Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

Silver-promoted selective fluorination of 2-aminopyrimidines: synthesis of 5-fluoro-2-aminopyrimidine derivatives

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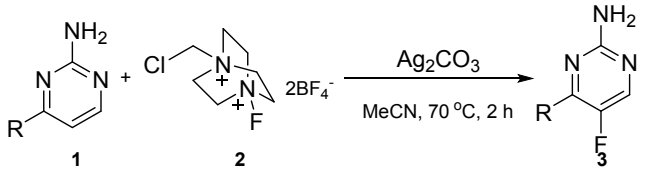
Table of Contents

1. General information

All reagents were purchased from commercial sources and used without further purification. ^{1}H NMR (TMS as the internal standard) and ^{19}F NMR spectra (without outside standard) and ^{13}C NMR was recorded on Bruker AM400 spectrometer. ^{1}H NMR spectra were obtained at 400 MHz and recorded relative to tetramethylsilane signal (0 ppm) or residual protio-solvent. ^{13}C NMR spectra were obtained at 101 MHz and chemical shifts were recorded relative to the solvent resonance ($CDCl_3$, 77.0 ppm; $(CD_3)_2SO$, 39.5 ppm). Data for ^{1}H NMR are recorded as follows: chemical shift (δ, ppm), multiplicity (s = singlet, d = doublet, t = triplet, m = multiplet or unresolved, br = broad singlet, coupling constant(s) in Hz, integration). ^{19}F NMR spectra were obtained at 376 MHz. For the compounds reported with ^{19}F NMR yields, $PhCF_3$ (1.0 equivalent) was added to the reaction mixture as internal standard added after the reaction completed. IR spectra were measured on Thermo Nicolet spectrometer. The X-ray diffraction experiments were carried out on Bruker D8 Discover. Melting point were measured on WRS-2A.

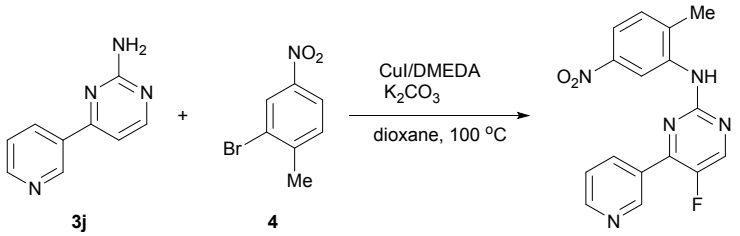
2. General procedure for fluorination of 4-substituted 2-aminopyrimidines with selectfluor



1 2 3

The mixture of 4-substituted 2-aminopyrimidine (0.2 mmol), selectfluor (85 mg, 0.24 mmol), Ag_2CO_3 (110 mg, 0.4 mmol) in a component solvent of MeCN and H_2O (100/3) (2.0 mL) was stirred at 70 °C for 2 h. After cooled to room temperature, the reaction mixture was diluted with ethyl acetate and then washed with water and brine. The organic phase was dried over anhydrous Na_2SO_4 and filtered. The filtrate was concentrated under reduced pressure and the residue was purified flash chromatography on silica gel to afford the desired compounds **3**. Compounds **3a–n** were obtained in the similar manner.

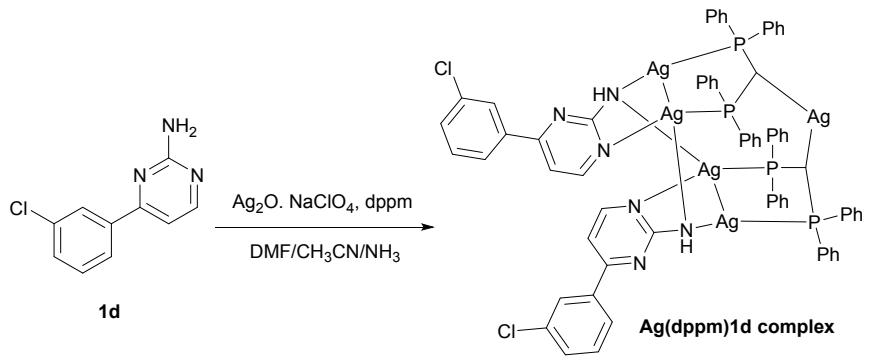
3. The procedure for the synthesis of fluorinated intermediate of *Imatinib* [1]



3j 4 5

The compound 5-fluoro-4-(pyridin-3-yl)pyrimidin-2-amine **3j** (38 mg, 0.2 mmol), CuI (9.5 mg, 0.05 mmol), and anhydrous K_2CO_3 (55 mg, 0.4 mmol) were added to a Schlenk sealed tube fitted with magnetic stirring bar. The tube was evacuated and back filled with argon three times. Dioxane (2 mL), 2-bromo-1-methyl-4-nitrobenzene **4** (43 mg, 0.2 mmol), and DMEDA (4.4 mg, 0.05 mmol) were added by syringe at room temperature. The reaction mixture was stirred at 100 °C for 30 h and then cooled to room temperature. After completion, the reaction mixture was diluted with AcOEt, washed with water and brine. The organic phase was dried over anhydrous Na_2SO_4 and filtered. The filtrate was concentrated in vacuo; and the residue was purified by column chromatography on silica gel to give the title compound **5** as yellowish powder.

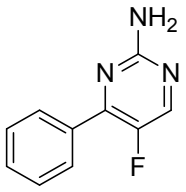
4. The procedure for the preparation of Ag(dppm)1d complex[2]



Reaction of Ag_2O (174 mg, 0.75 mmol), **1d** (102 mg, 0.5 mmol), dppm (192 mg, 0.5 mmol) and $NaClO_4 \cdot H_2O$ (210 mg, 1.5 mmol) in DMF/CH_3CN media (3 mL/5 mL) in the presence of ammonia in air under ultrasonic treatment at 60 °C for 15 min. The resultant pale yellow solution was allowed slowly to evaporate under argon atmosphere at room temperature to give yellow plate crystals of Ag(dppm)**1d** complex (224 mg, 52% yield) for about three weeks.

6. Compound characterization

5-Fluoro-4-phenyl-2-aminopyrimidine (3a) [3]:

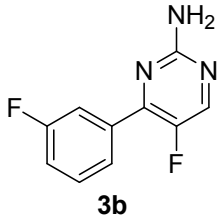


3a

White solid; yield: 61 % (23.1 mg); m.p.: 165.4–166.9 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.23 (d, J_{HF} = 3.4 Hz, 1H), 8.07 – 7.98 (m, 2H), 7.52 – 7.46 (m, 3H), 5.08 (s, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.64 (d, J_{CF} = 3.1 Hz), 152.61 (d, J_{CF} = 9.6 Hz), 150.72 (d, J_{CF} = 251.8 Hz), 147.02 (d, J_{CF} = 26.2 Hz), 133.49 (d, J_{CF} = 5.2 Hz), 130.77, 128.93 (d, J_{CF} = 6.2 Hz), 128.61; ^{19}F NMR (376 MHz, $CDCl_3$) δ -152.49 (s, 1F). IR (KBr) ν_{max} (cm^{-1}) = 3323, 3175, 1652, 1558, 1473, 1355, 1274, 1200. HRMS (ESI-TOF) m/z calcd. for $C_{11}H_9FN_3^+$ $[M+H]^+$: 190.0775; found: 190.0743.

5-Fluoro-4-(3-fluorophenyl)-2-aminopyrimidine (3b):

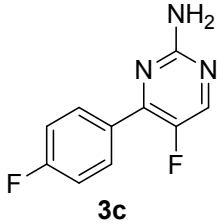


3b

White solid; yield: 65 % (26.9 mg); m.p.: 163.2–164.9 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25 (d, J_{HF} = 3.5 Hz, 1H), 7.84 (d, J = 7.8 Hz, 1H), 7.78 (d, J = 10.1 Hz, 1H), 7.45 (dd, J = 14.0, 8.0 Hz, 1H), 7.19 (td, J = 8.3, 2.1 Hz, 1H), 5.10 (s, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.83 (d, J_{CF} = 245.9 Hz), 159.58 (d, J_{CF} = 2.8 Hz), 150.94 (dd, J_{CF} = 9.2, 2.7 Hz), 150.83(d, J_{CF} = 253.72 Hz), 147.42 (d, J_{CF} = 26.3 Hz), 135.54 (dd, J_{CF} = 7.8, 5.4 Hz), 130.13 (d, J_{CF} = 8.0 Hz), 124.69 (dd, J_{CF} = 7.5, 3.0 Hz), 117.72 (d, J_{CF} = 21.2 Hz), 115.83 (dd, J_{CF} = 23.5, 6.1 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ -112.30 (s, 1F), -151.95 (s, 1F); IR (KBr) ν_{max} (cm^{-1}) = 3332, 3178, 1650, 1567, 1478, 1445, 1354, 1269, 1200; HRMS (ESI-TOF) m/z calcd. for $C_{10}H_8F_2N_3^+$ $[M+H]^+$: 208.0681; found: 208.0672.

5-Fluoro-4-(4-fluorophenyl)-2-aminopyrimidine (3c):



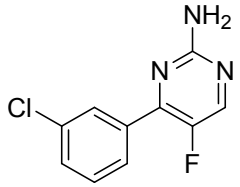
3c

White solid; yield: 68 % (28.0 mg); m.p.: 154.1–155.8°C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.22 (d, J_{HF}= 3.7 Hz, 1H), 8.07 (dd, J = 8.1, 5.5 Hz, 2H), 7.20 – 7.14 (m, 2H), 5.04 (s, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.33 (d, J_{CF} = 251.9 Hz), 159.55 (d, J_{CF} = 3.4 Hz), 151.33 (d, J_{CF} = 9.5 Hz), 150.55 (d, J_{CF} = 252.9 Hz), 147.13 (d, J_{CF} = 26.3 Hz), 131.16 (dd, J_{CF} = 8.7, 6.9 Hz), 129.59 (dd, J_{CF} = 5.5, 3.3 Hz), 115.72 (d, J_{CF} = 21.7 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ -109.05 (s, 1F), -152.45 (s, 1F); IR (KBr) ν_{max}

(cm^{-1}) = 3338, 3175, 1646, 1583, 1508, 1480, 1427, 1352, 1274, 1203; HRMS (ESI-TOF) m/z calcd. for $C_{10}H_8F_2N_3^+$ $[M+H]^+$: 208.0681; found: 208.0666.

5-Fluoro-4-(3-chlorophenyl)-2-aminopyrimidine (3d):

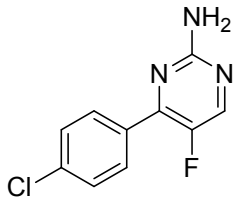


3d

White solid; yield: 62 % (27.6 mg); m.p.: 145.7–147.3 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25 (d, J_{CF} = 3.4 Hz, 1H), 8.06 (s, 1H), 7.93 (d, J = 7.6 Hz, 1H), 7.48 – 7.40 (m, 2H), 5.06 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.56 (d, J_{CF} = 2.8 Hz), 150.86 (d, J_{CF} = 9.3 Hz), 150.61 (d, J_{CF} = 259.6), 147.46 (d, J_{CF} = 26.1 Hz), 135.16 (d, J_{CF} = 5.4 Hz), 134.73, 130.77, 129.84, 128.90 (d, J_{CF} = 6.1 Hz), 127.11 (d, J_{CF} = 7.6 Hz).^{19}F NMR (376 MHz, $CDCl_3$) δ -151.98(s, 1F). IR (KBr) ν_{max} (cm^{-1}) = 3339, 3183, 1645, 1568, 1553, 1477, 1431, 1351, 1274, 1200. HRMS (ESI-TOF) m/z calcd. for $C_{10}H_8ClFN_3^+$ $[M+H]^+$: 224.0385; found: 224.0408.

5-Fluoro-4-(4-chlorophenyl)- 2-aminopyrimidine (3e):

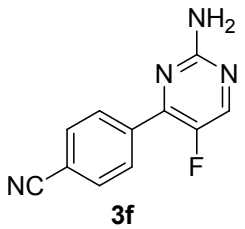


3e

White solid; yield: 73 % (32.5 mg); m.p.: 127.0–128.9 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.24 (s, 1H), 8.01 (d, J = 7.9 Hz, 2H), 7.46 (d, J = 7.3 Hz, 2H), 5.07 (s, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.60 (d, J_{CF} = 3.0 Hz), 151.17 (d, J_{CF} = 9.1 Hz), 151.16 (d, J_{CF} = 9.2), 150.88 (d, J_{CF} = 253.2),147.28 (d, J_{CF} = 26.2 Hz), 137.04, 131.89 (d, J_{CF} = 5.4 Hz), 130.29 (d, J_{CF} = 6.8 Hz), 128.88; ^{19}F NMR (376 MHz, $CDCl_3$) δ -152.03 (s, 1F); IR (KBr) ν_{max} (cm^{-1}) = 3331, 3186, 1647, 1594, 1574, 1473, 1422, 1353, 1281, 1203; HRMS (ESI-TOF) m/z calcd. for $C_{10}H_8ClFN_3^+$ $[M+H]^+$: 224.0385; found: 224.0361.

5-Fluoro-4-(4-cyanophenyl)-2-aminopyrimidine (3f):



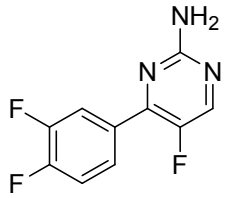
3f

White solid; yield: 52 % (22.2 mg); m.p.: 198.1–199.2 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.30 (d, J_{CF} = 3.3 Hz, 1H), 8.16 (d, J = 8.2 Hz, 2H), 7.78 (d, J = 8.4 Hz, 2H), 5.15 (s, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.68 (d, J_{CF} = 2.9 Hz), 150.71 (d, J_{CF} = 253.7 Hz), 150.01 (d, J_{CF} = 9.1 Hz), 147.94 (d, J_{CF} = 26.1 Hz), 137.66 (d, J_{CF} = 5.4 Hz), 132.28, 129.49 (d, J_{CF} = 6.8 Hz), 118.37, 114.16;

^{19}F NMR (376 MHz, $CDCl_3$) δ -151.66 (s, 1F); IR (KBr) ν_{max} (cm^{-1}) = 3292, 3160, 2223, 1641, 1569, 1483, 1354, 1220, 1202; HRMS (ESI-TOF) m/z calcd. for $C_{11}H_8FN_4^+$ $[M+H]^+$: 215.0728; found: 215.0731.

5-Fluoro-4-(3,4-difluorophenyl)-2-aminopyrimidine (3g):

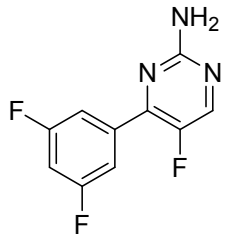


3g

White solid; yield: 66 % (29.7 mg); m.p.: 129.2–130.7 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.24 (d, J_{HF} = 3.6 Hz, 1H), 7.96 (ddd, J = 11.4, 7.8, 1.9 Hz, 1H), 7.90 – 7.82 (m, 1H), 7.26 (dd, J = 18.0, 8.8 Hz, 1H), 5.10 (s, 2H); ^{13}C NMR (101 MHz, CDCl3) δ 159.53 (d, J_{CF} = 2.9 Hz), 151.91 (ddd, J_{CF} = 254.9Hz, 12.8 Hz, 1.4 Hz), 150.51 (d, J_{CF} = 253.5Hz), 150.43 (dd, J_{CF} = 249.3Hz, 12.8 Hz), 150.11 – 149.68 (m), 147.52 (d, J_{CF} = 26.3 Hz), 130.49 – 130.33 (m), 125.92 – 125.36 (m), 118.18 (dd, J_{CF} = 19.2, 6.6 Hz), 117.46 (d, J_{CF} = 17.6 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ -133.57 (d, J = 21.5 Hz, 1F), -136.75 (d, J = 21.5 Hz, 1F), 152.08 (s, 1F); IR (KBr) ν_{max} (cm^{-1}) = 3310, 3176, 1645, 1582, 1558, 1508, 1474, 1419, 1351, 1284, 1203; HRMS (ESI-TOF) m/z calcd. for $C_{10}H_7F_3N_3^+$ $[M+H]^+$: 226.0587; found: 226.0663.

5-Fluoro-4-(3,5-difluorophenyl) -2-aminopyrimidine (3h):

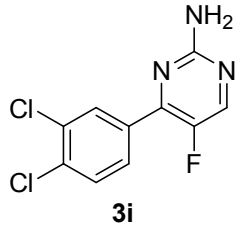


3h

White solid; yield: 60 % (27.0 mg); m.p.: 159.5–161.6 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.27 (d, J_{HF} = 3.5 Hz, 1H), 7.63 (d, J = 6.7 Hz, 2H), 6.95 (ddd, J = 8.6, 5.4, 2.2 Hz, 1H), 5.13 (s, 2H); ^{13}C NMR (101 MHz, CDCl3) δ 163.00 (dd, J_{CF} = 248.4Hz, J_{CF} = 12.5Hz), 159.53 (d, J_{CF} = 2.9Hz), 150.51(d, J_{CF} = 254.5Hz), 149.56 – 149.41 (m), 147.88 (d, J_{CF} = 26.2 Hz), 136.55 – 136.31 (m),112.11 – 111.768 (m). 106.11 (dd, J_{CF} = 25.4 Hz, J_{CF} = 25.4 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ -108.90 (s, 2F), -152.53(s, 1F); IR (KBr) ν_{max} (cm^{-1}) = 3345, 3198, 1647, 1603, 1572, 1474, 1440, 1355, 1312, 1200; HRMS (ESI-TOF) m/z calcd. for $C_{10}H_8F_2N_3^+$ $[M+H]^+$: 226.0587; found: 226.0600.

5-Fluoro-4-(3,4-dichlorophenyl)-2-aminopyrimidine (3i):



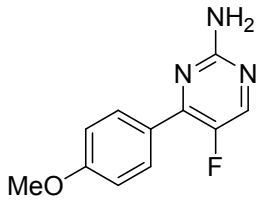
3i

White solid; yield: 61 % (31.4 mg); m.p.: 154.0–155.7 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25 (d, J_{CF} = 2.9 Hz, 1H), 8.20 (d, J = 1.8 Hz, 1H), 7.91 (dd, J = 8.5, 1.1 Hz, 1H), 7.55 (d, J = 8.5 Hz, 1H), 5.09 (s, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.57 (d, J_{CF} = 2.9 Hz), 150.13 (d, J_{CF} = 254.32 Hz), 149.68 (d, J_{CF} = 9.0 Hz), 147.62 (d, J_{CF} = 26.0 Hz), 135.14, 133.31 (d, J_{CF} = 5.5 Hz), 133.07, 130.73 (d, J_{CF} = 6.6 Hz), 130.58, 128.10 (d, J_{CF} = 8.0 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ -151.59 (s, 1F); IR (KBr) ν_{max}

(cm^{-1}) = 3336, 3203, 1642, 1588, 1462, 1415, 1345, 1196; HRMS (ESI-TOF) m/z calcd. for $C_{10}H_7Cl_2FN_3^+$ $[M+H]^+$: 257.9996; found: 257.9991.

5-Fluoro-4-(4-methoxyphenyl)-2-aminopyrimidine (3j):

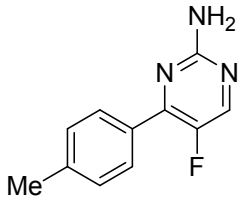


3j

White solid; yield: 50 % (21.9 mg); m.p.: 148.8–150.9 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 (d, J_{HF} = 3.9 Hz, 1H), 8.05 (d, J = 8.9 Hz, 2H), 6.99 (d, J = 9.0 Hz, 2H), 5.02 (s, 2H), 3.87 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.71, 159.50 (d, J_{CF} = 2.9 Hz), 152.08 (d, J_{CF} = 9.3 Hz), 150.57 (d, J_{CF} = 251.0 Hz), 146.58 (d, J_{CF} = 26.4 Hz), 130.64 (d, J_{CF} = 7.0 Hz), 125.93 (d, J_{CF}= 5.5 Hz), 114.00, 55.41; ^{19}F NMR (376 MHz, $CDCl_3$) δ -152.45(s, 1F); IR (KBr) ν_{max} (cm^{-1}) = 3323, 3196, 1652, 1576, 1558, 1507, 1472, 1457, 1257, 1203; HRMS (ESI-TOF) m/z calcd. for $C_{11}H_{11}FN_3O^+$ $[M+H]^+$: 220.0881; found: 220.0893.

5-Fluoro-4-(4-tolyl)-2-aminopyrimidine (3k):

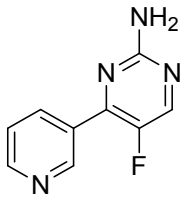


3k

White solid; yield: 51 % (20.7 mg); m.p.: 142.6–143.7 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.20 (d, J_{HF} = 2.7 Hz, 1H), 7.93 (d, J = 8.0 Hz, 2H), 7.29 (d, J = 7.8 Hz, 2H), 5.07 (s, 2H), 2.42 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.58 (d, J_{CF} = 3.0 Hz), 152.60 (d, J_{CF} = 9.4 Hz), 150.69 (d, J_{CF} = 251.6 Hz), 146.79 (d, J_{CF} = 26.3 Hz), 141.19, 130.68 (d, J_{CF} = 5.3 Hz), 129.35, 128.87 (d, J_{CF} = 6.5 Hz), 21.53; ^{19}F NMR (376 MHz, $CDCl_3$) δ -152.38(s, 1F); IR (KBr) ν_{max} (cm^{-1}) = 3326, 3182, 1648, 1573, 1473, 1421, 1351, 1200; HRMS (ESI-TOF) m/z calcd. for $C_{11}H_{11}FN_3^+$ $[M+H]^+$: 204.0932; found: 204.0944.

5-Fluoro-4-(pyridin-3-yl)-2-aminopyrimidine (3l):

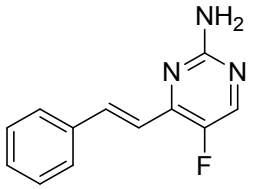


3l

White solid; yield: 50 % (19.0 mg); m.p.: 160.2–162.0 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.27 (s, 1H), 8.72 (d, J = 3.7 Hz, 1H), 8.34 (d, J = 8.0 Hz, 1H), 8.28 (d, J = 3.3 Hz, 1H), 7.43 (dd, J = 7.8, 4.8 Hz, 1H), 5.14 (s, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.72 (d, J_{CF} = 2.8 Hz), 151.37, 150.70 (d, J_{CF} = 253.7), 150.03 (d, J_{CF} = 8.4 Hz), 149.88 (d, J_{CF} = 10.3 Hz), 147.46 (d, J_{CF} = 25.6), 136.14 (d, J_{CF} = 6.1 Hz), 129.49 (d, J_{CF} = 5.8 Hz), 123.42; ^{19}F NMR (376 MHz, $CDCl_3$) δ -152.16(s, 1F); IR (KBr) ν_{max} (cm^{-1}) = 3321, 3175, 1642, 1588, 1468, 1350, 1270, 1203; HRMS (ESI-TOF) m/z calcd. for $C_9H_8FN_4^+$ $[M+H]^+$: 191.0728; found: 191.0708.

(*E*)-5-Fluoro-4-styryl-2-aminopyrimidine (3m):

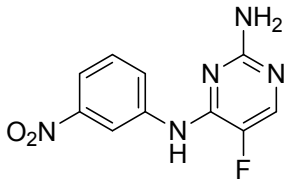


3m

White solid; yield: 52% (22.4 mg); m.p.: 143.6–145.7 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.15 (s, 1H), 7.90 (d, J = 16.0 Hz, 1H), 7.61 (d, J = 7.0 Hz, 2H), 7.42– 7.34 (m, 3H), 7.19 (d, J = 16.0 Hz, 1H), 4.96 (s, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.38 (d, J_{CF} = 2.8 Hz), 150.78 (d, J_{CF} = 11.1 Hz), 150.24 (d, J_{CF} = 252.8), 145.98 (d, J_{CF} = 23.9 Hz), 138.11 (d, J_{CF} = 4.0 Hz), 135.77, 129.57, 128.89, 127.86, 118.21; ^{19}F NMR (376 MHz, $CDCl_3$) δ -155.75(s, 1F); IR (KBr) ν_{max} (cm^{-1}) = 3333, 3200, 1648, 1578, 1469, 1422, 1352, 1255, 1214, 1192, 983; HRMS (ESI-TOF) m/z calcd. for $C_{12}H_{11}FN_3^+$ $[M+H]^+$: 216.0932; found: 216.0901.

5-Fluoro-*N*^{4}-(3-nitrophenyl)-2,4-diaminopyrimidine (3n):

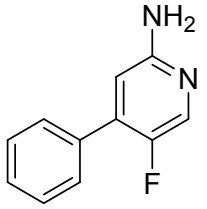


3n

Yellow powder; yield: 55% (27.4 mg); m.p.: 229.5–231.3 °C.

^{1}H NMR (400 MHz, DMSO) δ 9.60 (s, 1H), 8.65 (t, J = 1.9 Hz, 1H), 8.45 (d, J = 8.1 Hz, 1H), 7.97 (d, J = 3.7 Hz, 1H), 7.84 (dd, J = 8.1, 1.3 Hz, 1H), 7.57 (t, J = 8.2 Hz, 1H), 6.35 (s, 2H); ^{13}C NMR (101 MHz, DMSO) δ 159.73 (d, J_{CF} = 3.3 Hz), 149.71 (d, J_{CF} = 10.4 Hz), 148.41, 142.20 (d, J_{CF} = 19.2 Hz), 141.34, 140.21 (d, J_{CF} = 244.1 Hz), 130.24, 126.56, 117.01, 114.80; ^{19}F NMR (376 MHz, DMSO) δ -167.74 (s, 1F); IR (KBr) ν_{max} (cm^{-1}) = 3482, 3370, 3309, 3170, 1634, 1616, 1580, 1533, 1458, 1354, 1336, 1244, 1230; HRMS (ESI-TOF) m/z calcd. for $C_{10}H_8FN_5NaO_2^+$ $[M+Na]^+$: 272.0554; found: 272.0533.

3-Fluoro-4-phenylpyridin-2-amine (3p)[4]

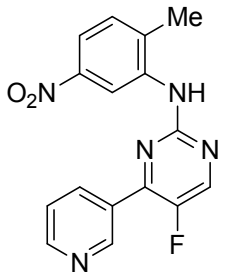


3p

Pale yellow solid; mp 125.9-127.3 °C; 5% yield (1.0 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.00 (d, J = 2.6 Hz, 1H), 7.55 (d, J = 7.2 Hz, 2H), 7.45 (t, J = 7.7 Hz, 3H), 6.56 (d, J = 5.2 Hz, 1H), 4.38 (s, 2H). ^{19}F NMR (376 MHz, $CDCl_3$) δ = -148.3.

5-Fluoro-*N*-(2-methyl-5-nitrophenyl)-4-(pyridin-3-yl)pyrimidin-2-amine (5):



5

Yellowish powder; yield: 70 % (45.3 mg); m.p.: 208.2–209.5 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.38 (d, J = 1.9 Hz, 2H), 8.77 (s, 1H), 8.56 (d, J = 8.0 Hz, 1H), 8.48 (d, J = 3.1 Hz, 1H), 7.87 (dd, J = 8.3, 2.1 Hz, 1H), 7.53 (dd, J = 7.8, 4.9 Hz, 1H), 7.36 (d, J = 8.3 Hz, 1H), 7.17 (s, 1H), 2.47 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 155.92 (d, J_{CF} = 2.7 Hz), 151.86, 151.25 (d, J_{CF} = 257.2 Hz), 150.17 (d, J_{CF} = 10.7 Hz), 149.70 (d, J_{CF} = 10.0 Hz), 147.87 (d, J_{CF} = 26.2 Hz), 147.08, 138.4, 136.25 (d, J_{CF} = 5.2 Hz), 133.53, 130.83, 129.92 (d, J_{CF} = 3.4 Hz), 123.85, 117.38, 114.19, 18.29; ^{19}F NMR (376 MHz, $CDCl_3$) δ -147.25(s, 1F); IR (KBr) ν_{max} (cm^{-1}) =3422, 1548, 1525, 1444, 1416, 1397, 1343, 1299, 1264; HRMS (ESI-TOF) m/z calcd. for $C_{16}H_{13}FN_5O_2^+$ $[M+H]^+$: 326.1048; found: 326.1052.

7. References

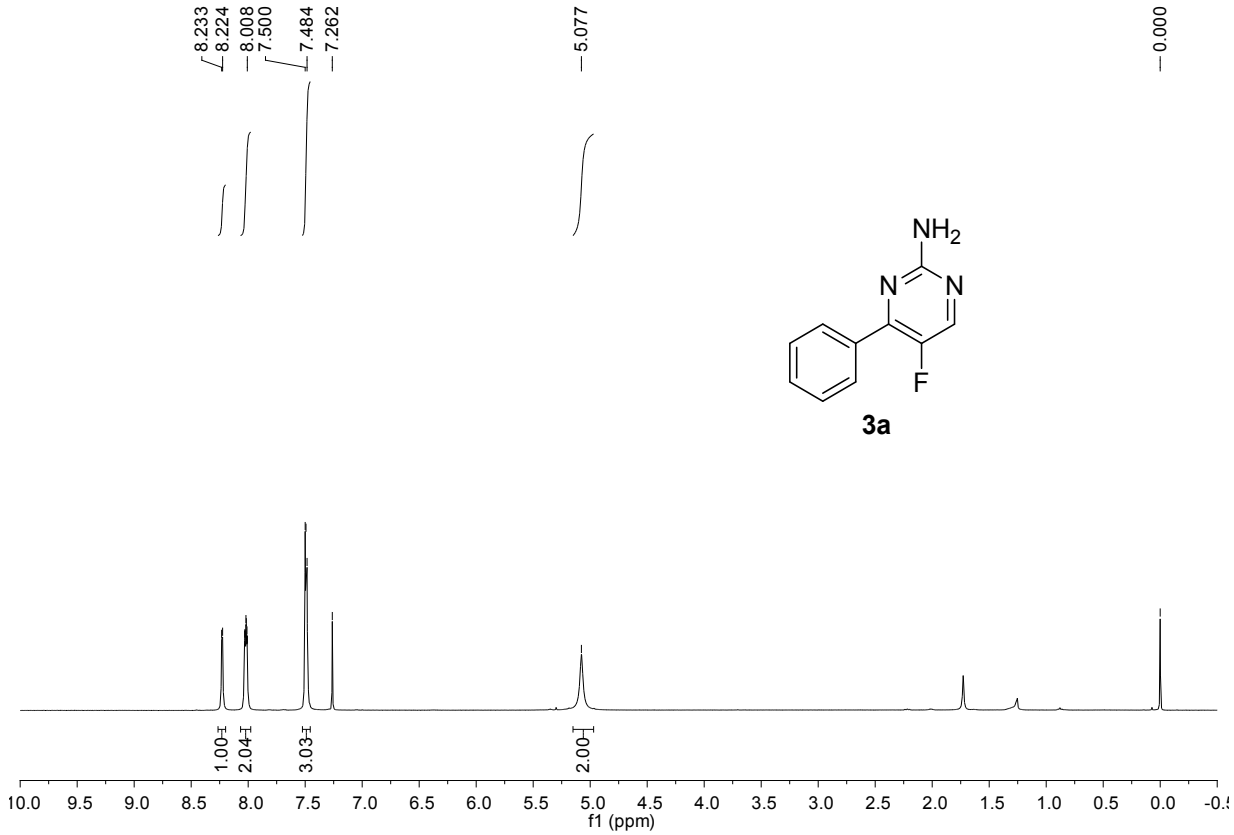
[1] Y. F. Liu, C. L. Wang, Y. J. Bai, N. Han, J. P. Jiao, X. L. Qi, *Organic Process Research & Development*, **2008**, *12*, 490-495.

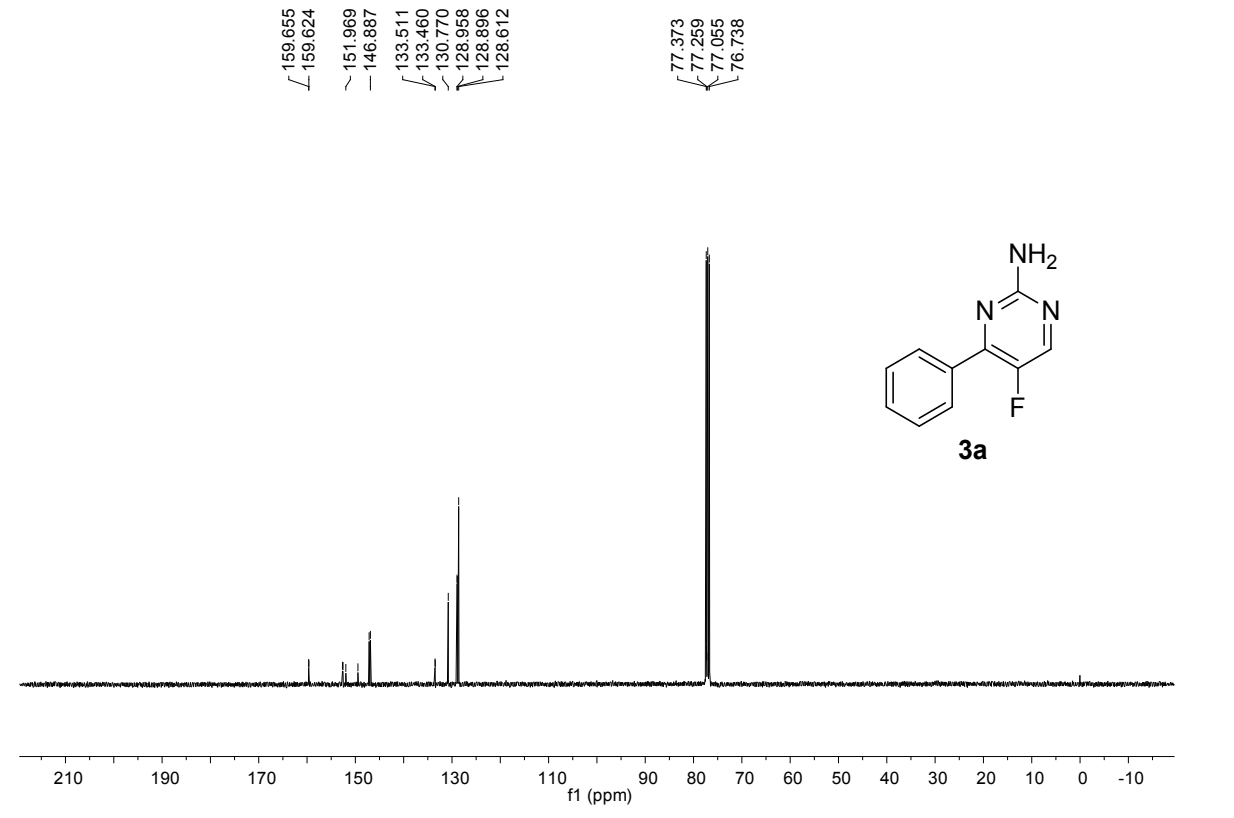
[2] D. Sun, N. Zhang, R. B. Huang, L. S. Zheng, *Inorg. Chem. Commun*, **2011**, *14*, 1039-1042.

