

Cu-Catalyzed Synthesis of Fluoroalkylated Isoxazoles from Commercially Available Amines and Alkynes

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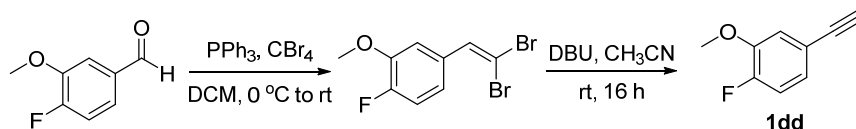
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1. General Information

Difluoroethylamine, trifluoroethylamine and *tert*-butyl nitrite were purified by distillation. Other purchased reagents were used without further purification unless otherwise noted. All solvents were dried over activated 4Å molecular sieves. Reactions were stirred using Teflon-coated magnetic stirrers. Analytical TLC was performed with 0.2 mm silica gel 60F plates with 254 nm fluorescent indicator. TLC plates were visualized by ultraviolet light or by treatment with a spray off Pancaldi reagent {(NH₄)₆MoO₄, Ce(SO₄)₂, H₂SO₄, H₂O} or a solution 0.5% ninhydrin in n-butanol. Chromatographic purification of products was carried out by flash column chromatography on silica gel (300-400 mesh). Melting points were determined using a WRX-4 visual melting point apparatus. NMR spectra were measured in CDCl₃ (TMS, ¹H δ = 0; CDCl₃, ¹H δ = 7.26, ¹³C δ = 77.36) or DMSO-d₆ or CD₃OD on a Bruker AV 400 (¹H at 400 MHz, ¹³C at 100 MHz, ¹⁹F at 376 MHz) magnetic resonance spectrometer. Chemical shifts (δ) are reported in ppm, and coupling constants (*J*) are in Hz. The following abbreviations were used to explain the multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet. What should be noted is that all petroleum ether and ethyl acetate (EtOAc) used for flash column chromatography were redistilled twice before using, but the trace amount of residue of impurities such as H-grease and silicone grease could still be seen on NMR spectra of some products (¹H NMR: δ 1.25/0.84-0.87 and 0.08; ¹³C NMR δ 29.7 and 1.19). (High-resolution mass spectra) HRMS were recorded on a SYNAPT G2Si High Definition MS System. The HRMS were measured under ESI model (specified in the section of characterization data). *Warning: Although no accident occurred during the course of this study, fluorinated diazoalkanes generated in situ are potentially explosive. Stringent safety precautions are necessary for all reactions involving (or indirectly involving) fluorinated diazoalkanes.*

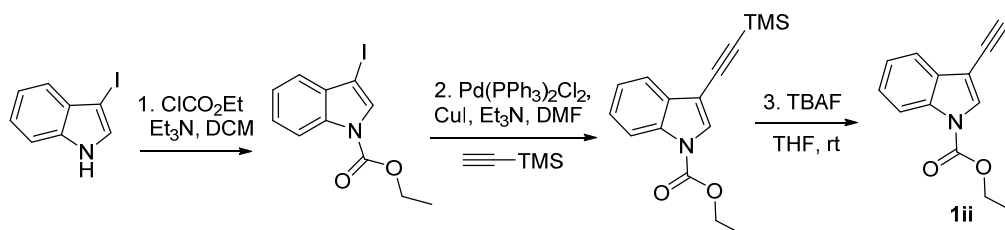
2. Experimental Section

2.1. Procedures for the synthesis **1dd**, **1ii** and **4a**



Following a reported procedure,^[1] 4-fluoro-3-methoxybenzaldehyde (1.55 g, 10 mmol, 1.0 equiv) in CH_2Cl_2 (10 mL) was added drop wise to a solution of CBr_4 (6.63 g, 20 mmol, 2.0 equiv) and PPh_3 (10.5 g, 40 mmol, 4.0 equiv) in CH_2Cl_2 (40 mL) at $0\text{ }^\circ\text{C}$ under N_2 atmosphere. After stirring for additional 3 h at room temperature, the reaction mixture was filtered and concentrated in vacuo. The resulting residue was purified by silica gel column chromatography to afford dibromoalkene as white solid (2.82 g, 91%).

To a solution of dibromoalkene (2.5 g, 8.1 mmol, 1 equiv) in anhydrous CH_3CN (20 mL) was added 4.84 mL of DBU (4.9 g, 32.4 mmol, 4 equiv) drop wise over a period of 10 min at room temperature. The reaction mixture was allowed to stir at this temperature for 16 h. After completion of the reaction (monitored by TLC), reaction mixture was cooled at $10\text{ }^\circ\text{C}$ and quenched by drop wise addition of 5 N aqueous HCl (20 mL) over a period of 15 min. The reaction mixture was extracted with Et_2O (2×30 mL); organic layers were washed with water (40 mL). The organic layers were dried over anhydrous K_2CO_3 , concentrated under reduced pressure and the resulting residue was purified by silica gel column chromatography to afford **1dd** as colorless oil (1.07 g, 78%).

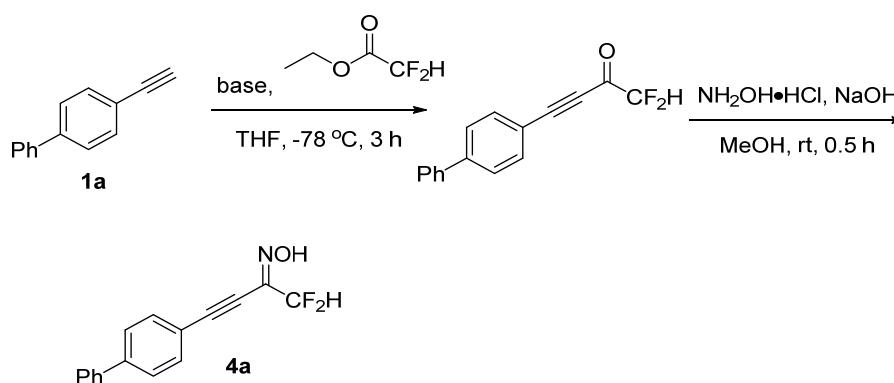


Following a reported procedure^[2], 3-Iodoindole (4.0 g, 16.5 mmol, 1 equiv) was dissolved in anhydrous CH_2Cl_2 (30 mL) at $0\text{ }^\circ\text{C}$ and treated sequentially with 6.9 mL of triethylamine (5.0 g, 49.5 mmol, 3 equiv) and 3.14 mL of ethyl chloroformate (3.58 g, 33.0 mmol, 2 equiv). The mixture was allowed to warm to room temperature over 3 h,

and the reaction was then quenched with the addition of water and extracted with CH_2Cl_2 . The organic layer was dried over Na_2SO_4 and the crude material was subjected to flash column chromatography to afford the corresponding protected product (4.4 g, 85%).

A 100 mL Schlenk tube was charge with the protected product (3.78 g, 12 mmol, 1 equiv), bis(triphenylphosphine)-palladium(II) chloride (168.5 mg, 0.24 mmol) and copper iodide (228.5 mg, 1.2 mmol) and purged with nitrogen three times. Then a 20 mL degassed solution of 5:1 (v/v) $\text{Et}_3\text{N}/\text{DMF}$ and trimethylsilylacetylene (373 μL , 0.258 g, 2.62 mmol) was added and the resulting solution was allowed to stir at 40 °C under nitrogen atmosphere. Upon completion, the reaction mixture was diluted with water (40 mL) and extracted with EtOAc (2×40 mL). The organic layer was dried with Na_2SO_4 and the crude material was collected and subjected to flash column chromatography (5% EtOAc -petroleum ether) to afford TMS-compound(2.56 g, 75%).

To a solution of TMS-compound (2.28 g, 8 mmol) in anhydrous THF (20 mL) was added Bu_4NF (2.5 g, 9.6 mmol). The reaction mixture was allowed to stir at room temperature under nitrogen atmosphere. Upon completion, the reaction mixture was diluted with the addition of water (30 mL) and extracted with EtOAc (2×20 mL). The organic layer was washed with brine (30 mL), dried over Na_2SO_4 and the crude product was purified via flash column chromatography (5% EtOAc -petroleum ether) to yield **1ii** as a white crystalline solid (1.23 g ,72%).



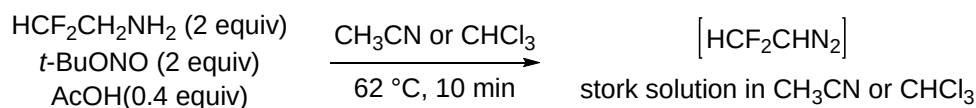
A hexane solution of *n*-butyllithium (15 mmol, 1.0 equiv) was added to a solution of alkyne **1a** (2.67 g, 15 mmol, 1.0 equiv) in 20 mL of anhydrous THF at -78°C under N_2 atmosphere. The solution was stirred for 30 min at -78°C , ethyl difluoroacetate (1.86 g, 15 mmol, 1.0 equiv) as a solution in tetrahydrofuran (5 mL) and boron triflu-

oride etherate (1.85 mL, 15 mmol, 1.0 equiv) were then added successively. The reaction mixture was stirred an additional 2 h at this temperature, saturated aqueous ammonium chloride (10 mL) was added, and the slurry was allowed to warm to ambient temperature. The tetrahydrofuran was removed under reduced pressure, and the residue was taken up in diethyl ether (30 mL), washed with brine (25 mL), and dried over anhydrous magnesium sulfate. The organic phase was concentrated under reduced pressure and the residue was purified by flash column chromatography to afford the difluoroketone product (2.4 g, 63%).

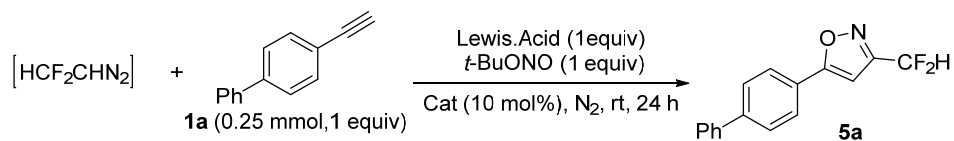
To a solution of difluoroketone (2.2 g, 8.6 mmol, 1 equiv) and hydroxylamine hydrochloride (0.72 g, 10.3 mmol, 1.2 equiv) in methanol (20 mL) was added sodium hydroxide (68 mg, 1.7 mmol, 0.2 equiv). The combined mixture was stirred at room temperature for 30 min, and TLC showed the starting material was completely consumed. The solvent was removed under reduced pressure, and the residue was taken up in EtOAc (25 mL), washed with water (25 mL) and brine (25 mL), and dried over anhydrous magnesium sulfate. The organic phase was concentrated under reduced pressure and the crude product was purification by silica gel column chromatography to afford the oxime product **4a** with a *E/Z* (2:1) mixture (1.8 g, 78%).

2.2. Reaction optimization

Preparation of the difluoromethyl diazomethane solution in CH₃CN or CHCl₃.^[4]



To a stirred solution of 2,2-difluoroethylamine (0.5 mmol, 2.0 equiv) in acetonitrile (or chloroform), *tert*-butyl nitrite (0.5 mmol, 2.0 equiv) and HOAc (0.4 equiv) were added successively under nitrogen atmosphere. The solution was heated at 62 °C for 10 min later, then cooled down to room temperature by external water bath. This stock solution was used directly in the following condition optimization (Table S1).

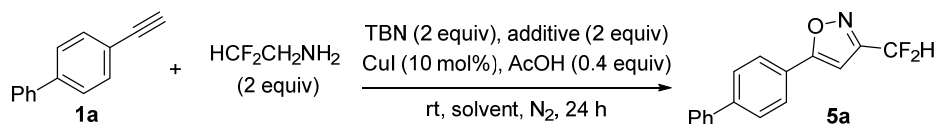
Table S1. Reaction optimization with prior formation of HCF₂CHN₂^a

Entry	Catalytics (10 mol%)	solvent	Additives (1 equiv)	Yield [%] ^b
1	Pd(OAc) ₂	MeCN	FeCl ₃	0
2		MeCN	AlCl ₃	0
3		MeCN	BF ₃ .Et ₂ O	0
4		MeCN	ZnCl ₂	0
5	Pd(OAc) ₂	CHCl ₃	FeCl ₃	0
6		CHCl ₃	AlCl ₃	0
7		CHCl ₃	BF ₃ .Et ₂ O	0
8		CHCl ₃	ZnCl ₂	0
9	Pd(PPh ₃) ₂ Cl ₂	MeCN	FeCl ₃	0
10		MeCN	AlCl ₃	0
11		MeCN	BF ₃ .Et ₂ O	0
12		MeCN	ZnCl ₂	0
13	Pd(PPh ₃) ₂ Cl ₂	CHCl ₃	FeCl ₃	0
14		CHCl ₃	AlCl ₃	0
15		CHCl ₃	BF ₃ .Et ₂ O	0
16		CHCl ₃	ZnCl ₂	0
17	CuI	MeCN	FeCl ₃	0
18		MeCN	AlCl ₃	0
19		MeCN	BF ₃ .Et ₂ O	0
20		MeCN	ZnI ₂	0
21	CuI	CHCl ₃	FeCl ₃	0
22		CHCl ₃	AlCl ₃	0

23		CHCl ₃	BF ₃ .Et ₂ O	0
24		CHCl ₃	ZnCl ₂	28

^a Reaction conditions: **1a** (0.25 mmol), CF₂HCHN₂ solution in CHCl₃ or CH₃CN (0.50 mmol, 2 equiv), TBN (0.25 mmol, 1 equiv), catalyst (10 mol%), additive (0.25 mmol, 1 equiv), at room temperature under N₂ for 24 h. ^b Isolated yield.

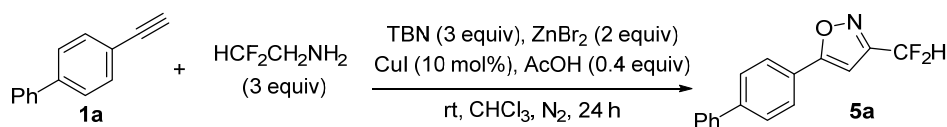
Table S2. Reaction optimization without prior formation of HCF₂CHN₂^a



entry	additive	yield [%] ^b	entry	additive	yield [%] ^b
1	FeCl ₃	0	10	ZnCl ₂	43
2	Fe(SO ₄) ₂	0	11	ZnBr ₂	66
3	Fe(NO ₃) ₃	0	12	ZnI ₂	0
4	BF ₃ .Et ₂ O	0	13	Zn(OTf) ₂	0
5	LiCl	0	14 ^c	ZnBr ₂	87
6	AlCl ₃	0	15 ^{c,d}	ZnBr ₂	52%
7	AgNO ₃	0	16 ^{c,e}	ZnBr ₂	3%
8	CuCl	0	17 ^{c,f}	ZnBr ₂	48%
9	CuBr	0			

^a Reaction conditions: **1a** (0.25 mmol), CF₂HCH₂NH₂ (0.50 mmol, 2 equiv), TBN (0.50 mmol, 2 equiv), CuI (10 mol %), additive (0.5 mmol, 2 equiv), AcOH (0.4 equiv), in CH₂Cl₂ (2.0 mL) at rt under N₂ for 24 h; ^b Isolated yield; ^c 3 equiv TBN and CF₂HCH₂NH₂ were used; ^d CH₂Cl₂ as the solvent; ^e THF as the solvent; ^f Toluene as the solvent.

Table S3. Selected examples of other conditions screened ^a



entry	change from above conditions	yield [%] ^b
1	none	87
2	without CuI	0
3	without ZnBr ₂	0
4	ZnBr ₂ (1 equiv)	42
5	CuI (5 mol%)	73
6	CuSO ₄ • 5H ₂ O (instead of CuI)	44
7	Cu(OAc) ₂ (instead of CuI)	56
8	Cu(acac) ₂ (instead of CuI)	50
9	Cu(TC) (instead of CuI)	48
10	CuBr (instead of CuI)	64
11	CuCl (instead of CuI)	61
12	CuCN (instead of CuI)	68
13	Cu(OTf) ₂ (instead of CuI)	62
14	AgNO ₃ (instead of CuI)	0
15	Ag ₂ CO ₃ (instead of CuI)	0
16	Ag ₂ O (instead of CuI)	5
17	AgOTf (instead of CuI)	8
18	Pd(OAc) ₂ (instead of CuI)	7
19	Pd(CF ₃ CO ₂) ₂ (instead of CuI)	0
20	Pd(PPh ₃) ₄ (instead of CuI)	41
21	PdCl ₂ (instead of CuI)	5
22	Pd(PPh ₃) ₂ Cl ₂ (instead of CuI)	46
23	[Rh(OAc) ₂] ₂ (instead of CuI)	0
24	[Ru(<i>p</i> -cymene)Cl ₂] ₂ (instead of CuI)	0

^a Reaction conditions: **1a** (0.25 mmol), CF₂HCH₂NH₂ (0.75 mmol, 3 equiv), TBN (0.75 mmol, 3 equiv), CuI (10 mol%), ZnBr₂ (0.5 mmol, 2 equiv), AcOH (0.4 equiv), in CHCl₃ (2.0 mL) at rt under N₂ for 24 h. ^b Isolated yield.

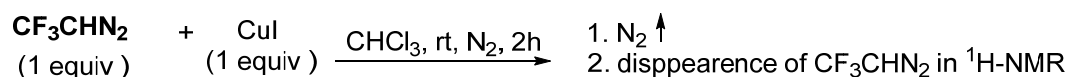
2.3. General Procedure for the synthesis of fluoroalkylated isoxazoles

A solution of alkyne **1** (0.25 mmol, 1 equiv) in chloroform (2 mL), acetic acid (5.7 μ L, 0.1 mmol, 0.4 equiv), perfluoroalkyl amine (0.75 mmol, 3.0 equiv) and *tert*-butyl nitrite (89 μ L, 0.75 mmol, 3.0 equiv), were added successively to a 15 mL Schlenk tube charged with CuI (4.8 mg, 10 mol %), ZnBr₂ (113 mg, 0.5 mmol, 2.0 equiv) and a magnetic stirring bar under nitrogen atmosphere. The mixture was stirred at room temperature for 24 h, then concentrated under vacuum and purified by flash column chromatography.

2.4. Procedure for the gram-scale synthesis of fluoroalkylated isoxazoles **5g**

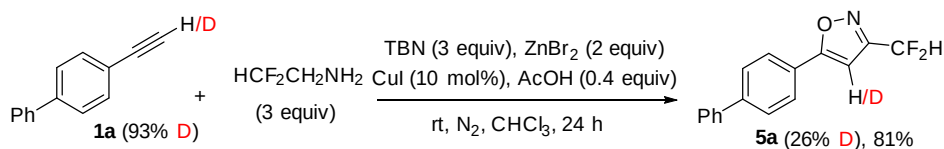
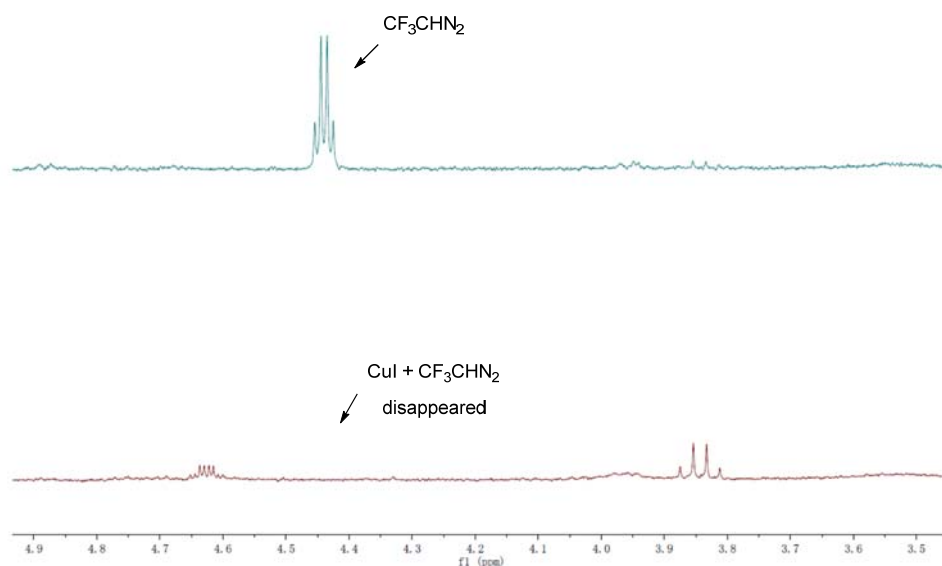
A solution of 4-bromophenylacetylene **1g** (1.2 g, 6.6 mmol, 1 equiv) in chloroform (20 mL), acetic acid (151 μ L, 2.64 mmol, 0.4 equiv), 2,2-difluoroethylamine (1.4 mL, 19.8 mmol, 3.0 equiv) were added successively to a 100 mL Schlenk tube charged with CuI (63 mg, 5 mol%), ZnBr₂ (2.97 g, 13.2 mmol, 2.0 equiv) and a magnetic stirring bar under N₂ atmosphere. The combined mixture was stirred in an ice-water bath. After 15 min, *tert*-butyl nitrite (2.4 mL, 19.8 mmol, 3.0 equiv) was slowly injected over 20 minutes (during this time, ZnBr₂ was dissolved gradually and the color of solution turned to light green). Then, the ice-water bath was removed and the reaction mixture was stirred at room temperature. After stirring 10 min, the reaction mixture became very viscous and the magnetic stirring bar even could not be stirred properly. 15 min later, the viscous mixture gradually became clear. After 24 h, the reaction mixture was filtered over a plug of celite (dichloromethane as eluent) and the filtrate was washed with saturated aqueous sodium thiosulfate (30 mL), and dried over anhydrous magnesium sulfate. The organic phase was concentrated under reduced pressure and the resulting residue was purified by flash column chromatography to afford the product **5g** (1.48 g, 82%).

2.5. Procedure for the control experiments

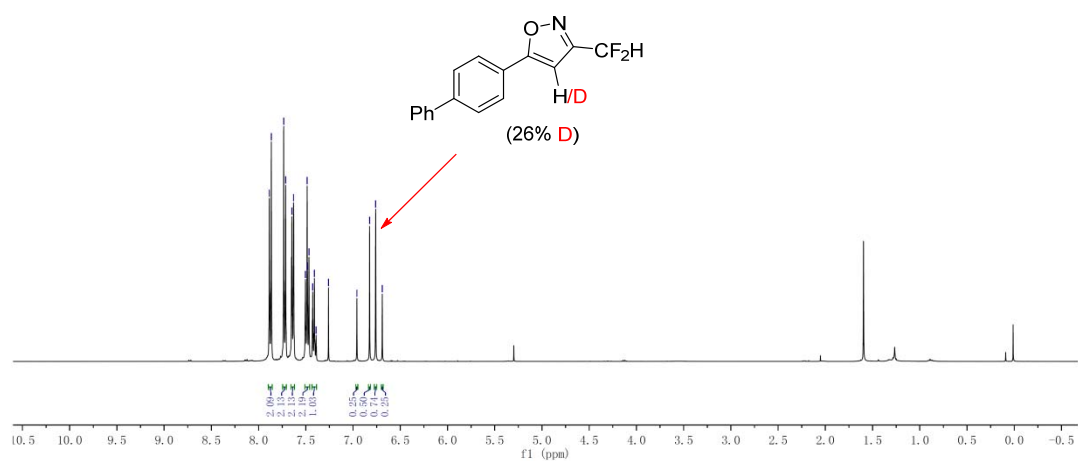


A solution of 2,2,2-trifluoromethyl diazomethane (0.2 mmol, 1.0 equiv) in chloroform was added to a 25 mL Schlenk tube charged with CuI (0.2 mmol, 1.0 equiv) at room temperature. Once the solution was added, the reaction mixture began to emit bubbles.

After stirring for 2 h, the reaction mixture was settled down. The top layer of the mixture was taken out and analyzed by ^1H -NMR.

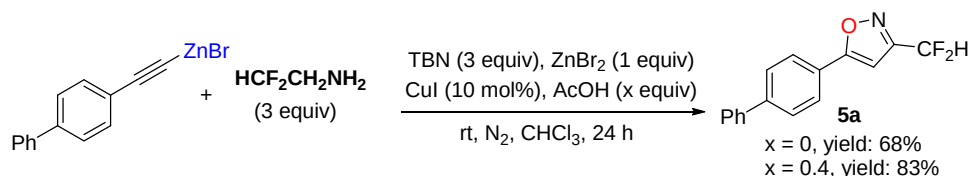


A solution of deuterated alkyne **1a** (0.25 mmol, 1 equiv) in chloroform (2 mL), acetic acid (5.7 μL , 0.1 mmol, 0.4 equiv), 2,2-difluoroethylamine (53 μL , 0.75 mmol, 3.0 equiv), *tert*-butyl nitrite (89 μL , 0.75 mmol, 3.0 equiv), were added successively to a 25 mL Schlenk tube charged with CuI (4.8 mg, 10 mol %), ZnBr₂ (113 mg, 0.5 mmol, 2.0 equiv) and a magnetic stirring bar under nitrogen atmosphere. The mixture was stirred at room temperature for 24 h, then concentrated under vacuum and purified by flash column chromatography.



Following a reported procedure for the synthesis of cuprous acetylide^[5]: A solution of alkyne **1a** (10 mmol) in ethanol (60 mL) was added to an ice-cooled mixture of copper sulfate pentahydrate (2.5 g, 10 mmol), 28% aqueous ammonia (10 mL), water (100 mL) and hydroxylamine hydrochloride (1.4 g, 20 mmol). The combined mixture was stirred for 5 min at this temperature. The precipitate was filtered, washed with water (20 mL), ethanol (20 mL) and diethyl ether (2 × 20 mL), and dried in vacuo overnight.

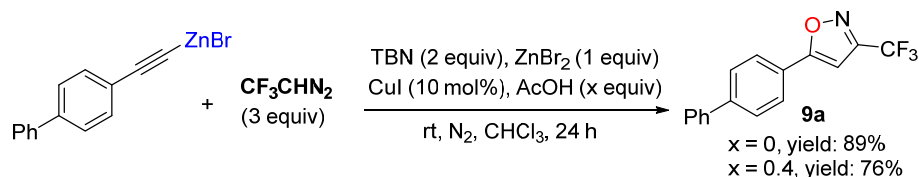
To a 25 mL of Schlenk tube charged with above cuprous acetylide (0.25 mmol, 1.0 equiv), ZnBr₂ (113 mg, 0.5 mmol, 2.0 equiv) and CuI (0 or 10 mol%) were added chloroform (2 mL), 2,2-difluoroethylamine (53 μ L, 0.75 mmol, 3.0 equiv), acetic acid (0 or 0.4 equiv) and *tert*-butyl nitrite (89 μ L, 0.75 mmol, 3.0 equiv) successively under nitrogen atmosphere. The reaction mixture was stirred at room temperature for 24 h, no reaction was occurred via the TLC or crude NMR analysis.



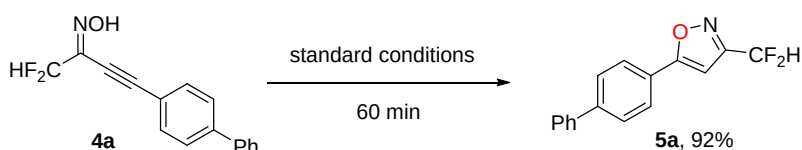
Following a reported procedure for the synthesis of alkynylzinc reagent^[6]: A trace amount of iodine was added to a 25 mL of Schlenk tube containing active zinc (0.275 mmol, 1.1 equiv) and 4-(bromoethynyl)-1,1'-biphenyl (0.25 mmol, 1.0 equiv) in dry THF (3 mL) under nitrogen atmosphere. The combined mixture was stirred at room temperature, the brown color of the mixture disappeared after 4 min then turned grey after 15 min.

After 4 h, the dark grey mixture was stood still for 5 min and the top layer was cannulated into another 25 mL of Schlenk tube charged with CuI (4.8 mg, 10 mol%), ZnBr₂ (0.25 mmol, 1.0 equiv) and a magnetic stirring bar by syringe under nitrogen atmosphere. The solvent was slowly evaporated under vacuum using a double row vacuum gas distributor. After completely drying of the solvent, the reaction tube was back-filled with nitrogen. Then, chloroform (2 mL), 2,2-difluoroethylamine (0.75 mmol, 3.0 equiv), HOAc (0 or 0.4 equiv) and *tert*-butyl nitrite (0.75 mmol, 3.0 equiv) was added successively to the reaction mixture under nitrogen atmosphere. The reaction

mixture was stirred at room temperature for 24 h, then concentrated under vacuum and the residue was purified by flash column chromatography.



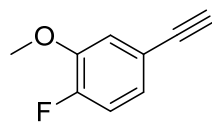
A trace amount of iodine was added to a 25 mL of Schlenk tube containing active zinc (0.275 mmol, 1.1 equiv) and 4-(bromoethynyl)-1,1'-biphenyl (0.25 mmol, 1.0 equiv) in dry THF (3 mL) under nitrogen atmosphere. The combined mixture was stirred at room temperature, the brown color of the mixture disappeared after 4 min then turned grey after 15 min. After 4 h, the dark grey mixture was stood still for 5 min and the top layer was cannulated into another 25 mL of Schlenk tube charged with CuI (4.8 mg, 10 mol %), ZnBr₂ (0.25 mmol, 1.0 equiv) and a magnetic stirring bar by syringe under nitrogen atmosphere. The solvent of this mixture was slowly evaporated under vacuum using a double row vacuum gas distributor. After completely drying the solvent, the reaction tube was backfilled with nitrogen. Then, a solution of trifluoromethyl dizaomethane (0.75 mmol, 3.0 equiv) in chloroform, HOAc (0 or 0.4 equiv) and *tert*-butyl nitrite (0.5 mmol, 2.0 equiv) was added successively to the reaction mixture under nitrogen atmosphere. After stirring at room temperature for 24 h, the reaction mixture was concentrated under reduce pressure and the residue was purified by flash column chromatography.



A solution of oxime **4a** (0.25 mmol, 1 equiv) in chloroform (2 mL), acetic acid (0.1 mmol, 0.4 equiv), 2,2-difluoroethylamine (0.75 mmol, 3.0 equiv) and *tert*-butyl nitrite (0.75 mmol, 3.0 equiv), was added successively to a 25 mL Schlenk tube charged with CuI (4.8 mg, 10 mol%), ZnBr₂ (113 mg, 0.5 mmol, 2.0 equiv) and a magnetic stirring bar under nitrogen atmosphere. The reaction mixture was stirred at room temperature for 60 min and TLC showed the starting material was completely consumed. The reaction mixture was concentrated under reduced pressure and the resulting resi-

due was purified by flash column chromatography to afford the isoxazole **5a** in 92% yield.

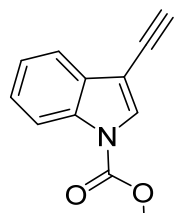
3. Characterization data of Compounds



1dd

4-ethynyl-1-fluoro-2-methoxybenzene

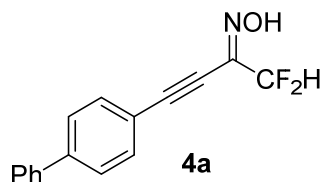
Prepared according to the general procedure, purified by flash column chromatography (petroleum ether/AcOEt = 200:1), pale yellow oil (1.07 g, 78%). **¹H NMR** (400 MHz, CDCl₃) δ 7.09 – 6.98 (m, 3 H), 3.88 (s, 3 H), 3.03 (s, 1 H); **¹³C NMR** (100 MHz, CDCl₃) δ 153.2 (d, J = 249.6 Hz), 147.8 (d, J = 11.1 Hz), 125.6 (d, J = 7.01 Hz), 118.6 (d, J = 4.2 Hz), 117.3 (d, J = 2.1 Hz), 116.5 (d, J = 19.3 Hz), 83.2 (d, J = 1.5 Hz), 77.0 (d, J = 1.6 Hz), 56.5; **¹⁹F NMR** (376 MHz, CDCl₃) δ -132.38 – -132.45 (m, 1 F); **¹⁹F {¹H} NMR** (376 MHz, CDCl₃) δ -132.42 (s, 1 F); **HRMS (ESI)** m/z calcd for C₉H₈OF⁺ [M+H]⁺ 151.0554, found 151.0553.



1ii

ethyl 3-ethynyl-1H-indole-1-carboxylate

White crystalline solid (1.23g, 72%); mp: 56.6 – 57.2; **¹H NMR** (400 MHz, CDCl₃) δ 8.17 (d, J = 8.0 Hz, 1 H), 7.85 (s, 1 H), 7.69 (d, J = 8.0 Hz, 1 H), 7.41 – 7.37 (m, 1 H), 7.34 – 7.31 (m, 1 H), 4.51 (q, J = 7.2 Hz, 2 H), 3.26 (s, 1 H), 1.48 (t, J = 7.2 Hz, 2 H); **¹³C NMR** (100 MHz, CDCl₃) δ 150.7, 134.9, 130.8, 129.9, 125.8, 123.9, 120.4, 115.6, 103.4, 81.3, 75.9, 64.0, 14.7; **HRMS (ESI)** m/z calcd for C₁₃H₁₂NO₂⁺ [M+H]⁺ 214.0863, found 214.0862.

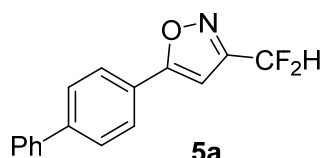


4a

4-([1,1'-biphenyl]-4-yl)-1,1-difluorobut-3-yn-2-one oxime

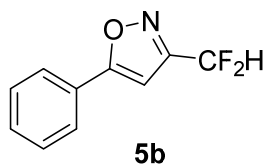
Prepared according to the general procedure, purified by flash column chromatography (petroleum ether/AcOEt = 10:1), white solid, (E/Z = 2:1); mp: 113.8 – 115.6; **¹H NMR** (400 MHz, CDCl₃) δ 9.40 (br s, 1 H), 7.69 – 7.59 (m, 6 H), 7.48 – 7.44 (m, 2 H), 7.42 – 7.37 (m, 1 H), 6.87 (t, J = 54.0 Hz, 0.64 H), 6.25 (t, J = 54.0 Hz, 0.36 H);

¹³C NMR (100 MHz, CDCl₃) δ 143.4, 143.0, 141.8 (t, J = 26.5 Hz), 140.3, 140.2, 138.5 (t, J = 29.1 Hz), 133.3, 133.0, 129.3, 129.3, 128.4, 128.3, 127.5, 127.4, 127.4, 120.1, 119.8, 111.9 (t, J = 241 Hz), 105.0 (t, J = 242 Hz), 104.4, 96.7, 79.1, 75.2; **¹⁹F NMR** (376 MHz, CDCl₃) δ -117.33 (d, J = 54.0 Hz), -124.16 (d, J = 54.0 Hz); **¹⁹F {¹H} NMR** (376 MHz, CDCl₃) δ -117.32 (s, 2 F), -124.16 (s, 2 F); **HRMS (ESI)** m/z calcd for C₁₆H₁₂ONF₂⁺ [M+H]⁺ 272.0882, found 272.0877.



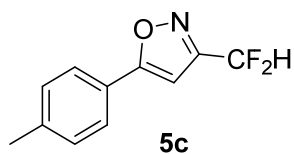
5-([1,1'-biphenyl]-4-yl)-3-(difluoromethyl)isoxazole

Purified by flash column chromatography (petroleum ether/AcOEt = 200:1), pale yellow solid (58.8 mg, 87% yield); mp: 124.5 – 124.8; **¹H NMR** (400 MHz, CDCl₃) δ 7.86 (d, J = 8.0 Hz, 2 H), 7.71 (d, J = 8.0 Hz, 2 H), 7.64 (d, J = 8.0 Hz, 2 H), 7.49 (t, J = 8.0 Hz, 2 H), 7.42 (t, J = 8.0 Hz, 1 H), 6.84 (t, J = 54.0 Hz, 1 H), 6.75 (s, 1 H); **¹³C NMR** (100 MHz, CDCl₃) δ 171.7, 159.7 (t, J = 30.0 Hz), 143.9, 140.0, 129.3, 128.4, 128.0, 127.4, 126.7, 125.6, 109.4 (t, J = 237.0 Hz), 96.4; **¹⁹F NMR** (376 MHz, CDCl₃) δ -115.15 (d, J = 54.0 Hz, 2 F); **¹⁹F {¹H} NMR** (376 MHz, CDCl₃) δ -115.15 (s, 2 F); **HRMS (ESI)** m/z calcd for C₁₆H₁₂ONF₂⁺ [M+H]⁺ 272.0882, found 272.0880.



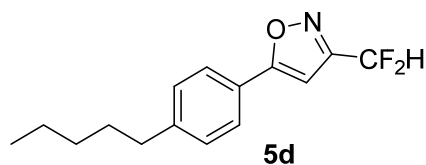
5-phenyl-3-(difluoromethyl)isoxazole

Purified by flash column chromatography (petroleum ether/AcOEt = 200:1), colorless oil (44.4 mg, 91% yield); **¹H NMR** (400 MHz, CDCl₃) δ 7.81 – 7.78 (m, 2 H), 7.49 – 7.47 (m, 3 H), 6.81 (t, J = 54.0 Hz, 1 H), 6.72 (s, 1 H); **¹³C NMR** (100 MHz, CDCl₃) δ 171.9, 159.7 (t, J = 30.0 Hz), 131.2, 129.5, 126.8, 126.3, 109.4 (t, J = 237.0 Hz), 96.4; **¹⁹F NMR** (376 MHz, CDCl₃) δ -115.27 (d, J = 54.0 Hz, 2 F); **¹⁹F {¹H} NMR** (376 MHz, CDCl₃) δ -115.27 (s, 2 F); **HRMS (ESI):** m/z calcd for C₁₀H₈ONF₂⁺ [M+H]⁺ 196.0569, found 196.0572.^[7]



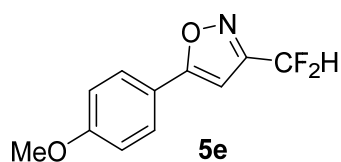
5-(p-tolyl)-3-(difluoromethyl)isoxazole

Purified by flash column chromatography (petroleum ether/AcOEt = 200:1), foamy solid (44.5 mg, 85% yield); **¹H NMR** (400 MHz, CDCl₃) δ 7.68 (d, J = 8.0 Hz, 2 H), 7.29 (d, J = 8.0 Hz, 2 H), 6.79 (t, J = 54.0 Hz, 1 H), 6.67 (s, 1 H), 2.41 (s, 3 H); **¹³C NMR** (100 MHz, CDCl₃) δ 172.2, 159.7 (t, J = 30 Hz), 141.7, 130.2, 126.2, 124.2, 109.5 (t, J = 237.0 Hz), 95.8, 21.9; **¹⁹F NMR** (376 MHz, CDCl₃) δ -115.26 (d, J = 54.0 Hz, 2 F); **¹⁹F {¹H} NMR** (376 MHz, CDCl₃) δ -115.26 (s, 2 F); **HRMS (ESI):** m/z calcd for C₁₁H₁₀ONF₂⁺ [M+H]⁺ 210.0725, found 210.0723. ^[8]



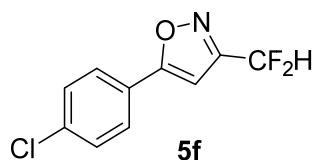
5-(4-pentylphenyl)-3-(difluoromethyl)isoxazole

Purified by flash column chromatography (petroleum ether/AcOEt = 200:1), colorless oil (53.2 mg, 80% yield); **¹H NMR** (400 MHz, CDCl₃) δ 7.71 (d, J = 8.0 Hz, 2 H), 7.30 (d, J = 8.0 Hz, 2 H), 6.80 (t, J = 54.0 Hz, 1 H), 6.67 (s, 1 H), 2.66 (t, J = 8.0 Hz, 2 H), 1.68-1.61 (m, 2H), 1.38 – 1.31 (m, 4 H), 0.90 (t, J = 7.0 Hz, 3 H); **¹³C NMR** (100 MHz, CDCl₃) δ 172.2, 159.7 (t, J = 30 Hz), 146.7, 129.5, 126.3, 124.4, 109.5 (t, J = 237 Hz), 95.8, 36.2, 31.8, 31.2, 22.8, 14.3; **¹⁹F NMR** (376 MHz, CDCl₃) δ -115.25 (d, J = 54.0 Hz, 2 F); **¹⁹F {¹H} NMR** (376 MHz, CDCl₃) δ -115.25 (s, 2 F); **HRMS (ESI)** m/z calcd for C₁₅H₁₈ONF₂⁺ [M+H]⁺ 266.1351, found 266.1346.



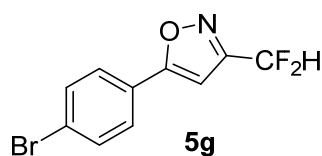
5-(4-methoxyphenyl)-3-(difluoromethyl)isoxazole

Purified by flash column chromatography (petroleum ether/AcOEt = 100:1), pale yellow solid (46.7 mg, 83% yield); mp: 72.3 – 73.1; **¹H NMR** (400 MHz, CDCl₃) δ 7.73 (d, J = 8.0 Hz, 2 H), 6.99 (d, J = 8.0 Hz, 2 H), 6.78 (t, J = 54.0 Hz, 1 H), 6.59 (s, 1 H), 3.87 (s, 3 H); **¹³C NMR** (100 MHz, CDCl₃) δ 172.0, 162.0, 159.7 (t, J = 30 Hz), 128.0, 119.7, 114.9, 109.5 (t, J = 235.0 Hz), 95.0, 55.8; **¹⁹F NMR** (376 MHz, CDCl₃) δ -115.28 (d, J = 54.0 Hz, 2 F); **¹⁹F {¹H} NMR** (376 MHz, CDCl₃) δ -115.28 (s, 2 F); **HRMS (ESI):** m/z calcd for C₁₁H₁₀O₂NF₂⁺ [M+H]⁺ 226.0674, found 226.0672.



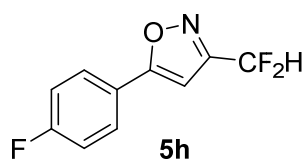
5-(4-chlorophenyl)-3-(difluoromethyl)isoxazole

Purified by flash column chromatography (petroleum ether/AcOEt = 200:1), white solid (54.6 mg, 95% yield); mp: 82.9 – 84.3; ^1H NMR (400 MHz, CDCl_3) δ 7.73 (d, J = 8.0 Hz, 2 H), 7.46 (d, J = 8.0 Hz, 2 H), 7.80 (t, J = 54.0 Hz, 1 H), 6.72 (s, 1 H); ^{13}C NMR (100 MHz, CDCl_3) δ 170.8, 159.8 (t, J = 38.0 Hz), 137.4, 129.8, 127.6, 125.3, 109.3 (t, J = 237 Hz), 96.8; ^{19}F NMR (376 MHz, CDCl_3) δ -115.29 (d, J = 54.0 Hz, 2 F); ^{19}F $\{^1\text{H}\}$ NMR (376 MHz, CDCl_3) δ -115.29 (s, 2 F); **HRMS (ESI):** m/z calcd for $\text{C}_{10}\text{H}_7\text{ONClF}_2^+$ $[\text{M}+\text{H}]^+$ 230.0179, found 230.0174.



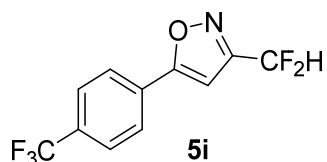
5-(4-bromophenyl)-3-(difluoromethyl)isoxazole

Purified by flash column chromatography (petroleum ether/AcOEt = 200:1), white solid (58.8 mg, 86% yield); mp: 103.7 – 104.5; ^1H NMR (400 MHz, CDCl_3) δ 7.68 – 7.62 (m, 4 H), 6.80 (t, J = 54.0 Hz, 1 H), 6.73 (s, 1 H); ^{13}C NMR (100 MHz, CDCl_3) δ 170.9, 159.9 (t, J = 30.0 Hz), 132.9, 127.8, 125.8, 109.3 (t, J = 235.0 Hz), 96.9; ^{19}F NMR (376 MHz, CDCl_3) δ -115.29 (d, J = 54.0 Hz, 2 F). ^{19}F $\{^1\text{H}\}$ NMR (376 MHz, CDCl_3) δ -115.29 (s, 2 F); **HRMS (ESI):** m/z calcd for $\text{C}_{10}\text{H}_7\text{ONF}_3\text{Br}^+$ $[\text{M}+\text{H}]^+$ 273.9674, found 273.9677.



5-(4-fluorophenyl)-3-(difluoromethyl)isoxazole

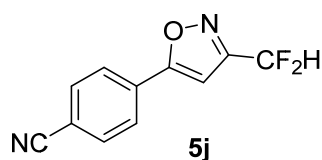
Purified by flash column chromatography (petroleum ether/AcOEt = 200:1), pale yellow foamy solid (48.9 mg, 92% yield); ^1H NMR (400 MHz, CDCl_3) δ 7.82 – 7.78 (m, 2 H), 7.21 – 7.17 (m, 2 H), 6.80 (t, J = 54.0 Hz, 1 H), 6.68 (s, 1 H); ^{13}C NMR (100 MHz, CDCl_3) δ 171.0, 164.5 (d, J = 252.0 Hz), 159.8 (t, J = 30 Hz), 128.5 (d, J = 9.0 Hz), 123.3 (d, J = 3.0 Hz), 116.8 (d, J = 23.0 Hz), 109.4 (t, J = 236 Hz), 96.3; ^{19}F NMR (376 MHz, CDCl_3) δ -108.11 – -108.18 (m, 1 F), -115.30 (d, J = 54.0 Hz, 2 F); ^{19}F $\{^1\text{H}\}$ NMR (376 MHz, CDCl_3) δ -108.14 (s, 1 F), -115.30 (s, 2 F); **HRMS (ESI):** m/z calcd for $\text{C}_{10}\text{H}_7\text{ONF}_3^+$ $[\text{M}+\text{H}]^+$ 214.0474, found 214.0471.



3-(difluoromethyl)-5-(4-

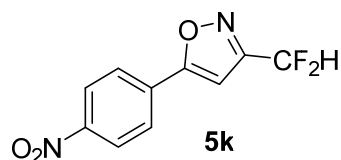
(trifluoromethyl)phenyl)isoxazole

Purified by flash column chromatography (petroleum ether/AcOEt = 100:1), white crystalline solid (50.9 mg, 77% yield); mp: 84.7 – 86.2; ¹H NMR (400 MHz, CDCl₃) δ 7.93 (d, *J* = 8.0 Hz, 2 H), 7.77 (d, *J* = 8.0 Hz, 2 H), 6.84 (s, 1 H), 6.83 (t, *J* = 54.0 Hz, 1 H); ¹³C NMR (100 MHz, CDCl₃) δ 170.3, 159.9 (t, *J* = 30 Hz), 132.8, 128.3 (q, *J* = 330 Hz), 126.7, 126.6 (q, *J* = 4.0 Hz), 122.6, 109.2 (t, *J* = 237.0 Hz), 98.0; ¹⁹F NMR (376 MHz, CDCl₃) δ -63.07 (s, 1 F), -115.31 (d, *J* = 54.0 Hz, 2 F); ¹⁹F {¹H} NMR (376 MHz, CDCl₃) δ -63.07 (s, 1 F), -115.31 (s, 2 F); HRMS (ESI): *m/z* calcd for C₁₁H₇ONF₅⁺ [M+H]⁺ 264.0442, found 264.0440.



4-(3-(difluoromethyl)isoxazol-5-yl)benzonitrile

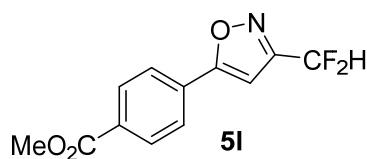
Purified by flash column chromatography (petroleum ether/AcOEt = 50:1), white solid (41.2 mg, 75% yield); mp: 112.7 – 114.2; ¹H NMR (400 MHz, CDCl₃) δ 7.92 (d, *J* = 8.0 Hz, 2 H), 7.80 (d, *J* = 8.0 Hz, 2 H), 6.87 (s, 1 H), 6.82 (t, *J* = 52.0 Hz, 1 H); ¹³C NMR (100 MHz, CDCl₃) δ 169.7, 160.0 (t, *J* = 30 Hz), 133.3, 130.5, 126.8, 118.2, 114.8, 109.1 (t, *J* = 236 Hz), 98.7; ¹⁹F NMR (376 MHz, CDCl₃) δ -115.34 (d, *J* = 52.0 Hz, 2 F); ¹⁹F {¹H} NMR (376 MHz, CDCl₃) δ -115.34 (s, 2 F); HRMS (ESI): *m/z* calcd for C₁₁H₇ON₂F₂⁺ [M+H]⁺ 221.0521, found 221.0518.



5-(4-nitrophenyl)-3-(difluoromethyl)isoxazole

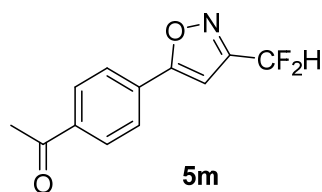
Purified by flash column chromatography (petroleum ether/AcOEt = 20:1), yellow solid (44.5 mg, 74% yield); mp: 163.6 – 165.3; ¹H NMR (400 MHz, CDCl₃) δ 8.38 (d, *J* = 8.0 Hz, 2 H), 8.00 (d, *J* = 8.0 Hz, 2 H), 6.93 (s, 1 H), 6.84 (t, *J* = 54.0 Hz, 1 H); ¹³C NMR (100 MHz, CDCl₃) δ 169.4, 160.1 (t, *J* = 30 Hz), 149.3, 132.1, 127.2, 124.9, 109.1 (t, *J* = 237.0 Hz), 99.2; ¹⁹F NMR (376 MHz, CDCl₃) δ -115.28 (d, *J* = 54.0 Hz,

2 F); **¹⁹F {¹H} NMR** (376 MHz, CDCl₃) δ -115.28 (s, 2 F); **HRMS (ESI):** m/z calcd for C₁₀H₇O₃N₂F₂⁺ [M+H]⁺ 241.0419, found 241.0415.



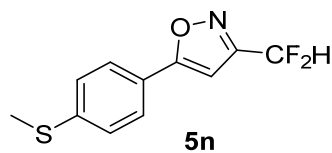
5l methyl 4-(3-(difluoromethyl)isoxazol-5-yl)benzoate

Purified by flash column chromatography (petroleum ether/AcOEt = 20:1), white solid (55.1 mg, 87% yield); mp: 123.4 – 124.4; **¹H NMR** (400 MHz, CDCl₃) δ 8.15 (d, *J* = 8.0 Hz, 2 H), 7.86 (d, *J* = 8.0 Hz, 2 H), 6.83 (s, 1 H), 6.81 (t, *J* = 54.0 Hz, 1 H), 3.95 (s, 3 H); **¹³C NMR** (100 MHz, CDCl₃) δ 170.8, 166.4, 159.9 (t, *J* = 30.0 Hz), 132.4, 130.7, 130.5, 126.2, 109.3 (t, *J* = 237 Hz), 98.0, 52.8; **¹⁹F NMR** (376 MHz, CDCl₃) δ -115.31 (d, *J* = 54.0 Hz, 2 F); **¹⁹F {¹H} NMR** (376 MHz, CDCl₃) δ -115.31 (s, 2 F); **HRMS (ESI)** m/z calcd for C₁₂H₁₀O₃NF₂⁺ [M+H]⁺ 254.0623, found 254.0619.



5m 1-(4-(3-(difluoromethyl)isoxazol-5-yl)phenyl)ethan-1-one

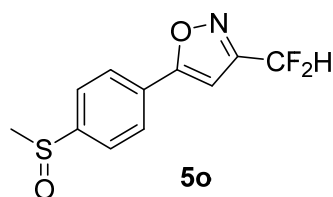
Purified by flash column chromatography (petroleum ether/AcOEt = 50:1), white solid (45.6 mg, 77% yield); mp: 125.0 – 126.2; **¹H NMR** (400 MHz, CDCl₃) δ 8.07 (d, *J* = 8.0 Hz, 2 H), 7.90 (d, *J* = 8.0 Hz, 2 H), 6.85 (s, 1 H), 6.82 (t, *J* = 54.0 Hz, 1 H), 2.65 (s, 3 H); **¹³C NMR** (100 MHz, CDCl₃) δ 197.4, 170.6, 159.9 (t, *J* = 30.0 Hz), 138.8, 130.5, 129.4, 126.5, 109.2 (t, *J* = 237.0 Hz), 98.1, 27.1; **¹⁹F NMR** (376 MHz, CDCl₃) δ -115.27 (d, *J* = 54.0 Hz, 2 F); **¹⁹F {¹H} NMR** (376 MHz, CDCl₃) δ -115.27 (s, 2 F); **HRMS (ESI)** m/z calcd for C₁₂H₁₂O₂NF₂⁺ [M+H]⁺ 240.0831, found 240.0824.



5n 5-(4-(methylthio)phenyl)-3-(difluoromethyl)isoxazole

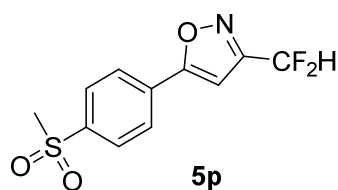
Purified by flash column chromatography (petroleum ether/AcOEt = 100:1), white solid (48.8 mg, 81% yield); mp: 87.8-88.3; **¹H NMR** (400 MHz, CDCl₃) δ 7.70 (d, *J* = 8.0 Hz, 2 H), 7.32 (d, *J* = 8.0 Hz, 2 H), 6.79 (t, *J* = 54.0 Hz, 1 H), 6.67 (s, 1 H), 2.53 (s, 3 H); **¹³C NMR** (100 MHz, CDCl₃) δ 171.6, 159.7 (t, *J* = 30.0 Hz), 143.2, 126.6, 126.4, 123.2, 109.4 (t, *J* = 237.0 Hz), 95.9, 15.4; **¹⁹F NMR** (376 MHz, CDCl₃) δ -

115.25 (d, $J = 54.0$ Hz, 2 F); **^{19}F { ^1H } NMR** (376 MHz, CDCl_3) δ -115.25 (s, 2 F); **HRMS (ESI):** m/z calcd for $\text{C}_{11}\text{H}_{10}\text{ONF}_2\text{S}^+$ $[\text{M}+\text{H}]^+$ 242.0446, found 242.0440.



5-(4-(methylsulfinyl)phenyl)-3-(difluoromethyl)isoxazole

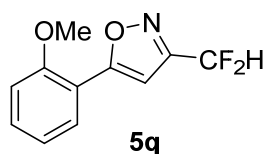
Purified by flash column chromatography (petroleum ether/AcOEt = 3:1), white solid (49.2 mg, 77% yield); mp: 111.7 – 113.3; **^1H NMR** (400 MHz, CDCl_3) δ 7.92 (d, $J = 8.0$ Hz, 2 H), 7.74 (d, $J = 8.0$ Hz, 2 H), 6.82 (s, 1 H), 6.79 (t, $J = 54.0$ Hz, 1 H), 2.74 (s, 3 H); **^{13}C NMR** (100 MHz, CDCl_3) δ 170.3, 159.7 (t, $J = 30.0$ Hz), 148.8, 129.0, 127.0, 124.7, 109.1 (t, $J = 237$ Hz), 97.7, 44.1; **^{19}F NMR** (376 MHz, CDCl_3) δ -115.35 (d, $J = 54.0$ Hz, 2 F); **^{19}F { ^1H } NMR** (376 MHz, CDCl_3) δ -115.35 (s, 2 F); **HRMS (ESI)** m/z calcd for $\text{C}_{11}\text{H}_{10}\text{O}_2\text{NF}_2\text{S}^+$ $[\text{M}+\text{H}]^+$ 258.0395, found 258.0392.



5-(4-(methylsulfonyl)phenyl)-3-

(difluoromethyl)isoxazole

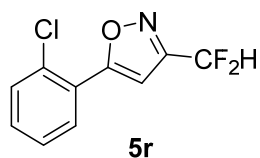
Purified by flash column chromatography (petroleum ether/AcOEt = 5:1), yellow solid (49.2 mg, 72% yield); mp: 159.0 – 160.9; **^1H NMR** (400 MHz, CDCl_3) δ 8.09 (d, $J = 8.0$ Hz, 2 H), 8.01 (d, $J = 8.0$ Hz, 2 H), 6.91 (s, 1 H), 6.84 (t, $J = 54.0$ Hz, 1 H), 3.11 (s, 3 H); **^{13}C NMR** (100 MHz, CDCl_3) δ 169.7, 160.0 (t, $J = 30.0$ Hz), 142.7, 131.5, 128.8, 127.2, 109.1 (t, $J = 237$ Hz), 98.8, 44.8; **^{19}F NMR** (376 MHz, CDCl_3) δ -115.28 (d, $J = 54.0$ Hz, 2 F); **^{19}F { ^1H } NMR** (376 MHz, CDCl_3) δ -115.28 (s, 2 F); **HRMS (ESI):** m/z calcd for $\text{C}_{11}\text{H}_{10}\text{O}_3\text{NF}_2\text{S}^+$ $[\text{M}+\text{H}]^+$ 274.0344, found 274.0339.



5-(2-methoxyphenyl)-3-(difluoromethyl)isoxazole

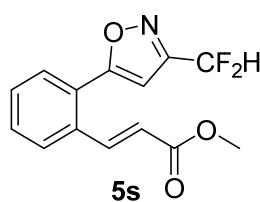
Purified by flash column chromatography (petroleum ether/AcOEt = 100:1), white solid (47.8 mg, 85% yield); mp: 48.8 – 49.5; **^1H NMR** (400 MHz, CDCl_3) δ 7.98 (dd, $J = 1.6, 8.0$ Hz, 1 H), 7.47 – 7.42 (m, 1 H), 7.08 (t, $J = 8.0$ Hz, 1 H), 7.03 (d, $J = 8.5$

Hz, 1 H), 7.00 (s, 1 H), 6.82 (t, $J = 54.0$ Hz, 1 H), 3.97 (s, 3 H); **^{13}C NMR** (100 MHz, CDCl_3) δ 168.0, 159.7 (t, $J = 30.0$ Hz), 156.7, 132.3, 128.0, 121.3, 115.9, 111.6, 109.7 (t, $J = 237.0$ Hz), 100.4, 55.9; **^{19}F NMR** (376 MHz, CDCl_3) δ -115.28 (d, $J = 54.0$ Hz, 2 F); **^{19}F { ^1H } NMR** (376 MHz, CDCl_3) δ -115.28 (s, 2 F); **HRMS (ESI)**: m/z calcd for $\text{C}_{11}\text{H}_{10}\text{O}_2\text{NF}_2^+$ $[\text{M}+\text{H}]^+$ 226.0674, found 226.0671.



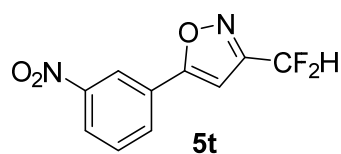
5-(2-chlorophenyl)-3-(difluoromethyl)isoxazole

Purified by flash column chromatography (petroleum ether/AcOEt = 200:1), colorless oil (47.1 mg, 82% yield); **^1H NMR** (400 MHz, CDCl_3) δ 7.98 – 7.94 (m, 1 H), 7.56 – 7.52 (m, 1 H), 7.44–7.40 (m, 2 H), 7.16 (s, 1 H), 6.84 (t, $J = 54.0$ Hz, 1 H); **^{13}C NMR** (100 MHz, CDCl_3) δ 168.3, 159.6 (t, $J = 30$ Hz), 132.4, 131.9, 131.4, 129.8, 127.7, 125.7, 109.4 (t, $J = 237$ Hz), 101.4; **^{19}F NMR** (376 MHz, CDCl_3) δ -115.33 (d, $J = 54.0$ Hz, 2 F); **^{19}F { ^1H } NMR** (376 MHz, CDCl_3) δ -115.33 (s, 2 F); **HRMS (ESI)**: m/z calcd for $\text{C}_{10}\text{H}_7\text{ONClF}_2^+$ $[\text{M}+\text{H}]^+$ 230.0179, found 230.0176.



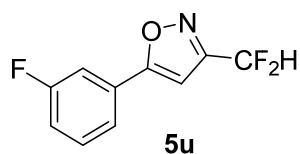
methyl (E)-3-(2-(3-(difluoromethyl)isoxazol-5-yl)phenyl)acrylate

Purified by flash column chromatography (petroleum ether/AcOEt = 20:1), colorless oil (53.7 mg, 77% yield); **^1H NMR** (400 MHz, CDCl_3) δ 7.95 (d, $J = 16.0$ Hz, 1 H), 7.76 – 7.74 (m, 1 H), 7.69 – 7.66 (m, 1 H), 7.53 – 7.51 (m, 2 H), 6.83 (t, $J = 54.0$ Hz, 1 H), 6.60 (s, 1 H), 6.43 (d, $J = 16.0$ Hz, 1 H), 3.82 (s, 3 H); **^{13}C NMR** (100 MHz, CDCl_3) δ 170.4, 166.9, 159.5 (t, $J = 30$ Hz), 142.1, 133.9, 131.4, 130.4, 129.6, 128.2, 126.7, 122.2, 109.3 (t, $J = 237.0$ Hz), 101.3, 52.3; **^{19}F NMR** (376 MHz, CDCl_3) δ -115.26 (d, $J = 54.0$ Hz, 2 F); **^{19}F { ^1H } NMR** (376 MHz, CDCl_3) δ -115.26 (s, 2 F); **HRMS (ESI)** m/z calcd for $\text{C}_{14}\text{H}_{12}\text{O}_3\text{NF}_2^+$ $[\text{M}+\text{H}]^+$ 280.0780, found 280.0774.



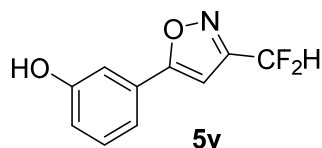
5-(3-nitrophenyl)-3-(difluoromethyl)isoxazole

Purified by flash column chromatography (petroleum ether/AcOEt = 30:1), pale yellow solid (49.9 mg, 83% yield); mp: 96.1 – 97.0; ¹H NMR (400 MHz, CDCl₃) δ 8.64 (t, *J* = 1.8 Hz, 1 H), 8.36 – 8.33 (m, 1 H), 8.16 – 8.13 (m, 1 H), 7.73 (t, *J* = 8.0 Hz, 1 H), 6.92 (s, 1 H), 6.83 (t, *J* = 54.0 Hz, 1 H); ¹³C NMR (100 MHz, CDCl₃) δ 169.3, 160.0 (t, *J* = 30.0 Hz), 149.0, 131.8, 130.9, 128.3, 125.6, 121.3, 109.1 (q, *J* = 237.0 Hz), 98.4; ¹⁹F NMR (376 MHz, CDCl₃) δ -115.34 (d, *J* = 54.0 Hz, 2 F); ¹⁹F {¹H} NMR (376 MHz, CDCl₃) δ -115.34 (s, 2 F); HRMS (ESI): *m/z* calcd for C₁₀H₇O₃N₂F₂⁺ [M+H]⁺ 241.0419, found 241.0414.



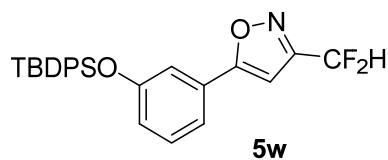
5-(3-fluorophenyl)-3-(difluoromethyl)isoxazole

Purified by flash column chromatography (petroleum ether/AcOEt = 200:1), pale yellow foamy solid (43.9 mg, 82% yield); ¹H NMR (400 MHz, CDCl₃) δ 7.59 – 7.58 (m, 1 H), 7.52 – 7.46 (m, 2 H), 7.21 – 7.16 (m, 1 H), 6.81 (t, *J* = 54.0 Hz, 1 H), 6.75 (s, 1 H); ¹³C NMR (100 MHz, CDCl₃) δ 170.6 (d, *J* = 2.0 Hz), 163.3 (d, *J* = 247.0 Hz), 159.8 (t, *J* = 30.0 Hz), 131.3 (d, *J* = 9.0 Hz), 128.7 (d, *J* = 9.0 Hz), 122.1 (d, *J* = 3.0 Hz), 118.2 (d, *J* = 21.0 Hz), 113.4 (d, *J* = 23.0 Hz), 109.3 (t, *J* = 237.0 Hz), 97.3; ¹⁹F NMR (376 MHz, CDCl₃) δ -111.08 – -111.14 (m, 1 F), -115.32 (d, *J* = 54.0 Hz, 2 F); ¹⁹F {¹H} NMR (376 MHz, CDCl₃) δ -111.11 (s, 1 F), -115.32 (s, 2 F); HRMS (ESI): *m/z* calcd for C₁₀H₇ONF₃⁺ [M+H]⁺ 214.0474, found 214.0471.



3-(3-(difluoromethyl)isoxazol-5-yl)phenol

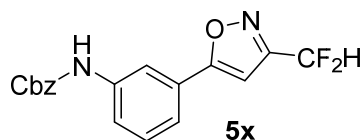
Purified by flash column chromatography (petroleum ether/AcOEt = 8:1), white solid (41.2 mg, 78% yield); mp: 134.4 – 134.9; ¹H NMR (400 MHz, CD₃OD) δ 7.32 – 7.30 (m, 2 H), 7.27 – 7.25 (m, 1 H), 6.95 (s, 1 H), 6.95 (t, *J* = 54.0 Hz, 1 H), 6.94 – 6.91 (m, 1 H); ¹³C NMR (100 MHz, CD₃OD) δ 173.1, 161.0 (t, *J* = 30.0 Hz), 159.3, 131.5, 128.9, 119.1, 118.2, 113.4, 110.9 (t, *J* = 237.0 Hz), 97.4; ¹⁹F NMR (376 MHz, CD₃OD) δ -117.64 (d, *J* = 54.0 Hz, 2 F); ¹⁹F {¹H} NMR (376 MHz, CD₃OD) δ -117.64 (s, 2 F); HRMS (ESI) *m/z* calcd for C₁₀H₈O₂NF₂⁺ [M+H]⁺ 212.0518, found 212.0513.



5-(3-((*tert*-butyldiphenylsilyl)oxy)phenyl)-3-

(difluoromethyl)isoxazole

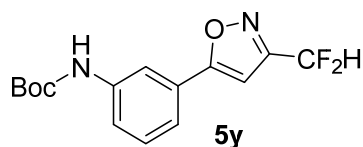
Purified by flash column chromatography (petroleum ether/AcOEt = 100:1), colorless oil (96.0 mg, 85% yield); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.77 – 7.75 (m, 4 H), 7.49 – 7.45 (m, 2 H), 7.43 – 7.39 (m, 4 H), 7.33 – 7.31 (m, 1 H), 7.23 (t, J = 2.0 Hz, 1 H), 7.19 (t, J = 8.0 Hz, 1 H), 6.85 (dd, J = 2.4, 8.0 Hz, 1 H), 6.78 (t, J = 54.0 Hz, 1 H), 6.5 (s, 1 H), 1.16 (s, 9 H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 171.7, 159.6 (t, J = 30.0 Hz), 156.5, 135.9, 132.7, 130.5, 130.4, 128.3, 127.8, 123.6, 119.1, 117.6, 109.4 (t, J = 237.0 Hz), 96.5, 26.9, 19.8; $^{19}\text{F NMR}$ (376 MHz, CDCl_3) δ -115.25 (d, J = 54.0 Hz, 2 F); $^{19}\text{F}\{^1\text{H}\}$ NMR (376 MHz, CDCl_3) δ -115.25 (s, 2 F); **HRMS (ESI)** m/z calcd for $\text{C}_{26}\text{H}_{26}\text{O}_2\text{NF}_2\text{Si}^+$ $[\text{M}+\text{H}]^+$ 450.1695, found 450.1686.



benzyl (3-(3-(difluoromethyl)isoxazol-5-

yl)phenyl)carbamate

Purified by flash column chromatography (petroleum ether/AcOEt = 6:1), yellow solid (80.2 mg, 93% yield); mp: 122.1 – 123.8; $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.92 (s, 1 H), 7.54 – 7.47 (m, 2 H), 7.43 – 7.36 (m, 6 H), 7.16 (s, 1 H), 6.76 (t, J = 54.0 Hz, 1 H), 6.72 (s, 1 H), 5.23 (s, 2 H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 171.6, 159.7 (t, J = 30.0 Hz), 153.6, 139.2, 136.1, 130.3, 129.0, 128.8, 128.7, 127.6, 121.2, 121.2, 116.1, 109.3 (t, J = 237.0 Hz), 97.0, 67.7; $^{19}\text{F NMR}$ (376 MHz, CDCl_3) δ -115.27 (d, J = 54.0 Hz, 2 F); $^{19}\text{F}\{^1\text{H}\}$ NMR (376 MHz, CDCl_3) δ -115.27 (s, 2 F); **HRMS (ESI)** m/z calcd for $\text{C}_{18}\text{H}_{15}\text{O}_3\text{N}_2\text{F}_2^+$ $[\text{M}+\text{H}]^+$ 345.1045, found 345.1039.

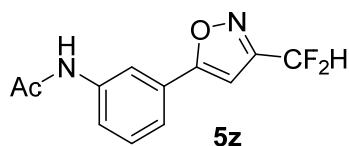


***tert*-butyl (3-(3-(difluoromethyl)isoxazol-5-**

yl)phenyl)carbamate

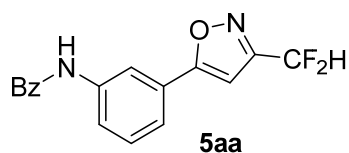
Purified by flash column chromatography (petroleum ether/AcOEt = 15:1), pale brown solid (67.4 mg, 87% yield); mp: 100.6 – 101.9; $^1\text{H NMR}$ (400 MHz, CDCl_3) δ

7.94 (s, 1 H), 7.47 – 7.44 (m, 1 H), 7.43 – 7.36 (m, 2 H), 6.80 (t, $J = 54.0$ Hz, 1 H), 6.77 (s, 1 H), 6.74 (s, 1 H), 1.53 (s, 9 H); ^{13}C NMR (100 MHz, CDCl_3) δ 171.8, 159.7 (t, $J = 30.0$ Hz), 152.9, 139.7, 130.1, 127.6, 121.0, 120.8, 116.0, 109.4 (t, $J = 237.0$ Hz), 28.6; ^{19}F NMR (376 MHz, CDCl_3) δ -115.29 (d, $J = 54.0$ Hz, 2 F); ^{19}F { ^1H } NMR (376 MHz, CDCl_3) δ -115.29 (s, 2 F); HRMS (ESI) m/z calcd for $\text{C}_{15}\text{H}_{17}\text{O}_3\text{N}_2\text{F}_2^+$ $[\text{M}+\text{H}]^+$ 311.1202, found 311.1196.



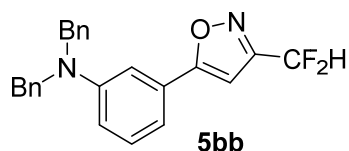
***N*-(3-(3-(difluoromethyl)isoxazol-5-yl)phenyl)acetamide**

Purified by flash column chromatography (petroleum ether/AcOEt = 3:1), pale yellow solid (52.2 mg, 83% yield); mp: 152.0 – 153.9; ^1H NMR (400 MHz, CD_3OD) δ 8.15 (t, $J = 1.8$ Hz, 1 H), 7.65 (d, $J = 8.0$ Hz, 1 H), 7.59 (d, $J = 8.0$ Hz, 1 H), 7.45 (t, $J = 8.0$ Hz, 1 H), 7.02 (s, 1 H), 6.97 (t, $J = 54.0$ Hz, 1 H), 2.16 (s, 3 H); ^{13}C NMR (100 MHz, CD_3OD) δ 172.8, 171.9, 161.1 (t, $J = 30.0$ Hz), 141.0, 130.9, 128.4, 123.2, 122.5, 118.0, 110.9 (q, $J = 237.0$ Hz), 97.8, 23.9; ^{19}F NMR (376 MHz, CD_3OD) δ -117.67 (d, $J = 54.0$ Hz, 2 F); ^{19}F { ^1H } NMR (376 MHz, CD_3OD) δ -117.67 (s, 2 F); HRMS (ESI) m/z calcd for $\text{C}_{12}\text{H}_{11}\text{O}_2\text{N}_2\text{F}_2^+$ $[\text{M}+\text{H}]^+$ 253.0783, found 253.0779.



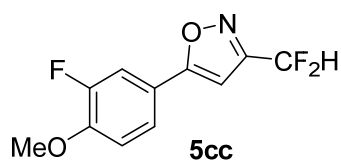
***N*-(3-(3-(difluoromethyl)isoxazol-5-yl)phenyl)benzamide**

Purified by flash column chromatography (petroleum ether/AcOEt = 4:1), white solid (58.0 mg, 74% yield); mp: 161.8 – 162.3; ^1H NMR (400 MHz, CDCl_3) δ 8.17 (s, 1 H), 8.09 (br s, 1 H), 7.90 – 7.88 (m, 2 H), 7.76 – 7.74 (m, 1 H), 7.59 – 7.56 (m, 2 H), 7.51 – 7.46 (m, 2 H), 6.78 (t, $J = 54.0$ Hz, 1 H), 6.75 (s, 1 H); ^{13}C NMR (100 MHz, CDCl_3) δ 171.5, 166.3, 159.8 (t, $J = 30.0$ Hz), 139.2, 134.8, 132.6, 130.3, 129.6, 127.7, 127.4, 122.8, 122.7, 122.3, 122.3, 117.9, 117.8, 109.4 (t, $J = 237.0$ Hz), 97.1; ^{19}F NMR (376 MHz, CDCl_3) δ -115.31 (d, $J = 54.0$ Hz, 2 F); ^{19}F { ^1H } NMR (376 MHz, CDCl_3) δ -115.31 (s, 2 F); HRMS (ESI) m/z calcd for $\text{C}_{17}\text{H}_{13}\text{O}_2\text{N}_2\text{F}_2^+$ $[\text{M}+\text{H}]^+$ 315.0940, found 315.0937.



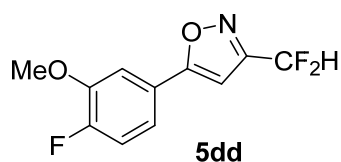
***N,N*-dibenzyl-3-(3-(difluoromethyl)isoxazol-5-yl)aniline**

Purified by flash column chromatography (petroleum ether/AcOEt = 20:1), white solid (61.6 mg, 63% yield); mp: 108.9 – 110.4; ¹H NMR (400 MHz, CDCl₃) δ 7.28 – 7.25 (m, 4 H), 7.21 – 7.15 (m, 8 H), 7.09 – 7.08 (m, 1 H), 7.02 (d, *J* = 8.0 Hz, 1 H), 6.75 (dd, *J* = 2.4, 8.4 Hz, 1 H), 6.67 (t, *J* = 54.0 Hz, 1 H), 6.48 (s, 1 H), 4.63 (s, 4 H); ¹³C NMR (100 MHz, CDCl₃) δ 172.7, 159.6 (t, *J* = 30.0 Hz), 149.9, 138.2, 130.4, 129.2, 127.6, 126.9, 115.3, 114.9, 109.7, 109.5 (t, *J* = 237.0 Hz), 96.3, 54.6; ¹⁹F NMR (376 MHz, CDCl₃) δ -115.22 (d, *J* = 54.0 Hz, 2 F); ¹⁹F {¹H} NMR (376 MHz, CDCl₃) δ -115.22 (s, 2 F); **HRMS (ESI)** *m/z* calcd for C₂₄H₂₁ON₂F₂⁺ [M+H]⁺ 391.1617, found 391.1610.



5-(3-fluoro-4-methoxyphenyl)-3-(difluoromethyl)isoxazole

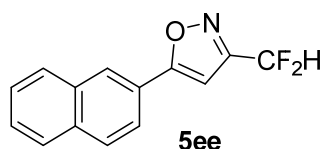
Purified by flash column chromatography (petroleum ether/AcOEt = 100:1), pale yellow solid (51.1 mg, 84% yield); mp: 90.9 – 91.6; ¹H NMR (400 MHz, CDCl₃) δ 7.53 – 7.47 (m, 2 H), 7.04 (t, *J* = 8.4 Hz, 1 H), 6.78 (t, *J* = 54.0 Hz, 1 H), 6.60 (s, 1 H), 3.94 (s, 3 H); ¹³C NMR (100 MHz, CDCl₃) δ 170.7 (d, *J* = 2.4 Hz), 159.8 (t, *J* = 30.0 Hz), 152.7 (d, *J* = 247.0 Hz), 150.2 (d, *J* = 10.5 Hz), 122.8 (d, *J* = 4.0 Hz), 119.8 (d, *J* = 7.4 Hz), 114.1 (d, *J* = 20.5 Hz), 113.9 (d, *J* = 2.4 Hz), 109.4 (t, *J* = 237.0 Hz), 95.8, 56.6; ¹⁹F NMR (376 MHz, CDCl₃) δ -115.39 (d, *J* = 54.0 Hz, 2 F), -133.40 – -133.45 (m, 1 F); ¹⁹F {¹H} NMR (376 MHz, CDCl₃) δ -115.39 (s, 2 F), -133.43 (s, 1 F); **HRMS (ESI)** *m/z* calcd for C₁₁H₉O₂NF₃⁺ [M+H]⁺ 244.0580, found 244.0576.



5-(4-fluoro-3-methoxyphenyl)-3-(difluoromethyl)isoxazole

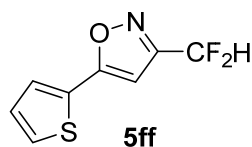
Purified by flash column chromatography (petroleum ether/AcOEt = 100:1), white solid (49.8 mg, 82% yield); mp: 77.3 – 78.3; ¹H NMR (400 MHz, CDCl₃) δ 7.39 (dd,

$J = 2.0, 8.0$ Hz, 1 H), 7.33 (dq, $J = 2.0, 8.0$ Hz, 1 H), 7.17 (dd, $J = 8.0, 10.0$ Hz, 1 H), 6.79 (t, $J = 54.0$ Hz, 1 H), 6.68 (s, 1 H), 3.96 (s, 3 H); ^{13}C NMR (100 MHz, CDCl_3) δ 171.1, 159.8 (t, $J = 30.0$ Hz), 154.3 (d, $J = 253.0$ Hz), 148.7 (d, $J = 11.0$ Hz), 123.4 (d, $J = 4.0$ Hz), 119.5 (d, $J = 7.8$ Hz), 117.2 (d, $J = 20.0$ Hz), 111.2 (d, $J = 2.6$ Hz), 111.3 (d, $J = 19.0$ Hz), 109.3 (t, $J = 237.0$ Hz), 96.4, 56.7; ^{19}F NMR (376 MHz, CDCl_3) δ -115.31 (d, $J = 54.0$ Hz, 2 F), -130.09 – -130.15 (m, 1 F); ^{19}F $\{^1\text{H}\}$ NMR (376 MHz, CDCl_3) δ -115.31 (s, 2 F), -130.12 (s, 1 F); **HRMS (ESI)** m/z calcd for $\text{C}_{11}\text{H}_9\text{O}_2\text{NF}_3^+$ $[\text{M}+\text{H}]^+$ 244.0580, found 244.0574.



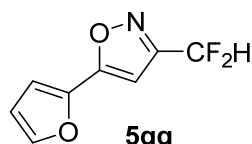
5-(naphthalen-2-yl)-3-(difluoromethyl)isoxazole

Purified by flash column chromatography (petroleum ether/AcOEt = 100:1), pale yellow solid (45.5 mg, 74% yield); mp: 75.3 – 75.9; ^1H NMR (400 MHz, CDCl_3) δ 8.30 (s, 1 H), 7.93 – 7.90 (m, 2 H), 7.88 – 7.85 (m, 1 H), 7.79 (dd, $J = 1.6, 8.6$ Hz, 1 H), 7.59 – 7.54 (m, 2 H), 6.85 (t, $J = 54.0$ Hz, 1 H), 6.82 (s, 1 H); ^{13}C NMR (100 MHz, CDCl_3) δ 172.0, 159.8 (t, $J = 30.0$ Hz), 134.5, 133.3, 129.4, 129.1, 128.2, 128.1, 127.5, 126.3, 124.0, 123.0, 109.5 (t, $J = 237.0$ Hz), 96.8; ^{19}F NMR (376 MHz, CDCl_3) δ -115.18 (d, $J = 54.0$ Hz, 2 F); ^{19}F $\{^1\text{H}\}$ NMR (376 MHz, CDCl_3) δ -115.18 (s, 2 F); **HRMS (ESI)** m/z calcd for $\text{C}_{14}\text{H}_{10}\text{ONF}_2^+$ $[\text{M}+\text{H}]^+$ 246.0725, found 246.0720.



5-(thiophen-2-yl)-3-(difluoromethyl)isoxazole

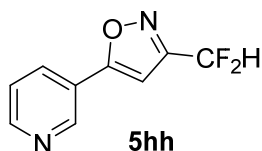
Purified by flash column chromatography (petroleum ether/AcOEt = 50:1), yellow oil (39.8 mg, 79% yield); ^1H NMR (400 MHz, CDCl_3) δ 7.57 (dd, $J = 1.0, 3.6$ Hz, 1 H), 7.51 (dd, $J = 1.0, 5.0$ Hz, 1 H), 7.16 (dd, $J = 3.8, 5.0$ Hz, 1 H), 6.78 (t, $J = 54.0$ Hz, 1 H), 6.59 (s, 1 H); ^{13}C NMR (100 MHz, CDCl_3) δ 167.0, 159.7 (t, $J = 30.0$ Hz), 129.3, 128.6, 128.5, 128.2, 109.3 (t, $J = 237.0$ Hz), 96.1; ^{19}F NMR (376 MHz, CDCl_3) δ -115.37 (d, $J = 54.0$ Hz, 2 F); ^{19}F $\{^1\text{H}\}$ NMR (376 MHz, CDCl_3) δ -115.37 (s, 2 F); **HRMS (ESI)** m/z calcd for $\text{C}_8\text{H}_6\text{ONF}_2\text{S}^+$ $[\text{M}+\text{H}]^+$ 202.0133, found 202.0130.^[7]



5gg

5-(furan-2-yl)-3-(difluoromethyl)isoxazole

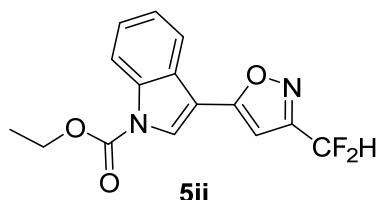
Purified by flash column chromatography (petroleum ether/AcOEt = 50:1), colorless oil (32.9 mg, 71% yield); ^1H NMR (400 MHz, CDCl_3) δ 7.58 (d, J = 1.4 Hz, 1 H), 6.98 (d, J = 3.4 Hz, 1 H), 6.79 (t, J = 54.0 Hz, 1 H), 6.65 (s, 1 H), 6.57 (dd, J = 1.8, 3.5 Hz, 1 H); ^{13}C NMR (100 MHz, CDCl_3) δ 163.4, 159.4 (t, J = 30.0 Hz), 145.1, 142.7, 112.4, 111.9, 109.2 (t, J = 237.0 Hz), 96.1; ^{19}F NMR (376 MHz, CDCl_3) δ -115.41 (d, J = 54.0 Hz, 2 F); ^{19}F $\{^1\text{H}\}$ NMR (376 MHz, CDCl_3) δ -115.41 (s, 2 F); HRMS (ESI) m/z calcd for $\text{C}_8\text{H}_6\text{O}_2\text{NF}_2^+$ $[\text{M}+\text{H}]^+$ 186.0361, found 186.0358.



5hh

5-(pyridin-3-yl)-3-(difluoromethyl)isoxazole

Purified by flash column chromatography (petroleum ether/AcOEt = 10:1), brown solid (28.5 mg, 58% yield); mp: 51.2 – 52.1; ^1H NMR (400 MHz, CDCl_3) δ 9.05 (s, 1 H), 8.73 (d, J = 4.0 Hz, 1 H), 8.11 (dt, J = 2.0, 8.0 Hz, 1 H), 7.46 (dd, J = 4.9, 8.0 Hz, 1 H), 6.84 (s, 1 H), 6.82 (t, J = 54.0 Hz, 1 H); ^{13}C NMR (100 MHz, CDCl_3) δ 169.2, 159.9 (t, J = 30.0 Hz), 152.0, 147.5, 133.4, 124.3, 123.2, 109.2 (t, J = 237.0 Hz), 97.6; ^{19}F NMR (376 MHz, CDCl_3) δ -115.31 (d, J = 54.0 Hz, 2 F); ^{19}F $\{^1\text{H}\}$ NMR (376 MHz, CDCl_3) δ -115.31 (s, 2 F); HRMS (ESI) m/z calcd for $\text{C}_9\text{H}_7\text{ON}_2\text{F}_2^+$ $[\text{M}+\text{H}]^+$ 197.0521, found 197.0516.

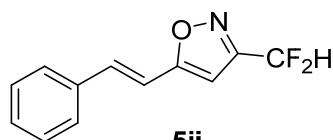


5ii

ethyl 3-(3-(difluoromethyl)isoxazol-5-yl)-1H-indole-1-carboxylate

Purified by flash column chromatography (petroleum ether/AcOEt = 100:1), pale yellow solid (54.5 mg, 71% yield); mp: 104.1 – 105.1; ^1H NMR (400 MHz, CDCl_3) δ 8.25 (d, J = 8.0 Hz, 1 H), 8.13 (s, 1 H), 7.91 (d, J = 8.0 Hz, 1 H), 7.46 – 7.37 (m, 2 H), 6.84 (t, J = 54.0 Hz, 1 H), 6.74 (s, 1 H), 4.55 (q, J = 7.2 Hz, 2 H), 1.51 (t, J = 7.2 Hz, 3 H); ^{13}C NMR (100 MHz, CDCl_3) δ 166.9, 159.5 (t, J = 30.0 Hz), 150.7, 135.8,

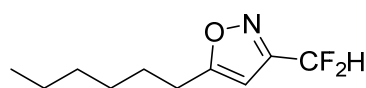
126.4, 126.1, 125.7, 124.5, 120.5, 115.9, 109.4 (t, $J = 237.0$ Hz), 109.2, 96.7, 64.4, 14.7; ^{19}F NMR (376 MHz, CDCl_3) δ -115.21 (d, $J = 54.0$ Hz, 2 F); ^{19}F { ^1H } NMR (376 MHz, CDCl_3) δ -115.21 (s, 2 F); HRMS (ESI) m/z calcd for $\text{C}_{15}\text{H}_{13}\text{O}_3\text{N}_2\text{F}_2^+$ $[\text{M}+\text{H}]^+$ 307.0889, found 307.0883.



5jj

(E)-5-styryl-3-(difluoromethyl)isoxazole

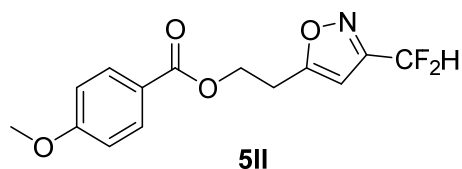
Purified by flash column chromatography (petroleum ether/AcOEt = 200:1), pale yellow solid (37.4 mg, 68% yield); mp: 68.1 – 71.4; ^1H NMR (400 MHz, CDCl_3) δ 7.55 – 7.52 (m, 2 H), 7.43 – 7.41 (m, 2 H), 7.39 – 7.37 (m, 2 H), 6.98 (d, $J = 16$ Hz, 1 H), 6.78 (t, $J = 54.0$ Hz, 1 H), 6.48 (s, 1 H); ^{13}C NMR (100 MHz, CDCl_3) δ 170.5, 159.5 (t, $J = 30.0$ Hz), 136.7, 135.4, 130.0, 129.3, 127.6, 112.6, 109.4 (t, $J = 237.0$ Hz), 98.1; ^{19}F NMR (376 MHz, CDCl_3) δ -115.29 (d, $J = 54.0$ Hz, 2 F); ^{19}F { ^1H } NMR (376 MHz, CDCl_3) δ -115.29 (s, 2 F); HRMS (ESI) m/z calcd for $\text{C}_{12}\text{H}_{10}\text{ONF}_2^+$ $[\text{M}+\text{H}]^+$ 222.0725, found 222.0721.



5kk

5-hexyl-3-(difluoromethyl)isoxazole

Purified by flash column chromatography (petroleum ether/AcOEt = 200:1), colorless oil (30.4 mg, 60% yield); ^1H NMR (400 MHz, CDCl_3) δ 6.72 (t, $J = 54.0$ Hz, 1 H), 6.20 (s, 1 H), 2.79 (t, $J = 7.6$ Hz, 1 H), 1.75 – 1.67 (m, 2 H), 1.39 – 1.27 (m, 6 H), 0.89 (t, $J = 7.0$ Hz, 3 H); ^{13}C NMR (100 MHz, CDCl_3) δ 176.0, 159.1 (t, $J = 30.0$ Hz), 109.6 (t, $J = 237.0$ Hz), 97.9, 31.7, 29.0, 27.7, 27.1, 22.8, 14.3; ^{19}F NMR (376 MHz, CDCl_3) δ -115.17 (d, $J = 54.0$ Hz, 2 F); ^{19}F { ^1H } NMR (376 MHz, CDCl_3) δ -115.17 (s, 2 F); HRMS (ESI) m/z calcd for $\text{C}_{10}\text{H}_{16}\text{ONF}_2^+$ $[\text{M}+\text{H}]^+$ 204.1195, found 204.1199.

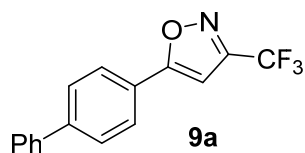


5ll

2-(3-(difluoromethyl)isoxazol-5-yl)ethyl 4-methoxybenzoate

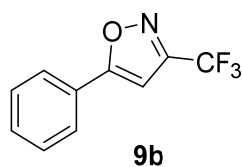
Purified by flash column chromatography (petroleum ether/AcOEt = 20:1), pale yellow oil (49.7 mg, 67% yield); ^1H NMR (400 MHz, CDCl_3) δ 7.97 – 7.93 (m, 2 H),

6.92 – 6.90 (m, 2 H), 6.74 (t, $J = 54.0$ Hz, 1 H), 6.37 (s, 1 H), 4.60 (t, $J = 6.4$ Hz, 1 H), 3.85 (s, 3 H), 3.28 (t, $J = 6.4$ Hz, 2 H); ^{13}C NMR (100 MHz, CDCl_3) δ 172.0, 166.2, 164.0, 159.2 (t, $J = 30.0$ Hz), 132.0, 122.2, 114.1, 109.4 (t, $J = 237.0$ Hz), 99.3, 61.4, 55.8, 27.1; ^{19}F NMR (376 MHz, CDCl_3) δ -115.23 (d, $J = 54.0$ Hz, 2 F); ^{19}F { ^1H } NMR (376 MHz, CDCl_3) δ -115.23 (s, 2 F); HRMS (ESI) m/z calcd for $\text{C}_{14}\text{H}_{14}\text{O}_4\text{NF}_2^+$ $[\text{M}+\text{H}]^+$ 298.0885, found 298.0881.



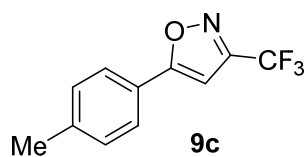
5-([1,1'-biphenyl]-4-yl)-3-(trifluoromethyl)isoxazole

Purified by flash column chromatography (petroleum ether/AcOEt = 200:1), pale yellow solid (60.7 mg, 84% yield); mp: 128.5 – 129.5; ^1H NMR (400 MHz, CDCl_3) δ 7.88 (d, $J = 8.0$ Hz, 2 H), 7.73 (d, $J = 8.0$ Hz, 2 H), 7.64 (d, $J = 8.0$ Hz, 2 H), 7.49 (t, $J = 8.0$ Hz, 2 H), 7.42 (d, $J = 8.0$ Hz, 1 H), 6.77 (s, 1 H); ^{13}C NMR (100 MHz, CDCl_3) δ 172.5, 156.4 (q, $J = 38.0$ Hz), 144.4, 140.0, 129.4, 128.6, 128.2, 127.4, 126.8, 125.2, 120.1 (q, $J = 270.0$ Hz), 97.1; ^{19}F NMR (376 MHz, CDCl_3) δ -63.19 (s, 3 F); ^{19}F { ^1H } NMR (376 MHz, CDCl_3) δ -63.19 (s, 3 F); HRMS (ESI) m/z calcd for $\text{C}_{16}\text{H}_{11}\text{ONF}_3^+$ $[\text{M}+\text{H}]^+$ 290.0787, found 290.0784.



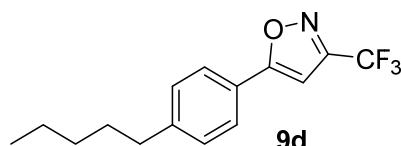
5-phenyl-3-(trifluoromethyl)isoxazole

Purified by flash column chromatography (petroleum ether/AcOEt = 200:1), pale yellow solid (46.7 mg, 88% yield); mp: 44.4 – 45.2; ^1H NMR (400 MHz, CDCl_3) δ 7.83 – 7.78 (m, 2 H), 7.53 – 7.50 (m, 3 H), 6.74 (s, 1 H); ^{13}C NMR (100 MHz, CDCl_3) δ 172.8, 156.4 (q, $J = 38.0$ Hz), 131.6, 129.6, 126.4, 120.1 (q, $J = 270$ Hz), 97.1; ^{19}F NMR (376 MHz, CDCl_3) δ -63.27 (s, 3 F); ^{19}F { ^1H } NMR (376 MHz, CDCl_3) δ -63.27 (s, 3 F); HRMS (ESI) m/z calcd for $\text{C}_{10}\text{H}_7\text{ONF}_3^+$ $[\text{M}+\text{H}]^+$ 214.0474, found 214.0471. ^[9]



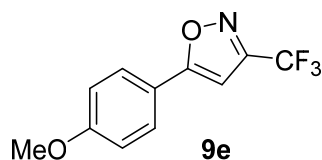
5-(p-tolyl)-3-(trifluoromethyl)isoxazole

Purified by flash column chromatography (petroleum ether/AcOEt = 200:1), white solid (49.6 mg, 87% yield); mp: 71.6 – 72.3; $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.69 (d, J = 8.0 Hz, 2 H), 7.30 (d, J = 8.0 Hz, 2 H), 6.68 (s, 1 H), 2.42 (s, 3 H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 173.0, 156.3 (q, J = 38.0 Hz), 142.2, 130.3, 126.3, 123.8, 120.1 (q, J = 270.0 Hz), 96.5, 21.8; $^{19}\text{F NMR}$ (376 MHz, CDCl_3) δ -63.30 (s, 3 F); $^{19}\text{F}\{^1\text{H}\}$ NMR (376 MHz, CDCl_3) δ -63.30 (s, 3 F); **HRMS (ESI)** m/z calcd for $\text{C}_{11}\text{H}_9\text{ONF}_3^+$ $[\text{M}+\text{H}]^+$ 228.0631, found 228.0628. ^[10]



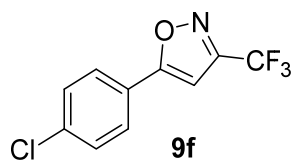
5-(4-pentylphenyl)-3-(trifluoromethyl)isoxazole

Purified by flash column chromatography (petroleum ether/AcOEt = 200:1), colorless oil (61.2 mg, 86% yield); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.71 (d, J = 8.0 Hz, 2 H), 7.31 (d, J = 8.0 Hz, 2 H), 6.68 (s, 1 H), 2.67 (t, J = 8.0 Hz, 2 H), 1.69 – 1.63 (m, 2H), 1.36 – 1.33 (m, 4 H), 0.91 (t, J = 6.8 Hz, 3 H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 173.0, 156.3 (q, J = 38.0 Hz), 147.2, 129.6, 126.4, 123.9, 120.1 (q, J = 270.0 Hz), 96.5, 36.2, 31.8, 31.2, 22.8, 14.3; $^{19}\text{F NMR}$ (376 MHz, CDCl_3) δ -63.29 (s, 3 F); $^{19}\text{F}\{^1\text{H}\}$ NMR (376 MHz, CDCl_3) δ -63.29 (s, 3 F); **HRMS (ESI)** m/z calcd for $\text{C}_{15}\text{H}_{17}\text{ONF}_3^+$ $[\text{M}+\text{H}]^+$ 284.1257, found 284.1254.



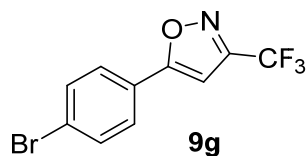
5-(4-methoxyphenyl)-3-(trifluoromethyl)isoxazole

Purified by flash column chromatography (petroleum ether/AcOEt = 100:1), yellow solid (49.4 mg, 81% yield); mp: 82.5 – 83.3; $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.74 (d, J = 8.0 Hz, 2 H), 7.00 (d, J = 8.0 Hz, 2 H), 6.61 (s, 1 H), 3.88 (s, 3 H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 172.8, 162.3, 156.3 (q, J = 38.0 Hz), 128.1, 120.1 (q, J = 270.0 Hz), 119.2, 115.0, 95.7, 55.8; $^{19}\text{F NMR}$ (376 MHz, CDCl_3) δ -63.30 (s, 3 F); $^{19}\text{F}\{^1\text{H}\}$ NMR (376 MHz, CDCl_3) δ -63.30 (s, 3 F); **HRMS (ESI)** m/z calcd for $\text{C}_{11}\text{H}_9\text{O}_2\text{NF}_3^+$ $[\text{M}+\text{H}]^+$ 244.0580, found 244.0579. ^[9]



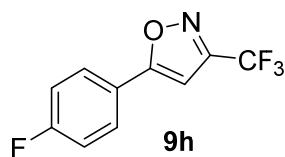
5-(4-chlorophenyl)-3-(trifluoromethyl)isoxazole

Purified by flash column chromatography (petroleum ether/AcOEt = 200:1), white crystalline solid (56.2 mg, 91% yield); mp: 97.4 – 97.7; ^1H NMR (400 MHz, CDCl_3) δ 7.74 (d, J = 8.0 Hz, 2 H), 7.49 (d, J = 8.0 Hz, 2 H), 6.74 (s, 1 H); ^{13}C NMR (100 MHz, CDCl_3) δ 171.7, 156.5 (q, J = 38.0 Hz), 137.9, 130.0, 127.6, 124.9, 120.0 (q, J = 270.0 Hz), 97.4; ^{19}F NMR (376 MHz, CDCl_3) δ -63.28 (s, 3 F); ^{19}F { ^1H } NMR (376 MHz, CDCl_3) δ -63.28 (s, 3 F); HRMS (ESI) m/z calcd for $\text{C}_{10}\text{H}_6\text{ONClF}_3^+$ $[\text{M}+\text{H}]^+$ 248.0085, found 248.0082.



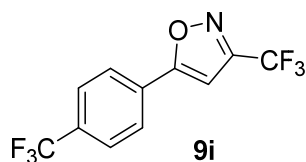
5-(4-bromophenyl)-3-(trifluoromethyl)isoxazole

Purified by flash column chromatography (petroleum ether/AcOEt = 200:1), white crystalline solid (62.9 mg, 86% yield); mp: 107.2 – 108.3; ^1H NMR (400 MHz, CDCl_3) δ 7.68 – 7.63 (m, 4 H), 6.75 (s, 1 H); ^{13}C NMR (100 MHz, CDCl_3) δ 171.7, 156.5 (q, J = 38.0 Hz), 132.9, 127.8, 126.2, 125.3, 119.9 (q, J = 270.0 Hz), 97.5; ^{19}F NMR (376 MHz, CDCl_3) δ -63.26 (s, 3 F); ^{19}F { ^1H } NMR (376 MHz, CDCl_3) δ -63.26 (s, 3 F); HRMS (ESI) m/z calcd for $\text{C}_{10}\text{H}_6\text{ONBrF}_3^+$ $[\text{M}+\text{H}]^+$ 291.9579, found 291.9576.^[9]



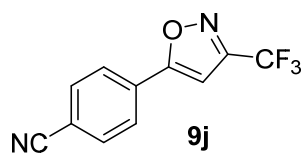
5-(4-fluorophenyl)-3-(trifluoromethyl)isoxazole

Purified by flash column chromatography (petroleum ether/AcOEt = 200:1), white solid (53.6 mg, 93% yield); mp: 59.4 – 60.4; ^1H NMR (400 MHz, CDCl_3) δ 7.83 – 7.78 (m, 2 H), 7.23 – 7.18 (m, 2 H), 6.70 (s, 1 H); ^{13}C NMR (100 MHz, CDCl_3) δ 171.8, 164.7 (d, J = 252 Hz), 156.5 (q, J = 38.0 Hz), 128.6 (d, J = 9.0 Hz), 122.9 (d, J = 4.0 Hz), 120.0 (q, J = 270.0 Hz), 117.0 (d, J = 22.0 Hz), 96.9; ^{19}F NMR (376 MHz, CDCl_3) δ -63.30 (s, 3 F), -107.38 – -107.46 (m, 1 F); ^{19}F { ^1H } NMR (376 MHz, CDCl_3) δ -63.30 (s, 3 F), -107.42 (s, 1 F); HRMS (ESI) m/z calcd for $\text{C}_{10}\text{H}_6\text{ONF}_4^+$ $[\text{M}+\text{H}]^+$ 232.0380, found 232.0378.^[11]



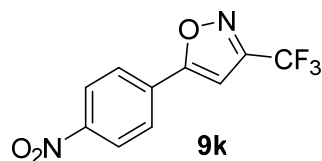
3-(trifluoromethyl)-5-(4-(trifluoromethyl)phenyl)isoxazole

Purified by flash column chromatography (petroleum ether/AcOEt = 200:1), white crystalline solid (58.4 mg, 83% yield); mp: 94.8 – 95.3; ¹H NMR (400 MHz, CDCl₃) δ 7.94 (d, *J* = 8.0 Hz, 2 H), 7.78 (d, *J* = 8.0 Hz, 2 H), 6.86 (s, 1 H); ¹³C NMR (100 MHz, CDCl₃) δ 171.2, 156.6 (q, *J* = 38.0 Hz), 133.3 (q, *J* = 33.0 Hz), 129.5, 126.8, 126.7 (q, *J* = 4.0 Hz), 123.9 (q, *J* = 270.0 Hz), 119.9 (q, *J* = 270.0 Hz), 98.6; ¹⁹F NMR (376 MHz, CDCl₃) δ -63.19 (s, 3 F), -63.31 (s, 3 F); ¹⁹F {¹H} NMR (376 MHz, CDCl₃) δ -63.19 (s, 3 F), -63.31 (s, 3 F); HRMS (ESI) *m/z* calcd for C₁₁H₆ONF₆⁺ [M+H]⁺ 282.0348, found 282.0346.



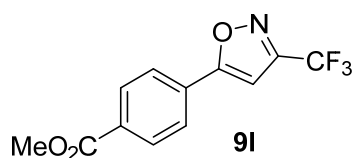
4-(3-(trifluoromethyl)isoxazol-5-yl)benzonitrile

Purified by flash column chromatography (petroleum ether/AcOEt = 20:1), white solid (42.1 mg, 71% yield); mp: 120.0 – 120.8; ¹H NMR (400 MHz, CDCl₃) δ 7.93 (d, *J* = 8.0 Hz, 2 H), 7.82 (d, *J* = 8.0 Hz, 2 H), 6.90 (s, 1 H); ¹³C NMR (100 MHz, CDCl₃) δ 170.5, 156.6 (q, *J* = 38.0 Hz), 133.4, 130.0, 126.9, 119.7 (q, *J* = 270.0 Hz), 118.1, 115.1, 99.3; ¹⁹F NMR (376 MHz, CDCl₃) δ -63.22 (s, 3 F); ¹⁹F {¹H} NMR (376 MHz, CDCl₃) δ -63.22 (s, 3 F); HRMS (ESI) *m/z* calcd for C₁₁H₆ON₂F₃⁺ [M+H]⁺ 239.0427, found 239.0425. ^[9]



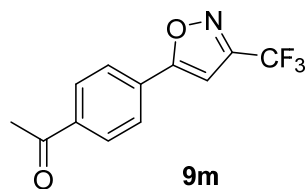
5-(4-nitrophenyl)-3-(trifluoromethyl)isoxazole

Purified by flash column chromatography (petroleum ether/AcOEt = 15:1), white solid (49.2 mg, 76% yield); mp: 126.5 – 127.3; ¹H NMR (400 MHz, CDCl₃) δ 8.38 (d, *J* = 8.0 Hz, 2 H), 8.01 (d, *J* = 8.0 Hz, 2 H), 6.96 (s, 1 H); ¹³C NMR (100 MHz, CDCl₃) δ 170.2, 156.7 (q, *J* = 38.0 Hz), 149.5, 131.7, 127.3, 125.0, 119.7 (q, *J* = 270.0 Hz), 99.7; ¹⁹F NMR (376 MHz, CDCl₃) δ -63.23 (s, 3 F). ¹⁹F {¹H} NMR (376 MHz, CDCl₃) δ -63.23 (s, 3 F); HRMS (ESI) *m/z* calcd for C₁₆H₆O₃N₂F₃⁺ [M+H]⁺ 259.0325, found 259.0321.



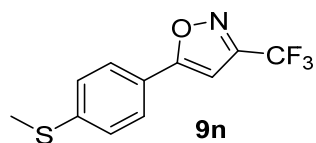
methyl 4-(3-(trifluoromethyl)isoxazol-5-yl)benzoate

Purified by flash column chromatography (petroleum ether/AcOEt = 40:1), white solid (57.5 mg, 85% yield); mp: 125.6 – 126.8; ^1H NMR (400 MHz, CDCl_3) δ 8.15 (d, J = 8.0 Hz, 2 H), 7.86 (d, J = 8.0 Hz, 2 H), 6.85 (s, 1 H), 3.95 (s, 3 H); ^{13}C NMR (100 MHz, CDCl_3) δ 171.6, 166.3, 156.5 (q, J = 38.0 Hz), 132.8, 130.8, 130.0, 126.3, 119.9 (q, J = 270.0 Hz), 98.5, 52.8; ^{19}F NMR (376 MHz, CDCl_3) δ -63.28 (s, 3 F); ^{19}F { ^1H } NMR (376 MHz, CDCl_3) δ -63.28 (s, 3 F); HRMS (ESI) m/z calcd for $\text{C}_{12}\text{H}_9\text{O}_3\text{NF}_3^+$ $[\text{M}+\text{H}]^+$ 272.0529, found 272.0526.



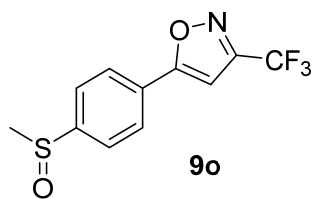
1-(4-(3-(trifluoromethyl)isoxazol-5-yl)phenyl)ethan-1-one

Purified by flash column chromatography (petroleum ether/AcOEt = 20:1), white crystalline solid (48.4 mg, 76% yield); mp: 168.1 – 169.3; ^1H NMR (400 MHz, CDCl_3) δ 8.08 (d, J = 8.0 Hz, 2 H), 7.91 (d, J = 8.0 Hz, 2 H), 6.86 (s, 1 H), 2.65 (s, 3 H); ^{13}C NMR (100 MHz, CDCl_3) δ 197.3, 171.5, 156.5 (q, J = 38.0 Hz), 139.2, 130.1, 129.5, 126.6, 119.9 (q, J = 270.0 Hz), 98.6, 27.0; ^{19}F NMR (376 MHz, CDCl_3) δ -63.24 (s, 3 F); ^{19}F { ^1H } NMR (376 MHz, CDCl_3) δ -63.24 (s, 3 F); HRMS (ESI) m/z calcd for $\text{C}_{12}\text{H}_9\text{O}_2\text{NF}_3^+$ $[\text{M}+\text{H}]^+$ 256.0580, found 256.0577.



5-(4-(methylthio)phenyl)-3-(trifluoromethyl)isoxazole

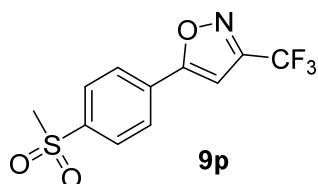
Purified by flash column chromatography (petroleum ether/AcOEt = 100:1), yellow solid (58.2 mg, 90% yield); mp: 89.1 – 90.2; ^1H NMR (400 MHz, CDCl_3) δ 7.68 (d, J = 8.0 Hz, 2 H), 7.31 (d, J = 8.0 Hz, 2 H), 6.68 (s, 1 H), 2.52 (s, 3 H); ^{13}C NMR (100 MHz, CDCl_3) δ 172.4, 156.3 (q, J = 38.0 Hz), 143.9, 126.6, 126.3, 122.6, 120.0 (q, J = 270.0 Hz), 96.5, 15.2; ^{19}F NMR (376 MHz, CDCl_3) δ -63.27 (s, 3 F); ^{19}F { ^1H } NMR (376 MHz, CDCl_3) δ -63.27 (s, 3 F); HRMS (ESI) m/z calcd for $\text{C}_{11}\text{H}_9\text{ONF}_3\text{S}^+$ $[\text{M}+\text{H}]^+$ 260.0352, found 260.0349.



9o

5-(4-(methylsulfinyl)phenyl)-3-(trifluoromethyl)isoxazole

Purified by flash column chromatography (petroleum ether/AcOEt = 3:1), pale yellow solid (51.1 mg, 74% yield); mp: 119.4 – 121.9; ^1H NMR (400 MHz, CDCl_3) δ 7.96 (d, J = 8.0 Hz, 2 H), 7.82 (d, J = 8.0 Hz, 2 H), 6.87 (s, 1 H), 2.88 (s, 3 H); ^{13}C NMR (100 MHz, CDCl_3) δ 171.0, 156.5 (q, J = 38.0 Hz), 147.2, 129.1, 127.3, 125.3, 119.8 (q, J = 270.0 Hz), 98.6, 43.5; ^{19}F NMR (376 MHz, CDCl_3) δ -63.22 (s, 3 F); ^{19}F { ^1H } NMR (376 MHz, CDCl_3) δ -63.22 (s, 3 F); HRMS (ESI) m/z calcd for $\text{C}_{11}\text{H}_9\text{O}_2\text{NF}_3\text{S}^+$ $[\text{M}+\text{H}]^+$ 276.0301, found 276.0298.

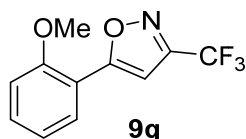


9p

5-(4-(methylsulfonyl)phenyl)-3-

(trifluoromethyl)isoxazole

Purified by flash column chromatography (petroleum ether/AcOEt = 7:1), white crystalline solid (54.9 mg, 75% yield); mp: 146.3 – 147.5; ^1H NMR (400 MHz, CDCl_3) δ 8.09 (d, J = 8.0 Hz, 2 H), 8.01 (d, J = 8.0 Hz, 2 H), 6.93 (s, 1 H), 3.10 (s, 3 H); ^{13}C NMR (100 MHz, CDCl_3) δ 170.5, 156.6 (q, J = 38.0 Hz), 143.1, 131.0, 128.8, 127.2, 119.8 (q, J = 270.0 Hz), 99.4, 44.7; ^{19}F NMR (376 MHz, CDCl_3) δ -63.20 (s, 3 F); ^{19}F { ^1H } NMR (376 MHz, CDCl_3) δ -63.20 (s, 3 F); HRMS (ESI) m/z calcd for $\text{C}_{11}\text{H}_9\text{O}_3\text{NF}_3\text{S}^+$ $[\text{M}+\text{H}]^+$ 292.0250, found 292.0245.

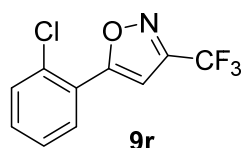


9q

5-(2-methoxyphenyl)-3-(trifluoromethyl)isoxazole

Purified by flash column chromatography (petroleum ether/AcOEt = 100:1), pale yellow solid (55.8 mg, 92% yield); mp: 41.8 – 43.0; ^1H NMR (400 MHz, CDCl_3) δ 7.98 (dd, J = 1.6, 8.0 Hz, 1 H), 7.49 – 7.44 (m, 1 H), 7.09 (t, J = 8.0 Hz, 1 H), 7.04 (d, J = 8.0 Hz, 1 H), 7.00 (s, 1 H), 3.98 (s, 3 H); ^{13}C NMR (100 MHz, CDCl_3) δ 168.8, 156.8, 156.4 (q, J = 38.0 Hz), 132.7, 128.1, 121.3, 120.3 (q, J = 270.0 Hz), 115.5, 111.7, 101.0, 55.9; ^{19}F NMR (376 MHz, CDCl_3) δ -63.25 (s, 3 F); ^{19}F { ^1H } NMR (376 MHz,

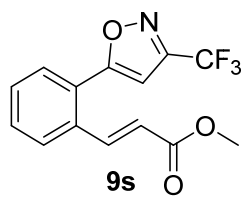
CDCl₃) δ -63.25 (s, 3 F); **HRMS (ESI)** m/z calcd for C₁₁H₉O₂NF₃⁺ [M+H]⁺ 244.0580, found 244.0577.



9r

5-(2-chlorophenyl)-3-(trifluoromethyl)isoxazole

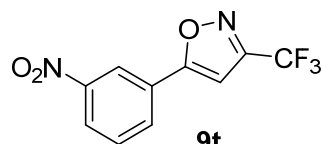
Purified by flash column chromatography (petroleum ether/AcOEt = 200:1), colorless oil (52.8 mg, 85% yield); **¹H NMR** (400 MHz, CDCl₃) δ 7.98 – 7.96 (m, 1 H), 7.55 – 7.53 (m, 1 H), 7.45 – 7.42 (m, 2 H), 7.18 (s, 1 H); **¹³C NMR** (100 MHz, CDCl₃) δ 169.1, 156.3 (q, J = 38.0 Hz), 132.4, 132.2, 131.4, 129.8, 127.8, 125.3, 120.0 (q, J = 270.0 Hz), 101.9; **¹⁹F NMR** (376 MHz, CDCl₃) δ -63.21 (s, 3 F); **¹⁹F {¹H} NMR** (376 MHz, CDCl₃) δ -63.21 (s, 3 F); **HRMS (ESI)** m/z calcd for C₁₀H₆ONClF₃⁺ [M+H]⁺ 248.0085, found 248.0082.



9s

methyl (E)-3-(2-(3-(trifluoromethyl)isoxazol-5-yl)phenyl)acrylate

Purified by flash column chromatography (petroleum ether/AcOEt = 20:1), white solid (61.9 mg, 83% yield); mp: 64.5 – 65.7; **¹H NMR** (400 MHz, CDCl₃) δ 7.92 (d, J = 16.0 Hz, 1 H), 7.76 – 7.74 (m, 1 H), 7.69 – 7.67 (m, 1 H), 7.56 – 7.50 (m, 2 H), 6.62 (s, 1 H), 6.44 (d, J = 16.0 Hz, 1 H), 3.81 (s, 3 H); **¹³C NMR** (100 MHz, CDCl₃) δ 171.2, 166.8, 156.1 (q, J = 38.0 Hz), 141.8, 134.0, 131.7, 130.5, 129.6, 128.2, 126.1, 122.5, 119.9 (q, J = 270.0 Hz), 101.7, 52.3; **¹⁹F NMR** (376 MHz, CDCl₃) δ -63.09 (s, 3 F); **¹⁹F {¹H} NMR** (376 MHz, CDCl₃) δ -63.09 (s, 3 F); **HRMS (ESI)** m/z calcd for C₁₄H₁₁O₃NF₃⁺ [M+H]⁺ 298.0686, found 298.0684.

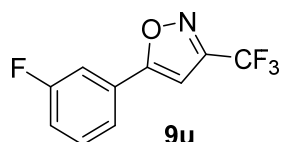


9t

5-(3-nitrophenyl)-3-(trifluoromethyl)isoxazole

Purified by flash column chromatography (petroleum ether/AcOEt = 25:1), white solid (54.7 mg, 85% yield); mp: 98.7 – 99.2; **¹H NMR** (400 MHz, CDCl₃) δ 8.65 (s, 1 H),

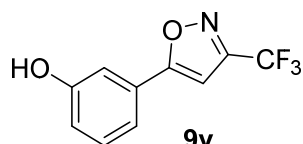
8.37 (d, $J = 8.0$ Hz, 1 H), 8.16 (d, $J = 8.0$ Hz, 1 H), 7.76 (t, $J = 8.0$ Hz, 1 H), 6.95 (s, 1 H); ^{13}C NMR (100 MHz, CDCl_3) δ 170.1, 156.7 (q, $J = 38.0$ Hz), 149.1, 131.8, 131.0, 127.8, 126.0, 121.4, 119.7 (q, $J = 270.0$ Hz), 99.0; ^{19}F NMR (376 MHz, CDCl_3) δ -63.26 (s, 3 F); ^{19}F { ^1H } NMR (376 MHz, CDCl_3) δ -63.26 (s, 3 F); HRMS (ESI) m/z calcd for $\text{C}_{16}\text{H}_6\text{O}_3\text{N}_2\text{F}_3^+$ $[\text{M}+\text{H}]^+$ 259.0325, found 259.0322.



9u

5-(3-fluorophenyl)-3-(trifluoromethyl)isoxazole

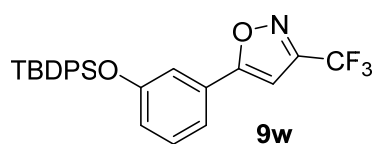
Purified by flash column chromatography (petroleum ether/AcOEt = 200:1), white solid (48.5 mg, 84% yield); mp: 47.2 – 47.7; ^1H NMR (400 MHz, CDCl_3) δ 7.60 – 7.58 (m, 1 H), 7.52 – 7.47 (m, 2 H), 7.24 – 7.19 (m, 1 H), 6.77 (s, 1 H); ^{13}C NMR (100 MHz, CDCl_3) δ 171.4 (d, $J = 3.0$ Hz), 163.3 (d, $J = 247.0$ Hz), 156.5 (q, $J = 38.0$ Hz), 131.5 (d, $J = 8.0$ Hz), 128.2 (d, $J = 9.0$ Hz), 122.2 (d, $J = 4.0$ Hz), 119.9 (q, $J = 270.0$ Hz), 118.6 (d, $J = 21.0$ Hz), 113.4 (d, $J = 24.0$ Hz), 97.9; ^{19}F NMR (376 MHz, CDCl_3) δ -63.31 (s, 3 F), -110.81 – -110.87 (m, 1 F); ^{19}F { ^1H } NMR (376 MHz, CDCl_3) δ -63.31 (s, 3 F), -110.84 (s, 1 F); HRMS (ESI) m/z calcd for $\text{C}_{10}\text{H}_6\text{ONF}_4^+$ $[\text{M}+\text{H}]^+$ 232.0380, found 232.0378.



