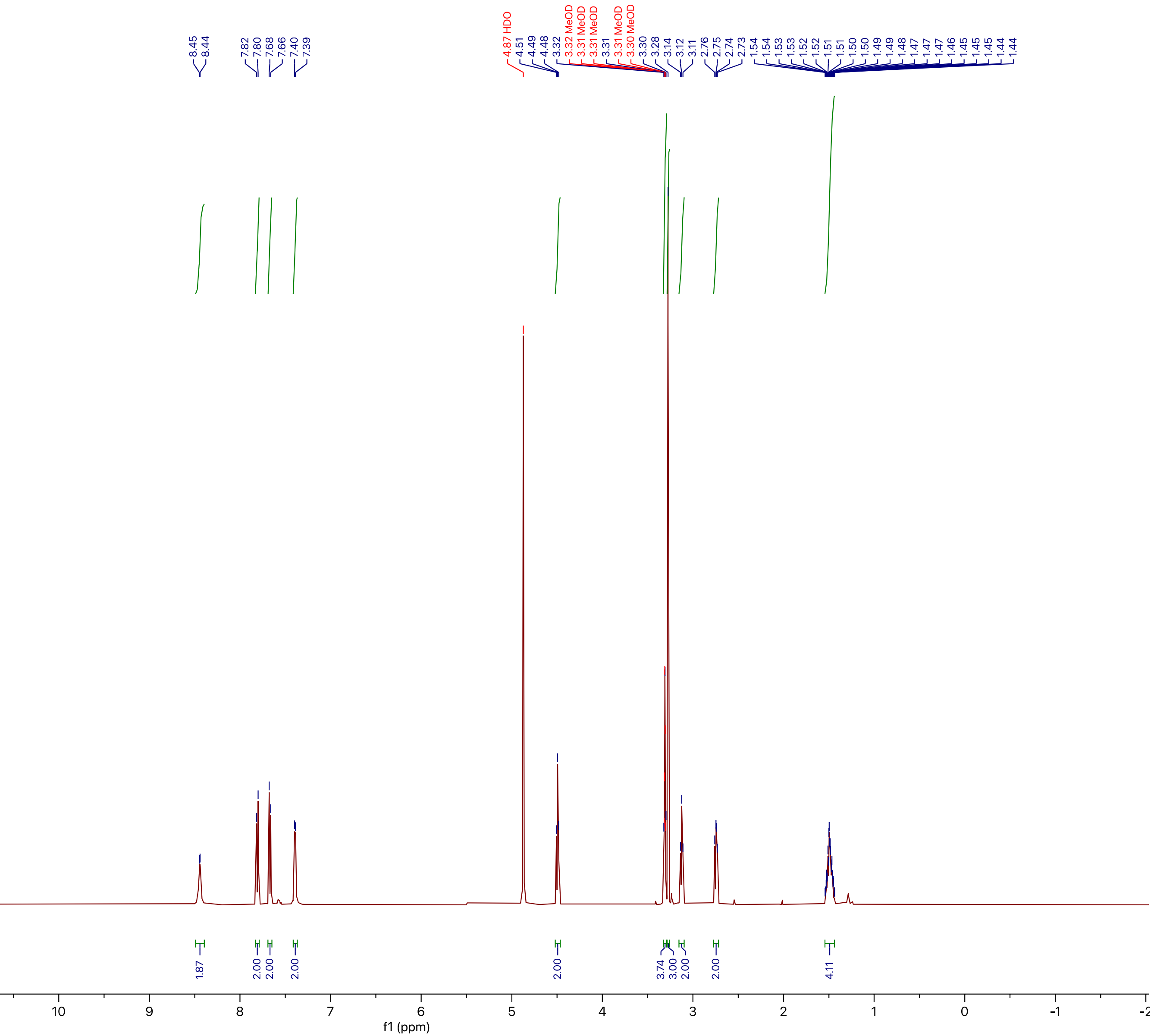
^{13}C NMR

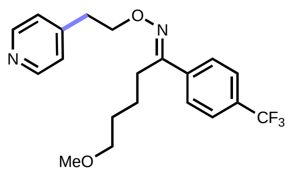
(126 MHz, $CDCl_3$)



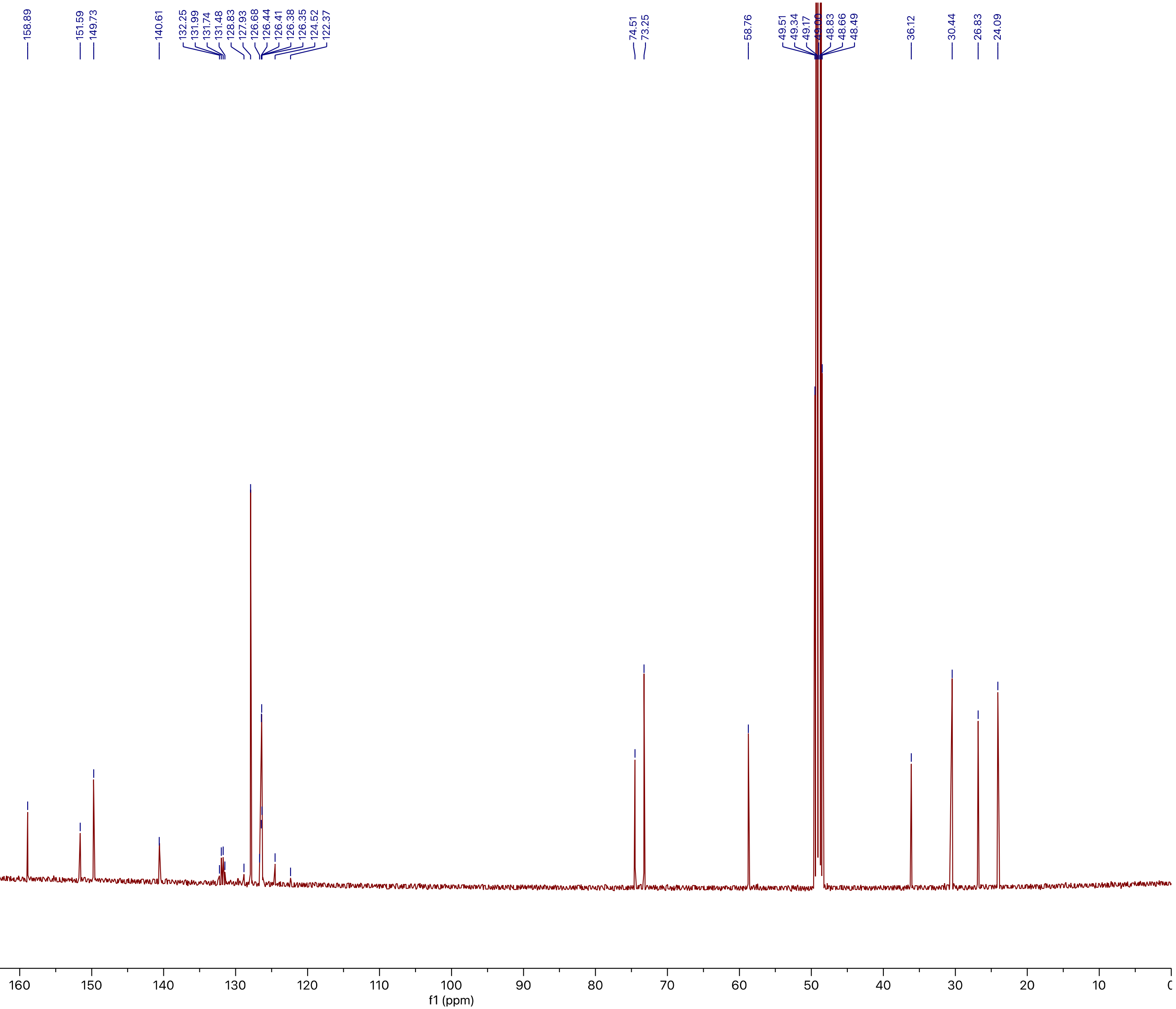


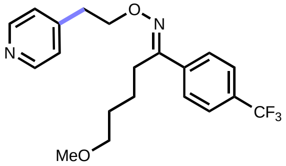
27
^{1}H NMR
(499 MHz, MeOD)



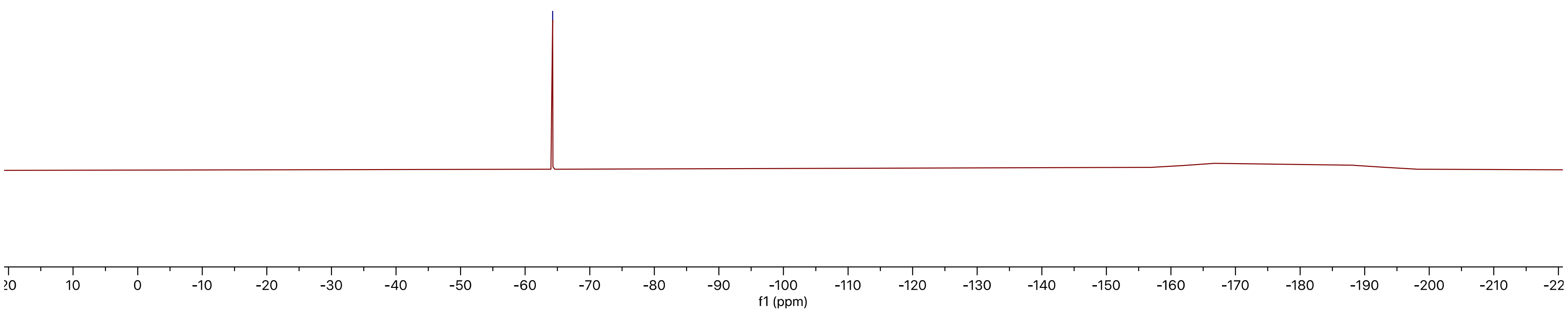


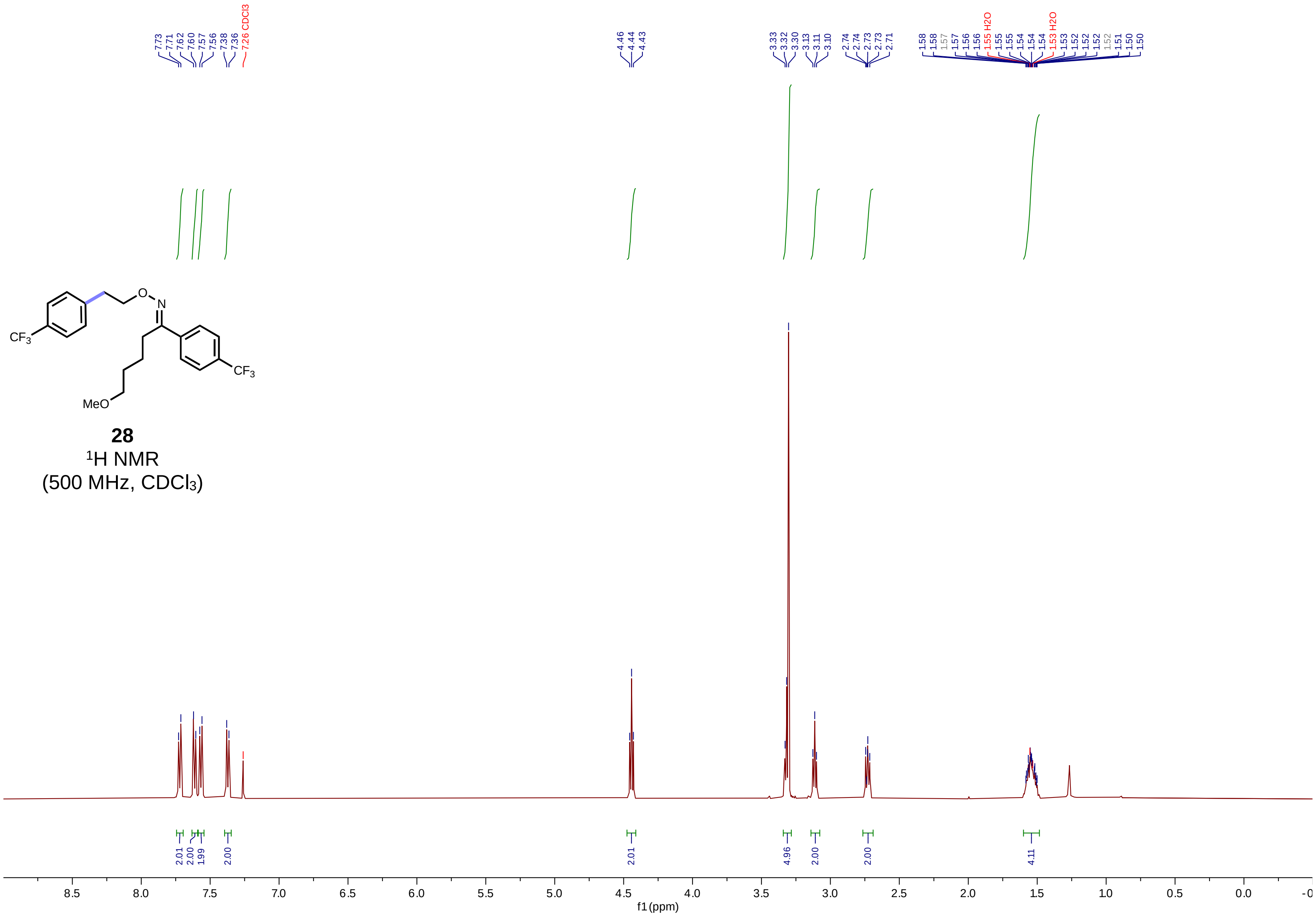
27
^{13}C NMR
(126 MHz, MeOD)



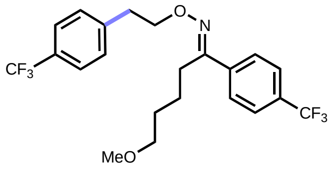


27
^{19}F NMR
(471 MHz, MeOD)





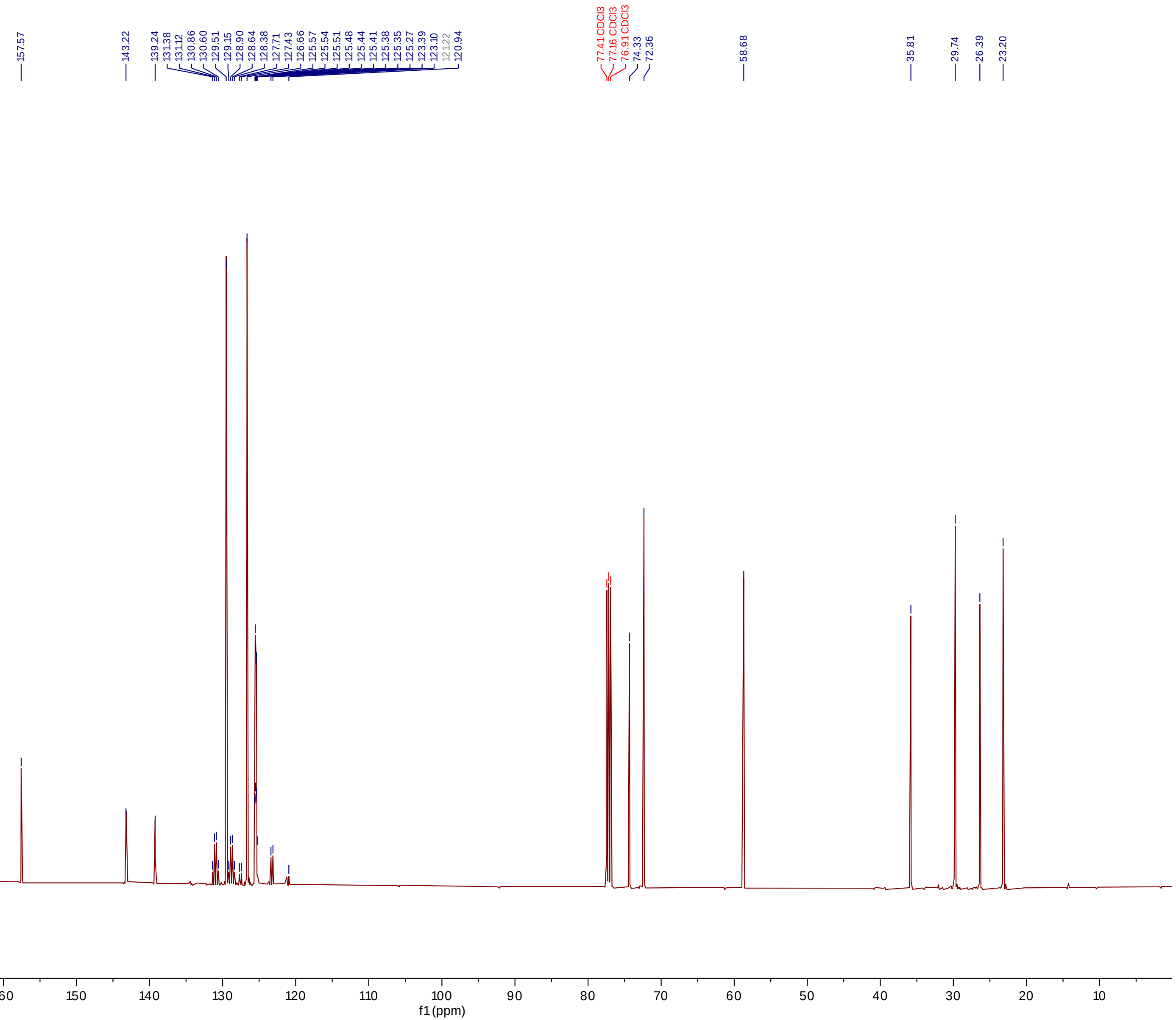
28
^{1}H NMR
(500 MHz, $CDCl_3$)

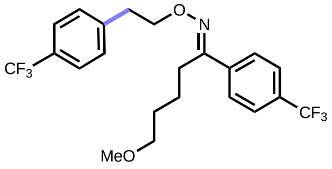


28

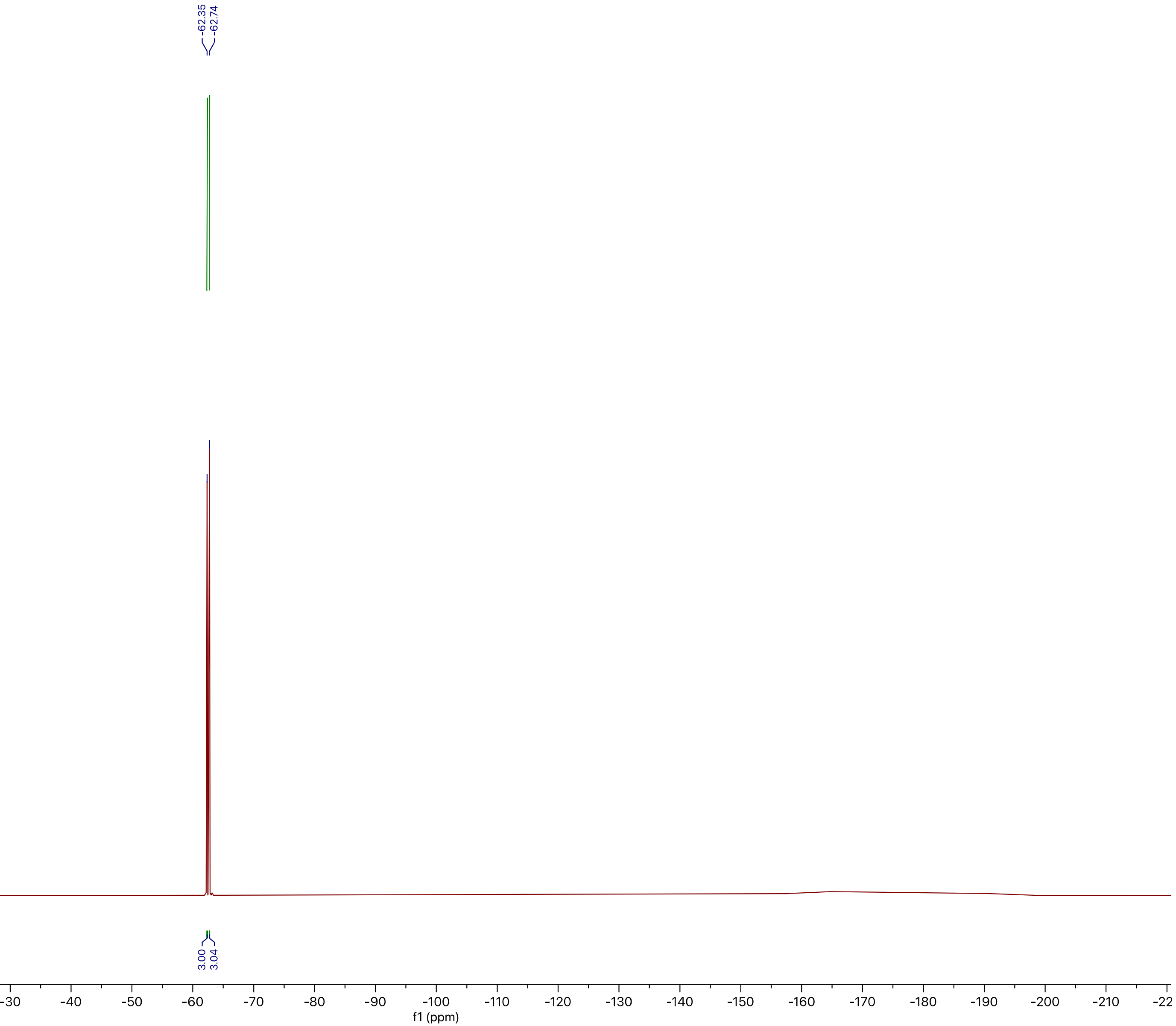
^{13}C NMR

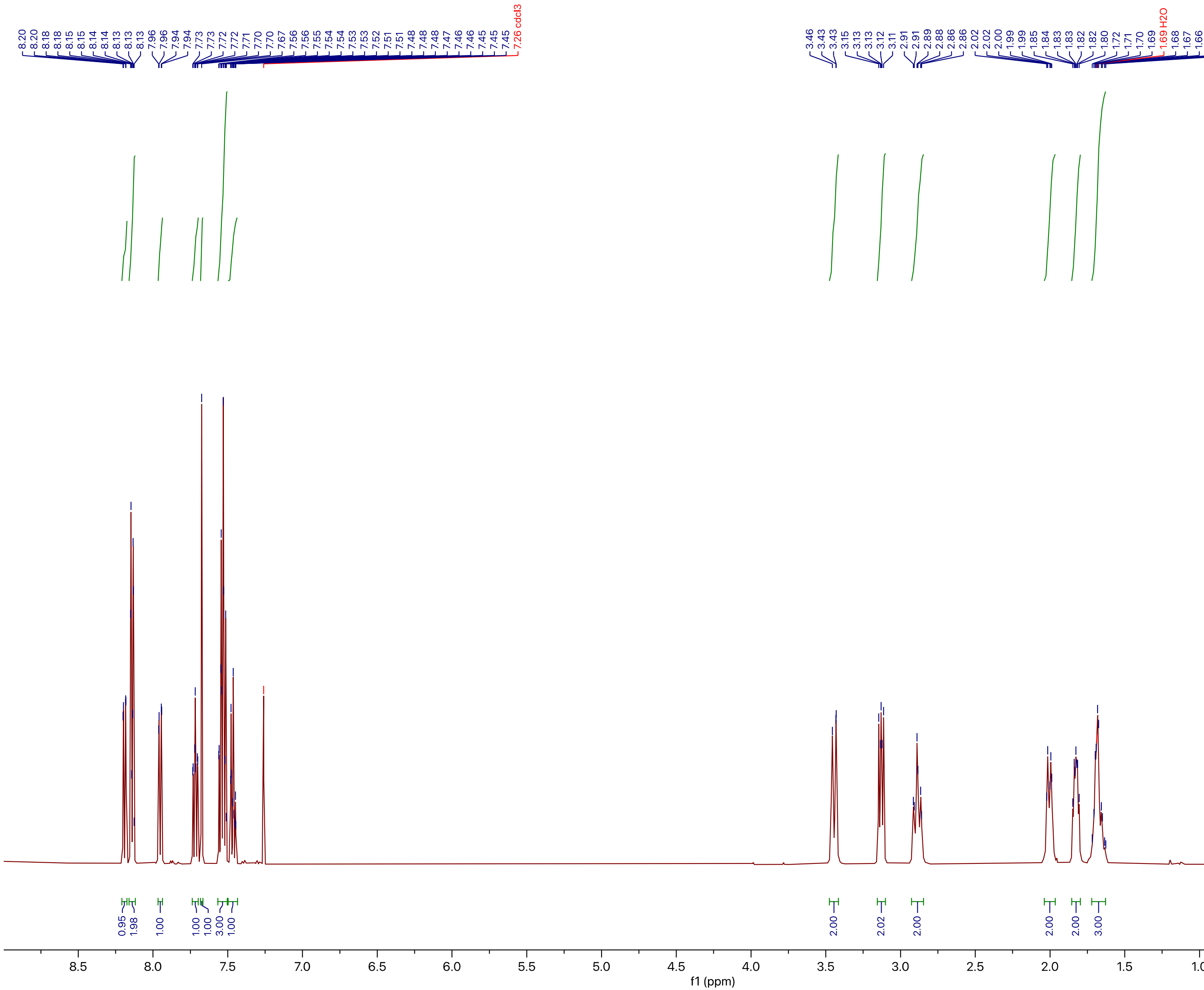
(126 MHz, $CDCl_3$)

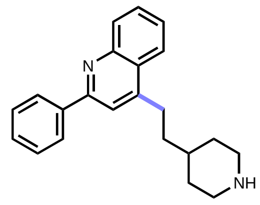




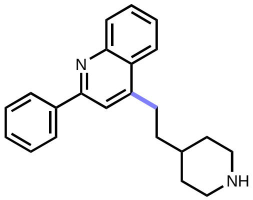
28
^{19}F NMR
(471 MHz, $CDCl_3$)



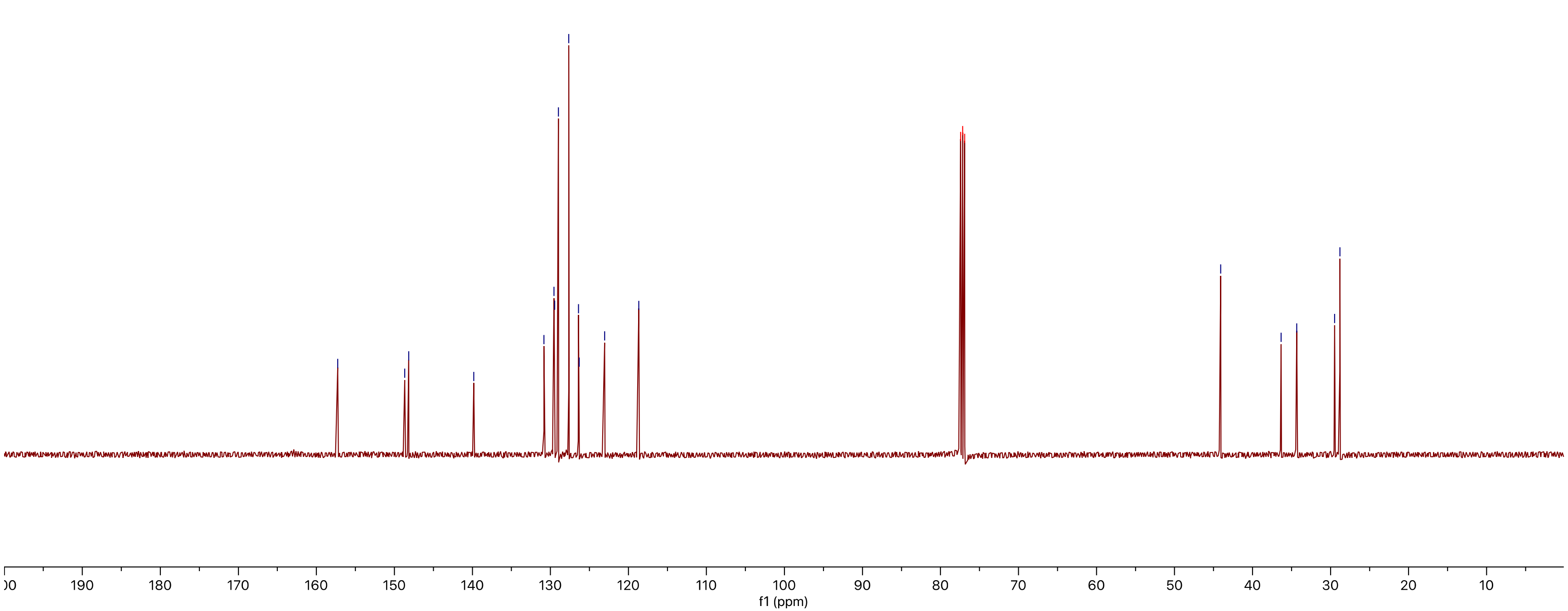


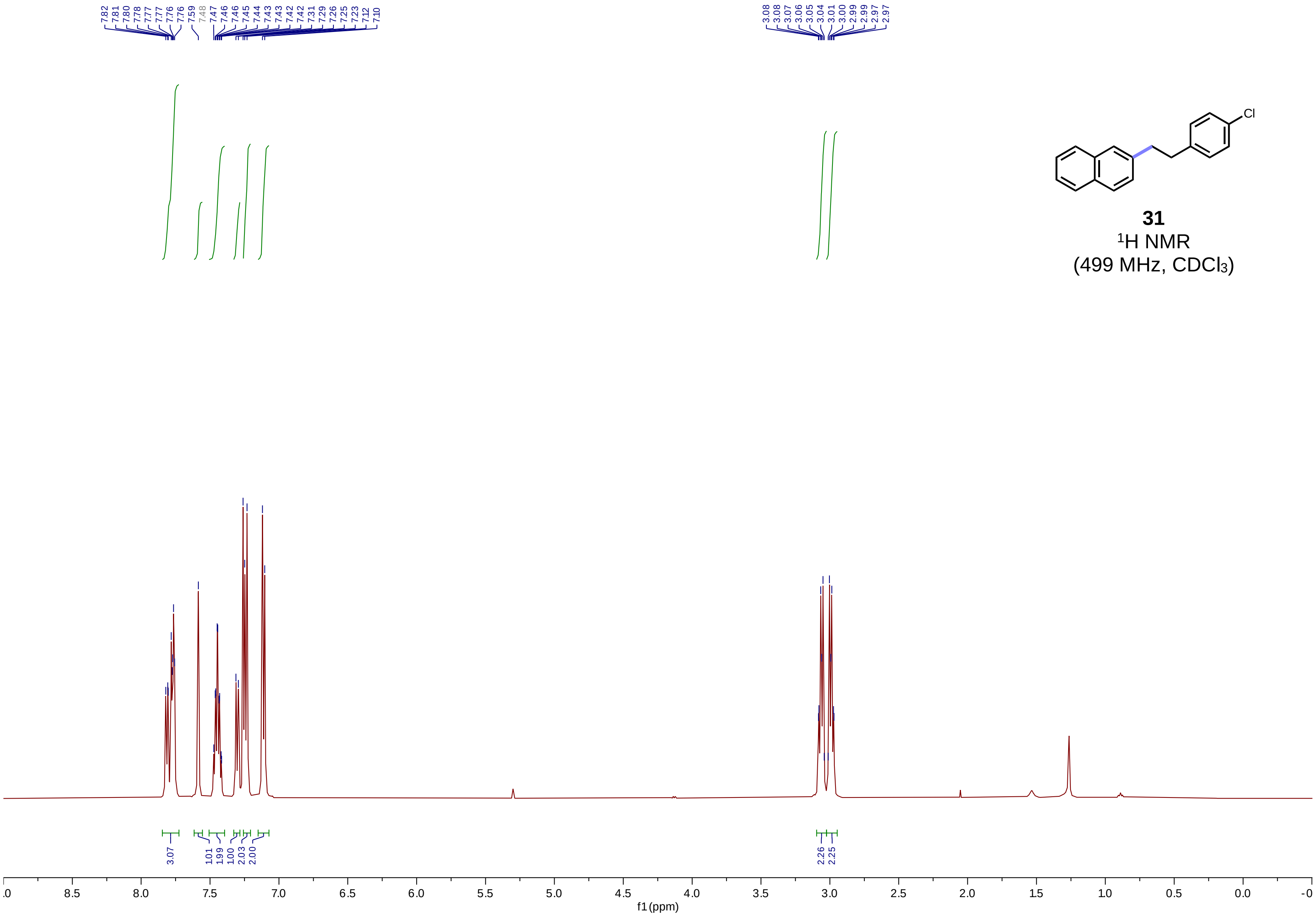


29
^{1}H NMR
(499 MHz, $CDCl_3$)

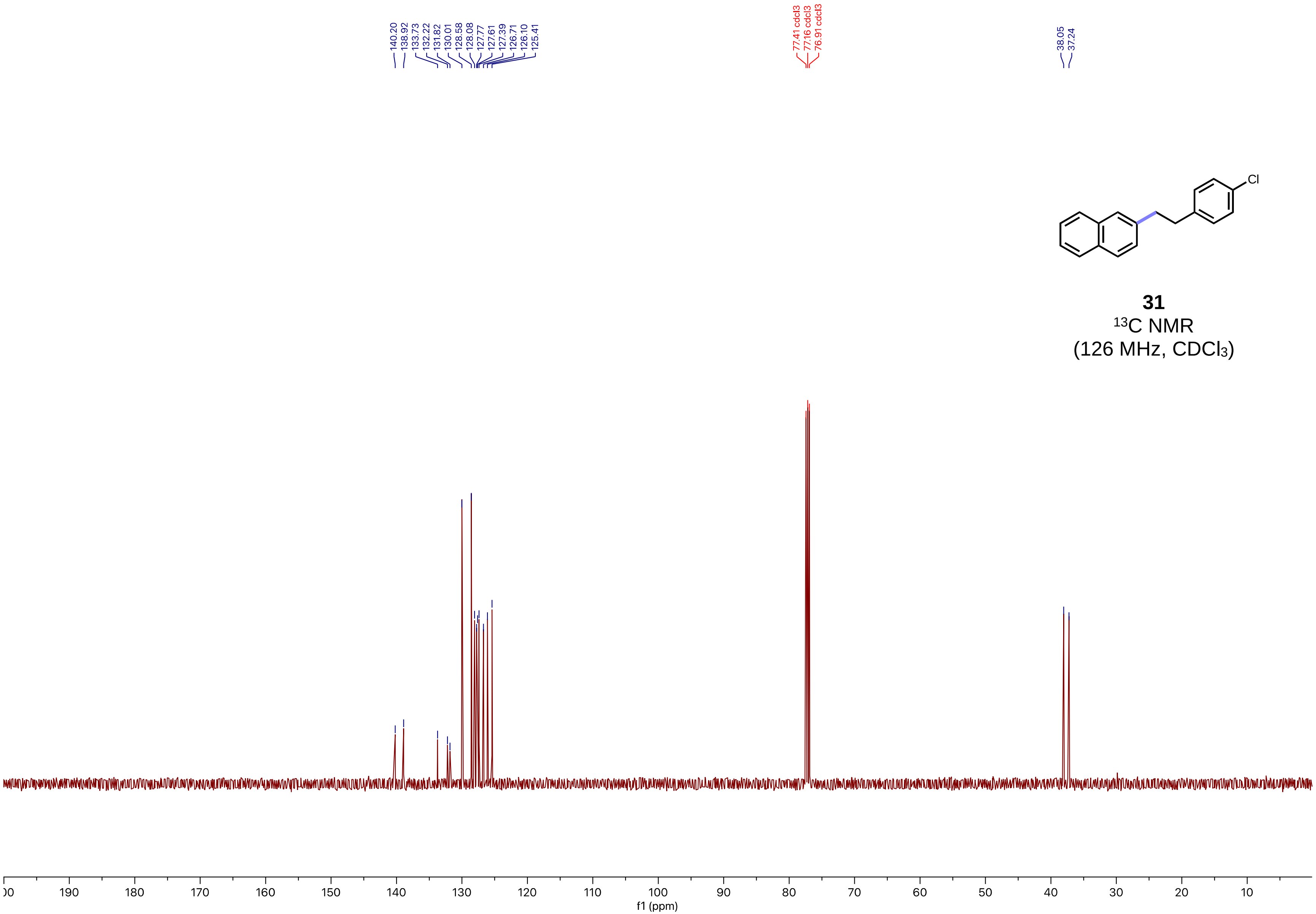


29
^{13}C NMR
(126 MHz, $CDCl_3$)

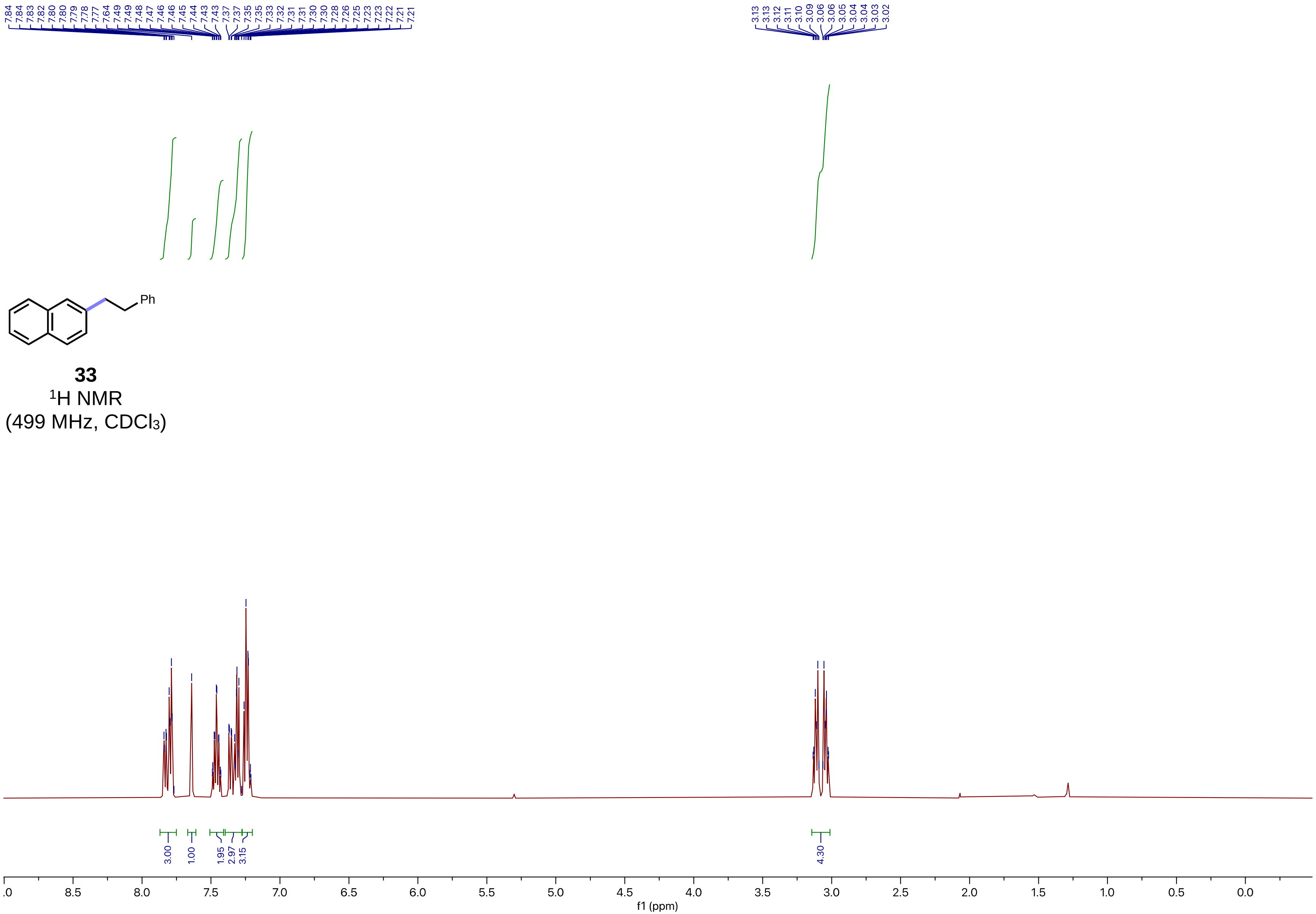




31
^{1}H NMR
(499 MHz, $CDCl_3$)



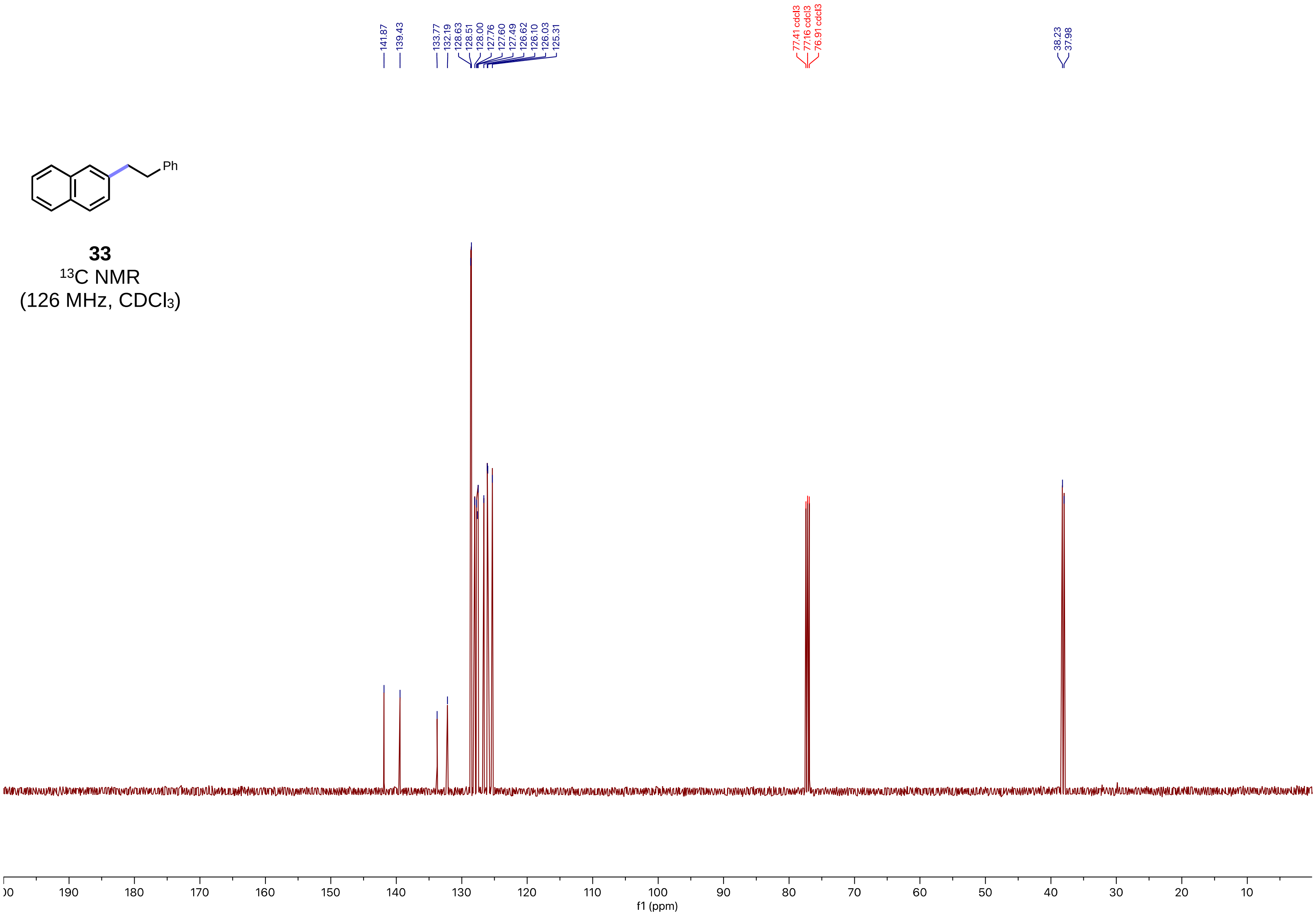
31
^{13}C NMR
(126 MHz, $CDCl_3$)



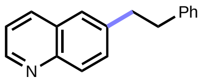
33

^{1}H NMR

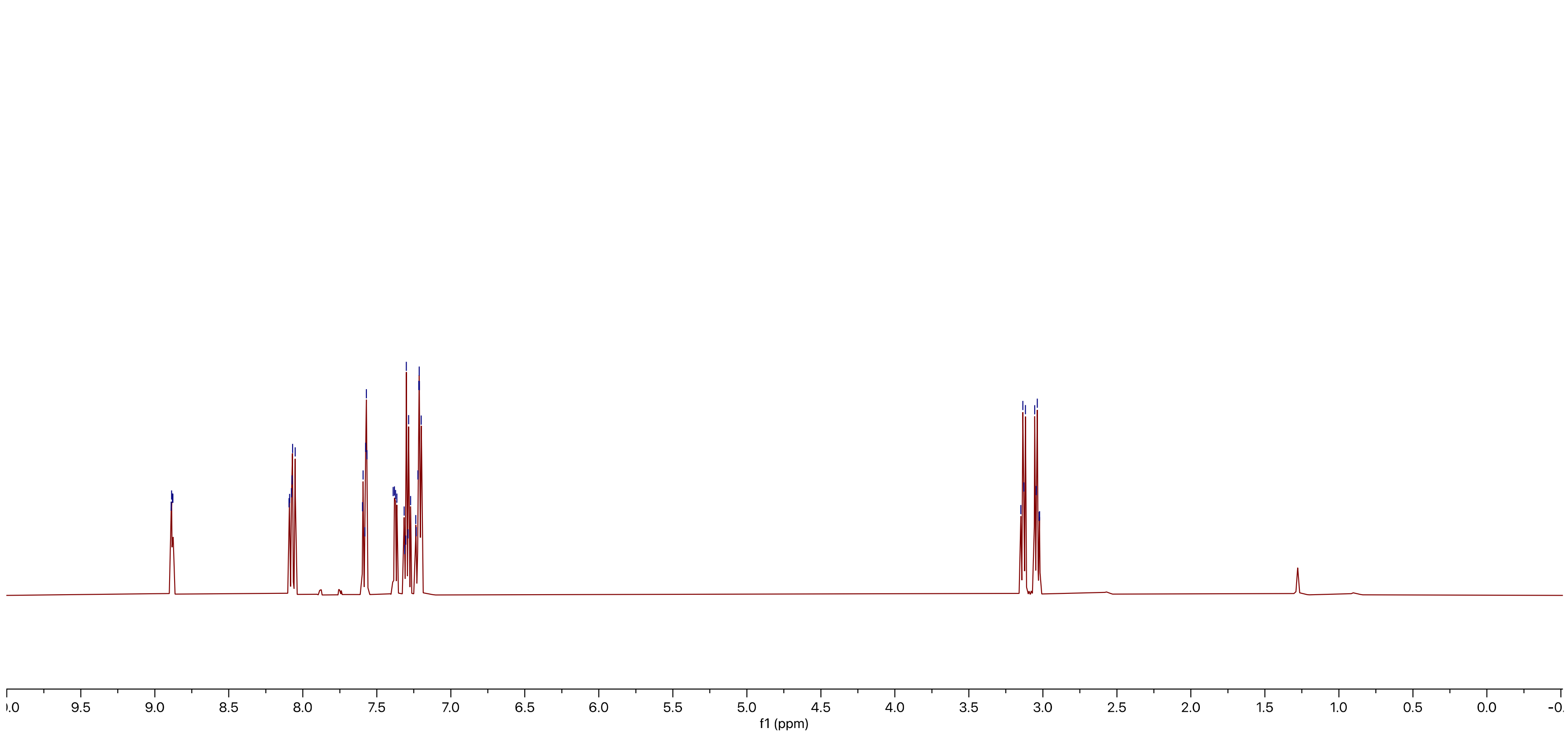
(499 MHz, $CDCl_3$)

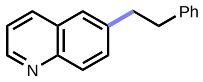


33
^{13}C NMR
(126 MHz, $CDCl_3$)



34
^{1}H NMR
(499 MHz, $CDCl_3$)

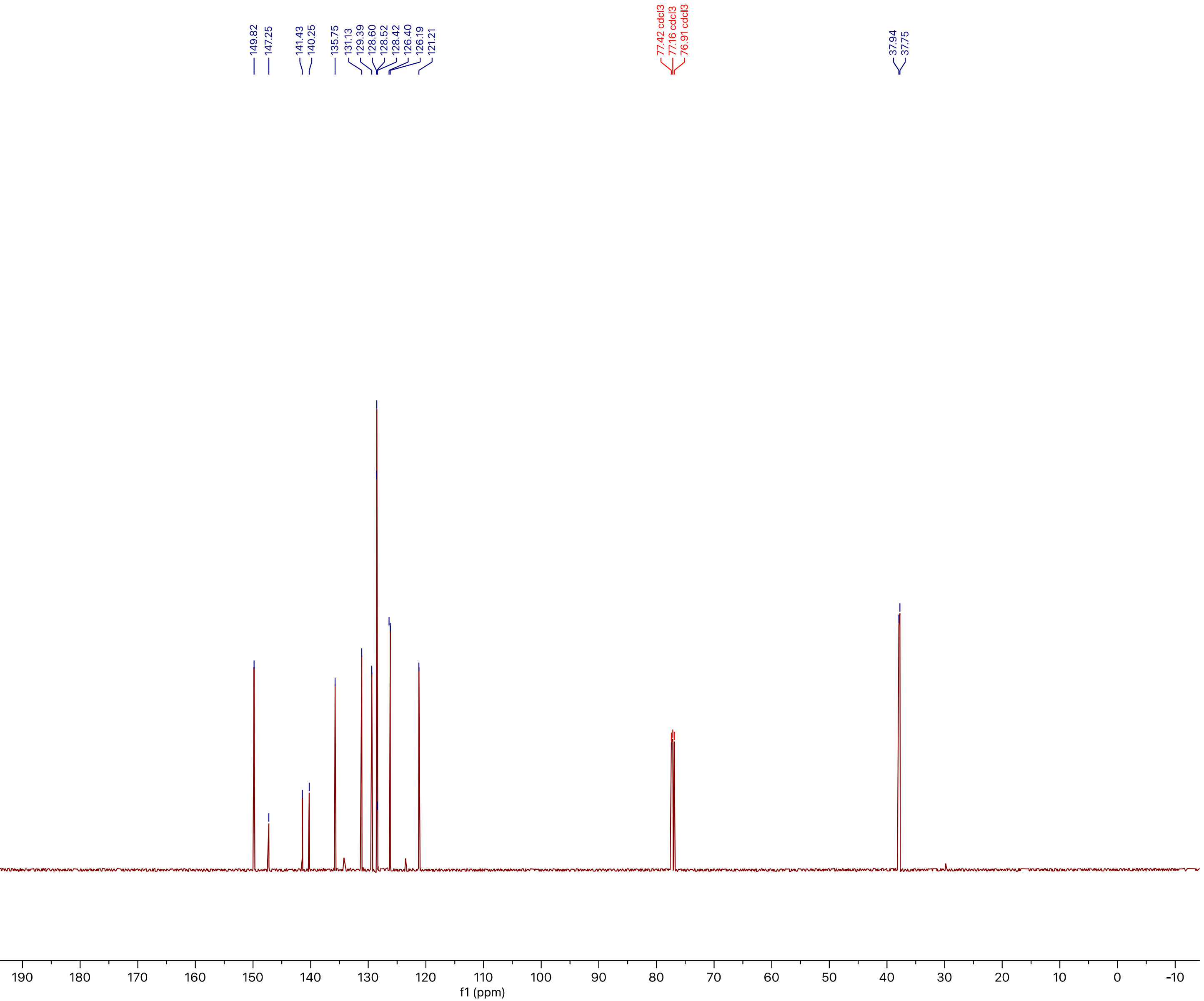


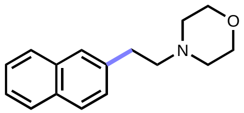


34

^{13}C NMR

(126 MHz, $CDCl_3$)

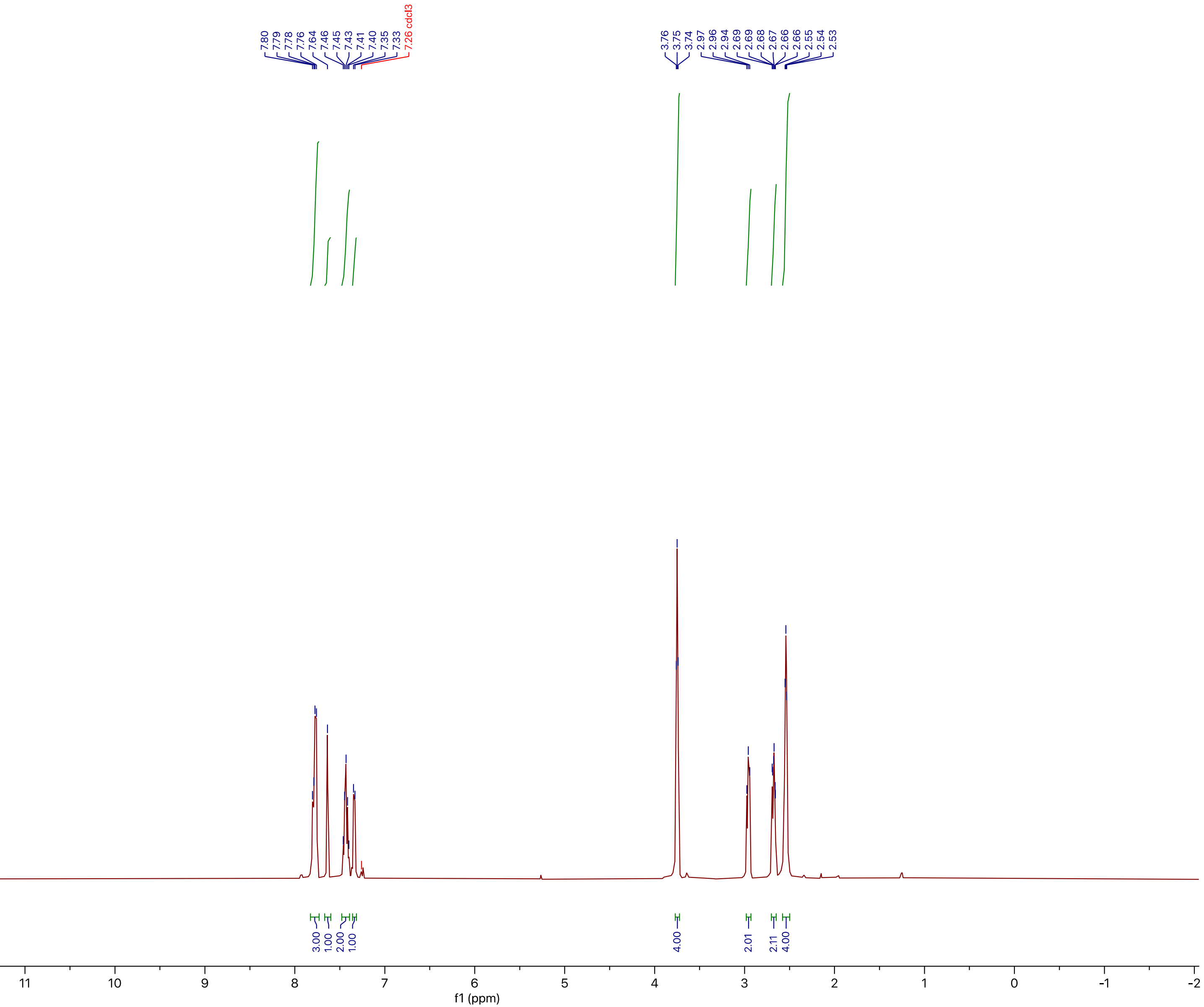


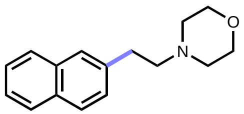


35

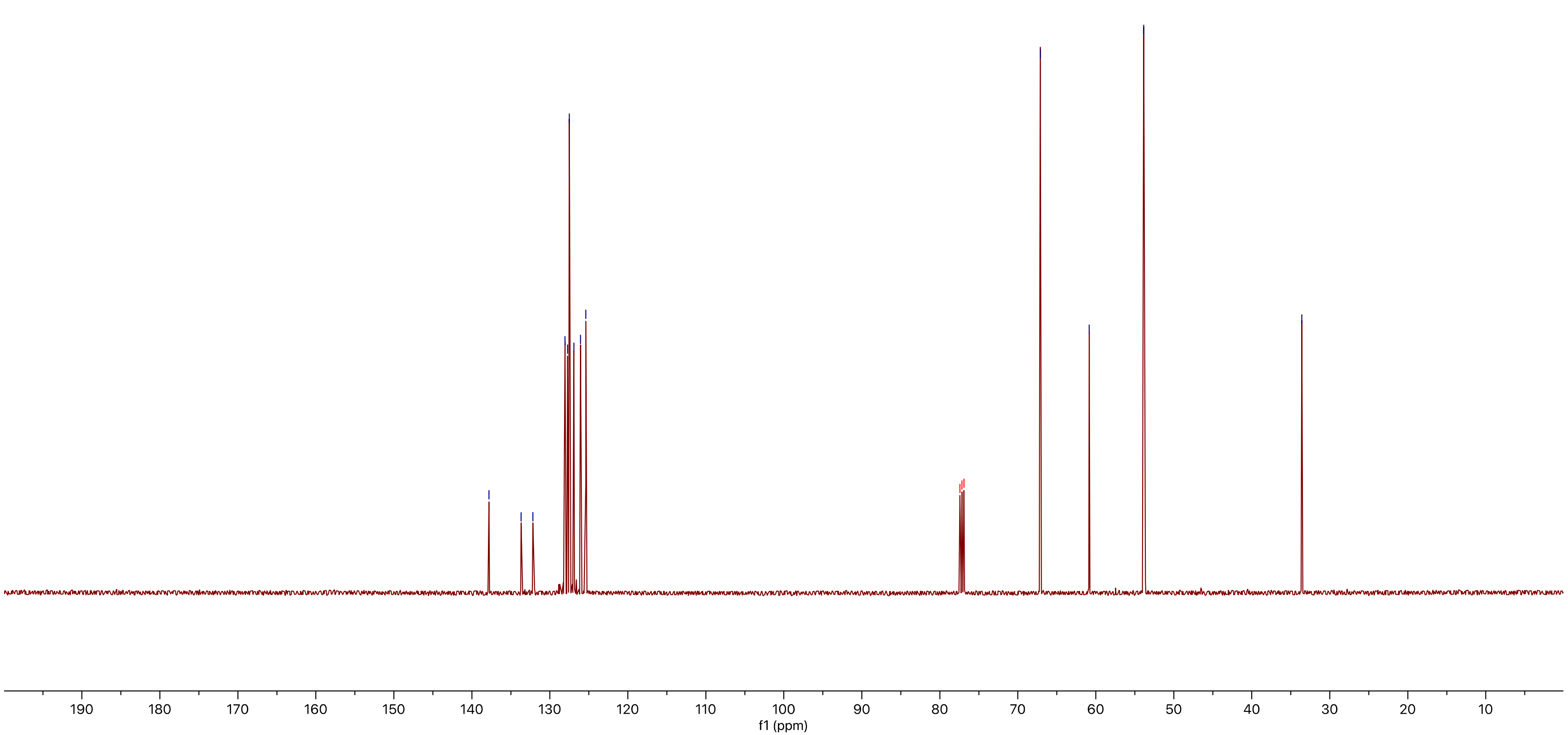
^{1}H NMR

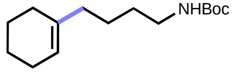
(499 MHz, $CDCl_3$)





35
^{13}C NMR
(126 MHz, $CDCl_3$)

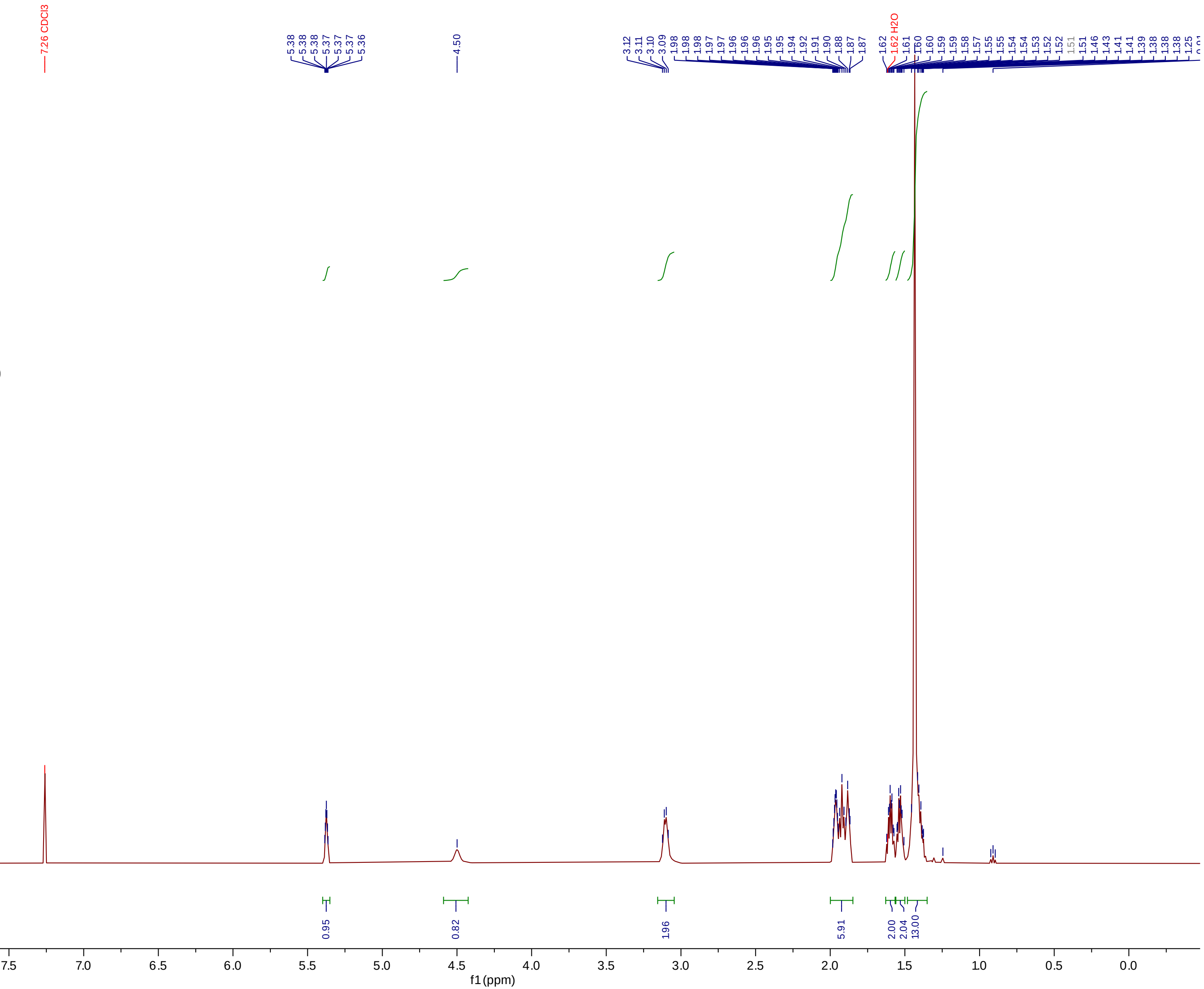


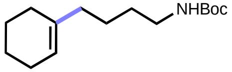


36

^{1}H NMR

(500 MHz, $CDCl_3$)

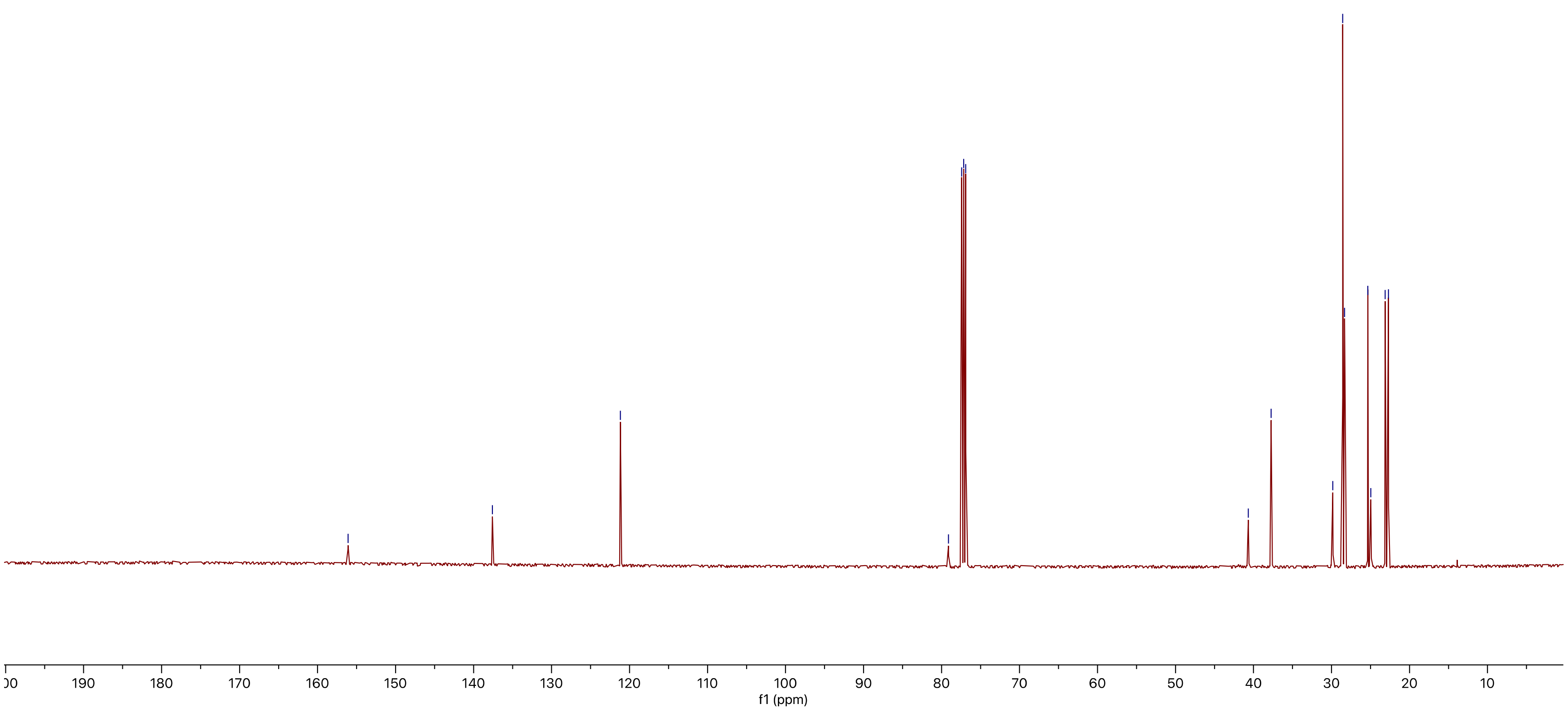


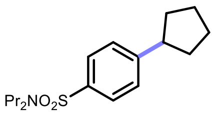


36

^{13}C NMR

(126 MHz, $CDCl_3$)

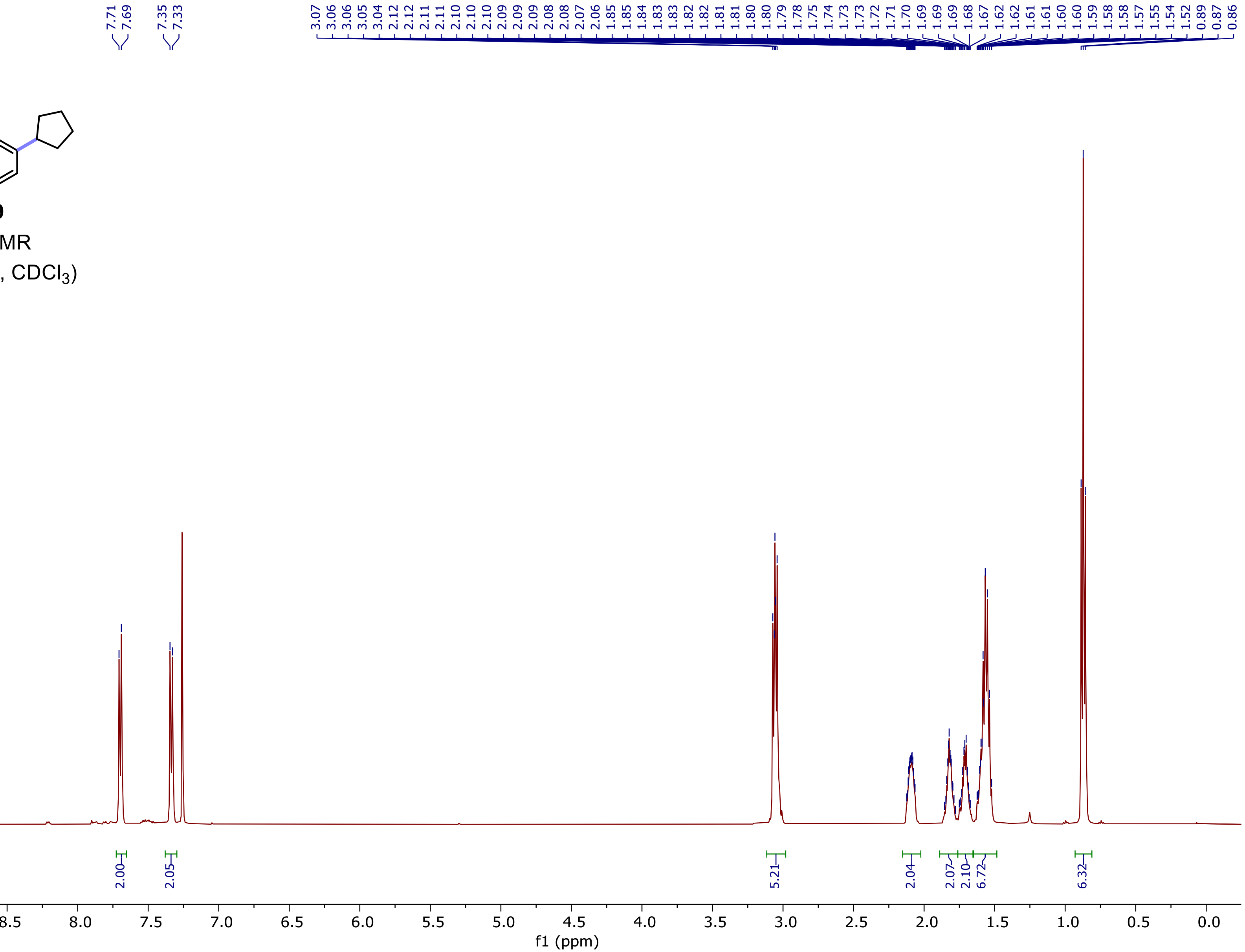


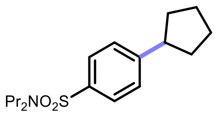


39

^1H NMR

(500 MHz, $CDCl_3$)

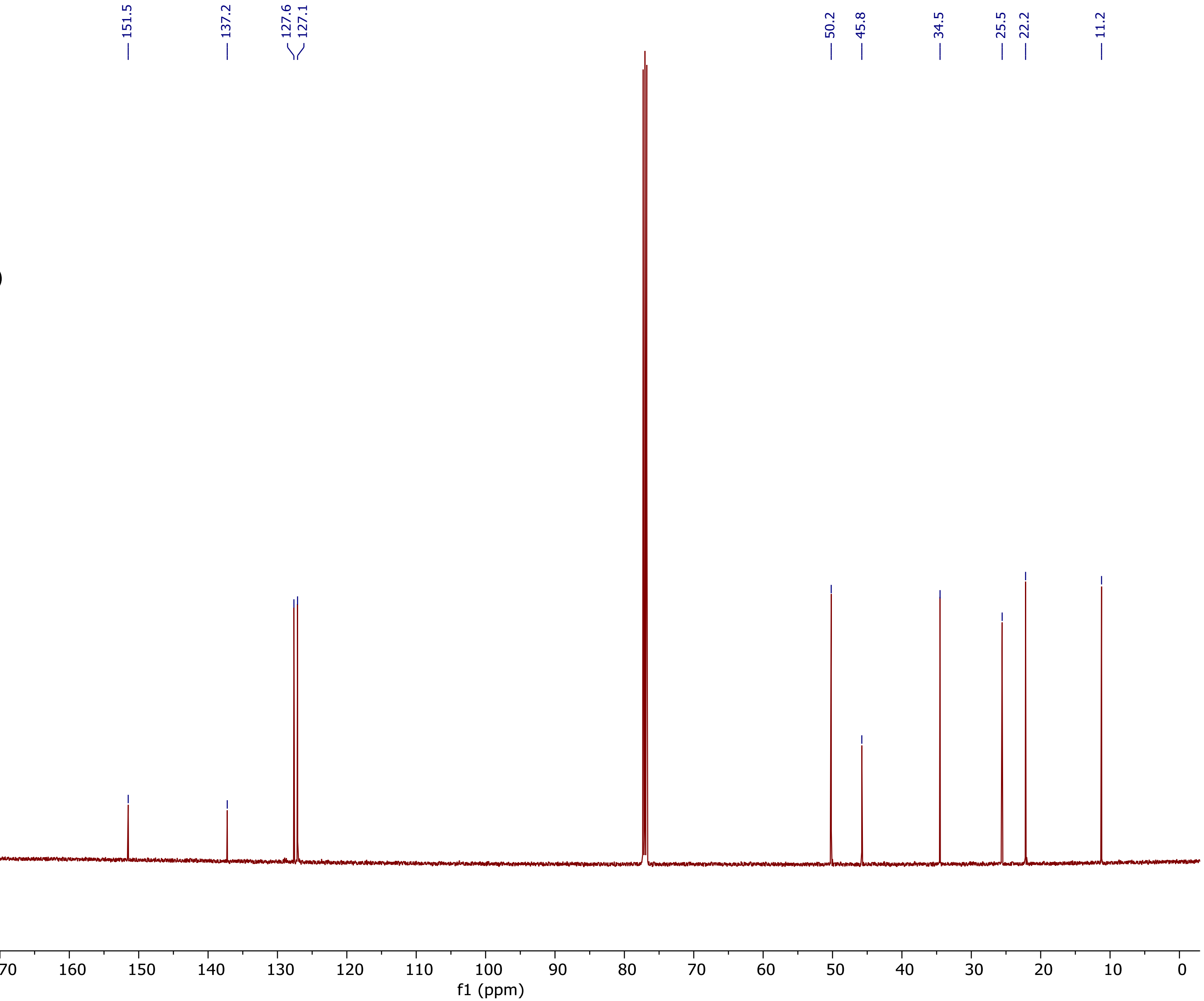


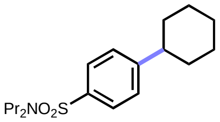


39

^{13}C NMR

(126 MHz, $CDCl_3$)

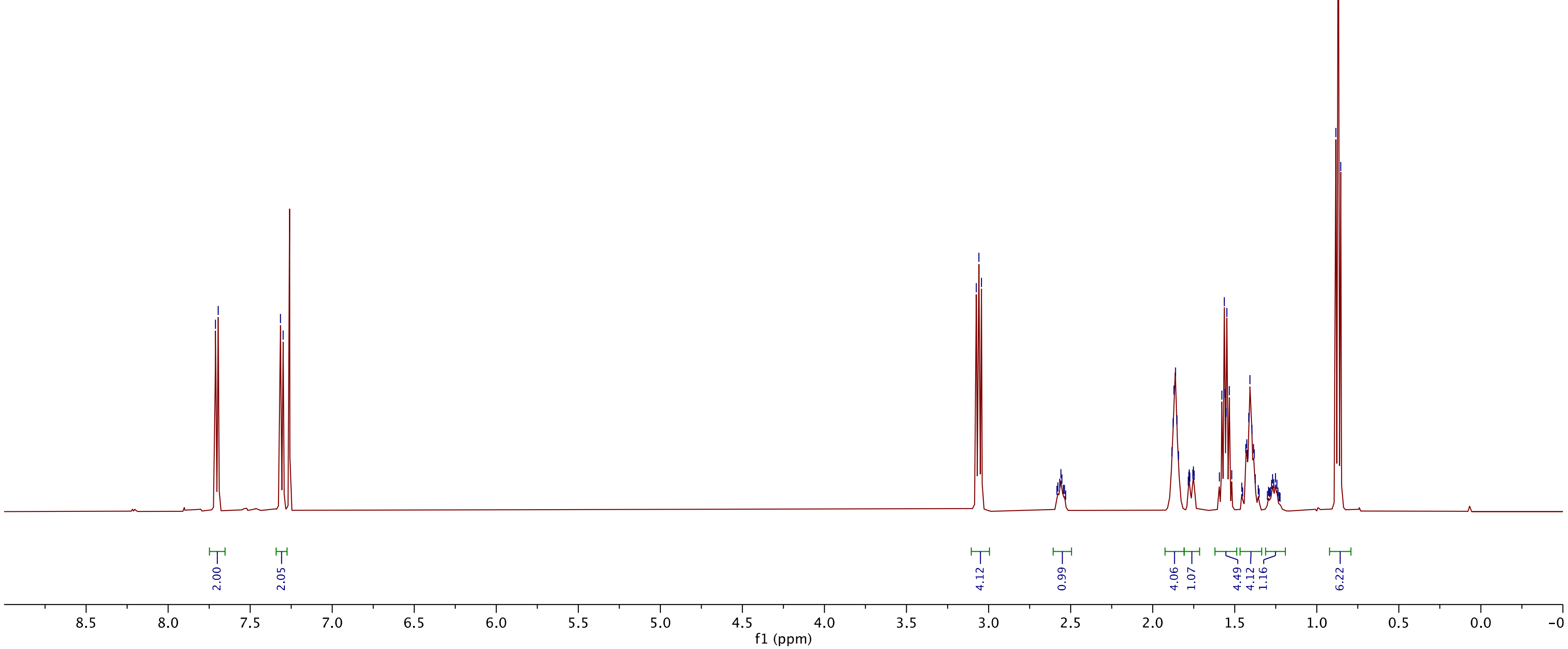


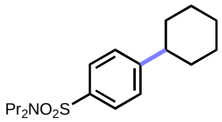


40

^{1}H NMR

(500 MHz, $CDCl_3$)

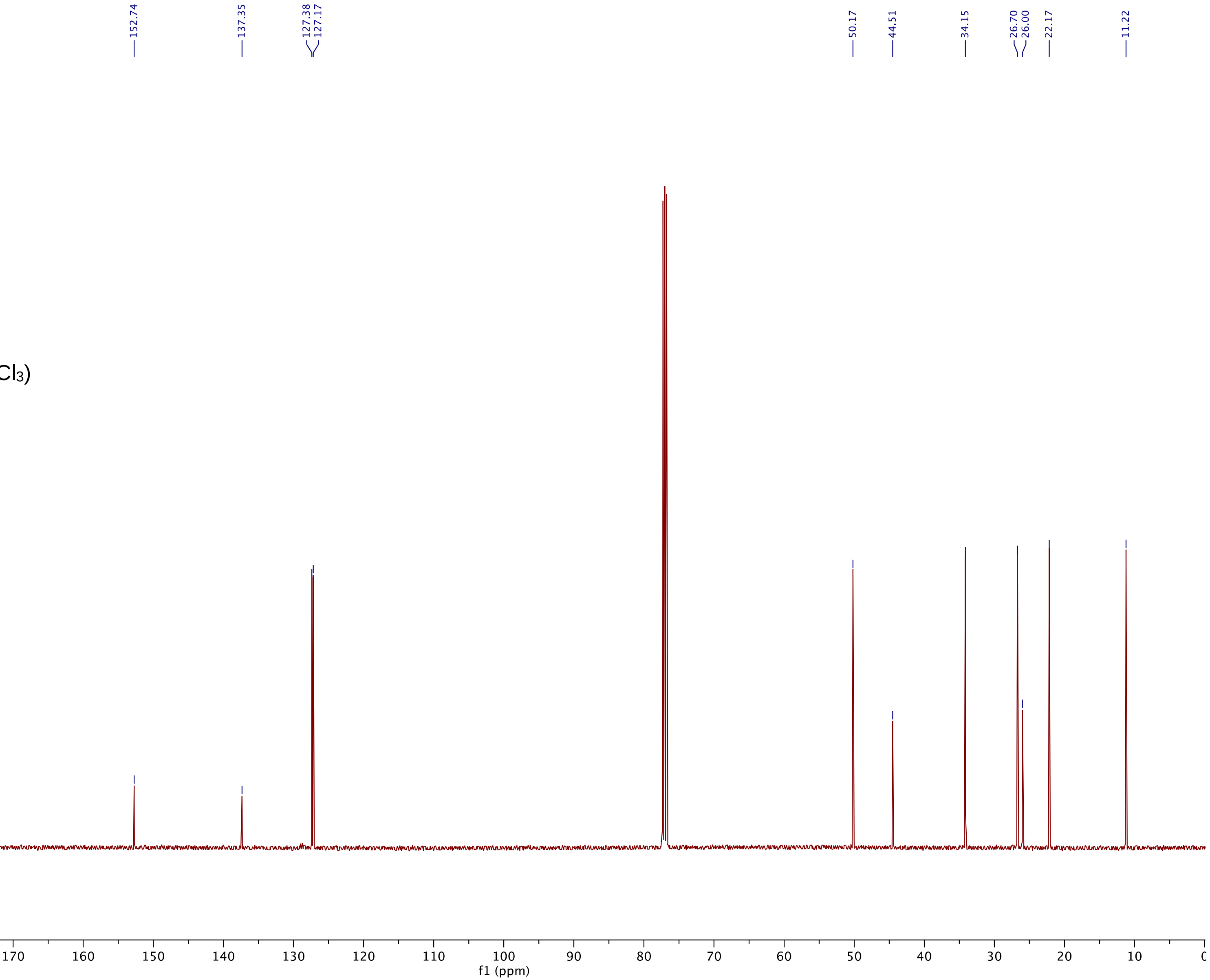


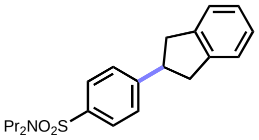


40

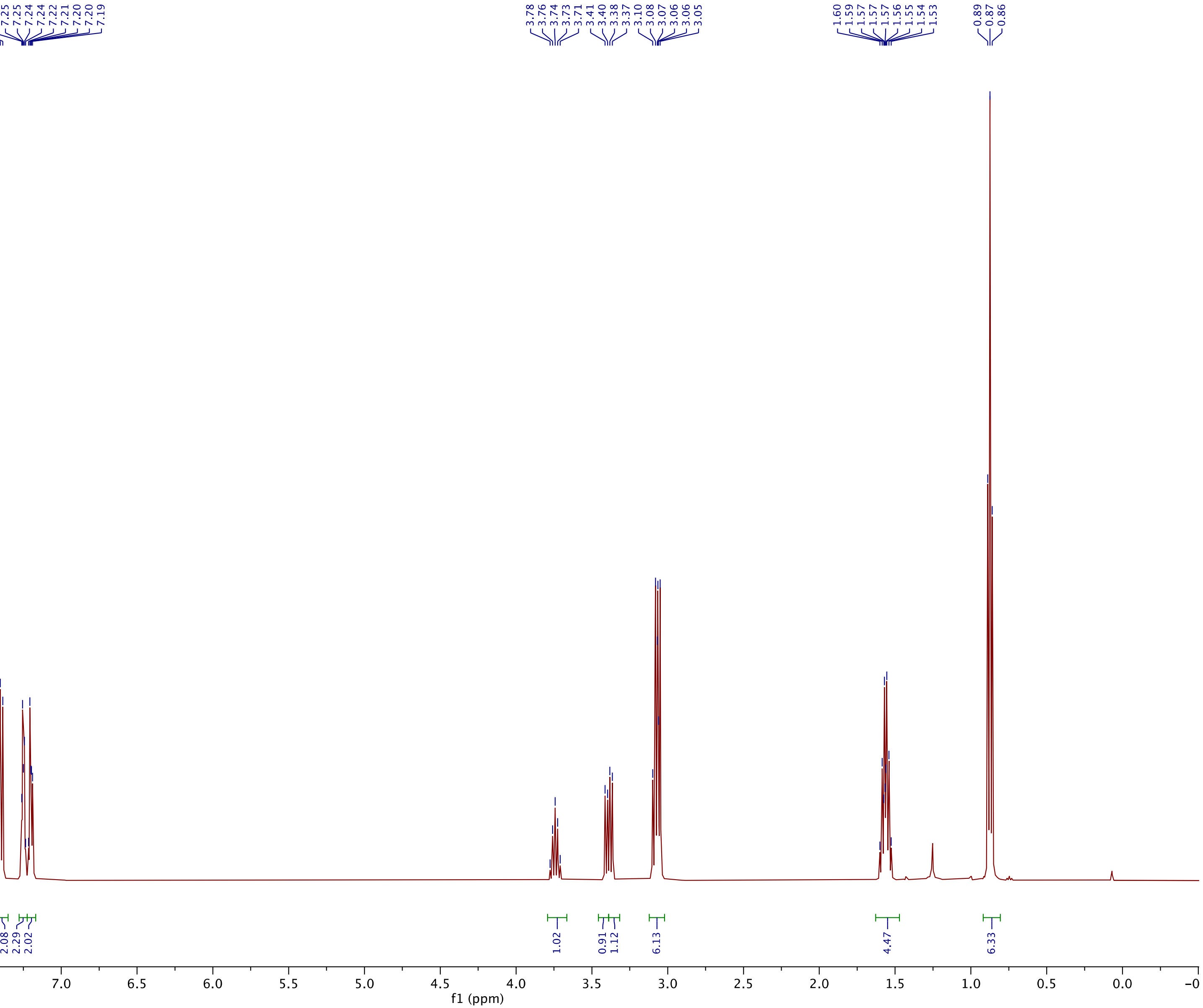
^{13}C NMR

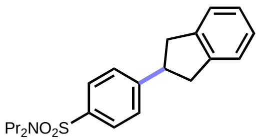
(126 MHz, $CDCl_3$)



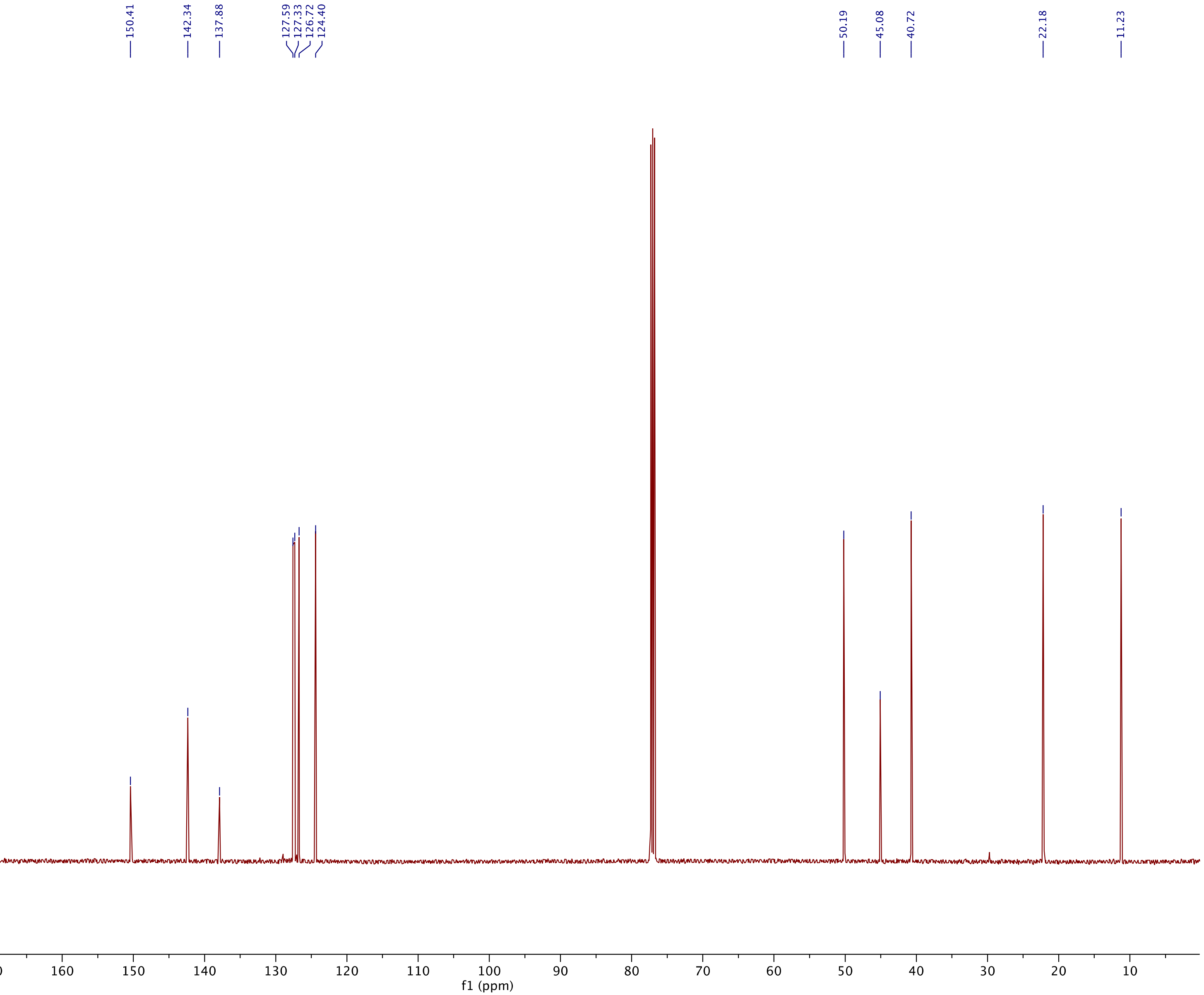


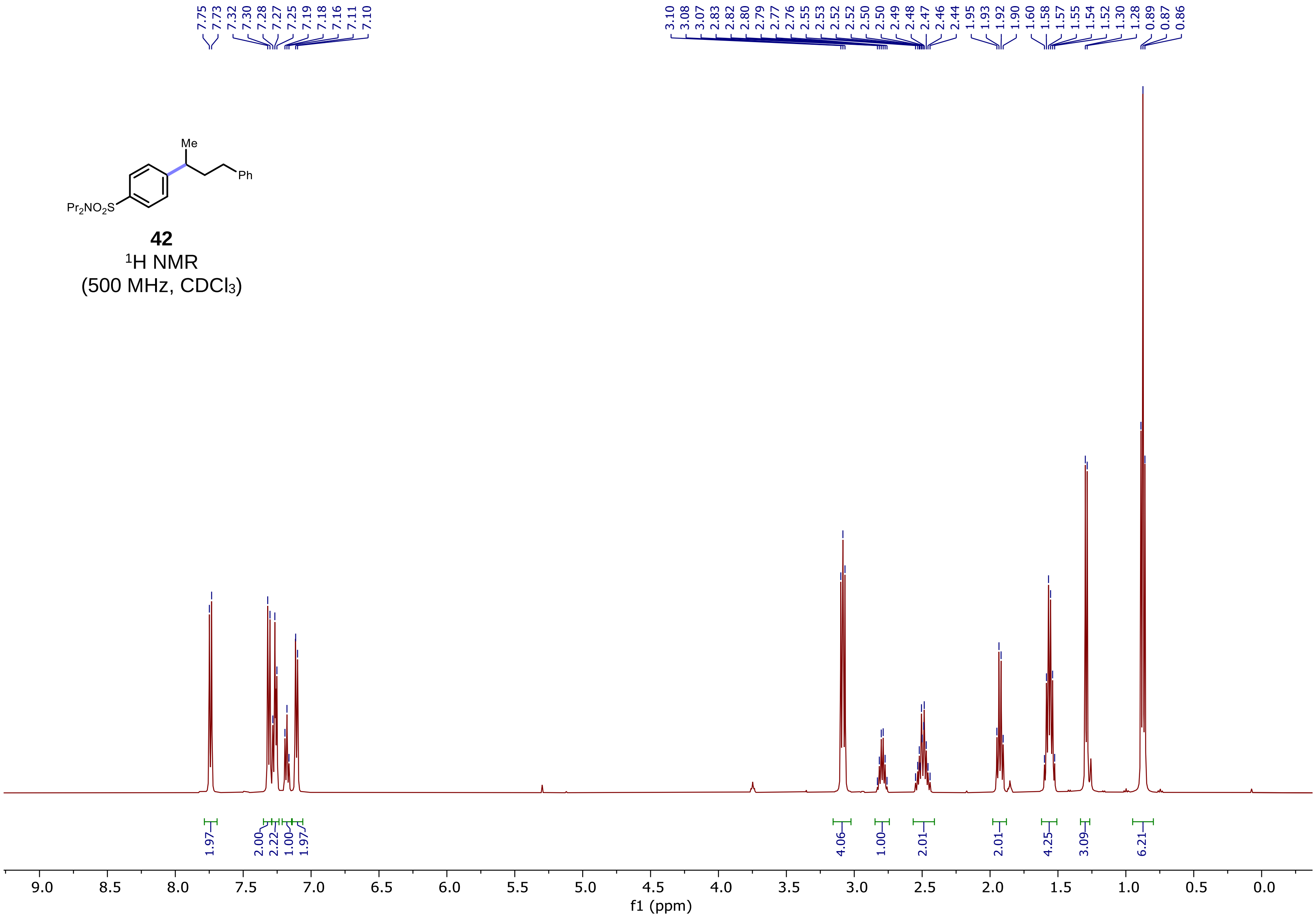
41
^1H NMR
(500 MHz, $CDCl_3$)

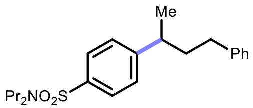




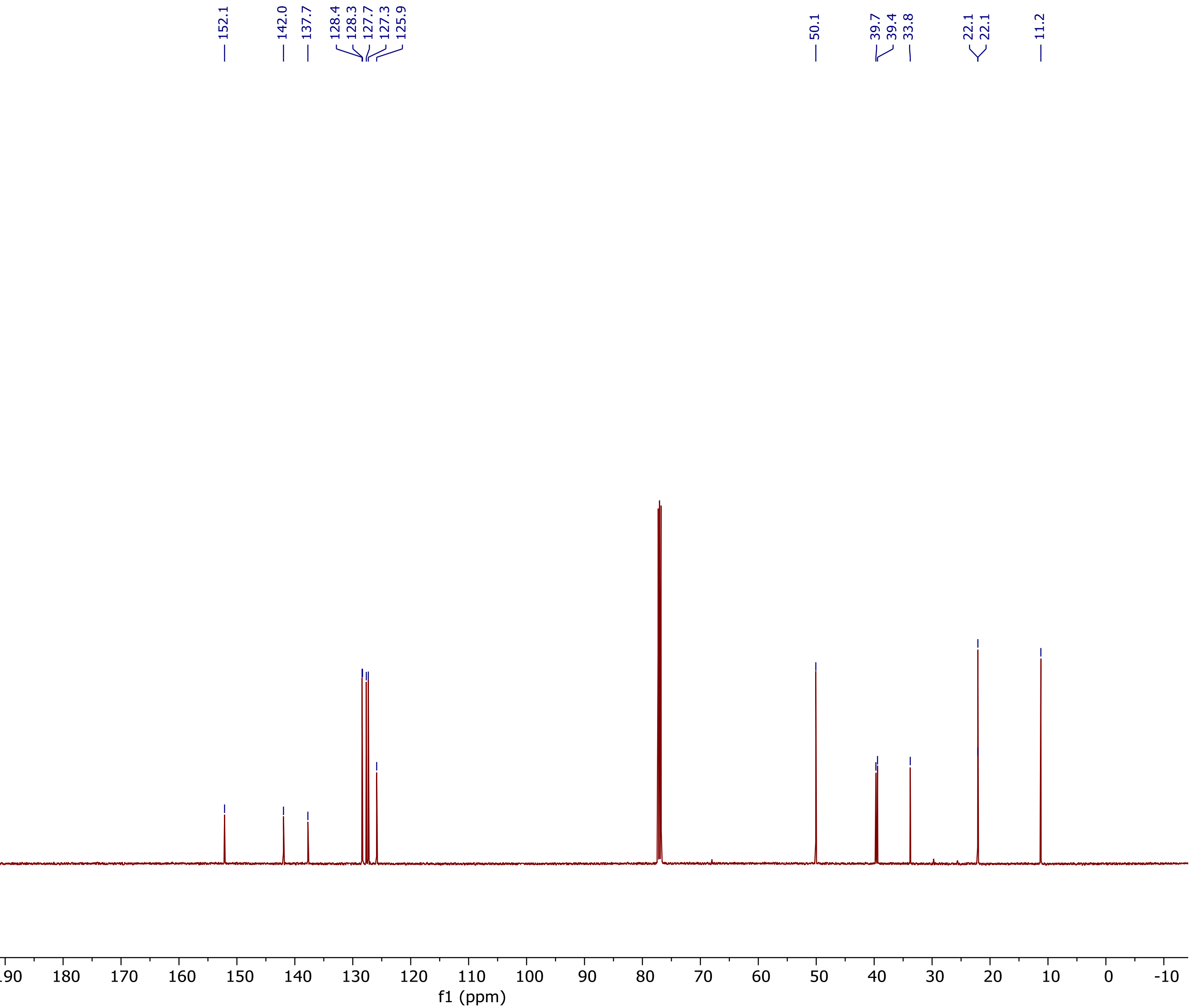
41
^{13}C NMR
(126 MHz, $CDCl_3$)

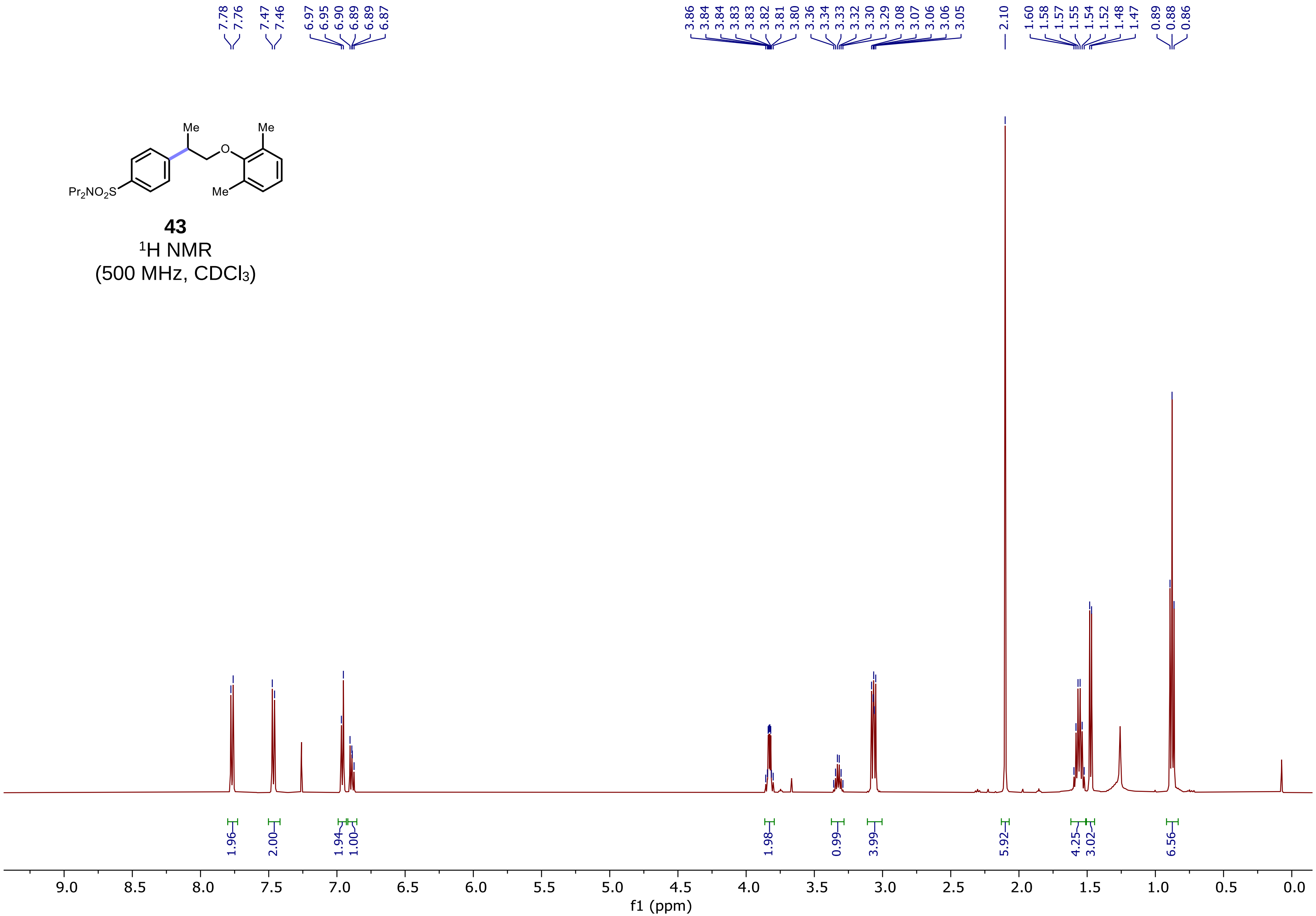


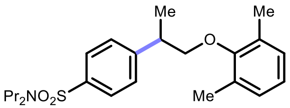

Me
Ph
Pr2NO2S
42
1H NMR
(500 MHz, CDCl3)
7.75
7.73
7.32
7.30
7.28
7.27
7.25
7.19
7.18
7.16
7.11
7.10
3.10
3.08
3.07
2.83
2.82
2.80
2.79
2.77
2.76
2.55
2.53
2.52
2.50
2.50
2.49
2.48
2.47
2.46
2.44
1.95
1.93
1.92
1.90
1.60
1.58
1.57
1.55
1.54
1.52
1.30
1.28
0.89
0.87
0.86
1.97
2.00
2.22
1.00
1.97
4.06
1.00
2.01
2.01
4.25
3.09
6.21
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)



42
^{13}C NMR
(126 MHz, $CDCl_3$)

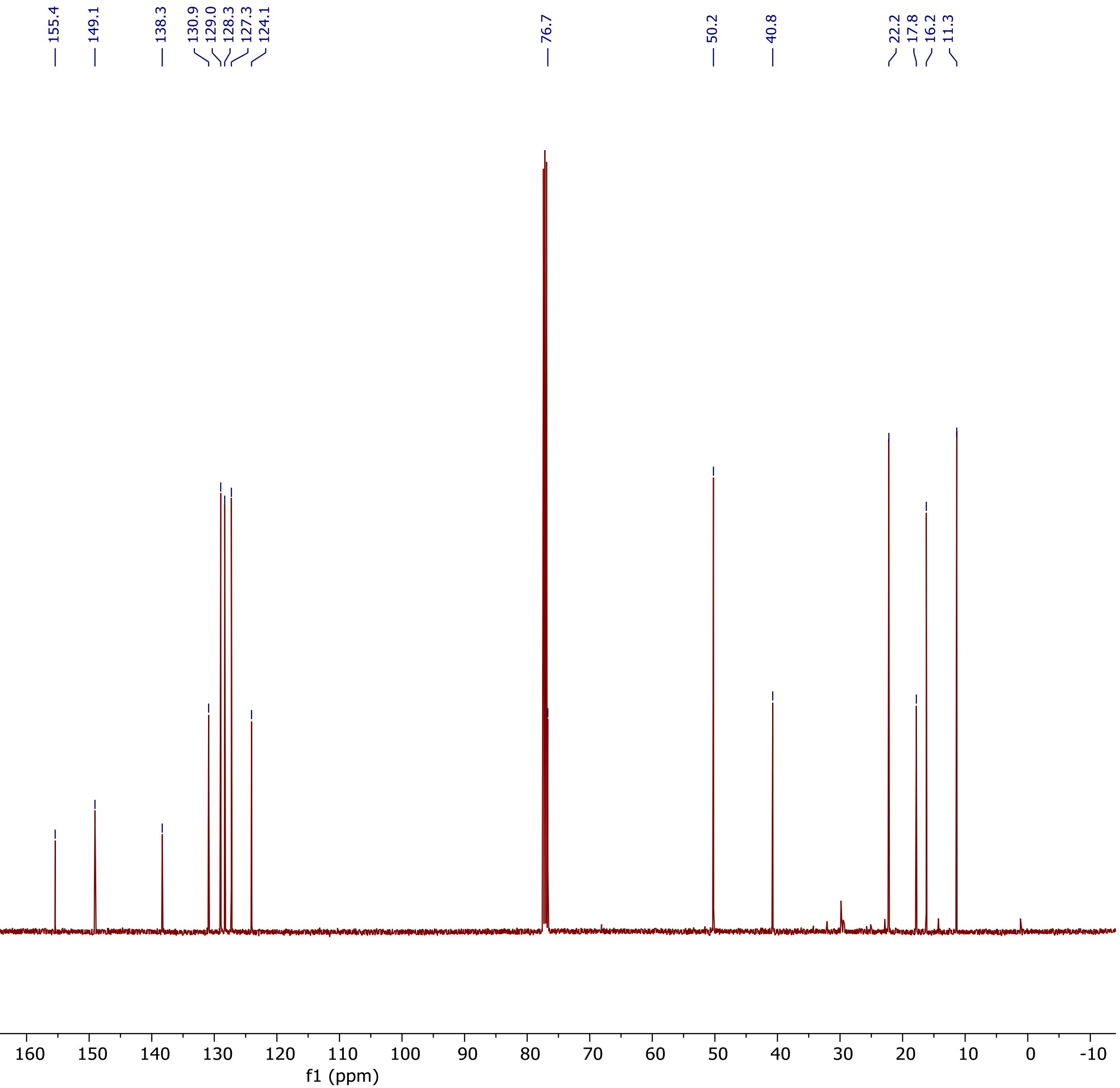


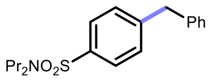

Me
Me
O
Pr$_2$NO$_2$S
Me
43
^{1}H NMR
(500 MHz, $CDCl_3$)
f1 (ppm)



43

^{13}C NMR
(126 MHz, $CDCl_3$)

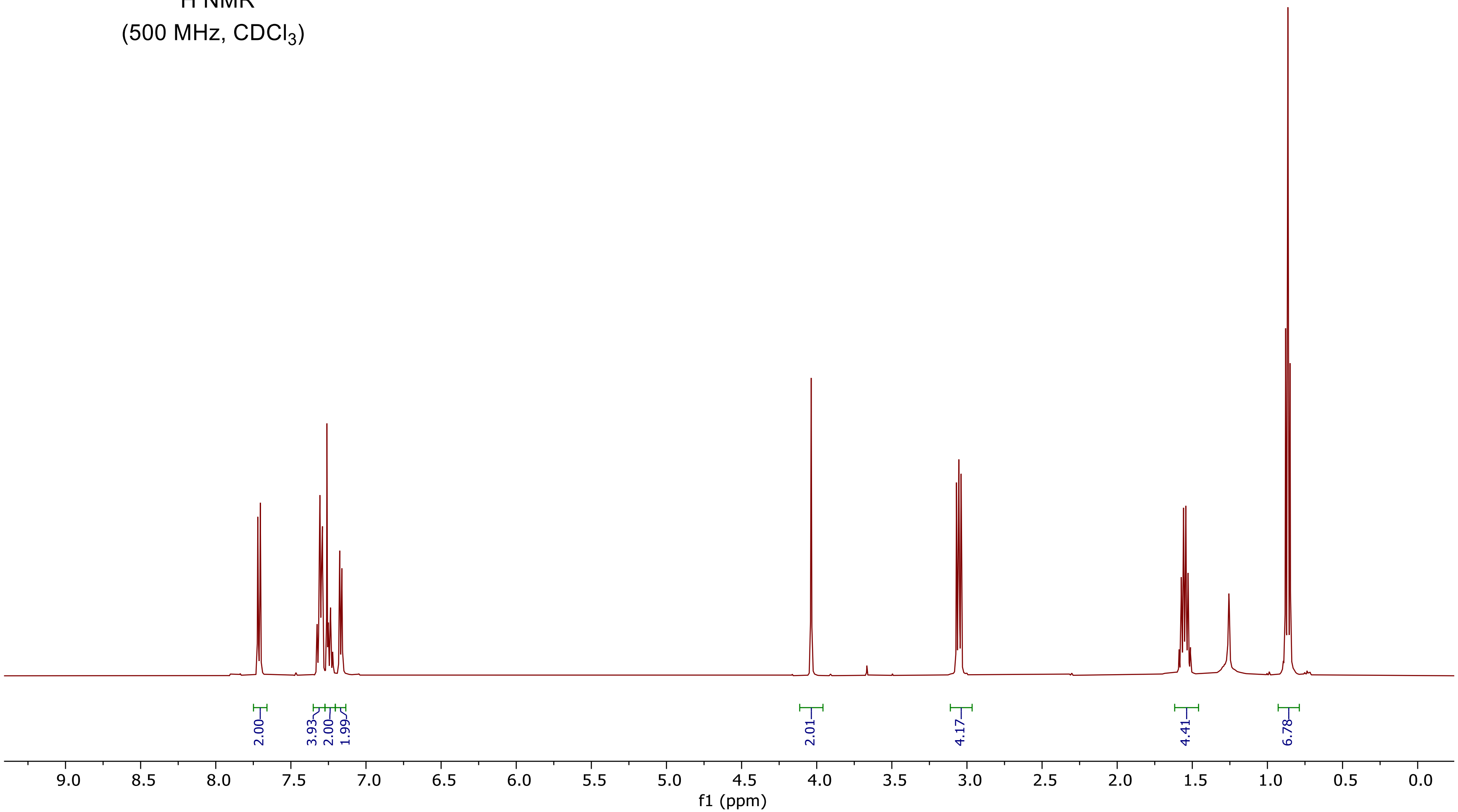


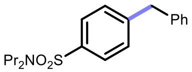


44

^{1}H NMR

(500 MHz, $CDCl_3$)

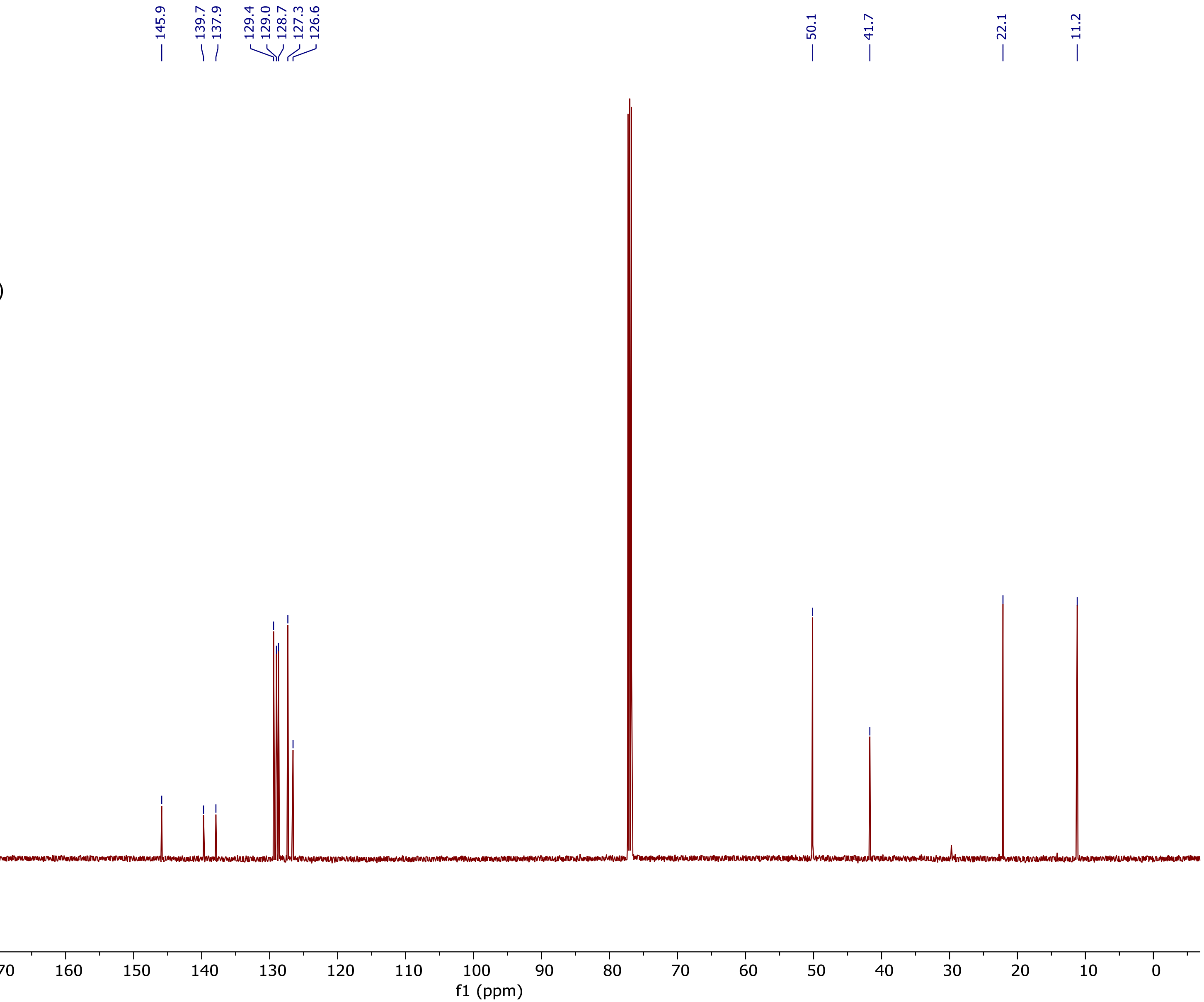




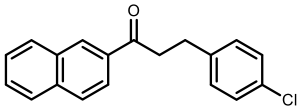
44

^{13}C NMR

(126 MHz, $CDCl_3$)



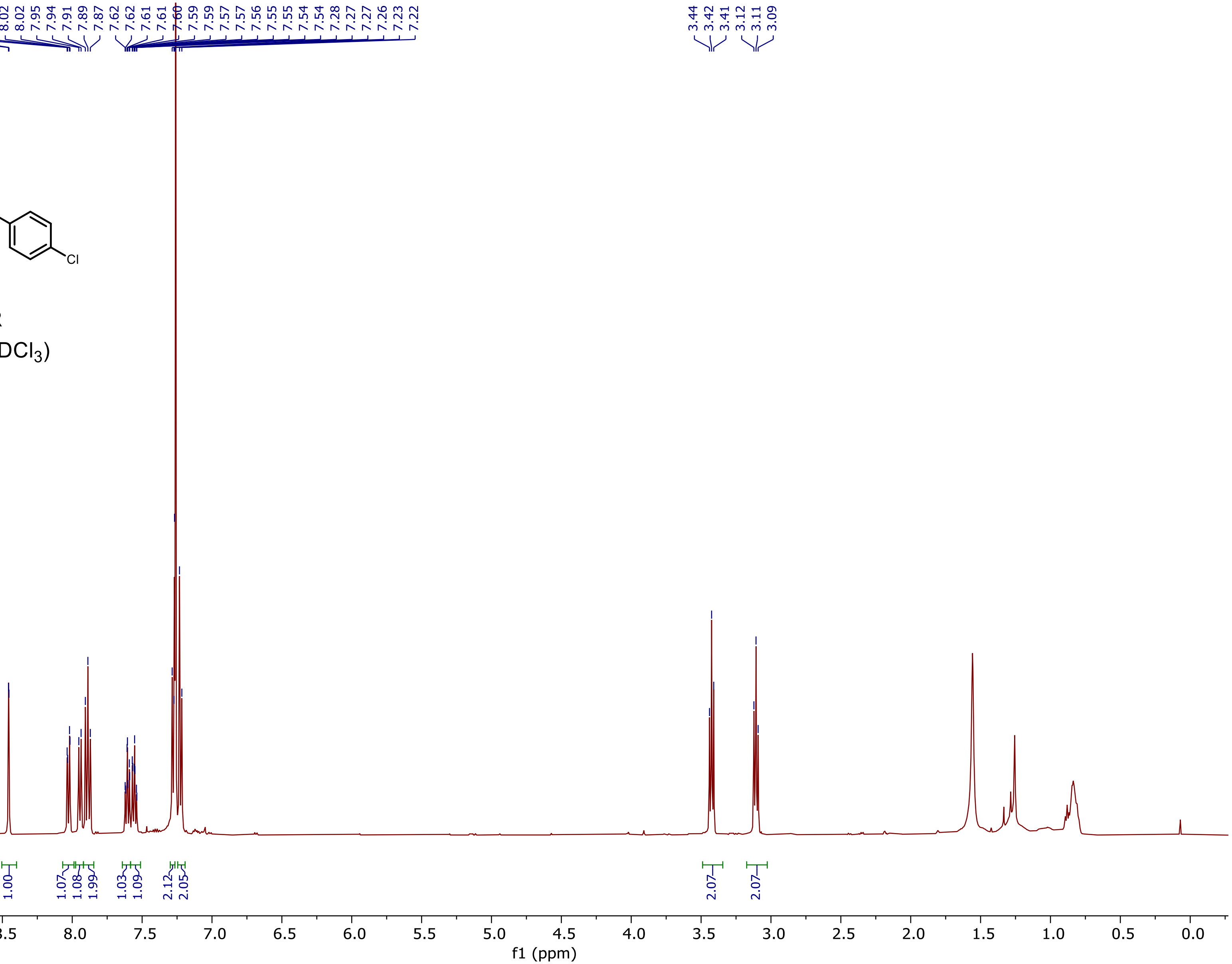
Ketones

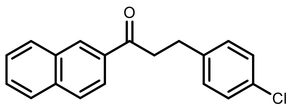


32

^{1}H NMR

(500 MHz, $CDCl_3$)

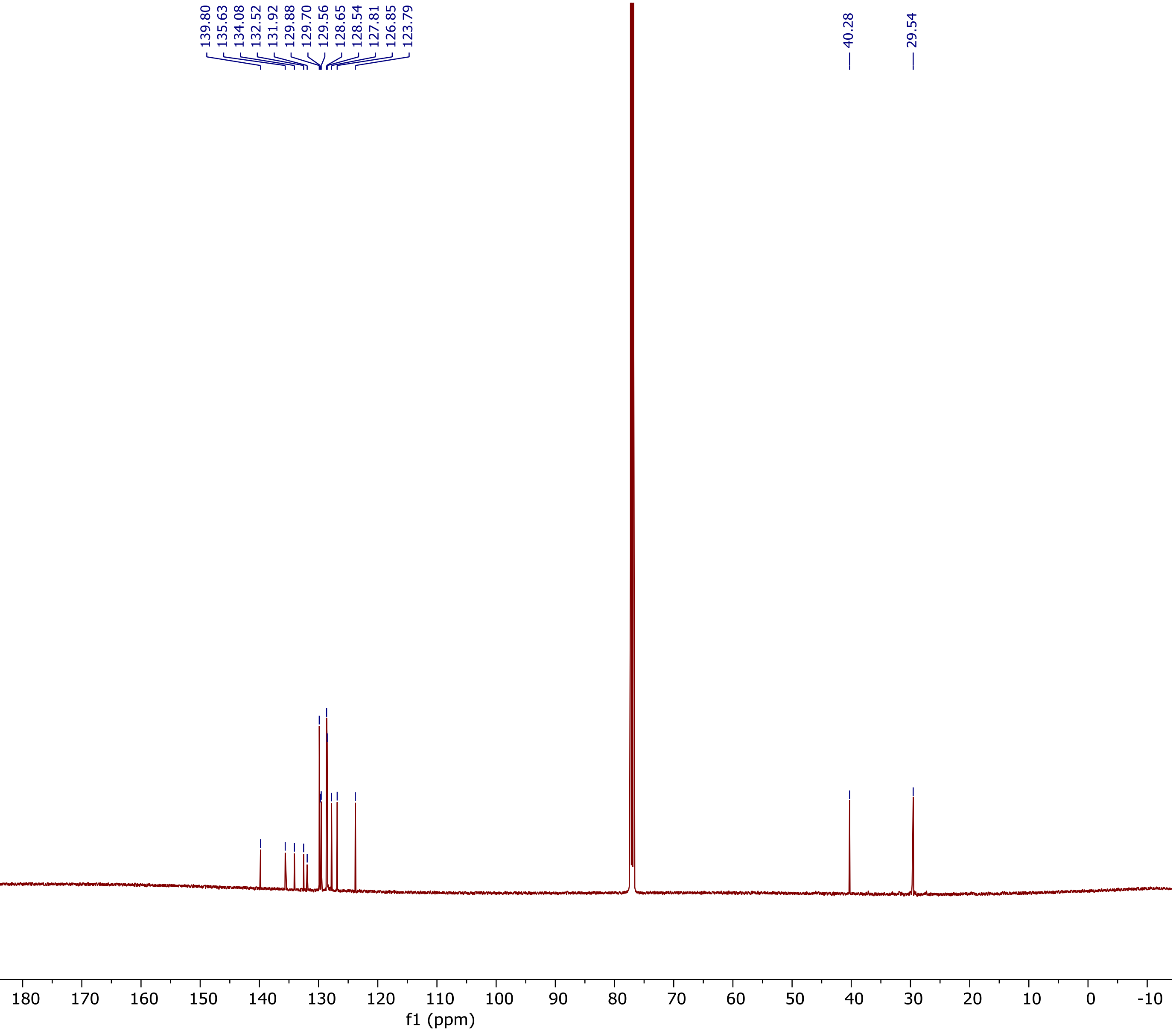


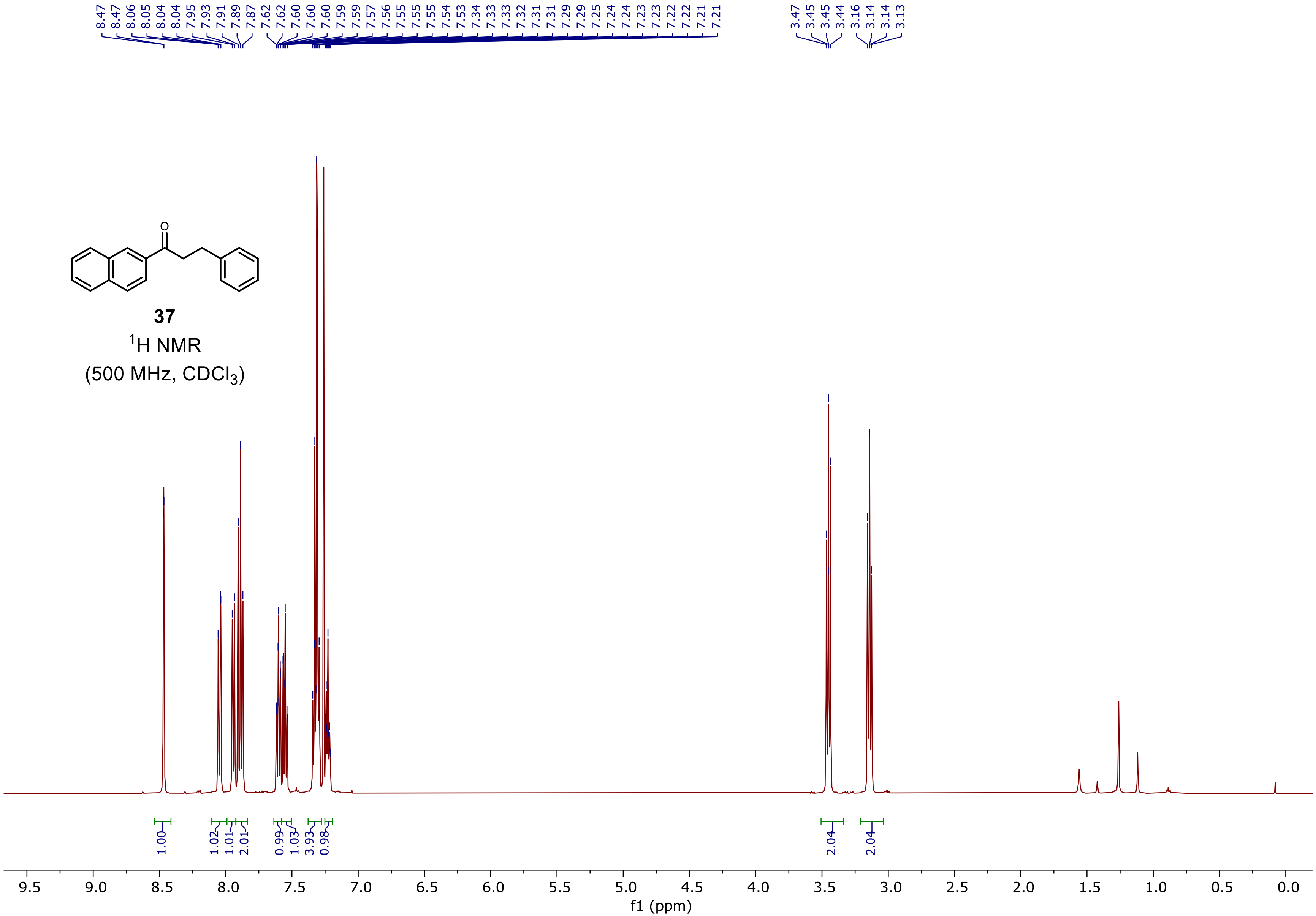


32

^{13}C NMR

(126 MHz, $CDCl_3$)

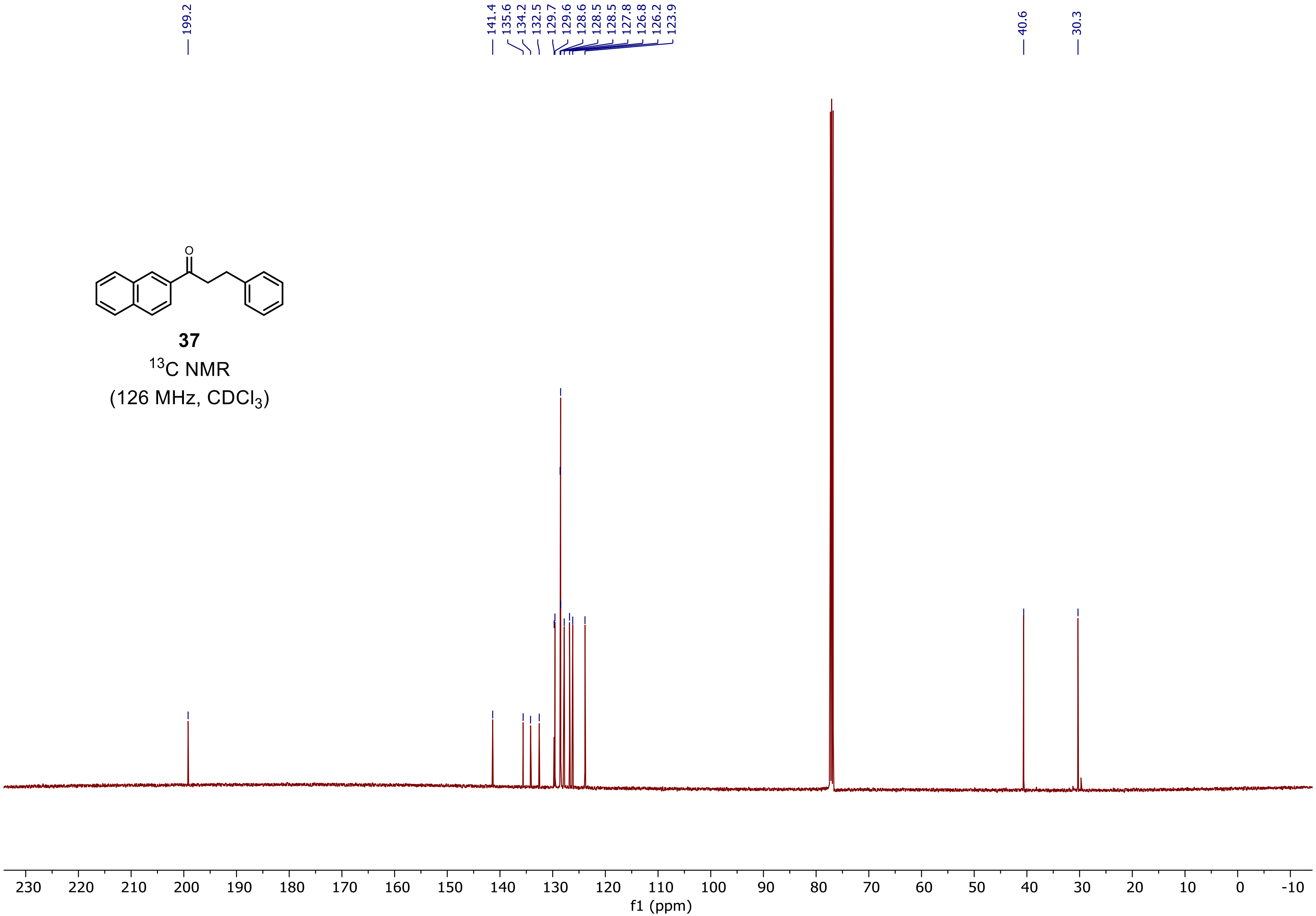


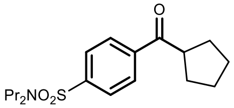

O
37
1H NMR
(500 MHz, CDCl3)
8.47 8.47 8.06 8.05 8.04 8.04 7.95 7.93 7.91 7.89 7.87 7.62 7.62 7.60 7.60 7.60 7.59 7.59 7.57 7.56 7.55 7.55 7.55 7.54 7.53 7.34 7.33 7.33 7.32 7.31 7.31 7.29 7.29 7.25 7.24 7.24 7.23 7.23 7.22 7.22 7.21 7.21
3.47 3.45 3.45 3.44 3.16 3.14 3.14 3.13
1.00 1.02 1.01 2.01 0.99 1.03 3.93 0.98 2.04 2.04
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

37

^{13}C NMR

(126 MHz, $CDCl_3$)

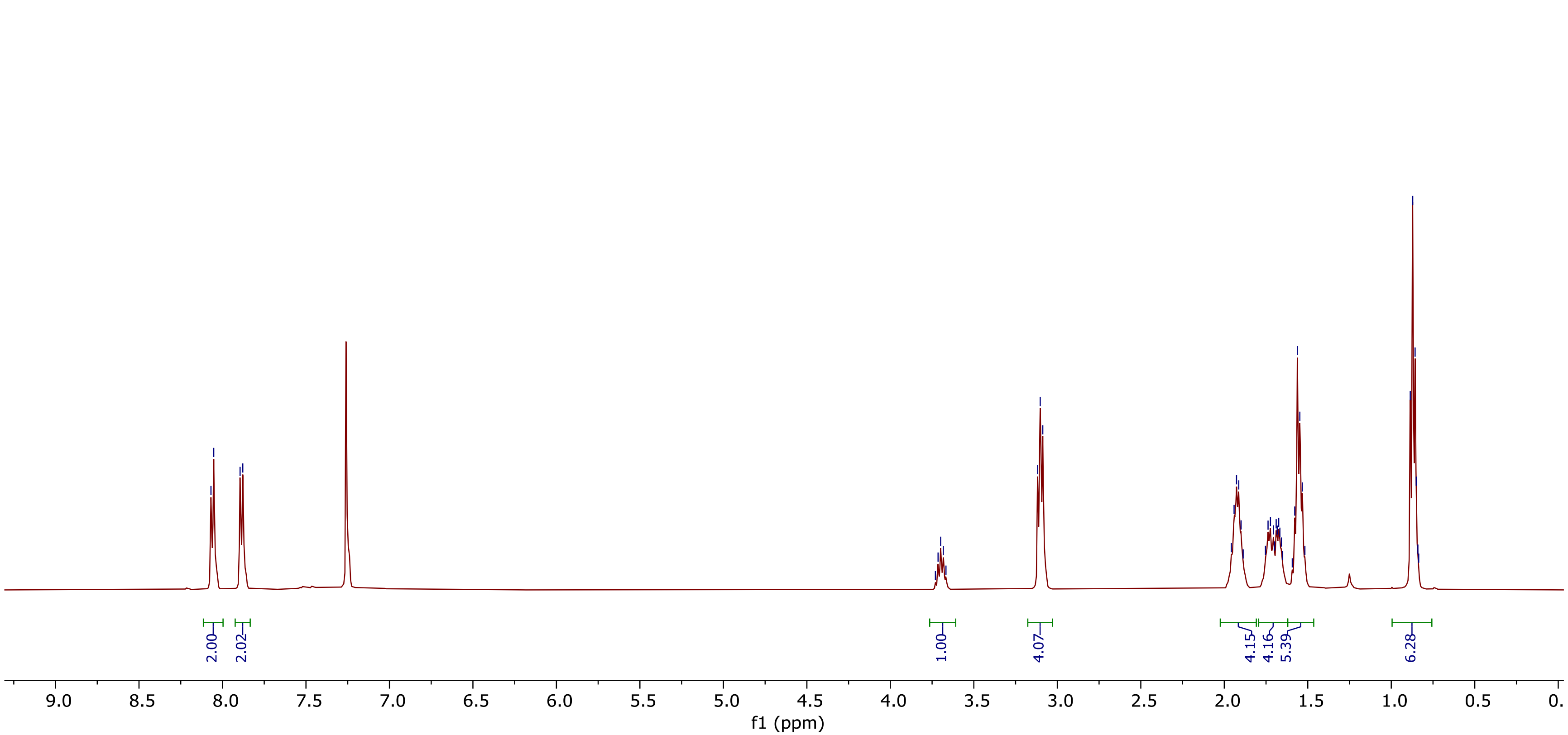


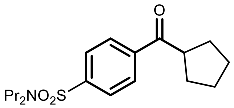


S49

^{1}H NMR

(500 MHz, $CDCl_3$)

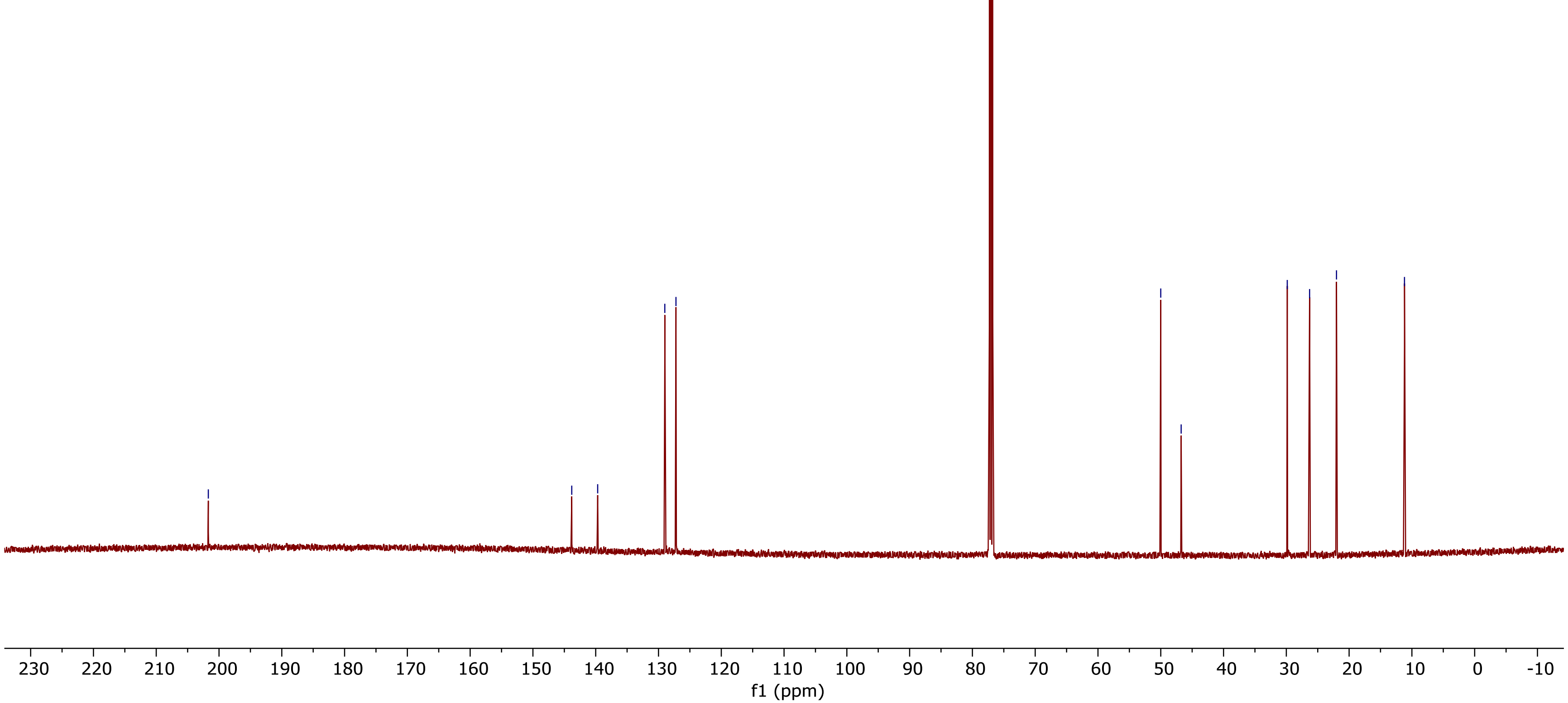


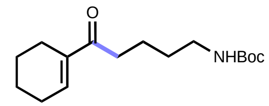


S49

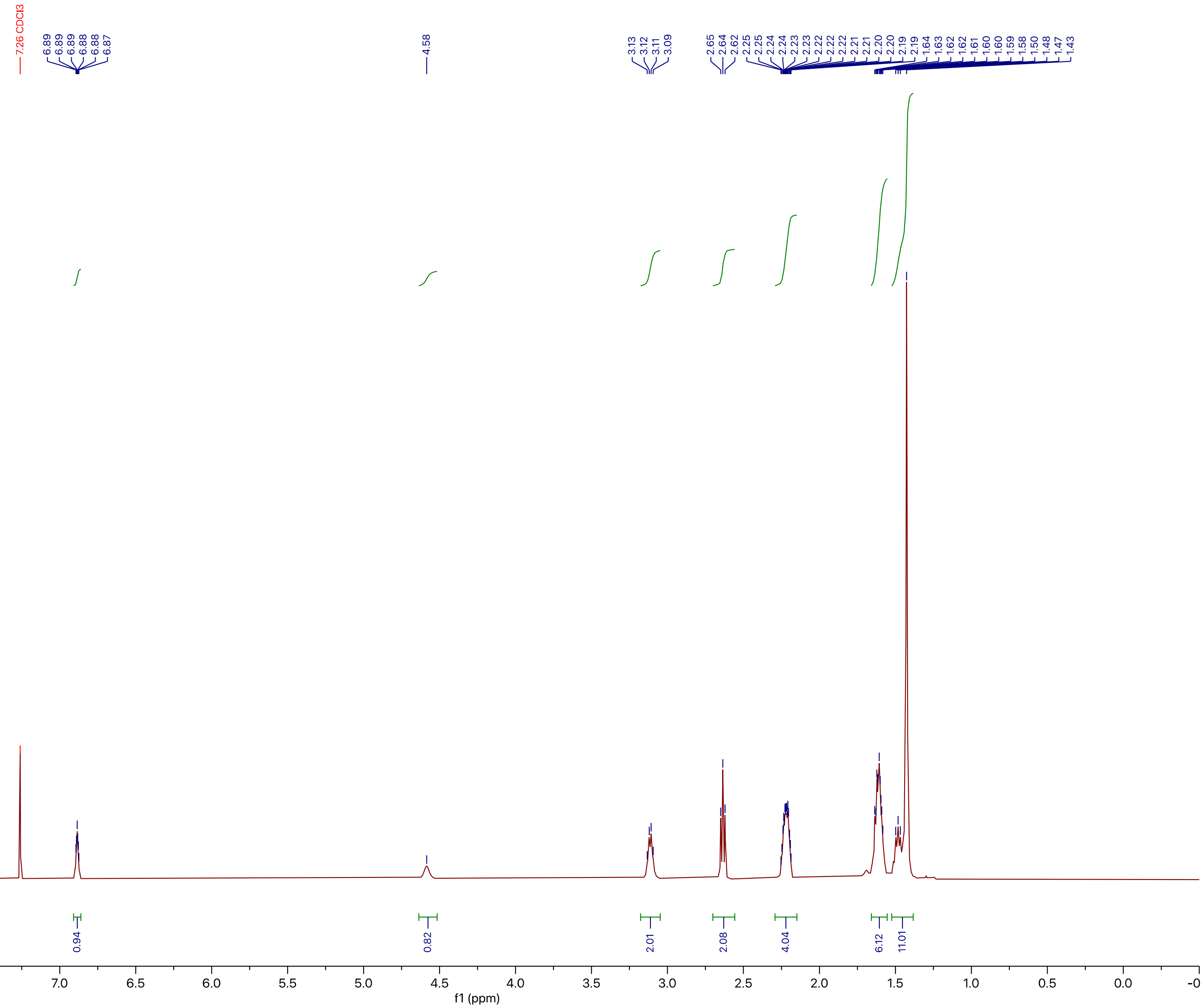
^{13}C NMR

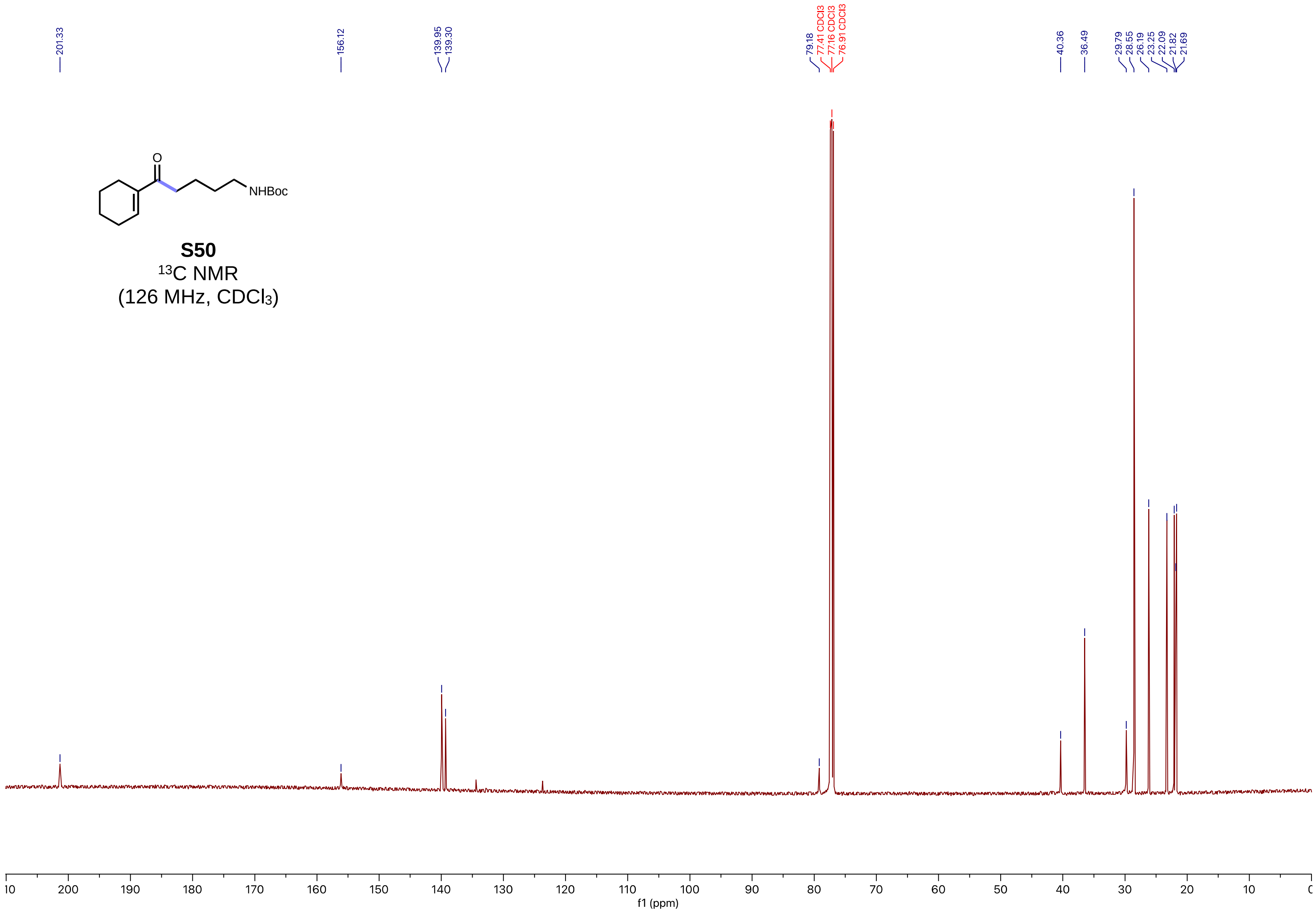
(126 MHz, $CDCl_3$)



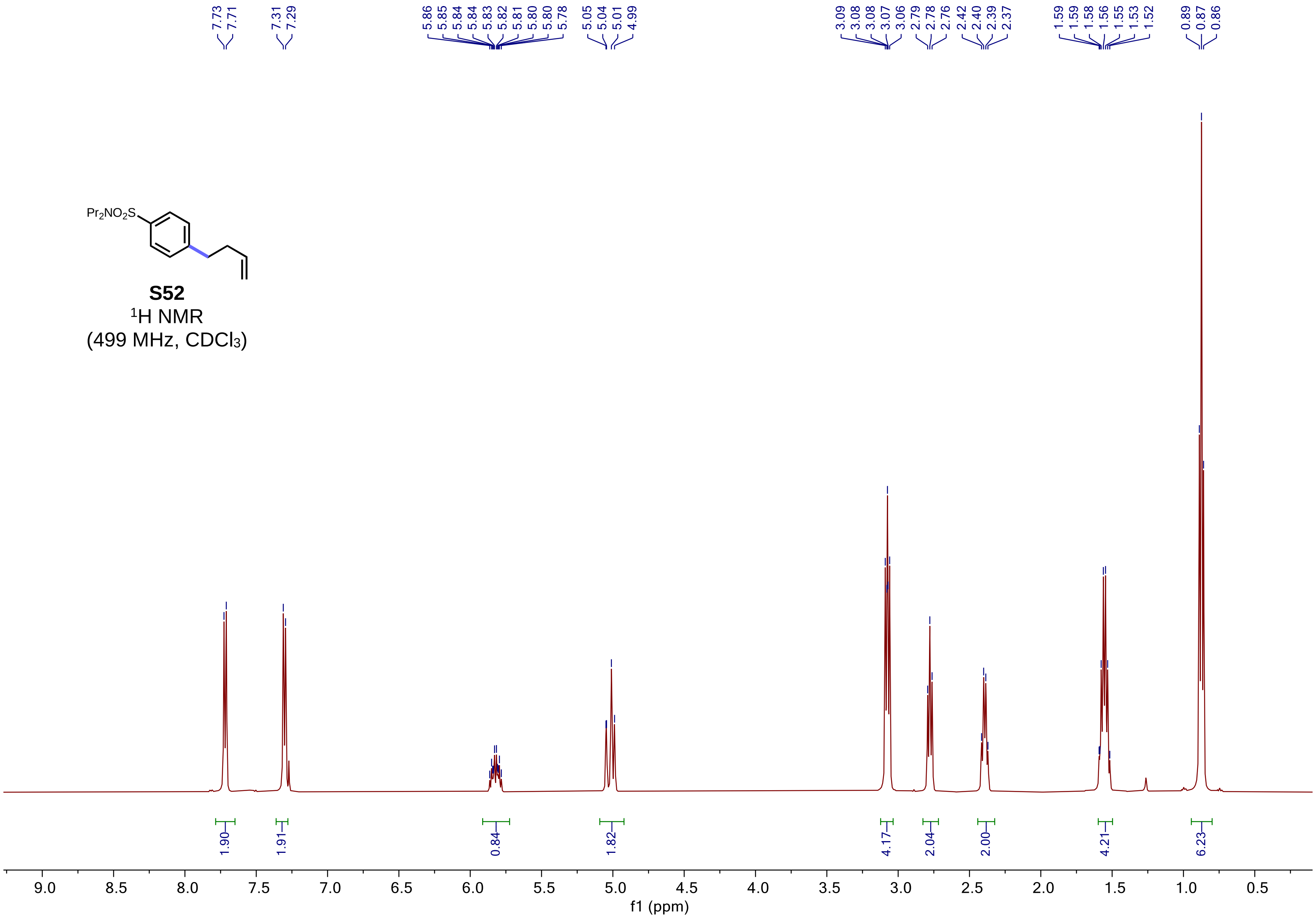


S50
^{1}H NMR
(500 MHz, $CDCl_3$)

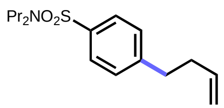



201.33
156.12
139.95
139.30
79.18
77.41 CDCl3
77.16 CDCl3
76.91 CDCl3
40.36
36.49
29.79
28.55
26.19
23.25
22.09
21.82
21.69
O
NHBoc
S50
13C NMR
(126 MHz, CDCl3)
f1 (ppm)

Mechanistic and Control Experiments



S52
^{1}H NMR
(499 MHz, $CDCl_3$)
Pr_2NO_2S
7.73 7.71 7.31 7.29 5.86 5.85 5.84 5.84 5.83 5.82 5.81 5.80 5.80 5.78 5.05 5.04 5.01 4.99 3.09 3.08 3.08 3.07 3.06 2.79 2.78 2.76 2.42 2.40 2.39 2.37 1.59 1.59 1.58 1.56 1.55 1.53 1.52 0.89 0.87 0.86
1.90 1.91 0.84 1.82 4.17 2.04 2.00 4.21 6.23
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)



S52

^{13}C NMR

(126 MHz, $CDCl_3$)