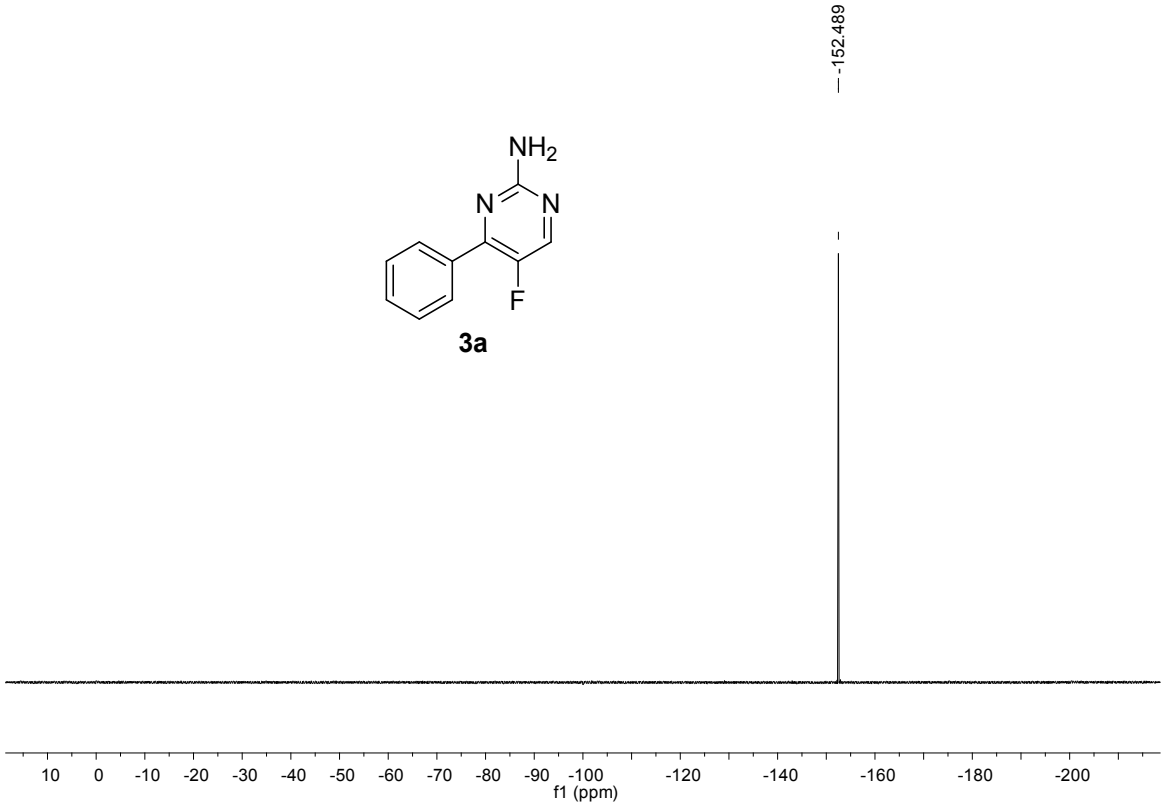
[3] K. Funabiki, T. Ohtsuki, T. Ishihara, H. Yamanaka, *Chemistry Letters*, **1995**, *3*, 239-240.

[4] G. Zhou, Y. Tian, X. Zhao, W. Dan, *Org. Lett.*, **2018**, *20*, 4858-4861.

8. NMR spectra data



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F
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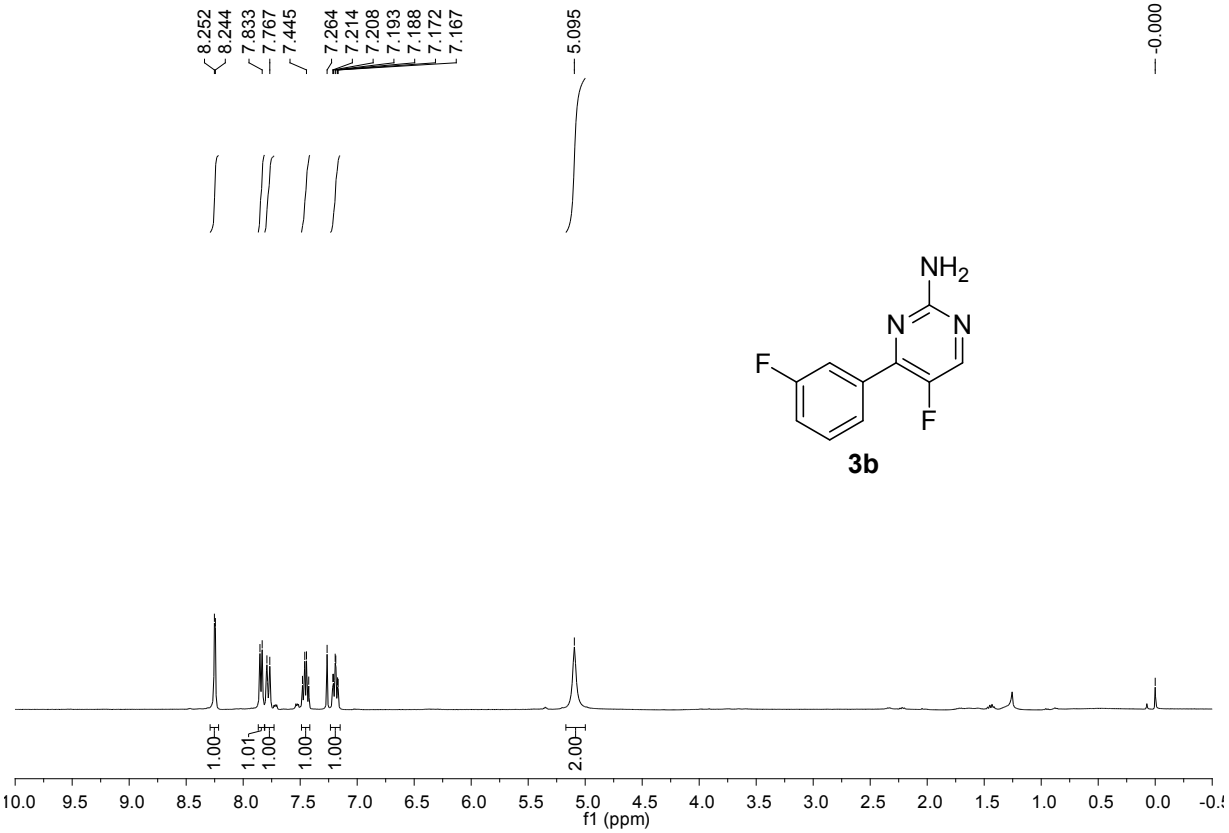
f1 (ppm)

3a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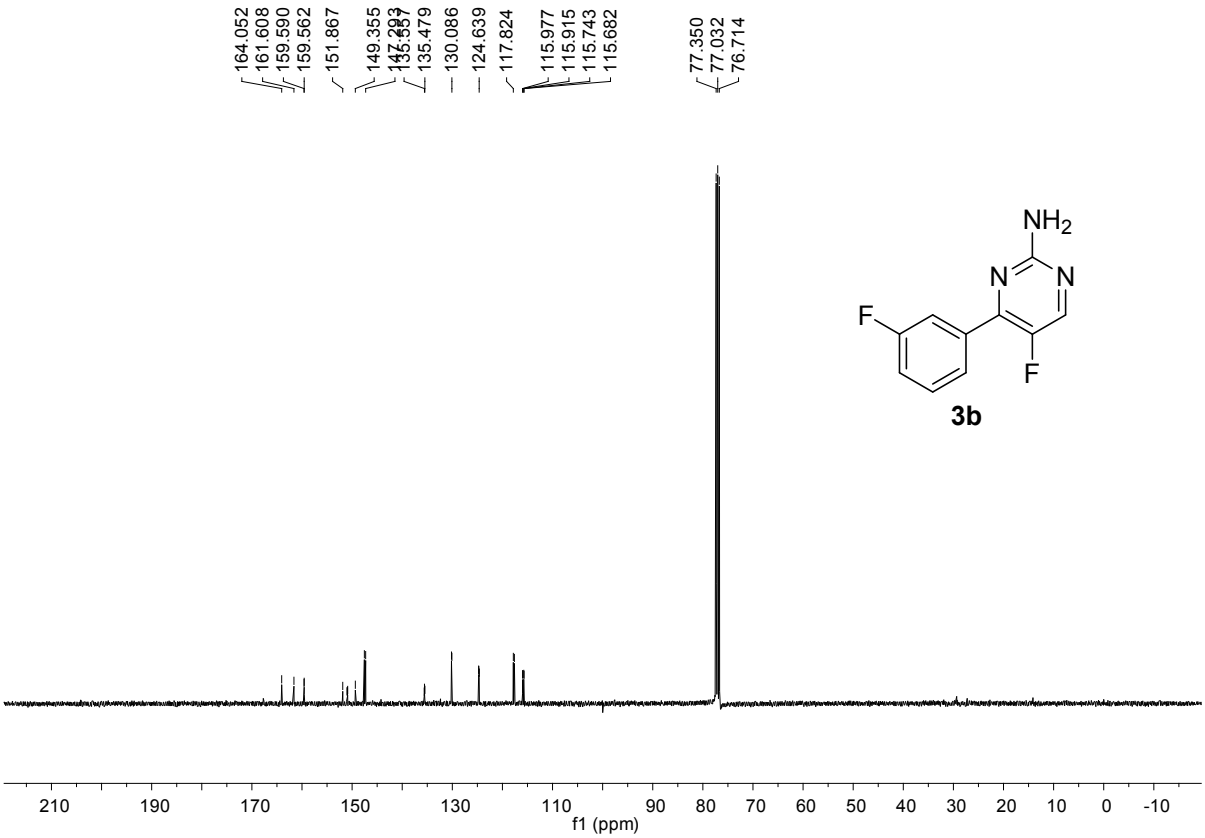
8.244
7.833
7.767
7.445
7.264
7.214
7.208
7.193
7.188
7.172
7.167
5.095
-0.000
NH2
N
N
F
F
1.00
1.01
1.00
1.00
1.00
2.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

