Supporting Information

Rh(III)-catalyzed C-H activation/annulation of *N*-carbamoylindoles with CF_3-imidoyl sulfoxonium ylides for the divergent synthesis of trifluoromethyl-substituted (dihydro)pyrimidoindolones

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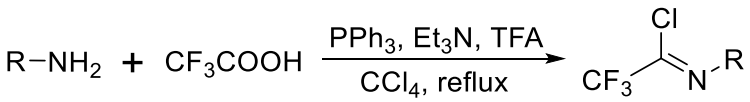
1. General Information

Unless otherwise noted, all reactions were carried out under air atmosphere. All reagents were from commercial sources and used as received without further purification. All solvents were dried by standard techniques and distilled prior to use. Column chromatography was performed on silica gel (200-300 meshes) using petroleum ether (bp. 60~90 °C) and ethyl acetate as eluent. ^{1}NMR spectra were recorded on a Bruker Avance operating at for ^{1}H NMR at 400 MHz, ^{13}C NMR at 100 MHz and ^{19}F NMR at 377 MHz and spectral data were reported in ppm relative to tetramethylsilane (TMS) as internal standard and $CDCl_3$ (^{1}H NMR δ 7.26, ^{13}C NMR δ 77.16) as solvent. All coupling constants (*J*) are reported in Hz. The following abbreviations were used to describe peak splitting patterns when appropriate: s = singlet, d = doublet, dd = double doublet, ddd = double doublet of doublets, t = triplet, dt = double triplet, q = quatriplet, m = multiplet, br = broad. Gas chromatography (GC) analyses were performed on a Shimadzu GC-2014C chromatograph equipped with a FID detector. Mass spectra (MS) were measured on spectrometer by direct inlet at 70 eV. Mass spectroscopy data of the products were collected on an HRMS-TOF instrument or Waters TOFMS GCT Premier using EI or ESI ionization. Melting points were measured with WRR digital point apparatus and not corrected.

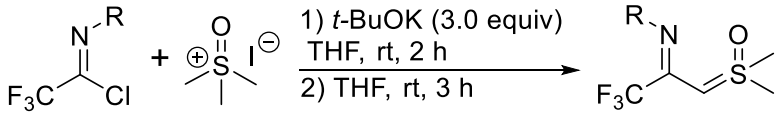
1.1 Preparation of Trifluoroacetimidoyl Chlorides[1]



A 100 mL two-necked flask equipped with a septum cap, a condenser, and a Tefloncoated magnetic stir bar was charged with PPh_3 (9.84 g, 37.5 mmol), Et_3N (2.1 mL, 15 mmol), CCl_4 (20.0 mL), and TFA (1.2 mL, 15 mmol). After the solution was stirred for about 10 min (ice bath), amine (15 mmol) dissolved in CCl_4 (20.0 mL) was added. The mixture was then refluxed under stirring (3 h). After the reaction was completed, residual solid Ph_3PO, PPh_3 and Et_3N-HCl were washed with hexane several times. Then the hexane was filtered and concentrated under vacuum. The crude product was purified by column chromatography on silica gel or neutral alumina to afford the

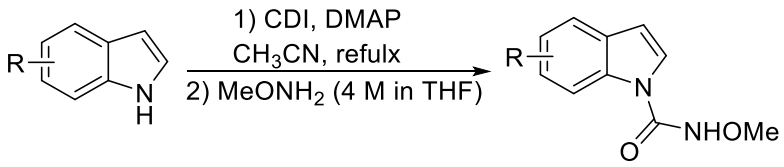
corresponding trifluoroacetimidoyl chloride product.

1.2 Preparation of CF_3-Imidoyl Sulfoxonium Ylides[2]



Trimethylsulfoxonium iodide (30 mmol, 3.0 equiv) was suspended in THF (150 mL) in a 250 mL round bottom flask, *t*-BuOK (30 mmol, 3.0 equiv) was added and the mixture was stirred at room temperature for 2 hours. Then, trifluoroacetimidoyl chloride (10 mmol, 1.0 equiv) was added. The mixture was stirred at room temperature for 3 hours and then filtered through a plug of celite before all volatiles were removed under vacuum. Purification by flash chromatography (petroleum ether/EtOAc = 2 : 1) afforded TFISY products. All the CF_3-imidoyl sulfoxonium ylides (TFISYs) are known compounds and have been reported previously by Cheng and our group.[2]

1.3 Preparation of *N*-methoxy-1H-indole-1-carboxamides [3]

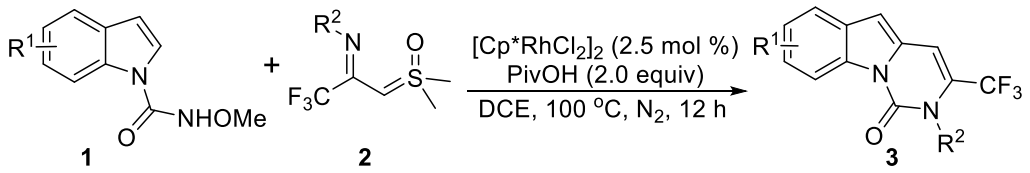


Step 1: Preparation of $MeONH_2$ solution: To a 100 mL round bottle charged with a stirring bar was added $MeONH_2$·HCl (80.0 mmol) and 20 mL THF. To the system was then added sodium hydroxide (powder, 1.0 equiv). The system was then stirred at room temperature for about 3 h until the system became clear.

Step 2: Preparation of *N*-methoxy-1H-indole-1-carboxamides: To a 100 mL round bottle charged with stirring bar, was added indole (5.0 mmol, 1.0 equiv), 1,1'-carbonyldiimidazole (CDI, 7.5 mmol, 1.5 equiv) and 4-dimethylaminepyridine (DMAP, 5.0 mol %). Then 20 mL anhydrous acetonitrile was added to bottle under the protection of argon. The system was refluxed at 85 °C for 10 h. After cooled to room temperature, $MeONH_2$ solution (4 M in THF, 2 equiv) was added and then stirred at 80 °C for another 6 hours (when the most of indole was consumed detected by TLC). After cooled to room temperature, the solvents were removed under reduced pressure. The residue was purified by silica chromatography in 15-75% yields without further optimization.

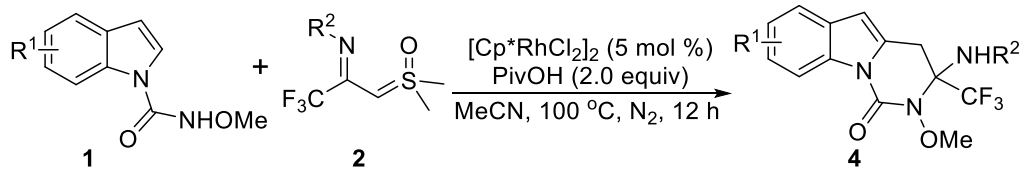
2. Experimental Procedures

2.1. General Procedure for the Synthesis of Products 3



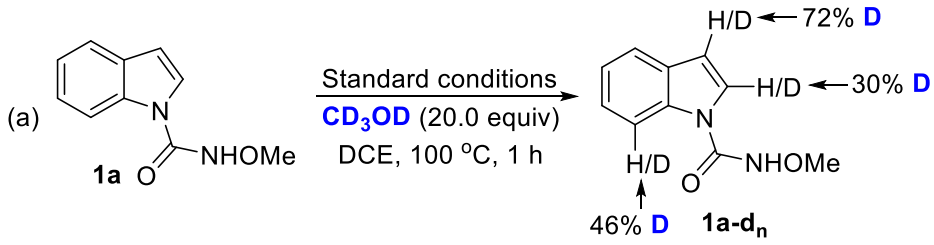
Under air atmosphere, *N*-methoxy-1H-indole-1-carboxamides **1** (0.2 mmol, 1.0 equiv), CF_3-imidoyl sulfoxonium ylides (TFISYs) **2** (0.3 mmol, 1.5 equiv), $[Cp^*RhCl_2]_2$ (3.1 mg, 0.005 mmol, 2.5 mol %), PivOH (40.9 mg, 0.4 mmol, 2.0 equiv) and DCE (2.0 mL) were added to an oven-dried 15 mL *In-Ex* tube. Then the tube was sealed and the mixture was stirred at 100 °C (oil bath) for 12 h. After the reaction was completed, the mixture was slowly cooled to room temperature, and extracted with EtOAc for three times (3×10 mL). The extract was combined and concentrated under vacuum. The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc) to yield the pyrimidoindolone products **3**.

2.2. General Procedure for the Synthesis of Products 4

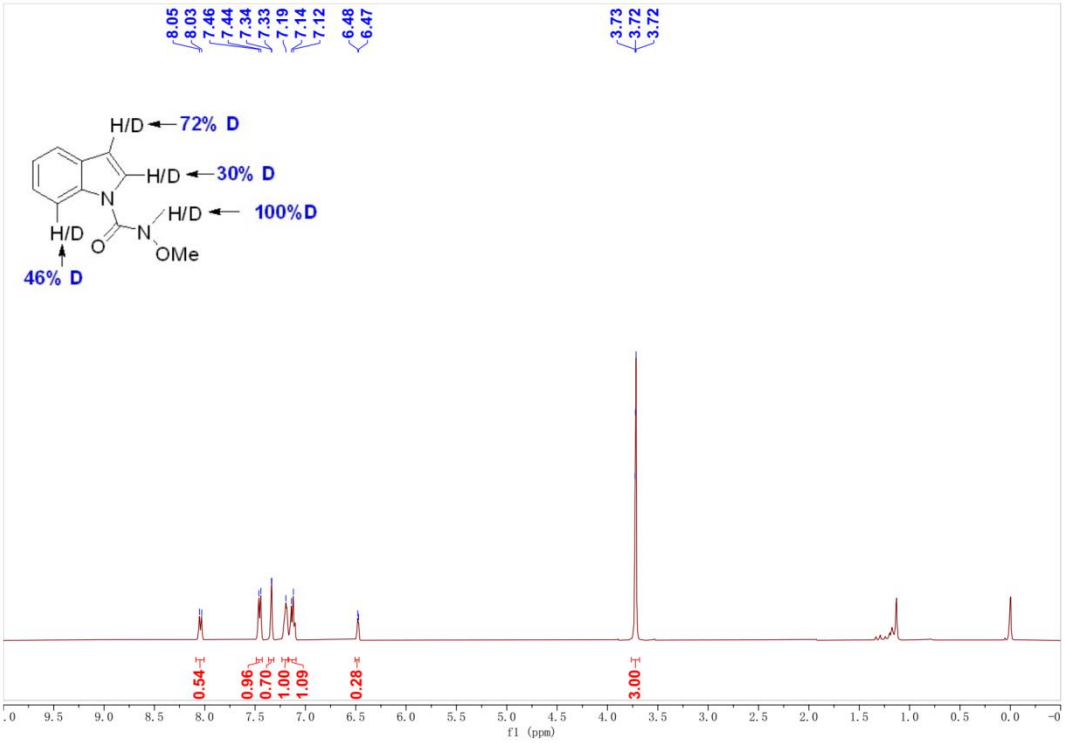


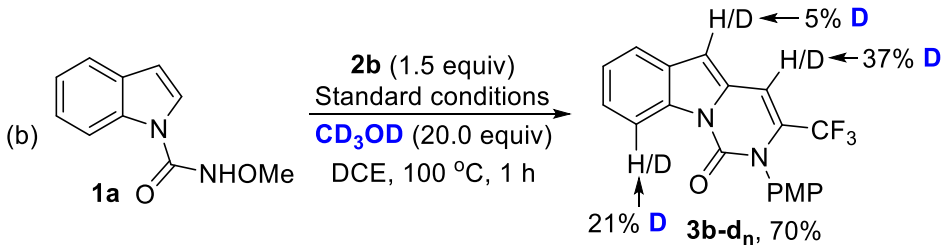
Under air atmosphere, *N*-methoxy-1H-indole-1-carboxamides **1** (0.2 mmol, 1.0 equiv), CF_3-imidoyl sulfoxonium ylides (TFISYs) **2** (0.3 mmol, 1.5 equiv), $[Cp^*RhCl_2]_2$ (6.2 mg, 0.01 mmol, 5 mol %), PivOH (40.8 mg, 0.4 mmol, 2.0 equiv) and MeCN (2.0 mL) were added to an oven-dried 15 mL *In-Ex* tube. Then the tube was sealed and the mixture was stirred at 100 °C (oil bath) for 12 h. After the reaction was completed, the mixture was slowly cooled to room temperature, and extracted with EtOAc for three times (3×10 mL). The extract was combined and concentrated under vacuum. The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc) to yield the dihydropyrimidoindolone products **4**.

2.3. Mechanistic Studies

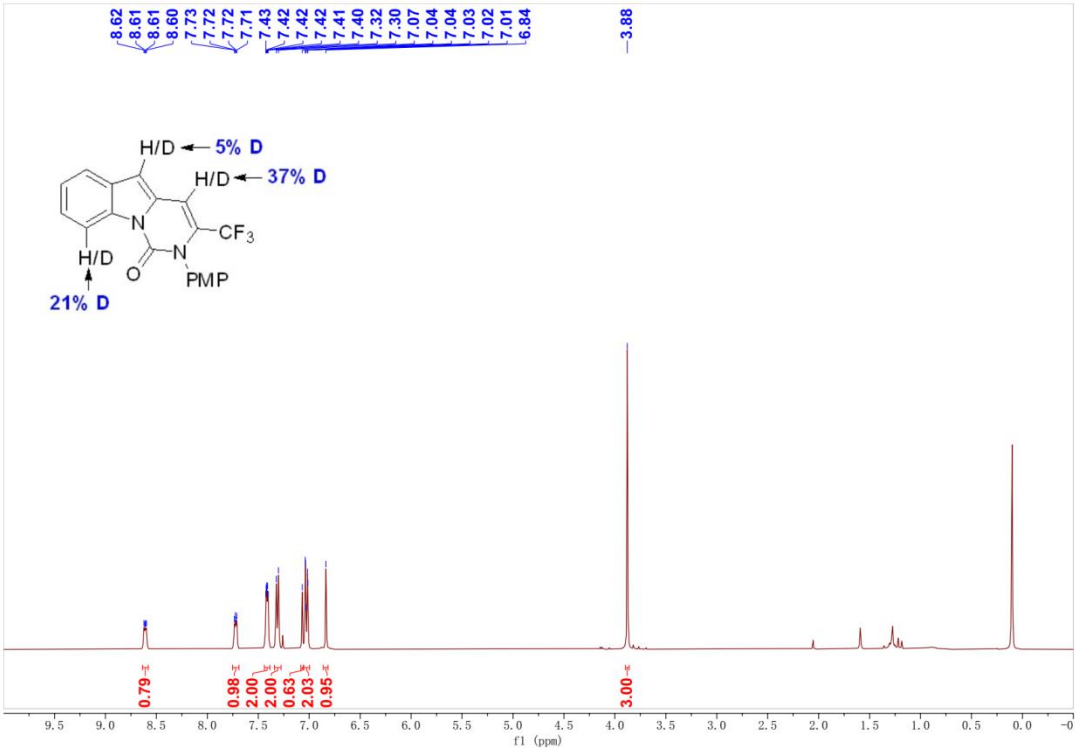


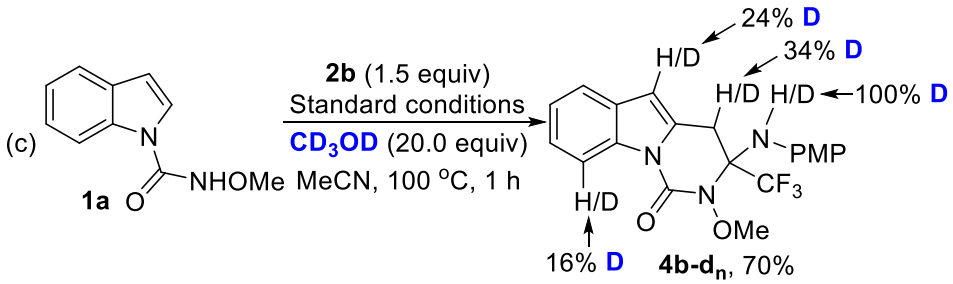
To a 15 mL Schlenk tube with a magneton was added *N*-methoxy-1H-indole-1-carboxamide **1a** (38 mg, 0.20 mmol, 1.0 equiv), $[Cp^*RhCl_2]_2$ (3.1 mg, 0.005 mmol, 2.5 mol %), PivOH (40.9 mg, 0.4 mmol, 2.0 equiv), CD_3OD (0.16 mL, 20.0 equiv) and DCE (2.0 mL) were added to an oven-dried 15 mL *In-Ex* tube. Then the tube was sealed and the mixture was stirred at 100 °C (oil bath) for 1 h. After the reaction was completed, the mixture was slowly cooled to room temperature, and extracted with EtOAc for three times (3×10 mL). The extract was combined and concentrated under vacuum. The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 10/1) to yield the product **$[D]_n$-1a**. The deuterium incorporation in **$[D]_n$-1a** was determined by ^{1}H NMR spectroscopy.



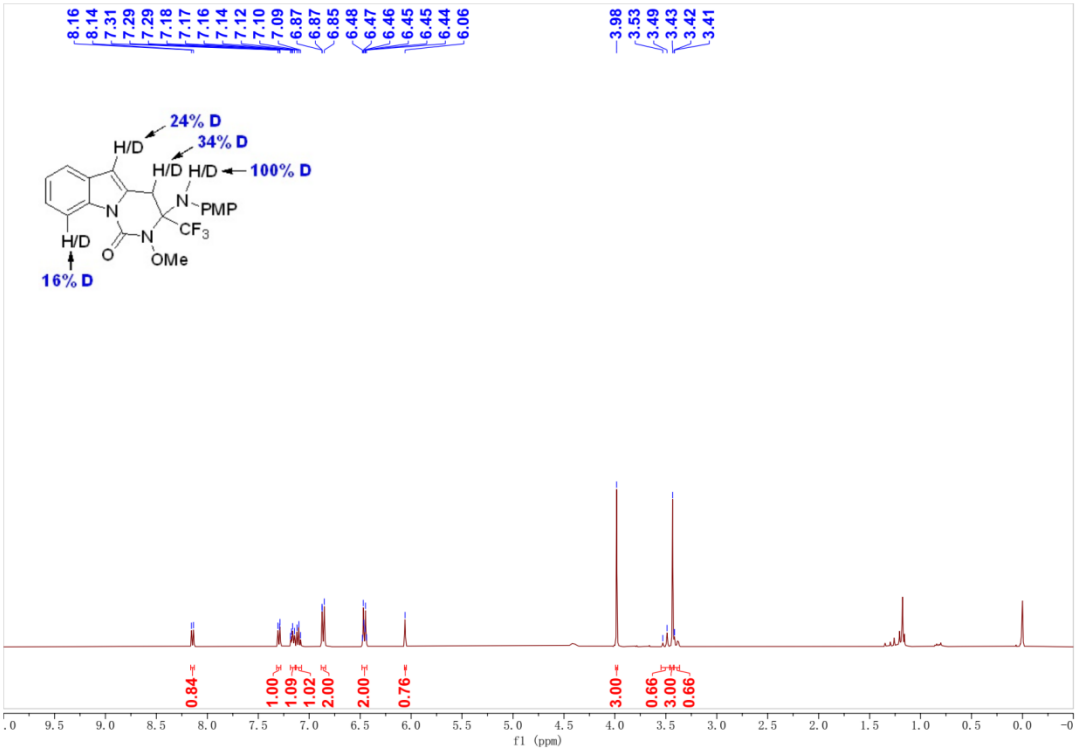


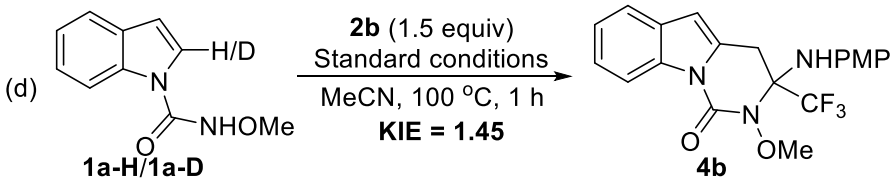
To a 15 mL Schlenk tube with a magneton was added *N*-methoxy-1H-indole-1-carboxamides **1a** (38 mg, 0.20 mmol, 1.0 equiv), TFISY **2b** (88.0 mg, 0.3 mmol, 1.5 equiv), $[Cp^*RhCl_2]_2$ (3.1 mg, 0.005 mmol, 2.5 mol %), PivOH (40.9 mg, 0.4 mmol, 2.0 equiv), CD_3OD (0.16 mL, 20.0 equiv) and DCE (2.0 mL). The reaction mixture was rapidly degassed several times, then it was sealed up and stirred vigorously at 100 °C (oil bath) for 1 h. After the reaction was completed, the mixture was slowly cooled to room temperature, and extracted with EtOAc for three times (3×10 mL). The extract was combined and concentrated under vacuum. The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 10/1) to yield the product **3b/[D]-3b** as a white solid in 70%. The deuterium incorporation in **3b/[D]-3b** was determined by ^{1}H NMR spectroscopy.



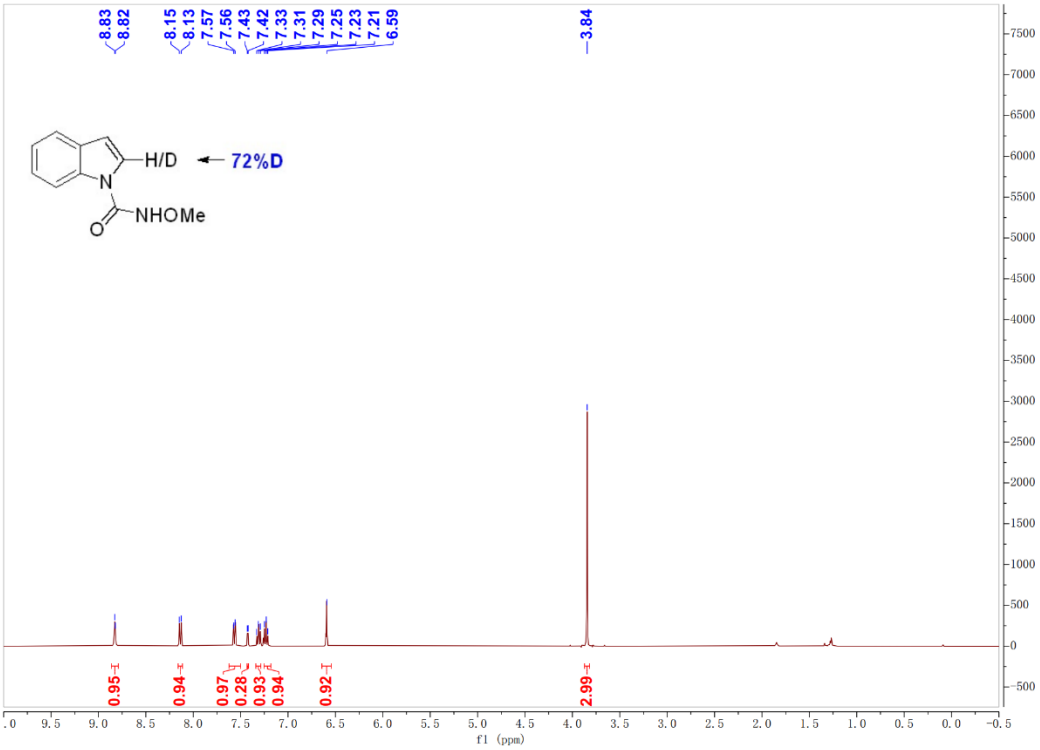


To a 15 mL Schlenk tube with a magneton was added **1a** (38 mg, 0.20 mmol, 1.0 equiv), TFISY **2b** (88.0 mg, 0.3 mmol, 1.5 equiv), $[Cp^*RhCl_2]_2$ (6.2 mg, 0.01 mmol, 5 mol %), PivOH (40.8 mg, 0.4 mmol, 2.0 equiv), CD_3OD (0.16 mL, 20.0 equiv) and MeCN (2.0 mL), The reaction mixture was sealed up and stirred vigorously at 100 °C (oil bath) for 1 h. After the reaction was completed, the mixture was slowly cooled to room temperature, and extracted with EtOAc for three times (3×10 mL). The extract was combined and concentrated under vacuum. The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 10/1) to yield the product **4b/[D]-4b** as a white solid in 70%. The deuterium incorporation in **4b/[D]-4b** was determined by ^{1}H NMR spectroscopy.

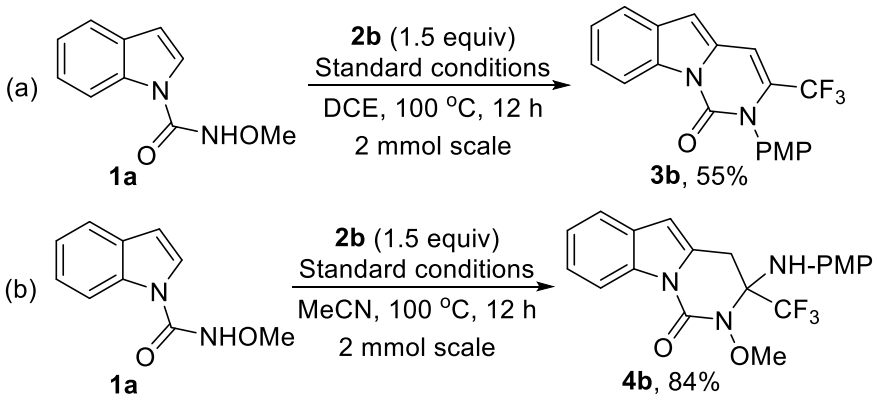




Two pressure tubes each was charged with $[Cp^*RhCl_2]_2$ (6.2 mg, 0.01 mmol, 5 mol %), PivOH (40.8 mg, 0.4 mmol, 2.0 equiv), TFISY **2b** (88.0 mg, 0.3 mmol, 1.5 equiv) and MeCN (2.0 mL). To the parallel tubes was then separately introduced **1a** (38.0 mg, 0.2 mmol) and **[D]-1a** (38.2 mg, 0.2 mmol). The reaction was sealed up and stirred vigorously at 100 °C (oil bath) for 1 h. After the reaction was completed, the mixture was slowly cooled to room temperature, and extracted with EtOAc for three times (3×10 mL). The extract was combined and concentrated under vacuum. The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 10/1) to yield the product **4b** (53.5 mg, 66.1%) and **[D]-4b** (51.7 mg, 63.2%), respectively. The KIE value (66.1%/63.2*0.72 = 1.45) was calculated according to the ratio of the isolated yields of **4b** and **[D]-4b** from the two reactions.



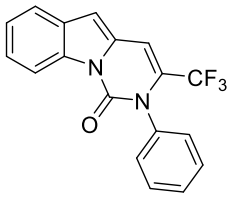
2.4. Scale-up Reactions



(a) Under air atmosphere, *N*-methoxy-1H-indole-1-carboxamide **1a** (380 mg, 2.0 mmol, 1.0 equiv), TFISY **2b** (789 mg, 3.0 mmol, 1.5 equiv), $[Cp^*RhCl_2]_2$ (31 mg, 0.05 mmol, 2.5 mol %), PivOH (408 mg, 4.0 mmol, 2.0 equiv) and DCE (20 mL) were added to an oven-dried 100 mL *In-Ex* tube. Then the tube was sealed and the mixture was stirred at 100 °C (oil bath) for 12 h. After the reaction was completed, the mixture was slowly cooled to room temperature, and extracted with EtOAc for three times (3×30 mL). The extract was combined and concentrated under vacuum. The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 5/1) to yield the product **3b** as a white solid (0.39 g, 55%).

(b) Under air atmosphere, *N*-methoxy-1H-indole-1-carboxamide **1a** (380 mg, 2.0 mmol, 1.0 equiv), TFISY **2a** (789 mg, 3.0 mmol, 1.5 equiv), $[Cp^*RhCl_2]_2$ (62 mg, 0.1 mmol, 5 mol %), PivOH (408 mg, 4.0 mmol, 2.0 equiv) and MeCN (20 mL) were added to an oven-dried 100 mL *In-Ex* tube. Then the tube was sealed and the mixture was stirred at 100 °C (oil bath) for 12 h. After the reaction was completed, the mixture was slowly cooled to room temperature, and extracted with EtOAc for three times (3×30 mL). The extract was combined and concentrated under vacuum. The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 5/1) to yield the product **4b** as a white solid (0.68 g, 84%).

3. Characterization Data of the Corresponding Products



2-phenyl-3-(trifluoromethyl)pyrimido[1,6-*a*]indol-1(*2H*)-one **(3a)**

Upon completion the mixture was concentrated and purified via flash column chromatography (petroleum ether / ethyl acetate = 10:1, R_f = 0.3) to give the titled product **3a** as a white solid (42.6 mg, 65%)

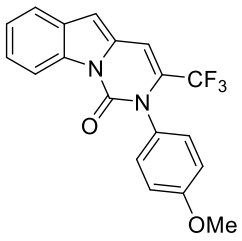
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.62 – 8.60 (m, 1H), 7.74-7.72 (m, 1H), 7.55 – 7.53 (m, 3H), 7.43 - 7.41 (m, 4H), 7.09 (s, 1H), 6.86 (s, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 148.3, 136.0, 134.0, 132.2, 130.3, 130.1, 129.8, 129.3, 127.5 (q, $^2J_{(C-F)}$ = 33.2 Hz), 124.5, 120.6, 120.1 (q, $^1J_{(C-F)}$ = 272.4 Hz), 116.4, 103.4, 101.9 (q, $^3J_{(C-F)}$ = 6.2 Hz).

^{19}F NMR (376 MHz, $CDCl_3$) δ -61.7.

M.p. 148.9 - 150.9 ºC.

HRMS (ESI): $[M+H]^+$ calcd. for $C_{18}H_{12}F_3N_2O^+$ 329.0896, found 329.0901.



2-(4-methoxyphenyl)-3-(trifluoromethyl)pyrimido[1,6-*a*]indol-1(*2H*)-one **(3b)**

Upon completion the mixture was concentrated and purified via flash column chromatography (petroleum ether / ethyl acetate = 10:1, R_f = 0.3) to give the titled product **3b** as a white solid (55.1 mg, 77%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.63 – 8.58 (m, 1H), 7.73 – 7.71 (m, 1H), 7.42 – 7.40 (m, 2H), 7.31 (d, *J* = 8.6 Hz, 2H), 7.07 (s, 1H), 7.02 (d, *J* = 8.9 Hz, 2H), 6.84 (s, 1H), 3.88 (s, 3H).

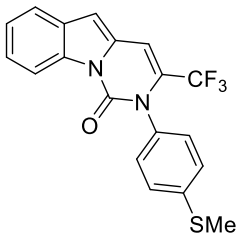
^{13}C NMR (101 MHz, $CDCl_3$) δ 160.3, 148.5, 134.0, 131.2, 131.1, 130.3, 128.4, 127.8

(q, $^{2}J_{(C-F)}$ = 33.3 Hz) 124.5, 120.5, 120.2 (q, $^{1}J_{(C-F)}$ = 272.5 Hz), 116.4, 114.5, 103.2, 101.7 (q, $^{3}J_{(C-F)}$ = 6.3 Hz), 55.5.

^{19}F NMR (377 MHz, CDCl$_3$) δ -61.9.

M.p. 202.7-203.8 ºC.

HRMS (ESI): $[M+H]^+$ calcd. for $C_{19}H_{14}F_3N_2O_2^+$ 359.1012, found 359.1008.



2-(4-(methylthio)phenyl)-3-(trifluoromethyl)pyrimido[1,6-*a*]indol-1(*2H*)-one **(3c)**

Upon completion the mixture was concentrated and purified via flash column chromatography (petroleum ether / ethyl acetate = 10:1, R_f = 0.3) to give the titled product **3c** as a yellow solid (41.9 mg, 56%).

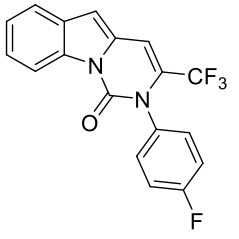
^{1}H NMR (400 MHz, CDCl$_3$) δ 8.59 (d, *J* = 5.5 Hz, 1H), 7.73 – 7.72 (m, 1H), 7.42 (dd, *J* = 4.4, 2.8 Hz, 2H), 7.36 (d, *J* = 8.4 Hz, 2H), 7.30 (d, *J* = 8.3 Hz, 2H), 7.09 (s, 1H), 6.86 (s, 1H), 2.54 (s, 3H).

^{13}C NMR (101 MHz, CDCl$_3$) δ 148.3, 141.1, 134.0, 132.5, 131.1, 130.3, 127.5 (q, $^{2}J_{(C-F)}$ = 33.6 Hz), 126.5, 124.5, 120.6, 120.1 (q, $^{1}J_{(C-F)}$ = 272.5 Hz), 116.4, 103.4, 101.94 (q, $^{3}J_{(C-F)}$ = 6.2 Hz), 15.4.

^{19}F NMR (376 MHz, CDCl$_3$) δ -61.9.

M.p. 209.3-210.4 ºC.

HRMS (ESI): $[M+H]^+$ calcd. for $C_{19}H_{14}F_3N_2OS^+$ 375.0773, found 375.0779.



2-(4-fluorophenyl)-3-(trifluoromethyl)pyrimido[1,6-*a*]indol-1(*2H*)-one **(3d)**

Upon completion the mixture was concentrated and purified via flash column

chromatography (petroleum ether / ethyl acetate = 10:1, R_f = 0.3) to give the titled product **3d** as a yellow solid (56.1 mg, 81%).

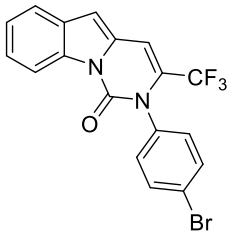
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.60 - 8.57 (m, 1H), 7.75 – 7.71 (m, 1H), 7.44 – 7.38 (m, 4H), 7.22 (t, *J* = 8.5 Hz, 2H), 7.08 (s, 1H), 6.85 (s, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 163.1 (d, $^1J_{(C-F)}$ = 250.0 Hz), 148.3, 134.0, 132.1 (d, $^3J_{(C-F)}$ = 8.9 Hz), 131.8, 131.1, 130.3, 127.4 (q, $^2J_{(C-F)}$ = 33.6 Hz), 124.7, 120.7, 120.2 (q, $^1J_{(C-F)}$ = 272.6 Hz), 116.4 (d, $^2J_{(C-F)}$ = 23.1 Hz), 116.4, 103.7, 102.2 (q, $^3J_{(C-F)}$ = 6.2 Hz).

^{19}F NMR (376 MHz, $CDCl_3$) δ -61.8, -111.5.

M.p. 150.5-152.3 ºC.

HRMS (ESI): $[M+H]^+$ calcd. for $C_{18}H_{11}F_4N_2O^+$ 347.0802, found 347.0808.



2-(4-bromophenyl)-3-(trifluoromethyl)pyrimido[1,6-*a*]indol-1(*2H*)-one **(3e)**

Upon completion the mixture was concentrated and purified via flash column chromatography (petroleum ether / ethyl acetate = 10:1, R_f = 0.3) to give the titled product **3e** as a yellow solid (44.7 mg, 55%).

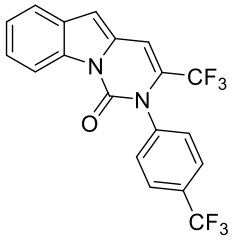
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.49 - 8.47 (m, 1H), 7.72 (dd, *J* = 5.5, 3.1 Hz, 1H), 7.66 (d, *J* = 8.4 Hz, 2H), 7.42 (dd, *J* = 6.0, 3.1 Hz, 2H), 7.27 (d, *J* = 8.3 Hz, 2H), 7.09 (s, 1H), 6.86 (s, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 147.9, 135.0, 134.0, 132.6, 131.8, 130.9, 130.2, 127.1 (q, $^2J_{(C-F)}$ = 33.9 Hz), 124.7, 124.7, 124.0, 120.7, 120.1 (q, $^1J_{(C-F)}$ = 272.4 Hz), 117.3, 116.3, 103.8, 102.2 (q, $^3J_{(C-F)}$ = 6.2 Hz).

^{19}F NMR (376 MHz, $CDCl_3$) δ -61.7.

M.p. 212.8-214.2 ºC.

HRMS (ESI): $[M+H]^+$ calcd. for $C_{18}H_{11}BrF_3N_2O^+$ 407.0001, found 407.0005.



3-(trifluoromethyl)-2-(4-(trifluoromethyl)phenyl)pyrimido[1,6-*a*]indol-1(*2H*)-one **(3f)**

Upon completion the mixture was concentrated and purified via flash column chromatography (petroleum ether / ethyl acetate = 10:1, R_f = 0.3) to give the titled product **3f** as a white solid (47.5 mg, 60 %).

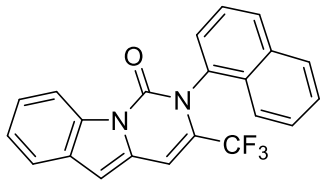
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.57 - 8.54 (m, 1H), 7.81 (d, *J* = 8.3 Hz, 2H), 7.75 – 7.73 (m, 1H), 7.55 (d, *J* = 8.2 Hz, 2H), 7.44 - 7.42 (m, 2H), 7.26 (s, 1H), 7.13 (s, 1H), 6.89 (s, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 147.8, 139.2, 134.0, 131.9 (q, $^2J_{(C-F)}$ = 33.0 Hz), 130.8, 130.2, 126.9 (q, $^2J_{(C-F)}$ = 33.8 Hz), 126.5 (q, $^3J_{(C-F)}$ = 3.6 Hz), 124.8, 124.7, 123.6 (q, $^1J_{(C-F)}$ = 272.7 Hz), 120.8, 120.0 (q, $^1J_{(C-F)}$ = 272.5 Hz), 116.3, 104.1, 102.5 (q, $^3J_{(C-F)}$ = 6.2 Hz).

^{19}F NMR (376 MHz, $CDCl_3$) δ -61.6, -63.3.

M.p. 230.0-233.6 ºC.

HRMS (ESI): $[M+H]^+$ calcd. for $C_{19}H_{11}F_6N_2O^+$ 397.0770, found 397.0774.



2-(naphthalen-1-yl)-3-(trifluoromethyl)pyrimido[1,6-*a*]indol-1(*2H*)-one **(3g)**

Upon completion the mixture was concentrated and purified via flash column chromatography (petroleum ether / ethyl acetate = 10:1, R_f = 0.3) to give the titled product **3g** as a white solid (45.4 mg, 60%).

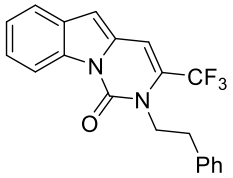
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.61 - 8.59 (m, 1H), 8.00 (d, *J* = 8.7 Hz, 1H), 7.96 – 7.89 (m, 3H), 7.76 – 7.74 (m, 1H), 7.62 – 7.54 (m, 2H), 7.47 (d, *J* = 8.7 Hz, 1H), 7.43 – 7.41 (m, 2H), 7.14 (s, 1H), 6.89 (s, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 148.4, 134.0, 133.5, 133.4, 133.2, 131.2, 130.3, 129.4, 129.2, 128.4, 127.9, 127.7 (q, $^2J_{(C-F)}$ = 34.1 Hz), 127.4, 127.1, 126.8, 124.5, 120.6, 120.2 (q, $^1J_{(C-F)}$ = 272.6 Hz), 116.4, 103.5, 102.0 (q, $^3J_{(C-F)}$ = 6.1 Hz).

^{19}F NMR (376 MHz, $CDCl_3$) δ -61.6.

M.p. 199.7-201.9 ºC.

HRMS (ESI): $[M+H]^+$ calcd. for $C_{22}H_{14}F_3N_2O^+$ 379.1053, found 379.1057.



2-phenethyl-3-(trifluoromethyl)pyrimido[1,6-*a*]indol-1(*2H*)-one **(3h)**

Upon completion the mixture was concentrated and purified via flash column chromatography (petroleum ether / ethyl acetate = 10:1, R_f = 0.3) to give the titled product **3h** as a white solid (58.4 mg, 82%).

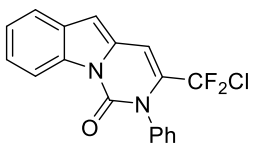
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.74 (d, *J* = 7.9 Hz, 1H), 7.72 (d, *J* = 7.4 Hz, 1H), 7.45 (t, *J* = 8.0 Hz, 2H), 7.38 (s, 2H), 7.37 (s, 2H), 7.32 – 7.26 (m, 1H), 7.02 (s, 1H), 6.78 (s, 1H), 4.26 – 4.21 (m, 2H), 3.12 – 3.08 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 148.0, 137.8, 133.7, 131.1, 130.2, 129.0, 128.8, 126.9, 126.2 (q, $^2J_{(C-F)}$ = 33.7 Hz), 124.4, 124.3, 120.9 (q, $^1J_{(C-F)}$ = 272.3 Hz), 120.5, 116.4, 102.6, 102.3 (q, $^3J_{(C-F)}$ = 7.0 Hz), 47.7, 35.1.

^{19}F NMR (376 MHz, $CDCl_3$) δ -62.9.

M.p. 209.3-210.4 ºC.

HRMS (ESI): $[M+H]^+$ calcd. for $C_{20}H_{16}F_3N_2O^+$ 357.1209, found 357.1214.



3-(chlorodifluoromethyl)-2-phenylpyrimido[1,6-*a*]indol-1(*2H*)-one **(3i)**

Upon completion the mixture was concentrated and purified via flash column chromatography (petroleum ether / ethyl acetate = 10:1, R_f = 0.3) to give the titled

product **3i** as a yellow solid (50.9 mg, 74%).

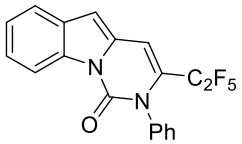
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.60 - 8.57 (m, 1H), 7.72 (s, 1H), 7.53 (s, 3H), 7.45 (s, 2H), 7.42 – 7.40 (m, 2H), 7.10 (s, 1H), 6.87 (s, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 148.5, 135.9, 134.1, 132.0 (t, $^{2}J_{(C-F)}$ = 28.3 Hz), 131.2, 131.0, 130.4, 129.7, 129.1, 124.6, 124.6, 120.6 (t, $^{1}J_{(C-F)}$ = 289.6 Hz), 120.6, 116.5, 103.7, 101.0 (t, $^{3}J_{(C-F)}$ = 8.2 Hz).

^{19}F NMR (376 MHz, $CDCl_3$) δ -48.9.

M.p. 171.2-172.4 ºC.

HRMS (ESI): $[M+H]^+$ calcd. for $C_{18}H_{12}ClF_2N_2O^+$ 345.0601, found 345.0606.



3-(perfluoroethyl)-2-phenylpyrimido[1,6-*a*]indol-1(*2H*)-one **(3j)**

Upon completion the mixture was concentrated and purified via flash column chromatography (petroleum ether / ethyl acetate = 10:1, Rf = 0.3) to give the titled product **3j** as a yellow solid (25.0 mg, 33%).

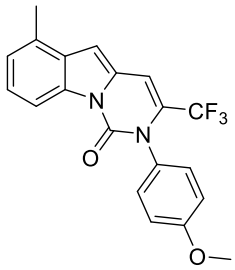
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.59 – 8.57 (m, 1H), 7.75 – 7.73 (m, 1H), 7.53 – 7.51 (m, 3H), 7.43 – 7.39 (m, 4H), 7.05 (s, 1H), 6.89 (s, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 148.6, 136.9, 134.1, 131.1, 130.4, 130.1, 130.1, 129.6, 129.2, 125.8 (t, $^{3}J_{(C-F)}$ = 24.0 Hz), 124.8, 124.7, 120.8, 118.7 (qt, $^{1}J_{(C-F)}$ = 250.0, 33.9 Hz), 116.6, 111.2 (tq, $^{2}J_{(C-F)}$ = 258.2, 39.5 Hz), 104.9 (t, $^{4}J_{(C-F)}$ = 7.3 Hz), 103.9.

^{19}F NMR (376 MHz, $CDCl_3$) δ -82.0, -107.0.

M.p. 131.9-141.4 ºC.

HRMS (ESI): $[M+H]^+$ calcd. for $C_{19}H_{12}F_5N_2O^+$ 379.0864, found 379.0871.



2-(4-methoxyphenyl)-6-methyl-3-(trifluoromethyl)pyrimido[1,6-*a*]indol-1(*2H*)-one **(3k)**

Upon completion the mixture was concentrated and purified via flash column chromatography (petroleum ether / ethyl acetate = 10:1, R_f = 0.3) to give the titled product **3k** as a yellow solid (72.2 mg, 97%).

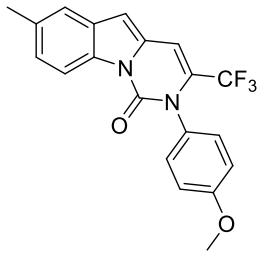
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.43 (d, *J* = 8.4 Hz, 1H), 7.33 – 7.29 (m, 3H), 7.21 (d, *J* = 7.3 Hz, 1H), 7.07 (s, 1H), 7.03 – 7.01 (m, 2H), 6.86 (s, 1H), 3.88 (s, 3H), 2.62 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 160.3, 148.6, 133.8, 131.1, 130.8, 130.2, 130.0, 128.4, 127.5 (q, $^2J_{(C-F)}$ = 32.6 Hz), 124.6, 124.6, 120.2 (q, $^1J_{(C-F)}$ = 273.6 Hz), 114.5, 113.9, 101.8 (q, $^3J_{(C-F)}$ = 7.6 Hz), 101.8, 55.6, 18.8.

^{19}F NMR (376 MHz, $CDCl_3$) δ -61.8.

M.p. 154.5-155.1 ºC.

HRMS (ESI): $[M+H]^+$ calcd. for $C_{20}H_{16}F_3N_2O_2^+$ 373.1158, found 373.1166.



2-(4-methoxyphenyl)-7-methyl-3-(trifluoromethyl)pyrimido[1,6-*a*]indol-1(*2H*)-one **(3l)**

Upon completion the mixture was concentrated and purified via flash column chromatography (petroleum ether / ethyl acetate = 10:1, R_f = 0.3) to give the titled product **3l** as a white solid (53.6 mg, 72%).

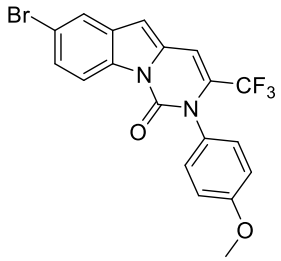
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.50 (d, *J* = 8.5 Hz, 1H), 7.54 (s, 1H), 7.34 (d, *J* = 8.5 Hz, 2H), 7.30 – 7.26 (m, 1H), 7.08– 7.05 (m, 3H), 6.80 (s, 1H), 3.91 (s, 3H), 2.55 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 160.2, 148.5, 134.2, 132.2, 131.3, 131.1, 130.6, 128.4, 127.5 (q, $^2J_{(C-F)}$ = 33.2 Hz), 126.1, 124.3, 120.23 120.2 (q, $^1J_{(C-F)}$ = 272.5 Hz), 116.0, 114.4, 102.9, 101.8 (q, $^3J_{(C-F)}$ = 6.2 Hz), 55.6, 21.7.

^{19}F NMR (376 MHz, $CDCl_3$) δ -61.8.

M.p. 215.0-215.9 ºC.

HRMS (ESI): $[M+H]^+$ calcd. for $C_{20}H_{16}F_3N_2O_2^+$ 373.1158, found 373.1168.



7-bromo-2-(4-methoxyphenyl)-3-(trifluoromethyl)pyrimido[1,6-*a*]indol-1(*2H*)-one

(3m)

Upon completion the mixture was concentrated and purified via flash column chromatography (petroleum ether / ethyl acetate = 10:1, R_f = 0.3) to give the titled product **3m** as a white solid (66.3 mg, 76%).

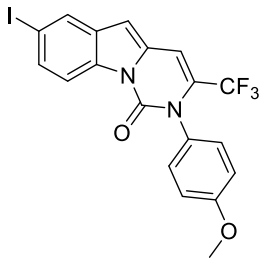
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.46 (d, *J* = 8.9 Hz, 1H), 7.84 (s, 1H), 7.48 (dd, *J* = 8.9, 1.9 Hz, 1H), 7.30 (d, *J* = 8.4 Hz, 2H), 7.06 – 7.01 (m, 3H), 6.76 (s, 1H), 3.88 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 160.4, 148.2, 132.5, 132.3, 131.9, 131.0, 128.5 (q, $^2J_{(C-F)}$ = 33.5 Hz), 127.3, 123.0, 120.0 (q, $^1J_{(C-F)}$ = 272.8 Hz), 118.0, 117.7, 114.5, 102.2, 101.4 (q, $^3J_{(C-F)}$ = 6.2 Hz), 55.6.

^{19}F NMR (376 MHz, $CDCl_3$) δ -62.0.

M.p. 196.8-197.9 ºC.

HRMS (ESI): $[M+H]^+$ calcd. for $C_{19}H_{13}BrF_3N_2O_2^+$ 437.0107, found 437.0109.



7-iodo-2-(4-methoxyphenyl)-3-(trifluoromethyl)pyrimido[1,6-*a*]indol-1(*2H*)-one **(3n)**

Upon completion the mixture was concentrated and purified via flash column chromatography (petroleum ether / ethyl acetate = 10:1, R_f = 0.3) to give the titled product **3n** as a white solid (58.1 mg, 60%).

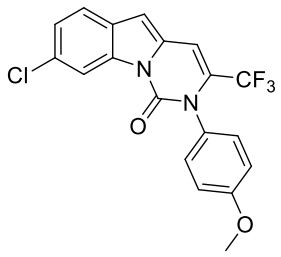
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.34 (d, *J* = 8.8 Hz, 1H), 8.07 (d, *J* = 1.4 Hz, 1H), 7.66 (dd, *J* = 8.8, 1.4 Hz, 1H), 7.30 (d, *J* = 8.7 Hz, 2H), 7.07 (s, 1H), 7.02 (d, *J* = 8.8 Hz, 2H), 6.76 (s, 1H), 3.88 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 160.4, 148.3, 133.1, 132.9, 132.5, 131.9, 131.0, 129.4, 128.6 (q, $^2J_{(C-F)}$ = 33.8 Hz), 128.0, 120.0 (q, $^1J_{(C-F)}$ = 273.0 Hz), 118.1, 114.5, 101.9, 101.5 (q, $^3J_{(C-F)}$ = 6.4 Hz), 89.1, 55.6.

^{19}F NMR (376 MHz, $CDCl_3$) δ -62.0.

M.p. 196.8-197.9 ºC.

HRMS (ESI): $[M+H]^+$ calcd. for $C_{19}H_{13}F_3IN_2O_2^+$ 484.9968, found 484.9972.



