Supporting information

Synthesis of 6-trifluoromethylindolo[1,2-*c*]quinazolines and related heterocycles using *N*-(2-iodophenyl)trifluoroacetimidoyl chlorides as starting material *via* C-H Bond functionalization

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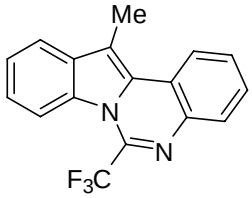
General:

^{1}H NMR spectra were recorded on a Bruker AM-300 spectrometer (300 MHz) with TMS as internal standard. ^{19}F NMR spectra were taken on a Bruker AM-300 (282 MHz) spectrometer using $CFCl_3$ as external standard. ^{13}C NMR spectra were taken on a Bruker AM-400 (101 MHz) spectrometer. Chemical shifts (δ) are reported in ppm, and coupling constants (*J*) are in Hertz (Hz). All reagents were used as received from commercial sources. DMF was distilled from CaH_2 and all reactions were performed under nitrogen. Column chromatography over silica gel (mesh 300-400) and petroleum ether/ethyl acetate combination was used as the eluent.

General procedure for the palladium-catalyzed direct arylation of the intermediates

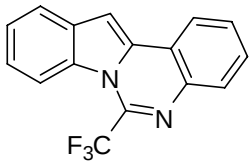
The mixture of the compounds **2** (0.3 mmol), $Pd(OAc)_2$ (3.4 mg, 0.015 mmol), PPh_3 (8 mg, 0.03 mmol) and KOAc (59 mg, 0.6 mmol) in DMF (2 mL) was stirred at 100 ^{o}C for 15 min. Then water (10 mL) was added and the mixture was extracted with ethyl acetate (15 mL × 2). The organic layer was washed with brine, dried over $MgSO_4$, and concentrated under vacuo. The residue was purified by column chromatography on silica gel to provide the desired products **3**.

12-Methyl-6-(trifluoromethyl)indolo[1,2-c]quinazolines (**3a**)



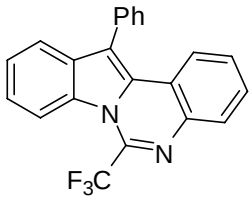
Yellow Solid, mp: 175 – 177 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.25 (d, *J* = 7.8 Hz, 1H), 8.17 (d, *J* = 8.1 Hz, 1H), 7.88 (d, *J* = 7.8 Hz, 1H), 7.83 (d, *J* = 7.6 Hz, 1H), 7.64 – 7.41 (m, 4H), 2.79 (s, 3H); ^{19}F NMR (282 MHz, $CDCl_3$): δ -68.08 (s, 3F); ^{13}C NMR (101 MHz, $CDCl_3$): δ 136.9, 135.9 (q, *J* = 37.8 Hz), 131.1, 129.5, 129.1, 128.6, 128.2, 123.7, 123.5, 123.4, 123.3, 119.0 (q, *J* = 273.6 Hz), 118.5, 114.3 (q, *J* = 7.8 Hz), 108.5, 10.9; MS (EI): m/z (%): 300 (100.00) [M^+]; Anal. Cacld. For $C_{17}H_{11}F_3N_2$: C, 68.00, H, 3.69, N, 9.33; Found: C, 68.39, H, 3.74, N, 9.37; IR (KBr): ν 3069, 2944, 2869, 1628, 1464, 1455, 1402, 1313, 1267, 1247, 1213, 1145, 1119, 953 cm^{-1}.

6-(Trifluoromethyl)indolo[1,2-c]quinazolines (**3b**)



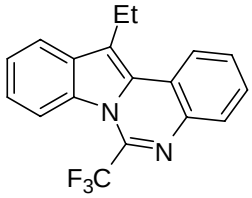
Yellow Solid, mp: 126 – 127 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.16 (d, *J* = 6.8 Hz, 1H), 8.12 – 8.00 (m, 1H), 7.88 – 7.81 (m, 2H), 7.68 – 7.52 (m, 2H), 7.52 – 7.38 (m, 2H), 7.35 (s, 1H); ^{19}F NMR (282 MHz, $CDCl_3$): δ -67.84 (s, 3F); ^{13}C NMR (101 MHz, $CDCl_3$): δ 136.2, 135.6 (q, *J* = 38.1 Hz), 134.8, 130.2, 130.1, 129.5, 129.2, 128.7, 124.3, 123.2, 122.6, 121.7, 120.8, 118.9 (q, *J* = 273.4 Hz), 114.5 (q, *J* = 7.5 Hz), 97.5 (s); MS (EI): m/z (%): 286 (100.00) [M^+]; HRMS (EI) calculated for $C_{16}H_9F_3N_2$: 286.0718, Found: 286.0721; IR (KBr): ν 3044, 1626, 1452, 1400, 1247, 1206, 1141, 967 cm^{-1}.

12-Phenyl-6-(trifluoromethyl)indolo[1,2-c]quinazolines (**3c**)



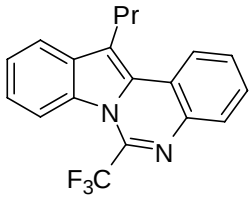
Yellow Solid, mp: 188 – 190 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.22 (d, *J* = 8.0 Hz, 1H), 7.85 (d, *J* = 8.0 Hz, 1H), 7.70 – 7.34 (m, 10H), 7.25 (d, *J* = 4.5 Hz, 1H); ^{19}F NMR (282 MHz, $CDCl_3$): δ -67.44 (s, 3F); ^{13}C NMR (101 MHz, $CDCl_3$): δ 137.0, 135.9 (q, *J* = 37.9 Hz), 134.0, 131.4, 130.7, 129.6, 129.3, 129.1, 128.9, 128.9, 128.8, 128.2, 124.3, 123.8, 123.6, 122.2, 119.7, 119.1 (q, *J* = 275.3 Hz), 115.0, 114.4 (q, *J* = 7.8 Hz); MS (ESI): m/z: 363 [M+H^{+}]; Anal. Cacld. For $C_{22}H_{13}F_3N_2$: C, 72.92, H, 3.62, N, 7.73; Found: C, 73.02, H, 3.58, N, 7.70; IR (KBr): ν 3068, 1626, 1604, 1453, 1397, 1220, 1139, 969 cm^{-1}.

2-Ethyl-12-methyl-6-(trifluoromethyl)indolo[1,2-c]quinazolines (**3d**)



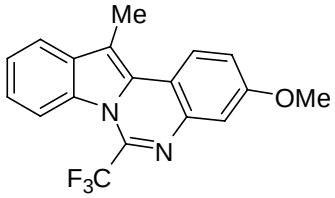
Yellow Solid, mp: 184 – 186 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.20 (d, *J* = 8.0 Hz, 1H), 8.15 (d, *J* = 8.0 Hz, 1H), 7.85 (t, *J* = 8.7 Hz, 2H), 7.66 – 7.40 (m, 4H), 3.29 (q, *J* = 7.5 Hz, 2H), 1.41 (t, *J* = 7.5 Hz, 3H); ^{19}F NMR (282 MHz, $CDCl_3$): δ -67.37 (s, 3F); ^{13}C NMR (101 MHz, $CDCl_3$): δ 137.0, 136.1 (q, *J* = 37.8 Hz), 130.5, 129.4, 129.0, 128.9, 128.9, 128.4, 123.9, 123.5, 123.3, 123.0, 119.0 (q, *J* = 273.6 Hz), 118.4, 115.4, 114.5 (q, *J* = 7.8 Hz), 18.2, 13.6; MS (EI): m/z (%): 299 (100.00), 314 (38.60) [M^{+}]; Anal. Cacld. For $C_{18}H_{13}F_3N_2$: C, 68.78, H, 4.17, N, 8.91; Found: C, 68.79, H, 4.09, N, 8.84; IR (KBr): ν 2964, 2875, 1624, 1604, 1454, 1402, 1310, 1244, 1212, 1136 cm^{-1}.

12-Propyl-6-(trifluoromethyl)indolo[1,2-c]quinazoline (**3e**)



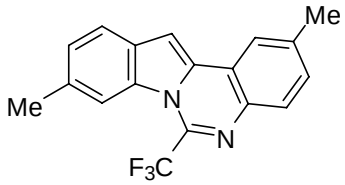
Yellow Solid, mp: 122 – 123 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.17 (m, 2H), 7.85 (t, *J* = 8.4 Hz, 2H), 7.71 – 7.37 (m, 4H), 3.30 – 3.19 (m, 2H), 3.63 – 2.72 (m, 2H), 1.12 (t, *J* = 7.3 Hz, 3H); ^{19}F NMR (282 MHz, $CDCl_3$): δ -67.40 (s, 3F); ^{13}C NMR (101 MHz, $CDCl_3$): δ 137.0, 136.1 (q, *J* = 37.6 Hz), 131.1, 129.3, 129.2, 128.9, 128.7, 128.3, 123.8, 123.5, 123.3, 123.1, 119.0 (q, *J* = 275.4 Hz), 118.7, 114.4 (q, *J* = 7.9 Hz), 114.1, 26.9, 22.5, 14.4; MS (EI): m/z (%): 299 (100.00), 328 (26.25) [M^{+}]; HRMS (EI) calculated for $C_{19}H_{15}F_3N_2$: 328.1187, Found: 328.1190; IR (KBr): ν 2955, 2931, 2870, 1624, 1453, 1400, 1310, 1245, 1212, 1147 cm^{-1}.

3-Methoxy-12-methyl-6-(trifluoromethyl)indolo[1,2-c]quinazoline (**3f**)



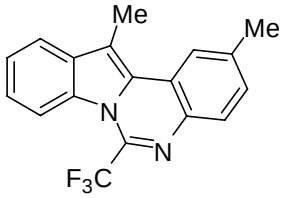
Yellow Solid, mp: 157 – 159 °C; ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.18 (d, *J* = 8.9 Hz, 1H), 8.13 (d, *J* = 8.6 Hz, 1H), 7.79 (d, *J* = 7.7 Hz, 1H), 7.46 (m, 2H), 7.34 (d, *J* = 2.5 Hz, 1H), 7.19 (dd, *J* = 8.9, 2.5 Hz, 1H), 3.92 (s, 3H), 2.75 (s, 3H); ^{19}F NMR (282 MHz, $CDCl_3$): δ -67.70 (s, 3F); ^{13}C NMR (101 MHz, $CDCl_3$): δ 159.6, 138.5, 136.5 (q, *J* = 37.8 Hz), 131.5, 129.8, 128.5, 124.7, 123.8, 122.8, 119.0 (q, *J* = 273.7 Hz), 118.2, 118.1, 116.7, 114.3 (q, *J* = 7.8 Hz), 110.7, 106.4, 55.5, 10.8; MS (ESI): m/z: 331 [M+H$^+$]; Anal. Cacld. For $C_{18}H_{13}F_3N_2O$: C, 65.45, H, 3.97, N, 8.48; Found: C, 65.13, H, 3.76, N, 8.37; IR (KBr): ν 2945, 2842, 1602, 1452, 1396, 1292, 1216, 1152 cm^{-1}.

2,9-Dimethyl-6-(trifluoromethyl)indolo[1,2-c]quinazoline (**3g**)



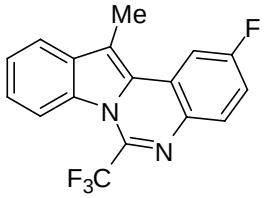
Yellow Solid, mp: 175 – 176 °C; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.93 (s, 1H), 7.83 (s, 1H), 7.74 (d, *J* = 8.2 Hz, 1H), 7.69 (d, *J* = 8.1 Hz, 1H), 7.35 (d, *J* = 8.2 Hz, 1H), 7.31 – 7.18 (m, 2H), 2.59 (s, 3H), 2.53 (s, 3H); ^{19}F NMR (282 MHz, $CDCl_3$): δ -67.45 (s, 3F); ^{13}C NMR (101 MHz, $CDCl_3$): δ 139.9, 134.9 (q, *J* = 38.0 Hz), 134.4, 134.1, 133.0, 130.5, 130.3, 128.5, 128.0, 125.9, 122.4, 121.7, 120.3, 119.0 (q, *J* = 274.8 Hz), 114.4 (q, *J* = 7.4 Hz), 97.0, 22.3, 21.7; MS (ESI): m/z: 315 [M+H$^+$]; Anal. Cacld. For $C_{18}H_{13}F_3N_2$: C, 68.78, H, 4.17, N, 8.91; Found: C, 68.50, H, 4.03, N, 8.83; IR (KBr): ν 2912, 2861, 1625, 1482, 1396, 1301, 1249, 1217, 1146 cm^{-1}.

2,12-Dimethyl-6-(trifluoromethyl)indolo[1,2-c]quinazoline (**3h**)



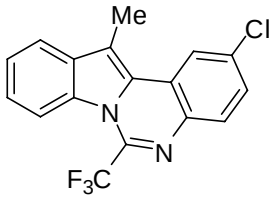
Yellow Solid, mp: 155 – 156 °C; ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.13 (d, *J* = 7.7 Hz, 1H), 8.03 (s, 1H), 7.80 (d, *J* = 7.9 Hz, 1H), 7.74 (d, *J* = 8.1 Hz, 1H), 7.57 – 7.38 (m, 2H), 7.33 (d, *J* = 8.1 Hz, 1H), 2.77 (s, 3H), 2.54 (s, 3H); ^{19}F NMR (282 MHz, $CDCl_3$): δ -67.32 (s, 3F); ^{13}C NMR (101 MHz, $CDCl_3$): δ 139.3, 135.2 (q, *J* = 38.0 Hz), 134.8, 131.1, 129.4, 129.3, 128.6, 128.4, 123.6, 123.5, 123.2, 123.1, 119.1 (q, *J* = 273.5 Hz), 118.4, 114.2 (q, *J* = 7.7 Hz), 108.1, 22.0, 10.9; MS (ESI): m/z: 315 [M+H$^+$]; Anal. Cacld. For $C_{18}H_{13}F_3N_2$: C, 68.78, H, 4.17, N, 8.91; Found: C, 68.94, H, 4.00, N, 8.98; IR (KBr): ν 2922, 2870, 1623, 1597, 1450, 1398, 1297, 1244, 1215, 1144 cm^{-1}.

2-Fluoro-12-methyl-6-(trifluoromethyl)indolo[1,2-c]quinazoline (**3i**)



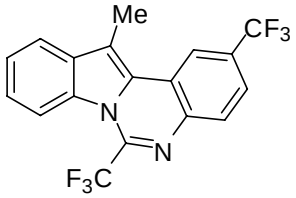
Yellow Solid, mp: 190 – 192 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.13 (d, *J* = 7.1 Hz, 1H), 7.88 (d, *J* = 12.4 Hz, 1H), 7.82 (m, 2H), 7.57 – 7.40 (m, 2H), 7.23 (d, *J* = 9.0 Hz, 1H), 2.76 (s, 3H); ^{19}F NMR (282 MHz, $CDCl_3$): δ -67.60 (s, 3F), -109.08 (m, 1F); ^{13}C NMR (101 MHz, $CDCl_3$): δ 162.5 (d, *J* = 248.8 Hz), 135.4 (q, *J* = 38.2 Hz), 133.4, 130.9, 130.9, 130.8, 128.8, 128.7, 124.8 (d, *J* = 10.6 Hz), 123.9, 118.9 (q, *J* = 273.4 Hz), 118.7, 115.9 (d, *J* = 23.6 Hz), 114.4 (q, *J* = 7.7 Hz), 109.7, 109.4 (d, *J* = 9.2 Hz), 10.8; MS (ESI): m/z: 319 [M+H$^+$]; HRMS (ESI) calculated for $C_{17}H_{11}F_4N_2^+$: 319.0862, Found: 319.0852; IR (KBr): ν 2931, 2875, 1624, 1613, 1570, 1478, 1399, 1289, 1215, 1148 cm^{-1}.

2-Chloro-12-methyl-6-(trifluoromethyl)indolo[1,2-c]quinazoline (**3j**)



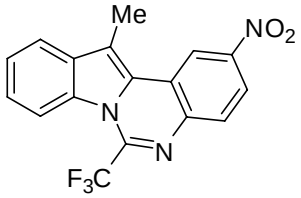
Yellow Solid, mp: 200 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.18 (s, 1H), 8.13 (d, *J* = 7.6 Hz, 1H), 7.83 (d, *J* = 8.3 Hz, 1H), 7.78 (d, *J* = 8.6 Hz, 1H), 7.49 (m, 3H), 2.78 (s, 3H); ^{19}F NMR (282 MHz, $CDCl_3$): δ -67.50 (s, 3F); ^{13}C NMR (101 MHz, $CDCl_3$): δ 136.1 (q, *J* = 38.7 Hz), 135.4, 134.9, 131.0, 130.0, 128.7, 128.5, 128.3, 124.5, 124.1, 124.0, 123.1, 118.9 (q, *J* = 274.1 Hz), 118.7, 114.4 (q, *J* = 7.9 Hz), 109.7, 10.9; MS (ESI): m/z: 355 [M+H$^+$]; Anal. Cacld. For $C_{17}H_{10}ClF_3N_2$: C, 61.00, H, 3.01, N, 8.37; Found: C, 60.86, H, 2.86, N, 8.37; IR (KBr): ν 2950, 2865, 1623, 1606, 1547, 1400, 1289, 1247, 1211, 1138 cm^{-1}.

12-Methyl-2,6-bis(trifluoromethyl)indolo[1,2-c]quinazoline (**3k**)



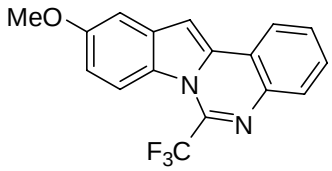
Yellow Solid, mp: 174 – 175 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.47 (s, 1H), 8.15 (d, *J* = 7.8 Hz, 1H), 7.95 (d, *J* = 8.4 Hz, 1H), 7.86 (d, *J* = 7.8 Hz, 1H), 7.75 (d, *J* = 8.4 Hz, 1H), 7.62 – 7.44 (m, 2H), 2.81 (s, 3H); ^{19}F NMR (282 MHz, $CDCl_3$): δ -62.44 (s, 3F), -67.86 (s, 3F); ^{13}C NMR (101 MHz, $CDCl_3$): δ 139.2, 137.7 (q, *J* = 38.6 Hz), 131.1, 130.8 (q, *J* = 32.6 Hz), 129.3, 128.8, 128.5, 124.7 (q, *J* = 3.5 Hz), 124.3, 124.2, 123.9 (q, *J* = 68.1 Hz), 120.7 (q, *J* = 4.1 Hz), 118.8, 118.7 (q, *J* = 273.9 Hz), 114.5 (q, *J* = 7.8 Hz), 110.2, 10.9; MS (ESI): m/z: 369 [M+H$^+$]; Anal. Cacld. For $C_{18}H_{10}F_6N_2$: C, 58.70, H, 2.74, N, 7.61; Found: C, 58.62, H, 2.60, N, 7.55; IR (KBr): ν 2931, 2875, 1630, 1599, 1576, 1401, 1293, 1243, 1214, 1155, 1122 cm^{-1}.

12-Methyl-2-nitro-6-(trifluoromethyl)indolo[1,2-c]quinazoline (**3l**)



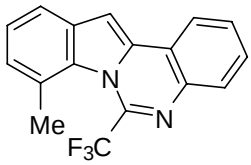
Yellow Solid, mp: 250 – 252 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$): δ 9.09 (d, *J* = 2.2 Hz, 1H), 8.35 (dd, *J* = 8.8, 2.2 Hz, 1H), 8.17 (d, *J* = 7.5 Hz, 1H), 7.97 (d, *J* = 8.8 Hz, 1H), 7.90 (d, *J* = 7.2 Hz, 1H), 7.66 – 7.48 (m, 2H), 2.88 (s, 3H); ^{19}F NMR (282 MHz, $CDCl_3$): δ -67.84 (d, *J* = 1.7 Hz, 3F); ^{13}C NMR (101 MHz, $CDCl_3$): δ 147.2, 141.3, 138.6 (q, *J* = 38.5 Hz), 131.1, 129.6, 128.9, 128.0, 124.8, 123.8, 122.8, 119.1, 119.1, 118.6 (q, *J* = 276.2 Hz), 114.7 (q, *J* = 7.8 Hz), 111.5, 10.9; MS (EI): m/z (%): 345 (100.00) [M^+]; Anal. Cacld. For $C_{17}H_{10}F_3N_3O_2$: C, 59.14, H, 2.92, N, 12.17; Found: C, 58.71, H, 2.88, N, 11.77; IR (KBr): ν 3124, 1601, 1581, 1515, 1405, 1346, 1292, 1242, 1211, 1156, 1092 cm^{-1}.

10-Methoxy-6-(trifluoromethyl)indolo[1,2-c]quinazoline (**3m**)



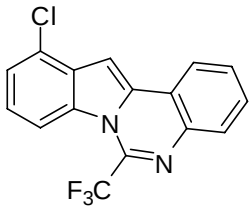
Yellow Solid, mp: 250 – 252 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.10 – 7.97 (m, 1H), 7.92 – 7.79 (m, 1H), 7.66 – 7.47 (m, 1H), 7.23 (s, 1H), 7.17 (d, *J* = 2.3 Hz, 1H), 7.03 (dd, *J* = 9.4, 2.5 Hz, 1H), 3.91 (s, 3H); ^{19}F NMR (282 MHz, $CDCl_3$): δ -68.05 (s, 3F); ^{13}C NMR (101 MHz, $CDCl_3$): δ 156.8, 136.2, 135.5, 135.2 (q, *J* = 38.2 Hz), 131.4, 129.3, 129.0, 128.6, 124.9, 122.5, 121.3, 118.9 (q, *J* = 275.2 Hz), 115.4 (q, *J* = 7.6 Hz), 113.1, 101.5, 97.2, 55.5; MS (EI): m/z (%): 316 (100.00) [M^+]; HRMS (EI) calculated for $C_{17}H_{11}F_3N_2O$: 316.0823, Found: 316.0822; IR (KBr): ν 3002, 2960, 2828, 1613, 1463, 1450, 1401, 1232, 1140 cm^{-1}.

8-Methyl-6-(trifluoromethyl)indolo[1,2-c]quinazoline (**3n**)



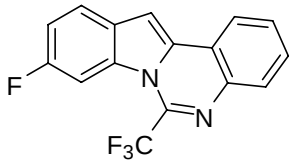
Yellow Solid, mp: 106 – 108 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.08 – 7.91 (m, 1H), 7.91 – 7.76 (m, 1H), 7.67 – 7.45 (m, 3H), 7.36 (t, *J* = 7.5 Hz, 1H), 7.29 – 7.12 (m, 2H), 2.68 (s, 3H); ^{19}F NMR (282 MHz, $CDCl_3$): δ –63.22 (s, 3F); ^{13}C NMR (101 MHz, $CDCl_3$): δ 139.6 (q, *J* = 37.6 Hz), 137.0, 136.5, 133.3, 131.8, 129.2, 129.1, 127.7, 126.9, 126.1, 124.8, 122.7, 121.7, 118.9 (q, *J* = 277.3 Hz), 117.8, 98.6, 20.5 (q, *J* = 6.1 Hz); MS (ESI): m/z: 301 [M+H^+]; Anal. Cacld. For $C_{17}H_{11}F_3N_2$: C, 68.00, H, 3.69, N, 9.33; Found: C, 67.72, H, 3.64, N, 9.25; IR (KBr): ν 2978, 2922, 1613, 1463, 1450, 1379, 1196, 1145 cm^{-1}.

11-Chloro-6-(trifluoromethyl)indolo[1,2-c]quinazoline (**3o**)



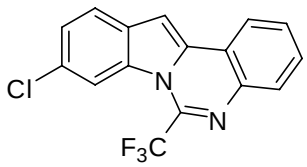
Yellow Solid, mp: 174 – 176 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.22 – 8.11 (m, 1H), 8.07 (d, *J* = 8.5 Hz, 1H), 7.98 – 7.83 (m, 1H), 7.73 – 7.56 (m, 2H), 7.55 – 7.43 (m, 2H), 7.36 (t, *J* = 8.2 Hz, 1H); ^{19}F NMR (282 MHz, $CDCl_3$): δ –67.51 (s, 3F); ^{13}C NMR (101 MHz, $CDCl_3$): δ 136.3, 135.4, 135.3 (q, *J* = 38.4 Hz), 130.6, 130.0, 129.7, 129.1, 128.96, 126.0, 123.8, 123.4, 122.8, 121.4, 118.7 (q, *J* = 275.2 Hz), 113.1 (q, *J* = 7.6 Hz), 95.9; MS (EI): m/z (%): 320 (100.00) [M^+]; Anal. Cacld. For $C_{16}H_8ClF_3N_2$: C, 59.92, H, 2.51, N, 8.74; Found: C, 59.67, H, 2.56, N, 8.68; IR (KBr): ν 1626, 1431, 1450, 1388, 1255, 1204, 1135 cm^{-1}.

9-Fluoro-6-(trifluoromethyl)indolo[1,2-c]quinazoline (**3p**)



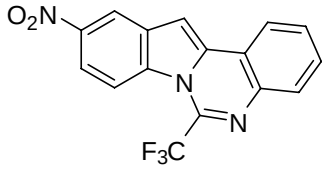
Yellow Solid, mp: 148 – 150 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.04 (d, *J* = 8.5 Hz, 1H), 7.95 – 7.81 (m, 2H), 7.75 (dd, *J* = 8.6, 5.8 Hz, 1H), 7.67 – 7.51 (m, 2H), 7.31 (s, 1H), 7.30 – 7.15 (m, 1H); ^{19}F NMR (282 MHz, $CDCl_3$): δ -67.51 (s, 3F), -116.62 – -116.78 (m, 1F); ^{13}C NMR (101 MHz, $CDCl_3$): δ 159.7 (d, *J* = 240.0 Hz), 136.0, 135.4, 135.3 (q, *J* = 43.5 Hz), 129.8, 129.7 (d, *J* = 12.3 Hz), 129.3, 129.0, 126.6, 122.4, 121.8, 121.4 (d, *J* = 9.8 Hz), 118.7 (q, *J* = 275.2 Hz), 113.3 (d, *J* = 24.6 Hz), 101.8 (dq, *J* = 29.6, 7.8 Hz), 97.2; MS (ESI): m/z: 305 [M+H^+]; Anal. Cacld. For $C_{16}H_8F_4N_2$: C, 63.16, H, 2.65, N, 9.21; Found: C, 63.17, H, 2.82, N, 9.06; IR (KBr): ν 3162, 3058, 1625, 1468, 1466, 1396, 1217, 1136 cm^{-1}.