9v

3-(3-(trifluoromethyl)isoxazol-5-yl)phenol

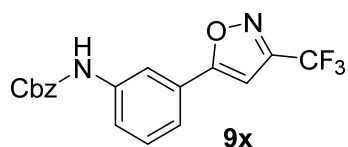
Purified by flash column chromatography (petroleum ether/AcOEt = 10:1), white solid (42.8 mg, 75% yield); mp: 115.4 – 116.5; ^1H NMR (400 MHz, CDCl_3) δ 7.48 (t, $J = 2.0$ Hz, 1 H), 7.40 – 7.32 (m, 2 H), 7.04 – 7.01 (m, 1 H), 6.75 (s, 1 H), 6.31 (s, 1 H); ^{13}C NMR (100 MHz, CDCl_3) δ 172.7, 157.0, 156.4 (q, $J = 38.0$ Hz), 131.1, 127.4, 119.9 (q, $J = 270.0$ Hz), 119.2, 118.8, 113.0, 97.5; ^{19}F NMR (376 MHz, CDCl_3) δ -63.31 (s, 3 F); ^{19}F { ^1H } NMR (376 MHz, CDCl_3) δ -63.31 (s, 3 F); HRMS (ESI) m/z calcd for $\text{C}_{10}\text{H}_7\text{O}_2\text{NF}_3^+$ $[\text{M}+\text{H}]^+$ 230.0423, found 230.0423.



9w

5-(3-((tert-butyldiphenylsilyl)oxy)phenyl)-3-(trifluoromethyl)isoxazole

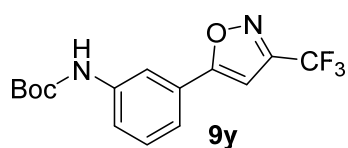
Purified by flash column chromatography (petroleum ether/AcOEt = 30:1), bright yellow oil (112.0 mg, 96% yield); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.64 – 7.62 (m, 4 H), 7.33 – 7.31 (m, 2 H), 7.29 – 7.26 (m, 4 H), 7.19 – 7.17 (m, 1 H), 7.09 – 7.04 (m, 2 H), 6.76 – 6.73 (m, 1 H), 6.37 (s, 1 H), 1.04 (s, 9 H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 172.5, 156.6, 156.2 (q, $J = 38.0$ Hz), 135.9, 132.7, 130.5, 130.5, 128.3, 127.4, 123.0, 120.0 (q, $J = 270.0$ Hz), 119.1, 117.7, 97.2 (q, $J = 1.0$ Hz), 26.9, 19.8; $^{19}\text{F NMR}$ (376 MHz, CDCl_3) δ -63.24 (s, 3 F); $^{19}\text{F}\{^1\text{H}\}$ NMR (376 MHz, CDCl_3) δ -63.24 (s, 3 F); **HRMS (ESI)** m/z calcd for $\text{C}_{26}\text{H}_{25}\text{O}_2\text{NF}_3\text{Si}^+$ $[\text{M}+\text{H}]^+$ 468.1601, found 468.1597.



benzyl (3-(3-(trifluoromethyl)isoxazol-5-

yl)phenyl)carbamate

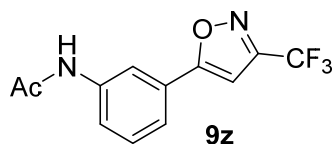
Purified by flash column chromatography (petroleum ether/AcOEt = 20:1), white solid (83.2 mg, 92% yield); mp: 137.3 – 137.9; $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.94 (s, 1 H), 7.49 – 7.47 (m, 2 H), 7.45 – 7.35 (m, 6 H), 7.05 (s, 1 H), 6.71 (s, 1 H), 5.23 (s, 2 H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 172.3, 156.3 (q, $J = 38.0$ Hz), 153.6, 139.2, 136.1, 130.3, 129.0, 128.8, 128.7, 127.1, 121.5, 121.2, 120.0 (q, $J = 270.0$ Hz), 116.3, 97.5, 67.7; $^{19}\text{F NMR}$ (376 MHz, CDCl_3) δ -63.22 (s, 3 F); $^{19}\text{F}\{^1\text{H}\}$ NMR (376 MHz, CDCl_3) δ -63.22 (s, 3 F); **HRMS (ESI)** m/z calcd for $\text{C}_{18}\text{H}_{14}\text{O}_3\text{N}_2\text{F}_3^+$ $[\text{M}+\text{H}]^+$ 363.0951, found 363.0947.



tert-butyl (3-(3-(trifluoromethyl)isoxazol-5-

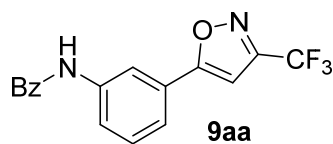
yl)phenyl)carbamate

Purified by flash column chromatography (petroleum ether/AcOEt = 10:1), white crystalline solid (67.2 mg, 82% yield); mp: 153.8 – 154.6; $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.97 (s, 1 H), 7.47 – 7.45 (m, 1 H), 7.40 – 7.39 (m, 2 H), 6.77 (s, 1 H), 6.75 (s, 1 H), 1.53 (s, 9 H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 172.6, 156.3 (q, $J = 38.0$ Hz), 152.9, 139.8, 130.2, 127.1, 121.3, 120.8, 120.0 (q, $J = 270.0$ Hz), 116.0, 97.5, 81.5, 28.6; $^{19}\text{F NMR}$ (376 MHz, CDCl_3) δ -63.27 (s, 3 F); $^{19}\text{F}\{^1\text{H}\}$ NMR (376 MHz, CDCl_3) δ -63.27 (s, 3 F); **HRMS (ESI)** m/z calcd for $\text{C}_{15}\text{H}_{16}\text{O}_3\text{N}_2\text{F}_3^+$ $[\text{M}+\text{H}]^+$ 329.1108, found 329.1103.



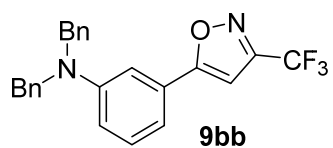
***N*-(3-(3-(trifluoromethyl)isoxazol-5-yl)phenyl)acetamide**

Purified by flash column chromatography (petroleum ether/AcOEt = 5:1), white crystalline solid (54.3 mg, 80% yield); mp: 174.4 – 175.8; **¹H NMR** (400 MHz, acetone-*d*₆) δ 9.47 (s, 1 H), 8.34 (s, 1 H), 7.78 – 7.76 (m, 1 H), 7.65 – 7.63 (m, 1 H), 7.50 (t, *J* = 8.0 Hz, 1 H), 7.33 (s, 1 H), 2.14 (s, 3 H); **¹³C NMR** (100 MHz, acetone-*d*₆) δ 173.6, 169.4, 156.7 (q, *J* = 38.0 Hz), 141.4, 130.7, 127.3, 122.6, 121.7, 120.9 (q, *J* = 269.0 Hz), 117.1, 98.4, 24.3; **¹⁹F NMR** (376 MHz, acetone-*d*₆) δ -64.06 (s, 3 F); **¹⁹F {¹H} NMR** (376 MHz, acetone-*d*₆) δ -64.06 (s, 3 F); **HRMS (ESI)** *m/z* calcd for C₁₂H₁₀O₂N₂F₃⁺ [M+H]⁺ 271.0689, found 271.0687.



***N*-(3-(3-(trifluoromethyl)isoxazol-5-yl)phenyl)benzamide**

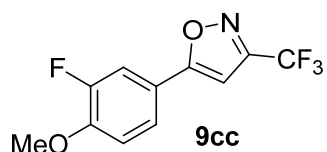
Purified by flash column chromatography (petroleum ether/AcOEt = 6:1), white crystalline solid (64.9 mg, 78% yield); mp: 195.6 – 196.3; **¹H NMR** (400 MHz, acetone-*d*₆) δ 9.78 (s, 1 H), 8.52 (s, 1 H), 8.05 – 8.02 (m, 3 H), 8.71 – 7.69 (m, 1 H), 7.61 – 7.50 (m, 4 H), 7.35 (s, 1 H); **¹³C NMR** (100 MHz, acetone-*d*₆) δ 173.6, 166.7, 156.8 (q, *J* = 38.0 Hz), 141.4, 135.9, 132.7, 130.8, 129.4, 128.5, 127.4, 123.8, 123.7, 122.3, 121.0 (q, *J* = 270.0 Hz), 118.3, 118.2, 98.5; **¹⁹F NMR** (376 MHz, acetone-*d*₆) δ -64.00 (s, 3 F); **¹⁹F {¹H} NMR** (376 MHz, acetone-*d*₆) δ -64.00 (s, 3 F); **HRMS (ESI)** *m/z* calcd for C₁₇H₁₂O₂N₂F₃⁺ [M+H]⁺ 333.0845, found 333.0844.



***N,N*-dibenzyl-3-(3-(trifluoromethyl)isoxazol-5-yl)aniline**

Purified by flash column chromatography (petroleum ether/AcOEt = 15:1), yellow solid (78.4 mg, 77% yield); mp: 104.8 – 106.8; **¹H NMR** (400 MHz, CDCl₃) δ 7.25 – 7.21 (m, 4 H), 7.17 – 7.11 (m, 8 H), 7.06 – 7.05 (m, 1 H), 6.97 (d, *J* = 8.0 Hz, 1 H), 6.74 (dd, *J* = 2.4, 8.4 Hz, 1 H), 6.44 (s, 1 H), 4.60 (s, 4 H); **¹³C NMR** (100 MHz, CDCl₃) δ 173.5, 156.1 (q, *J* = 38.0 Hz), 149.9, 138.1, 130.5, 129.2, 127.5, 127.2, 126.9, 120.1 (q, *J* = 270.0 Hz), 115.6, 114.8, 109.7, 97.0, 54.7; **¹⁹F NMR** (376 MHz,

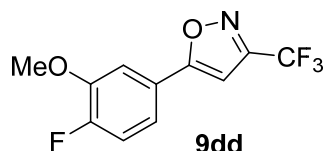
CDCl₃) δ -63.15 (s, 3 F); **¹⁹F {¹H} NMR** (376 MHz, CDCl₃) δ -63.15 (s, 3 F); **HRMS (ESI)** m/z calcd for C₂₄H₂₀ON₂F₃⁺ [M+H]⁺ 409.1522, found 409.1520.



5-(3-fluoro-4-methoxyphenyl)-3-

(trifluoromethyl)isoxazole

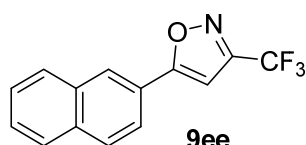
Purified by flash column chromatography (petroleum ether/AcOEt = 100:1), pale yellow solid (56.7 mg, 87% yield); mp: 116.5 – 117.1; **¹H NMR** (400 MHz, CDCl₃) δ 7.55 (dd, J = 3.2, 8.8 Hz, 1 H), 7.50 (dd, J = 2.0, 11.2 Hz, 1 H), 7.18 (t, J = 8.8 Hz, 1 H), 6.63 (s, 1 H), 3.95 (s, 3 H); **¹³C NMR** (100 MHz, CDCl₃) δ 171.6 (d, J = 2.5 Hz), 156.4 (q, J = 38.0 Hz), 152.7 (d, J = 247.0 Hz), 150.6 (d, J = 11.0 Hz), 123.0 (d, J = 3.0 Hz), 120.0 (q, J = 269.0 Hz), 119.3 (d, J = 7.0 Hz), 114.2 (d, J = 21.0 Hz), 114.0 (d, J = 3.0 Hz), 96.5 (d, J = 1.0 Hz), 56.6; **¹⁹F NMR** (376 MHz, CDCl₃) δ -63.36 (s, 3 F), -133.09 – -133.14 (m, 1 F); **¹⁹F {¹H} NMR** (376 MHz, CDCl₃) δ -63.36 (s, 3 F), -133.12 (s, 1 F); **HRMS (ESI)** m/z calcd for C₁₁H₈O₂NF₄⁺ [M+H]⁺ 262.0486, found 262.0482.



5-(4-fluoro-3-methoxyphenyl)-3-

(trifluoromethyl)isoxazole

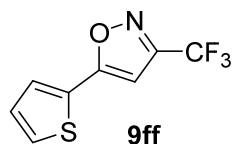
Purified by flash column chromatography (petroleum ether/AcOEt = 100:1), white solid (59.3 mg, 91% yield); mp: 95.9 – 97.0; **¹H NMR** (400 MHz, CDCl₃) δ 7.39 (dd, J = 2.0, 7.6 Hz, 1 H), 7.33 (dq, J = 2.0, 8.4 Hz, 1 H), 7.18 (dd, J = 8.4, 10.8 Hz, 1 H), 6.69 (s, 1 H), 3.96 (s, 3 H); **¹³C NMR** (100 MHz, CDCl₃) δ 171.9 (d, J = 1.4 Hz), 156.4 (q, J = 38.0 Hz), 154.5 (d, J = 251 Hz), 148.8 (d, J = 11 Hz), 123.0 (d, J = 4.0 Hz), 120.0 (q, J = 270.0 Hz), 119.6 (d, J = 7.0 Hz), 117.3 (d, J = 19.0 Hz), 111.3 (d, J = 19.0 Hz), 97.1, 56.7; **¹⁹F NMR** (376 MHz, CDCl₃) δ -63.34 (s, 3 F), -129.35 – -129.41 (m, 1 F); **¹⁹F {¹H} NMR** (376 MHz, CDCl₃) δ -63.34 (s, 3 F), -129.38 (s, 1 F); **HRMS (ESI)** m/z calcd for C₁₁H₈O₂NF₄⁺ [M+H]⁺ 262.0486, found 262.0482.



9ee

5-(naphthalen-2-yl)-3-(trifluoromethyl)isoxazole

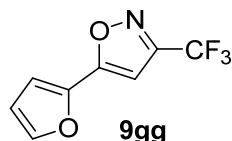
Purified by flash column chromatography (petroleum ether/AcOEt = 200:1), white solid (53.5 mg, 81% yield); mp: 96.9 – 97.5; $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.31 (s, 1 H), 7.95 – 7.91 (m, 2 H), 7.89-7.86 (m, 1 H), 7.79 (dd, J = 2.0, 8.4 Hz, 1 H), 7.59 – 7.57 (m, 2 H), 6.83 (s, 1 H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 172.8, 156.4 (q, J = 38.0 Hz), 134.7, 133.2, 129.6, 129.1, 128.3, 128.3, 127.6, 126.6, 123.6, 122.8, 120.1 (q, J = 270.0 Hz), 97.4; $^{19}\text{F NMR}$ (376 MHz, CDCl_3) δ -63.19 (s, 3 F); $^{19}\text{F}\{^1\text{H}\}$ NMR (376 MHz, CDCl_3) δ -63.19 (s, 3 F); **HRMS (ESI)** m/z calcd for $\text{C}_{14}\text{H}_9\text{ONF}_3^+$ $[\text{M}+\text{H}]^+$ 264.0631, found 264.0629.



9ff

5-(thiophen-2-yl)-3-(trifluoromethyl)isoxazole

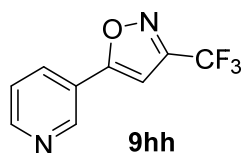
Purified by flash column chromatography (petroleum ether/AcOEt = 50:1), brown oil (38.2 mg, 70% yield); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.60 (dd, J = 1.2, 3.6 Hz, 1 H), 7.54 (dd, J = 1.2, 4.2 Hz, 1 H), 7.17 (dd, J = 3.6, 4.8 Hz, 1 H), 6.60 (s, 1 H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 167.7, 156.3 (q, J = 38.0 Hz), 129.8, 128.7, 128.7, 128.0, 119.9 (q, J = 270.0 Hz), 96.7; $^{19}\text{F NMR}$ (376 MHz, CDCl_3) δ -63.27 (s, 3 F); $^{19}\text{F}\{^1\text{H}\}$ NMR (376 MHz, CDCl_3) δ -63.27 (s, 3 F); **HRMS (ESI)** m/z calcd for $\text{C}_8\text{H}_5\text{ONSF}_3^+$ $[\text{M}+\text{H}]^+$ 220.0039, found 220.0040.



9gg

5-(furan-2-yl)-3-(trifluoromethyl)isoxazole

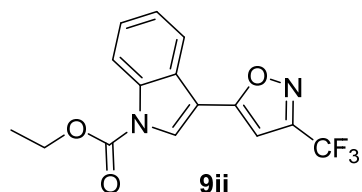
Purified by flash column chromatography (petroleum ether/AcOEt = 50:1), pale brown oil (38.4 mg, 76% yield); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.60 – 7.59 (m, 1 H), 7.02 (d, J = 4.0 Hz, 1 H), 6.65 (s, 1 H), 6.58 (dd, J = 1.6, 3.6 Hz, 1 H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 164.2, 156.1 (q, J = 38.0 Hz), 145.5, 142.3, 119.9 (q, J = 270.0 Hz), 112.6, 112.4, 96.6; $^{19}\text{F NMR}$ (376 MHz, CDCl_3) δ -63.23 (s, 3 F); $^{19}\text{F}\{^1\text{H}\}$ NMR (376 MHz, CDCl_3) δ -63.23 (s, 3 F); **HRMS (ESI)** m/z calcd for $\text{C}_8\text{H}_5\text{NO}_2\text{F}_3^+$ $[\text{M}+\text{H}]^+$ 204.0267, found 204.0261.



9hh

5-(pyridin-3-yl)-3-(trifluoromethyl)isoxazole

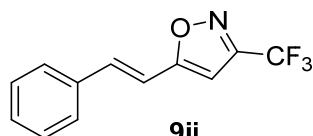
Purified by flash column chromatography (petroleum ether/AcOEt = 10:1), yellow solid (33.5 mg, 63% yield); mp: 64.1 – 65.9; $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 9.06 (s, 1 H), 8.76 (d, J = 4.0 Hz, 1 H), 8.13 (dt, J = 2.0, 8.0 Hz, 1 H), 7.48 (dd, J = 4.8, 8.0 Hz, 1 H), 6.86 (s, 1 H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 170.1, 156.6 (q, J = 38.0 Hz), 152.4, 147.5, 133.5, 124.3, 122.8, 119.9 (q, J = 269.0 Hz), 98.2; $^{19}\text{F NMR}$ (376 MHz, CDCl_3) δ -63.20 (s, 3 F); $^{19}\text{F}\{^1\text{H}\}$ NMR (376 MHz, CDCl_3) δ -63.20 (s, 3 F); **HRMS (ESI)** m/z calcd for $\text{C}_9\text{H}_6\text{ON}_2\text{F}_3^+$ $[\text{M}+\text{H}]^+$ 215.0427, found 215.0426.



9ii

ethyl 3-(3-(trifluoromethyl)isoxazol-5-yl)-1H-indole-1-carboxylate

Purified by flash column chromatography (petroleum ether/AcOEt = 20:1), yellow solid (68.3 mg, 84% yield); mp: 126.1 – 127.2; $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.23 (d, J = 8.0 Hz, 1 H), 8.13 (s, 1 H), 7.86 (t, J = 8.0 Hz, 1 H), 7.45 – 7.36 (m, 2 H), 6.73 (s, 1 H), 4.55 (q, J = 8.0 Hz, 2 H), 1.52 (t, J = 8.0 Hz, 3 H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 167.7, 154.1 (q, J = 38 Hz), 150.6, 135.8, 126.2, 126.0, 124.6, 120.4, 120.1 (q, J = 270 Hz), 115.9, 108.7, 97.2, 64.5, 14.6; $^{19}\text{F NMR}$ (376 MHz, CDCl_3) δ -63.13 (s, 3 F); $^{19}\text{F}\{^1\text{H}\}$ NMR (376 MHz, CDCl_3) δ -63.13 (s, 3 F); **HRMS (ESI)** m/z calcd for $\text{C}_{15}\text{H}_{12}\text{O}_3\text{N}_2\text{F}_3^+$ $[\text{M}+\text{H}]^+$ 325.0795, found 325.0794.

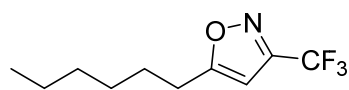


9jj

(E)-5-styryl-3-(trifluoromethyl)isoxazole

Purified by flash column chromatography (petroleum ether/AcOEt = 20:1), yellow solid (43.5 mg, 73% yield); mp: 80.8 – 82.0; $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.55 – 7.53 (m, 2 H), 7.46 – 7.38 (m, 4 H), 6.98 (d, J = 16 Hz, 1 H), 6.49 (s, 1 H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 171.3, 156.1 (q, J = 38.0 Hz), 137.5, 135.2, 130.2, 129.4, 127.7, 120.0 (q, J = 270.0 Hz), 112.1, 98.6; $^{19}\text{F NMR}$ (376 MHz, CDCl_3) δ -63.28 (s, 3 F);

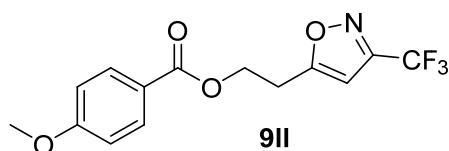
¹⁹F {¹H} NMR (376 MHz, CDCl₃) δ -63.28 (s, 3 F); **HRMS (ESI)** m/z calcd for C₁₂H₉ONF₃⁺ [M+H]⁺ 240.0631, found 240.0628.



9kk

5-hexyl-3-(trifluoromethyl)isoxazole

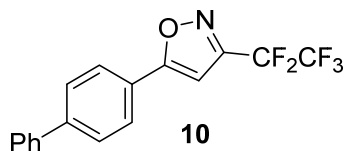
Purified by flash column chromatography (petroleum ether/AcOEt = 200:1), colorless oil (30.4 mg, 55% yield); **¹H NMR** (400 MHz, CDCl₃) δ 6.23 (s, 1 H), 2.81 (t, *J* = 7.8 Hz, 2 H), 1.76 – 1.68 (m, 2 H), 1.38 – 1.30 (m, 6 H), 0.89 (t, *J* = 6.8 Hz, 3 H); **¹³C NMR** (100 MHz, CDCl₃) δ 176.9, 155.7 (q, *J* = 38 Hz), 120.2 (t, *J* = 270 Hz), 98.7, 31.7, 29.0, 27.6, 27.1, 22.8, 14.3; **¹⁹F NMR** (376 MHz, CDCl₃) δ -63.31 (s, 3 F); **¹⁹F {¹H} NMR** (376 MHz, CDCl₃) δ -63.31 (s, 3 F); **HRMS (ESI)** m/z calcd for C₁₀H₁₅ONF₃⁺ [M+H]⁺ 222.1100, found 222.1101.^[12]



9ll

2-(3-(trifluoromethyl)isoxazol-5-yl)ethyl 4-methoxybenzoate

Purified by flash column chromatography (petroleum ether/AcOEt = 50:1), colorless oil (78.9 mg, 63% yield); **¹H NMR** (400 MHz, CDCl₃) δ 7.96 – 7.93 (m, 2 H), 6.93 – 6.90 (m, 2 H), 6.39 (s, 1 H), 4.60 (t, *J* = 6.3 Hz, 2 H), 3.85 (s, 3 H), 3.31 (t, *J* = 6.3 Hz, 2 H); **¹³C NMR** (100 MHz, CDCl₃) δ 172.9, 166.2, 164.1, 155.9 (q, *J* = 38.0 Hz), 132.0, 122.1, 120.0 (t, *J* = 271.0 Hz), 114.1, 100.1, 61.2, 55.8, 27.1; **¹⁹F NMR** (376 MHz, CDCl₃) δ -63.26 (s, 3 F); **¹⁹F {¹H} NMR** (376 MHz, CDCl₃) δ -63.26 (s, 3 F); **HRMS (ESI)** m/z calcd for C₁₄H₁₃O₄NF₃⁺ [M+H]⁺ 316.0791, found 316.0793.

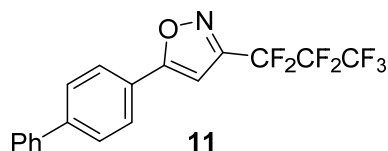


10

5-([1,1'-biphenyl]-4-yl)-3-(perfluoroethyl)isoxazole

Purified by flash column chromatography (petroleum ether/AcOEt = 200:1), white solid (70.5 mg, 83% yield); mp: 114.0 – 114.3; **¹H NMR** (400 MHz, CDCl₃) δ 7.89 (d, *J* = 8.0 Hz, 2 H), 7.74 (d, *J* = 8.0 Hz, 2 H), 7.64 (d, *J* = 8.0 Hz, 2 H), 7.49 (t, *J* = 8.0 Hz, 2 H), 7.42 (t, *J* = 8.0 Hz, 1 H), 6.79 (s, 1 H); **¹³C NMR** (100 MHz, CDCl₃) δ 172.7, 155.5 (t, *J* = 28.0 Hz), 144.5, 140.0, 129.4, 128.6, 128.2, 127.5, 126.9, 125.1, 120.1 118.7 (tq, *J* = 36.0, 284.0 Hz), 111.3 (tq, *J* = 40.0, 252.0 Hz), 98.0; **¹⁹F NMR**

(376 MHz, CDCl₃) δ -84.2 (t, J = 2.5 Hz, 3 F), -144.5 (q, J = 2.5 Hz, 2 F); **¹⁹F {¹H} NMR** (376 MHz, CDCl₃) δ -84.2 (t, J = 2.5 Hz, 3 F), -144.5 (q, J = 2.5 Hz, 2 F); **HRMS (ESI)** m/z calcd for C₁₇H₁₁ONF₅⁺ [M+H]⁺ 340.0755, found 340.0748.

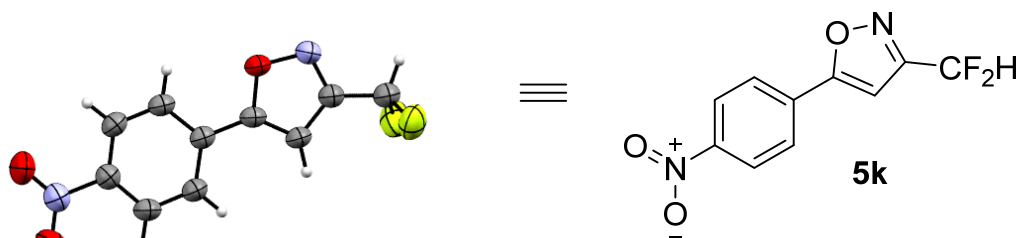


5-([1,1'-biphenyl]-4-yl)-3-(perfluoropropyl)isoxazole

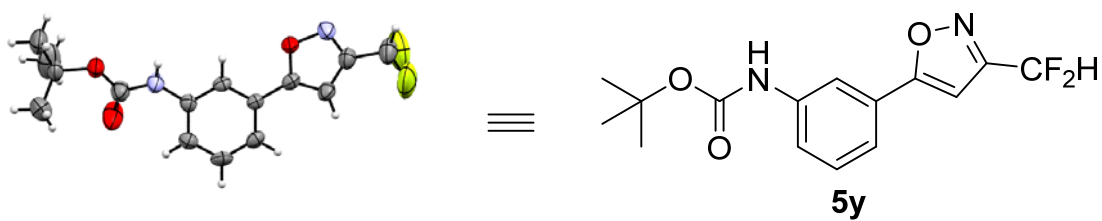
Purified by flash column chromatography (petroleum ether/AcOEt = 200:1), white solid (83.6 mg, 86% yield); mp: 112.9 – 114.2; **¹H NMR** (400 MHz, CDCl₃) δ 7.89 (d, J = 8.0 Hz, 2 H), 7.74 (d, J = 8.0 Hz, 2 H), 7.64 (d, J = 8.0 Hz, 2 H), 7.49 (t, J = 8.0 Hz, 2 H), 7.42 (t, J = 8.0 Hz, 1 H), 6.78 (s, 1 H); **¹³C NMR** (100 MHz, CDCl₃) δ 172.7, 155.6 (t, J = 28.0 Hz), 144.5, 140.0, 129.4, 128.6, 128.2, 127.5, 126.9, 125.1, 119.5 (m), 116.6 (m), 112.0 (m), 98.3; **¹⁹F NMR** (376 MHz, CDCl₃) δ -80.6 (t, J = 9.8 Hz, 3 F), -112.3 (m, 2 F), -126.8 (t, J = 7.5 Hz, 2 F); **¹⁹F {¹H} NMR** (376 MHz, CDCl₃) δ -80.6 (t, J = 9.8 Hz, 3 F), -112.3 (m, 2 F), -126.8 (t, J = 7.5 Hz, 2 F); **HRMS (ESI)** m/z calcd for C₁₈H₁₁ONF₇⁺ [M+H]⁺ 390.0723, found 390.0716.

4. X-ray Structure of 5k, 5y, 9c

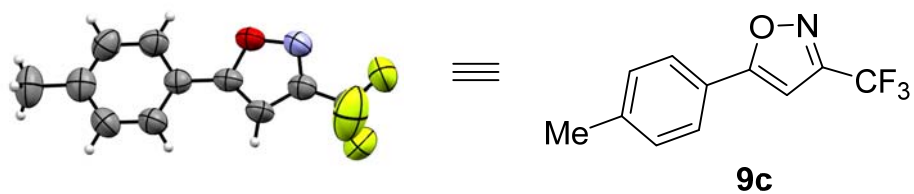
compound 5k (CCDC 1577898)



compound 5y (CCDC 1577913)



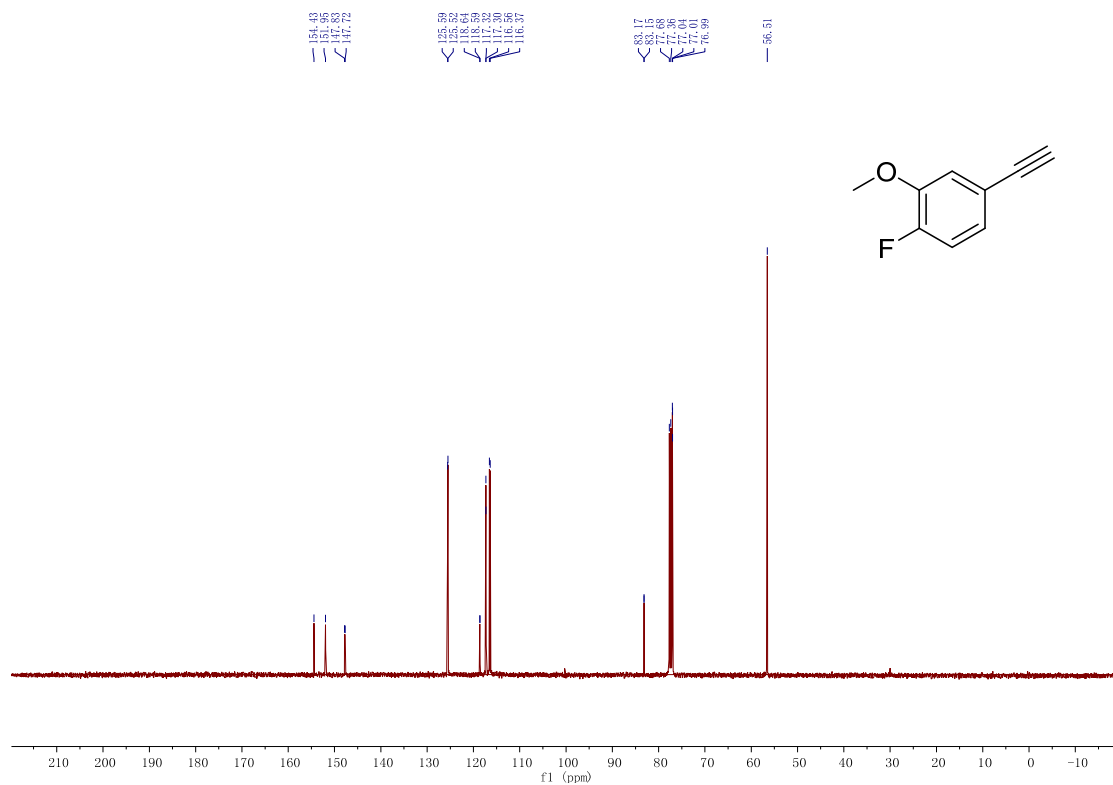
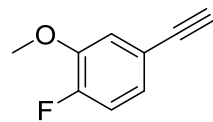
compound 9c (CCDC 1577906)



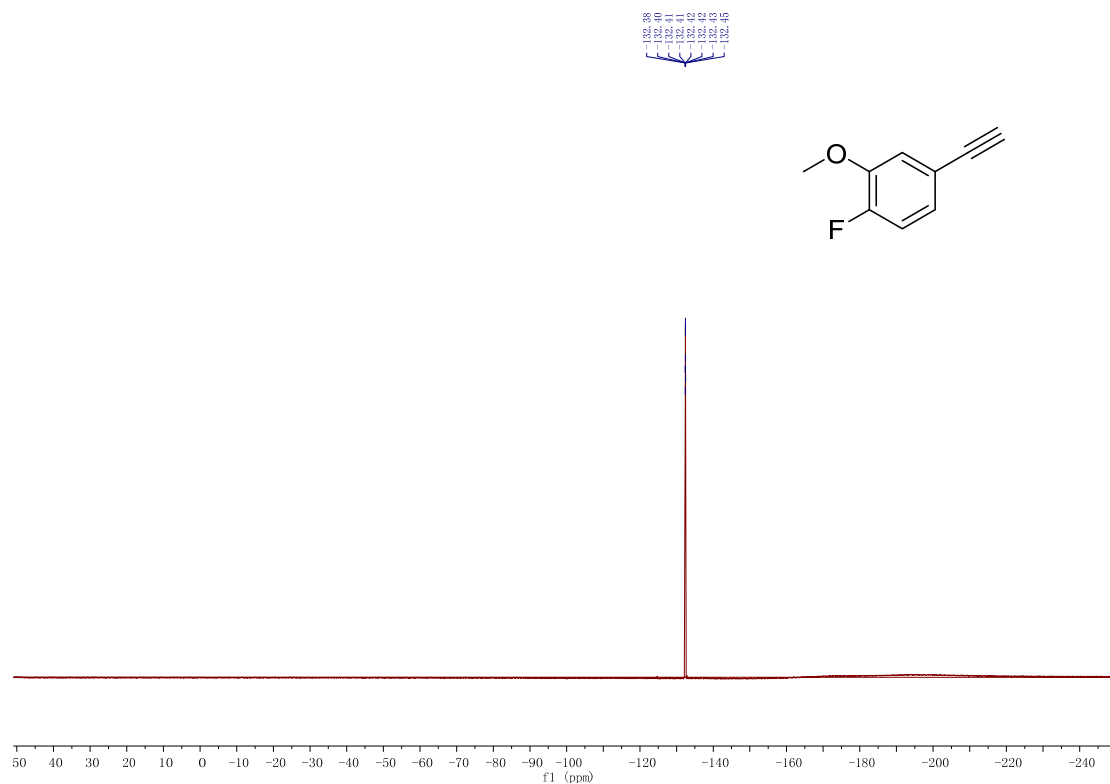
5. References

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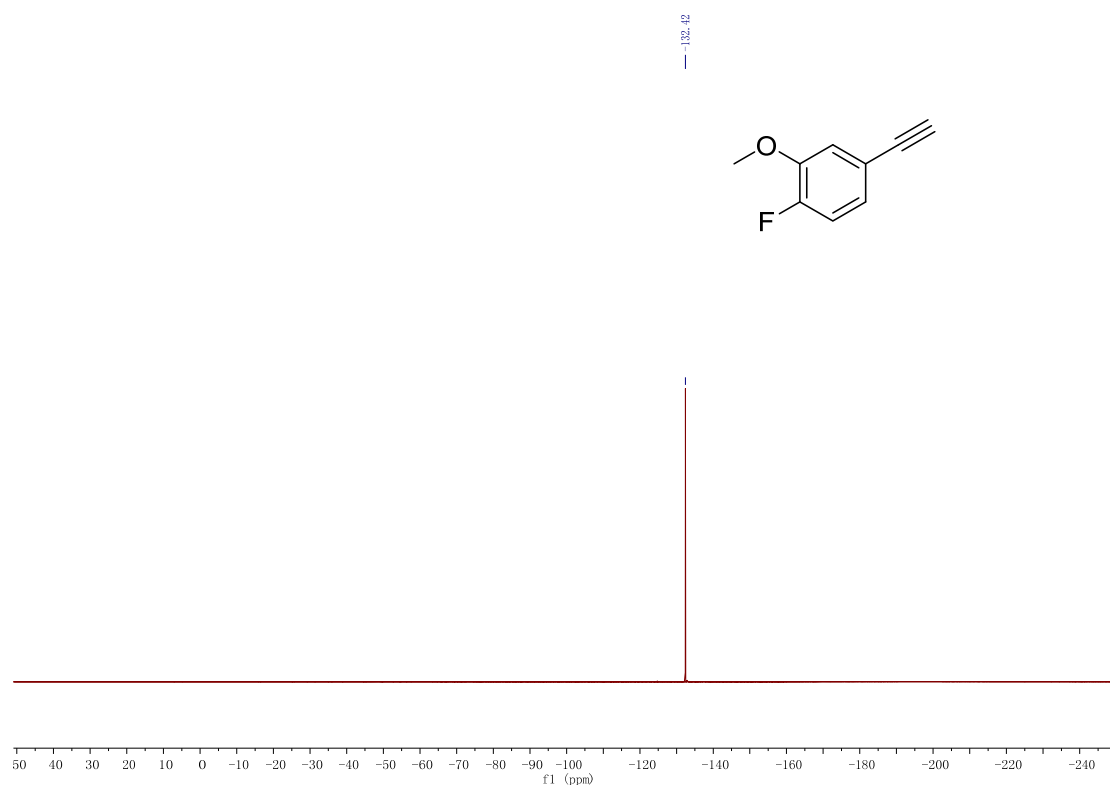
¹H NMR (CDCl₃, 400 MHz) of **1dd**



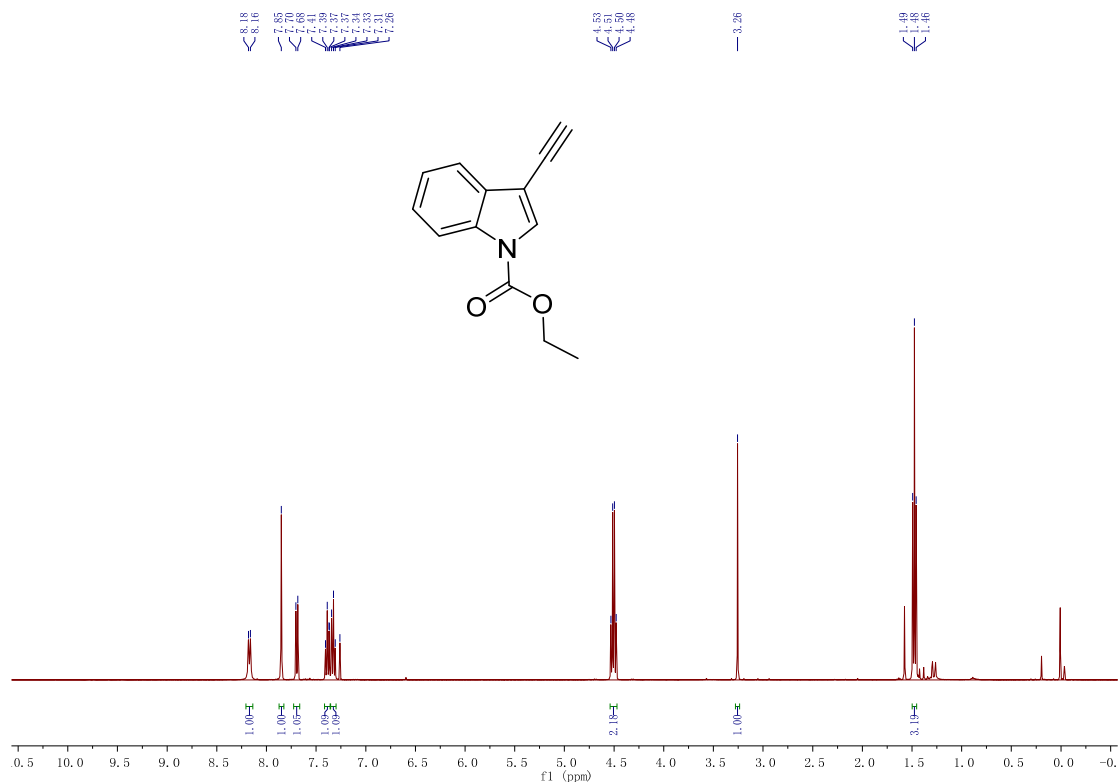
^{19}F NMR (CDCl₃, 376 MHz) of **1dd**



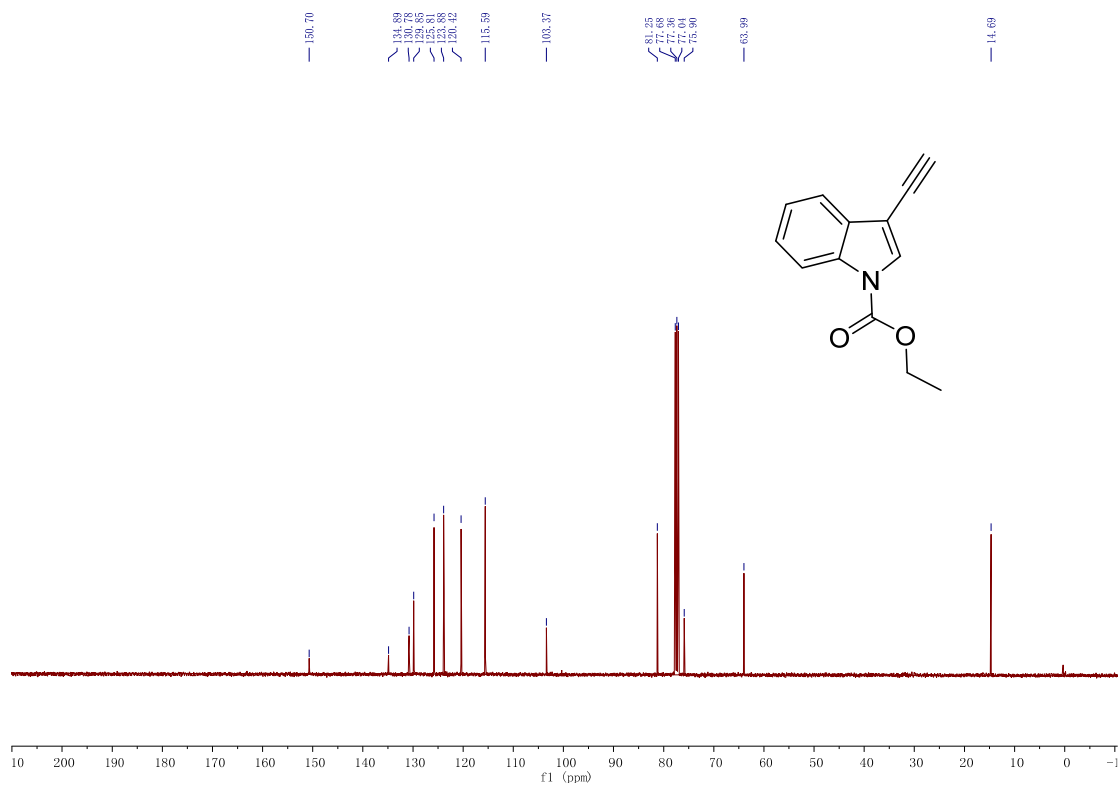
^{19}F { ^1H } NMR (CDCl₃, 376 MHz) of **1dd**



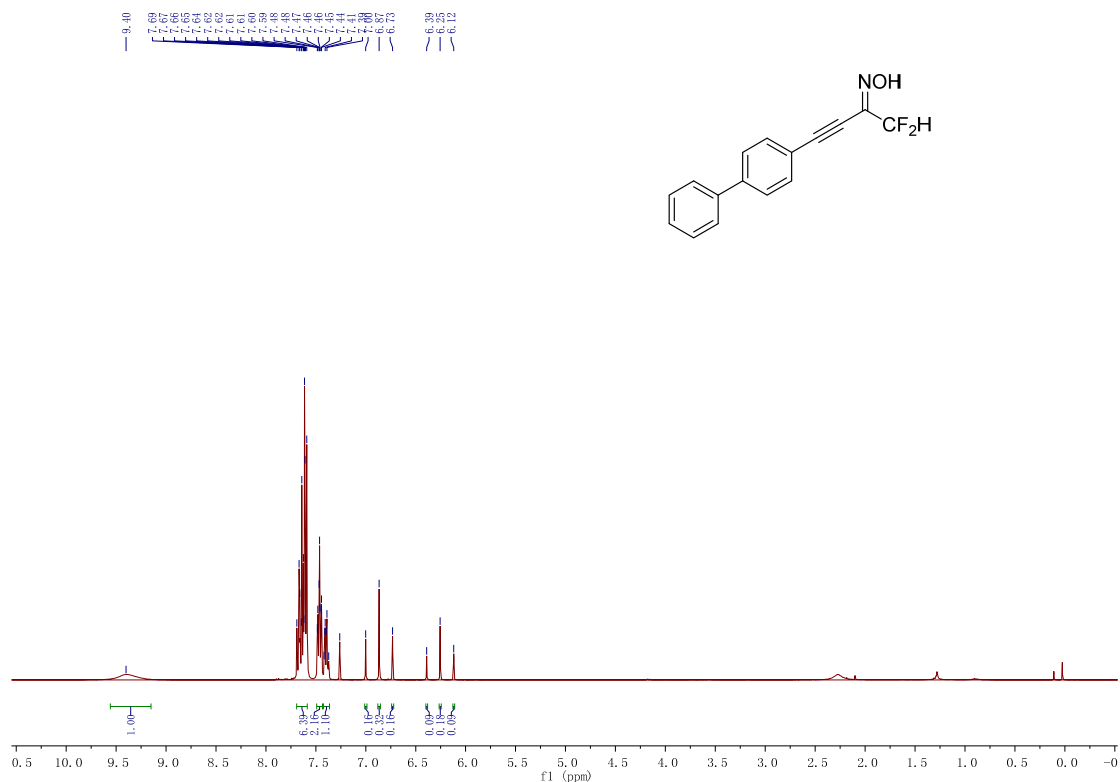
^1H NMR (CDCl₃, 400 MHz) of **1ii**



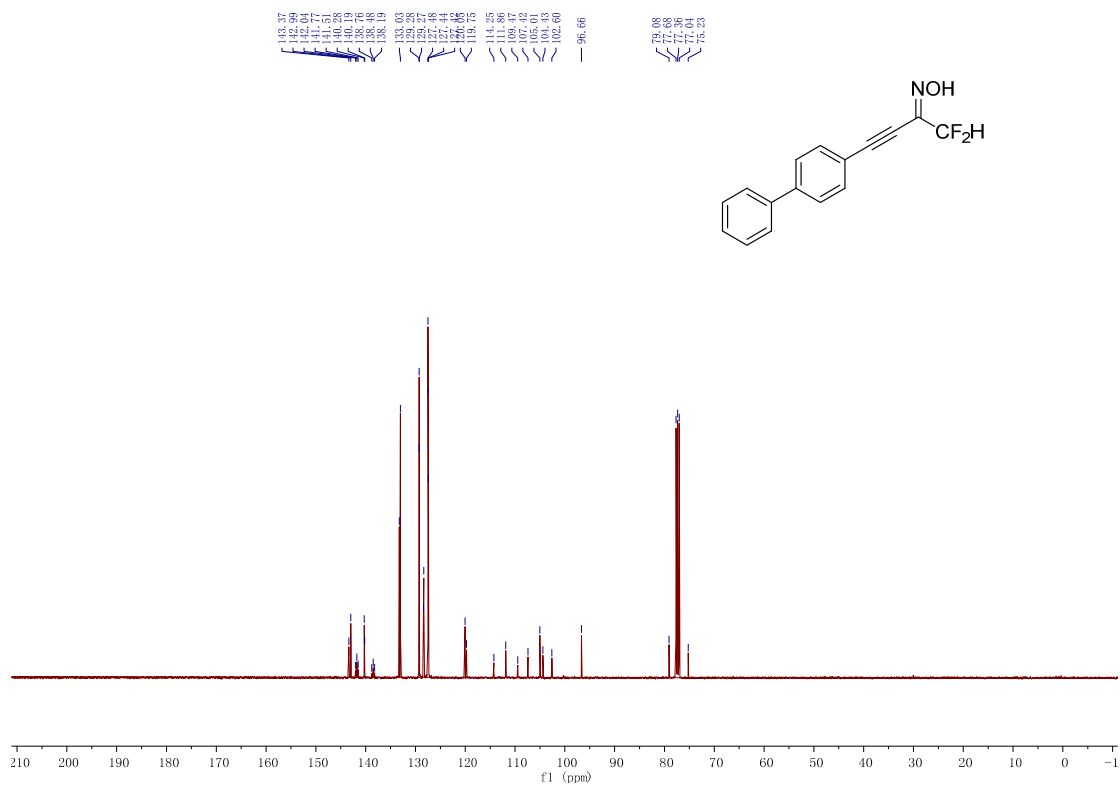
^{13}C NMR (CDCl₃, 100 MHz) of **1ii**



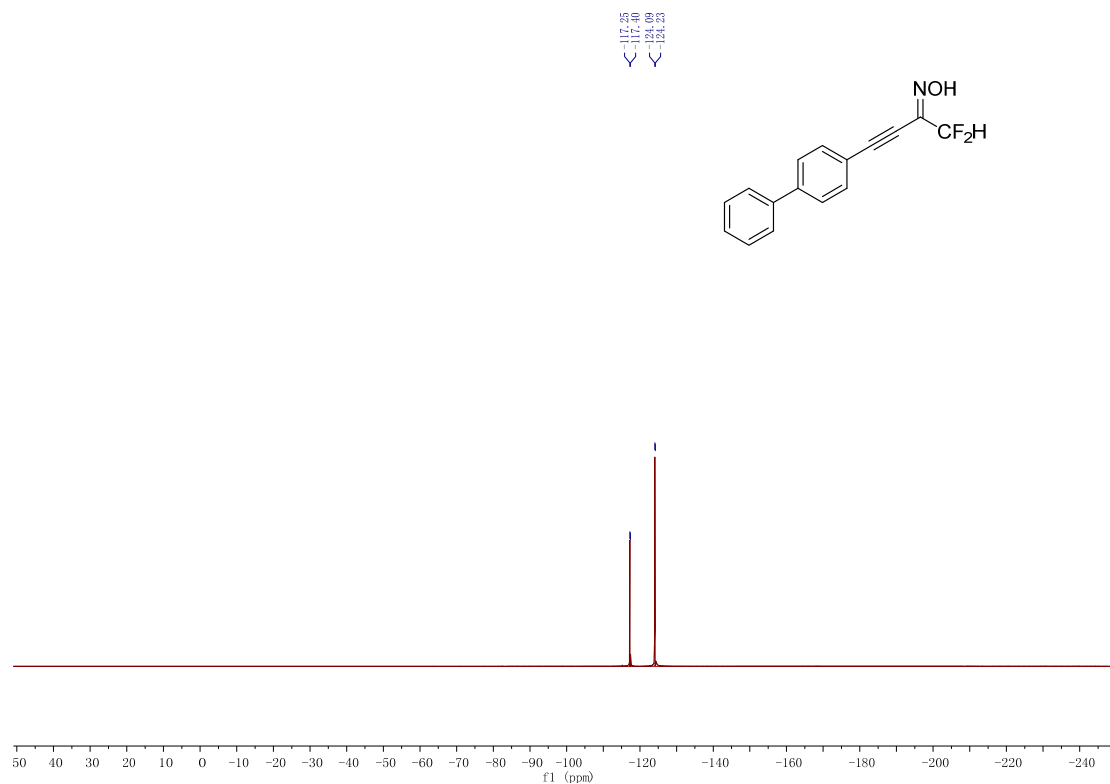
^1H NMR (CDCl_3 , 400 MHz) of **4a** ($E/Z = 2:1$)



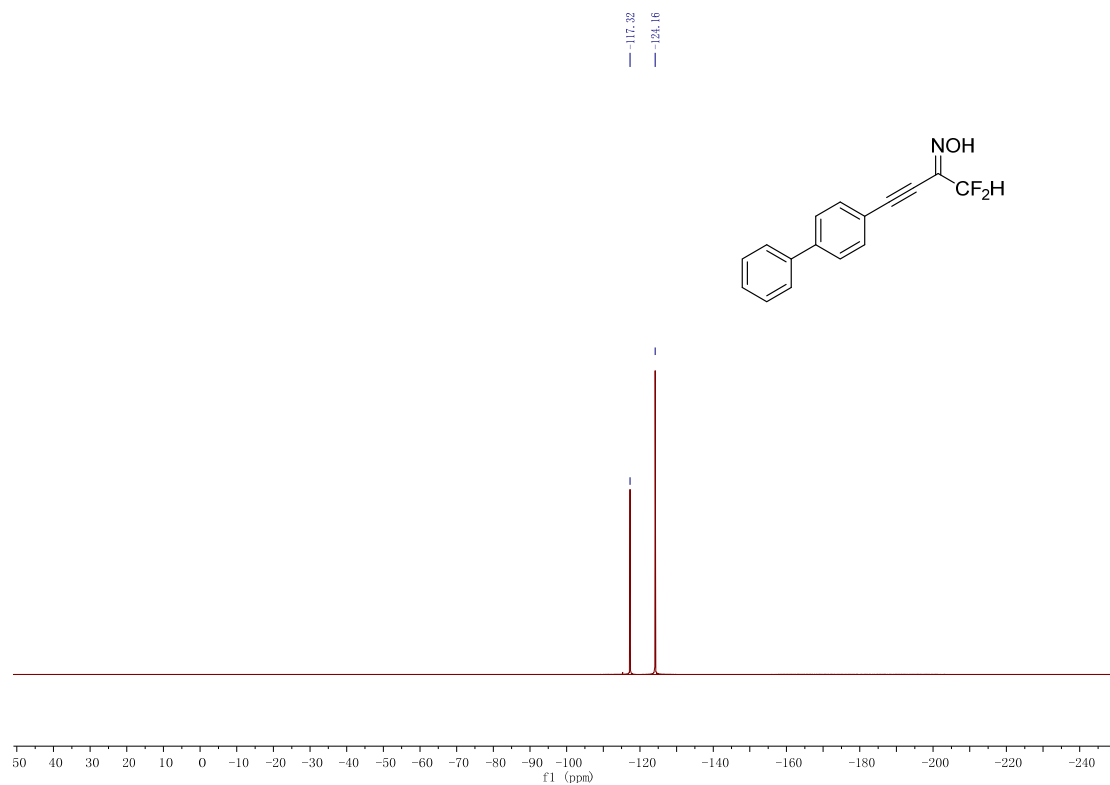
^{13}C NMR (CDCl_3 , 100 MHz) of **4a** ($E/Z = 2:1$)



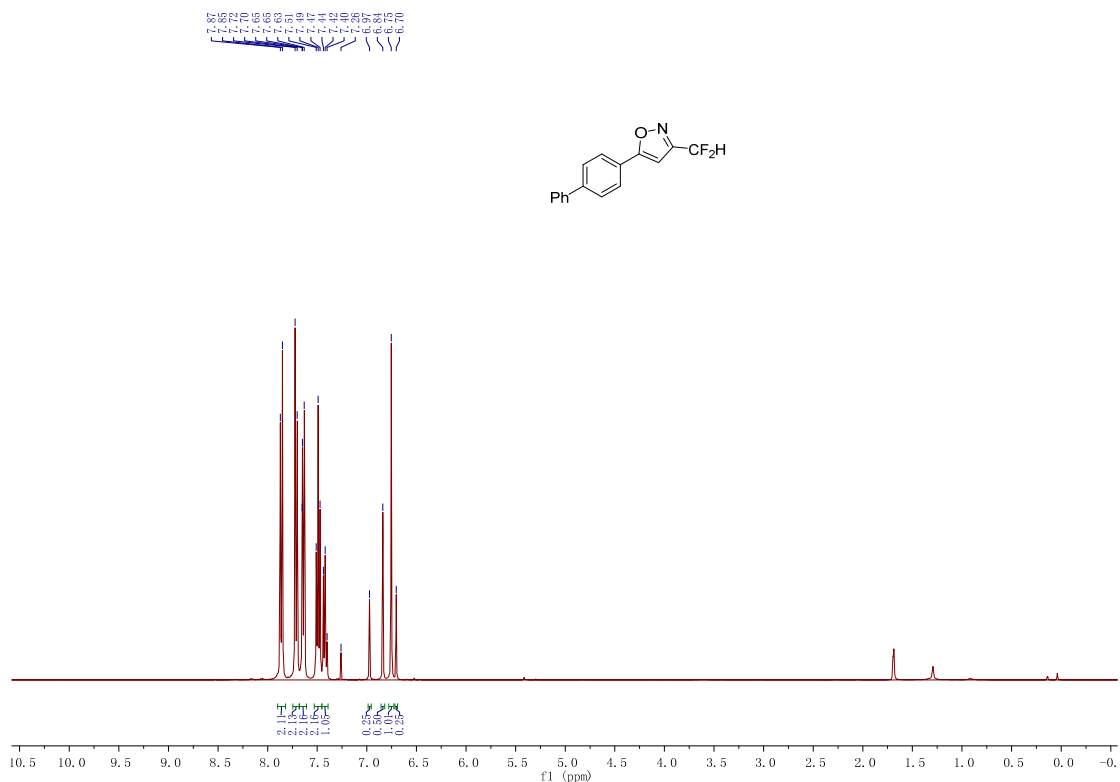
^{19}F NMR (CDCl_3 , 376 MHz) of **4a** ($E/Z = 2:1$)



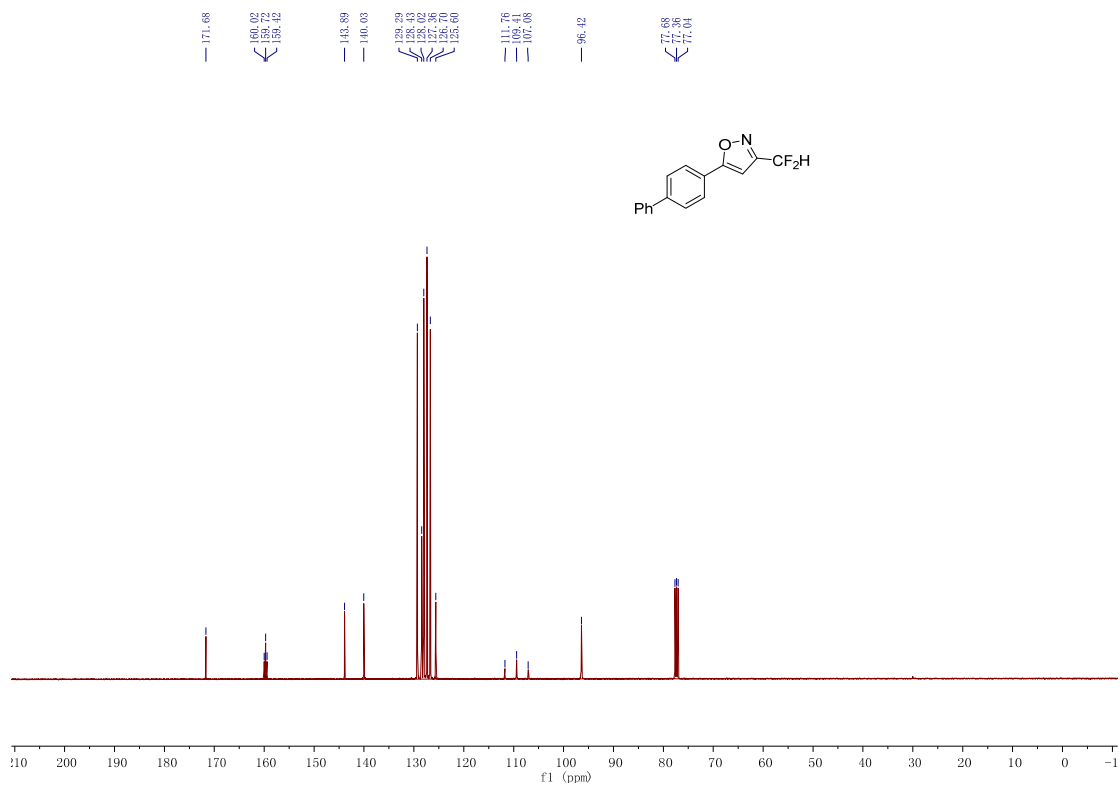
^{19}F $\{^1\text{H}\}$ NMR (CDCl_3 , 376 MHz) of **4a** ($E/Z = 2:1$)



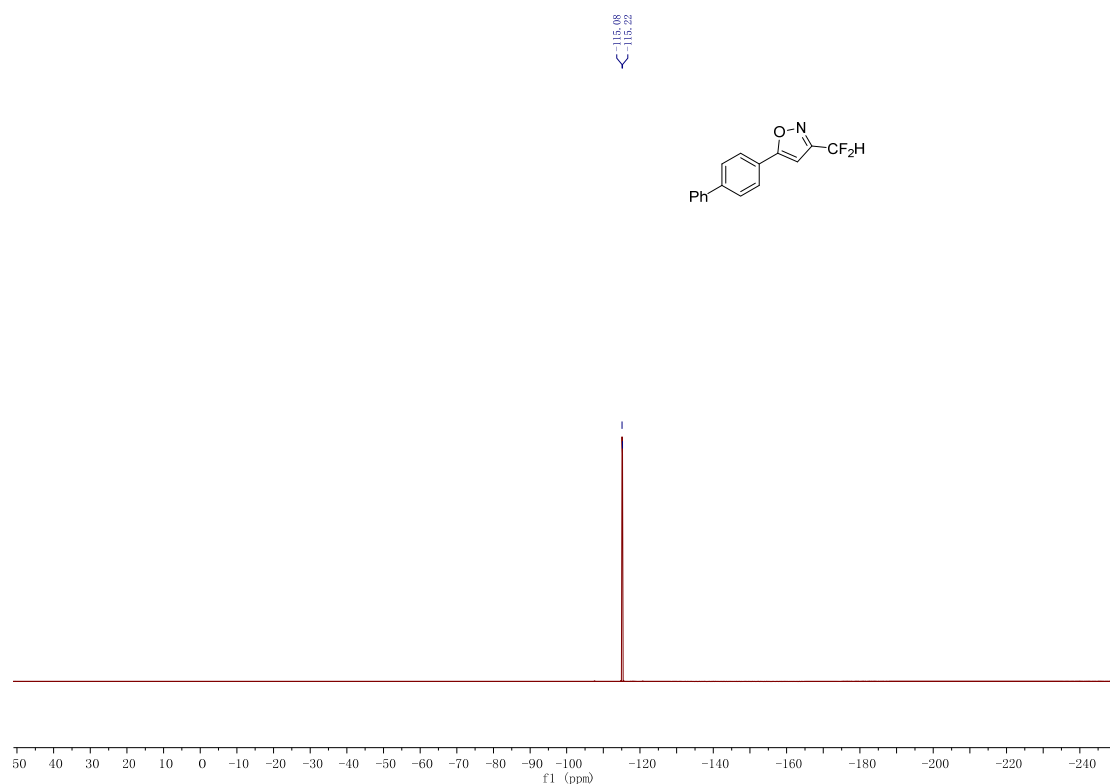
^1H NMR (CDCl_3 , 400 MHz) of 5a



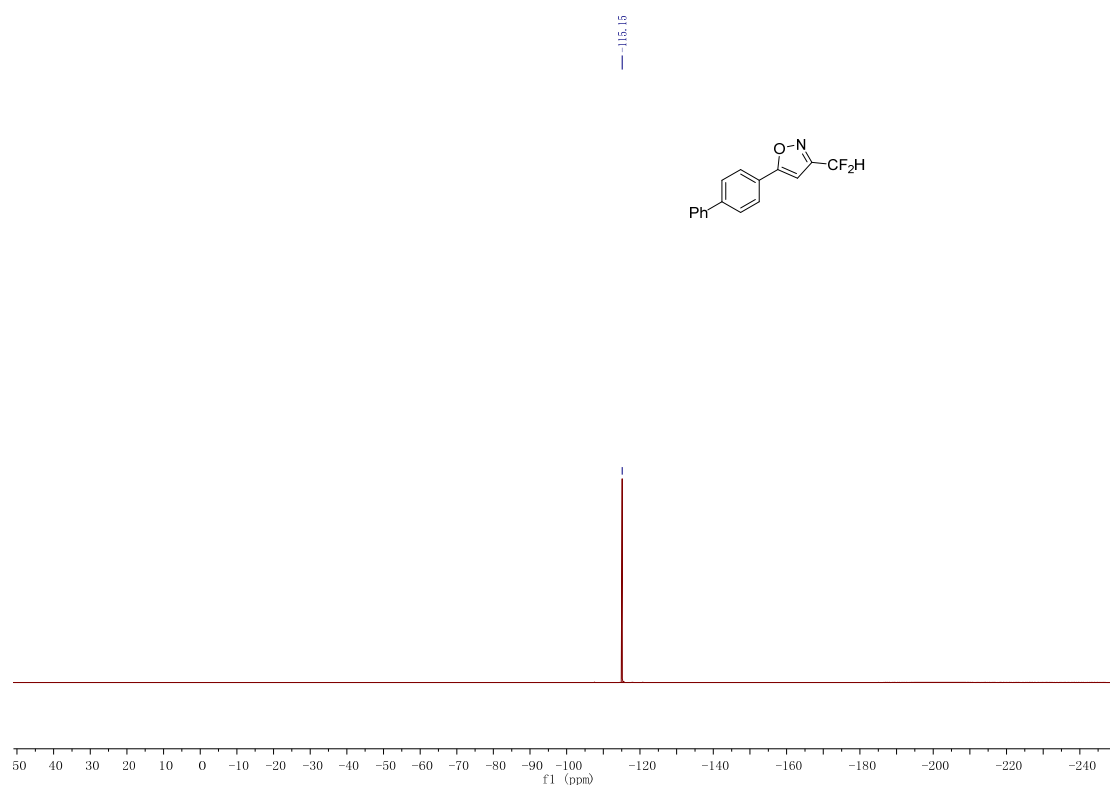
^{13}C NMR (CDCl_3 , 100 MHz) of 5a



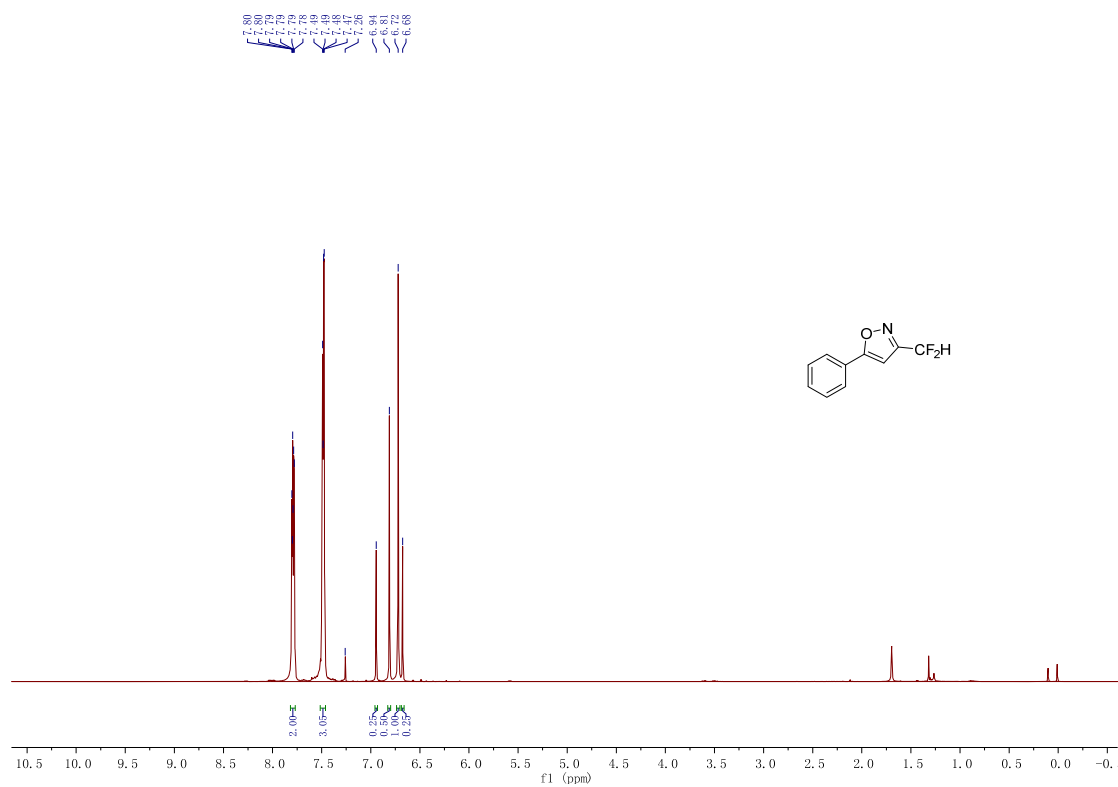
^{19}F NMR (CDCl₃, 376 MHz) of **5a**



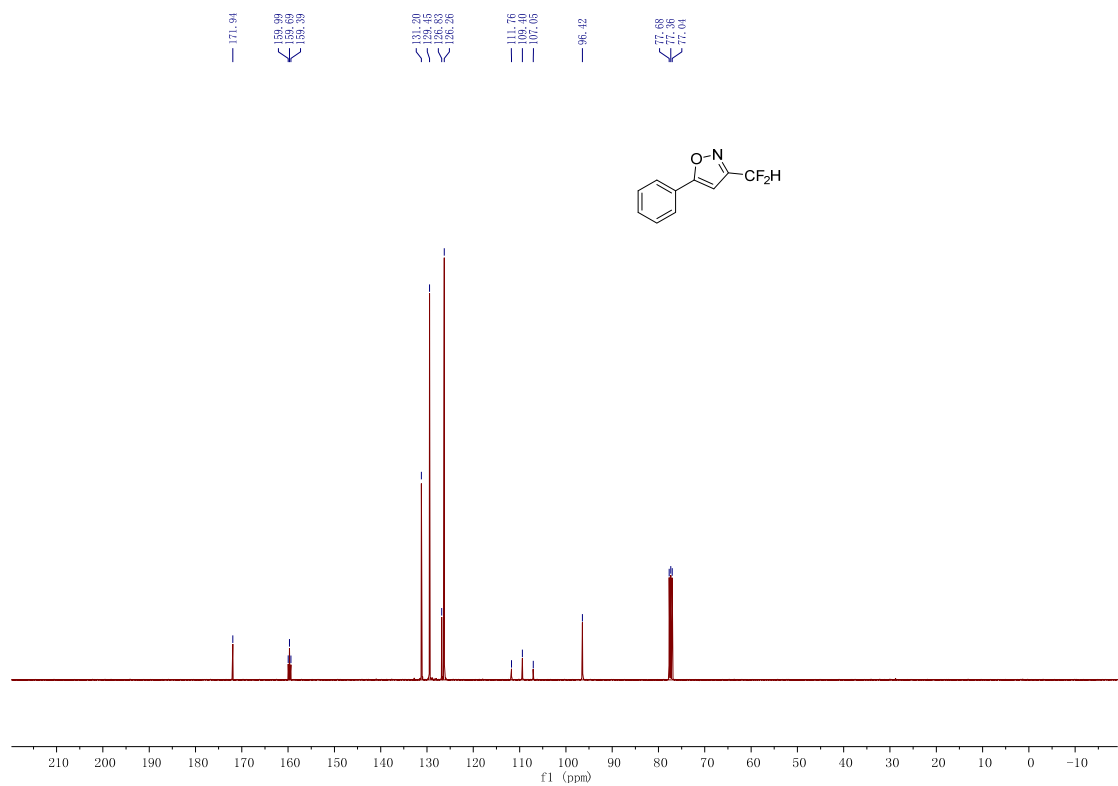
^{19}F { ^1H } NMR (CDCl₃, 376 MHz) of **5a**



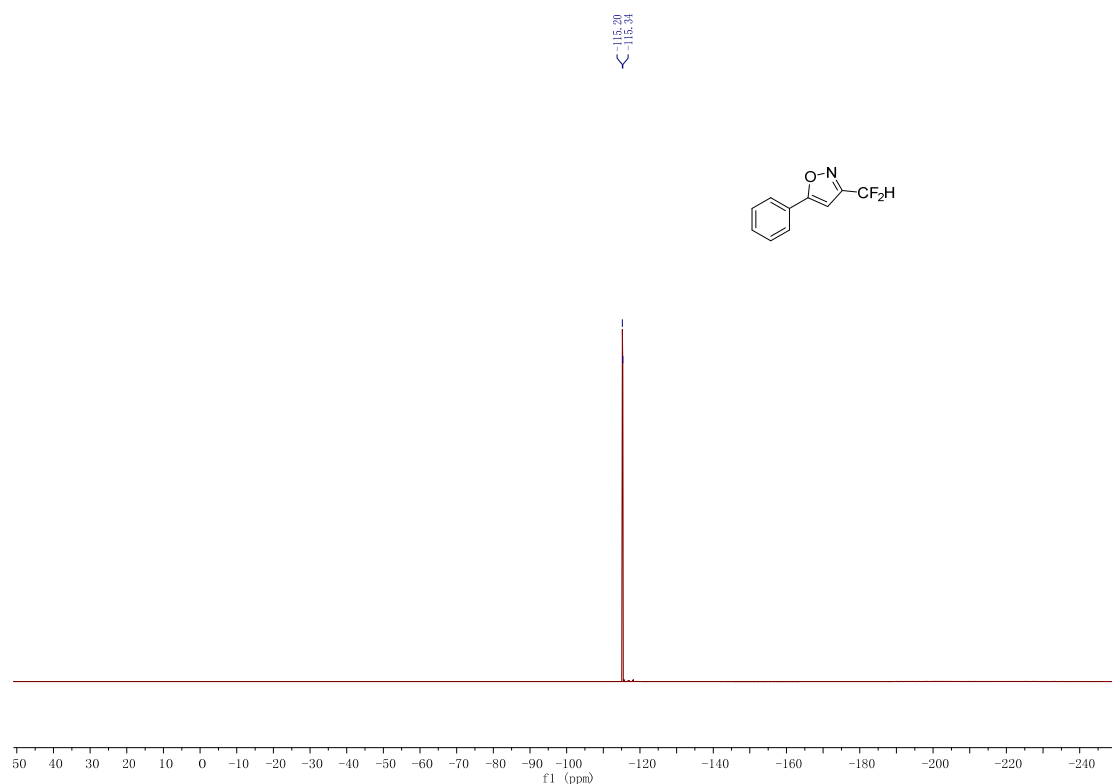
^1H NMR (CDCl₃, 400 MHz) of **5b**



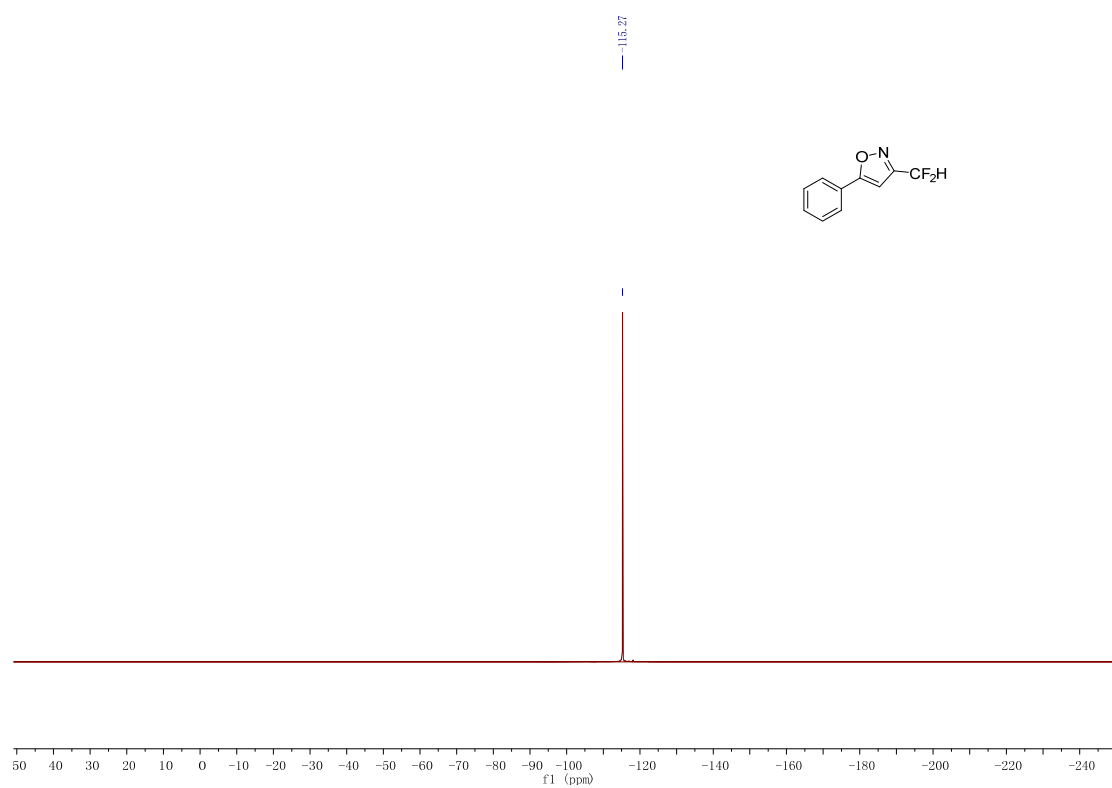
^{13}C NMR (CDCl₃, 100 MHz) of **5b**



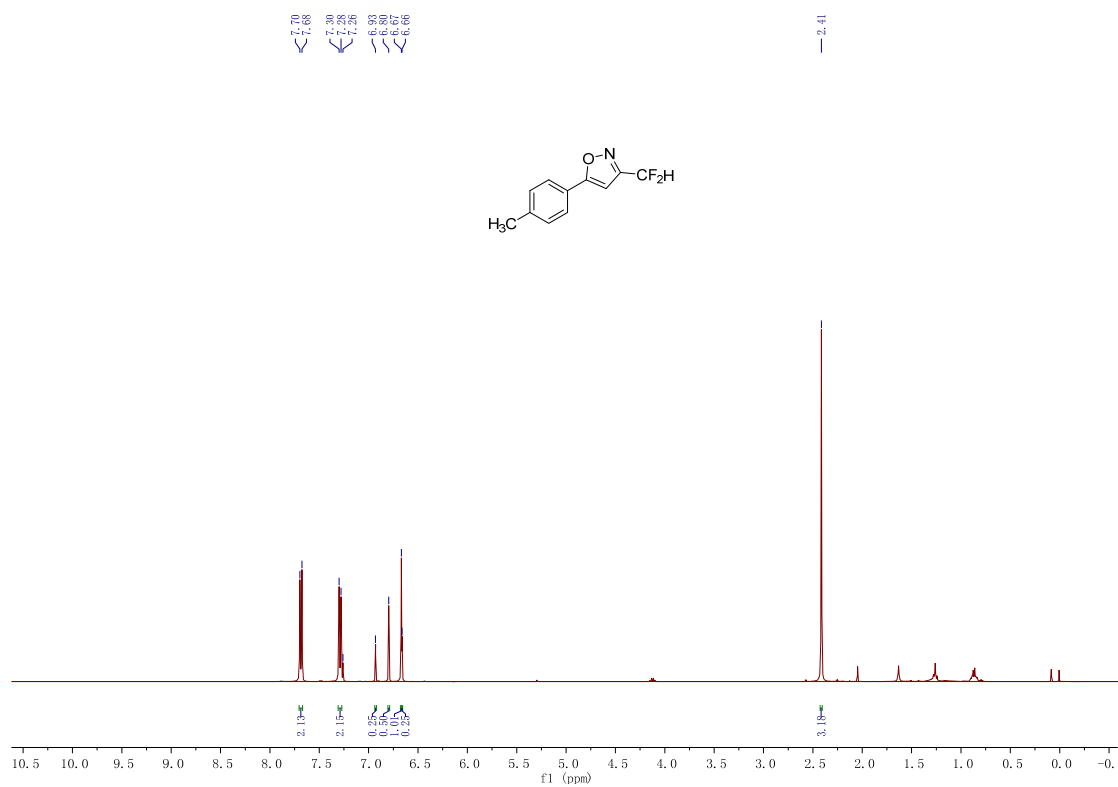
^{19}F NMR (CDCl₃, 376 MHz) of **5b**



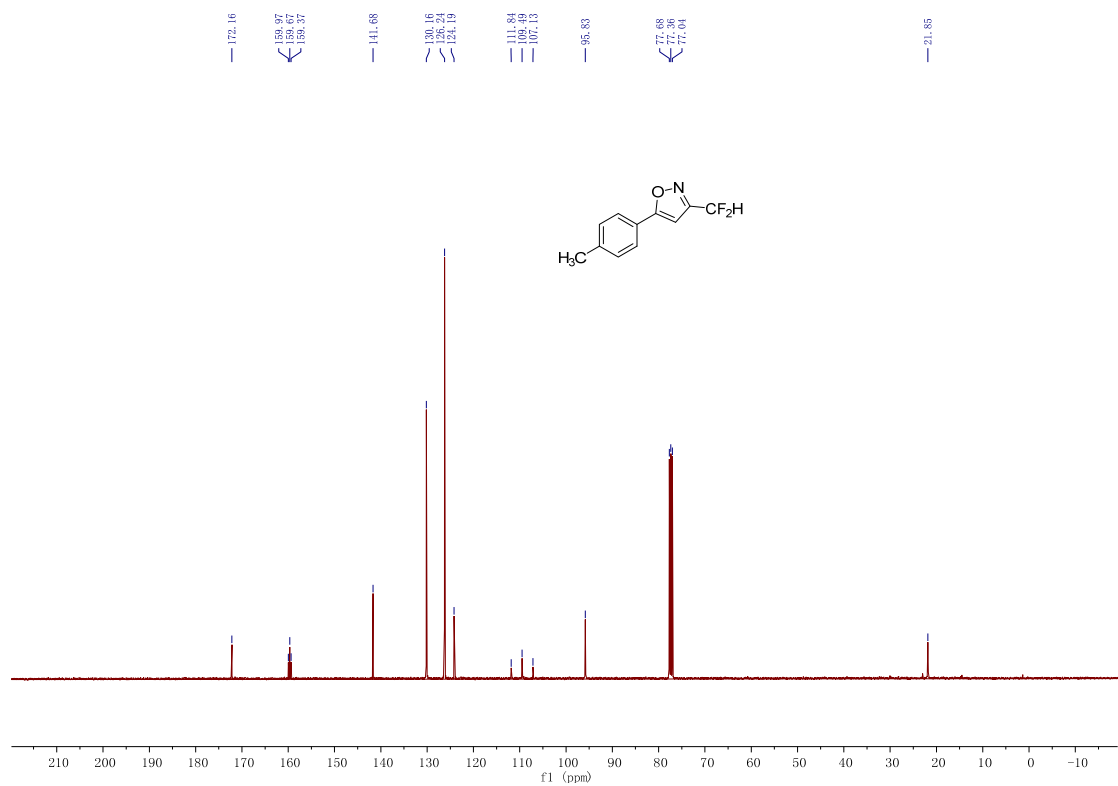
^{19}F { ^1H } NMR (CDCl₃, 376 MHz) of **5b**



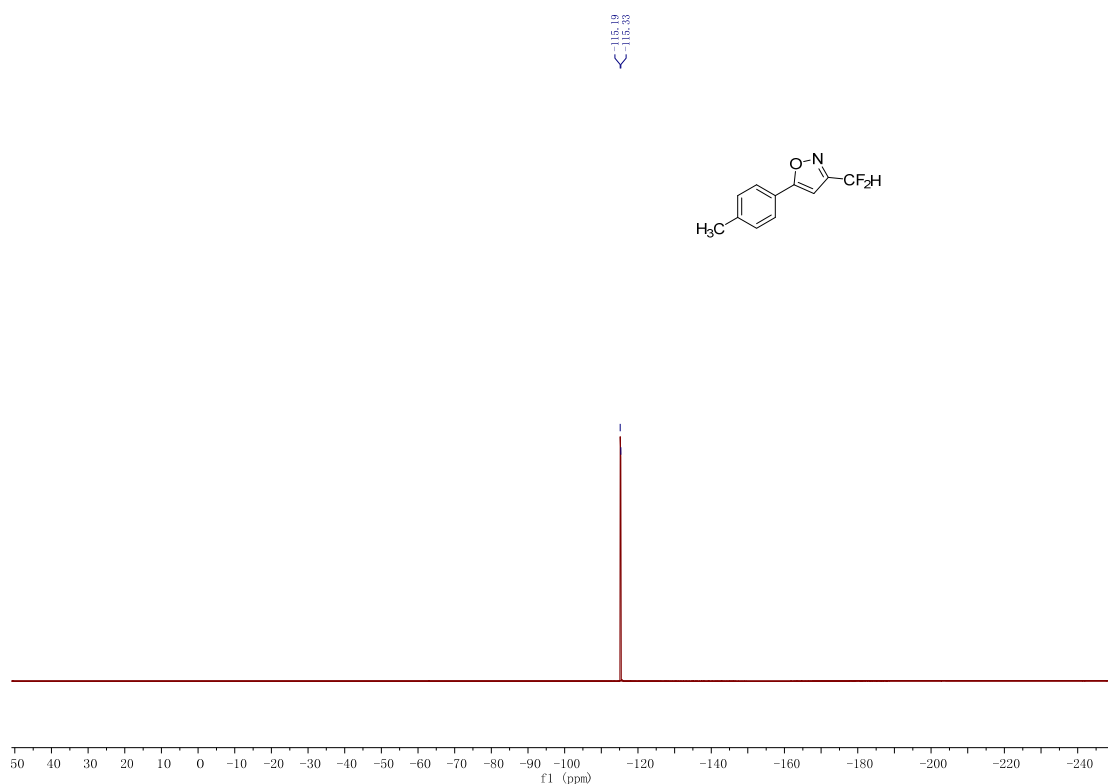
^1H NMR (CDCl₃, 400 MHz) of 5c



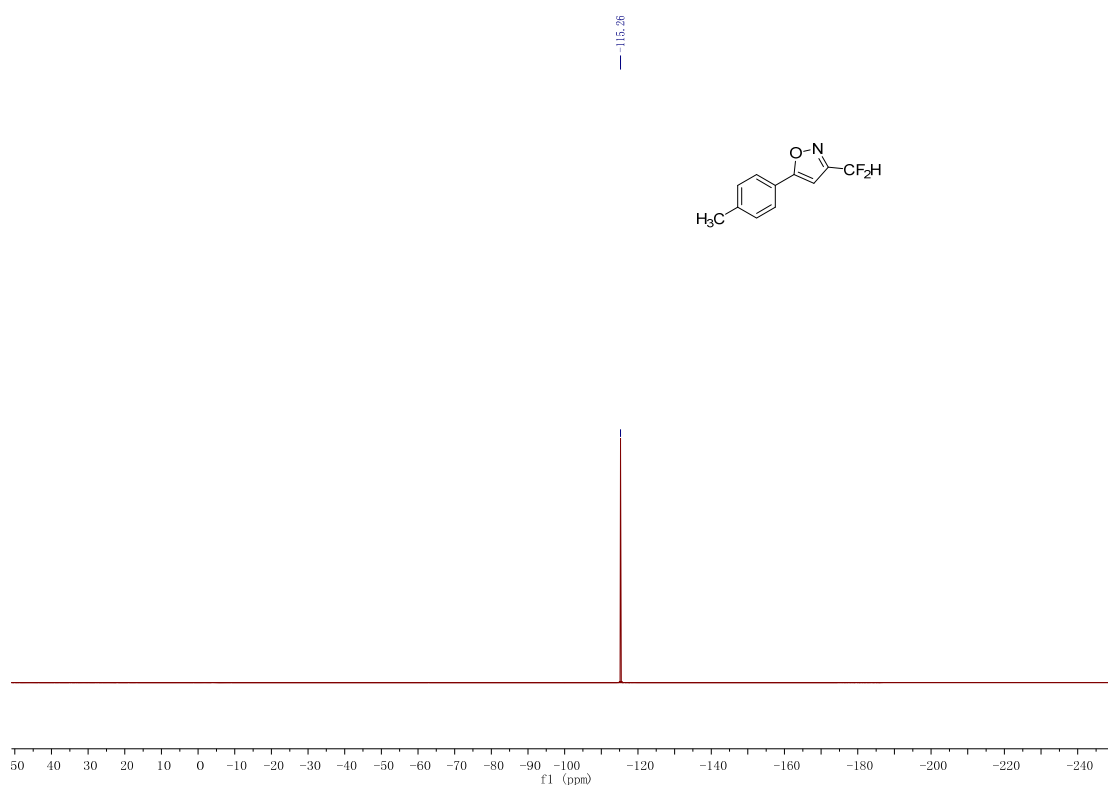
^{13}C NMR (CDCl₃, 100 MHz) of 5c



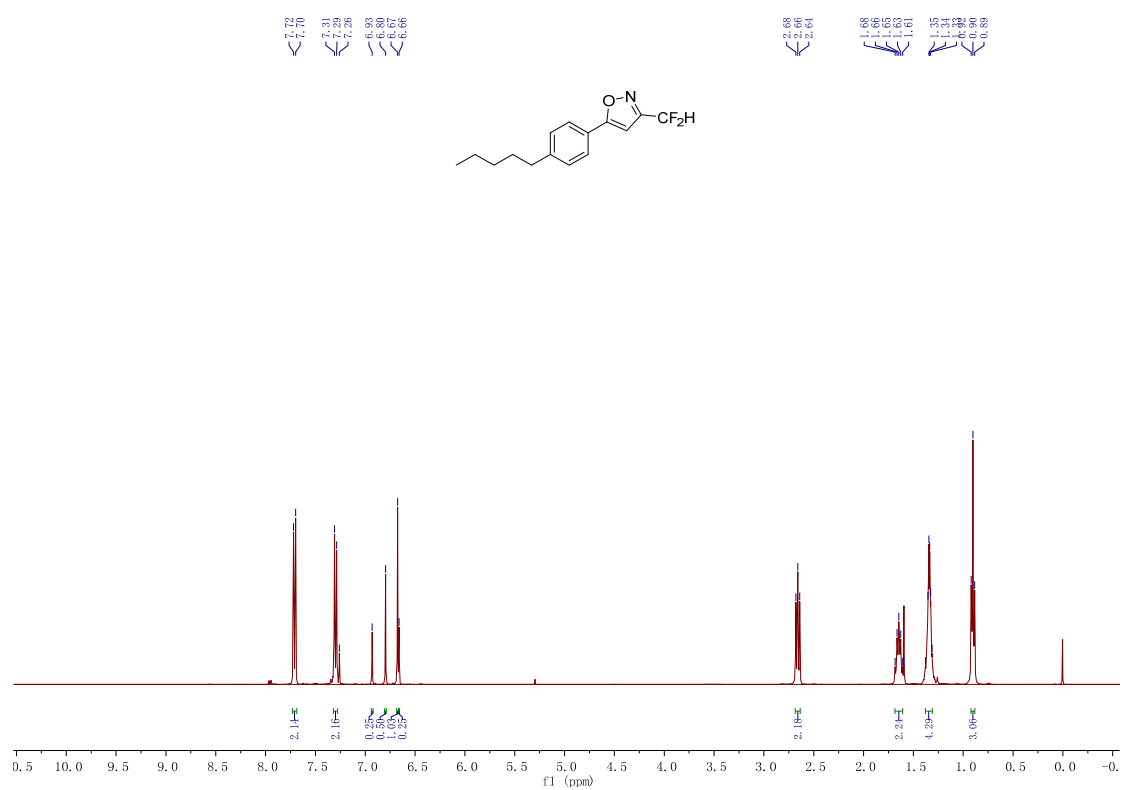
^{19}F NMR (CDCl_3 , 376 MHz) of **5c**



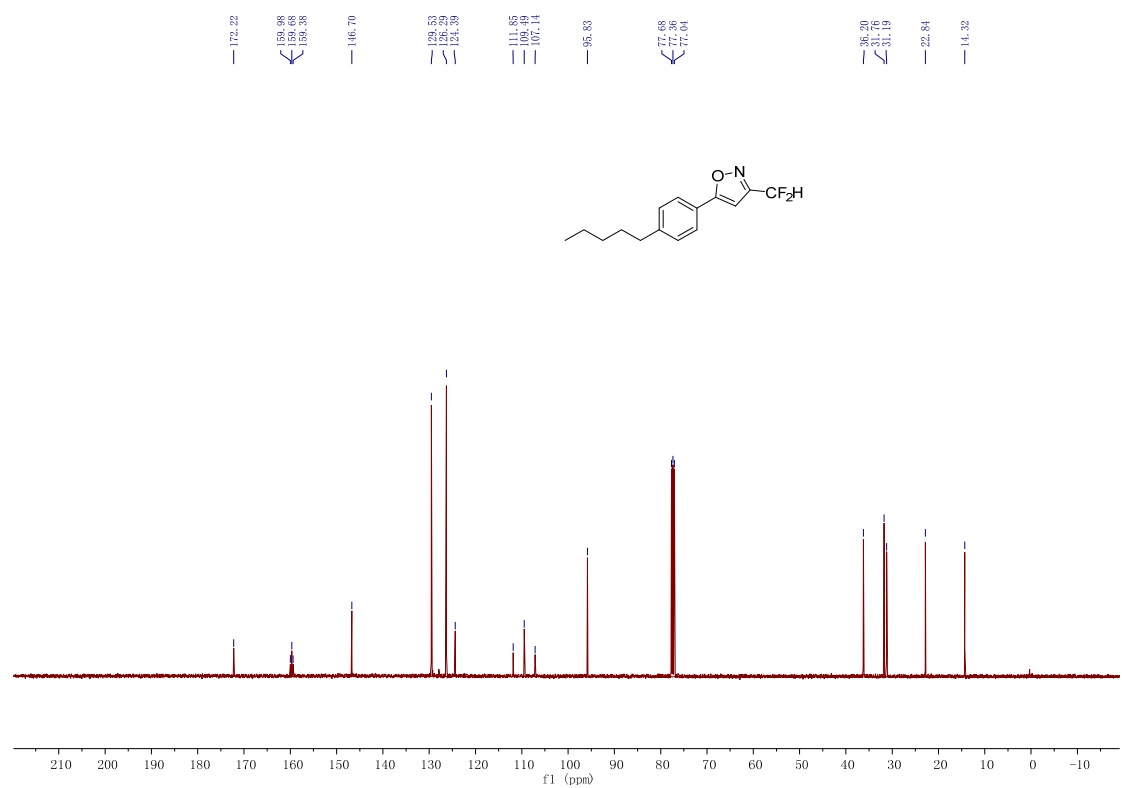
^{19}F { ^1H } NMR (CDCl_3 , 376 MHz) of **5c**



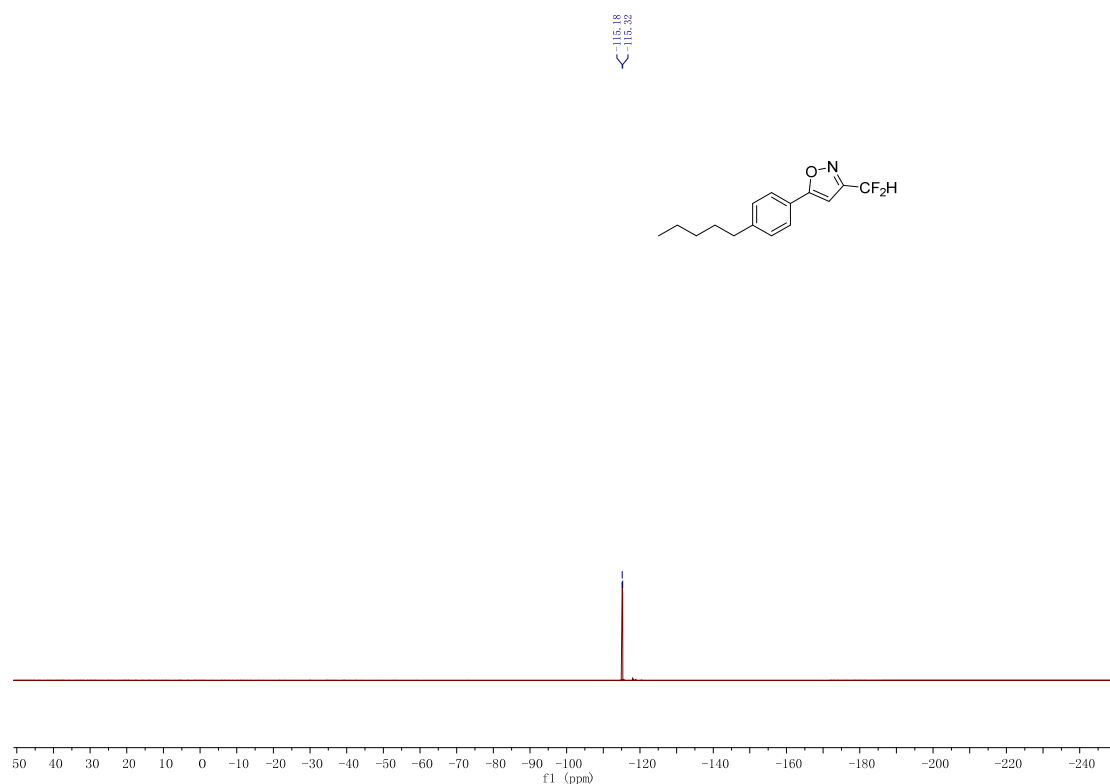
^1H NMR (CDCl₃, 400 MHz) of 5d



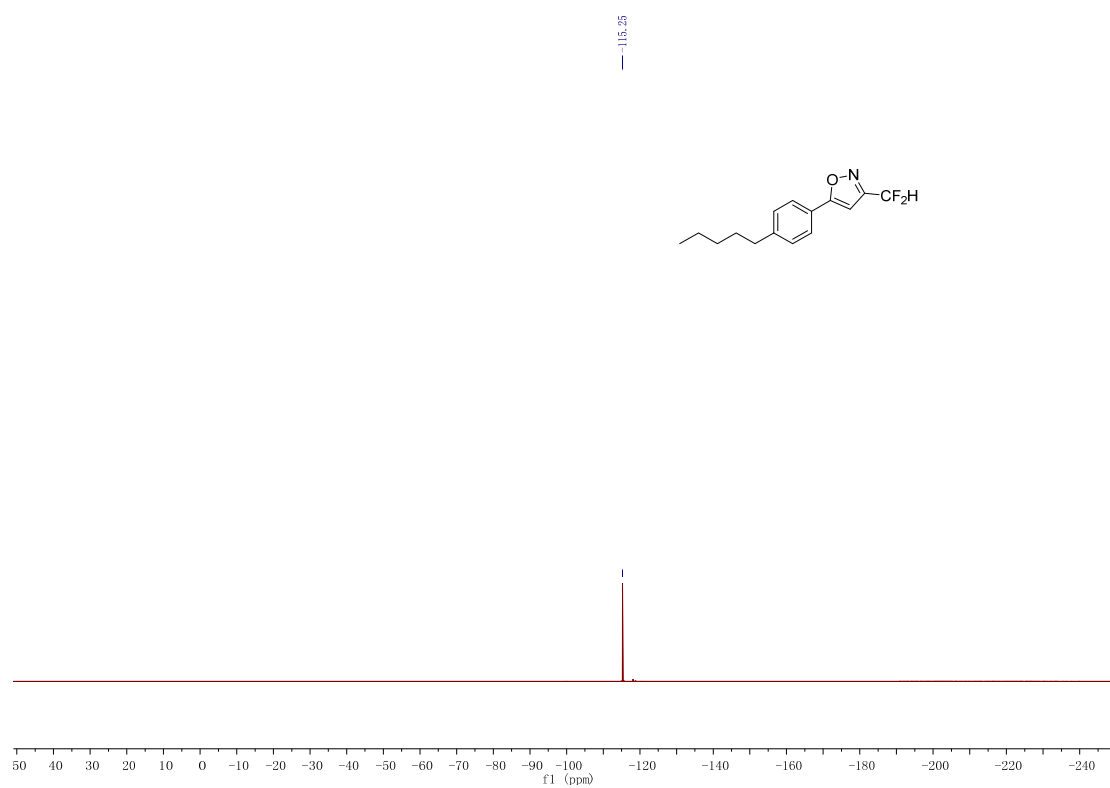
^{13}C NMR (CDCl₃, 100 MHz) of 5d



^{19}F NMR (CDCl_3 , 376 MHz) of **5d**



^{19}F $\{^1\text{H}\}$ NMR (CDCl_3 , 376 MHz) of **5d**



Chemical structure of 4-methoxy-2-(2-fluoromethyl-1H-imidazol-1-yl)phenol (10):

COc1ccc(cc1Oc2cc[nH]2)C(F)F

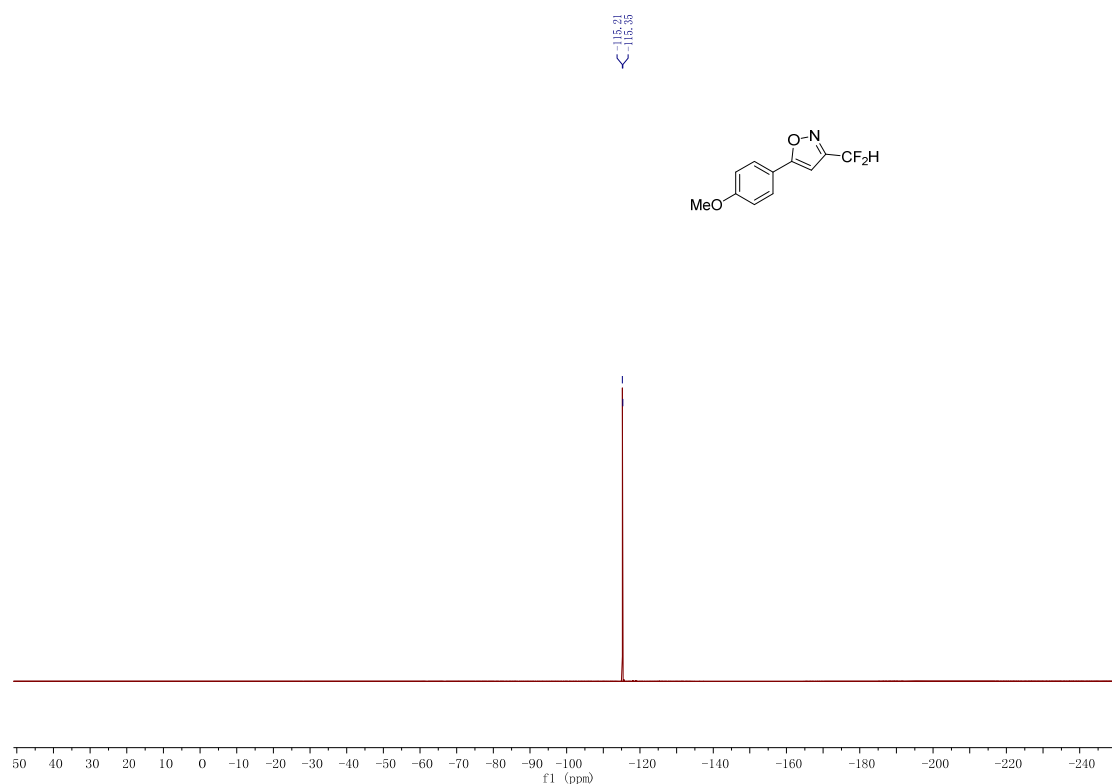
¹H NMR spectrum (CDCl₃) showing peaks at 7.70 (d, 2H), 7.50 (d, 2H), 7.20 (t, 1H), 7.10 (t, 1H), 7.00 (t, 1H), 6.90 (t, 1H), 6.80 (t, 1H), 6.70 (t, 1H), 6.60 (t, 1H), 6.50 (t, 1H), 6.40 (t, 1H), 6.30 (t, 1H), 6.20 (t, 1H), 6.10 (t, 1H), 6.00 (t, 1H), 5.90 (t, 1H), 5.80 (t, 1H), 5.70 (t, 1H), 5.60 (t, 1H), 5.50 (t, 1H), 5.40 (t, 1H), 5.30 (t, 1H), 5.20 (t, 1H), 5.10 (t, 1H), 5.00 (t, 1H), 4.90 (t, 1H), 4.80 (t, 1H), 4.70 (t, 1H), 4.60 (t, 1H), 4.50 (t, 1H), 4.40 (t, 1H), 4.30 (t, 1H), 4.20 (t, 1H), 4.10 (t, 1H), 4.00 (t, 1H), 3.90 (t, 1H), 3.80 (t, 1H), 3.70 (t, 1H), 3.60 (t, 1H), 3.50 (t, 1H), 3.40 (t, 1H), 3.30 (t, 1H), 3.20 (t, 1H), 3.10 (t, 1H), 3.00 (t, 1H), 2.90 (t, 1H), 2.80 (t, 1H), 2.70 (t, 1H), 2.60 (t, 1H), 2.50 (t, 1H), 2.40 (t, 1H), 2.30 (t, 1H), 2.20 (t, 1H), 2.10 (t, 1H), 2.00 (t, 1H), 1.90 (t, 1H), 1.80 (t, 1H), 1.70 (t, 1H), 1.60 (t, 1H), 1.50 (t, 1H), 1.40 (t, 1H), 1.30 (t, 1H), 1.20 (t, 1H), 1.10 (t, 1H), 1.00 (t, 1H), 0.90 (t, 1H), 0.80 (t, 1H), 0.70 (t, 1H), 0.60 (t, 1H), 0.50 (t, 1H), 0.40 (t, 1H), 0.30 (t, 1H), 0.20 (t, 1H), 0.10 (t, 1H), 0.00 (t, 1H).

Chemical structure of 4-methoxy-2-(hydrodifluoromethyl)furo[2,3-b]pyridine is shown above the spectrum.

