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Supporting Information for:

Palladium-Catalyzed Dearomative Cyclocarbonylation of Allyl Alcohol for the Synthesis of Quinolizinones

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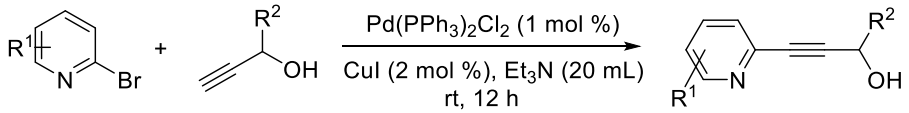
Contents

1. General experiment details and materials

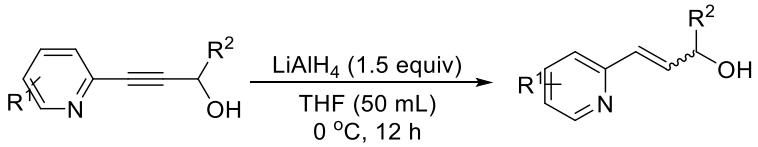
All non-aqueous reactions and manipulations were used by standard Schlenk techniques. All solvents before used were dried by standard methods and stored under argon atmosphere. All reactions were monitored by TLC with silica gel-coated plates. NMR spectra were recorded on BRUKER Avance III (400 MHz) spectrometers. Chemical shifts were reported in parts per million (ppm) down field from tetramethylsilane (TMS) with the solvent resonance as the internal standard. Coupling constants (J) were reported in Hz and referred to apparent peak multiplications. High resolution mass spectra (HRMS) were recorded on Bruker MicroTOF-QII mass instrument (ESI). GC-MS analysis were performed with Agilent 7890B/5975B GC-MS system. All chemicals were purchased from commercial sources.

2. Preparation of starting materials

2.1. Method A:

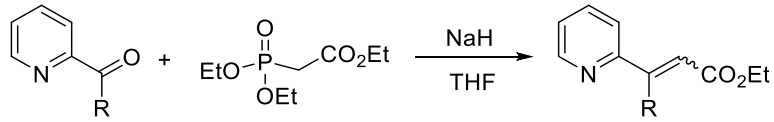


2-Bromopyridine (10 mmol, 1 equiv), prop-2-yn-1-ol (12 mmol, 1.2 equiv), $Pd(PPh)_2Cl_2$ (0.1 mmol, 1 mol %), CuI (0.2 mmol, 2 mol %), and Et_3N (50 mmol) were added to a 100 mL Schlenk flask under nitrogen atmosphere. The reaction mixture was stirred at room temperature for 12 hours and monitored by TLC. Then the reaction mixture was concentrated under reduced pressure. The crude product was purified by flash chromatography employing mixtures of petroleum ether/ EtOAc as eluents.

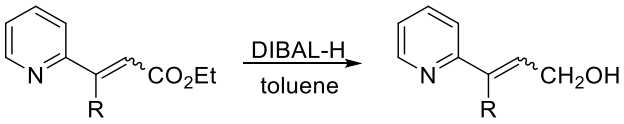


The above residue and anhydrous THF (50 mL) were added to 100 mL flask under nitrogen atmosphere. Then $LiAlH_4$ was carefully added in a few portions at 0 ^oC. The reaction mixture was gradually warmed to room temperature and stirred overnight. The reaction mixture was then cooled to 0 ^oC and quenched with EtOAc, followed by water. The solid aluminum salts was filtered, then the organic layer was separated and the aqueous layer was extracted with EtOAc (20 mL×3). The combined organic layer was dried over Na_2SO_4, filtered, and concentrated under reduced pressure. The crude residue was purified by flash column chromatography on silica gel and eluted with EtOAc/petroleum ether (1/3~1/1) afford the corresponding allylic alcohols **1a** (0. 86 g, 67% yield).

2.2. Method B:

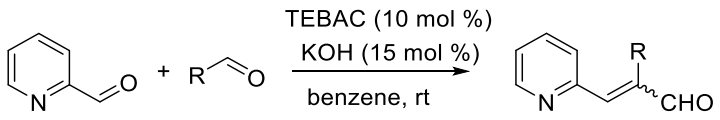


To a 100 mL round bottom flask containing NaH (20 mmol, 60% mineraldispersion) and anhydrous THF (40 mL) at 0 ^{o}C, triethyl phosphonoacetate (21.5 mmol) was dropwise added. The reaction mixture was naturally warmed to room temperature, followed by a dropwise addition of a 2-acetylpyridine solution (13 mmol, in 20 mL anhydrous THF). The reaction mixture was stirred for 12 hours, and then poured into aseparating funnel containing water. The organic layer was collected, and the aqueouslayer was extracted with diethyl ether (3×50 mL). The combined organic layer wasdried over Na_2SO_4, filtered, and concentrated under reduced pressure. The crude residue was subjected to flash chromatography (EtOAc/petroleum ether = 1/80~1/20) to afford the corresponding *α,β*-unsaturated ester (1.74 g, 70% yield)

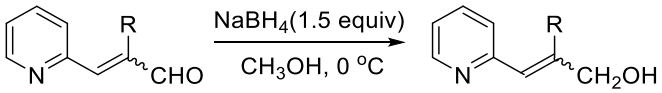


To a flame-dried 100 mL flask containing the unsaturated ester (20 mmol) obtained above and anhydrous toluene (30 mL), DIBAL-H (40 mmol) was carefully dropwise added at -78 ^{o}C. The reaction mixture was gradually warmed to room temperature and stirred overnight. The reaction mixture was then cooled to 0 ^{o}C and quenched with saturated aqueous NH_4Cl. The solid aluminum salts was filtered, then the organic layer was separated and the aqueous layer was extracted with EtOAc (50 mL×3). The combined organic layer was dried over Na_2SO_4, filtered, and concentrated under reduced pressure. The crude residue was subjected to flash chromatography (EtOAc/petroleum ether = 1/3~1/1) to afford the corresponding allylic alcohol (1.4 g, 47% yield).

2.3. Method C:

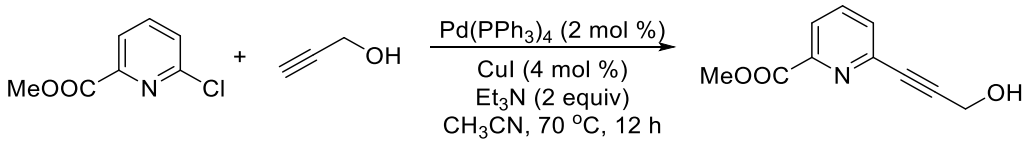


The solution of picolinaldehyde (18 mmol) in benzene (10 mL) and the solution of propionaldehyde (21.6 mmol) in benzene (10 mL) were added successively to vigorously stirred suspension of powdery KOH (2.7 mmol) and TEBAC (1.8 mmol) in benzene (10 mL) at room temperature. The reaction mixture was vigorously stirred at the same temperature until the condensation was finished (TLC monitoring). The organic solution was decanted from the wet TEBAC/KOH solid phase, and the residue was extracted with benzene (3×10 mL). The combined benzene extract was washed with water (2×10 mL) and dried over anhydrous Na_2SO_4. The solvent was evaporated under reduced pressure, and the residue was used in the next step without further purification.

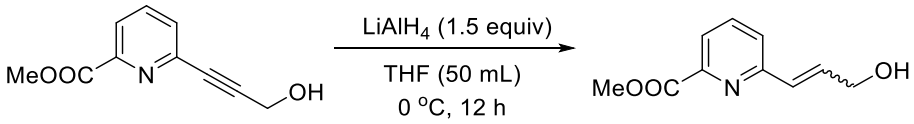


The residue of step **1** and CH_3OH (20 mL) were added to 100 mL flask. Then $NaBH_4$ was carefully added in a few portions at 0°C. The reaction mixture was stirred until the reaction was finished (TLC monitoring). The reaction mixture was quenched with NH_4Cl and concentrated under reduced pressure. After removing most of the solvent, the residue was extracted with EtOAc (20 mL×3). The EtOAc extractwas dried over anhydrous Na_2SO_4. The solvent was removed under reduced pressureand the residue was purified by flash column chromatography on silica gel and eluted with EtOAc/petroleum ether (1/3~1/1) to afford 2-methyl-3-(pyridin-2-yl)prop-2-en-1-ol (21 g, 78% yield).

2.4. Method D:

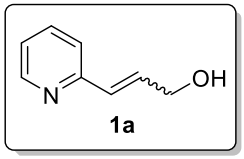


Ethyl 2-chloronicotinate (3.42 g, 20 mmol), prop-2-yn-1-ol (26 mmol, 1.3 equiv), $Pd(PPh_3)_4$ (0.6 mmol, 2 mol %), CuI (2.7 mmol, 4 mol %), Et_3N (60 mmol) and CH_3CN (50 mL) were added to a 250 mL Schlenk flask under nitrogen atmosphere. The reaction mixture was stirred at 70 ^oC for 12 hours and monitored by TLC. Then the reaction mixture was concentrated under reduced pressure, The ethyl 2-(3-hydroxyprop-1-yn-1-yl)nicotinate, thus obtained, was used in the next step without further purification.

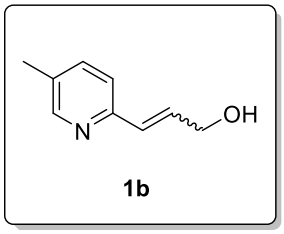


The above residue and anhydrous THF (50 mL) were added to 100 mL flask under nitrogen atmosphere. Then $LiAlH_4$ was carefully added in a few portions at 0 ^oC. The reaction mixture was gradually warmed to room temperature and stirred overnight. The reaction mixture was then cooled to 0 ^oC and quenched with EtOAc, followed by water. The solid aluminum salts was filtered, then the organic layer was separated and the aqueous layer was extracted with EtOAc (20 mL×3). The combined organic layer was dried over Na_2SO_4, filtered, and concentrated under reduced pressure. The crude residue was purified by flash column chromatography on silica gel andeluted with EtOAc/petroleum ether (1/3~1/1) afford 3-(3-(hydroxymethyl)pyridin-2-yl)prop-2-en-1-ol (1. 97 g, 51% yield).

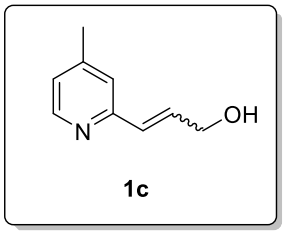
3. Experimental characterization data for starting materials



3-(Pyridin-2-yl)prop-2-en-1-ol (1a): The title compound was prepared according to the general procedure (method **A**) and purified by flash column chromatography to give the corresponding product as a yellow oil (56% yield, *E/Z* = 70:30). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 2.94 (br, 1H), 4.39 (dd, J_1 = 1.6 Hz, J_2 = 4.8 Hz, 2H), 6.73(t, *J* = 1.5 Hz, 0.3H), 6.77 (t, *J* = 1.5 Hz, 0.7H), 6.82 (t, *J* = 4.8 Hz, 0.7H), 6.86 (t, *J* = 4.8 Hz, 0.3H), 7.12-7.15 (m, 1H), 7.27-7.31 (m, 1H), 7.61-7.65 (m, 1H), 8.53-8.54 (m, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 63.1, 121.7, 122.3, 129.7, 134.1, 136.8, 149.5, 155.4; **HRMS (ESI)** calcd. for $C_8H_{10}NO$ [M+H]: 136.0757, found: 136.0766.

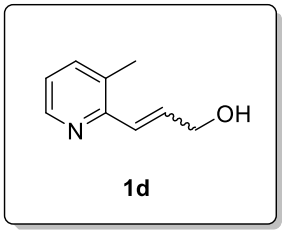


3-(5-Methylpyridin-2-yl)prop-2-en-1-ol (1b): The title compound was prepared according to the general procedure (method **A**) and purified by flash column chromatography to give the corresponding product as a yellow oil (66% yield, *E/Z* = 76:24). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 2.32 (s, 3H), 2.34 (br, 1H), 4.38 (d, *J* = 4.2 Hz, 2H), 6.68 (t, *J* = 1.2 Hz, 0.2H), 6.72 (t, *J* = 1.2 Hz, 0.8H), 6.76 (t, *J* = 4.8 Hz, 0.7H), 6.80 (t, *J* = 4.8 Hz, 0.3H), 7.21(d, *J* = 8.0 Hz, 1H), 7.43 (dd, J_1 = 1.6 Hz, J_2 = 8.0 Hz, 1H), 8.37 (d, *J* = 2.4 Hz, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 18.4, 63.3, 121.2, 130.0, 131.9, 132.7, 137.2, 150.0, 152.7; **HRMS (ESI)** calcd. for $C_9H_{12}NO$ [M+H]: 150.0913, found: 150.0917.

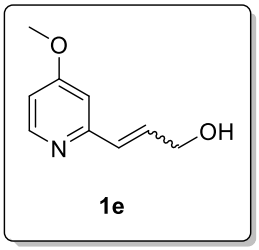


3-(4-Methylpyridin-2-yl)prop-2-en-1-ol (1c): The title compound was prepared according to the general procedure (method **A**) and purified by flash column chromatography to give the corresponding product as a yellow oil (65% yield, *E/Z* = 69:31). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 2.33 (s, 3H), 2.96 (br, 1H), 4.36(dd, J_1 = 1.6 Hz, J_2 = 4.8 Hz, 2H), 6.68 (t, *J* = 1.5 Hz, 0.3H), 6.72 (t, *J* = 1.2 Hz, 0.7H), 6.78 (t, *J* = 4.8 Hz, 0.7H), 6.82 (t, *J* = 4.8 Hz, 0.3H), 6.94-9.96 (m, 1H), 7.11 (t, *J* = 1.0 Hz, 1H), 8.36 (d, *J* = 4.8 Hz, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 21.1, 62.9, 122.6, 123.3, 129.6, 134.1, 147.9, 149.1, 155.2; **HRMS (ESI)** calcd. for

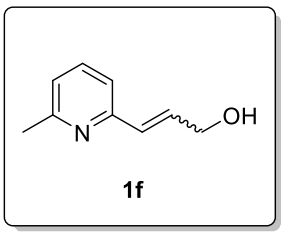
$C_9H_{12}NO$ [M+H]: 150.0913, found: 150.0968.



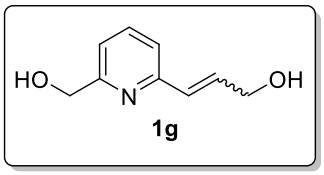
3-(3-Methylpyridin-2-yl)prop-2-en-1-ol (1d): The title compound was prepared according to the general procedure (method **A**) and purified by flash column chromatography to give the corresponding product as a yellow oil (57% yield, *E/Z* = 94:6). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 2.28 (s, 3H), 4.35 (d, *J* = 3.1 Hz, 3H), 6.69 (s, 0.1H), 6.73 (s, 0.9H), 6.73 (d, *J* = 3.6 Hz, 0.9H), 6.77 (d, *J* = 3.6 Hz, 0.1H), 7.19 (d, *J* = 8.0 Hz,1H), 7.40-7.43 (m, 1H), 8.32 (d, *J* = 2.0 Hz, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 18.2, 62.7, 121.0, 129.3, 131.7, 133.5, 137.3, 149.6, 152.9; **HRMS (ESI)** calcd. for $C_9H_{12}NO$ [M+H]: 150.0913, found: 150.0915.



3-(4-Methoxypyridin-2-yl)prop-2-en-1-ol (1e): The title compound was prepared according to the general procedure (method **A**) and purified by flash column chromatography to give the corresponding product as a yellow oil (70% yield, *E/Z* = 85:15). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 3.12 (br, 1H), 3.77 (s, 3H), 4.27 (d, *J* = 3.9 Hz, 2H), 6.55 (t, *J* = 3.7 Hz, 0.1H), 6.59 (t, *J* = 3.7 Hz, 0.9H), 6.61 (s, 0.9H), 6.65 (s, 0.1H), 7.06 (dd, J_1 = 2.9 Hz, J_2 = 8.6 Hz, 1H), 7.17 (d, *J* = 8.6 Hz, 1H), 8.15 (d, *J* = 3.0 Hz, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 55.6, 63.0, 121.1, 121.8, 129.3, 131.6, 136.8, 148.1, 154.7; **HRMS (ESI)** calcd. for $C_9H_{12}NO_2$ [M+H]: 166.0863, found: 166.0859.

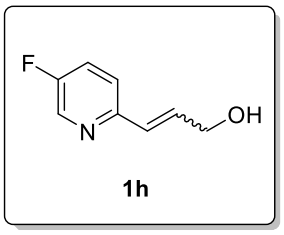


3-(6-Methylpyridin-2-yl)prop-2-en-1-ol (1f): The title compound was prepared according to the general procedure (method **A**) and purified by flash column chromatography to give the corresponding product as a yellow oil (43% yield, *E/Z* = 90:10). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 2.53 (s, 3H), 3.17 (br, 1H), 4.36 (d, *J* = 3.2Hz, 2H), 6.70 (s, 0.1H), 6.74 (s, 0.9H), 6.75 (d, *J* = 3.6 Hz, 0.9H), 6.79 (d, *J* = 3.6 Hz, 0.1H), 6.98 (d, *J* = 8.0 Hz, 1H), 7.12 (d, *J* = 7.8 Hz, 1H), 7.51 (t, *J* = 7.6 Hz, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 24.4, 62.8, 118.5, 121.9, 129.8, 134.0, 137.0, 155.0, 158.1; **HRMS (ESI)** calcd. for $C_9H_{12}NO$ [M+H]: 150.0913, found: 150.0918.



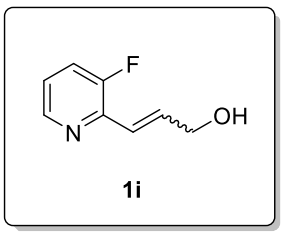
1g

3-(3-(Hydroxymethyl)pyridin-2-yl)prop-2-en-1-ol (1g): The title compound was prepared according to the general procedure (method **D**) and purified by flash column chromatography to give the corresponding product as a yellow oil (39% yield, *E/Z* = 63:37). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 3.45 (br, 2H), 4.34 (dd, J_1 = 1.6 Hz, J_2 = 4.8 Hz, 2H), 4.71 (s, 2H), 6.66 (t, *J* = 1.7 Hz, 0.4H), 6.70 (t, *J* = 1.7 Hz, 0.6H), 6.80 (t, *J* = 0.9 Hz, 0.6H), 6.84 (t, *J* = 0.9 Hz, 0.4H), 7.09 (d, *J* = 7.6 Hz, 1H), 7.14 (d, *J* = 7.6 Hz, 1H), 7.62 (t, *J* = 7.6 Hz, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 63.0, 64.0, 119.1, 120.4, 129.2, 134.1, 137.4, 154.0, 158.6; **HRMS (ESI)** calcd. for $C_9H_{12}NO_2$ [M+H]: 166.0868, found: 166.0935.



1h

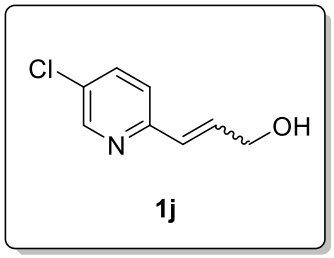
3-(5-Fluoropyridin-2-yl)prop-2-en-1-ol (1h): The title compound was prepared according to the general procedure (method **A**) and purified by flash column chromatography to givethe corresponding product as a yellow oil (85% yield, *E/Z* = 91:9). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 3.03 (br, 1H), 4.38 (d, *J* = 4.0 Hz, 2H), 6.69 (s, 0.1H), 6.73 (s, 0.9H), 6.75 (d, *J* = 10.8 Hz, 0.9H), 6.78 (d, *J* = 10.8 Hz, 0.1H), 7.27-7.38 (m, 2H), 8.38 (d, *J* = 2.6 Hz, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 62.7, 122.3 (d, *J* = 4.0 Hz), 123.5 (d, *J* = 19.0 Hz), 128.3, 134.1 (d, *J* = 3.0 Hz), 137.5 (d, *J* = 2.4 Hz), 151.8 (d, *J* = 4.0 Hz), 159.5 (d, *J* = 254 Hz); **^{19}F NMR** (376 MHz, $CDCl_3$) δ -128.8; **HRMS (ESI)** calcd. for C_8H_9FNO [M+H]: 154.0663, found: 150.0664.



1i

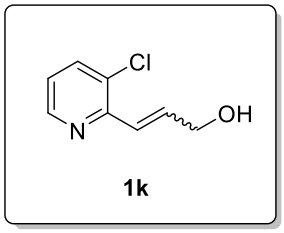
3-(3-Fluoropyridin-2-yl)prop-2-en-1-ol(1i): The title compound was prepared according to the general procedure (method **A**) and purified by flash column chromatography to givethe corresponding product as a yellow oil (54% yield, *E/Z* = 67:33). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 4.41 (d, *J* = 2.1 Hz, 3H), 6.90 (d, *J* = 1.4 Hz, 0.3H), 6.94 (d, *J* = 1.4 Hz, 0.7H), 7.01 (t, *J* = 3.5 Hz, 0.7H), 7.01 (t, *J* = 3.5 Hz, 0.3H), 7.12-7.16 (m, 1H), 7.31-7.36 (m, 1H), 8.31 (d, *J* = 4.8 Hz, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 62.7, 121.3, 123.1 (d, *J* = 4.0 Hz), 123.4 (d, *J* = 19.0 Hz), 136.8 (d, *J* = 5.0 Hz), 143.8 (d, *J* = 12.0 Hz), 144.8 (d, *J* = 6.0 Hz),

156.8 (d, J = 259.0 Hz); **^{19}F NMR** δ -126.07 (376 MHz $CDCl_3$); **HRMS (ESI)** calcd. for C_8H_9FNO [M+H]: 154.0663, found: 150.0668.



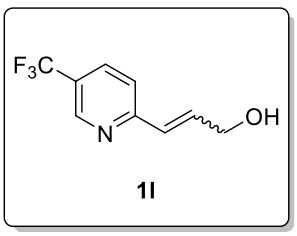
1j

3-(5-Chloropyridin-2-yl)prop-2-en-1-ol (1j): The title compound was prepared according to the general procedure (method **A**) and purified by flash column chromatography to give the corresponding product as a yellow oil (58% yield, E/Z = 67:33). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 3.10 (t, J = 5.4 Hz, 1H), 4.38 (t, J = 4.3 Hz, 2H), 6.68 (t, J = 1.7 Hz, 0.3H), 6.72 (t, J = 1.7 Hz, 0.7H), 6.79 (t, J = 4.8 Hz, 0.7H), 6.83 (t, J = 4.8 Hz, 0.3H), 7.21 (d, J = 8.4 Hz, 1H), 7.58 (dd, J_1 = 2.8 Hz, J_2 = 8.4 Hz, 1H), 8.46 (d, J = 2.4 Hz, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 62.8, 122.3, 128.4, 130.3, 134.9, 136.4, 148.3, 153.6; **HRMS (ESI)** calcd. for C_8H_9ClNO [M+H]: 170.0367, found: 170.0360.



1k

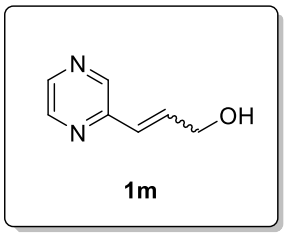
3-(3-Chloropyridin-2-yl)prop-2-en-1-ol (1k): The title compound was prepared according to the general procedure (method **A**) and purified by flash column chromatography to give the corresponding product as a yellow oil (59% yield, E/Z = 77:23). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 2.35 (br, 1H), 4.44 (dd, J_1 = 1.6 Hz, J_2 = 4.4 Hz, 2H), 7.06-7.14 (m, 2H), 7.14 (t, J = 1.5 Hz, 0.8H), 7.18 (t, J = 1.5 Hz, 0.2H), 7.64 (dd, J_1 = 1.2Hz, J_2 = 8.0 Hz, 1H), 8.44 (dd, J_1 = 1.6 Hz, J_2 = 4.8 Hz, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 63.2, 123.1, 124.4, 130.3, 137.0, 137.6, 147.5, 151.9; **HRMS (ESI)** calcd. for C_8H_9ClNO [M+H]: 170.0373, found: 170.0449.



1l

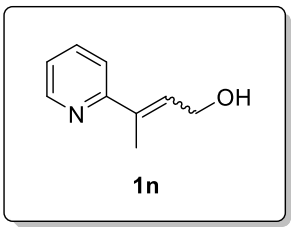
3-(5-(Trifluoromethyl)pyridin-2-yl)prop-2-en-1-ol (1l): The title compound was prepared according to the general procedure (method **A**) and purified by flash column chromatography to give the corresponding product as a yellow oil (58% yield, E/Z = 58:42). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 2.85 (br, 1H), 4.43 (dd, J_1 = 2.0 Hz, J_2 = 4.8 Hz, 2H), 6.79 (t, J = 1.9 Hz, 0.4H), 6.83 (t, J = 1.9 Hz, 0.6H), 6.97(t, J = 4.6 Hz, 0.6H), 7.01 (t, J = 4.6 Hz, 0.4H), 7.38 (d, J = 8.0 Hz, 1H), 7.84 (dd, J_1 = 2.4 Hz, J_2 = 8.4 Hz, 1H), 8.78-8.79 (m, 1H);

^{13}C NMR (100 MHz, $CDCl_3$) δ 62.7, 121.3, 122.3, 124.8 (dd, J_1 = 66.0 Hz, J_2 = 30.0 Hz), 128.1, 133.9 (dd, J_1 = 7.0 Hz, J_2 = 3.0 Hz), 137.3, 146.4 (dd, J_1 = 9.0 Hz, J_2 = 4.0 Hz), 158.6 (d, J = 2.0 Hz); **^{19}F NMR** (376 MHz $CDCl_3$) δ -62.3; **HRMS (ESI)** calcd. for $C_9H_9F_3NO$ [M+H]: 204.0626, found: 204.0770.



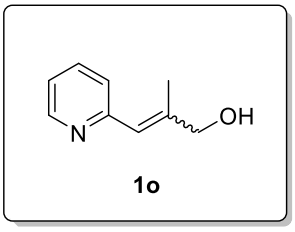
1m

3-(Pyrimidin-4-yl)prop-2-en-1-ol (1m): The title compound was prepared according to the general procedure (method **A**) and purified by flash column chromatography to give the corresponding product as a yellow oil (42% yield, *E/Z* = 56:44). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 2.83 (br, 1H), 4.42 (dd, J_1 = 2.0 Hz, J_2 = 4.4 Hz, 2H), 6.83 (t, J = 2.0 Hz,0.4H), 6.87 (t, J = 2.0 Hz, 0.6H), 7.11 (t, J = 4.9 Hz, 1H), 7.24 (t, J = 4.5 Hz, 0.6H), 7.29 (t, J = 4.5 Hz, 0.4H), 8.66 (d, J = 4.9 Hz, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 62.4, 118.9, 128.3, 140.8, 157.1, 164.3; **HRMS (ESI)** calcd. for $C_7H_9N_2O$ [M+H]: 137.0715, found: 137.0775.



1n

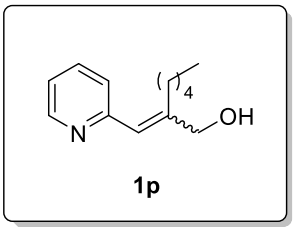
3-(Pyridin-2-yl)but-2-en-1-ol (1n): The title compound was prepared according to the general procedure (method **B**) and purified by flash column chromatography to give the corresponding product as ayellow oil (59% yield, *E/Z* = 56:44). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 2.09 (br, 1H), 2.13 (d, J = 1.2 Hz, 3H), 4.43 (dd, J_1 = 1.2 Hz, J_2 = 6.4 Hz, 2H), 6.48-6.52 (m, 1H), 7.14-7.18 (m, 1H), 7.43 (t, J = 1.0 Hz, 0.4H), 7.45 (t, J = 1.0 Hz, 0.6H), 7.63-7.67 (m, 1H), 8.56-8.58(m, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 14.7, 60.1, 120.1, 122.1, 130.0, 136.6, 136.9, 149.0, 159.3; **HRMS (ESI)** calcd. for $C_9H_{12}NO$ [M+H]: 150.0913, found: 150.0968.



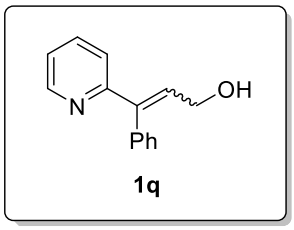
1o

2-Methyl-3-(pyridin-2-yl)prop-2-en-1-ol (1o): The title compound was prepared according to the general procedure (method **C**) and purified by flash column chromatography to give the corresponding product as a yellow oil (58% yield, *E/Z* > 99:1). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 2.01 (s, 3H), 2.95 (br, 1H), 4.20 (d, J = 1.6 Hz, 2H), 6.65 (d, J = 1.6 Hz, 1H), 7.09-7.13 (m, 1H), 7.26 (d, J = 8.2 Hz, 1H), 7.64 (m, 1H), 8.56-8.58 (m, 1H); **^{13}C NMR** (100 MHz,

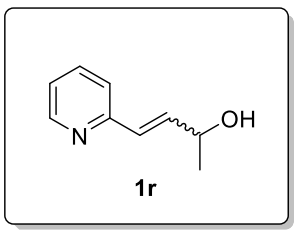
$CDCl_3$) δ 15.5, 68.1, 121.2, 123.3, 124.2, 136.3, 143.1, 149.0, 156.9; **HRMS (ESI)** calcd. for $C_9H_{12}NO$ [M+H]: 150.0913, found: 150.0993.



2-(Pyridin-2-ylmethylene)heptan-1-ol (1p): The title compound was prepared according to the general procedure (method **C**) and purified by flash column chromatography to give the corresponding product as a yellow oil (61% yield, *E/Z* > 99:1). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 0.82-0.85 (m, 3H), 1.25-1.26 (m, 4H), 1.42-1.49 (m, 2H), 2.41-2.45 (m, 2H), 4.23 (s, 2H), 4.93 (br, 1H), 6.65 (s, 1H), 7.06-7.10 (m, 1H), 7.20 (d, *J* = 8.0 Hz, 1H), 7.59-7.63 (m, 1H), 8.52-8.54 (m, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 14.0, 22.4, 28.0, 28.9, 32.0, 65.8, 121.0, 122.9, 123.8, 136.2, 147.9, 148.8, 157.0; **HRMS (ESI)** calcd. for $C_{13}H_{20}NO$ [M+H]: 206.1539, found: 206.1545.



3-Phenyl-3-(pyridin-2-yl)prop-2-en-1-ol (1q): The title compound was prepared according to the general procedure (method **B**) and purified by flash column chromatography to give the corresponding product as a yellow oil (64% yield, *E/Z* = 72:28). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 3.08 (br, 1H), 4.47 (dd, J_1 = 1.6 Hz, J_2 = 4.4 Hz, 2H), 6.91 (t, *J* = 4.4 Hz, 0.3H), 6.95 (t, *J* = 4.4 Hz, 0.7H), 6.99 (t, *J* = 1.6 Hz, 0.7H), 7.03 (t, *J* = 1.6 Hz, 0.7H), 7.44-7.55 (m, 4H), 7.64-7.72 (m, 2H), 7.77 (dd, J_1 = 1.6 Hz, J_2 = 8.4 Hz, 1H), 8.05-8.10 (m, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 67.0, 121.3, 123.9, 125.2, 127.7, 128.4, 128.7, 135.7, 138.3, 147.2, 148.7, 156.1; **HRMS (ESI)** calcd. for $C_{14}H_{14}NO$ [M+H]: 212.1070, found: 212.1072.



4-(Pyridin-2-yl)but-3-en-2-ol (1r): The title compound was prepared according to the general procedure (method **A**) and purified by flash column chromatography to give the corresponding product as a yellow oil (57% yield, *E/Z* = 69:31). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 1.40 (d, *J* = 6.8 Hz, 3H), 2.28 (br, 1H), 4.53-4.59 (m, 1H), 6.66 (s, 0.3H), 6.70 (s, 0.7H), 6.76 (d, *J* = 8.0 Hz, 0.7H), 6.80 (d, *J* = 8.0 Hz, 0.3H), 7.12-7.15 (m, 1H), 7.27-7.30 (m, 1H), 7.61-7.65 (m, 1H), 8.54-8.56 (m, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 23.4, 68.4,

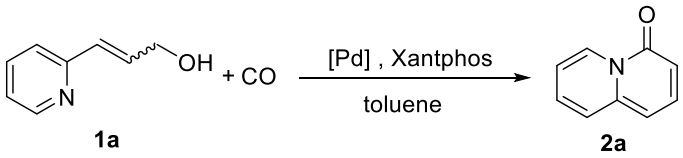
121.9, 122.3, 128.8, 136.7, 138.5, 149.6, 155.4; **HRMS (ESI)** calcd. for $C_9H_{12}NO$ [M+H]: 150.0913, found: 150.0968.

4. General procedure for the synthesis of product

A mixture of catalyst, ligand, and allylic alcohols were added into a glass tube which was placed in an autoclave. Then the autoclave was purged and charged with CO at the designed pressure. The reaction mixture was stirred at the designed temperature for 12 hours. After the reaction finished, the autoclave was cooled to room temperature and the pressure was carefully released. The yield was determined by GC analysis relative to the **1** with *n*-hexadecane as internal standard. Then the corresponding reactionmixture was purified by flash column chromatography on a silica gel column EtOAc/petroleum ether (1/50~1/10) to give the desired product.

5. Optimization of the reaction conditions

Table S1. Screening of the [Pd] catalysts.[a]

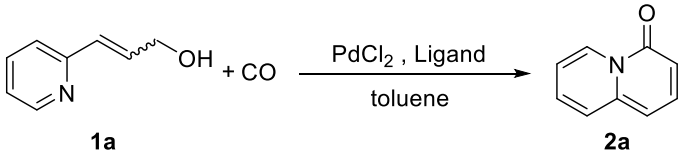


1a **2a**

Entry	[Pd]	Yield (%)[b]
1	PdI_2	20
2	$PdBr_2$	70
3	**$PdCl_2$**	**88**
4	$Pd(TFA)_2$	51
5	$[Pd(allyl)Cl]_2$	75
6	$Pd(OAc)_2$	54
7	$Pd_2(dba)_3$	ND
8	$Pd(CH_3CN)_2Cl_2$	79

[a] Reaction conditions: **1a** (0.5 mmol), [Pd] (0.025 mmol, 5 mol %), Xantphos (0.03 mmol, 6 mol %), toluene (2 mL), CO (20 atm), 120 ^{o}C, 12 h. [b] Yields were determined by GC analysis using *n*-hexadecane as an internal standard.

Table S2. Screening of the ligands.[a]



1a **2a**

Entry	Ligand	Yield (%)[b]
1	**XantPhos**	**88**
2	DPPM	34
3	DPPE	33
4	DPPB	16
5	DPPF	20
6	PPh_3	25[c]
7	P(*o*-Tolyl)$_3$	Trace[c]
8	P(*m*-Tolyl)$_3$	Trace[c]
9	PCy_3	16[c]
10	$P(C_6F_5)_3$	23[c]
11	DPEPhos	41

[a] Reaction conditions: **1a** (0.5 mmol), $PdCl_2$ (0.025 mmol, 5 mol%), ligands (0.03 mmol, 6 mol %), toluene (2 mL), CO (20 atm), 120 ^{o}C, 12 h. Yields were determined by GC analysis using *n*-hexadecane as an internal standard. [b] Yields were determined by GC analysis using n-hexadecane as an internal standard. [c] Ligand (12 mol%).

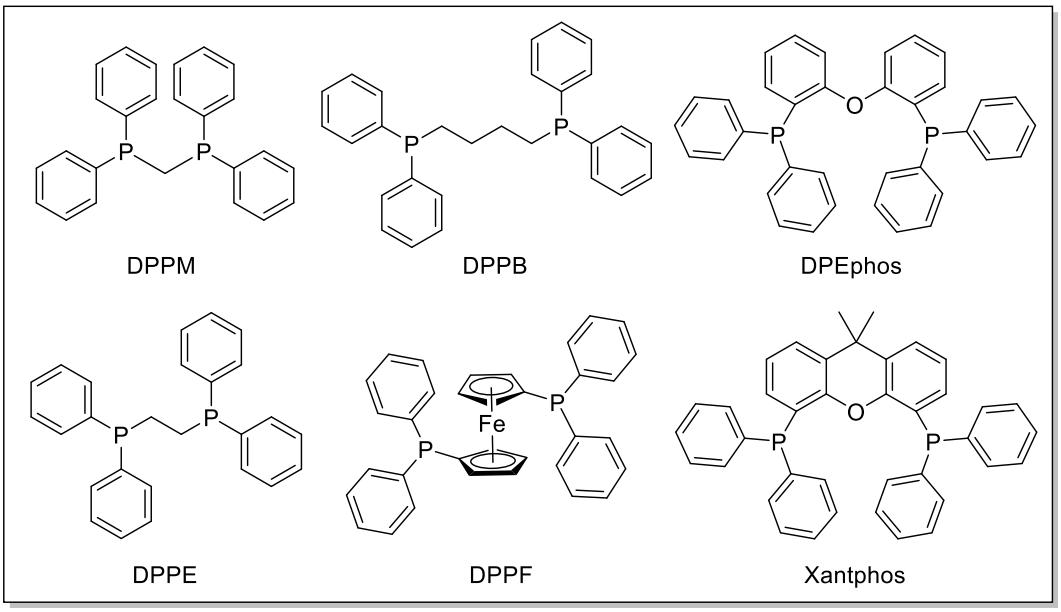
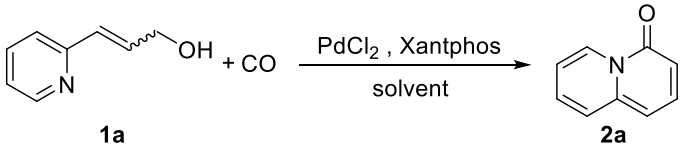


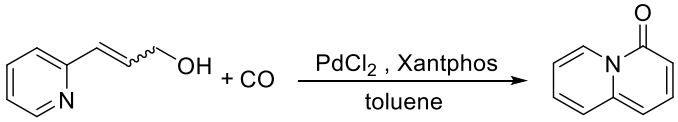
Table S3. Screening of the solvents.[a]



Entry	Solvent	Yield (%)[b]
1	toluene	88
2	*i*-PrOH	58
3	THF	62
4	CH_3CN	55
5	NMP	67
6	DMF	trace
7	anisole	48
8	xylene	85
9	mesitylene	81
10	$PhCF_3$	70

[a] Reaction conditions: **1a** (0.5 mmol), $PdCl_2$ (0.025 mmol, 5 mol %), XantPhos (0.03 mmol, 6 mol %), solvent (2 mL), CO (20 atm), 120 ^oC, 12 h. [b] Yields were determined by GC analysis using n-hexadecane as an internal standard.

Table S4. Screening of temperature.[a]

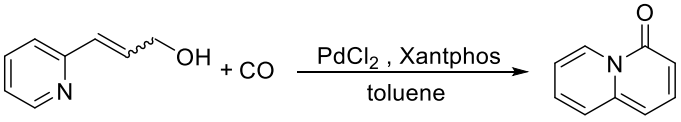


1a 2a

Entry	temperature (^{o}C)	Yield (%)[b]
1	**120**	**88**
2	100	87
3	80	86
4	60	62

[a] Reaction conditions: **1a** (0.5 mmol), $PdCl_2$ (0.025 mmol, 5 mol %), XantPhos (0.03 mmol, 6 mol %), toluene (2 mL), CO (20 atm), 12 h. [b] Yields were determined by GC analysis using *n*-hexadecane as an internal standard.

Table S5. Screening of pressure of CO.[a]

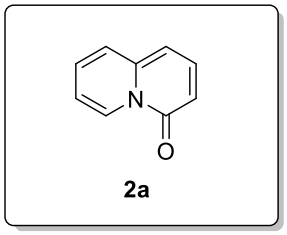


1a 2a

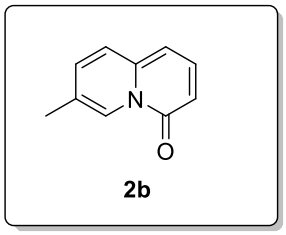
Entry	pressure of CO (atm)	Yield (%)[b]
1	30	88
2	20	88
3	10	85
4	1	85(86)[c]

[a] Reaction conditions: **1a** (0.5 mmol), $PdCl_2$ (0.025 mmol, 5 mol %), XantPhos(0.03 mmol, 6 mol %), toluene (2 mL), CO, 80 ^{o}C,12 h. [b] Yields were determined by GC analysis using *n*-hexadecane as an internal standard. [c] Isolated yield.

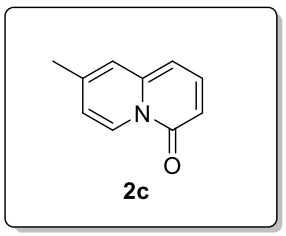
6. Experimental characterization data for products



4*H*-quinolizin-4-one (2a): The title compound was prepared according to the general procedure and purified by flash column chromatography to give the corresponding product as a yellow solid, 62 mg, 86% yield. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 6.61-6.66 (m, 2H), 6.98-7.02 (m, 1H), 7.31-7.35 (m, 1H), 7.45-7.48 (m, 1H), 7.64-7.68 (m, 1H), 9.12 (dd, J_1 = 1.2Hz, J_2 = 7.6Hz, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 103.3, 109.2, 115.0, 125.5, 127.4, 129.4, 138.2, 142.8, 158.8; **HRMS (ESI)** calcd. for C_9H_8NO [M+H]: 146.0600, found: 146.0605.

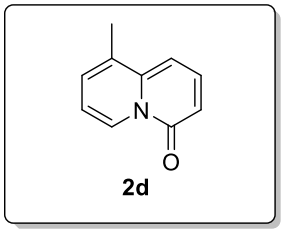


7-Methyl-4*H*-quinolizin-4-one (2b): The title compound was prepared according to the general procedure and purified by flash column chromatography to give the corresponding product as a yellow solid, 64 mg, 80% yield. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 2.38 (d, J = 1.2 Hz, 3H), 6.63 (dd, J_1 = 7.6 Hz, J_2 = 12.4 Hz, 2H), 7.19 (dd, J_1 = 1.6 Hz, J_2 = 8.8 Hz, 1H), 7.40 (d, J = 8.8 Hz, 1H), 7.59 (dd, J_1 = 8.0 Hz, J_2 = 8.8 Hz, 1H), 8.95 (s, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 18.7, 103.2, 108.8, 124.6, 125.0, 125.2, 132.5, 137.4, 141.5, 158.5; **HRMS (ESI)** calcd. for $C_{10}H_{10}NO$ [M+H]: 160.0757, found: 160.0755.

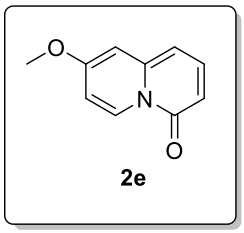


8-Methyl-4*H*-quinolizin-4-one (2c): The title compound was prepared according to the general procedure and purified by flash column chromatography to give the corresponding product as a yellow solid, 72 mg, 91% yield. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 2.4 (d, J = 1.2 Hz, 3H), 6.50-6.54 (m, 2H), 6.82 (dd, J_1 = 2.0 Hz, J_2 = 7.6 Hz, 1H), 7.22-7.23 (m, 1H), 7.58 (dd, J_1 = 7.6 Hz, J_2 = 8.4 Hz, 1H), 9.03 (d, J = 7.6 Hz, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 21.2, 102.2, 107.6, 117.9, 123.4, 126.9, 138.3, 140.8, 143.0, 158.7; **HRMS (ESI)** calcd. for $C_{10}H_{10}NO$ [M+H]: 160.0757, found: 160.0754.

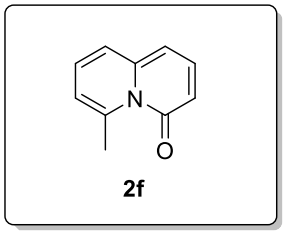
9-Methyl-4H-quinolizin-4-one (2d): The title compound was prepared according to the general procedure and purified by flash column chromatography to give the



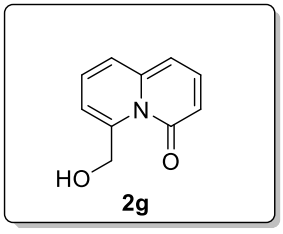
corresponding product as a yellow solid, 52 mg, 65% yield. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 2.48 (s, 3H), 6.62 (dd, J_1 = 1.2 Hz, J_2 = 8.8 Hz, 1H), 6.67-6.69 (m, 1H), 6.93 (t, J = 7.2 Hz, 1H), 7.19-7.21 (m, 1H),7.66 (dd, J_1 = 8.0 Hz, J_2 = 8.8 Hz, 1H), 9.08 (dd, J_1 = 1.2 Hz, J_2 = 7.6 Hz, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 19.3, 100.0, 109.1, 114.5, 126.0, 129.3, 132.2, 137.8, 143.0, 159.3; **HRMS (ESI)** calcd. for $C_{10}H_{10}NO$ [M+H]: 160.0757, found: 160.0862.



8-Methoxy-4*H*-quinolizin-4-one (2e): The title compound was prepared according to the general procedure and purified by flash column chromatography to give the the corresponding product as a yellow solid, 56 mg, 64% yield. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 3.94 (s, 3 H), 6.65 (dd, J_1 = 7.6 Hz, J_2 = 14.2 Hz, 2H), 7.15 (dd, J_1 = 2.5 Hz, J_2 = 9.5 Hz, 1H), 7.42 (d, J = 9.5 Hz, 1H), 7.58 (dd, J_1 = 7.6 Hz, J_2 = 8.8 Hz, 1H), 8.67 (d, J = 2.4 Hz, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 56.1, 103.8, 106.8, 108.7, 125.4, 126.1, 136.1, 139.5, 150.9, 158.2; **HRMS (ESI)** calcd. for $C_{10}H_{10}NO_2$ [M+H]: 176.0706, found: 176.0710.

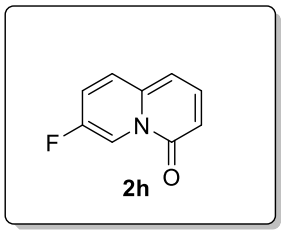


6-Methyl-4*H*-quinolizin-4-one (2f): The title compound was prepared according to the general procedure and purified by flash column chromatography to give the corresponding product as a yellow solid, 29 mg, 36% yield. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 3.02 (s, 3 H), 6.42 (s, 1H), 6.44 (s, 1H),6.45-6.47(m, 1H), 6.95-6.99 (m, 1H), 7.13 (dd, J_1 = 1.2 Hz, J_2 = 8.8 Hz, 1H), 7.45 (t, J = 8.0 Hz, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 25.0, 103,8, 112.4, 118.0, 124.6, 128.3, 137.3, 142.9, 145.1, 163.2; **HRMS (ESI)** calcd. for $C_{10}H_{10}NO$ [M+H]: 160.0757, found: 160.0754.

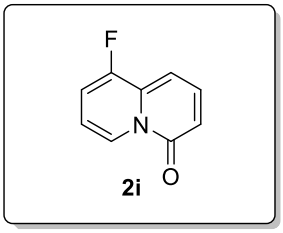


6-(Hydroxymethyl)-4*H*-quinolizin-4-one (2g): The title compound was prepared according to the general procedure and purified by flash column chromatography to give the corresponding product as a yellow solid, 52 mg, 24% yield.