9-Chloro-6-(trifluoromethyl)indolo[1,2-c]quinazoline (**3q**)



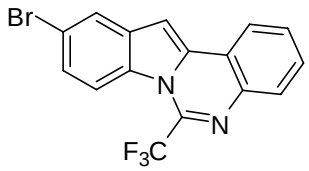
Yellow Solid, mp: 146 – 147 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.13 (s, 1H), 8.09 – 7.98 (m, 1H), 7.93 – 7.80 (m, 1H), 7.72 (d, *J* = 8.5 Hz, 1H), 7.65 – 7.52 (m, 2H), 7.42 (d, *J* = 7.8 Hz, 1H), 7.29 (s, 1H); ^{19}F NMR (282 MHz, $CDCl_3$): δ -67.57 (s, 3F); ^{13}C NMR (101 MHz, $CDCl_3$): δ 136.1, 135.6, 135.2 (q, *J* = 38.5 Hz), 130.2, 129.9, 129.6, 129.1, 129.0, 128.6, 125.1, 122.6, 121.6, 121.5, 118.7 (q, *J* = 275.1 Hz), 114.7 (q, *J* = 8.0 Hz), 97.3; MS (ESI): m/z: 321 [M+H^+]; Anal. Cacld. For $C_{16}H_8ClF_3N_2$: C, 59.92, H, 2.51, N, 8.74; Found: C, 59.69, H, 2.48, N, 8.68; IR (KBr): ν 1626, 1464, 1391, 1242, 1204, 1128 cm^{-1}.

10-Nitro-6-(trifluoromethyl)indolo[1,2-c]quinazoline (**3r**)



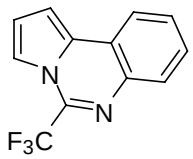
Red Solid, mp: 196 – 198 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.75 (s, 1H), 8.39 – 8.20 (m, 2H), 8.20 – 8.09 (m, 1H), 8.05 – 7.87 (m, 1H), 7.78 – 7.59 (m, 2H), 7.52 (s, 1H); ^{19}F NMR (282 MHz, $CDCl_3$): δ –67.55 (s, 3F); ^{13}C NMR (101 MHz, $CDCl_3$): δ 144.5, 137.8, 136.1, 135.0 (q, *J* = 39.1 Hz), 132.5, 130.5, 130.5, 130.0, 129.3, 123.1, 121.0, 118.7 (q, *J* = 276.2 Hz), 117.8, 117.0, 115.1 (q, *J* = 7.3 Hz), 98.5; MS (EI): m/z (%): 331 (100.00) [M^+]; HRMS (EI) calculated for $C_{16}H_8F_3N_3O_2$: 331.0569, Found: 331.0572; IR (KBr): ν 1597, 1505, 1333, 1246, 1188, 1132 cm^{-1}.

10-Bromo-6-(trifluoromethyl)indolo[1,2-c]quinazoline (**3s**)



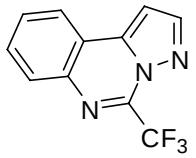
Yellow Solid, mp: 198 – 200 ^{o}C; ^{1}H NMR (300 MHz, DMSO): δ 8.42 (d, *J* = 6.3 Hz, 1H), 8.18 (s, 1H), 8.03 (d, *J* = 7.3 Hz, 1H), 7.93 (d, *J* = 6.5 Hz, 1H), 7.86 – 7.56 (m, 4H); ^{19}F NMR (282 MHz, DMSO): δ –66.84 (s, 3F); ^{13}C NMR (101 MHz, $CDCl_3$): δ 136.3, 136.1, 135.3 (q, *J* = 38.2 Hz), 131.9, 129.9, 129.8, 129.0, 128.8, 126.1, 123.2, 122.8, 121.4, 118.8 (q, *J* = 275.2 Hz), 118.0, 115.9 (q, *J* = 7.7 Hz), 96.7; MS (EI): m/z (%): 364 (100.00) [M^+]; HRMS (EI) calculated for $C_{16}H_8F_3N_2Br$: 363.9823, Found: 363.9819; IR (KBr): ν 1625, 1469, 1391, 1249, 1208, 1132 cm^{-1}.

5-(Trifluoromethyl)pyrrolo[1,2-c]quinazoline (**3t**)



Yellow Solid, mp: 62 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.94 (d, *J* = 7.8 Hz, 1H), 7.87 (d, *J* = 7.8 Hz, 1H), 7.65 – 7.40 (m, 3H), 7.00 (d, *J* = 3.2 Hz, 1H), 6.88 (t, *J* = 3.2 Hz, 1H); ^{19}F NMR (282 MHz, $CDCl_3$): δ –70.52 (s, 3F); ^{13}C NMR (101 MHz, $CDCl_3$): δ 135.5, 134.8 (q, *J* = 37.6 Hz), 130.8, 129.7, 129.1, 127.6, 122.0, 121.6, 118.7 (q, *J* = 275.8 Hz), 115.4, 113.8 (q, *J* = 3.4 Hz), 101.6; MS (EI): m/z (%): 236 (100.00) [M^+]; HRMS (EI) calculated for $C_{12}H_7F_3N_2$: 236.0561, Found: 236.0560; IR (KBr): ν 3155, 3057, 1626, 1473, 1413, 1255, 1200, 1136 cm^{-1}.

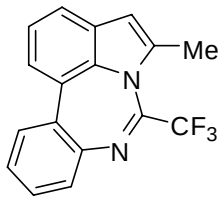
5-(Trifluoromethyl)pyrazolo[1,5-c]quinazoline (**3u**)



White Solid, mp: 234 – 236 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.22 (d, *J* = 1.9 Hz, 1H), 8.17 – 8.01 (m,

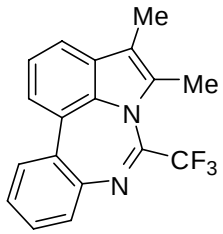
2H), 7.82 – 7.66 (m, 2H), 7.10 (d, J = 1.9 Hz, 1H); ^{19}F NMR (282 MHz, $CDCl_3$): δ –69.73 (s, 3F); ^{13}C NMR (101 MHz, $CDCl_3$): δ 144.7, 140.6, 137.6, 136.0 (q, J = 39.1 Hz), 130.3, 130.1, 129.7, 123.2, 120.8, 118.2 (q, J = 276.2 Hz), 98.9; MS (EI): m/z (%): 237 (100.00) [M^+]; HRMS (EI) calculated for $C_{11}H_6F_3N_3$: 237.0514, Found: 237.0516; IR (KBr): ν 3129, 1630, 1482, 1436, 1325, 1257, 1197, 1152, 1067 cm^{-1}.

4a



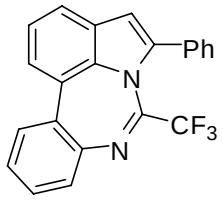
Yellow Solid, mp: 75 °C; ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.23 – 7.60 (m, 7H), 6.94 (s, 1H), 3.02 (s, 3H); ^{19}F NMR (282 MHz, $CDCl_3$): δ –64.27 (s, 3F); ^{13}C NMR (101 MHz, $CDCl_3$): δ 149.7, 143.1, 140.7 (q, J = 36.3 Hz), 138.8, 131.2, 131.0, 129.6, 129.1, 128.6, 128.3, 125.1, 125.0, 120.4, 118.6, 117.6 (q, J = 279.8 Hz), 110.9, 14.75 (q, J = 5.3 Hz). MS (EI): m/z (%): 300 (100.00) [M^+]; Anal. Cacld. For $C_{17}H_{11}F_3N_2$: C, 68.00, H, 3.69, N, 9.33; Found: C, 68.09, H, 3.64, N, 9.28; IR (KBr): ν 3063, 3021, 2941, 1690, 1469, 1411, 1336, 1272, 1226, 1194, 1139 cm^{-1}.

4b



Yellow Solid, mp: 84 °C; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.66 – 6.81 (m, 7H), 2.34 (s, 3H), 2.12 (s, 3H); ^{19}F NMR (282 MHz, $CDCl_3$): δ –64.85 (s, 3F); ^{13}C NMR (101 MHz, $CDCl_3$): δ 148.9, 143.3, 141.2 (q, J = 35.8 Hz), 133.8, 132.3, 131.3, 129.5, 128.9, 128.5, 128.1, 125.0, 124.8, 120.4, 117.1 (q, J = 280.3 Hz), 117.5, 116.9, 12.6 (q, J = 5.3 Hz), 8.9; MS (ESI): m/z: 315 [M+H^+]; Anal. Cacld. For $C_{18}H_{13}F_3N_2$: C, 68.78, H, 4.17, N, 8.91; Found: C, 68.80, H, 4.14, N, 8.80; IR (KBr): ν 3058, 3030, 2941, 1680, 1417, 1350, 1276, 1225, 1170, 1137 cm^{-1}.

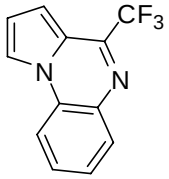
4c



Yellow Solid, mp: 132 °C; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.91 – 7.14 (m, 12H), 6.77 (s, 1H); ^{19}F NMR (282 MHz, $CDCl_3$): δ –64.05 (s, 3F); ^{13}C NMR (101 MHz, $CDCl_3$): δ 149.8, 143.9, 143.1, 141.5 (q, J = 35.8 Hz), 132.4, 131.1, 130.7, 129.6, 128.7, 128.7, 128.6, 128.1, 127.6, 125.5, 125.5, 121.4, 119.6,

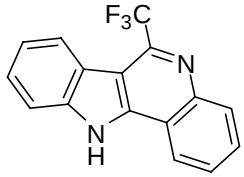
117.2 (q, J = 281.2 Hz), 110.4; MS (ESI): m/z: 363 [M+H$^+$]; Anal. Cacld. For $C_{22}H_{13}F_3N_2$: C, 72.92, H, 3.62, N, 7.73; Found: C, 72.89, H, 3.61, N, 7.79; IR (KBr): ν 3054, 3025, 1673, 1466, 1410, 1350, 1321, 1184, 1150 cm^{-1}.

4-(Trifluoromethyl)pyrrolo[1,2-a]quinoxaline (**5a**)



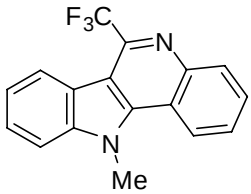
White Solid, mp: 98 – 100 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.06 (m, 2H), 7.89 (d, J = 8.2 Hz, 1H), 7.63 (t, J = 7.7 Hz, 1H), 7.50 (t, J = 7.6 Hz, 1H), 7.14 (s, 1H), 7.01 – 6.93 (m, 1H); ^{19}F NMR (282 MHz, $CDCl_3$): δ –67.89 (s, 3F); ^{13}C NMR (101 MHz, DMSO): δ 141.5 (q, J = 35.5 Hz), 133.4, 130.9, 130.6, 127.9, 126.5, 121.3 (q, J = 275.9 Hz), 120.9, 118.5, 115.6, 115.5, 107.9; MS (ESI): m/z: 237 [M+H$^+$]; Anal. Cacld. For $C_{12}H_7F_3N_2$: C, 61.02, H, 2.99, N, 11.86; Found: C, 61.30, H, 3.03, N, 11.98; IR (KBr): ν 3121, 1549, 1481, 1432, 1385, 1257, 1195, 1178, 1125 cm^{-1}.

6-(Trifluoromethyl)-11H-indolo[3,2-c]quinoline (**6a**)



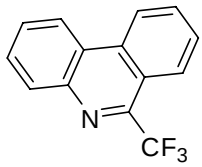
White Solid, mp: 128 – 130 ^{o}C; ^{1}H NMR (400 MHz, DMSO): δ 13.23 (s, 1H), 8.75 – 8.60 (m, 1H), 8.33 – 8.25 (m, 1H), 8.23 (d, J = 8.0 Hz, 1H), 7.95 – 7.85 (m, 2H), 7.83 (d, J = 8.2 Hz, 1H), 7.61 (t, J = 7.3 Hz, 1H), 7.44 (t, J = 7.6 Hz, 1H); ^{19}F NMR (282 MHz, $CDCl_3$): δ –64.85 (s, 3F); ^{13}C NMR (101 MHz, DMSO): δ 143.3, 142.7, 140.81 (q, J = 35.1 Hz), 139.7, 130.4, 129.8, 128.5, 126.9, 122.8 (q, J = 274.6 Hz), 122.6, 122.1 (q, J = 4.6 Hz), 121.9, 119.7, 118.0, 112.8, 110.0; MS (EI): m/z (%): 286 (16.60) [M$^+$], 238 (100.00); HRMS (EI) calculated for $C_{16}H_9F_3N_2$: 286.0718, Found: 286.0713; IR (KBr): ν 3336, 1566, 1507, 1450, 1362, 1253, 1190, 1165, 1123 cm^{-1}.

11-Methyl-6-(trifluoromethyl)-11H-indolo[3,2-c]quinoline (**6b**)

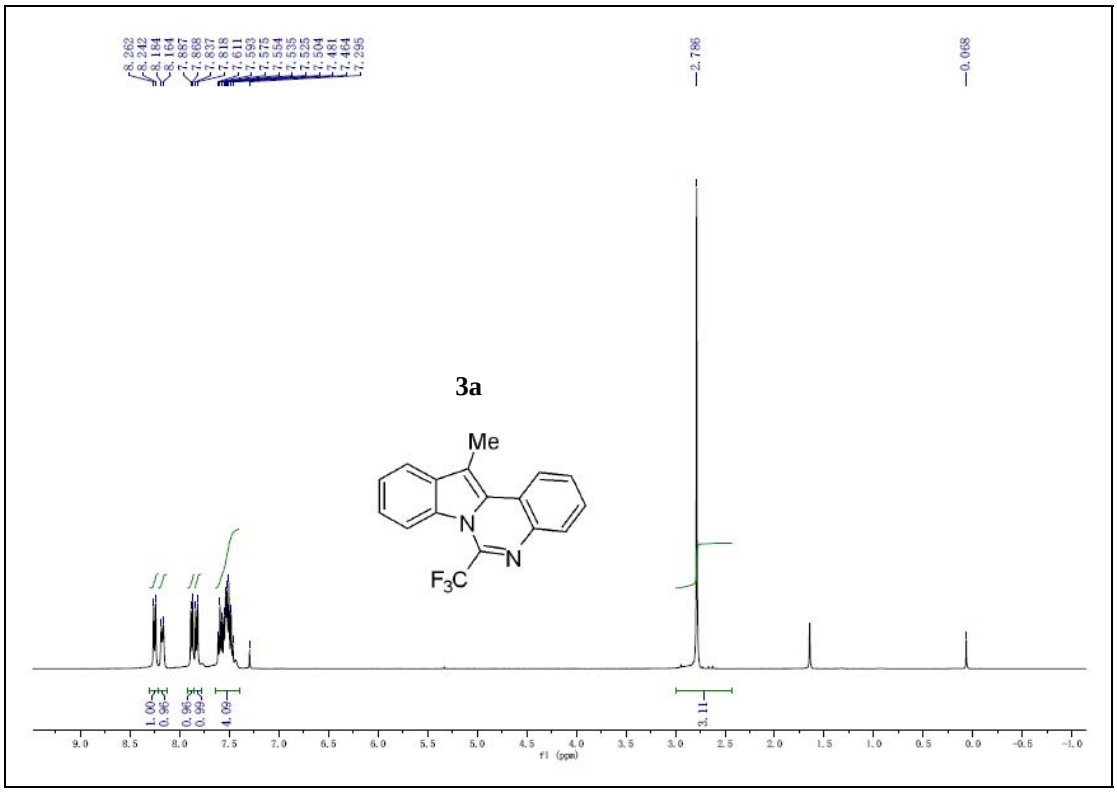


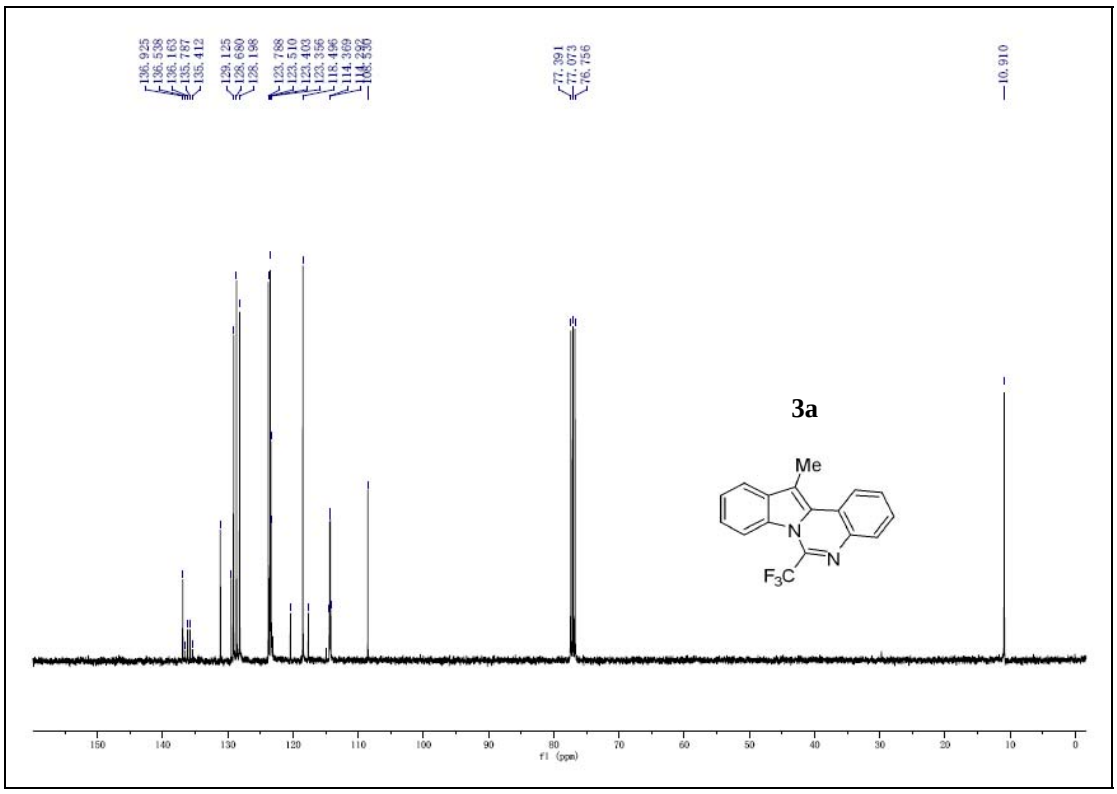
White Solid, mp: 176 – 178 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.44 (d, J = 8.3 Hz, 1H), 8.35 (d, J = 7.8 Hz, 1H), 8.28 (d, J = 8.2 Hz, 1H), 7.66 (t, J = 7.3 Hz, 1H), 7.62 – 7.54 (m, 1H), 7.53 – 7.27 (m, 3H), 4.18 (s, 3H); ^{19}F NMR (282 MHz, $CDCl_3$): δ –67.33 (s, 3F); ^{13}C NMR (101 MHz, $CDCl_3$): δ 144.4, 141.6, 141.5 (q, J = 35.2 Hz), 140.6, 131.2, 128.3, 127.2, 126.3, 122.7 (q, J = 5.2 Hz), 122.4 (q, J = 273.2 Hz), 121.7, 121.6, 119.2, 118.5, 110.9, 109.2, 33.5; MS (EI): m/z (%): 300 (100.00) [M$^+$]; Anal. Cacld. For $C_{17}H_{11}F_3N_2$: C, 68.00, H, 3.69, N, 9.33; Found: C, 67.88, H, 3.58, N, 9.33; IR (KBr): ν 3054, 1567, 1512, 1444, 1370, 1319, 1257, 1174, 1119 cm^{-1}.

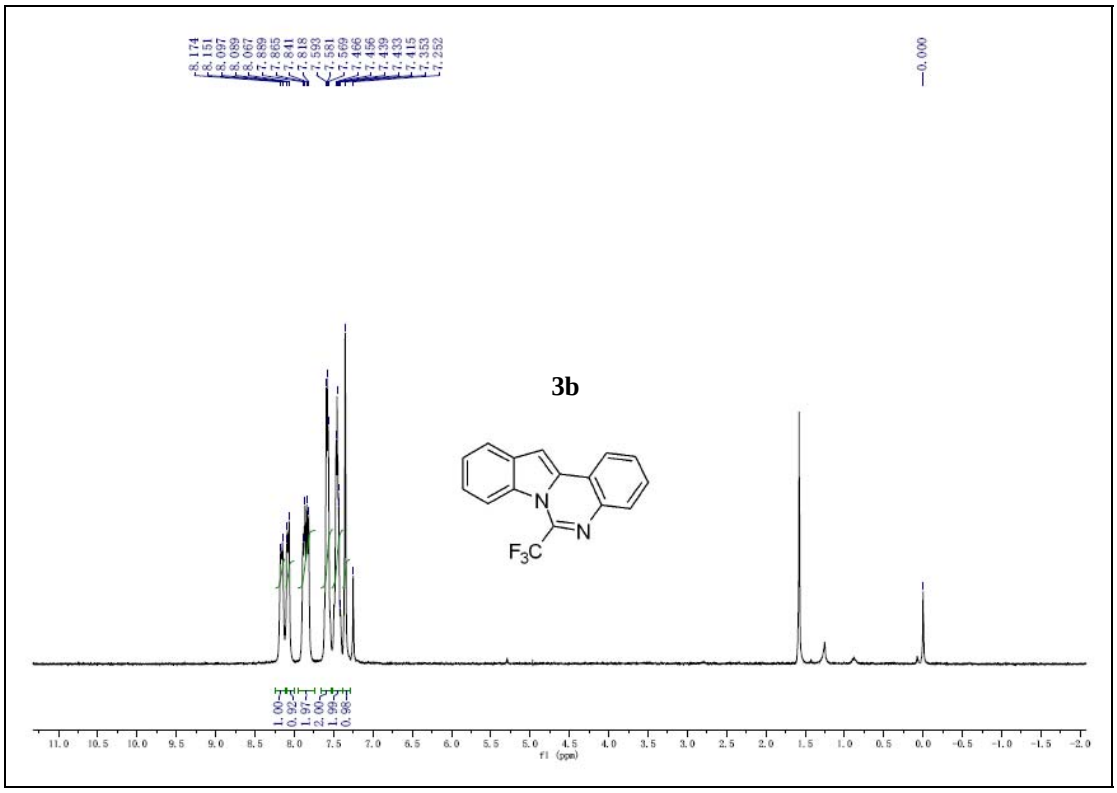
6-(Trifluoromethyl)phenanthridine (**7a**)



White Solid, mp: 73 – 74 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.71 (d, *J* = 8.3 Hz, 1H), 8.67 – 8.51 (m, 1H), 8.39 (d, *J* = 7.8 Hz, 1H), 8.34 – 8.16 (m, 1H), 7.93 (t, *J* = 7.5 Hz, 1H), 7.88 – 7.65 (m, 3H); ^{19}F NMR (282 MHz, $CDCl_3$): δ –63.33 (s, 3F); ^{13}C NMR (101 MHz, $CDCl_3$): δ 146.5 (q, *J* = 33.0 Hz), 141.7, 133.9, 131.3, 131.1, 129.3, 129.1, 128.0, 125.8 (q, *J* = 3.3 Hz), 125.0, 122.5, 122.0, 121.9 (q, *J* = 277.1 Hz), 121.7; MS (EI): m/z (%): 247 (100.00) [M^+]; Anal. Cacld. For $C_{14}H_8F_3N$: C, 68.02, H, 3.26, N, 5.67; Found: C, 67.94, H, 3.24, N, 5.42; IR (KBr): ν 3082, 1609, 1529, 1464, 1381, 1336, 1255,, 1182, 1117 cm^{-1}.