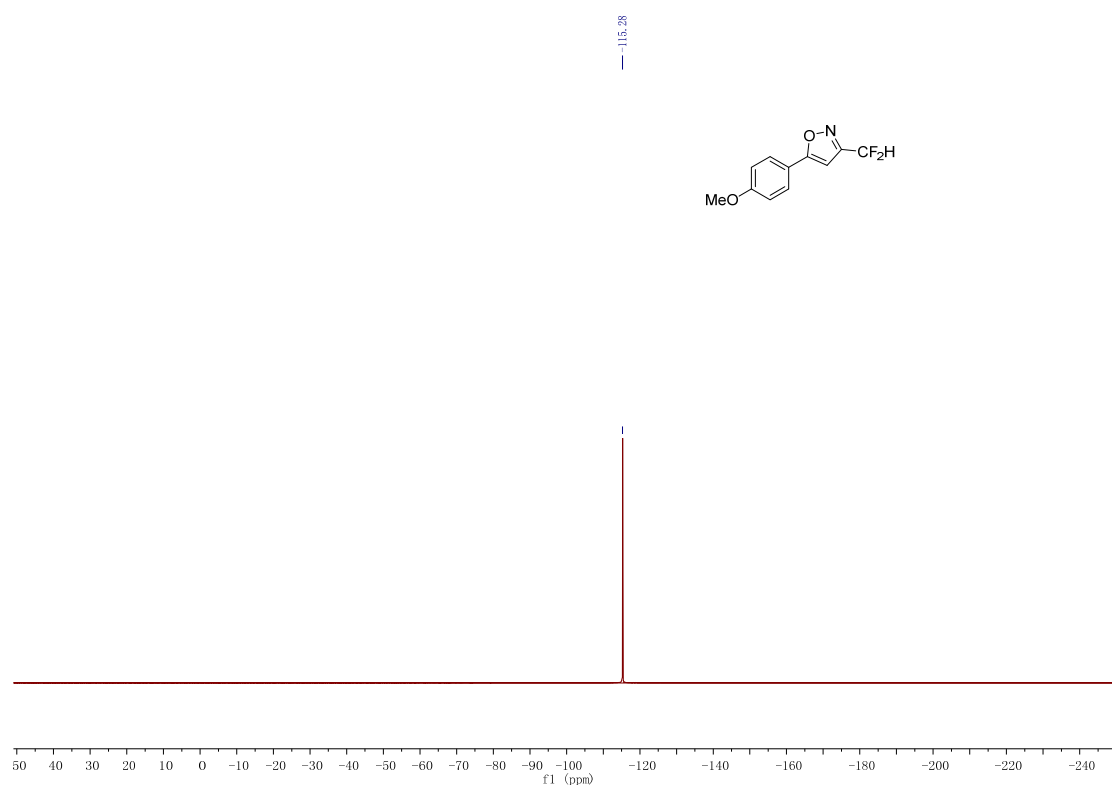
¹³C NMR peaks (ppm):

- 171.96
- 163.66
- 159.96
- 159.68
- 159.38
- 127.96
- 119.67
- 114.89
- 111.86
- 109.13
- 107.16
- 95.01
- 77.68
- 77.06
- 76.44
- 55.76

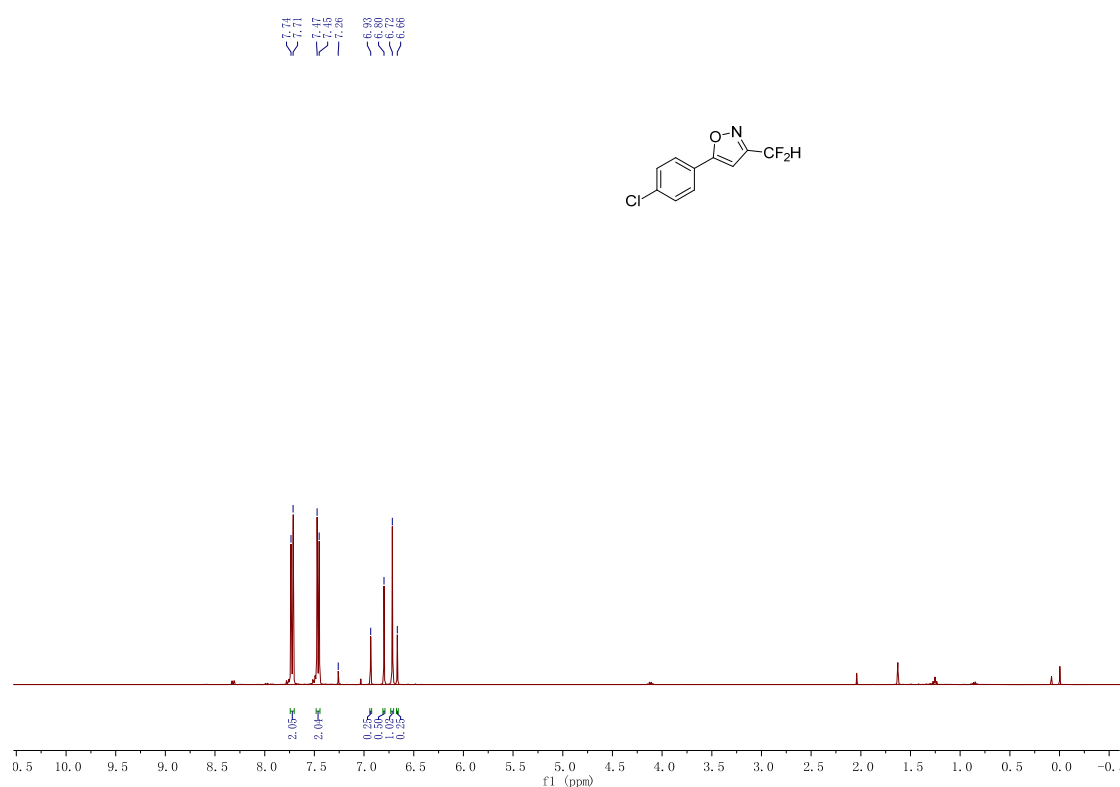
^{19}F NMR (CDCl₃, 376 MHz) of **5e**



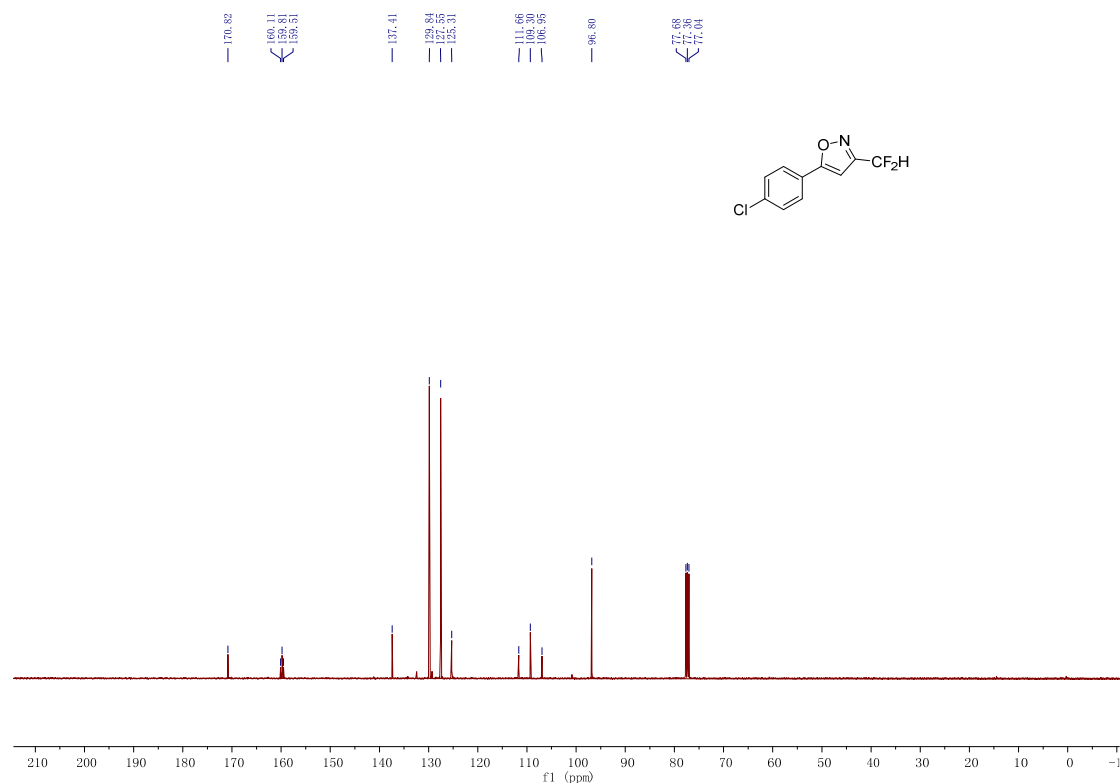
^{19}F { ^1H } NMR (CDCl₃, 376 MHz) of **5e**



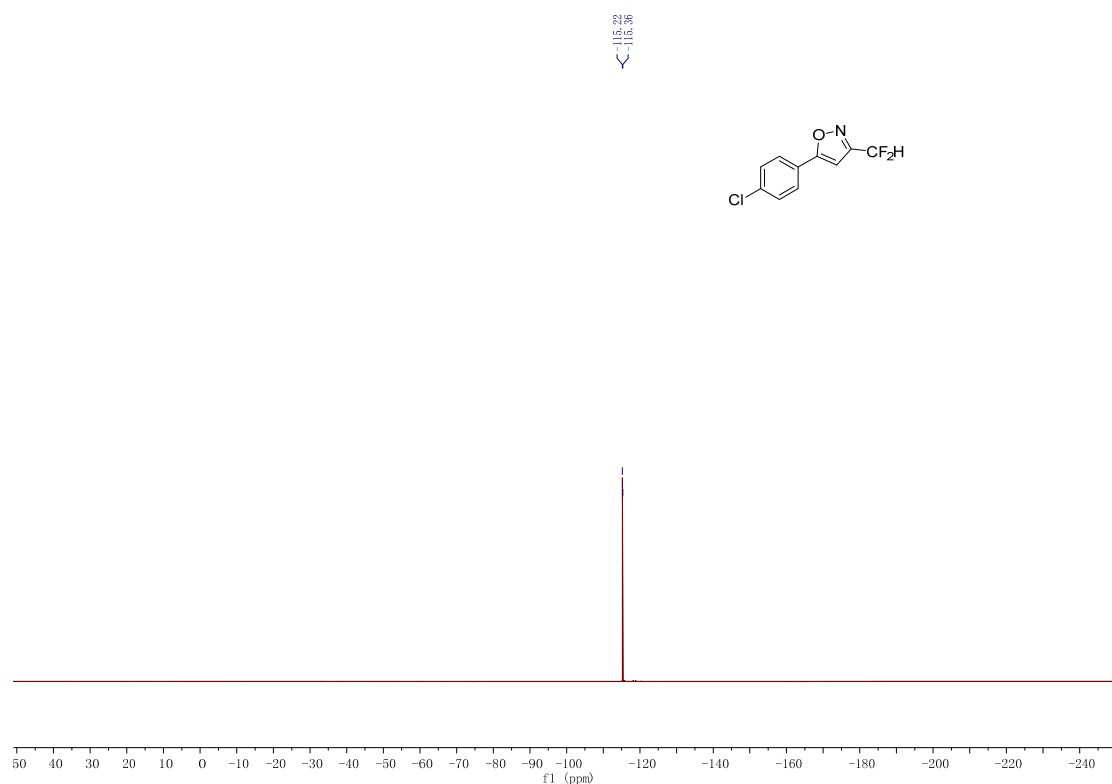
^1H NMR (CDCl₃, 400 MHz) of **5f**



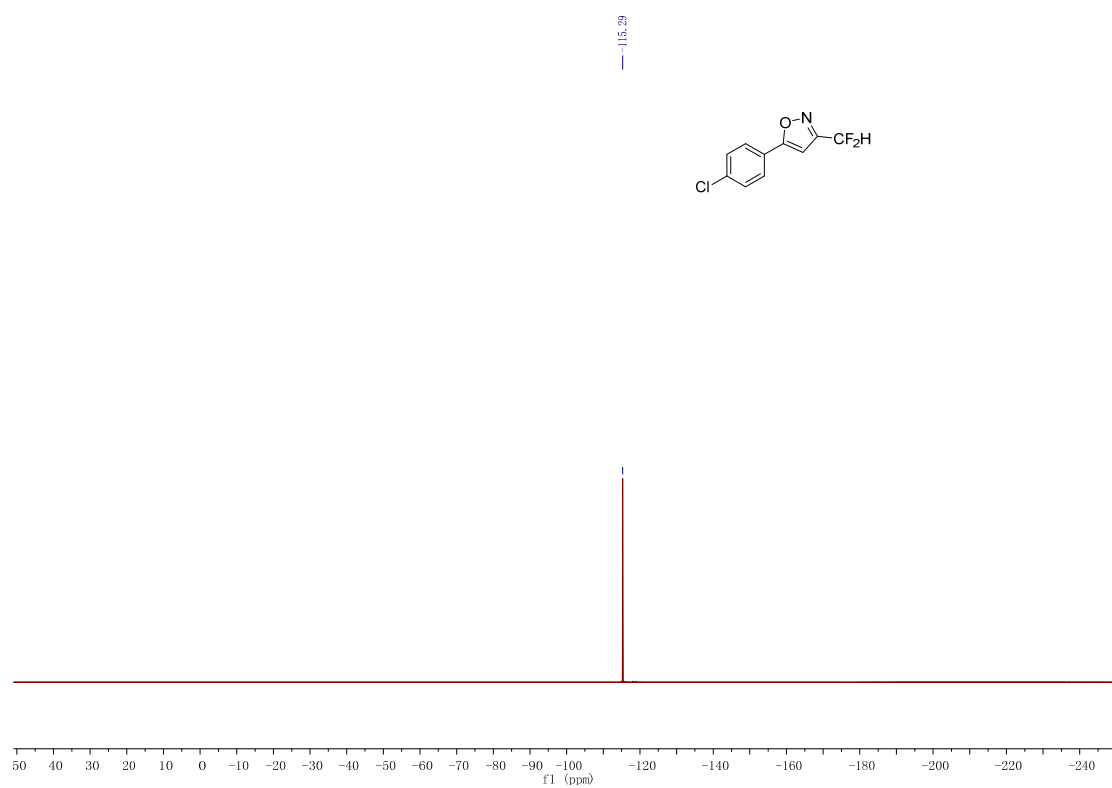
^{13}C NMR (CDCl₃, 100 MHz) of **5f**



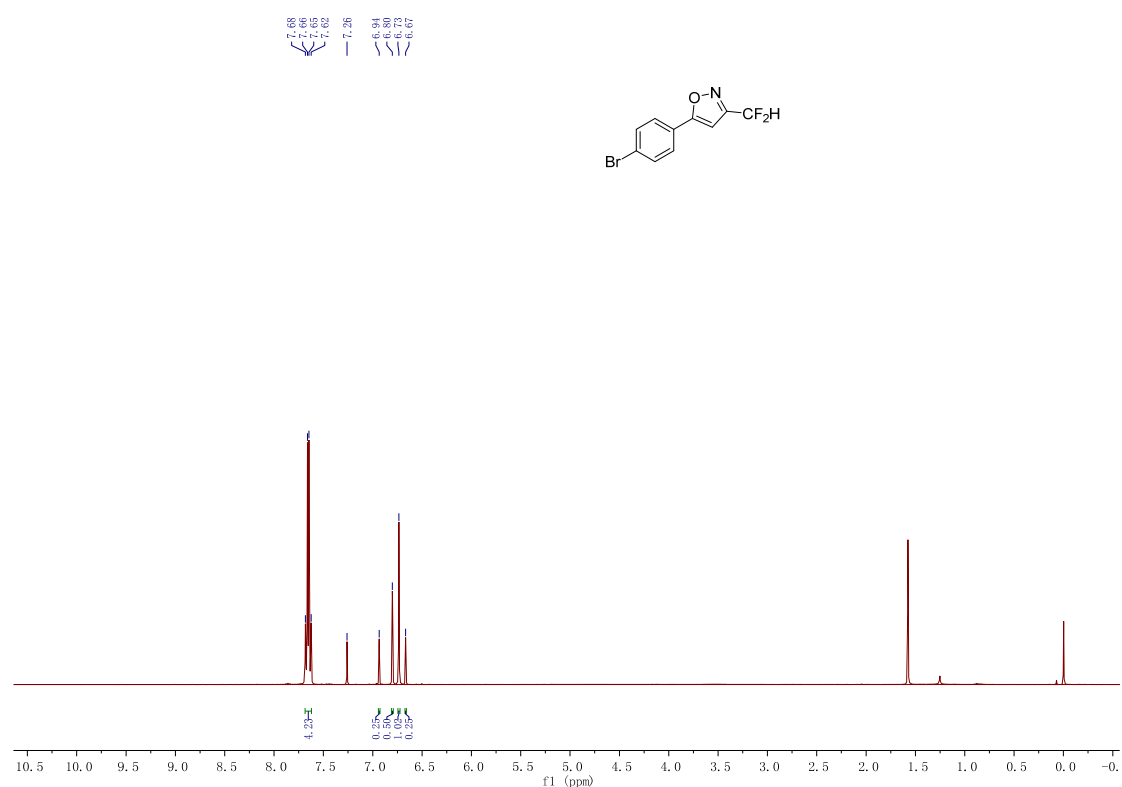
^{19}F NMR (CDCl₃, 376 MHz) of **5f**



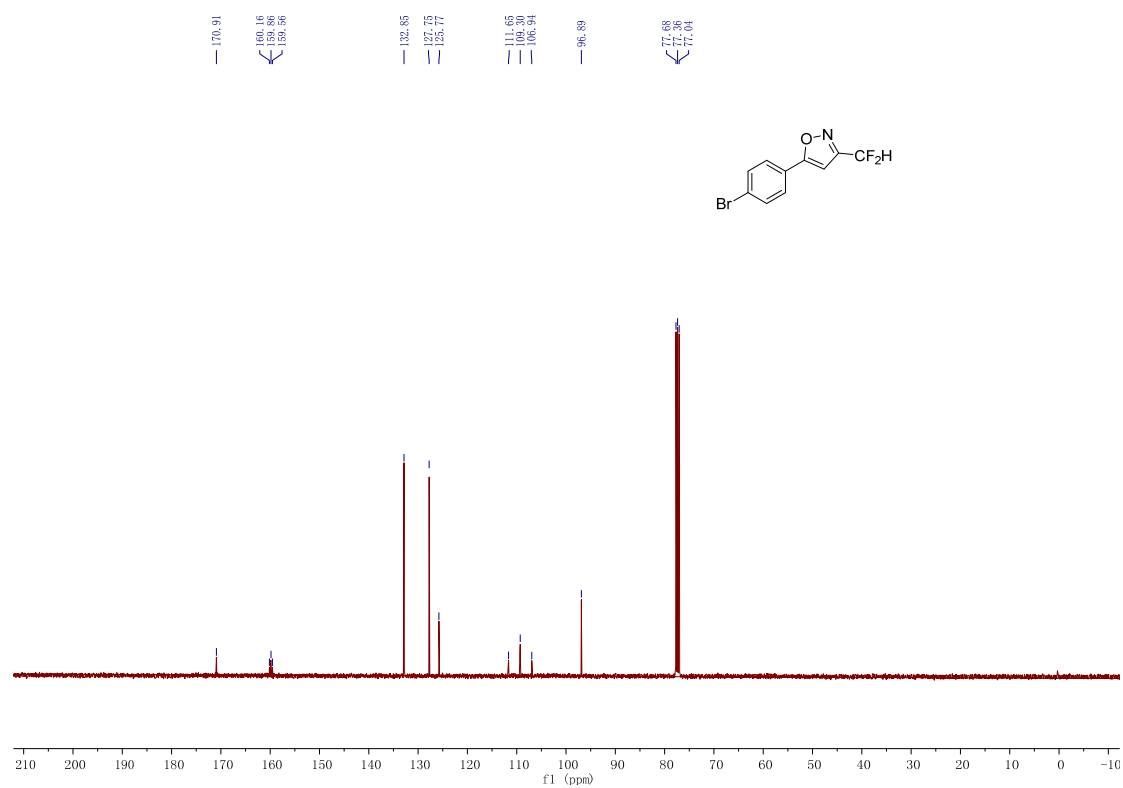
^{19}F { ^1H } NMR (CDCl₃, 376 MHz) of **5f**



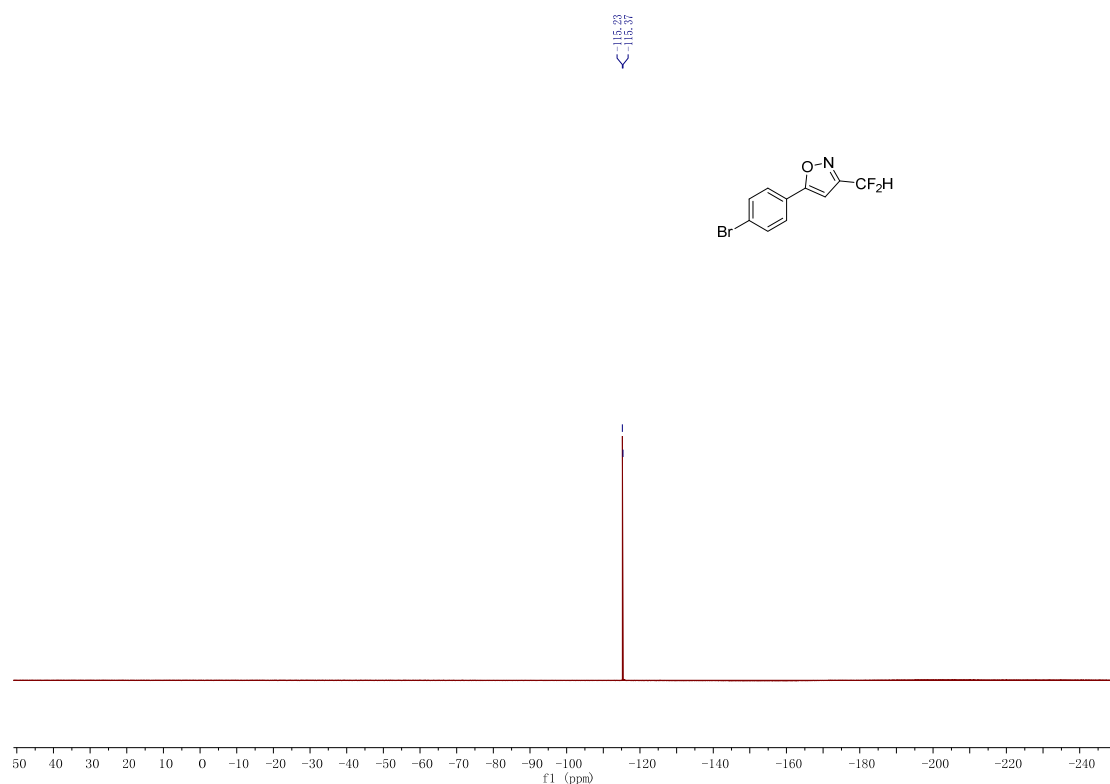
^1H NMR (CDCl₃, 400 MHz) of 5g



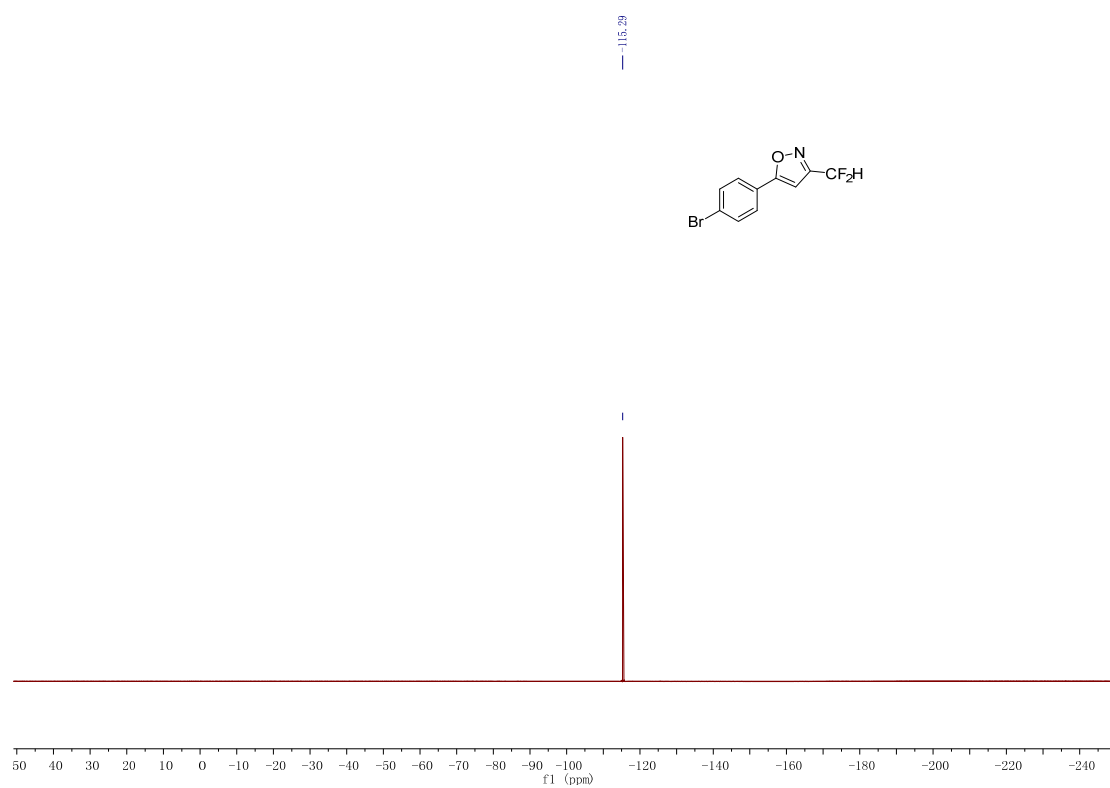
^{13}C NMR (CDCl₃, 100 MHz) of 5g



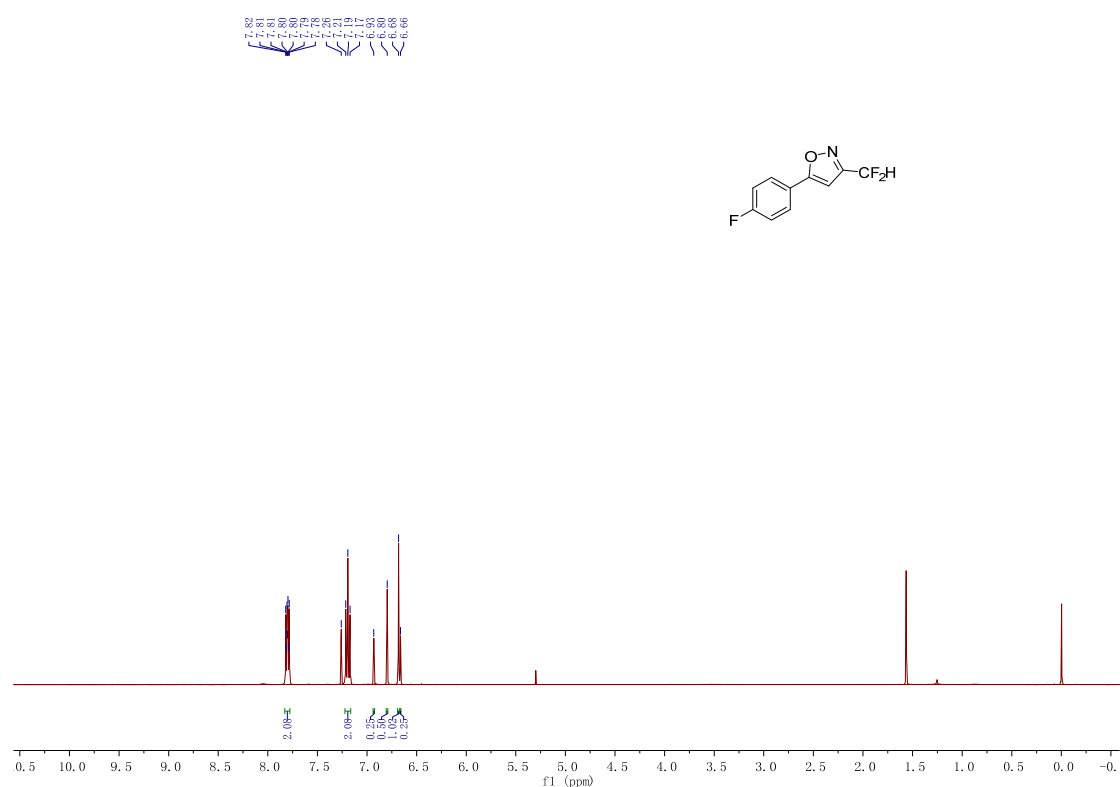
^{19}F NMR (CDCl₃, 376 MHz) of **5g**



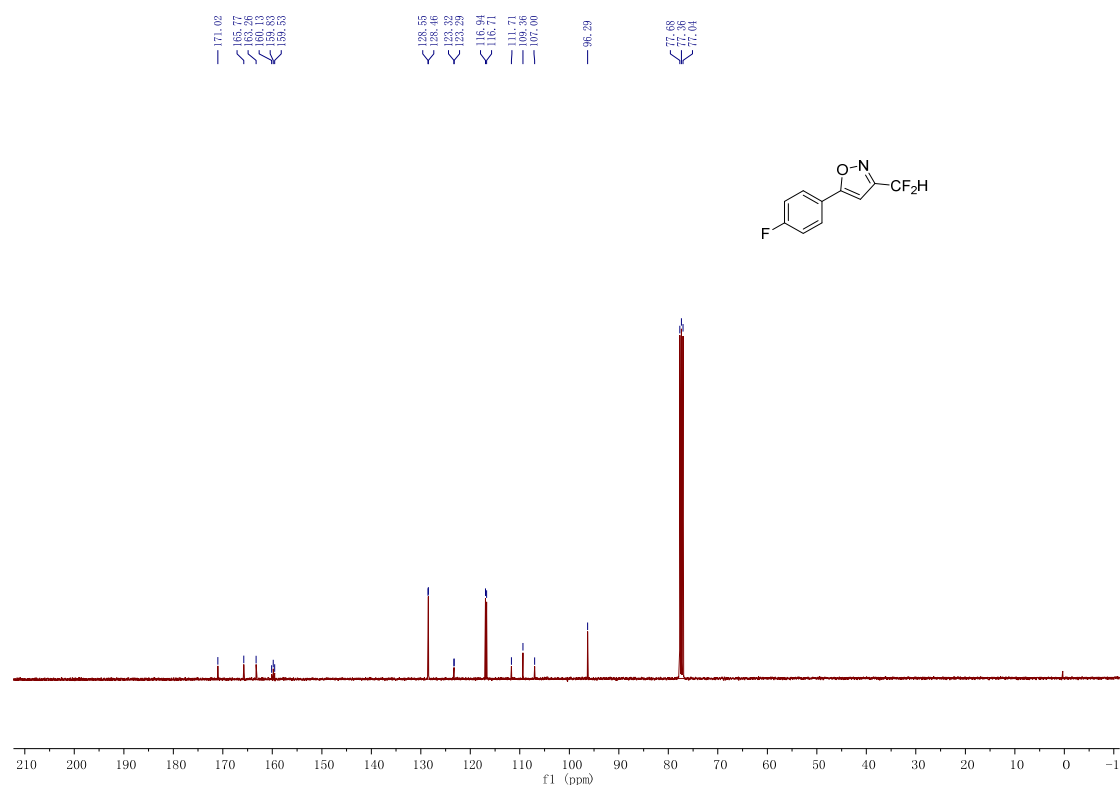
^{19}F { ^1H } NMR (CDCl₃, 376 MHz) of **5g**



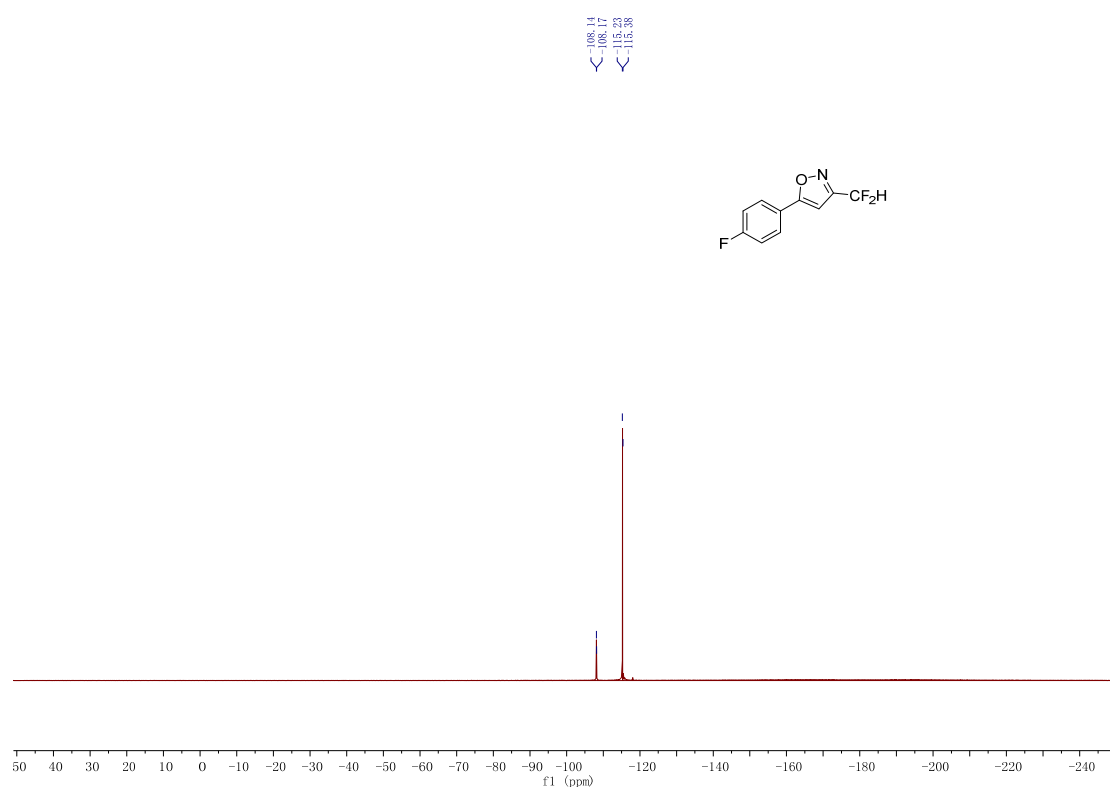
^1H NMR (CDCl₃, 400 MHz) of 5h



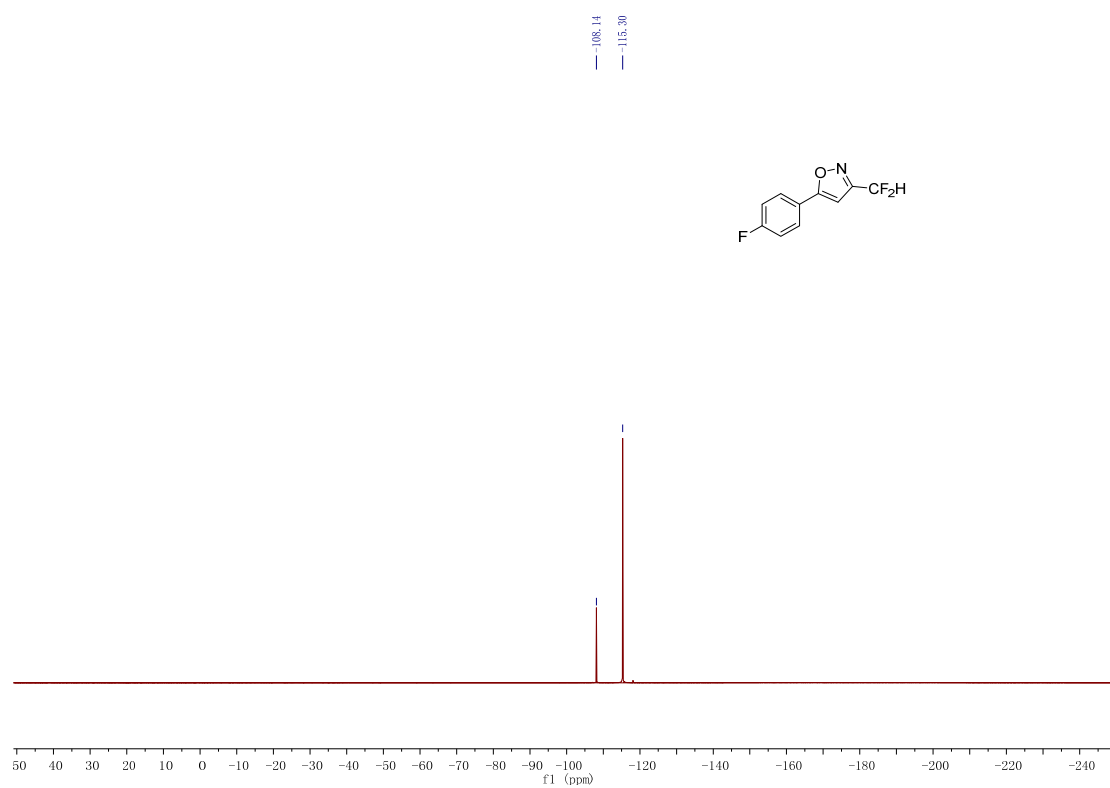
^{13}C NMR (CDCl₃, 100 MHz) of 5h



^{19}F NMR (CDCl₃, 376 MHz) of **5h**



^{19}F { ^1H } NMR (CDCl₃, 376 MHz) of **5h**



Chemical structure of 4-(4-(trifluoromethyl)phenyl)-2-(difluoromethyl)furo[3,2-b]pyridine is shown above the spectrum.

¹H NMR spectrum (CDCl₃) showing chemical shifts (ppm) on the x-axis (ranging from -0.5 to 10.5) and integration values below the peaks. The spectrum displays several multiplets in the aromatic region (6.5-8.0 ppm) and a doublet in the aliphatic region (1.2-1.6 ppm).

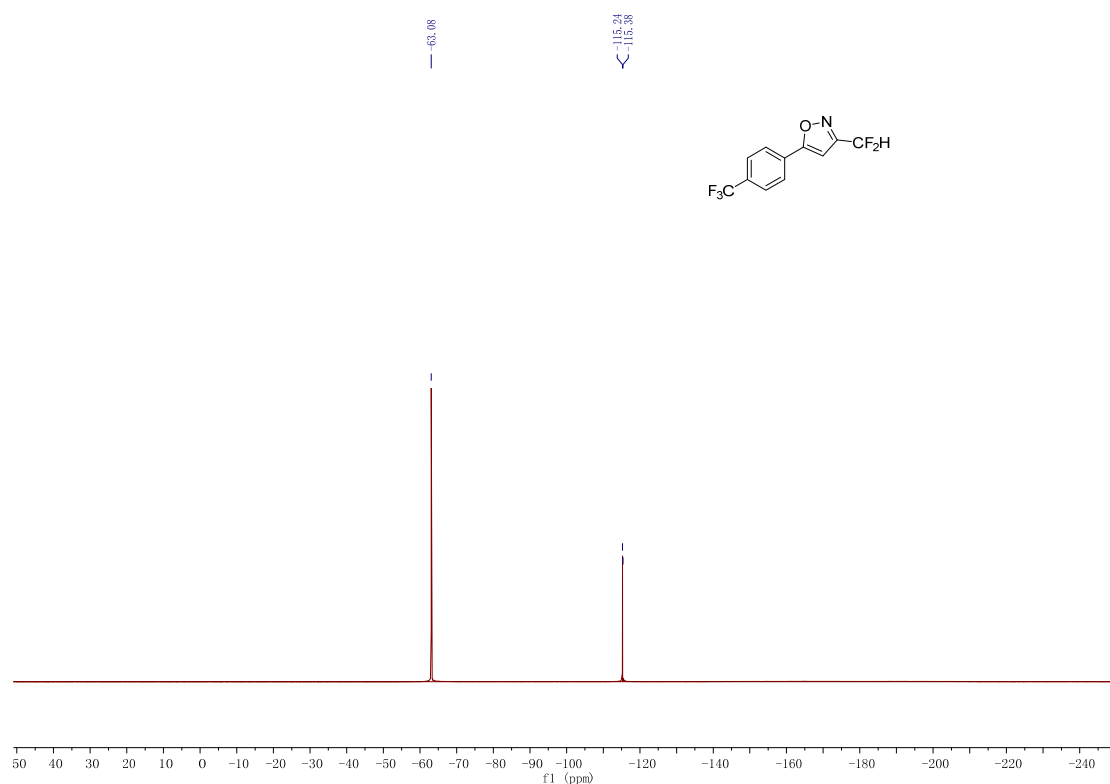
Chemical structure: FC(F)(F)c1ccc(cc1)-c2cc(C(F)F)n(O)c2

¹³C NMR spectrum (ppm):

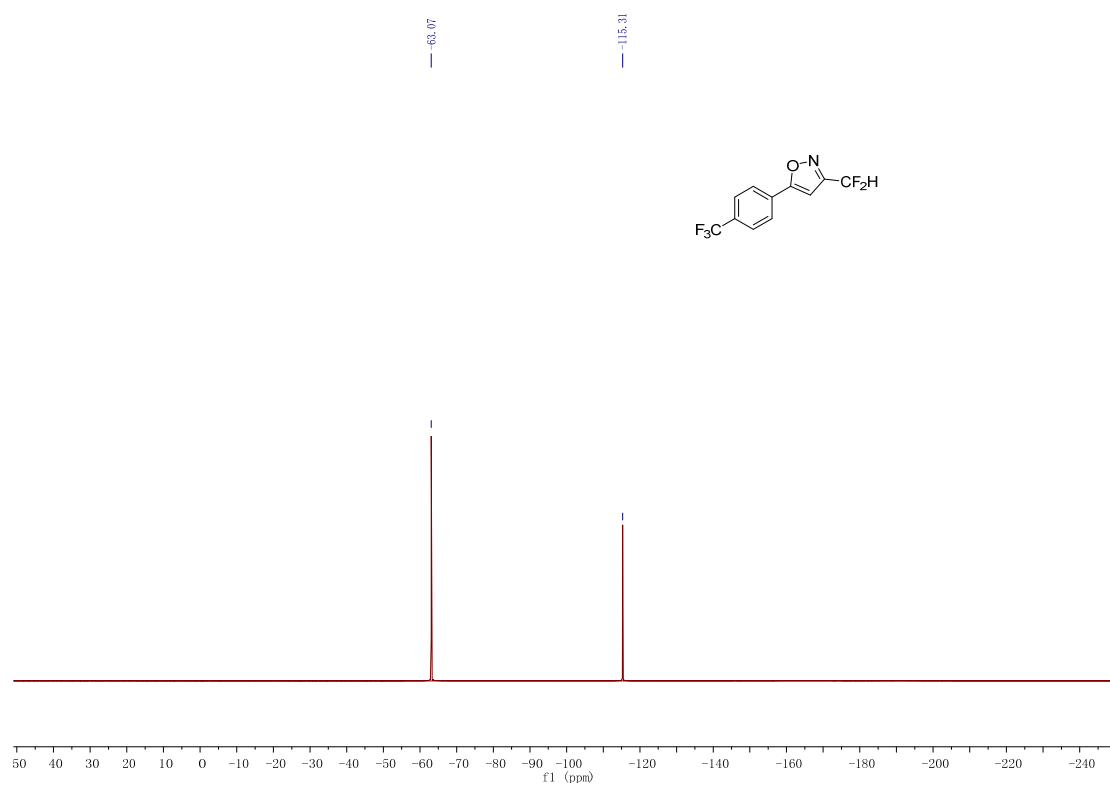
- 170.34
- 160.24
- 158.94
- 158.64
- 133.15
- 132.52
- 132.52
- 128.67
- 128.67
- 128.53
- 128.53
- 128.56
- 128.56
- 127.29
- 127.29
- 127.58
- 127.58
- 111.58
- 108.22
- 106.87
- 98.01
- 77.68
- 77.36
- 77.04

Chemical structure: FC(F)(F)c1ccc(cc1)-c2cc(C(F)F)n(O)c2

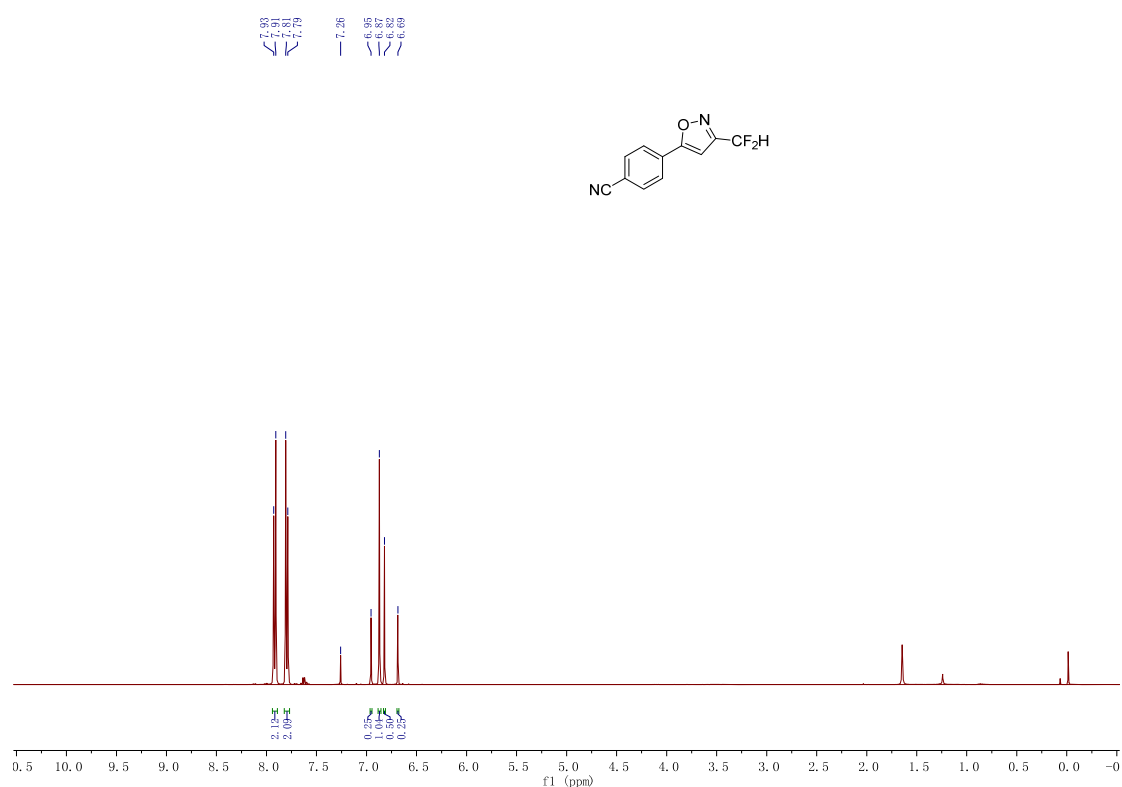
^{19}F NMR (CDCl₃, 376 MHz) of **5i**



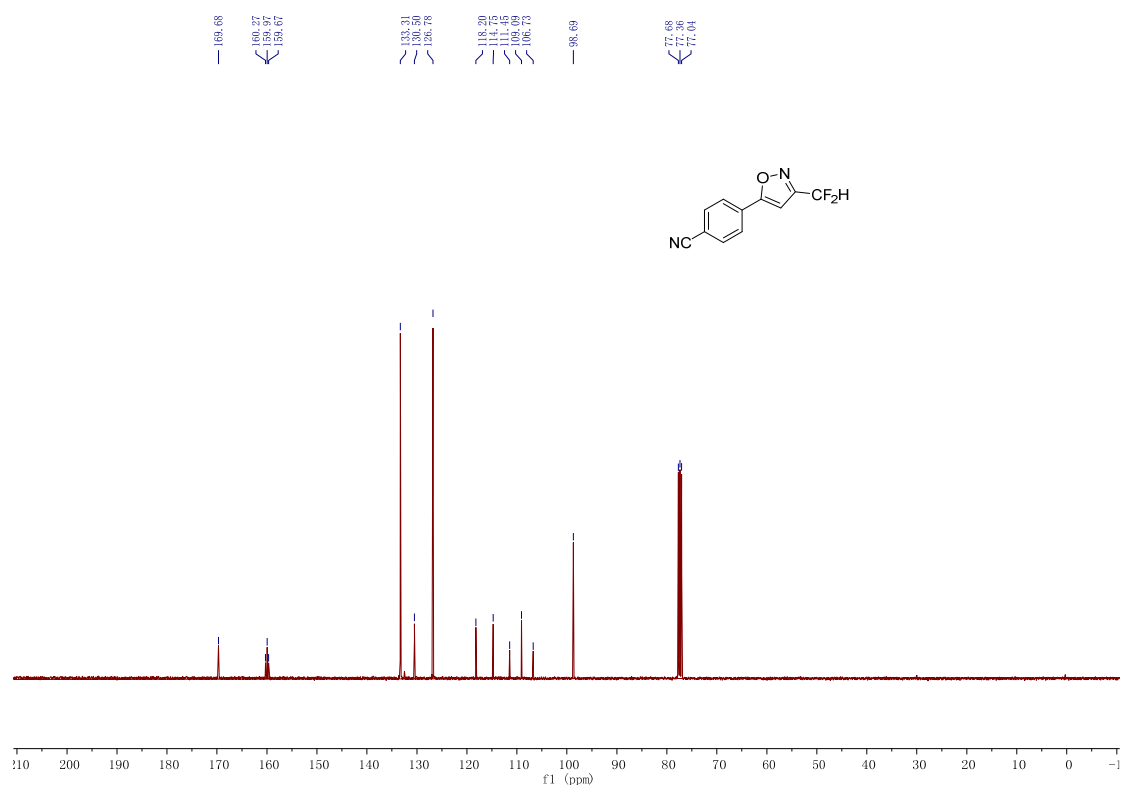
^{19}F { ^1H } NMR (CDCl₃, 376 MHz) of **5i**



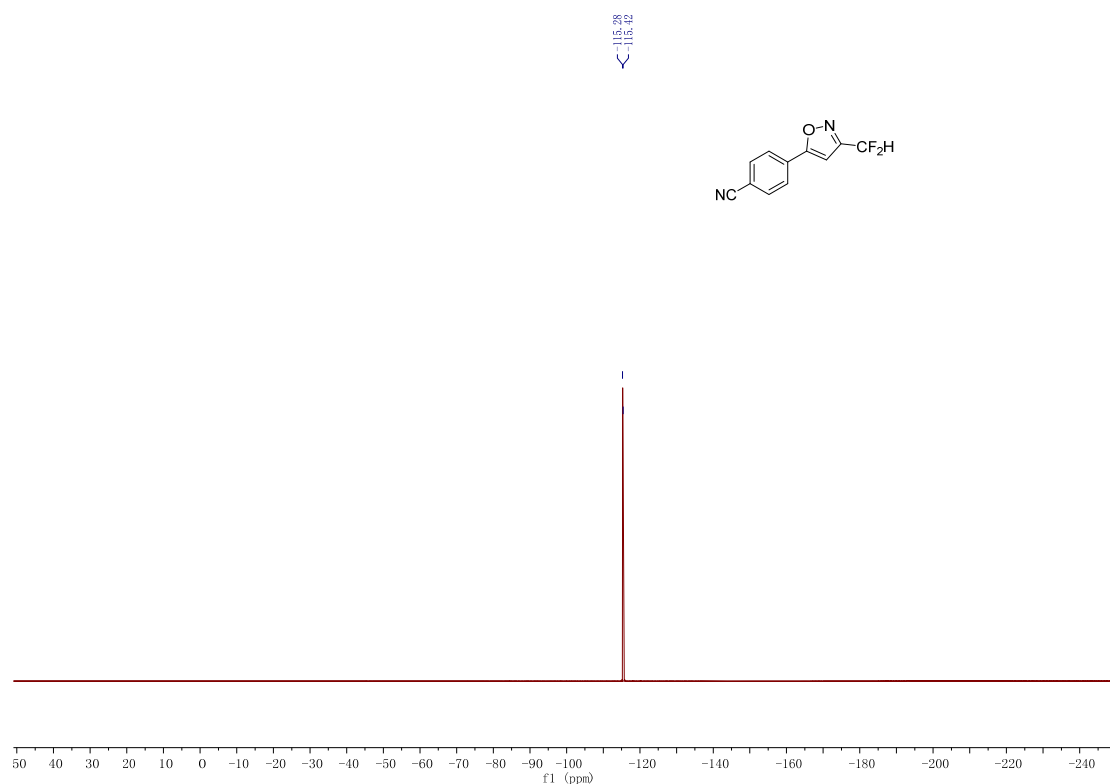
¹H NMR (CDCl₃, 400 MHz) of 5j



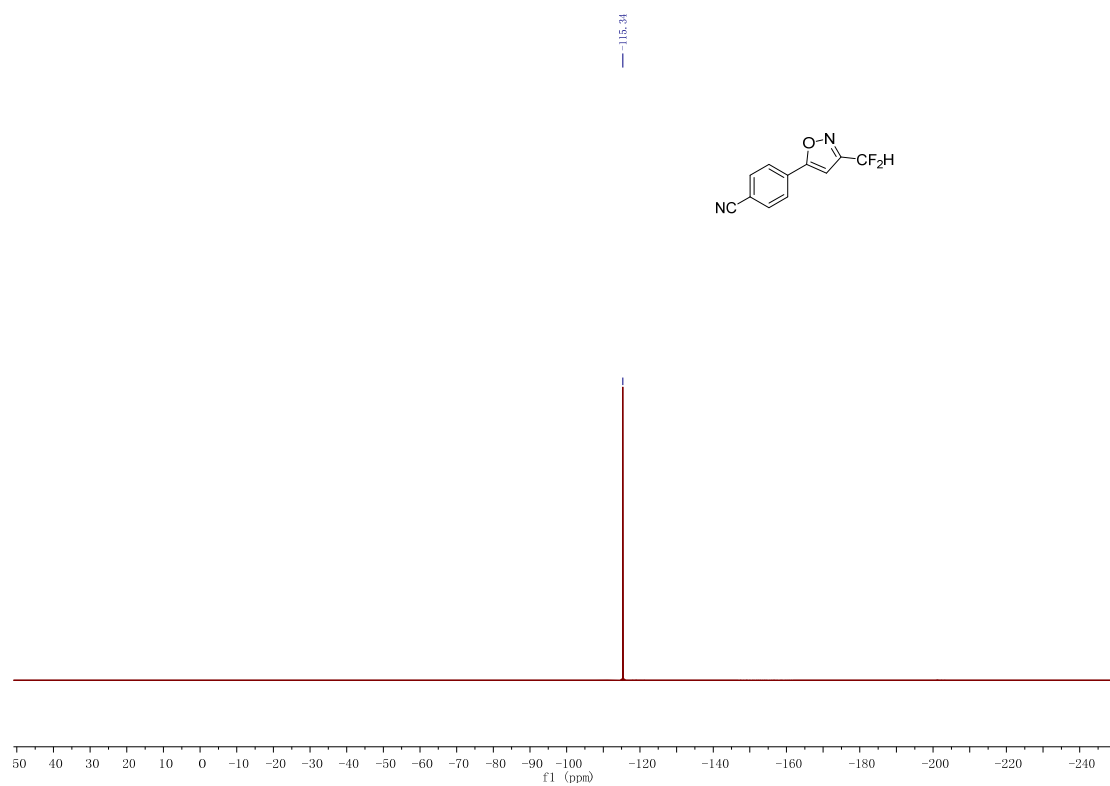
¹³C NMR (CDCl₃, 100 MHz) of 5j



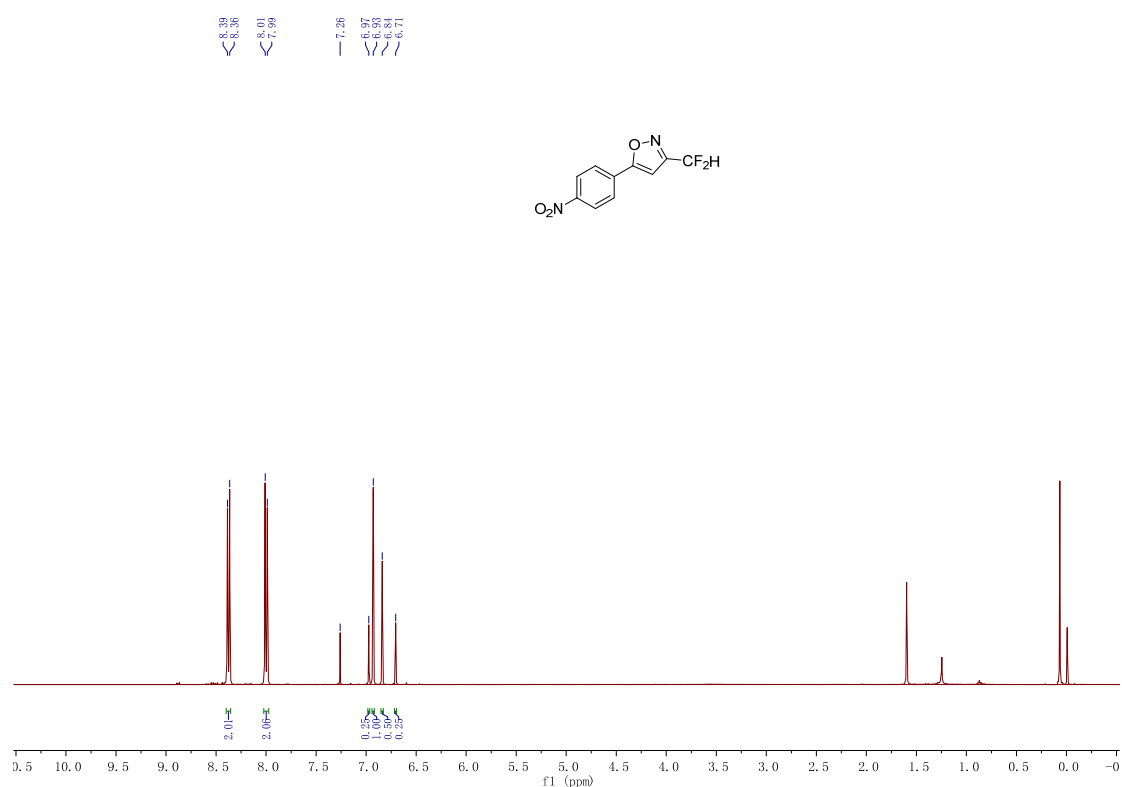
^{19}F NMR (CDCl₃, 376 MHz) of **5j**



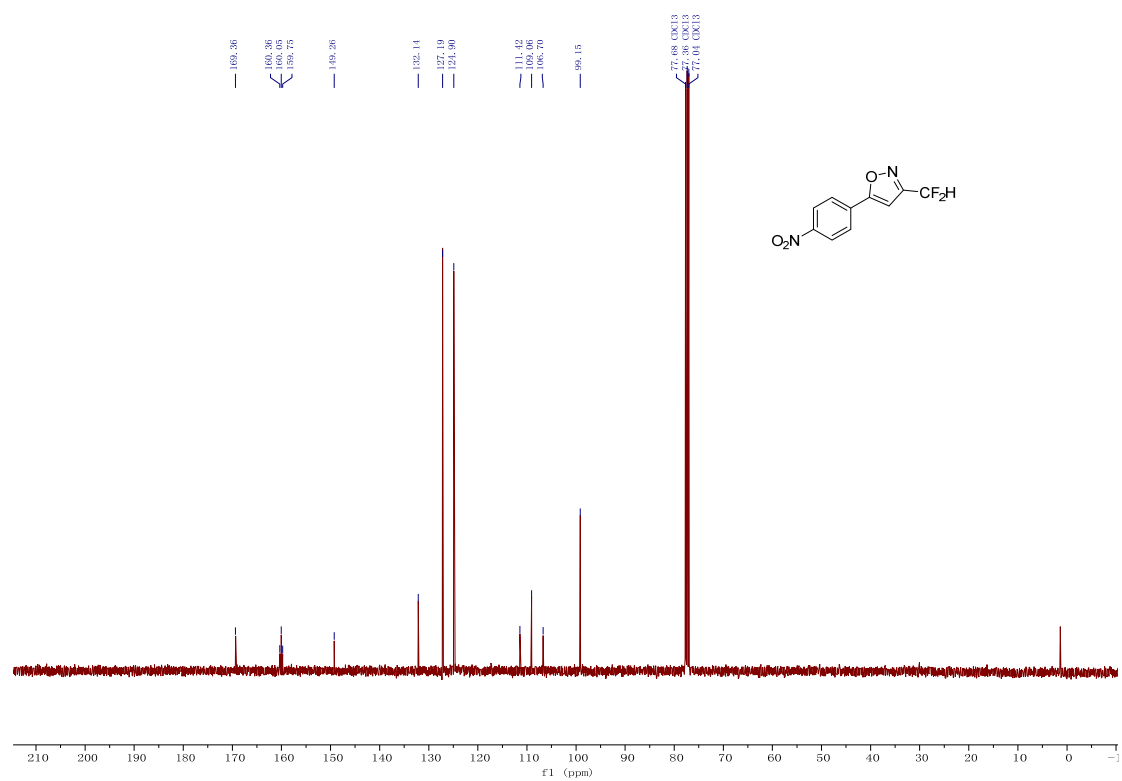
^{19}F { ^1H } NMR (CDCl₃, 376 MHz) of **5j**



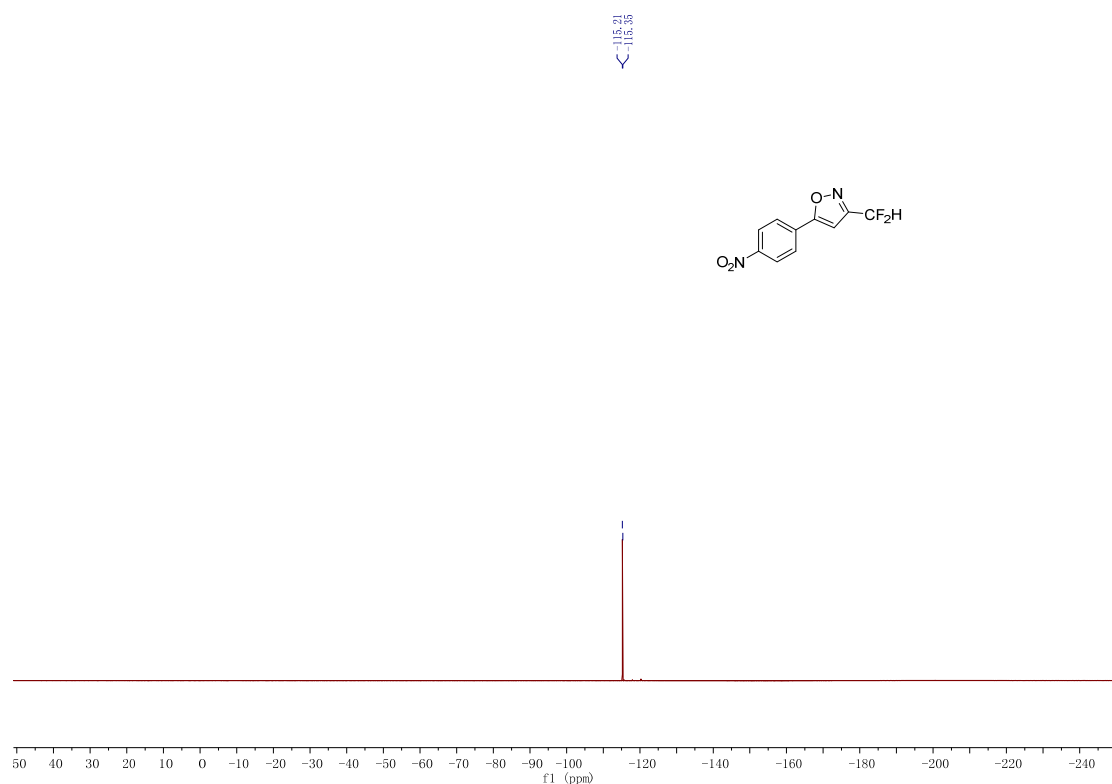
^1H NMR (CDCl₃, 400 MHz) of 5k



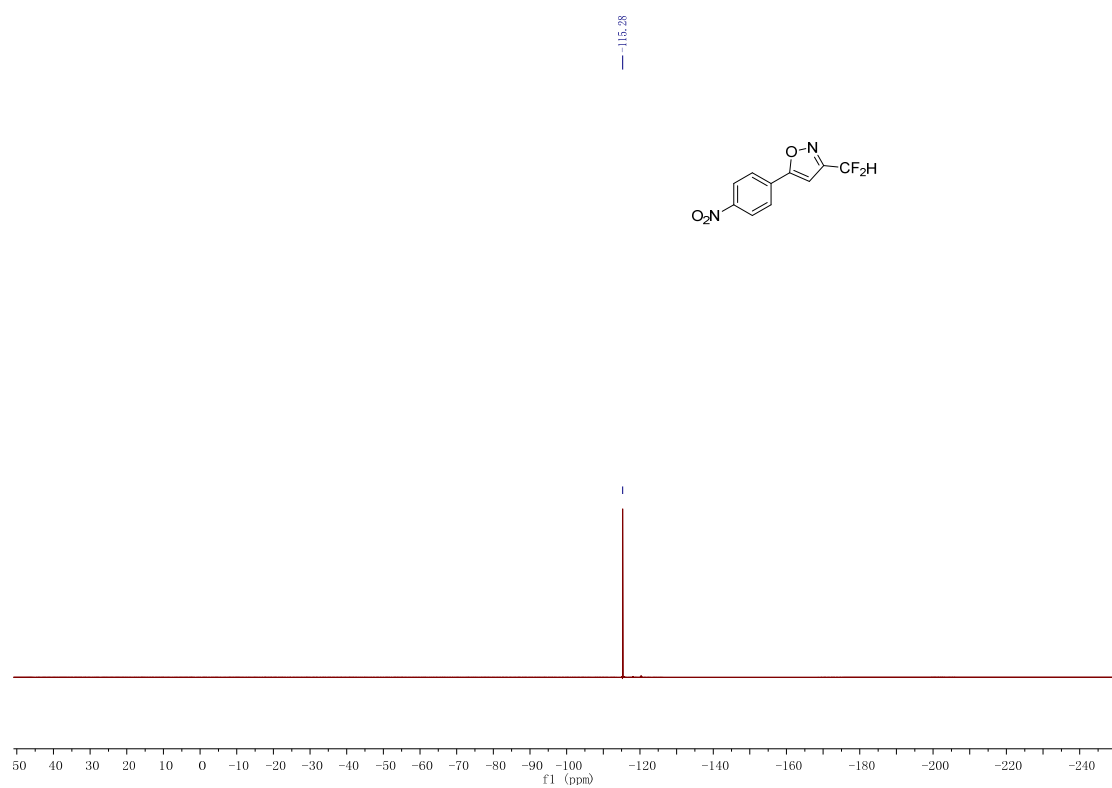
^{13}C NMR (CDCl₃, 100 MHz) of 5k



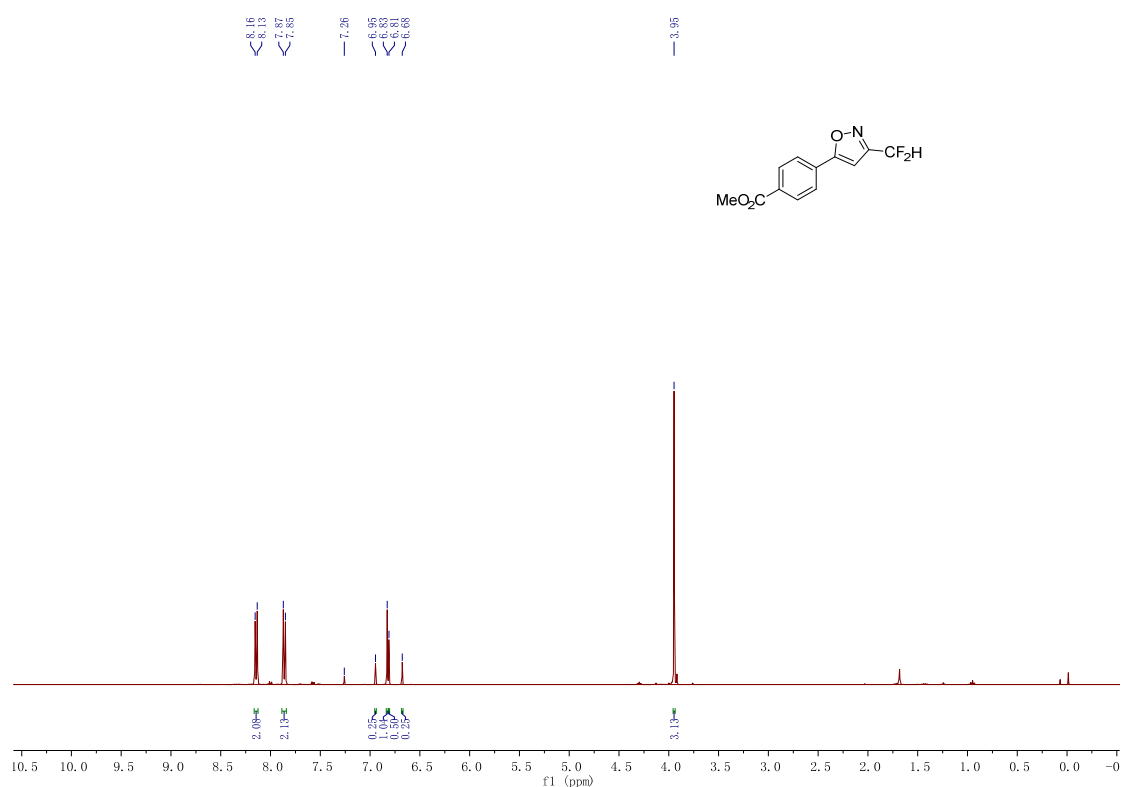
^{19}F NMR (CDCl₃, 376 MHz) of **5k**



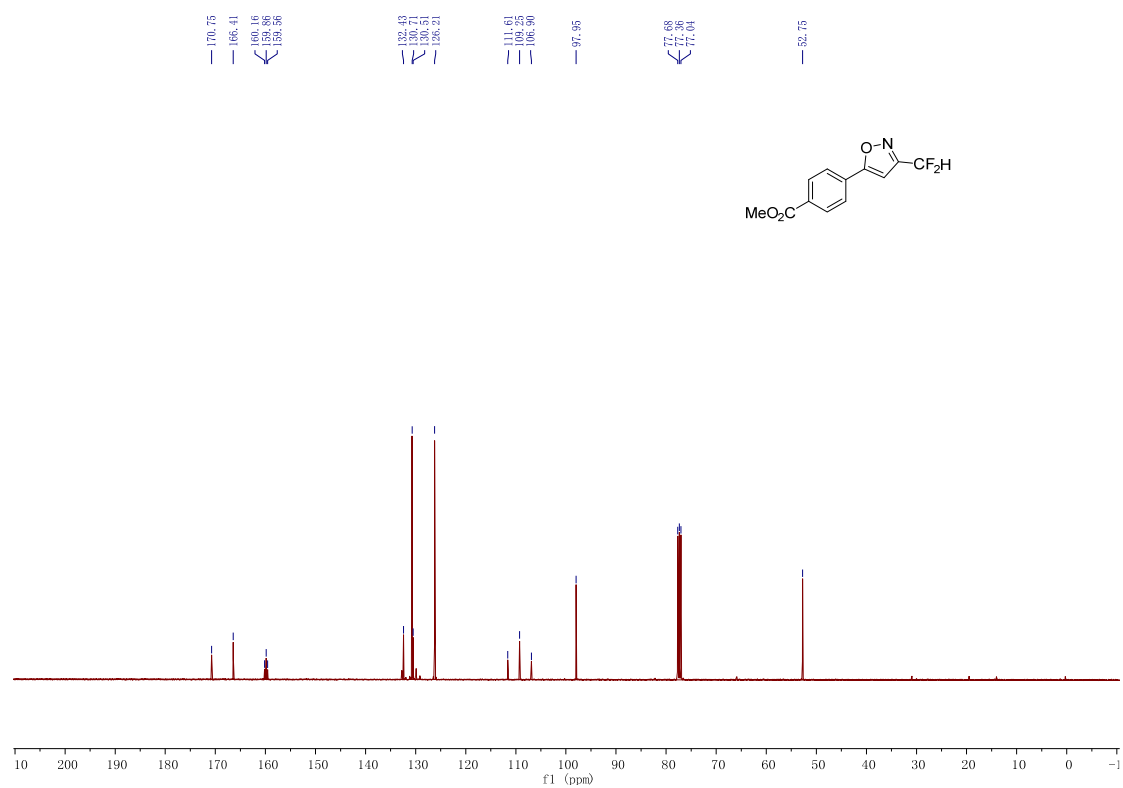
^{19}F { ^1H } NMR (CDCl₃, 376 MHz) of **5k**



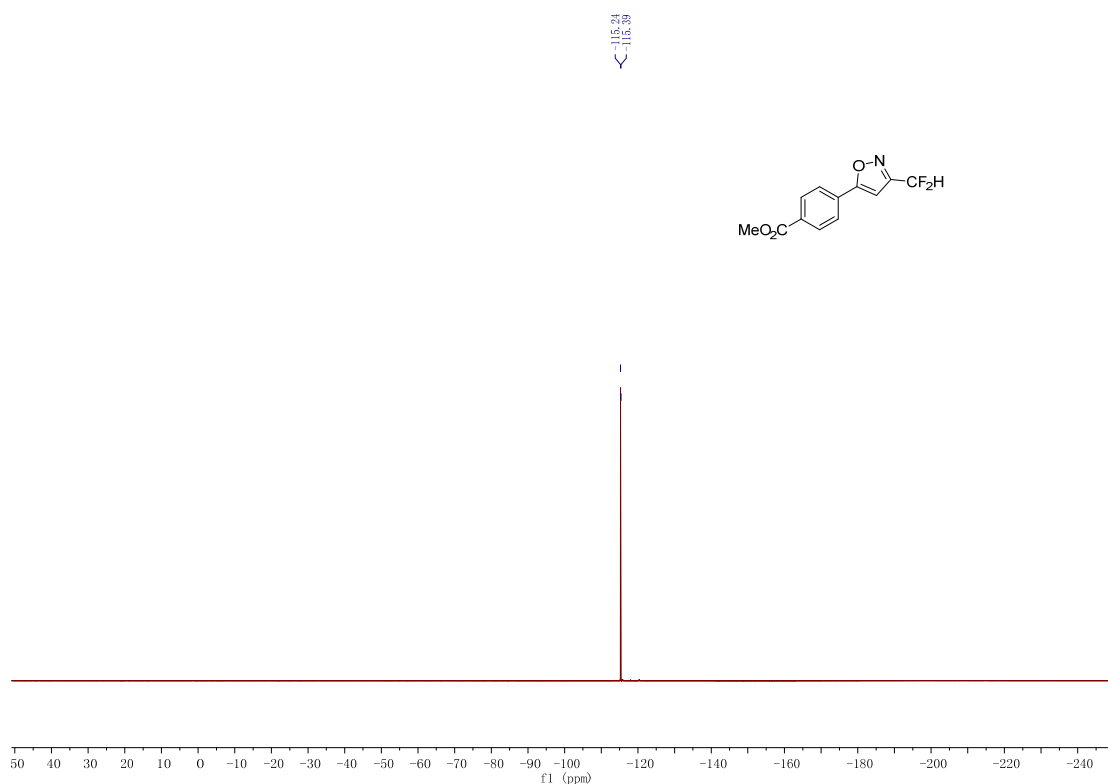
^1H NMR (CDCl₃, 400 MHz) of 5I



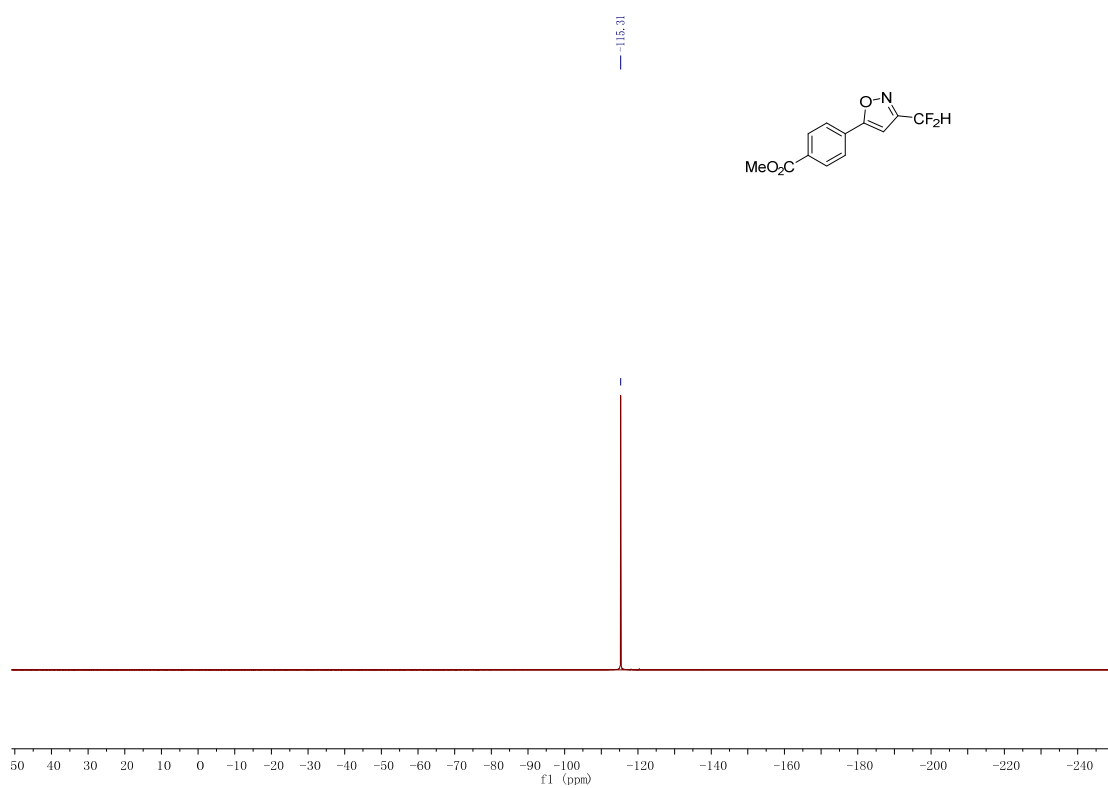
^{13}C NMR (CDCl₃, 100 MHz) of 5I



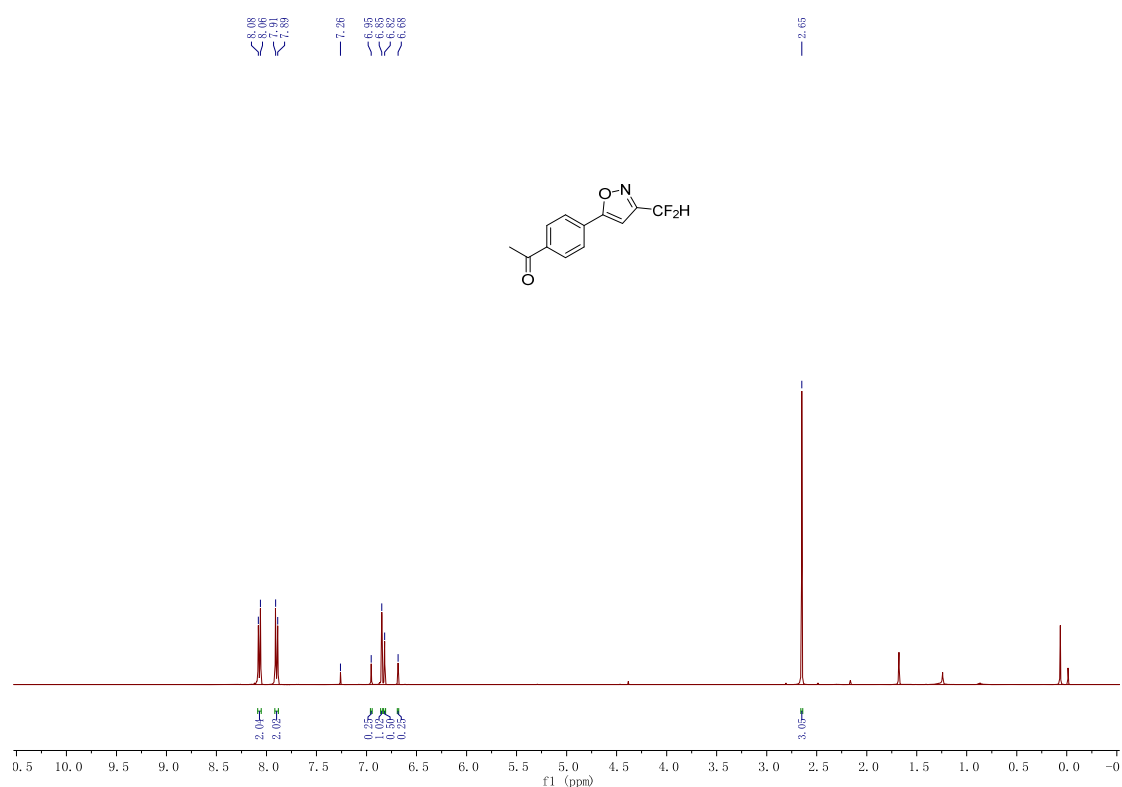
^{19}F NMR (CDCl₃, 376 MHz) of 5I



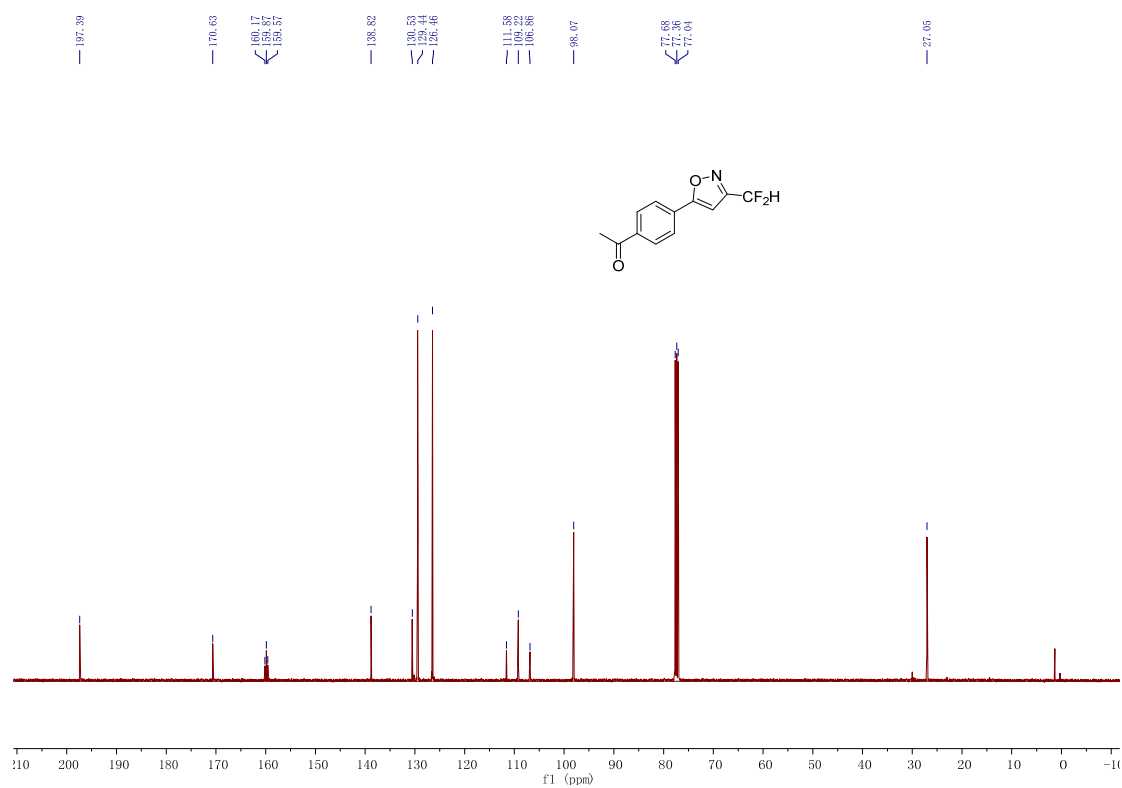
^{19}F { ^1H } NMR (CDCl₃, 376 MHz) of 5I



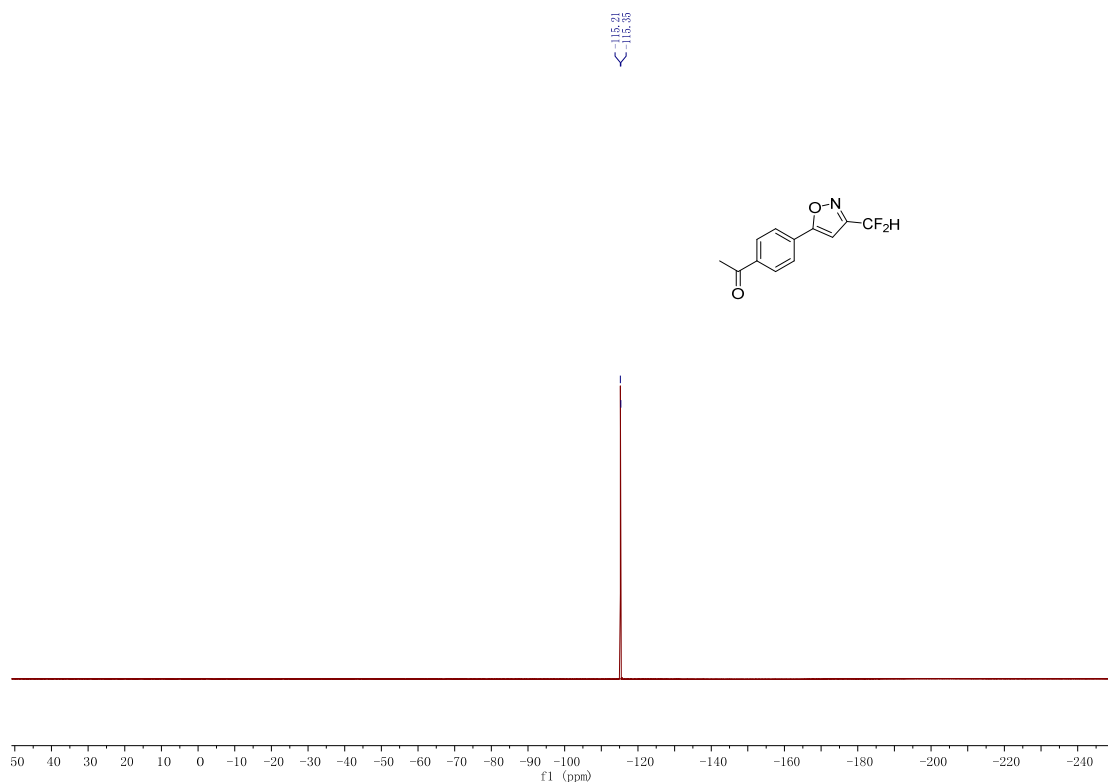
^1H NMR (CDCl₃, 400 MHz) of 5m



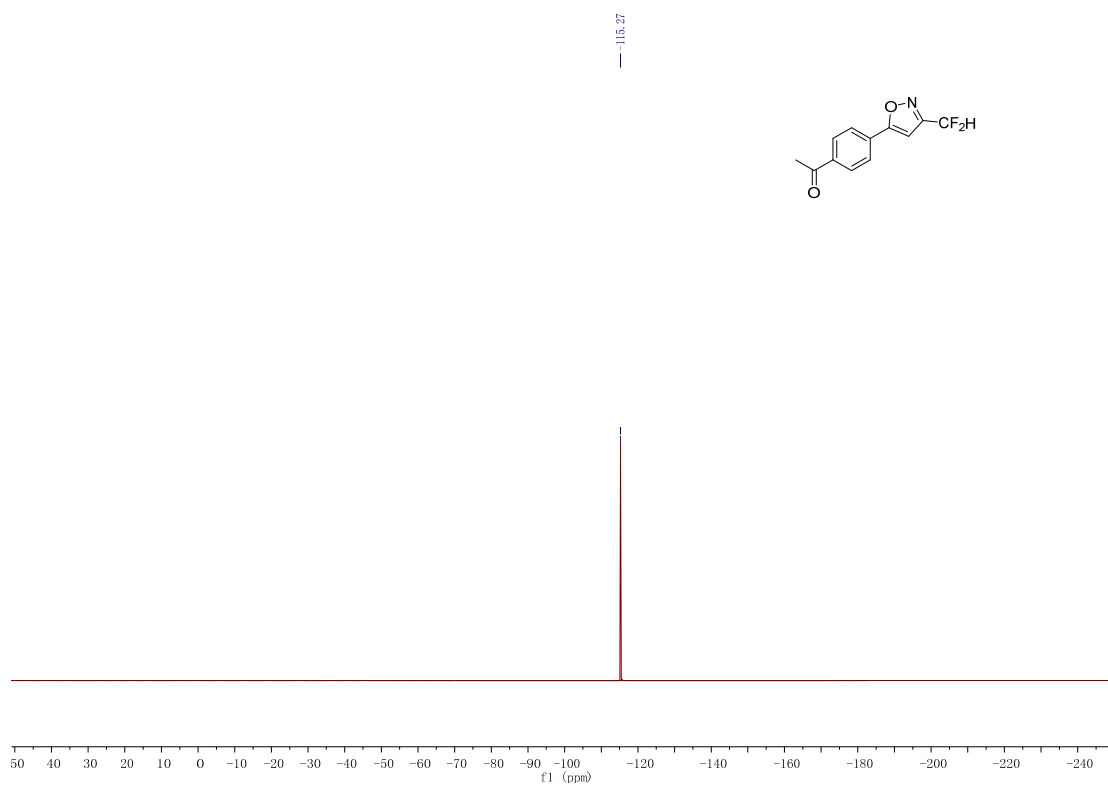
^{13}C NMR (CDCl₃, 100 MHz) of 5m



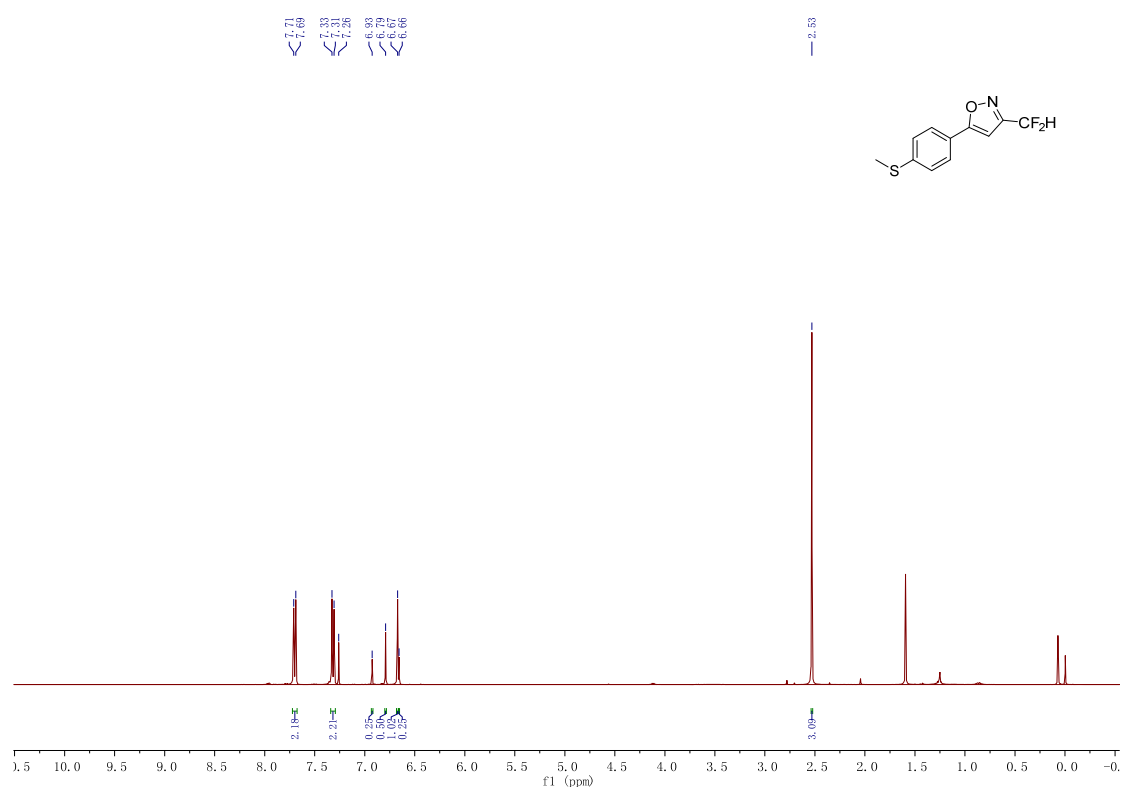
^{19}F NMR (CDCl_3 , 376 MHz) of **5m**



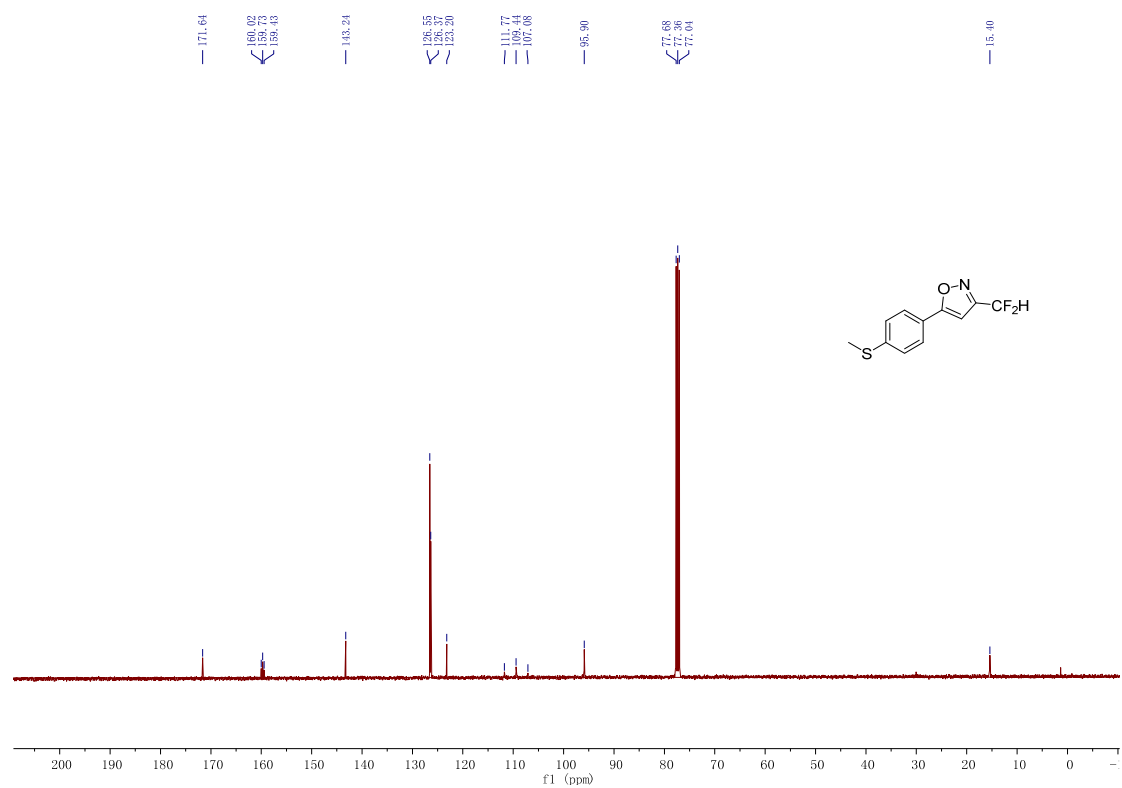
^{19}F { ^1H } NMR (CDCl_3 , 376 MHz) of **5m**



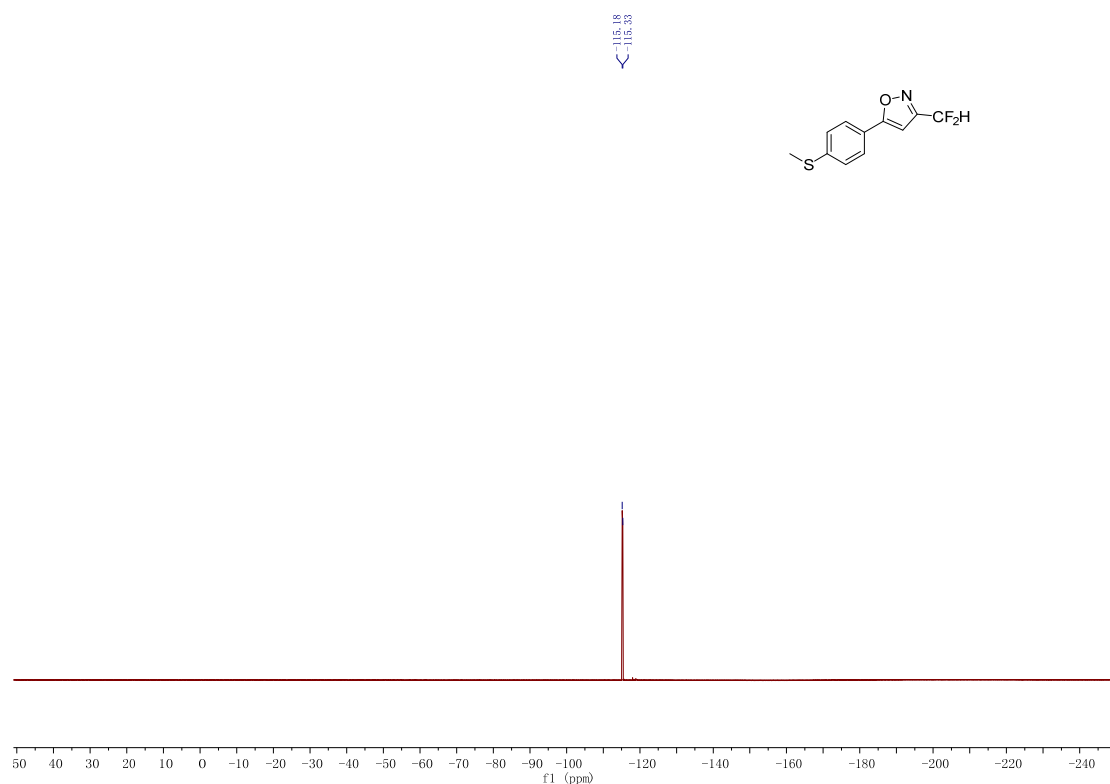
^1H NMR (CDCl₃, 400 MHz) of **5n**



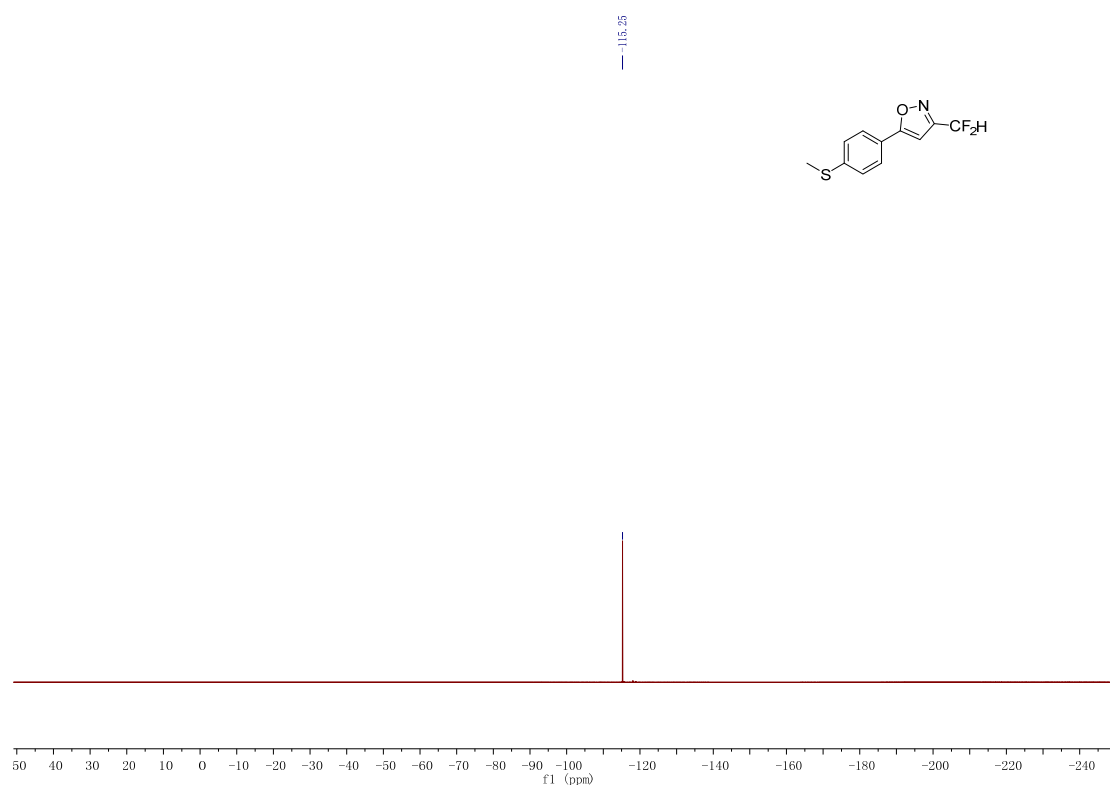
^{13}C NMR (CDCl₃, 100 MHz) of **5n**



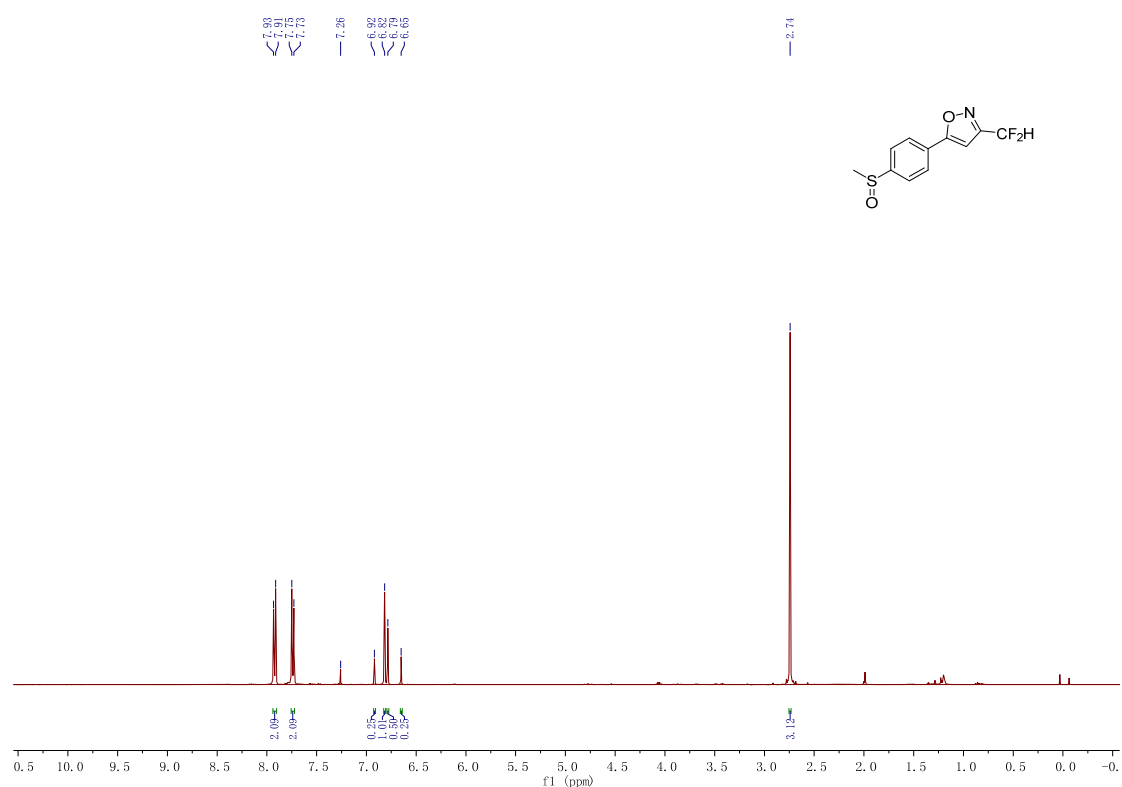
^{19}F NMR (CDCl₃, 376 MHz) of **5n**



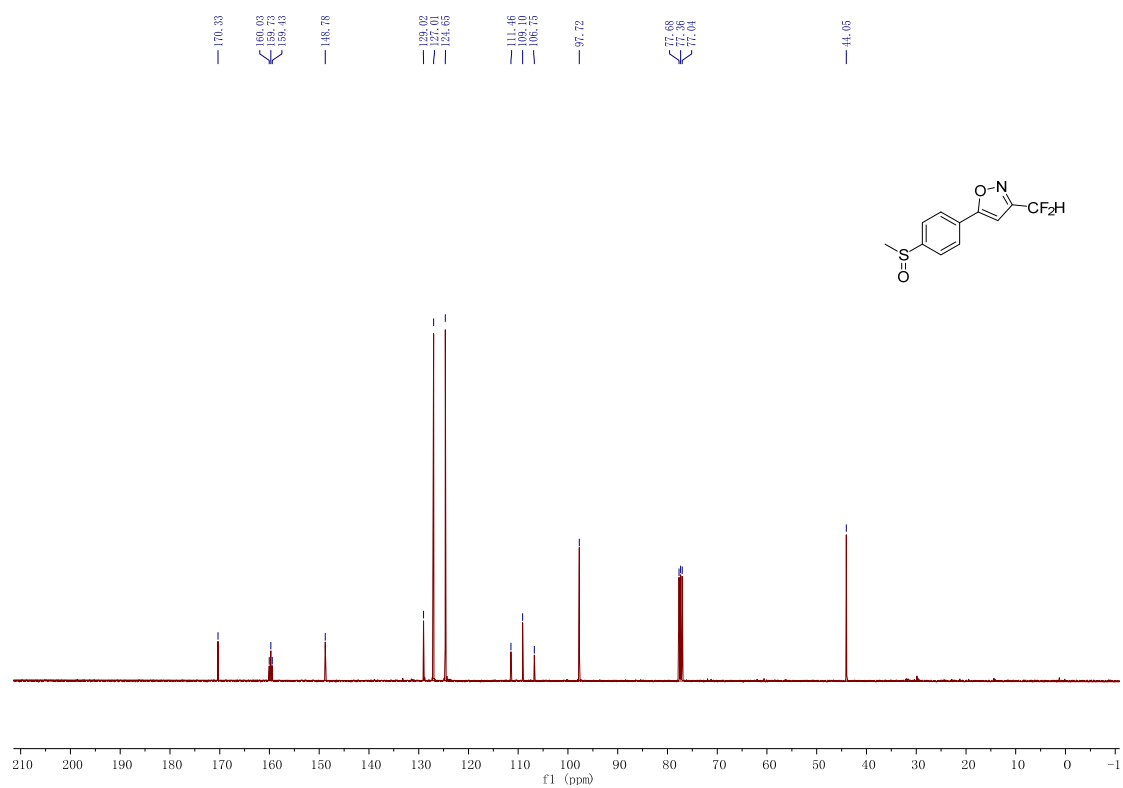
^{19}F { ^1H } NMR (CDCl₃, 376 MHz) of **5n**



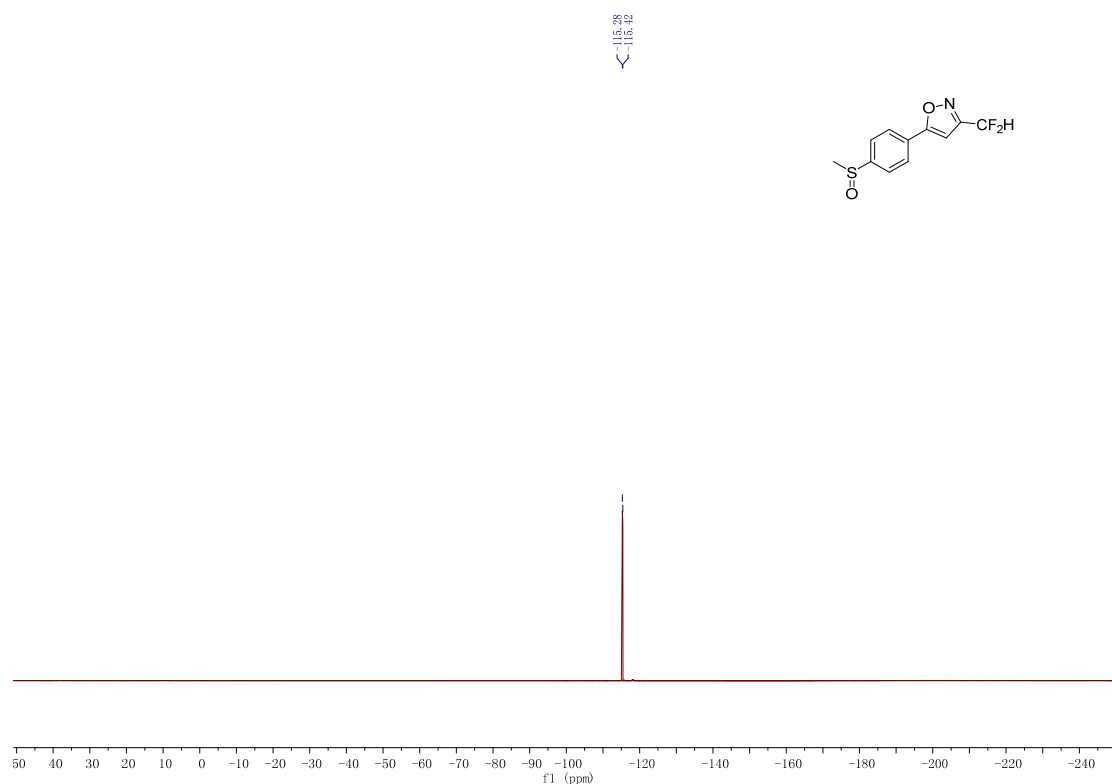
^1H NMR (CDCl₃, 400 MHz) of **5o**



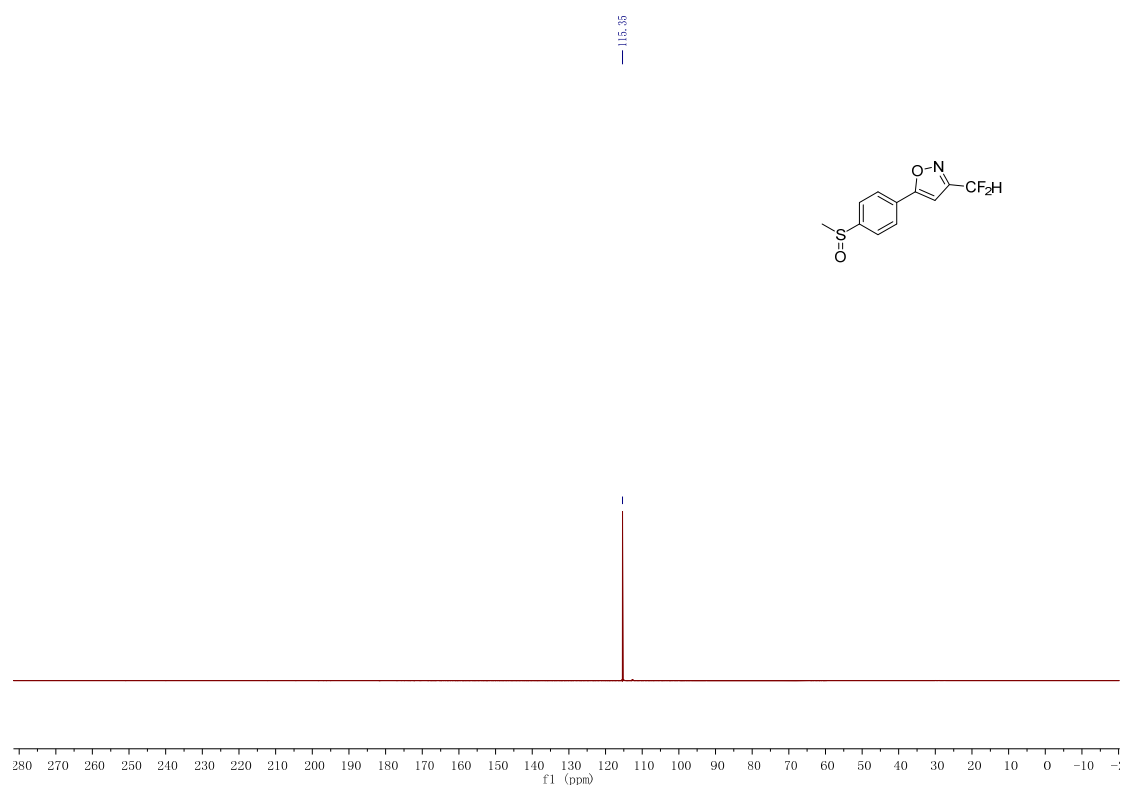
^{13}C NMR (CDCl₃, 100 MHz) of **5o**



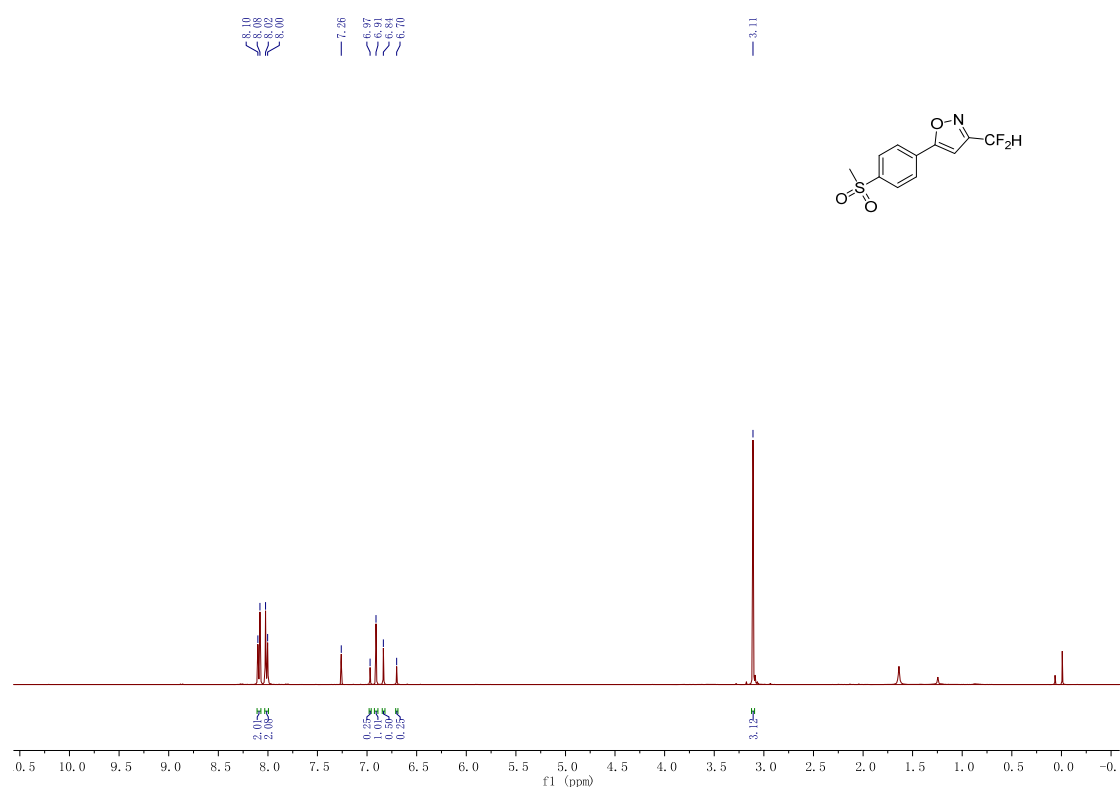
^{19}F NMR (CDCl₃, 376 MHz) of **5o**



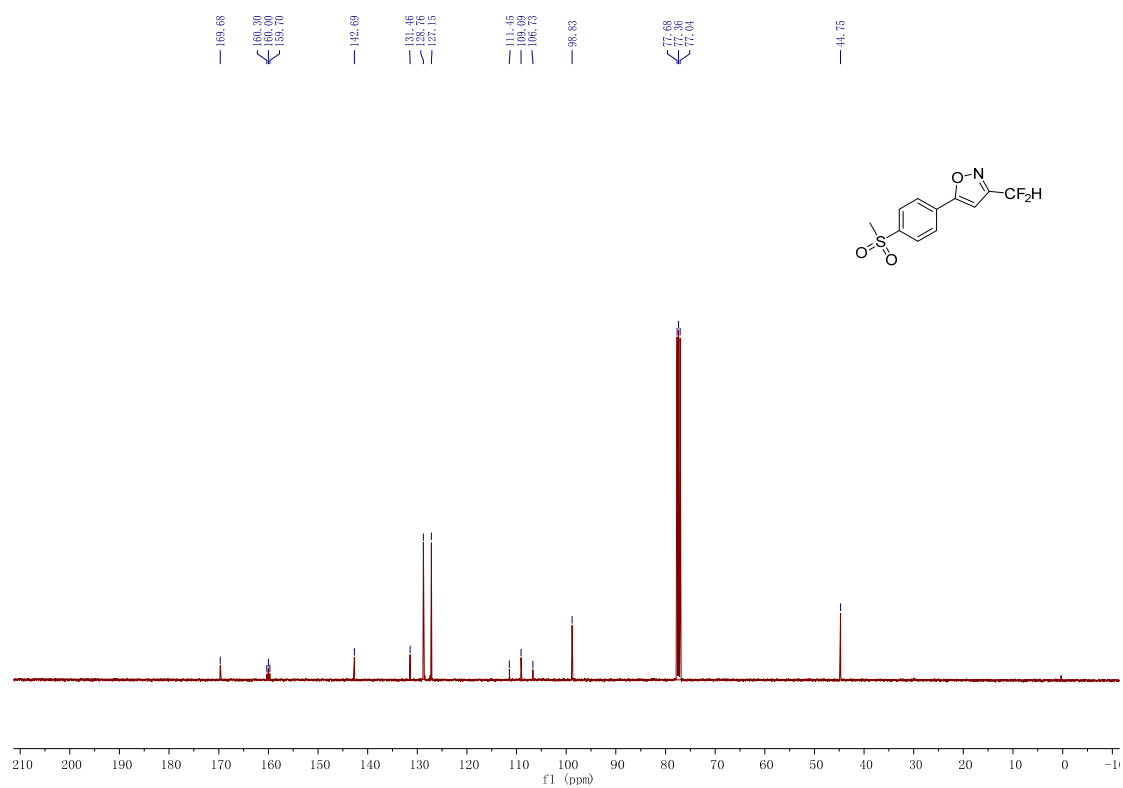
^{19}F { ^1H } NMR (CDCl₃, 376 MHz) of **5o**



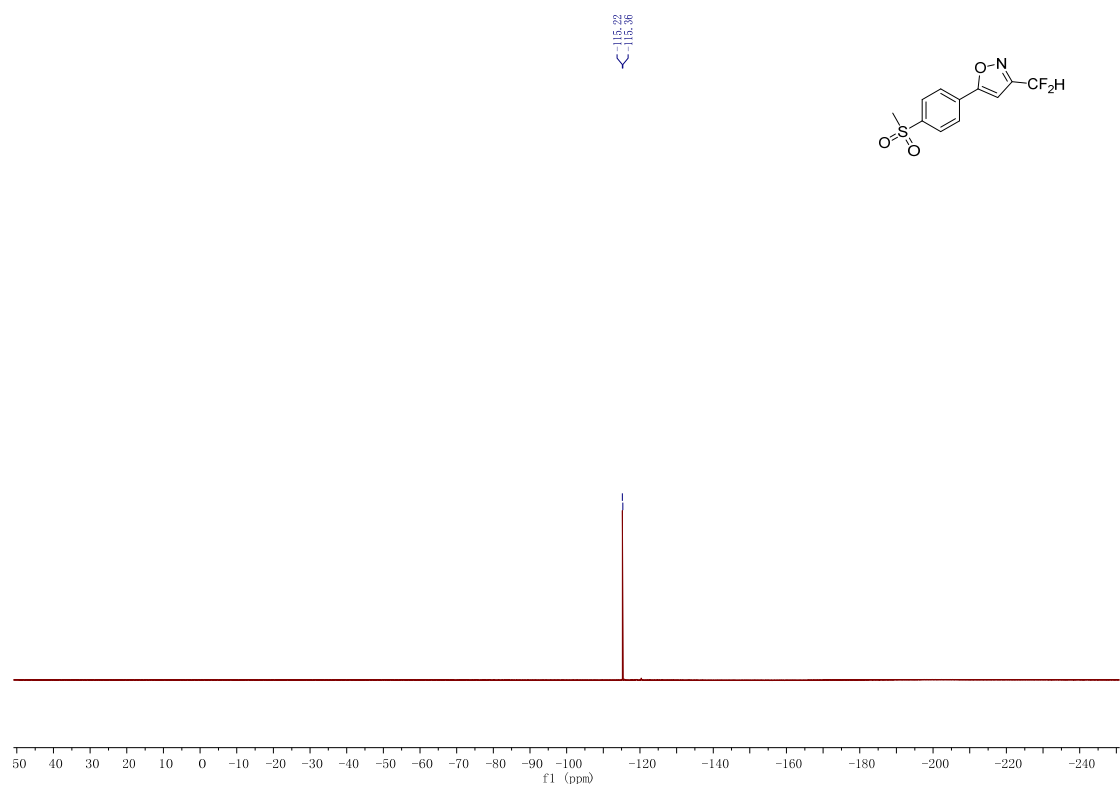
^1H NMR (CDCl₃, 400 MHz) of 5p



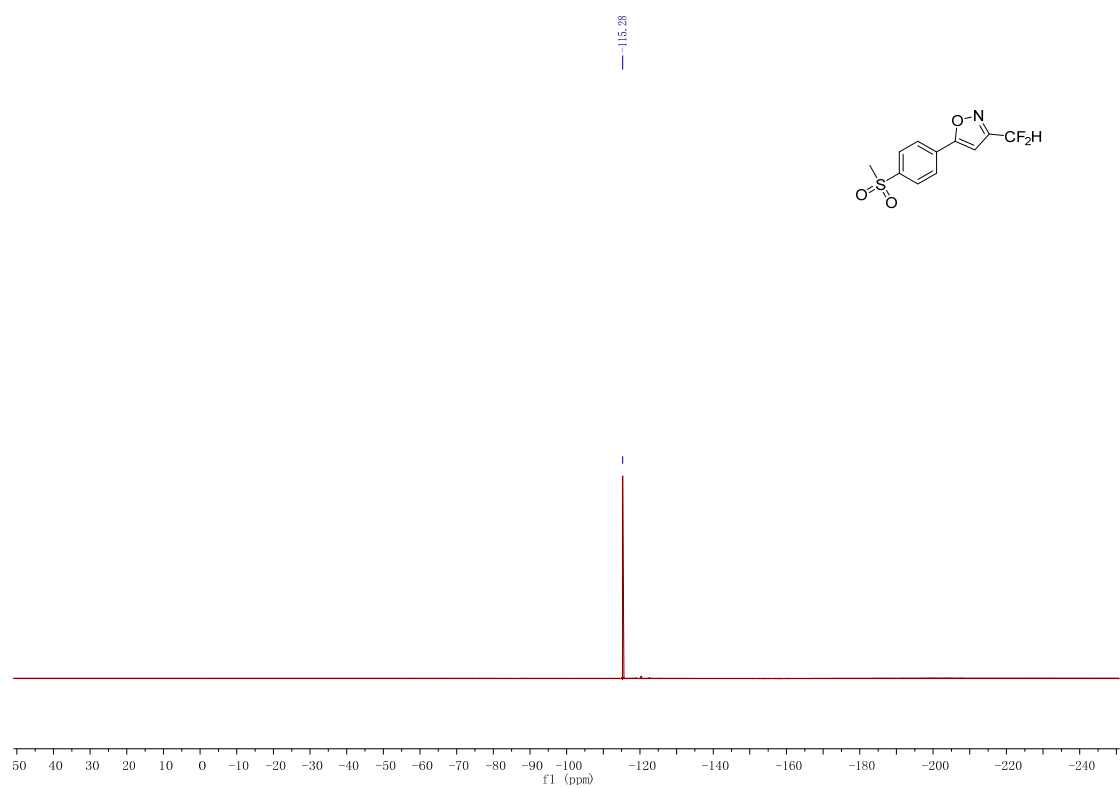
^{13}C NMR (CDCl₃, 100 MHz) of 5p



^{19}F NMR (CDCl₃, 376 MHz) of **5p**



^{19}F { ^1H } NMR (CDCl₃, 376 MHz) of **5p**



Chemical structure: COc1ccccc1-c2cc(C(F)(F)F)no2

¹H NMR spectrum (CDCl₃) showing peaks in the aromatic region (6.5-8.1 ppm) and aliphatic region (2.8 ppm). Integration values are provided below the peaks.