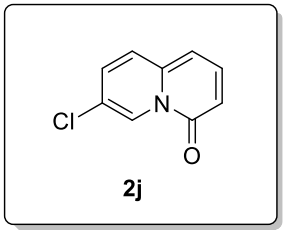
^{1}H NMR (400 MHz, $CDCl_3$) δ 4.94-5.01 (m, 3H), 6.62-6.67 (m, 2H), 6.78 (dd, J_1 = 1.6 Hz, J_2 = 6.8 Hz, 1H), 7.11 (dd, J_1 = 6.7 Hz, J_2 = 8.9 Hz, 1H), 7.35 (dd, J_1 = 1.6 Hz, J_2 = 8.9 Hz, 1 H), 7.59 (dd, J_1 = 7.4 Hz, J_2 = 8.7 Hz, 1 H), **^{13}C NMR** (100 MHz, $CDCl_3$) δ 65.3, 106.1, 113.2, 119.6, 127.2, 128.2, 137.8, 143.5, 144.5, 162.5; **HRMS (ESI)** calcd. for $C_{10}H_9NNaO_2$ [M+Na]: 198.0525, found: 198.0526.



7-Fluoro-4*H*-quinolizin-4-one (2h): The title compound was prepared according to the general procedure and purified by flash column chromatography to give the corresponding product as a yellow solid, 69 mg, 85% yield. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 6.64 (dd, J_1 = 1.2 Hz, J_2 = 8.8 Hz, 1H), 6.72 (d, J = 7.6 Hz, 1H), 7.25-7.30 (m, 1H), 7.49 (dd, J_1 = 5.6 Hz, J_2 = 9.6 Hz, 1H), 7.64 (dd, J_1 = 7.6 Hz, J_2 = 8.8 Hz, 1H), 9.03 (dd, J_1 = 2.4 Hz, J_2 = 6.0 Hz, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 104.1, 109.6, 113.0, 113.4, 122.3, 122.6, 127.4, 127.4, 137.5, 140.5, 153.3, 155.7, 158.2, 158.2; **^{19}F NMR** (376 MHz $CDCl_3$) δ -133.7; **HRMS** (ESI) calcd. for C_9H_7FNO [M+H]: 164.0506, found: 164.0502.

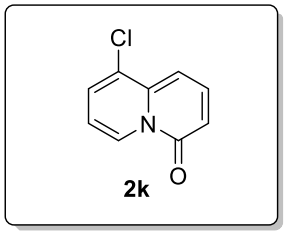


9-Fluoro-4*H*-quinolizin-4-one (2i): The title compound was prepared according to the general procedure and purified by flash column chromatography to give the corresponding product as a yellow solid, 51 mg, 63% yield. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 6.67 (dd, J_1 = 1.2 Hz, J_2 = 8.8 Hz, 1H), 6.90 (t, J = 7.2 Hz, 1H), 7.07 (d, J = 7.6 Hz, 1H), 7.43 (dd, J_1 = 1.2 Hz, J_2 = 7.2 Hz, 1H), 7.72 (dd, J_1 = 8.0 Hz, J_2 = 9.2 Hz, 1H), 9.06 (d, J = 7.6 Hz, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 101.0, 110.8, 113.3, 126.6, 128.9, 129.5, 138.6, 140.3, 158.8; **^{19}F NMR** (376 MHz $CDCl_3$) δ -122.7; **HRMS (ESI)** calcd. for C_9H_7FNO [M+H]: 164.0506, found: 164.0501.

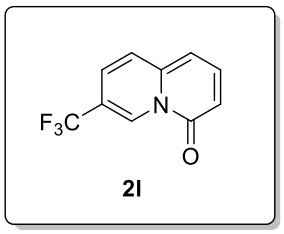


7-Chloro-4*H*-quinolizin-4-one (2j): The title compound was prepared according to the general procedure and purified by flash column chromatography to give the corresponding product as a yellow solid, 63 mg, 70% yield. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 6.67 (dd, J_1 = 1.2 Hz, J_2 = 9.2 Hz, 1H), 6.90 (t, J = 7.2 Hz, 1H), 7.06

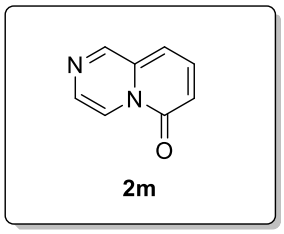
(d, J = 8.0 Hz, 1H), 7.43 (dd, J_1 = 1.2 Hz, J_2 = 7.2 Hz, 1H), 7.71 (dd, J_1 = 8.0 Hz, J_2 = 9.2 Hz, 1H), 9.04 (d, J = 7.6 Hz, 1 H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 100.9, 110.8, 113.3, 126.5, 128.7, 129.5, 138.6, 140.2, 158.7; **HRMS (ESI)** calcd. for C_9H_7ClNO [M+H]: 180.0211, found: 180.0209.



9-Chloro-4*H*-quinolizin-4-one (2k): The title compound was prepared according to the general procedure and purified by flash column chromatography to give the corresponding product as a yellow solid, 56 mg, 63% yield. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 6.67 (dd, J_1 = 1.2 Hz, J_2 = 9.2 Hz, 1H), 6.89 (t, J = 7.2 Hz, 1H), 7.07 (d, J = 7.6 Hz, 1H), 7.42 (dd, J_1 = 1.2 Hz, J_2 = 7.2 Hz, 1H), 7.71 (dd, J_1 = 8.0 Hz, J_2 = 8.8 Hz, 1H), 9.04-9.07 (m, 1 H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 100.9, 110.7, 113.3, 126.5, 128.9, 129.4, 138.5, 140.2, 158.7; **HRMS (ESI)** calcd. for C_9H_7ClNO [M+H]: 180.0211, found: 180.0206.

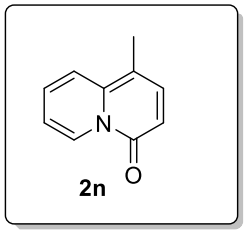


7-(Trifluoromethyl)-4H-quinolizin-4-one (2l): The title compound was prepared according to the general procedure and purified by flash column chromatography to give the corresponding product as a yellow solid, 76 mg, 71% yield. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 6.63-6.67 (m, 2H), 7.27 (dd, J_1 = 1.2 Hz, J_2 = 7.2 Hz, 1H), 7.46 (d, J = 7.2 Hz, 1H), 7.66 (dd, J_1 = 6.0 Hz, J_2 = 7.2 Hz, 1H), 9.35 (t, J = 1.6 Hz, 1 H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 103.9, 111.7, 118.7 (d, J = 28.0 Hz), 124.1 (q, J = 2.0 Hz), 124.2, 126.7 (d, J = 5.0 Hz), 126.8, 139.7, 142.1, 158.7; **^{19}F NMR** (376 MHz $CDCl_3$) δ -63.7; **HRMS (ESI)** calcd. for $C_{10}H_7F_3NO$ [M+H]: 214.0474, found: 214.0843.

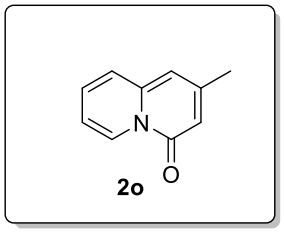


6*H*-pyrido[1,2-a]pyrazin-6-one (2m): The title compound was prepared according to the general procedure and purified by flash columnchromatography to give the corresponding product as a yellow solid, 40 mg, 55% yield. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 6.87 (s, 1H), 6.89-6.90 (m, 1H), 7.78 (dd, J_1 = 7.6 Hz, J_2 = 9.2 Hz, 1H), 7.89 (d, J = 5.2 Hz, 1H), 8.67-8.69 (m, 1H), 8.88 (d, J = 1.2 Hz, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 105.0, 116.0, 117.2, 130.9, 135.6, 138.8,

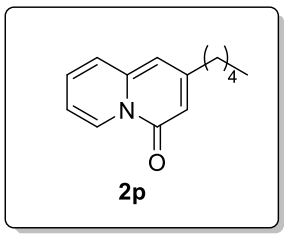
152.5, 157.4; **HRMS (ESI)** calcd. for $C_8H_7N_2O$ [M+H]: 147.0553, found: 147.0775.



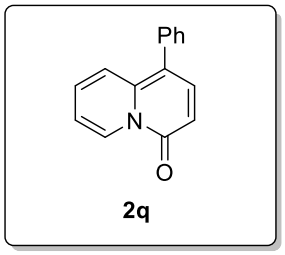
Methyl-4*H*-quinolizin-4-one (2n): The title compound was prepared according to the general procedure and purified by flash column chromatography to give the corresponding product as a yellow solid, 68 mg, 85% yield. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 2.41 (s, 3H), 6.57 (d, J = 8.8 Hz, 1H), 7.00-7.04 (m, 1H), 7.36-7.40 (m, 1H), 7.54 (d, J = 8.9 Hz, 1H), 7.58-7.61 (m, 1H), 9.20 (d, J = 7.4 Hz, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 17.1, 108.5, 109.4, 114.7, 122.3, 128.0, 129.0, 140.1, 140.5, 158.2; **HRMS (ESI)** calcd. for $C_{10}H_{10}NO$ [M+H]: 160.0757, found: 160.0888.



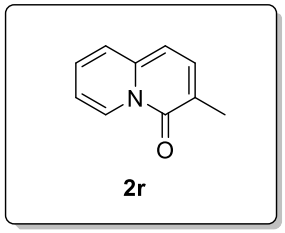
2-Methyl-4*H*-quinolizin-4-one (2o): The title compound was prepared according to the general procedure and purified by flash column chromatography to give the corresponding product as a yellow solid, 72 mg, 90% yield. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 2.36 (s, 3 H), 6.44 (dd, J_1 = 1.6 Hz, J_2 = 10.4 Hz, 2H), 6.87-6.91 (m, 1H), 7.24-7.28 (m, 1H), 7.33-7.36 (m, 1H), 9.00-9.03 (m, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 21.8, 104.7, 109.3, 114.2, 124.8, 127.0, 129.3, 141.7, 149.9, 158.4; **HRMS (ESI)** calcd. for $C_{10}H_{10}NO$ [M+H]: 160.0757, found: 160.0801.



Pentyl-4*H*-quinolizin-4-one (2p): The title compound was prepared according tothe general procedure and purified by flash column chromatographyto give the corresponding product as a yellow solid, 71 mg, 66% yield. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 0.88-0.91 (m, 3H), 1.32-1.36 (m, 4H), 1.63-1.71 (m, 2H), 2.61 (t, J = 7.6 Hz, 2H), 6.48 (dd, J_2 = 1.4 Hz, J_2 = 6.4 Hz, 2H), 6.89-6.92 (m, 1H), 7.24-7.28 (m, 1H), 7.36-7.39 (m, 1H), 9.02 (dd, J_1 = 0.8 Hz, J_2 = 7.6 Hz, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 14.1, 22.6, 29.8, 31.5, 36.0, 104.2, 108.8, 114.3, 125.1, 127.2, 129.2, 141.9, 154.6, 158.7; **HRMS (ESI)** calcd. for $C_{14}H_{18}NO$ [M+H]: 216.1383, found: 216.1386.

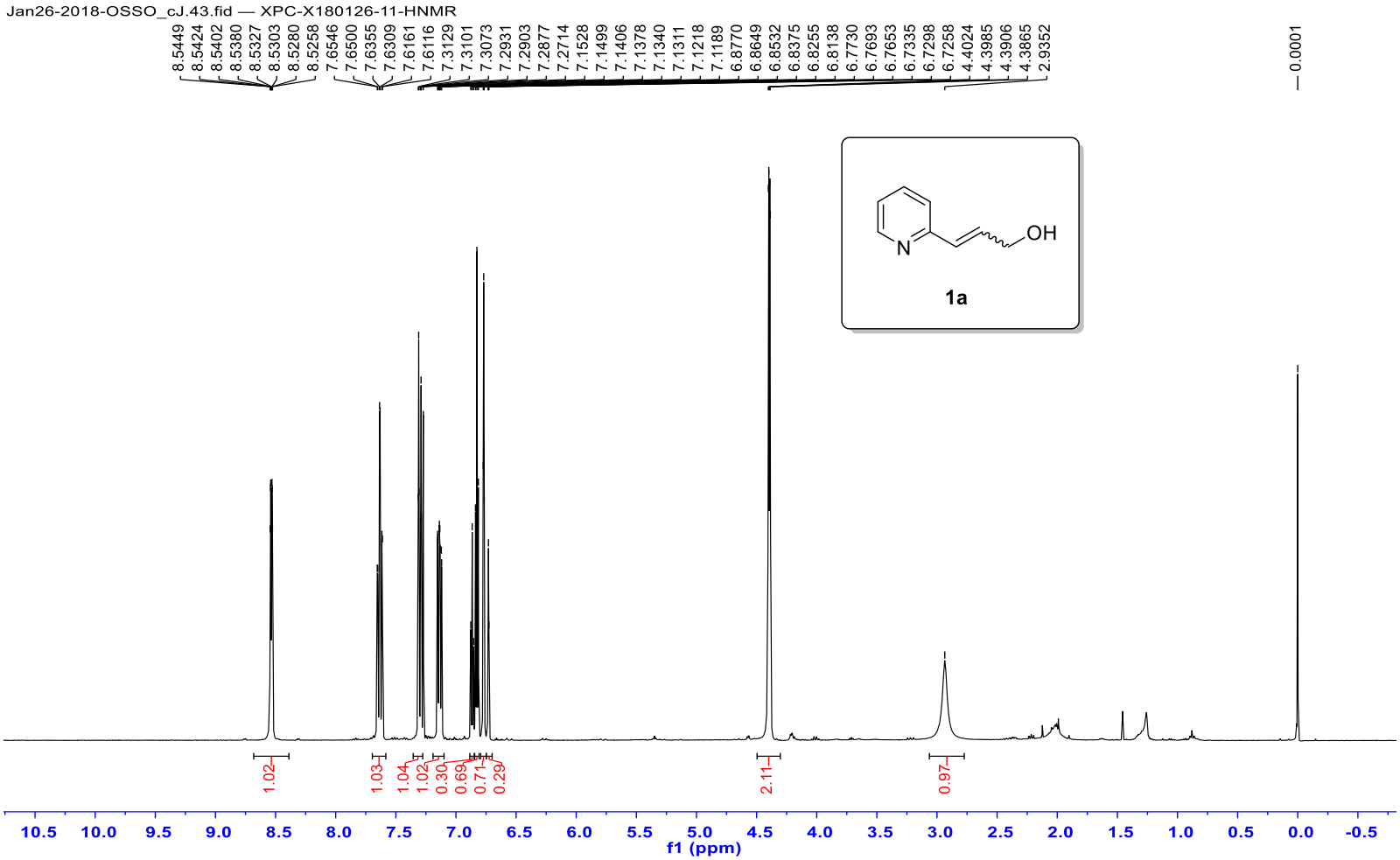


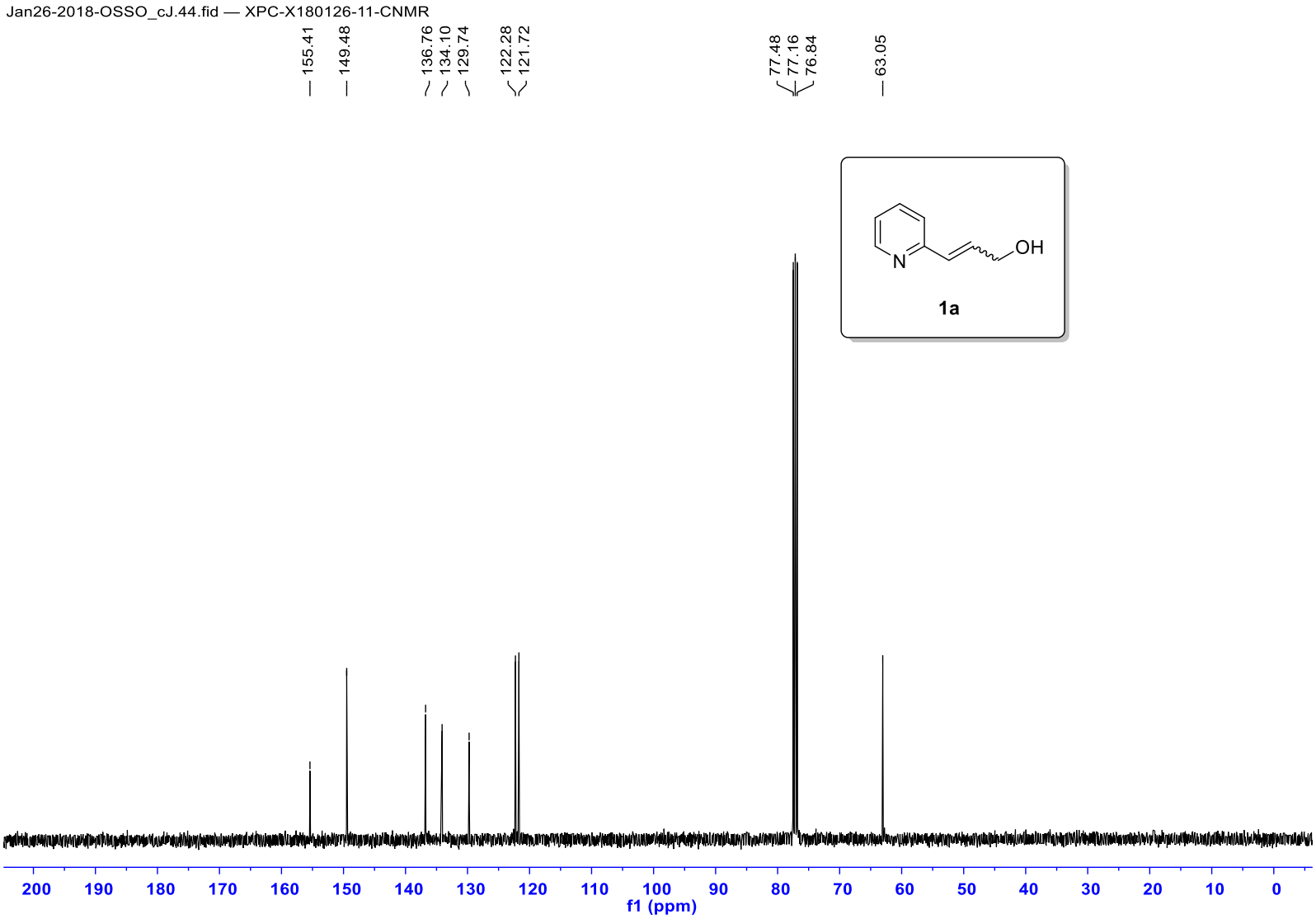
1-Phenyl-4*H*-quinolizin-4-one (2q): The title compound was prepared according to the general procedure and purified by flash column chromatography to give the corresponding product as a yellow solid, 85 mg, 77% yield. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 6.87-6.89 (m, 2H), 6.97-7.00 (m, 1H), 7.32-7.36 (m, 1H), 7.43-7.53 (m, 4H), 7.68-7.71 (m, 2H), 9.11 (d, J = 7.4 Hz, 1 H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 102.1, 106.6, 114.8, 125.6, 127.2, 127.2, 129.0, 129.2, 129.6, 138.4, 142.3, 150.4, 158.74; **HRMS (ESI)** calcd. for $C_{15}H_{12}NO$ [M+H]: 222.0913, found: 222.0913.



7-Methyl-4*H*-quinolizin-4-one (2r): The title compound was prepared according to the general procedure and purified by flash column chromatography to give the corresponding product as a yellow solid, 8 mg, 10% yield. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 2.29 (s, 3 H), 6.53 (d, J = 7.6 Hz, 1H), 6.84-6.88 (m, 1H), 7.10-7.15 (m, 1H), 7.33 (d, J = 8.8 Hz, 1H), 7.51 (dd, J_1 = 1.0 Hz, J_2 = 7.7 Hz, 1H), 9.00 (d, J = 7.6 Hz, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 17.6, 102.7, 114.6, 119.0, 125.3, 126.6, 127.3, 137.0, 140.5, 158.5; **HRMS (ESI)** calcd. for$C_{10}H_{10}NO$ [M+H]: 160.0757, found: 160.0985.

7. Copies of NMR of staring materials and products

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77.48
77.16
76.84
63.05
OH
N
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200
190
180
170
160
150
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130
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110
100
90
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70
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50
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30
20
10
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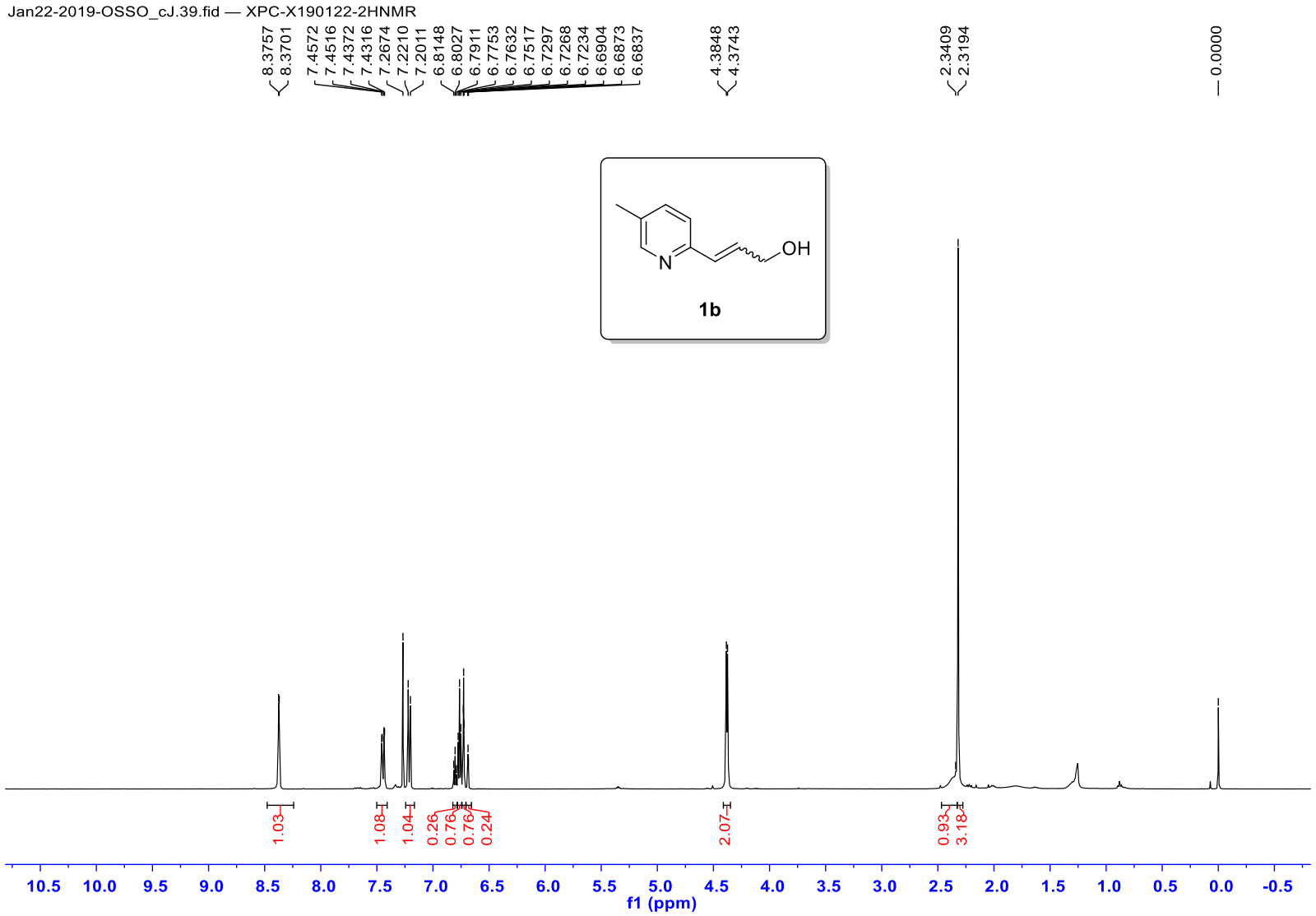
f1 (ppm)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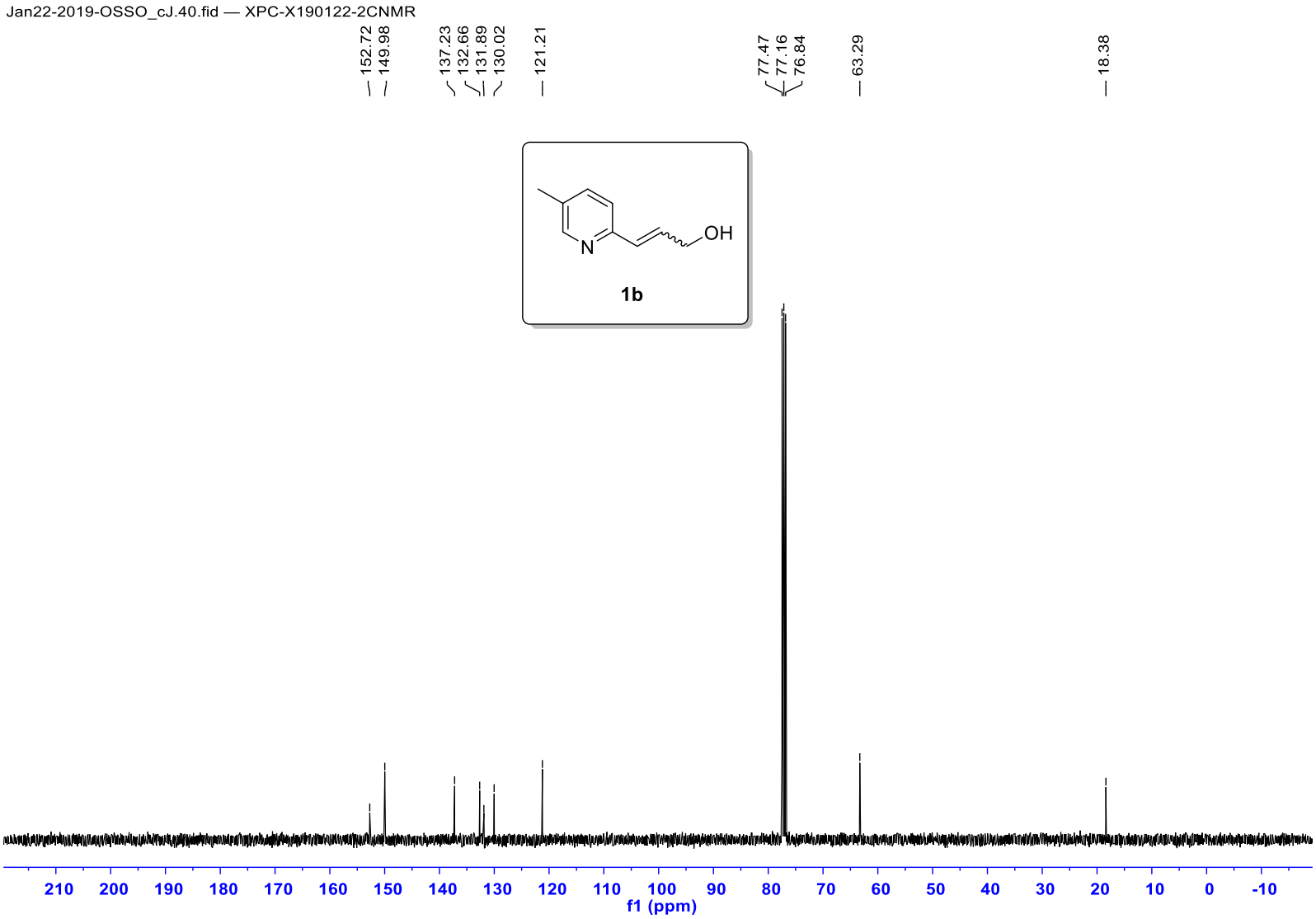
1.08
1.04
0.26
0.76
0.76
0.24
2.07
0.93
3.18
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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77.16
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63.29
18.38
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1b
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200
190
180
170
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110
100
90
80
70
60
50
40
30
20
10
0
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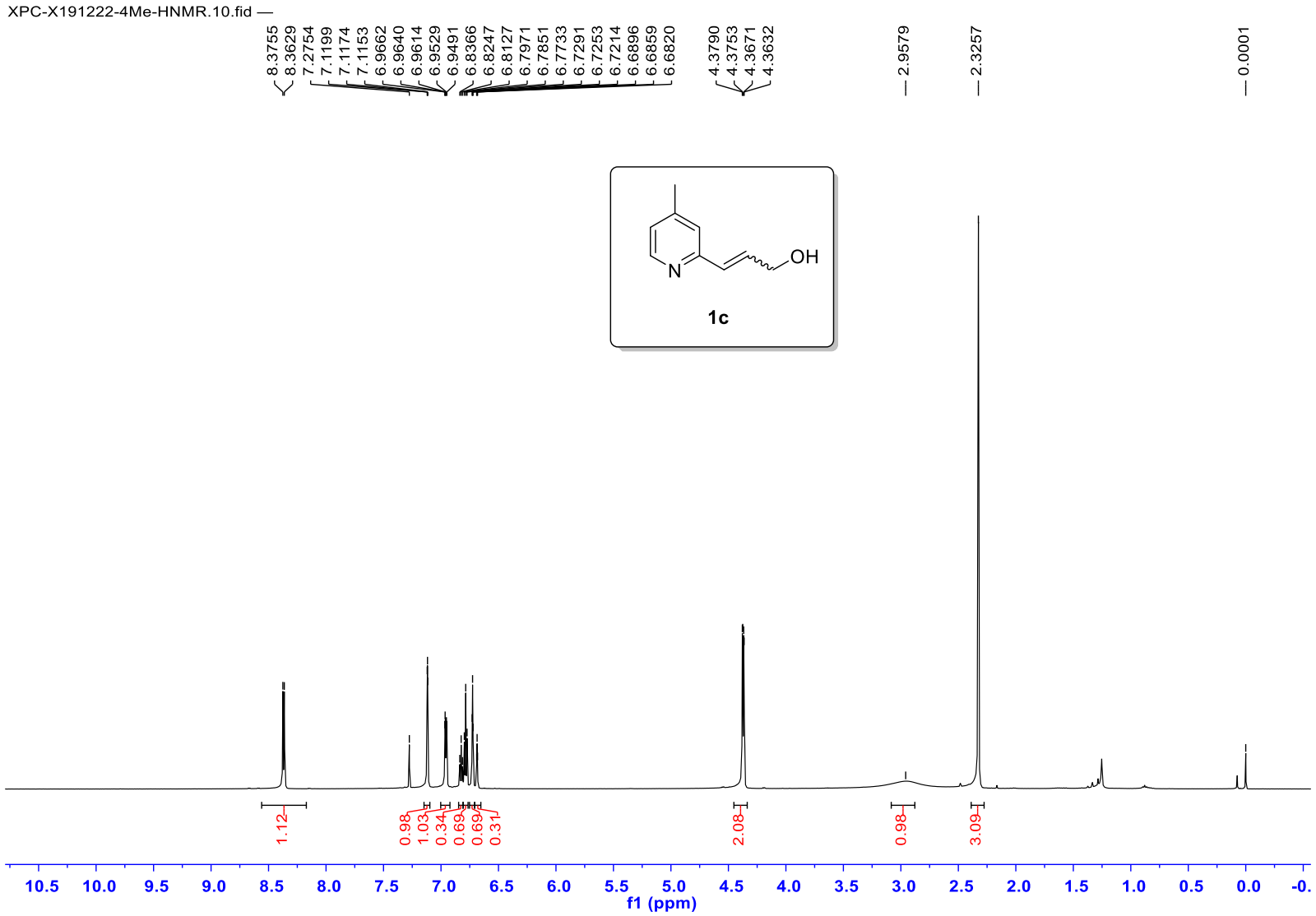
f1 (ppm)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0.69
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0.98
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9.0
8.5
8.0
7.5
7.0
6.5
6.0
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5.0
4.5
4.0
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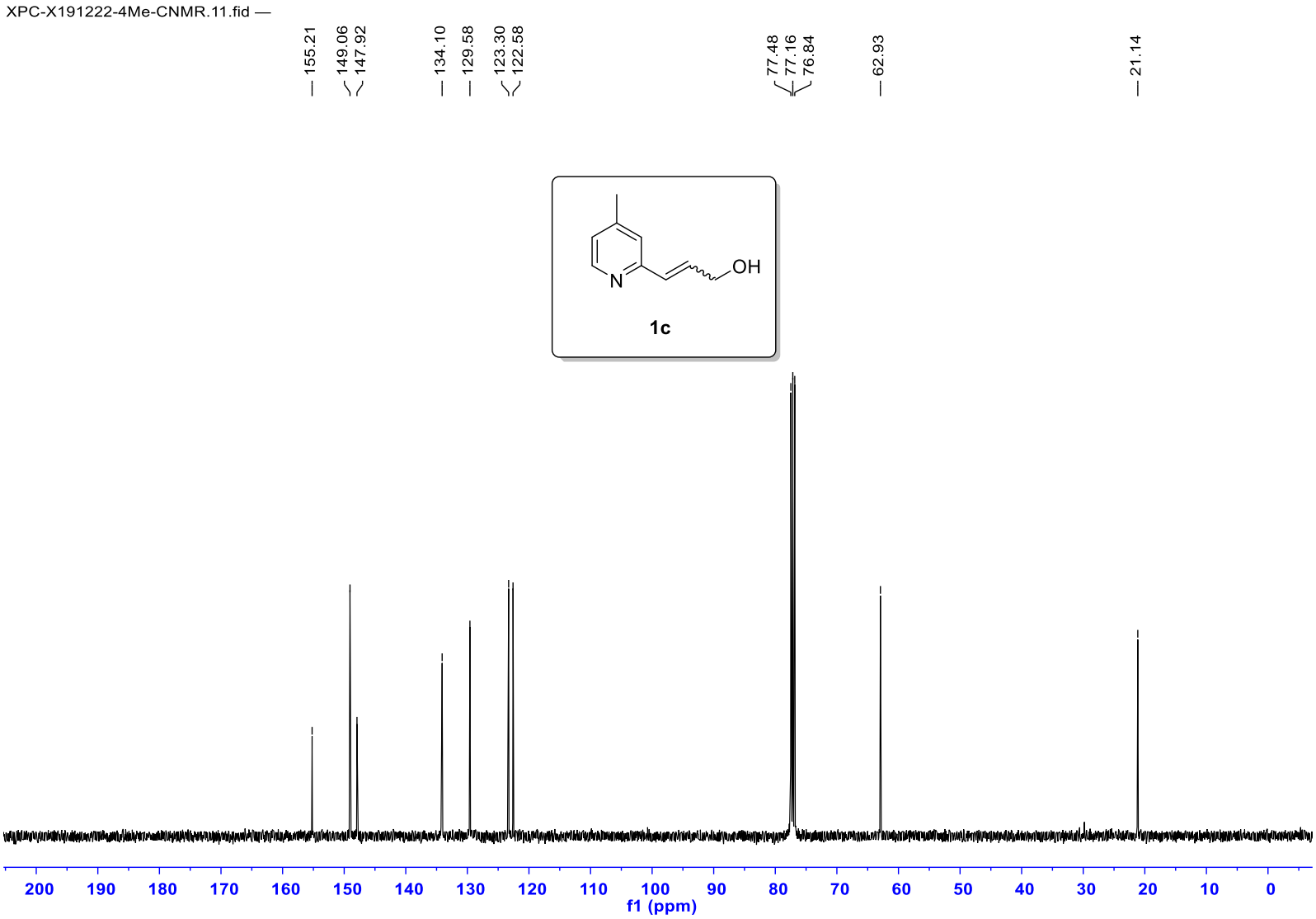
-0.
f1 (ppm)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200
190
180
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120
110
100
90
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70
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50
40
30
20
10
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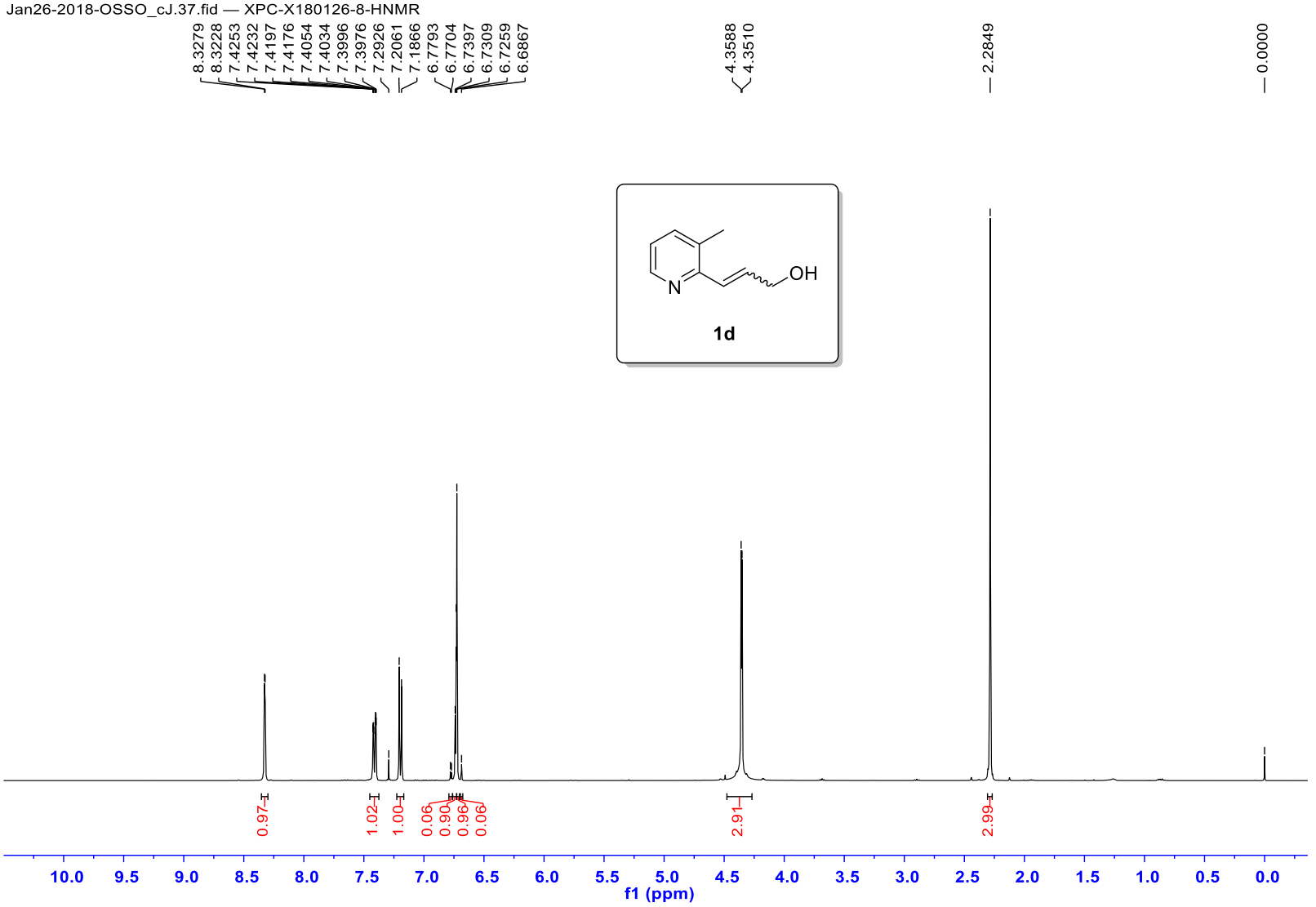
f1 (ppm)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4.3510
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N
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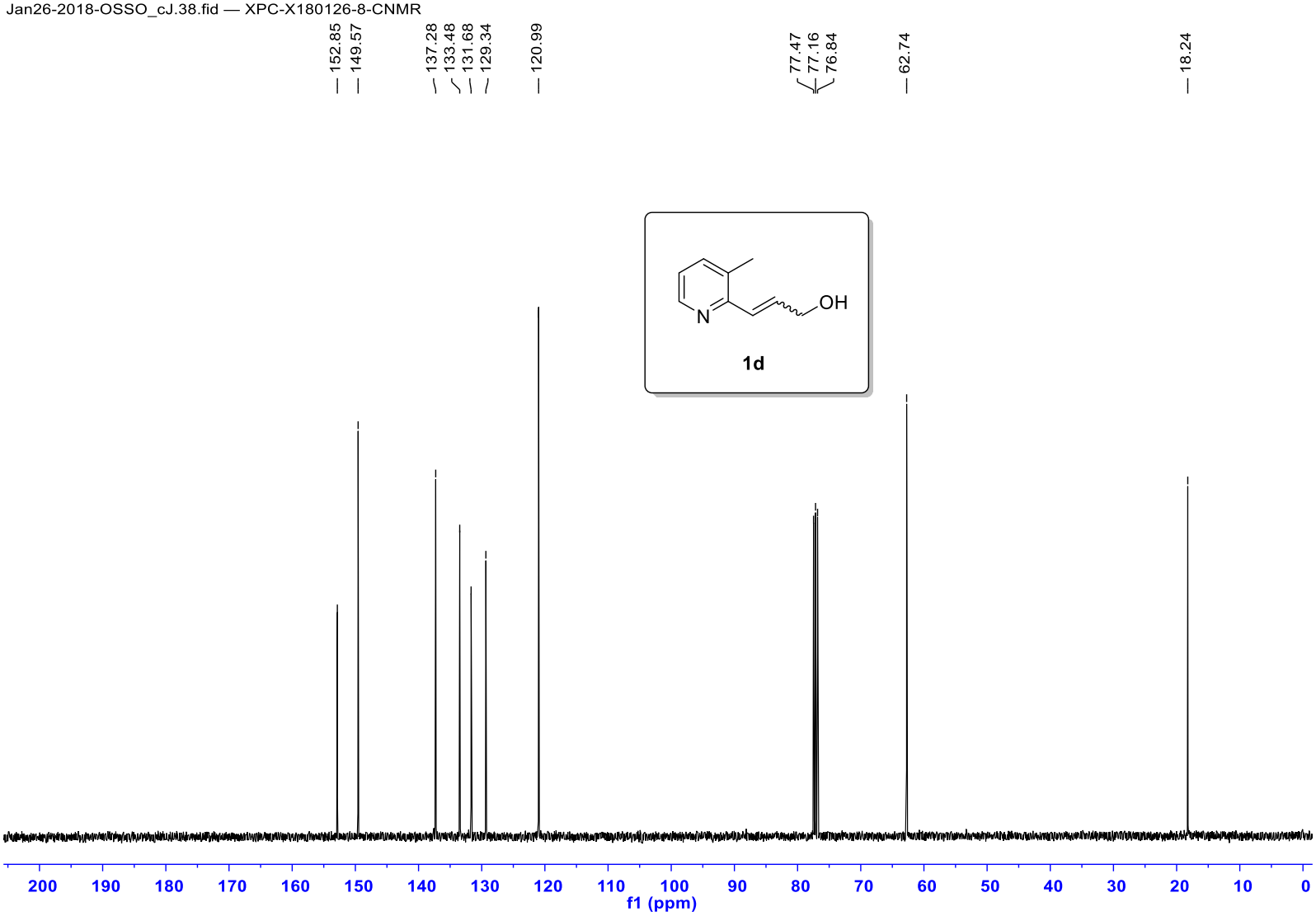
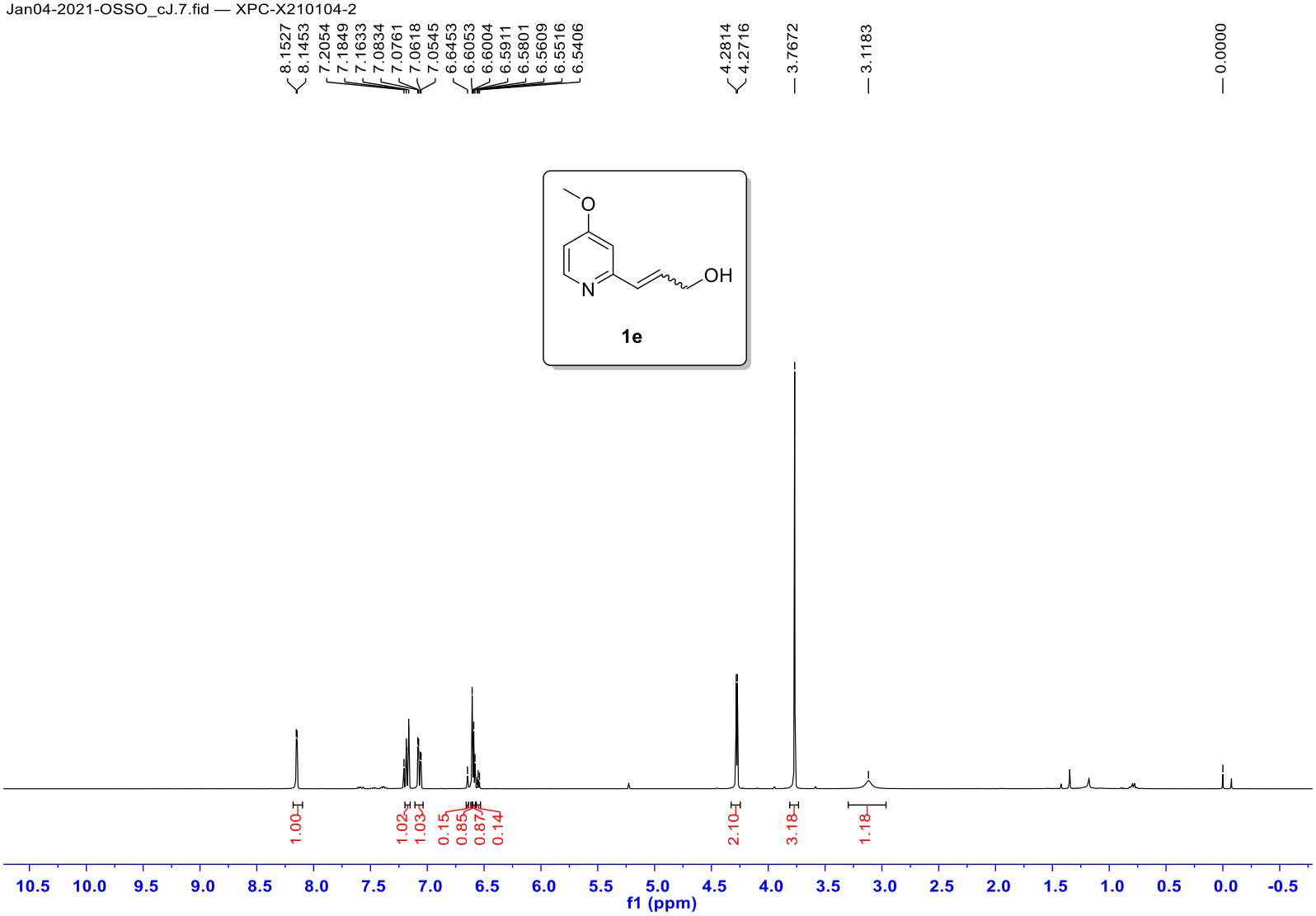
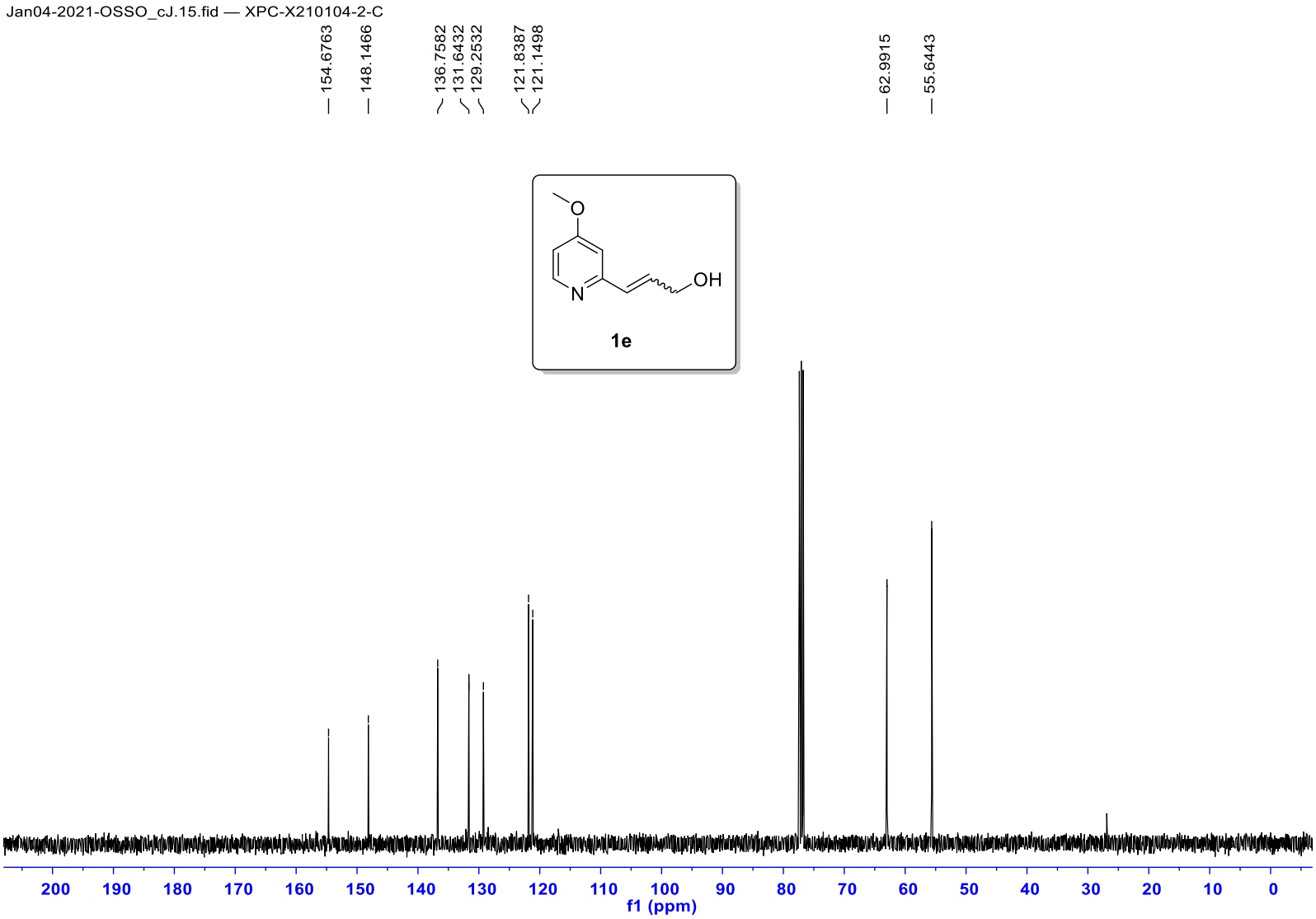
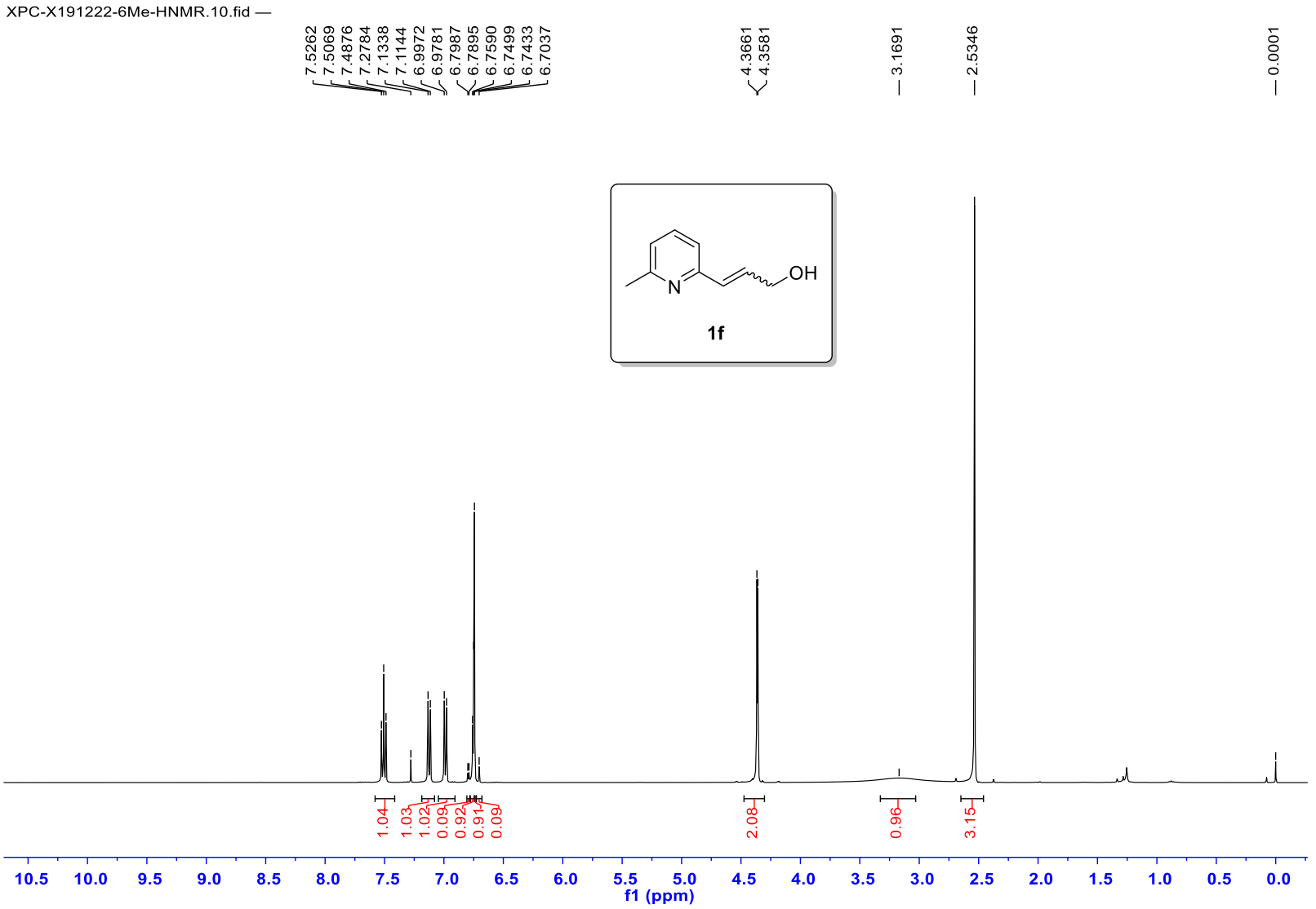
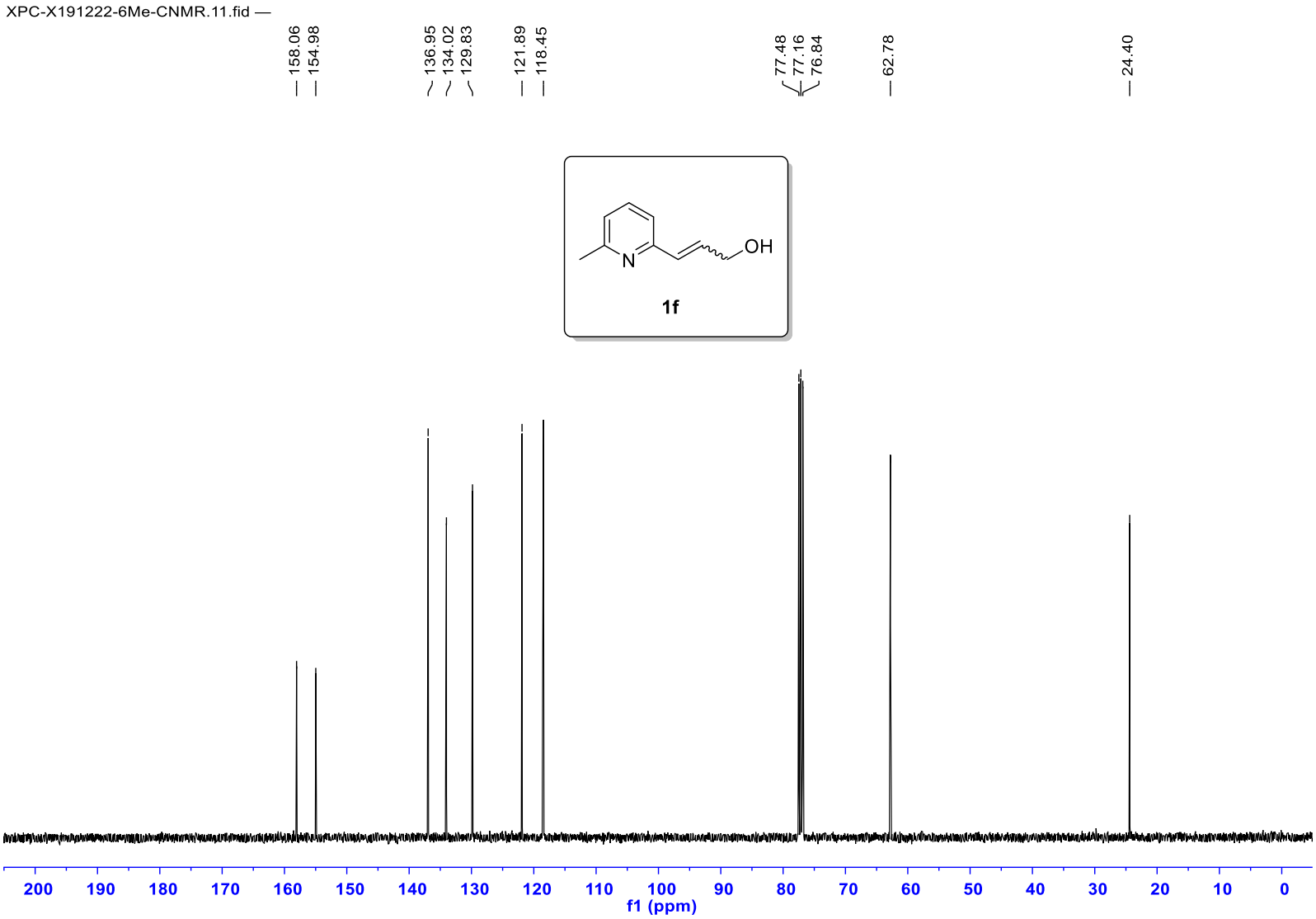
1.00
0.06
0.90
0.96
0.06
2.91
2.99
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

