Electronic Supplementary Material (ESI) for ChemComm.

Supporting Information *for*

Elemental tellurium mediated synthesis 2-(trifluoromethyl)oxazoles using trifluoroacetic anhydride as reagent

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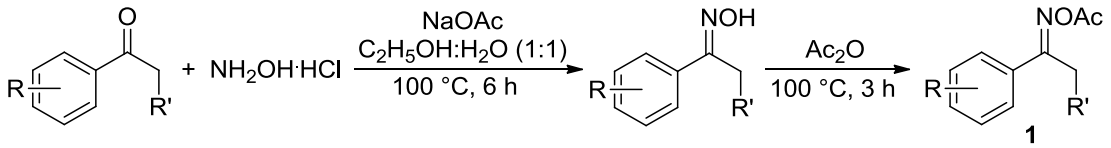
General information

^{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. Coupling constants (*J*) are reported in Hertz (Hz). The residual solvent peak was used as an internal reference: ^{1}H NMR (chloroform δ 7.26) and ^{13}C NMR (chloroform δ 77.0). 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 Waters GCT-TOF at the Shanghai Institute of Organic Chemistry and State Key Discipline Testing Center for Physical Chemistry of Fuzhou University. 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 for preparation of oxime acetate substrates

Oxime acetates were synthesized according to the published procedures:[1-6]

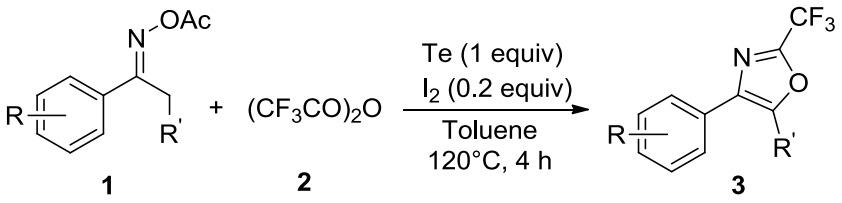


1

To a solution of aromatic ketones (2 mmol) in the mixture of C_2H_5OH/H_2O (v/v = 1:1) was added hydroxylamine hydrochloride (2.2 mmol), NaOAc (3 mmol) in one portion, and the reaction mixture was stirred at 100 °C for 6 h. Upon completion of the reaction as indicated by TLC, the reaction mixture was diluted with water, and extracted with ethyl acetate (15 mL × 3), dried over $MgSO_4$. The solvent was removed under reduced pressure to give oximes.

The mixture of aromatic ketoxime (2.0 mmol), anhydride (4.0 mmol) was stirred at 100 °C for 3 h. Upon completion of the reaction as indicated by TLC, the reaction mixture was diluted with water, and extracted with ethyl acetate (15 mL × 3), dried over $MgSO_4$. The solvent was removed by rotary evaporation and the resulting product was purified by column chromatography over silica gel with hexanes as the eluent to afford aromatic ketoxime acetates.

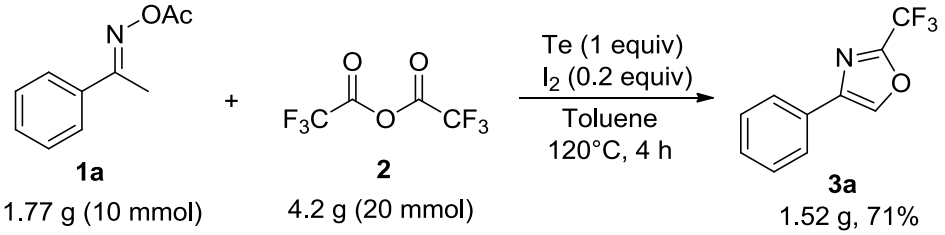
General procedure of the tellurium-mediated synthesis of 2-(trifluoromethyl)oxazoles



1 **2** **3**

The aromatic ketoxime acetates derivatives (**1**) (1.0 mmol), trifluoroacetic anhydride (**2**) (2.0 mmol, 2.0 equiv), Te (1.0 mmol, 1.0 equiv), I_2 (0.2 mmol, 0.2 equiv), and toluene (4.0 mL) were added to a oven-dried 25.0 mL test tube with Teflon screw cap. The tube was sealed and the mixture solution was placed into a preheated 120 °C oil bath for 4 h. The tube was removed from the oil bath and cooled to r.t. The reaction mixture was diluted with ethyl acetate (15 mL × 3), washed with saturated sodium bicarbonate (30 mL), and water (20 mL), dried over $MgSO_4$. The solvent was removed by rotary evaporation and the resulting crude product **3** was purified by column chromatography over silica gel (*n*-pentanes).

Procedure for the synthesis of 4-phenyl-2-(trifluoromethyl)oxazole (3a) on a 10.0 mmol scale



1a
1.77 g (10 mmol)

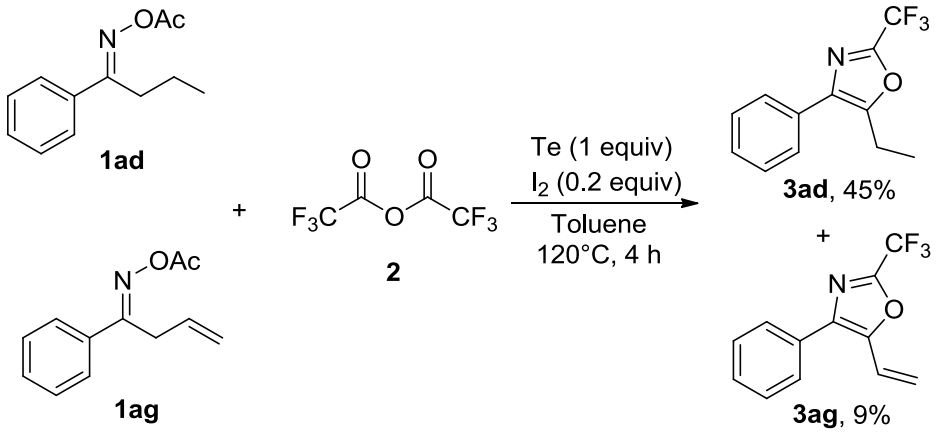
2
4.2 g (20 mmol)

3a
1.52 g, 71%

The acetophenone oxime acetate (**1a**) (1.77 g, 10.0 mmol), trifluoroacetic anhydride (**2**) (2.8 mL, 4.20 g, 20.0 mmol, 2.0 equiv), Te (1.30 g, 10.0 mmol), I_2 (0.50 g, 2.0 mmol), and toluene (40.0 mL) were added to a oven-dried 100 mL test tube with Teflon screw cap. The tube was sealed and the mixture solution was placed into a preheated 120 °C oil bath for 4 h. The tube was removed from the oil bath and cooled to r.t. The reaction mixture was diluted with ethyl acetate (40 mL × 5), washed with saturated sodium bicarbonate (500 mL), and water (200 mL), dried over $MgSO_4$. The solvent was removed by rotary evaporation and the crude product was purified by column chromatography over silica gel (*n*-pentanes). The product 4-phenyl-2-(trifluoromethyl)oxazole (**3a**) was isolated as a white solid in 71% (1.52 g).

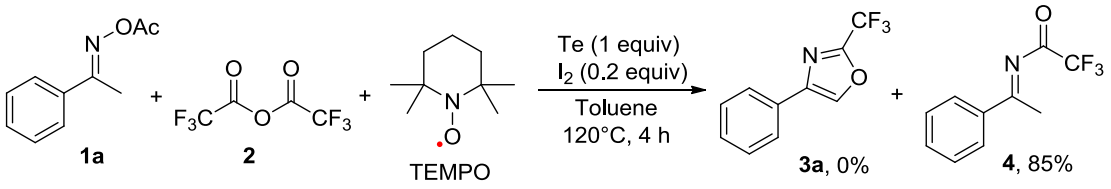
Experiments for Mechanistic Investigations

(a) Competition reaction of ketoxime acetates derivatives 1ae and 1ag with 2.



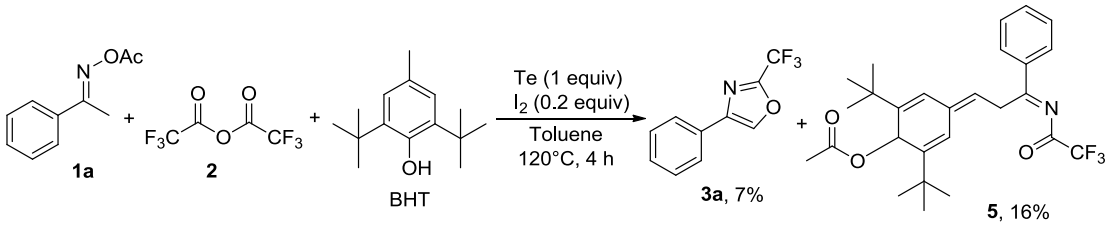
The aromatic ketoxime acetates derivatives **1ad** (17.7 mg, 0.10 mmol), **1ag** (21.7 mg, 0.10 mmol), trifluoroacetic anhydride (**2**) (42 μL, 63 mg, 0.30 mmol), Te (13 mg, 0.10 mmol), I_2 (5.0 mg, 0.020 mmol), and 1.0 mL toluene were added to a oven-dried 5 mL test tube with Teflon screw cap. The tube was sealed and the mixture solution was placed into a preheated 120 °C oil bath for 4 h. The tube was removed from the oil bath and cooled to r.t. 10 μL (Trifluoromethoxy)benzene was then added as an internal standard. The reaction mixture was filtered through a layer of celite. The filtrate was analyzed by ^{19}F NMR and GC-MS, and the products **3ad** and **3ag** were calculated to be 45% and 9%, respectively.

(b) Procedure for the reaction of acetophenone oxime acetate (1a) with trifluoroacetic anhydride (2) mediated by tellurium in the presence of 2.0 equiv TEMPO



In a dry-box, acetophenone oxime acetate (**1a**) (177 mg, 1.0 mmol), trifluoroacetic anhydride (**2**) (280 μL, 420 mg, 2.0 mmol, 2.0 equiv), Te (130 mg, 1.0 mmol, 1.0 equiv), I_2 (50 mg, 0.20 mmol, 0.20 equiv), TEMPO (312 mg, 2.0 mmoL, 2.0 equiv), and 1.0 mL toluene were added to a oven-dried 5 mL test tube with Teflon screw cap. The tube was sealed and the mixture solution was placed into a preheated 120 °C oil bath for 4 h. The tube was removed from the oil bath and cooled to r.t. 10 µL (Trifluoromethoxy)benzene was then added as an internal standard. The reaction mixture was filtered through a layer of celite. The filtrate was analyzed by ^{19}F NMR and GC-MS, and no trace of 4-phenyl-2-(trifluoromethyl)oxazole (**3a**) was detected. Compound 2,2,2-trifluoro-*N*-(1-phenylethylidene)acetamide (**4**) was formed in 85% NMR yield.

(c) Procedure for the reaction of acetophenone oxime acetate (1a) with trifluoroacetic anhydride mediated by tellurium in the presence of 2.0 equiv BHT

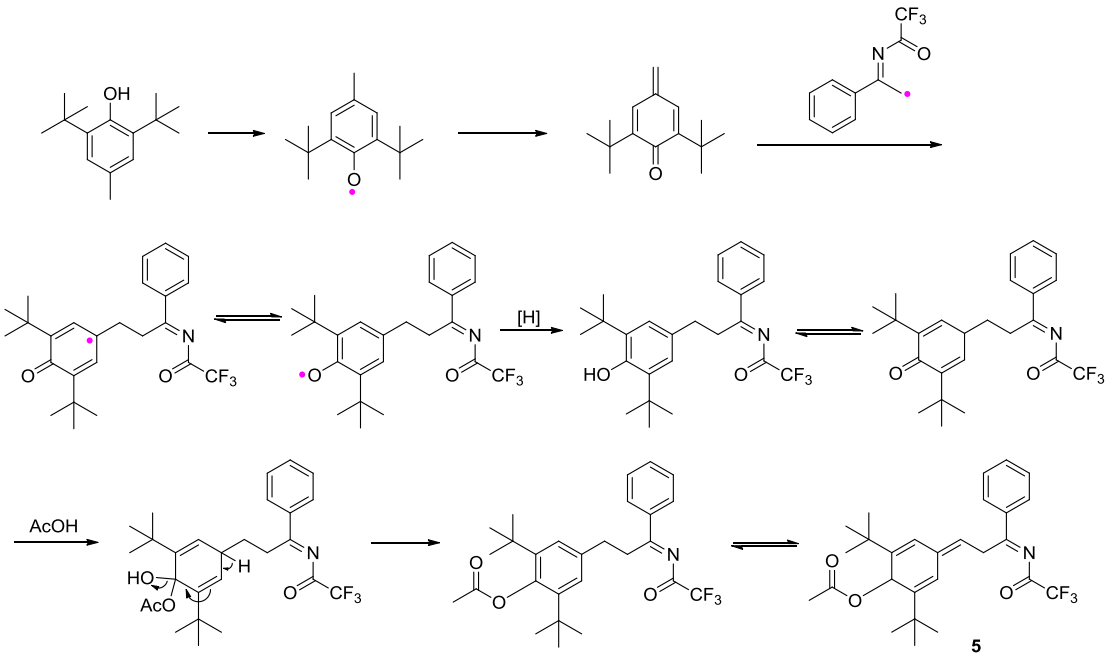


In a dry-box, acetophenone oxime acetate (**1a**) (177 mg, 1.0 mmol), trifluoroacetic anhydride (**2**) (280 μL, 420 mg, 2.0 mmol, 2.0 equiv), Te (130 mg, 1.0 mmol, 1.0 equiv), I_2 (50 mg, 0.20 mmol, 0.20 equiv), BHT (441 mg, 2.0 mmoL, 2.0 equiv), and 4.0 mL toluene were added to a oven-dried 25 mL test tube with Teflon screw cap. The tube was sealed and the mixture solution was placed into a preheated 120 °C oil bath for 4 h. The tube was removed from the oil bath and cooled to r.t. 10 μL (Trifluoromethoxy)benzene was then added as an internal standard. The reaction mixture was filtered through a layer of celite. The filtrate was analyzed by ^{19}F NMR and GC-MS, and the yields of 4-phenyl-2-(trifluoromethyl)oxazole (**3a**) and BHT-adduct (**5**) were calculated to be 7% and 16%, respectively.

The reaction mixture was diluted with ethyl acetate (15 mL × 3), washed with saturated sodium bicarbonate (30 mL), and water (20 mL), dried over $MgSO_4$. The solvent was removed by rotary evaporation and the resulting product **7** was purified by column chromatography over silica gel (*n*-pentane/ethyl acetate = 10:1). *N*-(2-(2,6-di-*tert*-butyl-4-methylphenoxy)-1-phenylethylidene)-2,2,2-trifluoroacetami de (**5**): Obtained as a light yellow solid. M.p. 141–142 °C. R_f (*n*-pentane/ethyl acetate = 10:1) = 0.52. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47 – 7.35 (m, 6H), 7.22 (s, 2H), 6.26 (t, J = 7.2 Hz, 1H), 3.50 (d, J = 7.0 Hz, 2H), 2.38 (s, 3H), 1.38 (s, 18H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -75.1 (s, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.3 (s), 155.3 (q, J = 37.0 Hz), 146.6 (s), 142.7 (s), 136.0 (s), 135.8 (s), 131.2 (s), 128.8 (s), 128.7 (s), 127.2 (s), 126.6 (s), 125.6 (s), 115.9 (q, J = 289.1 Hz), 35.4 (s), 34.5 (s), 31.5 (s), 22.7 (s). IR (KBr): ν 3277, 2964, 2165, 2034, 1717, 1526, 1483, 1425, 1367, 1203, 1164,

804, 758, 694, 515 cm^{-1}. GC-MS m/z 475 (M^+). HRMS (EI) m/z: calcd. for $C_{27}H_{32}F_3NO_3$: 475.2334; found: 475.2324.

A proposed reaction pathway for the formation of 5



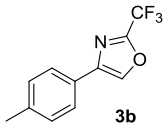
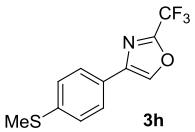
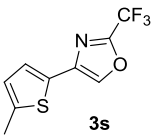
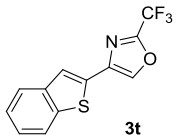
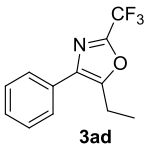
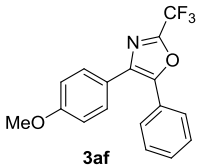
The procedure for the biological assay

Evaluations of fungicidal activities of the synthesized compounds:

Each of the test compounds (4 mg) was first dissolved in 5 mL of mixture of acetone and methanol (1:1 by volume), and then 5 mL of water containing 0.1% Tween 80 was added to generate a 10 mL stock solution of 400 mg/L concentration.

Briefly, a whole plant is used in this test, and the testing solution is sprayed to the host plant by a special plant sprayer. The plant is inoculated with fungus after 24 h. According to the infecting characteristics of fungus, the plant is stored in a humidity chamber and then transferred into a greenhouse after infection is finished. The other plants are placed in a greenhouse directly. The activity of each compound was estimated by visual inspection after 7 days, and screening results were reported as a range from 0% (no control) to 100% (complete control).

The general screening of the title compounds on bactericidal activity

compound	bactericidal activity (% control at the concentration of 400 mg/L)			
	CDM	WPM	CSR	CA
 **3b**	0	0	0	0
 **3h**	0	60	20	0
 **3s**	0	30	0	0
 **3t**	0	0	60	0
 **3ad**	0	0	75	0
 **3af**	0	0	40	0
Mancozeb (25 mg/L)	90	-	-	-
Azoxystrobin (25 mg/L)	-	100	100	100

CDM = cucumber downy mildew; WPM = wheat powdery mildew; CSR = corn rust; CA = cucumber anthracnose

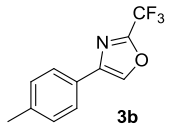
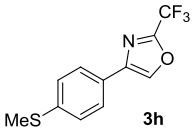
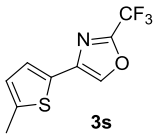
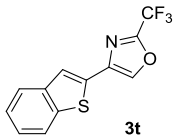
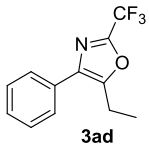
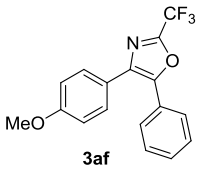
Insecticidal activities:

Each of the test compounds was first dissolved in 5 mL of mixture of acetone and methanol (1:1 by volume), and then 5 mL of water containing 0.1% Tween 80 was added to generate a 10 mL stock solution of 600 mg/L concentration.

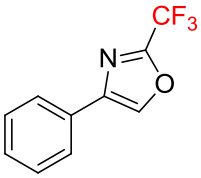
The cabbage leaves were cut into small circular pieces (ϕ = 30 mm), and placed on the glass Petri dishes (ϕ = 60 mm) layered with filter papers that had been wet with sterilized distilled water. The cabbage leaves were prayed with the aforementioned solutions using a Airbrush sprayer (dosage 0.5 mL). After they were air dried, the third-instar insects were introduced to the cabbage leaves. They were kept in a special room for normal cultivation (temperature: 23-25 °C; RH: 40-60%, L/D: 13 h/11 h). Assessments were made after 72 h by the number of killed and size of live insects relative to that in the negative control, and evaluations were based on a percentage scale of 0-100, in which 100 was total kill and 0 was no activity. To compare their activities, the commercial products abamectin and imidacloprid was tested at the concentration of 10 mg/L under the same conditions.

For the insecticidal activities against leucania separate, the corn leaf disks (2 mm $\times$ 5 mm) were used instead of the cabbage leaves.

The general screening of the title compounds on insecticidal activity

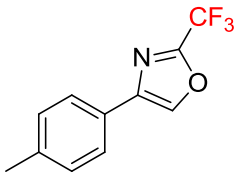
compound	insecticidal activity (% mortality at the concentration of 600 mg/L)			
	plutella xylostella	leucania separate	myzus persicae	tetranychus cinnabarinus
 **3b**	0	0	0	0
 **3h**	0	0	0	0
 **3s**	0	0	0	0
 **3t**	42.9	0	0	0
 **3ad**	0	0	0	0
 **3af**	16.7	0	0	0
96.2% Abamectin (10 mg/L)	100	100	-	100
96% Imidacloprid (10 mg/L)	-	-	100	-

Data for compounds 3.



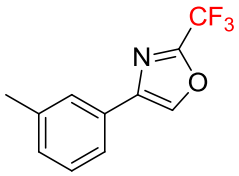
4-Phenyl-2-(trifluoromethyl)oxazole (3a)

Obtained as a white solid in 95% yield (202 mg). M.p. 51–52 °C. R_f (*n*-pentane) = 0.75. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (s, 1H), 7.79 (d, *J* = 7.6 Hz, 2H), 7.53 – 7.37 (m, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -65.9 (s, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 150.9 (q, *J* = 44.0 Hz), 142.1 (s), 135.4 (q, *J* = 1.2 Hz), 129.2 (s), 129.1 (s), 128.9 (s), 125.8 (s), 116.5 (q, *J* = 270.7 Hz). IR (KBr): ν 1598, 1580, 1486, 1450, 1378, 1243, 1155, 1125, 938, 754, 691, 548 cm^{-1}. GC-MS m/z 213 (M^+). HRMS (ESI) m/z: calcd. for $C_{10}H_6F_3NO$: 213.0401; found: 213.0399.



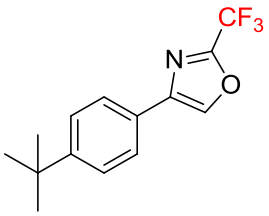
4-(*p*-Tolyl)-2-(trifluoromethyl)oxazole (3b)

Obtained as a white solid in 98% yield (222 mg). M.p. 76–77 °C. R_f (*n*-pentane) = 0.69. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (s, 1H), 7.68 (d, *J* = 8.2 Hz, 2H), 7.28 (d, *J* = 8.2 Hz, 2H), 2.42 (s, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -65.8 (s, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 150.9 (q, *J* = 43.9 Hz), 142.1 (s), 139.1 (s), 134.9 (q, *J* = 1.2 Hz), 129.6 (s), 126.4 (s), 125.7 (s), 116.5 (q, *J* = 270.6 Hz), 21.3 (s). IR (KBr): ν 2177, 2141, 2055, 1980, 1582, 1379, 1207, 1160, 954, 902, 822, 769, 545, 476 cm^{-1}. GC-MS m/z 227 (M^+). HRMS (EI) m/z: calcd. for $C_{11}H_8F_3NO$: 227.0558; found: 227.0559.



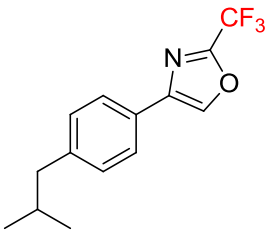
4-(*m*-Tolyl)-2-(trifluoromethyl)oxazole (3c)

Obtained as a white solid in 82% yield (186mg). M.p. 30–31 °C. R_f (*n*-pentane) = 0.65. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 (s, 1H), 7.64 (s, 1H), 7.57 (d, *J* = 7.7 Hz, 1H), 7.36 (t, *J* = 7.6 Hz, 1H), 7.23 (d, *J* = 7.6 Hz, 1H), 2.44 (s, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -65.9 (s, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 150.9 (q, *J* = 44.0 Hz), 142.2 (s), 138.8 (s), 135.4 (q, *J* = 1.2 Hz), 129.9 (s), 129.1 (s), 128.8 (s), 126.5 (s), 122.9 (s), 116.5 (q, *J* = 270.7 Hz), 21.3 (s). IR (KBr): ν 2815, 2213, 1585, 1377, 1243, 1207, 1159, 1126, 1106, 951, 836, 769, 548 cm^{-1}. GC-MS m/z 227 (M^+). HRMS (EI) m/z: calcd. for $C_{11}H_8F_3NO$: 227.0558; found: 227.0548.



4-(4-(*tert*-Butyl)phenyl)-2-(trifluoromethyl)oxazole (3d)

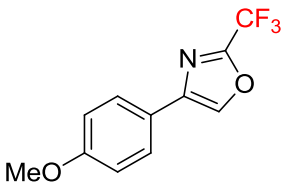
Obtained as a white liquid in 97% yield (261 mg). R_f (*n*-pentane) = 0.75. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 (s, 1H), 7.78 – 7.67 (m, 2H), 7.53 – 7.47 (m, 2H), 1.40 (s, 9H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -65.8 (s, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 152.4 (s), 150.9 (q, *J* = 44.0 Hz), 142.1 (s), 135.1 (q, *J* = 1.2 Hz), 126.4 (s), 125.9 (s), 125.6 (s), 116.5 (q, *J* = 270.7 Hz), 34.8 (s), 31.2 (s). IR (KBr): ν 2965, 2789, 2205, 1597, 1498, 1378, 1244, 1204, 1156, 954, 939, 755, 557 cm^{-1}. GC-MS m/z 269 (M^+). HRMS (EI) m/z: calcd. for $C_{14}H_{14}F_3NO$: 269.1027; found: 269.1029.



4-(4-Isobutylphenyl)-2-(trifluoromethyl)oxazole (3e)

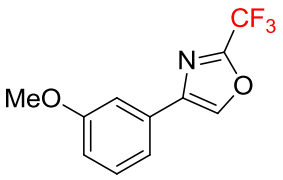
Obtained as a white solid in 79% yield (213 mg). M.p. 40–41 °C. R_f (*n*-pentane) = 0.69. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 (s, 1H), 7.70 (d, *J* = 8.1 Hz, 2H), 7.25 (d, *J*

= 8.1 Hz, 2H), 2.55 (d, *J* = 7.2 Hz, 2H), 1.93 (dp, *J* = 13.6, 6.8 Hz, 1H), 0.97 (d, *J* = 6.6 Hz, 6H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -65.9 (s, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 150.9 (q, *J* = 44.0 Hz), 142.9 (s), 142.2 (s), 135.0 (q, *J* = 1.2 Hz), 129.7 (s), 126.7 (s), 125.6 (s), 116.6 (q, *J* = 270.6 Hz), 45.2 (s), 30.2 (s), 22.3 (s). IR (KBr): ν 2957, 2870, 1597, 1465, 1378, 1301, 1242, 1156, 1125, 1103, 953, 798, 767, 532 cm^{-1}. GC-MS m/z 269 (M^+). HRMS (EI) m/z: calcd. for $C_{14}H_{14}F_3NO$: 269.1027; found: 269.1033.



4-(4-Methoxyphenyl)-2-(trifluoromethyl)oxazole (3f)

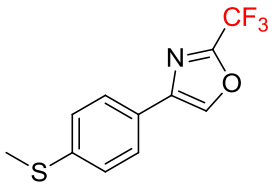
Obtained as a white solid in 71% yield (173 mg). M.p. 68–69 °C. R_f (*n*-pentane/ethyl acetate = 15:1) = 0.63. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 (s, 1H), 7.71 (d, *J* = 8.5 Hz, 2H), 6.99 (d, *J* = 8.5 Hz, 2H), 3.87 (s, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -65.8 (s, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.3 (s), 150.8 (q, *J* = 44.0 Hz), 141.9 (s), 134.4 (q, *J* = 1.3 Hz), 127.2 (s), 121.8 (s), 116.5 (q, *J* = 270.6 Hz), 114.4 (s), 55.3 (s). IR (KBr): ν 2788, 2253, 2150, 1619, 1502, 1380, 1255, 1207, 1162, 939, 835, 635, 546 cm^{-1}. GC-MS m/z 243 (M^+). HRMS (EI) m/z: calcd. for $C_{11}H_8F_3NO_2$: 243.0507; found: 243.0508.



4-(3-Methoxyphenyl)-2-(trifluoromethyl)oxazole (3g)

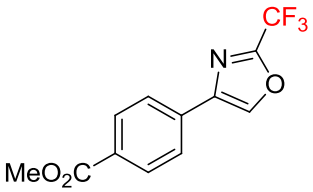
Obtained as a white solid in 62% yield (151 mg). M.p. 34–35 °C. R_f (*n*-pentane/ethyl acetate = 15:1) = 0.59. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (s, 1H), 7.42 – 7.31 (m, 3H), 6.96 (d, *J* = 7.2 Hz, 1H), 3.90 (s, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -65.8 (s, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.1 (s), 150.9 (q, *J* = 44.1 Hz), 142.0 (s), 135.6

(q, J = 1.2 Hz), 130.5 (s), 130.0 (s), 118.2 (s), 116.5 (q, J = 270.8 Hz), 114.9 (s), 111.2 (s), 55.4 (s). IR (KBr): ν 2927, 1583, 1490, 1466, 1377, 1320, 1288, 1246, 1159, 952, 838, 771, 549 cm^{-1}. GC-MS m/z 243 (M^+). HRMS (EI) m/z: calcd. for $C_{11}H_8F_3NO_2$: 243.0507; found: 243.0500.



4-(4-(Methylthio)phenyl)-2-(trifluoromethyl)oxazole (3h)

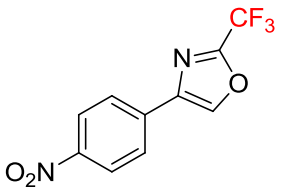
Obtained as a white solid in 73% yield (189 mg). M.p. 94–95 °C. R_f (*n*-pentane) = 0.40. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (s, 1H), 7.70 (d, J = 8.2 Hz, 2H), 7.32 (d, J = 8.2 Hz, 2H), 2.54 (s, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -65.8 (s, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 150.9 (q, J = 44.2 Hz), 141.7 (s), 140.0 (s), 135.1 (q, J = 0.9 Hz), 126.5 (s), 126.2 (s), 125.8 (s), 116.5 (q, J = 270.6 Hz), 15.5 (s). IR (KBr): ν 3152, 3126, 2919, 2323, 1989, 1611, 1591, 1487, 1380, 1256, 1153, 954, 863, 756, 497 cm^{-1}. GC-MS m/z 259 (M^+). HRMS (EI) m/z: calcd. for $C_{11}H_8F_3NOS$: 259.0279; found: 259.0284.



Methyl 4-(2-(trifluoromethyl)oxazol-4-yl)benzoate (3i)

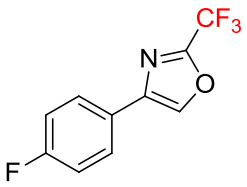
Obtained as a white solid in 45% yield (122 mg). M.p. 96–97 °C. R_f (*n*-pentane/ethyl acetate = 15:1) = 0.50. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 – 8.11 (m, 3H), 7.87 (d, J = 8.3 Hz, 2H), 3.97 (s, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -65.9 (s, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.5 (s), 151.2 (q, J = 44.3 Hz), 141.2 (s), 136.6 (q, J = 1.2 Hz), 133.4 (s), 130.5 (s), 130.3 (s), 125.7 (s), 116.3 (q, J = 270.9 Hz), 52.3 (s). IR (KBr): ν 3126, 2960, 2920, 2852, 1709, 1616, 1594, 1475, 1381, 1284, 1134, 956, 862, 774,

507 cm^{-1}. GC-MS m/z 271 (M^+). HRMS (EI) m/z: calcd. for $C_{12}H_8F_3NO_3$: 271.0456; found: 271.0457.



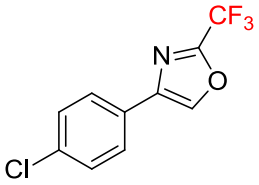
4-(4-Nitrophenyl)-2-(trifluoromethyl)oxazole (3j)

Obtained as a deep red solid in 40% yield (103 mg). M.p. 118–119 °C. R_f (*n*-pentane/ethyl acetate = 15:1) = 0.58. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.33 (d, *J* = 8.8 Hz, 2H), 8.24 (s, 1H), 7.98 (d, *J* = 8.8 Hz, 2H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -65.9 (s, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 151.6 (q, *J* = 44.6 Hz), 148.0 (s), 140.2 (s), 137.3 (q, *J* = 1.0 Hz), 135.4 (s), 126.5 (s), 124.4 (s), 116.2 (q, *J* = 271.1 Hz). IR (KBr): ν 3126, 2919, 2163, 2074, 1591, 1519, 1417, 1343, 1207, 1137, 939, 854, 718, 695 cm^{-1}. GC-MS m/z 258 (M^+). HRMS (EI) m/z: calcd. for $C_{10}H_5F_3N_2O_3$: 258.0252; found: 258.0247.



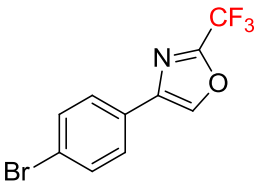
4-(4-Fluorophenyl)-2-(trifluoromethyl)oxazole (3k)

Obtained as a white solid in 58% yield (135 mg). M.p. 35–36 °C. R_f (*n*-pentane/ethyl acetate = 15:1) = 0.65. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 (s, 1H), 7.76 (dd, *J* = 8.5, 5.4 Hz, 2H), 7.16 (t, *J* = 8.6 Hz, 2H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -65.9 (s, 3F), -111.7 – -111.9 (m, 1F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.4 (s), 161.9 (s), 151.0 (q, *J* = 44.2 Hz), 141.3 (s), 135.1 (s), 127.7 (d, *J* = 8.3 Hz), 125.4 (d, *J* = 3.3 Hz), 116.4 (q, *J* = 270.7 Hz), 116.2 (s), 115.9 (s). IR (KBr): ν 2150, 2098, 1500, 1379, 1241, 1208, 1158, 1127, 1107, 904, 841, 614 cm^{-1}. GC-MS m/z 231 (M^+). HRMS (EI) m/z: calcd. for $C_{10}H_5F_4NO$: 231.0307; found: 231.0305.



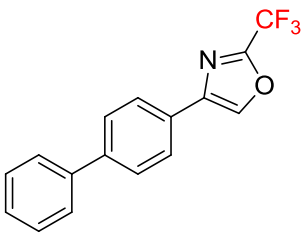
4-(4-Chlorophenyl)-2-(trifluoromethyl)oxazole (3l)

Obtained as a white liquid in 63% yield (156 mg). R_f (*n*-pentane) = 0.72. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (s, 1H), 7.75 – 7.68 (m, 2H), 7.46 – 7.39 (m, 2H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -65.9 (s, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 151.1 (q, *J* = 44.2 Hz), 141.1 (s), 135.5 (q, *J* = 1.2 Hz), 134.9 (s), 129.2 (s), 127.7 (s), 127.1 (s), 116.4 (q, *J* = 270.8 Hz). IR (KBr): ν 3180, 2795, 2048, 1613, 1597, 1485, 1377, 1242, 1155, 1091, 937, 834, 732, 548, 508 cm^{-1}. GC-MS m/z 247 (M^+). HRMS (EI) m/z: calcd. for $C_{10}H_5ClF_3NO$: 247.0012; found: 247.0003.



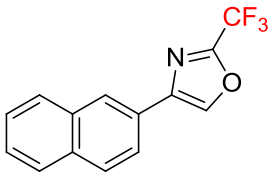
4-(4-Bromophenyl)-2-(trifluoromethyl)oxazole (3m)

Obtained as a white solid in 61% yield (178 mg). M.p. 32–33 °C. R_f (*n*-pentane) = 0.73. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 (s, 1H), 7.65 (d, *J* = 8.5 Hz, 2H), 7.58 (d, *J* = 8.5 Hz, 2H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -65.9 (s, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 151.1 (q, *J* = 44.2 Hz), 141.2 (s), 135.6 (q, *J* = 1.2 Hz), 132.2 (s), 128.2 (s), 127.3 (s), 123.2 (s), 116.4 (q, *J* = 270.8 Hz). IR (KBr): ν 2244, 1596, 1481, 1376, 1243, 1207, 1159, 1126, 954, 938, 832, 549 cm^{-1}. GC-MS m/z 290 (M^+). HRMS (EI) m/z: calcd. for $C_{10}H_5BrF_3NO$: 290.9507; found: 290.9503.



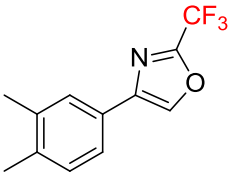
4-([1,1'-Biphenyl]-4-yl)-2-(trifluoromethyl)oxazole (3n)

Obtained as a white solid in 97% yield (280 mg). M.p.146–147 °C. R_f (*n*-pentane) = 0.45. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.09 (s, 1H), 7.87 (d, *J* = 8.0 Hz, 2H), 7.71 (d, *J* = 8.0 Hz, 2H), 7.66 (d, *J* = 8.0 Hz, 2H), 7.50 (t, *J* = 7.6 Hz, 2H), 7.41 (t, *J* = 7.8 Hz, 1H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -65.8 (s, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 151.0 (q, *J* = 44.2 Hz), 141.9 (s), 141.8 (s), 140.3 (s), 135.4 (q, *J* = 1.2 Hz), 128.9 (s), 128.2 (s), 127.7 (s), 127.6 (s), 127.1 (s), 126.3 (s), 116.5 (q, *J* = 270.6 Hz). IR (KBr): ν 3036, 2209, 2013, 1581, 1483, 1385, 1245, 1202, 1130, 957, 841, 761, 551 cm^{-1}. GC-MS m/z 289 (M^+). HRMS (EI) m/z: calcd. for $C_{16}H_{10}F_3NO$: 289.0714; found: 289.0711.



4-(Naphthalen-2-yl)-2-(trifluoromethyl)oxazole (3o)

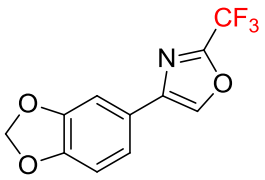
Obtained as a white solid in 64% yield (168 mg). M.p. 99–100 °C. R_f (*n*-pentane) = 0.42. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.35 (s, 1H), 8.15 (s, 1H), 7.98 – 7.86 (m, 3H), 7.80 (d, *J* = 8.5 Hz, 1H), 7.62 – 7.50 (m, 2H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -65.8 (s, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 151.1 (q, *J* = 44.2 Hz), 142.2 (s), 135.7 (q, *J* = 1.2 Hz), 133.5 (s), 133.4 (s), 128.8 (s), 128.4 (s), 127.8 (s), 126.8 (s), 126.7 (s), 126.5 (s), 125.2 (s), 123.2 (s), 116.5 (q, *J* = 270.7 Hz). IR (KBr): ν 2251, 2155, 1381, 1247, 1209, 1163, 1124, 953, 902, 811, 476 cm^{-1}. GC-MS m/z 263 (M^+). HRMS (EI) m/z: calcd. for $C_{14}H_8F_3NO$: 263.0558; found: 263.0564.



4-(3,4-Dimethylphenyl)-2-(trifluoromethyl)oxazole (3p)

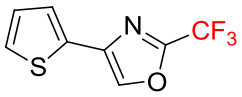
Obtained as a white solid in 56% yield (136 mg). M.p. 28–29 °C. R_f (*n*-pentane) = 0.67. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (s, 1H), 7.58 (s, 1H), 7.50 (dd, *J* = 7.8, 1.6

Hz, 1H), 7.22 (d, *J* = 7.8 Hz, 1H), 2.34 (s, 3H), 2.33 (s, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -65.8 (s, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 150.8 (q, *J* = 43.9 Hz), 142.2 (s), 137.8 (s), 137.3 (s), 134.9 (q, *J* = 1.3 Hz), 130.2 (s), 126.9 (s), 126.7 (s), 123.2 (s), 116.5 (q, *J* = 270.7 Hz), 19.7 (s), 19.6 (s). IR (KBr): ν 2973, 2195, 1583, 1492, 1385, 1242, 1206, 1158, 1123, 952, 862, 820, 548 cm^{-1}. GC-MS m/z 241 (M^+). HRMS (EI) m/z: calcd. for $C_{12}H_{10}F_3NO$: 241.0714; found: 241.0718.



4-(Benzo[*d*][1,3]dioxol-5-yl)-2-(trifluoromethyl)oxazole (3q)

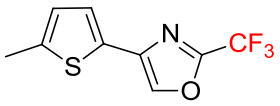
Obtained as a white solid in 89% yield (229 mg). M.p. 79–80 °C. R_f (*n*-pentane/ethyl acetate = 15:1) = 0.57. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94 (s, 1H), 7.32 – 7.27 (m, 1H), 7.23 (s, 1H), 6.89 (d, *J* = 8.1 Hz, 1H), 6.04 (s, 2H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -65.9 (s, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 150.8 (q, *J* = 43.9 Hz), 148.3 (s), 148.2 (s), 141.9 (s), 134.6 (q, *J* = 1.2 Hz), 123.3 (s), 119.9 (s), 116.4 (q, *J* = 270.7 Hz), 108.8 (s), 106.3 (s), 101.4 (s). IR (KBr): ν 2853, 1586, 1505, 1483, 1448, 1383, 1287, 1235, 1198, 1124, 951, 873, 767, 682 cm^{-1}. GC-MS m/z 257 (M^+). HRMS (EI) m/z: calcd. for $C_{11}H_6F_3NO_3$: 257.0300; found: 257.0304.



4-(Thiophen-2-yl)-2-(trifluoromethyl)oxazole (3r)

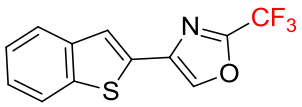
Obtained as a white solid in 72% yield (158 mg). M.p. 45–46 °C. R_f (*n*-pentane) = 0.52. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 (s, 1H), 7.50 – 7.43 (m, 1H), 7.39 (d, *J* = 5.0 Hz, 1H), 7.12 (dd, *J* = 4.7, 3.9 Hz, 1H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -65.8 (s, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 150.9 (q, *J* = 44.3 Hz), 137.2 (s), 134.5 (q, *J* = 1.2 Hz), 131.4 (s), 127.9 (s), 126.3 (s), 125.6 (s), 116.3 (q, *J* = 271.0 Hz). IR (KBr): ν 3160,

2926, 2189, 1381, 1251, 1206, 1160, 1100, 952, 849, 701, 489 cm^{-1}. GC-MS m/z 218 (M^+). HRMS (EI) m/z: calcd. for $C_8H_4F_3NOS$: 218.9966; found: 218.9962.



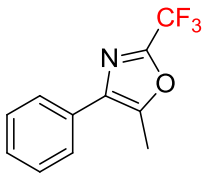
4-(5-Methylthiophen-2-yl)-2-(trifluoromethyl)oxazole (3s)

Obtained as a white solid in 66% yield (154 mg). M.p. 46–47 °C. R_f (*n*-pentane) = 0.42. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 (s, 1H), 7.25 (d, *J* = 3.5 Hz, 1H), 6.76 (d, *J* = 3.5 Hz, 1H), 2.54 (s, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -65.8 (s, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 150.7 (q, *J* = 44.2 Hz), 141.1 (s), 137.4 (s), 133.9 (q, *J* = 1.3 Hz), 128.9 (s), 126.0 (s), 125.7 (s), 116.4 (q, *J* = 270.9 Hz), 15.3 (s). IR (KBr): ν 3139, 2926, 2050, 1979, 1585, 1467, 1394, 1254, 1140, 1096, 955, 811, 786, 512 cm^{-1}. GC-MS m/z 233 (M^+). HRMS (EI) m/z: calcd. for $C_9H_6F_3NOS$: 233.0122; found: 233.0124.



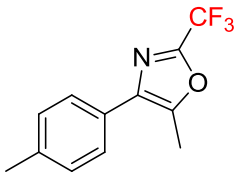
4-(Benzo[*b*]thiophen-2-yl)-2-(trifluoromethyl)oxazole (3t)

Obtained as a white solid in 62% yield (167 mg). M. p. 118–119 °C. R_f (*n*-pentane) = 0.35. ^{1}H NMR (400 MHz, acetone-d_6) δ 8.79 (s, 1H), 8.00 – 7.95 (m, 1H), 7.92 – 7.88 (m, 1H), 7.87 (s, 1H), 7.55 – 7.36 (m, 2H). ^{19}F NMR (376 MHz, acetone-d_6) δ -66.7 (s, 3F). ^{13}C NMR (101 MHz, acetone-d_6) δ 150.3 (q, *J* = 44.0 Hz), 139.9 (s), 139.5 (s), 137.8 (q, *J* = 1.0 Hz), 137.0 (s), 131.6 (s), 125.3 (s), 124.9 (s), 124.1 (s), 122.4 (s), 122.3 (s), 116.6 (q, *J* = 269.9 Hz). IR (KBr): ν 2253, 1637, 1517, 1380, 1208, 1126, 1100, 953, 867, 525, 478 cm^{-1}. GC-MS m/z 269 (M^+). HRMS (EI) m/z: calcd. for $C_{12}H_6F_3NOS$: 269.0122; found: 269.0123.



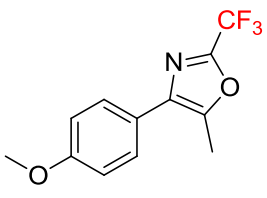
5-Methyl-4-phenyl-2-(trifluoromethyl)oxazole (3u)

Obtained as a white liquid in 76% yield (173 mg). R_f (*n*-pentane) = 0.65. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 (d, *J* = 7.4 Hz, 2H), 7.49 (t, *J* = 7.4 Hz, 2H), 7.40 (t, *J* = 7.4 Hz, 1H), 2.63 (s, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -65.8 (s, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 148.5 (q, *J* = 43.8 Hz), 146.7 (q, *J* = 0.9 Hz), 136.0 (s), 130.6 (s), 128.8 (s), 128.2 (s), 126.9 (s), 116.7 (q, *J* = 270.3 Hz), 11.8 (s). IR (KBr): ν 2927, 1587, 1495, 1446, 1397, 1371, 1349, 1198, 1144, 1118, 972, 771, 734, 662 cm^{-1}. GC-MS m/z 227 (M^+). HRMS (EI) m/z: calcd. for $C_{11}H_8F_3NO$: 227.0558; found: 227.0553.



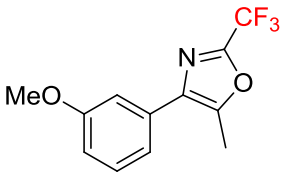
5-Methyl-4-(*p*-tolyl)-2-(trifluoromethyl)oxazole (3v)

Obtained as a white liquid in 82% yield (198 mg). R_f (*n*-pentane) = 0.72. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 (d, *J* = 8.1 Hz, 2H), 7.29 (d, *J* = 8.1 Hz, 2H), 2.62 (s, 3H), 2.43 (s, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -65.8 (s, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 148.4 (q, *J* = 43.7 Hz), 146.3 (q, *J* = 1.2 Hz), 138.1 (s), 136.1 (s), 129.5 (s), 127.7 (s), 126.8 (s), 116.7 (q, *J* = 270.3 Hz), 21.2 (s), 11.8 (s). IR (KBr): ν 2926, 1589, 1513, 1399, 1371, 1346, 1199, 1149, 1121, 1031, 972, 759, 733, 692 cm^{-1}. GC-MS m/z 241 (M^+). HRMS (EI) m/z: calcd. for $C_{12}H_{10}F_3NO$: 241.0714; found: 241.0710.



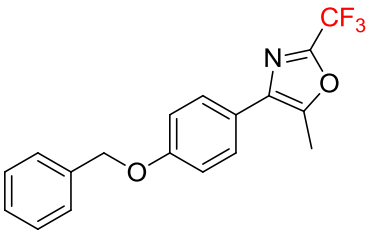
4-(4-Methoxyphenyl)-5-methyl-2-(trifluoromethyl)oxazole (3w)

Obtained as a white solid in 82% yield (212mg). M.p. 62–63 °C. R_f (n-pentane) = 0.60.^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 (d, J = 8.6 Hz, 2H), 6.99 (d, J = 8.6 Hz, 2H), 3.86 (s, 3H), 2.59 (s, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -65.9 (s, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.6 (s), 148.3 (q, J = 43.6 Hz), 145.7 (q, J = 1.0 Hz), 135.8 (s), 128.2 (s), 123.1 (s), 116.7 (q, J = 270.2 Hz), 114. 2 (s), 55.2 (s), 11.7 (s). IR (KBr): ν 2749, 2243, 1607, 1590, 1511, 1464, 1309, 1295, 1175, 1106, 956, 834, 786, 534 cm^{-1}. GC-MS m/z 257 (M^+). HRMS (EI) m/z: calcd. for $C_{12}H_{10}F_3NO_2$: 257.0664; found: 257.0662.



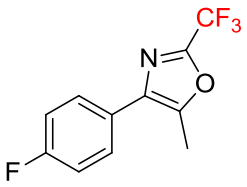
4-(3-Methoxyphenyl)-5-methyl-2-(trifluoromethyl)oxazole (3x)

Obtained as a white liquid in 68% yield (175 mg). R_f (*n*-pentane) = 0.45. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39 (t, J = 7.9 Hz, 1H), 7.26 (s, 1H), 7.25 (d, J = 7.3 Hz, 1H), 7.00 – 6.89 (m, 1H), 3.89 (s, 3H), 2.64 (s, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -65.8 (s, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.9 (s), 148.4 (q, J = 43.8 Hz), 146.9 (q, J = 1.2 Hz), 135.9 (s), 131.9 (s), 129.8 (s), 119.2 (s), 116.6 (q, J = 270.4 Hz), 113.9 (s), 112.4 (s), 55.4 (s), 12.2 (s). IR (KBr): ν 2926, 2623, 1579, 1492, 1465, 1447, 1396, 1370, 1287, 1144, 1028, 972, 849, 738, 553 cm^{-1}. GC-MS m/z 257 (M^+). HRMS (EI) m/z: calcd. for $C_{12}H_{10}F_3NO_2$: 257.0664; found: 257.0671.



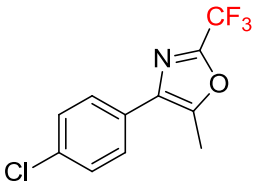
4-(4-(Benzyloxy)phenyl)-5-methyl-2-(trifluoromethyl)oxazole (3y)

Obtained as a white solid in 74% yield (229 mg). M.p. 87–88 °C. R_f (*n*-pentane/ethyl acetate = 15:1) = 0.65. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (d, *J* = 8.5 Hz, 2H), 7.53 – 7.34 (m, 5H), 7.09 (d, *J* = 8.5 Hz, 2H), 5.14 (s, 2H), 2.61 (s, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -65.8 (s, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.8 (s), 148.4 (q, *J* = 43.7 Hz), 145.7 (q, *J* = 1.1 Hz), 136.8 (s), 135.8 (s), 128.7 (s), 128.2 (s), 128.1 (s), 127.5 (s), 123.4 (s), 116.7 (q, *J* = 270.2 Hz), 115.2 (s), 70.1 (s), 11.8 (s). IR (KBr): ν 2978, 2235, 1606, 1590, 1509, 1454, 1371, 1349, 1291, 1123, 957, 833, 761, 534 cm^{-1}. GC-MS m/z 333 (M^+). HRMS (EI) m/z: calcd. for $C_{18}H_{14}F_3NO_2$: 333.0977; found: 333.0969.



4-(4-Fluorophenyl)-5-methyl-2-(trifluoromethyl)oxazole (3z)

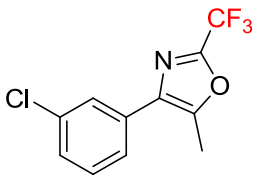
Obtained as a white solid in 47% yield (116 mg). M.p. 29–30 °C. R_f (*n*-pentane) = 0.75. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 – 7.58 (m, 2H), 7.24 – 7.08 (m, 2H), 2.60 (s, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -65.9 (s, 3F), -113.2 – -113.3 (m, 1F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.8 (s), 161.3 (s), 148.5 (q, *J* = 43.9 Hz), 146.5 (q, *J* = 1.2 Hz), 135.2 (s), 128.6 (d, *J* = 8.3 Hz), 126.7 (d, *J* = 3.3 Hz), 116.6 (q, *J* = 270.3 Hz), 115.9 (s), 115.7 (s), 11.7 (s). IR (KBr): ν 2183, 2050, 1607, 1592, 1399, 1371, 1346, 1204, 1152, 1120, 1025, 973, 840, 760, 528 cm^{-1}. GC-MS m/z 245 (M^+). HRMS (EI) m/z: calcd. for $C_{11}H_7F_4NO$: 245.0464; found: 245.0458.



4-(4-Chlorophenyl)-5-methyl-2-(trifluoromethyl)oxazole (3aa)

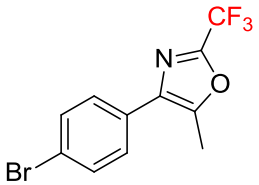
Obtained as a white solid in 74% yield (194 mg). M.p. 42–43 °C. R_f (*n*-pentane) = 0.68. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 (d, *J* = 8.5 Hz, 2H), 7.42 (d, *J* = 8.5 Hz, 2H),

2.61 (s, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -65.9 (s, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 148.6 (q, *J* = 43.9 Hz), 146.9 (q, *J* = 1.2 Hz), 135.1 (s), 134.1 (s), 129.1 (s), 128.9 (s), 128.0 (s), 116.6 (q, *J* = 270.4 Hz), 11.8 (s). IR (KBr): ν 2250, 1604, 1588, 1584, 1492, 1379, 1371, 1345, 1200, 1150, 1120, 972, 833, 762, 554 cm^{-1}. GC-MS m/z 261 (M^+). HRMS (EI) m/z: calcd. for $C_{11}H_7ClF_3NO$: 261.0168; found: 261.0164.



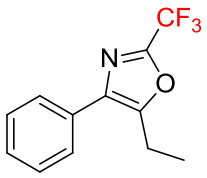
4-(3-Chlorophenyl)-5-methyl-2-(trifluoromethyl)oxazole (3ab)

Obtained as a white liquid in 35% yield (92 mg). R_f (*n*-pentane) = 0.70. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 (s, 1H), 7.55 (d, *J* = 7.5 Hz, 1H), 7.44 – 7.31 (m, 2H), 2.63 (s, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -65.9 (s, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 148.6 (q, *J* = 44.0 Hz), 147.3 (q, *J* = 0.9 Hz), 134.8 (s), 132.3 (s), 130.0 (s), 128.2 (s), 126.8 (s), 124.8 (s), 116.5 (q, *J* = 270.4 Hz), 11.9 (s). IR (KBr): ν 2250, 1608, 1598, 1580, 1472, 1369, 1348, 1205, 1145, 952, 853, 755, 558 cm^{-1}. GC-MS m/z 261 (M^+) HRMS (ESI) m/z: calcd. for $C_{11}H_7ClF_3NO$: 261.0168; found: 261.0164.



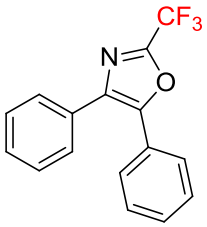
4-(4-Bromophenyl)-5-methyl-2-(trifluoromethyl)oxazole (3ac)

Obtained as a white solid in 66% yield (210 mg). M.p. 53–54 °C. R_f (*n*-pentane) = 0.72. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 – 7.48 (m, 4H), 2.61 (s, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -65.9 (s, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 148.6 (q, *J* = 44.0 Hz), 146.9 (q, *J* = 1.1 Hz), 135.1 (s), 131.9 (s), 129.5 (s), 128.3 (s), 122.3 (s), 116.5 (q, *J* = 270.4 Hz), 11.9 (s). IR (KBr): ν 2842, 2236, 1819, 1602, 1582, 1487, 1394, 1346, 1202, 1007, 957, 831, 765, 521 cm^{-1}. GC-MS m/z 304 (M^+). HRMS (EI) m/z: calcd. for $C_{11}H_7BrF_3NO$: 304.9663; found: 304.9668.



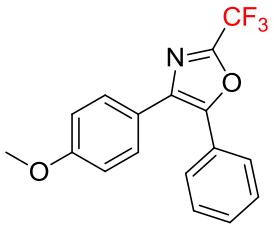
5-Ethyl-4-phenyl-2-(trifluoromethyl)oxazole (3ad)

Obtained as a white liquid in 56% yield (135 mg). R_f (*n*-pentane) = 0.52. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 – 7.66 (m, 2H), 7.50 (t, *J* = 7.6 Hz, 2H), 7.40 (t, *J* = 7.6 Hz, 1H), 3.01 (q, *J* = 7.5 Hz, 2H), 1.40 (t, *J* = 7.5 Hz, 2H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -65.8 (s, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 151.7 (q, *J* = 1.2 Hz), 148.6 (q, *J* = 43.7 Hz), 135.4 (s), 130.7 (s), 128.8 (s), 128.3 (s), 127.1 (s), 116.7 (q, *J* = 270.3 Hz), 19.5 (s), 12.1 (s). IR (KBr): ν 2981, 2875, 2164, 1584, 1495, 1447, 1391, 1377, 1271, 1148, 1072, 989, 969, 772, 562 cm^{-1}. GC-MS m/z 241 (M^+). HRMS (EI) m/z: calcd. for $C_{12}H_{10}F_3NO$: 241.0714; found: 241.0717.



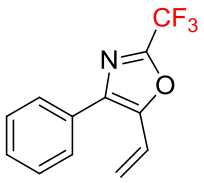
4-(4-Methoxyphenyl)-5-phenyl-2-(trifluoromethyl)oxazole (3ae)

Obtained as a colorless oil in 48% yield (138 mg). M.p. 73–74 °C. R_f (*n*-pentane/ethyl acetate = 15:1) = 0.50. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 – 7.64 (m, 4H), 7.50 – 7.41 (m, 6H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -65.7 (s, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 149.2 (q, *J* = 43.9 Hz), 148.0 (q, *J* = 1.2 Hz), 136.0 (s), 130.8 (s), 129.9 (s), 129.0 (s), 128.9 (s), 128.8 (s), 128.0 (s), 127.3 (s), 127.1 (s), 116.7 (q, *J* = 270.7 Hz). IR (KBr): ν 3062, 1580, 1504, 1482, 1445, 1383, 1354, 1206, 1145, 1120, 1073, 970, 763, 734, 690, 565 cm^{-1}. GC-MS m/z 288 (M^+). HRMS (EI) m/z: calcd. for $C_{16}H_{10}F_3NO$: 289.0714; found: 289.0711.



4-(4-Methoxyphenyl)-5-phenyl-2-(trifluoromethyl)oxazole (3af)

Obtained as a white solid in 52% yield (166 mg). M.p. 113–114 °C. R_f (*n*-pentane/ethyl acetate = 15:1) = 0.63. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 – 7.55 (m, 4H), 7.51 – 7.37 (m, 3H), 6.96 (d, *J* = 8.6 Hz, 2H), 3.88 (s, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -65.7 (s, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.1 (s), 149.0 (q, *J* = 44.0 Hz), 147.2 (q, *J* = 1.0 Hz), 135.7 (s), 129.7 (s), 129.4 (s), 128.9 (s), 127.5 (s), 126.9 (s), 123.1 (s), 116.7 (q, *J* = 270.6 Hz), 114.2 (s), 55.3 (s). IR (KBr): ν 2839, 2182, 2025, 1616, 1515, 1447, 1355, 1251, 1209, 972, 836, 718, 565 cm^{-1}. GC-MS m/z 319 (M^+). HRMS (EI) m/z: calcd. for $C_{17}H_{12}F_3NO_2$: 319.0820; found: 319.0824.



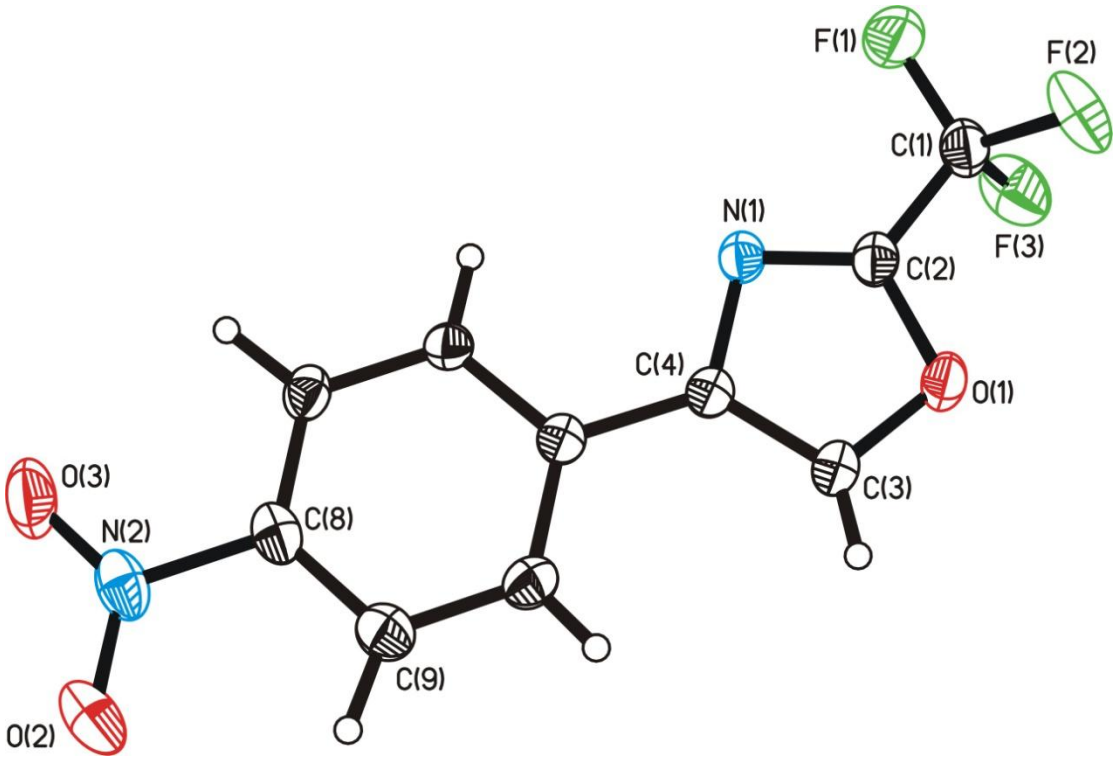
4-Phenyl-2-(trifluoromethyl)-5-vinyloxazole (3ag)

Obtained as a colorless oil in 38% yield (90 mg). R_f (*n*-pentane) = 0.55. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 – 7.34 (m, 5H), 7.31 (s, 1H), 6.44 (d, *J* = 21.7 Hz, 2H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -68.9 (s, 3F). ^{13}C NMR (101 MHz, $CDCl_3$) δ 137.2 (s), 132.3 (s), 128.9 (s), 128.1 (s), 127.9 (s), 121.4 (q, *J* = 4.7 Hz), 117.3 (s), 115.5 (q, *J* = 288.0 Hz), 114.6 (s). IR (KBr): ν 2925, 1752, 1602, 1511, 1477, 1404, 1363, 1293, 1217, 1153, 1110, 892, 865, 824, 757, 694, 675, 586 cm^{-1}. GC-MS m/z 239 (M^+). HRMS (EI) m/z: calcd. for $C_{12}H_8F_3NO$: 239.0558; found: 239.0553.

Crystal structure analyses

The suitable crystals of **3j** (CCDC 1835965) 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.[7] Structure solution and refinement were carried out with the SHELXTL suite of programs.[7] The structure was solved by direct methods to locate the heavy atoms, followed by difference maps for the light non-hydrogen atoms.

ORTEP diagrams



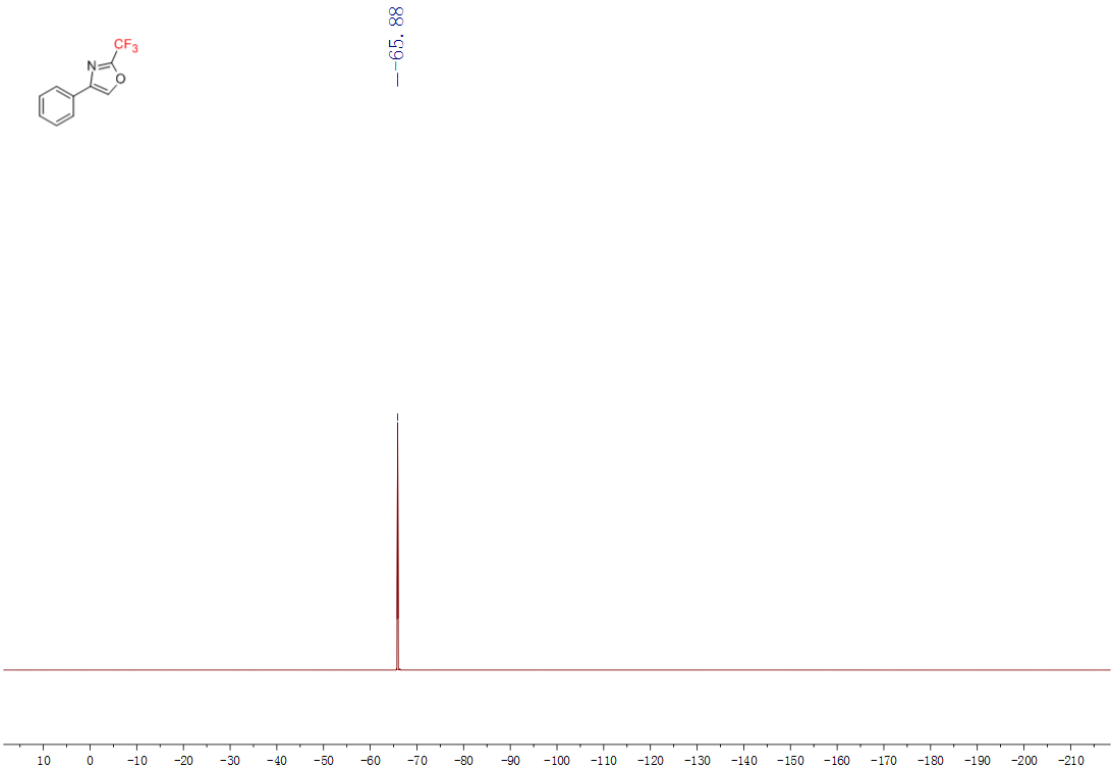
ORTEP diagram of compound 3j. Thermal ellipsoids are drawn at 40% probability

References:

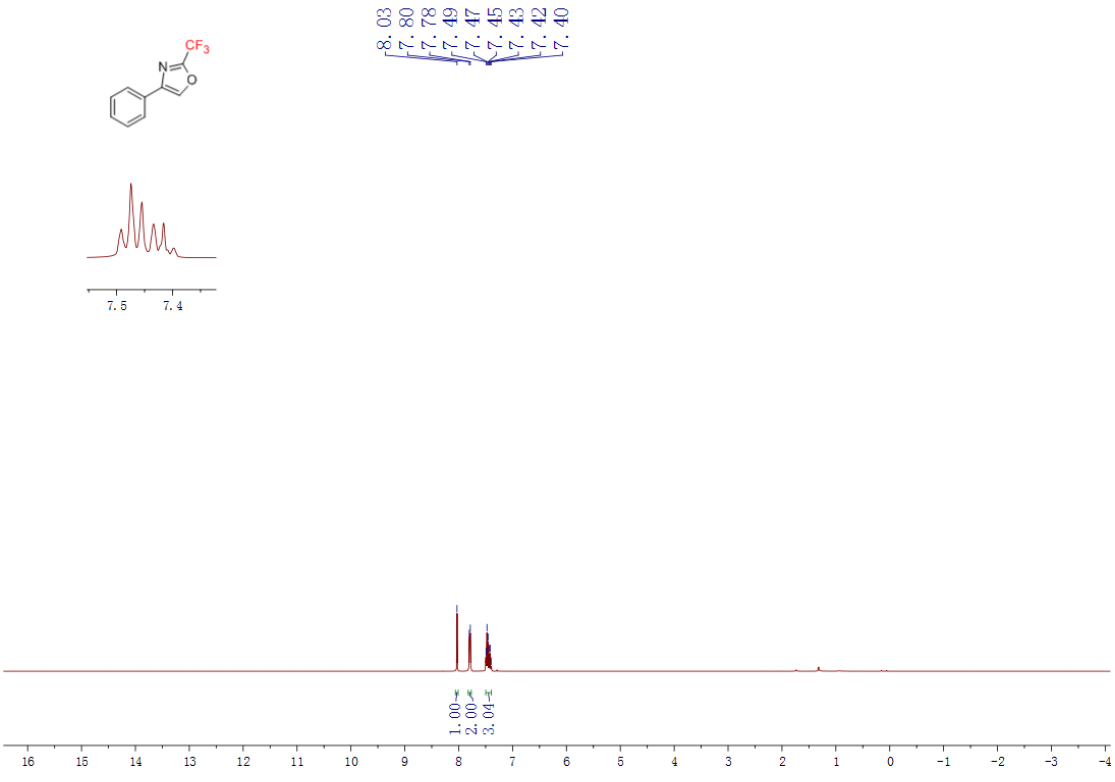
1. P. C. Too, Y.-F. Wang and S. Chiba, *Org. Lett.*, 2010, **12**, 5688-5691.
2. J. Ke, Y. Tang, H. Yi, Y. Li, Y. Cheng, C. Liu and A. Lei, *Angew. Chem. Int. Ed.*, 2015, **54**, 6604-6607.
3. H. Huang, J. Cai, X. Ji, F. Xiao, Y. Chen and G.-J. Deng, *Angew. Chem. Int. Ed.*, 2016, **55**, 307-311.
4. X. Tang, J. Yang, Z. Zhu, M. Zheng, W. Wu and H. Jiang, *J. Org. Chem.*, 2016, **81**, 11461-11466.
5. C. Zhu, R. Zhu, H. Zeng, F. Chen, C. Liu, W. Wu and H. Jiang, *Angew. Chem. Int. Ed.*, 2017, **56**, 13324-13328.
6. H. Huang, J. Cai, H. Xie, J. Tan, F. Li and G.-J. Deng, *Org. Lett.*, 2017, **19**, 3743-3746.
7. 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

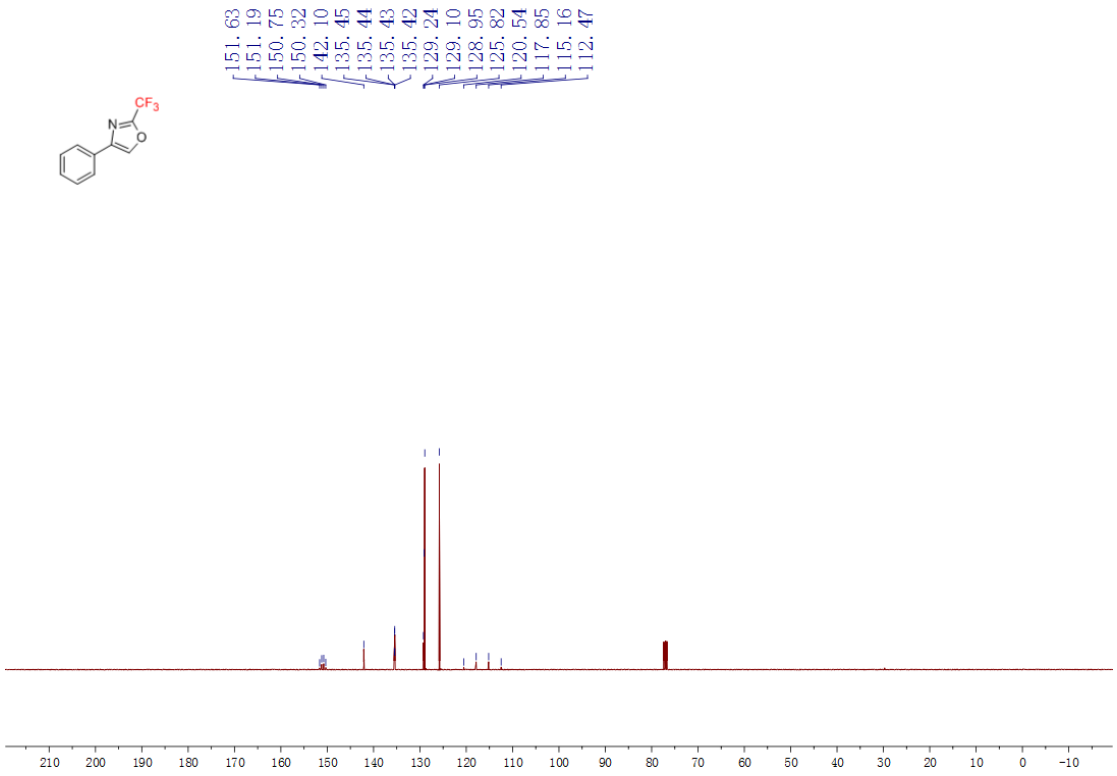
^{19}F NMR spectrum of **3a** in $CDCl_3$



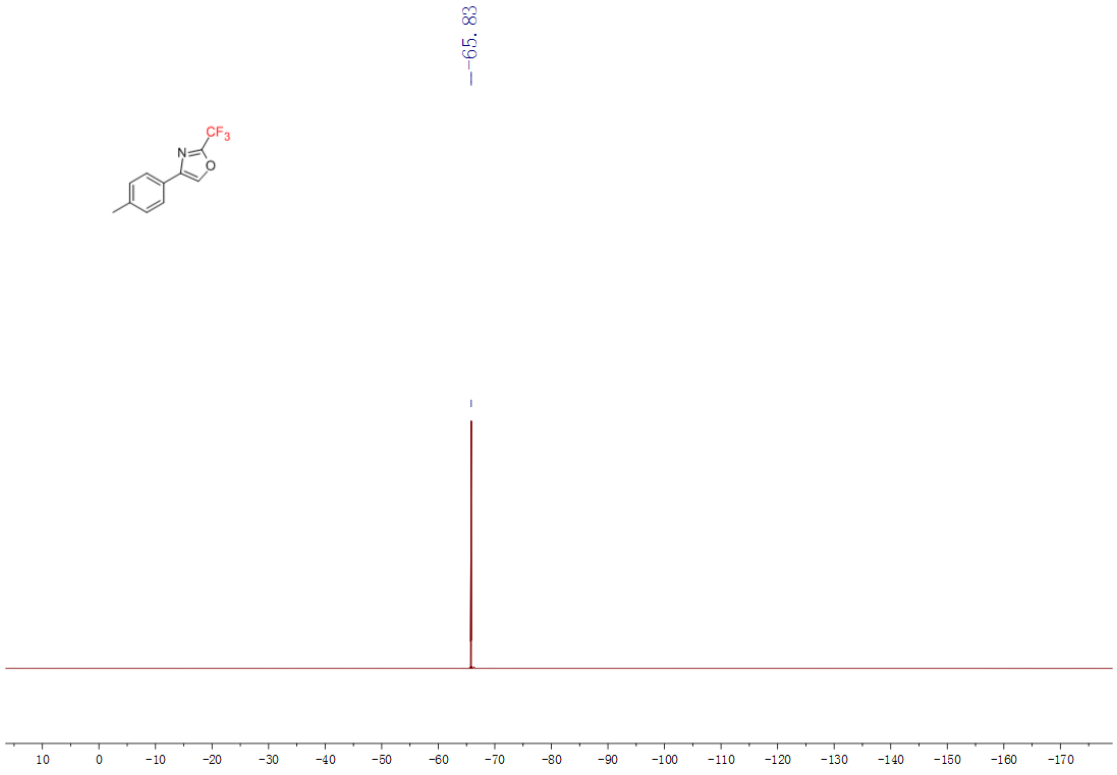
^{1}H NMR spectrum of **3a** in $CDCl_3$



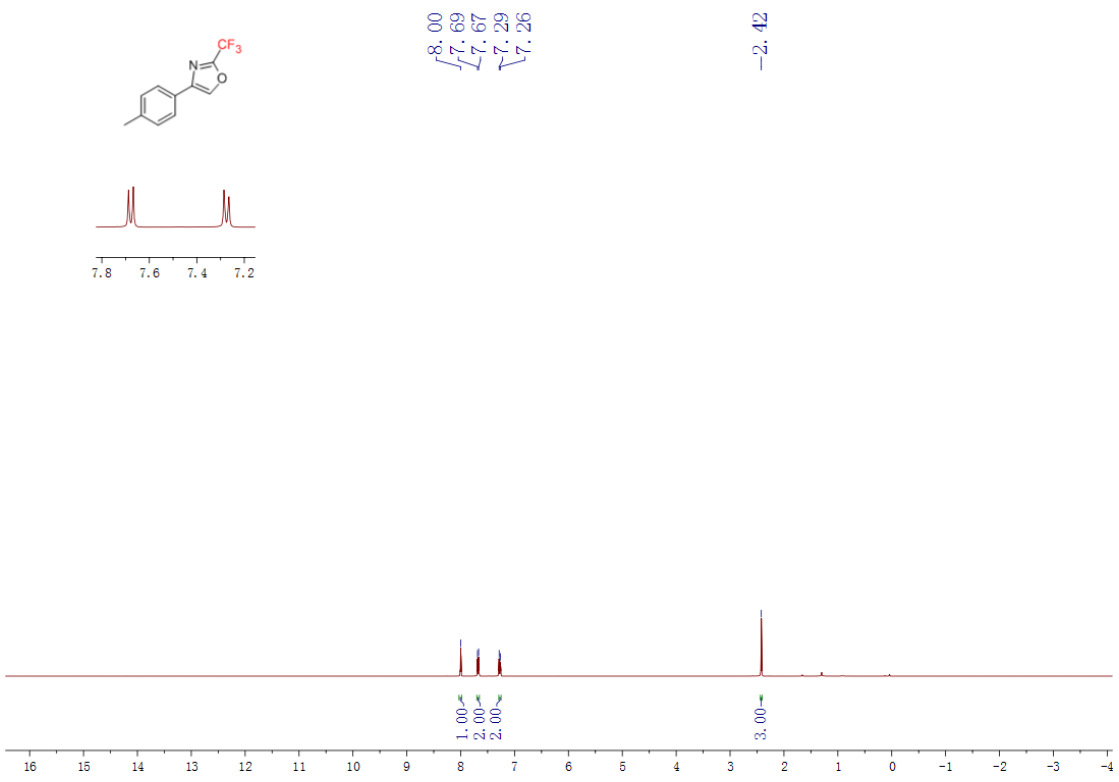
^{13}C NMR spectrum of **3a** in $CDCl_3$



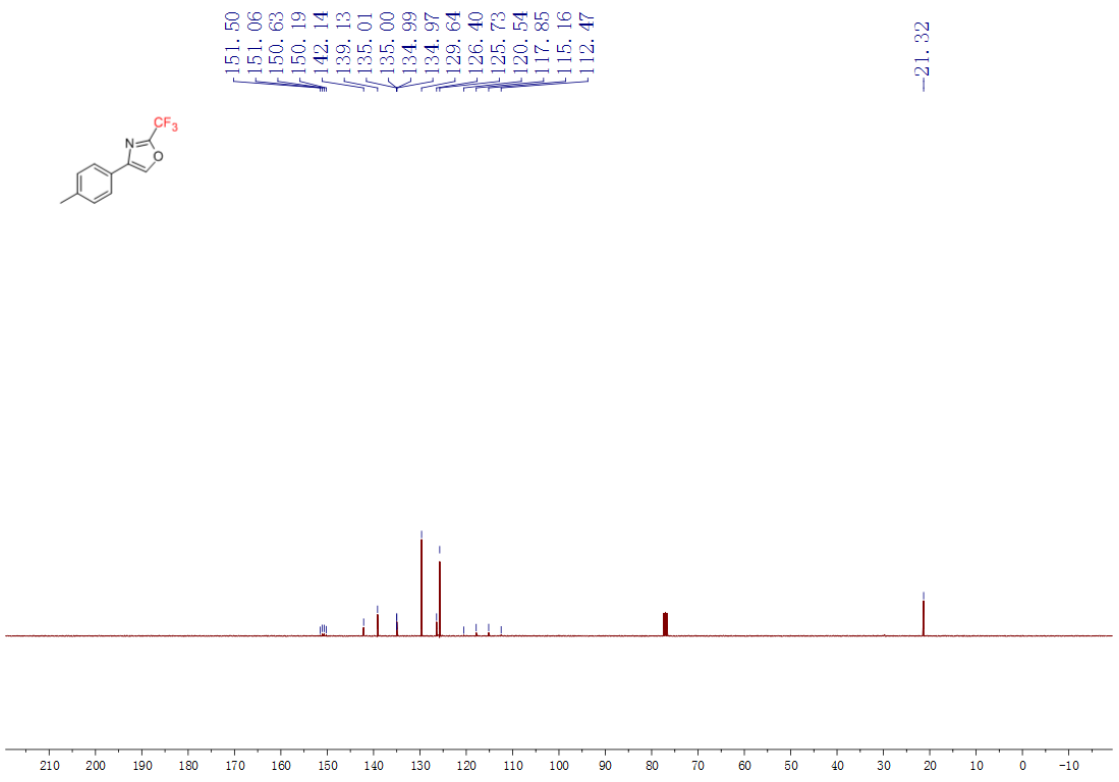
^{19}F NMR spectrum of **3b** in $CDCl_3$



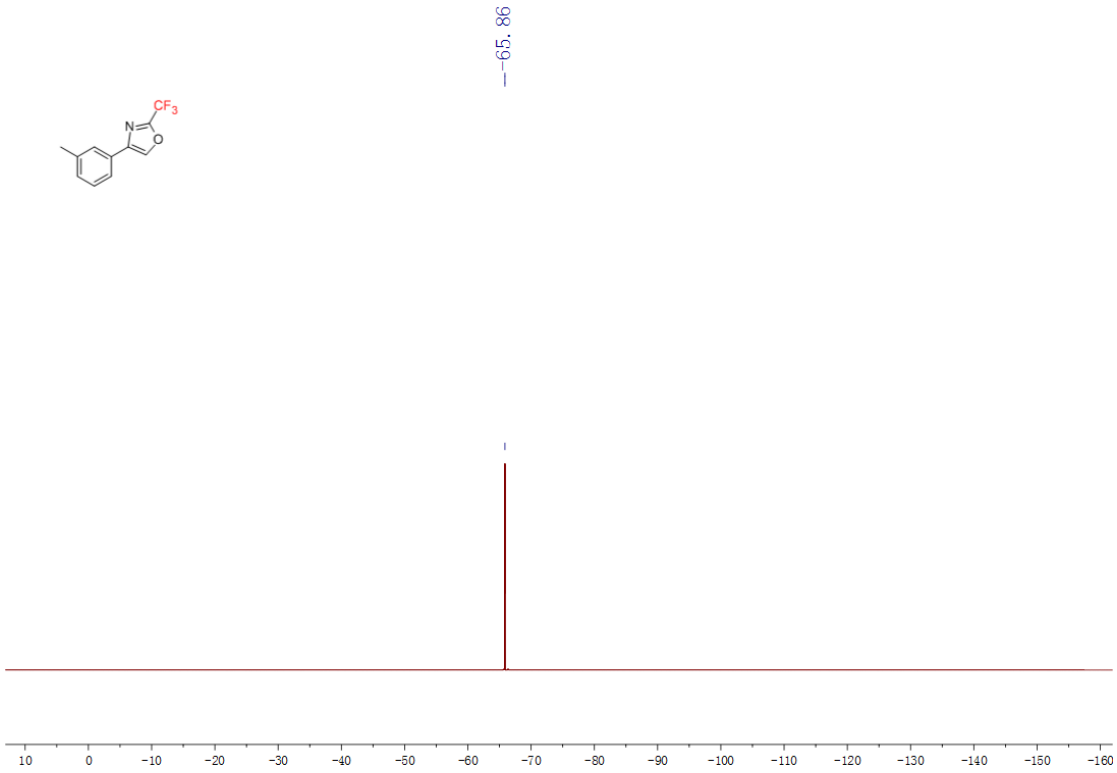
^{1}H NMR spectrum of **3b** in $CDCl_3$



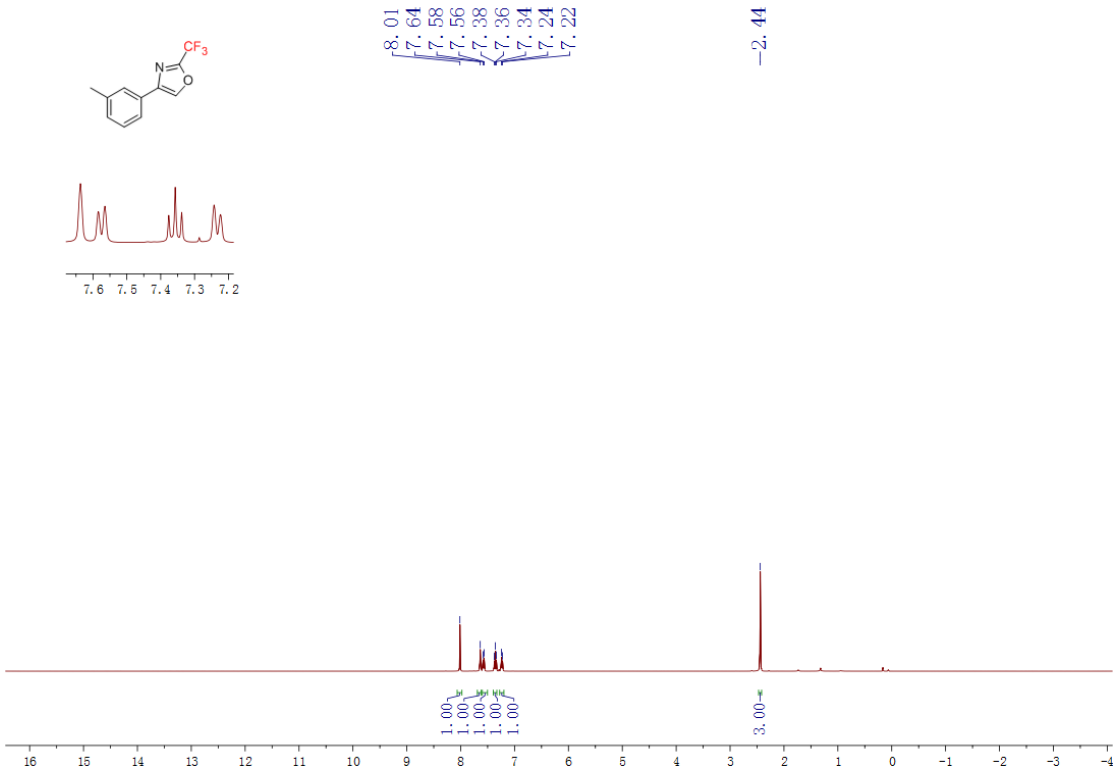
^{13}C NMR spectrum of **3b** in $CDCl_3$



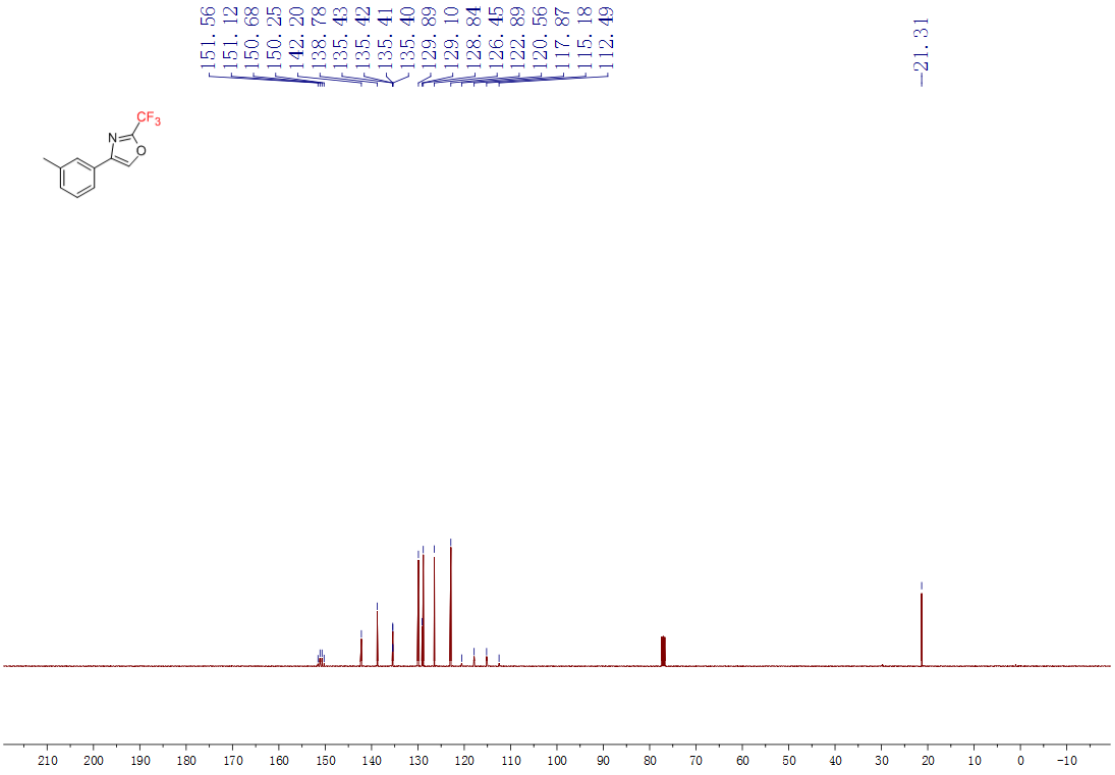
^{19}F NMR spectrum of **3c** in $CDCl_3$



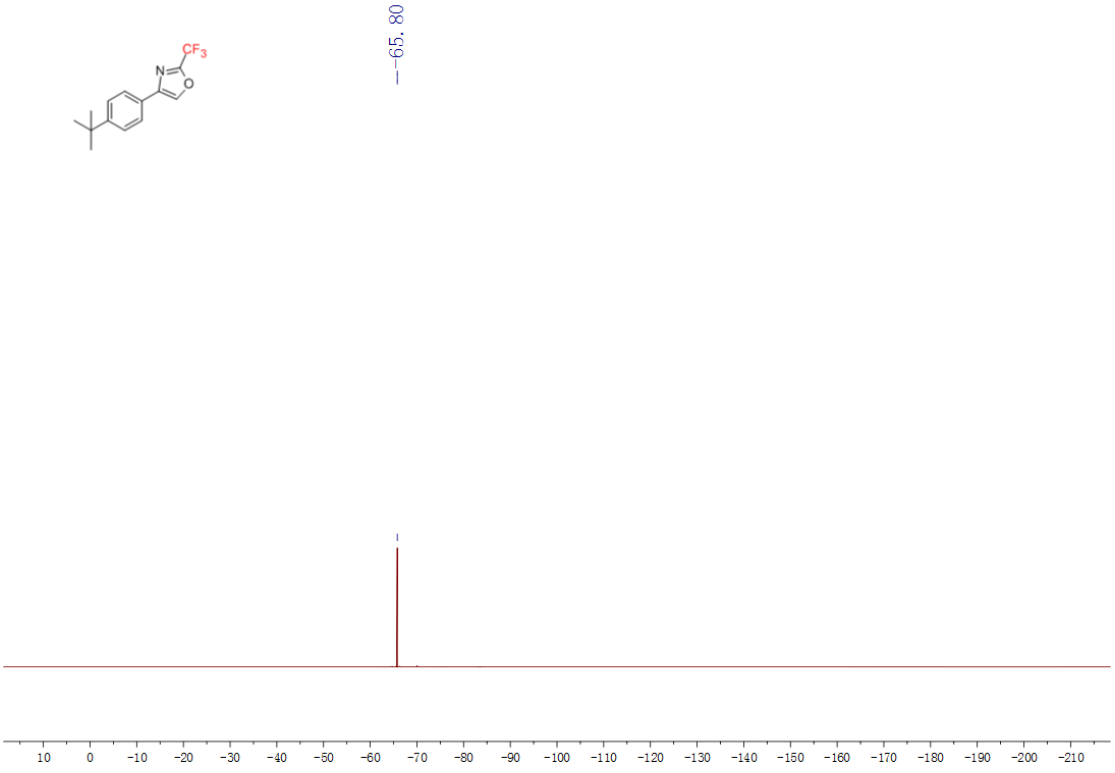
^{1}H NMR spectrum of **3c** in $CDCl_3$



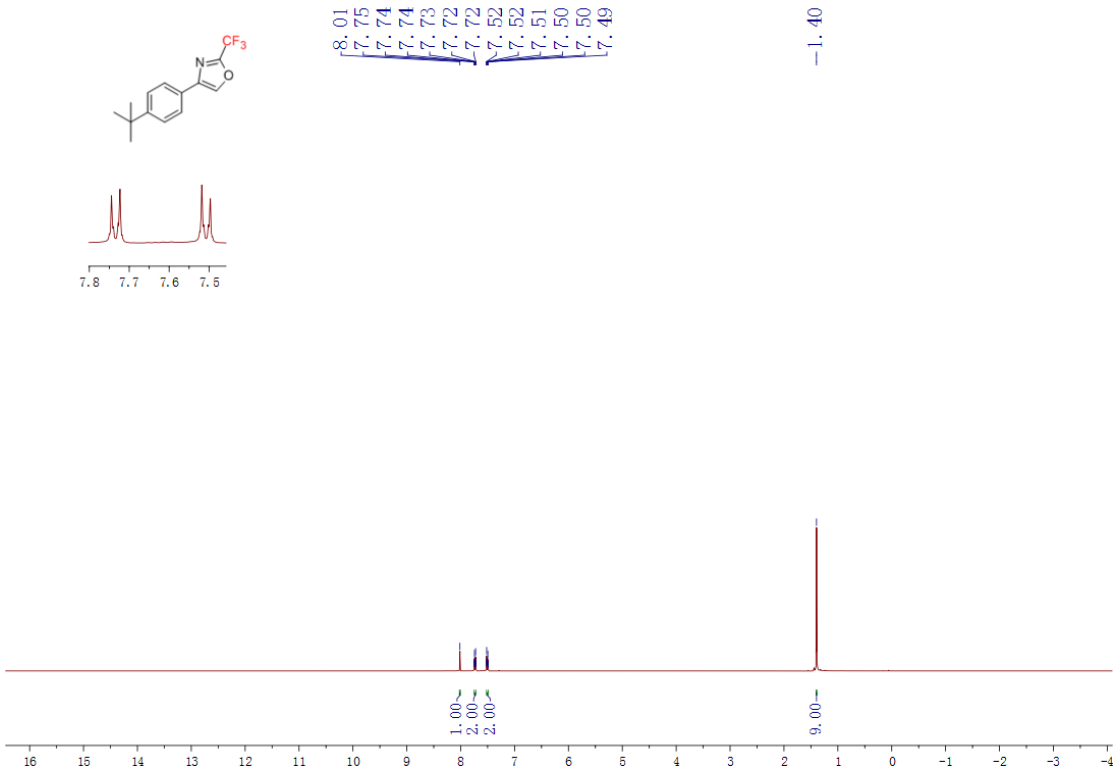
^{13}C NMR spectrum of **3c** in $CDCl_3$



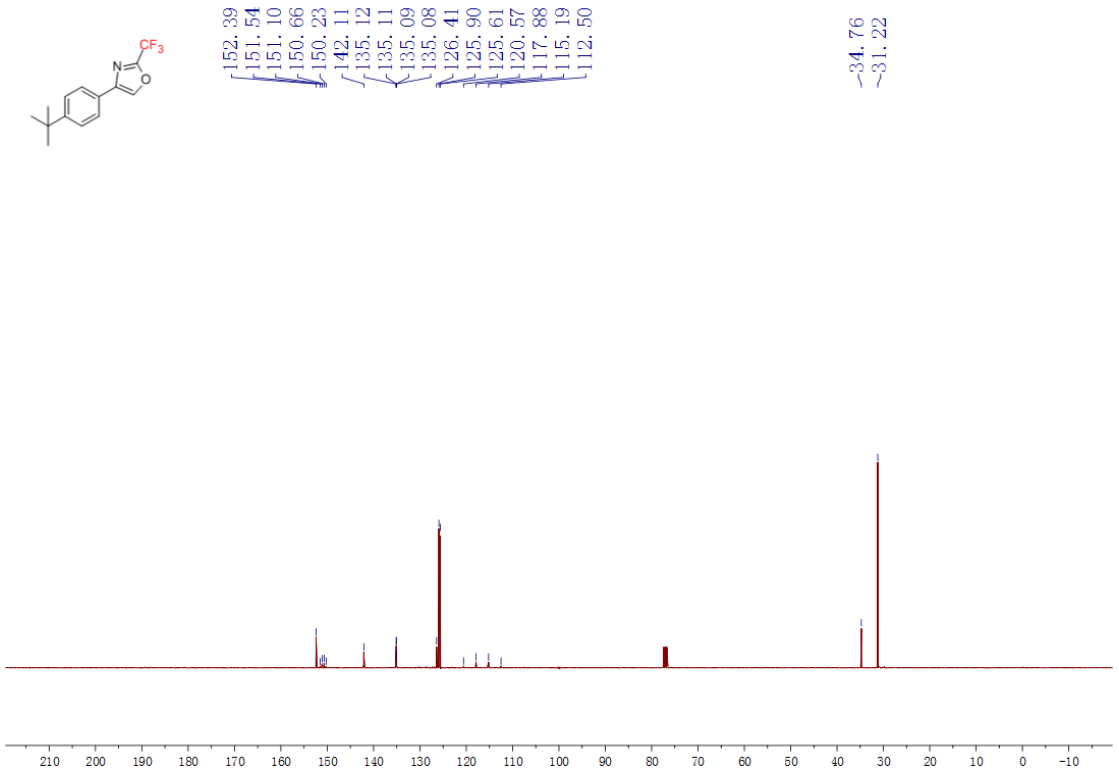
^{19}F NMR spectrum of **3d** in $CDCl_3$



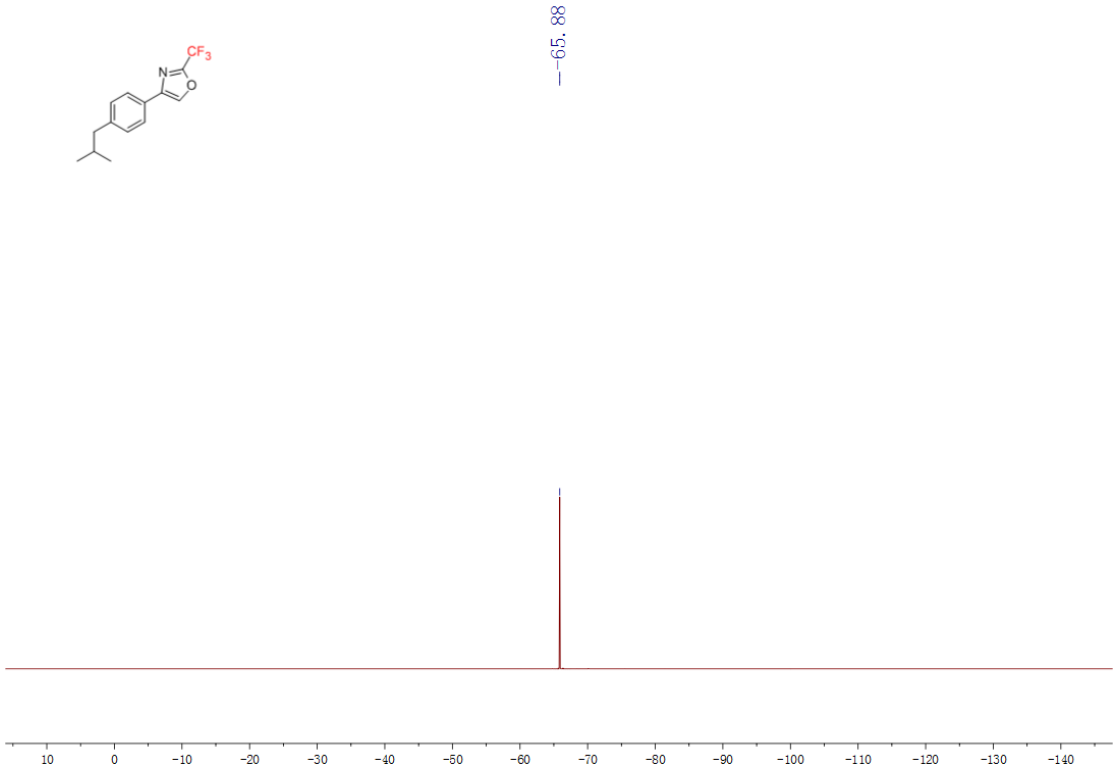
^{1}H NMR spectrum of **3d** in $CDCl_3$



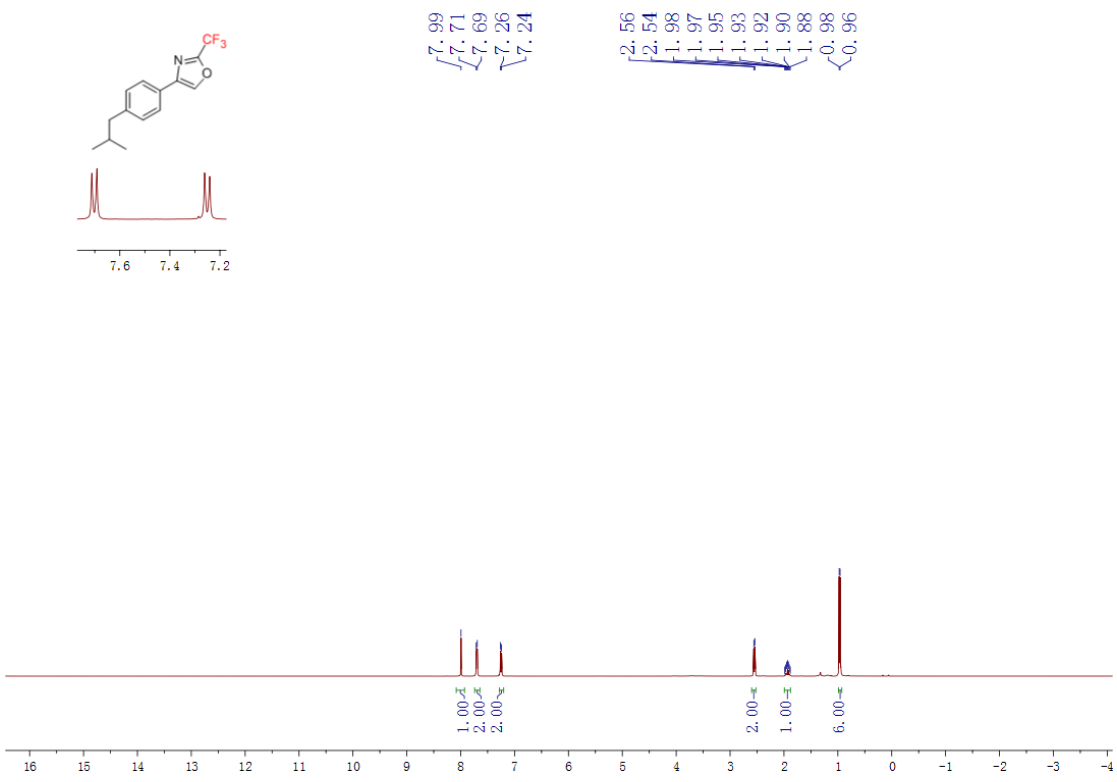
^{13}C NMR spectrum of **3d** in $CDCl_3$



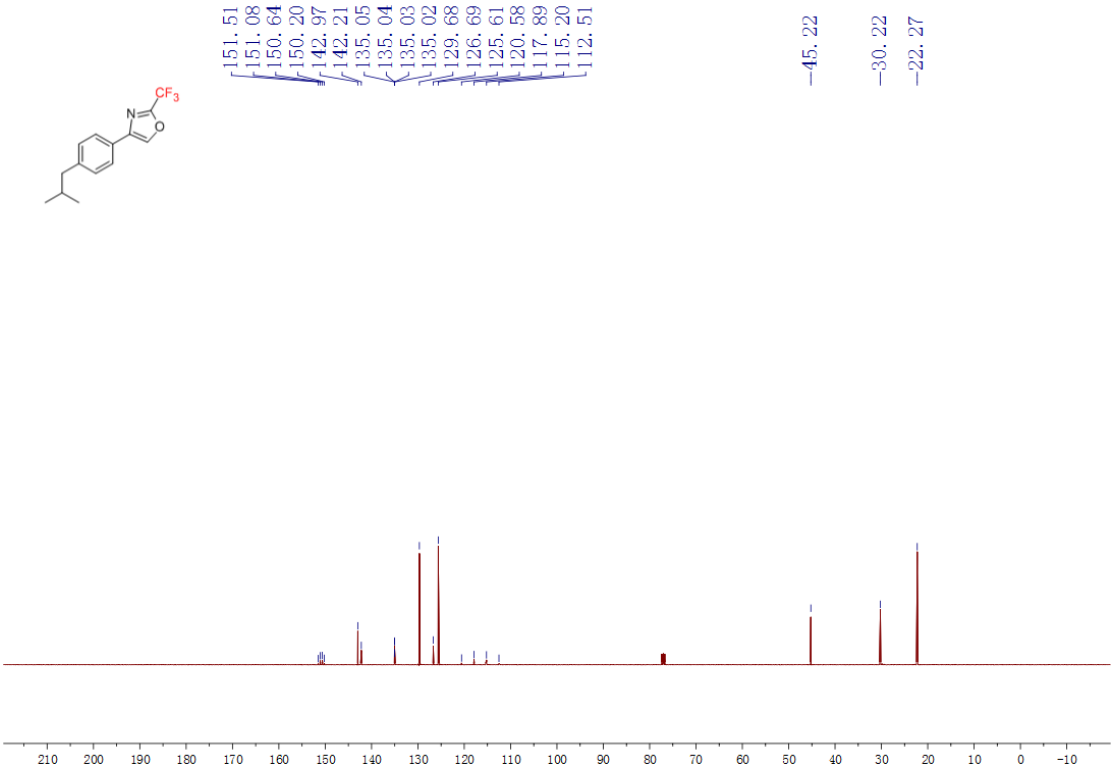
^{19}F NMR spectrum of **3e** in $CDCl_3$



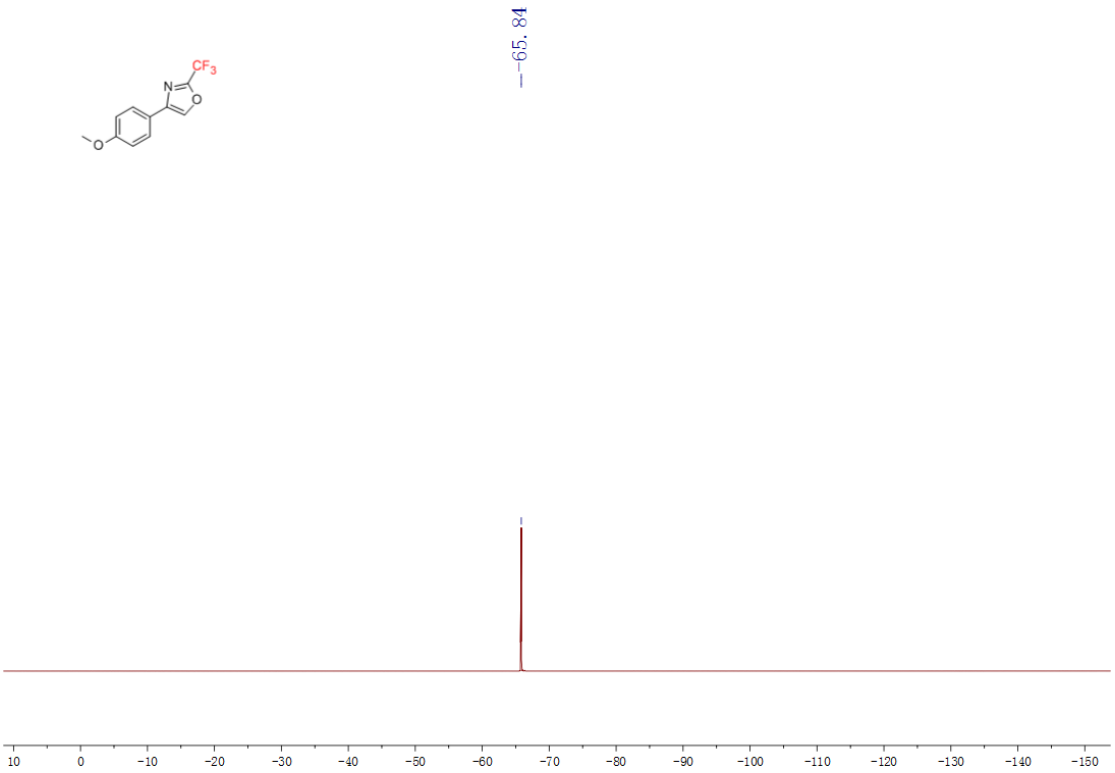
^{1}H NMR spectrum of **3e** in $CDCl_3$



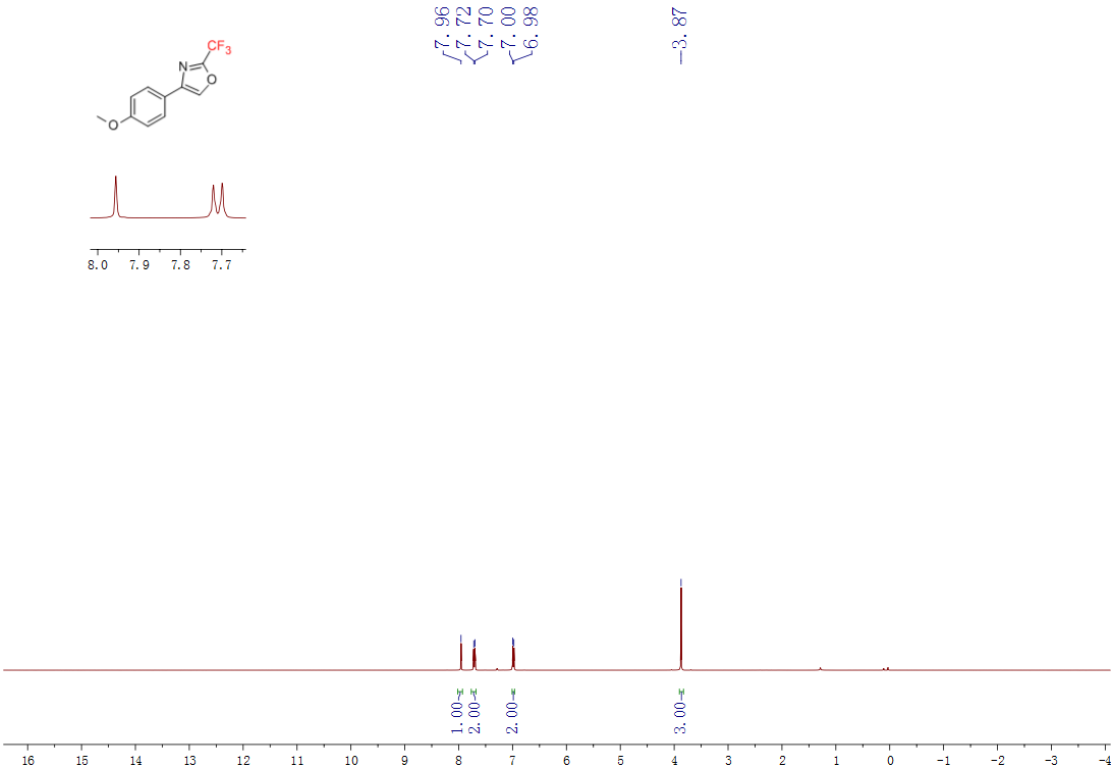
^{13}C NMR spectrum of **3e** in $CDCl_3$



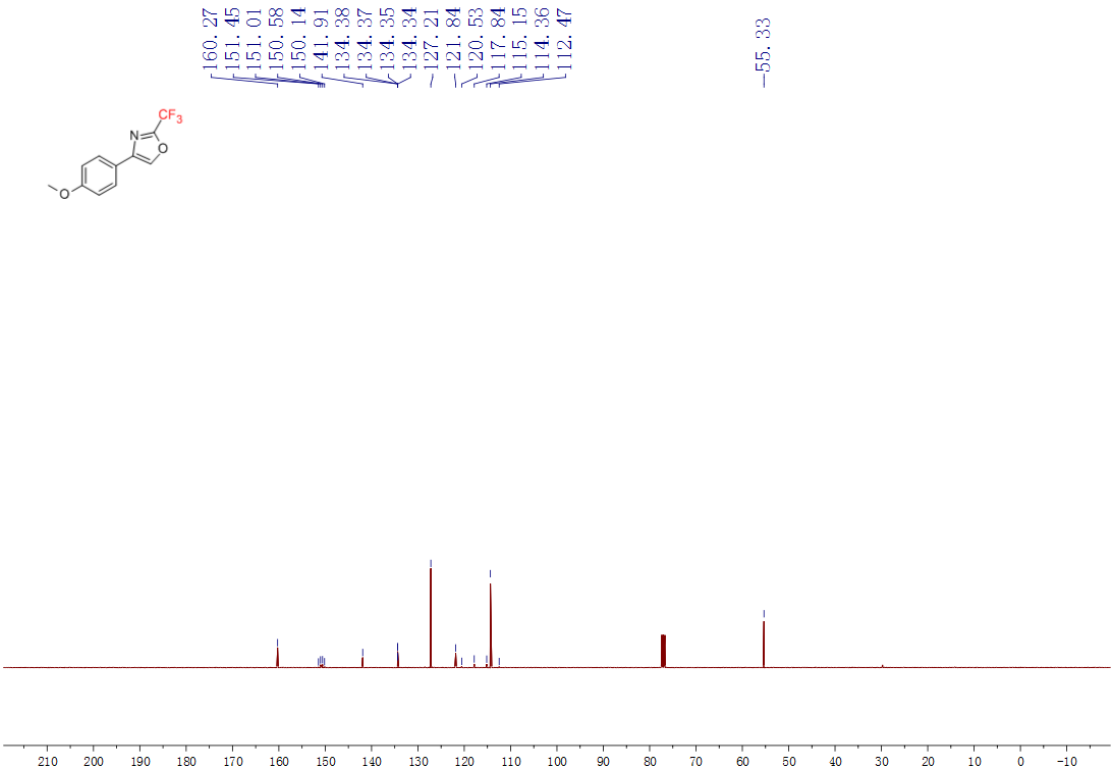
^{19}F NMR spectrum of **3f** in $CDCl_3$



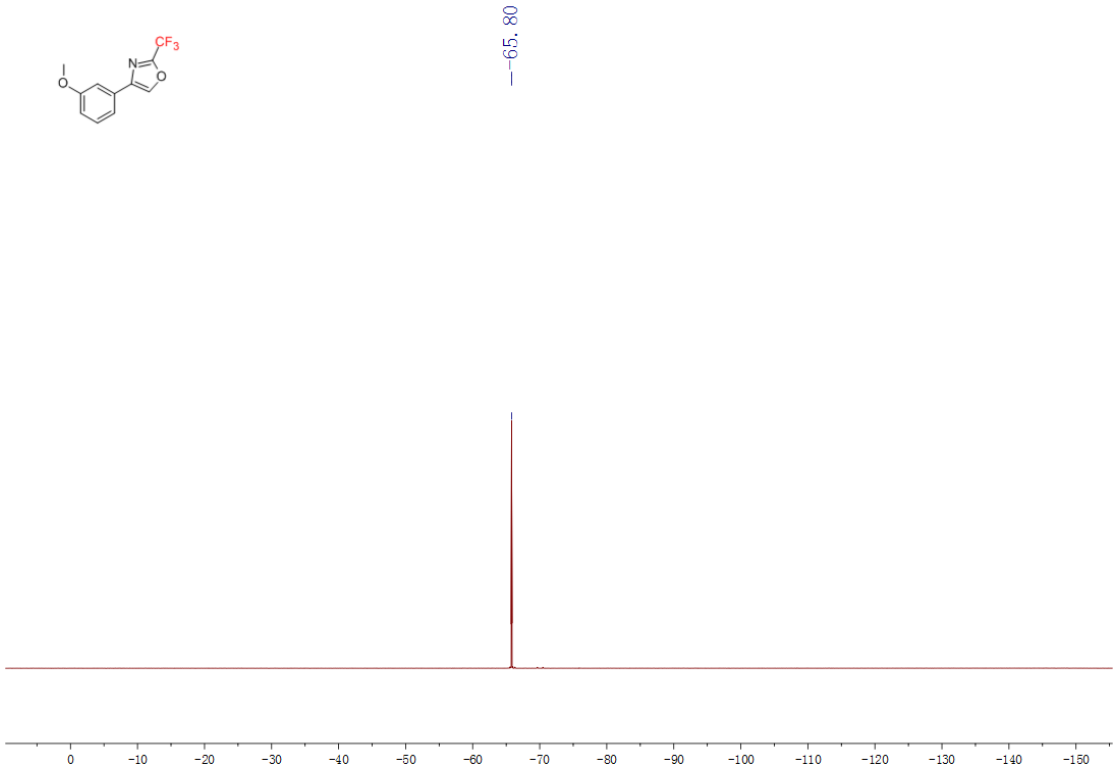
^{1}H NMR spectrum of **3f** in $CDCl_3$



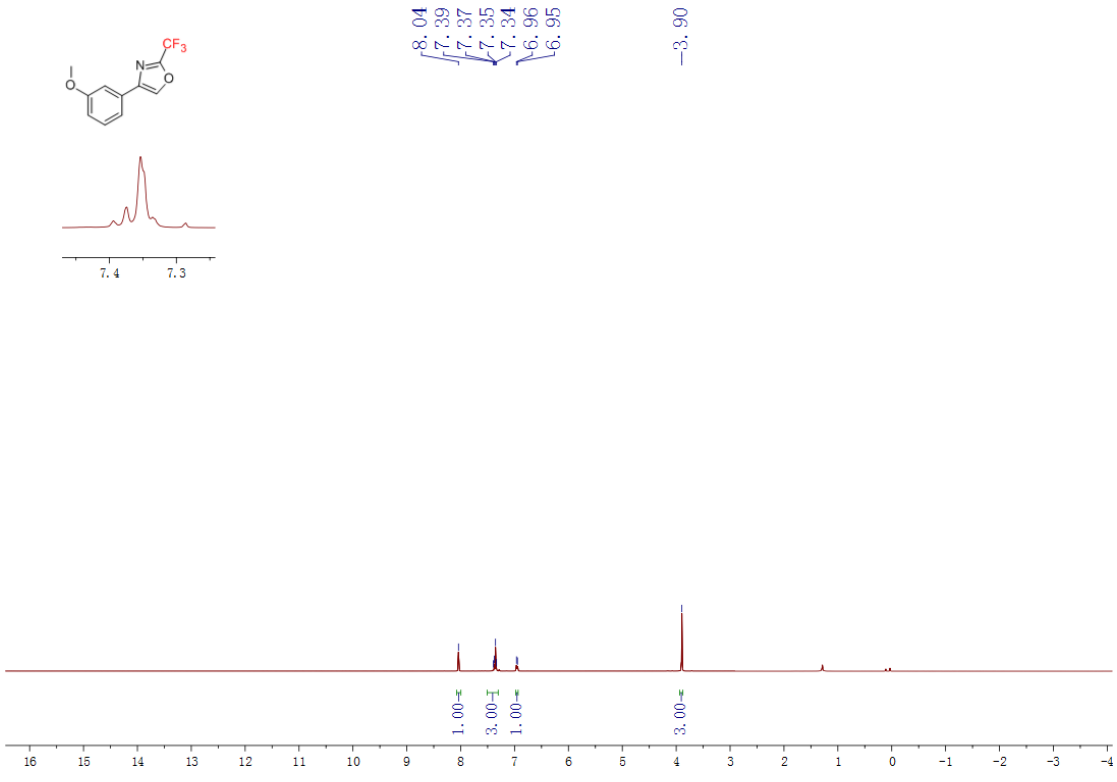
^{13}C NMR spectrum of **3f** in $CDCl_3$



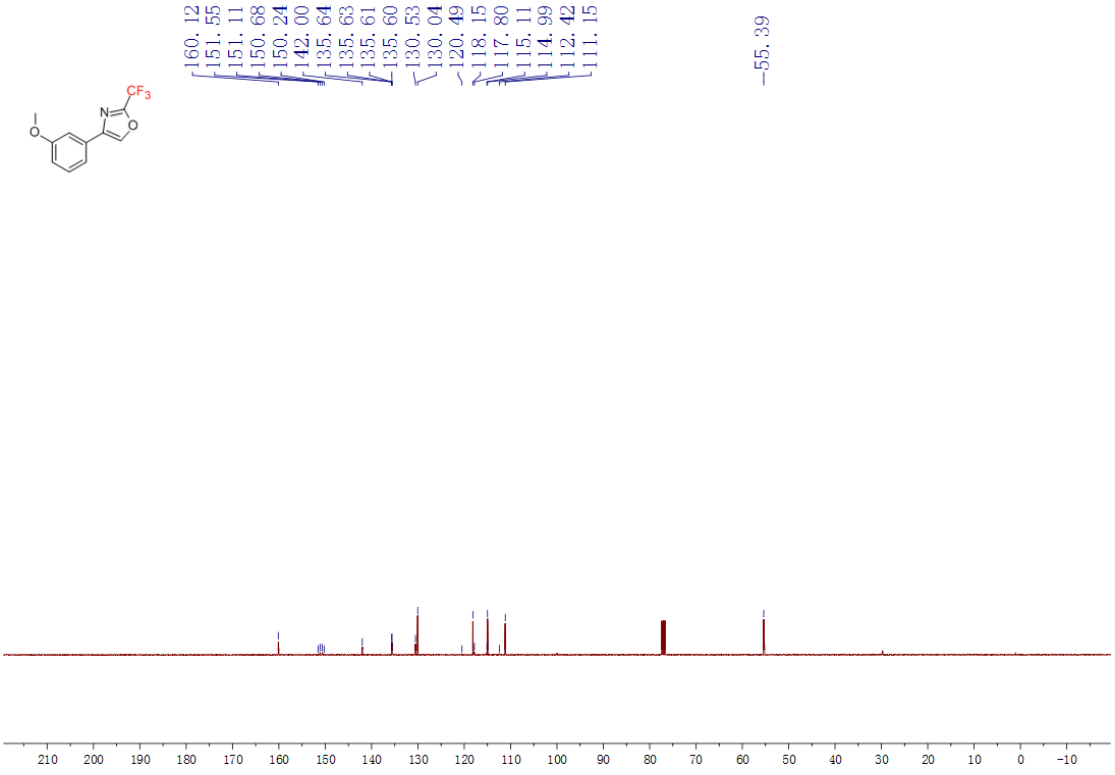
^{19}F NMR spectrum of **3g** in $CDCl_3$



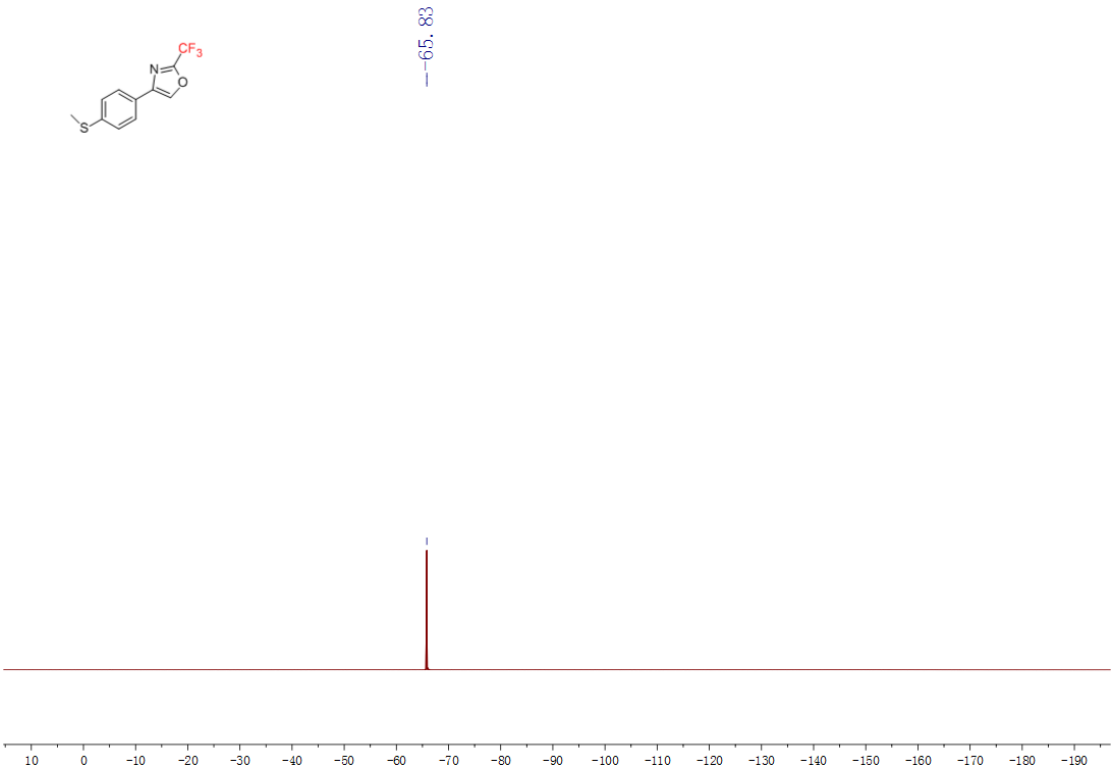
^{1}H NMR spectrum of **3g** in $CDCl_3$



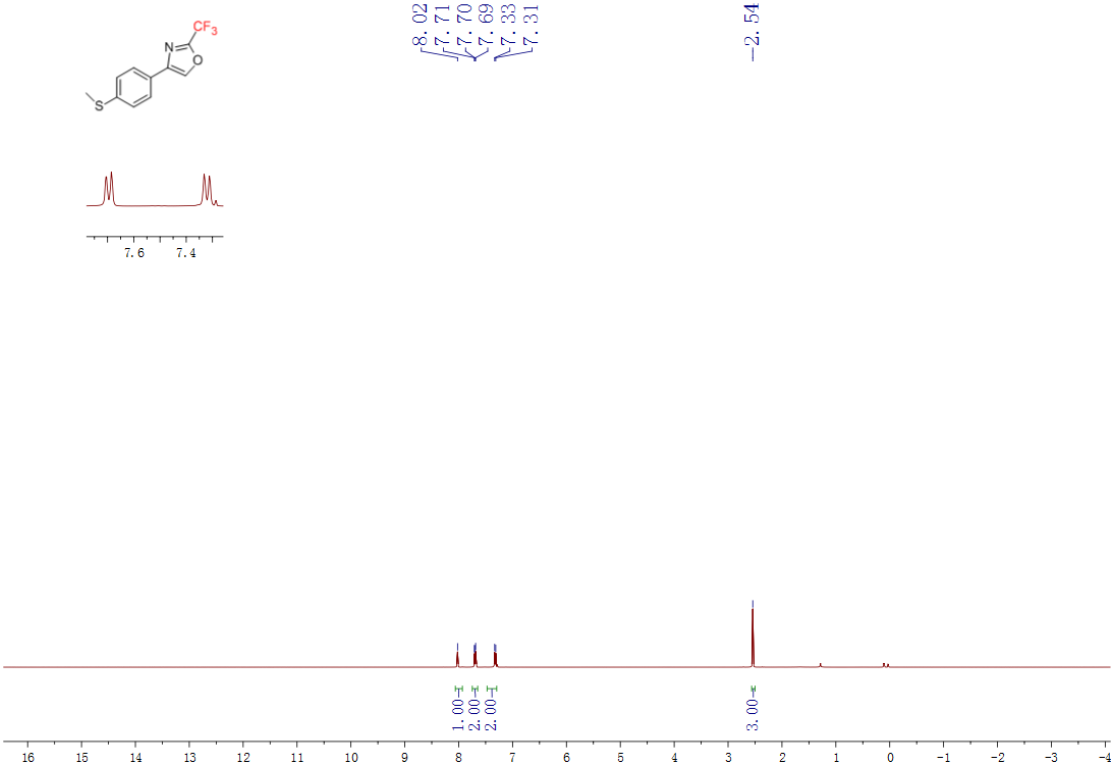
^{13}C NMR spectrum of **3g** in $CDCl_3$



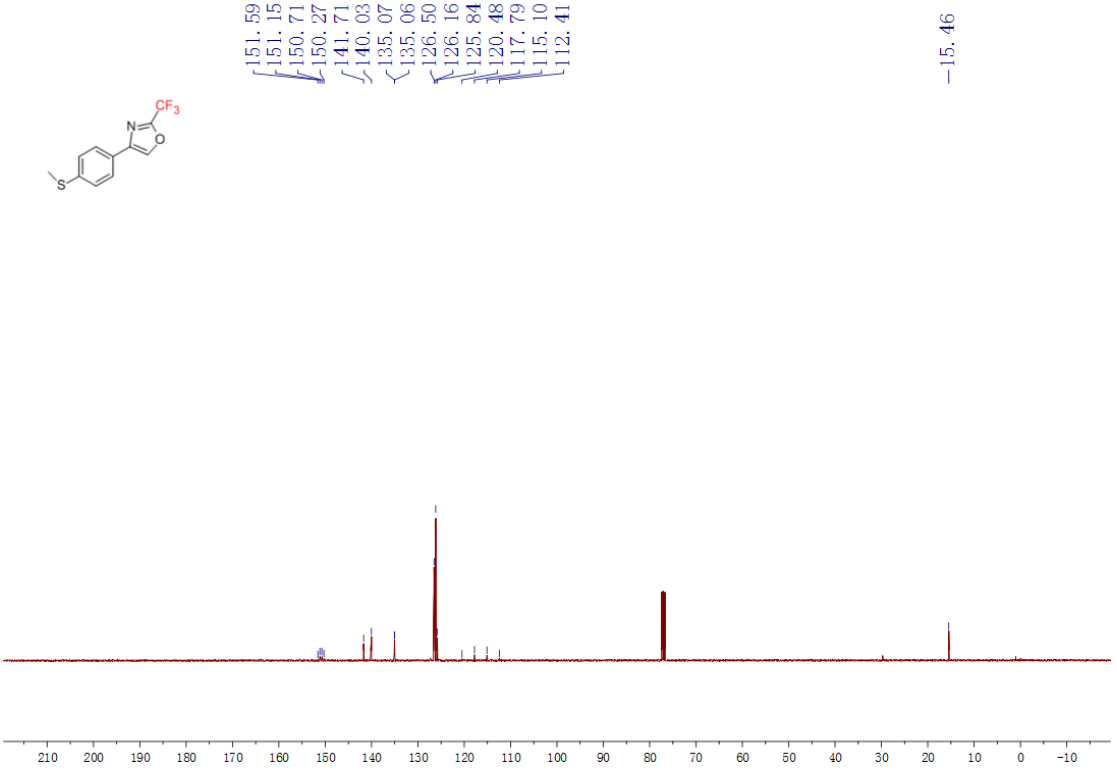
^{19}F NMR spectrum of **3h** in $CDCl_3$



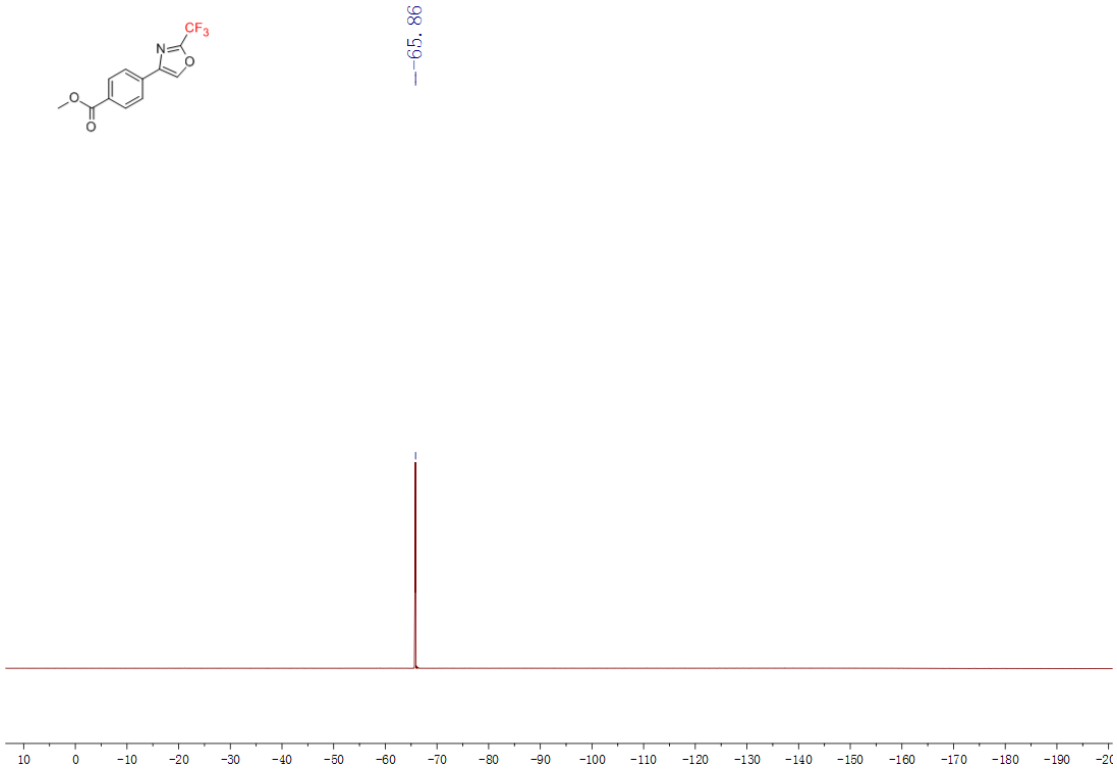
^{1}H NMR spectrum of **3h** in $CDCl_3$



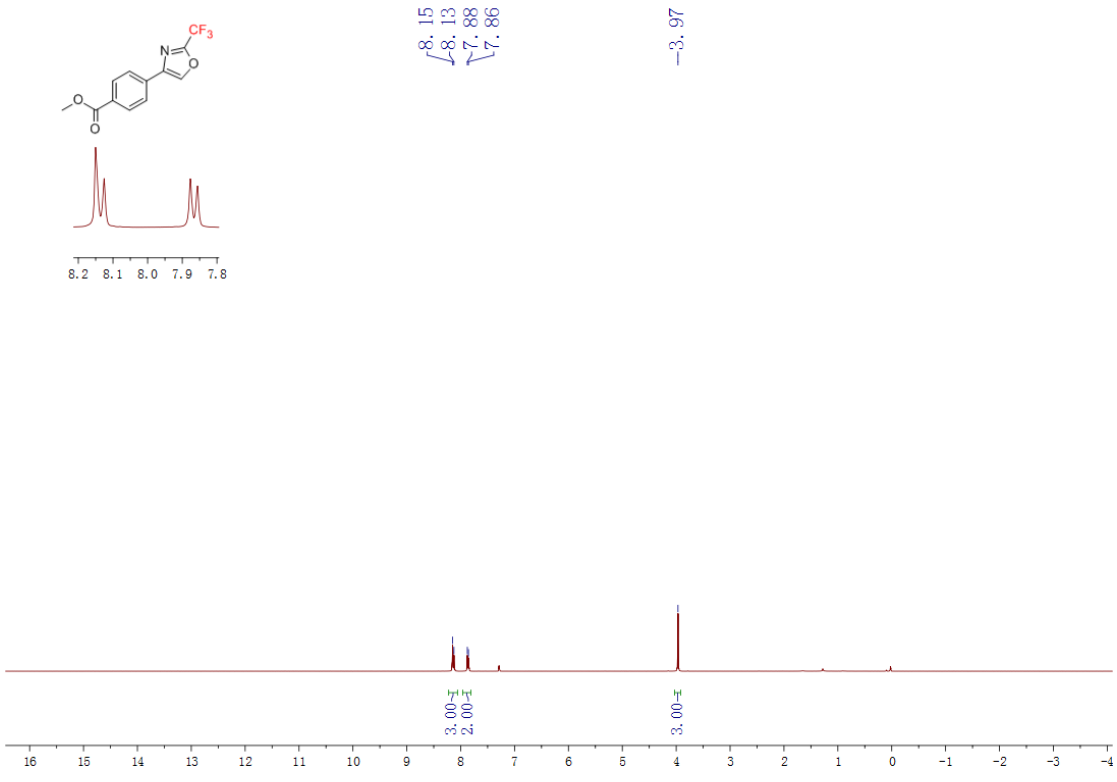
^{13}C NMR spectrum of **3h** in $CDCl_3$



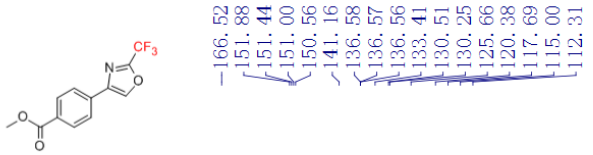
^{19}F NMR spectrum of **3i** in $CDCl_3$

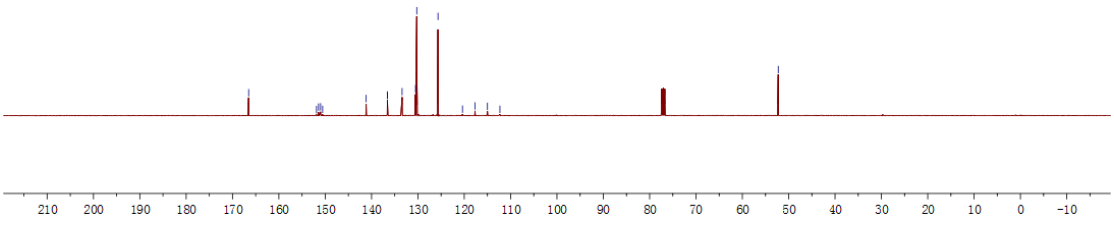


^{1}H NMR spectrum of **3i** in $CDCl_3$

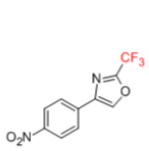


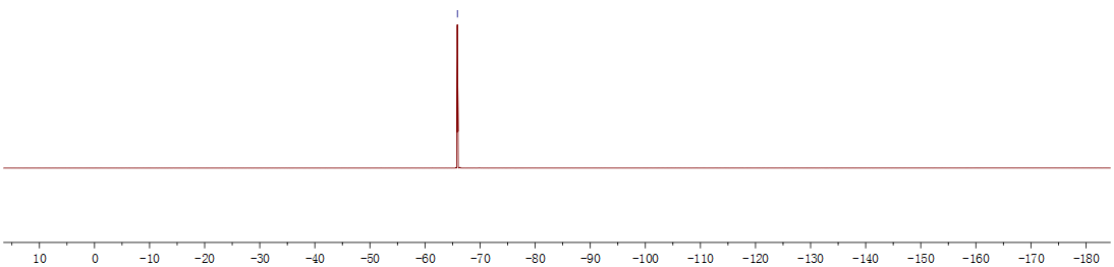
^{13}C NMR spectrum of **3i** in $CDCl_3$



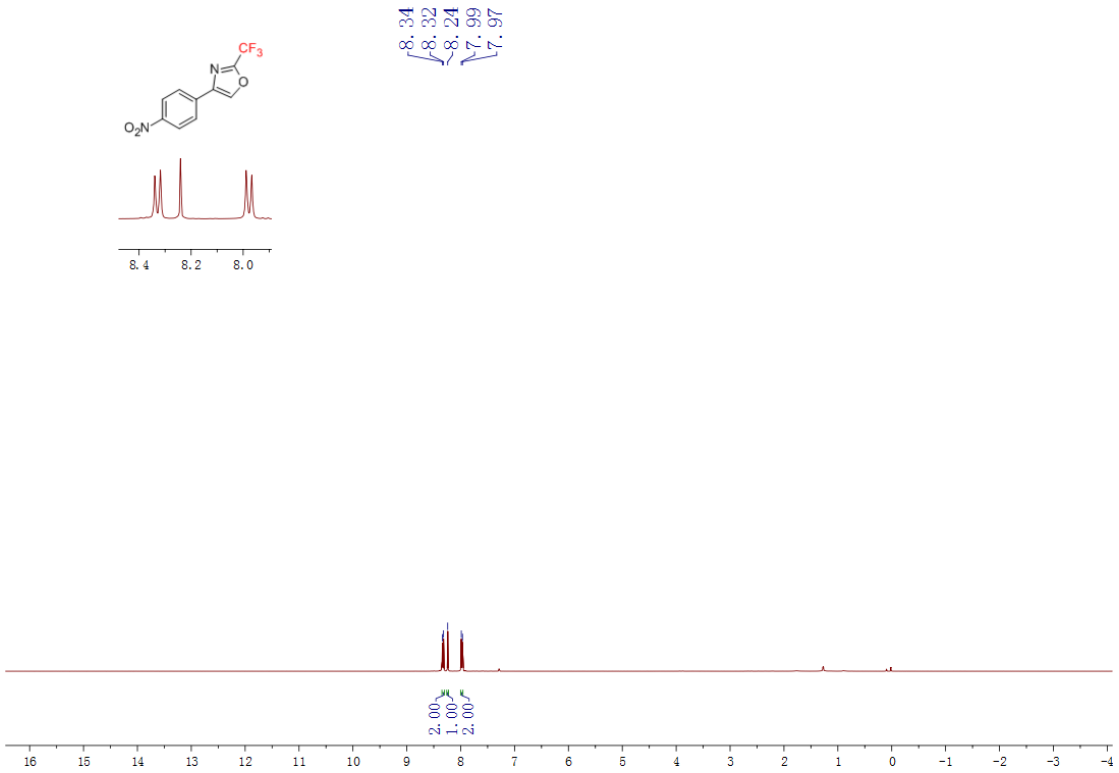


^{19}F NMR spectrum of **3j** in $CDCl_3$

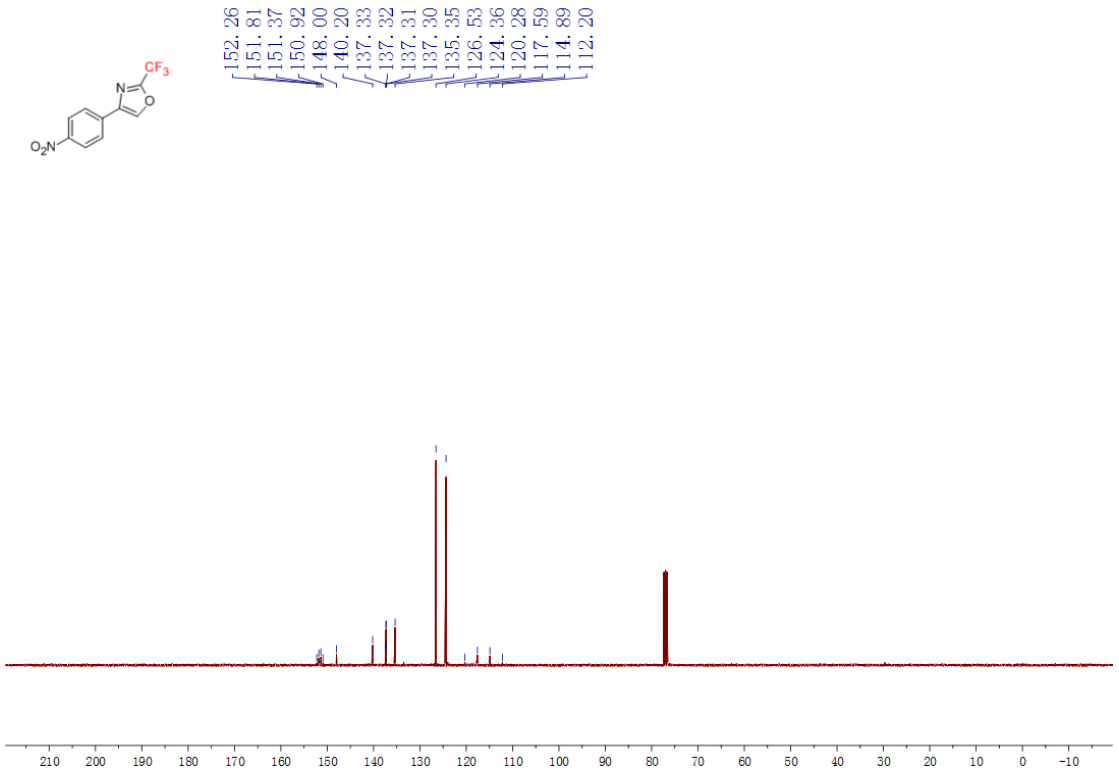




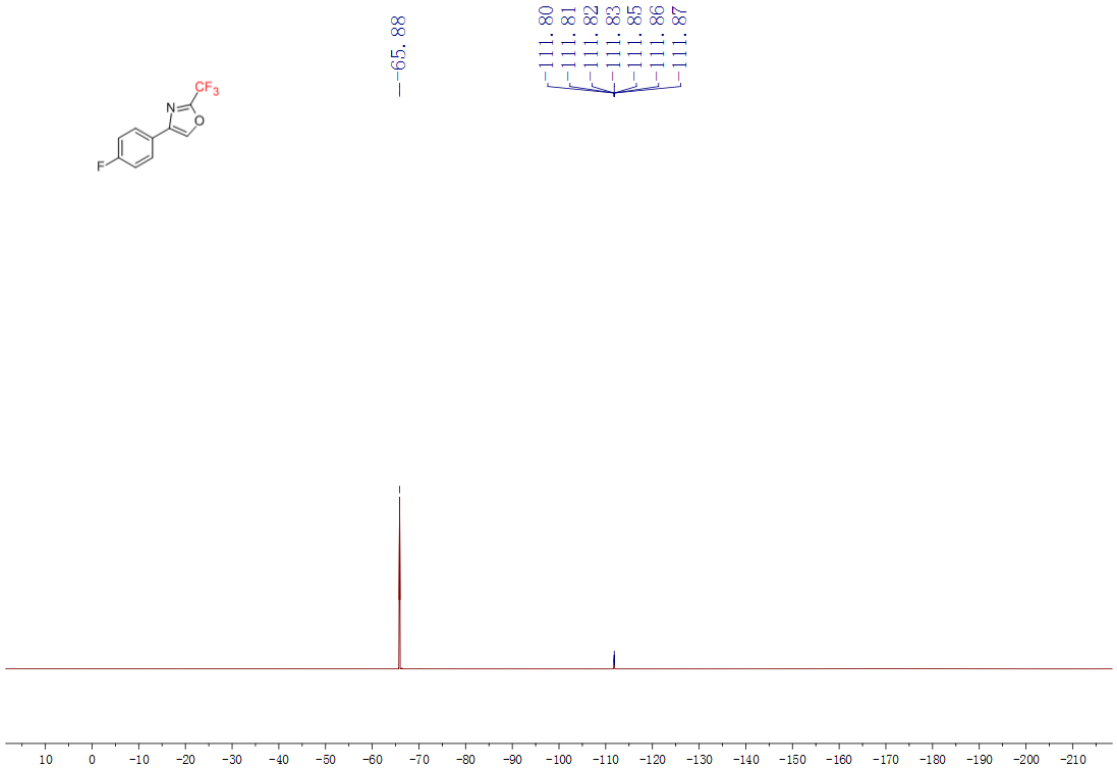
^{1}H NMR spectrum of **3j** in $CDCl_3$



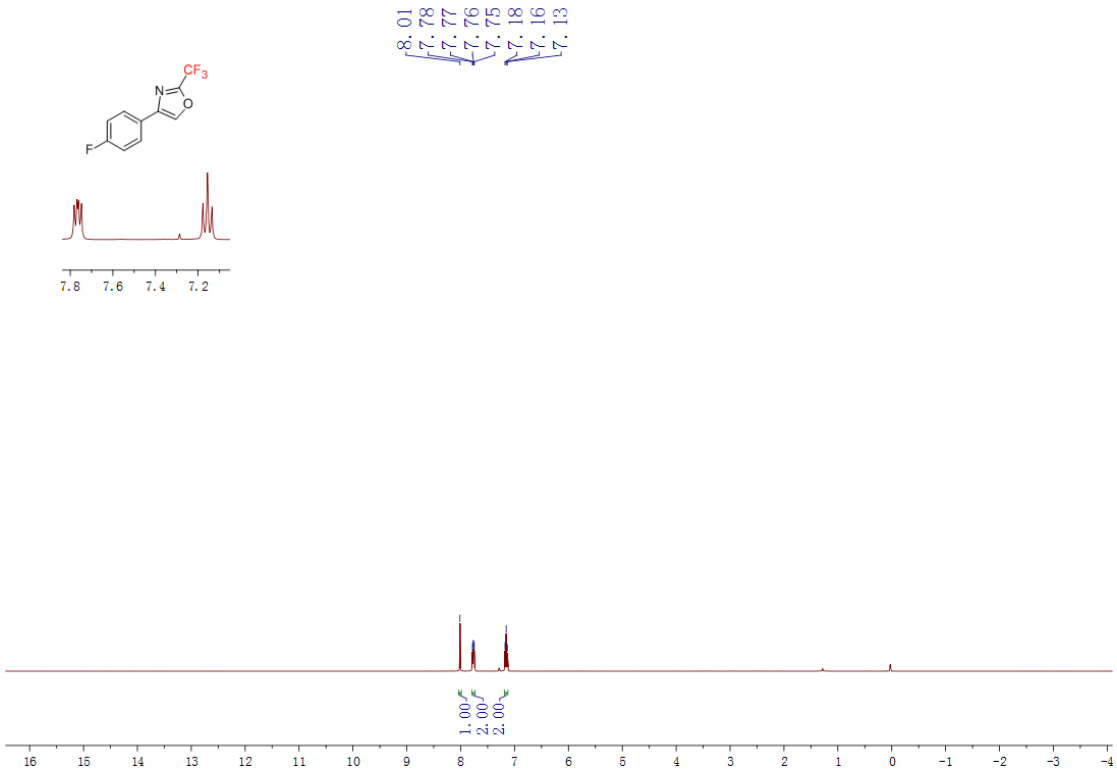
^{13}C NMR spectrum of **3j** in $CDCl_3$



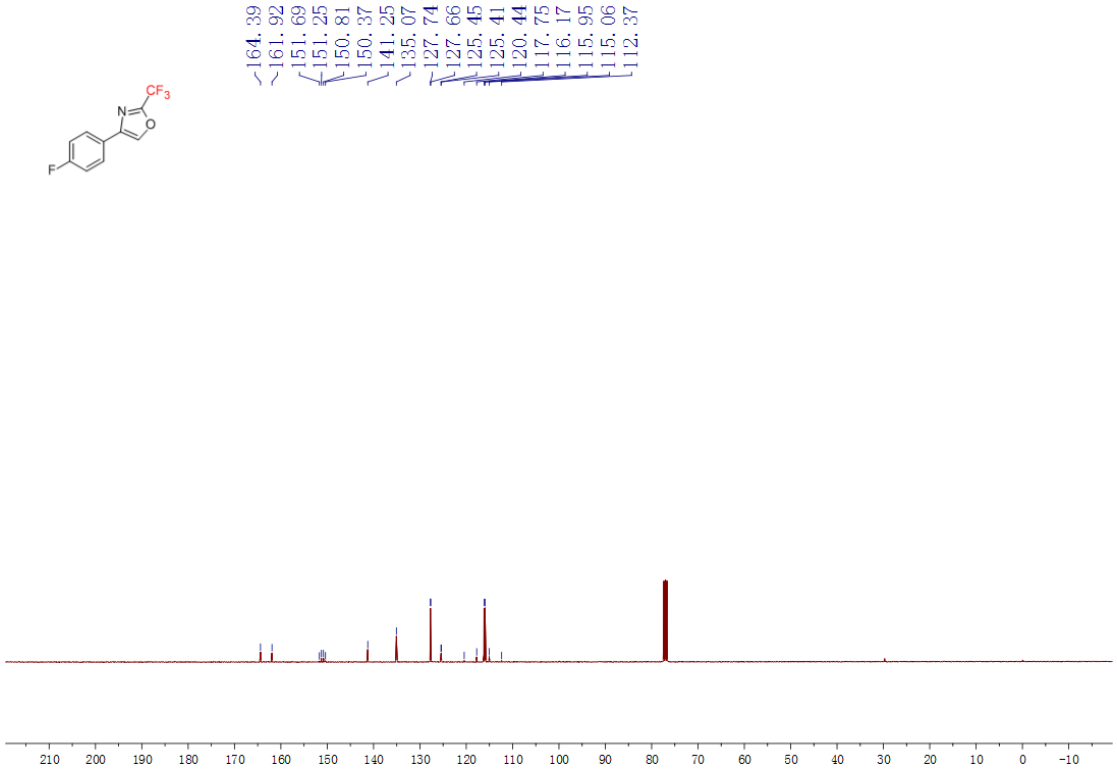
^{19}F NMR spectrum of **3k** in $CDCl_3$



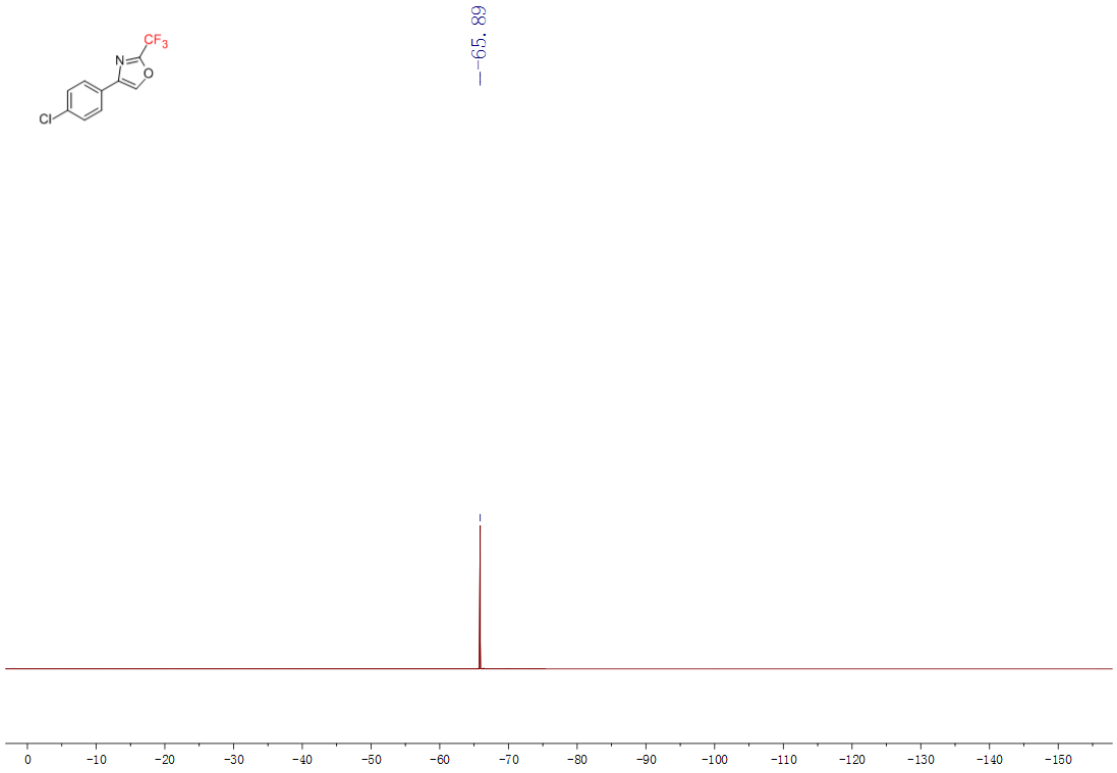
^{1}H NMR spectrum of **3k** in $CDCl_3$



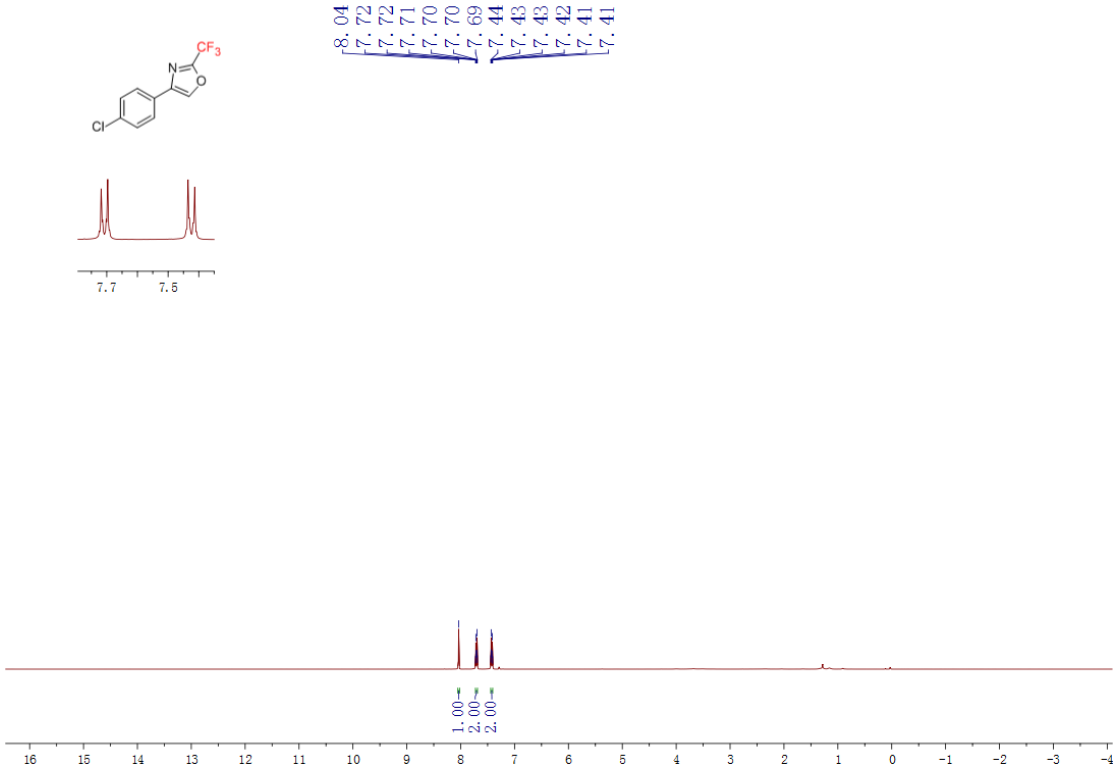
^{13}C NMR spectrum of **3k** in $CDCl_3$



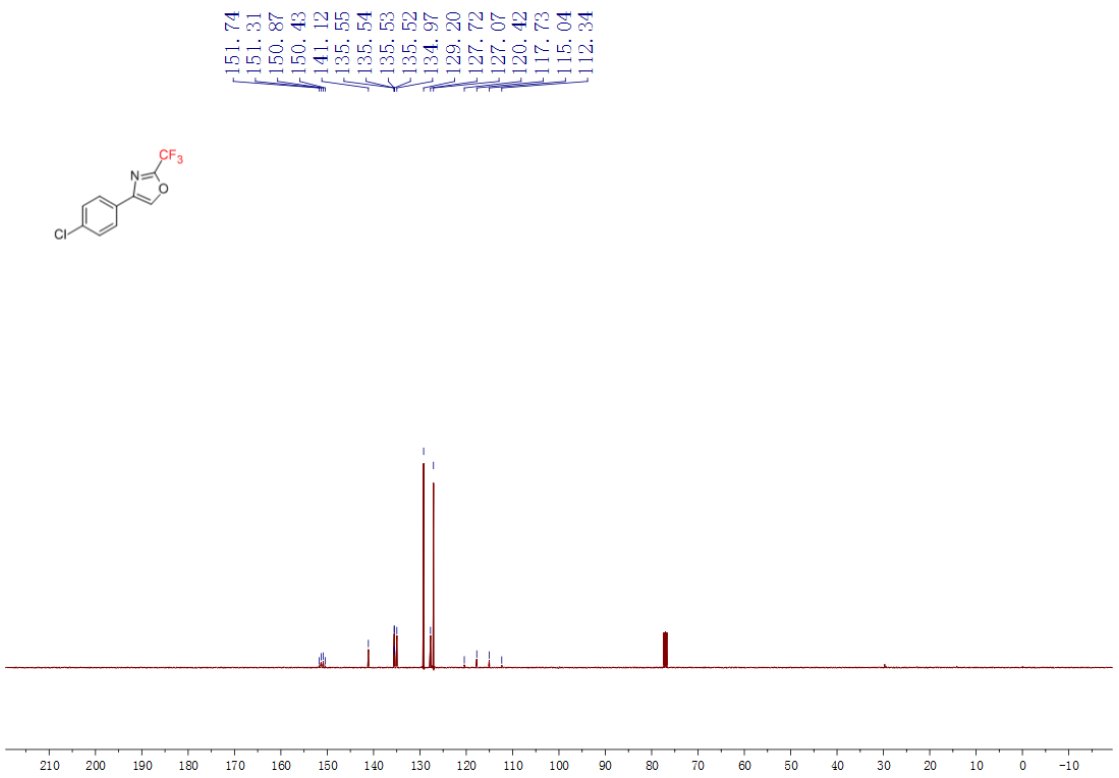
^{19}F NMR spectrum of **3l** in $CDCl_3$



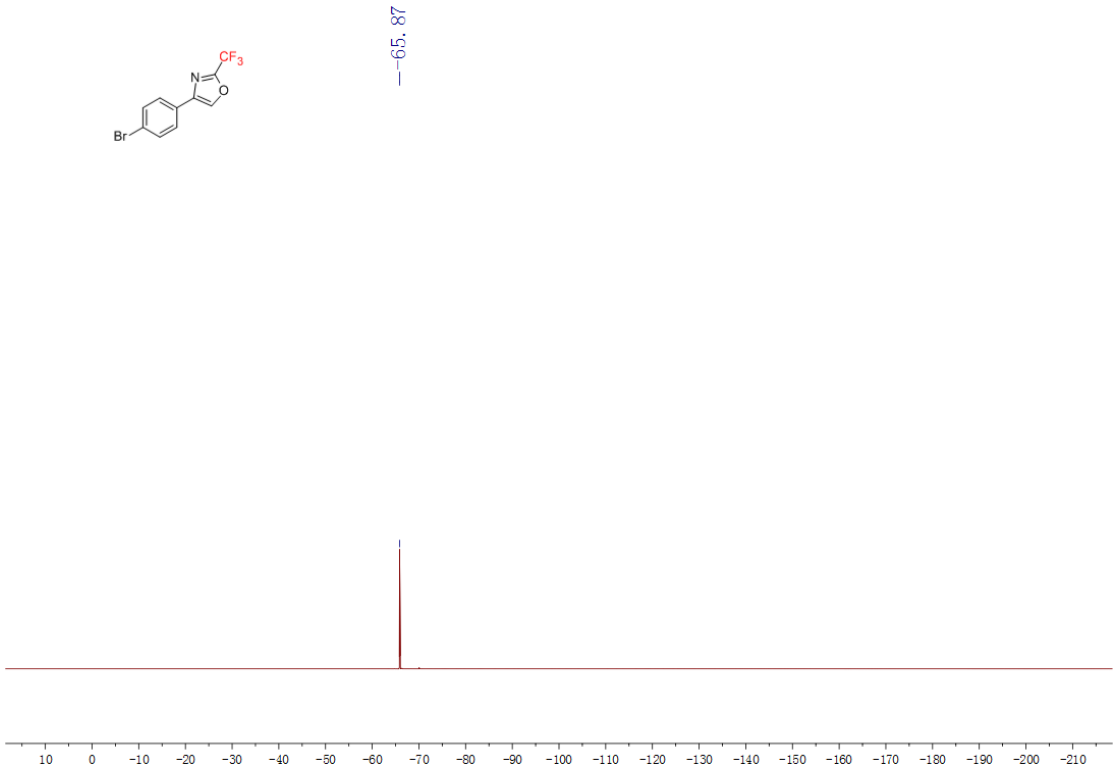
^{1}H NMR spectrum of **3l** in $CDCl_3$



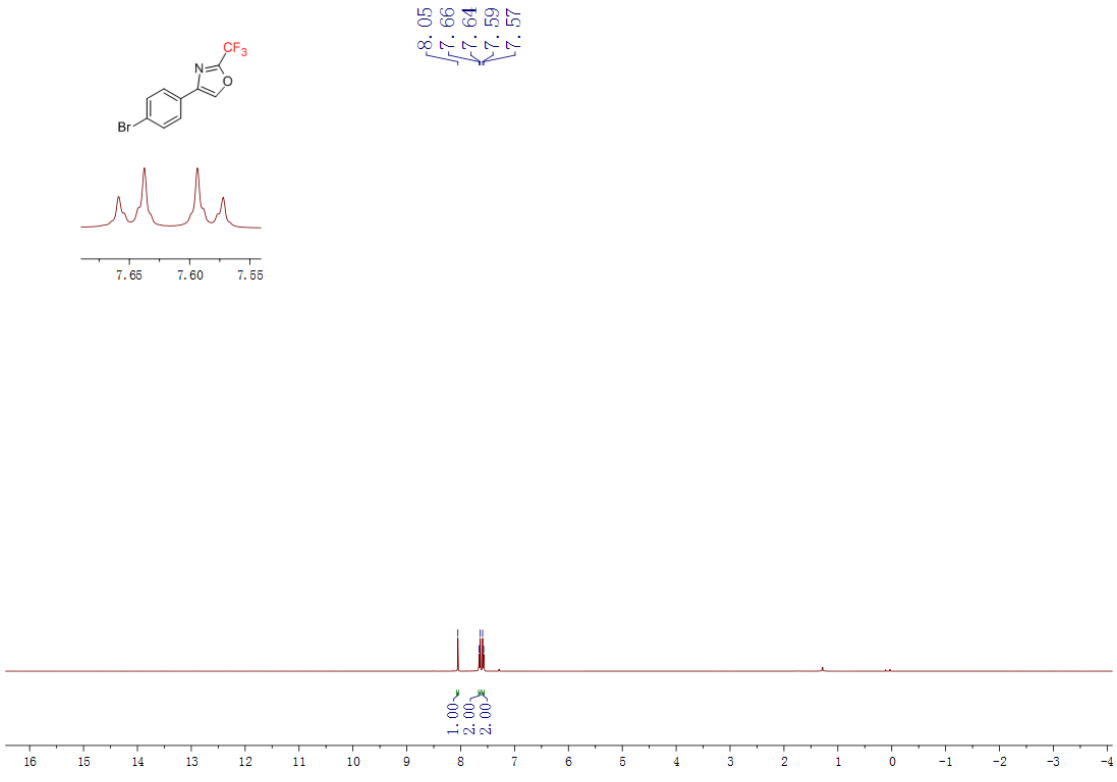
^{13}C NMR spectrum of **3l** in $CDCl_3$



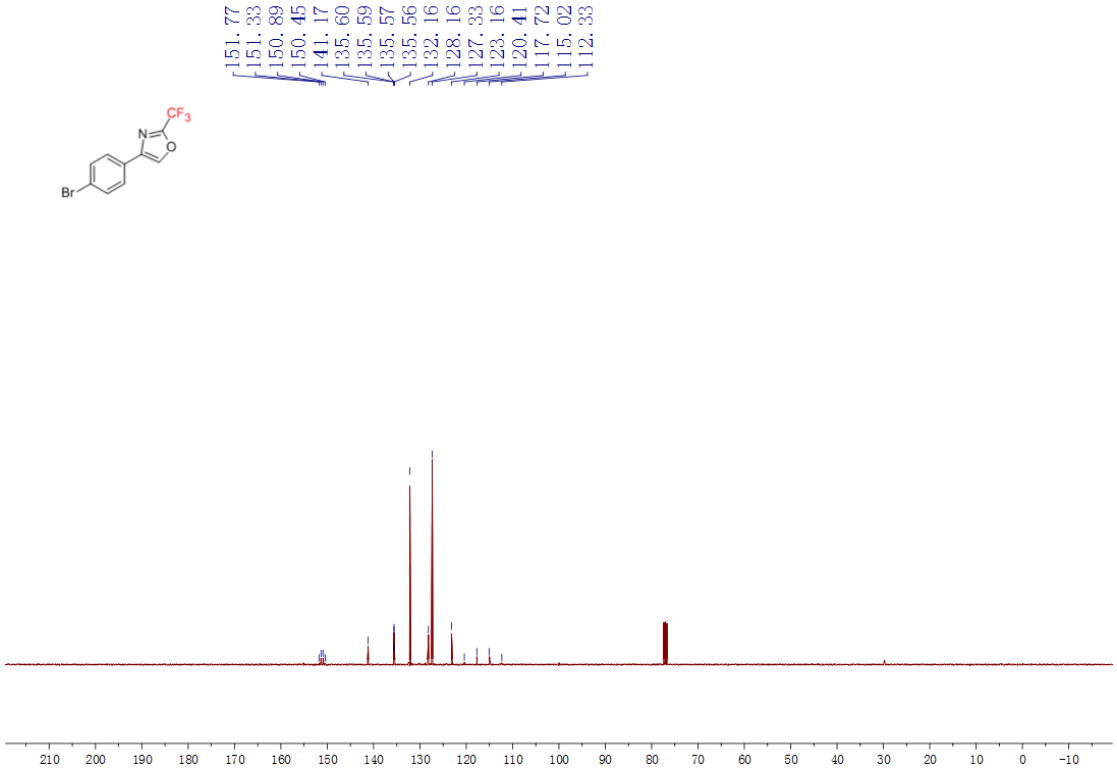
^{19}F NMR spectrum of **3m** in $CDCl_3$



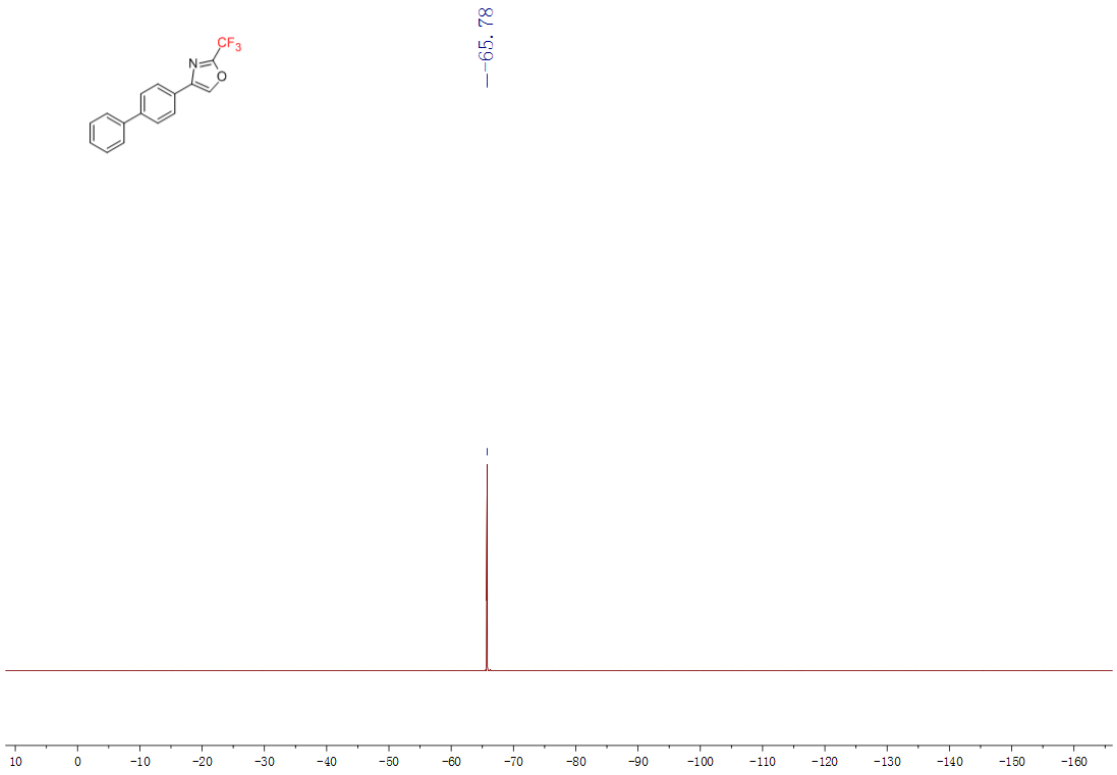
^{1}H NMR spectrum of **3m** in $CDCl_3$



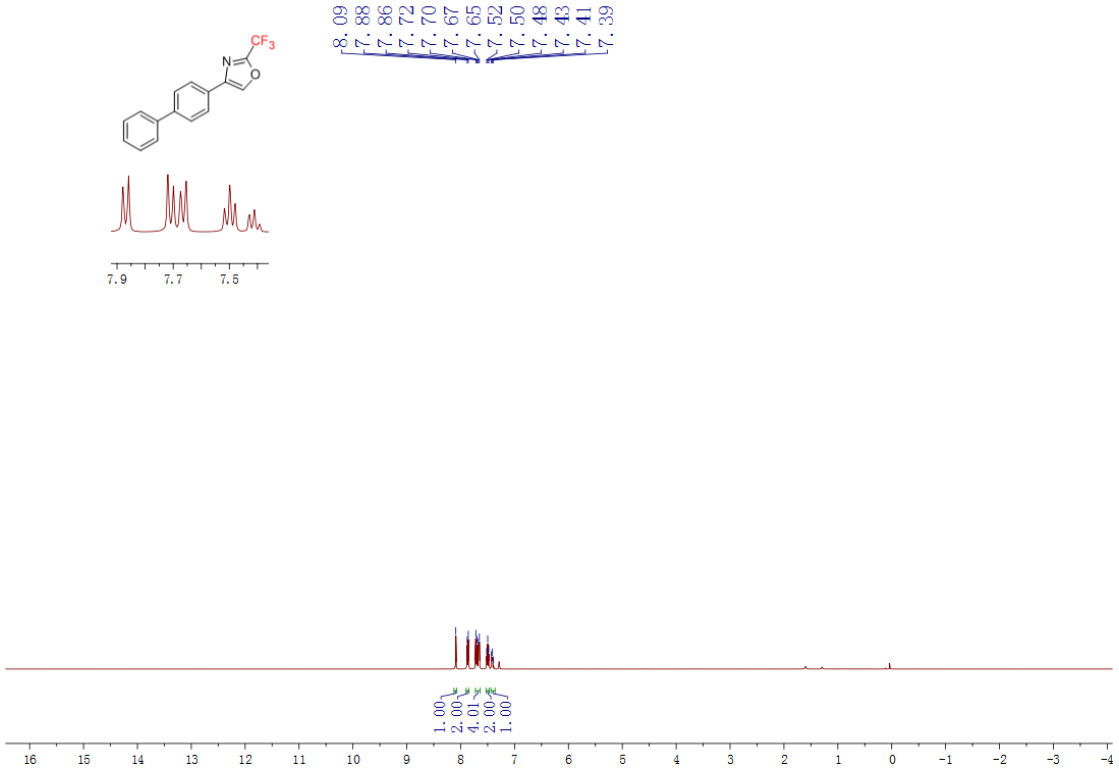
^{13}C NMR spectrum of **3m** in $CDCl_3$



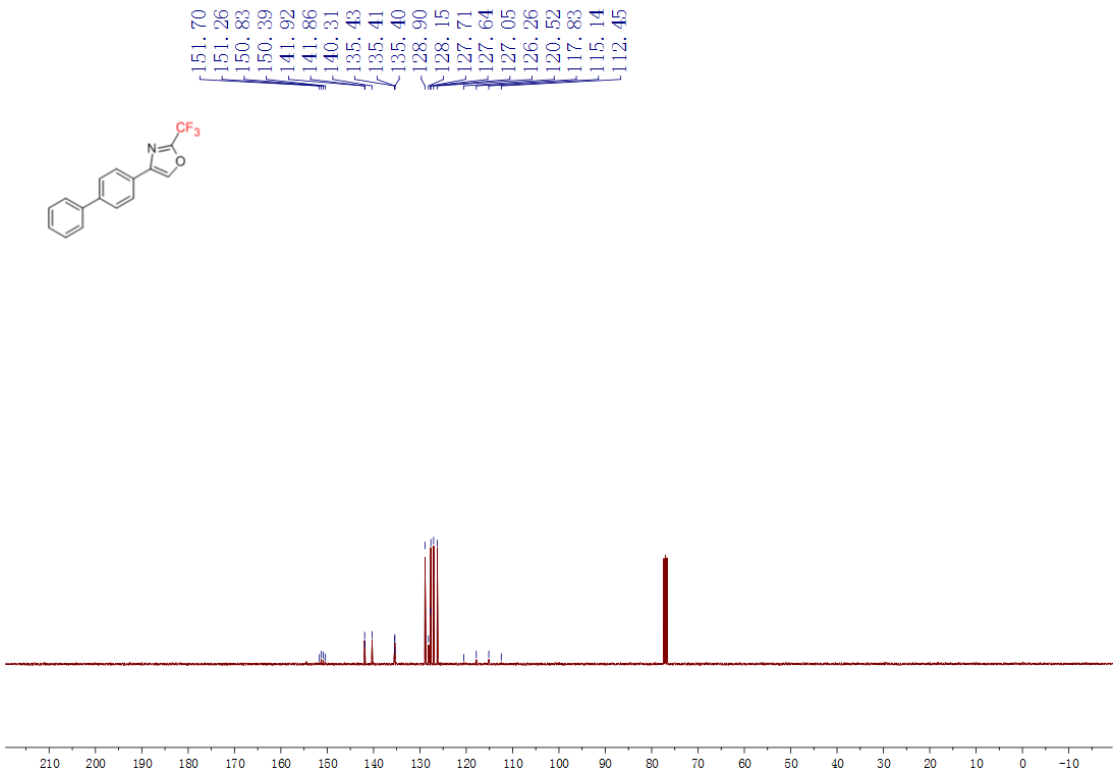
^{19}F NMR spectrum of **3n** in $CDCl_3$



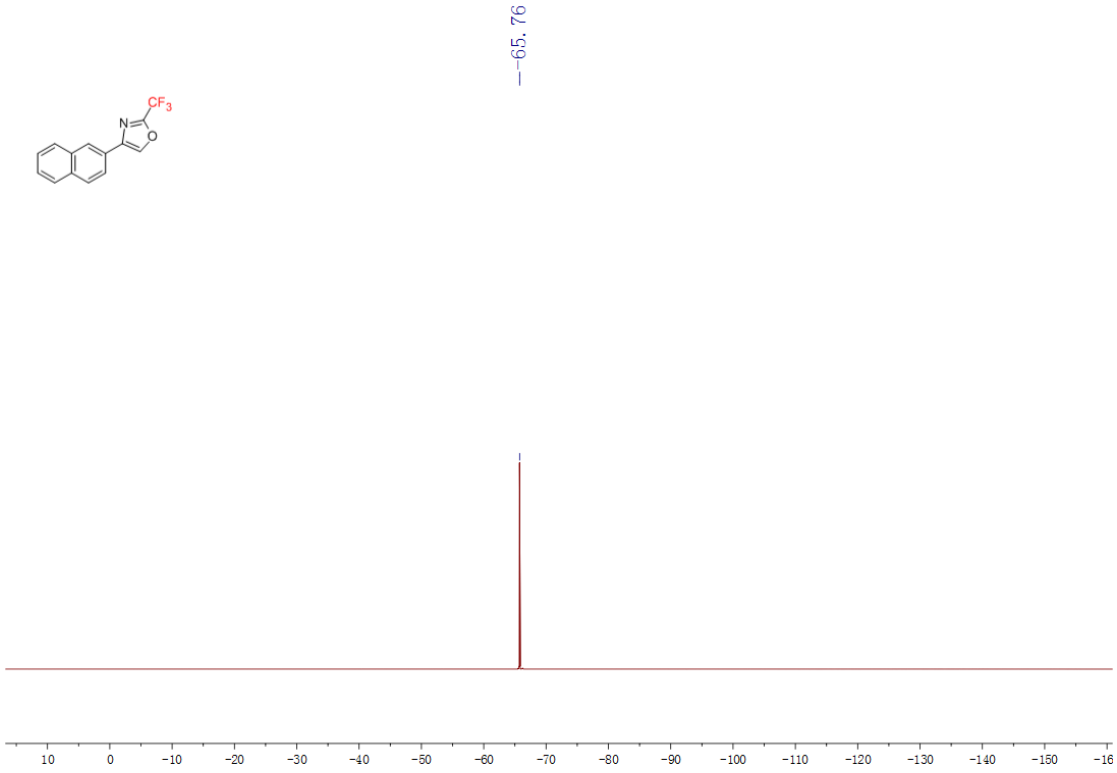
^{1}H NMR spectrum of **3n** in $CDCl_3$



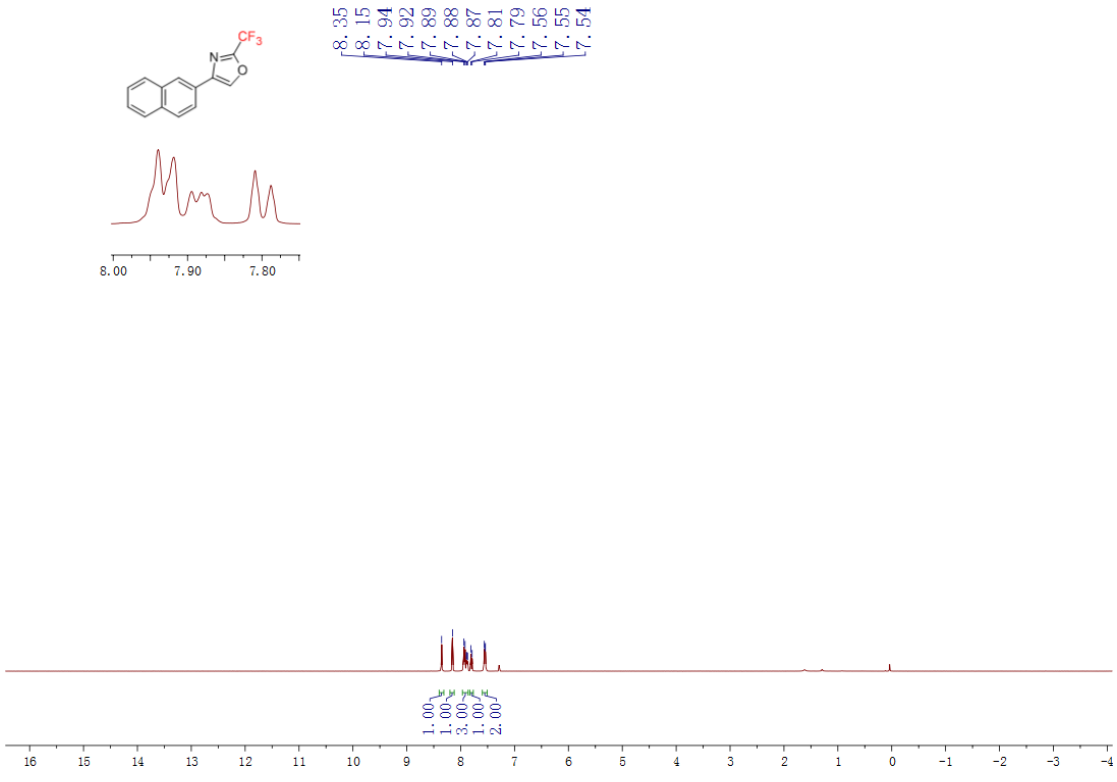
^{13}C NMR spectrum of **3n** in $CDCl_3$



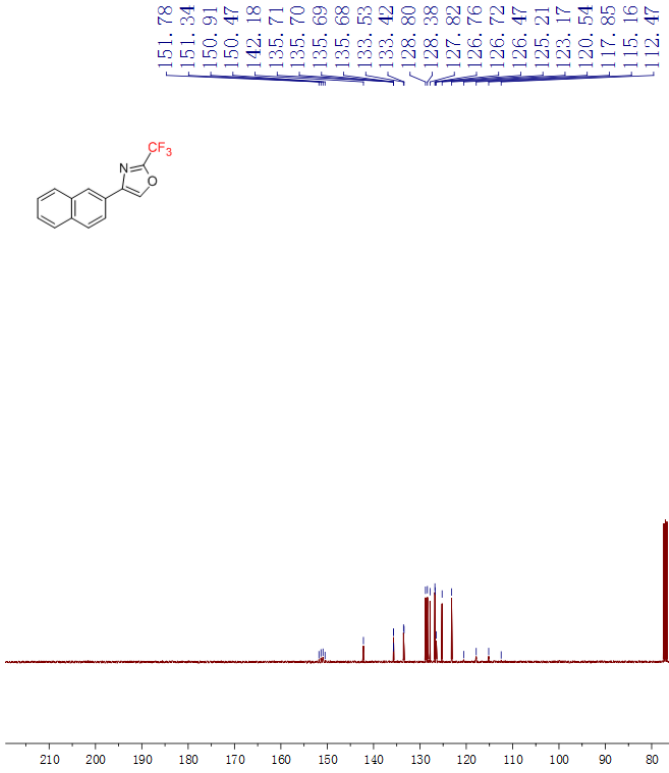
^{19}F NMR spectrum of **3o** in $CDCl_3$



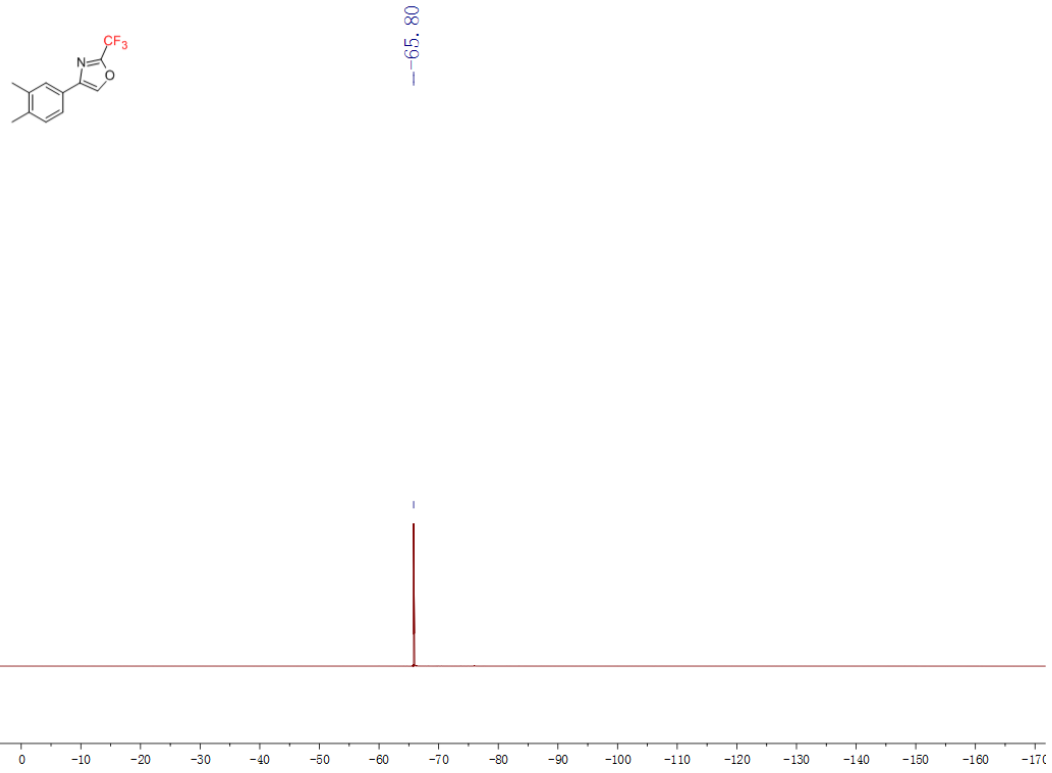
^{1}H NMR spectrum of **3o** in $CDCl_3$



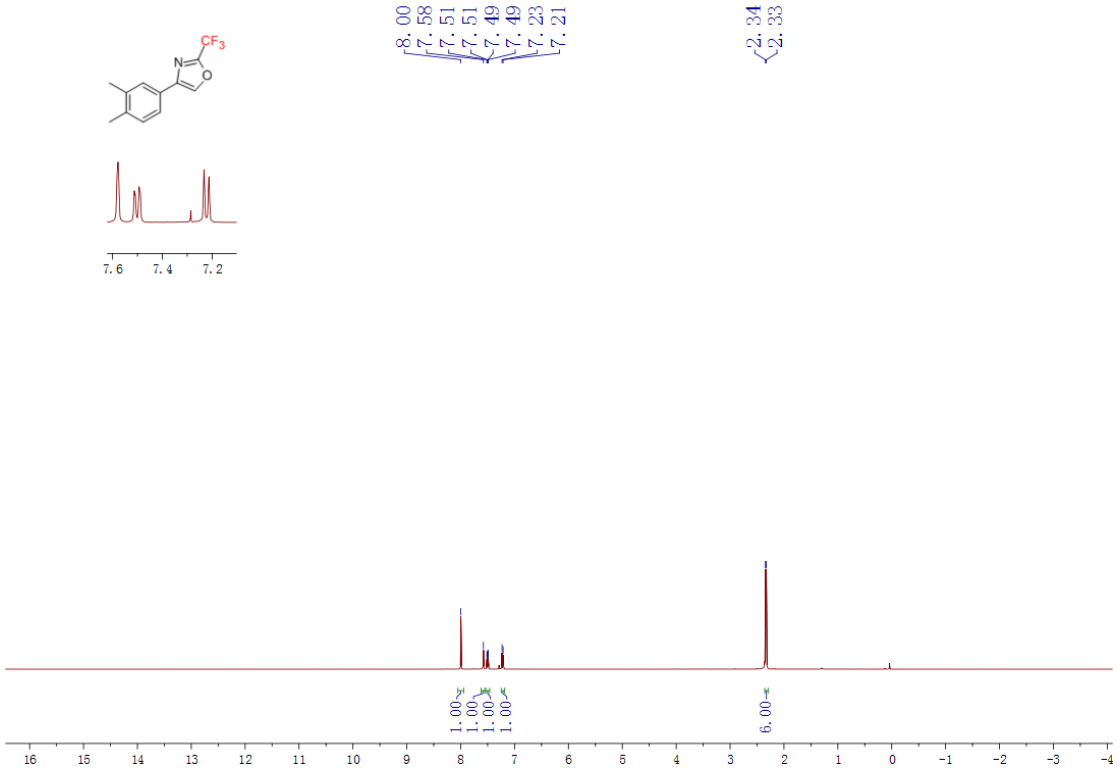
^{13}C NMR spectrum of **3o** in $CDCl_3$



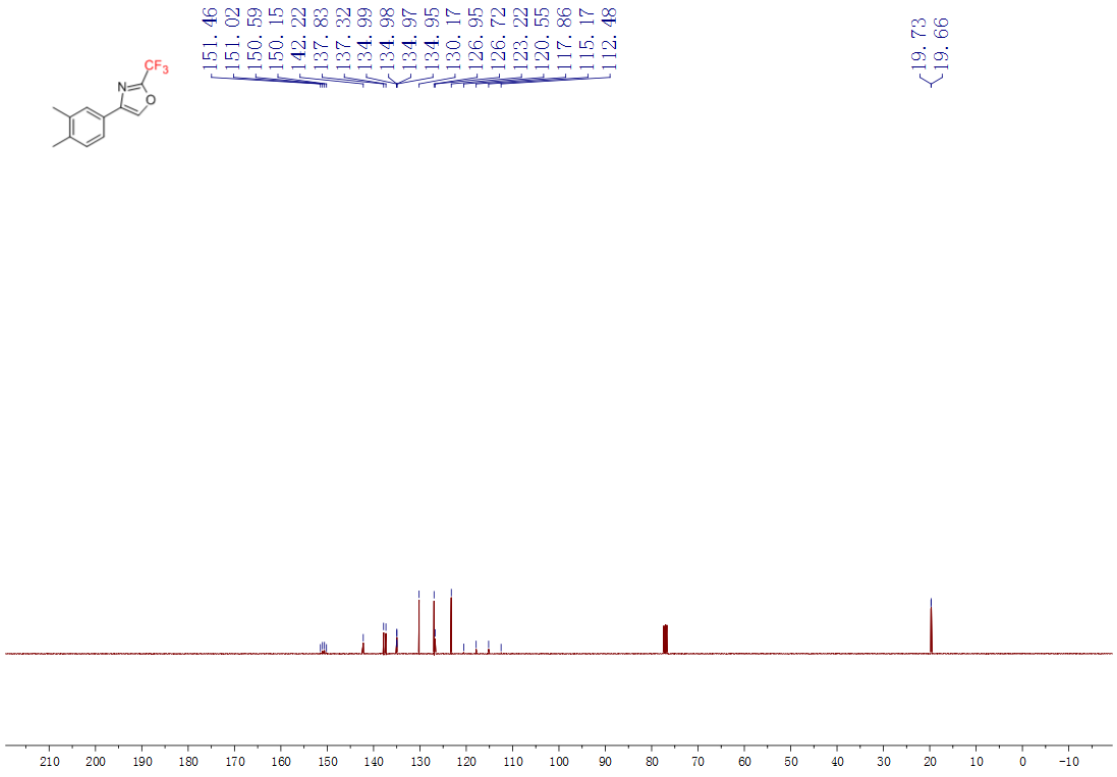
^{19}F NMR spectrum of **3p** in $CDCl_3$



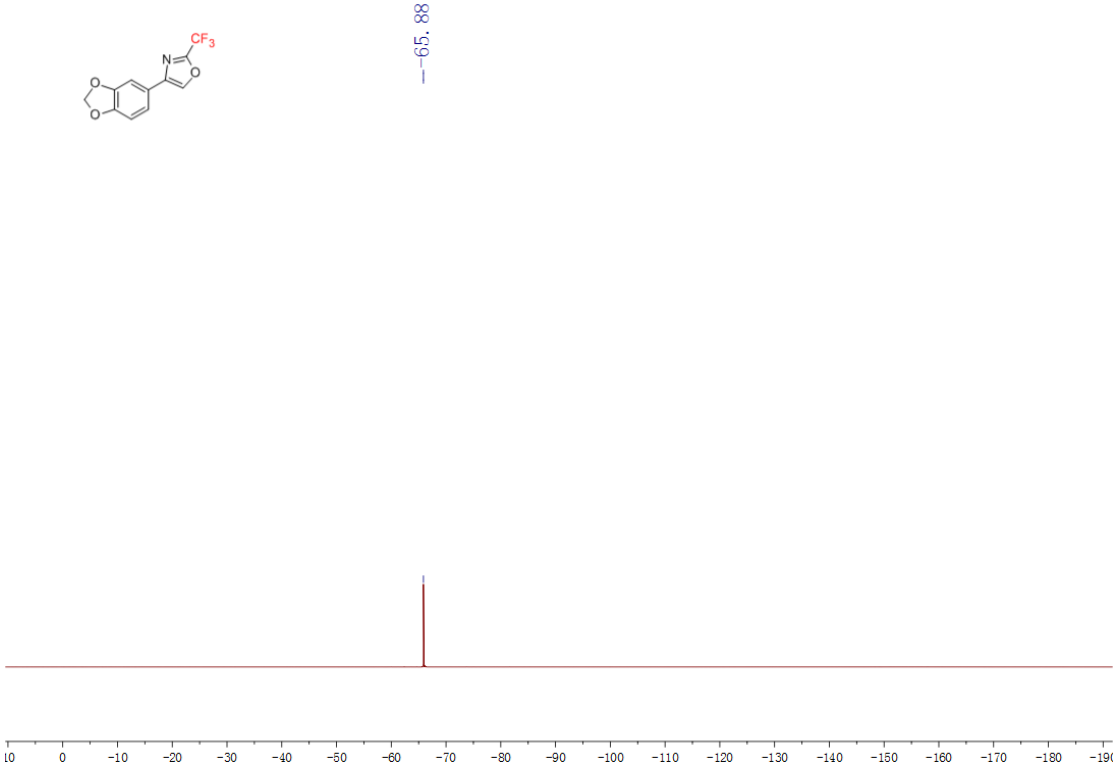
^{1}H NMR spectrum of **3p** in $CDCl_3$



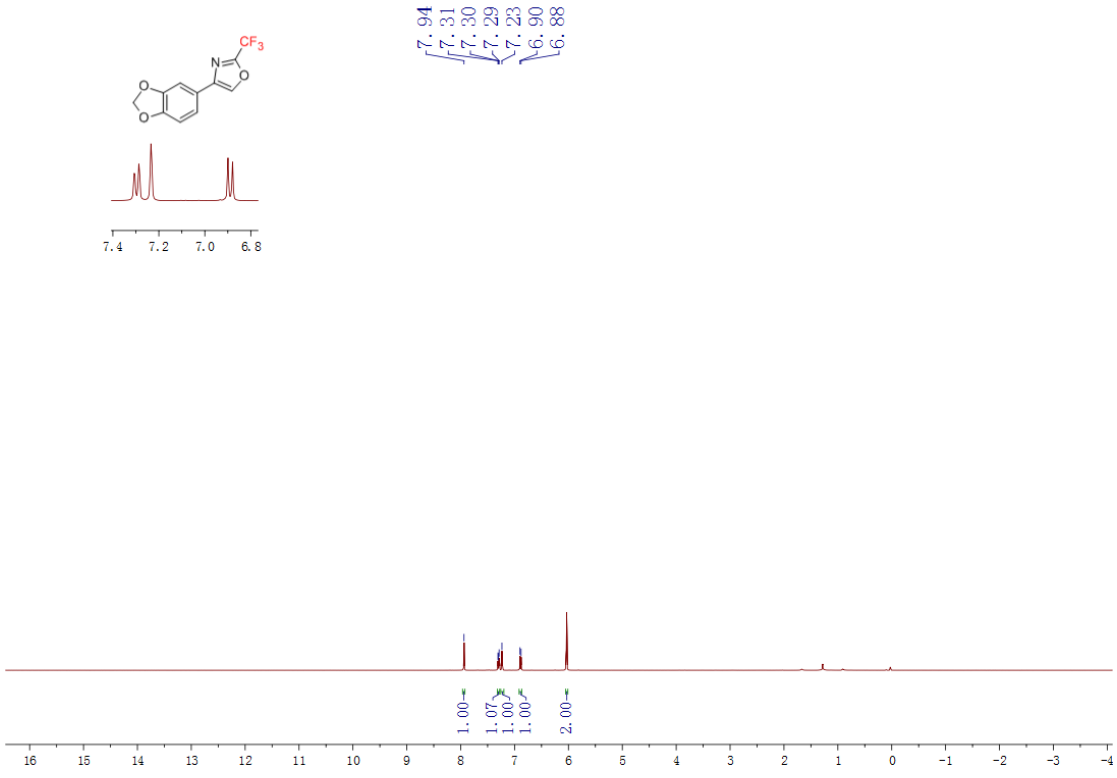
^{13}C NMR spectrum of **3p** in $CDCl_3$



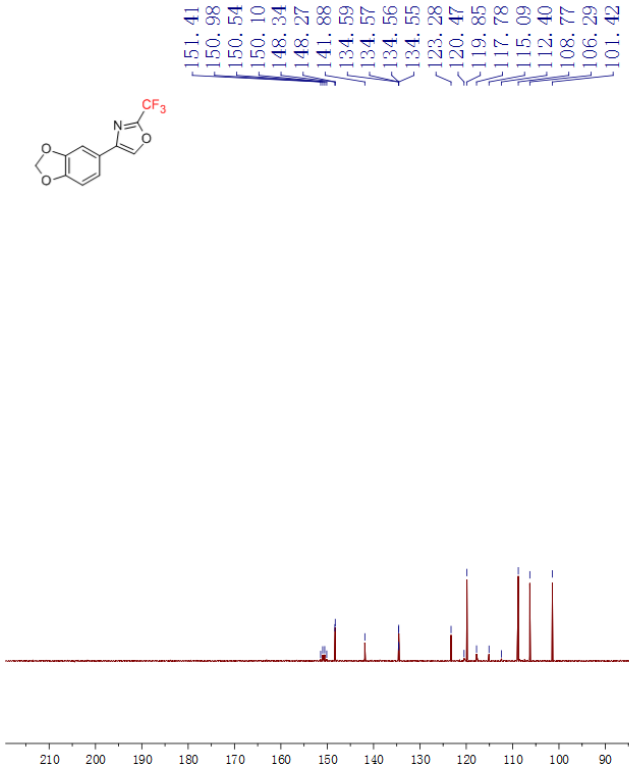
^{19}F NMR spectrum of **3q** in $CDCl_3$



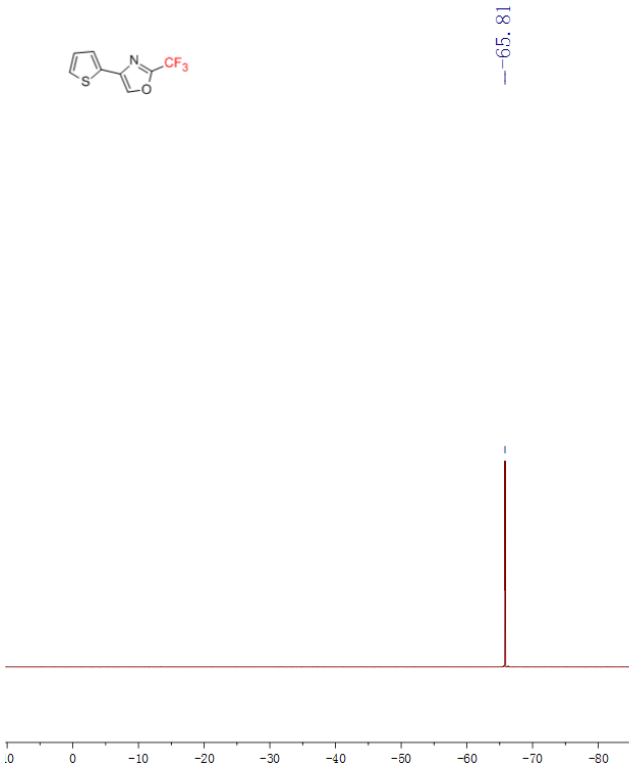
^{1}H NMR spectrum of **3q** in $CDCl_3$



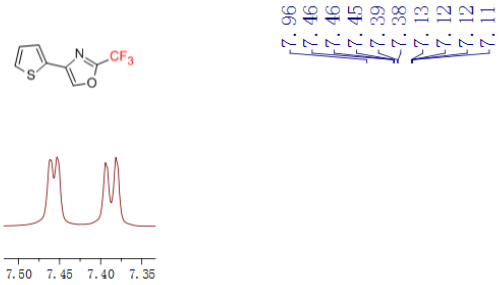
^{13}C NMR spectrum of **3q** in $CDCl_3$

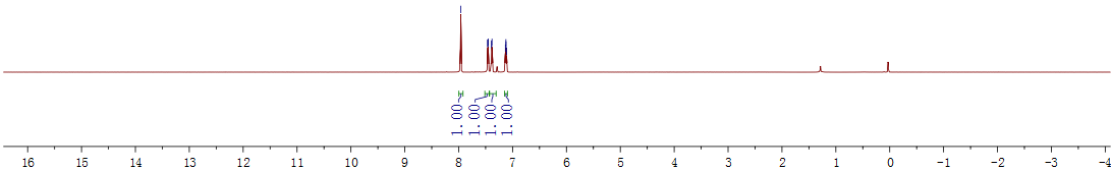


^{19}F NMR spectrum of **3r** in $CDCl_3$

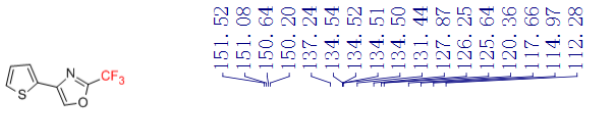


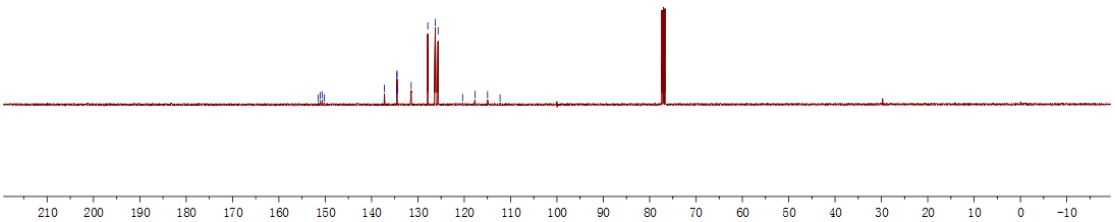
^{1}H NMR spectrum of **3r** in $CDCl_3$



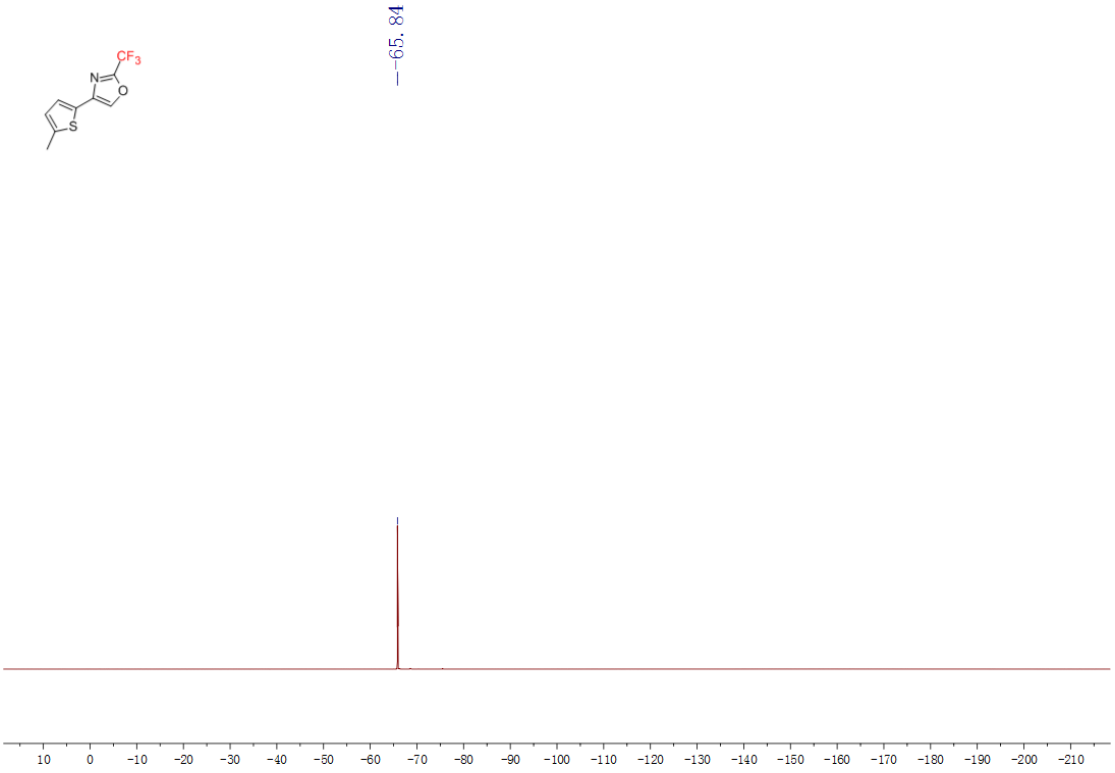


^{13}C NMR spectrum of **3r** in $CDCl_3$

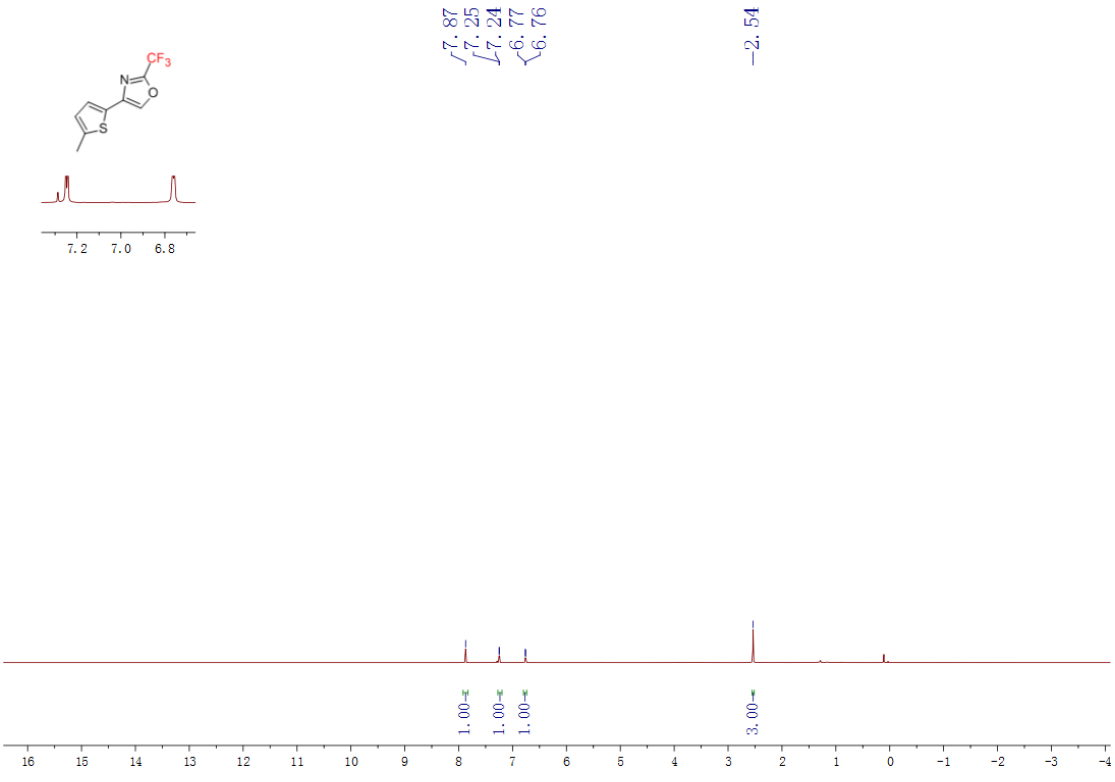




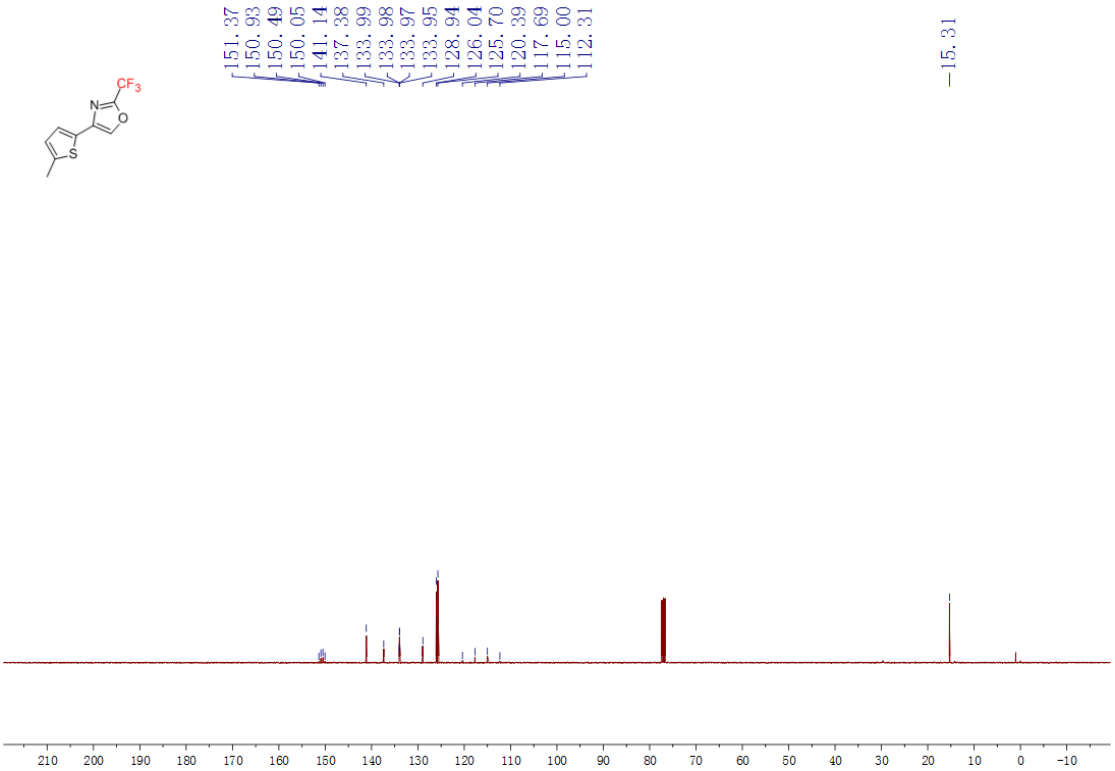
^{19}F NMR spectrum of **3s** in $CDCl_3$



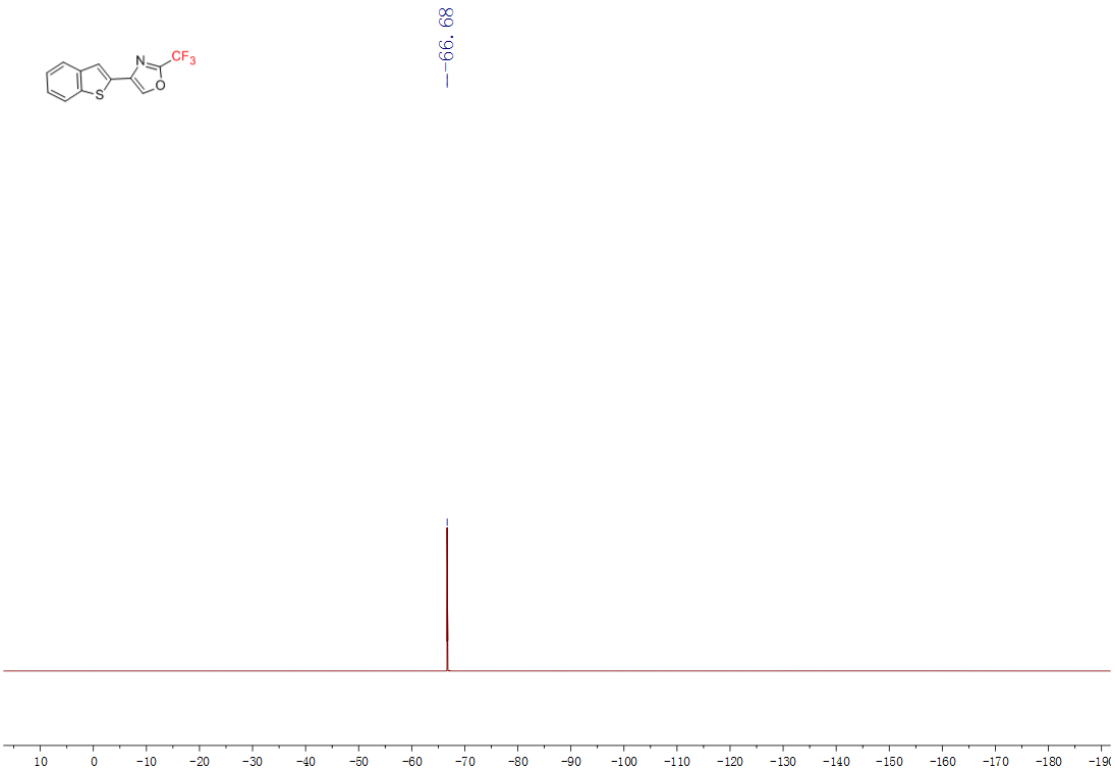
^{1}H NMR spectrum of **3s** in $CDCl_3$



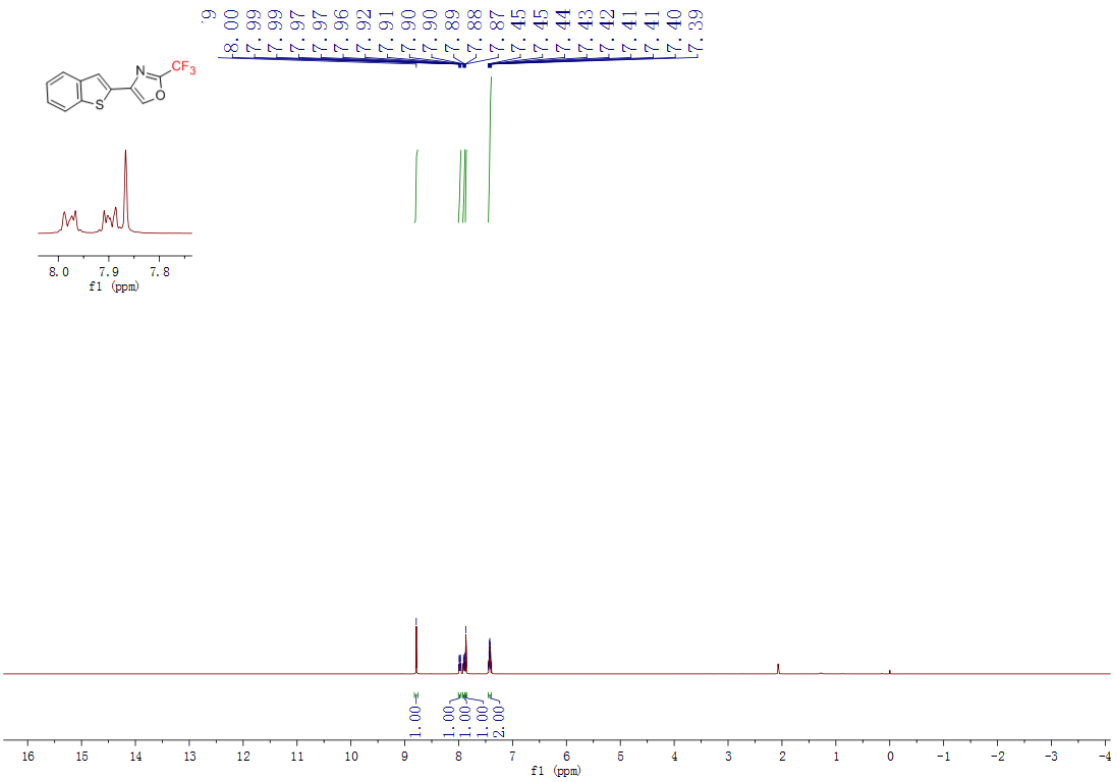
^{13}C NMR spectrum of **3s** in $CDCl_3$



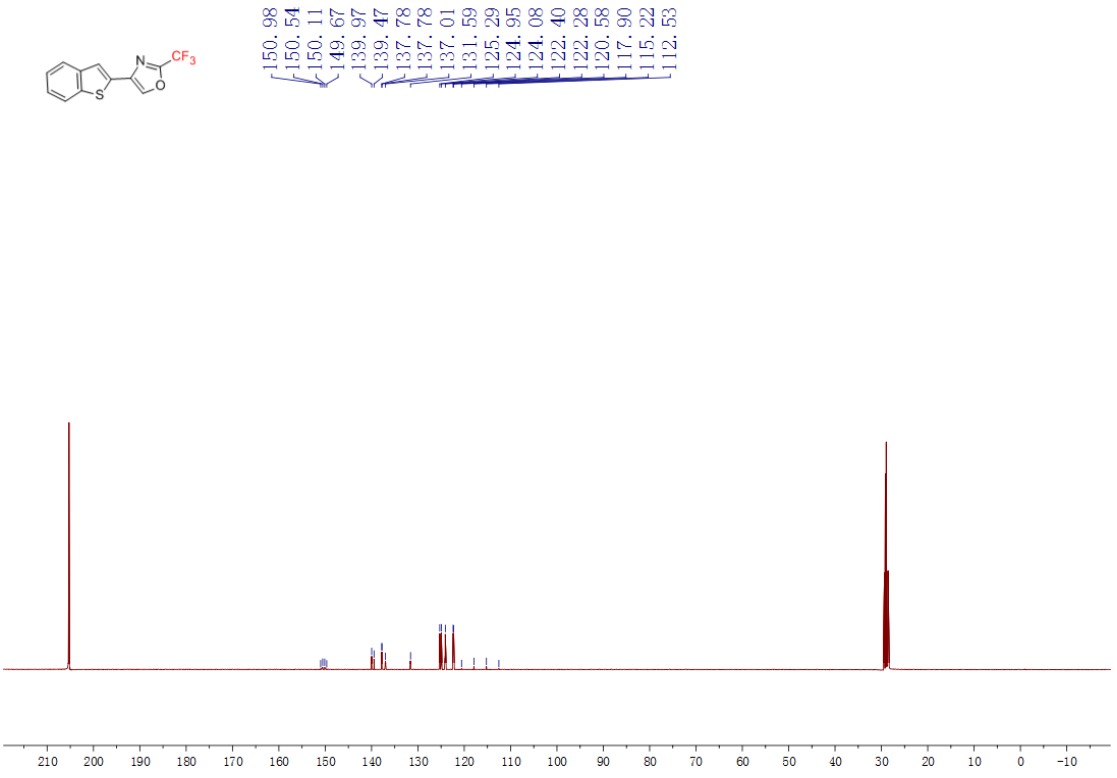
^{19}F NMR spectrum of **3t** in acetone-d_6



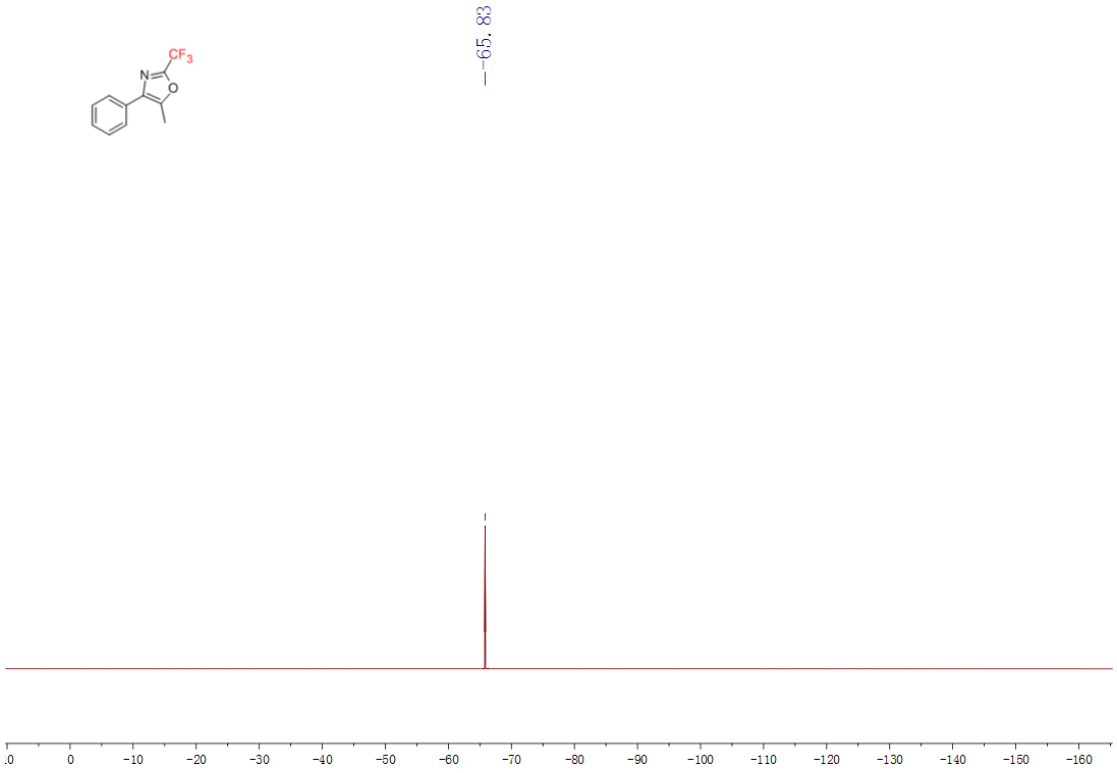
^{1}H NMR spectrum of **3t** in acetone-d_6



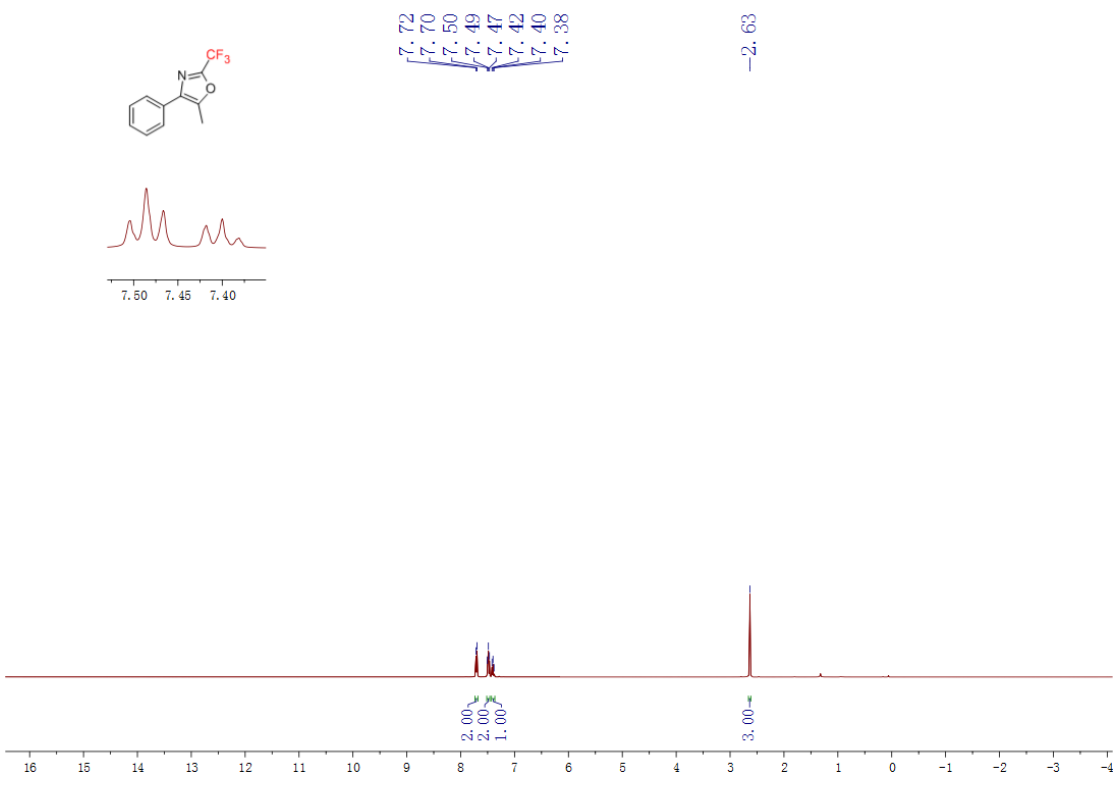
^{13}C NMR spectrum of **3t** in acetone-d_6



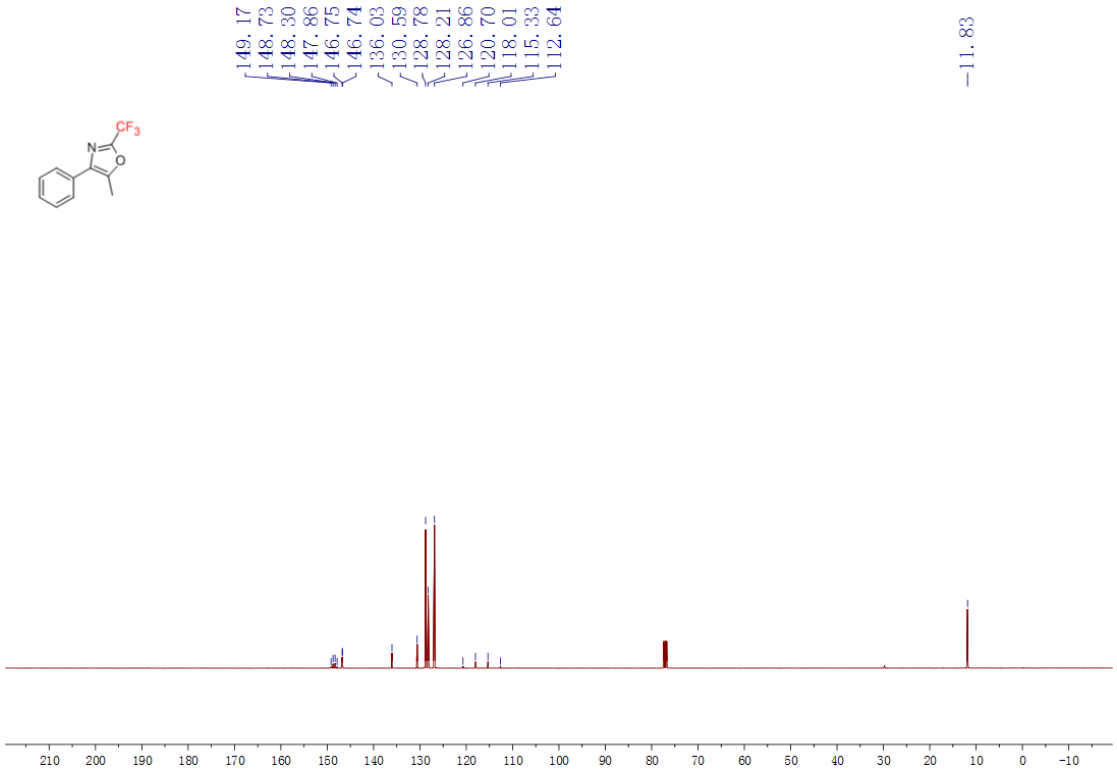
^{19}F NMR spectrum of **3u** in $CDCl_3$



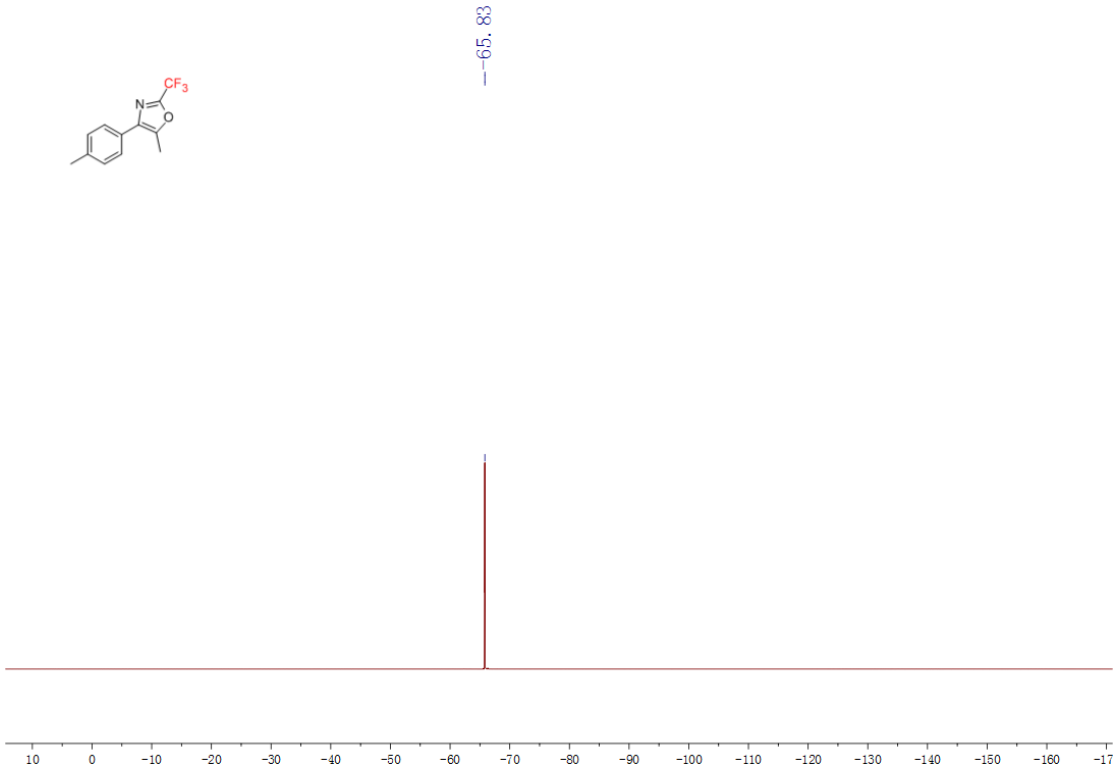
^{1}H NMR spectrum of **3u** in $CDCl_3$



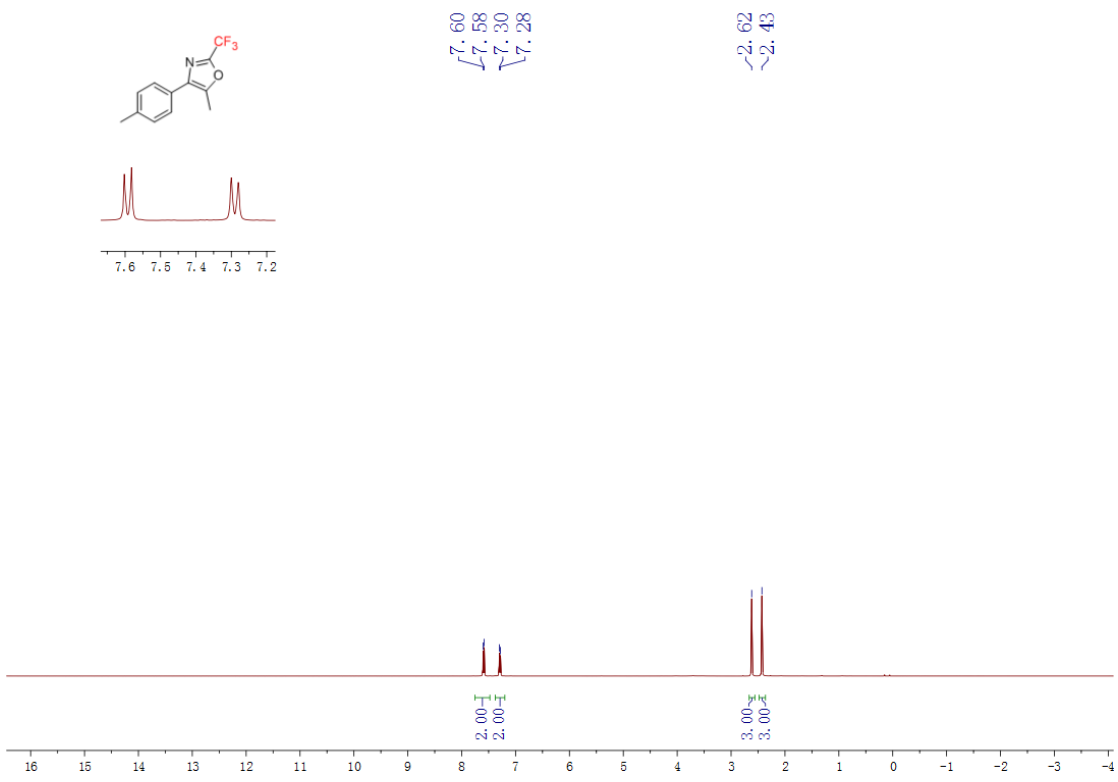
^{13}C NMR spectrum of **3u** in $CDCl_3$



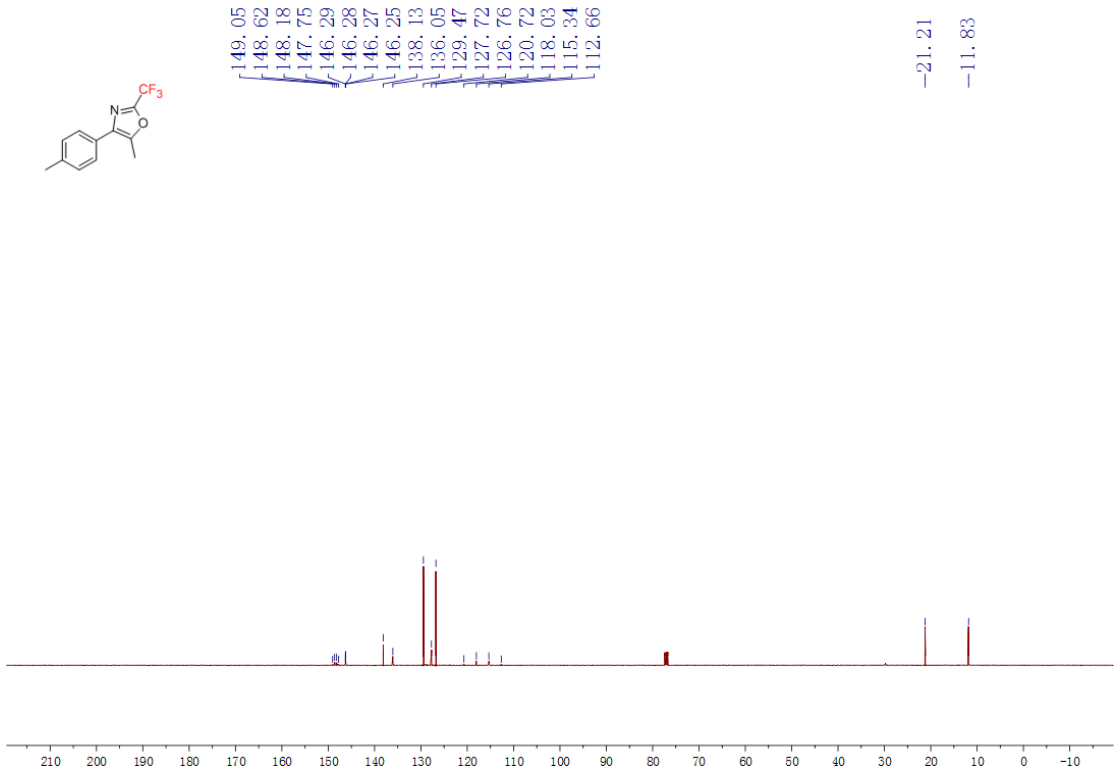
^{19}F NMR spectrum of **3v** in $CDCl_3$



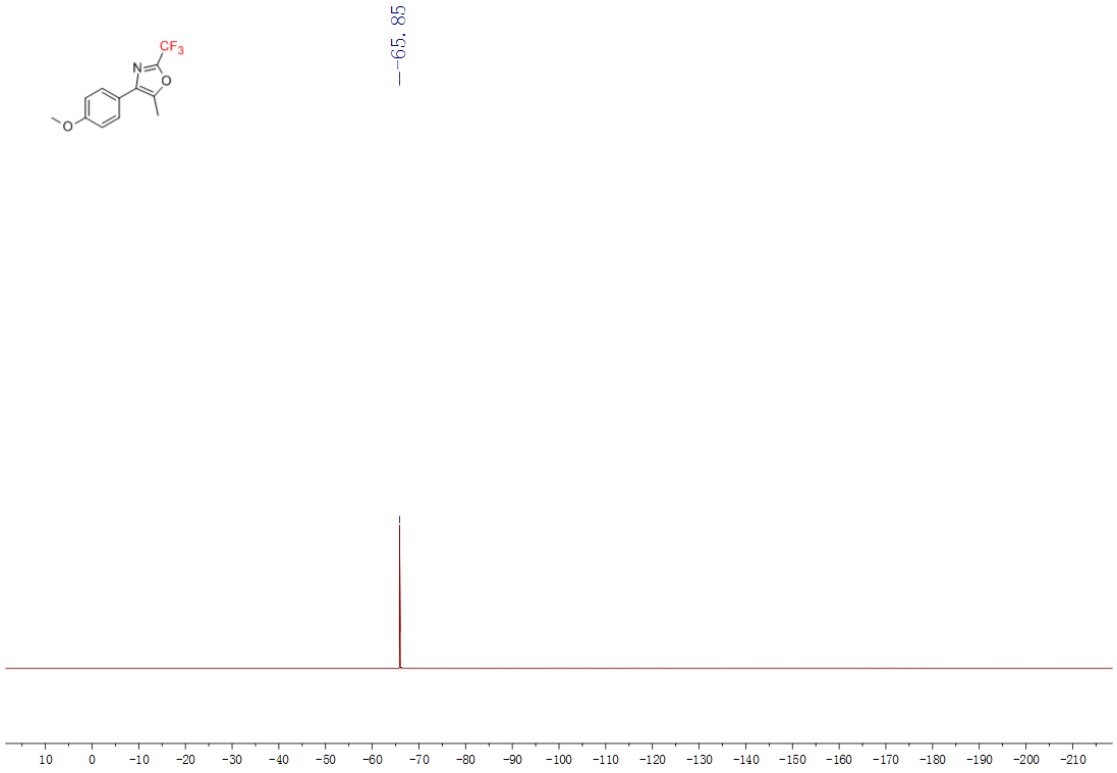
^{1}H NMR spectrum of **3v** in $CDCl_3$



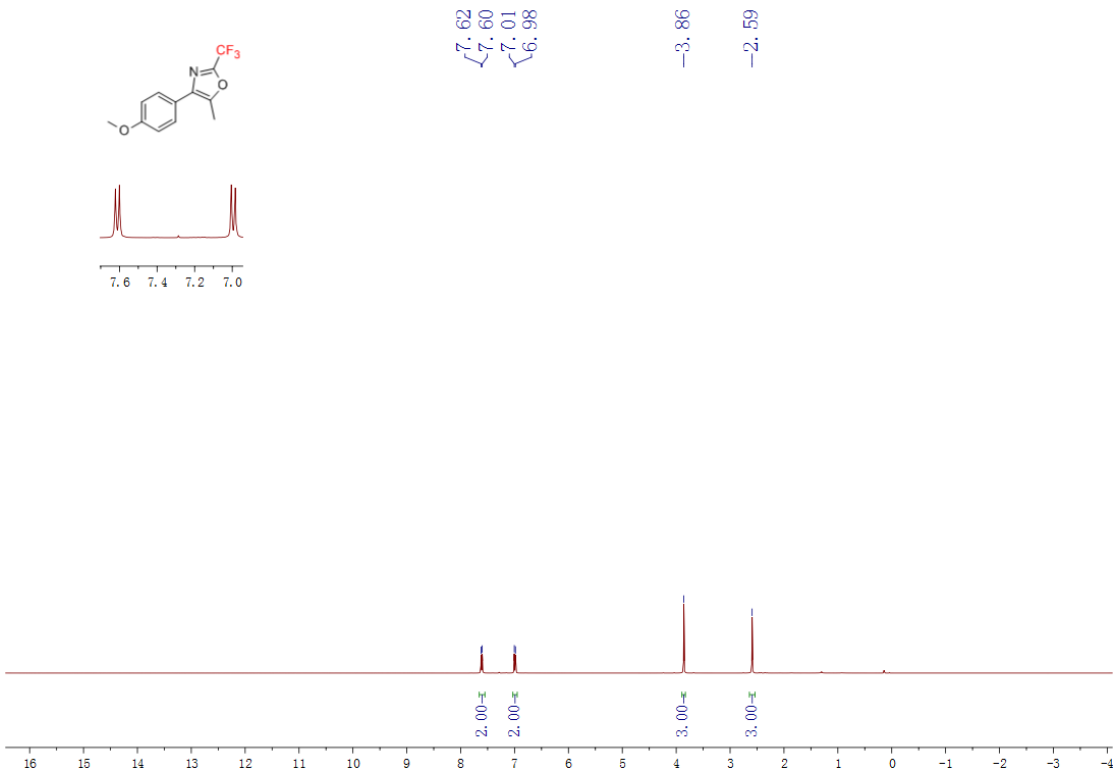
^{13}C NMR spectrum of **3v** in $CDCl_3$



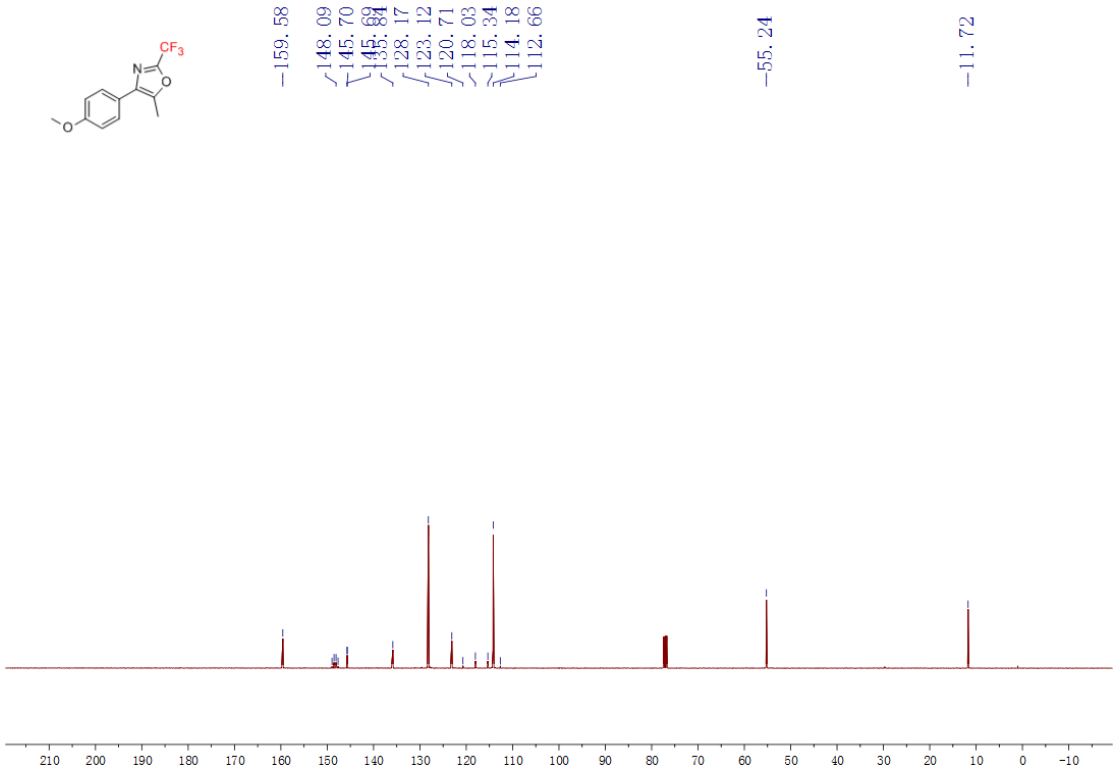
^{19}F NMR spectrum of **3w** in $CDCl_3$



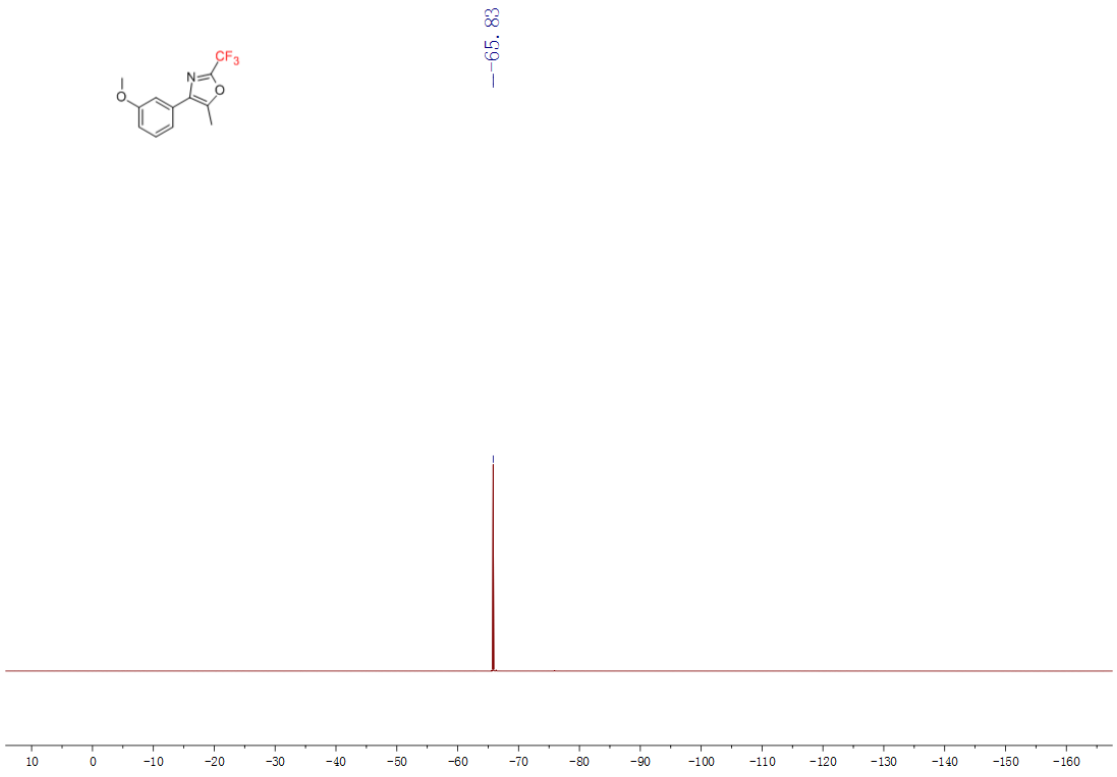
^{1}H NMR spectrum of **3w** in $CDCl_3$



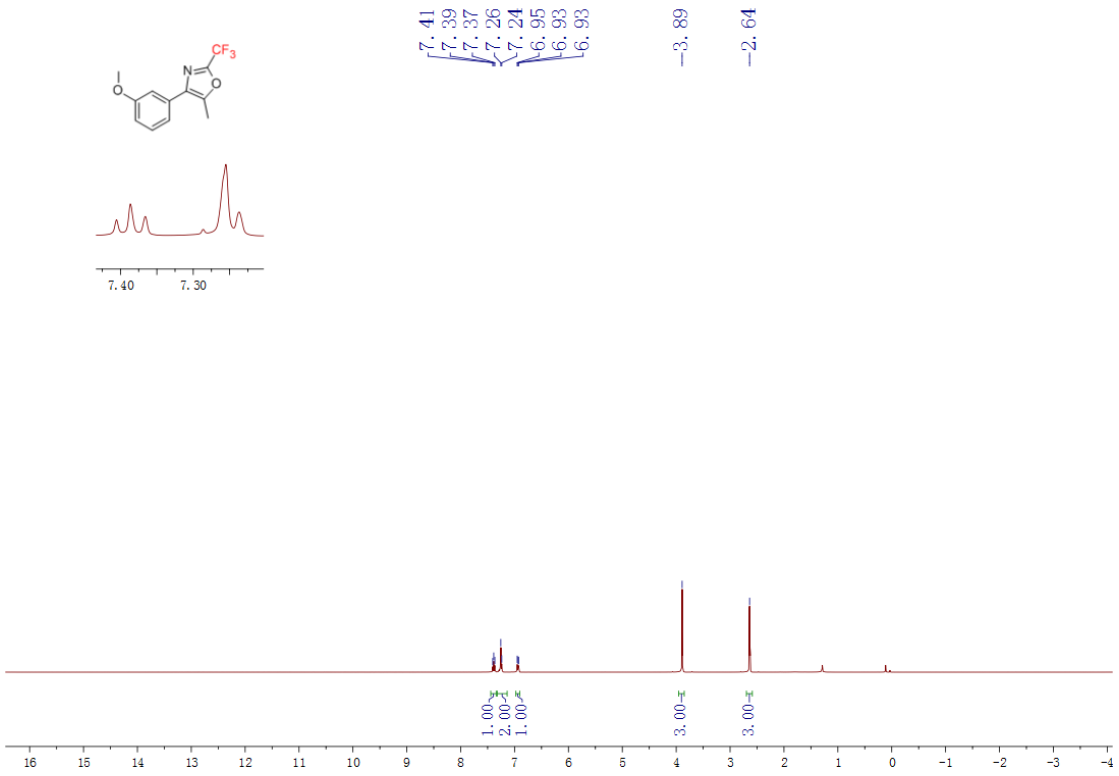
^{13}C NMR spectrum of **3w** in $CDCl_3$



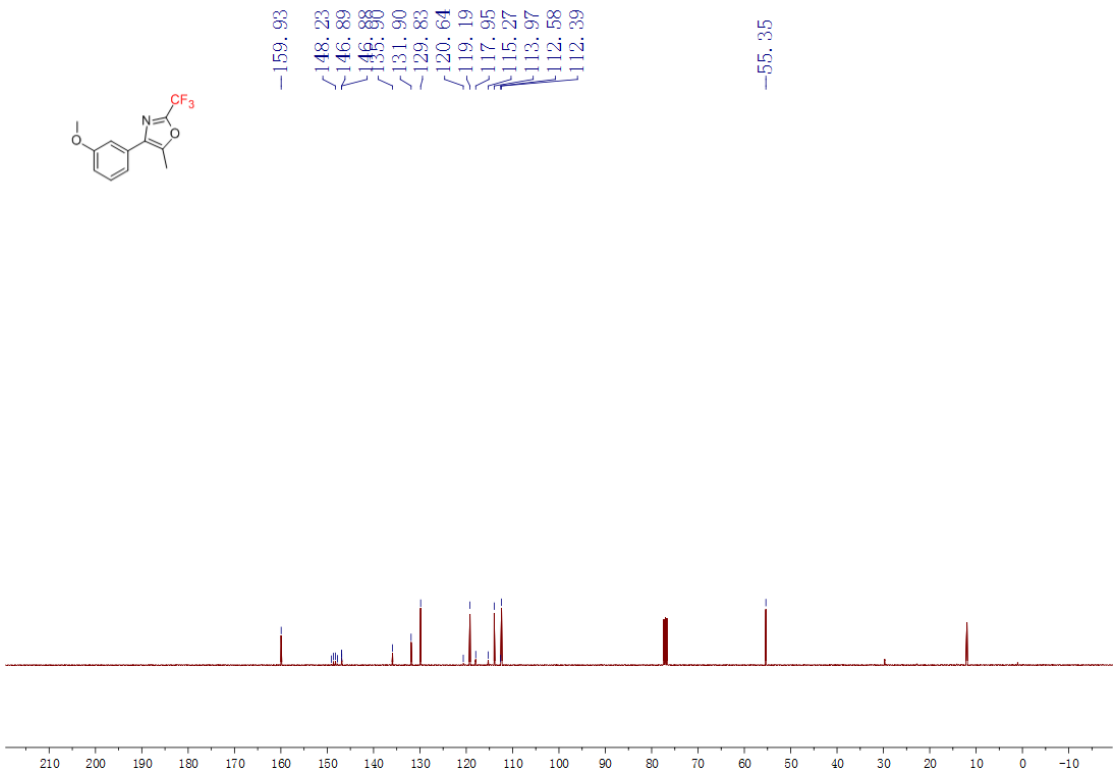
^{19}F NMR spectrum of **3x** in $CDCl_3$



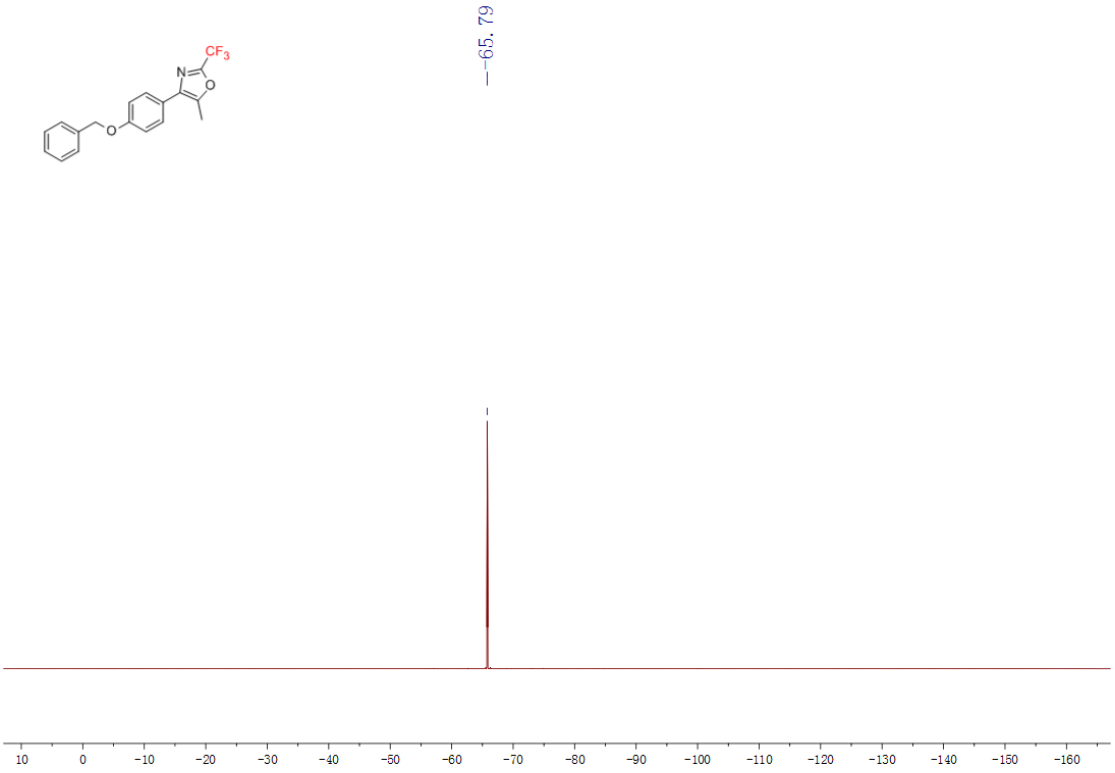
^{1}H NMR spectrum of **3x** in $CDCl_3$



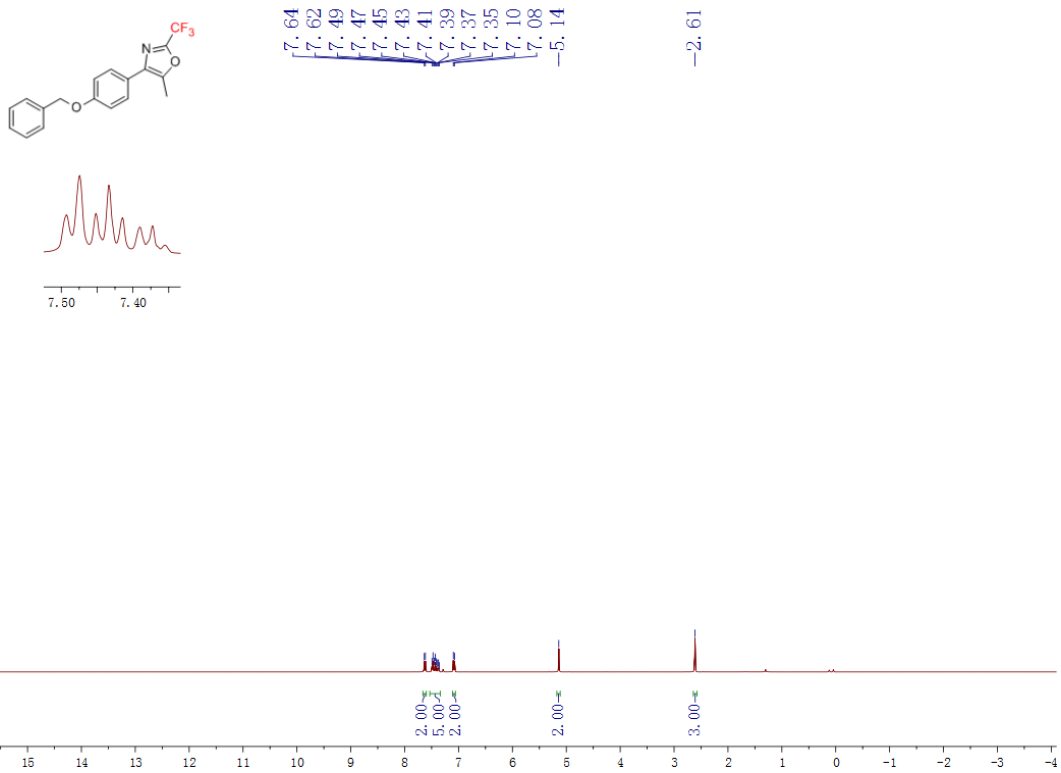
^{13}C NMR spectrum of **3x** in $CDCl_3$



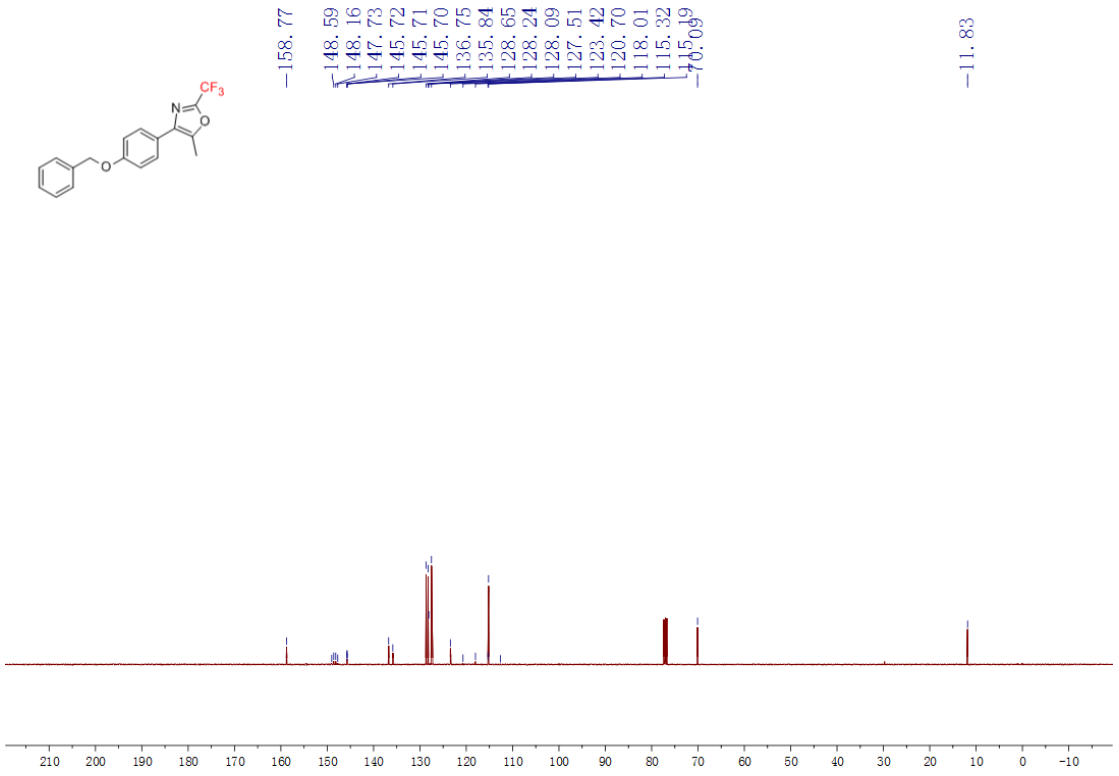
^{19}F NMR spectrum of **3y** in $CDCl_3$



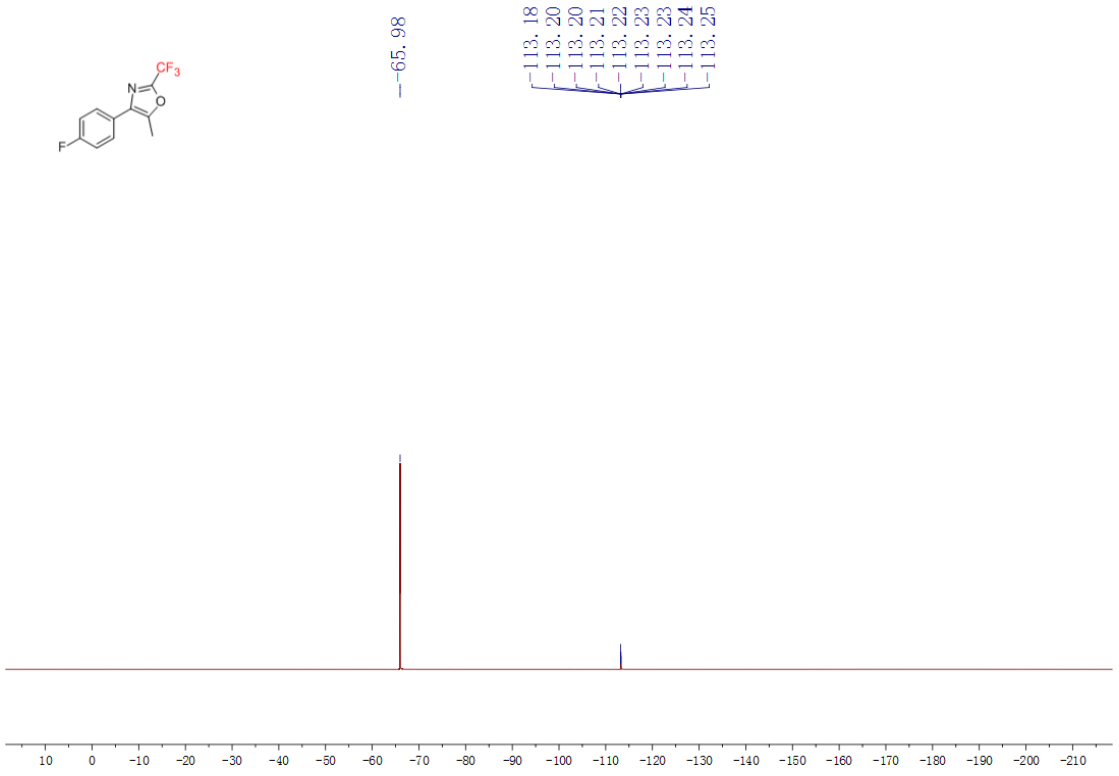
^{1}H NMR spectrum of **3y** in $CDCl_3$



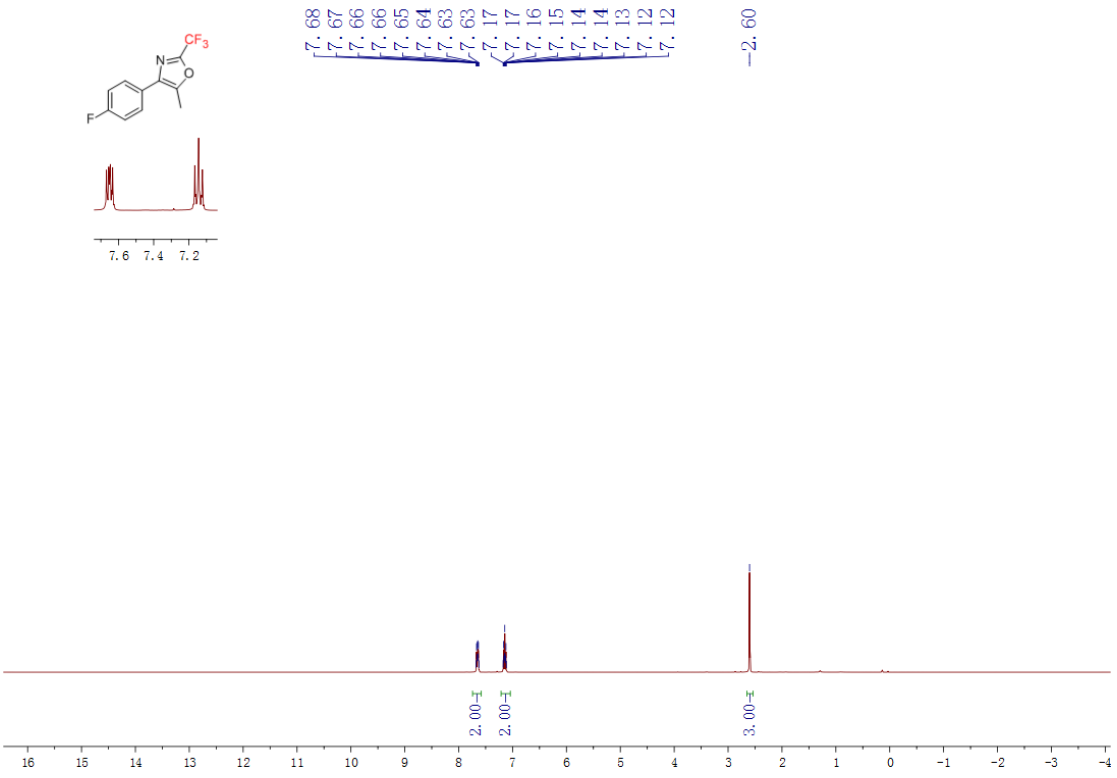
^{13}C NMR spectrum of **3y** in $CDCl_3$



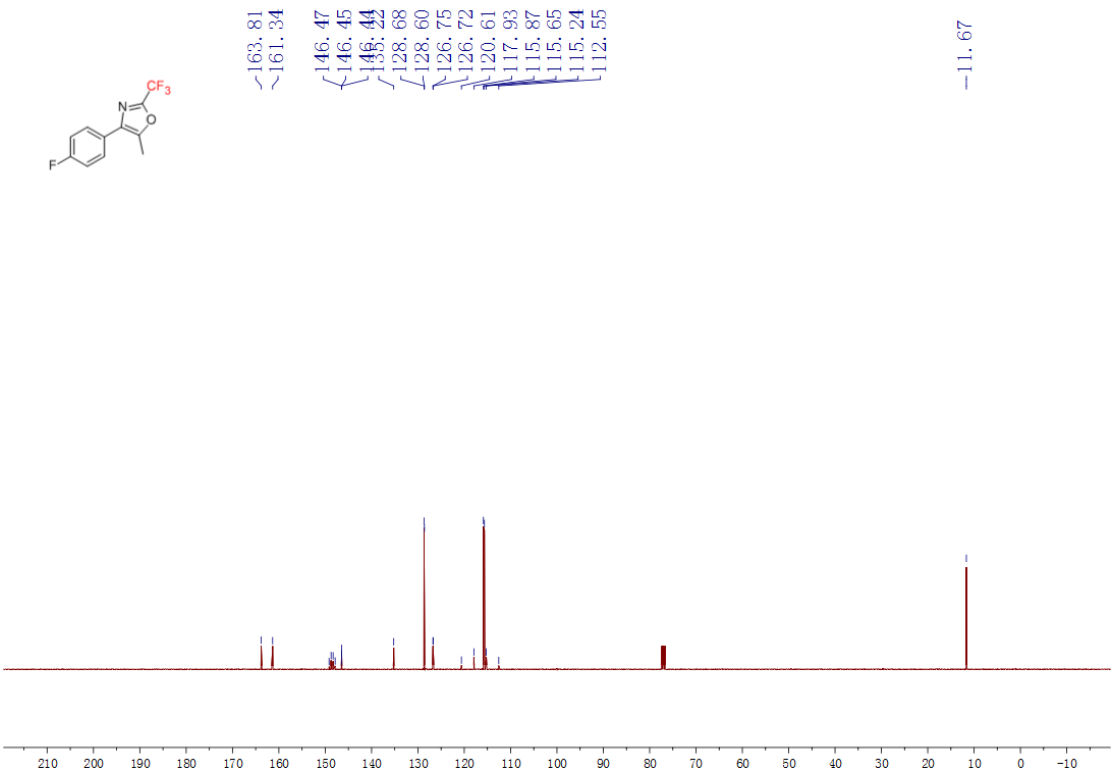
^{19}F NMR spectrum of **3z** in $CDCl_3$



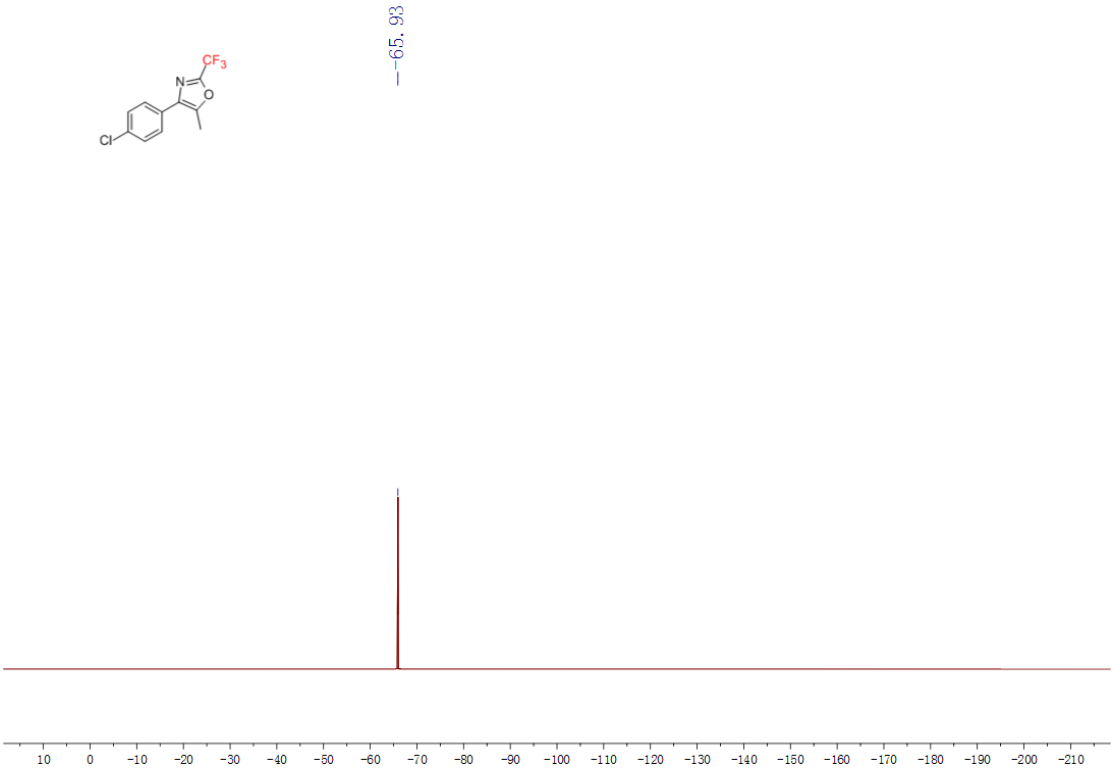
^{1}H NMR spectrum of **3z** in $CDCl_3$



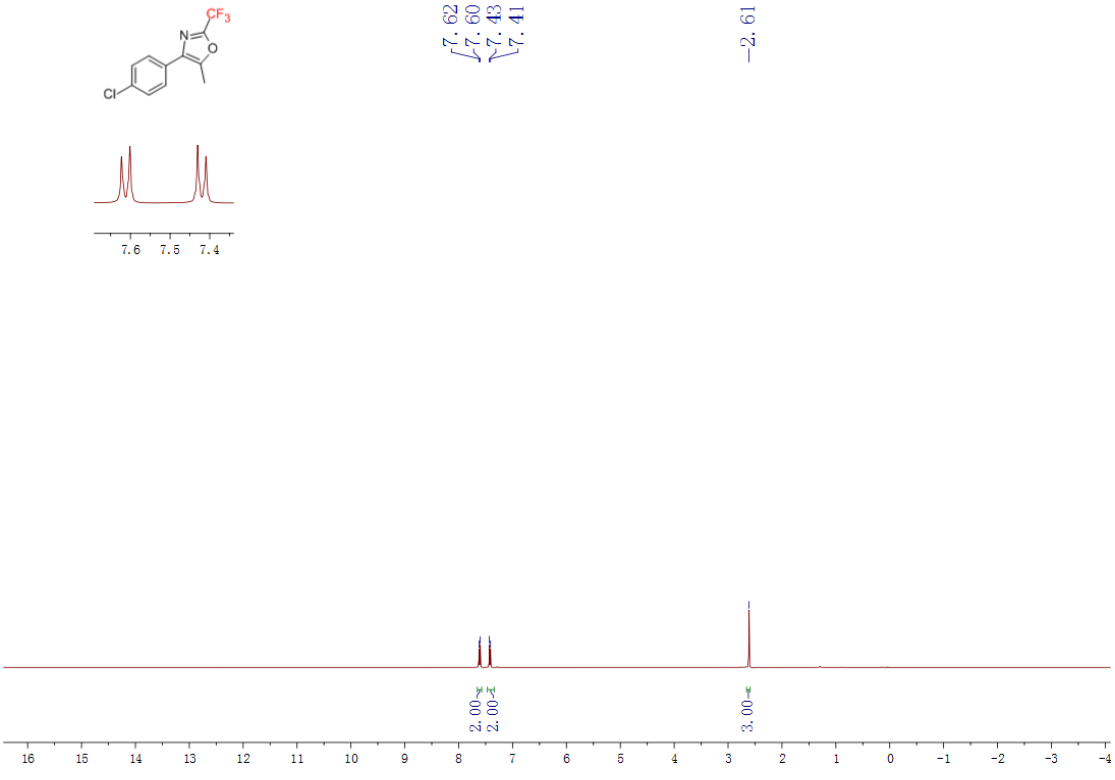
^{13}C NMR spectrum of **3z** in $CDCl_3$



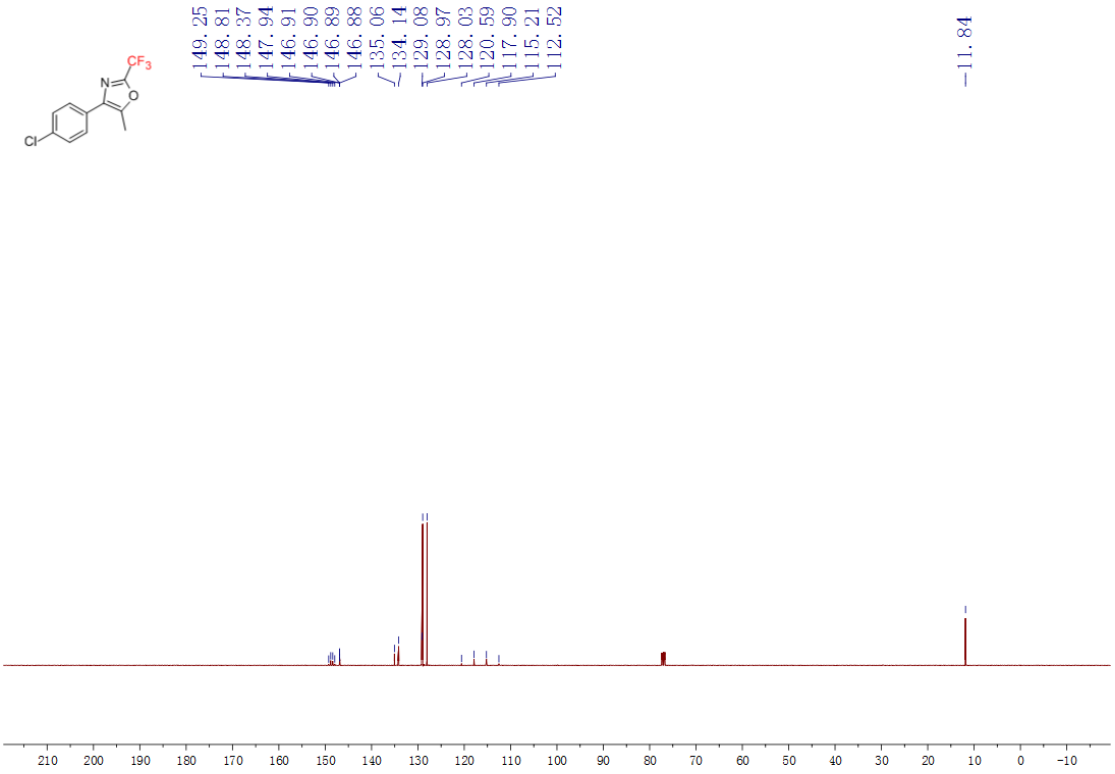
^{19}F NMR spectrum of **3aa** in $CDCl_3$



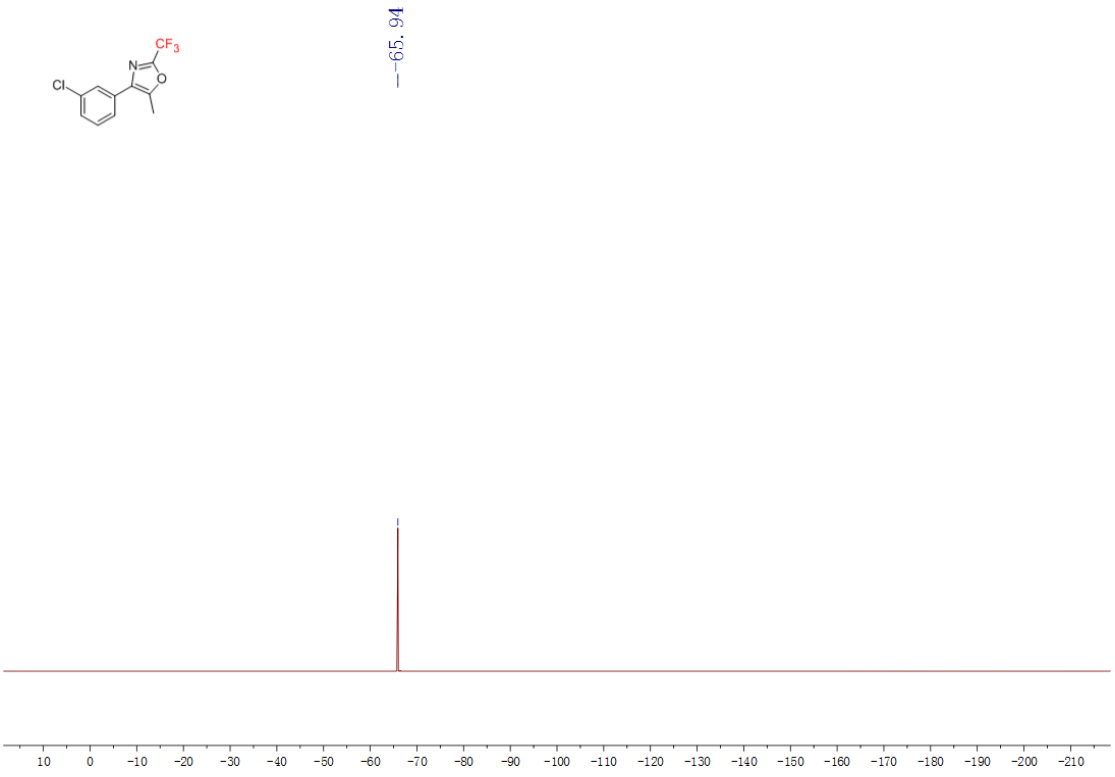
^{1}H NMR spectrum of **3aa** in $CDCl_3$



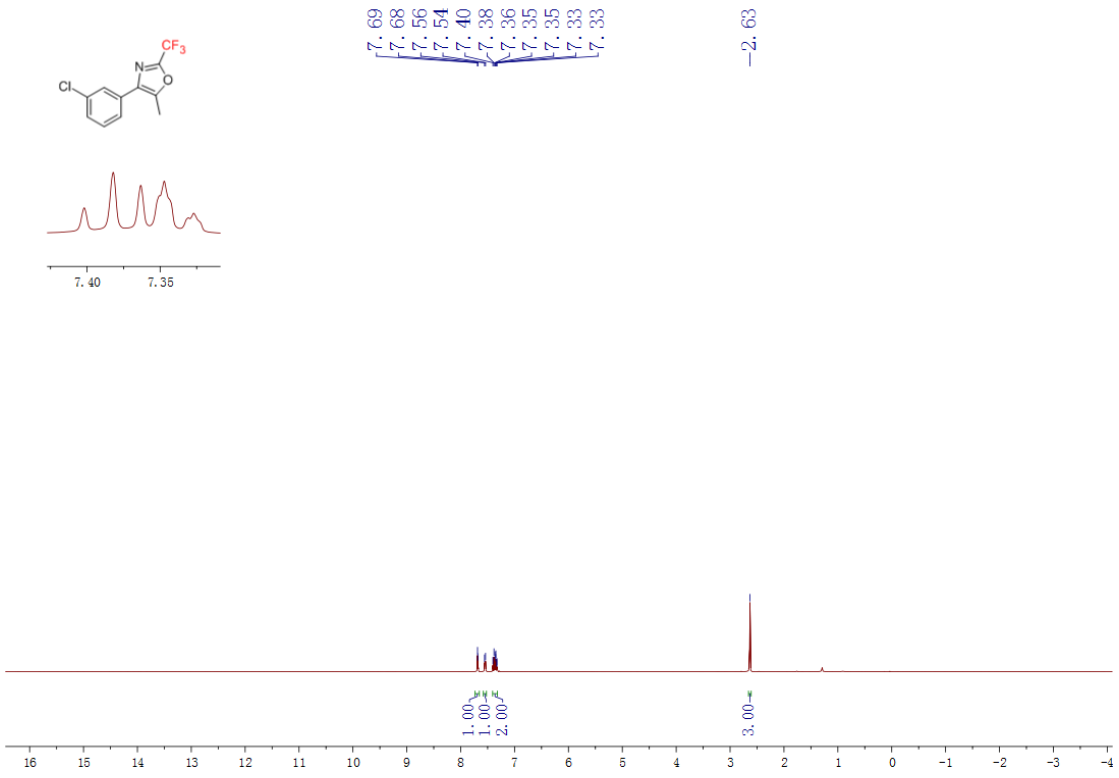
^{13}C NMR spectrum of **3aa** in $CDCl_3$



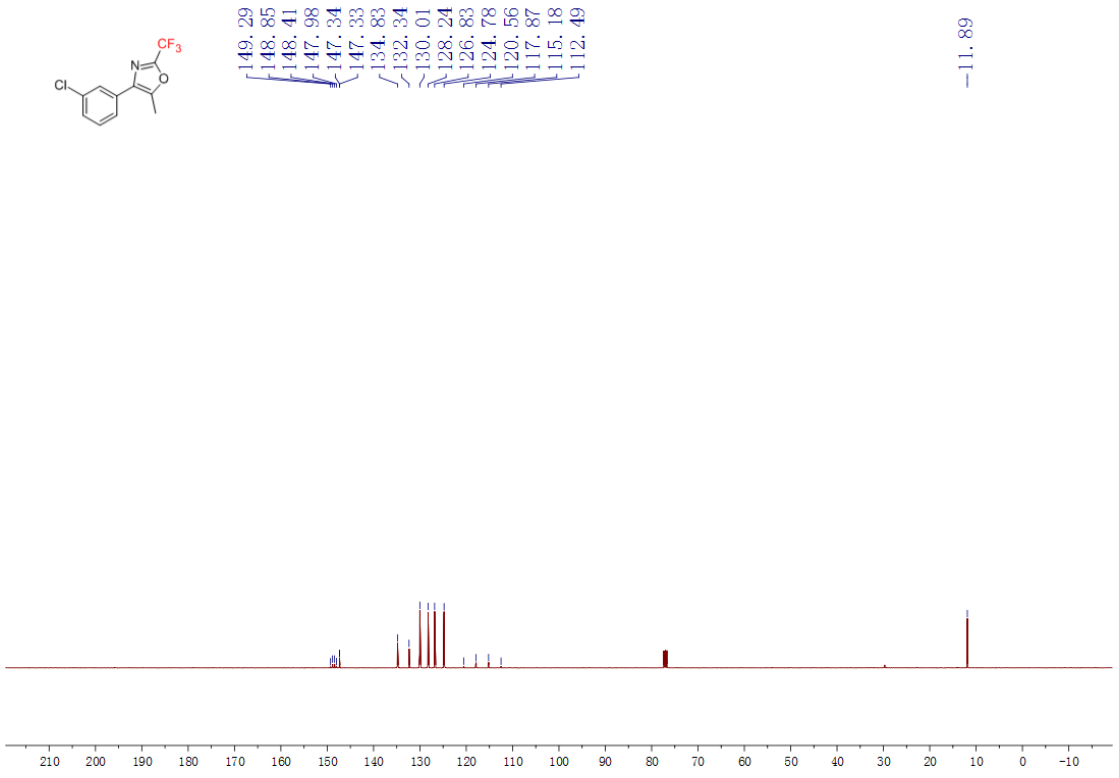
^{19}F NMR spectrum of **3ab** in $CDCl_3$



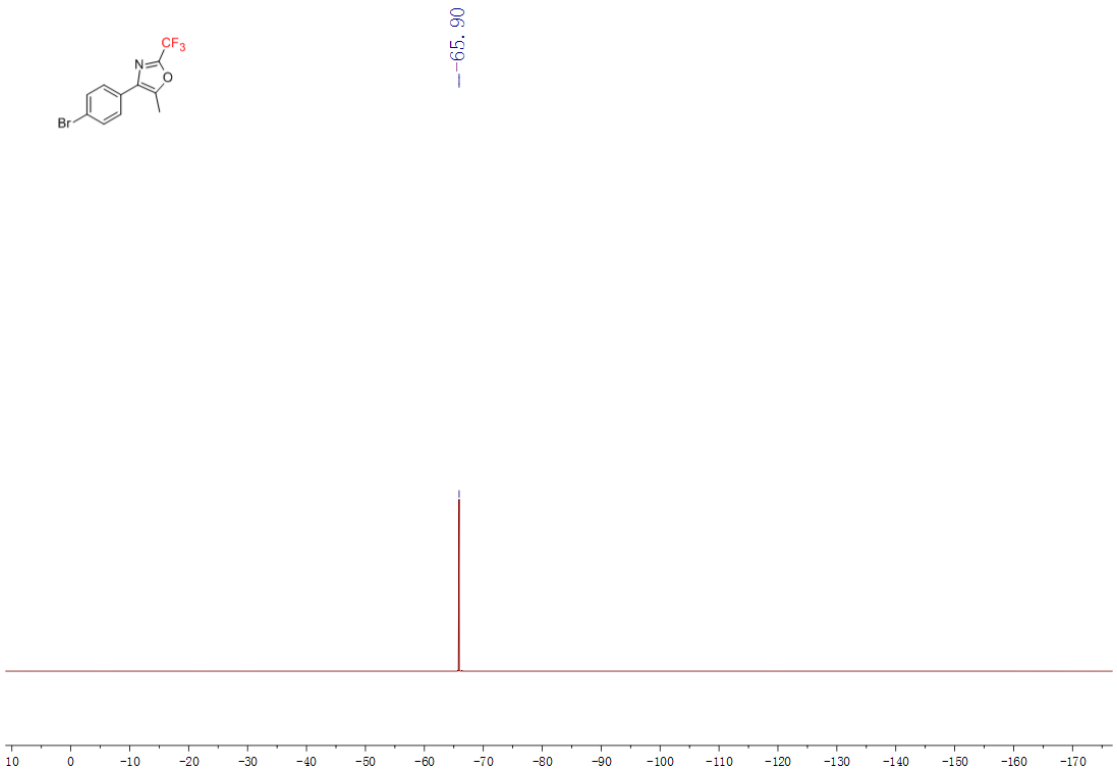
^{1}H NMR spectrum of **3ab** in $CDCl_3$



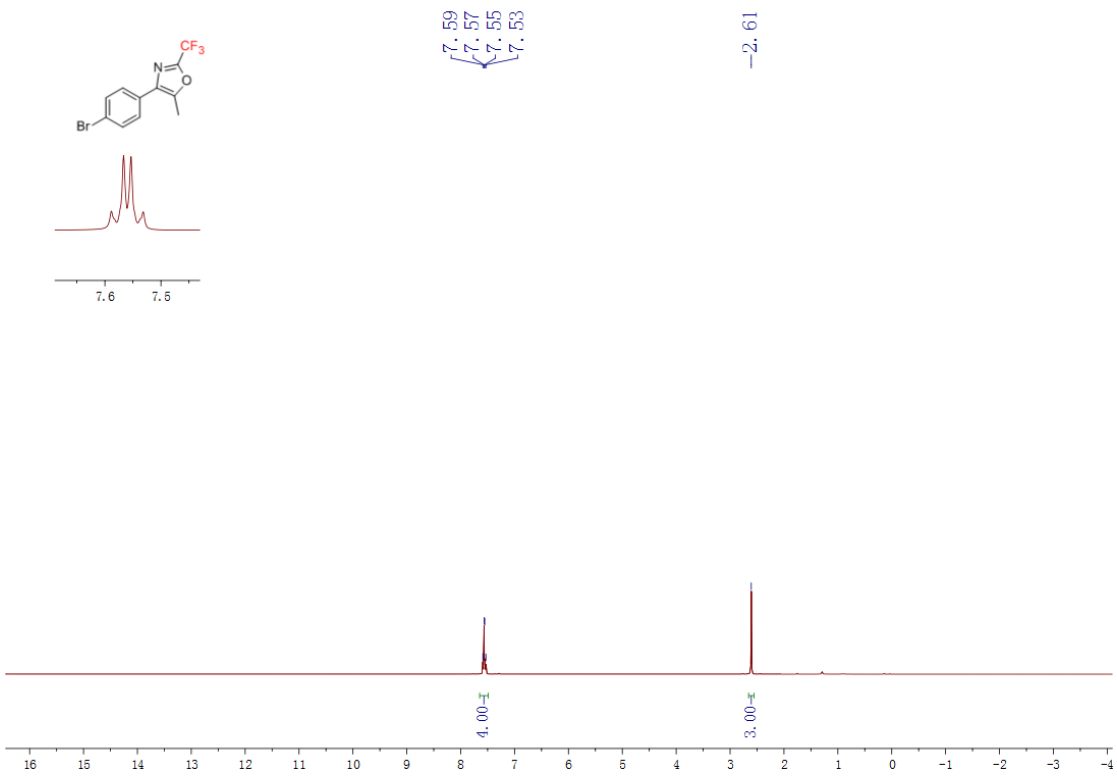
^{13}C NMR spectrum of **3ab** in $CDCl_3$



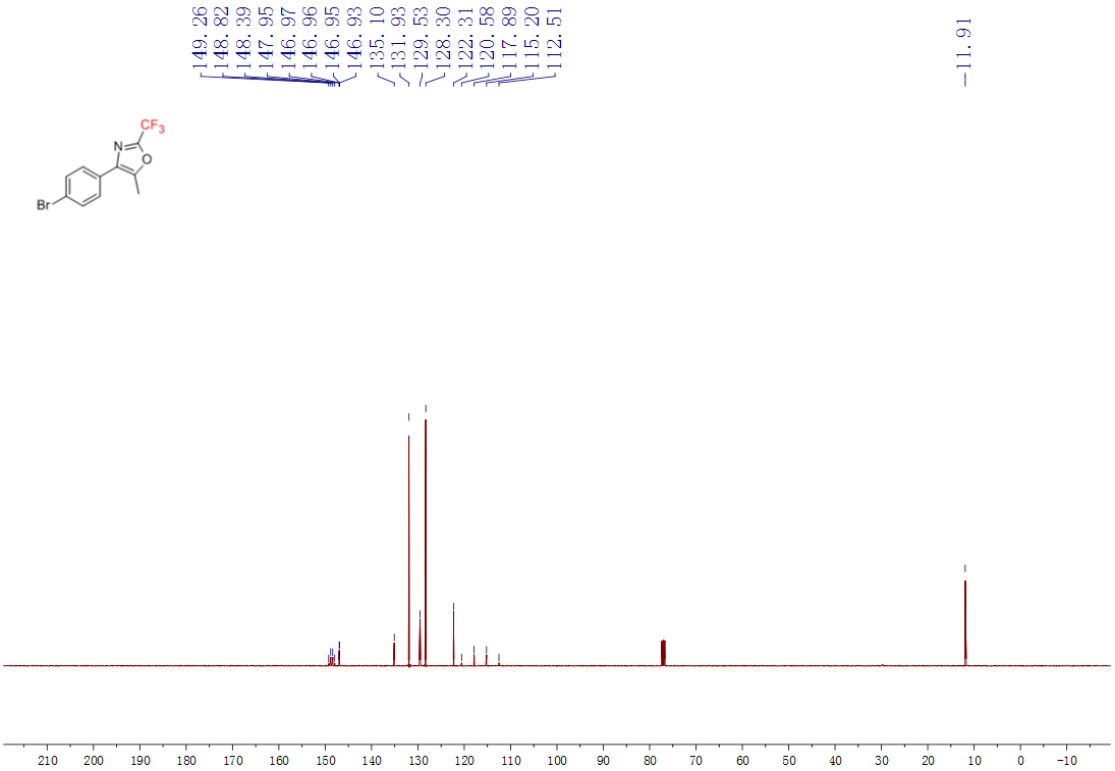
^{19}F NMR spectrum of **3ac** in $CDCl_3$



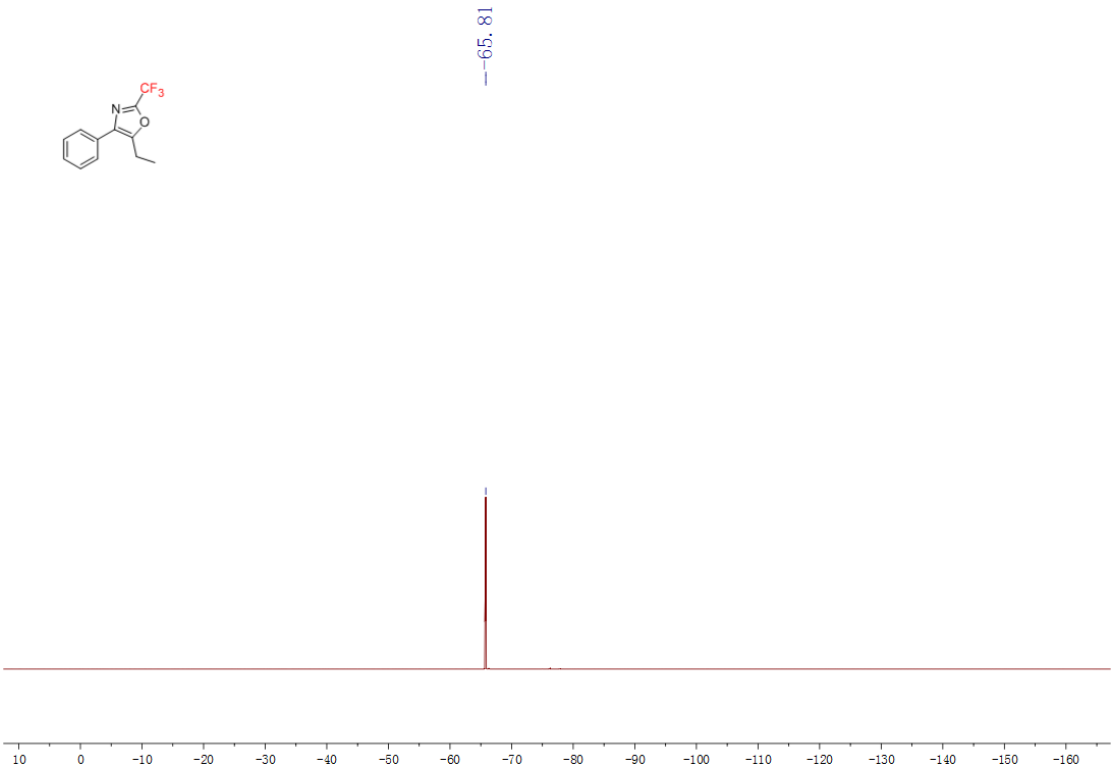
^{1}H NMR spectrum of **3ac** in $CDCl_3$



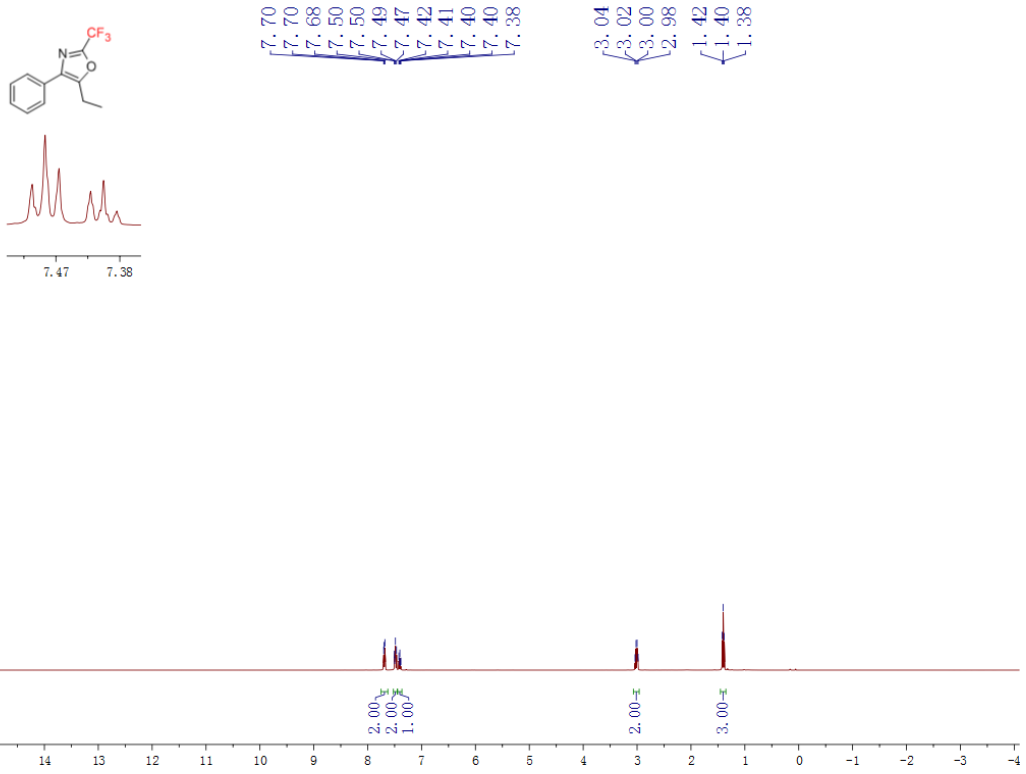
^{13}C NMR spectrum of **3ac** in $CDCl_3$



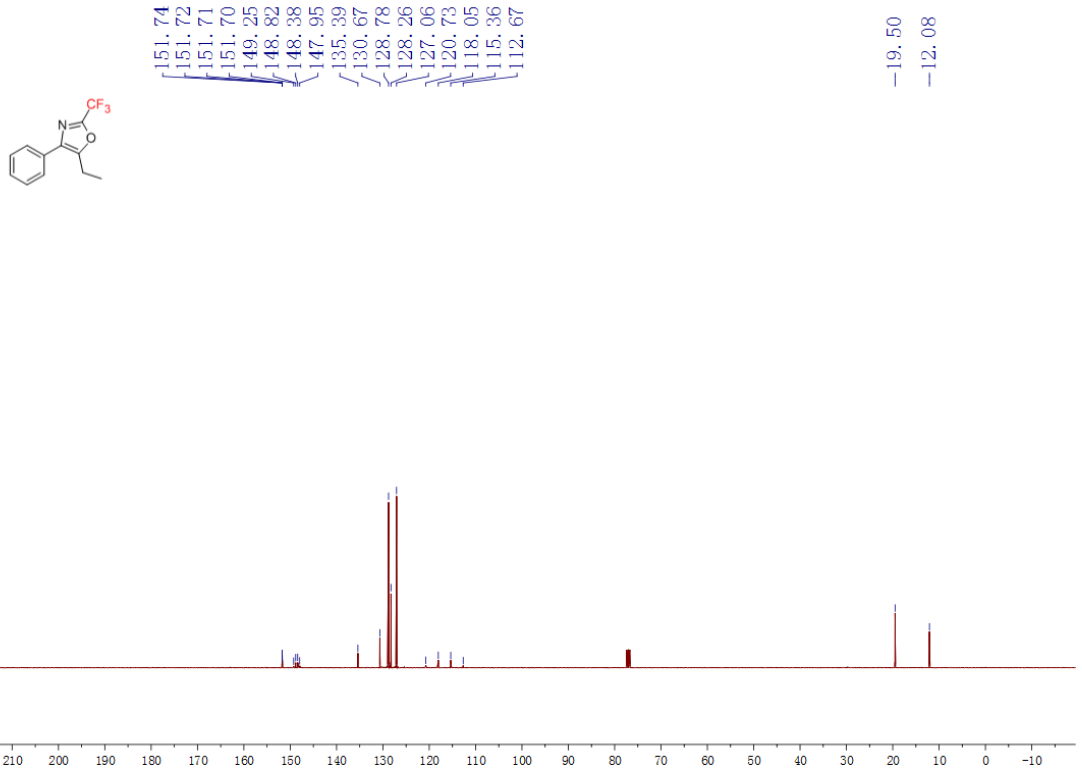
^{19}F NMR spectrum of compound **3ad** in $CDCl_3$



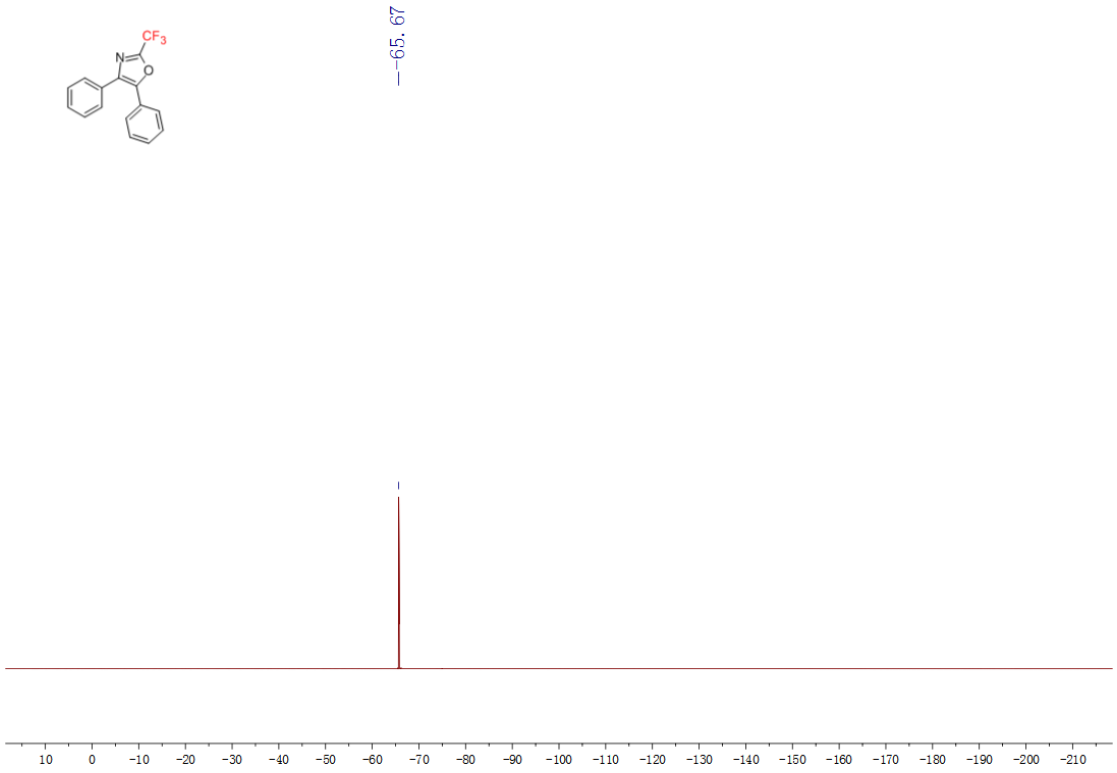
^{1}H NMR spectrum of compound **3ad** in $CDCl_3$



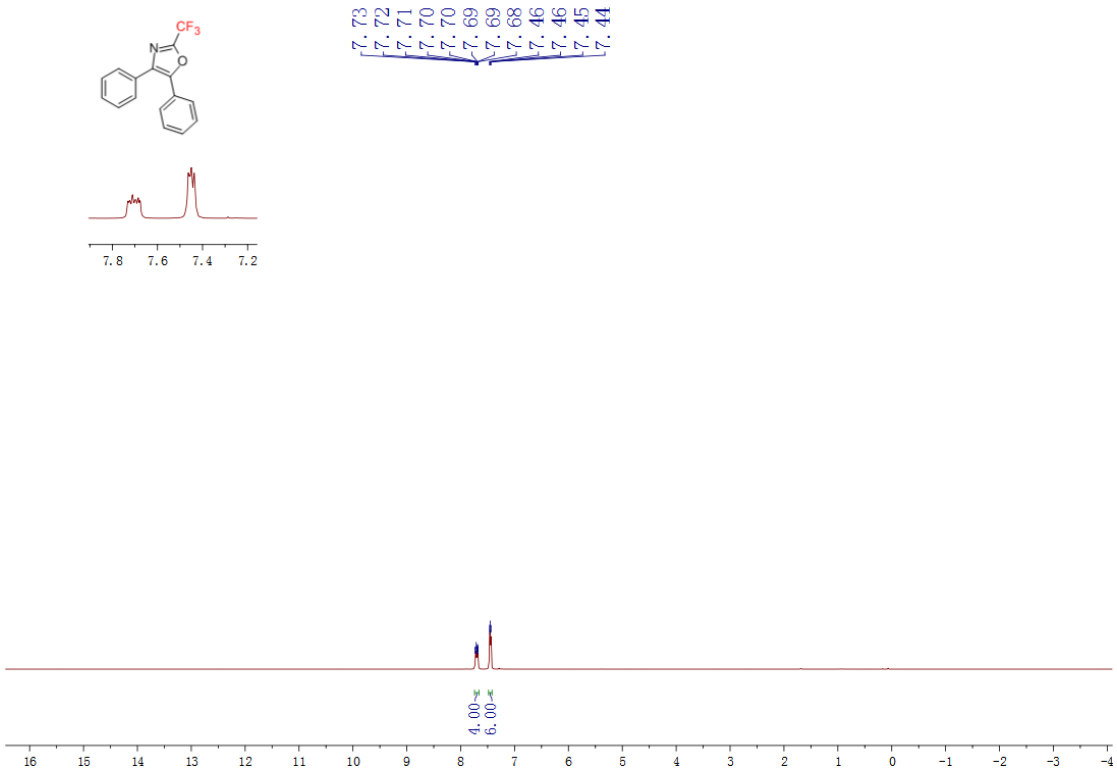
^{13}C NMR spectrum of compound **3ad** in $CDCl_3$



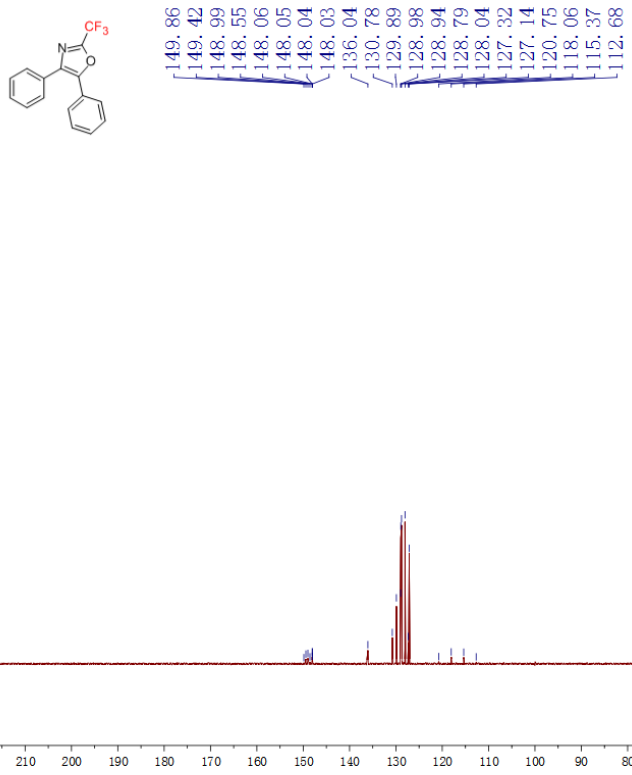
^{19}F NMR spectrum of compound **3ae** in $CDCl_3$



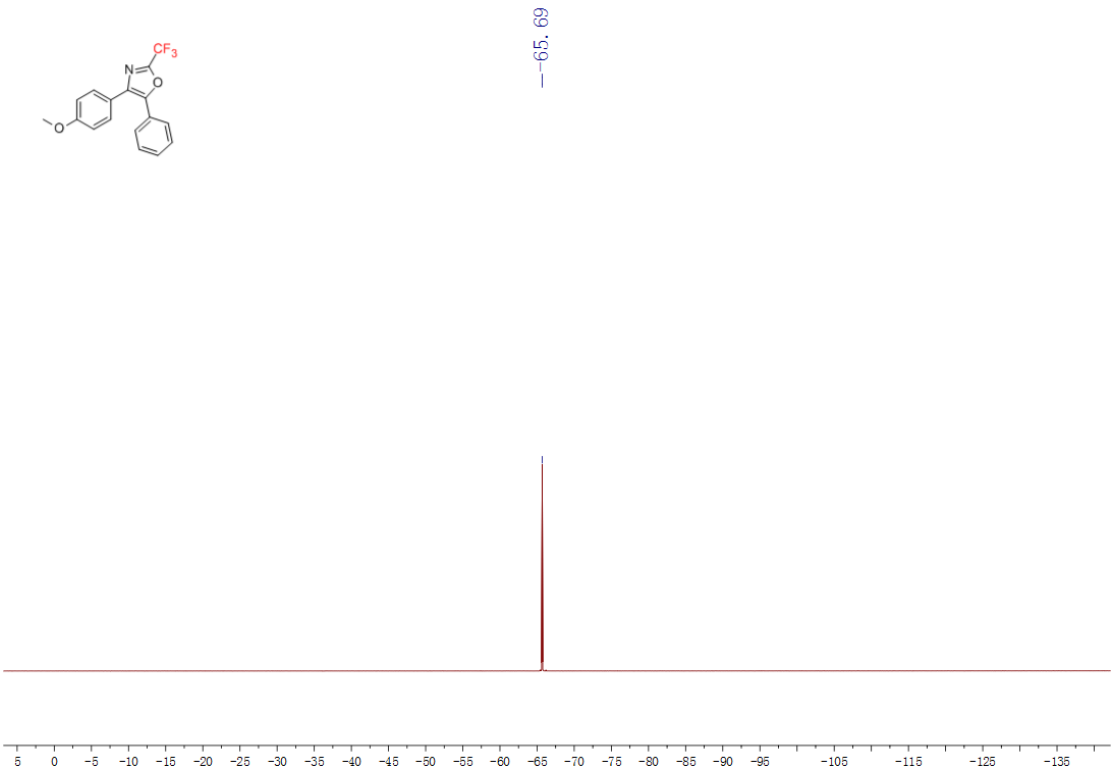
^{1}H NMR spectrum of compound **3ae** in $CDCl_3$



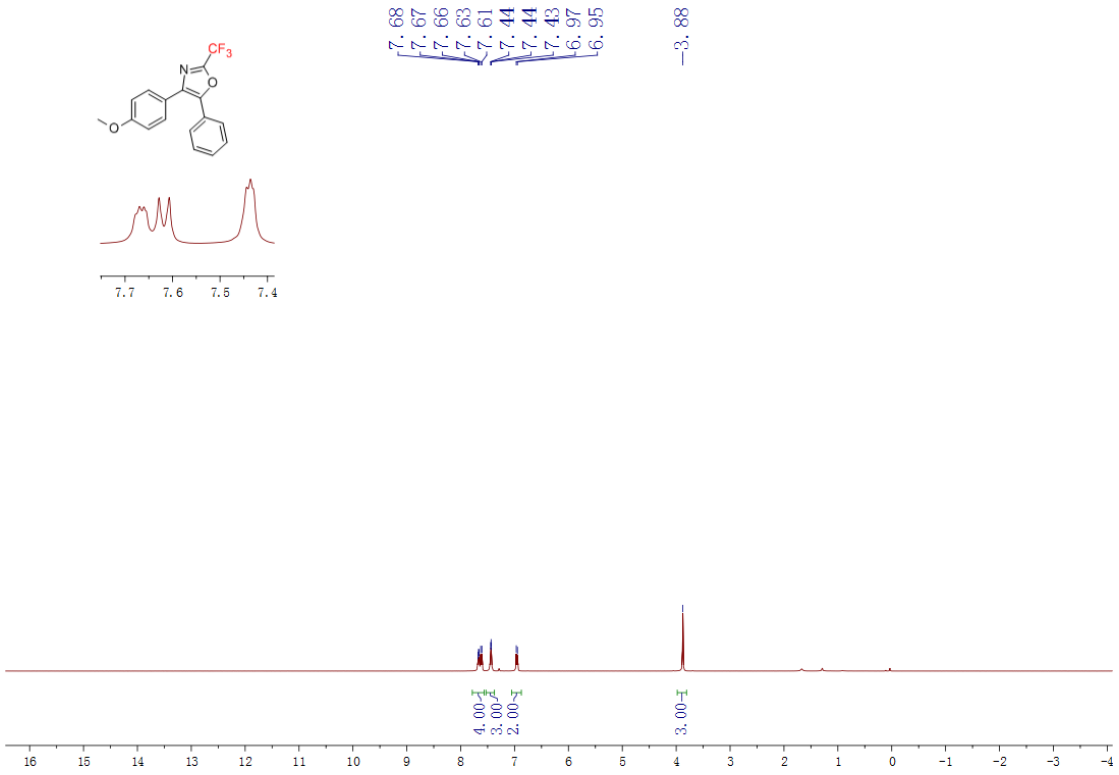
^{13}C NMR spectrum of compound **3ae** in $CDCl_3$



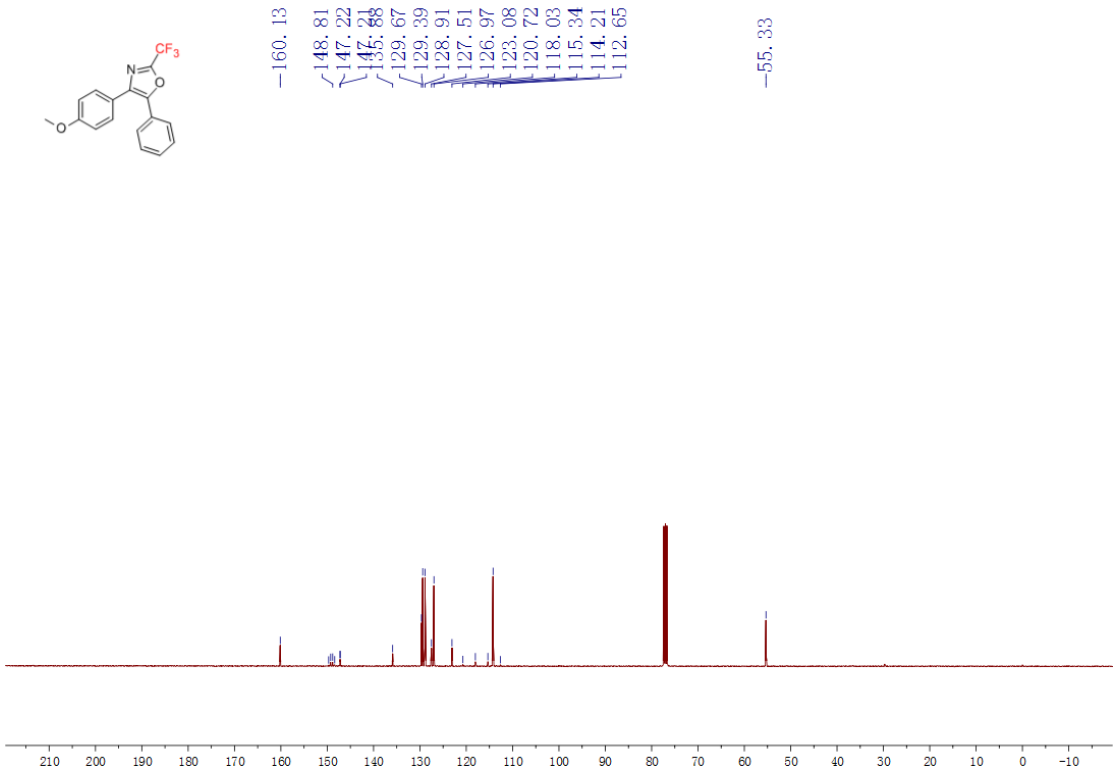
^{19}F NMR spectrum of compound **3af** in $CDCl_3$



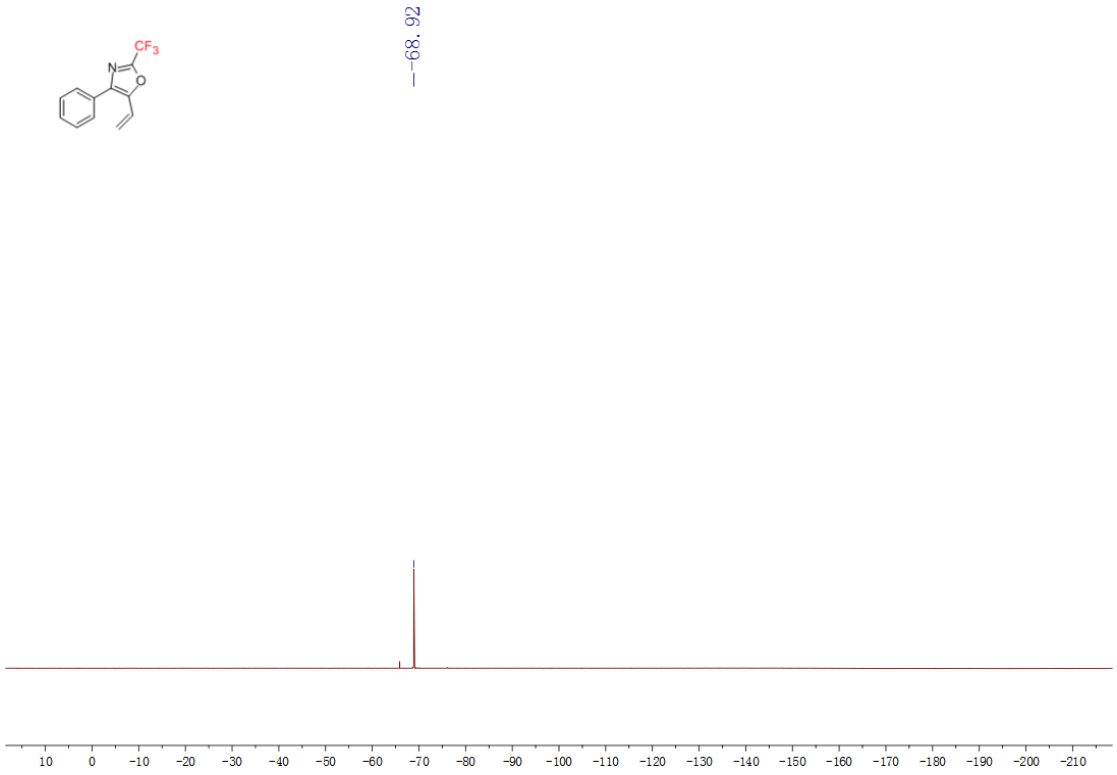
^{1}H NMR spectrum of compound **3af** in $CDCl_3$



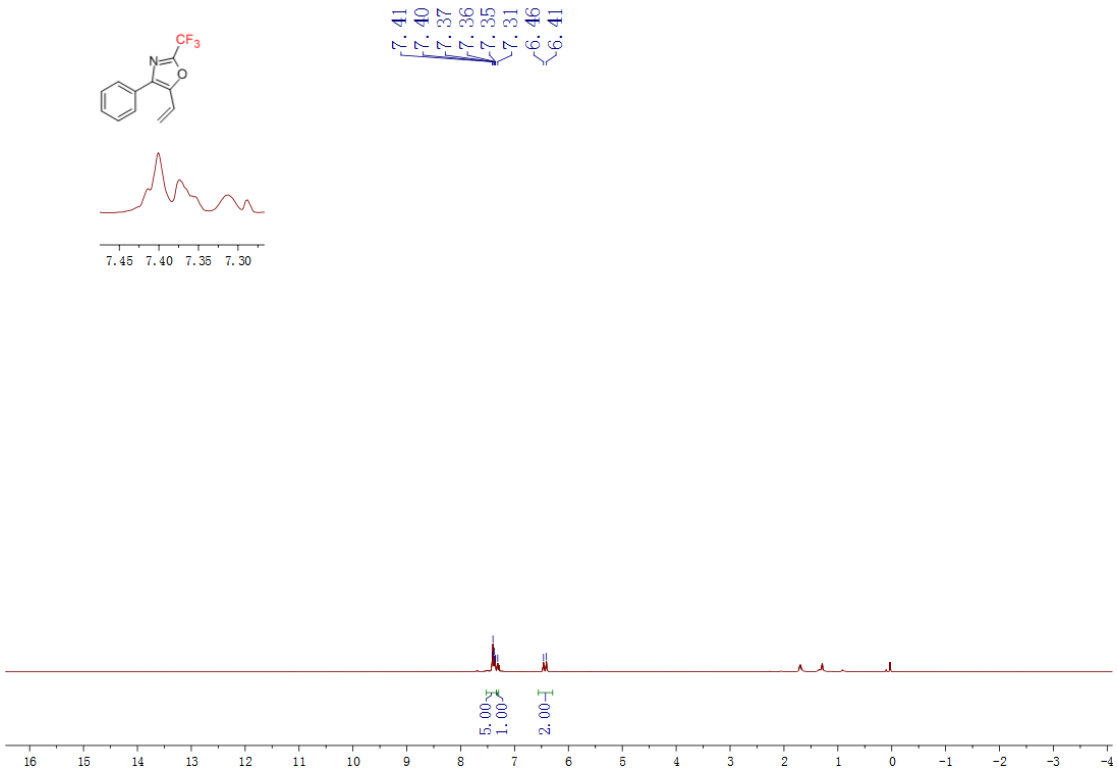
^{13}C NMR spectrum of compound **3af** in $CDCl_3$



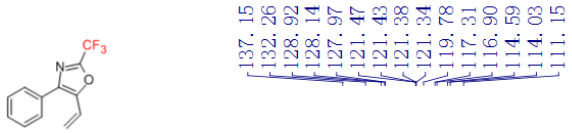
^{19}F NMR spectrum of **3ag** in $CDCl_3$

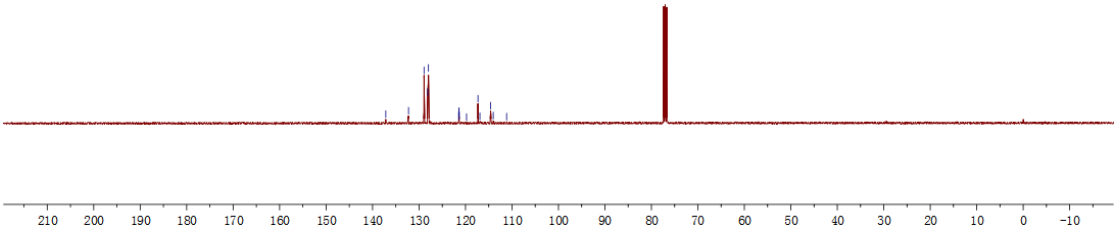


^{1}H NMR spectrum of **3ag** in $CDCl_3$

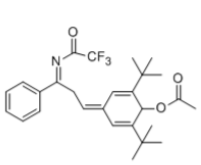


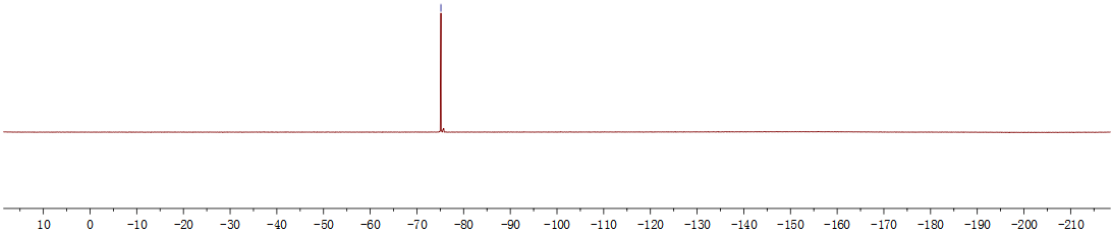
^{13}C NMR spectrum of **3ag** in $CDCl_3$



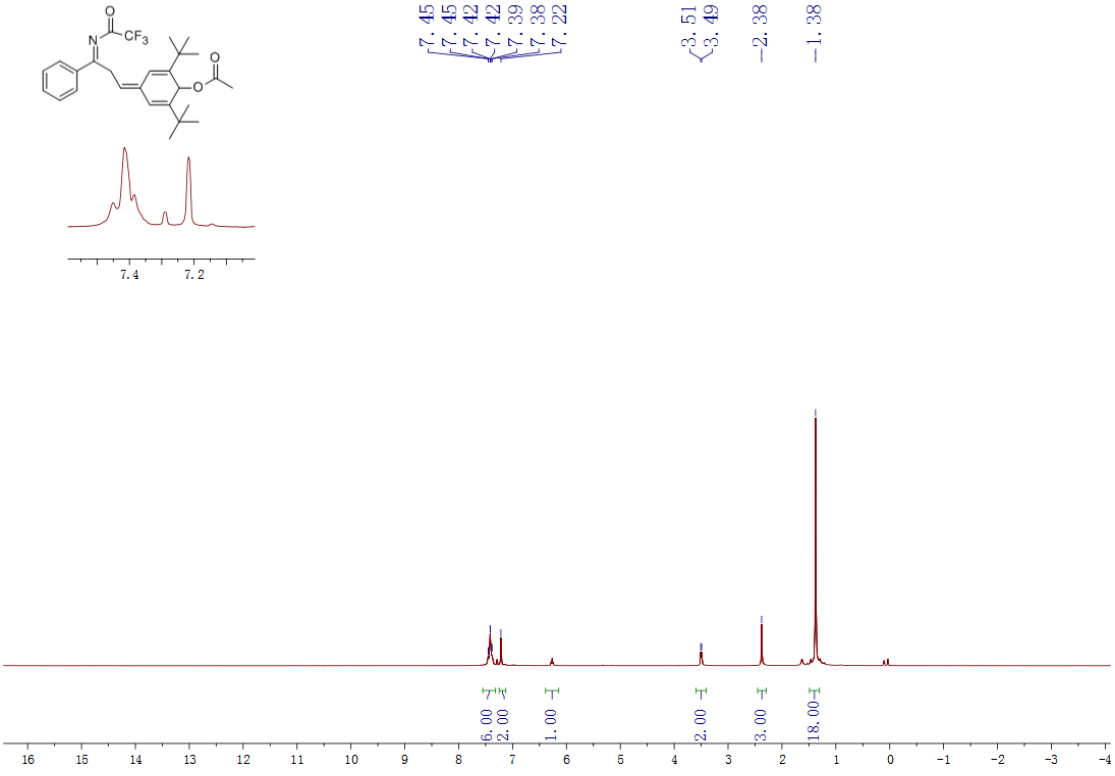


^{19}F NMR spectrum of compound **5** in $CDCl_3$





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



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