3b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159.562
151.867
149.355
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130.086
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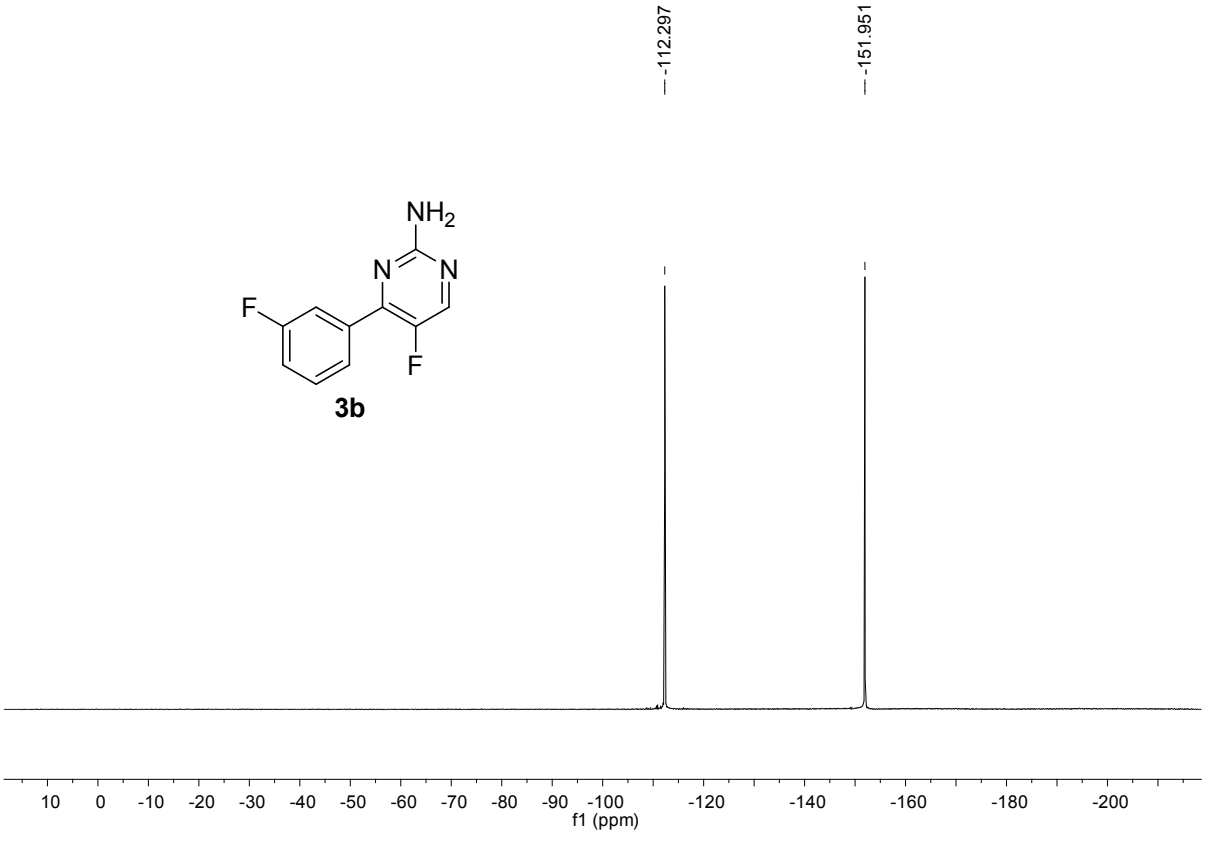
115.977
115.915
115.743
115.682
77.350
77.032
76.714
NH2
N
N
F
F
3b
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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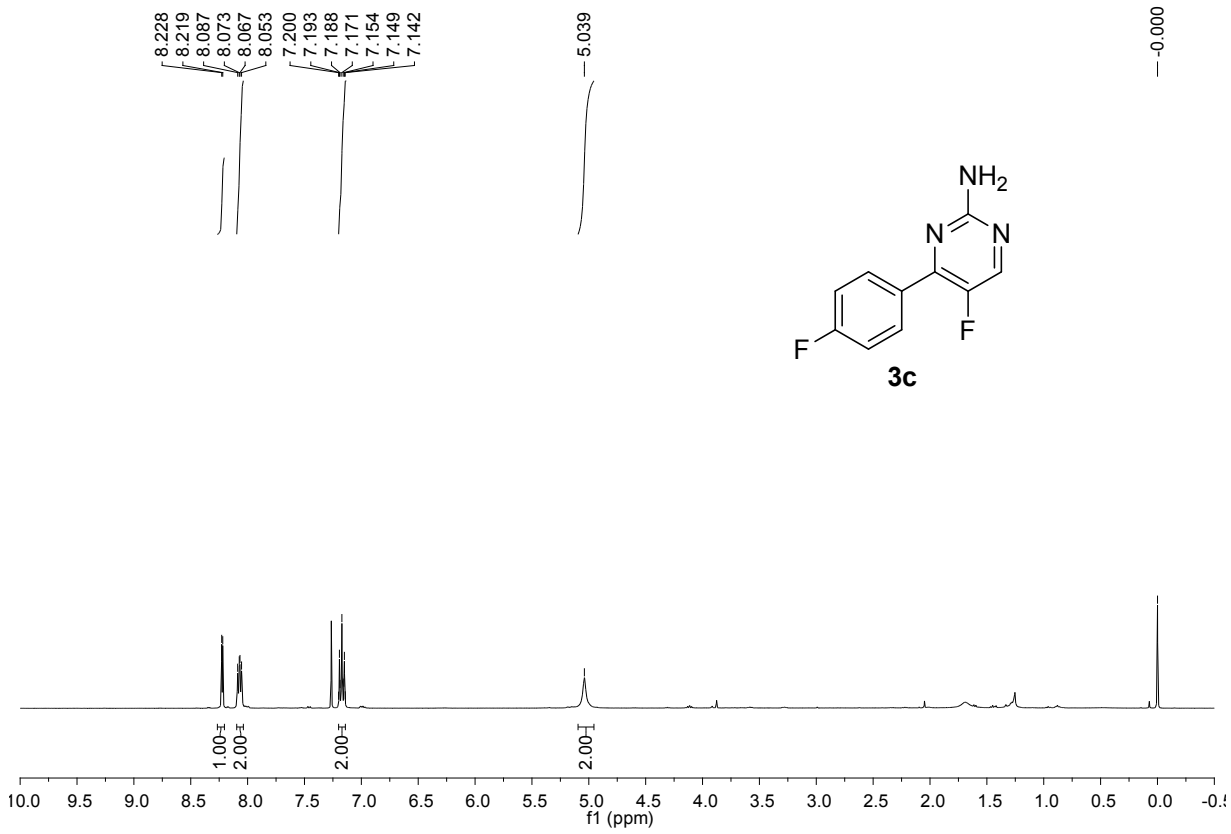
-50
-60
-70
-80
-90
-100
-120
-140
-160
-180
-200
f1 (ppm)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8.087
8.073
8.067
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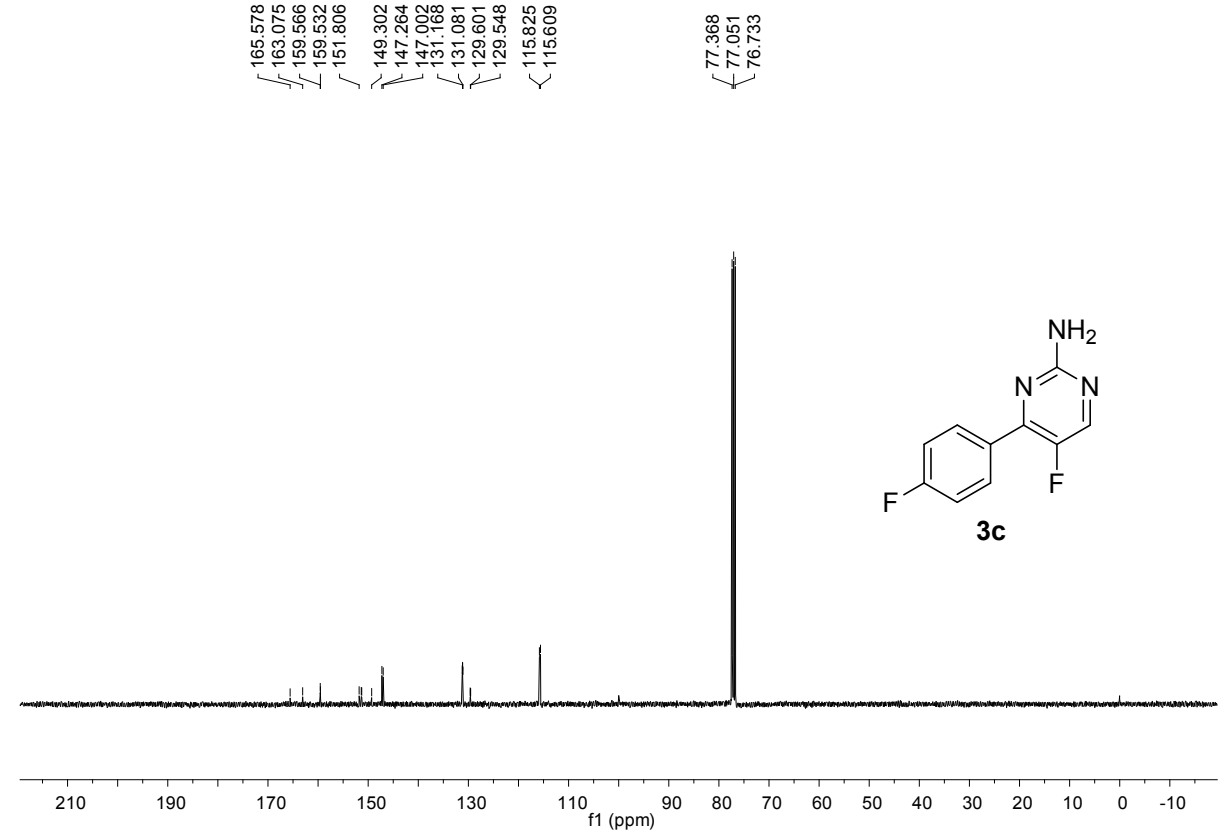
7.188
7.171
7.154
7.149
7.142
5.039
-0.000
NH2
N
N
F
F
3c
1.00
2.00
2.00
2.00
f1 (ppm)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159.566
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147.264
147.002
131.168
131.081
129.601
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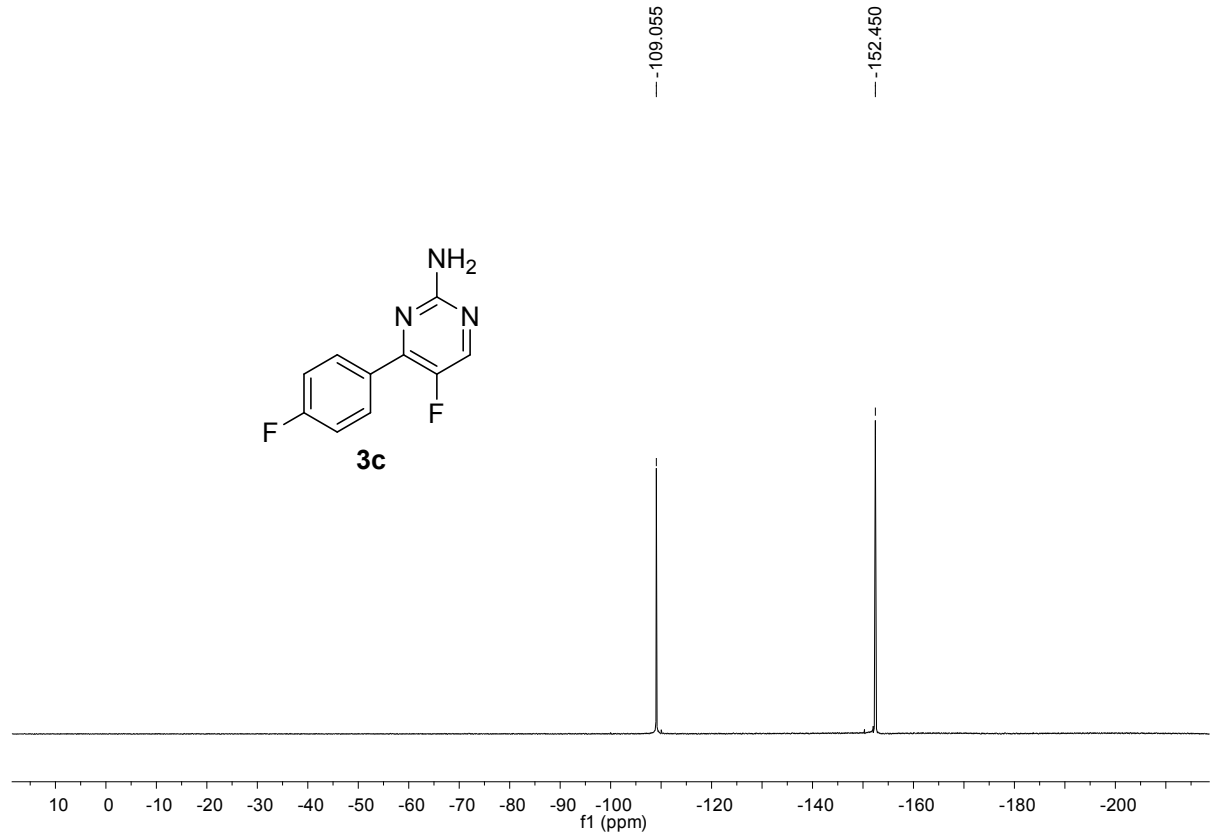
115.609
77.368
77.051
76.733
NH2
N
N
F
F
3c
f1 (ppm)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N
F
F
3c
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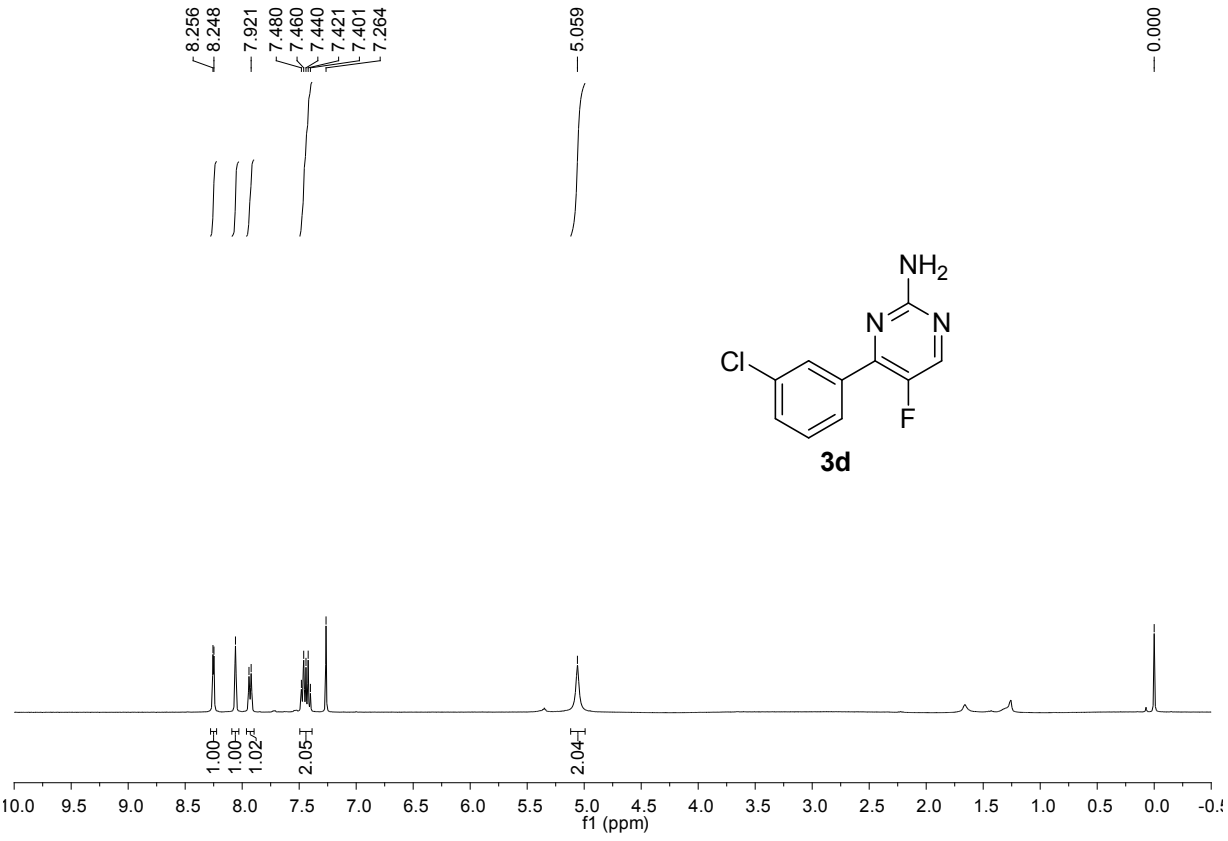
f1 (ppm)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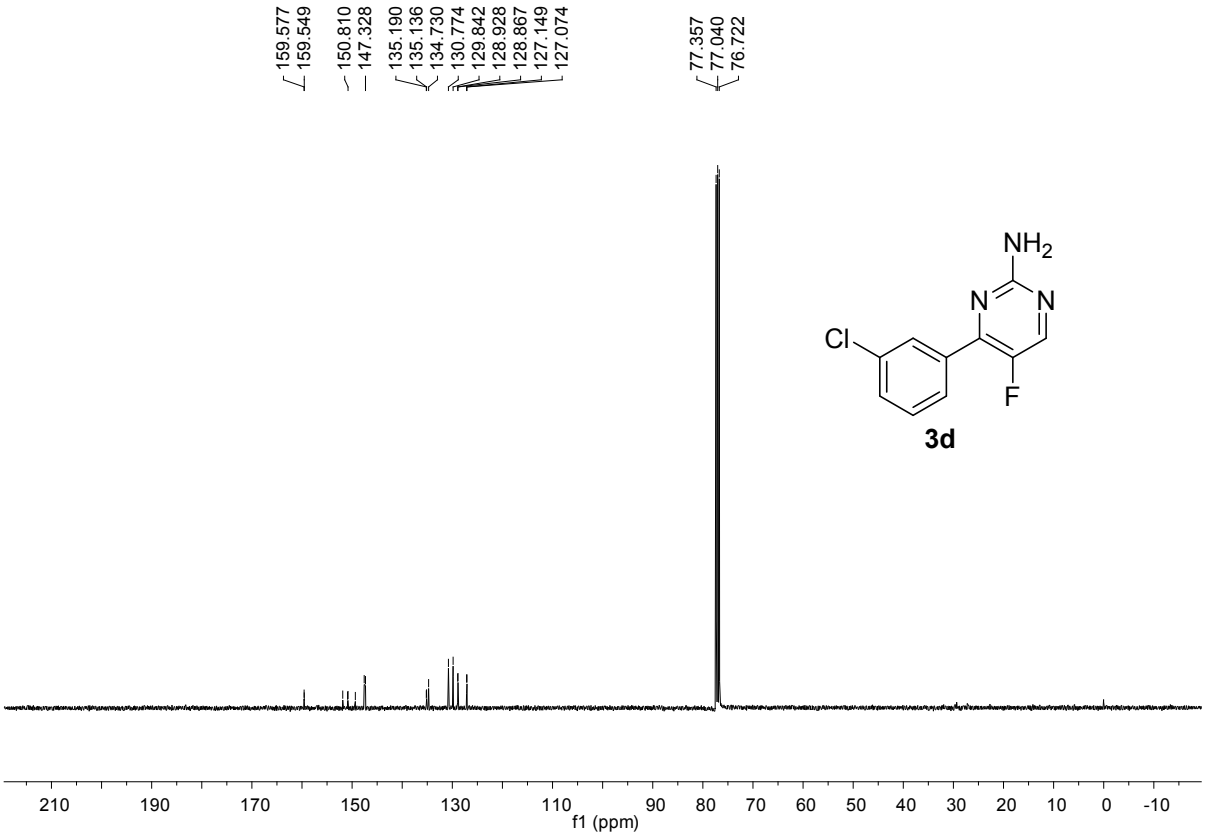
N
N
Cl
F
3d
1.00
1.00
1.02
2.05
2.04
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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135.190
135.136
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127.149
127.074
77.357
77.040
76.722
NH2
N
N
Cl
F
3d
210
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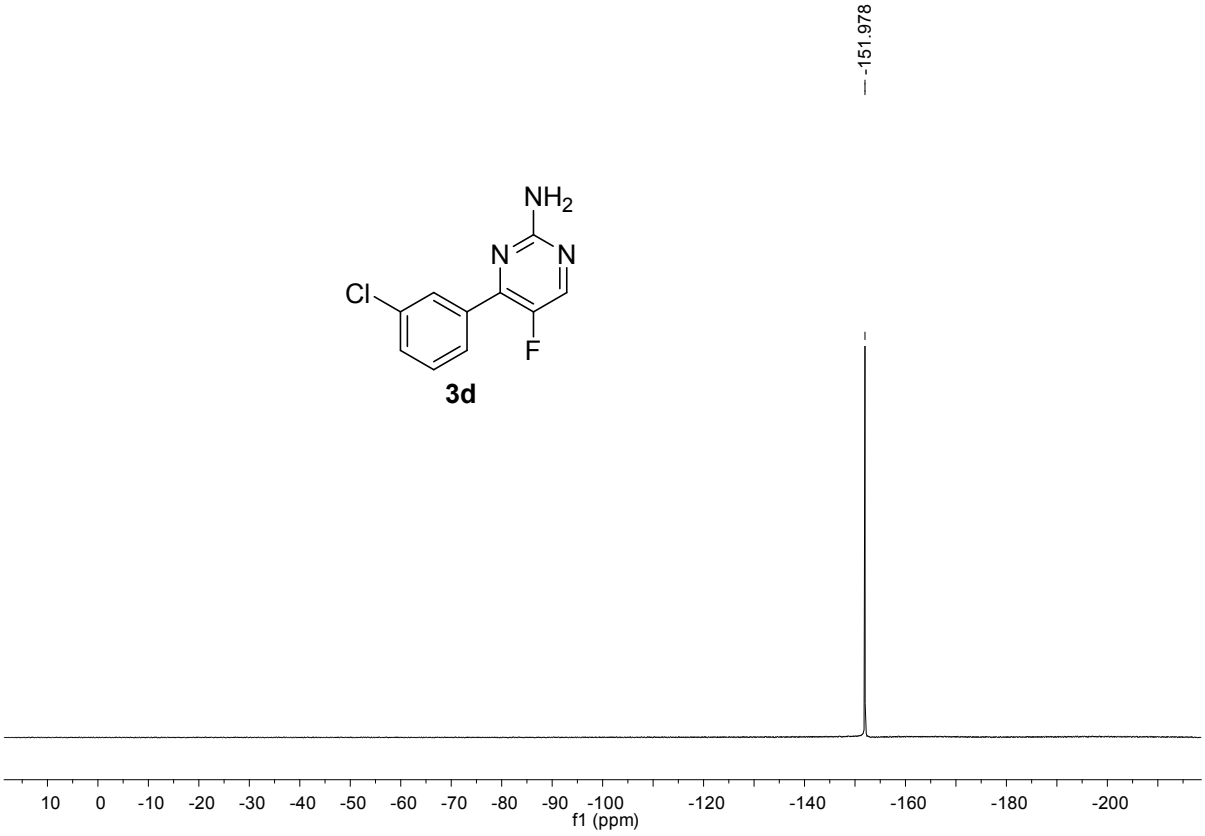
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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Cl
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3d
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0
-10
-20
-30
-40
-50
-60
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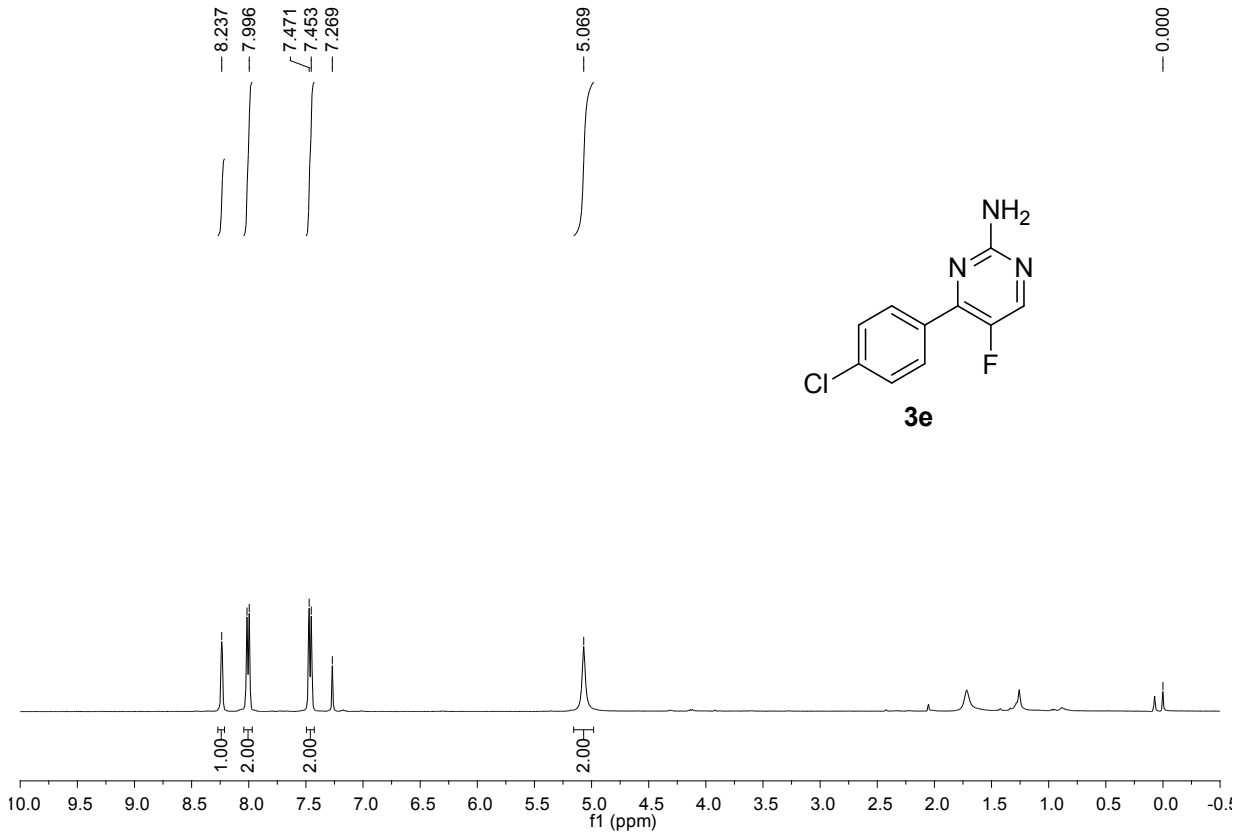
-120
-140
-160
-180
-200
f1 (ppm)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N
F
Cl
3e
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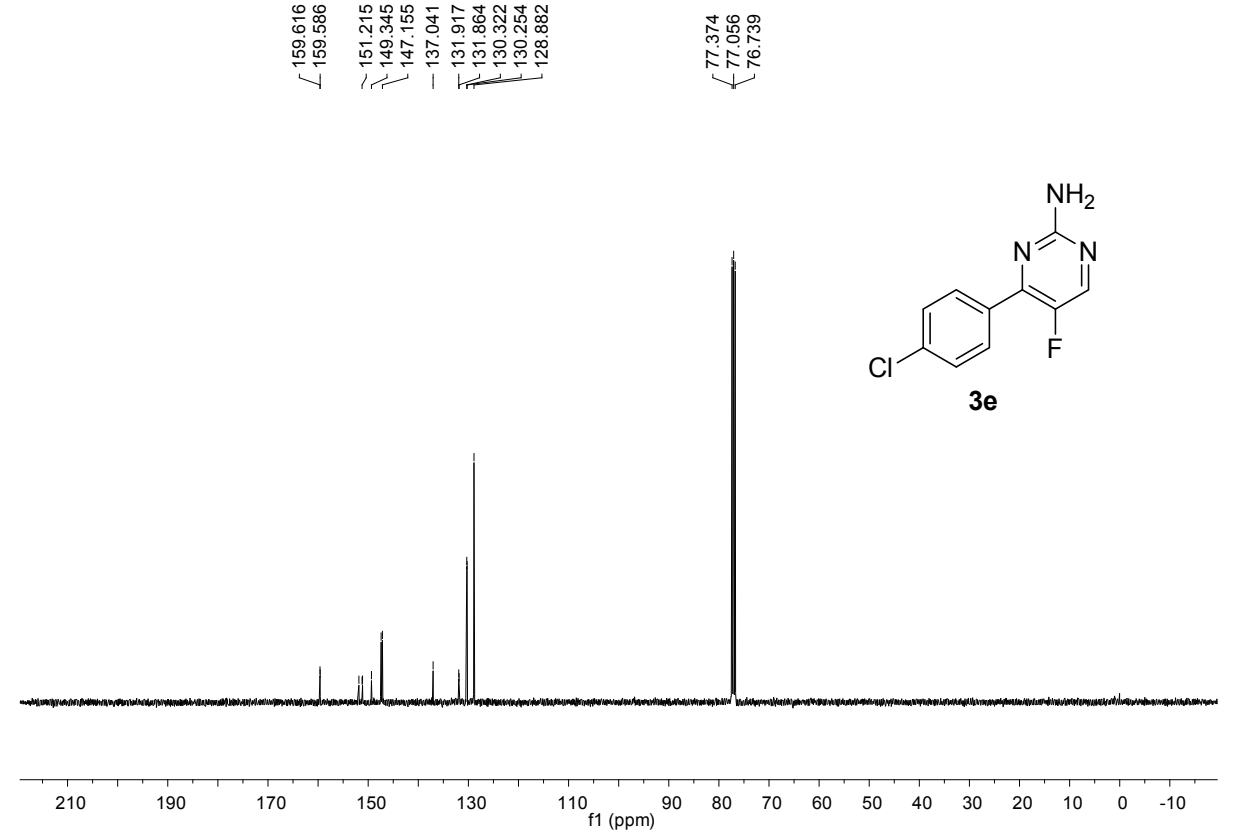
2.00
2.00
2.00
f1 (ppm)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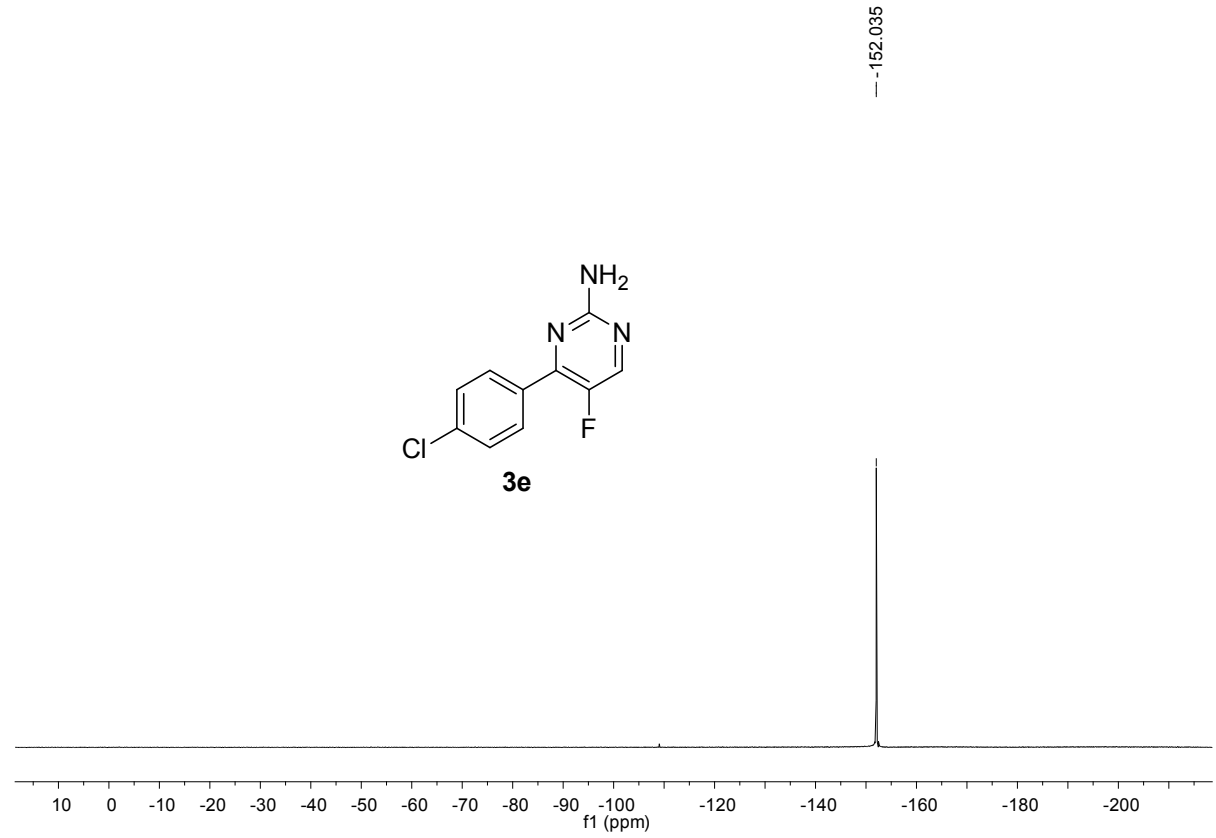
N
F
Cl
3e
f1 (ppm)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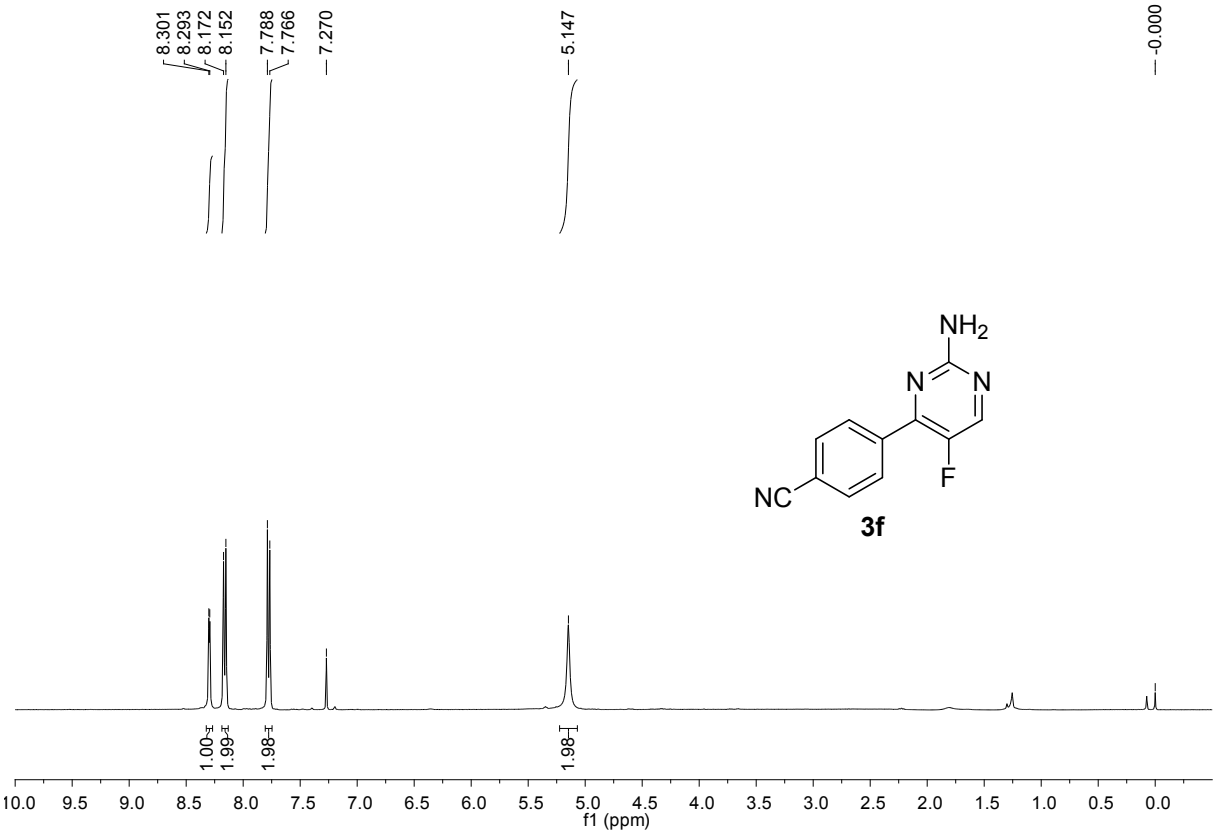
f1 (ppm)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NC
3f
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1.98
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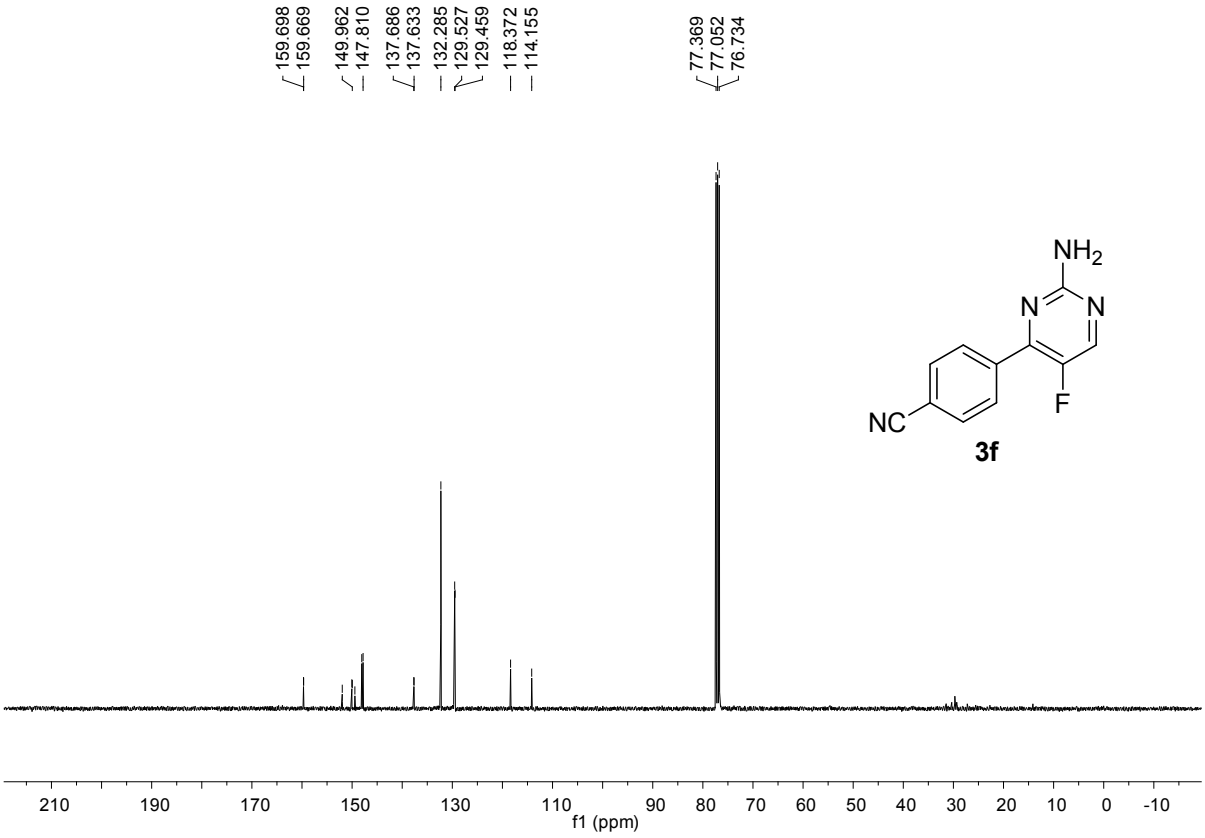
f1 (ppm)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N
N
F
NC
3f
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150
130
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90
80
70
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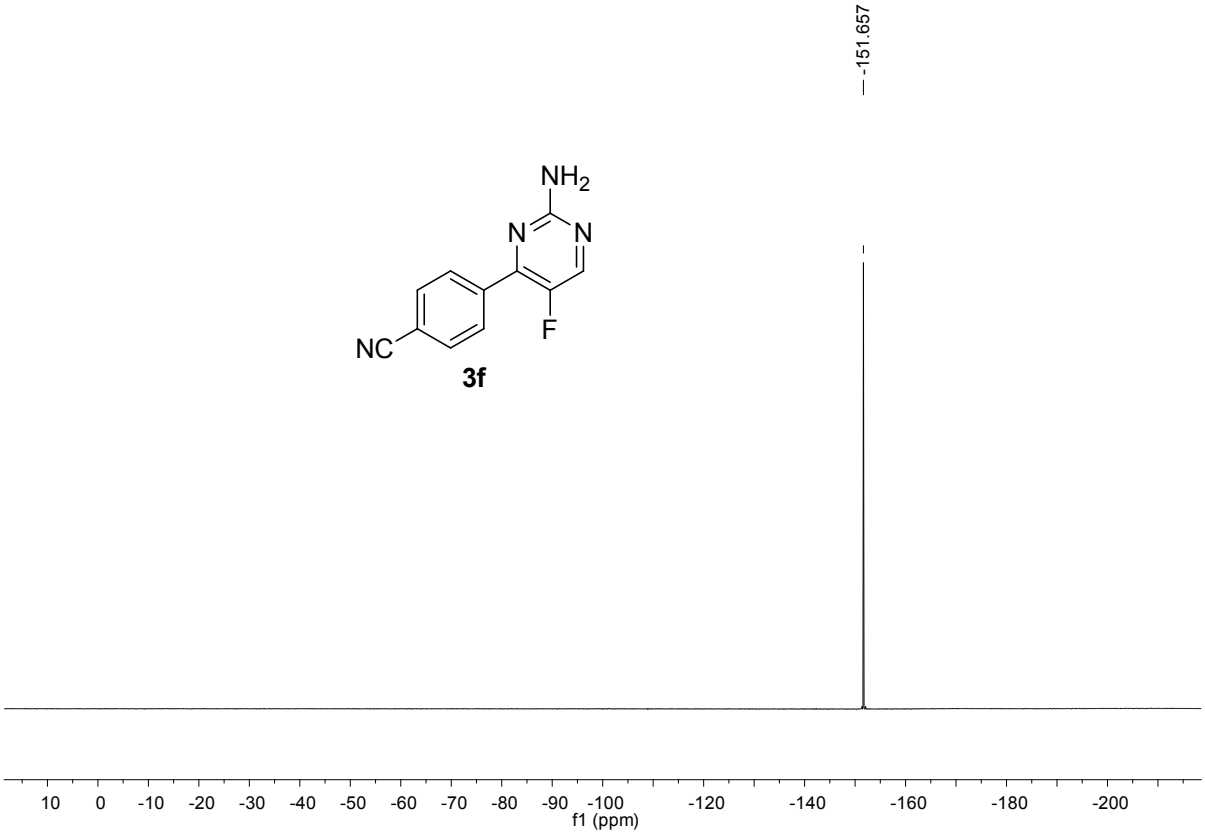
50
40
30
20
10
0
-10
f1 (ppm)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-120
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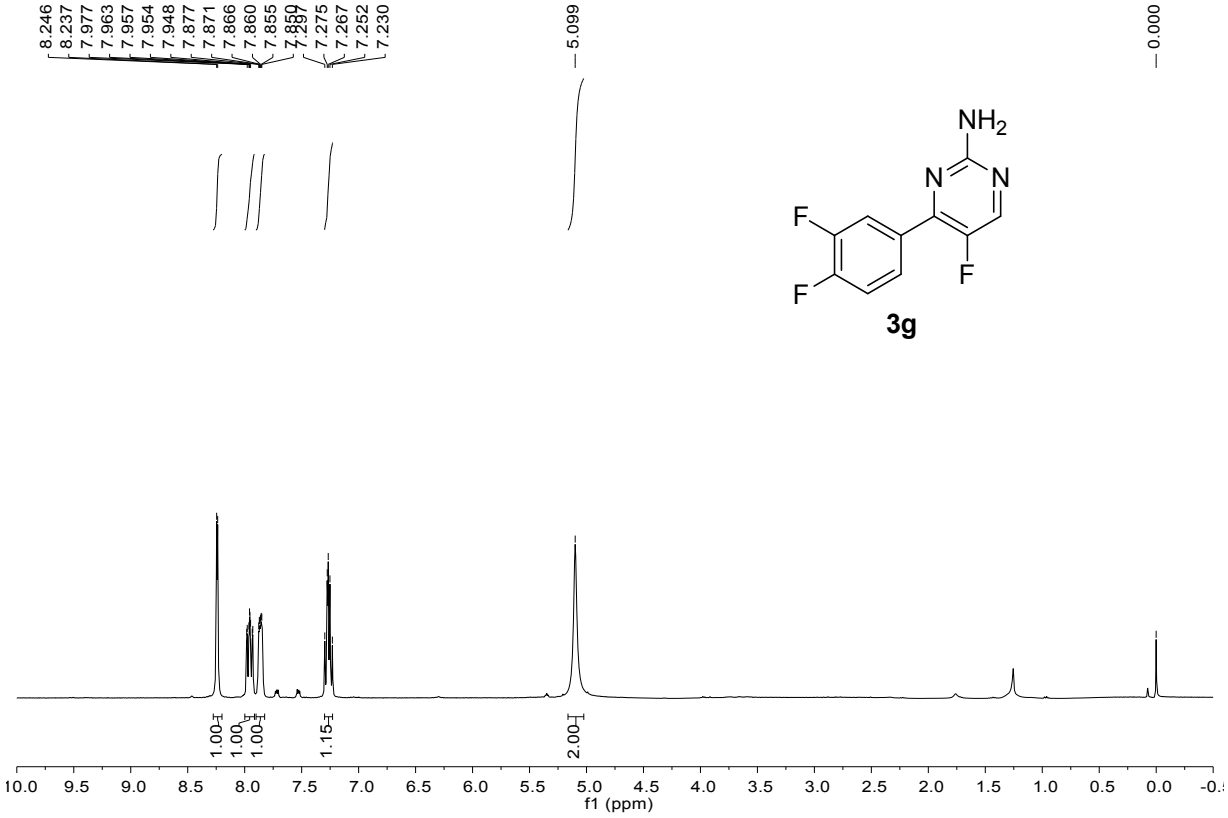
-180
-200
f1 (ppm)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7.275
7.267
7.252
7.230
5.099
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N
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F
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3g
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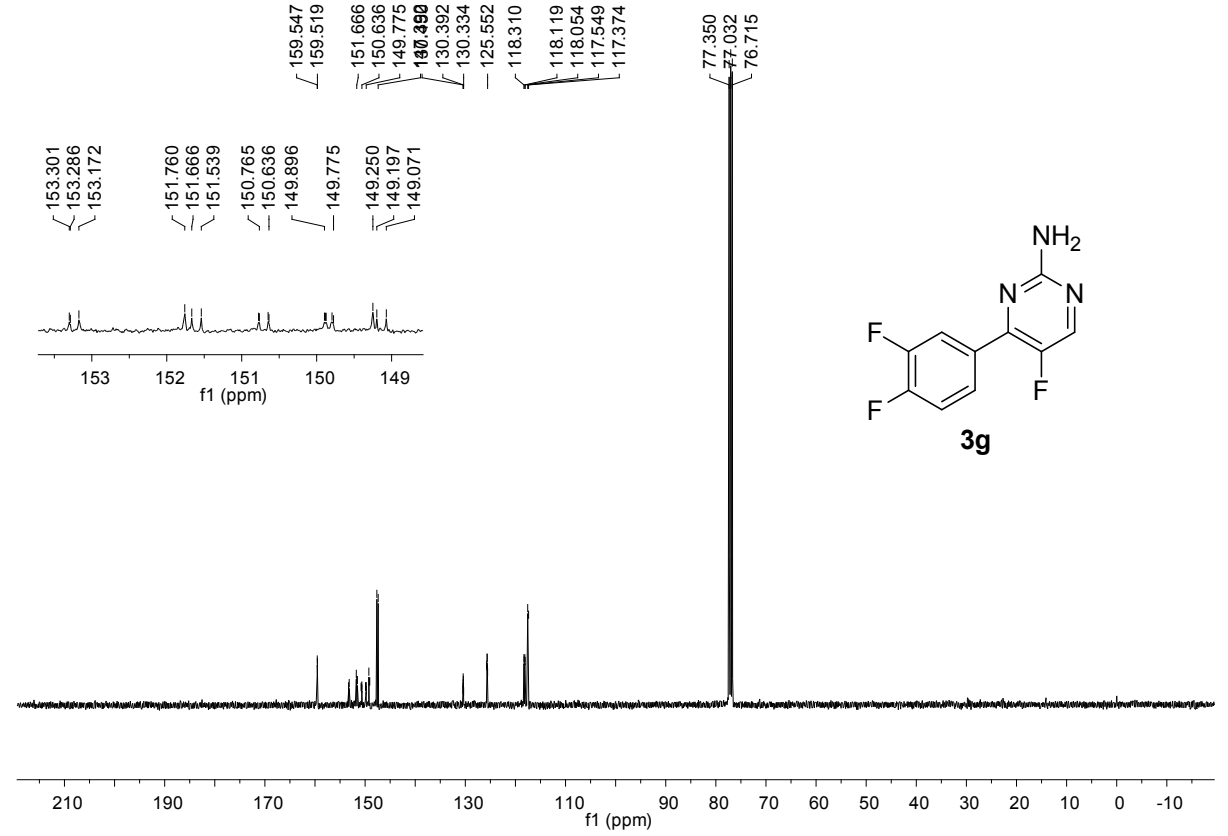
2.00
f1 (ppm)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117.549
117.374
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77.032
76.715
153.301
153.286
153.172
151.760
151.666
151.539
150.765
150.636
149.896
149.775
149.250
149.197
149.071
153
152
151
150
149
f1 (ppm)
NH2
N
N
F
F
F
3g
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190
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150
130
110
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80
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60
50
40
30
20
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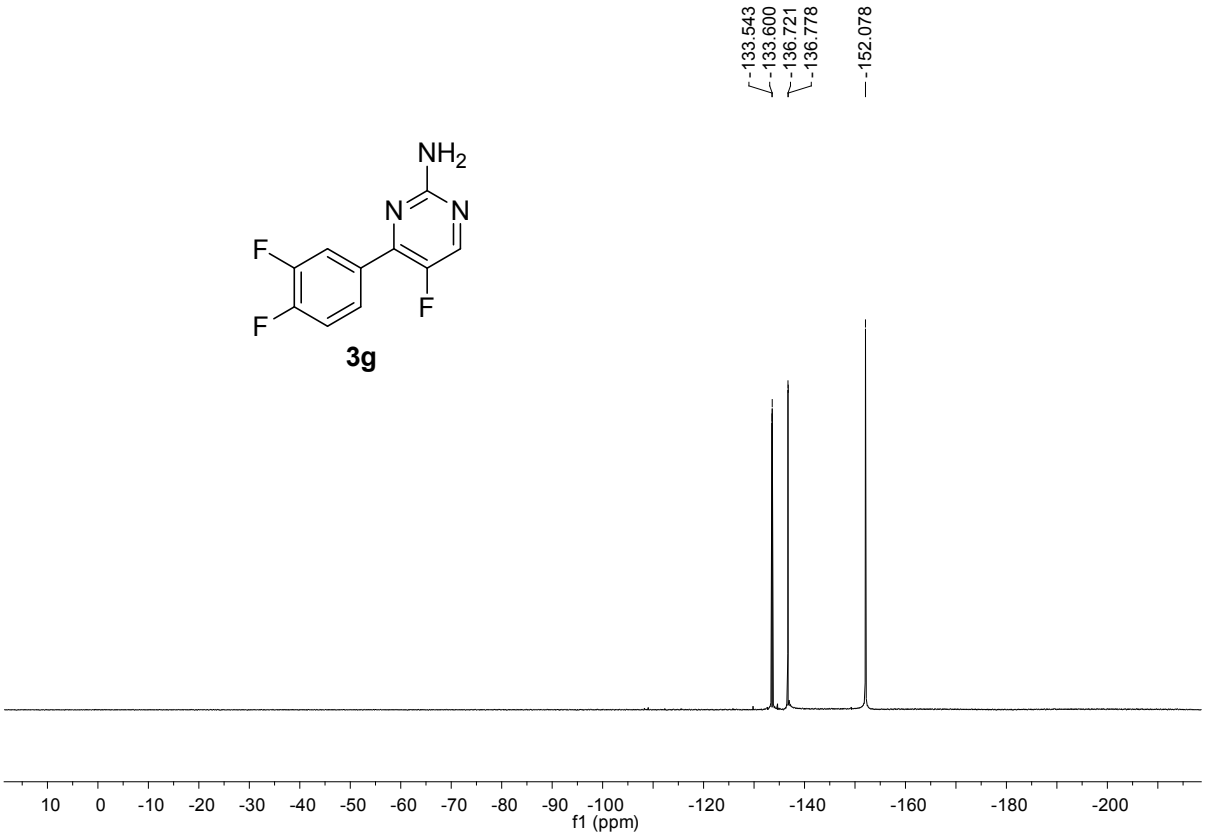
0
-10
f1 (ppm)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F
F
3g
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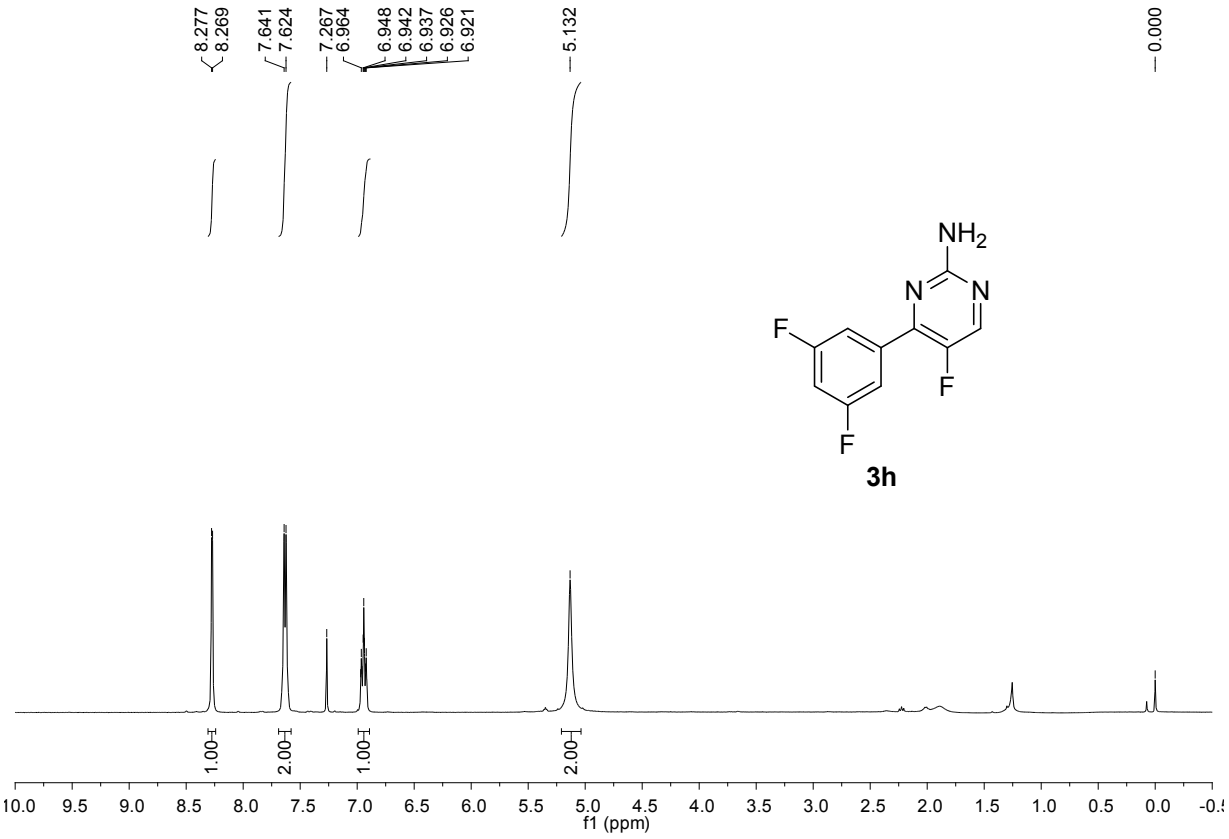
f1 (ppm)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0.000
NH2
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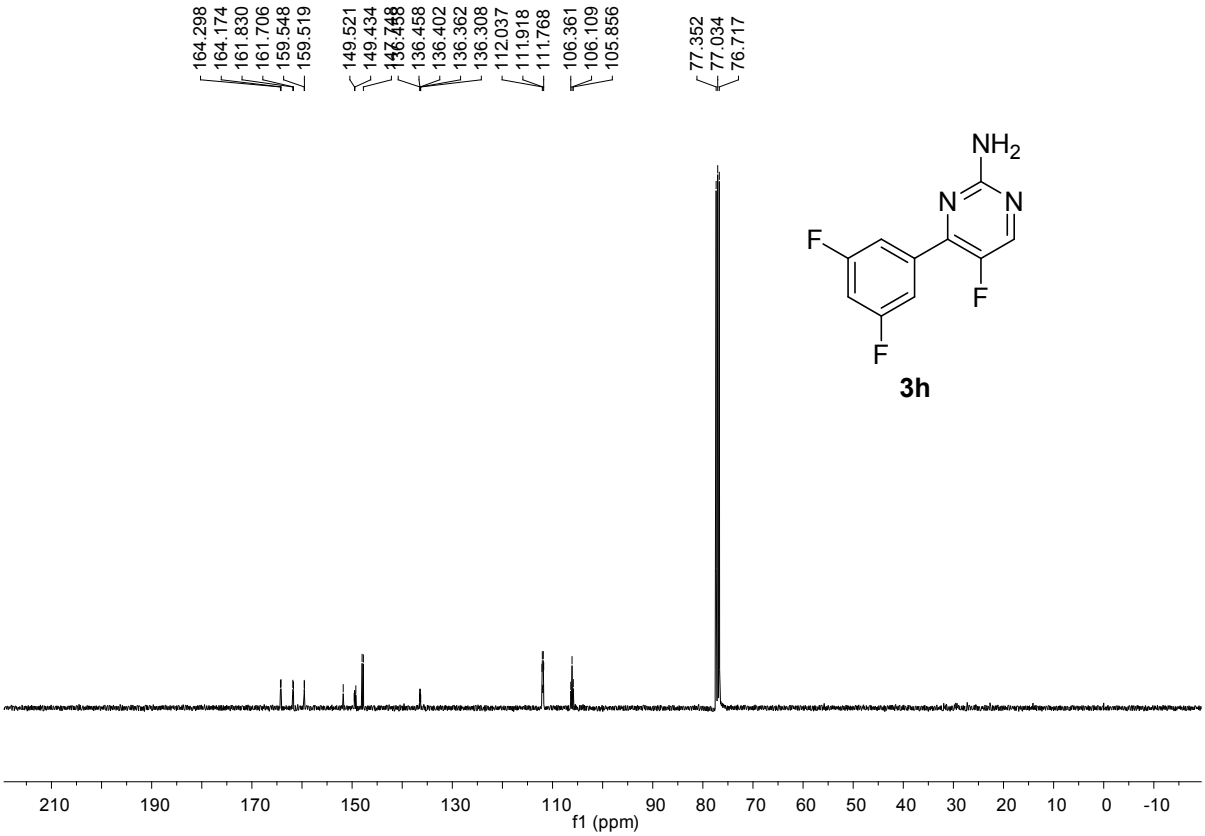
N
F
F
F
3h
1.00
2.00
1.00
2.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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106.361
106.109
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77.034
76.717
NH2
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N
F
F
F
3h
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190
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150
130
110
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80
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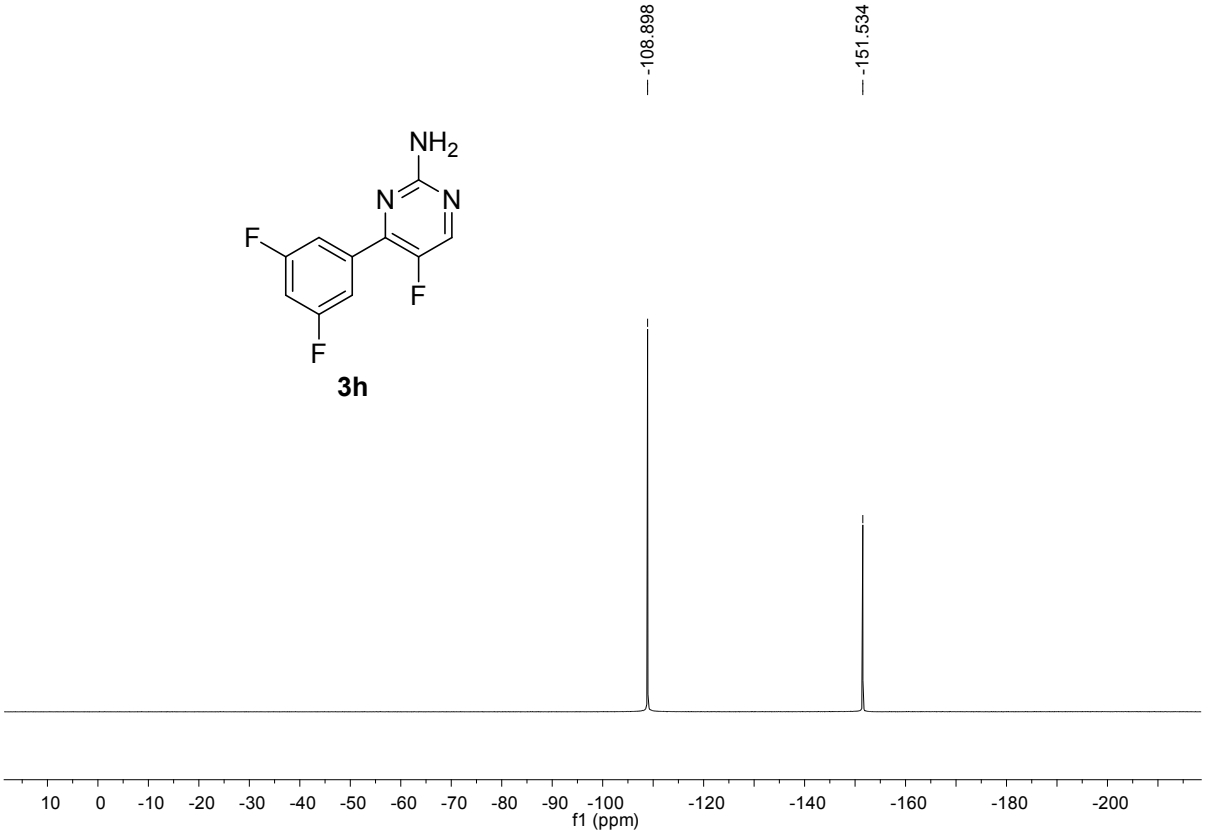
60
50
40
30
20
10
0
-10
f1 (ppm)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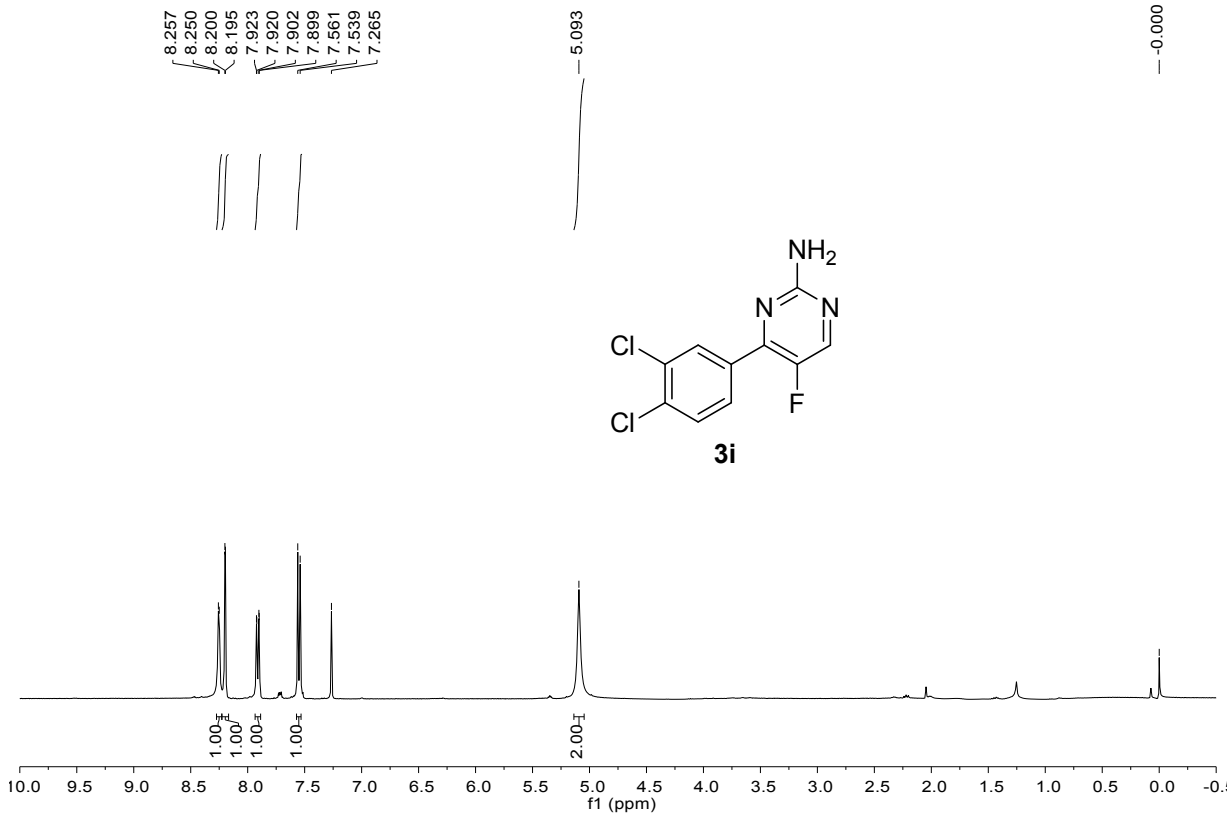
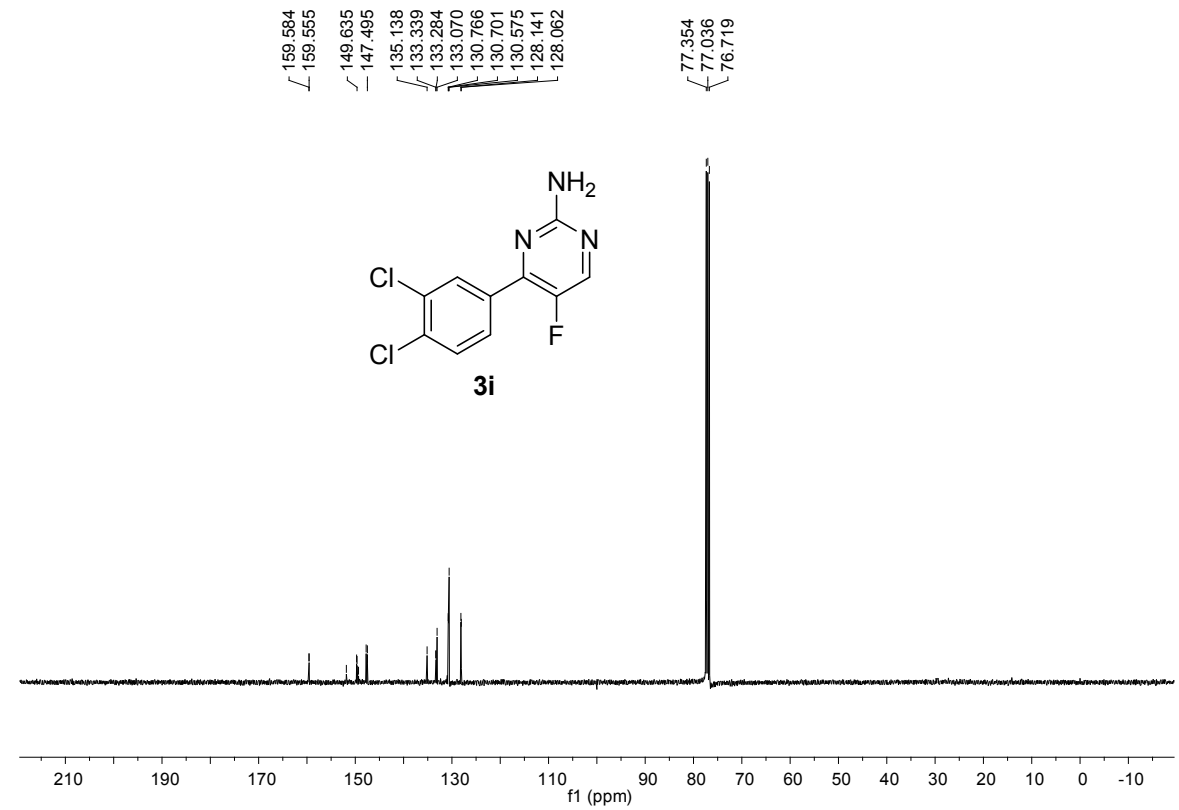
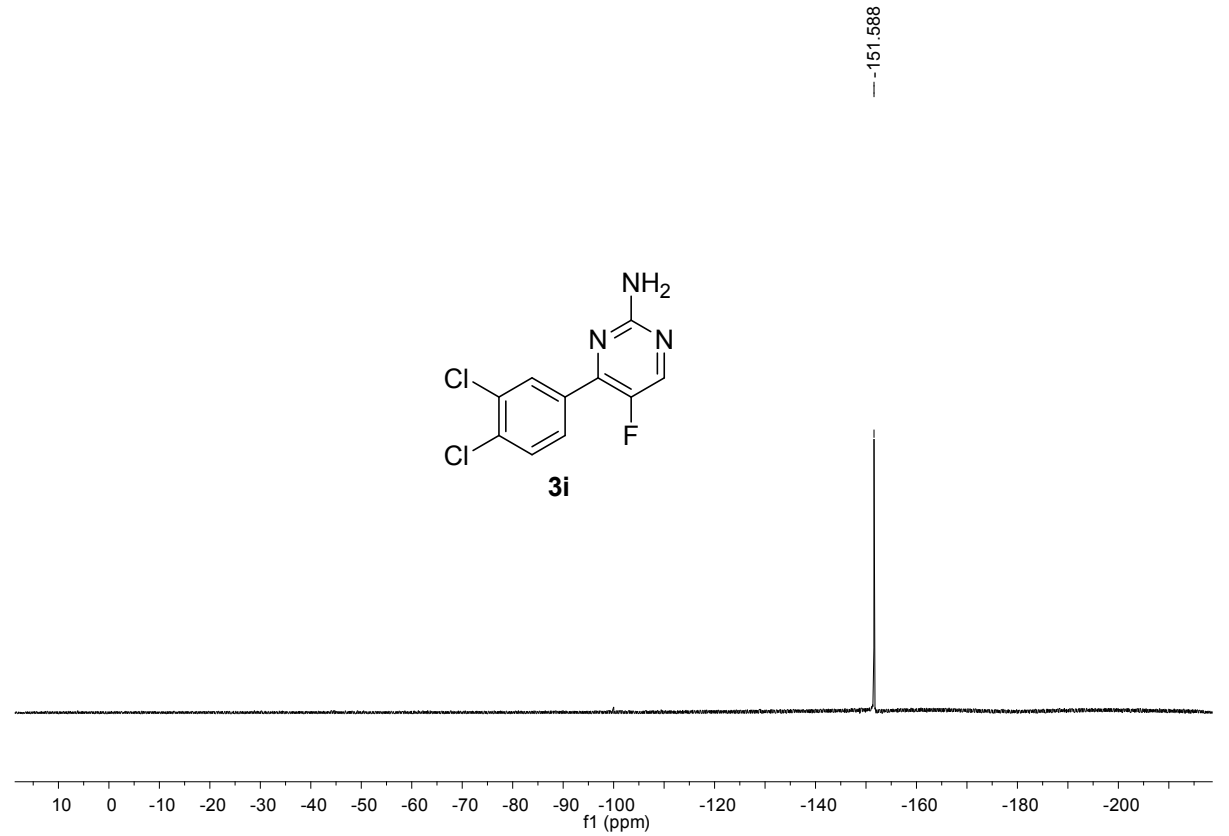
-60
-70
-80
-90
-100
-120
-140
-160
-180
-200
f1 (ppm)