3a
Me
N
N
F3C


3a
Me
N
N
F3C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8.151
8.097
8.089
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7.889
7.865
7.841
7.818
7.593
7.581
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7.466
7.456
7.439
7.433
7.415
7.353
7.252
0.000
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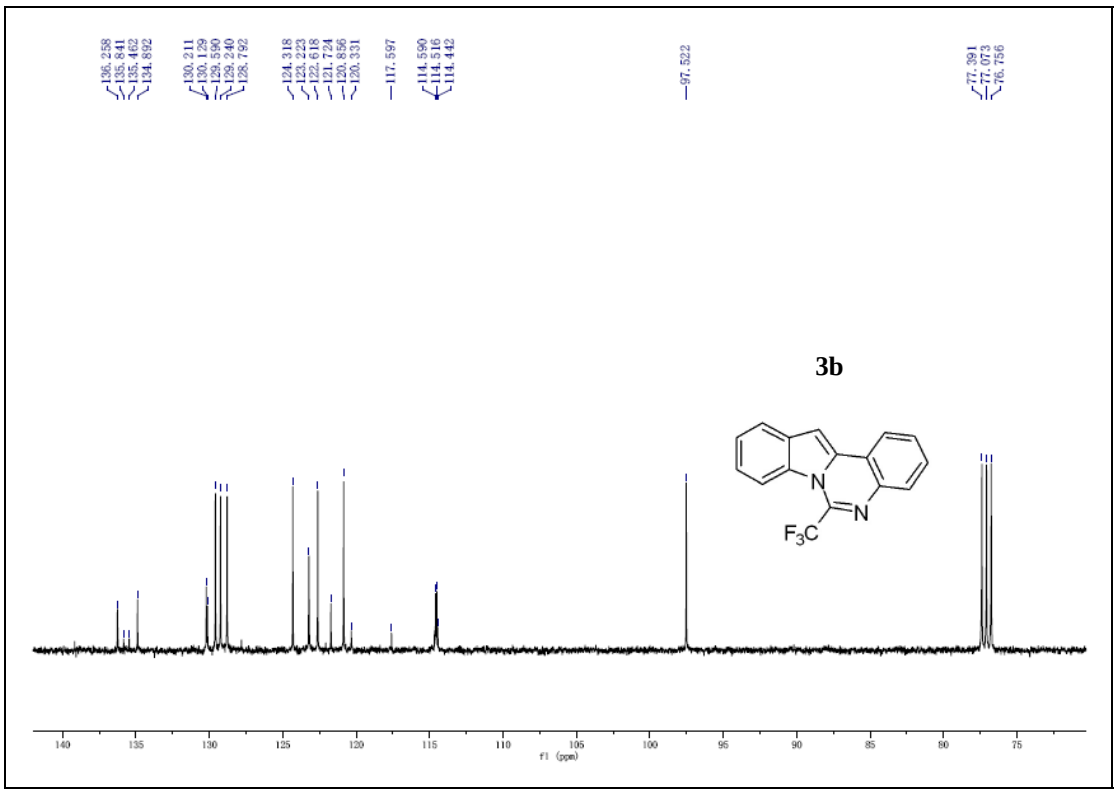
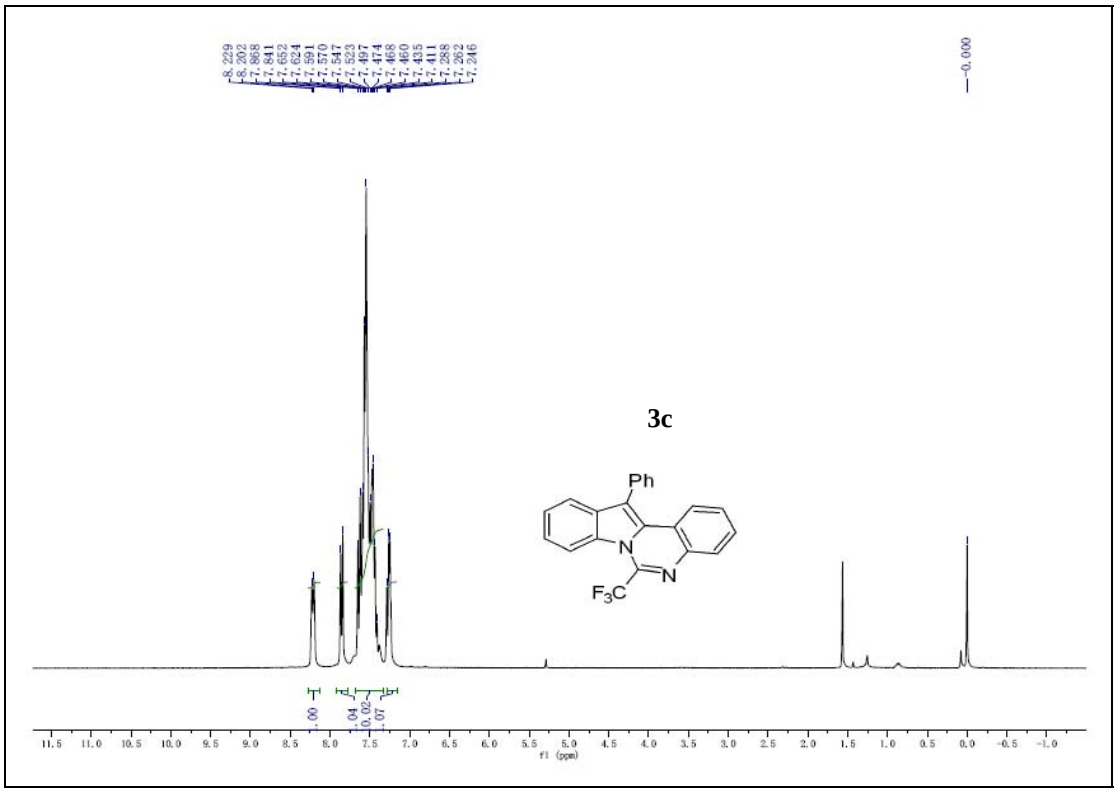
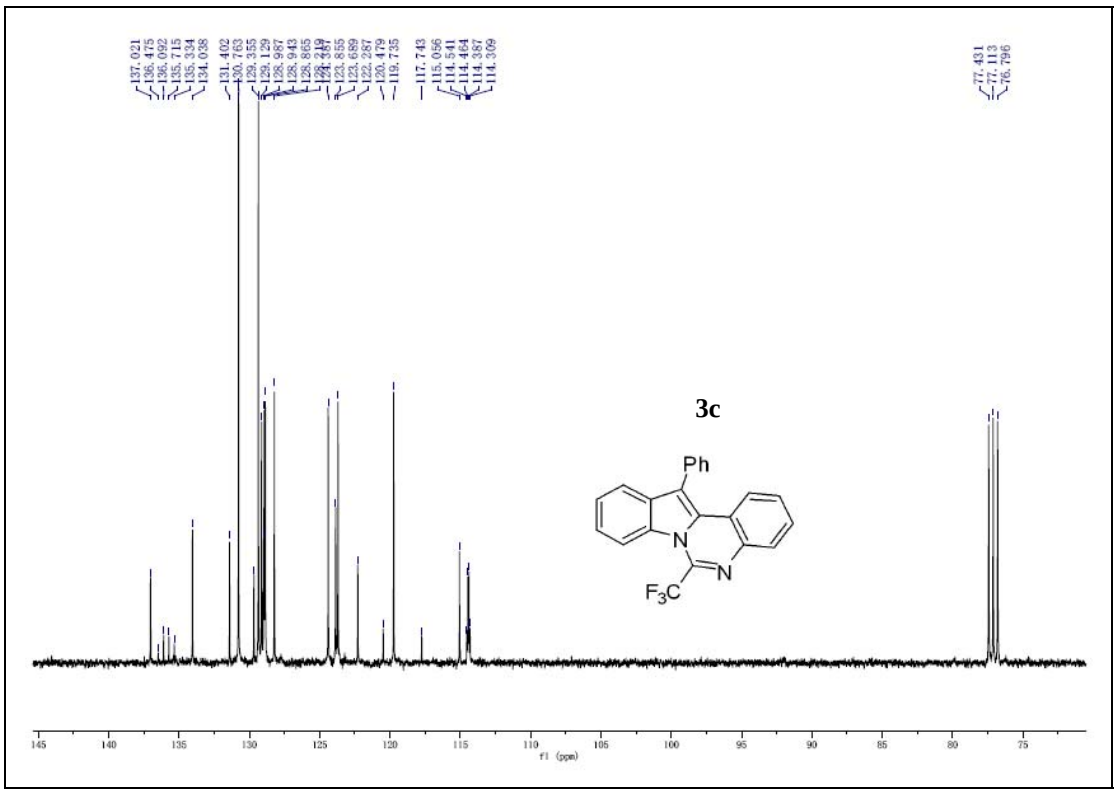
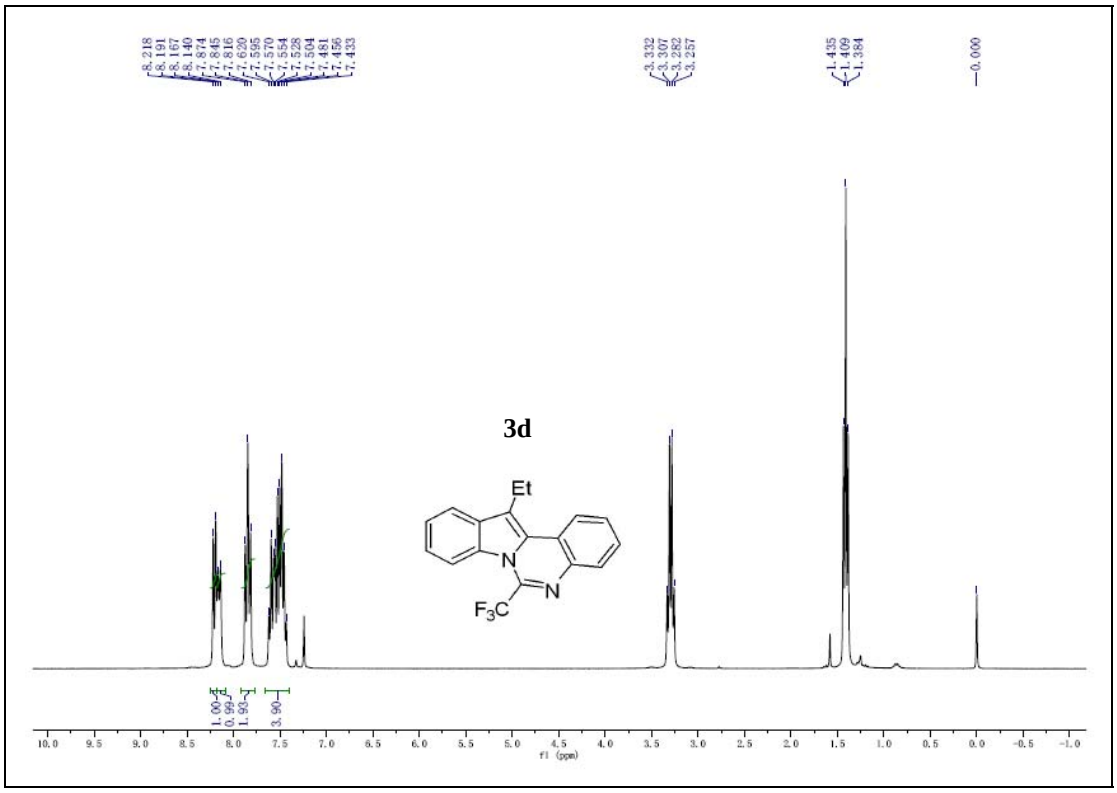
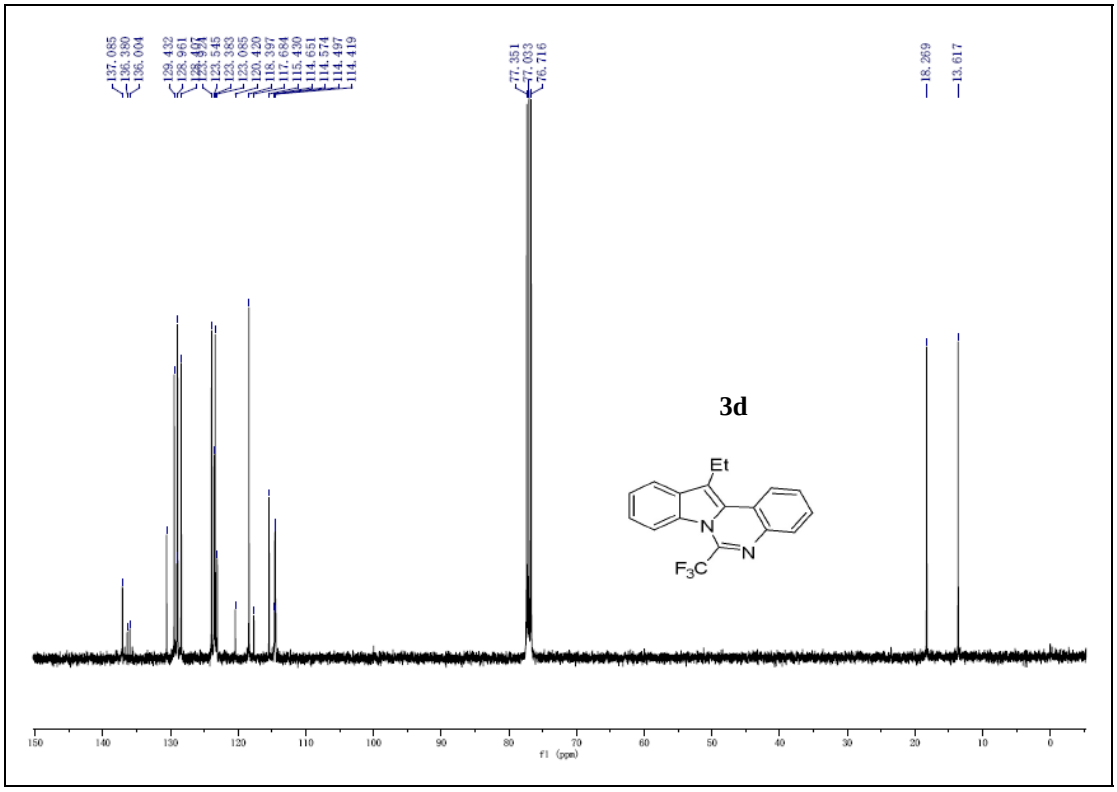
N
N
F3C
1.00
0.92
1.97
2.00
1.99
0.98
f1 (ppm)

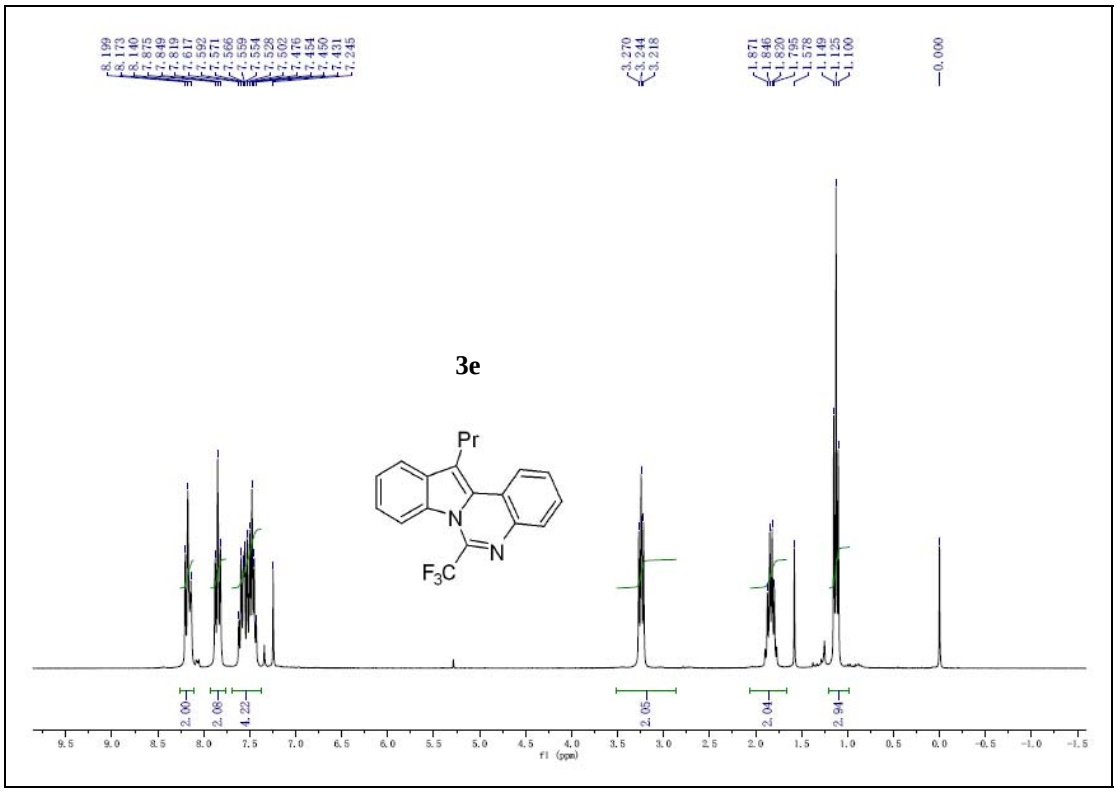

136.258
135.841
135.462
134.892
130.211
130.129
129.590
129.240
128.792
124.318
123.223
122.618
121.724
120.856
120.331
117.597
114.590
114.516
114.442
97.522
77.391
77.073
76.756
3b
N
N
F3C
f1 (ppm)

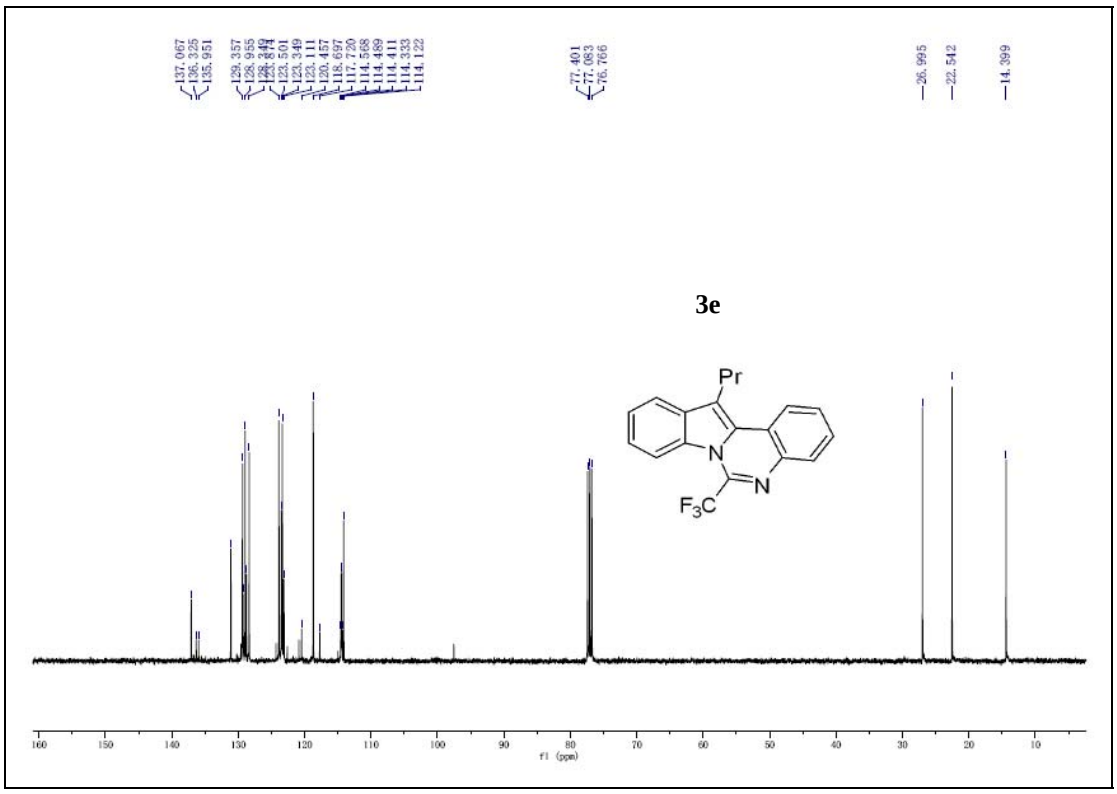

3c
Ph
N
N
F3C

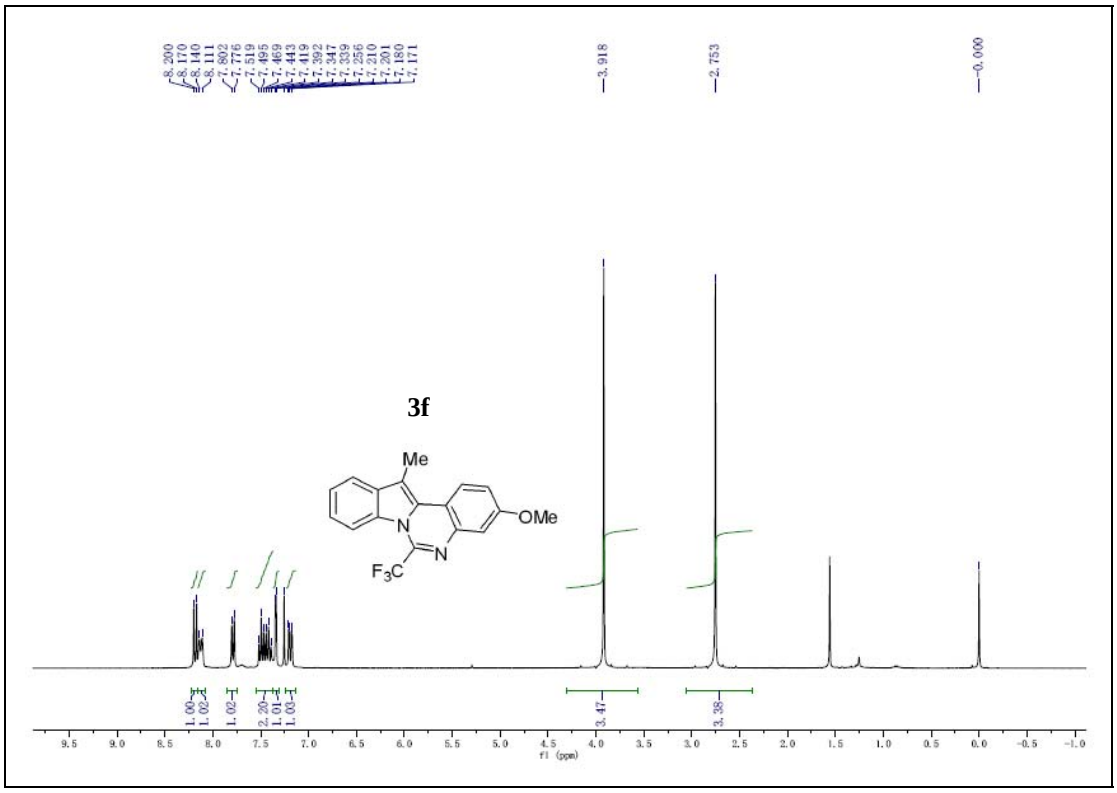

3c
Ph
N
N
F3C

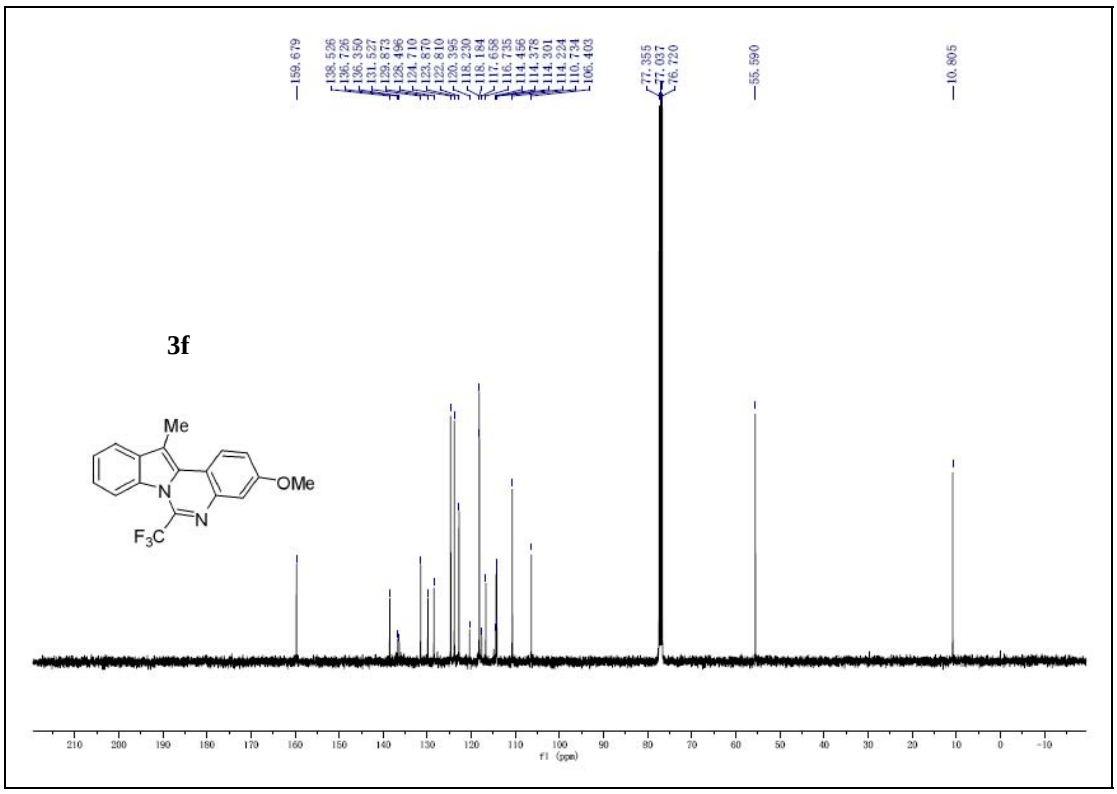

8.218
8.191
8.167
8.140
7.874
7.845
7.816
7.620
7.595
7.570
7.554
7.528
7.504
7.481
7.456
7.433
3.332
3.307
3.282
3.257
1.435
1.409
1.384
0.000
3d
Et
N
N
F3C
1.00
0.99
1.93
3.90
f1 (ppm)

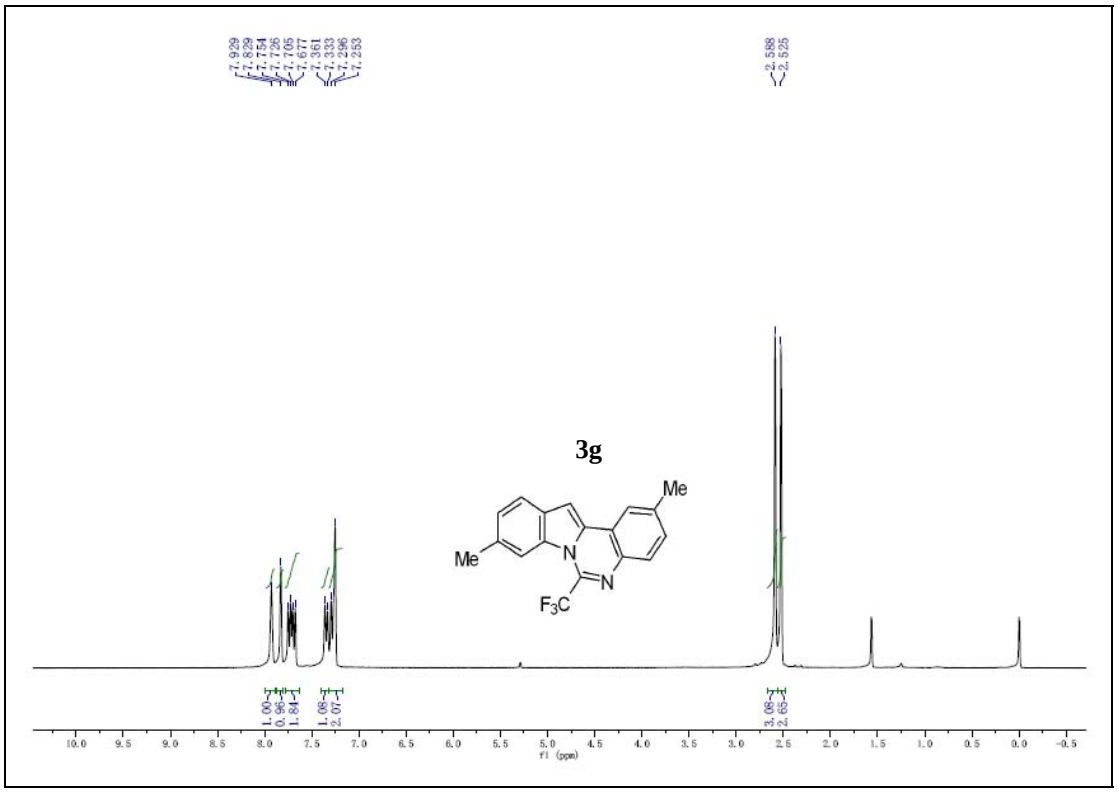

137.085
136.380
136.004
129.432
128.961
128.491
123.945
123.383
123.085
120.420
118.397
117.684
115.430
114.651
114.474
114.497
114.419
77.351
77.033
76.716
18.269
13.617
3d
Et
N
N
F3C
f1 (ppm)