Chemical Shift (ppm)	Integration
8.05	1.00
7.55	1.00
7.15	0.99
7.05	0.99
6.95	0.99
6.85	0.99
6.75	0.99
6.65	0.99
3.80	3.00
2.80	2.00

Chemical structure: COc1ccccc1-c2cc(C(F)(F)F)on2

¹³C NMR spectrum (ppm):

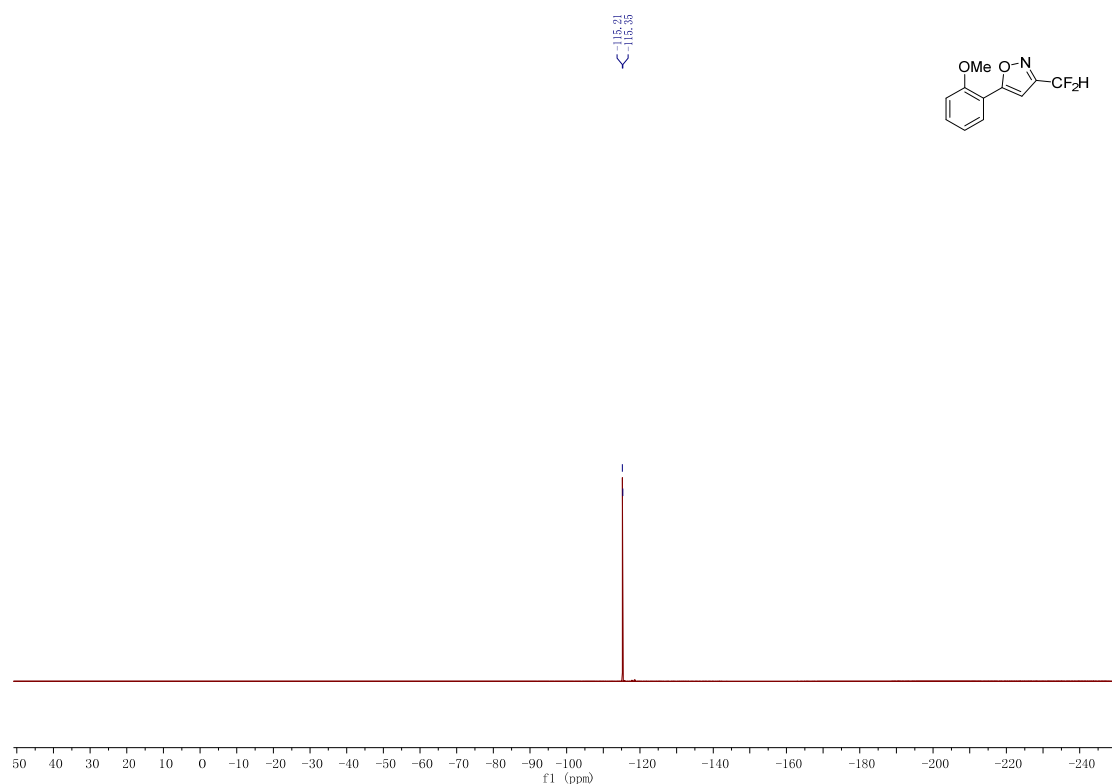
- 167.96
- 156.01
- 156.72
- 156.72
- 132.26
- 128.04
- 121.25
- 115.88
- 114.65
- 114.62
- 109.70
- 107.35
- 100.38
- 77.68
- 77.36
- 77.04
- 55.90

Chemical structure: COc1ccc(cc1)-c2cc(C=O)on2

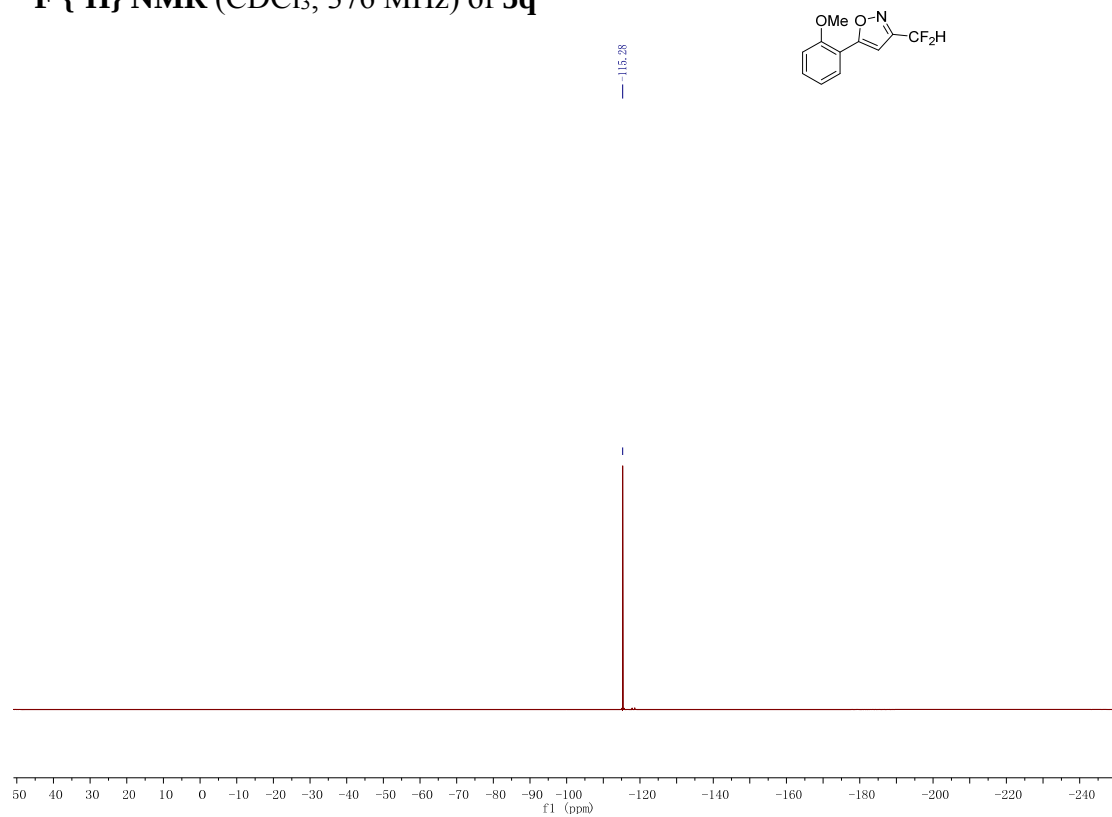
¹³C NMR spectrum (ppm):

- 167.96
- 156.01
- 156.72
- 156.72
- 132.26
- 128.04
- 121.25
- 115.88
- 114.65
- 114.62
- 109.70
- 107.35
- 100.38
- 77.68
- 77.36
- 77.04
- 55.90

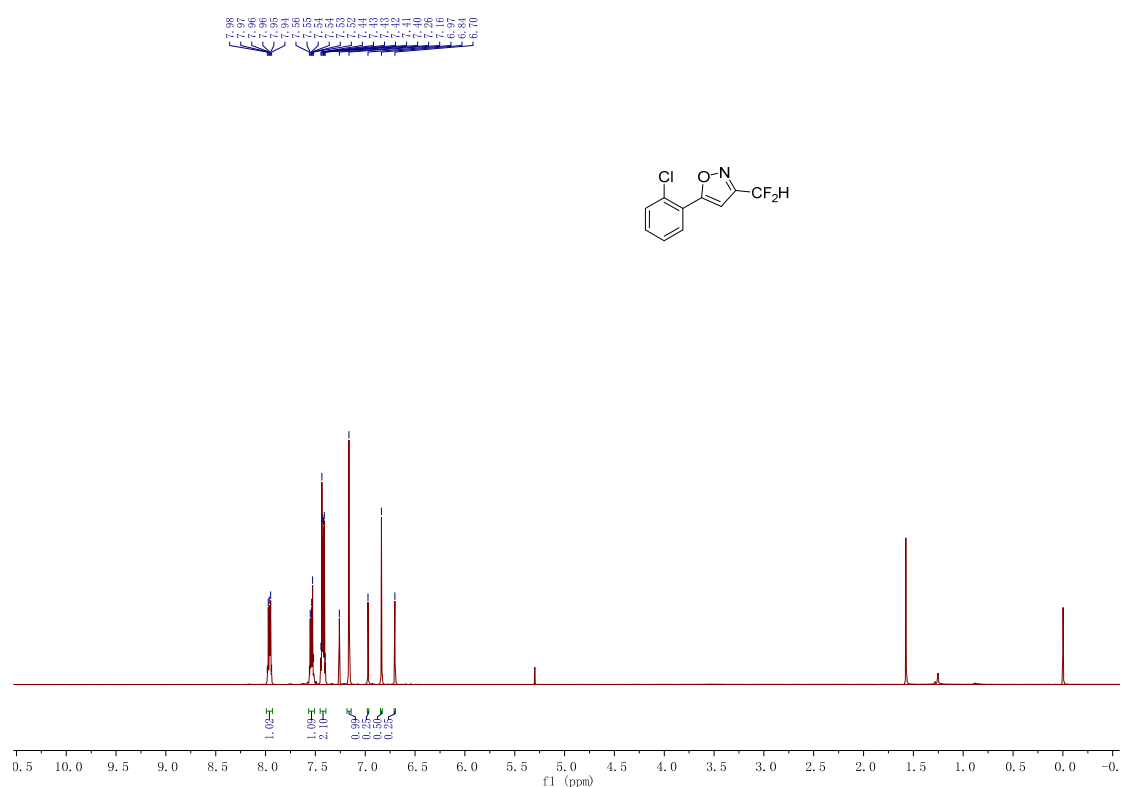
^{19}F NMR (CDCl₃, 376 MHz) of **5q**



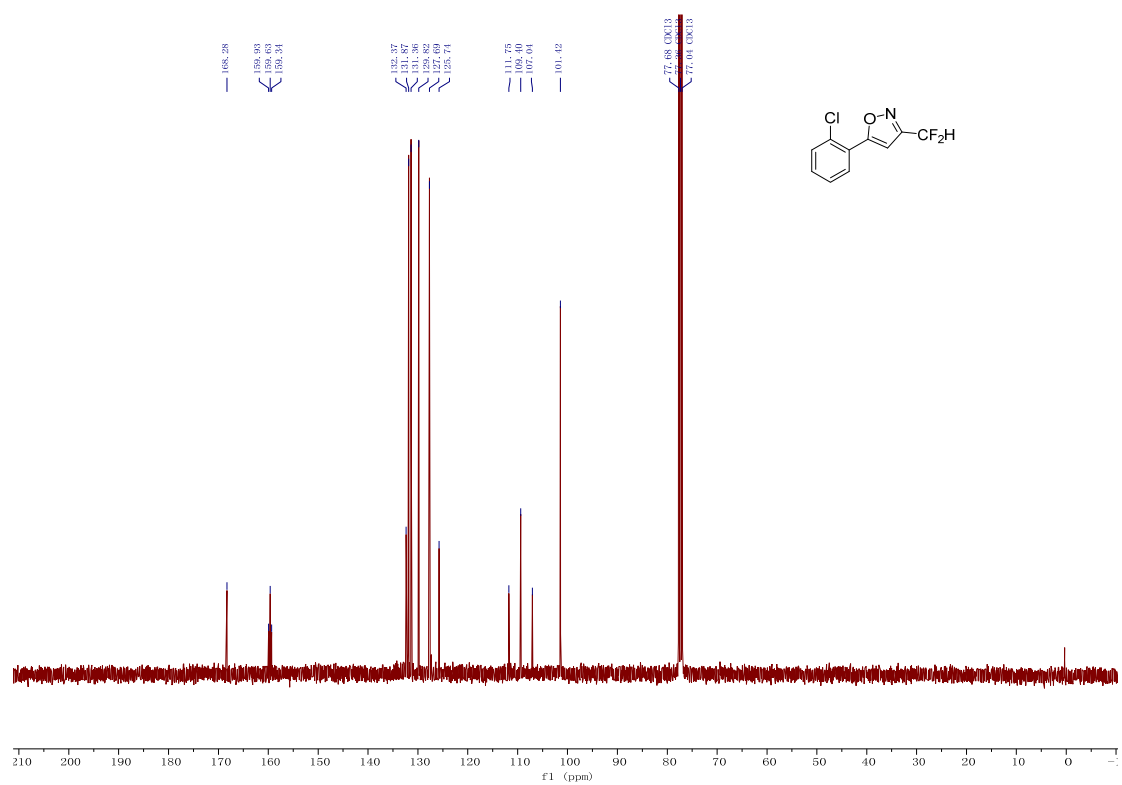
^{19}F { ^1H } NMR (CDCl₃, 376 MHz) of **5q**



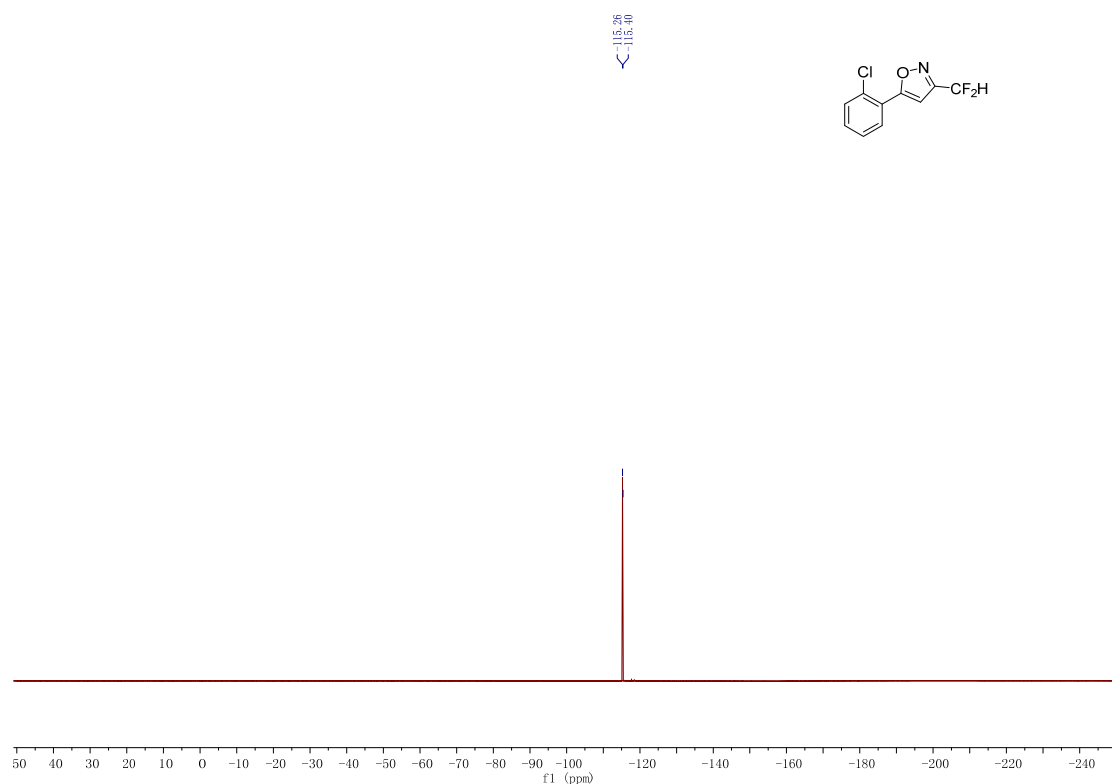
^1H NMR (CDCl₃, 400 MHz) of 5r



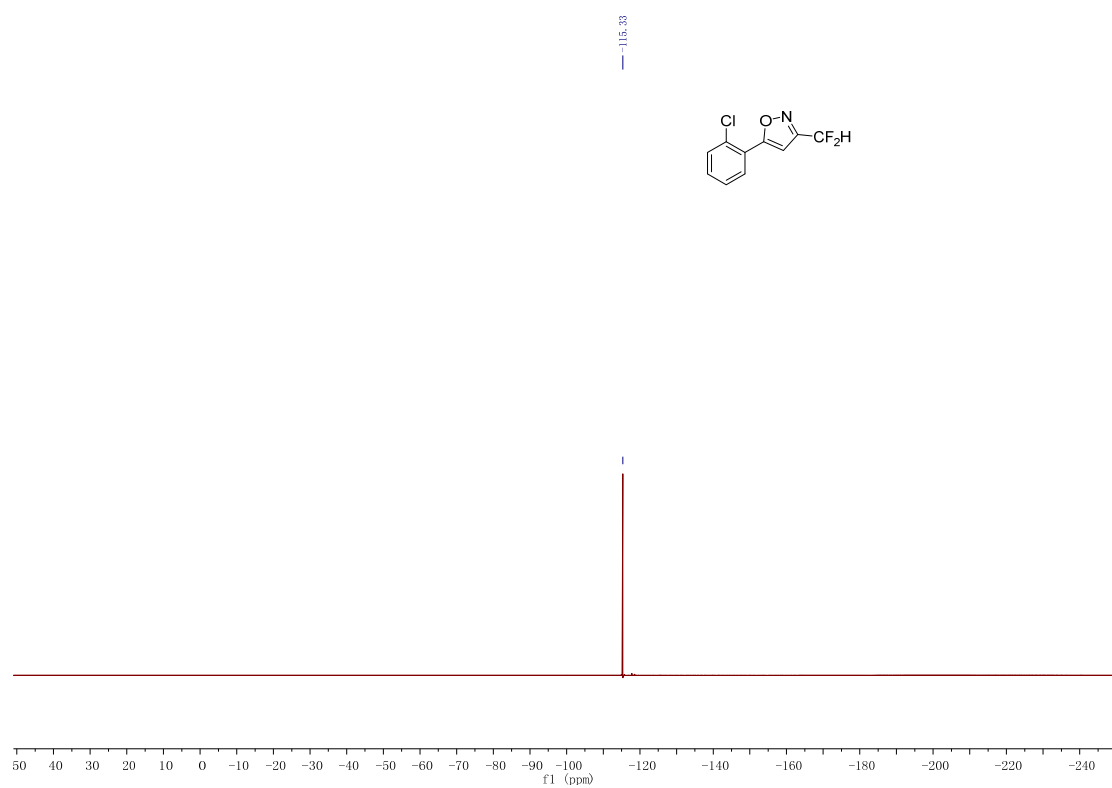
^{13}C NMR (CDCl₃, 100 MHz) of 5r



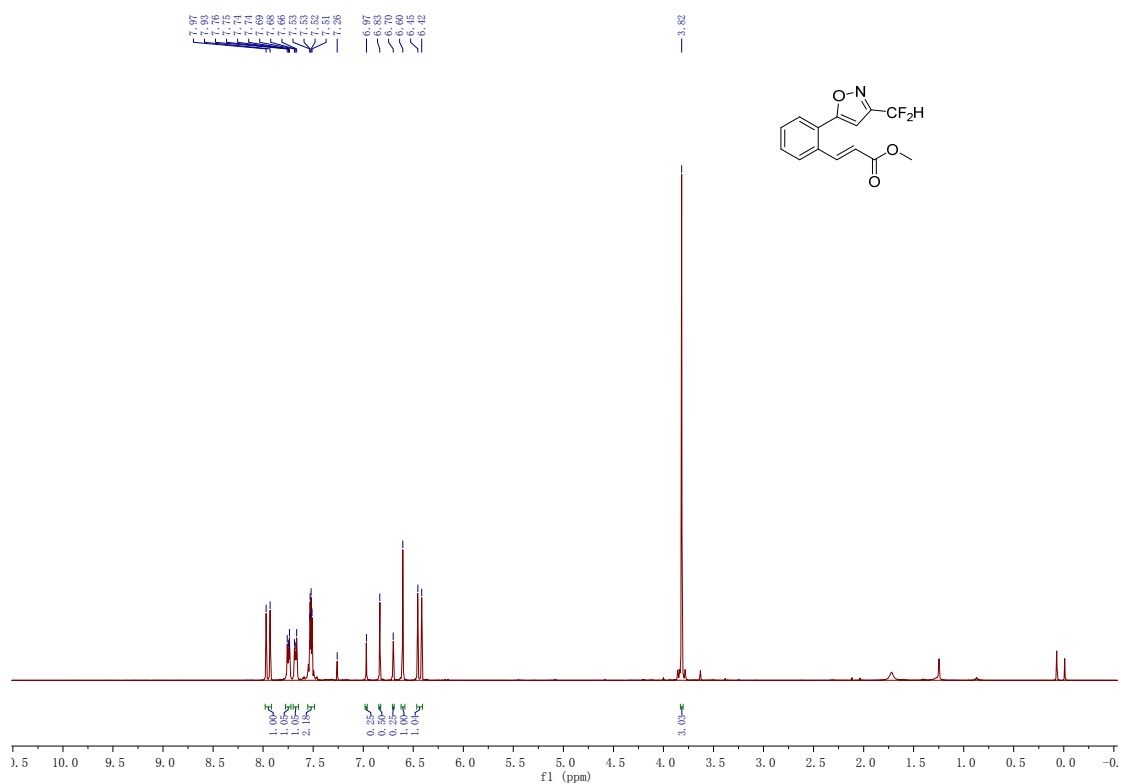
^{19}F NMR (CDCl₃, 376 MHz) of **5r**



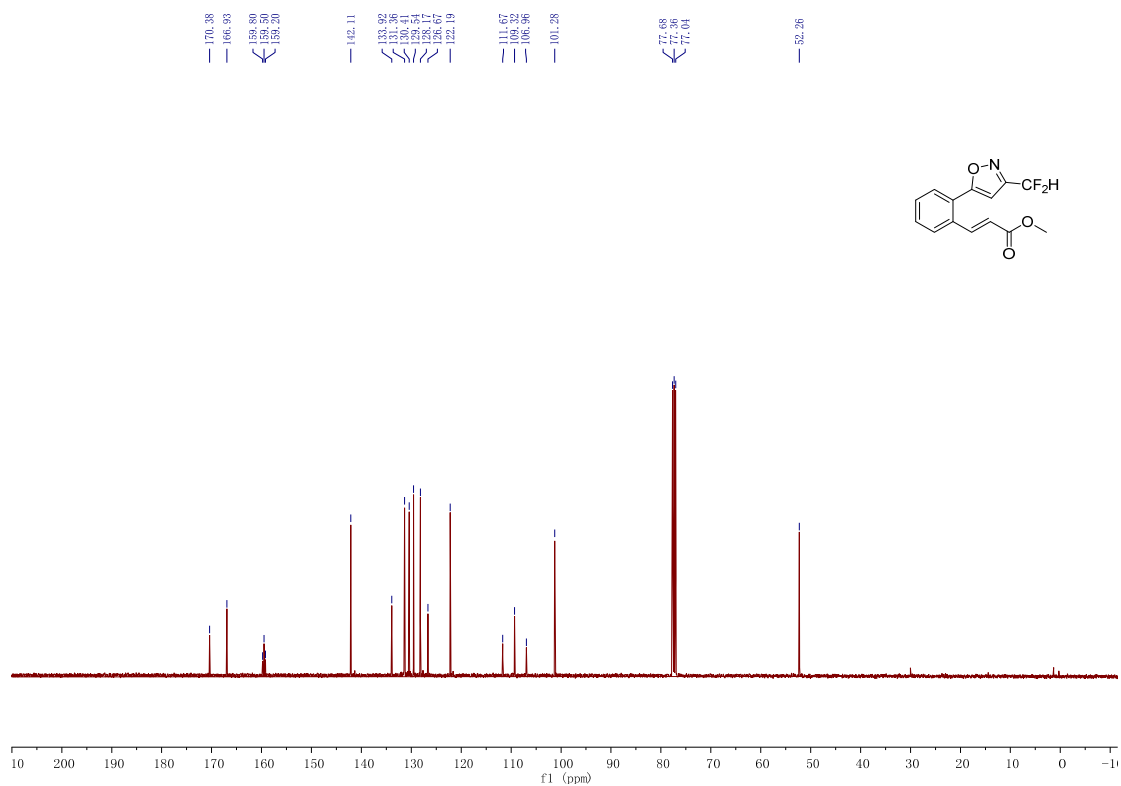
^{19}F { ^1H } NMR (CDCl₃, 376 MHz) of **5r**



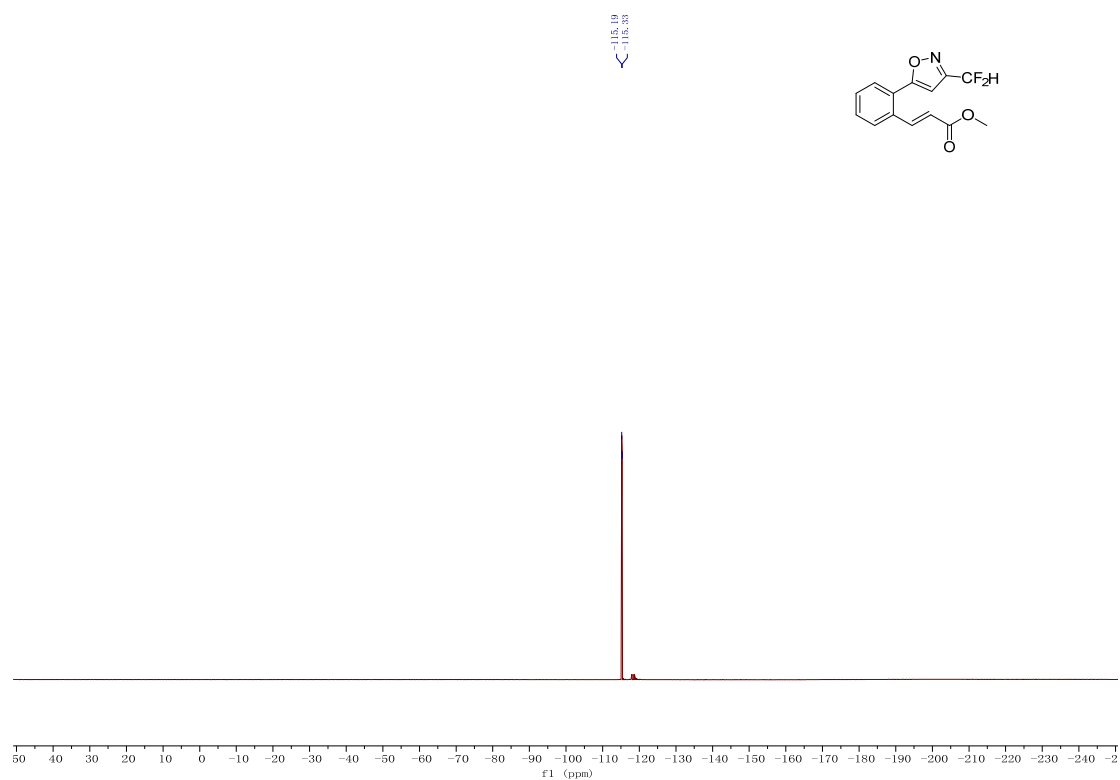
¹H NMR (CDCl₃, 400 MHz) of 5s



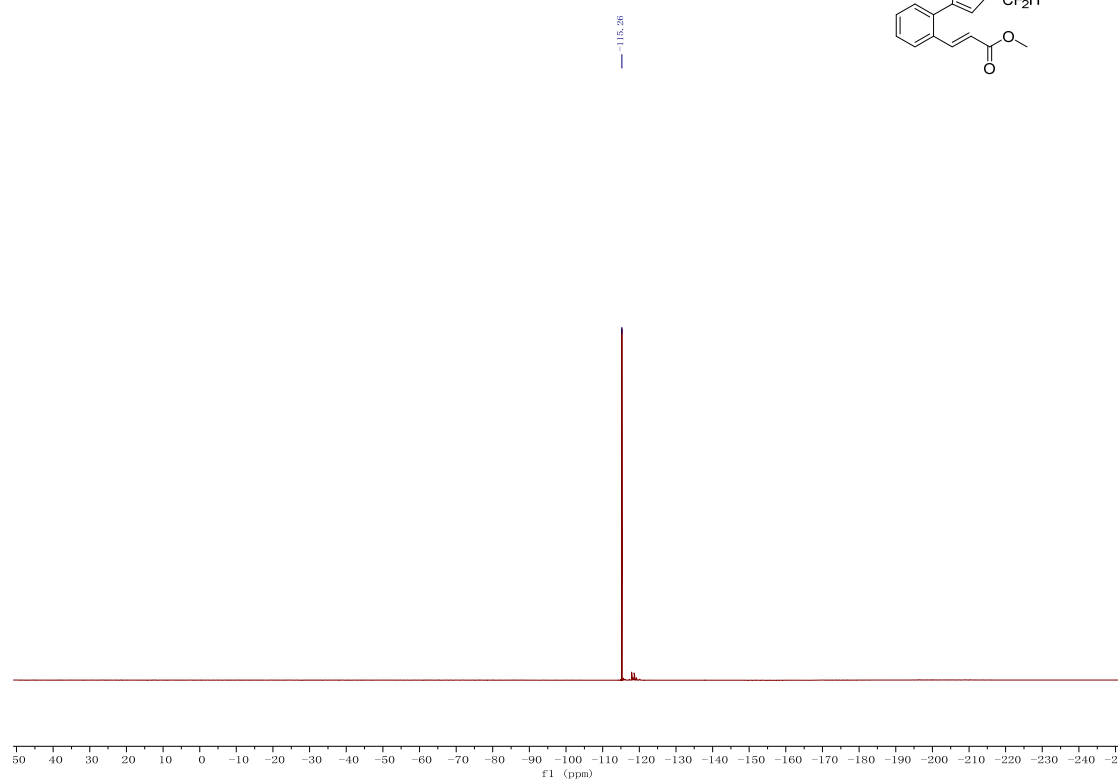
¹³C NMR (CDCl₃, 100 MHz) of 5s



^{19}F NMR (CDCl₃, 376 MHz) of **5s**



^{19}F { ^1H } NMR (CDCl₃, 376 MHz) of **5s**



Chemical structure: O=[N+]([O-])c1ccc(cc1-c2cc(F)cc2O)

¹H NMR spectrum (CDCl₃) showing peaks in the aromatic region (6.5-8.7 ppm) and aliphatic region (0.8-1.8 ppm). Integration values are provided below the peaks.

Chemical Shift (ppm)	Integration
8.65, 8.64, 8.63, 8.62, 8.61, 8.60, 8.59, 8.58, 8.57, 8.56, 8.55, 8.54, 8.53, 8.52, 8.51, 8.50, 8.49, 8.48, 8.47, 8.46, 8.45, 8.44, 8.43, 8.42, 8.41, 8.40, 8.39, 8.38, 8.37, 8.36, 8.35, 8.34, 8.33, 8.32, 8.31, 8.30, 8.29, 8.28, 8.27, 8.26, 8.25, 8.24, 8.23, 8.22, 8.21, 8.20, 8.19, 8.18, 8.17, 8.16, 8.15, 8.14, 8.13, 8.12, 8.11, 8.10, 8.09, 8.08, 8.07, 8.06, 8.05, 8.04, 8.03, 8.02, 8.01, 8.00, 7.99, 7.98, 7.97, 7.96, 7.95, 7.94, 7.93, 7.92, 7.91, 7.90, 7.89, 7.88, 7.87, 7.86, 7.85, 7.84, 7.83, 7.82, 7.81, 7.80, 7.79, 7.78, 7.77, 7.76, 7.75, 7.74, 7.73, 7.72, 7.71, 7.70, 7.69, 7.68, 7.67, 7.66, 7.65, 7.64, 7.63, 7.62, 7.61, 7.60, 7.59, 7.58, 7.57, 7.56, 7.55, 7.54, 7.53, 7.52, 7.51, 7.50, 7.49, 7.48, 7.47, 7.46, 7.45, 7.44, 7.43, 7.42, 7.41, 7.40, 7.39, 7.38, 7.37, 7.36, 7.35, 7.34, 7.33, 7.32, 7.31, 7.30, 7.29, 7.28, 7.27, 7.26, 7.25, 7.24, 7.23, 7.22, 7.21, 7.20, 7.19, 7.18, 7.17, 7.16, 7.15, 7.14, 7.13, 7.12, 7.11, 7.10, 7.09, 7.08, 7.07, 7.06, 7.05, 7.04, 7.03, 7.02, 7.01, 7.00, 6.99, 6.98, 6.97, 6.96, 6.95, 6.94, 6.93, 6.92, 6.91, 6.90, 6.89, 6.88, 6.87, 6.86, 6.85, 6.84, 6.83, 6.82, 6.81, 6.80, 6.79, 6.78, 6.77, 6.76, 6.75, 6.74, 6.73, 6.72, 6.71, 6.70, 6.69, 6.68, 6.67, 6.66, 6.65, 6.64, 6.63, 6.62, 6.61, 6.60, 6.59, 6.58, 6.57, 6.56, 6.55, 6.54, 6.53, 6.52, 6.51, 6.50, 6.49, 6.48, 6.47, 6.46, 6.45, 6.44, 6.43, 6.42, 6.41, 6.40, 6.39, 6.38, 6.37, 6.36, 6.35, 6.34, 6.33, 6.32, 6.31, 6.30, 6.29, 6.28, 6.27, 6.26, 6.25, 6.24, 6.23, 6.22, 6.21, 6.20, 6.19, 6.18, 6.17, 6.16, 6.15, 6.14, 6.13, 6.12, 6.11, 6.10, 6.09, 6.08, 6.07, 6.06, 6.05, 6.04, 6.03, 6.02, 6.01, 6.00, 5.99, 5.98, 5.97, 5.96, 5.95, 5.94, 5.93, 5.92, 5.91, 5.90, 5.89, 5.88, 5.87, 5.86, 5.85, 5.84, 5.83, 5.82, 5.81, 5.80, 5.79, 5.78, 5.77, 5.76, 5.75, 5.74, 5.73, 5.72, 5.71, 5.70, 5.69, 5.68, 5.67, 5.66, 5.65, 5.64, 5.63, 5.62, 5.61, 5.60, 5.59, 5.58, 5.57, 5.56, 5.55, 5.54, 5.53, 5.52, 5.51, 5.50, 5.49, 5.48, 5.47, 5.46, 5.45, 5.44, 5.43, 5.42, 5.41, 5.40, 5.39, 5.38, 5.37, 5.36, 5.35, 5.34, 5.33, 5.32, 5.31, 5.30, 5.29, 5.28, 5.27, 5.26, 5.25, 5.24, 5.23, 5.22, 5.21, 5.20, 5.19, 5.18, 5.17, 5.16, 5.15, 5.14, 5.13, 5.12, 5.11, 5.10, 5.09, 5.08, 5.07, 5.06, 5.05, 5.04, 5.03, 5.02, 5.01, 5.00, 4.99, 4.98, 4.97, 4.96, 4.95, 4.94, 4.93, 4.92, 4.91, 4.90, 4.89, 4.88, 4.87, 4.86, 4.85, 4.84, 4.83, 4.82, 4.81, 4.80, 4.79, 4.78, 4.77, 4.76, 4.75, 4.74, 4.73, 4.72, 4.71, 4.70, 4.69, 4.68, 4.67, 4.66, 4.65, 4.64, 4.63, 4.62, 4.61, 4.60, 4.59, 4.58, 4.57, 4.56, 4.55, 4.54, 4.53, 4.52, 4.51, 4.50, 4.49, 4.48, 4.47, 4.46, 4.45, 4.44, 4.43, 4.42, 4.41, 4.40, 4.39, 4.38, 4.37, 4.36, 4.35, 4.34, 4.33, 4.32, 4.31, 4.30, 4.29, 4.28, 4.27, 4.26, 4.25, 4.24, 4.23, 4.22, 4.21, 4.20, 4.19, 4.18, 4.17, 4.16, 4.15, 4.14, 4.13, 4.12, 4.11, 4.10, 4.09, 4.08, 4.07, 4.06, 4.05, 4.04, 4.03, 4.02, 4.01, 4.00, 3.99, 3.98, 3.97, 3.96, 3.95, 3.94, 3.93, 3.92, 3.91, 3.90, 3.89, 3.88, 3.87, 3.86, 3.85, 3.84, 3.83, 3.82, 3.81, 3.80, 3.79, 3.78, 3.77, 3.76, 3.75, 3.74, 3.73, 3.72, 3.71, 3.70, 3.69, 3.68, 3.67, 3.66, 3.65, 3.64, 3.63, 3.62, 3.61, 3.60, 3.59, 3.58, 3.57, 3.56, 3.55, 3.54, 3.53, 3.52, 3.51, 3.50, 3.49, 3.48, 3.47, 3.46, 3.45, 3.44, 3.43, 3.42, 3.41, 3.40, 3.39, 3.38, 3.37, 3.36, 3.35, 3.34, 3.33, 3.32, 3.31, 3.30, 3.29, 3.28, 3.27, 3.26, 3.25, 3.24, 3.23, 3.22, 3.21, 3.20, 3.19, 3.18, 3.17, 3.16, 3.15, 3.14, 3.13, 3.12, 3.11, 3.10, 3.09, 3.08, 3.07, 3.06, 3.05, 3.04, 3.03, 3.02, 3.01, 3.00, 2.99, 2.98, 2.97, 2.96, 2.95, 2.94, 2.93, 2.92, 2.91, 2.90, 2.89, 2.88, 2.87, 2.86, 2.85, 2.84, 2.83, 2.82, 2.81, 2.80, 2.79, 2.78, 2.77, 2.76, 2.75, 2.74, 2.73, 2.72, 2.71, 2.70, 2.69, 2.68, 2.67, 2.66, 2.65, 2.64, 2.63, 2.62, 2.61, 2.60, 2.59, 2.58, 2.57, 2.56, 2.55, 2.54, 2.53, 2.52, 2.51, 2.50, 2.49, 2.48, 2.47, 2.46, 2.45, 2.44, 2.43, 2.42, 2.41, 2.40, 2.39, 2.38, 2.37, 2.36, 2.35, 2.34, 2.33, 2.32, 2.31, 2.30, 2.29, 2.28, 2.27, 2.26, 2.25, 2.24, 2.23, 2.22, 2.21, 2.20, 2.19, 2.18, 2.17,	

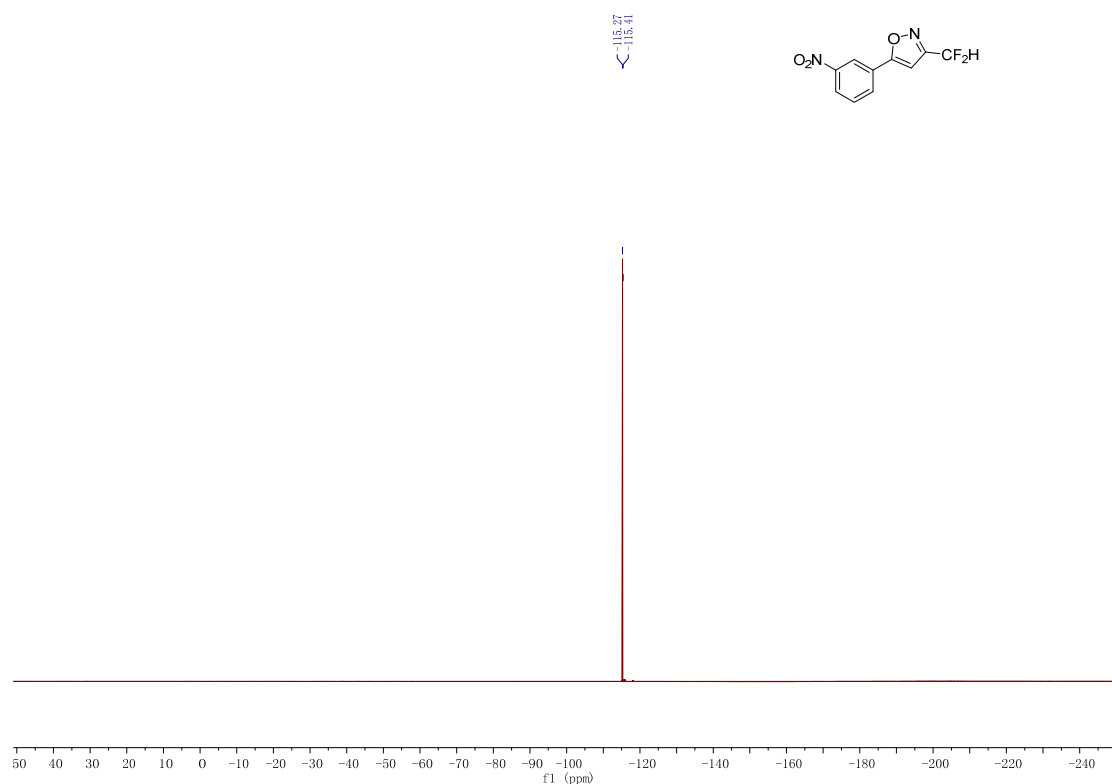
Chemical structure: O=[N+]([O-])c1ccc(cc1)c2cc(C(F)F)no2

¹³C NMR spectrum (ppm):

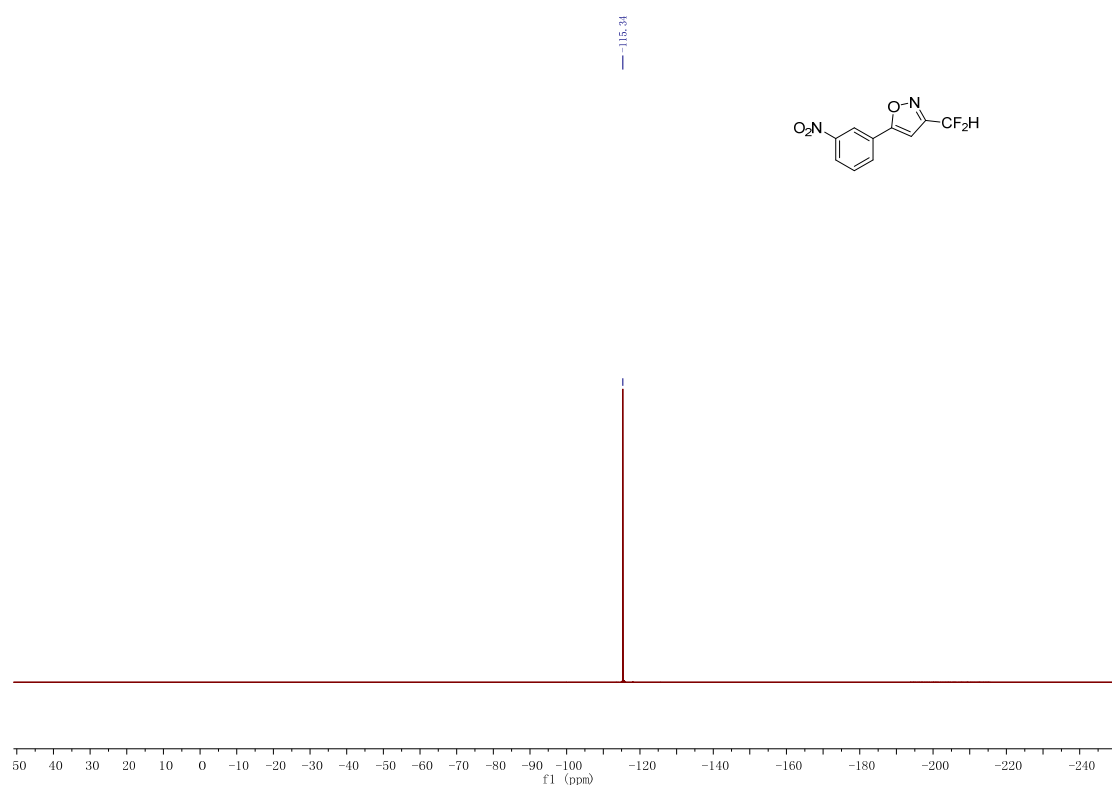
- 168.30
- 160.31
- 160.01
- 158.71
- 148.03
- 131.75
- 130.85
- 129.69
- 129.59
- 127.27
- 111.44
- 109.08
- 106.72
- 98.35
- 77.68
- 77.36
- 77.04

Chemical structure: O=[N+]([O-])c1ccc(cc1)c2cc(C(F)F)no2

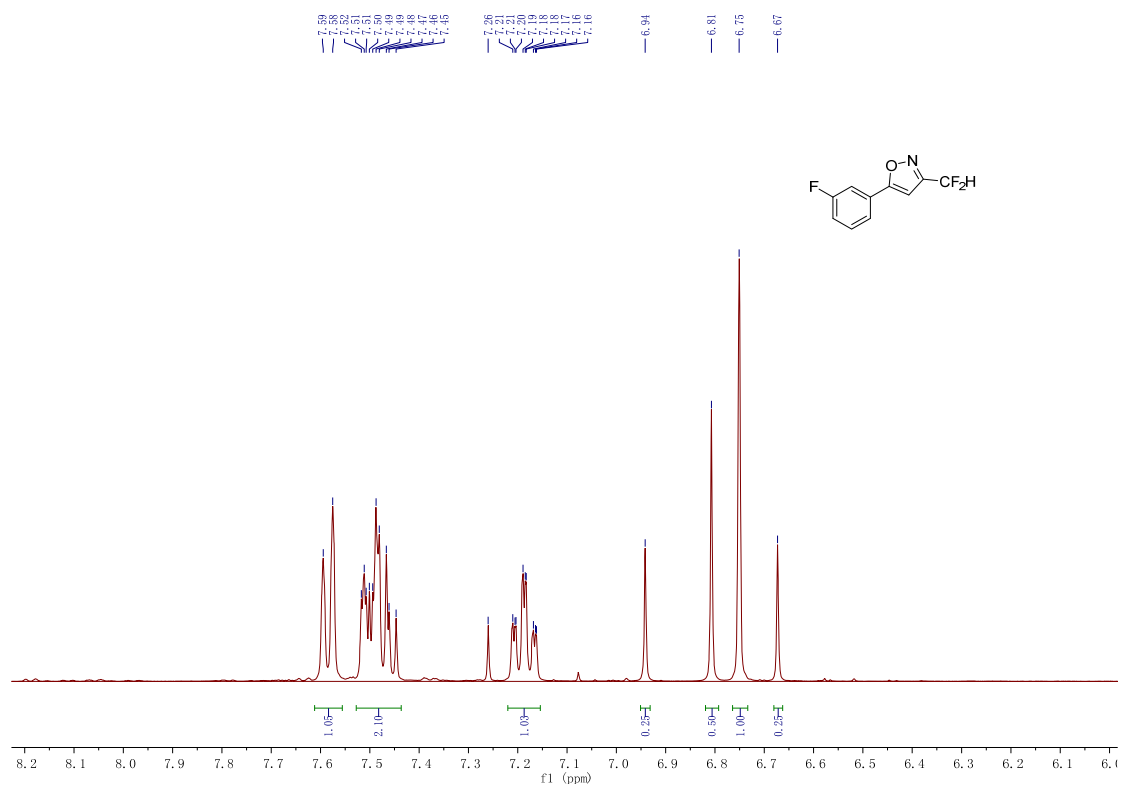
^{19}F NMR (CDCl₃, 376 MHz) of 5t



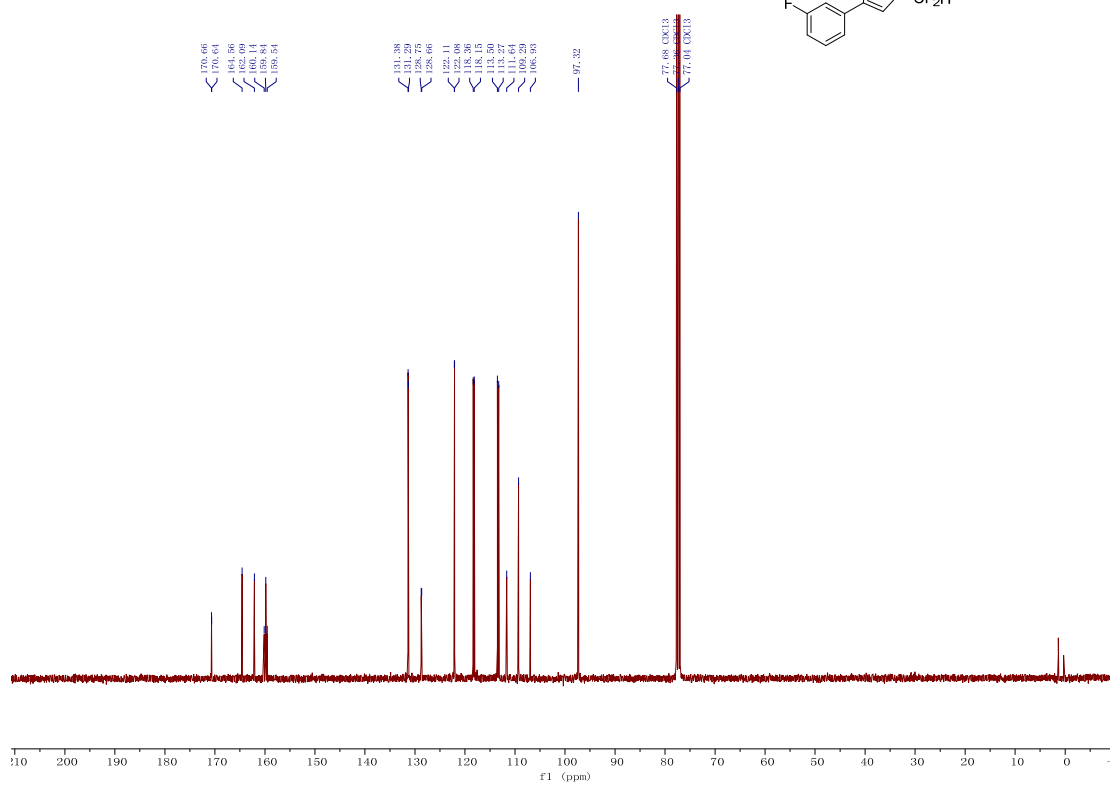
^{19}F { ^1H } NMR (CDCl₃, 376 MHz) of 5t



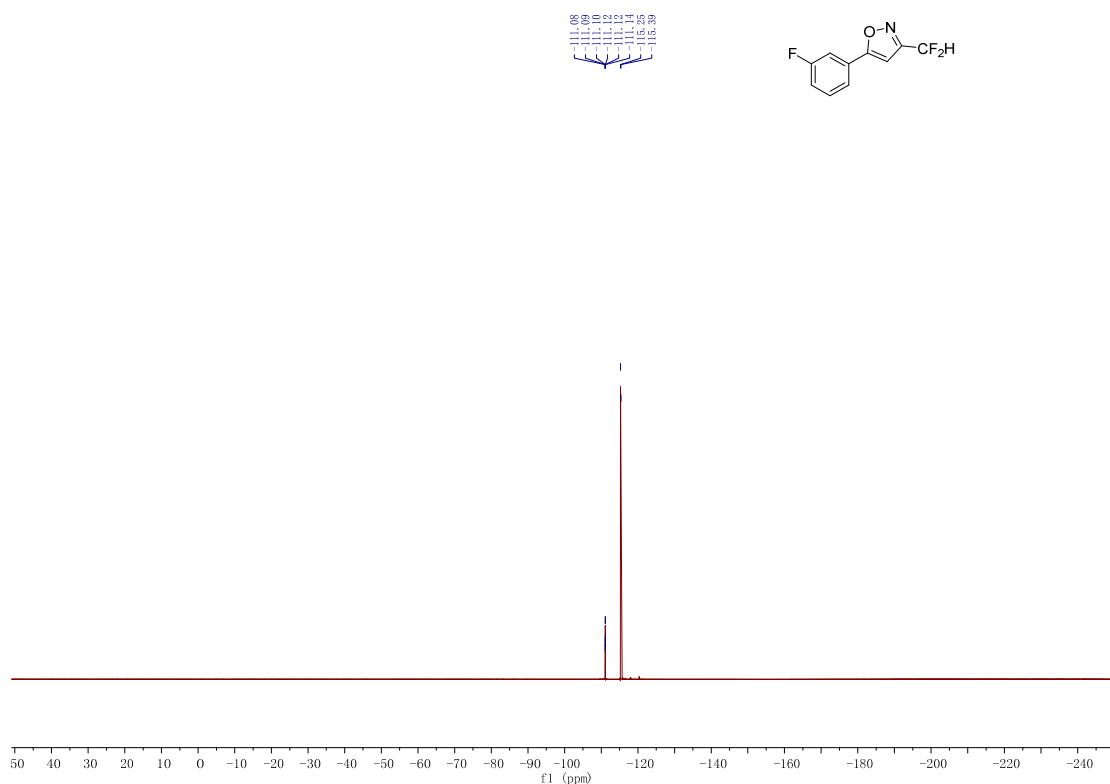
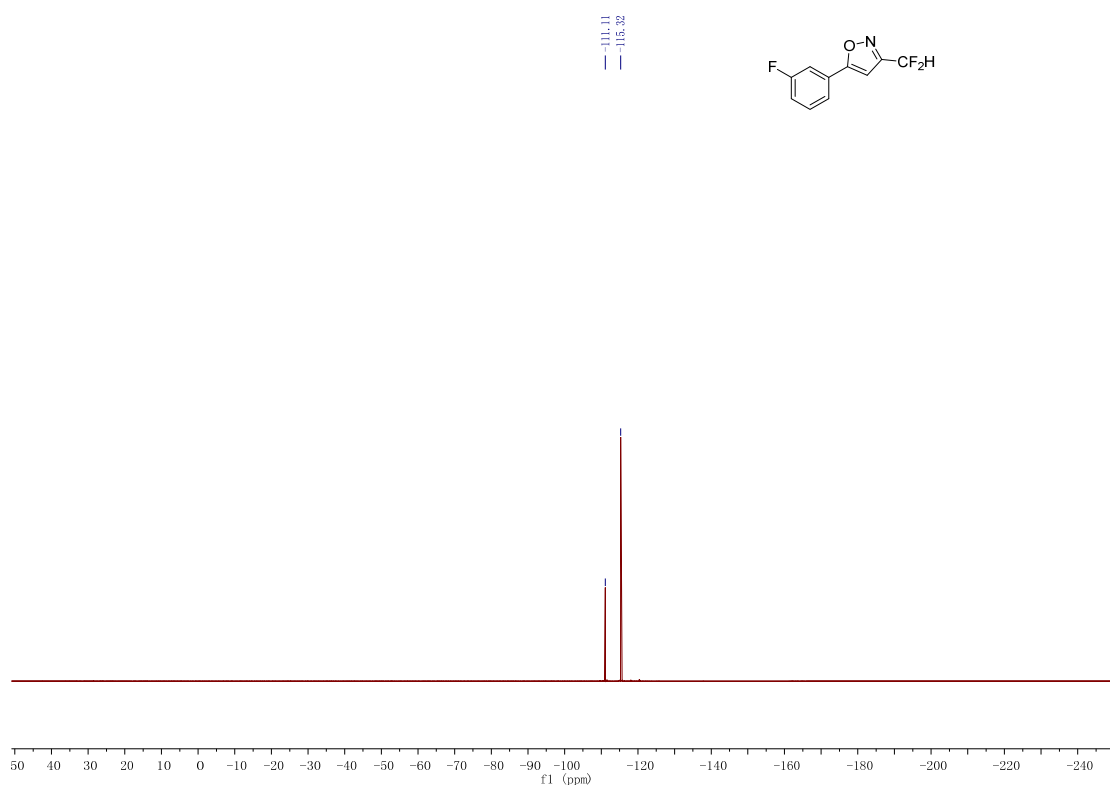
^1H NMR (CDCl₃, 400 MHz) of **5u**



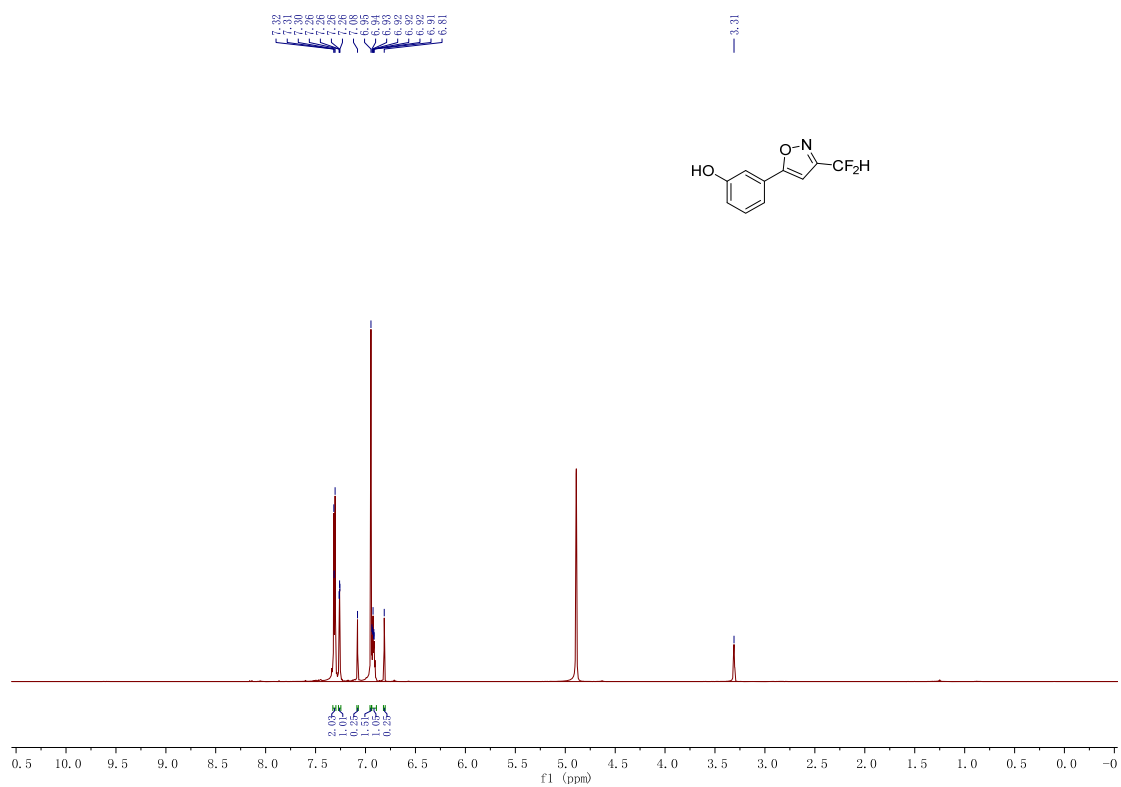
^{13}C NMR (CDCl₃, 100 MHz) of **5u**



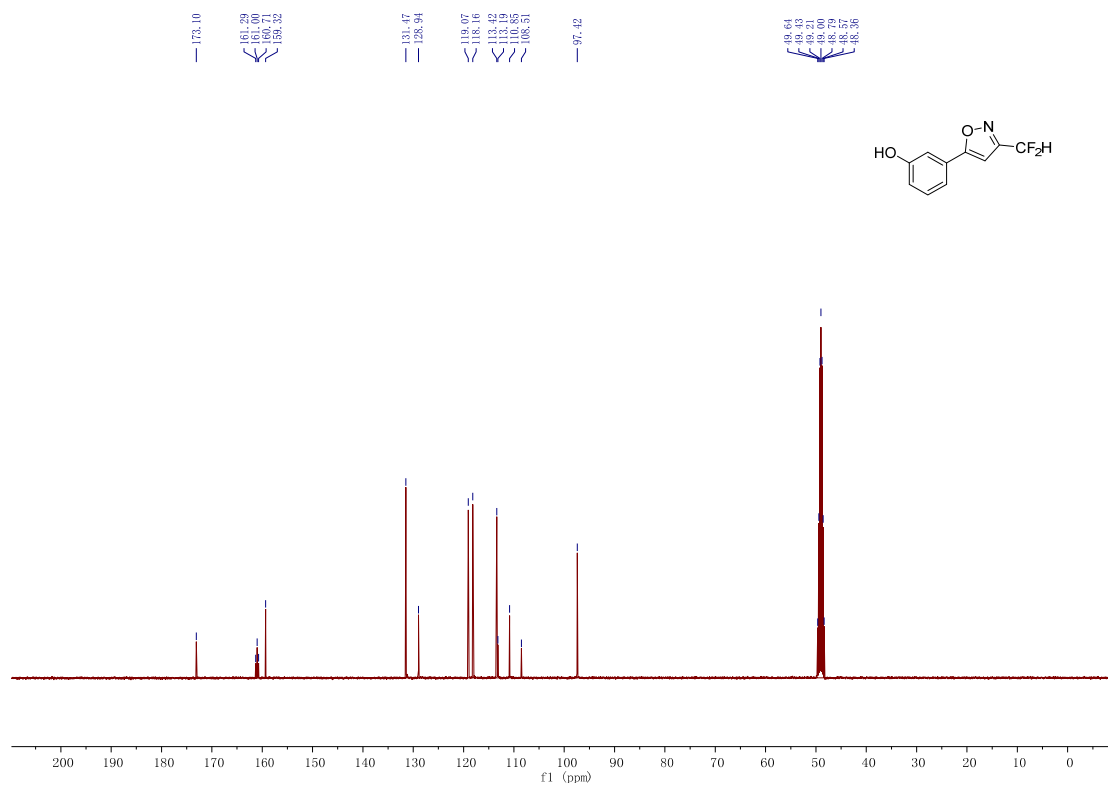
¹⁹F NMR (CDCl₃, 376 MHz) of **5u**

 ^{19}F $\{^1\text{H}\}$ NMR (CDCl_3 , 376 MHz) of **5u**

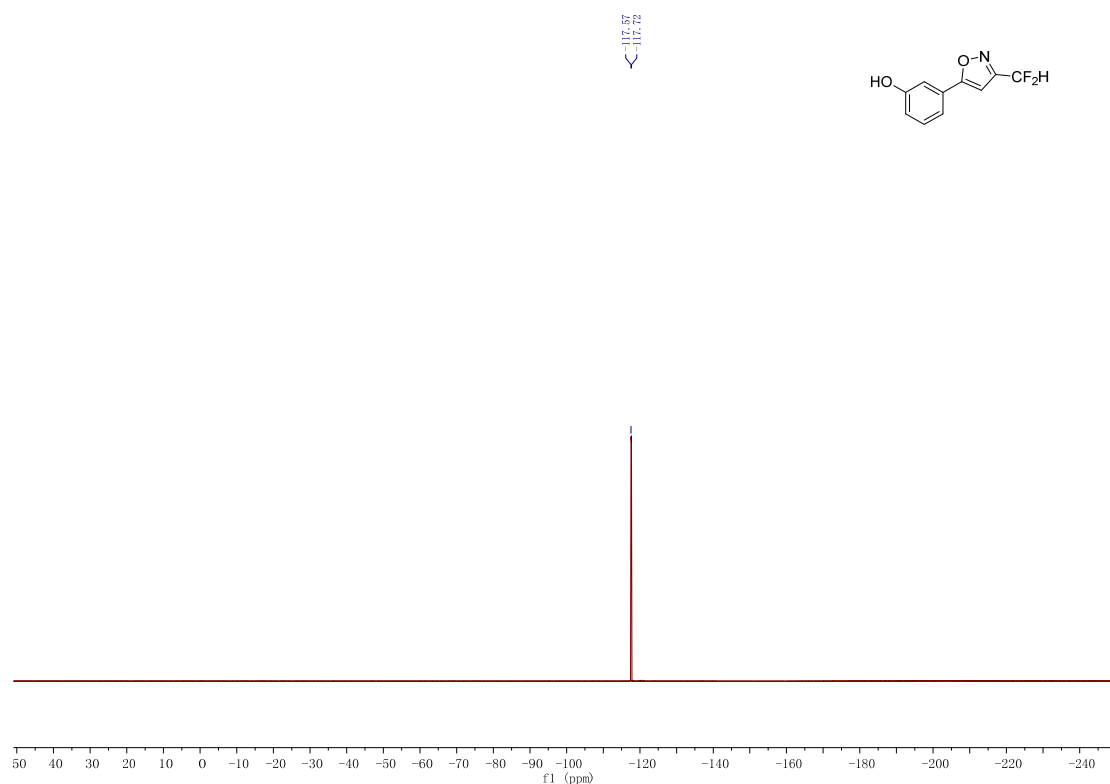
¹H NMR (CD₃OD, 400 MHz) of 5v



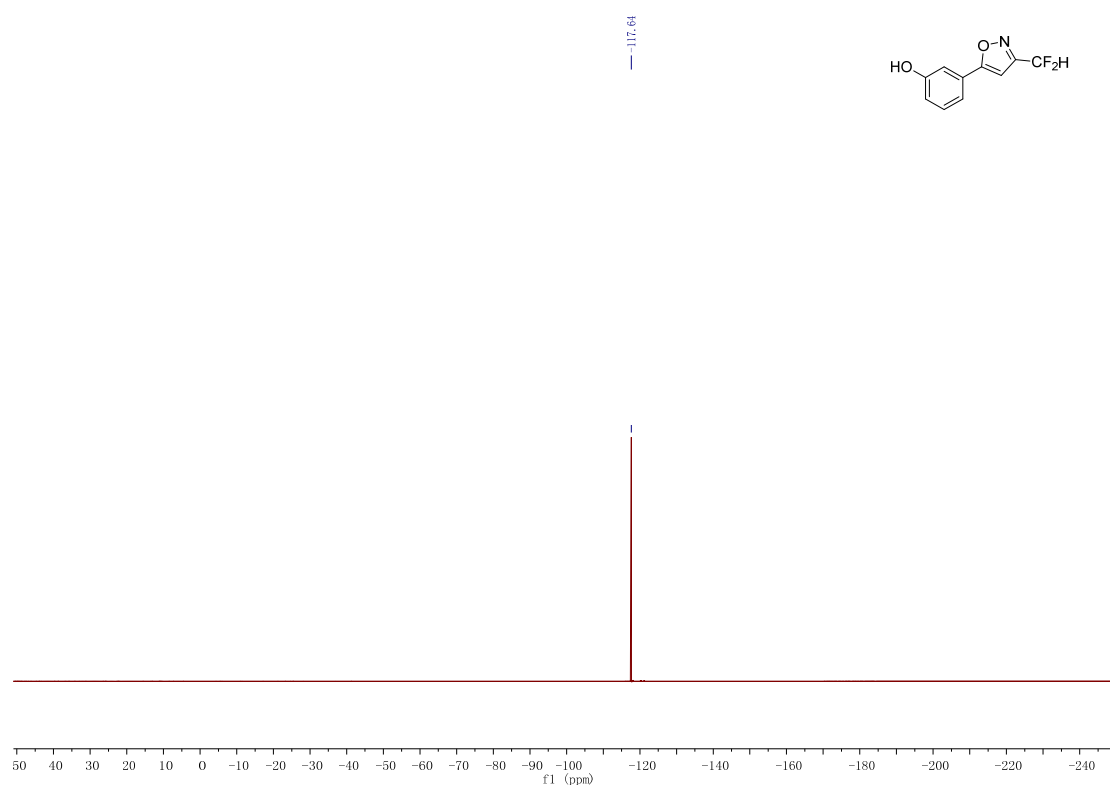
¹³C NMR (CD₃OD, 100 MHz) of 5v



^{19}F NMR (CD₃OD, 376 MHz) of 5v



^{19}F { ^1H } NMR (CD₃OD, 376 MHz) of 5v



Chemical structure: CC(C)(C)Si(C)(C)OC1=CC=C(C=C1C2=CC(=CC=C2)[N+](=O)[O-])C3=CC(=CC=C3)C(F)F

¹H NMR spectrum (CDCl₃) showing peaks and integration values:

Chemical Shift (ppm)	Integration
7.72, 7.71, 7.70, 7.69, 7.68, 7.67, 7.66, 7.65, 7.64, 7.63, 7.62, 7.61, 7.60, 7.59, 7.58, 7.57, 7.56, 7.55, 7.54, 7.53, 7.52, 7.51, 7.50, 7.49, 7.48, 7.47, 7.46, 7.45, 7.44, 7.43, 7.42, 7.41, 7.40, 7.39, 7.38, 7.37, 7.36, 7.35, 7.34, 7.33, 7.32, 7.31, 7.30, 7.29, 7.28, 7.27, 7.26, 7.25, 7.24, 7.23, 7.22, 7.21, 7.20, 7.19, 7.18, 7.17, 7.16, 7.15, 7.14, 7.13, 7.12, 7.11, 7.10, 7.09, 7.08, 7.07, 7.06, 7.05, 7.04, 7.03, 7.02, 7.01, 7.00, 6.99, 6.98, 6.97, 6.96, 6.95, 6.94, 6.93, 6.92, 6.91, 6.90, 6.89, 6.88, 6.87, 6.86, 6.85, 6.84, 6.83, 6.82, 6.81, 6.80, 6.79, 6.78, 6.77, 6.76, 6.75, 6.74, 6.73, 6.72, 6.71, 6.70, 6.69, 6.68, 6.67, 6.66, 6.65, 6.64, 6.63, 6.62, 6.61, 6.60, 6.59, 6.58, 6.57, 6.56, 6.55, 6.54, 6.53, 6.52, 6.51, 6.50, 6.49, 6.48, 6.47, 6.46, 6.45, 6.44, 6.43, 6.42, 6.41, 6.40, 6.39, 6.38, 6.37, 6.36, 6.35, 6.34, 6.33, 6.32, 6.31, 6.30, 6.29, 6.28, 6.27, 6.26, 6.25, 6.24, 6.23, 6.22, 6.21, 6.20, 6.19, 6.18, 6.17, 6.16, 6.15, 6.14, 6.13, 6.12, 6.11, 6.10, 6.09, 6.08, 6.07, 6.06, 6.05, 6.04, 6.03, 6.02, 6.01, 6.00, 5.99, 5.98, 5.97, 5.96, 5.95, 5.94, 5.93, 5.92, 5.91, 5.90, 5.89, 5.88, 5.87, 5.86, 5.85, 5.84, 5.83, 5.82, 5.81, 5.80, 5.79, 5.78, 5.77, 5.76, 5.75, 5.74, 5.73, 5.72, 5.71, 5.70, 5.69, 5.68, 5.67, 5.66, 5.65, 5.64, 5.63, 5.62, 5.61, 5.60, 5.59, 5.58, 5.57, 5.56, 5.55, 5.54, 5.53, 5.52, 5.51, 5.50, 5.49, 5.48, 5.47, 5.46, 5.45, 5.44, 5.43, 5.42, 5.41, 5.40, 5.39, 5.38, 5.37, 5.36, 5.35, 5.34, 5.33, 5.32, 5.31, 5.30, 5.29, 5.28, 5.27, 5.26, 5.25, 5.24, 5.23, 5.22, 5.21, 5.20, 5.19, 5.18, 5.17, 5.16, 5.15, 5.14, 5.13, 5.12, 5.11, 5.10, 5.09, 5.08, 5.07, 5.06, 5.05, 5.04, 5.03, 5.02, 5.01, 5.00, 4.99, 4.98, 4.97, 4.96, 4.95, 4.94, 4.93, 4.92, 4.91, 4.90, 4.89, 4.88, 4.87, 4.86, 4.85, 4.84, 4.83, 4.82, 4.81, 4.80, 4.79, 4.78, 4.77, 4.76, 4.75, 4.74, 4.73, 4.72, 4.71, 4.70, 4.69, 4.68, 4.67, 4.66, 4.65, 4.64, 4.63, 4.62, 4.61, 4.60, 4.59, 4.58, 4.57, 4.56, 4.55, 4.54, 4.53, 4.52, 4.51, 4.50, 4.49, 4.48, 4.47, 4.46, 4.45, 4.44, 4.43, 4.42, 4.41, 4.40, 4.39, 4.38, 4.37, 4.36, 4.35, 4.34, 4.33, 4.32, 4.31, 4.30, 4.29, 4.28, 4.27, 4.26, 4.25, 4.24, 4.23, 4.22, 4.21, 4.20, 4.19, 4.18, 4.17, 4.16, 4.15, 4.14, 4.13, 4.12, 4.11, 4.10, 4.09, 4.08, 4.07, 4.06, 4.05, 4.04, 4.03, 4.02, 4.01, 4.00, 3.99, 3.98, 3.97, 3.96, 3.95, 3.94, 3.93, 3.92, 3.91, 3.90, 3.89, 3.88, 3.87, 3.86, 3.85, 3.84, 3.83, 3.82, 3.81, 3.80, 3.79, 3.78, 3.77, 3.76, 3.75, 3.74, 3.73, 3.72, 3.71, 3.70, 3.69, 3.68, 3.67, 3.66, 3.65, 3.64, 3.63, 3.62, 3.61, 3.60, 3.59, 3.58, 3.57, 3.56, 3.55, 3.54, 3.53, 3.52, 3.51, 3.50, 3.49, 3.48, 3.47, 3.46, 3.45, 3.44, 3.43, 3.42, 3.41, 3.40, 3.39, 3.38, 3.37, 3.36, 3.35, 3.34, 3.33, 3.32, 3.31, 3.30, 3.29, 3.28, 3.27, 3.26, 3.25, 3.24, 3.23, 3.22, 3.21, 3.20, 3.19, 3.18, 3.17, 3.16, 3.15, 3.14, 3.13, 3.12, 3.11, 3.10, 3.09, 3.08, 3.07, 3.06, 3.05, 3.04, 3.03, 3.02, 3.01, 3.00, 2.99, 2.98, 2.97, 2.96, 2.95, 2.94, 2.93, 2.92, 2.91, 2.90, 2.89, 2.88, 2.87, 2.86, 2.85, 2.84, 2.83, 2.82, 2.81, 2.80, 2.79, 2.78, 2.77, 2.76, 2.75, 2.74, 2.73, 2.72, 2.71, 2.70, 2.69, 2.68, 2.67, 2.66, 2.65, 2.64, 2.63, 2.62, 2.61, 2.60, 2.59, 2.58, 2.57, 2.56, 2.55, 2.54, 2.53, 2.52, 2.51, 2.50, 2.49, 2.48, 2.47, 2.46, 2.45, 2.44, 2.43, 2.42, 2.41, 2.40, 2.39, 2.38, 2.37, 2.36, 2.35, 2.34, 2.33, 2.32, 2.31, 2.30, 2.29, 2.28, 2.27, 2.26, 2.25, 2.24, 2.23, 2.22, 2.21, 2.20, 2.19, 2.18, 2.17, 2.16, 2.15, 2.14, 2.13, 2.12, 2.11, 2.10, 2.09, 2.08, 2.07, 2.06, 2.05, 2.04, 2.03, 2.02, 2.01, 2.00, 1.99, 1.98, 1.97, 1.96, 1.95, 1.94, 1.93, 1.92, 1.91, 1.90, 1.89, 1.88, 1.87, 1.86, 1.85, 1.84, 1.83, 1.82, 1.81, 1.80, 1.79, 1.78, 1.77, 1.76, 1.75, 1.74, 1.73, 1.72, 1.71, 1.70, 1.69, 1.68, 1.67, 1.66, 1.65, 1.64, 1.63, 1.62, 1.61, 1.60, 1.59, 1.58, 1.57, 1.56, 1.55, 1.54, 1.53, 1.52, 1.51, 1.50, 1.49, 1.48, 1.47, 1.46, 1.45, 1.44, 1.43, 1.42, 1.41, 1.40, 1.39, 1.38, 1.37, 1.36, 1.35, 1.34, 1.33, 1.32, 1.31, 1.30, 1.29,	

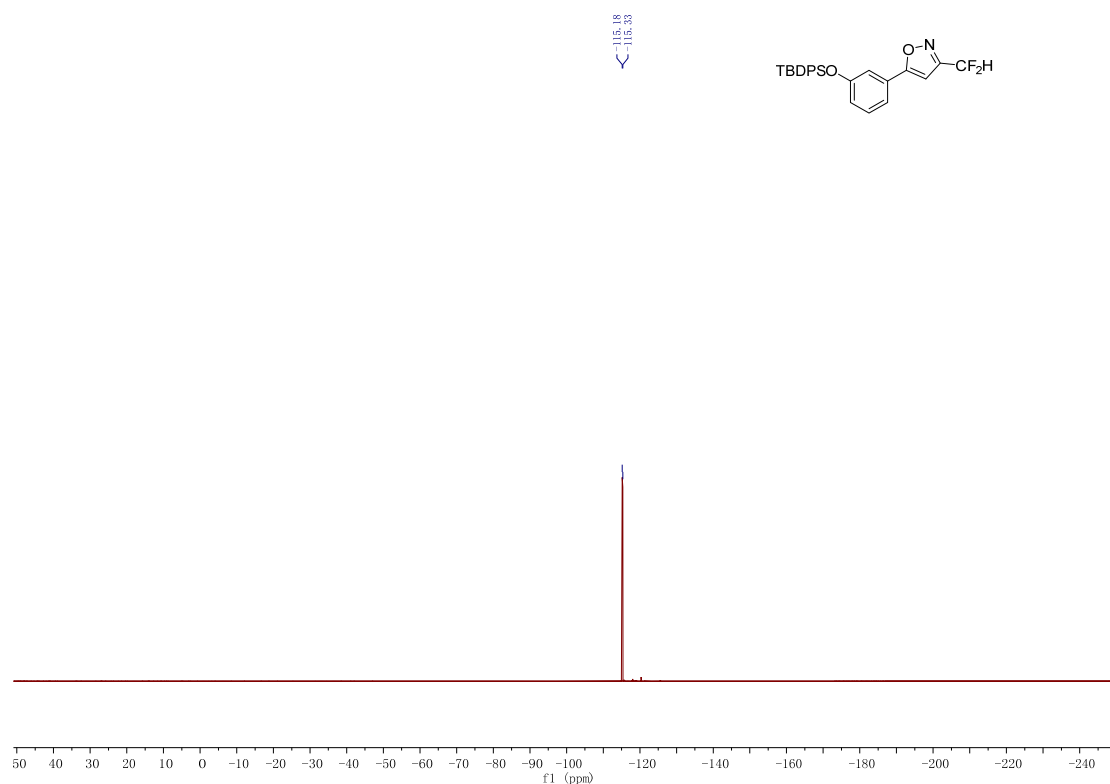
Chemical structure of the compound is shown above the spectrum:

CC(F)(F)c1cc(Oc2ccc(cc2)OSi(C)(C)C(C)(C)C)cn1

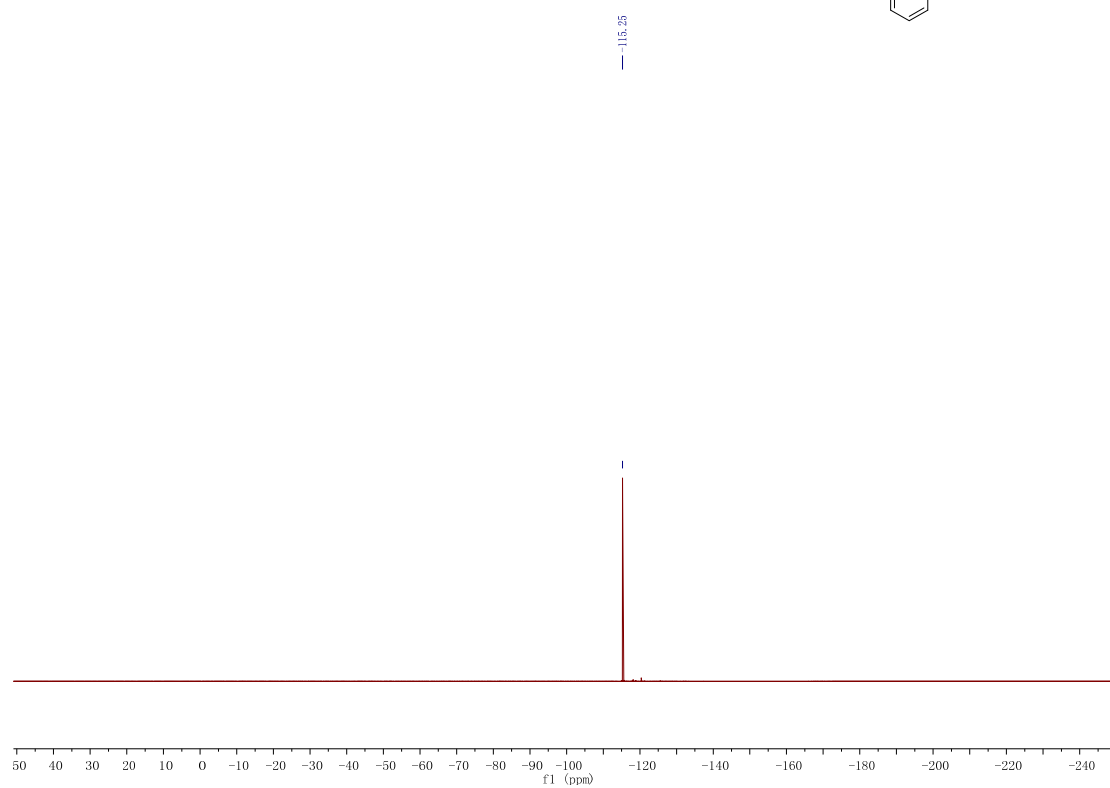
The spectrum displays the following chemical shifts (ppm):

Chemical Shift (ppm)
171.74
156.58
156.50
156.29
138.85
138.73
138.39
138.30
128.27
127.83
122.63
117.04
117.44
111.75
108.39
107.04
96.52
77.68
77.36
77.04
26.85
19.83

^{19}F NMR (CDCl_3 , 376 MHz) of **5w**



^{19}F { ^1H } NMR (CDCl_3 , 376 MHz) of **5w**



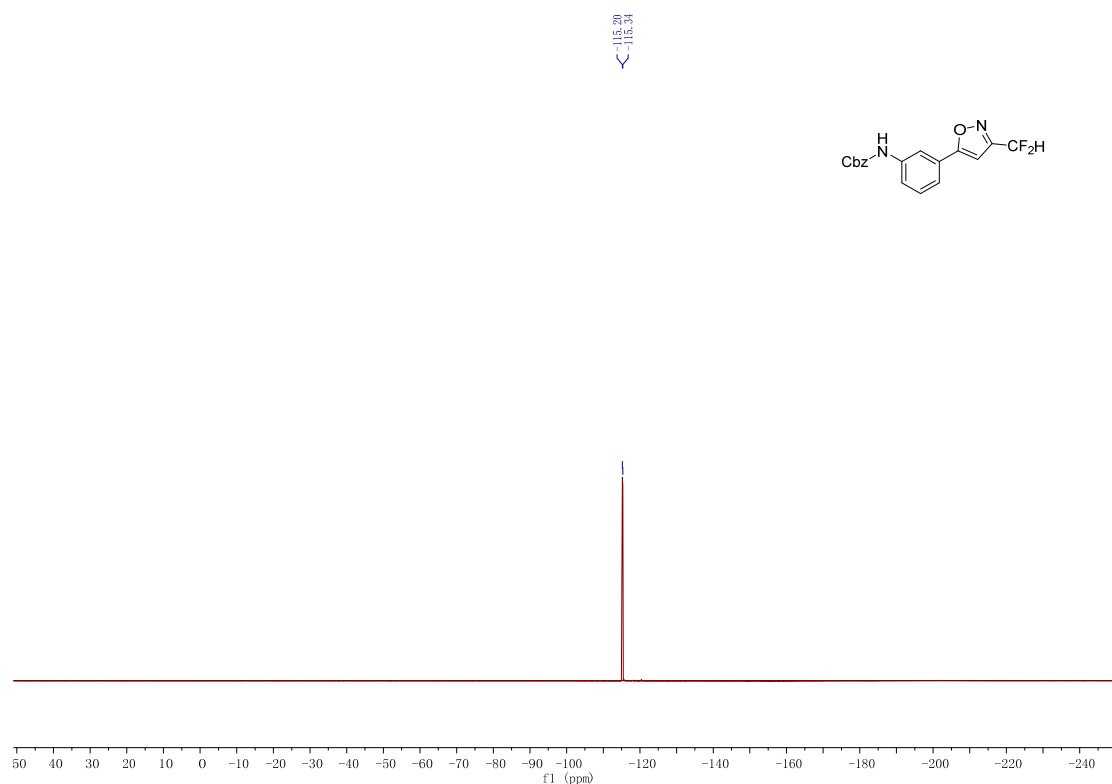
[illegible]

Chemical structure of compound 10b: CC(F)(F)c1cc([N+](=O)[O-])cc1Cc2ccc(NC3CCCCC3)cc2

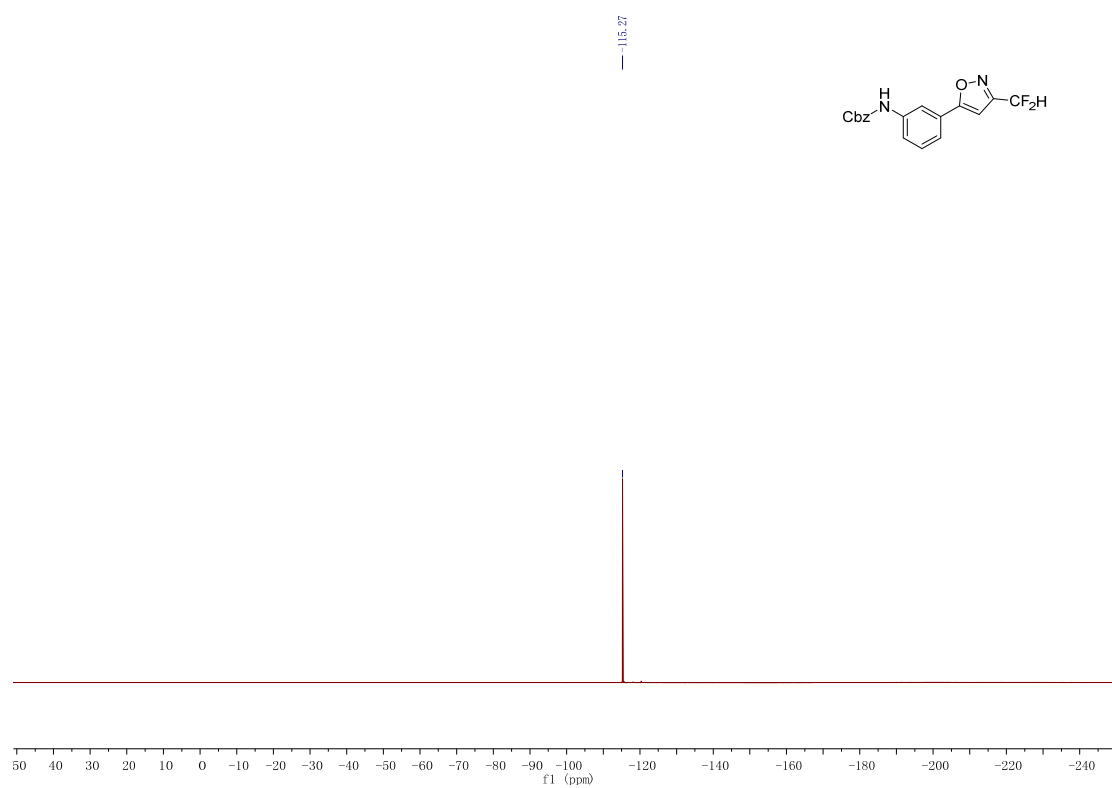
¹³C NMR spectrum (CDCl₃) of compound 10b. The x-axis represents the chemical shift in ppm, ranging from 0 to 180. The spectrum shows several peaks, with the following chemical shifts labeled:

- 171.57
- 160.04
- 159.74
- 156.45
- 153.60
- 139.17
- 136.07
- 130.28
- 129.63
- 129.74
- 127.57
- 127.25
- 124.17
- 116.14
- 111.65
- 106.25
- 104.89
- 96.95
- 77.68 (CDCl₃)
- 77.41 (CDCl₃)
- 77.06 (CDCl₃)
- 67.67

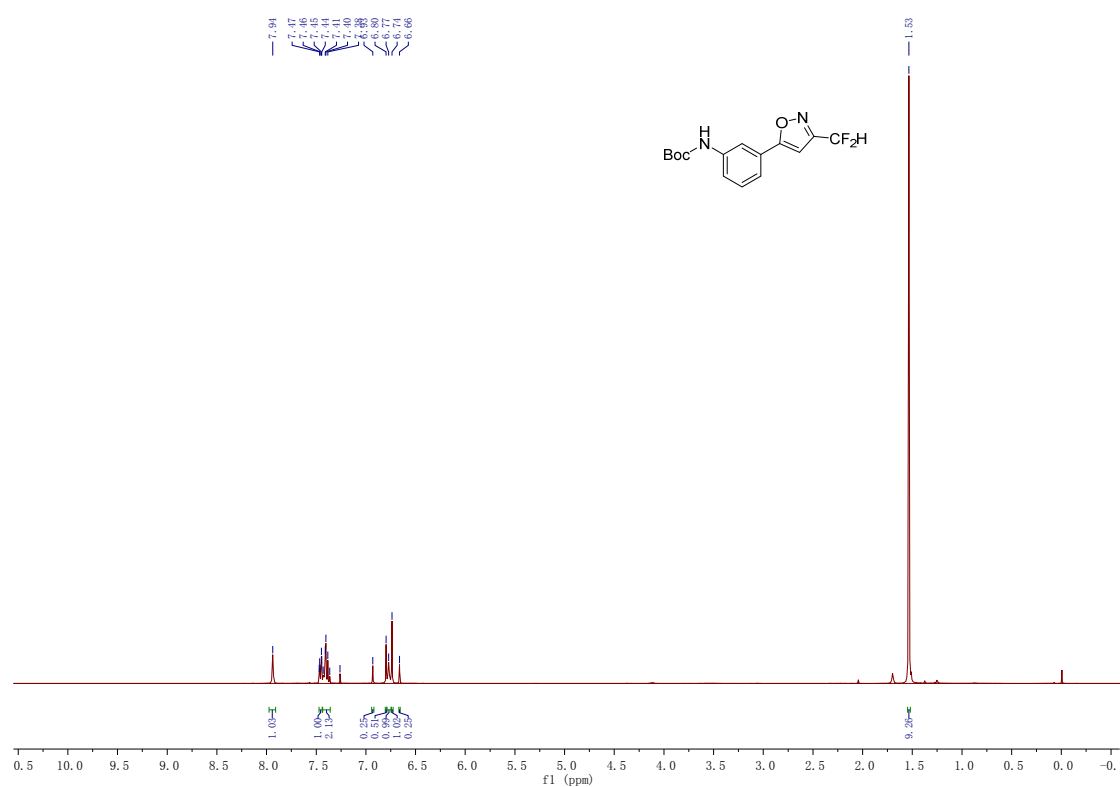
^{19}F NMR (CDCl₃, 376 MHz) of **5x**



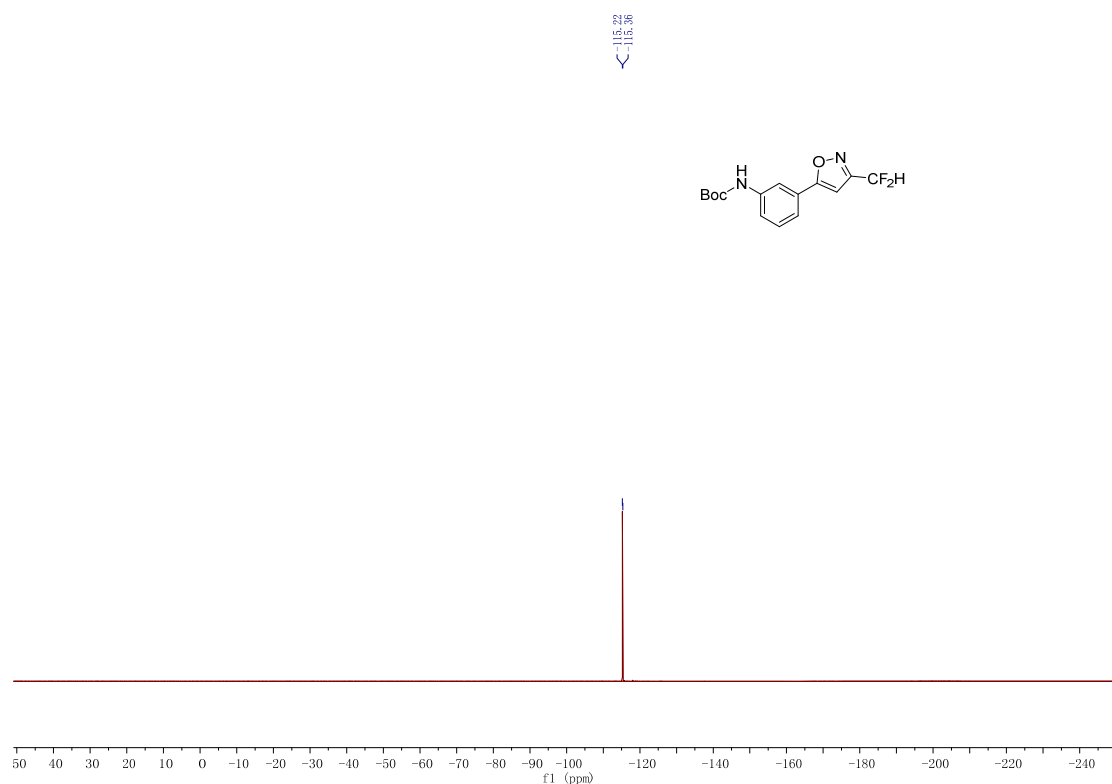
^{19}F { ^1H } NMR (CDCl₃, 376 MHz) of **5x**



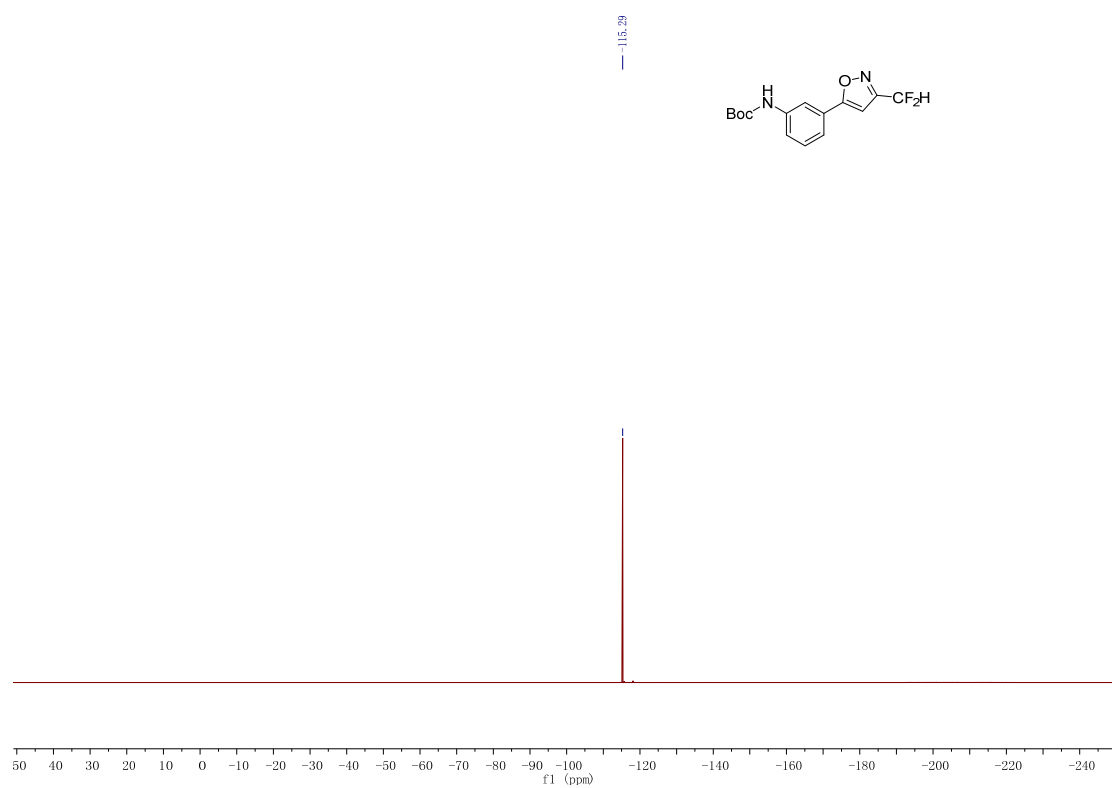
^1H NMR (CDCl₃, 400 MHz) of 5y



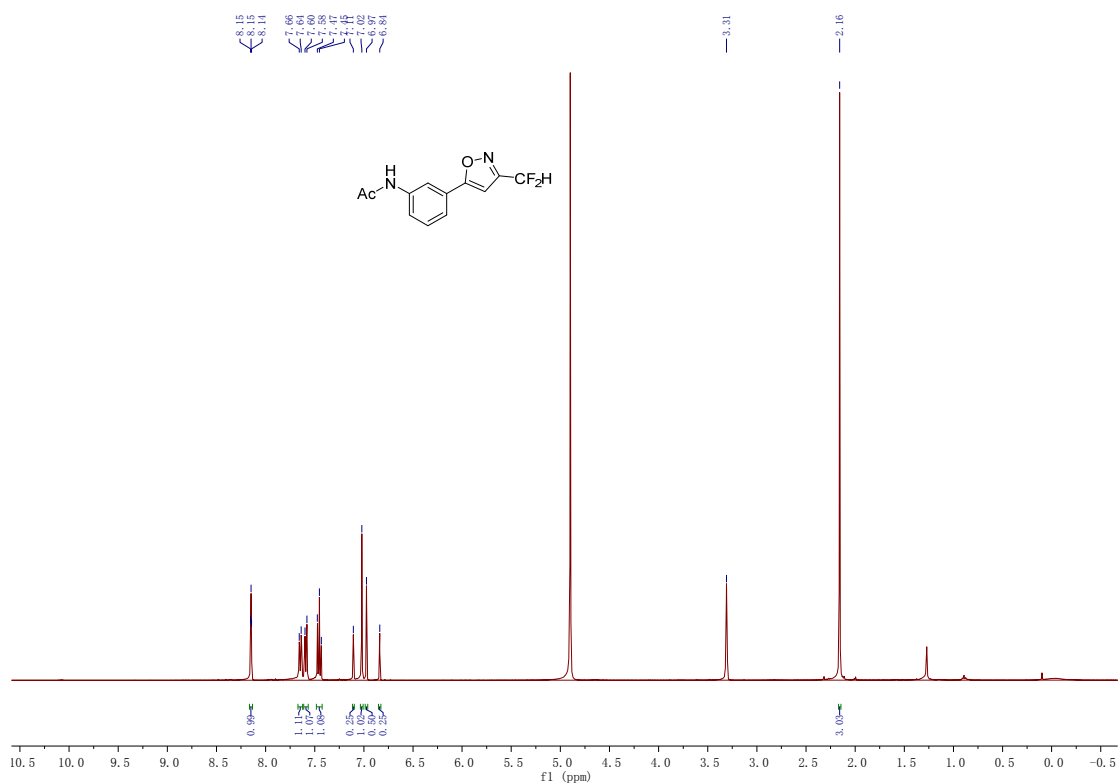
^{19}F NMR (CDCl₃, 376 MHz) of **5y**



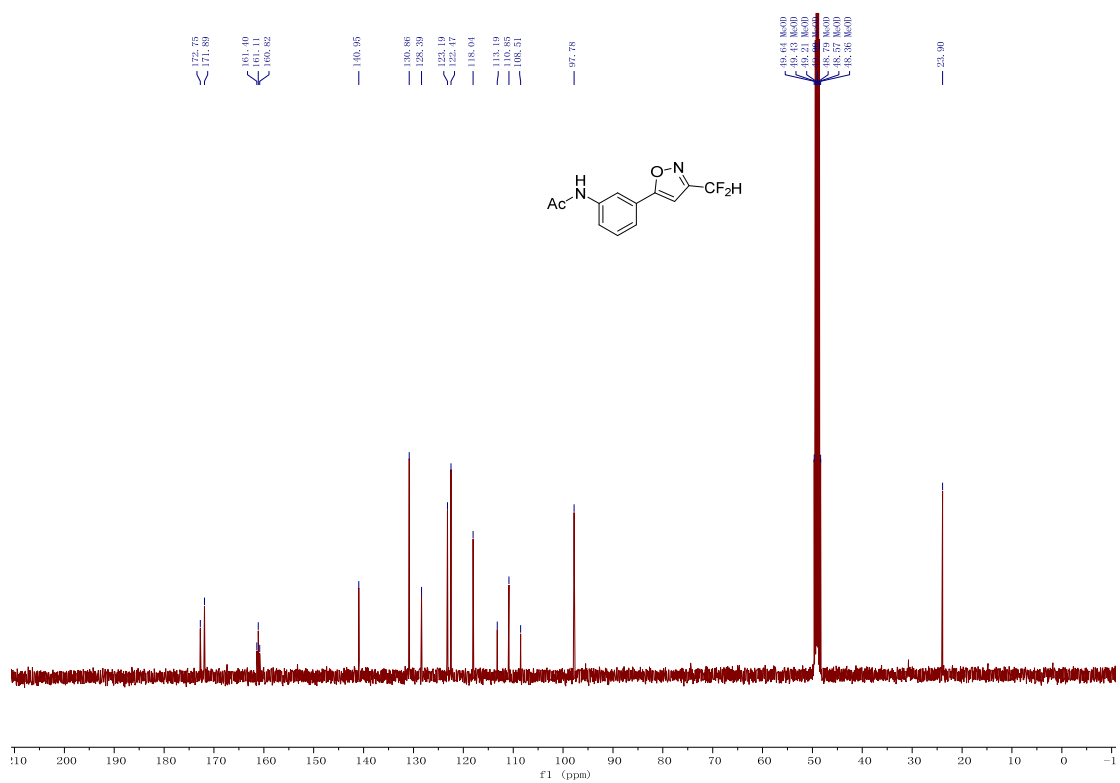
^{19}F { ^1H } NMR (CDCl₃, 376 MHz) of **5y**



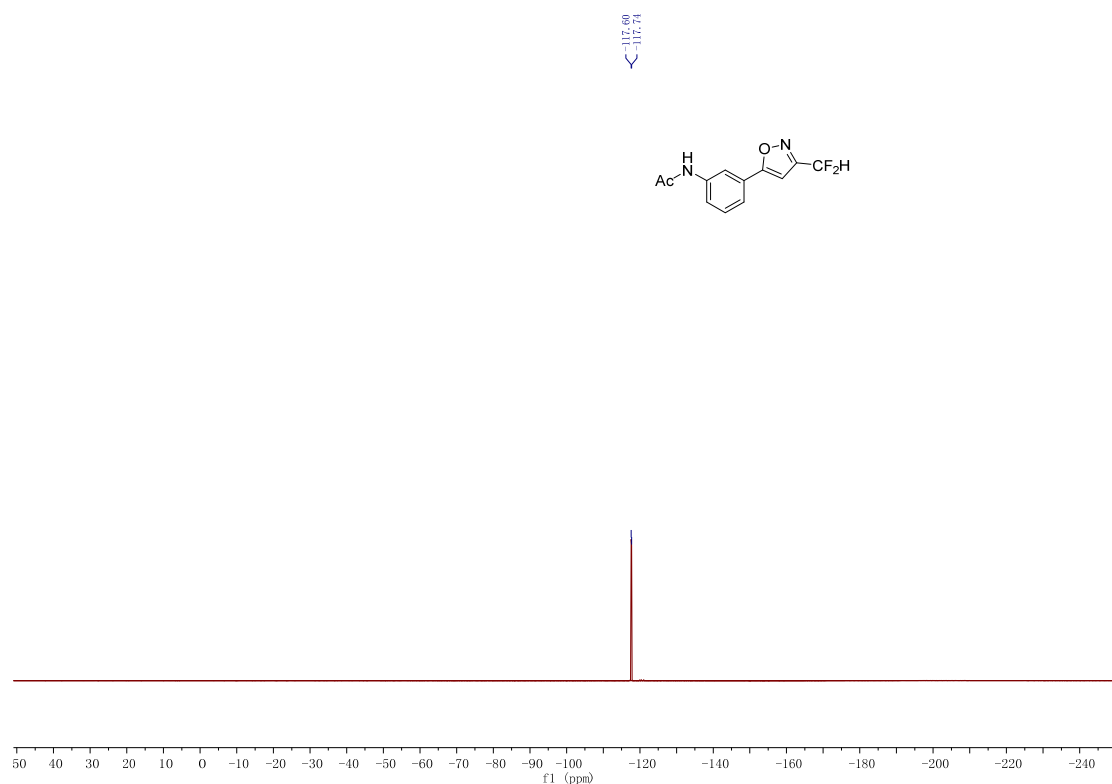
^1H NMR (CD₃OD, 400 MHz) of **5z**



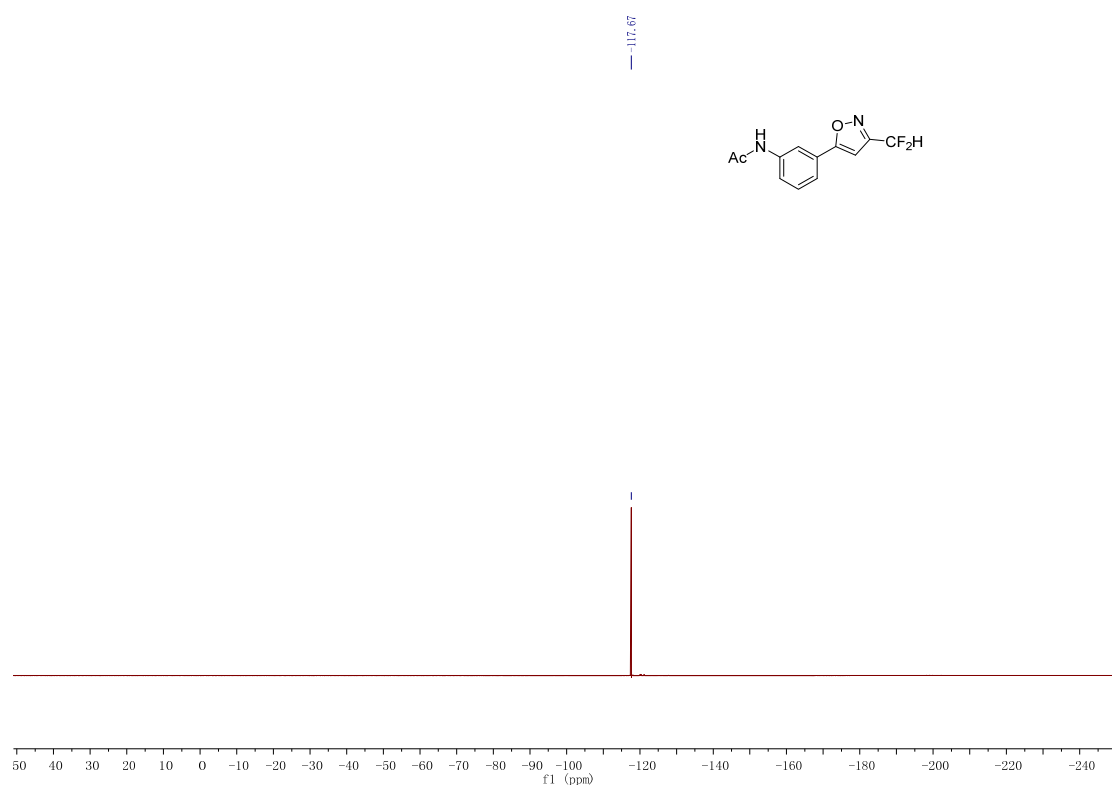
^{13}C NMR (CD₃OD, 100 MHz) of **5z**



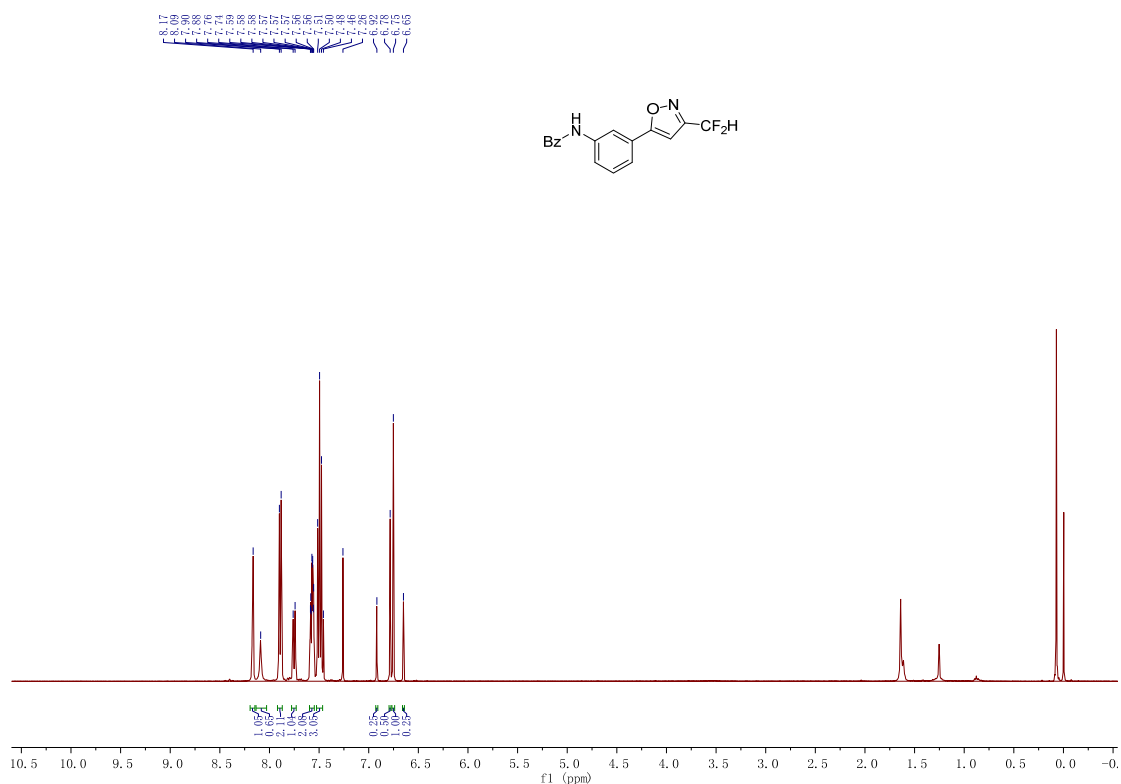
^{19}F NMR (CD₃OD, 376 MHz) of **5z**



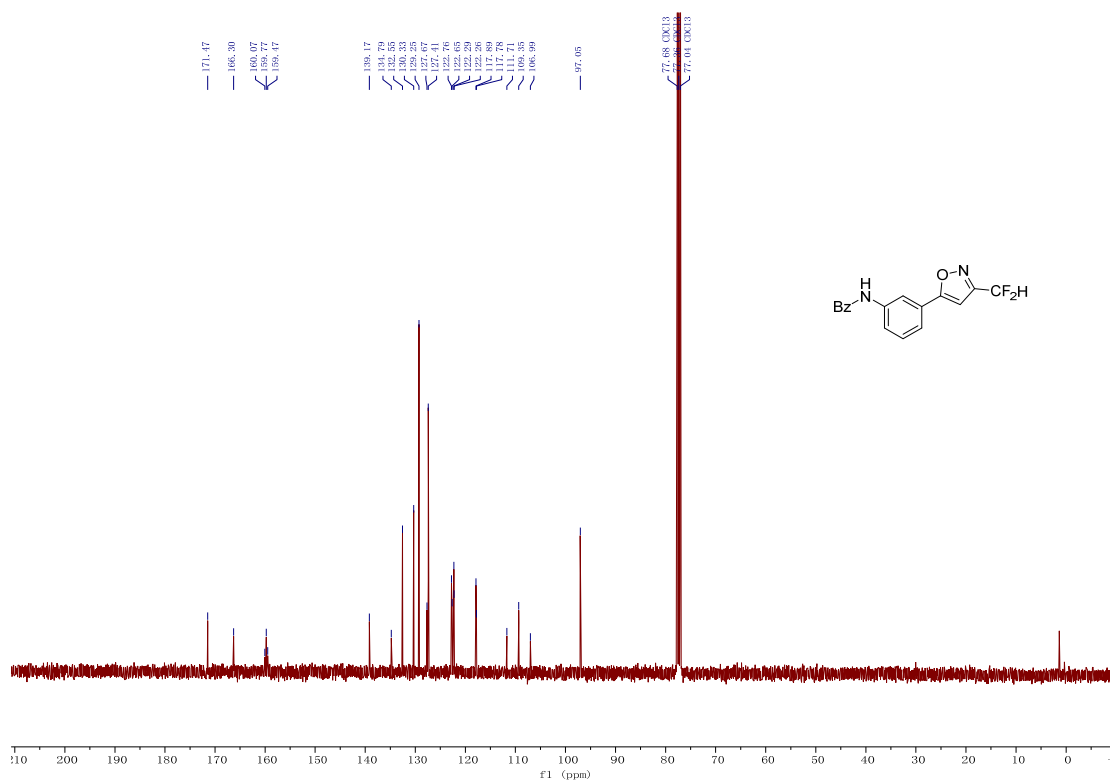
^{19}F { ^1H } NMR (CD₃OD, 376 MHz) of **5z**



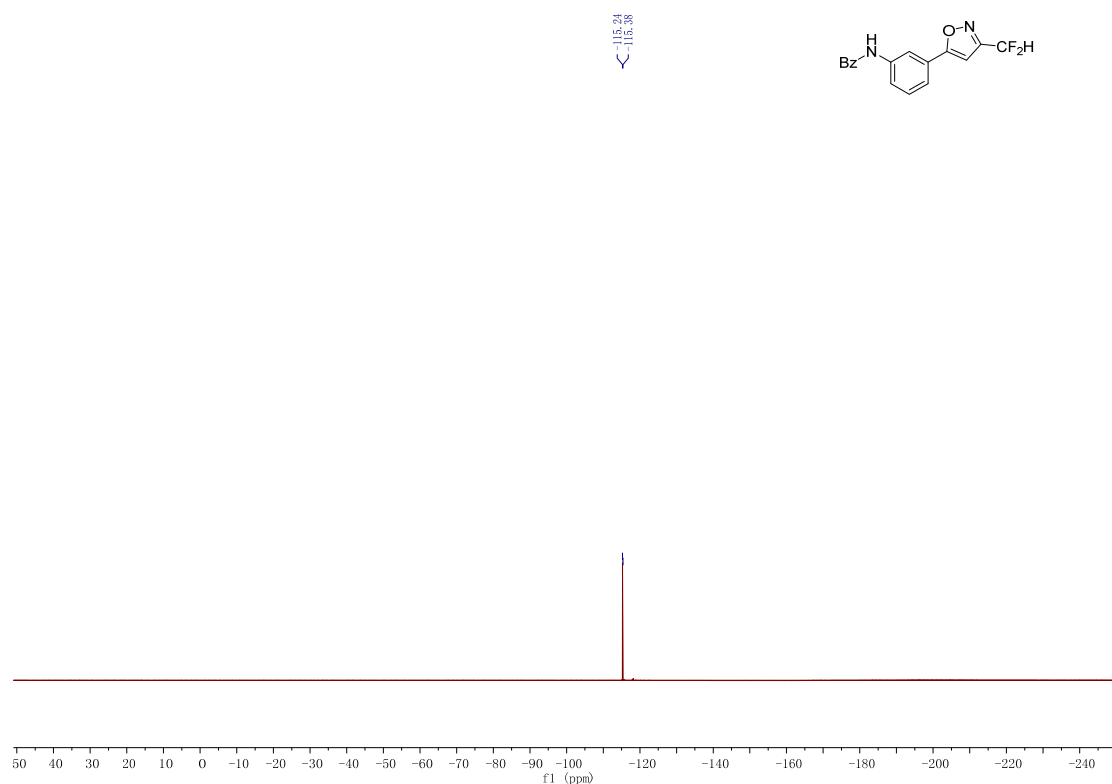
¹H NMR (CDCl₃, 400 MHz) of 5aa



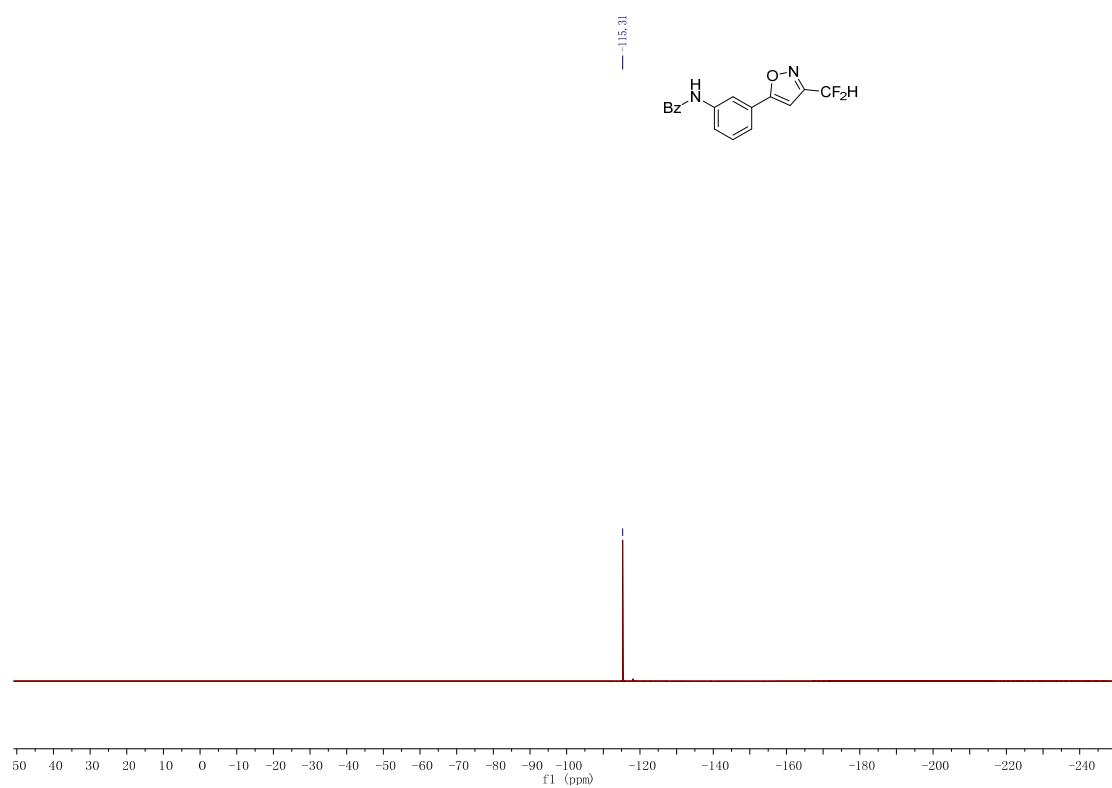
¹³C NMR (CDCl₃, 100 MHz) of 5aa



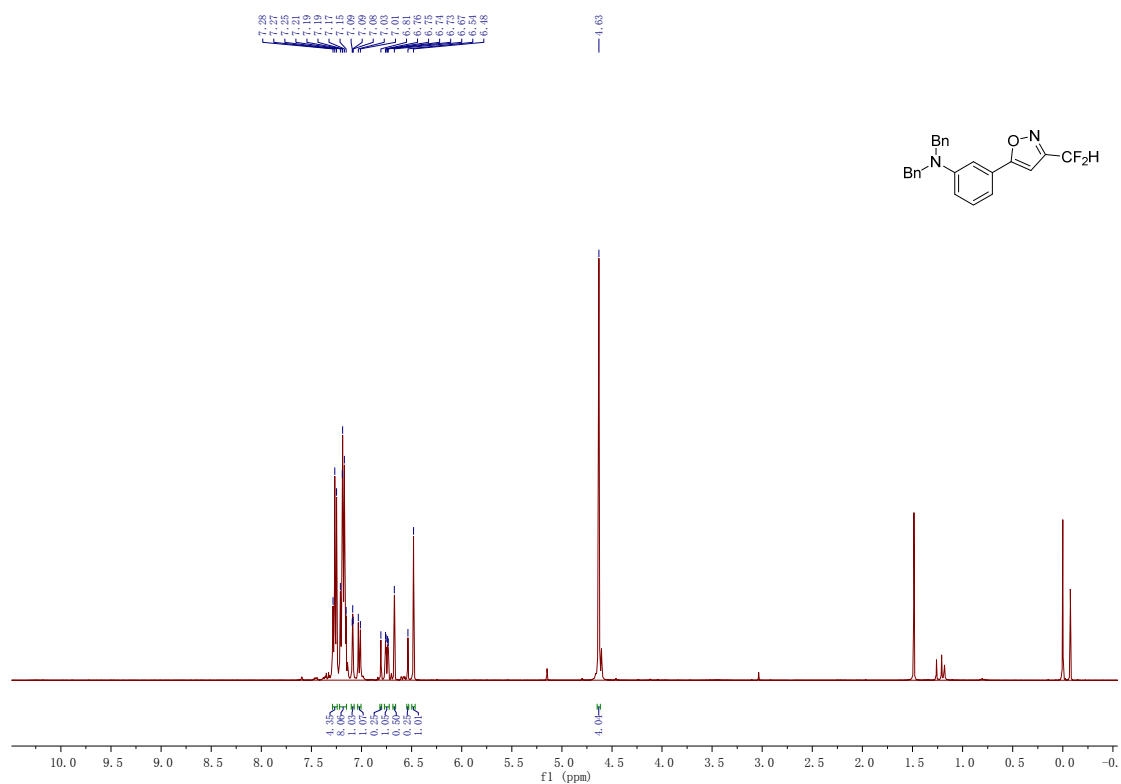
^{19}F NMR (CDCl_3 , 376 MHz) of **5aa**



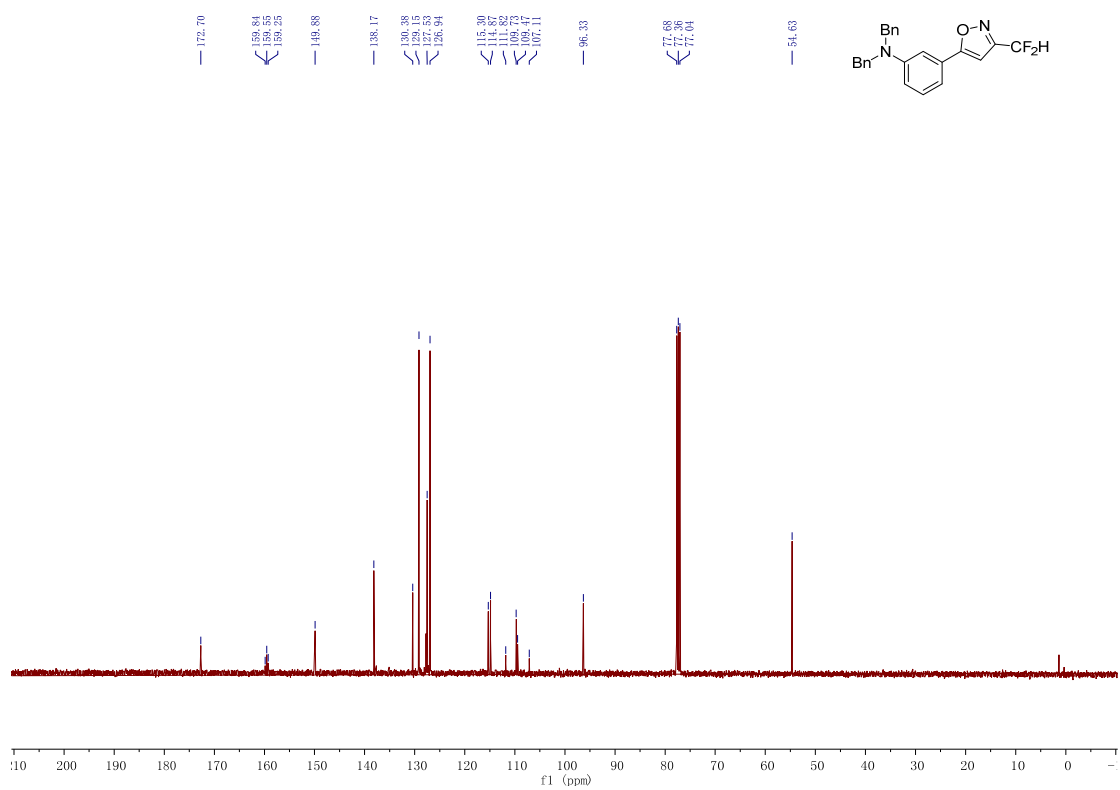
^{19}F { ^1H } NMR (CDCl_3 , 376 MHz) of **5aa**