8.257
8.250
8.200
8.195
7.923
7.920
7.902
7.899
7.561
7.539
7.265
5.093
-0.000
NH2
N
N
Cl
Cl
F
3i
1.00
1.00
1.00
1.00
2.00
f1 (ppm)


159.584
159.555
149.635
147.495
135.138
133.339
133.284
133.070
130.766
130.701
130.575
128.141
128.062
77.354
77.036
76.719
NH2
N
N
Cl
Cl
F
3i
f1 (ppm)


-151.588
NH2
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N
Cl
Cl
F
3i
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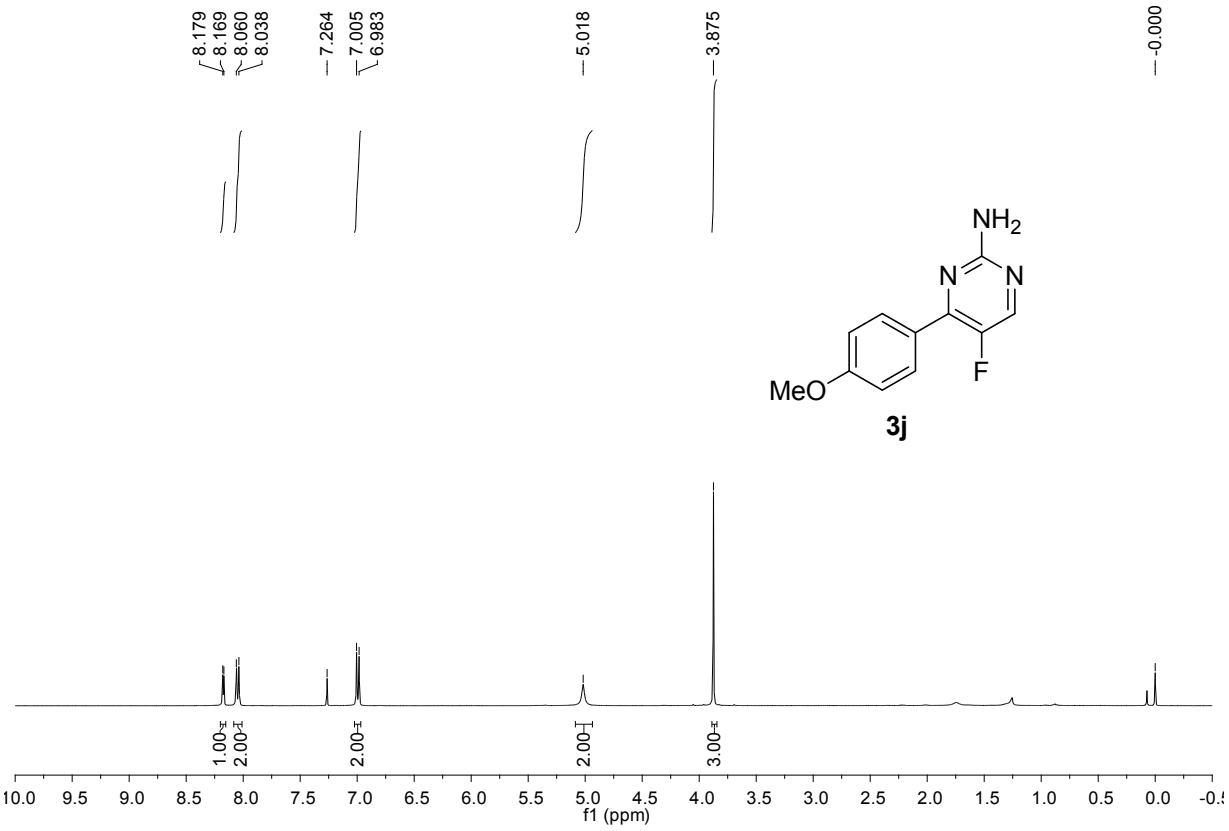
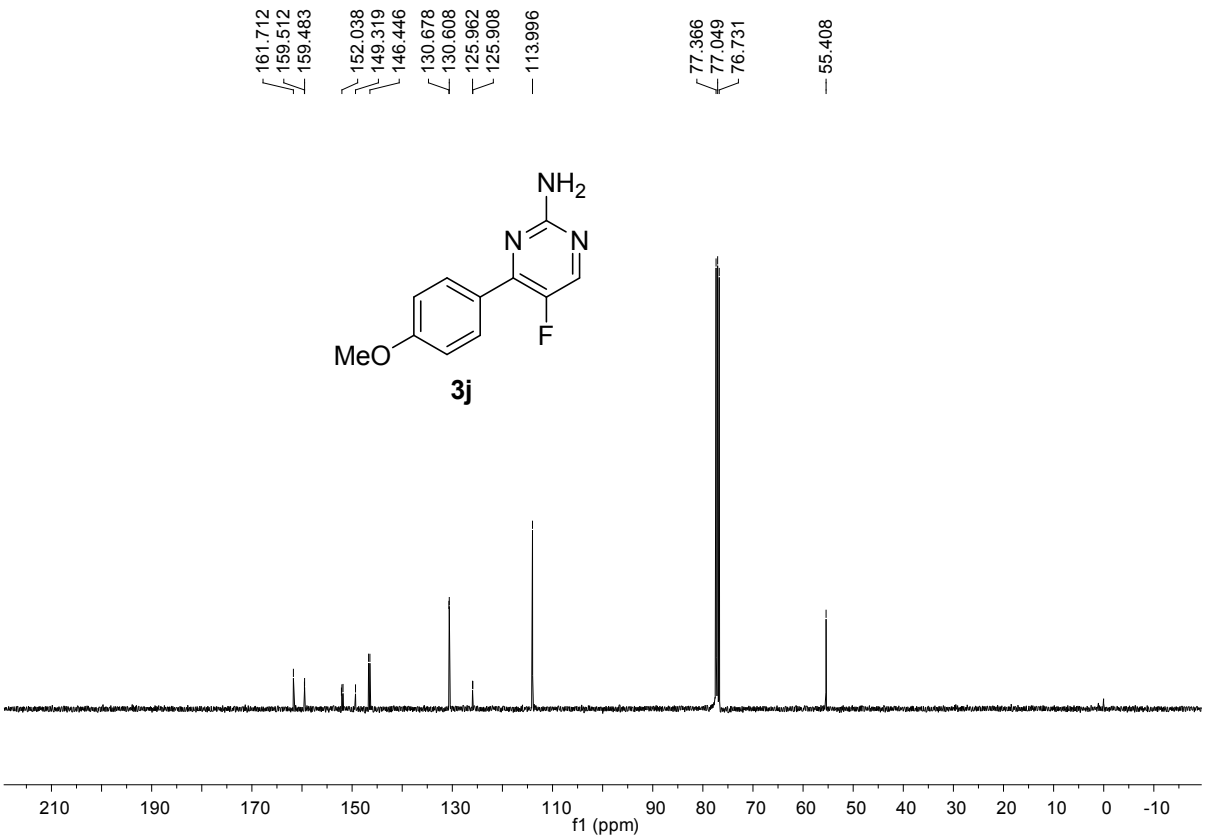
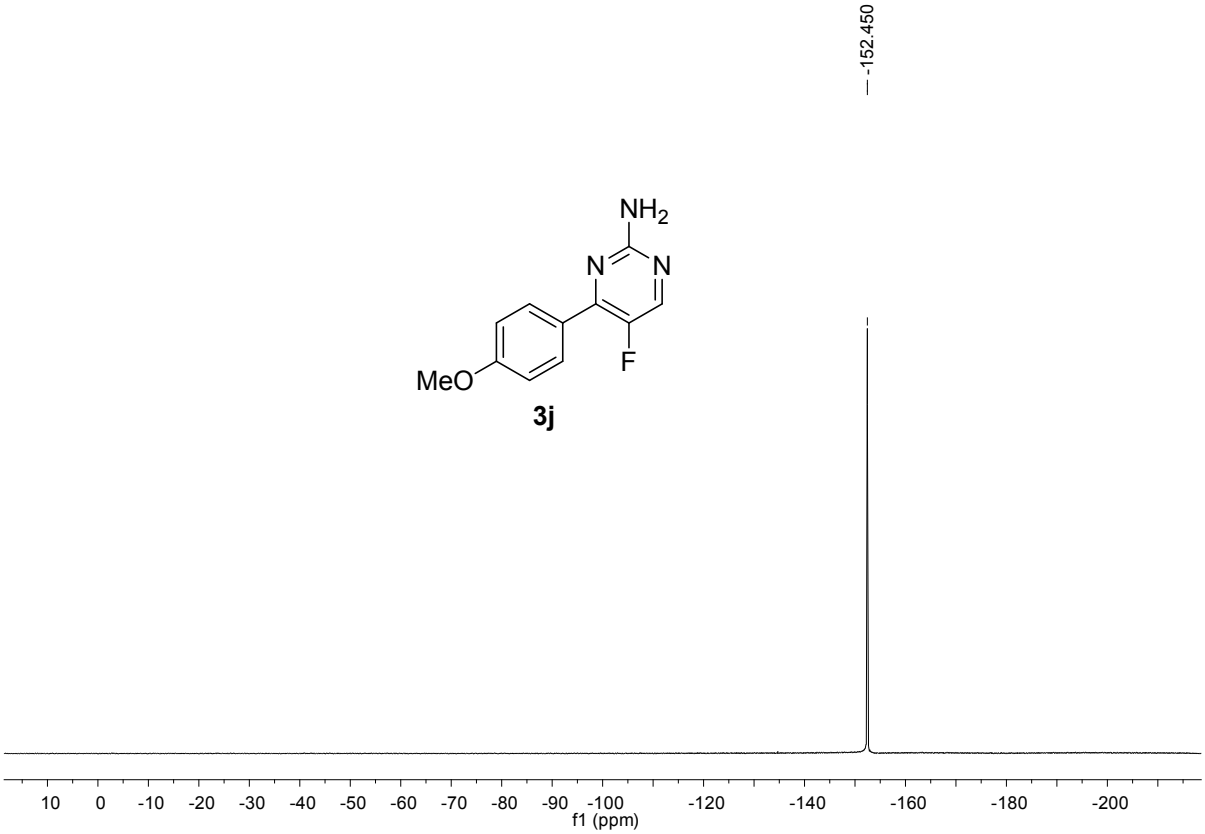
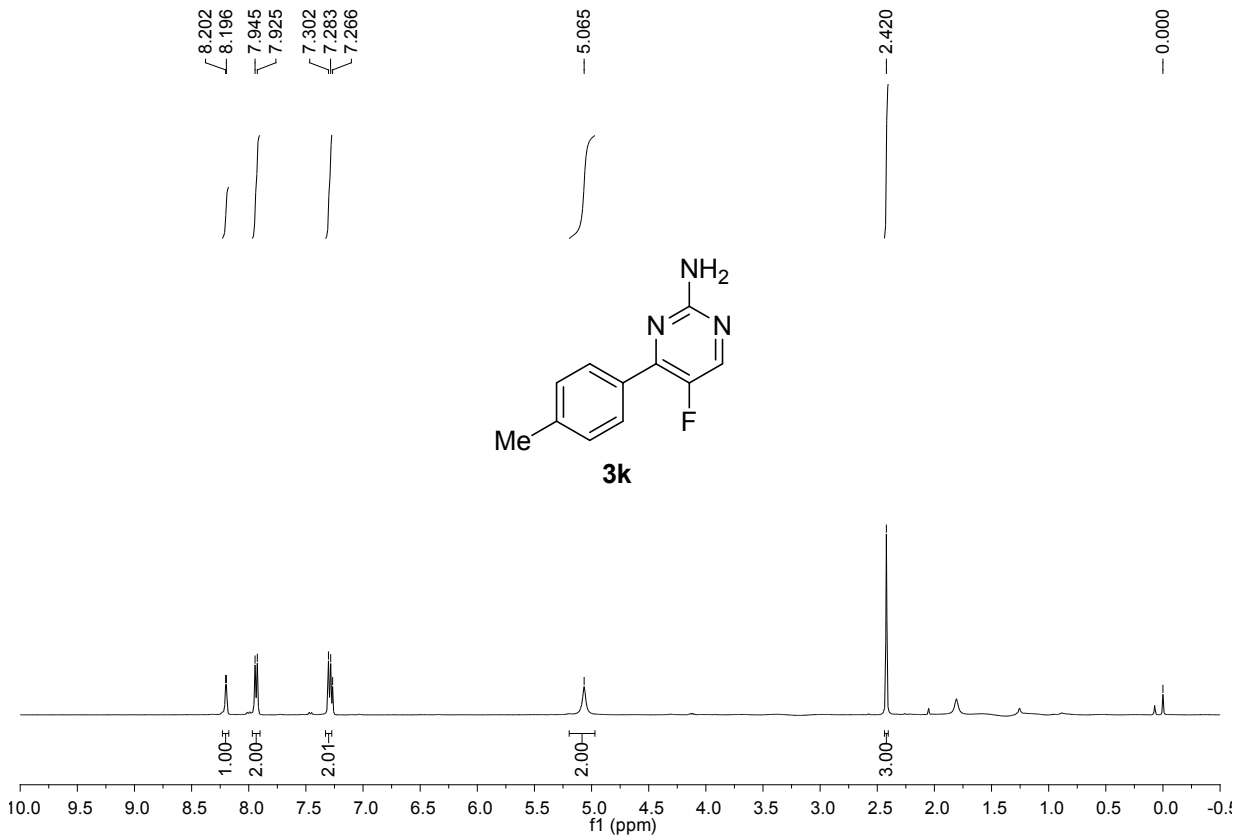
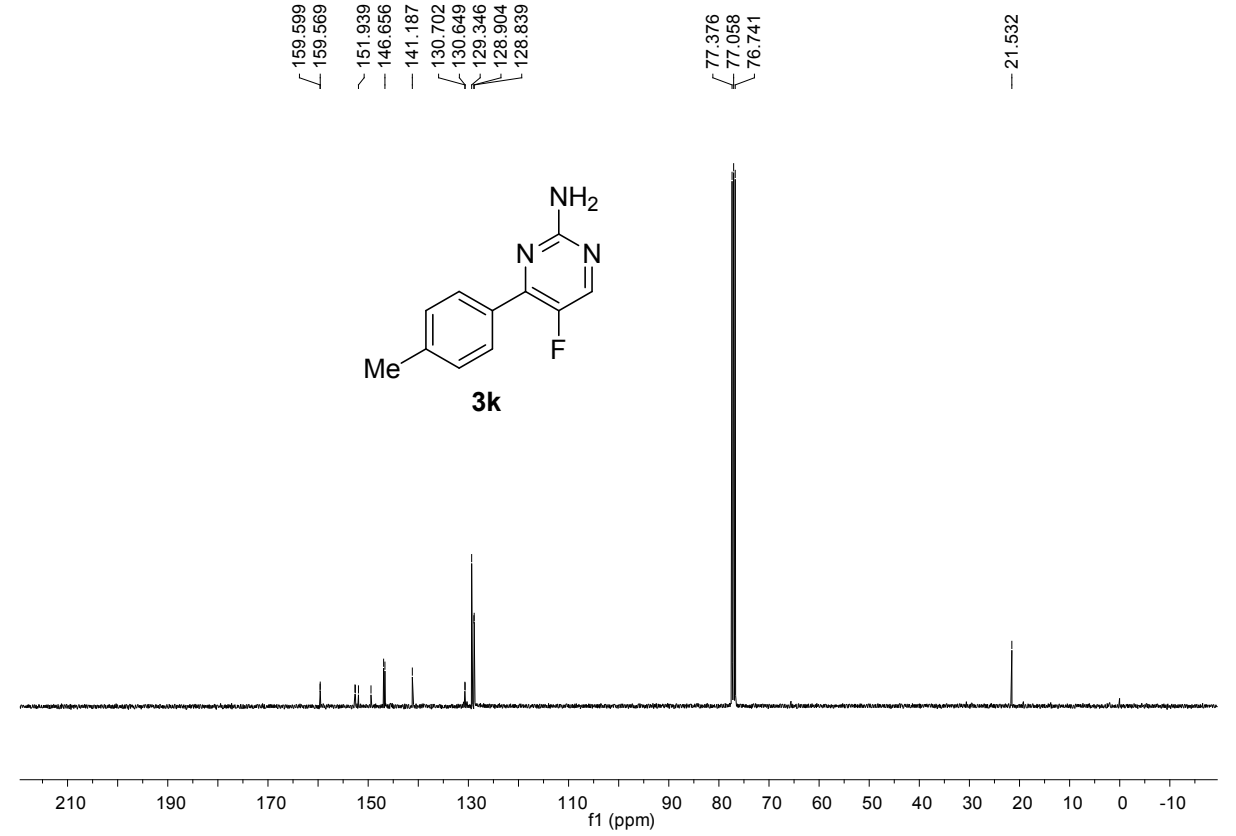
f1 (ppm)

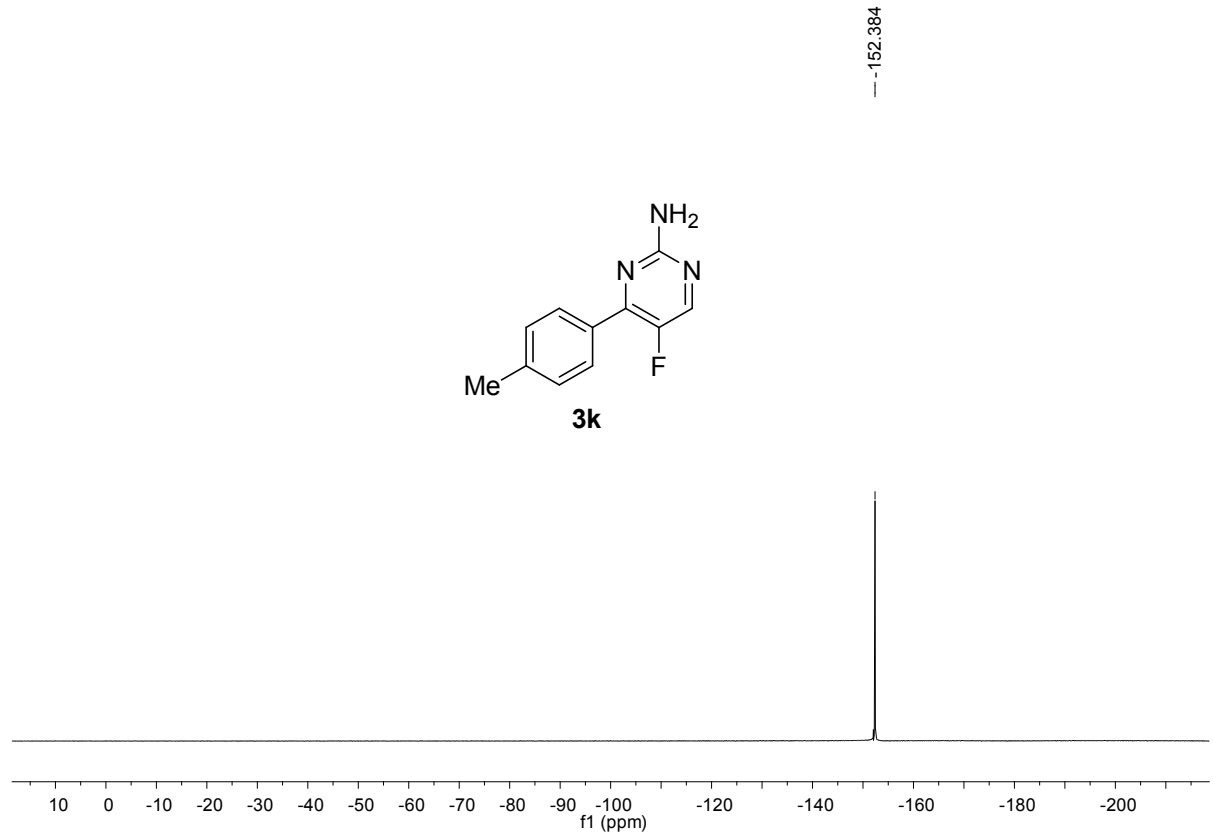

8.179
8.169
8.060
8.038
7.264
7.005
6.983
5.018
3.875
-0.000
NH2
N
N
F
MeO
3j
1.00
2.00
2.00
2.00
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