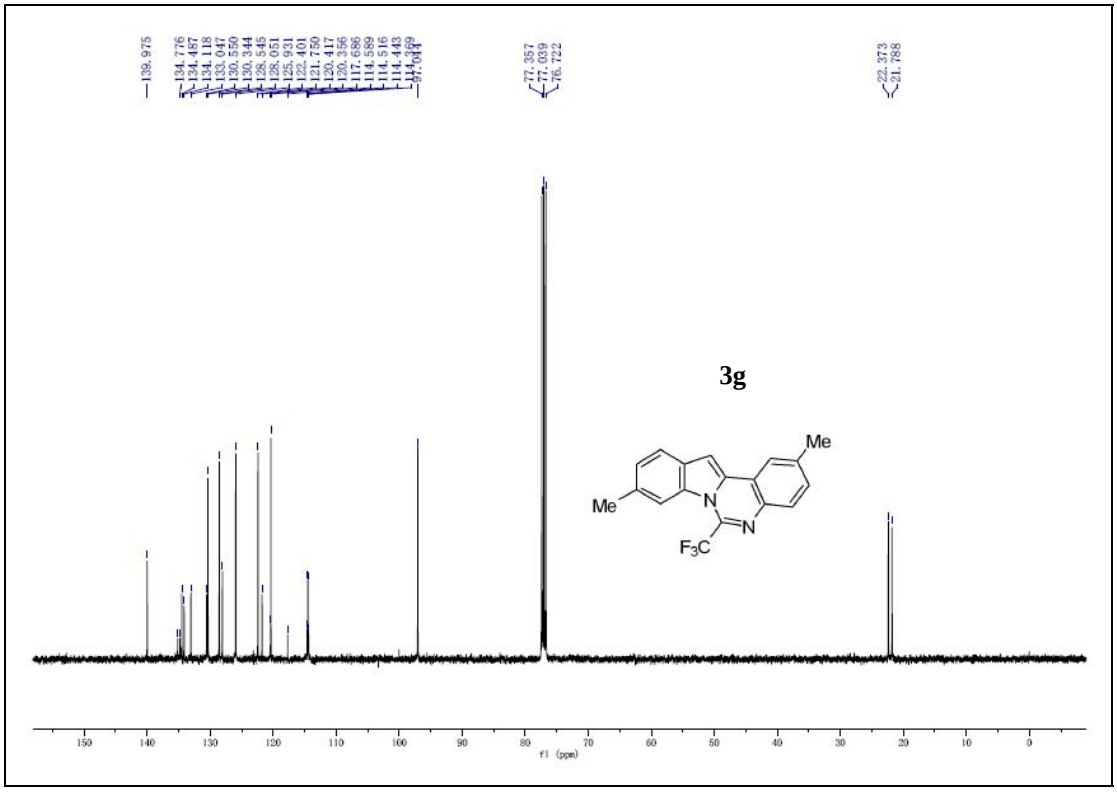

3e
Pr
N
N
F3C
f1 (ppm)

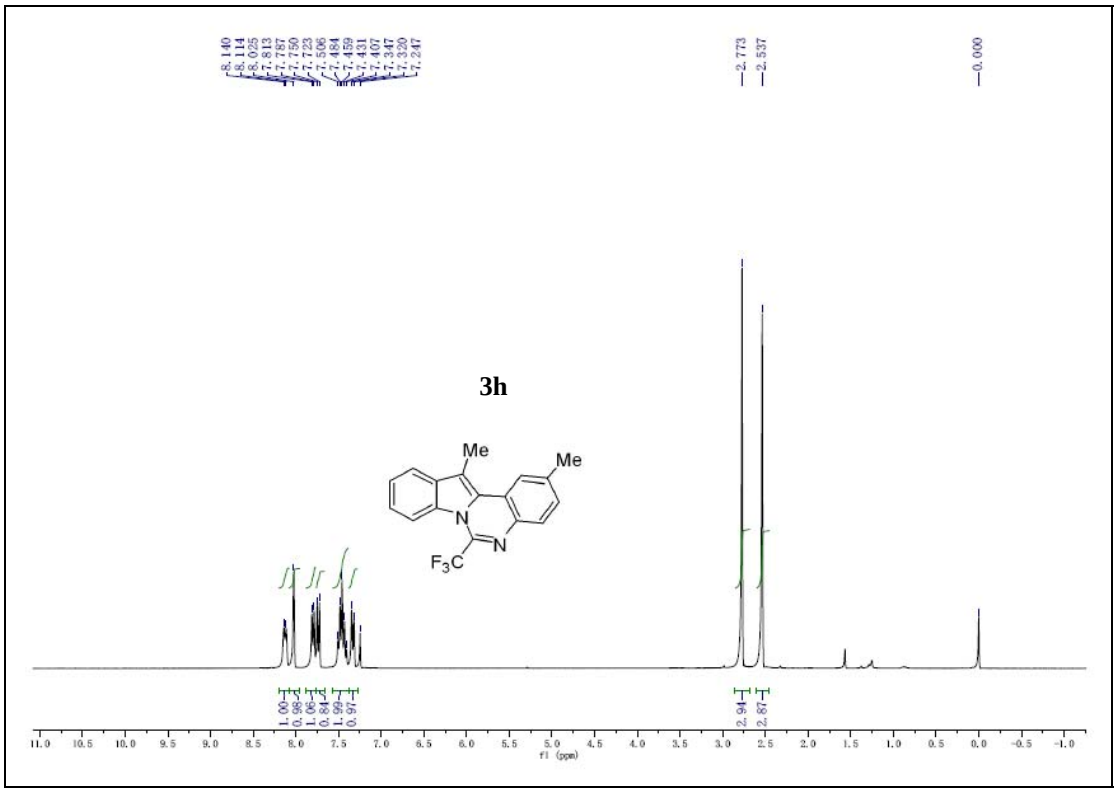

3e
Pr
N
N
F3C
f1 (ppm)

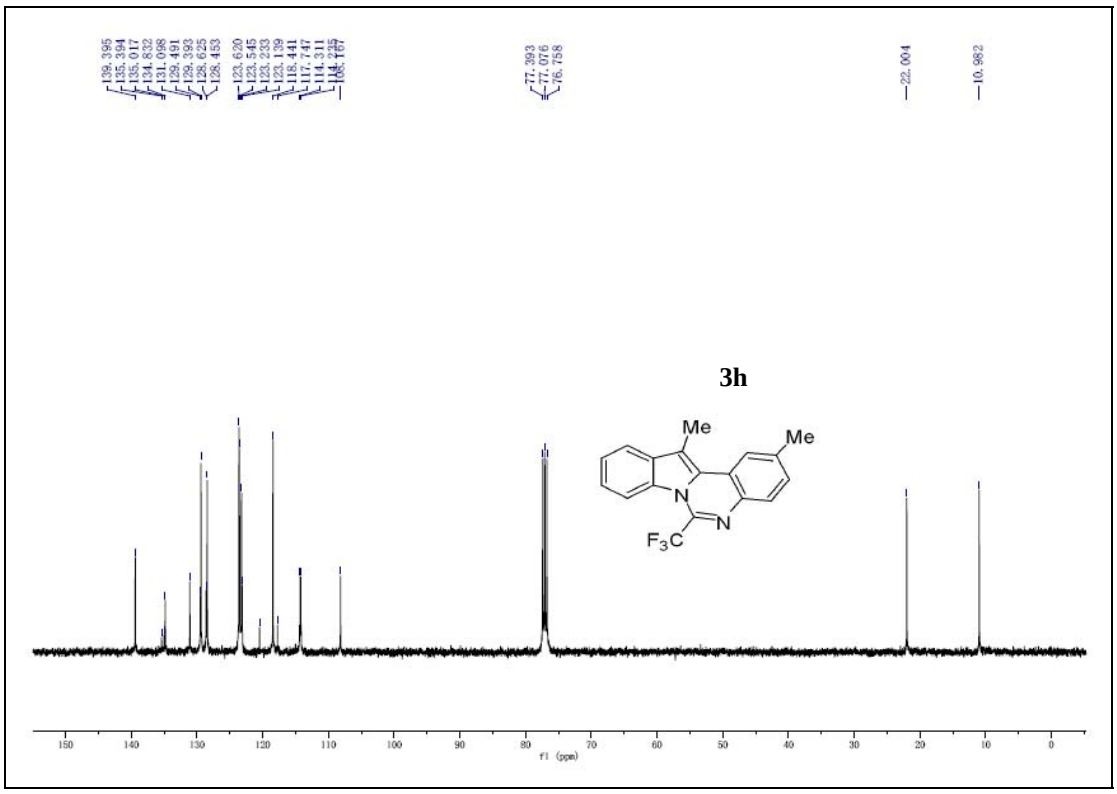

3f
Me
OMe
N
N
F3C
f1 (ppm)

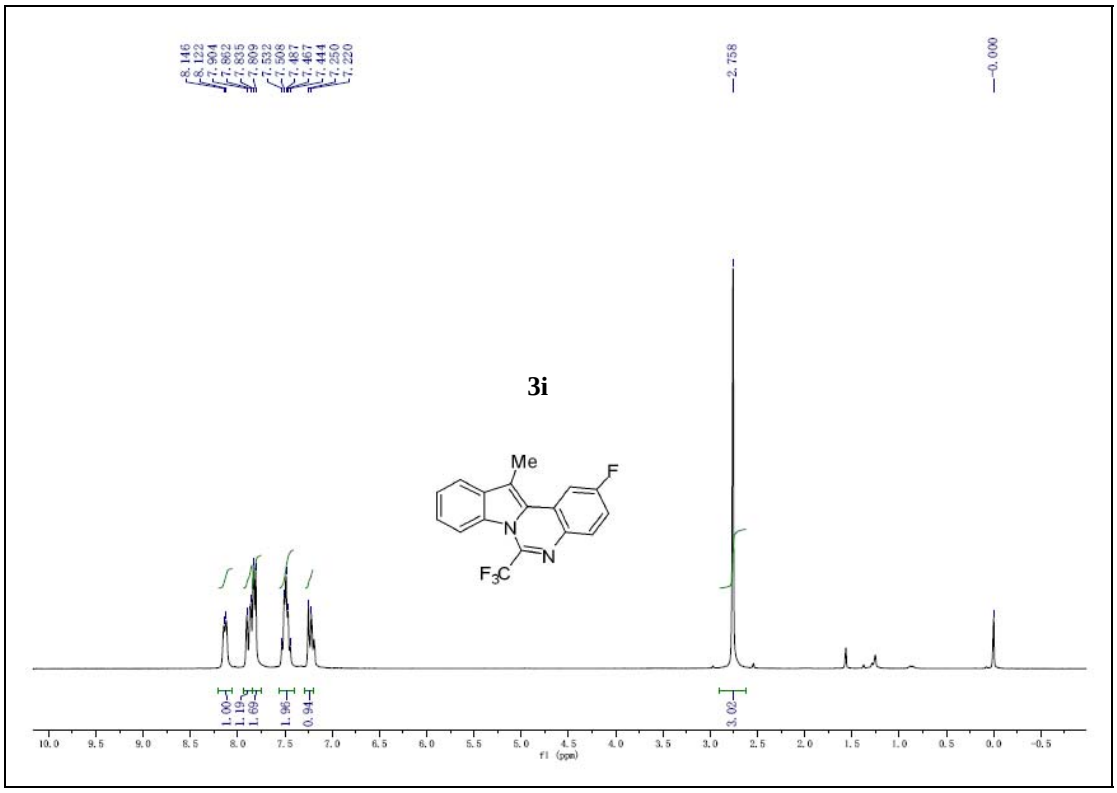

3f
Me
OMe
N
N
F3C
f1 (ppm)

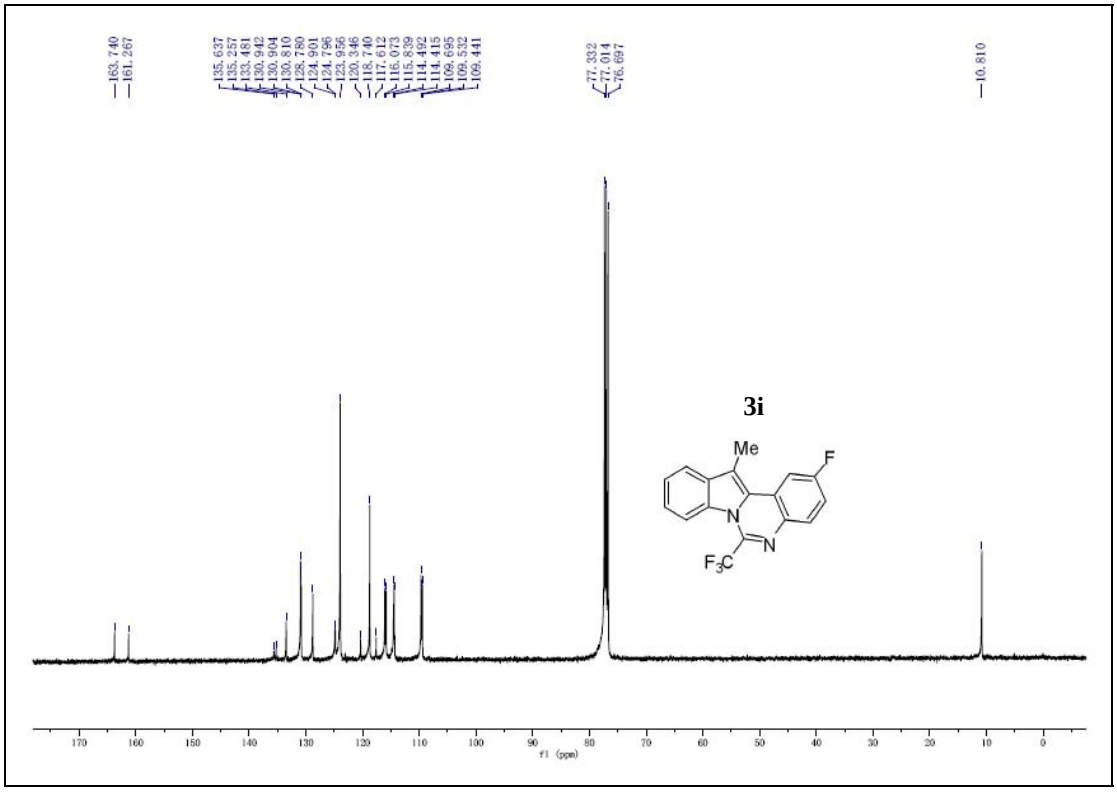

7.929
7.829
7.754
7.726
7.705
7.677
7.361
7.333
7.296
7.253
2.588
2.525
3g
Me
Me
N
N
F3C
1.00
0.96
1.84
1.06
2.07
3.06
2.65
f1 (ppm)

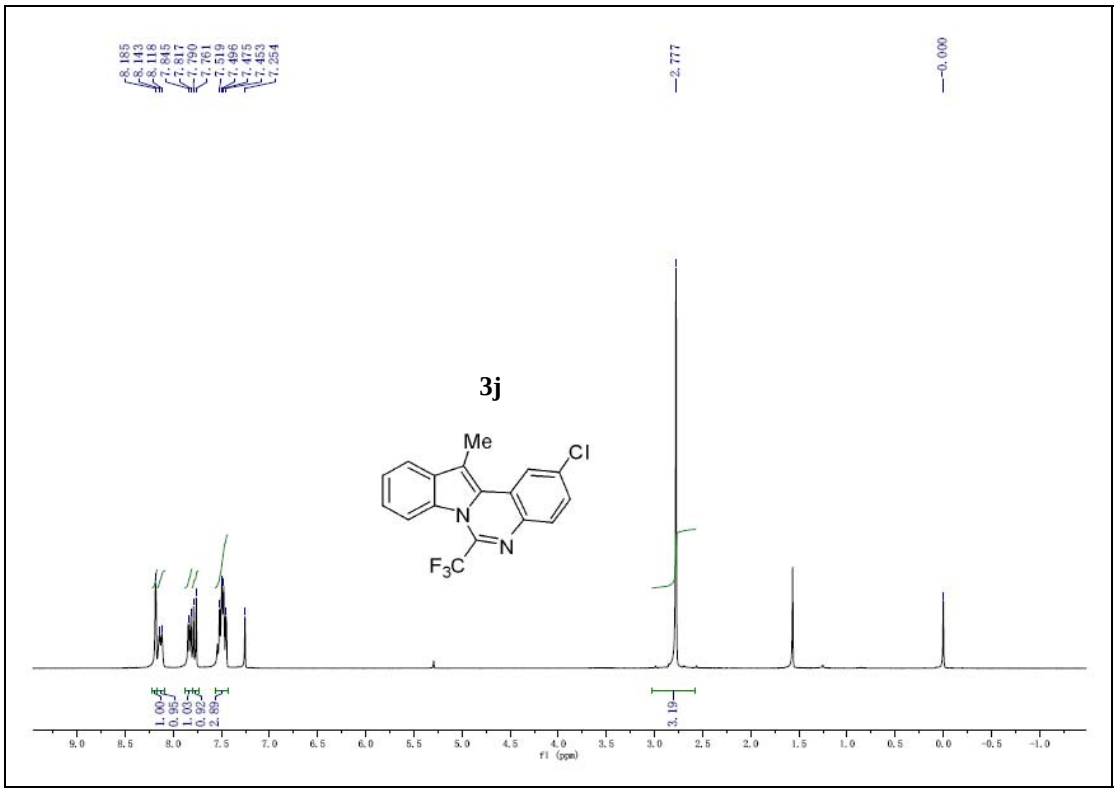

139.975
134.776
134.487
134.118
133.047
130.550
130.344
128.545
128.051
125.931
122.401
121.750
120.417
120.356
117.686
114.589
114.516
114.443
77.357
77.039
76.722
22.373
21.788
3g
Me
Me
N
N
F3C
f1 (ppm)

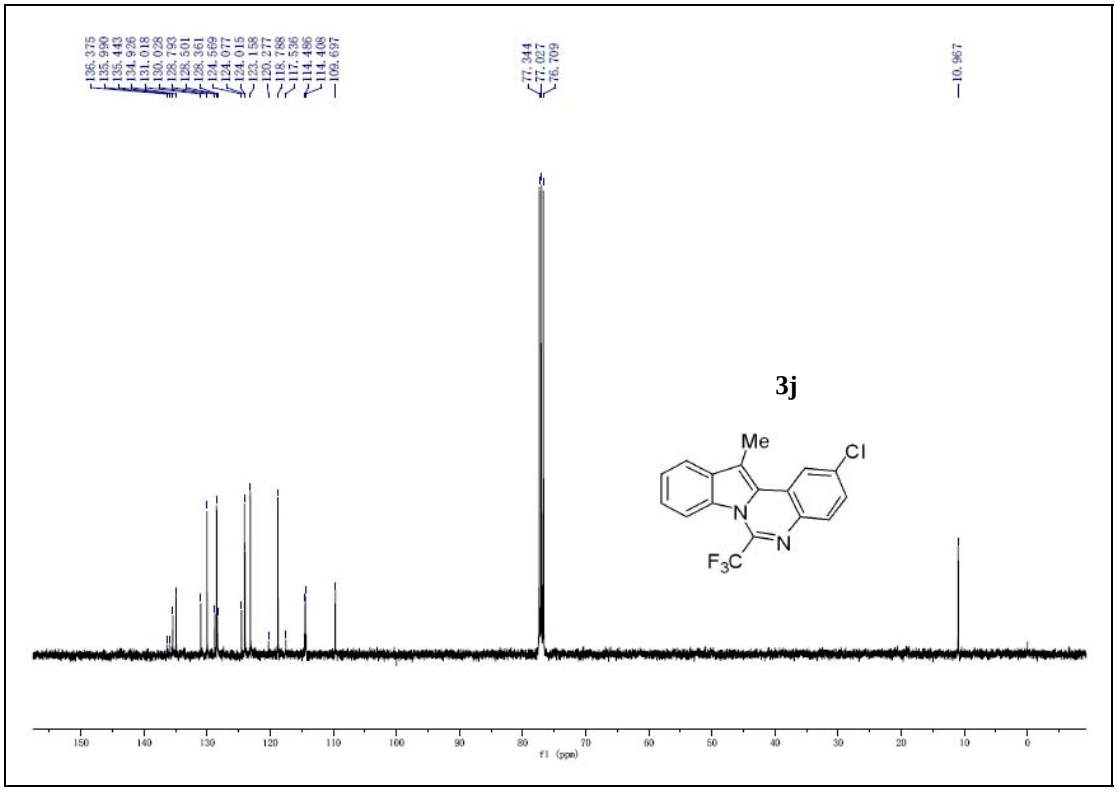

3h
Me
Me
N
N
F3C
f1 (ppm)

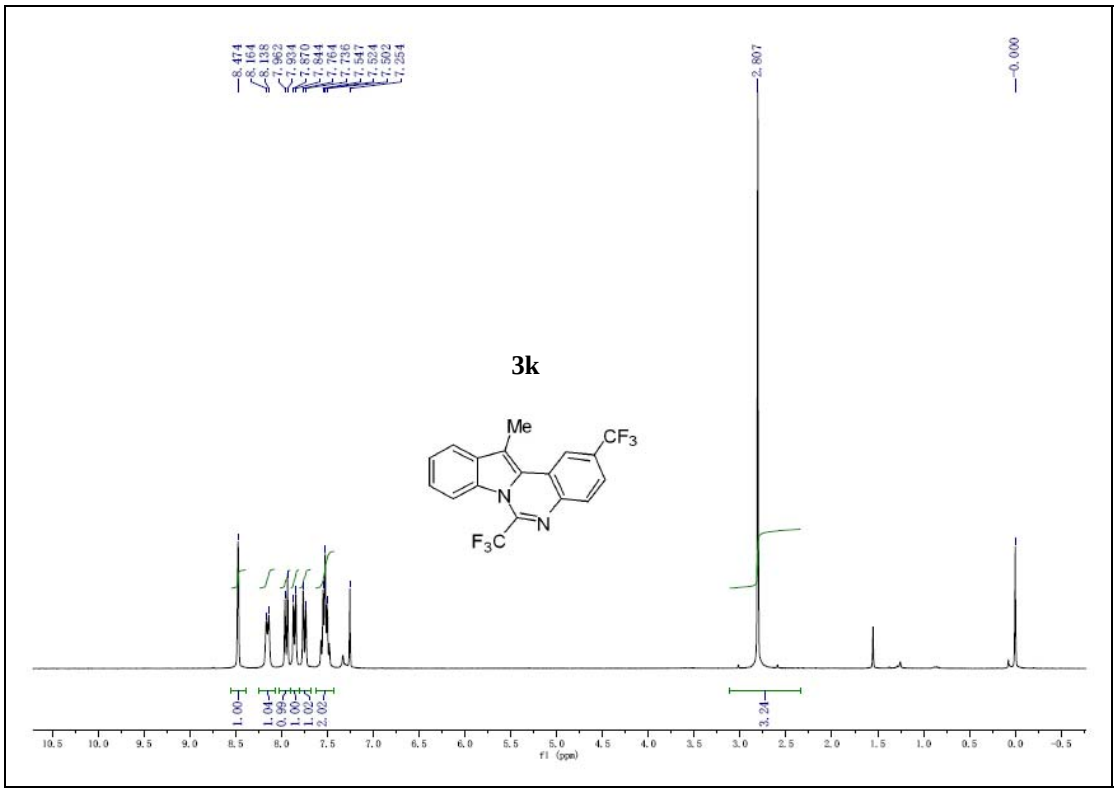

3h
Me
Me
N
N
F3C
f1 (ppm)

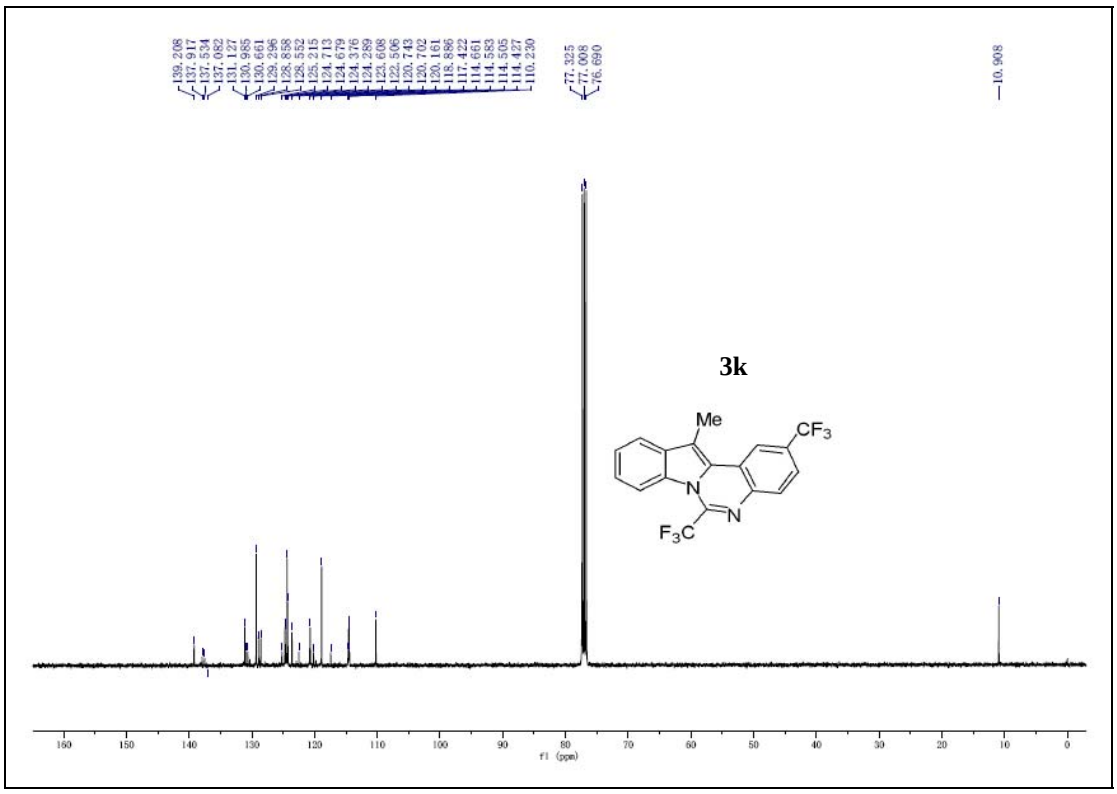

8.146
8.122
7.904
7.882
7.865
7.593
7.508
7.487
7.467
7.444
7.250
7.220
2.758
0.000
3i
Me
F
N
N
F3C
1.00
1.19
1.69
1.96
0.94
3.02
f1 (ppm)