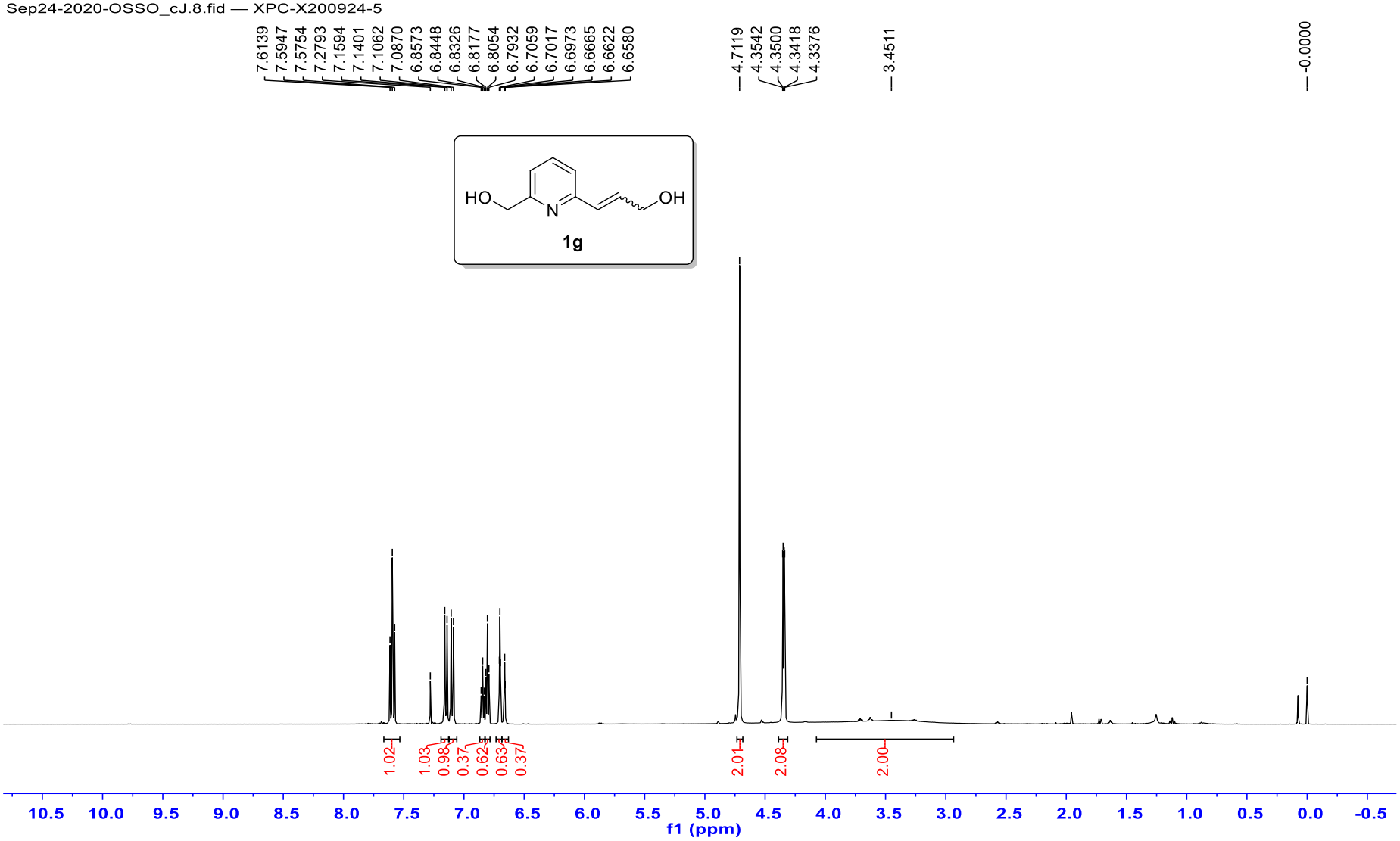

Jan26-2018-OSSO_cJ.38.fid — XPC-X180126-8-CNMR
152.85
149.57
137.28
133.48
131.68
129.34
120.99
77.47
77.16
76.84
62.74
18.24
N
OH
1d
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

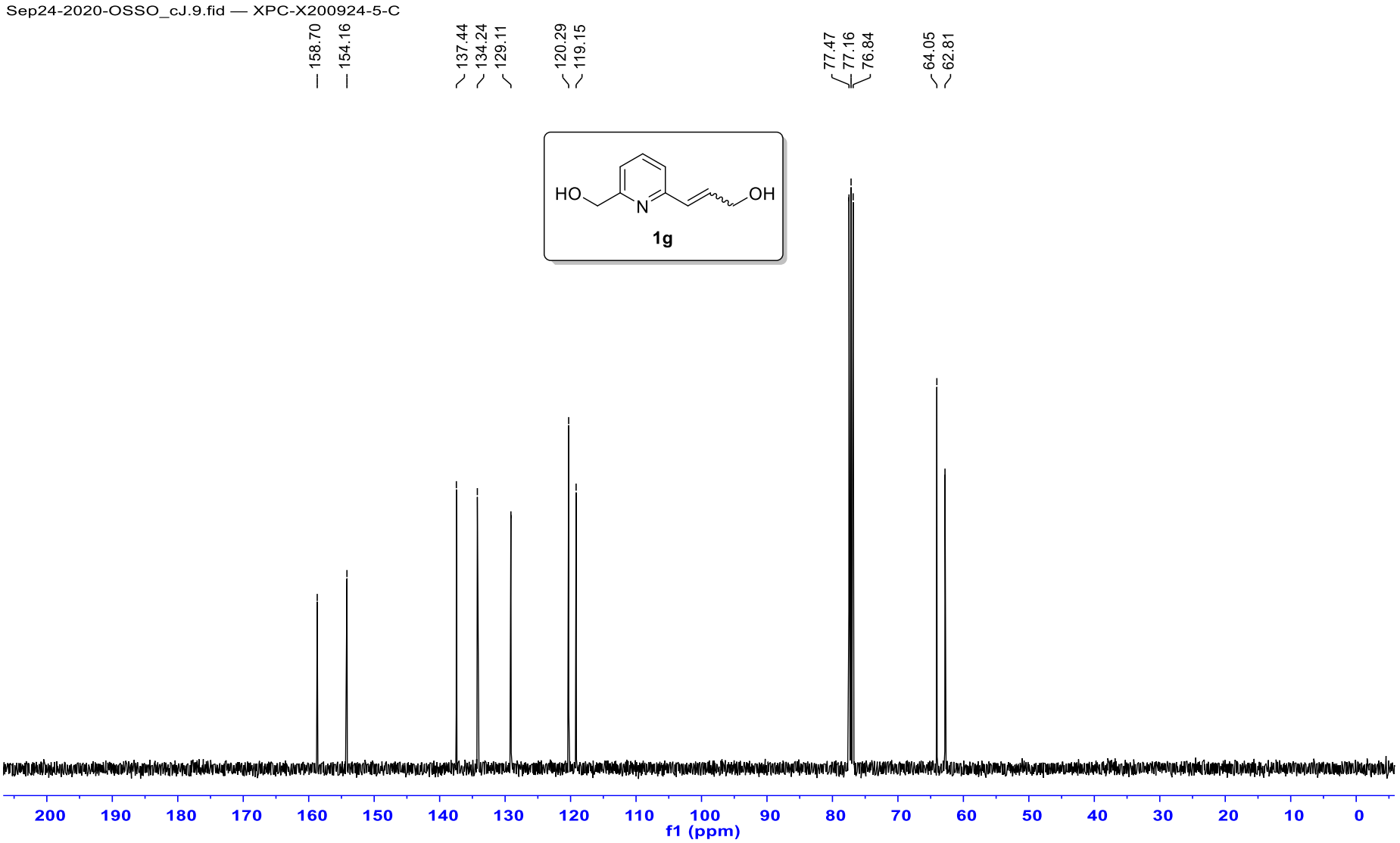

Jan04-2021-OSSO_cJ.7.fid — XPC-X210104-2
8.1527
8.1453
7.2054
7.1849
7.1633
7.0834
7.0761
7.0618
7.0545
6.6453
6.6053
6.6004
6.5911
6.5801
6.5609
6.5516
6.5406
4.2814
4.2716
3.7672
3.1183
0.0000
O
N
OH
1e
1.00
1.02
1.03
0.15
0.85
0.87
0.14
2.10
3.18
1.18
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

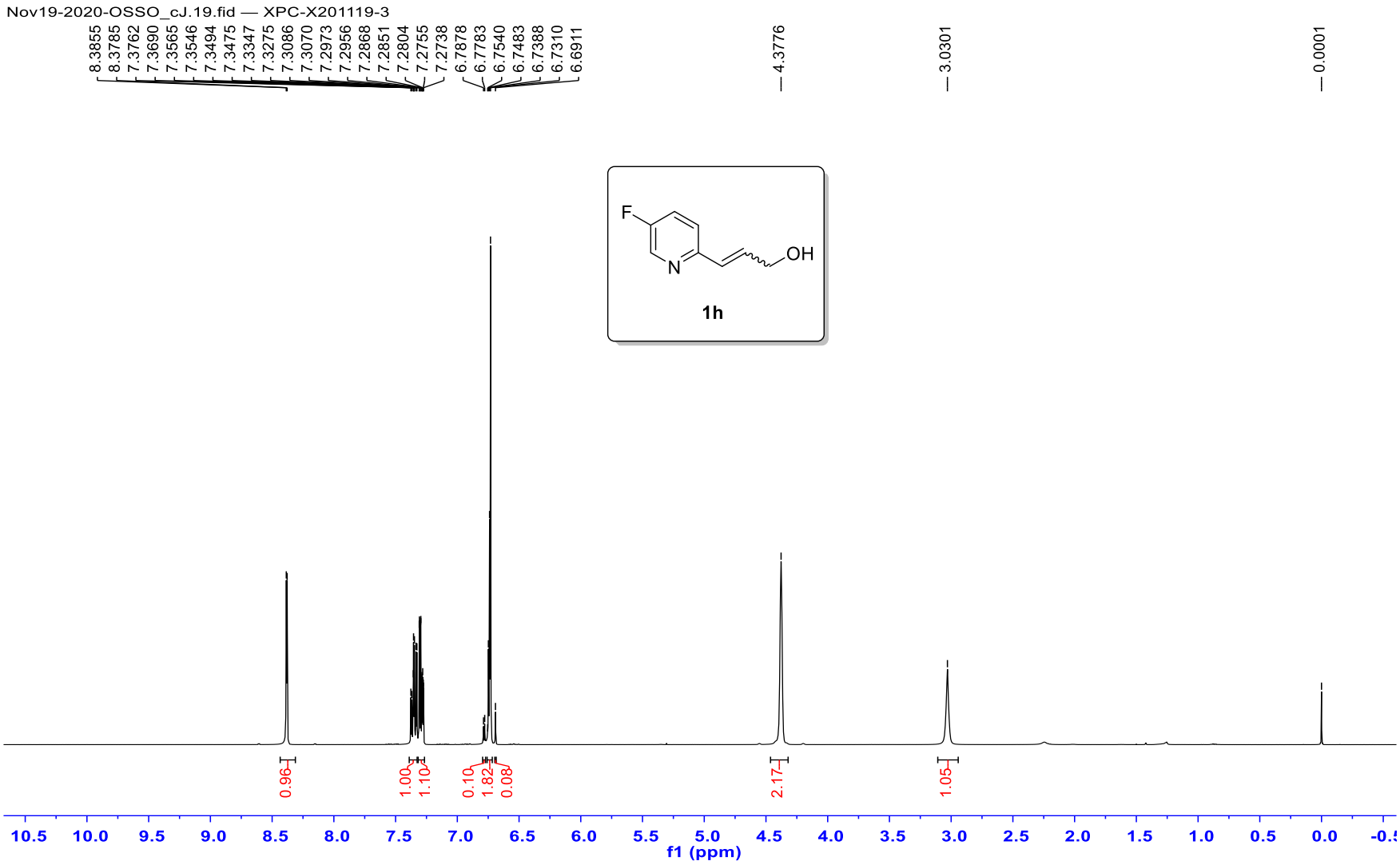

Jan04-2021-OSSO_cJ.15.fid — XPC-X210104-2-C
154.6763
148.1466
136.7582
131.6432
129.2532
121.8387
121.1498
62.9915
55.6443
O
N
OH
1e
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

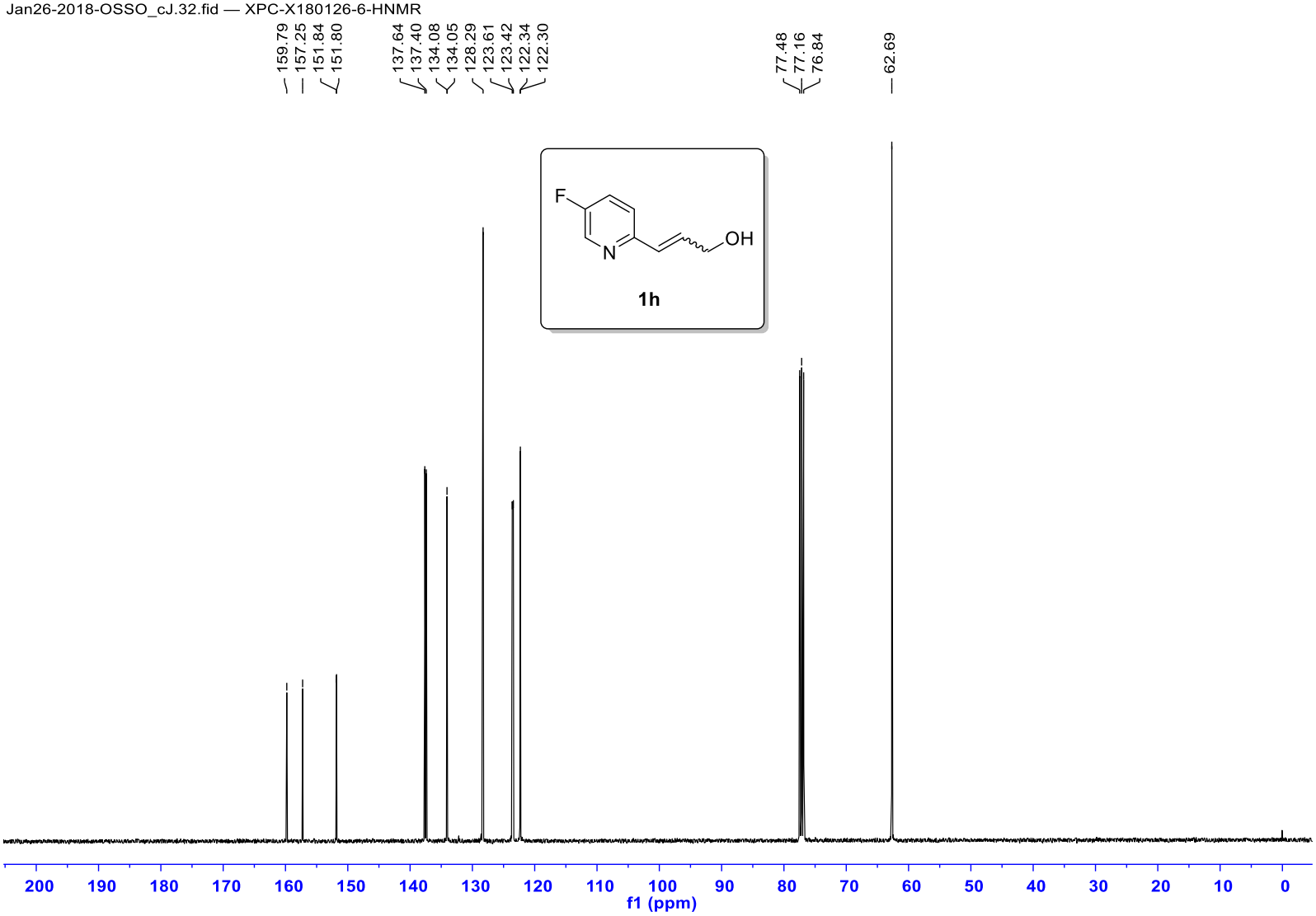

XPC-X191222-6Me-HNMR.10.fid
7.5262
7.5069
7.4876
7.2784
7.1338
7.1144
6.9972
6.9781
6.7987
6.7895
6.7590
6.7499
6.7433
6.7037
4.3661
4.3581
3.1691
2.5346
0.0001
OH
N
1f
1.04
1.03
1.02
0.09
0.92
0.91
0.09
2.08
0.96
3.15
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


XPC-X191222-6Me-CNMR.11.fid
158.06
154.98
136.95
134.02
129.83
121.89
118.45
77.48
77.16
76.84
62.78
24.40
OH
N
1f
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


Sep24-2020-OSSO_cJ.8.fid — XPC-X200924-5
7.6139
7.5947
7.5754
7.2793
7.1594
7.1401
7.1062
7.0870
6.8573
6.8448
6.8326
6.8177
6.8054
6.7932
6.7059
6.7017
6.6973
6.6665
6.6622
6.6580
4.7119
4.3542
4.3500
4.3418
4.3376
3.4511
-0.0000
HO
N
OH
1g
1.02
1.03
0.98
0.37
0.62
0.63
0.37
2.01
2.08
2.00
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
-0.5
f1 (ppm)

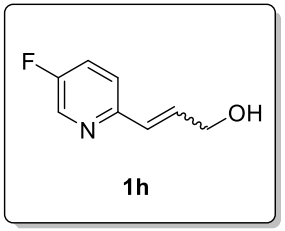

Sep24-2020-OSSO_cJ.9.fid — XPC-X200924-5-C
158.70
154.16
137.44
134.24
129.11
120.29
119.15
77.47
77.16
76.84
64.05
62.81
HO
N
OH
1g
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


Nov19-2020-OSSO_cJ.19.fid — XPC-X201119-3
8.3855
8.3785
7.3762
7.3690
7.3565
7.3546
7.3494
7.3475
7.3347
7.3275
7.3086
7.3070
7.2973
7.2956
7.2868
7.2851
7.2804
7.2755
7.2738
6.7878
6.7783
6.7540
6.7483
6.7388
6.7310
6.6911
4.3776
3.0301
0.0001
F
N
OH
1h
0.96
1.00
1.10
0.10
1.82
0.08
2.17
1.05
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)

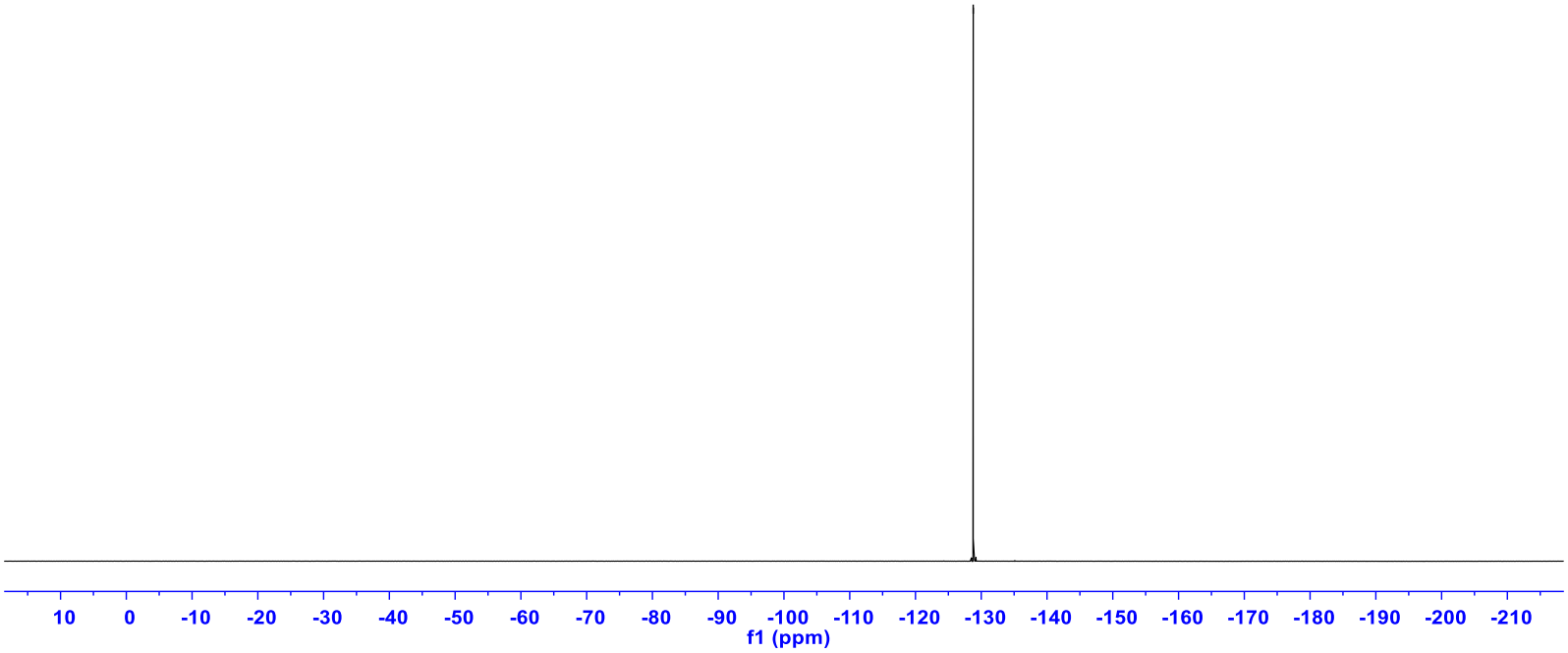

Jan26-2018-OSSO_cJ.32.fid — XPC-X180126-6-HNMR
159.79
157.25
151.84
151.80
137.64
137.40
134.08
134.05
128.29
123.61
123.42
122.34
122.30
77.48
77.16
76.84
62.69
F
N
OH
1h
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

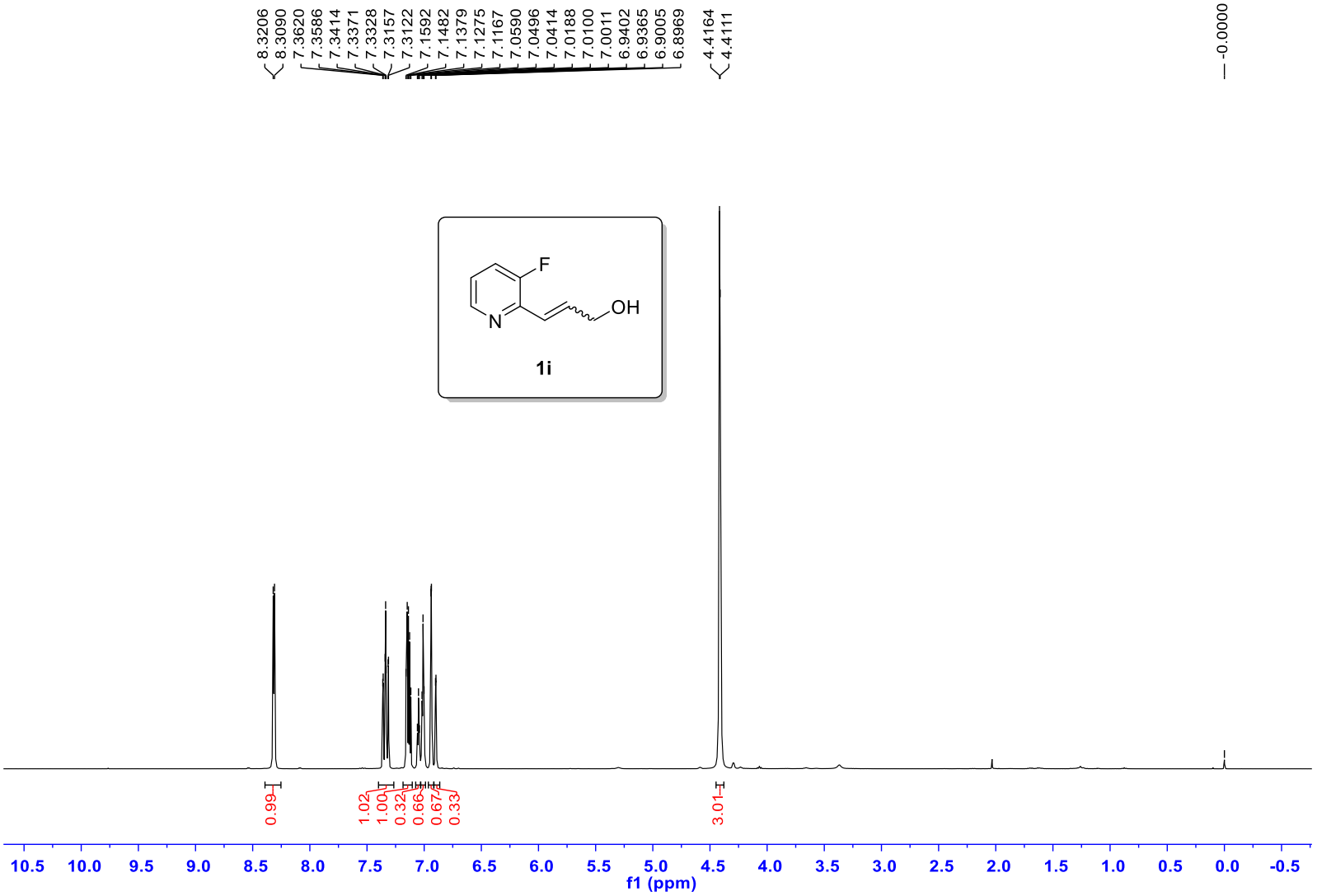
Jan26-2018-OSSO_cJ.34.fid — XPC-X180126-F-CNMR

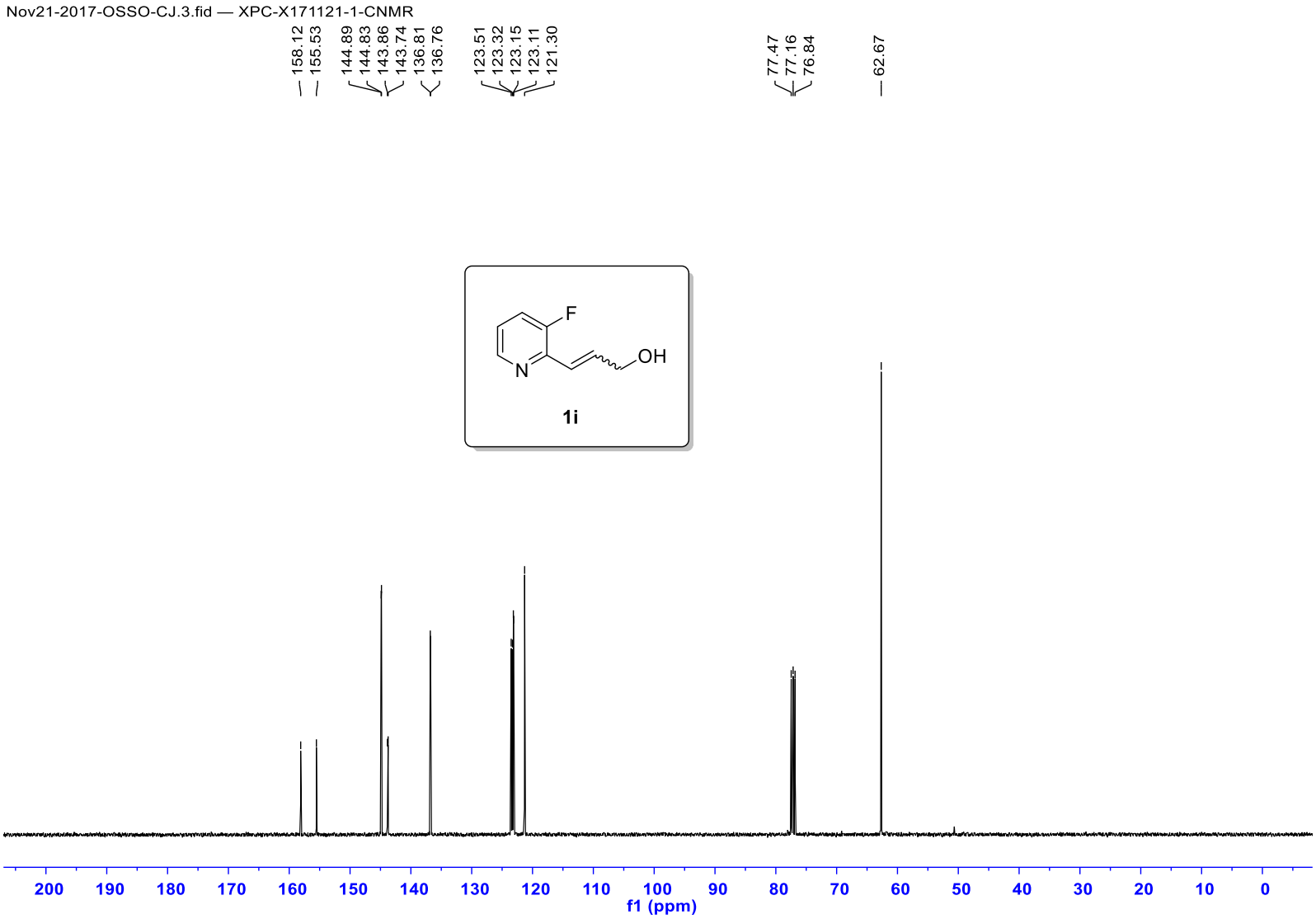
— -128.78



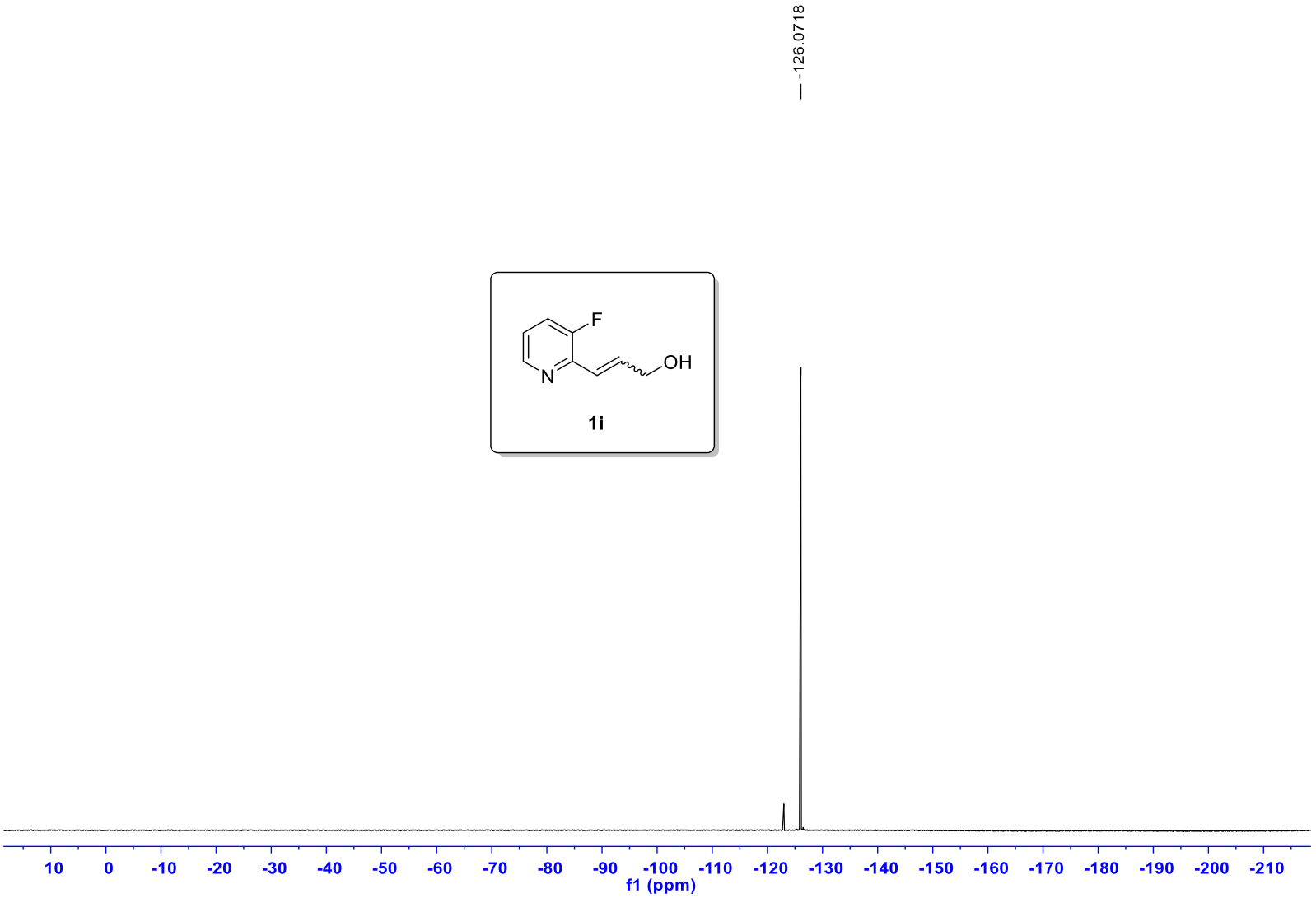
1h

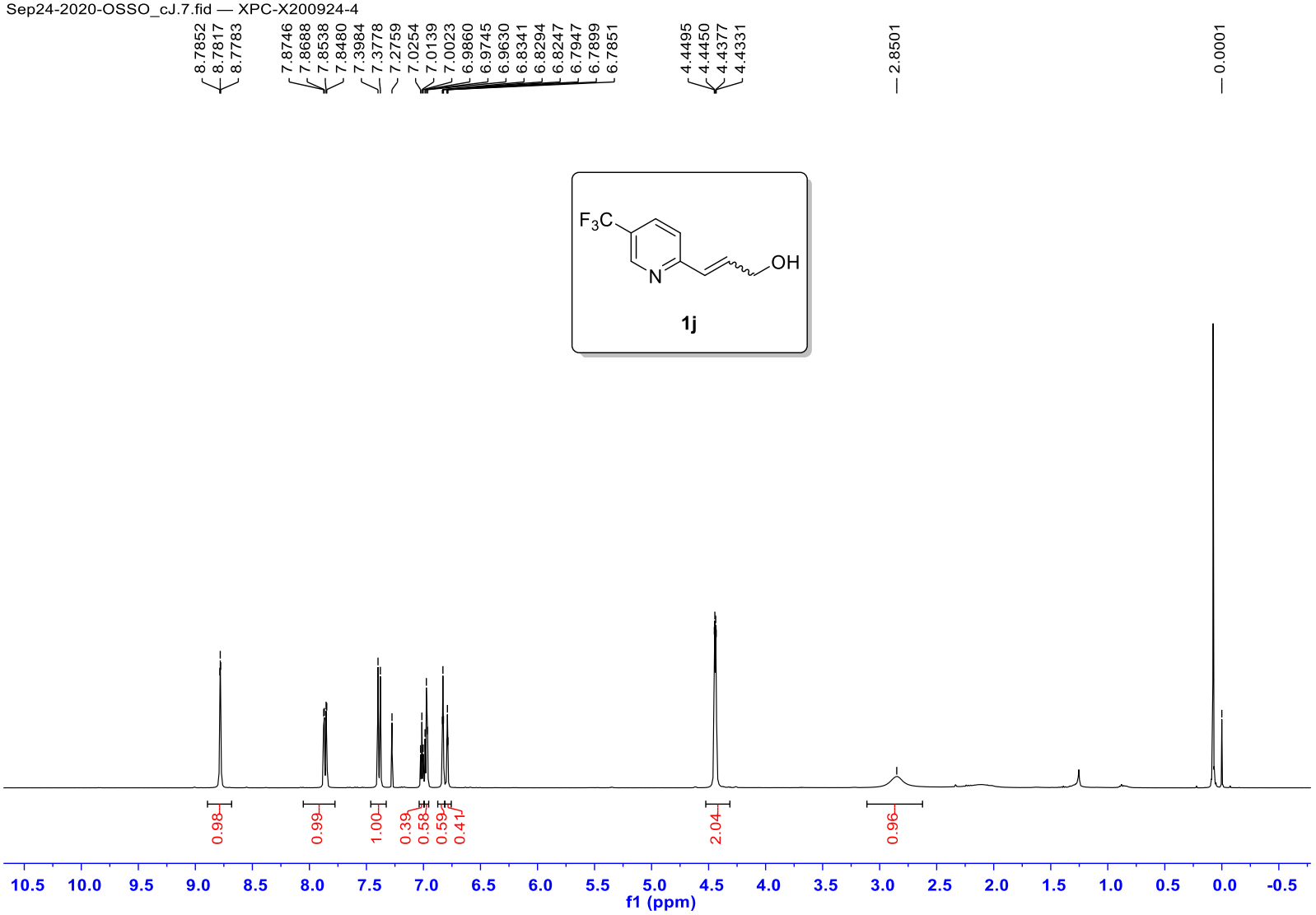


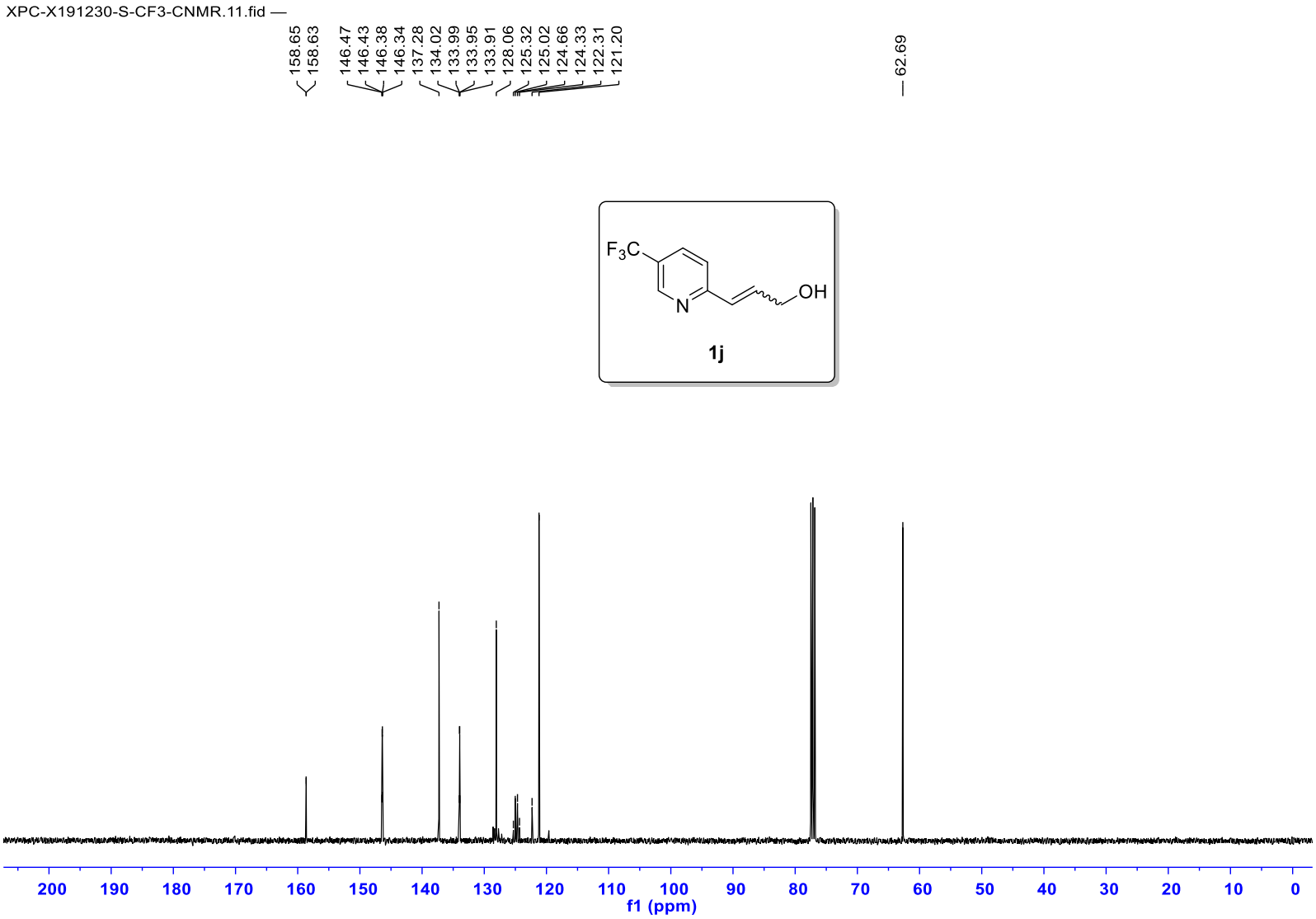

Nov21-2017-OSSO-CJ.2.fid — XPC-X171121-1-HNMR
8.3206
8.3090
7.3620
7.3586
7.3414
7.3371
7.3328
7.3157
7.3122
7.1592
7.1482
7.1379
7.1275
7.1167
7.0590
7.0496
7.0414
7.0188
7.0100
7.0011
6.9402
6.9365
6.9005
6.8969
4.4164
4.4111
-0.0000
F
N
OH
1i
0.99
1.02
1.00
0.32
0.66
0.67
0.33
3.01
10.5 10.0 9.5 9.0 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 -0.5
f1 (ppm)


Nov21-2017-OSSO-CJ.3.fid — XPC-X171121-1-CNMR
158.12
155.53
144.89
144.83
143.86
143.74
136.81
136.76
123.51
123.32
123.15
123.11
121.30
77.47
77.16
76.84
62.67
F
N
OH
1i
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

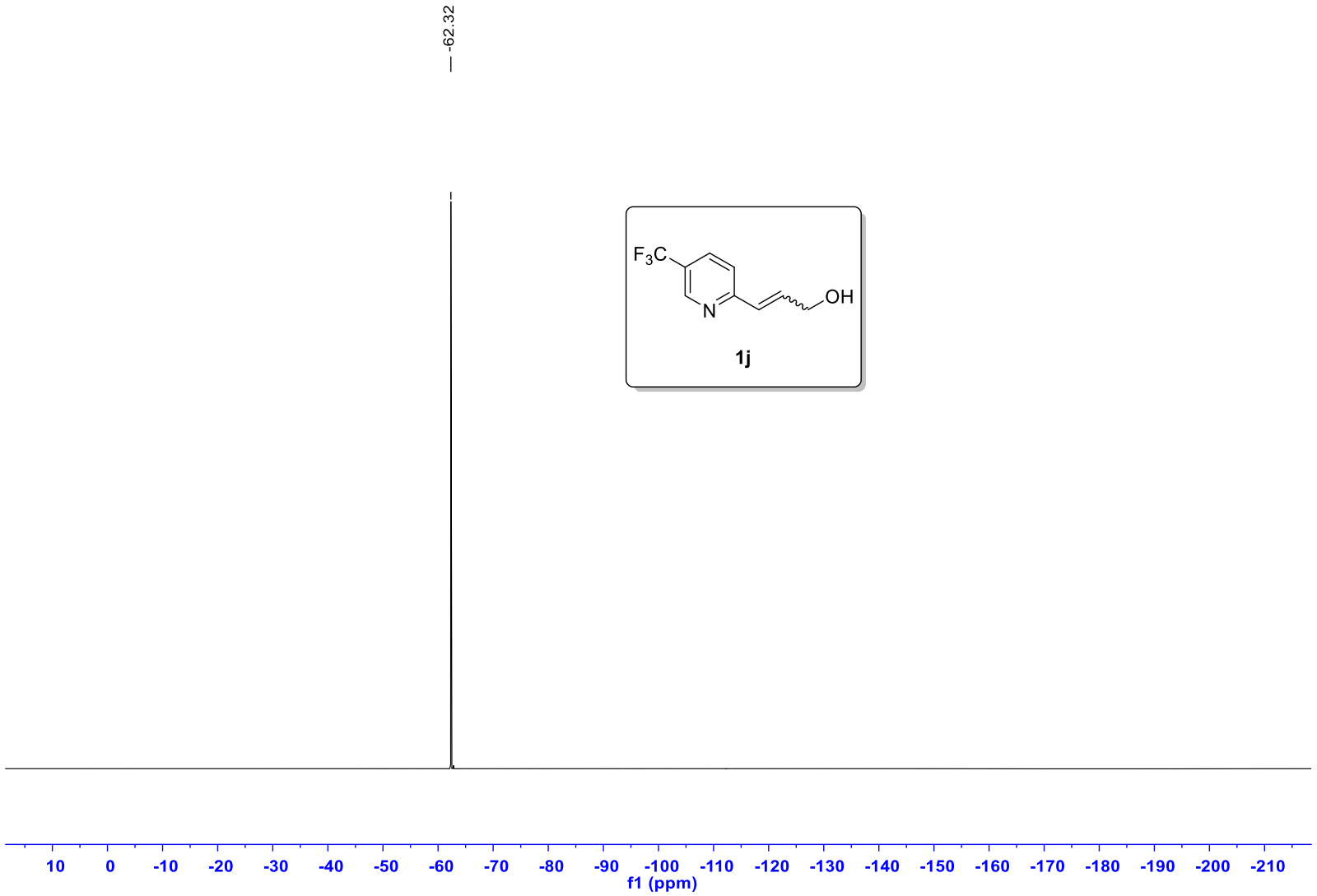
Nov17-2020-OSSO_cJ.15.fid — XPC-X201117-4

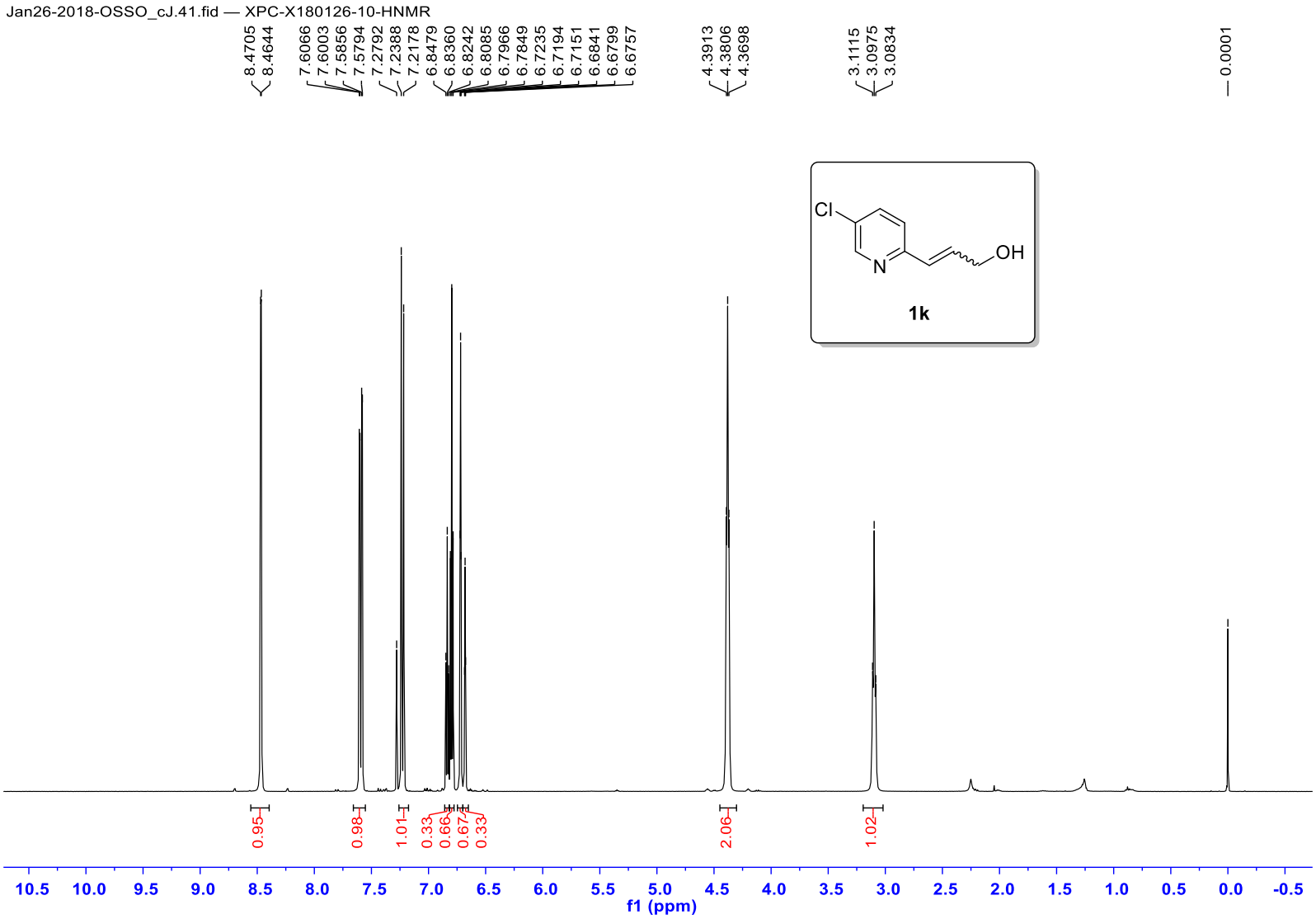


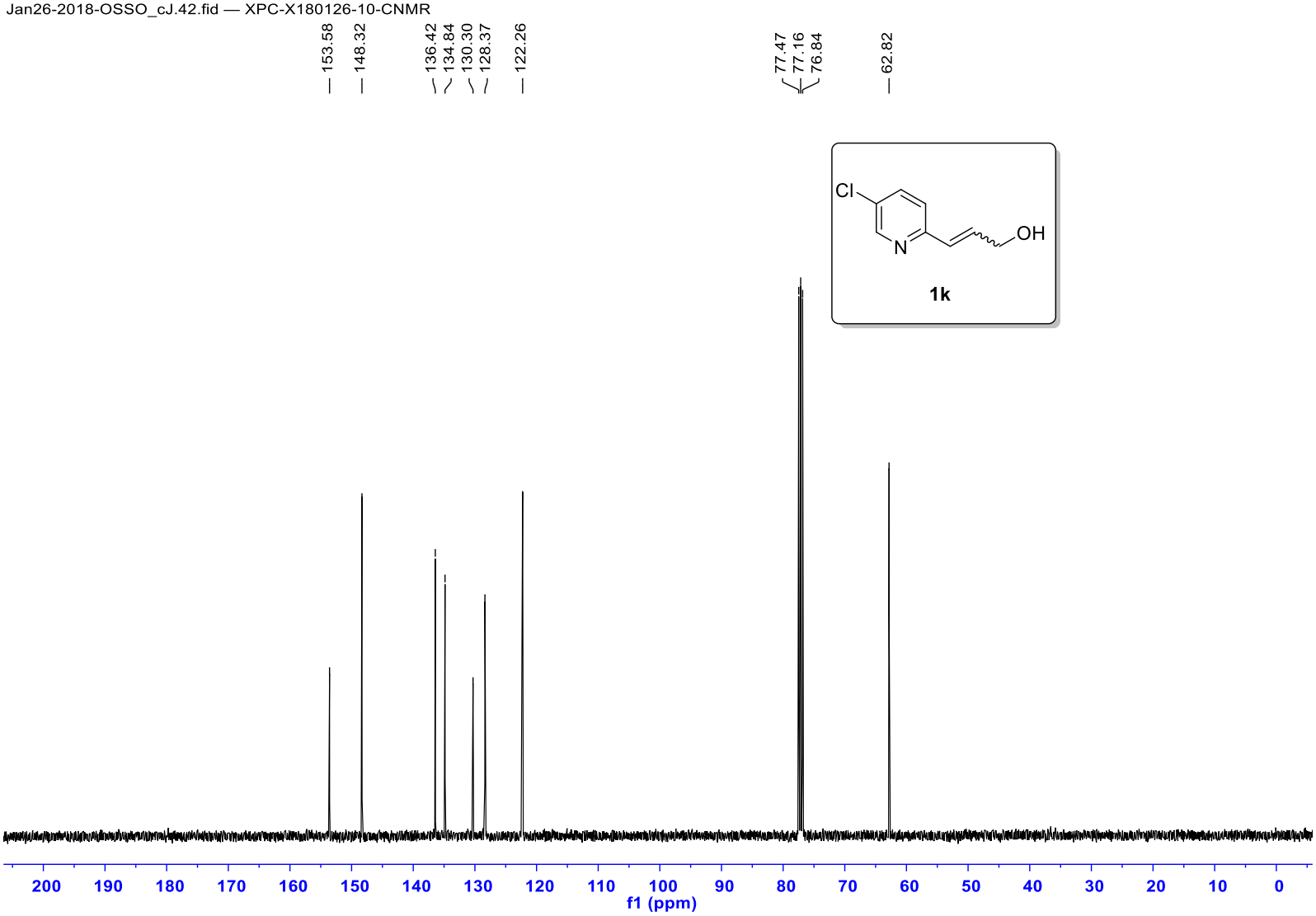

Sep24-2020-OSSO_cJ.7.fid — XPC-X200924-4
8.7852
8.7817
8.7783
7.8746
7.8688
7.8538
7.8480
7.3984
7.3778
7.2759
7.0254
7.0139
7.0023
6.9860
6.9745
6.9630
6.8341
6.8294
6.8247
6.7947
6.7899
6.7851
4.4495
4.4450
4.4377
4.4331
2.8501
0.0001
F3C
N
OH
1j
0.98
0.99
1.00
0.39
0.58
0.59
0.41
2.04
0.96
10.5 10.0 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 -0.5
f1 (ppm)

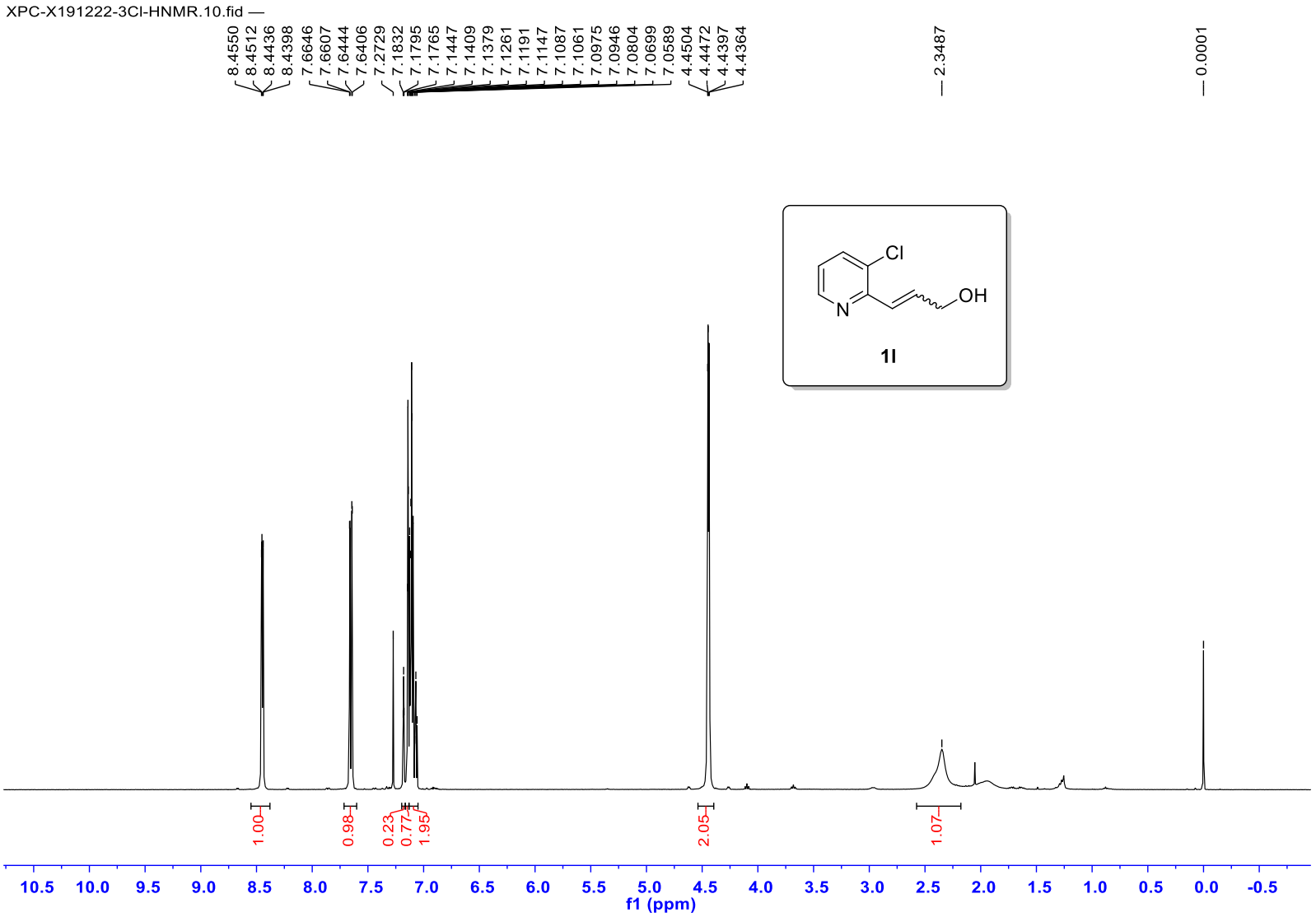

XPC-X191230-S-CF3-CNMR.11.fid
158.65
158.63
146.47
146.43
146.38
146.34
137.28
134.02
133.99
133.95
133.91
128.06
125.32
125.02
124.66
124.33
122.31
121.20
62.69
F3C
N
OH
1j
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

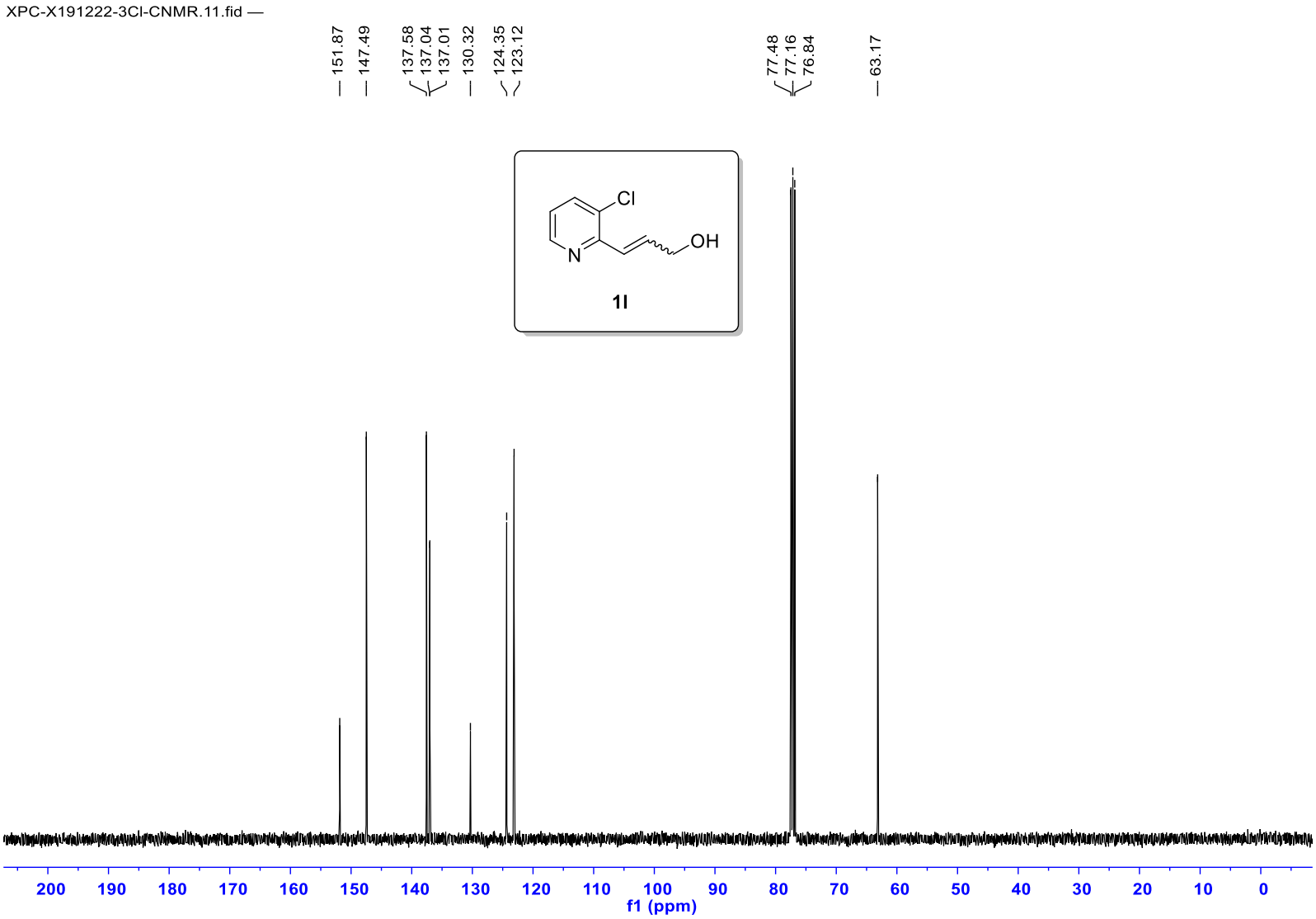
XPC-X191230-S-CF3-FNMR.12.fid —

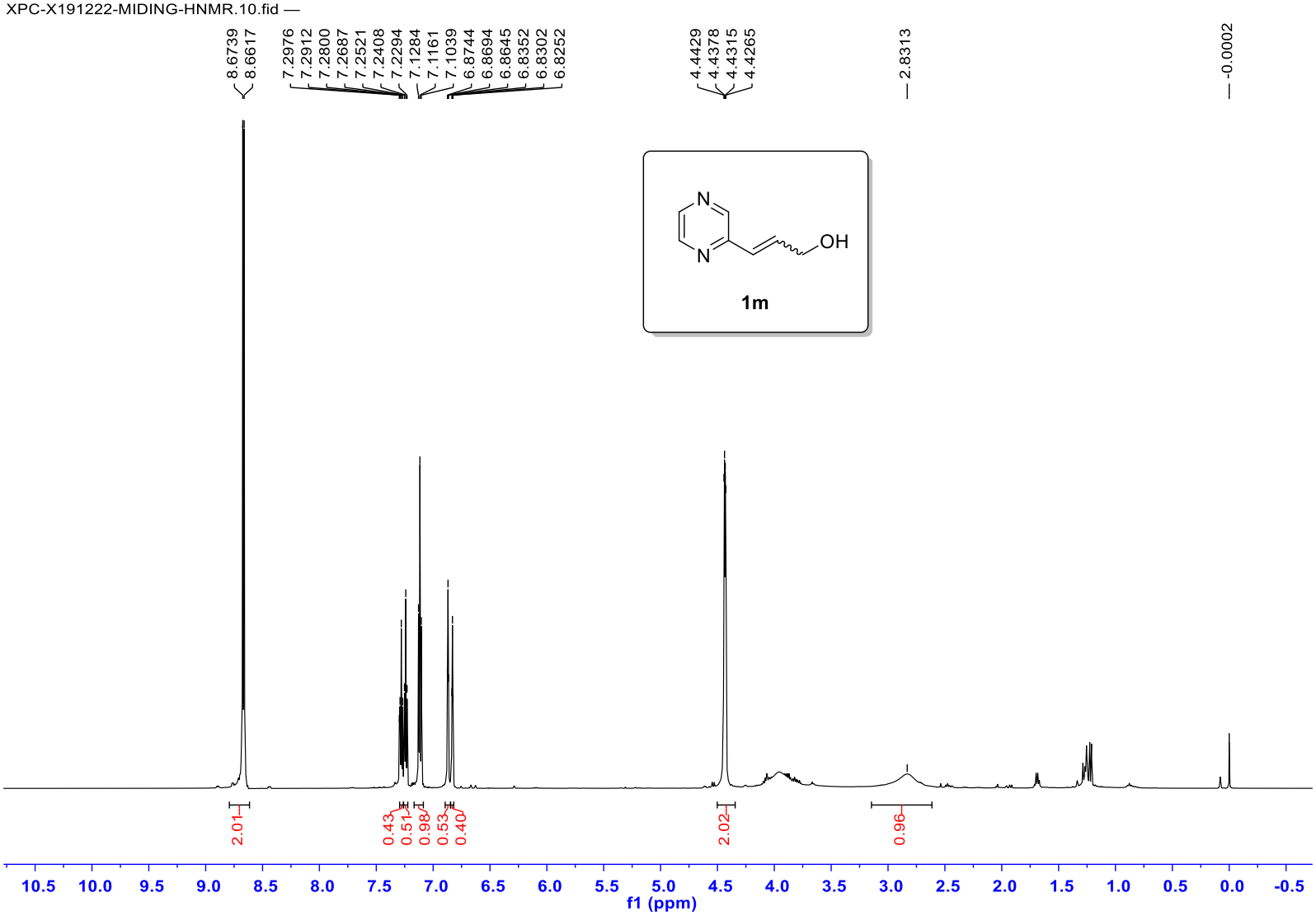


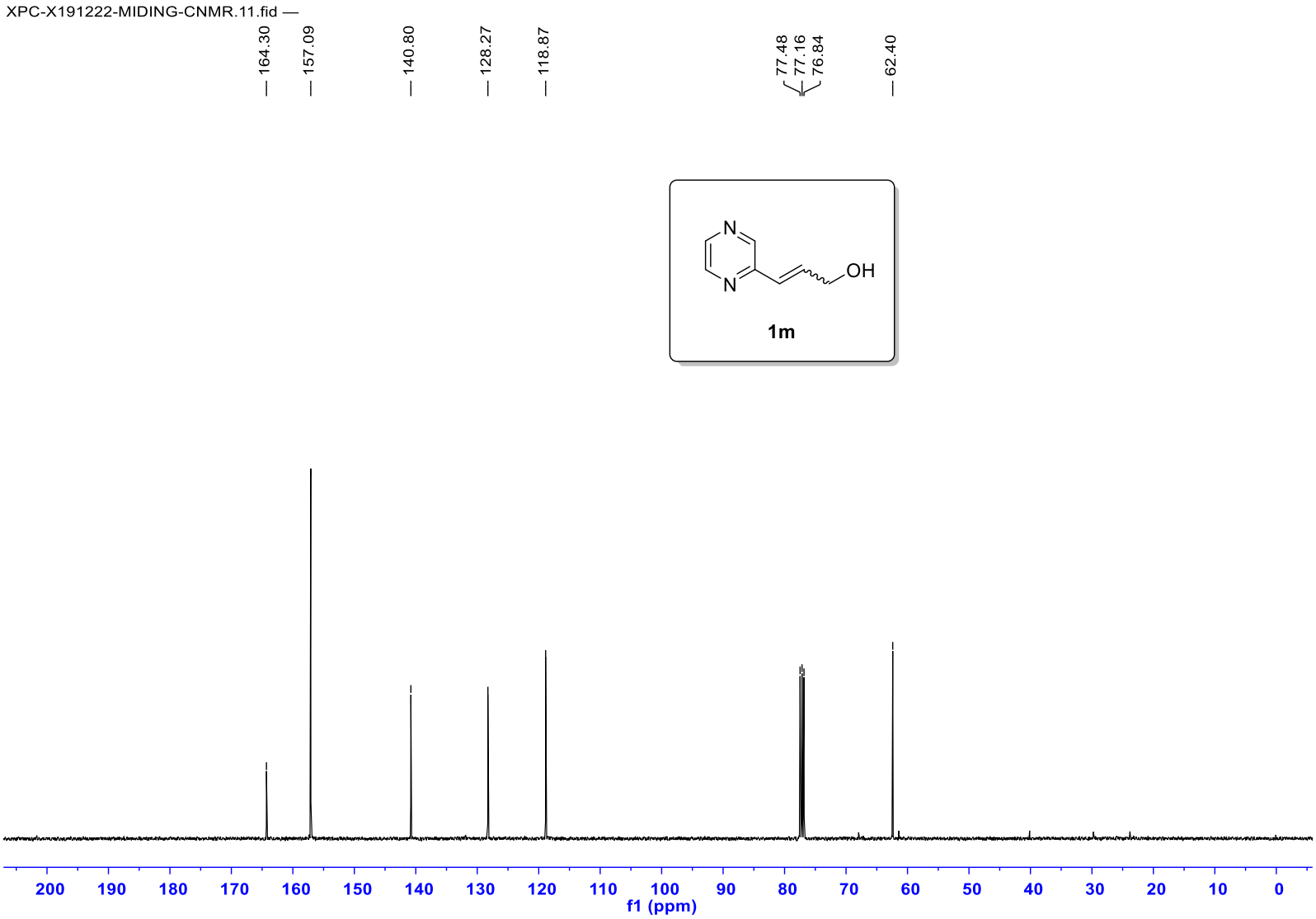

Jan26-2018-OSSO_cJ.41.fid — XPC-X180126-10-HNMR
8.4705
8.4644
7.6066
7.6003
7.5856
7.5794
7.2792
7.2388
7.2178
6.8479
6.8360
6.8242
6.8085
6.7966
6.7849
6.7235
6.7194
6.7151
6.6841
6.6799
6.6757
4.3913
4.3806
4.3698
3.1115
3.0975
3.0834
0.0001
Cl
N
OH
1k
0.95
0.98
1.01
0.33
0.66
0.67
0.33
2.06
1.02
10.5 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 -0.5
f1 (ppm)

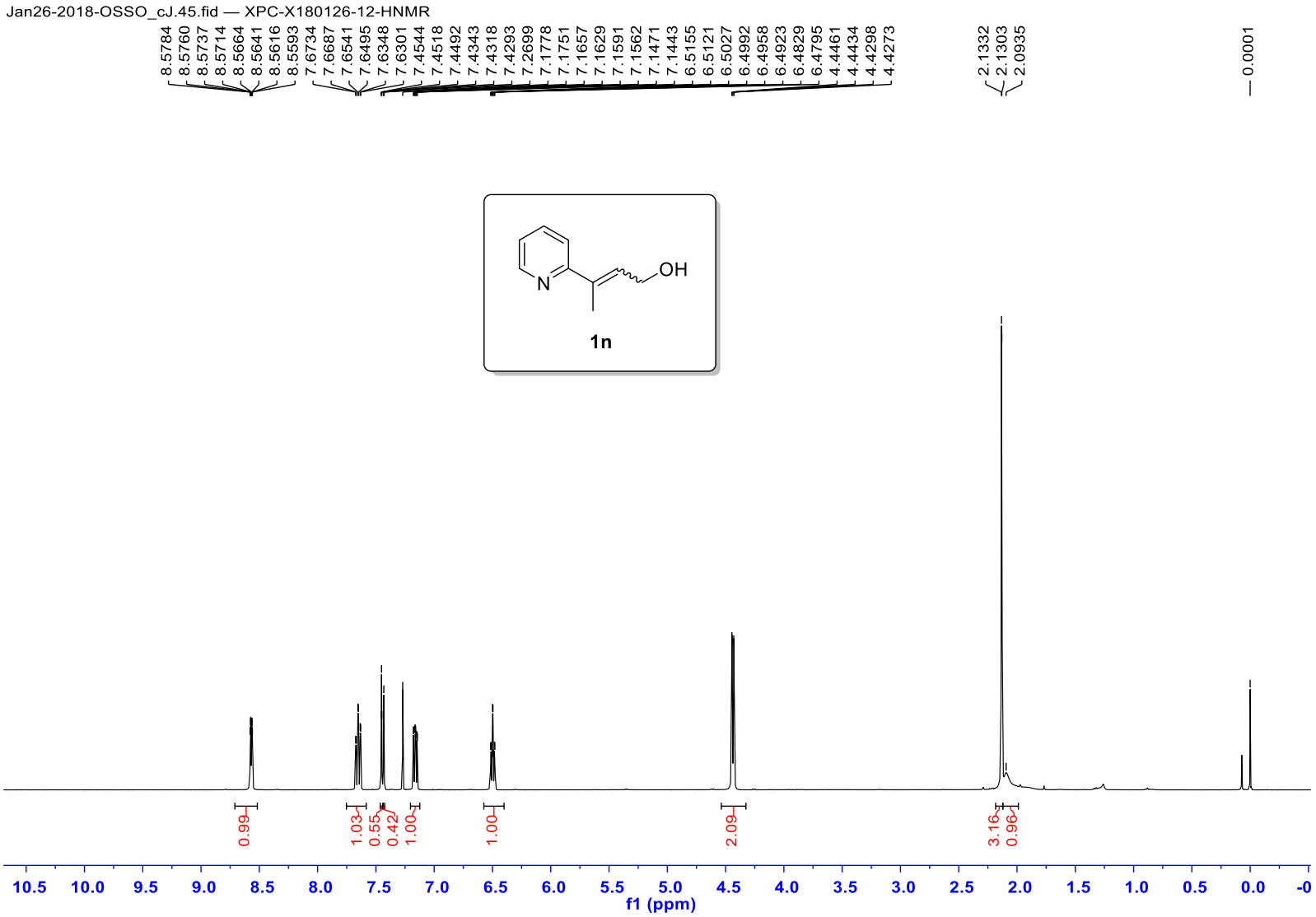

Jan26-2018-OSSO_cJ.42.fid — XPC-X180126-10-CNMR
153.58
148.32
136.42
134.84
130.30
128.37
122.26
77.47
77.16
76.84
62.82
Cl
N
OH
1k
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


XPC-X191222-3Cl-HNMR.10.fid
8.4550
8.4512
8.4436
8.4398
7.6646
7.6607
7.6444
7.6406
7.2729
7.1832
7.1795
7.1765
7.1447
7.1409
7.1379
7.1261
7.1191
7.1147
7.1087
7.1061
7.0975
7.0946
7.0804
7.0699
7.0589
4.4504
4.4472
4.4397
4.4364
2.3487
0.0001
Cl
N
OH
1l
1.00
0.98
0.23
0.77
1.95
2.05
1.07
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 -0.5
f1 (ppm)


XPC-X191222-3Cl-CNMR.11.fid
151.87
147.49
137.58
137.04
137.01
130.32
124.35
123.12
77.48
77.16
76.84
63.17
Cl
OH
N
1l
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


XPC-X191222-MIDING-HNMR.10.fid
8.6739
8.6617
7.2976
7.2912
7.2800
7.2687
7.2521
7.2408
7.2294
7.1284
7.1161
7.1039
6.8744
6.8694
6.8645
6.8352
6.8302
6.8252
4.4429
4.4378
4.4315
4.4265
2.8313
-0.0002
N
N
OH
1m
2.01
0.43
0.51
0.98
0.53
0.40
2.02
0.96
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 -0.5
f1 (ppm)


XPC-X191222-MIDING-CNMR.11.fid
164.30
157.09
140.80
128.27
118.87
77.48
77.16
76.84
62.40
N
N
OH
1m
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


