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Supporting Information

Expedient Stereospecific Co-catalyzed tandem *C-N* and *C-O* bond formation of *N*-methylanilines with styrene oxides

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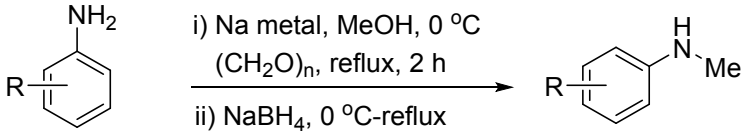
General Information: Anilines, styrenes, styrene oxides, *m*-CPBA (77%), $Cu(OTf)_2$ (98%), $Cu(OAc)_2$ (98%), $Fe(acac)_2$ (97%), $Fe(OAc)_2$ (95%), $Co(acac)_2$ (97%), $Co(OAc)_2{\cdot}4H_2O$ (98%), $CoCl_2$ (98%), TBHP in decane and DTBP of Aldrich, and 30% H_2O_2 and BHT (99%) of Merck were used as received. Solvents were purchased from Merck, distilled by the standard protocol and stored over molecular sieves under nitrogen atmosphere prior to use.[1] The reactions were monitored by analytical TLC on Merck silica gel G/GF 254 plates. The column chromatography was performed with Rankem silica gel (60-120 mesh). NMR (^1H and ^{13}C) spectra were recorded on 400/600 MHz NMR spectrometer using $CDCl_3$ as a solvent and TMS as an internal standard. The data are accounted as follows: chemical shifts (δ ppm) (multiplicity, coupling constant (Hz), integration). The abbreviations for multiplicity are as follows: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet and dd = doublet of doublets. FT-IR spectra recorded on a Perkin Elmer spectrometer. HRMS were analyzed with Agilent Q-TOF 6500. Optical rotation was determined using a polarimeter with a 50 mm path length cell at 589 nm. HPLC analysis was carried out with Daicel Chiralcel OJ-H column.

General Procedure for Preparation of *N*-Methylanilines.[2]

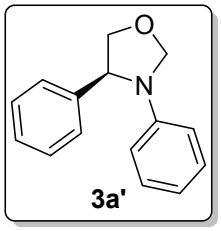


In an oven dried two-necked round bottom flask, NaOMe was prepared by adding sodium metal (10 mmol) portionwise in dry MeOH (20 mL) at 0 ºC. Aniline (2 mmol) and paraformaldehyde (5 mmol) were added to a freshly prepared NaOMe at room temperature (26 °C), and the reaction mixture was allowed to stirr for 2 h at 90 °C to generate an imine intermediate. The resultant mixture was reacted with $NaBH_4$ (3 mmol) at 0 ºC, and then refluxed for the additional 2 h. The reaction mixture was then cooled to room temperature, and the solvent was evaporated on a rotary evaporator to give a residue that was diluted with CH_2Cl_2 (15 mL) then washed with water (5 mL). Drying (Na_2SO_4) and evaporation of the solvent gave a residue that was purified on a silica gel column chromatography using hexane as an eluent.

General Procedure for Co-Catalyzed Stereospecific *C-N* and C-O Bond Formation of styrene oxides with *N*-Methylanilines. N-Methylaniline (0.5 mmol), epoxide (0.5 mmol) and $Co(OAc)_2 \cdot 4H_2O$ (10 mol%) were stirred in $(CH_2Cl)_2$ (2 mL) at 60 °C for 2 h. The reaction was cooled to room temperature and treated with TBHP (1 mmol). The mixture was then stirred at 60 °C for the appropriate time. The progress of the reaction was monitored by TLC using ethyl acetate and hexane. After completion, the reaction was allowed to cool to room temperature and treated with saturated Na_2SO_3 (1 mL). After stirrng for 1 h, the solution was extracted using CH_2Cl_2 (3x10 mL). The combined organic solution was then washed with brine (1x10 mL) and water (1x10 mL). Drying (Na_2SO_4) and evaporation of the solvent gave a residue that was puritifed on silica gel column chromatography using ethyl acetate and hexane as the solvent.

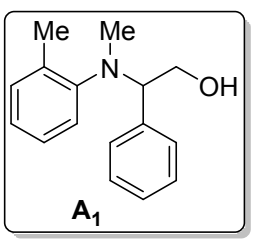
Characterization Data

3,4-Diphenyloxazolidine 3a. Analytical TLC on silica gel, 1:19 ethyl acetate/hexane R_f = 0.61;



Pale yellow liquid; 83 mg, yield 73%; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.37−7.34 (m, 4H), 7.30-7.28 (m, 1H), 7.19 (t, *J* = 7.2 Hz, 2H), 6.75 (t, *J* = 7.2 Hz, 1H), 6.49 (d, *J* = 8.4 Hz, 2H), 5.33 (d, *J* = 2.4 Hz, 1H), 5.04 (d, *J* = 2.4 Hz, 1H), 4.71 (dd, *J* = 6.6, 4.2 Hz, 1H), 4.42 (dd, *J* = 8.4, 6.6 Hz, 1H), 3.99 (dd, *J* = 8.4, 4.2 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 145.2, 141.6, 129.4, 129.0, 127.7, 126.4, 117.8, 112.9, 82.9, 75.9, 61.8; FT-IR (neat) 3060, 3029, 2929, 2867, 1600, 1504, 1391, 1346, 1211, 1164, 1089, 944, 749, 696 cm^{-1}; HRMS (ESI) m/z $[M+H]^+$ calcd for $[C_{15}H_{15}NO+H]^+$ 226.1226, found 226.1236; **(*S*)-3,4-Diphenyloxazolidine 3a**□. 81 mg, yield 72%; $[\alpha]_D^{23}$ = +156.0 (c= 0.32, $CHCl_3$); HPLC analysis: 98% ee [Daicel Chiralcel OJ-H column, hexane/*i*PrOH = 80:20, flow rate: 1 mL/min, λ = 254 nm, t_R = 9.70 min (minor), 14.37 min (major)].

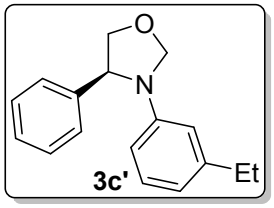
2-(Methyl(*o*-tolyl)amino)-2-phenylethan-1-ol A_1. Analytical TLC on silica gel, 1:5 ethyl



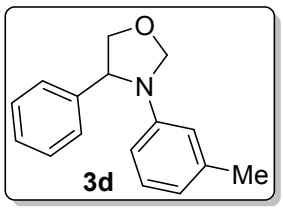
acetate/hexane R_f = 0.40; Yellow liquid; 97 mg, yield 81%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36-7.28 (m, 3H), 7.24-7.19 (m, 3H), 7.11-7.01 (m, 2H), 6.89 (dd, *J* = 8.0, 1.2 Hz, 1H), 4.12 (t, *J* = 6.8 Hz, 1H), 4.22 (dd, *J* = 10.8, 7.2 Hz, 1H), 3.82 (dd, *J* = 11.2, 6.4 Hz, 1H), 2.55 (s, 3H), 2.46 (s, 3H),

2.25 (br s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.7, 137.8, 134.3, 131.4, 128.9, 128.4, 127.9, 126.5, 124.5, 123.7, 68.6, 63.1, 38.0, 18.7; FT-IR (neat) 3434, 3062, 3028, 2949, 2881, 2796, 1637, 1598, 1491, 1452, 1252, 1033, 911,767 cm^{-1}; HRMS (ESI) m/z $[M+H]^+$ calcd for $[C_{16}H_{19}NO+H]^+$ 242.1539, found 242.1530.

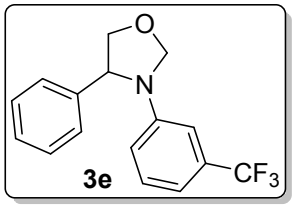
3-(3-Ethylphenyl)-4-phenyloxazolidine 3c. Analytical TLC on silica gel, 1:19 ethyl acetate/hexane R_f = 0.60; Yellow liquid; 91 mg, yield 72%; ^{1}H NMR (600 MHz, $CDCl_3$) δ 3.37-3.33 (m, 4H), 7.28-7.27 (m, 1H), 7.08 (t, *J* = 7.8 Hz, 1H), 6.61 (d, *J* = 7.8 Hz, 1H), 6.33-6.30 (m, 2H), 5.32 (d, *J* = 1.8 Hz, 1H), 5.03 (d, *J* = 2.4 Hz, 1H), 4.70 (dd, *J* = 7.2, 4.8 Hz, 1H), 4.39 (t, *J* = 7.2 Hz, 1H), 3.98 (dd, *J* = 8.4, 4.2 Hz, 1H), 2.57 (q, *J* = 7.8 Hz, 2H), 1.17 (t, *J* = 7.8 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 145.6, 145.3, 141.8, 129.3, 129.0, 127.7, 126.4, 117.6, 112.5, 110.5, 83.0, 75.9, 61.9, 29.3, 15.7; FT-IR (neat) 3063, 3032, 2963, 2928, 2867, 1604, 1493, 1453, 1390, 1355, 1089, 945, 755 cm^{-1}; HRMS (ESI) m/z $[M+H]^+$ calcd for $[C_{17}H_{19}NO+H]^+$ 254.1539, found 254.1549; **(*S*)-3-(3-Ethylphenyl)-4-phenyloxazolidine 3c**□. 95 mg, yield 75%; $[\alpha]_D^{23}$ = +27.0 (c= 0.31, $CHCl_3$); HPLC analysis: 98% ee [Daicel Chiralcel OJ-H column, hexane/*i*PrOH = 80:20, flow rate: 1 mL/min, λ = 254 nm, t_R = 6.11 min (minor), 10.84 min (major)].



4-Phenyl-3-(*m*-tolyl)oxazolidine 3d. Analytical TLC on silica gel, 1:19 ethyl acetate/hexane R_f = 0.60; Pale yellow liquid; 84 mg, yield 70%; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.36-7.33 (m, 4H), 7.29-7.27 (m, 1H), 7.05 (t, *J* = 7.8 Hz, 1H), 6.56 (d, *J* = 7.2 Hz, 1H), 6.30-6.28 (m, 2H), 5.31 (d, *J* = 1.8 Hz, 1H), 5.01 (d, *J* = 1.8 Hz, 1H), 4.69 (dd, *J* = 6.6, 4.2 Hz, 1H), 4.40 (dd, *J* = 8.4, 7.2 Hz, 1H), 3.98 (dd, *J* = 8.4, 4.2 Hz, 1H), 2.25 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 145.3, 141.8, 139.2, 129.3, 129.0, 127.7, 126.3, 118.8, 113.6, 110.2, 83.0, 75.9, 61.8, 22.0; FT-IR (neat) 3061, 3026, 2920, 2861, 1619, 1521, 1391, 1344, 1088, 944, 803 cm^{-1}; HRMS (ESI) m/z $[M+H]^+$ calcd for $[C_{16}H_{17}NO+H]^+$ 240.1383, found 240.1397.

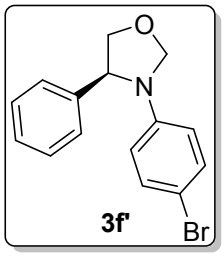


4-Phenyl-3-(3-(trifluoromethyl)phenyl)oxazolidine 3e. Analytical TLC on silica gel, 1:19 ethyl acetate/hexane R_f = 0.58; Colorless liquid; 96 mg, yield 65%; ^{1}H

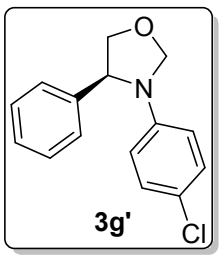


NMR (600 MHz, $CDCl_3$) δ 7.37-7.32 (m, 4H), 7.30-7.28 (m, 1H), 7.24 (t, *J* = 7.8 Hz, 1H), 6.97 (d, *J* = 7.8 Hz, 1H), 6.66 (s, 1H), 6.59 (dd, *J* = 8.4, 1.8 Hz, 1H), 5.33 (d, *J* = 2.4 Hz, 1H), 5.05 (d, *J* = 2.4 Hz, 1H), 4.73 (dd, *J* = 6.6, 4.2 Hz, 1H), 4.44 (dd, *J* = 9.0, 7.2 Hz, 1H), 4.01 (dd, *J* = 8.4, 4.2 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 145.1, 140.7, 132.0 (q, *J* = 31.5 Hz), 129.8, 129.2, 128.1, 126.3, 114.3 (q, *J* = 3.0 Hz), 109.1 (q, *J* = 3.0 Hz), 115.9, 82.7, 76.0, 61.8; FT-IR (neat) 3065, 6032, 2927, 2869, 1614, 1494, 1458, 1371, 1320, 1166, 1122, 1009, 948, 852 cm^{-1}; HRMS (ESI) m/z $[M+H]^+$ calcd for $[C_{16}H_{14}F_3NO+H]^+$ 294.1100, found 294.1124.

3-(4-Bromophenyl)-4-phenyloxazolidine 3f. Analytical TLC on silica gel, 1:19 ethyl acetate/hexane R_f = 0.60; Pale yellow liquid; 114 mg, yield 75%; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.36-7.27 (m, 5H), 7.25 (d, *J* = 9.0 Hz, 2H), 6.34 (d, *J* = 9.0 Hz, 2H), 5.28 (d, *J* = 2.4 Hz, 1H), 4.98 (d, *J* = 2.4 Hz, 1H), 4.66 (dd, *J* = 6.6, 4.2 Hz, 1H), 4.43 (dd, *J* = 8.4, 6.6 Hz, 1H), 3.98 (dd, *J* = 8.4, 4.8 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 143.8, 140.7, 131.9, 128.9, 127.8, 126.1, 114.3, 109.7, 82.6, 75.8, 61.7; FT-IR (neat) 3063, 3028, 2989, 2925, 2857, 1594, 1491, 1390, 1357, 1164, 1088, 944, 807, 753 cm^{-1}; HRMS (ESI) m/z $[M+H]^+$ calcd for $[C_{15}H_{14}BrNO+H]^+$ 304.0332, found 304.0333; **(*S*)-3-(4-Bromophenyl)-4-phenyloxazolidine 3f**□. 106 mg, yield 70%; $[\alpha]_D^{22}$ = +92.07 (c= 3.2, $CHCl_3$); HPLC analysis: 95% ee [Daicel Chiralcel OJ-H column, hexane/*i*PrOH = 80:20, flow rate: 1 mL/min, λ = 254 nm, t_R = 10.39 min (minor), 12.27 min (major)].

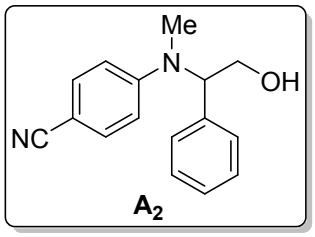


(*S*)-3-(4-Chlorophenyl)-4-phenyloxazolidine 3g. Analytical TLC on silica gel, 1:19 ethyl acetate/hexane R_f = 0.60; Pale yellow liquid; 94 mg, yield 72%; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.36-7.27 (m, 5H), 7.11 (d, *J* = 9.0 Hz, 2H), 6.38 (d, *J* = 9.0 Hz, 2H), 5.28 (d, *J* = 2.4 Hz, 1H), 4.99 (d, *J* = 2.4 Hz, 1H), 4.66 (dd, *J* = 6.6, 4.8 Hz, 1H), 4.43 (dd, *J* = 8.4, 7.2 Hz, 1H), 3.97 (dd, *J* = 8.4, 4.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.7, 141.0, 129.3, 129.1, 127.9, 126.3, 122.8, 114.0, 82.9, 76.0, 62.0; FT-IR (neat) 3063, 3026, 2925, 2858, 1600, 1493, 1391, 1354, 1092, 944, 809 cm^{-1}; HRMS (ESI) m/z $[M+H]^+$ calcd for $[C_{15}H_{14}ClNO+H]^+$ 260.0837, found 260.0847; **(*S*)-3-(4-Chlorophenyl)-4-phenyloxazolidine 3g**□**.** 93 mg, yield, 72%; $[\alpha]_D^{24}$ =

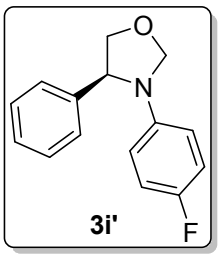


+72.6 (c= 0.22, $CHCl_3$); HPLC analysis: 99% ee [Daicel Chiralcel OJ-H column, hexane/*i*PrOH = 80:20, flow rate: 1 mL/min, λ = 254 nm, t_R = 10.34 min (minor), 13.42 min (major)].

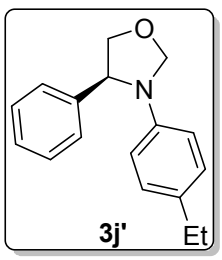
4-((2-Hydroxy-1-phenylethyl)(methyl)amino)benzonitrile A_2. Analytical TLC on silica gel, 1:4 ethyl acetate/hexane R_f = 0.38; yellow liquid; 85 mg, yield 68%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47 (d, *J* = 9.2 Hz, 2H), 7.37-7.31 (m, 3H), 7.20 (d, *J* = 7.2 Hz, 2H), 6.85 (d, *J* = 8.8 Hz, 2H), 5.17 (dd, *J* = 8.8, 5.2 Hz, 1H), 4.23 (dd, *J* = 11.2, 4.8 Hz, 1H), 4.15 (dd, *J* = 11.2, 8.8 Hz, 1H), 2.90 (s, 3H), 2.19 (br s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.4, 137.3, 133.6, 129.0, 128.9, 127.9, 126.9, 120.4, 112.6, 77.4, 63.2, 62.5, 32.5; FT-IR (neat) 3438, 3062, 2955, 2921, 2214, 1605, 1518, 1385, 1347, 1180, 1110, 1063, 817, 755, 702 cm^{-1}; HRMS (ESI) m/z $[M+H]^+$ calcd for $[C_{16}H_{16}N_2O+H]^+$ 253.1335, found 253.1352.



3-(4-Fluorophenyl)-4-phenyloxazolidine 3i. Analytical TLC on silica gel, 1:19 ethyl acetate/hexane R_f = 0.59; Yellow liquid; 84 mg, yield 69%; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.37-7.34 (m, 4H), 7.31-7.27 (m, 1H), 6.89 (t, *J* = 9.0, 2H), 6.41-6.39 (m, 2H), 5.29 (d, *J* = 2.4 Hz, 1H), 4.97 (d, *J* = 2.4 Hz, 1H), 4.64 (dd, *J* = 6.6, 4.8 Hz, 1H), 4.43 (dd, *J* = 8.4, 7.2 Hz, 1H), 3.96 (dd, *J* = 8.4, 4.2 Hz, 1H) ; ^{13}C NMR (150 MHz, $CDCl_3$) δ 156.9 (*J* = 234 Hz), 141.89 (*J* = 1.5 Hz), 141.3, 129.1, 127.9, 126.4, 115.97 (*J* = 22.5 Hz), 113.7 (*J* = 7.5 Hz), 83.4, 76.0, 62.4; FT-IR (neat) 3059, 3029, 2929, 2968, 1673, 1515, 1392, 1350, 1226, 1161, 1090, 945, 815 cm^{-1}; HRMS (ESI) m/z $[M+H]^+$ calcd for $[C_{15}H_{14}FNO+H]^+$ 244.1132, found 244.1142. **(*S*)-3-(4-Fluorophenyl)-4-phenyloxazolidine 3i′**. 88 mg, yield, 72%; $[\alpha]_D^{23}$ = +40.6 (c= 0.33, $CHCl_3$); HPLC analysis: 95% ee [Daicel Chiralcel OJ-H column, hexane/*i*PrOH = 80:20, flow rate: 1 mL/min, λ = 254 nm, t_R = 8.45 min (minor), 12.92 min (major)].

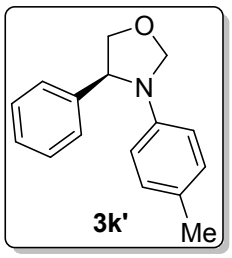


3-(4-Ethylphenyl)-4-phenyloxazolidine 3j. Analytical TLC on silica gel, 1:9 ethyl acetate/hexane R_f = 0.60; Yellow liquid; 93 mg, yield 73%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37-7.27 (m, 5H), 7.02 (d, *J* = 8.4 Hz, 2H), 6.44 (d, *J* = 8.4 Hz, 2H), 5.32 (d, *J* = 2.4 Hz, 1H), 5.00 (d, *J* = 2.0 Hz, 1H), 4.67 (dd, *J* = 6.8, 4.8 Hz, 1H), 4.38 (t, *J* = 7.6 Hz, 1H), 3.97 (dd, *J* = 8.4, 4.8 Hz, 1H), 2.55 (q, *J*

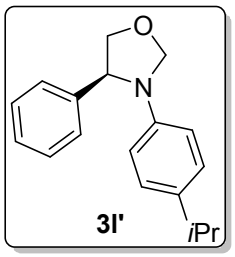


= 7.2 Hz, 2H), 1.16 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.4, 141.8, 133.7, 129.0, 128.8, 127.7, 126.4, 113.1, 83.3, 75.9, 62.2, 28.1, 16.1. FT-IR (neat) 3063, 3031, 2963, 2928, 2862, 1604, 1493, 1453, 1390, 1355, 1261,1166, 1089, 945 cm^{-1}; HRMS (ESI) m/z $[M+H]^+$ calcd for $[C_{17}H_{19}NO+H]^+$ 254.1539, found 254.1546. **(*S*)-3-(4-Ethylphenyl)-4-phenyloxazolidine 3j□.** 93 mg, yield, 73%; $[\alpha]_D^{23}$ = +26.6 (c= 0.33, $CHCl_3$); HPLC analysis: 98% ee [Daicel Chiralcel OJ-H column, hexane/*i*PrOH = 80:20, flow rate: 1 mL/min, λ = 254 nm, t_R = 6.87 min (minor), 9.52 min (major)].

4-Phenyl-3-(*p*-tolyl)oxazolidine 3k. Analytical TLC on silica gel, 1:19 ethyl acetate/hexane R_f= 0.62; Yellow liquid; 90 mg, yield 75%; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.37-7.33 (m, 4H), 7.29-7.27 (m, 1H), 7.00-6.99 (d, *J* = 8.4 Hz, 2H), 6.42 (d, *J* = 8.4 Hz, 2H), 5.32 (d, *J* = 2.4 Hz, 1H), 5.00 (d, *J* = 2.4 Hz, 1H), 4.67 (dd, *J* = 7.2, 4.8 Hz, 1H), 4.41 (dd, *J* = 8.4, 7.2 Hz, 1H), 3.97 (dd, *J* = 8.4, 4.8 Hz, 1H), 2.23 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 143.2, 141.7, 129.9, 129.0, 127.7, 127.1, 126.4, 113.0, 83.3, 75.9, 62.1, 20.5. FT-IR (neat) 3063, 3028, 2923, 2856, 1620, 1521, 1452, 1341, 1164, 1089, 944, 804, 755 cm^{-1}; HRMS (ESI) m/z $[M+H]^+$ calcd for $[C_{16}H_{17}NO+H]^+$ 240.1383, found 240.1392. **(*S*)-4-Phenyl-3-(*p*-tolyl)oxazolidine 3k′**. 90 mg, yield, 75%; $[\alpha]_D^{23}$ = +85.0 (c= 1.3, $CHCl_3$); HPLC analysis: 99% ee [Daicel Chiralcel OJ-H column, hexane/*i*PrOH = 80:20, flow rate: 1 mL/min, λ = 254 nm, t_R = 8.59 min (minor), 12.02 min (major)].

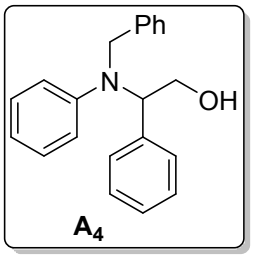


3-(4-*Iso*propylphenyl)-4-phenyloxazolidine 3l. Analytical TLC on silica gel, 1:19 ethyl acetate/hexane R_f= 0.62; Pale yellow liquid; 103 mg, yield 77%; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.37-7.32 (m, 4H), 7.28-7.27 (m, 1H), 7.05 (d, *J* = 8.4 Hz, 2H), 7.44 (d, *J* = 8.4 Hz, 2H), 5.31 (d, *J* = 1.8 Hz, 1H), 4.99 (d, *J* = 2.4 Hz, 1H), 4.65 (dd, *J* = 6.6, 4.2 Hz, 1H), 4.38 (dd, *J* = 8.4, 6.6 Hz, 1H), 3.96 (dd, *J* = 8.4, 4.2 Hz, 1H), 2.81-2.76 (m, 1H), 1.18 (d, *J* = 2.4 Hz, 3H), 1.17 (d, *J* = 2.4 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 143.5, 141.9, 138.3, 129.0, 127.7, 127.3, 126.4, 113.0, 83.3, 75.9, 62.9, 33.3, 24.4; FT-IR (neat) 3028, 2958, 2928, 2867, 2755, 1616, 1519, 1454, 1390, 1345, 1194, 1165, 1090, 946 cm^{-1}; HRMS (ESI) m/z $[M+H]^+$ calcd for $[C_{18}H_{21}NO+H]^+$ 268.1696, found 268.1699; **(*S*)-3-(4-*Iso*propylphenyl)-4-phenyloxazolidine**



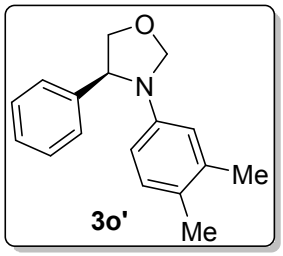
3l□. 102 mg, yield 76%; $[\alpha]_D^{23}$ = +46.0 (c= 0.2, $CHCl_3$); HPLC analysis: 97% ee [Daicel Chiralcel OJ-H column, hexane/*i*PrOH = 80:20, flow rate: 1 mL/min, λ = 254 nm, t_R = 4.80 min (minor), 8.10 min (major)].

2-(Benzyl(phenyl)amino)-2-phenylethan-1-ol A_4. Analytical TLC on silica gel, 1:5 ethyl acetate/hexane R_f= 0.40; Yellow liquid; 133 mg, yield 88%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.24-7.17 (m, 7H), 7.14-7.08 (m, 5H), 6.18 (d, *J* = 8.4 Hz, 2H), 6.71 (t, *J* = 7.2 Hz, 1H), 5.08 (t, *J* = 6.8 Hz, 1H), 4.45 (d, *J* = 17.1 Hz, 1H), 4.37 (d, *J* = 17.1 Hz, 1H) 4.00 (d, *J* = 6.8 Hz, 2H), 1.90 (br s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.8, 139.8, 138.1, 129.3, 128.9, 127.8, 127.7, 127.1, 126.9, 118.94, 116.1, 65.2, 63.2, 51.0; FT-IR (neat) 3559, 3060, 3029, 2926, 2884, 1597, 1499, 1451, 1348, 1249, 1158, 1033, 990, 949,746 cm^{-1}; HRMS (ESI) m/z $[M+H]^+$ calcd for $[C_{21}H_{21}NO+H]^+$ 304.1696, found 304.1696.



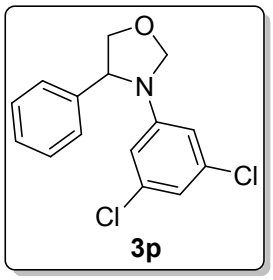
A_4

3-(3,4-dimethylphenyl)-4-phenyloxazolidine 3o. Analytical TLC on silica gel, 1:9 ethyl acetate/hexane R_f= 0.62; Yellow liquid; 98 mg, yield 77%; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.36-7.32 (m, 4H), 7.27-7.25 (m, 1H), 6.92 (d, *J* = 8.4 Hz, 1H), 6.31 (d, *J* = 1.8 Hz, 1H), 6.24 (dd, *J* = 7.8, 2.4 Hz, 1H), 5.30 (d, *J* = 1.8 Hz, 1H), 5.98 (d, *J* = 2.4 Hz, 1H), 4.66 (dd, *J* = 7.2, 4.8 Hz, 1H), 4.38 (dd, *J* = 8.4, 7.2 Hz, 1H), 3.95 (dd, *J* = 8.4, 4.2 Hz, 1H), 2.16 (s, 3H), 2.13 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 143.6, 141.9, 137.6, 130.4, 129.0, 127.6, 126.4, 126.0, 114.5, 110.6, 83.3, 75.9, 62.0, 20.4, 18.9; FT-IR (neat) 3063, 3026, 2923, 2854, 1617, 1512, 1453, 1346, 1166, 1088, 949, 800 cm^{-1}; HRMS (ESI) m/z $[M+H]^+$ calcd for $[C_{17}H_{19}NO+H]^+$ 254.1539, found 254.1544; **(*S*)-3-(3,4-dimethylphenyl)-4-phenyloxazolidine 3o□.** 93 mg, yield 73 %; $[\alpha]_D^{23}$ = +47.0 (c= 0.17, $CHCl_3$); HPLC analysis: 97% ee [Daicel Chiralcel OJ-H column, hexane/*i*PrOH = 80:20, flow rate: 1 mL/min, λ = 254 nm, t_R = 8.55 min (minor), 10.25 min (major)].



3o'

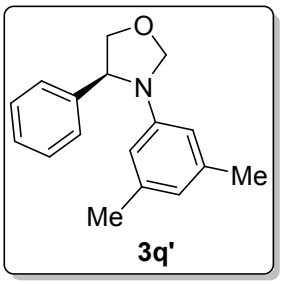
3-(3,5-dichlorophenyl)-4-phenyloxazolidine 3p. Analytical TLC on silica gel, 1:9 ethyl acetate/hexane R_f= 0.60; Colorless liquid; 99 mg, yield 67%; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.38-7.35 (m, 2H), 7.32-7.28 (m, 3H), 6.70 (t, *J* =



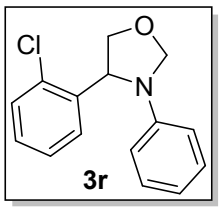
3p

1.8 Hz, 1H), 6.31 (d, J = 1.8 Hz, 2H), 5.24 (d, J = 6.6, 3.6 Hz, 1H), 4.97 (d, J = 8.4, 6.6 Hz, 1H), 4.67 (dd, J = 6.6, 3.6 Hz, 1H), 4.40 (dd, J = 8.4, 6.6 Hz, 1H), 3.99 (dd, J = 8.4, 4.2 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 146.3, 140.3, 135.7, 129.3, 128.2, 126.2, 117.6, 111.1, 82.4, 75.9, 61.6; FT-IR (neat) 3084, 3028, 2959, 2923, 2856, 1592, 1556, 1462, 1390, 1126, 1092, 1024, 982, 820, 705 cm^{-1}; HRMS (ESI) m/z $[M+H]^+$ calcd for $[C_{15}H_{13}Cl_2NO+H]^+$ 294.0447, found 294.0463.

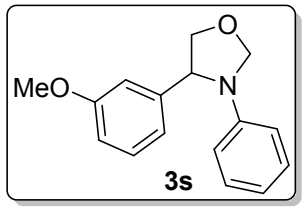
3-(3,5-Dimethylphenyl)-4-phenyloxazolidine 3q. Analytical TLC on silica gel, 1:19 ethyl acetate/hexane R_f = 0.62; Yellow liquid; 99 mg, yield 78%; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.35-7.33 (m, 4H), 7.29-7.27 (m, 1H), 6.42 (s, 1H), 6.12 (s, 2H), 5.30 (d, J = 2.4 Hz, 1H), 5.00 (d, J = 2.4 Hz, 1H), 4.69 (dd, J = 6.6, 4.2 Hz, 1H), 4.37 (dd, J = 8.4, 6.6 Hz, 1H), 3.97 (dd, J = 7.8, 3.6 Hz, 1H), 2.21 (s, 6H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 145.4, 142.0, 139.1, 129.0, 127.6, 126.4, 120.0, 110.9, 83.1, 75.9, 61.8, 21.8; FT-IR (neat) 3063, 3032, 2953, 2923, 2855, 1602, 1456, 1362, 1216, 1157, 1090, 945, 819, 754 cm^{-1}; HRMS (ESI) m/z $[M+H]^+$ calcd for $[C_{17}H_{19}NO+H]^+$ 254.1539, found 254.1546; **(S)-3-(3,5-Dimethylphenyl)-4-phenyloxazolidine 3q□.** yield 96 mg, 76%; $[\alpha]_D^{23}$ = +56.2 (c= 0.2, $CHCl_3$); HPLC analysis: 97% ee [Daicel Chiralcel OJ-H column, hexane/*i*PrOH = 80:20, flow rate: 1 mL/min, λ = 254 nm, t_R = 5.05 min (minor), 12.80 min (major)].

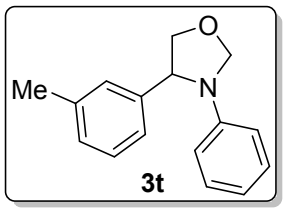


4-(2-Chlorophenyl)-3-phenyloxazolidine 3r. **A**alytical TLC on silica gel, 1:9 ethyl acetate/hexane R_f = 0.58; Colorless liquid; 94 mg, yield 72%; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.42 (dd, J = 7.8, 1.8 Hz, 1H), 7.37 (dd, J = 7.2, 1.8 Hz, 1H), 7.24-7.19 (m, 4H), 6.77 (t, J = 7.8 Hz, 1H), 6.43 (d, J = 8.4 Hz, 2H), 5.34 (d, J = 1.8 Hz, 1H), 5.10 (dd, J = 7.2, 3.0 Hz, 1H), 5.01 (d, J = 2.4 Hz, 1H), 4.47 (dd, J = 9.0, 7.0 Hz, 1H), 4.05 (dd, J = 8.4, 3.0 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 144.7, 138.6, 132.4, 129.8, 129.6, 128.9, 127.9, 127.4, 118.1, 112.9, 82.7, 74.5, 59.2; FT-IR (neat) 3063, 2993, 2926, 2864, 1600, 1505, 1391, 1348, 1264, 1170, 1091, 1035, 945, 746 cm^{-1}; HRMS (ESI) m/z $[M+H]^+$ calcd for $[C_{15}H_{14}ClNO+H]^+$ 260.0837, found 260.0845.



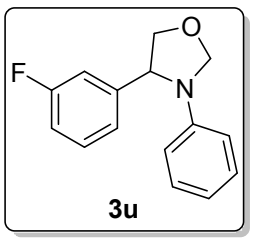
4-(3-Methoxyphenyl)-3-phenyloxazolidine 3s. Analytical TLC on silica gel, 1:19 ethyl acetate/hexane R_f = 0.40; Colorless liquid; 87 mg, yield 68%; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.28-7.25 (m, 1H), 7.19-7.16 (m, 2H), 6.95 (d, *J* = 7.8 Hz, 1H), 6.90 (s, 1H), 6.82 (dd, *J* = 8.4, 1.8 Hz, 1H), 6.74 (t, *J* = 7.8 Hz, 1H), 6.49 (d, *J* = 7.8 Hz, 2H), 5.31 (d, *J* = 2.4 Hz, 1H), 5.01 (d, J = 2.4 Hz, 1H), 4.66 (dd, *J* = 6.6, 4.2 Hz, 1H), 4.40 (dd, *J* = 8.4, 6.6 Hz, 1H), 3.98 (dd, *J* = 8.4, 4.2 Hz, 1H), 3.79 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 160.3, 145.3, 143.5, 130.1, 129.4, 118.7, 117.9, 113.0, 112.9, 112.1, 83.0, 75.8, 61.9, 55.4; FT-IR (neat) 3040, 2998, 2933, 2866, 2836, 1600, 1494, 1346, 1261, 1148, 1090, 1045, 973, 946, 786, 749 cm^{-1}; HRMS (ESI) m/z $[M+H]^+$ calcd for $[C_{16}H_{17}NO_2+H]^+$ 256.1332, found 256.1341.





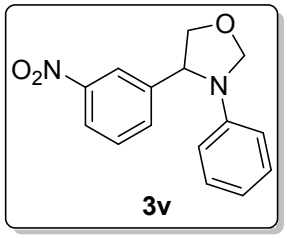
3-Phenyl-4-(*m*-tolyl)oxazolidine 3t. Analytical TLC on silica gel, 1:19 ethyl acetate/hexane R_f = 0.60; Colorless liquid; 89 mg, yield 74%; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.25 (t, *J* = 7.8 Hz, 1H), 7.21-7.16 (m, 4H), 7.12 (d, *J* = 7.2 Hz, 1H), 6.76 (t, *J* = 7.2 Hz, 1H), 6.51 (d, *J* = 7.8 Hz, 2H), 5.34 (d, *J* = 2.4 Hz, 1H), 5.04 (d, *J* = 2.4 Hz, 1H), 4.68 (dd, *J* = 7.2, 4.8 Hz, 1H), 4.41 (dd, *J* = 8.4, 6.6 Hz, 1H), 3.99 (dd, *J* = 8.4, 4.2 Hz, 1H), 2.36 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 145.3, 141.7, 138.7, 129.4, 128.9, 128.6, 126.9, 123.4, 117.8, 112.9, 83.0, 76.0, 61.9, 21.7; FT-IR (neat) 3032, 2961, 2920, 2860, 1601, 1506, 1390, 1345, 1258, 1172, 1090, 946, 748 cm^{-1}; HRMS (ESI) m/z $[M+H]^+$ calcd for $[C_{16}H_{17}NO+H]^+$ 240.1383, found 240.1389.

4-(3-Fluorophenyl)-3-phenyloxazolidine 3u. Analytical TLC on silica gel, 1:5 ethyl acetate/hexane R_f = 0.40; Brown liquid; 85 mg, yield 70%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35-7.30 (m, 1H), 7.21 (t, *J* = 7.6 Hz, 2H), 7.16 (d, *J* = 7.6 Hz, 1H), 7.10 (d, *J* = 9.6 Hz, 1H), 6.98 (t, *J* = 9.2 Hz, 1H), 6.78 (t, *J* = 7.6 Hz, 1H), 6.50 (d, *J* = 8.4 Hz, 2H), 5.33 (d, *J* = 2.0 Hz, 1H), 5.02 (d, *J* = 2.0 Hz, 1H), 4.71 (dd, *J* = 6.8, 4.4 Hz, 1H), 4.39 (t, *J* = 8.4 Hz, 1H), 4.00 (dd, *J* = 8.4, 4.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.7 (d, *J* = 245.0 Hz), 145.0, 130.6 (d, *J* = 8.0 Hz), 129.5, 122.0 (d, *J* = 3.0 Hz), 118.2, 114.8 (d, *J* = 22.0 Hz), 113.5 (d, *J* = 22.0 Hz), 113.0, 82.9, 75.6, 61.5, 61.51; FT-IR (neat) 3436, 3064, 2991, 2929, 2867, 1601, 1503,

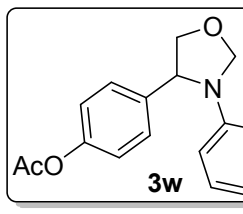


1448, 1391, 1347, 1173, 1089, 947, 871, 788, 750 cm^{-1}; HRMS (ESI) m/z $[M+H]^+$ calcd for $[C_{15}H_{14}FNO+H]^+$ 244.1132, found 244.1146.

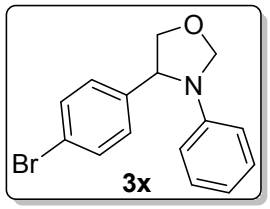
4-(3-Nitrophenyl)-3-phenyloxazolidine 3v. Analytical TLC on silica gel, 1:5 ethyl acetate/hexane R_f = 0.40; Brown liquid; 78 mg, yield 58%; ^1H NMR (400 MHz, $CDCl_3$) δ 8.23 (t, *J* = 2.0 Hz, 1H), 8.16-8.13 (m, 1H), 7.71 (d, *J* = 7.6 Hz, 1H), 7.53 (t, *J* = 8.0 Hz, 1H), 7.21 (dd, *J* = 8.8, 7.6 Hz, 2H), 6.78 (t, *J* = 7.2 Hz, 1H), 6.46 (d, *J* = 8.0 Hz, 2H), 5.38 (d, *J* = 2.4 Hz, 1H), 5.01 (d, *J* = 2.4 Hz, 1H), 4.80 (dd, *J* = 6.8, 4.4 Hz, 1H), 4.44 (dd, *J* = 8.8, 7.2 Hz, 1H), 4.01 (dd, *J* = 8.8, 3.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.9, 144.6, 144.4, 132.6, 130.1, 129.7, 123.0, 121.5, 118.6, 113.0, 83.1, 75.5, 61.6.; FT-IR (neat) 3032, 2965, 2929, 2867, 1600, 1496, 1454, 1355, 1201, 1172, 1091, 945, 848 cm^{-1}; HRMS (ESI) m/z $[M+H]^+$ calcd for $[C_{15}H_{14}N_2O_3+H]^+$ 271.1077, found 271.1070.



4-(3-Phenyloxazolidin-4-yl)phenyl acetate 3w. Analytical TLC on silica gel, 1:19 ethyl acetate/hexane R_f = 0.50; Colorless liquid; 114 mg, yield 80%; ^1H NMR (600 MHz, $CDCl_3$) δ 7.36 (d, *J* = 7.8 Hz, 2H), 7.18 (t, *J* = 7.2 Hz, 2H), 7.07 (d, *J* = 9.0 Hz, 2H), 6.75 (t, *J* = 7.2 Hz, 1H), 6.47 (d, *J* = 7.8 Hz, 2H), 5.31 (d, *J* = 2.4 Hz, 1H), 5.00 (d, *J* = 2.4 Hz, 1H), 4.69 (dd, *J* = 6.6, 4.2 Hz, 1H), 4.38 (dd, *J* = 8.4, 6.6 Hz, 1H), 3.97 (dd, *J* = 8.4, 4.2 Hz, 1H), 2.29 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 169.7, 150.2, 145.1, 139.9, 129.5, 127.4, 122.1, 118.0, 113.0, 83.0, 75.8, 61.4, 21.4; FT-IR (neat) 3063, 3035, 2957, 2924, 2854, 1761, 1600, 1505, 1366, 1196, 1088, 1014, 942, 749 cm^{-1}; HRMS (ESI) m/z $[M+H]^+$ calcd for $[C_{17}H_{17}NO_3+H]^+$ 284.1281, found 284.1286.

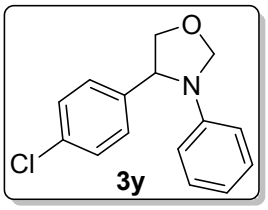


4-(4-Bromophenyl)-3-phenyloxazolidine 3x. Analytical TLC on silica gel, 1:19 ethyl acetate/hexane R_f = 0.60; Brown liquid; 114 mg, yield 75%; ^1H NMR (600 MHz, $CDCl_3$) δ 7.47 (d, *J* = 8.4 Hz, 2H), 7.24 (d, *J* = 8.4 Hz, 2H), 7.18 (t, *J* = 8.4 Hz, 2H), 6.76 (t, *J* = 7.2 Hz, 1H), 6.45 (d, *J* = 7.8 Hz, 2H), 5.31 (d, *J* = 2.4 Hz, 1H), 5.00 (d, *J* = 2.4 Hz, 1H), 4.65 (dd, *J* = 6.6, 4.2 Hz, 1H), 4.39 (dd, *J* = 8.4, 6.6 Hz, 1H), 4.95 (dd, *J* = 8.4, 4.2 Hz, 1H); ^{13}C NMR (150 MHz,

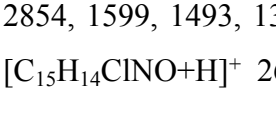


$CDCl_3$) δ 144.88, 140.79, 132.13, 129.50, 128.14, 121.54, 118.13, 112.91, 82.93, 75.67, 61.33; FT-IR (neat) 3043, 2989, 2926, 2864, 1599, 1505, 1403, 1346, 1263, 1165, 1070, 943, 749 cm^{-1}; HRMS (ESI) m/z $[M+H]^+$ calcd for $[C_{15}H_{14}BrNO+H]^+$ 304.0332, found 304.0330

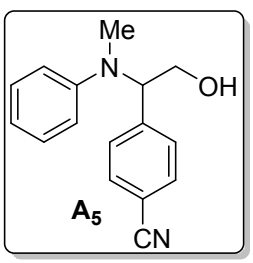
4-(4-Chlorophenyl)-3-phenyloxazolidine 3y. Analytical TLC on silica gel, 1:19 ethyl acetate/hexane R_f = 0.60; Pale yellow liquid; 101 mg, yield 78%; ^1H NMR (600 MHz, $CDCl_3$) δ 7.32-7.28 (m, 4H), 7.20 (dd, *J* = 8.4, 7.2 Hz, 2H), 6.76 (t, *J* = 7.2 Hz, 1H), 6.46 (d, *J* = 7.8 Hz, 2H), 5.31 (d, *J* = 2.4 Hz, 1H), 5.00 (d, *J* = 2.4 Hz, 1H), 4.67 (dd, *J* = 6.6, 4.2 Hz, 1H), 4.39 (dd, *J* = 8.4, 6.6 Hz, 1H), 3.95 (dd, *J* = 8.4, 4.2 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 144.9, 140.3, 133.5, 129.5, 129.2, 127.8, 118.1, 112.9, 82.9, 75.7, 61.3; FT-IR (neat) 3065, 3045, 2957, 2924, 2854, 1599, 1493, 1346, 1162, 1089, 1013, 643, 746cm^{-1}; HRMS (ESI) m/z $[M+H]^+$ calcd for $[C_{15}H_{14}ClNO+H]^+$ 260.0837, found 260.0838.



4-(4-Fluorophenyl)-3-phenyloxazolidine 3z. Analytical TLC on silica gel, 1:19 ethyl acetate/hexane R_f = 0.60; Brown liquid; 92 mg, yield 75%; ^1H NMR (600 MHz, $CDCl_3$) δ 7.36-7.34 (m, 2H), 7.21 (t, *J* = 7.8 Hz, 2H), 7.06 (t, *J* = 9.0 Hz, 2H), 6.78 (t, *J* = 7.2 Hz, 1H), 6.49 (d, *J* = 8.4 Hz, 2H), 5.35 (d, *J* = 2.4 Hz, 1H), 5.03 (d, *J* = 2.4 Hz, 1H), 4.71 (dd, *J* = 7.2, 4.2 Hz, 1H), 4.41 (dd, *J* = 8.4, 7.2 Hz, 1H), 3.98 (dd, *J* = 8.4, 4.2 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 163.2 (d, *J* = 224.5 Hz), 145.0, 137.4 (d, *J* = 3.0 Hz), 129.5, 127.9 (d, *J* = 9.0 Hz), 118.0, 116.0 (d, *J* = 21.0 Hz), 112.9, 82.9, 75.9, 61.2; FT-IR (neat) 3040, 2994, 2928, 2865, 1836, 1601, 1507, 1348, 1222, 1155, 1090, 943, 749 cm^{-1}; HRMS (ESI) m/z $[M+H]^+$ calcd for $[C_{15}H_{14}FNO+H]^+$ 244.1132, found 244.1144.

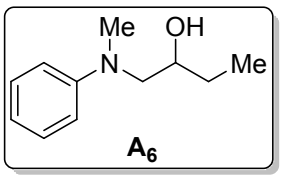


4-(2-Hydroxy-1-(methyl(phenyl)amino)ethyl)benzonitrile A_5. Analytical TLC on silica gel, 1:4 ethyl acetate/hexane R_f = 0.42; Yellow liquid; 103 mg, yield 82%; ^1H NMR (400 MHz, $CDCl_3$) 7.61 (d, *J* = 8.4 Hz, 2H), 7.29-7.25 (m, 4H), 6.91 (d, *J* = 8.0 Hz, 2H), 6.85 (t, *J* = 7.2 Hz, 1H), 5.08 (t, *J* = 7.2 Hz, 1H), 4.18-4.10 (m, 2H), 2.73 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.7, 143.7, 132.6, 129.7, 128.2, 119.2, 118.8, 115.0, 111.8, 64.6, 61.8, 32.7; FT-IR



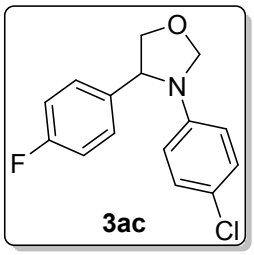
(neat) 3440, 3063, 3034, 2957, 2924, 2216, 1604, 1519, 1386, 1346, 1178, 1111, 1063, 818 cm^{-1}; HRMS (ESI) m/z $[M+H]^+$ calcd for $[C_{16}H_{16}N_2O+H]^+$ 253.1335, found 253.1350.