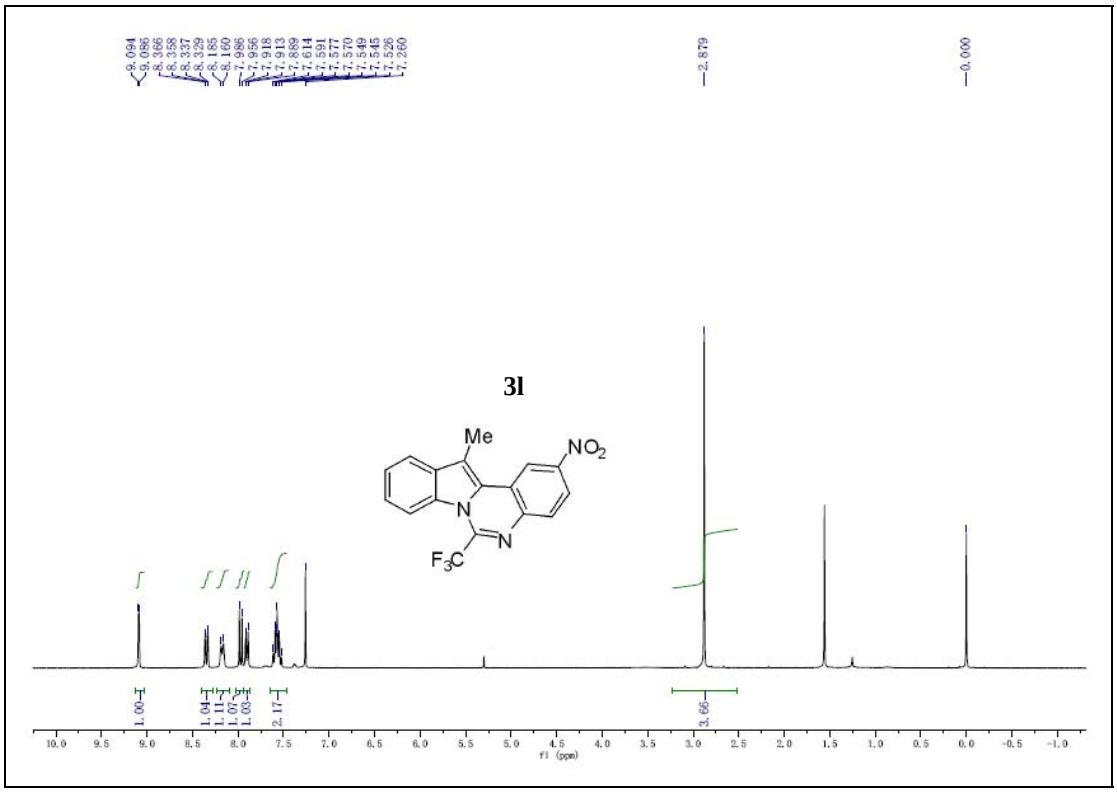

163.740
161.267
135.637
135.257
133.481
130.942
130.904
130.810
128.780
124.901
124.796
123.956
120.346
118.740
117.612
115.973
115.639
114.492
114.415
106.695
106.532
106.441
77.332
77.014
76.697
10.810
3i
Me
F
N
N
F3C
f1 (ppm)

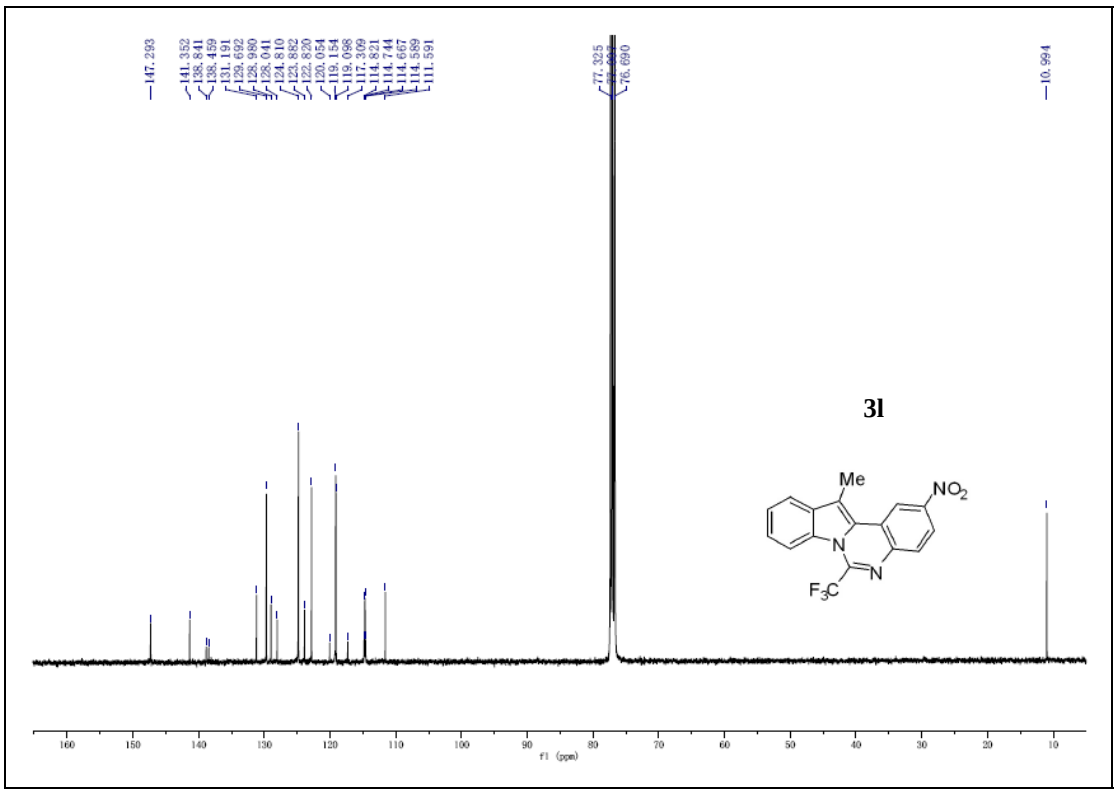

8.185
8.143
8.118
7.845
7.817
7.790
7.761
7.519
7.496
7.475
7.453
7.254
2.777
0.000
3j
Me
Cl
N
N
F3C
1.00
0.95
1.03
0.92
2.89
3.19
f1 (ppm)

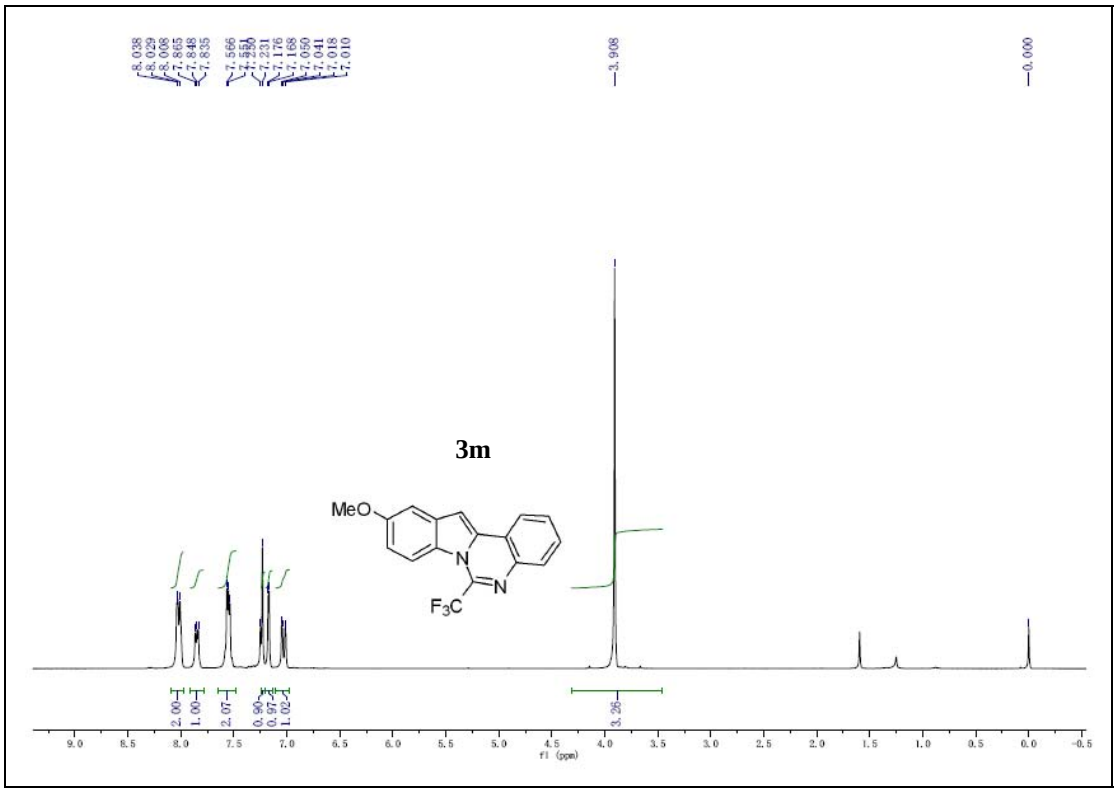

136.375
135.990
135.443
134.926
131.018
130.028
128.793
128.501
128.361
124.869
124.477
124.015
123.158
120.377
118.788
117.536
114.486
114.408
109.697
77.344
77.027
76.709
10.967
3j
Me
Cl
N
N
F3C
f1 (ppm)

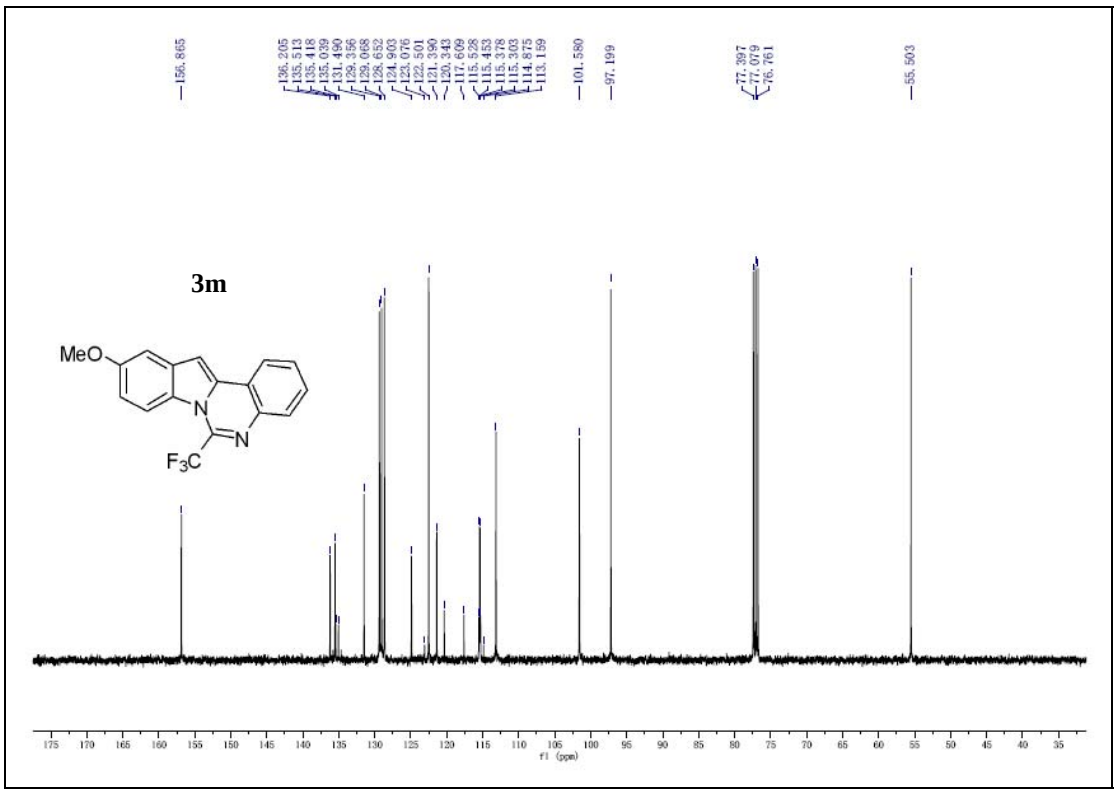

8.474
8.164
8.138
7.962
7.934
7.870
7.844
7.764
7.736
7.547
7.524
7.502
7.254
2.807
-0.000
3k
Me
CF3
N
N
F3C
1.00
1.04
0.98
1.02
2.02
3.24
f1 (ppm)

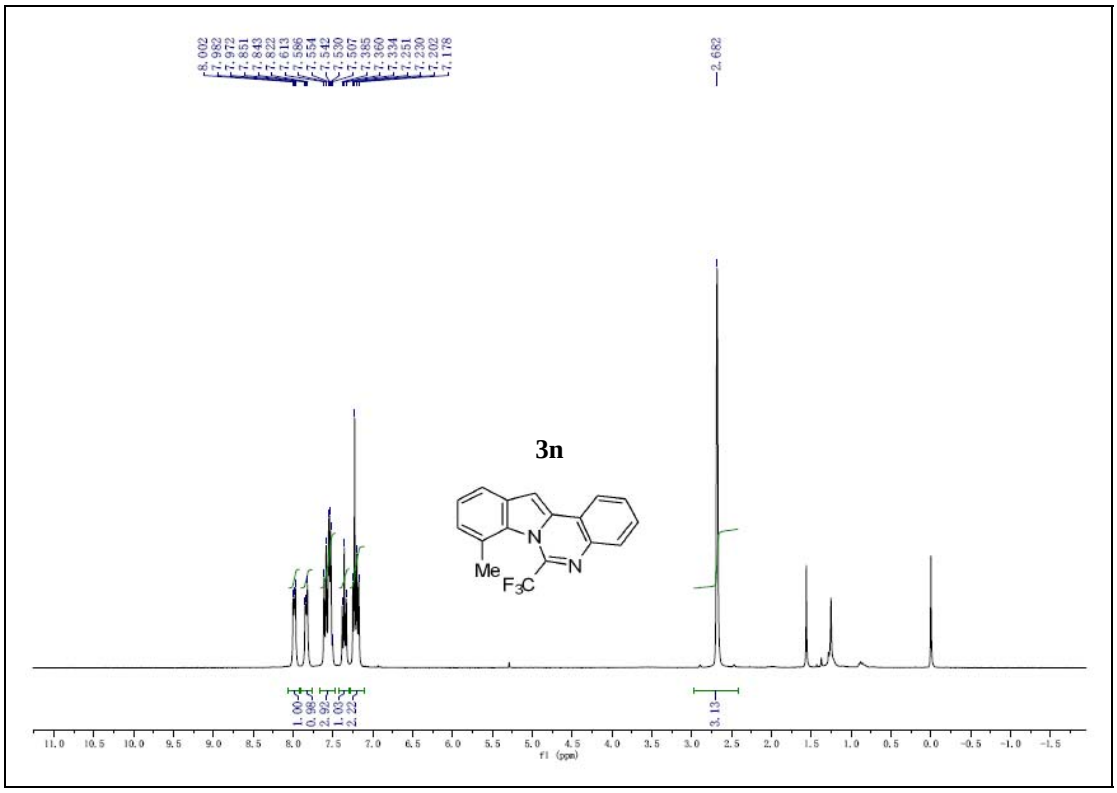

139.208
137.917
137.534
137.082
131.127
130.985
130.661
129.296
128.858
128.552
125.215
124.713
124.679
124.376
124.289
123.608
122.596
120.743
120.702
120.161
118.886
117.422
114.661
114.583
114.505
114.427
110.230
77.325
77.008
76.690
10.908
3k
Me
CF3
N
N
F3C
f1 (ppm)

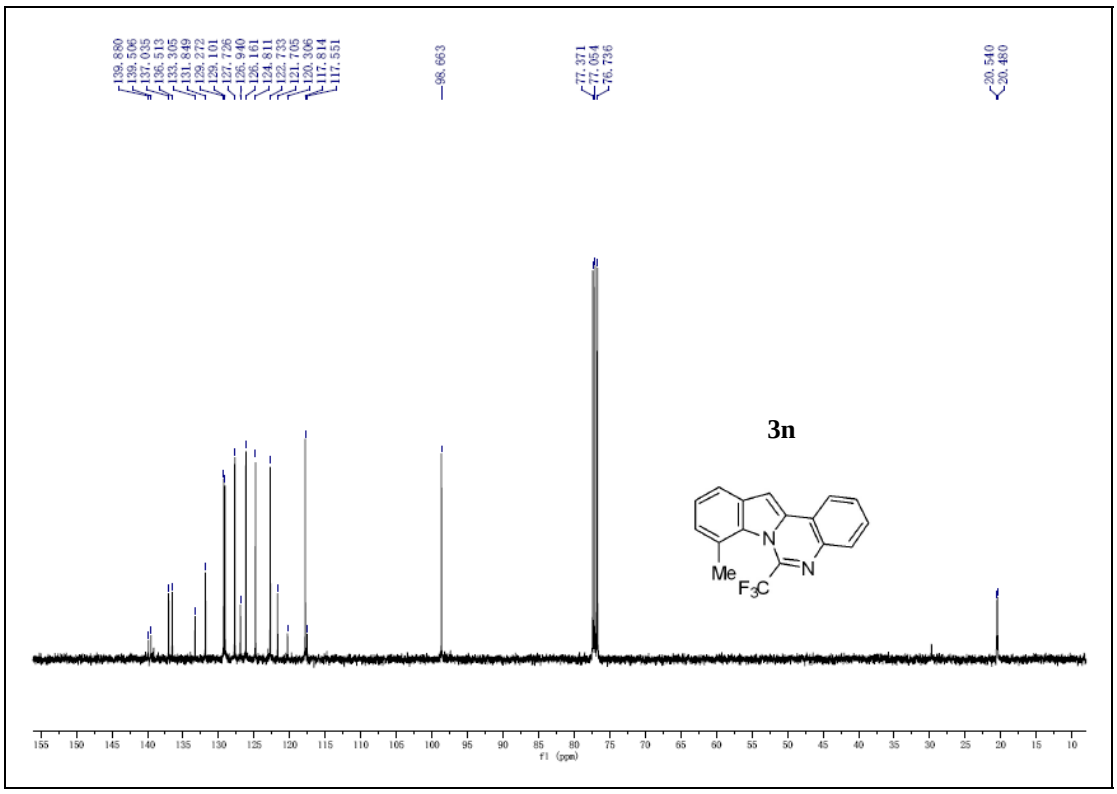

3l
Me
NO2
N
N
F3C
9.094
9.086
8.366
8.358
8.337
8.329
8.165
8.160
7.966
7.956
7.918
7.913
7.889
7.614
7.591
7.577
7.570
7.549
7.545
7.526
7.260
2.879
0.000
1.00
1.04
1.11
1.07
1.03
2.17
3.66
f1 (ppm)

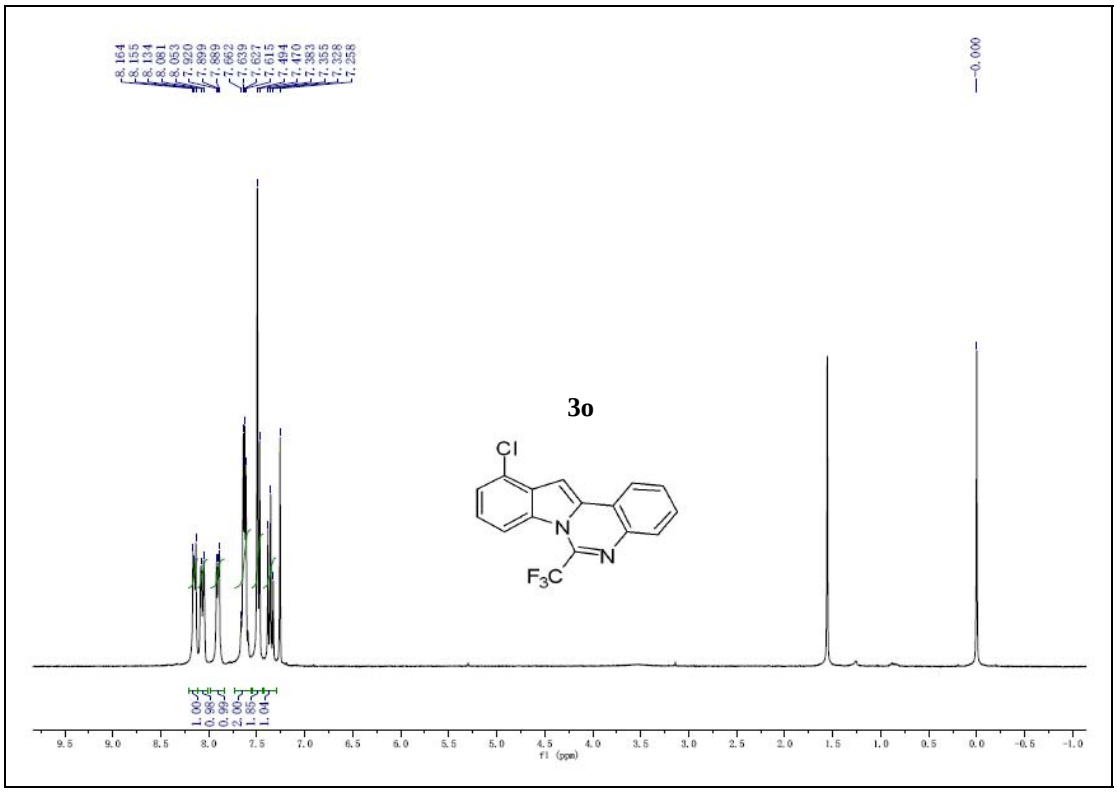

3l
Me
NO2
N
N
F3C
147.293
141.352
138.441
138.199
131.191
129.692
128.990
128.041
124.810
123.882
122.820
120.054
119.154
119.096
117.309
114.821
114.744
114.667
114.589
111.591
77.325
76.690
10.994
f1 (ppm)


3m
MeO
N
N
F3C
f1 (ppm)


3m
MeO
N
N
F3C
f1 (ppm)


3n
Me
F3C
N
N


3n
Me
F3C
N
N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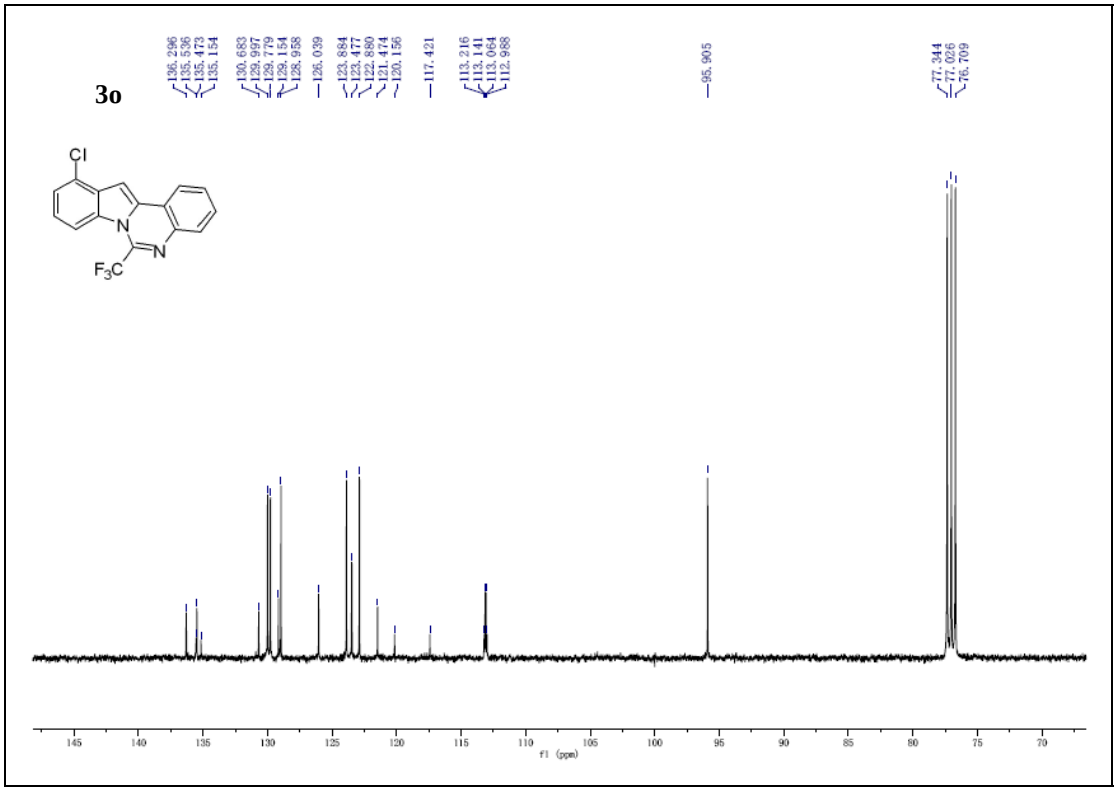
8.155
8.134
8.081
8.053
7.920
7.899
7.889
7.662
7.639
7.627
7.615
7.494
7.470
7.383
7.355
7.328
7.258
-0.000
3o
Cl
N
N
F3C
1.00
0.98
0.99
2.00
1.85
1.04
f1 (ppm)