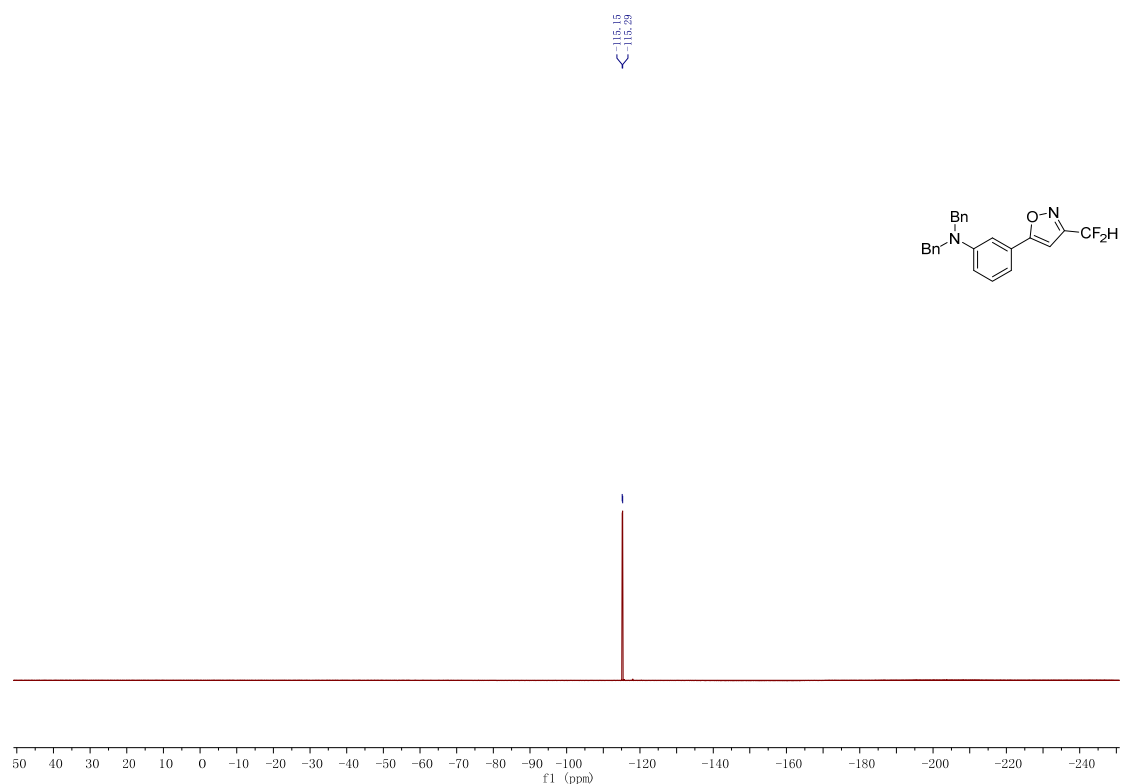
^1H NMR (CDCl₃, 400 MHz) of 5bb



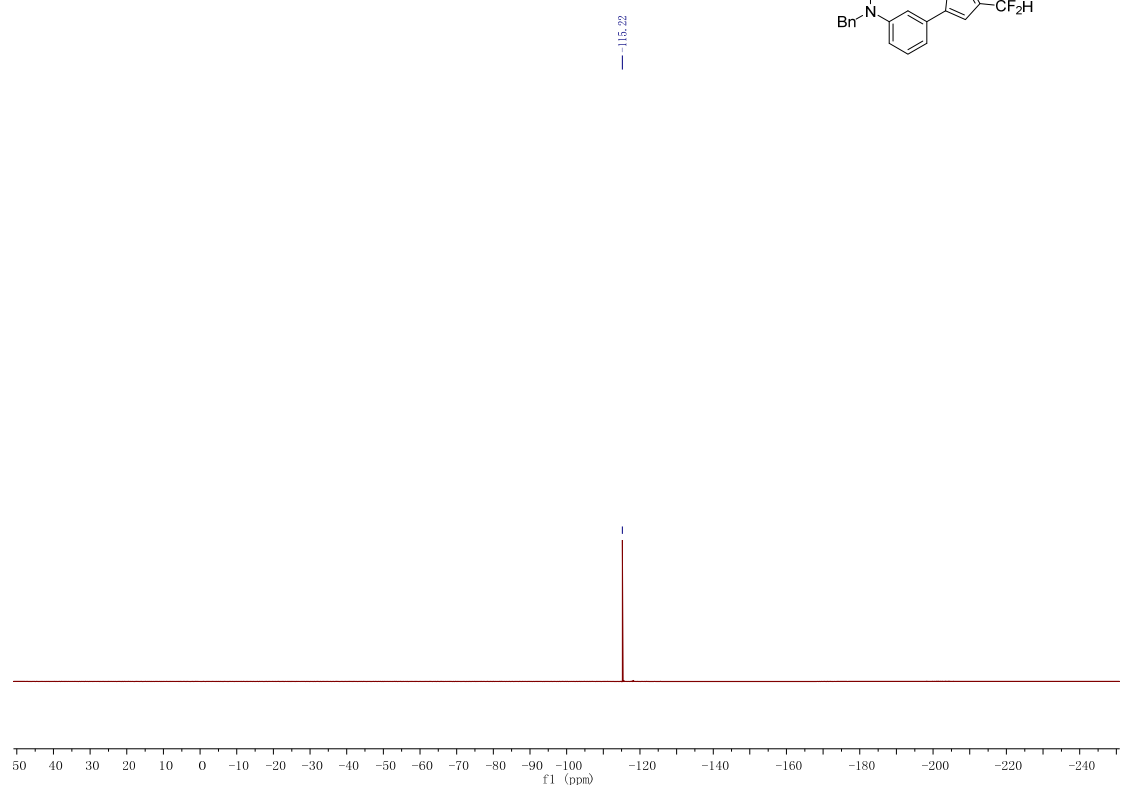
^{13}C NMR (CDCl₃, 100 MHz) of 5bb



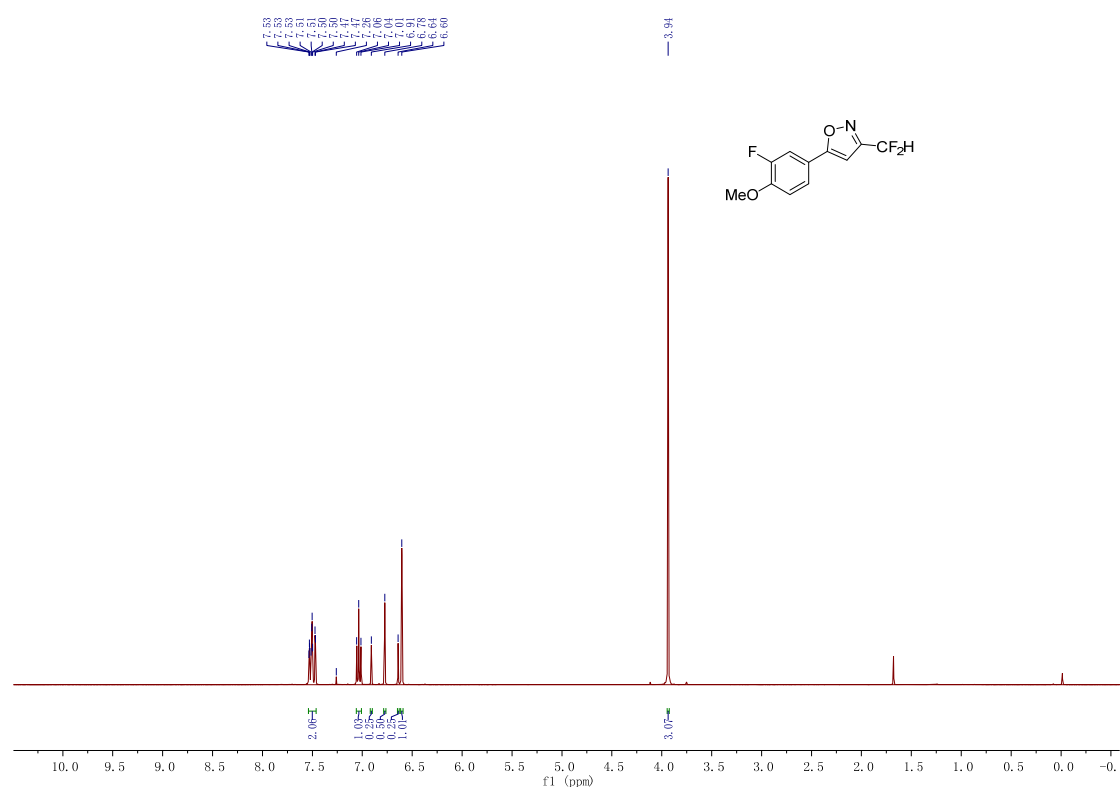
^{19}F NMR (CDCl₃, 376 MHz) of **5bb**



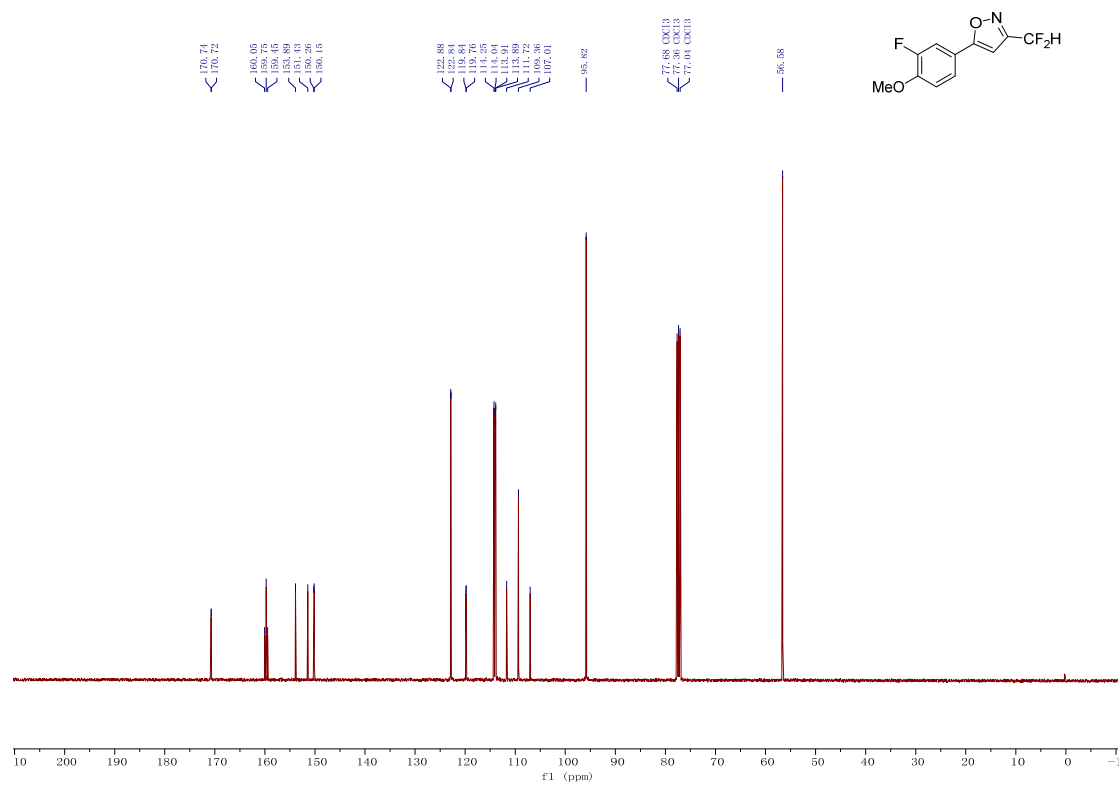
^{19}F { ^1H } NMR (CDCl₃, 376 MHz) of **5bb**



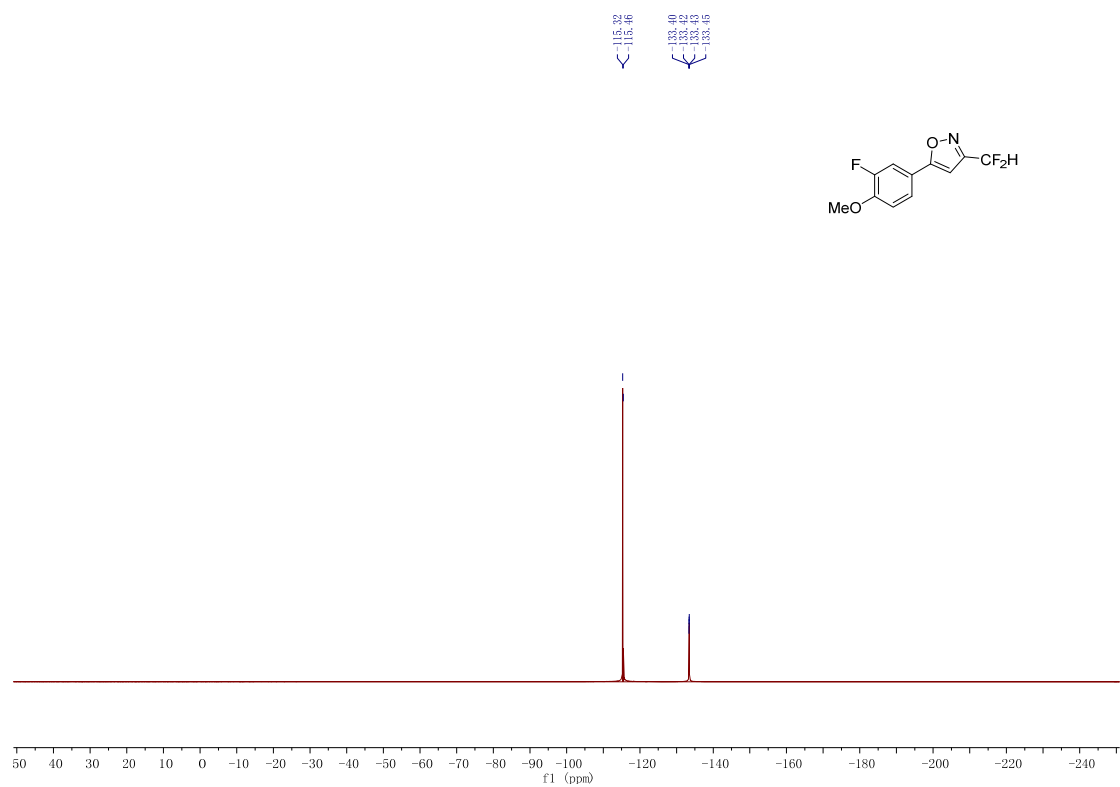
^1H NMR (CDCl₃, 400 MHz) of 5cc



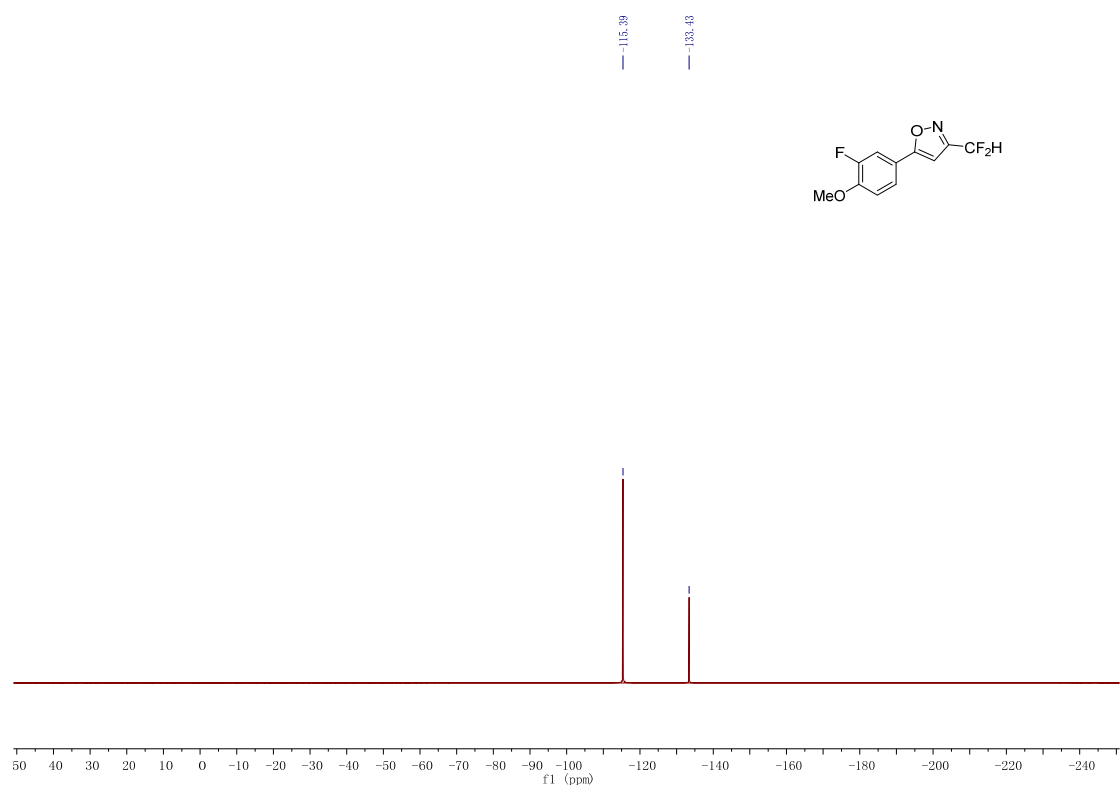
^{13}C NMR (CDCl₃, 100 MHz) of 5cc



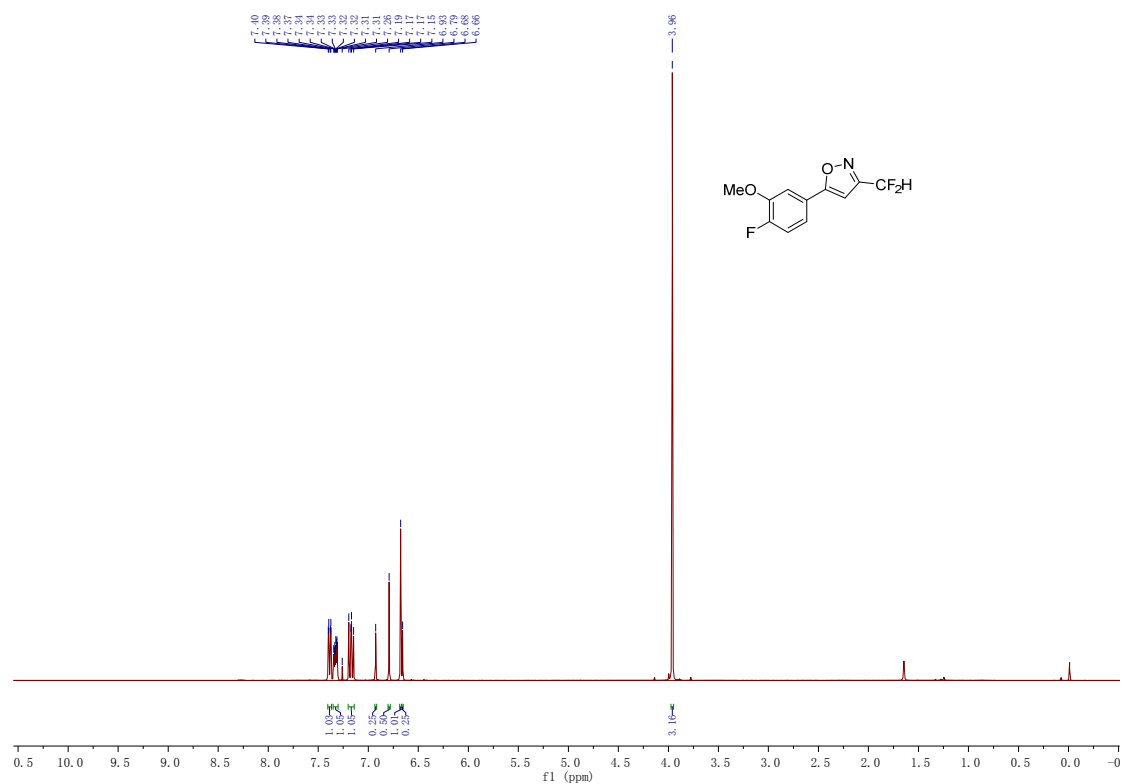
^{19}F NMR (CDCl₃, 376 MHz) of **5cc**



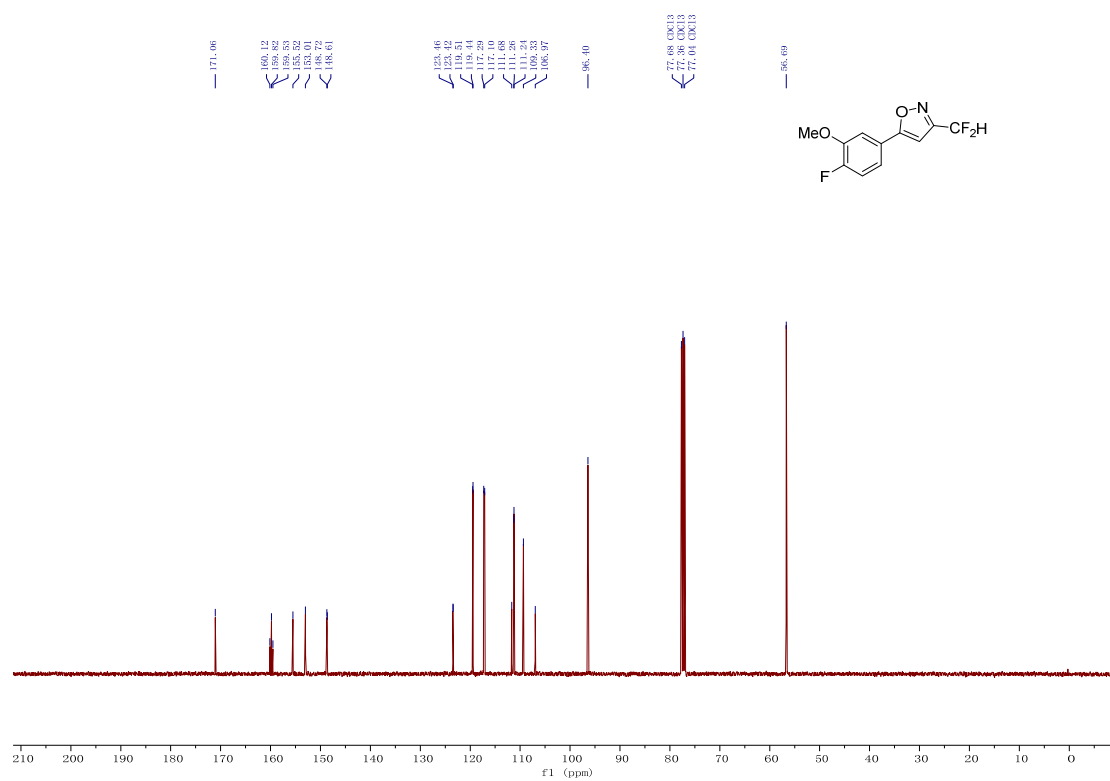
^{19}F { ^1H } NMR (CDCl₃, 376 MHz) of **5cc**



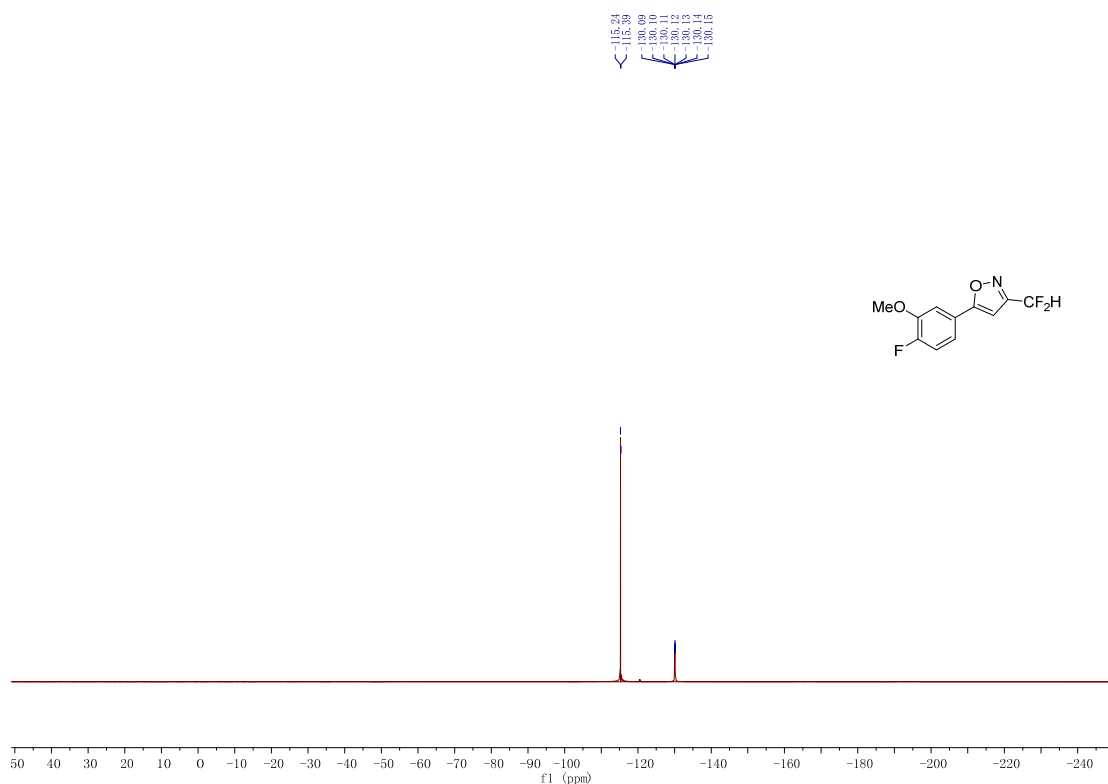
^1H NMR (CDCl₃, 400 MHz) of 5dd



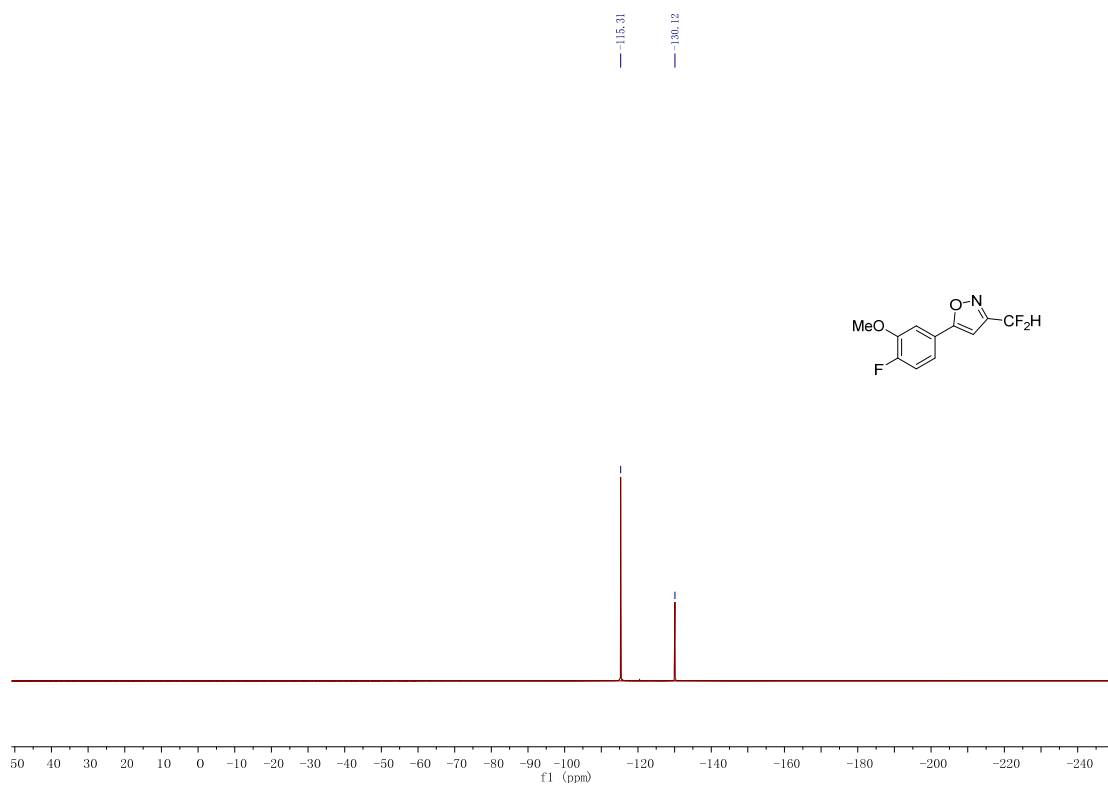
^{13}C NMR (CDCl₃, 100 MHz) of 5dd



^{19}F NMR (CDCl₃, 376 MHz) of 5dd



^{19}F { ^1H } NMR (CDCl₃, 376 MHz) of 5dd



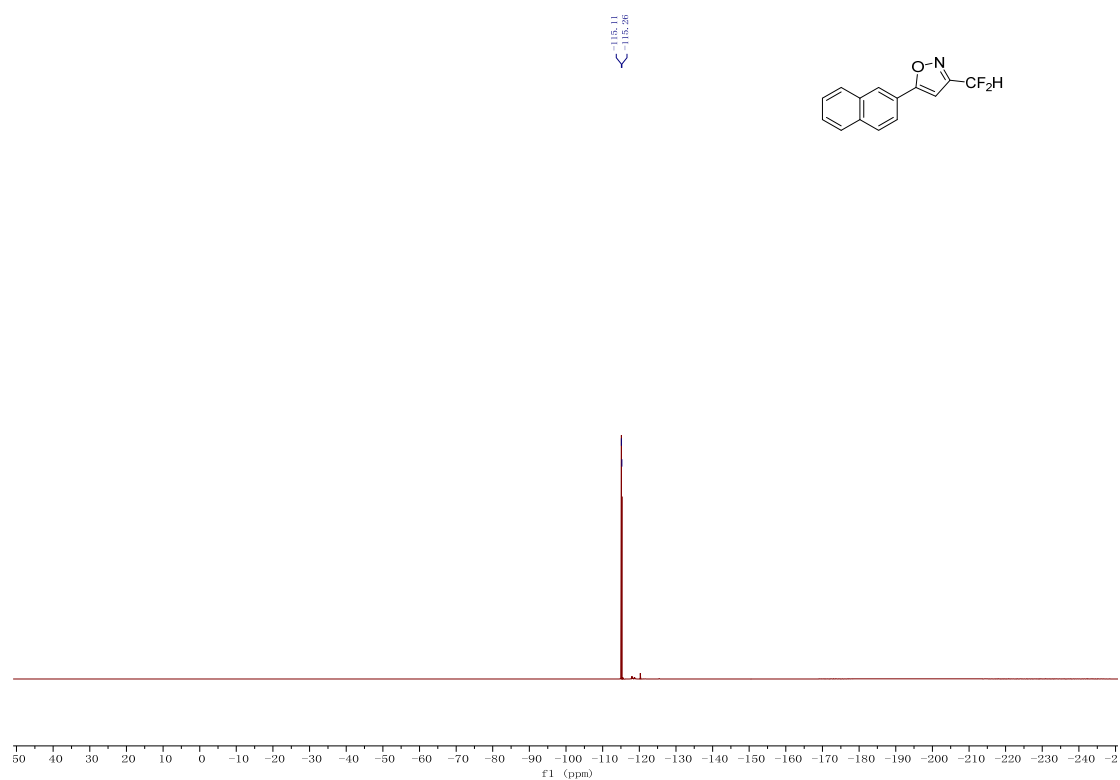
Chemical structure: c1ccc2c(c1)c(c3ccccc23)O[N+](=O)[O-]

¹H NMR spectrum (CDCl₃) showing peaks in the aromatic region (6.5-8.5 ppm) and a CF₂H group region (1.5-2.0 ppm). Integration values are provided below the peaks.

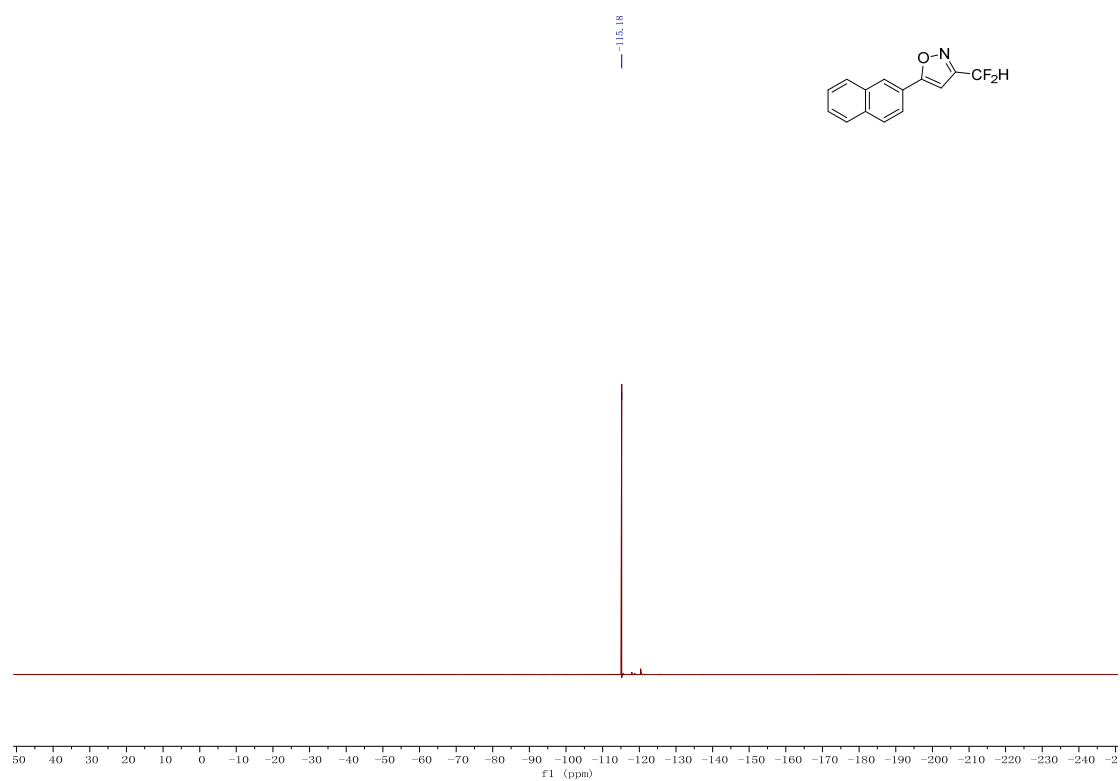
Chemical Shift (ppm)	Integration
8.45	1.00
8.05	1.00
7.95	1.00
7.85	1.00
7.75	1.00
7.65	1.00
7.55	1.00
7.45	1.00
7.35	1.00
7.25	1.00
7.15	1.00
7.05	1.00
6.95	1.00
6.85	1.00
6.75	1.00
6.65	1.00
6.55	1.00
6.45	1.00
6.35	1.00
6.25	1.00
6.15	1.00
6.05	1.00
6.95	1.00
6.85	1.00
6.75	1.00
6.65	1.00
6.55	1.00
6.45	1.00
6.35	1.00
6.25	1.00
6.15	1.00
6.05	1.00
6.95	1.00
6.85	1.00
6.75	1.00
6.65	1.00
6.55	1.00
6.45	1.00
6.35	1.00
6.25	1.00
6.15	1.00
6.05	1.00
6.95	1.00
6.85	1.00
6.75	1.00
6.65	1.00
6.55	1.00
6.45	1.00
6.35	1.00
6.25	1.00
6.15	1.00
6.05	1.00
6.95	1.00
6.85	1.00
6.75	1.00
6.65	1.00
6.55	1.00
6.45	1.00
6.35	1.00
6.25	1.00
6.15	1.00
6.05	1.00
6.95	1.00
6.85	1.00
6.75	1.00
6.65	1.00
6.55	1.00
6.45	1.00
6.35	1.00
6.25	1.00
6.15	1.00
6.05	1.00
6.95	1.00
6.85	1.00
6.75	1.00
6.65	1.00
6.55	1.00
6.45	1.00
6.35	1.00
6.25	1.00
6.15	1.00
6.05	1.00
6.95	1.00
6.85	1.00
6.75	1.00
6.65	1.00
6.55	1.00
6.45	1.00
6.35	1.00
6.25	1.00
6.15	1.00
6.05	1.00
6.95	1.00
6.85	1.00
6.75	1.00
6.65	1.00
6.55	1.00
6.45	1.00
6.35	1.00
6.25	1.00
6.15	1.00
6.05	1.00
6.95	1.00
6.85	1.00
6.75	1.00
6.65	1.00
6.55	1.00
6.45	1.00
6.35	1.00
6.25	1.00
6.15	1.00
6.05	1.00
6.95	1.00
6.85	1.00
6.75	1.00
6.65	1.00
6.55	1.00
6.45	1.00
6.35	1.00
6.25	1.00
6.15	1.00
6.05	1.00
6.95	1.00
6.85	1.00
6.75	1.00
6.65	1.00
6.55	1.00
6.45	1.00
6.35	1.00
6.25	1.00
6.15	1.00
6.05	1.00
6.95	1.00
6.85	1.00
6.75	1.00
6.65	1.00
6.55	1.00
6.45	1.00
6.35	1.00
6.25	1.00
6.15	1.00
6.05	1.00
6.95	1.00
6.85	1.00
6.75	1.00
6.65	1.00
6.55	1.00
6.45	1.00
6.35	1.00
6.25	1.00
6.15	1.00
6.05	1.00
6.95	1.00
6.85	1.00
6.75	1.00
6.65	1.00
6.55	1.00
6.45	1.00
6.35	1.00
6.25	1.00
6.15	1.00
6.05	1.00
6.95	1.00
6.85	1.00
6.75	1.00
6.65	1.00
6.55	1.00
6.45	1.00
6.35	1.00
6.25	1.00
6.15	1.00
6.05	1.00
6.95	1.00
6.85	1.00
6.75	1.00
6.65	1.00
6.55	1.0

[illegible]

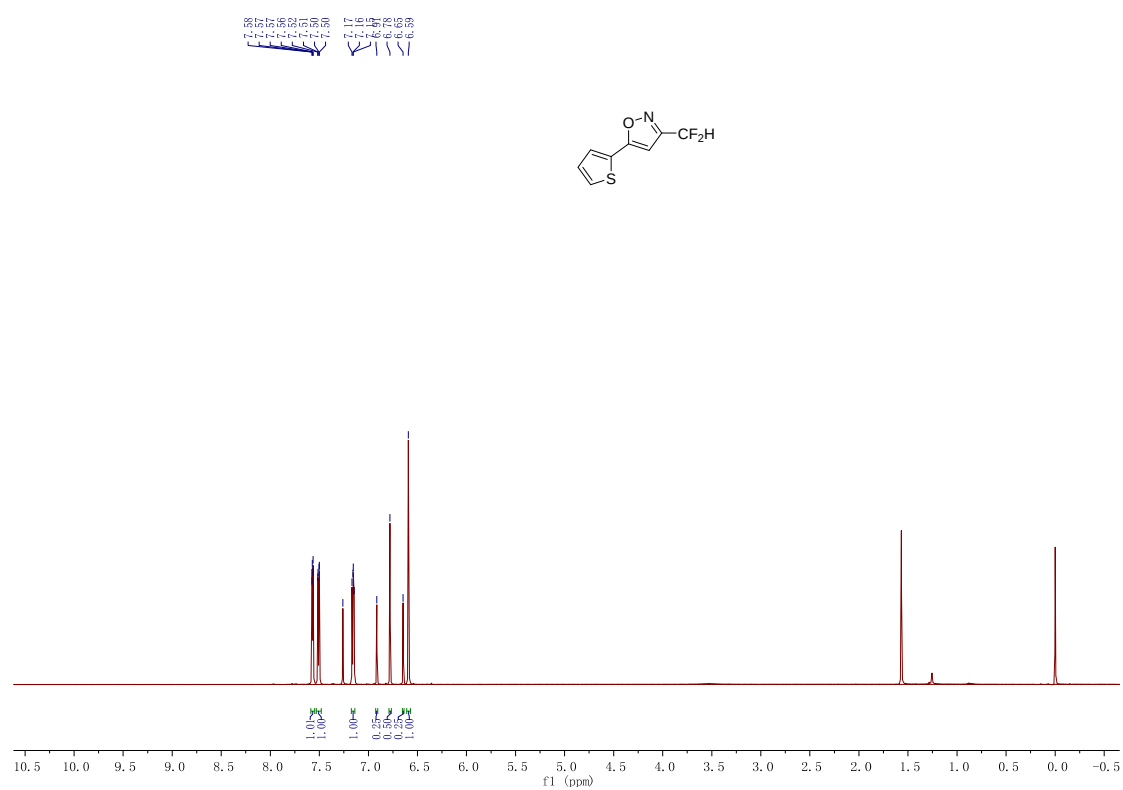
^{19}F NMR (CDCl₃, 376 MHz) of **5ee**



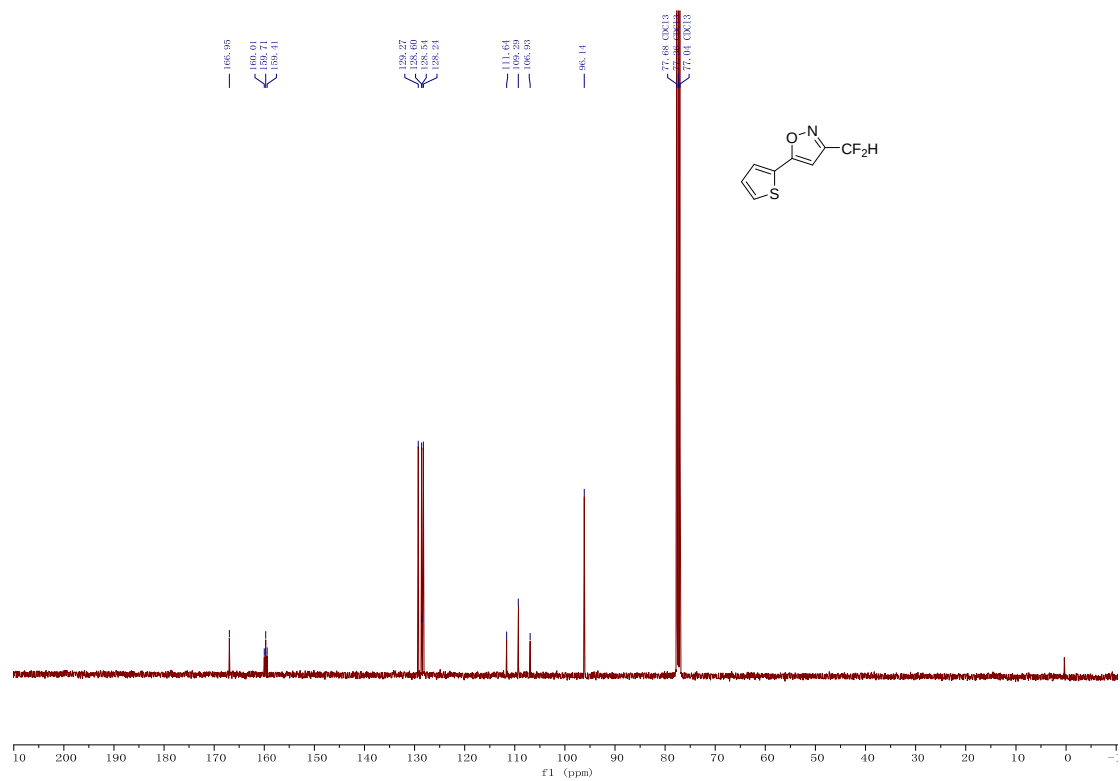
^{19}F { ^1H } NMR (CDCl₃, 376 MHz) of **5ee**



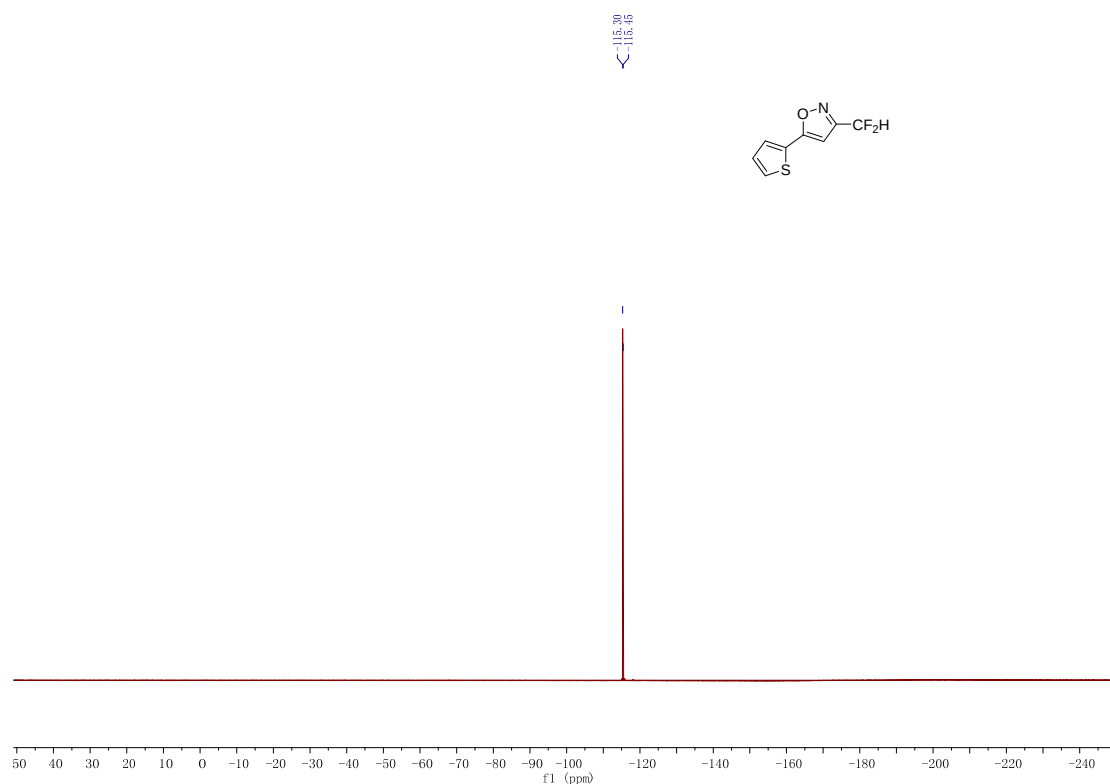
^1H NMR (CDCl₃, 400 MHz) of **5ff**



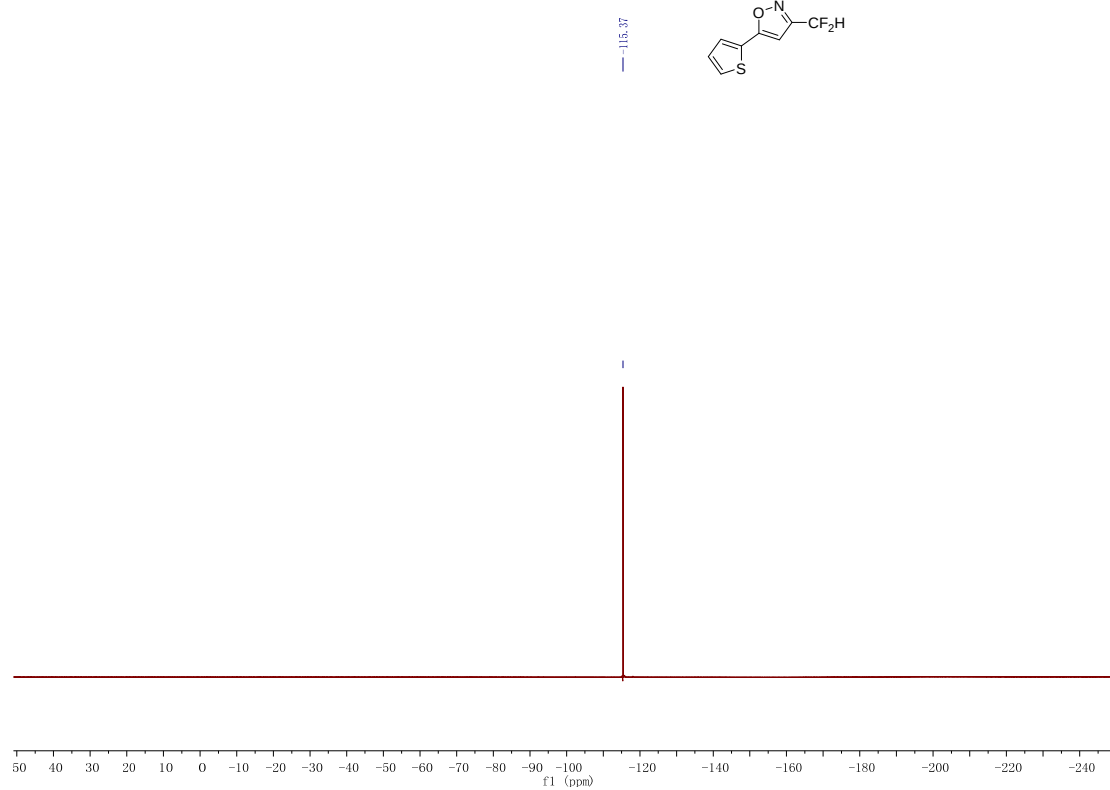
^{13}C NMR (CDCl₃, 100 MHz) of **5ff**



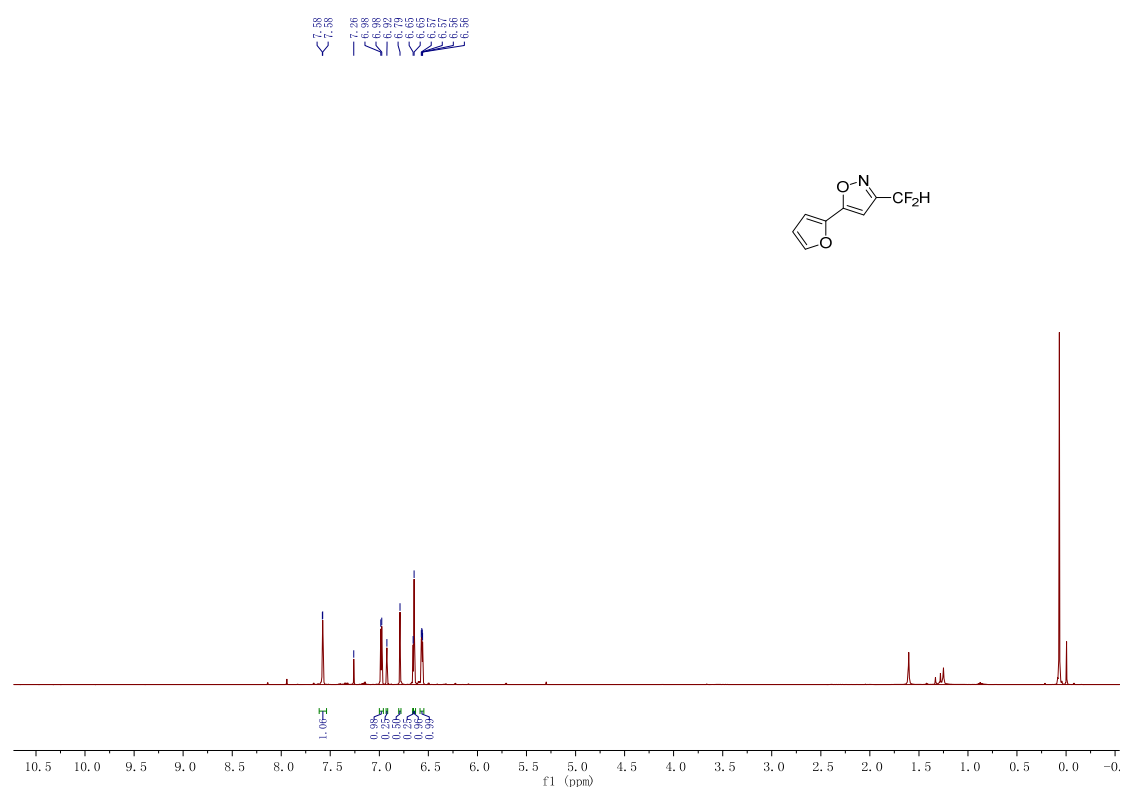
^{19}F NMR (CDCl_3 , 376 MHz) of **5ff**



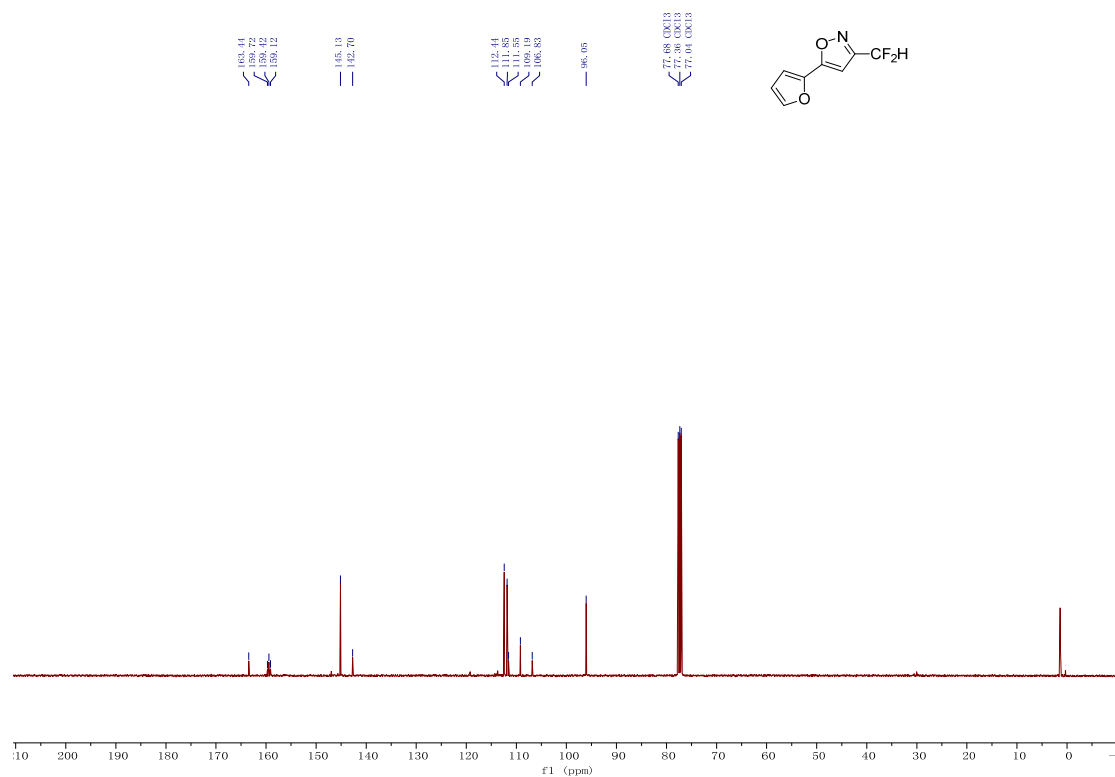
^{19}F { ^1H } NMR (CDCl_3 , 376 MHz) of **5ff**



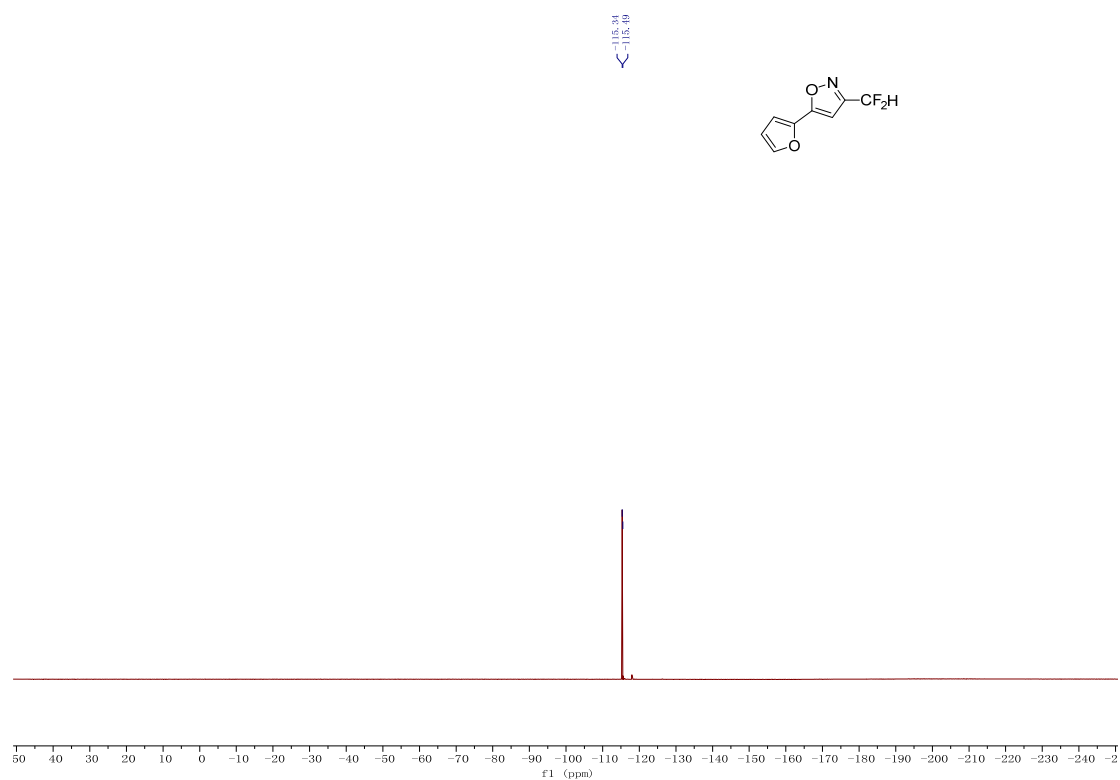
^1H NMR (CDCl₃, 400 MHz) of 5gg



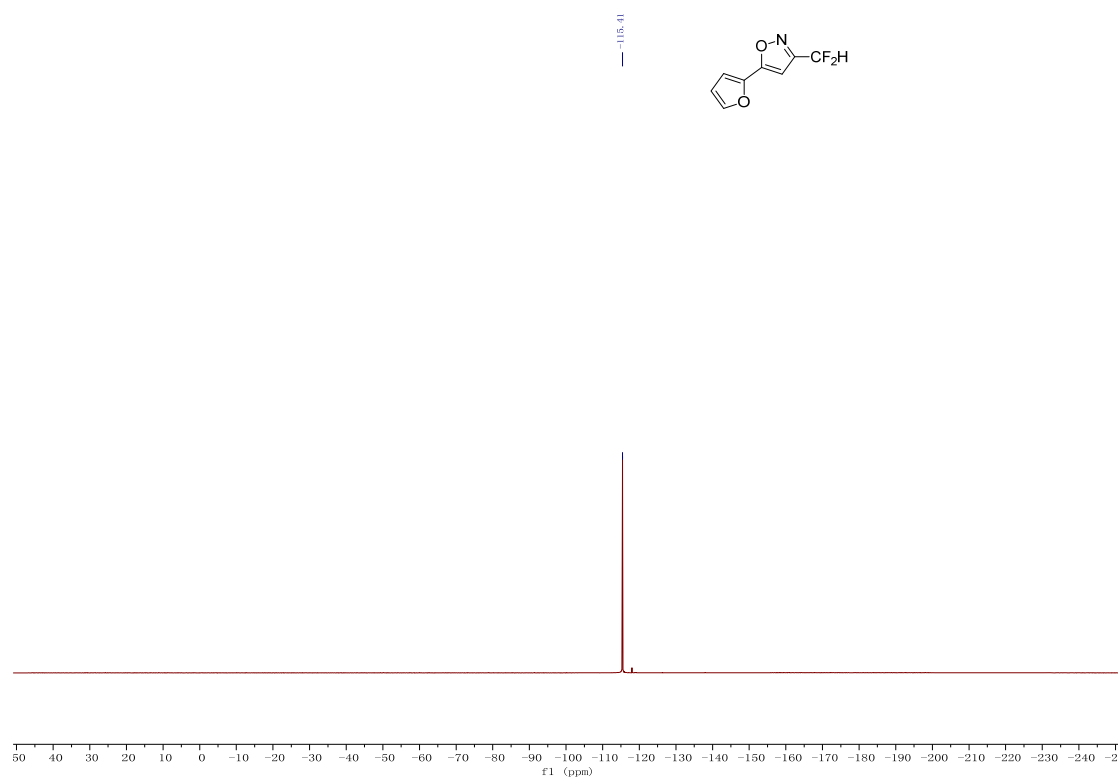
^{13}C NMR (CDCl₃, 100 MHz) of 5gg



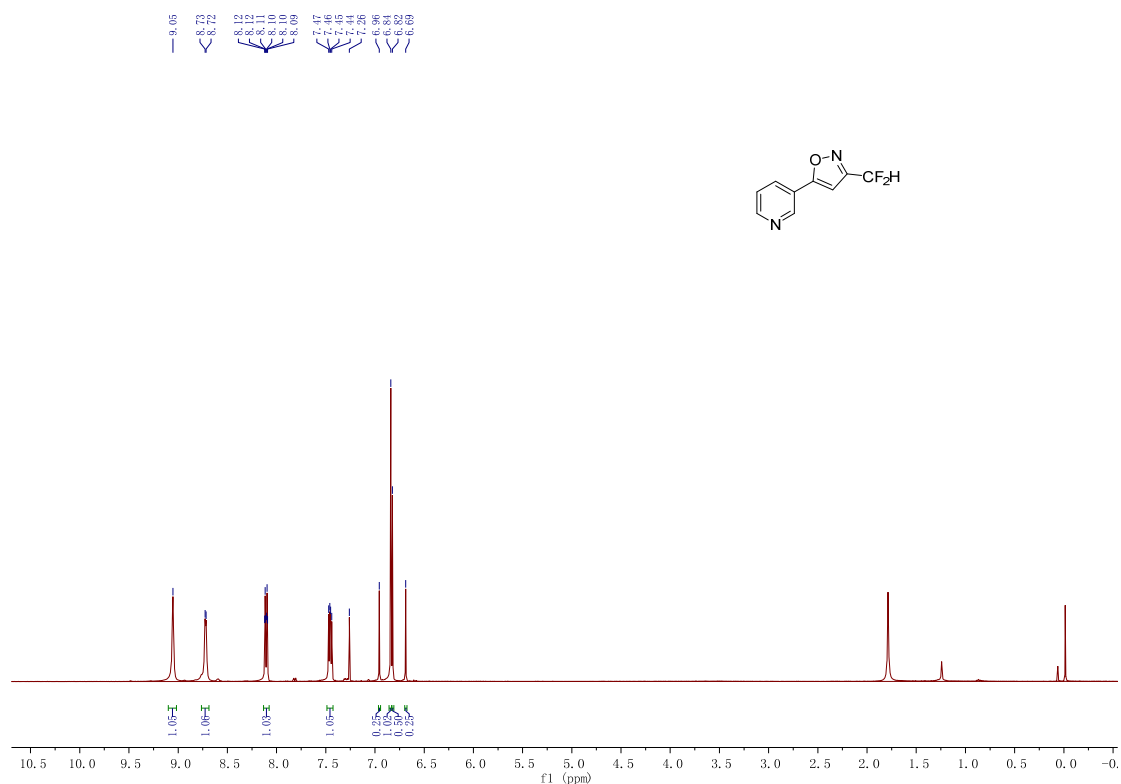
^{19}F NMR (CDCl_3 , 376 MHz) of **5gg**



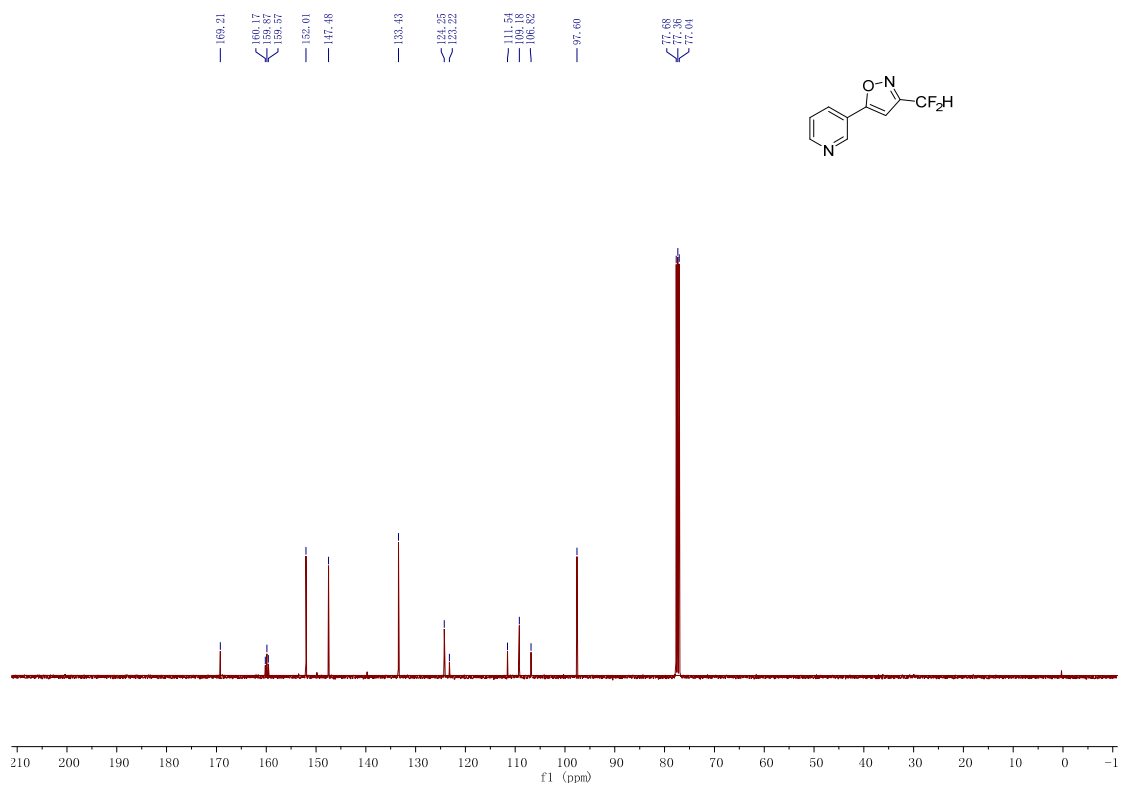
^{19}F $\{^1\text{H}\}$ NMR (CDCl_3 , 376 MHz) of **5gg**



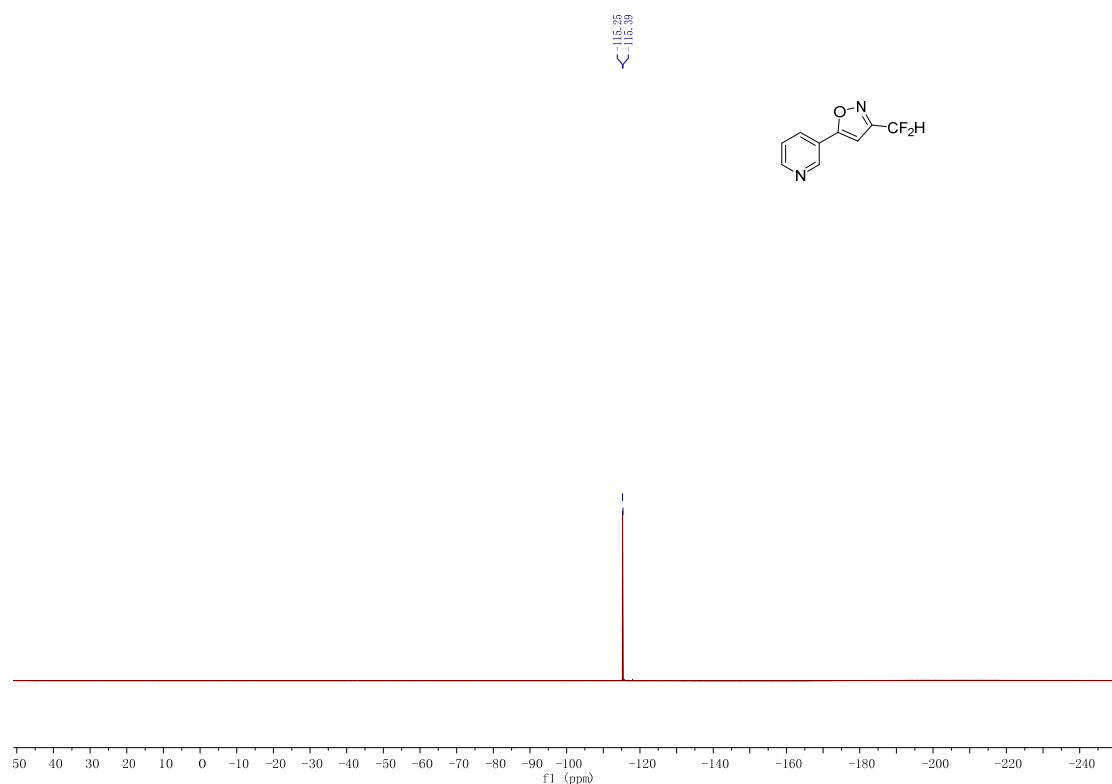
^1H NMR (CDCl₃, 400 MHz) of 5hh



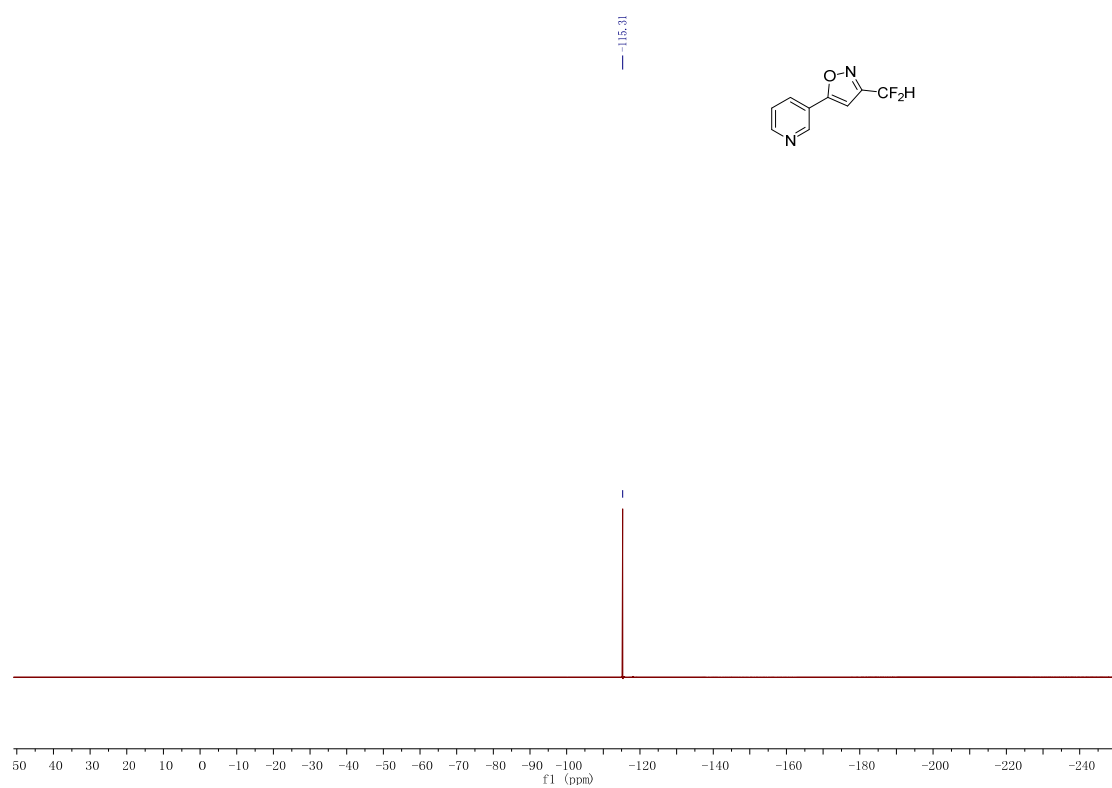
^{13}C NMR (CDCl₃, 100 MHz) of 5hh



^{19}F NMR (CDCl₃, 376 MHz) of **5hh**



^{19}F { ^1H } NMR (CDCl₃, 376 MHz) of **5hh**



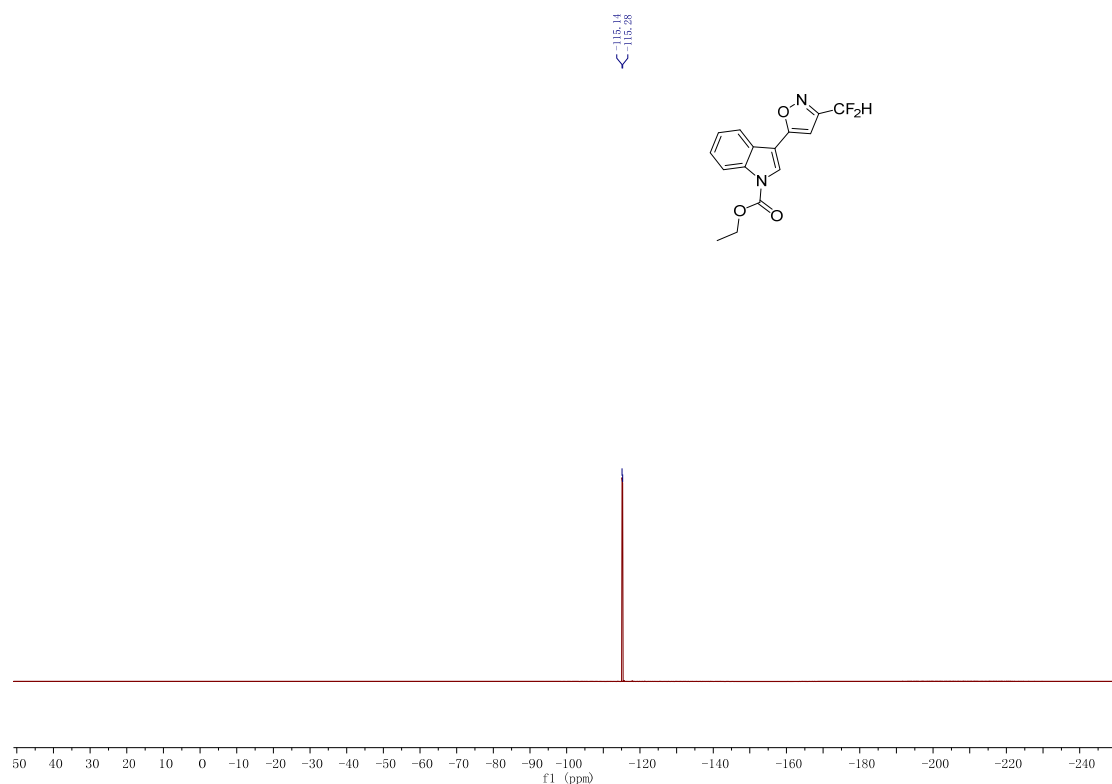
[illegible]

Chemical structure of the compound is shown above the spectrum. The spectrum displays peaks corresponding to the chemical shifts (ppm) listed on the right:

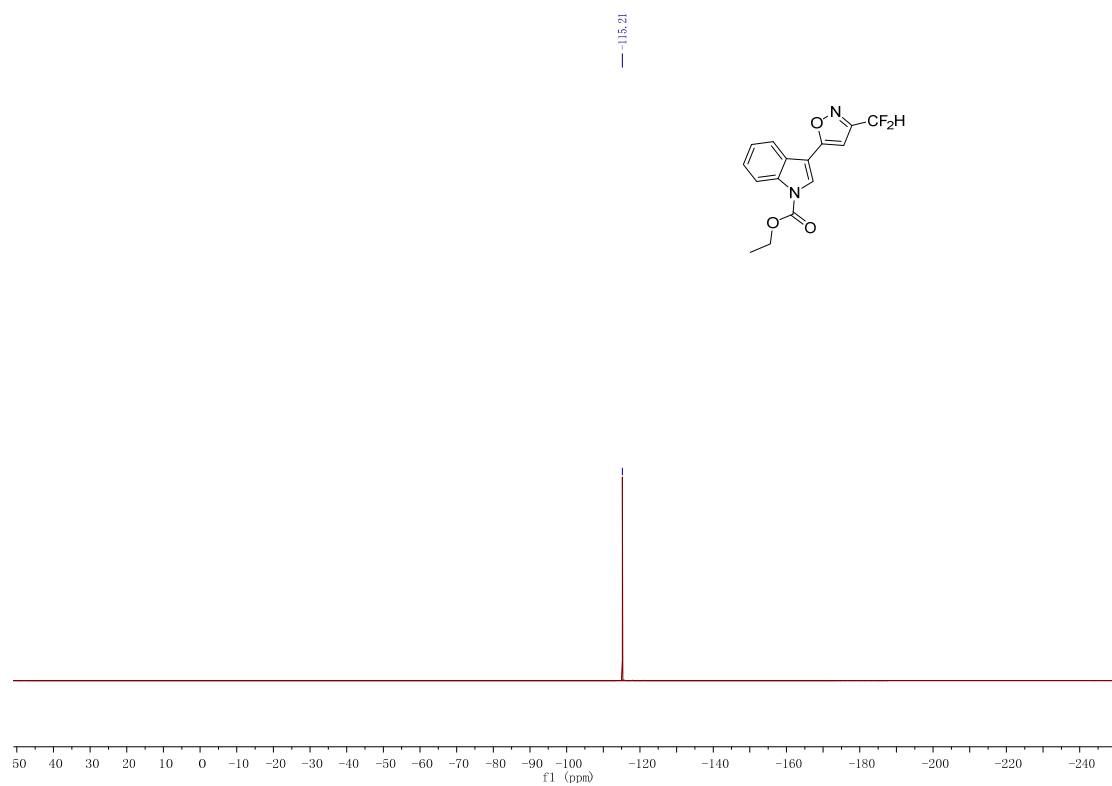
- 166.87
- 159.76
- 159.47
- 159.17
- 150.67
- 135.92
- 126.41
- 126.11
- 124.49
- 120.47
- 115.90
- 115.82
- 109.84
- 109.18
- 107.09
- 98.69
- 77.68
- 77.36
- 77.04
- 64.38
- 14.66

CCOC(=O)n1c(-c2cc(C(F)(F)F)nn2)c3ccccc31

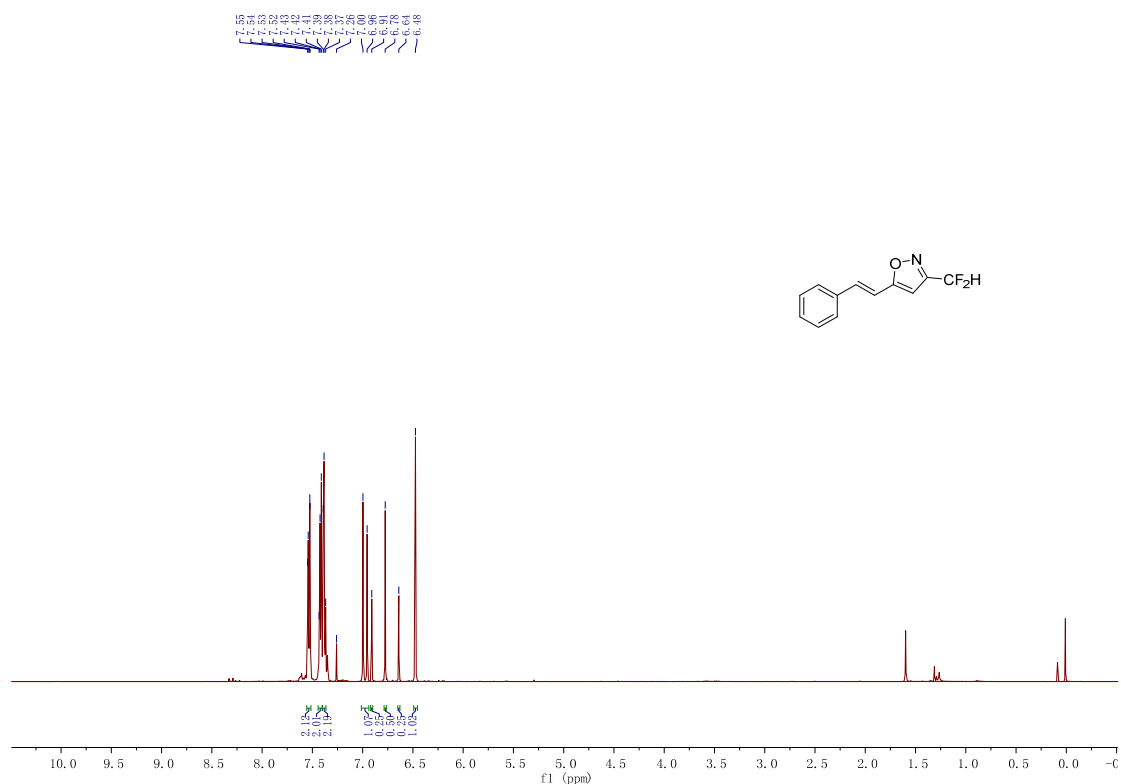
^{19}F NMR (CDCl₃, 376 MHz) of **5ii**



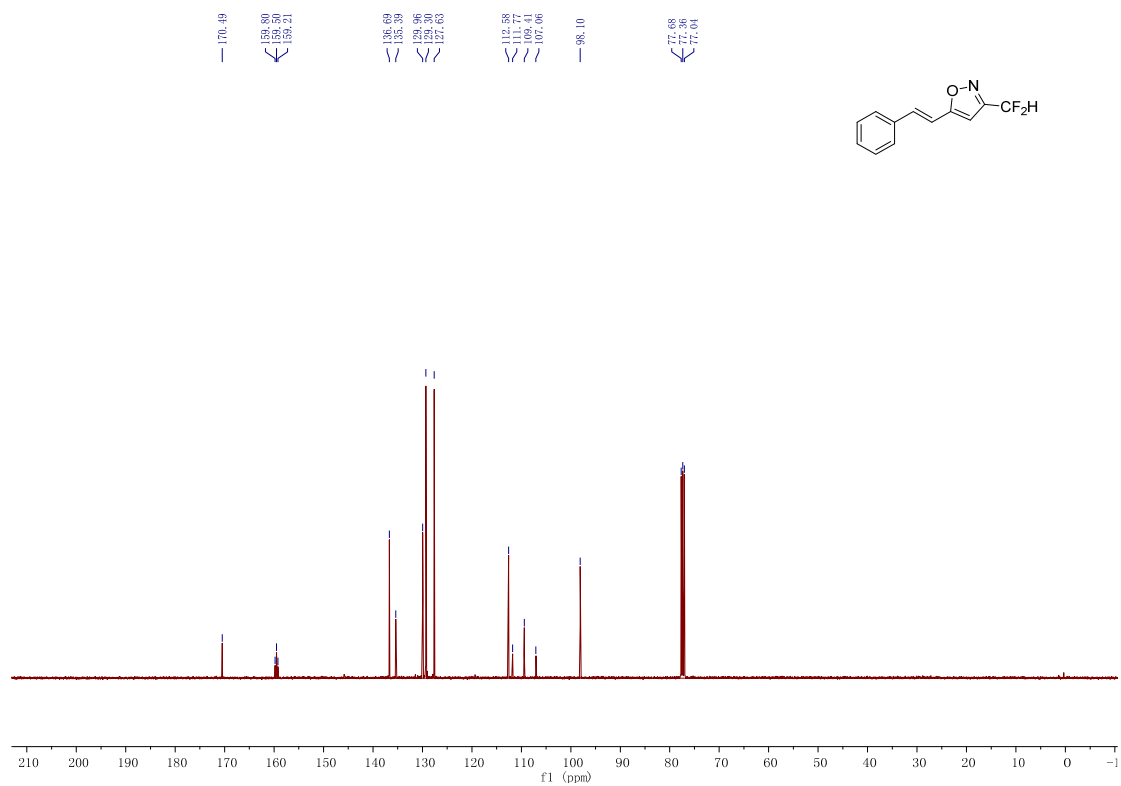
^{19}F { ^1H } NMR (CDCl₃, 376 MHz) of **5ii**



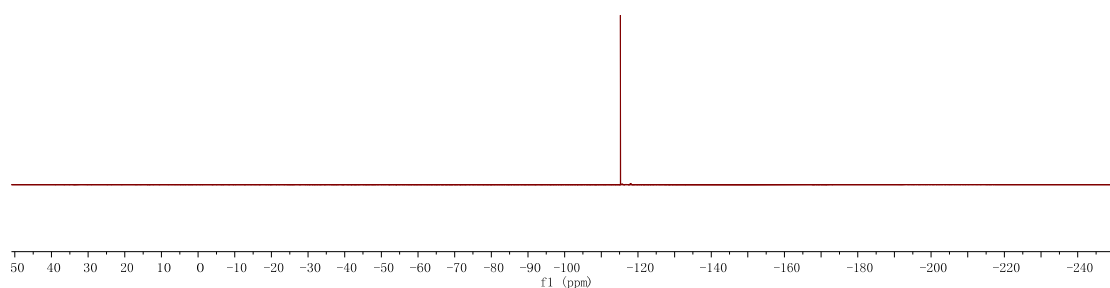
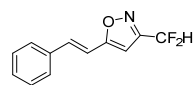
¹H NMR (CDCl₃, 400 MHz) of 5jj



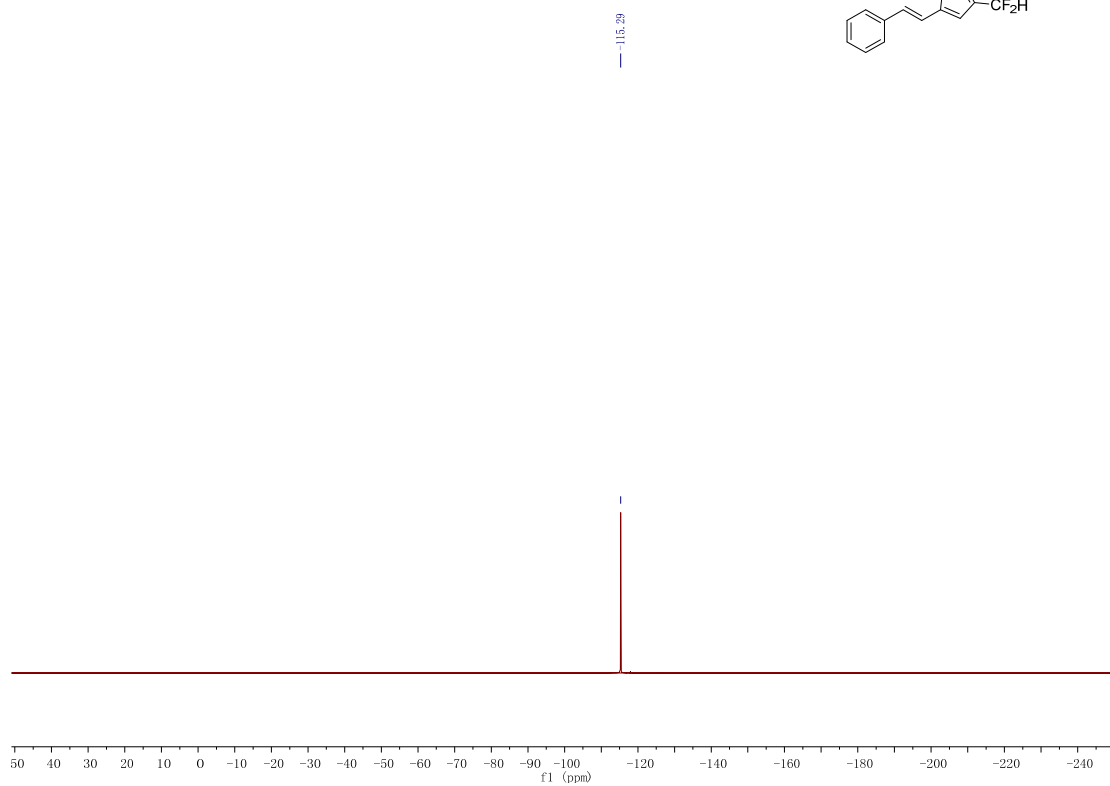
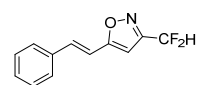
¹³C NMR (CDCl₃, 100 MHz) of 5jj



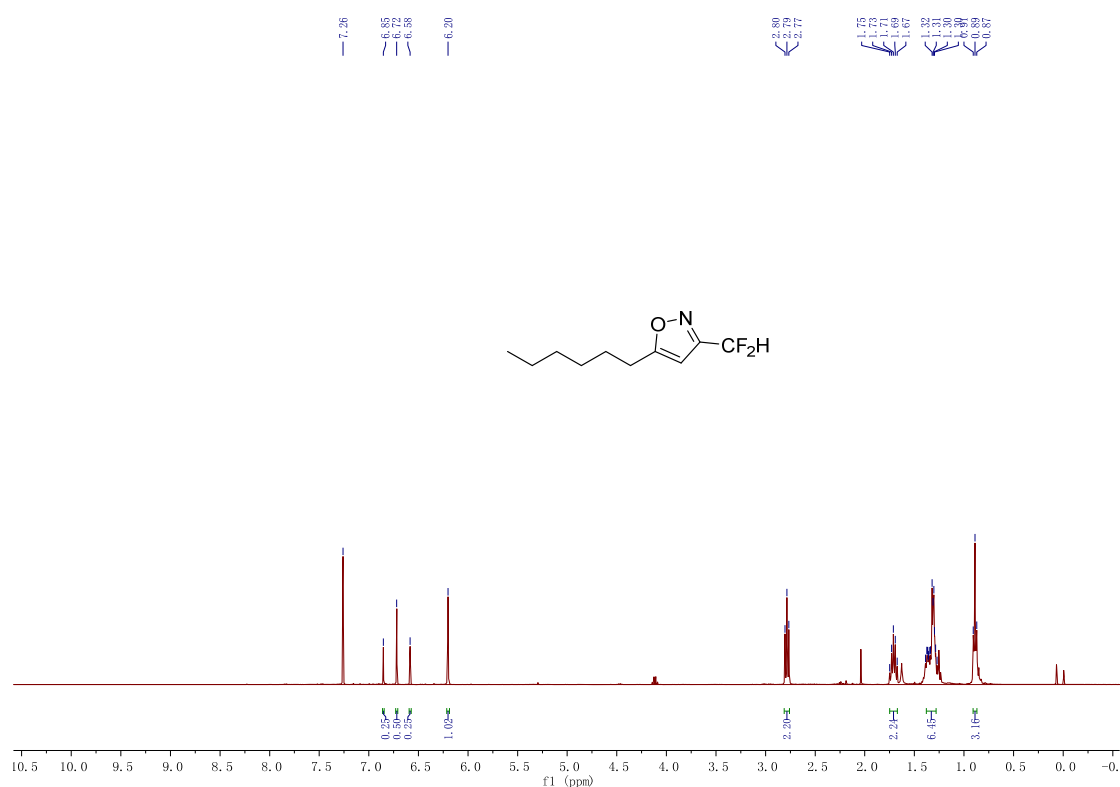
^{19}F NMR (CDCl_3 , 376 MHz) of **5jj**



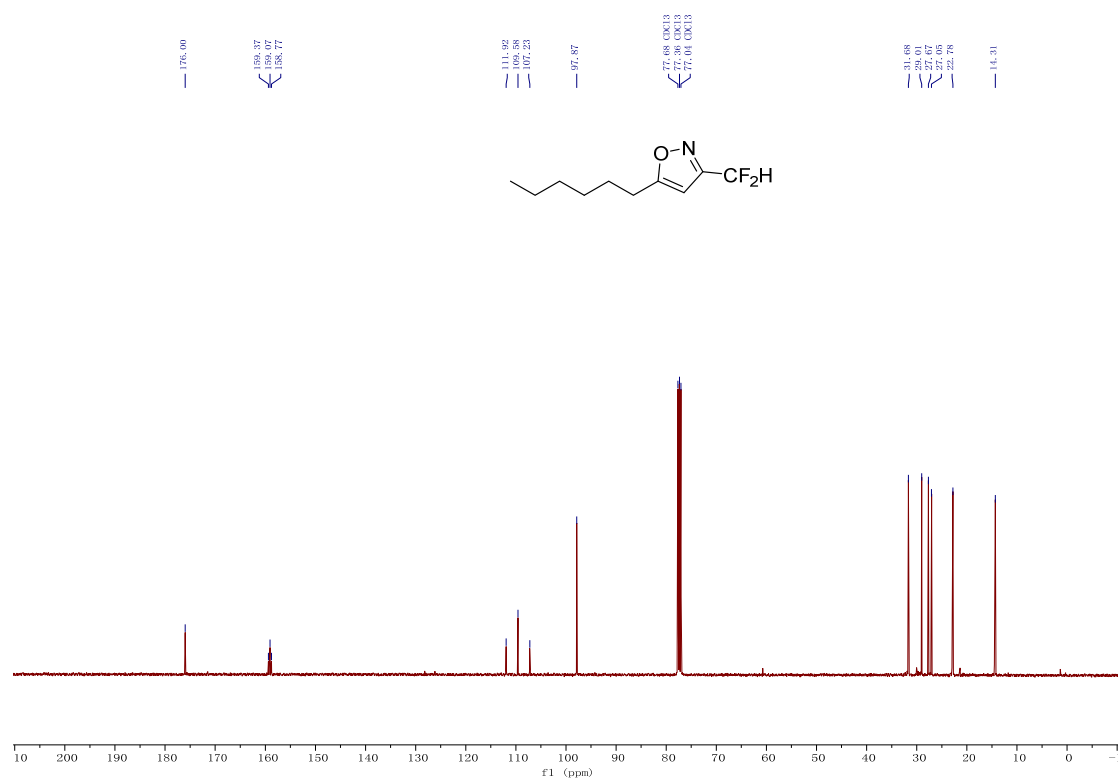
^{19}F { ^1H } NMR (CDCl_3 , 376 MHz) of **5jj**



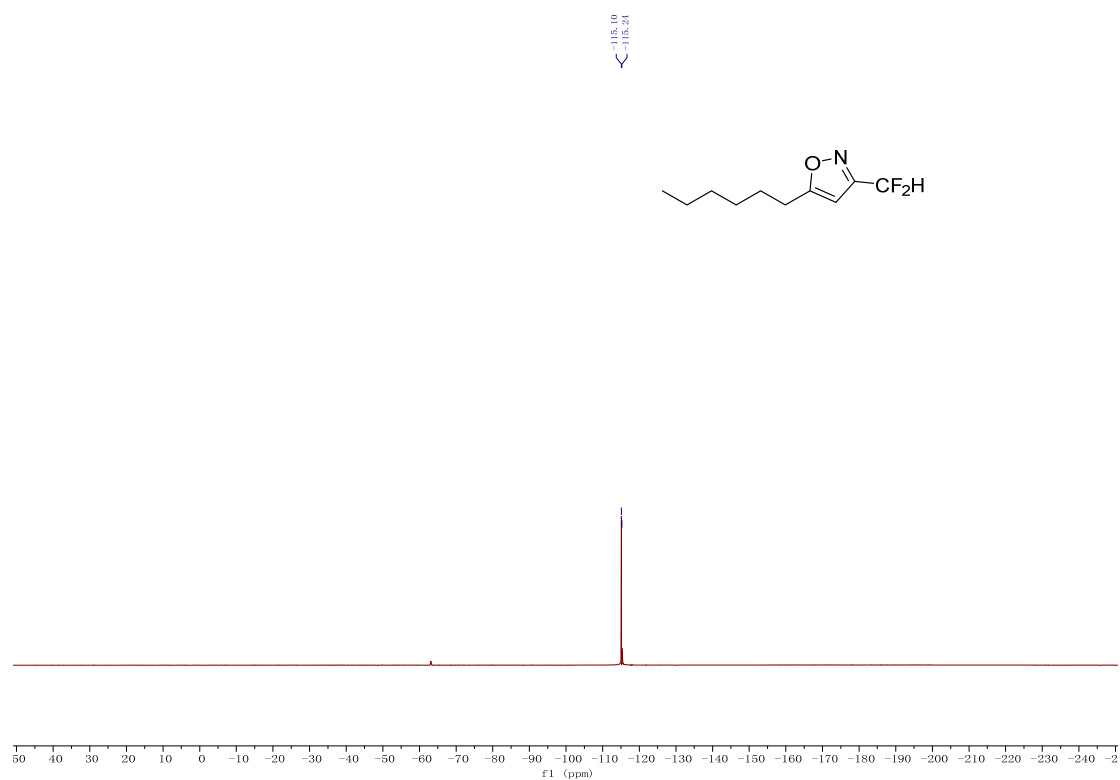
^1H NMR (CDCl₃, 400 MHz) of **5kk**



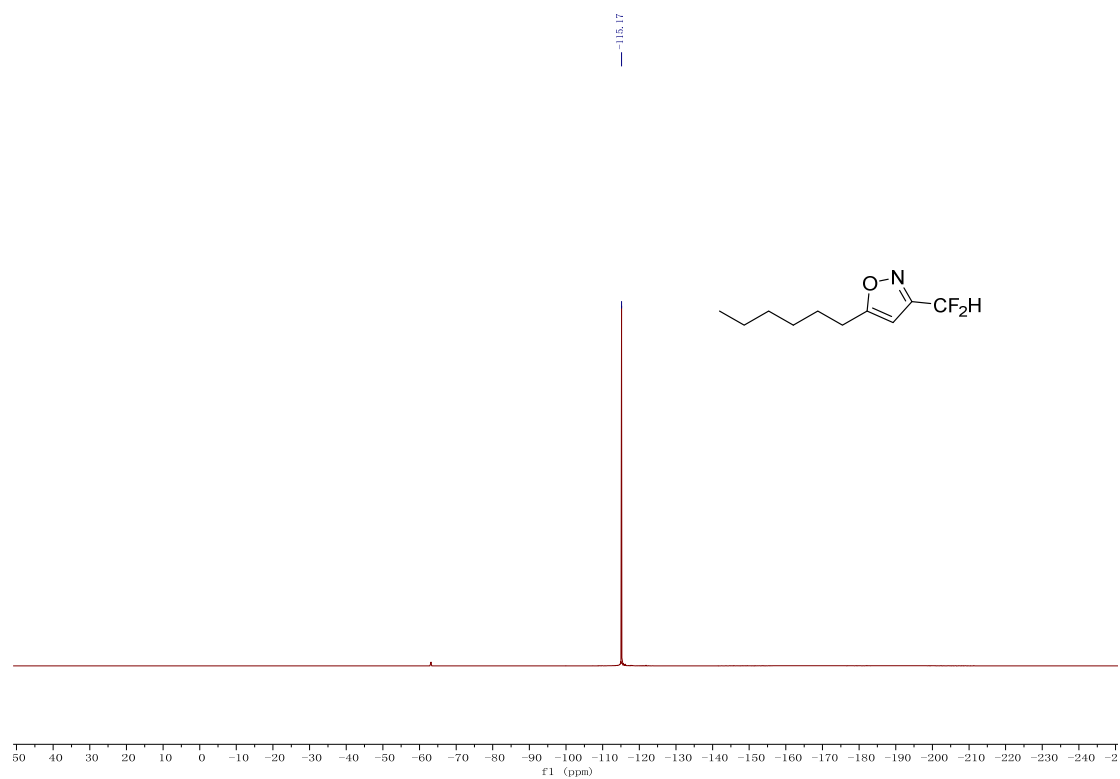
^{13}C NMR (CDCl₃, 100 MHz) of **5kk**



^{19}F NMR (CDCl_3 , 376 MHz) of **5kk**



^{19}F $\{^1\text{H}\}$ NMR (CDCl_3 , 376 MHz) of **5kk**

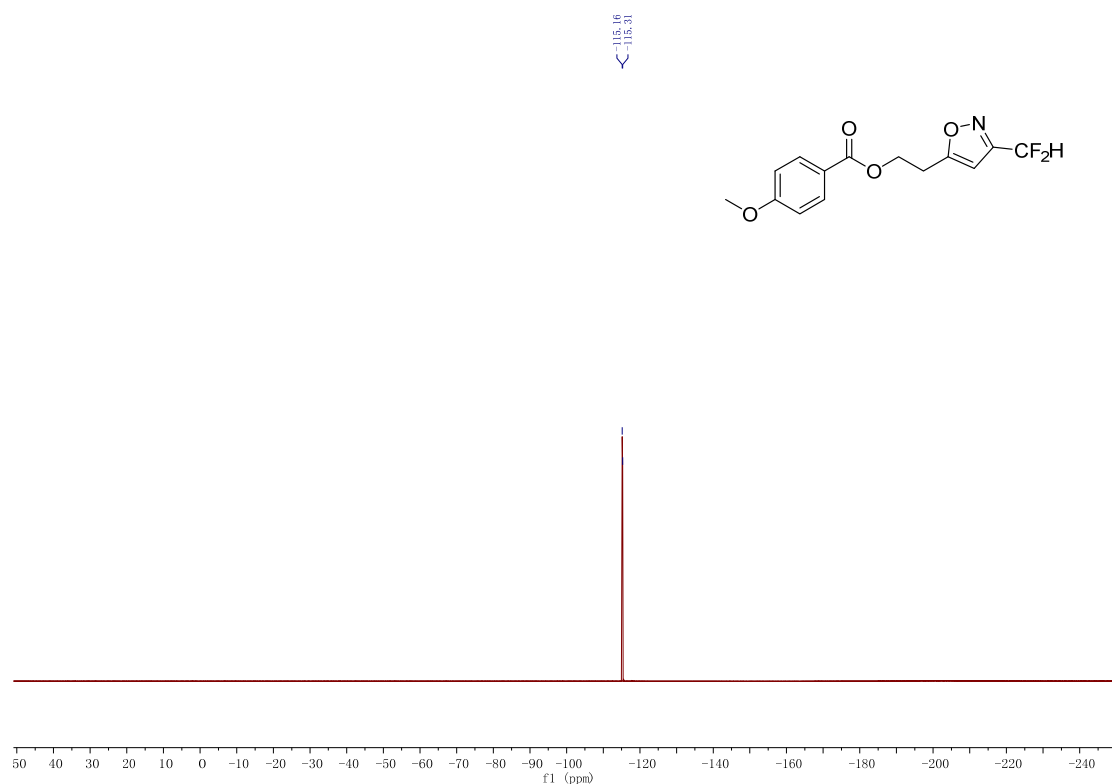


Chemical structure of 4-methoxybenzoic acid 2-(2-(difluoromethyl)-2H-isoxazol-3-yl)ethyl ester:

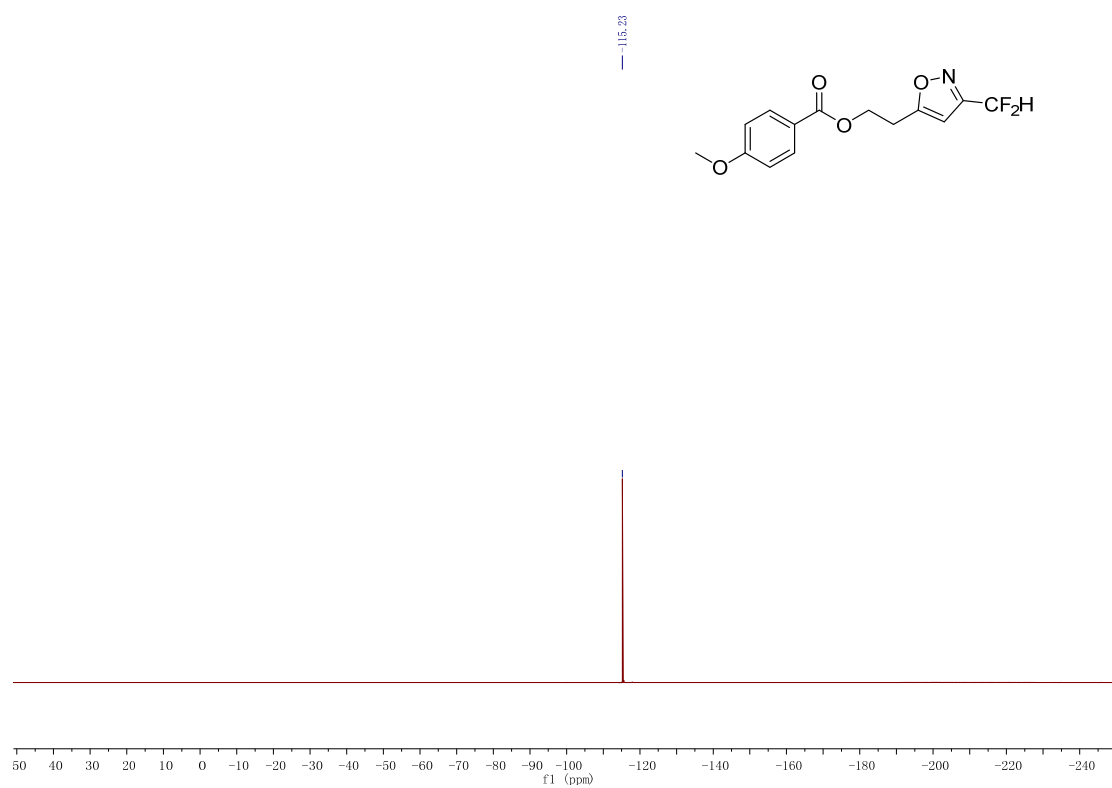
COc1ccc(cc1)C(=O)OCCc2cc(C(F)F)n2

¹H NMR spectrum (CDCl₃) showing peaks from 0.0 to 10.0 ppm. The spectrum includes a broad singlet at ~7.8 ppm (1H, COOH), aromatic signals between 6.5-7.5 ppm (4H), a singlet at ~3.8 ppm (3H, OCH₃), and a singlet at ~3.3 ppm (2H, CH₂). Integration values are provided below the peaks.