161.712
159.512
159.483
152.038
149.319
146.446
130.678
130.608
125.962
125.908
113.996
77.366
77.049
76.731
55.408
NH2
N
N
F
MeO
3j
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

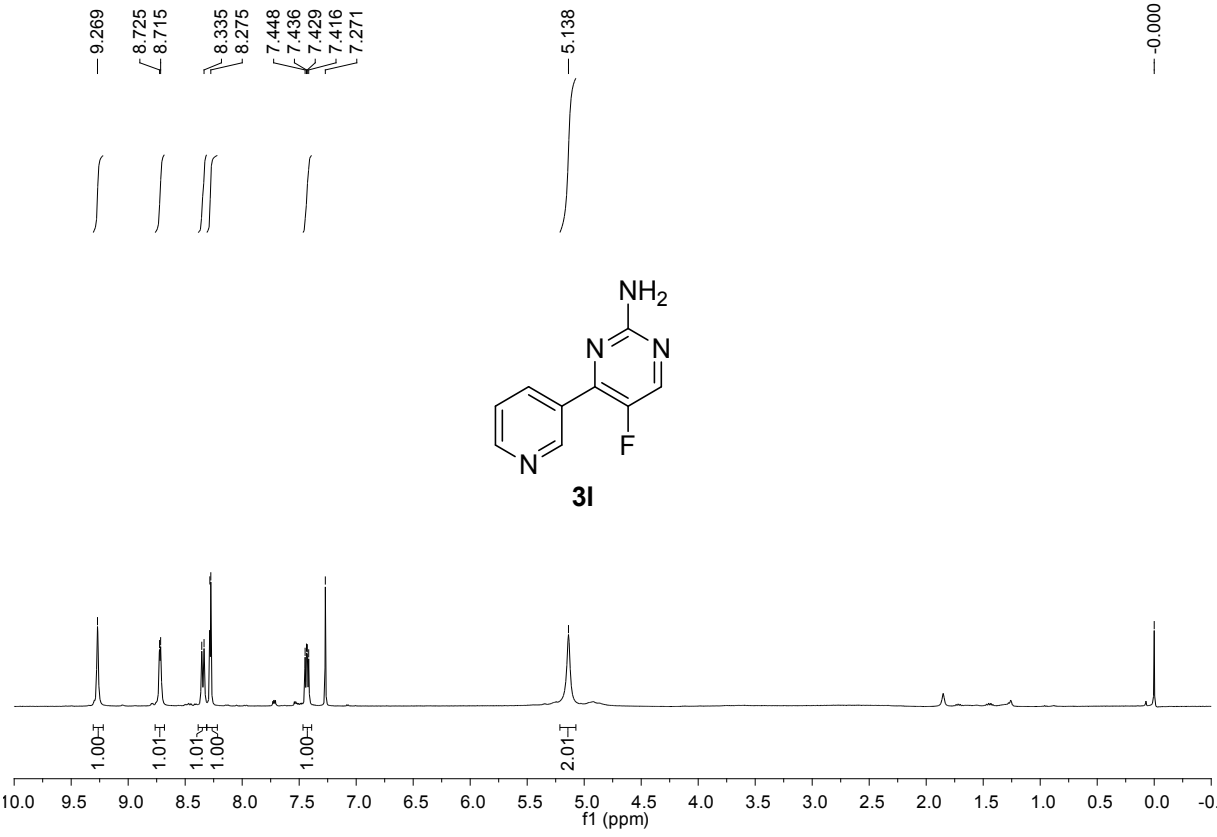

-152.450
NH2
N
N
F
MeO
3j
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-120
-140
-160
-180
-200
f1 (ppm)


8.202
8.196
7.945
7.925
7.302
7.283
7.266
5.065
2.420
0.000
NH2
N
N
F
Me
3k
1.00
2.00
2.01
2.00
3.00
f1 (ppm)

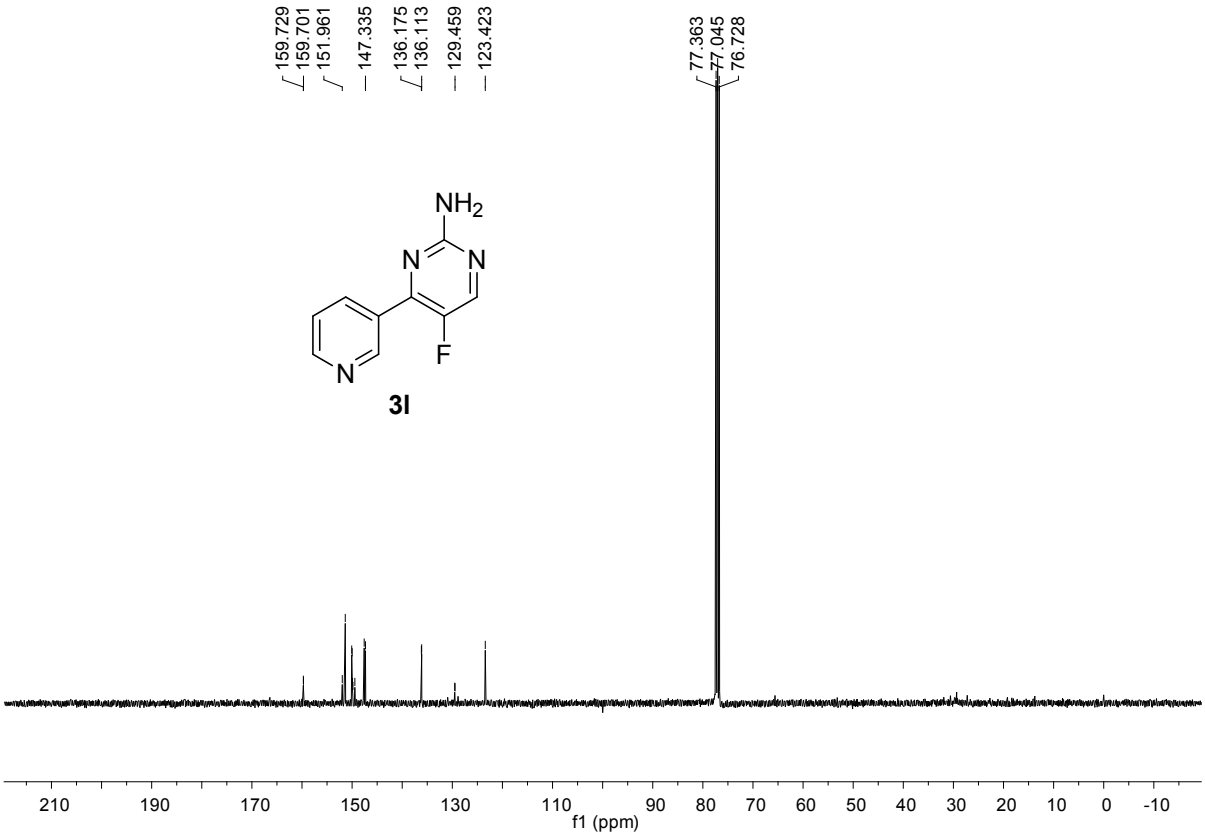

159.599
159.569
151.939
146.656
141.187
130.702
130.649
129.346
128.904
128.839
77.376
77.058
76.741
21.532
NH2
N
N
F
Me
3k
f1 (ppm)

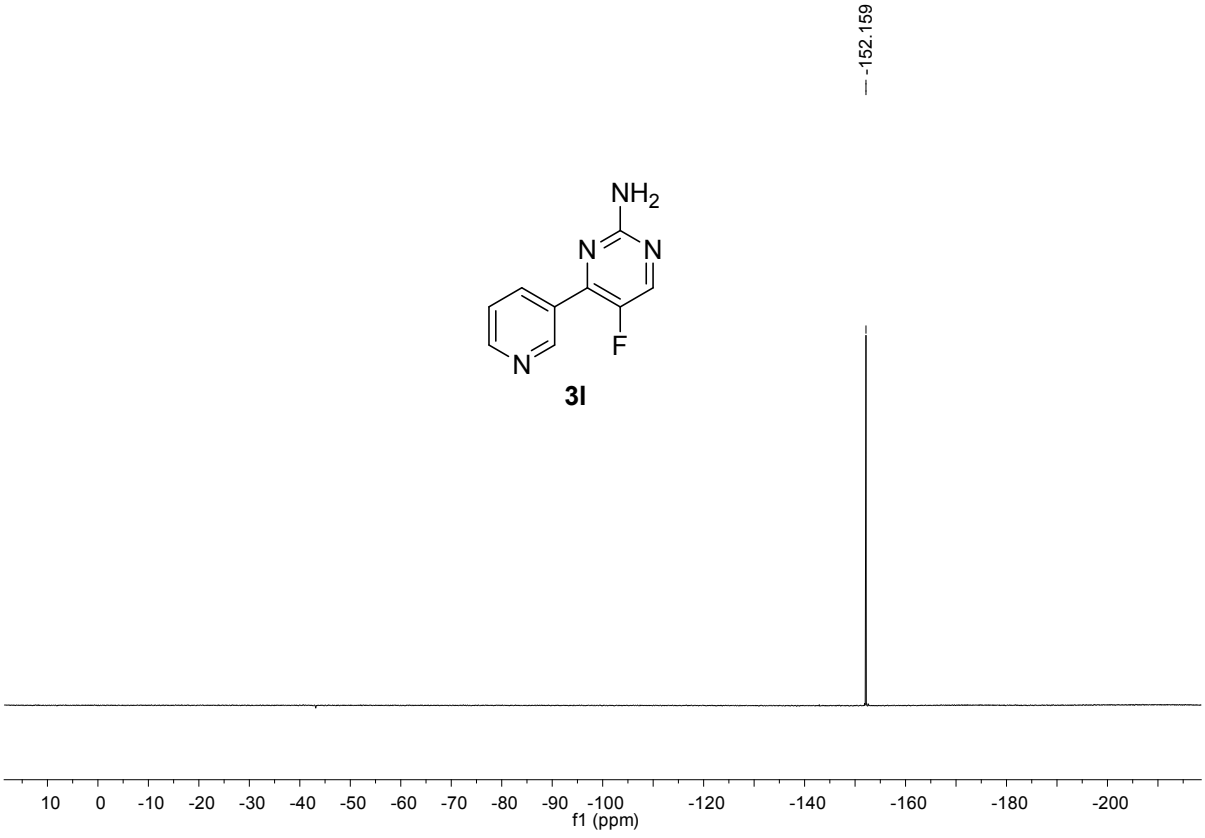

-152.384
NH2
N
N
F
Me
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -120 -140 -160 -180 -200
f1 (ppm)

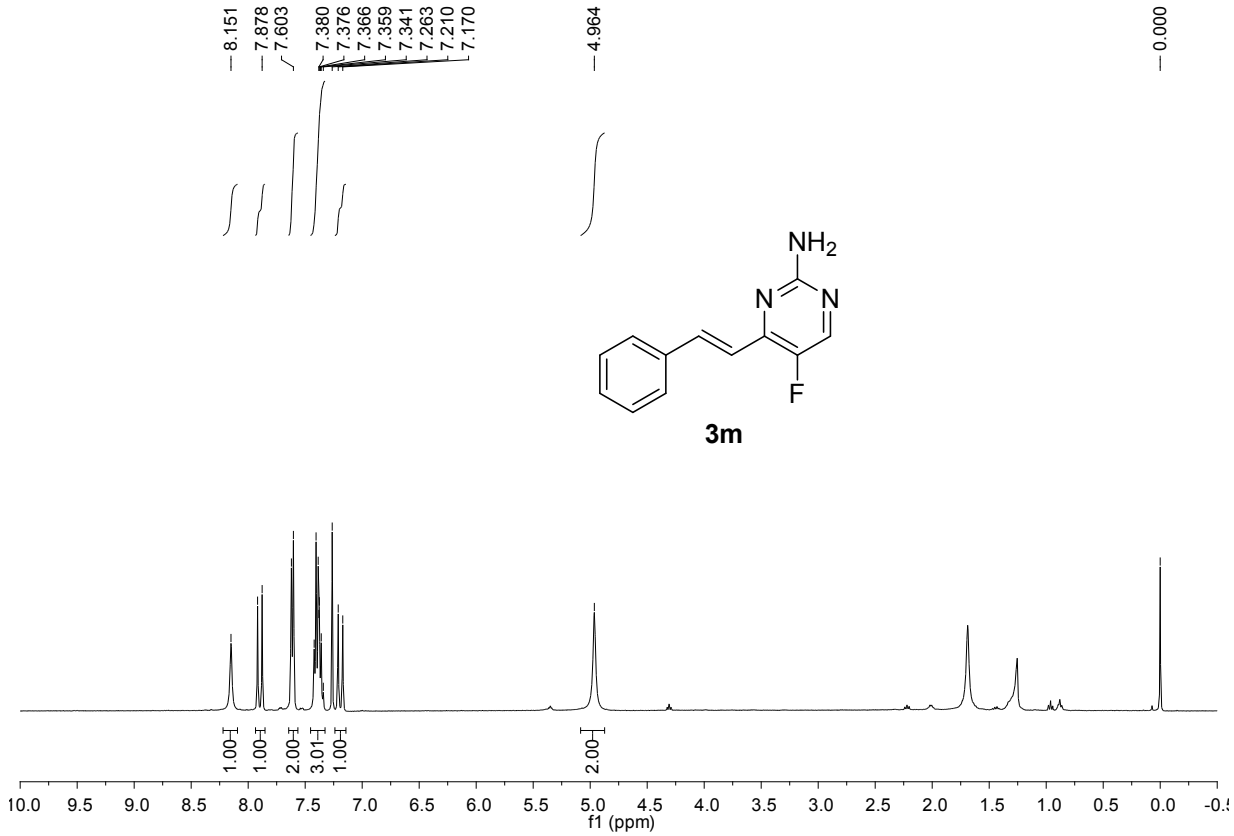
3k

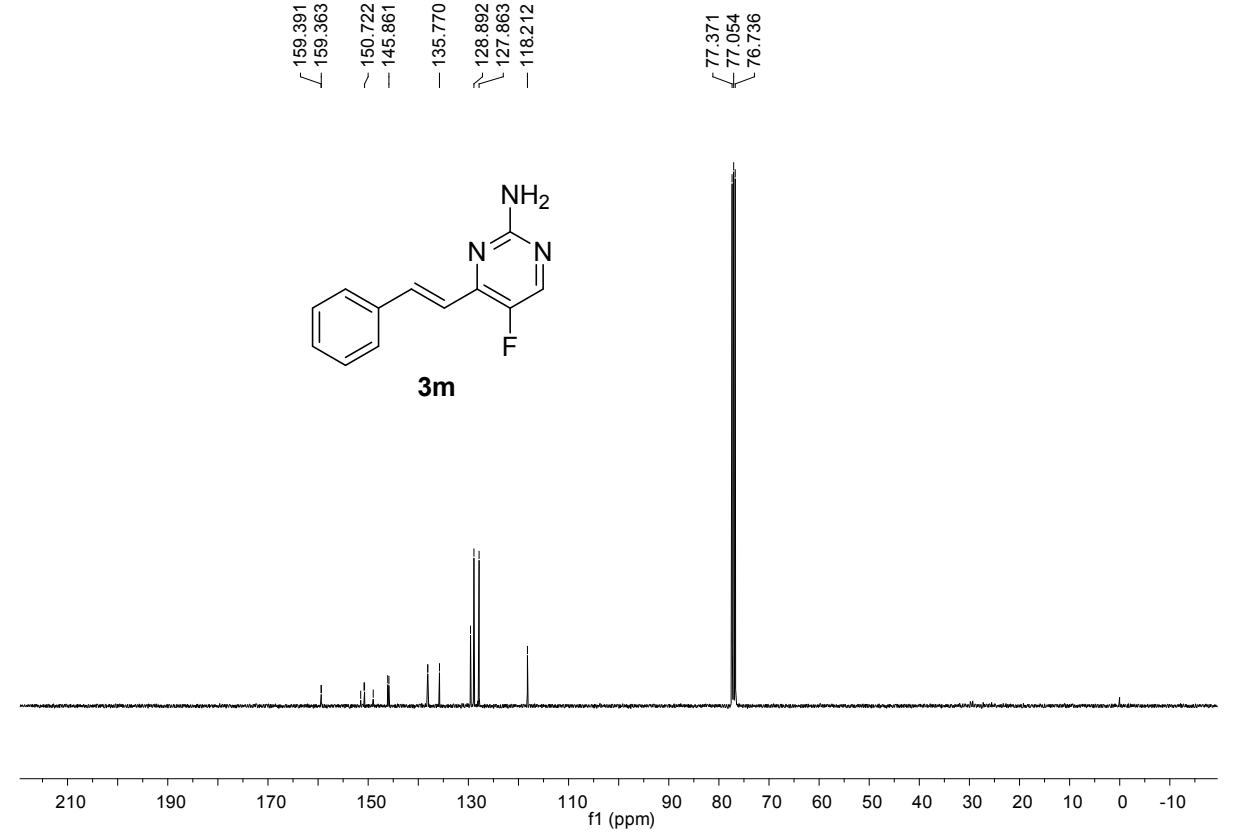

9.269
8.725
8.715
8.335
8.275
7.448
7.436
7.429
7.416
7.271
5.138
-0.000
NH2
N
N
F
N
1.00
1.01
1.01
1.00
1.00
2.01
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

3l


159.729
159.701
151.961
147.335
136.175
136.113
129.459
123.423
77.363
77.045
76.728
NH2
N
N
F
N
3l
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


-152.159
NH2
N
N
F
N
3l
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-120
-140
-160
-180
-200
f1 (ppm)


8.151
7.878
7.603
7.380
7.376
7.366
7.359
7.341
7.263
7.210
7.170
4.964
0.000
NH2
N
N
F
3m
1.00
1.00
2.00
3.01
1.00
2.00
f1 (ppm)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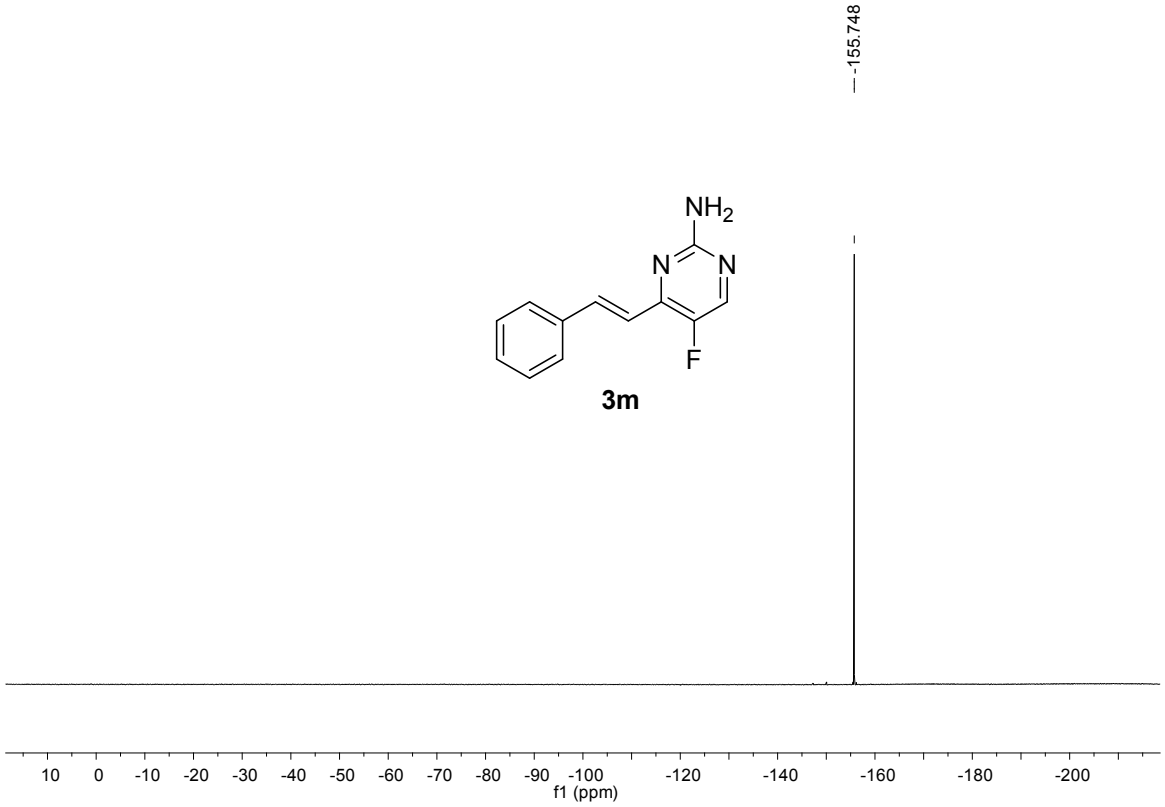
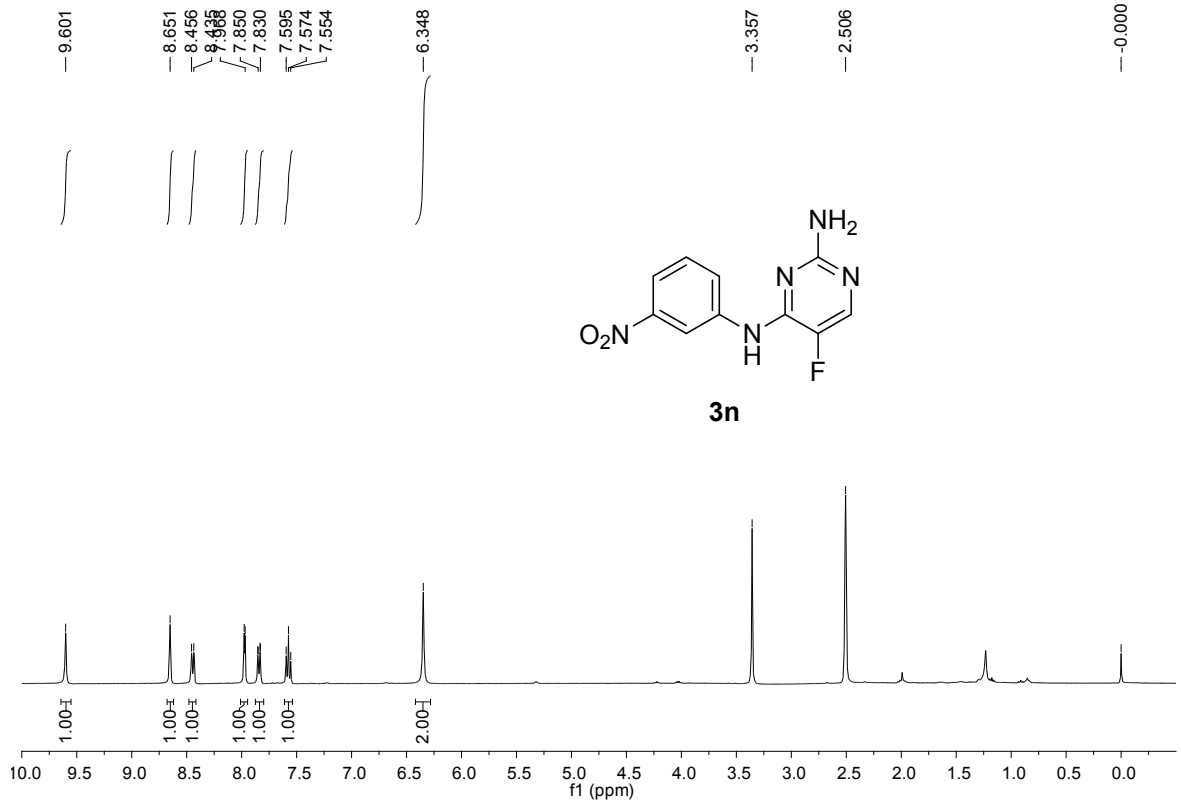
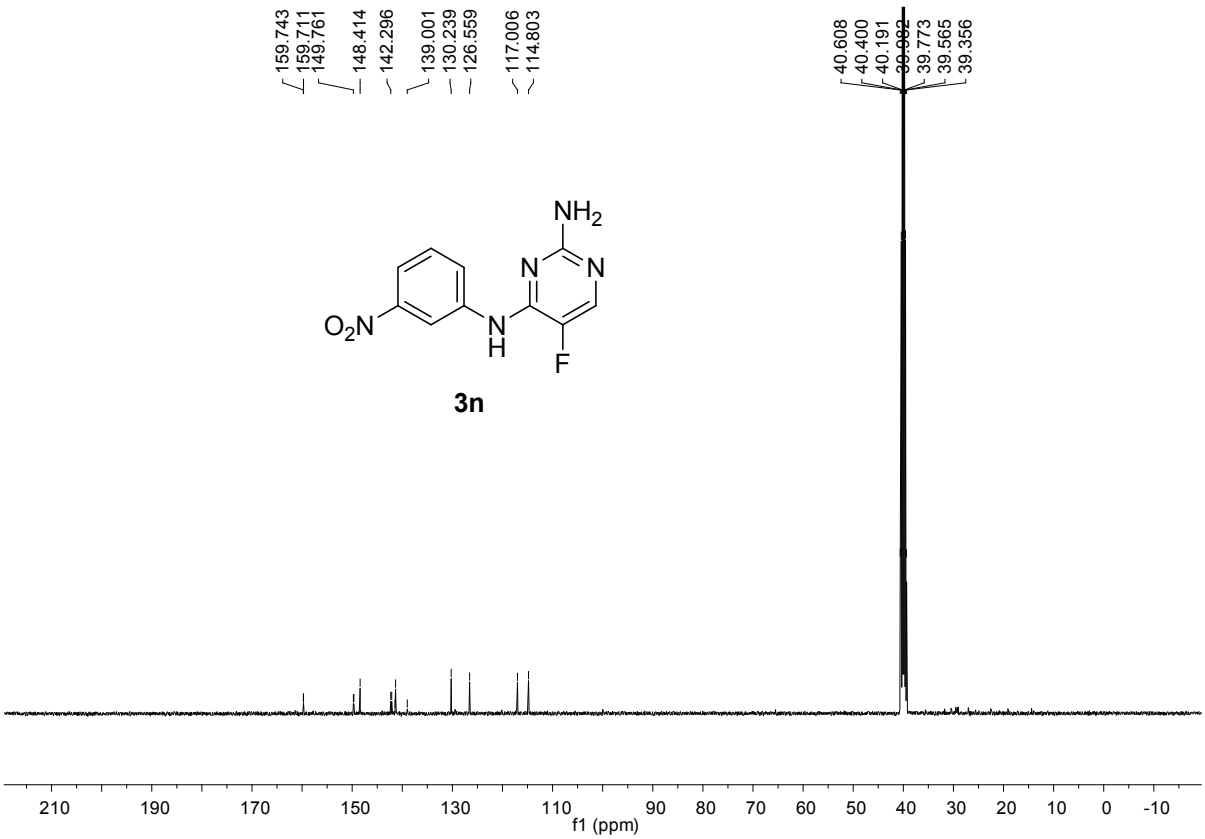
159.363
150.722
145.861
135.770
128.892
127.863
118.212
77.371
77.054
76.736
NH2
N
N
F
3m
f1 (ppm)

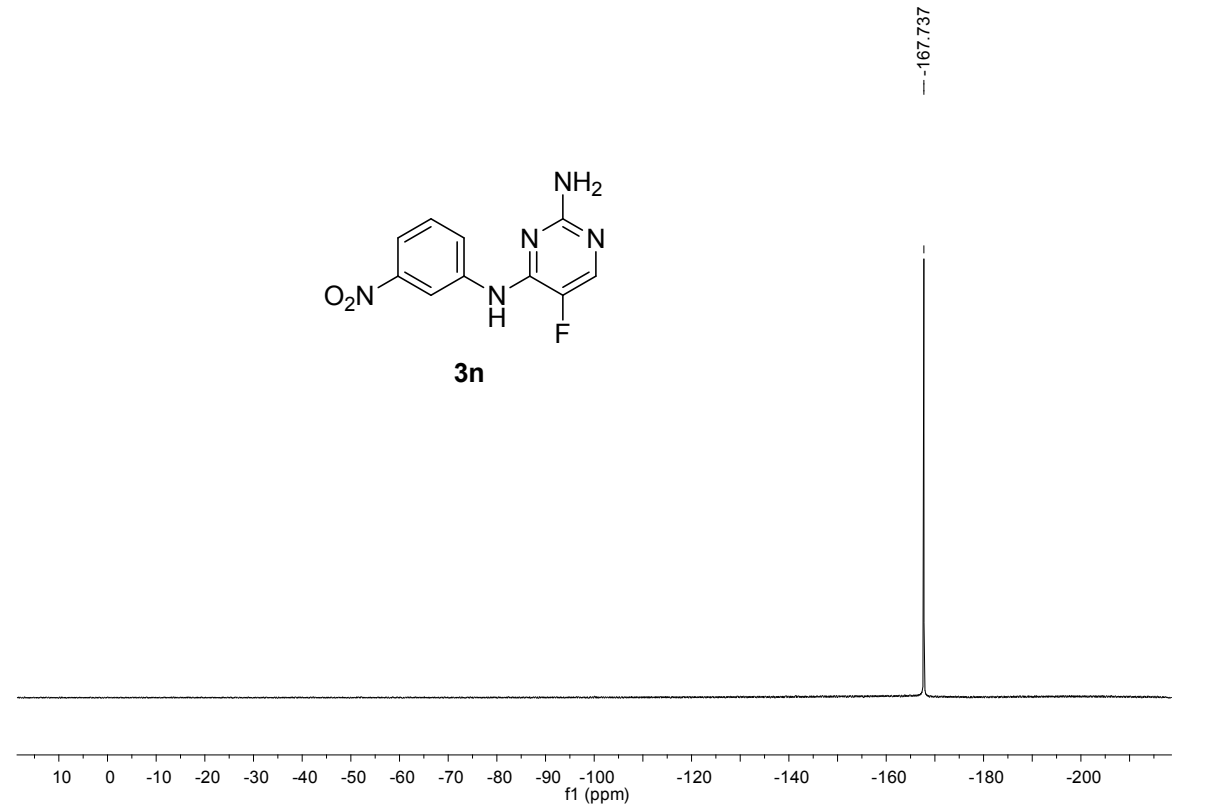

-155.748
NH2
N
N
F
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -120 -140 -160 -180 -200
f1 (ppm)

3m

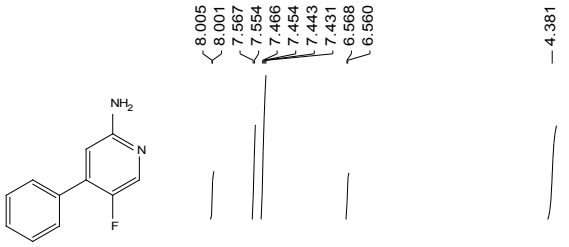

9.601
8.651
8.456
7.850
7.830
7.595
7.574
7.554
6.348
3.357
2.506
-0.000
NH2
N
N
O2N
N
H
F
1.00
1.00
1.00
1.00
1.00
2.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

3n

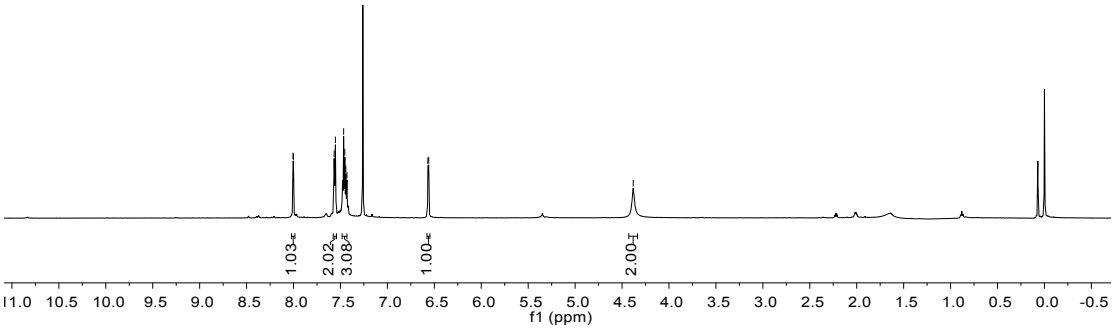

159.743
159.711
149.761
148.414
142.296
139.001
130.239
126.559
117.006
114.803
40.608
40.400
40.191
39.982
39.773
39.565
39.356
NH2
N
N
O2N
N
H
F
3n
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