3o
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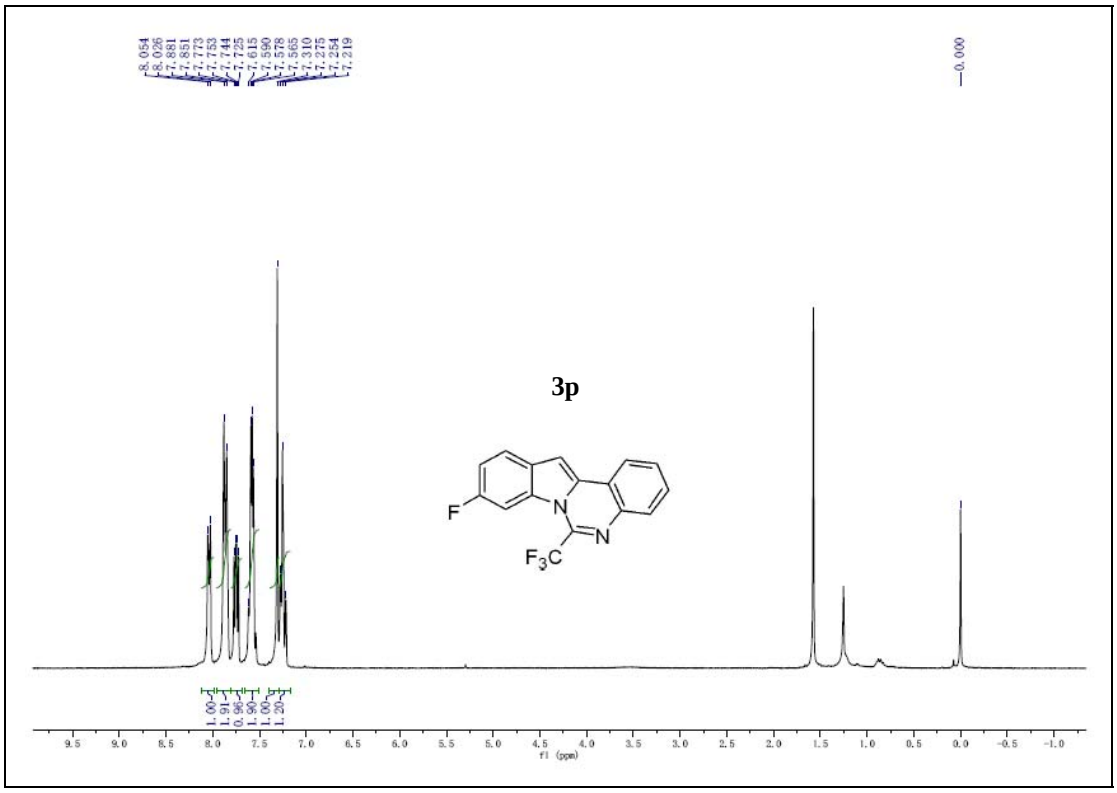
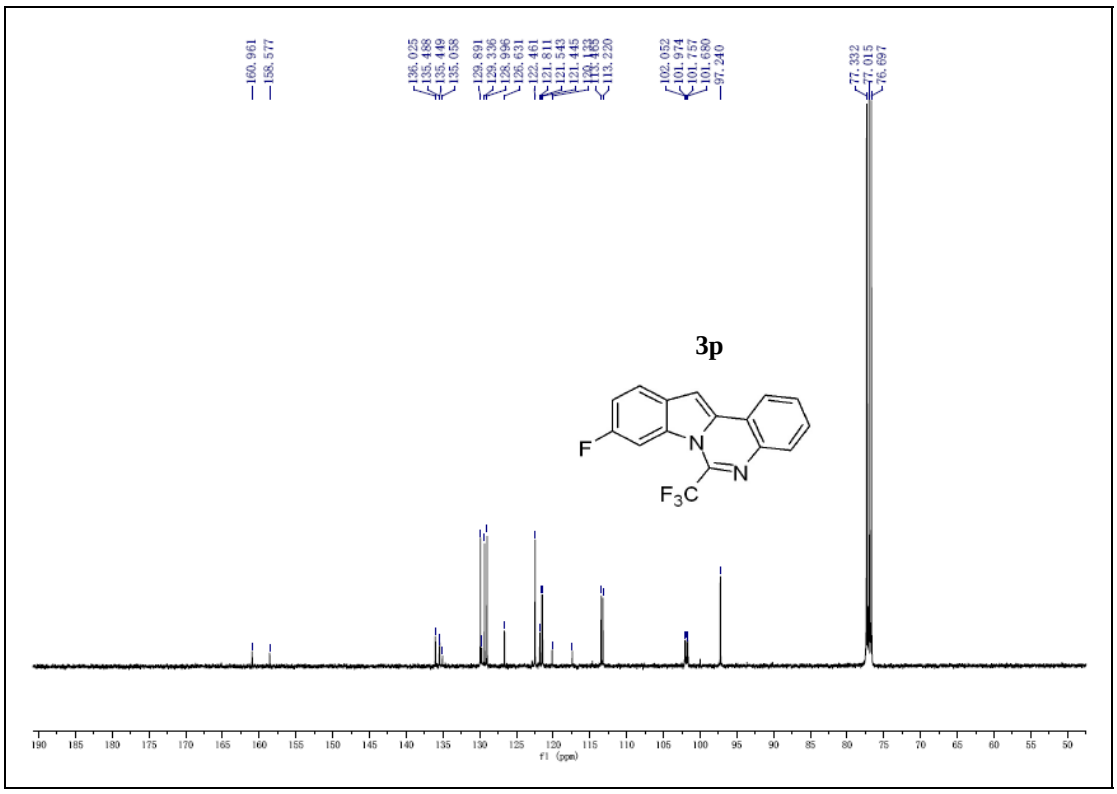
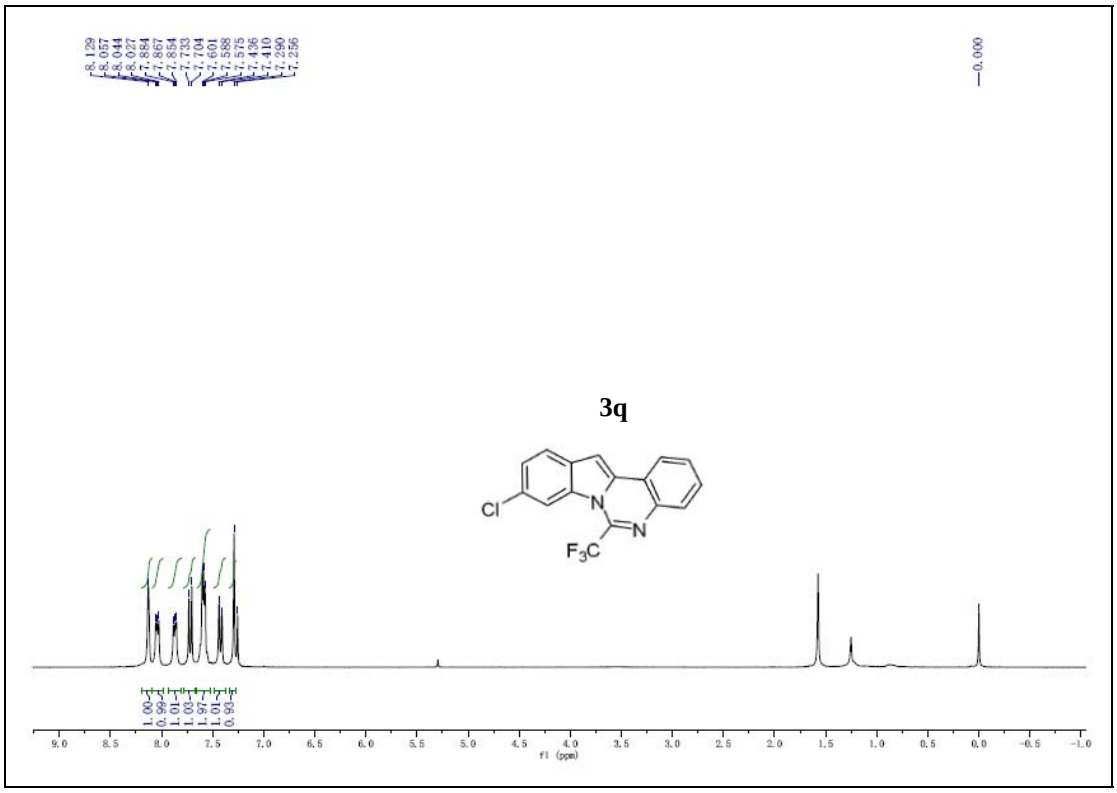
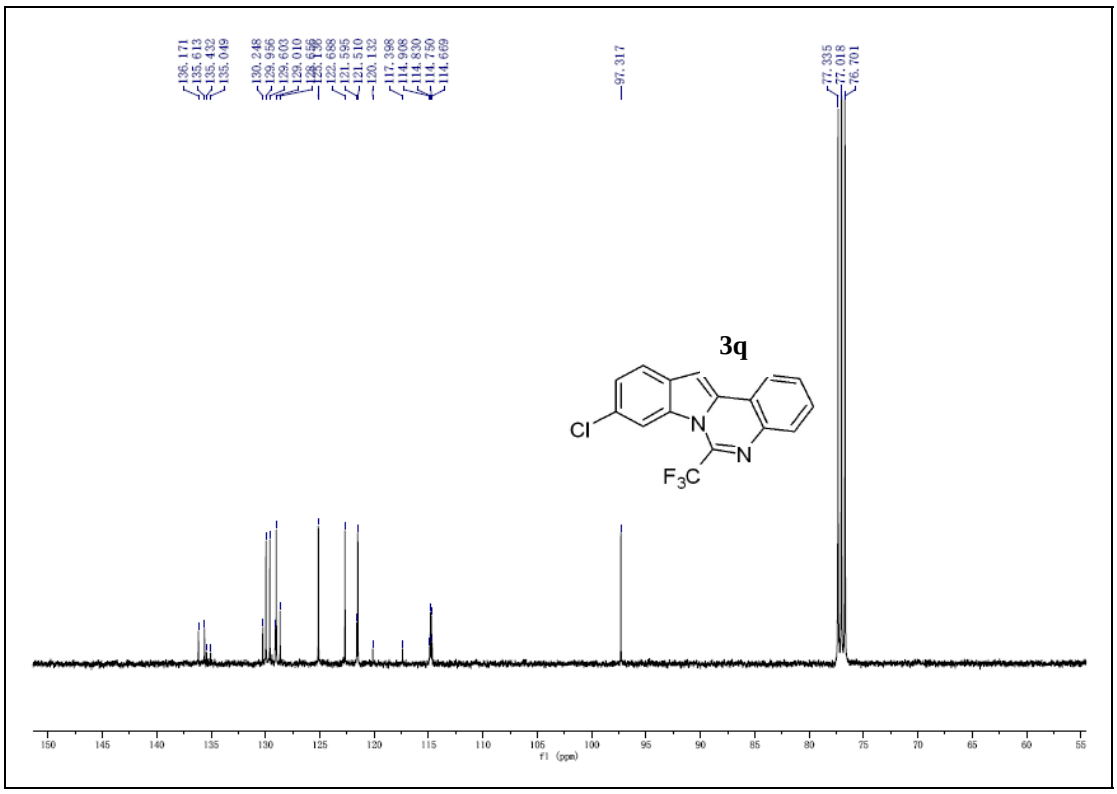
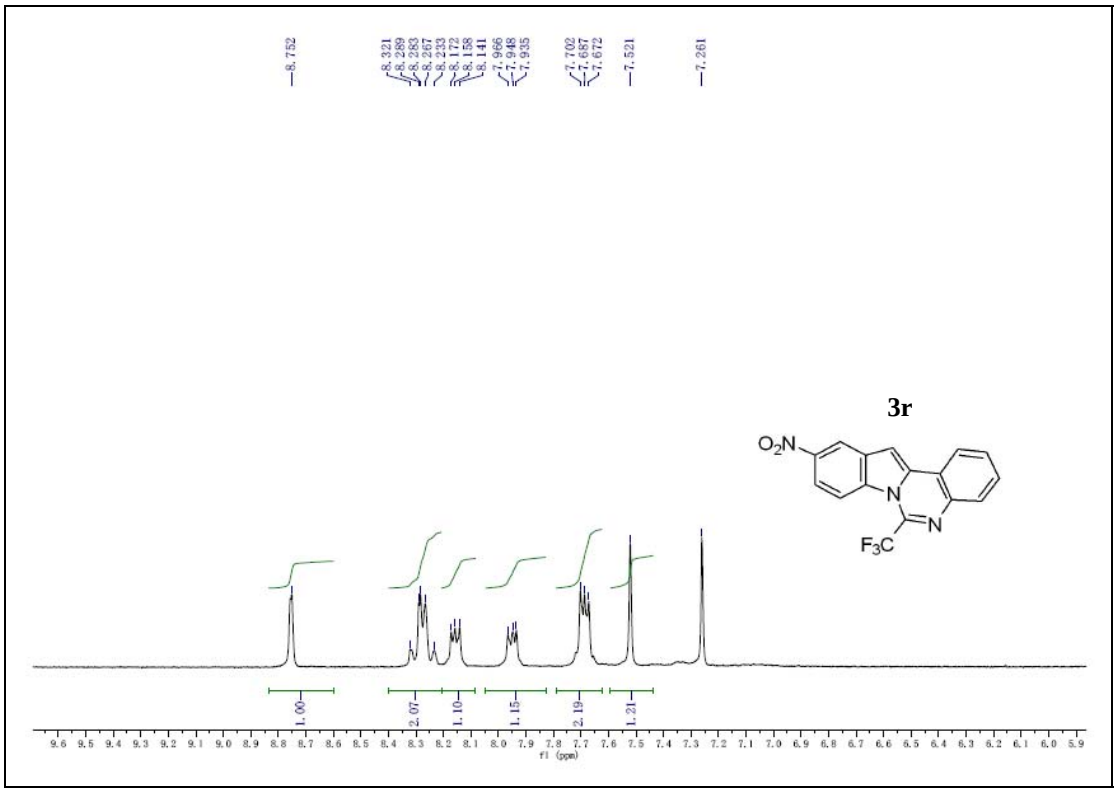
135.473
135.154
130.683
129.997
129.179
129.154
128.958
126.039
123.884
123.477
122.880
121.474
120.156
117.421
113.216
113.141
113.064
112.988
95.905
77.344
77.026
76.709
Cl
N
N
F3C
f1 (ppm)


3p
F
N
N
F3C
f1 (ppm)


3p
F
N
N
F3C
f1 (ppm)


3q
Cl
N
N
F3C
f1 (ppm)


3q
Cl
N
N
F3C
f1 (ppm)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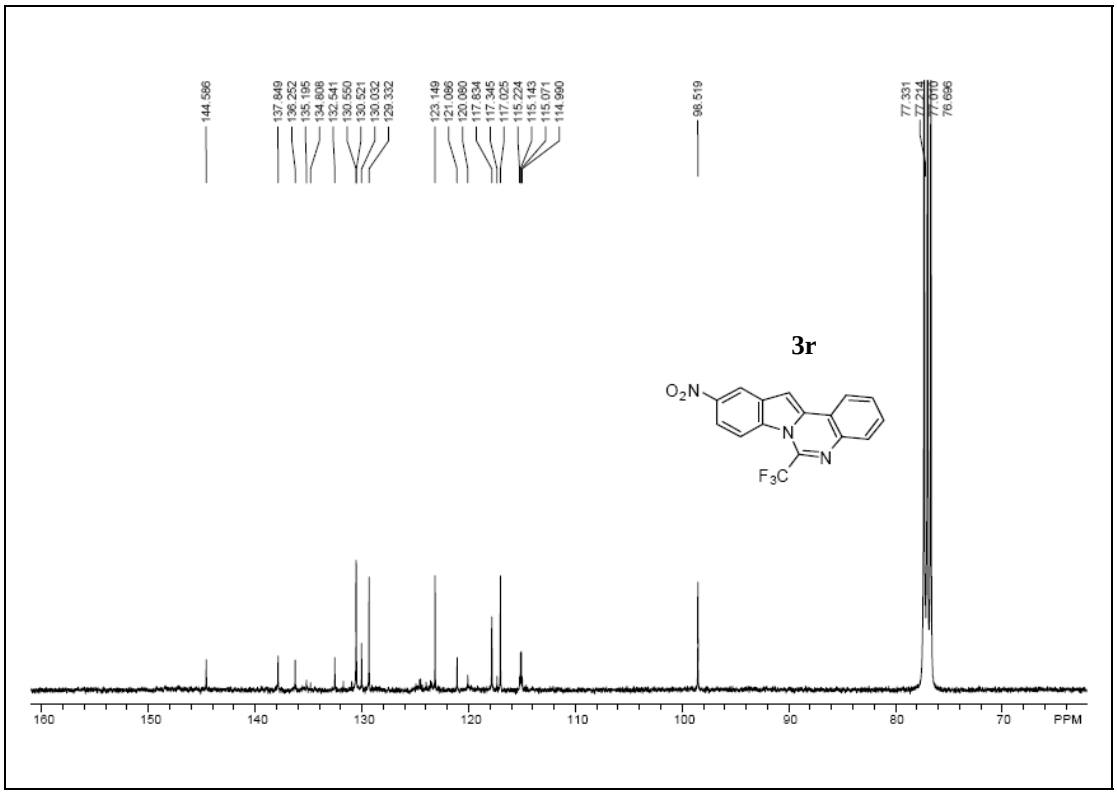
8.289
8.283
8.267
8.233
8.172
8.158
8.141
7.966
7.948
7.935
7.702
7.687
7.672
7.521
7.261
3r
O_2N
N
N
F_3C
1.00
2.07
1.10
1.15
2.19
1.21
f1 (ppm)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135.195
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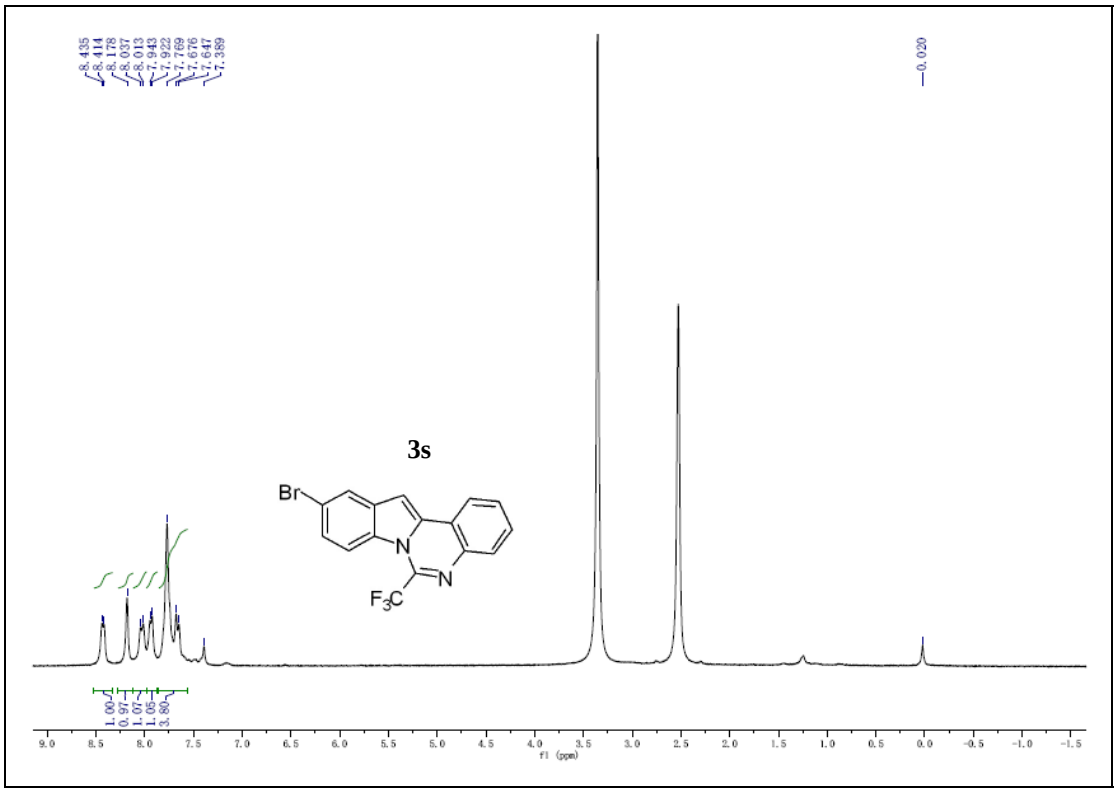
132.541
130.550
130.521
130.032
129.332
123.149
121.096
120.080
117.834
117.345
117.025
115.224
115.143
115.071
114.990
98.519
77.331
77.214
77.010
76.696
3r
O_2N
N
N
F_3C
160
150
140
130
120
110
100
90
80
70
PPM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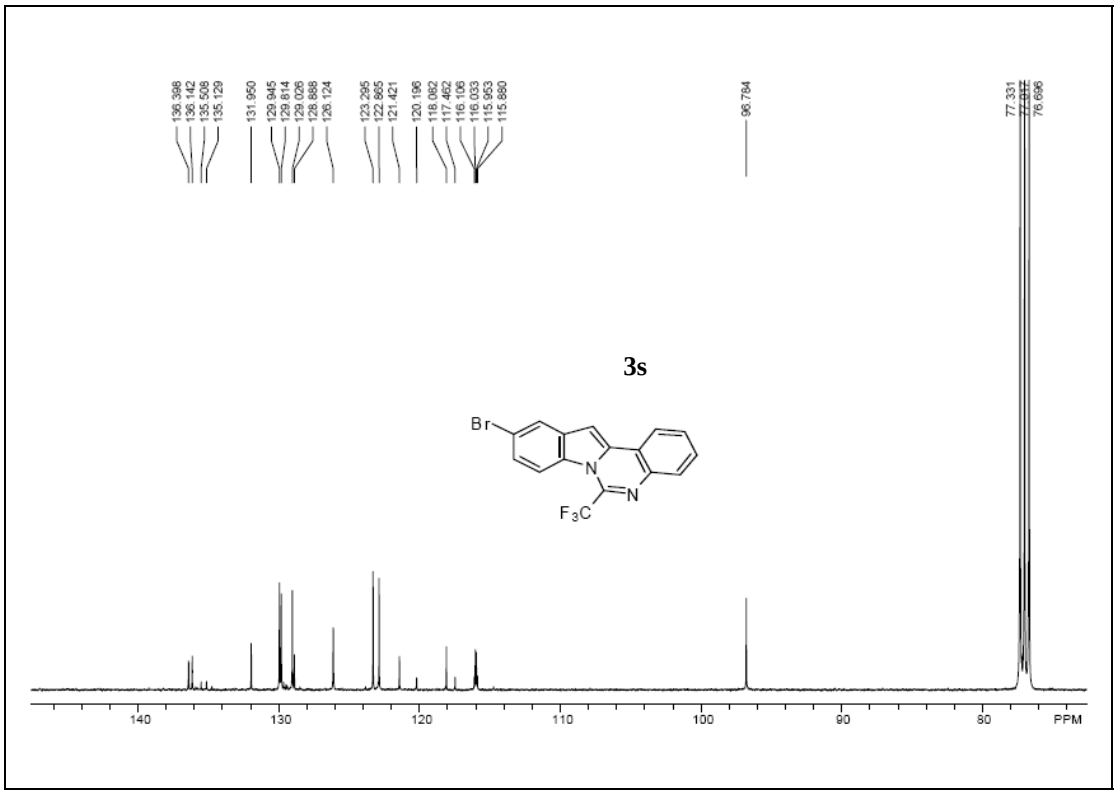
8.414
8.178
8.057
8.013
7.943
7.922
7.769
7.676
7.647
7.389
0.020
3s
Br
N
N
F3C
1.00
0.97
1.07
1.05
3.80
f1 (ppm)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129.945
129.614
129.026
128.888
126.124
123.295
122.865
121.421
120.196
118.082
117.462
116.106
116.033
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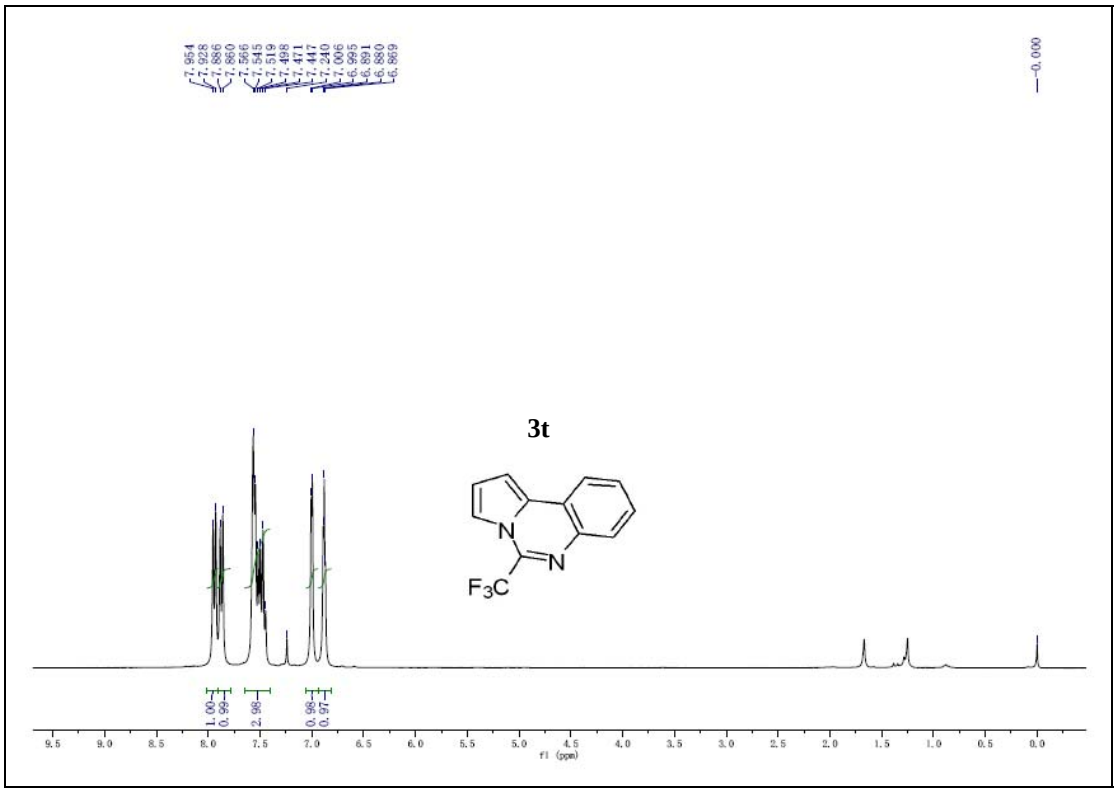
115.880
96.784
77.331
77.012
76.696
3s
Br
N
N
F3C
PPM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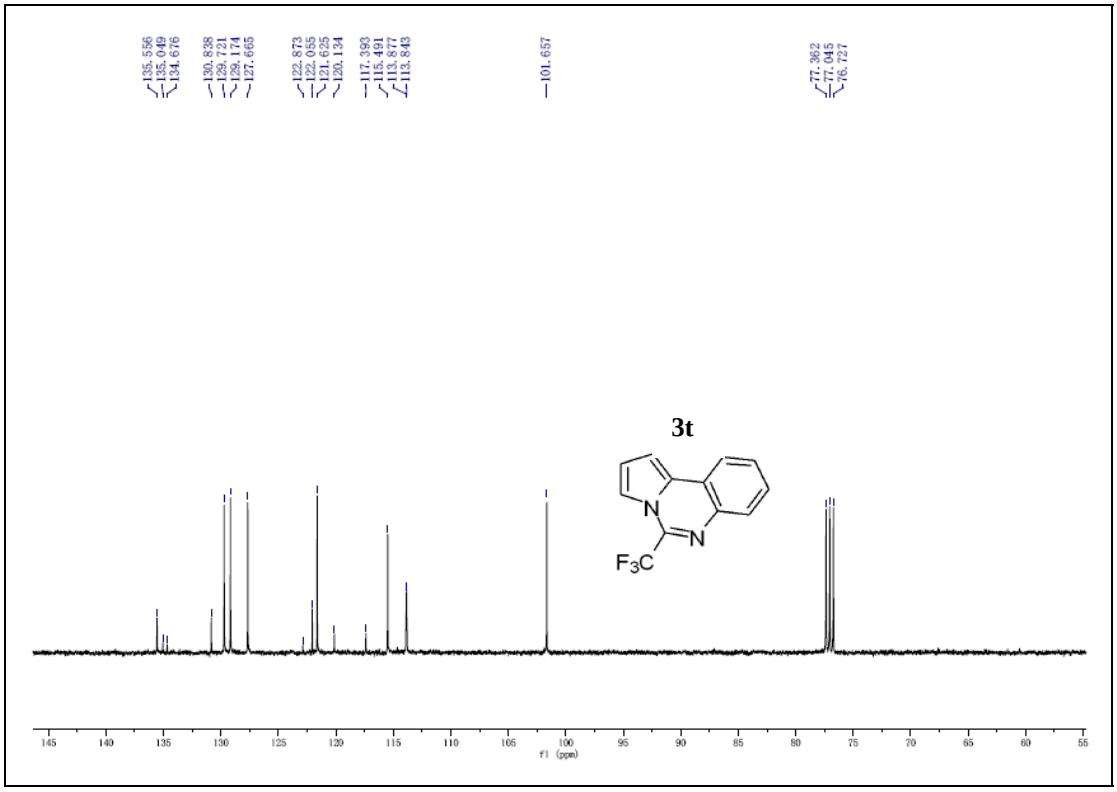
7.545
7.519
7.498
7.471
7.447
7.240
7.006
6.995
6.891
6.880
6.869
0.000
3t
N
N
F3C
1.00
0.98
2.98
0.96
0.97
f1 (ppm)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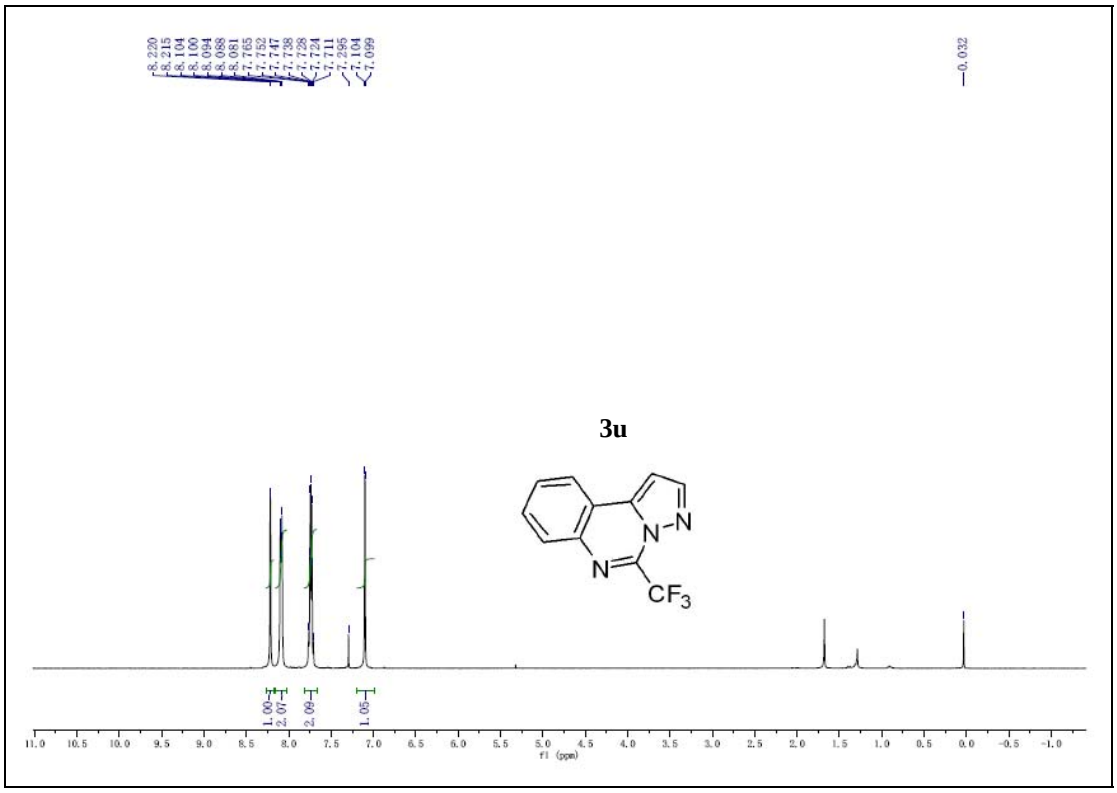
134.676
130.838
129.721
129.174
127.665
122.673
122.055
121.625
120.134
117.393
115.491
113.877
113.843
101.657
77.362
77.045
76.727
3t
N
N
F3C
f1 (ppm)