^{19}F NMR (CDCl₃, 376 MHz) of **5II**

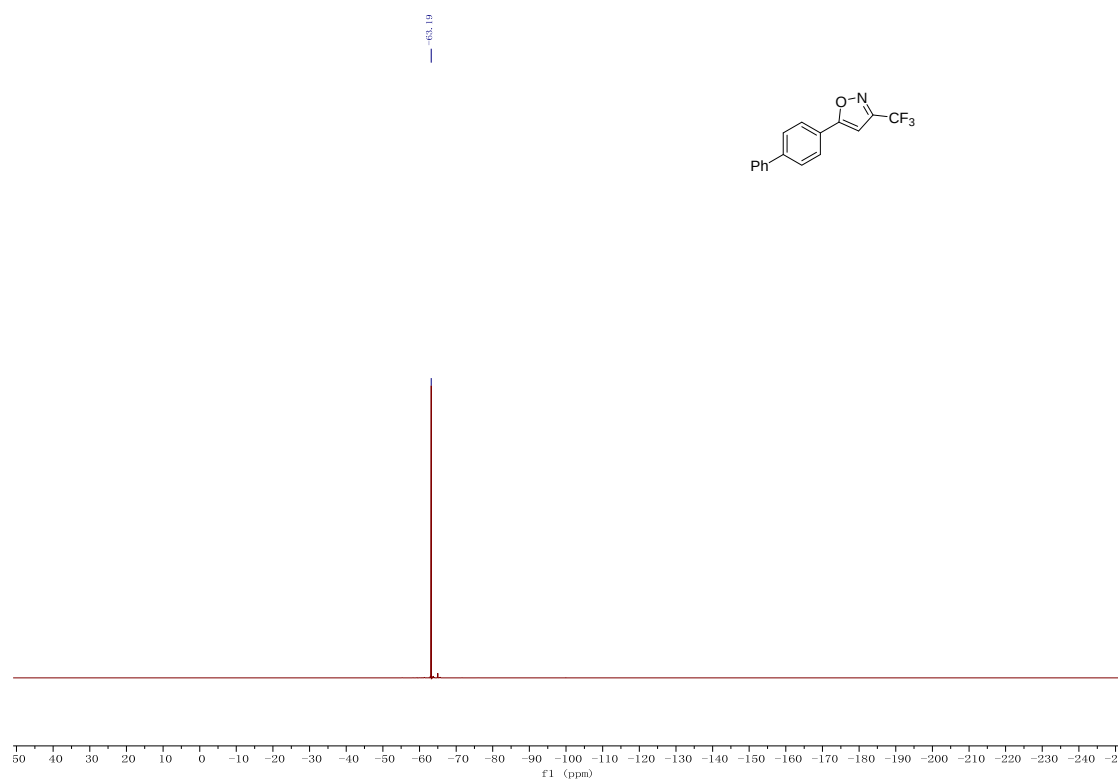


^{19}F { ^1H } NMR (CDCl₃, 376 MHz) of **5II**

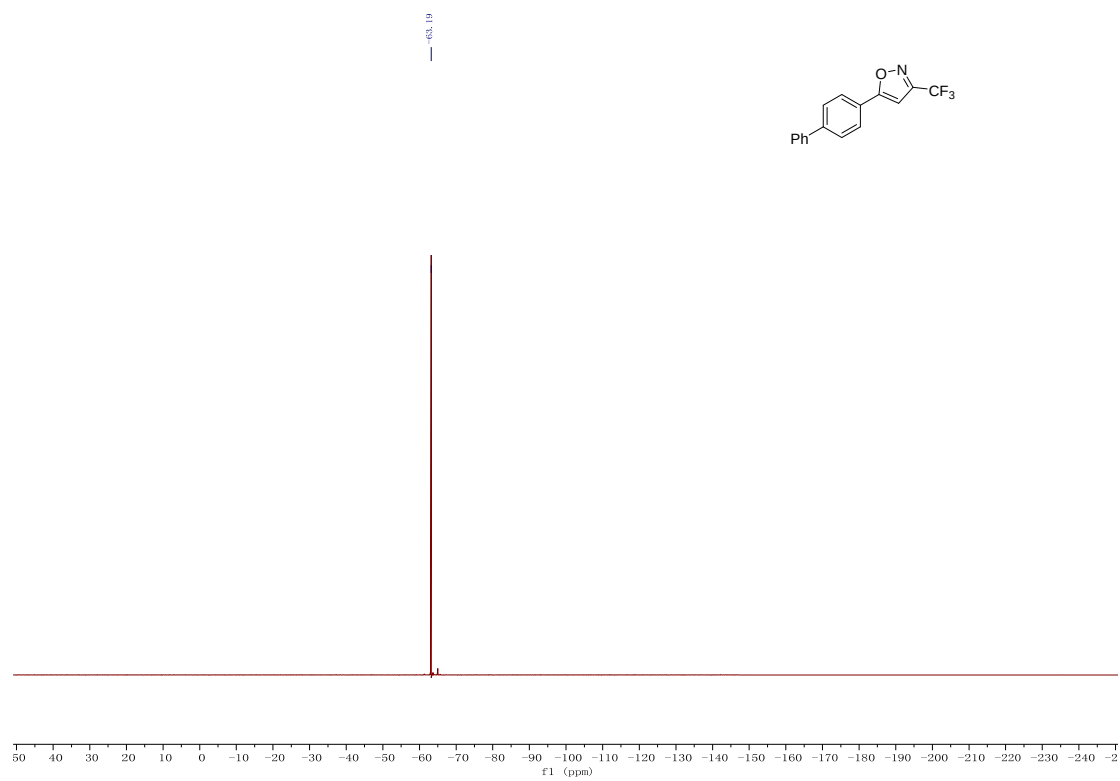


[illegible][illegible]

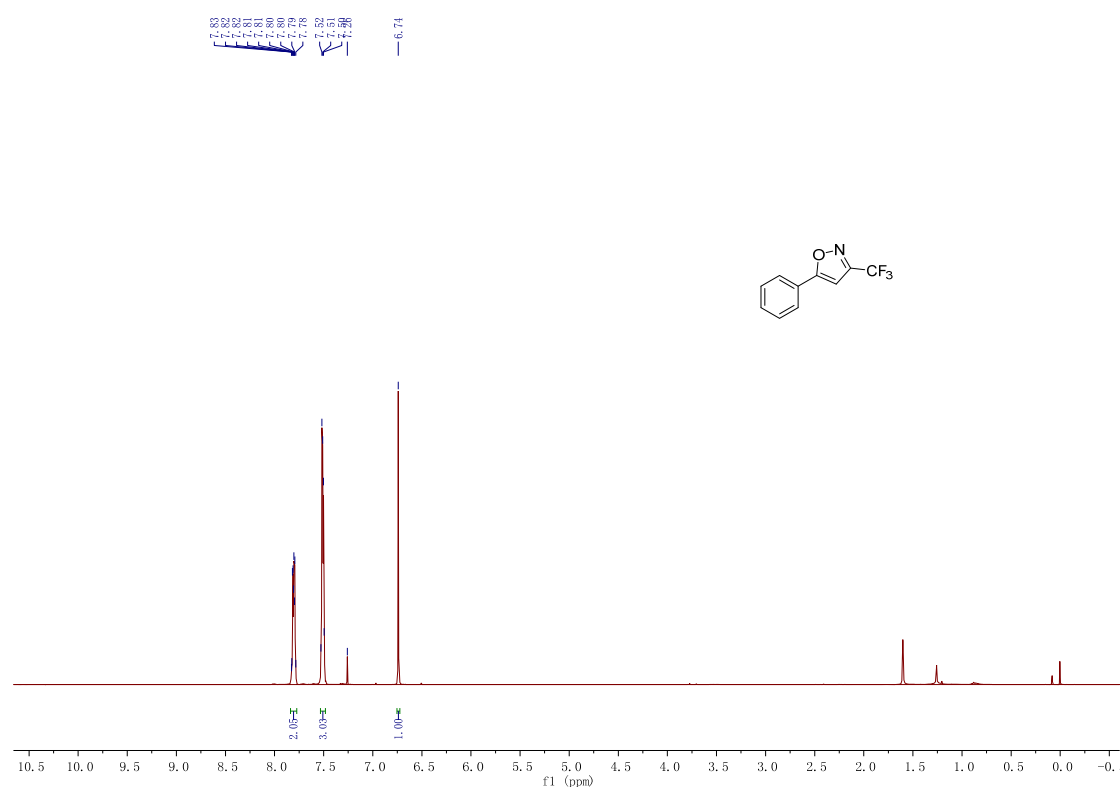
^{19}F NMR (CDCl_3 , 376 MHz) of **9a**



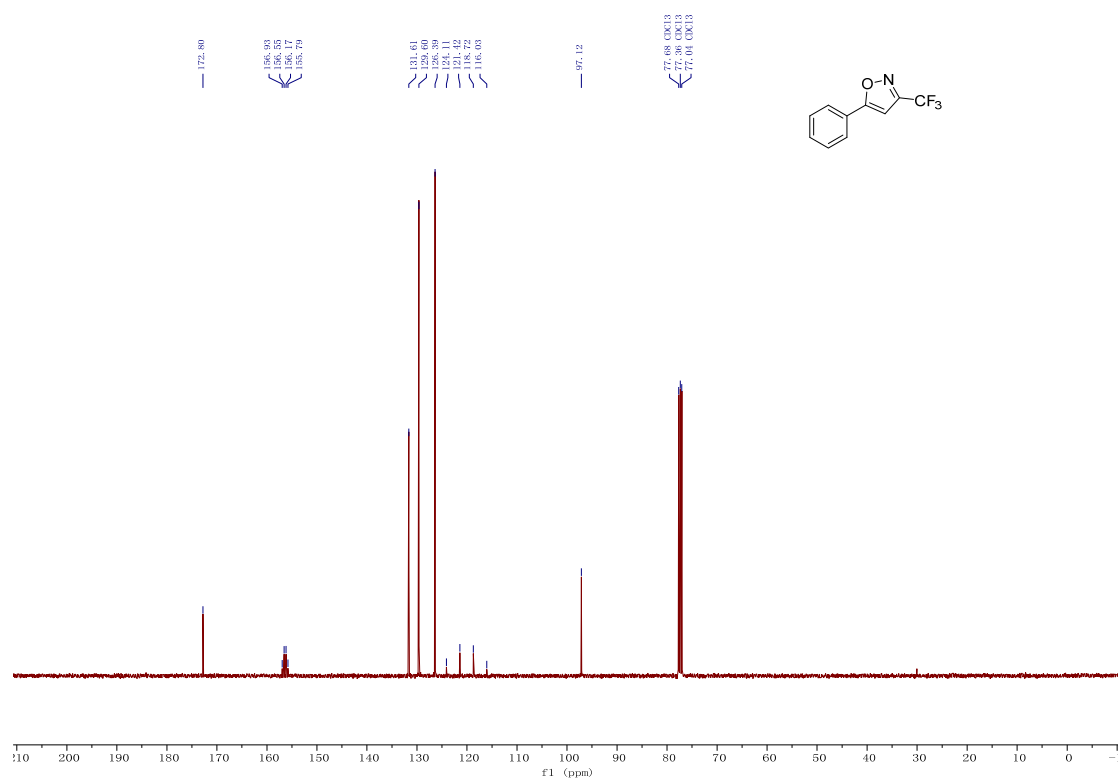
^{19}F $\{^1\text{H}\}$ NMR (CDCl_3 , 376 MHz) of **9a**



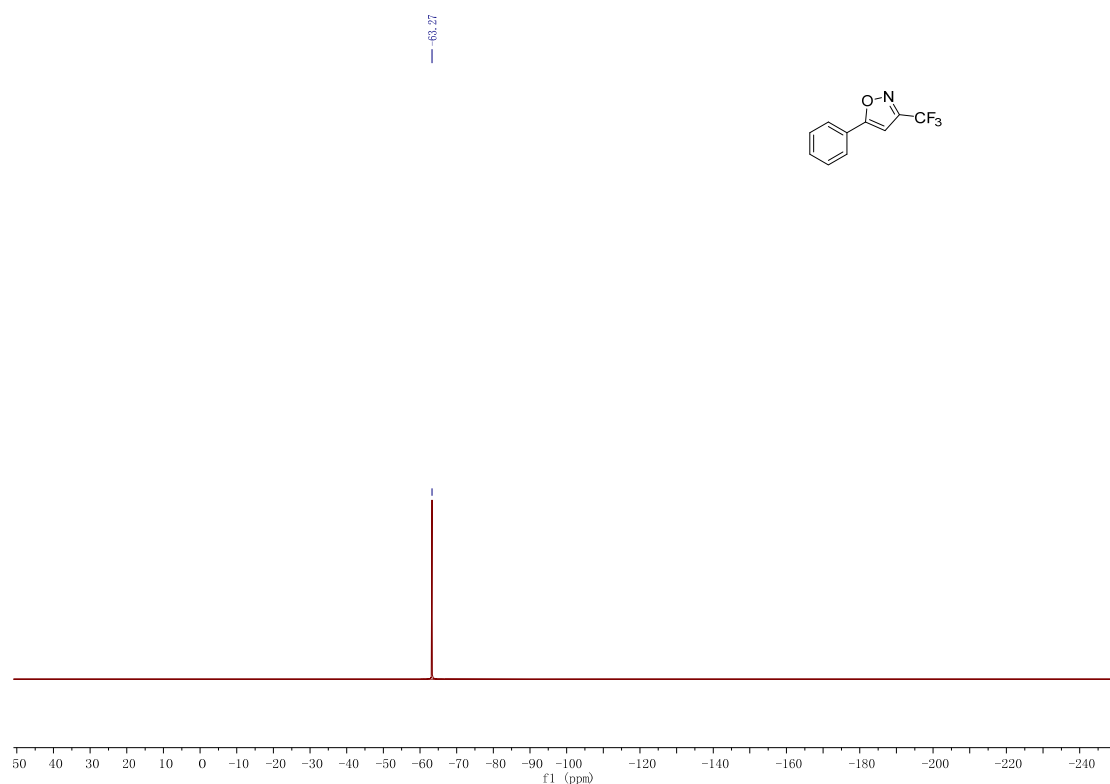
^1H NMR (CDCl₃, 400 MHz) of **9b**



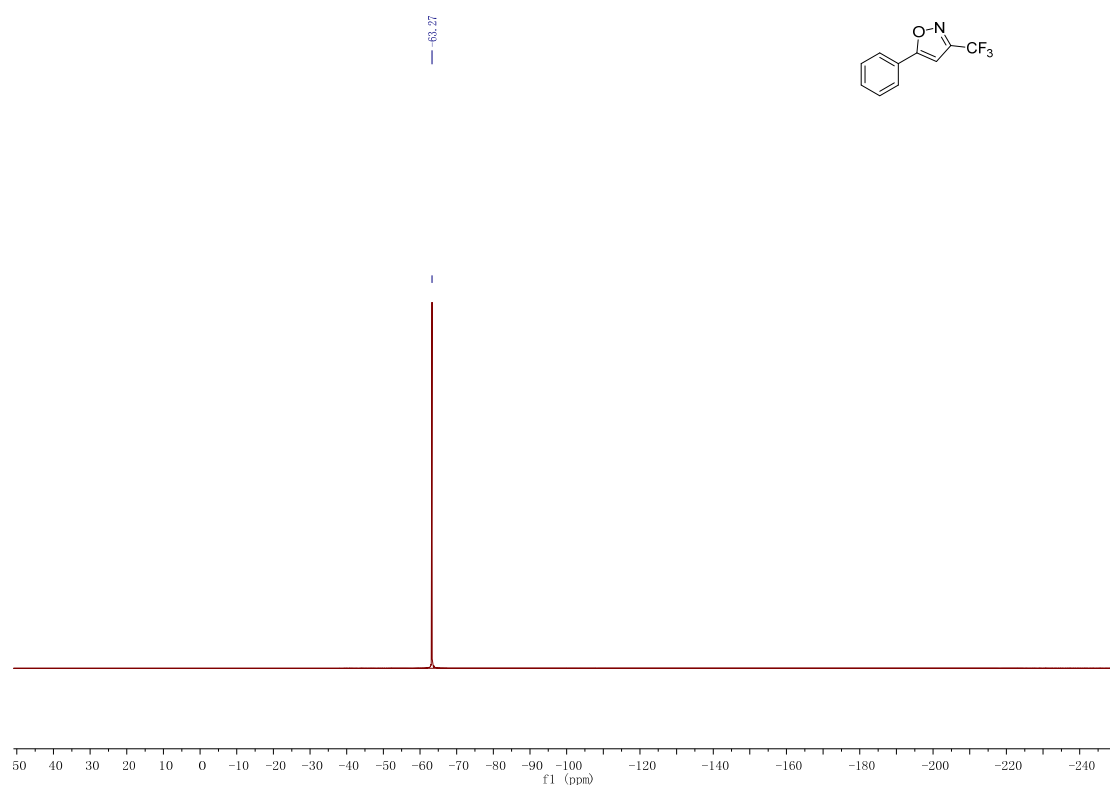
^{13}C NMR (CDCl₃, 100 MHz) of **9b**



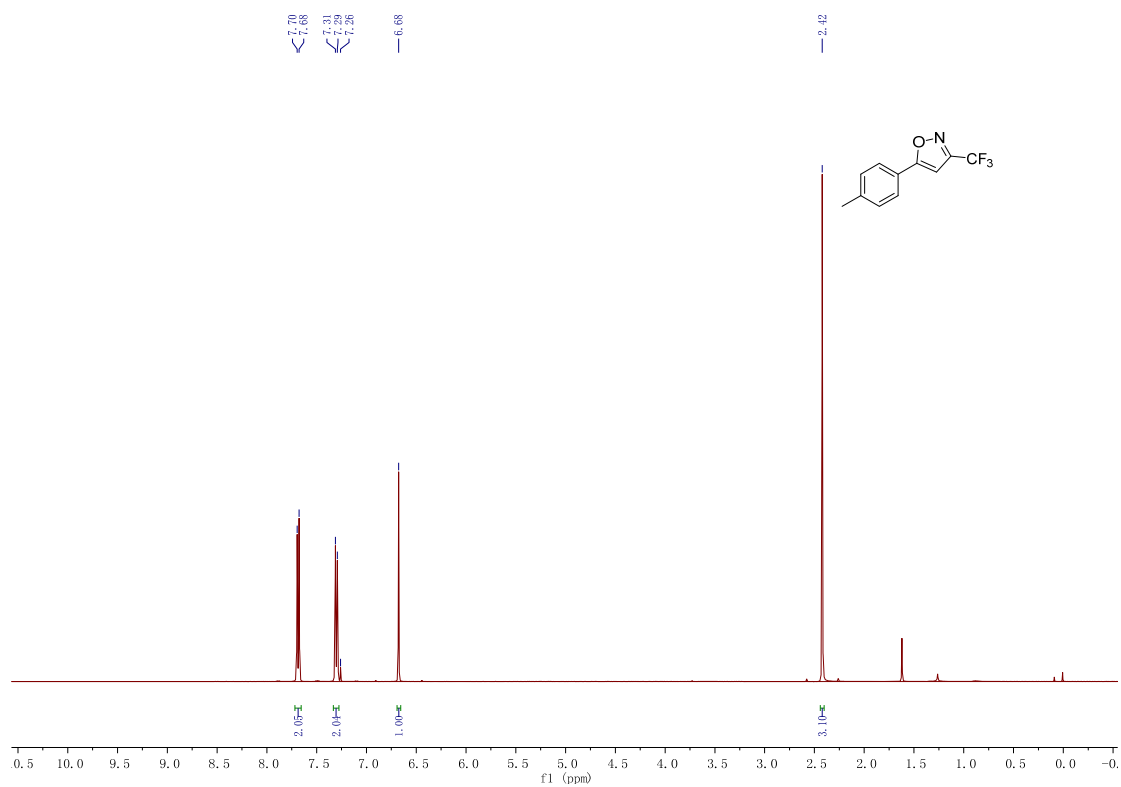
^{19}F NMR (CDCl₃, 376 MHz) of **9b**



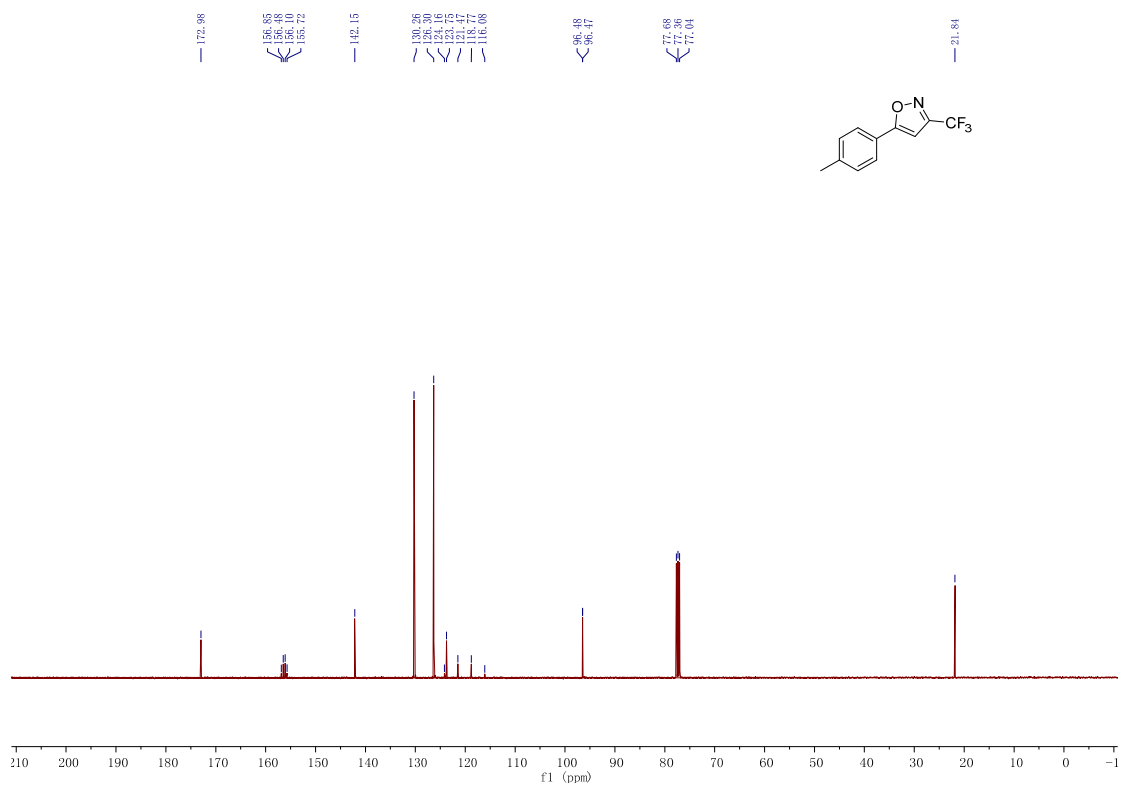
^{19}F { ^1H } NMR (CDCl₃, 376 MHz) of **9b**



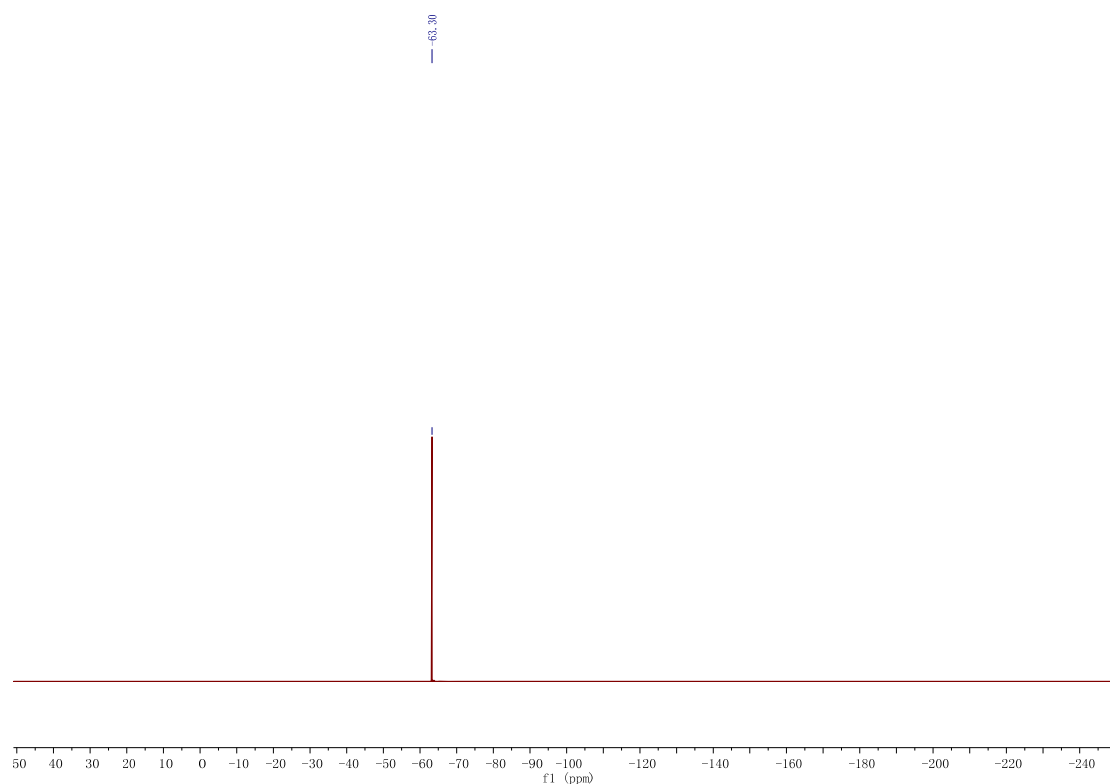
^1H NMR (CDCl₃, 400 MHz) of **9c**



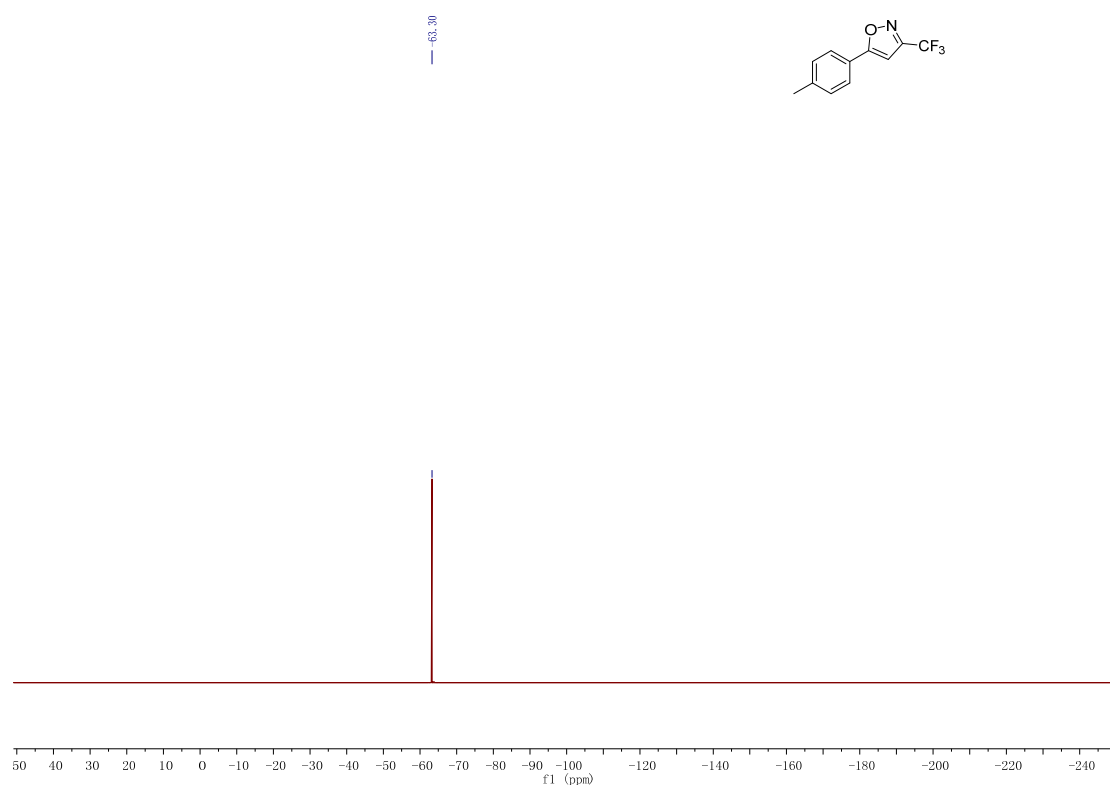
^{13}C NMR (CDCl₃, 100 MHz) of **9c**



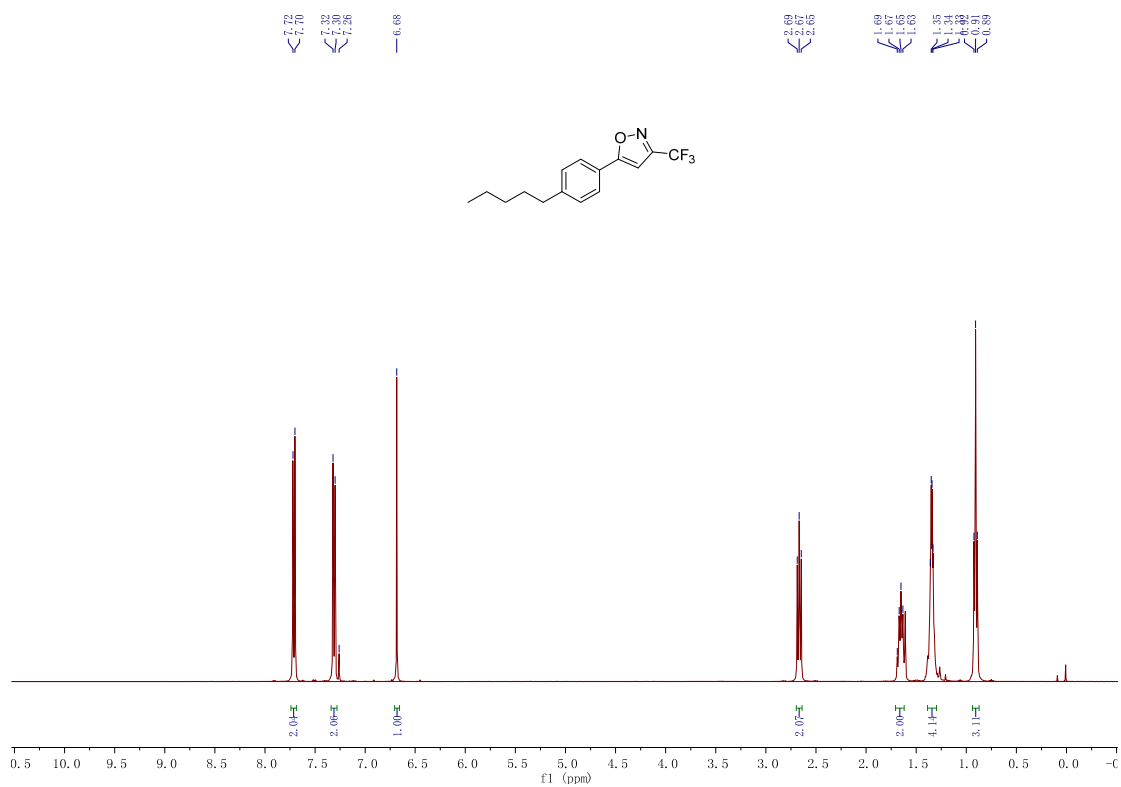
^{19}F NMR (CDCl_3 , 376 MHz) of **9c**



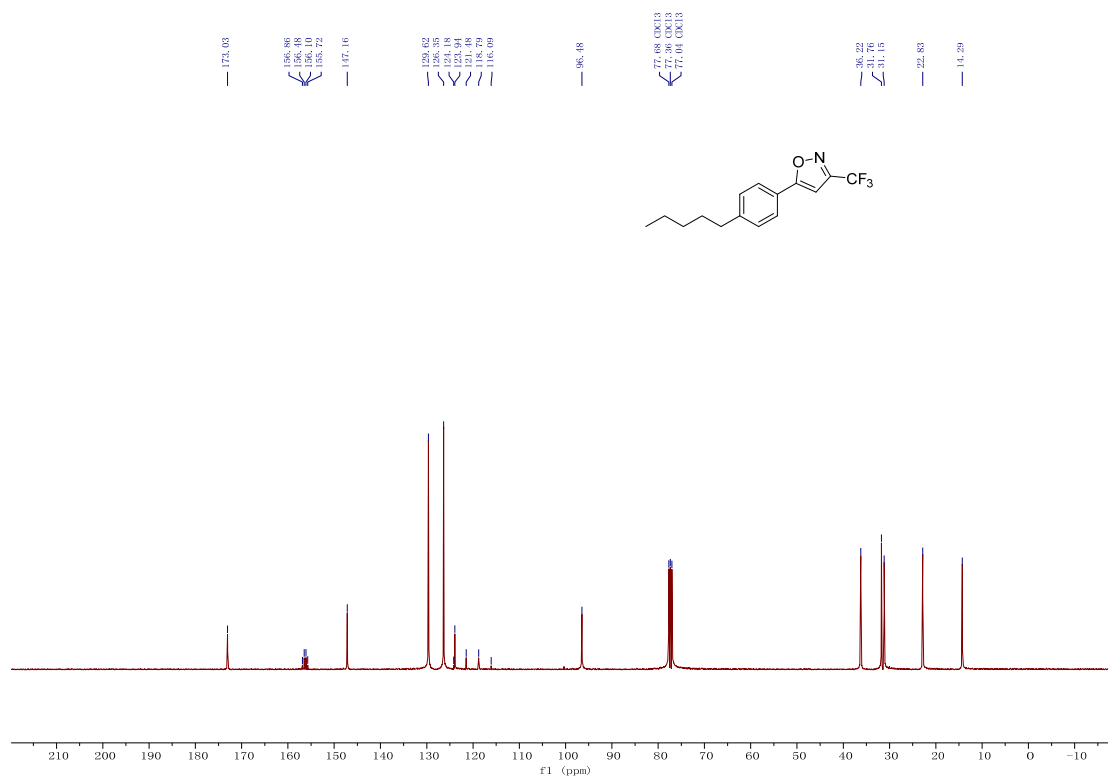
^{19}F { ^1H } NMR (CDCl_3 , 376 MHz) of **9c**



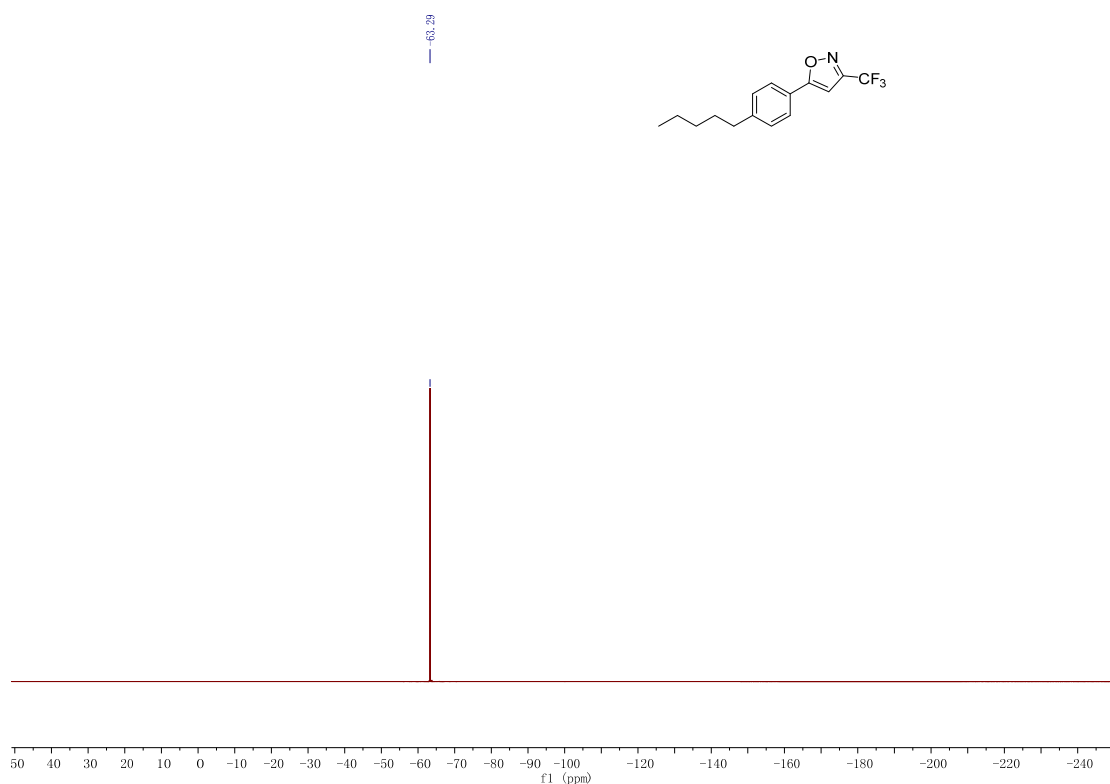
^1H NMR (CDCl₃, 400 MHz) of **9d**



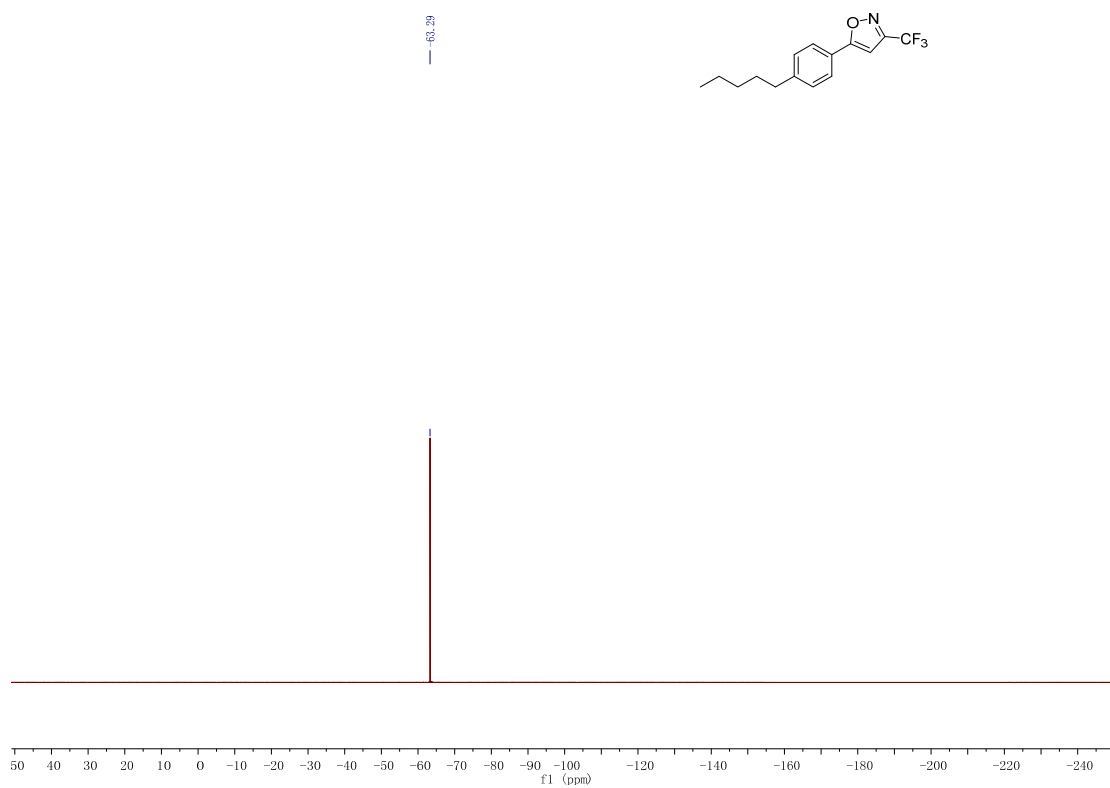
^{13}C NMR (CDCl₃, 100 MHz) of **9d**



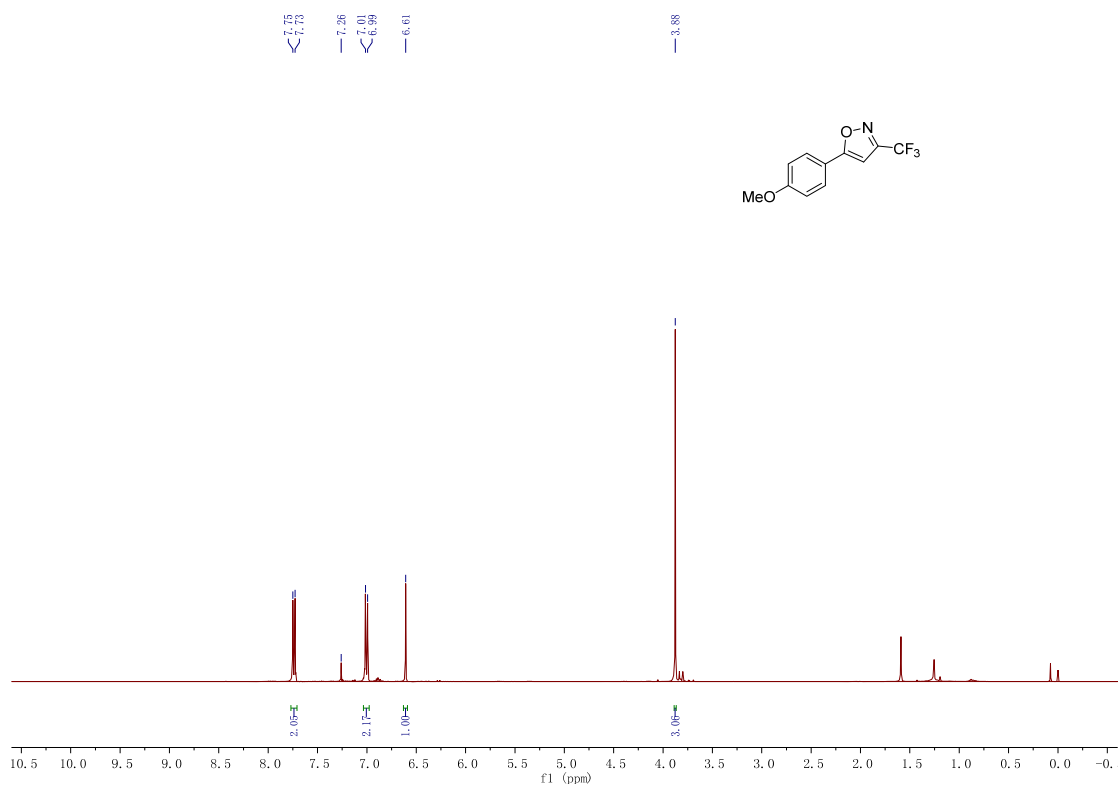
^{19}F NMR (CDCl₃, 376 MHz) of **9d**



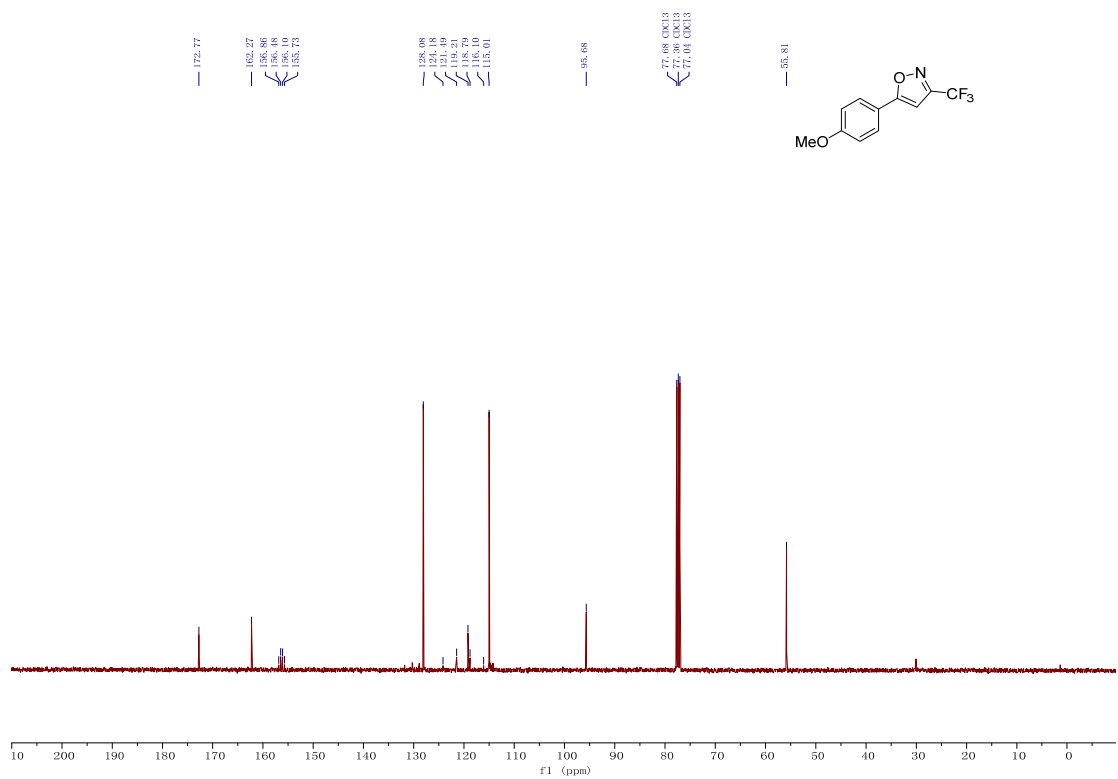
^{19}F { ^1H } NMR (CDCl₃, 376 MHz) of **9d**



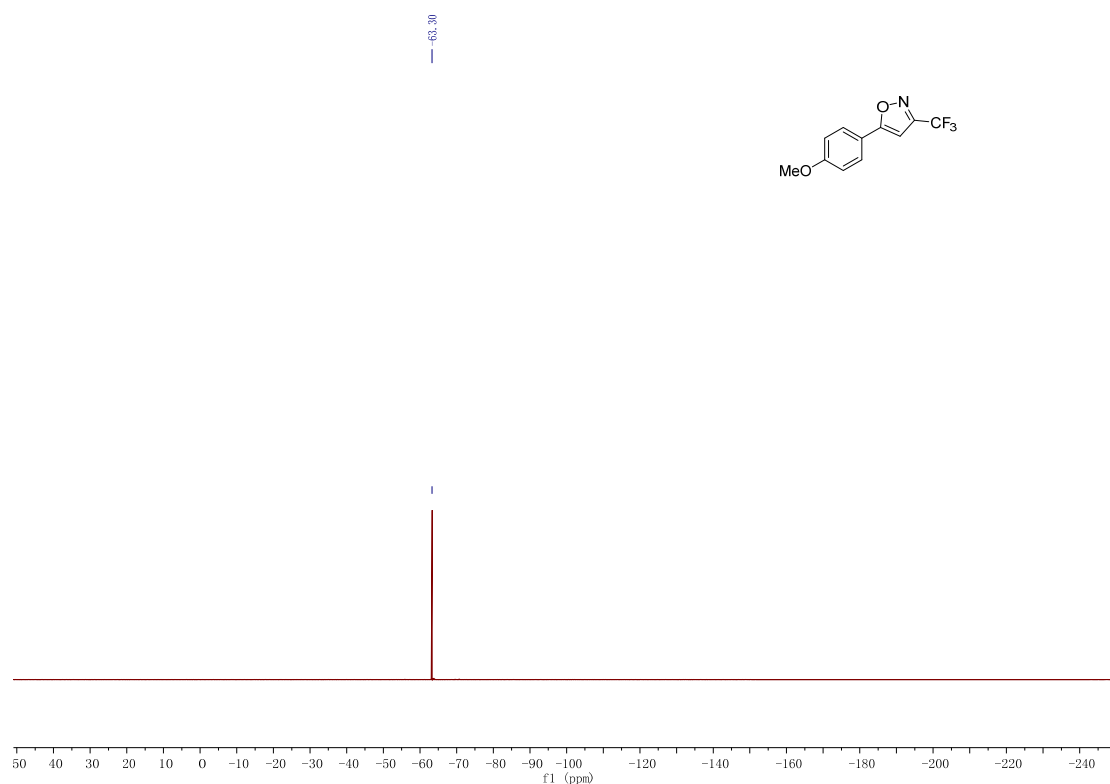
^1H NMR (CDCl₃, 400 MHz) of **9e**



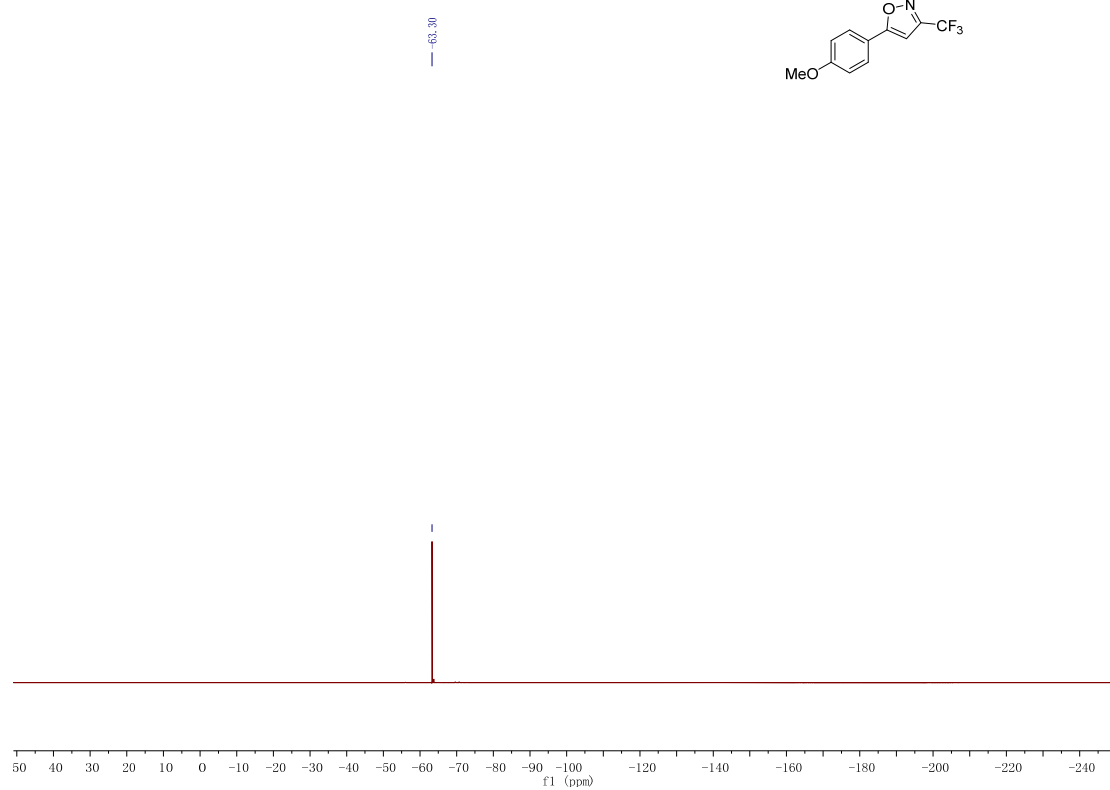
^{13}C NMR (CDCl₃, 100 MHz) of **9e**



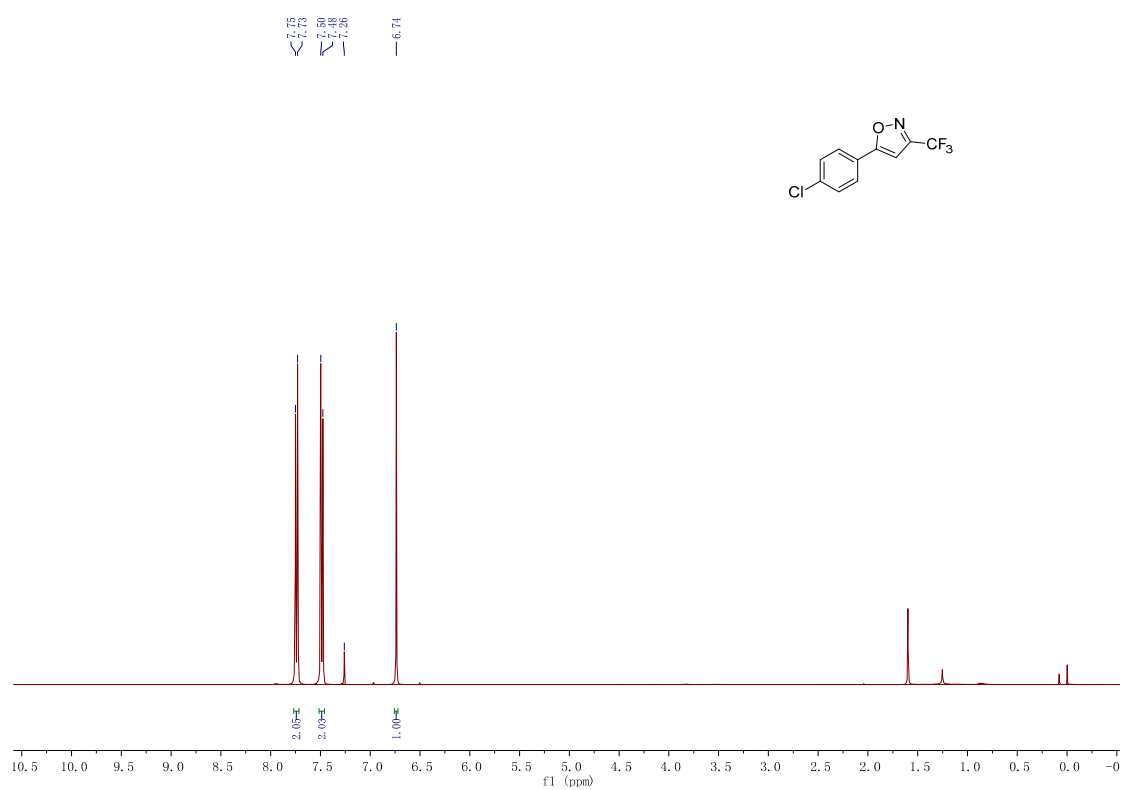
^{19}F NMR (CDCl₃, 376 MHz) of **9e**



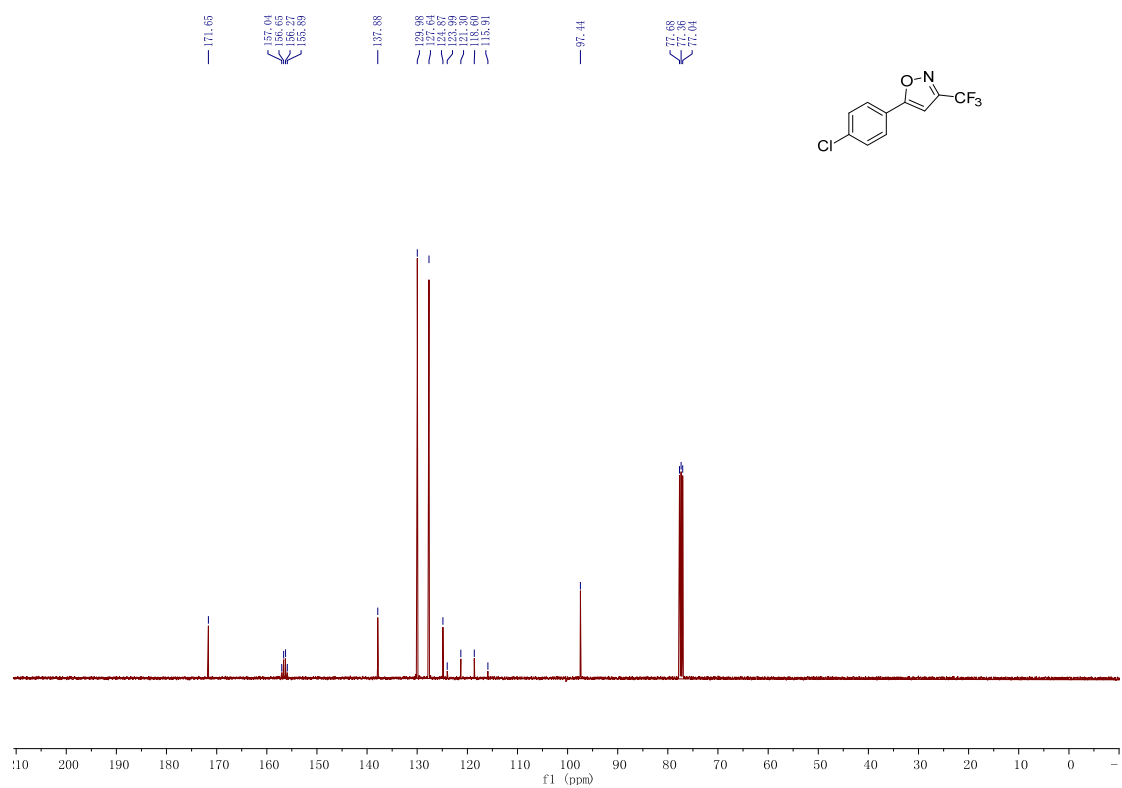
^{19}F { ^1H } NMR (CDCl₃, 376 MHz) of **9e**



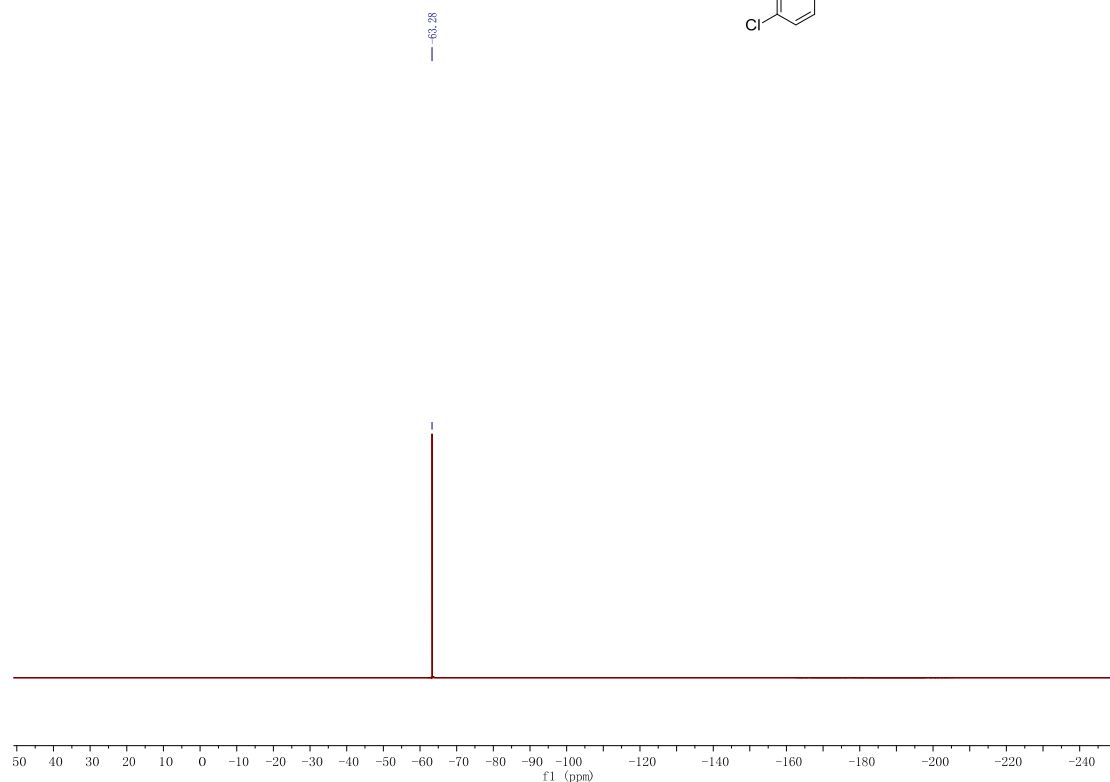
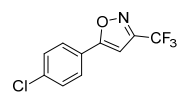
¹H NMR (CDCl₃, 400 MHz) of **9f**



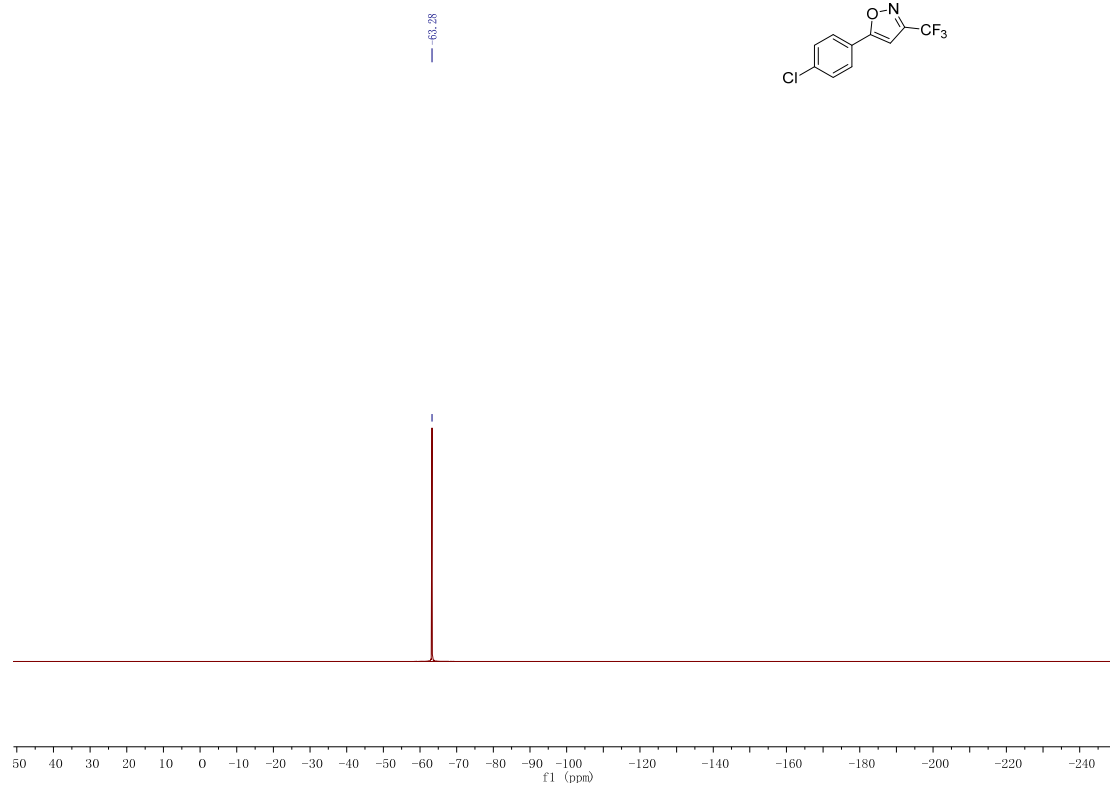
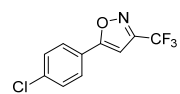
¹³C NMR (CDCl₃, 100 MHz) of **9f**



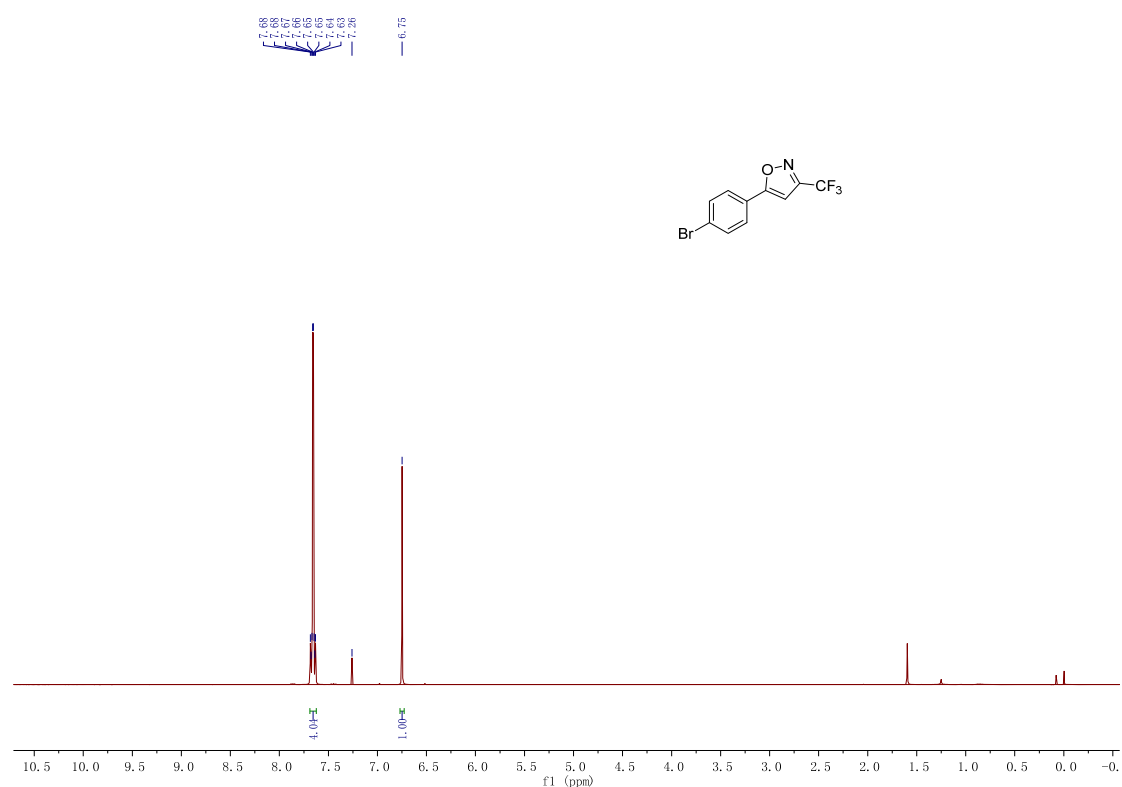
^{19}F NMR (CDCl_3 , 376 MHz) of **9f**



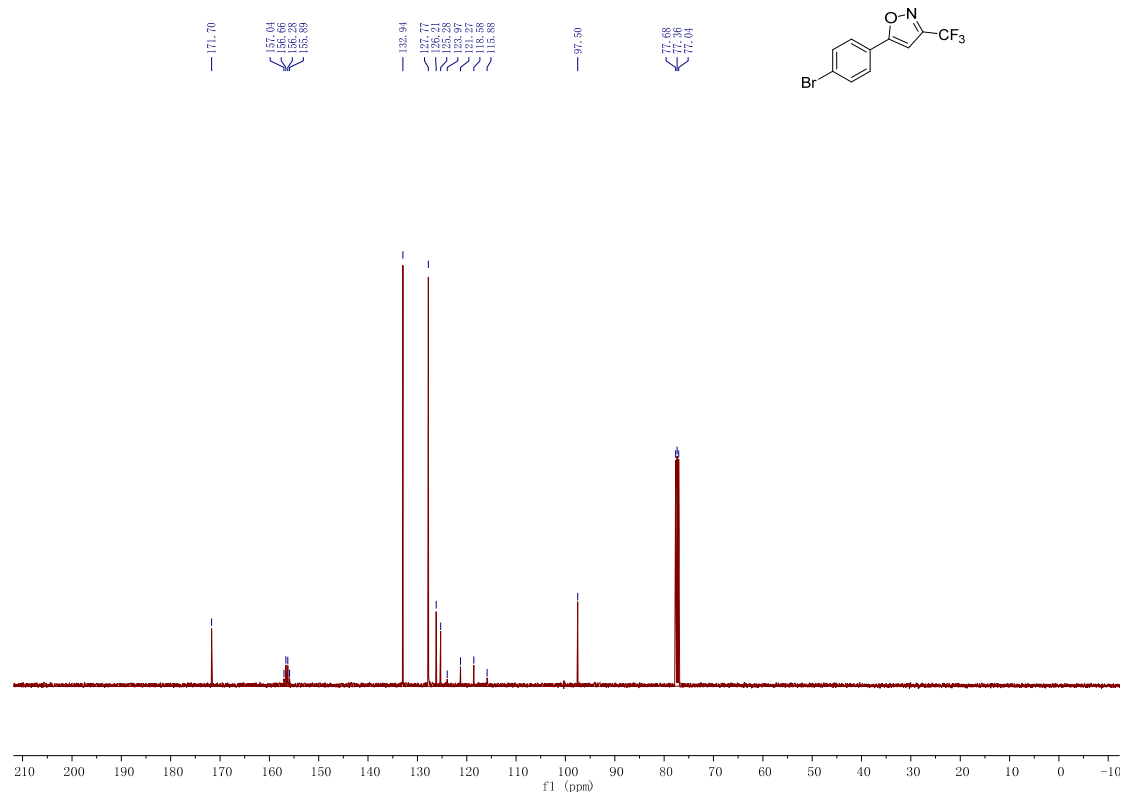
^{19}F { ^1H } NMR (CDCl_3 , 376 MHz) of **9f**



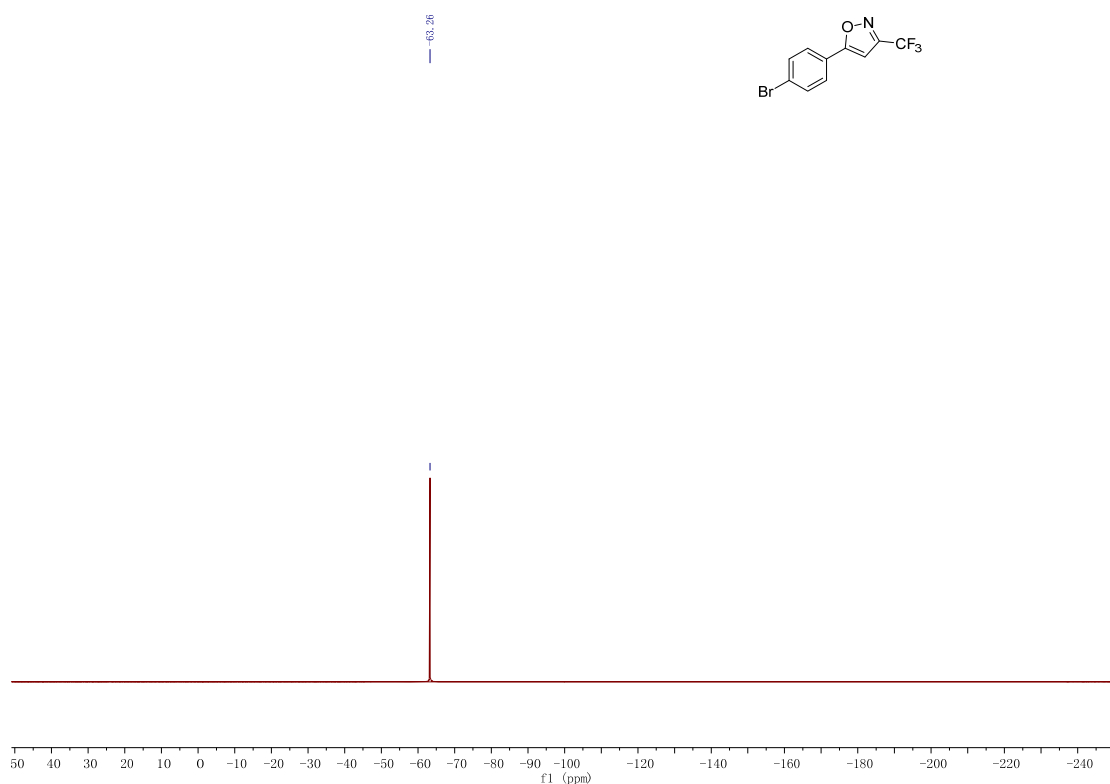
^1H NMR (CDCl₃, 400 MHz) of **9g**



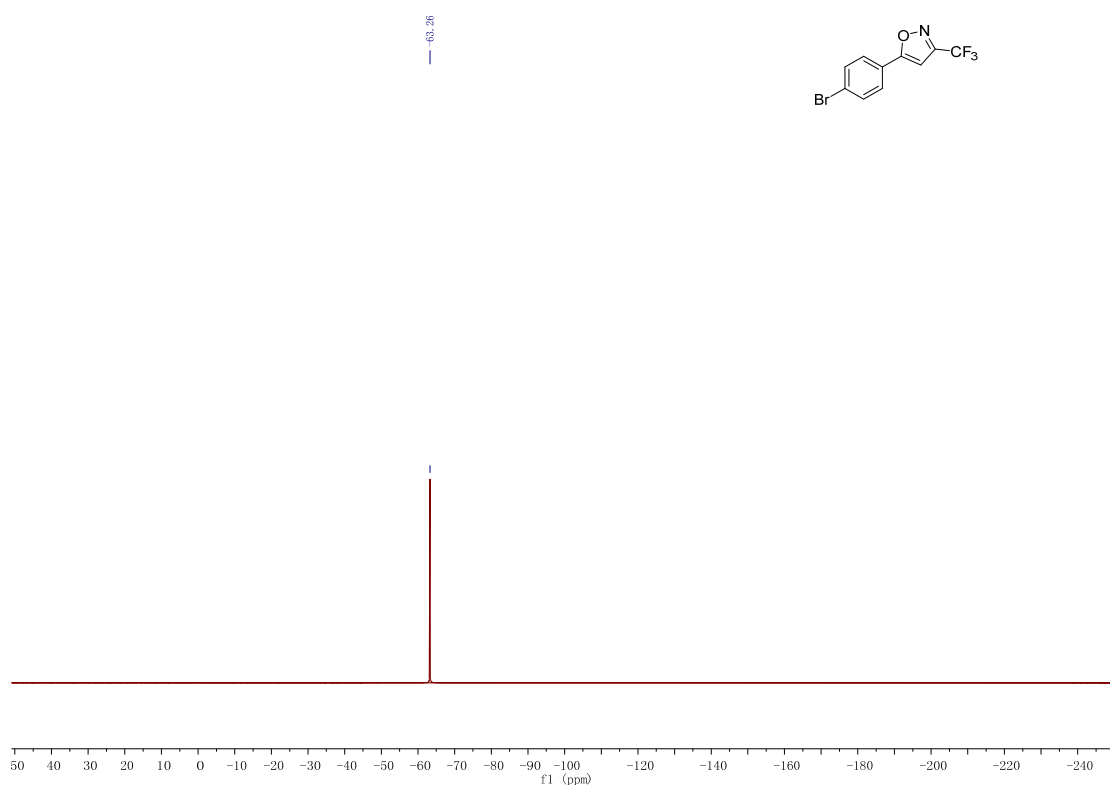
^{13}C NMR (CDCl₃, 100 MHz) of **9g**



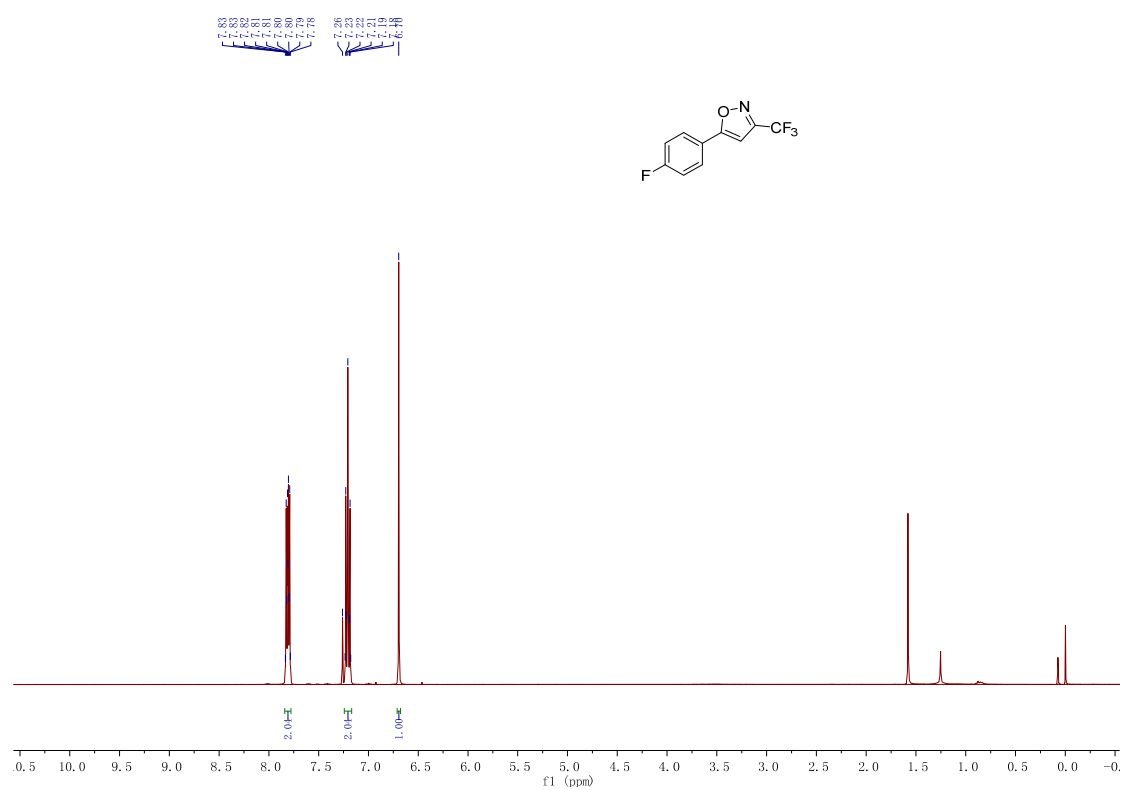
^{19}F NMR (CDCl_3 , 376 MHz) of **9g**



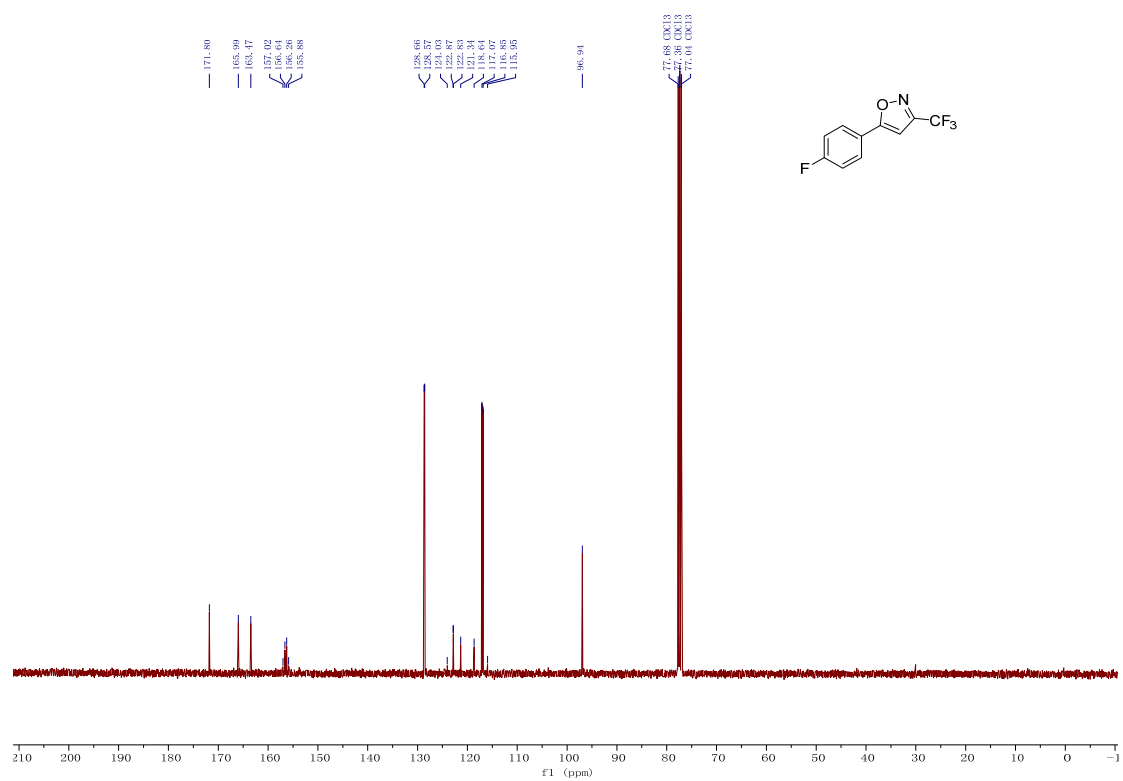
^{19}F { ^1H } NMR (CDCl_3 , 376 MHz) of **9g**



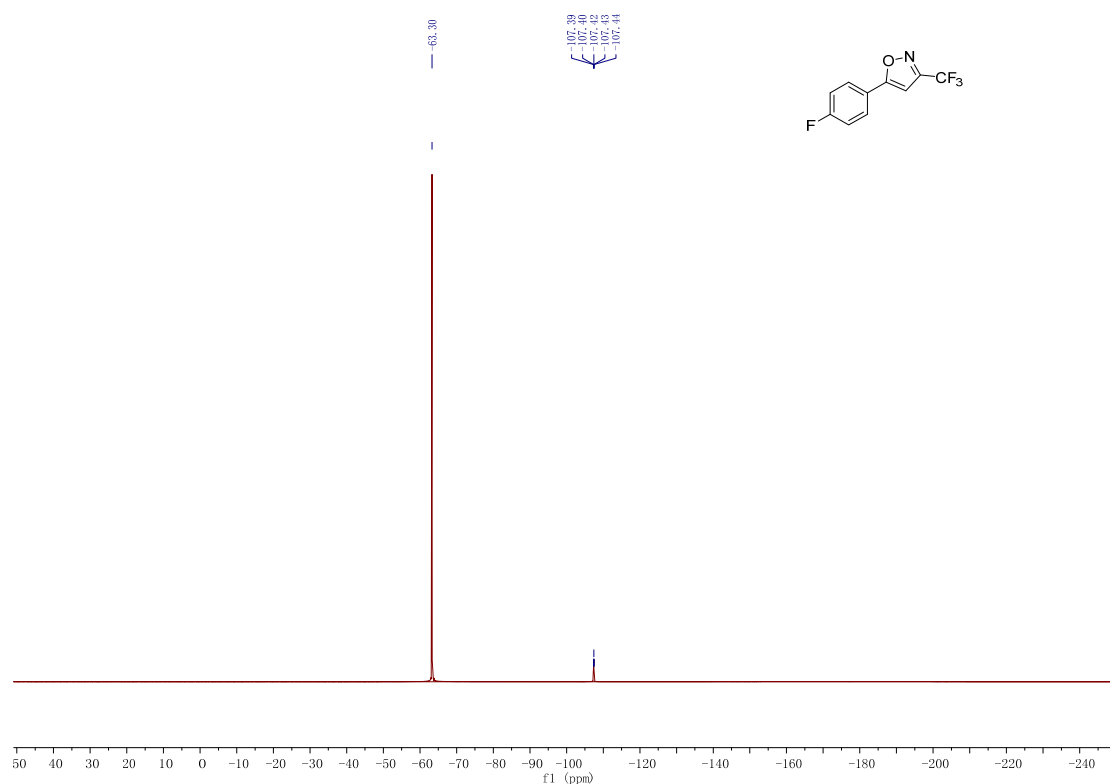
^1H NMR (CDCl₃, 400 MHz) of 9h



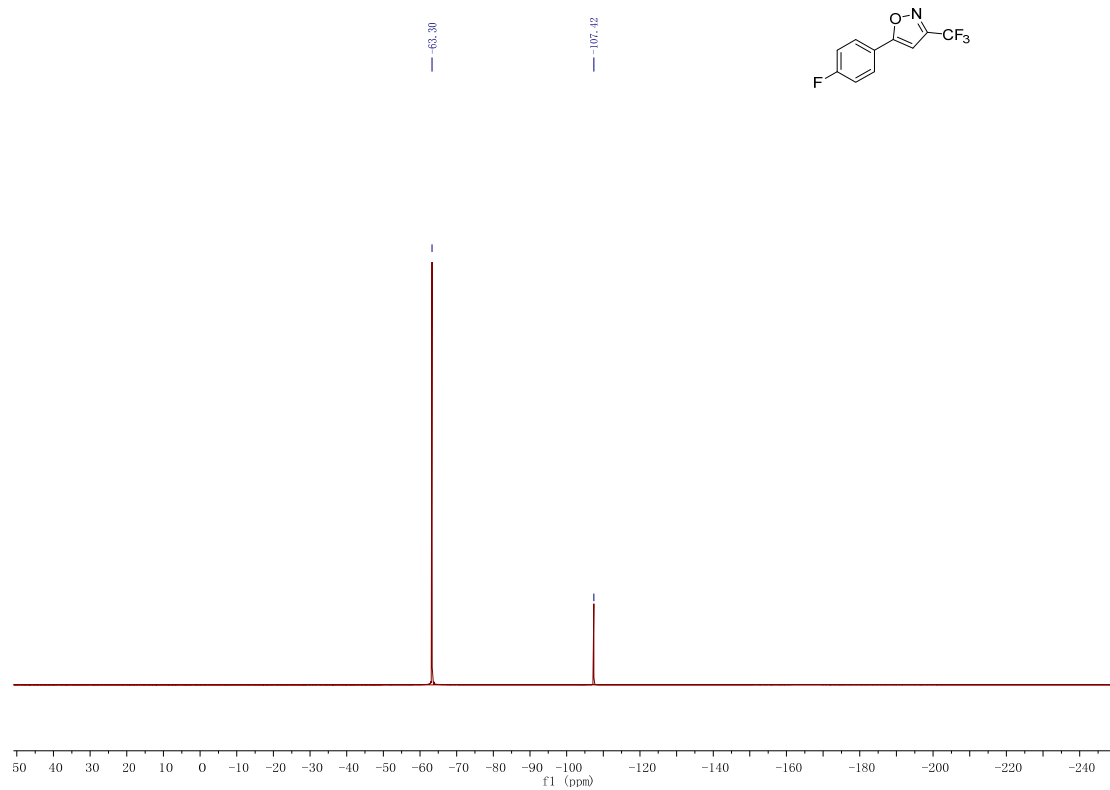
^{13}C NMR (CDCl₃, 100 MHz) of 9h



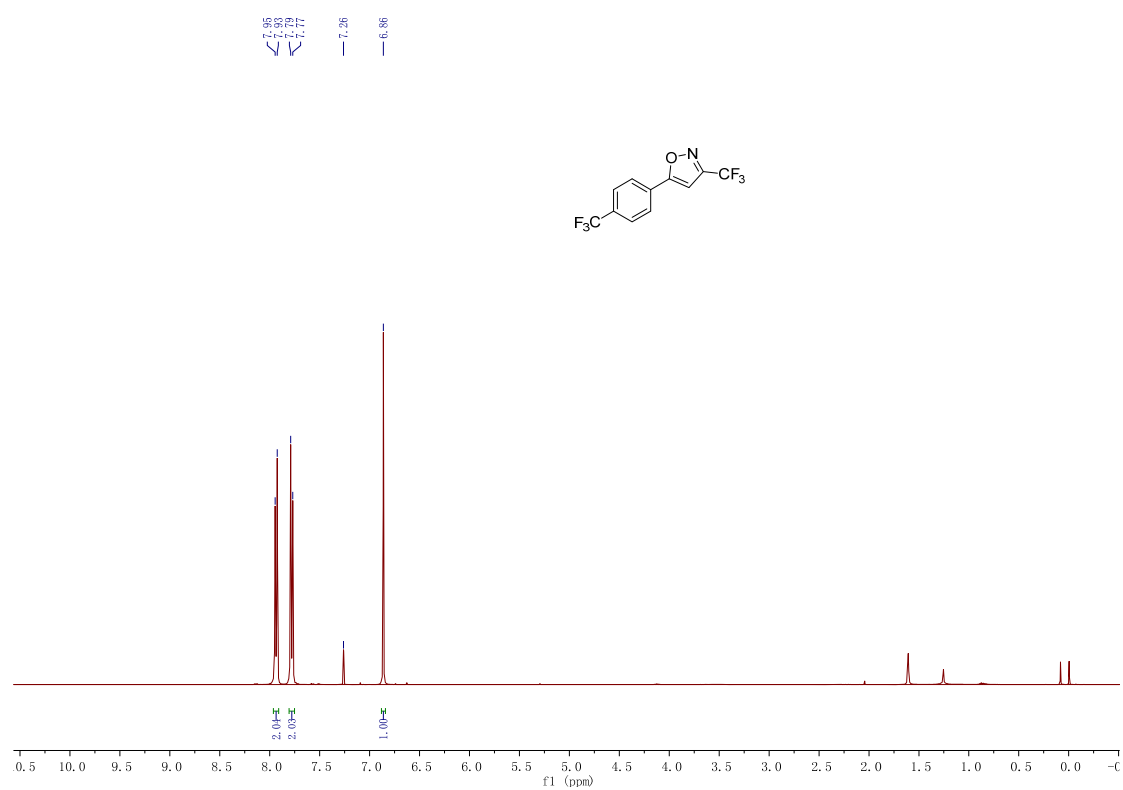
^{19}F NMR (CDCl₃, 376 MHz) of **9h**



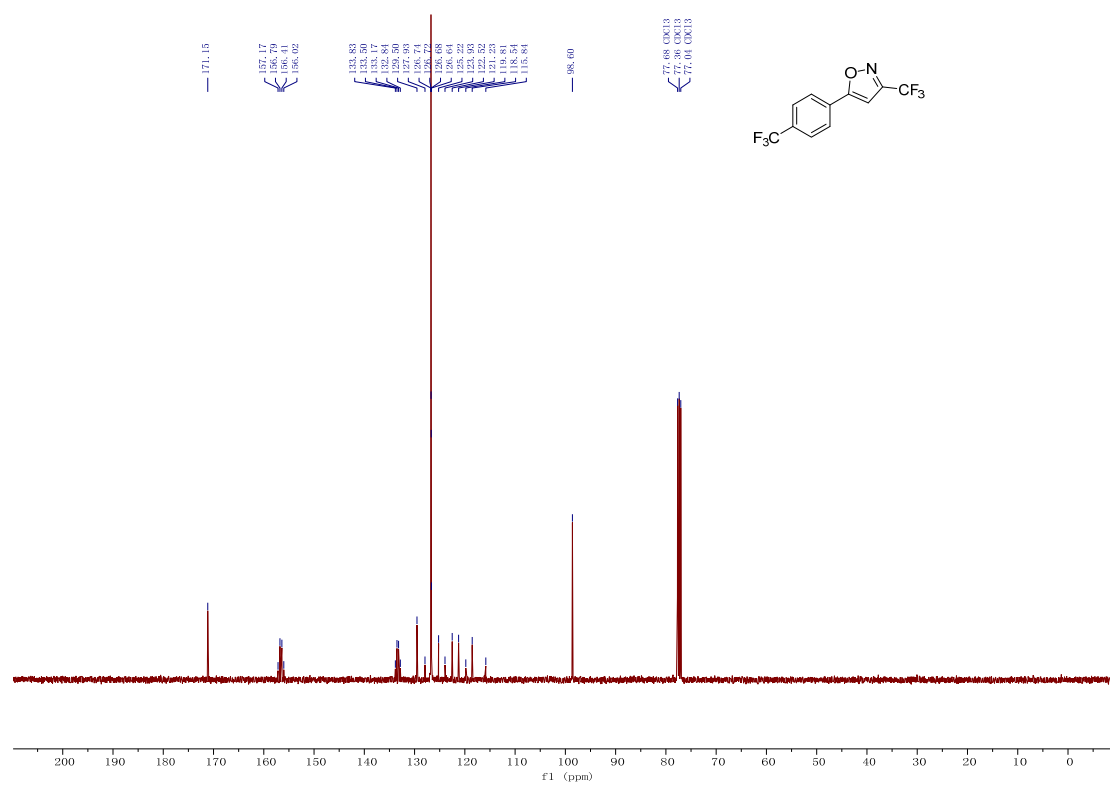
^{19}F { ^1H } NMR (CDCl₃, 376 MHz) of **9h**



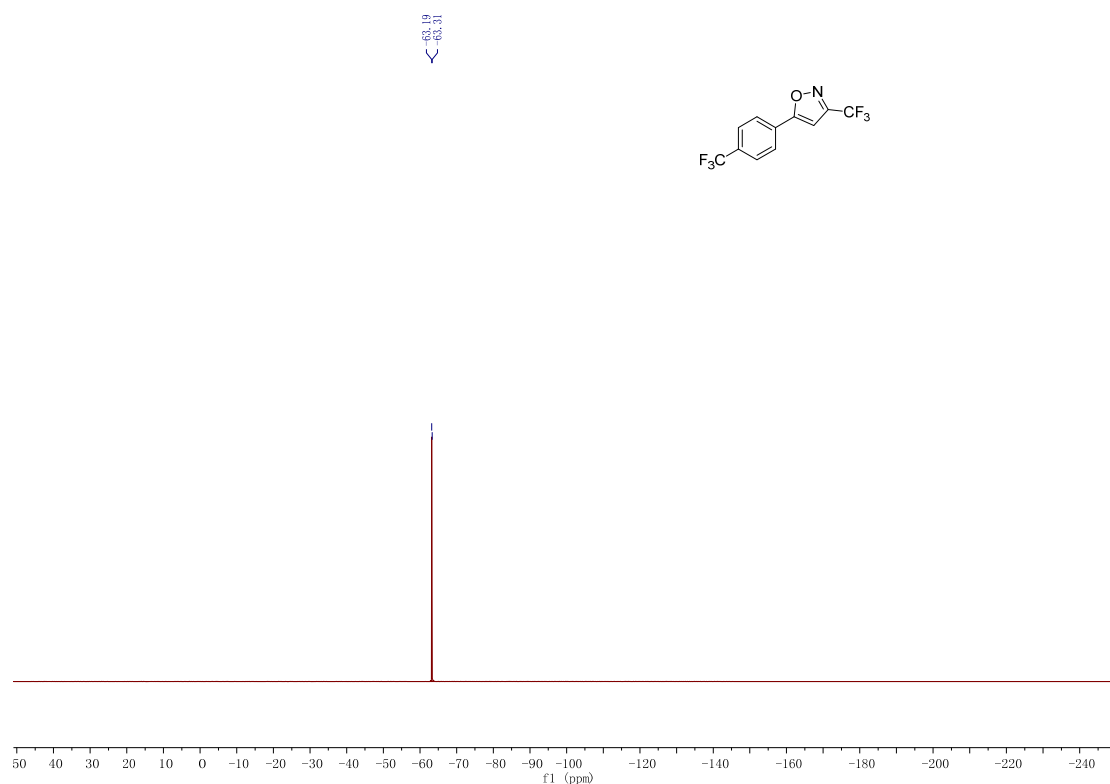
^1H NMR (CDCl₃, 400 MHz) of **9i**



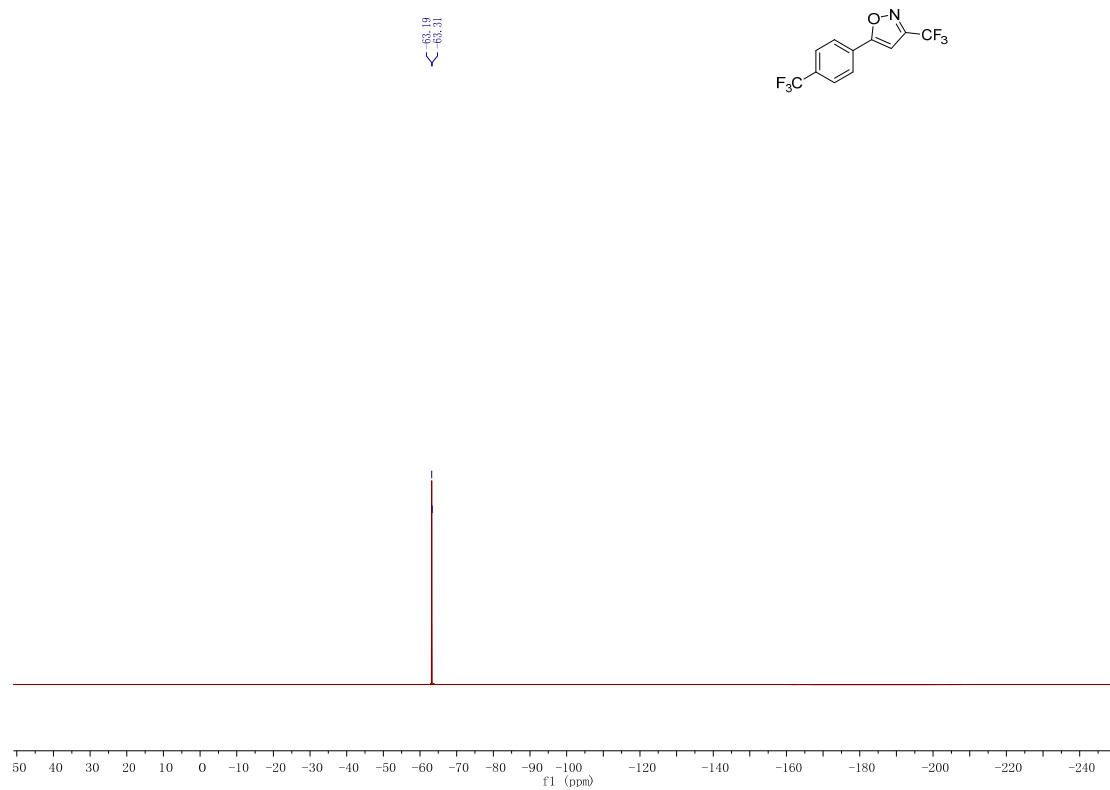
^{13}C NMR (CDCl₃, 100 MHz) of **9i**



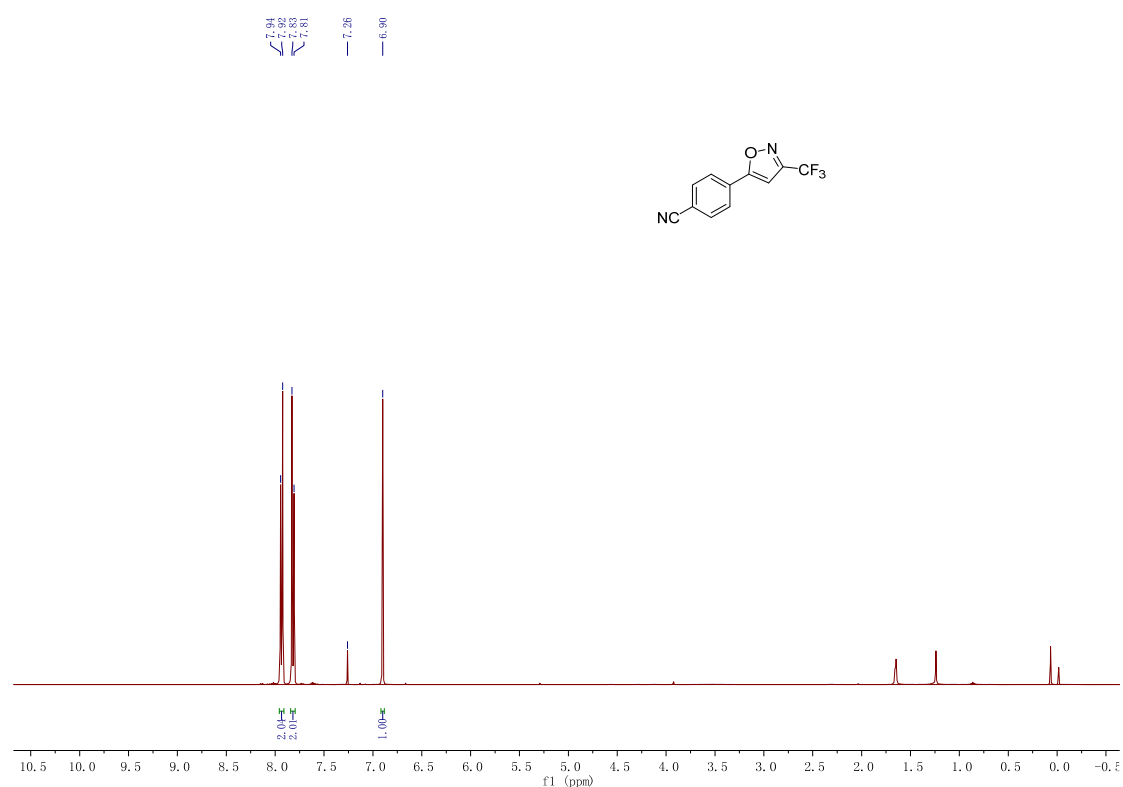
^{19}F NMR (CDCl₃, 376 MHz) of **9i**



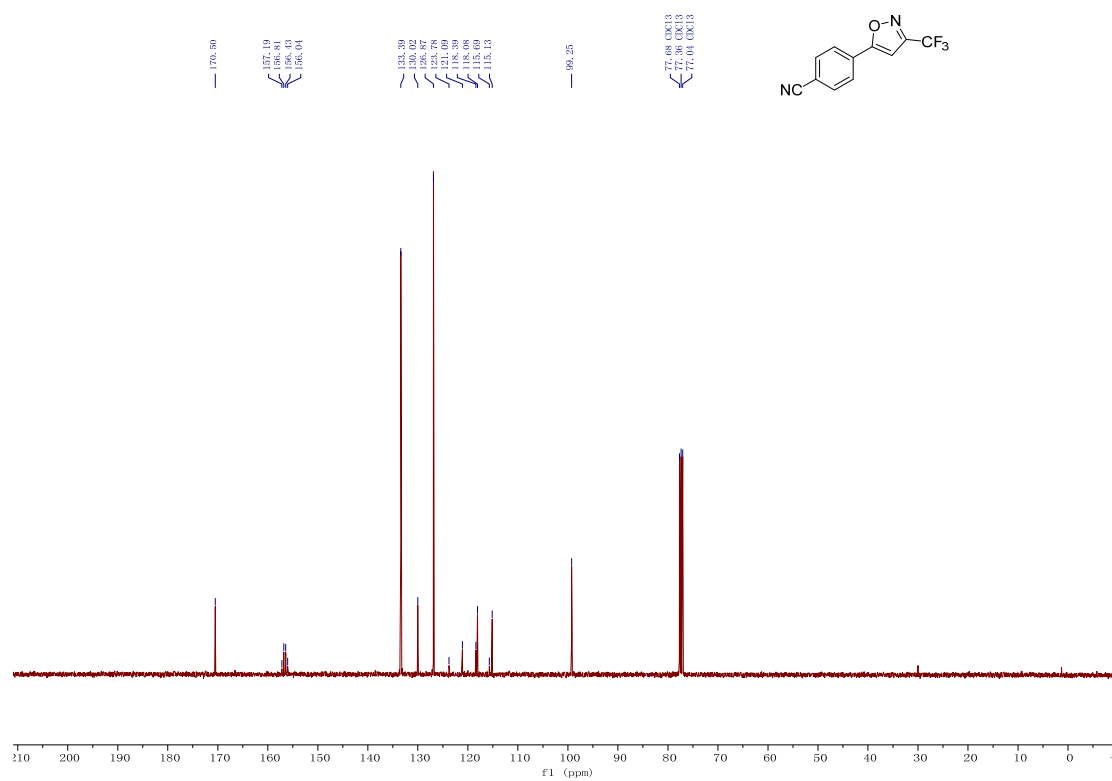
^{19}F { ^1H } NMR (CDCl₃, 376 MHz) of **9i**



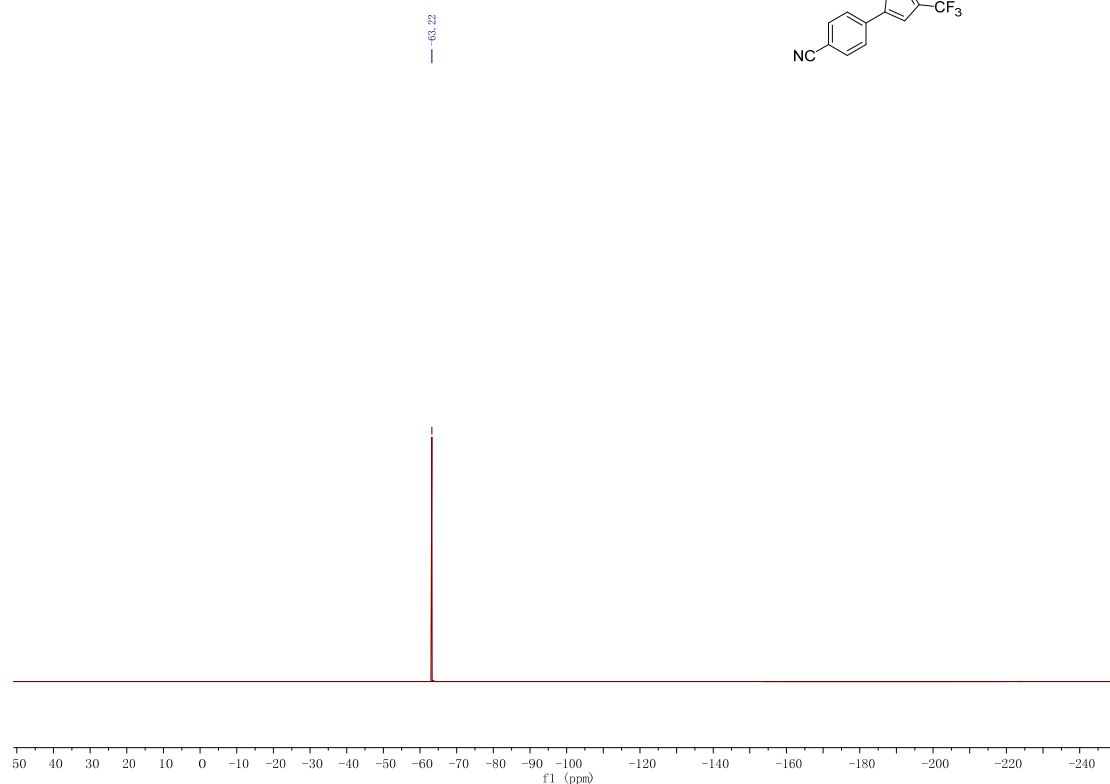
¹H NMR (CDCl₃, 400 MHz) of **9j**



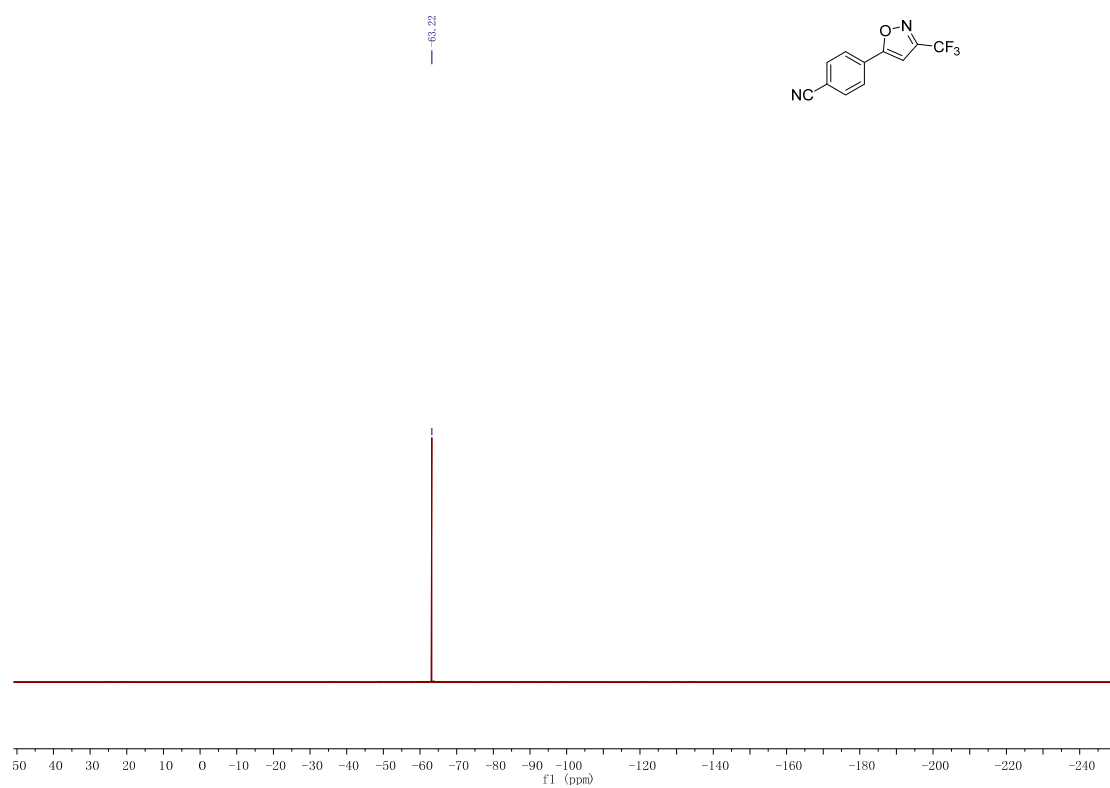
¹³C NMR (CDCl₃, 100 MHz) of **9j**



^{19}F NMR (CDCl_3 , 376 MHz) of **9j**



^{19}F { ^1H } NMR (CDCl_3 , 376 MHz) of **9j**



Chemical structure of 4-(4-nitrophenyl)-2-(trifluoromethyl)furan (1): CC1=CC=C(C=C1)C2=CC(=CC=C2)[N+](=O)[O-]

¹H NMR spectrum (CDCl₃) of compound 1:

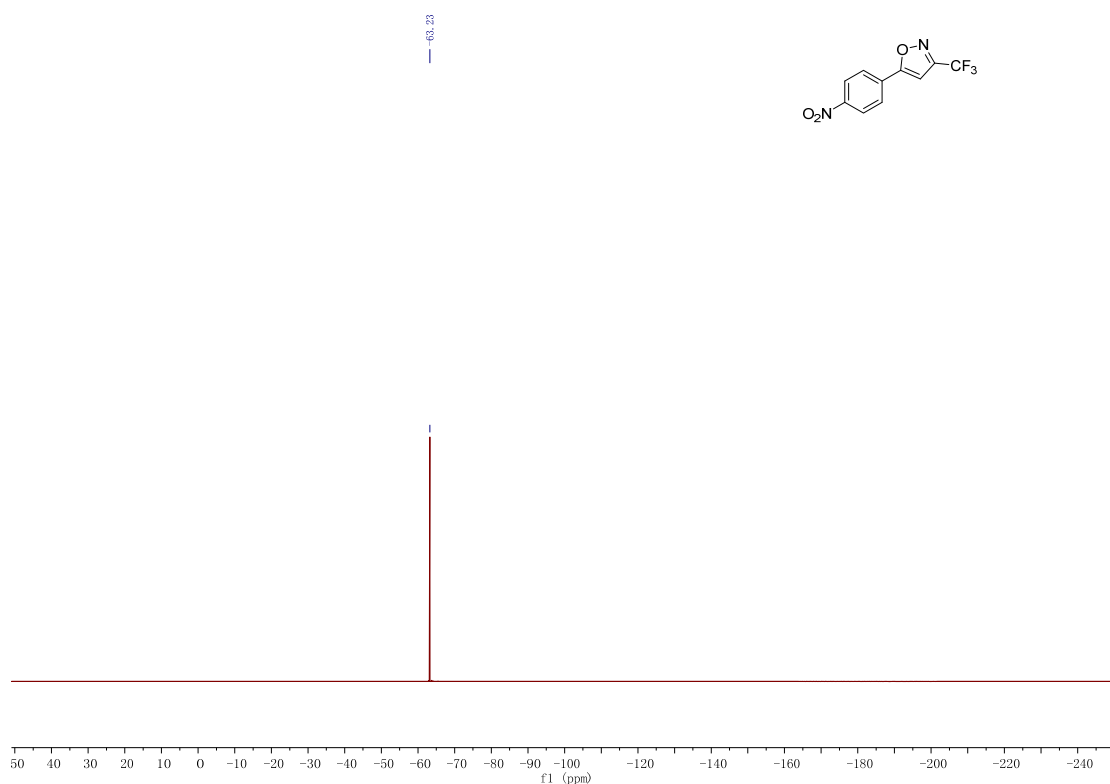
Chemical shift (ppm): 8.48, 8.47, 8.03, 8.02, 7.01, 6.99, 3.92, 2.01, 1.97, 1.95, 1.93, 1.91, 1.89, 1.87, 1.85, 1.83, 1.81, 1.79, 1.77, 1.75, 1.73, 1.71, 1.69, 1.67, 1.65, 1.63, 1.61, 1.59, 1.57, 1.55, 1.53, 1.51, 1.49, 1.47, 1.45, 1.43, 1.41, 1.39, 1.37, 1.35, 1.33, 1.31, 1.29, 1.27, 1.25, 1.23, 1.21, 1.19, 1.17, 1.15, 1.13, 1.11, 1.09, 1.07, 1.05, 1.03, 1.01, 0.99, 0.97, 0.95, 0.93, 0.91, 0.89, 0.87, 0.85, 0.83, 0.81, 0.79, 0.77, 0.75, 0.73, 0.71, 0.69, 0.67, 0.65, 0.63, 0.61, 0.59, 0.57, 0.55, 0.53, 0.51, 0.49, 0.47, 0.45, 0.43, 0.41, 0.39, 0.37, 0.35, 0.33, 0.31, 0.29, 0.27, 0.25, 0.23, 0.21, 0.19, 0.17, 0.15, 0.13, 0.11, 0.09, 0.07, 0.05, 0.03, 0.01, -0.01, -0.03, -0.05, -0.07, -0.09, -0.11, -0.13, -0.15, -0.17, -0.19, -0.21, -0.23, -0.25, -0.27, -0.29, -0.31, -0.33, -0.35, -0.37, -0.39, -0.41, -0.43, -0.45, -0.47, -0.49, -0.51, -0.53, -0.55, -0.57, -0.59, -0.61, -0.63, -0.65, -0.67, -0.69, -0.71, -0.73, -0.75, -0.77, -0.79, -0.81, -0.83, -0.85, -0.87, -0.89, -0.91, -0.93, -0.95, -0.97, -0.99, -1.01, -1.03, -1.05, -1.07, -1.09, -1.11, -1.13, -1.15, -1.17, -1.19, -1.21, -1.23, -1.25, -1.27, -1.29, -1.31, -1.33, -1.35, -1.37, -1.39, -1.41, -1.43, -1.45, -1.47, -1.49, -1.51, -1.53, -1.55, -1.57, -1.59, -1.61, -1.63, -1.65, -1.67, -1.69, -1.71, -1.73, -1.75, -1.77, -1.79, -1.81, -1.83, -1.85, -1.87, -1.89, -1.91, -1.93, -1.95, -1.97, -1.99, -2.01, -2.03, -2.05, -2.07, -2.09, -2.11, -2.13, -2.15, -2.17, -2.19, -2.21, -2.23, -2.25, -2.27, -2.29, -2.31, -2.33, -2.35, -2.37, -2.39, -2.41, -2.43, -2.45, -2.47, -2.49, -2.51, -2.53, -2.55, -2.57, -2.59, -2.61, -2.63, -2.65, -2.67, -2.69, -2.71, -2.73, -2.75, -2.77, -2.79, -2.81, -2.83, -2.85, -2.87, -2.89, -2.91, -2.93, -2.95, -2.97, -2.99, -3.01, -3.03, -3.05, -3.07, -3.09, -3.11, -3.13, -3.15, -3.17, -3.19, -3.21, -3.23, -3.25, -3.27, -3.29, -3.31, -3.33, -3.35, -3.37, -3.39, -3.41, -3.43, -3.45, -3.47, -3.49, -3.51, -3.53, -3.55, -3.57, -3.59, -3.61, -3.63, -3.65, -3.67, -3.69, -3.71, -3.73, -3.75, -3.77, -3.79, -3.81, -3.83, -3.85, -3.87, -3.89, -3.91, -3.93, -3.95, -3.97, -3.99, -4.01, -4.03, -4.05, -4.07, -4.09, -4.11, -4.13, -4.15, -4.17, -4.19, -4.21, -4.23, -4.25, -4.27, -4.29, -4.31, -4.33, -4.35, -4.37, -4.39, -4.41, -4.43, -4.45, -4.47, -4.49, -4.51, -4.53, -4.55, -4.57, -4.59, -4.61, -4.63, -4.65, -4.67, -4.69, -4.71, -4.73, -4.75, -4.77, -4.79, -4.81, -4.83, -4.85, -4.87, -4.89, -4.91, -4.93, -4.95, -4.97, -4.99, -5.01, -5.03, -5.05, -5.07, -5.09, -5.11, -5.13, -5.15, -5.17, -5.19, -5.21, -5.23, -5.25, -5.27, -5.29, -5.31, -5.33, -5.35, -5.37, -5.39, -5.41, -5.43, -5.45, -5.47, -5.49, -5.51, -5.53, -5.55, -5.57, -5.59, -5.61, -5.63, -5.65, -5.67, -5.69, -5.71, -5.73, -5.75, -5.77, -5.79, -5.81, -5.83, -5.85, -5.87, -5.89, -5.91, -5.93, -5.95, -5.97, -5.99, -6.01, -6.03, -6.05, -6.07, -6.09, -6.11, -6.13, -6.15, -6.17, -6.19, -6.21, -6.23, -6.25, -6.27, -6.29, -6.31, -6.33, -6.35, -6.37, -6.39, -6.41, -6.43, -6.45, -6.47, -6.49, -6.51, -6.53, -6.55, -6.57, -6.59, -6.61, -6.63, -6.65, -6.67, -6.69, -6.71, -6.73, -6.75, -6.77, -6.79, -6.81, -6.83, -6.85, -6.87, -6.89, -6.91, -6.93, -6.95, -6.97, -6.99, -7.01, -7.03, -7.05, -7.07, -7.09, -7.11, -7.13, -7.15, -7.17, -7.19, -7.21, -7.23, -7.25, -7.27, -7.29, -7.31, -7.33, -7.35, -7.37, -7.39, -7.41, -7.43, -7.45, -7.47, -7.49, -7.51, -7.53, -7.55, -7.57, -7.59, -7.61, -7.63, -7.65, -7.67, -7.69, -7.71, -7.73, -7.75, -7.77, -7.79, -7.81, -7.83, -7.85, -7.87, -7.89, -7.91, -7.93, -7.95, -7.97, -7.99, -8.01, -8.03, -8.05, -8.07, -8.09, -8.11, -8.13, -8.15, -8.17, -8.19, -8.21, -8.23, -8.25, -8.27, -8.29, -8.31, -8.33, -8.35, -8.37, -8.39, -8.41, -8.43, -8.45, -8.47, -8.49, -8.51, -8.53, -8.55, -8.57, -8.59, -8.61, -8.63, -8.65, -8.67, -8.69, -8.71, -8.73, -8.75, -8.77, -8.79, -8.81, -8.83, -8.85, -8.87, -8.89, -8.91, -8.93, -8.95, -8.97, -8.99, -9.01, -9.03, -9.05, -9.07, -9.09, -9.11, -9.13, -9.15, -9.17, -9.19, -9.21, -9.23, -9.25, -9.27, -9.29, -9.31, -9.33, -9.35, -9.37, -9.39, -9.41, -9.43, -9.45, -9.47, -9.49, -9.51, -9.53, -9.55, -9.57, -9.59, -9.61, -9.63, -9.65, -9.67, -9.69, -9.71, -9.73, -9.75, -9.77, -9.79, -9.81, -9.83, -9.85, -9.87, -9.89, -9.91, -9.93, -9.95, -9.97, -9.99, -10.01, -10.03, -10.05, -10.07, -10.09, -10.11, -10.13, -10.15, -10.17, -10.19, -10.21, -10.23, -10.25, -10.27, -10.29, -10.31, -10.33, -10.35, -10.37, -10.39, -10.41, -10.43, -10.45, -10.47, -10.49, -10.51, -10.53, -10.55, -10.57, -10.59, -10.61, -10.63, -10.65, -10.67, -10.69, -10.71, -10.73, -10.75, -10.77, -10.79, -10.81, -10.83, -10.85, -10.87, -10.89, -10.91, -10.93, -10.95, -10.97, -10.99, -11

Chemical structure: CC1=CC=C(C=C1C2=CC(=CC=C2)[N+](=O)[O-])OC3=CC(=C(C=C3)N)C(F)(F)F

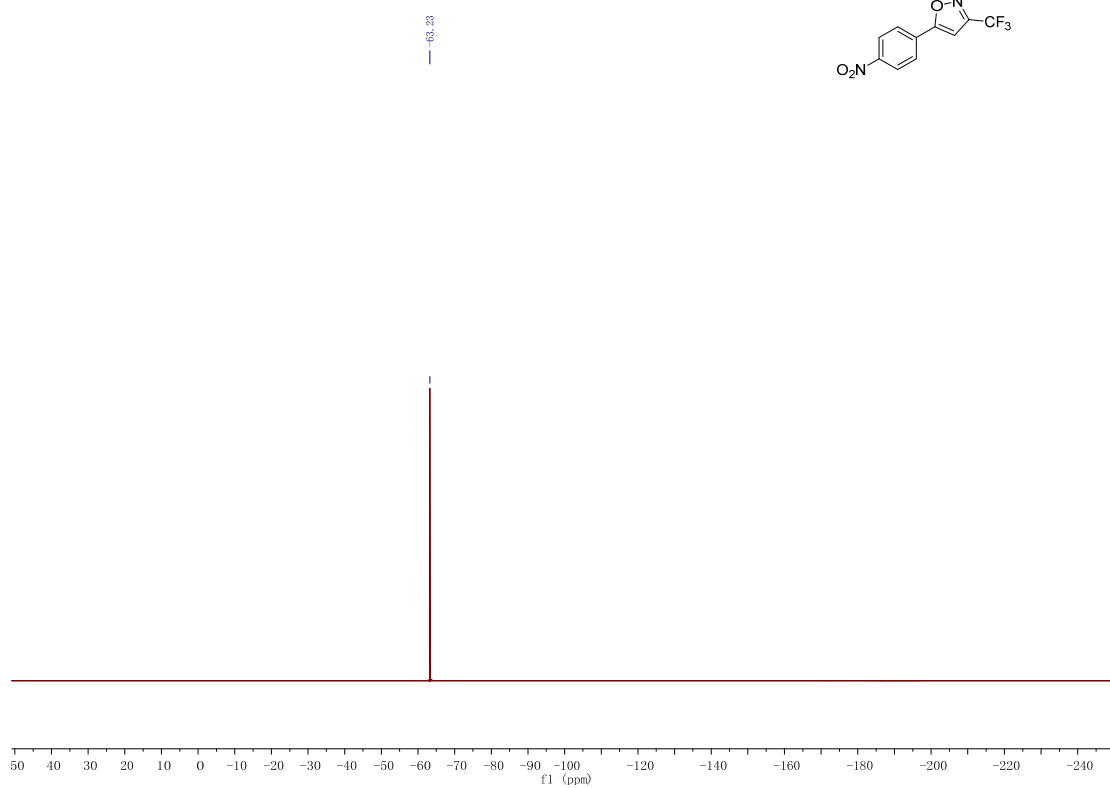
¹³C NMR spectrum (CDCl₃) showing peaks at the following chemical shifts (ppm):

- 170.19
- 157.28
- 156.89
- 156.51
- 156.13
- 149.49
- 131.65
- 127.31
- 124.90
- 124.72
- 121.68
- 118.38
- 115.68
- 99.68
- 77.68 (CDCl₃)
- 77.46 (CDCl₃)
- 77.24 (CDCl₃)

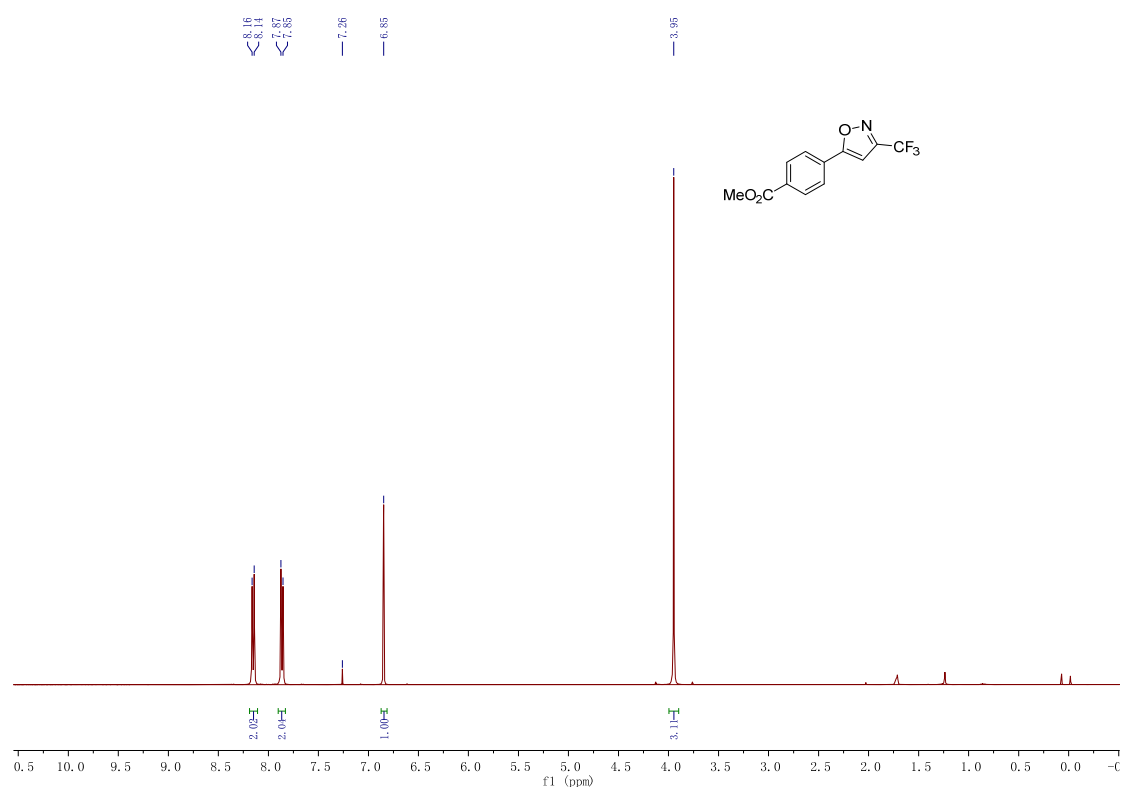
^{19}F NMR (CDCl₃, 376 MHz) of **9k**



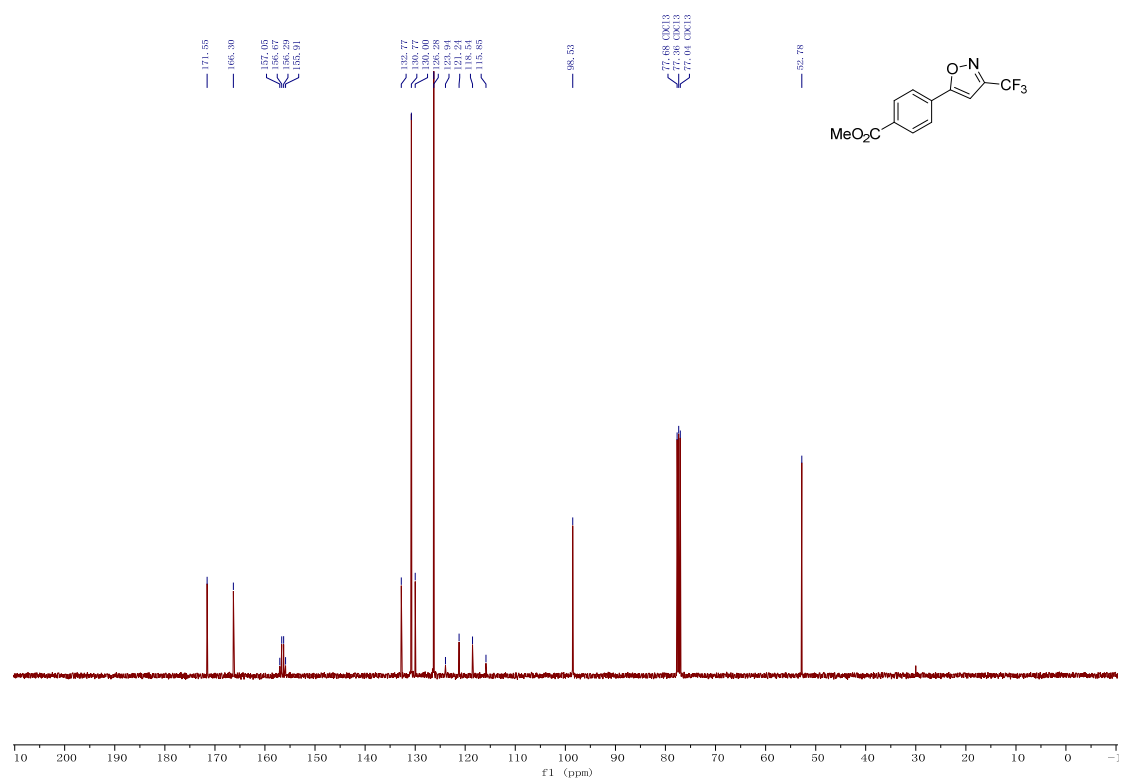
^{19}F { ^1H } NMR (CDCl₃, 376 MHz) of **9k**



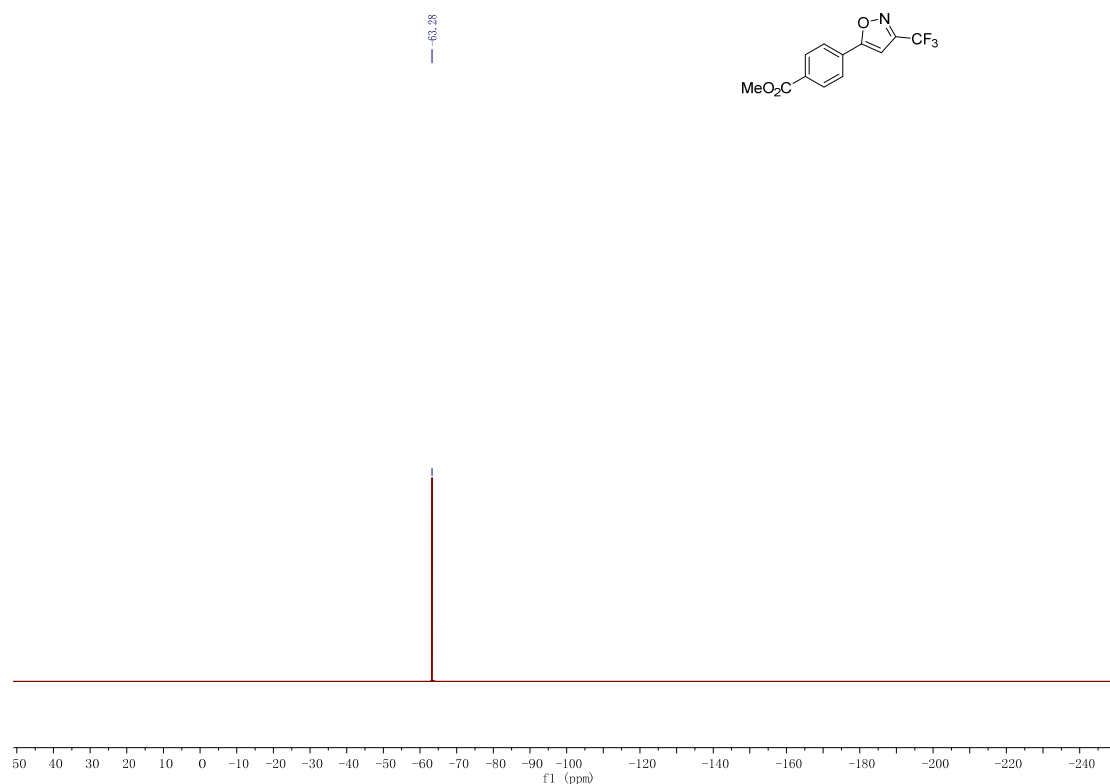
^1H NMR (CDCl₃, 400 MHz) of **9l**



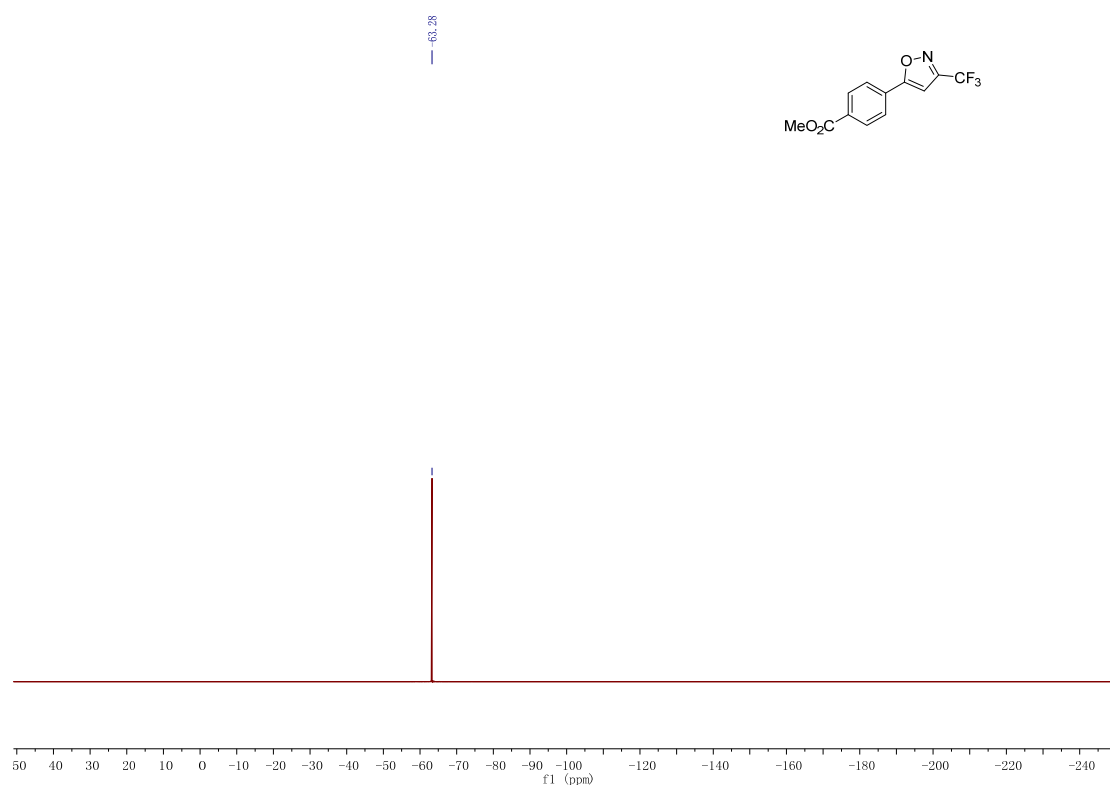
^{13}C NMR (CDCl₃, 100 MHz) of **9l**



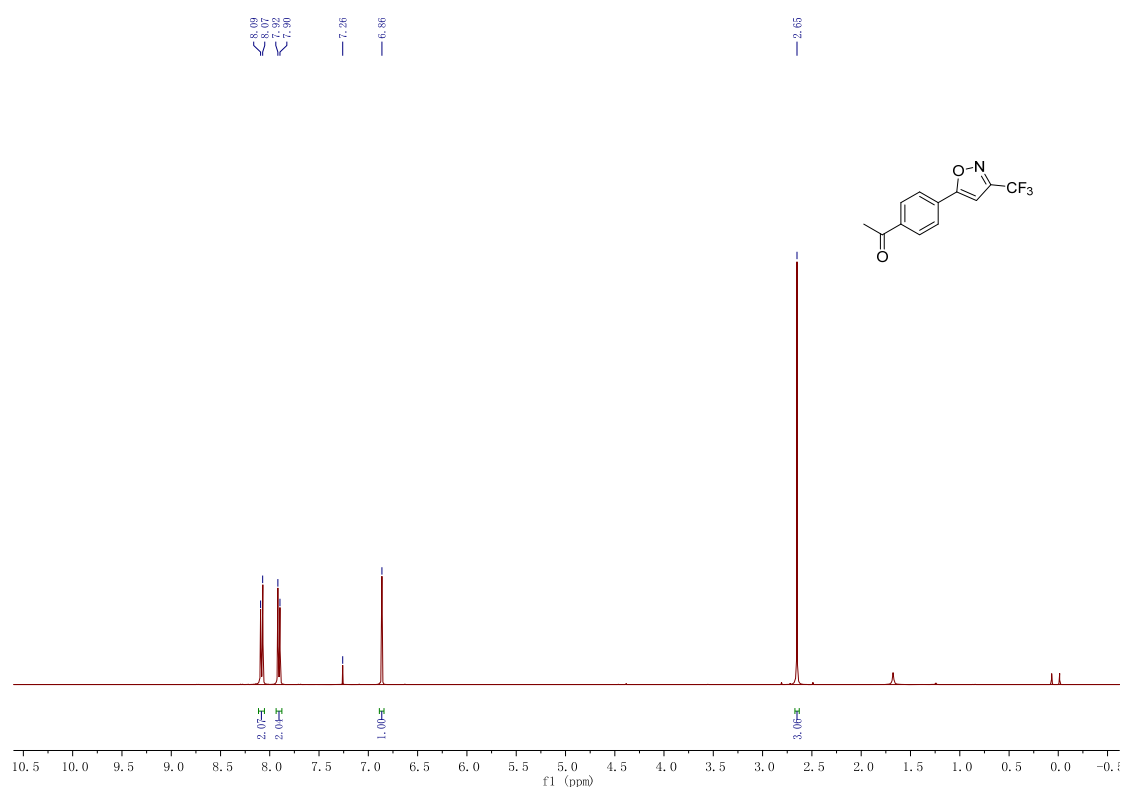
^{19}F NMR (CDCl₃, 376 MHz) of **9l**



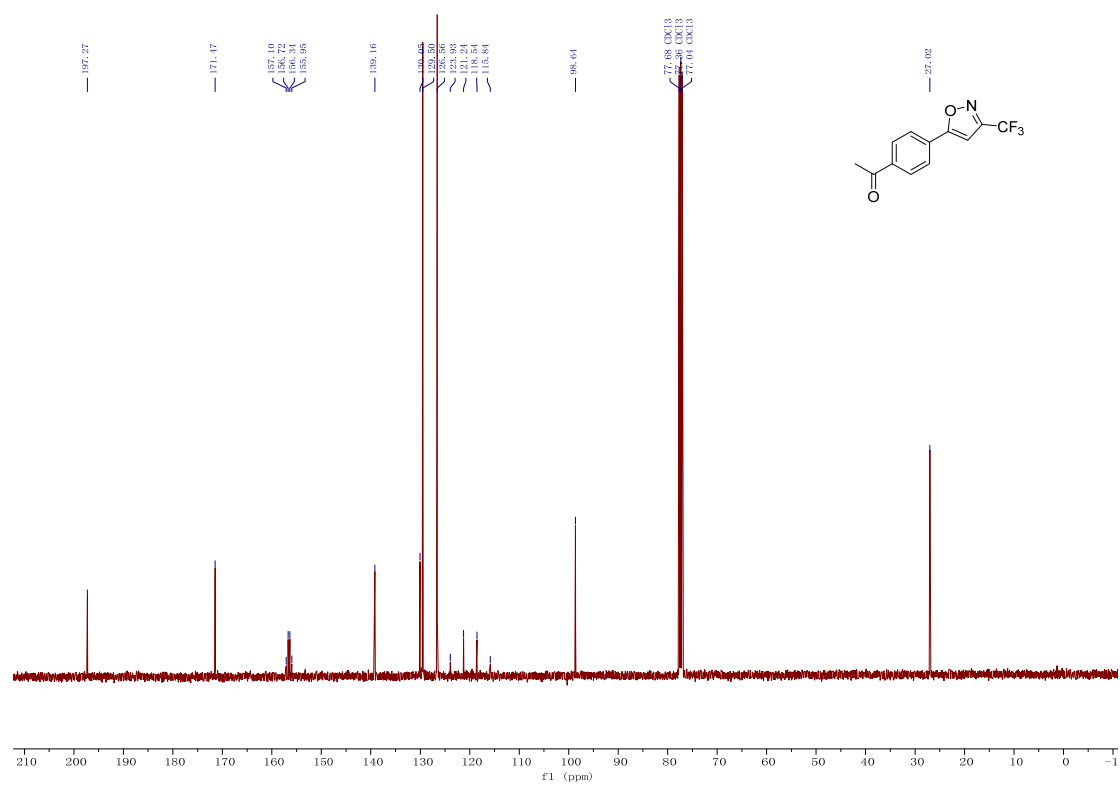
^{19}F { ^1H } NMR (CDCl₃, 376 MHz) of **9l**



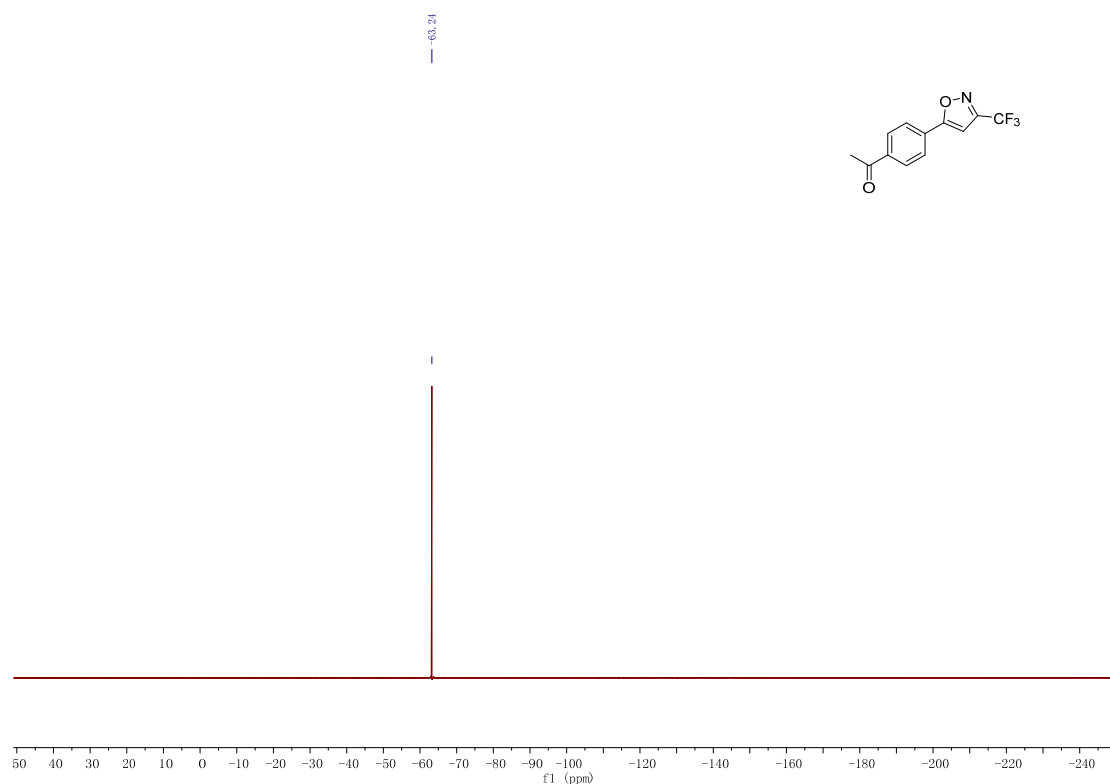
^1H NMR (CDCl₃, 400 MHz) of **9m**



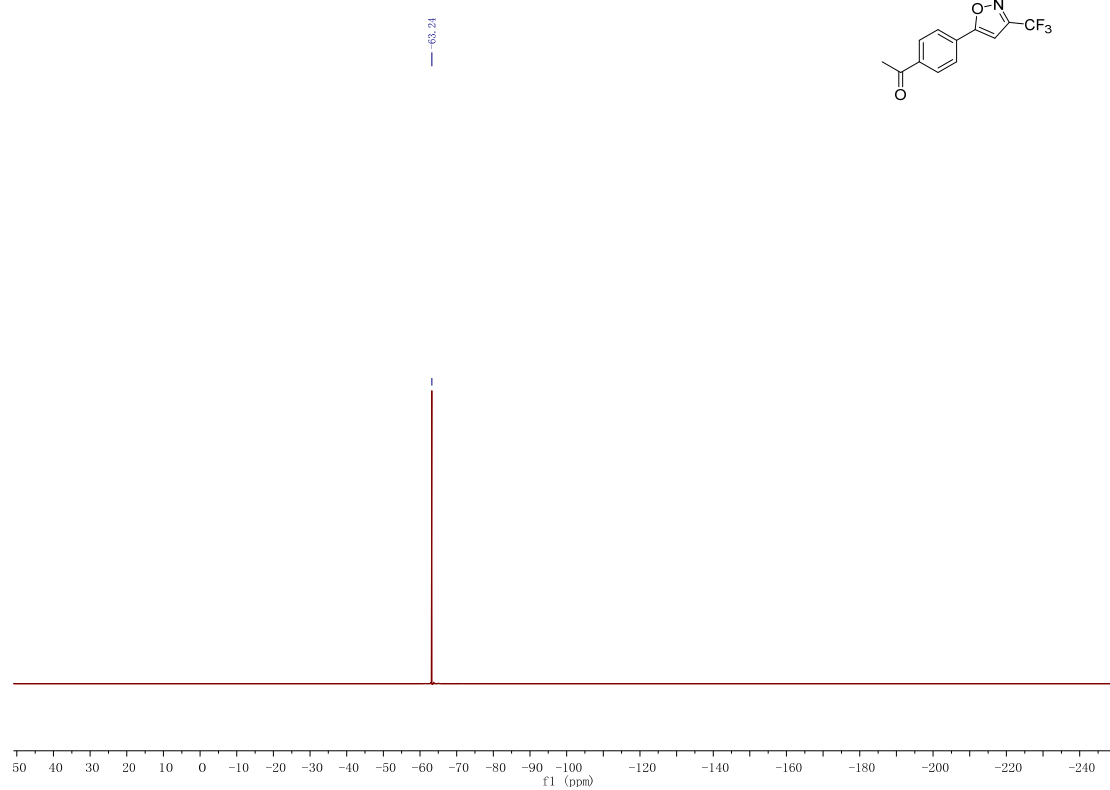
^{13}C NMR (CDCl₃, 100 MHz) of **9m**



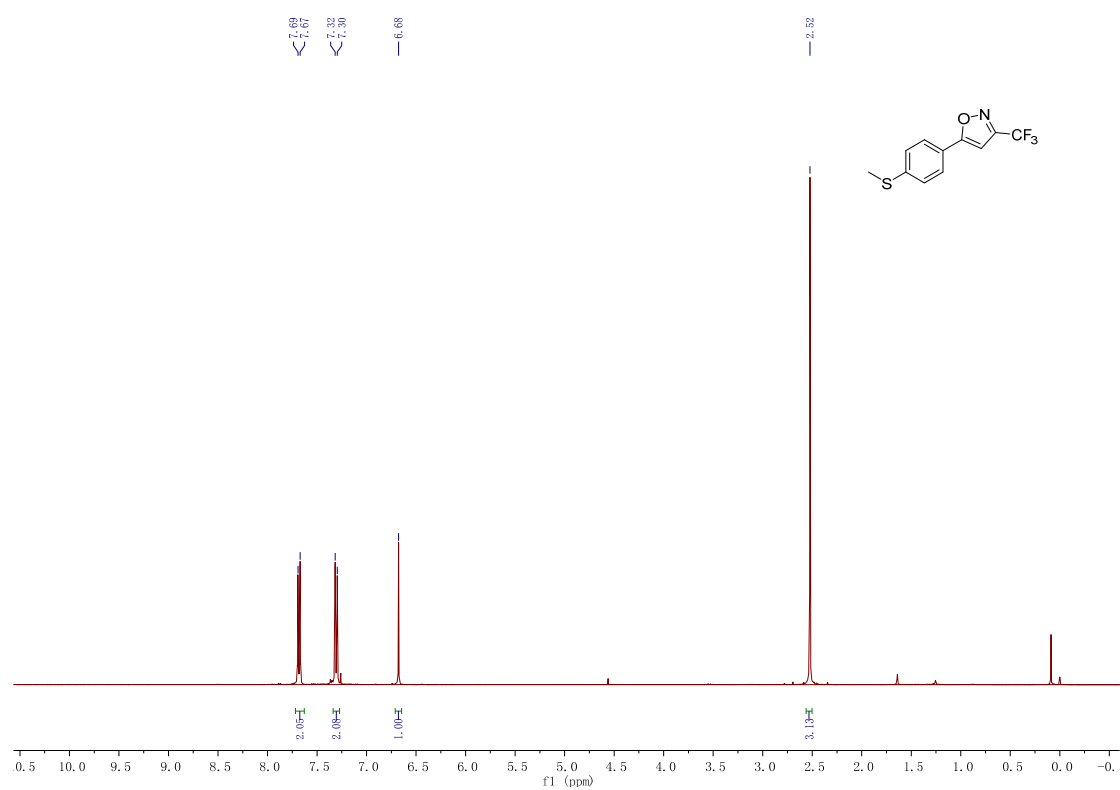
^{19}F NMR (CDCl₃, 376 MHz) of **9m**



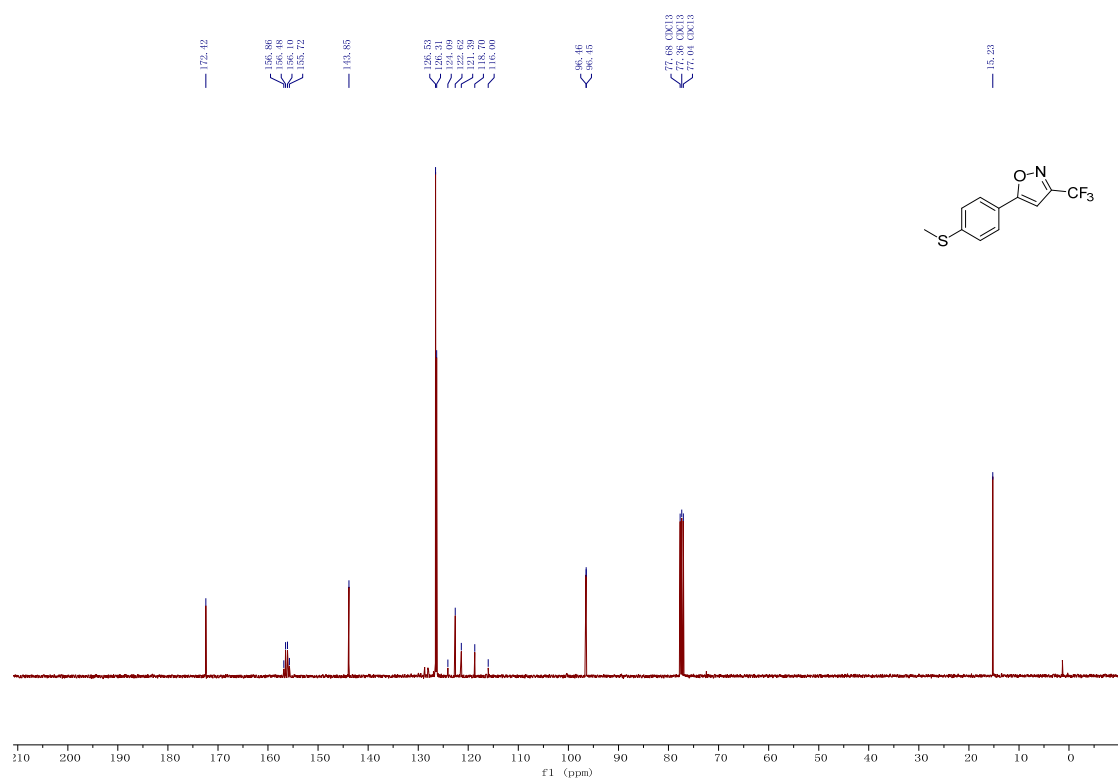
^{19}F { ^1H } NMR (CDCl₃, 376 MHz) of **9m**



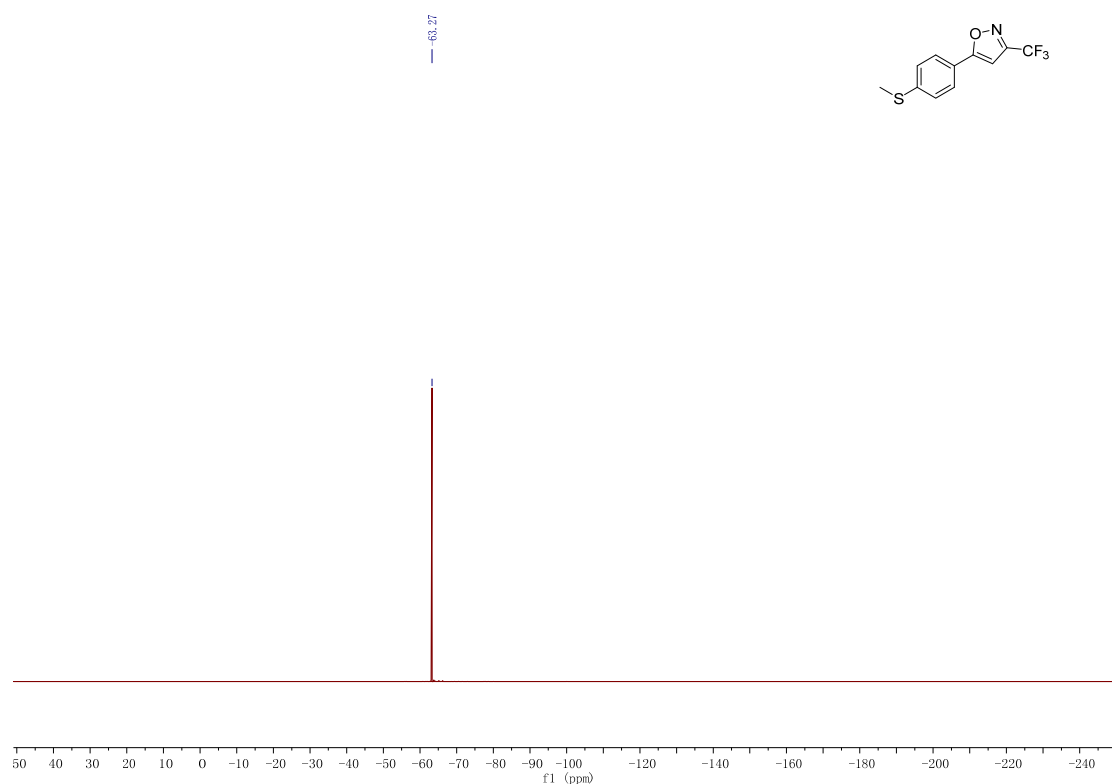
^1H NMR (CDCl₃, 400 MHz) of **9n**



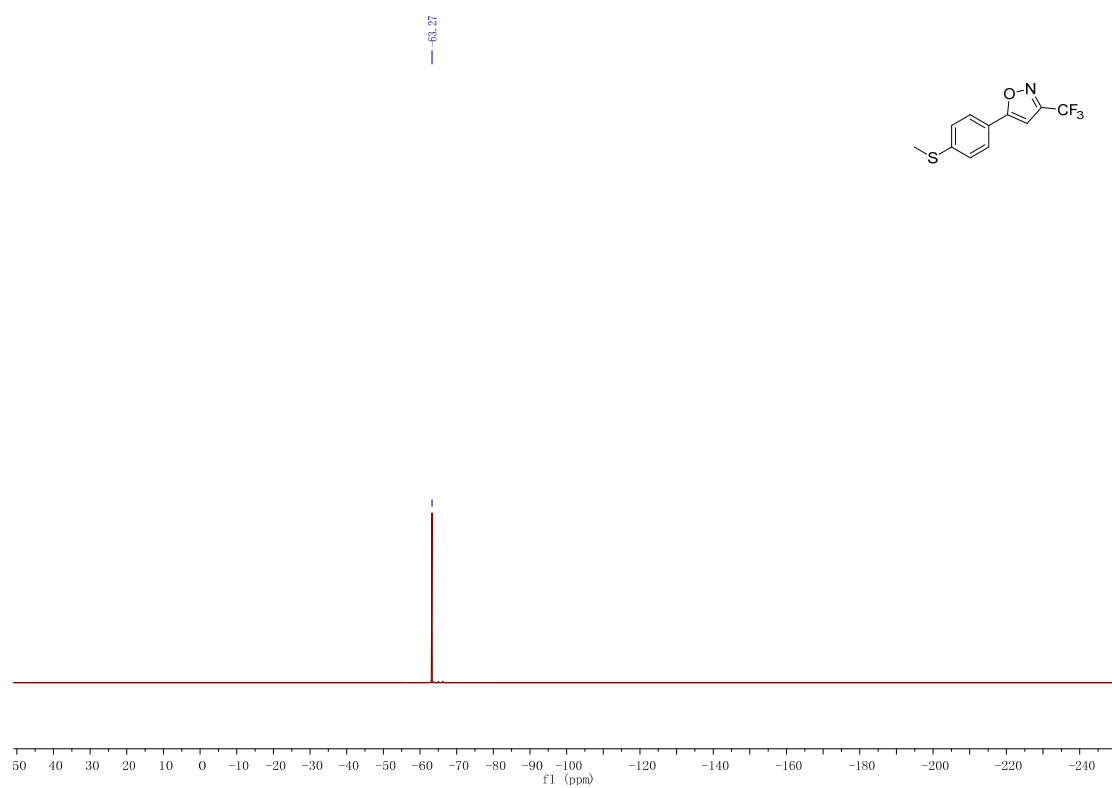
^{13}C NMR (CDCl₃, 100 MHz) of **9n**



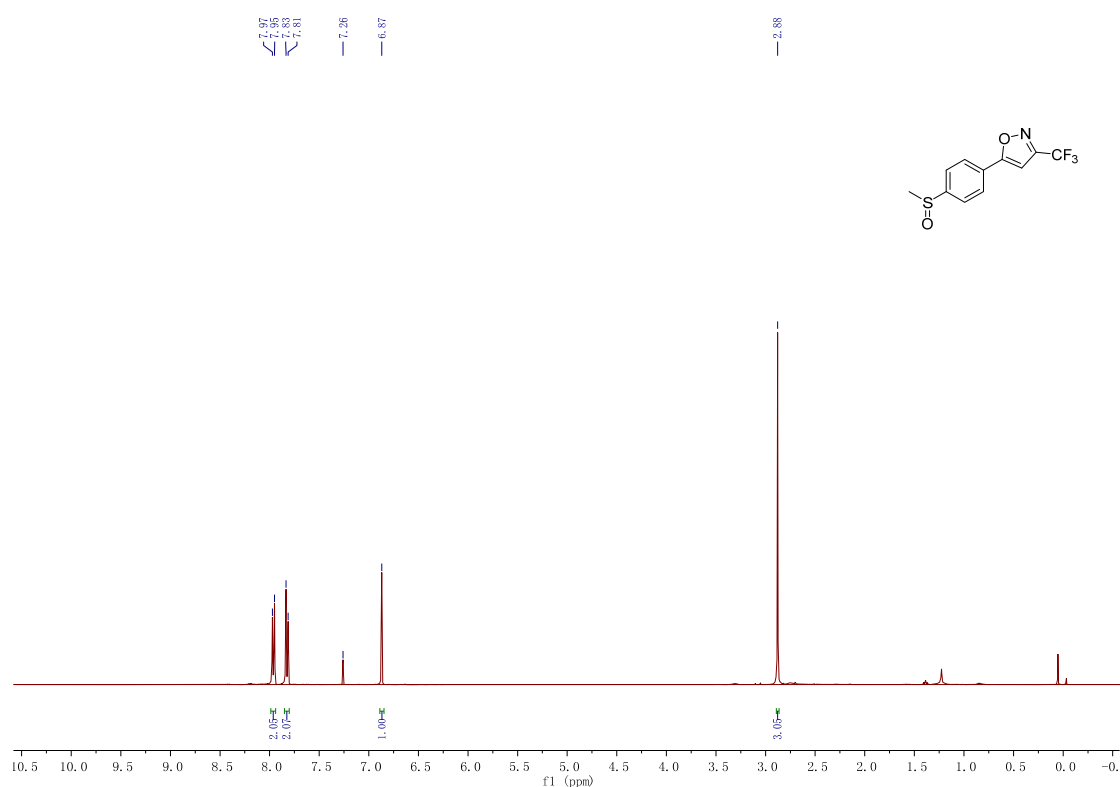
^{19}F NMR (CDCl₃, 376 MHz) of **9n**



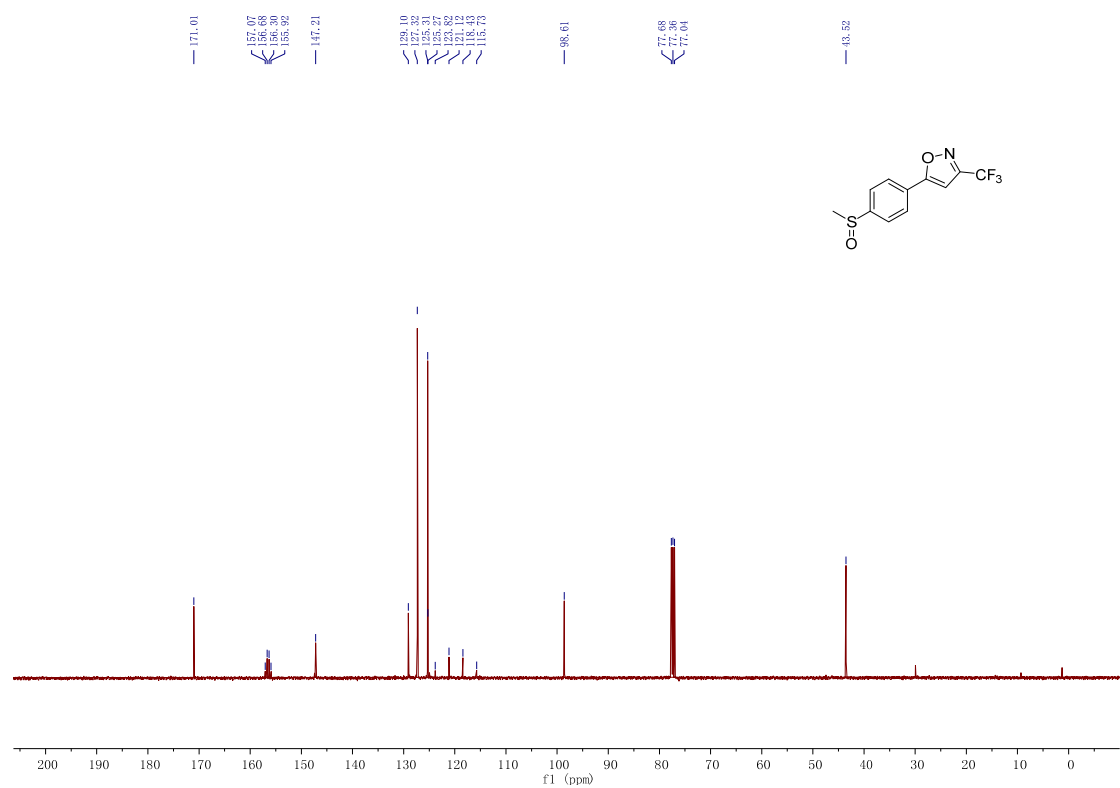
^{19}F { ^1H } NMR (CDCl₃, 376 MHz) of **9n**



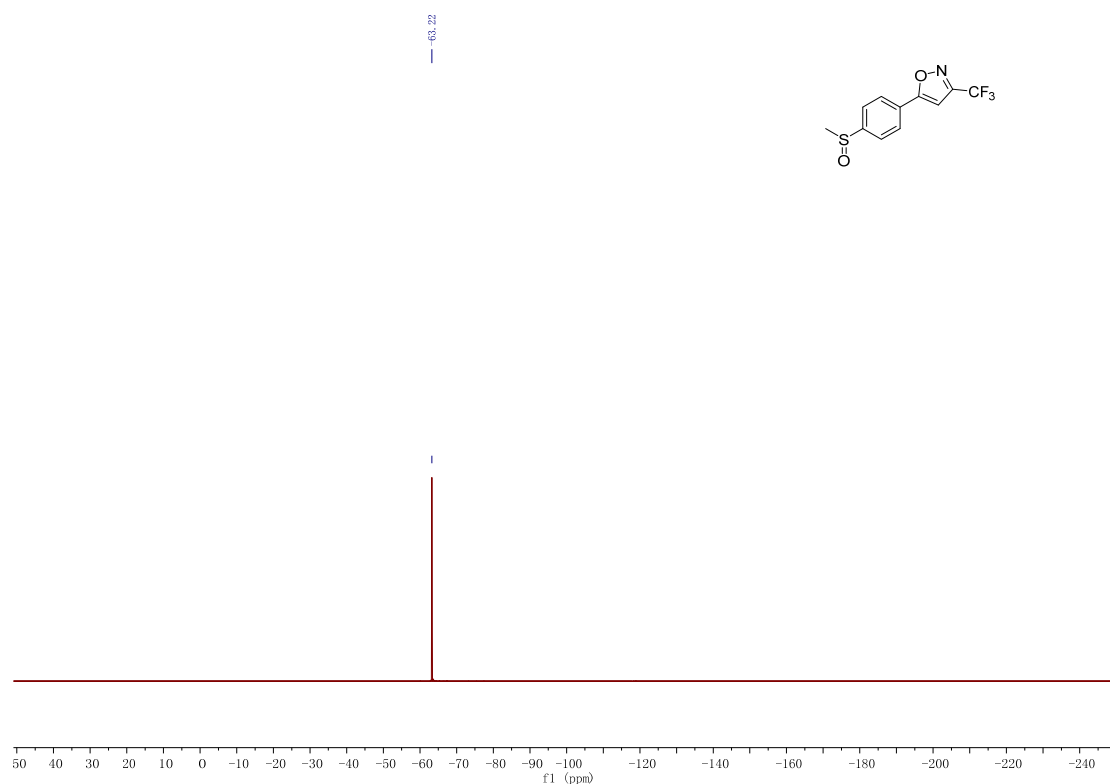
^1H NMR (CDCl₃, 400 MHz) of **9o**



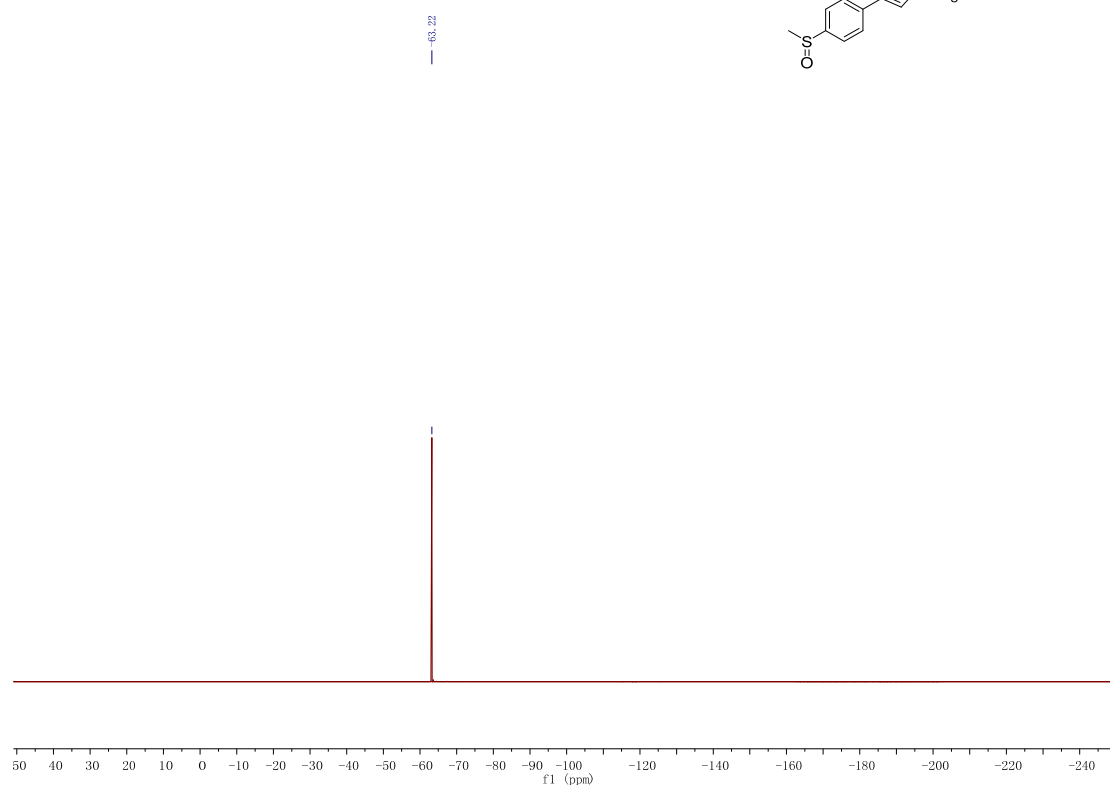
^{13}C NMR (CDCl₃, 100 MHz) of **9o**



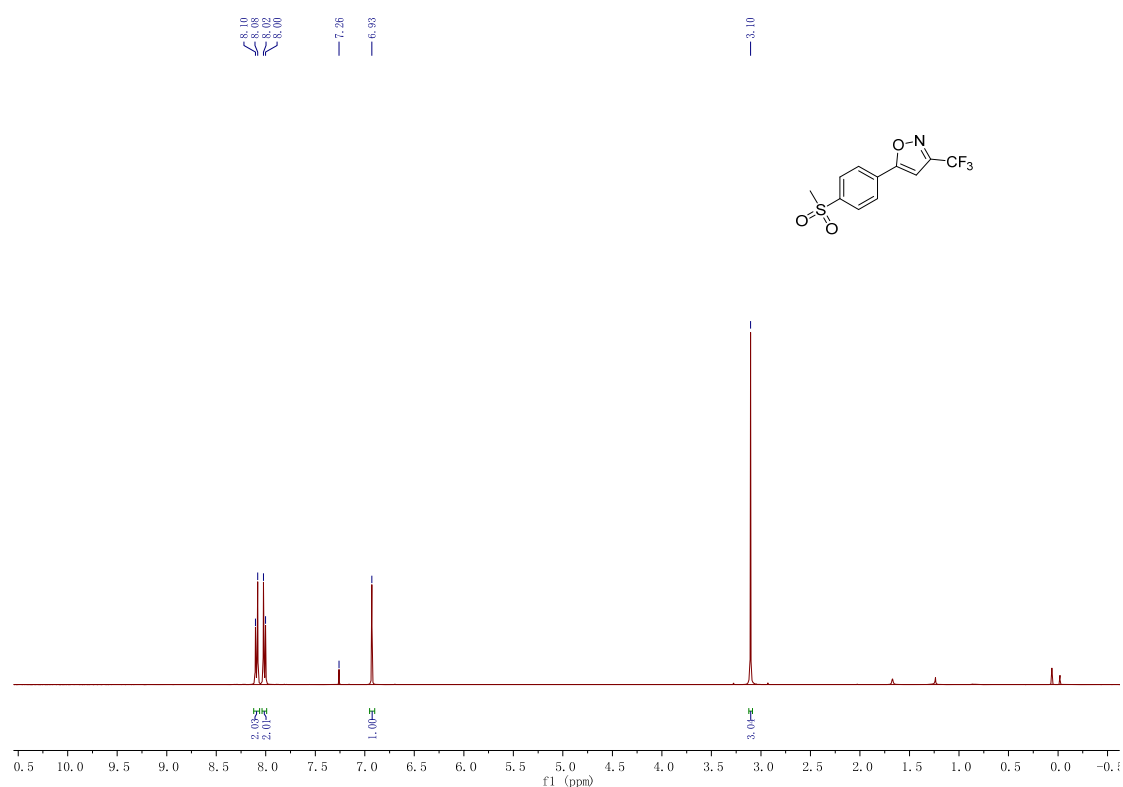
^{19}F NMR (CDCl₃, 376 MHz) of **9o**



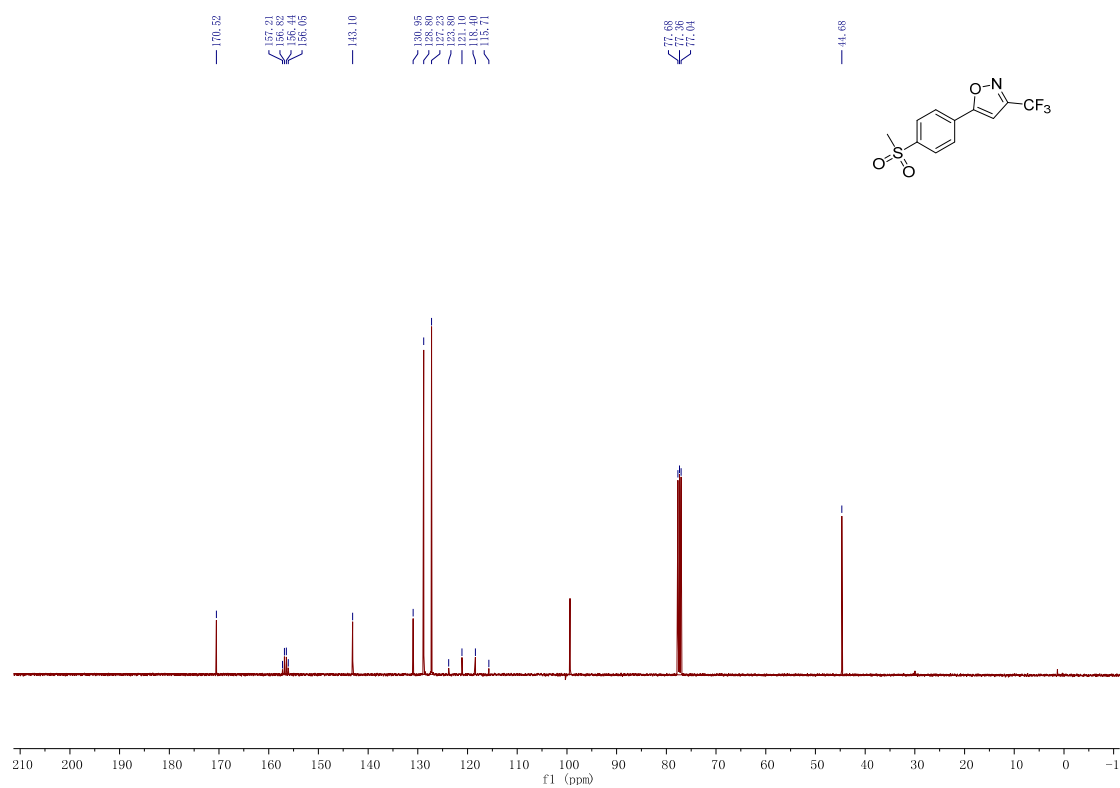
^{19}F { ^1H } NMR (CDCl₃, 376 MHz) of **9o**



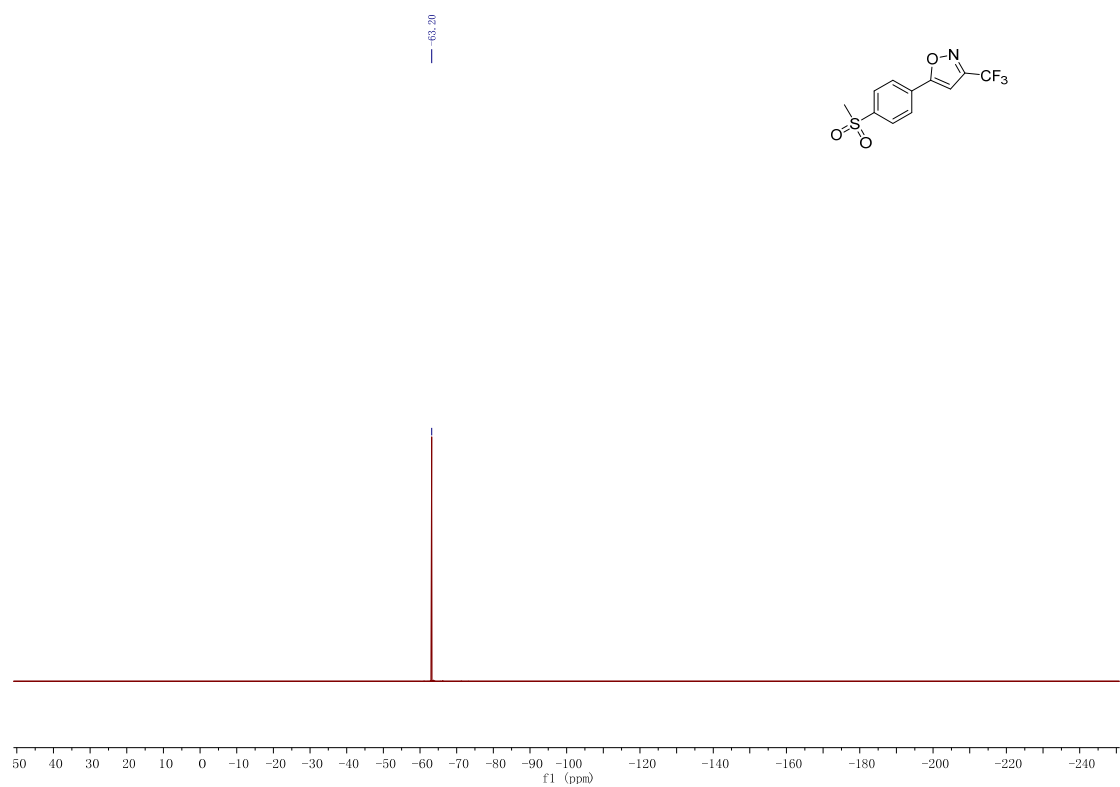
^1H NMR (CDCl₃, 400 MHz) of **9p**



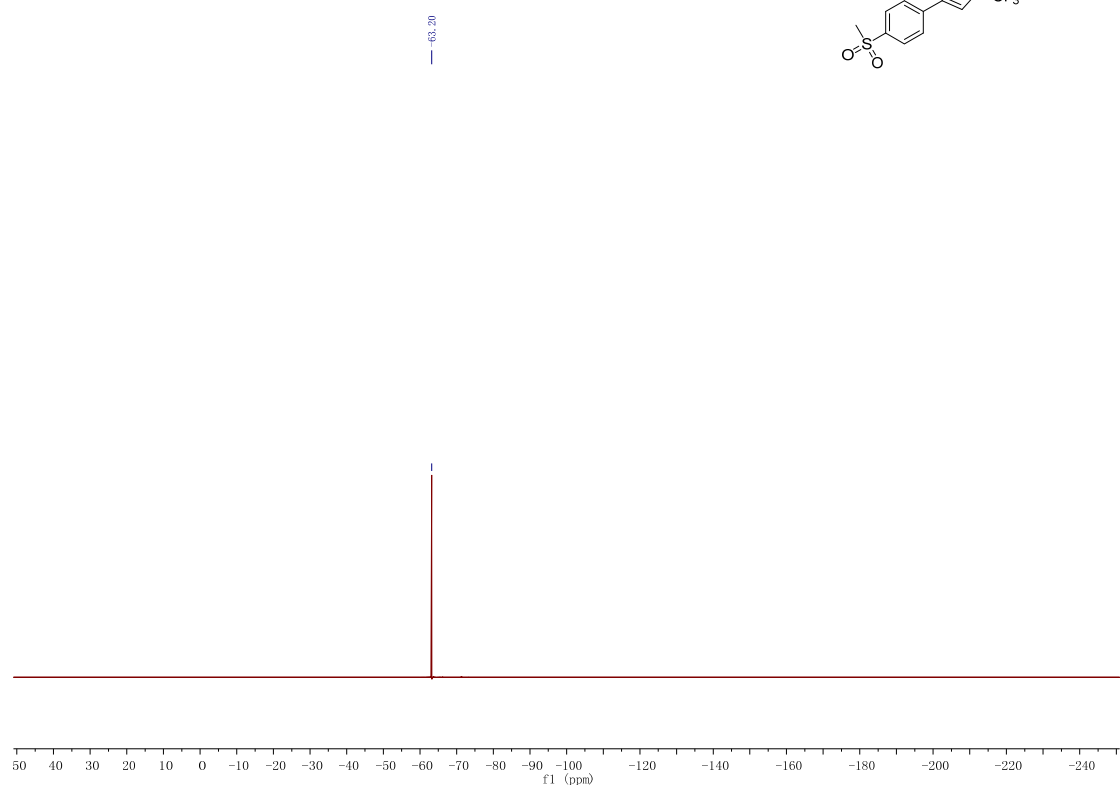
^{13}C NMR (CDCl₃, 100 MHz) of **9p**



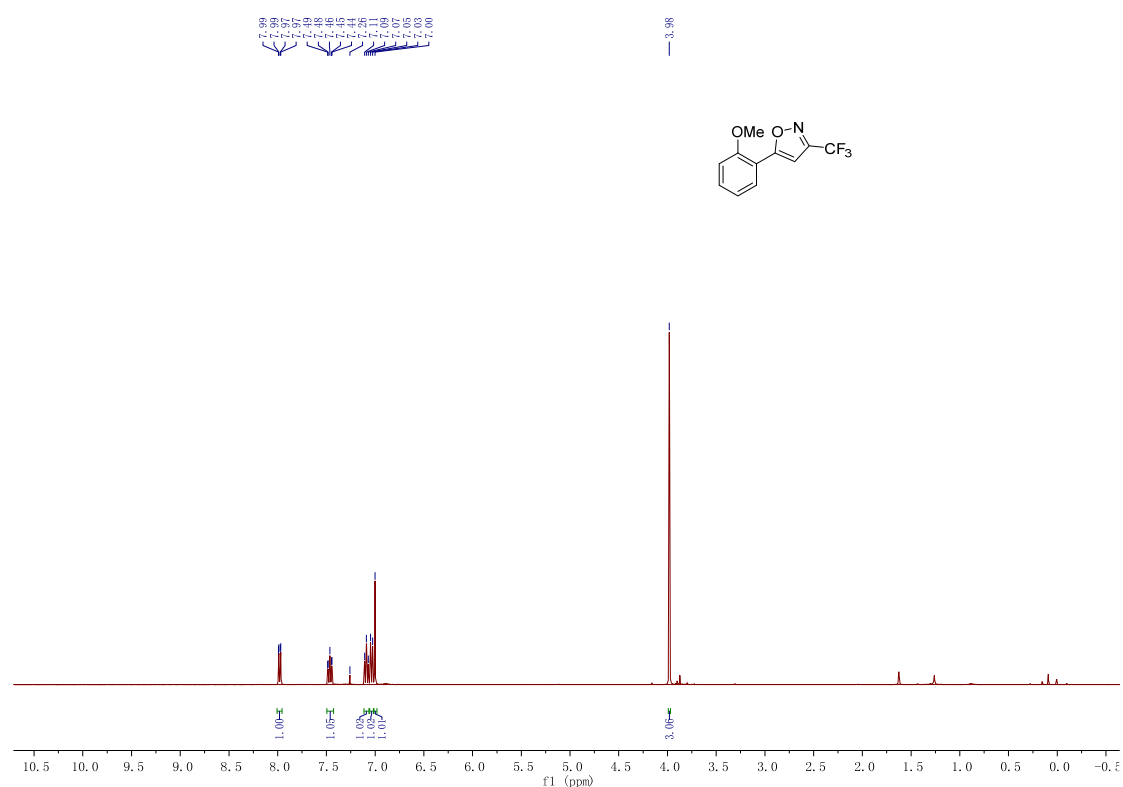
^{19}F NMR (CDCl₃, 376 MHz) of **9p**



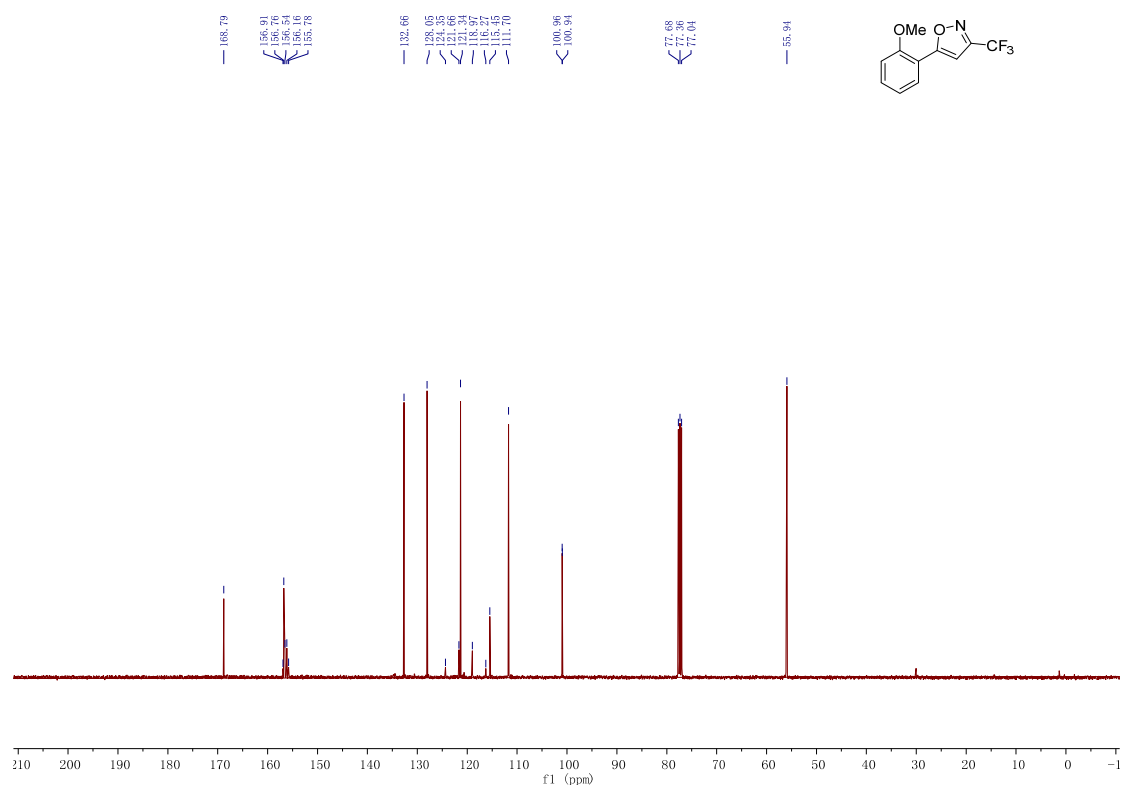
^{19}F { ^1H } NMR (CDCl₃, 376 MHz) of **9p**



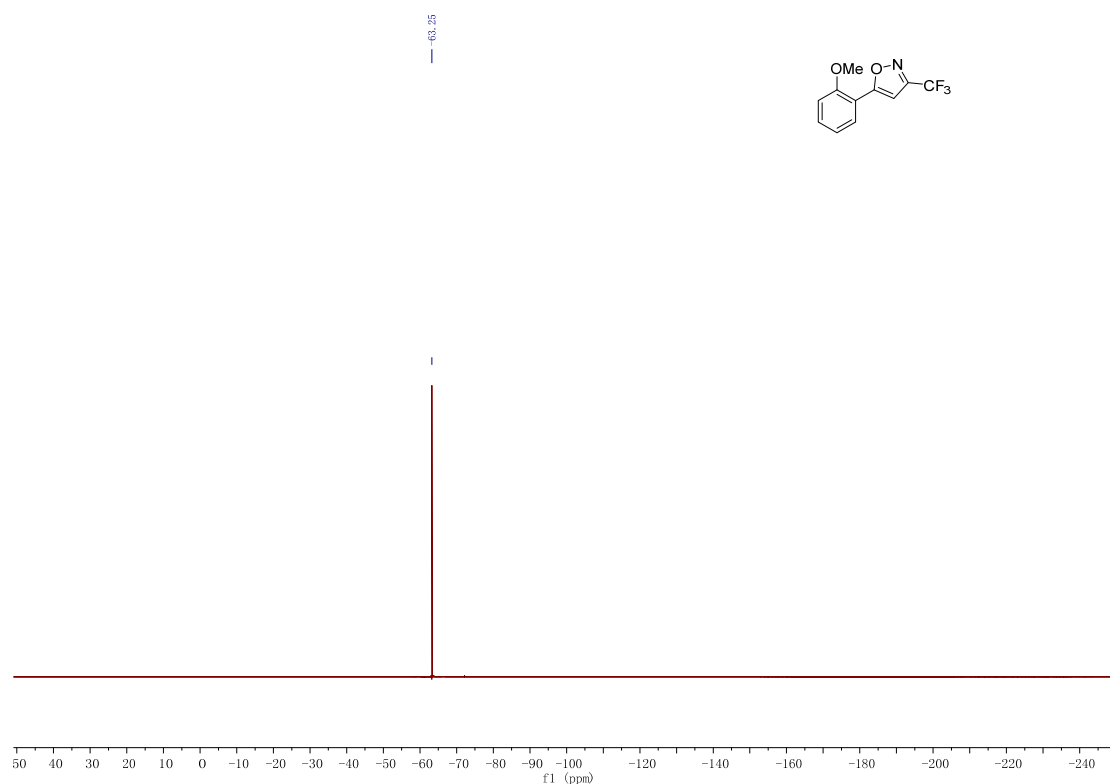
¹H NMR (CDCl₃, 400 MHz) of 9q



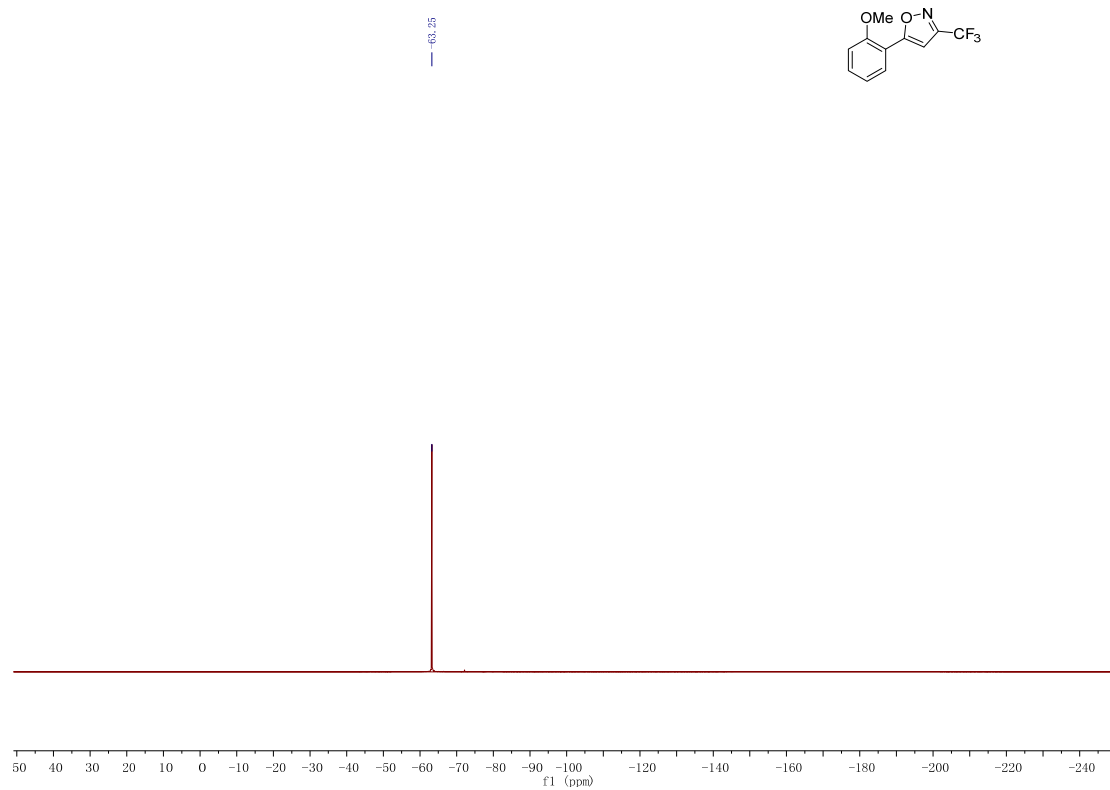
¹³C NMR (CDCl₃, 100 MHz) of 9q



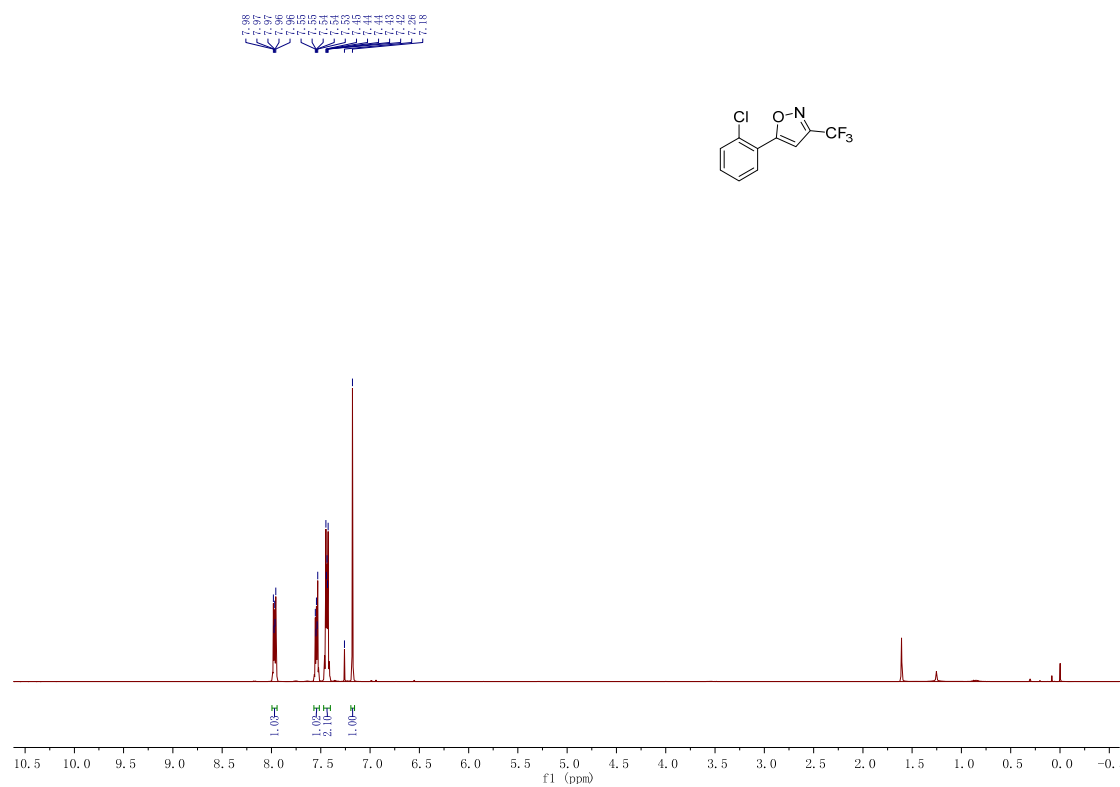
^{19}F NMR (CDCl₃, 376 MHz) of **9q**



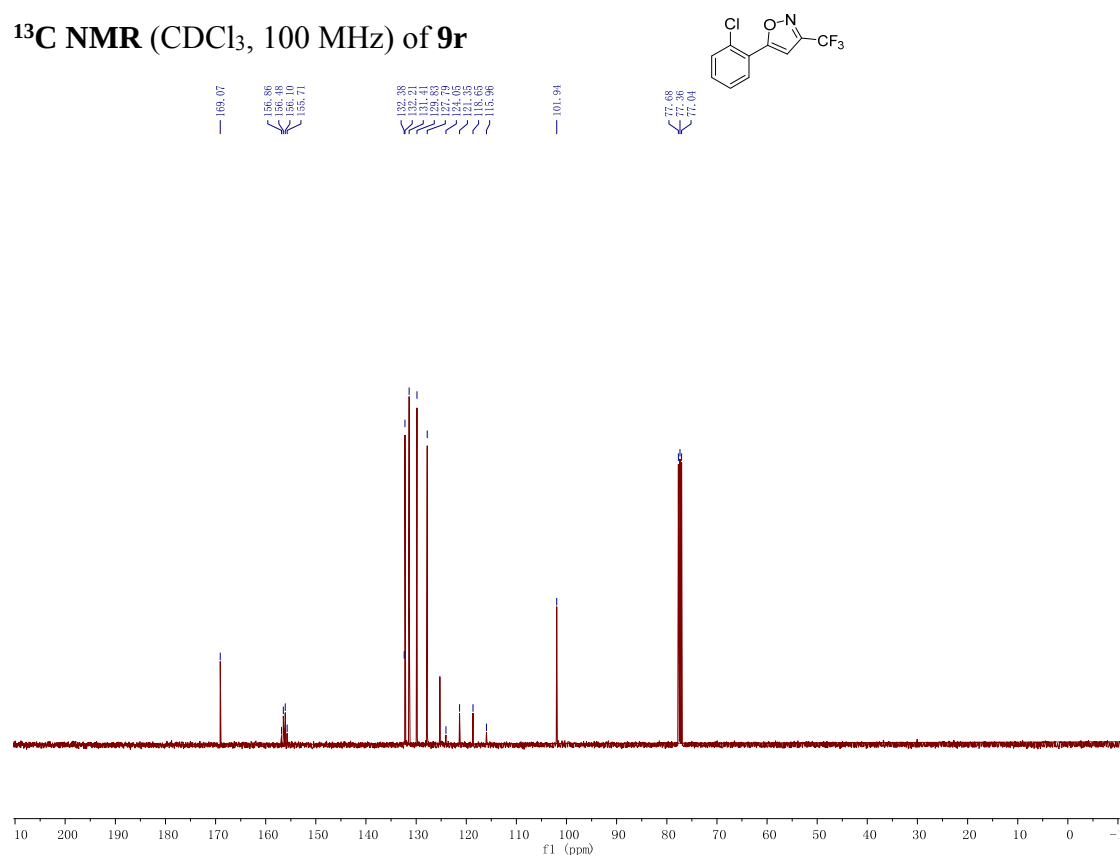
^{19}F { ^1H } NMR (CDCl₃, 376 MHz) of **9q**



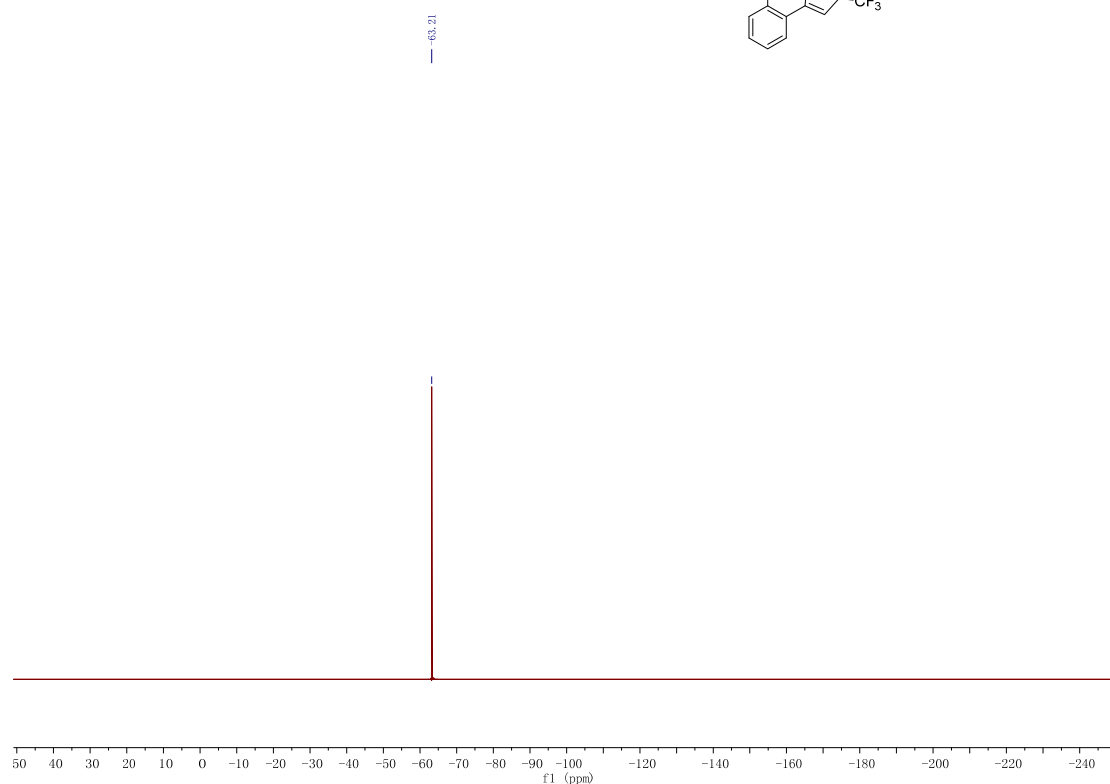
^1H NMR (CDCl₃, 400 MHz) of **9r**



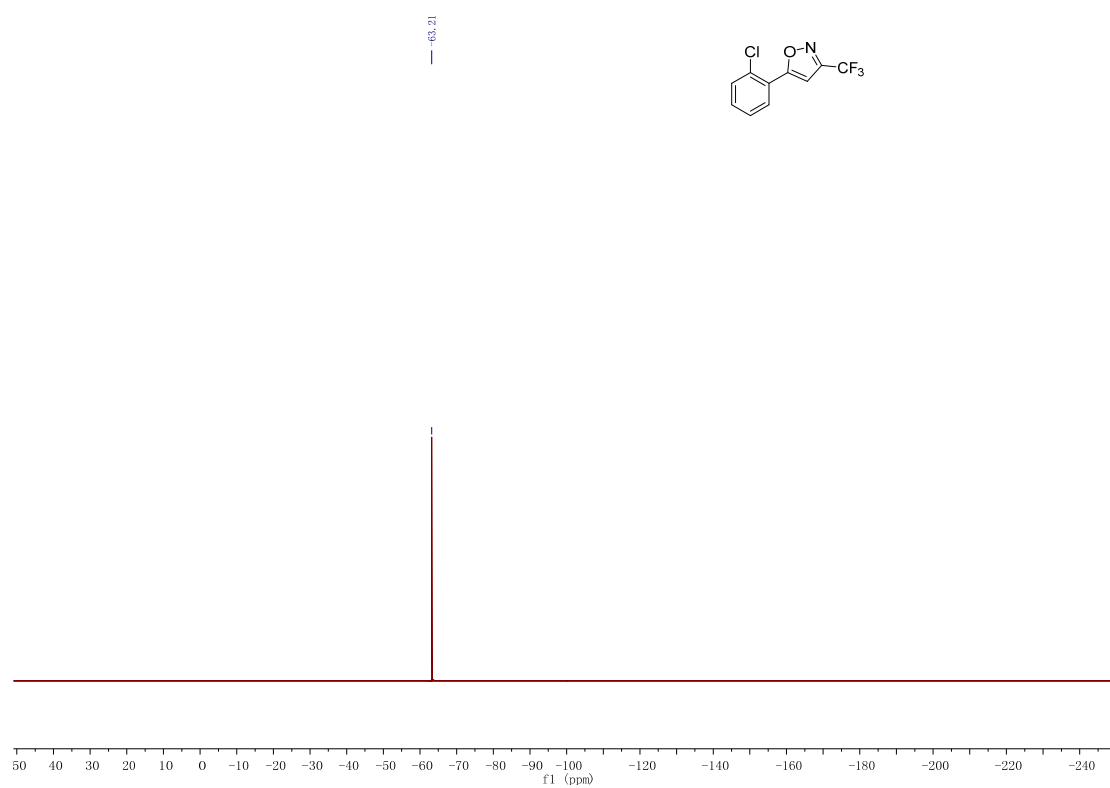
^{13}C NMR (CDCl₃, 100 MHz) of **9r**



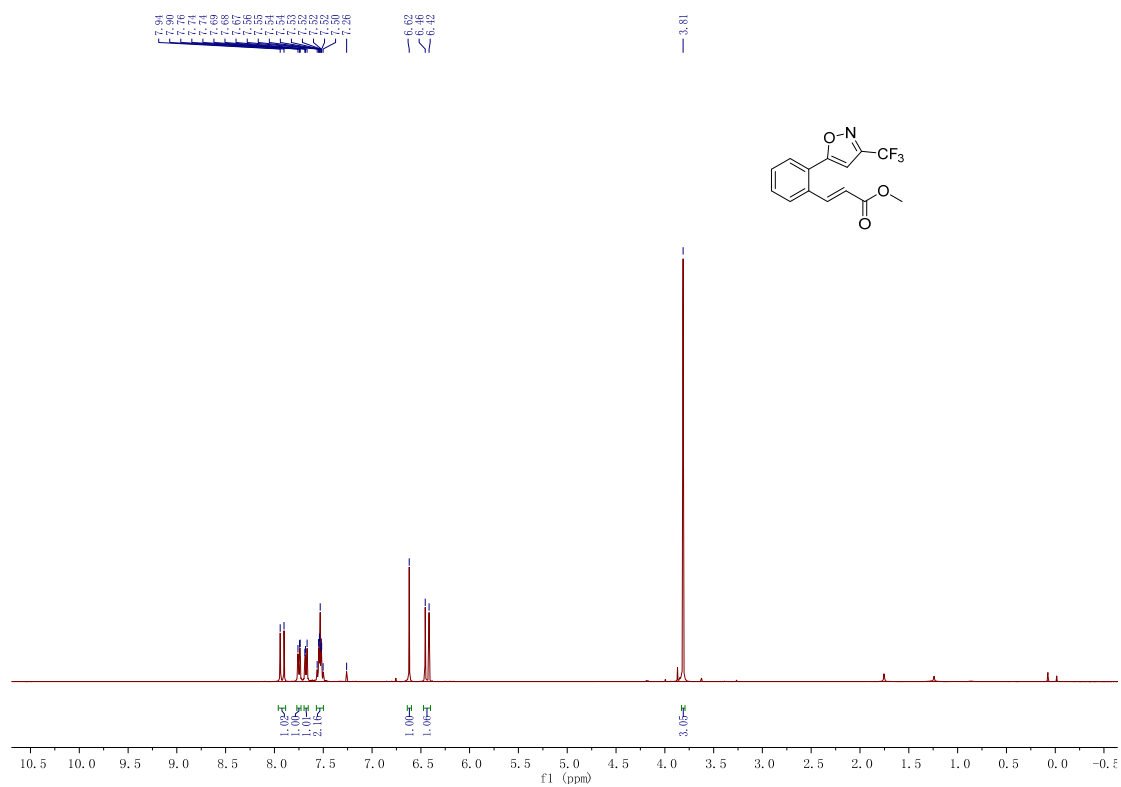
^{19}F NMR (CDCl₃, 376 MHz) of **9r**



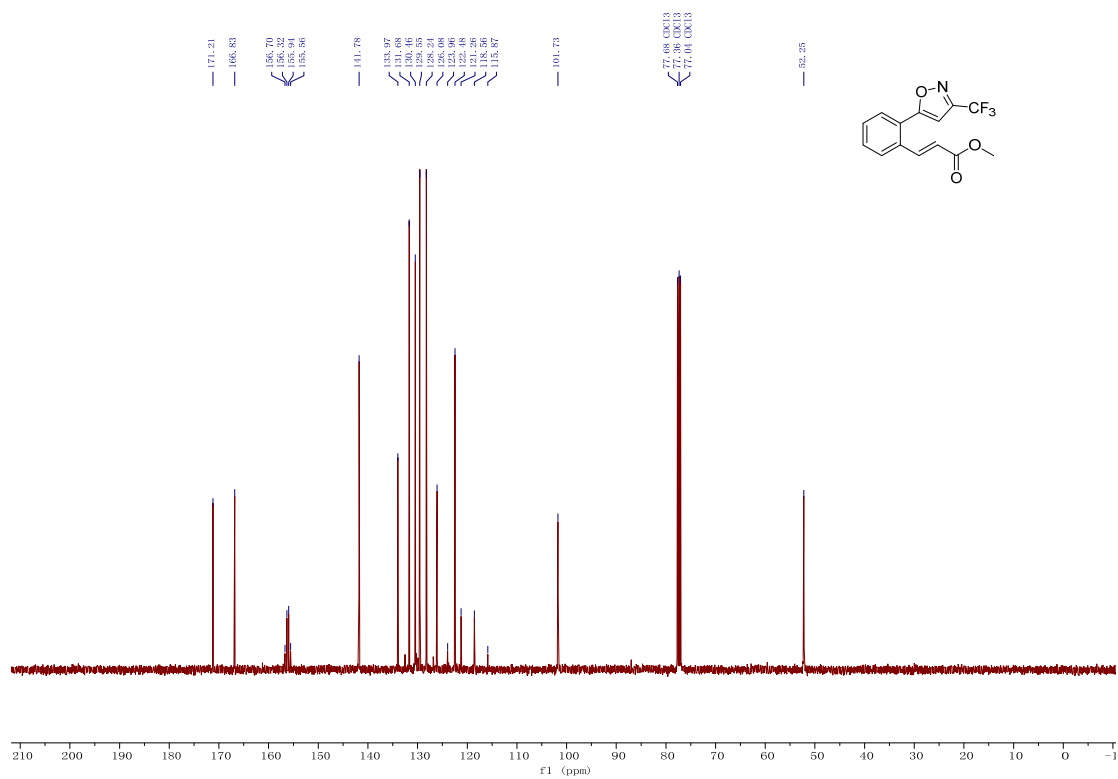
^{19}F { ^1H } NMR (CDCl₃, 376 MHz) of **9r**



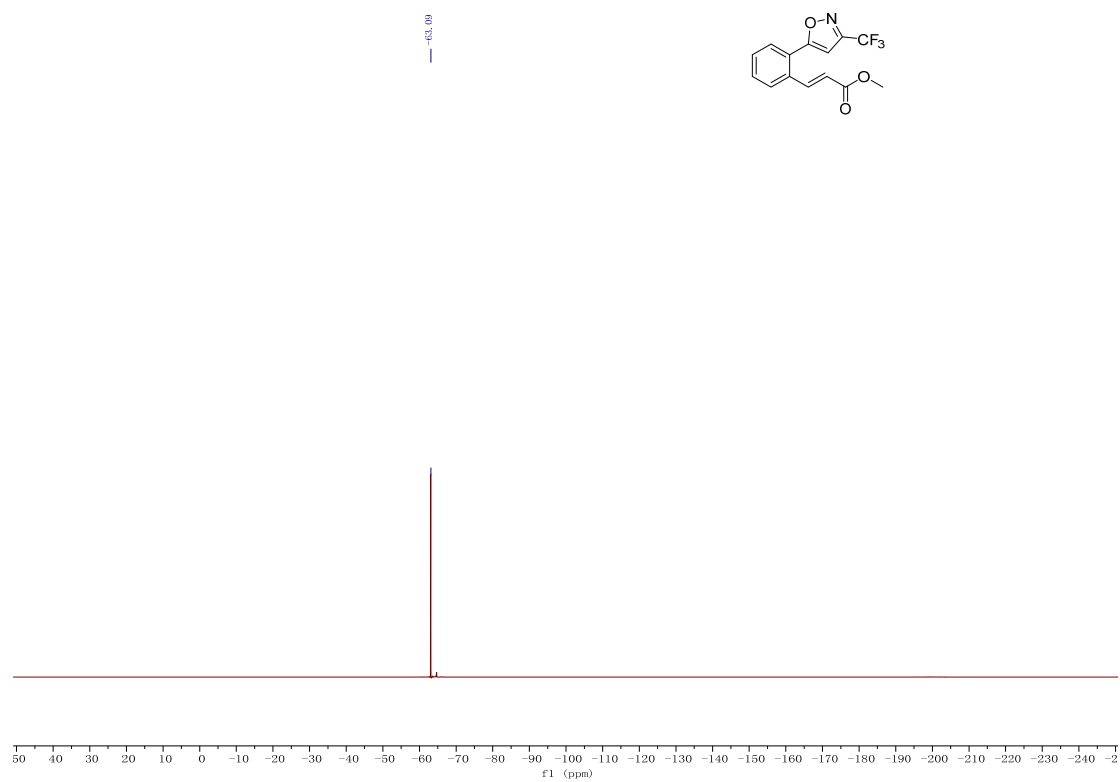
^1H NMR (CDCl₃, 400 MHz) of **9s**



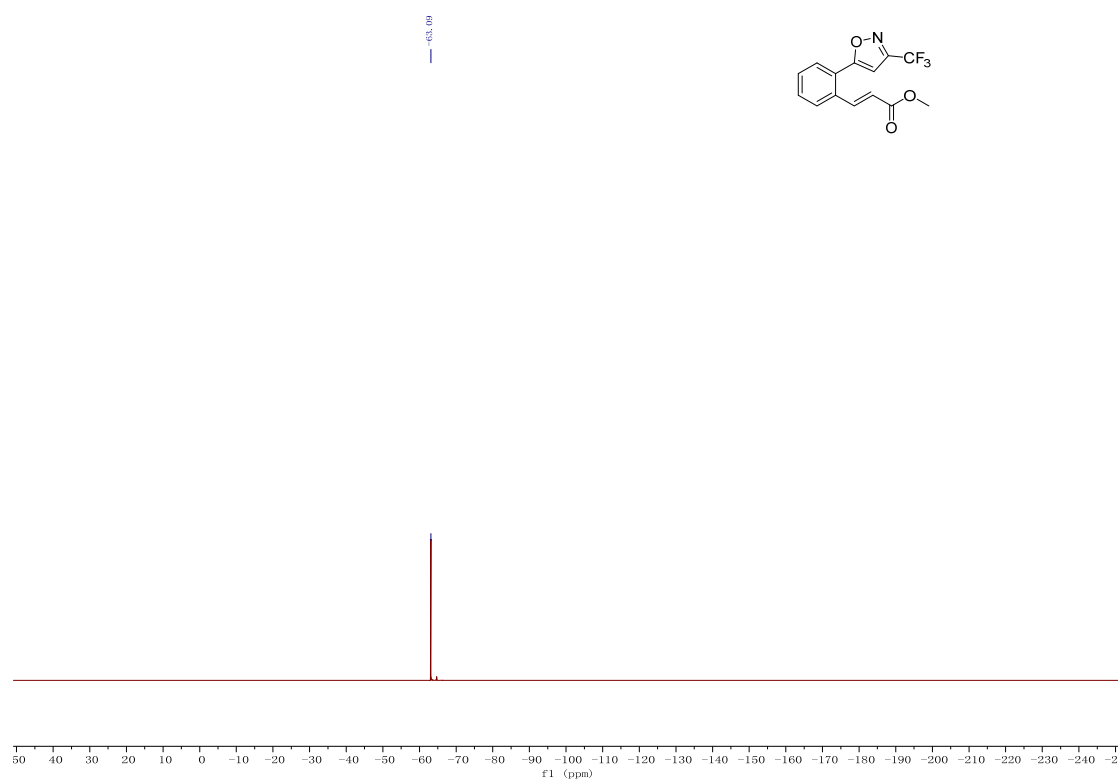
^{13}C NMR (CDCl₃, 100 MHz) of **9s**



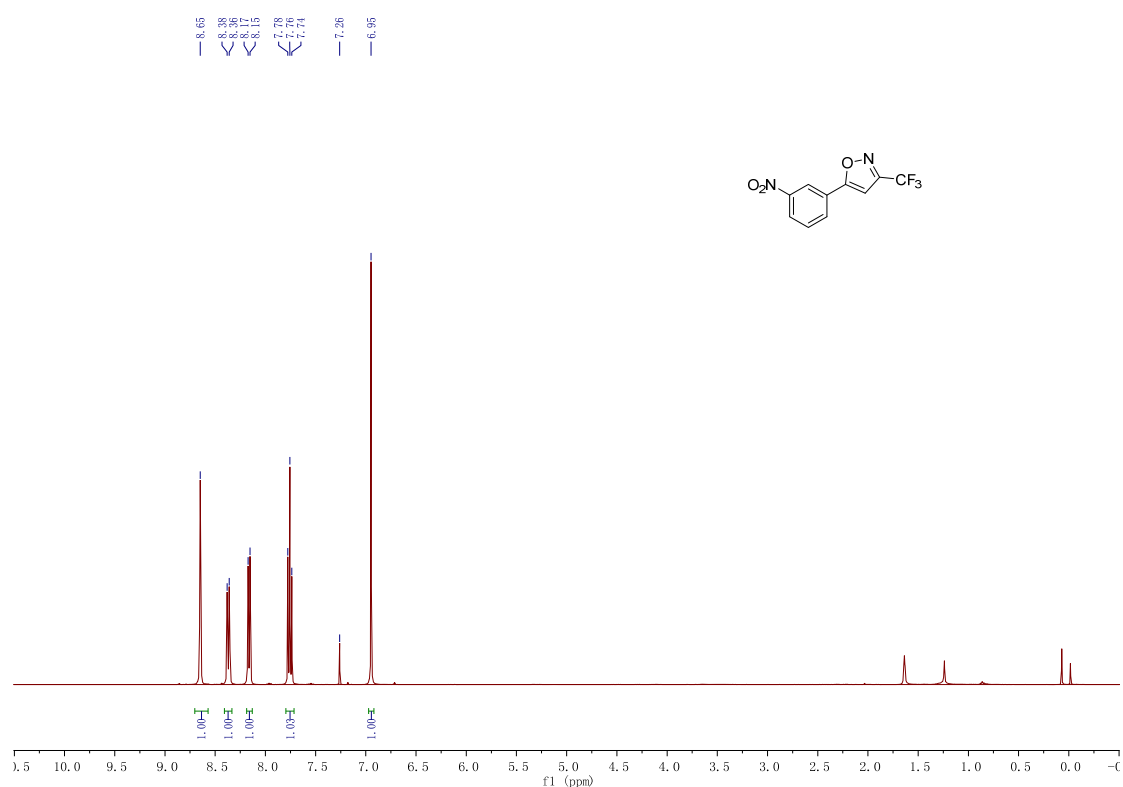
^{19}F NMR (CDCl₃, 376 MHz) of **9s**



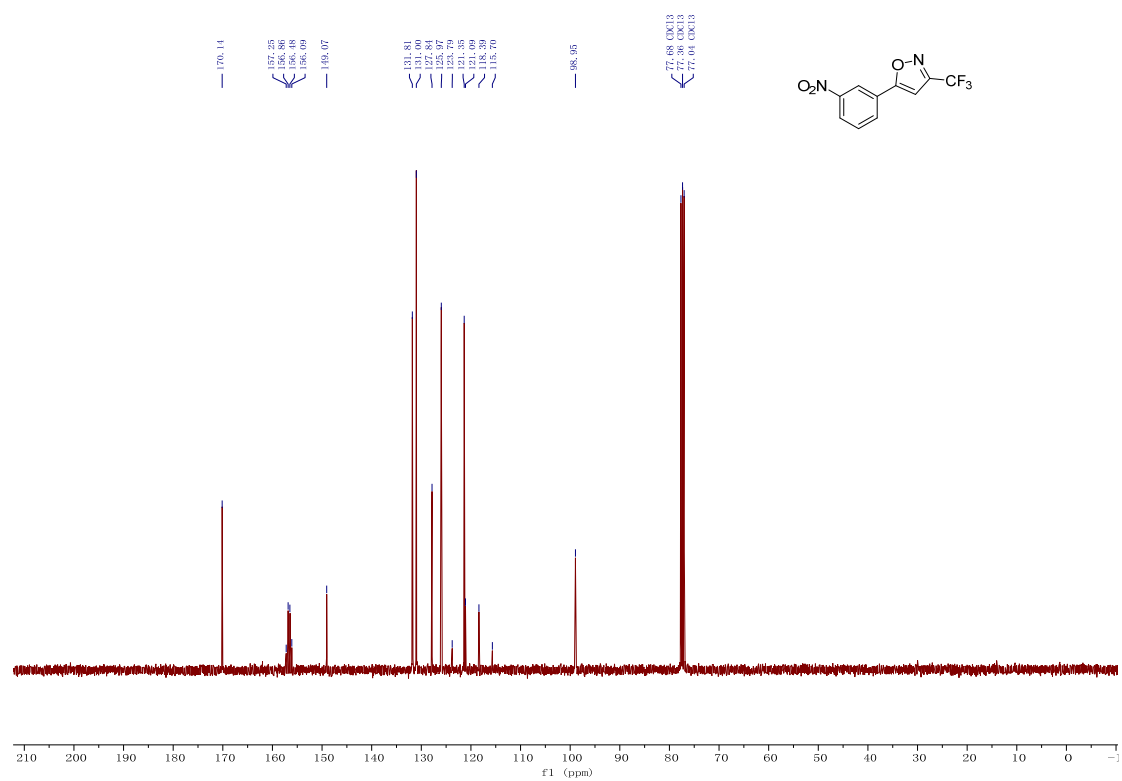
^{19}F { ^1H } NMR (CDCl₃, 376 MHz) of **9s**



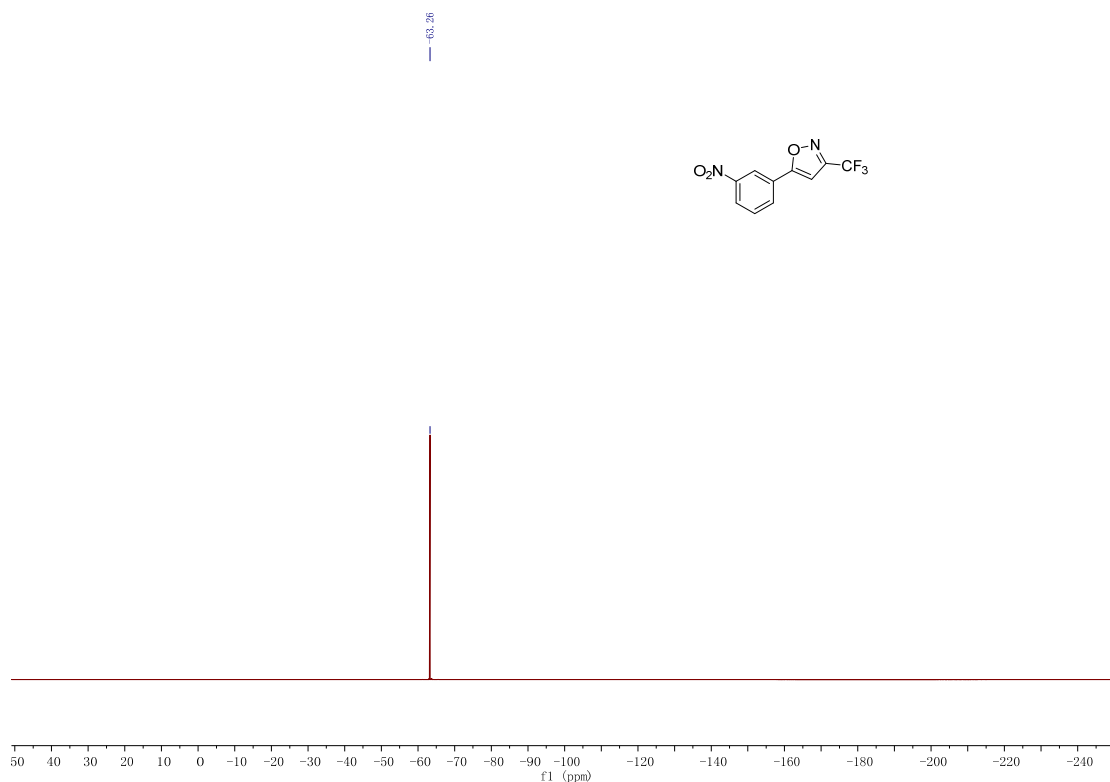
^1H NMR (CDCl₃, 400 MHz) of **9t**



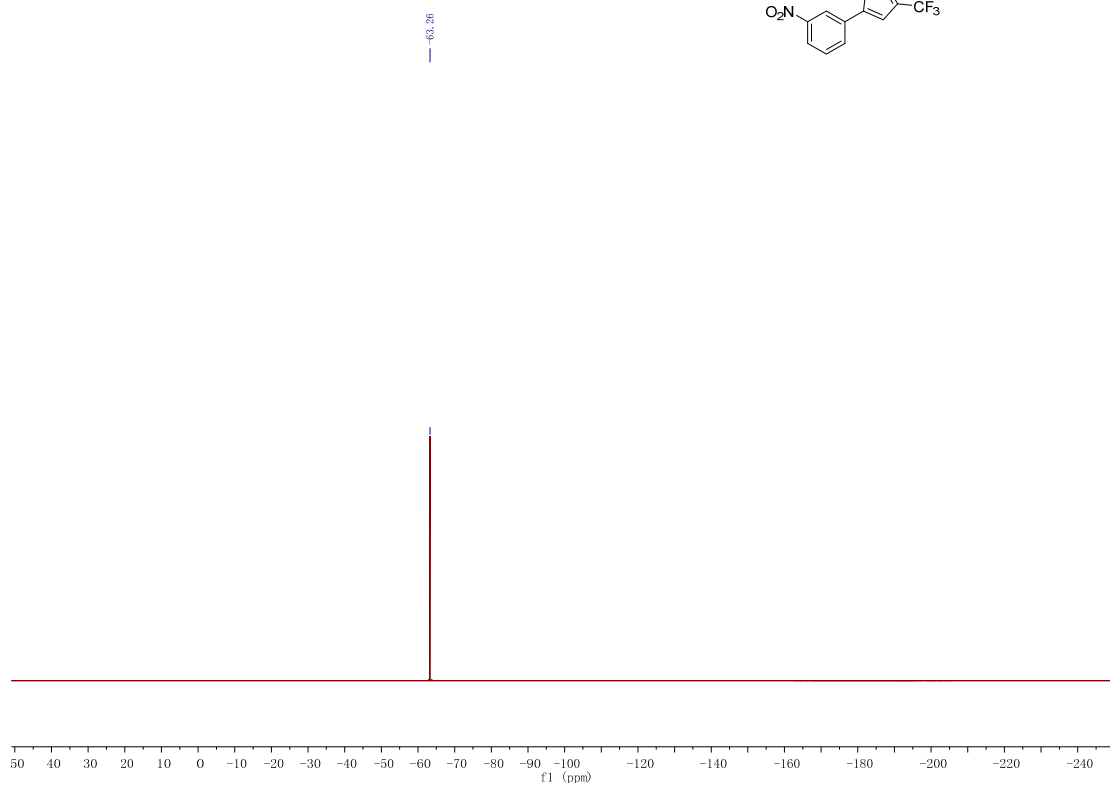
^{13}C NMR (CDCl₃, 100 MHz) of **9t**



^{19}F NMR (CDCl₃, 376 MHz) of **9t**



^{19}F { ^1H } NMR (CDCl₃, 376 MHz) of **9t**



FC(F)(F)c1cc(oc1-c2ccc(F)cc2)[N+]([O-])=O

Chemical structure of 2-(4-fluorophenyl)-5-(trifluoromethyl)-1,3,4-oxadiazole.

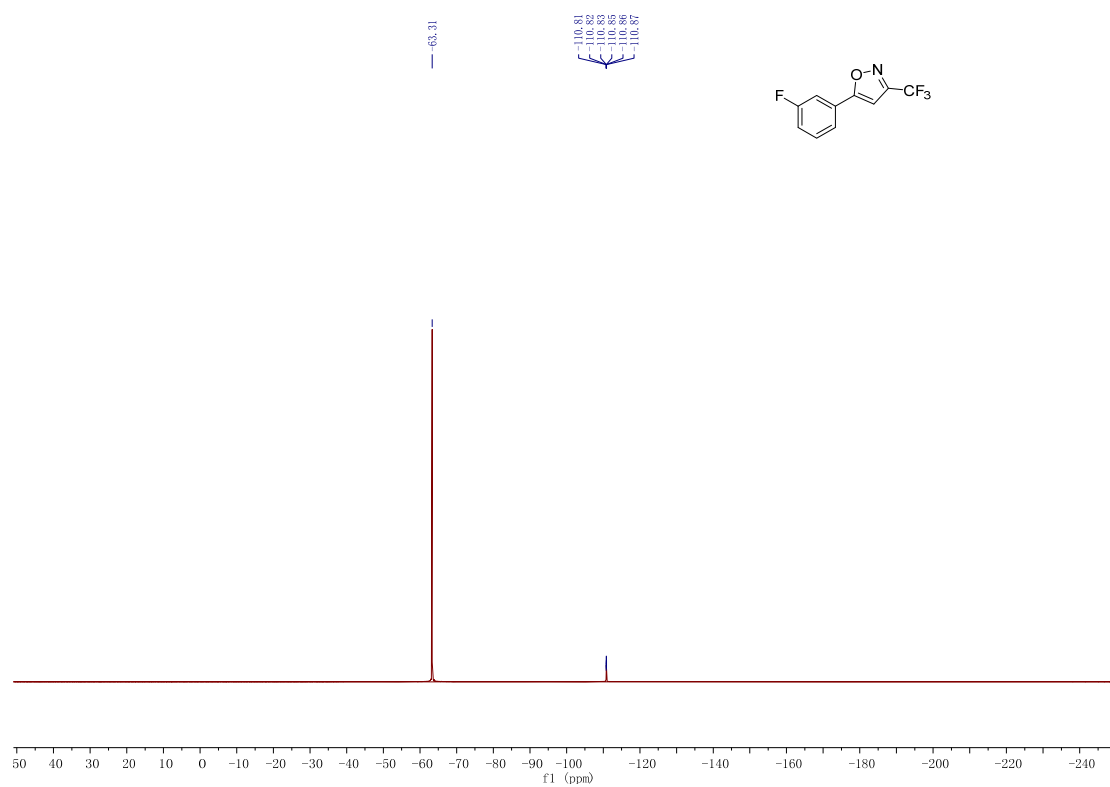
¹H NMR spectrum (CDCl₃) showing peaks at 7.64 (d, 2H), 7.54 (d, 2H), 7.44 (t, 2H), 7.34 (t, 2H), 7.24 (t, 2H), 7.14 (t, 2H), 7.04 (t, 2H), 6.94 (t, 2H), 6.84 (t, 2H), 6.74 (t, 2H), 6.64 (t, 2H), 6.54 (t, 2H), 6.44 (t, 2H), 6.34 (t, 2H), 6.24 (t, 2H), 6.14 (t, 2H), 6.04 (t, 2H), 5.94 (t, 2H), 5.84 (t, 2H), 5.74 (t, 2H), 5.64 (t, 2H), 5.54 (t, 2H), 5.44 (t, 2H), 5.34 (t, 2H), 5.24 (t, 2H), 5.14 (t, 2H), 5.04 (t, 2H), 4.94 (t, 2H), 4.84 (t, 2H), 4.74 (t, 2H), 4.64 (t, 2H), 4.54 (t, 2H), 4.44 (t, 2H), 4.34 (t, 2H), 4.24 (t, 2H), 4.14 (t, 2H), 4.04 (t, 2H), 3.94 (t, 2H), 3.84 (t, 2H), 3.74 (t, 2H), 3.64 (t, 2H), 3.54 (t, 2H), 3.44 (t, 2H), 3.34 (t, 2H), 3.24 (t, 2H), 3.14 (t, 2H), 3.04 (t, 2H), 2.94 (t, 2H), 2.84 (t, 2H), 2.74 (t, 2H), 2.64 (t, 2H), 2.54 (t, 2H), 2.44 (t, 2H), 2.34 (t, 2H), 2.24 (t, 2H), 2.14 (t, 2H), 2.04 (t, 2H), 1.94 (t, 2H), 1.84 (t, 2H), 1.74 (t, 2H), 1.64 (t, 2H), 1.54 (t, 2H), 1.44 (t, 2H), 1.34 (t, 2H), 1.24 (t, 2H), 1.14 (t, 2H), 1.04 (t, 2H), 1.00 (s, 3H), 0.94 (t, 2H), 0.84 (t, 2H), 0.74 (t, 2H), 0.64 (t, 2H), 0.54 (t, 2H), 0.44 (t, 2H), 0.34 (t, 2H), 0.24 (t, 2H), 0.14 (t, 2H), 0.04 (t, 2H), 0.00 (s, 3H).