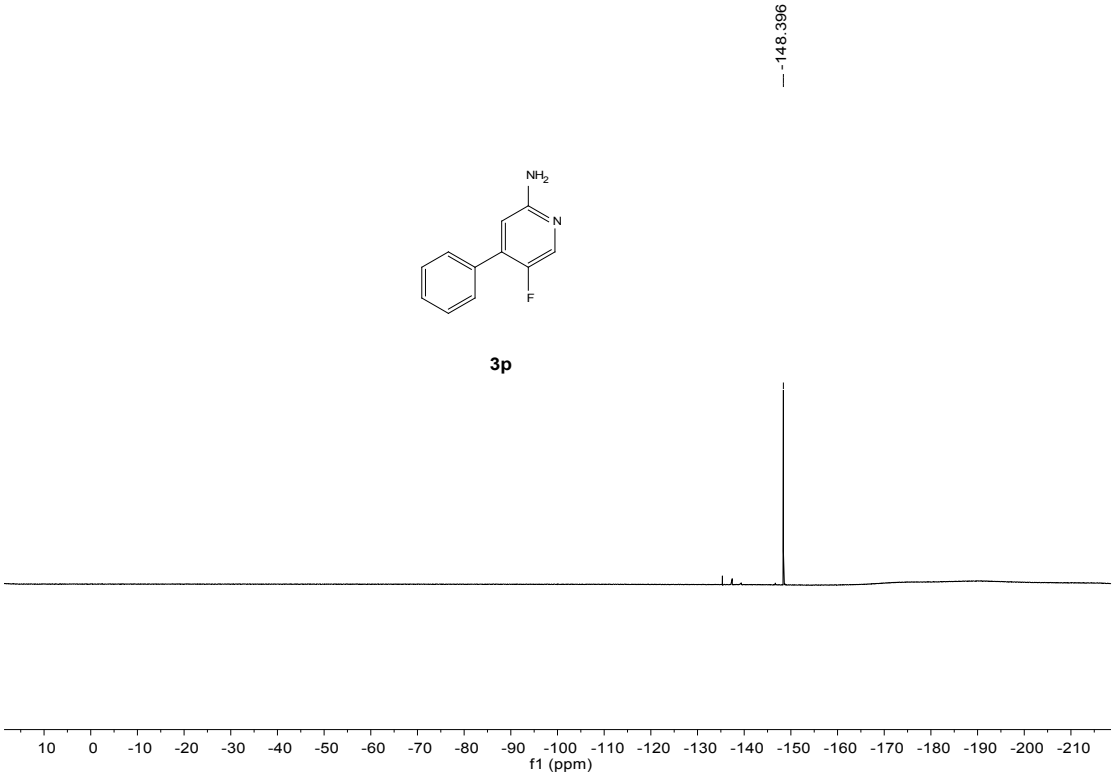

-167.737
NH2
N
N
O2N
N
H
F
3n
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-120
-140
-160
-180
-200
f1 (ppm)

NH2

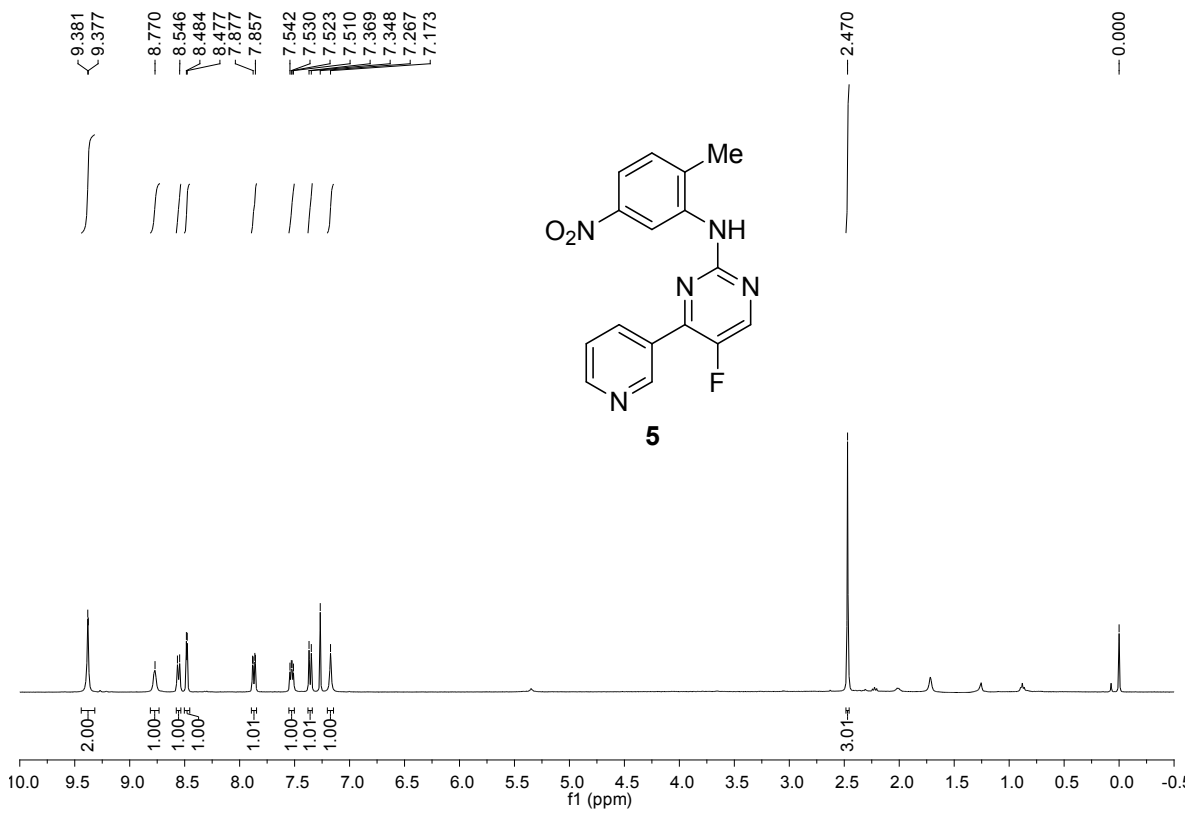

8.005
8.001
7.567
7.554
7.466
7.454
7.443
7.431
6.568
6.560
4.381
NH2
N
F

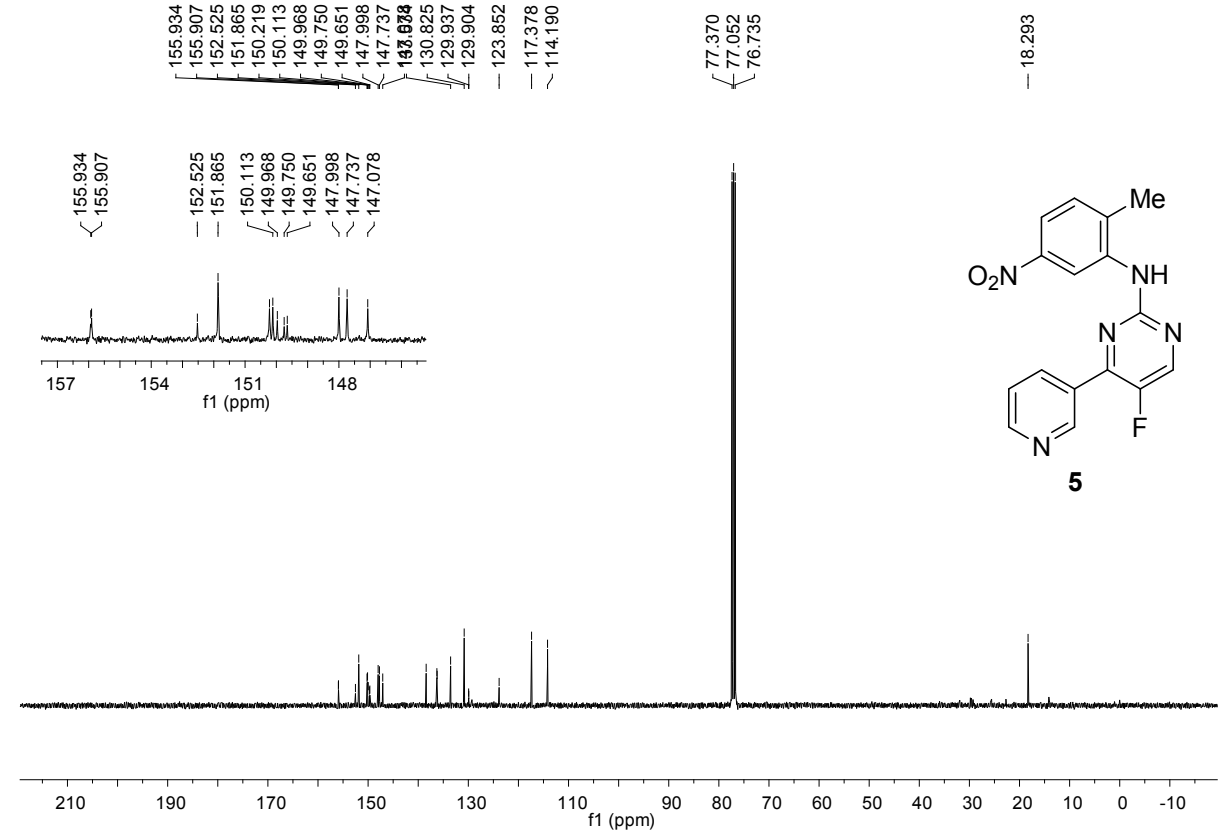
3p

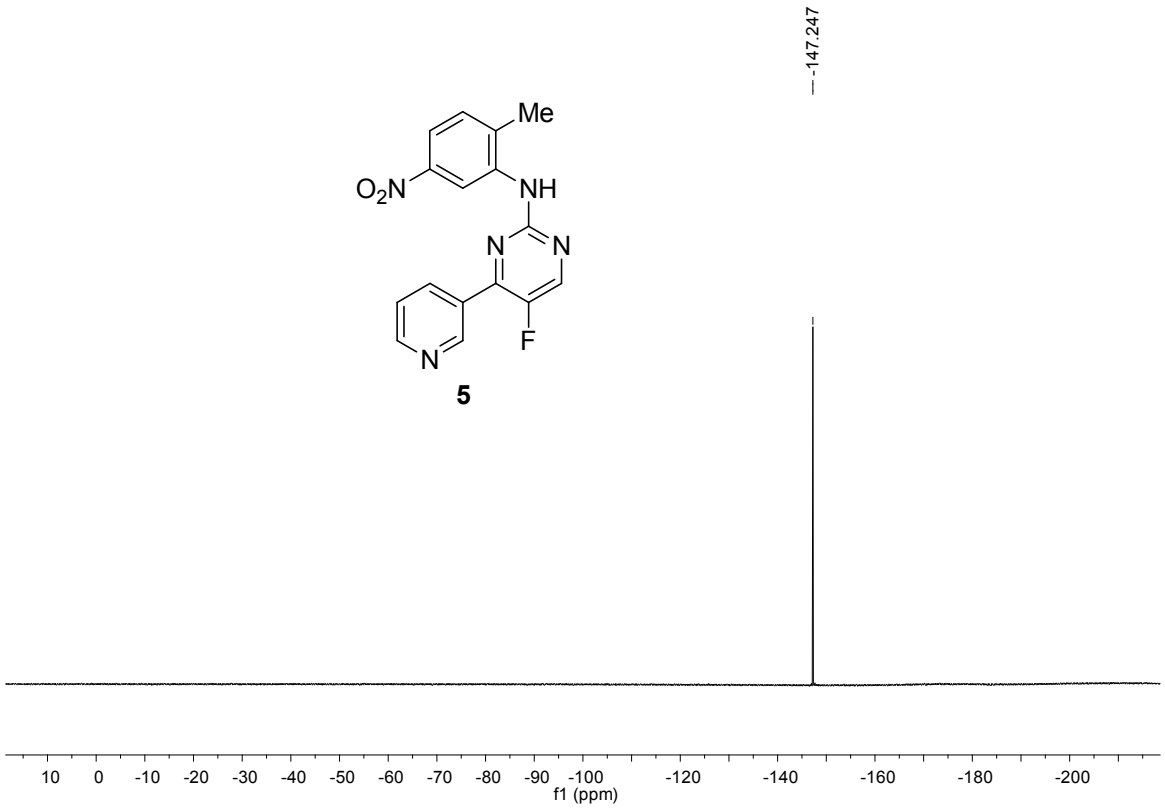

1.03
2.02
3.08
1.00
2.00
f1 (ppm)


-148.396
NH2
N
F
f1 (ppm)

3p

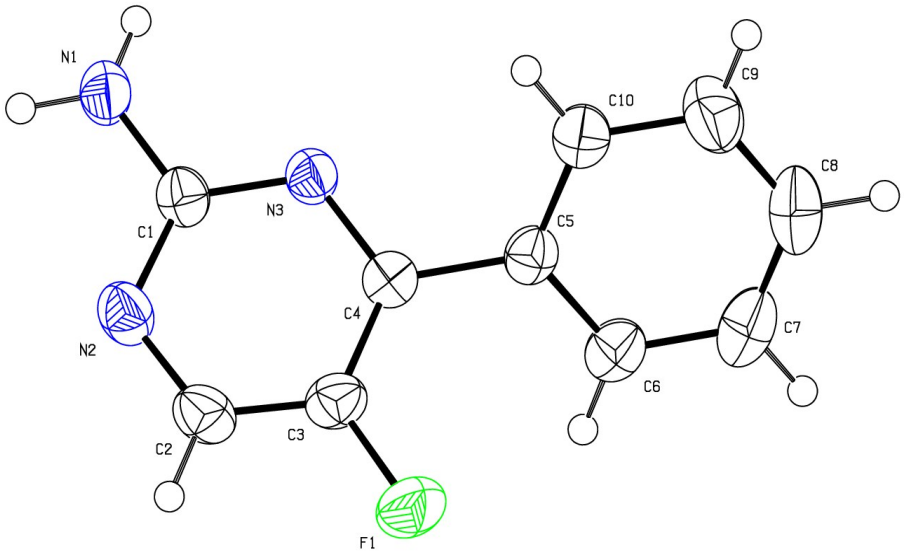

9.381
9.377
8.770
8.546
8.484
8.477
8.877
7.857
7.542
7.530
7.523
7.510
7.369
7.348
7.267
7.173
2.470
0.000
Me
O2N
NH
N
N
F
N
5
2.00
1.00
1.00
1.00
1.01
1.00
1.01
1.00
3.01
f1 (ppm)


155.934
155.907
152.525
151.865
150.219
150.113
149.968
149.750
149.651
147.998
147.737
130.825
129.937
129.904
123.852
117.378
114.190
77.370
77.052
76.735
18.293
155.934
155.907
152.525
151.865
150.113
149.968
149.750
149.651
147.998
147.737
147.078
157
154
151
148
f1 (ppm)
Me
O2N
NH
N
N
F
N
5
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


-147.247
Me
O2N
NH
N
N
F
N
5
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-120
-140
-160
-180
-200
f1 (ppm)

9. X-ray crystallography of 3a, 3l, 5 and Ag(dppm)1d complex

X-ray crystallography of 3a



3a

Table 1. Crystal data and structure refinement for Mo_160314ba.

Identification code	Mo_160314ba	
Empirical formula	C10 H8 F N3	
Formula weight	189.19	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	Pbca	
Unit cell dimensions	a = 7.4865(8) Å	α= 90°.
	b = 11.7277(13) Å	β= 90°.
	c = 20.913(3) Å	γ = 90°.
Volume	1836.1(4) $Å^3$	
Z	8	
Density (calculated)	1.369 Mg/m^3	
Absorption coefficient	0.100 mm^{-1}	
F(000)	784	
Crystal size	0.300 x 0.150 x 0.150 mm^3	
Theta range for data collection	3.347 to 27.582°.	
Index ranges	-9<=h<=9, -15<=k<=15, -27<=l<=26	
Reflections collected	47406	
Independent reflections	2114 [R(int) = 0.0361]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Refinement method	Full-matrix least-squares on F^2	

Data / restraints / parameters	2114 / 2 / 135
Goodness-of-fit on F^2	1.106
Final R indices [I>2sigma(I)]	R1 = 0.0436, wR2 = 0.0997
R indices (all data)	R1 = 0.0552, wR2 = 0.1080
Extinction coefficient	n/a
Largest diff. peak and hole	0.212 and -0.221 e.$Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for Mo_160314ba. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
F(1)	4707(1)	3876(1)	6350(1)	59(1)
N(1)	4664(2)	7772(1)	5026(1)	47(1)
C(1)	4693(2)	6790(1)	5356(1)	34(1)
N(2)	3200(2)	6143(1)	5342(1)	40(1)
C(2)	3258(2)	5181(1)	5675(1)	42(1)
N(3)	6204(1)	6529(1)	5675(1)	33(1)
C(3)	4749(2)	4859(1)	6010(1)	38(1)
C(4)	6249(2)	5549(1)	6007(1)	32(1)
C(5)	7911(2)	5280(1)	6362(1)	34(1)
C(6)	8552(2)	4168(1)	6402(1)	41(1)
C(7)	10070(2)	3933(2)	6753(1)	52(1)
C(8)	10961(2)	4793(2)	7067(1)	56(1)
C(9)	10359(2)	5899(2)	7021(1)	56(1)
C(10)	8847(2)	6145(1)	6666(1)	45(1)

Table 3. Bond lengths [Å] and angles [°] for Mo_160314ba.

F(1)-C(3)	1.3557(16)
N(1)-C(1)	1.3428(18)
N(1)-H(1A)	0.891(14)
N(1)-H(1B)	0.875(14)
C(1)-N(3)	1.3483(16)
C(1)-N(2)	1.3515(17)
N(2)-C(2)	1.3257(18)
C(2)-C(3)	1.371(2)
C(2)-H(2)	0.9300
N(3)-C(4)	1.3434(16)
C(3)-C(4)	1.3834(19)
C(4)-C(5)	1.4833(18)
C(5)-C(10)	1.388(2)
C(5)-C(6)	1.3918(19)
C(6)-C(7)	1.382(2)
C(6)-H(6)	0.9300
C(7)-C(8)	1.376(3)
C(7)-H(7)	0.9300
C(8)-C(9)	1.377(2)
C(8)-H(8)	0.9300
C(9)-C(10)	1.384(2)
C(9)-H(9)	0.9300
C(10)-H(10)	0.9300
C(1)-N(1)-H(1A)	117.7(12)
C(1)-N(1)-H(1B)	120.6(12)
H(1A)-N(1)-H(1B)	118.1(16)
N(1)-C(1)-N(3)	117.52(12)
N(1)-C(1)-N(2)	117.21(12)
N(3)-C(1)-N(2)	125.27(12)
C(2)-N(2)-C(1)	116.05(12)
N(2)-C(2)-C(3)	121.94(13)
N(2)-C(2)-H(2)	119.0
C(3)-C(2)-H(2)	119.0
C(4)-N(3)-C(1)	118.06(11)
F(1)-C(3)-C(2)	118.92(12)

F(1)-C(3)-C(4)	121.24(13)
C(2)-C(3)-C(4)	119.83(13)
N(3)-C(4)-C(3)	118.85(12)
N(3)-C(4)-C(5)	117.47(11)
C(3)-C(4)-C(5)	123.66(12)
C(10)-C(5)-C(6)	118.91(13)
C(10)-C(5)-C(4)	119.87(12)
C(6)-C(5)-C(4)	121.22(12)
C(7)-C(6)-C(5)	120.17(14)
C(7)-C(6)-H(6)	119.9
C(5)-C(6)-H(6)	119.9
C(8)-C(7)-C(6)	120.39(15)
C(8)-C(7)-H(7)	119.8
C(6)-C(7)-H(7)	119.8
C(7)-C(8)-C(9)	119.93(15)
C(7)-C(8)-H(8)	120.0
C(9)-C(8)-H(8)	120.0
C(8)-C(9)-C(10)	120.13(16)
C(8)-C(9)-H(9)	119.9
C(10)-C(9)-H(9)	119.9
C(9)-C(10)-C(5)	120.43(14)
C(9)-C(10)-H(10)	119.8
C(5)-C(10)-H(10)	119.8

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for Mo_160314ba. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
F(1)	50(1)	47(1)	81(1)	25(1)	2(1)	-8(1)
N(1)	32(1)	53(1)	57(1)	20(1)	-9(1)	-4(1)
C(1)	30(1)	40(1)	31(1)	1(1)	2(1)	1(1)
N(2)	30(1)	51(1)	40(1)	4(1)	0(1)	-4(1)
C(2)	33(1)	47(1)	44(1)	2(1)	4(1)	-8(1)
N(3)	30(1)	35(1)	33(1)	2(1)	-1(1)	-1(1)
C(3)	39(1)	36(1)	41(1)	6(1)	6(1)	-3(1)
C(4)	32(1)	34(1)	29(1)	-1(1)	4(1)	1(1)
C(5)	34(1)	37(1)	30(1)	5(1)	3(1)	2(1)
C(6)	42(1)	39(1)	42(1)	4(1)	5(1)	5(1)
C(7)	51(1)	55(1)	50(1)	12(1)	4(1)	18(1)
C(8)	46(1)	79(1)	42(1)	7(1)	-8(1)	15(1)
C(9)	50(1)	66(1)	51(1)	-4(1)	-15(1)	0(1)
C(10)	46(1)	41(1)	47(1)	1(1)	-8(1)	2(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for Mo_160314ba.

	x	y	z	U(eq)
H(1A)	3720(20)	7906(15)	4776(8)	55(5)
H(1B)	5655(19)	8142(15)	4947(8)	55(5)
H(2)	2257	4711	5681	50
H(6)	7956	3582	6191	49
H(7)	10492	3188	6778	62
H(8)	11970	4628	7309	67
H(9)	10969	6482	7229	67
H(10)	8456	6895	6632	53

Table 6. Torsion angles [°] for Mo_160314ba.

N(1)-C(1)-N(2)-C(2)	-179.60(13)
N(3)-C(1)-N(2)-C(2)	0.4(2)
C(1)-N(2)-C(2)-C(3)	-0.5(2)
N(1)-C(1)-N(3)-C(4)	-179.99(12)
N(2)-C(1)-N(3)-C(4)	0.02(19)
N(2)-C(2)-C(3)-F(1)	178.75(12)
N(2)-C(2)-C(3)-C(4)	0.1(2)
C(1)-N(3)-C(4)-C(3)	-0.36(18)
C(1)-N(3)-C(4)-C(5)	-179.22(11)
F(1)-C(3)-C(4)-N(3)	-178.29(12)
C(2)-C(3)-C(4)-N(3)	0.3(2)
F(1)-C(3)-C(4)-C(5)	0.5(2)
C(2)-C(3)-C(4)-C(5)	179.08(12)
N(3)-C(4)-C(5)-C(10)	38.07(17)
C(3)-C(4)-C(5)-C(10)	-140.73(14)
N(3)-C(4)-C(5)-C(6)	-142.52(13)
C(3)-C(4)-C(5)-C(6)	38.68(19)
C(10)-C(5)-C(6)-C(7)	1.6(2)
C(4)-C(5)-C(6)-C(7)	-177.79(12)
C(5)-C(6)-C(7)-C(8)	0.0(2)
C(6)-C(7)-C(8)-C(9)	-1.2(3)
C(7)-C(8)-C(9)-C(10)	0.7(3)
C(8)-C(9)-C(10)-C(5)	0.9(3)
C(6)-C(5)-C(10)-C(9)	-2.1(2)
C(4)-C(5)-C(10)-C(9)	177.32(14)

Symmetry transformations used to generate equivalent atoms:

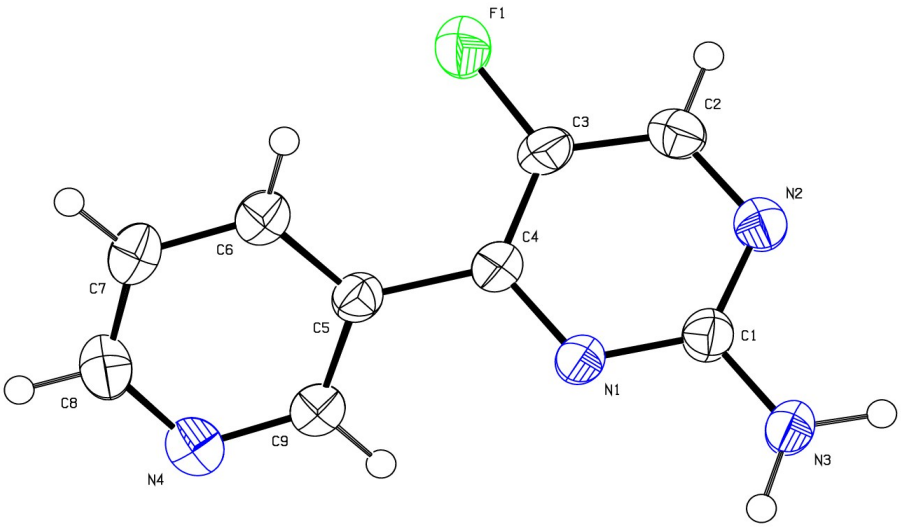
Table 7. Hydrogen bonds for Mo_160314ba [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1B)...N(2)#1	0.875(14)	2.168(14)	3.0361(17)	171.7(17)
N(1)-H(1A)...N(3)#2	0.891(14)	2.210(14)	3.0870(16)	167.9(15)

Symmetry transformations used to generate equivalent atoms:

#1 x+1/2,-y+3/2,-z+1 #2 x-1/2,-y+3/2,-z+1

X-ray crystallography of 3l



3l

Table 1. Crystal data and structure refinement for mo_160518e.

Identification code	mo_160518e	
Empirical formula	C9 H7 F N4	
Formula weight	190.07	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 6.185(2) Å	α= 90°.
	b = 7.487(2) Å	β= 96.138(11)°.
	c = 18.728(6) Å	γ = 90°.
Volume	862.2(5) $Å^3$	
Z	4	
Density (calculated)	1.457 Mg/m^3	
Absorption coefficient	0.107 mm^{-1}	
F(000)	392	
Crystal size	0.250 x 0.250 x 0.080 mm^3	
Theta range for data collection	2.932 to 27.597°.	
Index ranges	-8<=h<=8, -9<=k<=9, -24<=l<=24	
Reflections collected	20099	
Independent reflections	1996 [R(int) = 0.0389]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Semi-empirical from equivalents	

Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1996 / 1 / 136
Goodness-of-fit on F^2	1.050
Final R indices [I>2sigma(I)]	R1 = 0.0546, wR2 = 0.1129
R indices (all data)	R1 = 0.0746, wR2 = 0.1211
Extinction coefficient	0.020(3)
Largest diff. peak and hole	0.408 and -0.181 e.$Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for mo_160518e. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
F(1)	9276(2)	1852(2)	6046(1)	49(1)
N(1)	4470(2)	3538(2)	6841(1)	33(1)
C(1)	4026(3)	2040(3)	7197(1)	35(1)
N(2)	5159(3)	497(2)	7200(1)	40(1)
C(2)	6854(3)	505(3)	6821(1)	40(1)
N(3)	2339(3)	2083(3)	7592(1)	49(1)
C(3)	7430(3)	1982(3)	6451(1)	36(1)
C(4)	6192(3)	3520(3)	6460(1)	30(1)
C(5)	6584(3)	5160(3)	6050(1)	32(1)
C(6)	8636(3)	5726(3)	5918(1)	44(1)
C(7)	8817(4)	7247(3)	5510(1)	52(1)
C(8)	6966(4)	8146(3)	5248(1)	49(1)
N(4)	4975(3)	7649(3)	5372(1)	47(1)
C(9)	4830(3)	6176(3)	5765(1)	40(1)

Table 3. Bond lengths [Å] and angles [°] for mo_160518e.

F(1)-C(3)	1.440(2)
N(1)-C(4)	1.344(2)
N(1)-C(1)	1.347(2)
C(1)-N(2)	1.351(3)
C(1)-N(3)	1.342(3)
N(2)-C(2)	1.327(3)
C(2)-C(3)	1.371(3)
C(2)-H(2)	0.9300
N(3)-H(3A)	0.97(3)
N(3)-H(3B)	0.95(3)
C(3)-C(4)	1.384(3)
C(4)-C(5)	1.482(3)
C(5)-C(6)	1.385(3)
C(5)-C(9)	1.384(3)
C(6)-C(7)	1.382(3)
C(6)-H(6)	0.9300
C(7)-C(8)	1.373(3)
C(7)-H(7)	0.9300
C(8)-N(4)	1.331(3)
C(8)-H(8)	0.9300
N(4)-C(9)	1.334(3)
C(9)-H(9)	0.9300
C(4)-N(1)-C(1)	117.98(16)
N(2)-C(1)-N(1)	125.49(17)
N(2)-C(1)-N(3)	116.86(18)
N(1)-C(1)-N(3)	117.65(18)
C(2)-N(2)-C(1)	115.67(17)
N(2)-C(2)-C(3)	122.43(19)
N(2)-C(2)-H(2)	118.8
C(3)-C(2)-H(2)	118.8
C(1)-N(3)-H(3A)	118.4(14)
C(1)-N(3)-H(3B)	122.5(15)
H(3A)-N(3)-H(3B)	119(2)
C(2)-C(3)-C(4)	119.38(17)
C(2)-C(3)-F(1)	118.35(17)

C(4)-C(3)-F(1)	122.25(17)
N(1)-C(4)-C(3)	119.05(17)
N(1)-C(4)-C(5)	116.74(16)
C(3)-C(4)-C(5)	124.17(16)
C(6)-C(5)-C(9)	117.29(18)
C(6)-C(5)-C(4)	123.38(18)
C(9)-C(5)-C(4)	119.32(17)
C(5)-C(6)-C(7)	118.7(2)
C(5)-C(6)-H(6)	120.6
C(7)-C(6)-H(6)	120.6
C(8)-C(7)-C(6)	119.2(2)
C(8)-C(7)-H(7)	120.4
C(6)-C(7)-H(7)	120.4
N(4)-C(8)-C(7)	123.5(2)
N(4)-C(8)-H(8)	118.2
C(7)-C(8)-H(8)	118.2
C(8)-N(4)-C(9)	116.45(19)
N(4)-C(9)-C(5)	124.79(19)
N(4)-C(9)-H(9)	117.6
C(5)-C(9)-H(9)	117.6

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for mo_160518e. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
F(1)	57(1)	43(1)	50(1)	9(1)	19(1)	3(1)
N(1)	33(1)	30(1)	38(1)	1(1)	12(1)	-1(1)
C(1)	37(1)	31(1)	37(1)	0(1)	10(1)	-2(1)
N(2)	46(1)	33(1)	44(1)	4(1)	15(1)	4(1)
C(2)	43(1)	36(1)	42(1)	4(1)	10(1)	9(1)
N(3)	53(1)	34(1)	66(1)	9(1)	35(1)	4(1)
C(3)	31(1)	42(1)	36(1)	1(1)	12(1)	4(1)
C(4)	29(1)	33(1)	30(1)	-1(1)	4(1)	-2(1)
C(5)	32(1)	32(1)	31(1)	-1(1)	9(1)	-1(1)
C(6)	33(1)	45(1)	56(1)	11(1)	10(1)	-1(1)
C(7)	41(1)	49(1)	70(2)	15(1)	18(1)	-6(1)
C(8)	57(1)	40(1)	51(1)	12(1)	14(1)	-2(1)
N(4)	46(1)	43(1)	53(1)	11(1)	8(1)	5(1)
C(9)	34(1)	41(1)	45(1)	6(1)	9(1)	1(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for mo_160518e.

	x	y	z	U(eq)
H(2)	7682	-528	6806	48
H(3A)	1900(40)	980(40)	7807(13)	58(7)
H(3B)	1460(40)	3110(30)	7622(13)	53(7)
H(6)	9868	5094	6099	53
H(7)	10177	7656	5415	63
H(8)	7112	9157	4969	58
H(9)	3449	5804	5854	47

Table 6. Torsion angles [°] for mo_160518e.

C(4)-N(1)-C(1)-N(2)	-0.7(3)
C(4)-N(1)-C(1)-N(3)	178.25(19)
N(1)-C(1)-N(2)-C(2)	0.7(3)
N(3)-C(1)-N(2)-C(2)	-178.2(2)
C(1)-N(2)-C(2)-C(3)	0.2(3)
N(2)-C(2)-C(3)-C(4)	-1.0(3)
N(2)-C(2)-C(3)-F(1)	-179.06(18)
C(1)-N(1)-C(4)-C(3)	-0.2(3)
C(1)-N(1)-C(4)-C(5)	177.52(17)
C(2)-C(3)-C(4)-N(1)	1.0(3)
F(1)-C(3)-C(4)-N(1)	179.01(17)
C(2)-C(3)-C(4)-C(5)	-176.54(18)
F(1)-C(3)-C(4)-C(5)	1.4(3)
N(1)-C(4)-C(5)-C(6)	148.7(2)
C(3)-C(4)-C(5)-C(6)	-33.6(3)
N(1)-C(4)-C(5)-C(9)	-32.8(3)
C(3)-C(4)-C(5)-C(9)	144.8(2)
C(9)-C(5)-C(6)-C(7)	-0.4(3)
C(4)-C(5)-C(6)-C(7)	178.1(2)
C(5)-C(6)-C(7)-C(8)	-0.2(4)
C(6)-C(7)-C(8)-N(4)	1.0(4)
C(7)-C(8)-N(4)-C(9)	-1.1(4)
C(8)-N(4)-C(9)-C(5)	0.4(3)
C(6)-C(5)-C(9)-N(4)	0.3(3)
C(4)-C(5)-C(9)-N(4)	-178.23(19)

Symmetry transformations used to generate equivalent atoms:

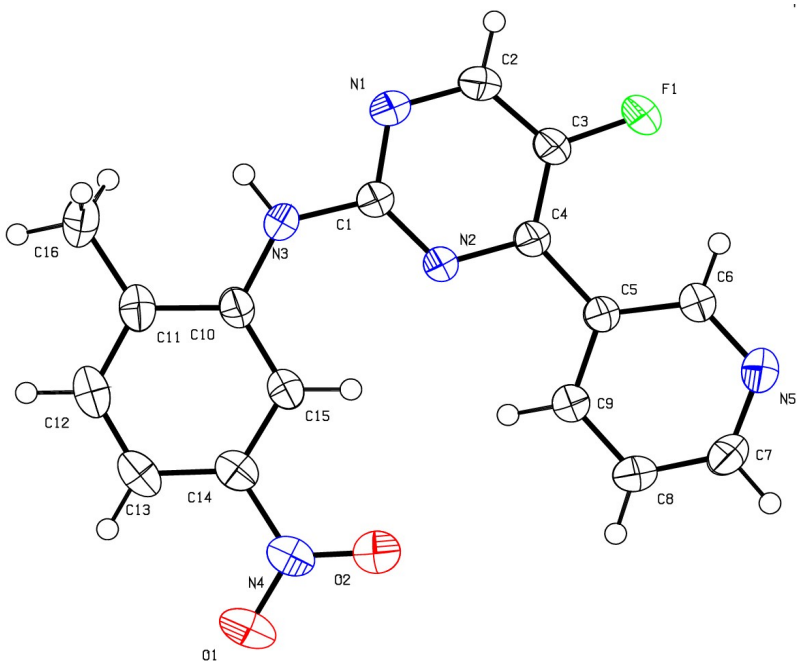
Table 7. Hydrogen bonds for mo_160518e [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(3)-H(3B)...N(2)#1	0.95(3)	2.09(3)	3.033(3)	172(2)
N(3)-H(3A)...N(1)#2	0.97(3)	2.15(3)	3.111(3)	171(2)
C(6)-H(6)...F(1)	0.93	2.46	2.934(3)	112.0

Symmetry transformations used to generate equivalent atoms:

#1 -x+1/2,y+1/2,-z+3/2 #2 -x+1/2,y-1/2,-z+3/2

X-ray crystallography of the fluorinated intermediate 5



5

Table 1. Crystal data and structure refinement for mo_160711a.