Jan26-2018-OSSO_cJ.45.fid — XPC-X180126-12-HNMR
8.5784
8.5760
8.5737
8.5714
8.5664
8.5641
8.5616
8.5593
7.6734
7.6687
7.6541
7.6495
7.6348
7.6301
7.4544
7.4518
7.4492
7.4343
7.4318
7.4293
7.2699
7.1778
7.1751
7.1657
7.1629
7.1591
7.1562
7.1471
7.1443
6.5155
6.5121
6.5027
6.4992
6.4958
6.4923
6.4829
6.4795
4.4461
4.4434
4.4298
4.4273
2.1332
2.1303
2.0935
0.0001
N
OH
1n
0.99
1.03
0.55
0.42
1.00
1.00
2.09
3.16
0.96
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
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3.0
2.5
2.0
1.5
1.0
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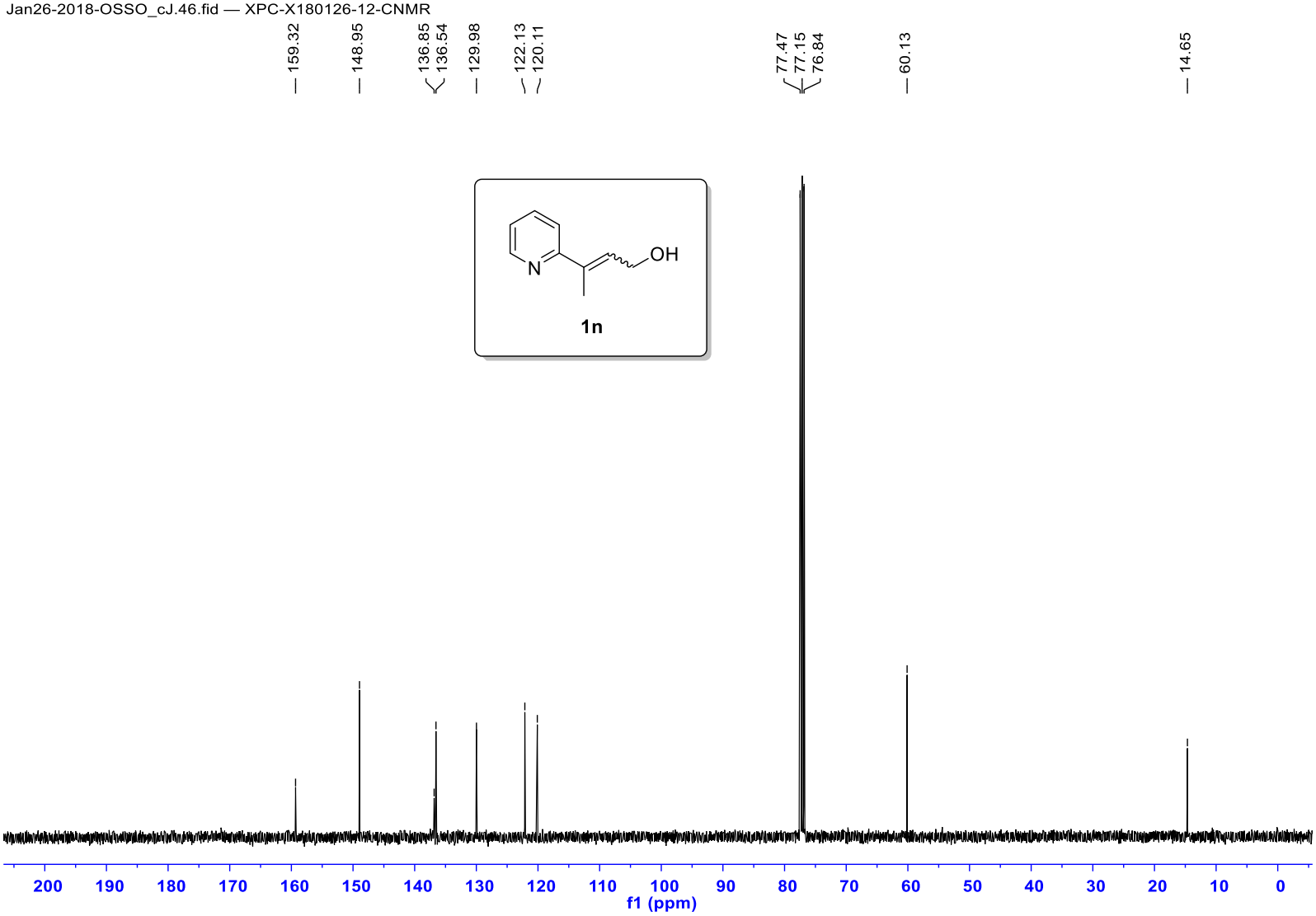
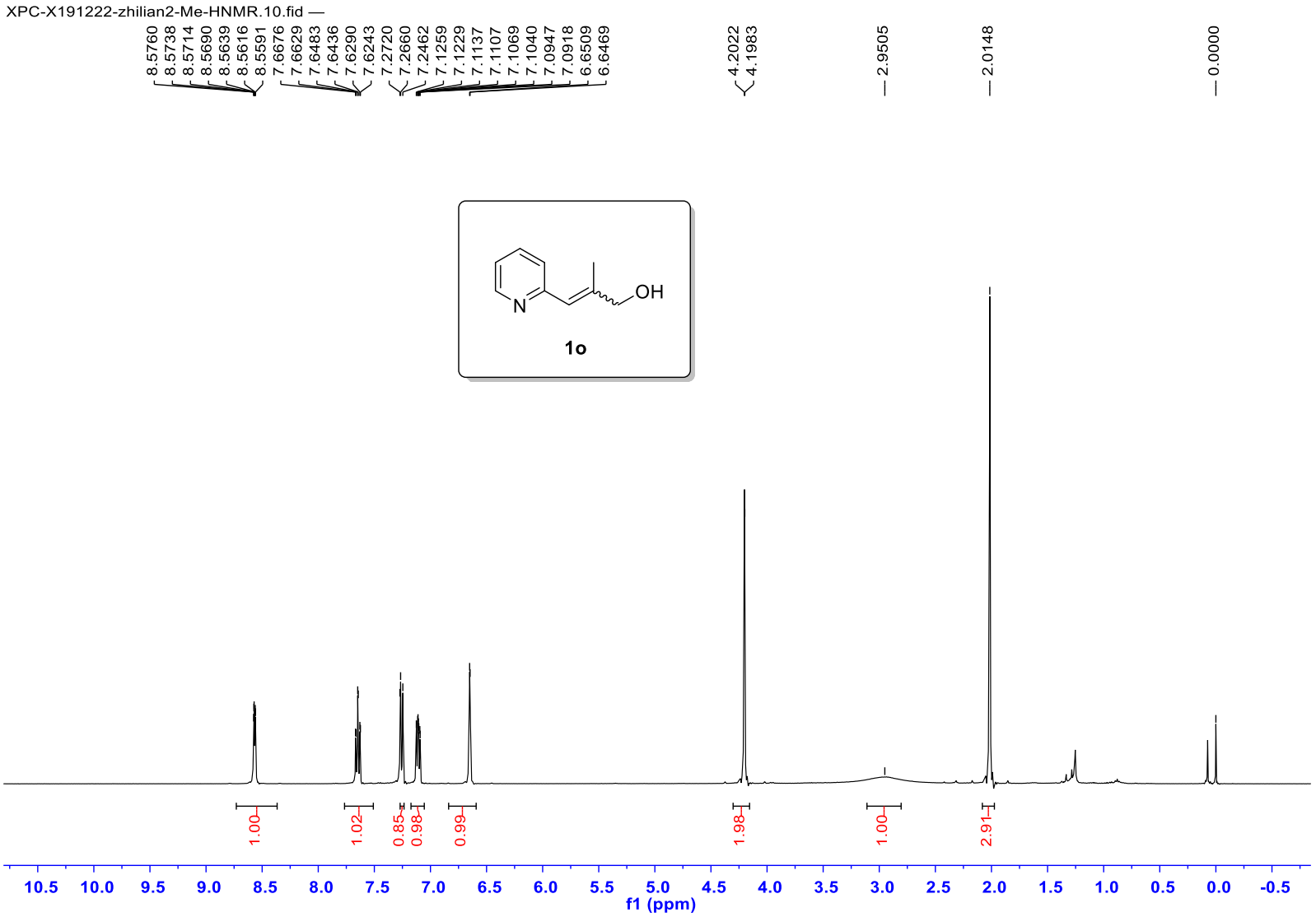
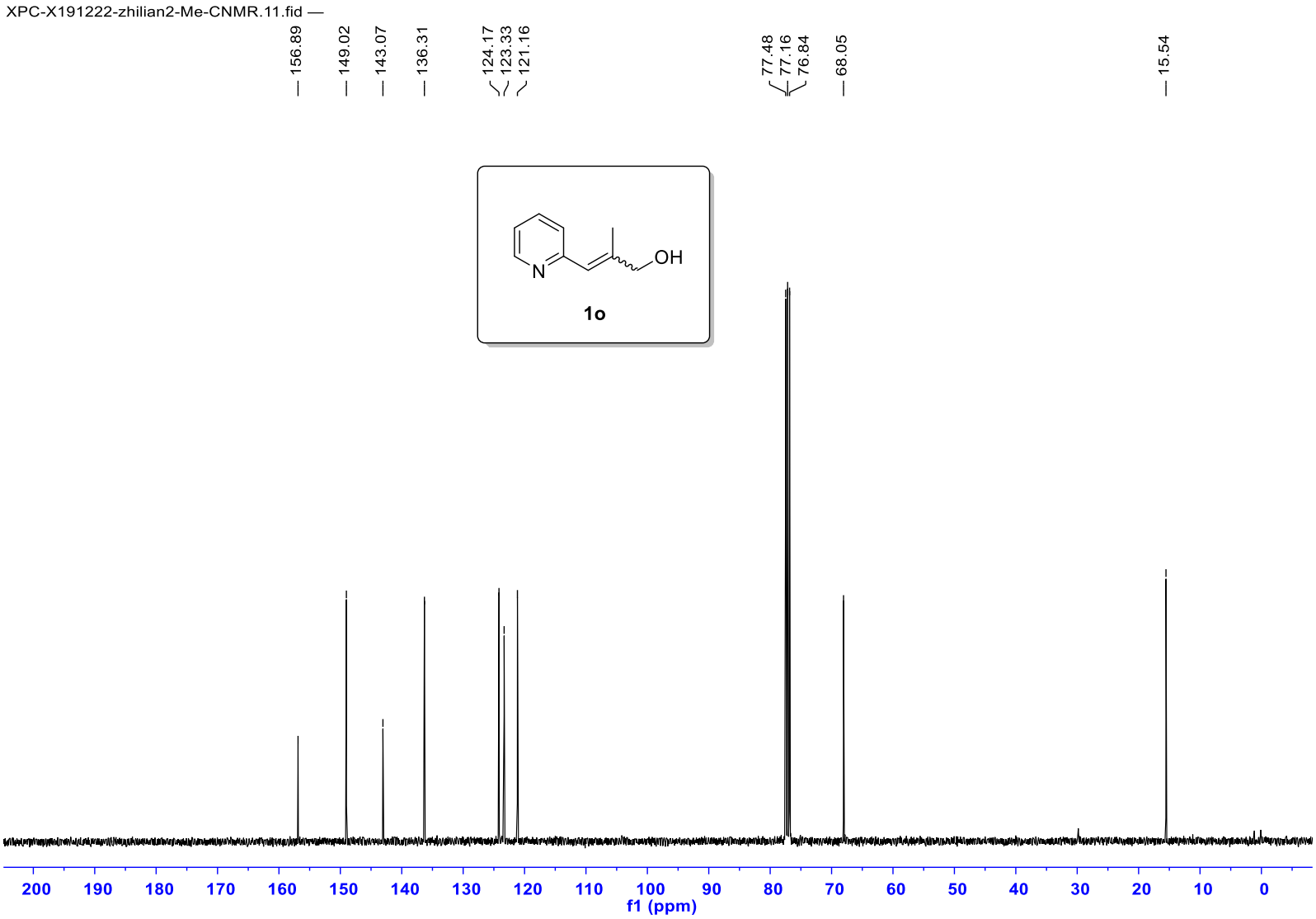
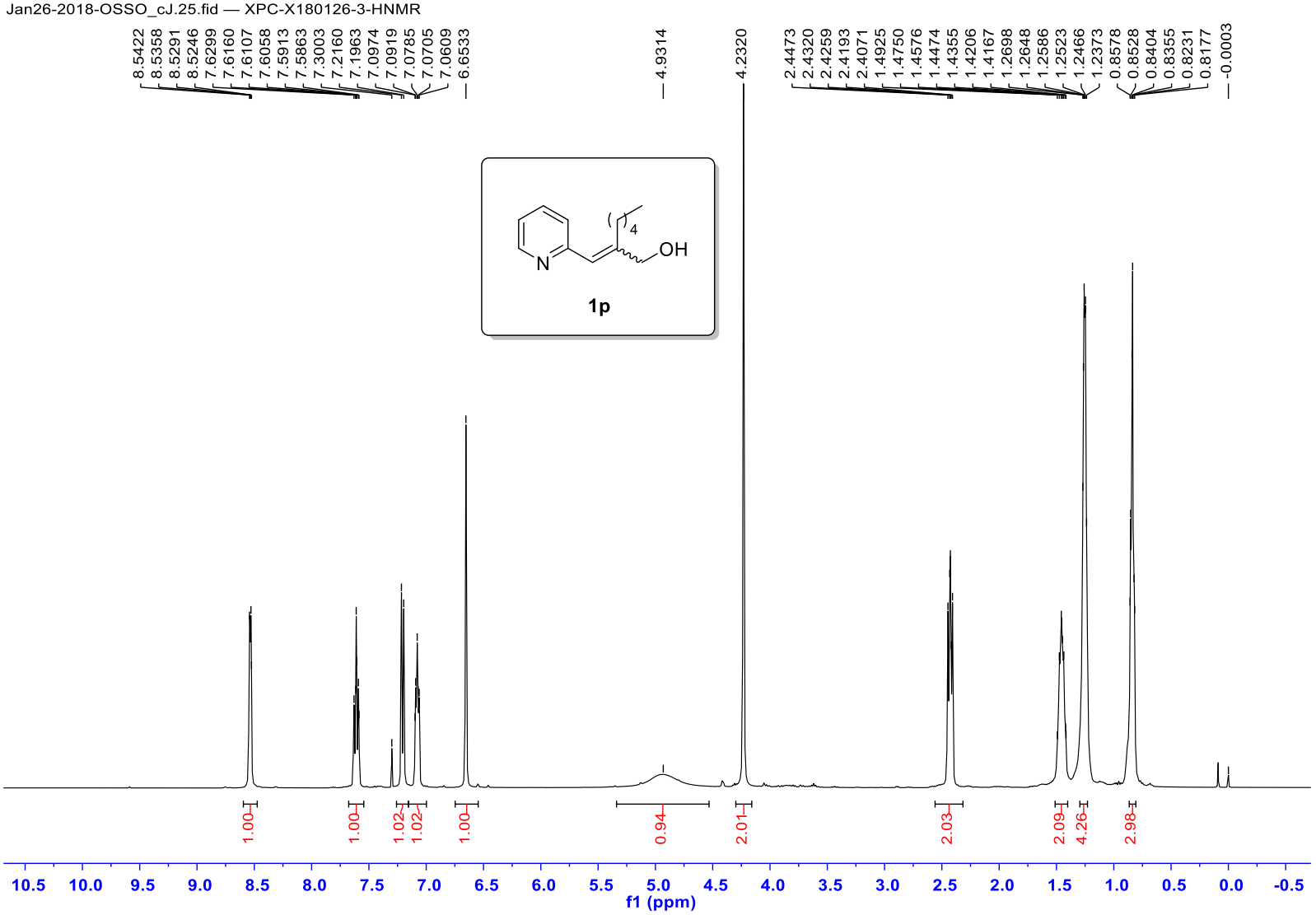
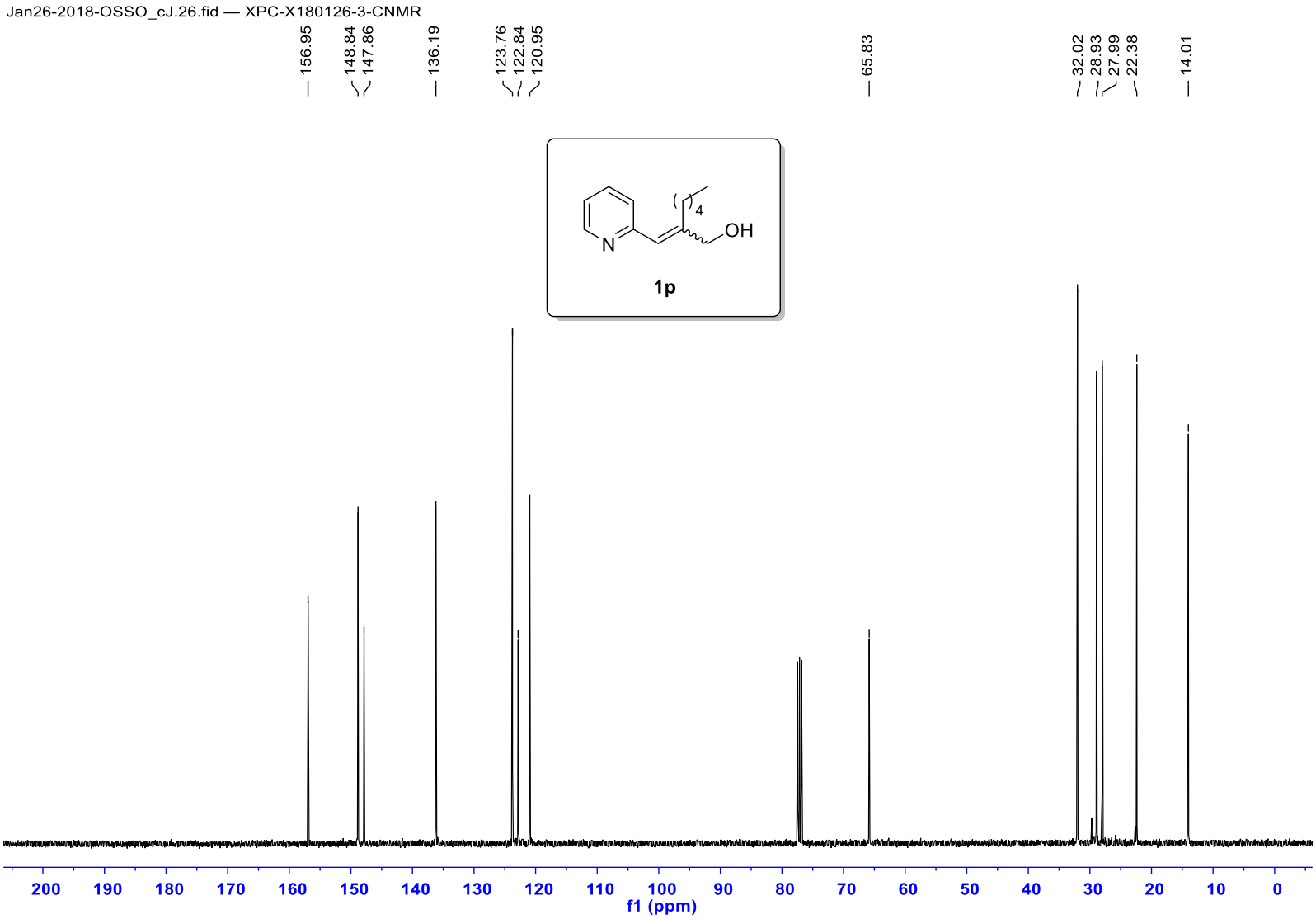
0.0
-0
f1 (ppm)

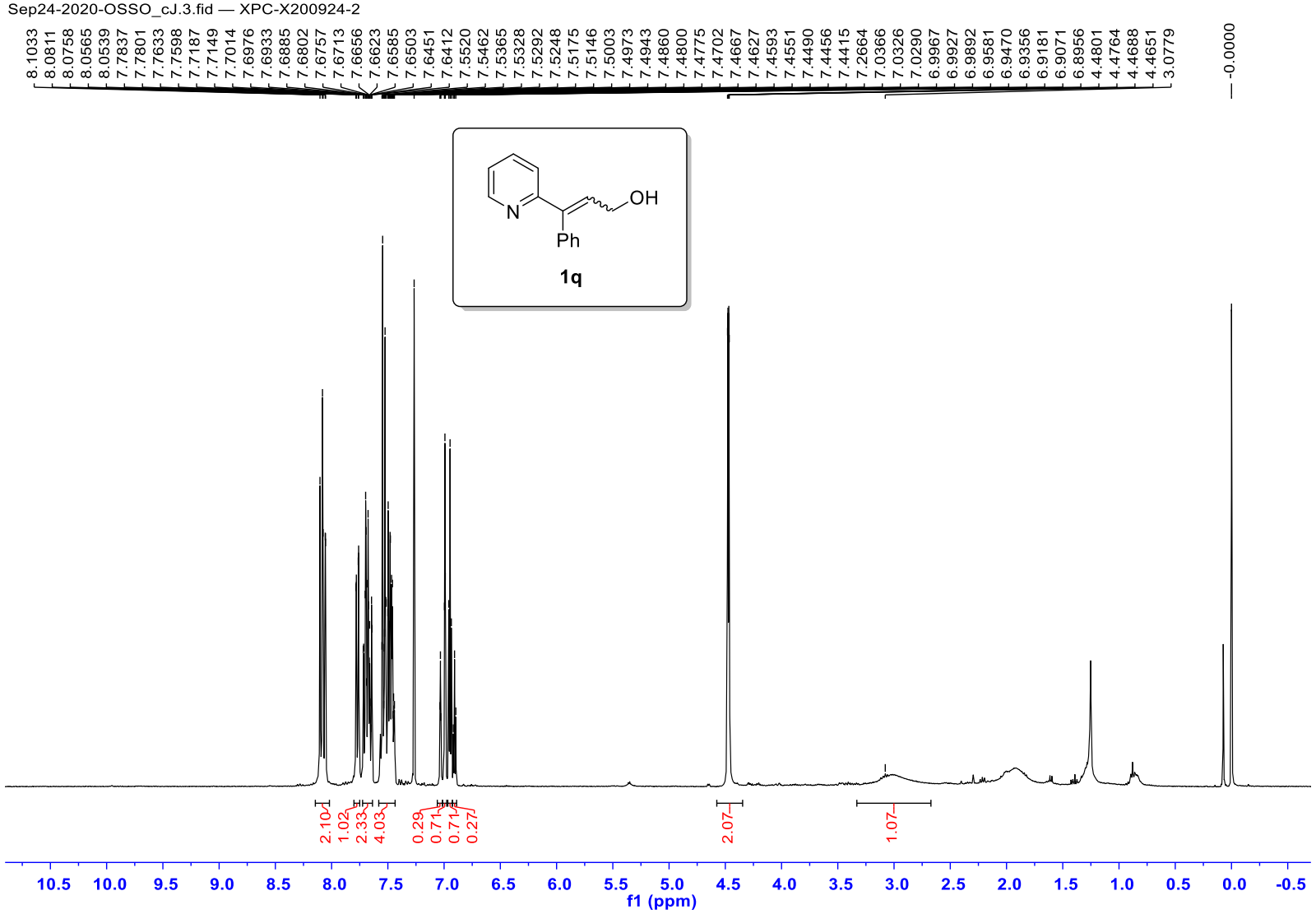

Jan26-2018-OSSO_cJ.46.fid — XPC-X180126-12-CNMR
159.32
148.95
136.85
136.54
129.98
122.13
120.11
77.47
77.15
76.84
60.13
14.65
OH
N
1n
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

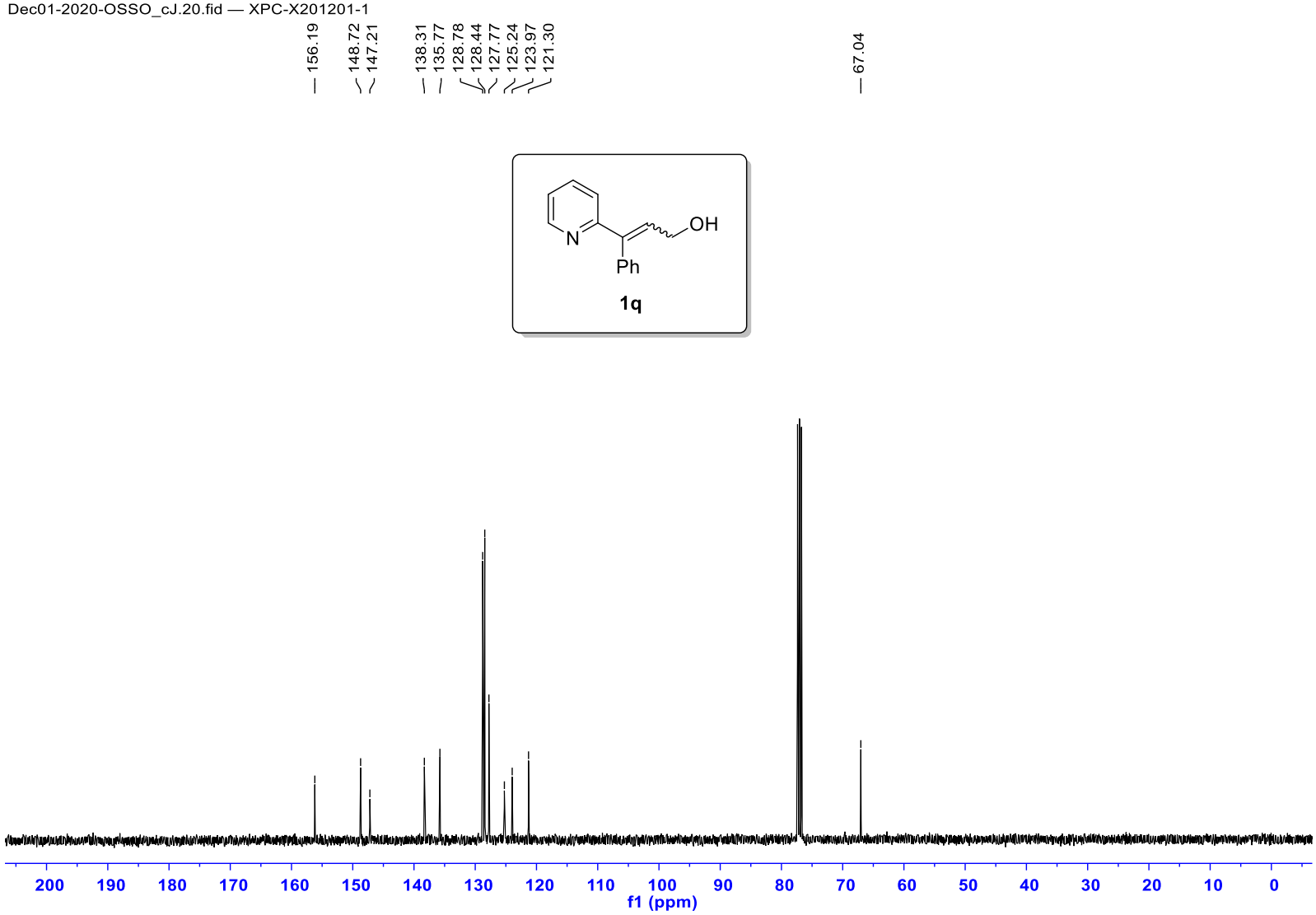

XPC-X191222-zhilian2-Me-HNMR.10.fid
8.5760
8.5738
8.5714
8.5690
8.5639
8.5616
8.5591
7.6676
7.6629
7.6483
7.6436
7.6290
7.6243
7.2720
7.2660
7.2462
7.1259
7.1229
7.1137
7.1107
7.1069
7.1040
7.0947
7.0918
6.6509
6.6469
4.2022
4.1983
2.9505
2.0148
0.0000
OH
N
1o
1.00
1.02
0.85
0.98
0.99
1.98
1.00
2.91
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
-0.5
f1 (ppm)

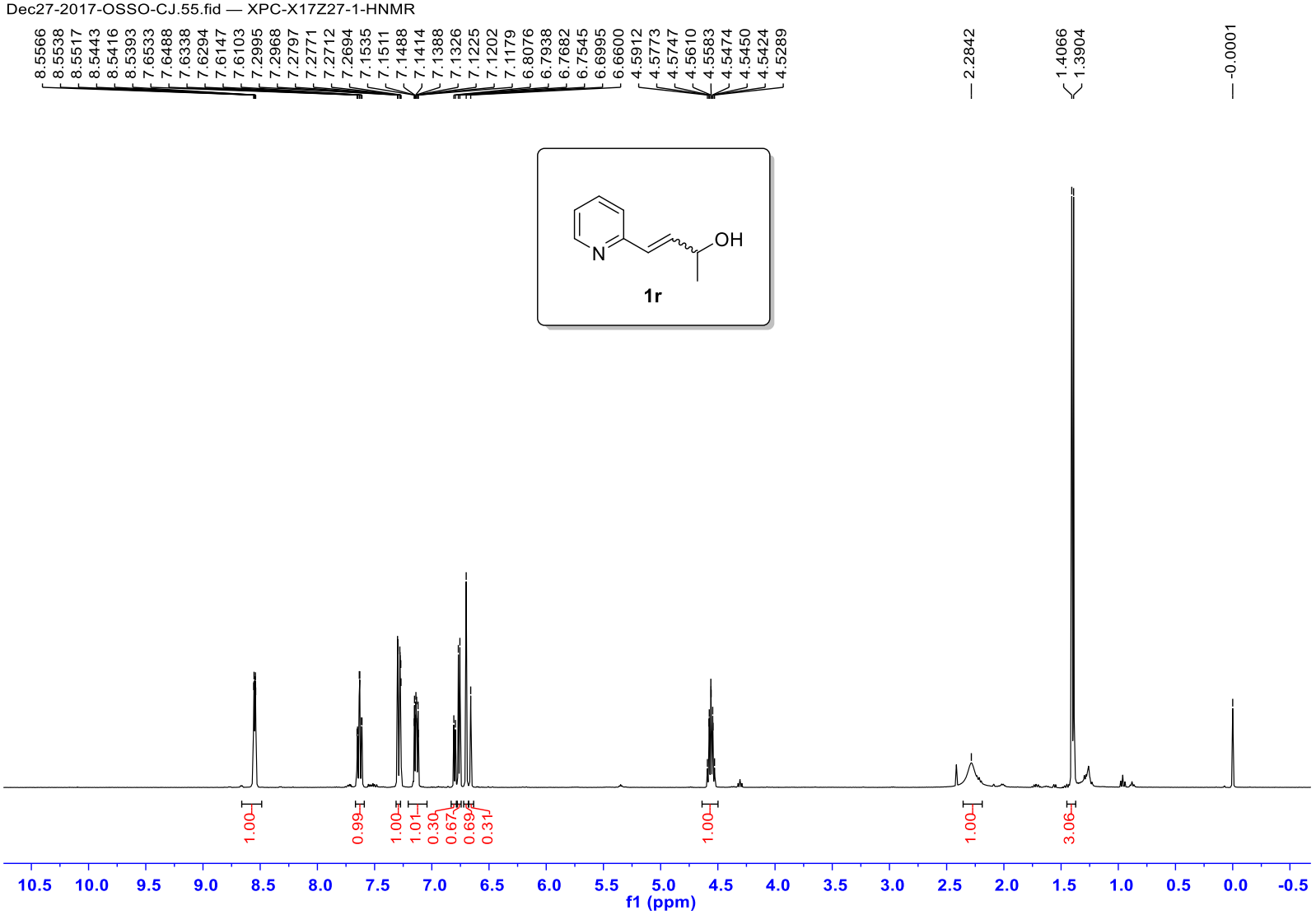

XPC-X191222-zhilian2-Me-CNMR.11.fid
156.89
149.02
143.07
136.31
124.17
123.33
121.16
77.48
77.16
76.84
68.05
15.54
N
OH
1o
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

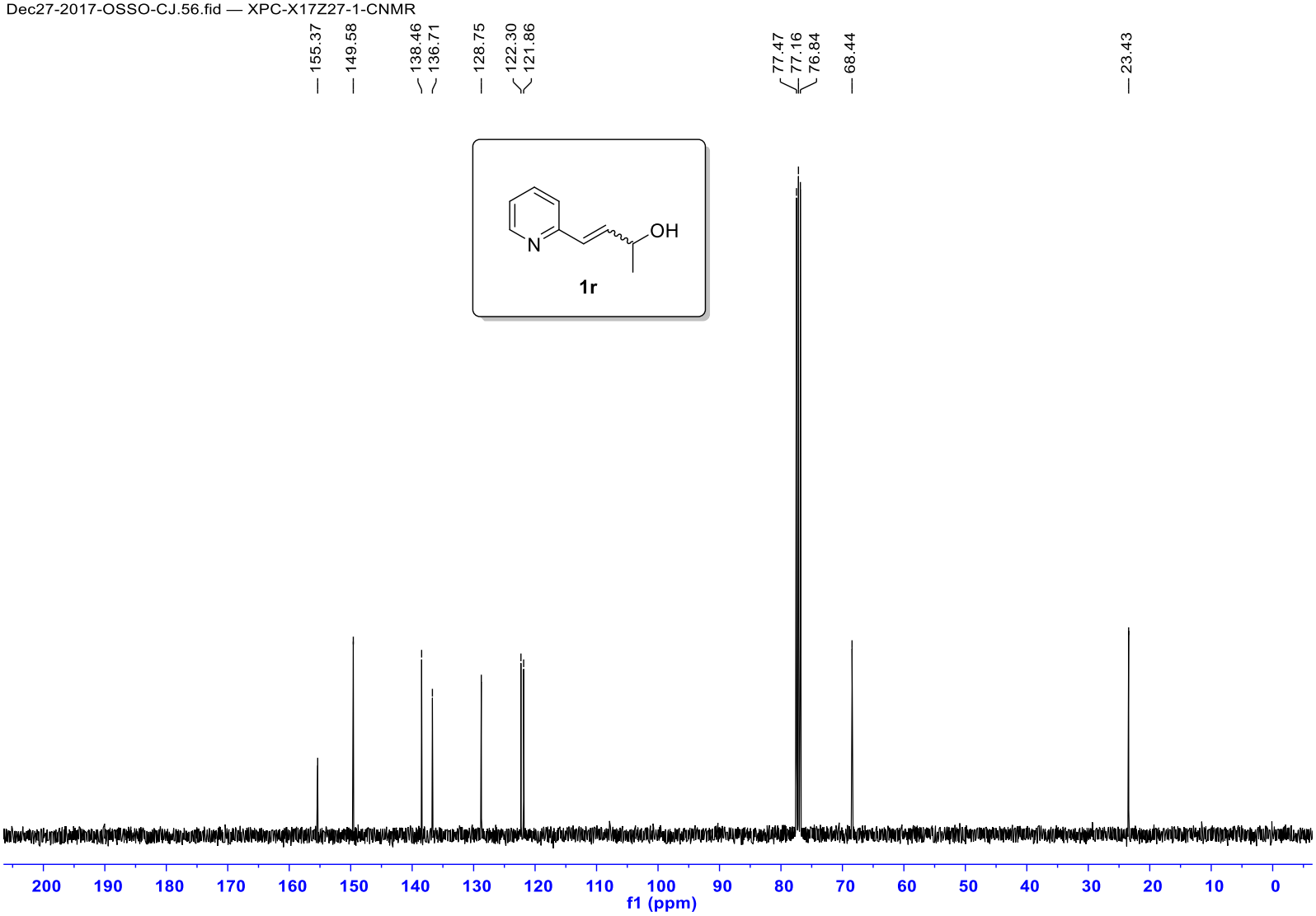

Jan26-2018-OSSO_cJ.25.fid — XPC-X180126-3-HNMR
8.5422
8.5358
8.5291
8.5246
7.6299
7.6160
7.6107
7.6058
7.5913
7.5863
7.3003
7.2160
7.1963
7.0974
7.0919
7.0785
7.0705
7.0609
6.6533
4.9314
4.2320
2.4473
2.4320
2.4259
2.4193
2.4071
1.4925
1.4750
1.4576
1.4474
1.4355
1.4206
1.4167
1.2698
1.2648
1.2586
1.2523
1.2466
1.2373
0.8578
0.8528
0.8404
0.8355
0.8231
0.8177
-0.0003
N
4
OH
1p
1.00
1.00
1.02
1.02
1.00
0.94
2.01
2.03
2.09
4.26
2.98
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
-0.5
f1 (ppm)

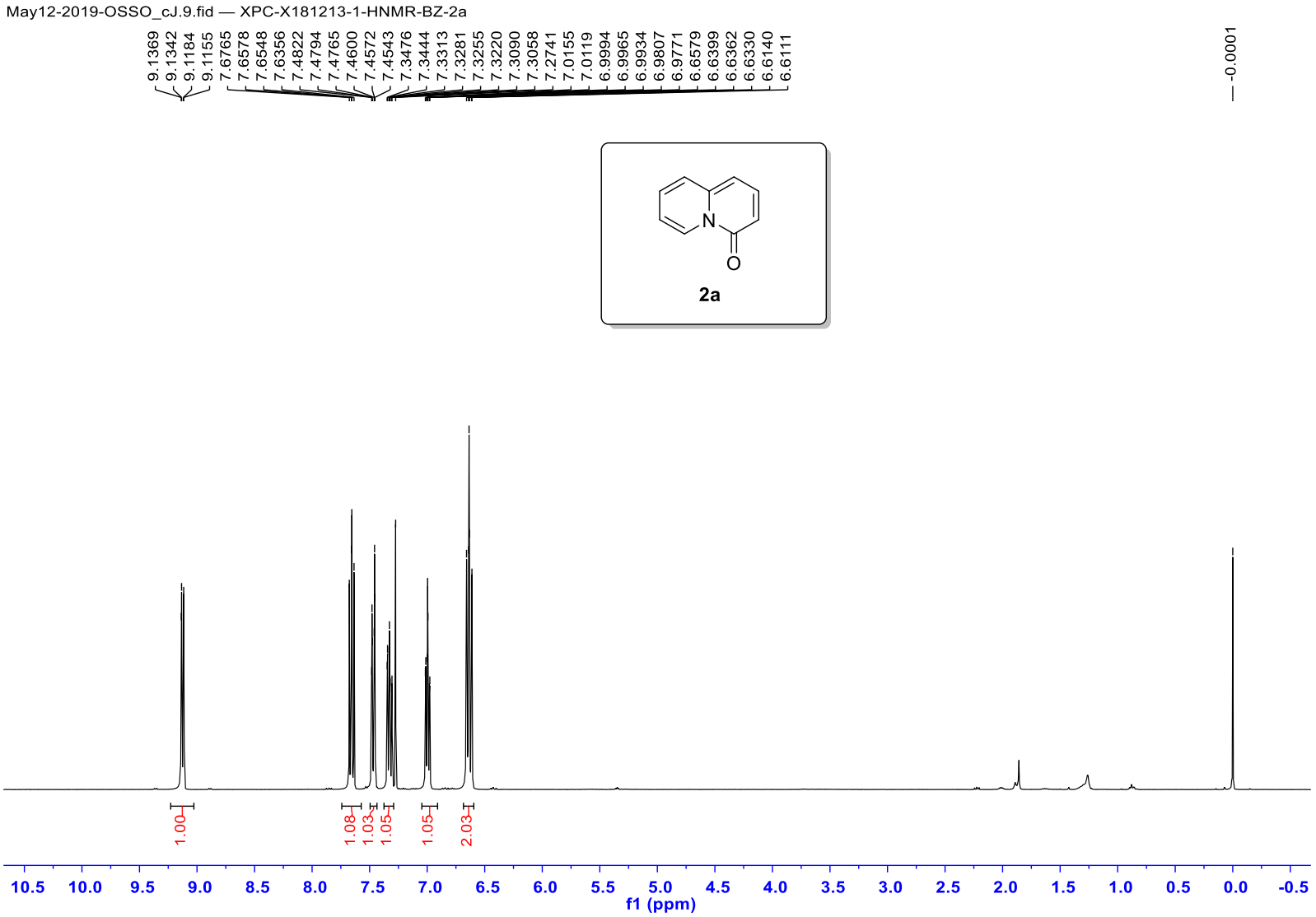

Jan26-2018-OSSO_cJ.26.fid — XPC-X180126-3-CNMR
156.95
148.84
147.86
136.19
123.76
122.84
120.95
65.83
32.02
28.93
27.99
22.38
14.01
N
OH
4
1p
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

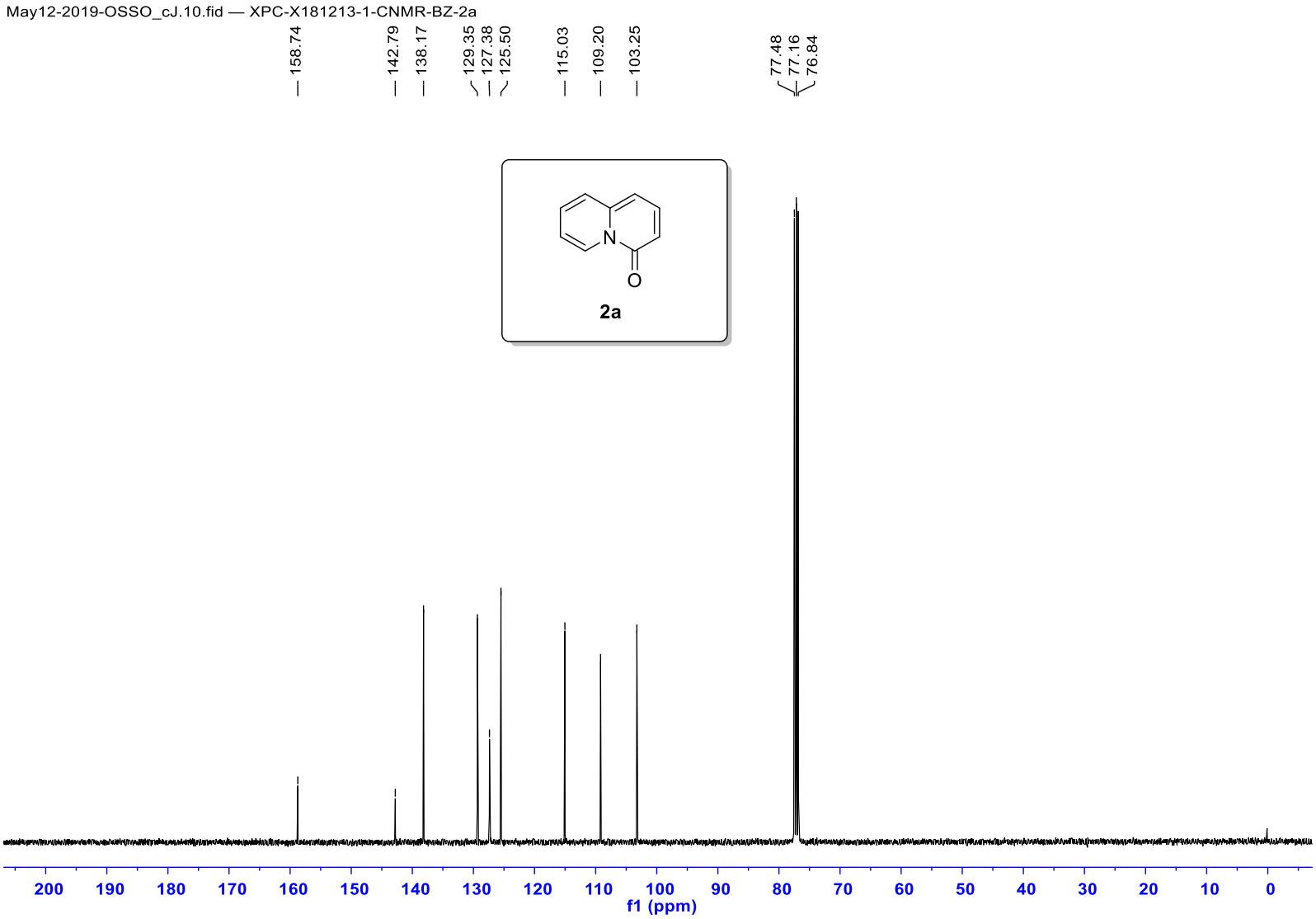

Sep24-2020-OSSO_cJ.3.fid — XPC-X200924-2
8.1033 8.0811 8.0758 8.0565 8.0539 7.7837 7.7801 7.7633 7.7598 7.7187 7.7149 7.7014 7.6976 7.6933 7.6885 7.6802 7.6757 7.6713 7.6656 7.6623 7.6585 7.6503 7.6451 7.6412 7.5520 7.5462 7.5365 7.5328 7.5292 7.5248 7.5175 7.5146 7.5003 7.4973 7.4943 7.4860 7.4800 7.4775 7.4702 7.4667 7.4627 7.4593 7.4551 7.4490 7.4456 7.4415 7.2664 7.0366 7.0326 7.0290 6.9967 6.9927 6.9892 6.9581 6.9470 6.9356 6.9181 6.9071 6.8956 4.4801 4.4764 4.4688 4.4651 3.0779
-0.0000
N
OH
Ph
1q
2.10
1.02
2.33
4.03
0.29
0.71
0.71
0.27
2.07
1.07
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 -0.5
f1 (ppm)

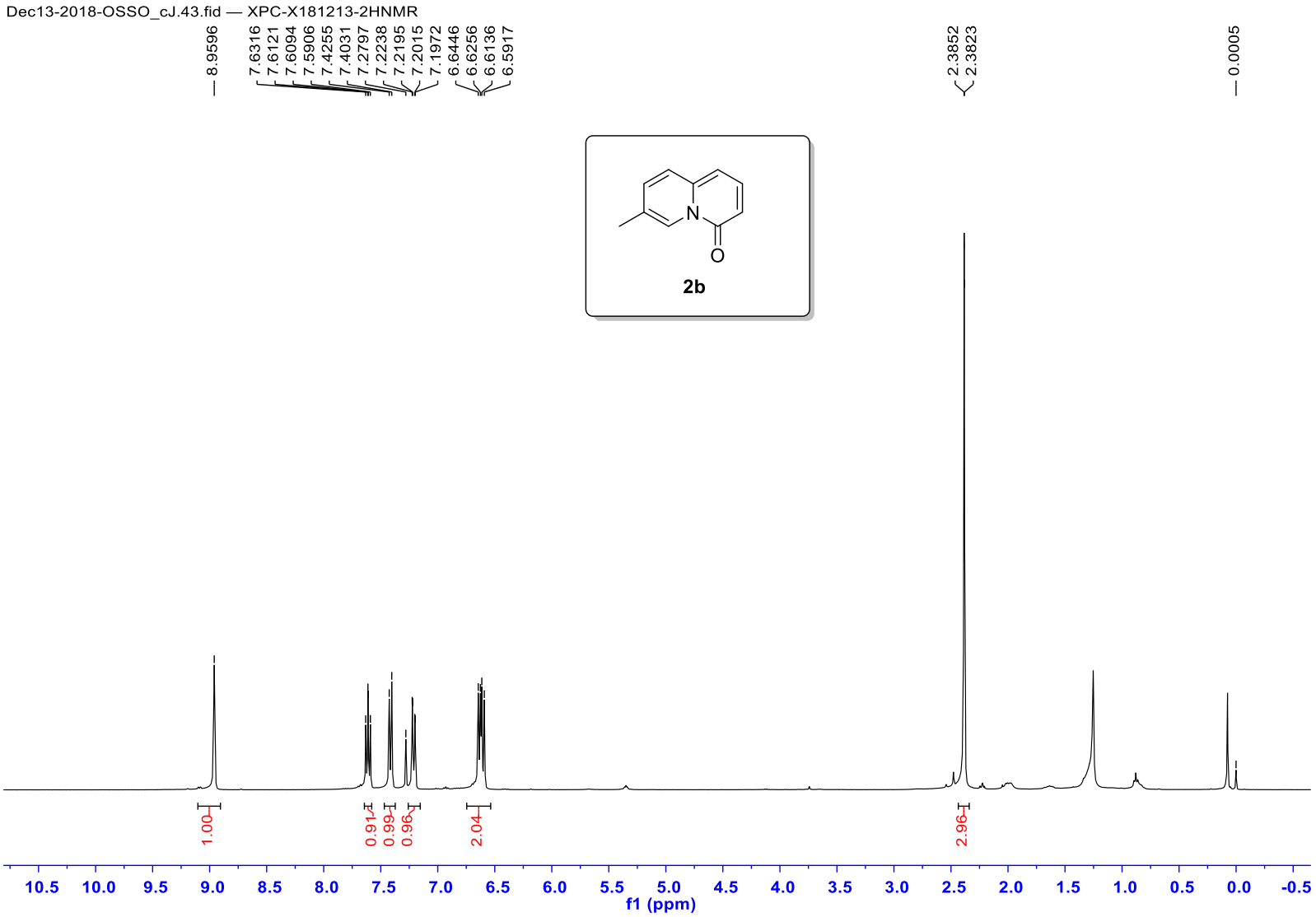

Dec01-2020-OSSO_cJ.20.fid — XPC-X201201-1
156.19
148.72
147.21
138.31
135.77
128.78
128.44
127.77
125.24
123.97
121.30
67.04
N
OH
Ph
1q
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

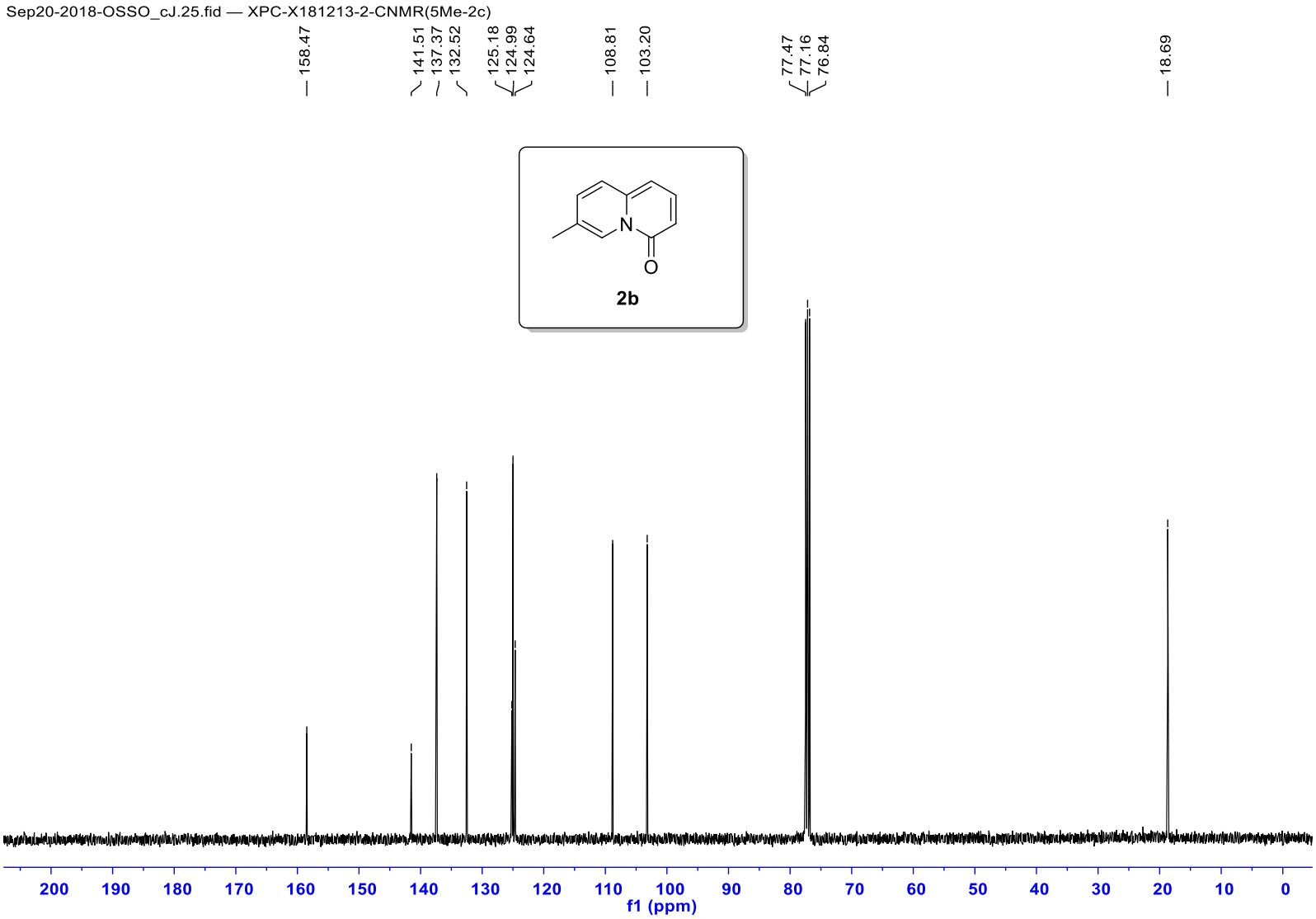

Dec27-2017-OSSO-CJ.55.fid — XPC-X17Z27-1-HNMR
8.5566
8.5538
8.5517
8.5443
8.5416
8.5393
7.6533
7.6488
7.6338
7.6294
7.6147
7.6103
7.2995
7.2968
7.2797
7.2771
7.2712
7.2694
7.1535
7.1511
7.1488
7.1414
7.1388
7.1326
7.1225
7.1202
7.1179
6.8076
6.7938
6.7682
6.7545
6.6995
6.6600
4.5912
4.5773
4.5747
4.5610
4.5583
4.5474
4.5450
4.5424
4.5289
2.2842
1.4066
1.3904
-0.0001
N
OH
1r
1.00
0.99
1.00
1.01
0.30
0.67
0.69
0.31
1.00
1.00
3.06
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
0.0
-0.5
f1 (ppm)

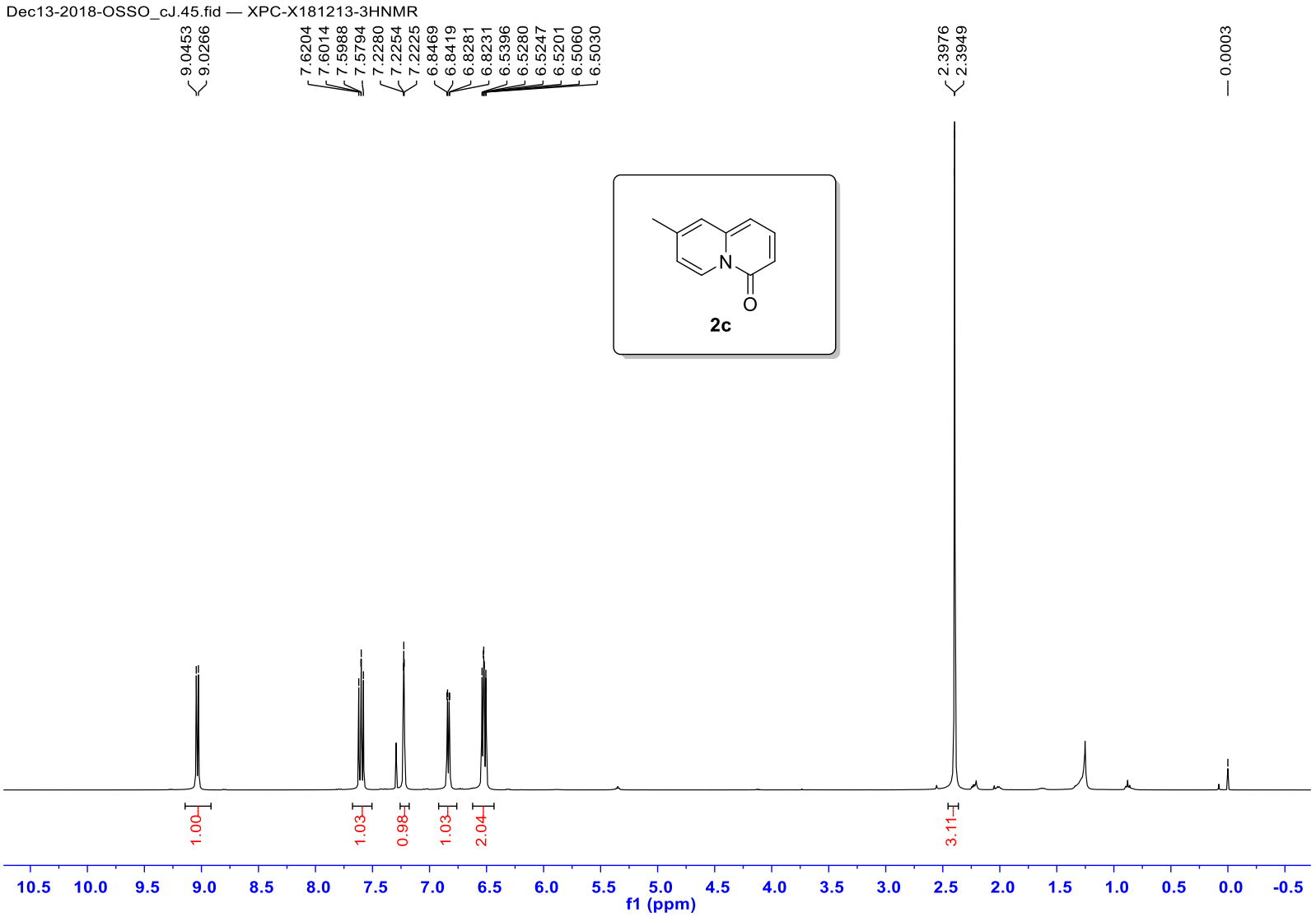

Dec27-2017-OSSO-CJ.56.fid — XPC-X17Z27-1-CNMR
155.37
149.58
138.46
136.71
128.75
122.30
121.86
77.47
77.16
76.84
68.44
23.43
N
OH
1r
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

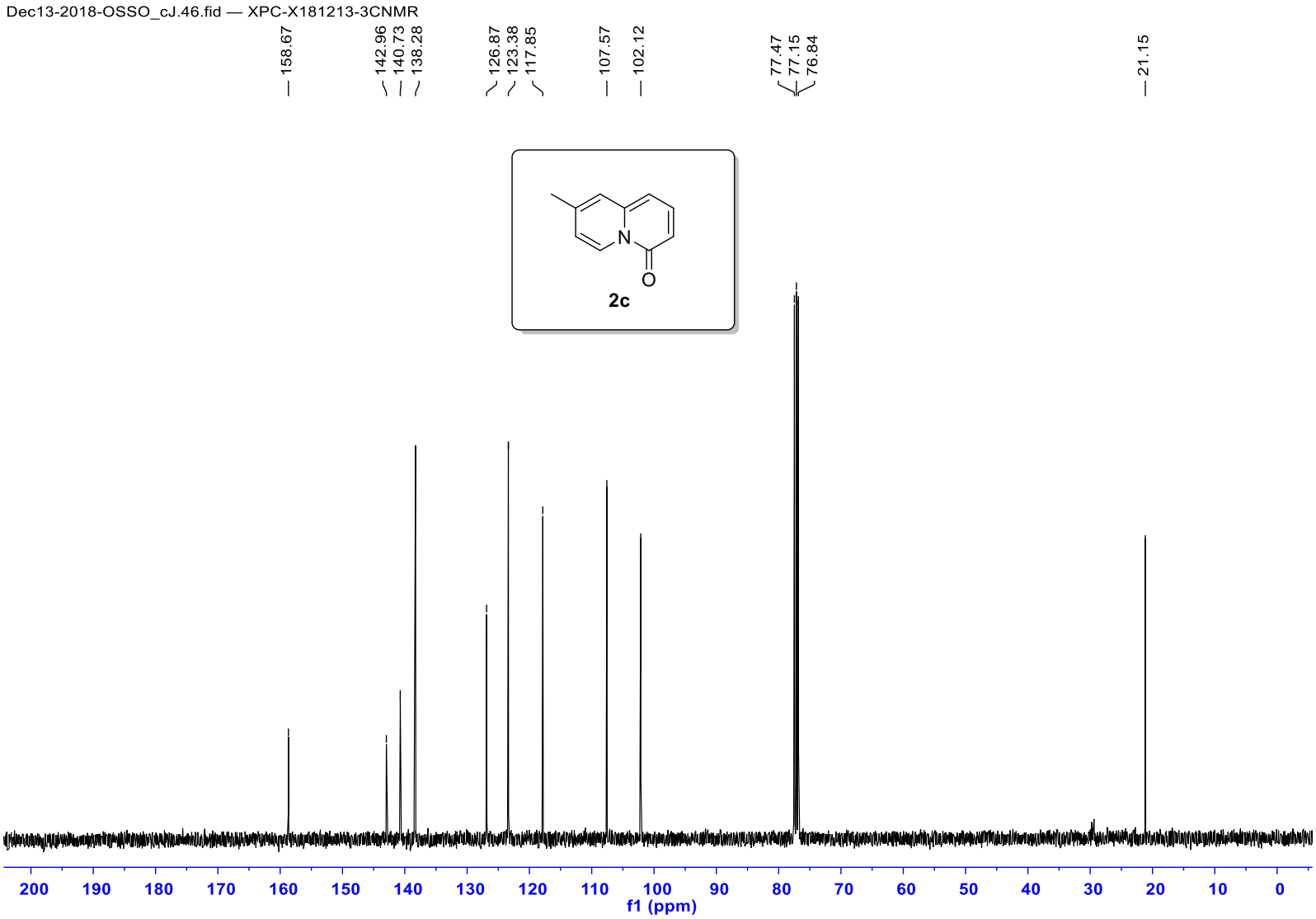

May12-2019-OSSO_cJ.9.fid — XPC-X181213-1-HNMR-BZ-2a
9.1369
9.1342
9.1184
9.1155
7.6765
7.6578
7.6548
7.6356
7.4822
7.4794
7.4765
7.4600
7.4572
7.4543
7.3476
7.3444
7.3313
7.3281
7.3255
7.3220
7.3090
7.3058
7.2741
7.0155
7.0119
6.9994
6.9965
6.9934
6.9807
6.9771
6.6579
6.6399
6.6362
6.6330
6.6140
6.6111
-0.0001
N
O
2a
1.00
1.08
1.03
1.05
1.05
2.03
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
-0.5
f1 (ppm)

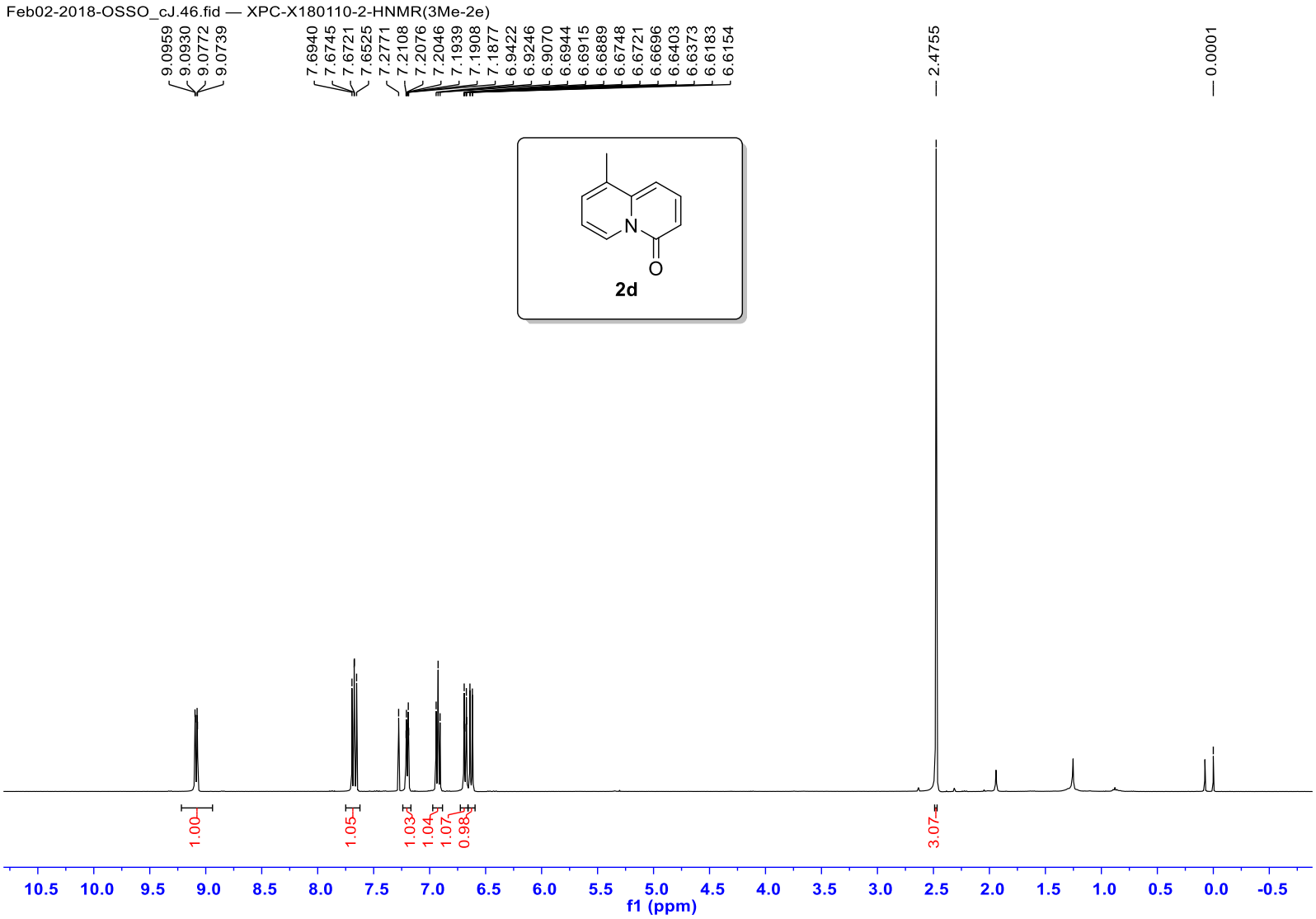

May12-2019-OSSO_cJ.10.fid — XPC-X181213-1-CNMR-BZ-2a
158.74
142.79
138.17
129.35
127.38
125.50
115.03
109.20
103.25
77.48
77.16
76.84
N
O
2a
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

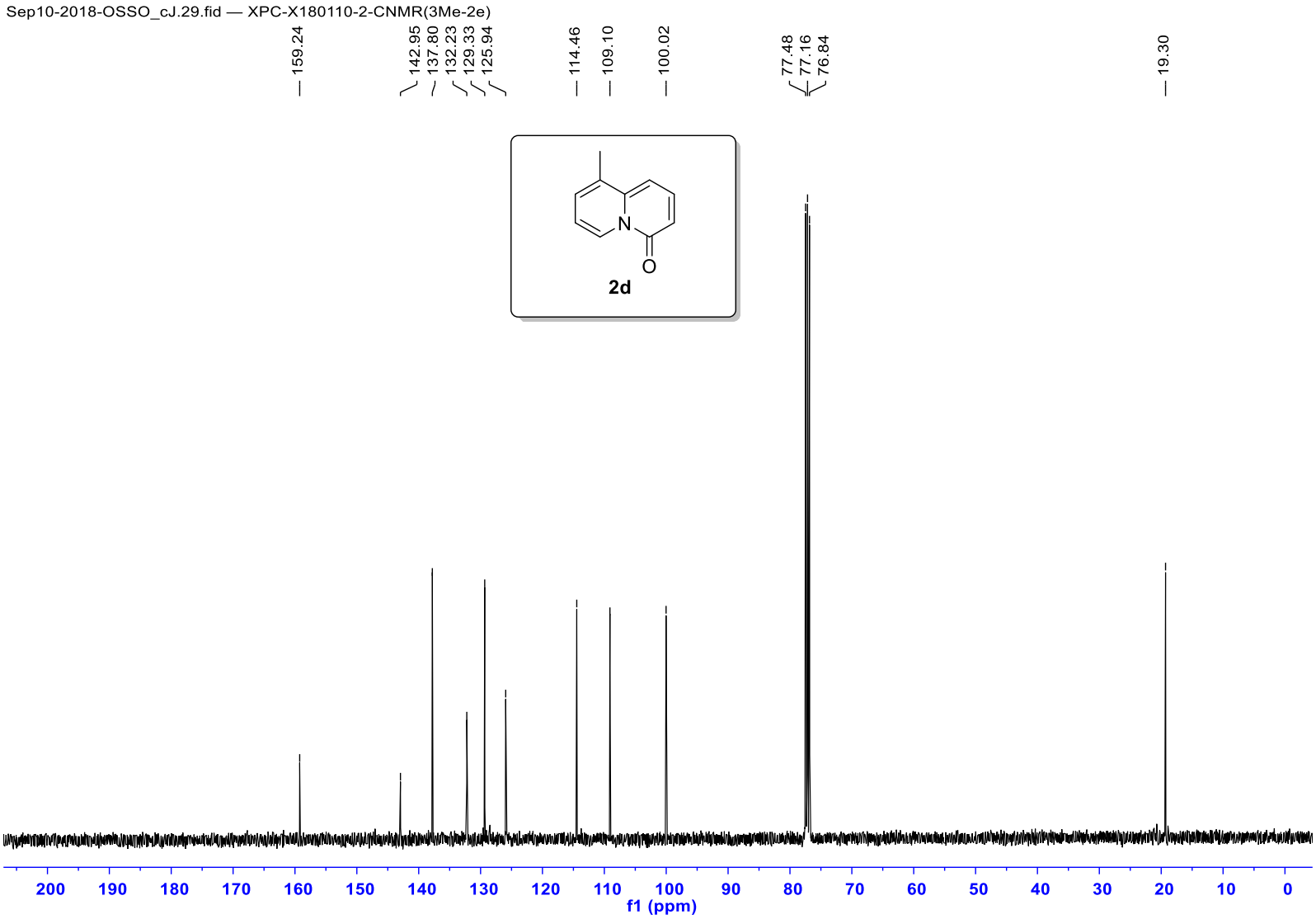

Dec13-2018-OSSO_cJ.43.fid — XPC-X181213-2HNMR
8.9596
7.6316
7.6121
7.6094
7.5906
7.4255
7.4031
7.2797
7.2238
7.2195
7.2015
7.1972
6.6446
6.6256
6.6136
6.5917
2.3852
2.3823
0.0005
N
O
2b
1.00
0.91
0.99
0.96
2.04
2.96
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

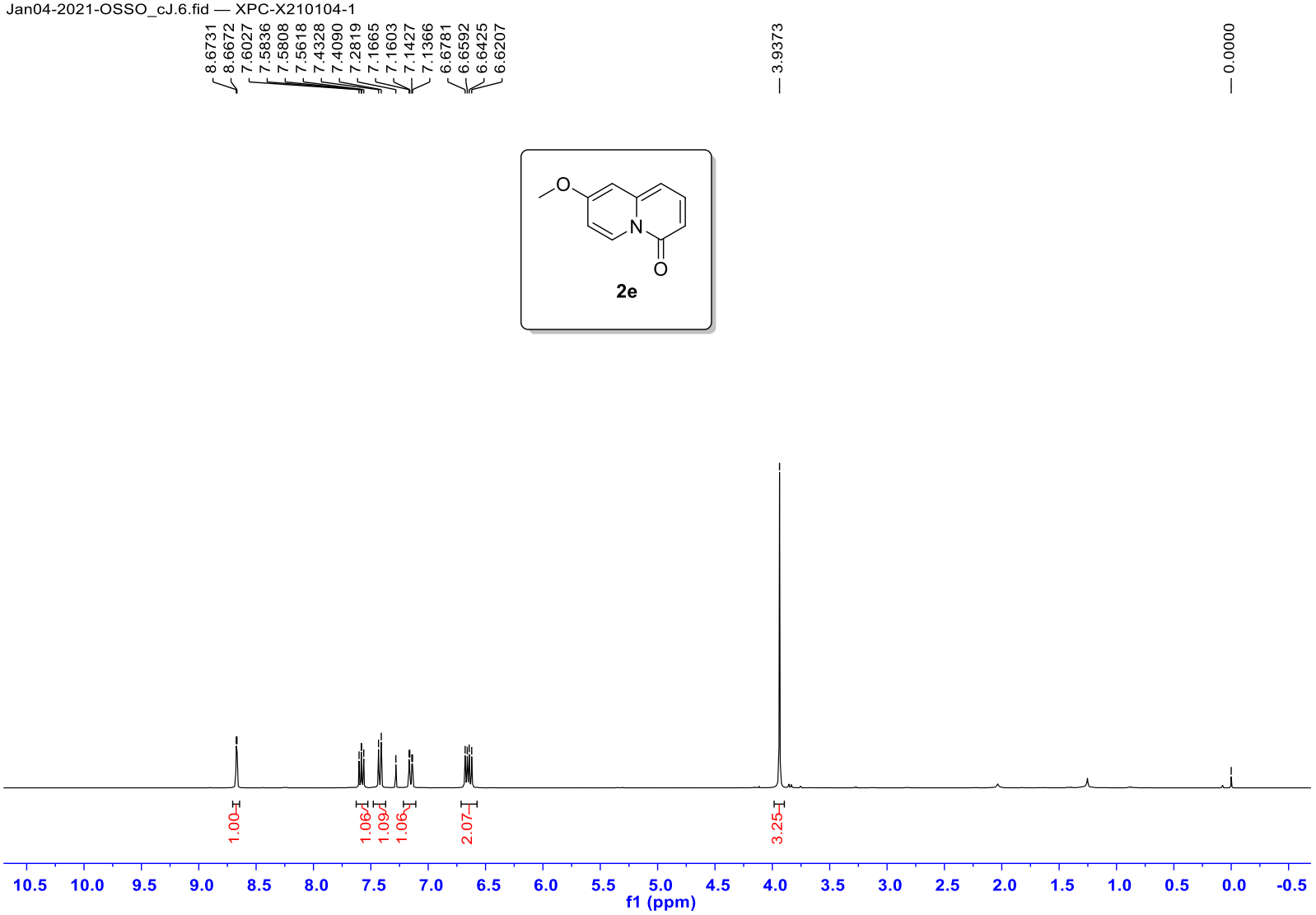

Sep20-2018-OSSO_cJ.25.fid — XPC-X181213-2-CNMR(5Me-2c)
158.47
141.51
137.37
132.52
125.18
124.99
124.64
108.81
103.20
77.47
77.16
76.84
18.69
N
O
2b
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

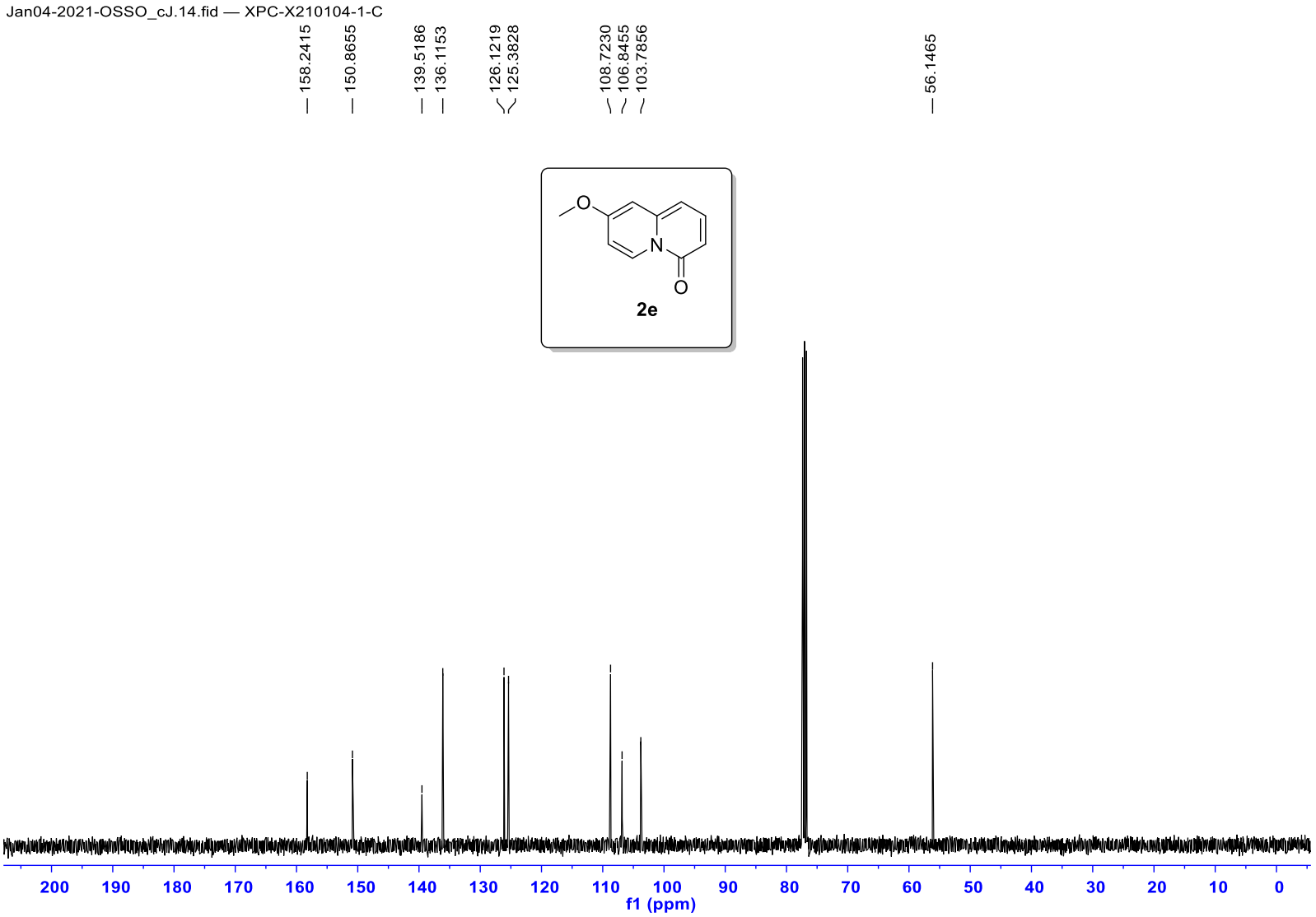

Dec13-2018-OSSO_cJ.45.fid — XPC-X181213-3HNMR
9.0453
9.0266
7.6204
7.6014
7.5988
7.5794
7.2280
7.2254
7.2225
6.8469
6.8419
6.8281
6.8231
6.5396
6.5280
6.5247
6.5201
6.5060
6.5030
2.3976
2.3949
0.0003
N
O
2c
1.00
1.03
0.98
1.03
2.04
3.11
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

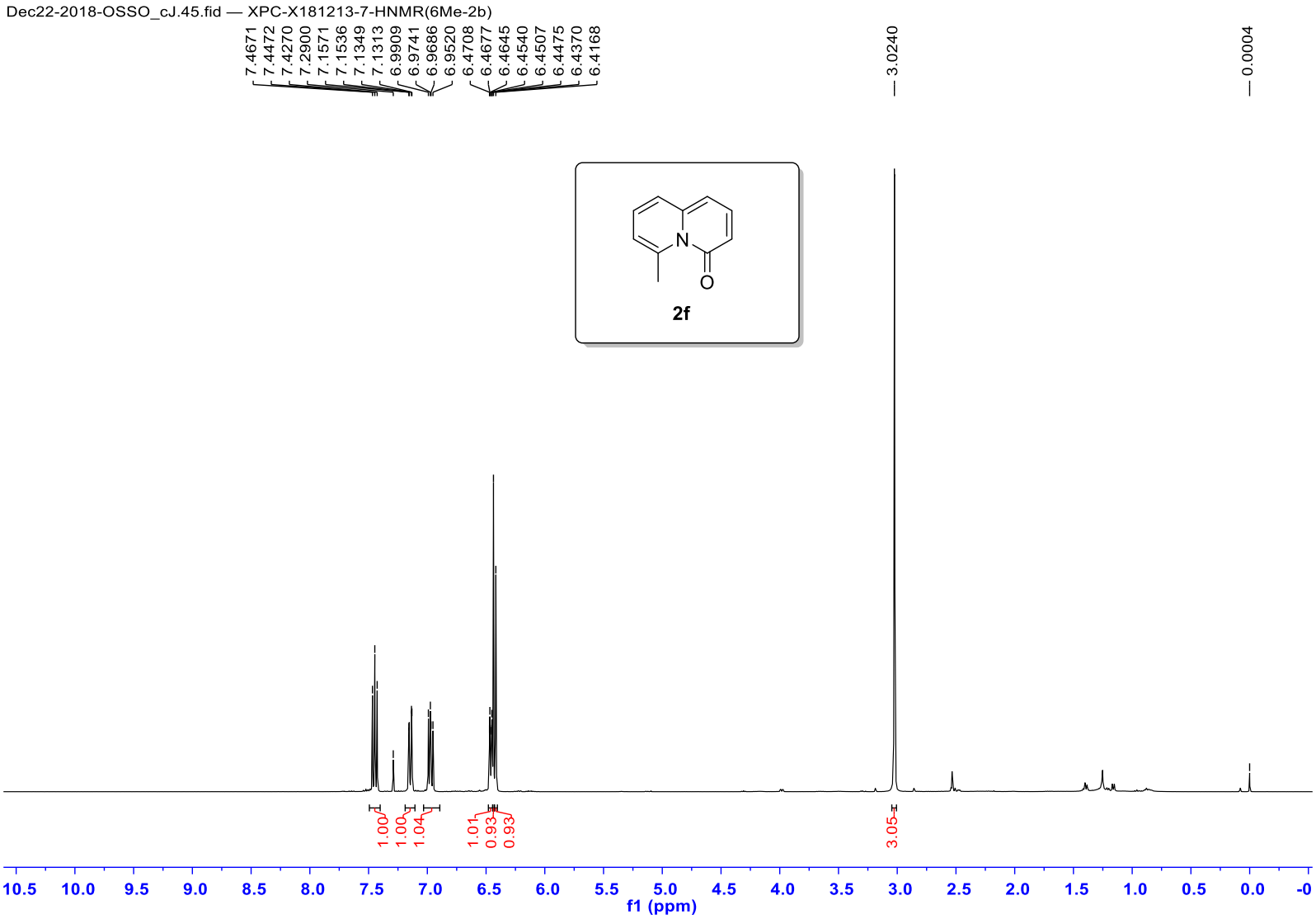

Dec13-2018-OSSO_cJ.46.fid — XPC-X181213-3CNMR
158.67
142.96
140.73
138.28
126.87
123.38
117.85
107.57
102.12
77.47
77.15
76.84
21.15
N
O
2c
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

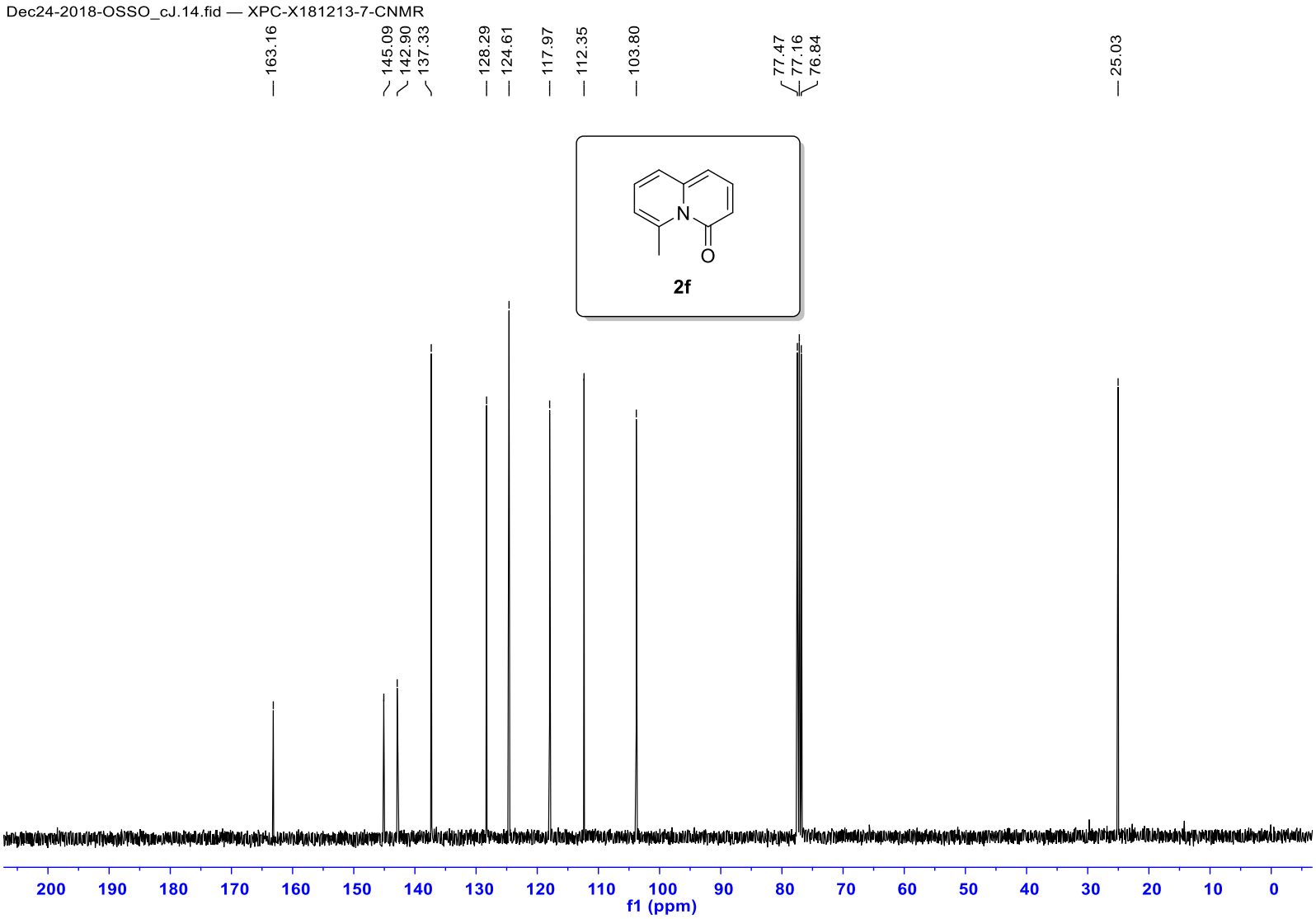

Feb02-2018-OSSO_cJ.46.fid — XPC-X180110-2-HNMR(3Me-2e)
9.0959
9.0930
9.0772
9.0739
7.6940
7.6745
7.6721
7.6525
7.2771
7.2108
7.2076
7.2046
7.1939
7.1908
7.1877
6.9422
6.9246
6.9070
6.6944
6.6915
6.6889
6.6748
6.6721
6.6696
6.6403
6.6373
6.6183
6.6154
2.4755
0.0001
N
O
2d
1.00
1.05
1.03
1.04
1.07
0.98
3.07
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
-0.5
f1 (ppm)

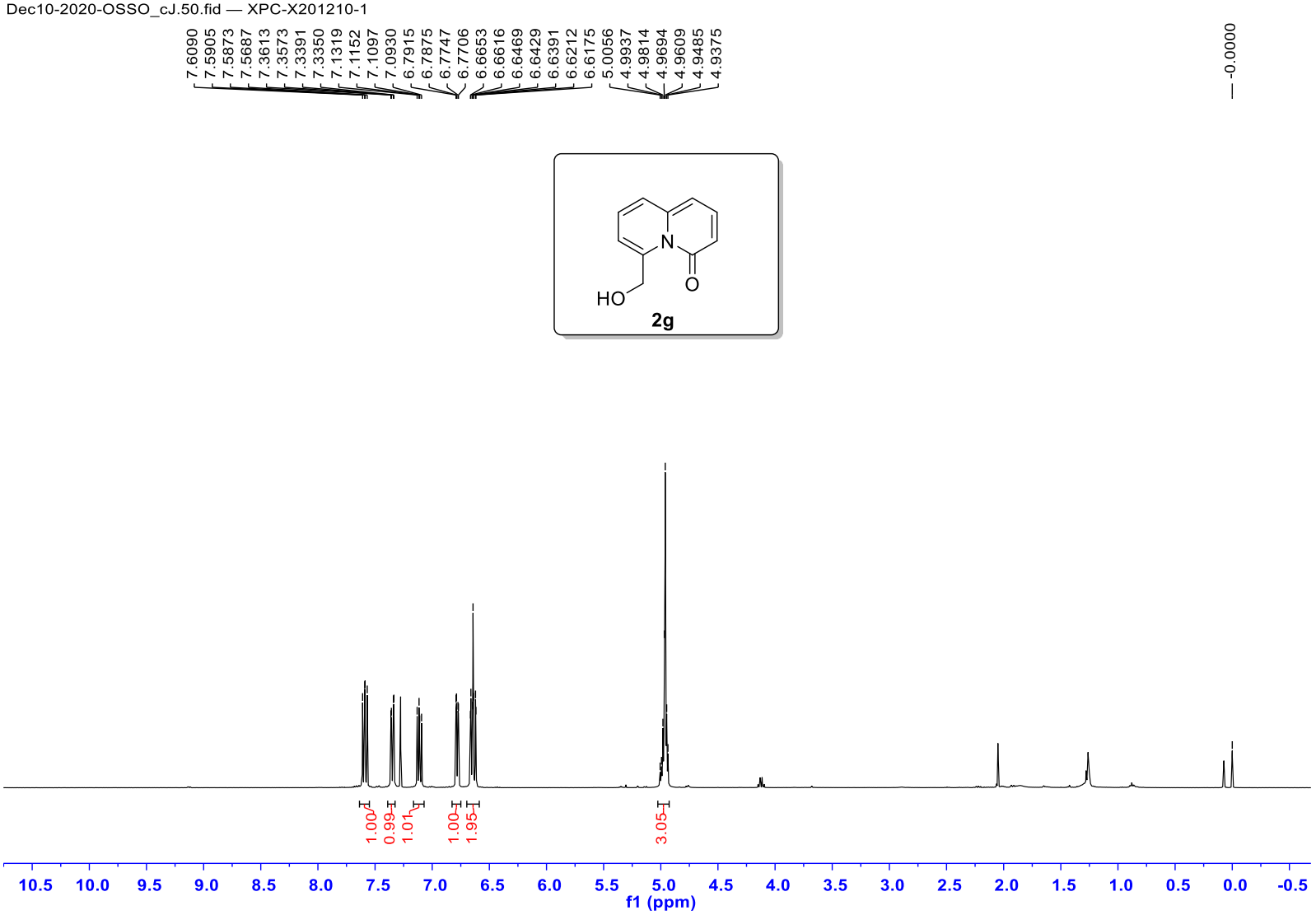

Sep10-2018-OSSO_cJ.29.fid — XPC-X180110-2-CNMR(3Me-2e)
159.24
142.95
137.80
132.23
129.33
125.94
114.46
109.10
100.02
77.48
77.16
76.84
19.30
N
O
2d
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

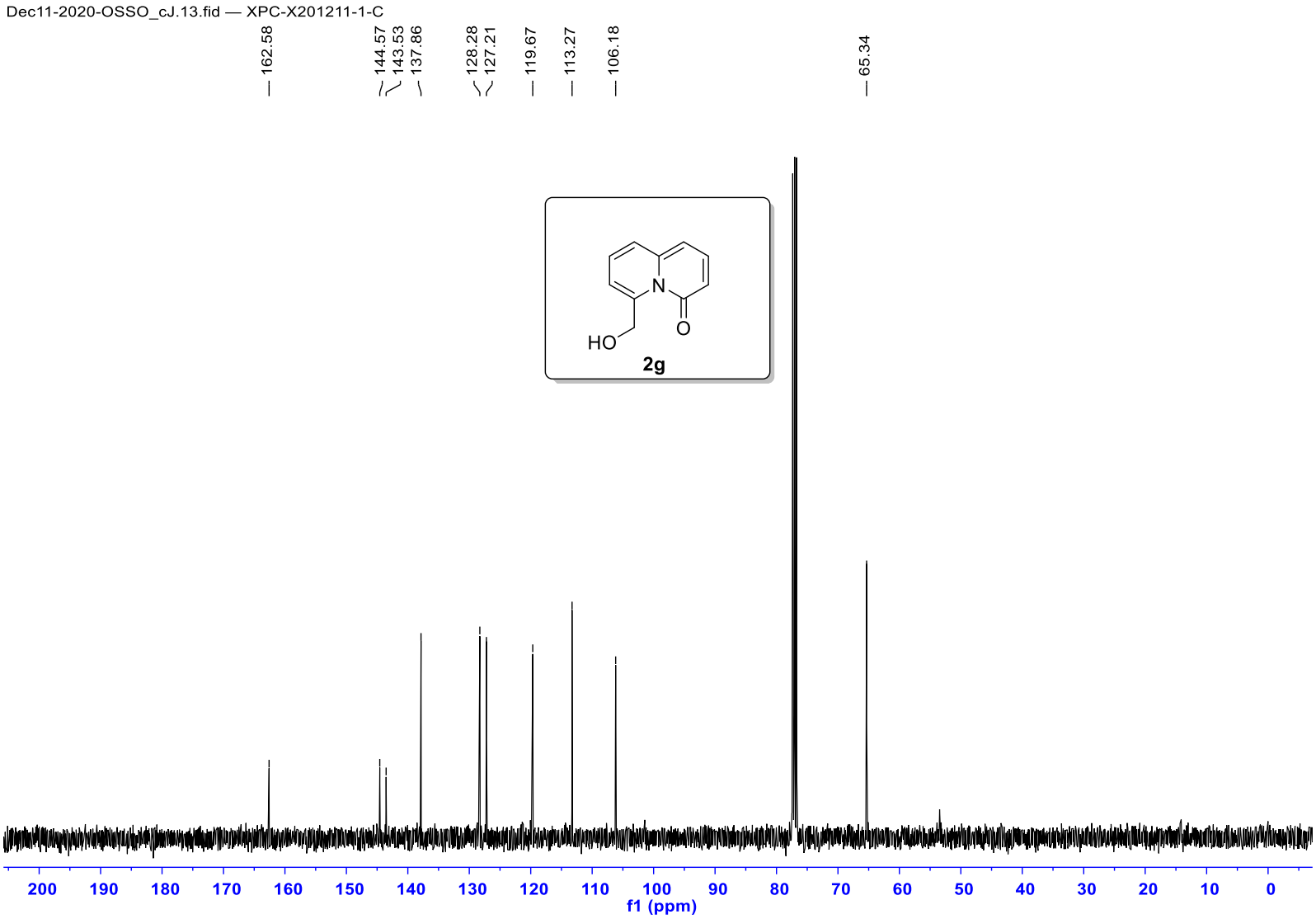

Jan04-2021-OSSO_cJ.6.fid — XPC-X210104-1
8.6731
8.6672
7.6027
7.5836
7.5808
7.5618
7.4328
7.4090
7.2819
7.1665
7.1603
7.1427
7.1366
6.6781
6.6592
6.6425
6.6207
3.9373
0.0000
O
N
O
2e
1.00
1.06
1.09
1.06
2.07
3.25
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

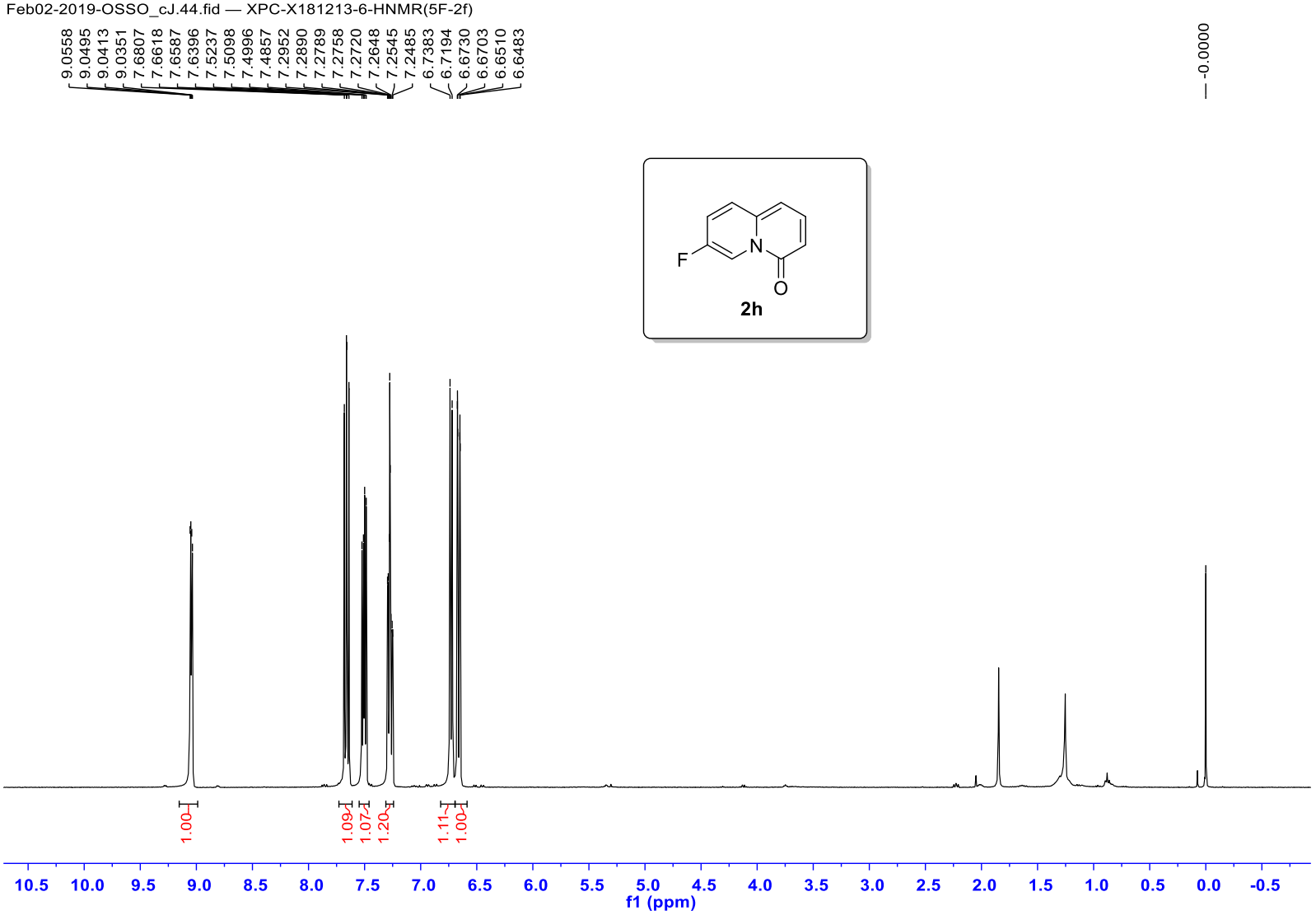

Jan04-2021-OSSO_cJ.14.fid — XPC-X210104-1-C
158.2415
150.8655
139.5186
136.1153
126.1219
125.3828
108.7230
106.8455
103.7856
56.1465
O
N
O
2e
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

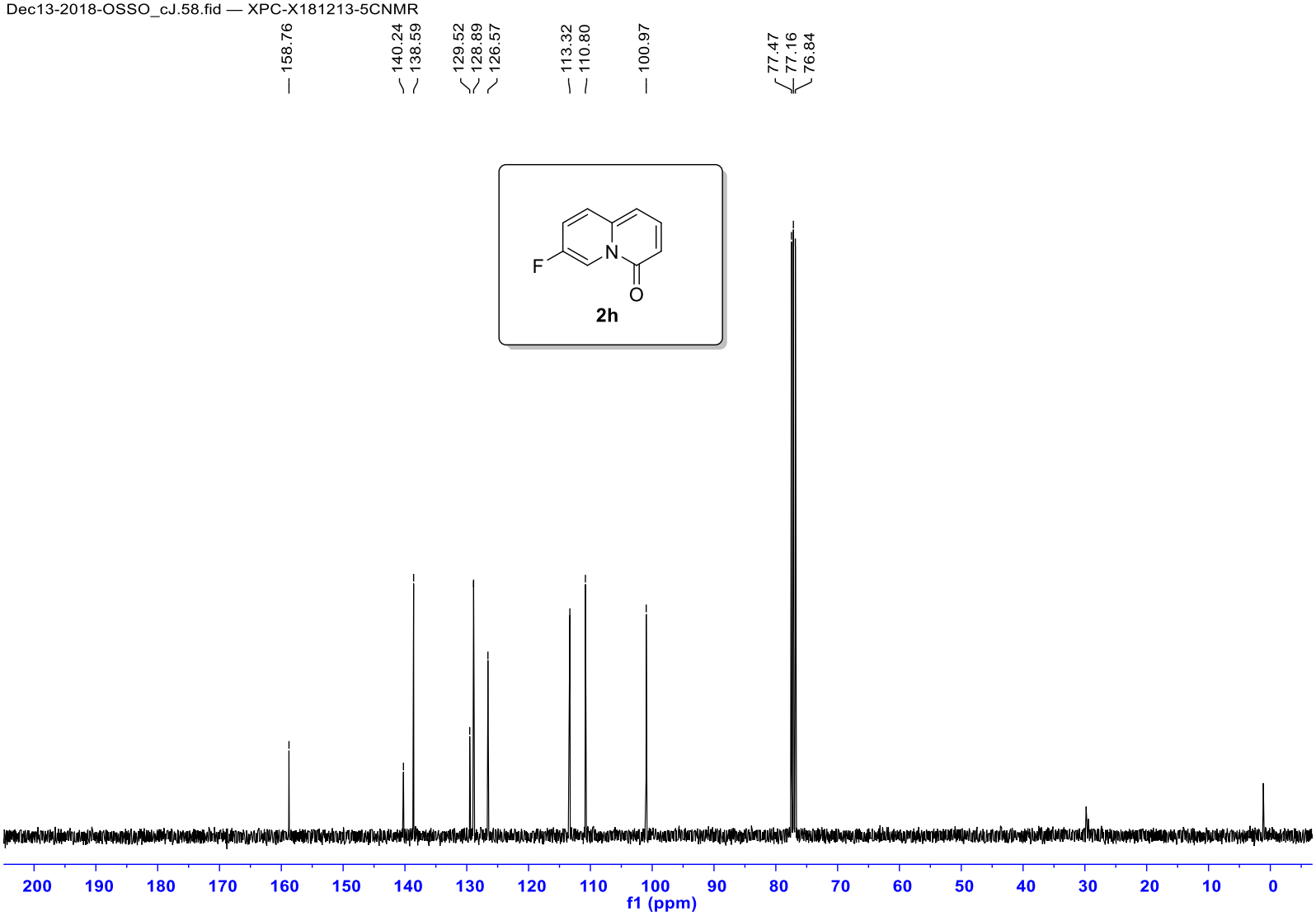

Dec22-2018-OSSO_cJ.45.fid — XPC-X181213-7-HNMR(6Me-2b)
7.4671
7.4472
7.4270
7.2900
7.1571
7.1536
7.1349
7.1313
6.9909
6.9741
6.9686
6.9520
6.4708
6.4677
6.4645
6.4540
6.4507
6.4475
6.4370
6.4168
3.0240
0.0004
N
O
2f
1.00
1.00
1.04
1.01
0.93
0.93
3.05
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0
f1 (ppm)


Dec24-2018-OSSO_cJ.14.fid — XPC-X181213-7-CNMR
163.16
145.09
142.90
137.33
128.29
124.61
117.97
112.35
103.80
77.47
77.16
76.84
25.03
N
O
2f
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