3u
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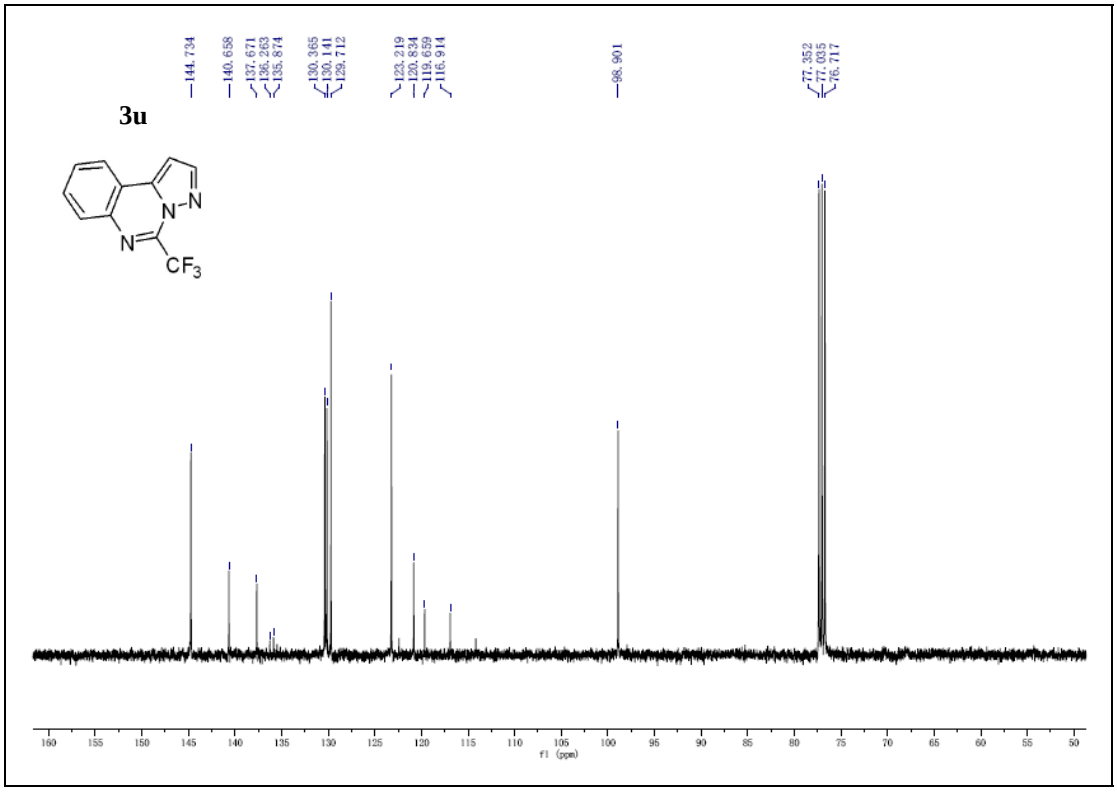
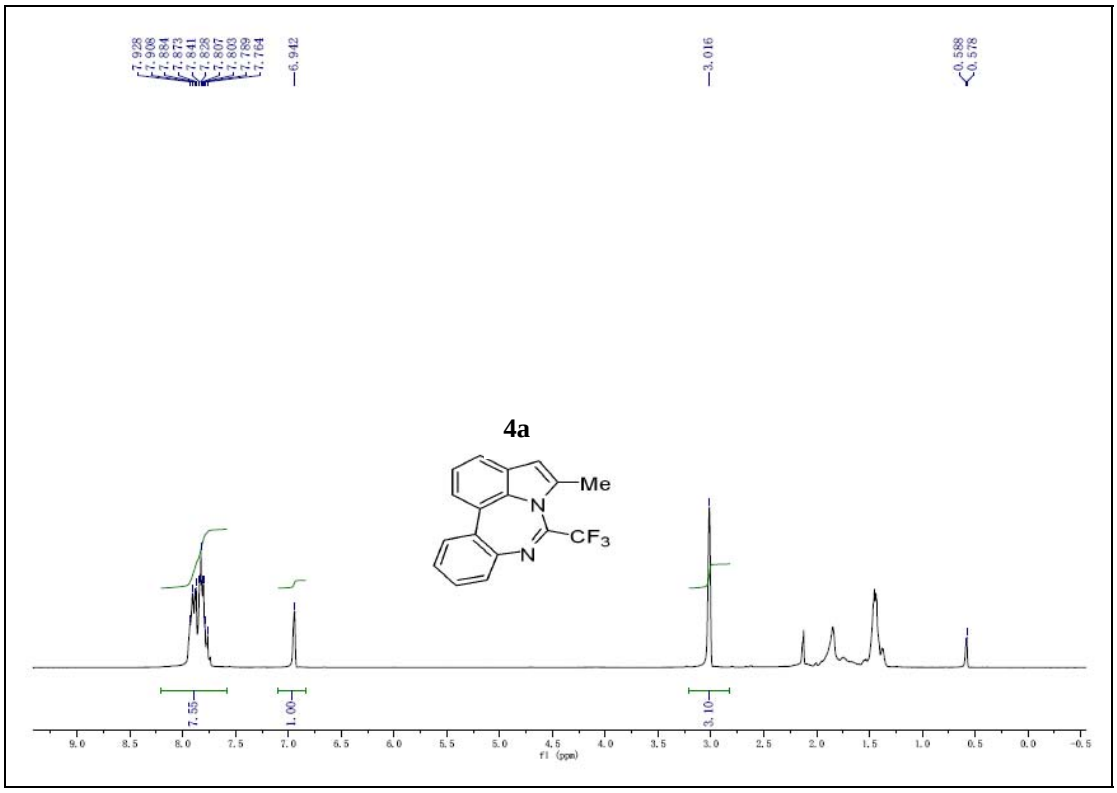
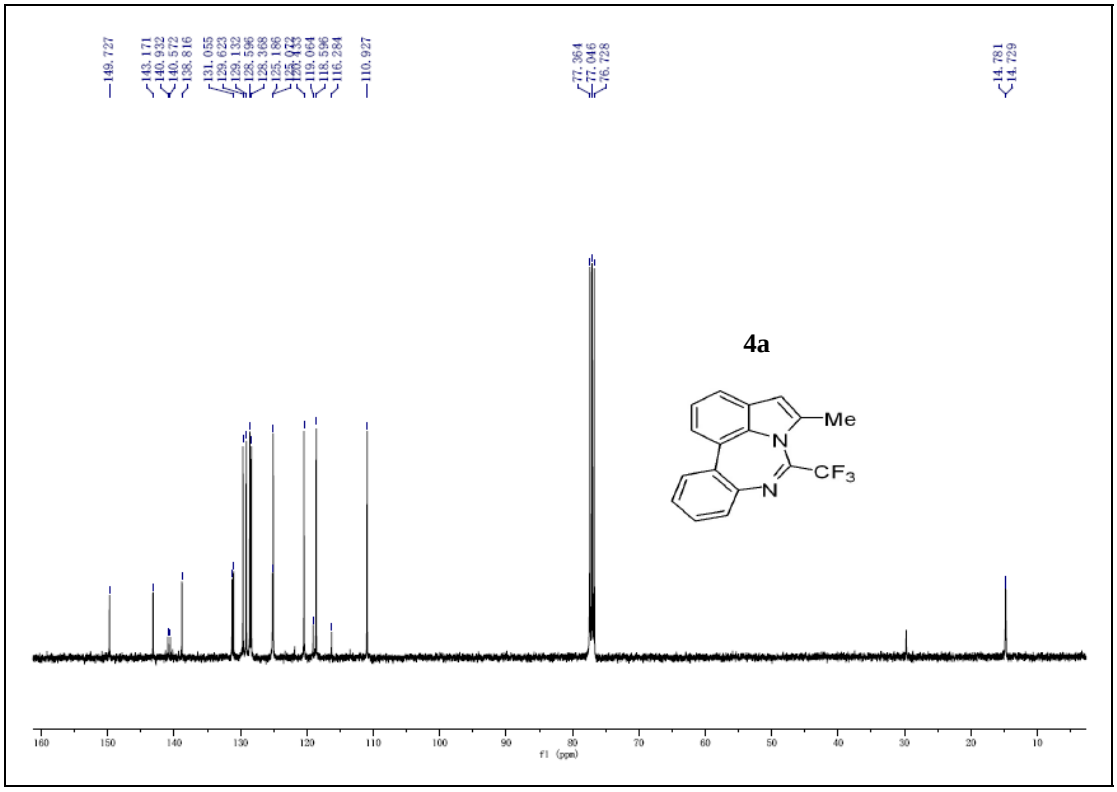
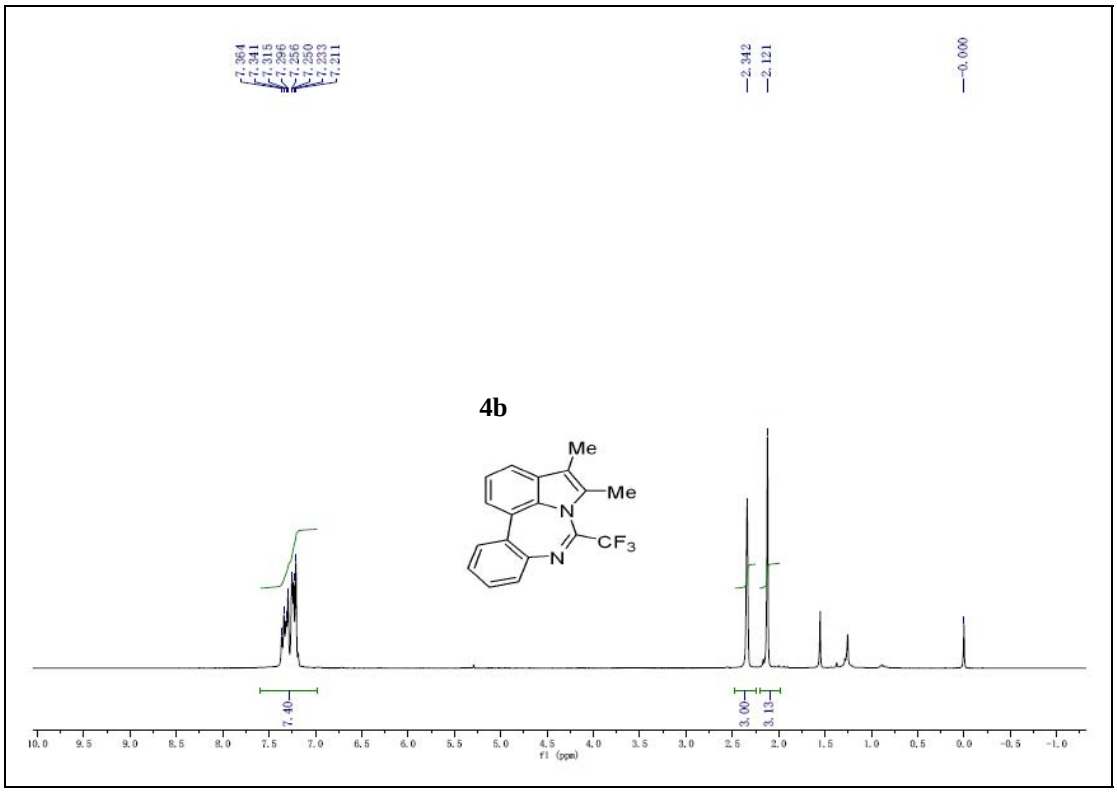
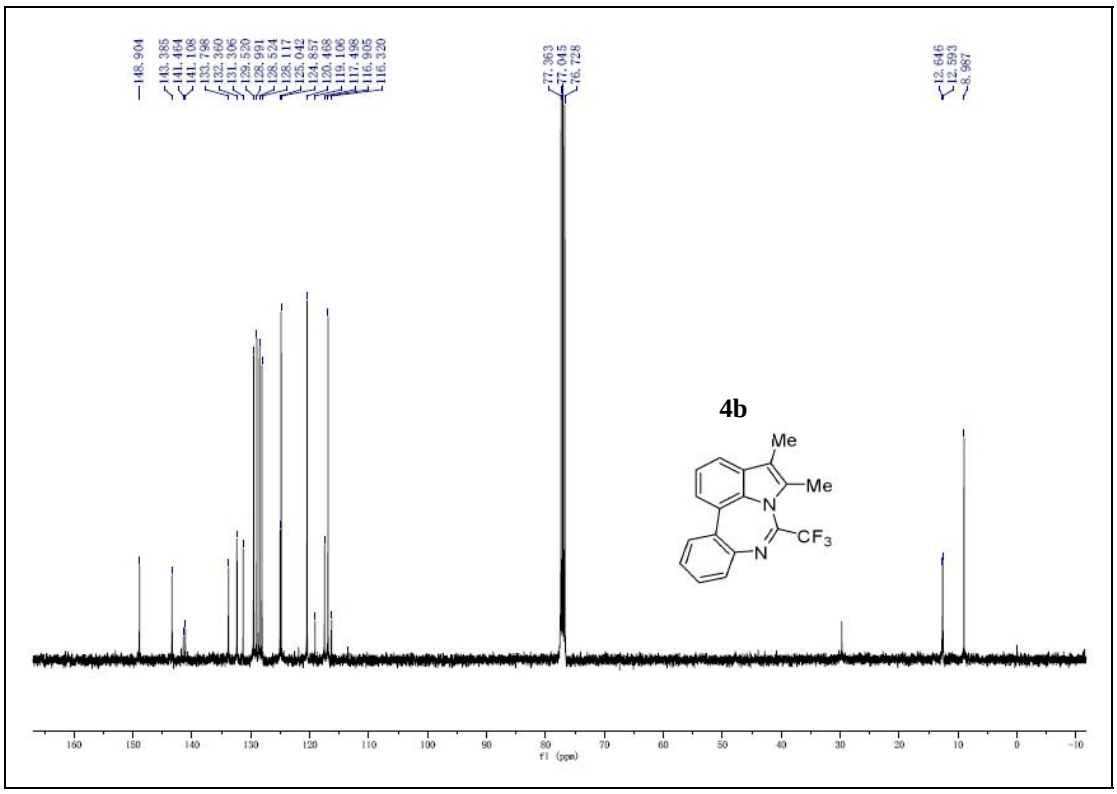
8.104
8.100
8.094
8.088
8.081
7.765
7.752
7.747
7.738
7.728
7.724
7.711
7.295
7.104
7.099
0.032
1.00
2.07
2.09
1.05
N
N
CF3
f1 (ppm)

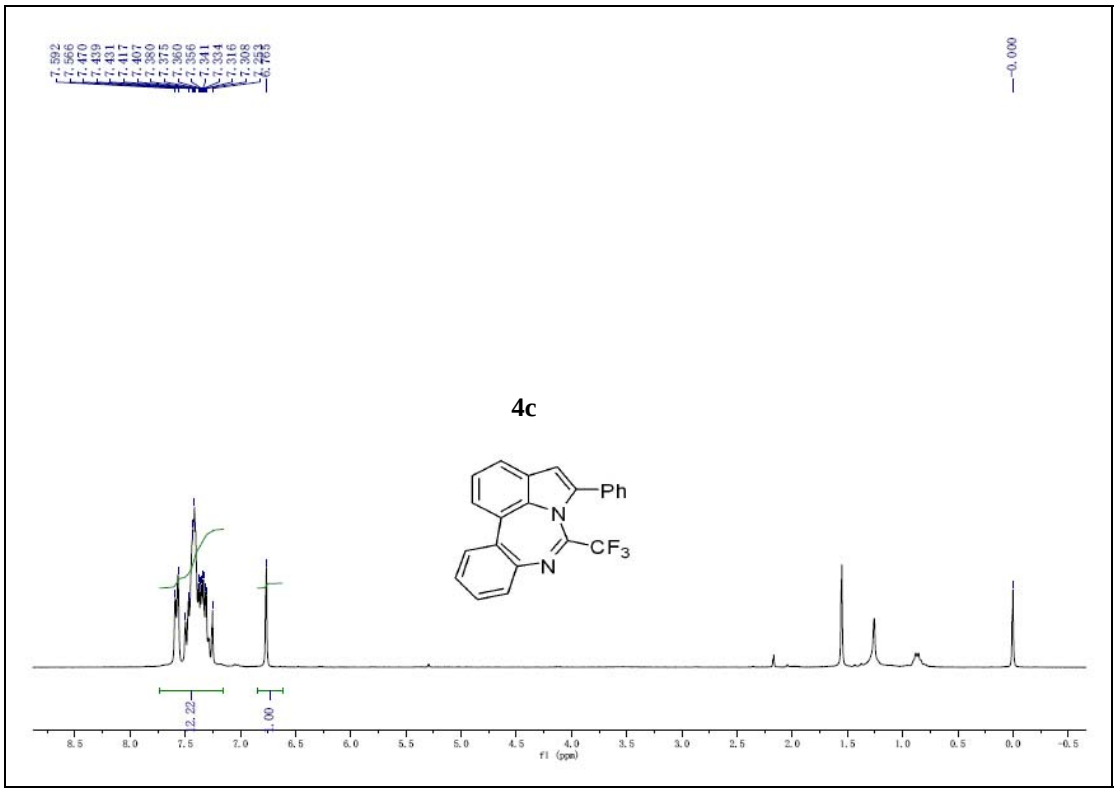

3u
144.734
140.658
137.671
136.263
135.874
130.365
130.141
129.712
123.219
120.834
119.659
116.914
98.901
77.352
77.035
76.717
N
N
CF3
f1 (ppm)

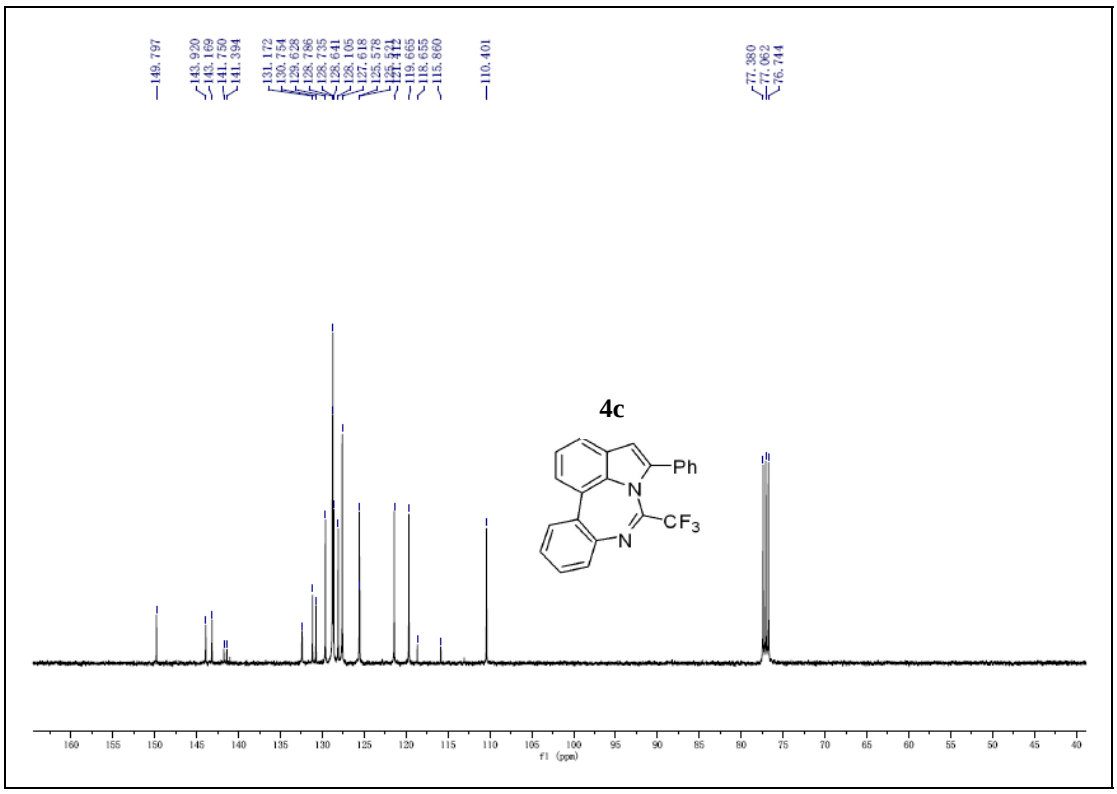

7.928
7.908
7.884
7.873
7.841
7.828
7.807
7.803
7.789
7.764
6.942
3.016
0.588
0.578
4a
Me
N
CF3
N
7.55
1.00
3.10
f1 (ppm)