8-chloro-2-(4-methoxyphenyl)-3-(trifluoromethyl)pyrimido[1,6-*a*]indol-1(*2H*)-one **(3o)**

Upon completion the mixture was concentrated and purified via flash column chromatography (petroleum ether / ethyl acetate = 10:1, R_f = 0.3) to give the titled product **3o** as a yellow solid (53.3 mg, 68%).

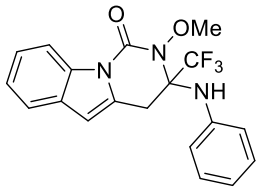
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.61 (s, 1H), 7.61 (d, *J* = 8.5 Hz, 1H), 7.37 (dd, *J* = 8.5, 1.1 Hz, 1H), 7.30 (d, *J* = 8.4 Hz, 2H), 7.05 – 7.01 (m, 3H), 6.78 (s, 1H), 3.88 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 160.4, 148.3, 134.0, 131.8, 131.0, 130.2, 128.7, 128.1, 128.1 (q, $^2J_{(C-F)}$ = 32.7 Hz), 125.3, 121.3, 120.1 (q, $^1J_{(C-F)}$ = 272.7 Hz), 116.5, 114.5, 102.9, 101.7 (q, $^3J_{(C-F)}$ = 6.2 Hz), 56.4.

^{19}F NMR (376 MHz, $CDCl_3$) δ -61.9.

M.p. 193.3-194.5 ºC.

HRMS (ESI): $[M+H]^+$ calcd. for $C_{19}H_{13}ClF_3N_2O_2^+$ 393.0612, found 393.0610.



2-methoxy-3-(phenylamino)-3-(trifluoromethyl)-3,4-dihydropyrimido[1,6-*a*]indol-1(*2H*)-one **(4a)**

Upon completion the mixture was concentrated and purified via flash column chromatography (petroleum ether / ethyl acetate = 10:1, R_f = 0.3) to give the titled product **4a** as a yellow solid (51.8 mg, 69%).

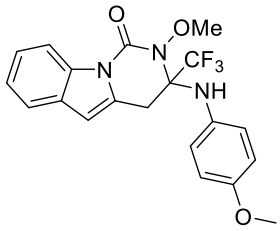
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.23 (d, *J* = 8.1 Hz, 1H), 7.39 (d, *J* = 7.5 Hz, 1H), 7.25 – 7.22 (m, 1H), 7.18 (t, *J* = 7.4 Hz, 1H), 7.08 (t, *J* = 7.7 Hz, 2H), 7.00 (d, *J* = 7.6 Hz, 2H), 6.91 (t, *J* = 7.3 Hz, 1H), 6.21 (s, 1H), 4.62 (s, 1H), 4.02 (s, 3H),3.63 (dd, *J* = 108.2, 17.0 Hz, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 151.8, 140.0, 135.3, 129.9, 129.0, 128.6, 125.7, 125.3, 124.4, 123.8 (q, $^1J_{(C-F)}$ = 289.2 Hz), 123.7, 120.2, 115.4, 105.6, 79.6 (q, $^2J_{(C-F)}$ = 27.7 Hz), 64.5, 27.4.

^{19}F NMR (376 MHz, $CDCl_3$) δ -77.0.

M.p. 150.9-152.1 ºC.

HRMS (ESI): $[M+H]^+$ calcd. for $C_{19}H_{17}F_3N_3O_2^+$ 376.1267, found 376.1266.



2-methoxy-3-((4-methoxyphenyl)amino)-3-(trifluoromethyl)-3,4-dihydropyrimido[1,6-*a*]indol-1(*2H*)-one **(4b)**

Upon completion the mixture was concentrated and purified via flash column chromatography (petroleum ether / ethyl acetate = 10:1, R_f = 0.3) to give the titled product **4b** as a yellow solid (67.3 mg, 83%).

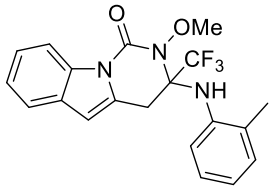
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.26 (d, *J* = 8.1 Hz, 1H), 7.41 (d, *J* = 7.6 Hz, 1H), 7.30 – 7.28 (m, 1H), 7.22 (t, *J* = 7.4 Hz, 1H), 6.99 – 6.97 (m, 2H), 6.59 – 6.57 (m, 2H), 6.18 (s, 1H), 4.52 (s, 1H), 4.10 (s, 3H),3.57 (q, *J* = 16.9 Hz, 2H), 3.56 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 157.9, 151.9, 135.3, 132.2, 129.8, 128.7, 128.6, 124.3, 123.8 (q, $^1J_{(C-F)}$ = 288.5 Hz), 123.6, 120.1, 115.3, 114.1, 105.4, 79.9 (q, $^2J_{(C-F)}$ = 27.7 Hz), 64.4, 55.5, 27.6.

^{19}F NMR (377 MHz, $CDCl_3$) δ -76.7.

M.p. 150.9-152.1 ºC.

HRMS (ESI): $[M+H]^+$ calcd. for $C_{20}H_{19}F_3N_3O_3^+$ 406.1373, found 406.1375.



2-methoxy-3-(o-tolylamino)-3-(trifluoromethyl)-3,4-dihydropyrimido[1,6-*a*]indol-1(*2H*)-one **(4c)**

Upon completion the mixture was concentrated and purified via flash column chromatography (petroleum ether / ethyl acetate = 10:1, Rf = 0.3) to give the titled product **4c** as a yellow solid (68.5 mg, 88%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.21 (d, *J* = 8.2 Hz, 1H), 7.30 (d, *J* = 7.6 Hz, 1H), 7.21 (d, *J* = 7.5 Hz, 1H), 7.12 (t, *J* = 7.5 Hz, 1H), 7.03 (d, *J* = 7.8 Hz, 1H), 6.96 (d, *J* = 7.4

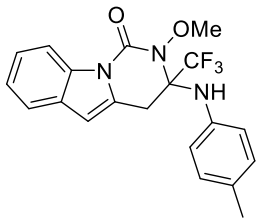
Hz, 1H), 6.85 (t, *J* = 7.5 Hz, 1H), 6.77 (t, *J* = 7.3 Hz, 1H), 6.06 (s, 1H), 4.30 (s, 1H), 3.97 (s, 3H), 3.59 (dd, *J* = 167.8, 17.1 Hz, 2H), 2.21 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 151.4, 138.4, 135.3, 133.1, 130.9, 129.7, 128.3, 126.3, 124.7, 124.3, 123.9 (q, *J* = 288.8 Hz), 123.5, 120.1, 115.3, 105.2, 79.2 (q, *J* = 21.9 Hz), 64.5, 32.4, 26.5, 17.8.

^{19}F NMR (376 MHz, $CDCl_3$) δ -78.1.

M.p. 91.6-92.8 ºC.

HRMS (ESI): $[M+H]^+$ calcd. for $C_{20}H_{19}F_3N_3O_2^+$ 390.1424, found 390.1426.



2-methoxy-3-(p-tolylamino)-3-(trifluoromethyl)-3,4-dihydropyrimido[1,6-*a*]indol-1(*2H*)-one **(4d)**

Upon completion the mixture was concentrated and purified via flash column chromatography (petroleum ether / ethyl acetate = 10:1, Rf = 0.3) to give the titled product **4d** as a yellow solid (61.5 mg, 79%).

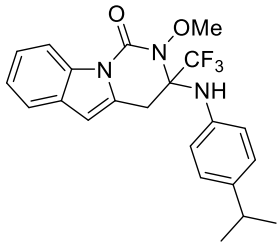
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 (d, *J* = 8.2 Hz, 1H), 7.33 (d, *J* = 7.6 Hz, 1H), 7.18 (t, *J* = 6.9 Hz, 1H), 7.12 (d, *J* = 6.9 Hz, 1H), 6.81 (q, *J* = 8.3 Hz, 4H), 6.12 (s, 1H), 4.47 (s, 1H), 3.97 (s, 3H), 3.51 (dd, *J* = 91.5, 16.9 Hz, 2H), 2.01 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 151.8, 137.1, 135.3, 135.3, 129.8, 129.5, 128.6, 126.1, 124.3, 123.8 (q, $^{1}J_{(C-F)}$ = 289.1 Hz), 123.5, 120.1, 115.3, 105.5, 79.6 (q, $^{2}J_{(C-F)}$ = 27.9 Hz), 64.4, 27.4, 20.7.

^{19}F NMR (376 MHz, $CDCl_3$) δ -76.9.

M.p. 89.6-90.4 ºC.

HRMS (ESI): $[M+H]^+$ calcd. for $C_{20}H_{19}F_3N_3O_2^+$ 390.1424, found 390.1425.



3-((4-isopropylphenyl)amino)-2-methoxy-3-(trifluoromethyl)-3,4-dihydropyrimido[1,6-*a*]indol-1(*2H*)-one **(4e)**

Upon completion the mixture was concentrated and purified via flash column chromatography (petroleum ether / ethyl acetate = 10:1, R_f = 0.3) to give the titled product **4e** as a yellow solid (55.1 mg, 66%).

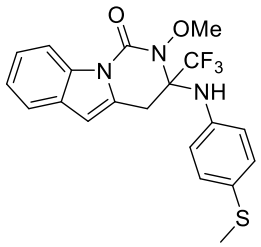
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.18 (d, *J* = 8.1 Hz, 1H), 7.34 (dd, *J* = 7.3, 1.6 Hz, 1H), 7.17 (dd, *J* = 14.2, 8.2 Hz, 2H), 6.95 (d, *J* = 8.4 Hz, 2H), 6.85 – 6.83 (m, 2H), 6.12 (s, 1H), 4.60 (s, 1H), 4.07 (s, 3H), 3.62 (dd, *J* = 72.4, 16.9 Hz, 2H), 2.59 (s, 1H), 0.91 (d, *J* = 6.9 Hz, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 151.7, 146.6, 136.9, 135.1, 129.7, 128.5, 126.6, 124.1, 123.7 (q, $^1J_{(C-F)}$ = 287.8 Hz), 123.4, 119.9, 115.1, 105.2, 79.6 (q, $^2J_{(C-F)}$ = 27.8 Hz), 64.2, 33.4, 27.6, 23.7.

^{19}F NMR (376 MHz, $CDCl_3$) δ -77.6.

M.p. 116.3-117.5 ºC.

HRMS (ESI): $[M+H]^+$ calcd. for $C_{22}H_{23}F_3N_3O_2^+$ 418.1737, found 418.1736.



2-methoxy-3-((4-(methylthio)phenyl)amino)-3-(trifluoromethyl)-3,4-dihydropyrimido[1,6-*a*]indol-1(*2H*)-one **(4f)**

Upon completion the mixture was concentrated and purified via flash column chromatography (petroleum ether / ethyl acetate = 10:1, R_f = 0.3) to give the titled product **4f** as a white solid (71.6 mg, 85%).

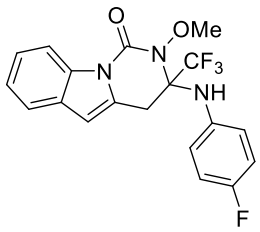
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.28 (d, *J* = 7.6 Hz, 1H), 7.44 (d, *J* = 7.5 Hz, 1H), 7.32 – 7.28 (m, 1H), 7.24 (t, *J* = 7.5 Hz, 1H), 6.98 (d, *J* = 3.3 Hz, 4H), 6.23 (s, 1H), 4.63 (s, 1H), 4.08 (s, 3H), 3.63 (dd, *J* = 72.5, 16.9 Hz, 2H), 2.22 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 151.7, 137.2, 135.5, 135.2, 129.7, 128.4, 127.9, 126.7, 124.4, 123.7 (q, $^1J_{(C-F)}$ = 287.4 Hz), 123.6, 120.1, 115.3, 105.6, 79.6 (q, $^2J_{(C-F)}$ = 27.8 Hz), 64.4, 27.4, 16.5.

^{19}F NMR (376 MHz, $CDCl_3$) δ -77.0.

M.p. 107.3-109.2 ºC.

HRMS (ESI): $[M+H]^+$ calcd. for $C_{20}H_{19}F_3N_3O_2S^+$ 422.1145, found 422.1146.



2-((4-fluorophenyl)amino)-2-methoxy-3-(trifluoromethyl)-3,4-dihydropyrimido[1,6-*a*]indol-1(*2H*)-one **(4g)**

Upon completion the mixture was concentrated and purified via flash column chromatography (petroleum ether / ethyl acetate = 10:1, R_f = 0.3) to give the titled product **4g** as a red solid (43.2 mg, 55%).

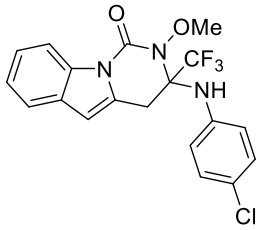
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.29 (d, *J* = 8.1 Hz, 1H), 7.46 (d, *J* = 7.6 Hz, 1H), 7.31 (d, *J* = 6.4 Hz, 1H), 7.26 (d, *J* = 7.3 Hz, 1H), 7.04 (dd, *J* = 7.3, 5.7 Hz, 2H), 6.79 (s, 2H), 6.25 (s, 1H), 4.60 (s, 1H), 4.11 (s, 3H), 3.62 (q, *J* = 16.9 Hz, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 160.8 (d, $^1J_{(C-F)}$ = 245.6 Hz), 151.8, 135.6 (d, $^4J_{(C-F)}$ = 2.8 Hz), 135.3, 129.8, 128.5 (d, $^3J_{(C-F)}$ = 8.4 Hz), 128.5, 124.6, 123.8, 123.7 (q, $^1J_{(C-F)}$ = 288.5 Hz), 120.2, 115.7 (d, $^2J_{(C-F)}$ = 22.6 Hz), 115.3, 105.6, 79.6 (q, $^2J_{(C-F)}$ = 27.2 Hz), 64.4, 27.5.

^{19}F NMR (376 MHz, $CDCl_3$) δ -76.9, -117.0.

M.p. 128.1-129.8 ºC.

HRMS (ESI): $[M+H]^+$ calcd. for $C_{19}H_{16}F_4N_3O_2^+$ 394.1173, found 394.1173.



3-((4-chlorophenyl)amino)-2-methoxy-3-(trifluoromethyl)-3,4-dihydropyrimido[1,6-*a*]indol-1(*2H*)-one **(4h)**

Upon completion the mixture was concentrated and purified via flash column chromatography (petroleum ether / ethyl acetate = 10:1, R_f = 0.3) to give the titled product **4h** as a yellow solid (49.1 mg, 60%).

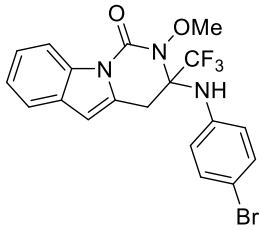
^{1}H NMR (400 MHz, CDCl$_3$) δ 8.28 (d, *J* = 8.2 Hz, 1H), 7.46 (d, *J* = 7.7 Hz, 1H), 7.31 (t, *J* = 7.7 Hz, 1H), 7.27 – 7.22 (m, 1H), 7.07 (d, *J* = 8.4 Hz, 2H), 6.96 (d, *J* = 8.5 Hz, 2H), 6.27 (s, 1H), 4.60 (s, 1H), 4.05 (s, 3H), 3.61 (dd, *J* = 71.9, 17.0 Hz, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 151.7, 138.5, 135.2, 131.0, 129.7, 129.0, 128.1, 127.0, 124.6, 123.8, 123.6 (q, $^1J_{(C-F)}$ = 288.9 Hz), 120.2, 115.3, 105.8, 79.4 (q, $^2J_{(C-F)}$ = 27.8 Hz), 64.4, 27.3.

^{19}F NMR (376 MHz, CDCl$_3$) δ -76.7.

M.p. 110.3-112.2 ºC.

HRMS (ESI): $[M+H]^+$ calcd. for $C_{19}H_{16}ClF_3N_3O_2^+$ 410.0878, found 410.0877.



3-((4-bromophenyl)amino)-2-methoxy-3-(trifluoromethyl)-3,4-dihydropyrimido[1,6-*a*]indol-1(*2H*)-one **(4i)**

Upon completion the mixture was concentrated and purified via flash column chromatography (petroleum ether / ethyl acetate = 10:1, R_f = 0.3) to give the titled

product **4i** as a yellow solid (56.2 mg, 62%).

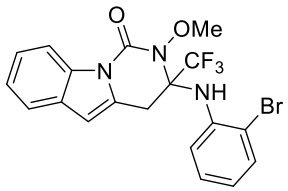
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.27 (d, *J* = 8.1 Hz, 1H), 7.46 (d, *J* = 7.6 Hz, 1H), 7.30 (t, *J* = 7.1 Hz, 1H), 7.24 – 7.21 (m, 3H), 6.89 (d, *J* = 8.6 Hz, 2H), 6.27 (s, 1H), 4.59 (s, 1H), 4.04 (s, 3H), 3.61 (dd, *J* = 76.4, 17.0 Hz, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 151.7, 139.1, 135.2, 132.0, 129.7, 128.1, 127.2, 124.6, 123.8, 123.6 (q, $^1J_{(C-F)}$ = 289.2 Hz), 120.2, 118.6, 115.3, 105.8, 79.3 (q, $^2J_{(C-F)}$ = 27.9 Hz), 64.4, 27.2.

^{19}F NMR (376 MHz, $CDCl_3$) δ -76.6.

M.p. 105.1-107.0 ºC.

HRMS (ESI): $[M+H]^+$ calcd. for $C_{19}H_{16}BrF_3N_3O_2^+$ 454.0373, found 454.0369.



3-((2-bromophenyl)amino)-2-methoxy-3-(trifluoromethyl)-3,4-dihydropyrimido[1,6-*a*]indol-1(*2H*)-one **(4j)**

Upon completion the mixture was concentrated and purified via flash column chromatography (petroleum ether / ethyl acetate = 10:1, R_f = 0.3) to give the titled product **4j** as a yellow solid (54.4 mg, 60%).

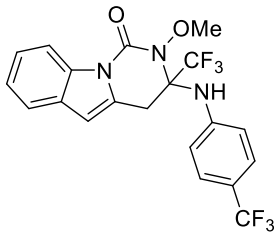
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.32 (d, *J* = 8.2 Hz, 1H), 7.40 (t, *J* = 6.9 Hz, 2H), 7.30 (t, *J* = 7.7 Hz, 1H), 7.21 (dd, *J* = 14.0, 7.6 Hz, 2H), 7.09 (t, *J* = 7.7 Hz, 1H), 6.77 (t, *J* = 7.6 Hz, 1H), 6.20 (s, 1H), 4.97 (s, 1H), 4.07 (s, 1H), 4.02 (s, 3H), 3.78 (dd, *J* = 210.4, 17.2 Hz, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 151.4, 139.0, 135.5, 133.2, 129.8, 128.0, 128.0, 124.7, 124.6, 123.7 (q, $^1J_{(C-F)}$ = 289.3 Hz), 123.8, 123.3, 120.3, 115.5, 105.8, 79.1 (q, $^2J_{(C-F)}$ = 29.0 Hz), 64.7, 27.0.

^{19}F NMR (376 MHz, $CDCl_3$) δ -77.5.

M.p. 117.3-120.6 ºC.

HRMS (ESI): $[M+H]^+$ calcd. for $C_{19}H_{16}BrF_3N_3O_2^+$ 454.0373, found 454.0377.



2-methoxy-3-(trifluoromethyl)-3-((4-(trifluoromethyl)phenyl)amino)-3,4-dihydropyrimido[1,6-*a*]indol-1(*2H*)-one **(4k)**

Upon completion the mixture was concentrated and purified via flash column chromatography (petroleum ether / ethyl acetate = 10:1, R_f = 0.3) to give the titled product **4k** as a yellow solid (67.4 mg, 76%).

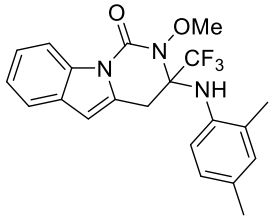
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.32 (d, *J* = 8.1 Hz, 1H), 7.49 (d, *J* = 7.7 Hz, 1H), 7.42 (d, *J* = 8.3 Hz, 2H), 7.34 (t, *J* = 7.7 Hz, 1H), 7.30 – 7.26 (m, 1H), 7.13 (d, *J* = 8.3 Hz, 2H), 6.34 (s, 1H), 4.86 (s, 1H), 4.05 (s, 3H), 3.75 (dd, *J* = 120.0, 17.2 Hz, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 151.6, 143.8, 135.3, 129.8, 127.9, 126.8 (q, $^3J_{(C-F)}$ = 34.0 Hz), 126.8 (q, $^2J_{(C-F)}$ = 34.0 Hz), 124.8, 124.0 (q, $^1J_{(C-F)}$ = 271.6 Hz), 124.0, 123.8, 123.6 (q, $^1J_{(C-F)}$ = 289.8 Hz), 120.4, 115.4, 106.2, 79.2 (q, $^2J_{(C-F)}$ = 28.4 Hz), 64.6, 28.7.

^{19}F NMR (376 MHz, $CDCl_3$) δ -62.9, -76.7.

M.p. 115.2-117.1 ºC.

HRMS (ESI): $[M+H]^+$ calcd. for $C_{20}H_{16}F_6N_3O_2^+$ 444.1141, found 444.1140.



3-((2,4-dimethylphenyl)amino)-2-methoxy-3-(trifluoromethyl)-3,4-dihydropyrimido[1,6-*a*]indol-1(*2H*)-one **(4l)**

Upon completion the mixture was concentrated and purified via flash column chromatography (petroleum ether / ethyl acetate = 10:1, R_f = 0.3) to give the titled product **4l** as a yellow solid (70.1 mg, 87%).

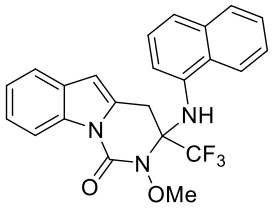
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.27 (d, *J* = 8.0 Hz, 1H), 7.42 (d, *J* = 7.6 Hz, 1H), 7.29 (dd, *J* = 9.7, 5.7 Hz, 1H), 7.22 (t, *J* = 7.4 Hz, 1H), 6.91 – 6.69 (m, 3H), 6.18 (s, 1H), 4.57 (s, 1H), 4.09 (s, 3H), 3.63 (dd, *J* = 83.5, 16.8 Hz, 2H), 1.98 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 151.9, 137.3, 137.2, 135.3, 134.2, 129.9, 129.8, 128.8, 127.6, 124.2, 123.9, 123.8 (q, $^1J_{(C-F)}$ = 288.4 Hz), 123.5, 120.0, 115.3, 105.3, 79.7 (q, $^2J_{(C-F)}$ = 27.7 Hz), 64.4, 27.6, 19.6, 19.0.

^{19}F NMR (376 MHz, $CDCl_3$) δ -77.3.

M.p. 106.9-108.8 ºC.

HRMS (ESI): $[M+H]^+$ calcd. for $C_{21}H_{21}F_3N_3O_2^+$ 404.1580, found 404.1582.



2-methoxy-3-(naphthalen-1-ylamino)-3-(trifluoromethyl)-3,4-dihydropyrimido[1,6-*a*]indol-1(*2H*)-one **(4m)**

Upon completion the mixture was concentrated and purified via flash column chromatography (petroleum ether / ethyl acetate = 10:1, R_f = 0.3) to give the titled product **4m** as a yellow solid (51.0 mg, 60%).

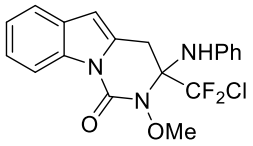
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.33 (d, *J* = 8.4 Hz, 1H), 8.19 (d, *J* = 8.2 Hz, 1H), 7.66 (d, *J* = 8.1 Hz, 1H), 7.53 (dd, *J* = 8.1, 7.1 Hz, 1H), 7.45 (t, *J* = 7.5 Hz, 1H), 7.33 (d, *J* = 8.3 Hz, 1H), 7.20 (d, *J* = 7.4 Hz, 2H), 7.13 (s, 2H), 6.99 (t, *J* = 7.8 Hz, 1H), 5.38 (s, 1H), 4.85 (s, 1H), 4.15 (s, 3H), 3.53 (dd, *J* = 120.3, 16.8 Hz, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 151.6, 135.6, 135.1, 134.2, 132.3, 129.5, 128.1, 127.9, 126.5, 126.3, 126.1, 124.9, 124.0, 123.9, 123.9 (q, $^1J_{(C-F)}$ = 287.0 Hz), 123.3, 122.7, 119.8, 115.1, 104.8, 79.9 (q, $^2J_{(C-F)}$ = 28.3 Hz), 64.4, 26.6.

^{19}F NMR (376 MHz, $CDCl_3$) δ -78.4.

M.p. 146.8-148.0 ºC.

HRMS (ESI): $[M+H]^+$ calcd. for $C_{23}H_{19}F_3N_3O_2^+$ 426.1424, found 426.1434.



3-(chlorodifluoromethyl)-2-methoxy-3-(phenylamino)-3,4-dihydropyrimido[1,6-*a*]indol-1(*2H*)-one **(4o)**

Upon completion the mixture was concentrated and purified via flash column chromatography (petroleum ether / ethyl acetate = 10:1, R_f = 0.3) to give the titled product **4o** as a yellow solid (34.4 mg, 44%).

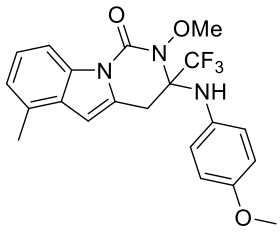
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.34 (d, *J* = 8.1 Hz, 1H), 7.47 (d, *J* = 7.6 Hz, 1H), 7.32 - 7.26 (m, 2H), 7.18 (t, *J* = 7.3 Hz, 2H), 7.09 (d, *J* = 7.8 Hz, 2H), 7.01 (t, *J* = 7.3 Hz, 1H), 6.29 (s, 1H), 4.79 (s, 1H), 4.12 (s, 3H), 3.78 (dd, *J* = 90.6, 17.1 Hz, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 151.7, 140.4, 135.4, 129.9, 129.3 (t, $^1J_{(C-F)}$ = 304.7 Hz), 129.1, 128.7, 125.2, 125.0, 124.4, 123.7, 120.2, 115.4, 105.5, 82.9 (t, $^2J_{(C-F)}$ = 24.0 Hz), 64.6, 28.2.

^{19}F NMR (376 MHz, $CDCl_3$) δ -61.7 (dd, *J* = 410.3, 167.4 Hz).

M.p. 117.8-119.5 °C.

HRMS (ESI): $[M+H]^+$ calcd. for $C_{19}H_{17}ClF_2N_3O_2^+$ 392.0972, found 392.0972.



2-methoxy-3-((4-methoxyphenyl)amino)-6-methyl-3-(trifluoromethyl)-3,4-dihydropyrimido[1,6-*a*]indol-1(*2H*)-one **(4p)**

Upon completion the mixture was concentrated and purified via flash column chromatography (petroleum ether / ethyl acetate = 10:1, R_f = 0.3) to give the titled product **4p** as a yellow solid (67.1 mg, 80%).

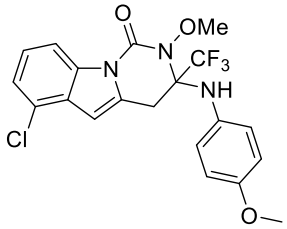
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (d, *J* = 8.1 Hz, 1H), 7.16 (t, *J* = 7.3 Hz, 1H), 7.00 (d, *J* = 7.2 Hz, 1H), 6.95 (d, *J* = 7.6 Hz, 2H), 6.55 (d, *J* = 7.6 Hz, 2H), 6.18 (s, 1H), 4.48 (s, 1H), 4.07 (s, 3H), 3.55 (s, 3H), 3.54 (q, *J* = 16.9 Hz, 2H), 2.43 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 157.7, 151.9, 135.0, 132.3, 129.4, 128.4, 128.0, 124.3, 123.9, 123.7 (q, $^1J_{(C-F)}$ = 288.7 Hz), 114.0, 112.8, 79.8 (q, $^2J_{(C-F)}$ = 27.3 Hz), 64.3, 55.4, 27.5, 18.4.

^{19}F NMR (376 MHz, $CDCl_3$) δ -77.0.

M.p. 127.9-129.4 ºC.

HRMS (ESI): $[M+H]^+$ calcd. for $C_{21}H_{21}F_3N_3O_3^+$ 420.1530, found 420.1530.



6-chloro-2-methoxy-3-((4-methoxyphenyl)amino)-3-(trifluoromethyl)-3,4-dihydropyrimido[1,6-*a*]indol-1(*2H*)-one **(4q)**

Upon completion the mixture was concentrated and purified via flash column chromatography (petroleum ether / ethyl acetate = 10:1, R_f = 0.3) to give the titled product **4q** as a yellow solid (80.8 mg, 92%).

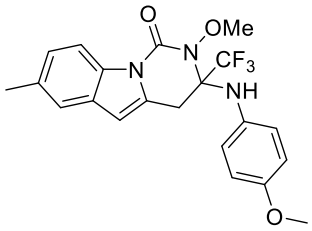
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12 (dd, *J* = 7.3, 1.4 Hz, 1H), 7.20 (s, 1H), 7.20 – 7.14 (m, 2H), 6.94 (d, *J* = 8.8 Hz, 2H), 6.54 (d, *J* = 8.8 Hz, 2H), 6.26 (s, 1H), 4.50 (s, 1H), 4.07 (s, 3H), 3.56 (q, *J* = 17.0 Hz, 2H), 3.54 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 157.9, 151.5, 135.7, 131.8, 129.4, 128.5, 128.5, 125.1, 125.0, 123.2, 120.7 (q, $^1J_{(C-F)}$ = 276.1 Hz), 114.0, 113.7, 103.4, 79.9 (q, $^2J_{(C-F)}$ = 27.5 Hz), 64.3, 55.4, 27.6.

^{19}F NMR (376 MHz, $CDCl_3$) δ -77.3.

M.p. 140.5-142.1 ºC.

HRMS (ESI): $[M+H]^+$ calcd. for $C_{20}H_{18}ClF_3N_3O_3^+$ 440.0983, found 440.0982.



2-methoxy-3-((4-methoxyphenyl)amino)-7-methyl-3-(trifluoromethyl)-3,4-dihydropyrimido[1,6-*a*]indol-1(*2H*)-one **(4r)**

Upon completion the mixture was concentrated and purified via flash column chromatography (petroleum ether / ethyl acetate = 10:1, R_f = 0.3) to give the titled product **4r** as a white solid (82.2 mg, 98%).

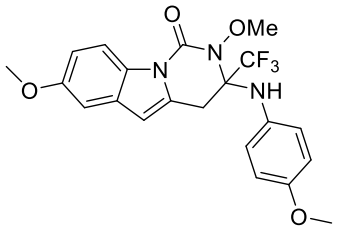
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (d, *J* = 8.4 Hz, 1H), 7.08 (s, 1H), 6.98 (d, *J* = 9.2 Hz, 1H), 6.85 (d, *J* = 8.8 Hz, 2H), 6.47 (d, *J* = 8.8 Hz, 2H), 5.98 (s, 1H), 4.39 (s, 1H), 3.97 (s, 3H), 3.45 (s, 3H), 3.42 (q, *J* = 16.9 Hz, 2H), 2.31 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 157.7, 151.8, 133.4, 133.0, 130.0, 128.6, 128.4, 125.5, 123.8 (q, $^1J_{(C-F)}$ = 288.5 Hz), 120.0, 114.8, 114.0, 105.2, 79.8 (q, $^2J_{(C-F)}$ = 27.4 Hz), 64.3, 55.3, 27.5, 21.4.

^{19}F NMR (376 MHz, $CDCl_3$) δ -77.0.

M.p. 147.2-148.5 ºC.

HRMS (ESI): $[M+H]^+$ calcd. For $C_{21}H_{21}F_3N_3O_3^+$ 420.1530, found 420.1534.



2,7-dimethoxy-3-((4-methoxyphenyl)amino)-3-(trifluoromethyl)-3,4-dihydropyrimido[1,6-*a*]indol-1(*2H*)-one **(4s)**

Upon completion the mixture was concentrated and purified via flash column chromatography (petroleum ether / ethyl acetate = 10:1, R_f = 0.3) to give the titled product **4s** as a yellow solid (70.5 mg, 81%).

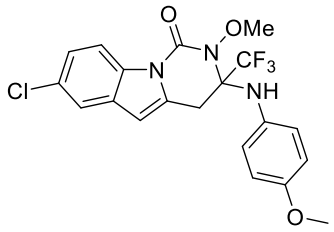
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10 (d, *J* = 7.9 Hz, 1H), 6.95 (d, *J* = 6.9 Hz, 1H), 6.86 (d, *J* = 7.5 Hz, 1H), 6.56 (d, *J* = 6.9 Hz, 2H), 6.08 (s, 1H), 4.49 (s, 1H), 4.06 (d, *J* = 1.3 Hz, 3H), 3.82 (s, 3H), 3.55 (s, 3H), 3.52 (q, *J* = 16.8 Hz, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 157.7, 156.5, 151.7, 132.2, 130.7, 129.8, 129.3, 128.4, 123.7 (q, $^{1}J_{(C-F)}$ = 288.6 Hz), 115.8, 114.0, 112.4, 105.2, 103.1, 79.9 (q, $^{2}J_{(C-F)}$ = 27.2 Hz), 64.3, 55.7, 55.4, 27.5.

^{19}F NMR (376 MHz, $CDCl_3$) δ -77.1.

M.p. 92.4-93.7 ºC.

HRMS (ESI): $[M+H]^+$ calcd. for $C_{21}H_{21}F_3N_3O_4^+$ 436.1479, found 436.1482.



7-chloro-2-methoxy-3-((4-methoxyphenyl)amino)-3-(trifluoromethyl)-3,4-dihydropyrimido[1,6-*a*]indol-1(*2H*)-one **(4t)**

Upon completion the mixture was concentrated and purified via flash column chromatography (petroleum ether / ethyl acetate = 10:1, R_f = 0.3) to give the titled product **4t** as a yellow solid (72.0 mg, 82%).

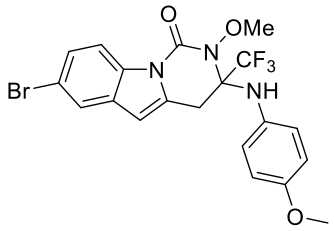
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12 (d, *J* = 8.8 Hz, 1H), 7.34 (d, *J* = 1.6 Hz, 1H), 7.19 (dd, *J* = 8.8, 1.8 Hz, 1H), 6.93 (d, *J* = 8.7 Hz, 2H), 6.53 (d, *J* = 8.7 Hz, 2H), 6.07 (s, 1H), 4.50 (s, 1H), 4.06 (s, 3H), 3.53 (s, 3H), 3.78 (q, *J* = 16.9 Hz, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 157.9, 151.5, 133.4, 131.8, 130.9, 130.1, 129.1, 128.6, 124.3, 123.6 (q, $^{1}J_{(C-F)}$ = 288.3 Hz), 119.6, 116.1, 114.0, 104.5, 79.9 (q, $^{2}J_{(C-F)}$ = 27.9 Hz), 64.3, 55.4, 27.6.

^{19}F NMR (376 MHz, $CDCl_3$) δ -77.4.

M.p. 117.8-120.5 ºC.

HRMS (ESI): $[M+H]^+$ calcd. for $C_{20}H_{18}ClF_3N_3O_3^+$ 440.0983, found 440.0982.



7-bromo-2-methoxy-3-((4-methoxyphenyl)amino)-3-(trifluoromethyl)-3,4-dihydropyrimido[1,6-*a*]indol-1(*2H*)-one **(4u)**

Upon completion the mixture was concentrated and purified via flash column chromatography (petroleum ether / ethyl acetate = 10:1, R_f = 0.3) to give the titled product **4u** as a yellow solid (86.9 mg, 90%).

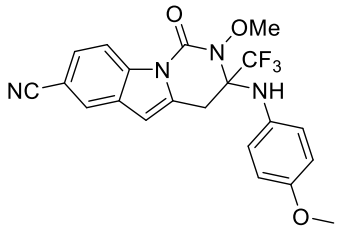
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12 (d, *J* = 8.8 Hz, 1H), 7.55 (d, *J* = 1.9 Hz, 1H), 7.38 (dd, *J* = 8.7, 2.0 Hz, 1H), 7.30 (s, 1H), 6.97 (d, *J* = 8.8 Hz, 2H), 6.57 (d, *J* = 8.8 Hz, 2H), 6.11 (s, 1H), 4.10 (s, 3H), 3.58 (s, 3H), 3.58 (q, *J* = 16.6 Hz, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 157.9, 151.5, 133.8, 131.8, 131.4, 123.0, 128.6, 127.0, 122.6, 123.6 (q, $^1J_{(C-F)}$ = 287.5 Hz), 119.3, 116.8, 116.5, 114.0, 104.4, 79.9 (q, $^2J_{(C-F)}$ = 27.4 Hz), 64.3, 55.4, 27.5.

^{19}F NMR (376 MHz, $CDCl_3$) δ -77.4.

M.p. 106.3-108.9 ºC.

HRMS (ESI): $[M+H]^+$ calcd. for $C_{20}H_{18}BrF_3N_3O_3^+$ 484.0478, found 484.0477.



2-methoxy-3-((4-methoxyphenyl)amino)-1-oxo-3-(trifluoromethyl)-1,2,3,4-tetrahydropyrimido[1,6-*a*]indole-7-carbonitrile **(4v)**

Upon completion the mixture was concentrated and purified via flash column chromatography (petroleum ether / ethyl acetate = 10:1, R_f = 0.3) to give the titled product **4v** as a yellow solid (62.8 mg, 73%).

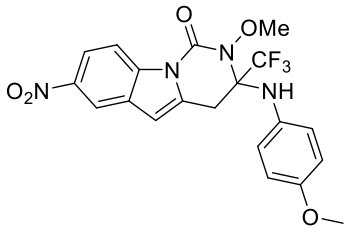
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.30 (d, *J* = 8.6 Hz, 1H), 7.70 (d, *J* = 1.6 Hz, 1H), 7.49 (d, *J* = 8.5 Hz, 1H), 6.94 (d, *J* = 8.5 Hz, 2H), 6.51 (d, *J* = 8.4 Hz, 2H), 6.19 (s, 1H), 4.52 (s, 1H), 4.07 (s, 3H), 3.59 (q, *J* = 16.7 Hz, 2H), 3.51 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 158.0, 151.2, 136.9, 131.5, 131.3, 129.7, 128.7, 127.4, 124.6, 123.4 (q, $^{1}J_{(C-F)}$ = 286.1 Hz), 119.6, 115.9, 114.0, 106.9, 104.6, 79.9 (q, $^{2}J_{(C-F)}$ = 27.8 Hz), 64.3, 55.4, 27.7.

^{19}F NMR (376 MHz, $CDCl_3$) δ -77.5.

M.p. 97.5-100.3 ºC.

HRMS (ESI): $[M+Na]^+$ calcd. for $C_{21}H_{17}F_3N_4NaO_3^+$ 453.1145, found 453.1131.



2-methoxy-3-((4-methoxyphenyl)amino)-7-nitro-3-(trifluoromethyl)-3,4-dihydropyrimido[1,6-*a*]indol-1(*2H*)-one **(4w)**

Upon completion the mixture was concentrated and purified via flash column chromatography (petroleum ether / ethyl acetate = 10:1, R_f = 0.3) to give the titled product **4w** as a yellow solid (56.7 mg, 63%).

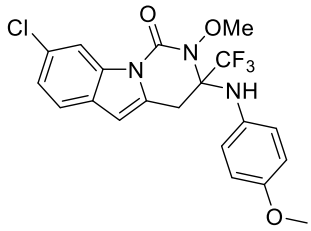
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.33 – 8.30 (m, 2H), 8.14 (dd, *J* = 9.0, 2.2 Hz, 1H), 6.96 – 6.94 (m, 2H), 6.52 (dd, *J* = 6.7, 2.1 Hz, 2H), 6.28 (s, 1H), 4.52 (s, 1H), 4.08 (s, 3H), 3.61 (q, *J* = 16.9 Hz, 2H), 3.50 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 158.1, 151.1, 144.3, 138.1, 132.0, 131.4, 129.5, 128.8, 123.4 (q, $^{1}J_{(C-F)}$ = 287.8 Hz), 119.5, 116.1, 115.2, 114.0, 105.4, 79.9 (q, $^{2}J_{(C-F)}$ = 27.7 Hz), 64.3, 55.3, 27.7.

^{19}F NMR (376 MHz, $CDCl_3$) δ -77.3.

M.p. 150.2-153.1 ºC.

HRMS (ESI): $[M+H]^+$ calcd. for $C_{20}H_{18}F_3N_4O_5^+$ 451.1224, found 451.1214.



8-chloro-2-methoxy-3-((4-methoxyphenyl)amino)-3-(trifluoromethyl)-3,4-dihydropyrimido[1,6-*a*]indol-1(*2H*)-one **(4x)**

Upon completion the mixture was concentrated and purified via flash column chromatography (petroleum ether / ethyl acetate = 10:1, R_f = 0.3) to give the titled product **4x** as a yellow solid (68.5 mg, 78%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.28 (s, 1H), 7.30 (d, *J* = 8.3 Hz, 1H), 7.18 (dd, *J* = 8.3, 1.5 Hz, 1H), 6.96 (d, *J* = 8.7 Hz, 2H), 6.56 (d, *J* = 8.7 Hz, 2H), 6.12 (s, 1H), 4.53 (s, 1H), 4.09 (s, 3H), 3.56 (s, 3H), 3.55 (q, *J* = 16.9 Hz, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 157.9, 151.5, 135.4, 131.9, 130.0, 129.3, 128.6, 128.2, 124.0, 123.6 (q, $^1J_{(C-F)}$ = 288.0 Hz), 120.6, 115.4, 114.0, 104.9, 79.8 (q, $^2J_{(C-F)}$ = 27.4 Hz), 64.3, 55.4, 27.5.

^{19}F NMR (376 MHz, $CDCl_3$) δ -77.4.

M.p. 108.0-109.6 ºC.

HRMS (ESI): $[M+H]^+$ calcd. for $C_{20}H_{18}ClF_3N_3O_3^+$ 440.0983, found 440.0984.

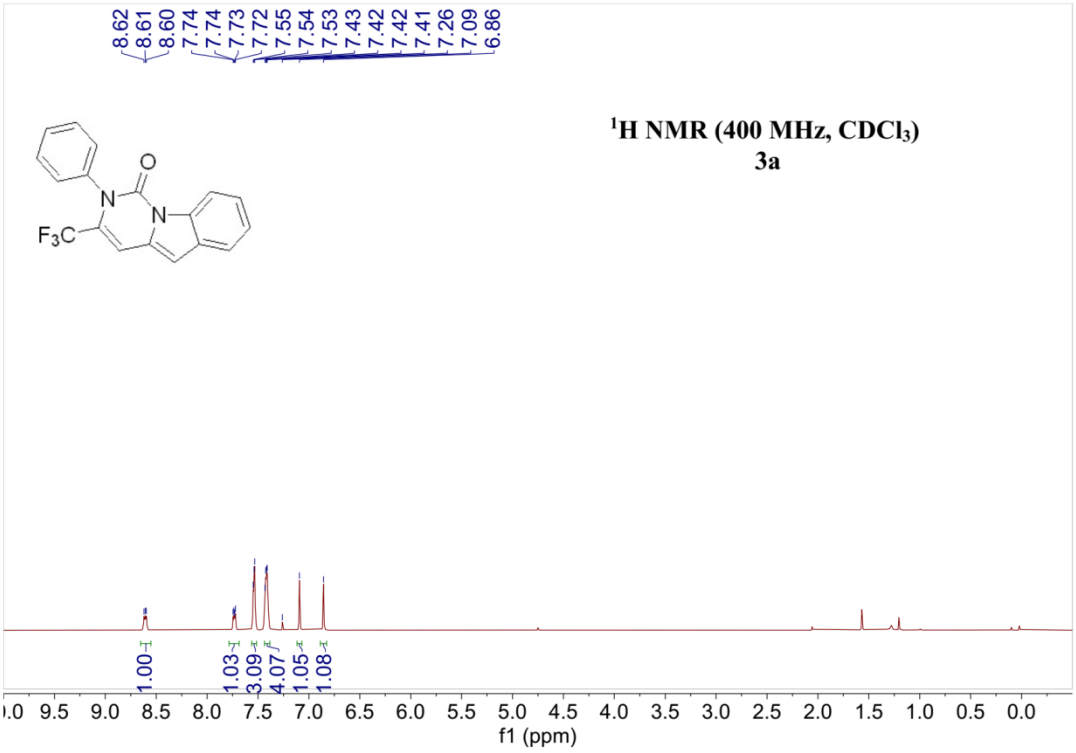
4. References

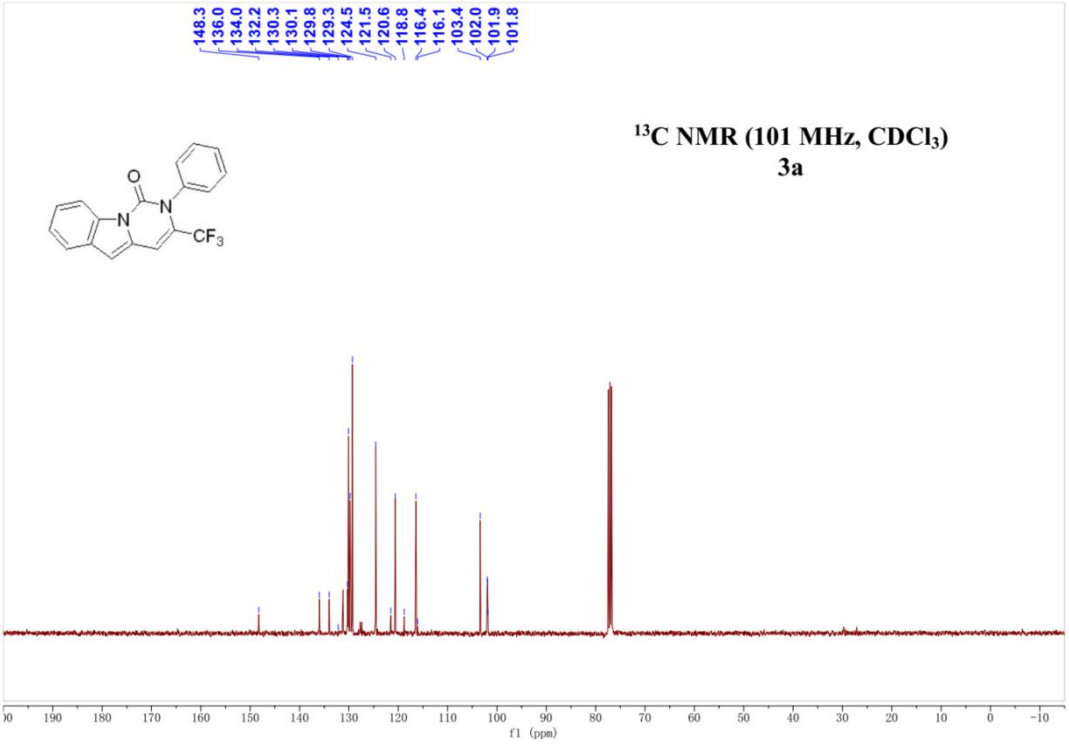
(1) Tamura, K.; Mizukami,H.; Maeda, K.; Watanabe, H.; Uneyama, K. One-pot synthesis of trifluoroacetimidoyl Halides. *J. Org. Chem.* **1993**, *58*, 32-35.

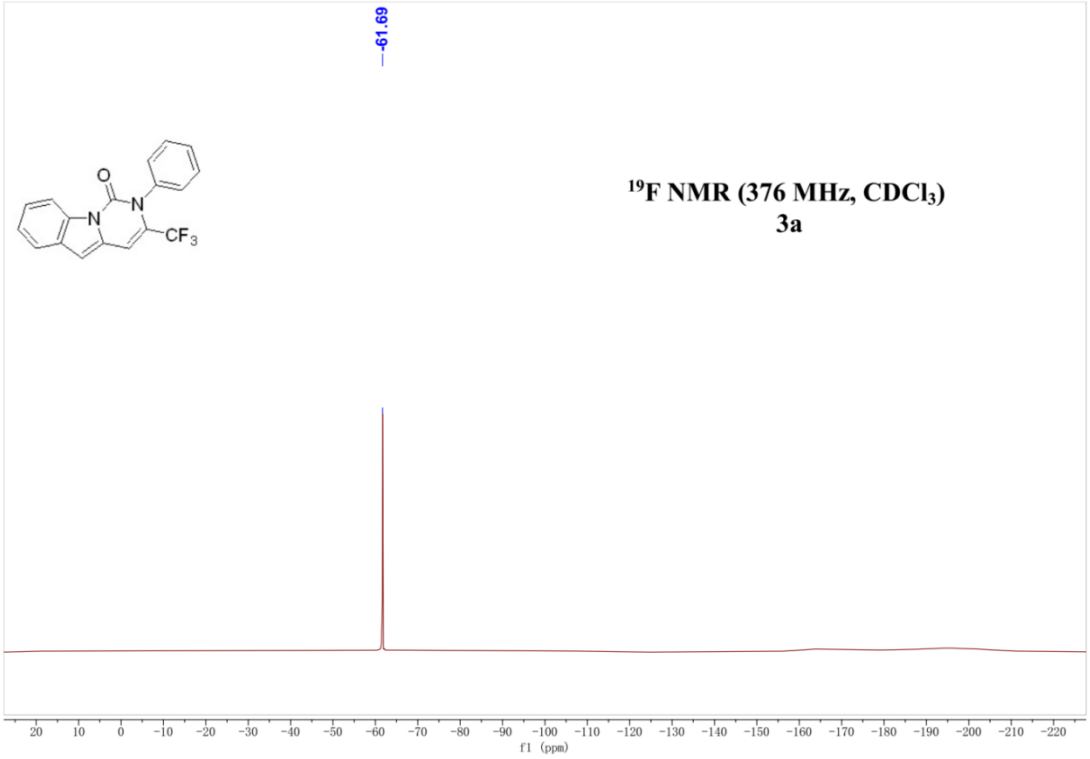
(2) (a) Wen, S.; Tian, Q.; Chen, Y.; Zhang, Y.; Cheng, G. Annulation of CF_3-imidoyl sulfoxonium ylides with 1,3-dicarbonyl compounds: Access to 1,2,3-trisubstituted 5-trifluoromethylpyrroles. *Org. Lett.* **2021**, *23*, 7407-7411. (b) Sun, Y.; Yang, Z.; Lu, S.-N.; Chen, Z.; Wu, X.-F., Formal [4+1] Annulation of Azoalkenes with CF_3-Imidoyl Sulfoxonium Ylides and Dual Double Bond Isomerization Cascade: Synthesis of Trifluoromethyl-Containing Pyrazole Derivatives. *Org. Lett.* **2022,** *24*, 6822-6827. (c) Yang, Z.; Tang, J.; Chen, Z.; Wu, X.-F., Ruthenium-Catalyzed Hydroxyl-Directed *peri*-Selective C-H Activation and Annulation of 1-Naphthols with CF_3-Imidoyl Sulfoxonium Ylides for the Synthesis of 2-(Trifluoromethyl)-2,3-dihydrobenzo[de]chromen-2-amines. *Org. Lett.* **2022,** *24*, 7288-7293.