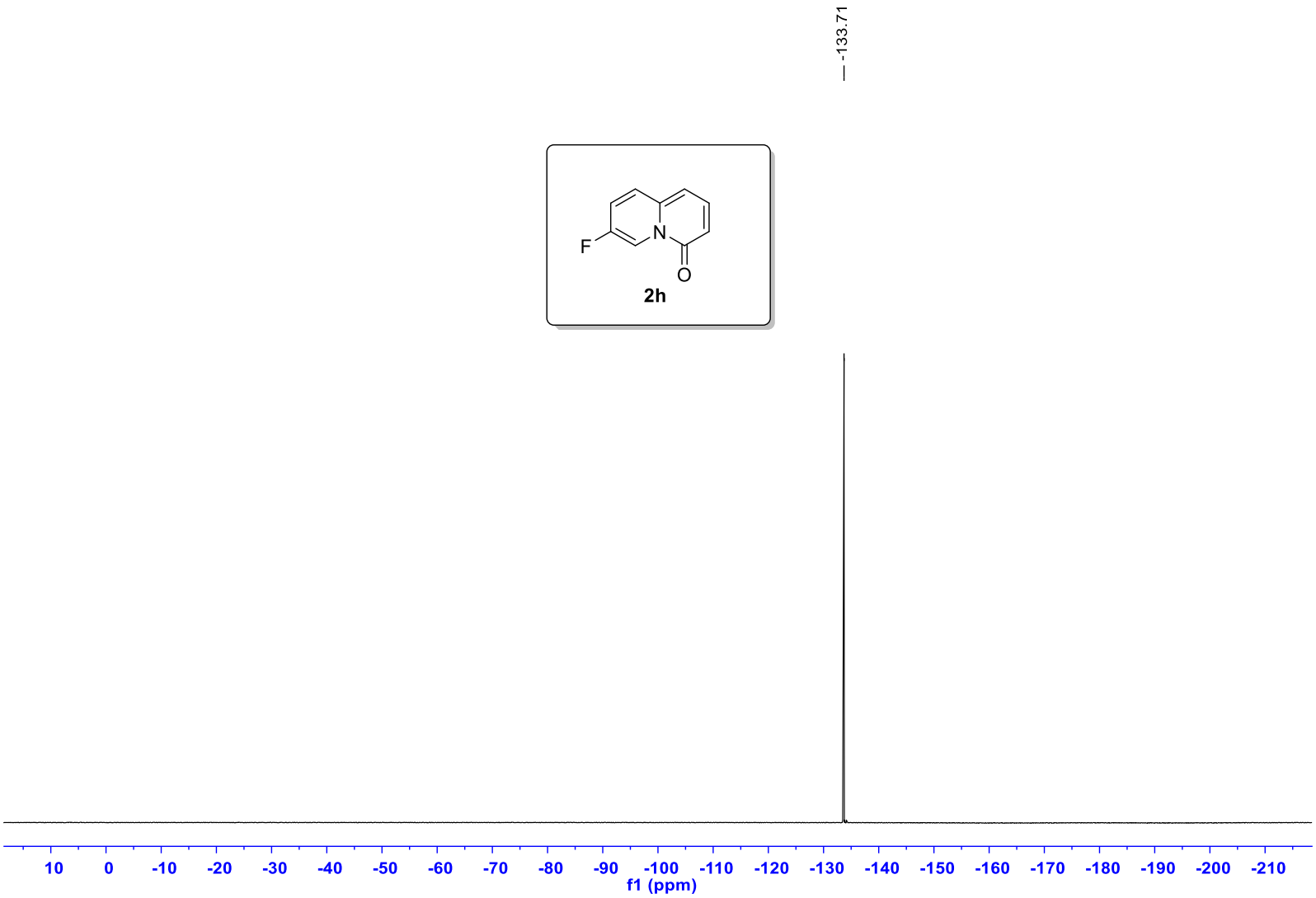

Dec10-2020-OSSO_cJ.50.fid — XPC-X201210-1
7.6090
7.5905
7.5873
7.5687
7.3613
7.3573
7.3391
7.3350
7.1319
7.1152
7.1097
7.0930
6.7915
6.7875
6.7747
6.7706
6.6653
6.6616
6.6469
6.6429
6.6391
6.6212
6.6175
5.0056
4.9937
4.9814
4.9694
4.9609
4.9485
4.9375
— -0.0000
N
O
HO
2g
1.00
0.99
1.01
1.00
1.95
3.05
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
-0.5
f1 (ppm)

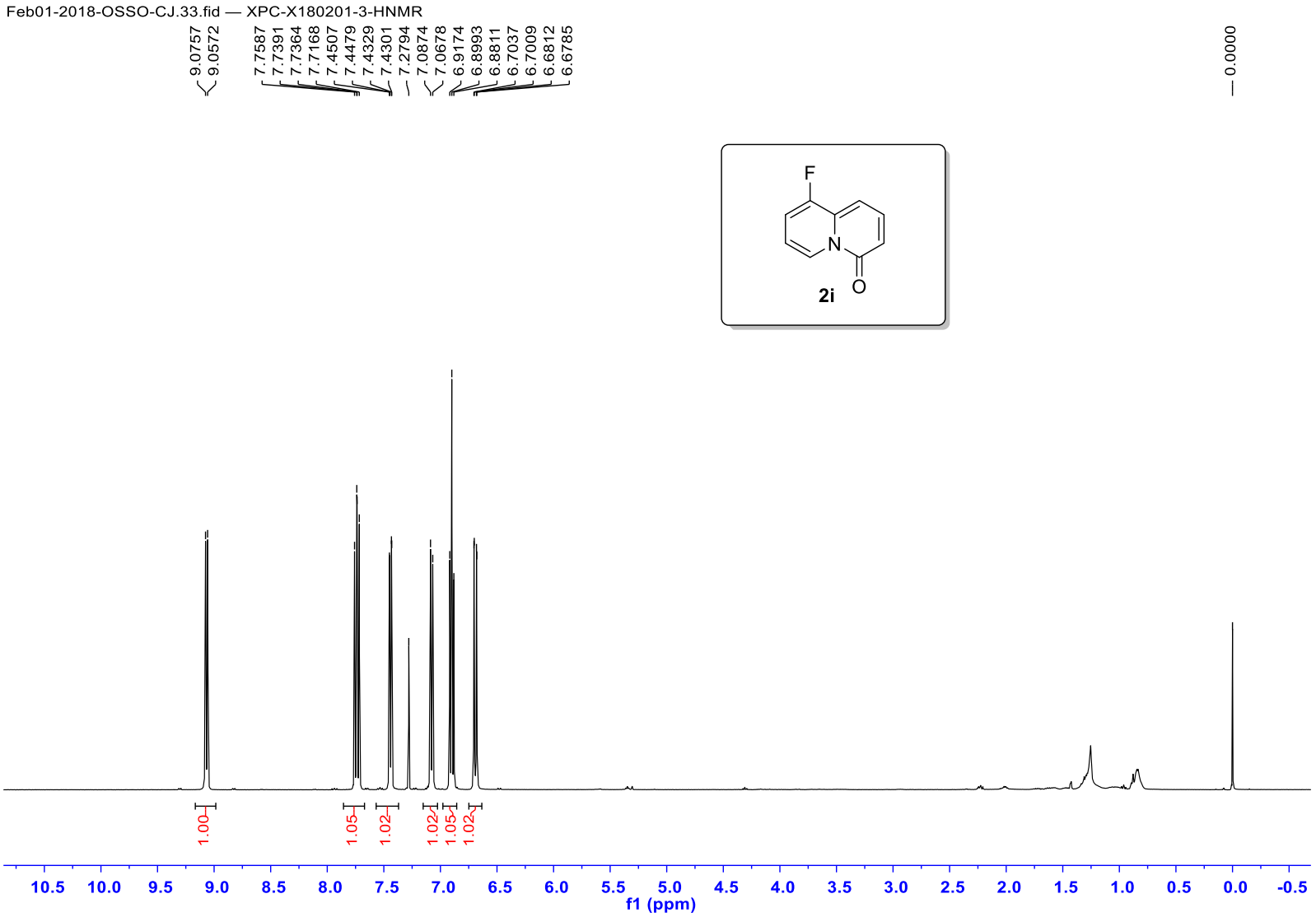

Dec11-2020-OSSO_cJ.13.fid — XPC-X201211-1-C
162.58
144.57
143.53
137.86
128.28
127.21
119.67
113.27
106.18
65.34
HO
N
O
2g
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

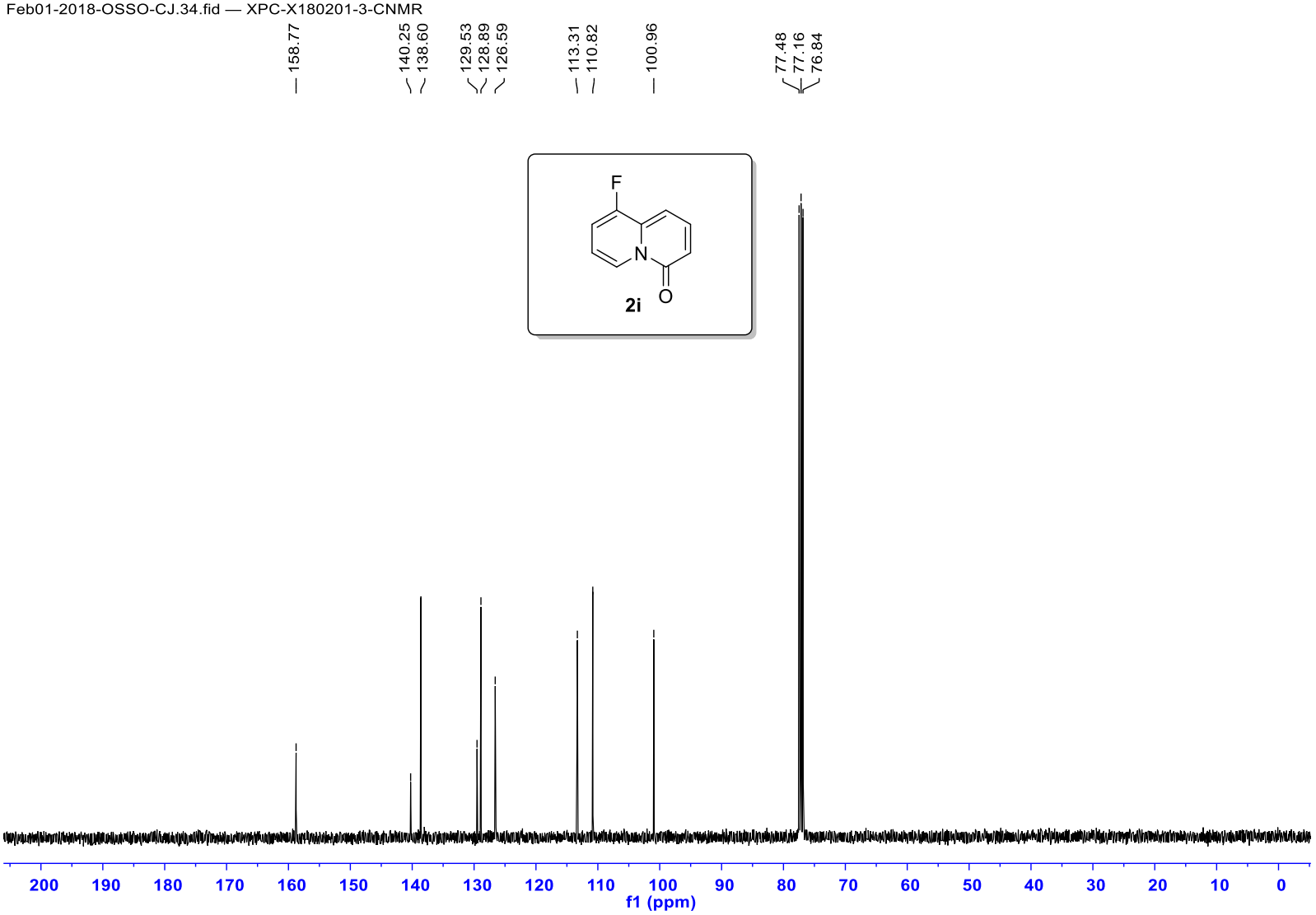

Feb02-2019-OSSO_cJ.44.fid — XPC-X181213-6-HNMR(5F-2f)
9.0558
9.0495
9.0413
9.0351
7.6807
7.6618
7.6587
7.6396
7.5237
7.5098
7.4996
7.4857
7.2952
7.2890
7.2789
7.2758
7.2720
7.2648
7.2545
7.2485
6.7383
6.7194
6.6730
6.6703
6.6510
6.6483
— -0.0000
F
N
O
2h
1.00
1.09
1.07
1.20
1.11
1.00
10.5 10.0 9.5 9.0 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 -0.5
f1 (ppm)


Dec13-2018-OSSO_cJ.58.fid — XPC-X181213-5CNMR
158.76
140.24
138.59
129.52
128.89
126.57
113.32
110.80
100.97
77.47
77.16
76.84
F
N
O
2h
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

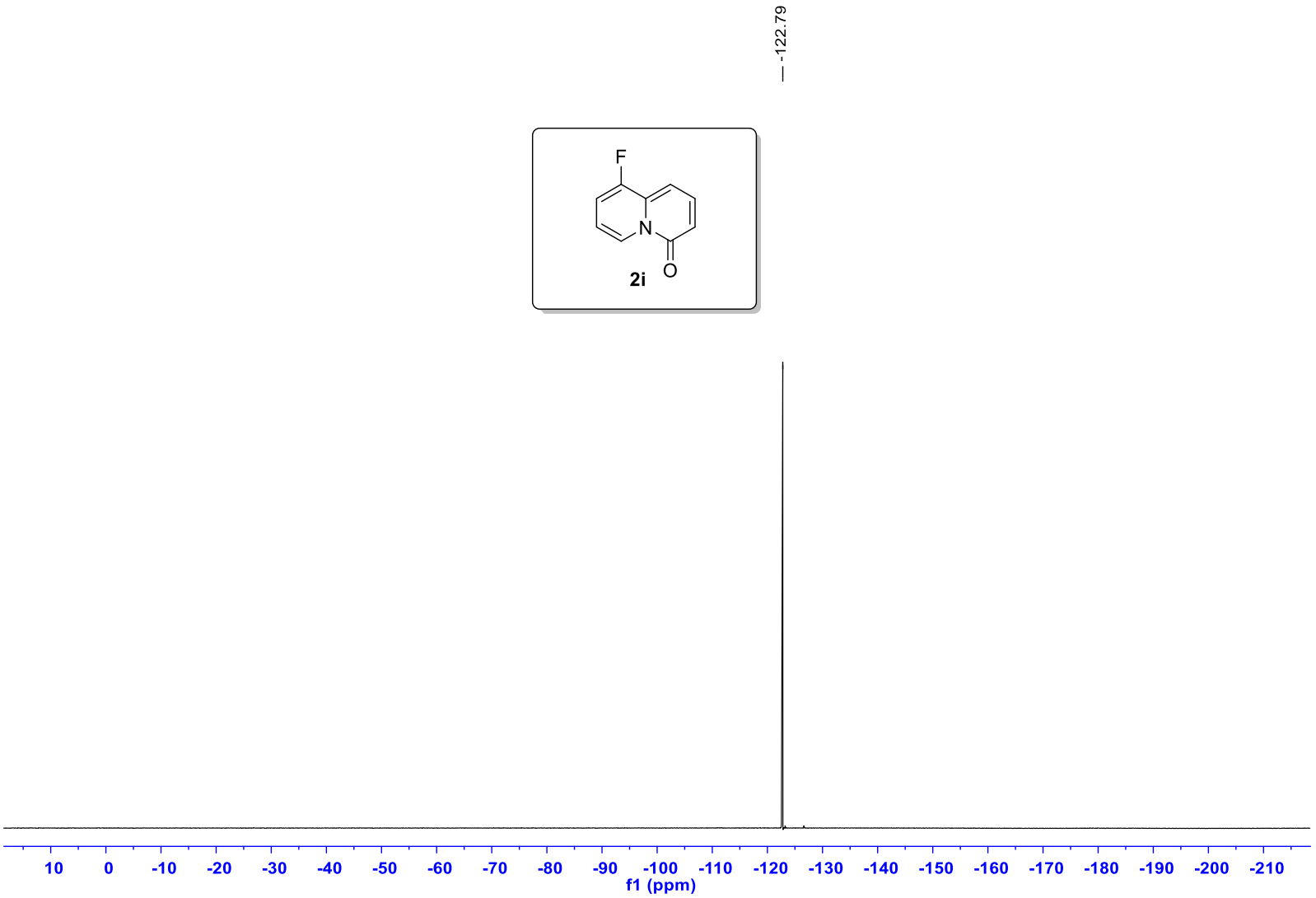
Feb02-2019-OSSO_cJ.45.fid — XPC-X181213-6-FNMR(5F-2f)

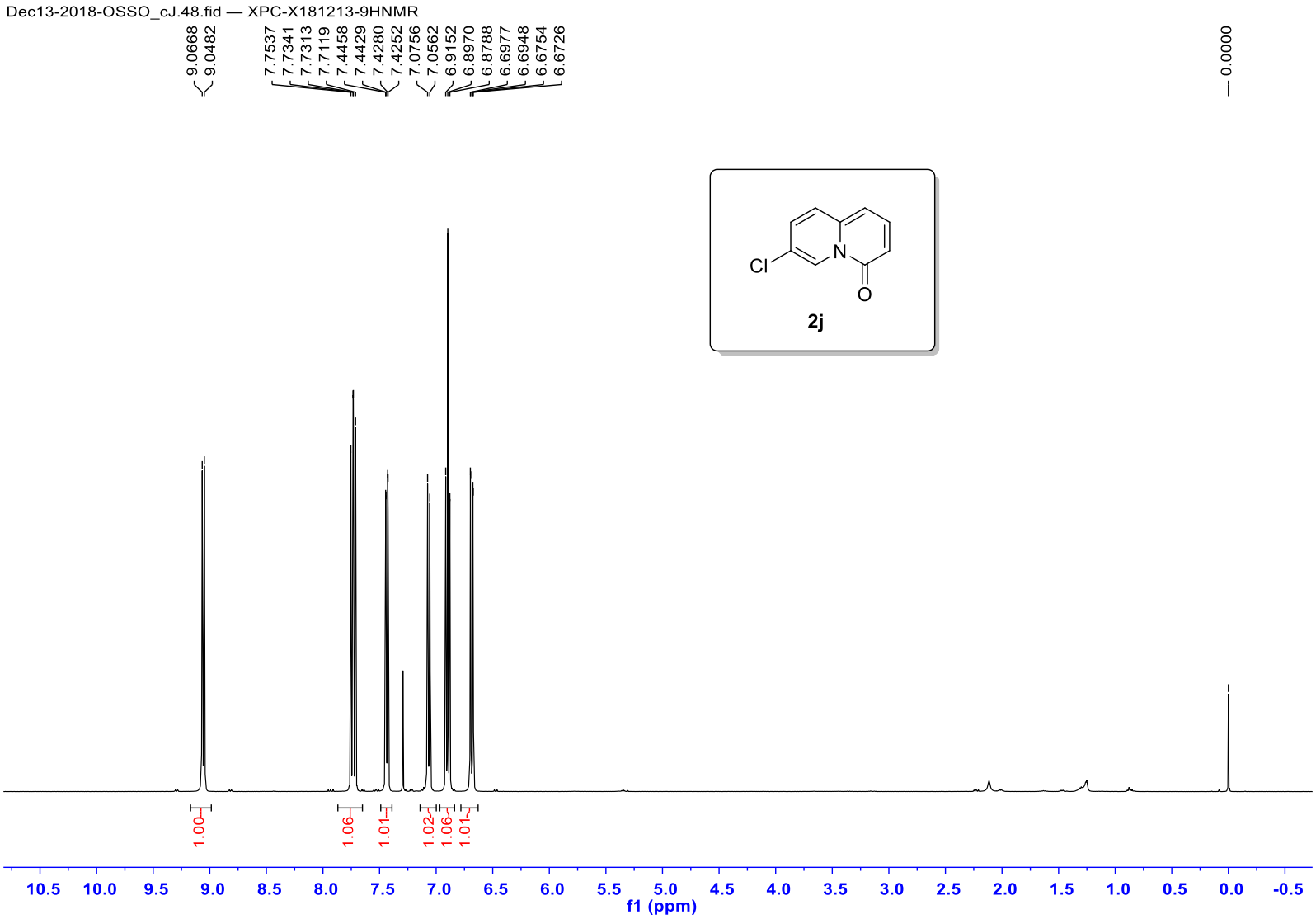


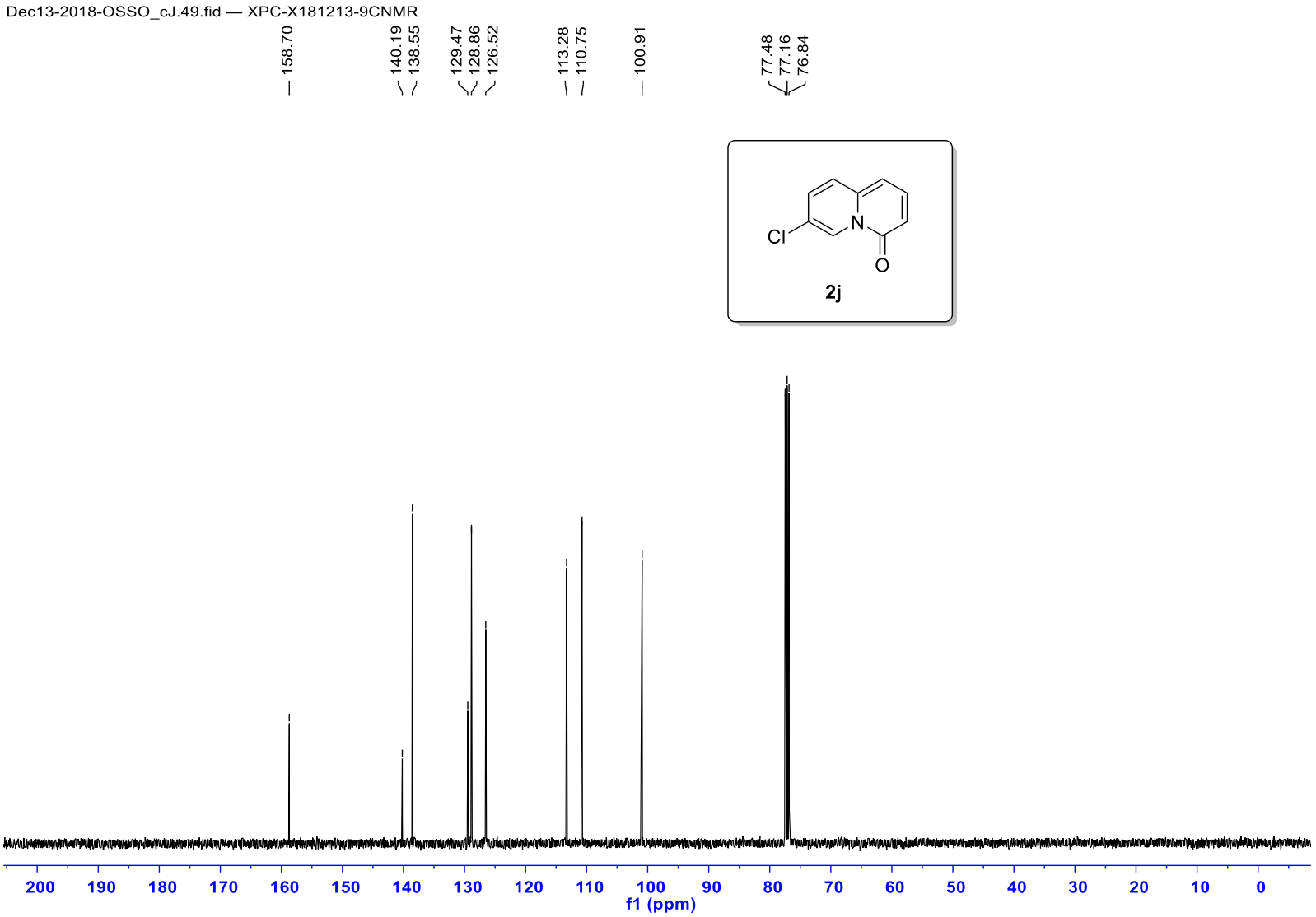

Feb01-2018-OSSO-CJ.33.fid — XPC-X180201-3-HNMR
9.0757
9.0572
7.7587
7.7391
7.7364
7.7168
7.4507
7.4479
7.4329
7.4301
7.2794
7.0874
7.0678
6.9174
6.8993
6.8811
6.7037
6.7009
6.6812
6.6785
0.0000
F
N
O
2i
1.00
1.05
1.02
1.02
1.05
1.02
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

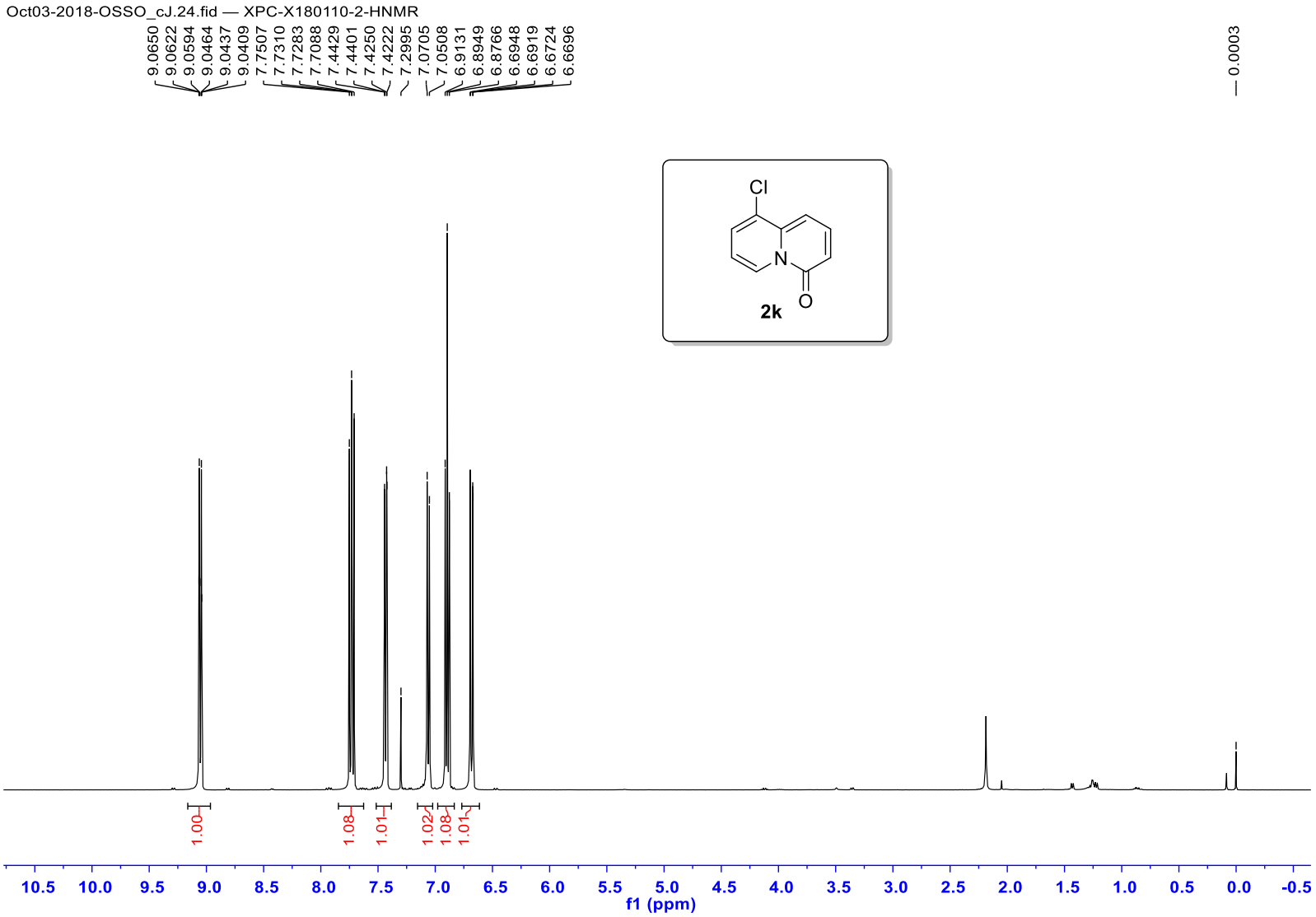

Feb01-2018-OSSO-CJ.34.fid — XPC-X180201-3-CNMR
158.77
140.25
138.60
129.53
128.89
126.59
113.31
110.82
100.96
77.48
77.16
76.84
F
N
O
2i
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

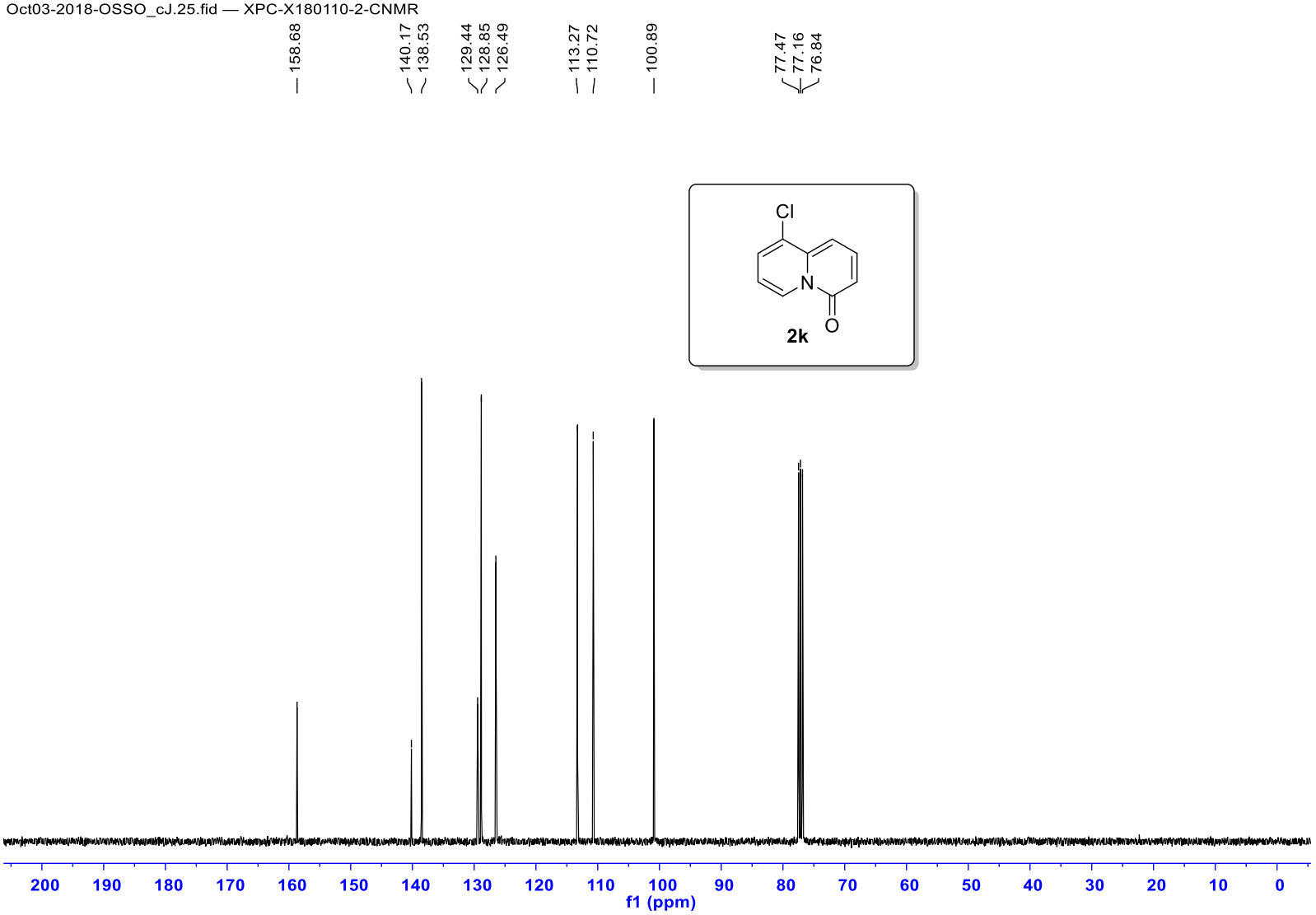
Feb02-2019-OSSO_cJ.41.fid — XPC-X181213-4-FNMR(5F-2f)

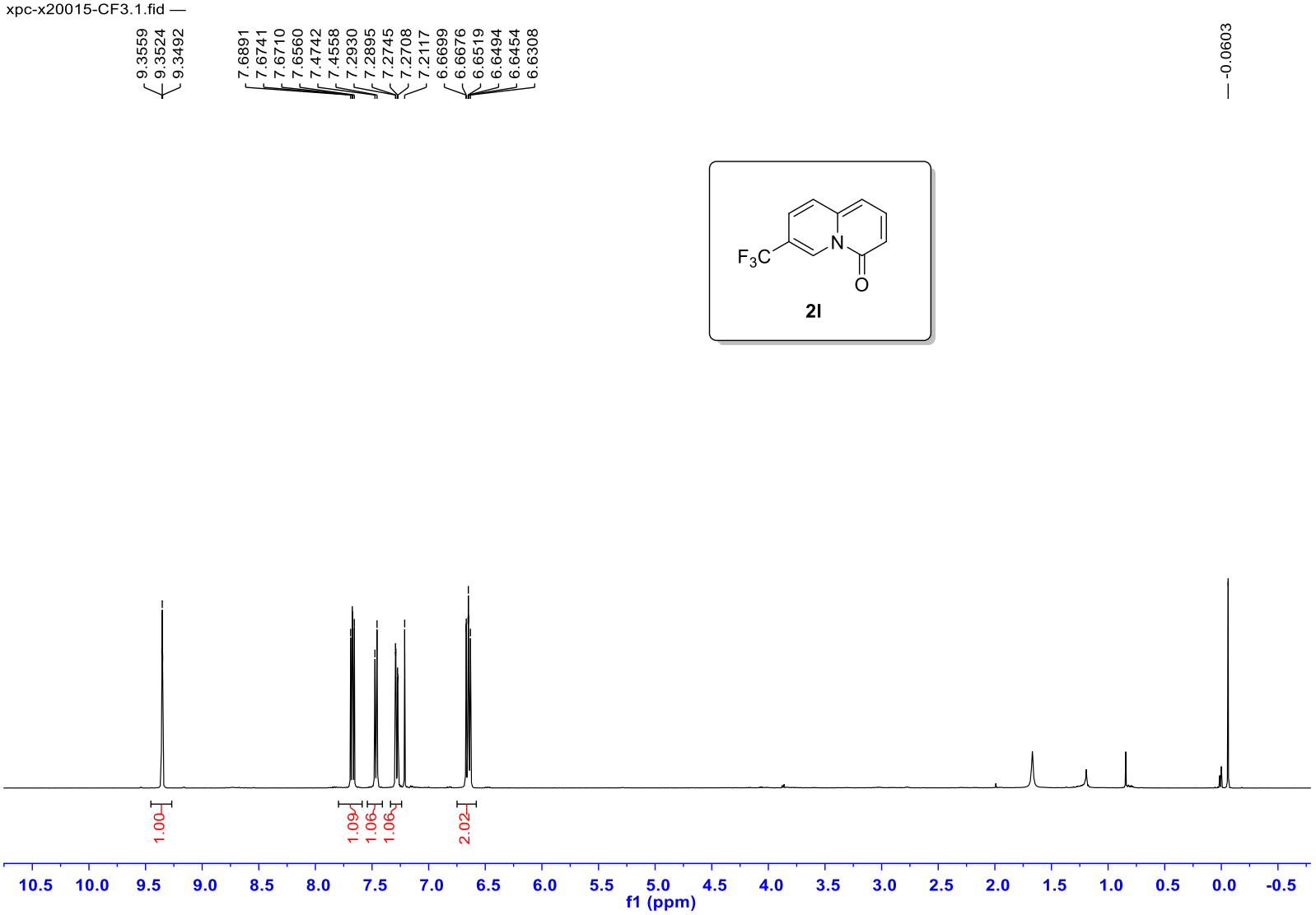


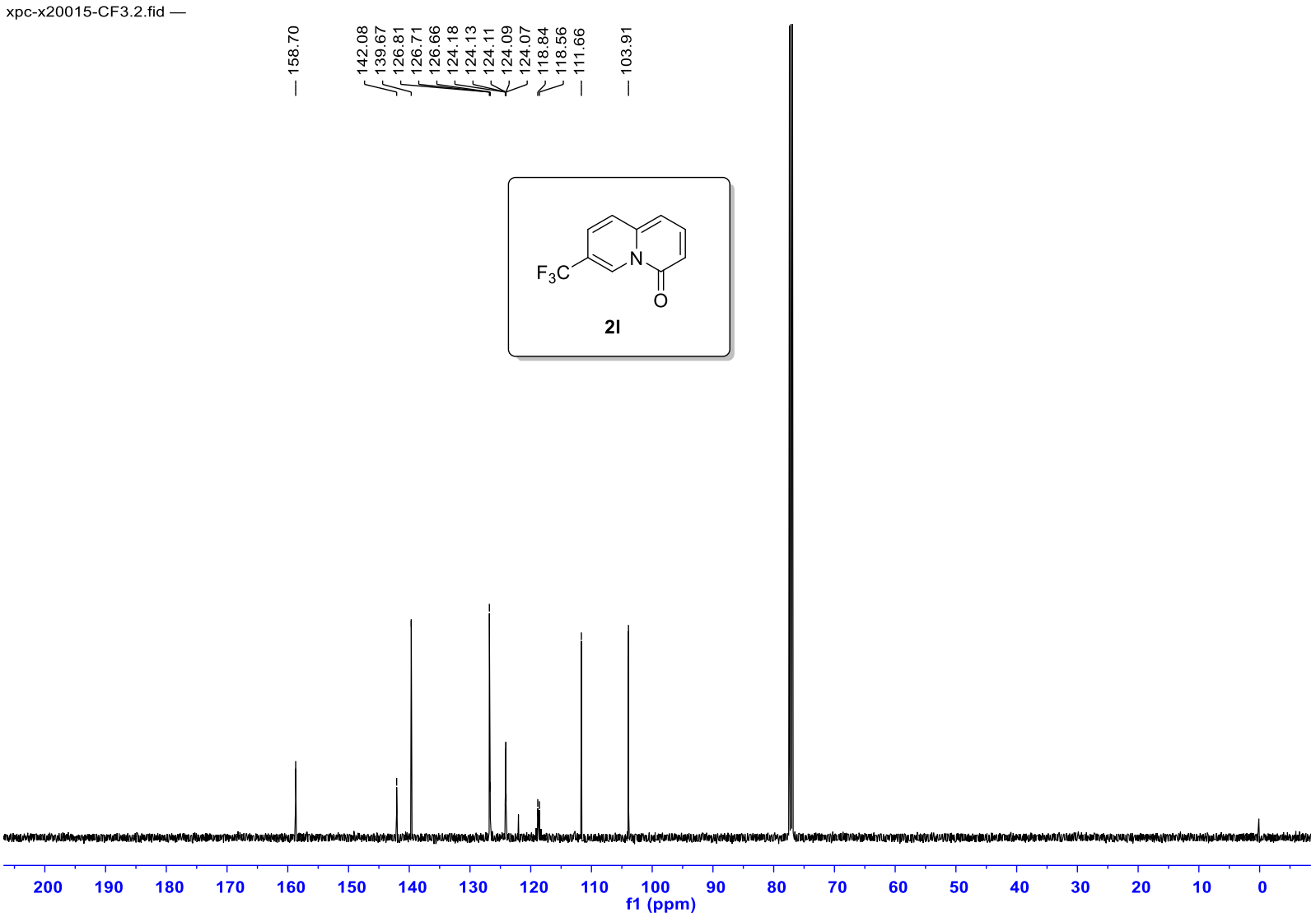

Dec13-2018-OSSO_cJ.48.fid — XPC-X181213-9HNMR
9.0668
9.0482
7.7537
7.7341
7.7313
7.7119
7.4458
7.4429
7.4280
7.4252
7.0756
7.0562
6.9152
6.8970
6.8788
6.6977
6.6948
6.6754
6.6726
0.0000
Cl
N
O
2j
1.00
1.06
1.01
1.02
1.06
1.01
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


Dec13-2018-OSSO_cJ.49.fid — XPC-X181213-9CNMR
158.70
140.19
138.55
129.47
128.86
126.52
113.28
110.75
100.91
77.48
77.16
76.84
Cl
N
O
2j
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

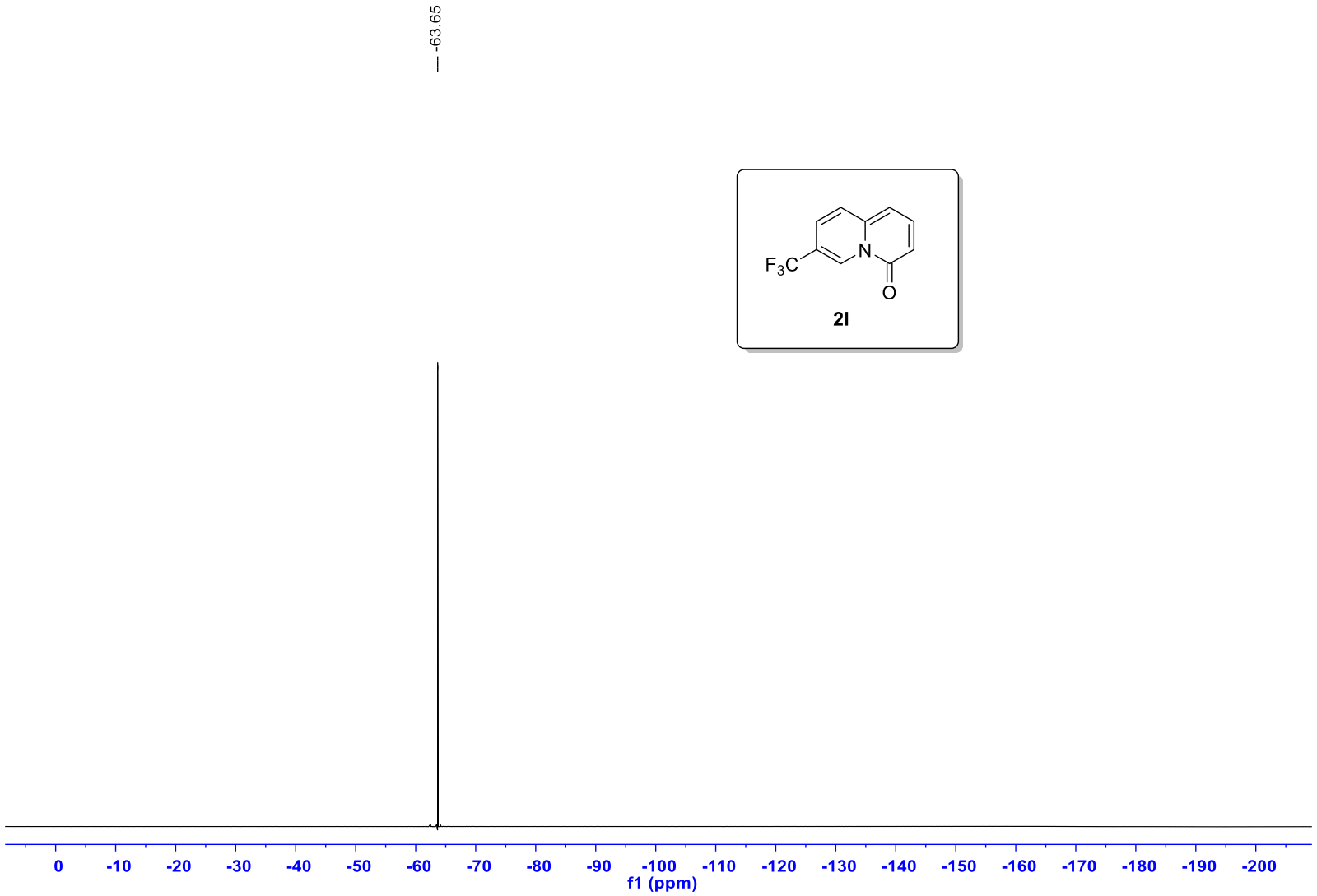

Oct03-2018-OSSO_cJ.24.fid — XPC-X180110-2-HNMR
9.0650
9.0622
9.0594
9.0464
9.0437
9.0409
7.7507
7.7310
7.7283
7.7088
7.4429
7.4401
7.4250
7.4222
7.2995
7.0705
7.0508
6.9131
6.8949
6.8766
6.6948
6.6919
6.6724
6.6696
— 0.0003
Cl
N
O
2k
1.00
1.08
1.01
1.02
1.08
1.01
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 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 -0.5
f1 (ppm)

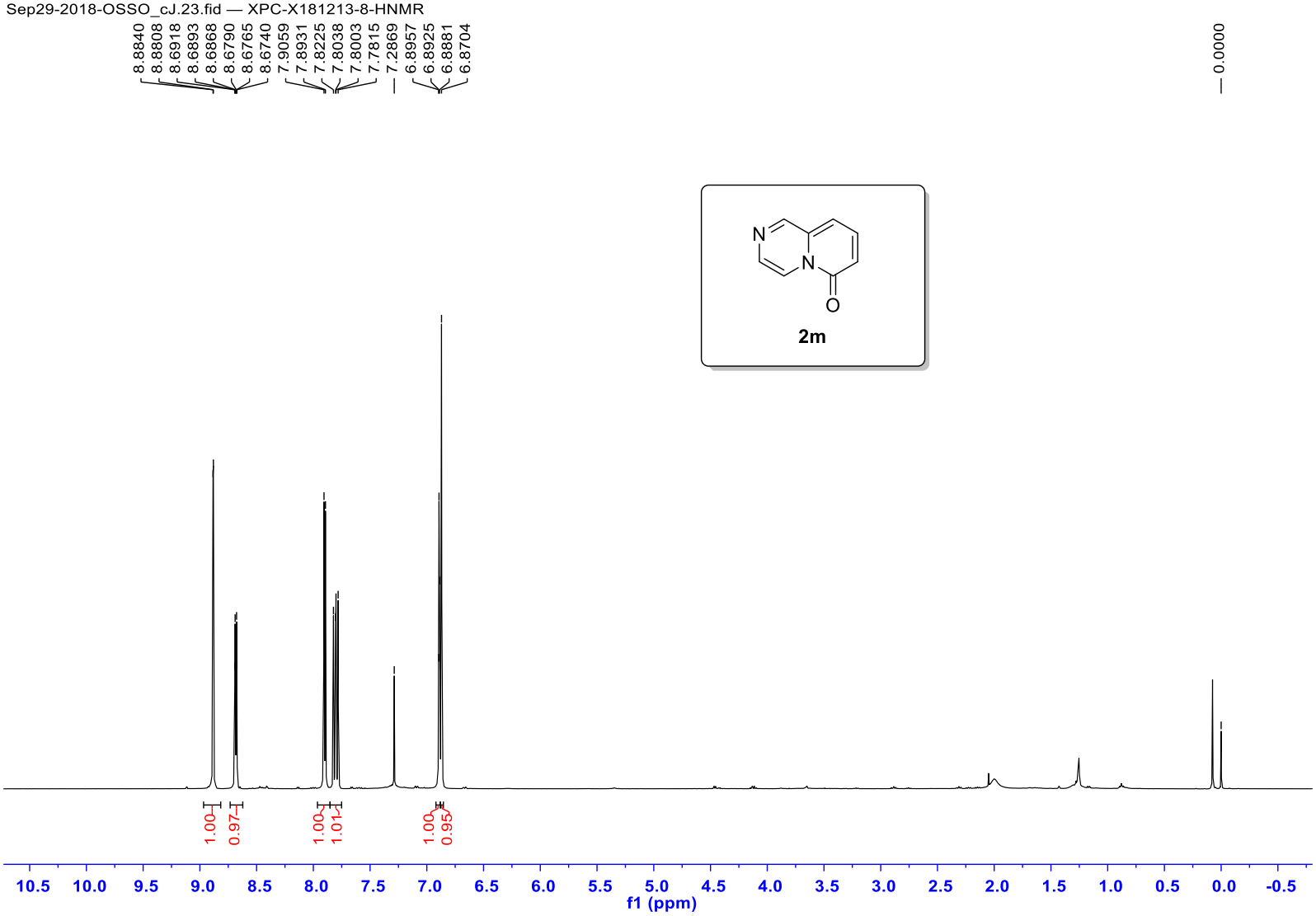

Oct03-2018-OSSO_cJ.25.fid — XPC-X180110-2-CNMR
158.68
140.17
138.53
129.44
128.85
126.49
113.27
110.72
100.89
77.47
77.16
76.84
Cl
N
O
2k
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


xpc-x20015-CF3.1.fid
9.3559
9.3524
9.3492
7.6891
7.6741
7.6710
7.6560
7.4742
7.4558
7.2930
7.2895
7.2745
7.2708
7.2117
6.6699
6.6676
6.6519
6.6494
6.6454
6.6308
-0.0603
F3C
N
O
2l
1.00
1.09
1.06
1.06
2.02
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 -0.5
f1 (ppm)