Identification code	mo_160711a	
Empirical formula	C16 H12 F N5 O2	
Formula weight	325.31	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 8.4745(7) Å	α= 90°.
	b = 13.4830(13) Å	β= 96.566(3)°.
	c = 12.5515(12) Å	γ = 90°.
Volume	1424.7(2) $Å^3$	
Z	4	
Density (calculated)	1.517 Mg/m^3	
Absorption coefficient	0.114 mm^{-1}	
F(000)	672	
Crystal size	0.220 x 0.160 x 0.120 mm^3	
Theta range for data collection	2.852 to 27.103°.	
Index ranges	-10<=h<=10, -17<=k<=17, -16<=l<=16	
Reflections collected	26719	
Independent reflections	3144 [R(int) = 0.0291]	
Completeness to theta = 25.242°	99.9 %	

Absorption correction	Semi-empirical from equivalents
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3144 / 1 / 222
Goodness-of-fit on F^2	1.046
Final R indices [I>2sigma(I)]	R1 = 0.0443, wR2 = 0.1115
R indices (all data)	R1 = 0.0581, wR2 = 0.1196
Largest diff. peak and hole	0.190 and -0.230 e.$Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for mo_160711a. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
F(1)	-149(1)	6855(1)	7635(1)	52(1)
O(1)	5411(2)	4545(1)	2092(1)	66(1)
O(2)	4598(2)	5593(1)	3200(1)	58(1)
N(1)	500(2)	4303(1)	7046(1)	44(1)
N(2)	1786(1)	5313(1)	5840(1)	33(1)
N(3)	1830(2)	3572(1)	5782(1)	42(1)
N(4)	4724(2)	4744(1)	2871(1)	44(1)
N(5)	2307(2)	8858(1)	5965(1)	56(1)
C(1)	1370(2)	4444(1)	6223(1)	34(1)
C(2)	26(2)	5124(1)	7493(1)	42(1)
C(3)	408(2)	6054(1)	7144(1)	35(1)
C(4)	1311(2)	6150(1)	6300(1)	31(1)
C(5)	1827(2)	7093(1)	5842(1)	33(1)
C(6)	1794(2)	8011(1)	6355(1)	45(1)
C(7)	2893(2)	8811(1)	5025(2)	53(1)
C(8)	2963(2)	7949(1)	4446(1)	51(1)
C(9)	2427(2)	7080(1)	4853(1)	42(1)
C(10)	2639(2)	3399(1)	4884(1)	35(1)
C(11)	2747(2)	2405(1)	4537(1)	40(1)
C(12)	3514(2)	2218(1)	3637(1)	48(1)
C(13)	4159(2)	2961(1)	3073(1)	46(1)
C(14)	4042(2)	3926(1)	3440(1)	38(1)
C(15)	3312(2)	4154(1)	4339(1)	36(1)
C(16)	2061(2)	1558(1)	5118(2)	55(1)

Table 3. Bond lengths [Å] and angles [°] for mo_160711a.

F(1)-C(3)	1.3557(16)
O(1)-N(4)	1.2238(17)
O(2)-N(4)	1.2257(18)
N(1)-C(2)	1.324(2)
N(1)-C(1)	1.3498(18)
N(2)-C(1)	1.3285(17)
N(2)-C(4)	1.3503(17)
N(3)-C(1)	1.3749(18)
N(3)-C(10)	1.4045(18)
N(3)-H(3A)	0.877(14)
N(4)-C(14)	1.468(2)
N(5)-C(7)	1.333(2)
N(5)-C(6)	1.334(2)
C(2)-C(3)	1.379(2)
C(2)-H(2)	0.9300
C(3)-C(4)	1.3818(19)
C(4)-C(5)	1.4817(18)
C(5)-C(9)	1.394(2)
C(5)-C(6)	1.397(2)
C(6)-H(6)	0.9300
C(7)-C(8)	1.377(2)
C(7)-H(7)	0.9300
C(8)-C(9)	1.375(2)
C(8)-H(8)	0.9300
C(9)-H(9)	0.9300
C(10)-C(15)	1.384(2)
C(10)-C(11)	1.415(2)
C(11)-C(12)	1.389(2)
C(11)-C(16)	1.508(2)
C(12)-C(13)	1.375(2)
C(12)-H(12)	0.9300
C(13)-C(14)	1.388(2)
C(13)-H(13)	0.9300
C(14)-C(15)	1.381(2)
C(15)-H(15)	0.9300
C(16)-H(16A)	0.9600

C(16)-H(16B)	0.9600
C(16)-H(16C)	0.9600

C(2)-N(1)-C(1)	115.12(12)
C(1)-N(2)-C(4)	118.54(12)
C(1)-N(3)-C(10)	130.71(12)
C(1)-N(3)-H(3A)	113.7(12)
C(10)-N(3)-H(3A)	115.5(12)
O(1)-N(4)-O(2)	122.75(15)
O(1)-N(4)-C(14)	118.31(14)
O(2)-N(4)-C(14)	118.94(12)
C(7)-N(5)-C(6)	117.04(14)
N(2)-C(1)-N(1)	126.33(13)
N(2)-C(1)-N(3)	120.57(12)
N(1)-C(1)-N(3)	113.09(12)
N(1)-C(2)-C(3)	122.16(13)
N(1)-C(2)-H(2)	118.9
C(3)-C(2)-H(2)	118.9
F(1)-C(3)-C(2)	118.25(12)
F(1)-C(3)-C(4)	121.74(13)
C(2)-C(3)-C(4)	120.00(13)
N(2)-C(4)-C(3)	117.86(12)
N(2)-C(4)-C(5)	115.86(11)
C(3)-C(4)-C(5)	126.28(12)
C(9)-C(5)-C(6)	116.76(13)
C(9)-C(5)-C(4)	119.22(12)
C(6)-C(5)-C(4)	124.00(13)
N(5)-C(6)-C(5)	124.35(14)
N(5)-C(6)-H(6)	117.8
C(5)-C(6)-H(6)	117.8
N(5)-C(7)-C(8)	123.37(15)
N(5)-C(7)-H(7)	118.3
C(8)-C(7)-H(7)	118.3
C(9)-C(8)-C(7)	119.16(15)
C(9)-C(8)-H(8)	120.4
C(7)-C(8)-H(8)	120.4
C(8)-C(9)-C(5)	119.31(14)
C(8)-C(9)-H(9)	120.3

C(5)-C(9)-H(9)	120.3
C(15)-C(10)-N(3)	122.77(13)
C(15)-C(10)-C(11)	119.94(13)
N(3)-C(10)-C(11)	117.29(13)
C(12)-C(11)-C(10)	118.32(15)
C(12)-C(11)-C(16)	119.85(14)
C(10)-C(11)-C(16)	121.83(14)
C(13)-C(12)-C(11)	122.48(14)
C(13)-C(12)-H(12)	118.8
C(11)-C(12)-H(12)	118.8
C(12)-C(13)-C(14)	117.66(14)
C(12)-C(13)-H(13)	121.2
C(14)-C(13)-H(13)	121.2
C(15)-C(14)-C(13)	122.33(15)
C(15)-C(14)-N(4)	117.92(13)
C(13)-C(14)-N(4)	119.74(13)
C(14)-C(15)-C(10)	119.24(13)
C(14)-C(15)-H(15)	120.4
C(10)-C(15)-H(15)	120.4
C(11)-C(16)-H(16A)	109.5
C(11)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(11)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for mo_160711a. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
F(1)	67(1)	38(1)	57(1)	-4(1)	36(1)	9(1)
O(1)	77(1)	74(1)	54(1)	-4(1)	38(1)	4(1)
O(2)	77(1)	47(1)	55(1)	-1(1)	27(1)	-6(1)
N(1)	57(1)	32(1)	46(1)	5(1)	24(1)	-1(1)
N(2)	42(1)	26(1)	34(1)	0(1)	14(1)	1(1)
N(3)	59(1)	24(1)	45(1)	1(1)	22(1)	-1(1)
N(4)	44(1)	52(1)	38(1)	-2(1)	13(1)	2(1)
N(5)	74(1)	29(1)	69(1)	-2(1)	33(1)	1(1)
C(1)	41(1)	29(1)	34(1)	1(1)	11(1)	1(1)
C(2)	50(1)	39(1)	42(1)	4(1)	23(1)	2(1)
C(3)	39(1)	32(1)	37(1)	-1(1)	14(1)	6(1)
C(4)	32(1)	29(1)	31(1)	1(1)	7(1)	2(1)
C(5)	35(1)	28(1)	36(1)	2(1)	11(1)	3(1)
C(6)	60(1)	30(1)	49(1)	-2(1)	25(1)	2(1)
C(7)	64(1)	30(1)	70(1)	9(1)	31(1)	1(1)
C(8)	68(1)	39(1)	52(1)	7(1)	31(1)	0(1)
C(9)	57(1)	30(1)	40(1)	-1(1)	20(1)	0(1)
C(10)	39(1)	29(1)	36(1)	-4(1)	7(1)	5(1)
C(11)	45(1)	31(1)	43(1)	-5(1)	2(1)	6(1)
C(12)	54(1)	37(1)	51(1)	-14(1)	7(1)	8(1)
C(13)	47(1)	50(1)	41(1)	-13(1)	11(1)	7(1)
C(14)	36(1)	43(1)	36(1)	-3(1)	7(1)	3(1)
C(15)	40(1)	32(1)	38(1)	-6(1)	11(1)	2(1)
C(16)	76(1)	27(1)	62(1)	-3(1)	12(1)	3(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for mo_160711a.

	x	y	z	U(eq)
H(2)	-584	5072	8061	51
H(6)	1387	8034	7012	54
H(7)	3275	9391	4746	64
H(8)	3367	7953	3788	61
H(9)	2465	6490	4473	50
H(12)	3593	1566	3407	57
H(13)	4656	2821	2467	55
H(15)	3274	4806	4575	44
H(16A)	2050	969	4687	82
H(16B)	996	1718	5249	82
H(16C)	2701	1446	5790	82
H(3A)	1510(20)	3040(11)	6097(13)	50(5)

Table 6. Torsion angles [°] for mo_160711a.

C(4)-N(2)-C(1)-N(1)	0.0(2)
C(4)-N(2)-C(1)-N(3)	-179.84(13)
C(2)-N(1)-C(1)-N(2)	0.4(2)
C(2)-N(1)-C(1)-N(3)	-179.78(14)
C(10)-N(3)-C(1)-N(2)	-5.0(3)
C(10)-N(3)-C(1)-N(1)	175.13(15)
C(1)-N(1)-C(2)-C(3)	-0.4(2)
N(1)-C(2)-C(3)-F(1)	178.93(14)
N(1)-C(2)-C(3)-C(4)	0.1(2)
C(1)-N(2)-C(4)-C(3)	-0.3(2)
C(1)-N(2)-C(4)-C(5)	179.42(13)
F(1)-C(3)-C(4)-N(2)	-178.49(13)
C(2)-C(3)-C(4)-N(2)	0.3(2)
F(1)-C(3)-C(4)-C(5)	1.8(2)
C(2)-C(3)-C(4)-C(5)	-179.43(14)
N(2)-C(4)-C(5)-C(9)	14.3(2)
C(3)-C(4)-C(5)-C(9)	-166.01(15)
N(2)-C(4)-C(5)-C(6)	-163.87(14)
C(3)-C(4)-C(5)-C(6)	15.8(2)
C(7)-N(5)-C(6)-C(5)	-0.3(3)
C(9)-C(5)-C(6)-N(5)	-0.6(3)
C(4)-C(5)-C(6)-N(5)	177.59(16)
C(6)-N(5)-C(7)-C(8)	1.1(3)
N(5)-C(7)-C(8)-C(9)	-1.0(3)
C(7)-C(8)-C(9)-C(5)	0.0(3)
C(6)-C(5)-C(9)-C(8)	0.7(2)
C(4)-C(5)-C(9)-C(8)	-177.55(15)
C(1)-N(3)-C(10)-C(15)	8.5(3)
C(1)-N(3)-C(10)-C(11)	-171.24(15)
C(15)-C(10)-C(11)-C(12)	-1.1(2)
N(3)-C(10)-C(11)-C(12)	178.70(14)
C(15)-C(10)-C(11)-C(16)	178.76(15)
N(3)-C(10)-C(11)-C(16)	-1.5(2)
C(10)-C(11)-C(12)-C(13)	-0.3(2)
C(16)-C(11)-C(12)-C(13)	179.84(16)
C(11)-C(12)-C(13)-C(14)	0.8(3)

C(12)-C(13)-C(14)-C(15)	0.1(2)
C(12)-C(13)-C(14)-N(4)	179.47(14)
O(1)-N(4)-C(14)-C(15)	177.99(15)
O(2)-N(4)-C(14)-C(15)	-1.3(2)
O(1)-N(4)-C(14)-C(13)	-1.4(2)
O(2)-N(4)-C(14)-C(13)	179.35(15)
C(13)-C(14)-C(15)-C(10)	-1.5(2)
N(4)-C(14)-C(15)-C(10)	179.15(13)
N(3)-C(10)-C(15)-C(14)	-177.82(14)
C(11)-C(10)-C(15)-C(14)	2.0(2)

Symmetry transformations used to generate equivalent atoms:

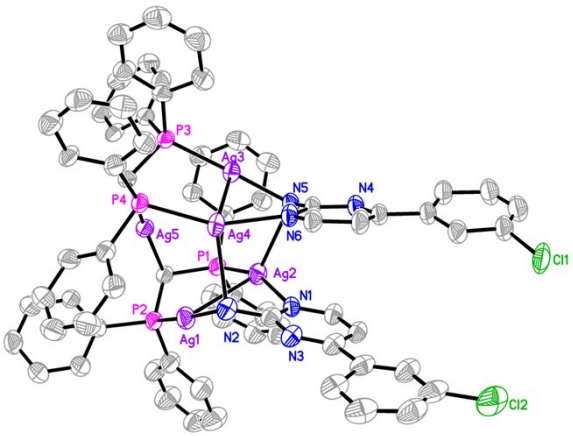
Table 7. Hydrogen bonds for mo_160711a [Å and °].

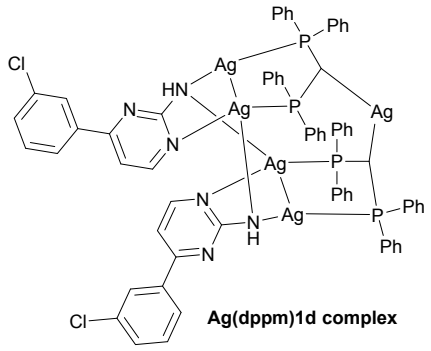
D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(2)-H(2)...N(5)#1	0.93	2.59	3.383(2)	143.3
C(6)-H(6)...F(1)	0.93	2.25	2.8856(18)	124.9
C(15)-H(15)...N(2)	0.93	2.24	2.8677(18)	123.8
N(3)-H(3A)...F(1)#1	0.877(14)	2.614(15)	3.4618(15)	162.7(16)

Symmetry transformations used to generate equivalent atoms:

#1 -x,y-1/2,-z+3/2

X-ray crystallography of the Ag(dppm)1d complex





Ag(dppm)1d complex

Table 1. Crystal data and structure refinement for 161012a_a_sq_d.

Identification code	161012a_a_sq_d	
Empirical formula	C70 H56 Ag5 Cl2 N6 P4	
Formula weight	1715.33	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	Aba2	
Unit cell dimensions	a = 27.38(3) Å	α= 90°.
	b = 26.90(3) Å	β= 90°.
	c = 24.03(3) Å	γ = 90°.
Volume	17696(31) $Å^3$	
Z	8	
Density (calculated)	1.288 Mg/m^3	
Absorption coefficient	1.255 mm^{-1}	
F(000)	6776	
Crystal size	0.350 x 0.320 x 0.300 mm^3	
Theta range for data collection	2.845 to 25.287°.	

Index ranges	-32<=h<=32, -32<=k<=31, -28<=l<=28
Reflections collected	91342
Independent reflections	15976 [R(int) = 0.0759]
Completeness to theta = 25.242°	99.8 %
Absorption correction	Semi-empirical from equivalents
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	15976 / 2531 / 803
Goodness-of-fit on F^2	1.112
Final R indices [I>2sigma(I)]	R1 = 0.0647, wR2 = 0.1672
R indices (all data)	R1 = 0.0794, wR2 = 0.1826
Absolute structure parameter	-0.030(16)
Largest diff. peak and hole	0.837 and -0.767 e.$Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 161012a_a_sq_d. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ag(1)	3437(1)	7578(1)	6164(1)	76(1)
Ag(2)	2977(1)	7648(1)	5054(1)	69(1)
Ag(3)	2468(1)	6491(1)	4952(1)	70(1)
Ag(4)	2338(1)	6942(1)	6074(1)	71(1)
Ag(5)	3600(1)	6400(1)	5550(1)	62(1)
P(1)	3684(1)	7264(1)	4668(2)	59(1)
P(2)	4189(1)	7361(1)	5757(2)	66(1)
P(3)	2707(1)	5727(1)	5339(2)	60(1)
P(4)	2777(1)	6236(1)	6441(2)	58(1)
N(1)	2538(4)	8199(4)	5520(5)	58(2)
N(2)	2710(5)	7783(5)	6370(6)	71(3)
N(3)	2183(5)	8449(4)	6391(6)	69(3)
N(4)	1495(4)	7697(5)	4704(6)	68(3)
N(5)	2181(4)	7209(4)	4743(6)	68(3)
N(6)	1762(4)	7347(4)	5579(6)	65(2)
C(1)	1655(7)	9124(7)	7053(9)	91(4)
C(2)	3089(5)	5864(5)	5937(6)	58(3)
C(3)	4072(5)	6965(5)	5165(6)	63(3)
C(4)	4639(5)	7024(6)	6188(8)	76(3)
C(5)	4857(6)	7287(7)	6635(9)	89(4)
C(6)	5196(7)	7054(7)	6962(9)	97(4)
C(7)	5328(7)	6568(8)	6867(9)	97(4)
C(8)	5123(6)	6317(7)	6437(9)	93(4)
C(9)	4764(5)	6542(5)	6138(8)	73(3)
C(10)	4555(6)	7884(6)	5528(9)	88(3)
C(11)	4368(7)	8372(7)	5554(11)	103(4)
C(12)	4655(9)	8775(8)	5359(12)	123(5)
C(13)	5096(8)	8683(8)	5134(12)	119(5)
C(14)	5010(7)	7851(7)	5314(9)	98(4)
C(15)	4515(7)	7502(8)	4008(10)	107(4)
C(16)	4060(6)	7646(7)	4218(9)	85(3)
C(17)	4785(8)	7790(9)	3676(11)	121(5)
C(18)	3472(6)	6790(6)	4164(8)	78(3)

C(19)	3686(6)	6297(6)	4128(8)	80(3)
C(20)	3509(7)	5966(7)	3732(8)	92(4)
C(21)	3111(8)	6090(8)	3395(9)	99(5)
C(22)	3094(6)	6911(7)	3818(8)	85(4)
C(23)	2920(8)	6558(8)	3428(9)	100(5)
C(24)	3044(5)	5292(5)	4909(7)	66(3)
C(25)	3534(6)	5191(5)	4962(7)	71(3)
C(26)	3765(7)	4837(6)	4611(8)	84(4)
C(27)	3514(8)	4602(7)	4217(10)	97(4)
C(28)	3025(7)	4701(7)	4161(8)	89(4)
C(29)	2802(7)	5037(6)	4513(7)	80(3)
C(30)	2203(5)	5337(5)	5565(7)	67(3)
C(31)	2251(6)	4894(6)	5854(8)	79(3)
C(32)	1878(6)	4605(7)	6037(8)	89(4)
C(33)	1419(7)	4734(8)	5919(10)	103(5)
C(34)	1329(7)	5164(8)	5633(10)	103(4)
C(35)	1722(5)	5500(7)	5415(8)	87(4)
C(36)	2427(6)	5790(6)	6870(7)	74(3)
C(37)	2661(5)	5418(5)	7157(7)	69(3)
C(38)	1928(6)	5818(6)	6850(7)	75(3)
C(39)	1658(7)	5429(7)	7164(8)	89(4)
C(40)	1889(7)	5103(7)	7429(8)	91(4)
C(41)	3229(5)	6456(5)	6925(7)	68(3)
C(42)	3117(7)	6852(7)	7319(8)	90(4)
C(43)	3450(8)	7014(9)	7696(10)	107(5)
C(44)	3893(8)	6829(8)	7720(10)	103(5)
C(45)	4020(7)	6451(7)	7393(9)	95(4)
C(46)	3702(6)	6256(7)	6976(8)	79(3)
C(47)	1078(5)	7880(6)	5544(8)	76(3)
C(48)	1398(5)	7563(6)	5831(8)	71(3)
C(49)	1588(6)	9138(6)	6467(8)	76(3)
C(50)	1292(6)	9465(6)	6253(9)	87(4)
C(51)	1002(6)	9768(6)	6541(9)	96(4)
C(52)	1008(8)	9758(7)	7098(10)	103(5)
C(53)	1353(8)	9454(8)	7352(10)	105(5)
C(54)	1145(5)	7933(5)	4981(7)	70(3)
C(55)	809(5)	8247(6)	4643(8)	81(3)
C(56)	523(5)	8601(6)	4869(9)	86(4)

C(57)	190(6)	8874(6)	4550(9)	95(4)
C(58)	192(7)	8808(8)	3974(11)	111(5)
C(59)	466(7)	8475(8)	3744(11)	105(5)
C(60)	789(7)	8165(7)	4072(9)	92(4)
C(63)	1964(5)	8866(5)	5571(7)	66(3)
C(64)	1804(5)	7408(5)	5001(7)	67(3)
C(65)	2285(5)	8556(5)	5268(7)	67(3)
C(66)	4633(9)	8222(9)	3504(11)	116(5)
C(67)	4206(9)	8387(10)	3654(11)	125(5)
C(68)	3939(8)	8103(8)	4058(10)	107(4)
C(69)	2380(7)	5068(7)	7435(8)	89(4)
C(71)	5288(8)	8232(9)	5106(12)	123(5)
C(72)	2462(5)	8153(5)	6096(7)	66(3)
C(73)	1945(5)	8800(5)	6146(7)	68(3)
Cl(1)	-146(6)	9344(5)	4932(13)	115(5)
Cl(2)	596(6)	10191(6)	6357(15)	131(5)
Cl(1')	-174(10)	9358(10)	4665(18)	106(7)
Cl(2')	605(8)	10154(9)	6104(15)	91(7)

Table 3. Bond lengths [Å] and angles [°] for 161012a_a_sq_d.

Ag(1)-N(2)	2.124(12)
Ag(1)-P(2)	2.354(4)
Ag(1)-Ag(2)	2.957(3)
Ag(2)-N(1)	2.213(12)
Ag(2)-P(1)	2.382(4)
Ag(2)-N(5)	2.588(12)
Ag(3)-N(5)	2.146(12)
Ag(3)-P(3)	2.347(4)
Ag(3)-Ag(4)	2.977(3)
Ag(4)-N(6)	2.255(11)
Ag(4)-P(4)	2.414(4)
Ag(4)-N(2)	2.583(13)
Ag(5)-C(3)	2.199(13)
Ag(5)-C(2)	2.216(13)
P(1)-C(3)	1.789(14)
P(1)-C(16)	1.812(17)
P(1)-C(18)	1.851(19)
P(2)-C(3)	1.805(16)
P(2)-C(10)	1.815(17)
P(2)-C(4)	1.847(15)
P(3)-C(24)	1.814(15)
P(3)-C(2)	1.816(14)
P(3)-C(30)	1.817(14)
P(4)-C(2)	1.788(14)
P(4)-C(41)	1.798(17)
P(4)-C(36)	1.848(17)
N(1)-C(65)	1.330(18)
N(1)-C(72)	1.40(2)
N(2)-C(72)	1.373(19)
N(2)-H(2A)	0.8599
N(3)-C(73)	1.288(19)
N(3)-C(72)	1.311(19)
N(4)-C(54)	1.33(2)
N(4)-C(64)	1.352(17)
N(5)-C(64)	1.317(19)
N(5)-H(5A)	0.8600

N(6)-C(48)	1.30(2)
N(6)-C(64)	1.40(2)
C(1)-C(53)	1.41(3)
C(1)-C(49)	1.42(3)
C(1)-H(1)	0.9300
C(2)-H(2)	0.9800
C(3)-H(3)	0.9800
C(4)-C(9)	1.35(2)
C(4)-C(5)	1.42(3)
C(5)-C(6)	1.37(3)
C(5)-H(5)	0.9300
C(6)-C(7)	1.37(3)
C(6)-H(6)	0.9300
C(7)-C(8)	1.35(3)
C(7)-H(7)	0.9300
C(8)-C(9)	1.36(2)
C(8)-H(8)	0.9300
C(9)-H(9)	0.9300
C(10)-C(14)	1.35(2)
C(10)-C(11)	1.41(3)
C(11)-C(12)	1.42(3)
C(11)-H(11)	0.9300
C(12)-C(13)	1.35(3)
C(12)-H(12)	0.9300
C(13)-C(71)	1.32(3)
C(13)-H(13)	0.9300
C(14)-C(71)	1.37(3)
C(14)-H(14)	0.9300
C(15)-C(17)	1.34(3)
C(15)-C(16)	1.40(3)
C(15)-H(15)	0.9300
C(16)-C(68)	1.33(3)
C(17)-C(66)	1.30(3)
C(17)-H(17)	0.9300
C(18)-C(22)	1.37(2)
C(18)-C(19)	1.45(2)
C(19)-C(20)	1.39(3)
C(19)-H(19)	0.9300

C(20)-C(21)	1.40(3)
C(20)-H(20)	0.9300
C(21)-C(23)	1.37(3)
C(21)-H(21)	0.9300
C(22)-C(23)	1.41(3)
C(22)-H(22)	0.9300
C(23)-H(23)	0.9300
C(24)-C(29)	1.35(2)
C(24)-C(25)	1.38(2)
C(25)-C(26)	1.42(2)
C(25)-H(25)	0.9300
C(26)-C(27)	1.33(3)
C(26)-H(26)	0.9300
C(27)-C(28)	1.37(3)
C(27)-H(27)	0.9300
C(28)-C(29)	1.38(2)
C(28)-H(28)	0.9300
C(29)-H(29)	0.9300
C(30)-C(31)	1.38(2)
C(30)-C(35)	1.43(2)
C(31)-C(32)	1.36(2)
C(31)-H(31)	0.9300
C(32)-C(33)	1.34(3)
C(32)-H(32)	0.9300
C(33)-C(34)	1.37(3)
C(33)-H(33)	0.9300
C(34)-C(35)	1.50(3)
C(34)-H(34)	0.9300
C(35)-H(35)	0.9300
C(36)-C(38)	1.37(2)
C(36)-C(37)	1.37(2)
C(37)-C(69)	1.39(2)
C(37)-H(37)	0.9300
C(38)-C(39)	1.49(2)
C(38)-H(38)	0.9300
C(39)-C(40)	1.25(3)
C(39)-H(39)	0.9300
C(40)-C(69)	1.35(3)

C(40)-H(40)	0.9300
C(41)-C(46)	1.41(2)
C(41)-C(42)	1.46(2)
C(42)-C(43)	1.36(3)
C(42)-H(42)	0.9300
C(43)-C(44)	1.31(3)
C(43)-H(43)	0.9300
C(44)-C(45)	1.33(3)
C(44)-H(44)	0.9300
C(45)-C(46)	1.43(2)
C(45)-H(45)	0.9300
C(46)-H(46)	0.9300
C(47)-C(54)	1.37(2)
C(47)-C(48)	1.40(2)
C(47)-H(47)	0.9300
C(48)-H(48)	0.9300
C(49)-C(50)	1.30(2)
C(49)-C(73)	1.54(2)
C(50)-C(51)	1.33(2)
C(50)-H(50)	0.9300
C(51)-C(52)	1.34(3)
C(51)-Cl(2)	1.65(2)
C(51)-Cl(2')	1.83(2)
C(52)-C(53)	1.39(3)
C(52)-H(52)	0.9300
C(53)-H(53)	0.9300
C(54)-C(55)	1.49(2)
C(55)-C(56)	1.35(2)
C(55)-C(60)	1.39(3)
C(56)-C(57)	1.40(2)
C(56)-H(56)	0.9300
C(57)-C(58)	1.40(3)
C(57)-Cl(1')	1.66(2)
C(57)-Cl(1)	1.81(2)
C(58)-C(59)	1.29(3)
C(58)-H(58)	0.9300
C(59)-C(60)	1.45(2)
C(59)-H(59)	0.9300

C(60)-H(60)	0.9300
C(63)-C(73)	1.39(2)
C(63)-C(65)	1.41(2)
C(63)-H(63)	0.9300
C(65)-H(65)	0.9300
C(66)-C(67)	1.30(3)
C(66)-H(66)	0.9300
C(67)-C(68)	1.44(3)
C(67)-H(67)	0.9300
C(68)-H(68)	0.9300
C(69)-H(69)	0.9300
C(71)-H(71)	0.9300

N(2)-Ag(1)-P(2)	168.9(4)
N(2)-Ag(1)-Ag(2)	78.1(4)
P(2)-Ag(1)-Ag(2)	90.77(13)
N(1)-Ag(2)-P(1)	158.2(3)
N(1)-Ag(2)-N(5)	89.7(4)
P(1)-Ag(2)-N(5)	111.9(3)
N(1)-Ag(2)-Ag(1)	79.4(3)
P(1)-Ag(2)-Ag(1)	88.71(12)
N(5)-Ag(2)-Ag(1)	126.2(3)
N(5)-Ag(3)-P(3)	169.3(4)
N(5)-Ag(3)-Ag(4)	78.5(4)
P(3)-Ag(3)-Ag(4)	91.81(12)
N(6)-Ag(4)-P(4)	157.1(3)
N(6)-Ag(4)-N(2)	89.8(4)
P(4)-Ag(4)-N(2)	113.1(3)
N(6)-Ag(4)-Ag(3)	78.7(3)
P(4)-Ag(4)-Ag(3)	87.18(12)
N(2)-Ag(4)-Ag(3)	124.0(3)
C(3)-Ag(5)-C(2)	176.6(5)
C(3)-P(1)-C(16)	108.3(8)
C(3)-P(1)-C(18)	108.2(7)
C(16)-P(1)-C(18)	100.3(9)
C(3)-P(1)-Ag(2)	114.7(5)
C(16)-P(1)-Ag(2)	116.7(6)
C(18)-P(1)-Ag(2)	107.4(5)

C(3)-P(2)-C(10)	108.5(9)
C(3)-P(2)-C(4)	105.8(7)
C(10)-P(2)-C(4)	100.5(8)
C(3)-P(2)-Ag(1)	108.6(5)
C(10)-P(2)-Ag(1)	114.6(6)
C(4)-P(2)-Ag(1)	118.2(6)
C(24)-P(3)-C(2)	106.8(6)
C(24)-P(3)-C(30)	100.6(7)
C(2)-P(3)-C(30)	108.5(7)
C(24)-P(3)-Ag(3)	118.8(5)
C(2)-P(3)-Ag(3)	107.3(4)
C(30)-P(3)-Ag(3)	114.4(5)
C(2)-P(4)-C(41)	107.0(7)
C(2)-P(4)-C(36)	105.2(7)
C(41)-P(4)-C(36)	102.1(7)
C(2)-P(4)-Ag(4)	115.5(5)
C(41)-P(4)-Ag(4)	108.7(5)
C(36)-P(4)-Ag(4)	117.1(5)
C(65)-N(1)-C(72)	115.8(12)
C(65)-N(1)-Ag(2)	122.3(10)
C(72)-N(1)-Ag(2)	121.4(9)
C(72)-N(2)-Ag(1)	122.7(10)
C(72)-N(2)-Ag(4)	107.9(9)
Ag(1)-N(2)-Ag(4)	94.5(5)
C(72)-N(2)-H(2A)	119.3
Ag(1)-N(2)-H(2A)	107.8
Ag(4)-N(2)-H(2A)	98.7
C(73)-N(3)-C(72)	119.4(14)
C(54)-N(4)-C(64)	117.5(14)
C(64)-N(5)-Ag(3)	122.9(10)
C(64)-N(5)-Ag(2)	109.8(10)
Ag(3)-N(5)-Ag(2)	92.0(4)
C(64)-N(5)-H(5A)	120.6
Ag(3)-N(5)-H(5A)	109.2
Ag(2)-N(5)-H(5A)	93.8
C(48)-N(6)-C(64)	118.0(12)
C(48)-N(6)-Ag(4)	120.4(11)
C(64)-N(6)-Ag(4)	121.4(9)