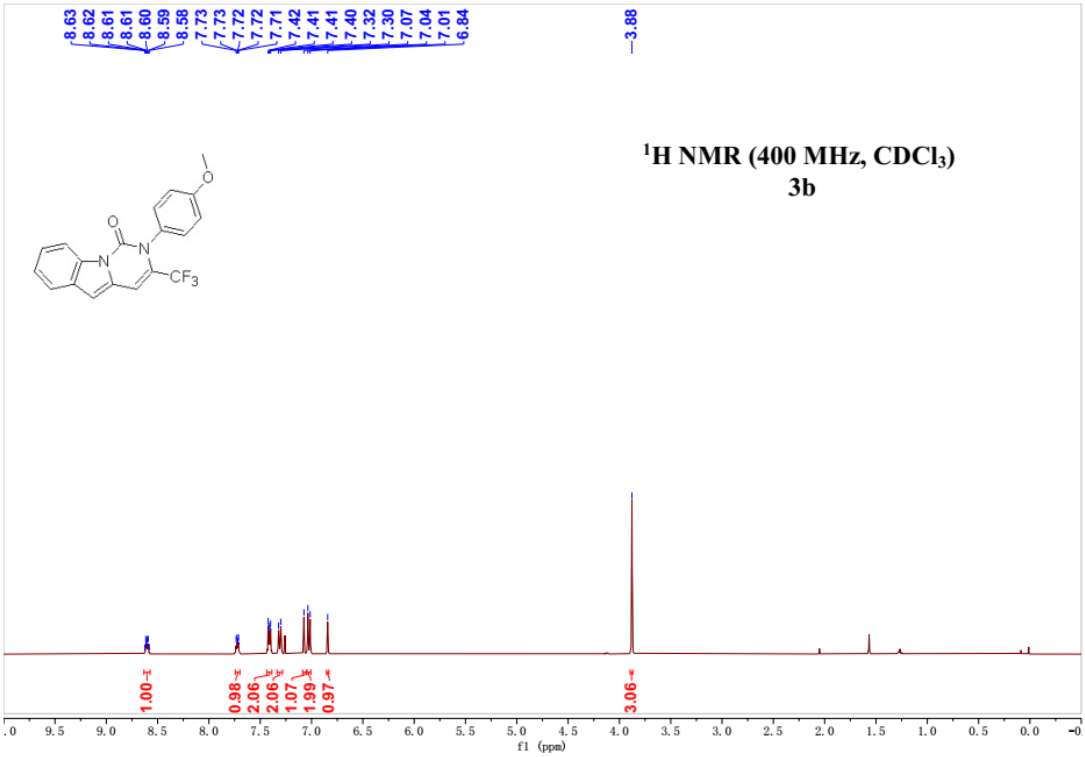
(3) (a) Xie, H.; Zhong, M.; Kang, H. J.; Shu, B.; Zhang, S. S., A Cascade Rh(III)-catalyzed C−H Activation/Chemodivergent Annulation of *N*-carbamoylindoles with Sulfoxonium Ylides for the Synthesis of Dihydropyrimidoindolone and Tricyclic [1,3]Oxazino[3,4-a]indol-1-ones Derivatives. *Adv. Synth. Catal.* **2021,** *363*, 1436-1442. (b) Chen, J.; Zhong, T.; Zheng, X.; Yin, C.; Zhang, L.; Zhou, J.; Jiang, X.; Yu, C., Selective Synthesis of Fused Tricyclic [1,3]oxazino[3,4-a]indolone and Dihydropyrimido [1,6-a]indolone via Rh(III)-catalyzed [3+3] or [4+2] C−H Annulation. *Adv. Synth. Catal.* **2021,** *363*, 446-452.

5. Copy of ^{1}H, ^{13}C and ^{19}F-NMR Spectra of Products

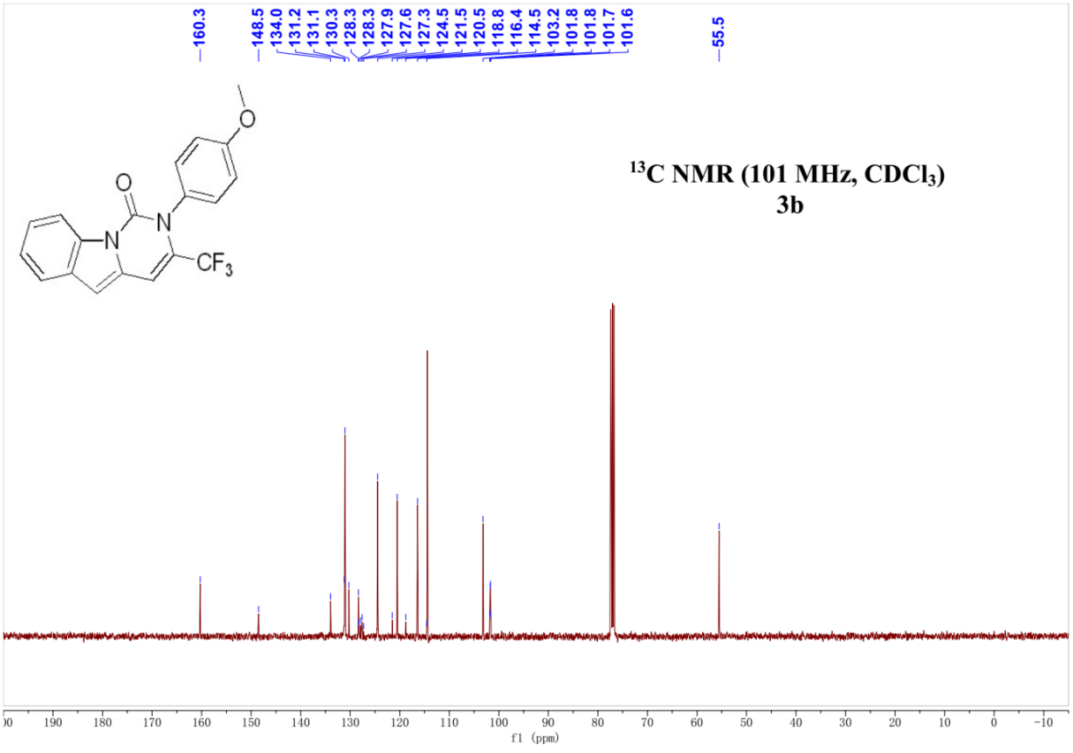




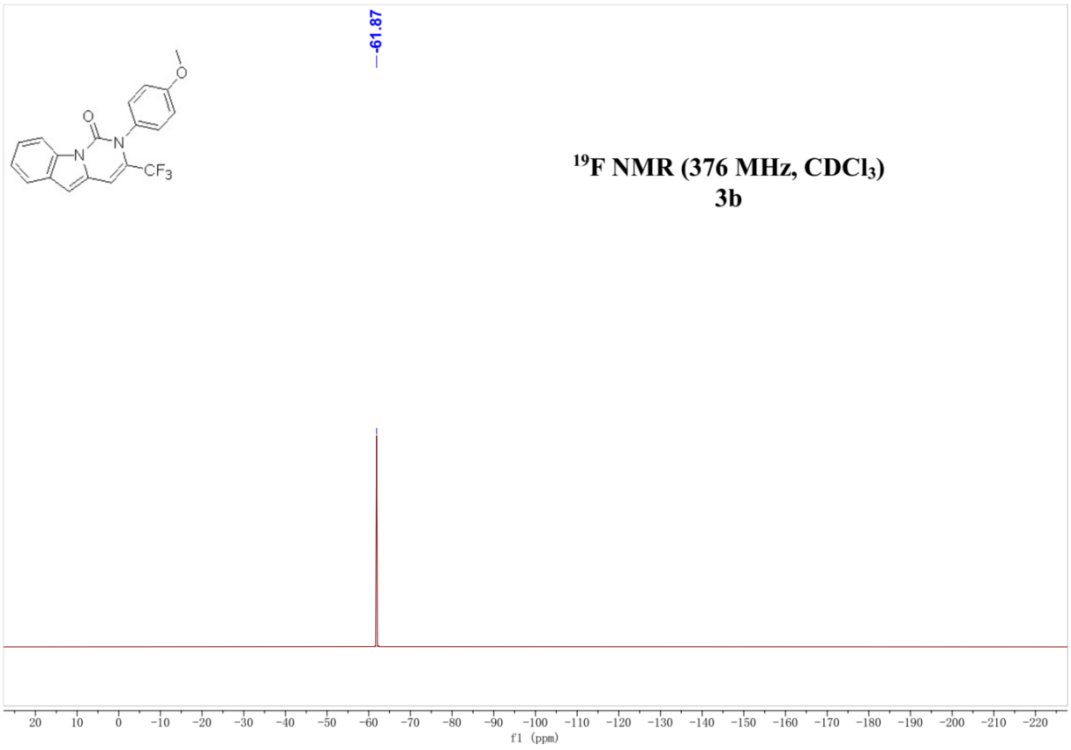

-61.69
O
N
N
CF3
19F NMR (376 MHz, CDCl3)
3a
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220
f1 (ppm)



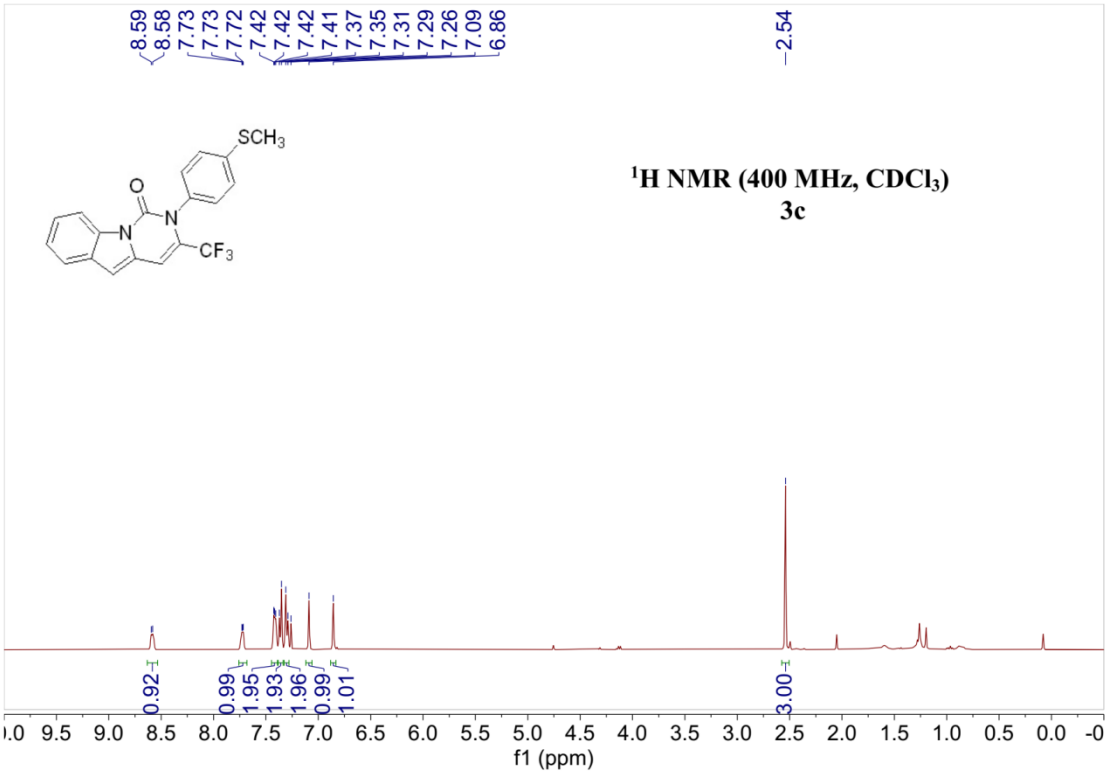
^{1}H NMR (400 MHz, $CDCl_3$)
3b



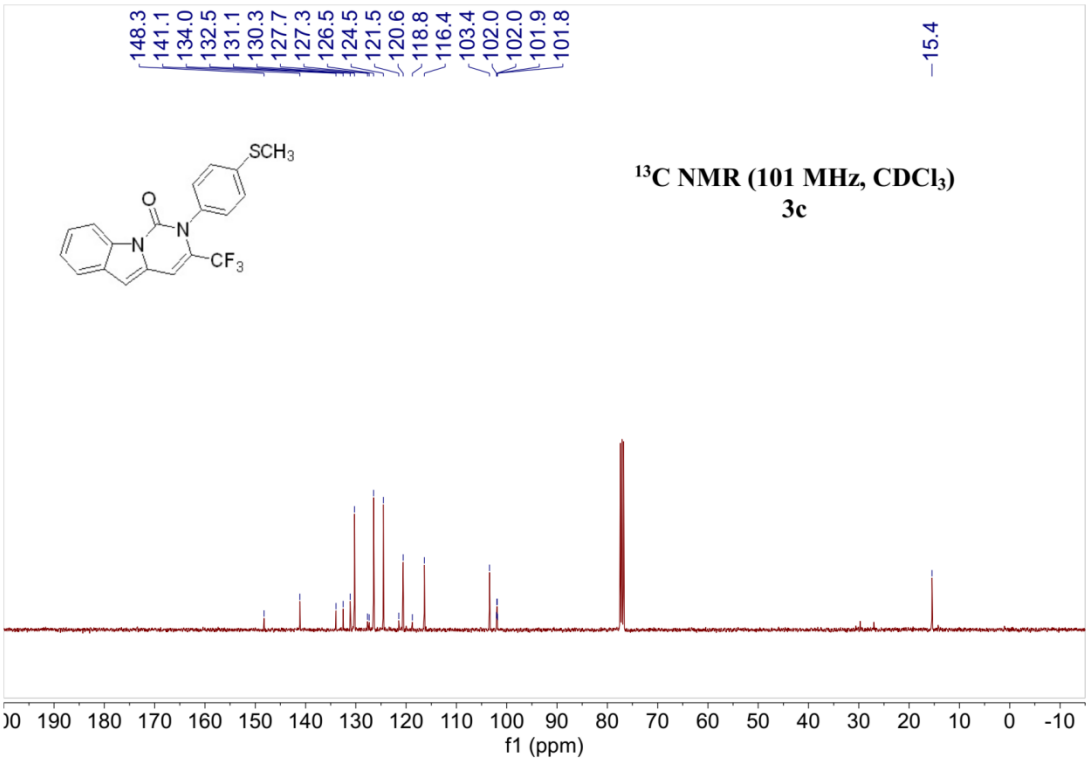
^{13}C NMR (101 MHz, $CDCl_3$)
3b



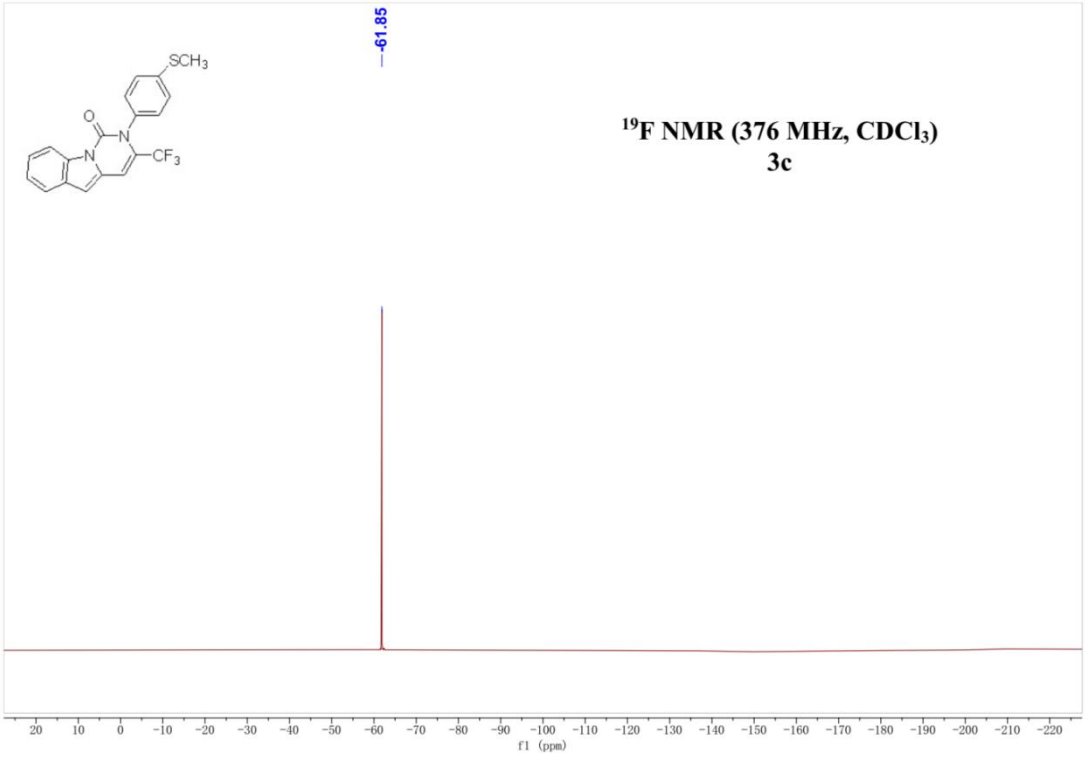
^{19}F NMR (376 MHz, $CDCl_3$)
3b



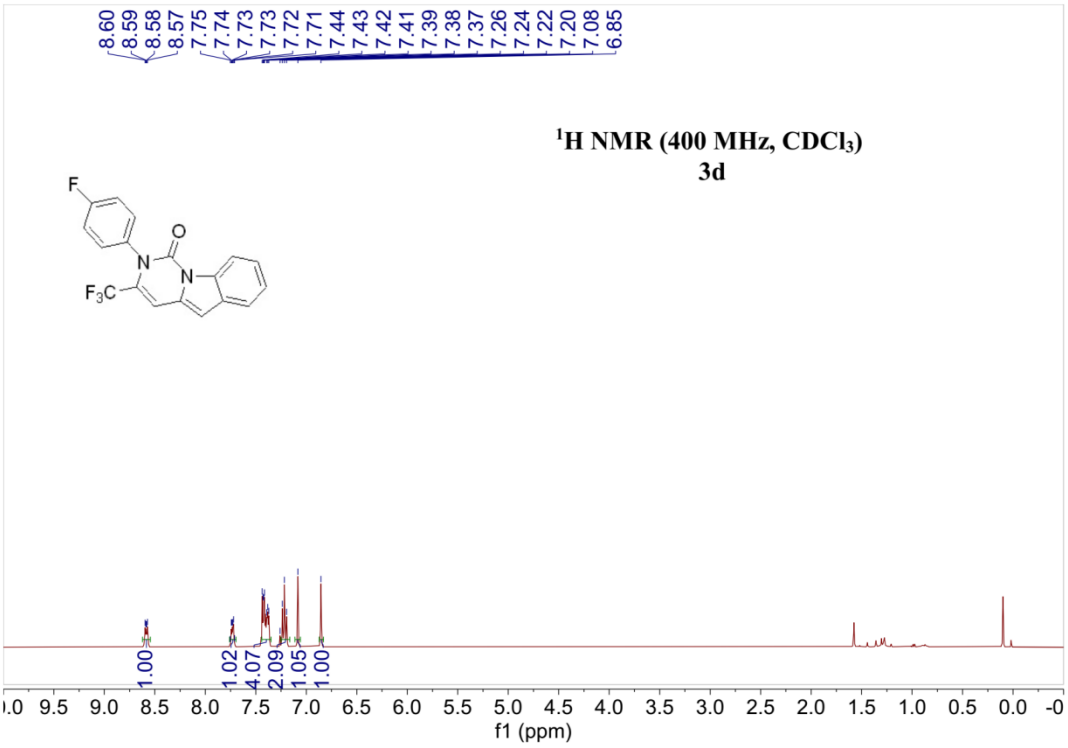
^{1}H NMR (400 MHz, $CDCl_3$)
3c

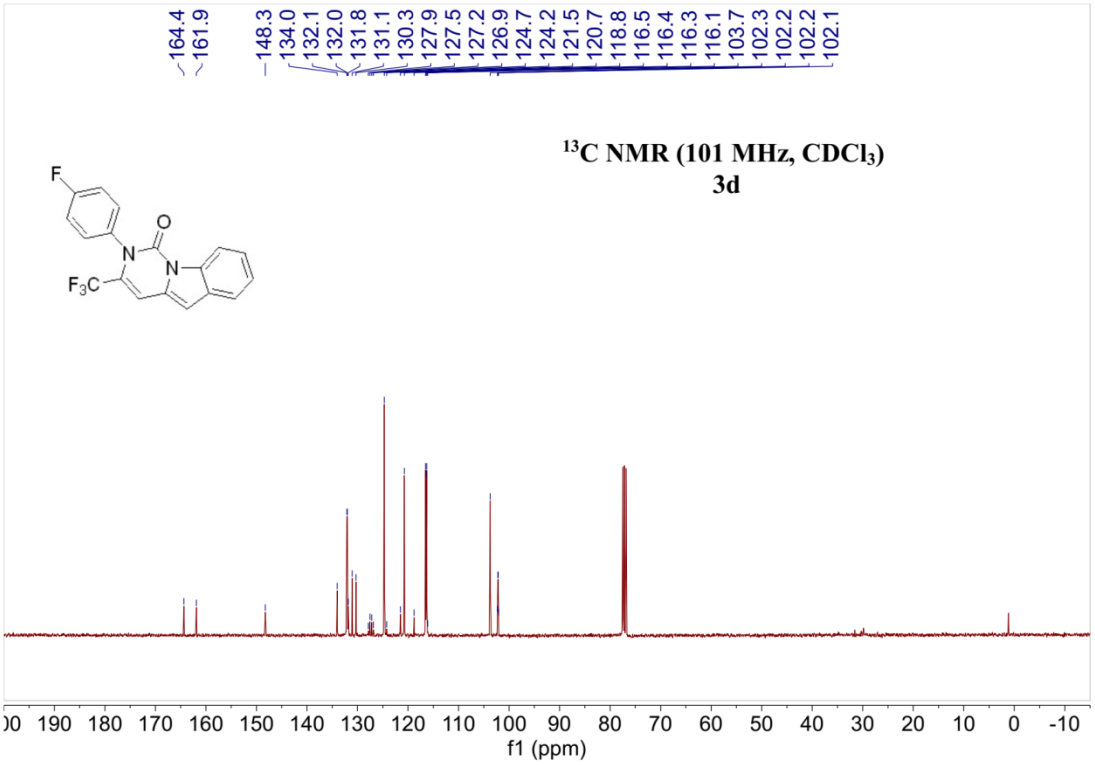


^{13}C NMR (101 MHz, $CDCl_3$)
3c



^{19}F NMR (376 MHz, $CDCl_3$)
3c


8.60
8.59
8.58
8.57
7.75
7.74
7.73
7.73
7.72
7.71
7.44
7.43
7.42
7.41
7.39
7.38
7.37
7.26
7.24
7.22
7.20
7.08
6.85
1H NMR (400 MHz, CDCl3)
3d
F
O
N
N
F3C
1.00
1.02
4.07
2.09
1.05
1.00
f1 (ppm)


164.4
161.9
148.3
134.0
132.1
132.0
131.8
131.1
130.3
127.9
127.5
127.2
126.9
124.7
124.2
121.5
120.7
118.8
116.5
116.4
116.3
116.1
103.7
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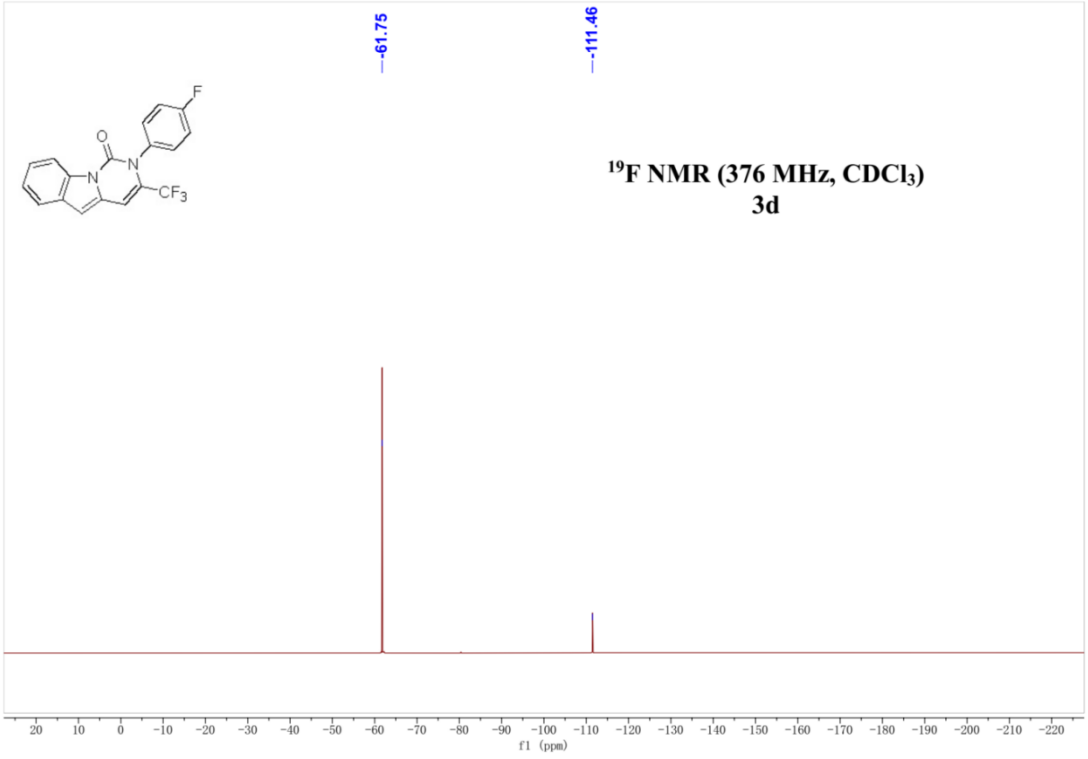
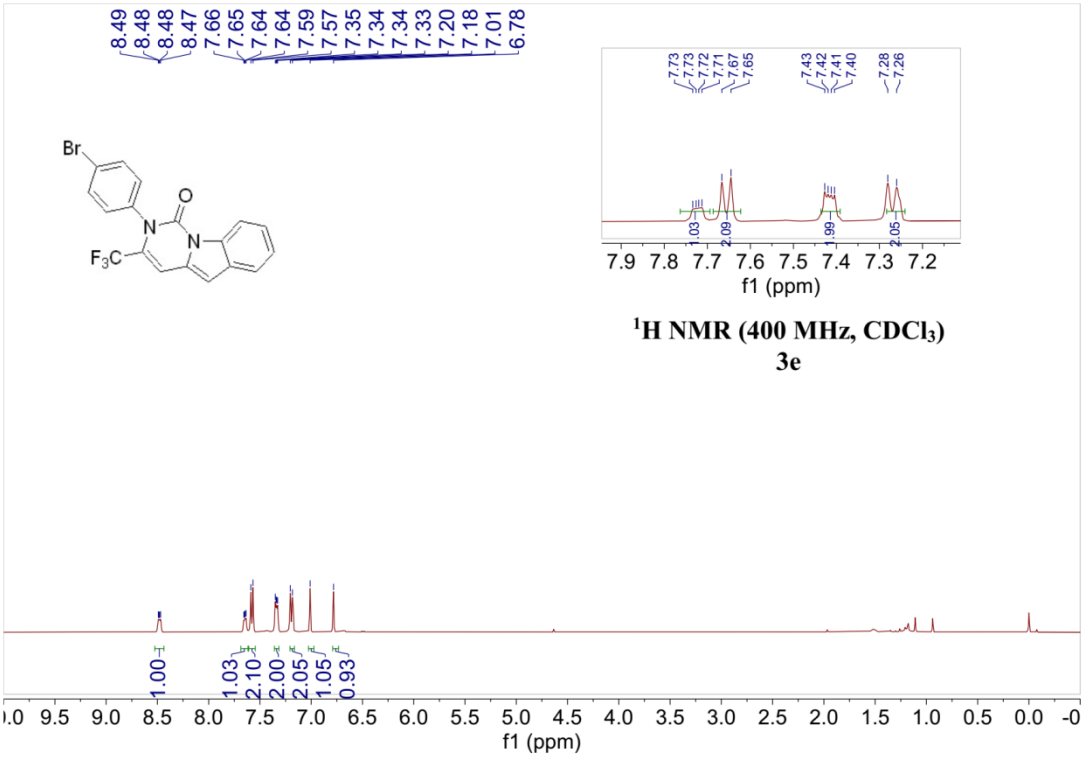
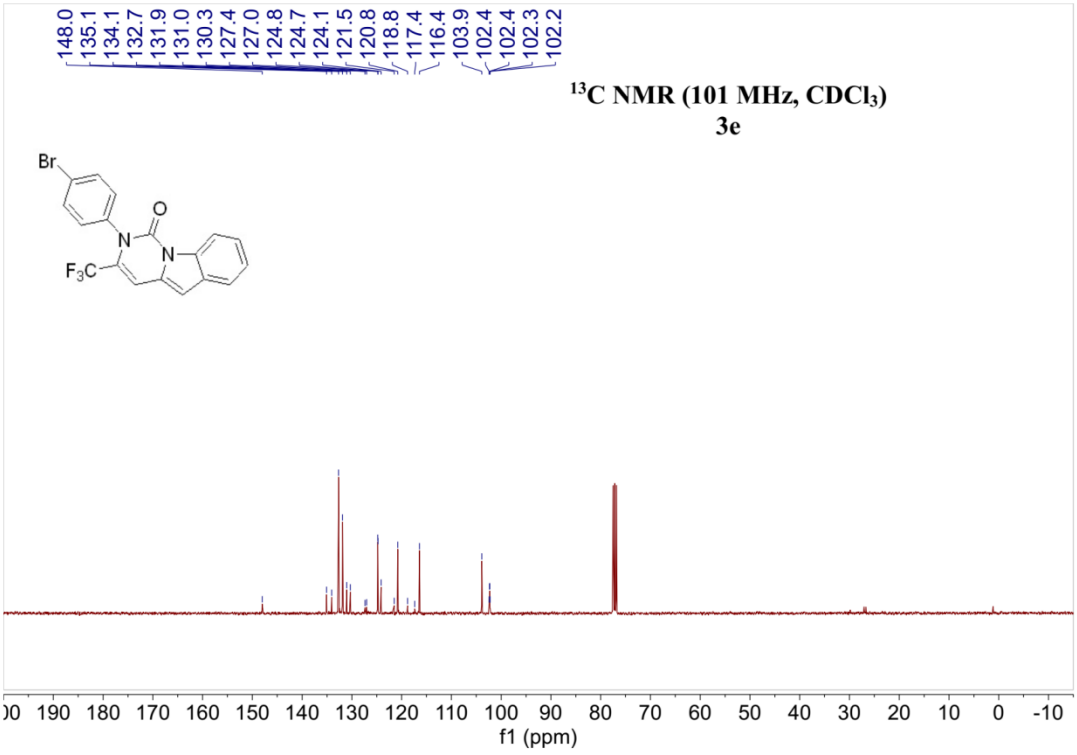
102.1
13C NMR (101 MHz, CDCl3)
3d
F
O
N
N
F3C
f1 (ppm)

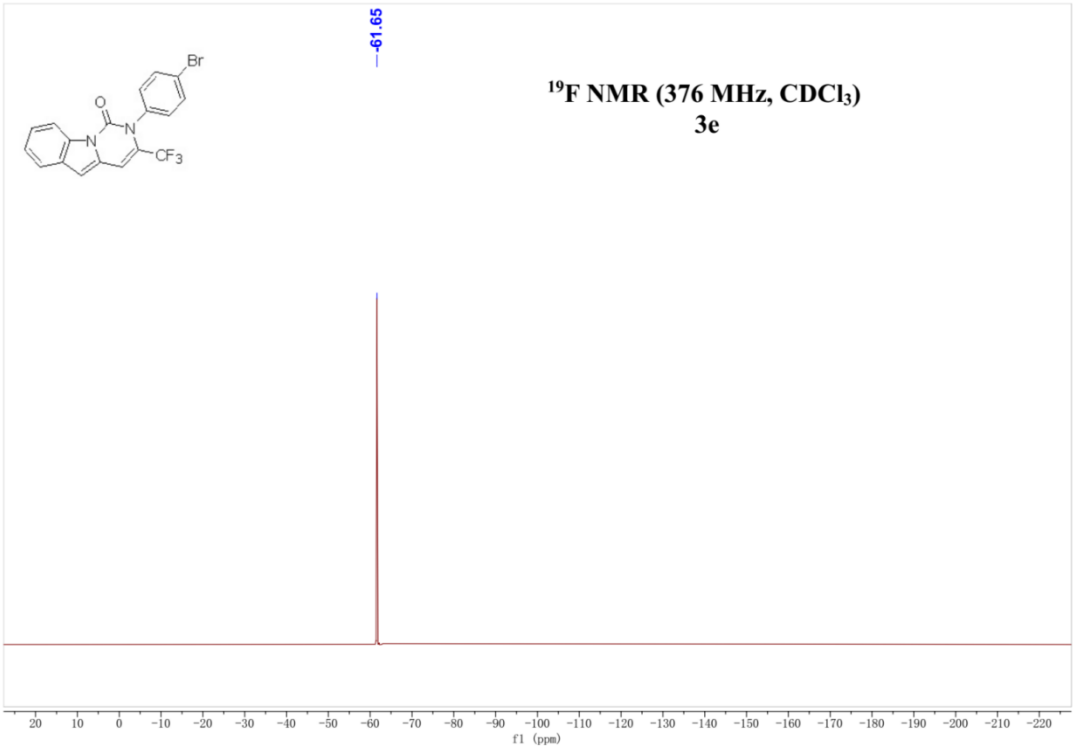

-61.75
-111.46
F
O
N
N
CF3
19F NMR (376 MHz, CDCl3)
3d
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220
f1 (ppm)



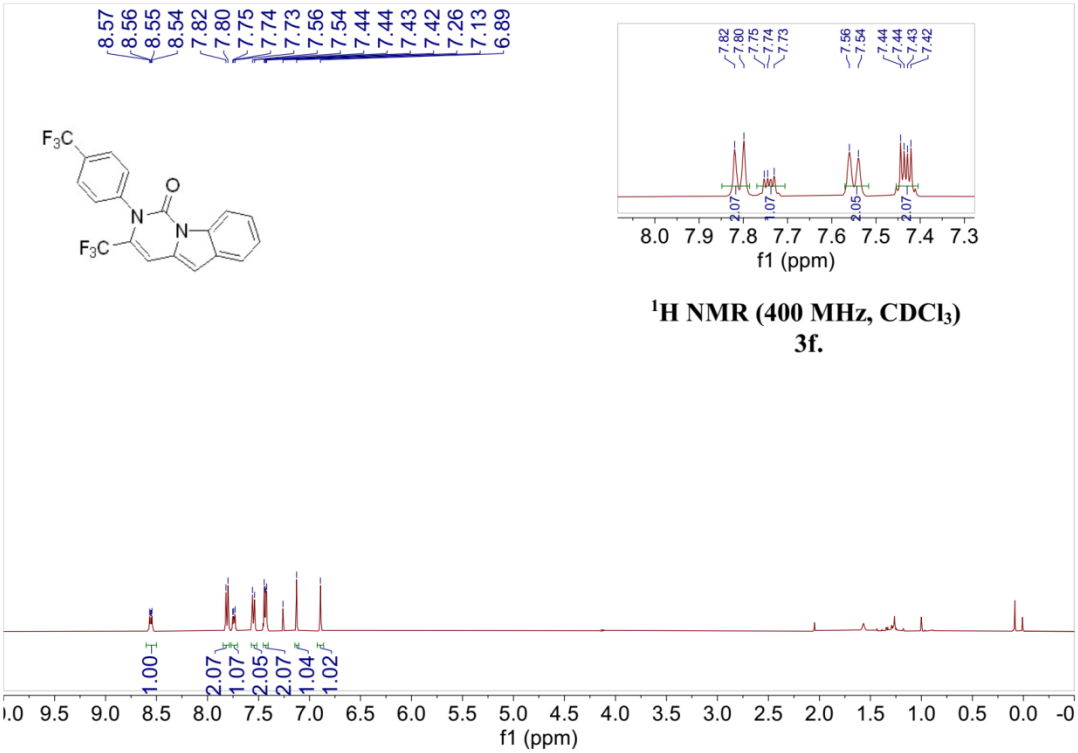
^{1}H NMR (400 MHz, $CDCl_3$)
3e



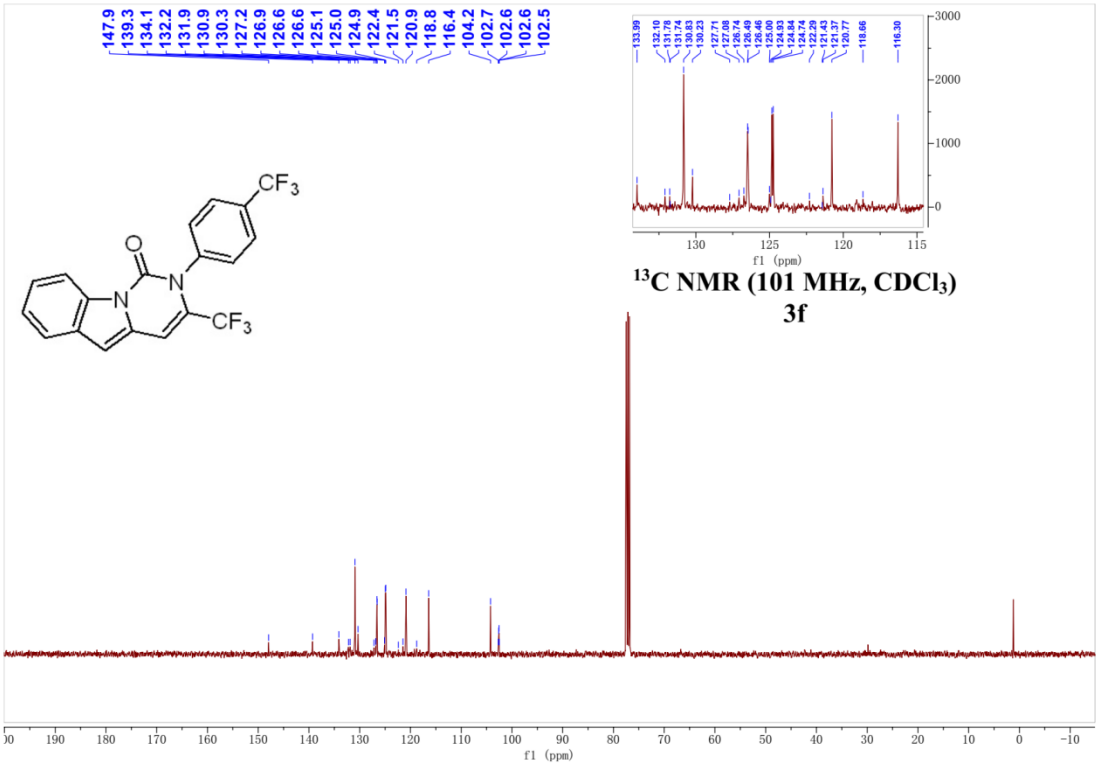
^{13}C NMR (101 MHz, $CDCl_3$)
3e



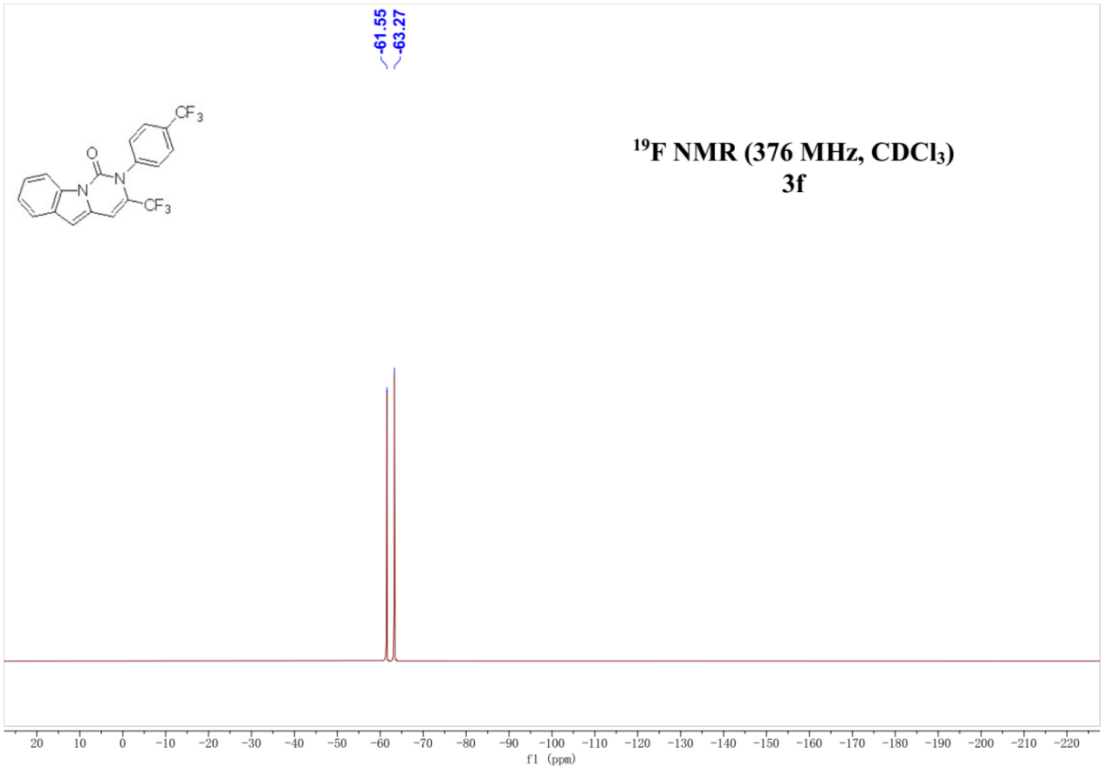
^{19}F NMR (376 MHz, $CDCl_3$)
3e

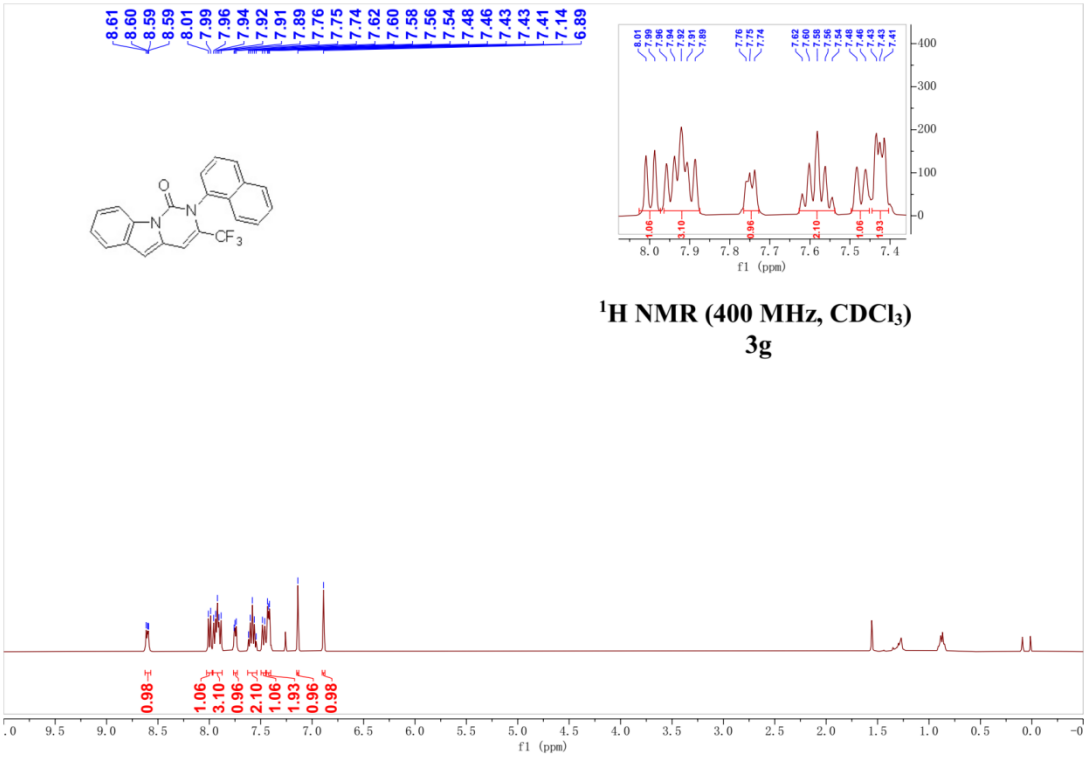


^{1}H NMR (400 MHz, $CDCl_3$)
3f.