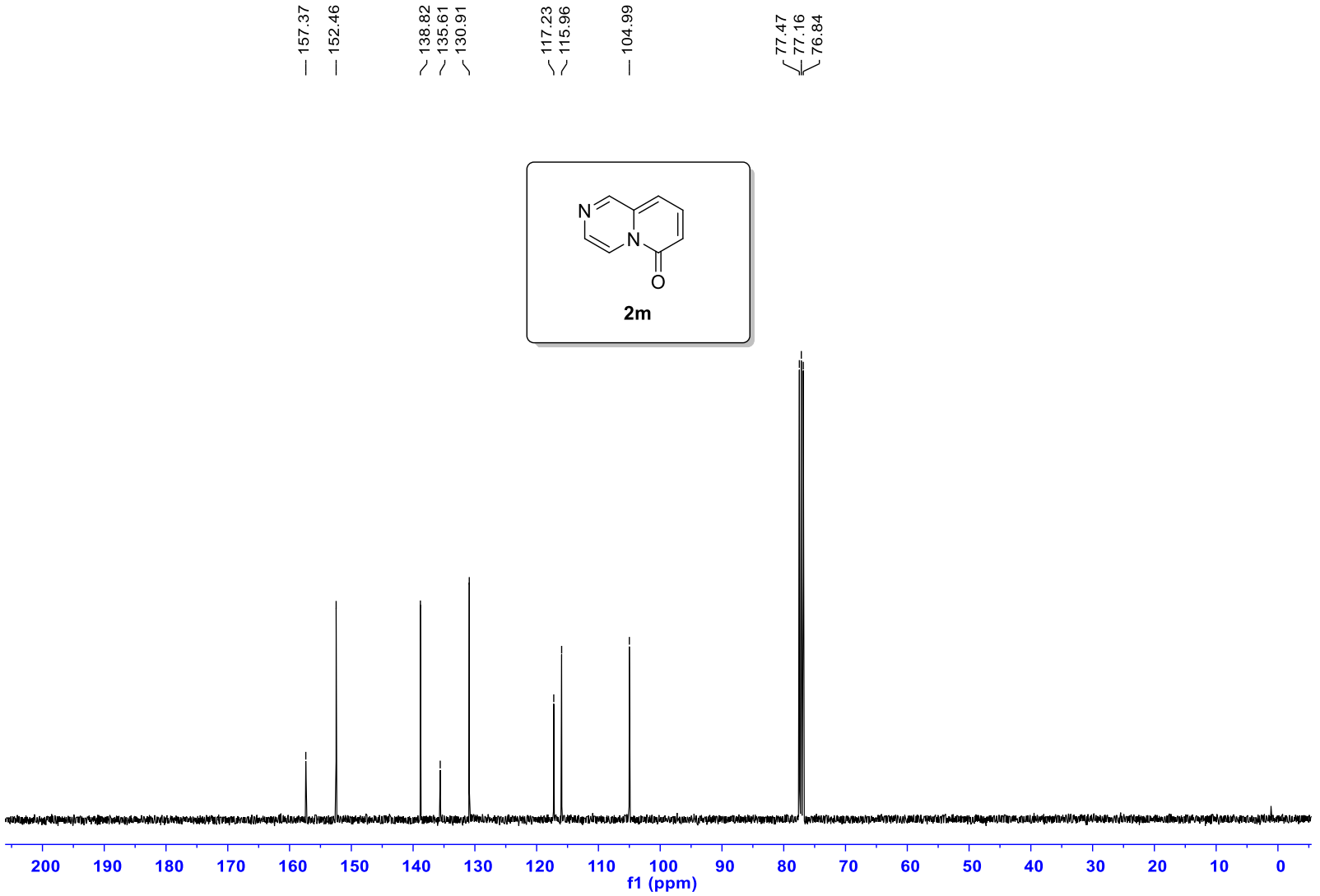

xpc-x20015-CF3.2.fid
158.70
142.08
139.67
126.81
126.71
126.66
124.18
124.13
124.11
124.09
124.07
118.84
118.56
111.66
103.91
F3C
N
O
2l
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

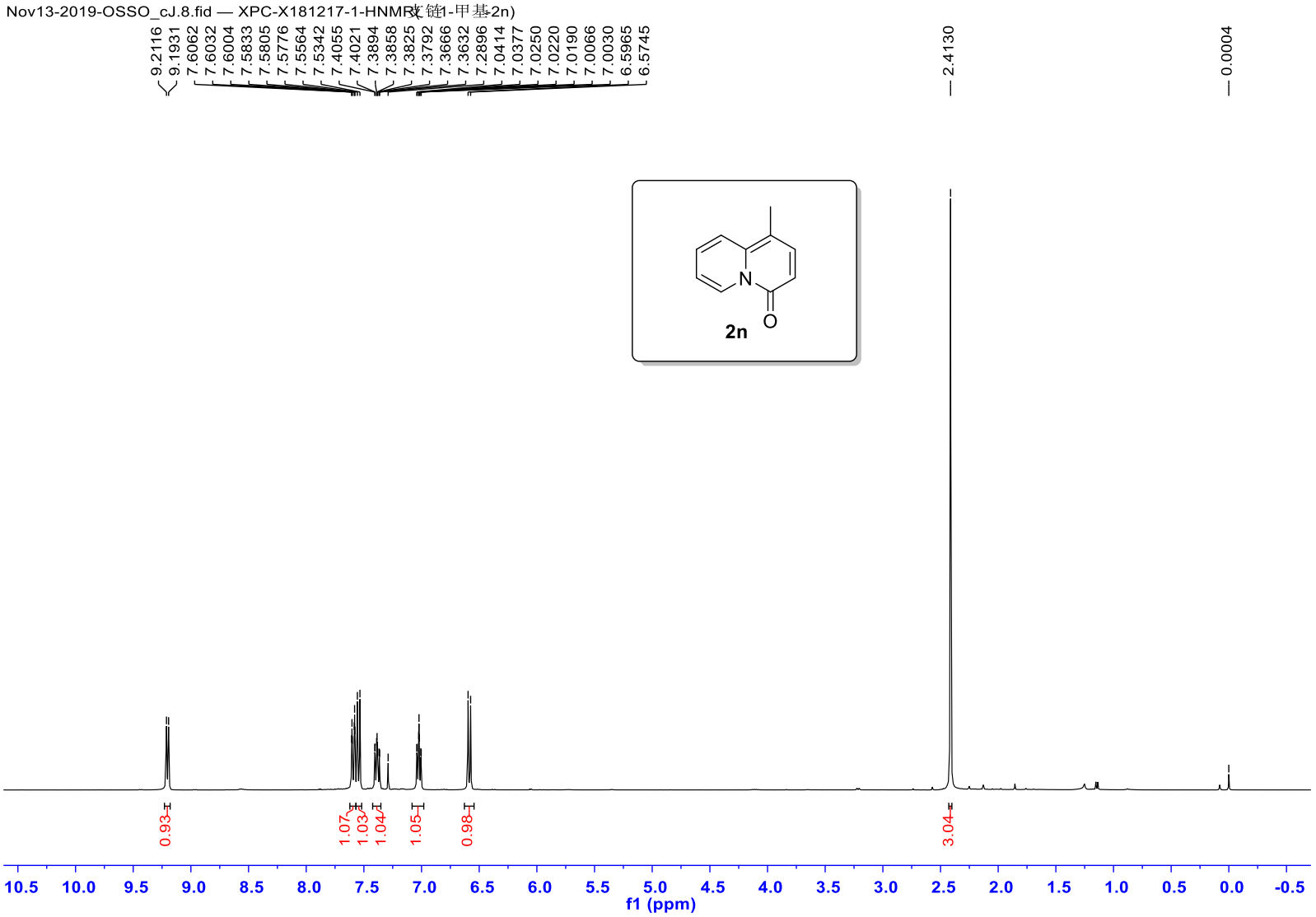
xpc-x20015-CF3.3.fid —

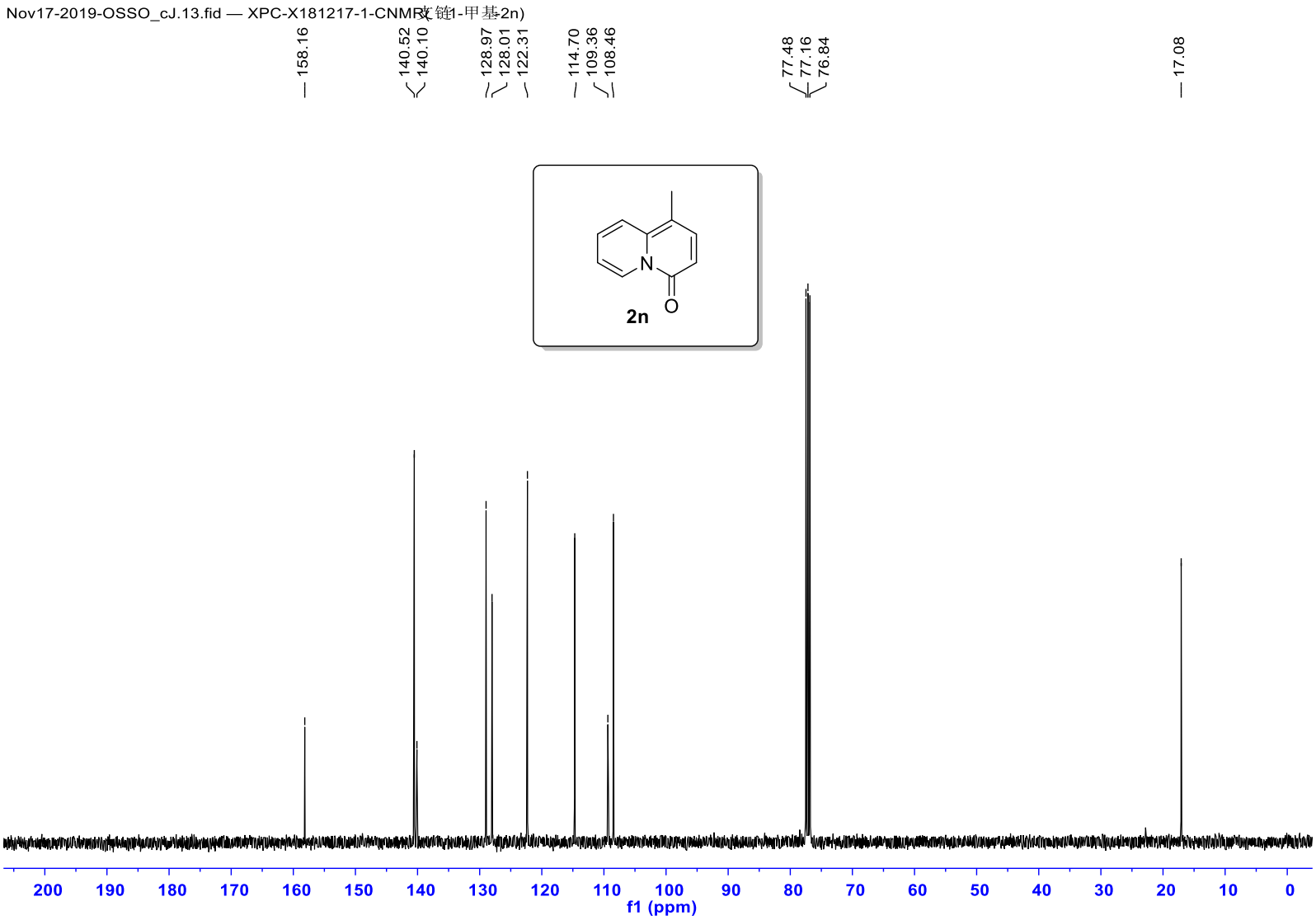


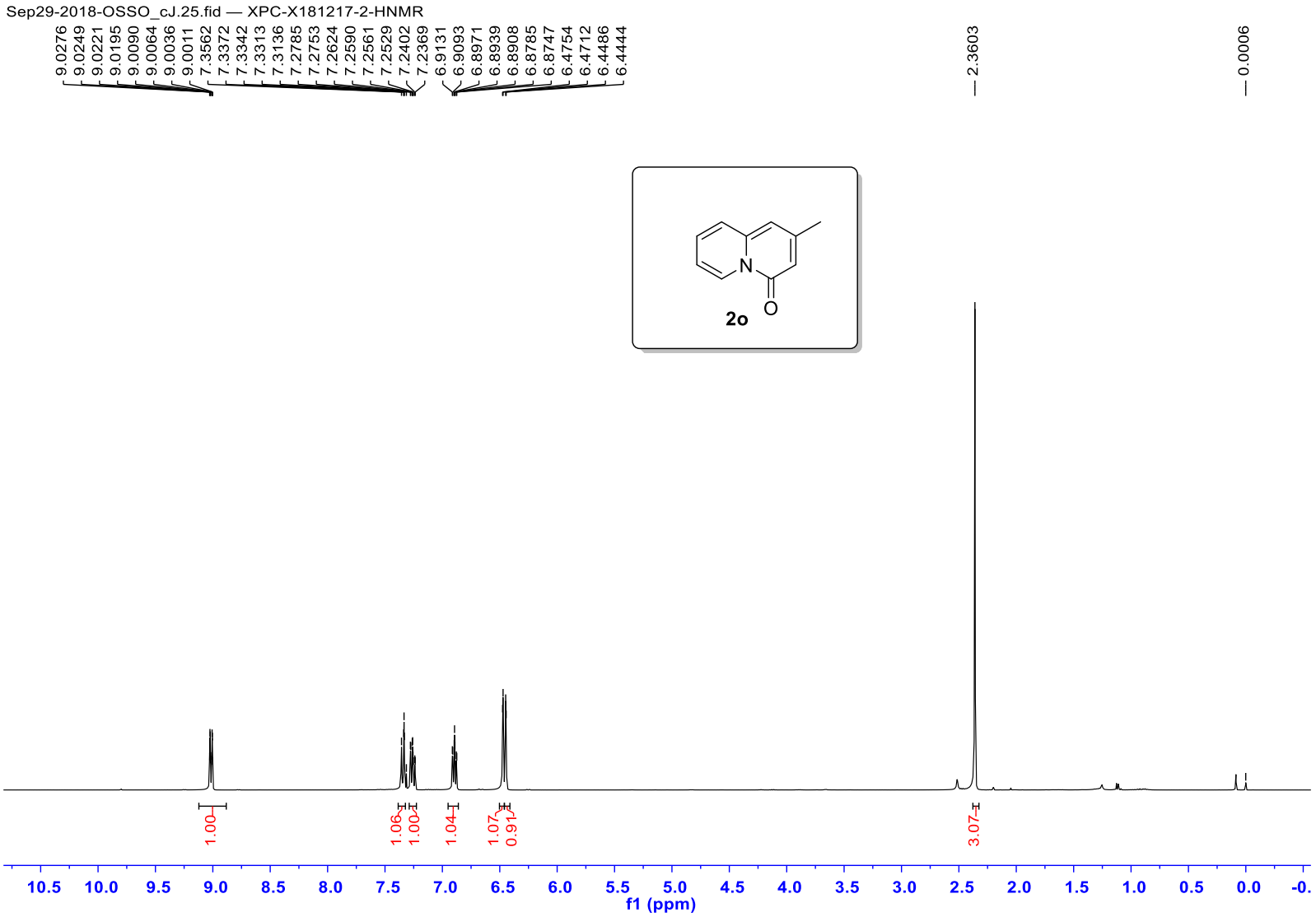

Sep29-2018-OSSO_cJ.23.fid — XPC-X181213-8-HNMR
8.8840
8.8808
8.6918
8.6893
8.6868
8.6790
8.6765
8.6740
7.9059
7.8931
7.8225
7.8038
7.8003
7.7815
7.2869
6.8957
6.8925
6.8881
6.8704
0.0000
N
N
O
2m
1.00
0.97
1.00
1.01
1.00
0.95
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

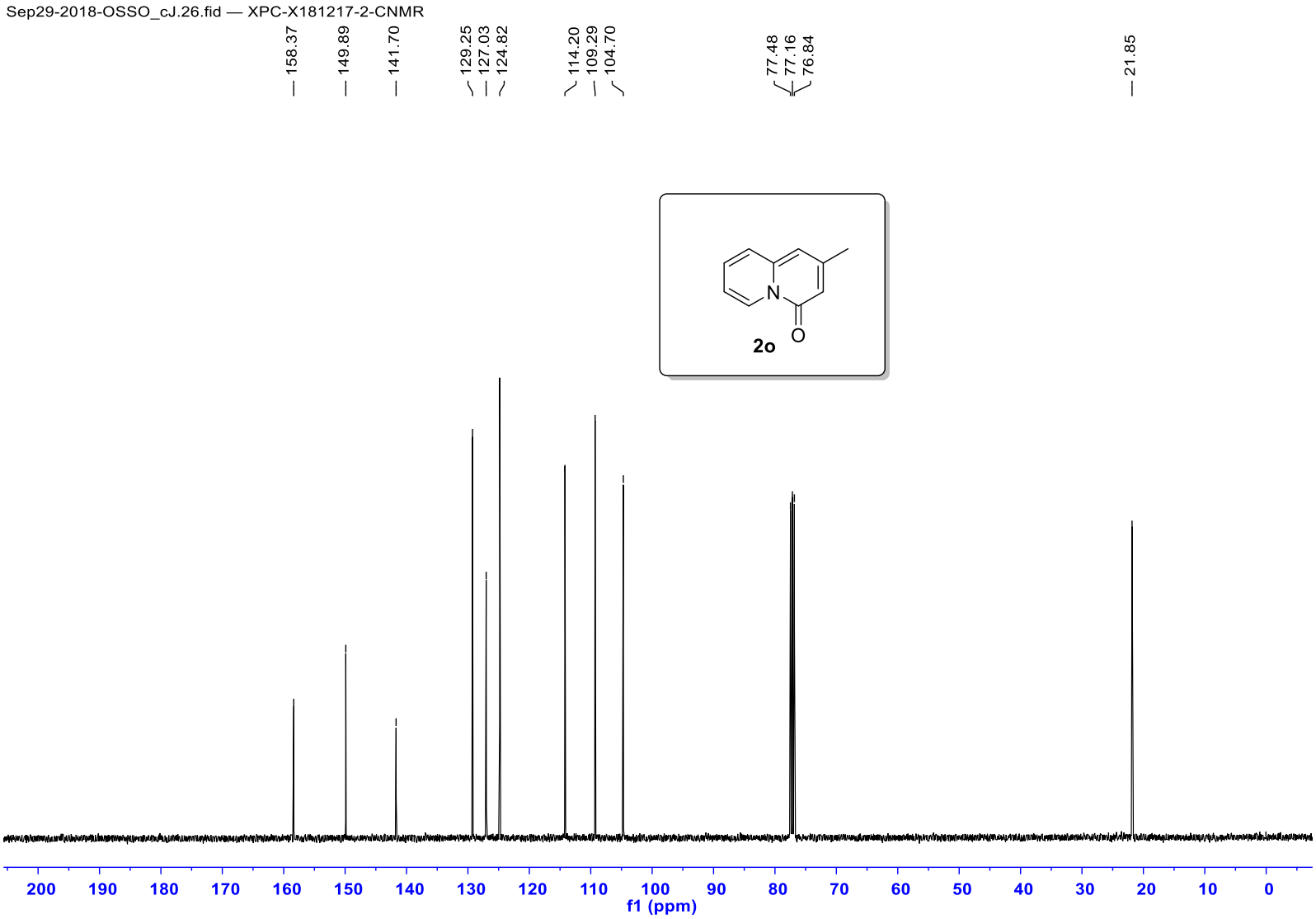
Sep29-2018-OSSO_cJ.24.fid — XPC-X181213-8-CNMR

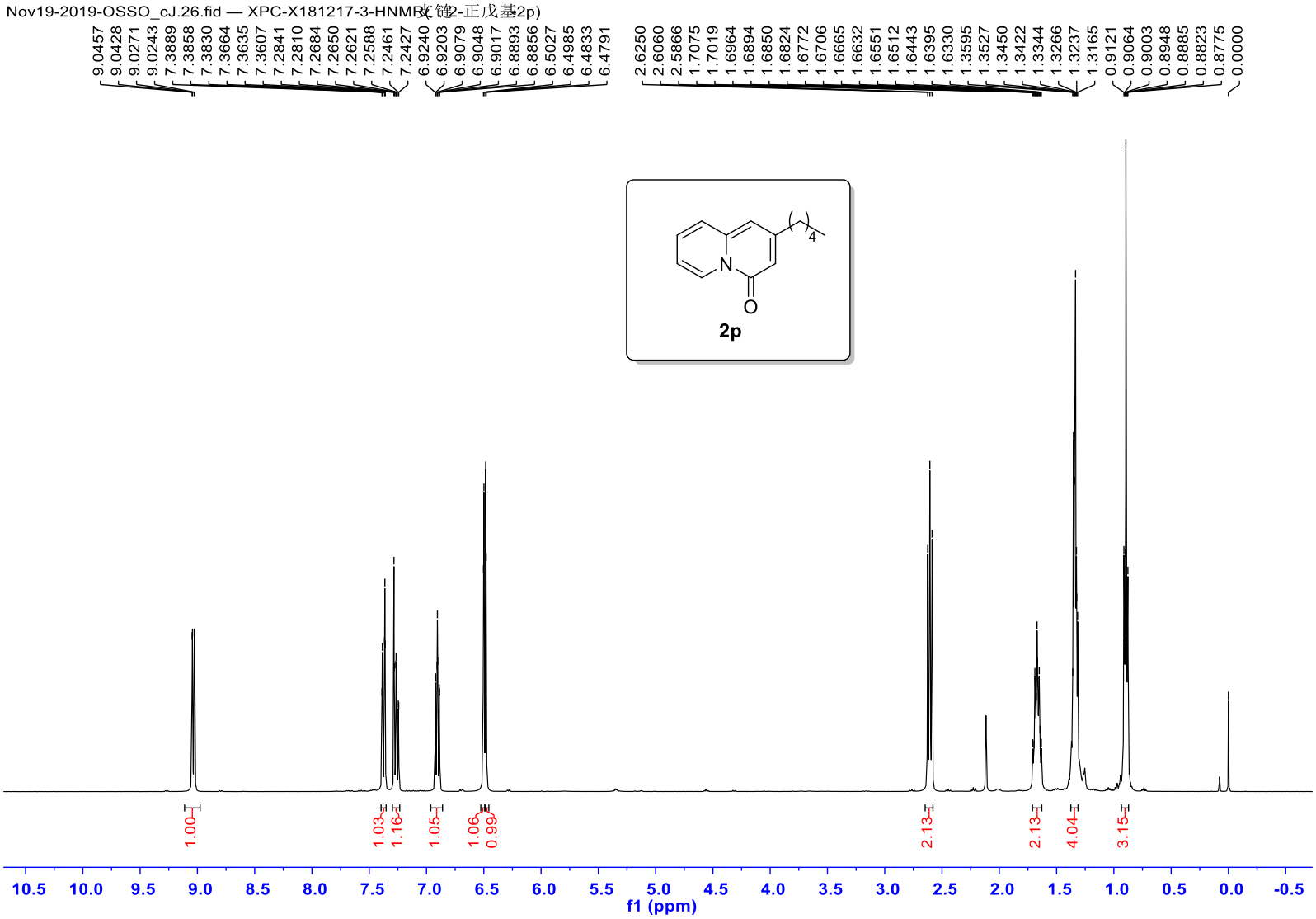


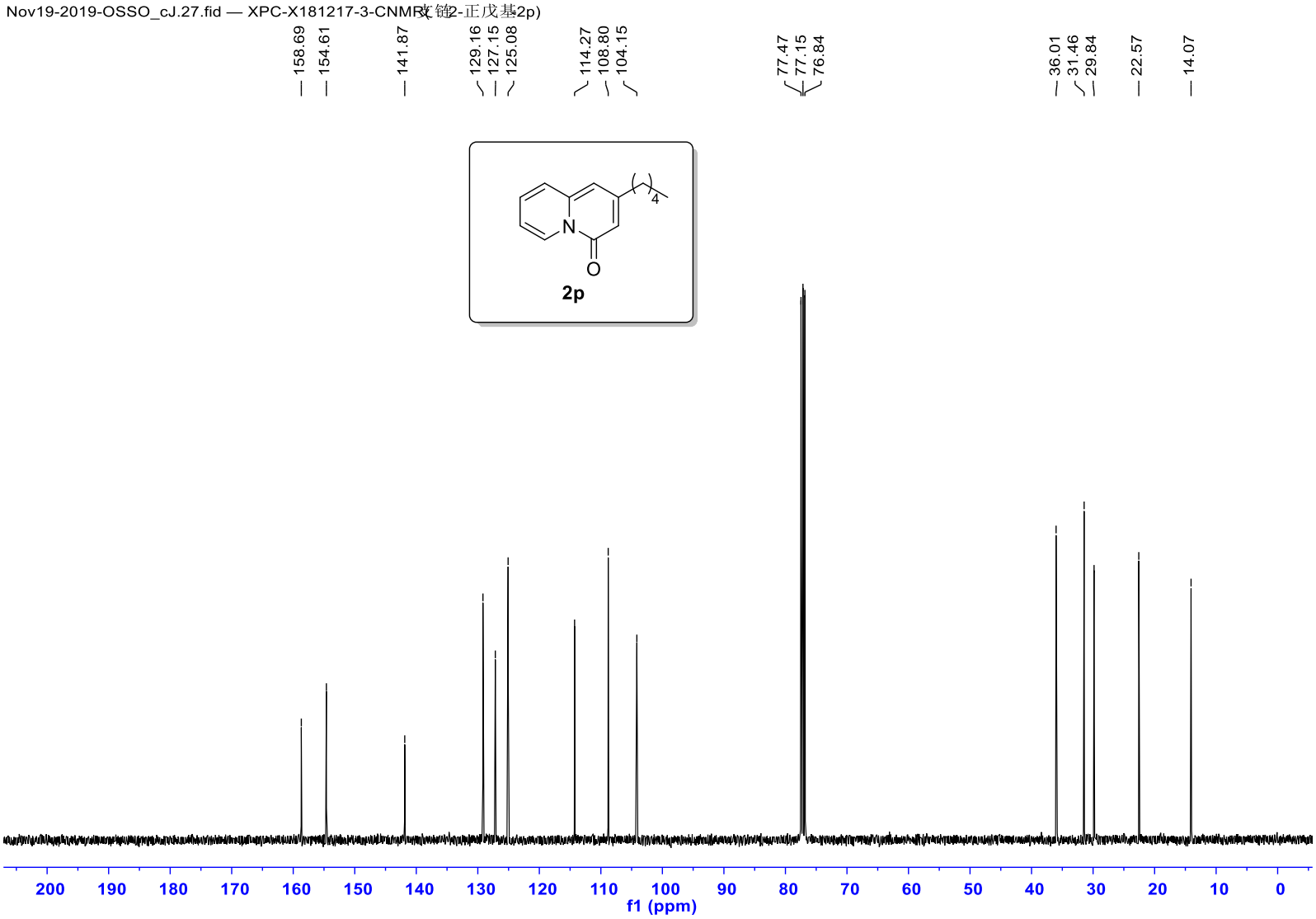

Nov13-2019-OSSO_cJ.8.fid — XPC-X181217-1-HNMR(支链1-甲基2n)
9.2116
9.1931
7.6062
7.6032
7.6004
7.5833
7.5805
7.5776
7.5564
7.5342
7.4055
7.4021
7.3894
7.3858
7.3825
7.3792
7.3666
7.3632
7.2896
7.0414
7.0377
7.0250
7.0220
7.0190
7.0066
7.0030
6.5965
6.5745
2.4130
0.0004
N
O
2n
0.93
1.07
1.03
1.04
1.05
0.98
3.04
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 -0.5
f1 (ppm)

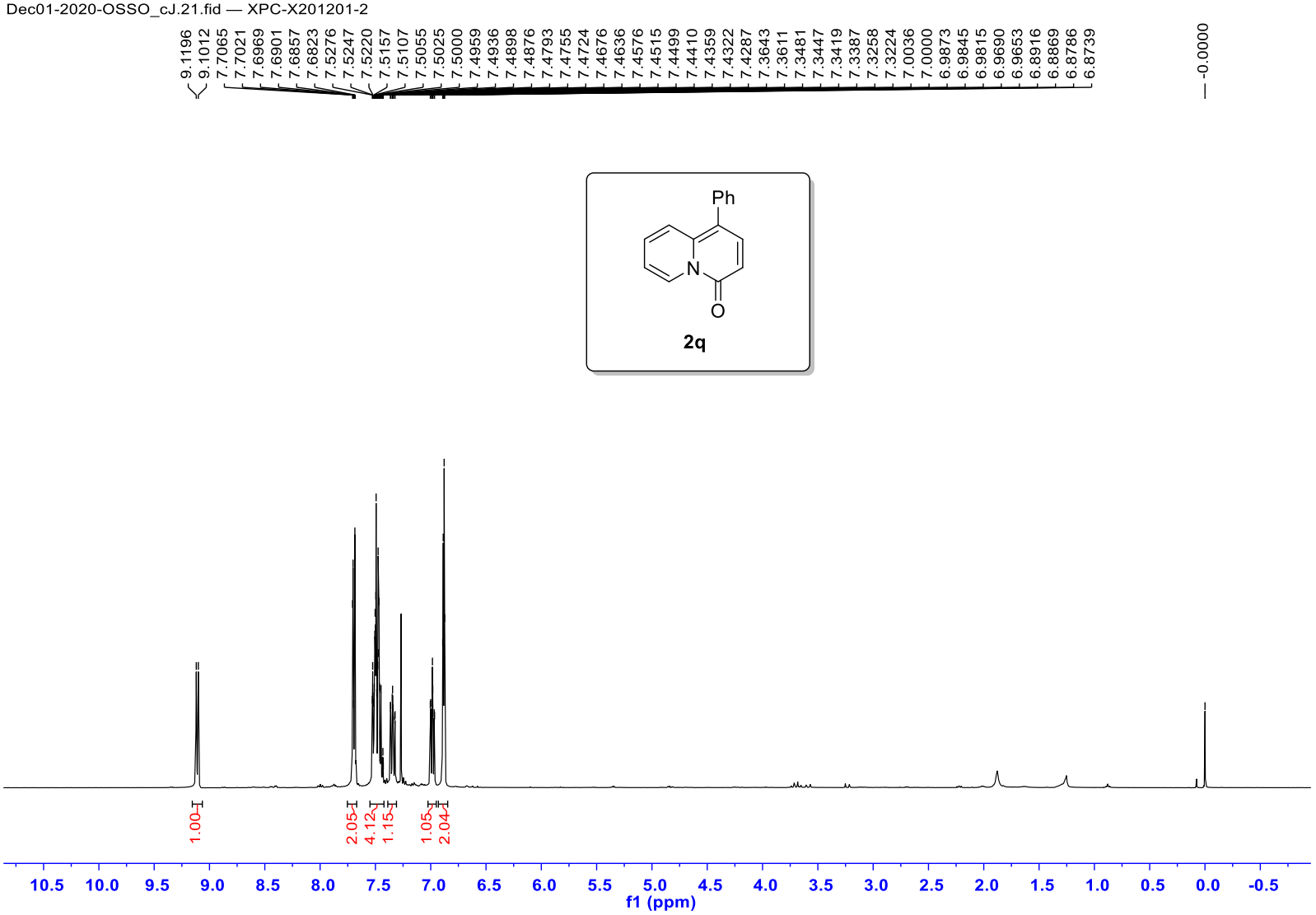

Nov17-2019-OSSO_cJ.13.fid — XPC-X181217-1-CNMR(支链1-甲基2n)
158.16
140.52
140.10
128.97
128.01
122.31
114.70
109.36
108.46
77.48
77.16
76.84
17.08
N
O
2n
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

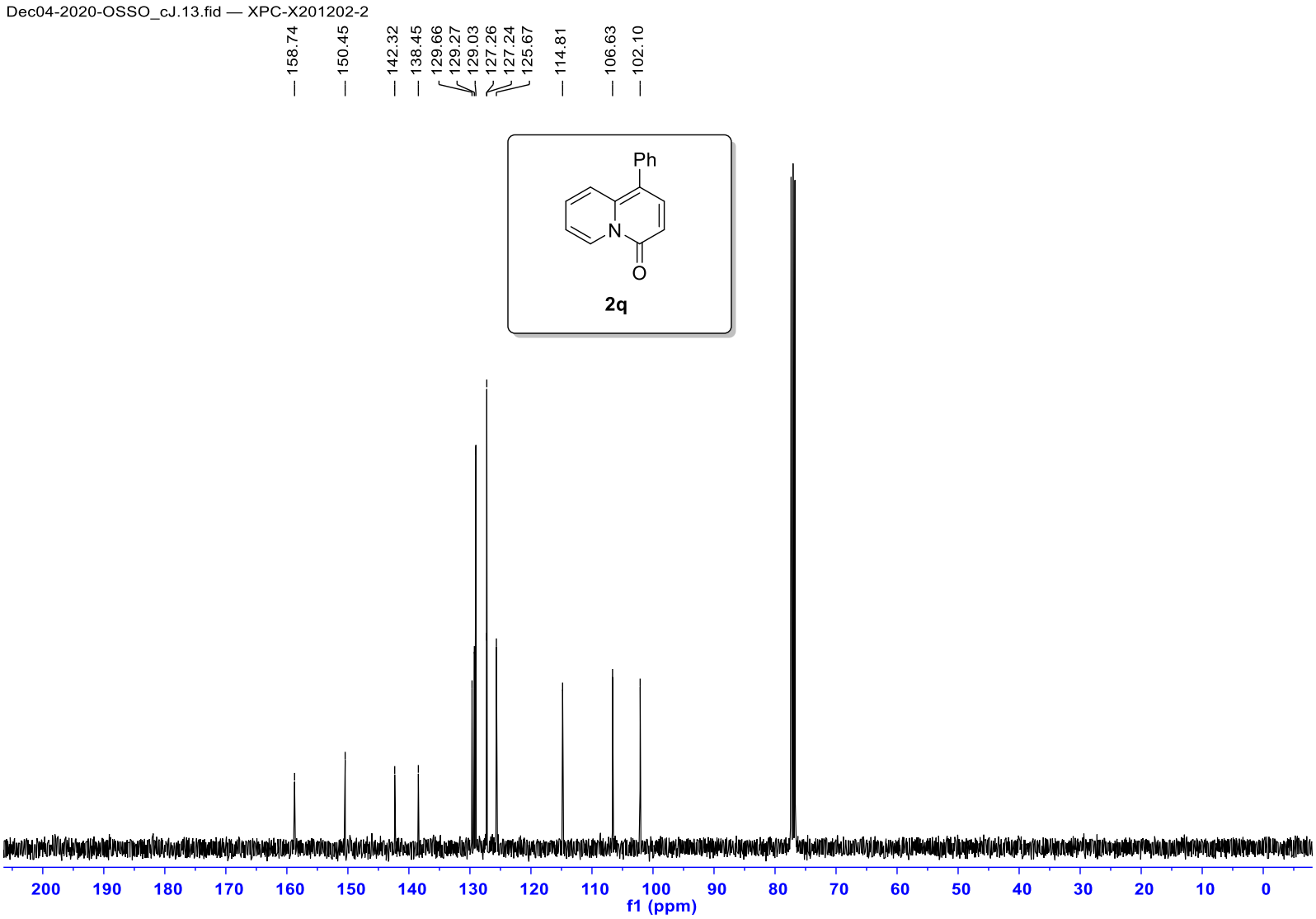

Sep29-2018-OSSO_cJ.25.fid — XPC-X181217-2-HNMR
9.0276
9.0249
9.0221
9.0195
9.0090
9.0064
9.0036
9.0011
7.3562
7.3372
7.3342
7.3313
7.3136
7.2785
7.2753
7.2624
7.2590
7.2561
7.2529
7.2402
7.2369
6.9131
6.9093
6.8971
6.8939
6.8908
6.8785
6.8747
6.4754
6.4712
6.4486
6.4444
2.3603
0.0006
2o
1.00
1.06
1.00
1.04
1.07
0.91
3.07
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
-0.
f1 (ppm)

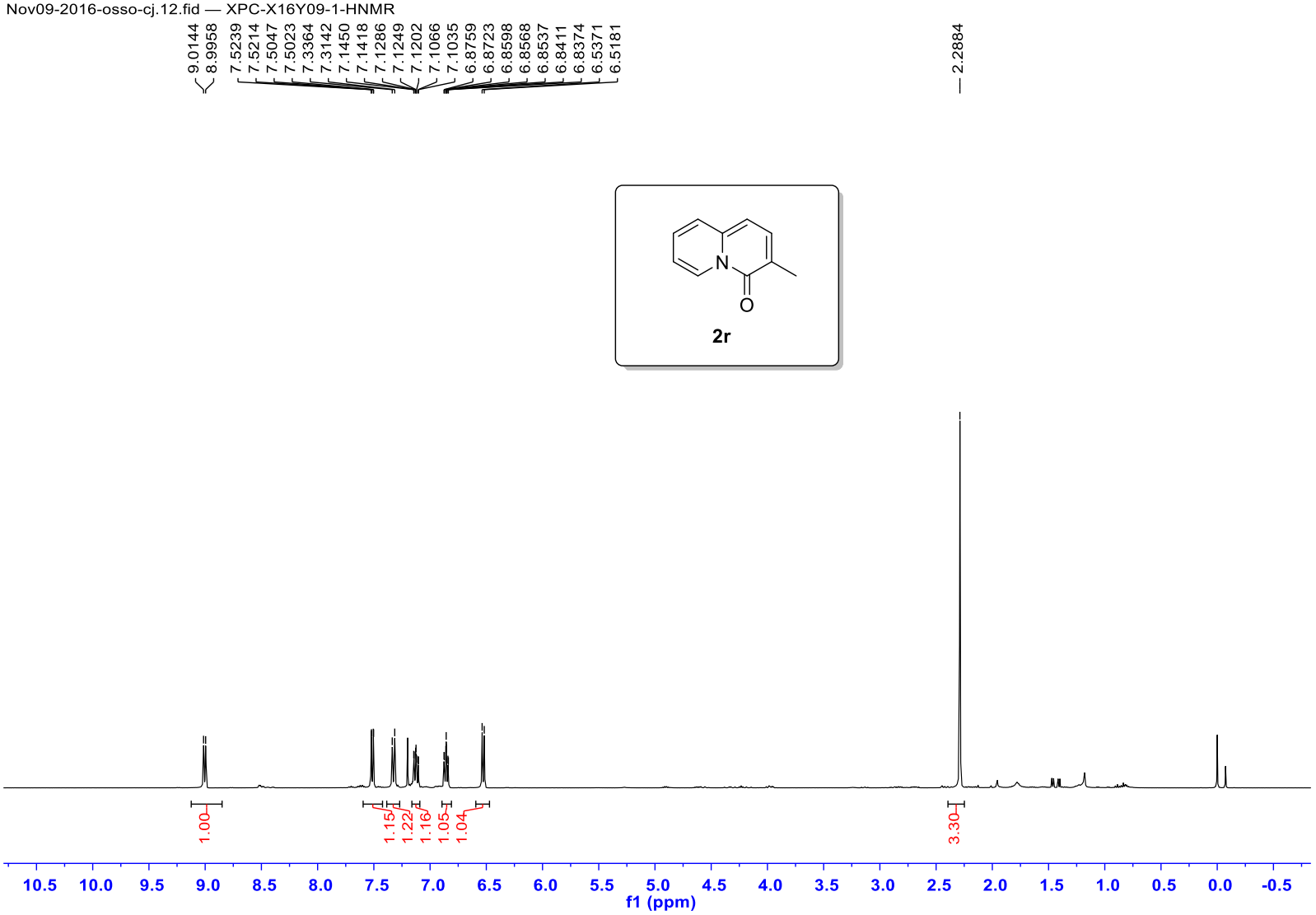

Sep29-2018-OSSO_cJ.26.fid — XPC-X181217-2-CNMR
158.37
149.89
141.70
129.25
127.03
124.82
114.20
109.29
104.70
77.48
77.16
76.84
21.85
N
O
2o
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

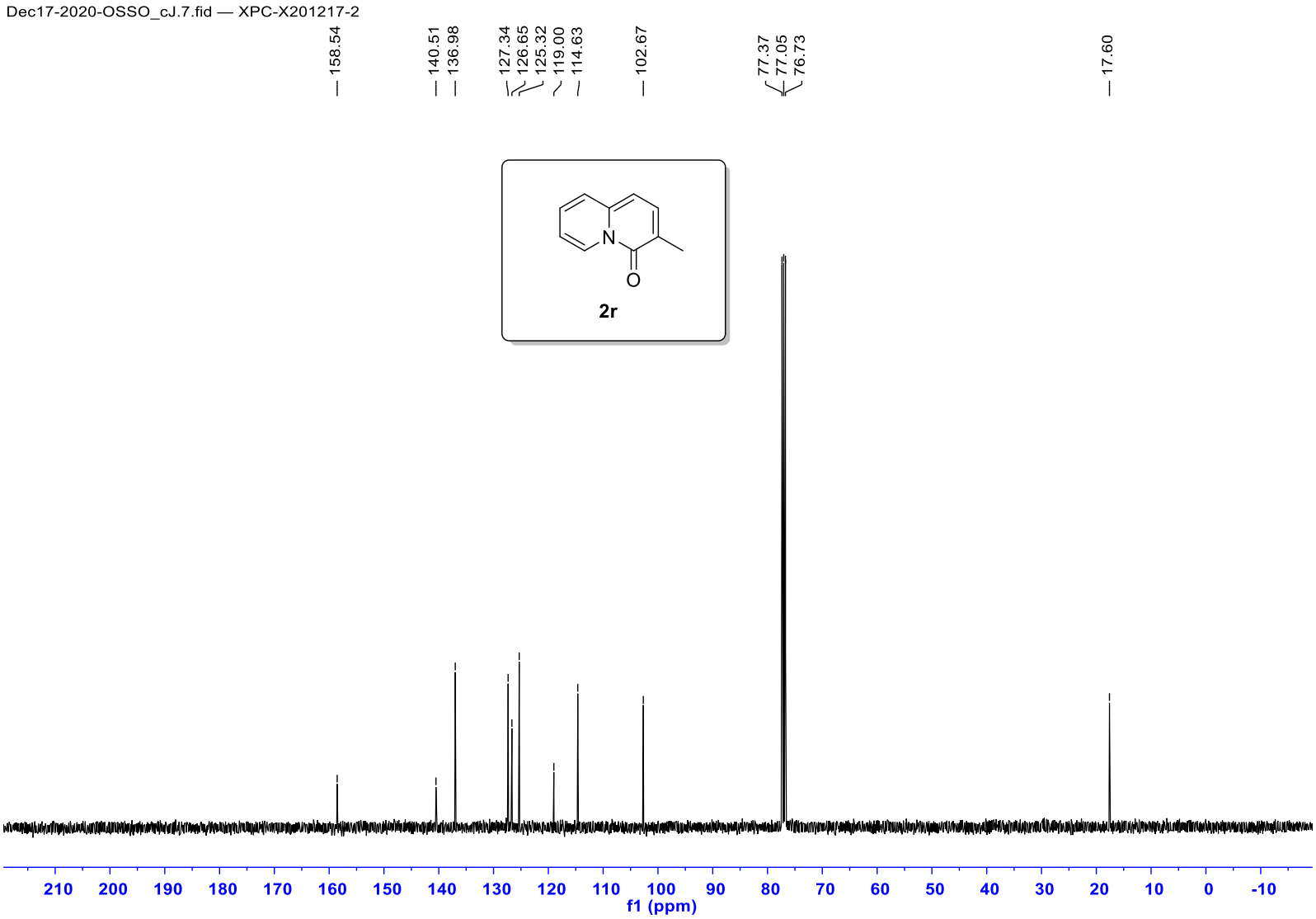

Nov19-2019-OSSO_cJ.26.fid — XPC-X181217-3-HNMR(改链2-正戊基2p)
9.0457 9.0428 9.0271 9.0243 7.3889 7.3858 7.3830 7.3664 7.3635 7.3607 7.2841 7.2810 7.2684 7.2650 7.2621 7.2588 7.2461 7.2427 6.9240 6.9203 6.9079 6.9048 6.9017 6.8893 6.8856 6.5027 6.4985 6.4833 6.4791
2.6250 2.6060 2.5866 1.7075 1.7019 1.6964 1.6894 1.6850 1.6824 1.6772 1.6706 1.6665 1.6632 1.6551 1.6512 1.6443 1.6395 1.6330 1.3595 1.3527 1.3450 1.3422 1.3344 1.3266 1.3237 1.3165 0.9121 0.9064 0.9003 0.8948 0.8885 0.8823 0.8775 0.0000
N
O
4
2p
1.00 1.03 1.16 1.05 1.06 0.99 2.13 2.13 4.04 3.15
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 -0.5
f1 (ppm)


Nov19-2019-OSSO_cJ.27.fid — XPC-X181217-3-CNMR(支链2-正戊基2p)
158.69
154.61
141.87
129.16
127.15
125.08
114.27
108.80
104.15
77.47
77.15
76.84
36.01
31.46
29.84
22.57
14.07
N
O
4
2p
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


Dec01-2020-OSSO_cJ.21.fid — XPC-X201201-2
9.1196
9.1012
7.7065
7.7021
7.6969
7.6901
7.6857
7.6823
7.5276
7.5247
7.5220
7.5157
7.5107
7.5055
7.5025
7.5000
7.4959
7.4936
7.4898
7.4876
7.4793
7.4755
7.4724
7.4676
7.4636
7.4576
7.4515
7.4499
7.4410
7.4359
7.4322
7.4287
7.3643
7.3611
7.3481
7.3447
7.3419
7.3387
7.3258
7.3224
7.0036
7.0000
6.9873
6.9845
6.9815
6.9690
6.9653
6.8916
6.8869
6.8786
6.8739
-0.0000
Ph
N
O
2q
1.00
2.05
4.12
1.15
1.05
2.04
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
-0.5
f1 (ppm)


Dec04-2020-OSSO_cJ.13.fid — XPC-X201202-2
158.74
150.45
142.32
138.45
129.66
129.27
129.03
127.26
127.24
125.67
114.81
106.63
102.10
Ph
N
O
2q
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


Nov09-2016-osso-cj.12.fid — XPC-X16Y09-1-HNMR
9.0144
8.9958
7.5239
7.5214
7.5047
7.5023
7.3364
7.3142
7.1450
7.1418
7.1286
7.1249
7.1202
7.1066
7.1035
6.8759
6.8723
6.8598
6.8568
6.8537
6.8411
6.8374
6.5371
6.5181
2.2884
N
O
2r
1.00
1.15
1.22
1.16
1.05
1.04
3.30
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 -0.5
f1 (ppm)


Dec17-2020-OSSO_cJ.7.fid — XPC-X201217-2
158.54
140.51
136.98
127.34
126.65
125.32
119.00
114.63
102.67
77.37
77.05
76.73
17.60
N
O
2r
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)