C(53)-C(1)-C(49)	114(2)
C(53)-C(1)-H(1)	122.8
C(49)-C(1)-H(1)	122.8
P(4)-C(2)-P(3)	112.0(7)
P(4)-C(2)-Ag(5)	102.8(6)
P(3)-C(2)-Ag(5)	99.4(6)
P(4)-C(2)-H(2)	113.8
P(3)-C(2)-H(2)	113.8
Ag(5)-C(2)-H(2)	113.8
P(1)-C(3)-P(2)	111.5(7)
P(1)-C(3)-Ag(5)	104.0(6)
P(2)-C(3)-Ag(5)	100.3(7)
P(1)-C(3)-H(3)	113.3
P(2)-C(3)-H(3)	113.3
Ag(5)-C(3)-H(3)	113.3
C(9)-C(4)-C(5)	116.2(15)
C(9)-C(4)-P(2)	126.2(13)
C(5)-C(4)-P(2)	117.5(12)
C(6)-C(5)-C(4)	119.4(18)
C(6)-C(5)-H(5)	120.3
C(4)-C(5)-H(5)	120.3
C(5)-C(6)-C(7)	121.3(19)
C(5)-C(6)-H(6)	119.4
C(7)-C(6)-H(6)	119.4
C(8)-C(7)-C(6)	119.4(18)
C(8)-C(7)-H(7)	120.3
C(6)-C(7)-H(7)	120.3
C(7)-C(8)-C(9)	118.7(18)
C(7)-C(8)-H(8)	120.6
C(9)-C(8)-H(8)	120.6
C(4)-C(9)-C(8)	124.4(17)
C(4)-C(9)-H(9)	117.8
C(8)-C(9)-H(9)	117.8
C(14)-C(10)-C(11)	114.5(17)
C(14)-C(10)-P(2)	125.0(14)
C(11)-C(10)-P(2)	120.5(14)
C(10)-C(11)-C(12)	120(2)
C(10)-C(11)-H(11)	120.2

C(12)-C(11)-H(11)	120.2
C(13)-C(12)-C(11)	119(2)
C(13)-C(12)-H(12)	120.4
C(11)-C(12)-H(12)	120.4
C(71)-C(13)-C(12)	123(2)
C(71)-C(13)-H(13)	118.5
C(12)-C(13)-H(13)	118.5
C(10)-C(14)-C(71)	127(2)
C(10)-C(14)-H(14)	116.6
C(71)-C(14)-H(14)	116.6
C(17)-C(15)-C(16)	123(2)
C(17)-C(15)-H(15)	118.3
C(16)-C(15)-H(15)	118.3
C(68)-C(16)-C(15)	111.9(17)
C(68)-C(16)-P(1)	123.6(15)
C(15)-C(16)-P(1)	124.5(14)
C(66)-C(17)-C(15)	122(2)
C(66)-C(17)-H(17)	119.0
C(15)-C(17)-H(17)	119.0
C(22)-C(18)-C(19)	119.0(17)
C(22)-C(18)-P(1)	118.1(13)
C(19)-C(18)-P(1)	122.9(13)
C(20)-C(19)-C(18)	119.0(17)
C(20)-C(19)-H(19)	120.5
C(18)-C(19)-H(19)	120.5
C(19)-C(20)-C(21)	121.1(18)
C(19)-C(20)-H(20)	119.4
C(21)-C(20)-H(20)	119.4
C(23)-C(21)-C(20)	118.9(19)
C(23)-C(21)-H(21)	120.6
C(20)-C(21)-H(21)	120.6
C(18)-C(22)-C(23)	120.0(19)
C(18)-C(22)-H(22)	120.0
C(23)-C(22)-H(22)	120.0
C(21)-C(23)-C(22)	122(2)
C(21)-C(23)-H(23)	119.1
C(22)-C(23)-H(23)	119.1
C(29)-C(24)-C(25)	116.4(15)

C(29)-C(24)-P(3)	118.8(11)
C(25)-C(24)-P(3)	124.8(12)
C(24)-C(25)-C(26)	120.7(16)
C(24)-C(25)-H(25)	119.6
C(26)-C(25)-H(25)	119.6
C(27)-C(26)-C(25)	120.7(17)
C(27)-C(26)-H(26)	119.6
C(25)-C(26)-H(26)	119.6
C(26)-C(27)-C(28)	118.9(19)
C(26)-C(27)-H(27)	120.5
C(28)-C(27)-H(27)	120.5
C(27)-C(28)-C(29)	119.8(18)
C(27)-C(28)-H(28)	120.1
C(29)-C(28)-H(28)	120.1
C(24)-C(29)-C(28)	123.4(17)
C(24)-C(29)-H(29)	118.3
C(28)-C(29)-H(29)	118.3
C(31)-C(30)-C(35)	118.5(14)
C(31)-C(30)-P(3)	125.0(11)
C(35)-C(30)-P(3)	116.5(12)
C(32)-C(31)-C(30)	125.8(17)
C(32)-C(31)-H(31)	117.1
C(30)-C(31)-H(31)	117.1
C(33)-C(32)-C(31)	119.3(19)
C(33)-C(32)-H(32)	120.4
C(31)-C(32)-H(32)	120.4
C(32)-C(33)-C(34)	119.8(18)
C(32)-C(33)-H(33)	120.1
C(34)-C(33)-H(33)	120.1
C(33)-C(34)-C(35)	123.9(18)
C(33)-C(34)-H(34)	118.1
C(35)-C(34)-H(34)	118.1
C(30)-C(35)-C(34)	112.7(16)
C(30)-C(35)-H(35)	123.7
C(34)-C(35)-H(35)	123.7
C(38)-C(36)-C(37)	121.5(15)
C(38)-C(36)-P(4)	117.5(13)
C(37)-C(36)-P(4)	120.7(12)

C(36)-C(37)-C(69)	118.5(15)
C(36)-C(37)-H(37)	120.8
C(69)-C(37)-H(37)	120.8
C(36)-C(38)-C(39)	116.1(16)
C(36)-C(38)-H(38)	121.9
C(39)-C(38)-H(38)	121.9
C(40)-C(39)-C(38)	119.8(18)
C(40)-C(39)-H(39)	120.1
C(38)-C(39)-H(39)	120.1
C(39)-C(40)-C(69)	123.9(18)
C(39)-C(40)-H(40)	118.1
C(69)-C(40)-H(40)	118.1
C(46)-C(41)-C(42)	114.6(15)
C(46)-C(41)-P(4)	124.3(13)
C(42)-C(41)-P(4)	121.0(12)
C(43)-C(42)-C(41)	121.7(18)
C(43)-C(42)-H(42)	119.1
C(41)-C(42)-H(42)	119.1
C(44)-C(43)-C(42)	122(2)
C(44)-C(43)-H(43)	119.0
C(42)-C(43)-H(43)	119.0
C(43)-C(44)-C(45)	120(2)
C(43)-C(44)-H(44)	119.9
C(45)-C(44)-H(44)	119.9
C(44)-C(45)-C(46)	122.5(19)
C(44)-C(45)-H(45)	118.8
C(46)-C(45)-H(45)	118.8
C(41)-C(46)-C(45)	118.8(17)
C(41)-C(46)-H(46)	120.6
C(45)-C(46)-H(46)	120.6
C(54)-C(47)-C(48)	117.7(15)
C(54)-C(47)-H(47)	121.2
C(48)-C(47)-H(47)	121.2
N(6)-C(48)-C(47)	121.4(16)
N(6)-C(48)-H(48)	119.3
C(47)-C(48)-H(48)	119.3
C(50)-C(49)-C(1)	119.3(17)
C(50)-C(49)-C(73)	126.5(17)

C(1)-C(49)-C(73)	113.5(16)
C(49)-C(50)-C(51)	125(2)
C(49)-C(50)-H(50)	117.3
C(51)-C(50)-H(50)	117.3
C(50)-C(51)-C(52)	119.9(19)
C(50)-C(51)-Cl(2)	133(2)
C(52)-C(51)-Cl(2)	107(2)
C(50)-C(51)-Cl(2')	113.7(19)
C(52)-C(51)-Cl(2')	126(2)
C(51)-C(52)-C(53)	117.5(18)
C(51)-C(52)-H(52)	121.3
C(53)-C(52)-H(52)	121.3
C(52)-C(53)-C(1)	123(2)
C(52)-C(53)-H(53)	118.5
C(1)-C(53)-H(53)	118.5
N(4)-C(54)-C(47)	122.7(13)
N(4)-C(54)-C(55)	116.4(15)
C(47)-C(54)-C(55)	120.9(15)
C(56)-C(55)-C(60)	119.1(16)
C(56)-C(55)-C(54)	122.7(18)
C(60)-C(55)-C(54)	118.2(16)
C(55)-C(56)-C(57)	122(2)
C(55)-C(56)-H(56)	119.1
C(57)-C(56)-H(56)	119.1
C(58)-C(57)-C(56)	118.4(17)
C(58)-C(57)-Cl(1')	105(2)
C(56)-C(57)-Cl(1')	135(2)
C(58)-C(57)-Cl(1)	126.3(17)
C(56)-C(57)-Cl(1)	114.7(18)
C(59)-C(58)-C(57)	120.9(19)
C(59)-C(58)-H(58)	119.6
C(57)-C(58)-H(58)	119.6
C(58)-C(59)-C(60)	121(2)
C(58)-C(59)-H(59)	119.3
C(60)-C(59)-H(59)	119.3
C(55)-C(60)-C(59)	118(2)
C(55)-C(60)-H(60)	121.0
C(59)-C(60)-H(60)	121.0

C(73)-C(63)-C(65)	117.2(13)
C(73)-C(63)-H(63)	121.4
C(65)-C(63)-H(63)	121.4
N(5)-C(64)-N(4)	118.4(15)
N(5)-C(64)-N(6)	118.9(12)
N(4)-C(64)-N(6)	122.5(13)
N(1)-C(65)-C(63)	121.0(15)
N(1)-C(65)-H(65)	119.5
C(63)-C(65)-H(65)	119.5
C(17)-C(66)-C(67)	120(2)
C(17)-C(66)-H(66)	119.9
C(67)-C(66)-H(66)	119.9
C(66)-C(67)-C(68)	118(2)
C(66)-C(67)-H(67)	121.2
C(68)-C(67)-H(67)	121.2
C(16)-C(68)-C(67)	124(2)
C(16)-C(68)-H(68)	117.9
C(67)-C(68)-H(68)	117.9
C(40)-C(69)-C(37)	120.1(17)
C(40)-C(69)-H(69)	120.0
C(37)-C(69)-H(69)	120.0
C(13)-C(71)-C(14)	117(2)
C(13)-C(71)-H(71)	121.7
C(14)-C(71)-H(71)	121.7
N(3)-C(72)-N(2)	118.0(14)
N(3)-C(72)-N(1)	124.4(13)
N(2)-C(72)-N(1)	117.5(13)
N(3)-C(73)-C(63)	121.9(14)
N(3)-C(73)-C(49)	121.5(15)
C(63)-C(73)-C(49)	116.3(14)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 161012a_a_sq_d. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ag(1)	56(1)	79(1)	93(1)	12(1)	-7(1)	6(1)
Ag(2)	56(1)	70(1)	81(1)	0(1)	7(1)	15(1)
Ag(3)	66(1)	62(1)	84(1)	6(1)	-8(1)	12(1)
Ag(4)	70(1)	64(1)	80(1)	13(1)	-4(1)	21(1)
Ag(5)	47(1)	55(1)	83(1)	7(1)	-2(1)	-4(1)
P(1)	47(2)	53(2)	77(2)	1(2)	4(2)	4(1)
P(2)	45(2)	59(2)	95(3)	11(2)	-8(2)	-1(1)
P(3)	50(2)	50(2)	79(2)	3(2)	-3(2)	2(1)
P(4)	47(2)	50(2)	77(2)	11(2)	-5(2)	3(1)
N(1)	50(4)	60(5)	63(5)	11(4)	-4(4)	4(4)
N(2)	73(6)	64(5)	77(6)	9(5)	8(5)	6(5)
N(3)	71(6)	56(5)	79(6)	5(5)	10(5)	5(5)
N(4)	48(5)	71(6)	85(6)	16(5)	-6(5)	11(5)
N(5)	48(5)	69(6)	86(6)	9(5)	-6(5)	10(5)
N(6)	50(5)	67(5)	78(5)	16(5)	-1(5)	11(4)
C(1)	93(8)	74(7)	105(8)	-4(7)	21(7)	-3(7)
C(2)	51(5)	48(5)	76(6)	3(5)	-1(5)	-5(4)
C(3)	45(5)	53(5)	89(6)	12(5)	0(5)	-4(4)
C(4)	59(6)	66(6)	102(7)	10(6)	-18(6)	-4(5)
C(5)	74(7)	78(7)	114(8)	11(7)	-22(7)	-9(6)
C(6)	81(8)	92(9)	118(10)	4(8)	-33(8)	-8(8)
C(7)	66(8)	96(9)	128(10)	29(9)	-23(8)	2(8)
C(8)	62(8)	84(8)	133(11)	4(9)	-17(8)	-9(7)
C(9)	49(6)	63(6)	108(8)	10(6)	-12(6)	-8(5)
C(10)	63(6)	75(6)	125(7)	11(7)	-1(6)	1(6)
C(11)	80(8)	90(8)	139(10)	13(9)	9(9)	0(7)
C(12)	108(10)	86(9)	175(12)	1(10)	24(10)	-9(9)
C(13)	98(10)	87(9)	172(12)	12(10)	18(10)	-26(8)
C(14)	71(7)	78(7)	146(8)	11(7)	11(7)	0(6)
C(15)	75(7)	104(8)	141(9)	35(8)	31(7)	-2(7)
C(16)	63(6)	80(6)	113(7)	20(6)	10(6)	-5(6)
C(17)	84(9)	119(11)	159(12)	25(10)	48(9)	3(9)
C(18)	62(6)	71(6)	99(7)	11(6)	12(6)	4(6)

C(19)	68(6)	77(7)	95(7)	10(6)	3(6)	-12(6)
C(20)	94(8)	77(7)	105(8)	-9(7)	13(7)	8(7)
C(21)	88(9)	103(10)	105(10)	-16(9)	6(8)	-16(8)
C(22)	67(7)	88(7)	98(8)	5(7)	-1(6)	-6(6)
C(23)	89(9)	109(10)	103(10)	-6(9)	-2(9)	-14(9)
C(24)	58(6)	57(5)	82(6)	2(5)	-5(5)	0(5)
C(25)	75(6)	47(5)	92(7)	9(6)	8(6)	0(5)
C(26)	74(8)	61(7)	116(9)	-3(7)	3(8)	7(6)
C(27)	98(9)	74(8)	119(10)	-6(8)	16(9)	-3(8)
C(28)	91(9)	76(8)	98(9)	-9(7)	-6(8)	-5(7)
C(29)	75(7)	70(7)	94(8)	2(7)	2(7)	11(6)
C(30)	53(5)	62(6)	88(6)	-1(6)	-4(5)	-12(5)
C(31)	66(6)	69(6)	102(7)	5(6)	11(6)	-6(6)
C(32)	78(8)	85(8)	104(9)	1(8)	9(7)	-14(7)
C(33)	77(8)	108(9)	124(10)	2(9)	13(8)	-25(8)
C(34)	67(8)	116(10)	127(10)	-6(9)	4(8)	-2(8)
C(35)	50(6)	98(8)	111(9)	8(7)	4(6)	-2(6)
C(36)	68(6)	65(6)	88(6)	0(6)	0(6)	-2(5)
C(37)	63(6)	52(6)	91(7)	20(6)	5(6)	-3(5)
C(38)	61(6)	78(7)	88(7)	4(6)	1(6)	-4(6)
C(39)	86(8)	93(8)	89(8)	-9(7)	6(7)	-12(7)
C(40)	92(9)	82(8)	101(9)	10(8)	12(8)	-26(7)
C(41)	52(6)	61(6)	90(7)	13(6)	8(5)	3(5)
C(42)	81(7)	83(7)	105(8)	4(7)	-8(7)	3(7)
C(43)	99(10)	103(10)	120(10)	-20(9)	-11(9)	-4(9)
C(44)	91(9)	98(10)	119(10)	-16(9)	-18(9)	-4(8)
C(45)	73(7)	99(8)	114(8)	1(8)	-21(7)	-6(7)
C(46)	69(6)	73(6)	96(7)	-5(6)	-4(6)	-9(6)
C(47)	54(6)	72(6)	104(7)	12(7)	-3(6)	17(5)
C(48)	54(6)	66(6)	93(7)	14(6)	-3(6)	5(5)
C(49)	75(7)	57(6)	96(7)	-13(6)	18(6)	-3(6)
C(50)	83(7)	65(7)	113(8)	-6(7)	20(7)	4(6)
C(51)	90(8)	66(7)	134(10)	-13(8)	29(8)	-18(7)
C(52)	98(9)	73(8)	138(10)	-23(9)	35(9)	2(8)
C(53)	107(9)	92(9)	117(10)	-19(8)	32(8)	-15(8)
C(54)	48(5)	63(5)	98(7)	20(6)	-10(6)	2(5)
C(55)	51(6)	70(7)	120(8)	18(7)	-18(6)	6(5)
C(56)	50(6)	79(7)	130(9)	19(7)	-8(7)	1(6)

C(57)	54(7)	83(8)	147(10)	22(8)	-14(8)	11(6)
C(58)	73(8)	98(9)	160(11)	34(10)	-28(9)	1(8)
C(59)	72(8)	107(9)	134(10)	26(9)	-24(8)	12(8)
C(60)	70(7)	82(8)	124(9)	24(8)	-18(7)	9(7)
C(63)	58(6)	55(6)	87(7)	8(6)	8(6)	7(5)
C(64)	47(5)	61(5)	92(6)	16(6)	-6(5)	9(5)
C(65)	61(6)	62(6)	77(6)	10(5)	4(5)	8(5)
C(66)	101(10)	109(10)	139(11)	25(10)	38(9)	-13(9)
C(67)	116(11)	108(10)	151(12)	35(10)	34(10)	9(10)
C(68)	92(8)	95(8)	134(9)	20(8)	28(8)	11(8)
C(69)	94(9)	77(8)	96(9)	18(8)	9(8)	-4(7)
C(71)	96(10)	100(10)	174(12)	12(10)	27(10)	-19(9)
C(72)	62(6)	60(5)	75(6)	7(5)	9(6)	-9(5)
C(73)	61(6)	59(6)	84(6)	8(6)	25(5)	-4(5)
Cl(1)	76(5)	83(5)	185(14)	51(8)	-13(9)	24(4)
Cl(2)	85(6)	112(7)	196(14)	-52(9)	41(9)	26(5)
Cl(1')	75(8)	87(10)	154(16)	39(11)	-36(11)	18(7)
Cl(2')	63(8)	76(9)	135(15)	-14(9)	32(9)	13(6)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 161012a_a_sq_d.

	x	y	z	U(eq)
H(2A)	2677	7754	6724	86
H(5A)	2231	7266	4395	82
H(1)	1879	8914	7225	109
H(2)	3249	5571	6095	70
H(3)	4369	6827	5000	75
H(5)	4771	7616	6706	106
H(6)	5340	7227	7254	116
H(7)	5556	6413	7095	116
H(8)	5227	5998	6347	112
H(9)	4592	6350	5883	88
H(11)	4058	8429	5698	124
H(12)	4539	9099	5387	148
H(13)	5274	8948	4991	143
H(14)	5150	7536	5308	118
H(15)	4636	7191	4105	128
H(17)	5092	7678	3564	145
H(19)	3938	6203	4366	96
H(20)	3657	5658	3690	110
H(21)	2978	5857	3151	118
H(22)	2951	7224	3838	102
H(23)	2668	6648	3188	121
H(25)	3716	5357	5231	85
H(26)	4095	4768	4657	100
H(27)	3667	4375	3983	117
H(28)	2844	4542	3886	106
H(29)	2468	5090	4475	95
H(31)	2567	4786	5929	95
H(32)	1942	4319	6243	107
H(33)	1161	4533	6031	124
H(34)	1006	5252	5569	124
H(35)	1660	5784	5206	104
H(37)	3000	5401	7165	82

H(38)	1767	6066	6652	90
H(39)	1318	5427	7164	107
H(40)	1711	4872	7633	110
H(42)	2809	6997	7312	108
H(43)	3362	7264	7944	129
H(44)	4119	6962	7968	123
H(45)	4328	6310	7437	114
H(46)	3806	6001	6743	95
H(47)	830	8049	5729	92
H(48)	1348	7505	6208	85
H(50)	1282	9489	5867	105
H(52)	790	9946	7306	124
H(53)	1386	9470	7737	126
H(56)	547	8665	5249	104
H(58)	-7	9007	3752	133
H(59)	455	8433	3360	125
H(60)	977	7919	3906	111
H(63)	1774	9105	5394	80
H(65)	2319	8601	4886	80
H(66)	4830	8413	3272	140
H(67)	4079	8679	3506	150
H(68)	3664	8247	4217	128
H(69)	2531	4810	7626	107
H(71)	5595	8177	4954	148

Table 6. Torsion angles [°] for 161012a_a_sq_d.

C(41)-P(4)-C(2)-P(3)	-167.4(7)
C(36)-P(4)-C(2)-P(3)	84.5(8)
Ag(4)-P(4)-C(2)-P(3)	-46.3(8)
C(41)-P(4)-C(2)-Ag(5)	-61.6(7)
C(36)-P(4)-C(2)-Ag(5)	-169.7(7)
Ag(4)-P(4)-C(2)-Ag(5)	59.5(6)
C(24)-P(3)-C(2)-P(4)	-173.4(7)
C(30)-P(3)-C(2)-P(4)	-65.8(9)
Ag(3)-P(3)-C(2)-P(4)	58.3(7)
C(24)-P(3)-C(2)-Ag(5)	78.6(7)
C(30)-P(3)-C(2)-Ag(5)	-173.8(6)
Ag(3)-P(3)-C(2)-Ag(5)	-49.8(5)
C(16)-P(1)-C(3)-P(2)	84.8(10)
C(18)-P(1)-C(3)-P(2)	-167.3(7)
Ag(2)-P(1)-C(3)-P(2)	-47.5(8)
C(16)-P(1)-C(3)-Ag(5)	-167.9(8)
C(18)-P(1)-C(3)-Ag(5)	-60.0(8)
Ag(2)-P(1)-C(3)-Ag(5)	59.8(7)
C(10)-P(2)-C(3)-P(1)	-67.4(9)
C(4)-P(2)-C(3)-P(1)	-174.5(7)
Ag(1)-P(2)-C(3)-P(1)	57.7(7)
C(10)-P(2)-C(3)-Ag(5)	-177.1(6)
C(4)-P(2)-C(3)-Ag(5)	75.8(7)
Ag(1)-P(2)-C(3)-Ag(5)	-52.0(5)
C(3)-P(2)-C(4)-C(9)	-13.8(18)
C(10)-P(2)-C(4)-C(9)	-126.6(17)
Ag(1)-P(2)-C(4)-C(9)	108.0(16)
C(3)-P(2)-C(4)-C(5)	169.8(14)
C(10)-P(2)-C(4)-C(5)	57.0(16)
Ag(1)-P(2)-C(4)-C(5)	-68.4(15)
C(9)-C(4)-C(5)-C(6)	4(3)
P(2)-C(4)-C(5)-C(6)	-179.4(16)
C(4)-C(5)-C(6)-C(7)	0(3)
C(5)-C(6)-C(7)-C(8)	1(3)
C(6)-C(7)-C(8)-C(9)	-5(3)
C(5)-C(4)-C(9)-C(8)	-9(3)

P(2)-C(4)-C(9)-C(8)	174.8(15)
C(7)-C(8)-C(9)-C(4)	10(3)
C(3)-P(2)-C(10)-C(14)	-63(2)
C(4)-P(2)-C(10)-C(14)	48(2)
Ag(1)-P(2)-C(10)-C(14)	175.8(18)
C(3)-P(2)-C(10)-C(11)	115.9(19)
C(4)-P(2)-C(10)-C(11)	-133(2)
Ag(1)-P(2)-C(10)-C(11)	-6(2)
C(14)-C(10)-C(11)-C(12)	0(3)
P(2)-C(10)-C(11)-C(12)	-178.3(19)
C(10)-C(11)-C(12)-C(13)	2(4)
C(11)-C(12)-C(13)-C(71)	-3(5)
C(11)-C(10)-C(14)-C(71)	-3(4)
P(2)-C(10)-C(14)-C(71)	176(2)
C(17)-C(15)-C(16)-C(68)	-2(4)
C(17)-C(15)-C(16)-P(1)	180(2)
C(3)-P(1)-C(16)-C(68)	-137.5(19)
C(18)-P(1)-C(16)-C(68)	109(2)
Ag(2)-P(1)-C(16)-C(68)	-6(2)
C(3)-P(1)-C(16)-C(15)	41(2)
C(18)-P(1)-C(16)-C(15)	-72(2)
Ag(2)-P(1)-C(16)-C(15)	172.3(18)
C(16)-C(15)-C(17)-C(66)	-3(5)
C(3)-P(1)-C(18)-C(22)	166.7(13)
C(16)-P(1)-C(18)-C(22)	-80.0(15)
Ag(2)-P(1)-C(18)-C(22)	42.3(15)
C(3)-P(1)-C(18)-C(19)	-12.5(16)
C(16)-P(1)-C(18)-C(19)	100.8(15)
Ag(2)-P(1)-C(18)-C(19)	-136.8(13)
C(22)-C(18)-C(19)-C(20)	2(2)
P(1)-C(18)-C(19)-C(20)	-179.1(13)
C(18)-C(19)-C(20)-C(21)	-4(3)
C(19)-C(20)-C(21)-C(23)	5(3)
C(19)-C(18)-C(22)-C(23)	-1(3)
P(1)-C(18)-C(22)-C(23)	-179.7(14)
C(20)-C(21)-C(23)-C(22)	-4(3)
C(18)-C(22)-C(23)-C(21)	2(3)
C(2)-P(3)-C(24)-C(29)	164.0(13)

C(30)-P(3)-C(24)-C(29)	50.8(14)
Ag(3)-P(3)-C(24)-C(29)	-74.8(14)
C(2)-P(3)-C(24)-C(25)	-14.6(15)
C(30)-P(3)-C(24)-C(25)	-127.8(14)
Ag(3)-P(3)-C(24)-C(25)	106.6(13)
C(29)-C(24)-C(25)-C(26)	0(2)
P(3)-C(24)-C(25)-C(26)	178.9(12)
C(24)-C(25)-C(26)-C(27)	1(3)
C(25)-C(26)-C(27)-C(28)	-1(3)
C(26)-C(27)-C(28)-C(29)	0(3)
C(25)-C(24)-C(29)-C(28)	-2(2)
P(3)-C(24)-C(29)-C(28)	179.4(14)
C(27)-C(28)-C(29)-C(24)	2(3)
C(24)-P(3)-C(30)-C(31)	58.2(17)
C(2)-P(3)-C(30)-C(31)	-53.6(17)
Ag(3)-P(3)-C(30)-C(31)	-173.3(14)
C(24)-P(3)-C(30)-C(35)	-120.0(14)
C(2)-P(3)-C(30)-C(35)	128.1(14)
Ag(3)-P(3)-C(30)-C(35)	8.4(15)
C(35)-C(30)-C(31)-C(32)	-3(3)
P(3)-C(30)-C(31)-C(32)	178.3(15)
C(30)-C(31)-C(32)-C(33)	3(3)
C(31)-C(32)-C(33)-C(34)	-2(3)
C(32)-C(33)-C(34)-C(35)	3(3)
C(31)-C(30)-C(35)-C(34)	3(2)
P(3)-C(30)-C(35)-C(34)	-178.4(14)
C(33)-C(34)-C(35)-C(30)	-3(3)
C(2)-P(4)-C(36)-C(38)	-115.1(14)
C(41)-P(4)-C(36)-C(38)	133.3(14)
Ag(4)-P(4)-C(36)-C(38)	14.8(16)
C(2)-P(4)-C(36)-C(37)	59.2(15)
C(41)-P(4)-C(36)-C(37)	-52.4(16)
Ag(4)-P(4)-C(36)-C(37)	-171.0(12)
C(38)-C(36)-C(37)-C(69)	-1(3)
P(4)-C(36)-C(37)-C(69)	-174.7(14)
C(37)-C(36)-C(38)-C(39)	1(3)
P(4)-C(36)-C(38)-C(39)	175.3(12)
C(36)-C(38)-C(39)-C(40)	0(3)

C(38)-C(39)-C(40)-C(69)	-2(3)
C(2)-P(4)-C(41)-C(46)	-15.9(15)
C(36)-P(4)-C(41)-C(46)	94.4(15)
Ag(4)-P(4)-C(41)-C(46)	-141.3(13)
C(2)-P(4)-C(41)-C(42)	167.0(13)
C(36)-P(4)-C(41)-C(42)	-82.7(14)
Ag(4)-P(4)-C(41)-C(42)	41.6(14)
C(46)-C(41)-C(42)-C(43)	1(3)
P(4)-C(41)-C(42)-C(43)	178.4(17)
C(41)-C(42)-C(43)-C(44)	1(4)
C(42)-C(43)-C(44)-C(45)	-4(4)
C(43)-C(44)-C(45)-C(46)	5(4)
C(42)-C(41)-C(46)-C(45)	0(2)
P(4)-C(41)-C(46)-C(45)	-177.5(14)
C(44)-C(45)-C(46)-C(41)	-3(3)
C(64)-N(6)-C(48)-C(47)	-5(2)
Ag(4)-N(6)-C(48)-C(47)	170.0(11)
C(54)-C(47)-C(48)-N(6)	4(2)
C(53)-C(1)-C(49)-C(50)	5(2)
C(53)-C(1)-C(49)-C(73)	176.2(14)
C(1)-C(49)-C(50)-C(51)	-7(3)
C(73)-C(49)-C(50)-C(51)	-177.0(16)
C(49)-C(50)-C(51)-C(52)	1(3)
C(49)-C(50)-C(51)-Cl(2)	-178.1(18)
C(49)-C(50)-C(51)-Cl(2')	-176.4(17)
C(50)-C(51)-C(52)-C(53)	5(3)
Cl(2)-C(51)-C(52)-C(53)	-175.1(16)
Cl(2')-C(51)-C(52)-C(53)	-177.2(17)
C(51)-C(52)-C(53)-C(1)	-7(3)
C(49)-C(1)-C(53)-C(52)	2(3)
C(64)-N(4)-C(54)-C(47)	-2(2)
C(64)-N(4)-C(54)-C(55)	-179.8(13)
C(48)-C(47)-C(54)-N(4)	0(2)
C(48)-C(47)-C(54)-C(55)	177.5(14)
N(4)-C(54)-C(55)-C(56)	-162.7(15)
C(47)-C(54)-C(55)-C(56)	20(2)
N(4)-C(54)-C(55)-C(60)	18(2)
C(47)-C(54)-C(55)-C(60)	-159.4(17)

C(60)-C(55)-C(56)-C(57)	3(3)
C(54)-C(55)-C(56)-C(57)	-176.5(15)
C(55)-C(56)-C(57)-C(58)	-6(3)
C(55)-C(56)-C(57)-Cl(1')	-173(2)
C(55)-C(56)-C(57)-Cl(1)	-178.1(14)
C(56)-C(57)-C(58)-C(59)	6(3)
Cl(1')-C(57)-C(58)-C(59)	176(2)
Cl(1)-C(57)-C(58)-C(59)	176.3(18)
C(57)-C(58)-C(59)-C(60)	-1(3)
C(56)-C(55)-C(60)-C(59)	1(3)
C(54)-C(55)-C(60)-C(59)	-179.3(16)
C(58)-C(59)-C(60)-C(55)	-2(3)
Ag(3)-N(5)-C(64)-N(4)	-145.9(11)
Ag(2)-N(5)-C(64)-N(4)	108.1(13)
Ag(3)-N(5)-C(64)-N(6)	39.4(18)
Ag(2)-N(5)-C(64)-N(6)	-66.6(14)
C(54)-N(4)-C(64)-N(5)	-173.5(13)
C(54)-N(4)-C(64)-N(6)	1(2)
C(48)-N(6)-C(64)-N(5)	177.4(13)
Ag(4)-N(6)-C(64)-N(5)	2.2(18)
C(48)-N(6)-C(64)-N(4)	3(2)
Ag(4)-N(6)-C(64)-N(4)	-172.3(10)
C(72)-N(1)-C(65)-C(63)	1(2)
Ag(2)-N(1)-C(65)-C(63)	172.6(11)
C(73)-C(63)-C(65)-N(1)	3(2)
C(15)-C(17)-C(66)-C(67)	0(5)
C(17)-C(66)-C(67)-C(68)	6(4)
C(15)-C(16)-C(68)-C(67)	8(4)
P(1)-C(16)-C(68)-C(67)	-173(2)
C(66)-C(67)-C(68)-C(16)	-11(4)
C(39)-C(40)-C(69)-C(37)	3(3)
C(36)-C(37)-C(69)-C(40)	-1(3)
C(12)-C(13)-C(71)-C(14)	1(5)
C(10)-C(14)-C(71)-C(13)	2(4)
C(73)-N(3)-C(72)-N(2)	-180.0(13)
C(73)-N(3)-C(72)-N(1)	3(2)
Ag(1)-N(2)-C(72)-N(3)	-140.7(11)
Ag(4)-N(2)-C(72)-N(3)	111.5(12)

Ag(1)-N(2)-C(72)-N(1)	36.9(17)
Ag(4)-N(2)-C(72)-N(1)	-70.9(13)
C(65)-N(1)-C(72)-N(3)	-4(2)
Ag(2)-N(1)-C(72)-N(3)	-175.8(11)
C(65)-N(1)-C(72)-N(2)	178.9(13)
Ag(2)-N(1)-C(72)-N(2)	6.7(16)
C(72)-N(3)-C(73)-C(63)	2(2)
C(72)-N(3)-C(73)-C(49)	176.3(13)
C(65)-C(63)-C(73)-N(3)	-5(2)
C(65)-C(63)-C(73)-C(49)	-179.3(13)
C(50)-C(49)-C(73)-N(3)	-172.0(16)
C(1)-C(49)-C(73)-N(3)	17(2)
C(50)-C(49)-C(73)-C(63)	3(2)
C(1)-C(49)-C(73)-C(63)	-168.1(14)

Symmetry transformations used to generate equivalent atoms: