Supporting Information *for*

Synthesis of Pertrifluoromethyl Pyridazine Derivatives via Tandem Reaction of Aryldiazonium Salts with Hexafluoroacetylacetone

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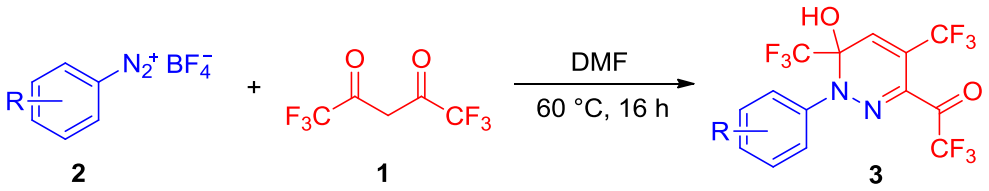
General information

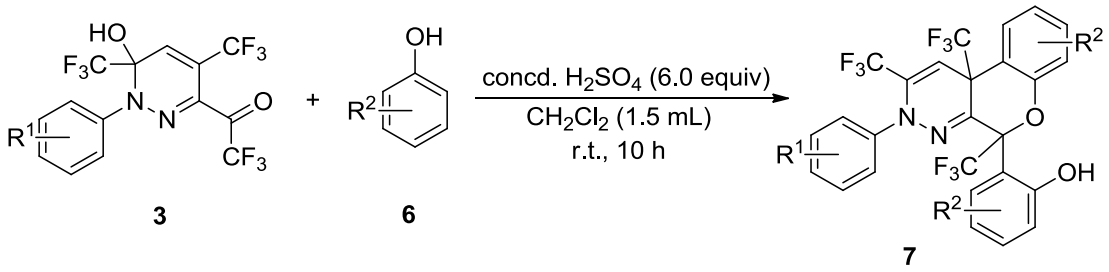
^{1}H NMR, ^{19}F NMR and ^{13}C NMR spectra were recorded using Bruker AVIII 400 spectrometer. ^{1}H NMR and ^{13}C NMR chemical shifts were reported in parts per million (ppm) downfield from tetramethylsilane and ^{19}F NMR chemical shifts were determined relative to $CFCl_3$ as the external standard and low field is positive. The residual solvent peak was used as an internal reference: ^{1}H NMR ($CDCl_3$ δ 7.26; DMSO-d_6 δ 2.50) and ^{13}C NMR ($CDCl_3$ δ 77.0; DMSO-d_6 δ 39.5). Coupling constants (*J*) are reported in Hertz (Hz). The following abbreviations were used to explain the multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br = broad. HRMS were obtained on State Key Discipline Testing Center for Physical Chemistry of Fuzhou University. The infrared (IR) spectra were recorded using a Nicolet iS50 at room temperature. Arenediazonium tetrafluoroborates were prepared according to the published procedures.[1] Other reagents were received from commercial sources. Solvents were freshly dried and degassed according to the published procedures prior to use. Column chromatography purifications were performed by flash chromatography using Merck silica gel 60.

General procedure of the synthesis of pertrifluoromethyl pyridazine derivatives 3



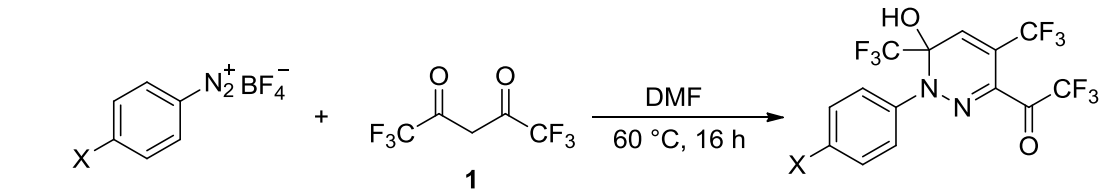
In a glove box filled with nitrogen, to an oven-dried 10 mL pressure tube equipped with a stir bar were added arenediazonium tetrafluoroborate **2** (0.30 mmol, 1.0 equiv), 1,1,1,5,5,5-hexafluoropentane-2,4-dione **1** (0.66 mmol, 2.2 equiv) and DMF (3.0 mL). The tube was sealed with Teflon screw cap and the solution was stirred at 60 °C for 16 h. After cool to room temperature, the crude mixture was diluted with ethyl acetate (30 mL) and water (10 mL), and the products were extracted. The organic phase was washed with saturated brine(5 mL × 2) and dried over Na_2SO_4, filtered, and the solvent was removed by rotary evaporation. The resulting pyridazine derivatives **3** were purified by column chromatography on silica gel with petroleum ether/ethyl acetate.

General procedure of the synthesis of 7



To an oven-dried 10 mL eggplant-shaped bottle equipped with a stir bar were added **3** (0.20 mmol, 1.0 equiv), **6** (0.60 mmol, 3.0 equiv), CH_2Cl_2 (1.5 mL) and concentrated H_2SO_4 (1.2 mmol, 6.0 equiv). The bottle was sealed with a glass cap, and the reaction mixture was stirred at room temperature for 10 h. The reaction was quenched by adding cold 5% $NaHCO_3$ solution, and the mixture was extracted with CH_2Cl_2 (10 mL × 3), washed with brine (5 mL × 3). The organic phase was collected and dried over Na_2SO_4, filtered, and the solvent was removed by rotary evaporation. The resulting product was purified by column chromatography on silica gel with petroleum ether/ethyl acetate or petroleum ether/CH_2Cl_2.

Procedure for gram scale reaction for synthesis of 3c and 3t



1

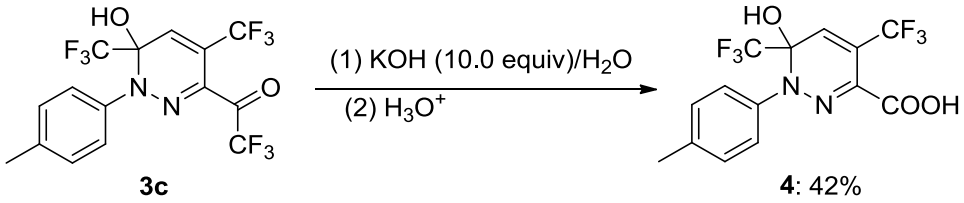
2c: X= CH_3, 1.03 g, 5.0 mmol — 2.29 g, 11.0 mmol — **3c**: 1.89 g, 90%

2t: X= Br, 0.96 g, 3.6 mmol — 1.65 g, 7.9 mmol — **3t**: 1.64 g, 92%

In a glove box filled with nitrogen, to an oven-dried 100 mL pressure tube equipped with a stir bar were added **2c** (1.03, 5.0 mmol, 1.0 equiv) or **2t** (0.96 g, 3.6 mmol, 1.0 equiv), 1,1,1,5,5,5-hexafluoropentane-2,4-dione (2.29g, 11.0 mmol, 2.2 equiv or 1.65 g, 7.9 mmol, 2.2 equiv) and DMF (30 mL or 20 mL). The tube was sealed with Teflon screw cap and the solution was stirred at 60 °C for 16 h. After cool to room temperature, the crude mixture was diluted with ethyl acetate (100 mL) and water (60 mL), and the products were extracted. The organic phase was washed with saturated brine(30 mL × 2) and dried over Na_2SO_4, filtered, and the solvent was removed by rotary evaporation. The resulting residue was purified by column chromatography on silica gel with petroleum ether/ethyl acetate (8:1) to give 1.89 g of product **3c** (90% yield) and 1.64 g of product **3t** (92% yield), respectively.

Synthetic utility of pertrifluoromethyl pyridazinols

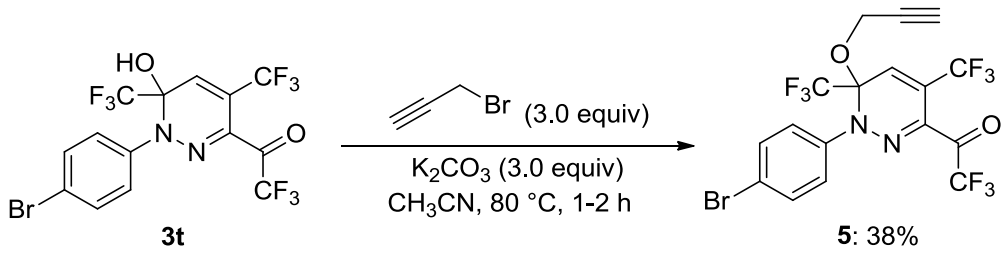
(1)



3c **4**: 42%

To an 10 mL eggplant-shaped bottle flask equipped with a stir bar were added **3c** (0.30 mmol, 1.0 equiv), KOH (3.0 mmol, 10.0 equiv) and H_2O (1.5 mL). The bottle was sealed with a glass cap, and the reaction mixture was stirred at room temperature for overnight. The reaction was acidified by adding 6 M HCl and the mixture was extracted with ethyl acetate (10 mL × 3). The organic phase was collected, washed with brine (5 mL × 3) and dried over Na_2SO_4, filtered, and the solvent was removed by rotary evaporation. The resulting residue was purified by column chromatography on silica gel with petroleum ether/ethyl acetate (1:1) to give 46 mg of product **4** (42% yield).

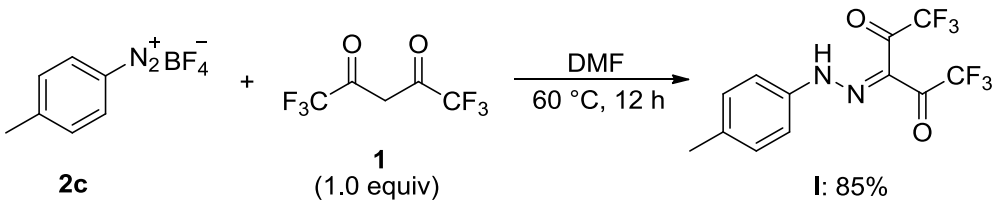
(2)



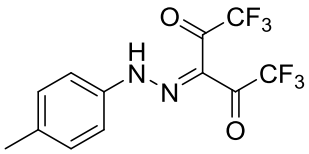
To an oven-dried 5 mL pressure tube equipped with a stir bar were added **3t** (145 mg, 0.30 mmol, 1.0 equiv), 3-bromopropyne (78 μL, 0.90 mmol, 3.0 equiv), K_2CO_3 (124 mg, 0.90 mmol, 3.0 equiv) and CH_3CN (3.0 mL). The tube was sealed with Teflon screw cap and the solution was stirred at 80 °C for 1-2 h. After cool to room temperature, the crude mixture was diluted with ethyl acetate (20 mL) and water (10 mL), and the products were extracted. The organic phase was washed with saturated brine(5 mL × 2) and dried over Na_2SO_4, filtered, and the solvent was removed by rotary evaporation. The resulting residue was purified by column chromatography on silica gel with petroleum ether/ethyl acetate (4:1) to give 60 mg of product **5** (38% yield).

Mechanism experiments

(a) Synthesis of intermediate I



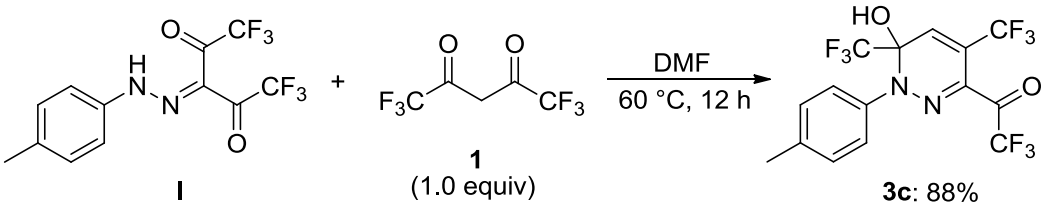
In a glove box filled with nitrogen, to an oven-dried 25 mL pressure tube equipped with a stir bar were added 4-methylbenzenediazonium tetrafluoroborate **2c** (124 mg, 0.60 mmol, 1.0 equiv), 1,1,1,5,5,5-hexafluoropentane-2,4-dione **1** (125 mg, 0.60 mmol, 1.0 equiv) and DMF (6.0 mL). The tube was sealed with Teflon screw cap and the solution was stirred at 60 °C for 12 h. After cool to room temperature, the crude mixture was diluted with ethyl acetate (20 mL) and water (10 mL), and the products were extracted. The organic phase was washed with saturated brine (5 mL × 2) and water (5 mL × 2). The organic phase was collected and dried over Na_2SO_4, filtered, and the solvent was removed by rotary evaporation. The resulting product was purified by column chromatography on silica gel with petroleum ether/ethyl acetate (8:1) to give 1,1,1,5,5,5-hexafluoro-3-(2-(*p-tolyl*)hydrazono)pentane-2,4-dione **I** in 85% yield (166 mg).



1,1,1,5,5,5-Hexafluoro-3-(2-(*p-tolyl*)hydrazono)pentane-2,4-dione (I)[2]

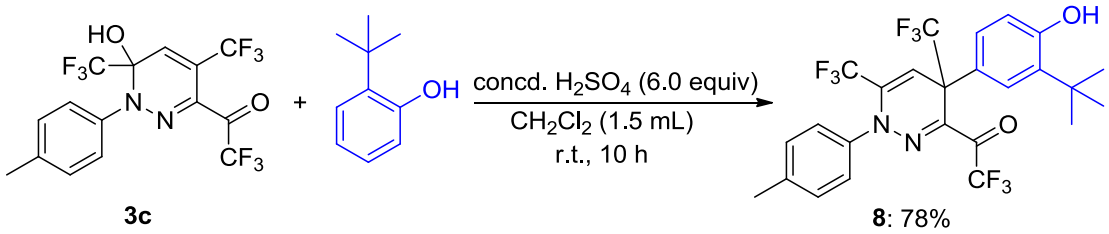
^{1}H NMR (400 MHz, $CDCl_3$) δ 14.58 (s, 1H), 7.47 (d, *J* = 7.6 Hz, 2H), 7.34 (d, *J* = 7.6 Hz, 2H), 2.44 (s, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -72.1 (s, 3F), -75.6 (s, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 176.5 (q, *J* = 40.1 Hz), 174.9 (q, *J* = 33.9 Hz), 140.0 (s), 137.7 (s), 130.8 (s), 123.9 (s), 117.9 (s), 116.9 (q, *J* = 292.0 Hz), 115.6 (q, *J* = 287.4 Hz), 21.1 (s).

(b) Reaction of intermediate I with 1



In a glove box filled with nitrogen, to an oven-dried 10 mL pressure tube equipped with a stir bar were added 1,1,1,5,5,5-hexafluoro-3-(2-(*p-tolyl*)hydrazono)pentane-2,4-dione **I** (98 mg, 0.30 mmol, 1.0 equiv), 1,1,1,5,5,5-hexafluoropentane-2,4-dione **1** (62 mg, 0.30 mmol, 1.0 equiv) and DMF (3.0 mL). The tube was sealed with Teflon screw cap and the solution was stirred at 60 °C for 12 h. After cool to room temperature, the crude mixture was diluted with ethyl acetate (20 mL) and water (10 mL), and the products were extracted. The organic phase was washed with saturated brine (5 mL × 2) and water (5 mL × 2), and dried over Na_2SO_4, filtered, and the solvent was removed by rotary evaporation. The resulting residue was purified by column chromatography on silica gel with petroleum ether /ethyl acetate (6:1) to give **3c** in 88% yield (111 mg).

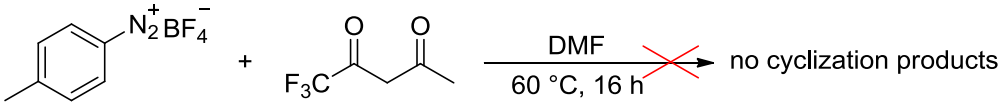
(c) Reaction of 3c with bulky *ortho*-substituted phenol

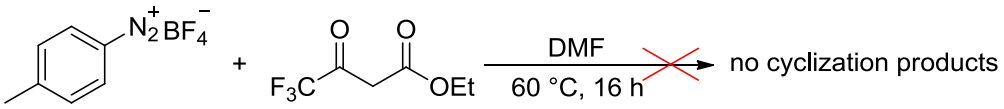


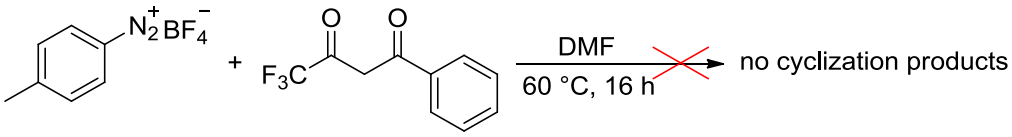
3c **8**: 78%

To an oven-dried 10 mL eggplant-shaped bottle equipped with a stir bar were added **3c** (84 mg, 0.20 mmol, 1.0 equiv), 2-(*tert*-butyl)phenol (90 mg, 0.60 mmol, 3.0 equiv), CH_2Cl_2 (1.5 mL) and concentrated H_2SO_4 (1.2 mmol, 6.0 equiv). The bottle was sealed with a glass cap, and the reaction mixture was stirred at room temperature for 10 h. The reaction was quenched by adding cold 5% $NaHCO_3$ solution, and the mixture was extracted with CH_2Cl_2 (10 mL × 3), washed with brine (5 mL × 3). The organic phase was collected and dried over $MgSO_4$, filtered, and the solvent was removed by rotary evaporation. The resulting product was purified by column chromatography on silica gel with petroleum ether/ethyl acetate (8:1) to give **8** in 78% yield (86 mg).

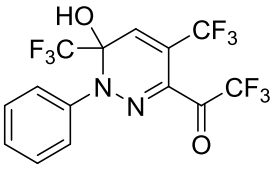
Unsuccessful reactions with other 1,3-diketone substrates





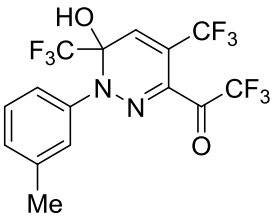


Data for compounds



2,2,2-Trifluoro-1-(6-hydroxy-1-phenyl-4,6-bis(trifluoromethyl)-1,6-dihydropyridazin-3-yl)ethanone (3a)

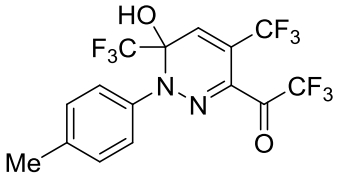
Following the general procedure and workup, and purification by column chromatography (silica gel, petroleum ether: ethyl acetate 6:1) gave final product **3a** as a light yellow solid in 90% yield (110 mg). Mp: 112.0–112.6 ℃. R_f (petroleum ether: ethyl acetate 6:1) = 0.62. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 – 7.54 (m, 2H), 7.50 – 7.43 (m, 3H), 6.53 (s, 1H), 4.93 (br s, 1H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.5 (s, 3F), -70.8 (s, 3F), -78.0 (s, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.4 (q, J = 34.6 Hz), 142.3 (s), 129.3 (s), 129.1 (s), 126.8 (s), 124.1 (q, J = 35.7 Hz), 121.5 (q, J = 289.2 Hz), 120.7 (q, J = 6.8 Hz), 120.6 (q, J = 273.5 Hz), 116.4 (q, J = 291.0 Hz), 83.2 (q, J = 34.1 Hz). IR (ATR): ν 3503, 3101, 2922, 1693, 1658, 1494, 1404, 1311, 1184, 1143, 1020, 977, 934, 881, 692, 673 cm^{-1}. HRMS (ESI) m/z: calcd. for $C_{14}H_6F_9N_2O_2$ [M-H]$^-$: 405.0280; found: 405.0280.



2,2,2-Trifluoro-1-(6-hydroxy-1-(*m*-tolyl)-4,6-bis(trifluoromethyl)-1,6-dihydropyridazin-3-yl)ethanone (3b)

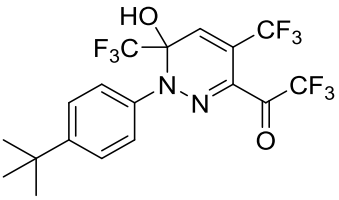
Following the general procedure and workup, and purification by column chromatography (silica gel, petroleum ether: ethyl acetate 6:1) gave final product **3b** as a white solid in 91% yield (115 mg). Mp: 93.0–94.2 ℃. R_f (petroleum ether: ethyl acetate 6:1) = 0.55. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39 – 7.32 (m, 3H), 7.31 – 7.26 (m,

1H), 6.52 (s, 1H), 4.58 (br s, 1H), 2.42 (s, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.5 (s, 3F), -70.7 (s, 3F), -78.1 (s, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.4 (q, *J* = 34.6 Hz), 142.0 (s), 139.3 (s), 130.2 (s), 128.9 (s), 127.5 (s), 126.7 (s), 124.2 (q, *J* = 35.7 Hz), 124.0 (s), 121.5 (q, *J* = 289.2 Hz), 120.6 (q, *J* = 273.6 Hz), 120.4 (q, *J* = 6.6 Hz), 116.4 (q, *J* = 291.0 Hz), 83.1 (q, *J* = 34.2 Hz), 21.3 (s). IR (ATR): ν 3377, 3109, 2931, 1700, 1505, 1403, 1310, 1246, 1198, 1171, 1138, 1076, 1045, 998, 950, 896, 876, 728, 706 cm^{-1}. HRMS (ESI) m/z: calcd. for $C_{15}H_8F_9N_2O_2$ [M-H]$^-$: 419.0437; found: 419.0419.



2,2,2-Trifluoro-1-(6-hydroxy-1-(*p*-tolyl)-4,6-bis(trifluoromethyl)-1,6-dihydropyridazin-3-yl)ethanone (3c)

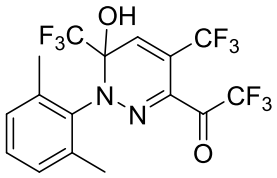
Following the general procedure and workup, and purification by column chromatography (silica gel, petroleum ether: ethyl acetate 6:1) gave final product **3c** as a yellow solid in 93% yield (117 mg). Mp: 99.1-100.0 ℃. R_f (petroleum ether: ethyl acetate 6:1) = 0.76. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 (d, *J* = 8.0 Hz, 2H), 7.28 (d, *J* = 6.8 Hz, 2H), 6.54 (s, 1H), 4.65 (s, 1H), 2.44 (s, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.4 (s, 3F), -70.8 (s, 3F), -78.0 (s, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.1 (q, *J* = 34.4 Hz), 139.6 (s), 129.8 (s), 126.9 (s), 126.7 (s), 124.4 (q, *J* = 36.6 Hz), 121.5 (q, *J* = 289.3 Hz), 120.7 (q, *J* = 273.5 Hz), 120.3 (q, *J* = 7.7 Hz), 116.4 (q, *J* = 291.4 Hz), 83.1 (q, *J* = 34.2 Hz), 21.2 (s). IR (ATR): ν 3479, 3107, 2977, 2928, 1701, 1656, 1503, 1403, 1308, 1214, 1148, 1037, 1017, 981, 937, 885, 821 cm^{-1}. HRMS (ESI) m/z: calcd. for $C_{15}H_8F_9N_2O_2$ [M-H]$^-$: 419.0437; found: 419.0452.



1-(1-(4-(*tert*-Butyl)phenyl)-6-hydroxy-4,6-bis(trifluoromethyl)-1,6-dihydropyrida

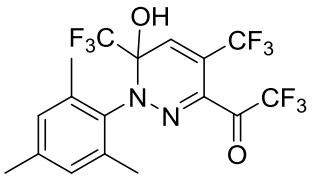
zin-3-yl)-2,2,2-trifluoroethanone (3d)

Following the general procedure and workup, and purification by column chromatography (silica gel, petroleum ether: ethyl acetate 6:1) gave final product **3d** as a yellow solid in 93% yield (129 mg). Mp: 149.5–150.5 ℃. R_f (petroleum ether: ethyl acetate 6:1) = 0.72. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 (s, 4H), 6.50 (s, 1H), 4.29 (s, 1H), 1.36 (s, 9H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.4 (s, 3F), -70.8 (s, 3F), -78.2 (s, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.1 (q, *J* = 34.6 Hz), 152.6 (s), 139.3 (s), 127.0 (s), 126.4 (s), 126.1 (s), 124.5 (q, *J* = 35.0 Hz), 121.6 (q, *J* = 289.7 Hz), 120.6 (q, *J* = 273.6 Hz), 120.2 (q, *J* = 6.1 Hz), 116.4 (q, *J* = 291.3 Hz), 83.2 (q, *J* = 33.9 Hz), 34.8 (s), 31.2 (s). IR (ATR): ν 3468, 2974, 1727, 1703, 1501, 1411, 1307, 1276, 1216, 1196, 1155, 1140, 1067, 1045, 999, 944, 840 cm^{-1}. HRMS (ESI) m/z: calcd. for $C_{18}H_{14}F_9N_2O_2$ [M-H]$^-$: 461.0906; found: 461.0909.



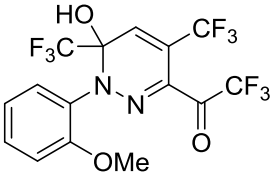
1-(1-(2,6-Dimethylphenyl)-6-hydroxy-4,6-bis(trifluoromethyl)-1,6-dihydropyrida zin-3-yl)-2,2,2-trifluoroethanone (3e)

Following the general procedure and workup, and purification by column chromatography (silica gel, petroleum ether: ethyl acetate 6:1) gave final product **3e** as a white solid in 58% yield (76 mg). Mp: 131.0–131.8 ℃. R_f (petroleum ether: ethyl acetate 6:1) = 0.75. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.29 (t, *J* = 7.6 Hz, 1H), 7.20 – 7.14 (m, 2H), 6.48 (s, 1H), 4.05 (s, 1H), 2.31 (s, 3H), 2.14 (s, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.9 (s, 3F), -71.0 (s, 3F), -80.6 (s, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.1 (q, *J* = 34.8 Hz), 138.6 (s), 138.2 (s), 138.1 (s), 129.9 (s), 129.3 (s), 129.2 (q, *J* = 65.4 Hz), 128.8 (s), 124.6 (q, *J* = 35.8 Hz), 121.8 (q, *J* = 288.6 Hz), 120.8 (q, *J* = 273.7 Hz), 118.5 (q, *J* = 6.5 Hz), 116.4 (q, *J* = 291.0 Hz), 82.7 (q, *J* = 34.0 Hz), 19.2 (s), 17.4 (q, *J* = 3.1 Hz). IR (ATR): ν 3103, 2815, 2676, 1730, 1527, 1463, 1403, 1354, 1312, 1258, 1216, 1153, 1115, 1021, 986, 937, 888, 843, 714, 628 cm^{-1}. HRMS (ESI) m/z: calcd. for $C_{16}H_{10}F_9N_2O_2$ [M-H]$^-$: 433.0593; found: 433.0595.



2,2,2-Trifluoro-1-(6-hydroxy-1-mesityl-4,6-bis(trifluoromethyl)-1,6-dihydropyridazin-3-yl)ethanone (3f)

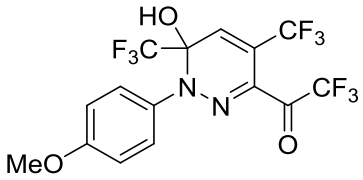
Following the general procedure and workup, and purification by column chromatography (silica gel, petroleum ether: ethyl acetate 6:1) gave final product **3f** as a off-white solid in 51% yield (69 mg). Mp: 135.5–136.2 ℃. R_f (petroleum ether: ethyl acetate 6:1) = 0.65. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.98 (s, 2H), 6.46 (s, 1H), 3.67 (s, 1H), 2.33 (s, 3H), 2.27 (s, 3H), 2.10 (s, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.9 (s, 3F), -71.0 (s, 3F), -80.7 (s, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.1 (q, *J* = 34.7 Hz), 140.0 (s), 137.7 (s), 137.6 (s), 136.1 (s), 130.0 (s), 129.6 (s), 129.5 (s), 124.6 (q, *J* = 35.9 Hz), 121.8 (q, *J* = 288.7 Hz), 120.8 (q, *J* = 273.6 Hz), 118.3 (q, *J* = 6.3 Hz), 116.4 (q, *J* = 290.8 Hz), 82.7 (q, *J* = 34.1 Hz), 21.0 (s), 19.0 (s), 17.3 (q, *J* = 3.0 Hz). IR (ATR): ν 3459, 3124, 2931, 1977, 1707, 1480, 1400, 1262, 1213, 1180, 1151, 1052, 1031, 997, 957, 932, 851, 743 cm^{-1}. HRMS (ESI) m/z: calcd. for $C_{17}H_{12}F_9N_2O_2$ [M-H]$^-$: 447.0750; found: 447.0752.



2,2,2-Trifluoro-1-(6-hydroxy-1-(2-methoxyphenyl)-4,6-bis(trifluoromethyl)-1,6-dihydropyridazin-3-yl)ethanone (3g)

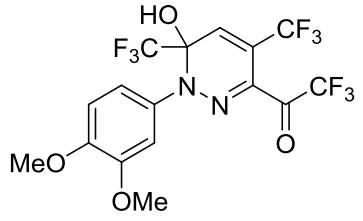
Following the general procedure and workup, and purification by column chromatography (silica gel, petroleum ether: ethyl acetate 6:1) gave final product **3g** as a yellow solid in 76% yield (99 mg). Mp: 81.5–82.1 ℃. R_f (petroleum ether: ethyl acetate 6:1) = 0.67. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 (t, *J* = 7.9 Hz, 1H), 7.37 (d, *J* = 7.7 Hz, 1H), 7.19 – 7.07 (m, 2H), 6.59 (s, 1H), 5.71 (s, 1H), 3.95 (s, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.2 (s, 3F), -71.0 (s, 3F), -79.2 (s, 3F). ^{13}C NMR (101 MHz,

$CDCl_3$) δ 174.1 (q, *J* = 34.7 Hz), 153.8 (s), 131.6 (s), 131.5 (s), 130.5 (s), 129.0 (s), 123.6 (q, *J* = 35.9 Hz), 122.4 (s), 122.1 (q, *J* = 6.5 Hz), 121.7 (q, *J* = 288.7 Hz), 120.9 (q, *J* = 273.4 Hz), 116.3 (q, *J* = 291.2 Hz), 112.6 (s), 82.7 (q, *J* = 33.5 Hz), 56.8 (s). IR (ATR): ν 3470, 3123, 2948, 2846, 1708, 1501, 1414, 1394, 1299, 1209, 1192, 1149, 1135, 1061, 1028, 982, 943, 877 cm^{-1}. HRMS (ESI) m/z: calcd. for $C_{15}H_8F_9N_2O_3$ $[M-H]^-$: 435.0386; found: 435.0390.



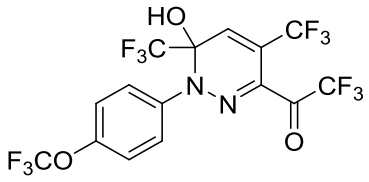
2,2,2-Trifluoro-1-(6-hydroxy-1-(4-methoxyphenyl)-4,6-bis(trifluoromethyl)-1,6-dihydropyridazin-3-yl)ethan-1-one (3h)

Following the general procedure and workup, and purification by column chromatography (silica gel, petroleum ether: ethyl acetate 6:1) gave final product **3h** as a yellow solid in 95% yield (124 mg). Mp: 99.0–100.7 ℃. R_f (petroleum ether: ethyl acetate 6:1) = 0.87. ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.69 (s, 1H), 7.48 (d, *J* = 8.3 Hz, 2H), 7.05 (d, *J* = 8.3 Hz, 2H), 6.72 (s, 1H), 3.81 (s, 3H). ^{19}F NMR (376 MHz, DMSO-d_6) δ -62.3 (s, 3F), -69.7 (s, 3F), -78.1 (s, 3F). ^{13}C NMR (101 MHz, DMSO-d_6) δ 173.0 (q, *J* = 33.1 Hz), 159.5 (s), 135.4 (s), 128.2 (s), 125.9 (s), 122.4 (q, *J* = 6.5 Hz), 122.0 (q, *J* = 35.4 Hz), 121.9 (q, *J* = 289.5 Hz), 121.0 (q, *J* = 273.2 Hz), 116.5 (q, *J* = 291.5 Hz), 114.1 (s), 83.0 (q, *J* = 33.1 Hz), 55.4 (s). IR (ATR): ν 3485, 3130, 2973, 1714, 1607, 1503, 1414, 1299, 1192, 1148, 1131, 987, 945, 874, 838, 738, 669, 581 cm^{-1}. HRMS (ESI) m/z: calcd. for $C_{15}H_8F_9N_2O_3$ $[M-H]^-$: 435.0386; found: 435.0385.



1-(1-(3,4-Dimethoxyphenyl)-6-hydroxy-4,6-bis(trifluoromethyl)-1,6-dihydropyridazin-3-yl)-2,2,2-trifluoroethanone (3i)

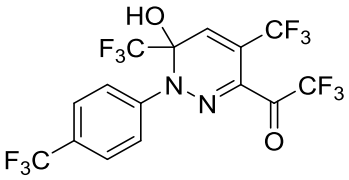
Following the general procedure and workup, and purification by column chromatography (silica gel, petroleum ether: ethyl acetate 6:1) gave final product **3i** as a brownish yellow solid in 93% yield (130 mg). Mp: 126.6–127.5 ℃. R_f (petroleum ether: ethyl acetate 6:1) = 0.29. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.27 (d, *J* = 7.7 Hz, 1H), 7.12 (s, 1H), 6.91 (d, *J* = 7.7 Hz, 1H), 6.51 (s, 1H), 5.23 (br s, 1H), 3.92 (s, 3H), 3.87 (s, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.6 (s, 3F), -70.7 (s, 3F), -77.9 (s, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.1 (q, *J* = 68.5, 34.3 Hz), 149.4 (s), 148.7 (s), 135.6 (s), 126.6 (s), 124.0 (q, *J* = 35.5 Hz), 121.6 (q, *J* = 290.1 Hz), 120.6 (q, *J* = 273.6 Hz), 120.5 (q, *J* = 6.8 Hz), 119.1 (s), 116.5 (q, *J* = 291.0 Hz), 110.7 (s), 110.3 (s), 83.4 (q, *J* = 34.1 Hz), 56.1 (s), 56.0 (s). IR (ATR): ν 3378, 2952, 2922, 2849, 1722, 1603, 1510, 1467, 1402, 1306, 1253, 1214, 1188, 1149, 1133, 1084, 1054, 1019, 991, 948, 899, 849, 771 cm^{-1}. HRMS (ESI) m/z: calcd. for $C_{16}H_{10}F_9N_2O_4$ $[M-H]^-$: 465.0491; found: 465.0468.



2,2,2-Trifluoro-1-(6-hydroxy-1-(4-(trifluoromethoxy)phenyl)-4,6-bis(trifluoromethyl)-1,6-dihydropyridazin-3-yl)ethanone (3j)

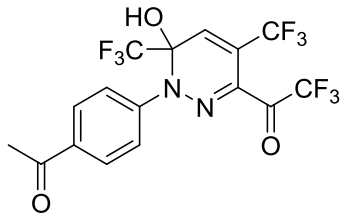
Following the general procedure and workup, and purification by column chromatography (silica gel, petroleum ether: ethyl acetate 6:1) gave final product **3j** as a yellow oily liquid in 45% yield (66 mg). Mp: 92.6–93.5 ℃. R_f (petroleum ether: ethyl acetate 6:1) = 0.62. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 (d, *J* = 7.9 Hz, 2H), 7.29 (d, *J* = 8.4 Hz, 2H), 6.55 (s, 1H), 5.37 (br s, 1H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -58.0 (s, 3F), -63.6 (s, 3F), -70.8 (s, 3F), -78.0 (s, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.5 (q, *J* = 34.7 Hz), 149.4 (s), 140.6 (s), 128.2 (s), 127.2 (s), 124.1 (q, *J* = 36.1 Hz), 121.5 (q, *J* = 289.0 Hz), 121.3 (s), 121.2 (q, *J* = 9.1 Hz), 120.5 (q, *J* = 273.5 Hz), 120.4 (q, *J* = 258.4 Hz), 116.4 (q, *J* = 290.9 Hz), 83.2 (q, *J* = 34.1 Hz). IR (ATR): ν 3432, 3104, 1713, 1504, 1406, 1259, 1210, 1148, 1105, 1034, 1016, 979, 939, 852, 747, 672 cm^{-1}. HRMS (ESI) m/z: calcd. for $C_{15}H_5F_{12}N_2O_3$ $[M-H]^-$: 489.0103; found:

489.0102.



2,2,2-Trifluoro-1-(6-hydroxy-4,6-bis(trifluoromethyl)-1-(4-(trifluoromethyl)phenyl)-1,6-dihydropyridazin-3-yl)ethanone (3k)

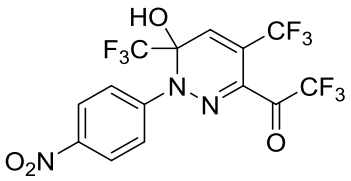
Following the general procedure and workup, and purification by column chromatography (silica gel, petroleum ether: ethyl acetate 6:1) gave final product **3k** as a white solid in 86% yield (122 mg). Mp: 85.6–87.1 ℃. R_f (petroleum ether: ethyl acetate 6:1) = 0.61. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 (d, *J* = 8.8 Hz, 2H), 7.72 (d, *J* = 8.8 Hz, 2H), 6.57 (s, 1H), 5.41 (s, 1H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.8 (s, 3F), -63.5 (s, 3F), -70.9 (s), -78.0 (s, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.4 (q, *J* = 34.8 Hz), 145.3 (s), 131.0 (q, *J* = 33.1 Hz), 127.5 (s), 126.8 (q, *J* = 3.7 Hz), 126.6 (s), 126.3 (q, *J* = 3.6 Hz), 124.1 (q, *J* = 35.8 Hz), 123.6 (q, *J* = 272.3 Hz), 121.7 (q, *J* = 7.2 Hz), 121.5 (q, *J* = 289.1 Hz), 120.5 (q, *J* = 273.6 Hz), 116.3 (q, *J* = 291.0 Hz), 83.4 (q, *J* = 34.4 Hz). IR (ATR): ν 3502, 3109, 2924, 1721, 1616, 1520, 1412, 1372, 1321, 1214, 1183, 1160, 1140, 1114, 1065, 1034, 1013, 967, 943, 890, 842, 681, 623 cm^{-1}. HRMS (ESI) m/z: calcd. for $C_{15}H_5F_{12}N_2O_2$ $[M-H]^-$: 473.0154; found: 473.0160.



1-(1-(4-Acetylphenyl)-6-hydroxy-4,6-bis(trifluoromethyl)-1,6-dihydropyridazin-3-yl)-2,2,2-trifluoroethanone (3l)

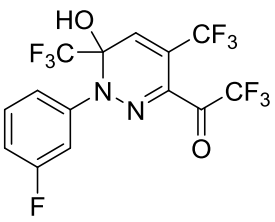
Following the general procedure and workup, and purification by column chromatography (silica gel, petroleum ether: ethyl acetate 6:1) gave final product **3l** as a white solid in 86% yield (116 mg). Mp: 136.5–137.6 ℃. R_f (petroleum ether: ethyl acetate 6:1) = 0.28. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 (d, *J* = 8.2 Hz, 2H), 7.73

(d, *J* = 8.3 Hz, 2H), 6.59 (s, 1H), 5.62 (br s, 1H), 2.62 (s, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.3 (s, 3F), -70.9 (s, 3F), -77.9 (s, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 198.7 (s), 173.9 (q, *J* = 35.0 Hz), 146.7 (s), 136.2 (s), 129.2 (s), 127.7 (s), 126.1 (s), 124.0 (q, *J* = 36.1 Hz), 122.1 (q, *J* = 6.8 Hz), 121.6 (q, *J* = 289.5 Hz), 120.5 (q, *J* = 273.6 Hz), 116.3 (q, *J* = 291.3 Hz), 83.5 (q, *J* = 34.6 Hz), 26.7 (s). IR (ATR): ν 3141, 2922, 1729, 1657, 1602, 1525, 1403, 1282, 1219, 1172, 1154, 1086, 1035, 1013, 979, 937, 844, 594 cm^{-1}. HRMS (ESI) m/z: calcd. for $C_{16}H_8F_9N_2O_3$ [M-H]$^-$: 447.0386; found: 447.0387.



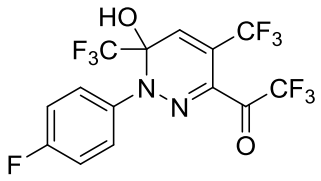
2,2,2-Trifluoro-1-(6-hydroxy-1-(4-nitrophenyl)-4,6-bis(trifluoromethyl)-1,6-dihydropyridazin-3-yl)ethanone (3m)

Following the general procedure and workup, and purification by column chromatography (silica gel, petroleum ether: ethyl acetate 6:1) gave final product **3m** as a brown liquid in 76% yield (103 mg). Mp: 117.0–118.2 ℃. R_f (petroleum ether: ethyl acetate 6:1) = 0.41. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.27 (d, *J* = 8.2 Hz, 2H), 7.88 (d, *J* = 8.2 Hz, 2H), 6.61 (s, 1H), 6.36 (br s, 1H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.5 (s, 3F), -70.9 (s, 3F), -78.2 (s, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.1 (q, *J* = 35.1 Hz), 148.0 (s), 146.7 (s), 128.0 (s), 126.4 (s), 124.5 (s), 123.9 (q, *J* = 36.2 Hz), 122.8 (q, *J* = 6.1 Hz), 121.6 (q, *J* = 289.5 Hz), 120.4 (q, *J* = 273.6 Hz), 116.3 (q, *J* = 291.1 Hz), 83.6 (q, *J* = 34.6 Hz). IR (ATR): ν 3404, 3099, 2931, 1730, 1595, 1524, 1492, 1402, 1343, 1312, 1213, 1150, 1107, 1029, 1014, 936, 856, 749, 692 cm^{-1}. HRMS (ESI) m/z: calcd. for $C_{14}H_5F_9N_3O_4$ [M-H]$^-$: 450.0131; found: 450.0111.



2,2,2-Trifluoro-1-(1-(3-fluorophenyl)-6-hydroxy-4,6-bis(trifluoromethyl)-1,6-dihydropyridazin-3-yl)ethanone (3n)

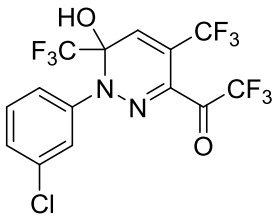
Following the general procedure and workup, and purification by column chromatography (silica gel, petroleum ether: ethyl acetate 6:1) gave final product **3n** as a white solid in 88% yield (112 mg). Mp: 97.0–98.6 ℃. R_f (petroleum ether: ethyl acetate 6:1) = 0.71. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48 – 7.33 (m, 3H), 7.17 (t, *J* = 8.1 Hz, 1H), 6.55 (s, 1H), 4.77 (s, 1H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.5 (s, 3F), -70.8 (s, 3F), -78.0 (s, 3F), -110.6 (dd, *J* = 14.7, 8.6 Hz, 1F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.4 (q, *J* = 34.9 Hz), 162.3 (d, *J* = 248.2 Hz), 143.4 (d, *J* = 9.8 Hz), 130.3 (d, *J* = 8.9 Hz), 127.1 (s), 124.1 (q, *J* = 36.0 Hz), 122.3 (d, *J* = 2.9 Hz), 121.5 (q, *J* = 289.3 Hz), 121.3 (q, *J* = 6.4 Hz), 120.5 (q, *J* = 273.6 Hz), 116.4 (q, *J* = 290.9 Hz), 116.3 (d, *J* = 21.1 Hz), 114.3 (d, *J* = 25.2 Hz), 83.3 (q, *J* = 34.4 Hz). IR (ATR): ν 3388, 3108, 2920, 2851, 1701, 1602, 1511, 1492, 1397, 1312, 1244, 1183, 1152, 1136, 1077, 1041, 991, 954, 884, 705 cm^{-1}. HRMS (ESI) m/z: calcd. for $C_{14}H_5F_{10}N_2O_2$ $[M-H]^-$: 423.0186; found: 423.0188.



2,2,2-Trifluoro-1-(1-(4-fluorophenyl)-6-hydroxy-4,6-bis(trifluoromethyl)-1,6-dihydropyridazin-3-yl)ethanone (3o)

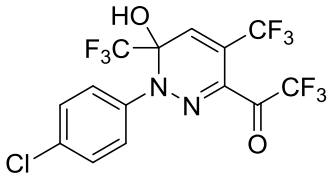
Following the general procedure and workup, and purification by column chromatography (silica gel, petroleum ether: ethyl acetate 6:1) gave final product **3o** as a yellow solid in 79% yield (100 mg). Mp: 119.2–120.8 ℃. R_f (petroleum ether: ethyl acetate 6:1) = 0.57. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55 (dd, *J* = 7.4, 4.9 Hz, 2H), 7.15 (t, *J* = 8.0 Hz, 2H), 6.55 (s, 1H), 4.40 (s, 1H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.4 (s, 3F), -70.8 (s, 3F), -77.8 (s, 3F), -110.8 – -110.9 (m). ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.2 (q, *J* = 34.8 Hz), 162.7 (d, *J* = 250.5 Hz), 138.2 (d, *J* = 3.3 Hz), 128.9 (d, *J* = 8.9 Hz), 127.1 (s), 124.4 (q, *J* = 36.6 Hz), 121.4 (q, *J* = 289.0 Hz), 120.6 (q, *J* = 6.2 Hz), 120.5 (q, *J* = 273.7 Hz), 116.3 (q, *J* = 291.0 Hz), 116.2 (d, *J* = 23.1 Hz),

83.1 (q, *J* = 34.2 Hz). IR (ATR): ν 3486, 3099, 1704, 1501, 1403, 1315, 1211, 1145, 1102, 1031, 1013, 978, 933, 840 cm^{-1}. HRMS (ESI) m/z: calcd. for $C_{14}H_5F_{10}N_2O_2$ $[M-H]^-$: 423.0186; found: 423.0190.



1-(1-(3-Chlorophenyl)-6-hydroxy-4,6-bis(trifluoromethyl)-1,6-dihydropyridazin-3-yl)-2,2,2-trifluoroethanone (3p)

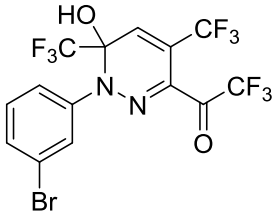
Following the general procedure and workup, and purification by column chromatography (silica gel, petroleum ether: ethyl acetate 6:1) gave final product **3p** as a yellow solid in 82% yield (108 mg). Mp: 82.3–83.8 ℃. R_f (petroleum ether: ethyl acetate 6:1) = 0.52. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62 (s, 1H), 7.53 – 7.35 (m, 3H), 6.55 (s, 1H), 4.97 (s, 1H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.5 (s, 3F), -70.8 (s, 3F), -78.0 (s, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.3 (q, *J* = 28.7 Hz), 143.2 (s), 134.6 (s), 130.1 (s), 129.4 (s), 127.3 (s), 126.9 (s), 124.9 (s), 124.1 (q, *J* = 31.5 Hz), 121.4 (q, *J* = 289.2 Hz), 121.3 (q, *J* = 6.9 Hz), 120.5 (q, *J* = 273.7 Hz), 116.3 (q, *J* = 290.9 Hz), 83.2 (q, *J* = 34.2 Hz). IR (ATR): ν 3387, 3100, 1728, 1703, 1590, 1510, 1477, 1402, 1351, 1306, 1215, 1182, 1146, 1074, 1040, 988, 948, 885, 867, 780, 702 cm^{-1}. HRMS (ESI) m/z: calcd. for $C_{14}H_5ClF_9N_2O_2$ $[M-H]^-$: 438.9890; found: 438.9895.



1-(1-(4-Chlorophenyl)-6-hydroxy-4,6-bis(trifluoromethyl)-1,6-dihydropyridazin-3-yl)-2,2,2-trifluoroethanone (3q)

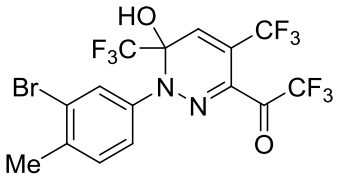
Following the general procedure and workup, and purification by column chromatography (silica gel, petroleum ether: ethyl acetate 6:1) gave final product **3q** as a light yellow solid in 92% yield (121 mg). Mp: 101.0–101.6 ℃. R_f (petroleum

ether: ethyl acetate 6:1) = 0.59. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 (d, *J* = 8.6 Hz, 2H), 7.43 (d, *J* = 8.6 Hz, 2H), 6.55 (s, 1H), 4.83 (s, 1H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.5 (s, 3F), -70.8 (s, 3F), -77.8 (s, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.4 (q, *J* = 34.8 Hz), 140.8 (s), 135.3 (s), 129.4 (s), 127.9 (s), 127.1 (s), 124.2 (q, *J* = 35.7 Hz), 121.4 (q, *J* = 289.4 Hz), 120.9 (q, *J* = 6.7 Hz), 120.5 (q, *J* = 273.8 Hz), 116.3 (q, *J* = 290.9 Hz), 83.2 (q, *J* = 34.2 Hz). IR (ATR): ν 3471, 3106, 2977, 2927, 1708, 1510, 1489, 1402, 1314, 1214, 1190, 1147, 1089, 1034, 1012, 982, 936, 888, 831 cm^{-1}. HRMS (ESI) m/z: calcd. for $C_{14}H_5ClF_9N_2O_2$ $[M-H]^-$: 438.9890; found: 438.9892.



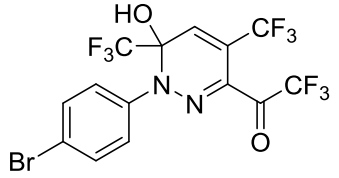
1-(1-(3-Bromophenyl)-6-hydroxy-4,6-bis(trifluoromethyl)-1,6-dihydropyridazin-3-yl)-2,2,2-trifluoroethanone (3r)

Following the general procedure and workup, and purification by column chromatography (silica gel, petroleum ether: ethyl acetate 6:1) gave final product **3r** as a white solid in 86% yield (111 mg). Mp: 93.8–94.7 ℃. R_f (petroleum ether: ethyl acetate 6:1) = 0.76. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 (s, 1H), 7.59 (d, *J* = 8.0 Hz, 1H), 7.53 (d, *J* = 8.0 Hz, 1H), 7.34 (t, *J* = 7.5 Hz, 1H), 6.55 (s, 1H), 5.25 (br s, 1H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.5 (s, 3F), -70.8 (s, 3F), -78.0 (s, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.4 (q, *J* = 34.9 Hz), 143.4 (s), 132.3 (s), 130.4 (s), 129.7 (s), 127.2 (s), 125.3 (s), 124.1 (q, *J* = 36.0 Hz), 122.2 (s), 121.5 (q, *J* = 289.5 Hz), 121.3 (q, *J* = 7.3 Hz), 120.5 (q, *J* = 273.6 Hz), 116.3 (q, *J* = 290.8 Hz), 83.2 (q, *J* = 34.2 Hz). IR (ATR): ν 3424, 3101, 1713, 1581, 1514, 1475, 1403, 1309, 1214, 1148, 1102, 1035, 982, 942, 885, 774, 746, 693 cm^{-1}. HRMS (ESI) m/z: calcd. for $C_{14}H_5BrF_9N_2O_2$ $[M-H]^-$: 482.9385; found: 482.9389.



1-(1-(3-Bromo-4-methylphenyl)-6-hydroxy-4,6-bis(trifluoromethyl)-1,6-dihydropyridazin-3-yl)-2,2,2-trifluoroethanone (3s)

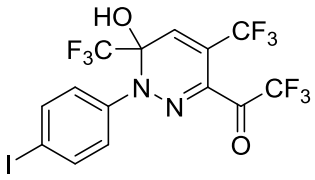
Following the general procedure and workup, and purification by column chromatography (silica gel, petroleum ether: ethyl acetate 6:1) gave final product **3s** as a yellow solid in 88% yield (131 mg). Mp: 100.5–101.1 ℃. R_f (petroleum ether: ethyl acetate 6:1) = 0.56. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 (s, 1H), 7.41 (d, *J* = 8.1 Hz, 1H), 7.32 (d, *J* = 7.6 Hz, 1H), 6.53 (s, 1H), 4.81 (br s, 1H), 2.46 (s, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.4 (s, 3F), -70.8 (s, 3F), -77.9 (s, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.0 (q, *J* = 34.9 Hz), 140.8 (s), 139.4 (s), 131.0 (s), 130.4 (s), 127.3 (s), 125.5 (s), 124.5 (s), 124.3 (q, *J* = 36.1 Hz), 121.5 (q, *J* = 289.3 Hz). 121.0 (q, *J* = 6.3 Hz), 120.6 (q, *J* = 273.6 Hz), 116.3 (q, *J* = 291.4 Hz), 83.1 (q, *J* = 34.2 Hz), 22.7 (s). IR (ATR): ν 3362, 3105, 2963, 1703, 1512, 1487, 1405, 1314, 1230, 1183, 1150, 1109, 1091, 1035, 977, 943, 892 cm^{-1}. HRMS (ESI) m/z: calcd. for $C_{15}H_7BrF_9N_2O_2$ [M-H]$^-$: 496.9542; found: 496.9546.



1-(1-(4-Bromophenyl)-6-hydroxy-4,6-bis(trifluoromethyl)-1,6-dihydropyridazin-3-yl)-2,2,2-trifluoroethanone (3t)

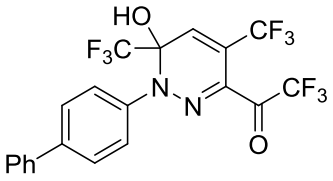
Following the general procedure and workup, and purification by column chromatography (silica gel, petroleum ether: ethyl acetate 6:1) gave final product **3t** as a yellow solid in 94% yield (136 mg). Mp: 98.2–100.1 ℃. R_f (petroleum ether: ethyl acetate 6:1) = 0.69. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 (d, *J* = 7.2 Hz, 2H), 7.46 (d, *J* = 7.2 Hz, 2H), 6.55 (s, 1H), 4.49 (br s, 1H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.4 (s, 3F), -70.9 (s, 3F), -77.8 (s, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.2 (q, *J* = 34.9

Hz), 141.3 (s), 132.4 (s), 128.2 (s), 127.3 (s), 124.3 (q, *J* = 35.9 Hz), 123.4 (s), 121.4 (q, *J* = 289.3 Hz), 120.9 (q, *J* = 6.7 Hz), 120.5 (q, *J* = 273.7 Hz), 116.3 (q, *J* = 291.2 Hz), 83.2 (q, *J* = 34.4 Hz). IR (ATR): ν 3370, 3104, 1712, 1578, 1512, 1486, 1405, 1356, 1312, 1218, 1199, 1146, 1070, 1036, 1010, 941, 832, 693 cm^{-1}. HRMS (ESI) m/z: calcd. for $C_{14}H_5BrF_9N_2O_2$ $[M-H]^-$: 482.9385; found: 482.9387.



2,2,2-Trifluoro-1-(6-hydroxy-1-(4-iodophenyl)-4,6-bis(trifluoromethyl)-1,6-dihydropyridazin-3-yl)ethanone (3u)

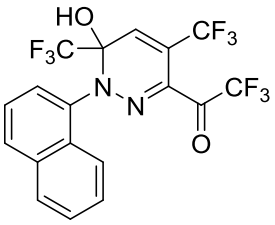
Following the general procedure and workup, and purification by column chromatography (silica gel, petroleum ether: ethyl acetate 6:1) gave final product **3u** as a yellow solid in 87% yield (139 mg). Mp: 99.0–99.6 ℃. R_f (petroleum ether: ethyl acetate 6:1) = 0.66. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80 (d, *J* = 7.8 Hz, 2H), 7.33 (d, *J* = 7.8 Hz, 2H), 6.54 (s, 1H), 4.51 (s, 1H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.5 (s, 3F), -70.8 (s, 3F), -77.8 (s, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.3 (q, *J* = 35.4 Hz), 142.1 (s), 138.4 (s), 128.3 (s), 127.3 (s), 124.4 (q, *J* = 36.2 Hz), 121.4 (q, *J* = 289.8 Hz), 120.9 (q, *J* = 6.4 Hz), 120.5 (q, *J* = 273.4 Hz), 116.3 (q, *J* = 291.0 Hz), 95.0 (s), 83.2 (q, *J* = 34.5 Hz). IR (ATR): ν 3364, 3103, 1711, 1513, 1484, 1405, 1357, 1312, 1172, 1142, 1035, 1005, 980, 939, 887, 828, 622 cm^{-1}. HRMS (ESI) m/z: calcd. for $C_{14}H_5F_9IN_2O_2$ $[M-H]^-$: 530.9247; found: 530.9247.



1-(1-([1,1'-Biphenyl]-4-yl)-6-hydroxy-4,6-bis(trifluoromethyl)-1,6-dihydropyridazin-3-yl)-2,2,2-trifluoroethanone (3v)

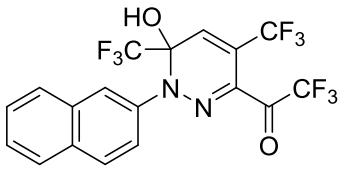
Following the general procedure and workup, and purification by column chromatography (silica gel, petroleum ether: ethyl acetate 6:1) gave final product **3v**

as a yellow solid in 92% yield (133 mg). Mp: 117.9–119.0 ℃. R_f (petroleum ether: ethyl acetate 6:1) = 0.58. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 – 7.61 (m, 6H), 7.48 (t, *J* = 7.4 Hz, 2H), 7.44 – 7.38 (m, 1H), 6.56 (s, 1H), 4.97 (br s, 1H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.4 (s, 3F), -70.7 (s, 3F), -77.9 (s, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.3 (q, *J* = 34.6 Hz), 142.9 (s), 142.0 (s), 141.4 (s), 139.6 (s), 129.1 (s), 129.0 (s), 128.9 (s), 128.1 (s), 128.0 (s), 127.7 (s), 127.2 (s), 126.9 (s), 126.3 (s), 124.2 (q, *J* = 35.9 Hz), 121.6 (q, *J* = 289.7 Hz), 120.8 (q, *J* = 5.9 Hz), 120.7 (q, *J* = 273.5 Hz), 116.5 (q, *J* = 291.0 Hz), 83.3 (q, *J* = 33.9 Hz). IR (ATR): ν 3446, 3090, 1727, 1527, 1486, 1406, 1302, 1195, 1139, 1084, 1034, 1017, 969, 939, 884, 842, 766, 700 cm^{-1}. HRMS (ESI) m/z: calcd. for $C_{20}H_{10}F_9N_2O_2$ [M-H]$^-$: 481.0593; found: 481.0597.



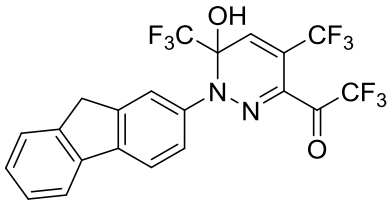
2,2,2-Trifluoro-1-(6-hydroxy-1-(naphthalen-1-yl)-4,6-bis(trifluoromethyl)-1,6-dihydropyridazin-3-yl)ethanone (3w)

Following the general procedure and workup, and purification by column chromatography (silica gel, petroleum ether: ethyl acetate 6:1) gave final product **3w** as a yellow solid in 83% yield (114 mg). Mp: 150.0–151.2 ℃. R_f (petroleum ether: ethyl acetate 6:1) = 0.47. ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.78 (s, 1H), 8.11 (d, *J* = 7.9 Hz, 1H), 8.04 (d, *J* = 7.2 Hz, 1H), 7.92 (d, *J* = 6.6 Hz, 1H), 7.75 (d, *J* = 6.9 Hz, 1H), 7.66 – 7.52 (m, 3H), 6.93 (s, 1H). ^{19}F NMR (376 MHz, DMSO-d_6) δ -62.1 (s, 3F), -69.7 (s, 3F), -76.9 (s, 3F). ^{13}C NMR (101 MHz, DMSO-d_6) δ 173.2 (q, *J* = 33.5 Hz), 137.4 (s), 134.0 (s), 130.0 (s), 129.5 (s), 128.3 (s), 127.2 (s), 126.5 (s), 124.9 (s), 122.5 (q, *J* = 5.8 Hz), 122.4 (s), 122.3 (q, *J* = 35.2 Hz), 121.7 (q, *J* = 288.8 Hz), 121.1 (q, *J* = 273.5 Hz), 116.2 (q, *J* = 291.5 Hz), 82.5 (q, *J* = 32.2 Hz). IR (ATR): ν 3471, 3128, 2961, 1710, 1497, 1393, 1301, 1248, 1195, 1153, 1134, 1055, 1008, 975, 935, 770 cm^{-1}. HRMS (ESI) m/z: calcd. for $C_{18}H_8F_9N_2O_2$ [M-H]$^-$: 455.0437; found: 455.0441.



2,2,2-Trifluoro-1-(6-hydroxy-1-(naphthalen-2-yl)-4,6-bis(trifluoromethyl)-1,6-dihydropyridazin-3-yl)ethanone (3x)

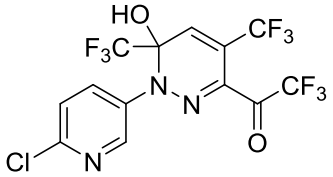
Following the general procedure and workup, and purification by column chromatography (silica gel, petroleum ether: ethyl acetate 6:1) gave final product **3x** as a yellow solid in 66% yield (90 mg). Mp: 95.8–96.7 ℃. R_f (petroleum ether: ethyl acetate 6:1) = 0.65. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.11 (s, 1H), 7.96 – 7.86 (m, 3H), 7.65 (d, *J* = 8.7 Hz, 1H), 7.58 (d, *J* = 4.6 Hz, 2H), 6.59 (s, 1H), 5.21 (br s, 1H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.4 (s, 3F), -70.7 (s, 3F), -77.9 (s, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.3 (q, *J* = 34.4 Hz), 139.6 (s), 133.0 (s), 132.8 (s), 129.3 (s), 128.6 (s), 127.8 (s), 127.4 (s), 127.1 (s), 125.7 (s), 124.4 (s), 124.2 (q, *J* = 35.4 Hz), 121.7 (q, *J* = 289.1 Hz), 120.8 (q, *J* = 6.3 Hz), 120.7 (q, *J* = 273.6 Hz), 116.5 (q, *J* = 291.0 Hz), 83.4 (q, *J* = 34.2 Hz). IR (ATR): ν 3463, 3393, 3109, 3069, 1707, 1505, 1408, 1303, 1244, 1198, 1170, 1139, 1069, 1034, 985, 959, 936, 890, 860, 808, 746, 724, 632, 474 cm^{-1}. HRMS (ESI) m/z: calcd. for $C_{18}H_8F_9N_2O_2$ $[M-H]^-$: 455.0437; found: 455.0440.



1-(1-(9*H*-Fluoren-2-yl)-6-hydroxy-4,6-bis(trifluoromethyl)-1,6-dihydropyridazin-3-yl)-2,2,2-trifluoroethan-1-one (3y)

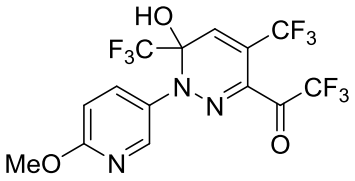
Following the general procedure and workup, and purification by column chromatography (silica gel, petroleum ether: ethyl acetate 6:1) gave final product **3y** as a yellow solid in 85% yield (126 mg). Mp: 201.4–202.3 ℃. R_f (petroleum ether: ethyl acetate 6:1) = 0.59. ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.84 (s, 1H), 8.03 (d, *J* = 8.1 Hz, 1H), 7.95 (d, *J* = 7.4 Hz, 1H), 7.79 (s, 1H), 7.61 (d, *J* = 7.2 Hz, 1H), 7.57 (d, *J*

= 7.2 Hz, 1H), 7.42 (t, *J* = 7.2 Hz, 1H), 7.37 (t, *J* = 7.2 Hz, 1H), 6.82 (s, 1H), 4.01 (s, 2H). ^{19}F NMR (376 MHz, DMSO-d_6) δ -62.0 (s, 3F), -69.5 (s, 3F), -77.8 (s, 3F). ^{13}C NMR (101 MHz, DMSO-d_6) δ 172.9 (q, *J* = 33.1 Hz), 143.6 (s), 143.5 (s), 141.7 (s), 141.1 (s), 139.8 (s), 127.5 (s), 127.0 (s), 126.1 (s), 125.6 (s), 125.2 (s), 123.5 (s), 122.8 (q, *J* = 6.5 Hz), 121.9 (q, *J* = 289.5 Hz), 121.8 (q, *J* = 35.2 Hz), 120.9 (q, *J* = 273.6 Hz), 120.6 (s), 120.2 (s), 116.4 (q, *J* = 291.7 Hz), 83.2 (q, *J* = 33.1 Hz), 36.5 (s). IR (ATR): ν 3373, 3110, 2963, 1726, 1700, 1505, 1401, 1309, 1250, 1200, 1171, 1152, 1134, 1078, 1038, 990, 951, 900, 738, 672 cm^{-1}. HRMS (ESI) m/z: calcd. for $C_{21}H_{10}F_9N_2O_2$ [M-H]$^-$: 493.0593; found: 493.0594.



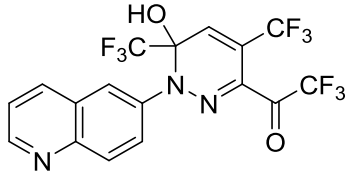
1-(1-(6-Chloropyridin-3-yl)-6-hydroxy-4,6-bis(trifluoromethyl)-1,6-dihydropyridazin-3-yl)-2,2,2-trifluoroethan-1-one (3z)

Following the general procedure and workup, and purification by column chromatography (silica gel, petroleum ether: ethyl acetate 6:1) gave final product **3z** as a white solid in 43% yield (57 mg). Mp: 163.0–164.5 ℃. R_f (petroleum ether: ethyl acetate 6:1) = 0.41. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.65 (s, 1H), 7.92 (d, *J* = 8.7 Hz, 1H), 7.45 (d, *J* = 8.8 Hz, 1H), 6.61 (s, 1H), 5.55 (br s, 1H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.3 (s, 3F), -71.0 (s, 3F), -78.1 (s, 3F). ^{13}C NMR (101 MHz, DMSO-d_6) δ 173.0 (q, *J* = 33.4 Hz), 149.8 (s), 146.9 (s), 138.6 (s), 137.2 (s), 127.6 (s), 124.8 (s), 124.2 (q, *J* = 7.1 Hz), 121.9 (q, *J* = 34.9 Hz), 121.8 (q, *J* = 290.2 Hz), 120.7 (q, *J* = 273.4 Hz), 116.2 (q, *J* = 291.8 Hz), 83.0 (q, *J* = 33.4 Hz). IR (ATR): ν 3102, 2959, 2919, 2849, 2676, 1730, 1526, 1462, 1402, 1354, 1312, 1258, 1216, 1154, 1114, 1020, 985, 936, 740 cm^{-1}. HRMS (ESI) m/z: calcd. for $C_{13}H_4ClF_9N_3O_2$ [M-H]$^-$: 439.9843; found: 439.9845.



2,2,2-Trifluoro-1-(6-hydroxy-1-(6-methoxypyridin-3-yl)-4,6-bis(trifluoromethyl)-1,6-dihydropyridazin-3-yl)ethanone (3aa)

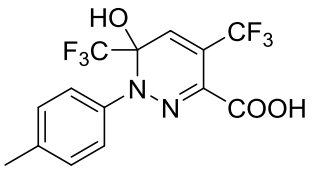
Following the general procedure and workup, and purification by column chromatography (silica gel, petroleum ether: ethyl acetate 6:1) gave final product **3aa** as a light yellow solid in 82% yield (108 mg). Mp: 123.5–124.3 ℃. R_f (petroleum ether: ethyl acetate 6:1) = 0.39. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.34 (s, 1H), 7.82 (dd, *J* = 8.9, 2.3 Hz, 1H), 6.83 (d, *J* = 8.9 Hz, 1H), 6.56 (s, 2H), 3.95 (s, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.4 (s, 3F), -70.8 (s, 3F), -78.1 (s, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.0 (q, *J* = 34.7 Hz), 163.7 (s), 144.7 (s), 137.7 (s), 133.6 (s), 127.5 (s), 124.0 (q, *J* = 35.4 Hz), 121.5 (q, *J* = 289.1 Hz), 121.3 (q, *J* = 5.8 Hz), 120.5 (q, *J* = 273.6 Hz), 116.3 (q, *J* = 291.0 Hz), 110.2 (s), 83.0 (q, *J* = 33.9 Hz), 54.5 (s). IR (ATR): ν 3101, 2953, 2852, 2751, 2630, 1722, 1621, 1523, 1496, 1386, 1297, 1211, 1154, 1017, 978, 935, 880, 841, 746 cm^{-1}. HRMS (ESI) m/z: calcd. for $C_{14}H_7F_9N_3O_3$ $[M-H]^-$: 436.0338; found: 436.0352.



2,2,2-Trifluoro-1-(6-hydroxy-1-(quinolin-6-yl)-4,6-bis(trifluoromethyl)-1,6-dihydropyridazin-3-yl)ethan-1-one (3ab)

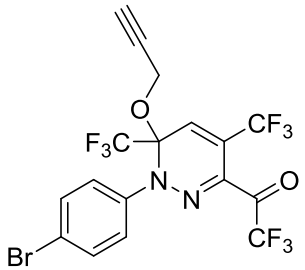
Following the general procedure and workup, and purification by column chromatography (silica gel, petroleum ether: ethyl acetate 2:1) gave final product **3ab** as a white solid in 63% yield (86 mg). Mp: 219.7–220.5 ℃. R_f (petroleum ether: ethyl acetate 2:1) = 0.68. ^{1}H NMR (400 MHz, DMSO-d_6) δ 10.01 (br s, 1H), 9.00 (s, 1H), 8.52 (d, *J* = 8.2 Hz, 1H), 8.26 (s, 1H), 8.17 (d, *J* = 9.0 Hz, 1H), 7.90 (d, *J* = 8.9 Hz, 1H), 7.63 (dd, *J* = 7.7, 3.8 Hz, 1H), 6.90 (s, 1H). ^{19}F NMR (376 MHz, DMSO-d_6) δ

-61.9 (s, 3F), -69.6 (s, 3F), -77.8 (s, 3F). ^{13}C NMR (101 MHz, DMSO-d_6) δ 173.0 (q, J = 33.6 Hz), 151.9 (s), 146.8 (s), 140.1 (s), 136.7 (s), 130.1 (s), 127.9 (s), 127.3 (s), 126.7 (s), 125.5 (s), 123.5 (q, J = 6.7 Hz), 122.5 (s), 121.9 (q, J = 290.0 Hz), 121.8 (q, J = 35.0 Hz), 120.8 (q, J = 273.0 Hz), 116.3 (q, J = 291.9 Hz), 83.3 (q, J = 33.5 Hz). IR (ATR): ν 3387, 1713, 1670, 1585, 1508, 1379, 1327, 1270, 1162, 1130, 1061, 1037, 990, 926, 799, 704, 671, 635 cm^{-1}. HRMS (ESI) m/z: calcd. for $C_{17}H_7F_9N_3O_2$ $[M-H]^-$: 456.0389; found: 456.0391.



6-Hydroxy-1-(*p*-tolyl)-4,6-bis(trifluoromethyl)-1,6-dihydropyridazine-3-carboxylic acid (4)

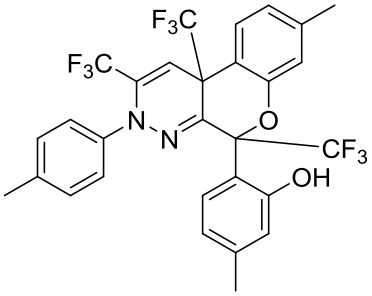
Following the procedure and workup, and purification by column chromatography (silica gel, petroleum ether: ethyl acetate 1:2) gave final product **4** as a white solid in 42% yield (46 mg). Mp: 105.9–107.5 ℃. R_f (petroleum ether: ethyl acetate 1:2) = 0.50. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41 (d, *J* = 7.7 Hz, 2H), 7.32 – 7.21 (m, 3H), 6.59 (s, 1H), 2.42 (s, 3H), COO*H* was not observed. ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.3 (s, 3F), -76.8 (s, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.0 (s), 139.8 (s), 139.5 (s), 130.0 (s), 129.7 (s), 128.1 (s), 123.8 (q, *J* = 34.2 Hz), 121.5 (q, *J* = 287.7 Hz), 121.1 (q, *J* = 7.9 Hz), 120.8 (q, *J* = 273.3 Hz), 83.2 (q, *J* = 33.0 Hz), δ 21.2 (s). IR (ATR): ν 3218, 2926, 2858, 1729, 1510, 1407, 1357, 1260, 1187, 1047, 985 cm^{-1}. HRMS (ESI) m/z: calcd. for $C_{14}H_9F_6N_2O_3$ $[M-H]^-$: 367.0512; found: 367.0523.



1-(1-(4-Bromophenyl)-6-(prop-2-yn-1-yloxy)-4,6-bis(trifluoromethyl)-1,6-dihydropyridazin-3-yl)-2,2,2-trifluoroethan-1-one (5)

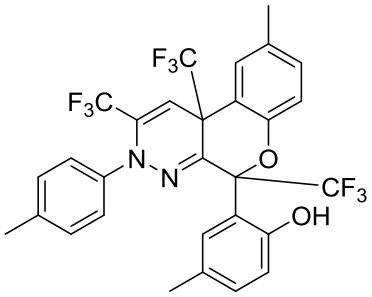
Following the procedure and workup, and purification by column chromatography (silica gel, petroleum ether: ethyl acetate 4:1) gave final product **5** as a brown solid in 38% yield (60 mg). Mp: 97.8–99.5 ℃. R_f (petroleum ether: ethyl acetate 4:1) = 0.47. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 (d, *J* = 8.6 Hz, 2H), 7.45 (d, *J* = 8.6 Hz, 2H), 6.57 (s, 1H), 4.32 (dd, *J* = 27.6, 16.0 Hz, 2H), 2.51 (s, 1H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.5 (s, 3F), -70.9 (s, 3F), -75.6 (s, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 173.7 (q, *J* = 34.9 Hz), 141.8 (s), 132.3 (s), 127.3 (s), 127.2 (q, *J* = 8.0 Hz), 123.2 (s), 120.9 (q, *J* =

289.2 Hz), 120.3 (q, *J* = 274.0 Hz), 119.6 (q, *J* = 8.0 Hz), 119.3 (q, *J* = 44.1 Hz), 116.3 (q, *J* = 291.2 Hz), 87.7 (q, *J* = 33.6 Hz), 77.3 (s), 76.2 (s), 53.0 (s). IR (ATR): ν 3305, 2930, 1732, 1519, 1488, 1405, 1275, 1215, 1166, 1052, 1013, 939, 829 cm^{-1}. HRMS (ESI) m/z: calcd. for $C_{17}H_7BrF_9N_2O_2$ $[M-H]^-$: 520.9542; found: 520.9543.



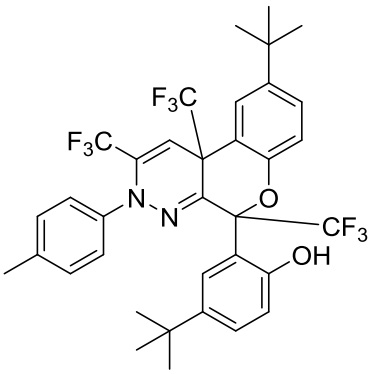
5-Methyl-2-(8-methyl-3-(*p*-tolyl)-2,5,10b-tris(trifluoromethyl)-3,10b-dihydro-5*H*-chromeno[3,4-*c*]pyridazin-5-yl)phenol (7a)

Following the general procedure and workup, and purification by column chromatography (silica gel, petroleum ether: ethyl acetate 8:1) gave final product **7a** as a white solid in 91% yield (109 mg). Mp: 182.1–183.0 ℃. R_f (petroleum ether: ethyl acetate 8:1) = 0.69. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (s, 1H), 7.50 – 7.22 (m, 6H), 7.11 (d, *J* = 7.6 Hz, 1H), 7.05 (d, *J* = 7.6 Hz, 1H), 6.81 (s, 1H), 6.70 (d, *J* = 6.1 Hz, 1H), 5.75 (s, 1H), 2.46 (s, 3H), 2.41 (s, 3H), 2.27 (s, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -61.4 (s, 3F), -73.7 (s, 3F), -77.1 (s, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 155.9 (s), 150.7 (s), 142.5 (s), 141.7 (s), 138.7 (s), 138.5 (s), 133.7 (q, *J* = 34.5 Hz), 129.7 (s), 129.6 (s), 129.3 (s), 126.3 (s), 126.0 (s), 125.6 (s), 124.4 (q, *J* = 289.5 Hz), 123.7 (q, *J* = 286.8 Hz), 120.9 (s), 119.9 (q, *J* = 274.9 Hz), 119.6 (s), 119.5 (s), 117.8 (s), 114.4 (s), 94.5 (q, *J* = 4.6 Hz), 84.8 (q, *J* = 30.8 Hz), 43.7 (q, *J* = 31.2 Hz), 21.2 (s), 21.0 (s), 20.7 (s). IR (ATR): ν 3539, 2925, 1625, 1570, 1511, 1294, 1263, 1170, 1152, 1116, 1033, 992, 811, 703 cm^{-1}. HRMS (ESI) m/z: calcd. for $C_{29}H_{20}F_9N_2O_2$ $[M-H]^-$: 599.1376; found: 599.1383.



4-Methyl-2-(9-methyl-3-(*p*-tolyl)-2,5,10b-tris(trifluoromethyl)-3,10b-dihydro-5*H*-chromeno[3,4-*c*]pyridazin-5-yl)phenol (7b)

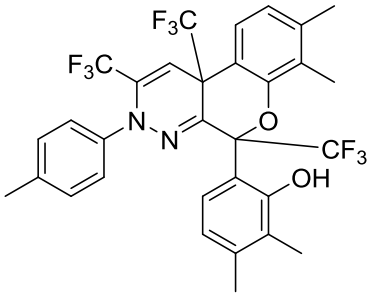
Following the general procedure and workup, and purification by column chromatography (silica gel, petroleum ether: ethyl acetate 8:1) gave final product **7b** as a white solid in 93% yield (112 mg). Mp: 221.9–222.7 ℃. R_f (petroleum ether: ethyl acetate 8:1) = 0.69. ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.54 (s, 1H), 7.72 (s, 1H), 7.25 (s, 4H), 7.16 – 7.04 (m, 3H), 6.94 (d, J = 8.2 Hz, 1H), 6.70 (d, J = 8.2 Hz, 1H), 6.17 (s, 1H), 2.31 (s, 3H), 2.27 (s, 3H), 2.13 (s, 3H). ^{19}F NMR (376 MHz, DMSO-d_6) δ -60.1 (s, 3F), -70.7 (s, 3F), -75.2 (s, 3F). ^{13}C NMR (101 MHz, DMSO-d_6) δ 154.3 (s), 149.8 (s), 139.3 (s), 137.7 (s), 133.4 (s), 131.8 (q, J = 33.1 Hz), 131.7 (s), 131.0 (s), 130.3 (s), 129.9 (s), 129.6 (s), 127.5 (s), 127.0 (s), 125.4 (s), 124.6 (q, J = 289.8 Hz), 123.8 (q, J = 286.8 Hz), 121.2 (s), 120.3 (q, J = 274.9 Hz), 119.3 (s), 119.2 (s), 117.6 (s), 96.3 (q, J = 4.4 Hz), 82.5 (q, J = 29.4 Hz), 44.6 (q, J = 30.0 Hz), 20.5 (s), 20.2 (s), 20.1 (s). IR (ATR): ν 3401, 2925, 1644, 1616, 1512, 1497, 1417, 1297, 1262, 1223, 1185, 1152, 993, 736, 703 cm^{-1}. HRMS (ESI) m/z: calcd. for $C_{29}H_{20}F_9N_2O_2$ [M-H]$^-$: 599.1376; found: 599.1382.



4-(*tert*-Butyl)-2-(9-(*tert*-butyl)-3-(*p*-tolyl)-2,5,10b-tris(trifluoromethyl)-3,10b-dihydro-5*H*-chromeno[3,4-*c*]pyridazin-5-yl)phenol (7c)

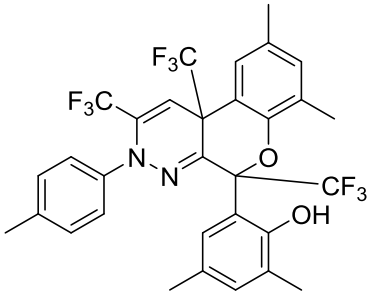
Following the general procedure and workup, and purification by column chromatography (silica gel, petroleum ether: ethyl acetate 8:1) gave final product **7c** as a white solid in 95% yield (130 mg). Mp: 209.0–209.7 ℃. R_f (petroleum ether: ethyl acetate 8:1) = 0.79. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 (s, 1H), 7.43 – 7.35 (m, 4H), 7.32 – 7.22 (m, 4H), 7.17 (s, 1H), 6.81 (d, J = 8.5 Hz, 1H), 5.61 (s, 1H), 2.42 (s, 3H), 1.31 (s, 9H), 1.18 (s, 9H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -61.2 (s, 3F), -73.8 (s, 3F), -77.0 (s, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 153.7 (s), 148.5 (s), 148.1 (s), 142.1

(s), 138.6 (s), 138.4 (s), 133.6 (q, *J* = 34.3 Hz), 129.8 (s), 129.3 (s), 128.8 (s), 128.0 (s), 126.7 (s), 125.2 (s), 124.2 (q, *J* = 289.9 Hz), 123.6 (q, *J* = 286.9 Hz), 123.4 (s), 119.9 (q, *J* = 275.2 Hz), 119.8 (s), 118.6 (s), 118.4 (s), 116.3 (s), 94.5 (q, *J* = 4.6 Hz), 84.8 (q, *J* = 30.7 Hz), 44.2 (q, *J* = 30.9 Hz), 34.7 (s), 34.1 (s), 31.3 (s), 31.2 (s), 21.1 (s). IR (ATR): ν 3543, 2964, 2871, 1577, 1511, 1494, 1295, 1265, 1174, 1094, 1034, 994, 826, 704 cm^{-1}. HRMS (ESI) m/z: calcd. for $C_{35}H_{32}F_9N_2O_2$ $[M-H]^-$: 683.2315; found: 683.2322.



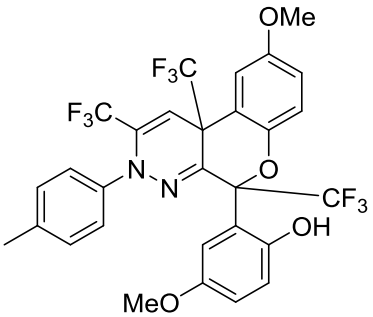
6-(7,8-Dimethyl-3-(*p*-tolyl)-2,5,10b-tris(trifluoromethyl)-3,10b-dihydro-5*H*-chromeno[3,4-*c*]pyridazin-5-yl)-2,3-dimethylphenol (7d)

Following the general procedure and workup, and purification by column chromatography (silica gel, petroleum ether: ethyl acetate 8:1) gave final product **7d** as a white solid in 86% yield (108 mg). Mp: 222.5–223.1 ℃. R_f (petroleum ether: ethyl acetate 8:1) = 0.82. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.35 (s, 1H), 7.56 (d, *J* = 7.5 Hz, 1H), 7.21 (d, *J* = 7.2 Hz, 2H), 7.15 (d, *J* = 7.2 Hz, 2H), 7.10 (d, *J* = 8.0 Hz, 1H), 6.94 (d, *J* = 7.4 Hz, 1H), 6.64 (d, *J* = 7.9 Hz, 1H), 6.09 (s, 1H), 2.30 (s, 3H), 2.15 (s, 3H), 2.10 (s, 3H), 2.09 (s, 3H), 1.97 (s, 3H). ^{19}F NMR (376 MHz, DMSO-d_6) δ -60.1 (s, 3F), -68.7 (s, 3F), -74.9 (s, 3F). ^{13}C NMR (101 MHz, DMSO-d_6) δ 153.5 (s), 149.5 (s), 139.5 (s), 139.3 (s), 139.2 (s), 137.5 (s), 132.3 (s), 131.5 (q, *J* = 32.9 Hz), 129.5 (s), 126.4 (s), 125.8 (s), 125.5 (s), 125.0 (s), 124.7 (q, *J* = 289.8 Hz), 124.6 (s), 124.0 (q, *J* = 286.8 Hz), 123.8 (s), 120.9 (s), 120.6 (s), 120.2 (q, *J* = 274.7 Hz), 118.6 (s), 82.7 (q, *J* = 28.9 Hz), 44.6 (q, *J* = 29.5 Hz), 20.5 (s), 19.9 (s), 19.4 (s), 12.7 (s), 11.7 (s). IR (ATR): ν 3424, 3052, 1650, 1513, 1266, 1188, 730, 702, 618 cm^{-1}. HRMS (ESI) m/z: calcd. for $C_{31}H_{24}F_9N_2O_2$ $[M-H]^-$: 627.1689; found: 627.1699.



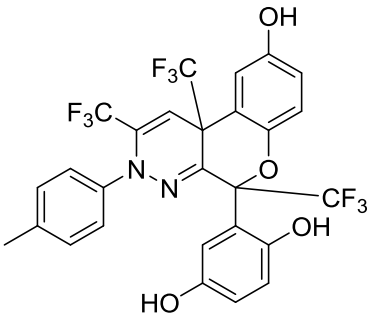
2-(7,9-Dimethyl-3-(*p*-tolyl)-2,5,10b-tris(trifluoromethyl)-3,10b-dihydro-5*H*-chromeno[3,4-*c*]pyridazin-5-yl)-4,6-dimethylphenol (7e)

Following the general procedure and workup, and purification by column chromatography (silica gel, petroleum ether: ethyl acetate 8:1) gave final product **7e** as a white solid in 85% yield (107 mg). Mp: 190.0–191.1 ℃. R_f (petroleum ether: ethyl acetate 8:1) = 0.81. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14 (s, 1H), 7.44 (d, *J* = 7.6 Hz, 2H), 7.33 (d, *J* = 7.6 Hz, 2H), 7.14 (d, *J* = 9.6 Hz, 2H), 6.97 (s, 1H), 6.90 (s, 1H), 5.78 (s, 1H), 2.60 (s, 3H), 2.46 (s, 3H), 2.35 (s, 3H), 2.26 (s, 3H), 2.20 (s, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -61.5 (s, 3F), -73.1 (s, 3F), -76.7 (s, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 152.2 (s), 147.7 (s), 138.8 (s), 138.5 (s), 133.9 (s), 133.8 (s), 133.6 (q, *J* = 34.5 Hz), 133.3 (s), 131.0 (s), 129.8 (s), 127.7 (s), 127.6 (s), 127.3 (s), 126.0 (s), 124.7 (s), 124.4 (q, *J* = 290.1 Hz), 124.0 (q, *J* = 287.2 Hz), 119.9 (q, *J* = 275.0 Hz), 119.1 (s), 116.6 (s), 94.7 (q, *J* = 4.7 Hz), 84.2 (q, *J* = 30.7 Hz), 44.1 (q, *J* = 30.4 Hz), 21.0 (s), 20.6 (s), 20.4 (s), 16.4 (s), 15.9 (s). IR (ATR): ν 3557, 3289, 2925, 1513, 1477, 1237, 1218, 1184, 1156, 1077, 1040, 992, 847 cm^{-1}. HRMS (ESI) m/z: calcd. for $C_{31}H_{24}F_9N_2O_2$ $[M-H]^-$: 627.1689; found: 627.1696.



4-Methoxy-2-(9-methoxy-3-(*p*-tolyl)-2,5,10b-tris(trifluoromethyl)-3,10b-dihydro-5*H*-chromeno[3,4-*c*]pyridazin-5-yl)phenol (7f)

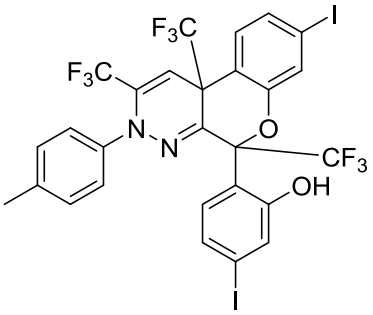
Following the general procedure and workup, and purification by column chromatography (silica gel, petroleum ether: ethyl acetate 8:1) gave final product **7f** as a light yellow solid in 83% yield (105 mg). Mp: 95.2–96.4 ℃. R_f (petroleum ether: ethyl acetate 8:1) = 0.43. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 (s, 1H), 7.47 – 7.27 (m, 5H), 7.01 (s, 1H), 6.93 (d, *J* = 8.8 Hz, 1H), 6.85 (s, 2H), 6.62 (s, 1H), 5.69 (s, 1H), 3.82 (s, 3H), 3.66 (s, 3H), 2.45 (s, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -61.4 (s, 3F), -73.2 (s, 3F), -76.7 (s, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 156.7 (s), 152.4 (s), 149.7 (s), 144.2 (s), 138.6 (s), 138.5 (s), 133.6 (q, *J* = 34.1 Hz), 129.8 (s), 128.9 (s), 125.4 (s), 124.2 (q, *J* = 289.7 Hz), 123.6 (q, *J* = 287.1 Hz), 121.8 (s), 120.0 (s), 119.9 (q, *J* = 275.0 Hz), 119.8 (s), 118.7 (s), 117.2 (s), 115.5 (s), 113.7 (s), 112.6 (s), 94.4 (q, *J* = 4.7 Hz), 85.0 (q, *J* = 30.8 Hz), 55.7 (s), 55.2 (s), 44.3 (q, *J* = 31.1 Hz), 21.1 (s). IR (ATR): ν 3525, 2940, 2840, 1579, 1511, 1494, 1432, 1270, 1223, 1191, 1175, 1072, 1039, 1026, 995, 818 cm^{-1}. HRMS (ESI) m/z: calcd. for $C_{29}H_{20}F_9N_2O_4$ $[M-H]^-$: 631.1274; found: 631.1279.



2-(9-Hydroxy-3-(*p*-tolyl)-2,5,10b-tris(trifluoromethyl)-3,10b-dihydro-5*H*-chromeno[3,4-*c*]pyridazin-5-yl)benzene-1,4-diol (7g)

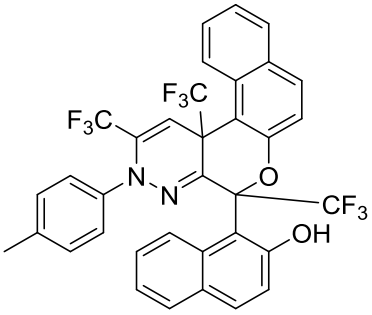
Following the general procedure and workup, and purification by column chromatography (silica gel, petroleum ether: ethyl acetate 1:1) gave final product **7g** as a white solid in 45% yield (54 mg). Mp: 244.0–245.2 ℃. R_f (petroleum ether: ethyl acetate 1: 1) = 0.36. ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.48 (s, 1H), 8.91 (d, *J* = 4.4 Hz, 2H), 7.28 (d, *J* = 7.6 Hz, 2H), 7.23 (d, *J* = 7.6 Hz, 2H), 7.15 (s, 1H), 6.95 (d, *J* = 8.4 Hz, 1H), 6.83 – 6.69 (m, 2H), 6.57 (s, 2H), 5.96 (s, 1H), 2.33 (s, 3H). ^{19}F NMR (376 MHz, DMSO-d_6) δ -60.0 (s, 3F), -70.8 (s, 3F), -75.2 (s, 3F). ^{13}C NMR (101 MHz, DMSO-d_6) δ 153.7 (s), 149.8 (s), 149.1 (s), 148.9 (s), 144.0 (s), 139.3 (s), 137.7 (s),

131.7 (q, *J* = 33.1 Hz), 130.3 (s), 129.6 (s), 125.4 (s), 124.5 (q, *J* = 289.7 Hz), 123.7 (q, *J* = 287.2 Hz), 122.5 (s), 120.4 (s), 120.1 (q, *J* = 275.0 Hz), 119.4 (s), 118.3 (s), 117.0 (s), 115.7 (s), 113.2 (s), 95.5 (q, *J* = 4.3 Hz), 82.3 (q, *J* = 29.0 Hz), 44.5 (q, *J* = 29.9 Hz), 20.6 (s). IR (ATR): ν 3420, 3050, 1656, 1512, 1266, 1189, 822, 729, 700, 615 cm^{-1}. HRMS (ESI) m/z: calcd. for $C_{27}H_{16}F_9N_2O_4$ $[M-H]^-$: 603.0961; found: 603.0969.



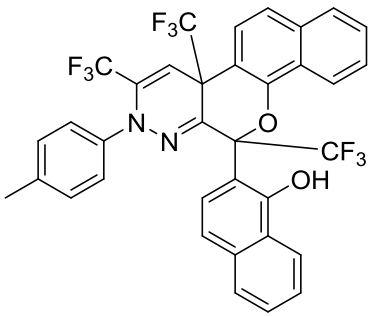
5-Iodo-2-(8-iodo-3-(*p*-tolyl)-2,5,10b-tris(trifluoromethyl)-3,10b-dihydro-5*H*-chromeno[3,4-*c*]pyridazin-5-yl)phenol (7h)

Following the general procedure and workup, and purification by column chromatography (silica gel, petroleum ether: ethyl acetate 8:1) gave final product **7h** as a white solid in 55% yield (91 mg). Mp: 237.0–237.4 ℃. R_f (petroleum ether: ethyl acetate 8:1) = 0.72. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94 (s, 1H), 7.75 (s, 1H), 7.61 (d, *J* = 7.8 Hz, 1H), 7.43 – 7.15 (m, 7H), 6.89 (d, *J* = 8.0 Hz, 1H), 5.64 (s, 1H), 2.45 (s, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -61.6 (s, 3F), -73.9 (s, 3F), -77.0 (s, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 156.2 (s), 151.0 (s), 139.0 (s), 138.2 (s), 134.6 (s), 134.0 (q, *J* = 34.4 Hz), 130.4 (s), 129.9 (s), 129.3 (s), 128.7 (s), 128.5 (s), 128.4 (s), 128.0 (s), 125.8 (s), 123.9 (q, *J* = 290.0 Hz), 123.1 (q, *J* = 287.3 Hz), 120.6 (s), 119.6 (q, *J* = 275.1 Hz), 117.0 (s), 97.9 (s), 95.8 (s), 93.6 (q, *J* = 4.9 Hz), 84.5 (q, *J* = 31.4 Hz), 43.7 (q, *J* = 31.2 Hz), 21.2 (s). IR (ATR): ν 3545, 3047, 1596, 1556, 1512, 1479, 1400, 1265, 1224, 1190, 1155, 1066, 1021, 990, 933, 862, 811, 705 cm^{-1}. HRMS (ESI) m/z: calcd. for $C_{27}H_{14}F_9I_2N_2O_2$ $[M-H]^-$: 822.8995; found: 822.9001.



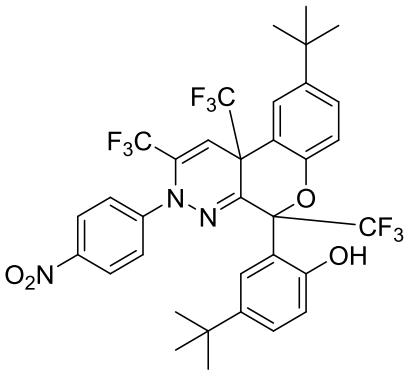
1-(3-(*p*-Tolyl)-2,5,12c-tris(trifluoromethyl)-3,12c-dihydro-5*H*-benzo[5,6]chromeno[3,4-*c*]pyridazin-5-yl)naphthalen-2-ol (7i)

Following the general procedure and workup, and purification by column chromatography (silica gel, petroleum ether: ethyl acetate 4:1) gave final product **7i** as a white solid in 72% yield (97 mg). Mp: 267.0–268.1 ℃. R_f (petroleum ether: ethyl acetate 4:1) = 0.42. ^{1}H NMR (400 MHz, DMSO-d_6) δ 10.04 (s, 1H), 8.35 (d, J = 6.5 Hz, 1H), 8.06 (d, J = 7.8 Hz, 1H), 7.92 (d, J = 6.8 Hz, 1H), 7.86 – 7.58 (m, 6H), 7.55 – 7.36 (m, 5H), 7.18 – 7.05 (m, 2H), 6.23 (s, 1H), 2.37 (s, 3H). ^{19}F NMR (376 MHz, DMSO-d_6) δ -60.1 (s, 3F), -72.4 (s, 3F), -73.8 (s, 3F). ^{13}C NMR (101 MHz, DMSO-d_6) δ 157.0 (s), 151.0 (s), 138.2 (s), 134.8 (s), 133.1 (s), 132.1 (q, J = 67.9, 33.9 Hz), 131.3 (s), 130.2 (s), 130.0 (s), 129.8 (s), 129.5 (s), 128.5 (s), 127.9 (s), 127.2 (s), 126.9 (s), 126.5 (s), 126.3 (s), 125.1 (s), 124.7 (s), 124.2 (s), 123.6 (s), 123.0 (q, J = 285.9 Hz), 120.6 (s), 120.0 (q, J = 275.4 Hz), 119.8 (s), 112.9 (s), 108.3 (s), 93.8 (q, J = 4.3 Hz), 82.1 (q, J = 29.7 Hz), 44.9 (q, J = 31.2 Hz), 20.6 (s). IR (ATR): ν 3362, 3054, 1631, 1605, 1512, 1396, 1292, 1265, 1230, 1190, 1086, 989, 730, 703 cm^{-1}. HRMS (ESI) m/z: calcd. for $C_{35}H_{20}F_9N_2O_2$ [M-H]$^-$: 671.1376; found: 671.1395.



2-(2-(*p*-Tolyl)-3,4a,12-tris(trifluoromethyl)-2,4a-dihydro-12*H*-benzo[7,8]chromeno[3,4-*c*]pyridazin-12-yl)naphthalen-1-ol (7j)

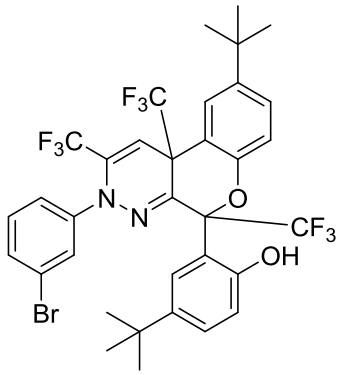
Following the general procedure and workup, and purification by column chromatography (silica gel, *n*-pentane: dichloromethane 1:1) gave final product **7j** as a white solid in 60% yield (81 mg). Mp: 240.6–241.1 ℃. R_f (*n*-pentane: dichloromethane 1:1) = 0.77. ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.71 (s, 1H), 8.26 – 8.18 (m, 1H), 8.12 – 8.01 (m, 2H), 7.91 – 7.85 (m, 1H), 7.80 (d, *J* = 8.7 Hz, 1H), 7.74 (d, *J* = 7.9 Hz, 2H), 7.55 – 7.36 (m, 5H), 7.19 (s, 4H), 6.37 (s, 1H), 2.27 (s, 3H). ^{19}F NMR (376 MHz, DMSO-d_6) δ -59.9 (s, 3F), -68.7 (s, 3F), -74.3 (s, 3F). ^{13}C NMR (101 MHz, DMSO-d_6) δ 152.3 (s), 147.8 (s), 139.4 (s), 137.6 (s), 134.4 (s), 134.0 (s), 132.1 (s), 131.7 (q, *J* = 33.2 Hz), 129.5 (s), 127.6 (s), 127.6 (s), 127.5 (s), 127.4 (s), 126.7 (s), 125.6 (s), 125.4 (s), 125.3 (s), 125.0 (s), 124.9 (d, *J* = 290.0 Hz), 124.1 (q, *J* = 287.3 Hz), 123.4 (s), 122.9 (s), 121.6 (s), 120.3 (d, *J* = 274.8 Hz), 119.4 (s), 117.4 (s), 116.0 (s), 96.8 (q, *J* = 4.5 Hz), 82.7 (q, *J* = 28.8 Hz), 44.9 (q, *J* = 29.6 Hz), 20.5 (s). IR (ATR): ν 3388, 2258, 1648, 1512, 1397, 1265, 1188, 1091, 997, 808, 753 cm^{-1}. HRMS (ESI) m/z: calcd. for $C_{35}H_20F_9N_2O_2$ [M-H]$^-$: 671.1376; found: 671.1387.



4-(*tert*-Butyl)-2-(9-(*tert*-butyl)-3-(4-nitrophenyl)-2,5,10b-tris(trifluoromethyl)-3,10b-dihydro-5*H*-chromeno[3,4-*c*]pyridazin-5-yl)phenol (7k)

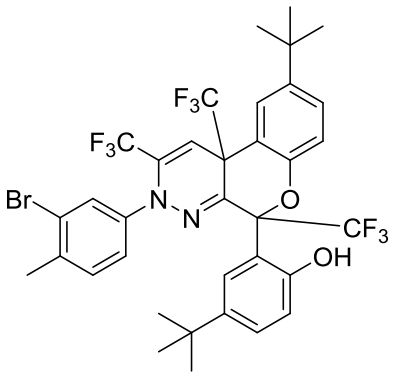
Following the general procedure and workup, and purification by column chromatography (silica gel, petroleum ether: ethyl acetate 8:1) gave final product **7k** as a white solid in 89% yield (127 mg). Mp: 182.0–183.0 ℃. R_f (petroleum ether: ethyl acetate 8:1) = 0.65. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.37 (d, *J* = 8.2 Hz, 2H), 7.66 (d, *J* = 8.3 Hz, 2H), 7.51 (s, 1H), 7.42 (s, 2H), 7.33 – 7.22 (m, 2H), 7.00 (s, 1H), 6.83 (d, *J* = 8.5 Hz, 1H), 5.87 (s, 1H), 1.32 (s, 9H), 1.16 (s, 9H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -60.0 (s, 3F), -73.5 (s, 3F), -76.2 (s, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ

153.6 (s), 148.6 (s), 148.2 (s), 146.3 (s), 145.9 (s), 142.3 (s), 133.1 (q, *J* = 35.0 Hz), 132.4 (s), 129.3 (s), 128.5 (s), 126.3 (s), 125.1 (s), 123.9 (q, *J* = 289.3 Hz), 123.7 (s), 123.5 (s), 123.4 (q, *J* = 287.0 Hz), 119.9 (q, *J* = 275.6 Hz), 118.9 (s), 118.6 (s), 118.5 (s), 115.5 (s), 99.5 (q, *J* = 3.7 Hz), 85.2 (q, *J* = 30.9 Hz), 45.0 (q, *J* = 30.8 Hz), 34.7 (s), 34.0 (s), 31.3 (s), 31.2 (s). IR (ATR): ν 3546, 2964, 2871, 1596, 1526, 1495, 1344, 1296, 1266, 1192, 1175, 1144, 1110, 1067, 1031, 995, 857, 830, 704 cm^{-1}. HRMS (ESI) m/z: calcd. for $C_{34}H_{29}F_9N_3O_4$ $[M-H]^-$: 714.2009; found: 714.2026.



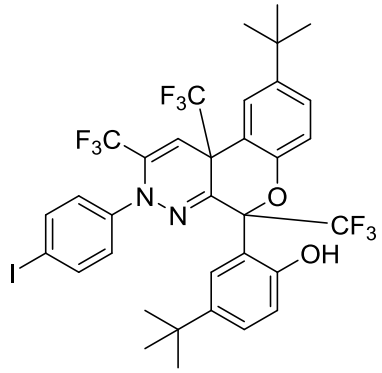
2-(3-(3-Bromophenyl)-9-(*tert*-butyl)-2,5,10b-tris(trifluoromethyl)-3,10b-dihydro-5*H*-chromeno[3,4-*c*]pyridazin-5-yl)-4-(*tert*-butyl)phenol (7l)

Following the general procedure and workup, and purification by column chromatography (silica gel, petroleum ether: ethyl acetate 8:1) gave final product **7l** as a white solid in 91% yield (136 mg). Mp: 152.5–153.3 ℃. R_f (petroleum ether: ethyl acetate 8:1) = 0.72. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 (s, 2H), 7.56 – 7.24 (m, 7H), 7.11 (s, 1H), 6.84 (d, *J* = 8.4 Hz, 1H), 5.74 (s, 1H), 1.33 (s, 9H), 1.20 (s, 9H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -60.8 (s, 3F), -73.5 (s, 3F), -76.6 (s, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 153.7 (s), 148.4 (s), 148.3 (s), 142.2 (s), 142.1 (s), 133.4 (q, *J* = 34.4 Hz), 131.2 (s), 130.5 (s), 129.0 (s), 128.2 (s), 128.1 (s), 126.5 (s), 124.1 (q, *J* = 290.0 Hz), 123.6 (q, *J* = 287.2 Hz), 123.5 (s), 122.5 (s), 119.9 (q, *J* = 275.3 Hz), 119.4 (s), 118.6 (s), 118.5 (s), 115.9 (s), 96.3 (q, *J* = 4.5 Hz), 85.1 (q, *J* = 31.0 Hz), 44.5 (q, *J* = 30.8 Hz), 34.7 (s), 34.0 (s), 31.3 (s), 31.2 (s). IR (ATR): ν 3543, 2964, 2871, 1589, 1498, 1477, 1296, 1265, 1191, 1174, 1035, 995, 830, 704 cm^{-1}. HRMS (ESI) m/z: calcd. for $C_{34}H_{29}BrF_9N_2O_2$ $[M-H]^-$: 749.1243; found: 749.1259.



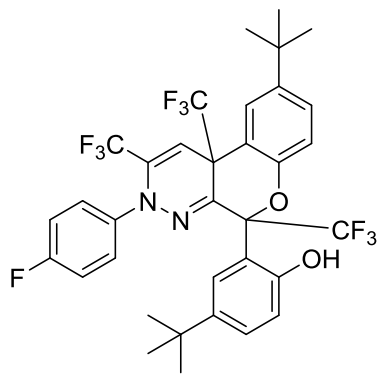
2-(3-(3-Bromo-4-methylphenyl)-9-(*tert*-butyl)-2,5,10b-tris(trifluoromethyl)-3,10b-dihydro-5*H*-chromeno[3,4-*c*]pyridazin-5-yl)-4-(*tert*-butyl)phenol (7m)

Following the general procedure and workup, and purification by column chromatography (silica gel, petroleum ether: ethyl acetate 8:1) gave final product **7m** as a white solid in 86% yield (131 mg). Mp: 192.8–194.0 ℃. R_f (petroleum ether: ethyl acetate 8:1) = 0.77. ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.64 (s, 1H), 7.80 (s, 1H), 7.56 (s, 1H), 7.44 – 7.25 (m, 4H), 7.16 (t, J = 6.3 Hz, 2H), 6.75 (d, J = 7.8 Hz, 1H), 6.37 (s, 1H), 2.33 (s, 3H), 1.26 (s, 9H), 1.14 (s, 9H). ^{19}F NMR (376 MHz, DMSO-d_6) δ -59.4 (s, 3F), -71.3 (s, 3F), -75.4 (s, 3F). ^{13}C NMR (101 MHz, DMSO-d_6) δ 154.4 (s), 149.6 (s), 146.8 (s), 140.4 (s), 140.3 (s), 137.3 (s), 131.7 (q, J = 33.6 Hz), 131.3 (s), 130.6 (s), 128.0 (s), 127.9 (s), 127.3 (s), 126.7 (s), 124.5 (q, J = 289.4 Hz), 124.4 (s), 123.9 (s), 123.8 (s), 123.6 (q, J = 286.8 Hz), 120.1 (s), 120.0 (q, J = 275.4 Hz), 118.9 (s), 117.9 (s), 117.4 (s), 97.5 (q, J = 2.8 Hz), 82.8 (q, J = 29.7 Hz), 44.8 (q, J = 30.0 Hz), 34.4 (s), 33.6 (s), 31.1 (s), 31.0 (s), 21.9 (s). IR (ATR): ν 3389, 2963, 2258, 1648, 1493, 1298, 1269, 1190, 1114, 995 cm^{-1}. HRMS (ESI) m/z: calcd. for $C_{35}H_{31}BrF_9N_2O_2$ [M-H]$^-$: 761.1420; found: 761.1417.



4-(*tert*-Butyl)-2-(9-(*tert*-butyl)-3-(4-iodophenyl)-2,5,10b-tris(trifluoromethyl)-3,10 b-dihydro-5*H*-chromeno[3,4-*c*]pyridazin-5-yl)phenol (7n)

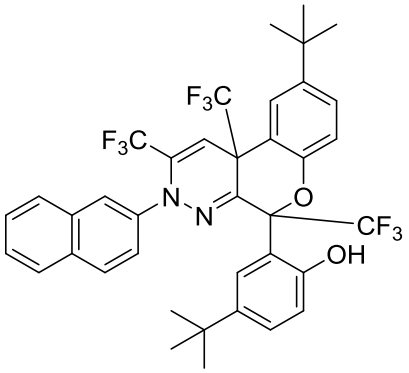
Following the general procedure and workup, and purification by column chromatography (silica gel, petroleum ether: ethyl acetate 8:1) gave final product **7n** as a white solid in 92% yield (146 mg). Mp: 231.0–232.0 ℃. R_f (petroleum ether: ethyl acetate 8:1) = 0.76. ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.62 (s, 1H), 7.97 – 7.74 (m, 3H), 7.36 (d, J = 7.2 Hz, 1H), 7.28 – 7.08 (m, 5H), 6.75 (d, J = 8.4 Hz, 1H), 6.39 (s, 1H), 1.26 (s, 9H), 1.13 (s, 9H). ^{19}F NMR (376 MHz, DMSO-d_6) δ -59.2 (s, 3F), -71.1 (s, 3F), -75.4 (s, 3F). ^{13}C NMR (101 MHz, DMSO-d_6) δ 154.4 (s), 149.6 (s), 146.8 (s), 141.3 (s), 140.3 (s), 138.2 (s), 131.6 (q, J = 34.2 Hz), 130.9 (s), 128.1 (s), 127.3 (s), 126.8 (s), 126.4 (s), 124.4 (s), 124.3 (q, J = 291.0 Hz), 123.6 (q, J = 286.9 Hz), 120.3 (s), 120.1 (q, J = 275.3 Hz), 119.0 (s), 117.7 (s), 117.5 (s), 97.7 (q, J = 2.9 Hz), 93.3 (s), 82.8 (q, J = 29.6 Hz), 44.9 (q, J = 29.7 Hz), 34.4 (s), 33.6 (s), 31.1 (s), 31.0 (s). IR (ATR): ν 3380, 2963, 1641, 1486, 1414, 1296, 1265, 1190, 1173, 995, 940, 734, 704 cm^{-1}. HRMS (ESI) m/z: calcd. for $C_{34}H_{29}F_9IN_2O_2$ [M-H]$^-$: 795.1125; found: 795.1143.



4-(*tert*-Butyl)-2-(9-(*tert*-butyl)-3-(4-fluorophenyl)-2,5,10b-tris(trifluoromethyl)-3,

10b-dihydro-5*H*-chromeno[3,4-*c*]pyridazin-5-yl)phenol (7o)

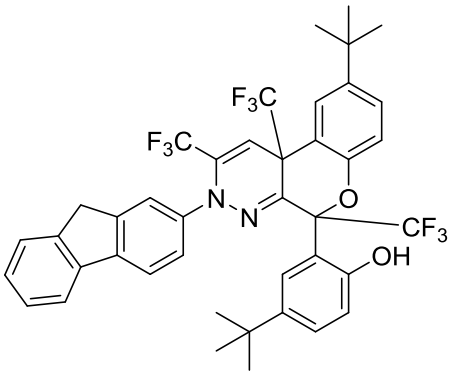
Following the general procedure and workup, and purification by column chromatography (silica gel, petroleum ether: ethyl acetate 8:1) gave final product **7o** as a white solid in 93% yield (128 mg). Mp: 151.5–152.3 ℃. R_f (petroleum ether: ethyl acetate 8:1) = 0.76. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 (s, 1H), 7.62 – 7.48 (m, 4H), 7.40 (d, *J* = 8.3 Hz, 1H), 7.33 (d, *J* = 8.4 Hz, 1H), 7.26 (s, 1H), 7.19 (t, *J* = 7.4 Hz, 2H), 6.92 (d, *J* = 8.3 Hz, 1H), 5.82 (s, 1H), 1.38 (s, 9H), 1.27 (s, 9H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -61.3 (s, 3F), -73.6 (s, 3F), -76.9 (s, 3F), -112.5 (s, 1F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.2 (d, *J* = 248.7 Hz), 153.8 (s), 148.5 (s), 148.3 (s), 142.2 (s), 137.1 (d, *J* = 2.8 Hz), 133.6 (q, *J* = 34.3 Hz), 130.1 (s), 129.0 (s), 128.2 (s), 127.4 (d, *J* = 8.7 Hz), 126.6 (s), 124.3 (q, *J* = 289.8 Hz), 123.7 (q, *J* = 286.9 Hz), 123.5 (s), 119.9 (q, *J* = 275.0 Hz), 119.7 (s), 118.7 (s), 118.6 (s), 116.3 (d, *J* = 23.2 Hz), 116.2 (s), 95.1 (q, *J* = 4.4 Hz), 85.1 (q, *J* = 30.7 Hz), 44.4 (q, *J* = 31.0 Hz), 34.6 (s), 34.1 (s), 31.2 (s). IR (ATR): ν 3546, 2965, 2872, 1508, 1295, 1266, 1192, 1175, 1151, 1094, 1033, 995, 831, 705 cm^{-1}. HRMS (ESI) m/z: calcd. for $C_{34}H_{29}F_{10}N_2O_2$ [M-H]$^-$: 687.2064; found: 687.2081.



4-(*tert*-Butyl)-2-(9-(*tert*-butyl)-3-(naphthalen-2-yl)-2,5,10b-tris(trifluoromethyl)-3 ,10b-dihydro-5*H*-chromeno[3,4-*c*]pyridazin-5-yl)phenol (7p)

Following the general procedure and workup, and purification by column chromatography (silica gel, petroleum ether: ethyl acetate 8:1) gave final product **7p** as a white solid in 85% yield (122 mg). Mp: 222.8–223.5 ℃. R_f (petroleum ether: ethyl acetate 8:1) = 0.72. ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.68 (s, 1H), 8.05 (d, *J* = 8.6 Hz, 1H), 8.02 – 7.97 (m, 2H), 7.87 (s, 1H), 7.84 (s, 1H), 7.67 – 7.52 (m, 3H), 7.37

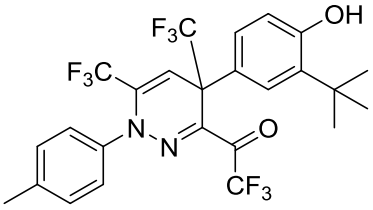
(d, J = 8.1 Hz, 1H), 7.28 (s, 1H), 7.18 (s, 2H), 6.78 (d, J = 8.3 Hz, 1H), 6.43 (s, 1H), 1.26 (s, 9H), 1.15 (s, 9H). ^{19}F NMR (376 MHz, DMSO-d_6) δ -59.2 (s, 3F), -71.0 (s, 3F), -75.4 (s, 3F). ^{13}C NMR (101 MHz, DMSO-d_6) δ 154.5 (s), 149.6 (s), 146.8 (s), 140.3 (s), 138.8 (s), 132.6 (s), 132.1 (q, J = 34.0 Hz), 132.0 (s), 130.4 (s), 129.4 (s), 128.1 (s), 127.9 (s), 127.7 (s), 127.3 (s), 127.1 (s), 126.9 (s), 126.8 (s), 124.5 (q, J = 289.9 Hz), 124.4 (s), 123.7 (q, J = 286.4 Hz), 123.0 (q, J = 275.5 Hz), 122.8 (s), 122.6 (s), 120.4 (s), 118.9 (s), 117.9 (s), 117.5 (s), 97.1 (q, J = 4.6 Hz), 83.0 (q, J = 30.4 Hz), 44.8 (q, J = 29.3 Hz), 34.5 (s), 33.6 (s), 31.1 (s), 31.0 (s). IR (ATR): ν 3395, 2963, 1632, 1601, 1500, 1398, 1297, 1265, 1223, 1171, 996, 736, 703 cm^{-1}. HRMS (ESI) m/z: calcd. for $C_{38}H_{32}F_9N_2O_2$ [M-H]$^-$: 719.2315; found: 719.2332.



2-(3-(2-9*H*-Fluorene)-9-(*tert*-butyl)-2,5,10b-tris(trifluoromethyl)-3,10b-dihydro-5*H*-chromeno[3,4-*c*]pyridazin-5-yl)-4-(*tert*-butyl)phenol (7q)

Following the general procedure and workup, and purification by column chromatography (silica gel, petroleum ether: ethyl acetate 8:1) gave final product **7q** as a white solid in 89% yield (135 mg). Mp: 150.0–151.5 ℃. R_f (petroleum ether: ethyl acetate 8:1) = 0.72. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 (s, 1H), 7.86 – 7.75 (m, 2H), 7.71 (s, 1H), 7.63 – 7.53 (m, 3H), 7.50 – 7.31 (m, 6H), 6.94 (d, J = 8.2 Hz, 1H), 5.80 (s, 1H), 3.88 (s, 2H), 1.38 (s, 9H), 1.30 (s, 9H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -60.9 (s, 3F), -73.5 (s, 3F), -76.8 (s, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 153.8 (s), 148.5 (s), 148.2 (s), 144.2 (s), 143.6 (s), 142.2 (s), 141.9 (s), 140.5 (s), 139.5 (s), 133.7 (q, J = 34.1 Hz), 129.5 (s), 128.9 (s), 128.1 (s), 127.2 (s), 126.9 (s), 126.8 (s), 125.0 (s), 124.4 (q, J = 289.8 Hz), 124.2 (s), 123.8 (q, J = 286.9 Hz), 123.5 (s), 122.1

(s), 120.2 (s), 120.0 (q, J = 276.1 Hz), 119.8 (s), 118.7 (s), 118.5 (s), 116.3 (s), 94.8 (q, J = 4.5 Hz), 85.0 (q, J = 30.7 Hz), 44.4 (q, J = 30.7 Hz), 36.8 (s), 34.6 (s), 34.1 (s), 31.3 (s), 31.3 (s). IR (ATR): ν 3542, 3055, 2964, 1580, 1491, 1459, 1397, 1296, 1265, 1176, 1036, 995, 829, 704 cm^{-1}. HRMS (ESI) m/z: calcd. for $C_{41}H_{34}F_9N_2O_2$ $[M-H]^-$: 757.2471; found: 757.2464.



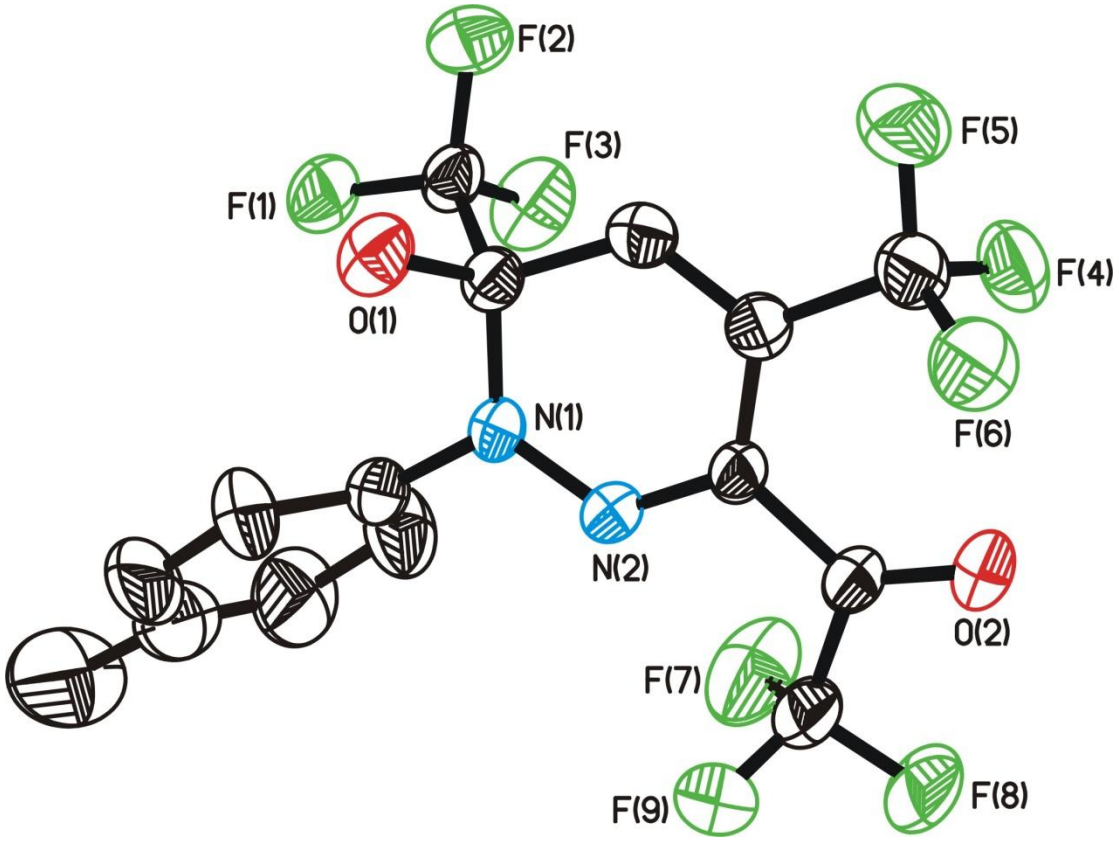
1-(4-(3-(*tert*-butyl)-4-hydroxyphenyl)-1-(*p*-tolyl)-4,6-bis(trifluoromethyl)-1,4-dihydropyridazin-3-yl)-2,2,2-trifluoroethan-1-one (8)

Obtained as a yellow solid in 78% yield (86 mg). Mp: 175.0–176.6 ℃. R_f (petroleum ether: ethyl acetate 8: 1) = 0.56. ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.81 (s, 1H), 7.33 (s, 4H), 7.13 (s, 1H), 7.08 (d, J = 7.6 Hz, 1H), 6.91 (d, J = 7.6 Hz, 1H), 6.03 (s, 1H), 2.35 (s, 3H), 1.33 (s, 9H). ^{19}F NMR (376 MHz, DMSO-d_6) δ -61.7 (s, 3F), -67.9 (s, 3F), -70.7 (s, 3F). ^{13}C NMR (101 MHz, DMSO-d_6) δ 175.6 (q, J = 33.1 Hz), 155.8 (s), 139.7 (s), 138.7 (s), 135.4 (s), 129.9 (s), 128.3 (q, J = 33.8 Hz), 128.1 (s), 128.0 (s), 126.4 (s), 126.2 (s), 125.2 (s), 124.8 (q, J = 286.9 Hz), 119.2 (q, J = 273.9 Hz), 116.6 (s), 116.0 (q, J = 292.0 Hz), 108.6 (s), 48.1 (q, J = 28.9 Hz), 34.4 (s), 29.0 (s), 20.6 (s). IR (ATR): ν 3446, 3050, 2981, 1511, 1422, 1267, 1178, 1162, 729, 701 cm^{-1}. HRMS (ESI) m/z: calcd. for $C_{25}H_{20}F_9N_2O_2$ $[M-H]^-$: 551.1376; found: 551.1389.

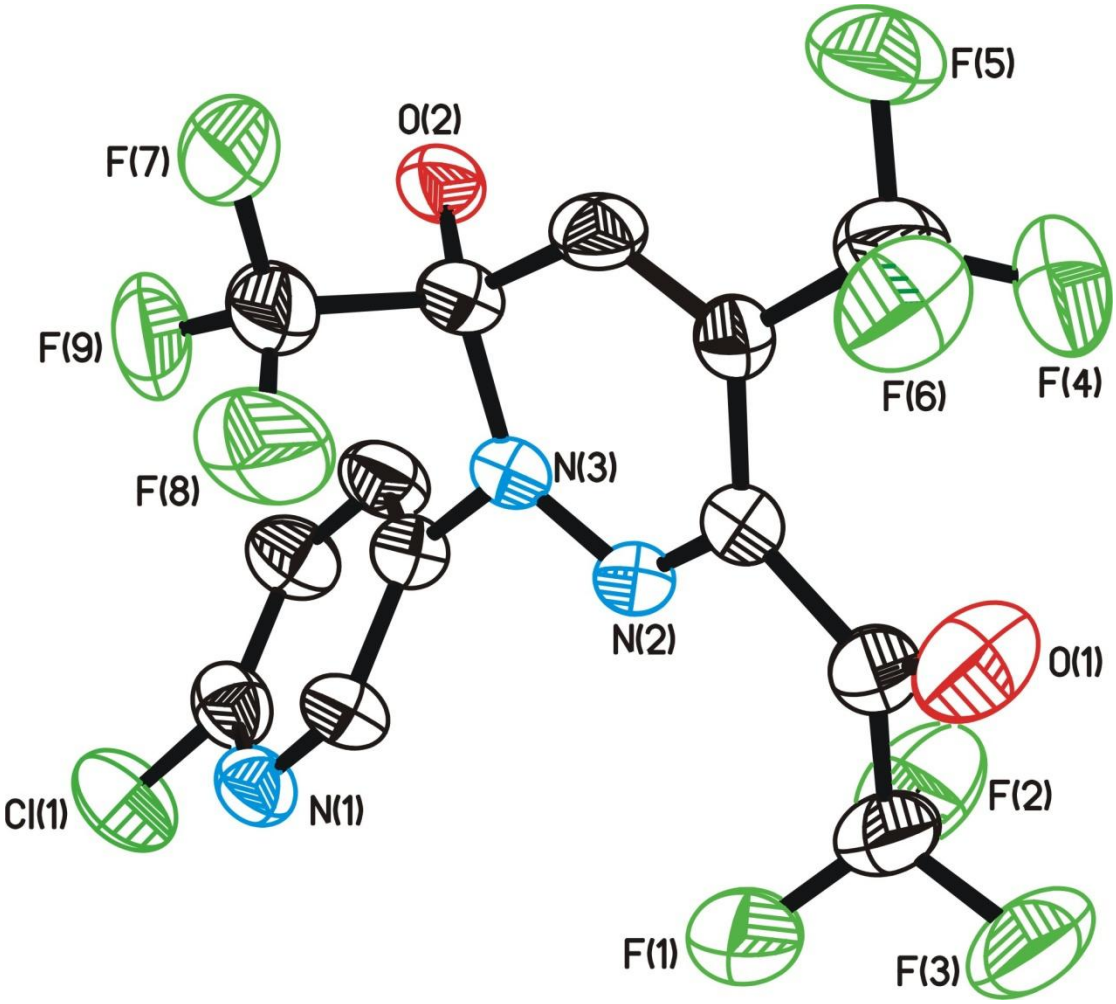
Crystal structure analyses.

The suitable crystals of **3c** (CCDC 2013786), **3z** (CCDC 2013787), **7c** (CCDC 2013788), and **8** (CCDC 2032426) were mounted on quartz fibers and X-ray data collected on a Bruker AXS APEX diffractometer, equipped with a CCD detector at -50 ºC, using MoKα radiation (λ 0.71073 Å). The data was corrected for Lorentz and polarisation effect with the **SMART** suite of programs and for absorption effects with SADABS.[3] Structure solution and refinement were carried out with the SHELXTL suite of programs.[3] The structure was solved by direct methods to locate the heavy atoms, followed by difference maps for the light non-hydrogen atoms.

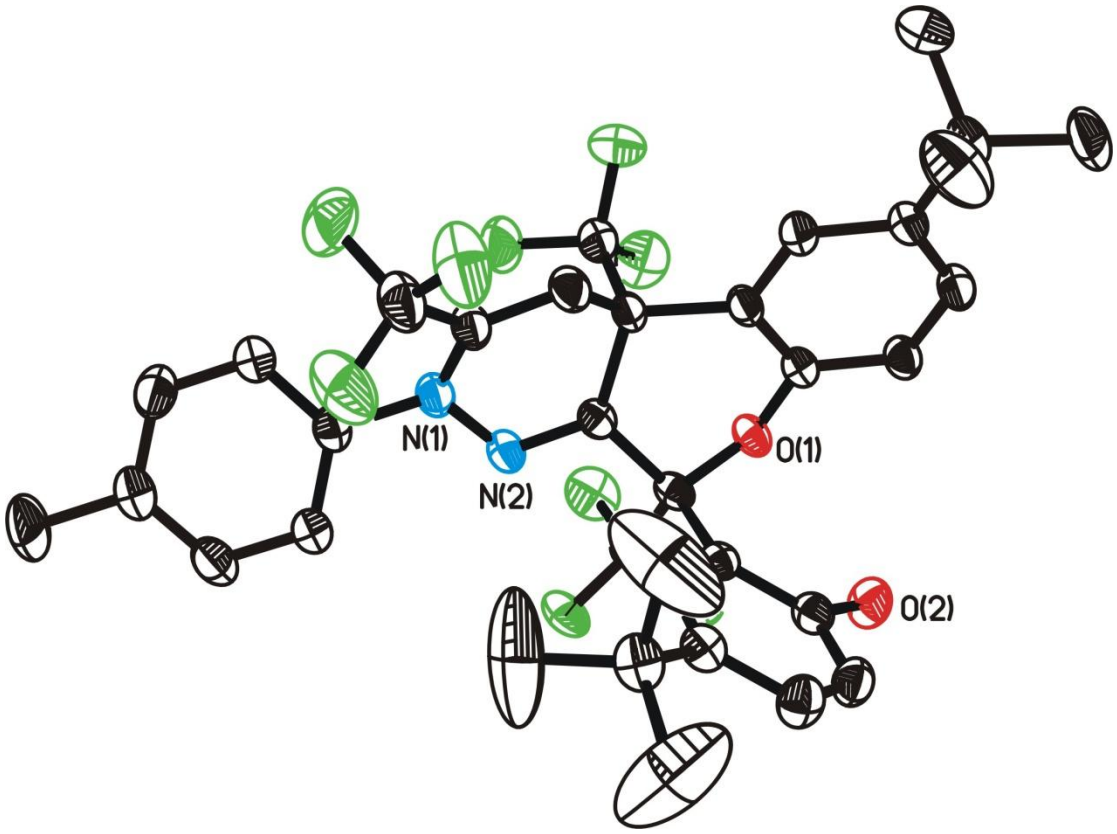
ORTEP diagrams



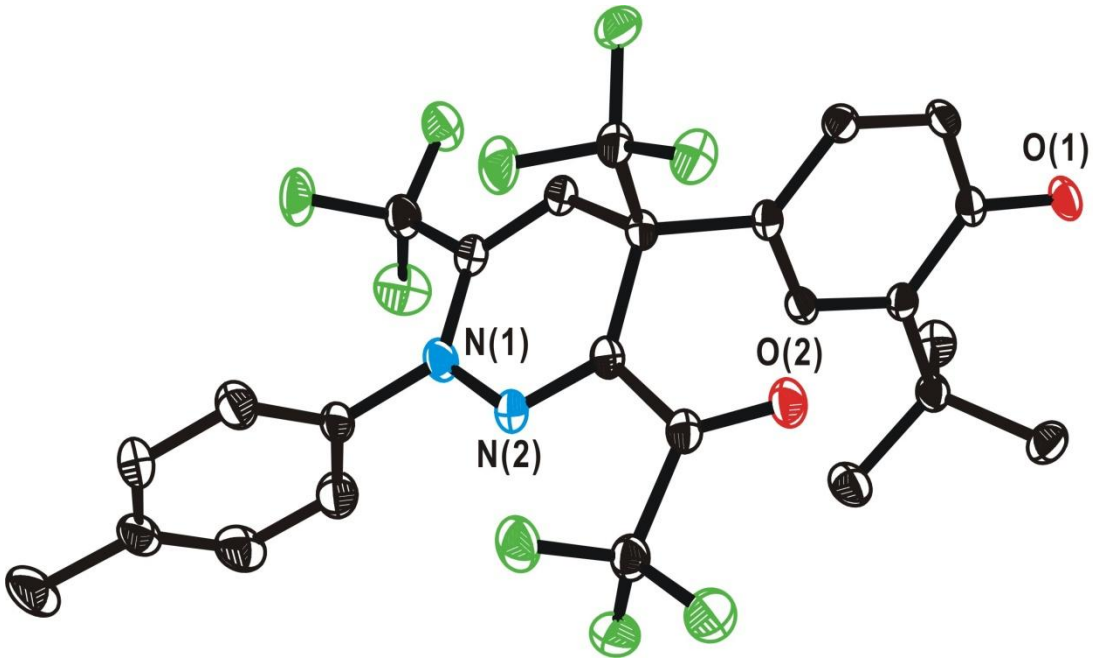
ORTEP diagram of compound **3c**. Thermal ellipsoids are drawn at 40% probability.



ORTEP diagram of compound **3z**. Thermal ellipsoids are drawn at 40% probability.



ORTEP diagram of compound **7c**. Thermal ellipsoids are drawn at 40% probability.



ORTEP diagram of compound **8**. Thermal ellipsoids are drawn at 40% probability.

References:

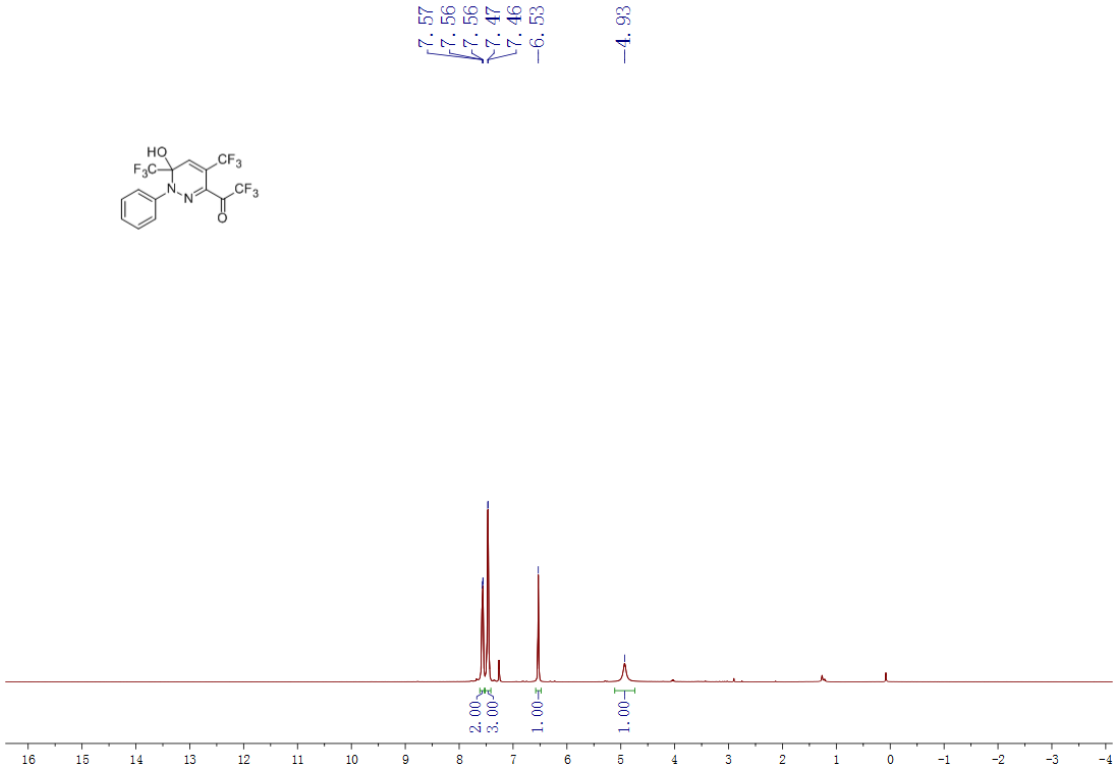
(1) (a) Reay, A. J.; Hammarback, L. A.; Bray, J. T. W.; Sheridan, T.; Turnbull, D.; Whitwood, A. C.; Fairlamb, I. J. S. *ACS Catalysis* **2017**, *7*, 5174; (b) Wang, M.; Fan, Q.; Jiang, X. *Green Chem.* **2018**, *20*, 5469; (c) Yang, Y.-M.; Yao, J.-F.; Yan, W.; Luo, Z.; Tang, Z.-Y. *Org. Lett.* **2019**, *21*, 8003.

(2) Khudina, O. G.; Shchegol'kov, E. V.; Burgart, Y. V.; Kodess, M. I.; Kazheva, O. N.; Chekhlov, A. N.; Shilov, G. V.; Dyachenko, O. A.; Saloutin, V. I.; Chupakhin, O. N. *J. Fluorine Chem.* **2005**, *126*, 1230.

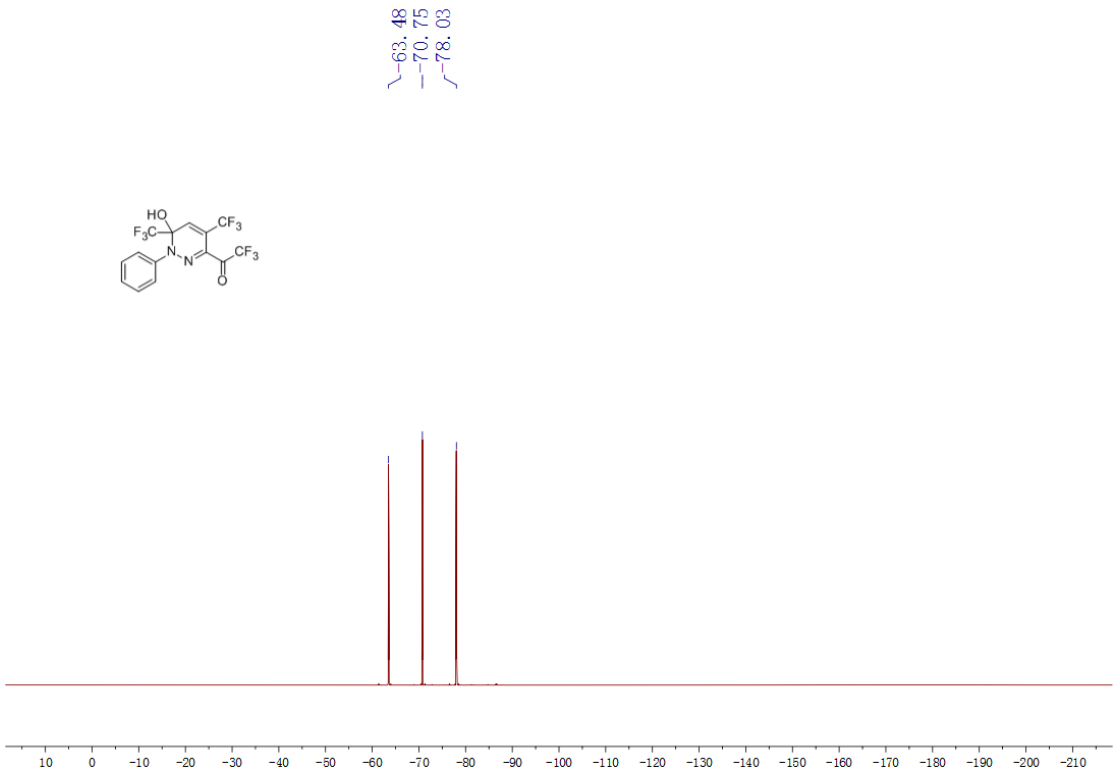
(3) SHELXTL version 5.03; Bruker Analytical X-ray Systems, Madison, WI, 1997.

Copies of ^{1}H NMR, ^{13}C NMR and ^{19}F NMR spectra

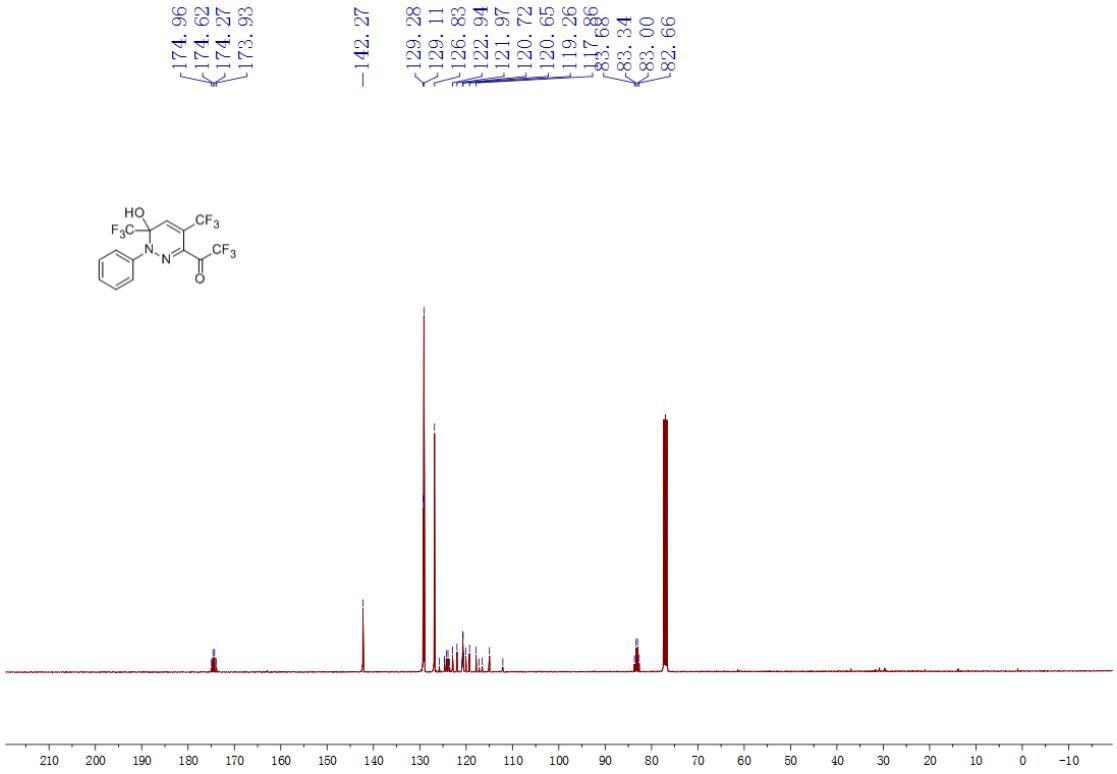
^{1}H NMR spectrum of **3a** in $CDCl_3$



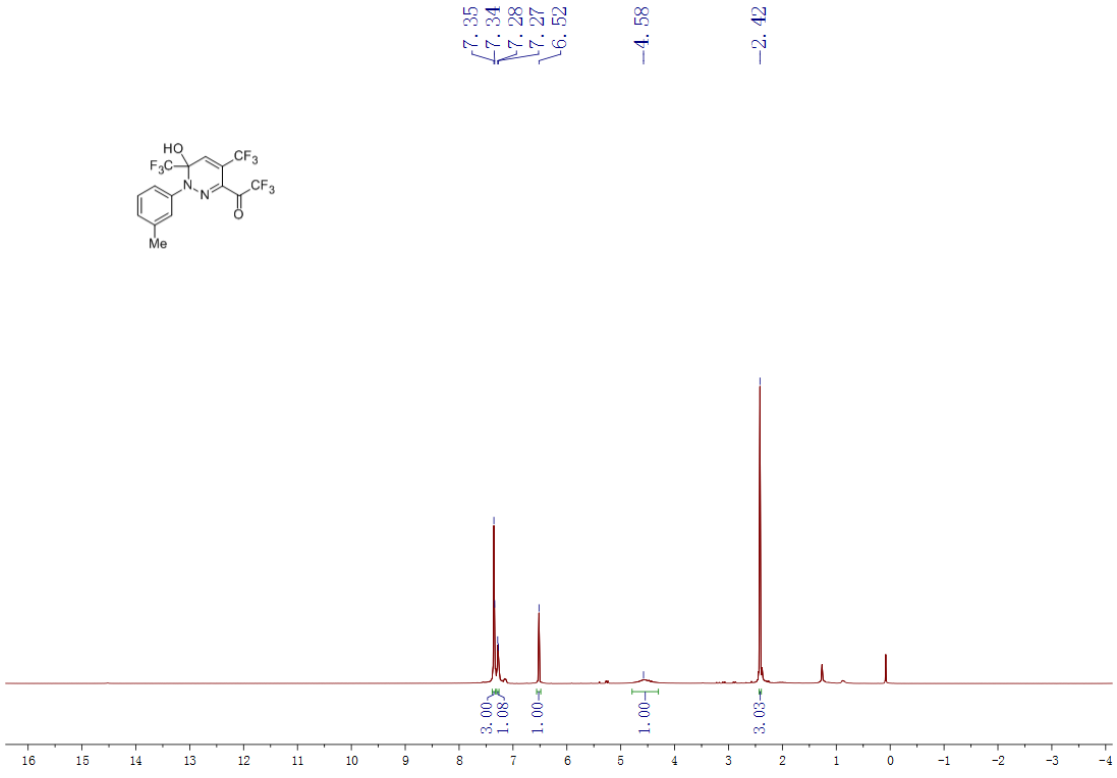
^{19}F NMR spectrum of **3a** in $CDCl_3$



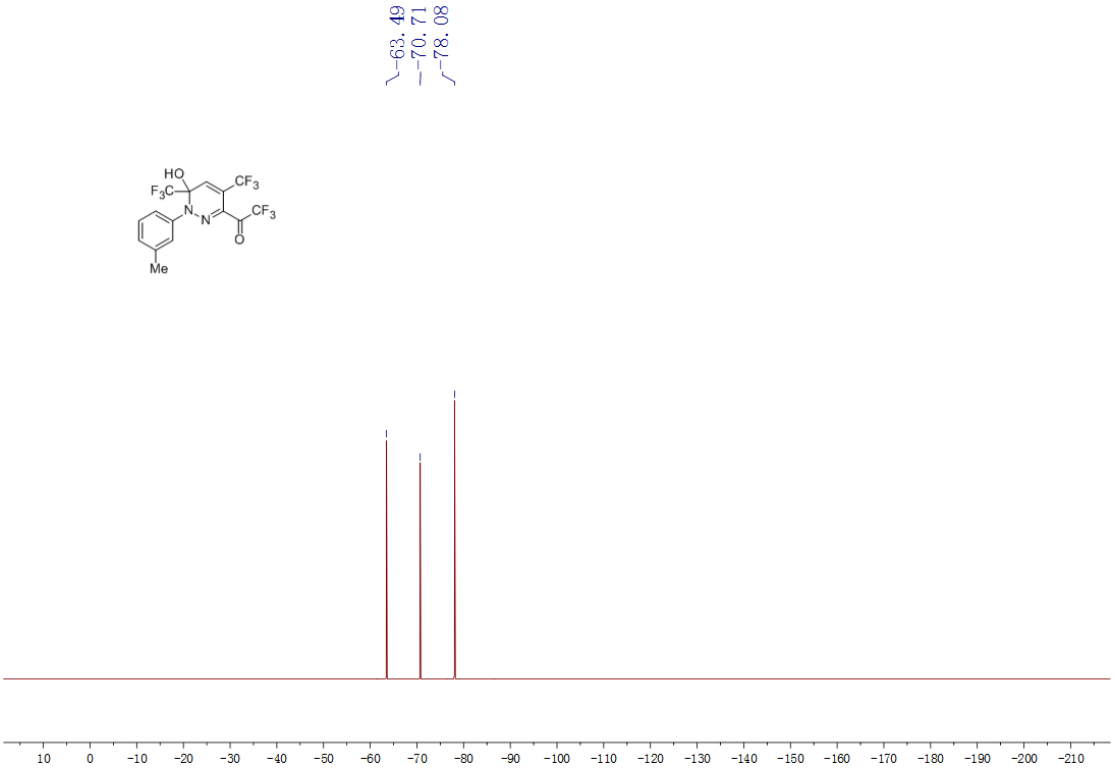
^{13}C NMR spectrum of **3a** in $CDCl_3$



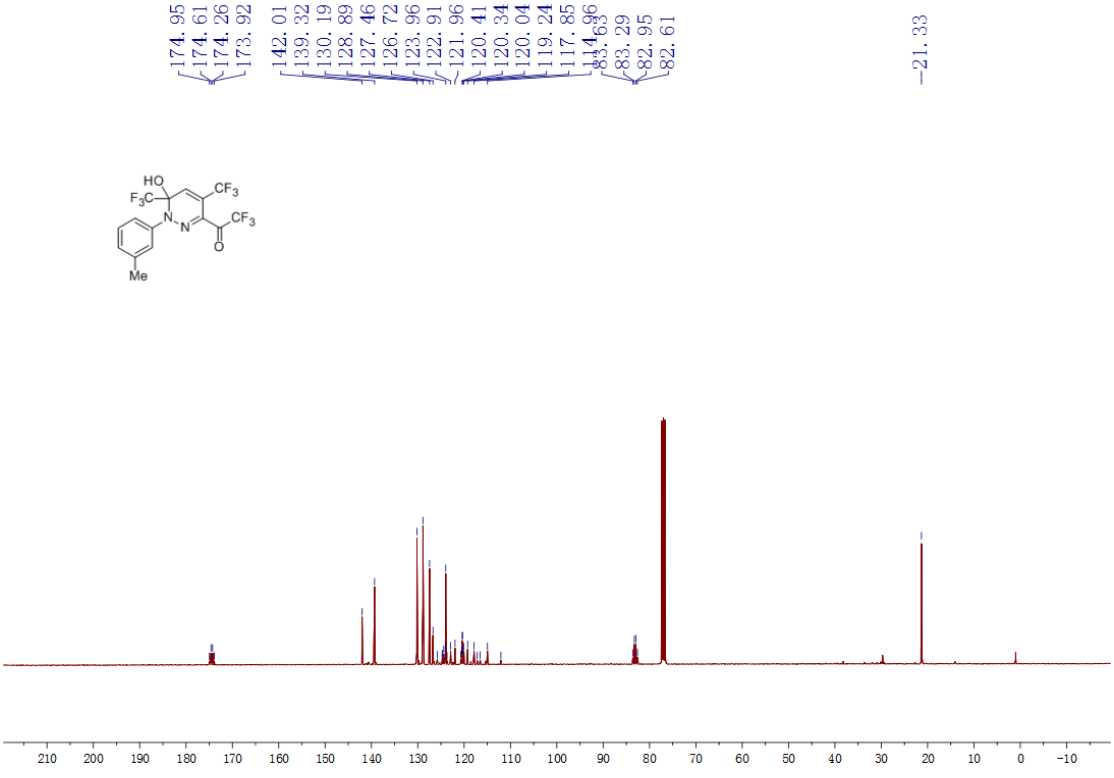
^{1}H NMR spectrum of **3b** in $CDCl_3$



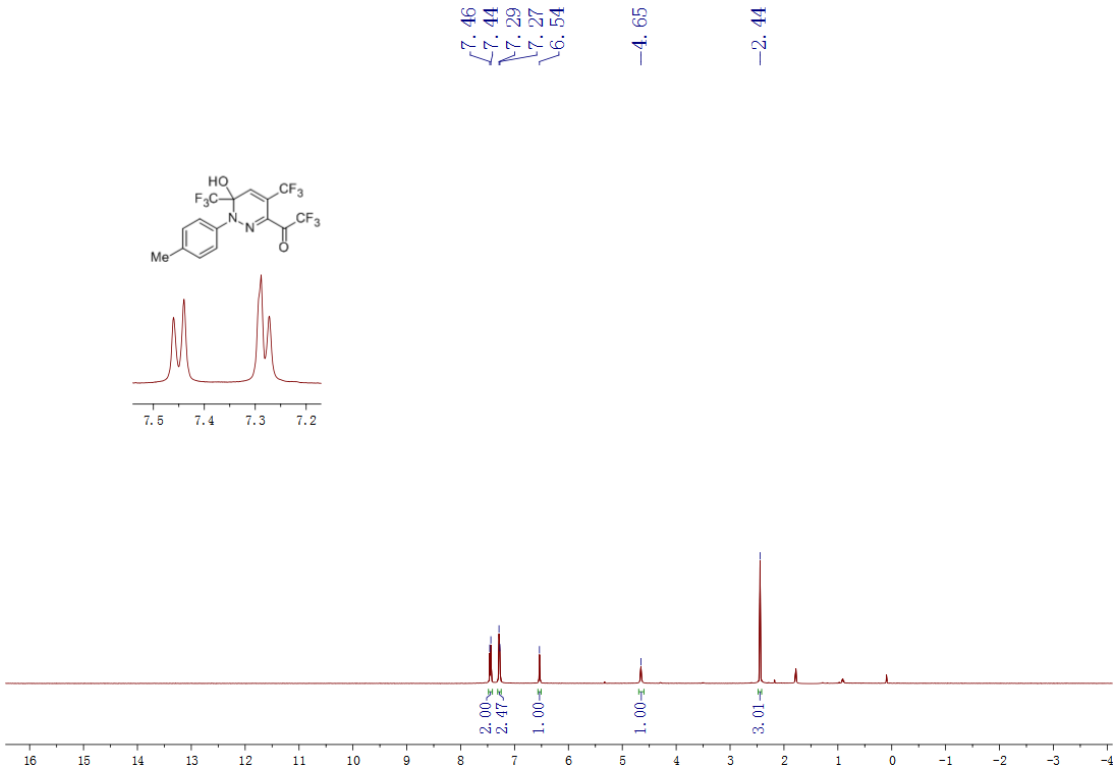
^{19}F NMR spectrum of **3b** in $CDCl_3$



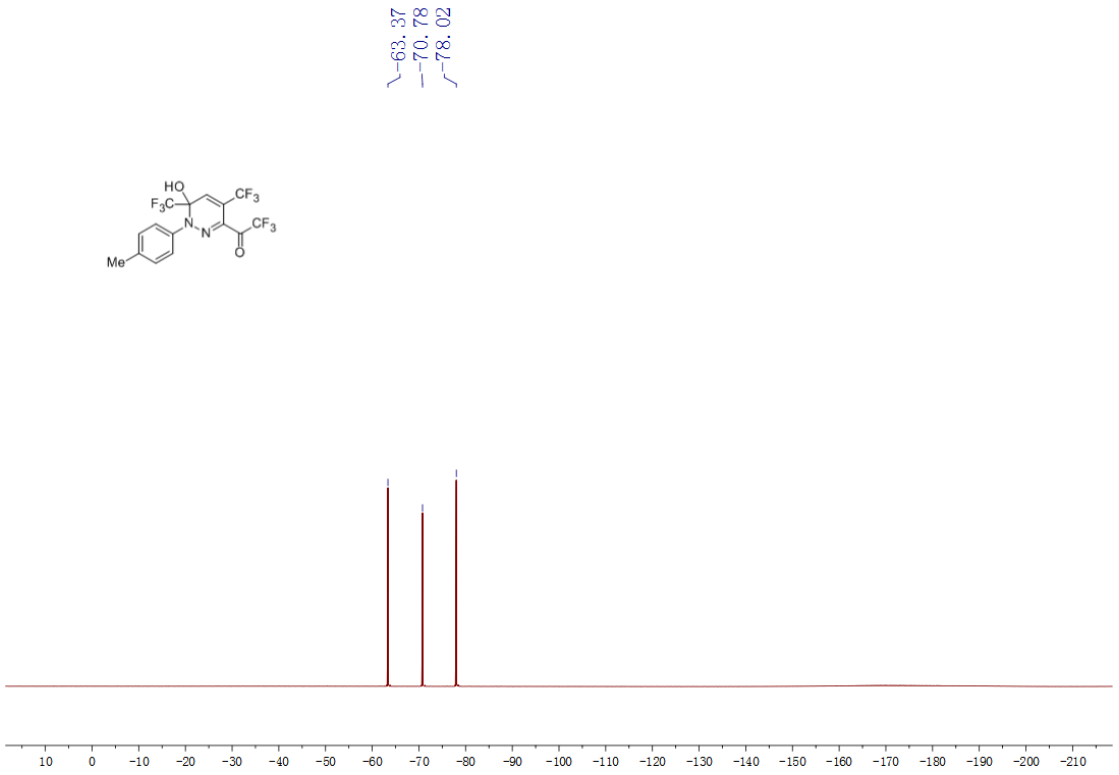
^{13}C NMR spectrum of **3b** in $CDCl_3$



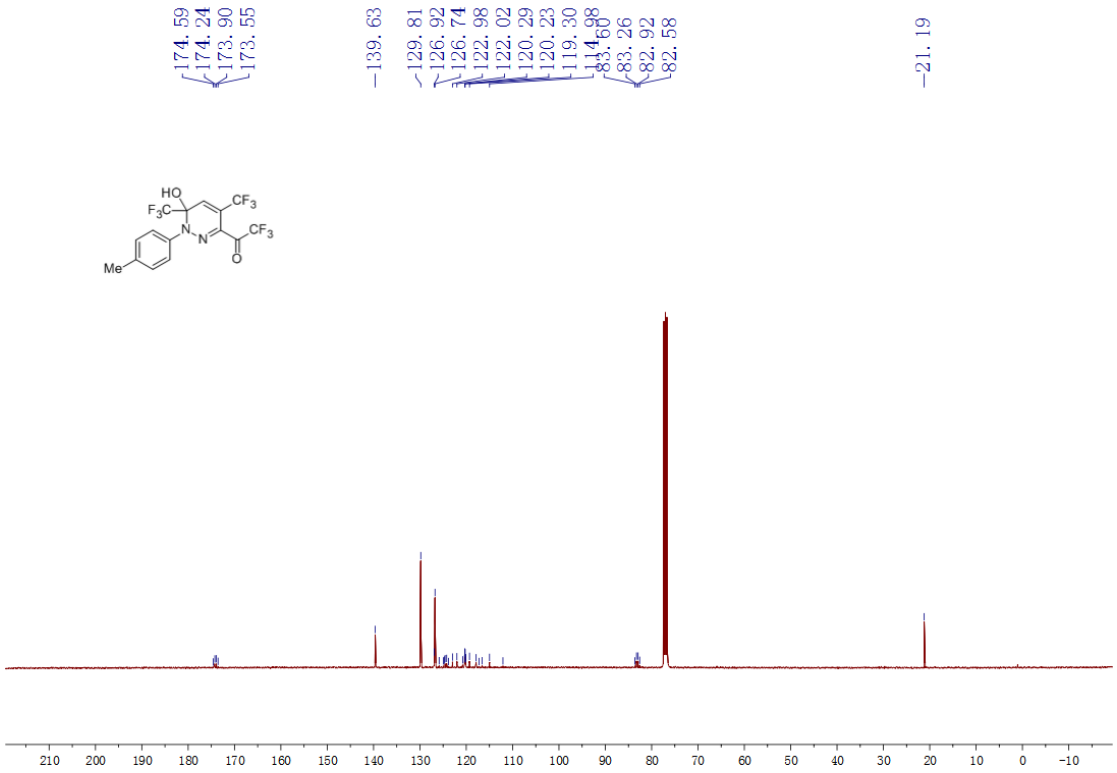
^{1}H NMR spectrum of **3c** in $CDCl_3$



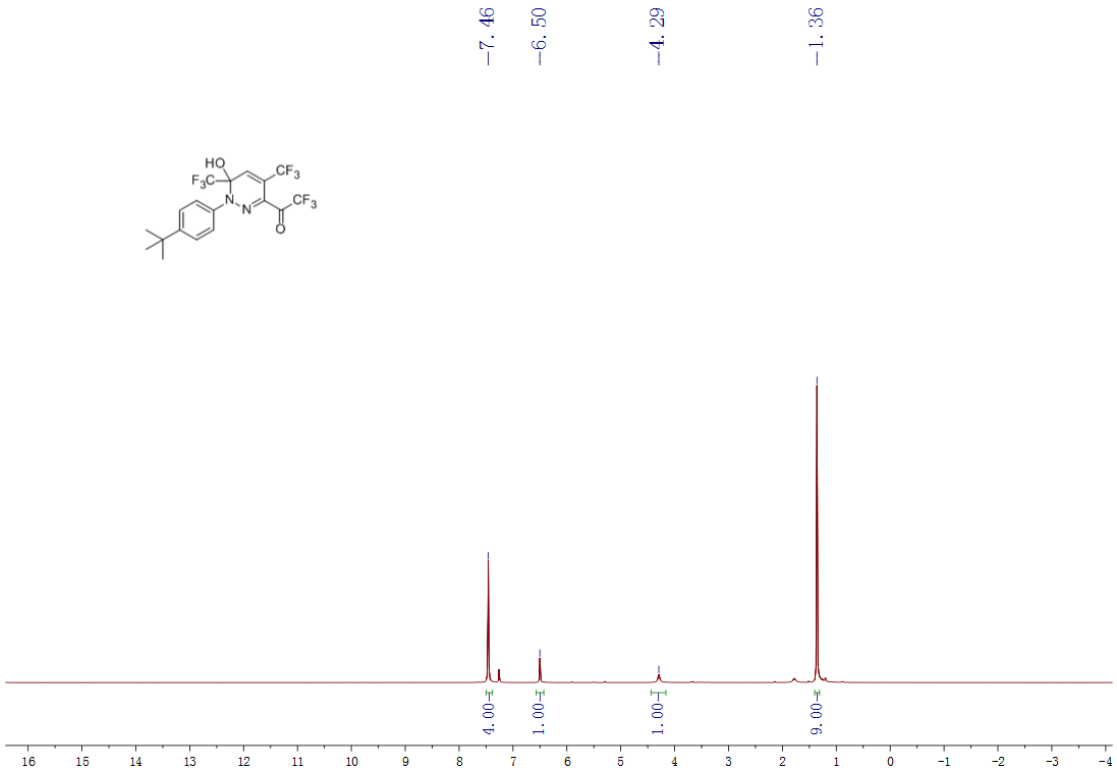
^{19}F NMR spectrum of **3c** in $CDCl_3$



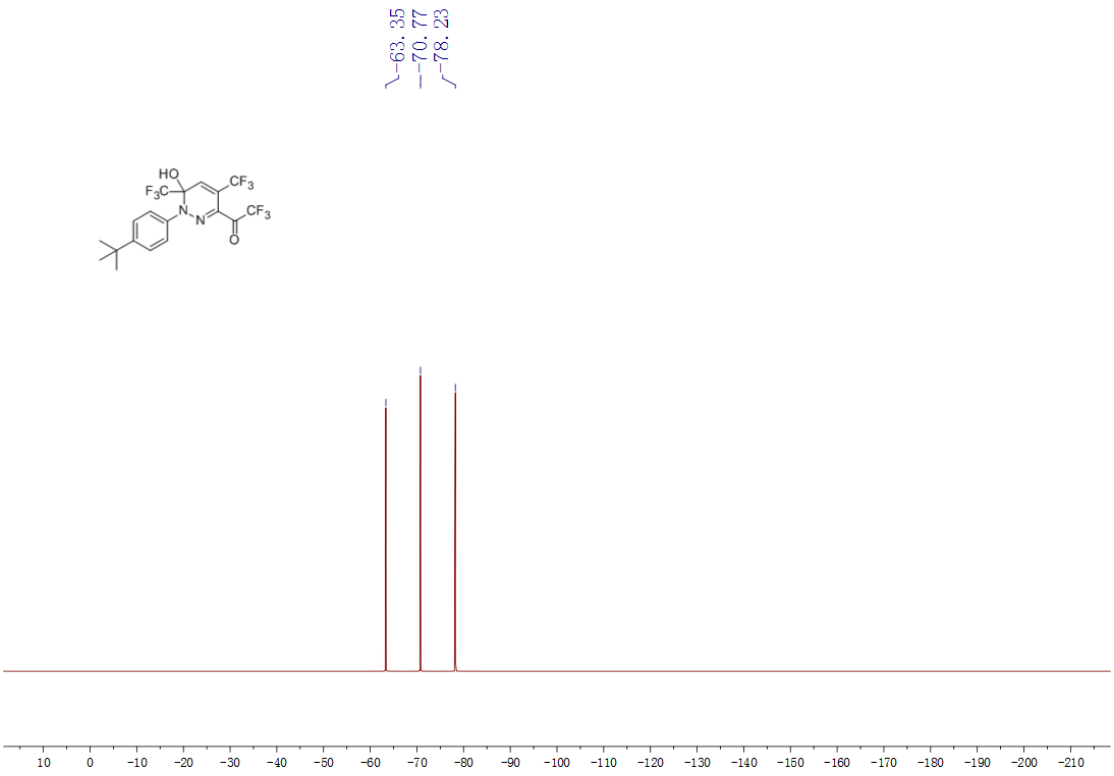
^{13}C NMR spectrum of **3c** in $CDCl_3$



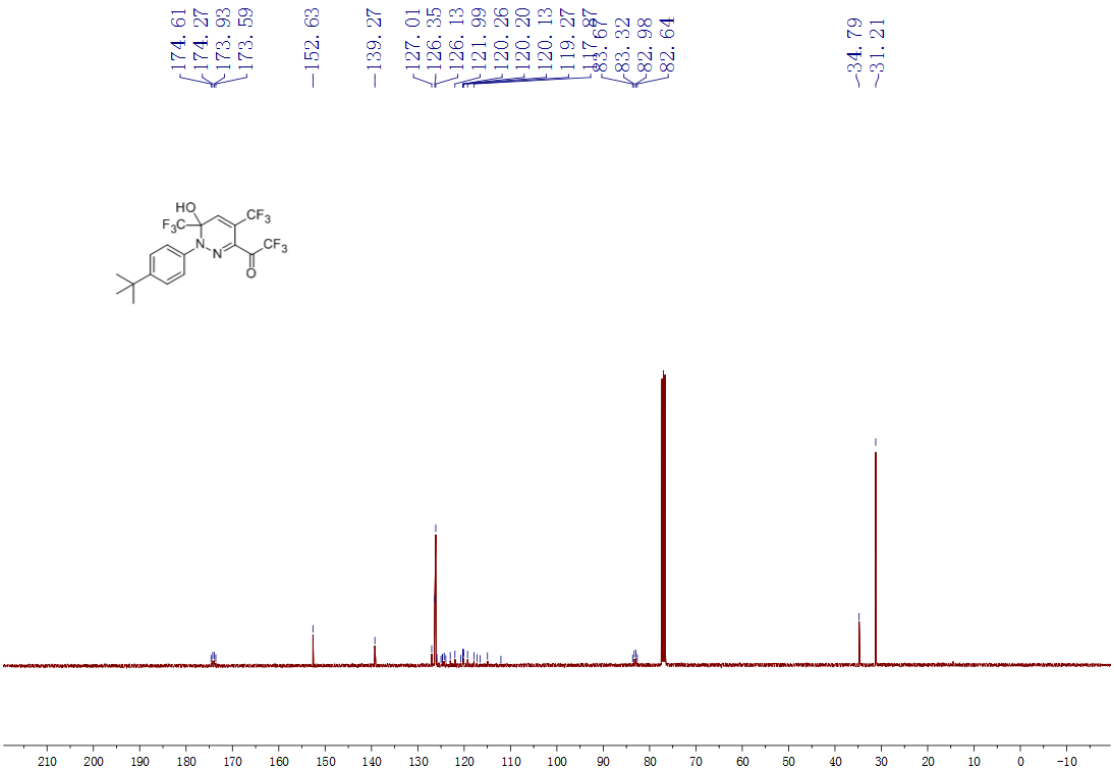
^{1}H NMR spectrum of **3d** in $CDCl_3$



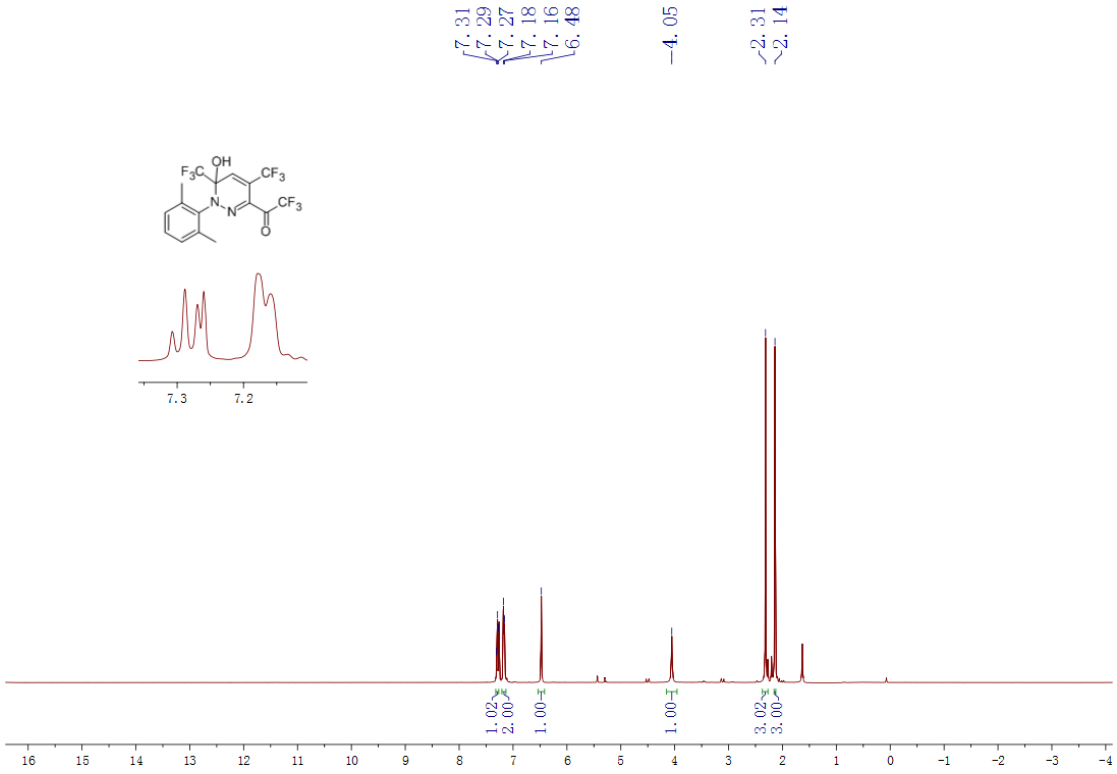
^{19}F NMR spectrum of **3d** in $CDCl_3$



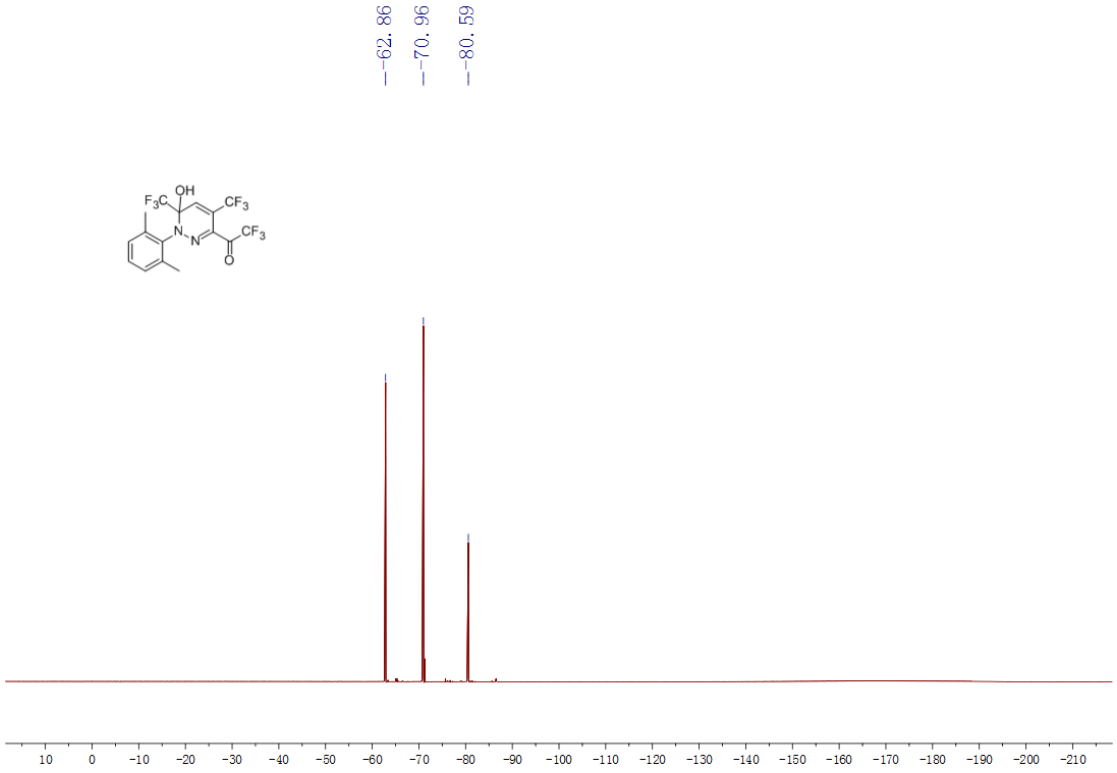
^{13}C NMR spectrum of **3d** in $CDCl_3$



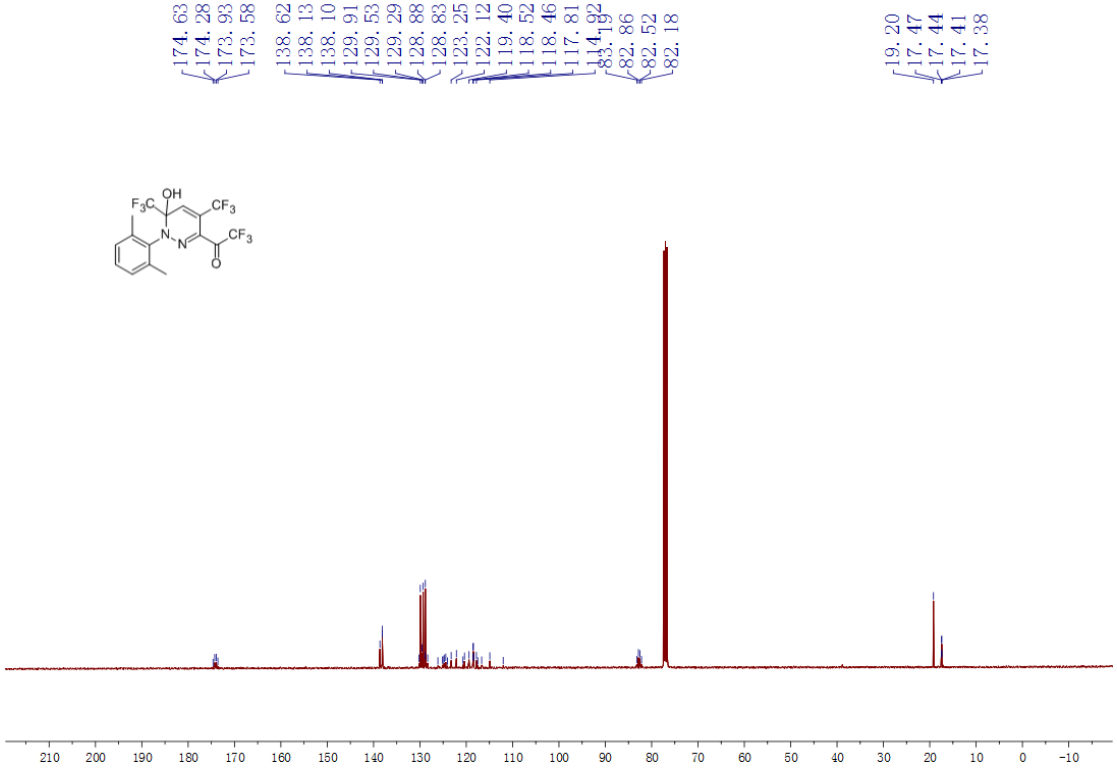
^{1}H NMR spectrum of **3e** in $CDCl_3$



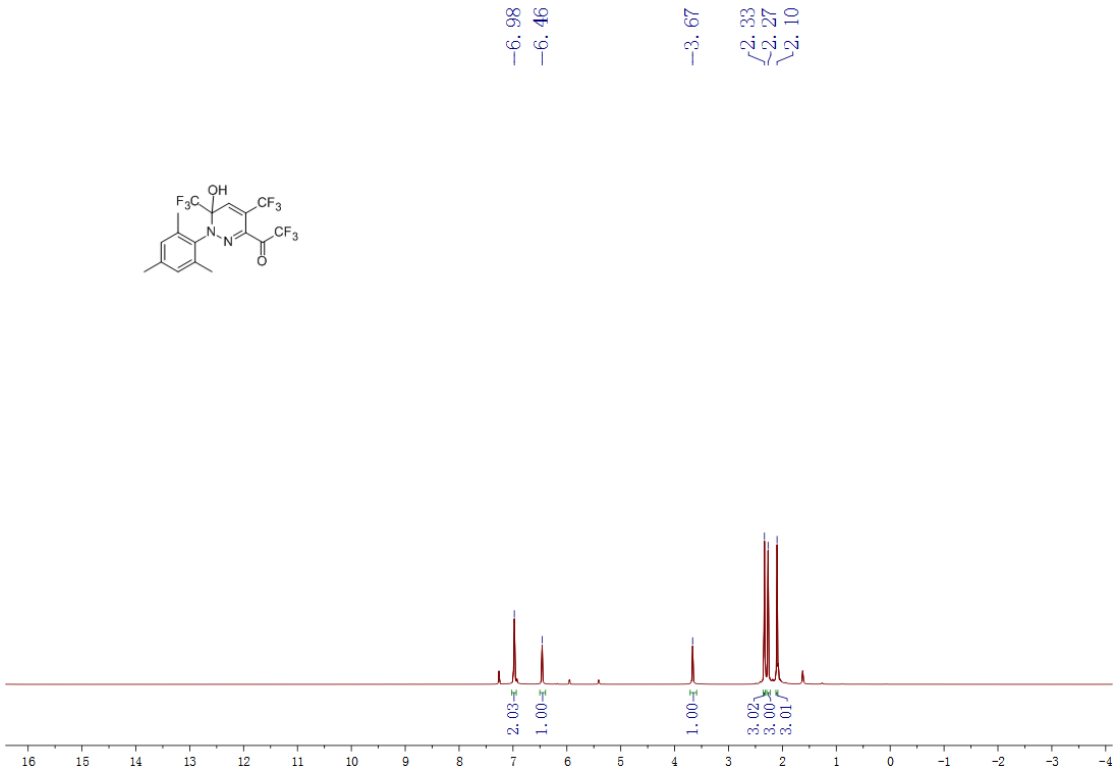
^{19}F NMR spectrum of **3e** in $CDCl_3$



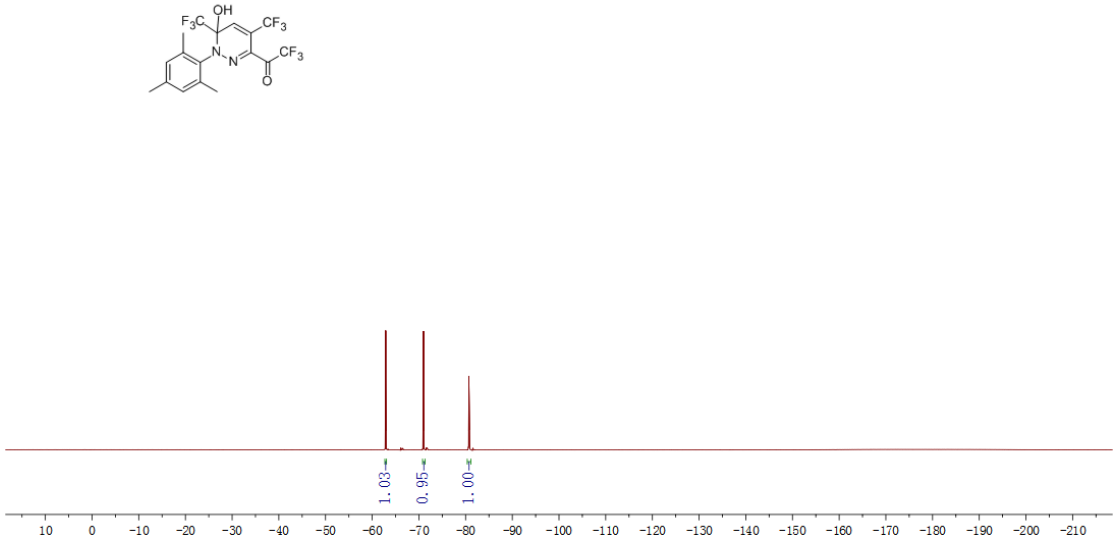
^{13}C NMR spectrum of **3e** in $CDCl_3$



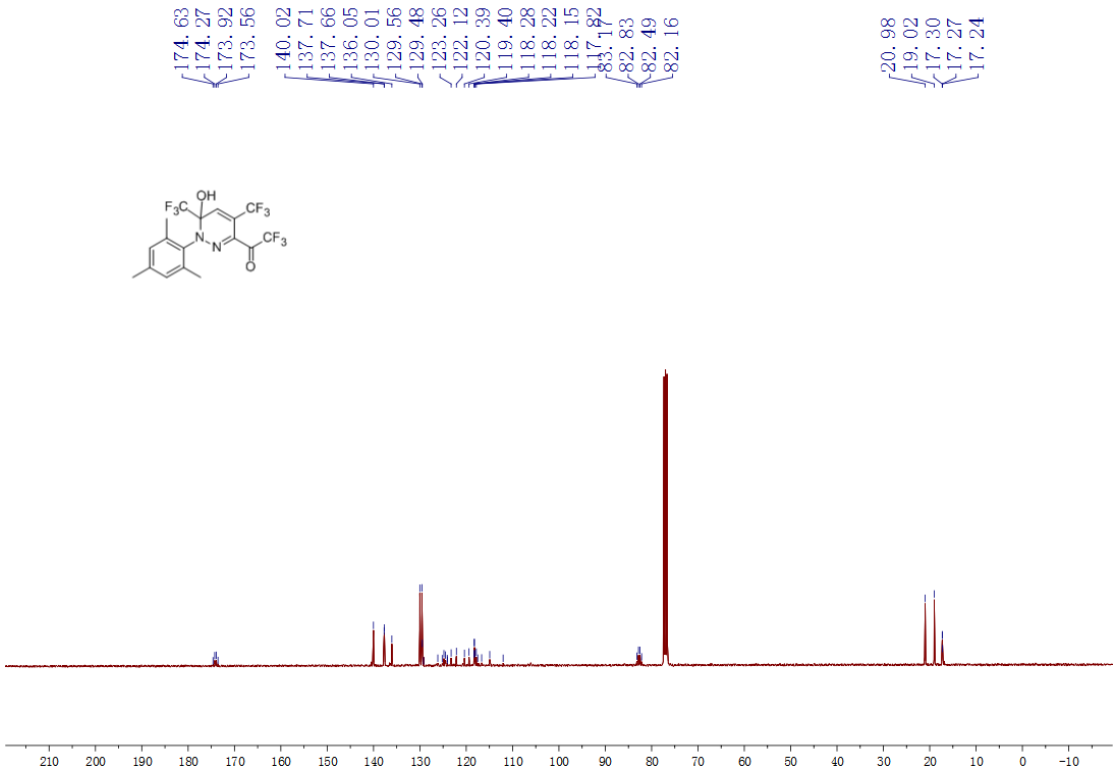
^{1}H NMR spectrum of **3f** in $CDCl_3$



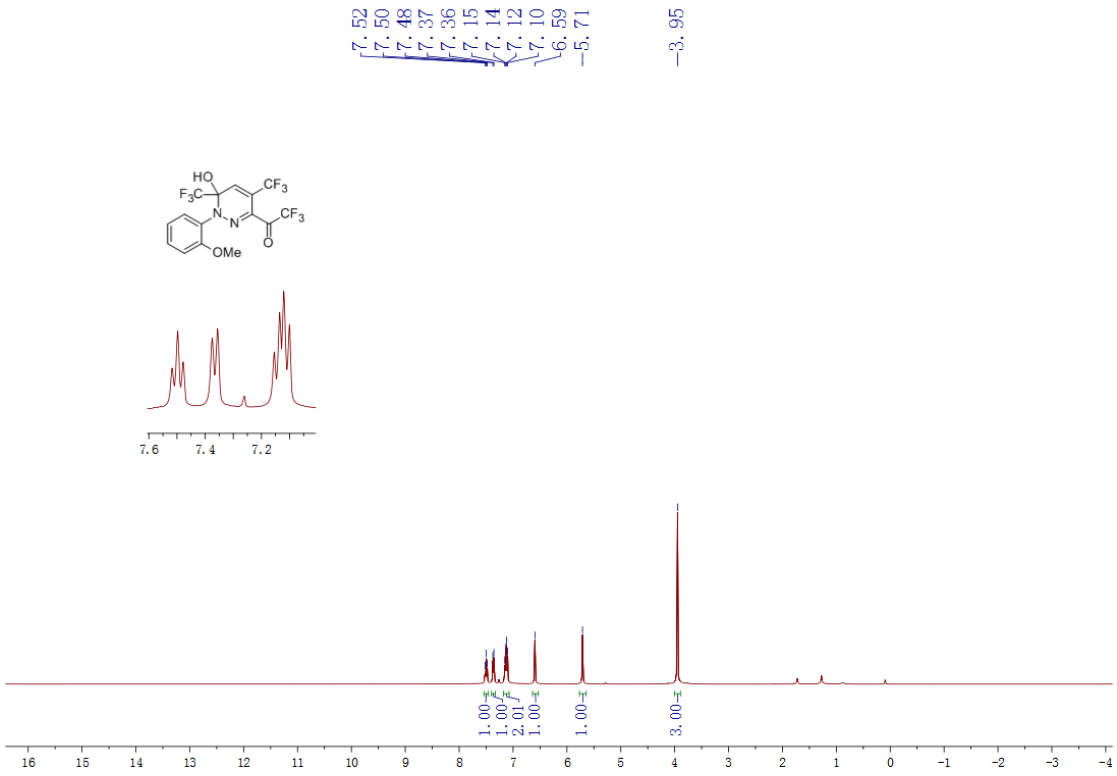
^{19}F NMR spectrum of **3f** in $CDCl_3$



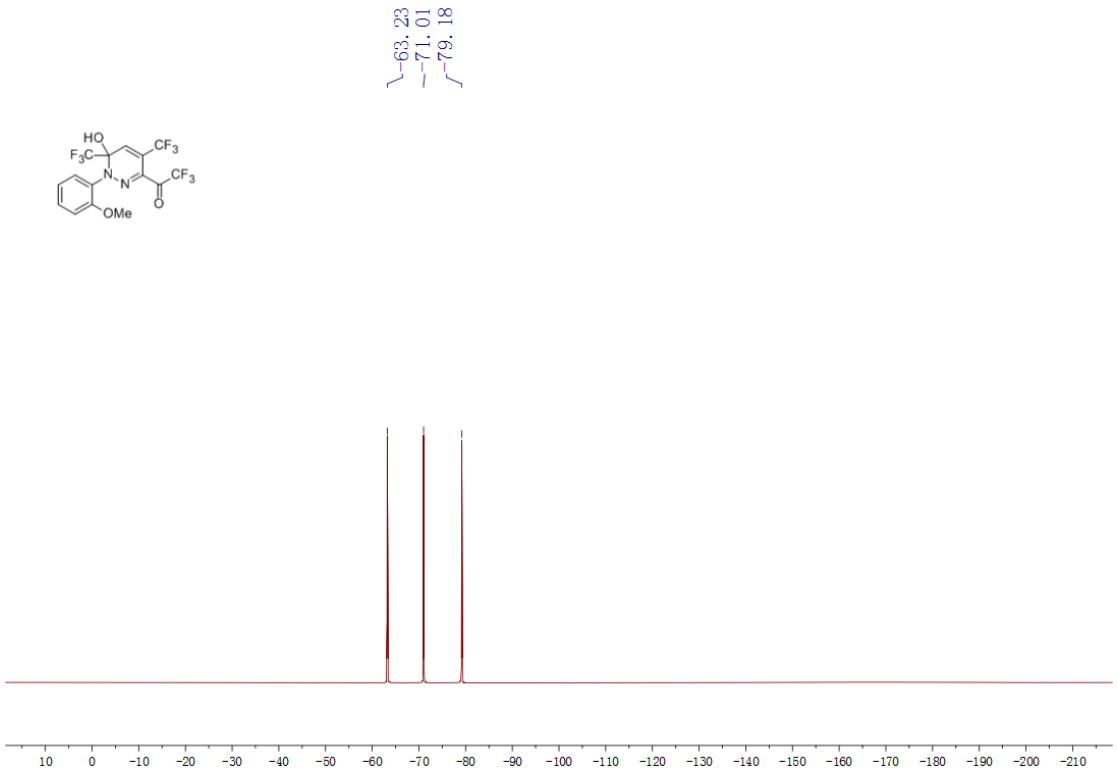
^{13}C NMR spectrum of **3f** in $CDCl_3$



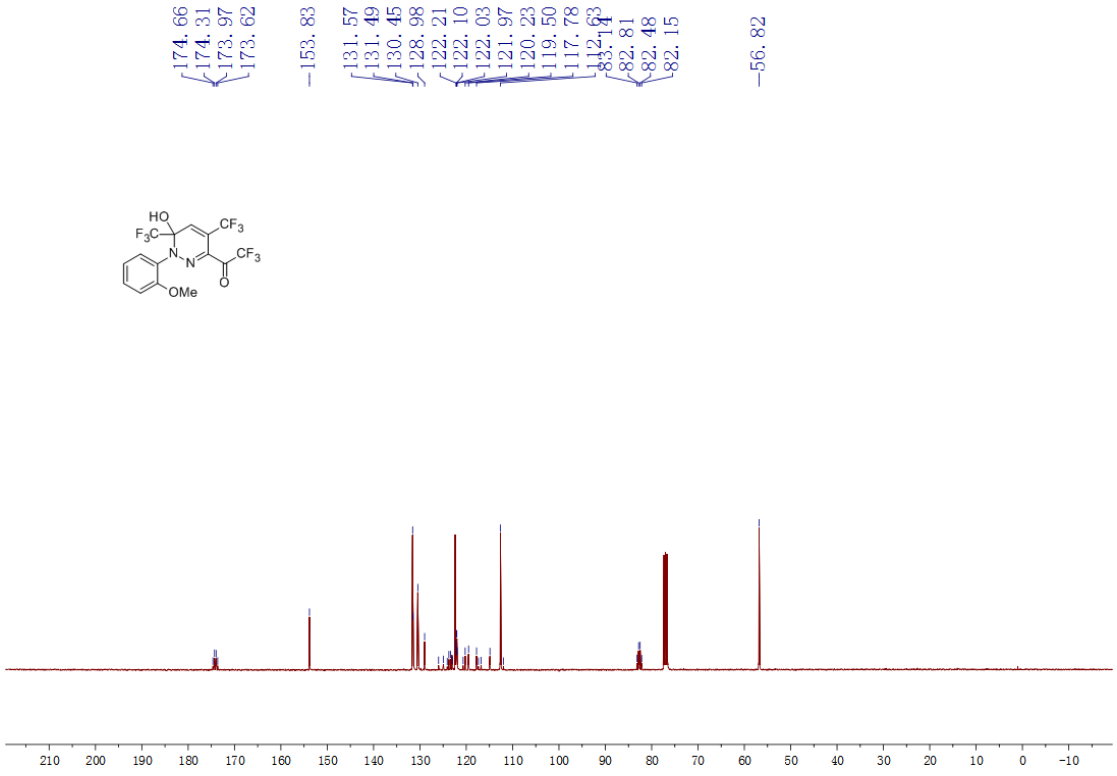
^{1}H NMR spectrum of **3g** in $CDCl_3$



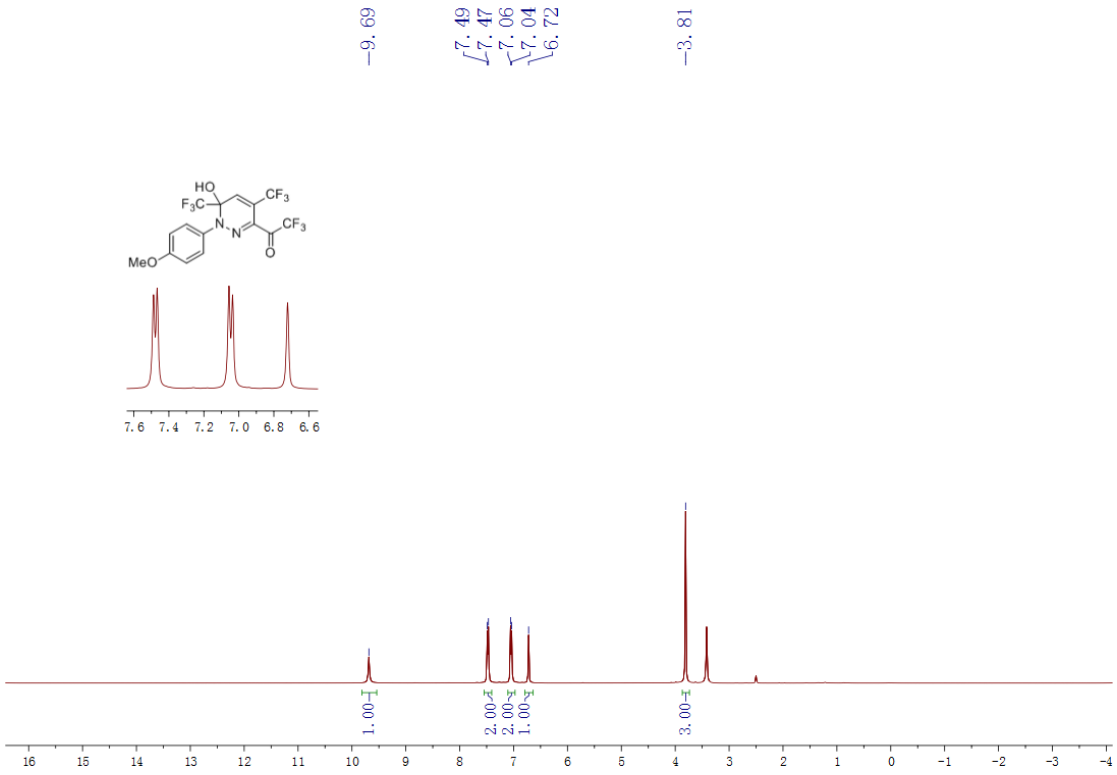
^{19}F NMR spectrum of **3g** in $CDCl_3$



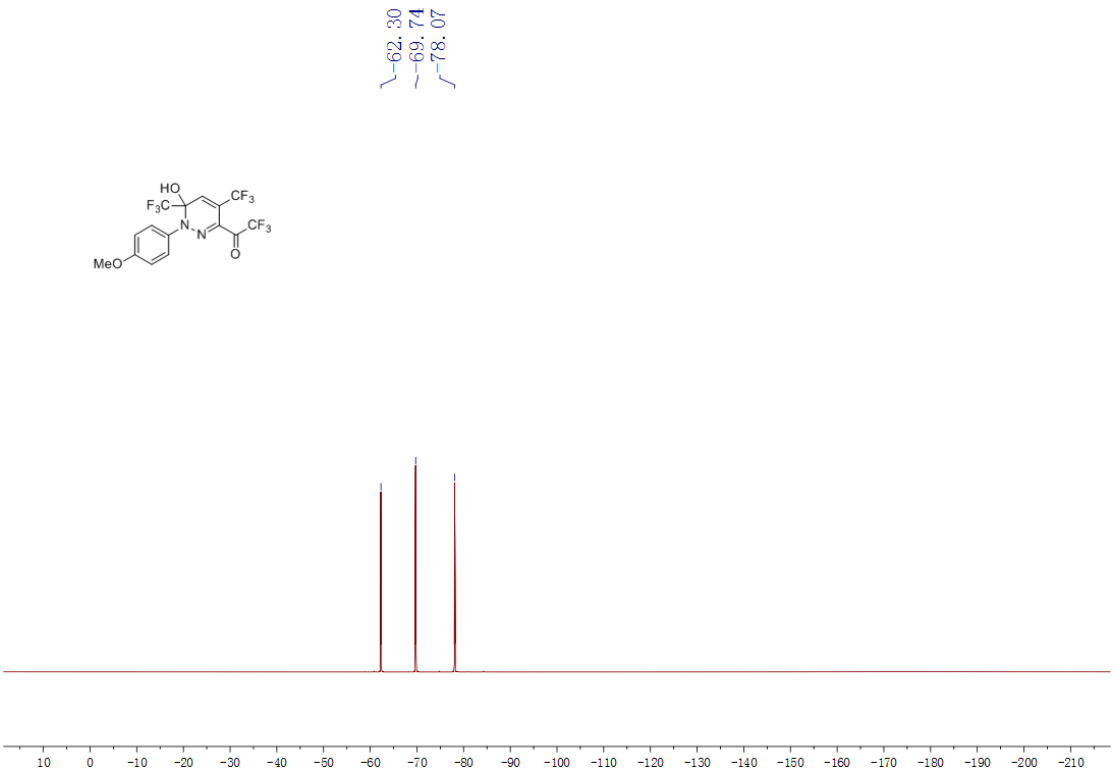
^{13}C NMR spectrum of **3g** in $CDCl_3$



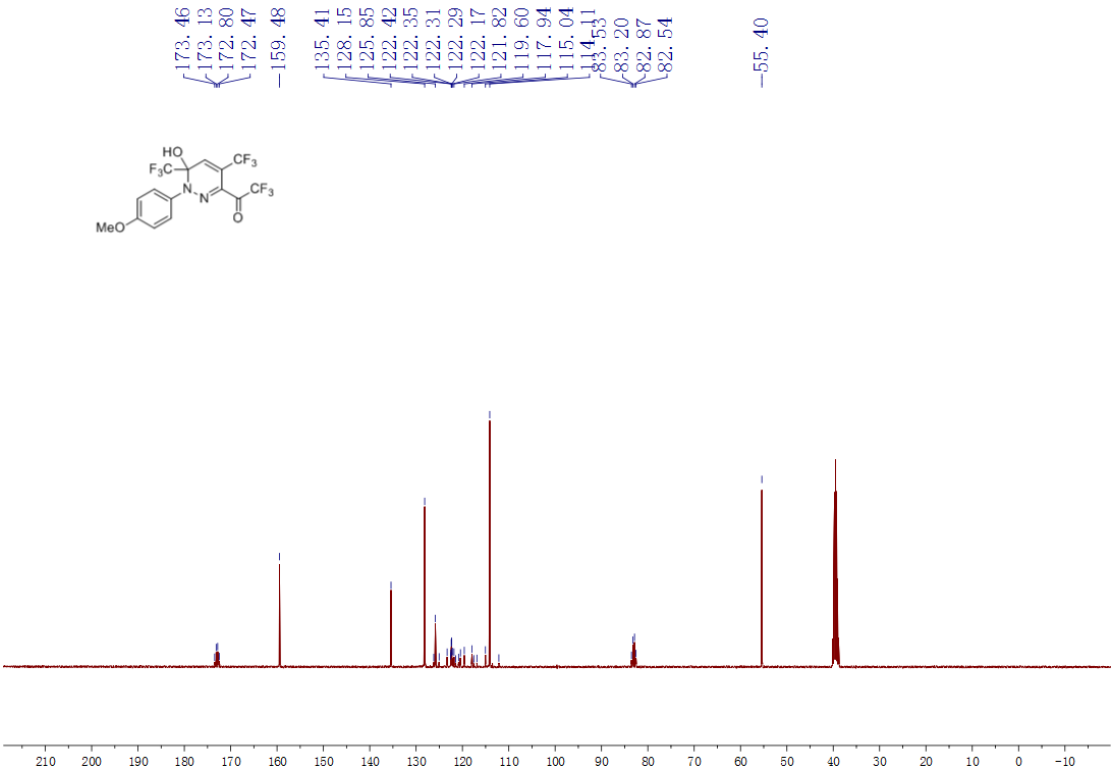
^{1}H NMR spectrum of **3h** in DMSO-d_6



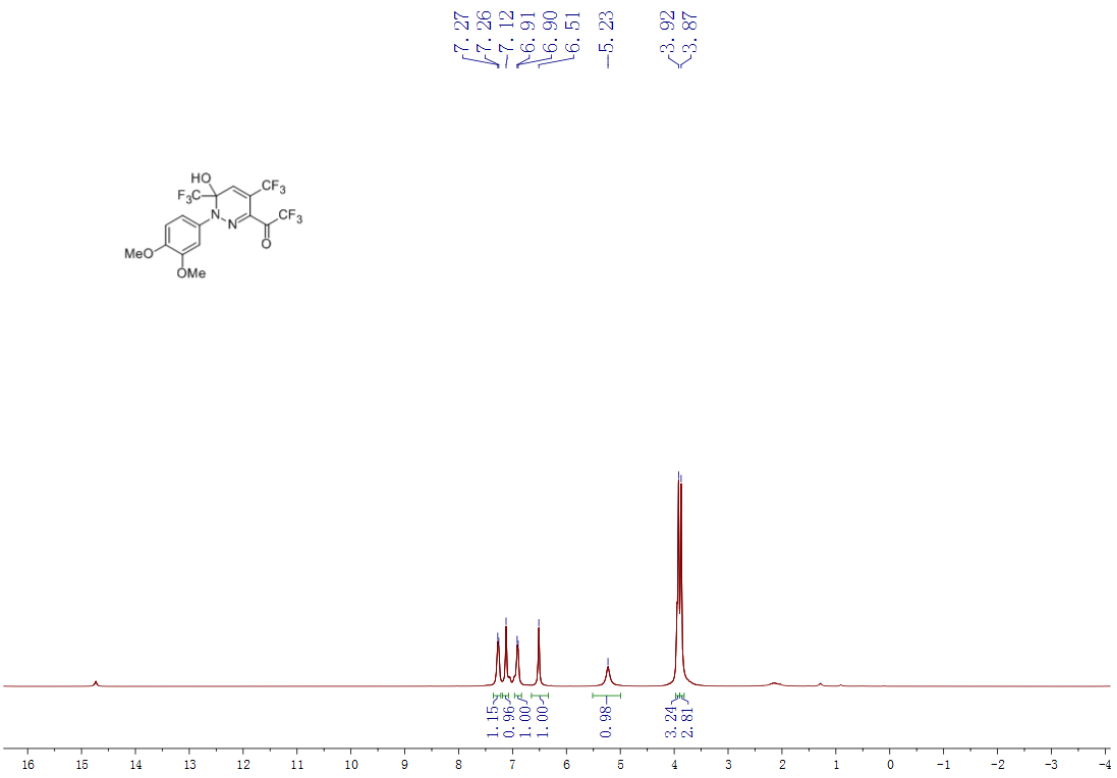
^{19}F NMR spectrum of **3h** in DMSO-d_6



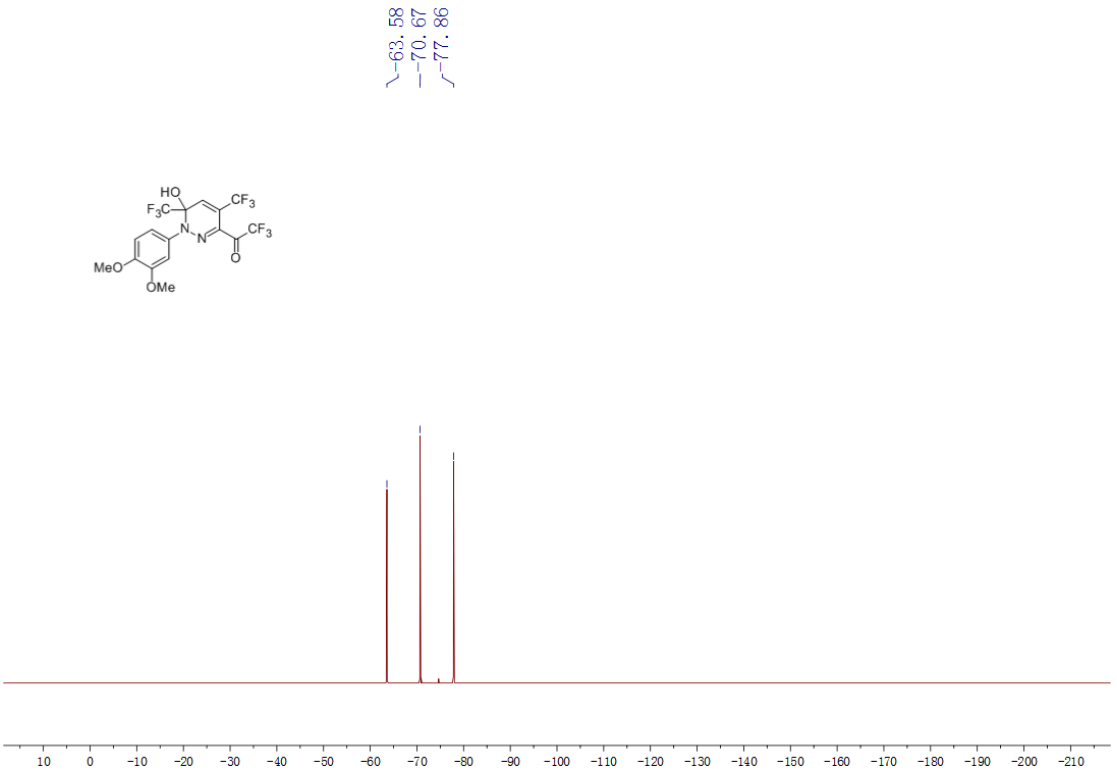
^{13}C NMR spectrum of **3h** in DMSO-d_6



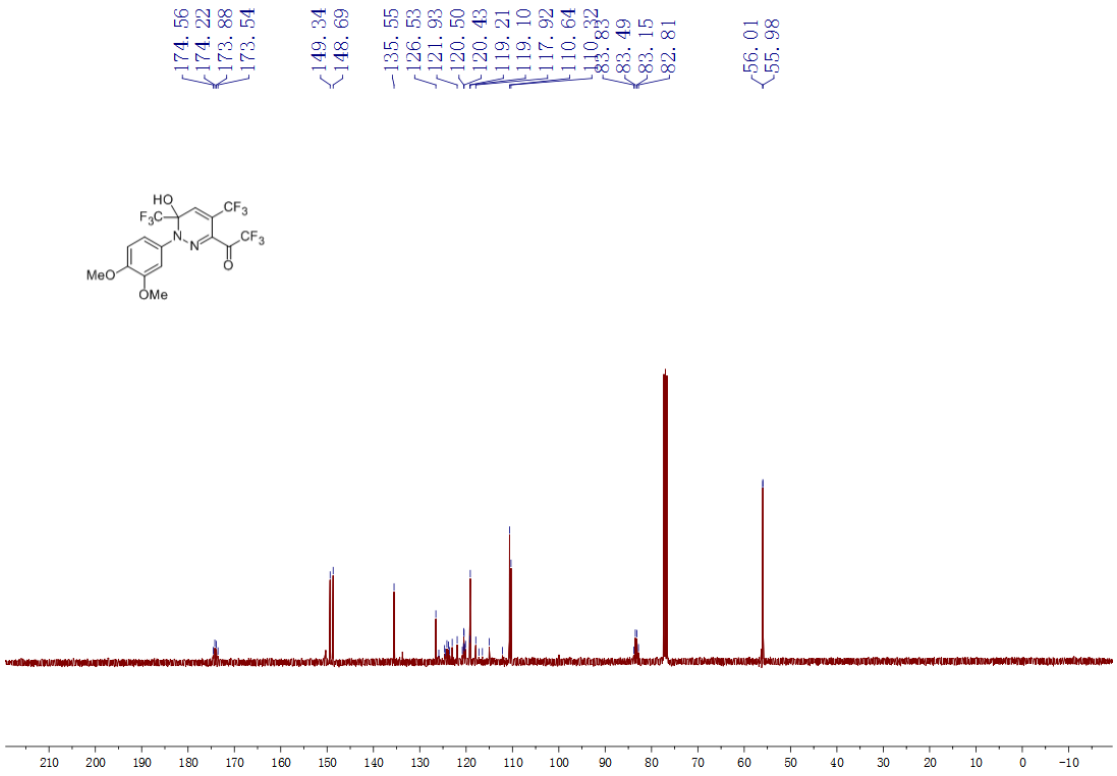
^{1}H NMR spectrum of **3i** in $CDCl_3$



^{19}F NMR spectrum of **3i** in $CDCl_3$



^{13}C NMR spectrum of **3i** in $CDCl_3$



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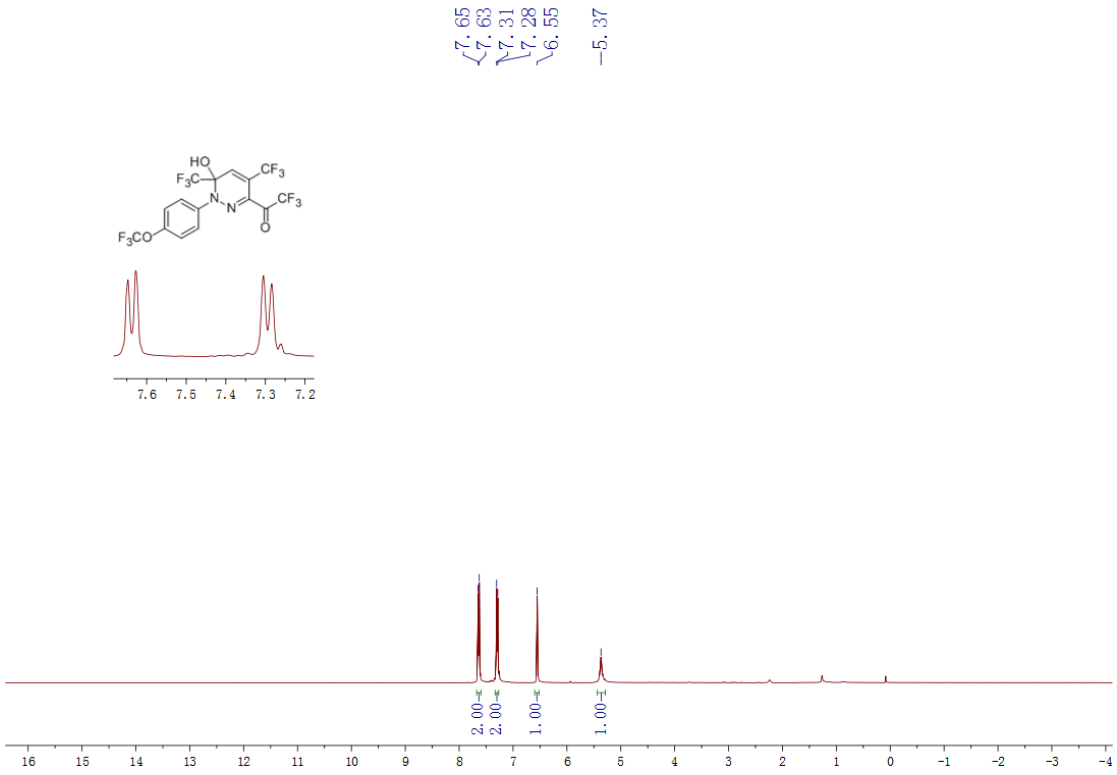

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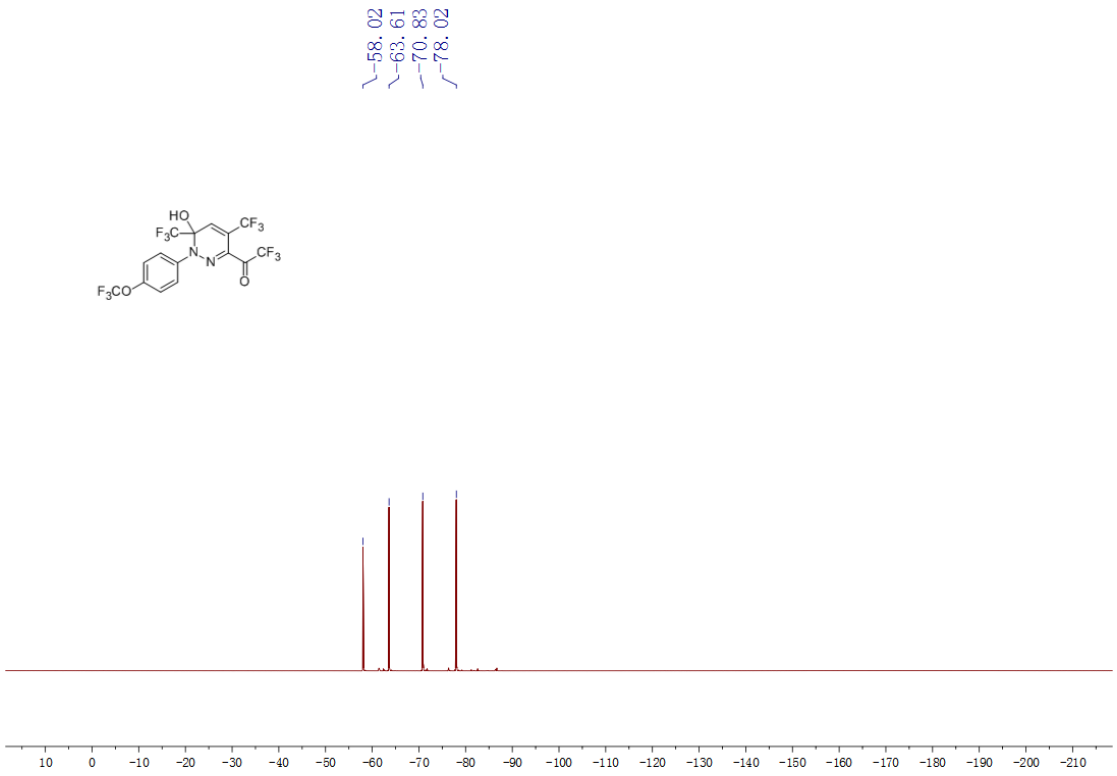

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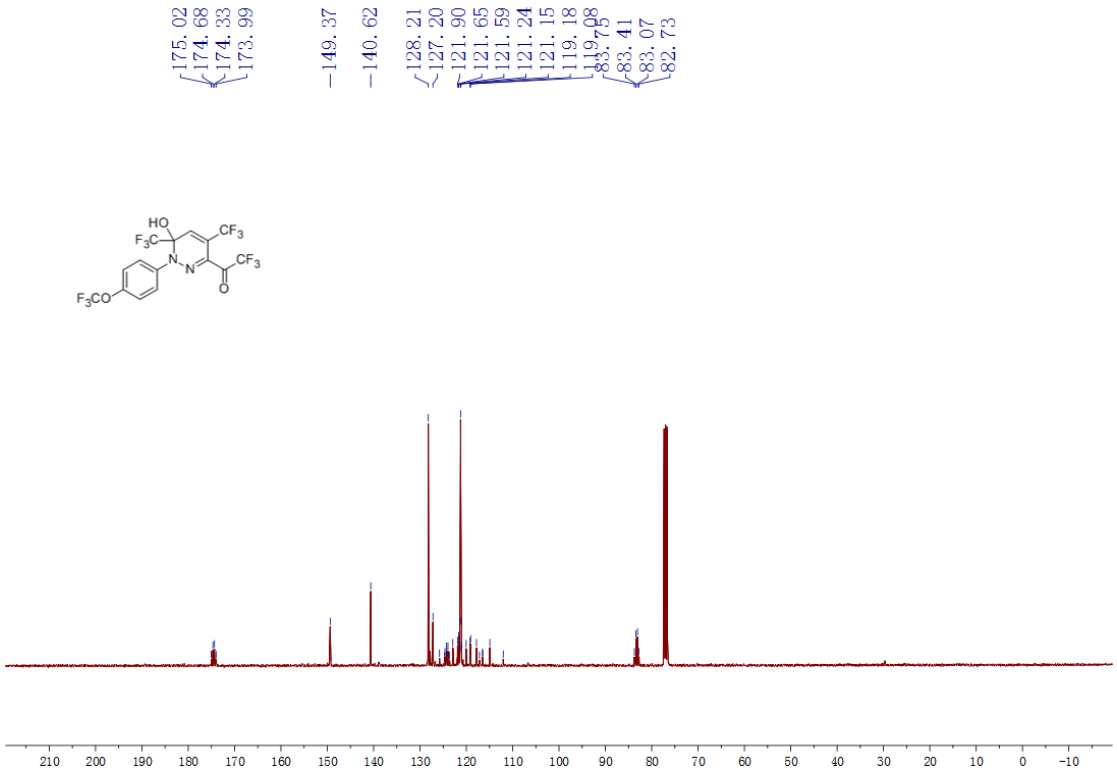
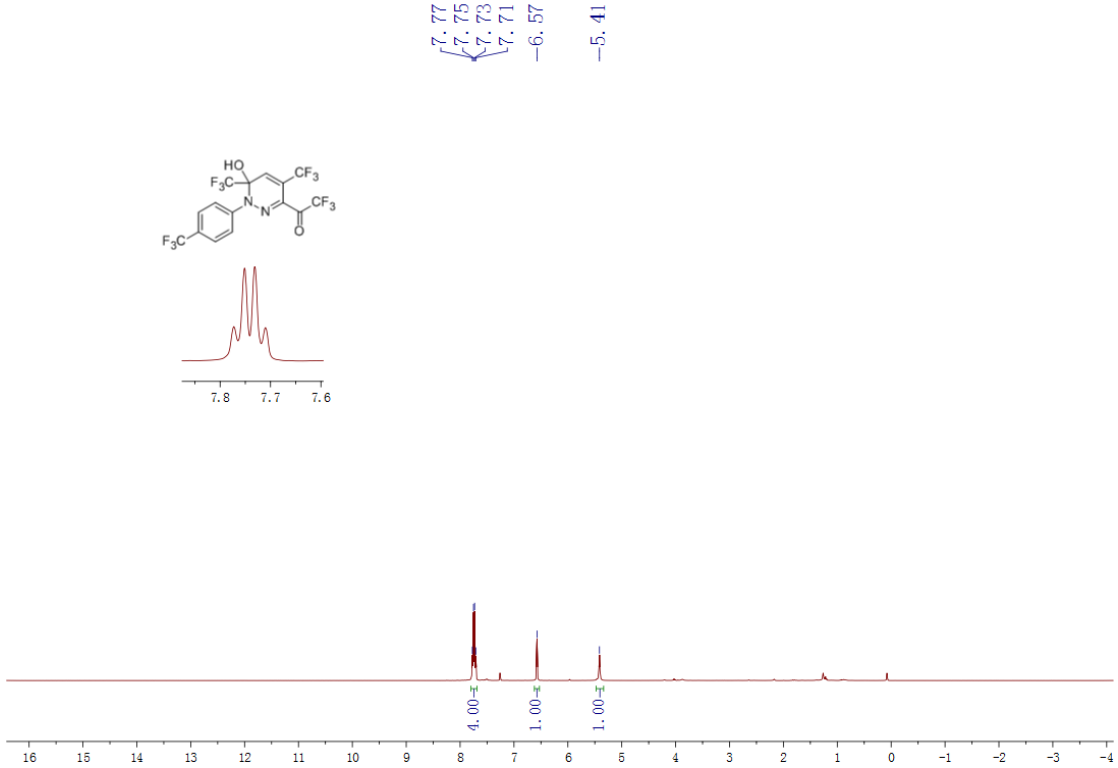
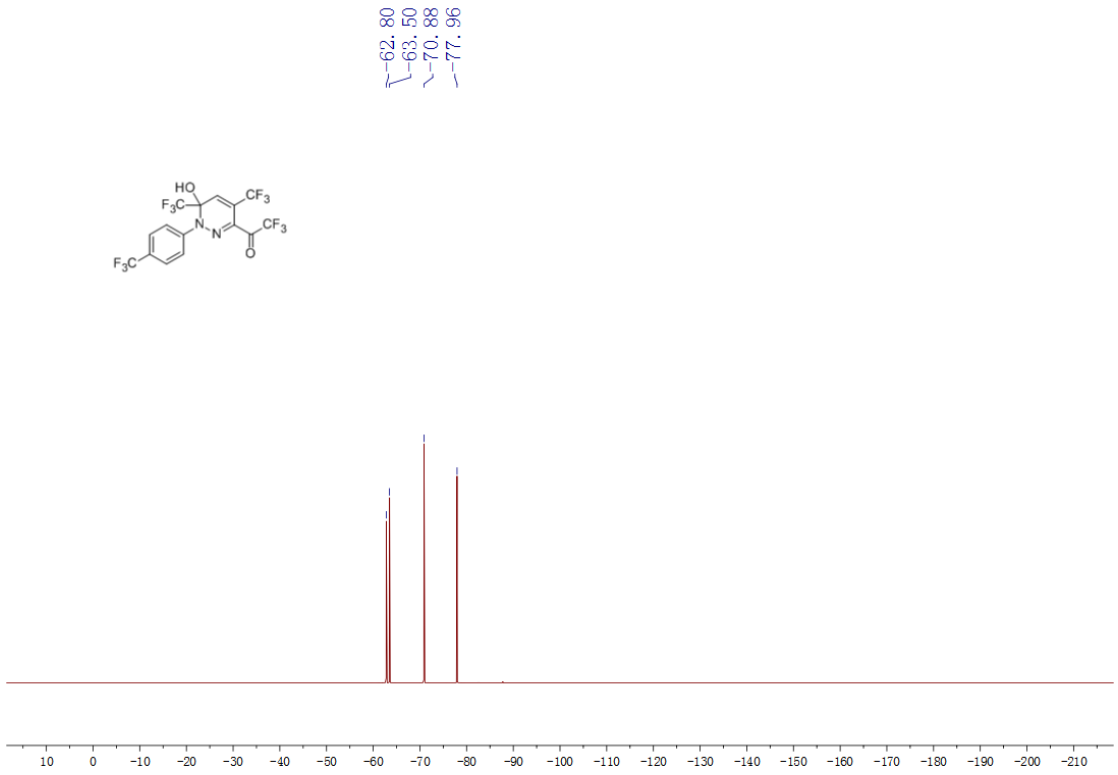


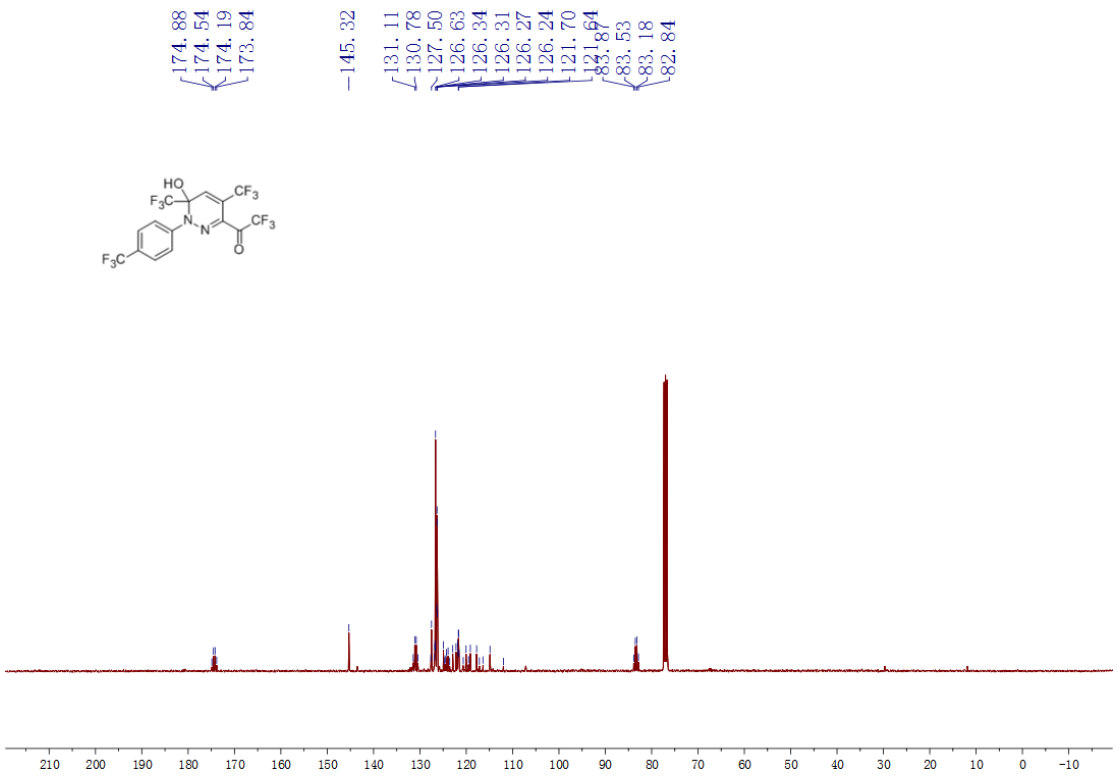
^{1}H NMR spectrum of **3k** in $CDCl_3$



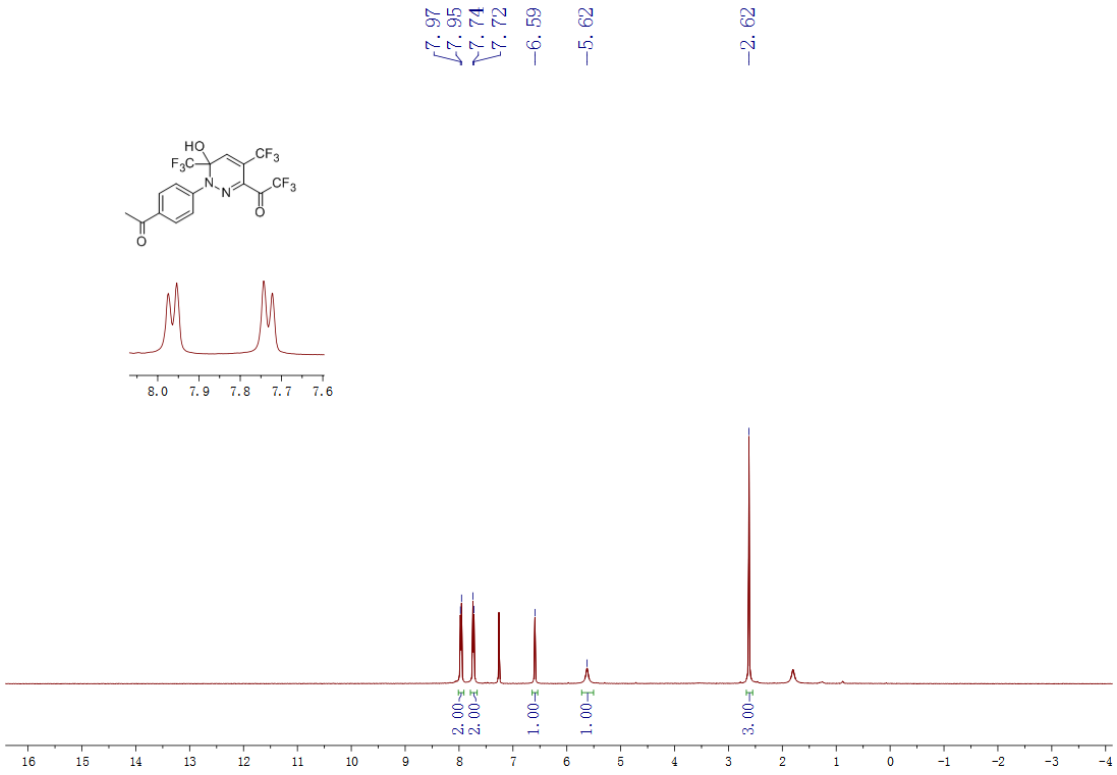
^{19}F NMR spectrum of **3k** in $CDCl_3$



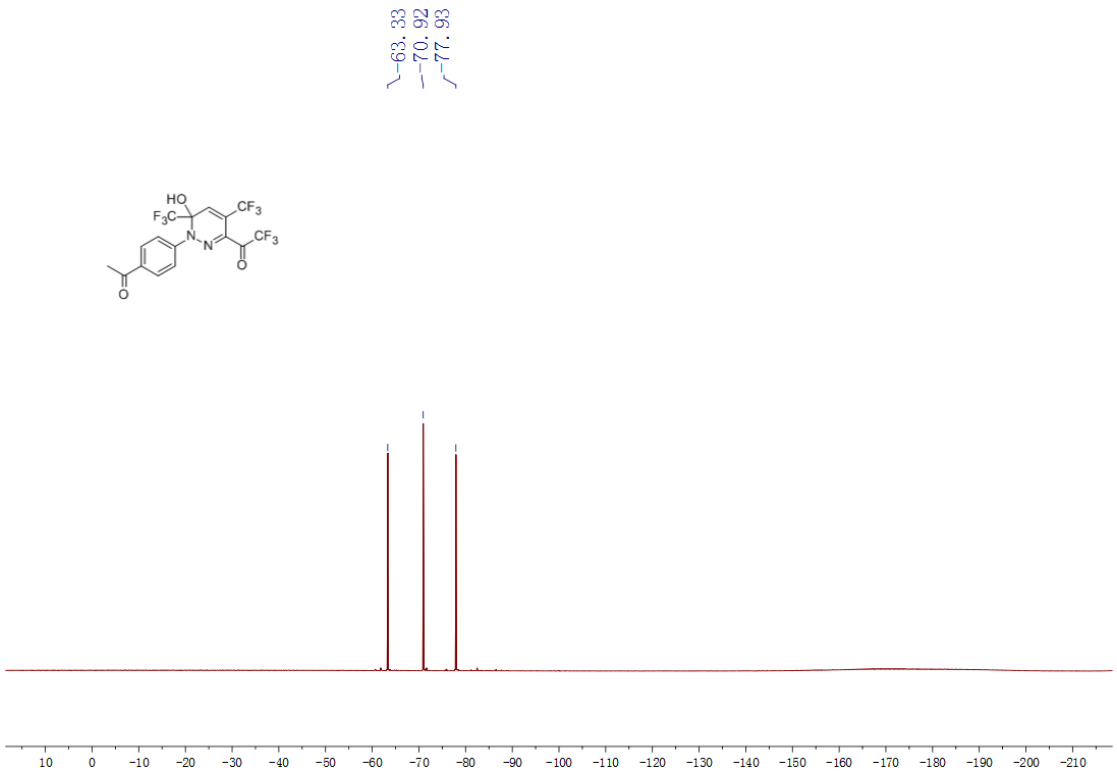
^{13}C NMR spectrum of **3k** in $CDCl_3$



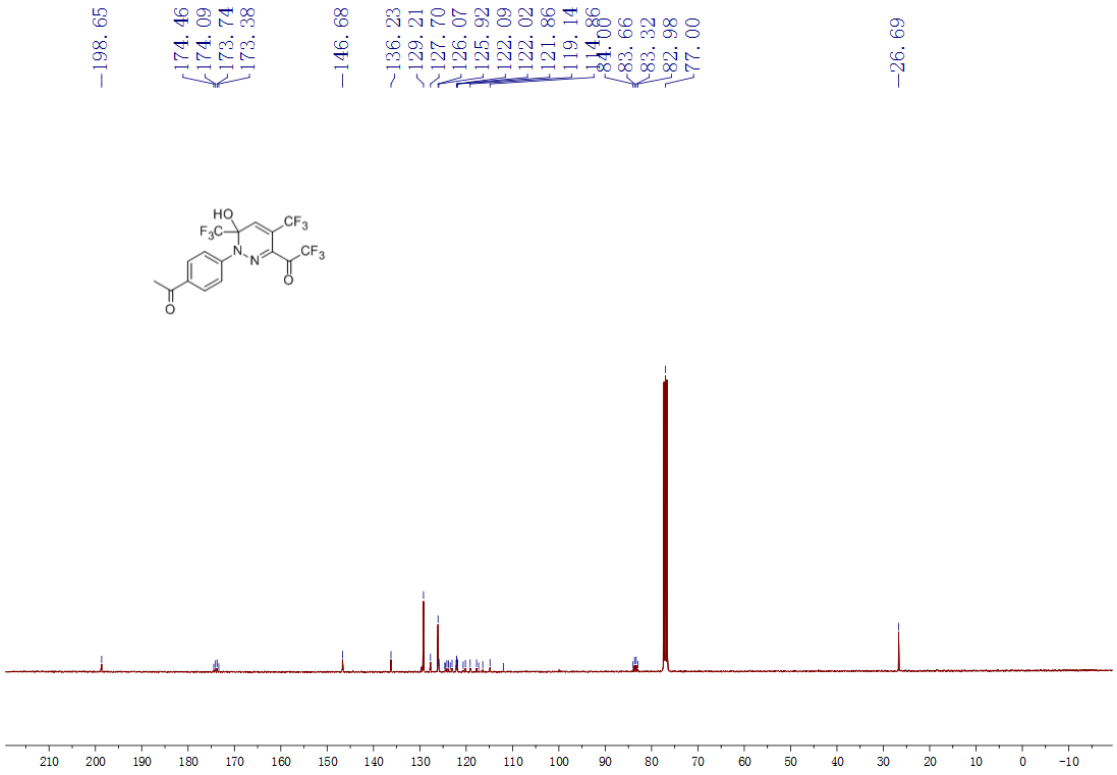
^{1}H NMR spectrum of **3l** in $CDCl_3$



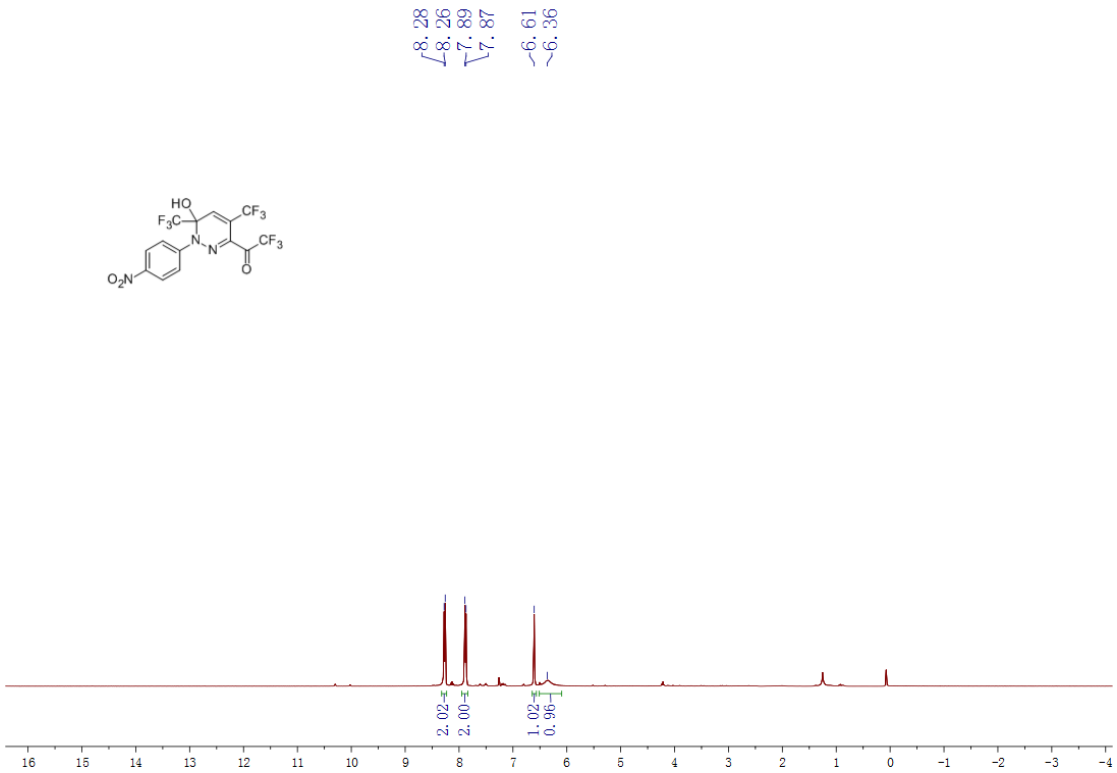
^{19}F NMR spectrum of **3l** in $CDCl_3$



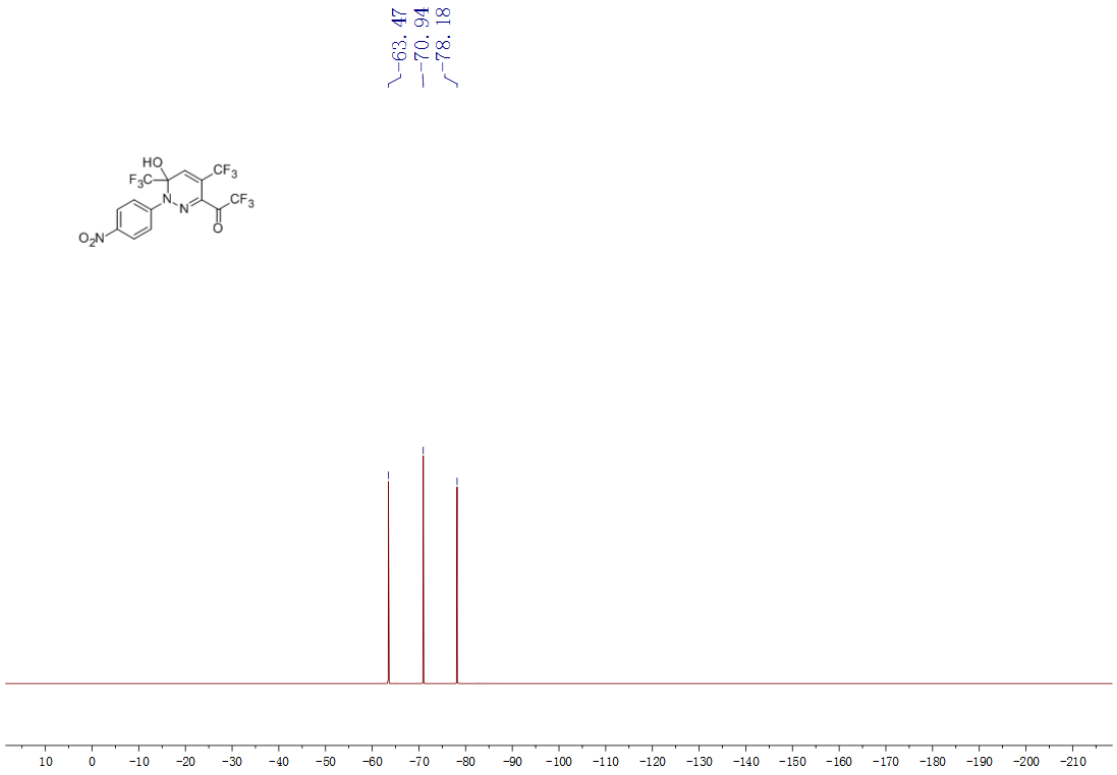
^{13}C NMR spectrum of **3l** in $CDCl_3$



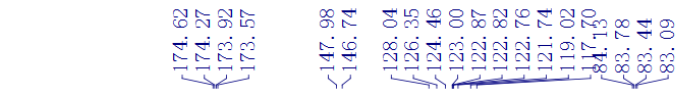
^{1}H NMR spectrum of **3m** in $CDCl_3$

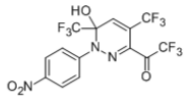


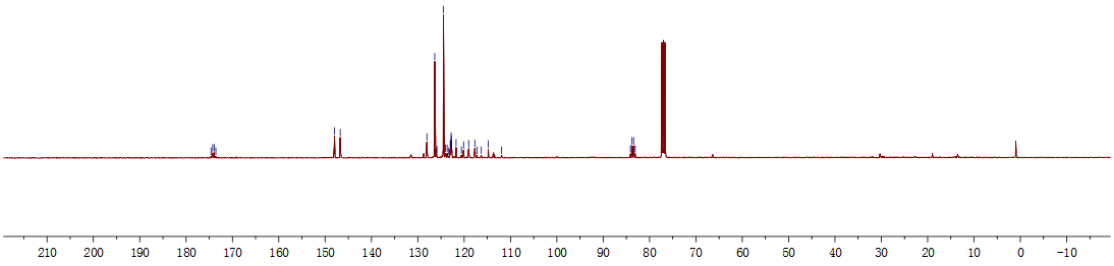
^{19}F NMR spectrum of **3m** in $CDCl_3$



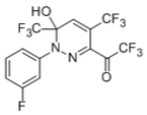
^{13}C NMR spectrum of **3m** in $CDCl_3$

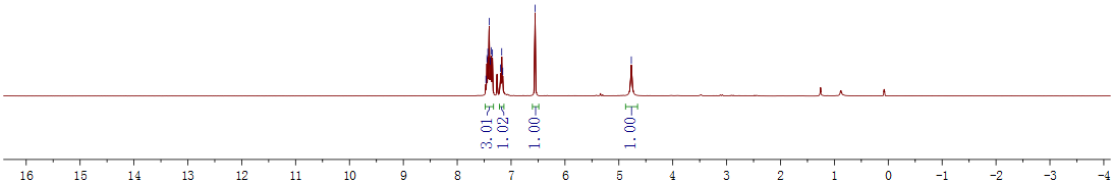




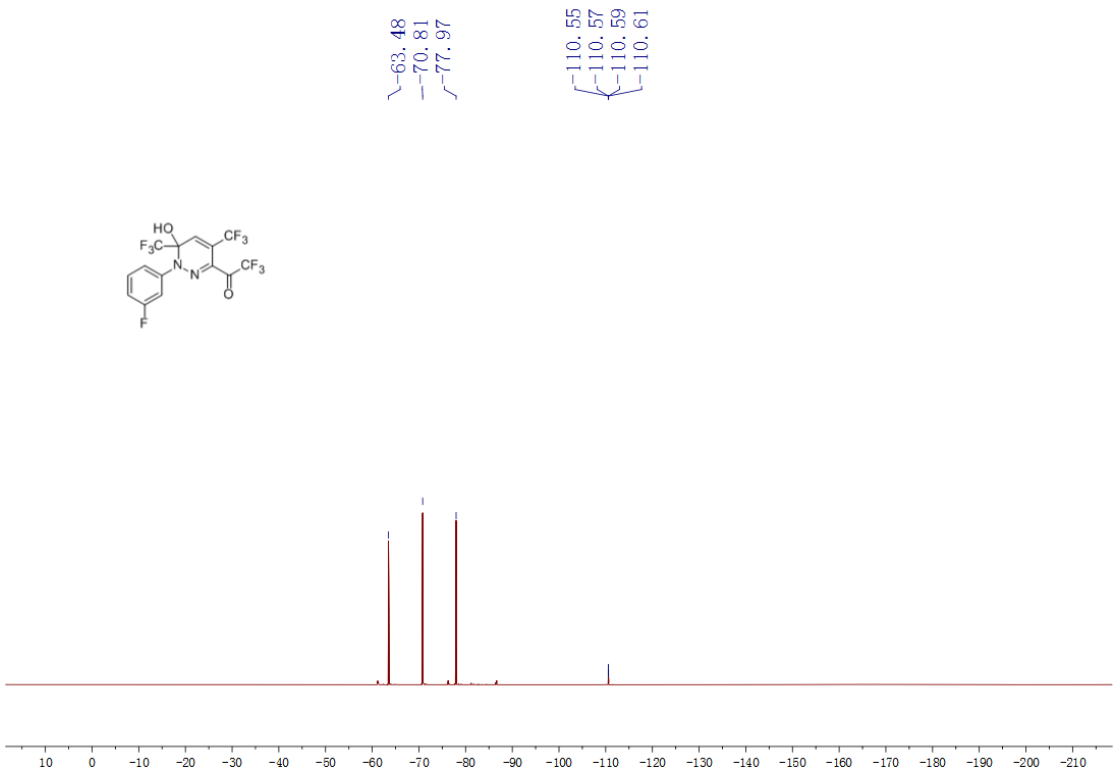


^{1}H NMR spectrum of **3n** in $CDCl_3$

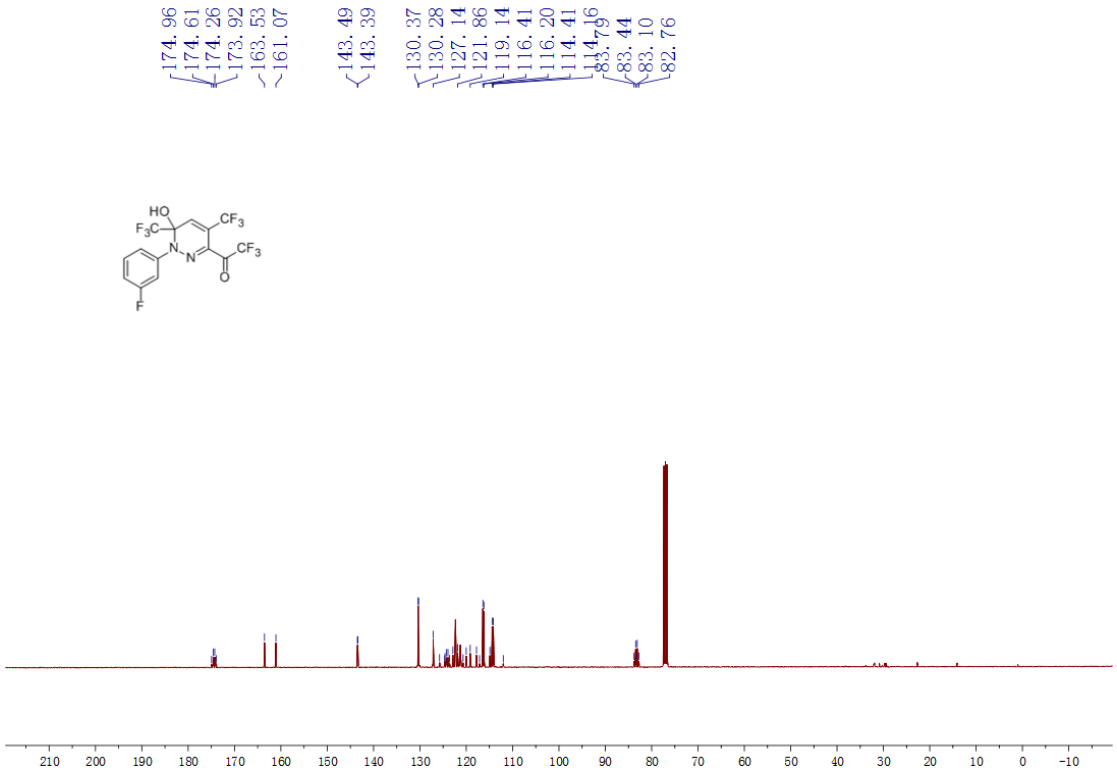




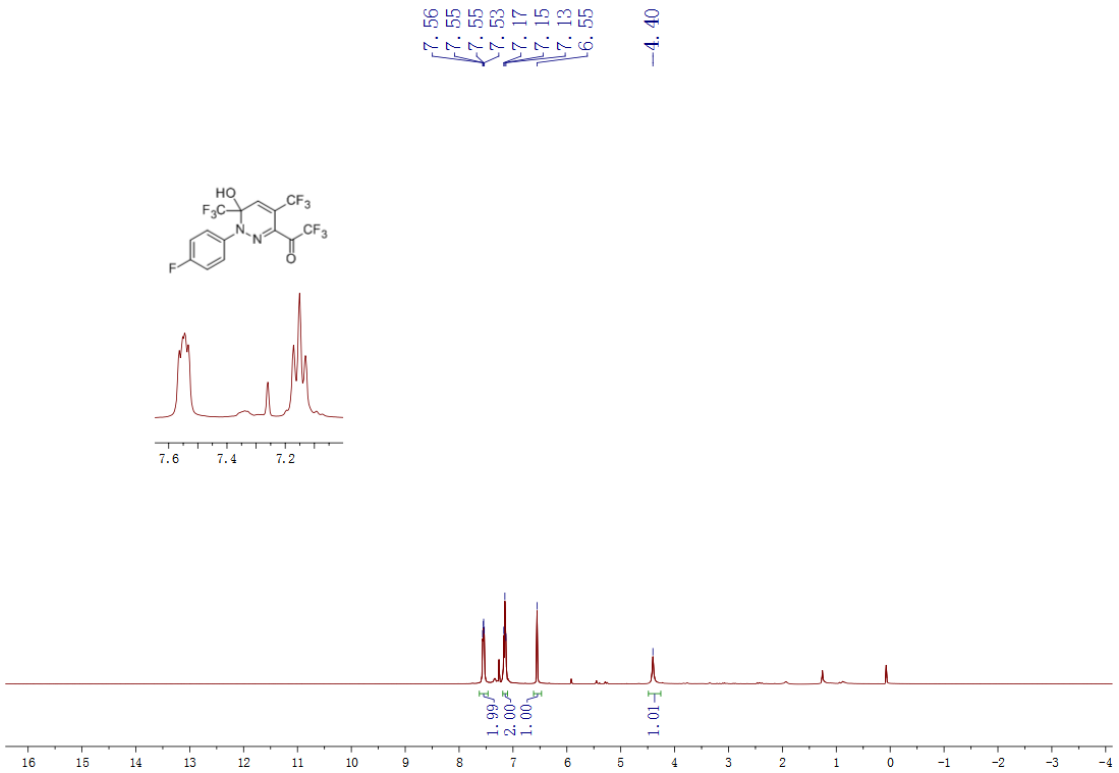
^{19}F NMR spectrum of **3n** in $CDCl_3$



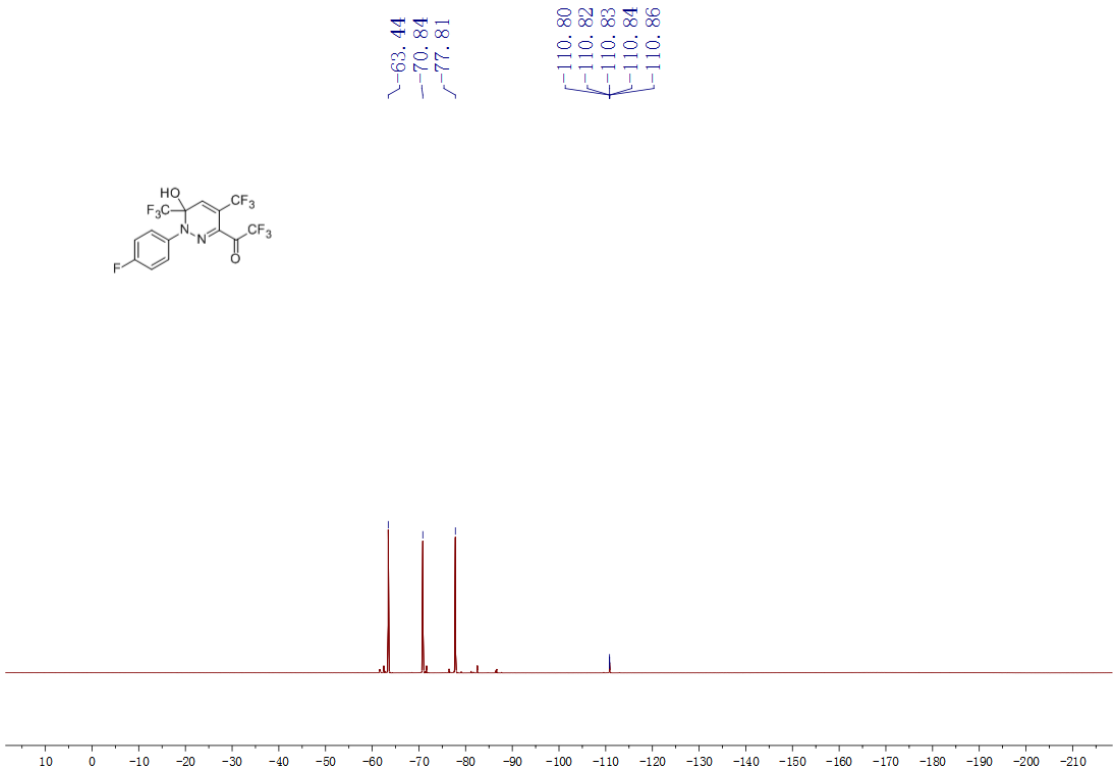
^{13}C NMR spectrum of **3n** in $CDCl_3$



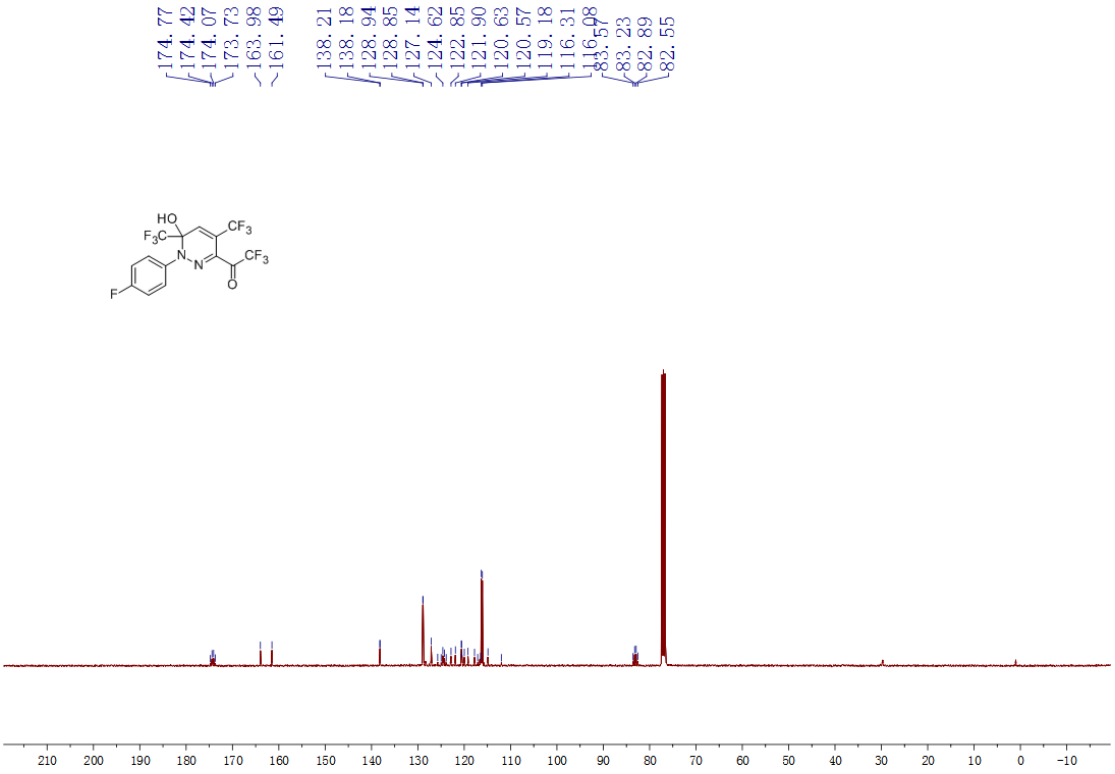
^{1}H NMR spectrum of **3o** in $CDCl_3$



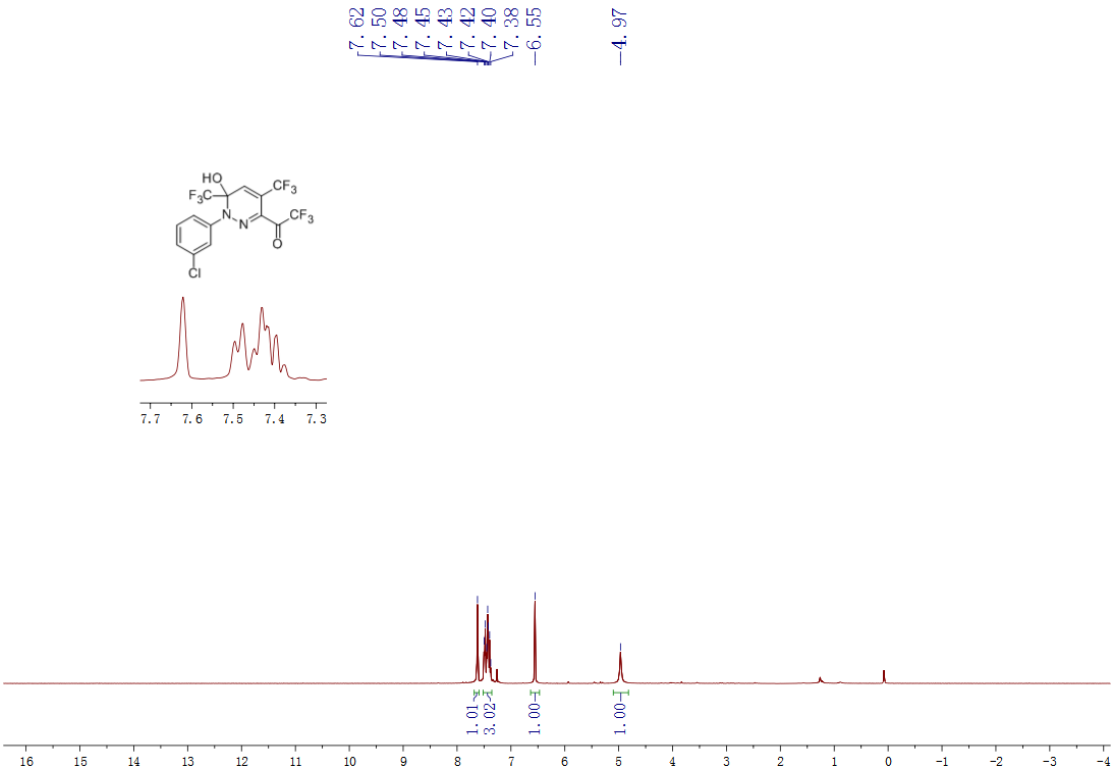
^{19}F NMR spectrum of **3o** in $CDCl_3$



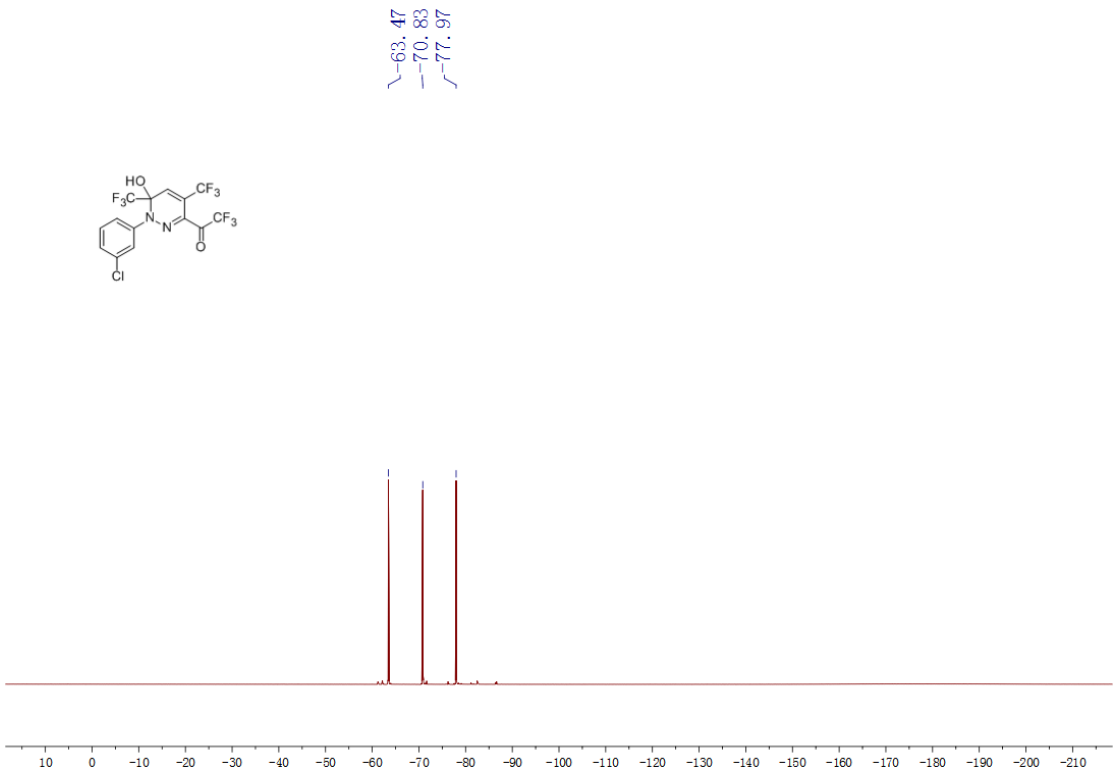
^{13}C NMR spectrum of **3o** in $CDCl_3$



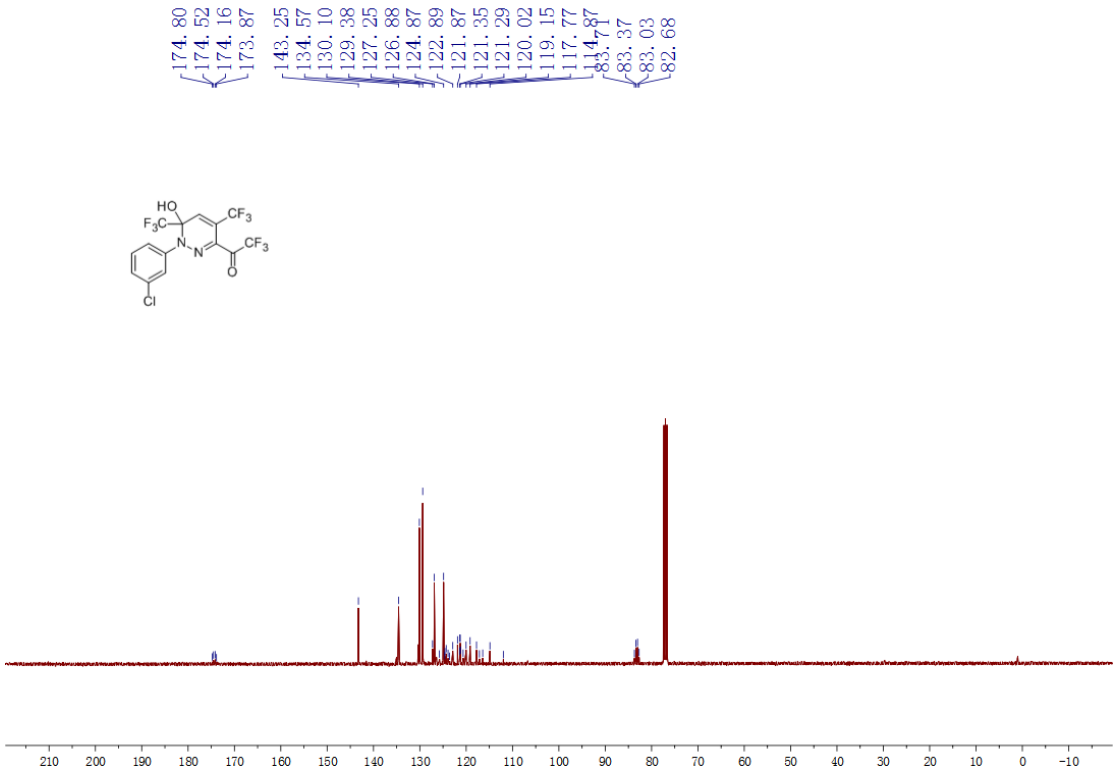
^{1}H NMR spectrum of **3p** in $CDCl_3$



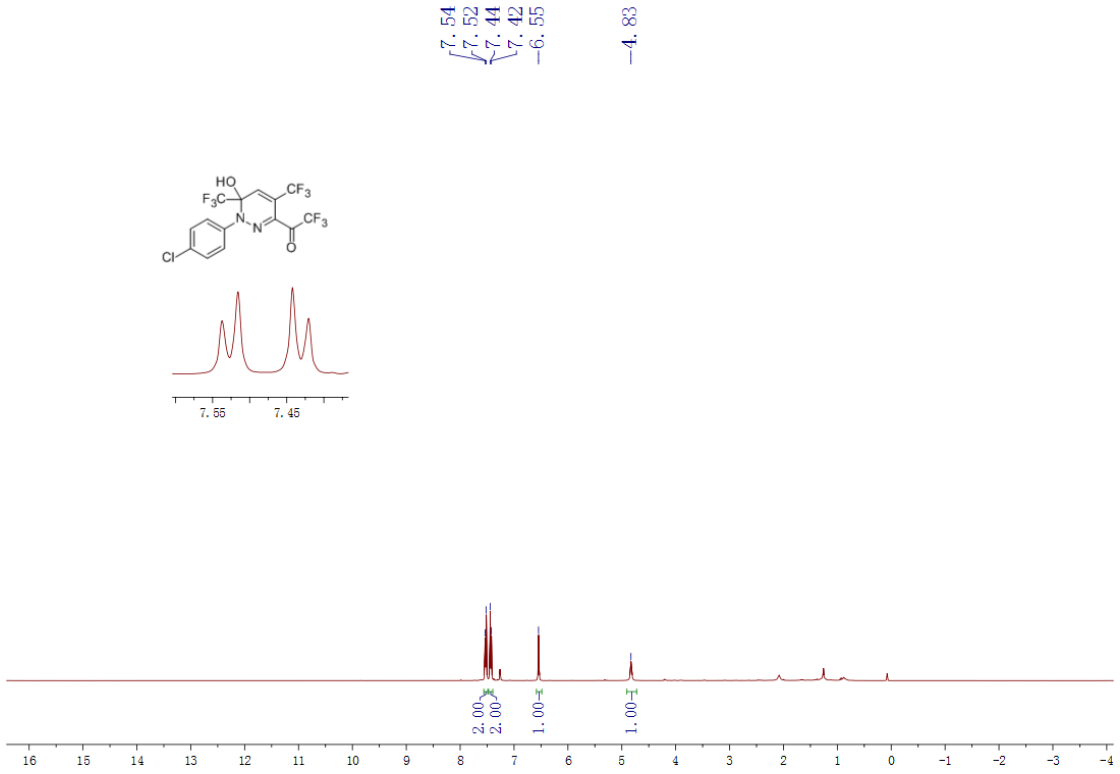
^{19}F NMR spectrum of **3p** in $CDCl_3$



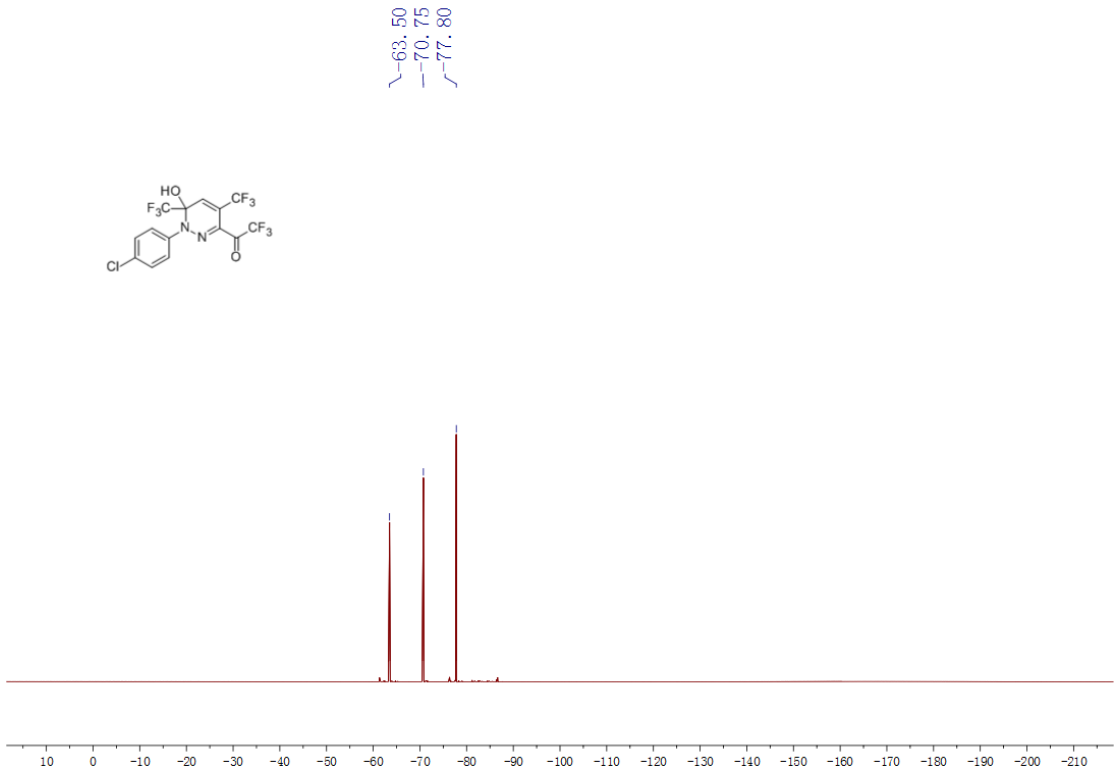
^{13}C NMR spectrum of **3p** in $CDCl_3$



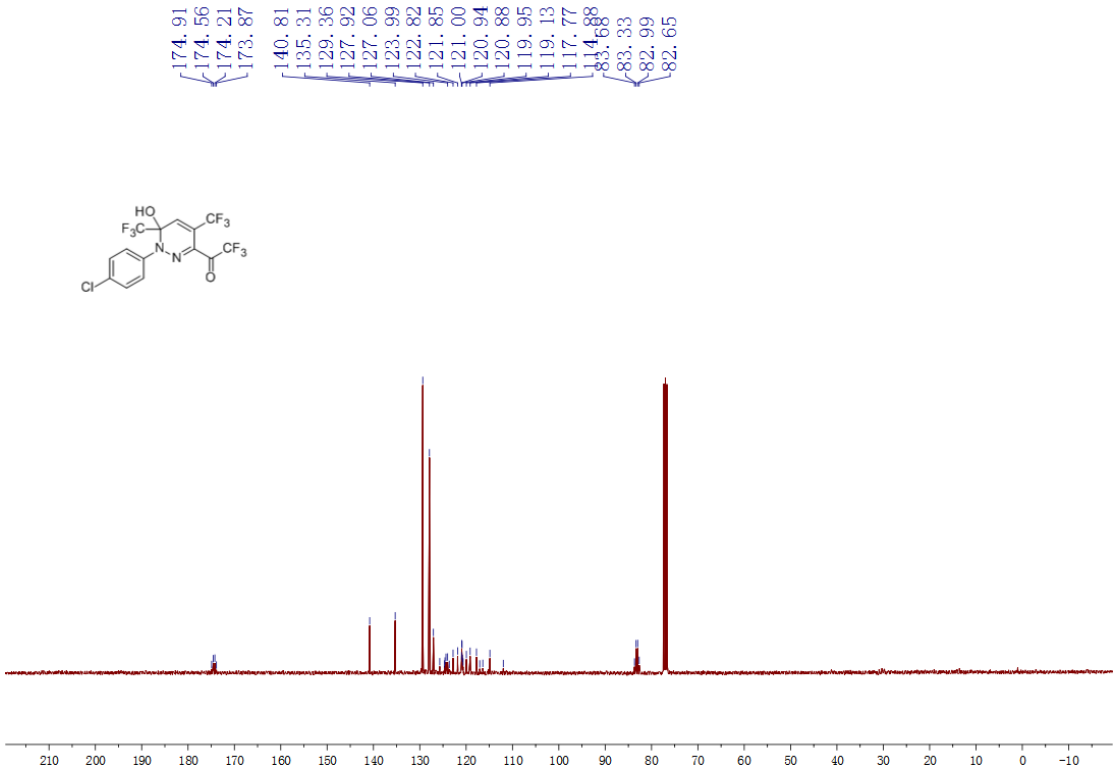
^{1}H NMR spectrum of **3q** in $CDCl_3$



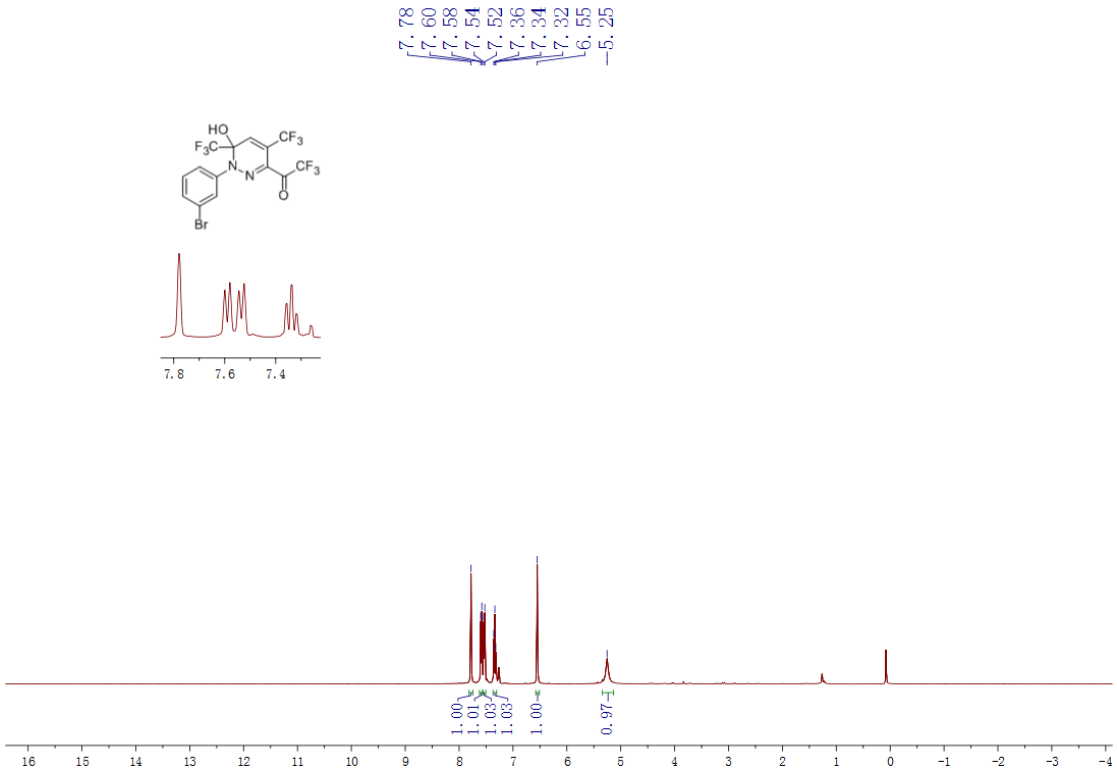
^{19}F NMR spectrum of **3q** in $CDCl_3$



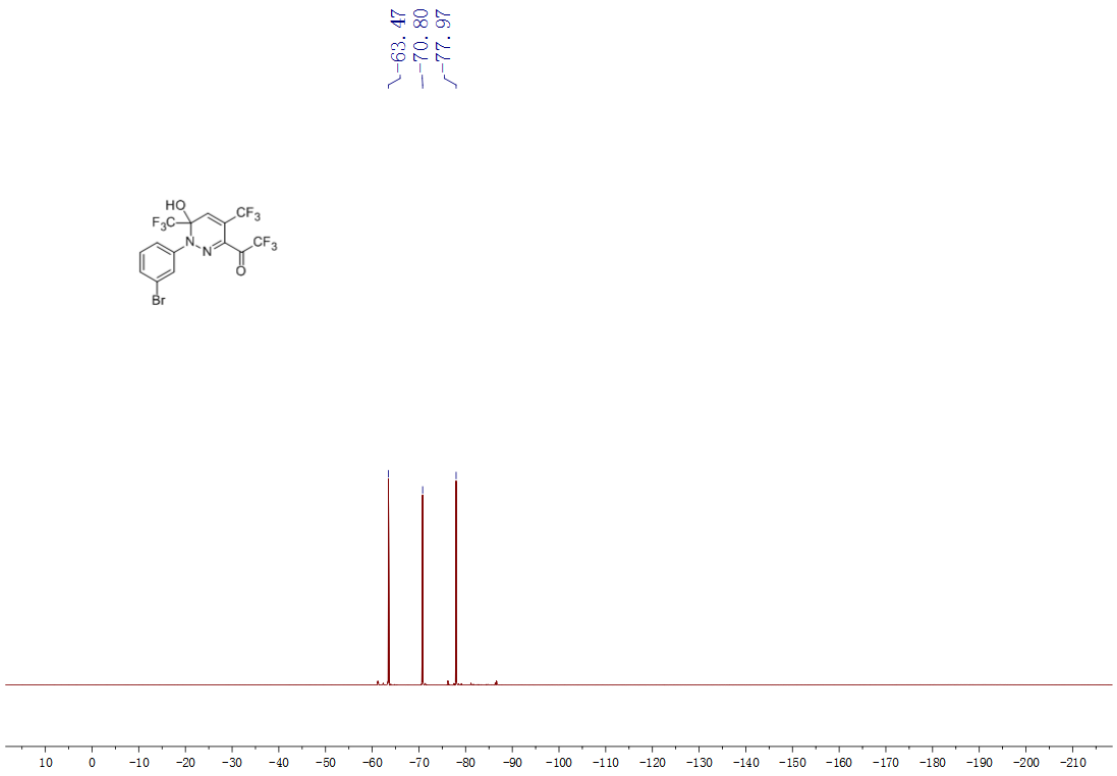
^{13}C NMR spectrum of **3q** in $CDCl_3$



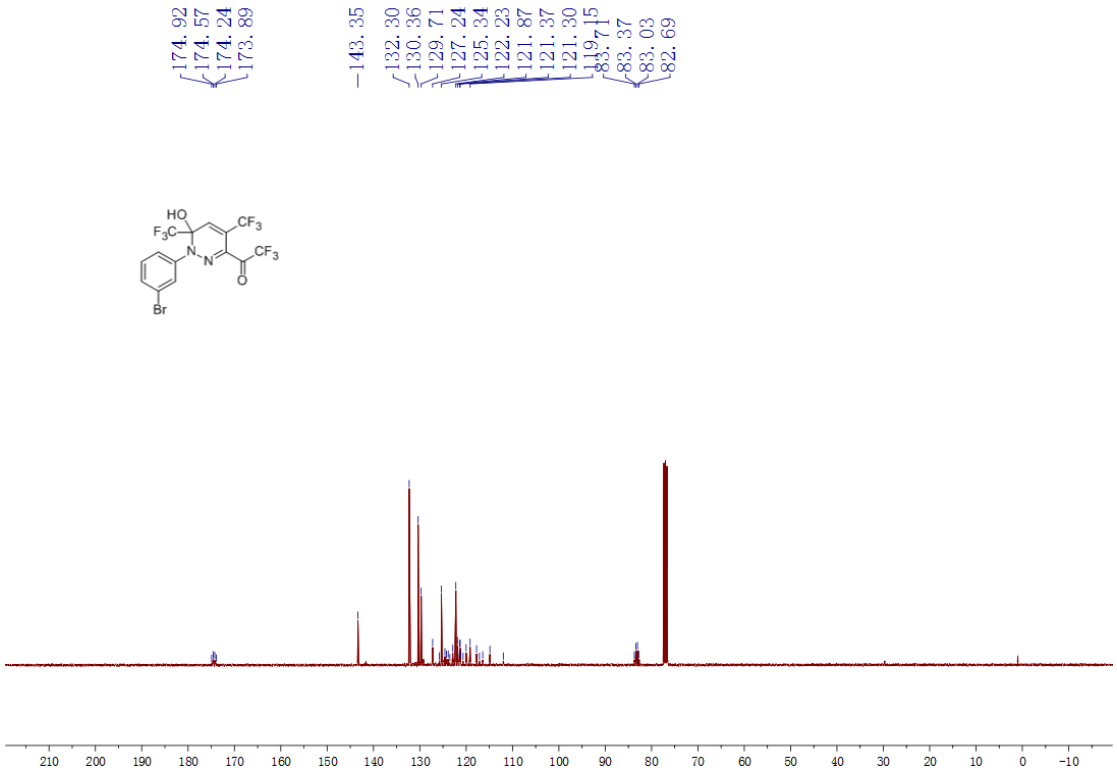
^{1}H NMR spectrum of **3r** in $CDCl_3$



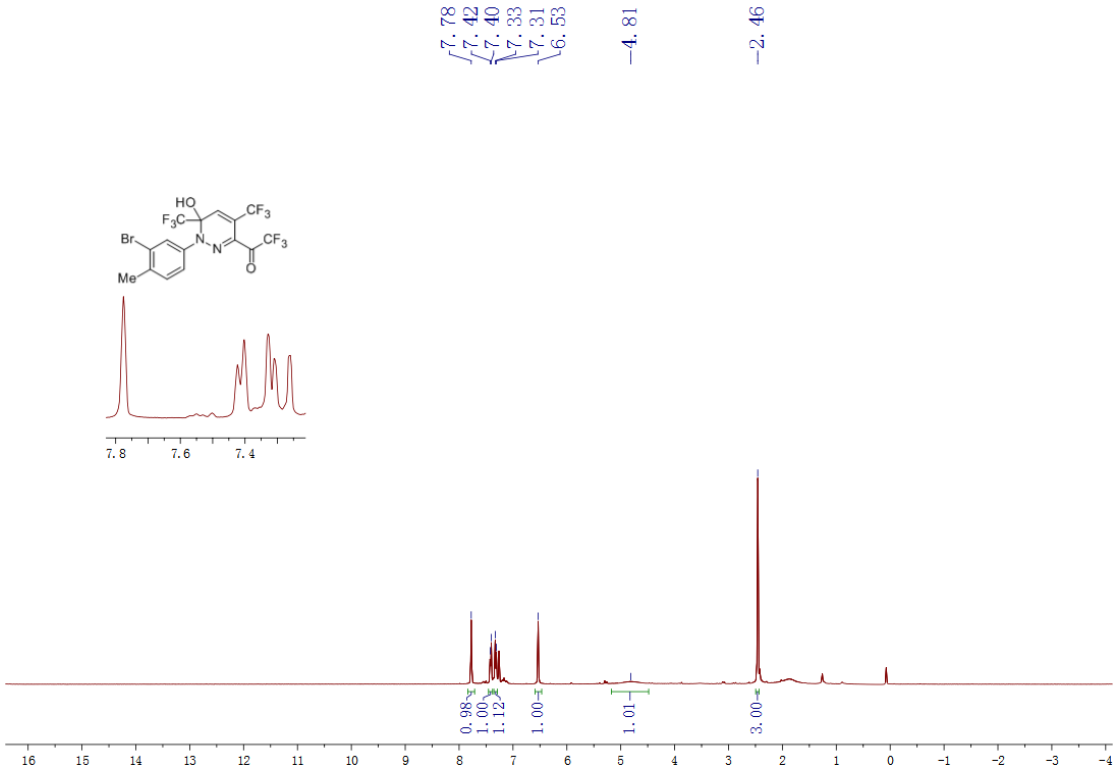
^{19}F NMR spectrum of **3r** in $CDCl_3$



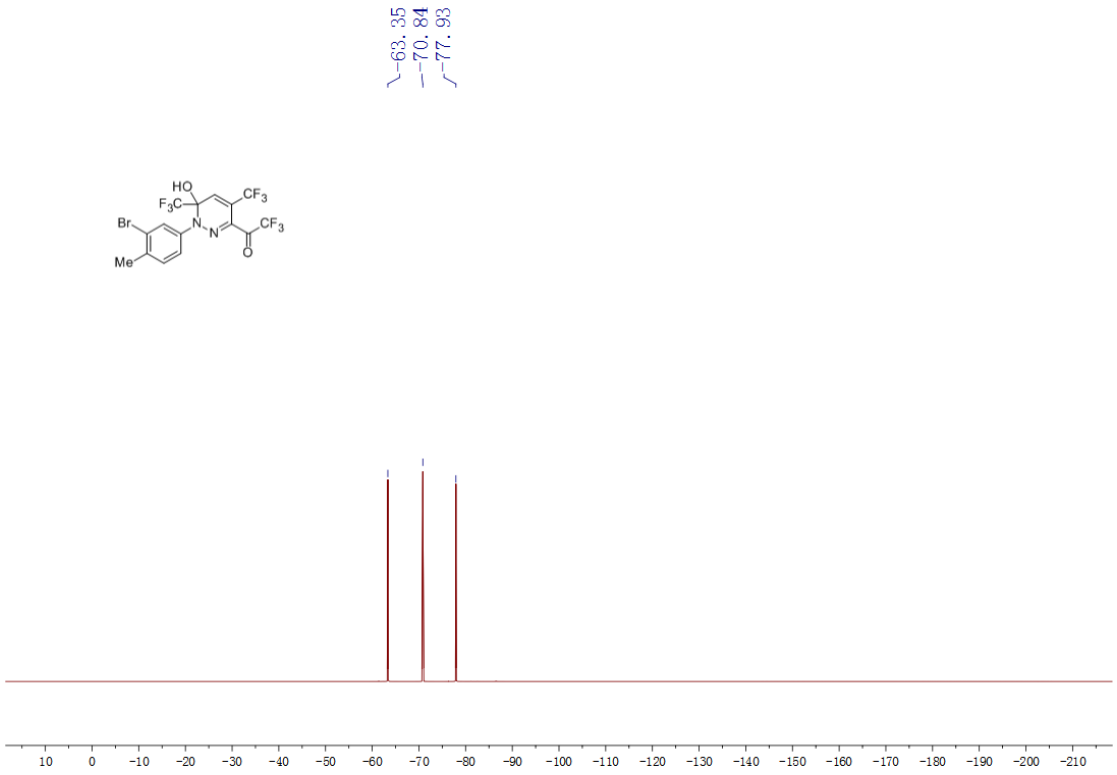
^{13}C NMR spectrum of **3r** in $CDCl_3$



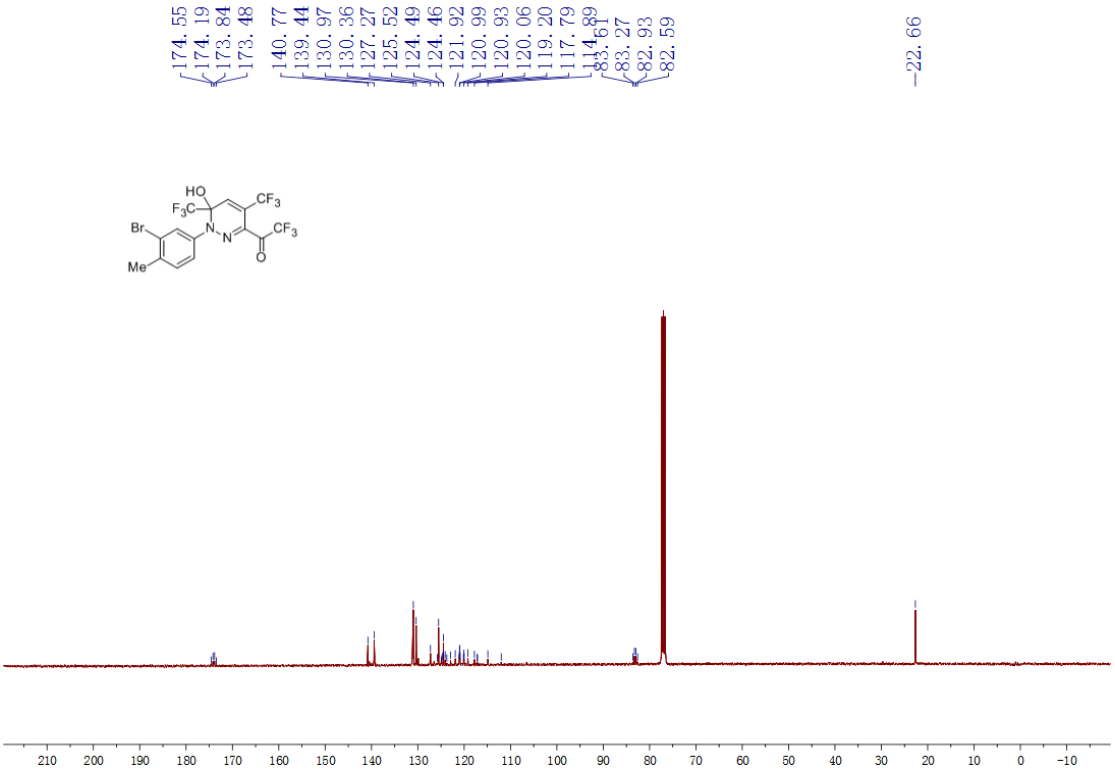
^{1}H NMR spectrum of **3s** in $CDCl_3$



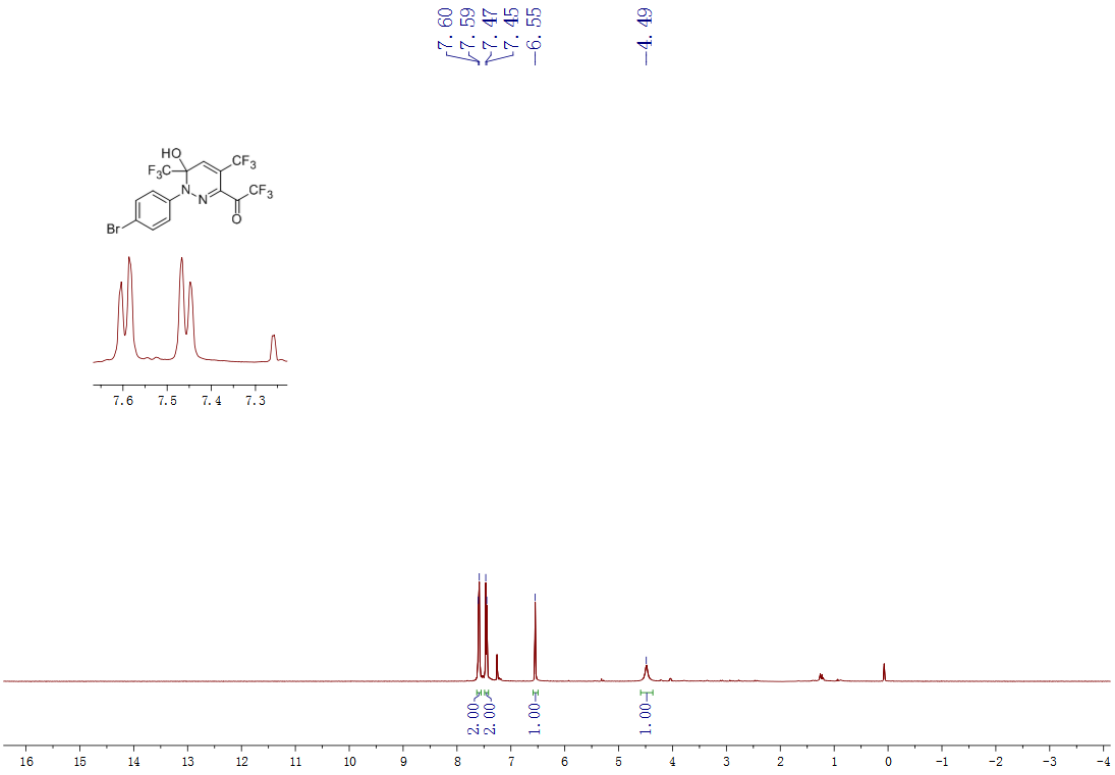
^{19}F NMR spectrum of **3s** in $CDCl_3$



^{13}C NMR spectrum of **3s** in $CDCl_3$

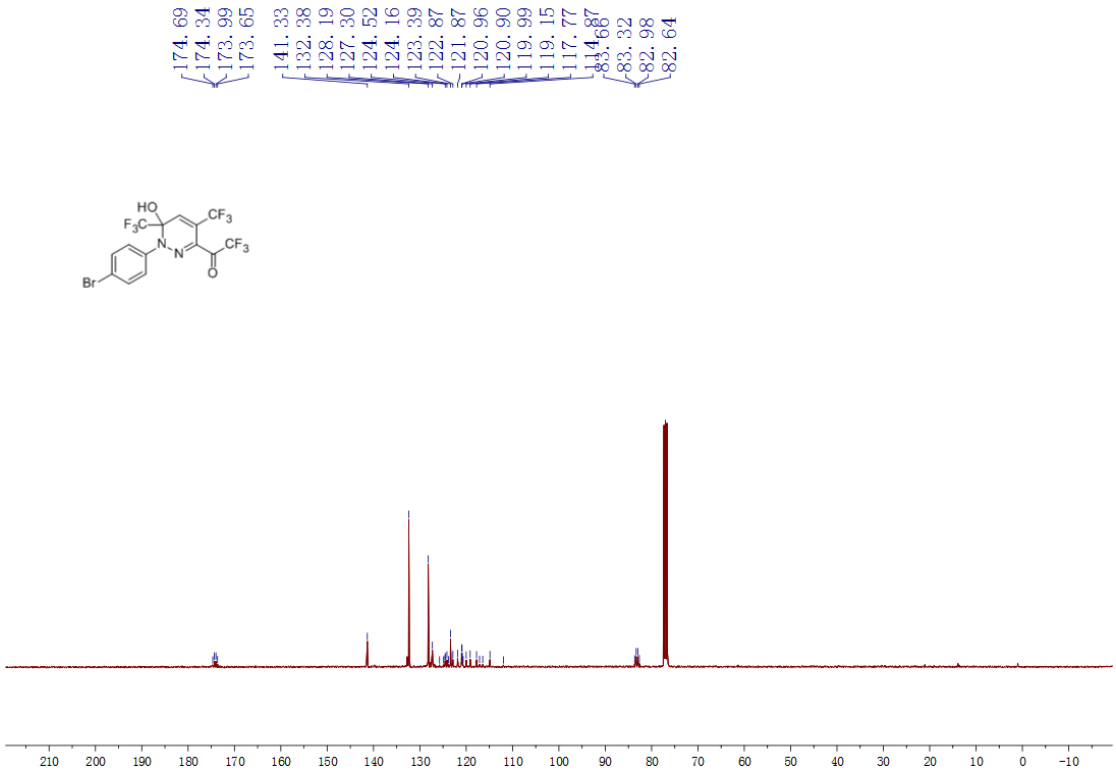


^{1}H NMR spectrum of **3t** in $CDCl_3$

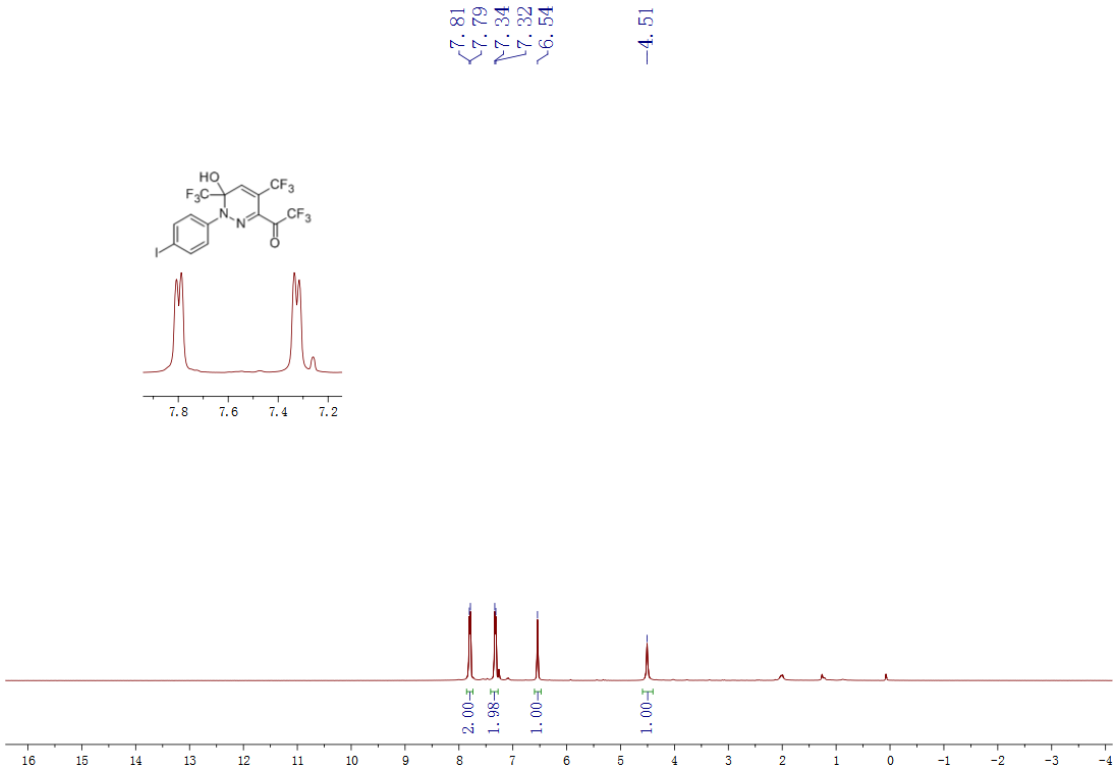


^{19}F NMR spectrum of **3t** in $CDCl_3$

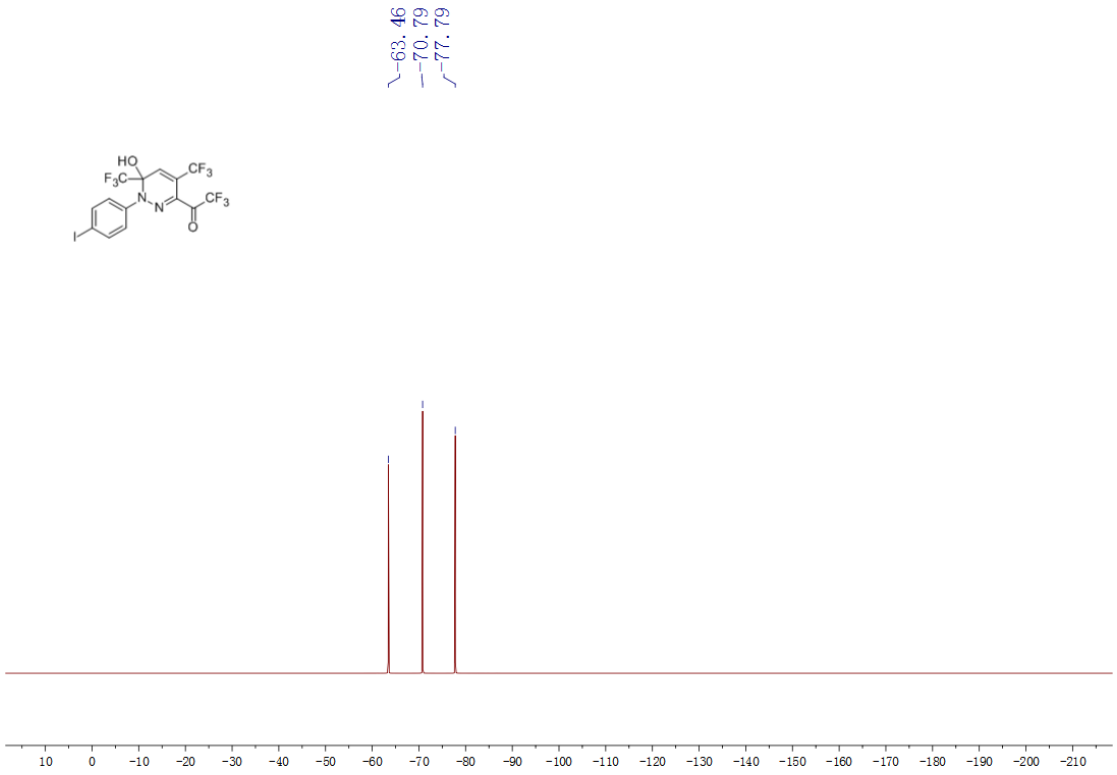
^{13}C NMR spectrum of **3t** in $CDCl_3$



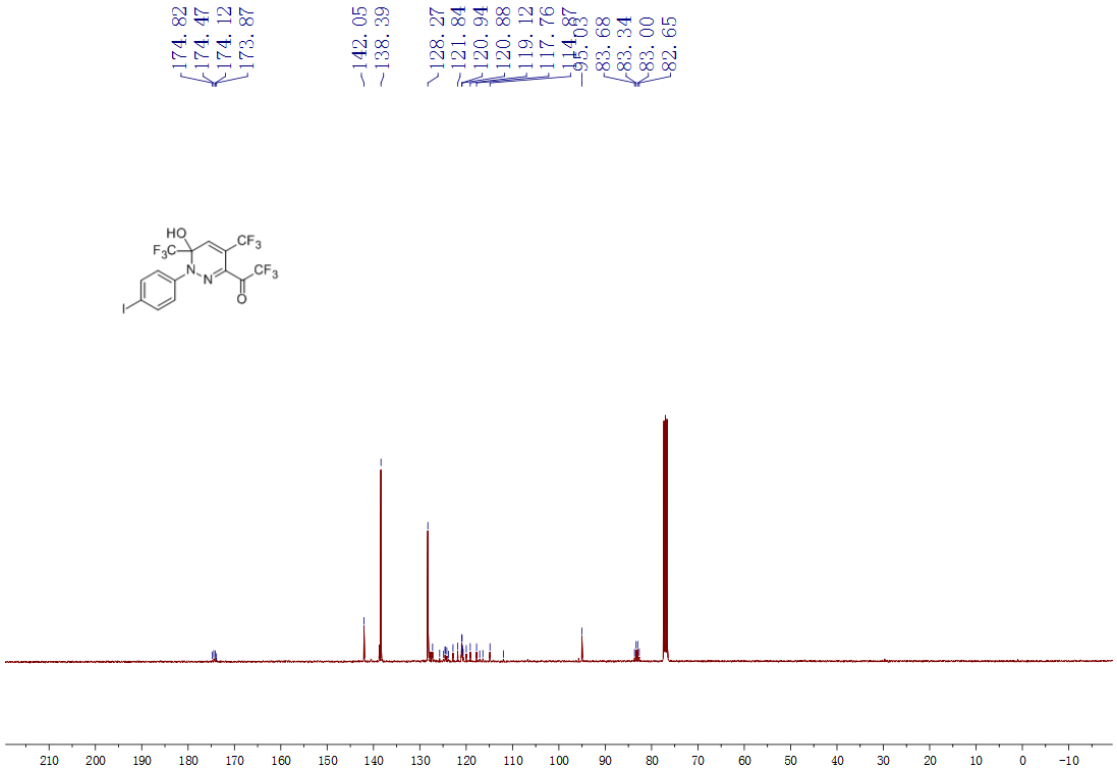
^{1}H NMR spectrum of **3u** in $CDCl_3$



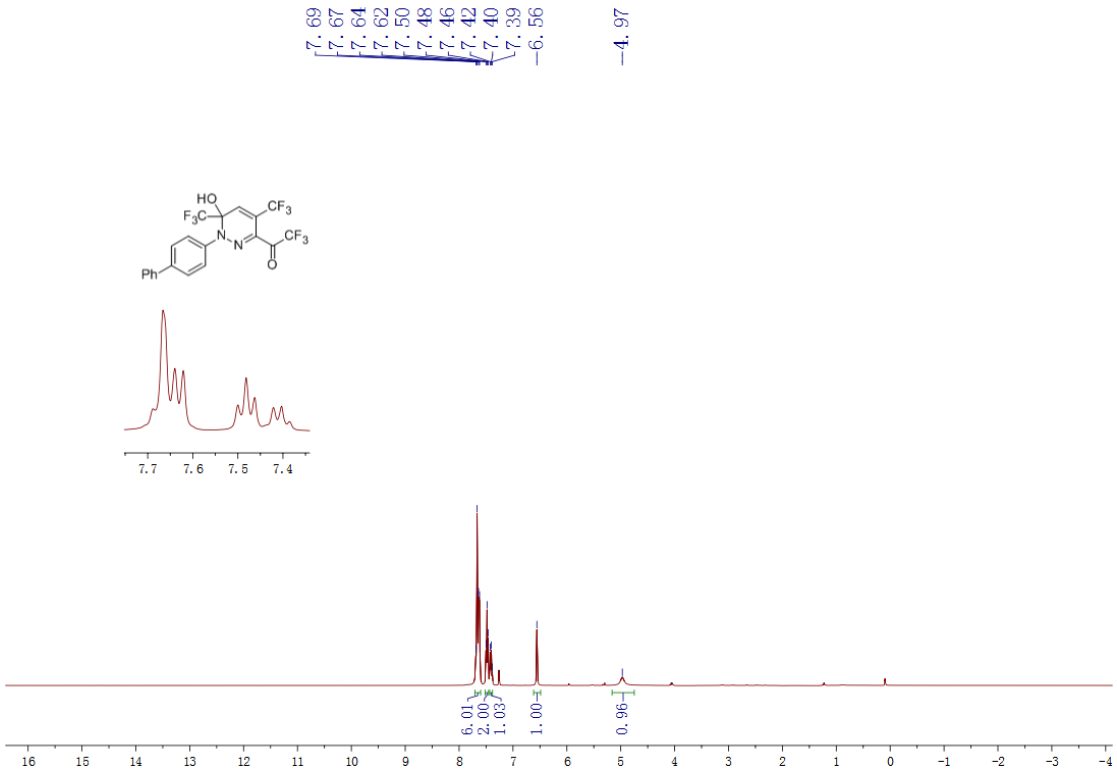
^{19}F NMR spectrum of **3u** in $CDCl_3$



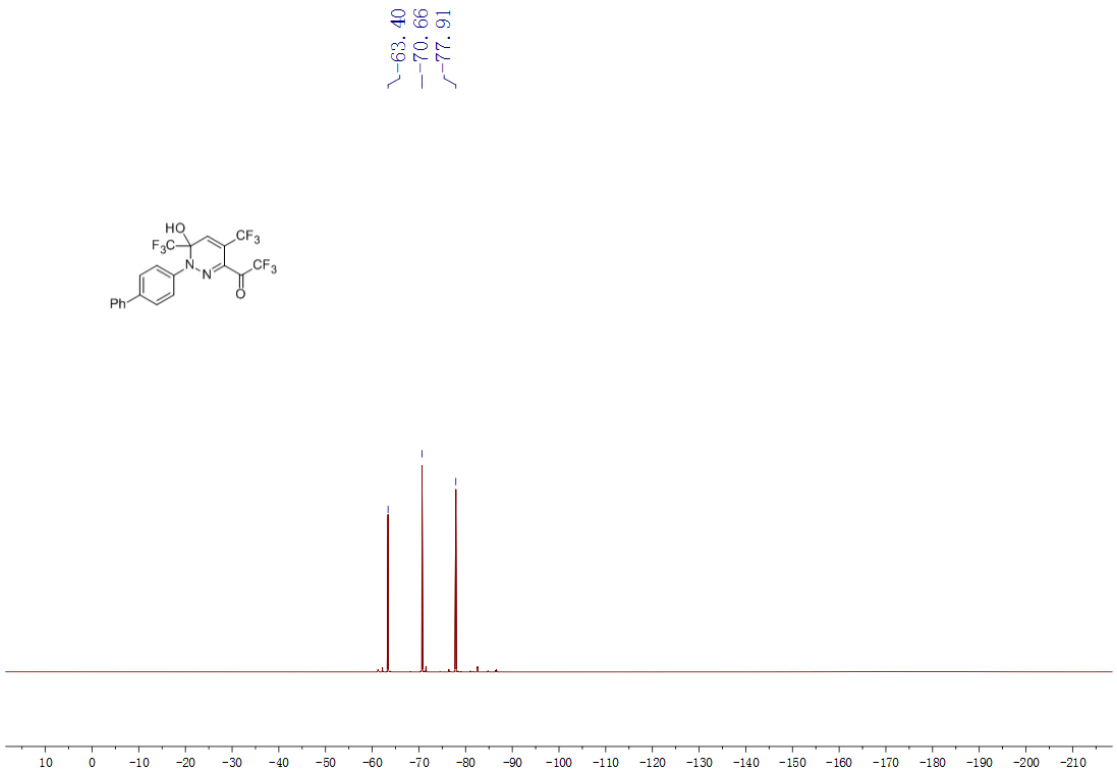
^{13}C NMR spectrum of **3u** in $CDCl_3$



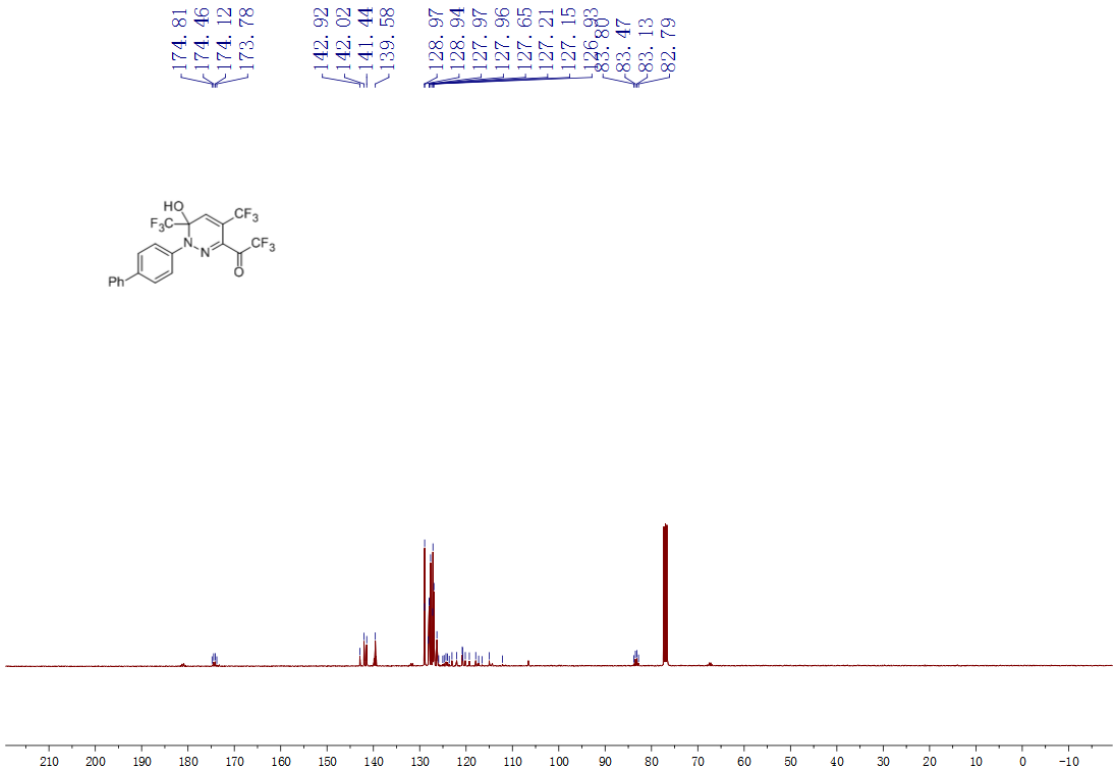
^{1}H NMR spectrum of **3v** in $CDCl_3$



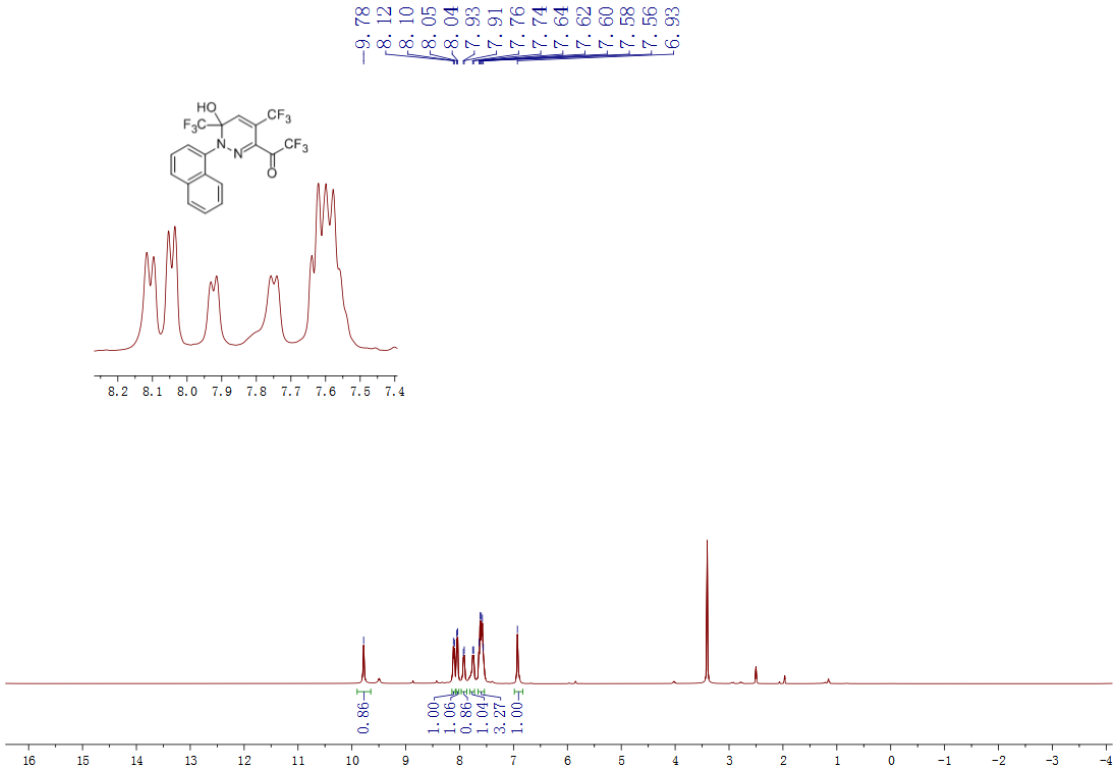
^{19}F NMR spectrum of **3v** in $CDCl_3$



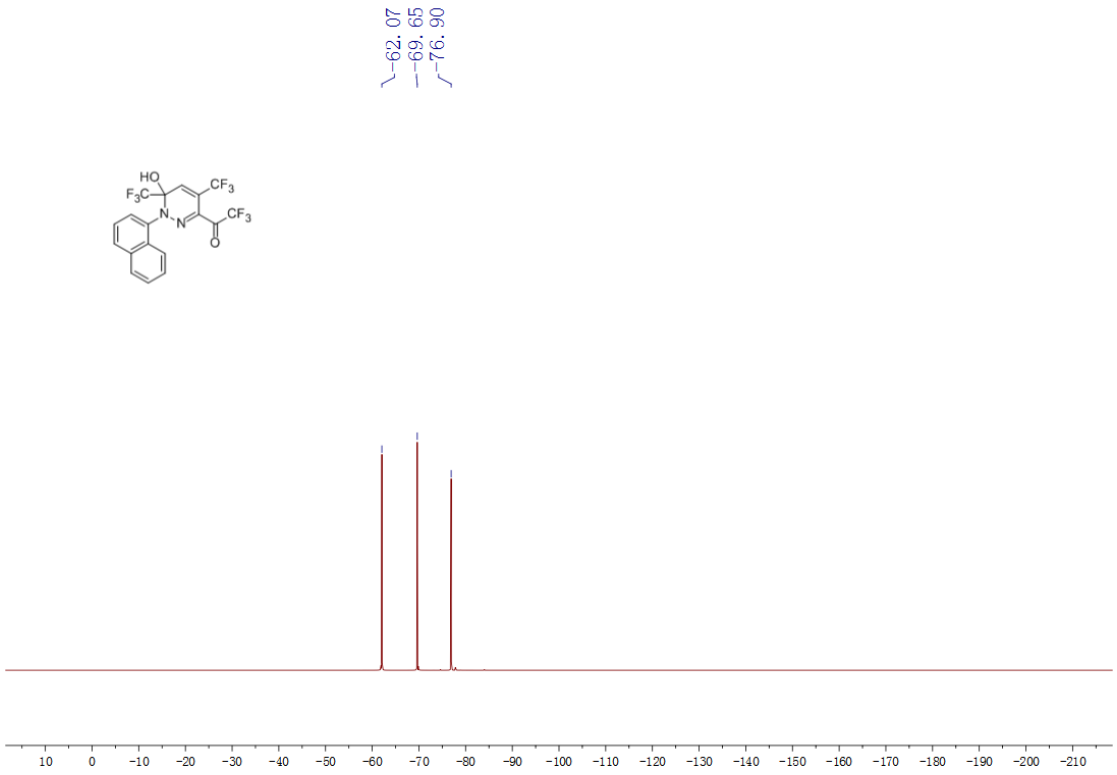
^{13}C NMR spectrum of **3v** in $CDCl_3$



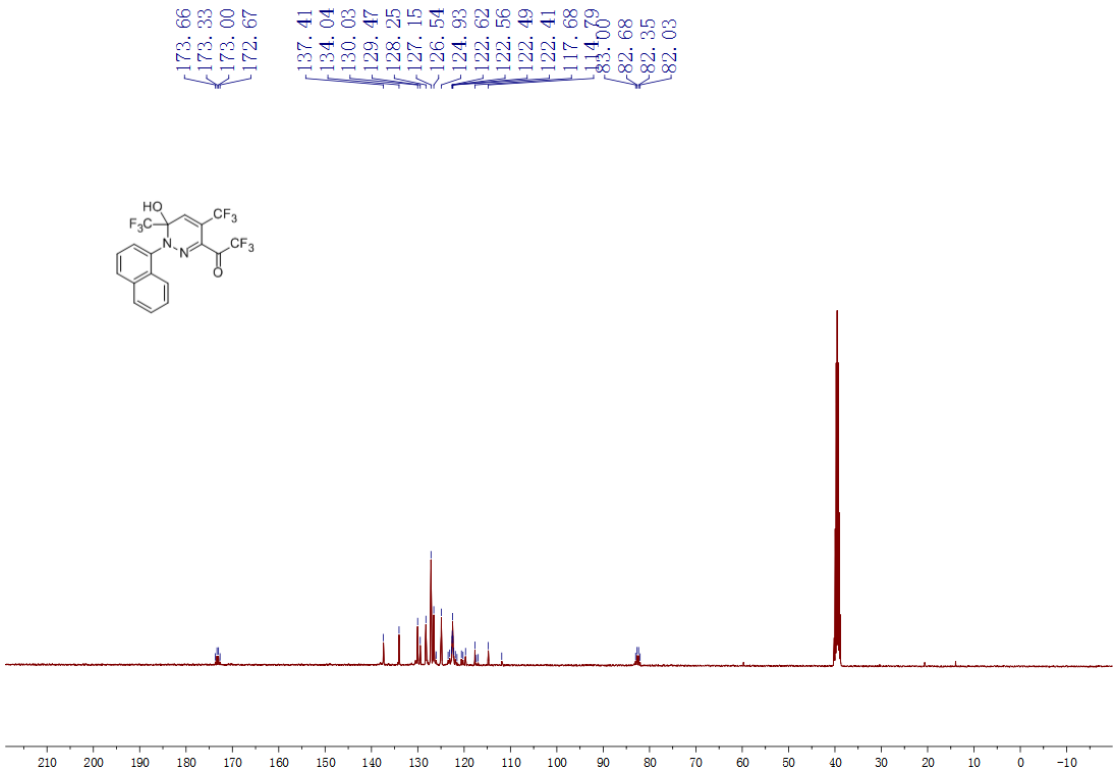
^{1}H NMR spectrum of **3w** in DMSO-d_6



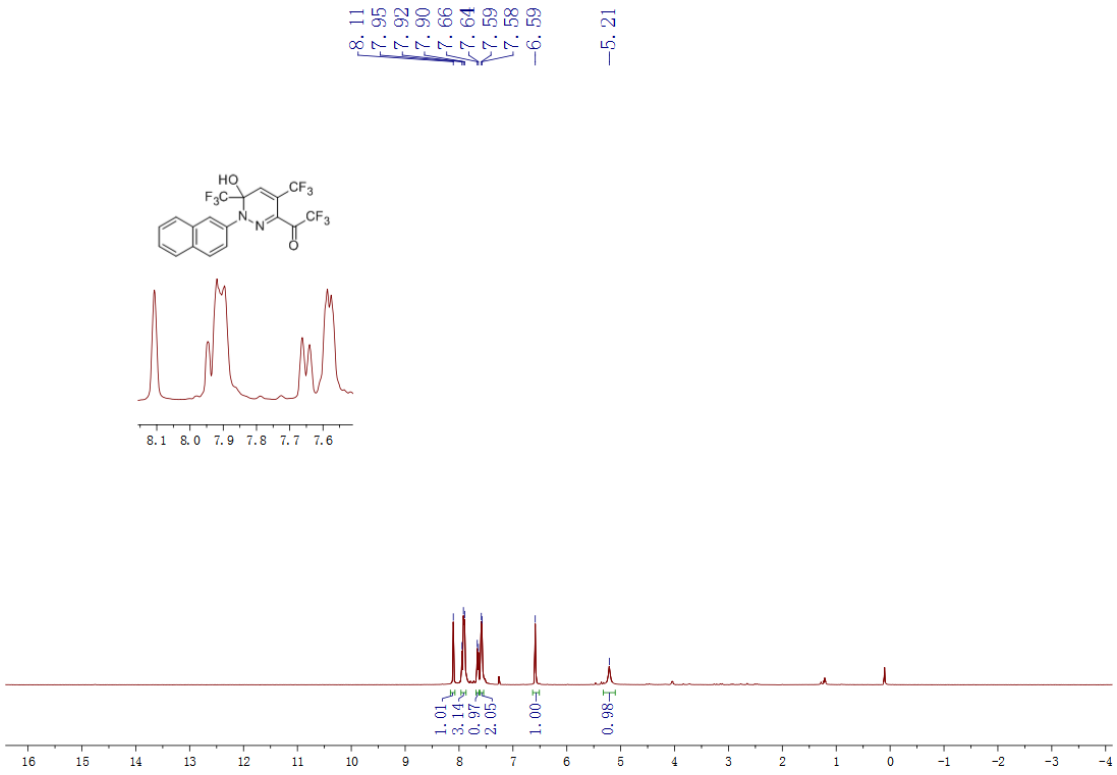
^{19}F NMR spectrum of **3w** in DMSO-d_6



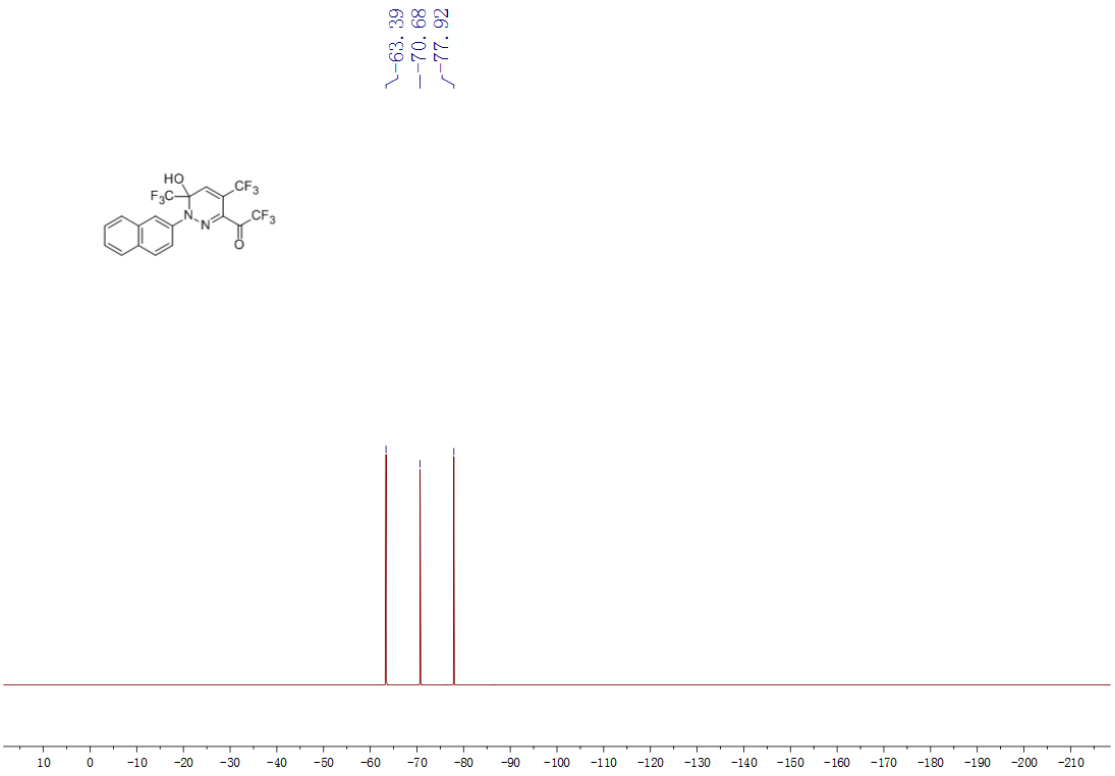
^{13}C NMR spectrum of **3w** in DMSO-d_6



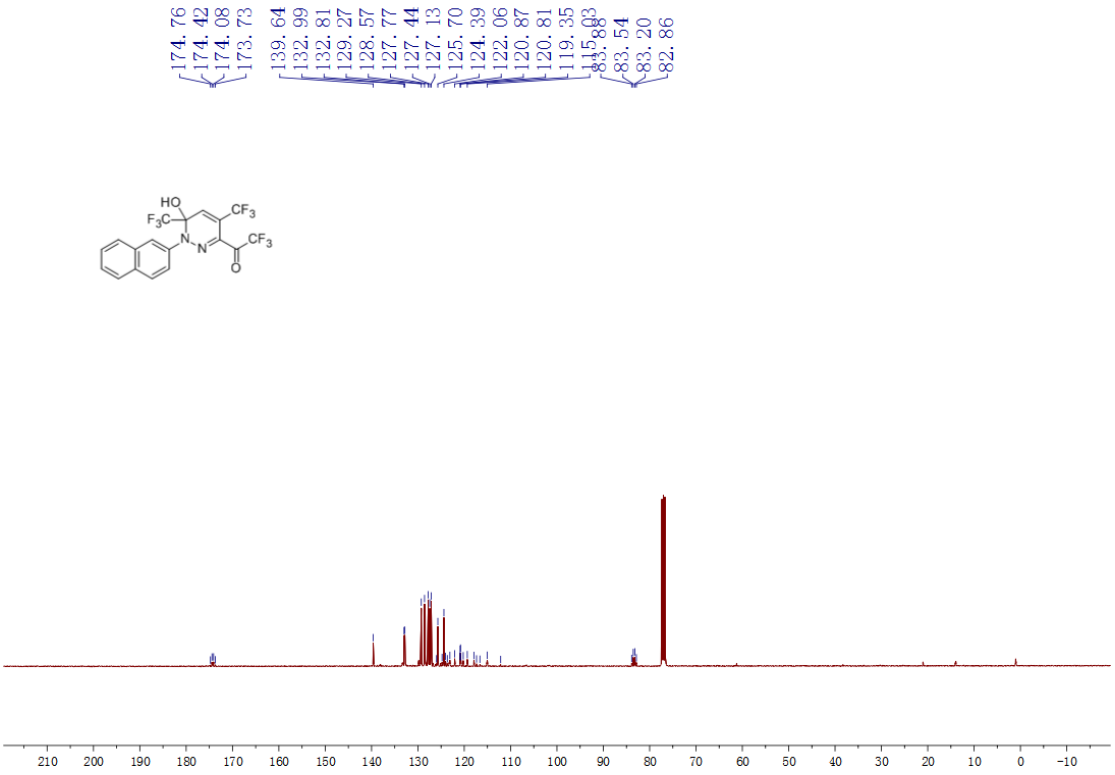
^{1}H NMR spectrum of **3x** in $CDCl_3$



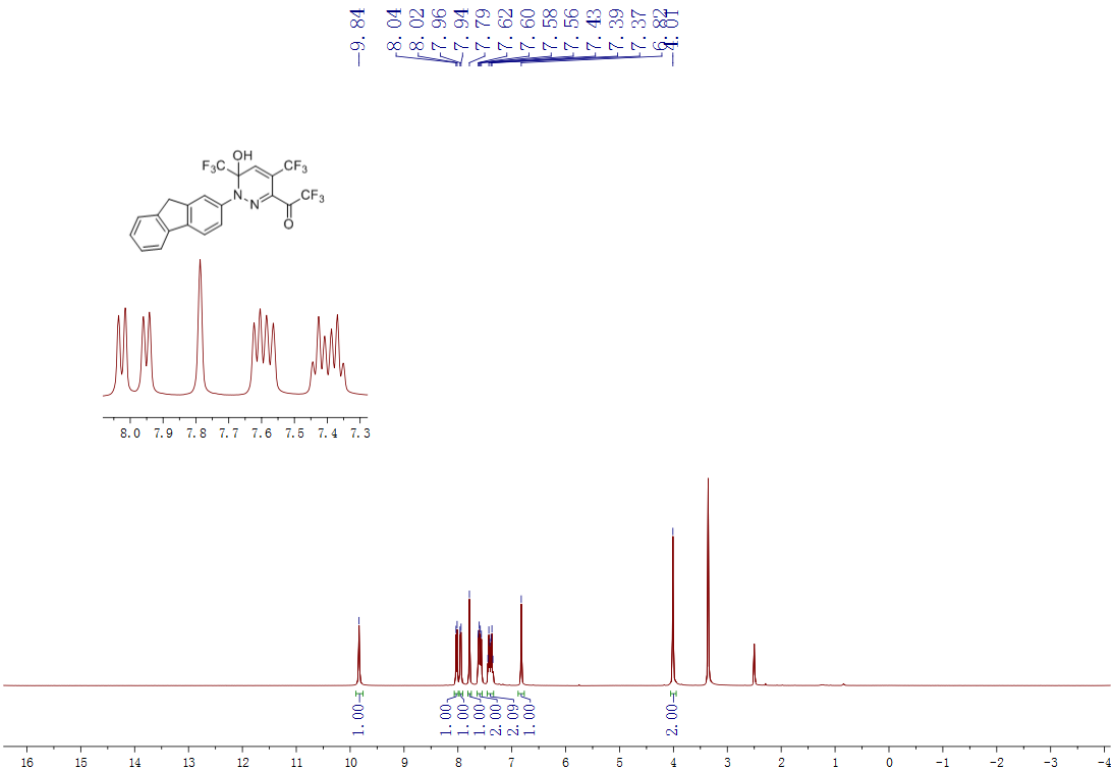
^{19}F NMR spectrum of **3x** in $CDCl_3$



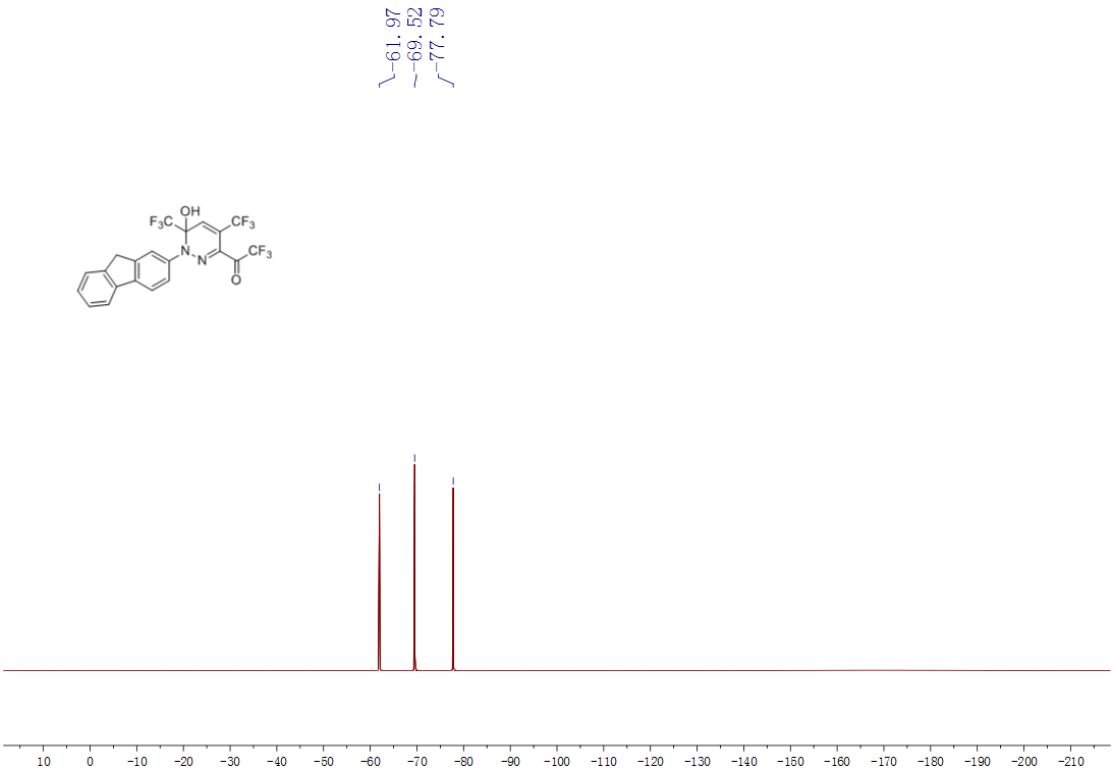
^{13}C NMR spectrum of **3x** in $CDCl_3$



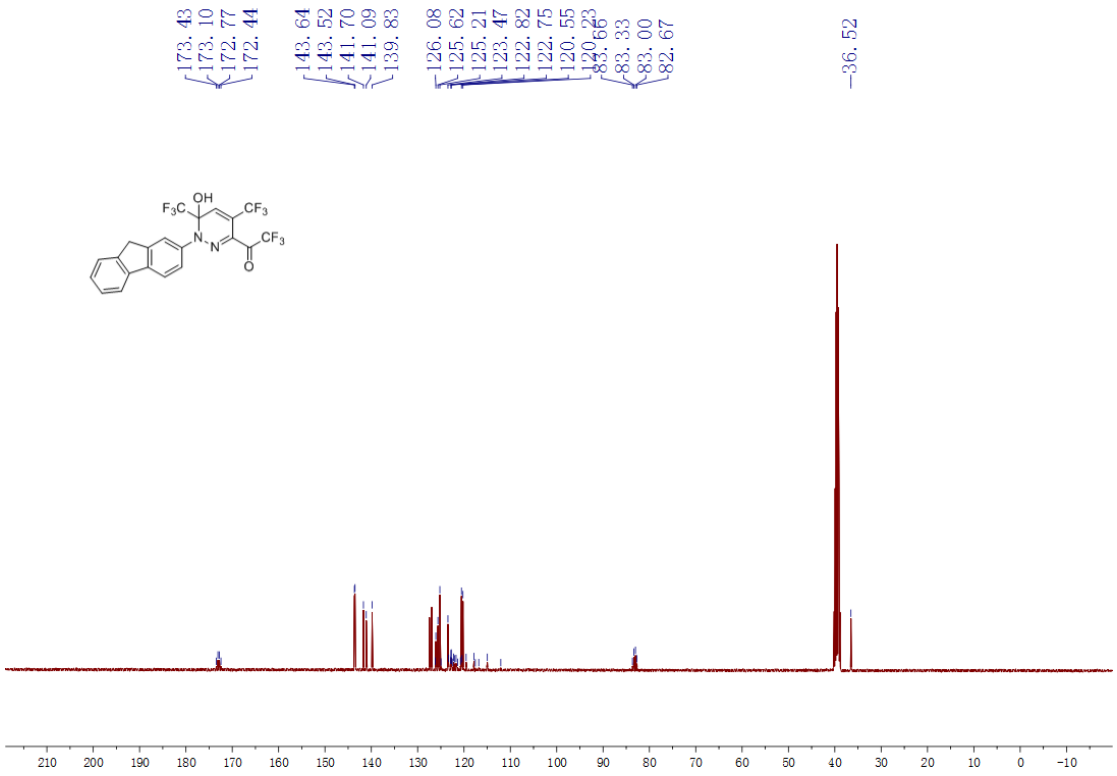
^{1}H NMR spectrum of **3y** in DMSO-d_6



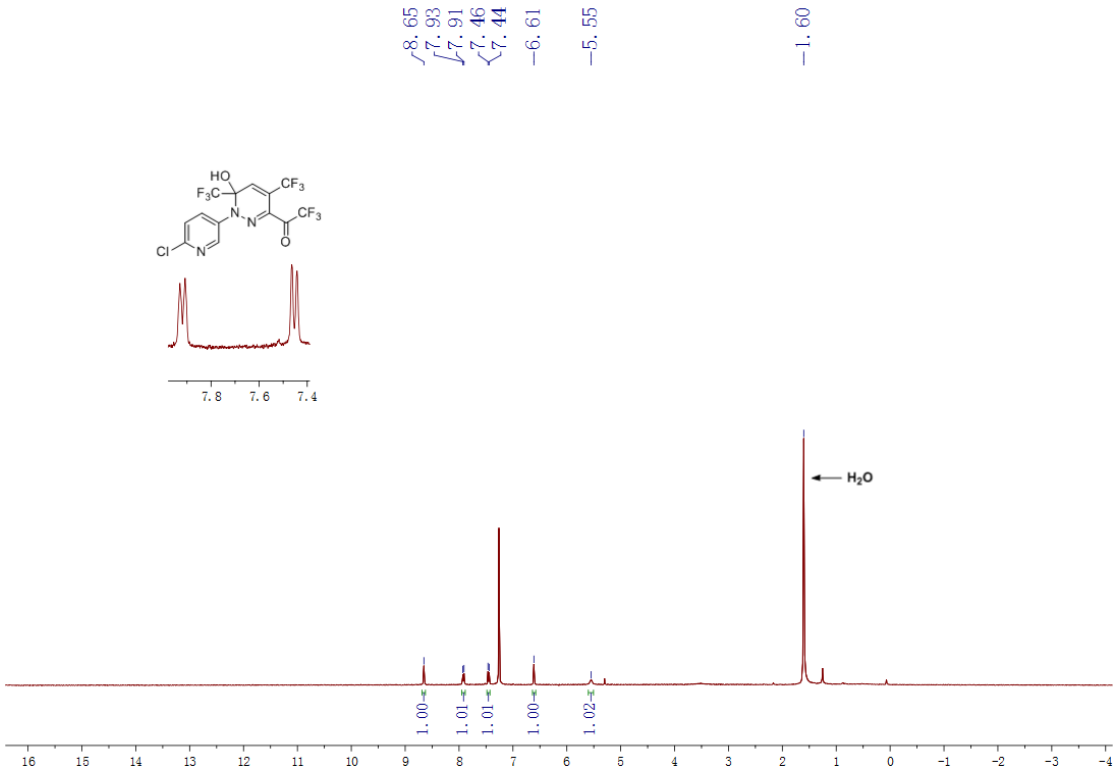
^{19}F NMR spectrum of **3y** in DMSO-d_6



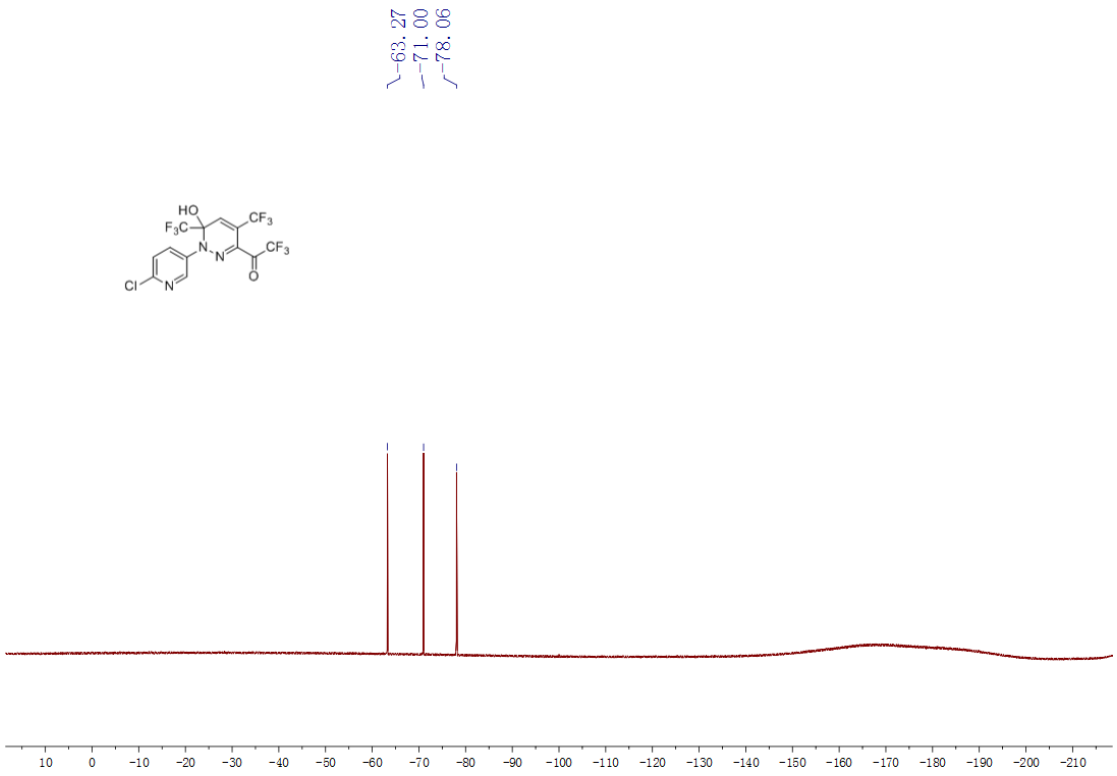
^{13}C NMR spectrum of **3y** in DMSO-d_6



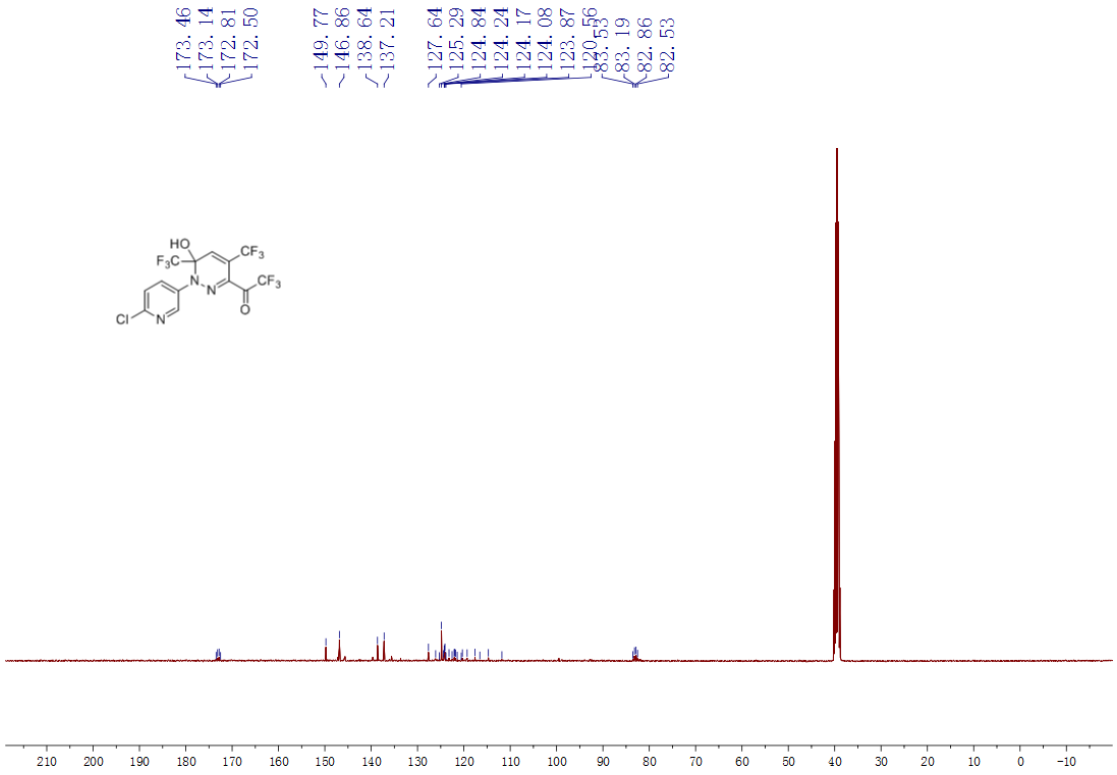
^{1}H NMR spectrum of **3z** in $CDCl_3$



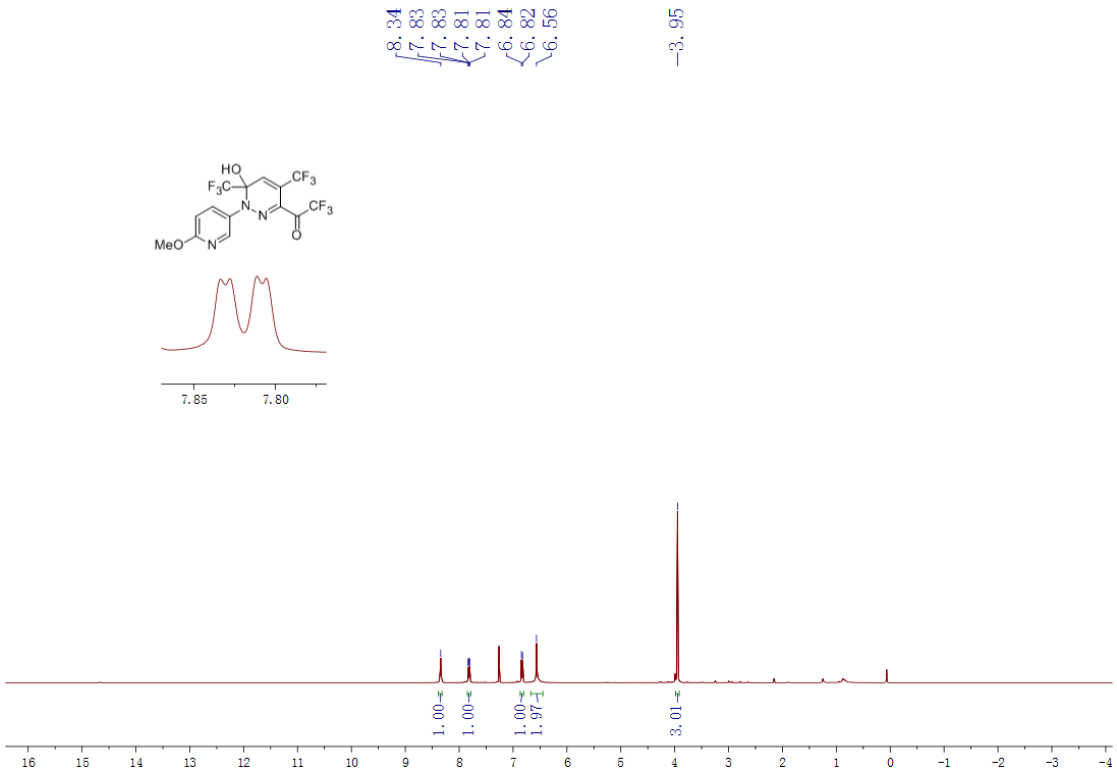
^{19}F NMR spectrum of **3z** in $CDCl_3$



^{13}C NMR spectrum of **3z** in DMSO-d_6

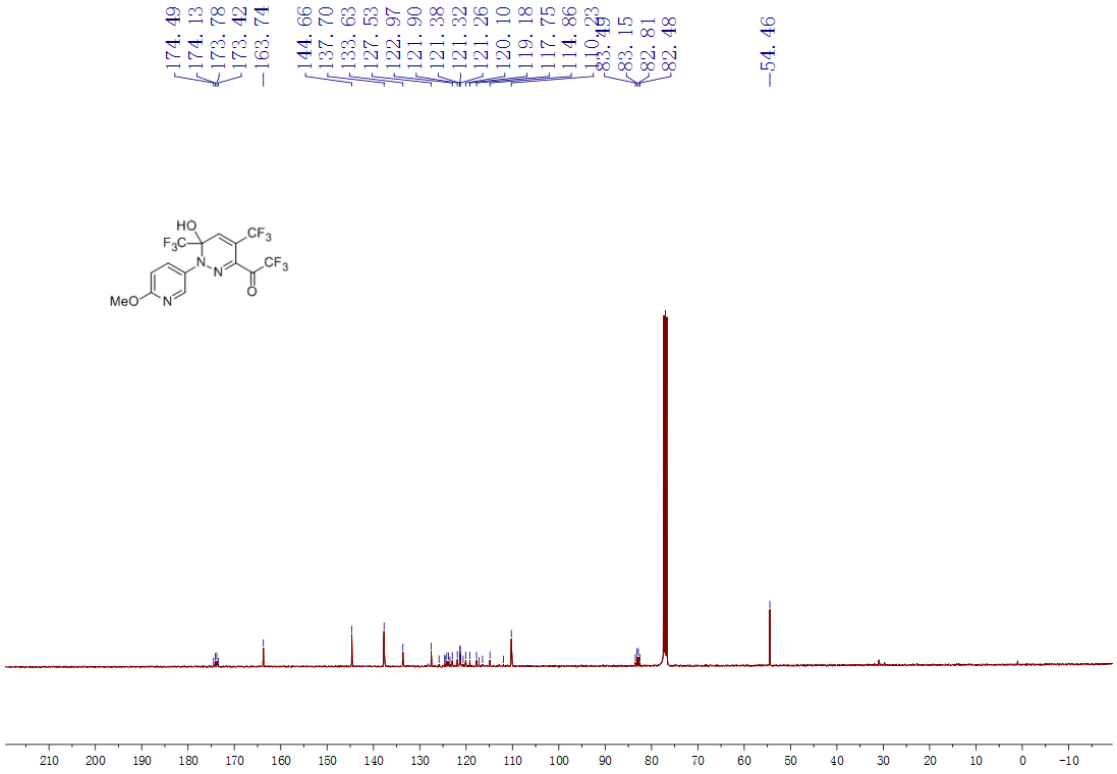


^{1}H NMR spectrum of **3aa** in $CDCl_3$

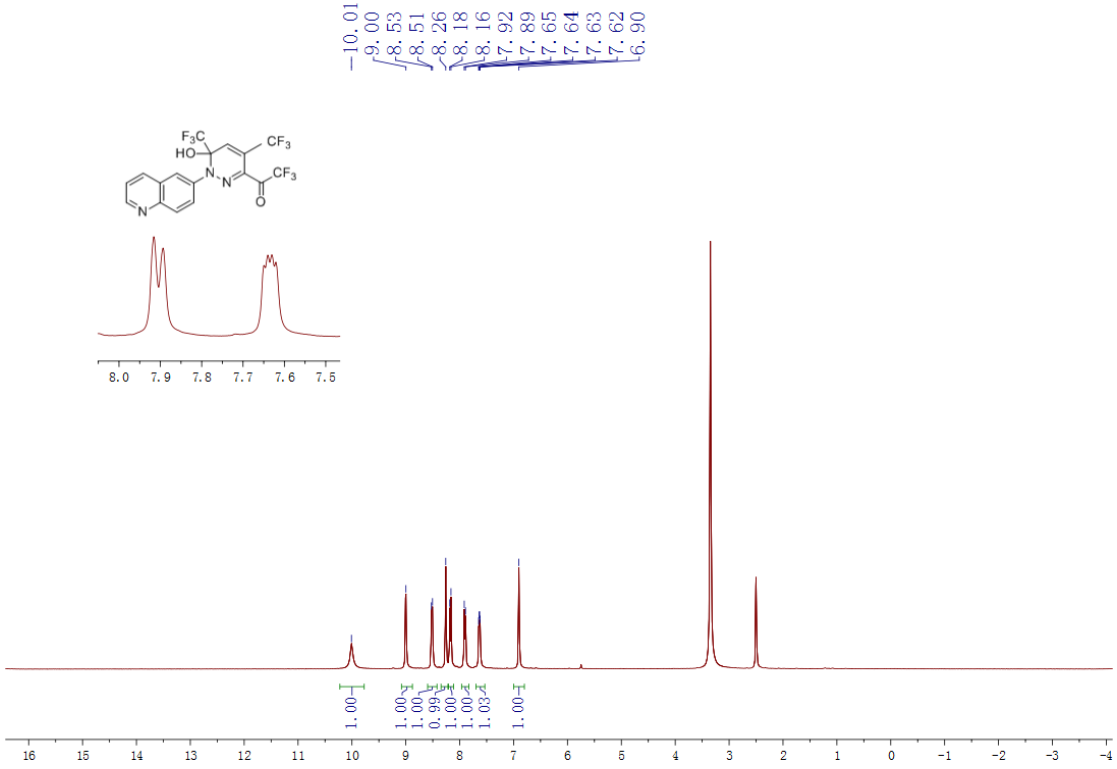


^{19}F NMR spectrum of **3aa** in $CDCl_3$

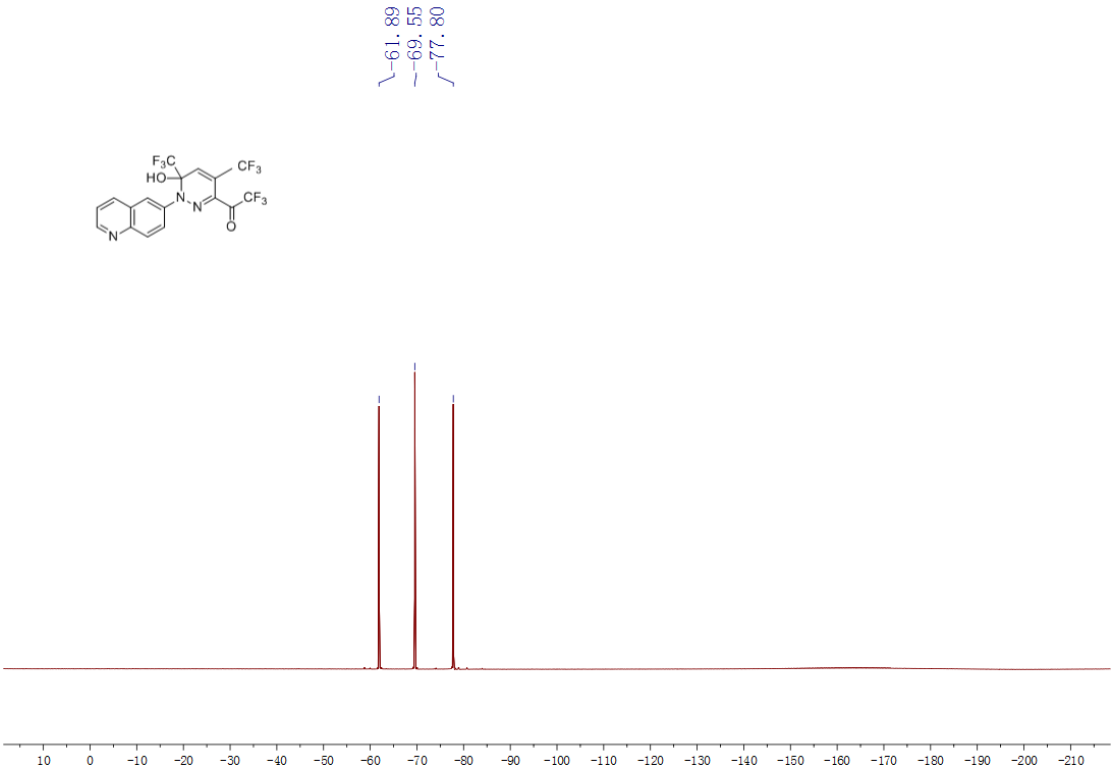
^{13}C NMR spectrum of **3aa** in $CDCl_3$



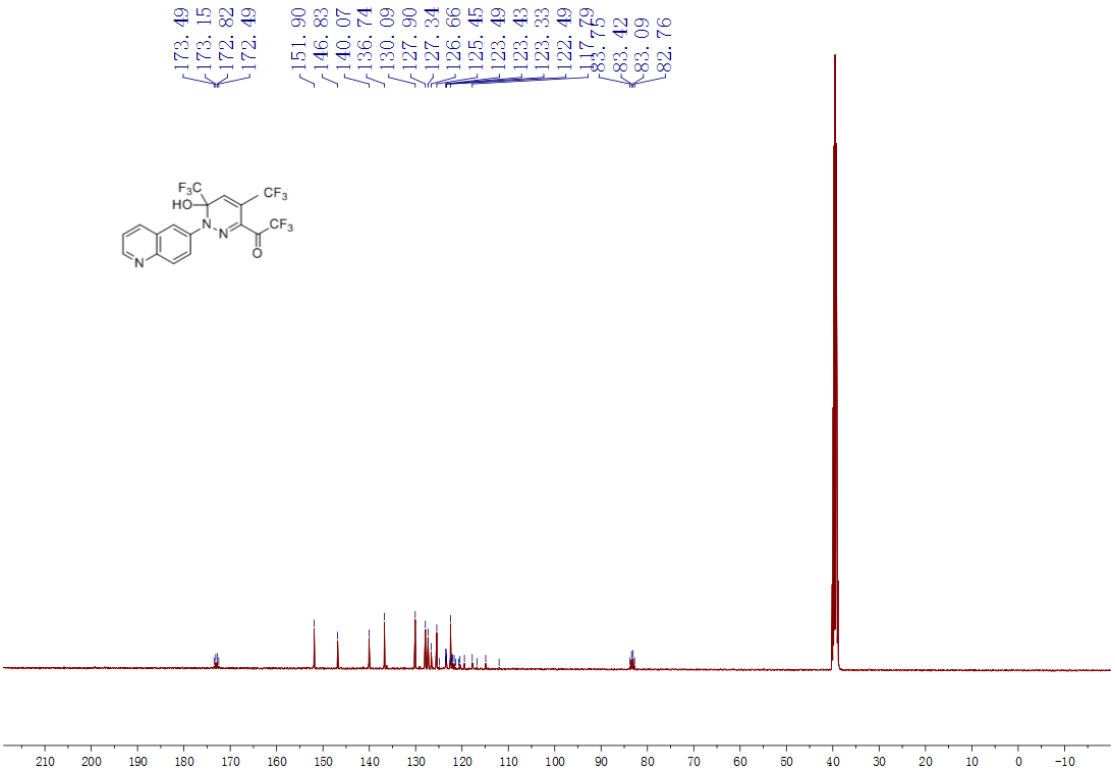
^{1}H NMR spectrum of **3ab** in DMSO-d_6



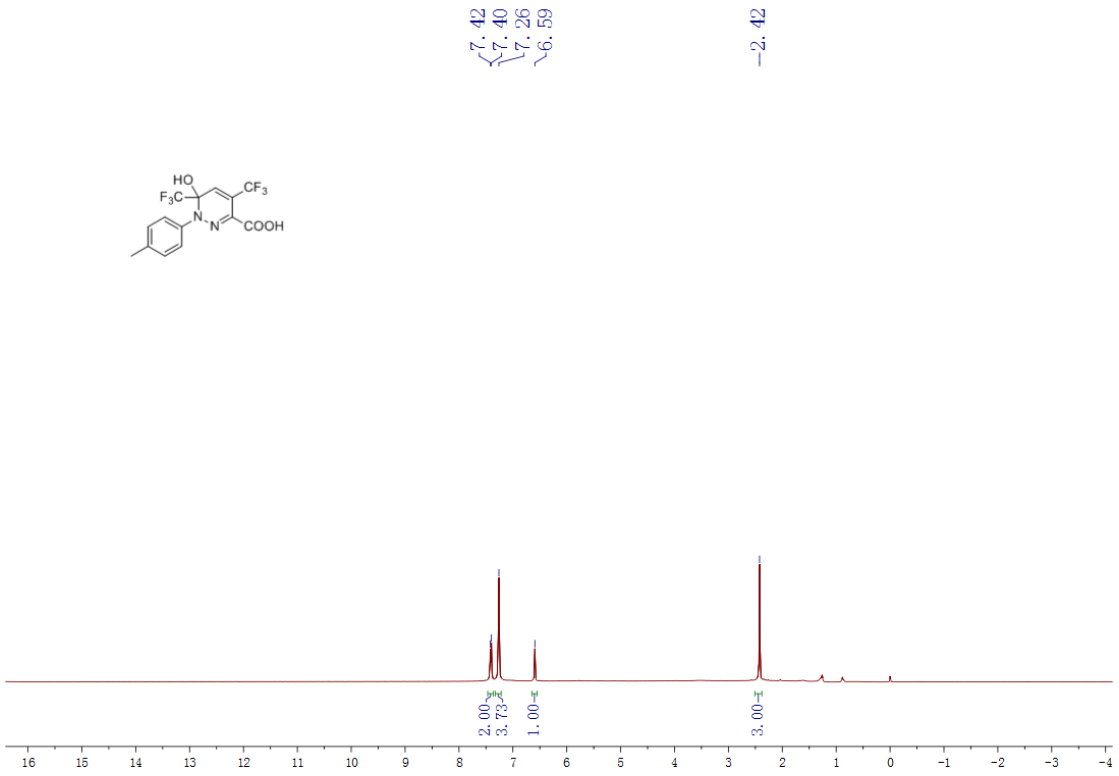
^{19}F NMR spectrum of **3ab** in DMSO-d_6



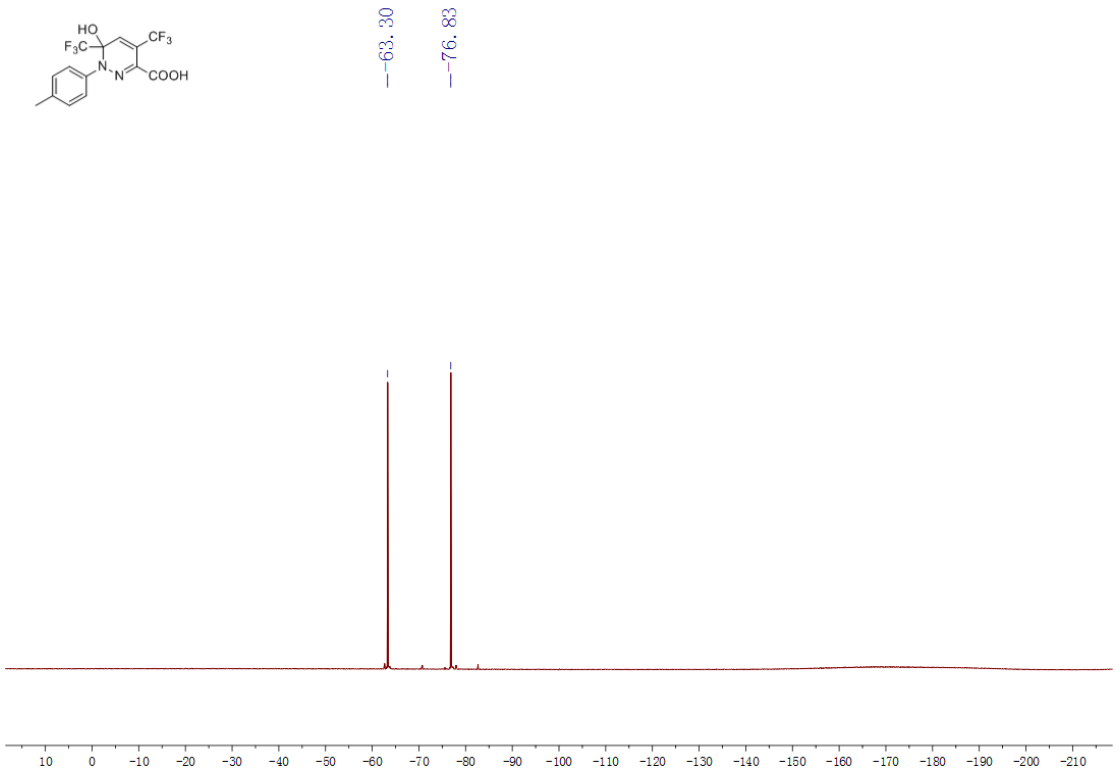
^{13}C NMR spectrum of **3ab** in DMSO-d_6



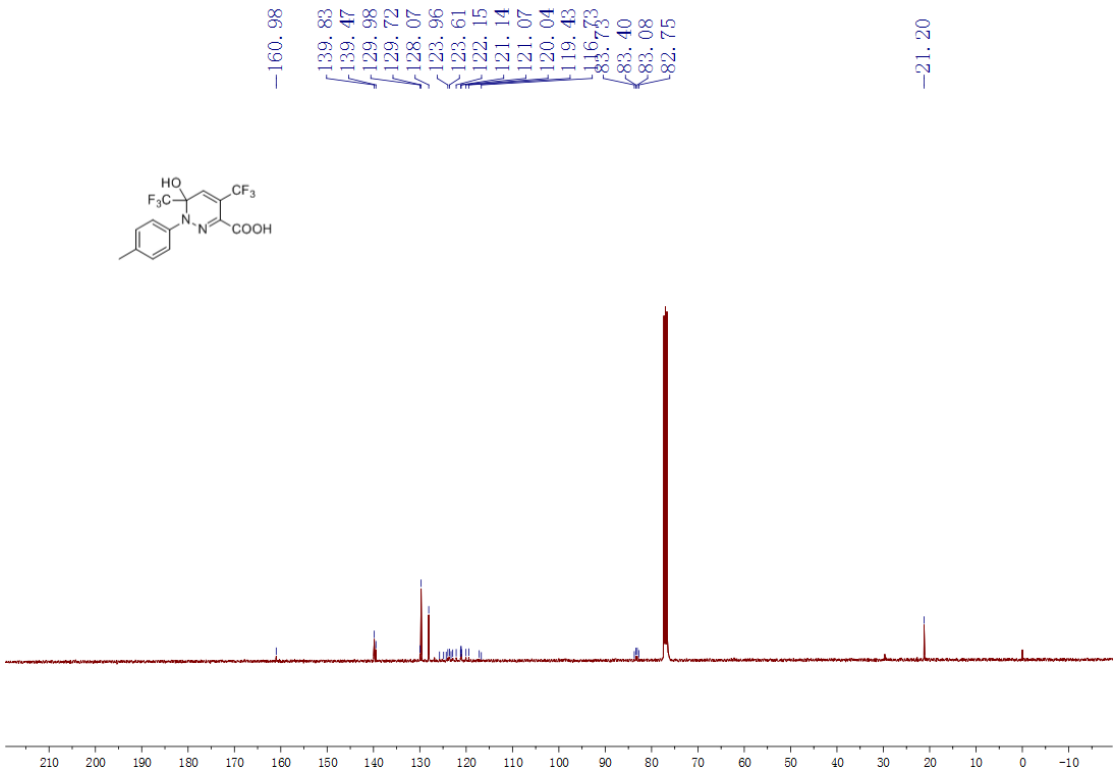
^{1}H NMR spectrum of **4** in $CDCl_3$



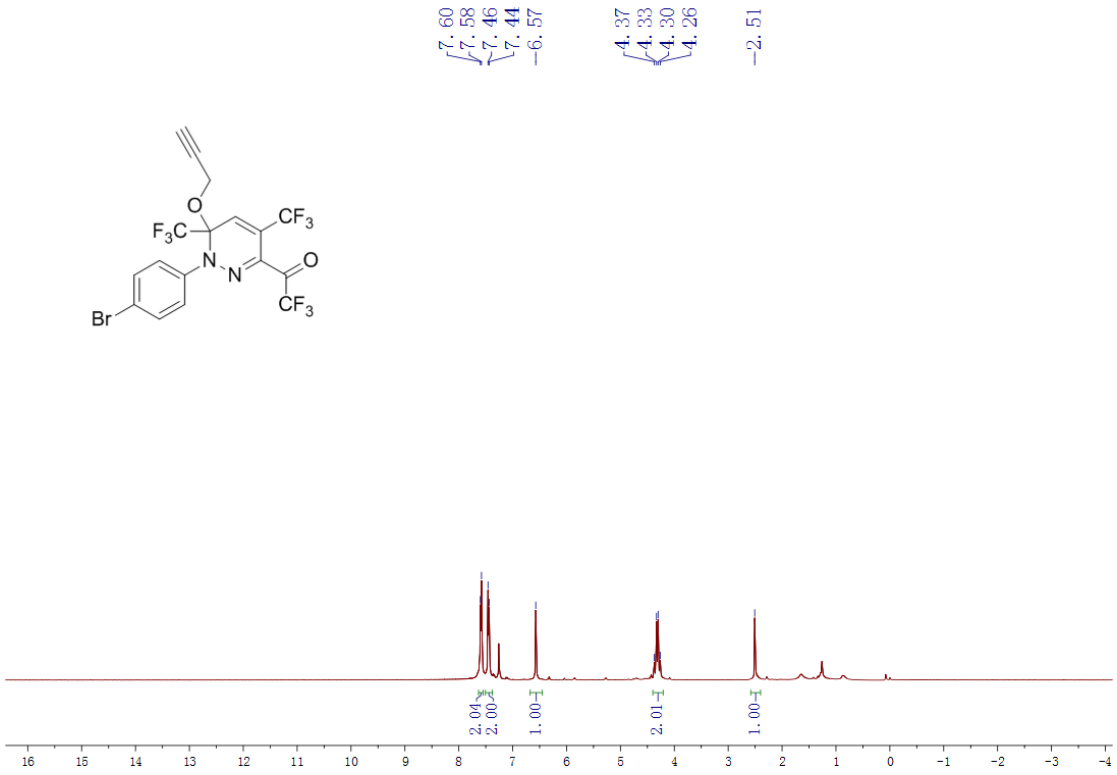
^{19}F NMR spectrum of **4** in $CDCl_3$



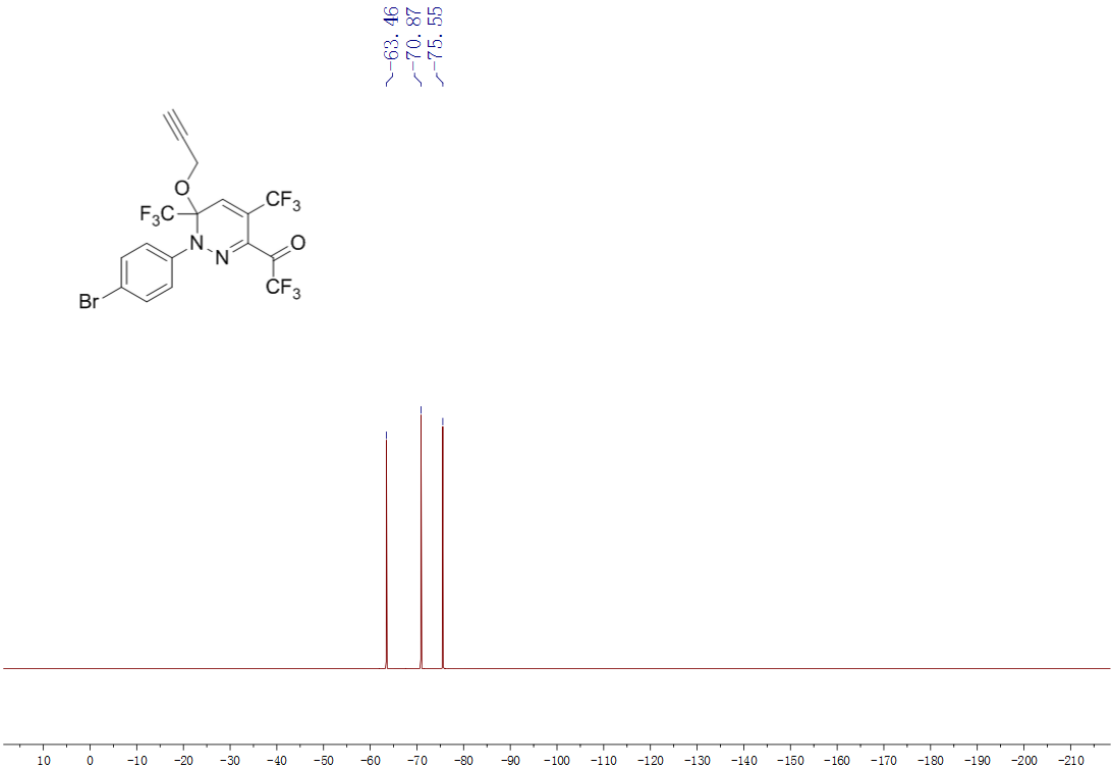
^{13}C NMR spectrum of **4** in $CDCl_3$



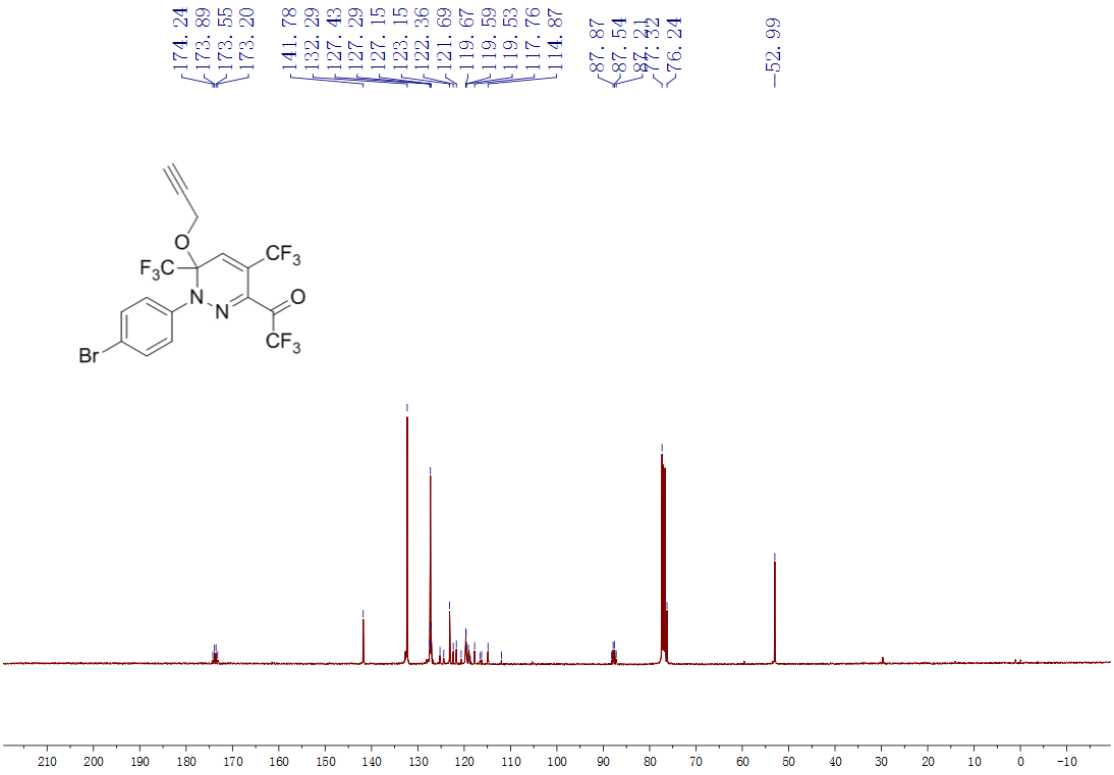
^{1}H NMR spectrum of **5** in $CDCl_3$



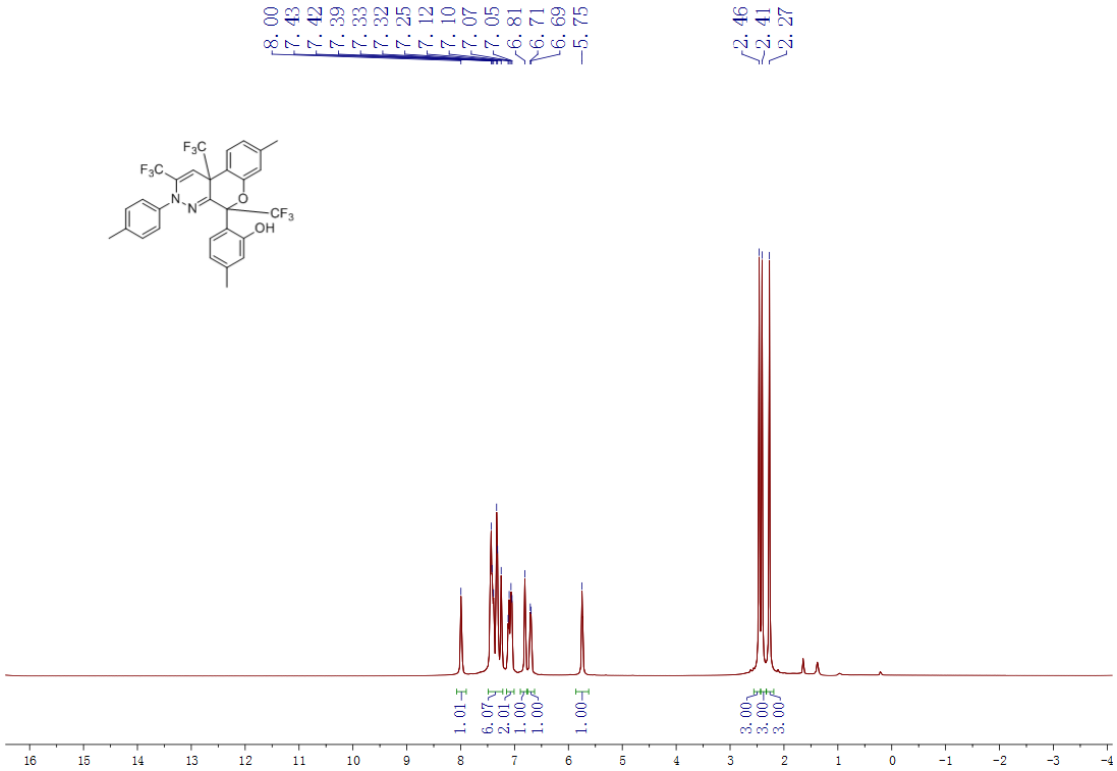
^{19}F NMR spectrum of **5** in $CDCl_3$



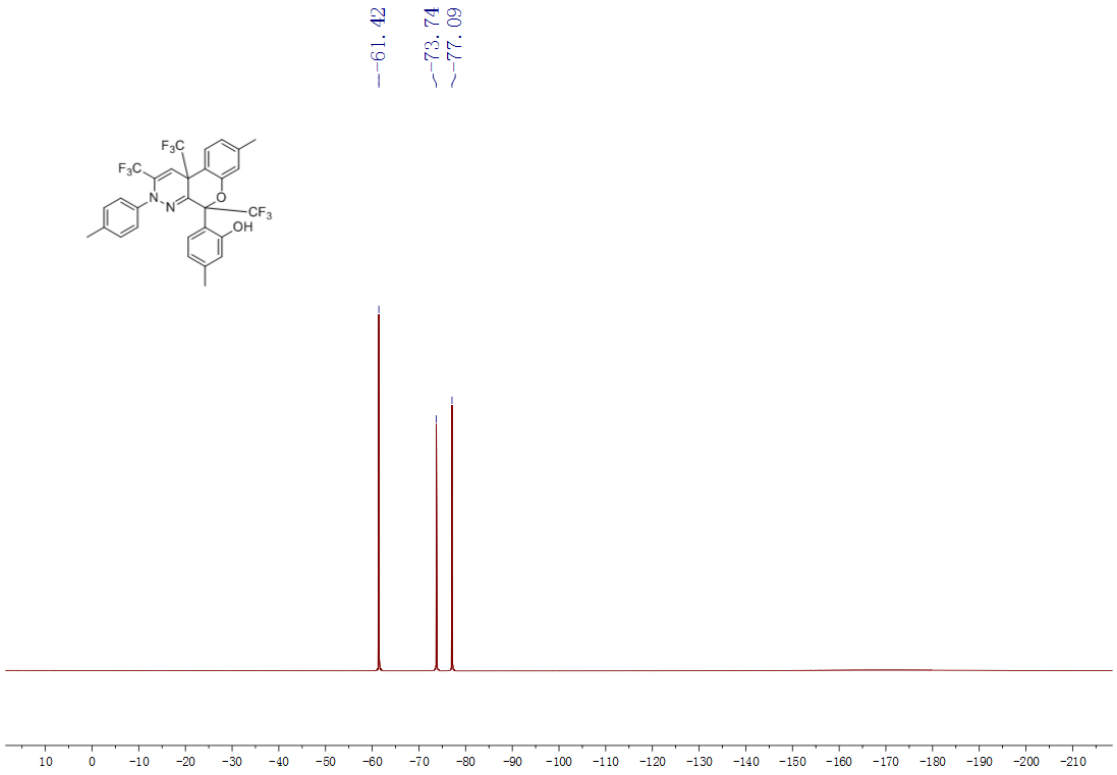
^{13}C NMR spectrum of **5** in $CDCl_3$



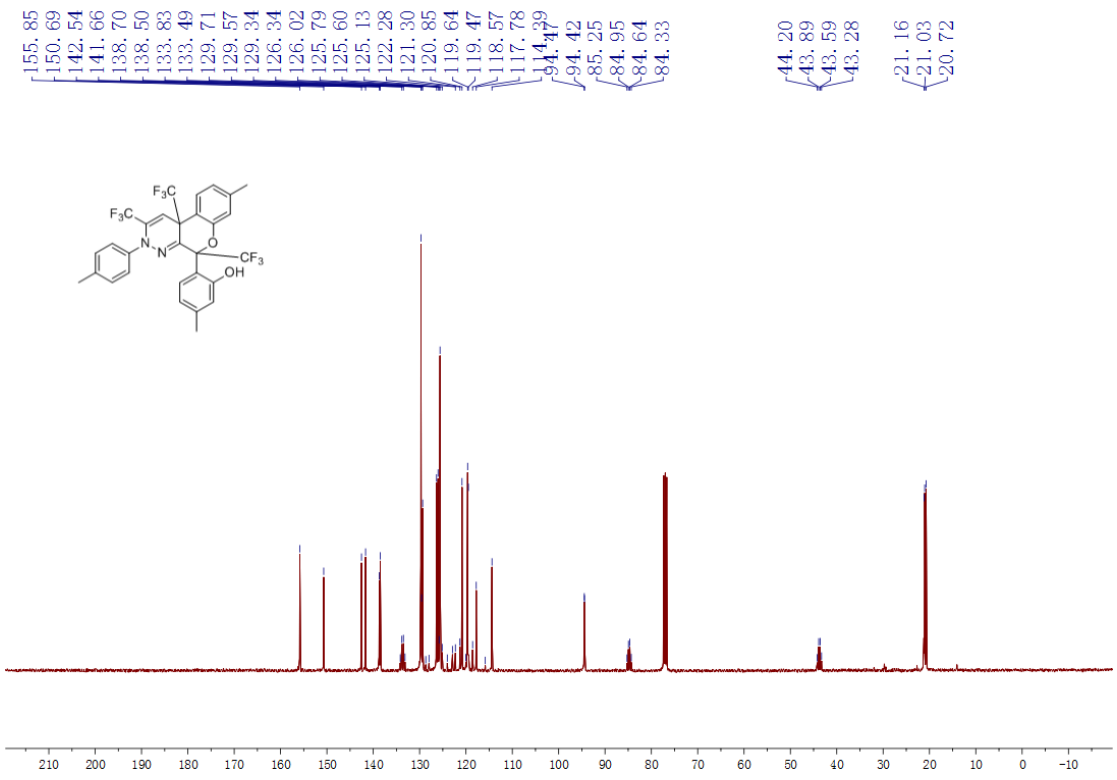
^{1}H NMR spectrum of **7a** in $CDCl_3$



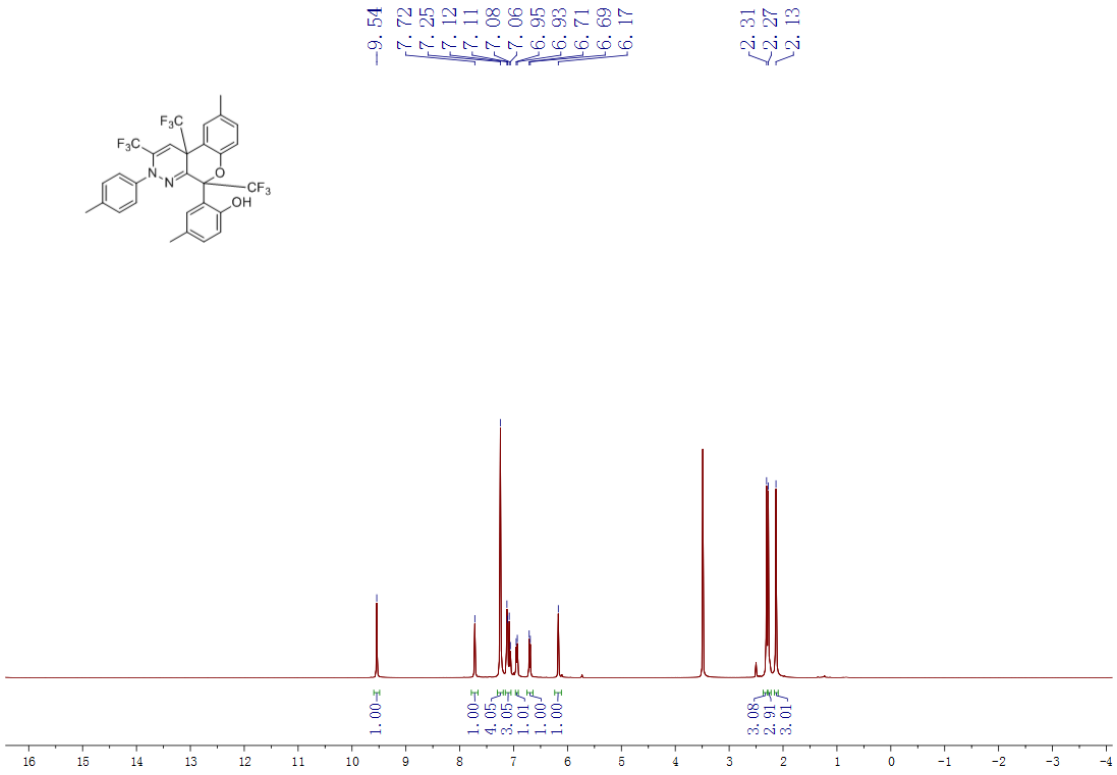
^{19}F NMR spectrum of **7a** in $CDCl_3$



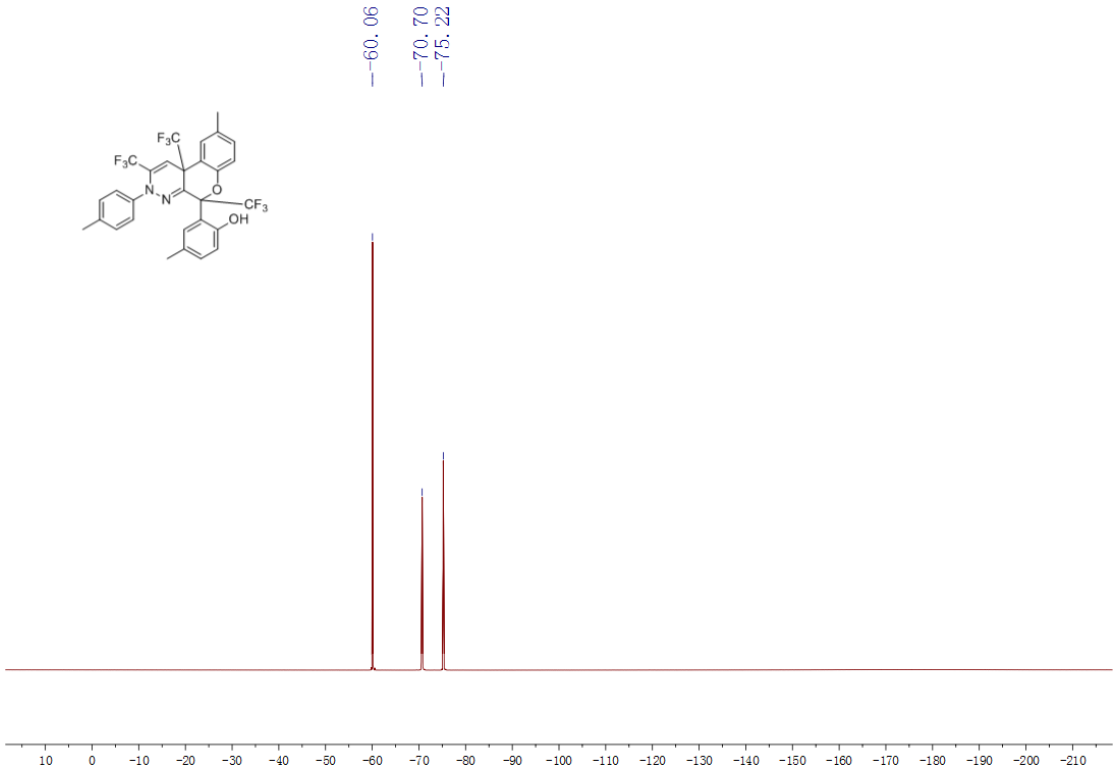
^{13}C NMR spectrum of **7a** in $CDCl_3$



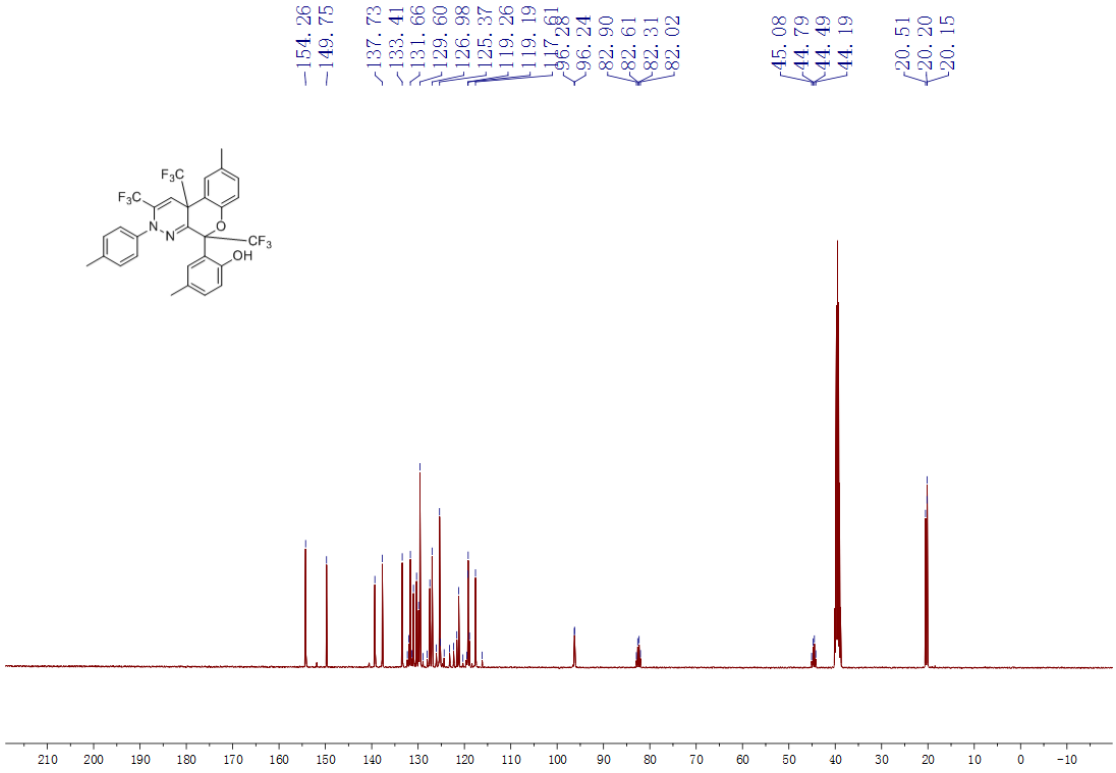
^{1}H NMR spectrum of **7b** in DMSO-d_6



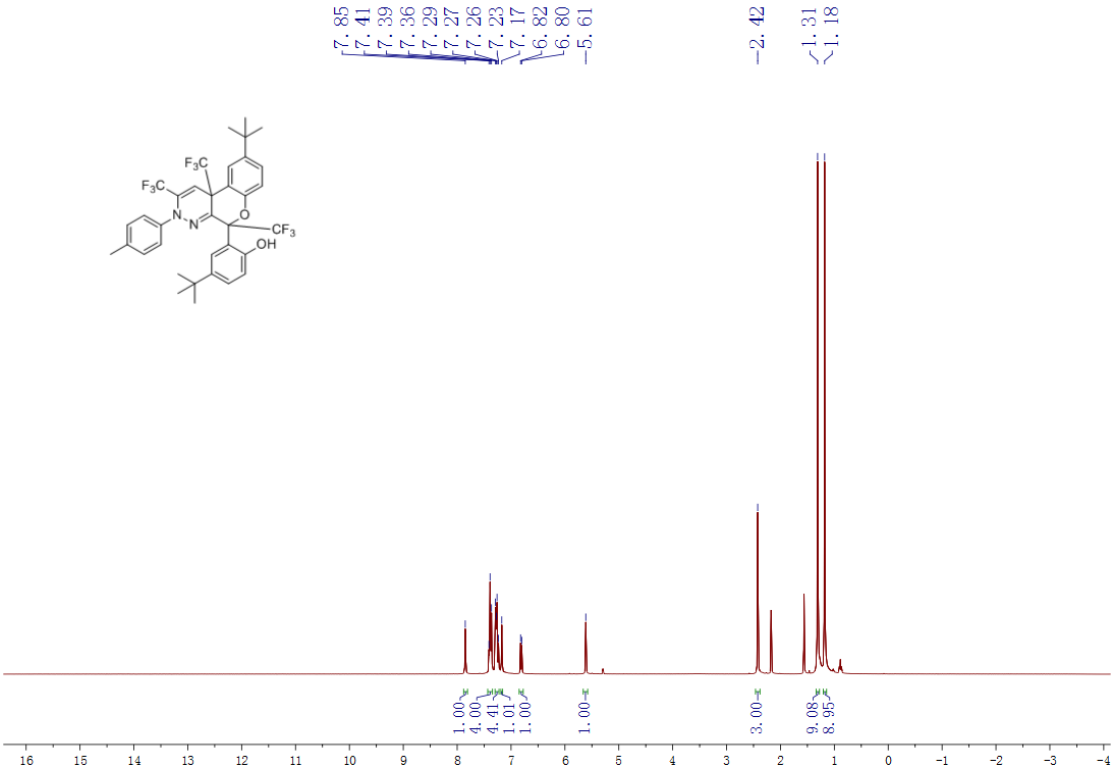
^{19}F NMR spectrum of **7b** in DMSO-d_6



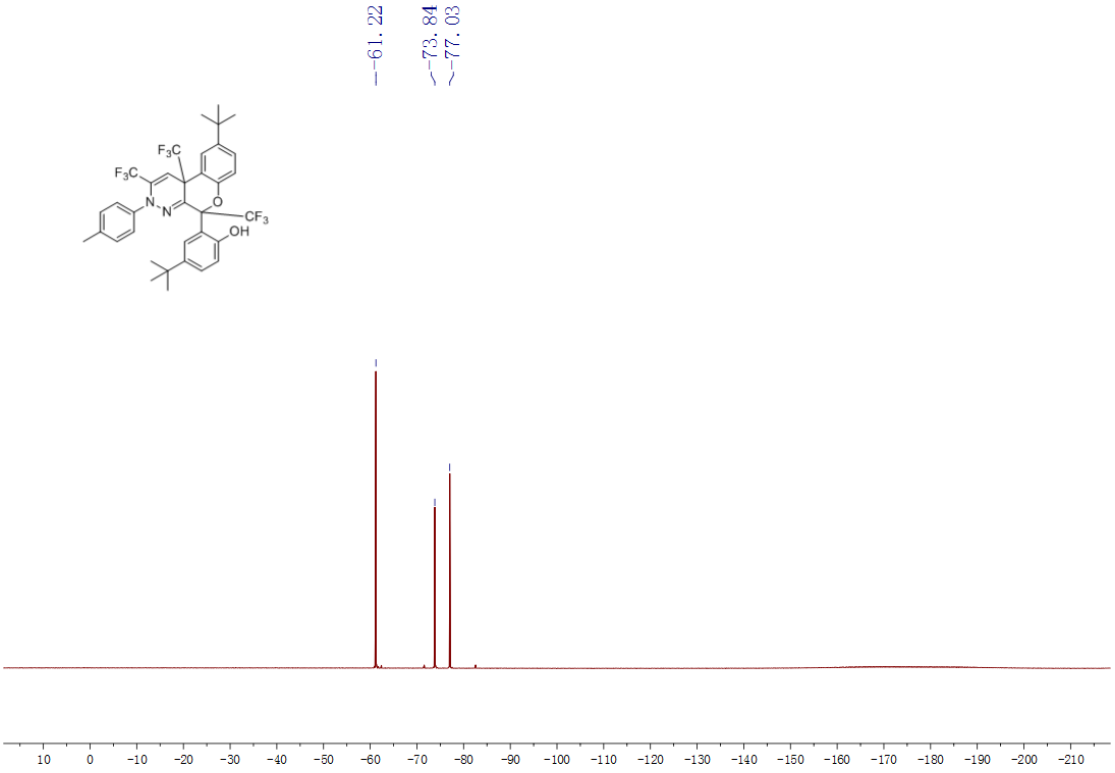
^{13}C NMR spectrum of **7b** in DMSO-d_6



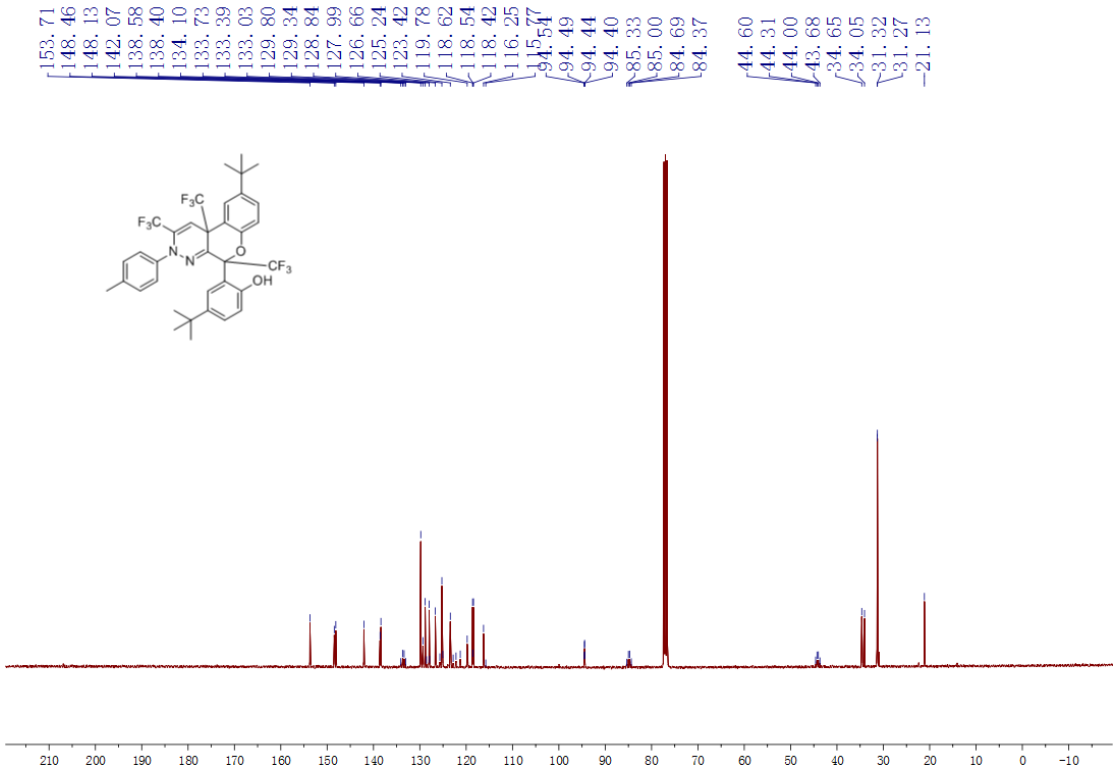
^{1}H NMR spectrum of **7c** in $CDCl_3$



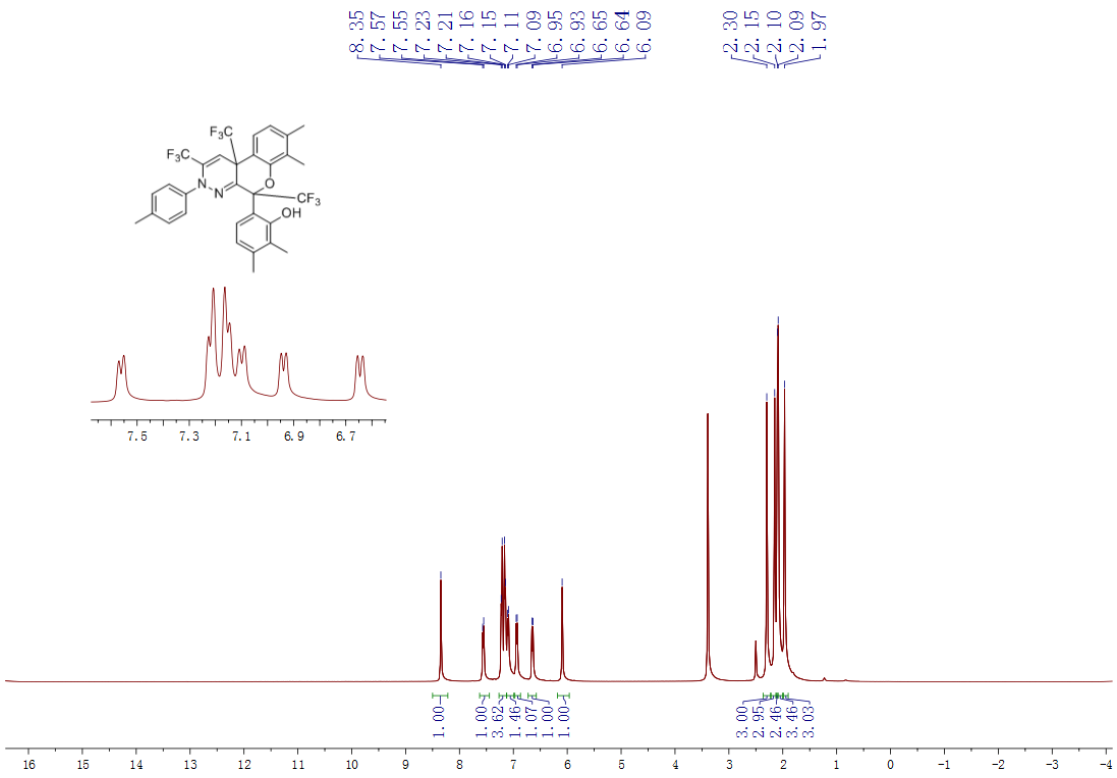
^{19}F NMR spectrum of **7c** in $CDCl_3$



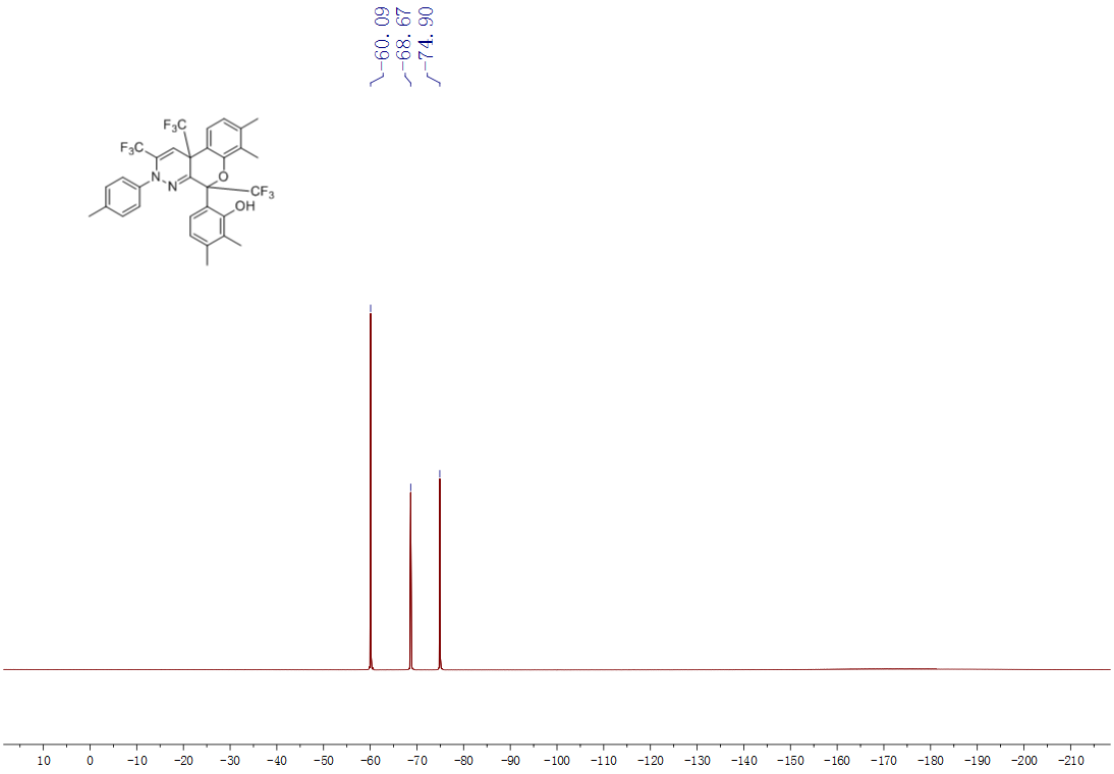
^{13}C NMR spectrum of **7c** in $CDCl_3$



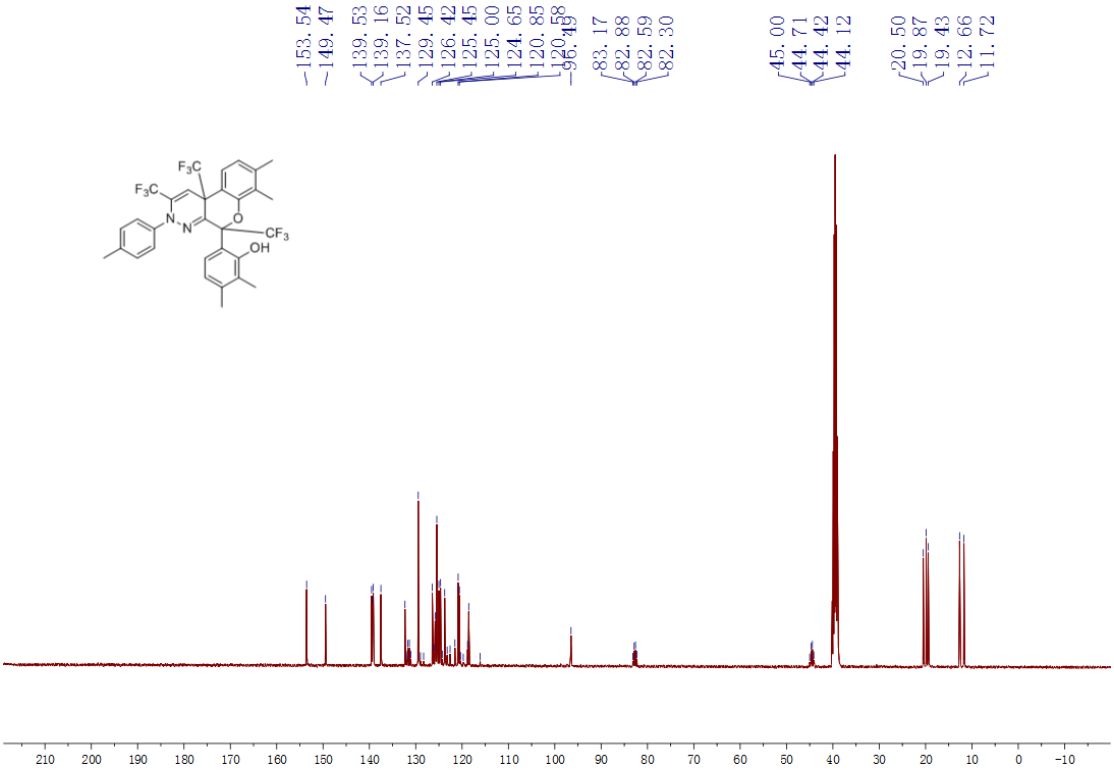
^{1}H NMR spectrum of **7d** in DMSO-d_6



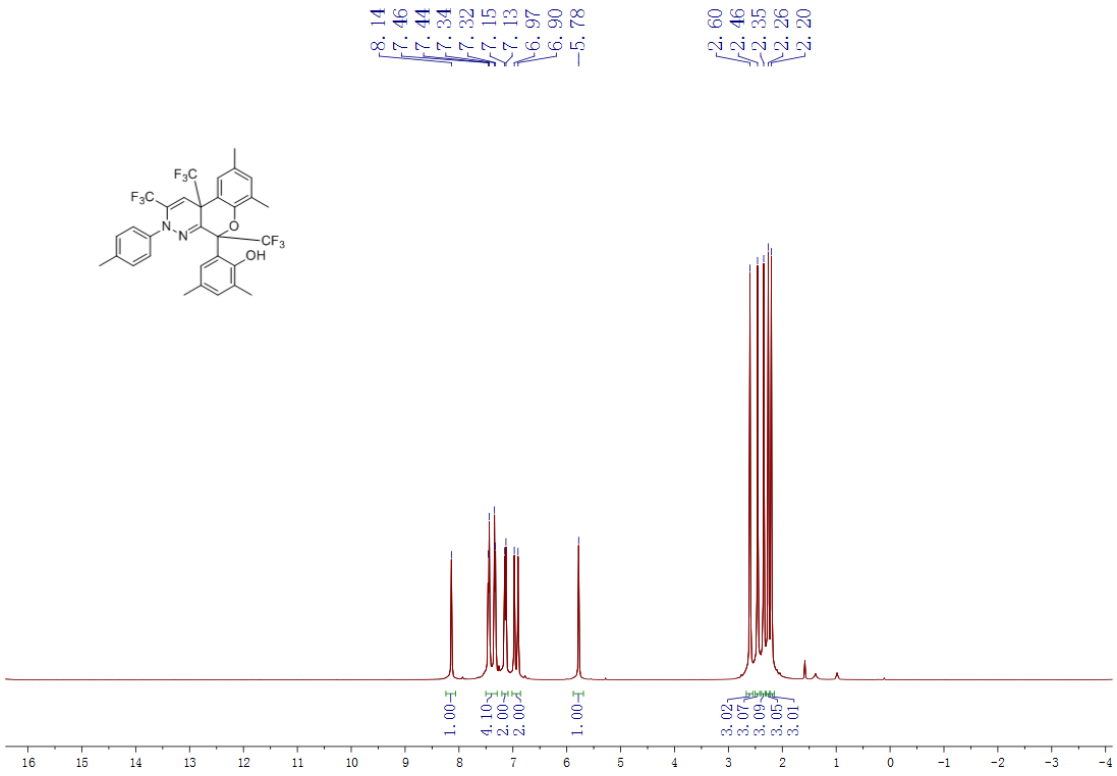
^{19}F NMR spectrum of **7d** in DMSO-d_6



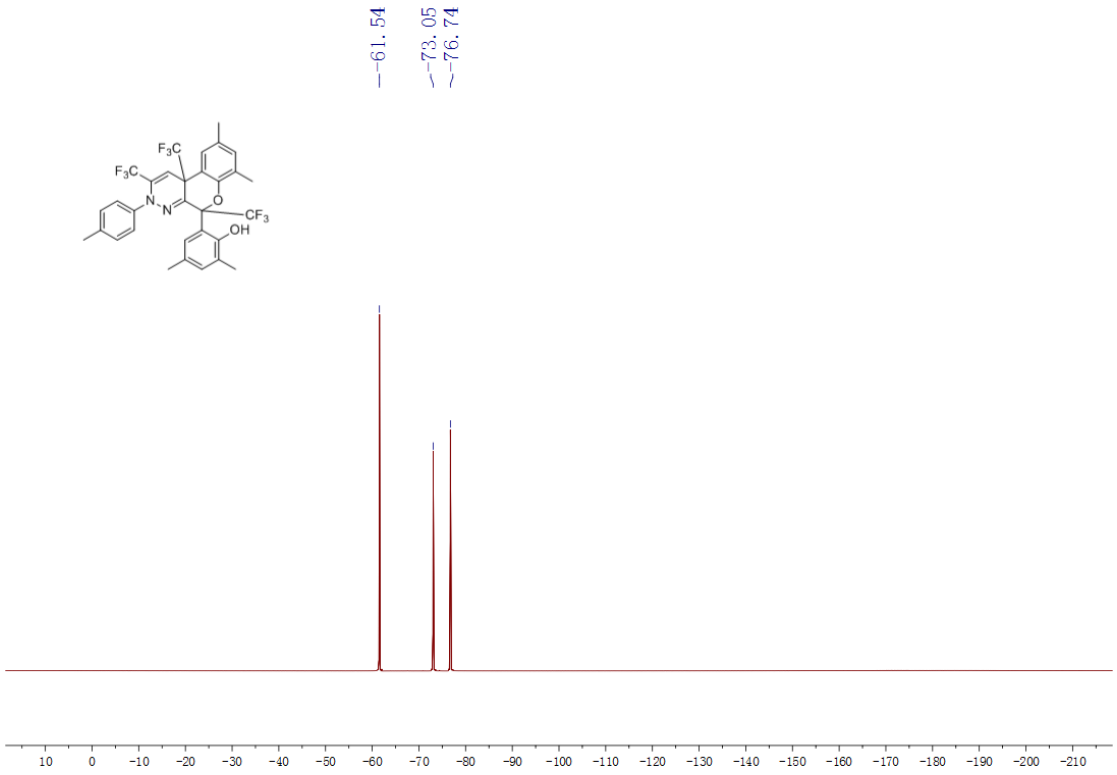
^{13}C NMR spectrum of **7d** in DMSO-d_6



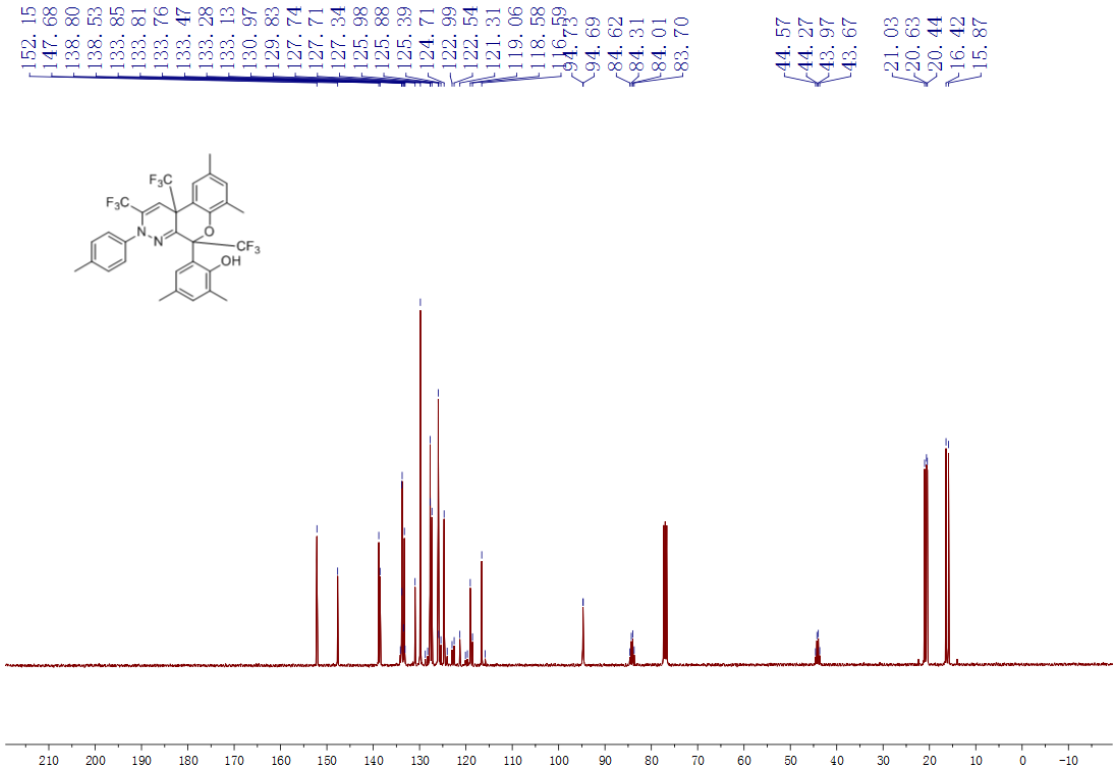
^{1}H NMR spectrum of **7e** in $CDCl_3$



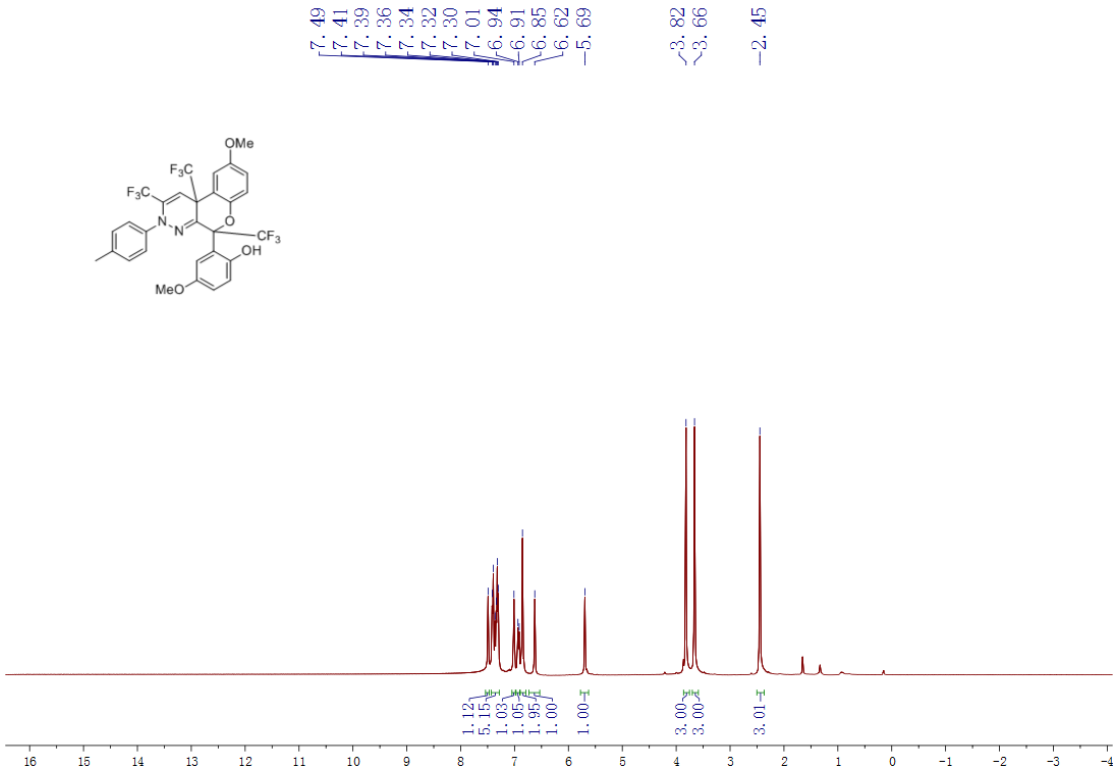
^{19}F NMR spectrum of **7e** in $CDCl_3$



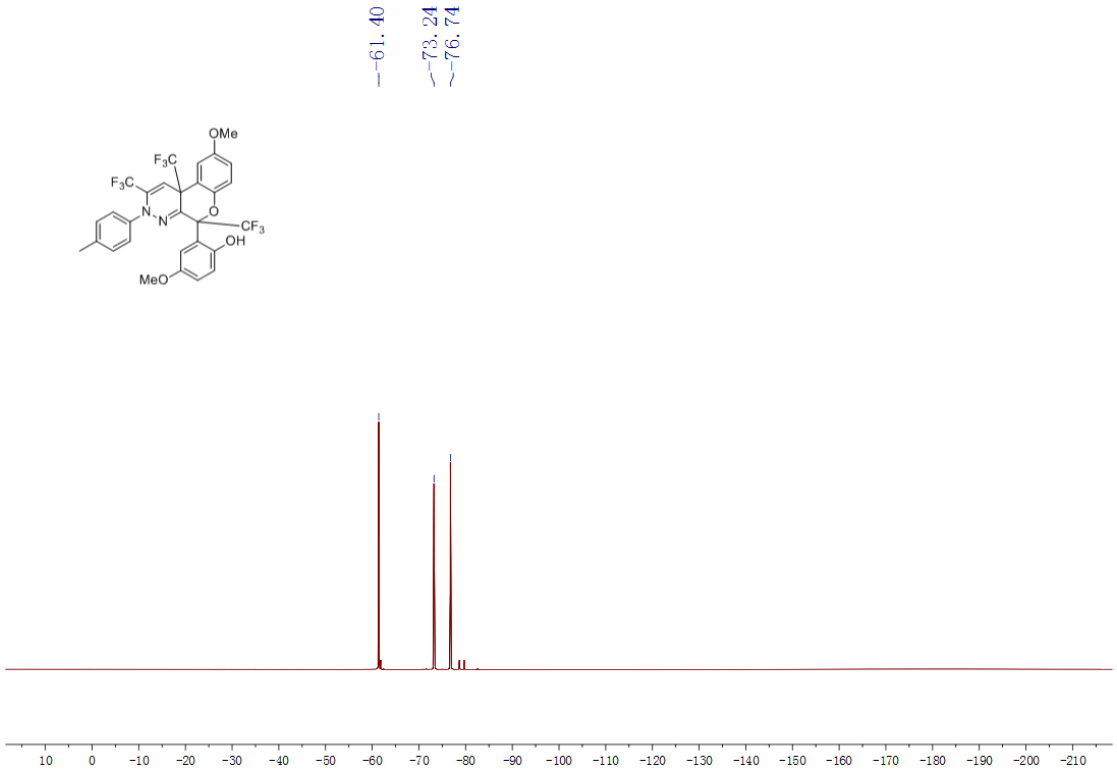
^{13}C NMR spectrum of **7e** in $CDCl_3$



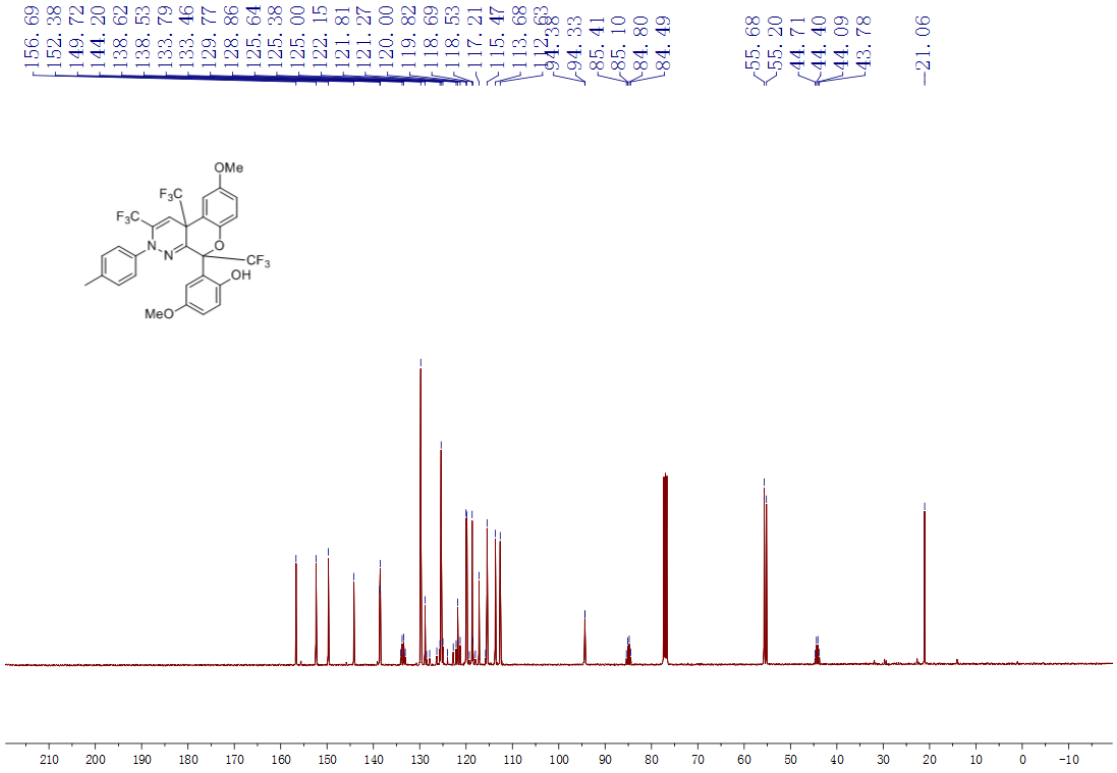
^{1}H NMR spectrum of **7f** in $CDCl_3$



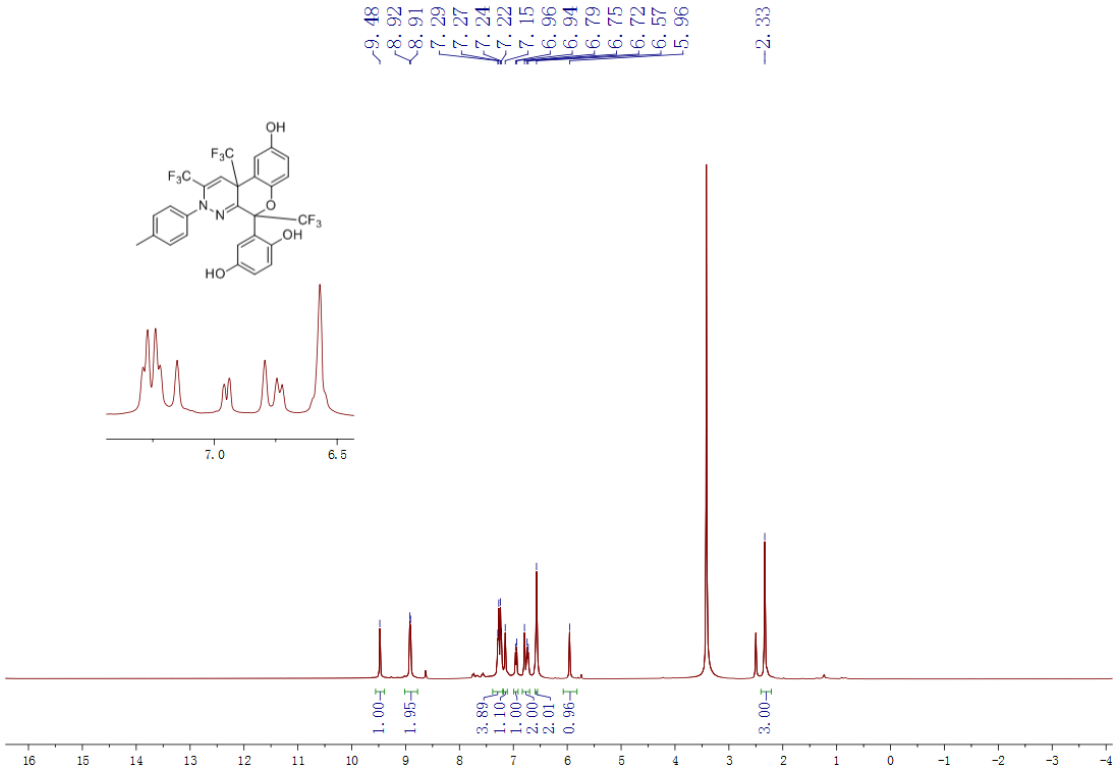
^{19}F NMR spectrum of **7f** in $CDCl_3$



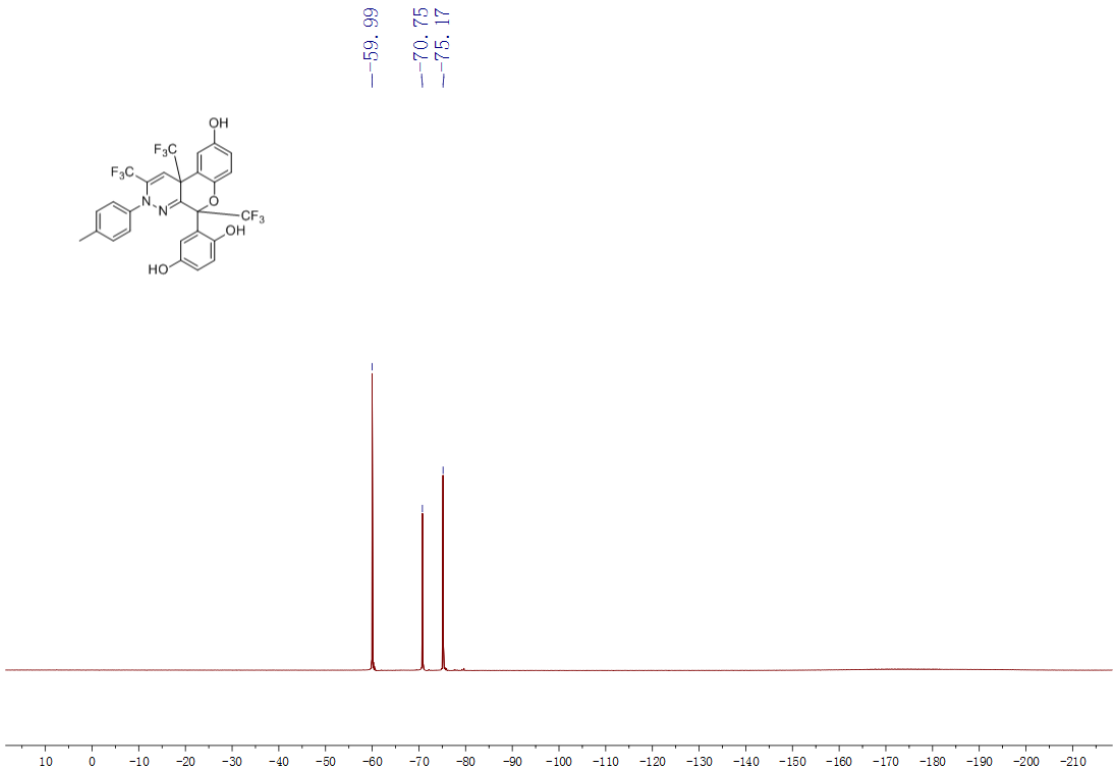
^{13}C NMR spectrum of **7f** in $CDCl_3$



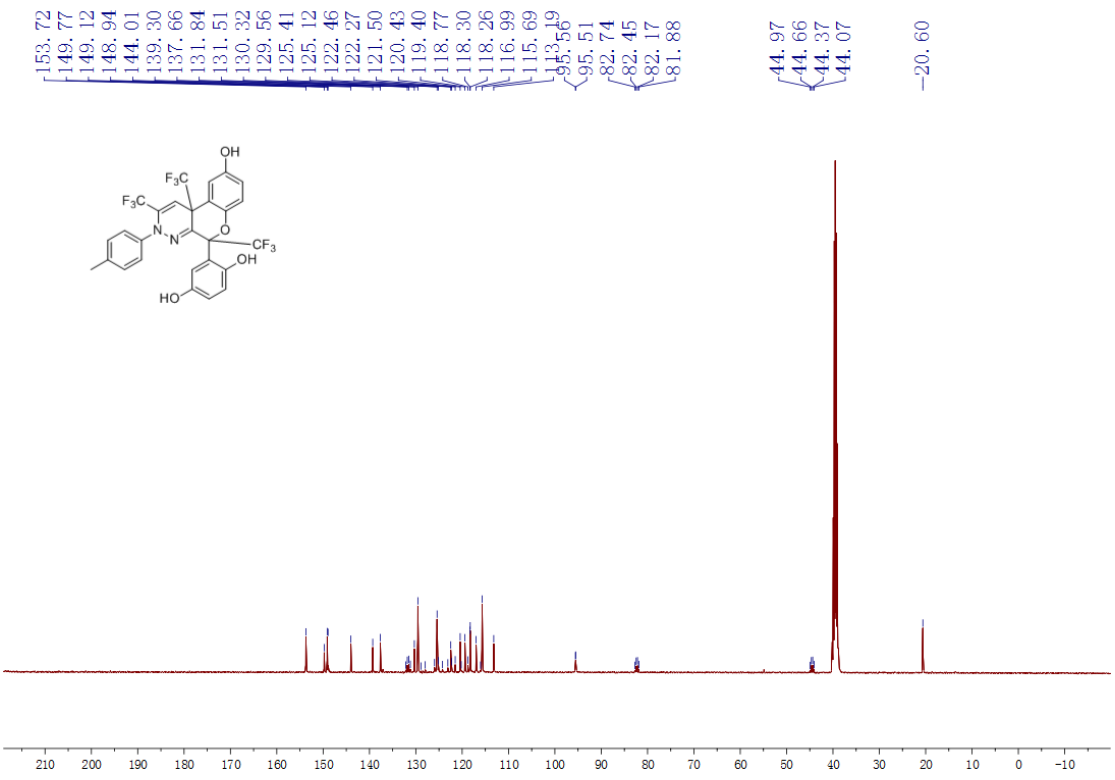
^{1}H NMR spectrum of **7g** in DMSO-d_6



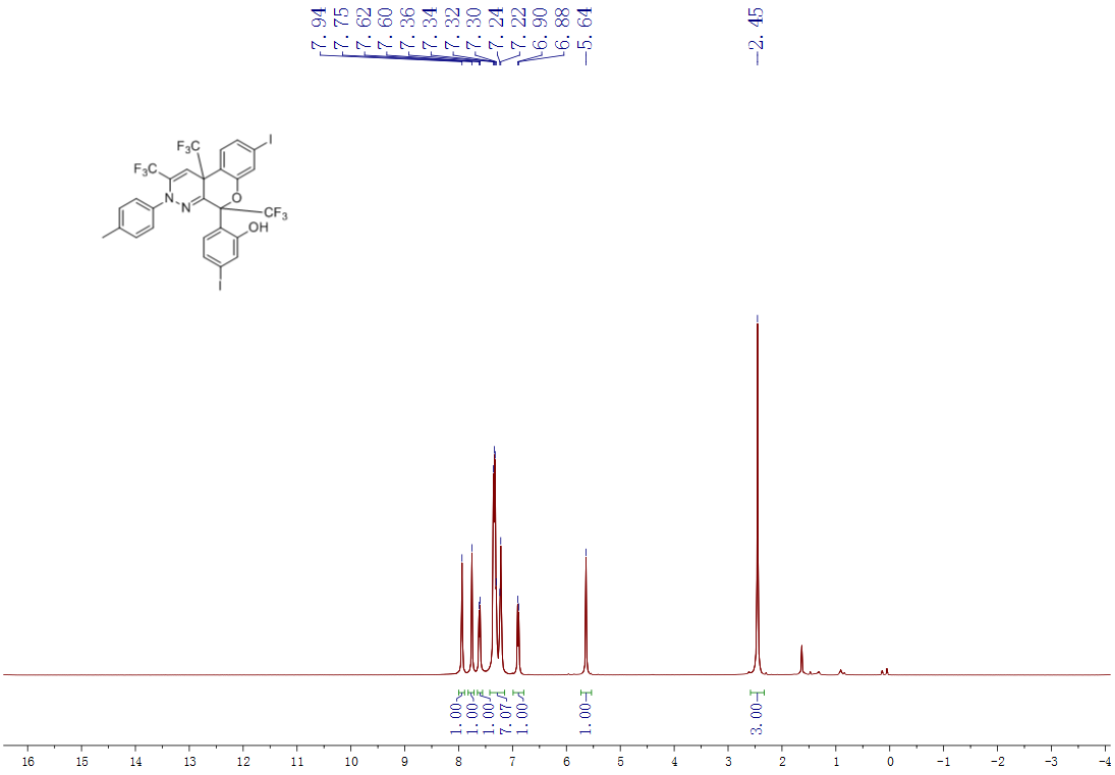
^{19}F NMR spectrum of **7g** in DMSO-d_6



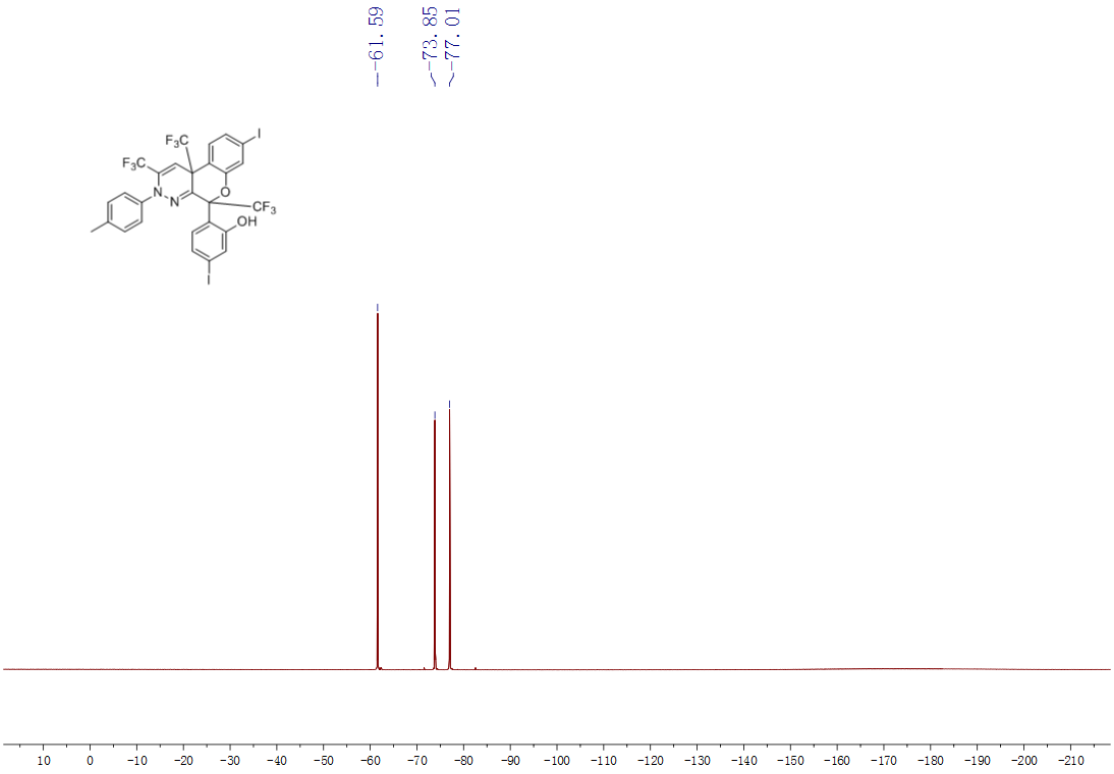
^{13}C NMR spectrum of **7g** in DMSO-d_6



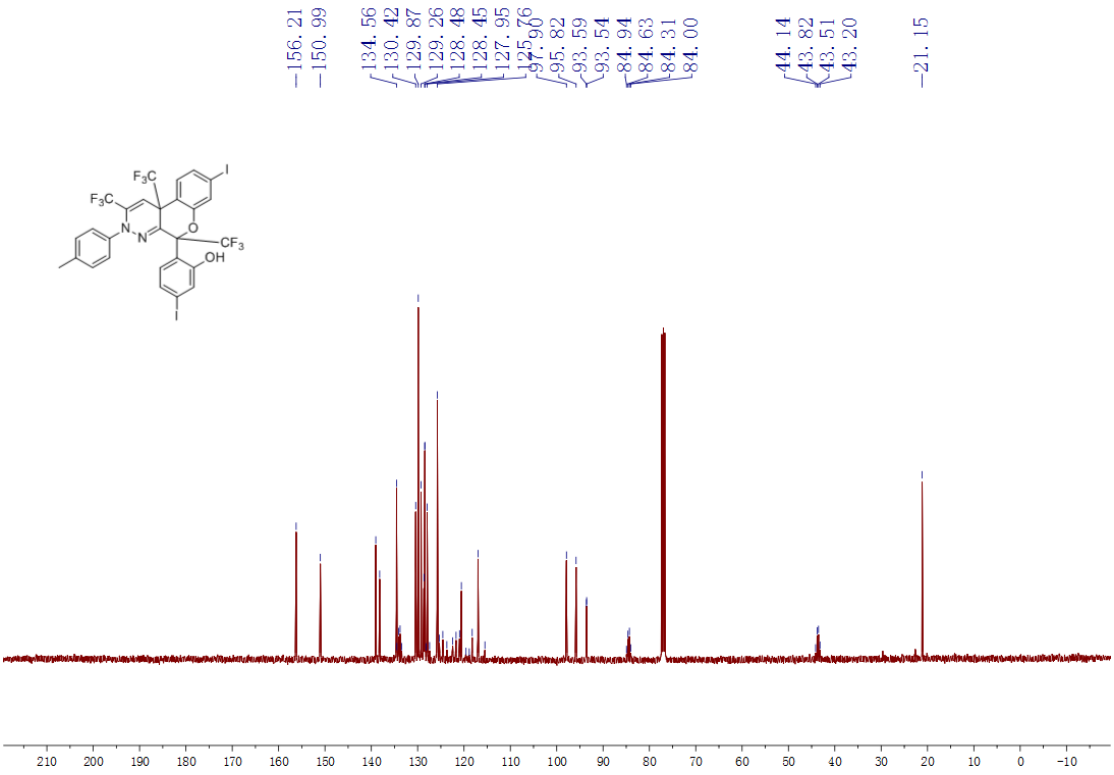
^{1}H NMR spectrum of **7h** in $CDCl_3$



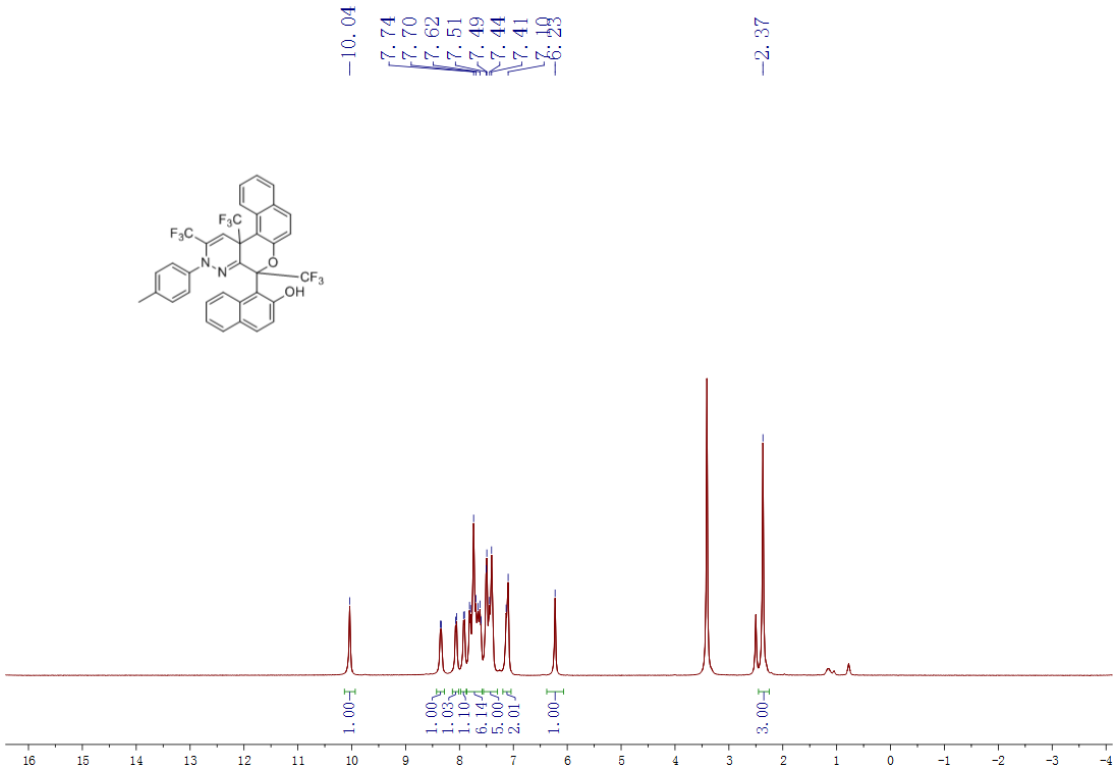
^{19}F NMR spectrum of **7h** in $CDCl_3$



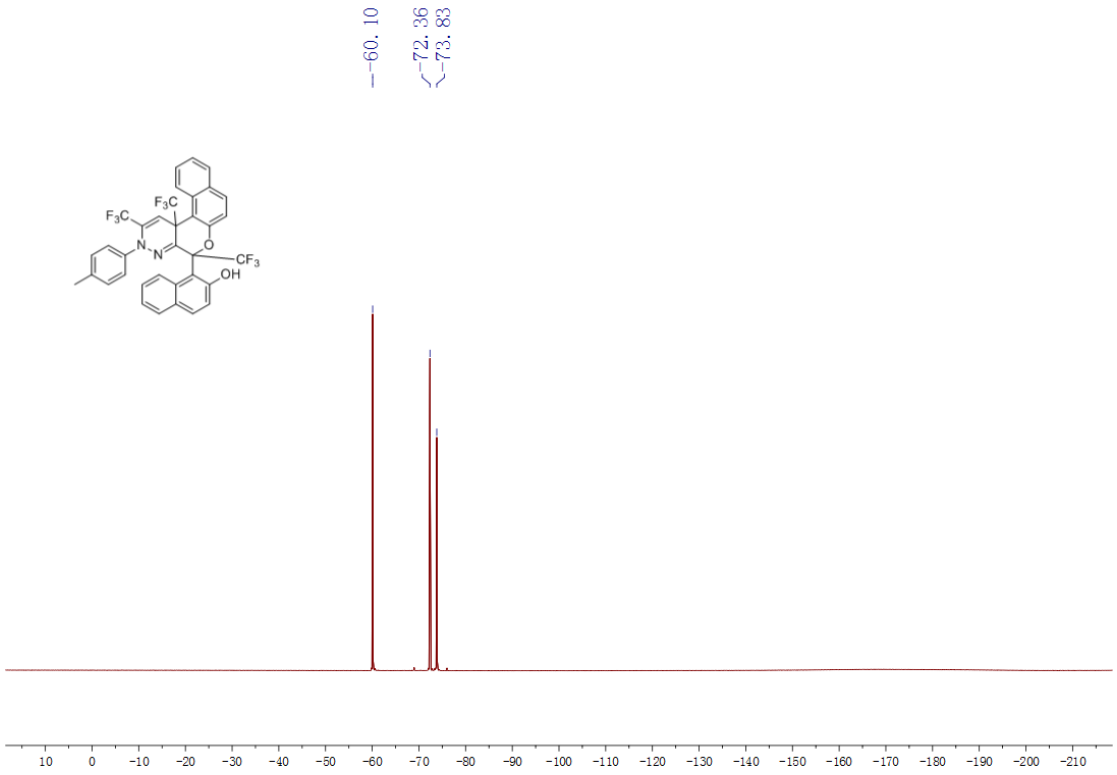
^{13}C NMR spectrum of **7h** in $CDCl_3$



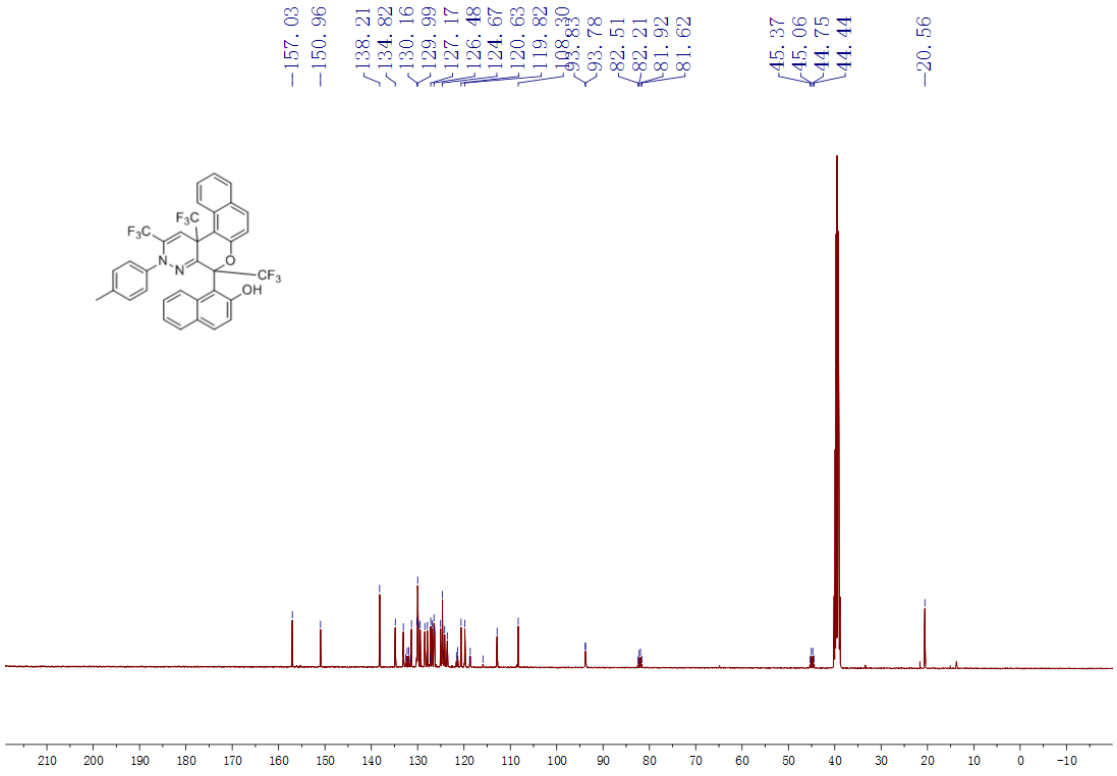
^{1}H NMR spectrum of **7i** in DMSO-d_6



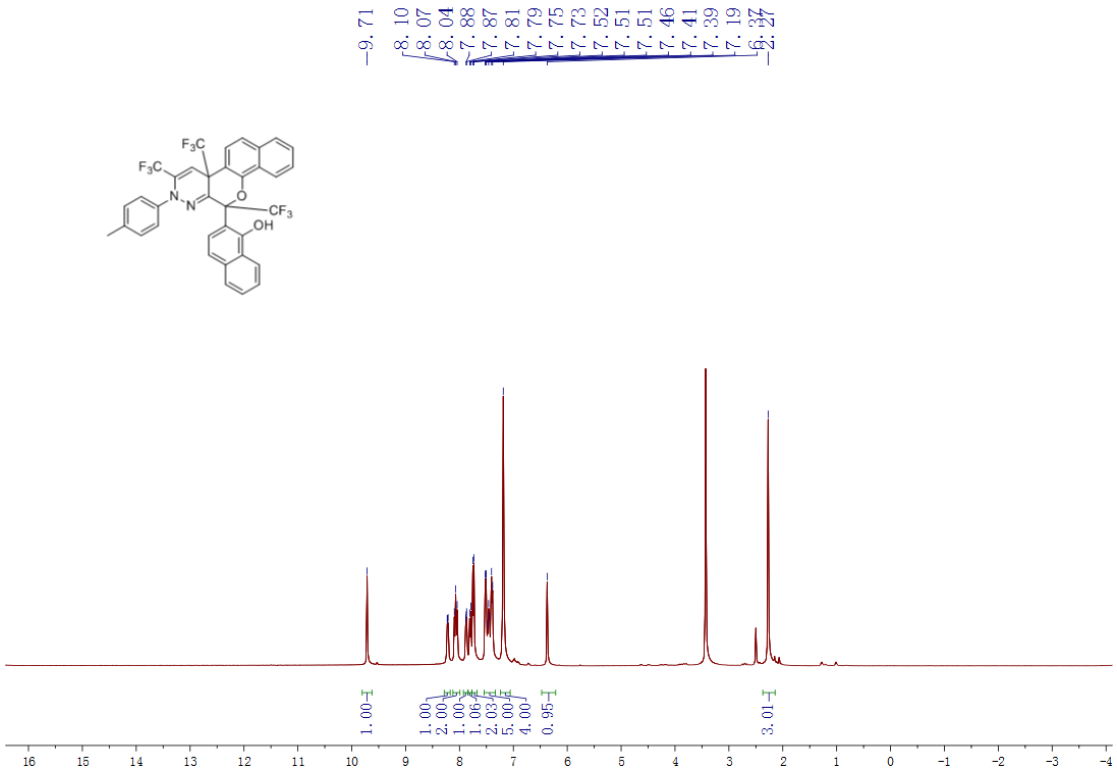
^{19}F NMR spectrum of **7i** in DMSO-d_6



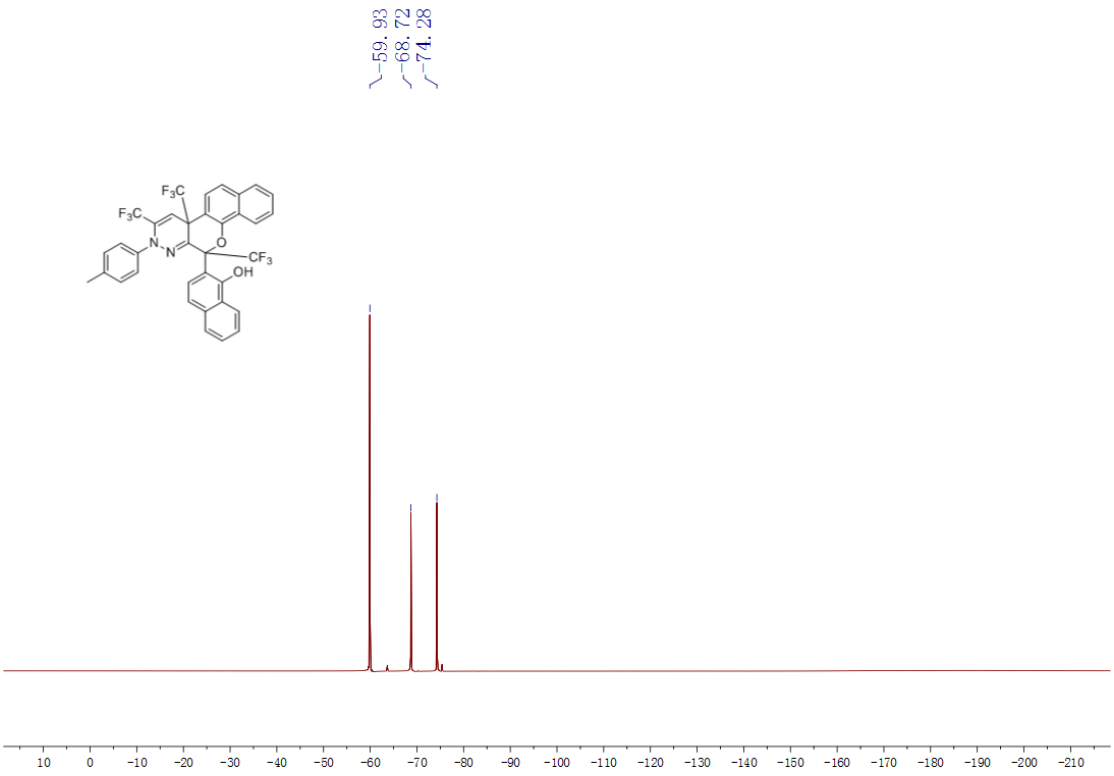
^{13}C NMR spectrum of **7i** in DMSO-d_6



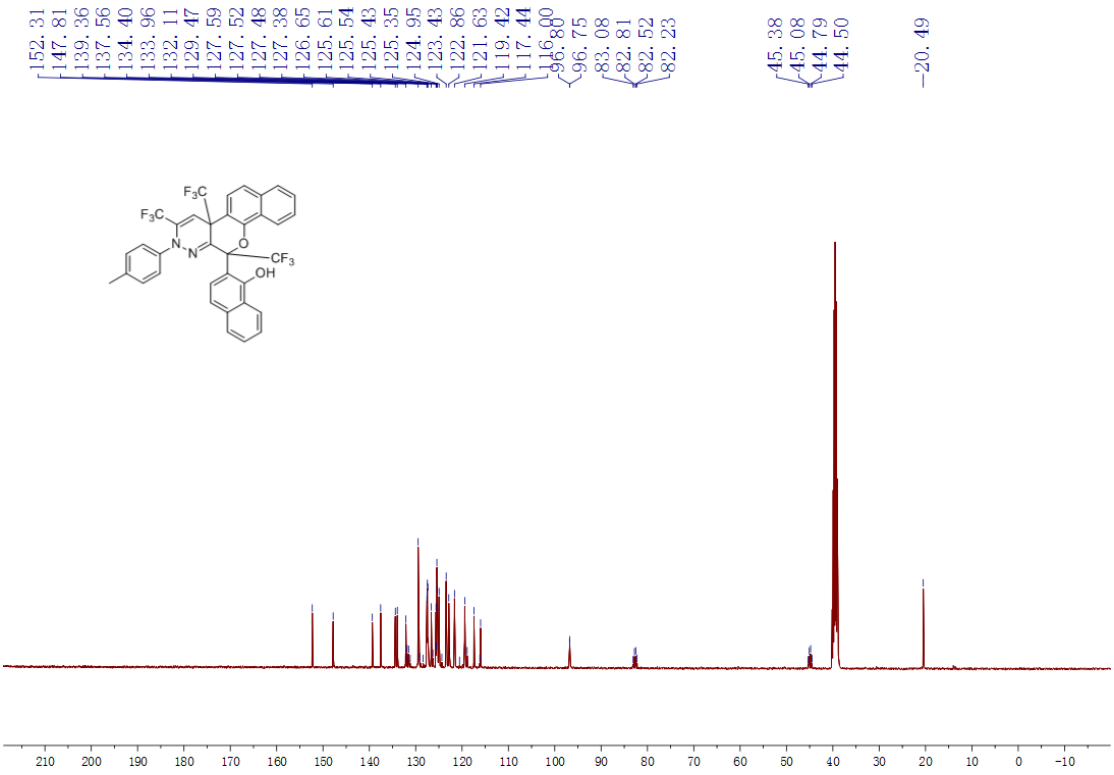
^{1}H NMR spectrum of **7j** in DMSO-d_6



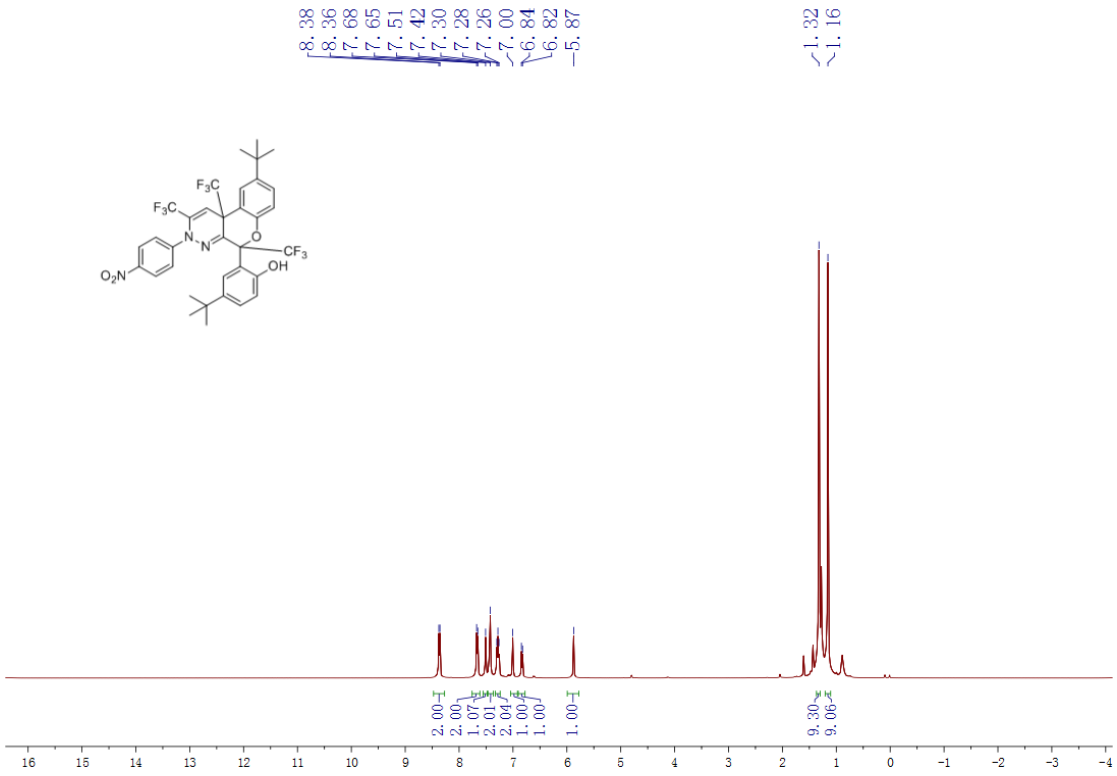
^{19}F NMR spectrum of **7j** in DMSO-d_6



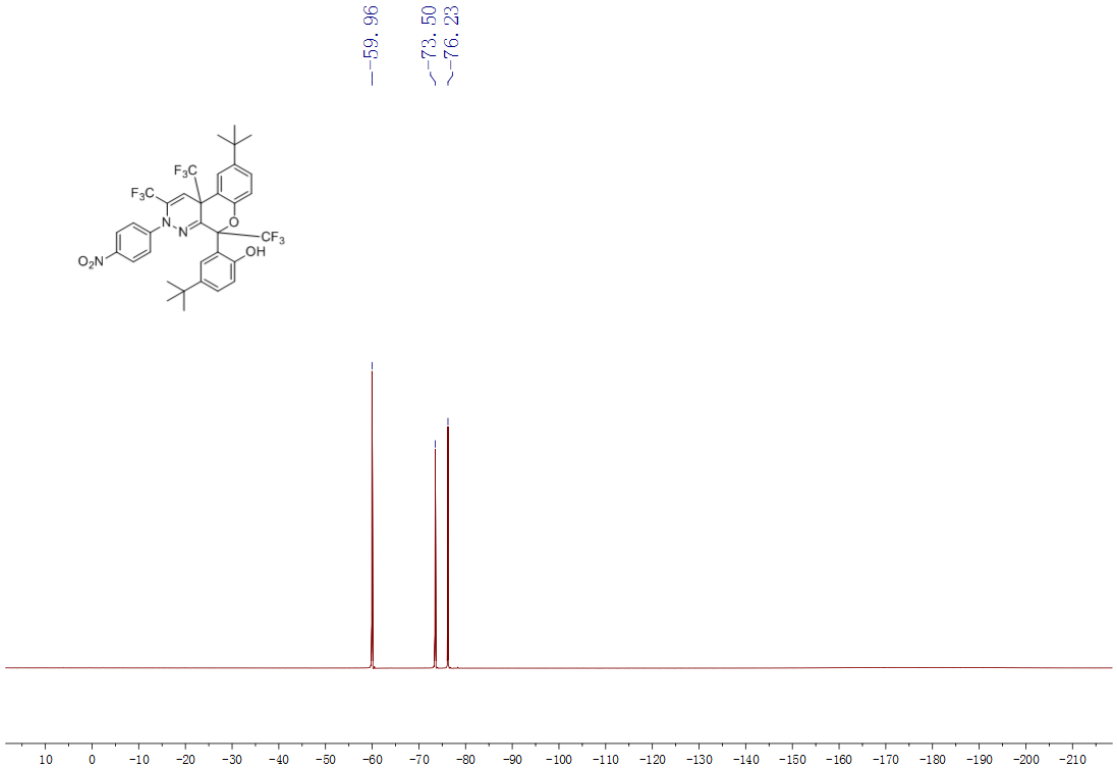
^{13}C NMR spectrum of **7j** in DMSO-d_6



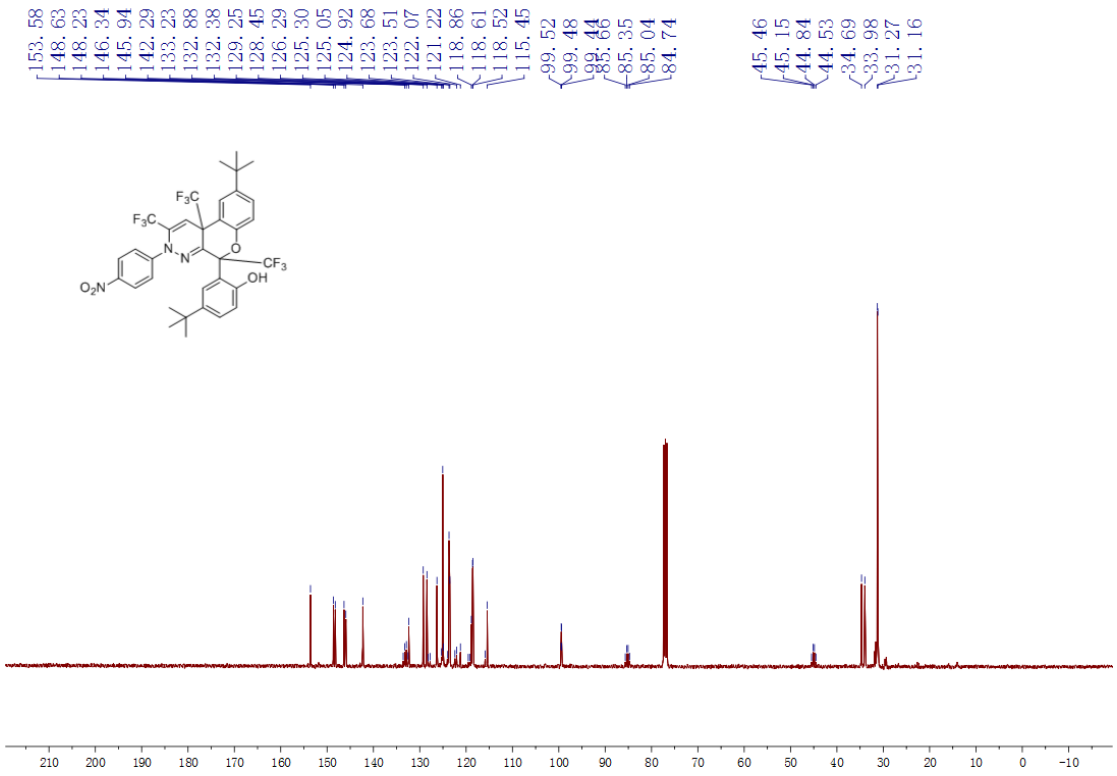
^{1}H NMR spectrum of **7k** in $CDCl_3$



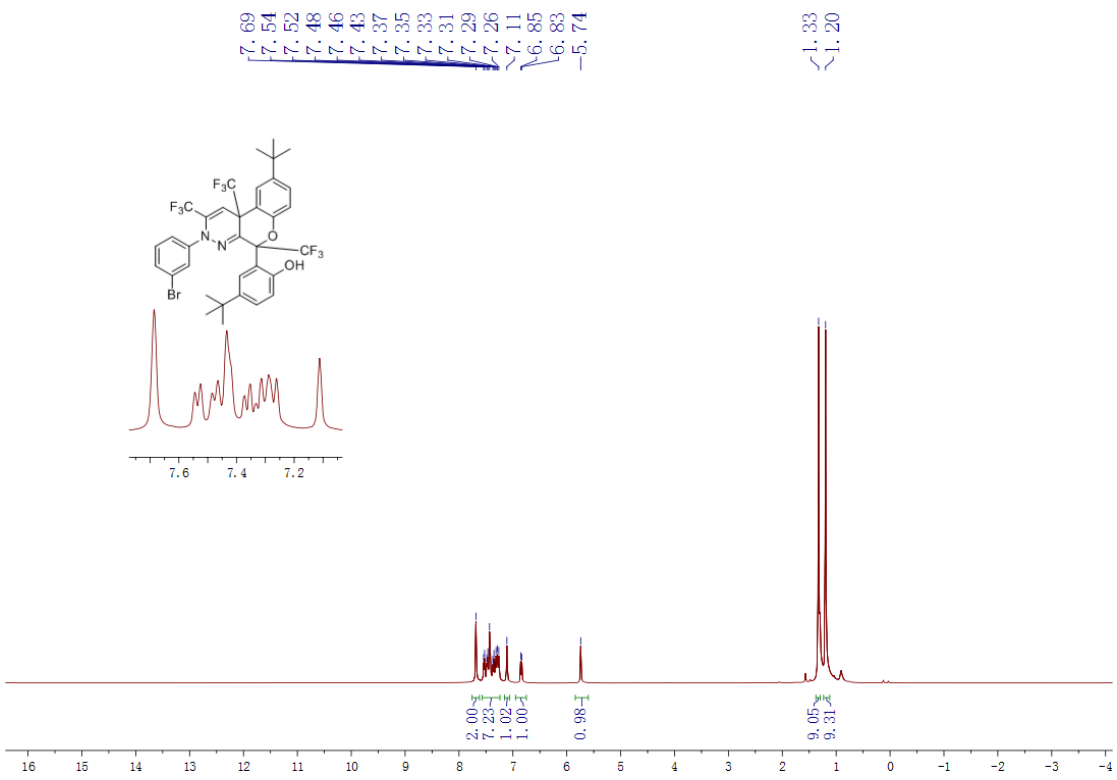
^{19}F NMR spectrum of **7k** in $CDCl_3$



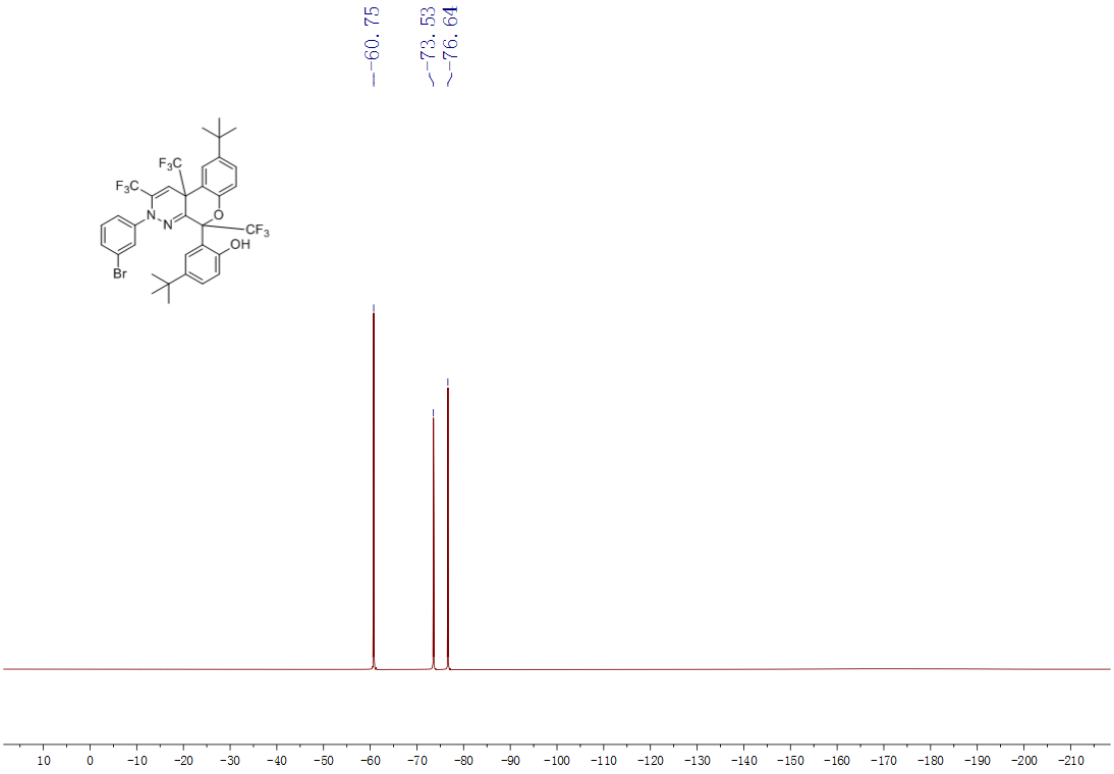
^{13}C NMR spectrum of **7k** in $CDCl_3$



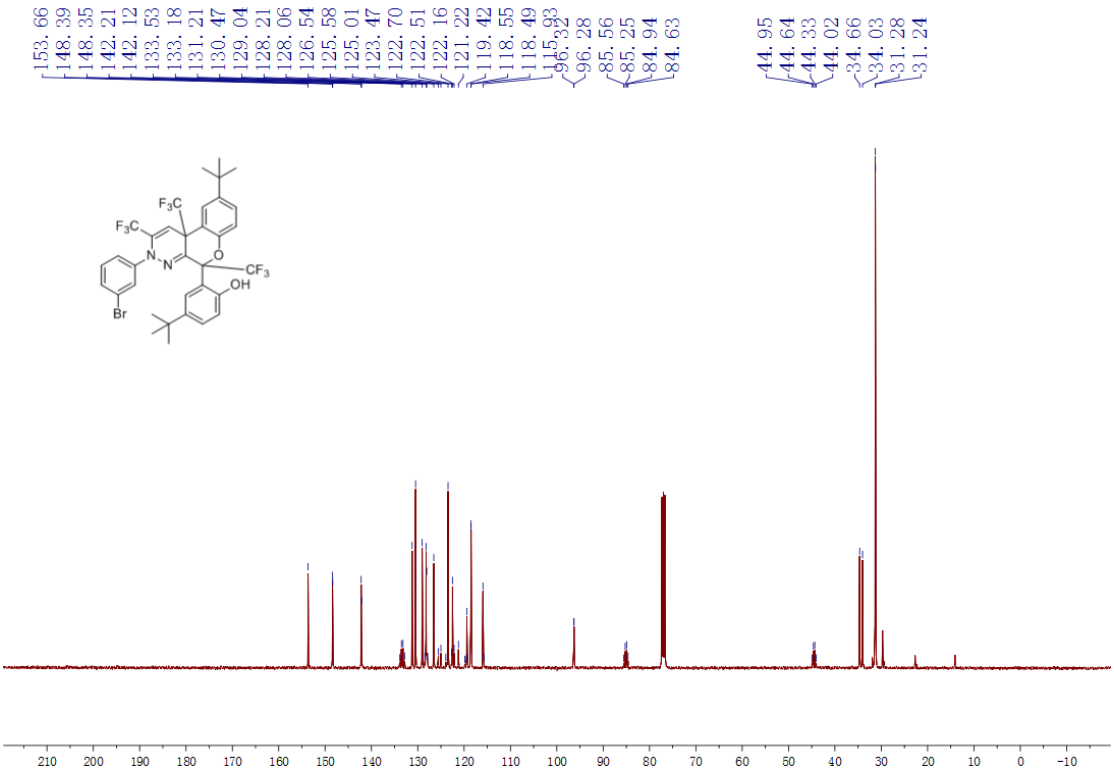
^{1}H NMR spectrum of **7l** in $CDCl_3$



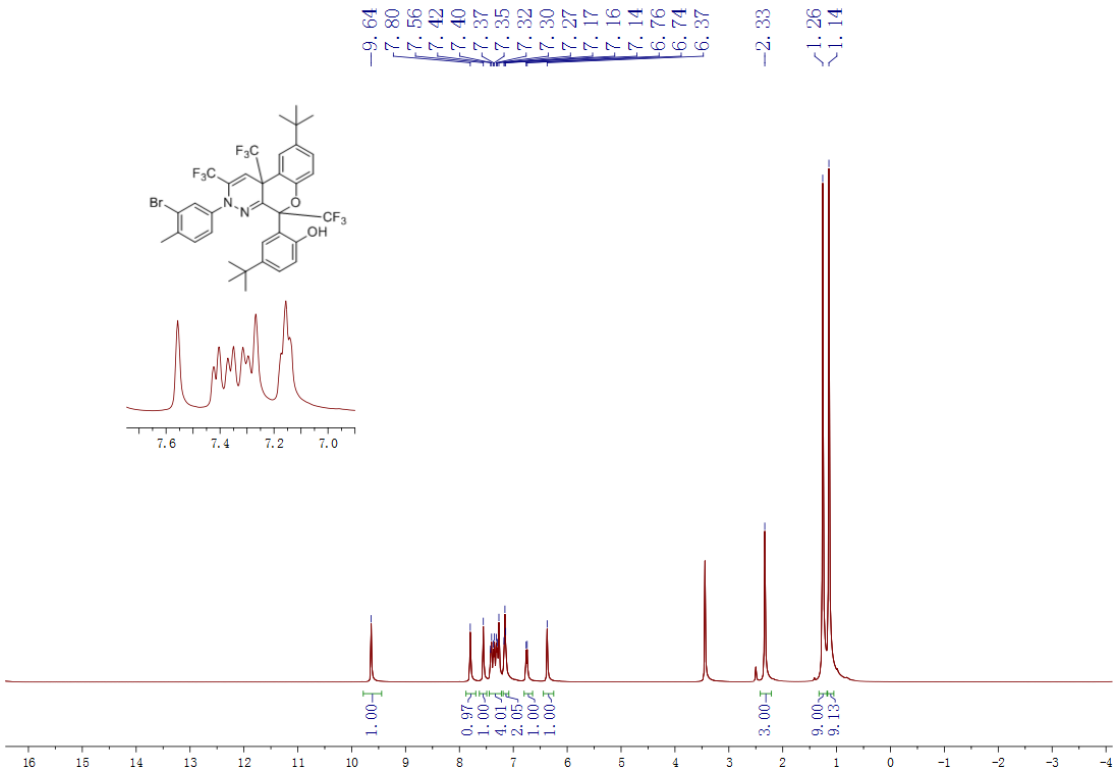
^{19}F NMR spectrum of **7l** in $CDCl_3$



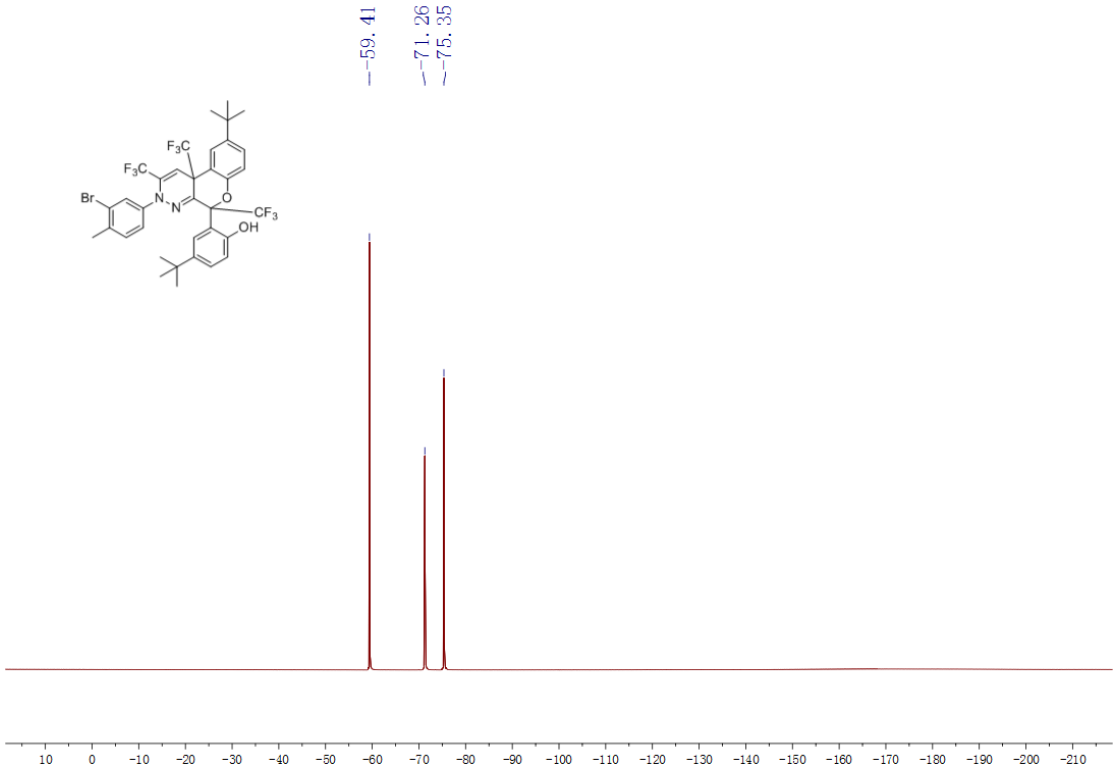
^{13}C NMR spectrum of **7l** in $CDCl_3$



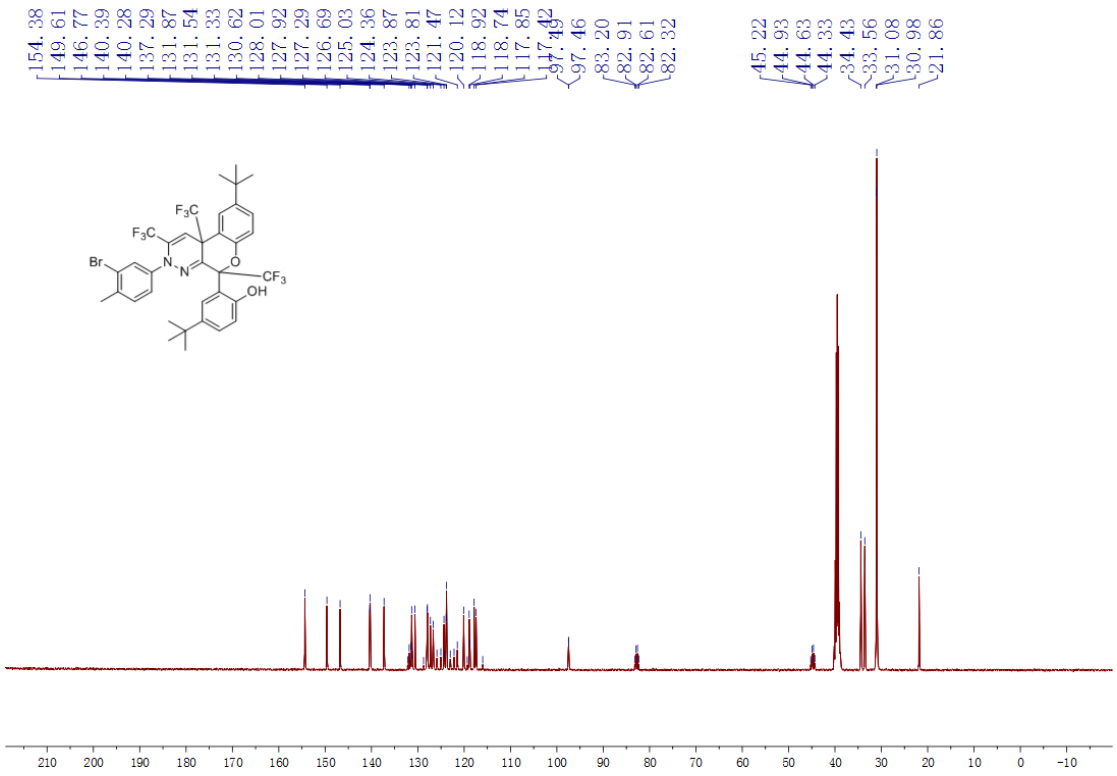
^{1}H NMR spectrum of **7m** in DMSO-d_6



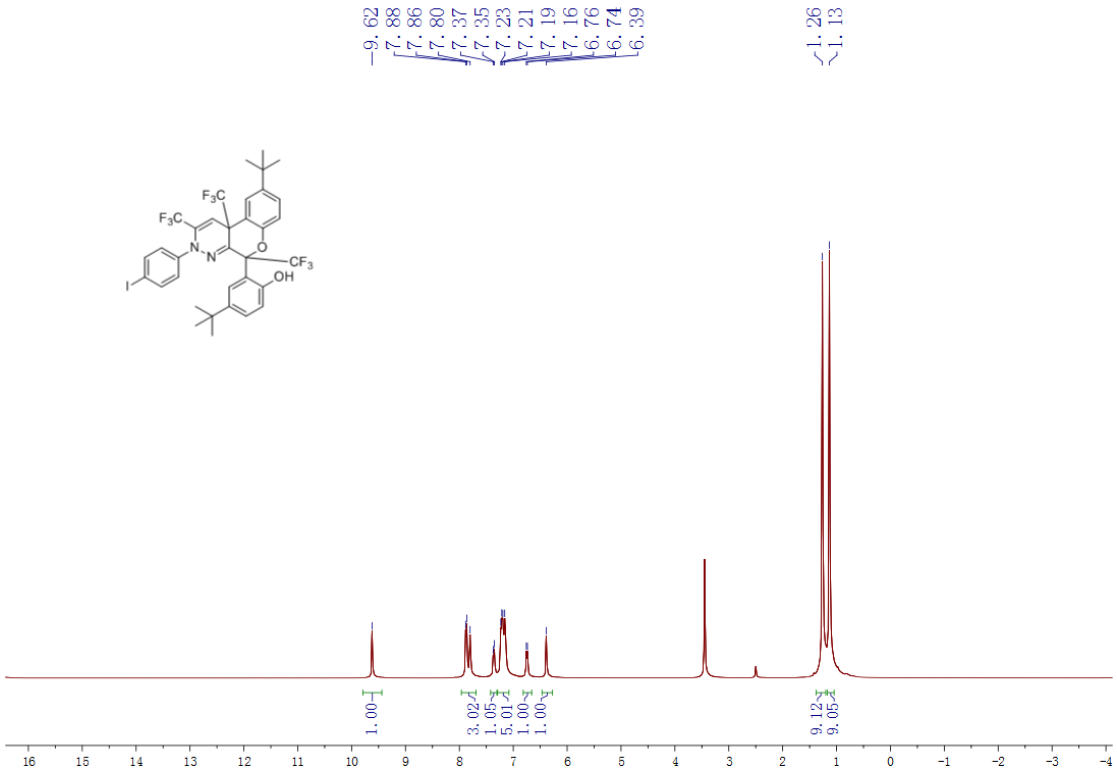
^{19}F NMR spectrum of **7m** in DMSO-d_6



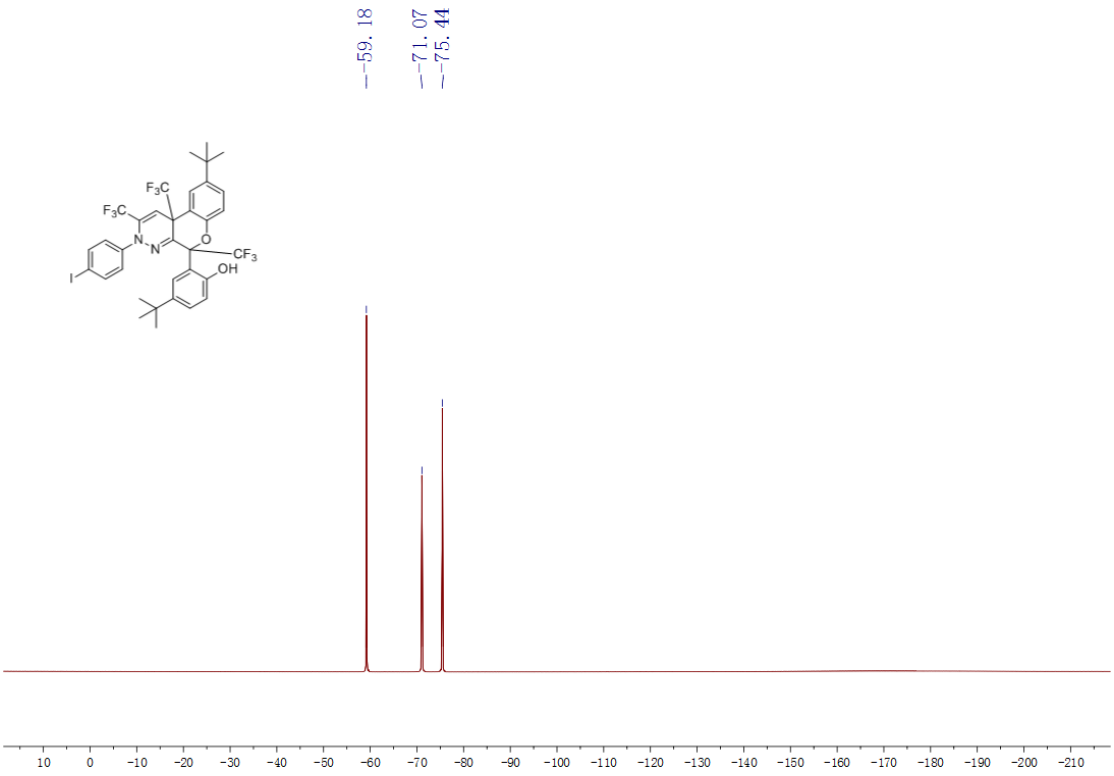
^{13}C NMR spectrum of **7m** in DMSO-d_6



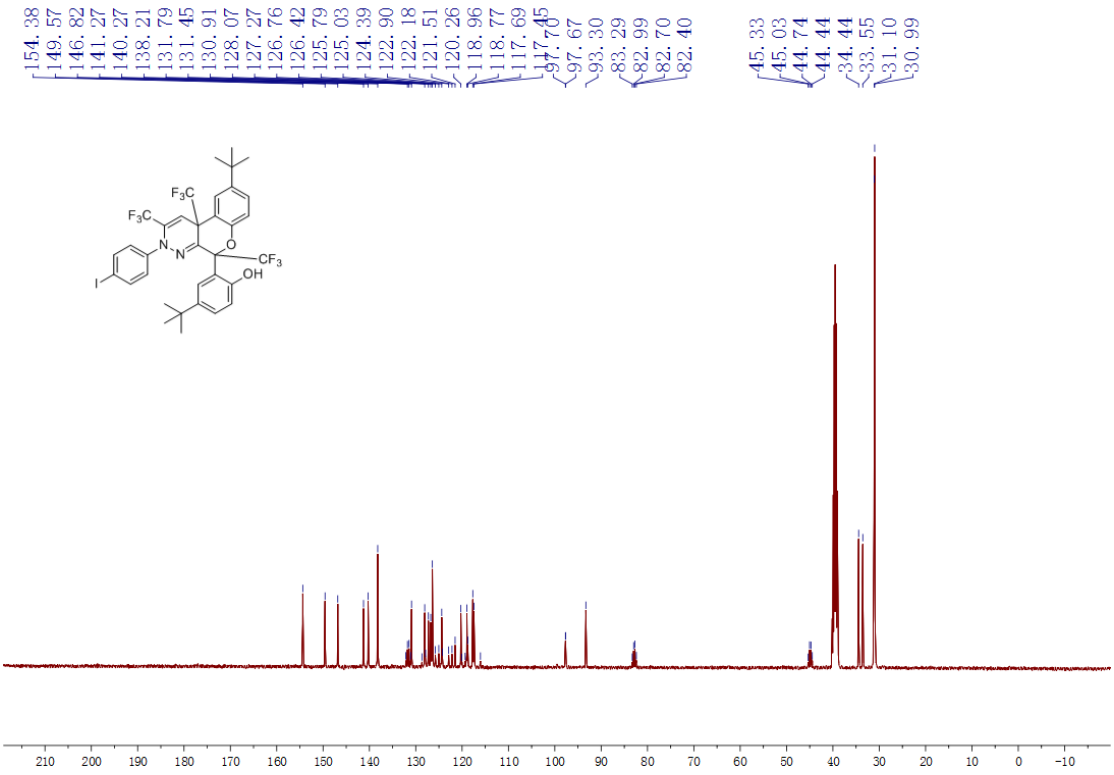
^{1}H NMR spectrum of **7n** in DMSO-d_6



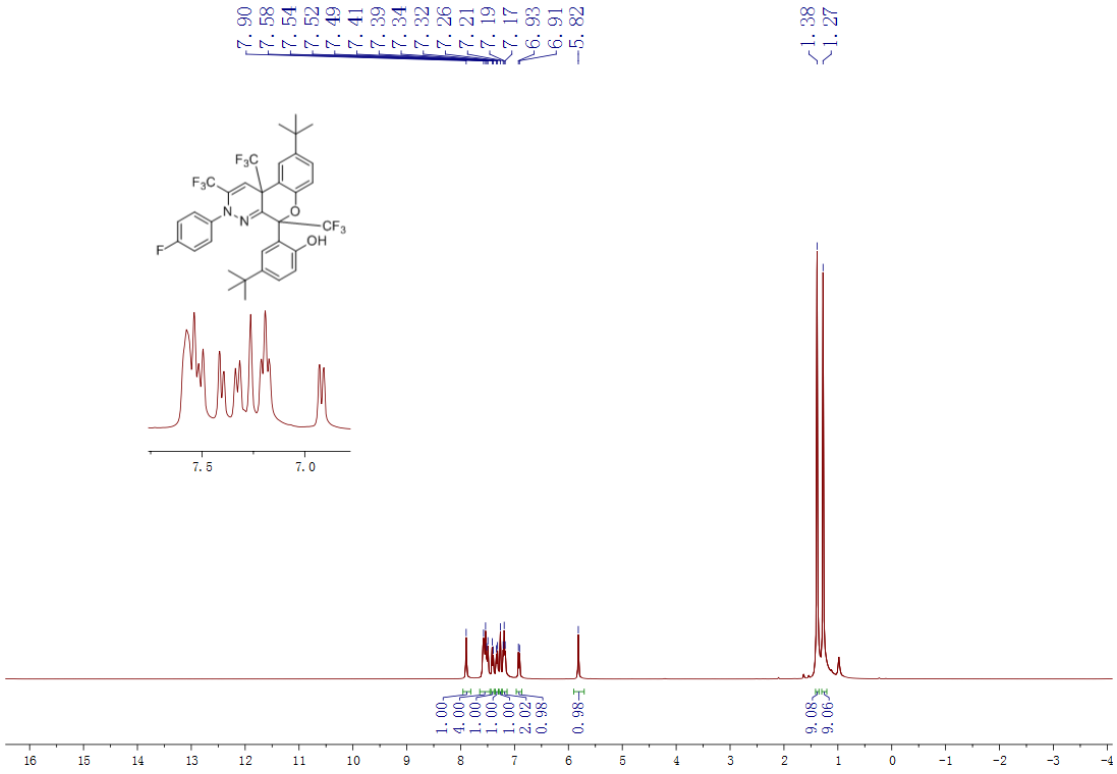
^{19}F NMR spectrum of **7n** in DMSO-d_6



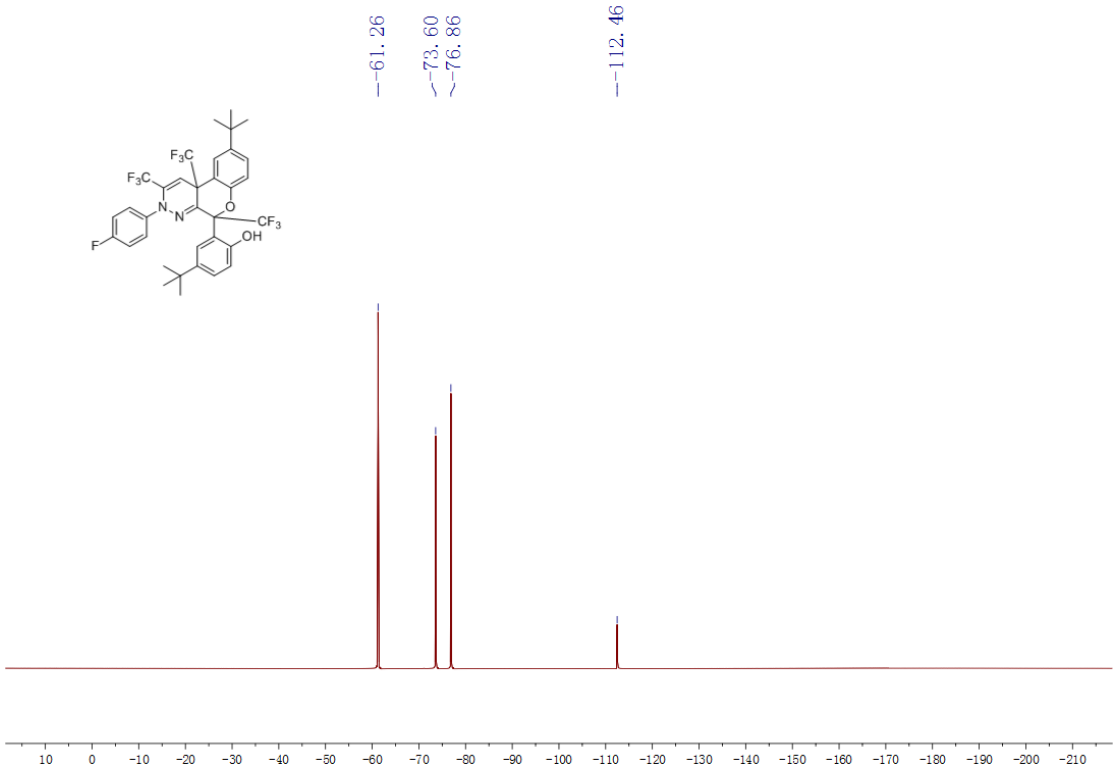
^{13}C NMR spectrum of **7n** in DMSO-d_6



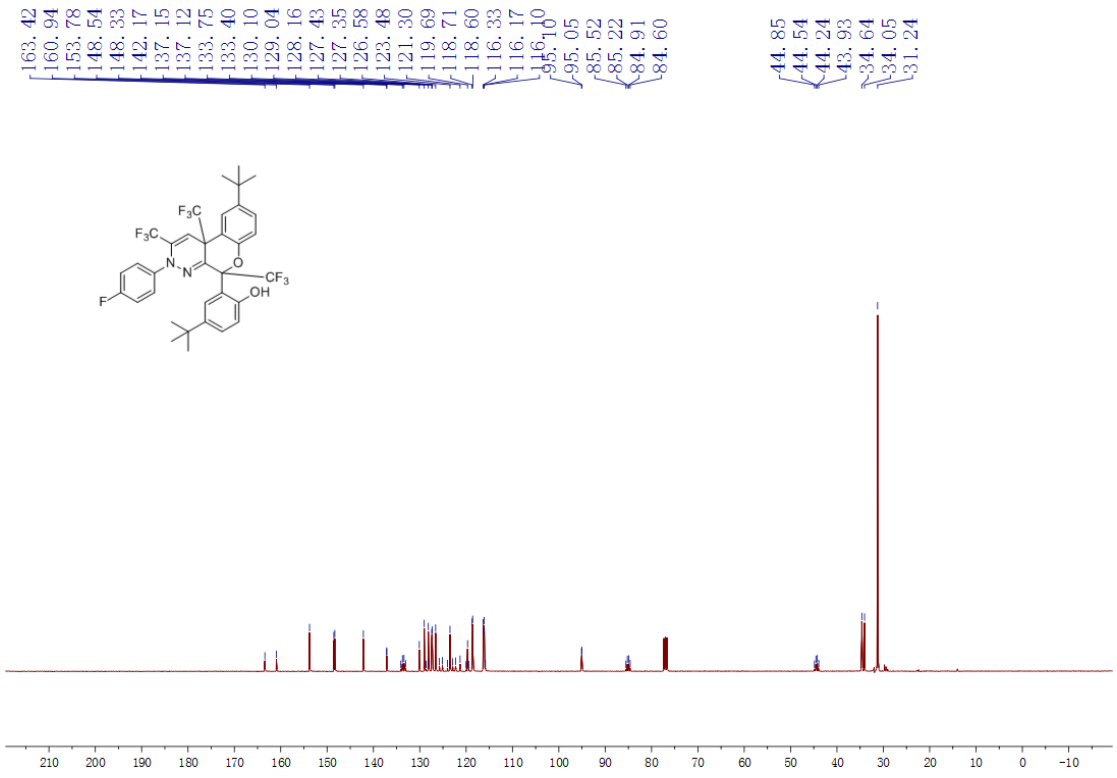
^{1}H NMR spectrum of **7o** in $CDCl_3$



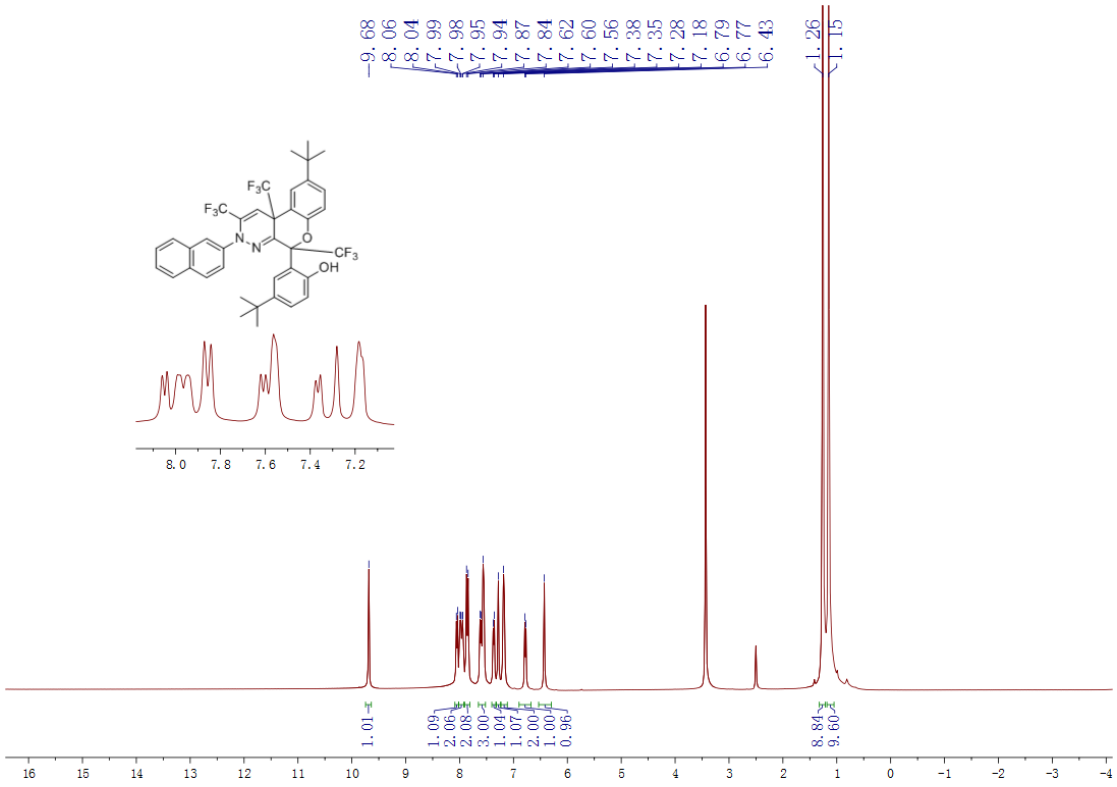
^{19}F NMR spectrum of **7o** in $CDCl_3$



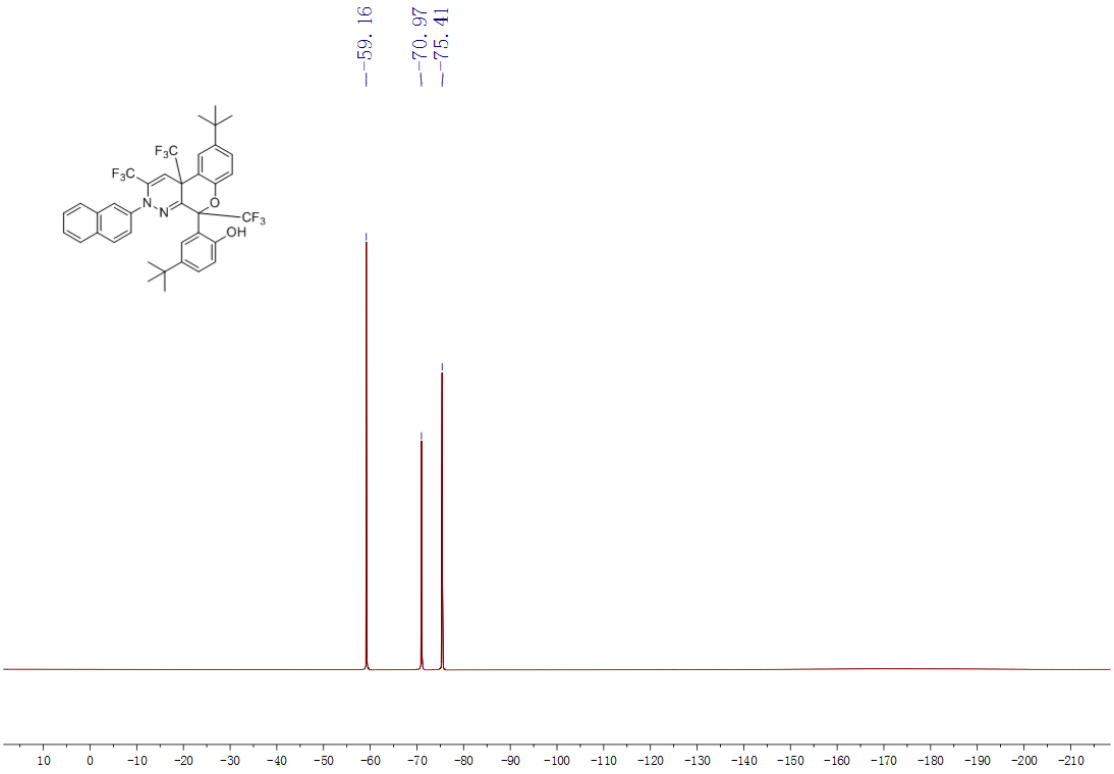
^{13}C NMR spectrum of **7o** in $CDCl_3$



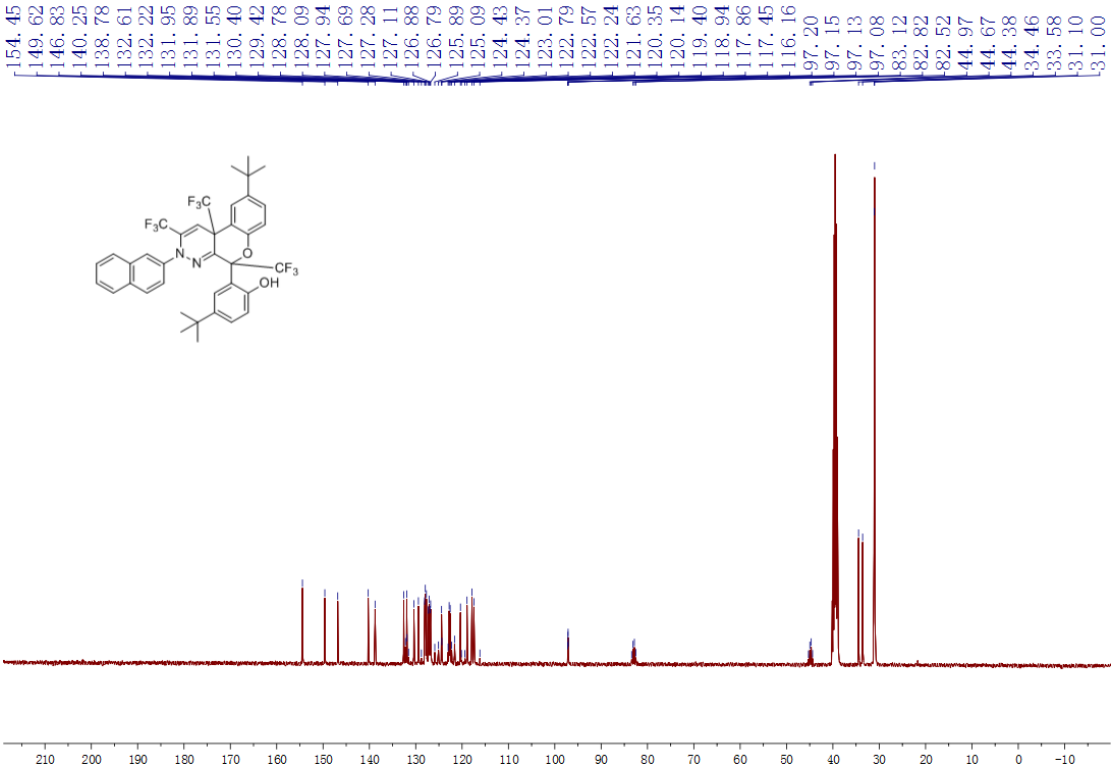
^{1}H NMR spectrum of **7p** in DMSO-d_6



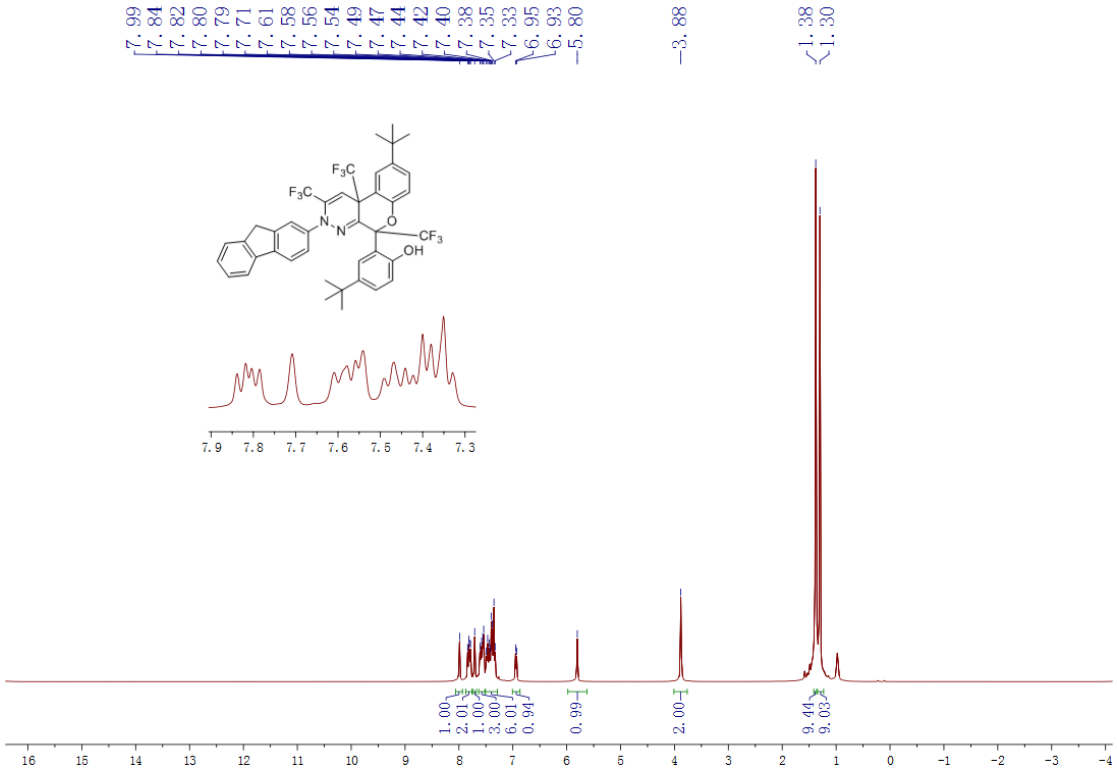
^{19}F NMR spectrum of **7p** in DMSO-d_6



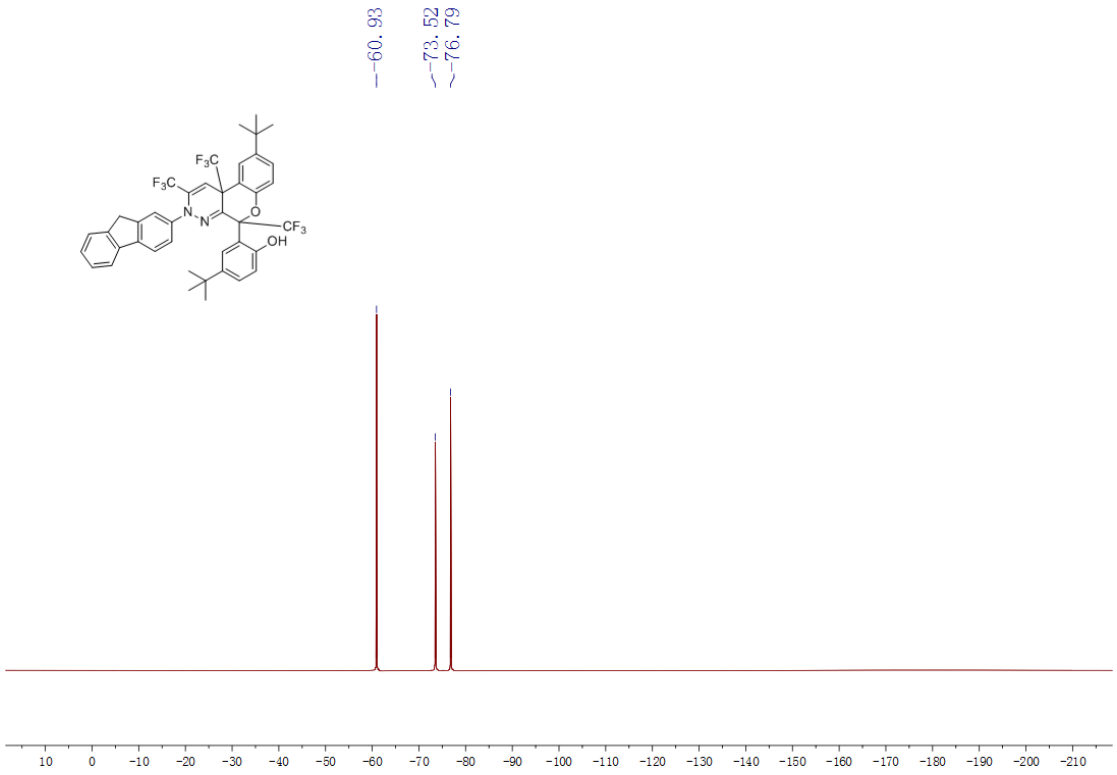
^{13}C NMR spectrum of **7p** in DMSO-d_6



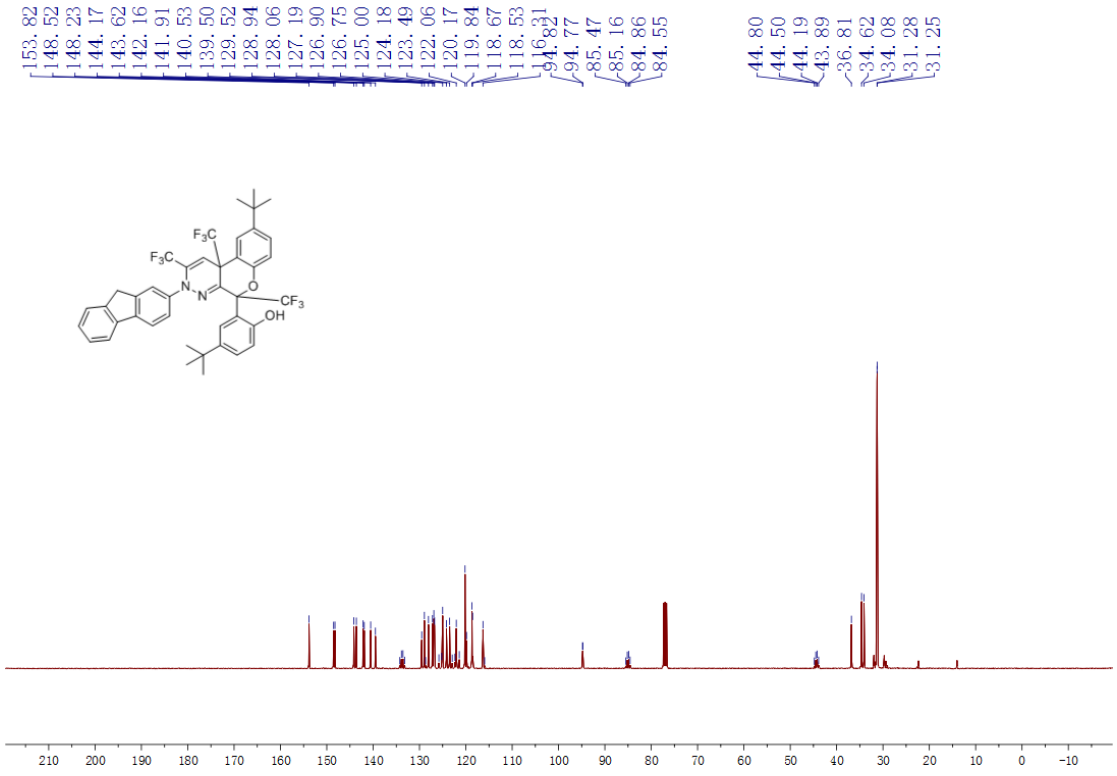
^{1}H NMR spectrum of **7q** in $CDCl_3$



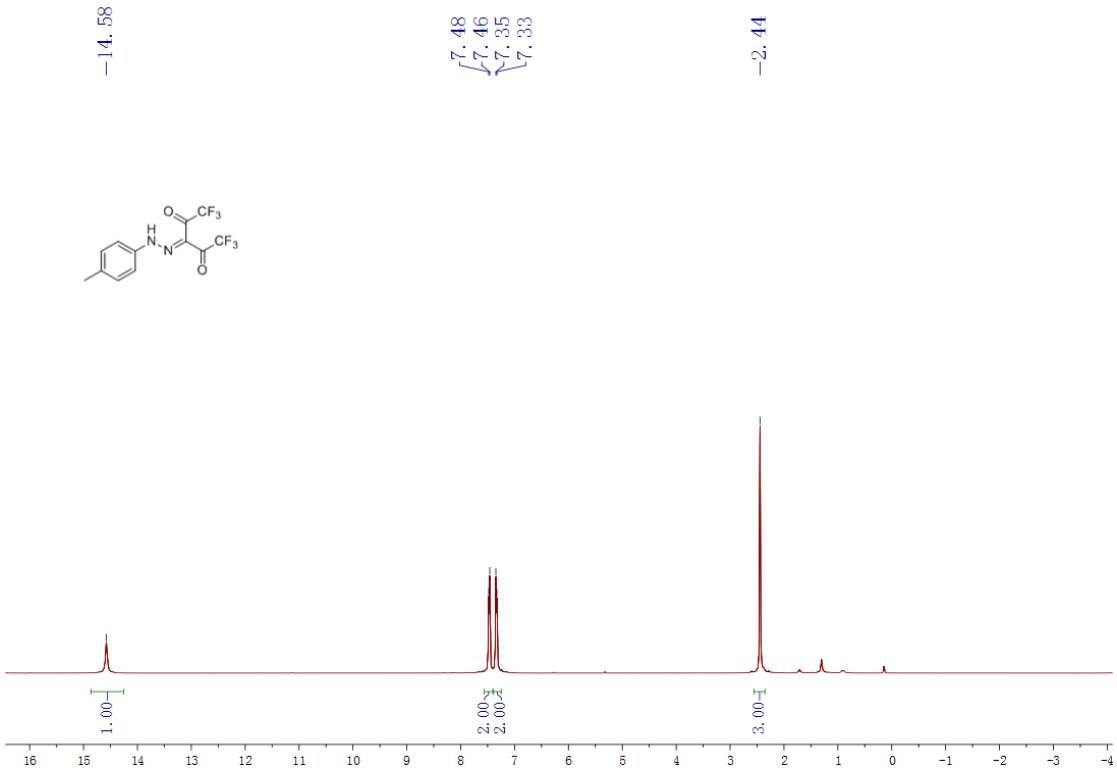
^{19}F NMR spectrum of **7q** in $CDCl_3$



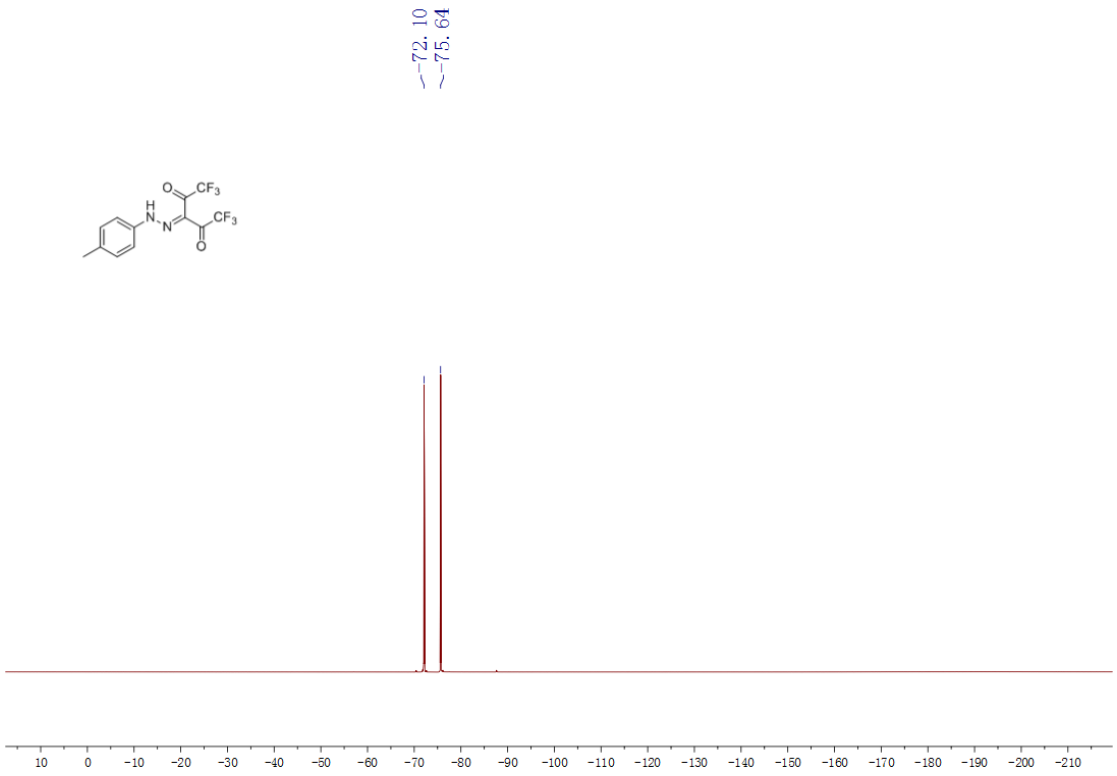
^{13}C NMR spectrum of **7q** in $CDCl_3$



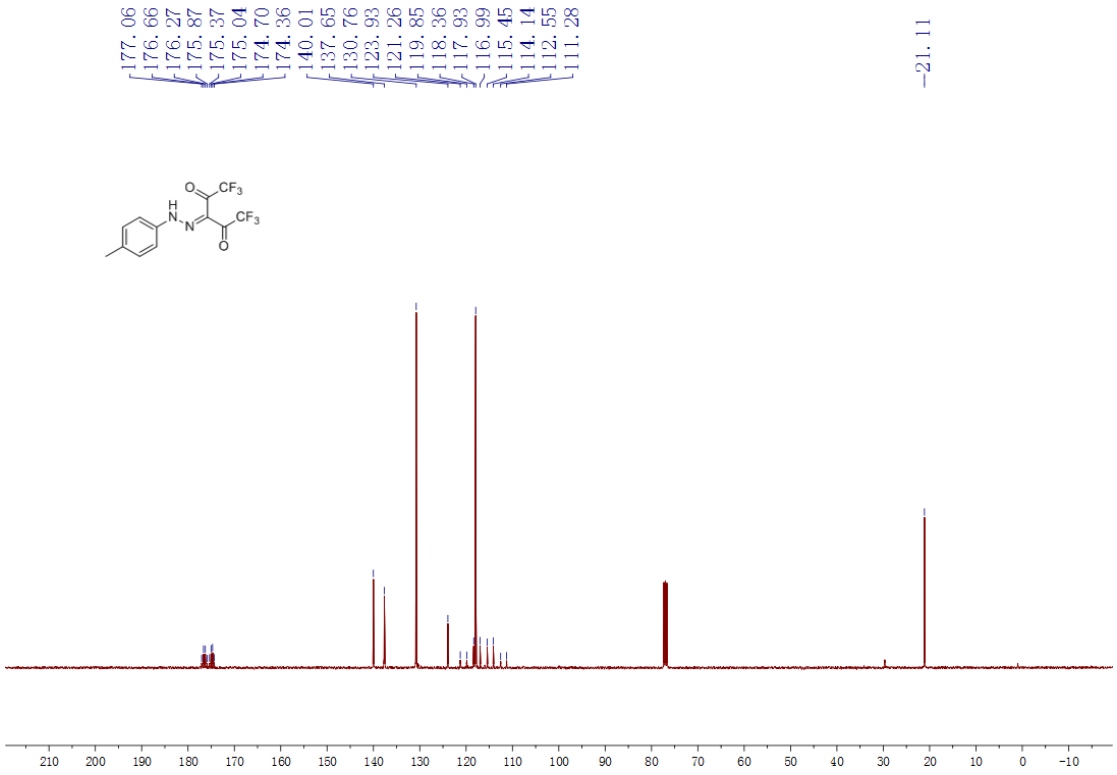
^{1}H NMR spectrum of intermediate **I** in $CDCl_3$



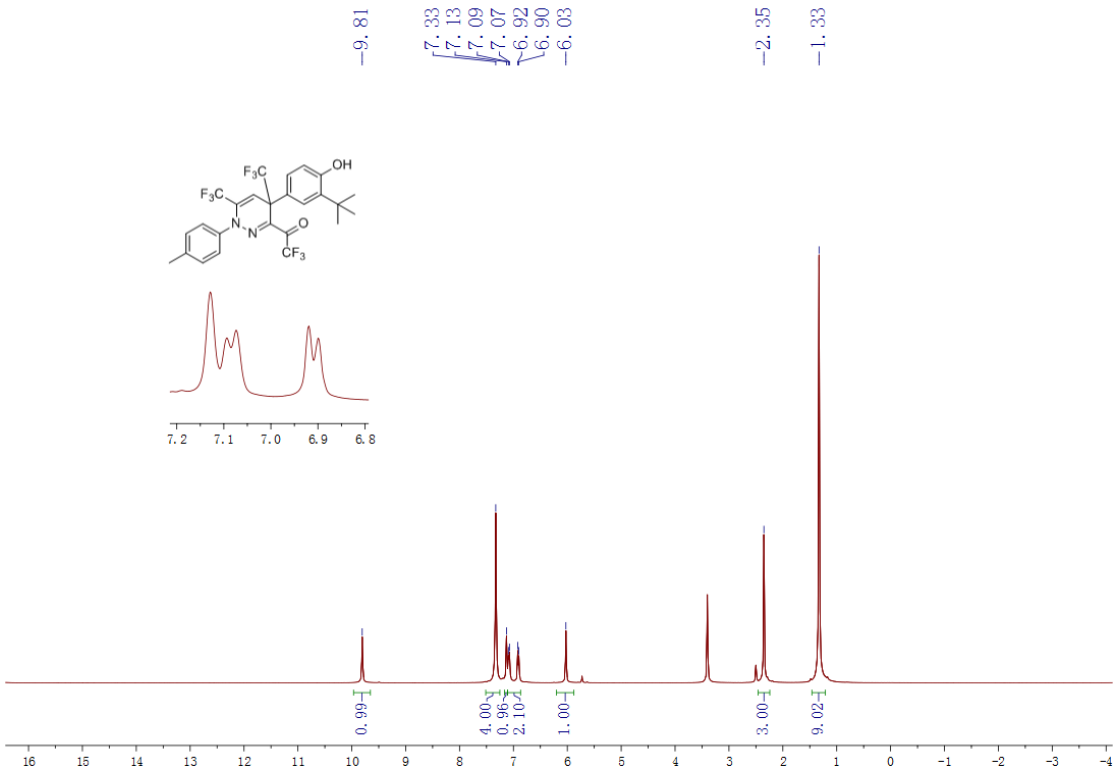
^{19}F NMR spectrum of intermediate **I** in $CDCl_3$



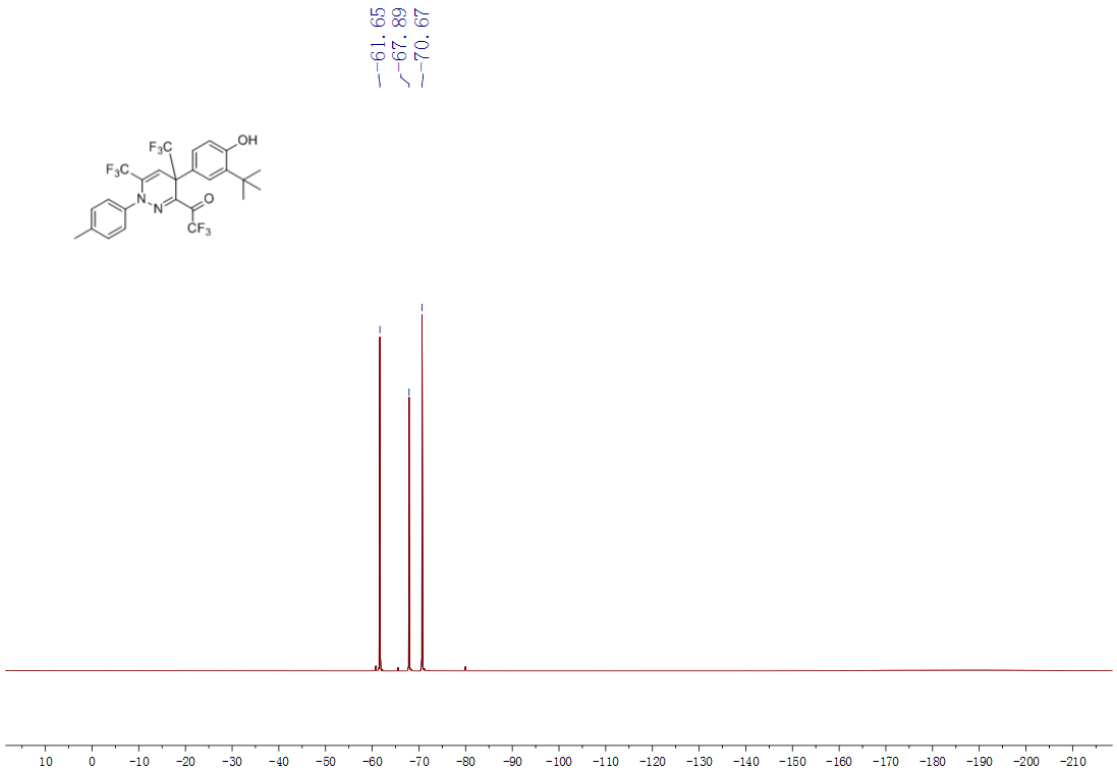
^{13}C NMR spectrum of intermediate **I** in $CDCl_3$



^{1}H NMR spectrum of **8** in DMSO-d_6



^{19}F NMR spectrum of **8** in DMSO-d_6



^{13}C NMR spectrum of **8** in DMSO-d_6