1-(Methyl(phenyl)amino)butan-2-ol A_6. Analytical TLC on silica gel, 1:5 ethyl acetate/hexane

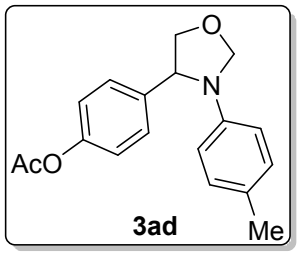


R_f = 0.40; Brown liquid; 81 mg, yield 90%; ^1H NMR (400 MHz, $CDCl_3$) δ 7.28 (m, 2H), 6.84 (d, *J* = 8.0 Hz, 2H), 6.78 (t, *J* = 7.2 Hz, 1H), 3.88-3.82 (m, 1H), 3.31-3.20 (m, 2H), 2.96 (s, 3H), 2.37 (br s, 1H), 1.61-1.47 (m, 2H), 1.05 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.6, 129.3, 117.5, 113.5, 70.7, 60.3, 39.5, 27.6, 10.1; FT-IR (neat) 3410, 3093, 3061, 2964, 2931, 2877, 1600, 1505, 1369, 1242, 1208, 987, 856, 749 cm^{-1}; HRMS (ESI) m/z $[M+H]^+$ calcd for $[C_{11}H_{17}NO+H]^+$ 180.1383, found 180.1408.

3-(4-Chlorophenyl)-4-(4-fluorophenyl)oxazolidine 3ac. Analytical TLC on silica gel, 1:19 ethyl acetate/hexane R_f = 0.58; Pale yellow liquid;101 mg, yield 73% ; ^1H NMR (600 MHz, $CDCl_3$) δ 7.30-7.27 (m, 2H), 7.12 (d, *J* = 9.0 Hz, 2H), 7.03 (t, *J* = 8.4 Hz, 2H), 6.36 (d, *J* = 9.0 Hz, 2H), 5.28 (d, *J* = 2.4 Hz, 1H), 4.96 (d, *J* = 2.4 Hz, 1H), 4.64 (dd, *J* = 6.6, 4.2 Hz, 1H), 4.40 (dd, *J* = 8.4, 6.6 Hz, 1H), 3.94 (dd, *J* = 9.0, 4.8 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 163.3 (d, *J* = 244.5 Hz), 143.5, 136.8 (d, *J* = 3.0 Hz), 129.3, 127.9 (d, *J* = 127.0 Hz), 123.0, 116.1 (d, *J* = 21.0 Hz), 114.0, 82.9, 75.9, 61.3; FT-IR (neat) 3073, 3049, 2992, 2925, 2860, 1601, 1507, 1391, 1356, 1223, 1156, 1093, 945, 810, 765 cm^{-1}; HRMS (ESI) m/z $[M+H]^+$ calcd for $[C_{15}H_{13}ClFNO+H]^+$ 278.0742 found 278.0749.

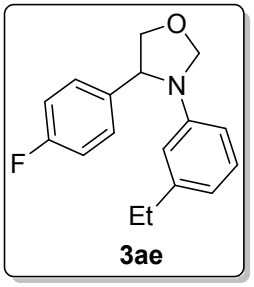


4-(3-(*p*-Tolyl)oxazolidin-4-yl)phenyl acetate 3ad. Analytical TLC on silica gel, 1:9 ethyl acetate/hexane R_f = 0.40; Yellow liquid; 113 mg, yield 76%; ^1H NMR (600 MHz, $CDCl_3$) δ 7.37 (d, *J* = 8.4 Hz, 2H), 7.06 (d, *J* = 8.4 Hz, 2H), 7.00 (d, *J* = 8.4 Hz, 2H), 6.40 (d, *J* = 8.4 Hz, 2H), 5.30 (d, *J* = 2.4 Hz, 1H), 4.97 (d, *J* = 2.4 Hz, 1H), 4.66 (dd, *J* = 7.2, 4.8 Hz, 1H), 4.38 (dd, *J* = 8.4, 6.6 Hz, 1H), 3.96 (dd, J = 8.4, 4.2 Hz, 1H), 2.29 (s, 3H), 2.22 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 169.7, 150.1, 143.1, 139.3, 130.0, 127.4, 127.3, 122.1, 113.1, 83.3, 75.8, 61.6, 21.4, 20.5; FT-IR (neat) 3006, 2923, 2860, 1763, 1619, 1521, 1366,



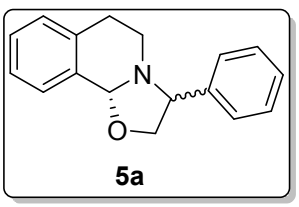
1214, 1088, 943,804 cm^{-1}. HRMS (ESI) m/z $[M+H]^+$ calcd for $[C_{18}H_{19}NO_3+H]^+$ 298.1438, found 298.1448.

3-(3-Ethylphenyl)-4-(4-fluorophenyl)oxazolidine 3ae. Analytical TLC on silica gel, 1:9 ethyl acetate/hexane R_f = 0.60; Brown liquid; 97 mg, yield 71%; ^1H NMR (600 MHz, $CDCl_3$) δ 7.34-7.31 (m, 2H), 7.09 (t, *J* = 7.8 Hz, 1H), 7.03 (t, *J* = 9.0 Hz, 2H), 6.62 (d, *J* = 7.2 Hz, 1H), 6.30-6.27 (m, 2H), 5.32 (d, *J* = 1.2 Hz, 1H), 5.00 (d, *J* = 2.4 Hz, 1H), 4.68 (dd, *J* = 7.2, 4.2 Hz, 1H), 4.37 (dd, *J* = 8.4, 6.6 Hz, 1H), 3.95 (dd, *J* = 8.4, 4.2 Hz, 1H), 2.56 (q, *J* = 7.2 Hz, 2H), 1.17 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 163.2 (d, *J* = 243.0 Hz), 145.7, 145.1, 137.6 (d, *J* = 3.0 Hz), 129.4, 128.0 (d, *J* = Hz), 117.7, 115.9 (d, *J* = 21.0 Hz), 112.5, 110.4, 83.0, 75.8, 61.2, 29.3, 15.7; FT-IR (neat) 3041, 2962, 2926, 2856, 1604, 1507, 1455, 1356, 1223, 1155, 1090, 945, 836, 752cm^{-1}; HRMS (ESI) m/z $[M+H]^+$ calcd for $[C_{17}H_{18}FNO+H]^+$ 272.1445, found 272.1447.



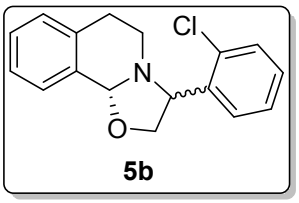
3ae

3-Phenyl-2,3,6,10b-tetrahydro-5H-oxazolo[2,3-a]isoquinoline 5a. Analytical TLC on silica gel, 1:19 ethyl acetate/hexane R_f = 0.50; Colorless liquid; 95 mg, yield 75%; 9:1 Mixture of diasteroisomers; ^1H NMR (600 MHz, $CDCl_3$) δ 7.46 (d, *J* = 7.2 Hz, 2H), 7.42-7.41 (m, 1H), 7.37 (t, *J* = 7.8 Hz, 2H), 7.29-7.25 (m, 3H), 7.19-7.17 (m, 1H), 5.45 (s, 1H), 4.47 (t, *J* = 7.8 Hz, 1H), 4.32 (t, *J* = 6.6 Hz, 1H), 3.82 (dd, *J* = 7.8, 6.0 Hz, 1H), 3.08-2.97 (m, 3H), 2.83-2.80 (m, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 141.9, 135.7, 132.9, 128.8, 128.7, 128.3, 128.3, 127.4, 126.8, 126.6, 90.3, 71.4, 68.8, 46.9, 29.3; FT-IR (neat) 3063, 3030, 2924, 2853, 1711, 1682, 1455, 1373, 1314, 1234, 1030, 941, 746, 699 cm^{-1}; HRMS (ESI) m/z $[M+H]^+$ calcd for $[C_{17}H_{17}NO+H]^+$ 252.1383, found 252.1394.



5a

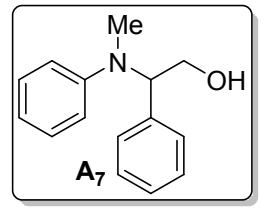
3-(2-Chlorophenyl)-2,3,6,10b-tetrahydro-5H-oxazolo[2,3-a]isoquinoline 5b. Analytical TLC on silica gel, 1:19 ethyl acetate/hexane R_f = 0.50; Colorless liquid; 97 mg, yield 68%; 9:1 mixture of diasteroisomers; ^1H NMR (400 MHz, $CDCl_3$) δ 7.79 (d, *J* = 7.2 Hz, 1H), 7.42 (m, 2H), 7.30-7.19 (m, 5H), 5.37 (s, 1H), 4.68-4.59 (m, 2H), 3.63 (dd, *J* = 7.6, 5.6 Hz, 1H), 3.14-2.99 (m, 3H), 2.84-2.78 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 135.8, 129.8, 128.9, 128.5,



5b

128.5, 128.3, 127.6, 127.2, 126.6, 100.2, 90.3, 70.9, 67.2, 47.2, 29.9; FT-IR (neat) 3066, 2953, 2924, 2853, 1649, 1464, 1440, 1396, 1257, 1127, 1034, 942, 750 cm^{-1}; HRMS (ESI) m/z $[M+H]^+$ calcd for $[C_{17}H_{16}ClNO+H]^+$ 286.0993, found 286.1003.

3-(4-Fluorophenyl)-2,3,6,10b-tetrahydro-5H-oxazolo[2,3-a]isoquinoline 5c. Analytical TLC on silica gel, 1:19 ethyl acetate/hexane R_f = 0.50; Colorless liquid; 97 mg, yield 72%; 9:1 Mixture of diasteroisomers; ^1H NMR (600 MHz, $CDCl_3$) δ 7.43-7.40 (m, 3H), 7.28-7.25 (m, 2H), 7.19-7.17 (m, 1H), 7.05 (t, *J* = 8.4 Hz, 2H), 5.42 (s, 1H), 4.45 (t, *J* = 7.8 Hz, 1H), 4.28 (t, *J* = 7.2 Hz, 1H), 3.77 (dd, *J* = 8.4, 6.6 Hz, 1H), 3.07-2.95 (m, 3H), 2.83-2.80 (m, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 163.1 (d, *J* = 244.5 Hz), 137.6 (d, *J* = 4.5 Hz), 135.6, 132.9, 128.7, 128.4 (d, *J* = 7.5 Hz), 128.4, 128.3, 126.7, 115.7 (d, *J* = 21 Hz), 90.2, 71.5, 68.1, 46.9, 29.2; FT-IR (neat) 3067, 2957, 2924, 2854, 1637, 1508, 1424, 1223, 1154, 1096, 1033, 834, 746 cm^{-1}; HRMS (ESI) m/z $[M+H]^+$ calcd for $[C_{17}H_{16}FNO+H]^+$ 270.1289, found 270.1301.

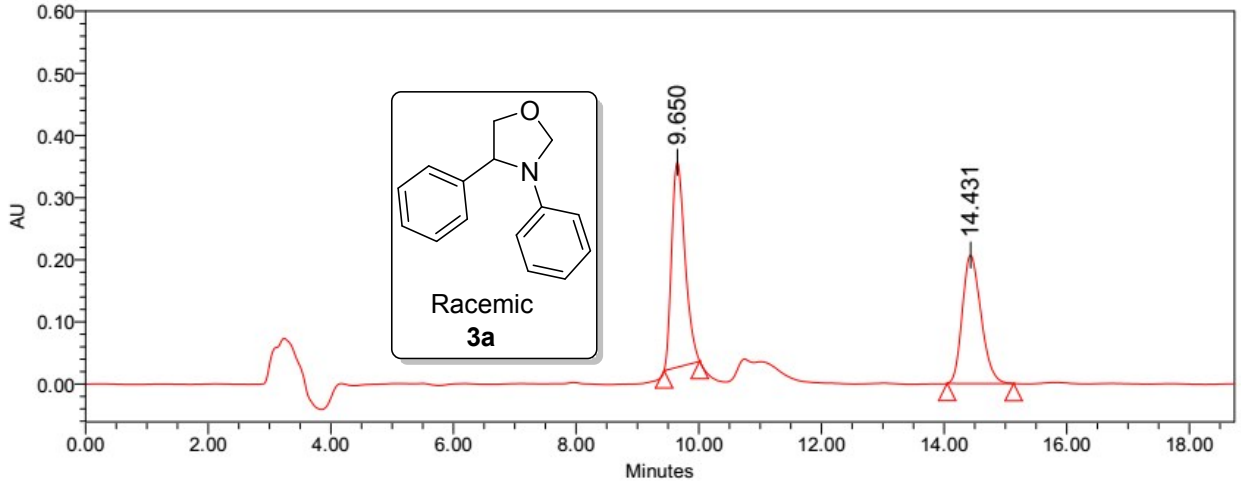


2-(Methyl(phenyl)amino)-2-phenylethan-1-ol A_7. Analytical TLC on silica gel, 1:5 ethyl acetate/hexane R_f = 0.40; Yellow liquid; 64 mg, yield 56%; ^1H NMR (400 MHz, $CDCl_3$) δ 7.35-7.27 (m, 5H), 7.17 (d, *J* = 6.8 Hz, 2H), 6.97 (d, *J* = 8.0 Hz, 2H), 6.84 (t, *J* = 7.2 Hz, 1H), 5.13 (dd, *J* = 8.4, 6.0 Hz, 1H), 4.18-4.10 (m, 2H), 2.74 (s, 3H), 2.22 (br s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.3, 137.7, 129.4, 128.7, 127.7, 127.4, 118.5, 114.9, 64.7, 61.9, 32.3; FT-IR (neat) 3401, 3087, 3060, 3027, 2943, 2816, 1598, 1504, 1450, 1379, 1319, 1065, 1030, 900, 750 cm^{-1}; HRMS (ESI) m/z $[M+H]^+$ calcd for $[C_{15}H_{17}NO+H]^+$ 228.1383, found 228.1398.

References

1. B. S. Furniss, A. J. Hannaford, P. W. G. Smith and A. R. Tatchell, *In Vogel's Textbook of Practical Organic Chemistry*, Fifth Edition, Pearson Education Pvt. Ltd., Indian Branch, Delhi, 2004, 928.
2. W. Qu, M.-P. Kung, C. Hou, T. E. Benedum and H. F. Kung, *J. Med. Chem*. 2007, **50**, 2157

HPLC Chromatograms of compounds 3



Peak Results

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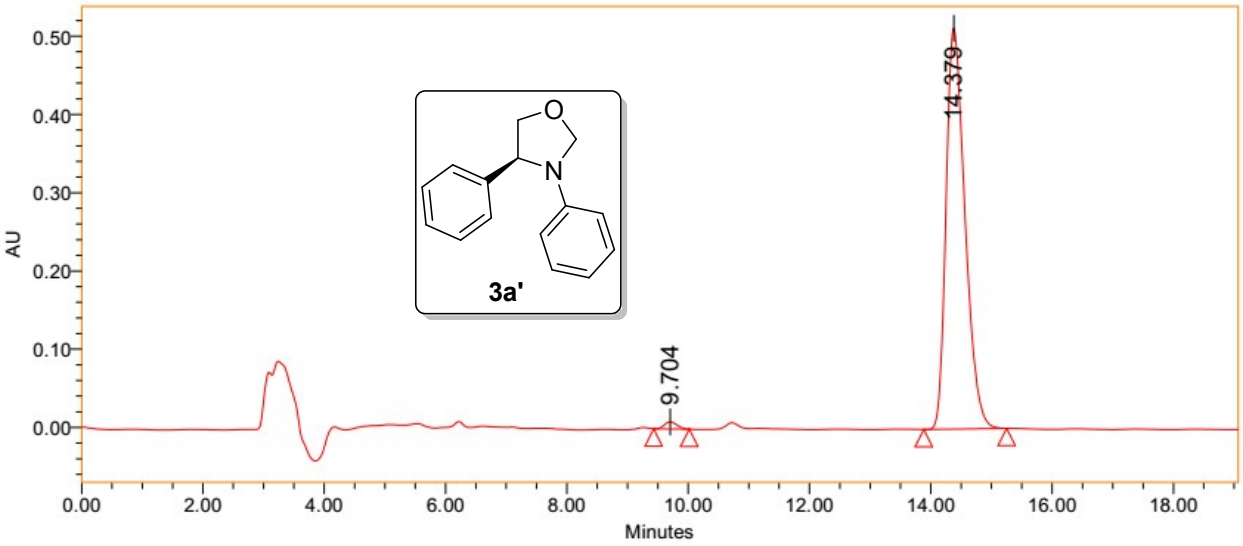

Peak Results

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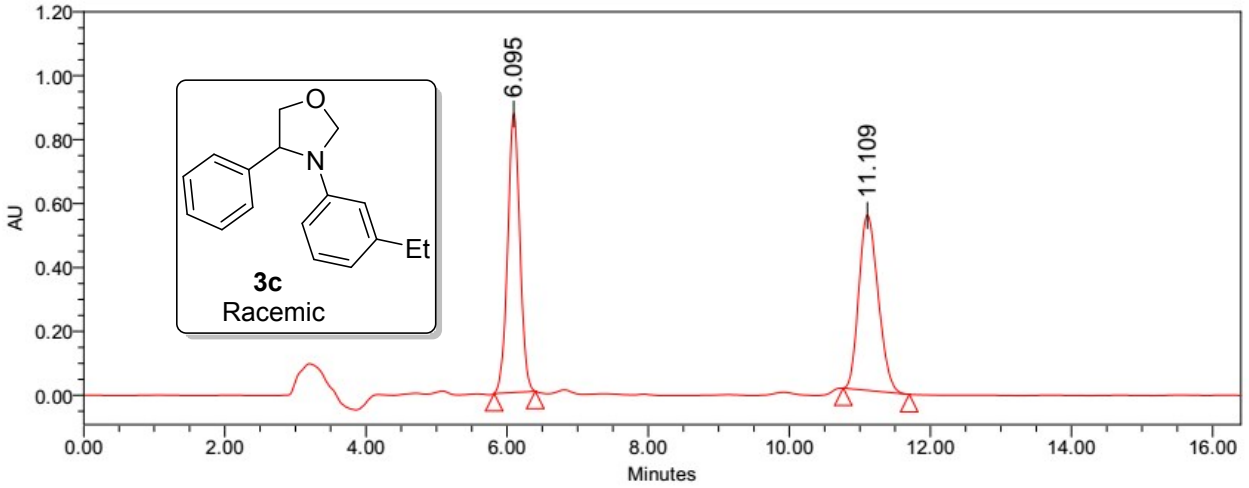

Peak Results

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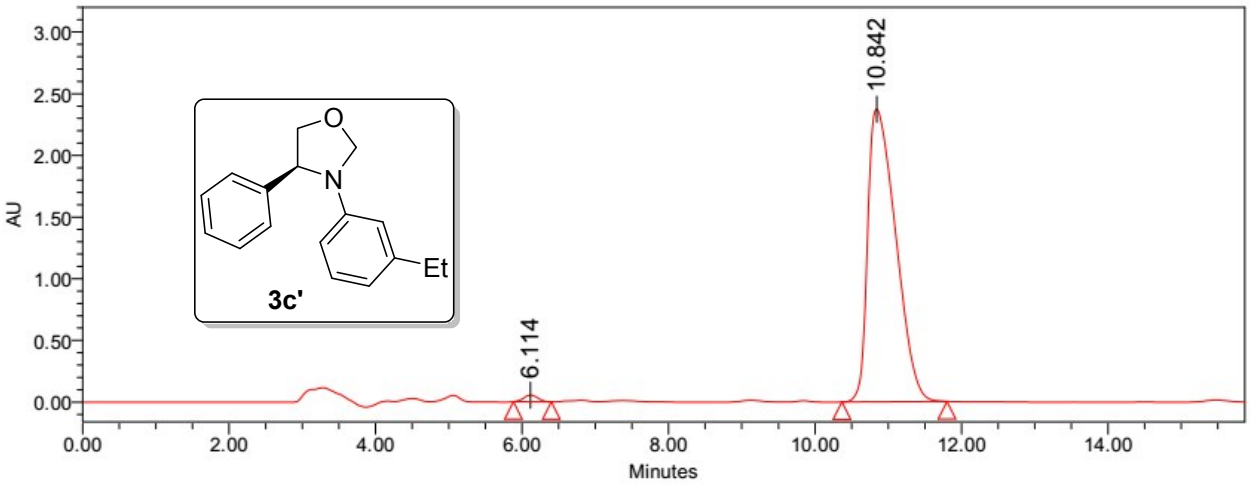

Peak Results

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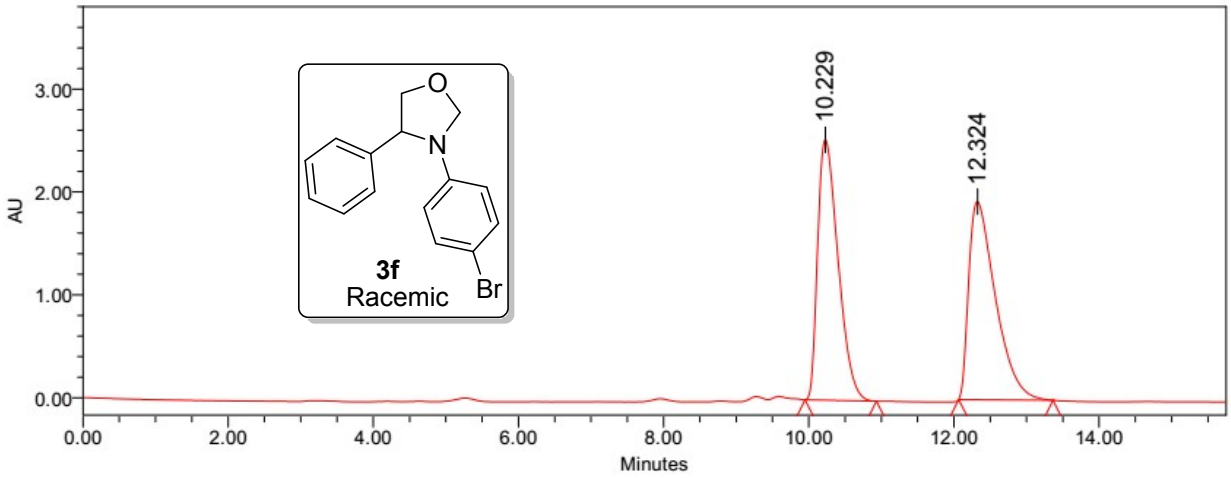

Peak Results

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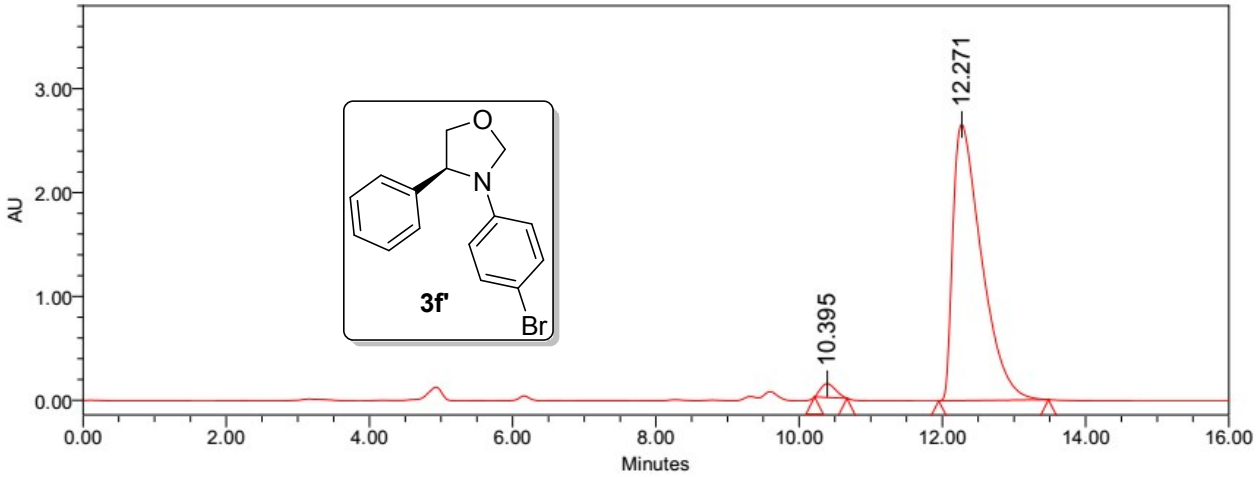

Peak Results

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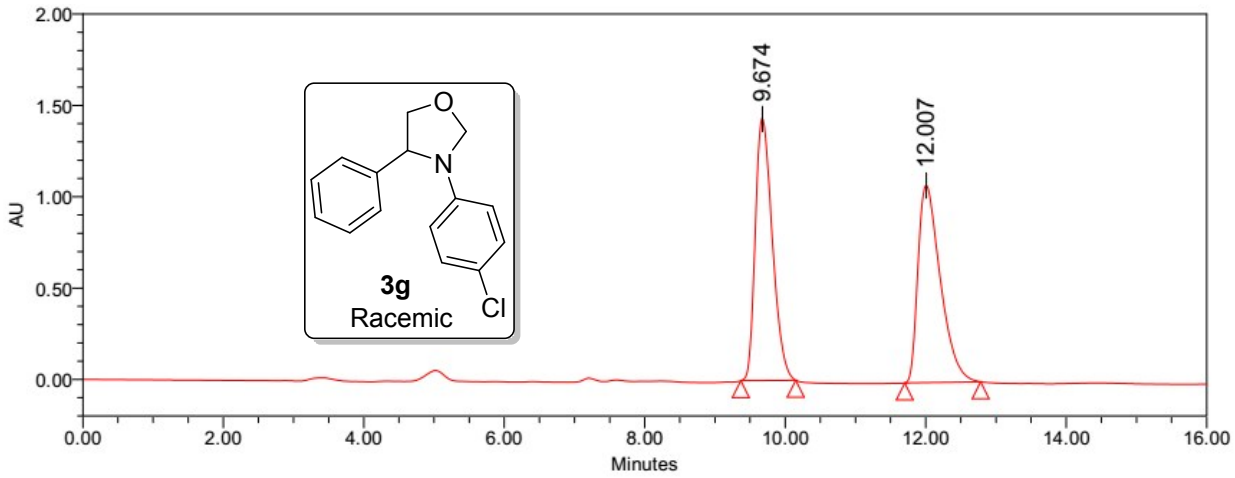

Peak Results

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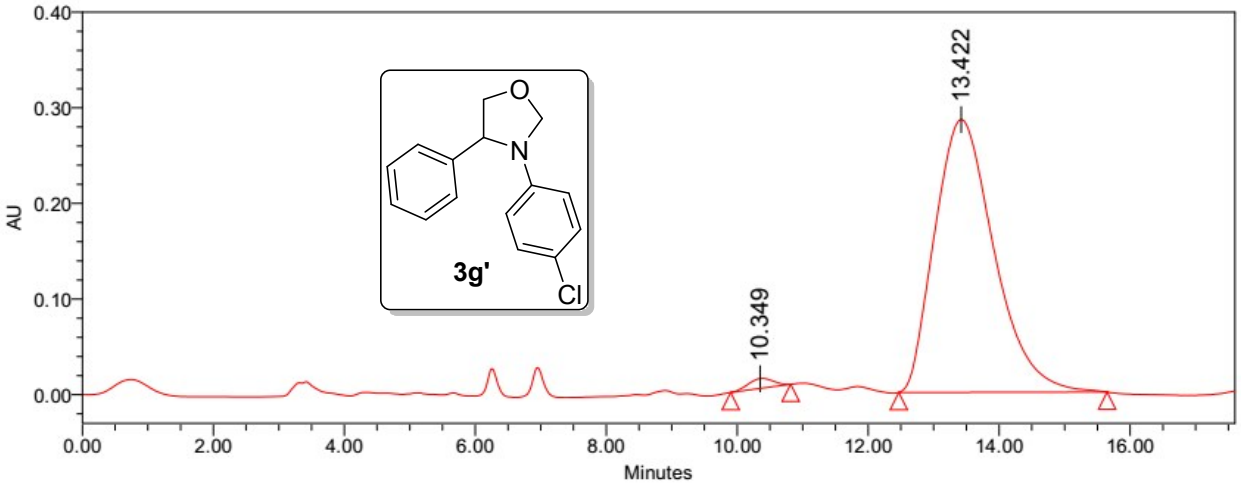

Peak Results

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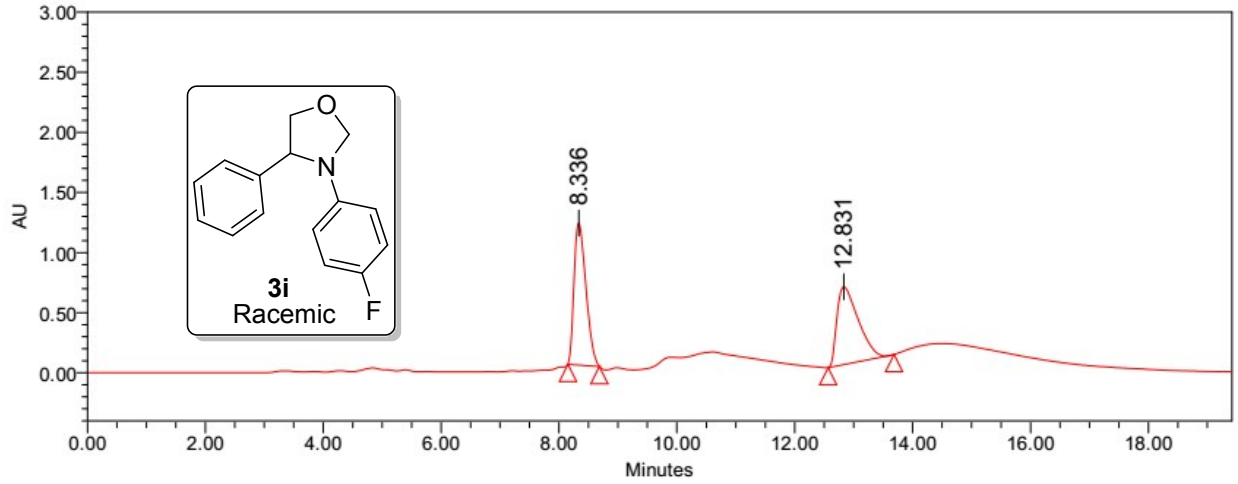

Peak Results

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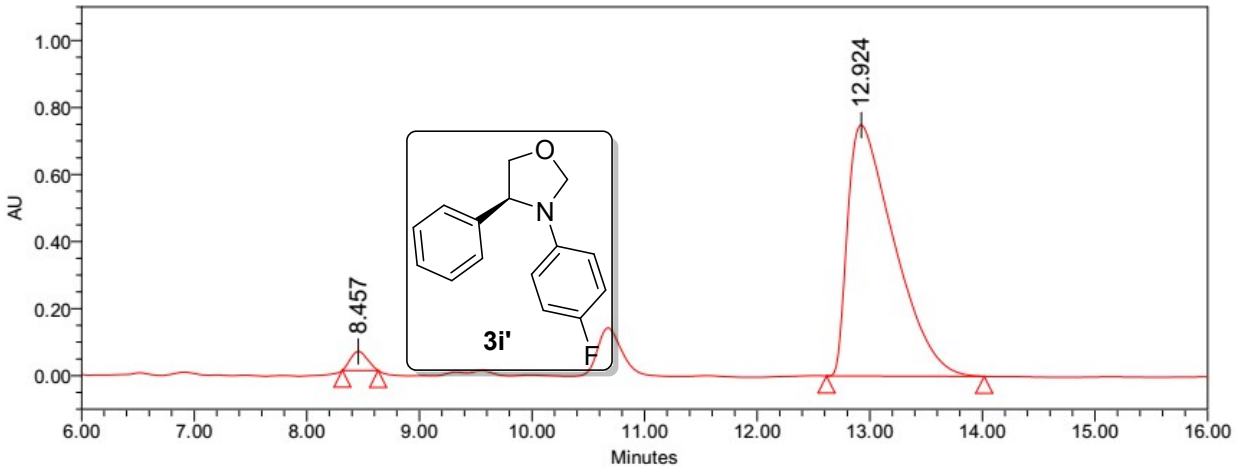

Peak Results

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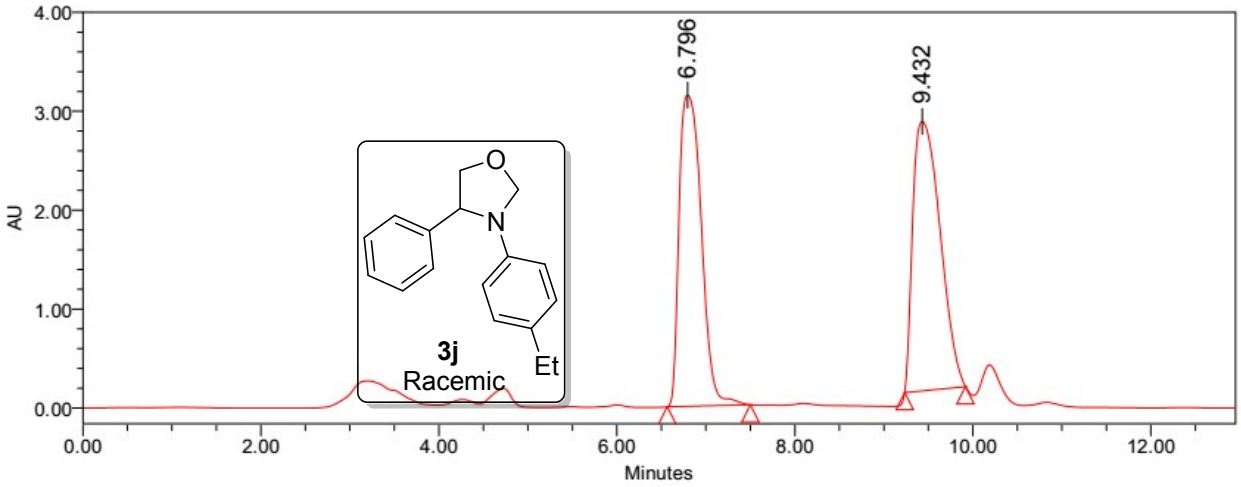
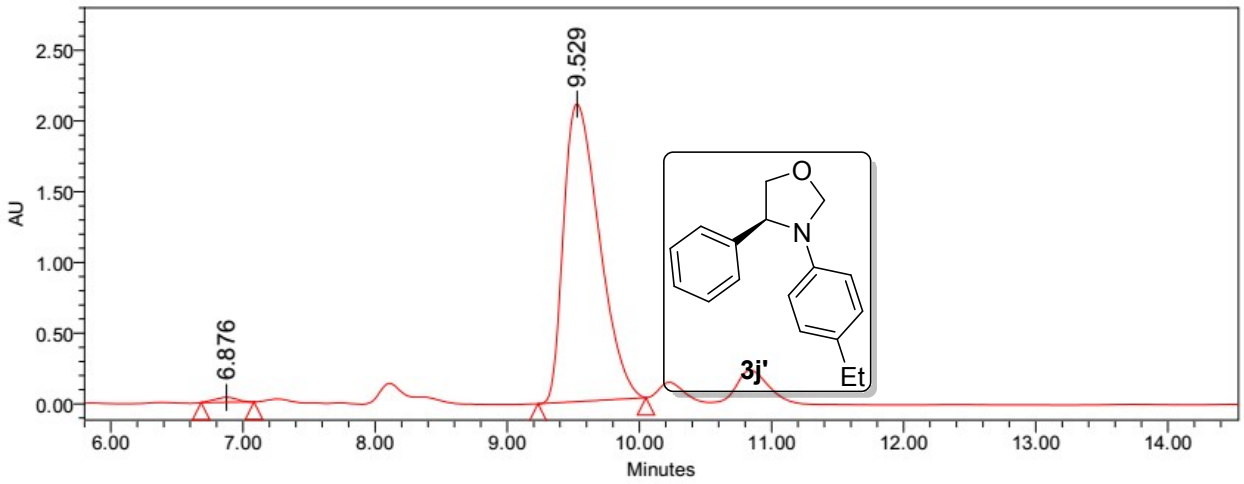
2	12.924	749816	97.34



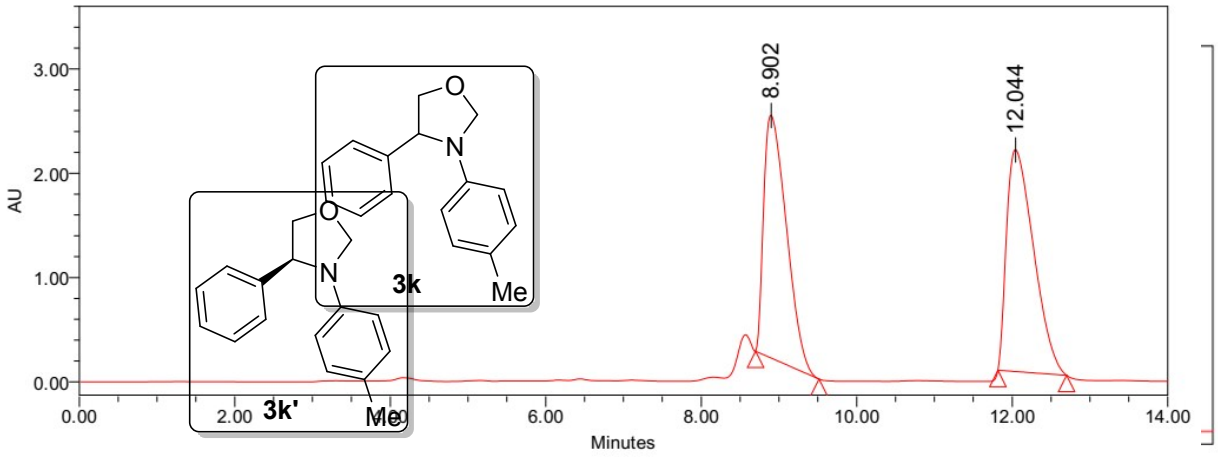
Peak Results

	RT	Height (μV)	% Area
1	6.796	3147644	48.45
2	9.432	2724719	51.55



Peak Results

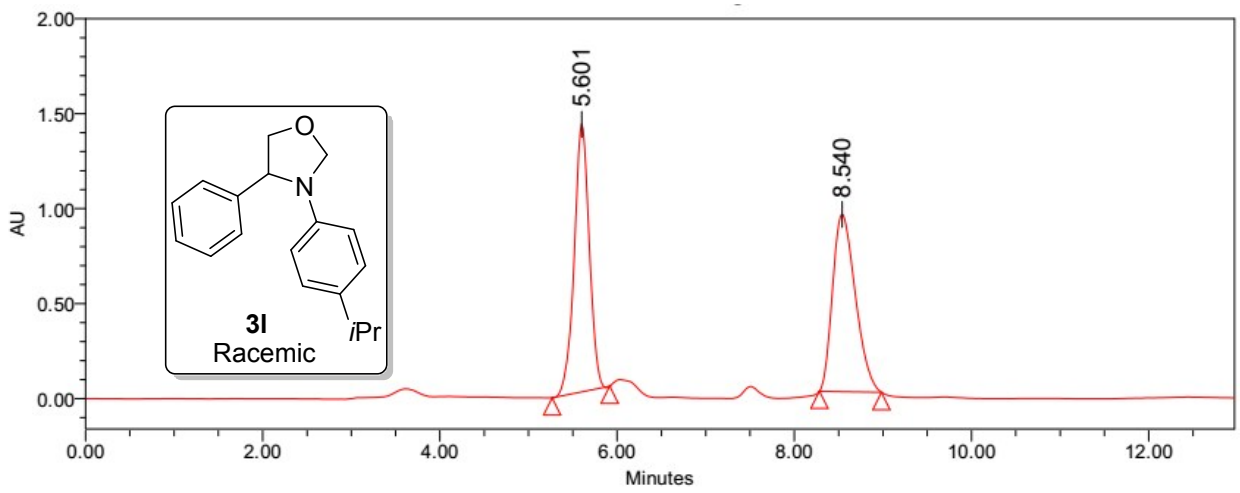
	RT	Height (μV)	% Area
1	6.876	35123	1.02
2	9.529	2105040	98.98



Peak Results

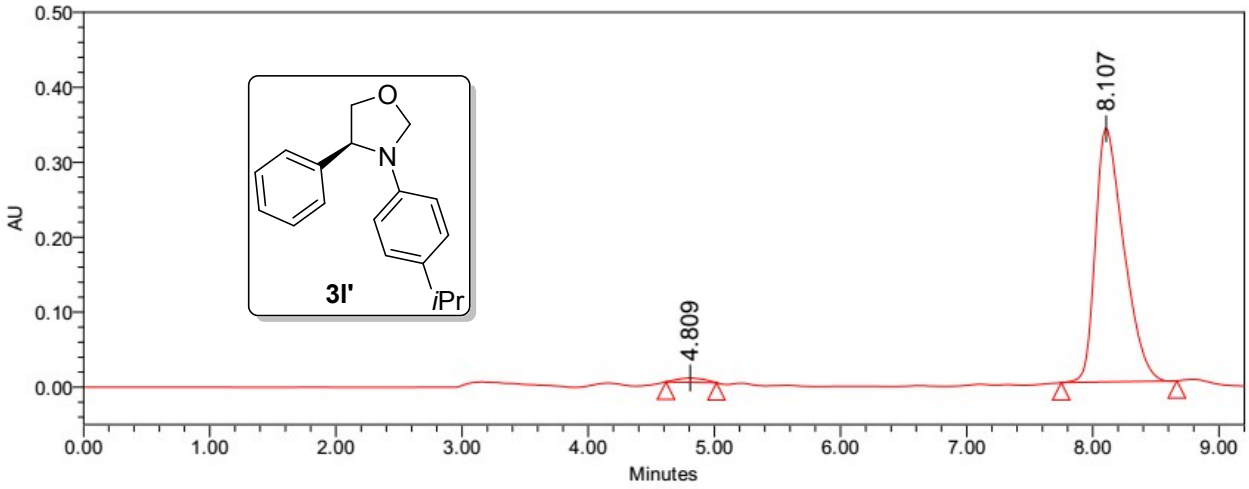
	RT	Height (μV)	% Area
1	8.902	2328562	47.96
2	12.044	2127078	52.04