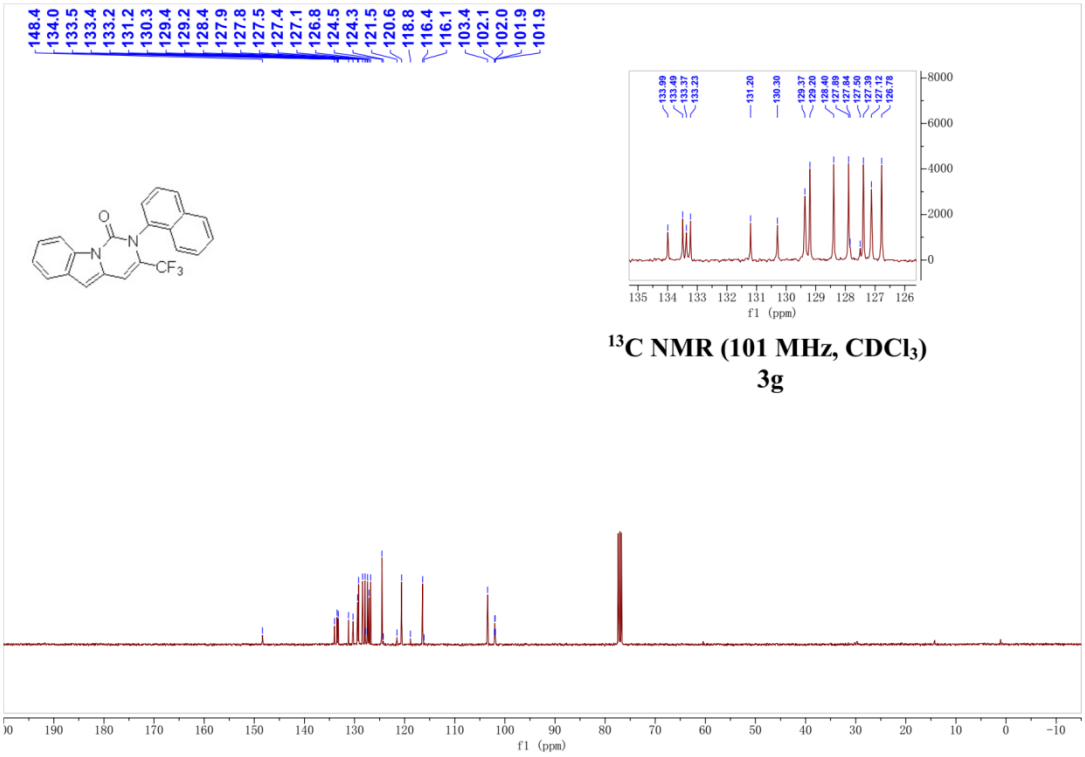


^{13}C NMR (101 MHz, $CDCl_3$)
3f

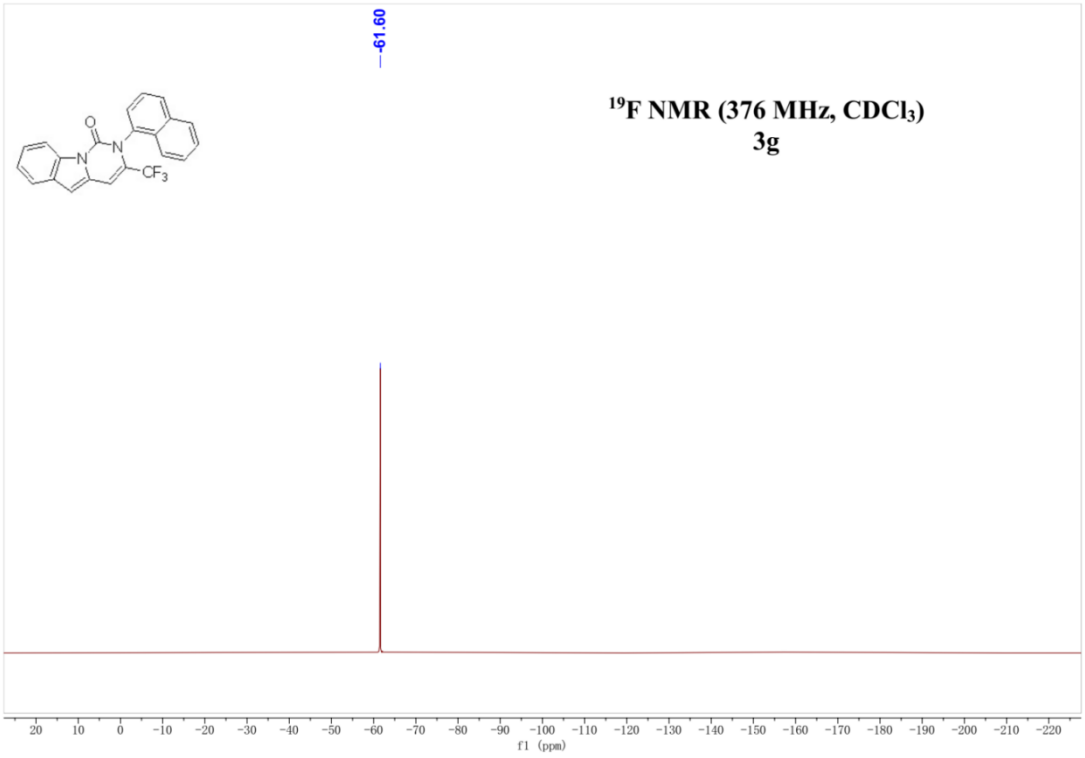

-61.55
-63.27
CF3
O
N
N
CF3
19F NMR (376 MHz, CDCl3)
3f
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220
f1 (ppm)



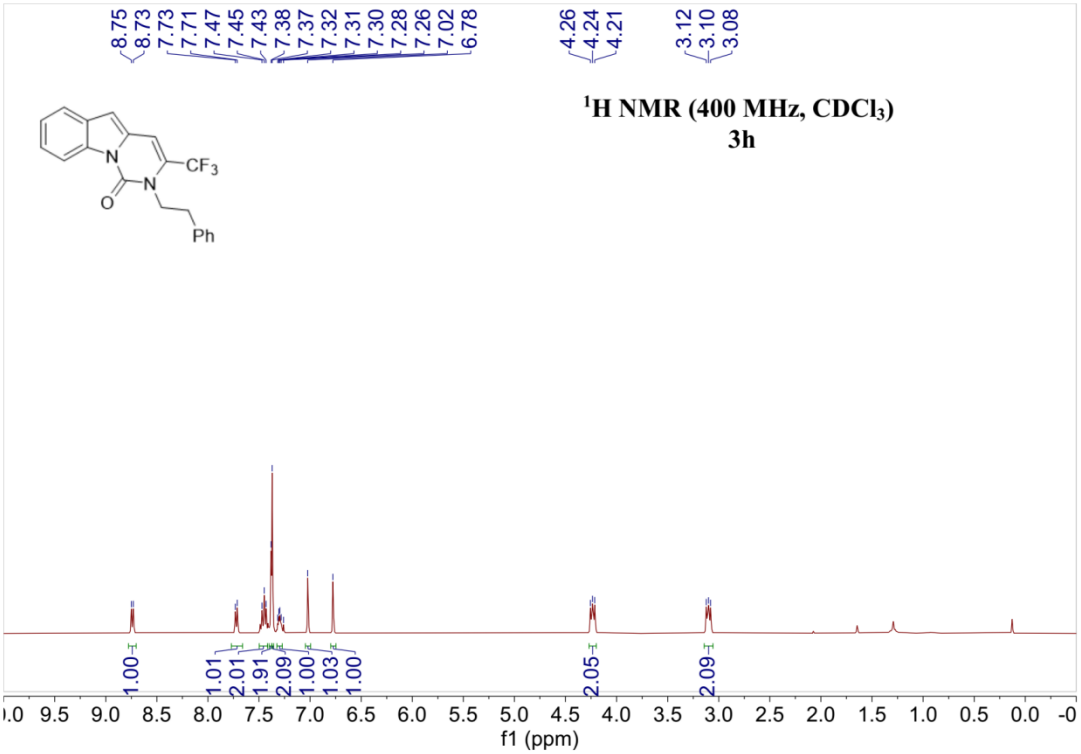
^{1}H NMR (400 MHz, $CDCl_3$)
3g

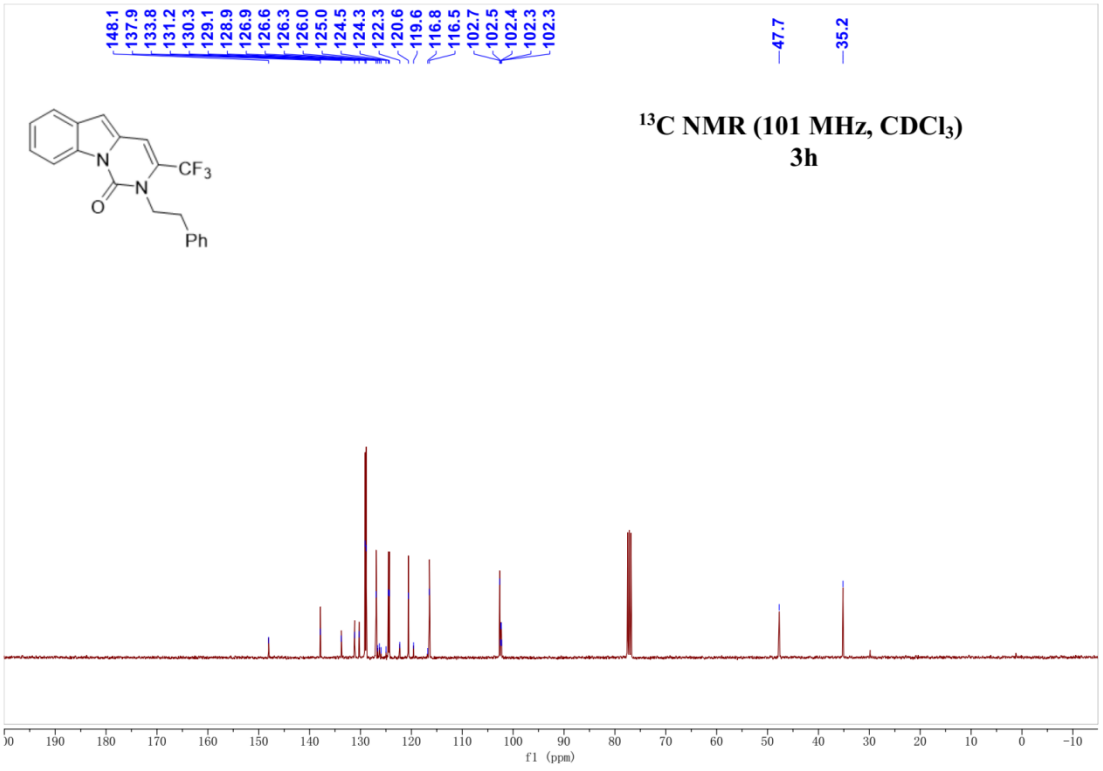


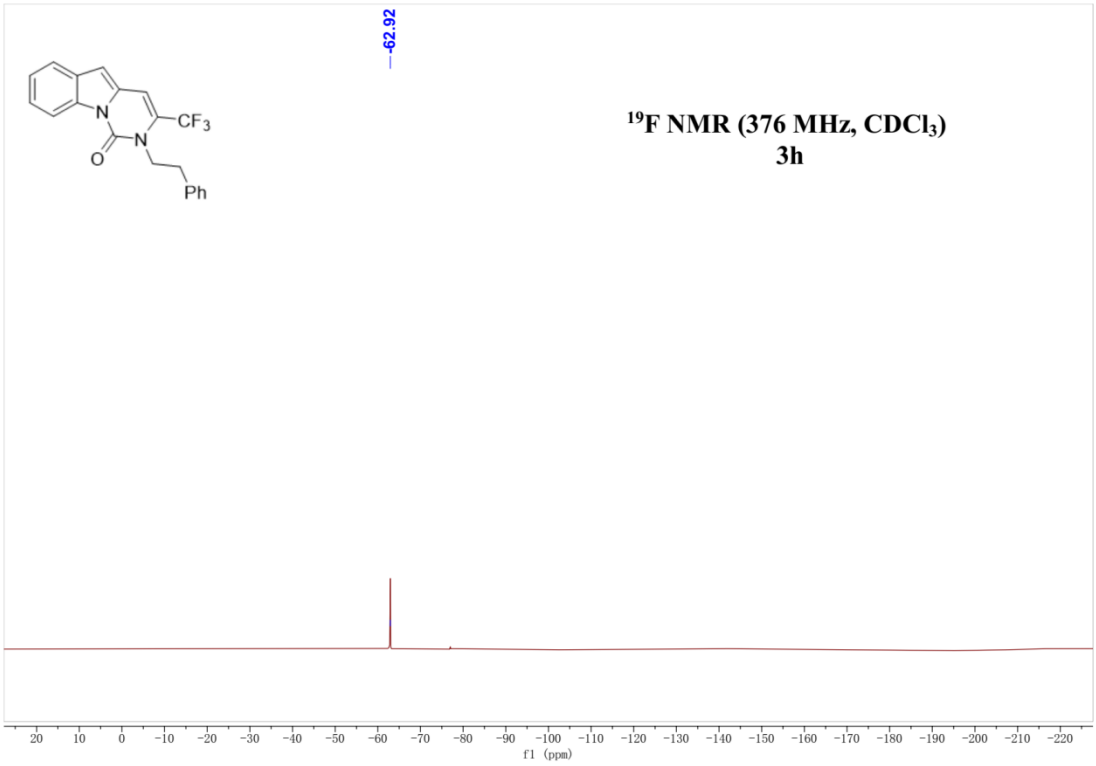
^{13}C NMR (101 MHz, $CDCl_3$)
3g

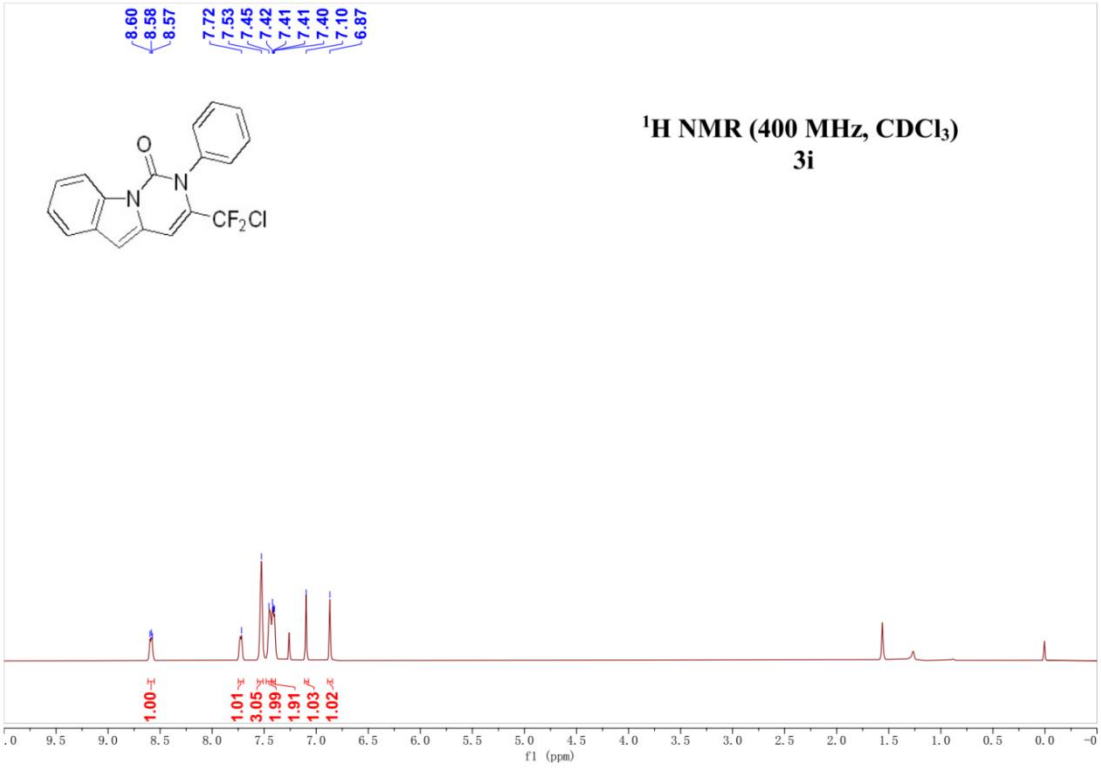


^{19}F NMR (376 MHz, $CDCl_3$)
3g

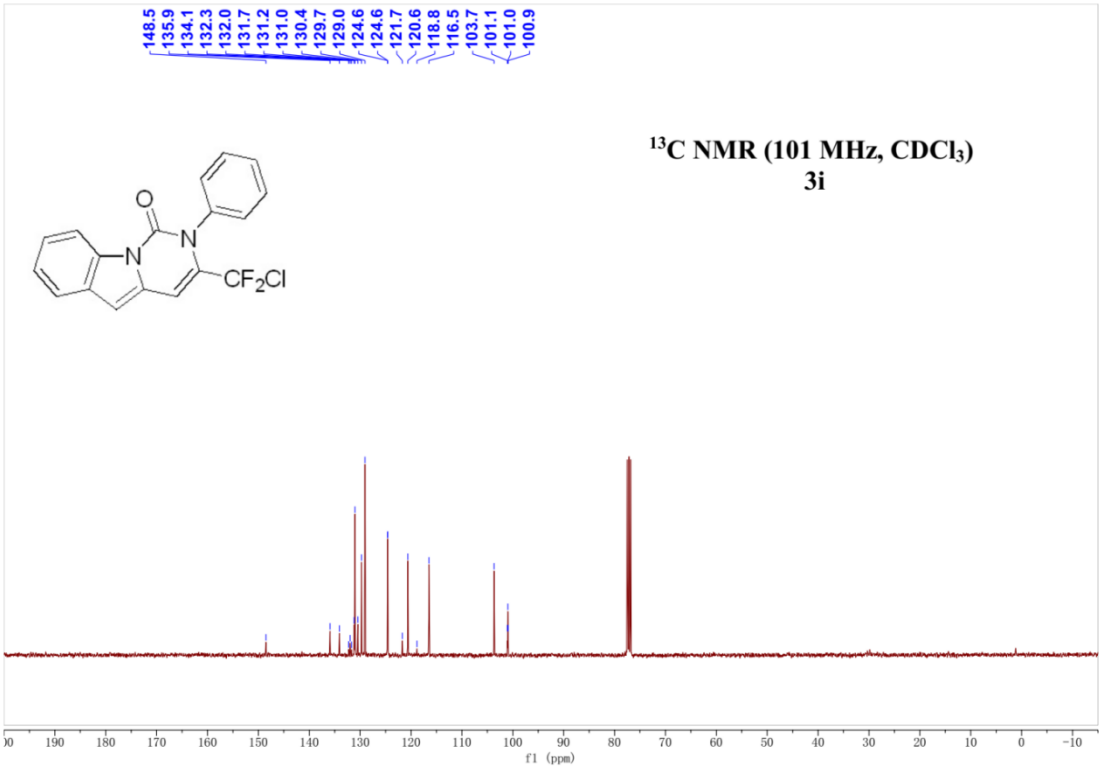

8.75
8.73
7.73
7.71
7.47
7.45
7.43
7.38
7.37
7.32
7.31
7.30
7.28
7.26
7.02
6.78
4.26
4.24
4.21
3.12
3.10
3.08
1H NMR (400 MHz, CDCl3)
3h
CF3
N
N
O
Ph
1.00
1.01
2.01
1.91
2.09
1.00
1.03
1.00
2.05
2.09
f1 (ppm)


148.1
137.9
133.8
131.2
130.3
129.1
128.9
126.9
126.6
126.3
126.0
125.0
124.5
124.3
122.3
120.6
119.6
116.8
116.5
102.7
102.5
102.4
102.3
102.3
47.7
35.2
13C NMR (101 MHz, CDCl3)
3h
CF3
N
N
O
Ph
f1 (ppm)

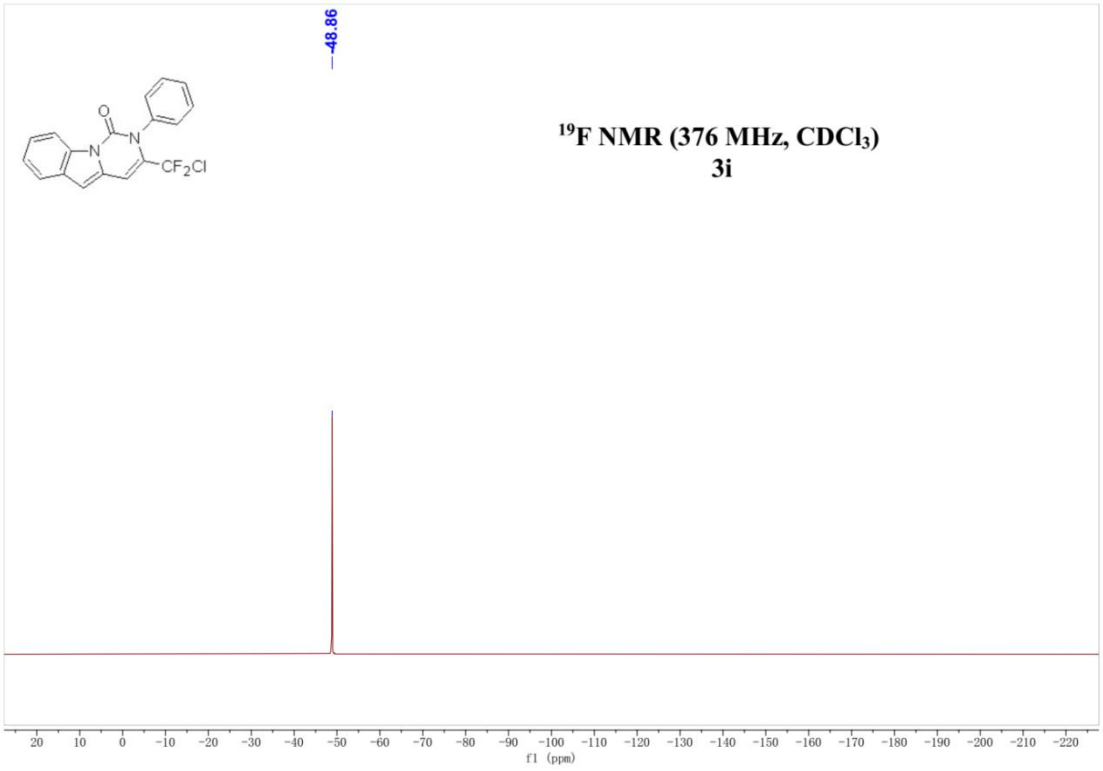

-62.92
CF3
N
N
O
Ph
19F NMR (376 MHz, CDCl3)
3h
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220
f1 (ppm)



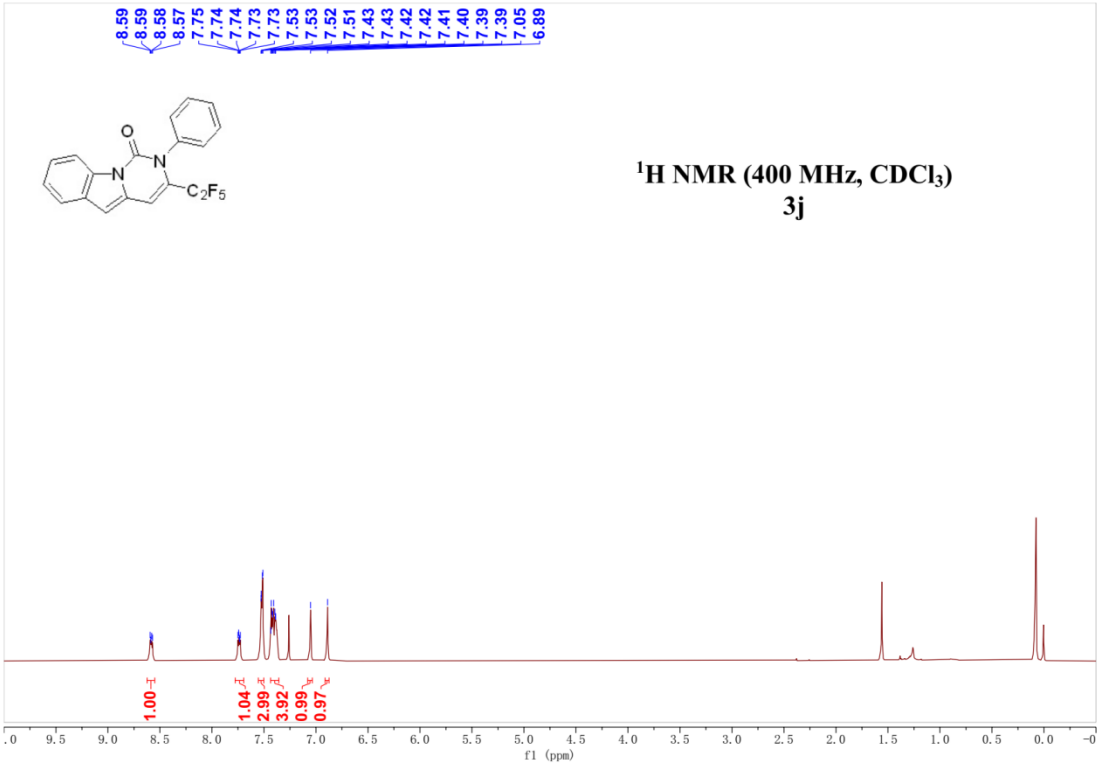
^{1}H NMR (400 MHz, $CDCl_3$)
3i



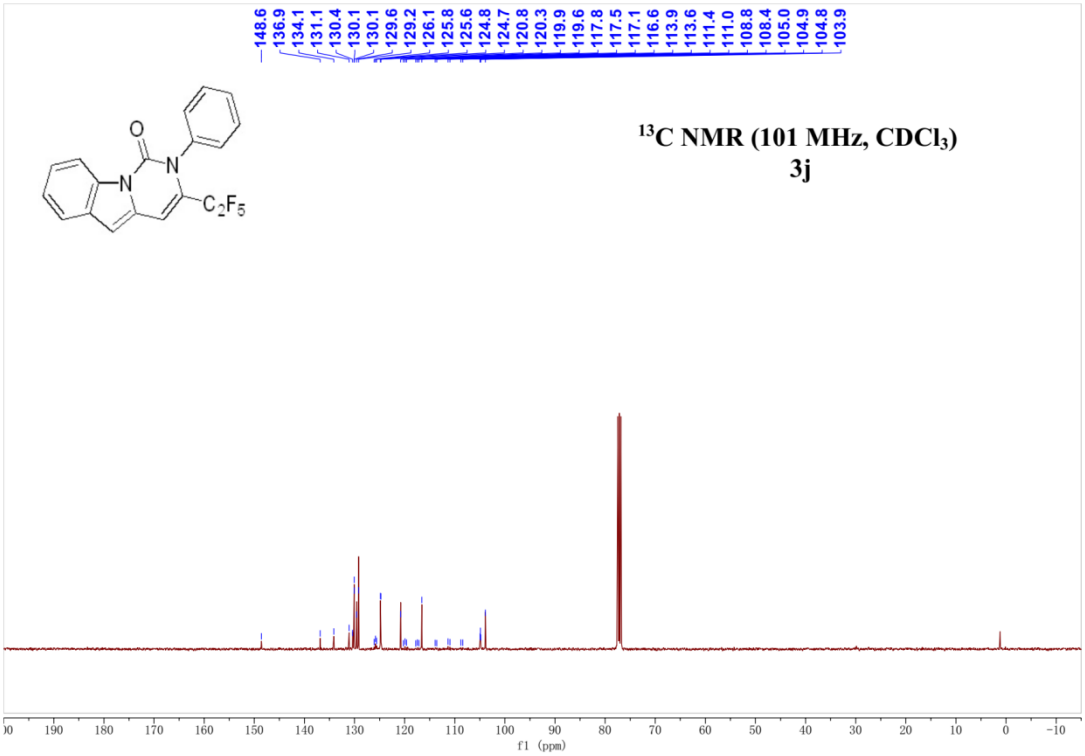
^{13}C NMR (101 MHz, $CDCl_3$)
3i



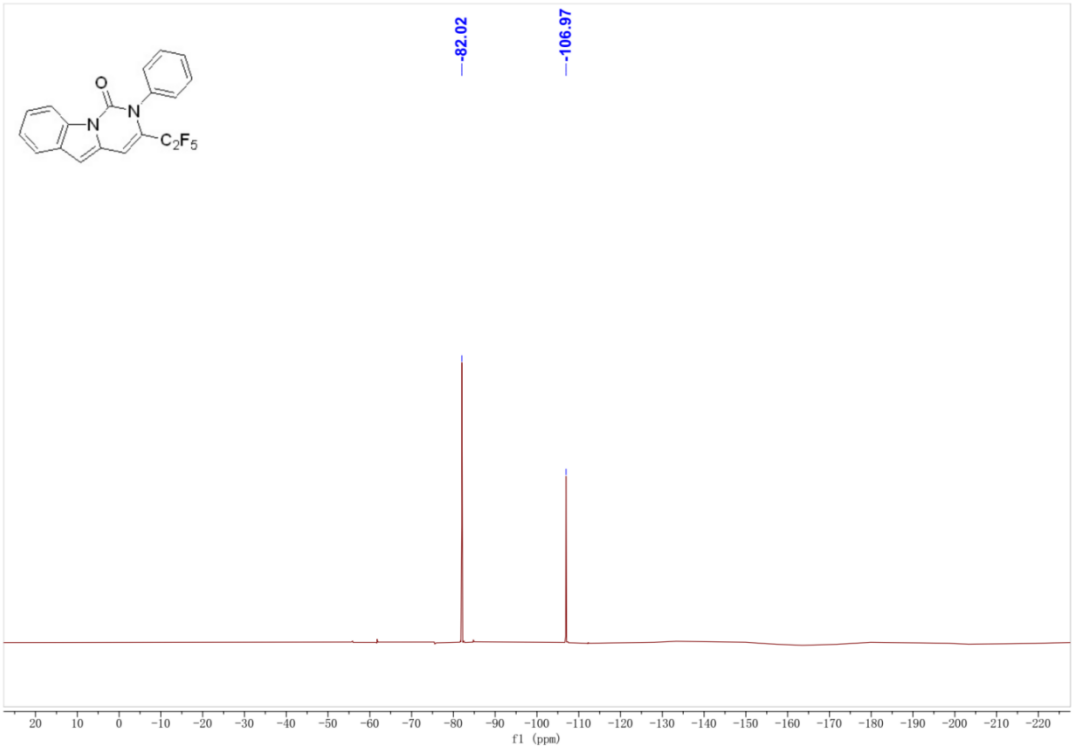
^{19}F NMR (376 MHz, $CDCl_3$)
3i

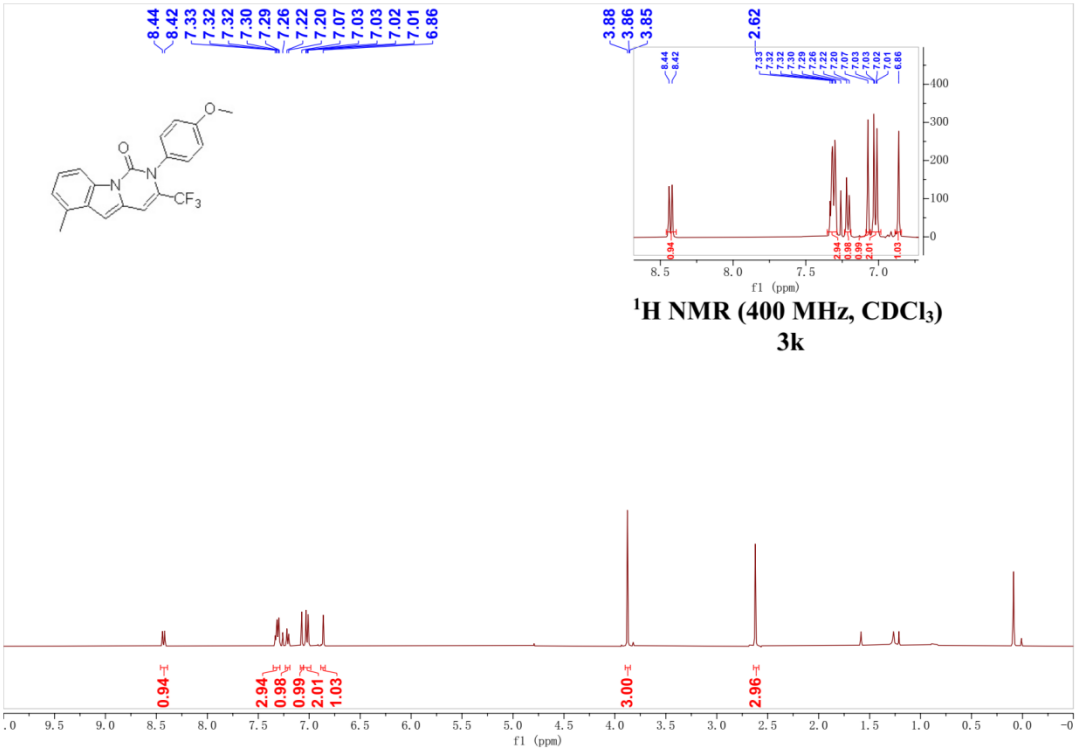


^{1}H NMR (400 MHz, $CDCl_3$)
3j

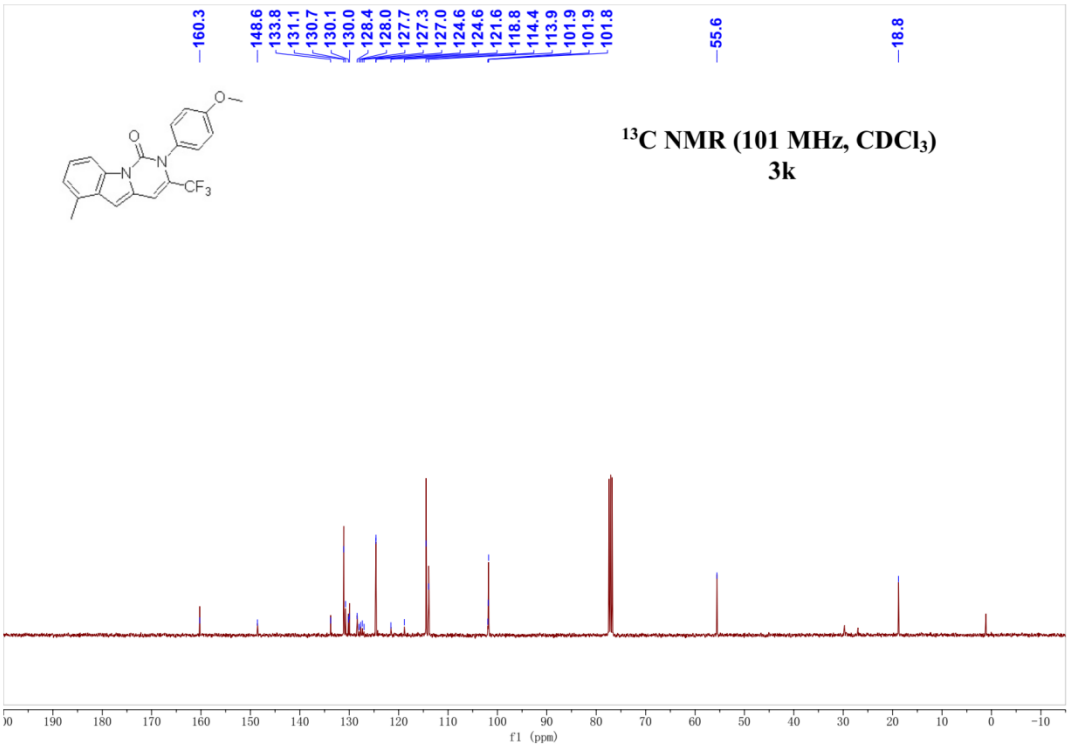


^{13}C NMR (101 MHz, $CDCl_3$)
3j

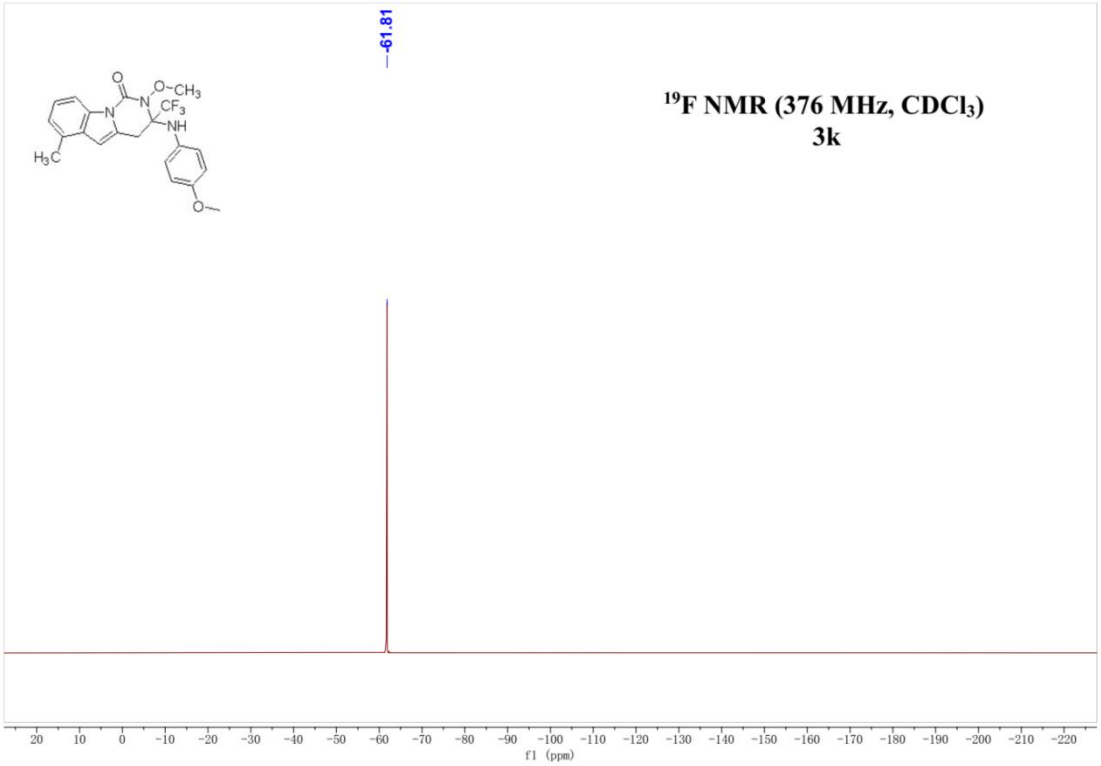

-82.02
-106.97
O
N
N
C_2F_5
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220
f1 (ppm)

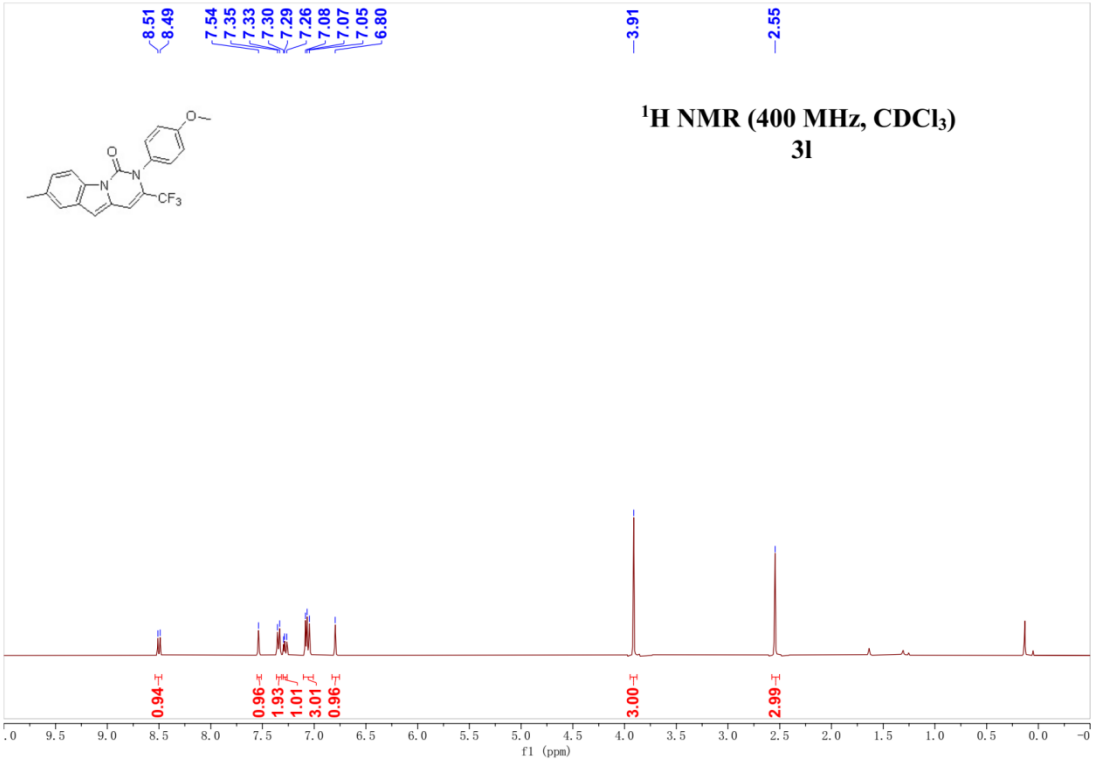


^{1}H NMR (400 MHz, $CDCl_3$)
3k

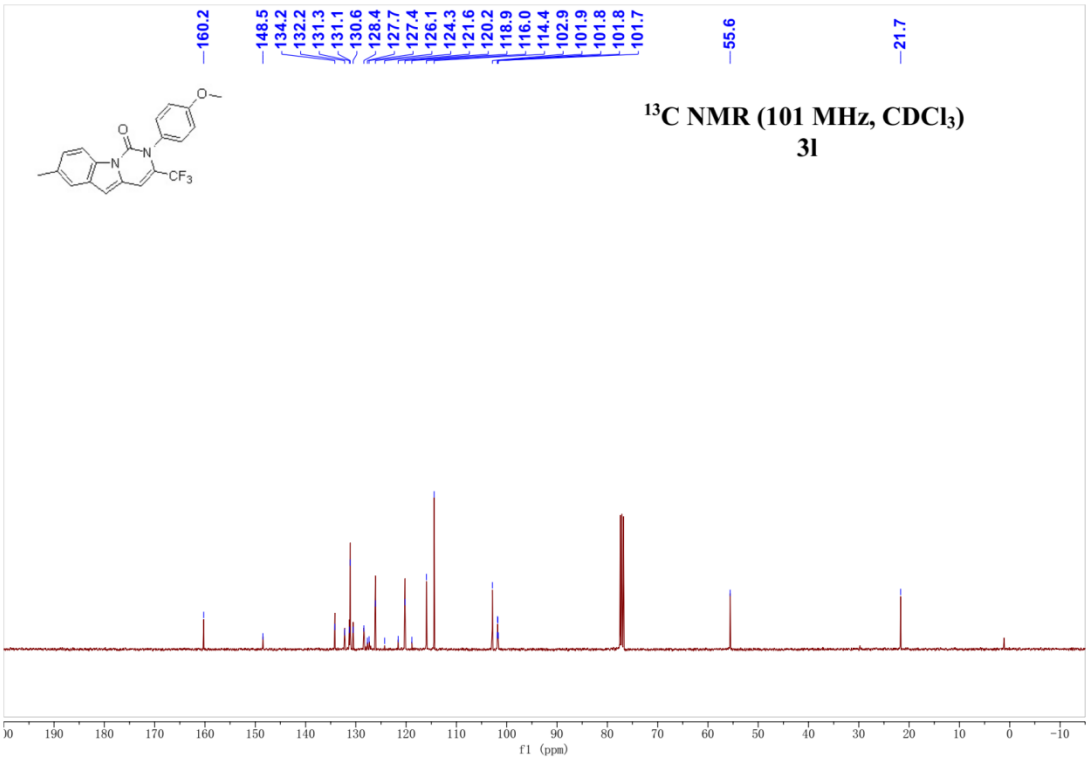


^{13}C NMR (101 MHz, $CDCl_3$)
3k

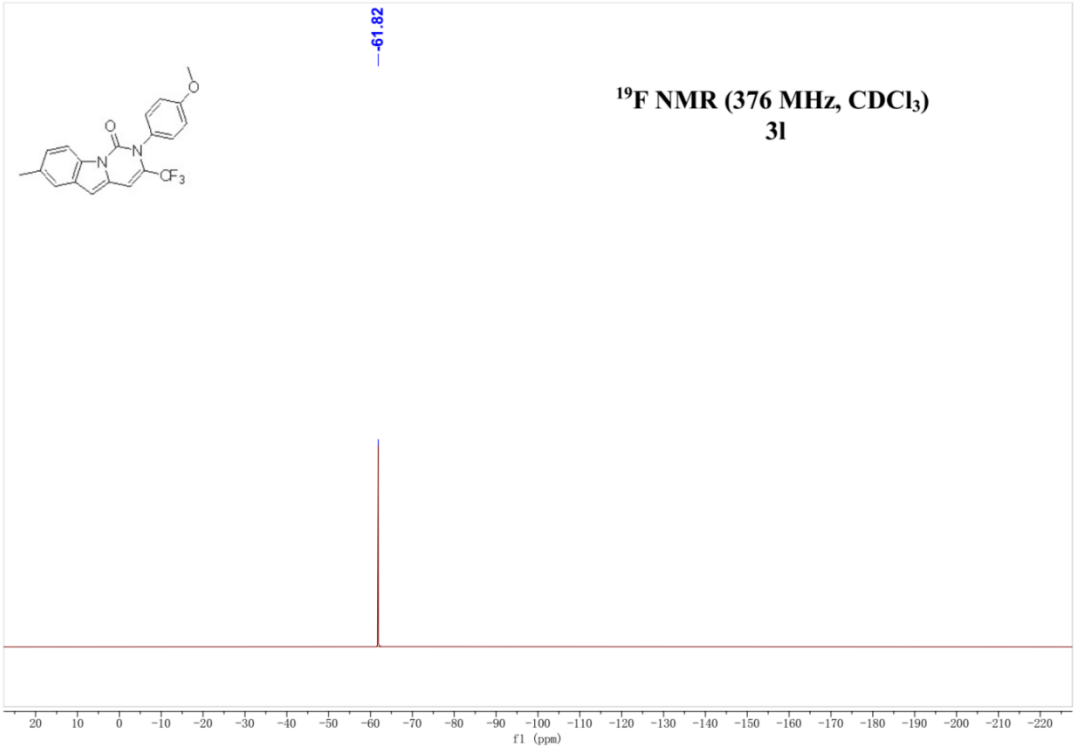

-61.81
O
O-CH3
N
CF3
NH
H3C
O
19F NMR (376 MHz, CDCl3)
3k
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220
f1 (ppm)

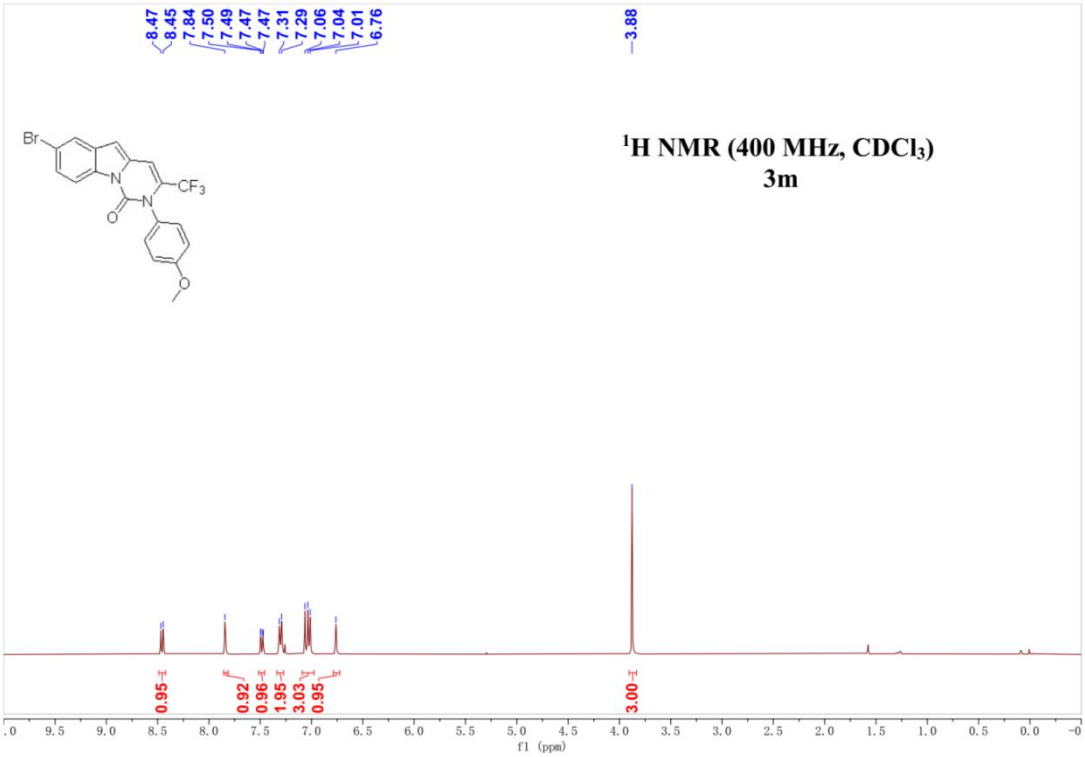


^{1}H NMR (400 MHz, $CDCl_3$)
3l

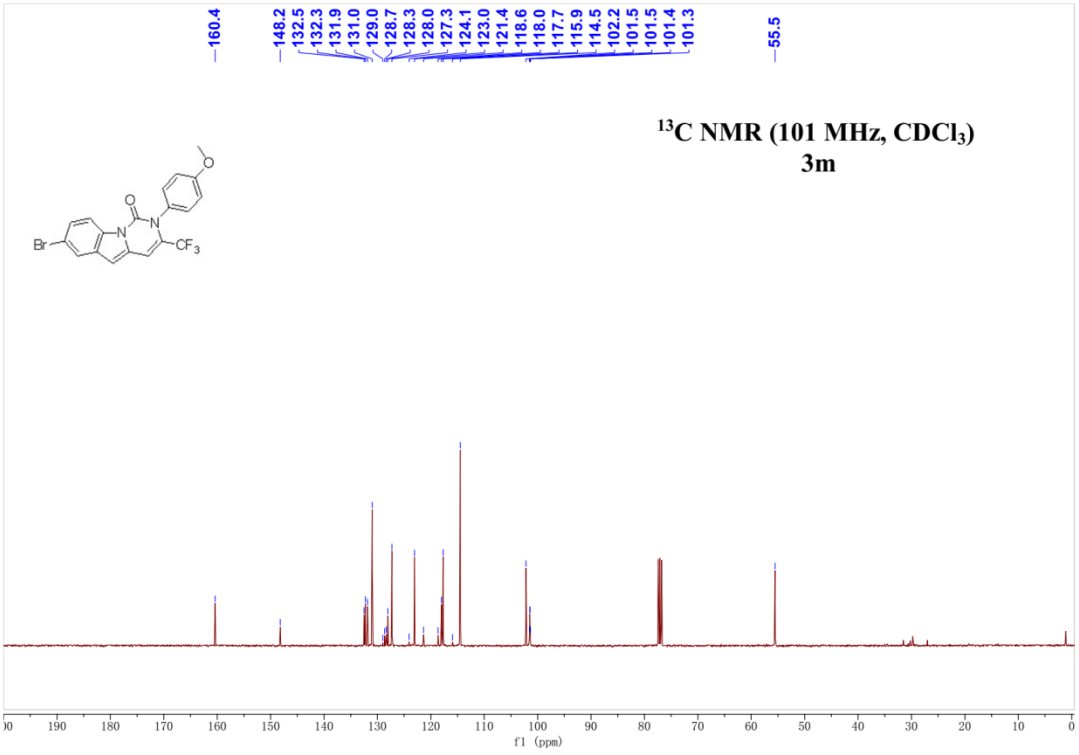


^{13}C NMR (101 MHz, $CDCl_3$)
3l

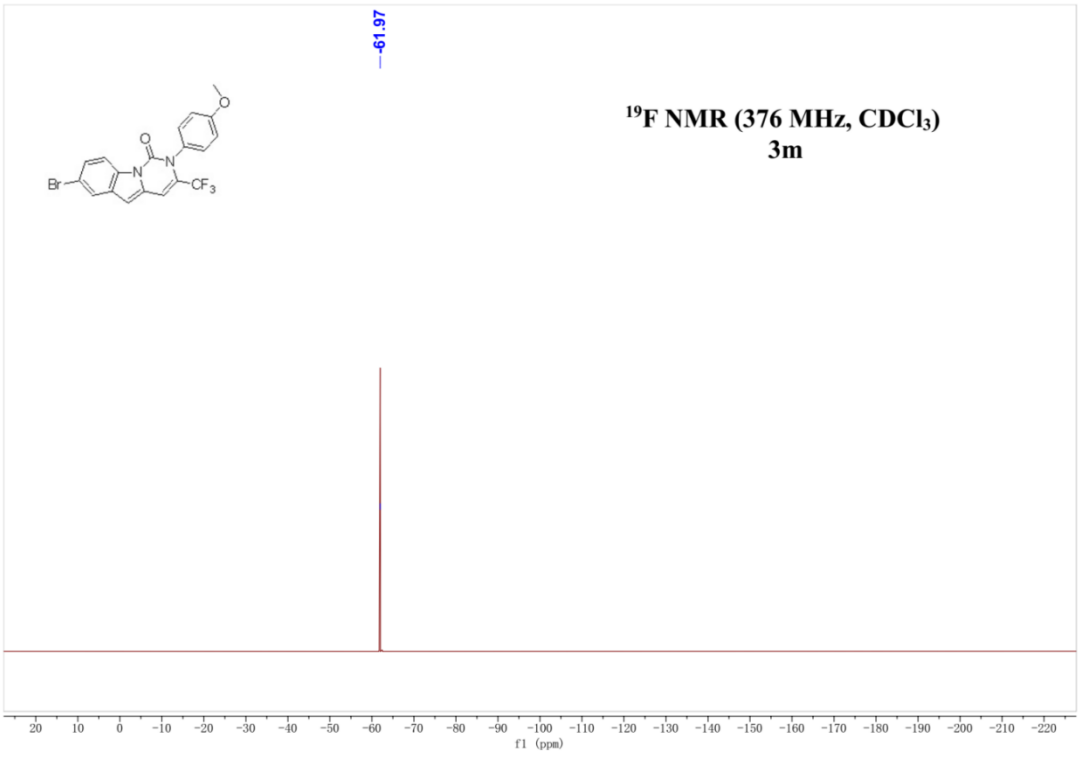

-61.82
^{19}F NMR (376 MHz, CDCl$_3$)
3l
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220
f1 (ppm)

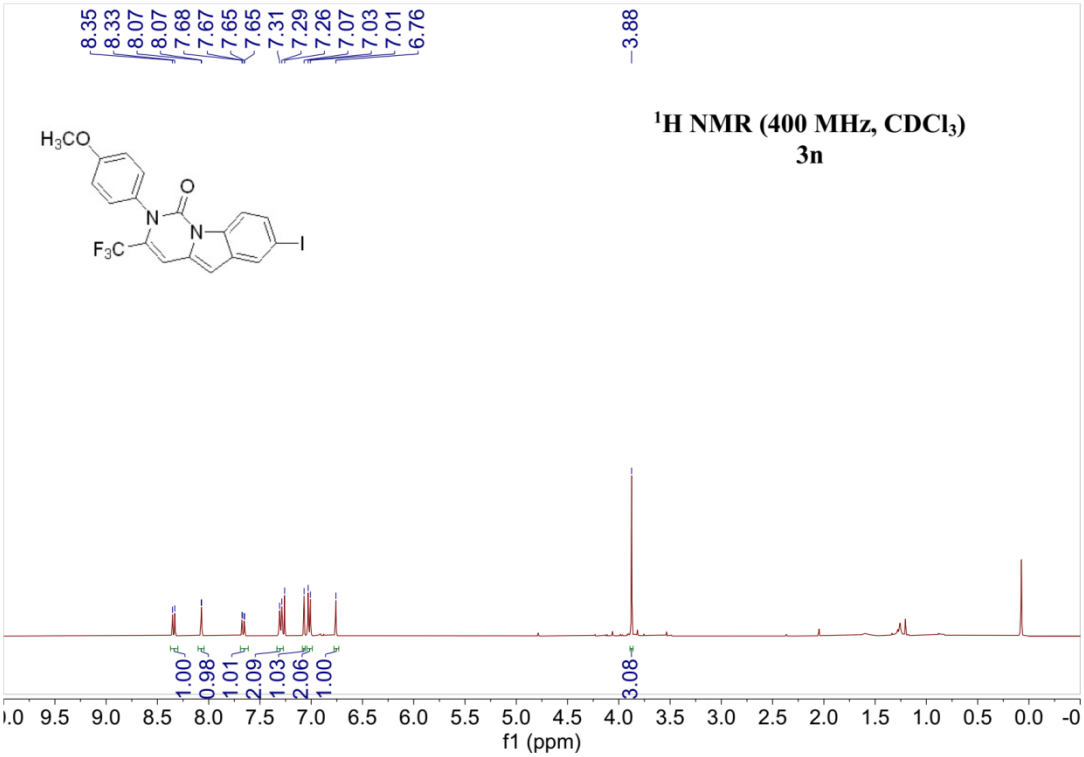


^{1}H NMR (400 MHz, $CDCl_3$)
3m

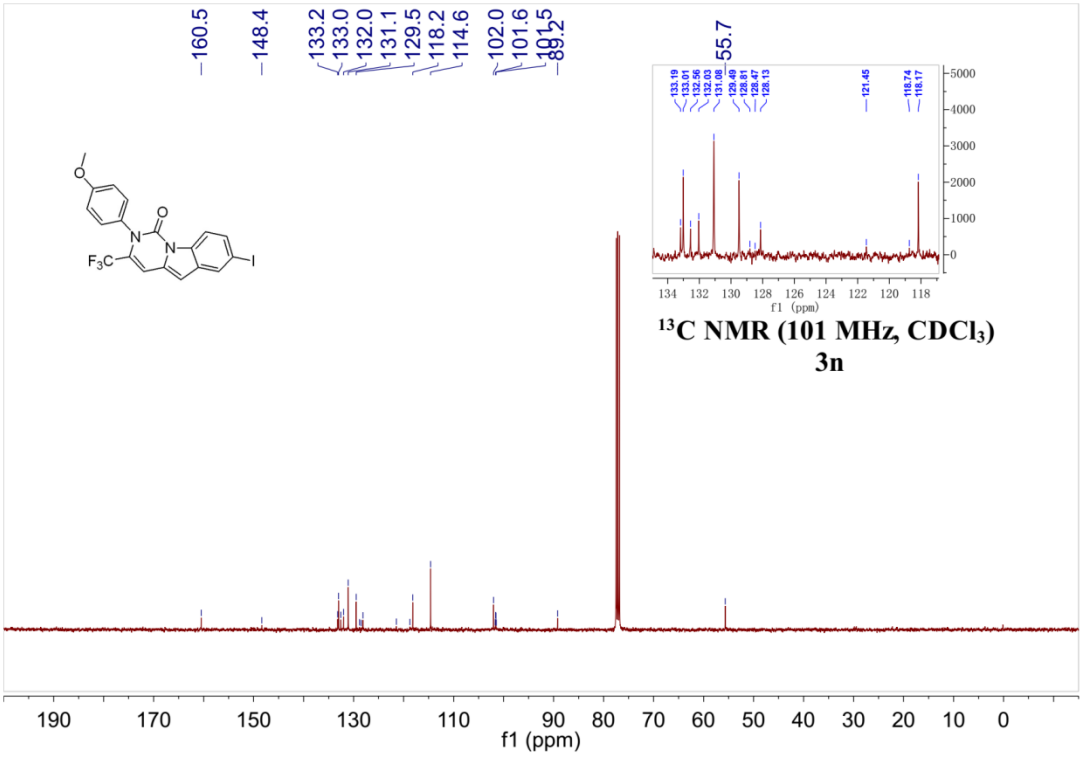


^{13}C NMR (101 MHz, $CDCl_3$)
3m

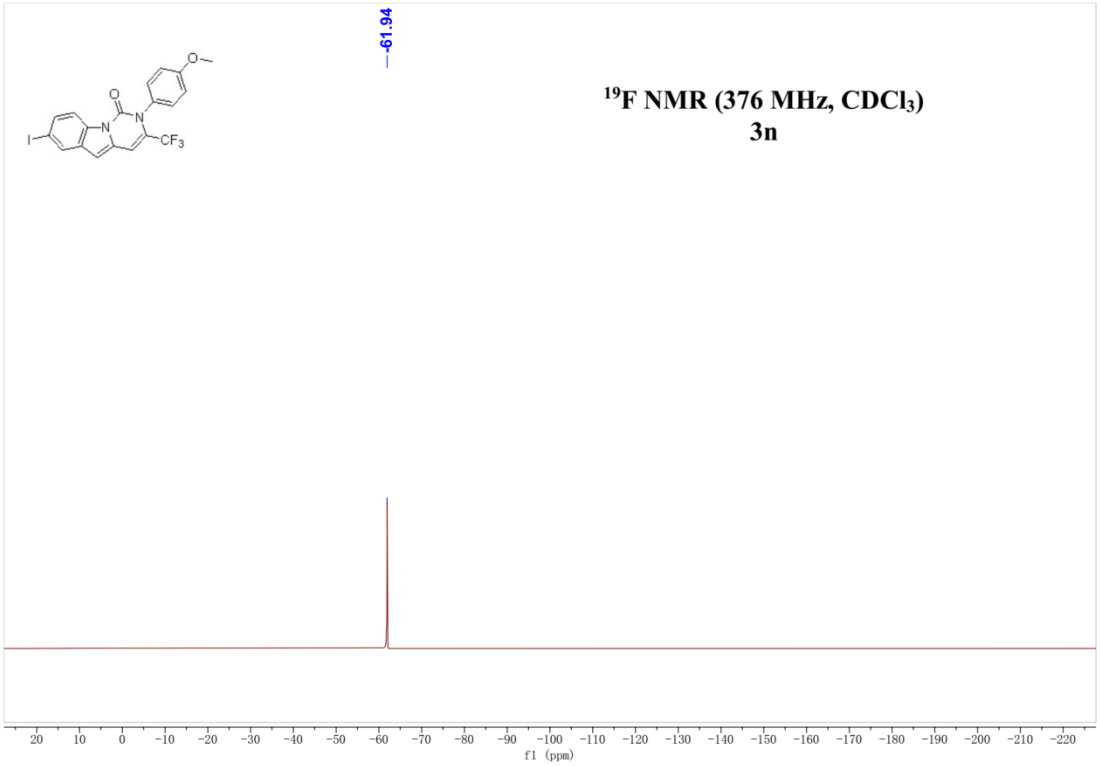

-61.97
O
N
O
Br
CF3
19F NMR (376 MHz, CDCl3)
3m
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220
f1 (ppm)



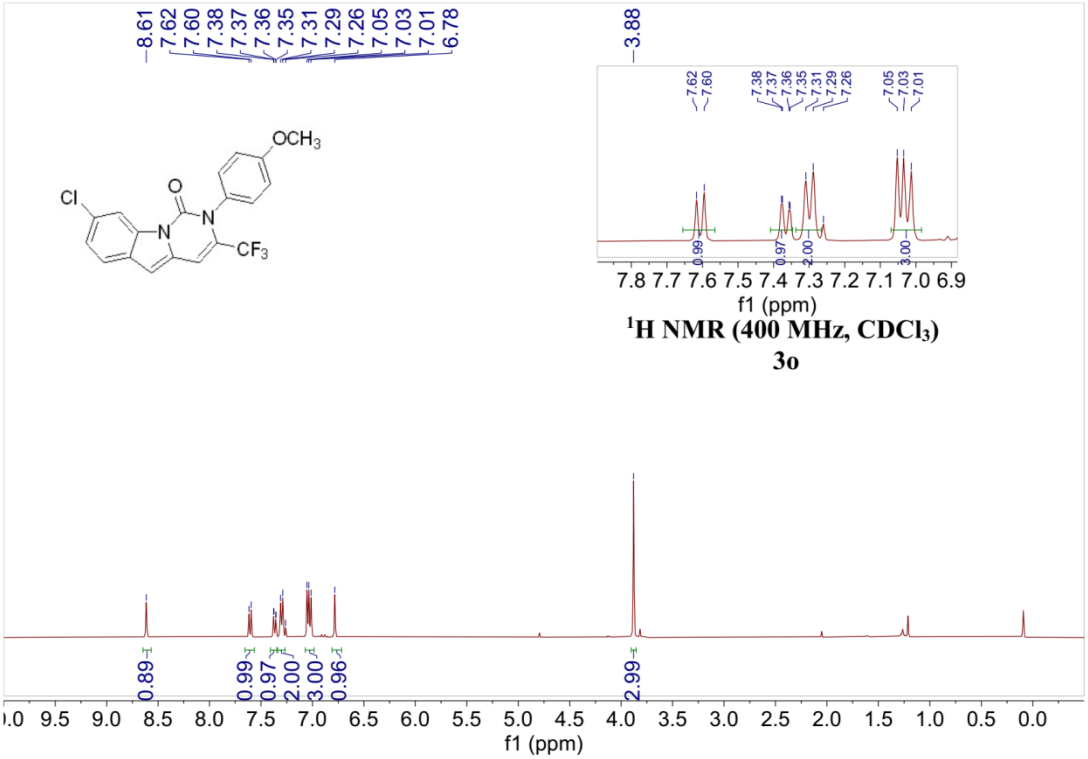
^{1}H NMR (400 MHz, $CDCl_3$)
3n



^{13}C NMR (101 MHz, $CDCl_3$)
3n

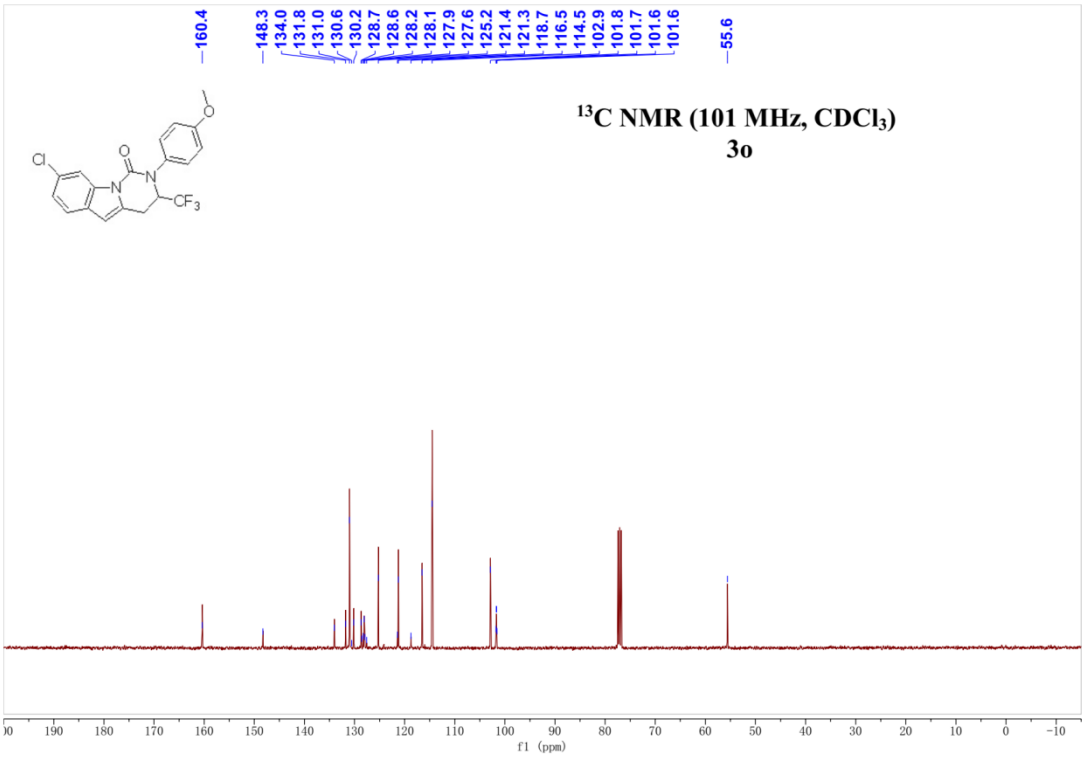


^{19}F NMR (376 MHz, $CDCl_3$)
3n



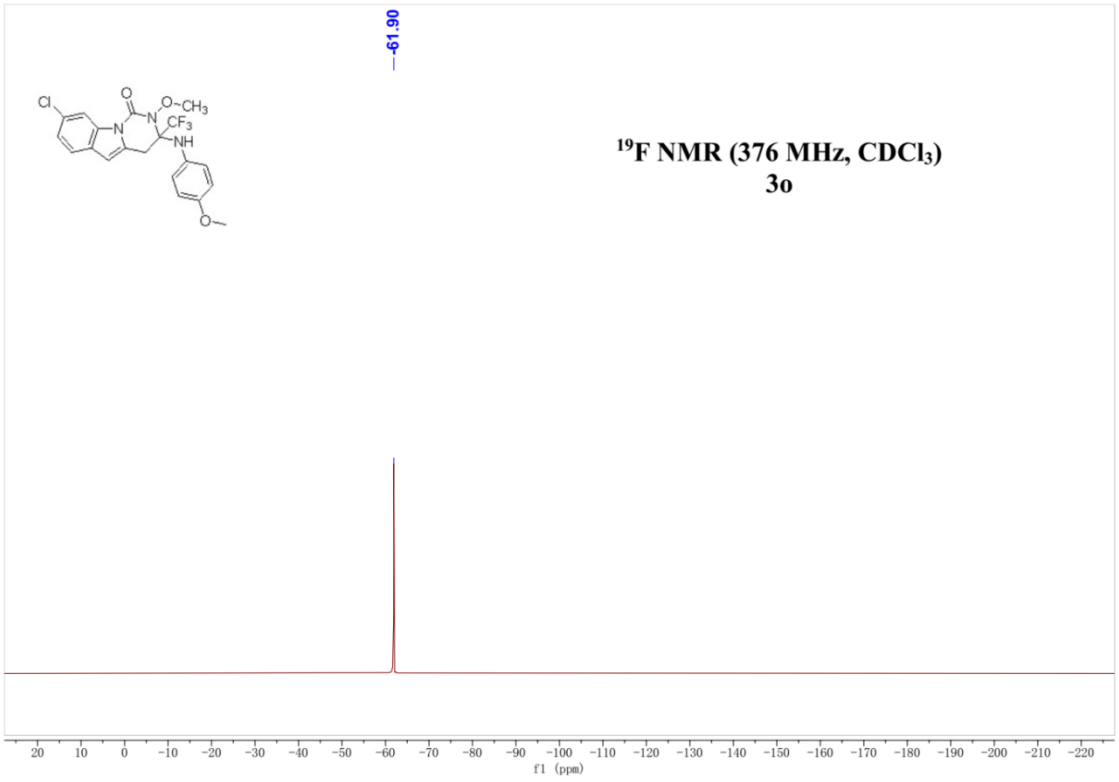
^{1}H NMR (400 MHz, $CDCl_3$)

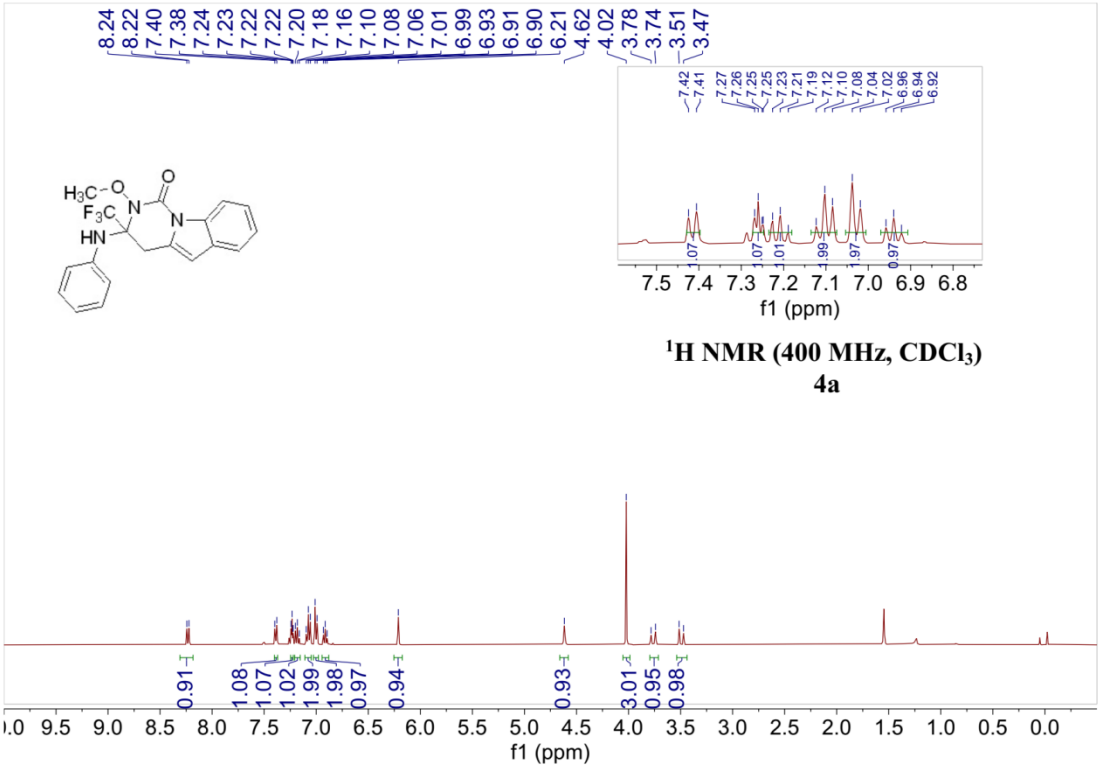
3o



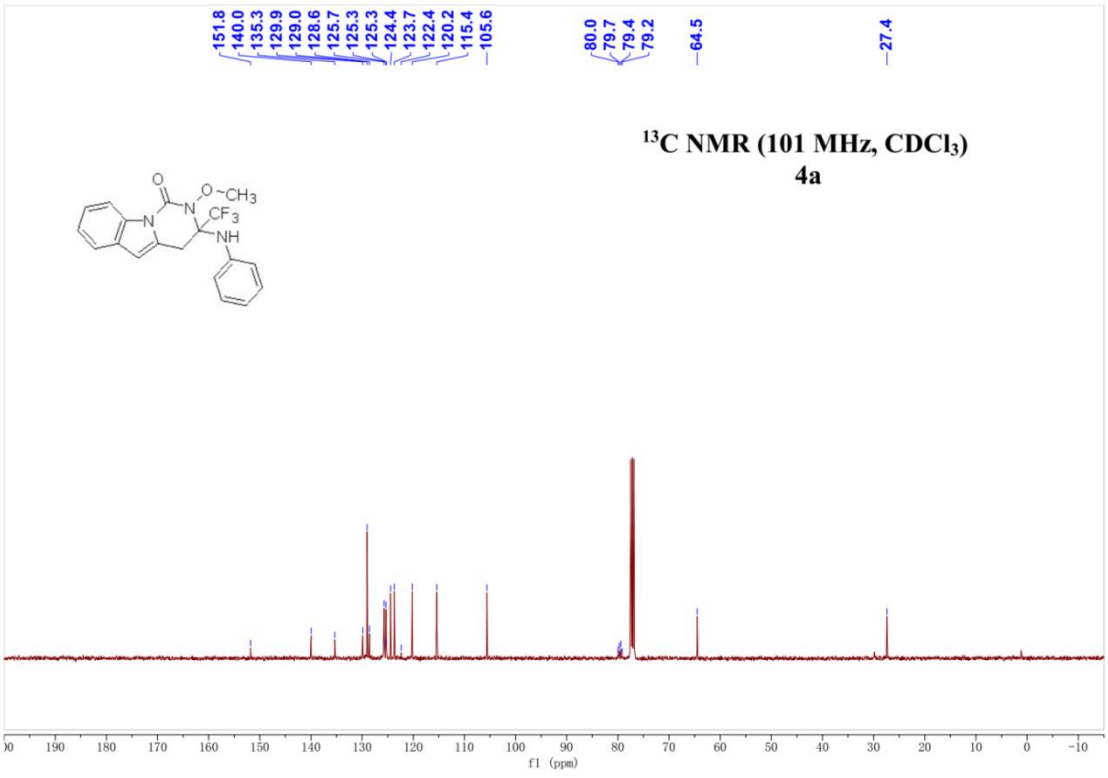
^{13}C NMR (101 MHz, $CDCl_3$)

3o

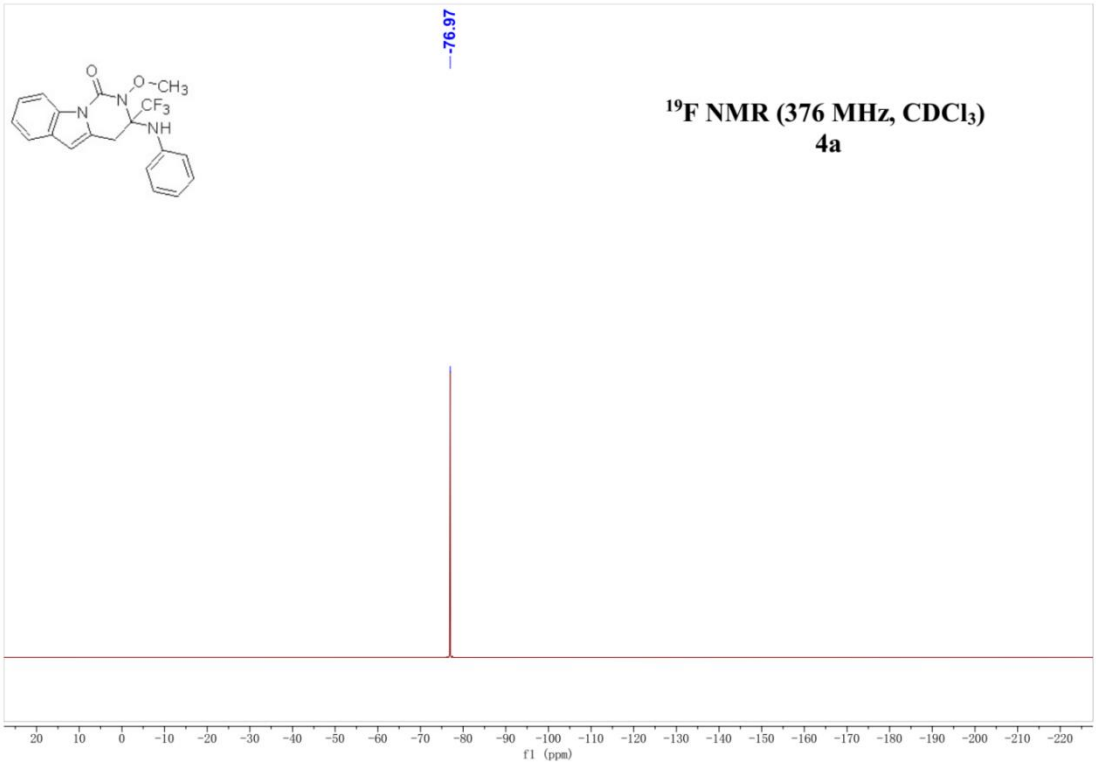

-61.90
Cl
O
N
O-CH3
CF3
NH
O
19F NMR (376 MHz, CDCl3)
3o
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220
f1 (ppm)

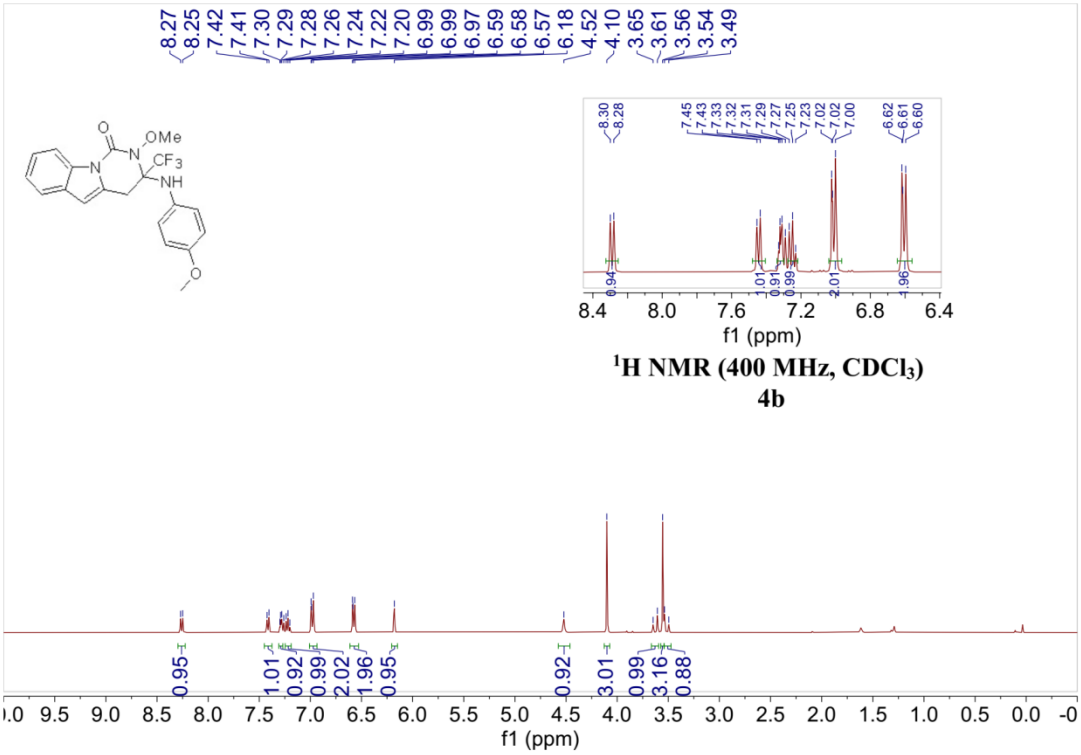


^{1}H NMR (400 MHz, $CDCl_3$)
4a

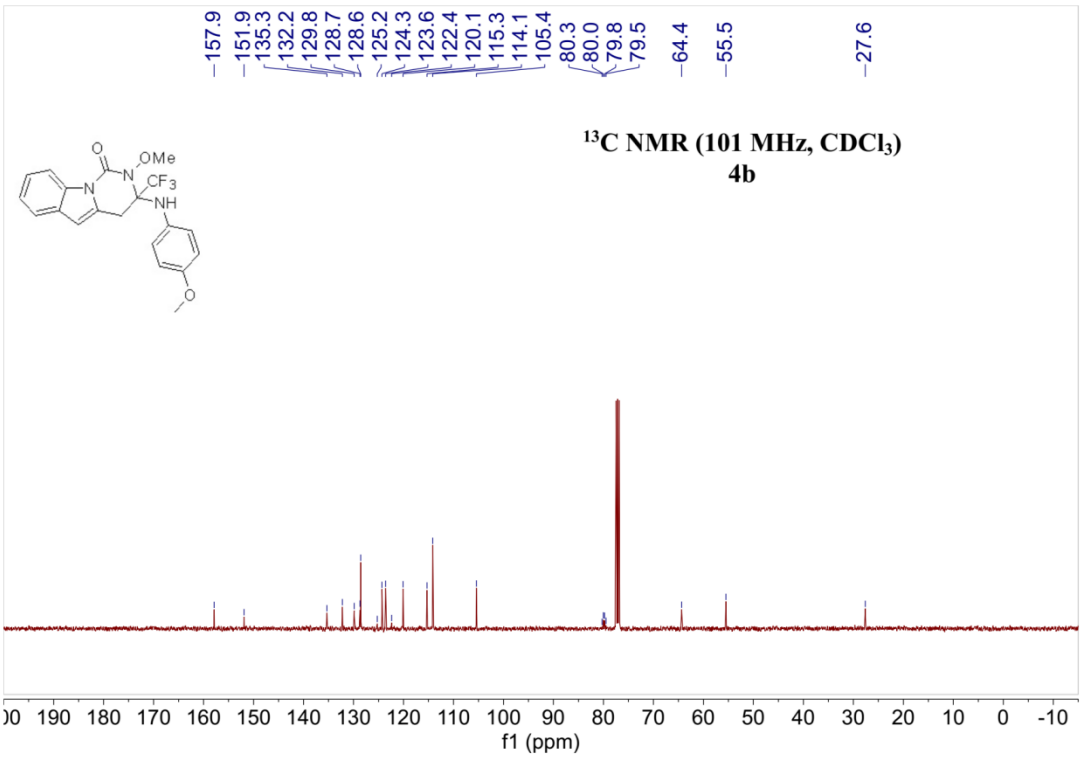


^{13}C NMR (101 MHz, $CDCl_3$)
4a

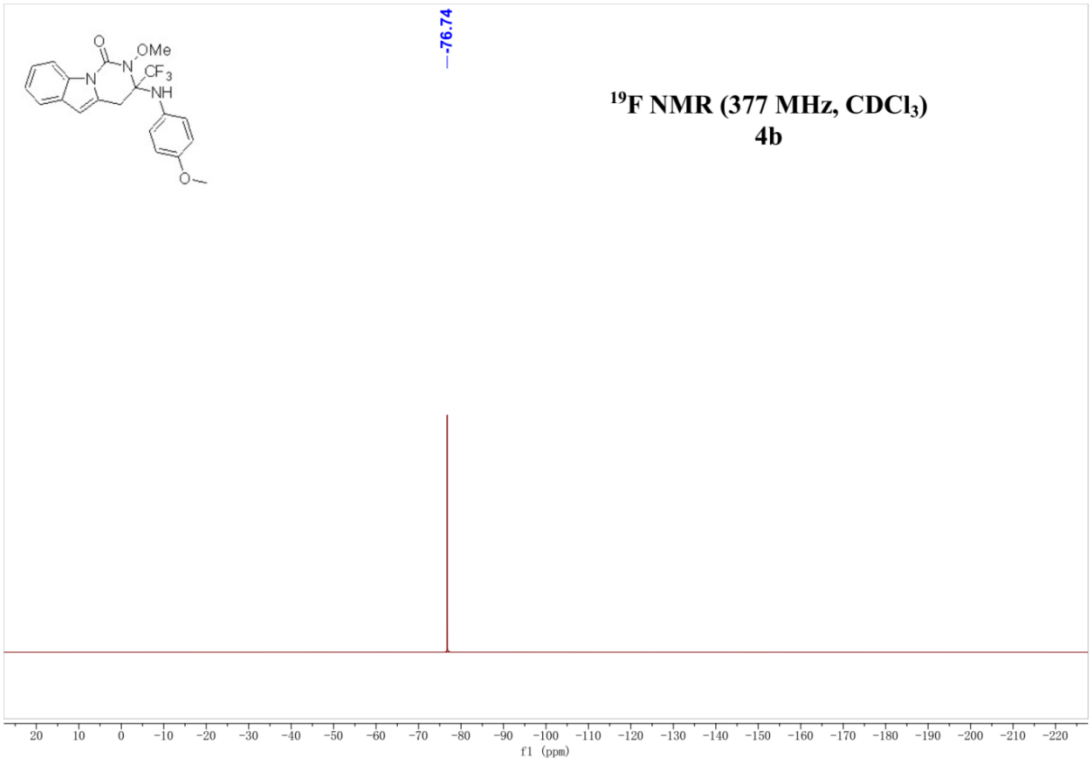

-76.97
O
O~CH3
N
N
CF3
NH
19F NMR (376 MHz, CDCl3)
4a
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220
f1 (ppm)

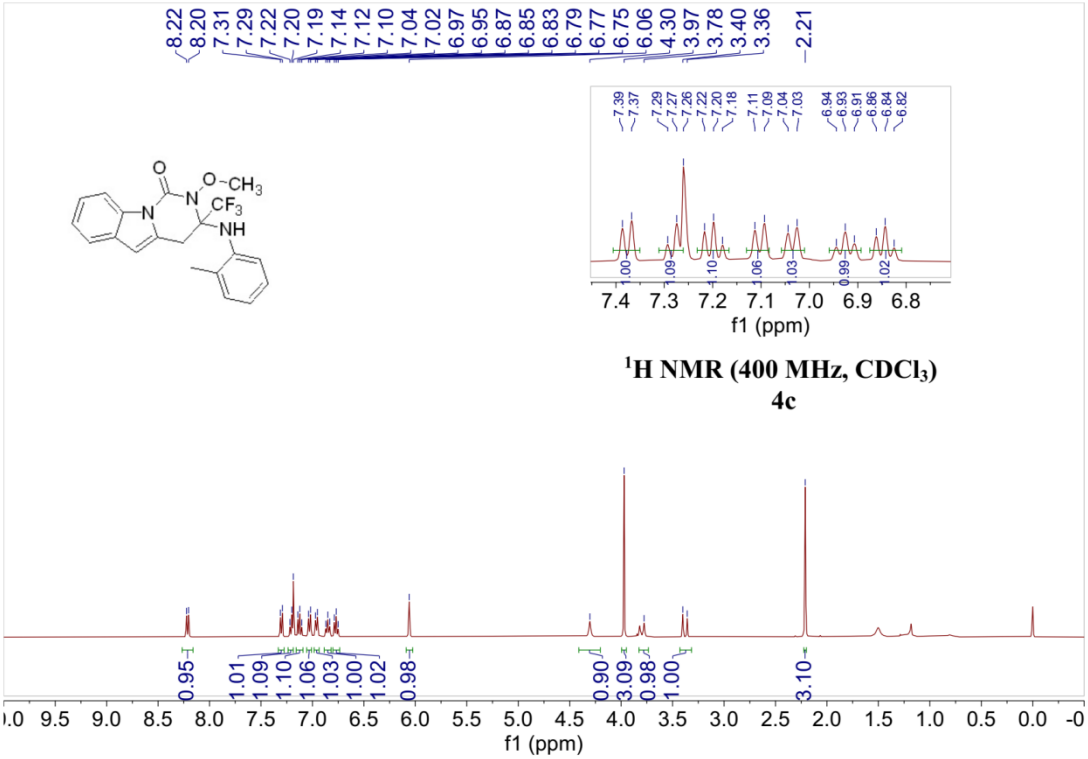


^{1}H NMR (400 MHz, $CDCl_3$)
4b

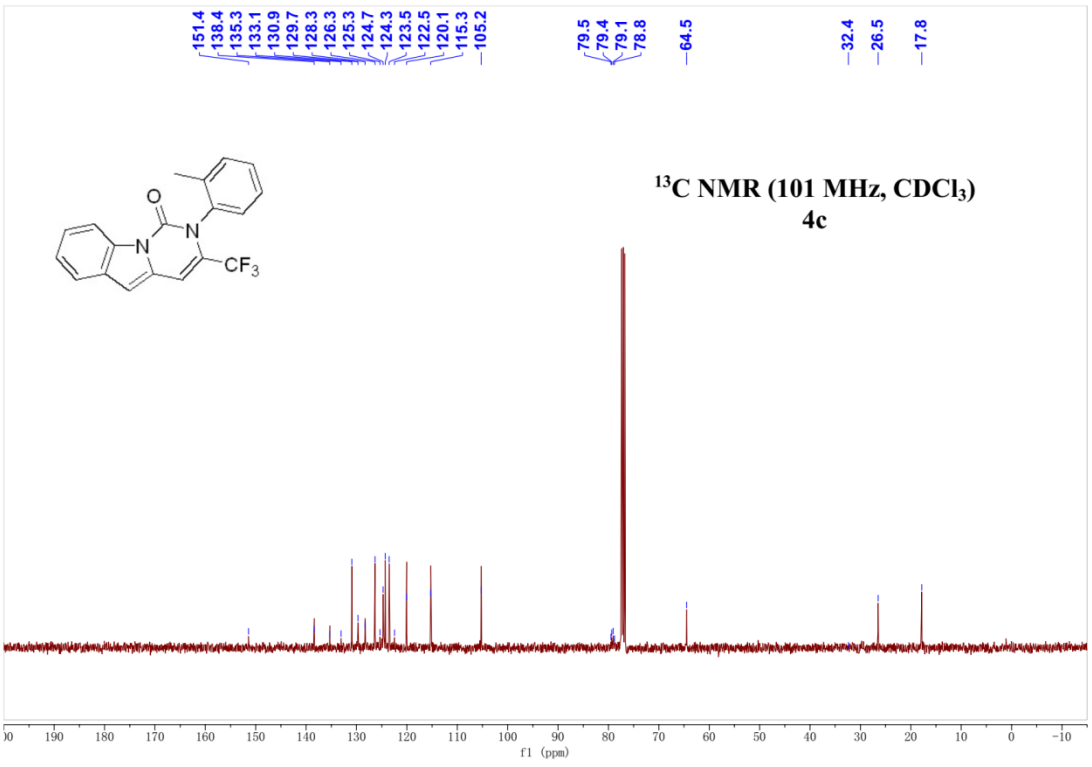


^{13}C NMR (101 MHz, $CDCl_3$)
4b

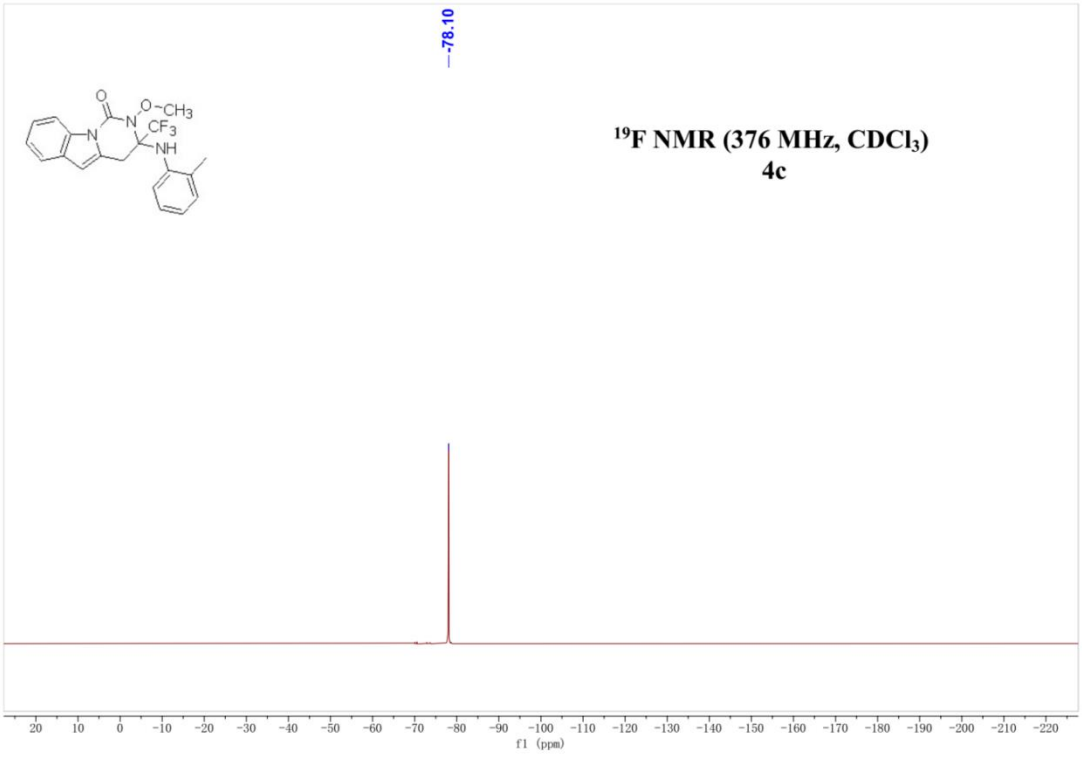

-76.74
OMe
CF3
NH
O
N
O
19F NMR (377 MHz, CDCl3)
4b
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220
f1 (ppm)



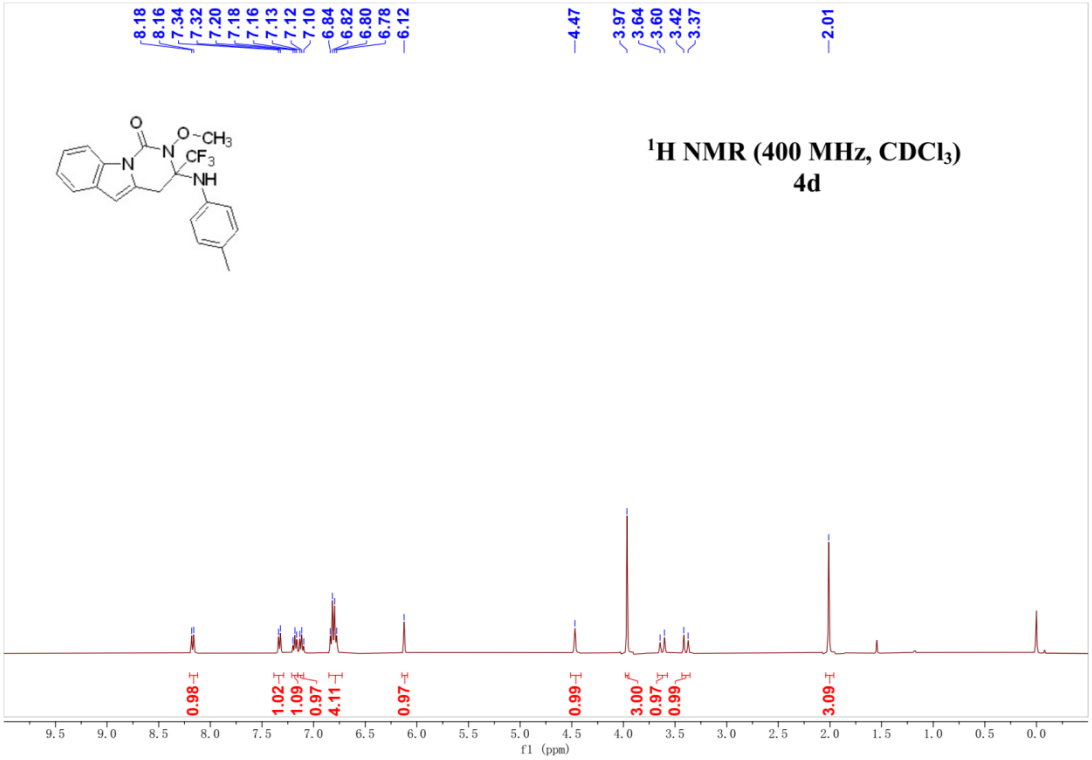
^{1}H NMR (400 MHz, $CDCl_3$)
4c



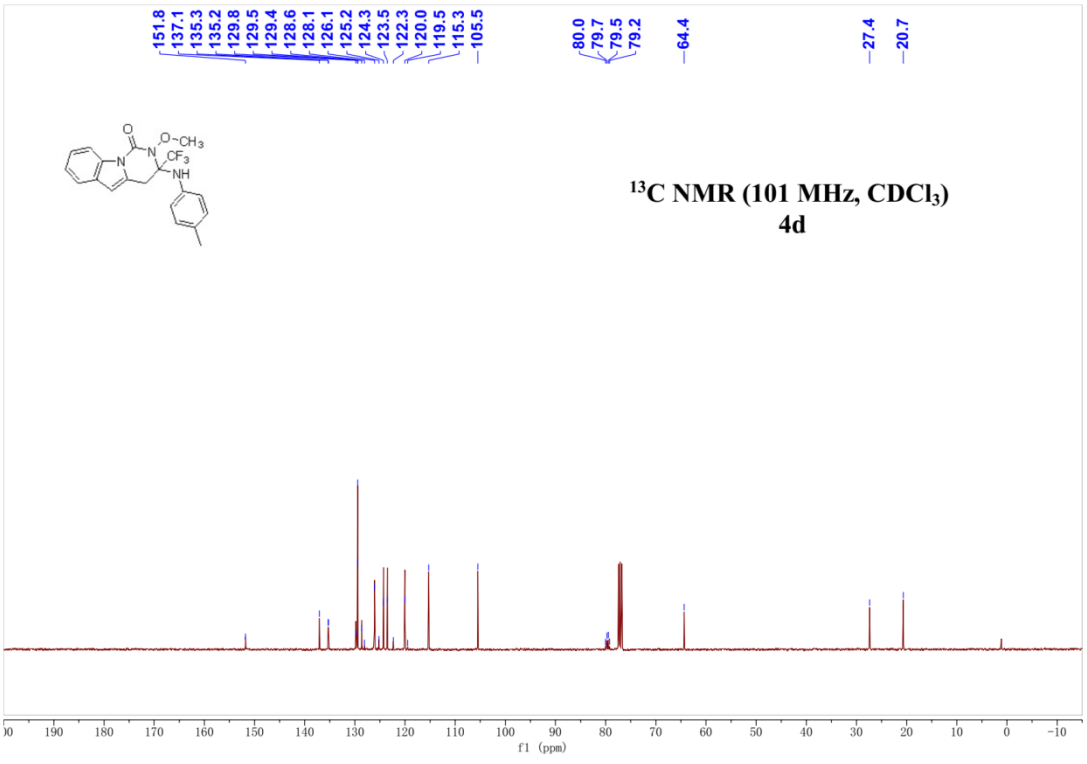
^{13}C NMR (101 MHz, $CDCl_3$)
4c



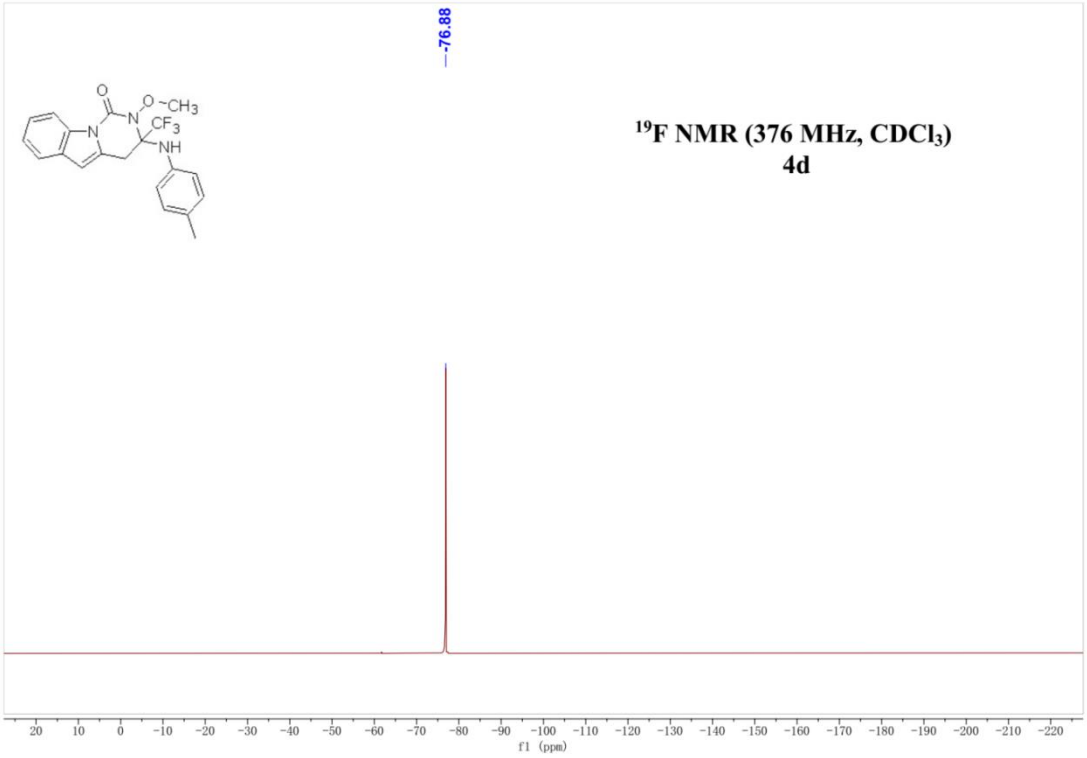
^{19}F NMR (376 MHz, $CDCl_3$)
4c

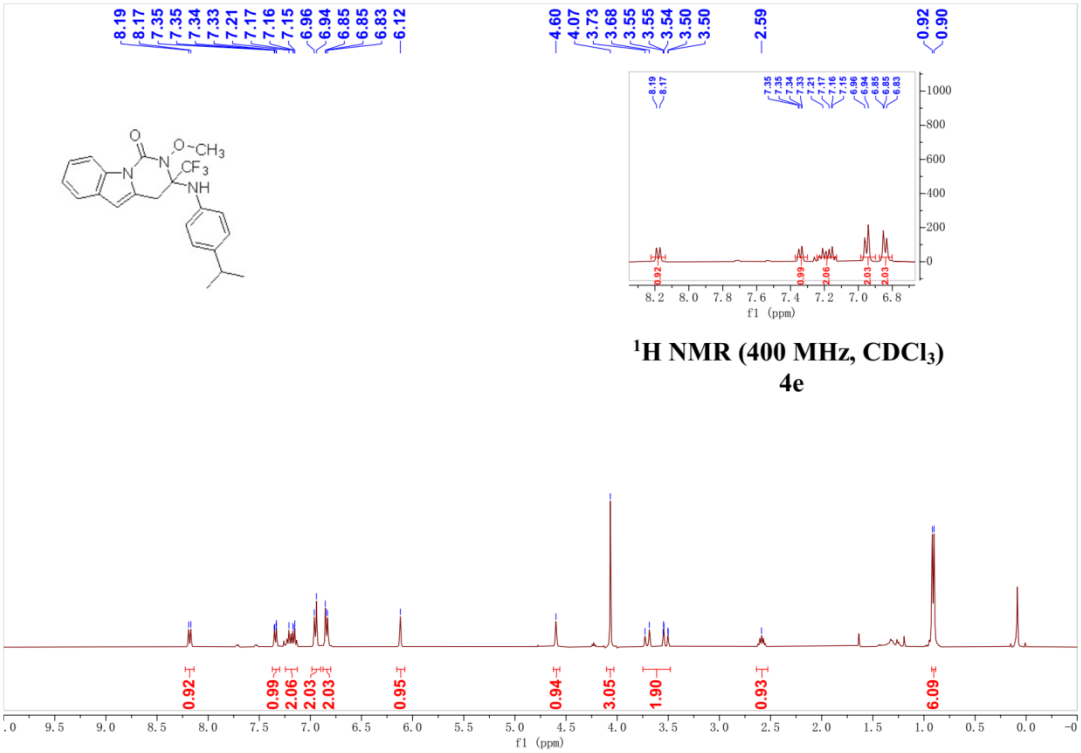


^{1}H NMR (400 MHz, $CDCl_3$)
4d

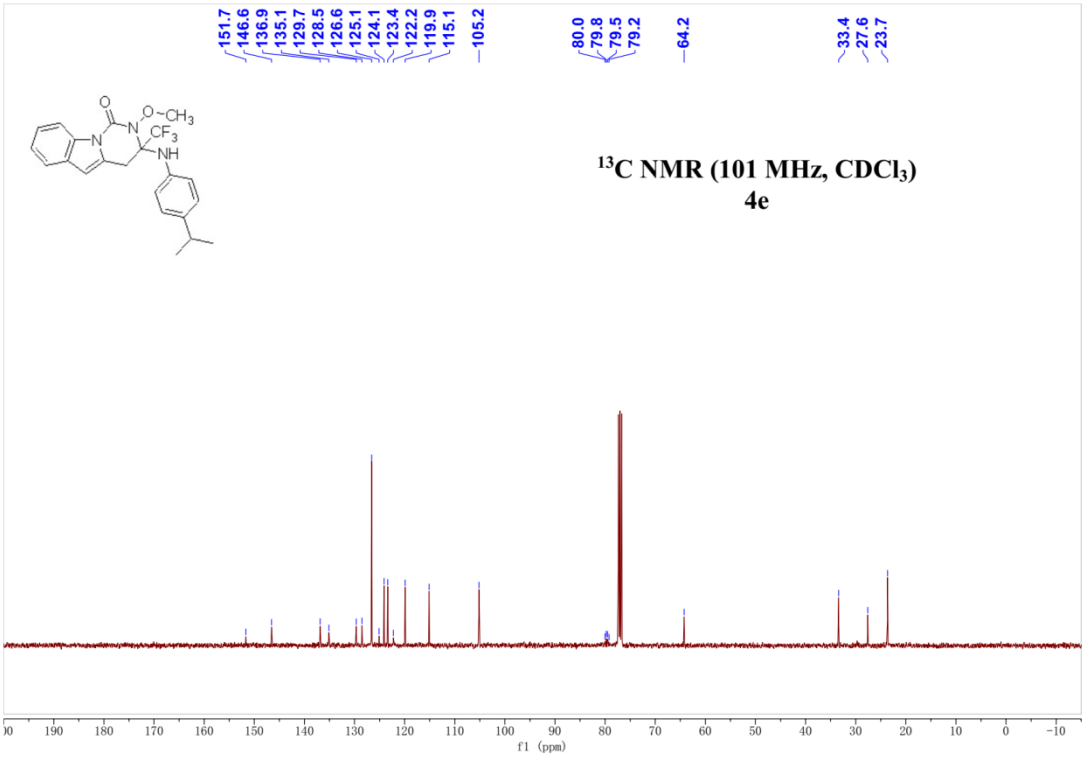


^{13}C NMR (101 MHz, $CDCl_3$)
4d

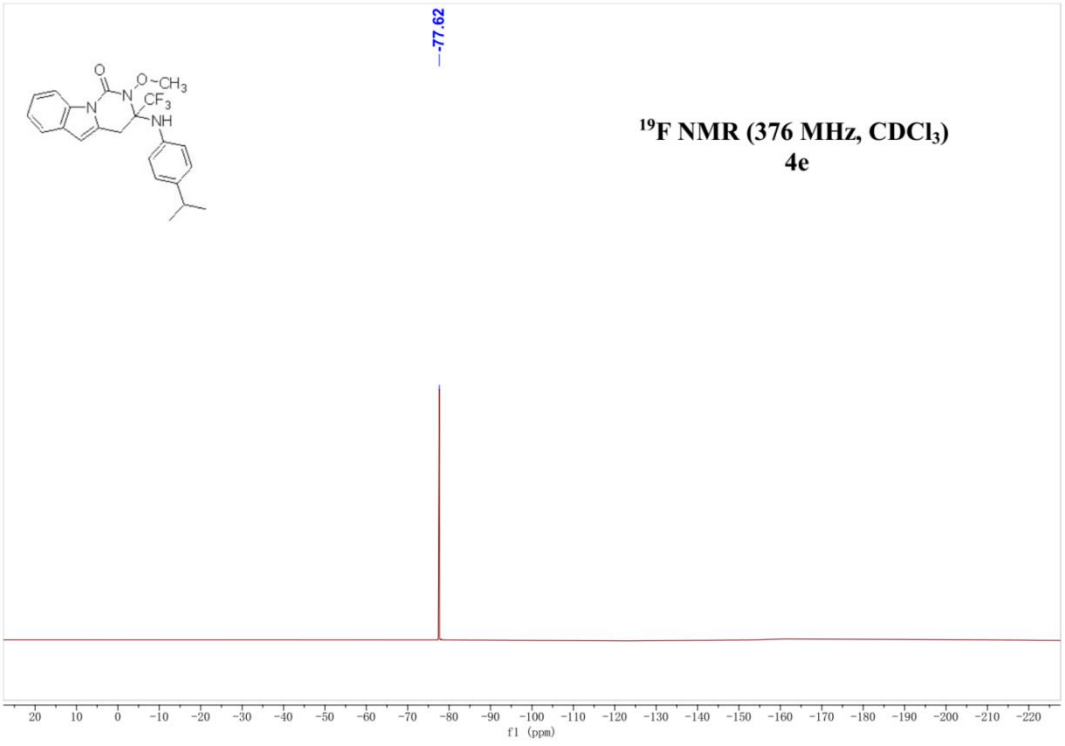

-76.88
O
N
O
CH3
CF3
NH
19F NMR (376 MHz, CDCl3)
4d
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220
f1 (ppm)

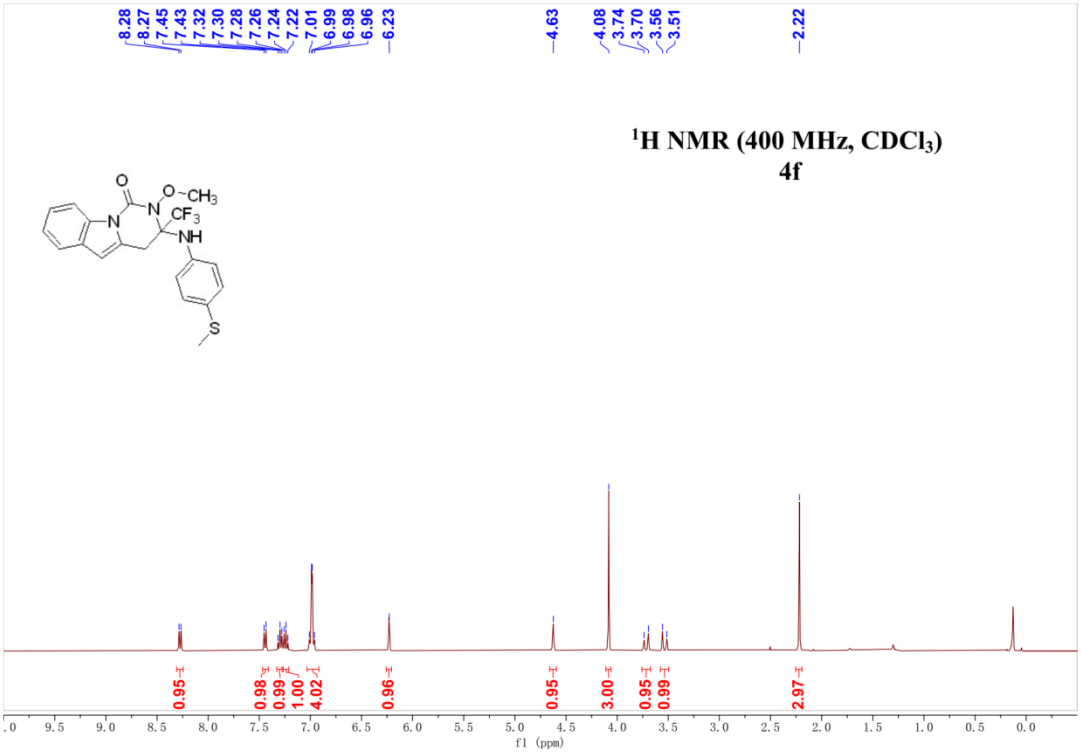


^{1}H NMR (400 MHz, $CDCl_3$)
4e

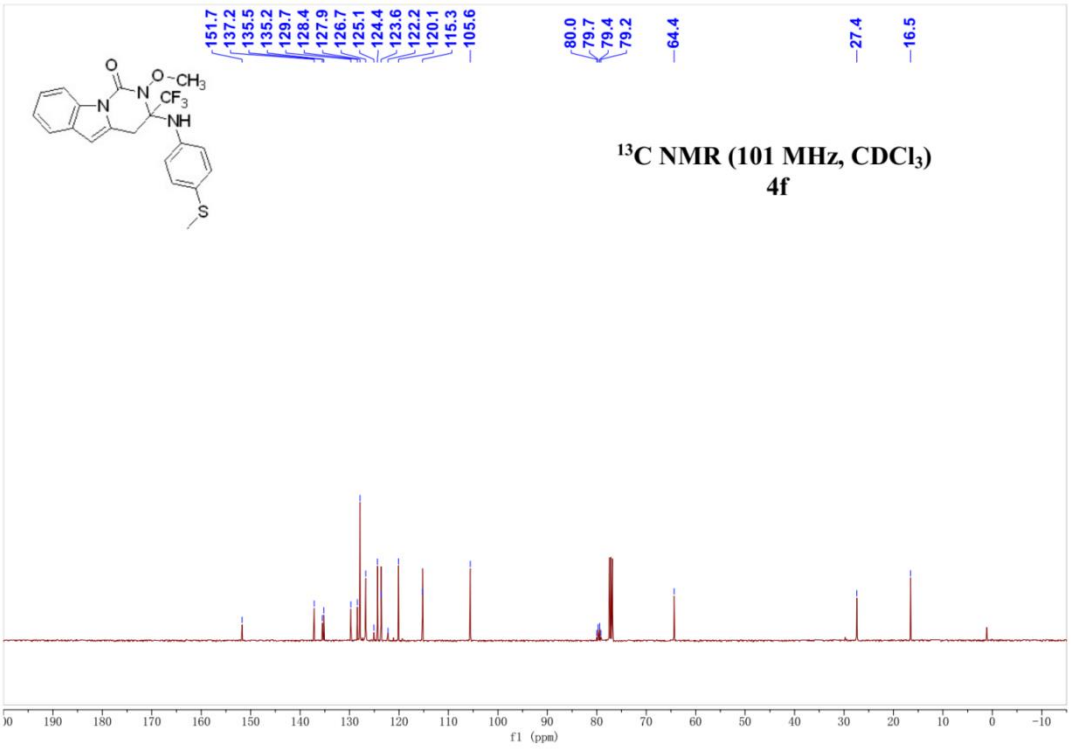


^{13}C NMR (101 MHz, $CDCl_3$)
4e

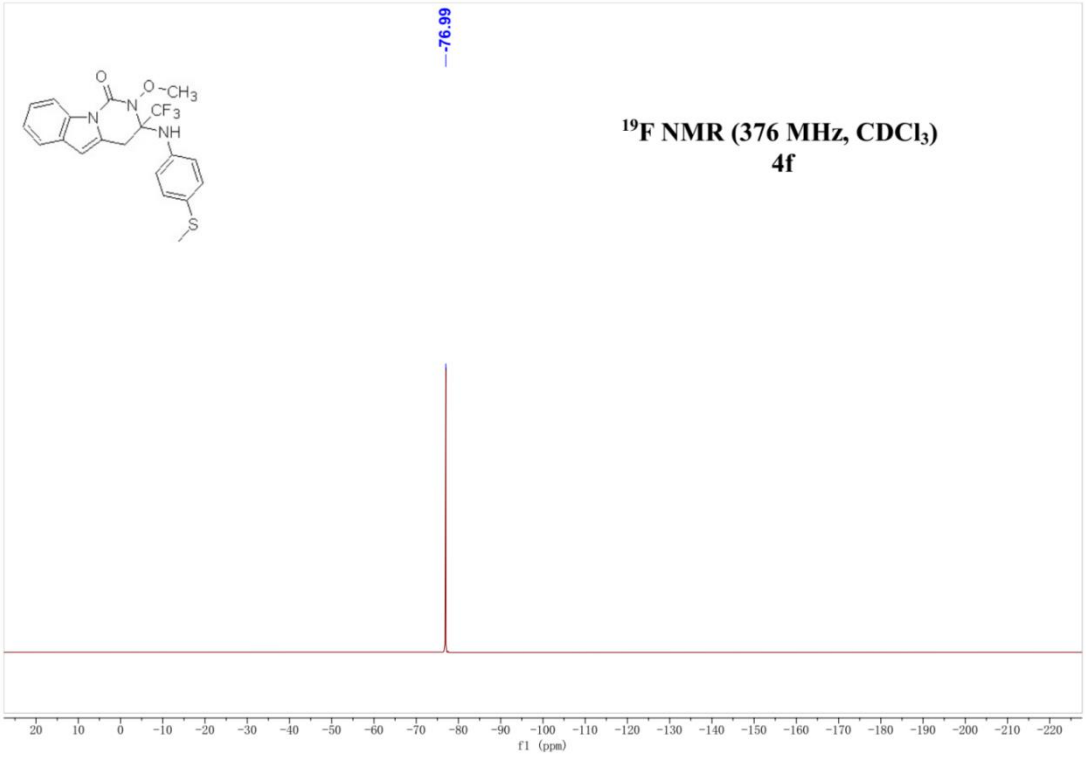

-77.62
O
O
CH3
N
CF3
NH
19F NMR (376 MHz, CDCl3)
4e
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220
f1 (ppm)



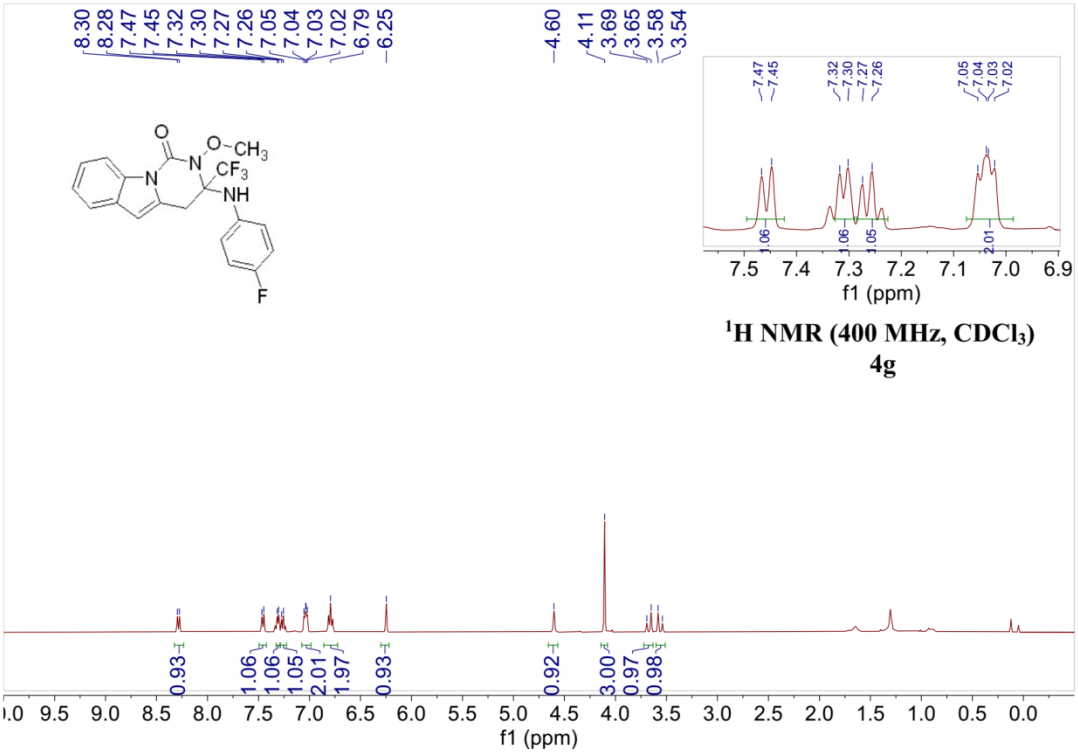
^{1}H NMR (400 MHz, $CDCl_3$)
4f



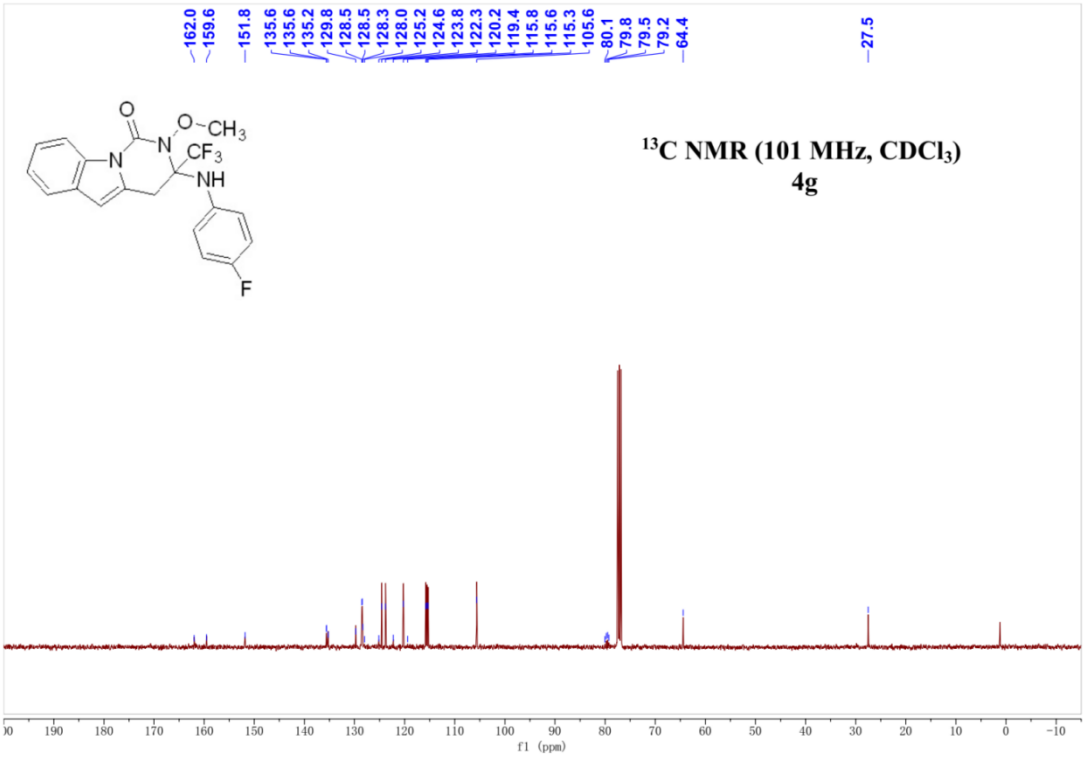
^{13}C NMR (101 MHz, $CDCl_3$)
4f



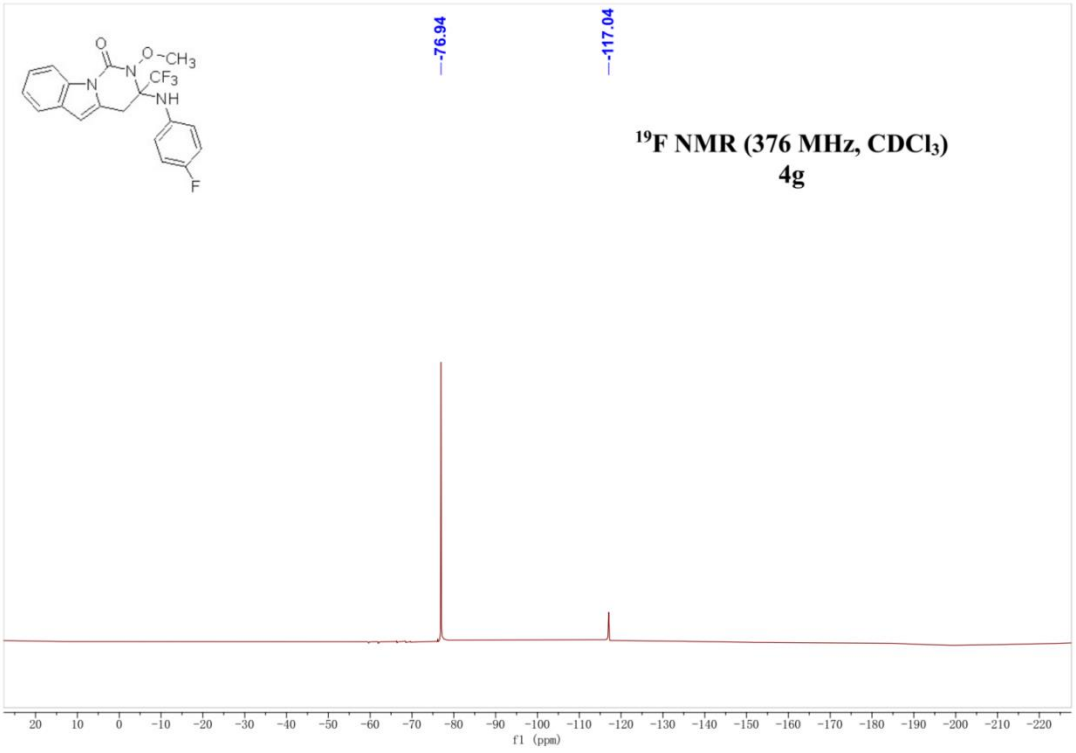
^{19}F NMR (376 MHz, $CDCl_3$)
4f

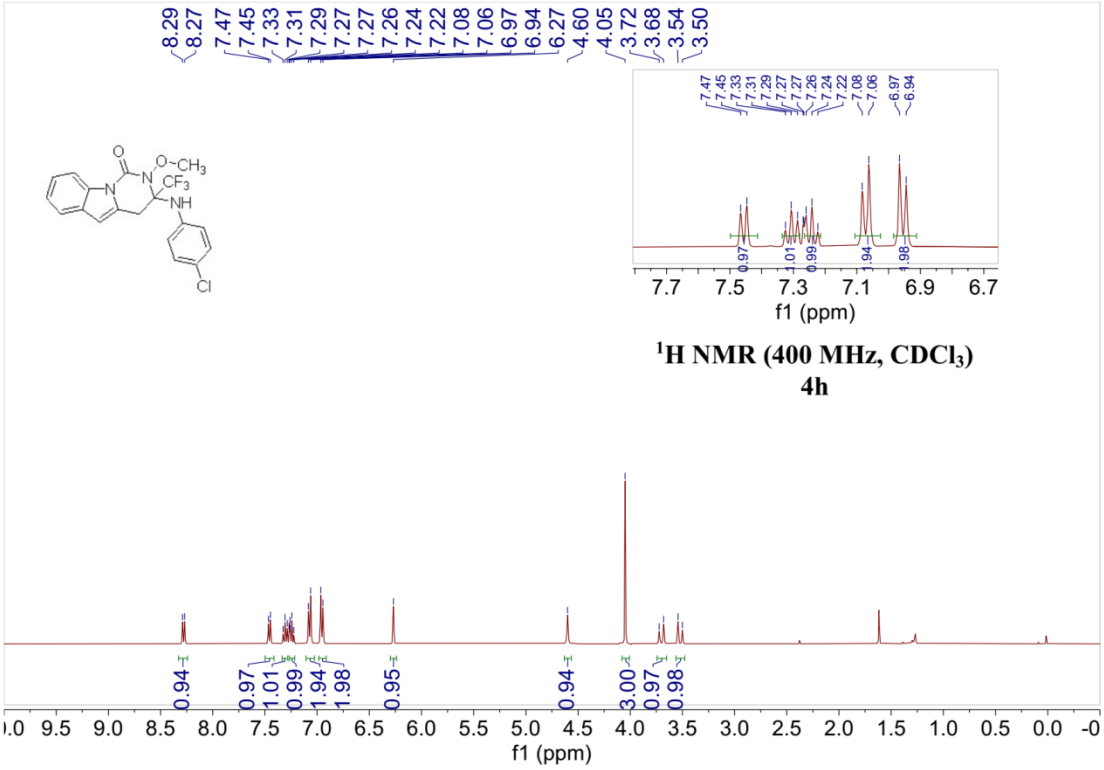


^{1}H NMR (400 MHz, $CDCl_3$)
4g

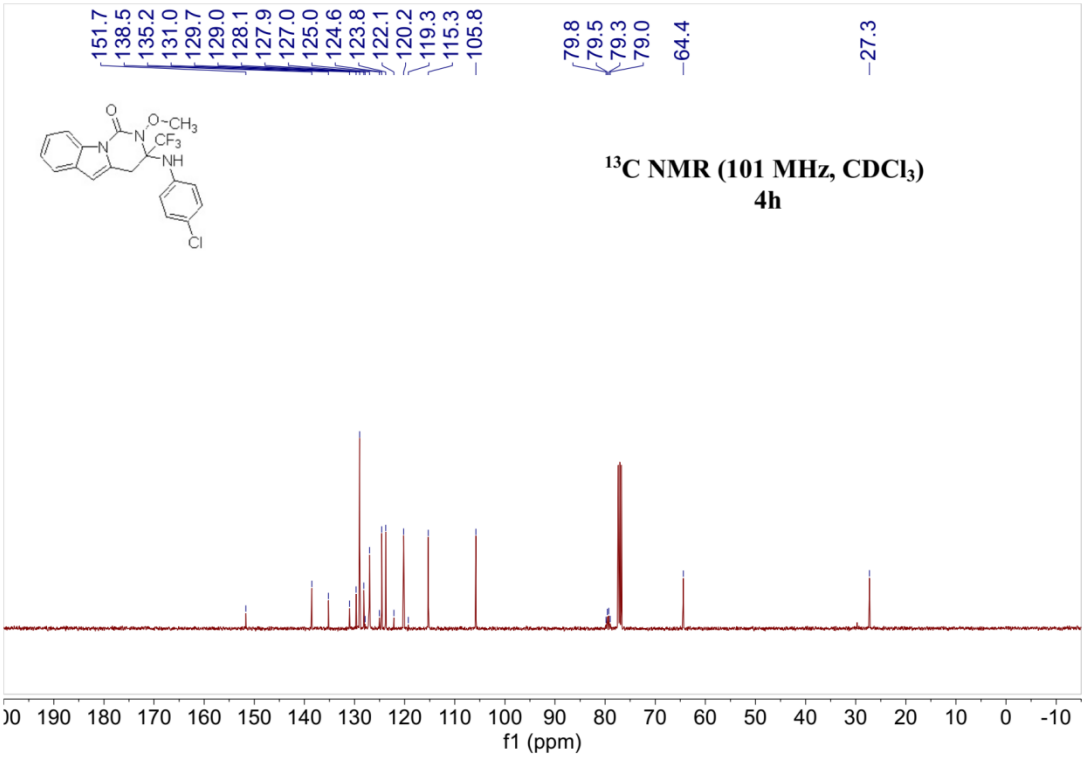


^{13}C NMR (101 MHz, $CDCl_3$)
4g

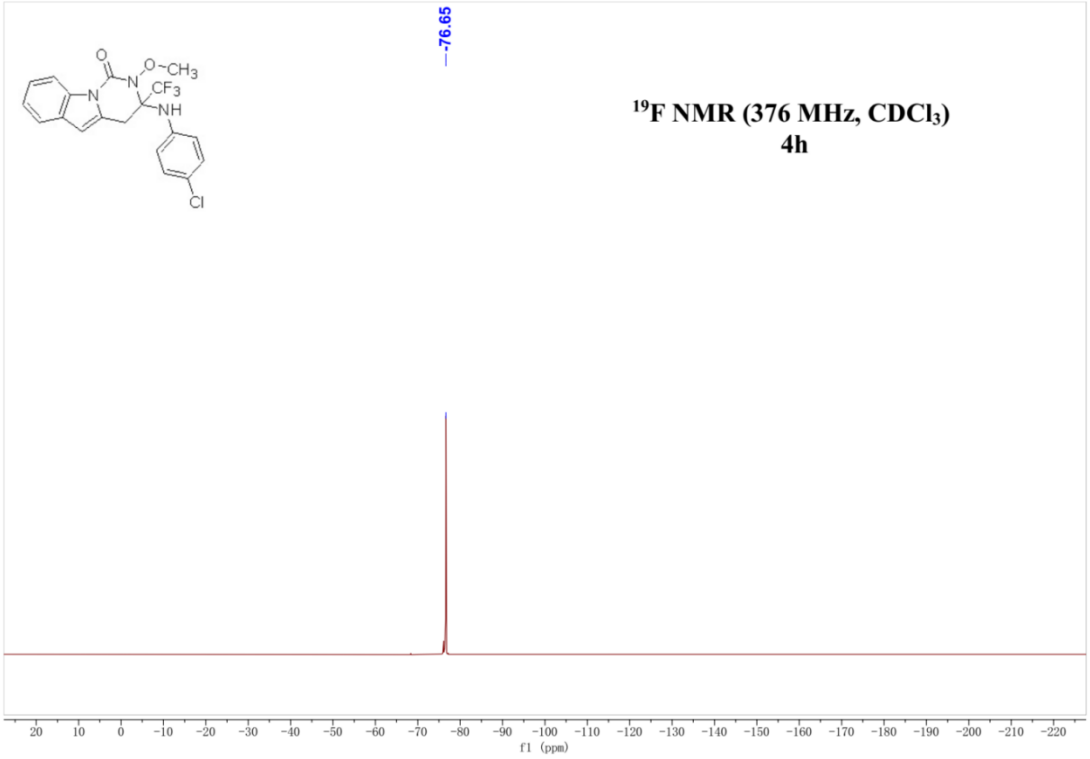

-76.94
-117.04
^{19}F NMR (376 MHz, CDCl$_3$)
4g
f1 (ppm)

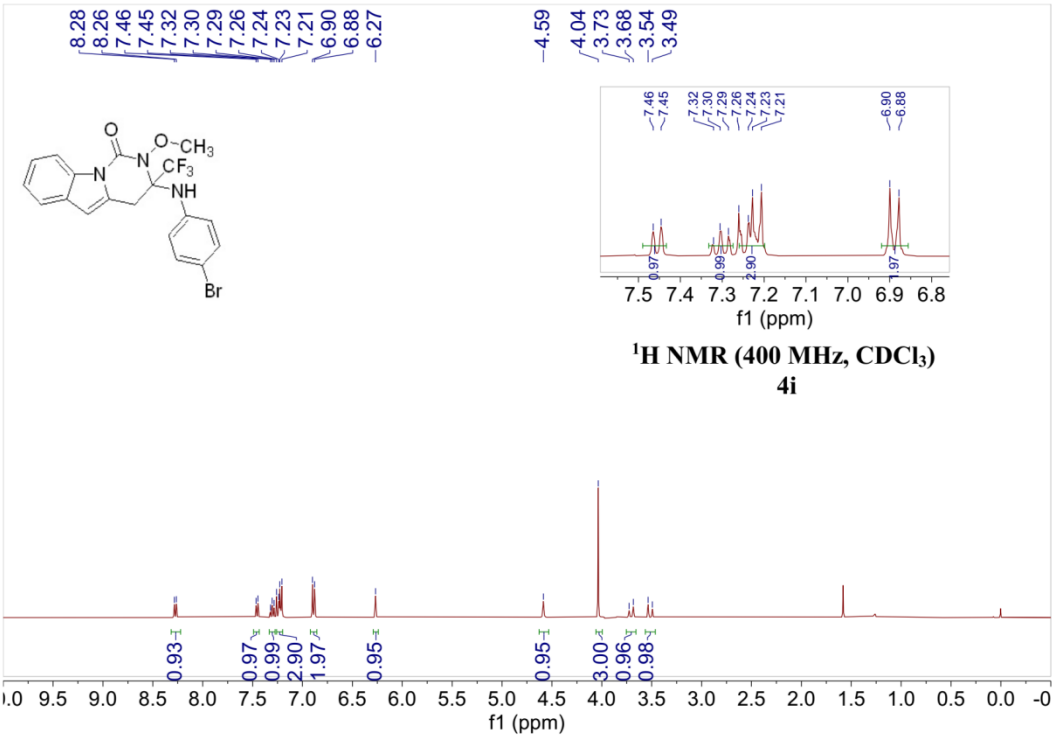


^{1}H NMR (400 MHz, $CDCl_3$)
4h

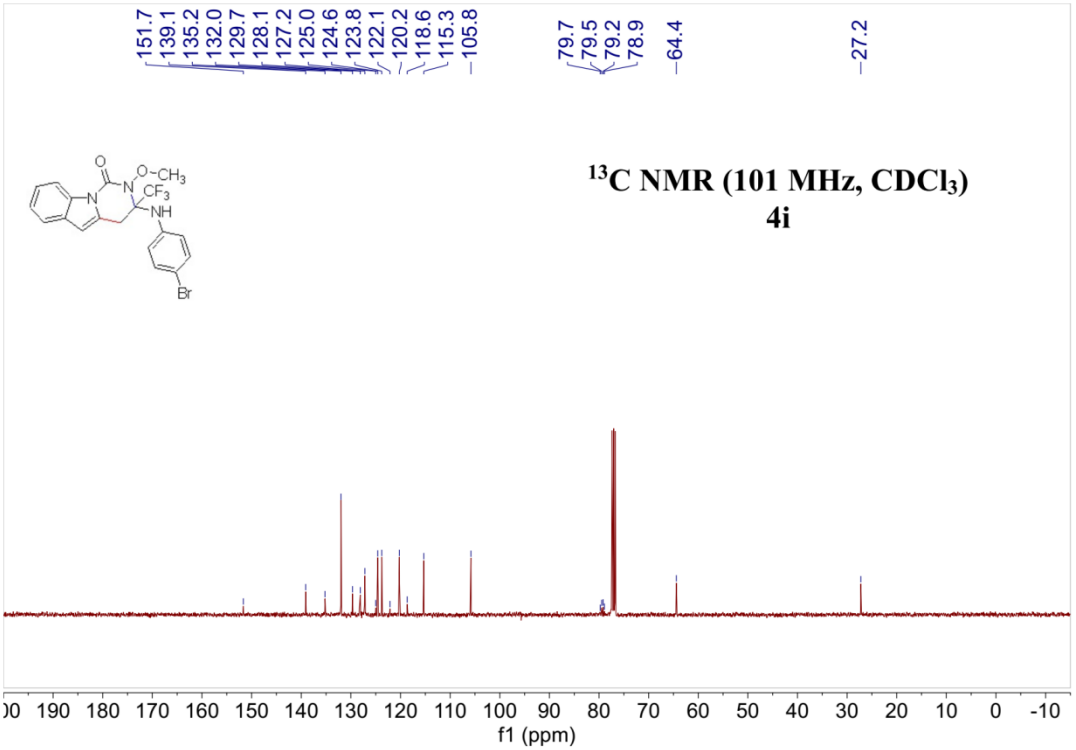


^{13}C NMR (101 MHz, $CDCl_3$)
4h

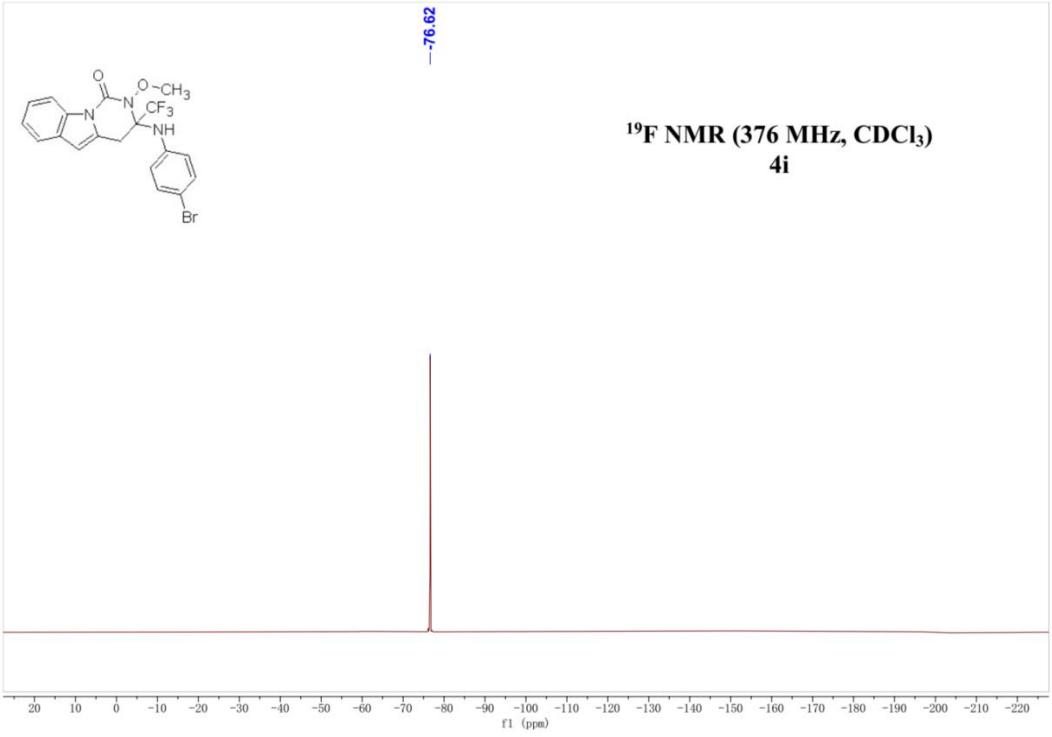

-76.65
O
N
O-CH3
CF3
NH
Cl
19F NMR (376 MHz, CDCl3)
4h
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220
f1 (ppm)

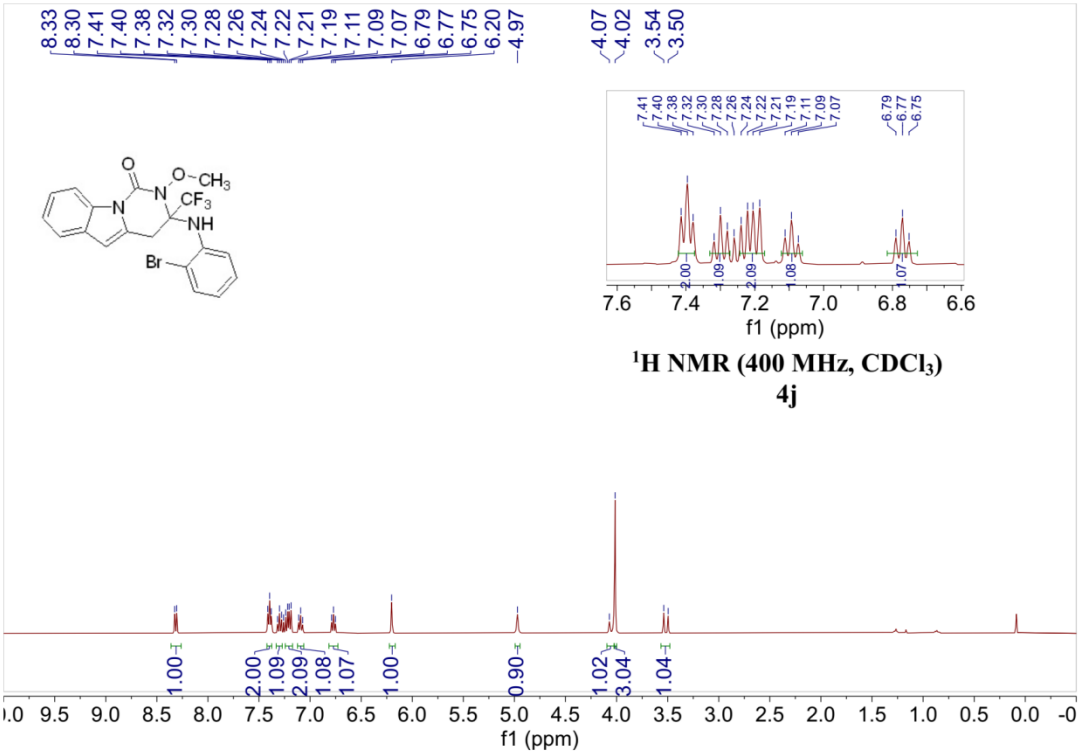


^{1}H NMR (400 MHz, $CDCl_3$)
4i

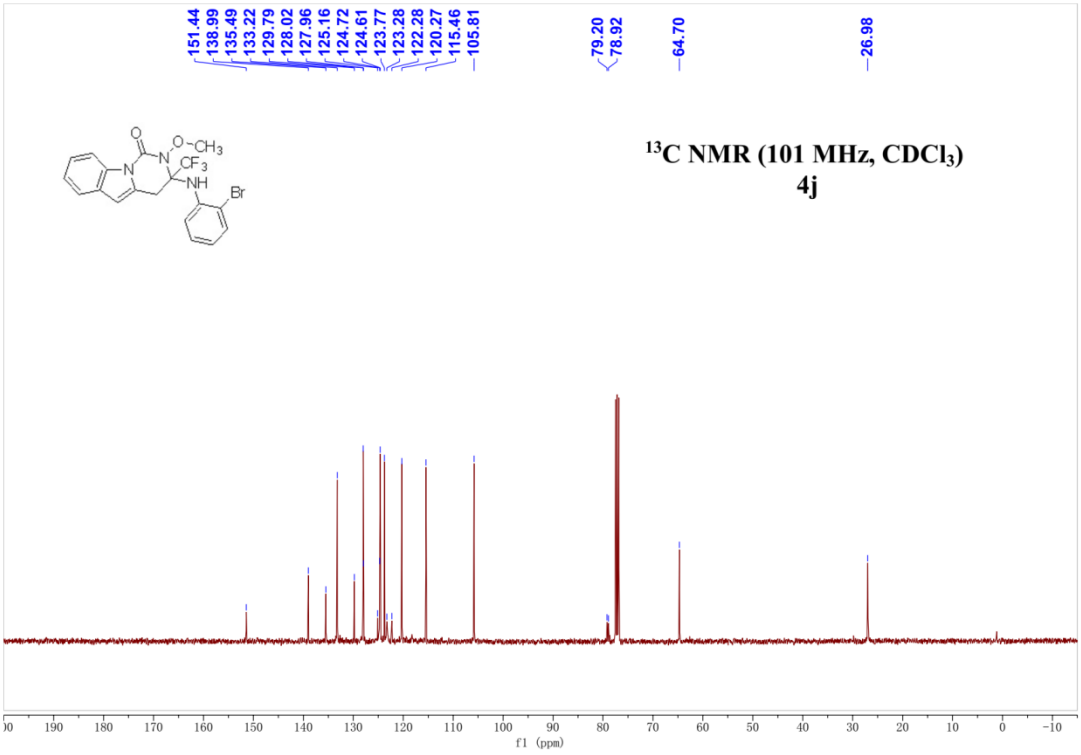


^{13}C NMR (101 MHz, $CDCl_3$)
4i

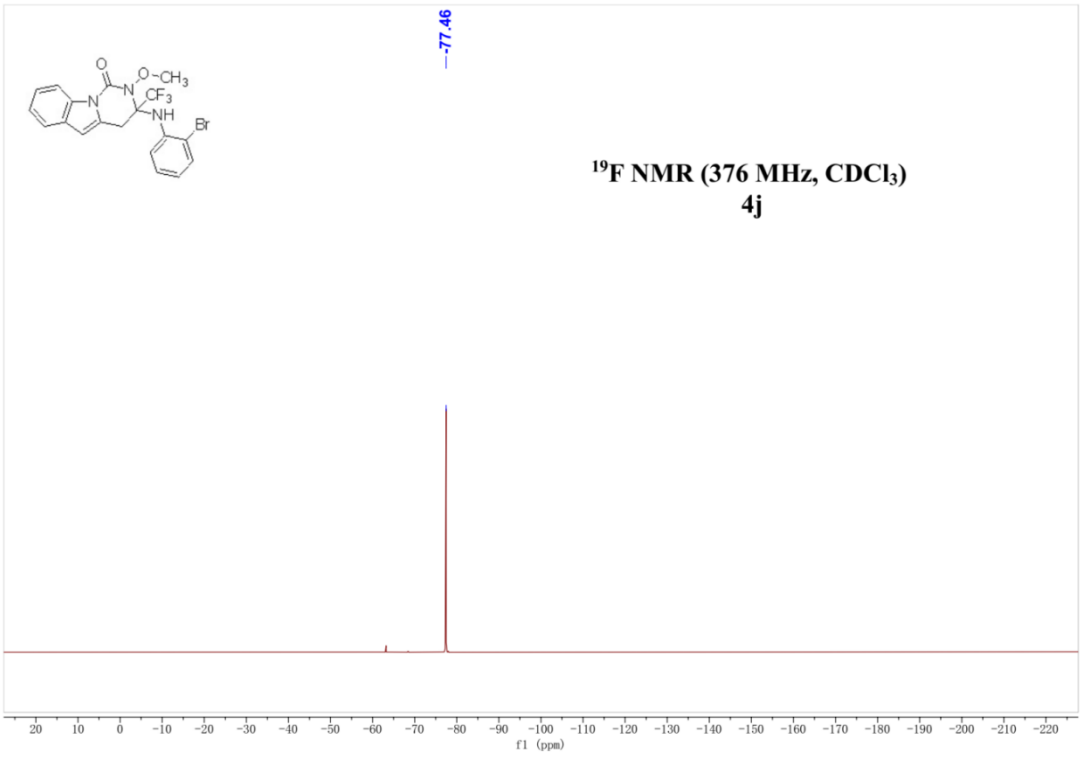

-76.62
O
O
CH3
N
N
CF3
NH
Br
19F NMR (376 MHz, CDCl3)
4i
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220
f1 (ppm)



^{1}H NMR (400 MHz, $CDCl_3$)
4j



^{13}C NMR (101 MHz, $CDCl_3$)
4j


-77.46
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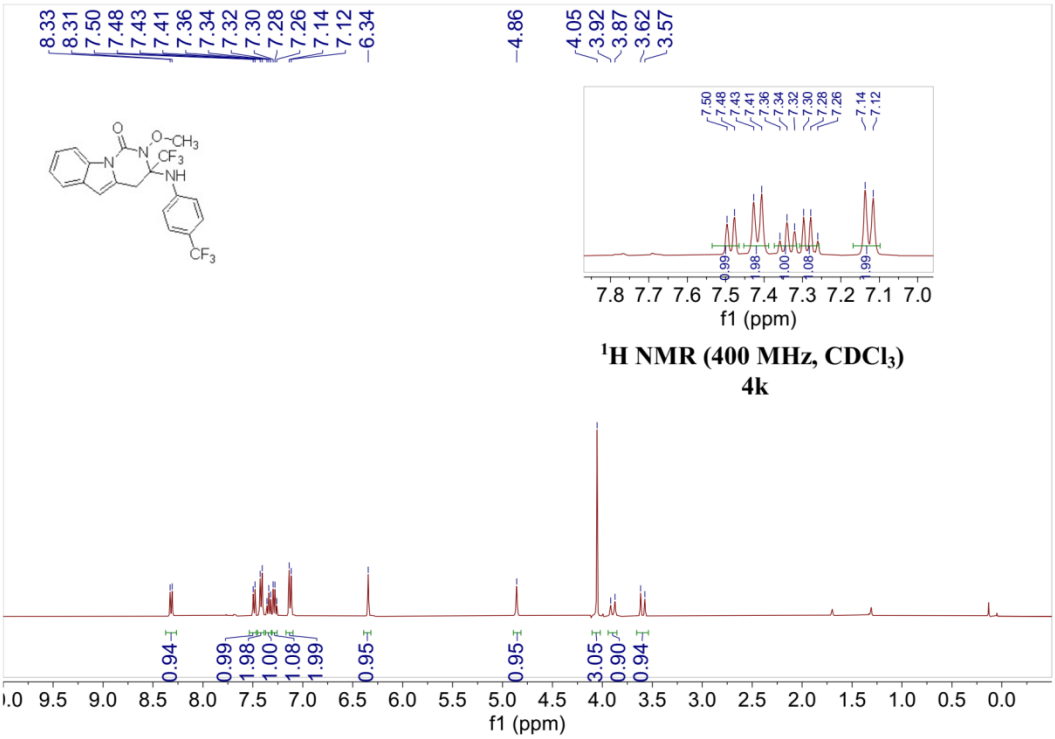
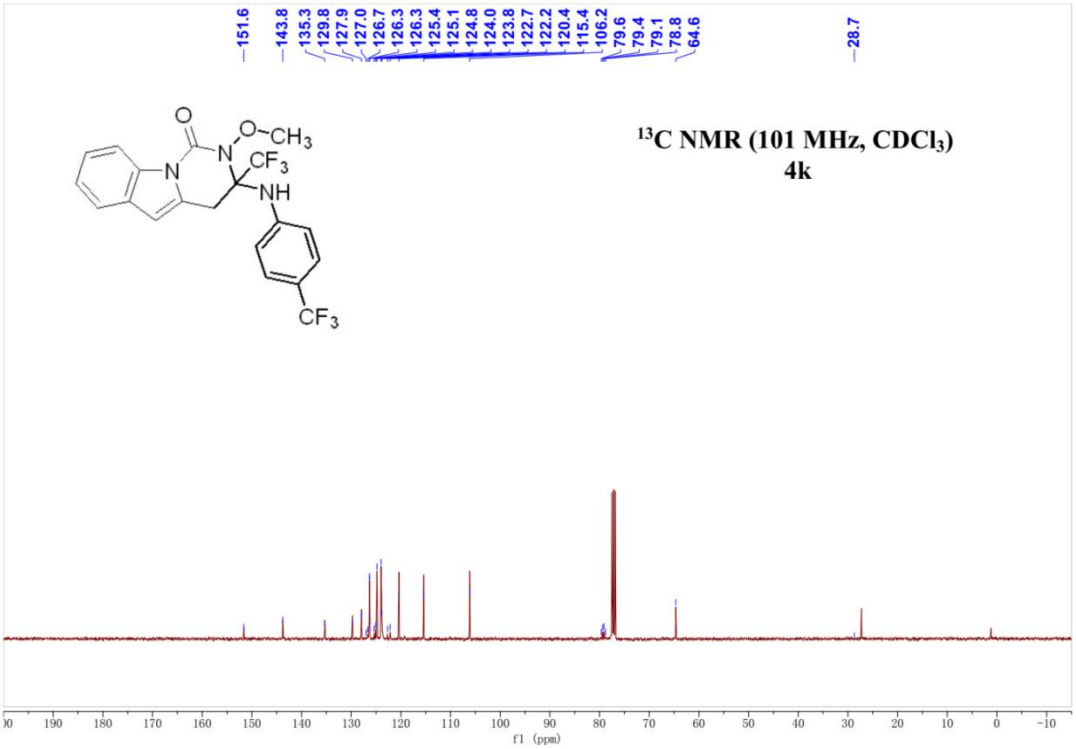
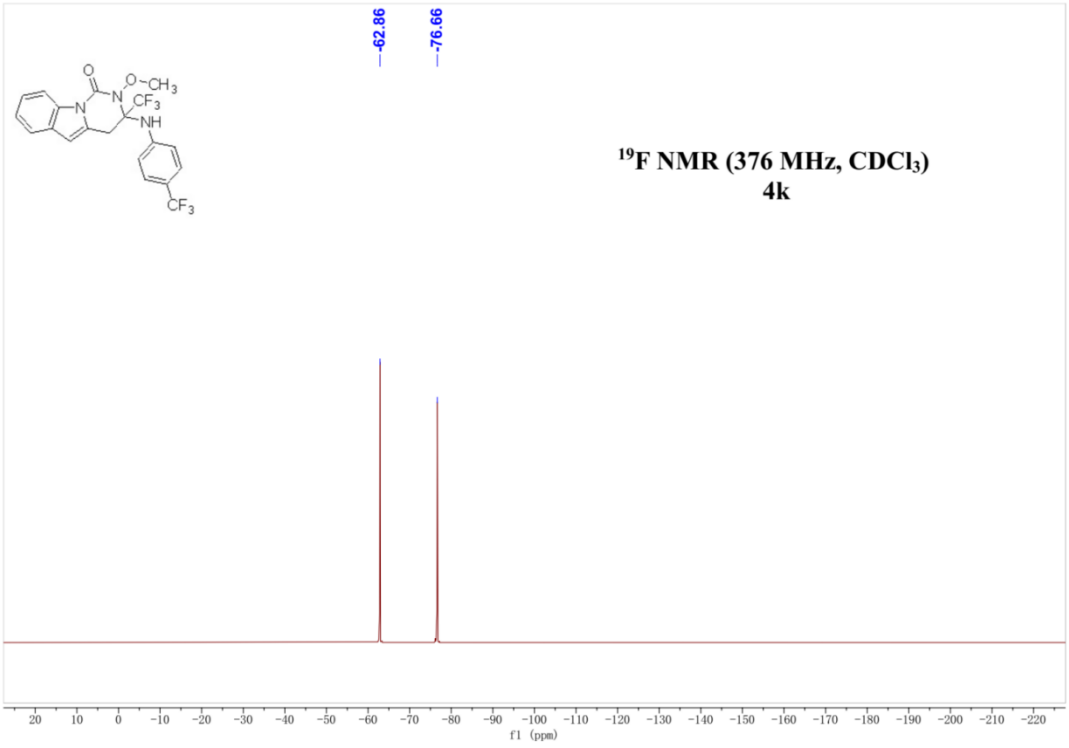
O-CH3
N
N
CF3
NH
Br
19F NMR (376 MHz, CDCl3)
4j
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220
f1 (ppm)

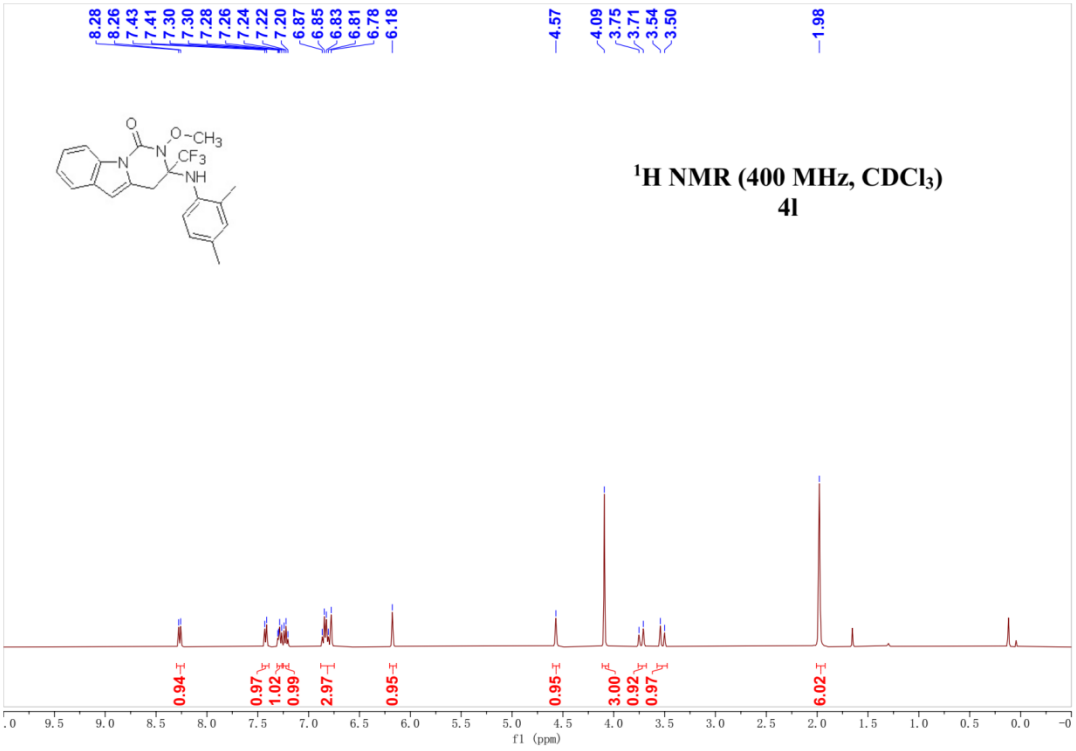


^{1}H NMR (400 MHz, $CDCl_3$)
4k

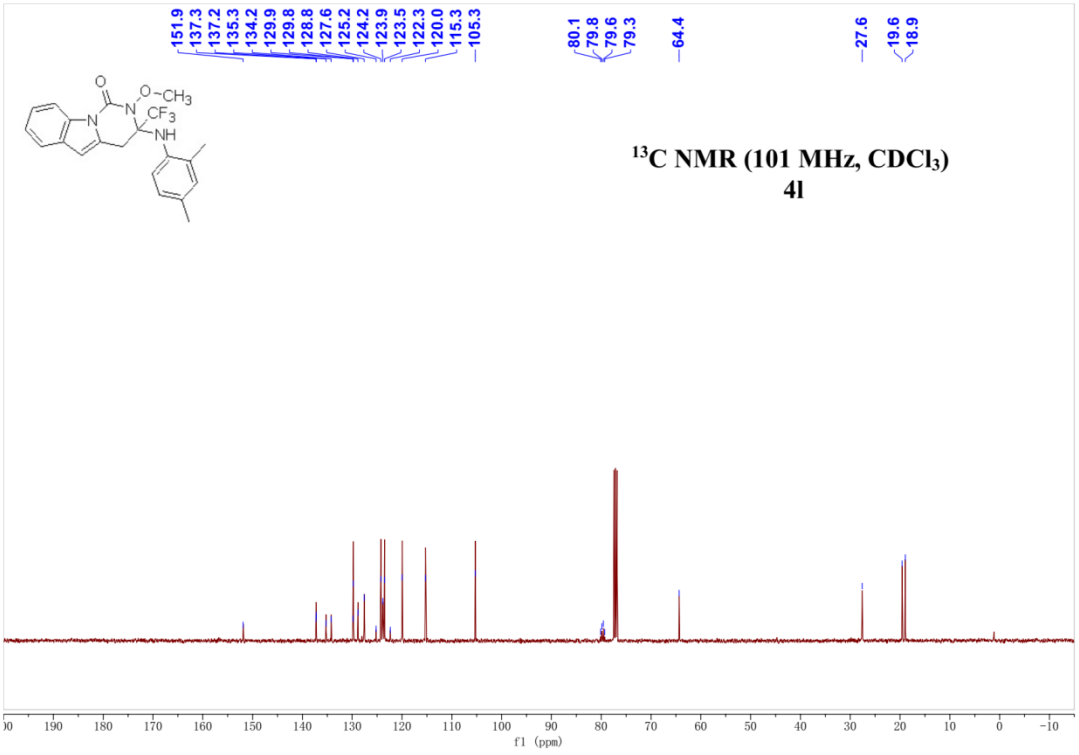


^{13}C NMR (101 MHz, $CDCl_3$)
4k

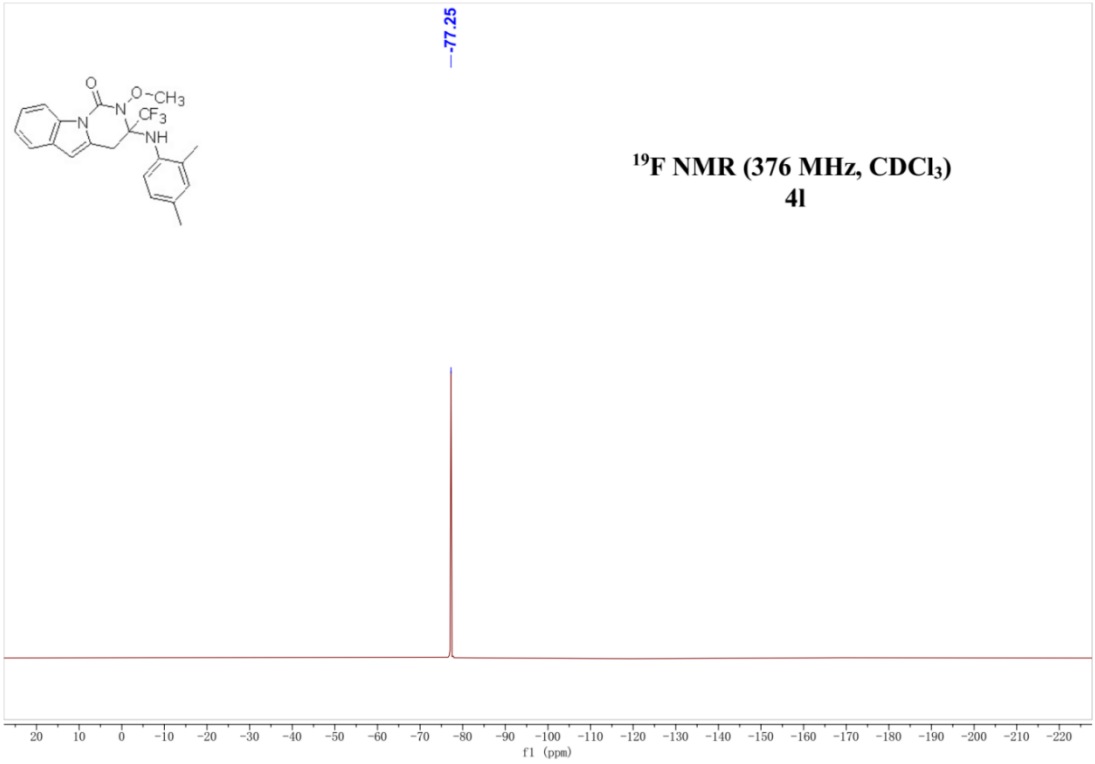

-62.86
-76.66
O
O
CH3
N
N
CF3
NH
CF3
19F NMR (376 MHz, CDCl3)
4k
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220
f1 (ppm)

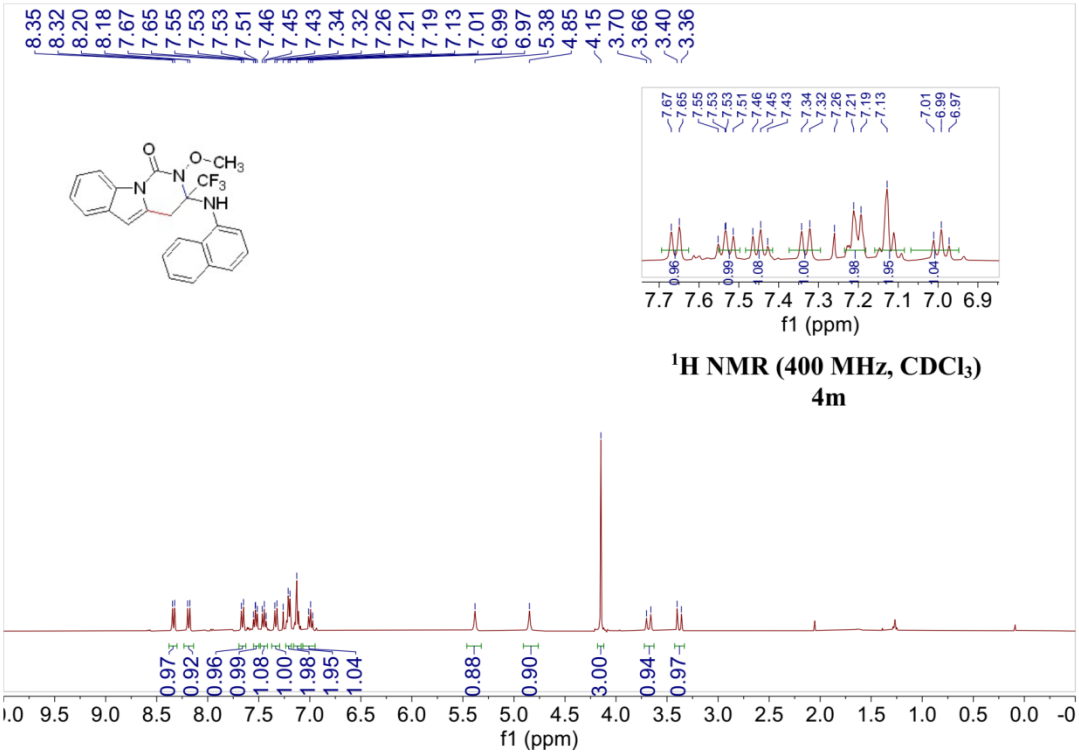


^{1}H NMR (400 MHz, $CDCl_3$)
4l

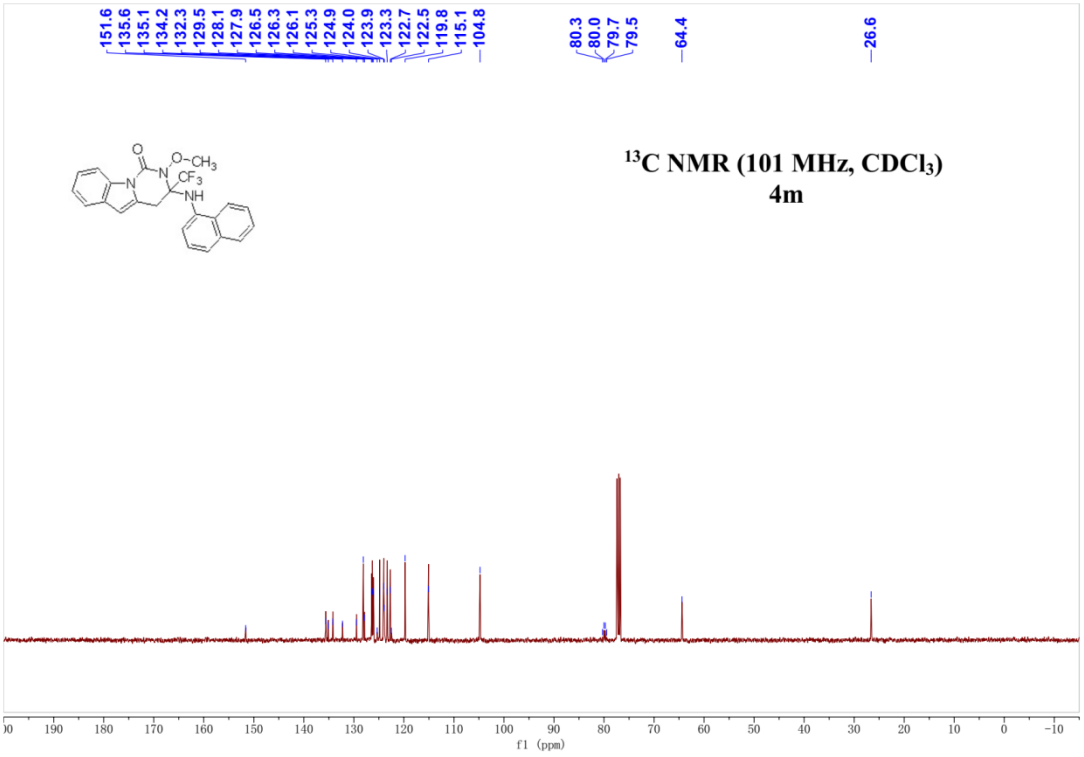


^{13}C NMR (101 MHz, $CDCl_3$)
4l

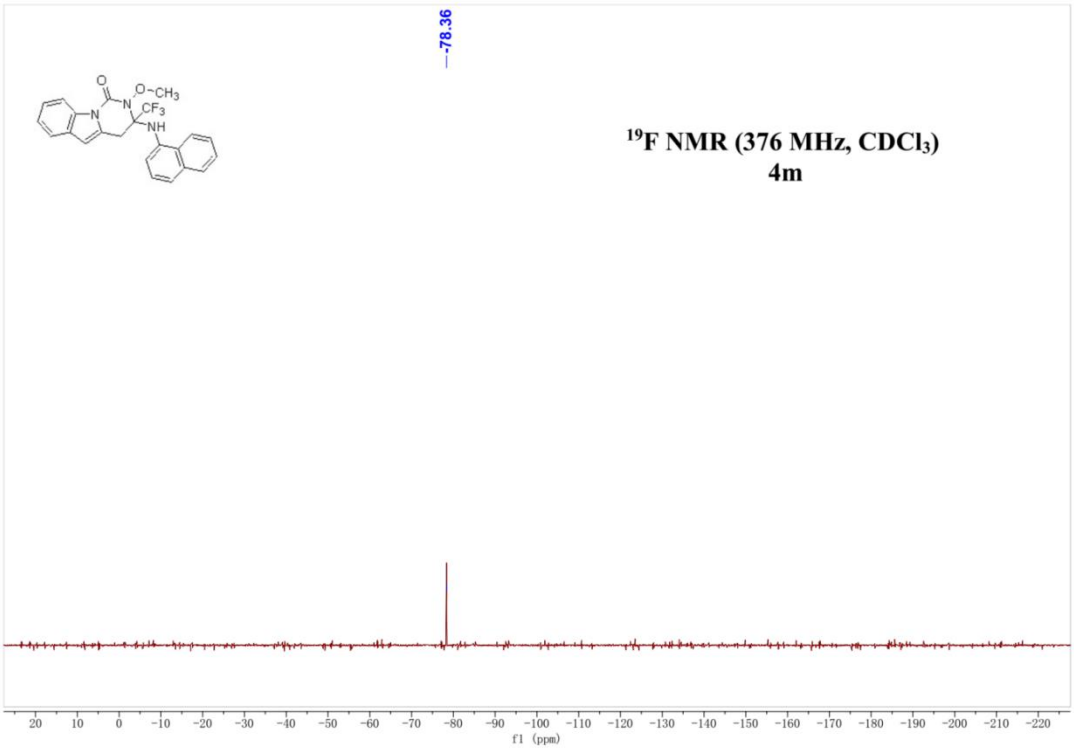

-77.25
O
N
O
CH3
CF3
NH
19F NMR (376 MHz, CDCl3)
4l
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220
f1 (ppm)

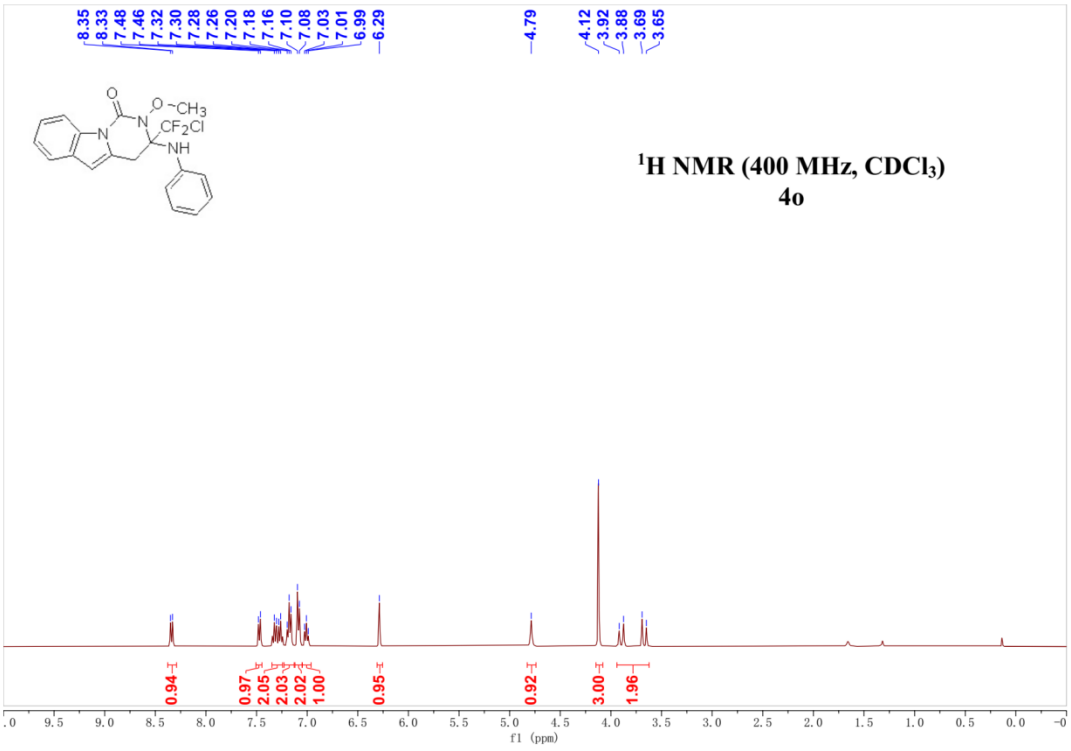


^{1}H NMR (400 MHz, $CDCl_3$)
4m

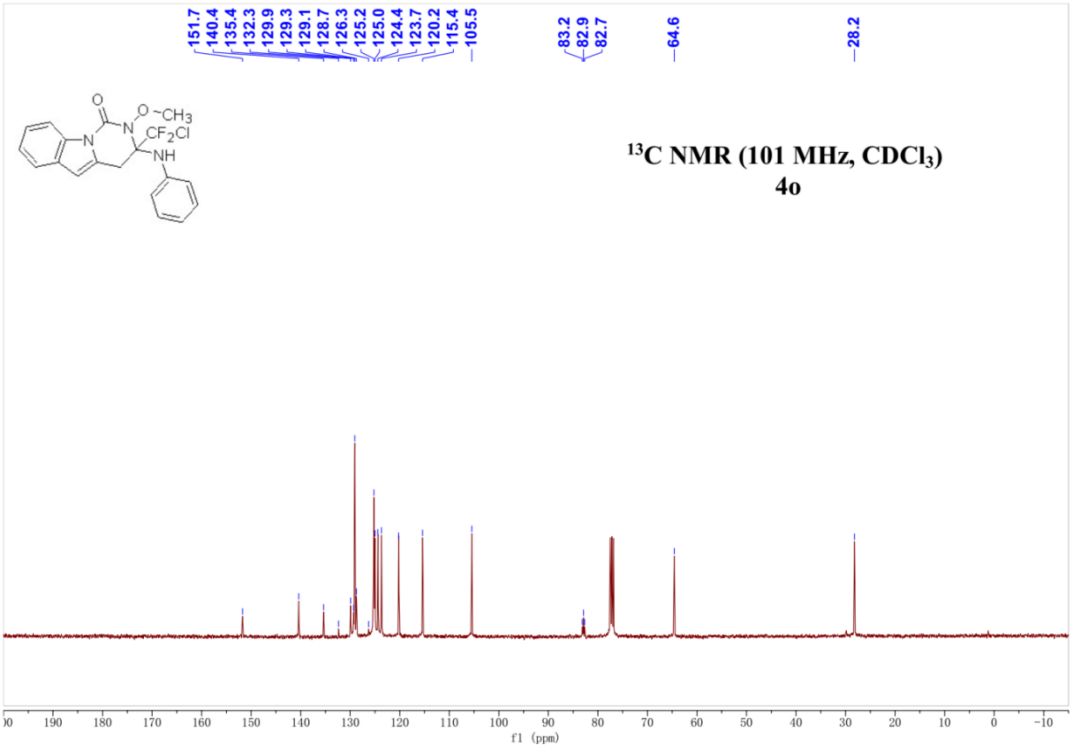


^{13}C NMR (101 MHz, $CDCl_3$)
4m

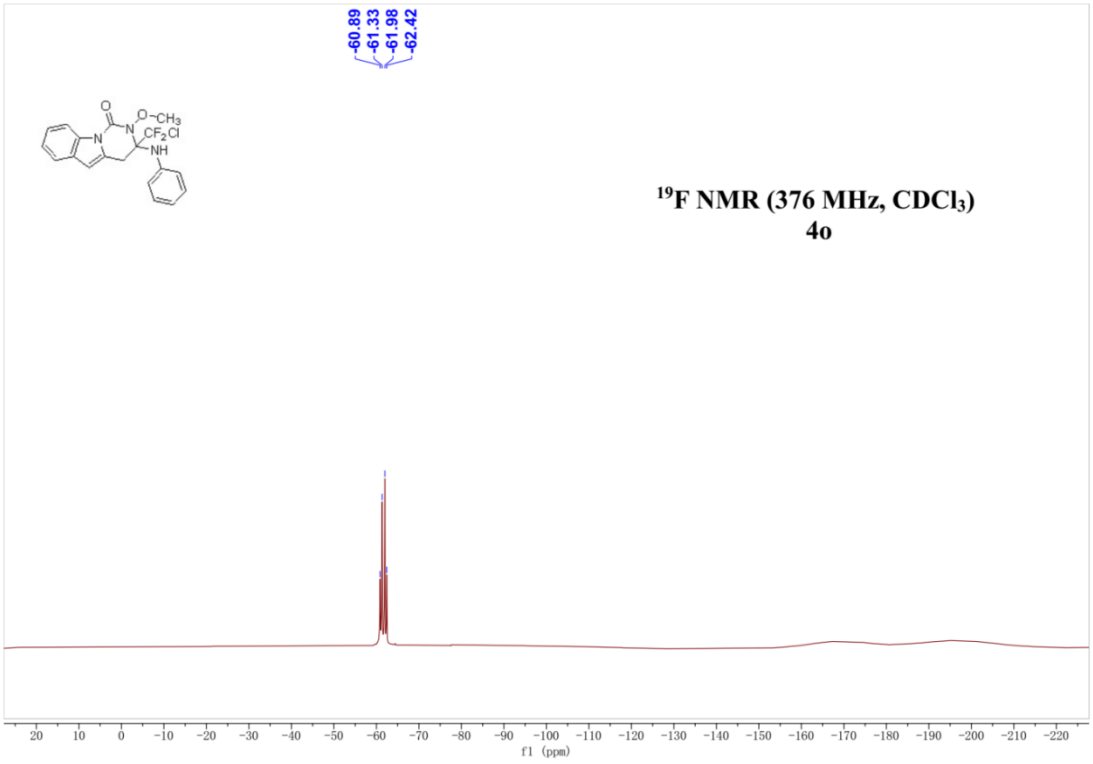

-78.36
O
O-CH3
N
N
CF3
NH
19F NMR (376 MHz, CDCl3)
4m
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220
f1 (ppm)

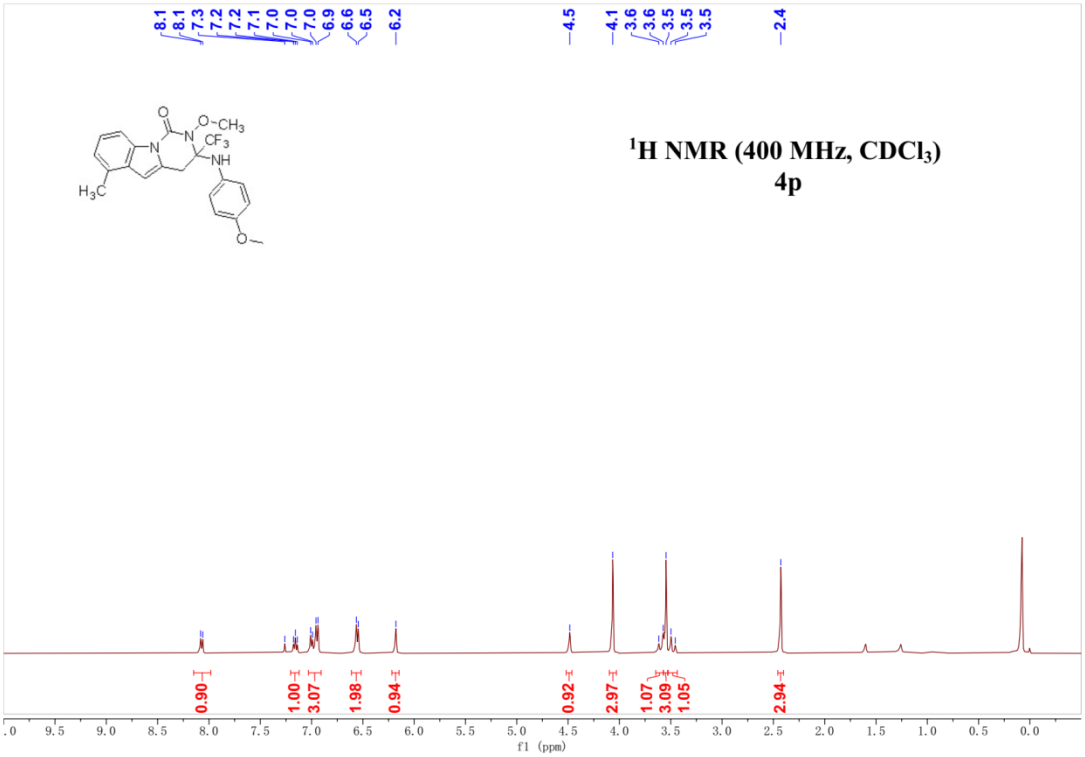


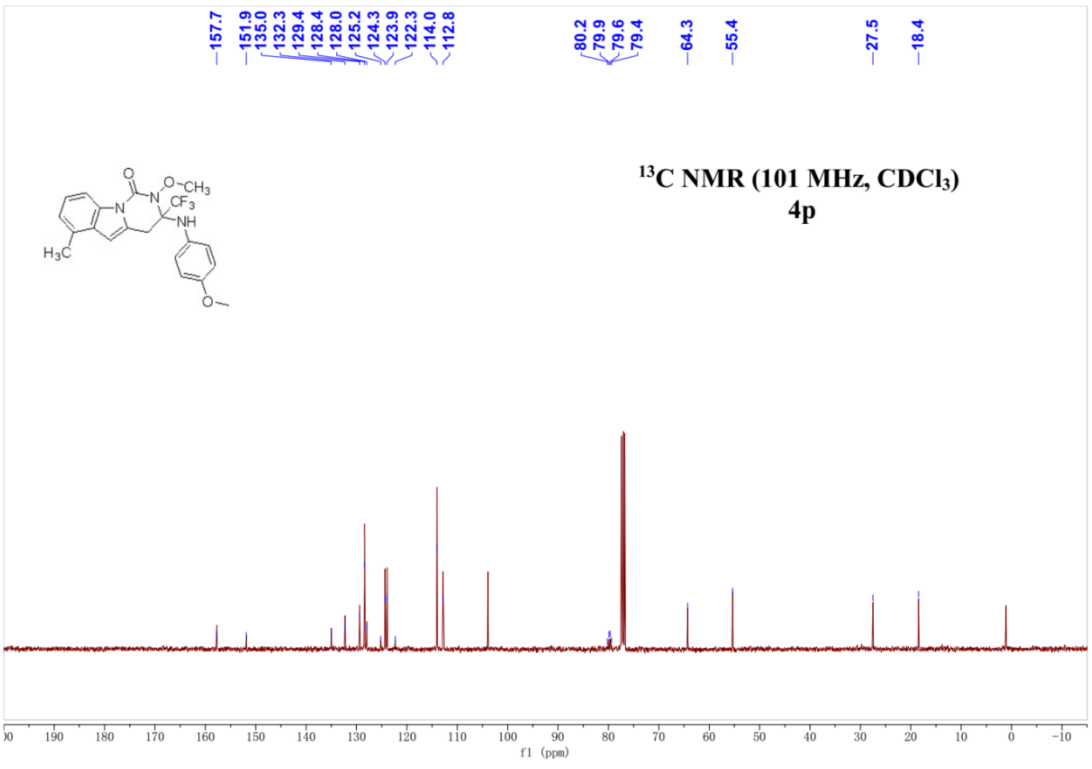
^{1}H NMR (400 MHz, $CDCl_3$)
4o

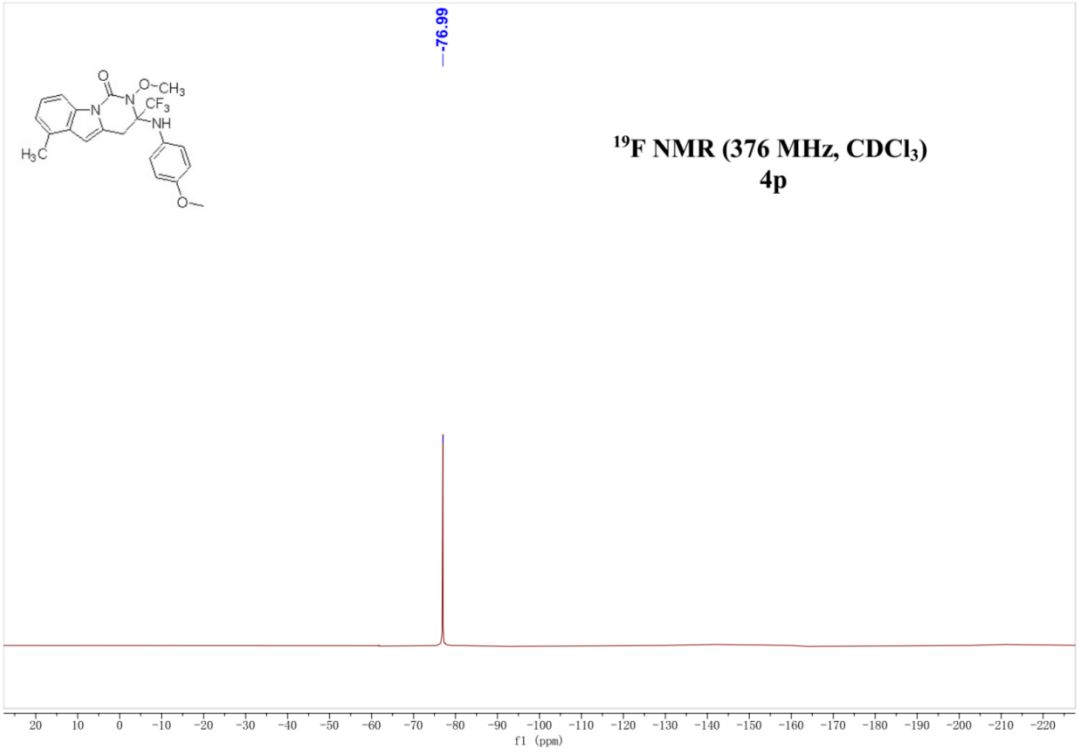


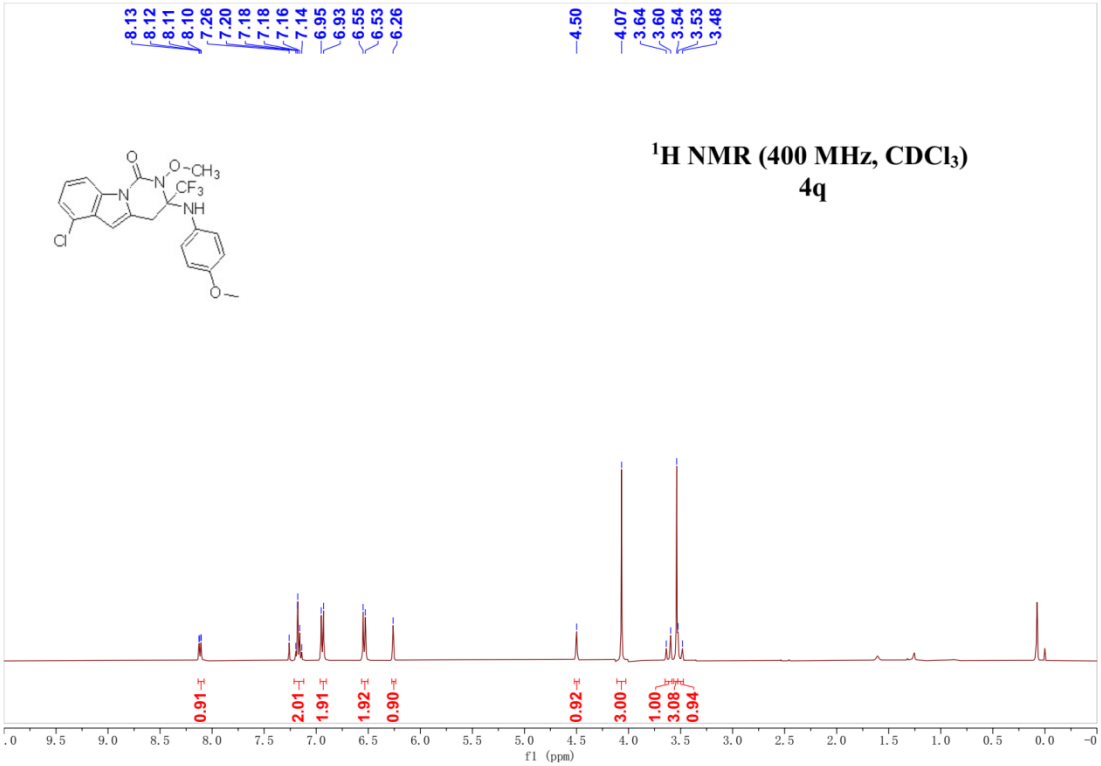
^{13}C NMR (101 MHz, $CDCl_3$)
4o


-60.89
-61.33
-61.98
-62.42
O
O-CH3
N
CF2Cl
NH
19F NMR (376 MHz, CDCl3)
4o
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220
f1 (ppm)

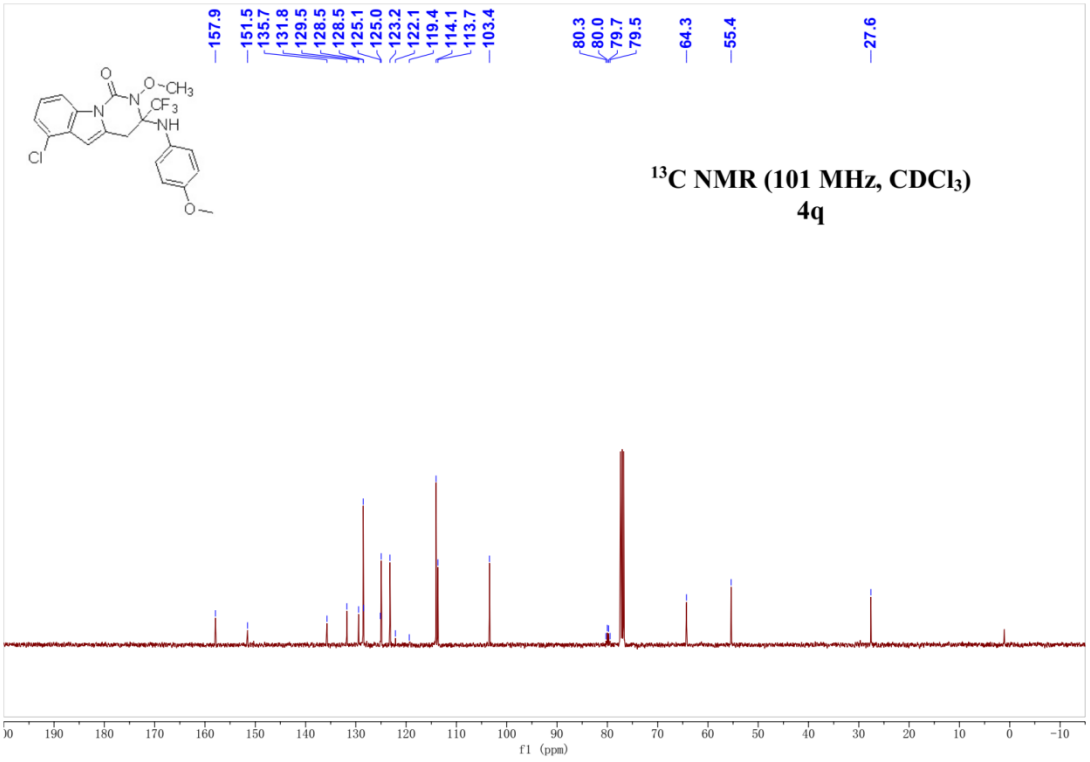

8.1
8.1
7.3
7.2
7.2
7.1
7.0
7.0
7.0
6.9
6.6
6.5
6.2
4.5
4.1
3.6
3.6
3.5
3.5
3.5
2.4
O
N
O-CH3
CF3
NH
H3C
O
1H NMR (400 MHz, CDCl3)
4p
0.90
1.00
3.07
1.98
0.94
0.92
2.97
1.07
3.09
1.05
2.94
f1 (ppm)


157.7
151.9
135.0
132.3
129.4
128.4
128.0
125.2
124.3
123.9
122.3
114.0
112.8
80.2
79.9
79.6
79.4
64.3
55.4
27.5
18.4
O
N
O-CH3
CF3
NH
H3C
O
13C NMR (101 MHz, CDCl3)
4p
f1 (ppm)

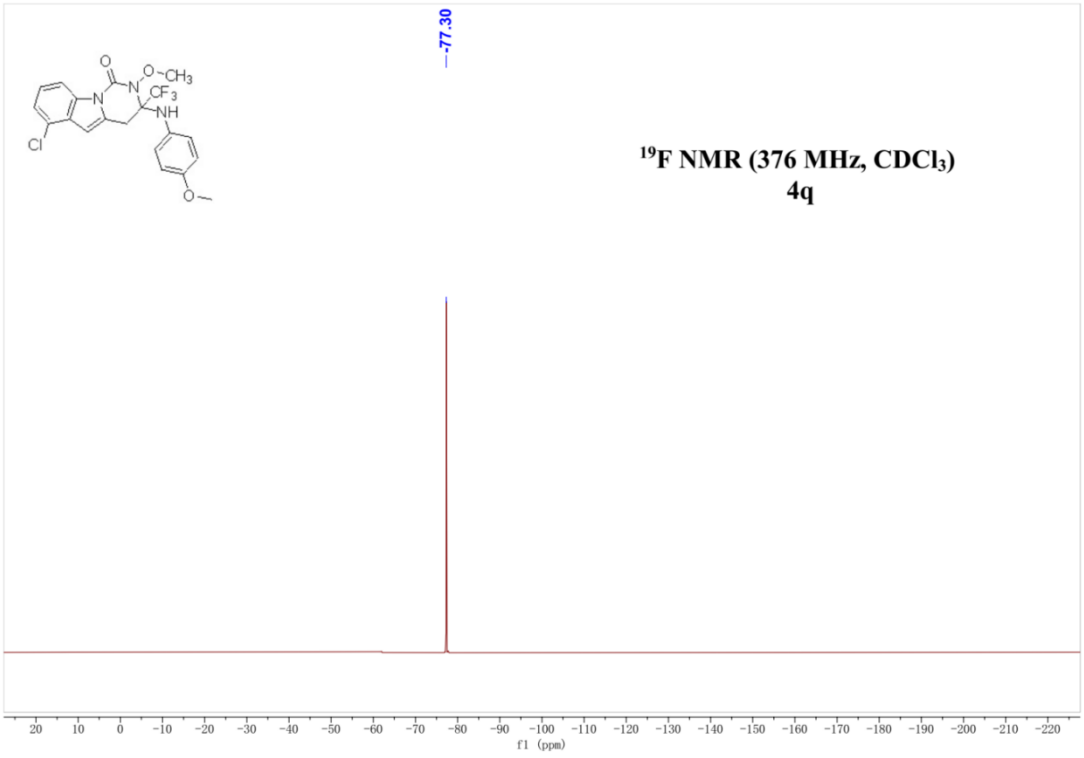

-76.99
O
O-CH3
N
CF3
NH
H3C
O
19F NMR (376 MHz, CDCl3)
4p
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220
f1 (ppm)

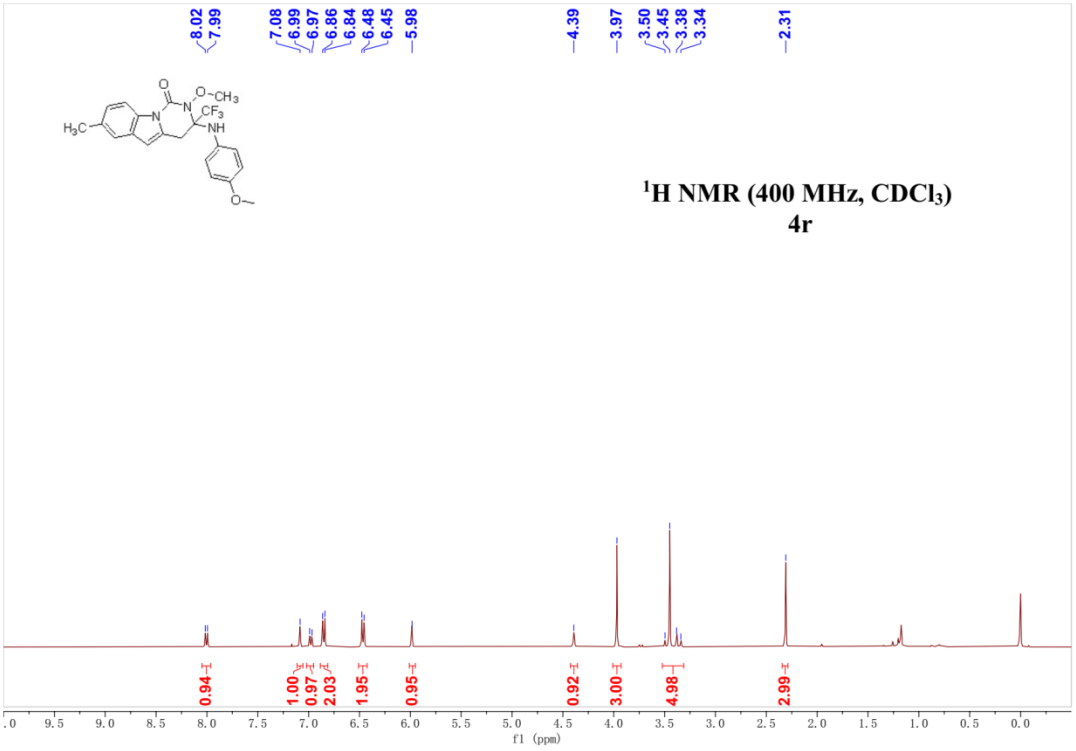


^{1}H NMR (400 MHz, $CDCl_3$)
4q

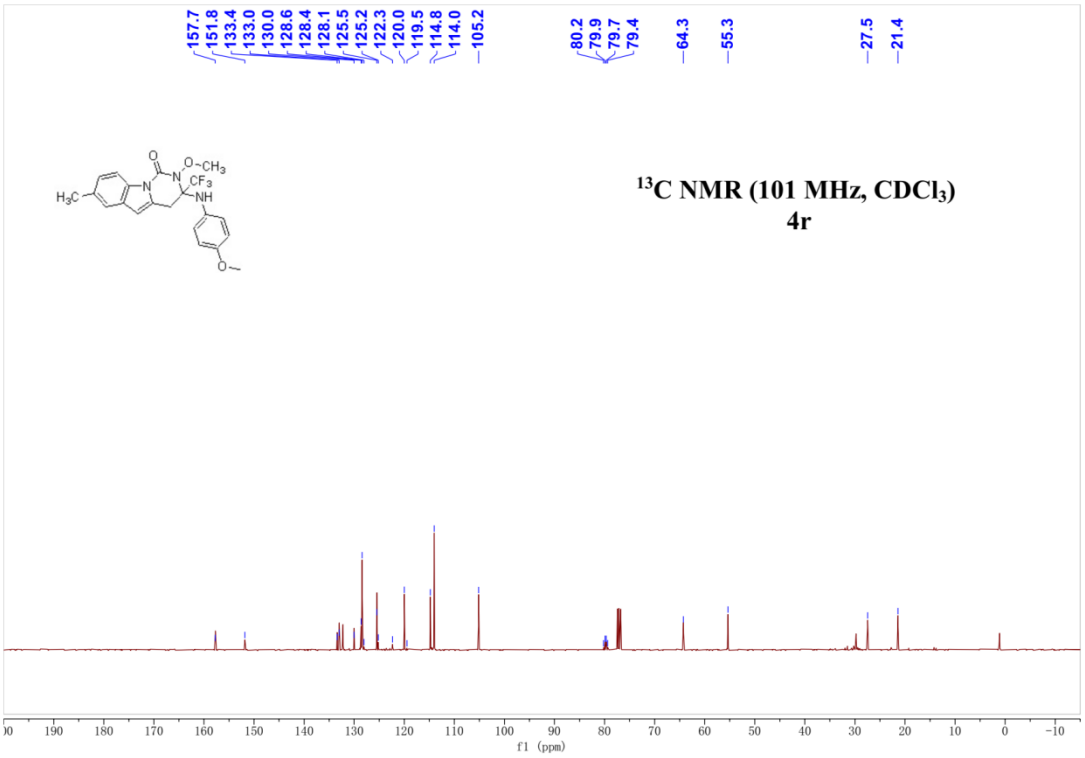


^{13}C NMR (101 MHz, $CDCl_3$)
4q

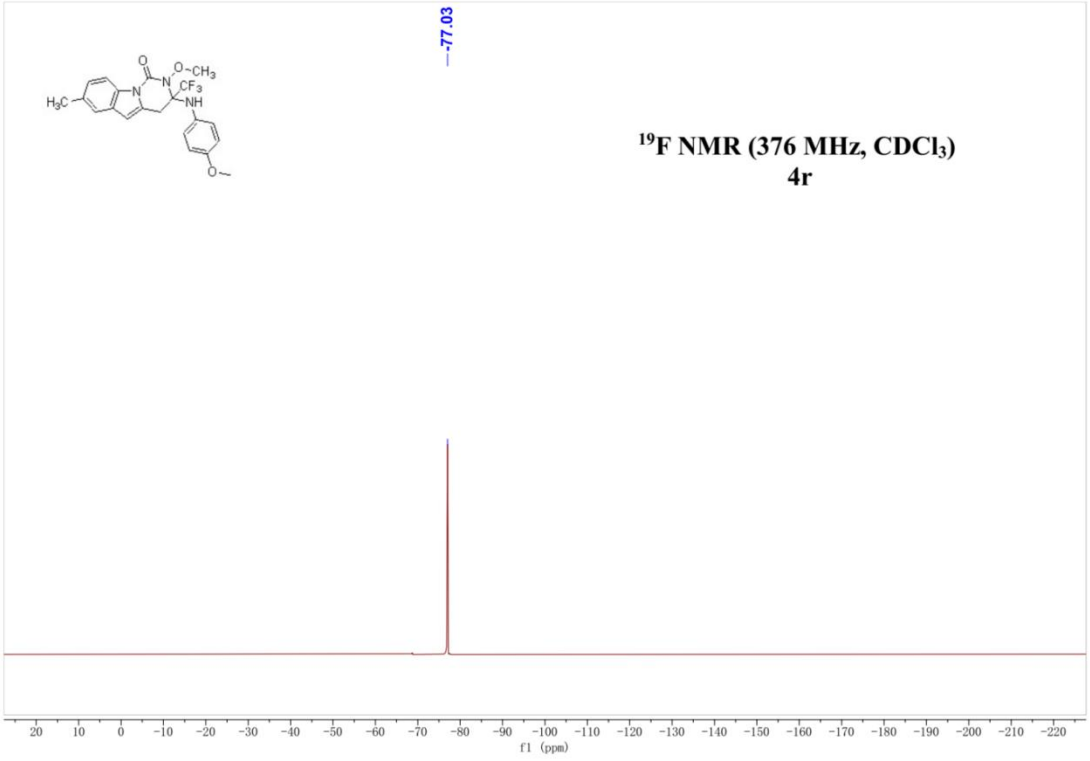

-77.30
^{19}F NMR (376 MHz, CDCl$_3$)
4q
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220
f1 (ppm)

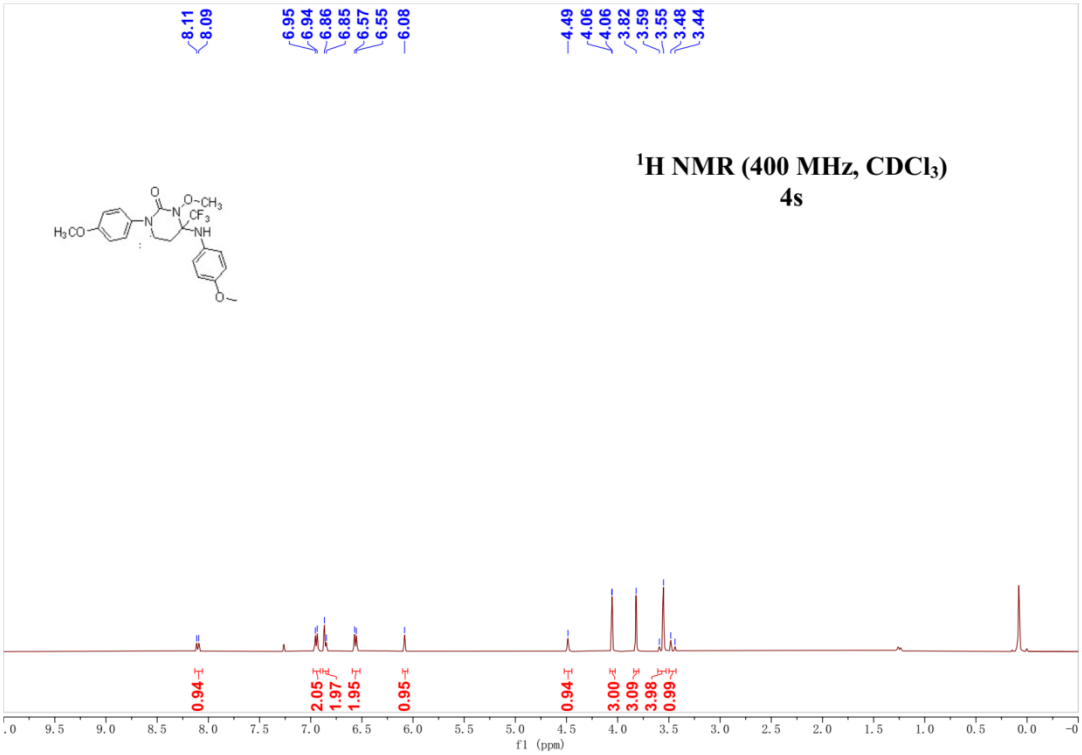


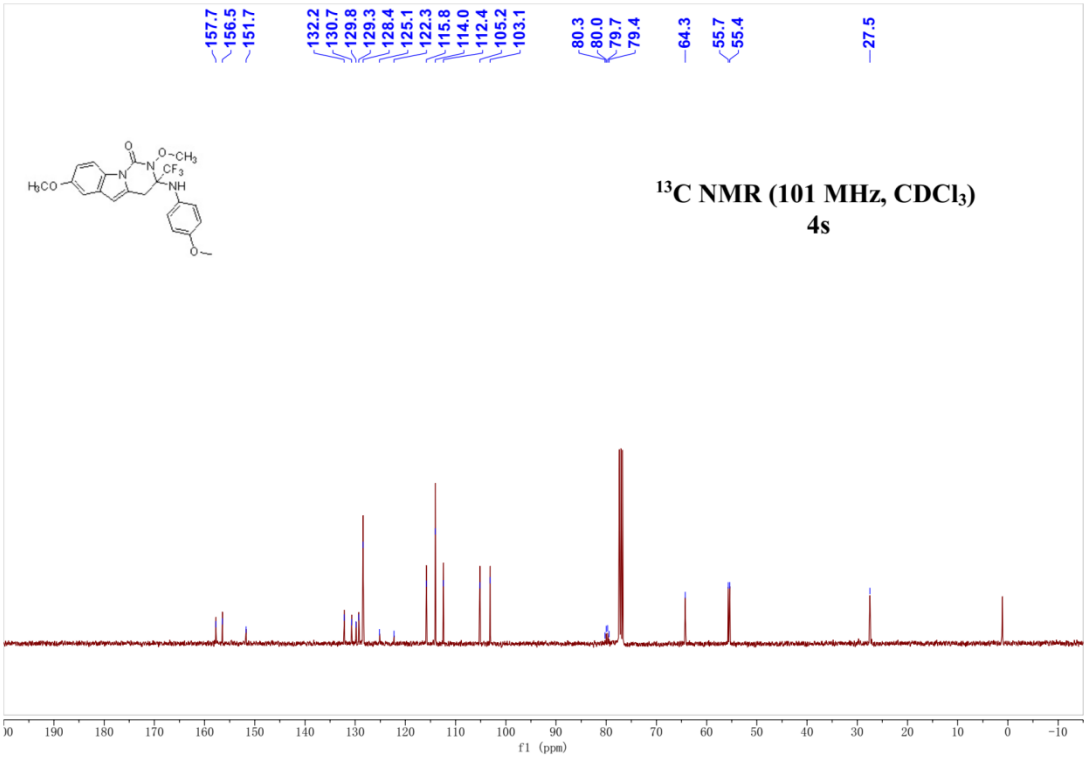
^{1}H NMR (400 MHz, $CDCl_3$)
4r

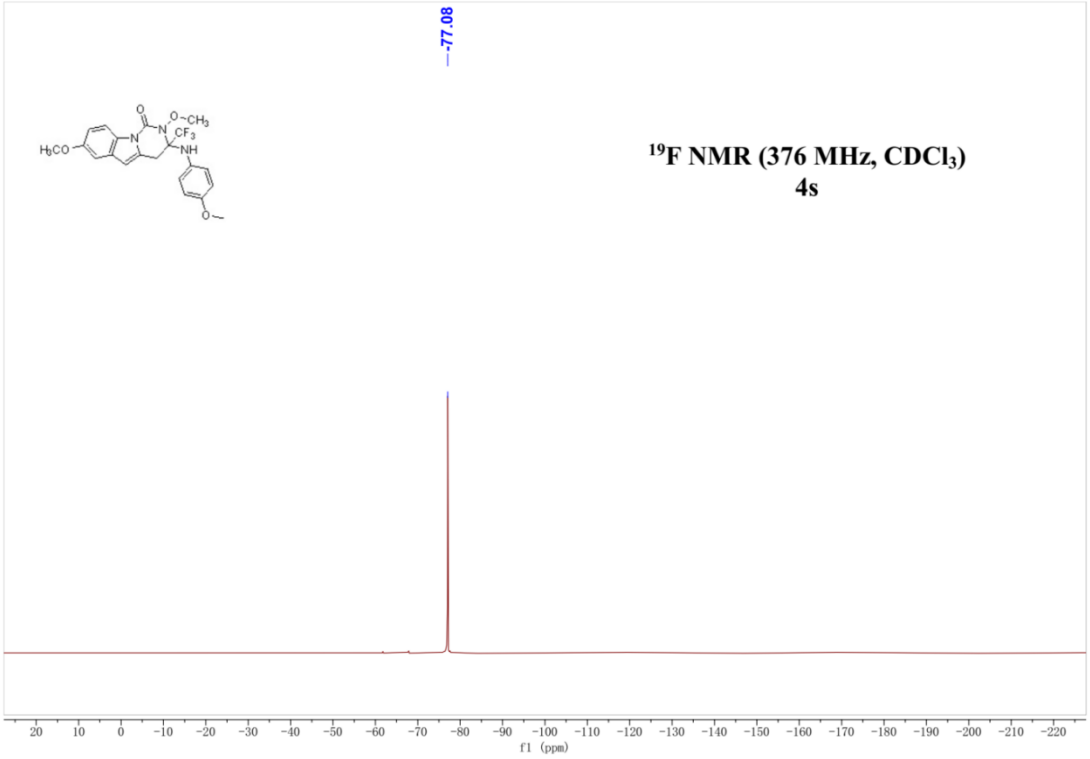


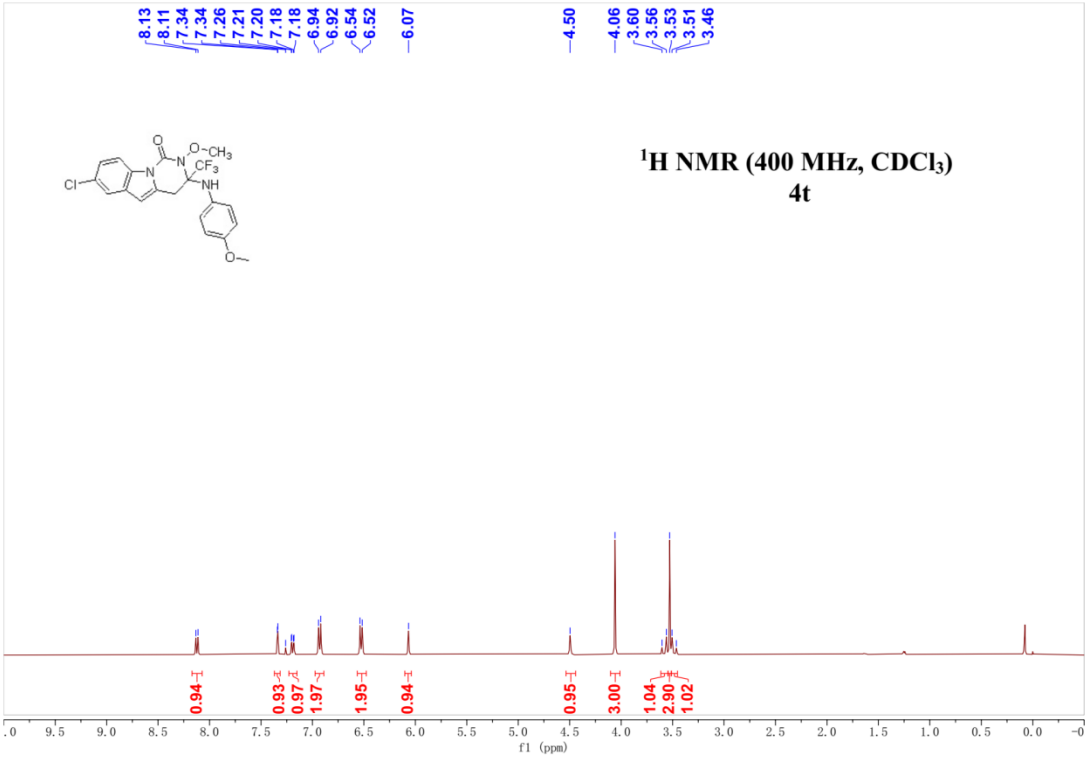
^{13}C NMR (101 MHz, $CDCl_3$)
4r


-77.03
^{19}F NMR (376 MHz, CDCl$_3$)
4r
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220
f1 (ppm)

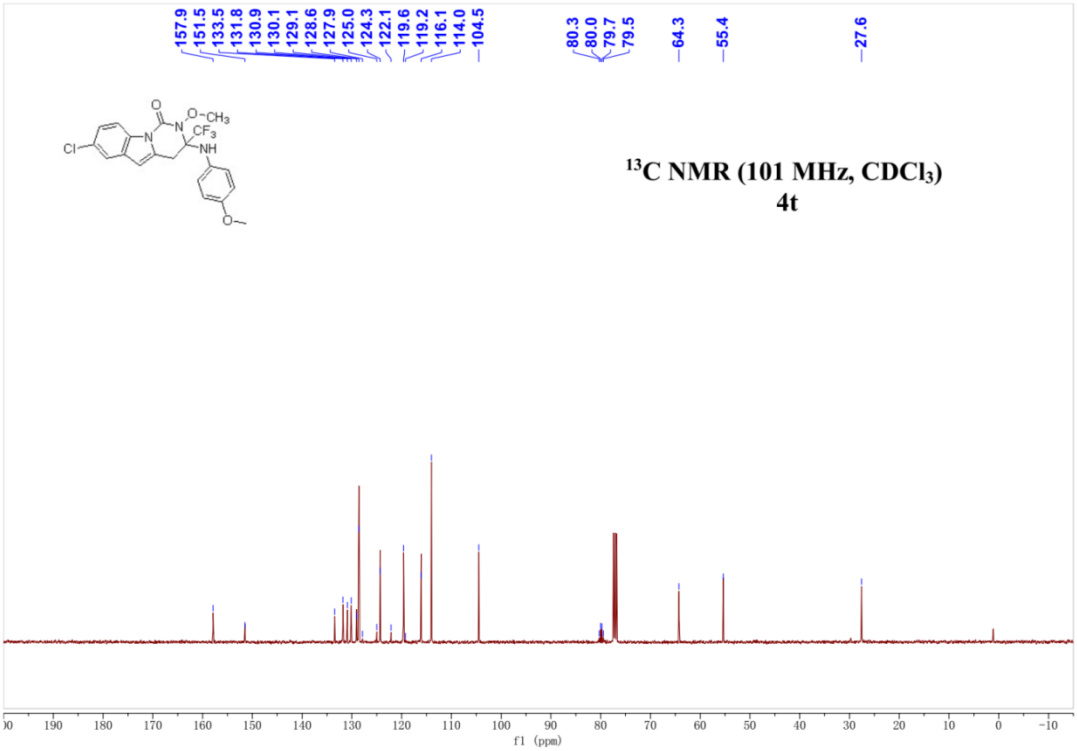

8.11
8.09
6.95
6.94
6.86
6.85
6.57
6.55
6.08
4.49
4.06
4.06
3.82
3.59
3.55
3.48
3.44
^{1}H NMR (400 MHz, CDCl$_3$)
4s
0.94
2.05
1.97
1.95
0.95
0.94
3.00
3.09
3.98
0.99
f1 (ppm)


157.7
156.5
151.7
132.2
130.7
129.8
129.3
128.4
125.1
122.3
115.8
114.0
112.4
105.2
103.1
80.3
80.0
79.7
79.4
64.3
55.7
55.4
27.5
^{13}C NMR (101 MHz, CDCl$_3$)
4s
f1 (ppm)

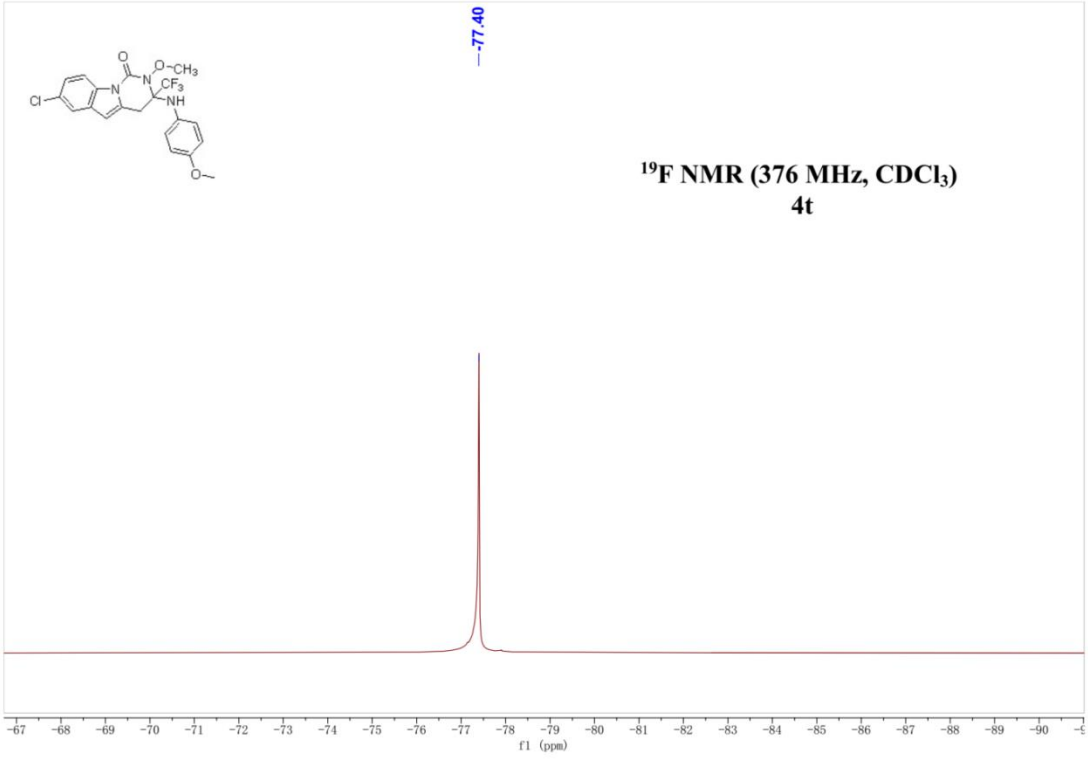

-77.08
^{19}F NMR (376 MHz, CDCl$_3$)
4s
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220
f1 (ppm)

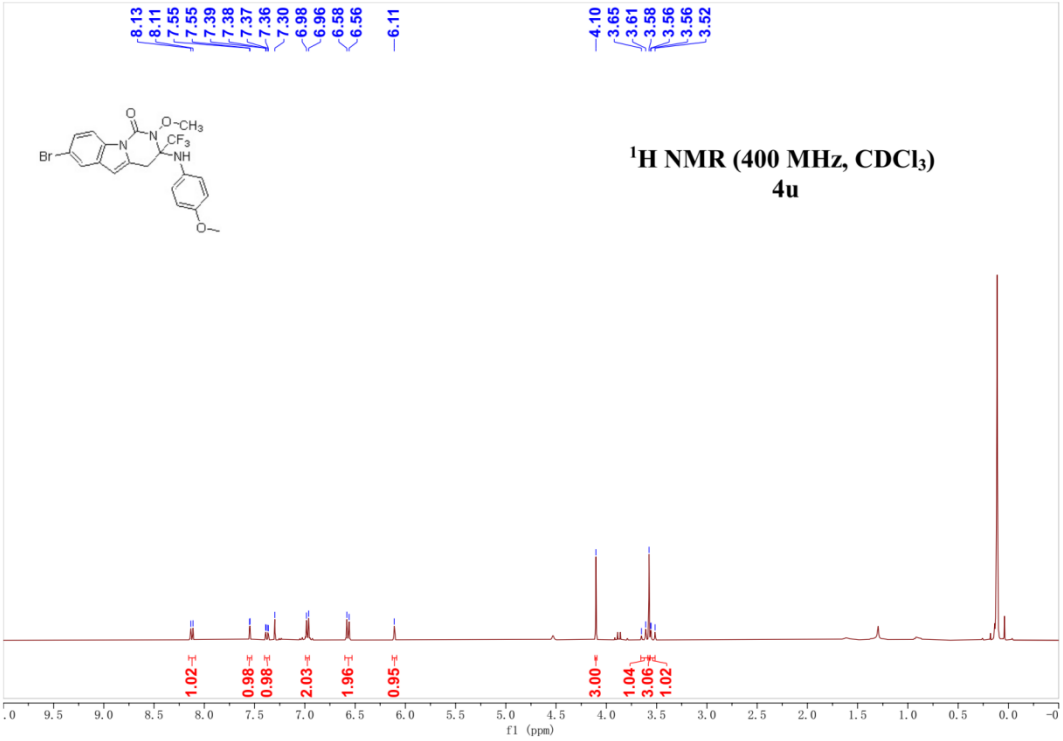


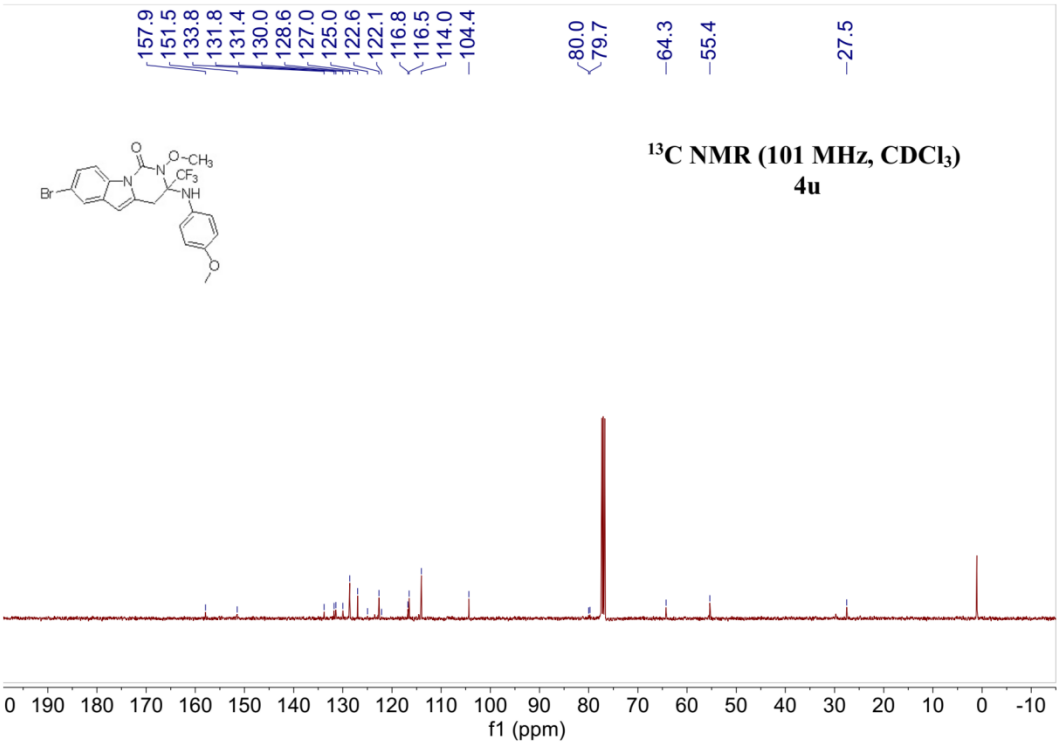
^{1}H NMR (400 MHz, $CDCl_3$)
4t

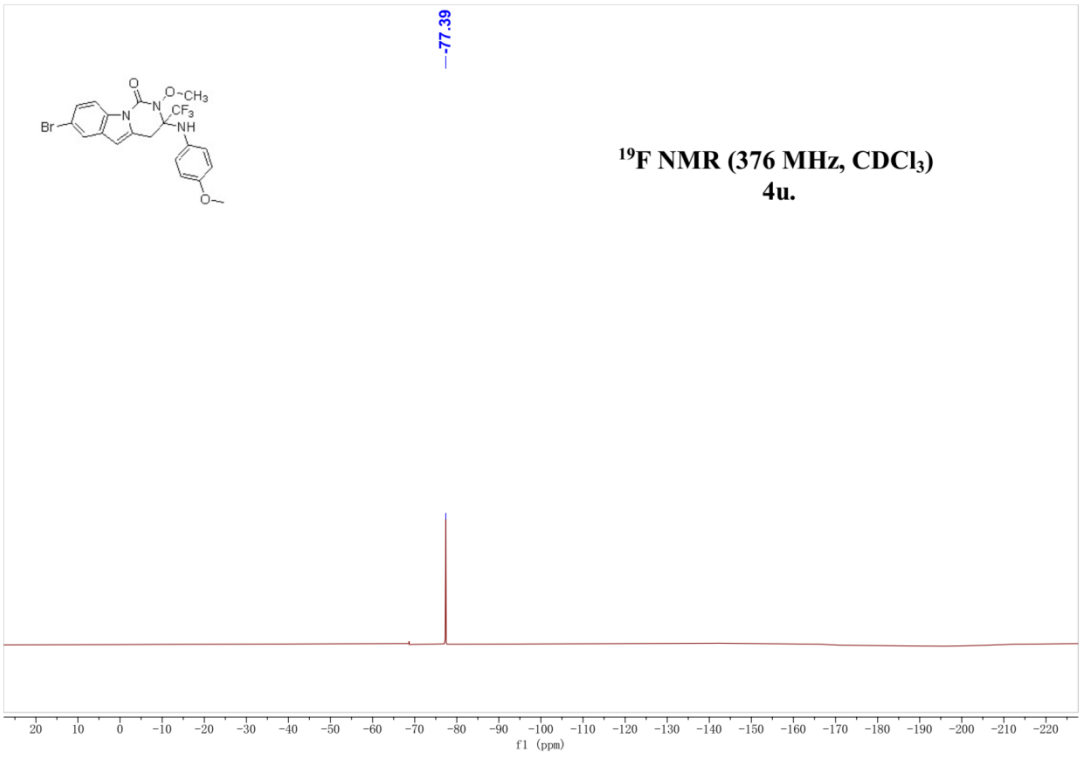


^{13}C NMR (101 MHz, $CDCl_3$)
4t

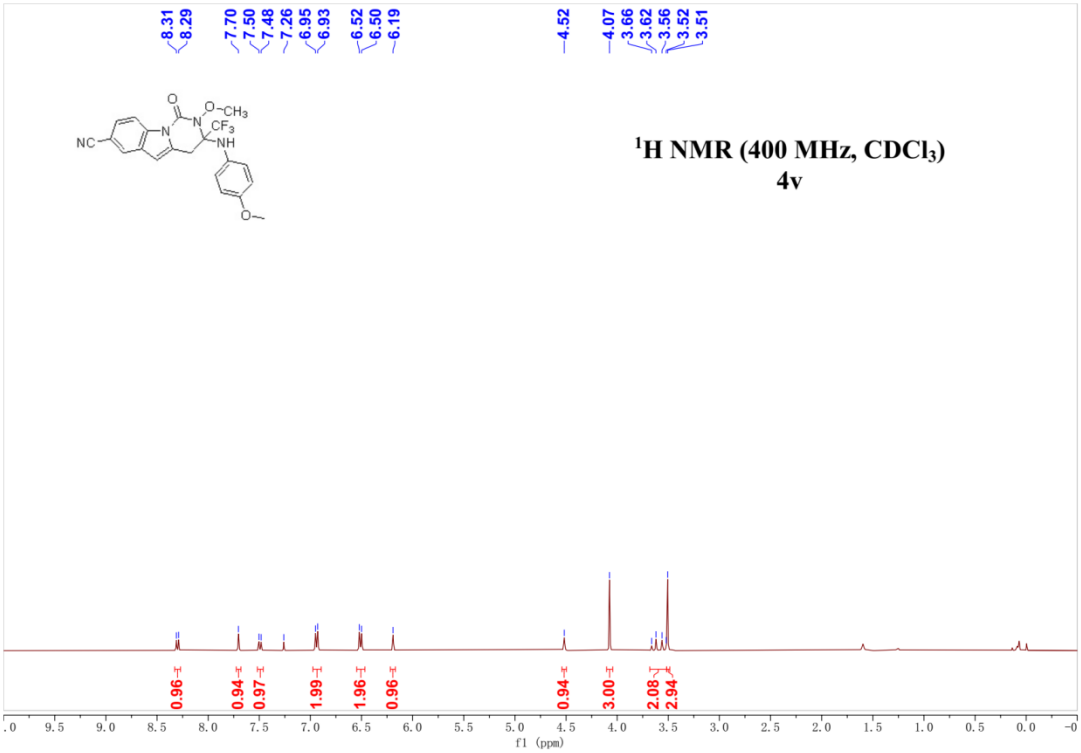

-77.40
Cl
O
N
O-CH3
CF3
NH
O
19F NMR (376 MHz, CDCl3)
4t
-67 -68 -69 -70 -71 -72 -73 -74 -75 -76 -77 -78 -79 -80 -81 -82 -83 -84 -85 -86 -87 -88 -89 -90
f1 (ppm)


8.13
8.11
7.55
7.55
7.39
7.38
7.37
7.36
7.30
6.98
6.96
6.58
6.56
6.11
4.10
3.65
3.61
3.58
3.56
3.56
3.52
Br
O
N
O-CH3
CF3
NH
O
1H NMR (400 MHz, CDCl3)
4u
1.02
0.98
0.98
2.03
1.96
0.95
3.00
1.04
3.06
1.02
f1 (ppm)

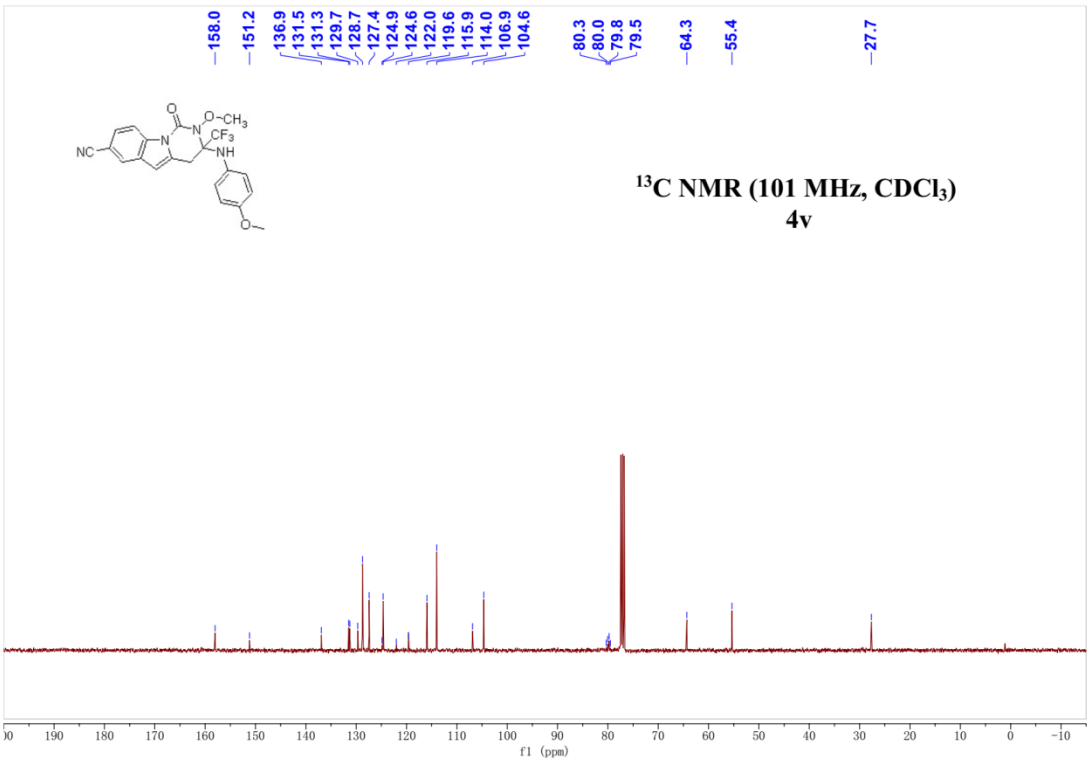

157.9
151.5
133.8
131.8
131.4
130.0
128.6
127.0
125.0
122.6
122.1
116.8
116.5
114.0
104.4
80.0
79.7
64.3
55.4
27.5
Br
O
N
O-CH3
CF3
NH
O
13C NMR (101 MHz, CDCl3)
4u
f1 (ppm)



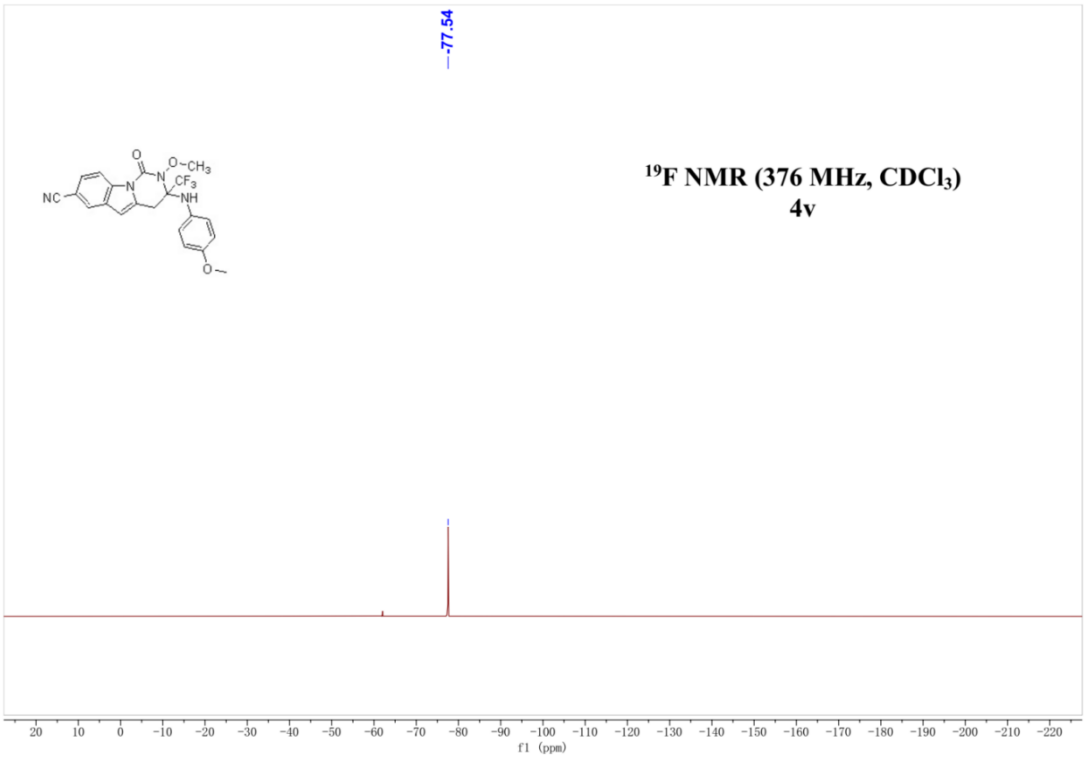
^{19}F NMR (376 MHz, $CDCl_3$)
4u.

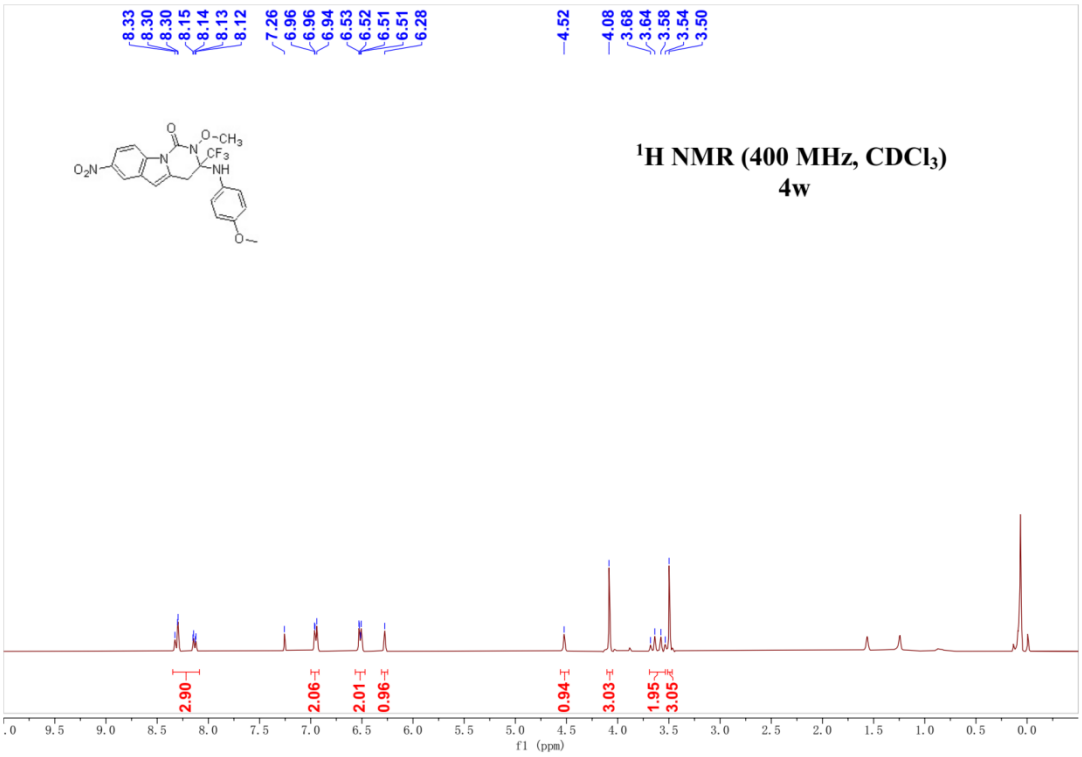


^{1}H NMR (400 MHz, $CDCl_3$)
4v

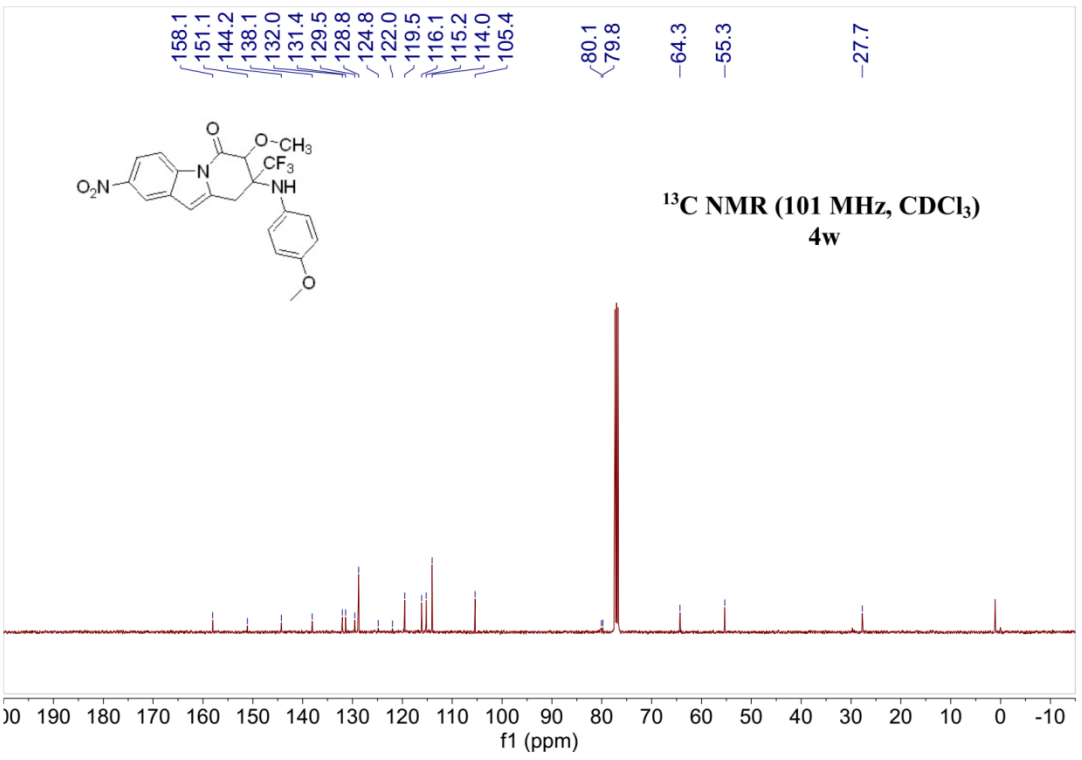


^{13}C NMR (101 MHz, $CDCl_3$)
4v

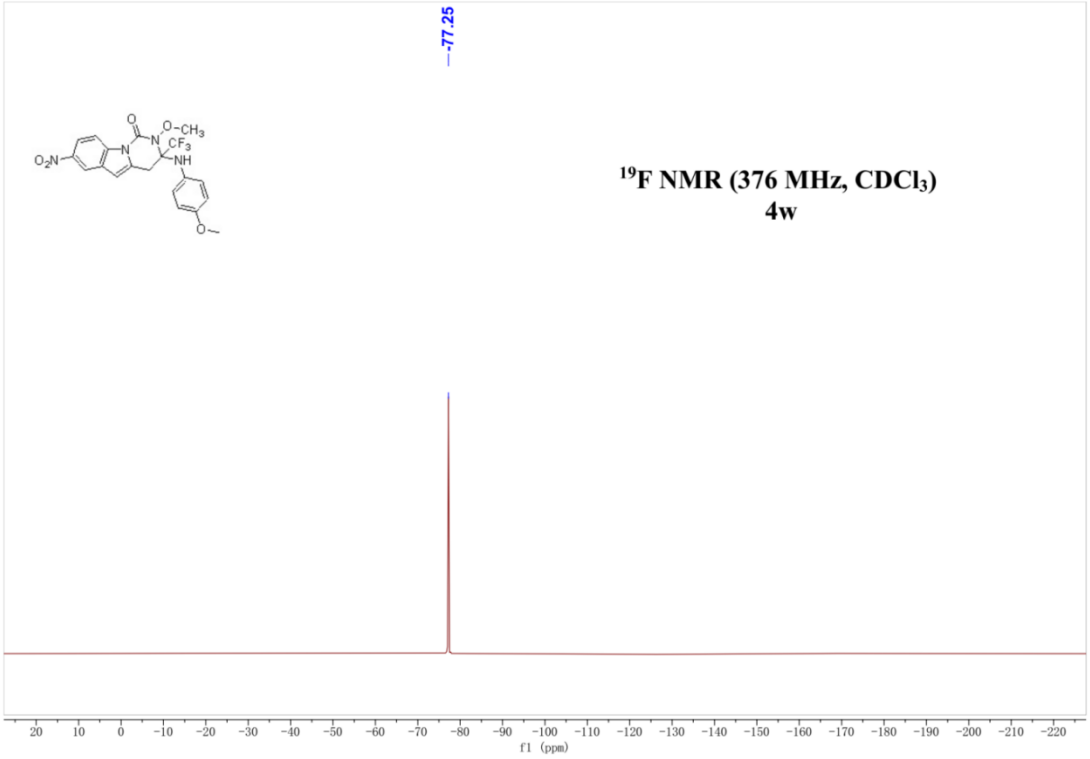

-77.54
NC
O
N
O–CH3
CF3
NH
O–
19F NMR (376 MHz, CDCl3)
4v
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220
f1 (ppm)

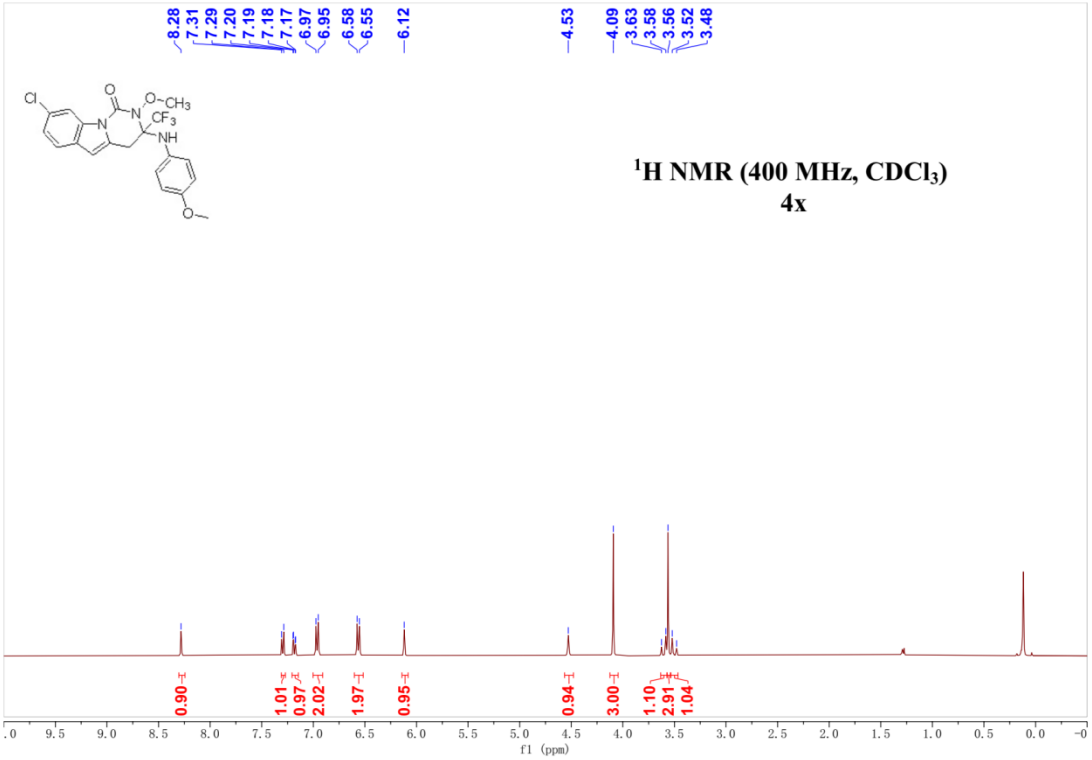


^{1}H NMR (400 MHz, $CDCl_3$)
4w

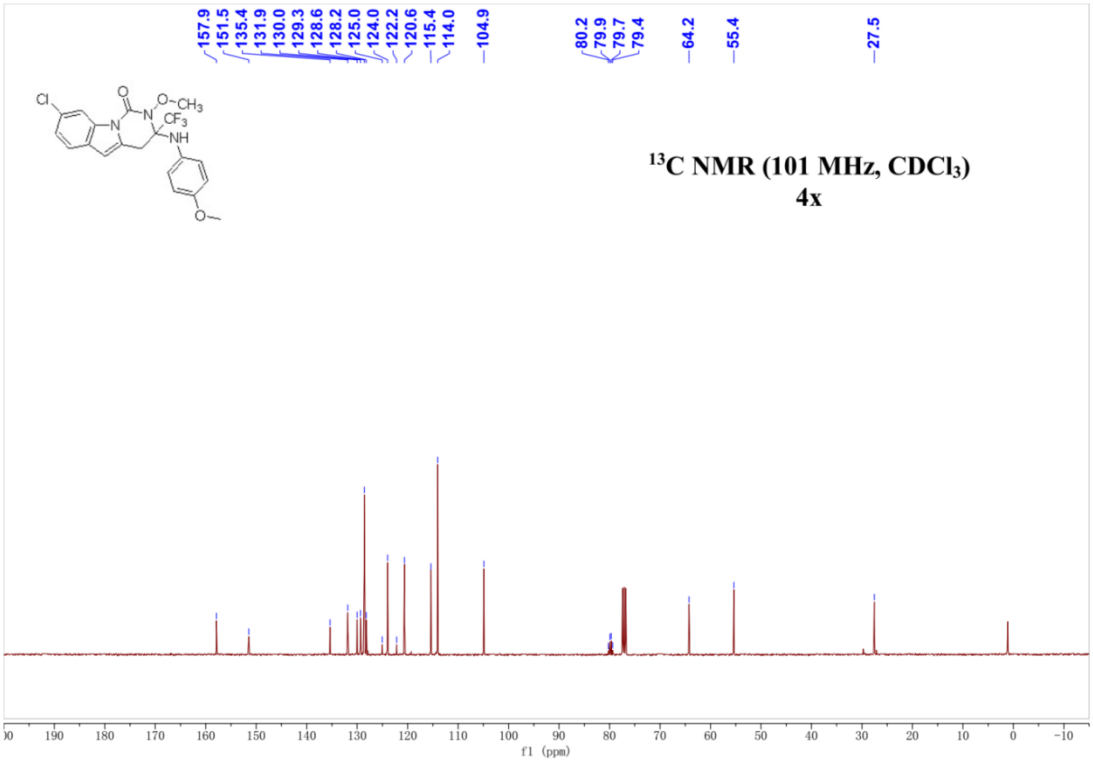


^{13}C NMR (101 MHz, $CDCl_3$)
4w

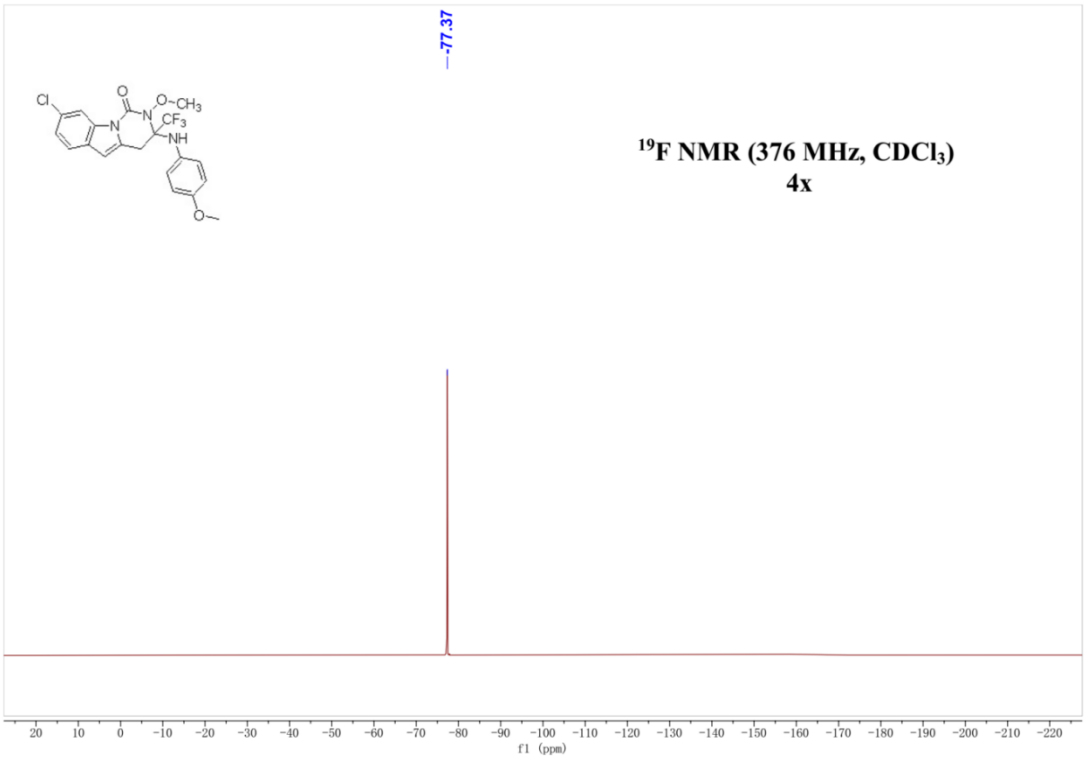

-77.25
O
O-CH3
CF3
NH
O2N
O
19F NMR (376 MHz, CDCl3)
4w
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220
f1 (ppm)



^{1}H NMR (400 MHz, $CDCl_3$)
4x



^{13}C NMR (101 MHz, $CDCl_3$)
4x


-77.37
Cl
O
N
O-CH3
CF3
NH
O
19F NMR (376 MHz, CDCl3)
4x
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220
f1 (ppm)