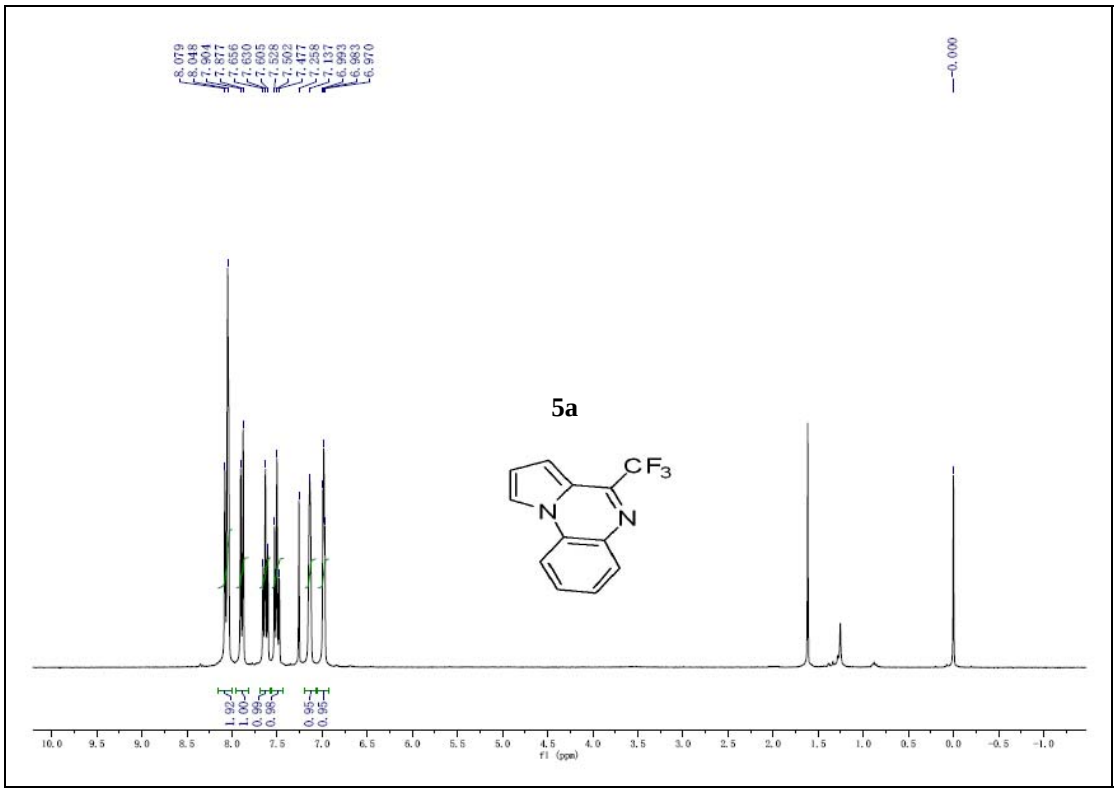

149.727
143.171
140.932
140.572
138.816
131.055
129.623
129.132
128.596
128.368
125.186
110.927
77.364
77.046
76.728
14.781
14.729
4a
Me
N
CF3
N
f1 (ppm)

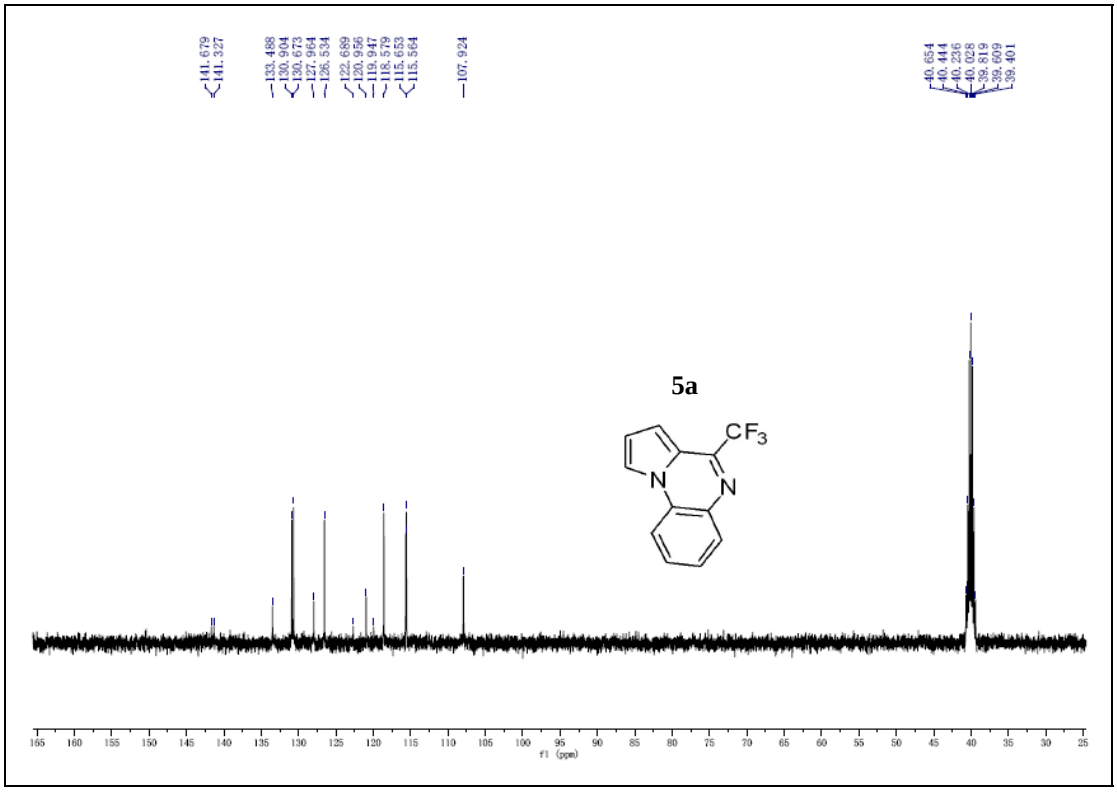

7.364
7.341
7.315
7.296
7.256
7.250
7.233
7.211
2.342
2.121
0.000
4b
Me
Me
N
N
CF3
7.40
3.00
3.13
f1 (ppm)

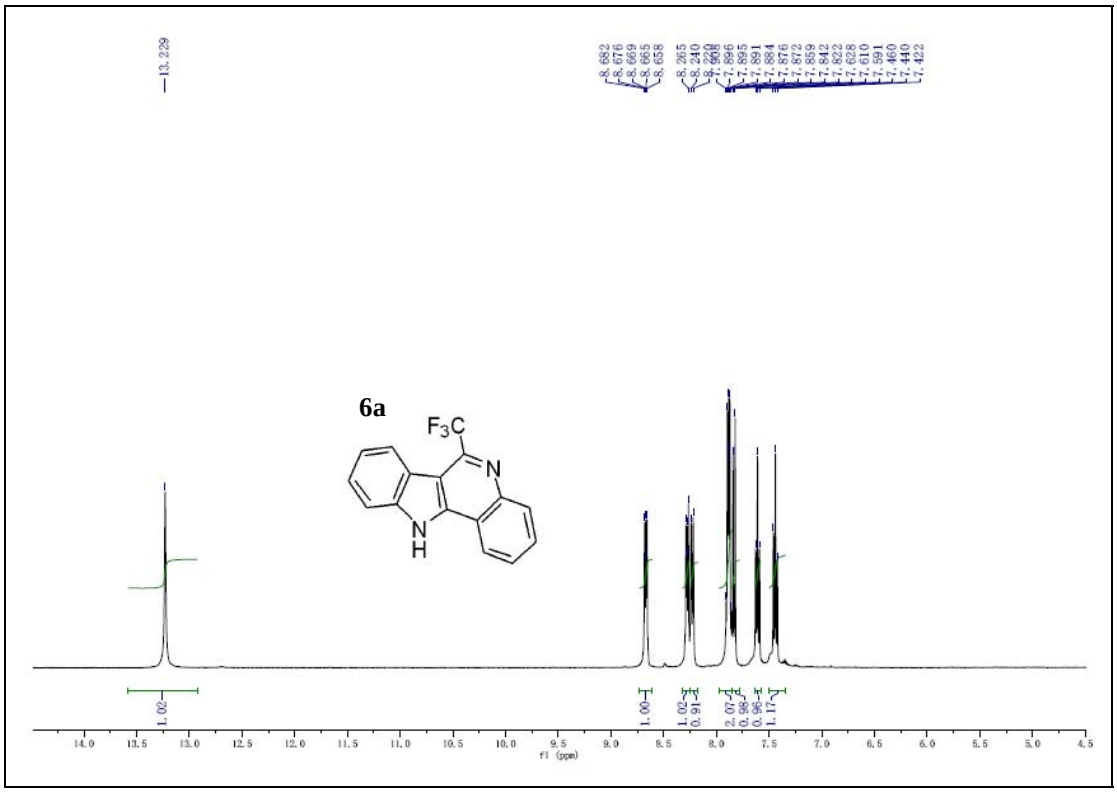

148.904
143.385
141.464
141.108
133.798
132.360
131.306
129.520
128.991
128.524
128.117
125.042
124.857
120.468
119.106
117.498
116.905
116.320
77.363
77.045
76.728
12.646
12.593
8.987
4b
Me
Me
N
N
CF3
f1 (ppm)

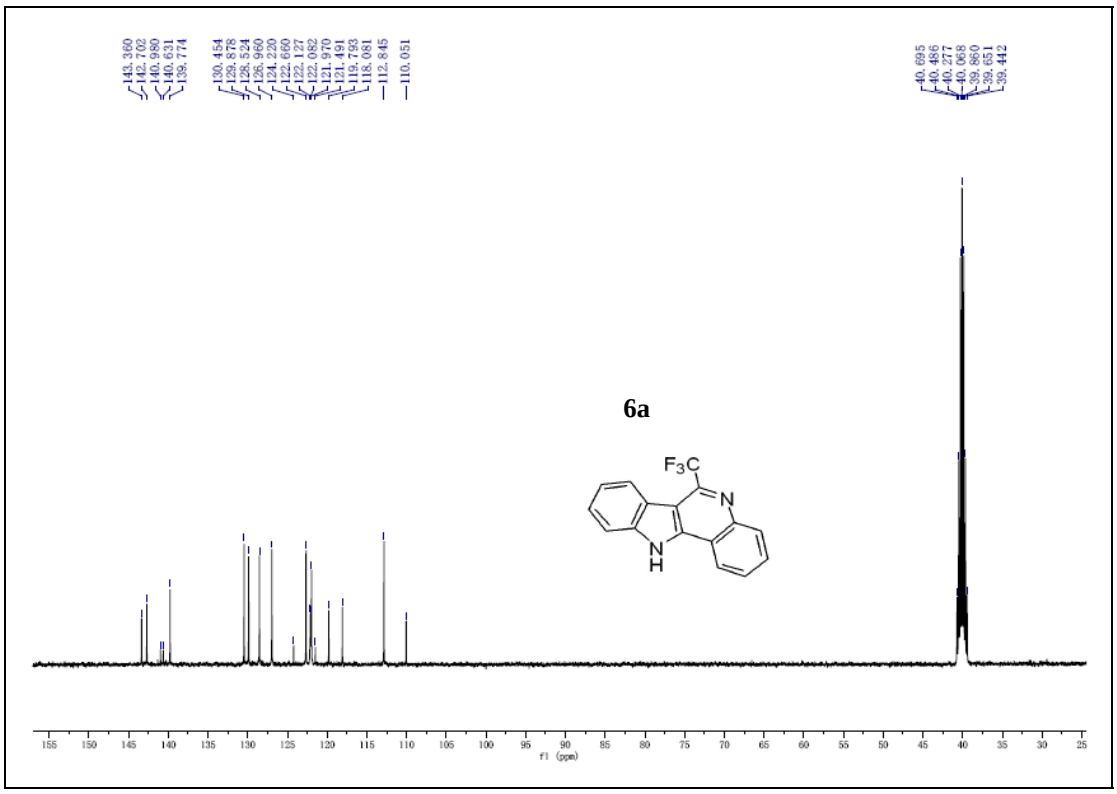

4c
Ph
N
CF3
N
2.22
1.00
f1 (ppm)

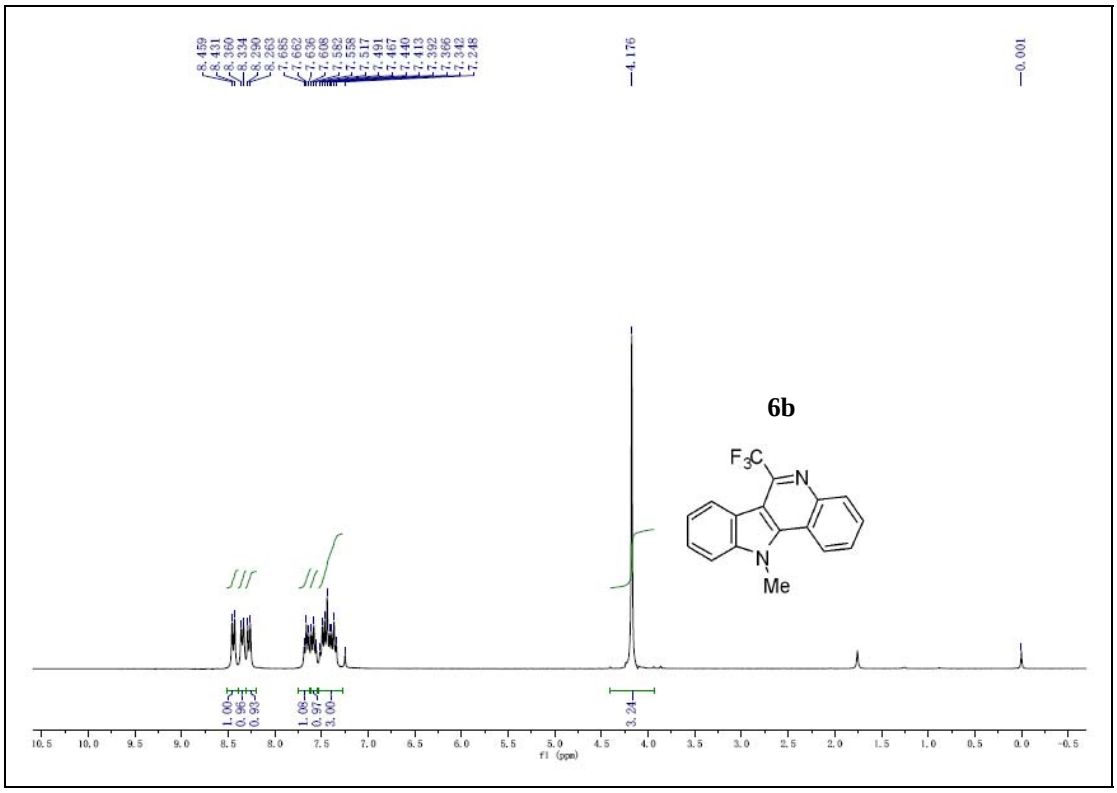

4c
Ph
N
CF3
N
f1 (ppm)

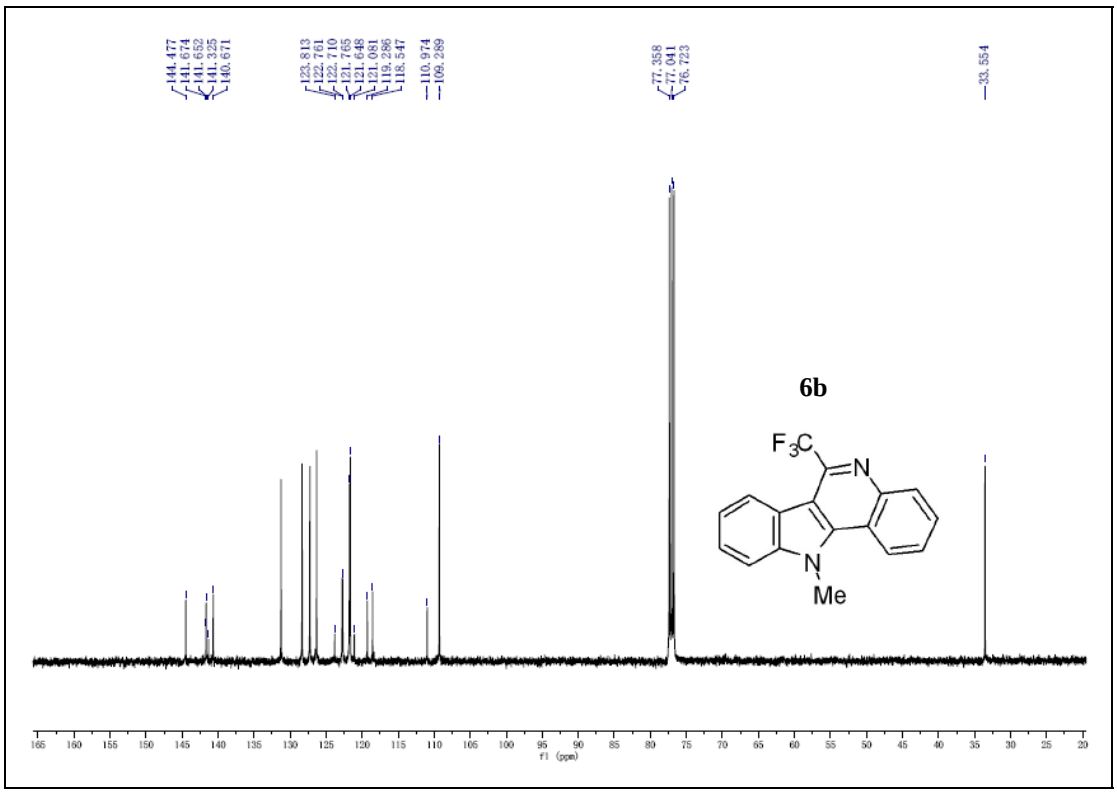

8.079
8.048
7.904
7.877
7.656
7.630
7.605
7.528
7.502
7.477
7.258
7.137
6.993
6.983
6.970
0.000
5a
CF3
N
N
1.92
1.00
0.99
0.98
0.95
0.95
f1 (ppm)

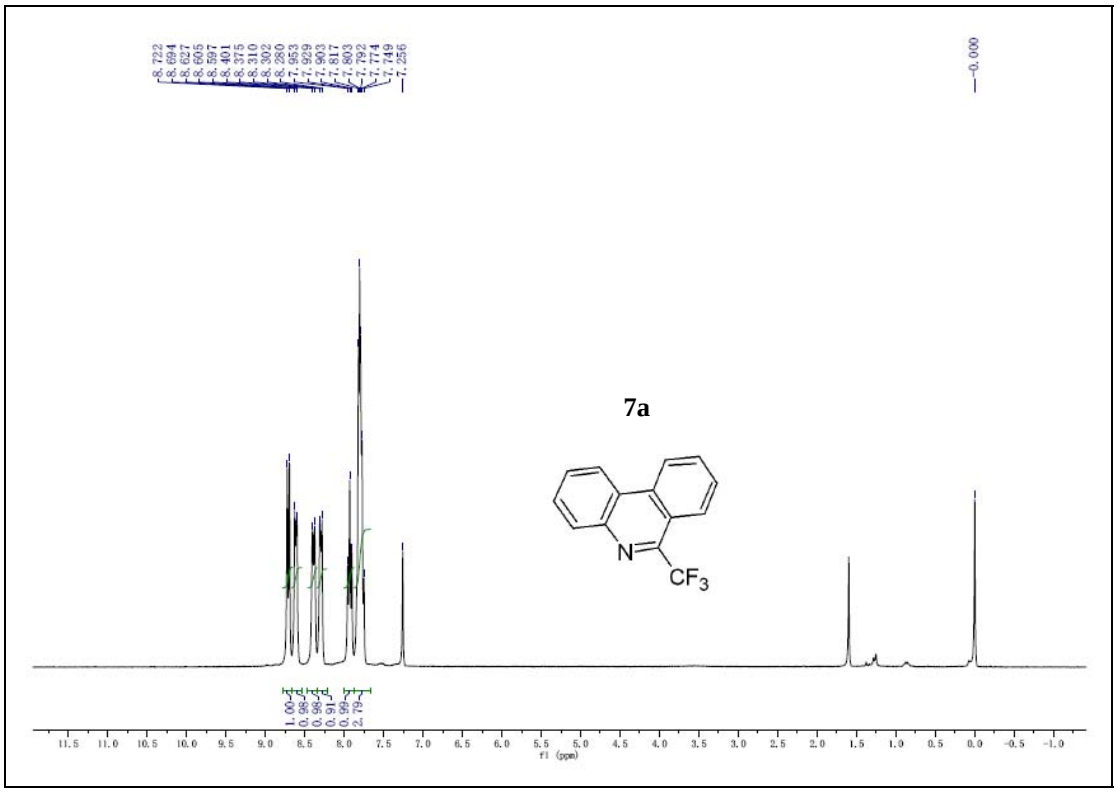

141.679
141.327
133.488
130.994
130.673
127.964
126.534
122.689
120.956
119.947
118.579
115.653
115.564
107.924
40.654
40.444
40.236
40.028
39.819
39.609
39.401
5a
CF3
N
N
f1 (ppm)

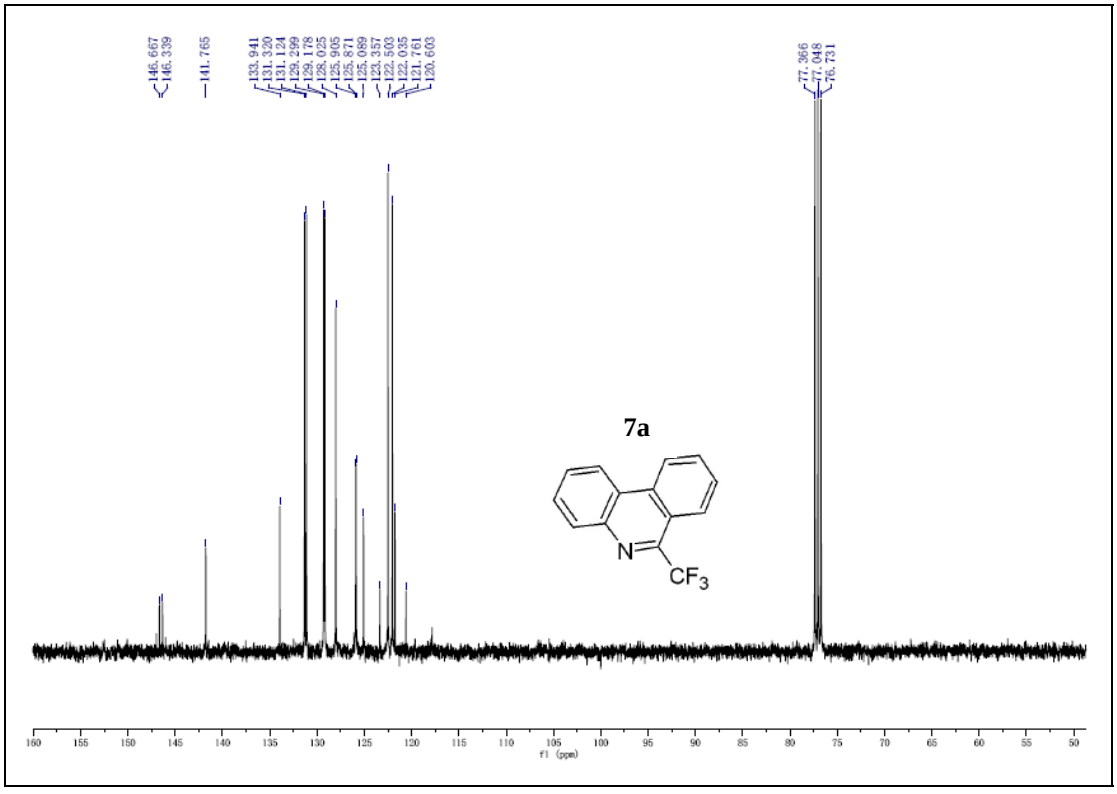

6a
F3C
N
N
H
f1 (ppm)


6a
F3C
N
N
H
f1 (ppm)


8.459
8.431
8.360
8.334
8.290
8.263
7.685
7.662
7.636
7.608
7.582
7.558
7.517
7.491
7.467
7.440
7.413
7.392
7.366
7.342
7.248
4.176
0.001
6b
F3C
N
N
Me
1.00
0.98
0.93
1.06
0.97
3.00
3.24
f1 (ppm)


144.477
141.674
141.552
141.325
140.671
123.813
122.761
122.710
121.765
121.648
121.081
119.286
118.547
110.974
109.289
77.358
77.041
76.723
33.554
6b
F3C
N
N
Me
f1 (ppm)


8.722
8.694
8.627
8.605
8.497
8.491
8.315
8.302
8.286
7.953
7.929
7.903
7.817
7.803
7.792
7.774
7.749
7.256
0.000
7a
N
CF3
1.00
0.98
0.96
0.91
0.99
2.79
f1 (ppm)


146.667
146.339
141.765
133.941
131.320
131.124
129.299
129.178
128.025
125.905
125.871
125.089
123.357
122.503
122.035
121.761
120.603
77.366
77.048
76.731
7a
N
CF3
f1 (ppm)