2	12.024	2101136	99.86



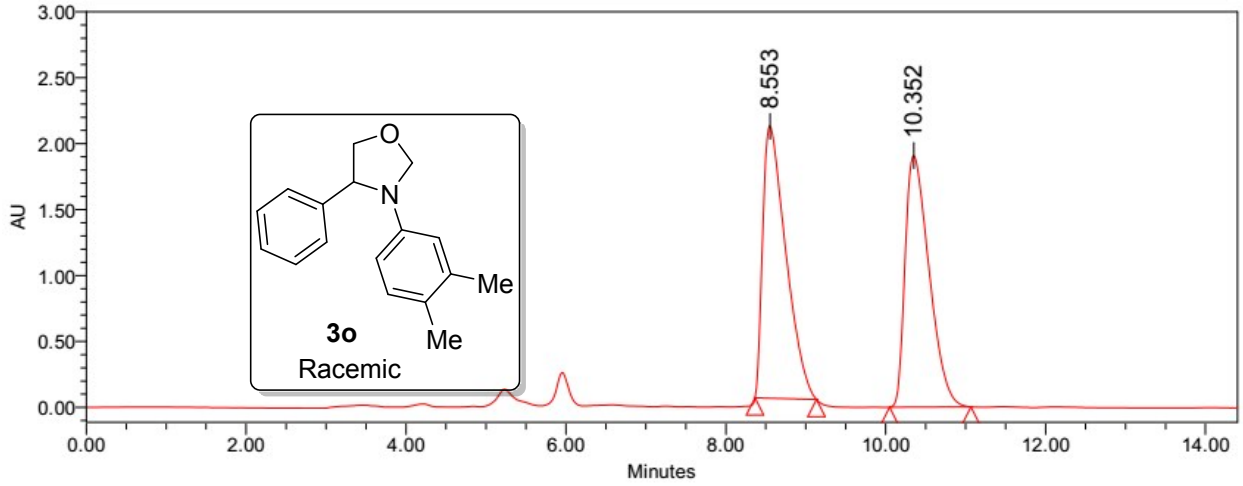
Peak Results

	RT	Height (μV)	% Area
1	5.601	1409422	49.90
2	8.540	935027	50.10



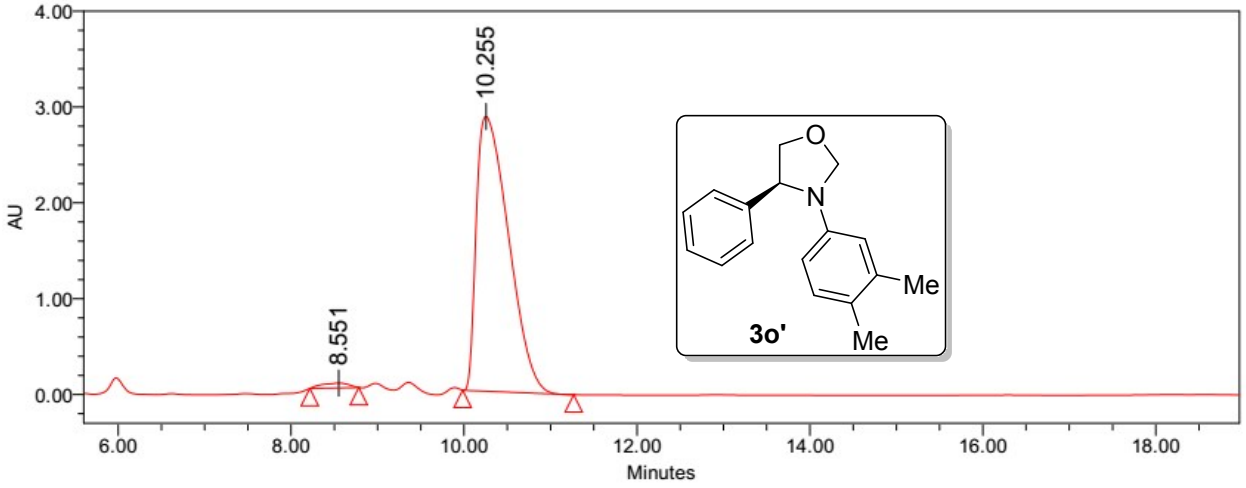
Peak Results

	RT	Height (μV)	% Area
1	4.809	5741	1.61
2	8.107	339400	98.39



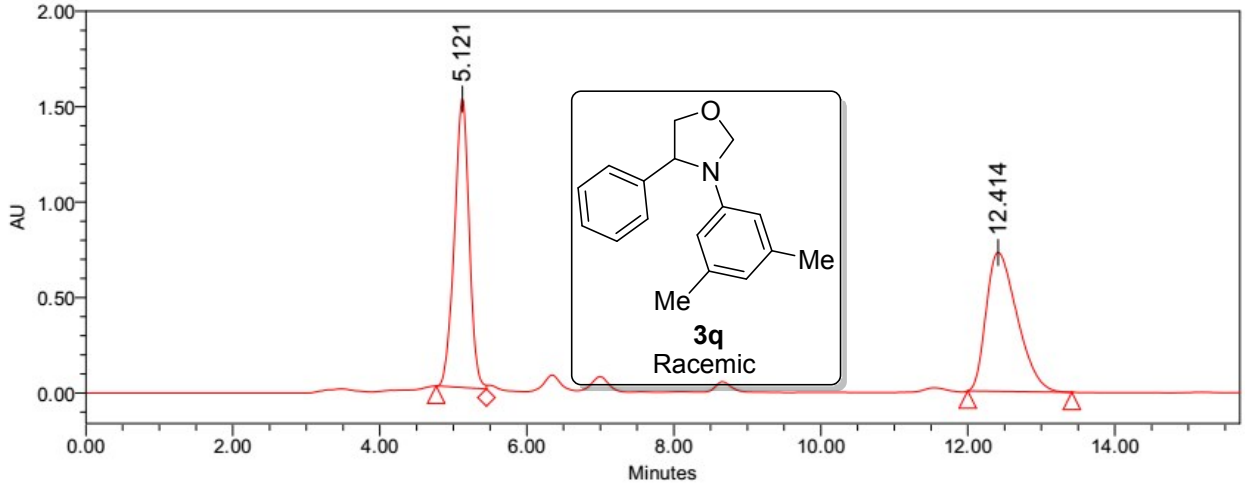
Peak Results

	RT	Height (μV)	% Area
1	8.553	2065959	50.99
2	10.352	1908580	49.01



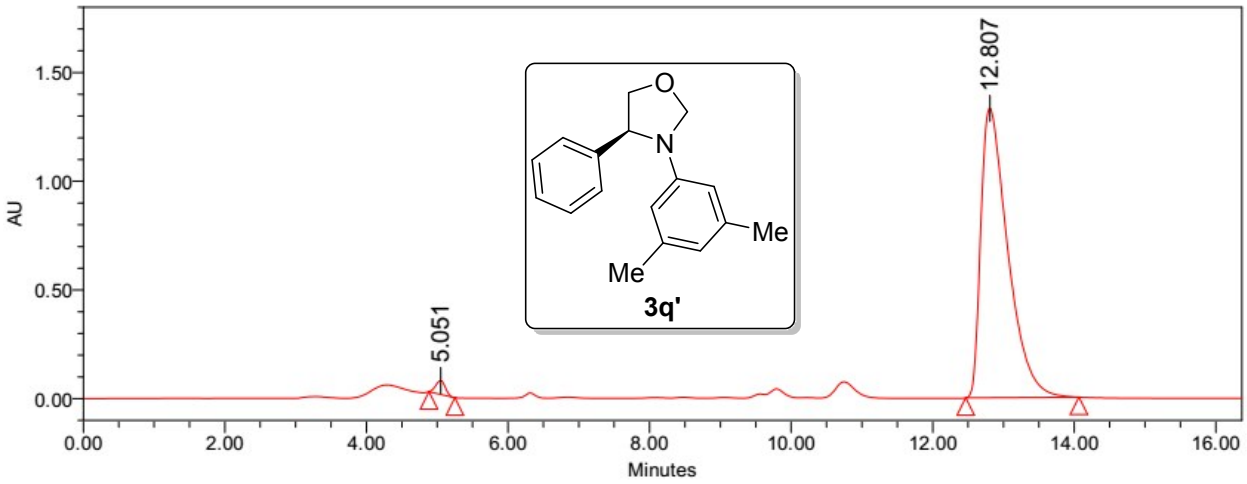
Peak Results

	RT	Height (μV)	% Area
1	8.551	49730	1.48
2	10.255	2870291	98.52



Peak Results

	RT	Height (μV)	% Area
1	5.121	1515064	49.71
2	12.414	728142	50.29

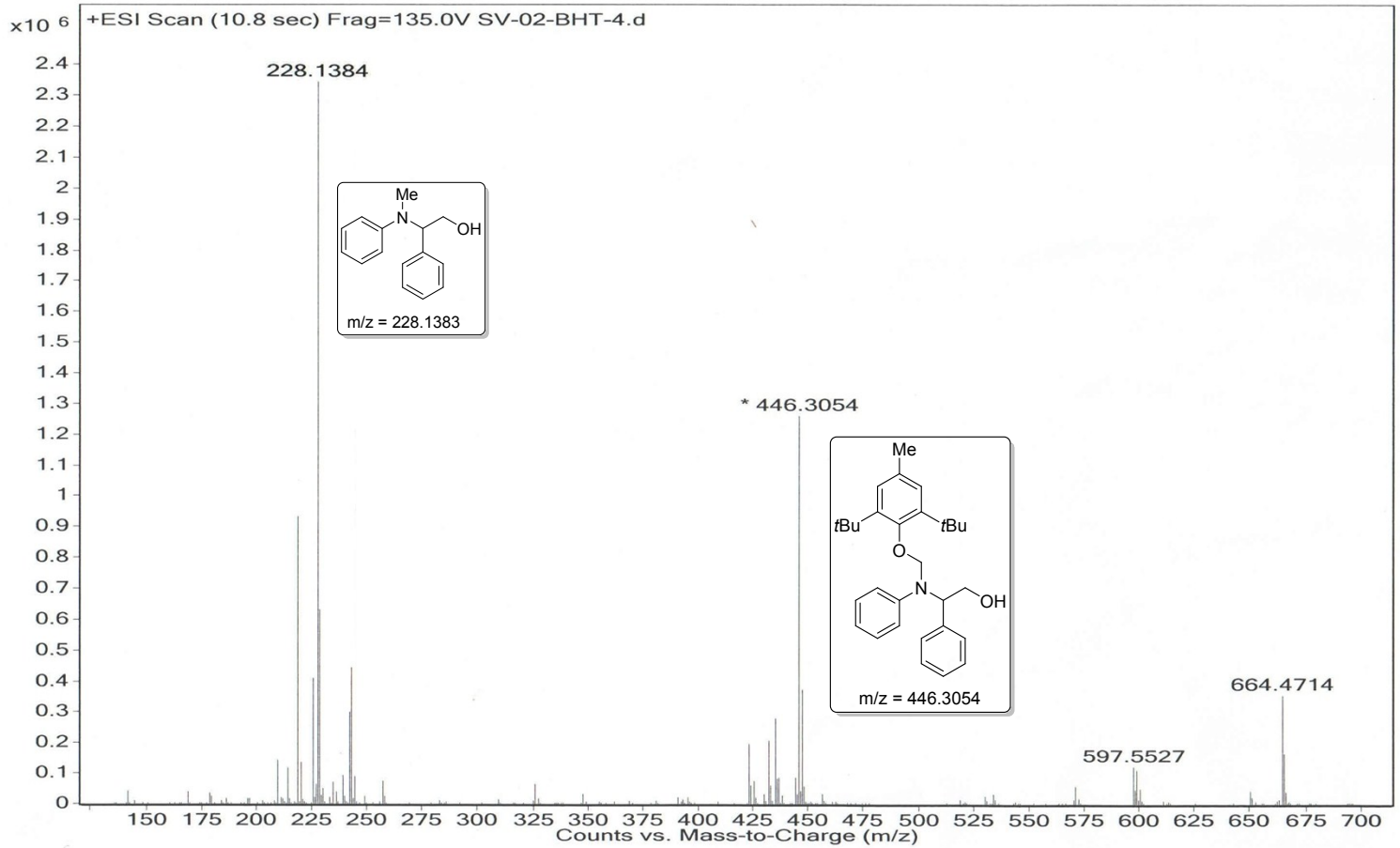


Peak Results

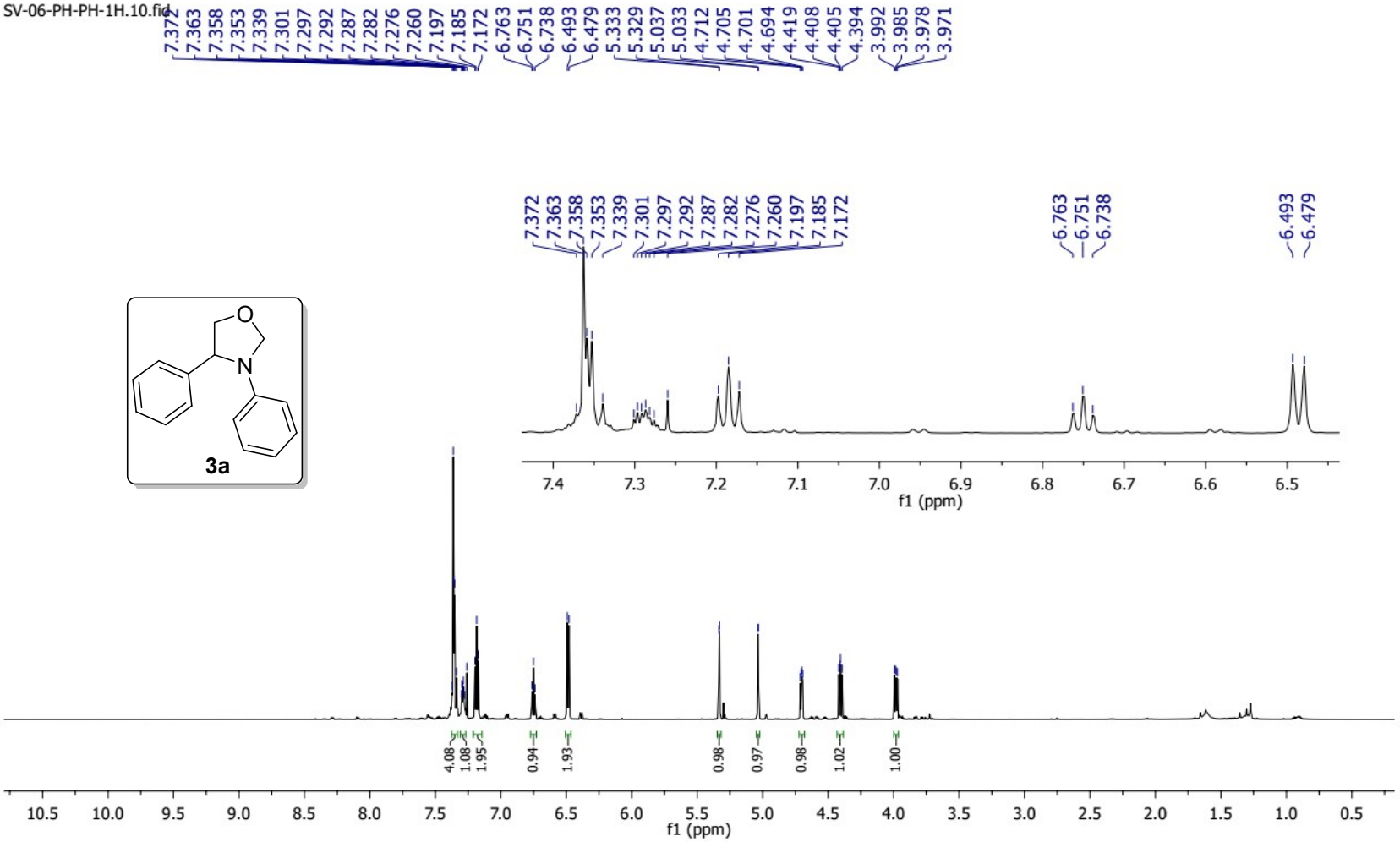
	RT	Height (μV)	% Area
1	5.051	64189	1.67
2	12.807	1333216	98.33

ESI-MS Spectrum of radical trapping experiment

Sample Name	Unavailable	**Position**	Unavailable	**Instrument Name**	Unavailable	**User Name**	Unavailable
Inj Vol	Unavailable	**InjPosition**	Unavailable	**SampleType**	Unavailable	**IRM Calibration Status**	Some Ions Missed
Data Filename	SV-02-BHT-4.d	**ACQ Method**		**Comment**	Sample information is unavailable	**Acquired Time**	Unavailable

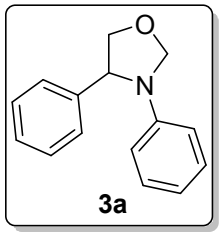


NMR Spectra of compounds A, 3 and 5

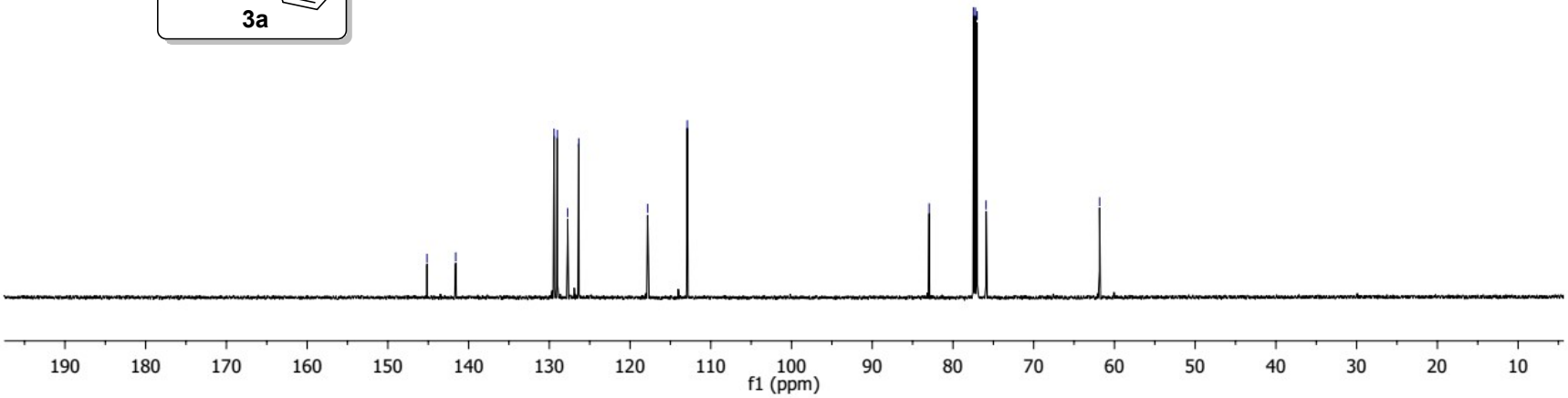


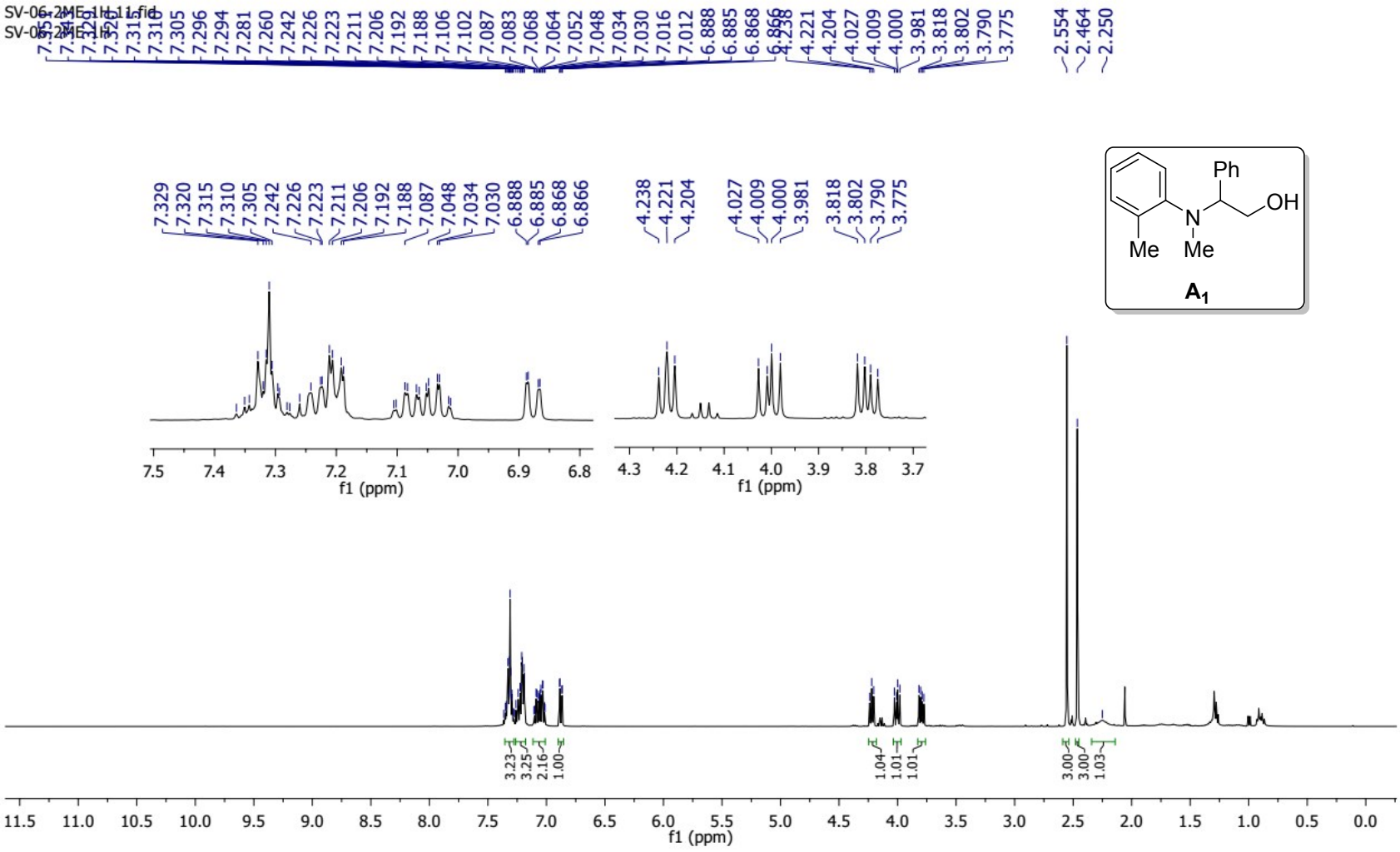
SV-06-PH-PH-13C/10

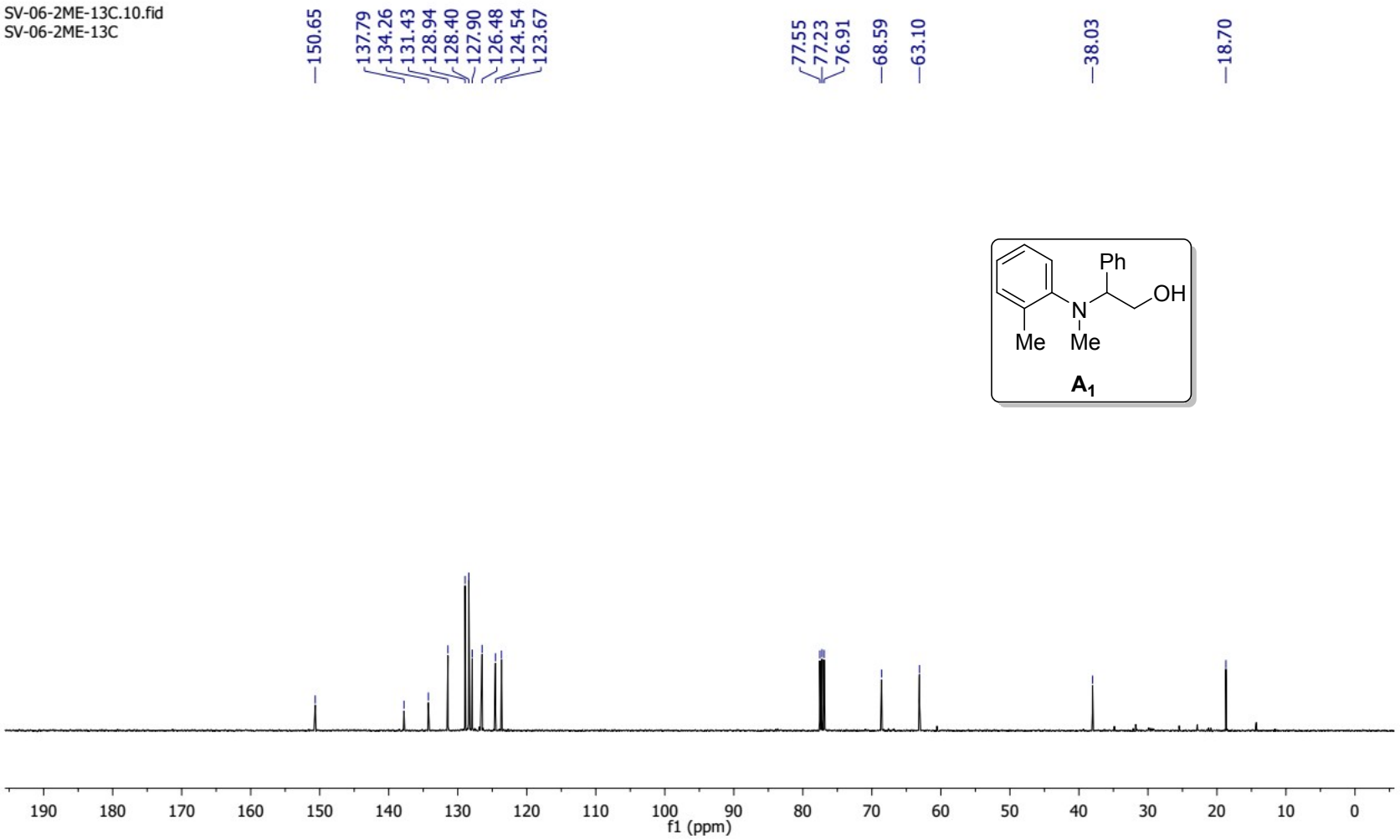
145.16
141.60
129.42
129.01
127.74
126.36
117.82
112.91
82.95
77.44
77.23
77.02
75.90
61.84

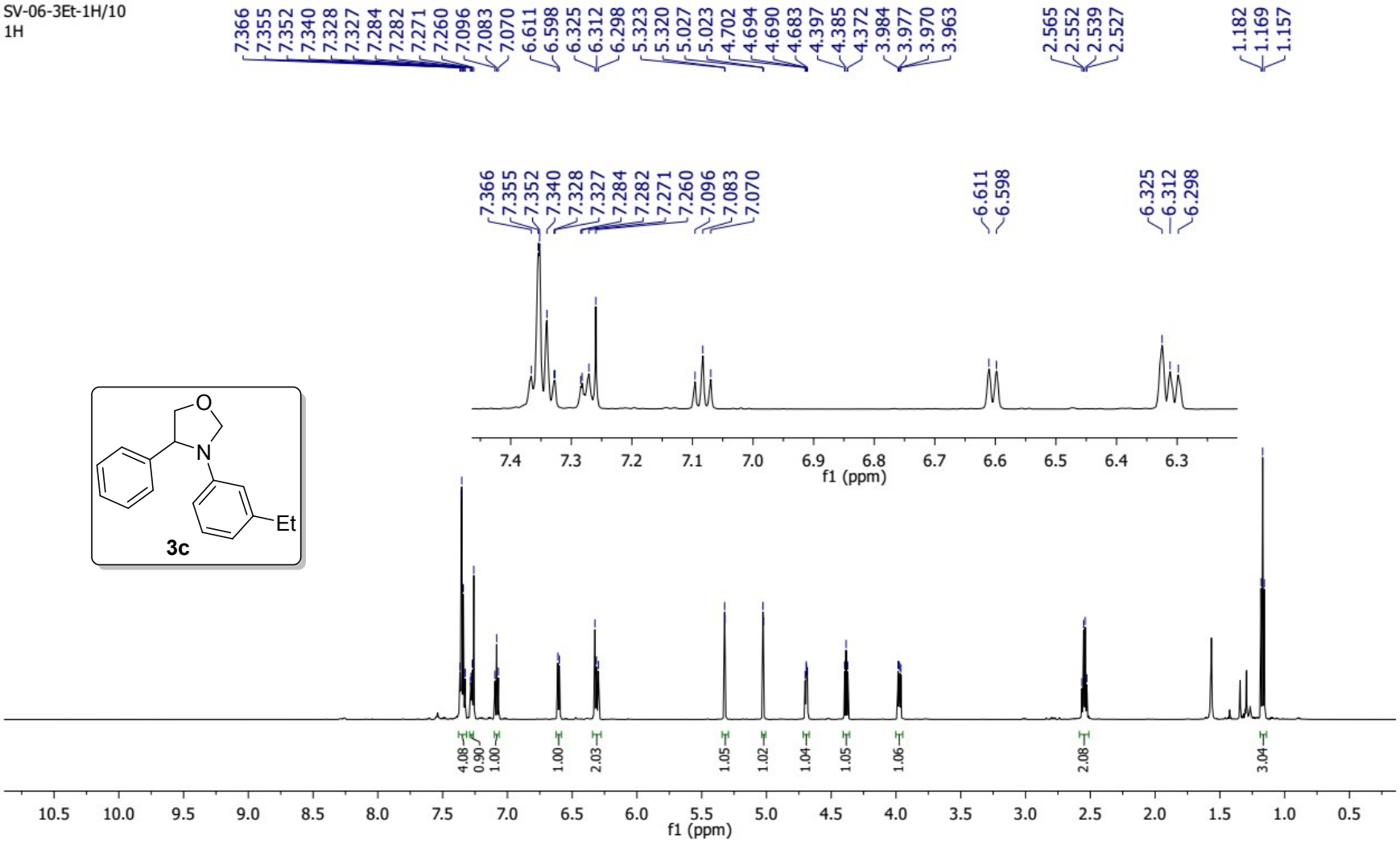


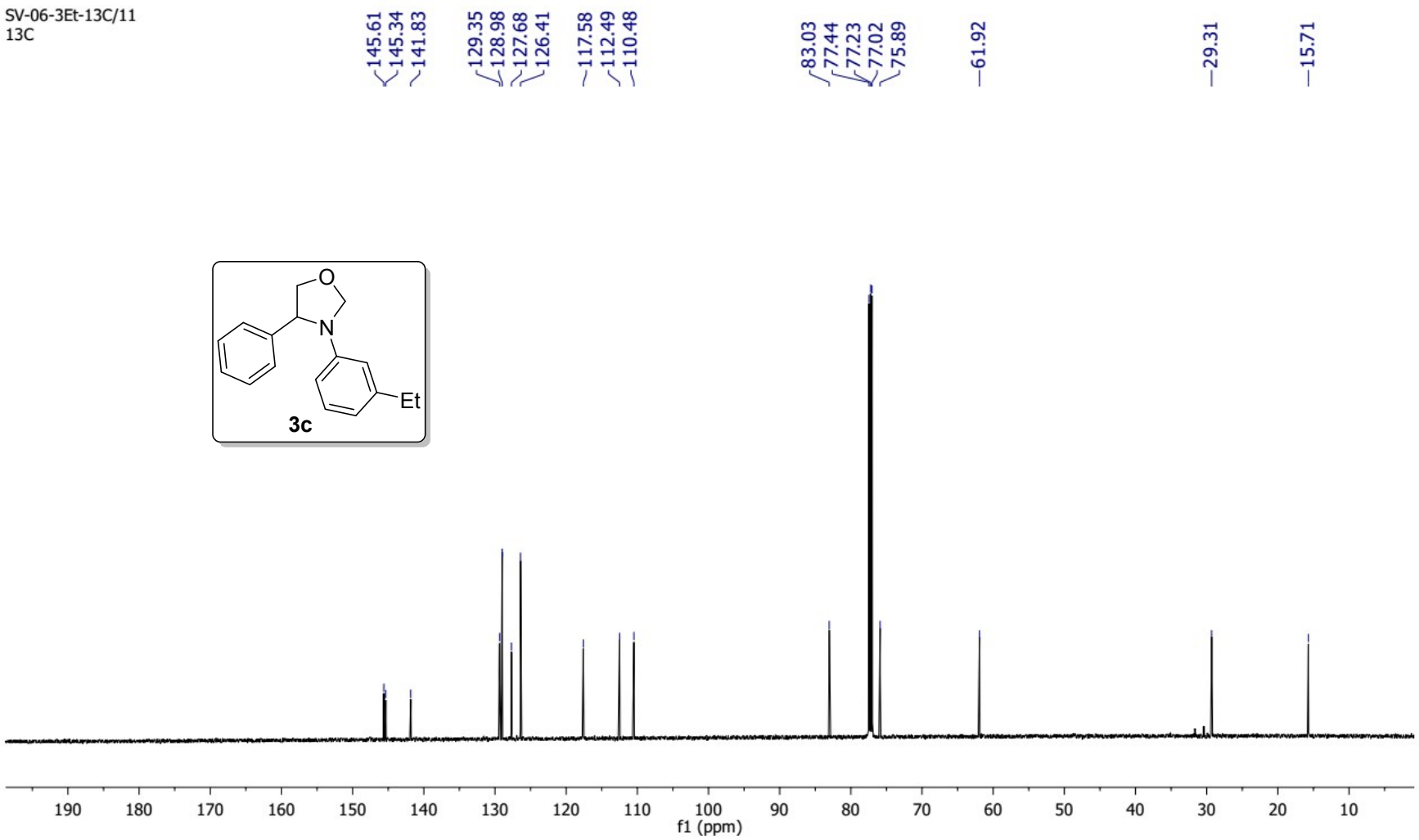
3a

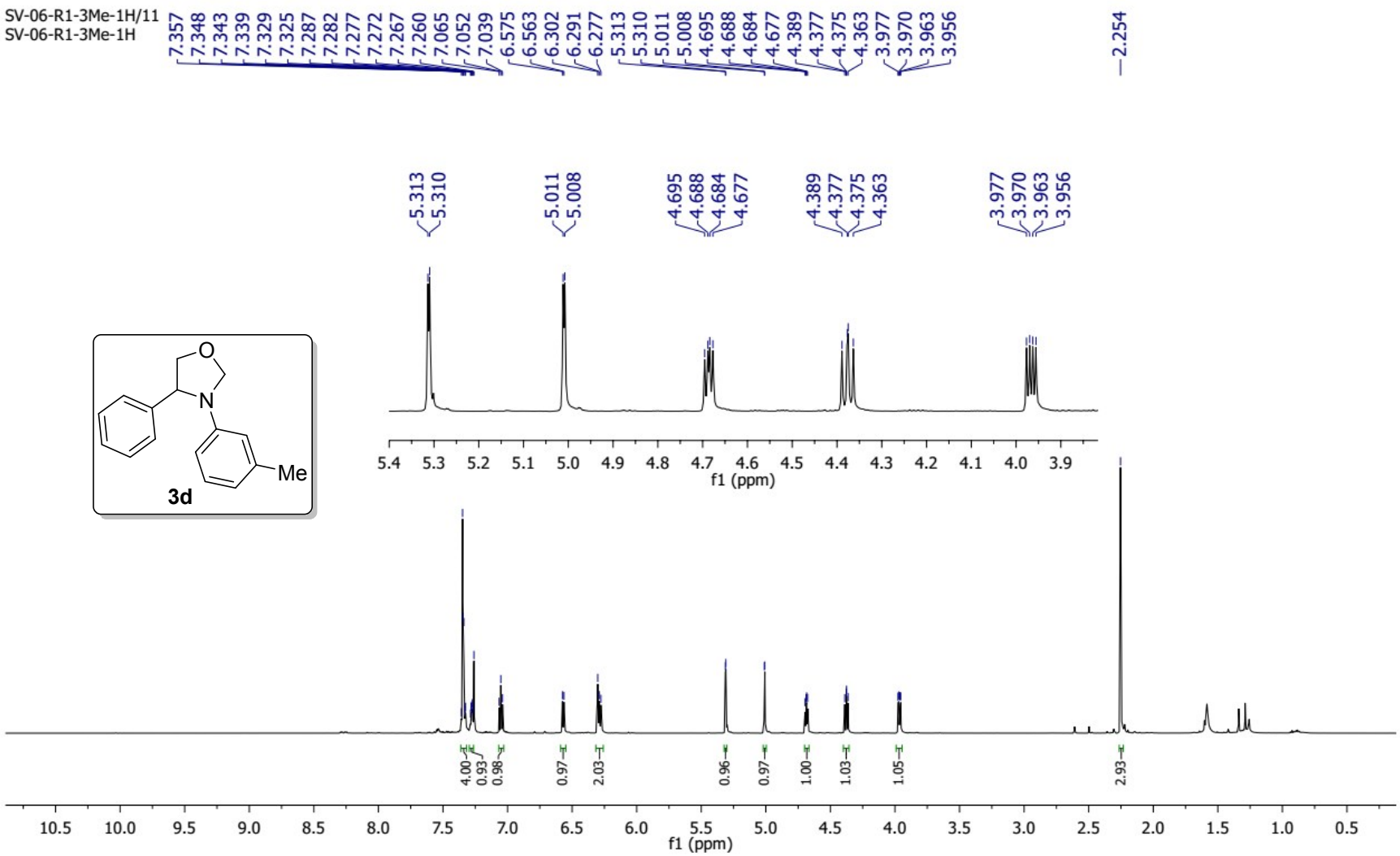



SV-06-2ME-1H_11.fid
7.329
7.320
7.315
7.310
7.305
7.242
7.226
7.223
7.211
7.206
7.192
7.188
7.087
7.048
7.034
7.030
6.888
6.885
6.868
6.866
4.238
4.221
4.204
4.027
4.009
4.000
3.981
3.818
3.802
3.790
3.775
2.554
2.464
2.250
Ph
OH
N
Me
Me
A1
f1 (ppm)
3.23
3.25
2.16
1.00
1.04
1.01
1.01
3.00
3.00
1.03

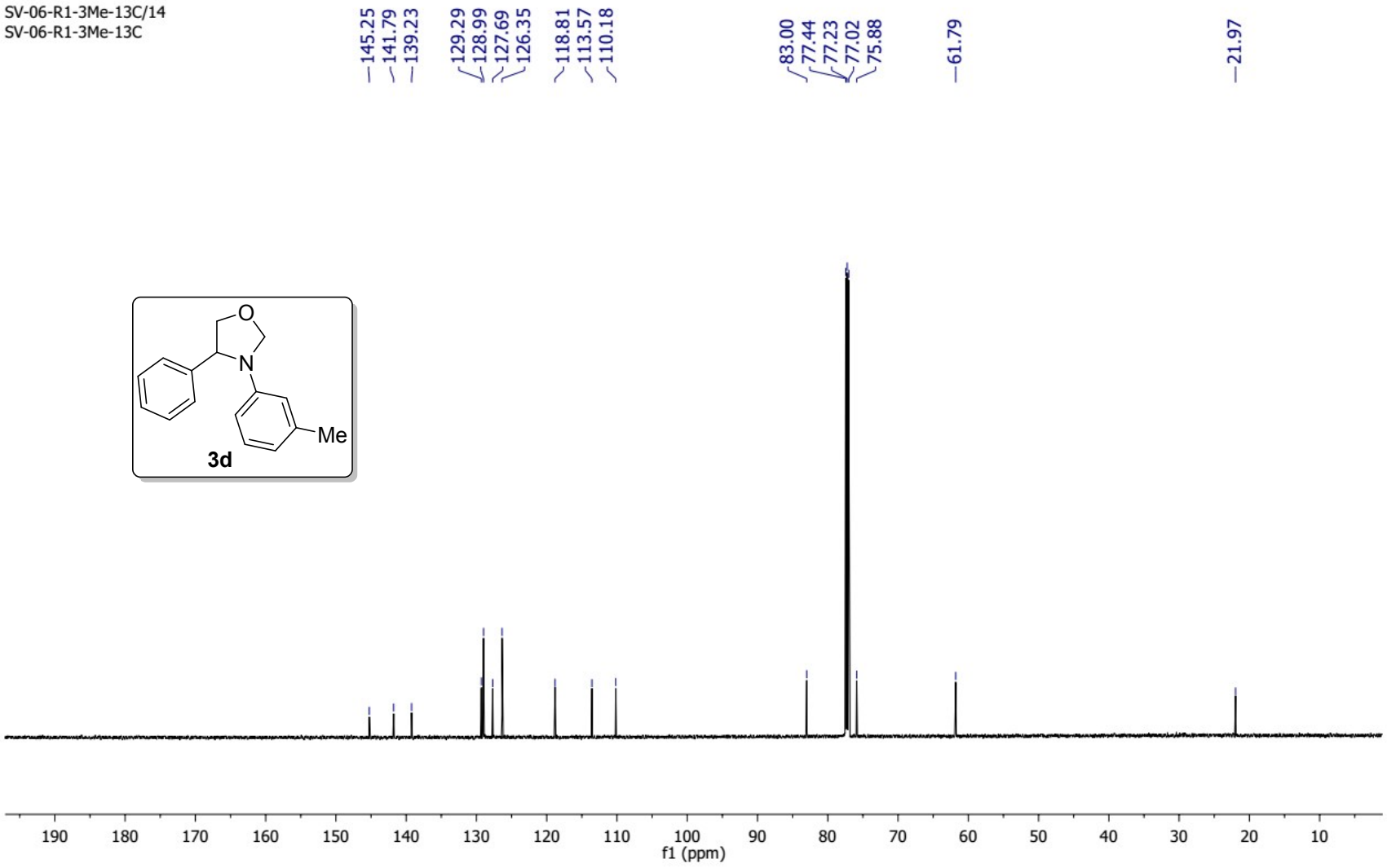

SV-06-2ME-13C.10.fid
SV-06-2ME-13C
150.65
137.79
134.26
131.43
128.94
128.40
127.90
126.48
124.54
123.67
77.55
77.23
76.91
68.59
63.10
38.03
18.70
Ph
OH
N
Me
Me
A1
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


SV-06-3Et-1H/10
1H
7.366
7.355
7.352
7.340
7.328
7.327
7.284
7.282
7.271
7.260
7.096
7.083
7.070
6.611
6.598
6.325
6.312
6.298
5.323
5.320
5.027
5.023
4.702
4.694
4.690
4.683
4.397
4.385
4.372
3.984
3.977
3.970
3.963
2.565
2.552
2.539
2.527
1.182
1.169
1.157
O
N
Et
3c
f1 (ppm)
4.08
0.90
1.00
1.00
2.03
1.05
1.02
1.04
1.05
1.06
2.08
3.04

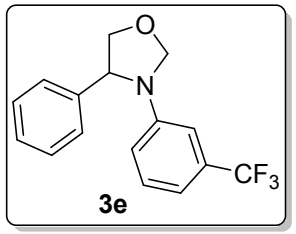

SV-06-3Et-13C/11
13C
145.61
145.34
141.83
129.35
128.98
127.68
126.41
117.58
112.49
110.48
83.03
77.44
77.23
77.02
75.89
61.92
29.31
15.71
O
N
Et
3c
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


SV-06-R1-3Me-1H/11
SV-06-R1-3Me-1H
7.357
7.348
7.343
7.339
7.329
7.325
7.287
7.282
7.277
7.272
7.267
7.260
7.065
7.052
7.039
6.575
6.563
6.302
6.291
6.277
5.313
5.310
5.011
5.008
4.695
4.688
4.684
4.677
4.389
4.377
4.375
4.363
3.977
3.970
3.963
3.956
2.254
O
N
Me
3d
f1 (ppm)
4.00
0.93
0.98
0.97
2.03
0.96
0.97
1.00
1.03
1.05
2.93

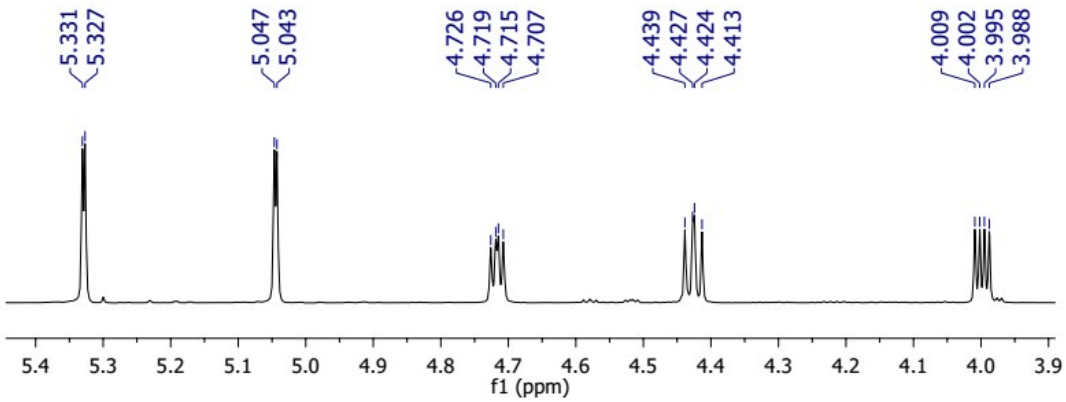
SV-06-R1-3Me-13C/14
SV-06-R1-3Me-13C

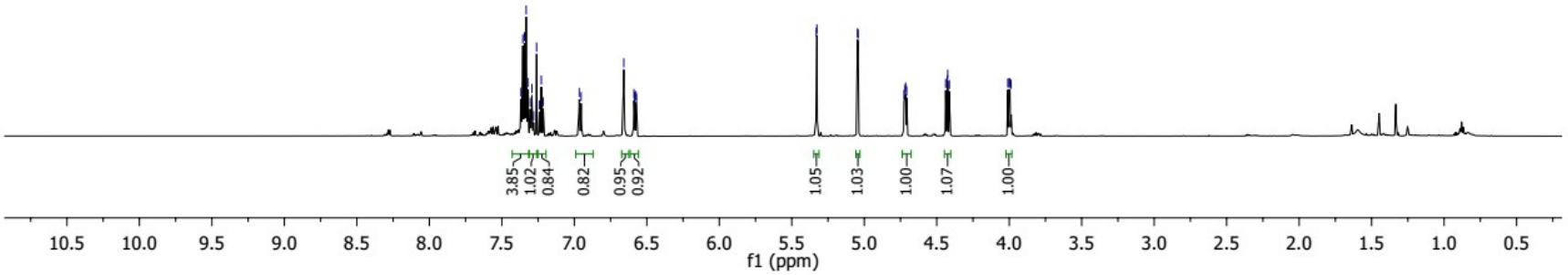


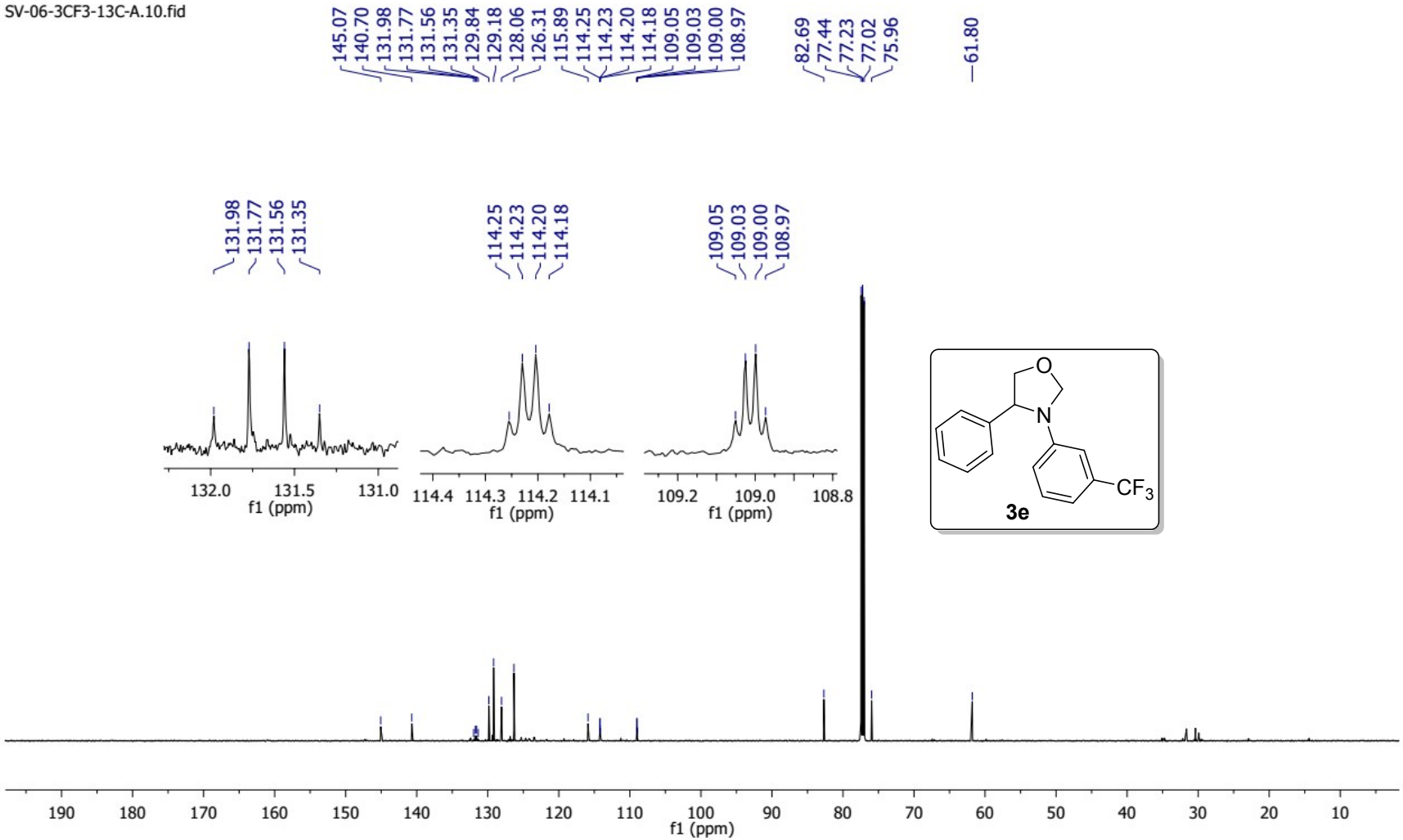
SV-06-3CF3-1H-a/13
SV-06-3CF3-1H-a

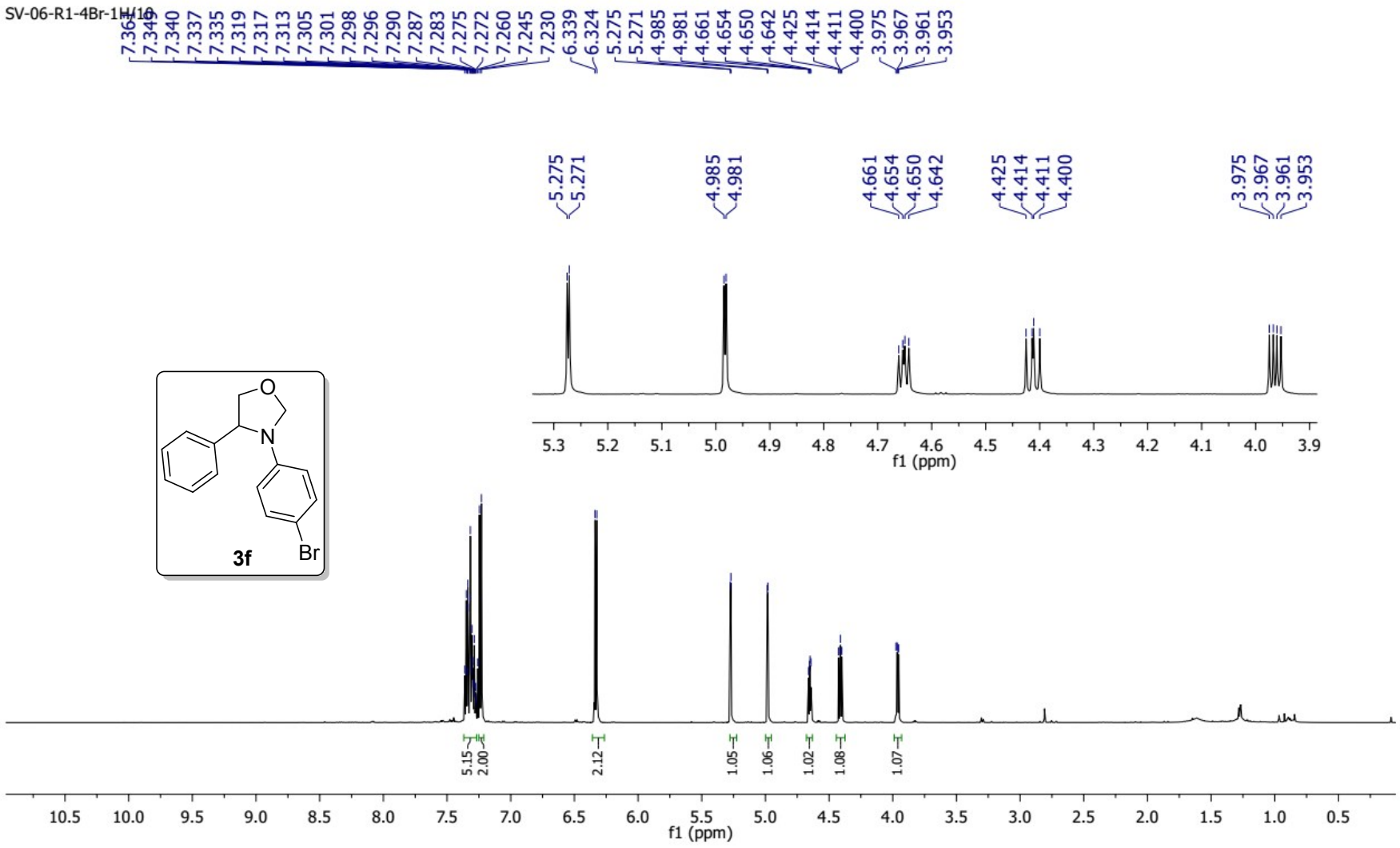


3e



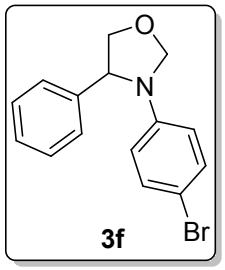



SV-06-3CF3-13C-A.10.fid
145.07
140.70
131.98
131.77
131.56
131.35
129.84
129.18
128.06
126.31
115.89
114.25
114.23
114.20
114.18
109.05
109.03
109.00
108.97
82.69
77.44
77.23
77.02
75.96
61.80
131.98
131.77
131.56
131.35
114.25
114.23
114.20
114.18
109.05
109.03
109.00
108.97
132.0
131.5
131.0
f1 (ppm)
114.4
114.3
114.2
114.1
f1 (ppm)
109.2
109.0
108.8
f1 (ppm)
O
N
CF3
3e
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

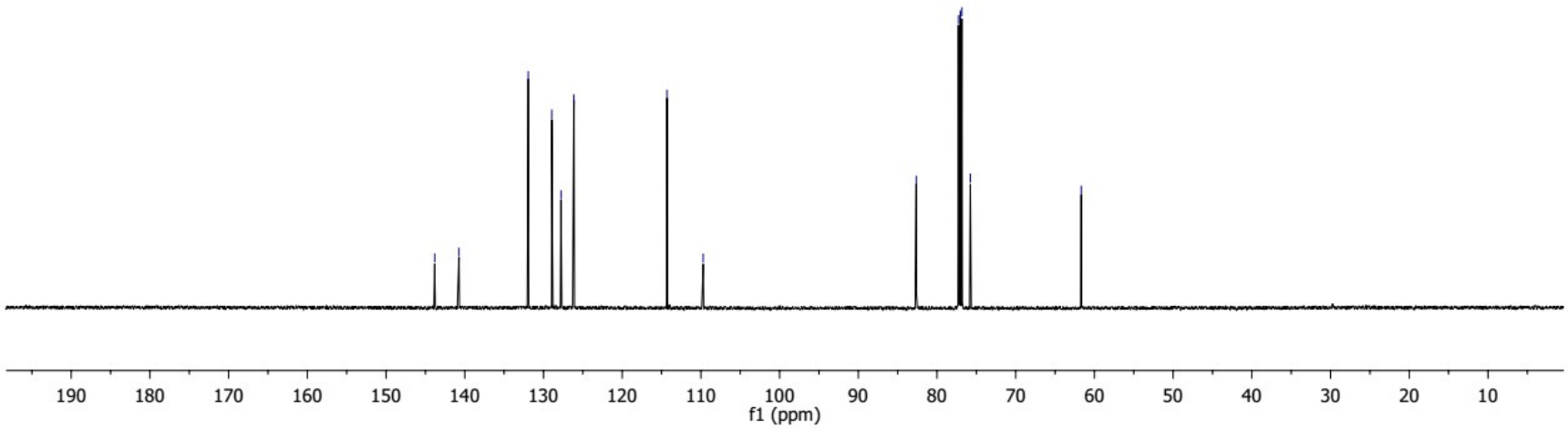

SV-06-R1-4Br-1H/1d
7.365
7.349
7.340
7.337
7.335
7.319
7.317
7.313
7.305
7.301
7.298
7.296
7.290
7.287
7.283
7.275
7.272
7.260
7.245
7.230
6.339
6.324
5.275
5.271
4.985
4.981
4.661
4.654
4.650
4.642
4.425
4.414
4.411
4.400
3.975
3.967
3.961
3.953
O
N
Br
3f
f1 (ppm)
f1 (ppm)

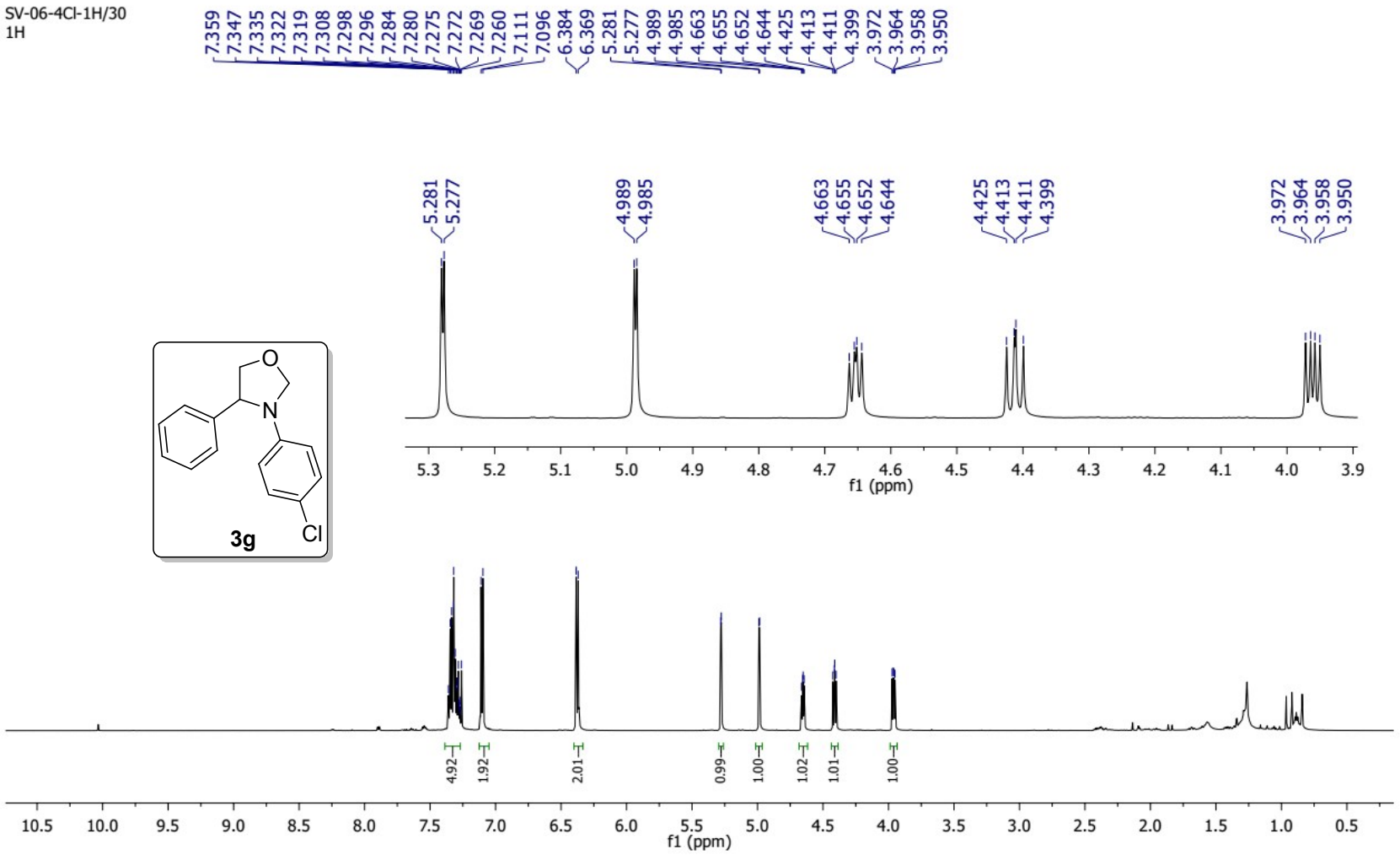
SV-06-R1-4Br-13C/11

143.81
140.74
131.93
128.94
127.77
126.13
114.31
109.71
82.63
77.26
77.05
76.84
75.77
61.67



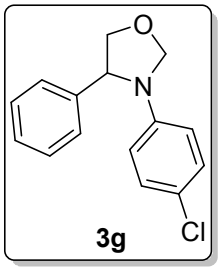
3f



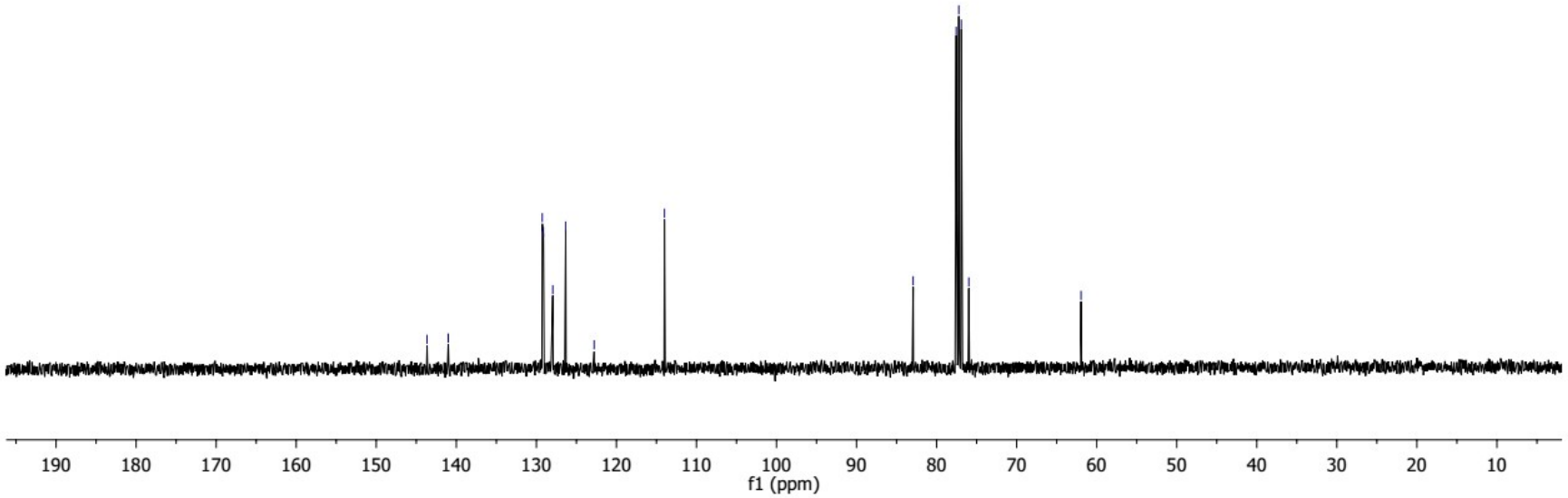

SV-06-4Cl-1H/30
1H
7.359
7.347
7.335
7.322
7.319
7.308
7.298
7.296
7.284
7.280
7.275
7.272
7.269
7.260
7.111
7.096
6.384
6.369
5.281
5.277
4.989
4.985
4.663
4.655
4.652
4.644
4.425
4.413
4.411
4.399
3.972
3.964
3.958
3.950
O
N
Cl
3g
f1 (ppm)
4.92
1.92
2.01
0.99
1.00
1.02
1.01
1.00
f1 (ppm)

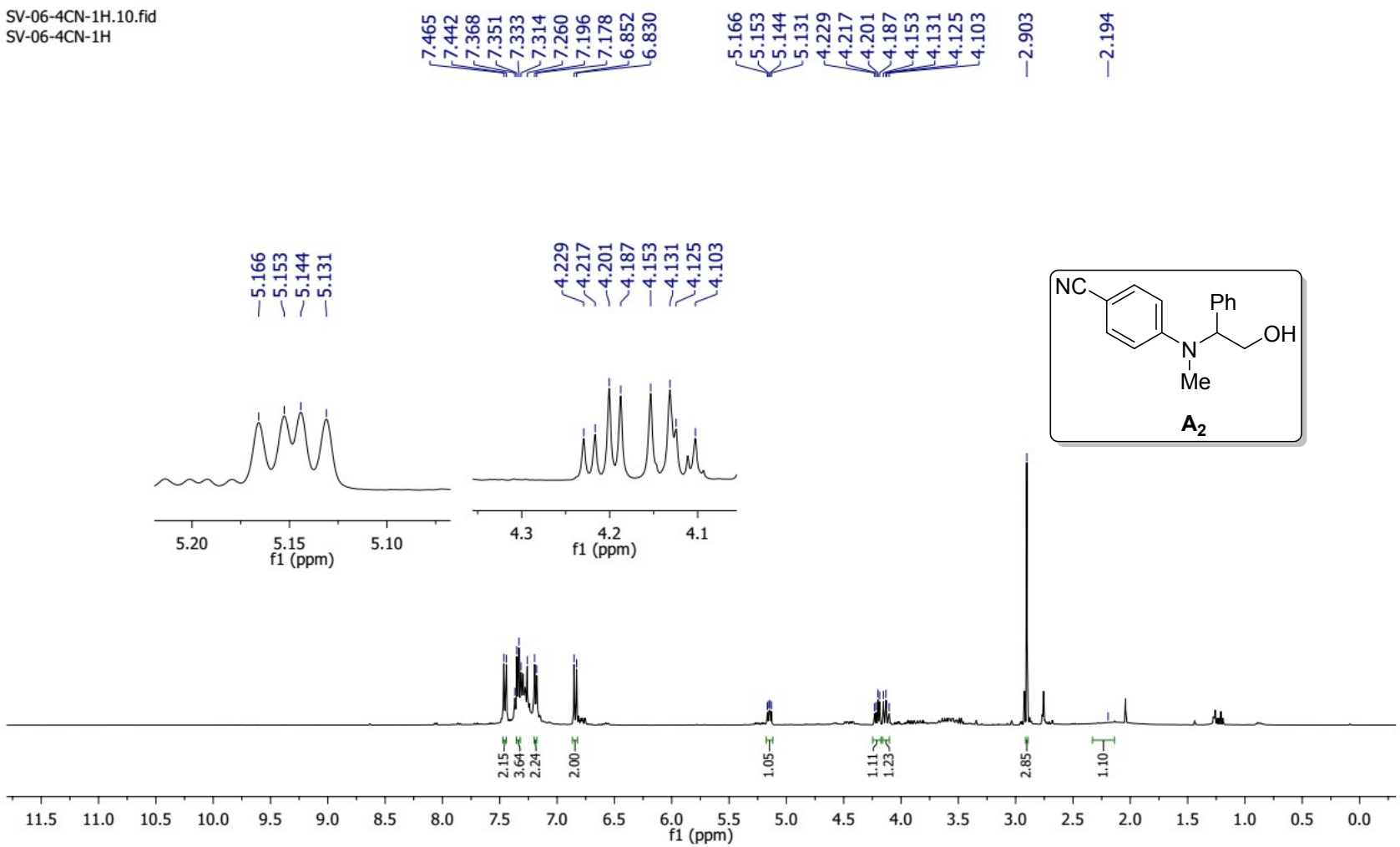
spa40718.526.fid
lab spaacr-4-cl
iitm_carbonshort CDCl3 /opt/topspin nmr 2

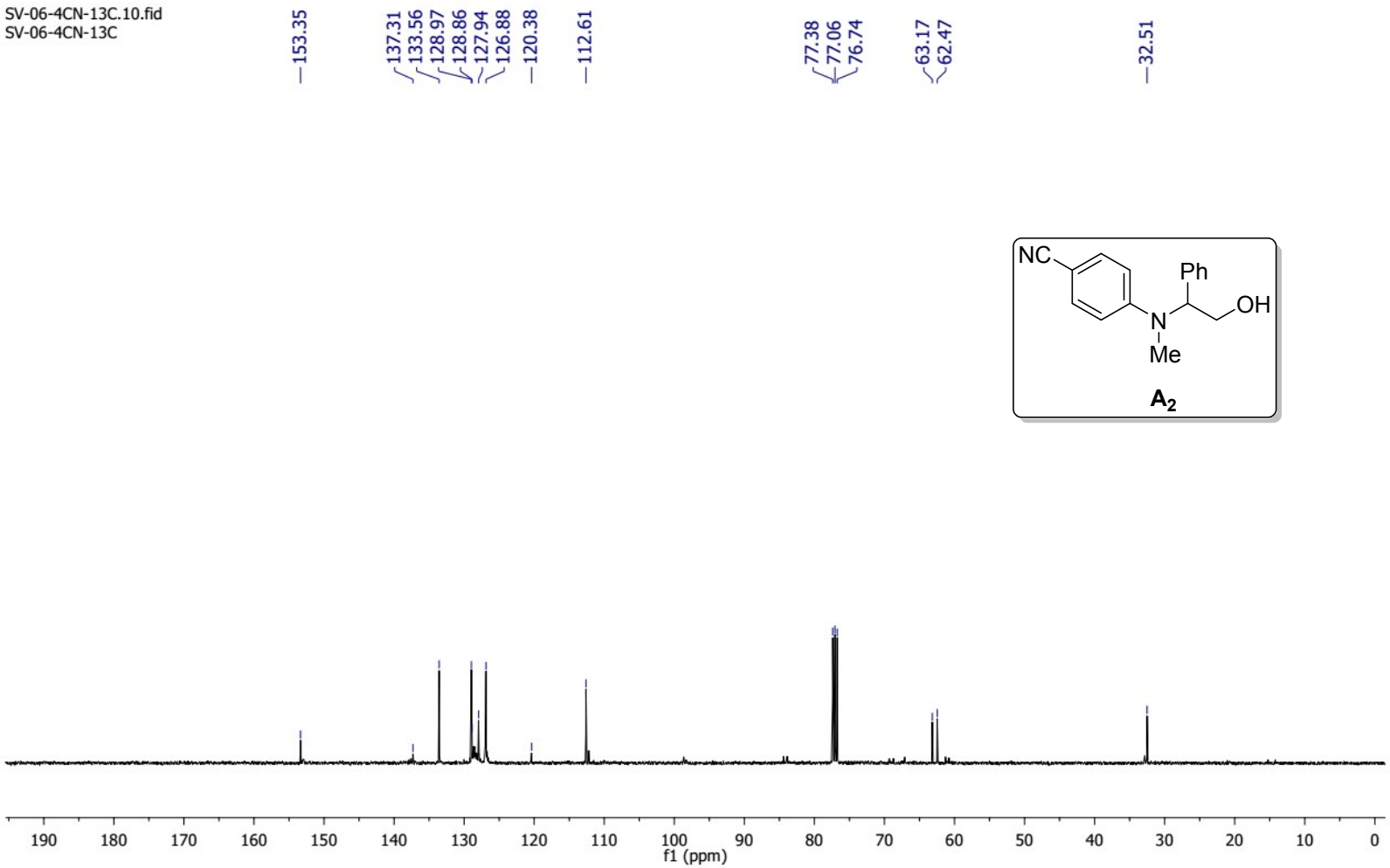
143.66
141.01
129.26
129.13
127.95
126.33
122.78
114.00
82.93
77.55
77.23
76.91
75.98
61.96

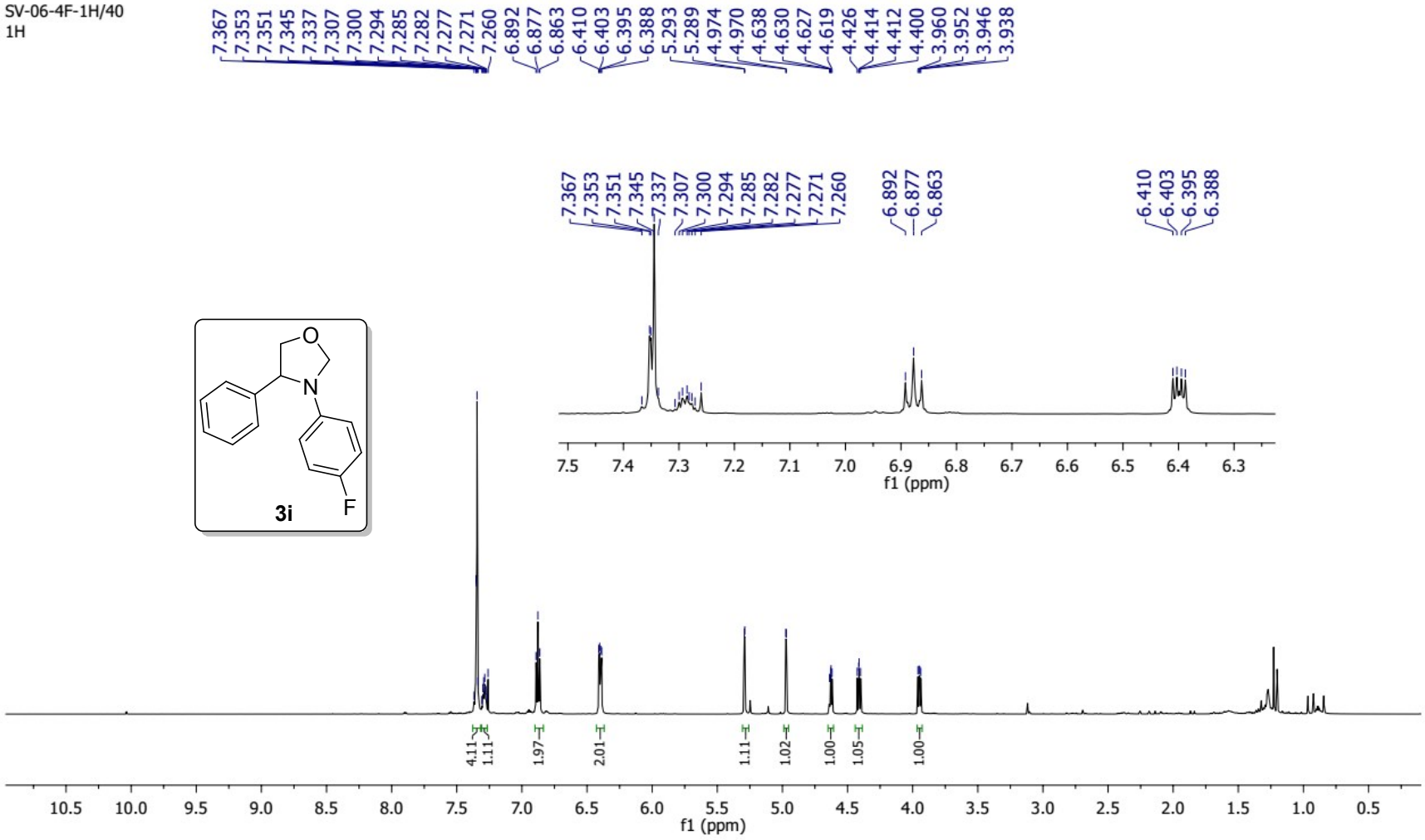


3g



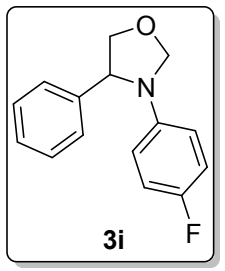

SV-06-4CN-1H.10.fid
SV-06-4CN-1H
7.465
7.442
7.368
7.351
7.333
7.314
7.260
7.196
7.178
6.852
6.830
5.166
5.153
5.144
5.131
4.229
4.217
4.201
4.187
4.153
4.131
4.125
4.103
2.903
2.194
NC
Ph
OH
N
Me
A2
f1 (ppm)
2.15
3.64
2.24
2.00
1.05
1.11
1.23
2.85
1.10


SV-06-4CN-13C.10.fid
SV-06-4CN-13C
153.35
137.31
133.56
128.97
128.86
127.94
126.88
120.38
112.61
77.38
77.06
76.74
63.17
62.47
32.51
NC
Ph
OH
N
Me
A2
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

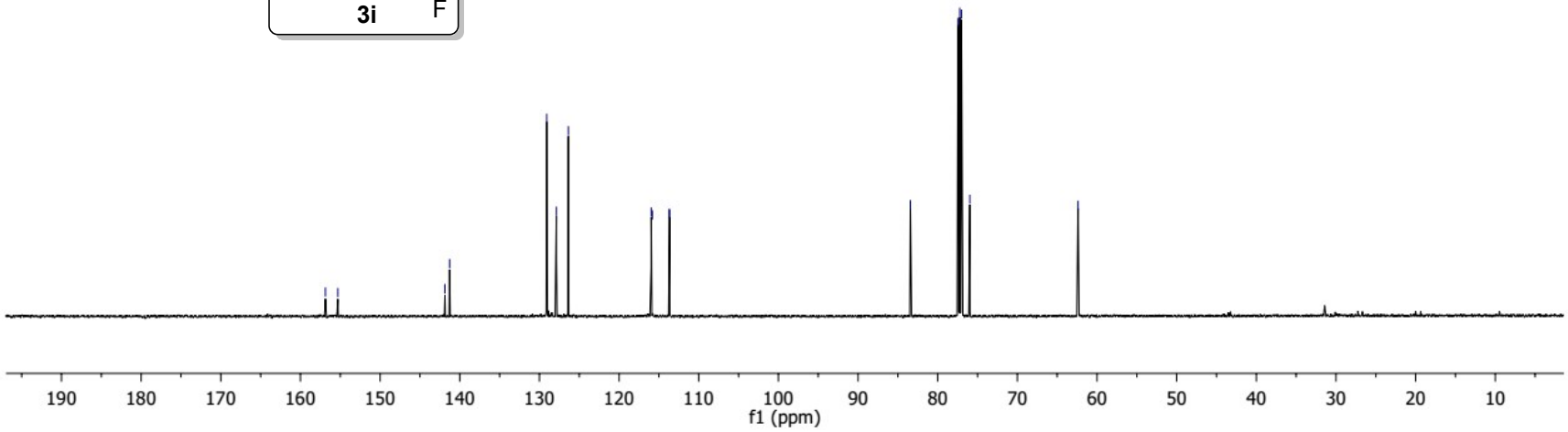

SV-06-4F-1H/40
1H
7.367
7.353
7.351
7.345
7.337
7.307
7.300
7.294
7.285
7.282
7.277
7.271
7.260
6.892
6.877
6.863
6.410
6.403
6.395
6.388
5.293
5.289
4.974
4.970
4.638
4.630
4.627
4.619
4.426
4.414
4.412
4.400
3.960
3.952
3.946
3.938
O
N
F
3i
f1 (ppm)
4.11
1.11
1.97
2.01
1.11
1.02
1.00
1.05
1.00

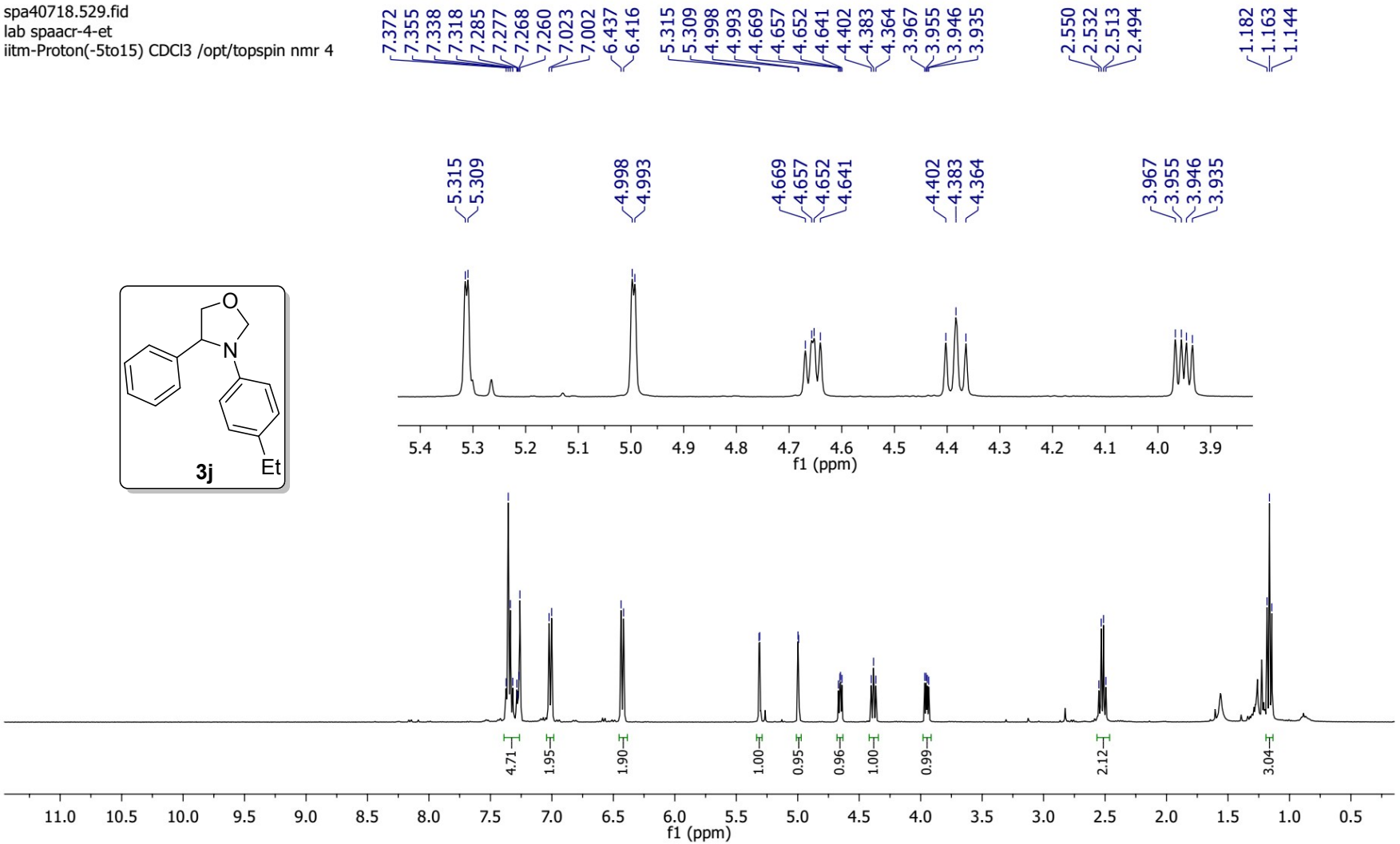
SV-06-R1-4F-13C/10

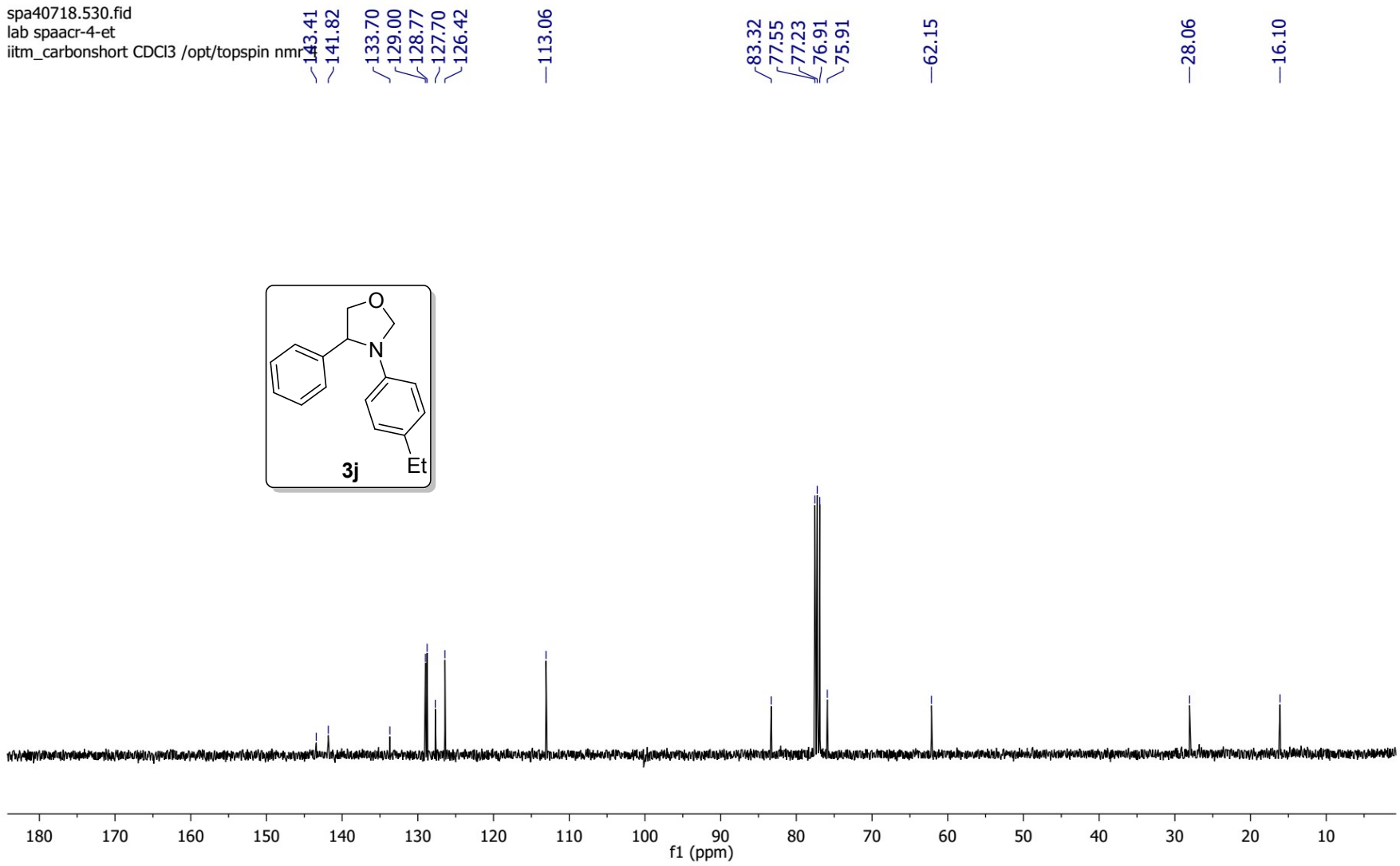
156.87
155.31
141.88
141.87
141.28
129.08
127.87
126.37
115.97
115.82
113.71
113.66
83.44
77.44
77.23
77.02
75.96
62.38

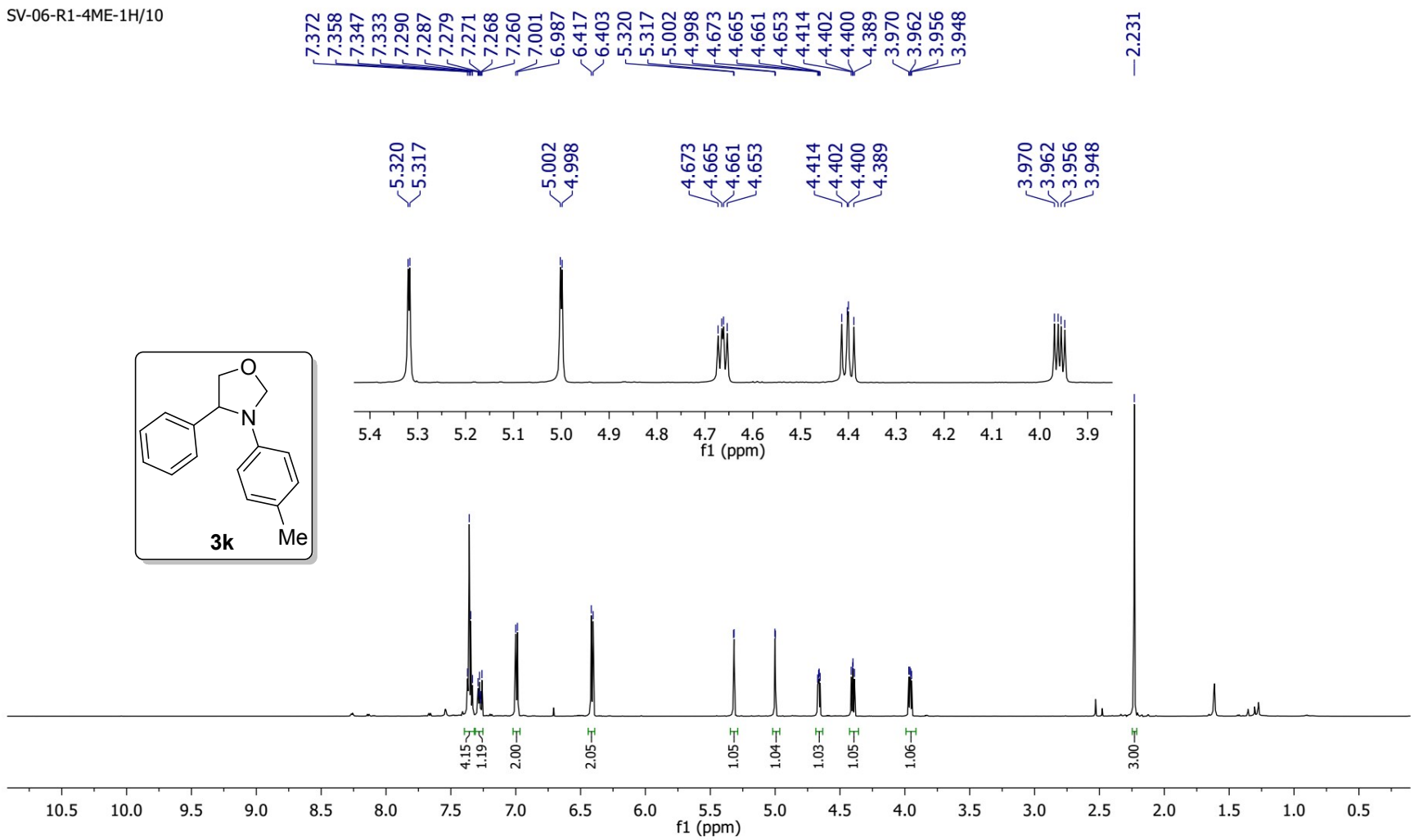


3i



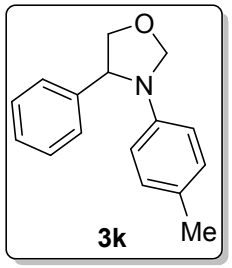

spa40718.529.fid
lab spaacr-4-et
iitm-Proton(-5to15) CDCl3 /opt/topspin nmr 4
7.372
7.355
7.338
7.318
7.285
7.277
7.268
7.260
7.023
7.002
6.437
6.416
5.315
5.309
4.998
4.993
4.669
4.657
4.652
4.641
4.402
4.383
4.364
3.967
3.955
3.946
3.935
2.550
2.532
2.513
2.494
1.182
1.163
1.144
3j
Et
f1 (ppm)
4.71
1.95
1.90
1.00
0.95
0.96
1.00
0.99
2.12
3.04


spa40718.530.fid
lab spaacr-4-et
iitm_carbonshort CDCl3 /opt/topspin nmr
143.41
141.82
133.70
129.00
128.77
127.70
126.42
113.06
83.32
77.55
77.23
76.91
75.91
62.15
28.06
16.10
O
N
Et
3j
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

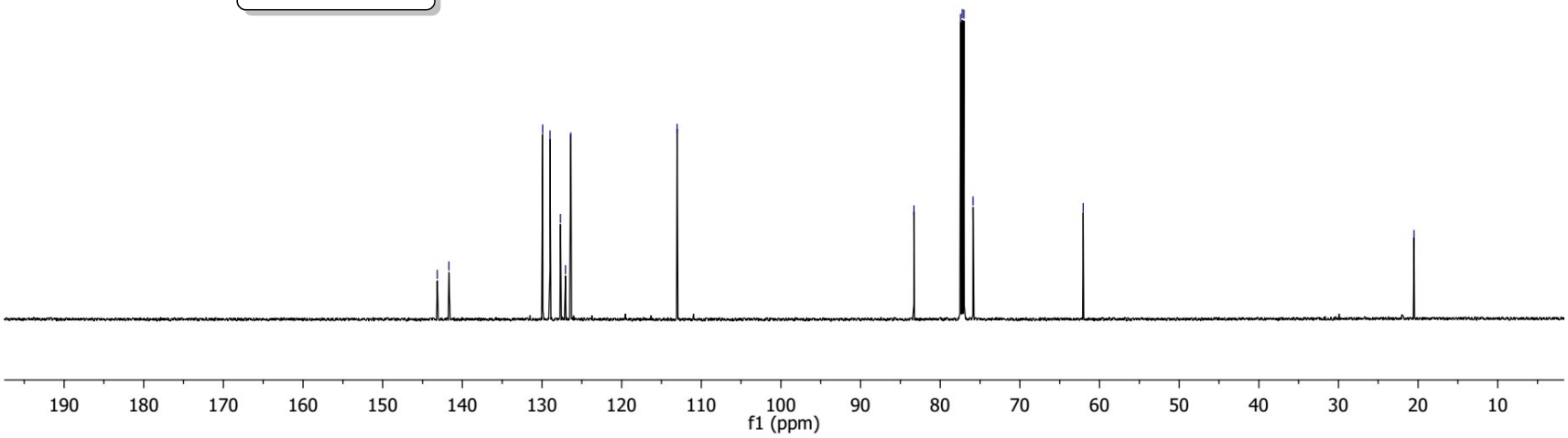

SV-06-R1-4ME-1H/10
7.372
7.358
7.347
7.333
7.290
7.287
7.279
7.271
7.268
7.260
7.001
6.987
6.417
6.403
5.320
5.317
5.002
4.998
4.673
4.665
4.661
4.653
4.414
4.402
4.400
4.389
3.970
3.962
3.956
3.948
2.231
O
N
Me
3k
f1 (ppm)
4.15
1.19
2.00
2.05
1.05
1.04
1.03
1.05
1.06
3.00

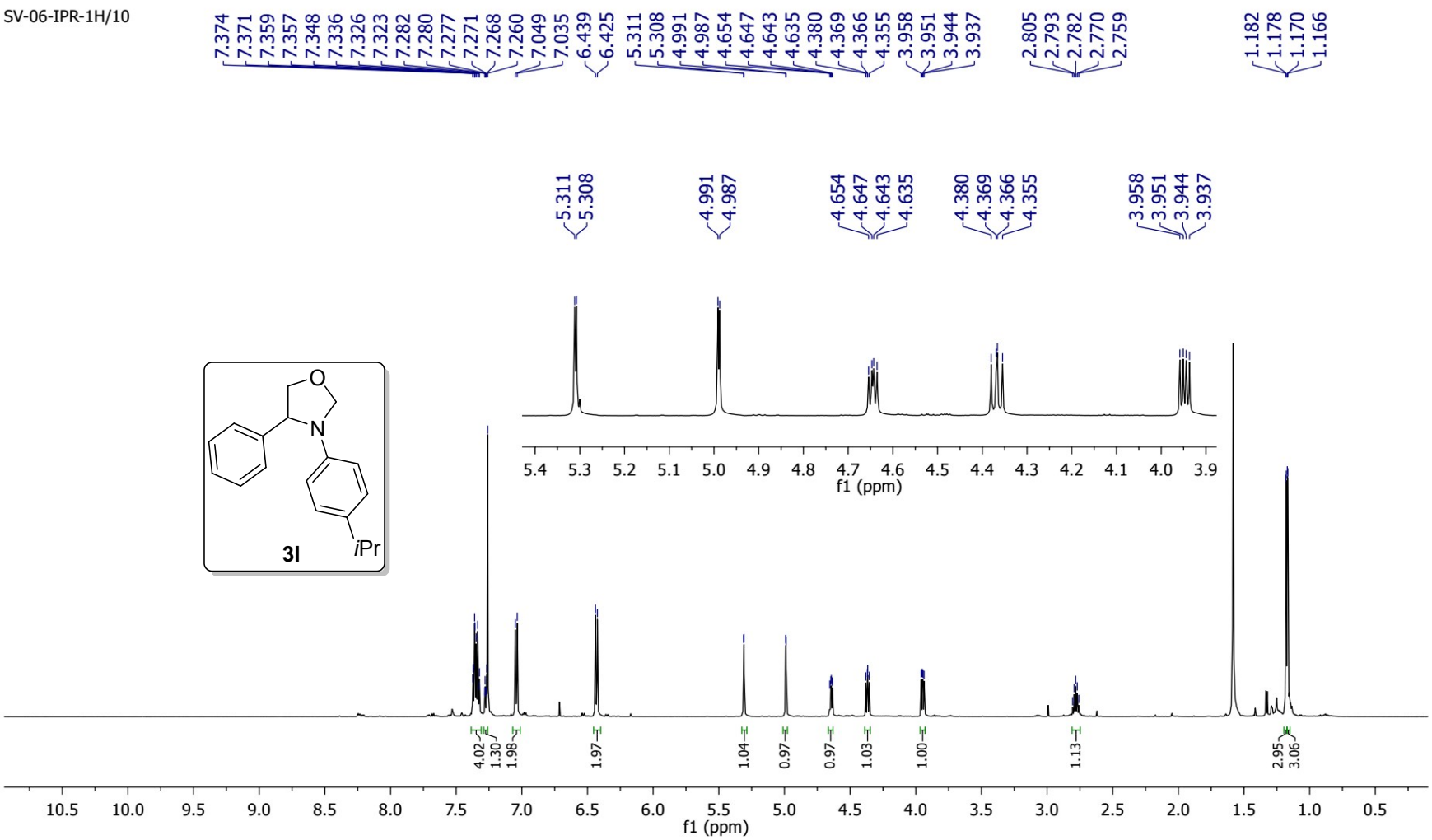
SV-06-R1-4ME-13C/10

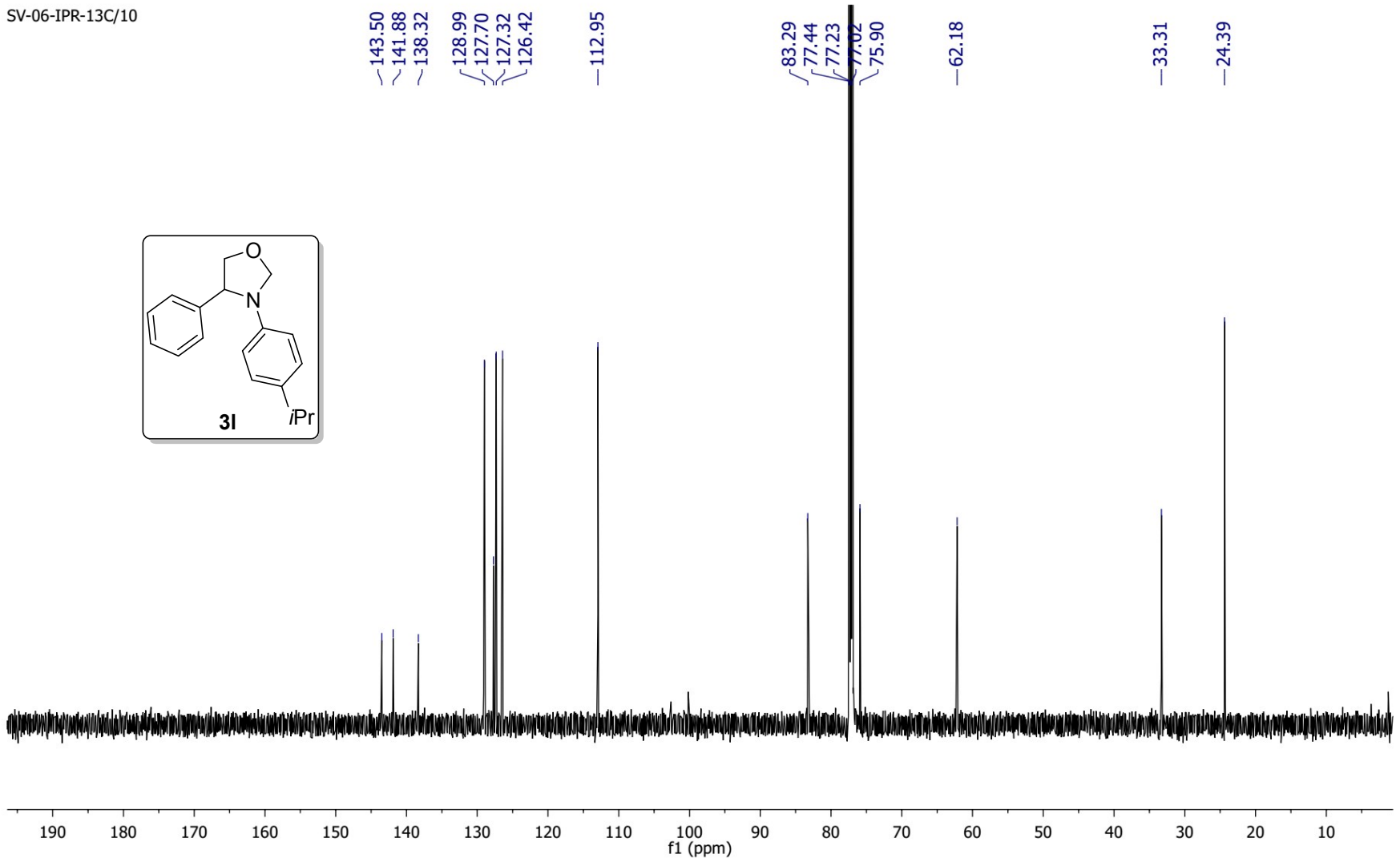
143.15
141.69
129.91
128.98
127.68
127.05
126.38
113.03
83.29
77.44
77.23
77.02
75.88
62.05
20.51

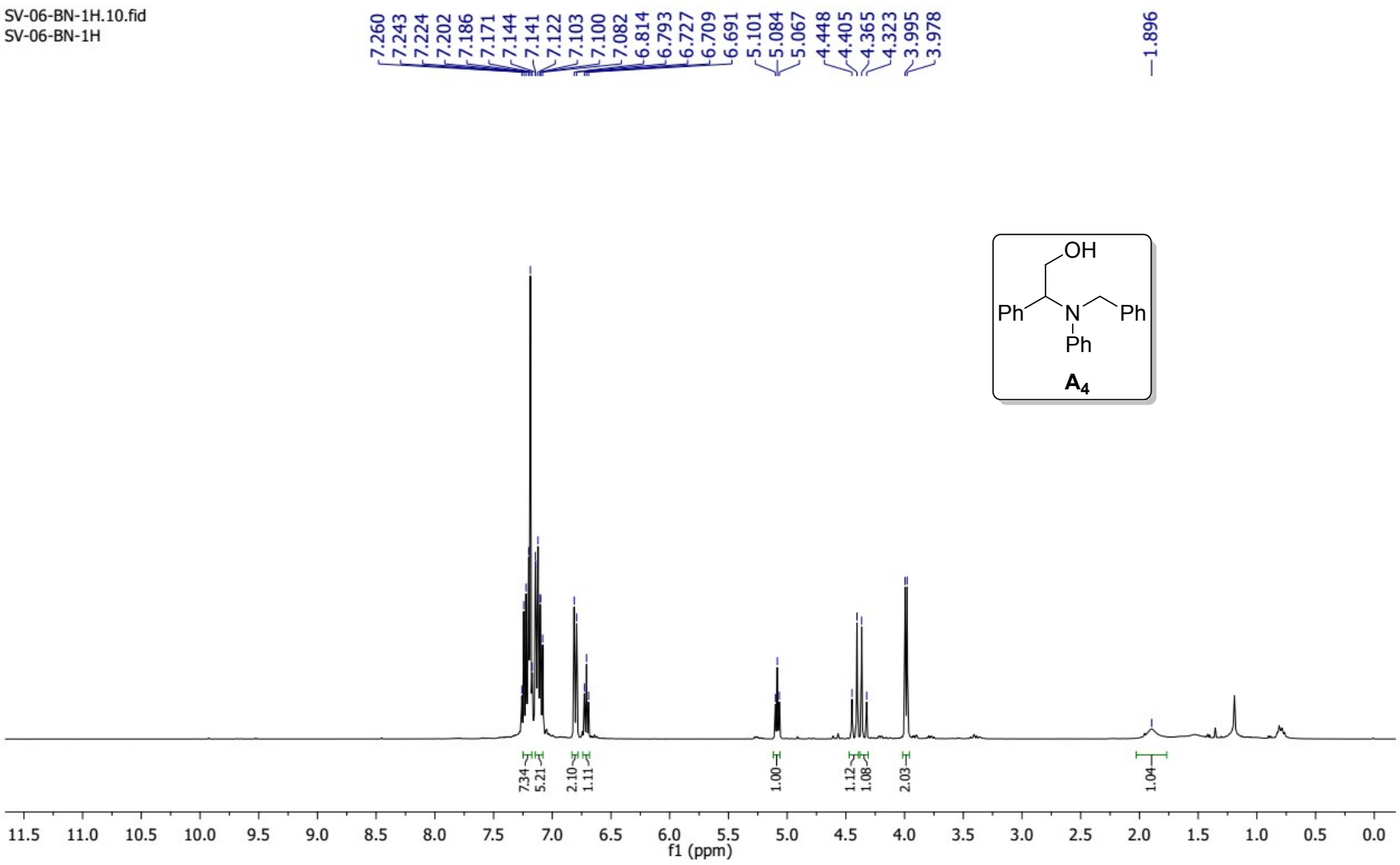


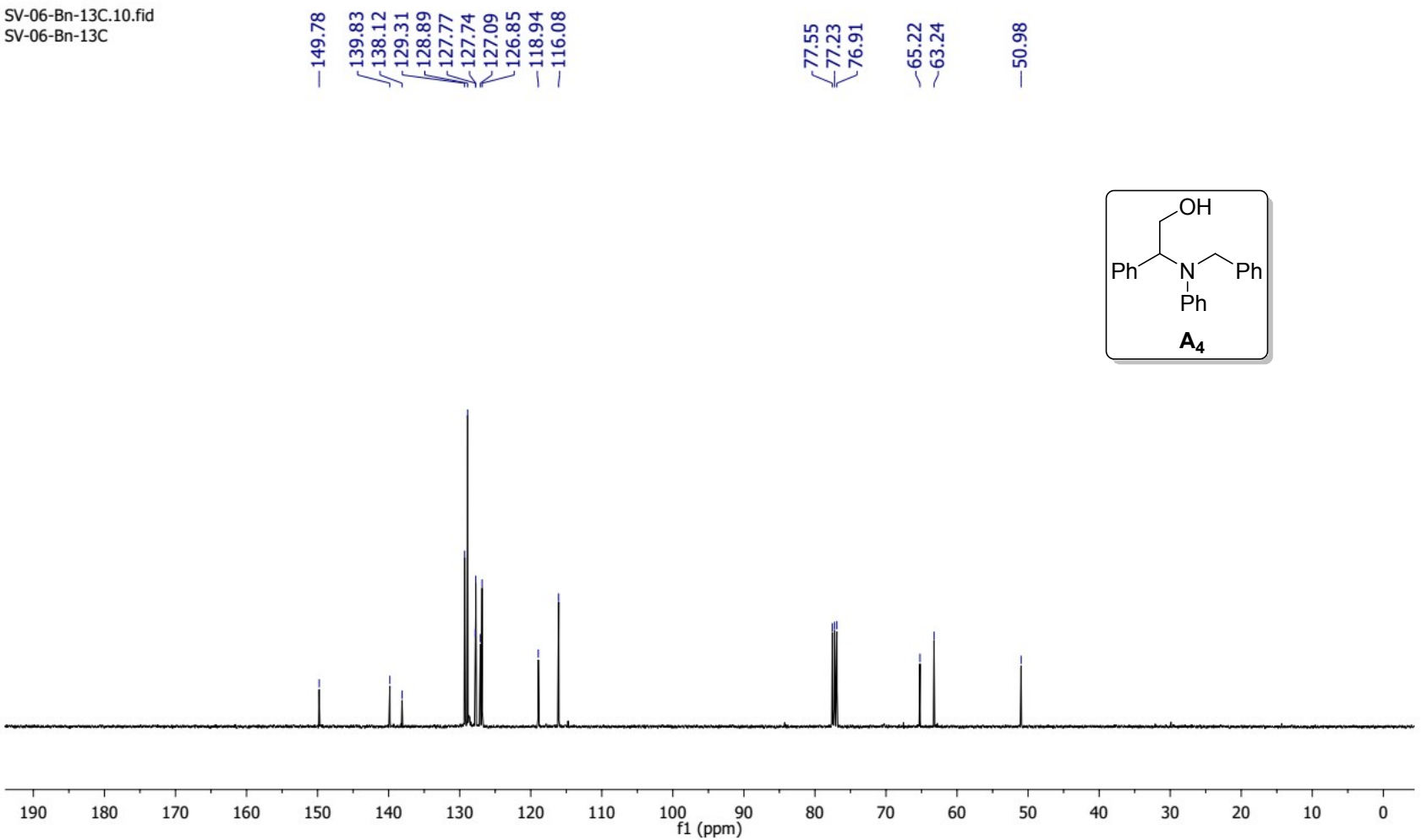
3k

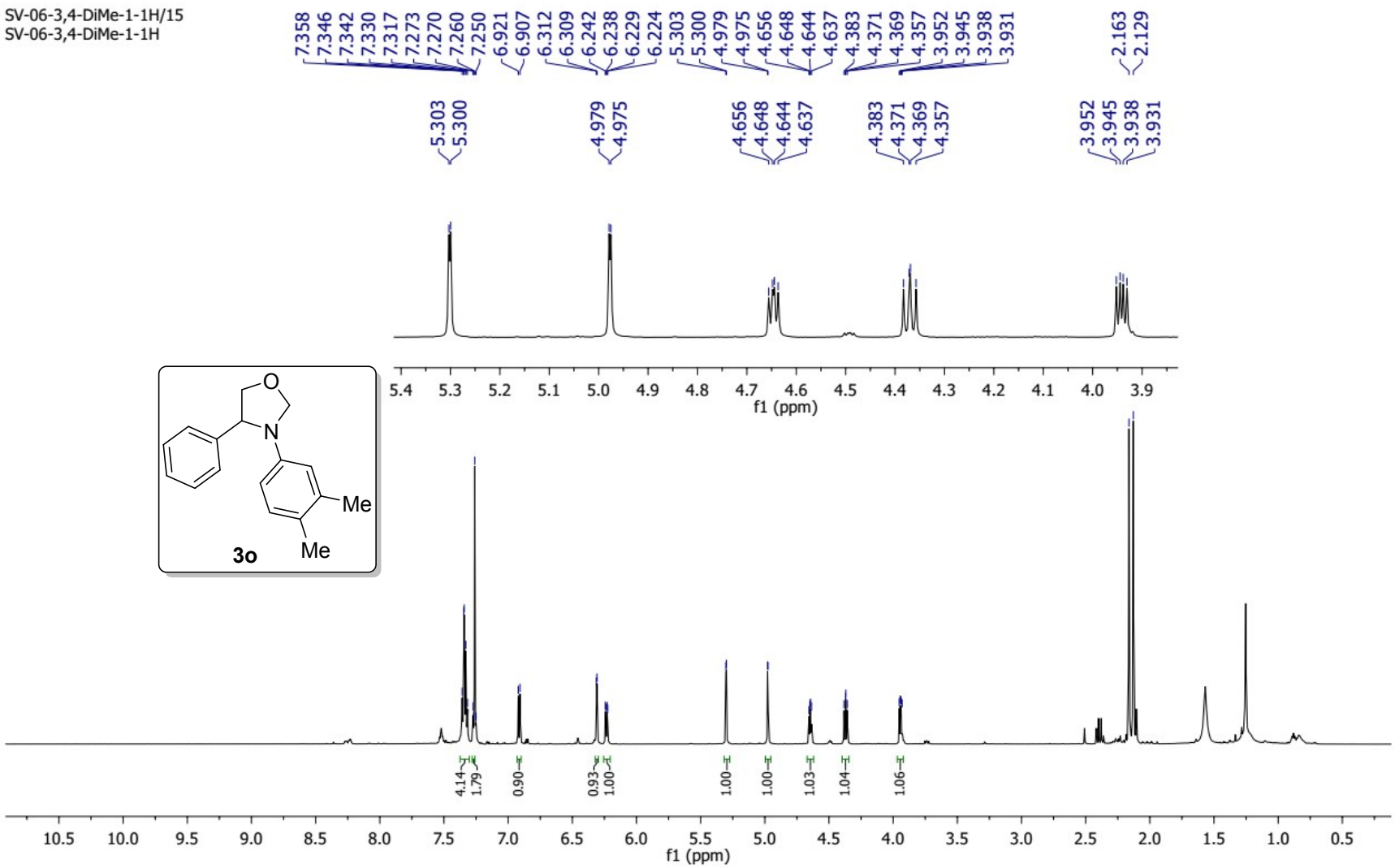


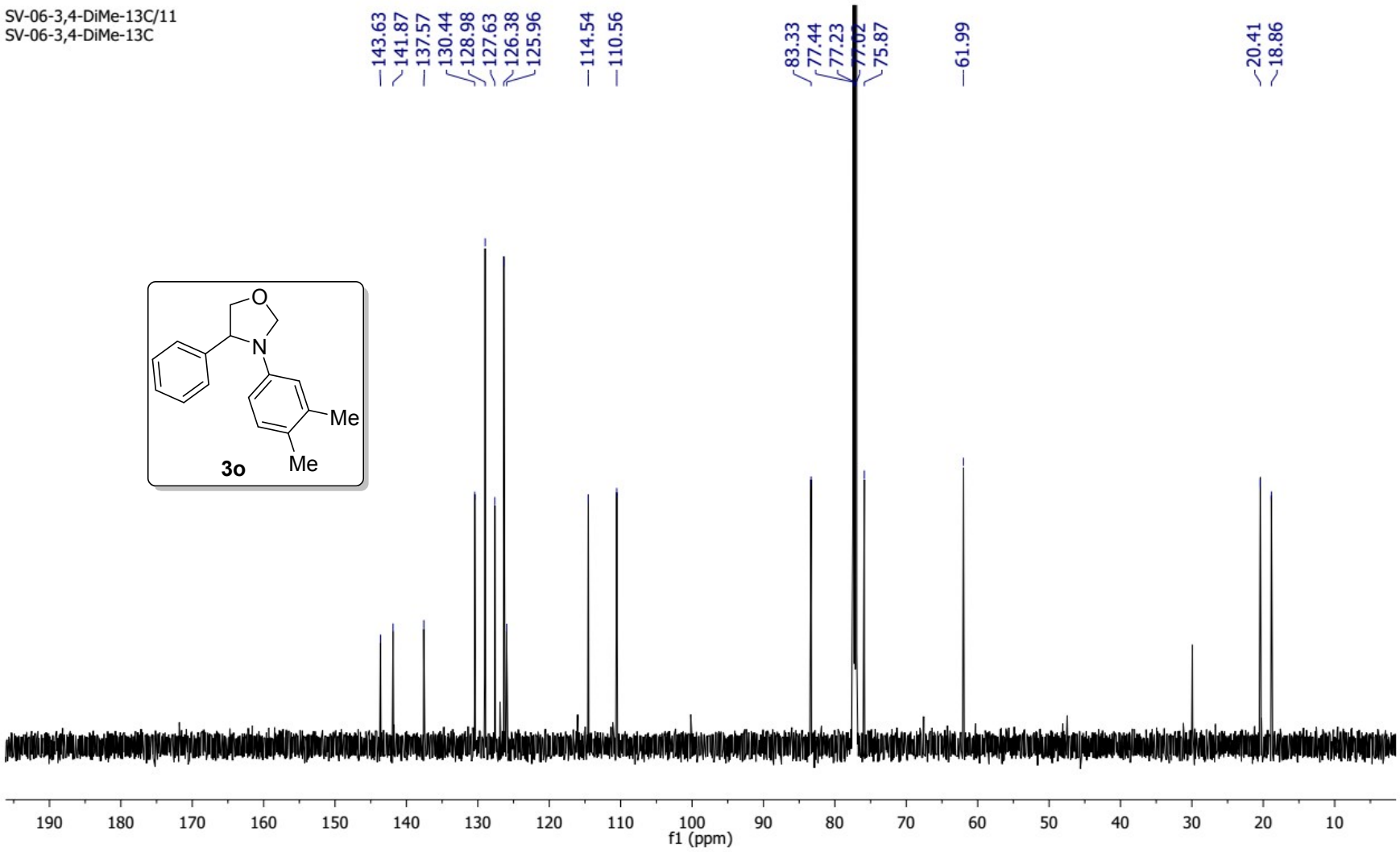

SV-06-IPR-1H/10
7.374
7.371
7.359
7.357
7.348
7.336
7.326
7.323
7.282
7.280
7.277
7.271
7.268
7.260
7.049
7.035
6.439
6.425
5.311
5.308
4.991
4.987
4.654
4.647
4.643
4.635
4.380
4.369
4.366
4.355
3.958
3.951
3.944
3.937
2.805
2.793
2.782
2.770
2.759
1.182
1.178
1.170
1.166
O
N
3l
iPr
4.02
1.30
1.98
1.97
1.04
0.97
0.97
1.03
1.00
1.13
2.95
3.06
f1 (ppm)

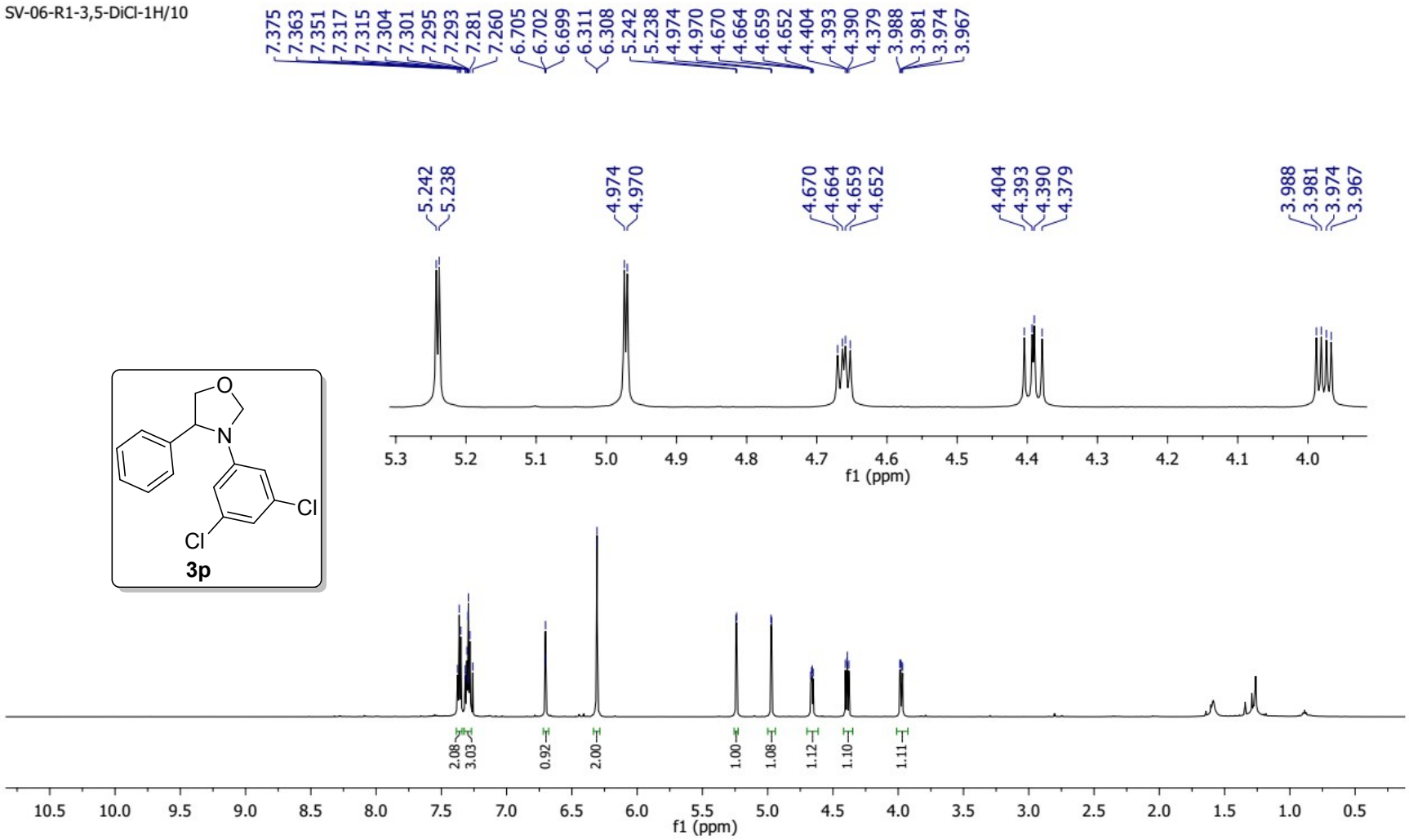

SV-06-IPR-13C/10
143.50
141.88
138.32
128.99
127.70
127.32
126.42
112.95
83.29
77.44
77.23
77.02
75.90
62.18
33.31
24.39
O
N
3l
iPr
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

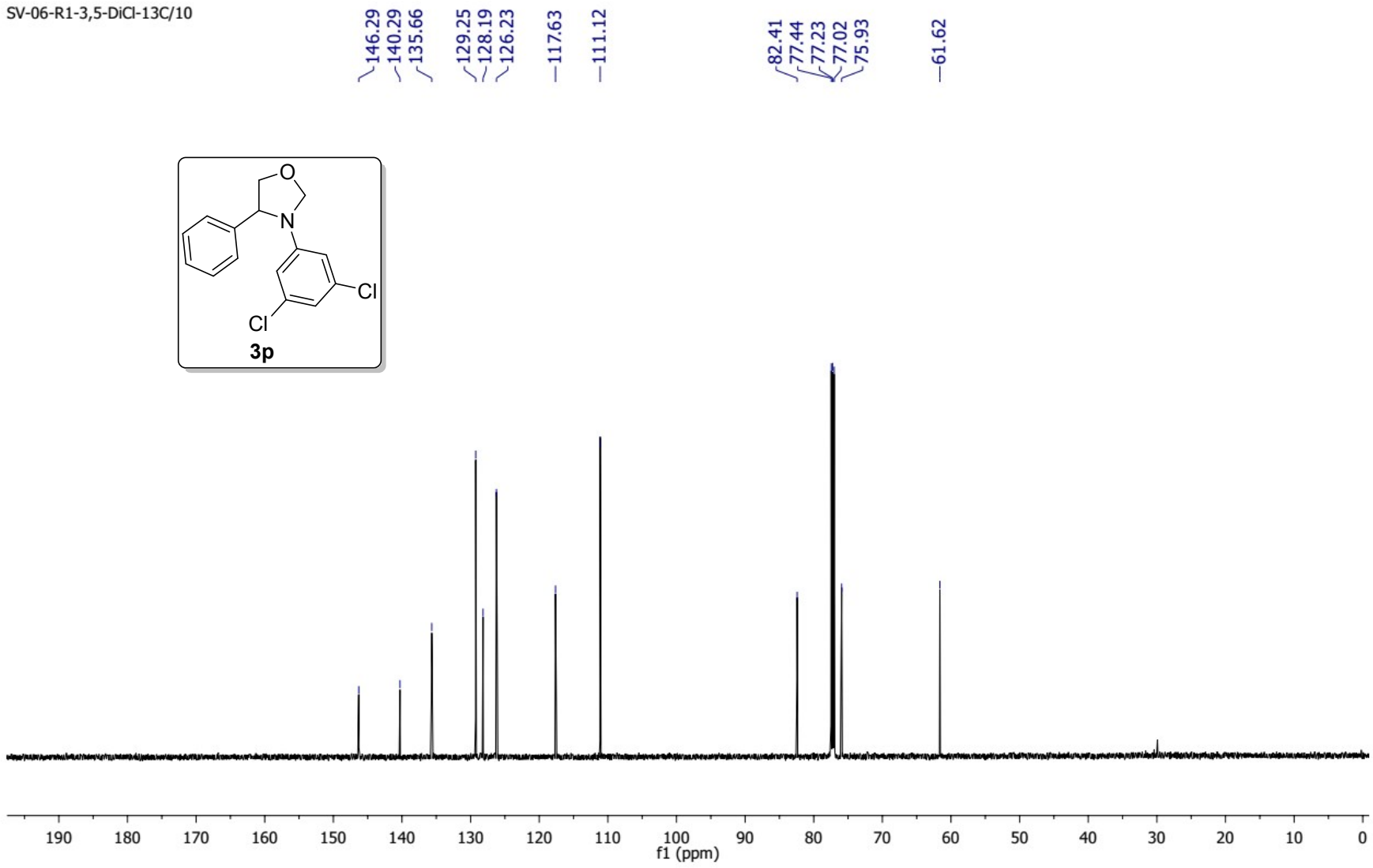

SV-06-BN-1H.10.fid
SV-06-BN-1H
7.260
7.243
7.224
7.202
7.186
7.171
7.144
7.141
7.122
7.103
7.100
7.082
6.814
6.793
6.727
6.709
6.691
5.101
5.084
5.067
4.448
4.405
4.365
4.323
3.995
3.978
1.896
OH
Ph
N
Ph
Ph
A4
7.34
5.21
2.10
1.11
1.00
1.12
1.08
2.03
1.04
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
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)

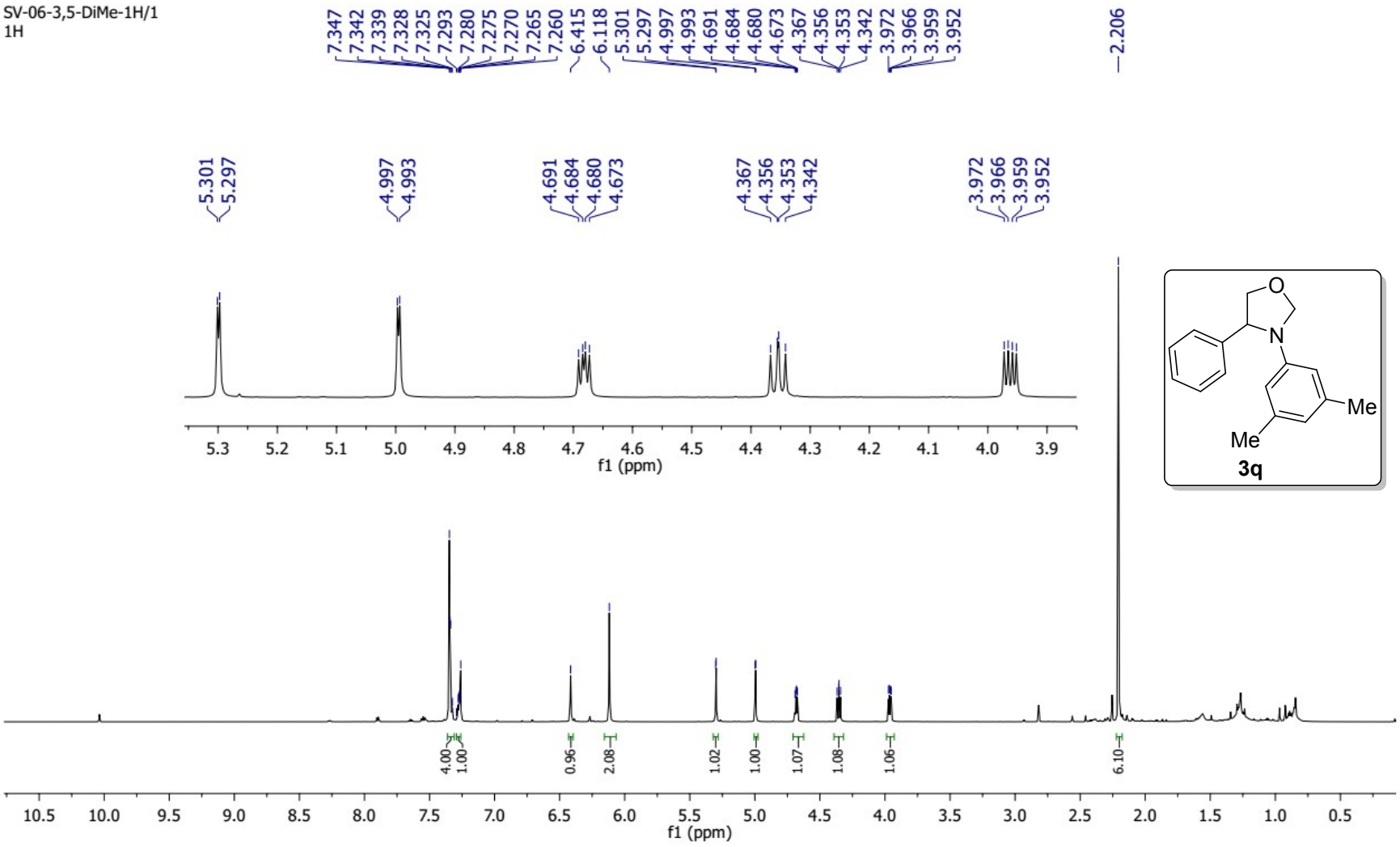

SV-06-Bn-13C.10.fid
SV-06-Bn-13C
149.78
139.83
138.12
129.31
128.89
127.77
127.74
127.09
126.85
118.94
116.08
77.55
77.23
76.91
65.22
63.24
50.98
OH
Ph
N
Ph
Ph
A4
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

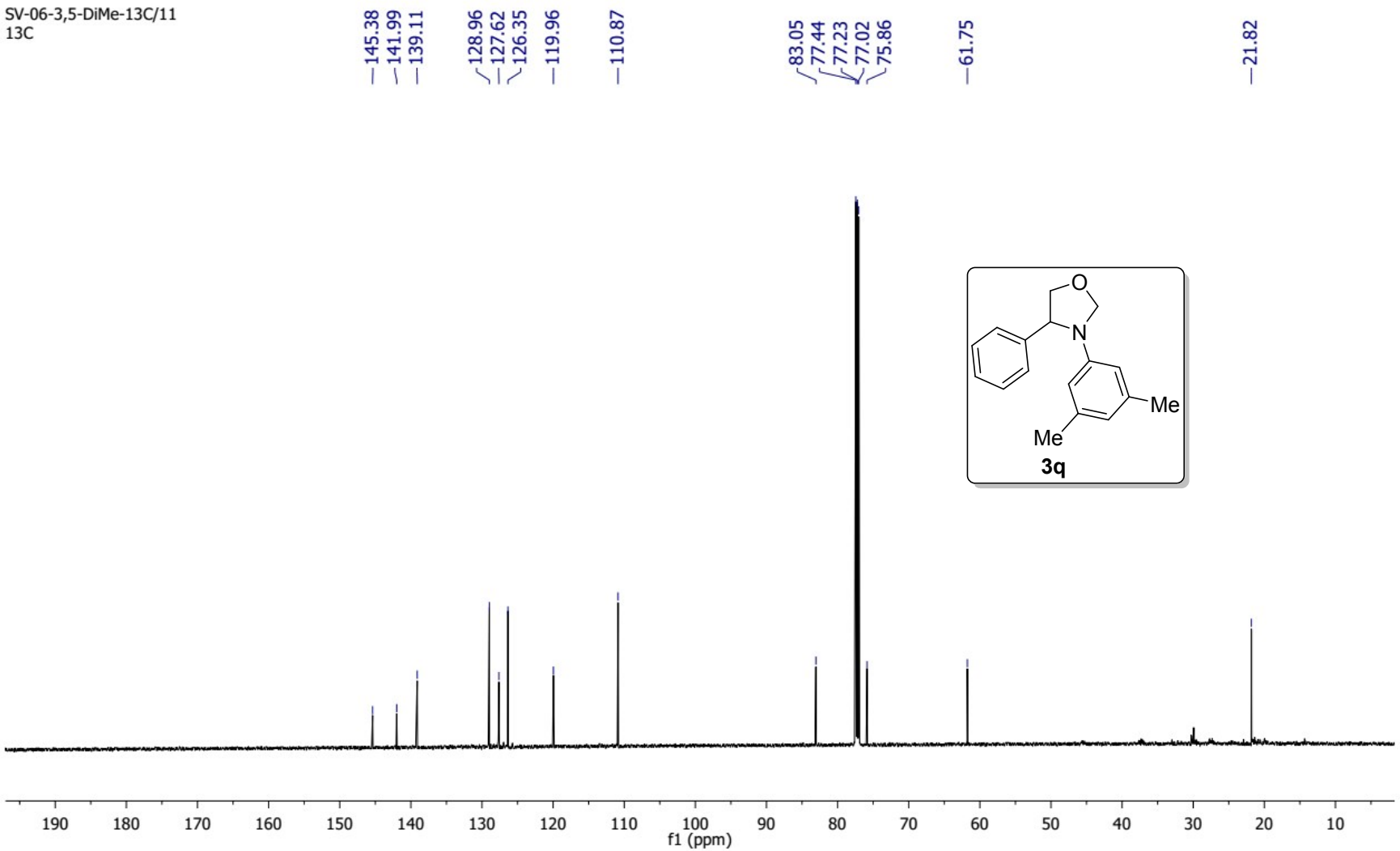

SV-06-3,4-DiMe-1-1H/15
SV-06-3,4-DiMe-1-1H
7.358
7.346
7.342
7.330
7.317
7.273
7.270
7.260
7.250
6.921
6.907
6.312
6.309
6.242
6.238
6.229
6.224
5.303
5.300
4.979
4.975
4.656
4.648
4.644
4.637
4.383
4.371
4.369
4.357
3.952
3.945
3.938
3.931
2.163
2.129
O
N
Me
Me
3o
f1 (ppm)
f1 (ppm)

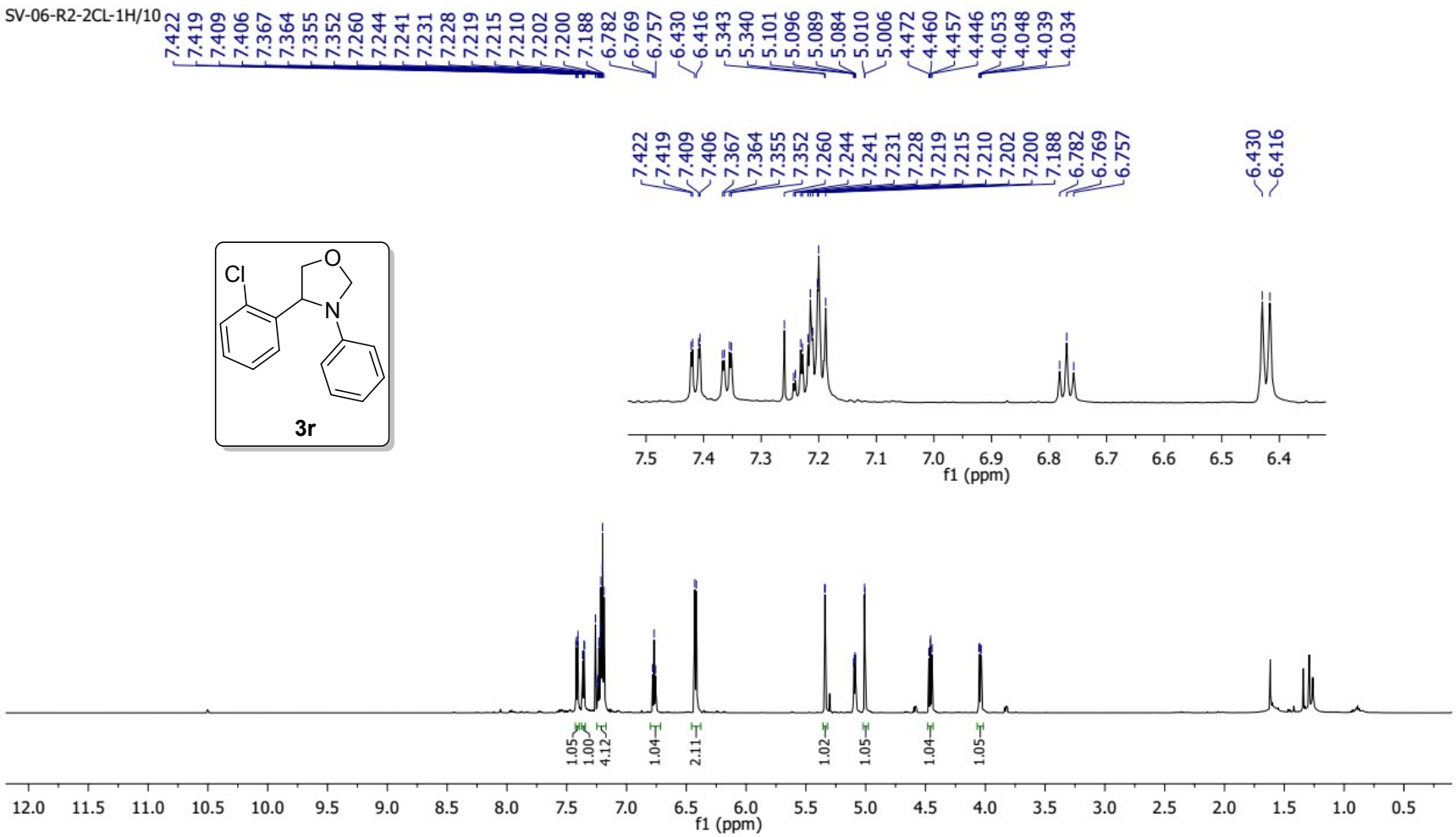

SV-06-3,4-DiMe-13C/11
SV-06-3,4-DiMe-13C
143.63
141.87
137.57
130.44
128.98
127.63
126.38
125.96
114.54
110.56
83.33
77.44
77.23
77.02
75.87
61.99
20.41
18.86
O
N
Me
Me
3o
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


SV-06-R1-3,5-DiCl-1H/10
7.375
7.363
7.351
7.317
7.315
7.304
7.301
7.295
7.293
7.281
7.260
6.705
6.702
6.699
6.311
6.308
5.242
5.238
4.974
4.970
4.670
4.664
4.659
4.652
4.404
4.393
4.390
4.379
3.988
3.981
3.974
3.967
O
N
Cl
Cl
3p
f1 (ppm)
2.08
3.03
0.92
2.00
1.00
1.08
1.12
1.10
1.11
f1 (ppm)


SV-06-R1-3,5-DiCl-13C/10
146.29
140.29
135.66
129.25
128.19
126.23
117.63
111.12
82.41
77.44
77.23
77.02
75.93
61.62
O
N
Cl
Cl
3p
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

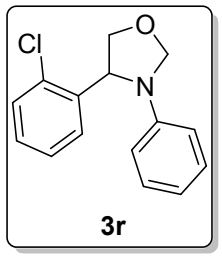

SV-06-3,5-DiMe-1H/1
1H
7.347
7.342
7.339
7.328
7.325
7.293
7.280
7.275
7.270
7.265
7.260
6.415
6.118
5.301
5.297
4.997
4.993
4.691
4.684
4.680
4.673
4.367
4.356
4.353
4.342
3.972
3.966
3.959
3.952
2.206
f1 (ppm)
Me
Me
3q


SV-06-3,5-DiMe-13C/11
13C
145.38
141.99
139.11
128.96
127.62
126.35
119.96
110.87
83.05
77.44
77.23
77.02
75.86
61.75
21.82
O
N
Me
Me
3q
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

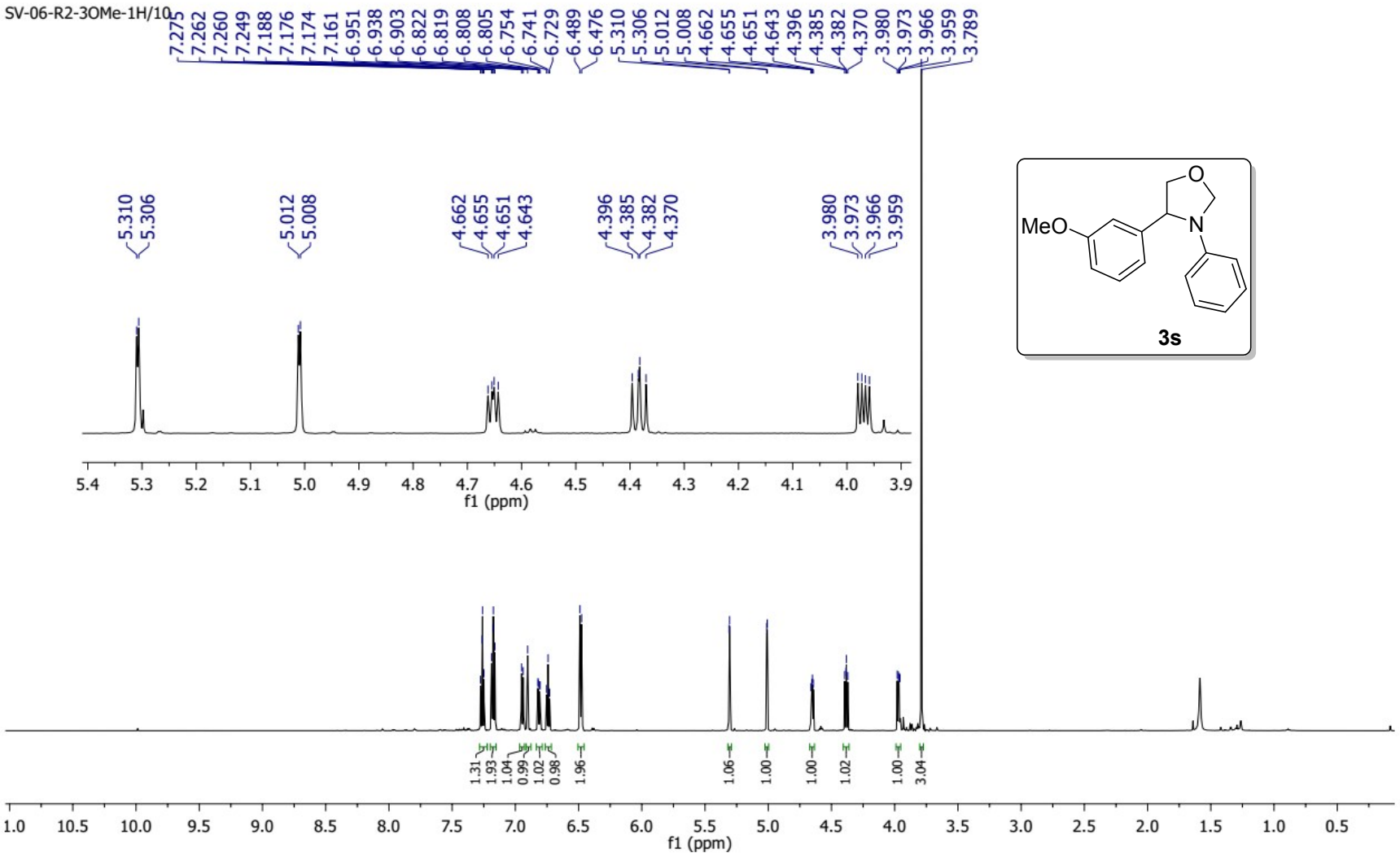

SV-06-R2-2CL-1H/10
7.422
7.419
7.409
7.406
7.367
7.364
7.355
7.352
7.260
7.244
7.241
7.231
7.228
7.219
7.215
7.210
7.202
7.200
7.188
6.782
6.769
6.757
6.430
6.416
5.343
5.340
5.101
5.096
5.089
5.084
5.010
5.006
4.472
4.460
4.457
4.446
4.053
4.048
4.039
4.034
Cl
O
N
3r
f1 (ppm)
1.05
1.00
4.12
1.04
2.11
1.02
1.05
1.04
1.05
f1 (ppm)

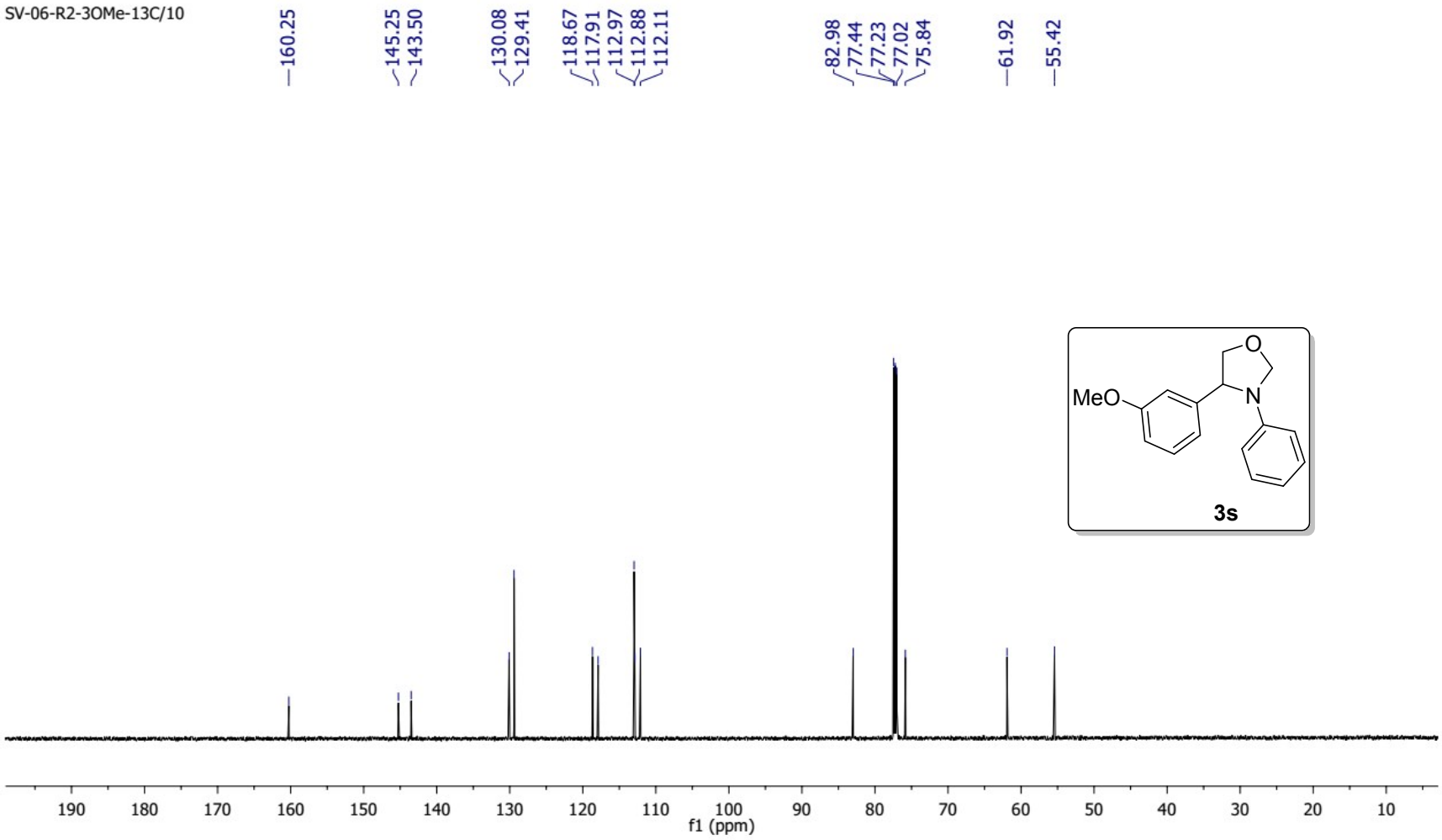
SV-06-R2-2CL-13C/10

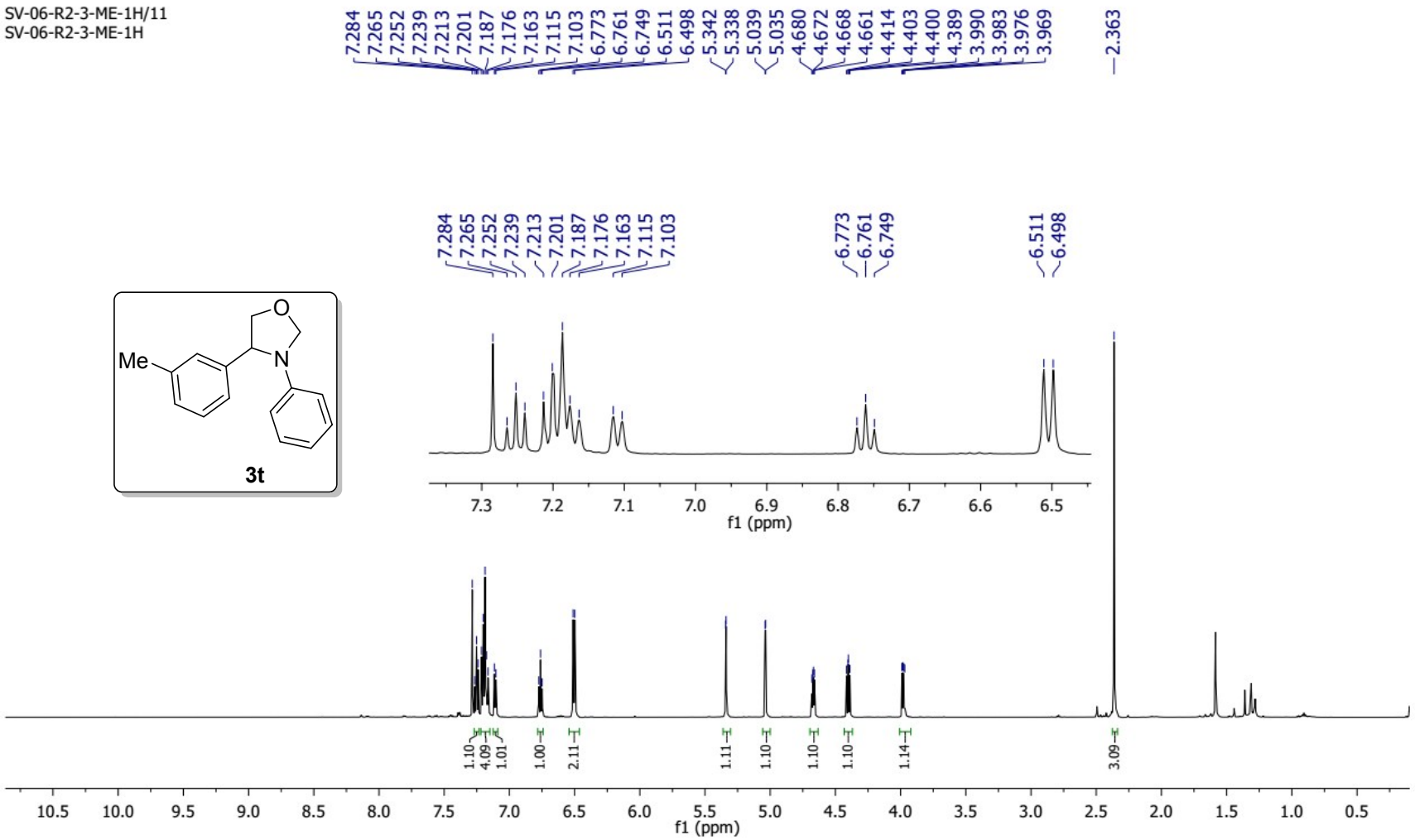
144.70
138.62
132.39
129.77
129.57
128.92
127.92
127.44
118.08
112.85
82.65
77.44
77.23
77.02
74.48
59.18



3r

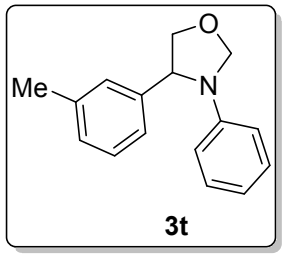

SV-06-R2-3OMe-1H/10
7.275
7.262
7.260
7.249
7.188
7.176
7.174
7.161
6.951
6.938
6.903
6.822
6.819
6.808
6.805
6.754
6.741
6.729
6.489
6.476
5.310
5.306
5.012
5.008
4.662
4.655
4.651
4.643
4.396
4.385
4.382
4.370
3.980
3.973
3.966
3.959
3.789
MeO
O
N
3s
f1 (ppm)
1.31
1.93
1.04
0.99
1.02
0.98
1.96
1.06
1.00
1.00
1.02
1.00
3.04


SV-06-R2-3OMe-13C/10
160.25
145.25
143.50
130.08
129.41
118.67
117.91
112.97
112.88
112.11
82.98
77.44
77.23
77.02
75.84
61.92
55.42
MeO
O
N
3s
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

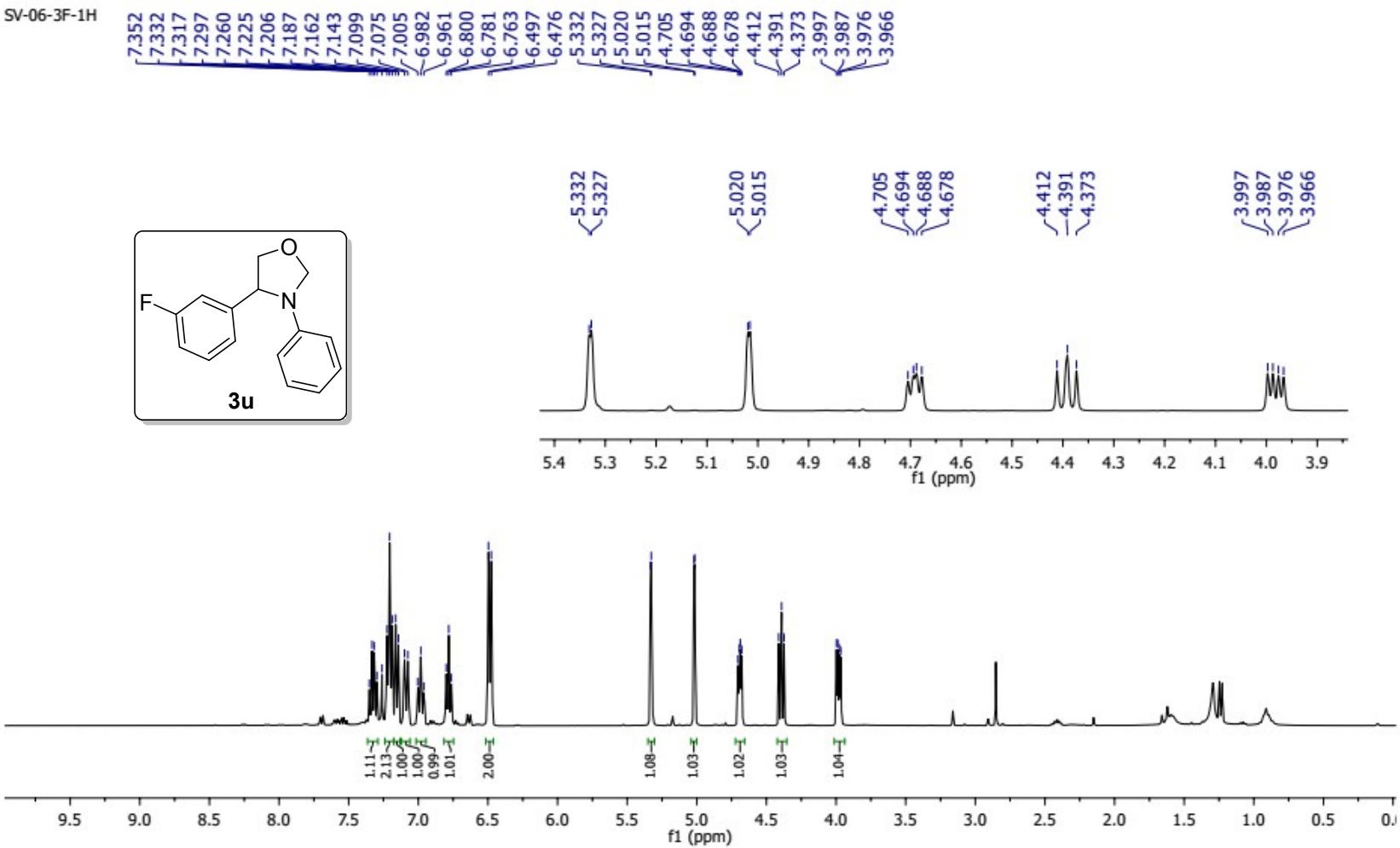

SV-06-R2-3-ME-1H/11
SV-06-R2-3-ME-1H
7.284
7.265
7.252
7.239
7.213
7.201
7.187
7.176
7.163
7.115
7.103
6.773
6.761
6.749
6.511
6.498
5.342
5.338
5.039
5.035
4.680
4.672
4.668
4.661
4.414
4.403
4.400
4.389
3.990
3.983
3.976
3.969
2.363
Me
O
N
3t
f1 (ppm)
1.10
4.09
1.01
1.00
2.11
1.11
1.10
1.10
1.10
1.14
3.09

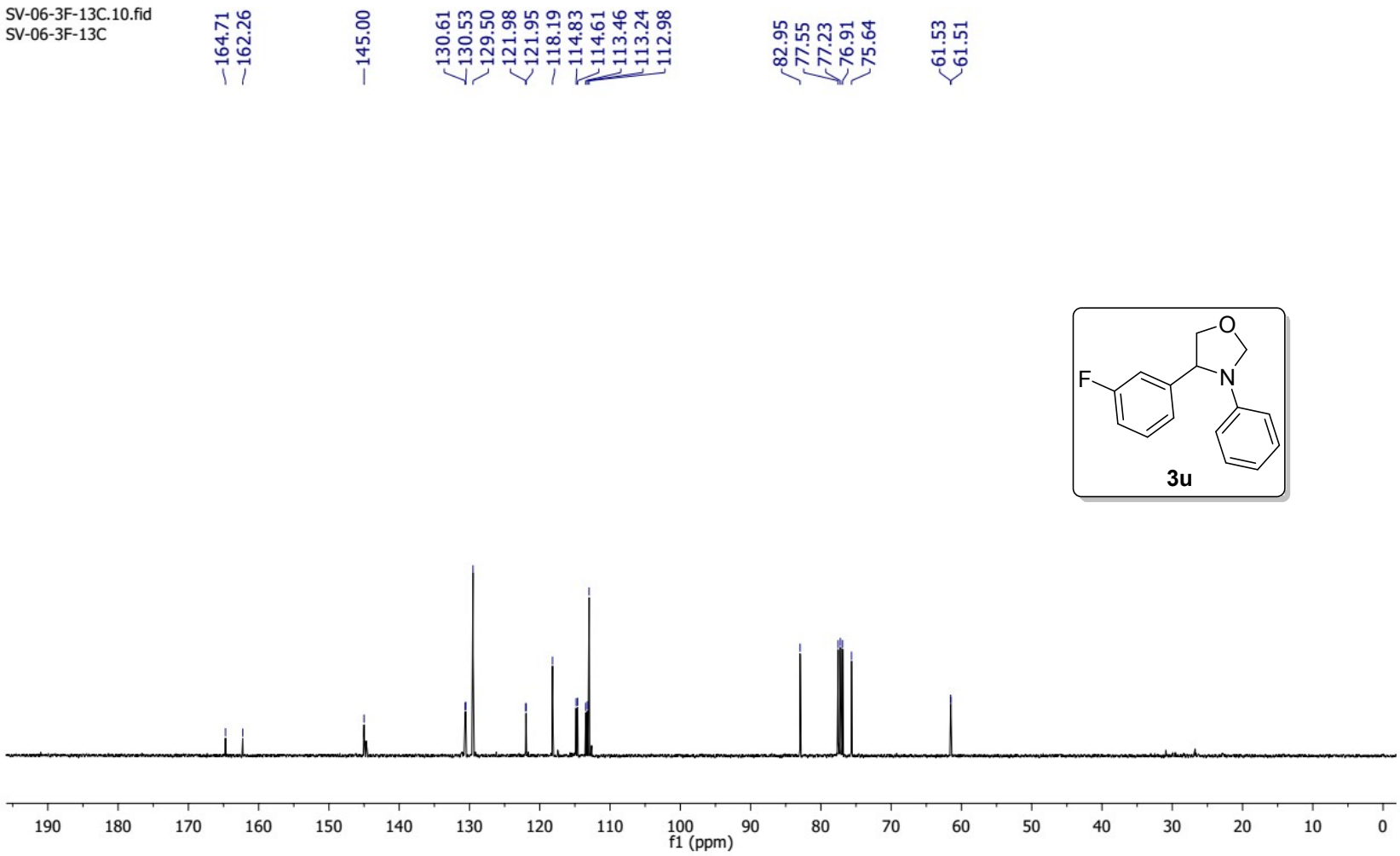
SV-06-R2-3-ME-13C/11
SV-06-R2-3-ME-13C

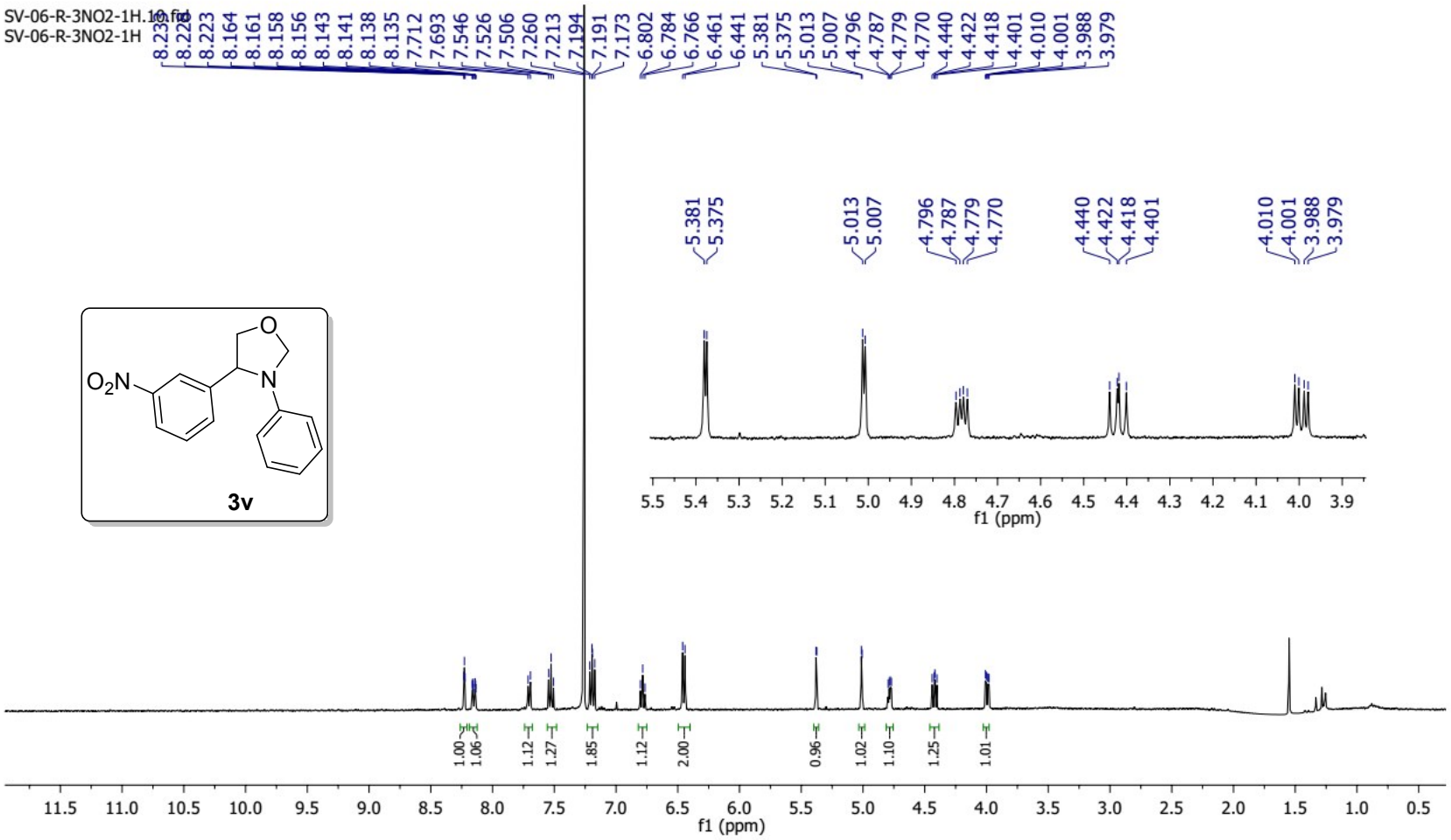
145.31
141.66
138.71
129.42
128.89
128.55
126.95
123.44
117.79
112.92
82.99
77.44
77.23
77.02
75.97
61.94
21.74

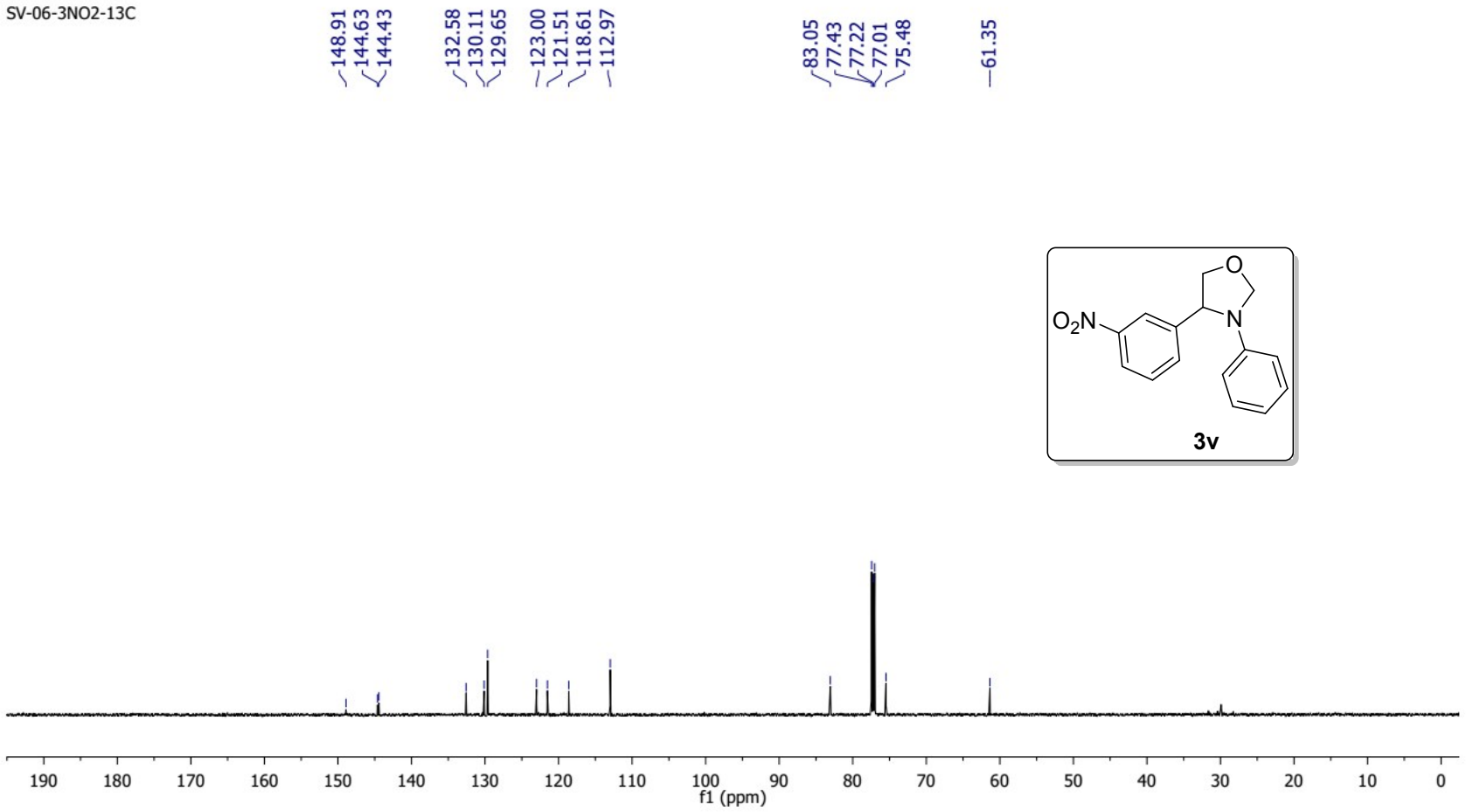


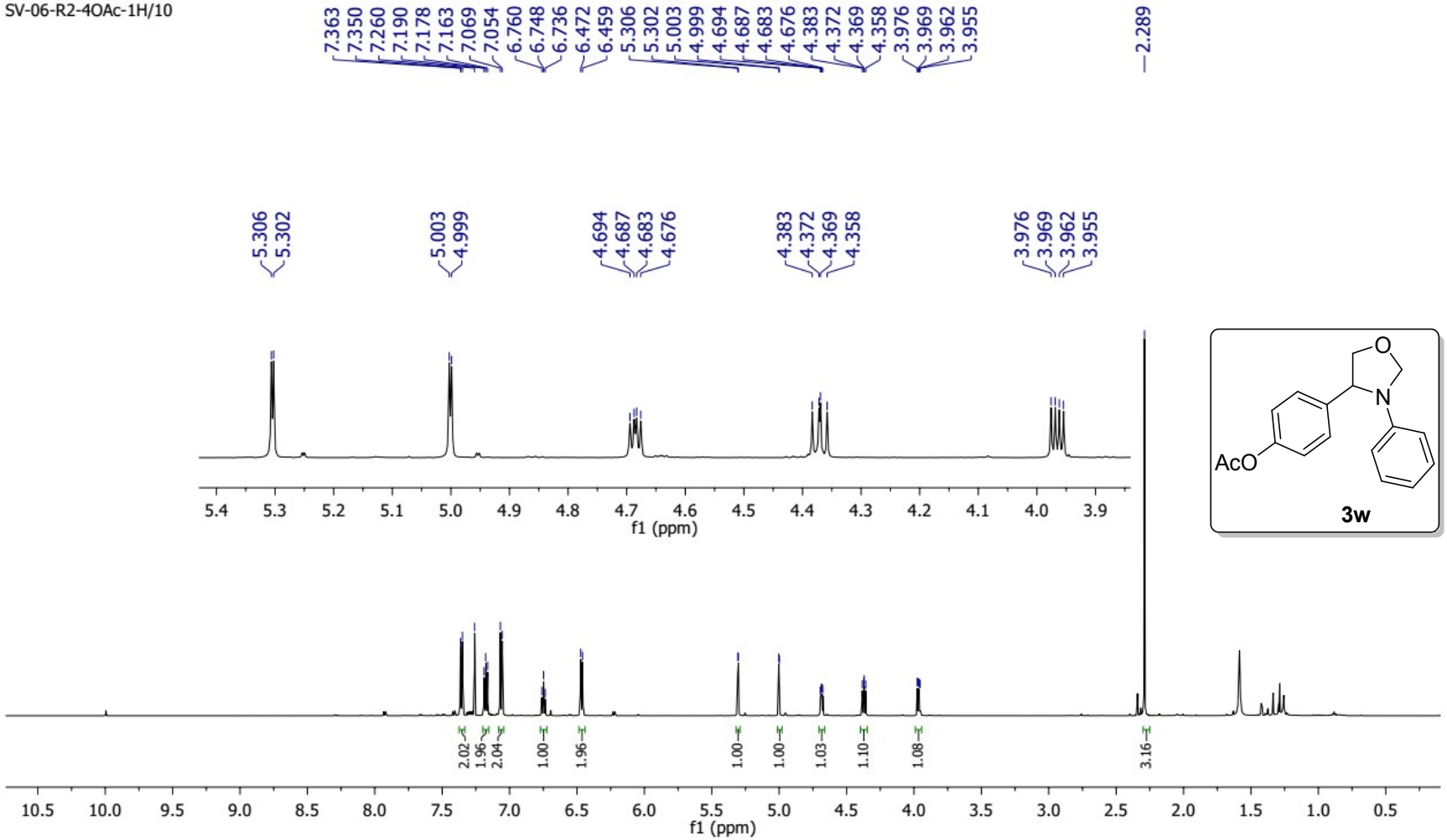
3t

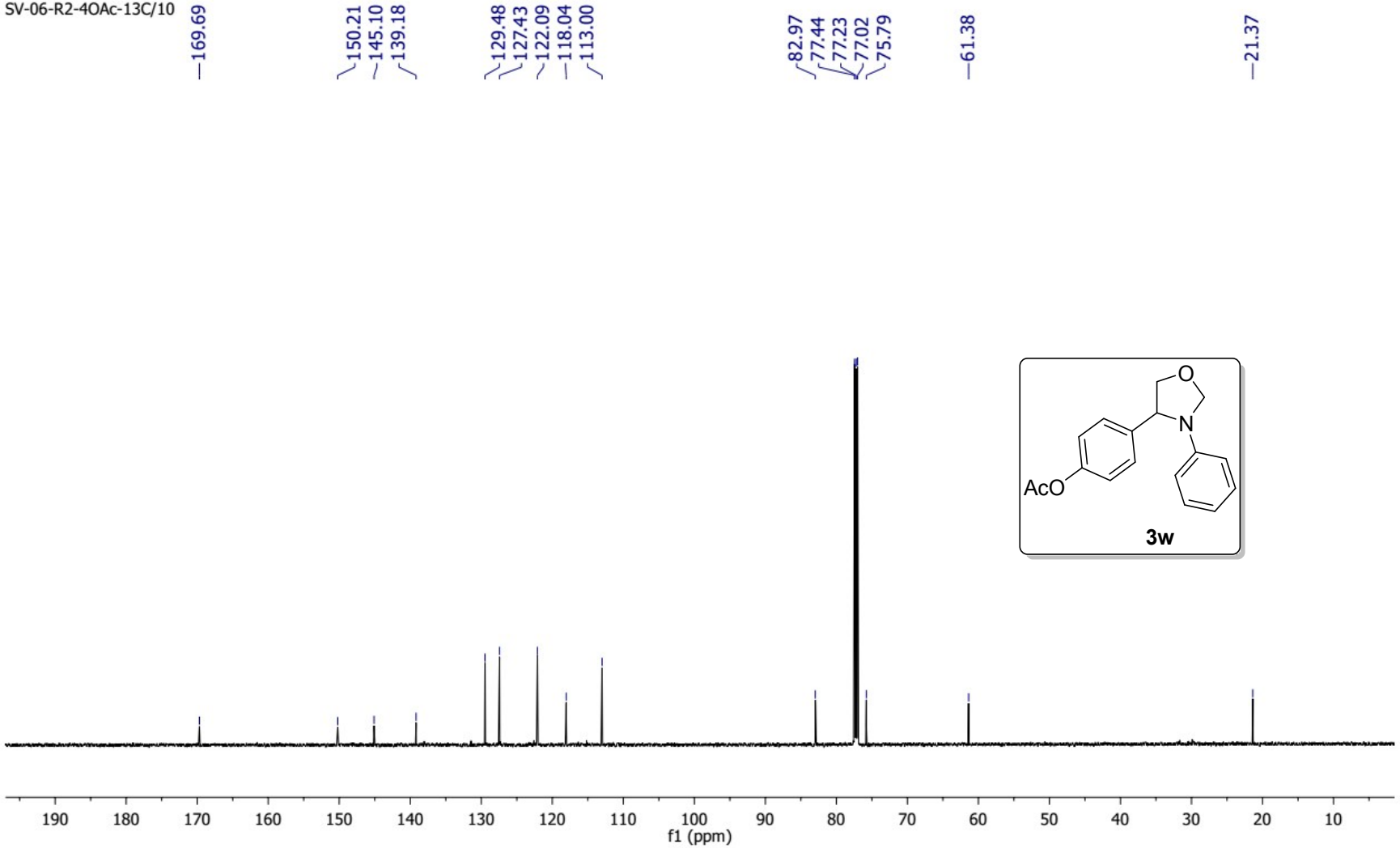

SV-06-3F-1H
7.352
7.332
7.317
7.297
7.260
7.225
7.206
7.187
7.162
7.143
7.099
7.075
7.005
6.982
6.961
6.800
6.781
6.763
6.497
6.476
5.332
5.327
5.020
5.015
4.705
4.694
4.688
4.678
4.412
4.391
4.373
3.997
3.987
3.976
3.966
O
N
F
3u
f1 (ppm)
1.11
2.13
1.00
1.00
0.99
1.01
2.00
1.08
1.03
1.02
1.03
1.04


SV-06-3F-13C.10.fid
SV-06-3F-13C
164.71
162.26
145.00
130.61
130.53
129.50
121.98
121.95
118.19
114.83
114.61
113.46
113.24
112.98
82.95
77.55
77.23
76.91
75.64
61.53
61.51
O
N
F
3u
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

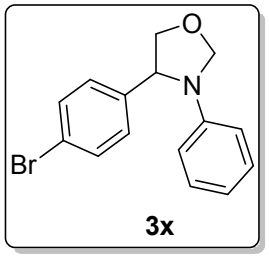

SV-06-R-3NO2-1H.10.fid
SV-06-R-3NO2-1H
8.232
8.228
8.223
8.164
8.161
8.158
8.156
8.143
8.141
8.138
8.135
7.712
7.693
7.546
7.526
7.506
7.260
7.213
7.194
7.191
7.173
6.802
6.784
6.766
6.461
6.441
5.381
5.375
5.013
5.007
4.796
4.787
4.779
4.770
4.440
4.422
4.418
4.401
4.010
4.001
3.988
3.979
O2N
O
N
3v
f1 (ppm)
1.00
1.06
1.12
1.27
1.85
1.12
2.00
0.96
1.02
1.10
1.25
1.01


SV-06-3NO2-13C
148.91
144.63
144.43
132.58
130.11
129.65
123.00
121.51
118.61
112.97
83.05
77.43
77.22
77.01
75.48
61.35
O
N
O2N
3v
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

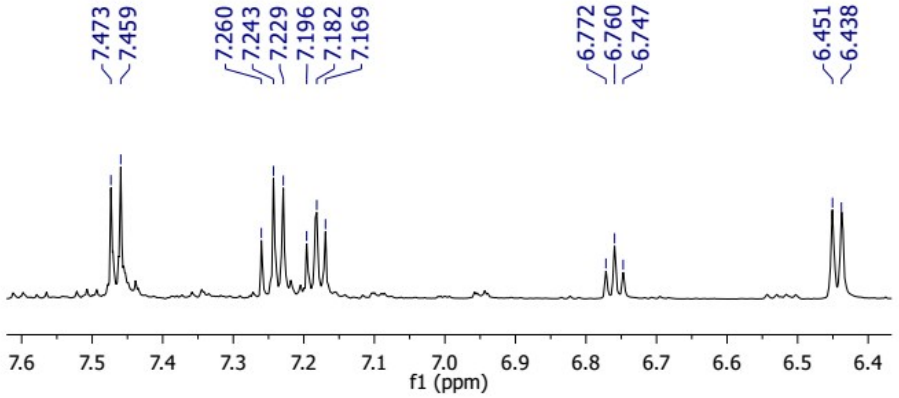

SV-06-R2-4OAc-1H/10
7.363
7.350
7.260
7.190
7.178
7.163
7.069
7.054
6.760
6.748
6.736
6.472
6.459
5.306
5.302
5.003
4.999
4.694
4.687
4.683
4.676
4.383
4.372
4.369
4.358
3.976
3.969
3.962
3.955
2.289
f1 (ppm)
AcO
O
N
3w
2.02
1.96
2.04
1.00
1.96
1.00
1.00
1.03
1.10
1.08
3.16
f1 (ppm)

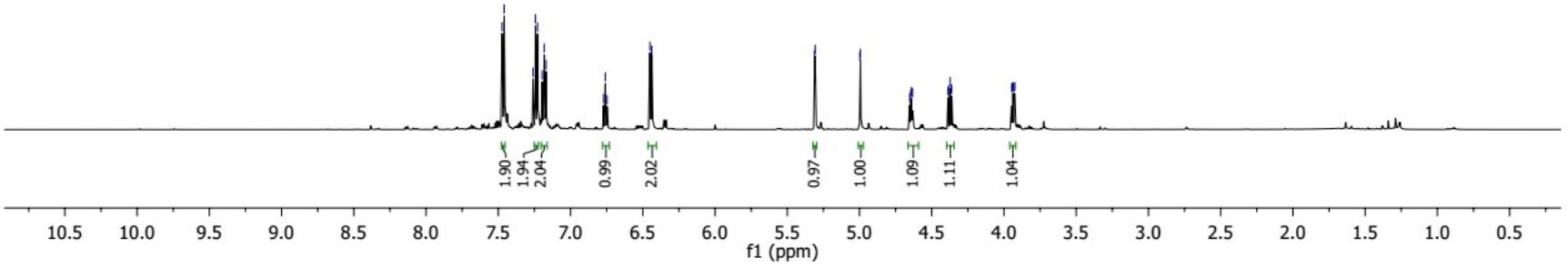

SV-06-R2-4OAc-13C/10
169.69
150.21
145.10
139.18
129.48
127.43
122.09
118.04
113.00
82.97
77.44
77.23
77.02
75.79
61.38
21.37
O
N
AcO
3w
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

SV-06-R2-4BR-1H/10



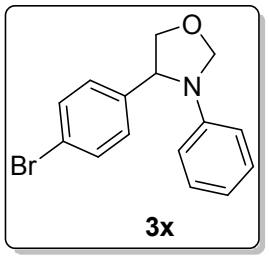
3x



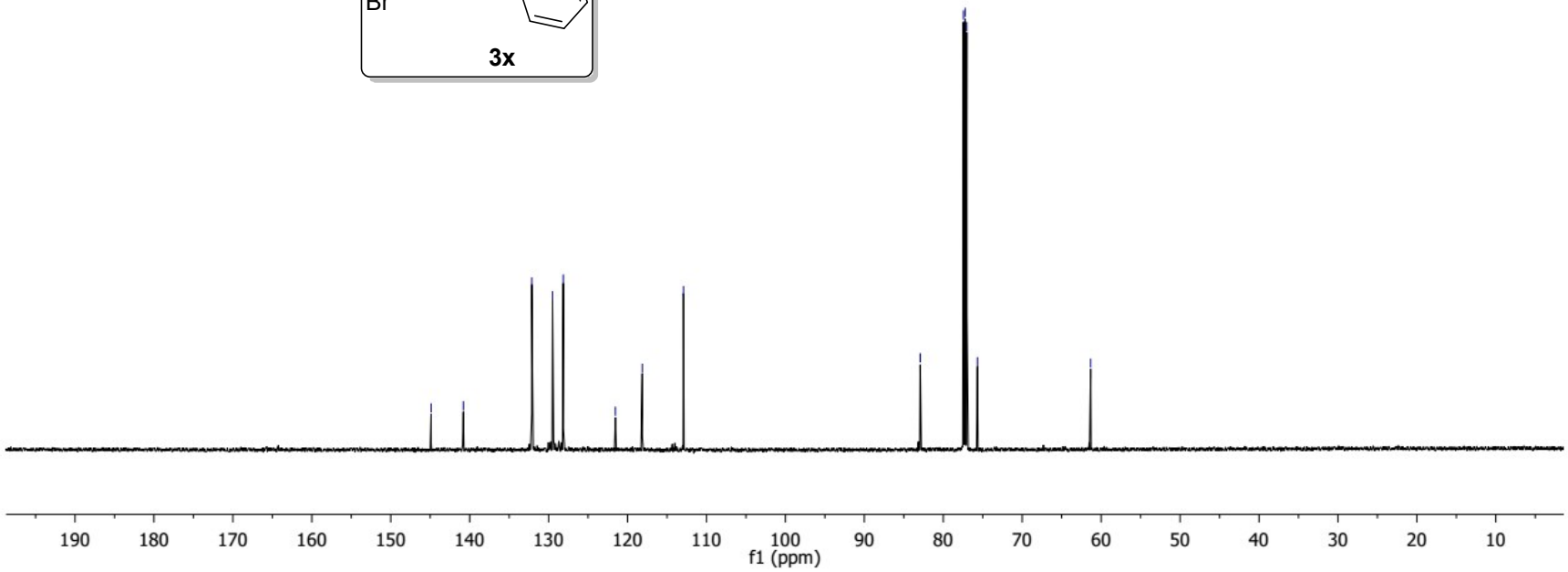


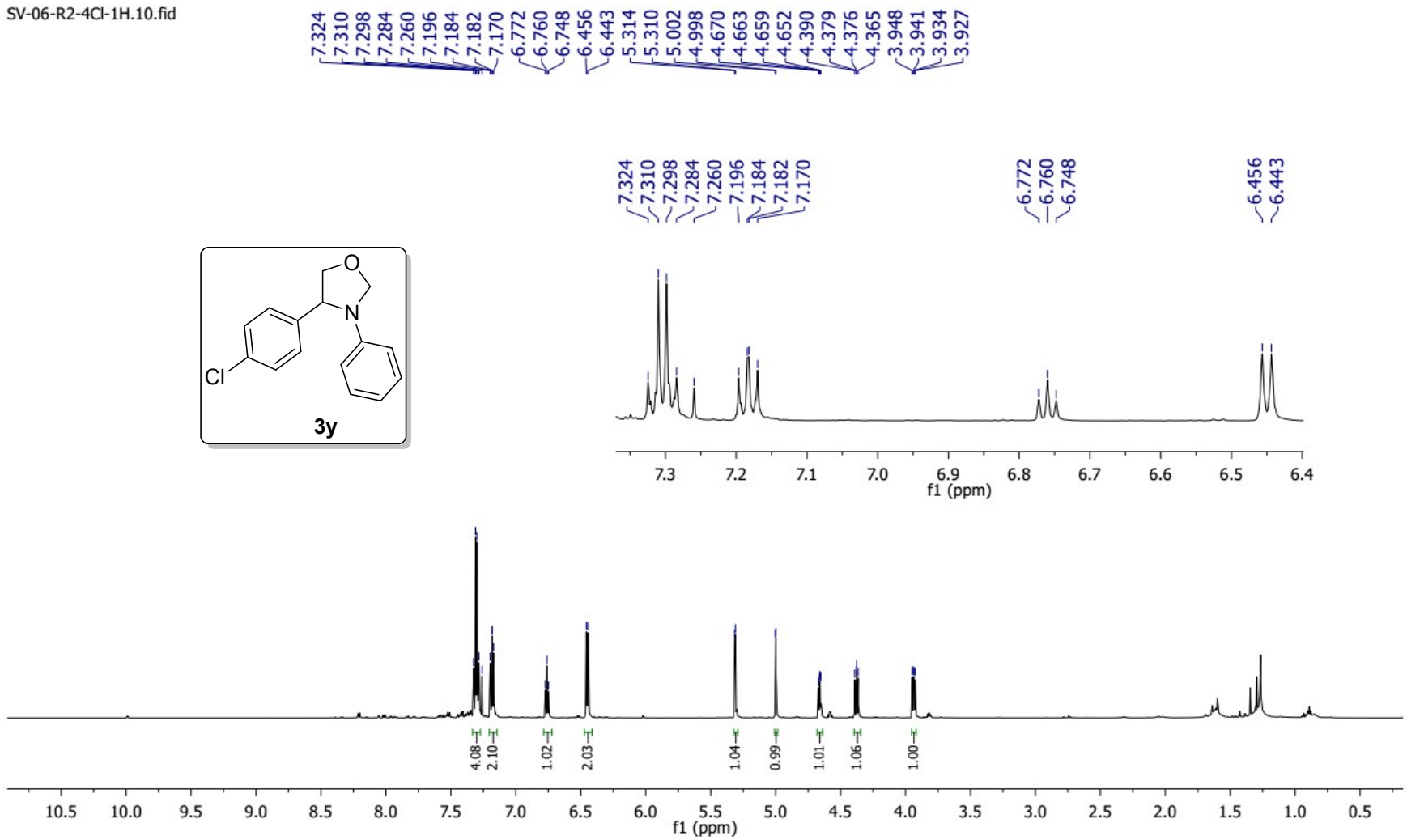
SV-06-R2-4BR-13C/10

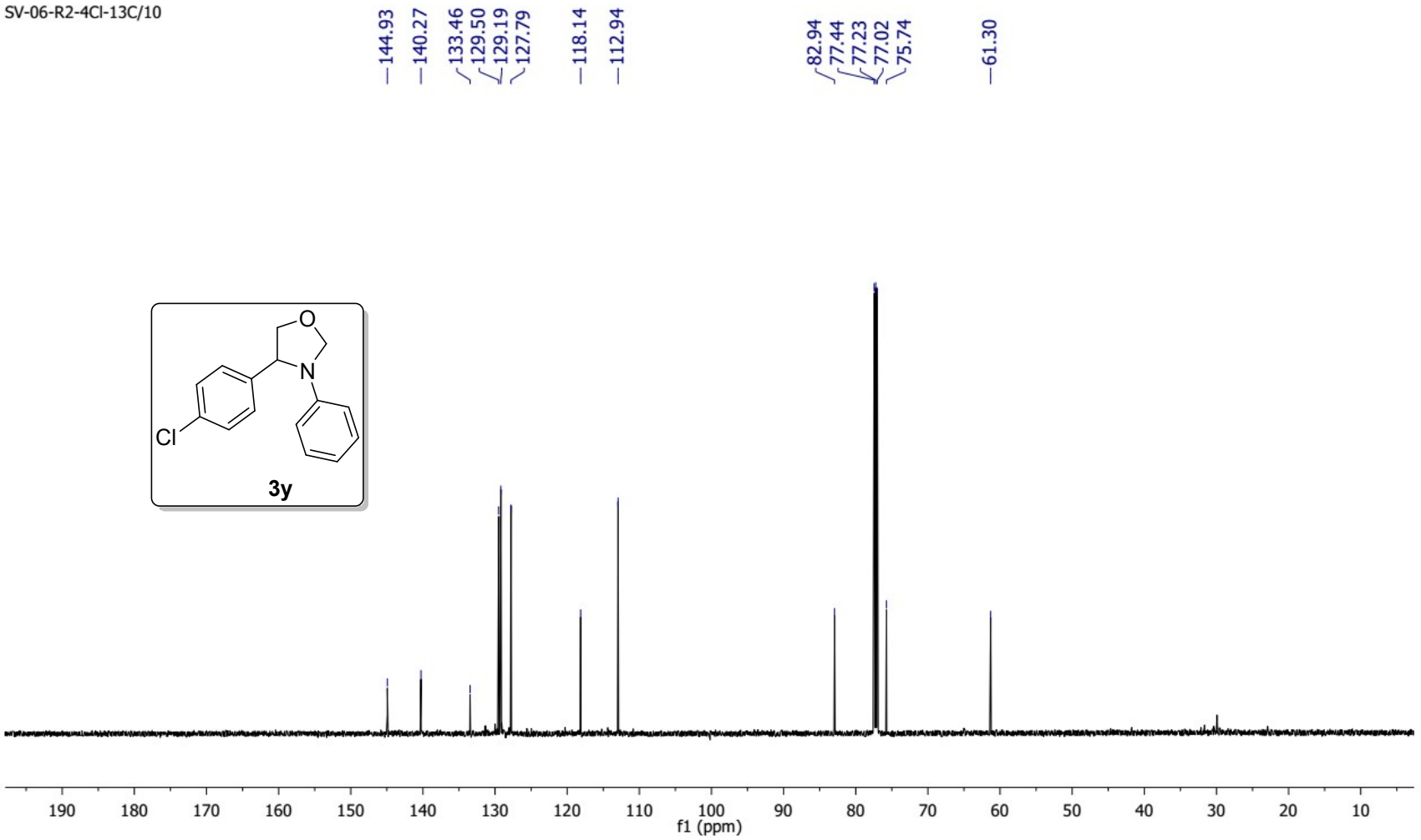
144.88
140.79
132.13
129.50
128.14
121.54
118.13
112.91
82.93
77.44
77.23
77.02
75.67
61.33

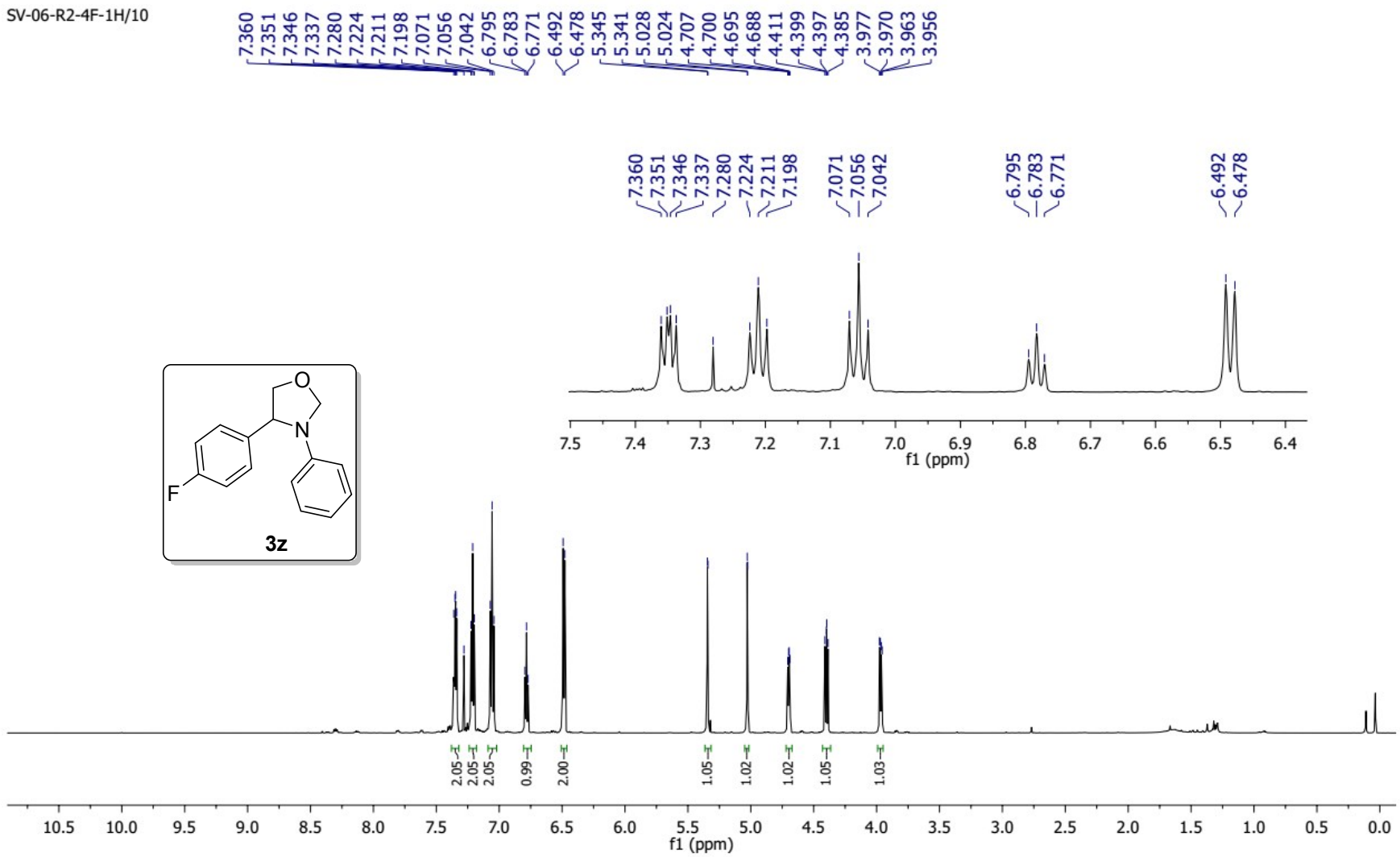


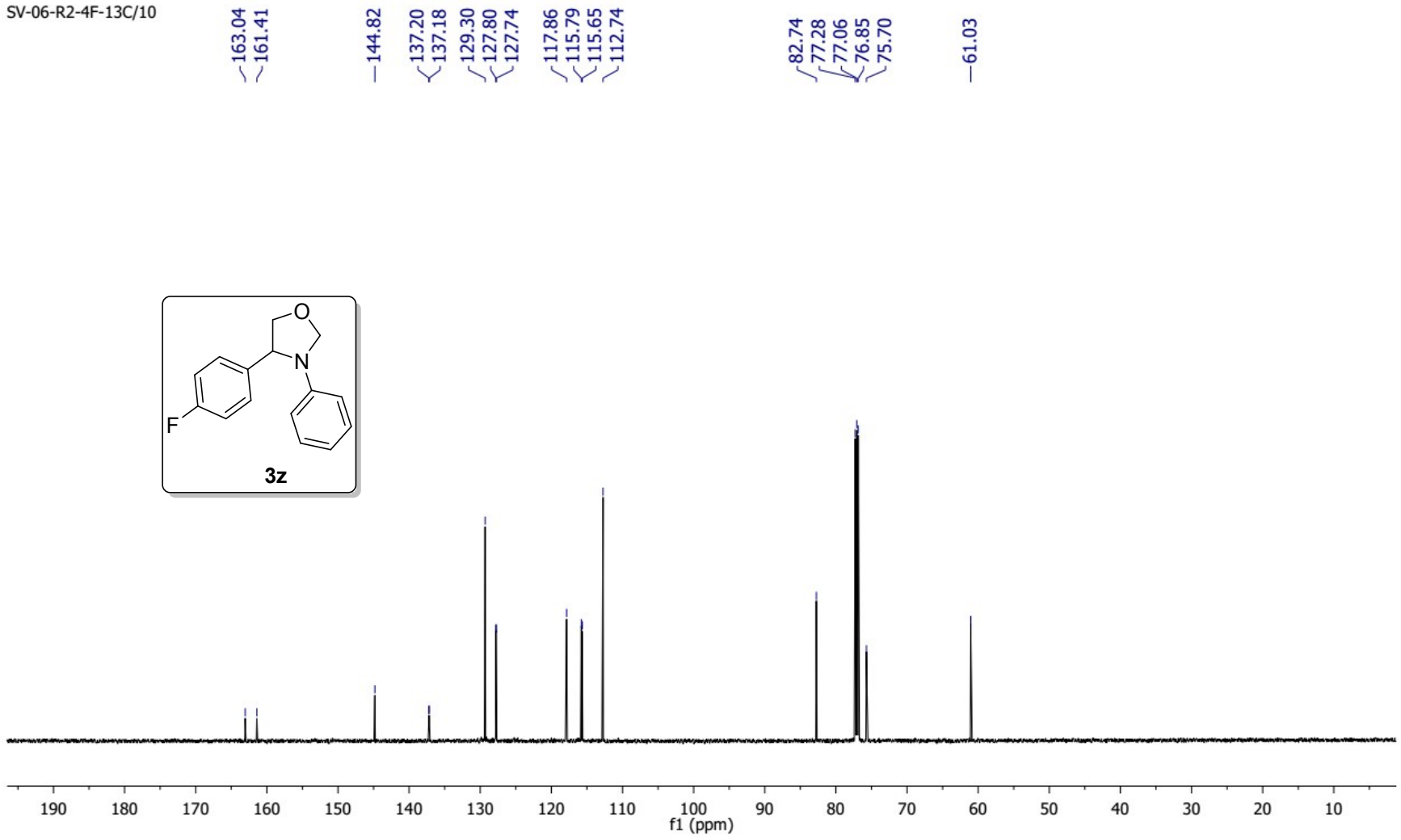
3x

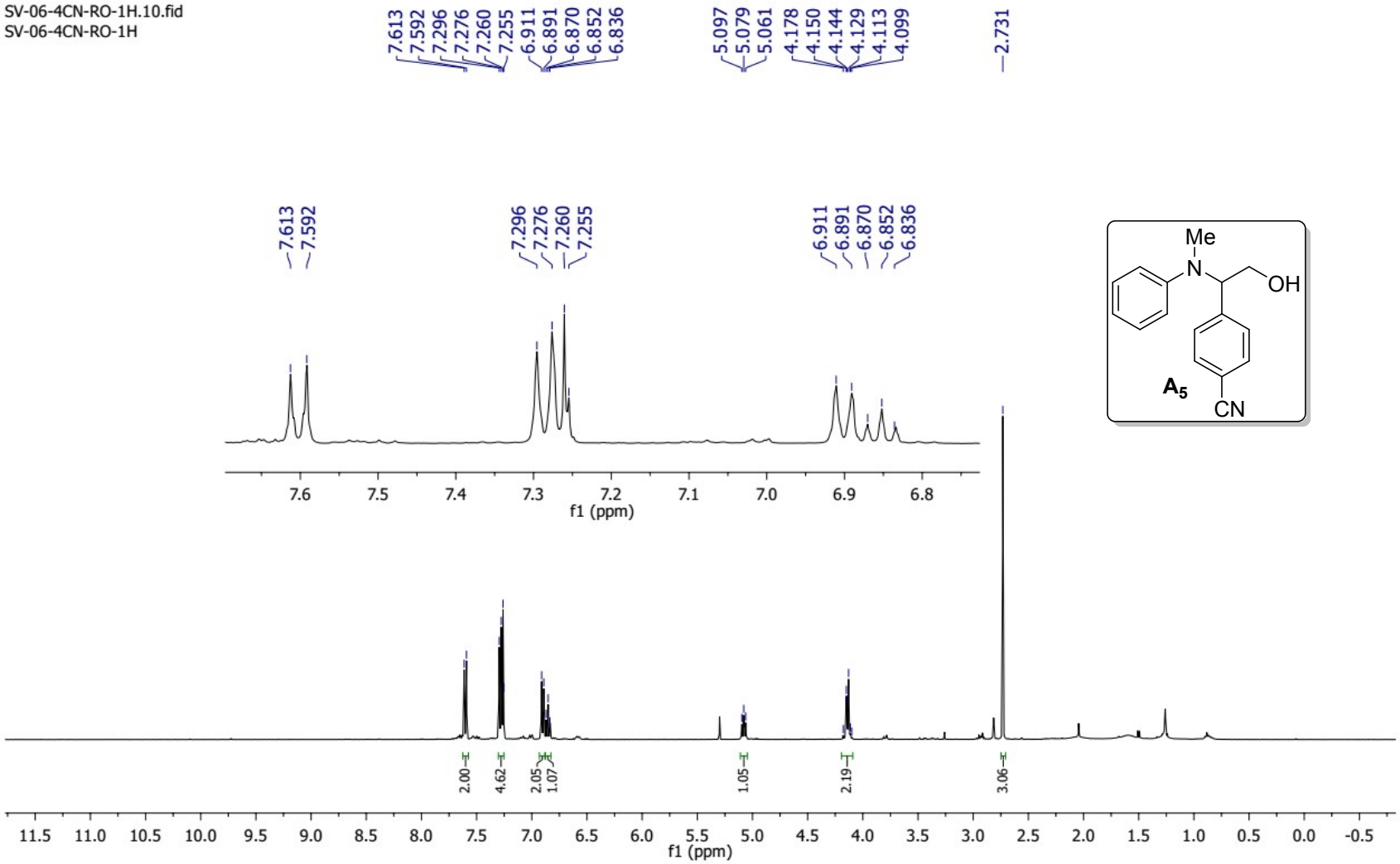


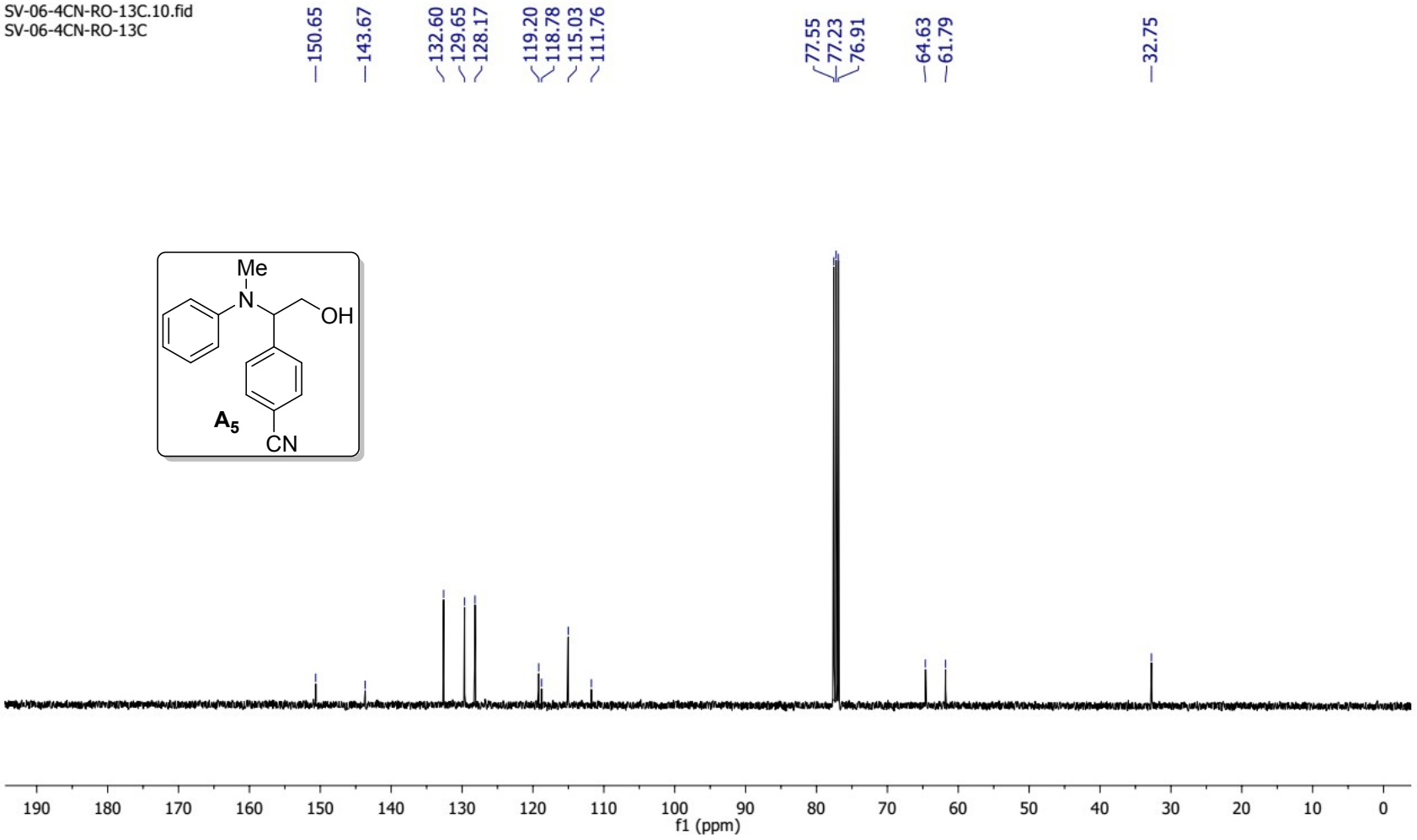

SV-06-R2-4Cl-1H.10.fid
7.324
7.310
7.298
7.284
7.260
7.196
7.184
7.182
7.170
6.772
6.760
6.748
6.456
6.443
5.314
5.310
5.002
4.998
4.670
4.663
4.659
4.652
4.390
4.379
4.376
4.365
3.948
3.941
3.934
3.927
Cl
O
N
3y
f1 (ppm)
4.08
2.10
1.02
2.03
1.04
0.99
1.01
1.06
1.00

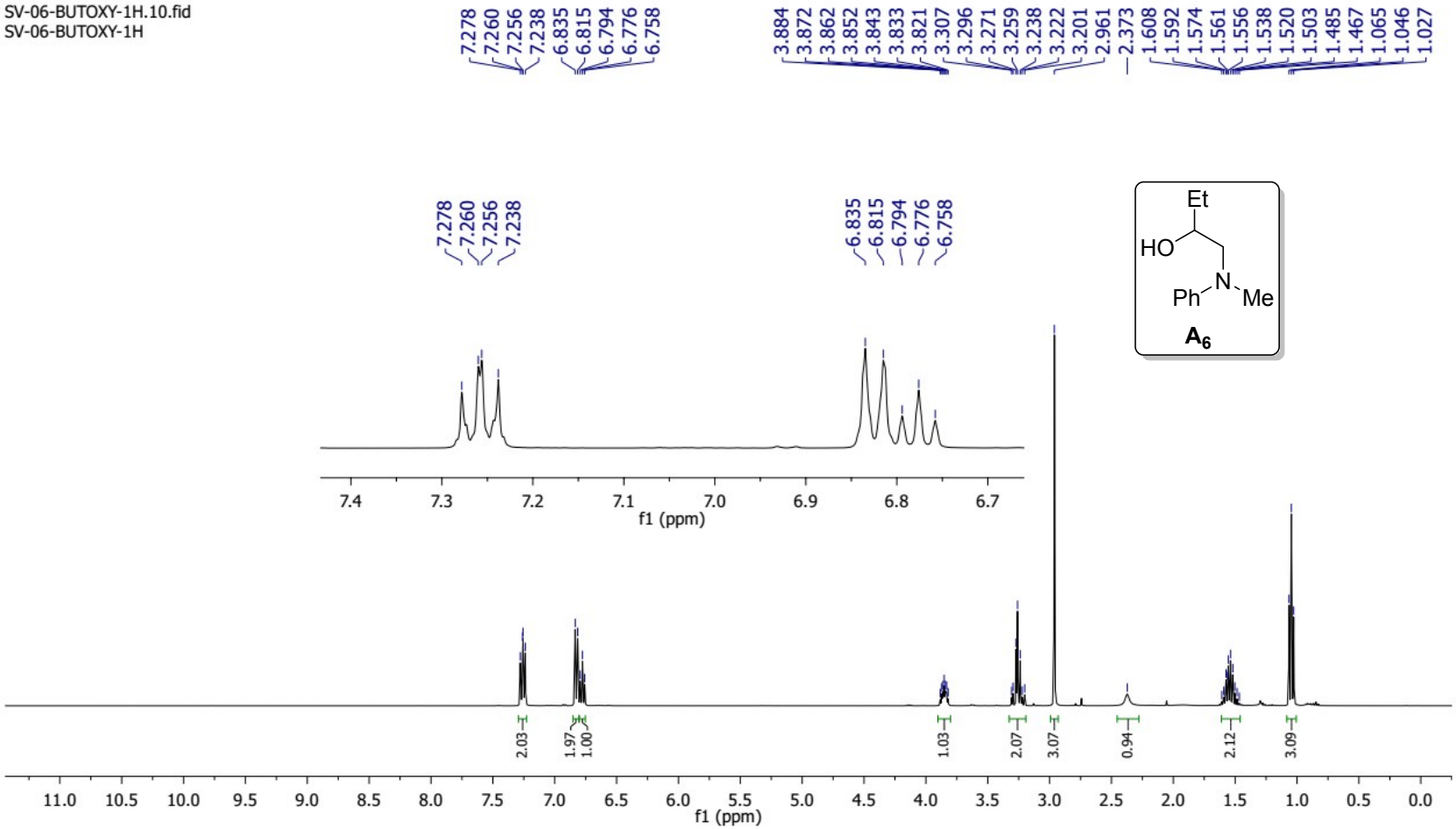

SV-06-R2-4Cl-13C/10
144.93
140.27
133.46
129.50
129.19
127.79
118.14
112.94
82.94
77.44
77.23
77.02
75.74
61.30
O
N
Cl
3y
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

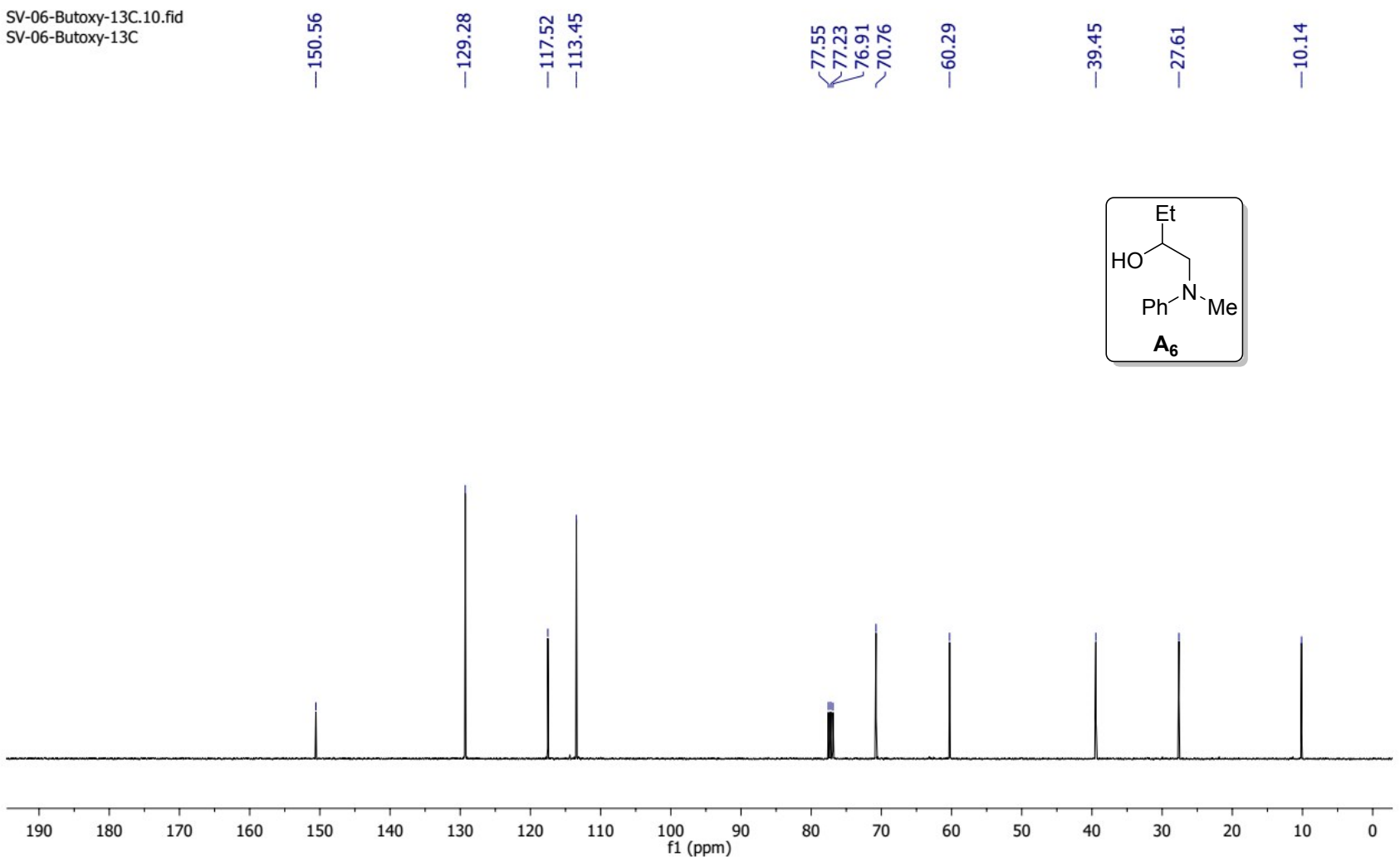

SV-06-R2-4F-1H/10
7.360
7.351
7.346
7.337
7.280
7.224
7.211
7.198
7.071
7.056
7.042
6.795
6.783
6.771
6.492
6.478
5.345
5.341
5.028
5.024
4.707
4.700
4.695
4.688
4.411
4.399
4.397
4.385
3.977
3.970
3.963
3.956
F
O
N
3z
f1 (ppm)
2.05
2.05
2.05
0.99
2.00
1.05
1.02
1.02
1.05
1.03

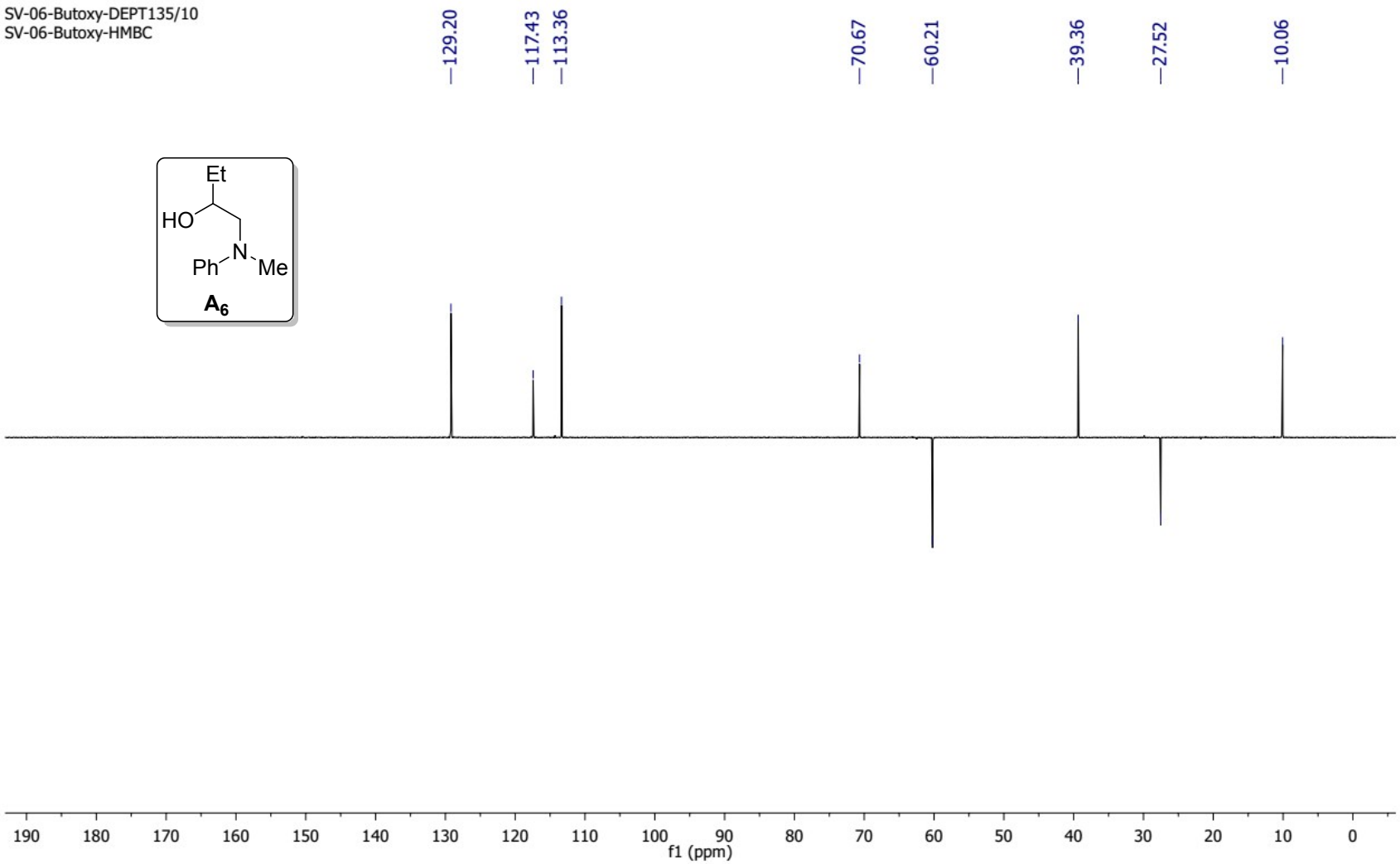

SV-06-R2-4F-13C/10
163.04
161.41
144.82
137.20
137.18
129.30
127.80
127.74
117.86
115.79
115.65
112.74
82.74
77.28
77.06
76.85
75.70
61.03
O
N
F
3z
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

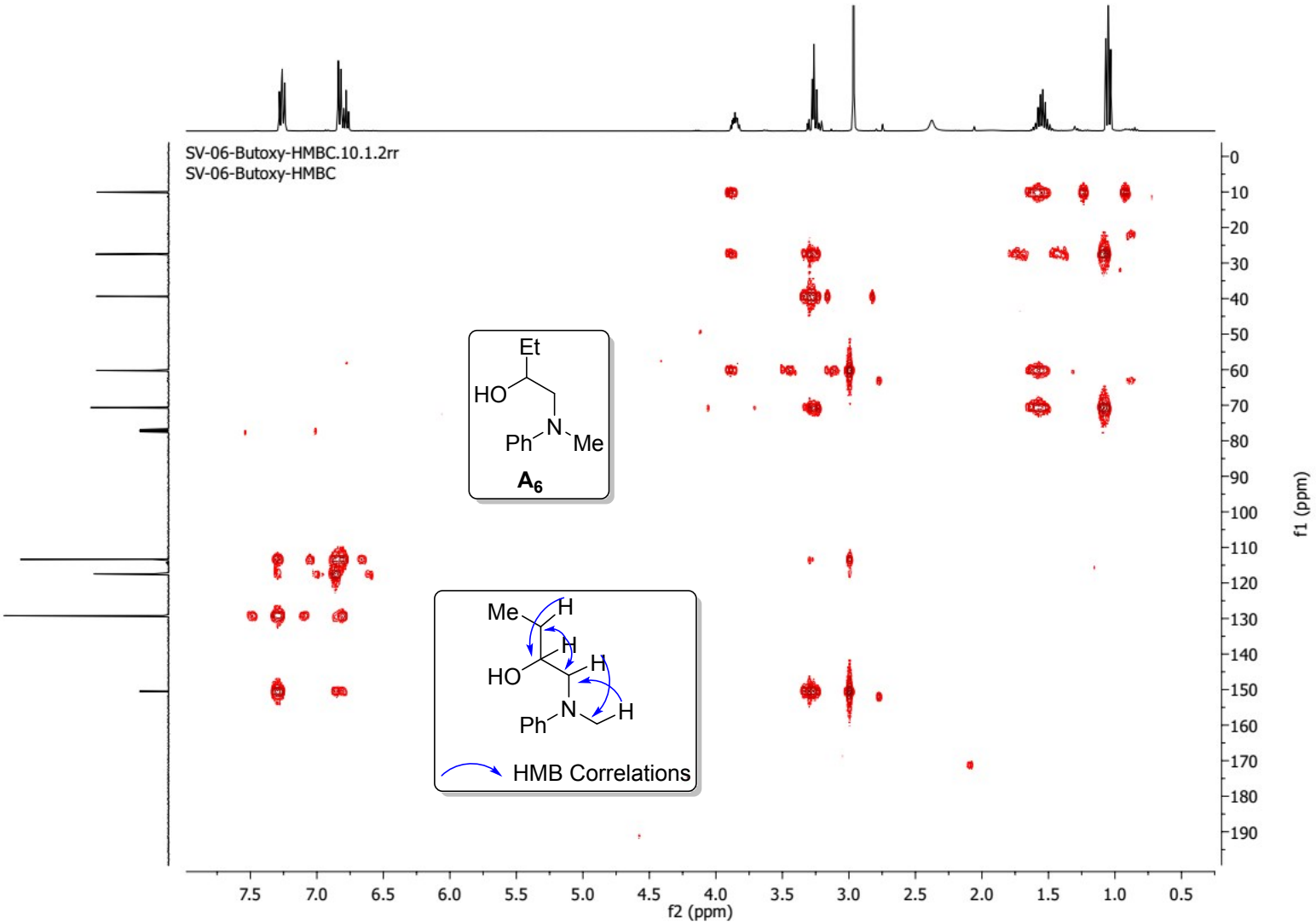

SV-06-4CN-RO-1H.10.fid
SV-06-4CN-RO-1H
7.613
7.592
7.296
7.276
7.260
7.255
6.911
6.891
6.870
6.852
6.836
5.097
5.079
5.061
4.178
4.150
4.144
4.129
4.113
4.099
2.731
Me
N
OH
CN
A5
f1 (ppm)
2.00
4.62
2.05
1.07
1.05
2.19
3.06


SV-06-4CN-RO-13C.10.fid
SV-06-4CN-RO-13C
150.65
143.67
132.60
129.65
128.17
119.20
118.78
115.03
111.76
77.55
77.23
76.91
64.63
61.79
32.75
Me
N
OH
A5
CN
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

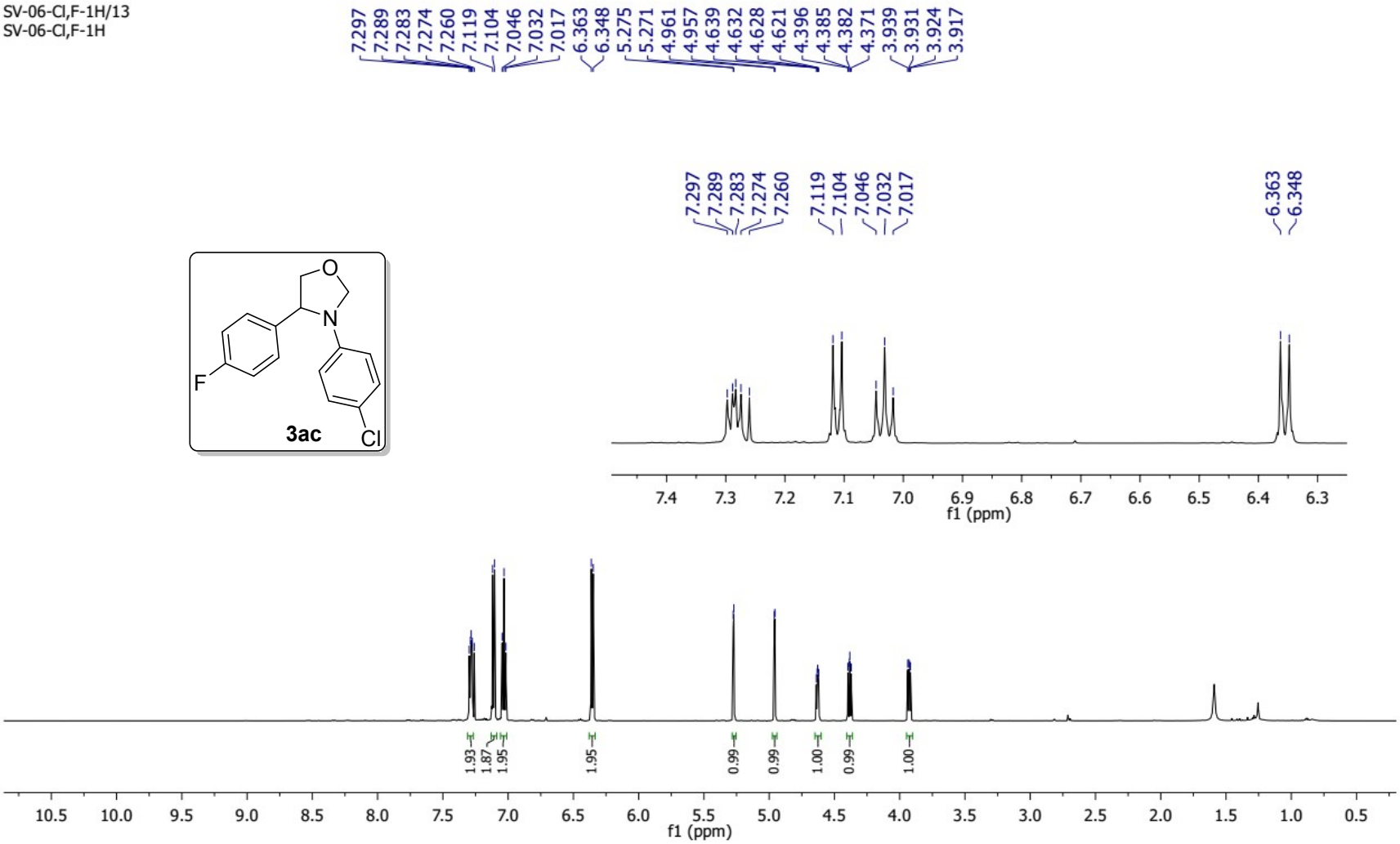

SV-06-BUTOXY-1H.10.fid
SV-06-BUTOXY-1H
7.278
7.260
7.256
7.238
6.835
6.815
6.794
6.776
6.758
3.884
3.872
3.862
3.852
3.843
3.833
3.821
3.307
3.296
3.271
3.259
3.238
3.222
3.201
2.961
2.373
1.608
1.592
1.574
1.561
1.556
1.538
1.520
1.503
1.485
1.467
1.065
1.046
1.027
Et
HO
N
Ph
Me
A6
f1 (ppm)
2.03
1.97
1.00
1.03
2.07
3.07
0.94
2.12
3.09

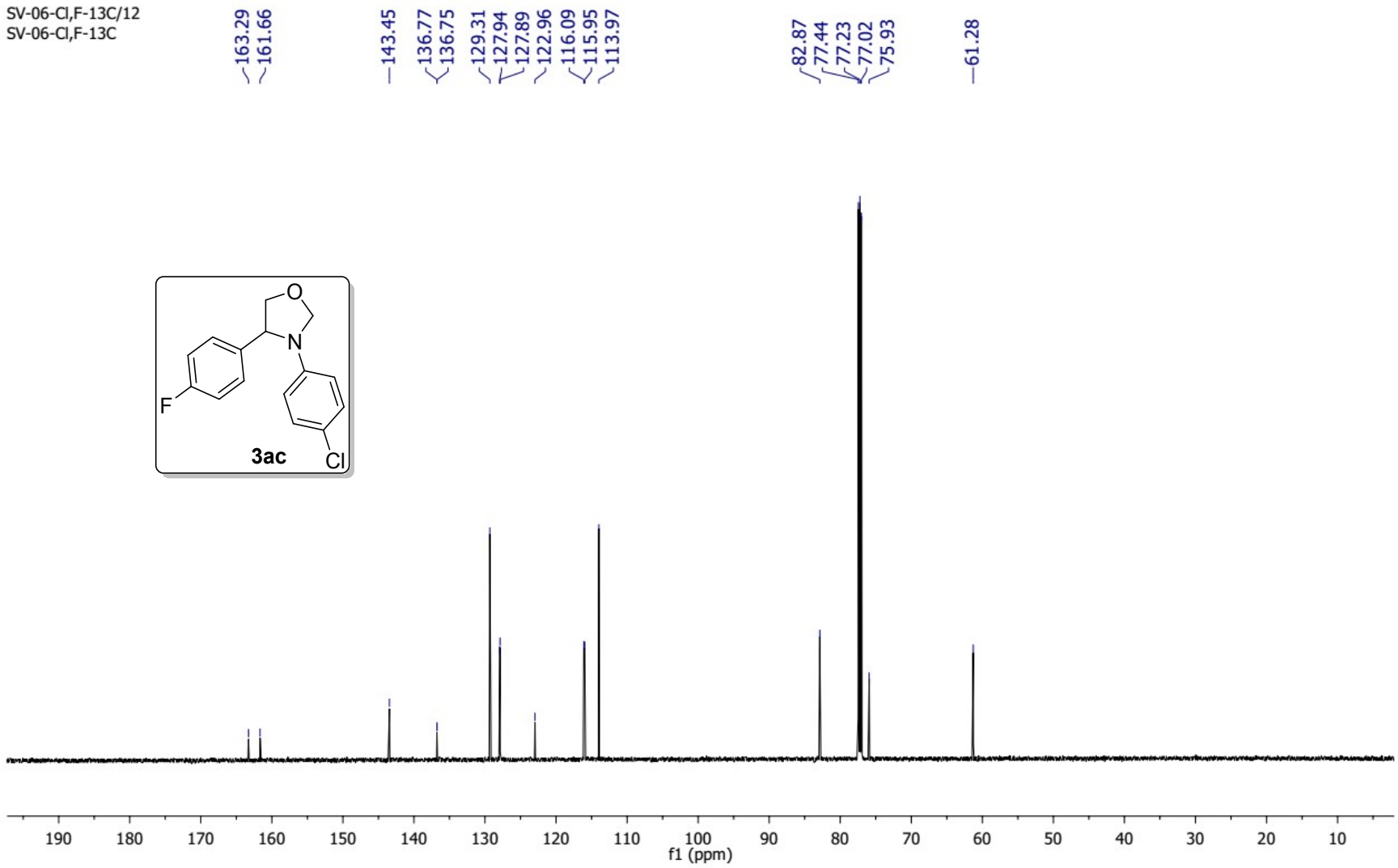

SV-06-Butoxy-13C.10.fid
SV-06-Butoxy-13C
150.56
129.28
117.52
113.45
77.55
77.23
76.91
70.76
60.29
39.45
27.61
10.14
Et
HO
N
Ph
Me
A6
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

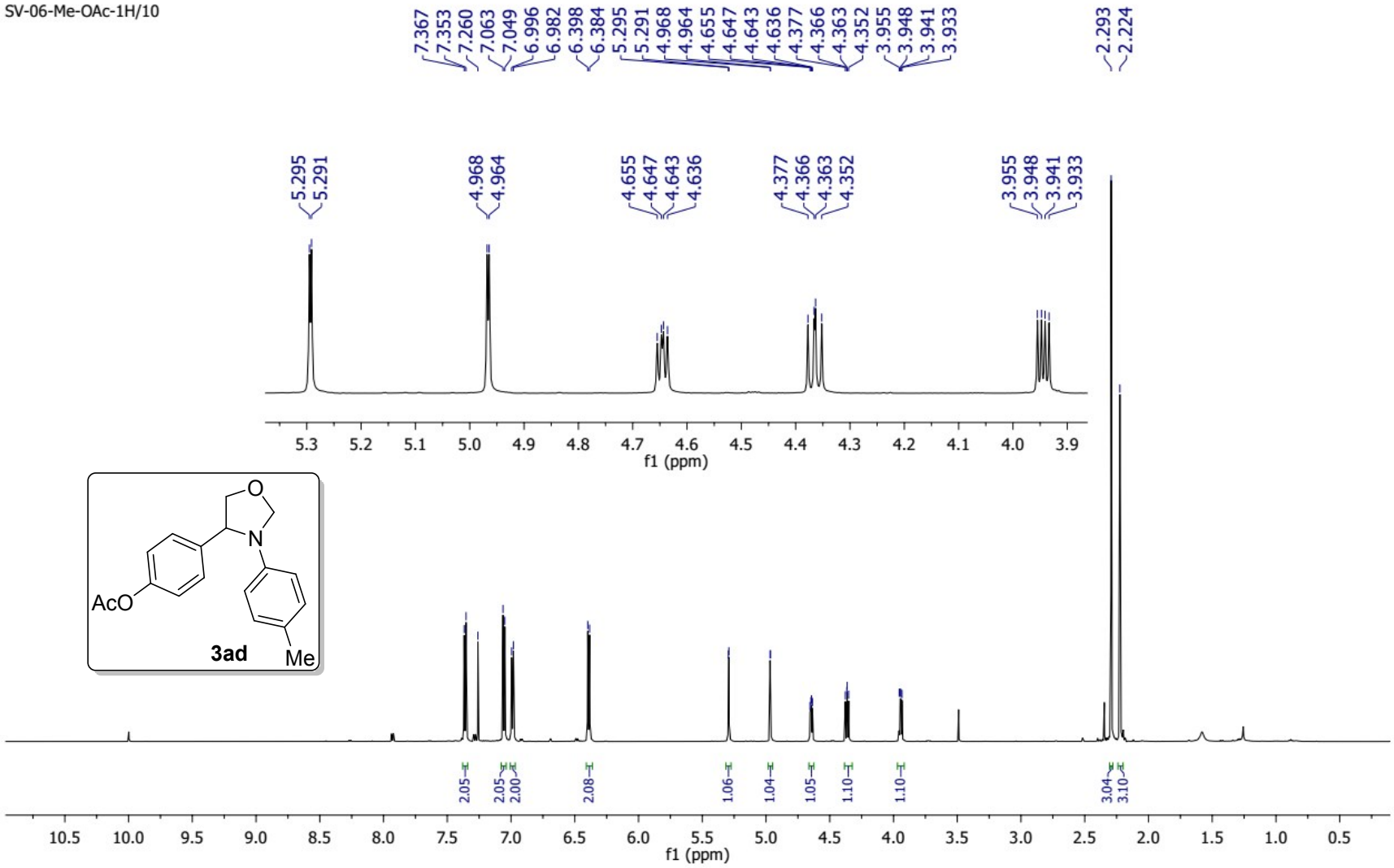

SV-06-Butoxy-DEPT135/10
SV-06-Butoxy-HMBC
129.20
117.43
113.36
70.67
60.21
39.36
27.52
10.06
Et
HO
N
Ph
Me
A6
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

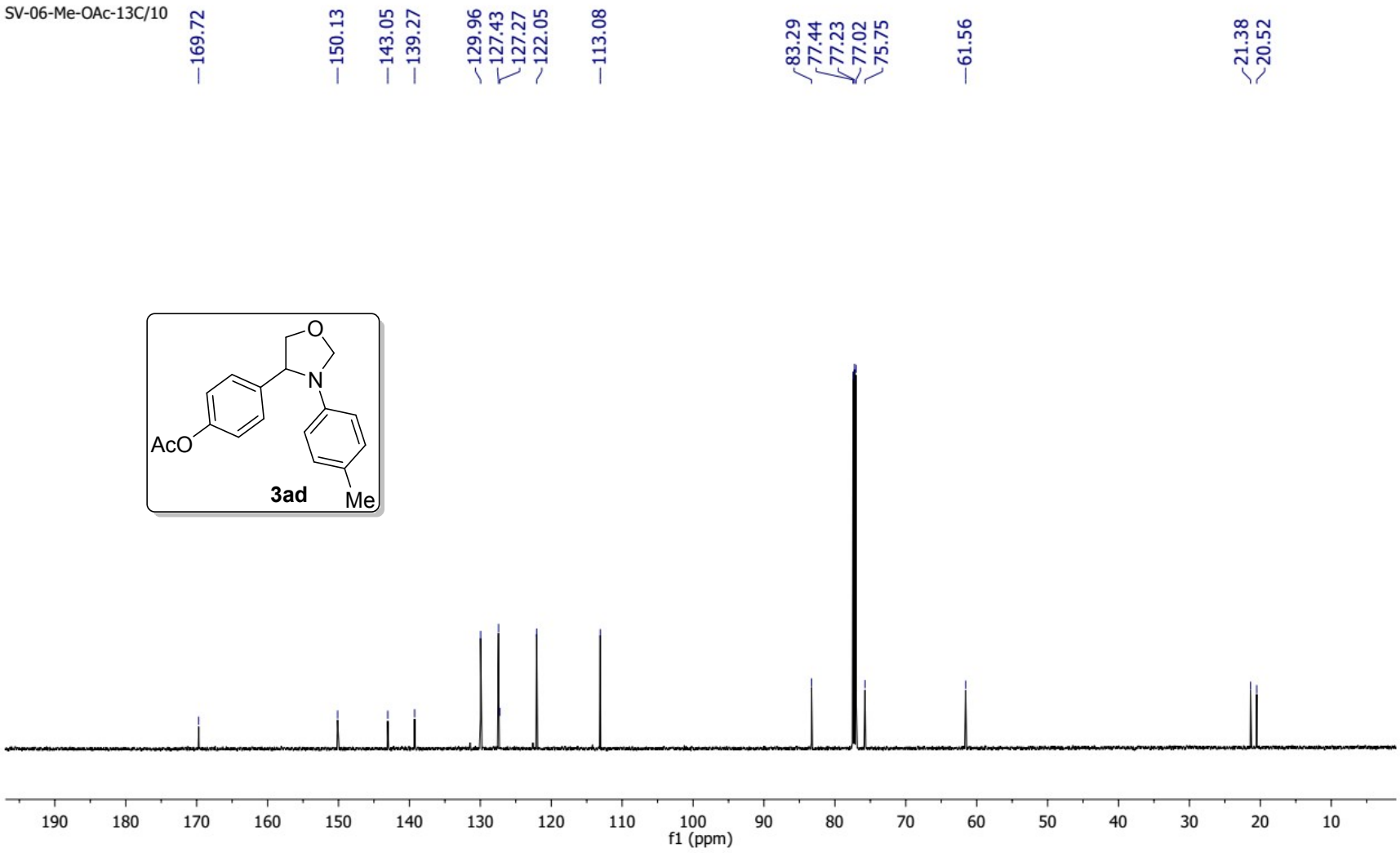

SV-06-Butoxy-HMBC.10.1.2rr
SV-06-Butoxy-HMBC
Et
HO
N
Ph
Me
A6
Me
H
H
HO
H
N
Ph
H
HMB Correlations
f2 (ppm)
f1 (ppm)

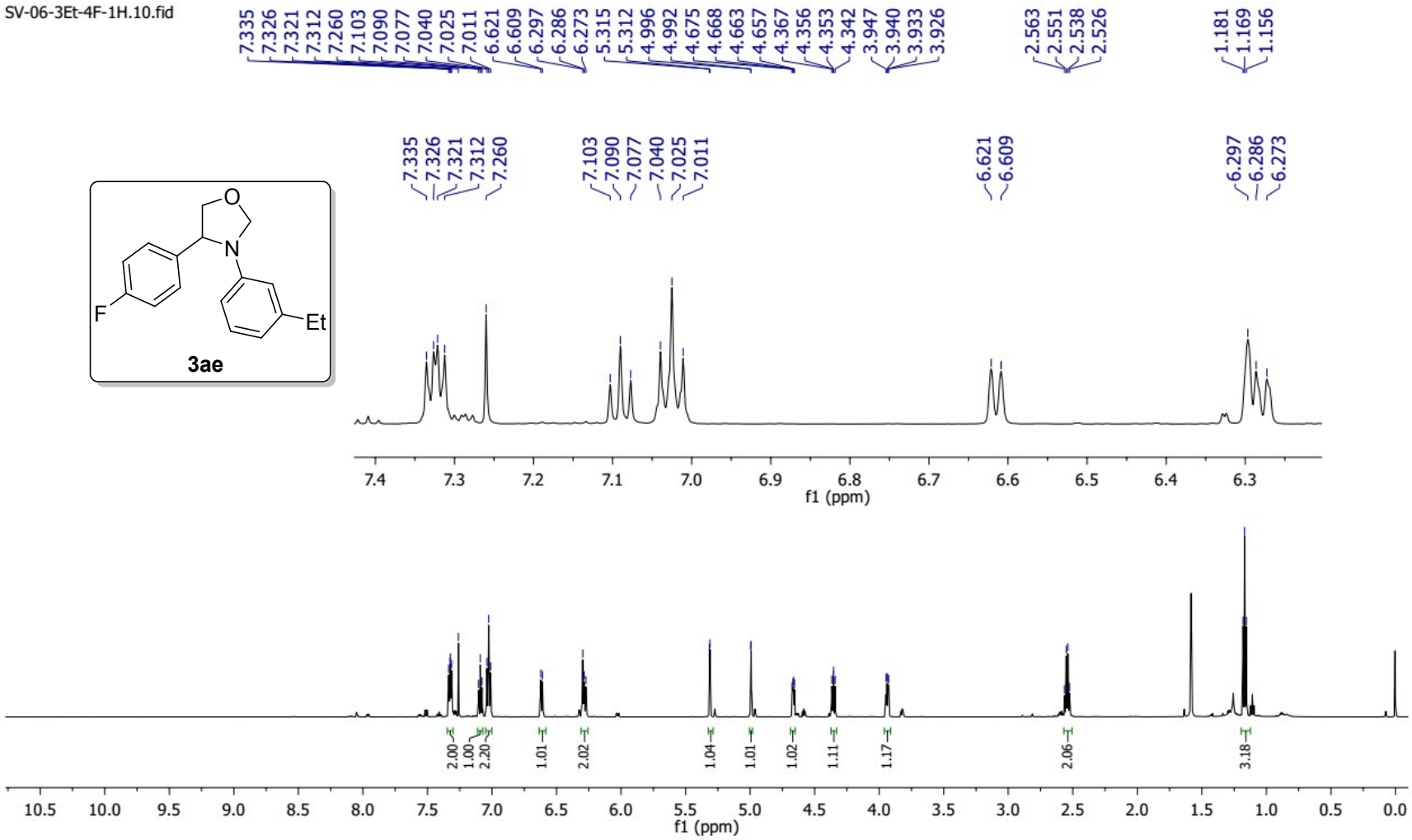
SV-06-Cl,F-1H/13
SV-06-Cl,F-1H

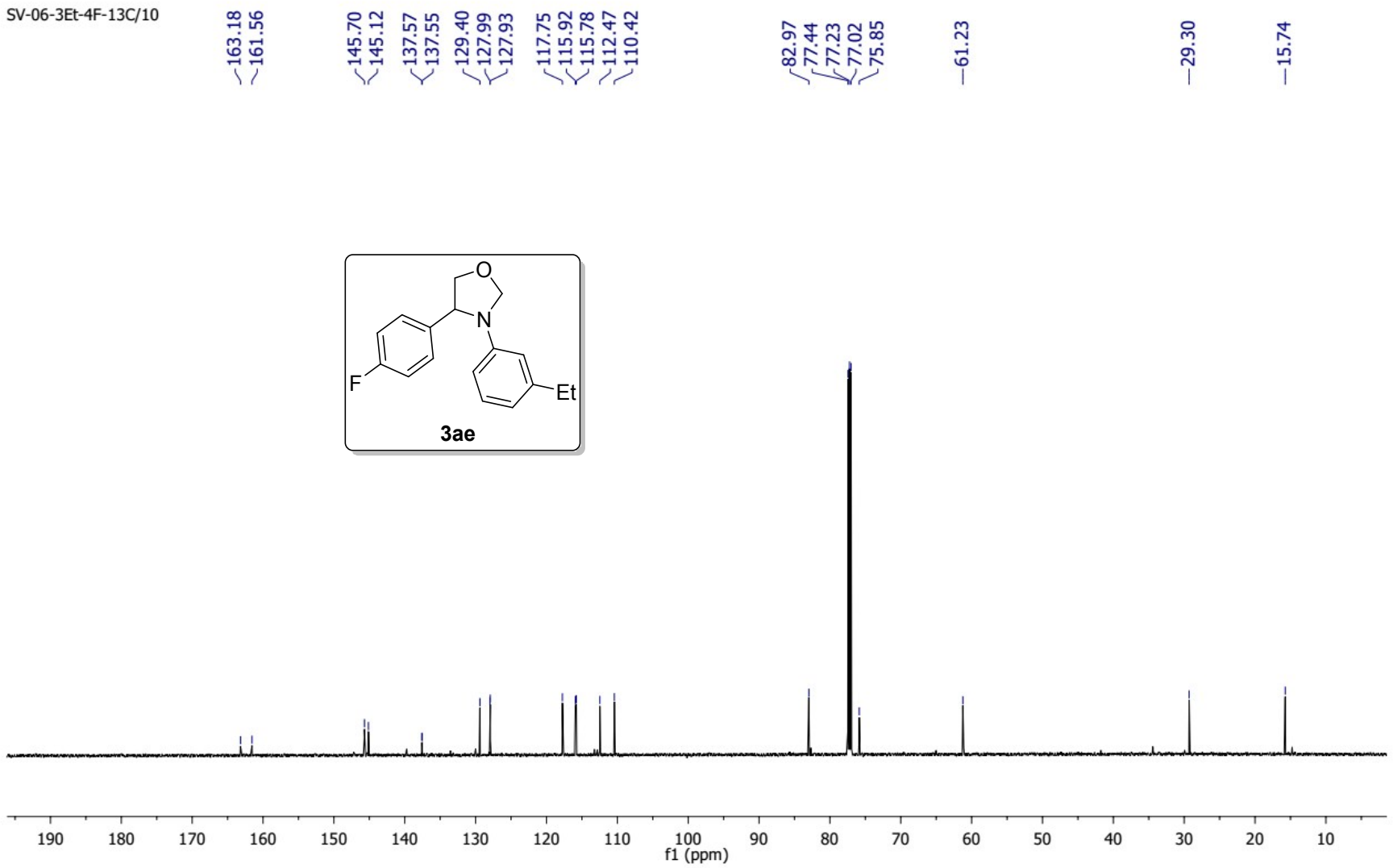



SV-06-Cl,F-13C/12
SV-06-Cl,F-13C
163.29
161.66
143.45
136.77
136.75
129.31
127.94
127.89
122.96
116.09
115.95
113.97
82.87
77.44
77.23
77.02
75.93
61.28
O
N
F
Cl
3ac
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


SV-06-Me-OAc-1H/10
7.367
7.353
7.260
7.063
7.049
6.996
6.982
6.398
6.384
5.295
5.291
4.968
4.964
4.655
4.647
4.643
4.636
4.377
4.366
4.363
4.352
3.955
3.948
3.941
3.933
2.293
2.224
f1 (ppm)
AcO
N
O
Me
3ad
2.05
2.05
2.00
2.08
1.06
1.04
1.05
1.10
1.10
3.04
3.10
f1 (ppm)

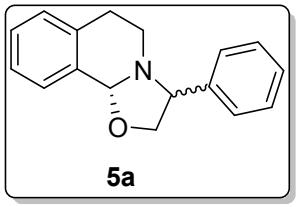

SV-06-Me-OAc-13C/10
169.72
150.13
143.05
139.27
129.96
127.43
127.27
122.05
113.08
83.29
77.44
77.23
77.02
75.75
61.56
21.38
20.52
O
N
AcO
3ad
Me
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


SV-06-3Et-4F-1H.10.fid
7.335
7.326
7.321
7.312
7.260
7.103
7.090
7.077
7.040
7.025
7.011
6.621
6.609
6.297
6.286
6.273
5.315
5.312
4.996
4.992
4.675
4.668
4.663
4.657
4.367
4.356
4.353
4.342
3.947
3.940
3.933
3.926
2.563
2.551
2.538
2.526
1.181
1.169
1.156
O
N
F
Et
3ae
f1 (ppm)
2.00
1.00
2.20
1.01
2.02
1.04
1.01
1.02
1.11
1.17
2.06
3.18

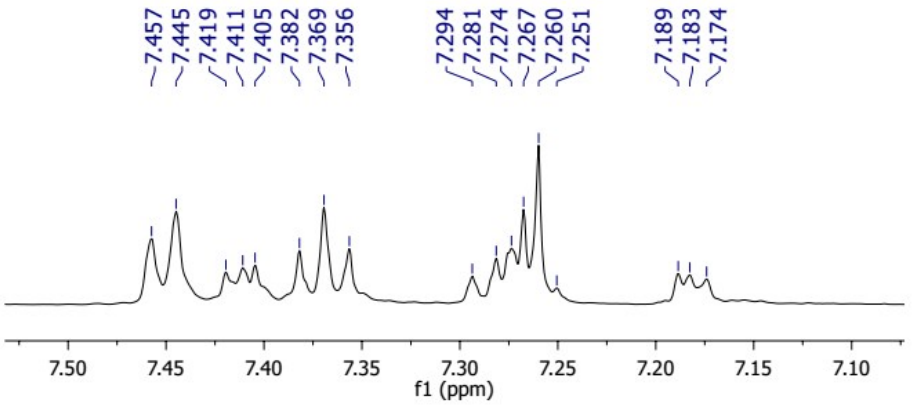

SV-06-3Et-4F-13C/10
163.18
161.56
145.70
145.12
137.57
137.55
129.40
127.99
127.93
117.75
115.92
115.78
112.47
110.42
82.97
77.44
77.23
77.02
75.85
61.23
29.30
15.74
O
N
F
Et
3ae
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

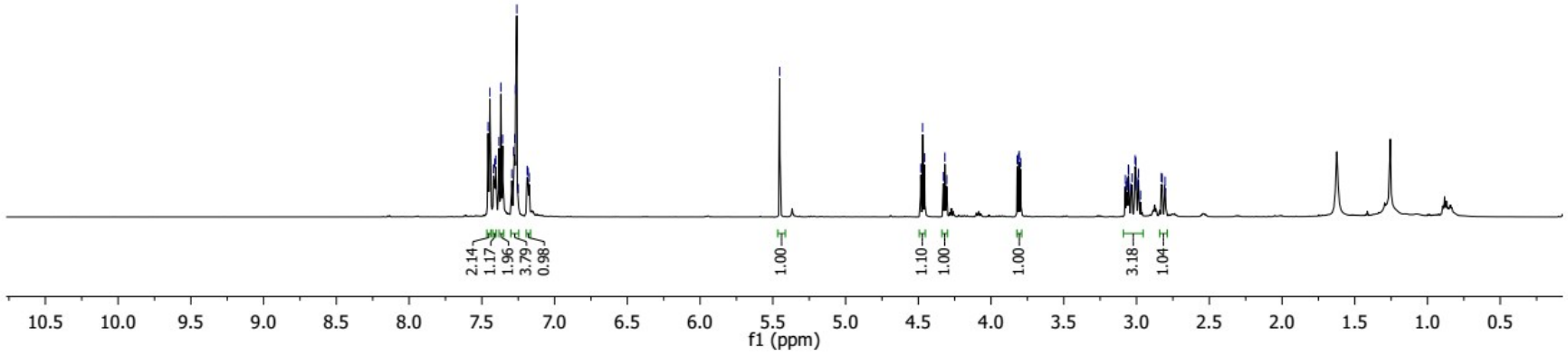
SV-06-THIQ-Ph-1H/11
SV-06-THIQ-Ph-1H

7.457 7.445 7.419 7.411 7.405 7.382 7.369 7.356 7.294 7.281 7.274 7.267 7.260 7.251 7.189 7.183 7.174 5.453 4.483 4.470 4.457 4.328 4.317 4.305 3.820 3.810 3.807 3.796 3.077 3.070 3.067 3.063 3.056 3.054 3.039 3.031 3.009 3.005 3.001 2.991 2.986 2.973 2.829 2.823 2.807 2.803

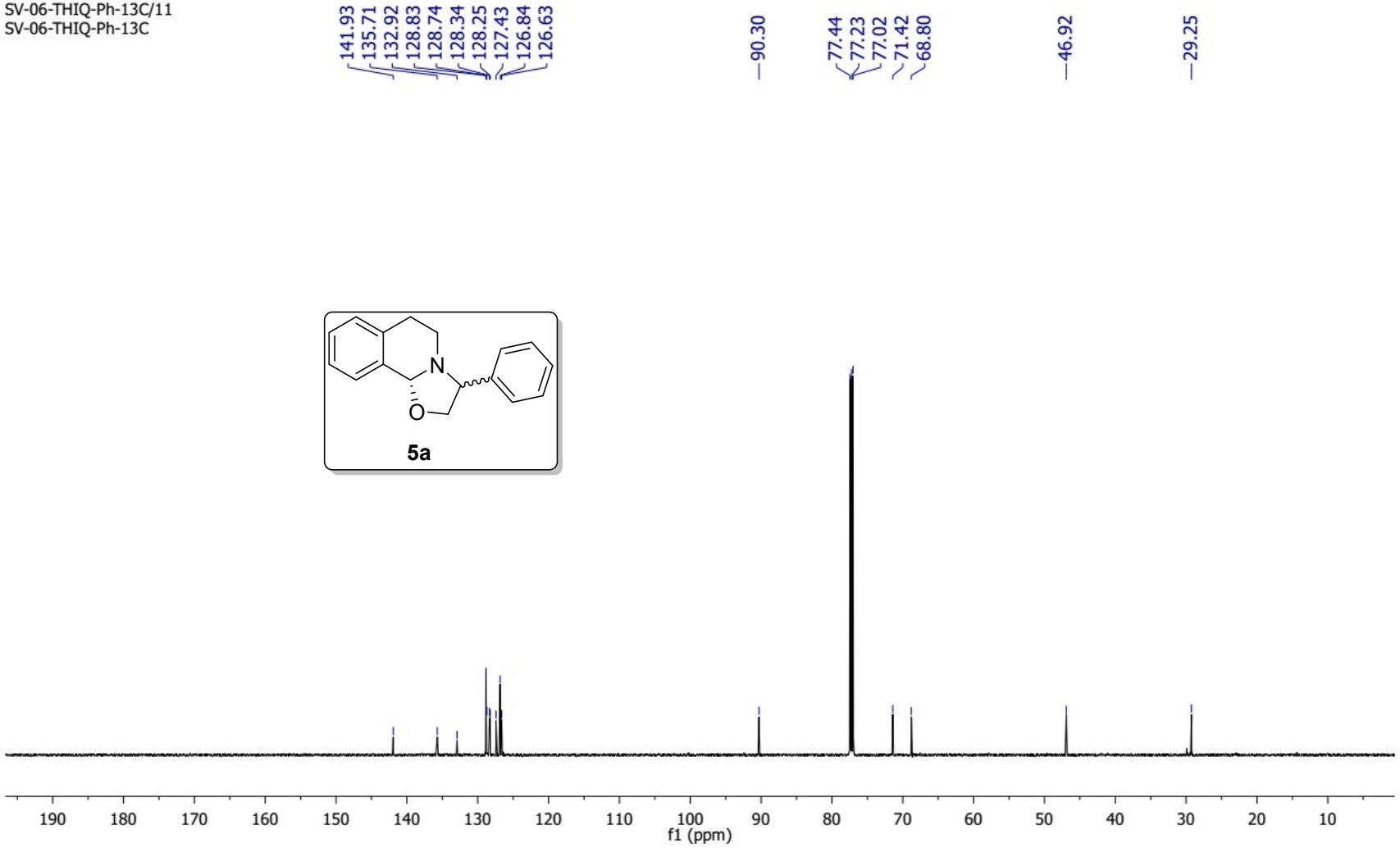


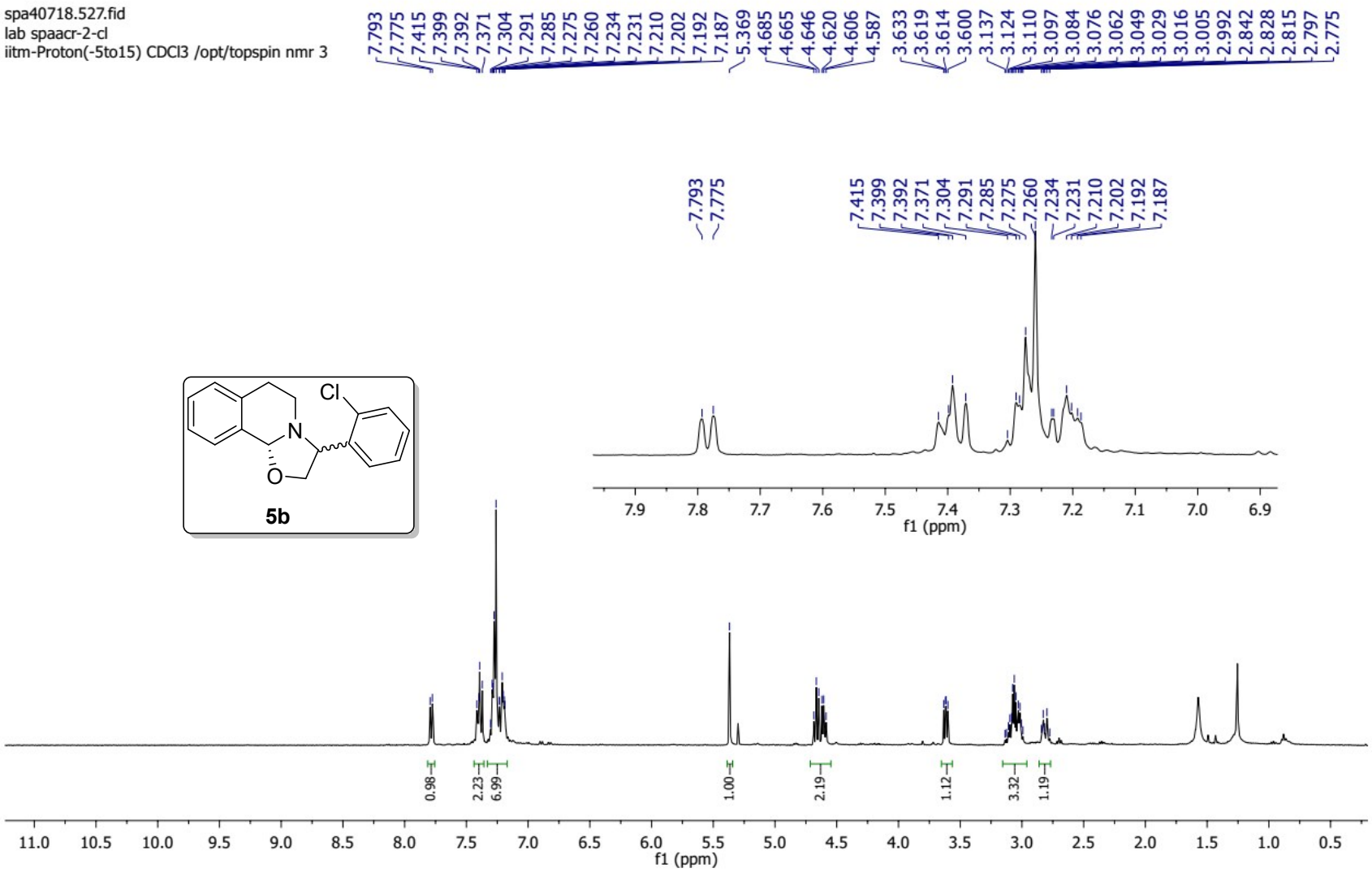
5a

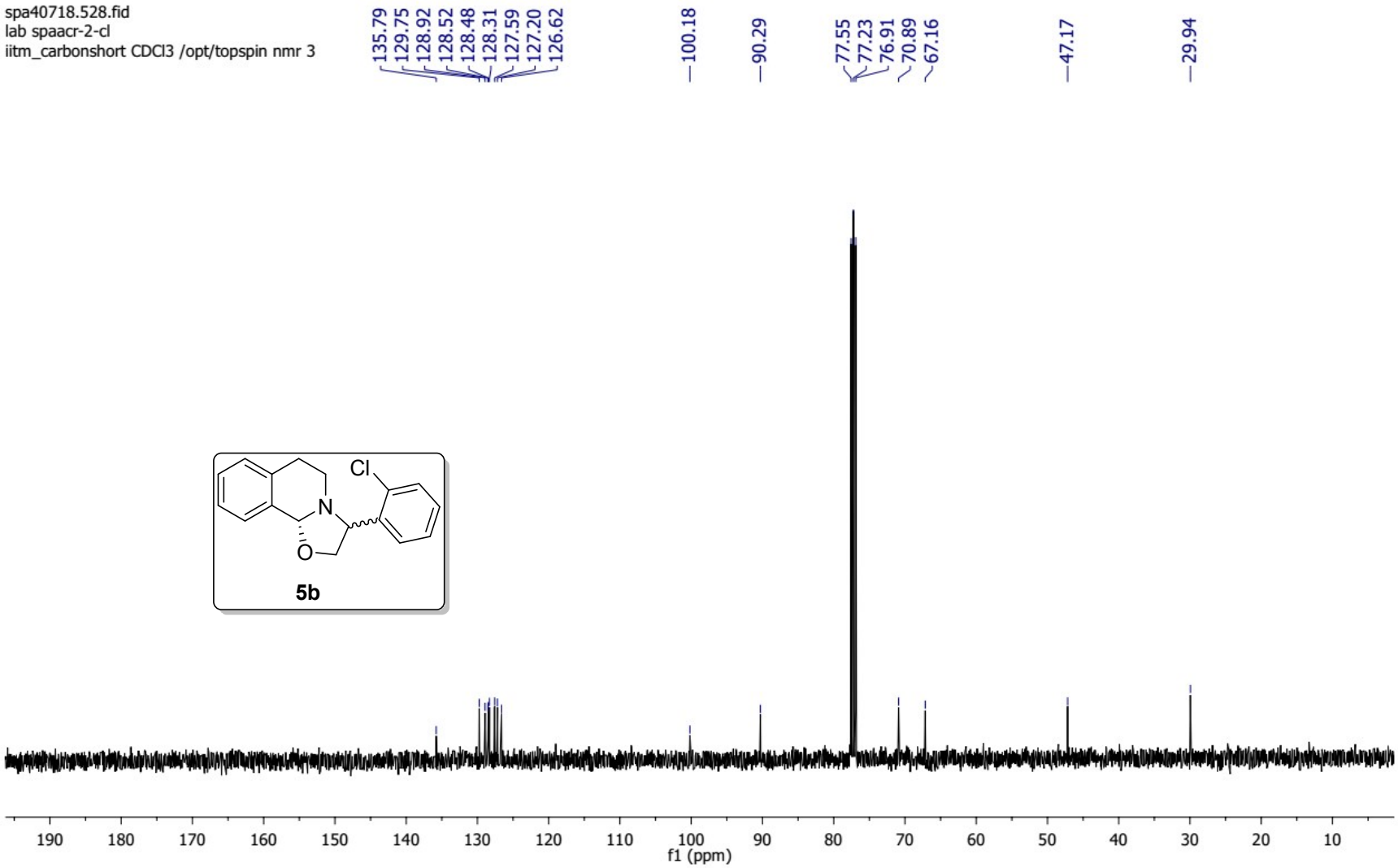


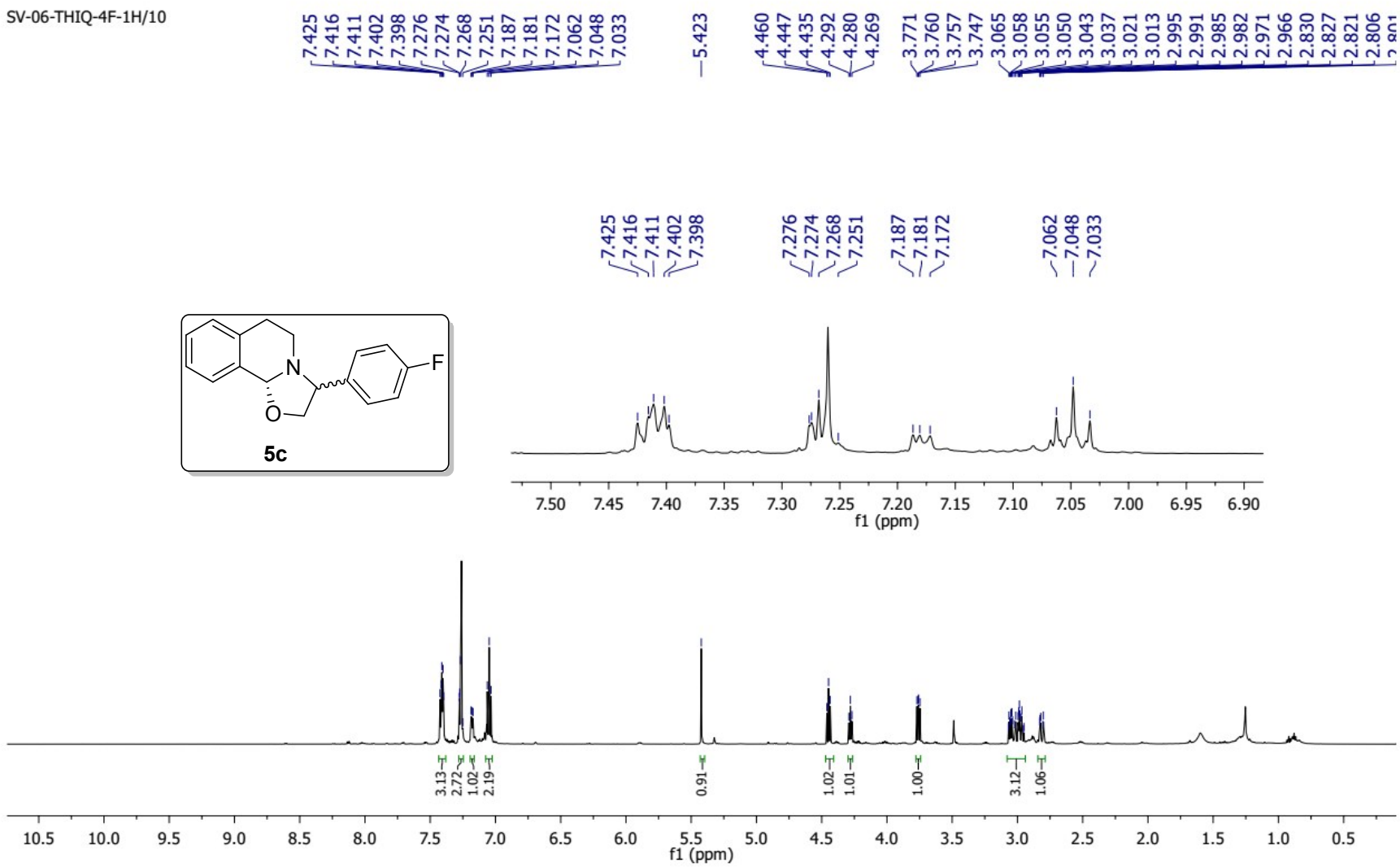


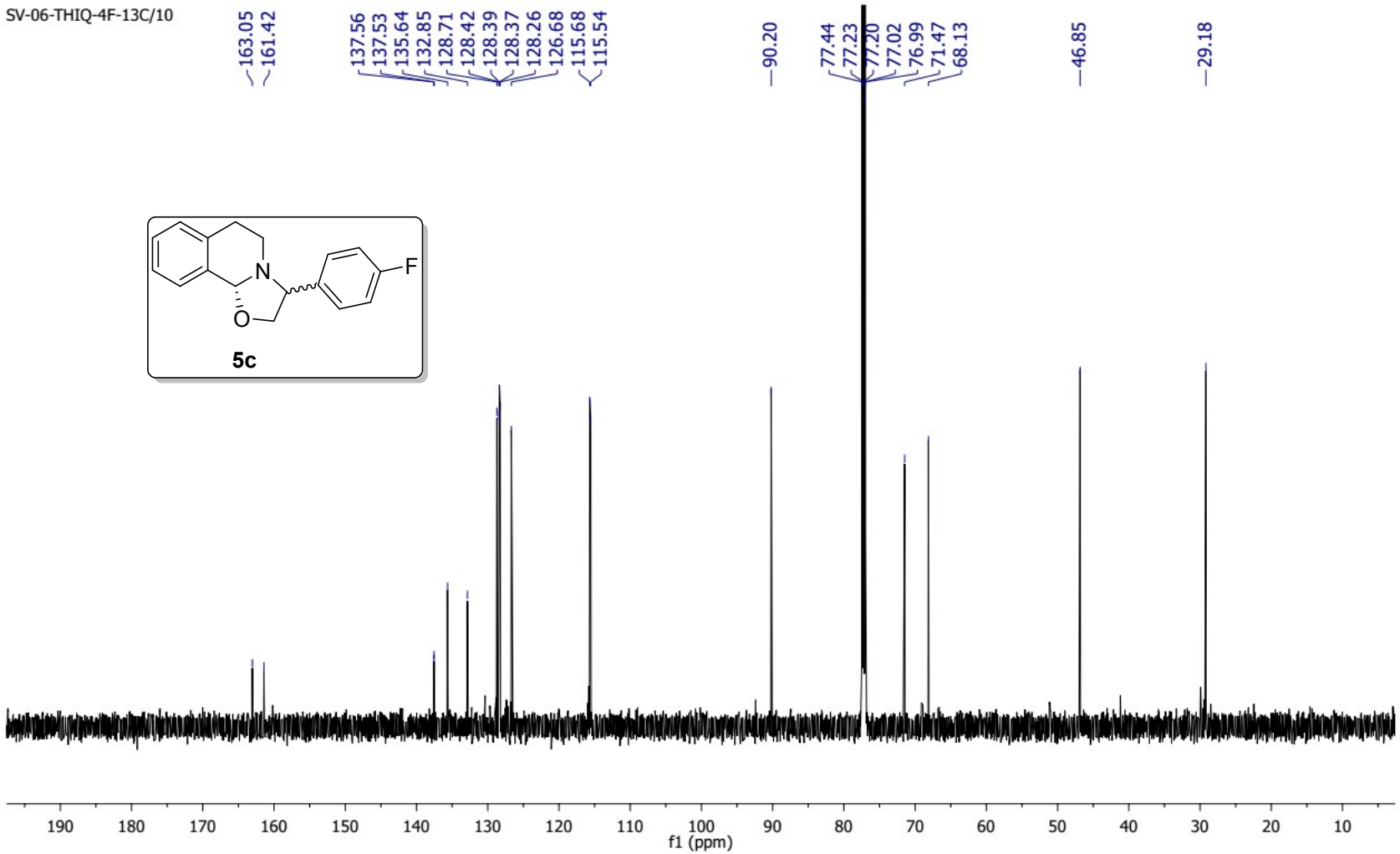
SV-06-THIQ-Ph-13C/11
SV-06-THIQ-Ph-13C

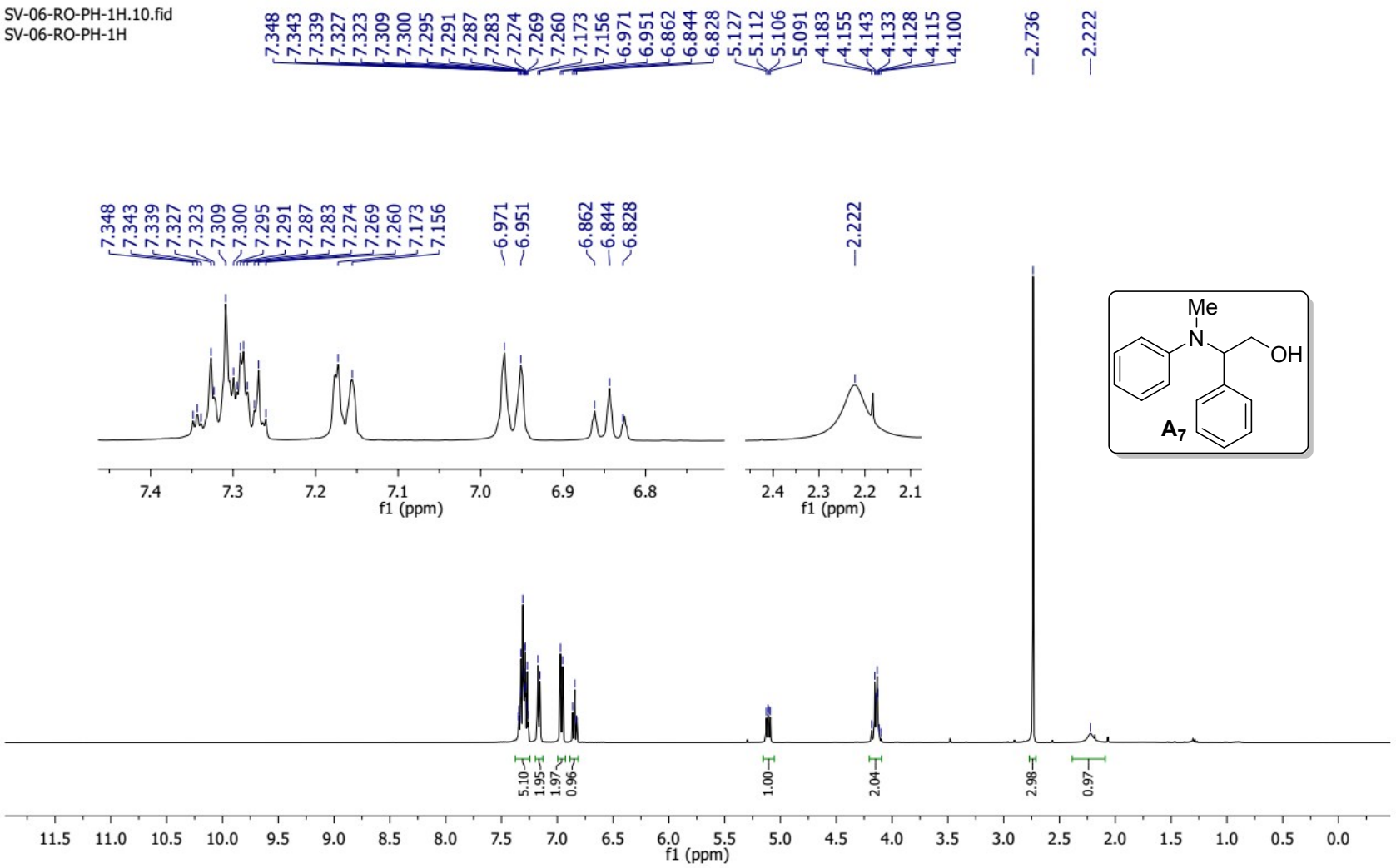


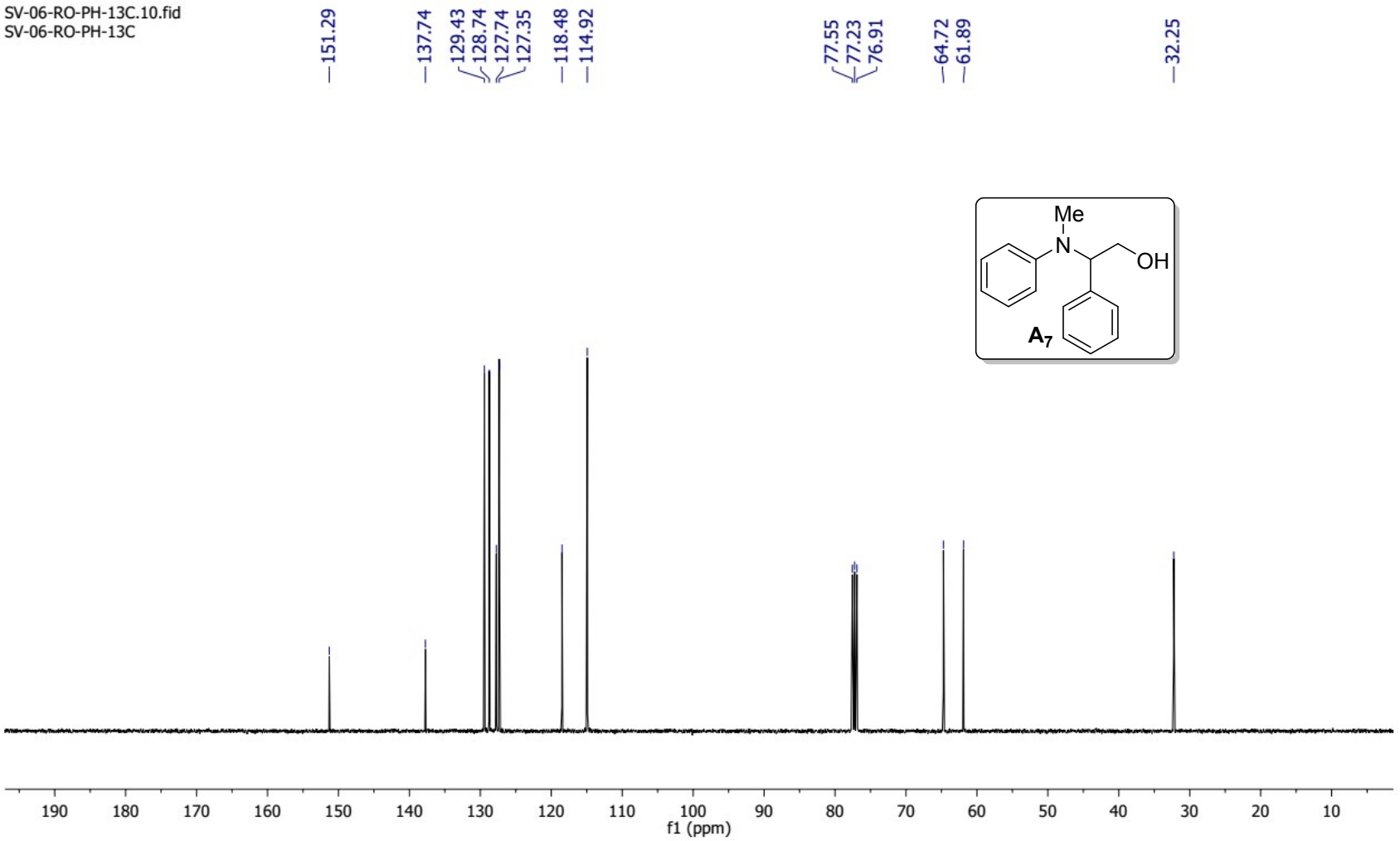

spa40718.527.fid
lab spaacr-2-cl
iitm-Proton(-5to15) CDCl3 /opt/topspin nmr 3
7.793
7.775
7.415
7.399
7.392
7.371
7.304
7.291
7.285
7.275
7.260
7.234
7.231
7.210
7.202
7.192
7.187
5.369
4.685
4.665
4.646
4.620
4.606
4.587
3.633
3.619
3.614
3.600
3.137
3.124
3.110
3.097
3.084
3.076
3.062
3.049
3.029
3.016
3.005
2.992
2.842
2.828
2.815
2.797
2.775
Cl
N
O
5b
f1 (ppm)
0.98
2.23
6.99
1.00
2.19
1.12
3.32
1.19

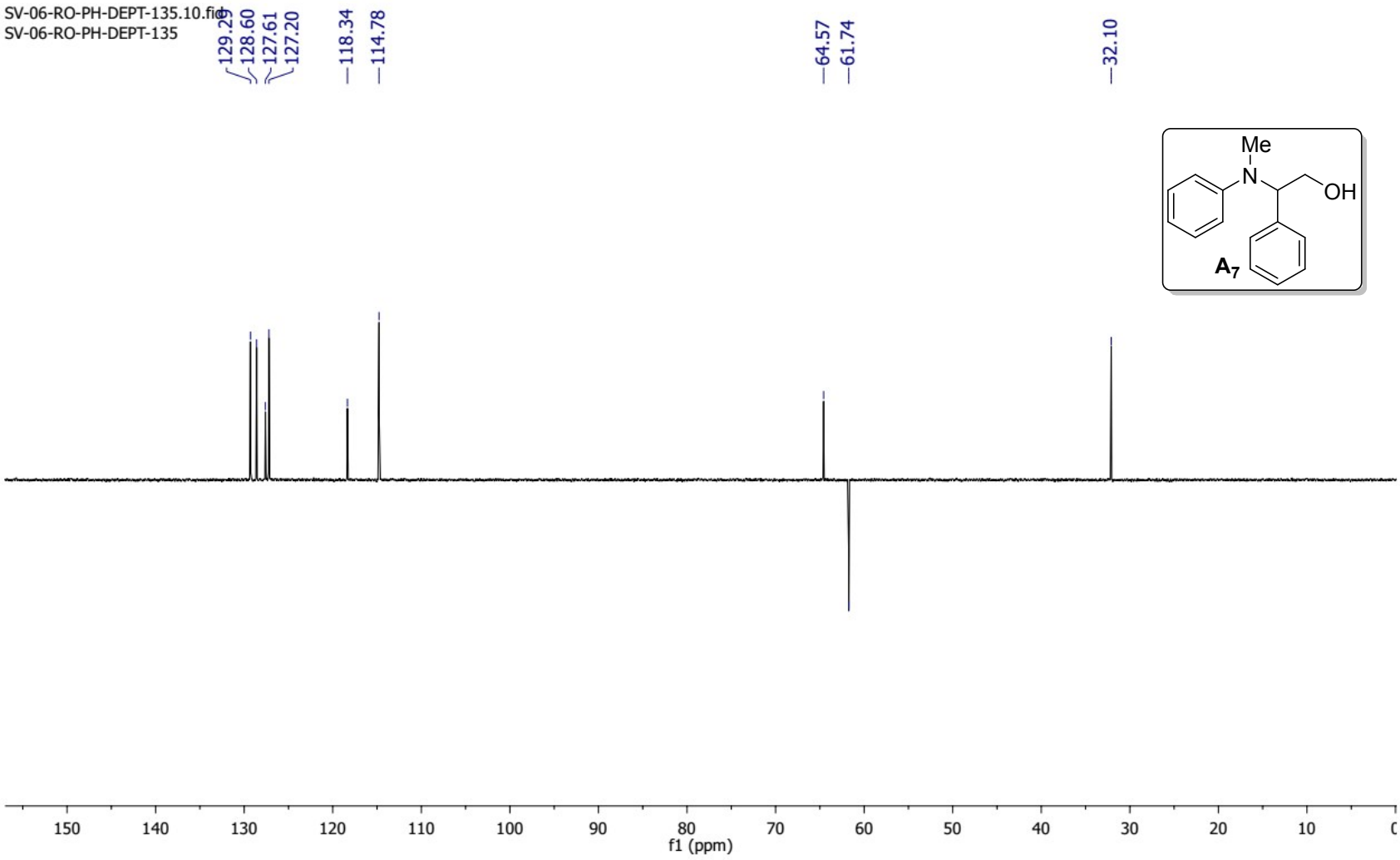

spa40718.528.fid
lab spaacr-2-cl
iitm_carbonshort CDCl3 /opt/topspin nmr 3
135.79
129.75
128.92
128.52
128.48
128.31
127.59
127.20
126.62
100.18
90.29
77.55
77.23
76.91
70.89
67.16
47.17
29.94
Cl
N
O
5b
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

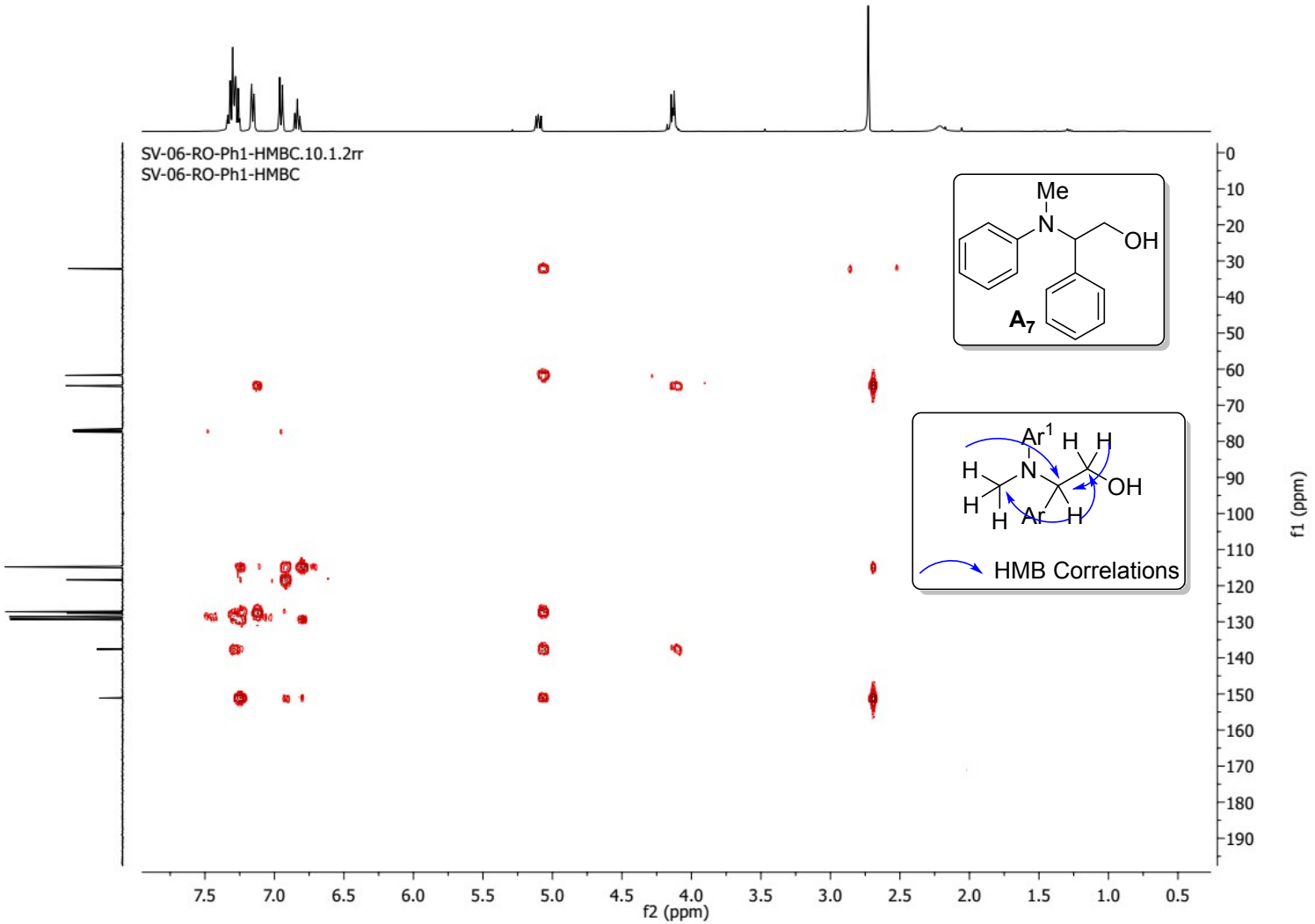

SV-06-THIQ-4F-1H/10
7.425
7.416
7.411
7.402
7.398
7.276
7.274
7.268
7.251
7.187
7.181
7.172
7.062
7.048
7.033
5.423
4.460
4.447
4.435
4.292
4.280
4.269
3.771
3.760
3.757
3.747
3.065
3.058
3.055
3.050
3.043
3.037
3.021
3.013
2.995
2.991
2.985
2.982
2.971
2.966
2.830
2.827
2.821
2.806
N
O
F
5c
7.50
7.45
7.40
7.35
7.30
7.25
7.20
7.15
7.10
7.05
7.00
6.95
6.90
f1 (ppm)
3.13
2.72
1.02
2.19
0.91
1.02
1.01
1.00
3.12
1.06
10.5
10.0
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
f1 (ppm)


SV-06-THIQ-4F-13C/10
163.05
161.42
137.56
137.53
135.64
132.85
128.71
128.42
128.39
128.37
128.26
126.68
115.68
115.54
90.20
77.44
77.23
77.20
77.02
76.99
71.47
68.13
46.85
29.18
N
O
F
5c
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


SV-06-RO-PH-1H.10.fid
SV-06-RO-PH-1H
7.348
7.343
7.339
7.327
7.323
7.309
7.300
7.295
7.291
7.287
7.283
7.274
7.269
7.260
7.173
7.156
6.971
6.951
6.862
6.844
6.828
5.127
5.112
5.106
5.091
4.183
4.155
4.143
4.133
4.128
4.115
4.100
2.736
2.222
Me
N
OH
A7
f1 (ppm)
5.10
1.95
1.97
0.96
1.00
2.04
2.98
0.97


SV-06-RO-PH-13C.10.fid
SV-06-RO-PH-13C
151.29
137.74
129.43
128.74
127.74
127.35
118.48
114.92
77.55
77.23
76.91
64.72
61.89
32.25
Me
N
OH
A7
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


SV-06-RO-PH-DEPT-135.10.fid
SV-06-RO-PH-DEPT-135
129.29
128.60
127.61
127.20
118.34
114.78
64.57
61.74
32.10
Me
N
OH
A7
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


SV-06-RO-Ph1-HMBC.10.1.2rr
SV-06-RO-Ph1-HMBC
Me
N
OH
A7
Ar1
H
H
H
N
OH
H
H
Ar
H
HMB Correlations
f2 (ppm)
f1 (ppm)