Chemical structure: N#Cc1nc(Oc2ccc(F)cc2)c1

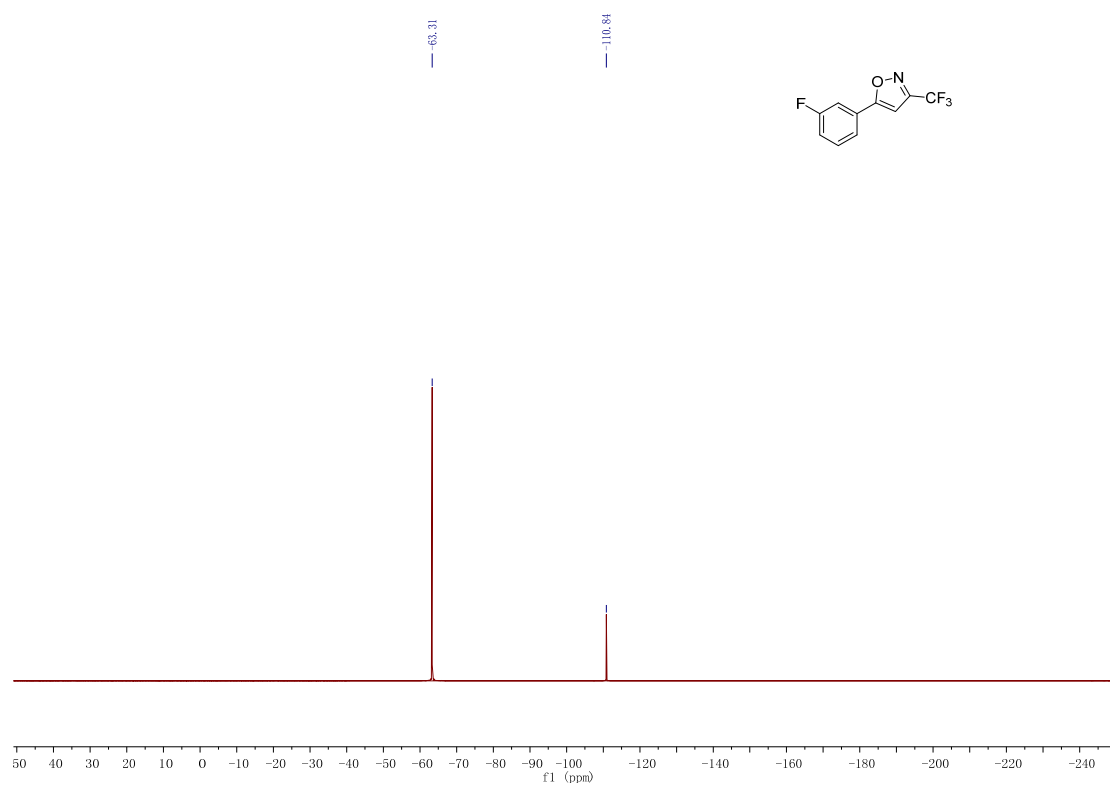
¹³C NMR spectrum (ppm):

- 171.46
- 171.43
- 164.56
- 162.09
- 157.04
- 156.60
- 156.59
- 155.89
- 131.51
- 131.43
- 128.25
- 128.23
- 125.96
- 122.78
- 122.77
- 121.57
- 118.75
- 118.54
- 118.54
- 113.88
- 113.82
- 97.94
- 77.68 CDCl₃
- 77.30 CDCl₃
- 77.04 CDCl₃
- 76.63

^{19}F NMR (CDCl₃, 376 MHz) of **9u**



^{19}F { ^1H } NMR (CDCl₃, 376 MHz) of **9u**



Chemical structure: Oc1ccc(cc1)-c2cc(C(F)(F)F)oc2=N

¹H NMR spectrum (ppm):

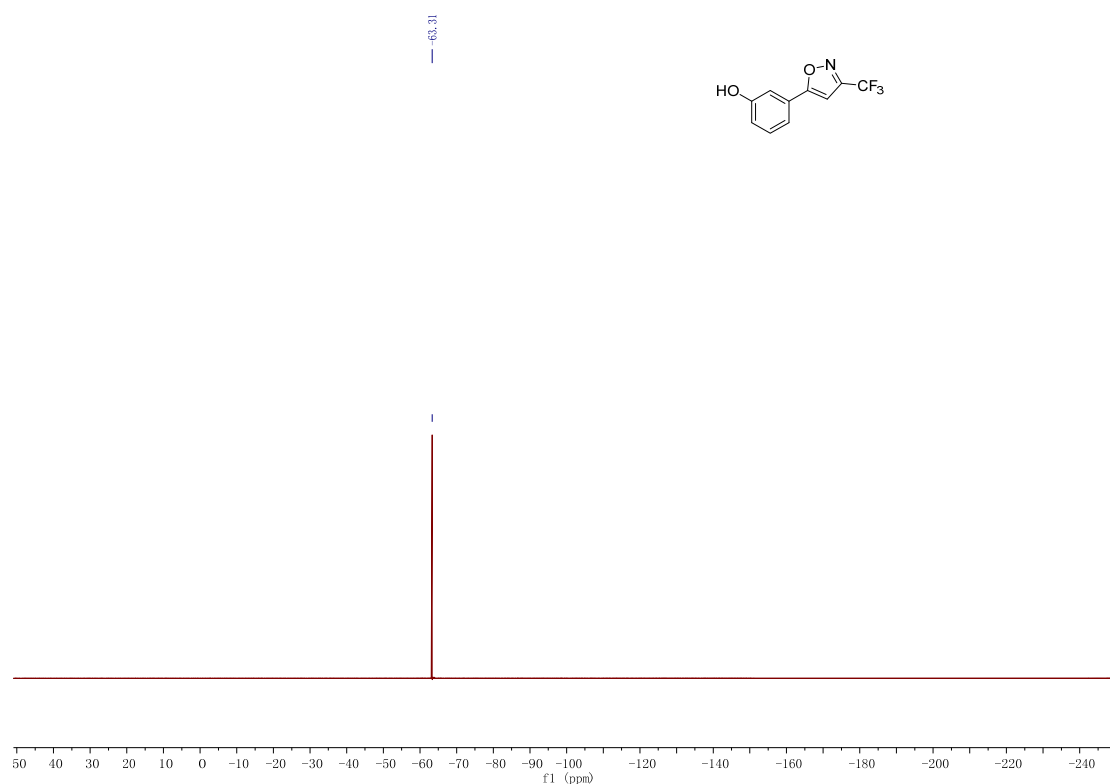
- 7.55 (d, 2H, integration 1.00)
- 7.45 (d, 2H, integration 2.00)
- 7.05 (d, 2H, integration 1.00)
- 6.95 (d, 2H, integration 1.00)
- 6.35 (s, 1H, integration 1.00)
- 6.55 (s, 1H, integration 1.00)

Chemical structure: Oc1ccc(cc1)-c2cc(C(F)(F)F)[n+]([O-])n2

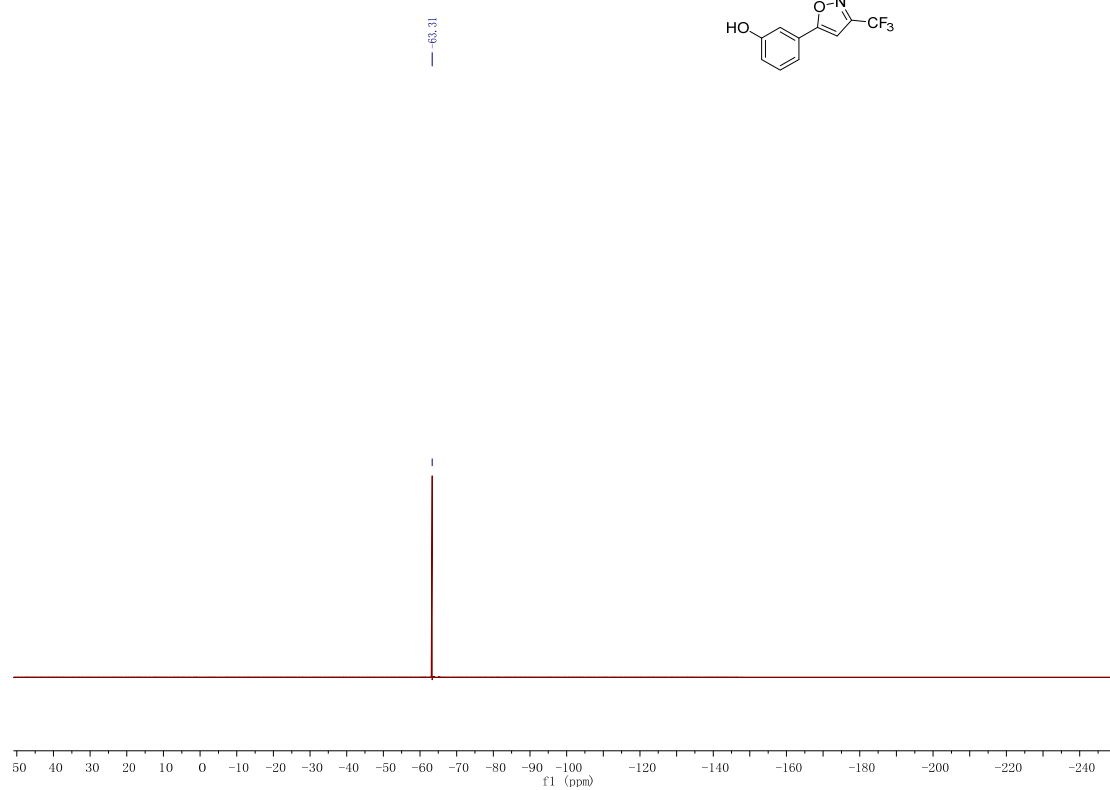
¹³C NMR spectrum (CDCl₃) peaks (ppm):

- 172.73
- 156.96
- 156.58
- 156.19
- 155.51
- 131.08
- 127.39
- 123.14
- 121.24
- 119.15
- 118.83
- 118.53
- 115.81
- 113.00
- 97.47
- 77.68 (CDCl₃)
- 77.36 (CDCl₃)
- 77.04 (CDCl₃)

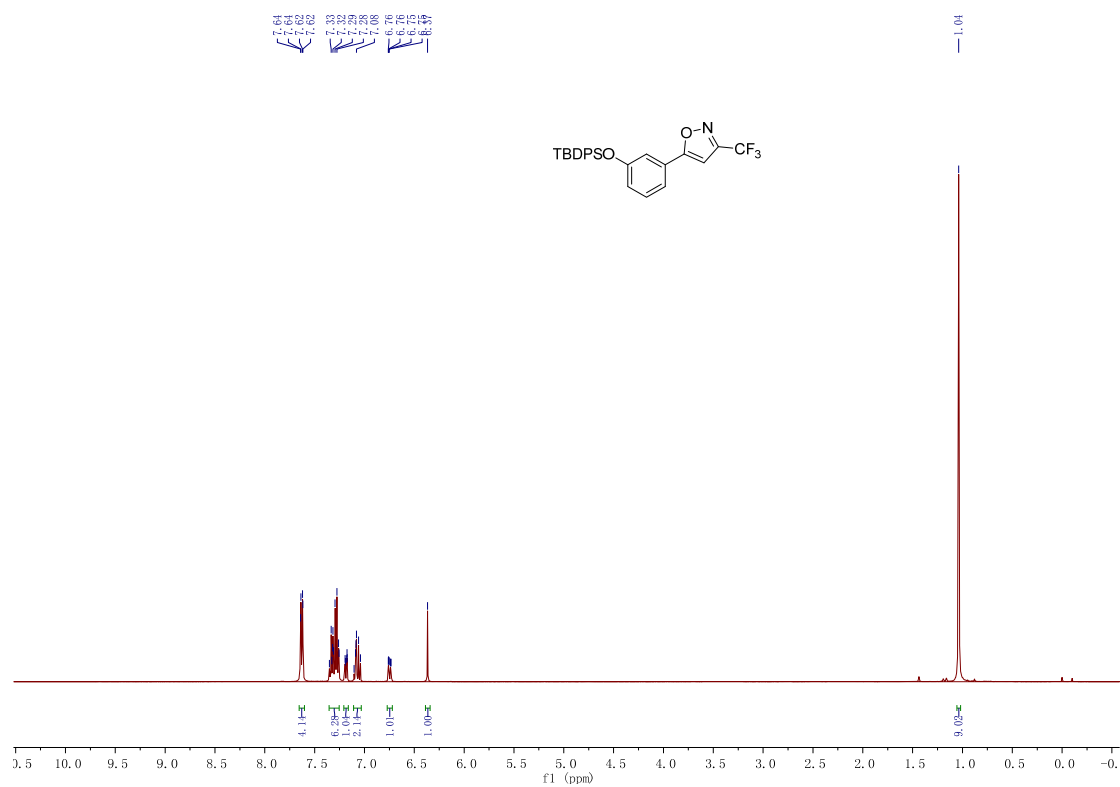
^{19}F NMR (CDCl₃, 376 MHz) of **9v**



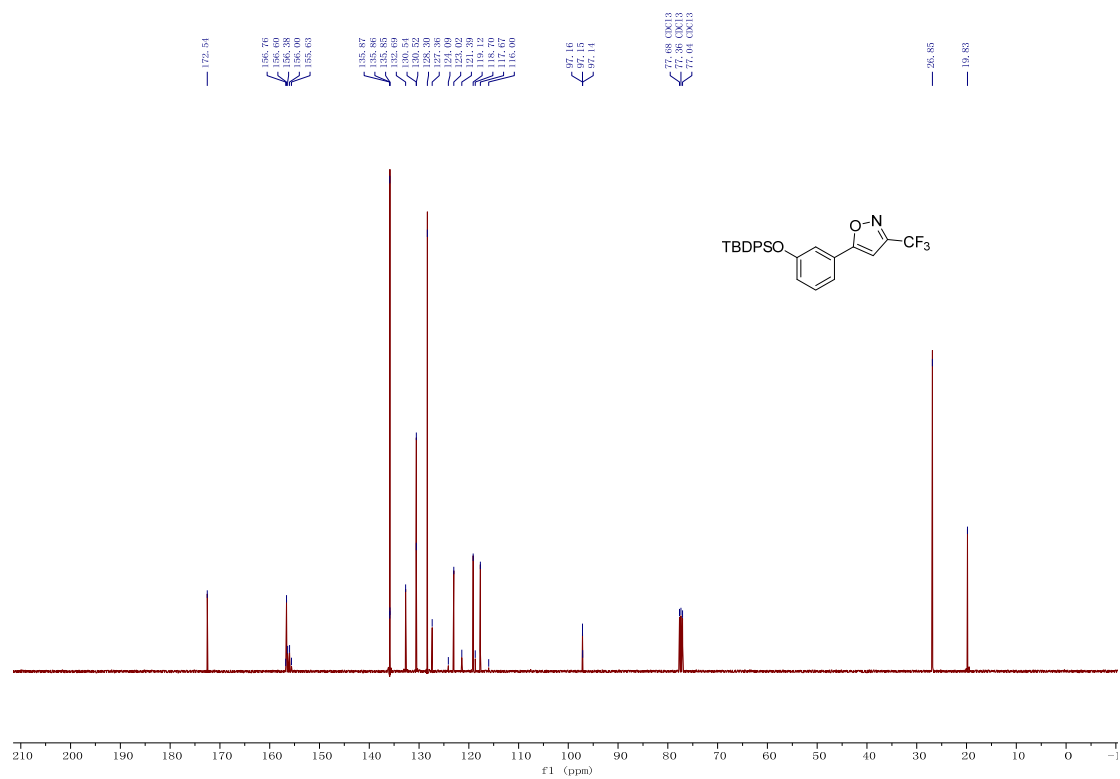
^{19}F { ^1H } NMR (CDCl₃, 376 MHz) of **9v**



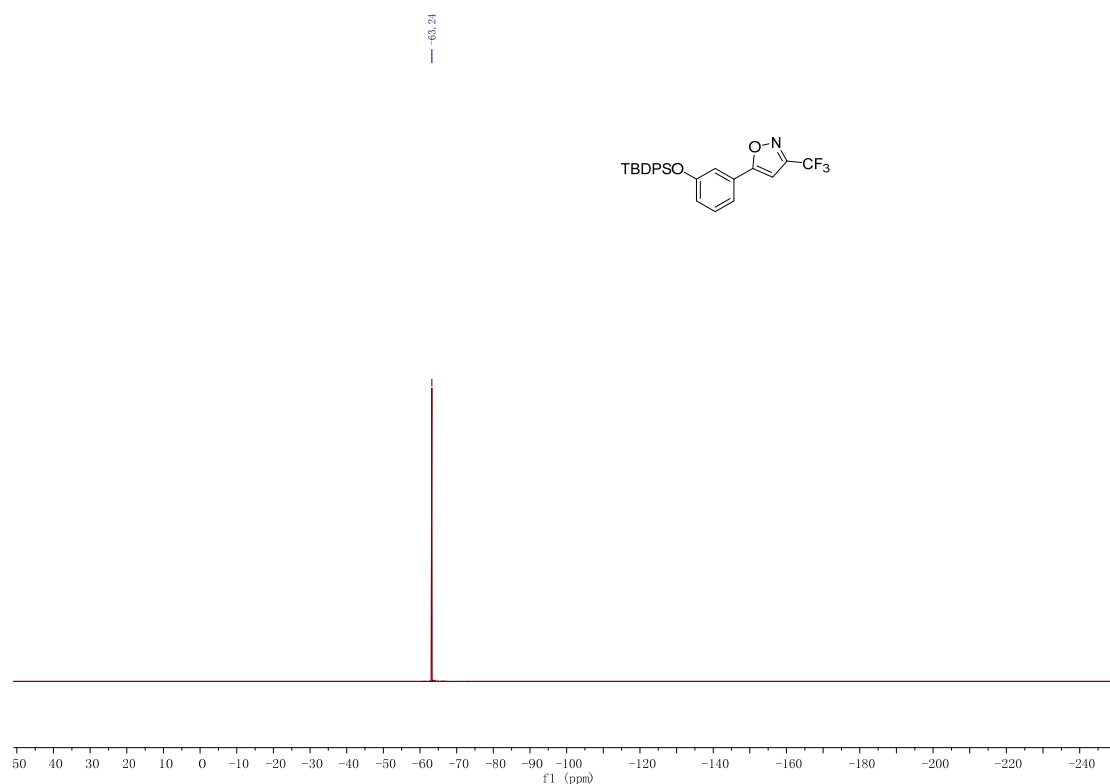
^1H NMR (CDCl₃, 400 MHz) of **9w**



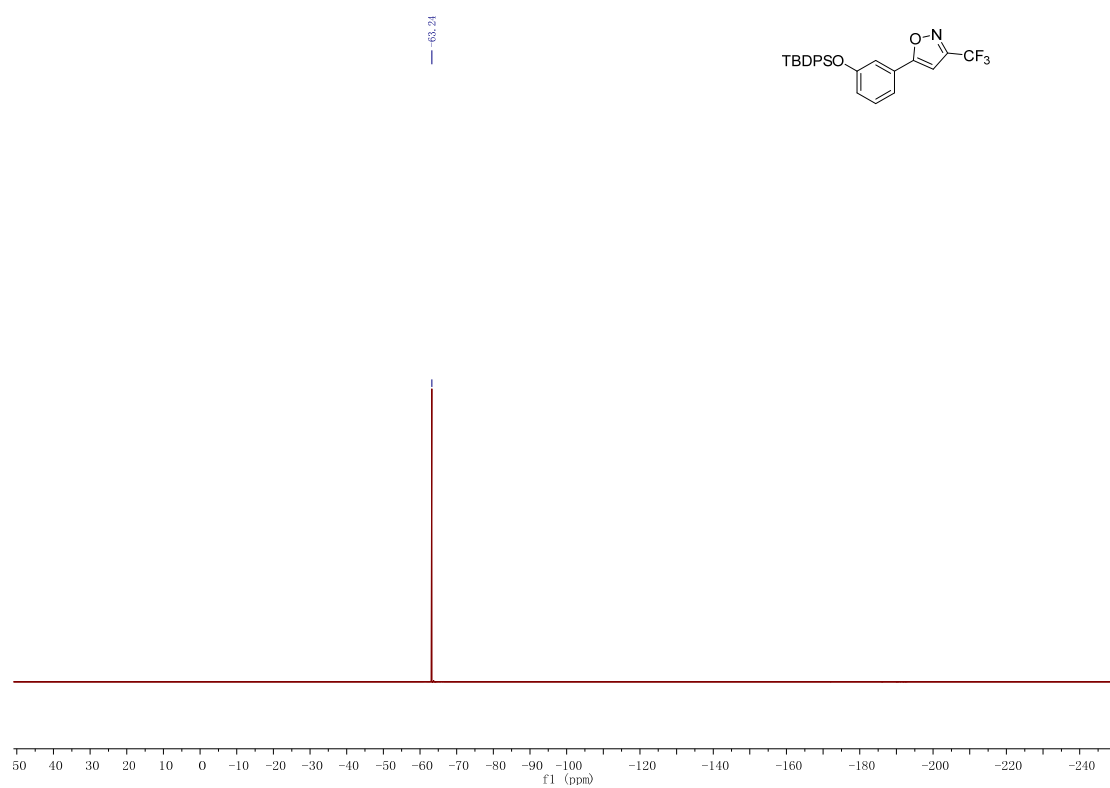
^{13}C NMR (CDCl₃, 100 MHz) of **9w**



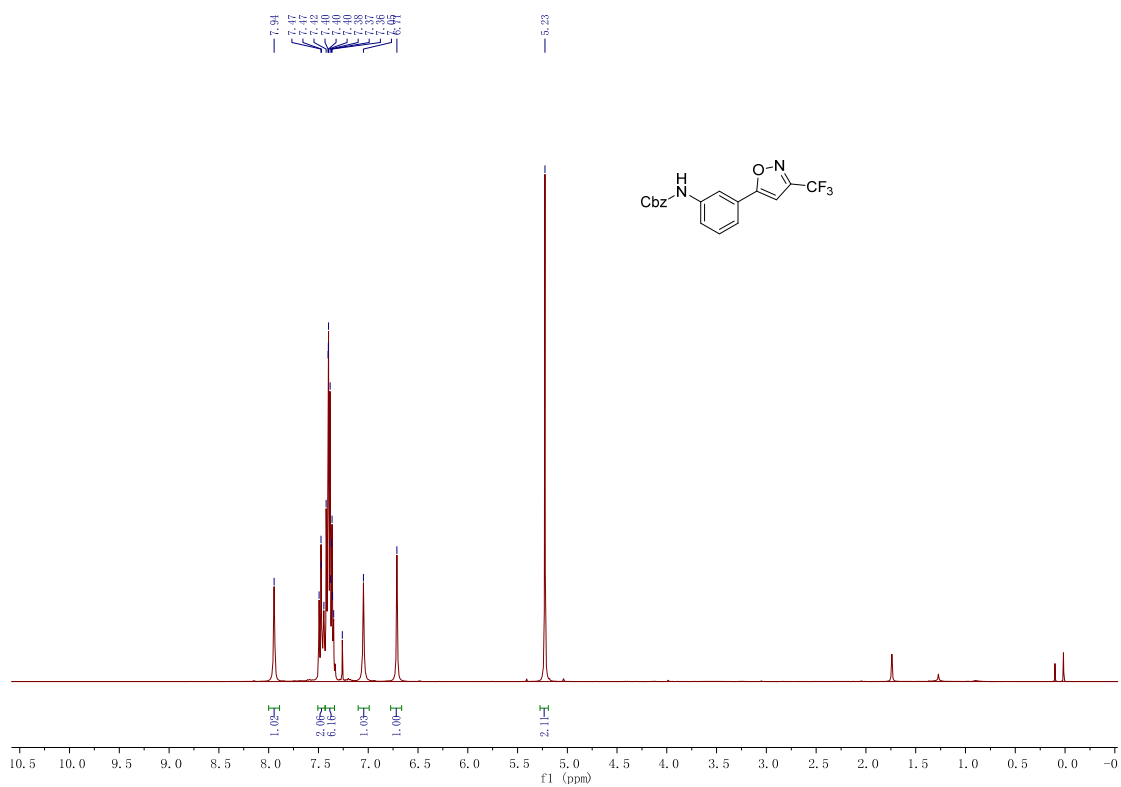
^{19}F NMR (CDCl_3 , 376 MHz) of **9w**



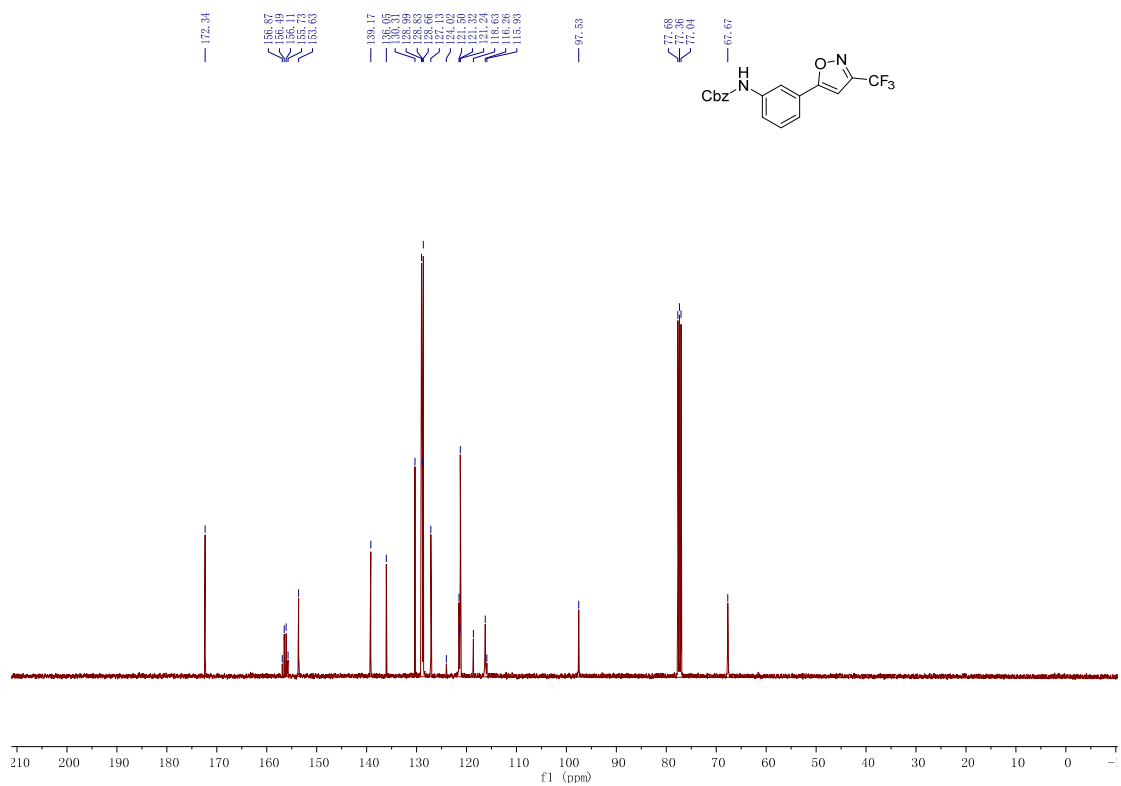
^{19}F { ^1H } NMR (CDCl_3 , 376 MHz) of **9w**



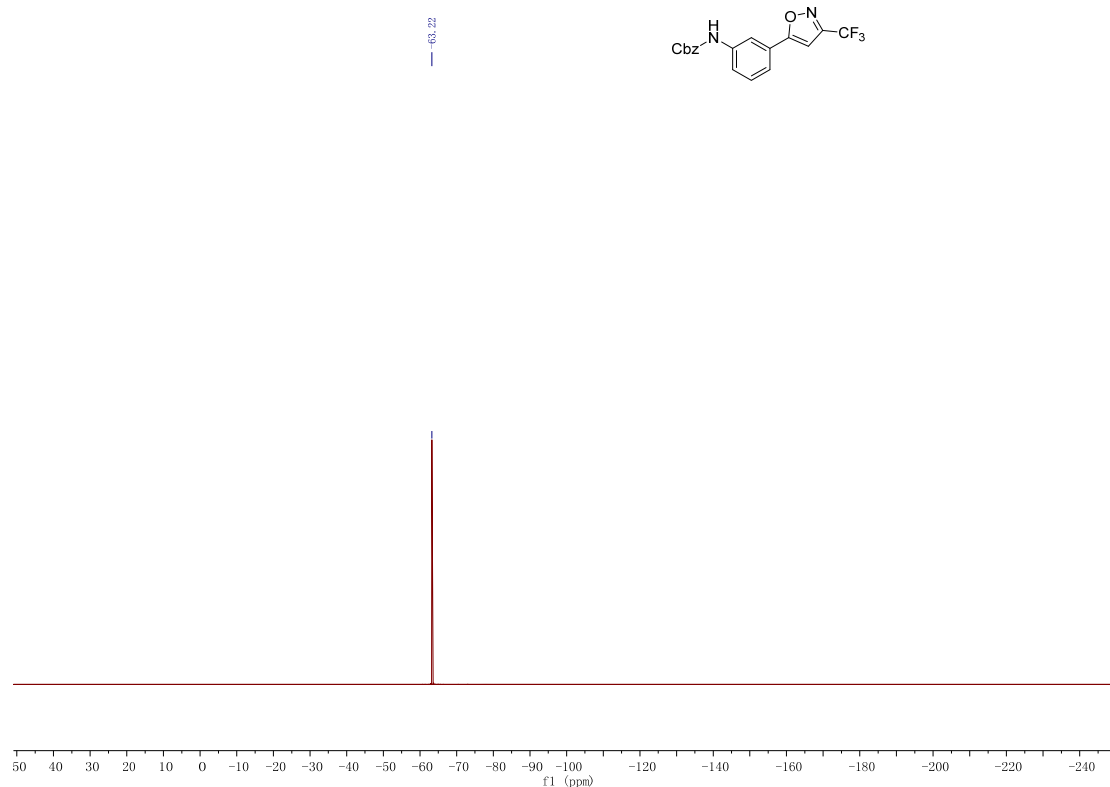
^1H NMR (CDCl₃, 400 MHz) of **9x**



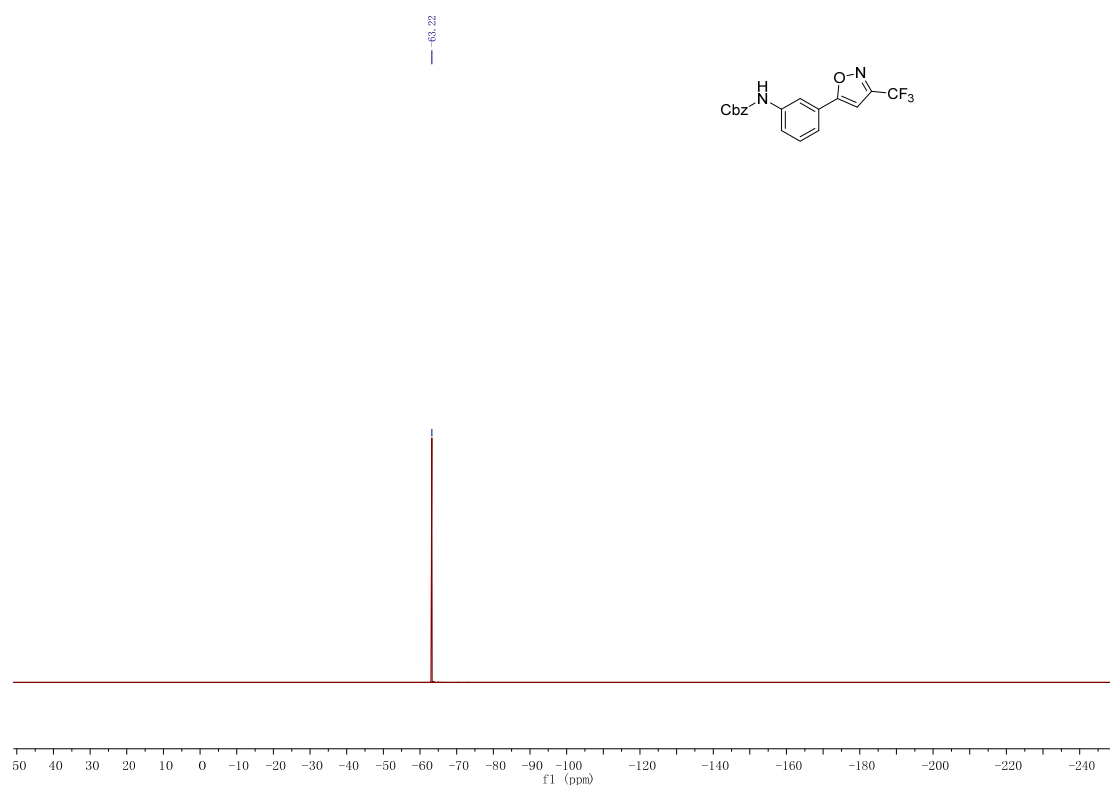
^{13}C NMR (CDCl₃, 100 MHz) of **9x**



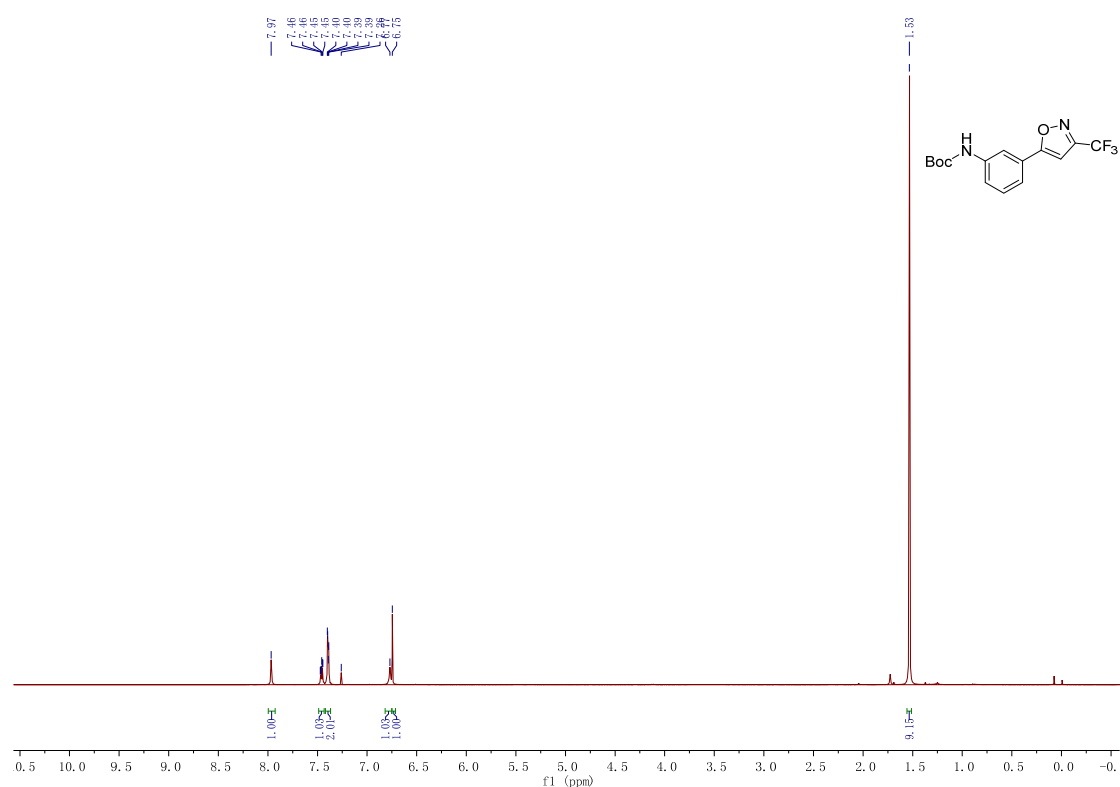
^{19}F NMR (CDCl₃, 376 MHz) of **9x**



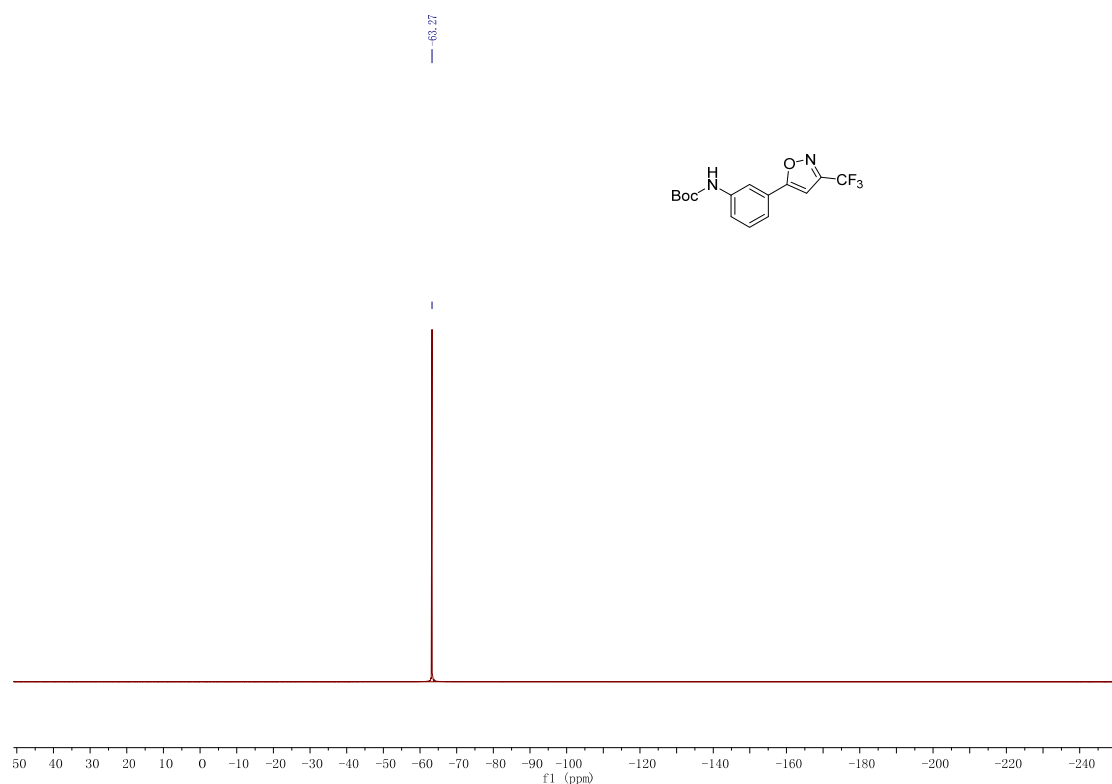
^{19}F { ^1H } NMR (CDCl₃, 376 MHz) of **9x**



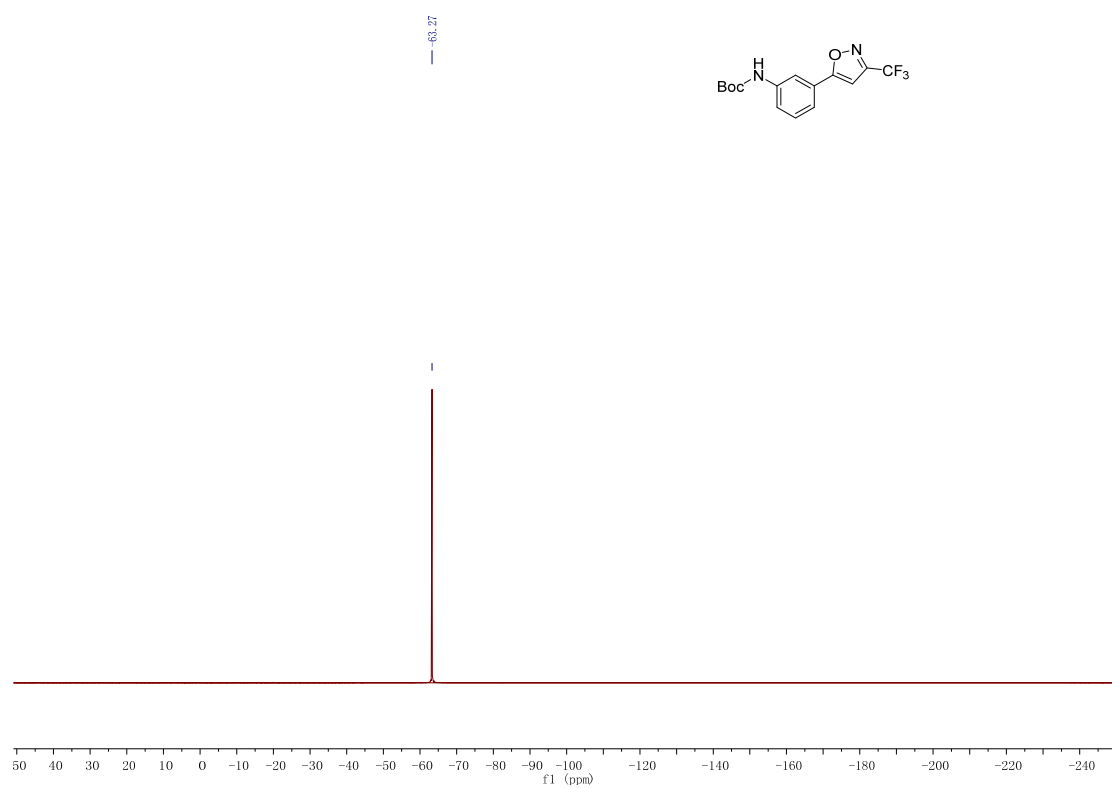
¹H NMR (CDCl₃, 400 MHz) of **9y**



^{19}F NMR (CDCl₃, 376 MHz) of **9y**



^{19}F { ^1H } NMR (CDCl₃, 376 MHz) of **9y**



Chemical structure: CC(=O)Nc1ccc(cc1)-c2cc(C(F)(F)F)[n+]([O-])o2

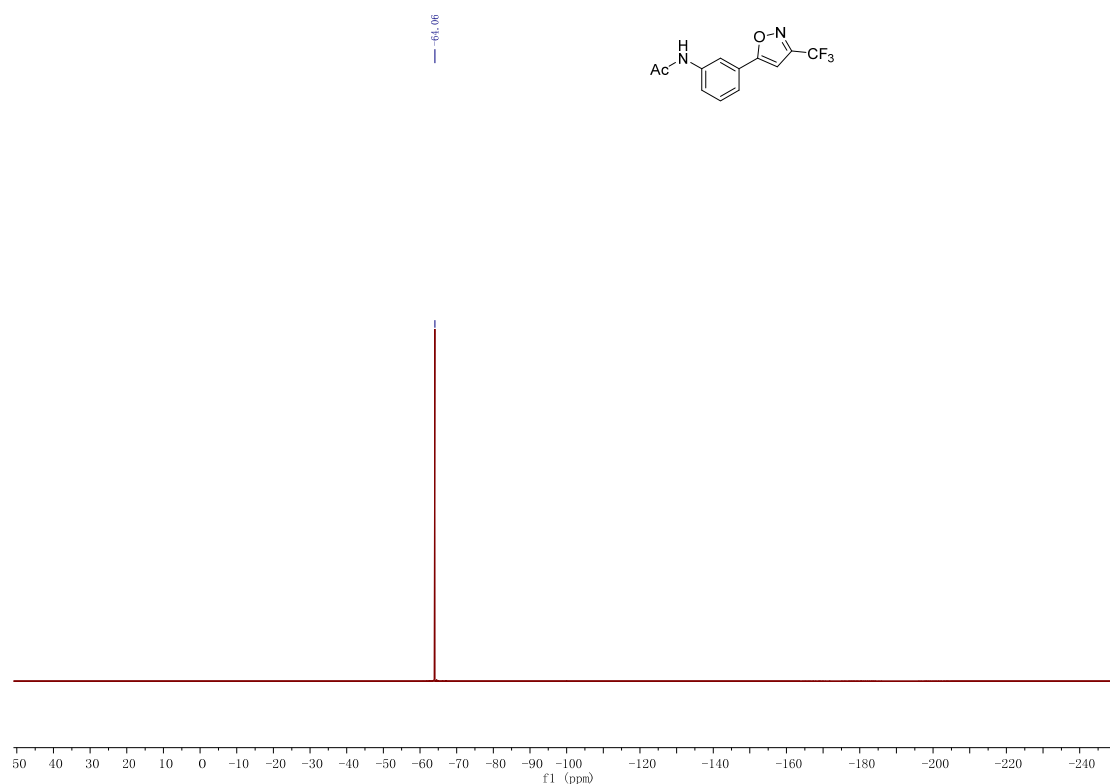
¹H NMR spectrum (DMSO-d₆) showing peaks at 9.50 (s, 1H), 7.50-7.60 (m, 4H), 7.65 (s, 1H), 2.95 (s, 3H), and 2.10 (s, 3H). Integration values are shown below the peaks: 1.00, 1.00, 1.00, 1.00, 1.00, 3.00, and 3.00.

Chemical structure: CC(=O)c1ccc(cc1)-c2cc(C(F)(F)F)[nH]2

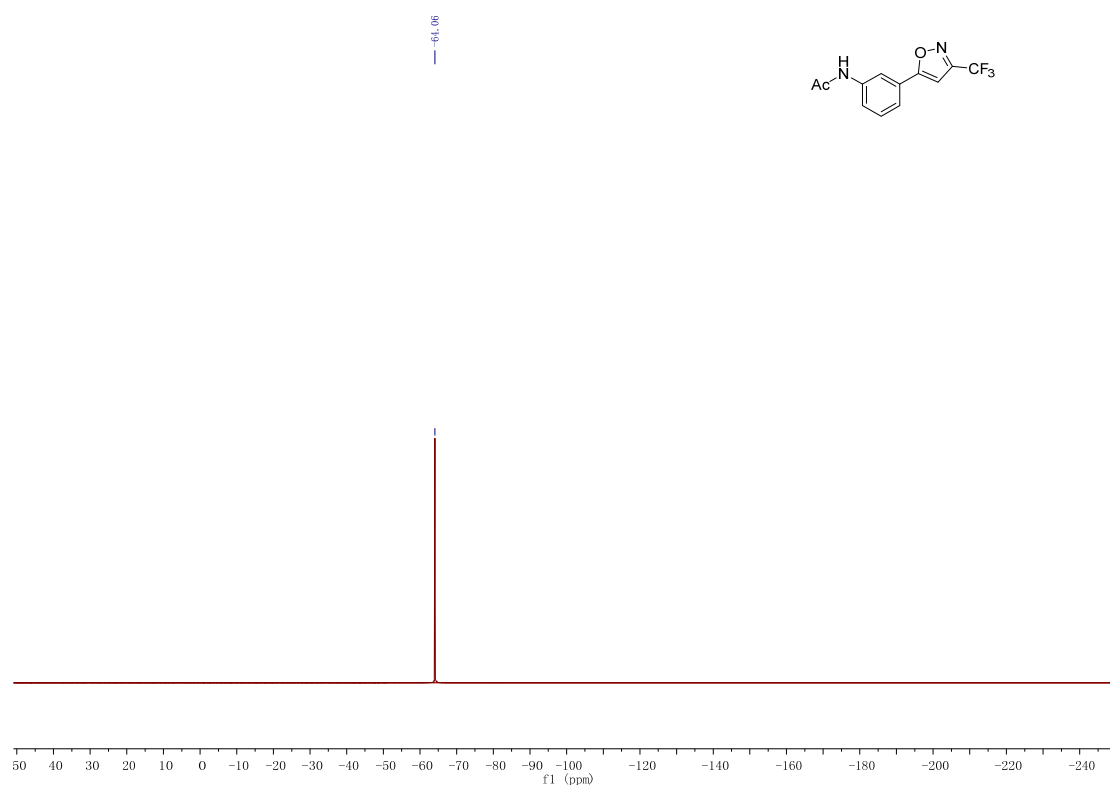
¹³C NMR spectrum (ppm):

- 206.26
- 173.55
- 169.40
- 156.54
- 136.24
- 130.71
- 127.32
- 124.95
- 122.72
- 121.72
- 116.89
- 98.44
- 30.21
- 21.26

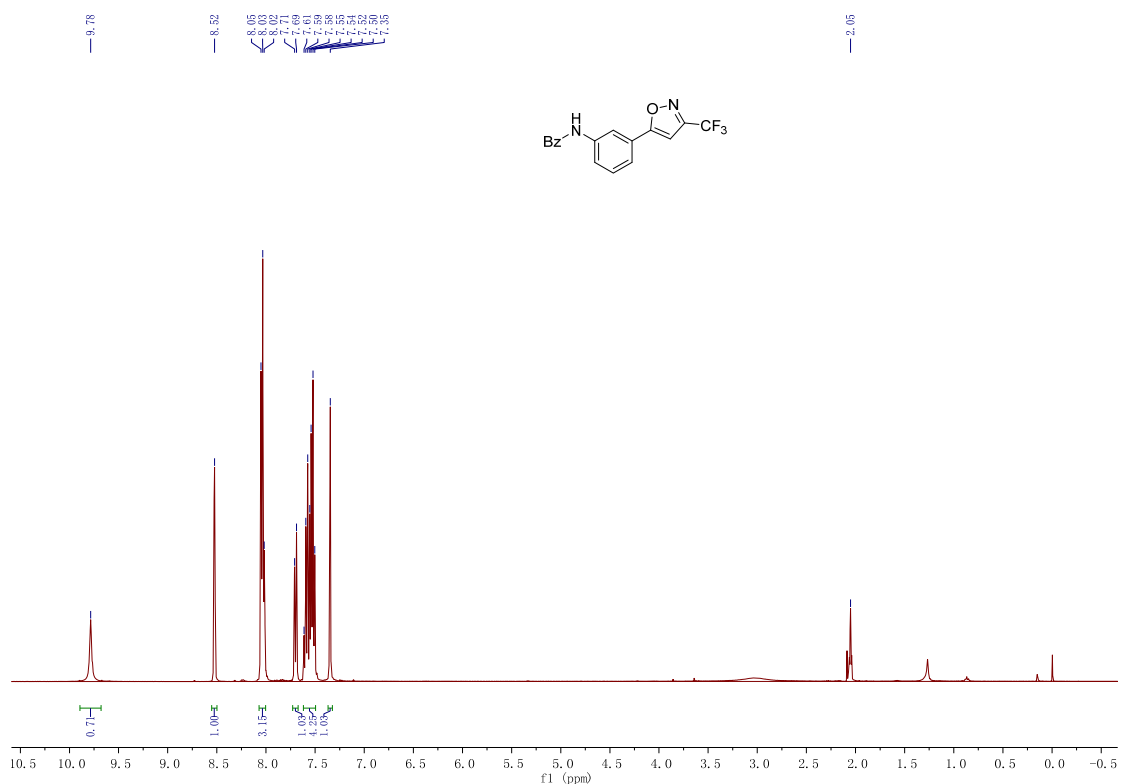
^{19}F NMR (acetone- d_6 , 376 MHz) of **9z**



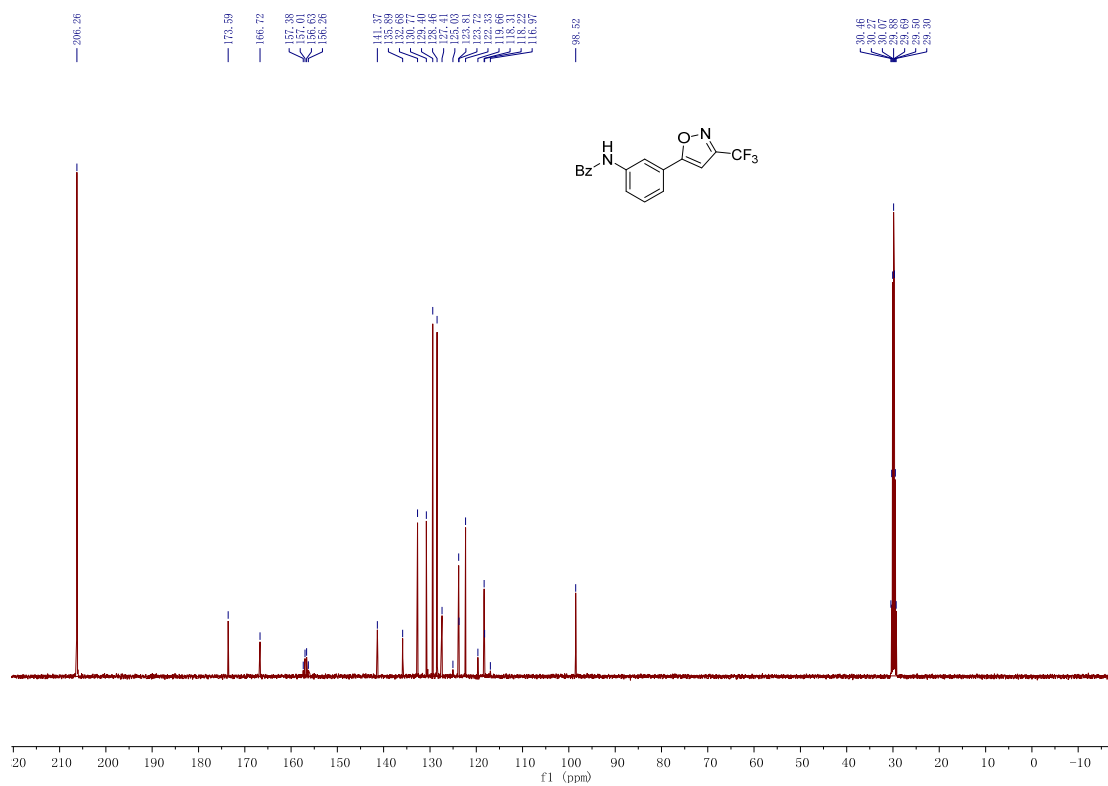
^{19}F { ^1H } NMR (acetone- d_6 , 376 MHz) of **9z**



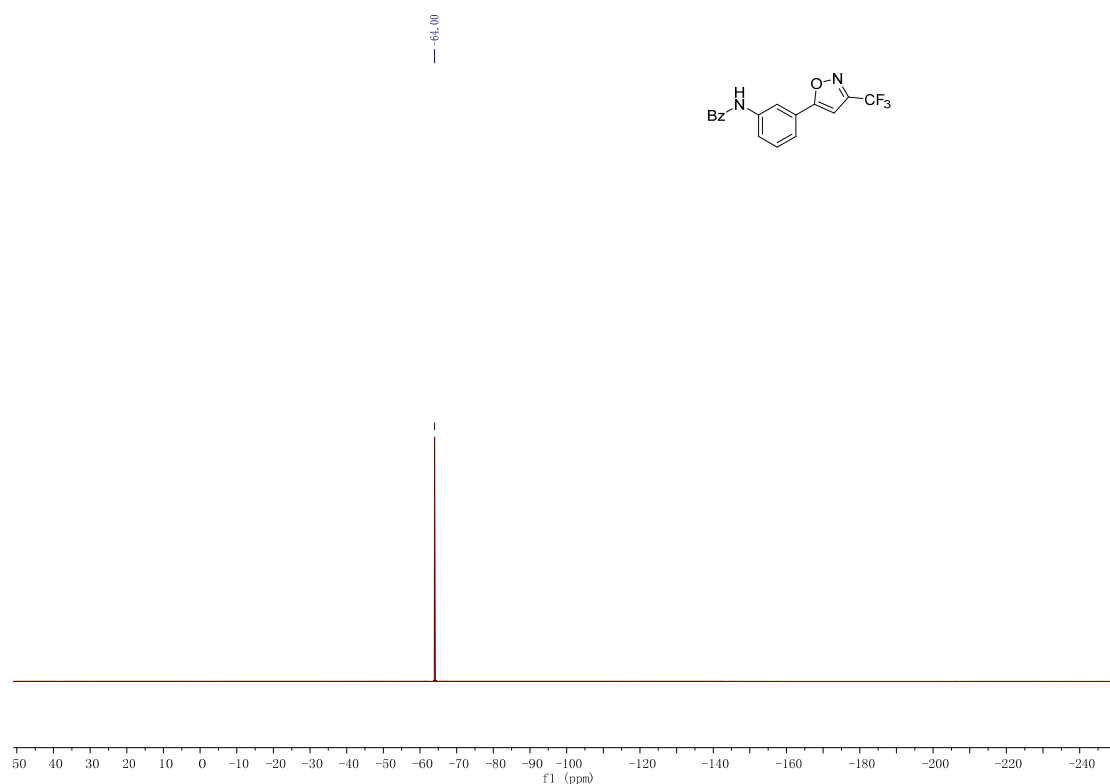
¹H NMR (acetone-*d*₆, 400 MHz) of 9aa



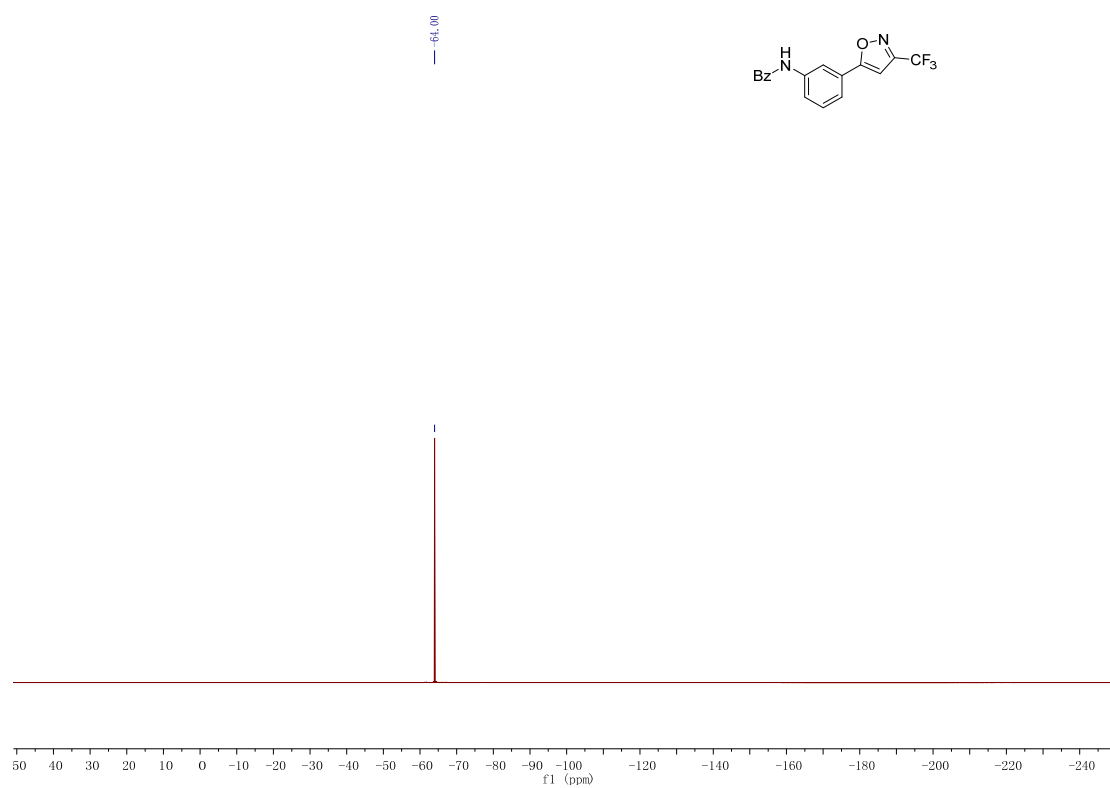
¹³C NMR (acetone-*d*₆, 100 MHz) of 9aa



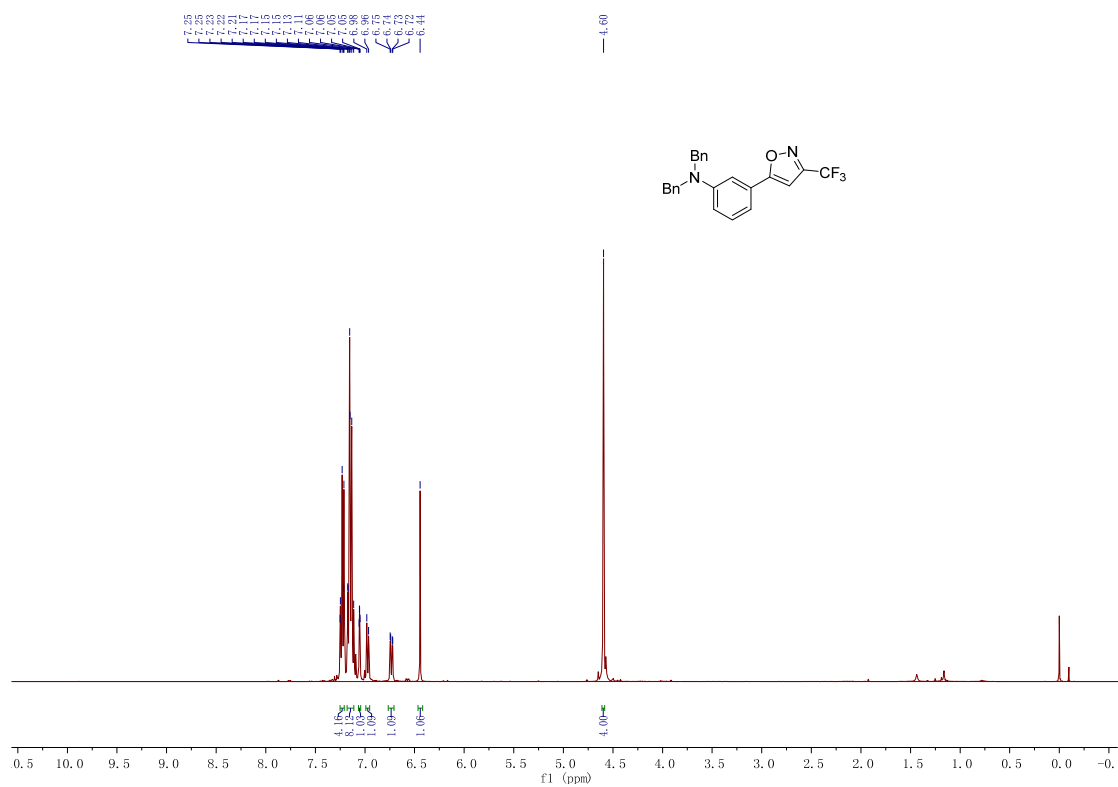
^{19}F NMR (acetone- d_6 , 376 MHz) of **9aa**



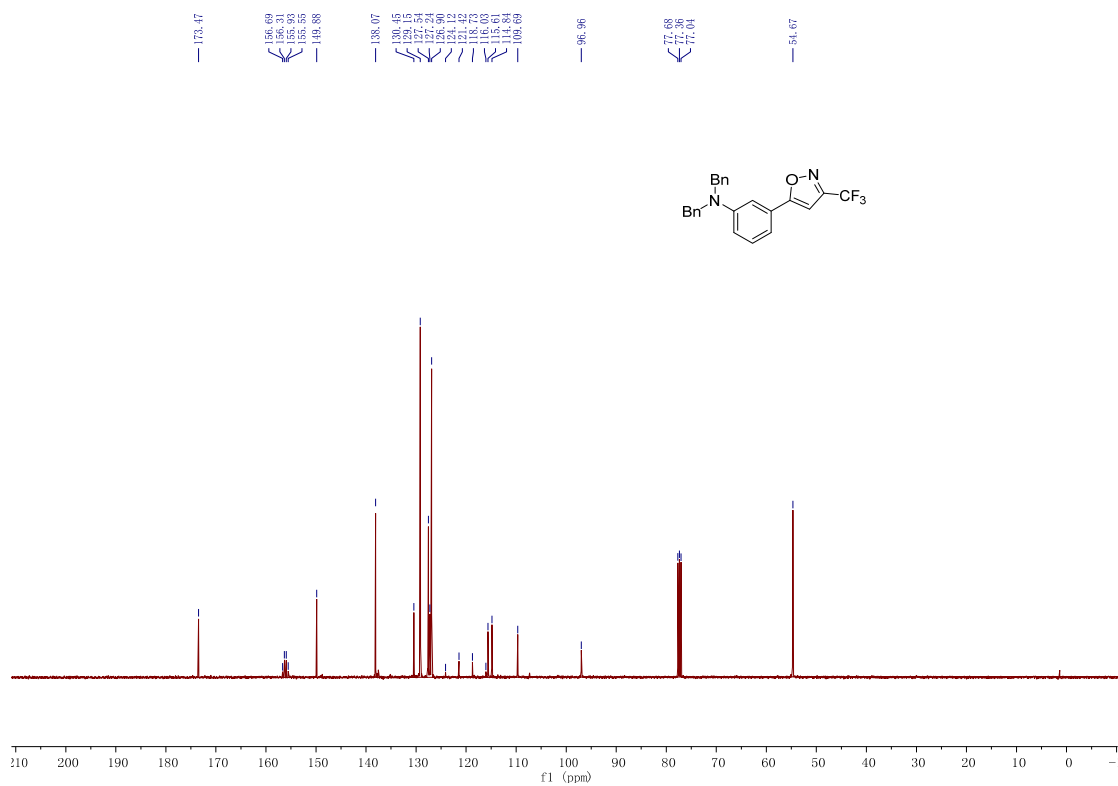
^{19}F { ^1H } NMR (acetone- d_6 , 376 MHz) of **9aa**



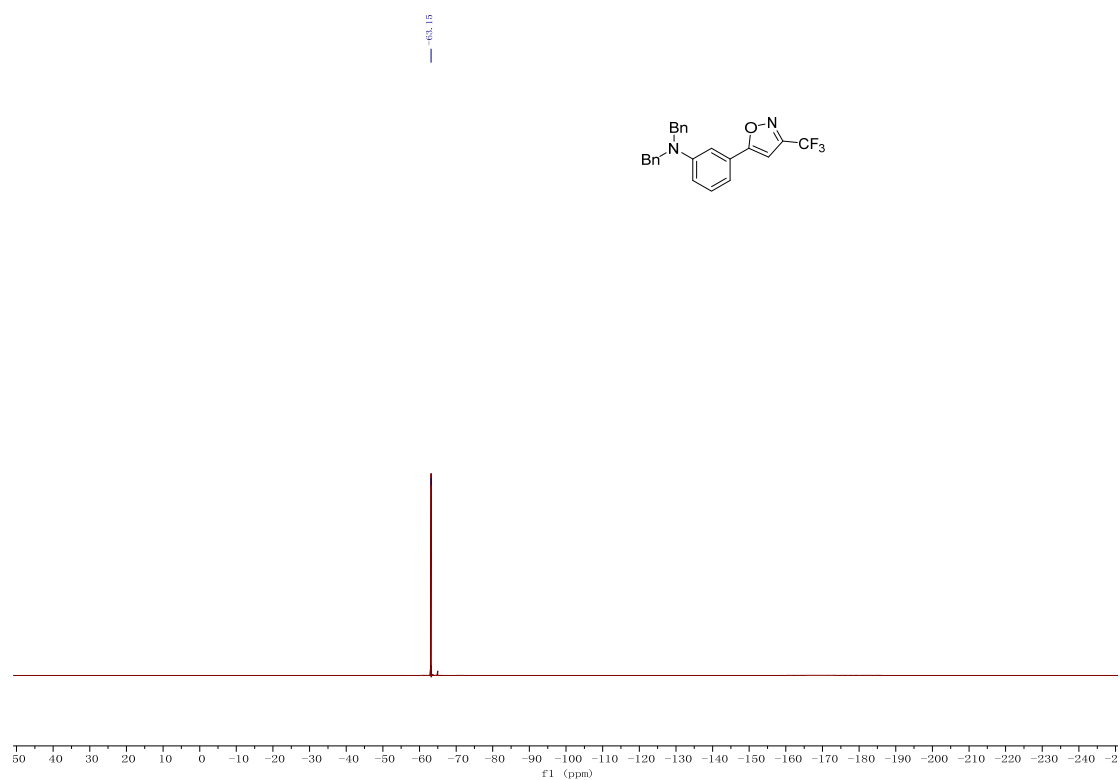
¹H NMR (CDCl₃, 400 MHz) of 9bb



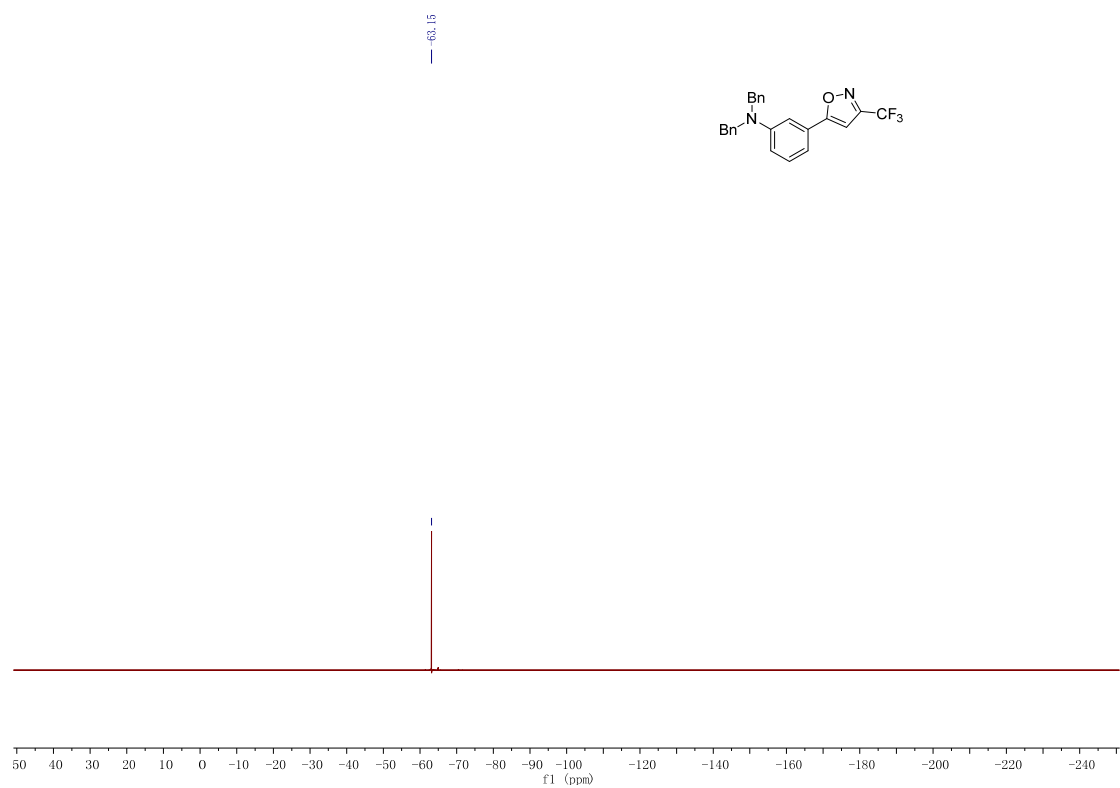
¹³C NMR (CDCl₃, 100 MHz) of 9bb



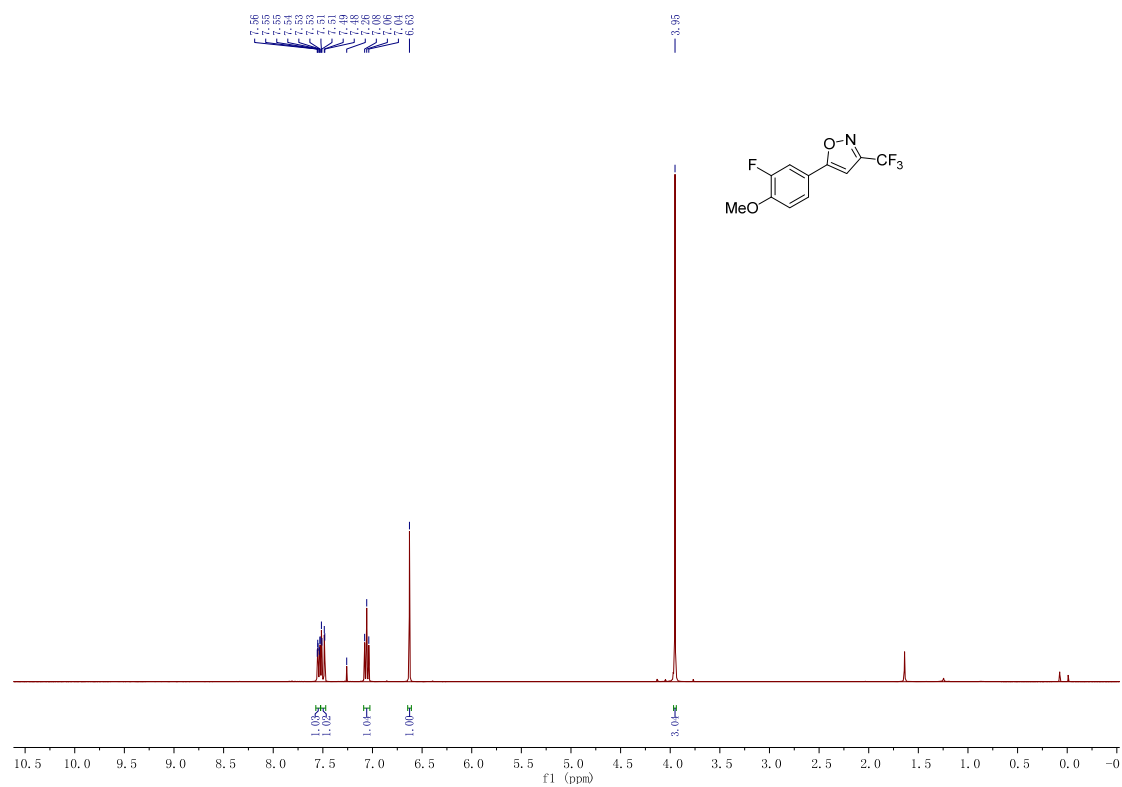
^{19}F NMR (CDCl₃, 376 MHz) of **9bb**



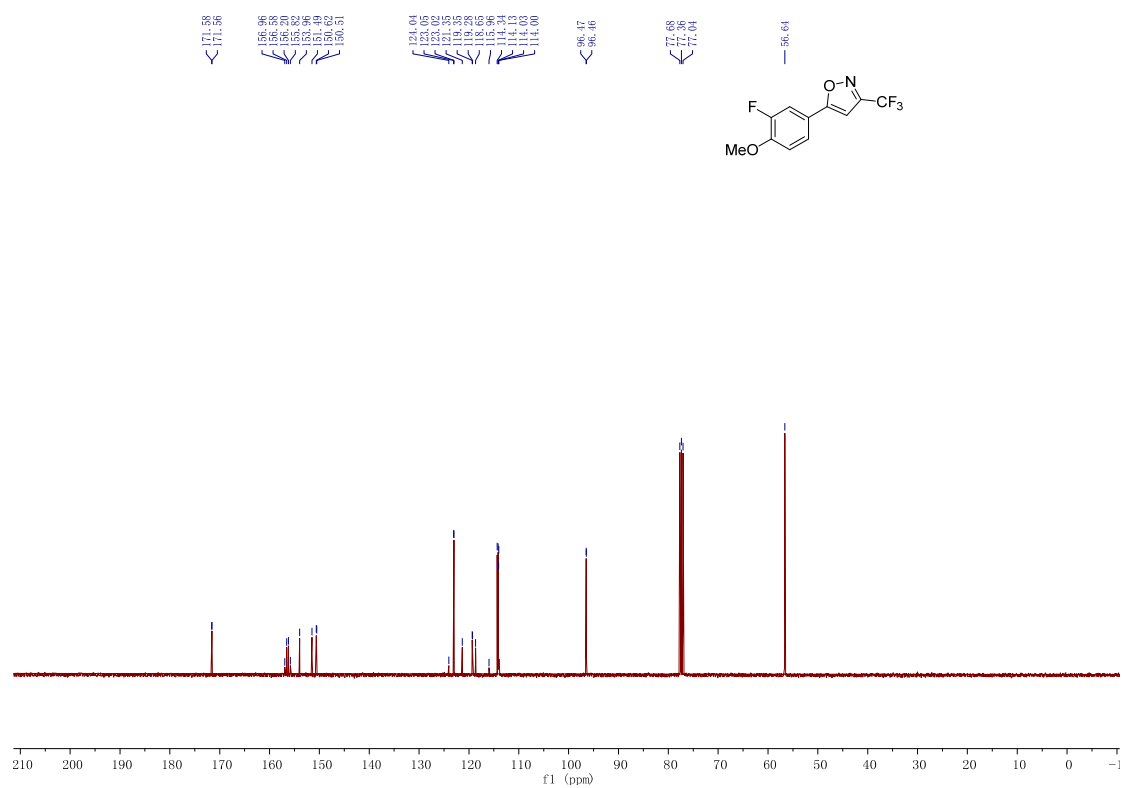
^{19}F { ^1H } NMR (CDCl₃, 376 MHz) of **9bb**



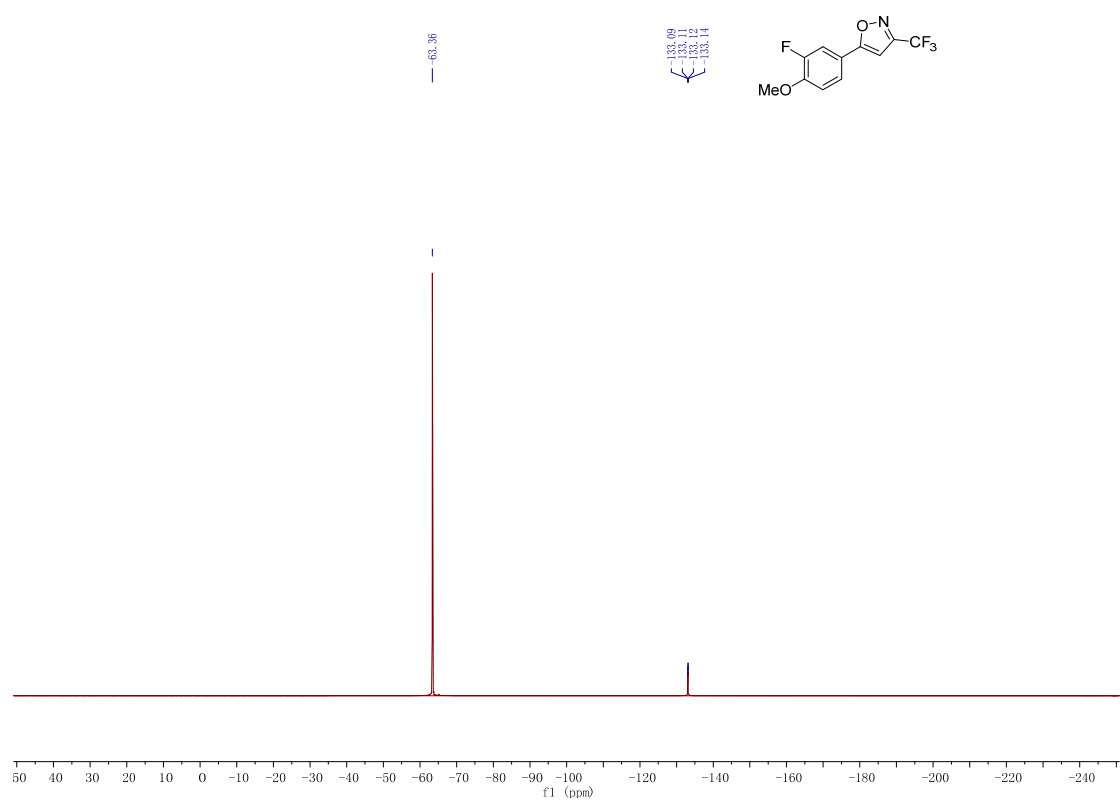
^1H NMR (CDCl₃, 400 MHz) of **9cc**



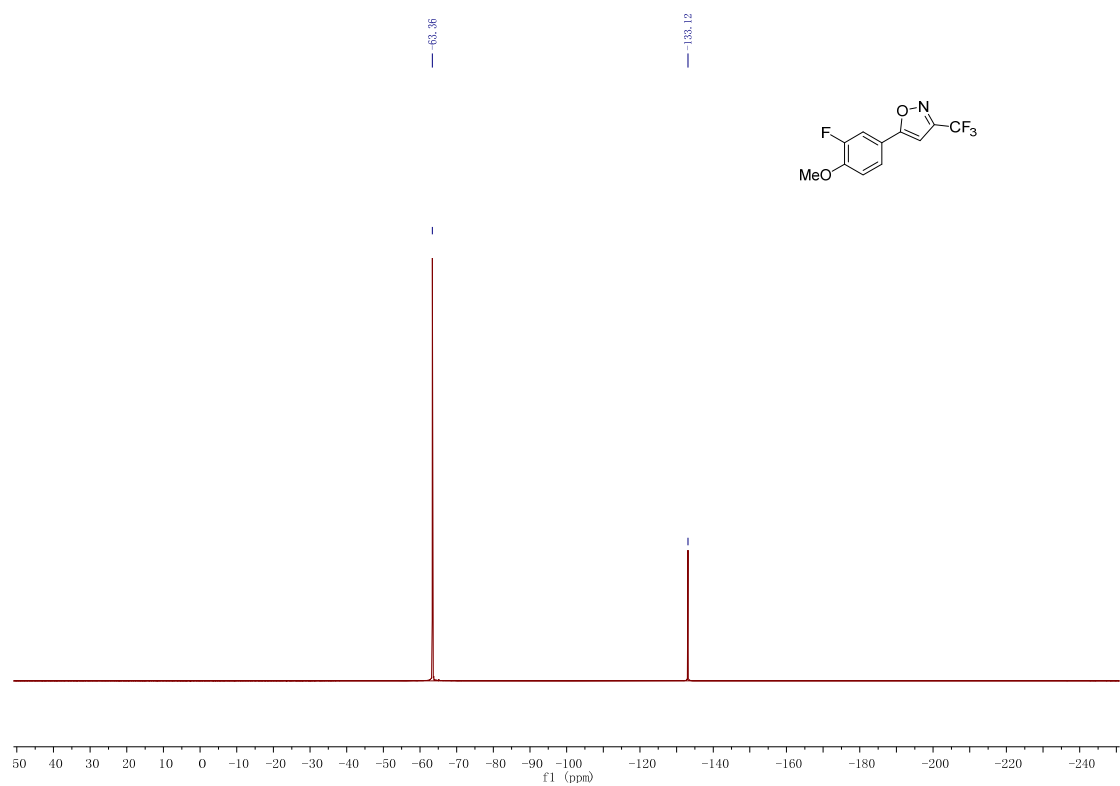
^{13}C NMR (CDCl₃, 100 MHz) of **9cc**



^{19}F NMR (CDCl₃, 376 MHz) of **9cc**



^{19}F { ^1H } NMR (CDCl₃, 376 MHz) of **9cc**



Chemical structure: COc1cc(cc(c1F)-c2cc(C(F)(F)F)nn2)C(F)(F)F

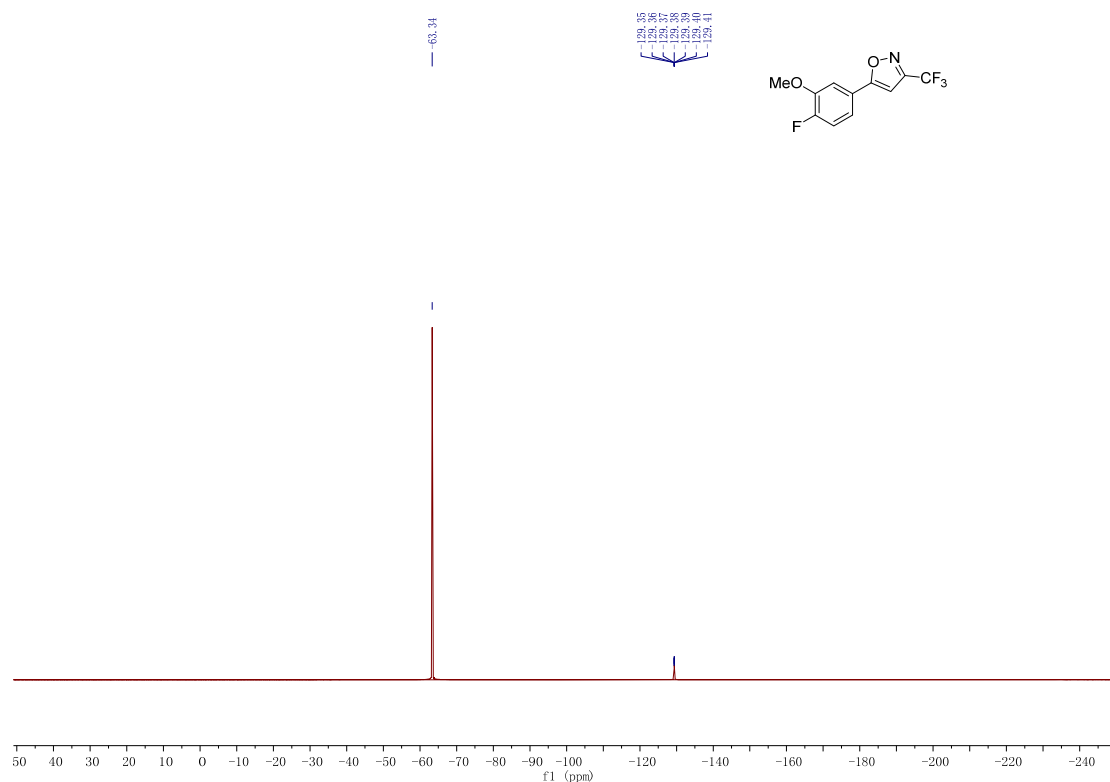
¹H NMR spectrum (CDCl₃) showing peaks at approximately 7.3-7.5 ppm (4H), 6.8 ppm (1H), 3.8 ppm (3H), and 1.8 ppm (TMS). The inset shows the chemical structure with atom numbering 1-10.

Chemical structure: COc1cc(F)ccc1-c2cc(C(F)(F)F)nn2

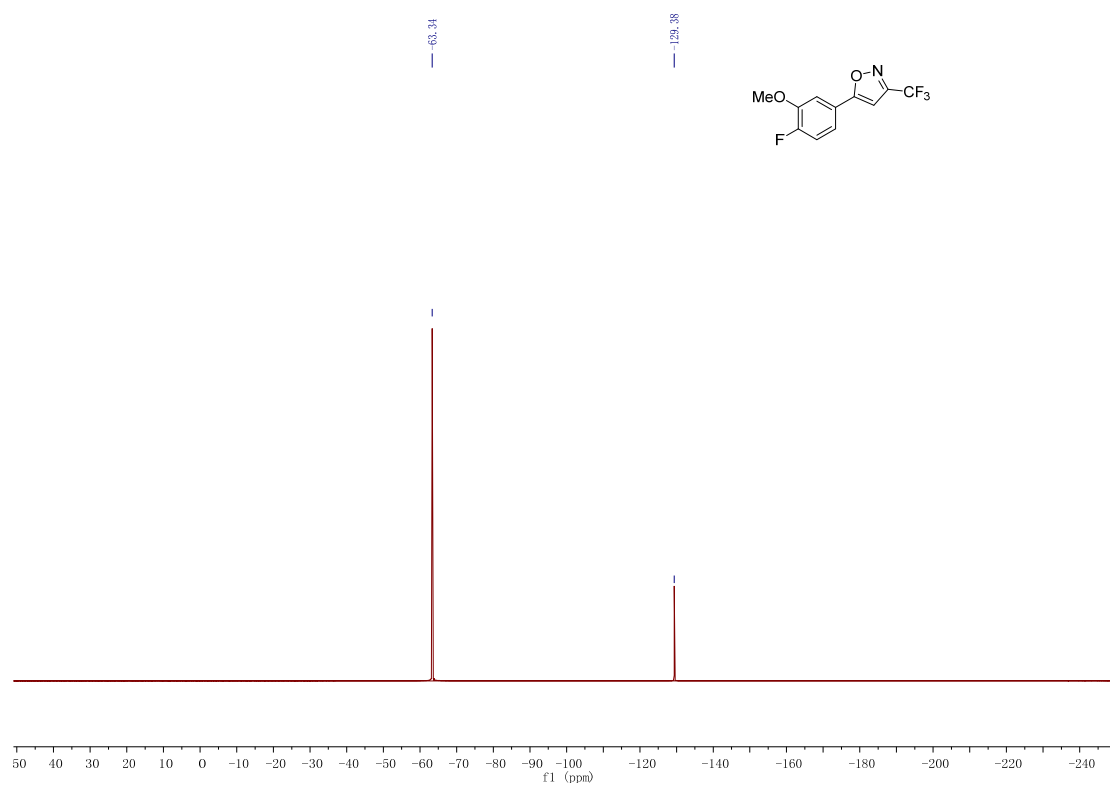
¹H NMR spectrum (ppm):

- 7.72, 7.70, 7.68 (m, 1H)
- 7.36 (m, 1H)
- 6.98 (m, 1H)
- 6.72, 6.70, 6.68 (m, 1H)
- 5.62 (s, 3H)
- 2.82 (s, 3H)

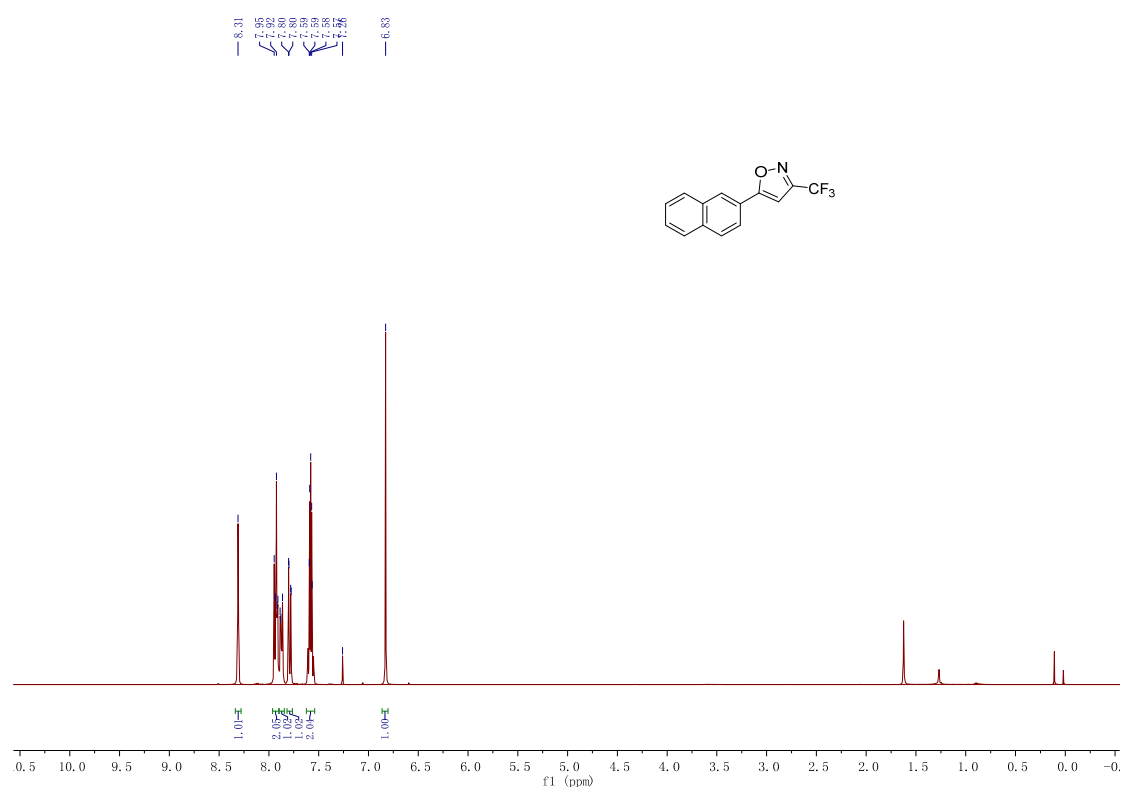
^{19}F NMR (CDCl₃, 376 MHz) of **9dd**



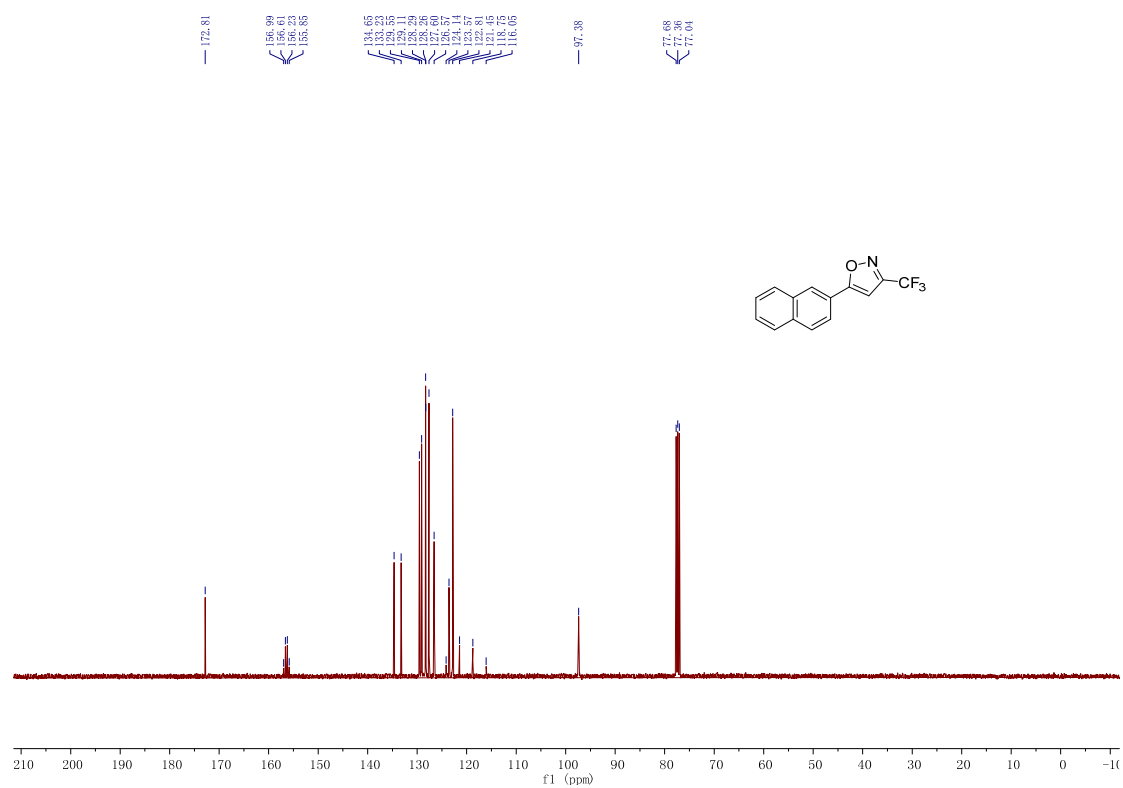
^{19}F { ^1H } NMR (CDCl₃, 376 MHz) of **9dd**



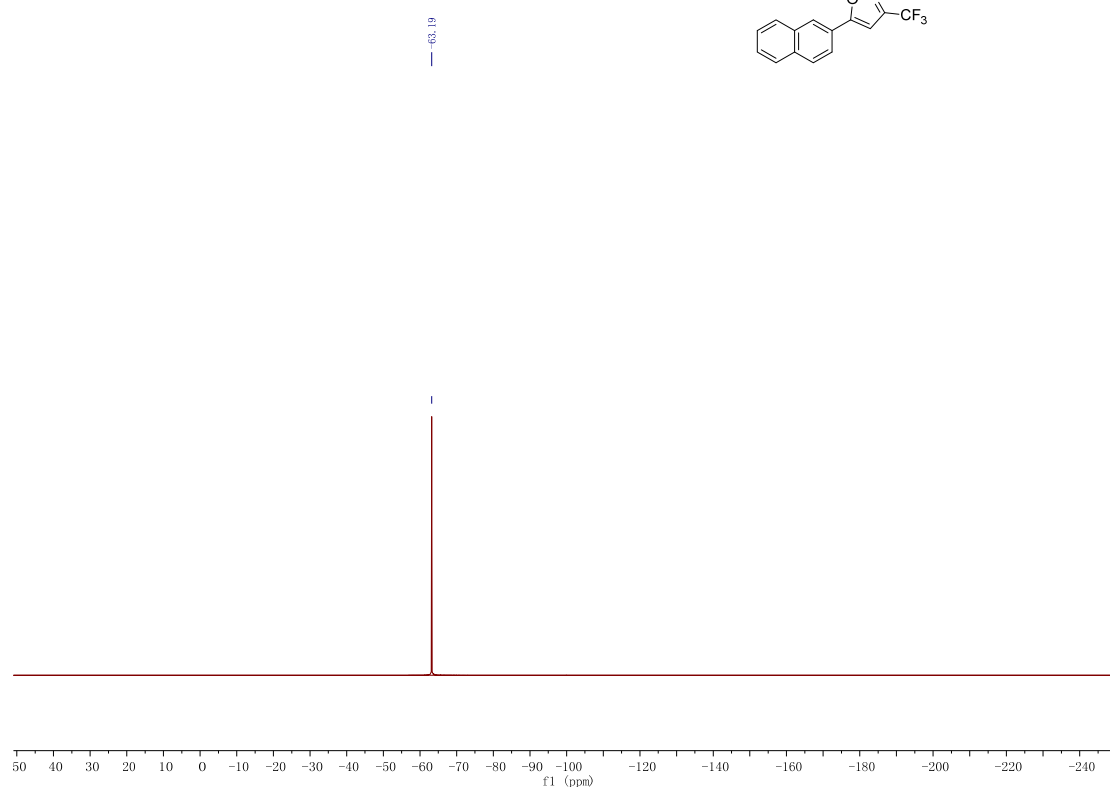
^1H NMR (CDCl₃, 400 MHz) of **9ee**



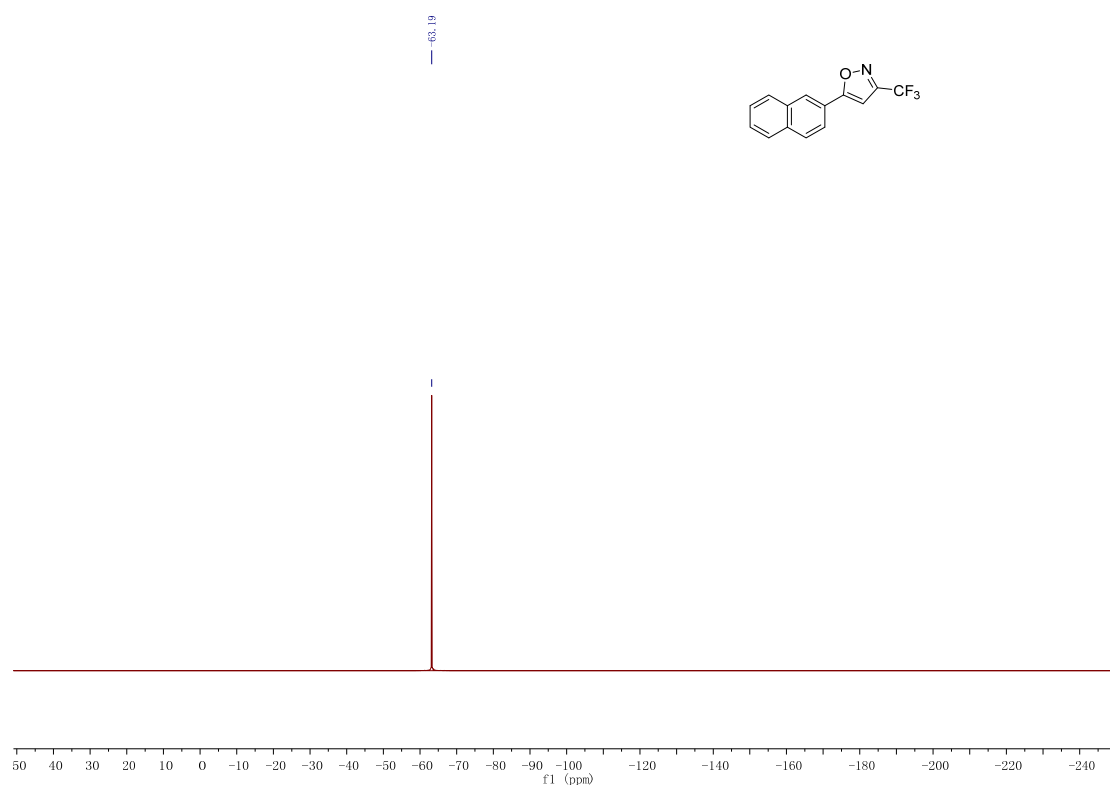
^{13}C NMR (CDCl₃, 100 MHz) of **9ee**



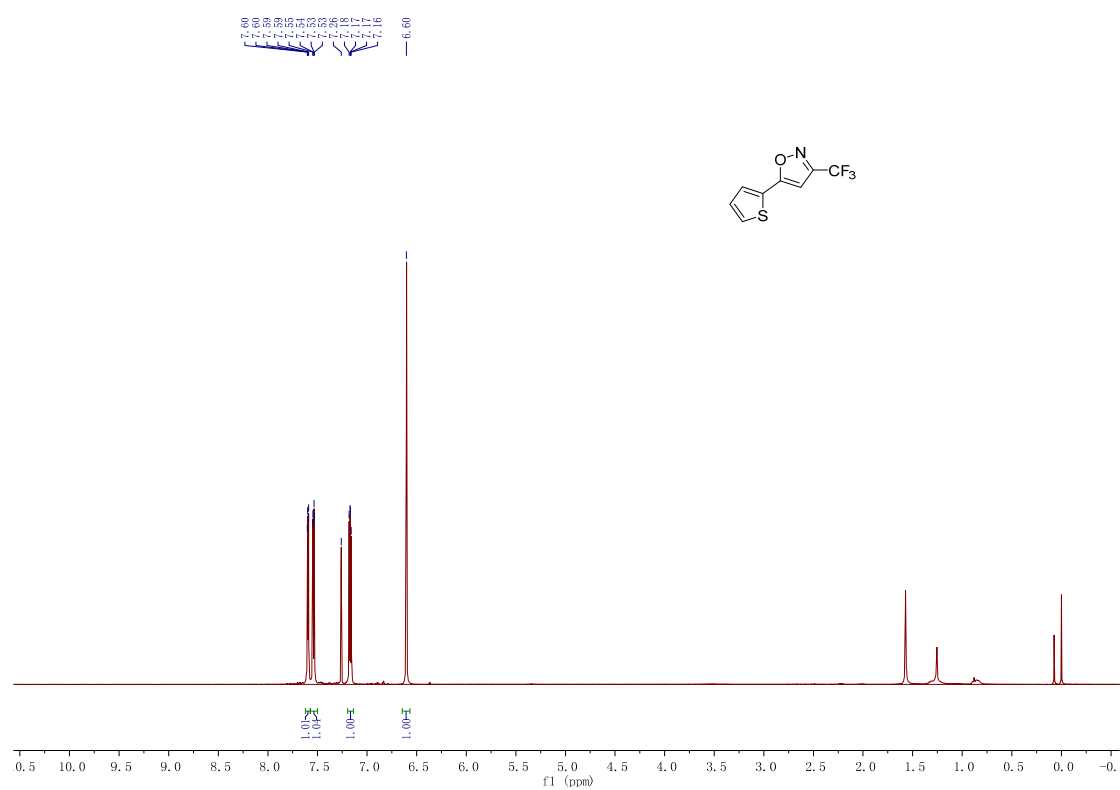
^{19}F NMR (CDCl₃, 376 MHz) of **9ee**



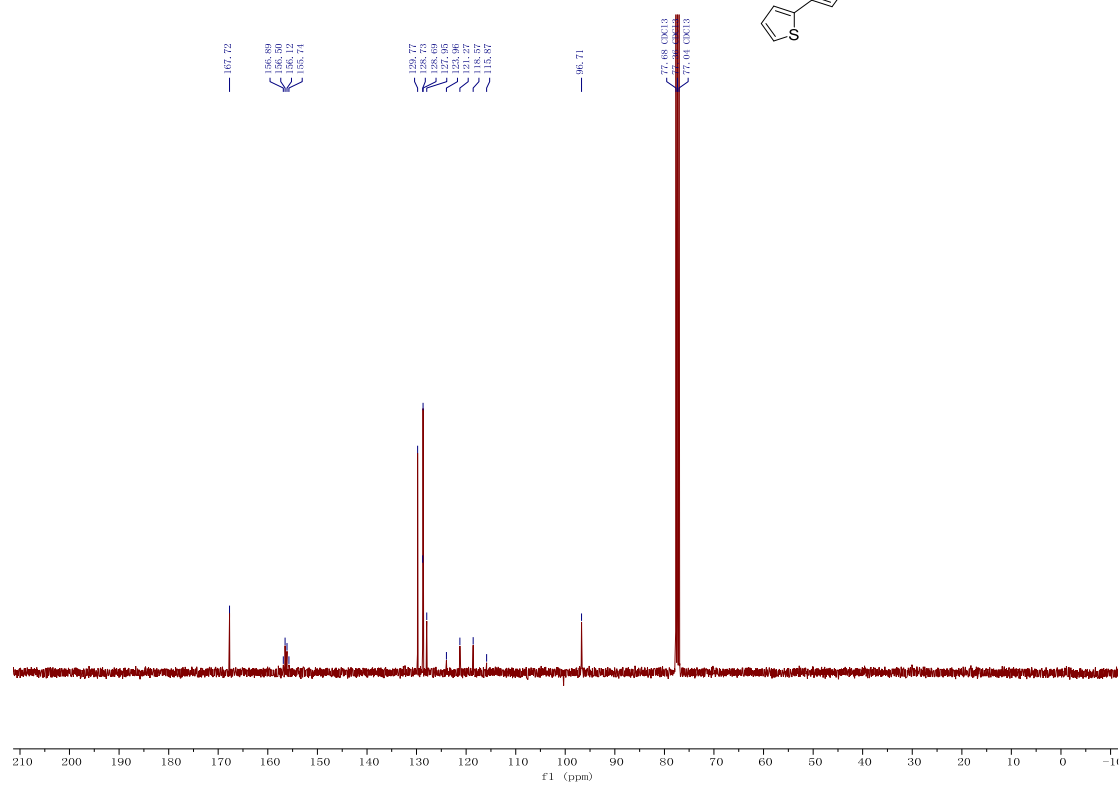
^{19}F { ^1H } NMR (CDCl₃, 376 MHz) of **9ee**



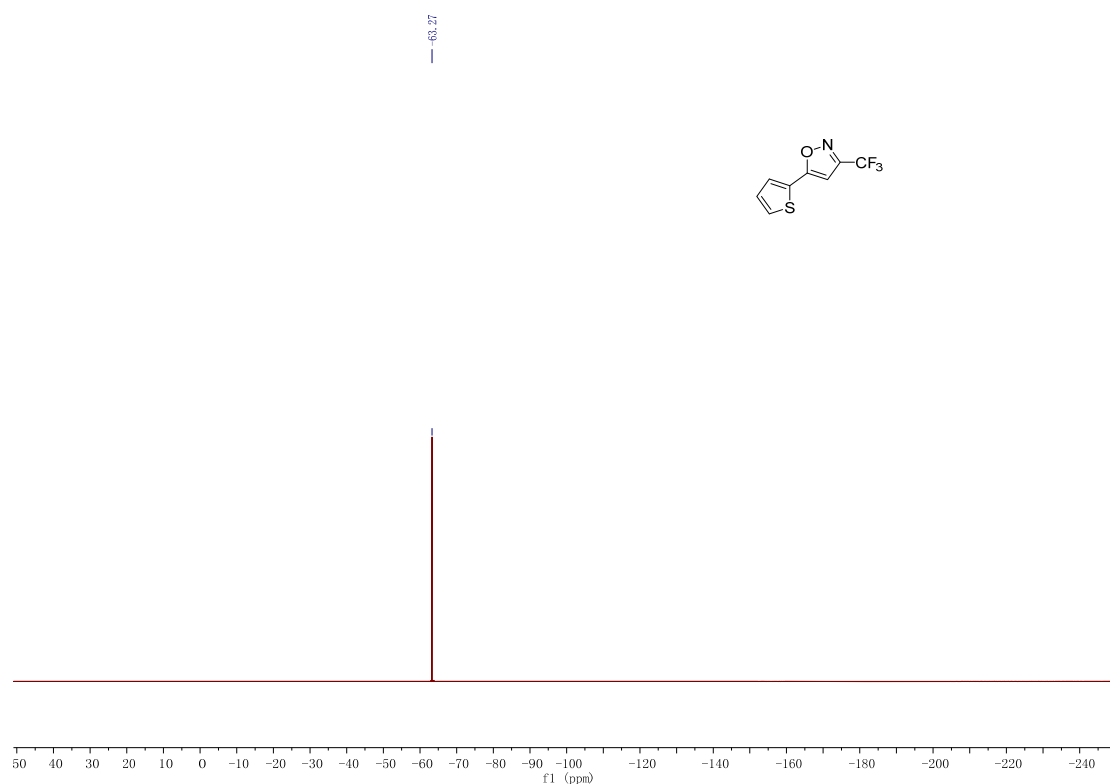
^1H NMR (CDCl₃, 400 MHz) of **9ff**



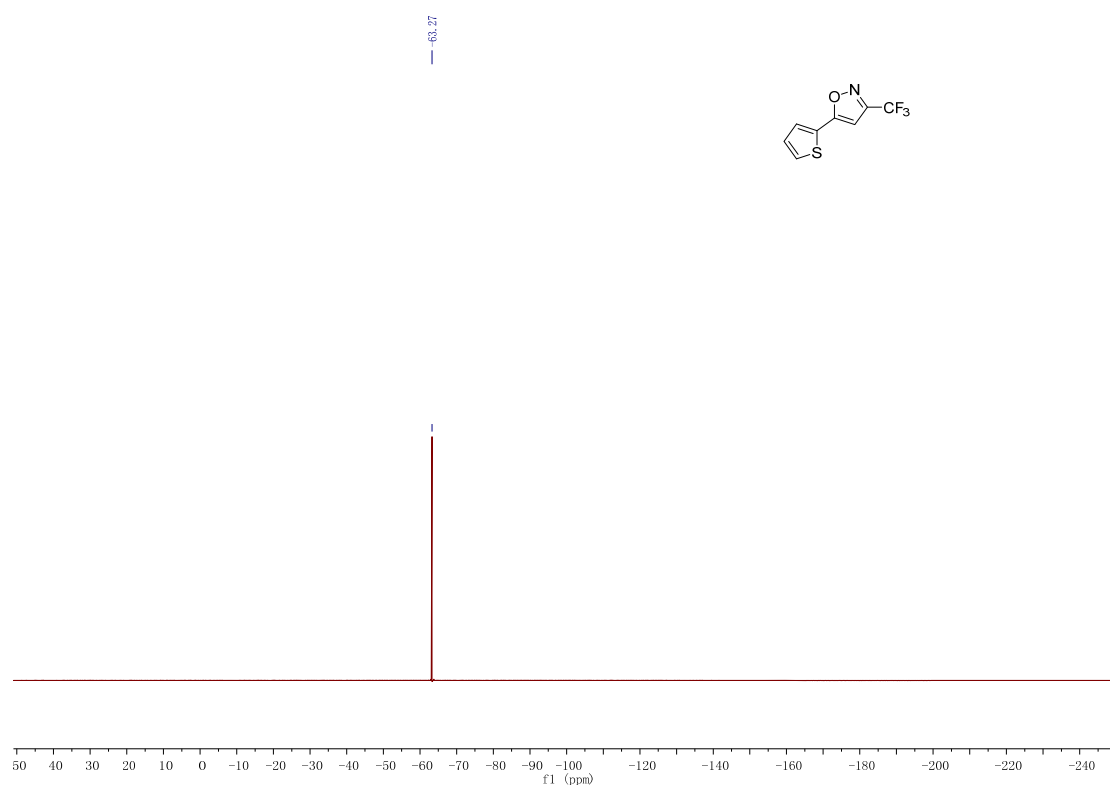
^{13}C NMR (CDCl₃, 100 MHz) of **9ff**



^{19}F NMR (CDCl₃, 376 MHz) of **9ff**



^{19}F { ^1H } NMR (CDCl₃, 376 MHz) of **9ff**



Chemical structure of 2-(2-(trifluoromethyl)-5-oxo-4,5-dihydroisoxazol-3-yl)furan (1):

Cc1cc2oc(=O)nn2c1C(F)(F)F

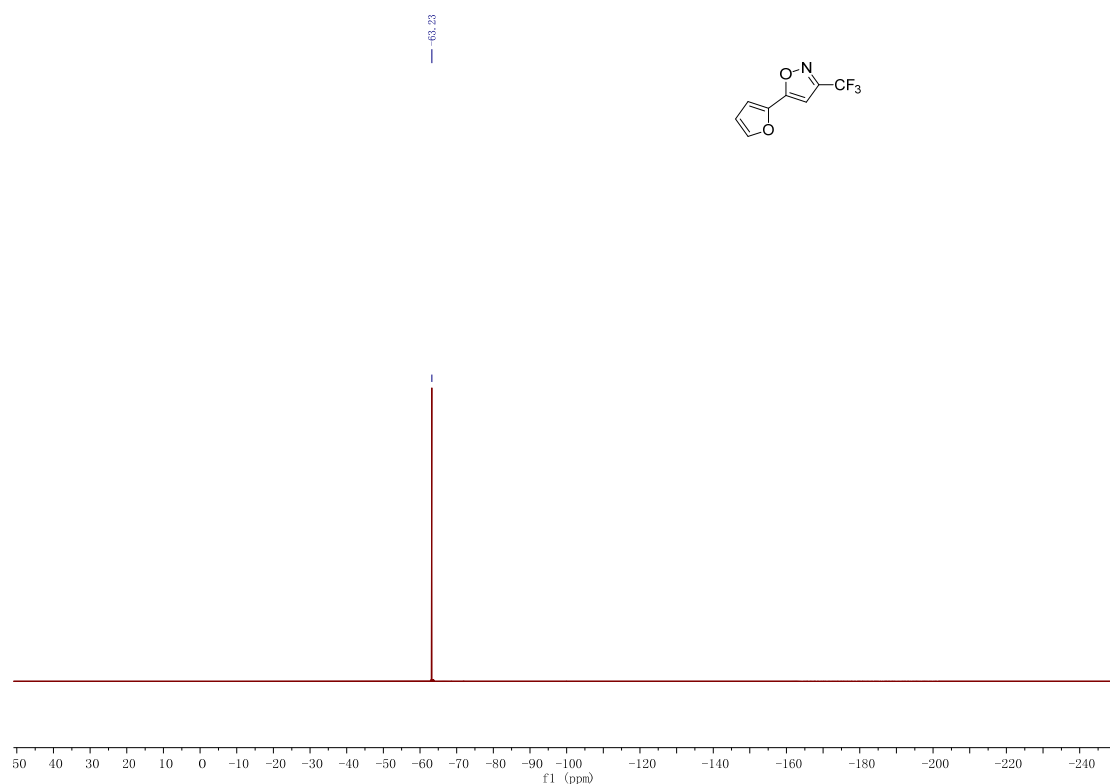
¹H NMR spectrum (CDCl₃) showing peaks at 7.70 (d, 1H), 7.50 (d, 1H), 7.20 (t, 1H), 6.80 (d, 1H), 6.60 (d, 1H), 4.10 (s, 2H), 2.10 (s, 3H), and 0.00 (TMS, 3H).

Chemical structure: Cc1cc2oc3cc(C(F)(F)F)nn3c2o1

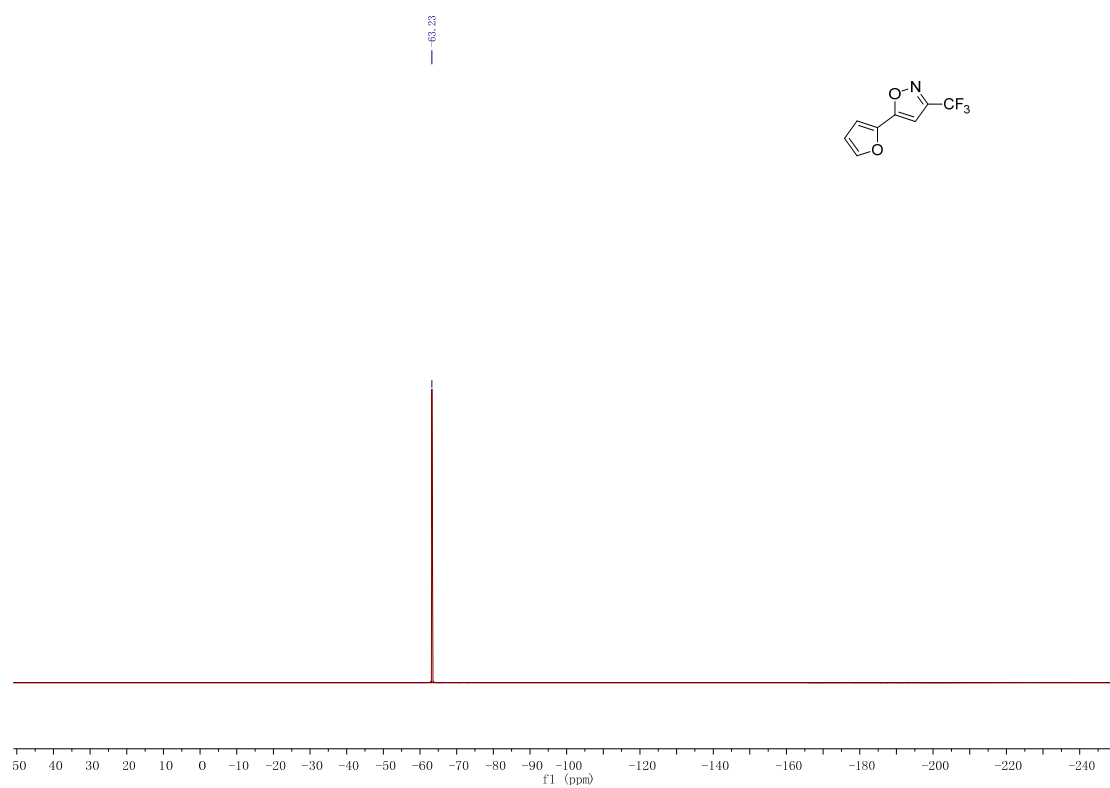
¹³C NMR spectrum (ppm):

- 164.19
- 156.60
- 156.55
- 156.22
- 155.54
- 145.47
- 142.26
- 123.97
- 121.27
- 119.55
- 118.98
- 112.57
- 112.44
- 96.63
- 96.61
- 77.68 CDCl₃
- 77.38 CDCl₃
- 77.01 CDCl₃

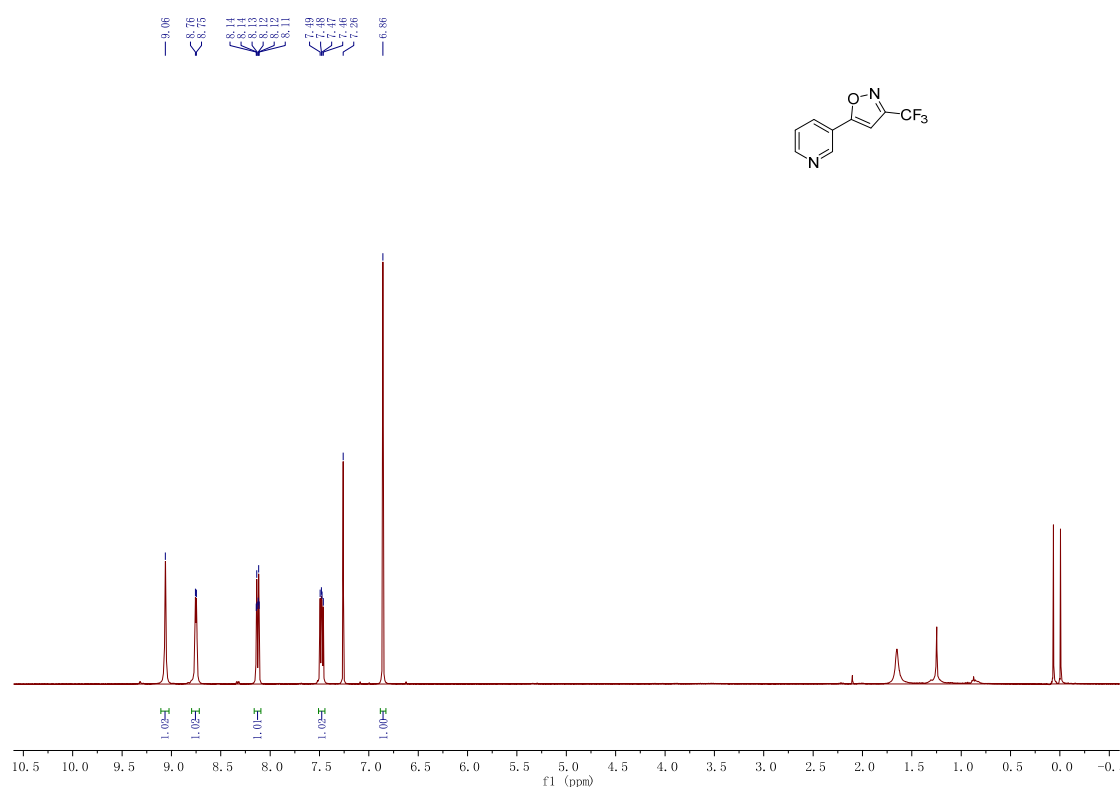
^{19}F NMR (CDCl₃, 376 MHz) of **9gg**



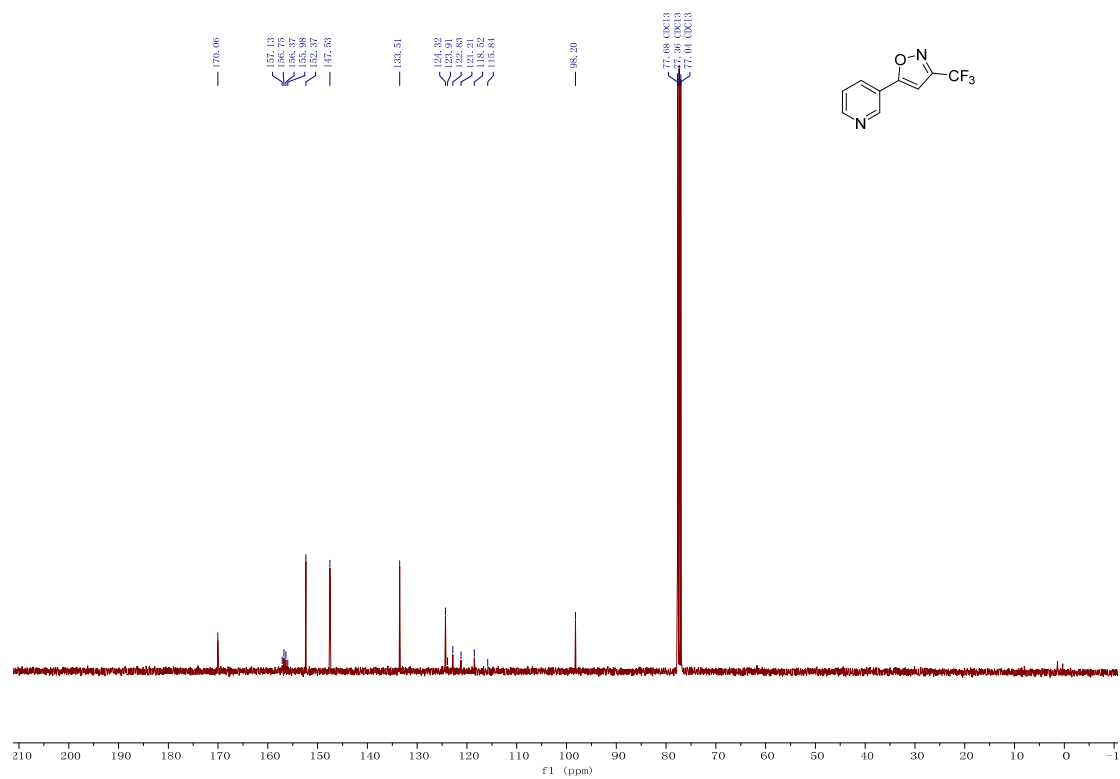
^{19}F { ^1H } NMR (CDCl₃, 376 MHz) of **9gg**



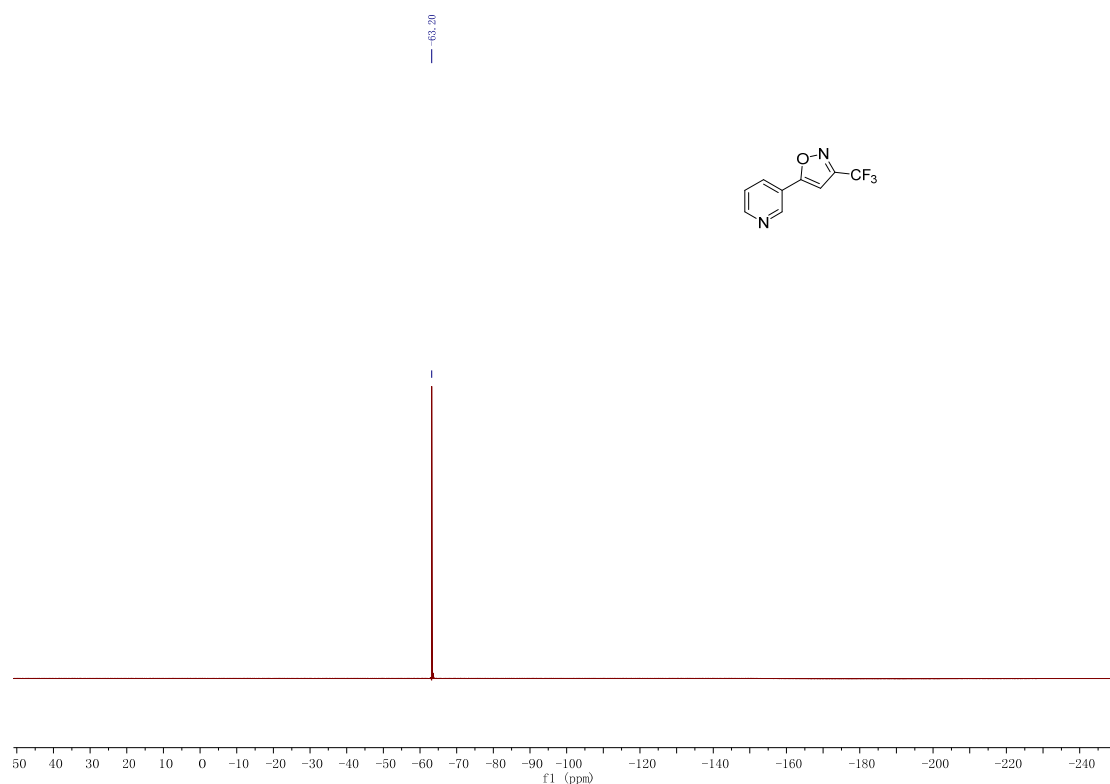
^1H NMR (CDCl₃, 400 MHz) of **9hh**



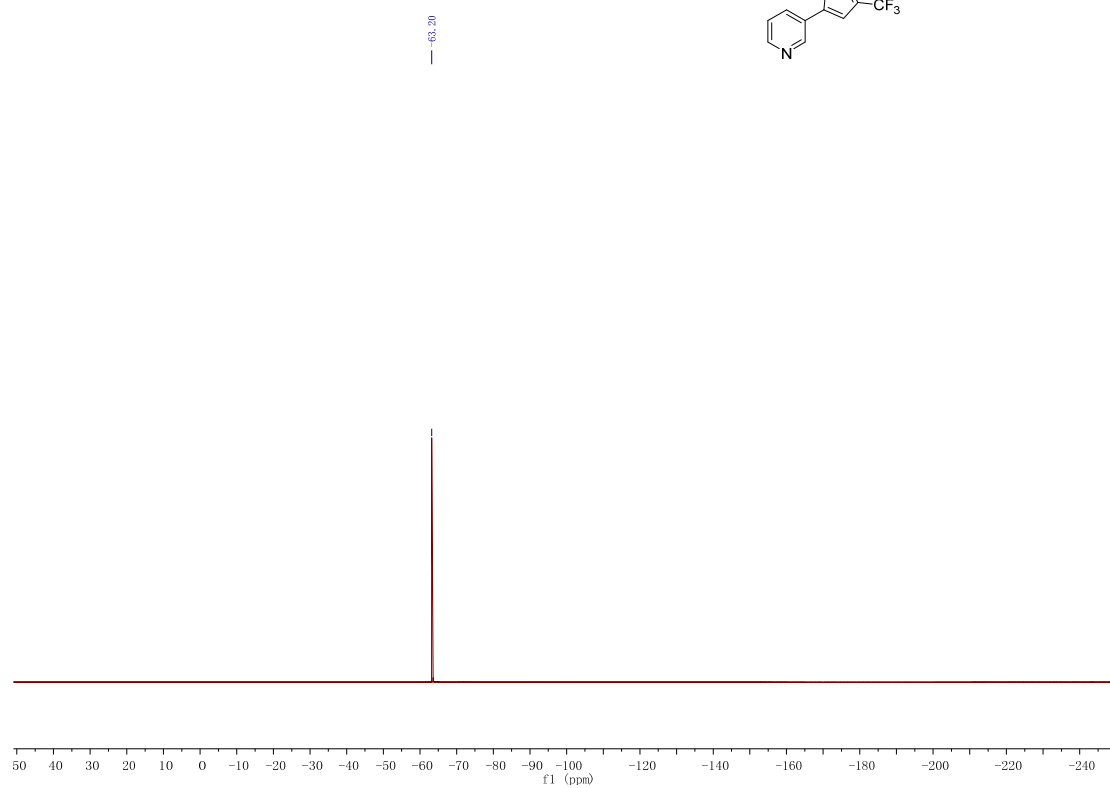
^{13}C NMR (CDCl₃, 100 MHz) of **9hh**



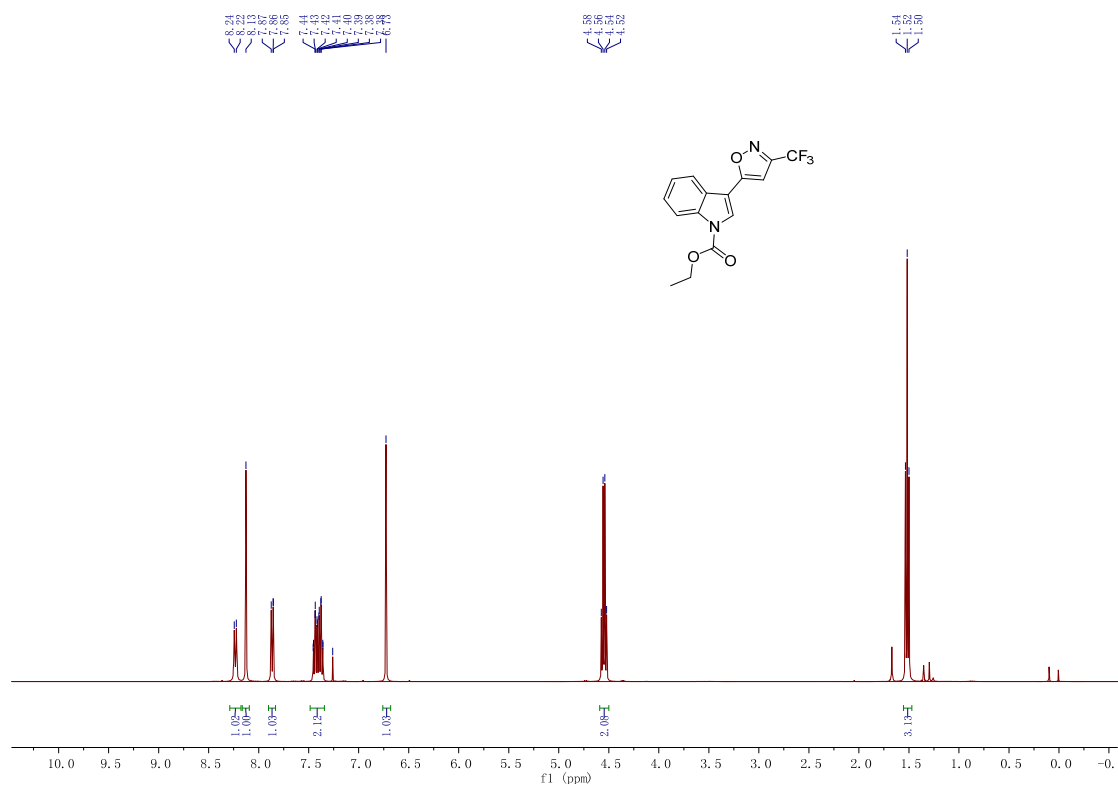
^{19}F NMR (CDCl_3 , 376 MHz) of **9hh**



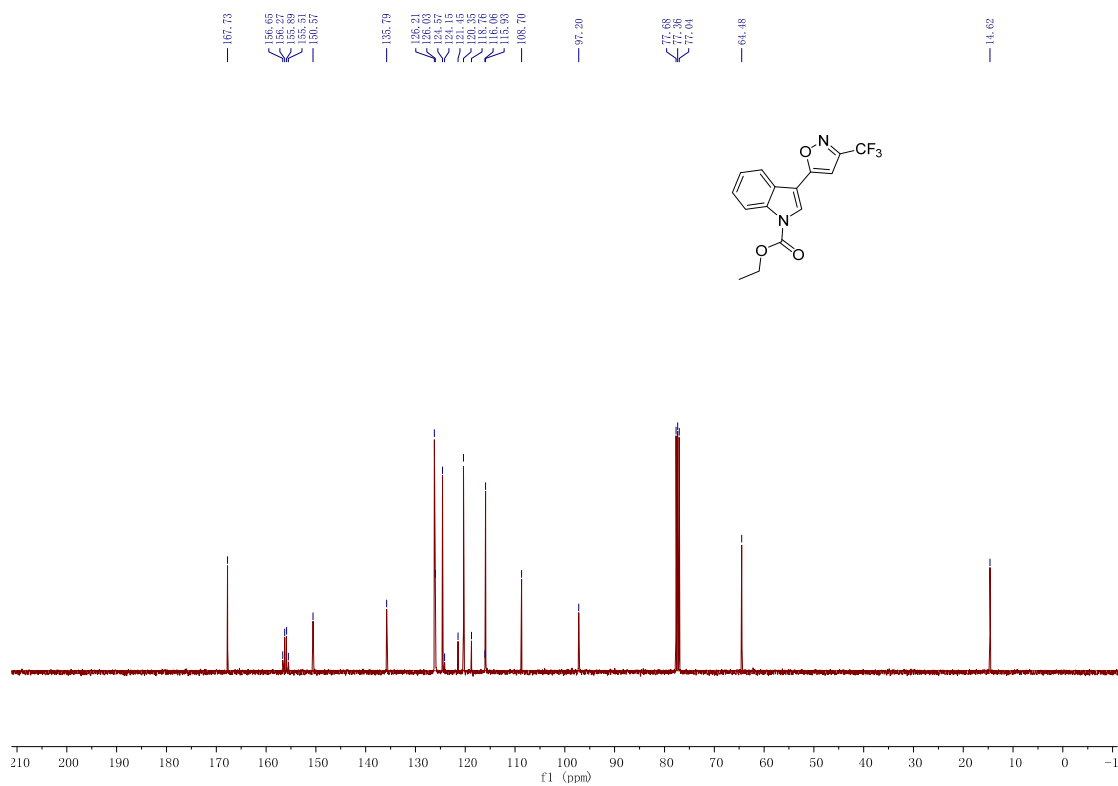
^{19}F { ^1H } NMR (CDCl_3 , 376 MHz) of **9hh**



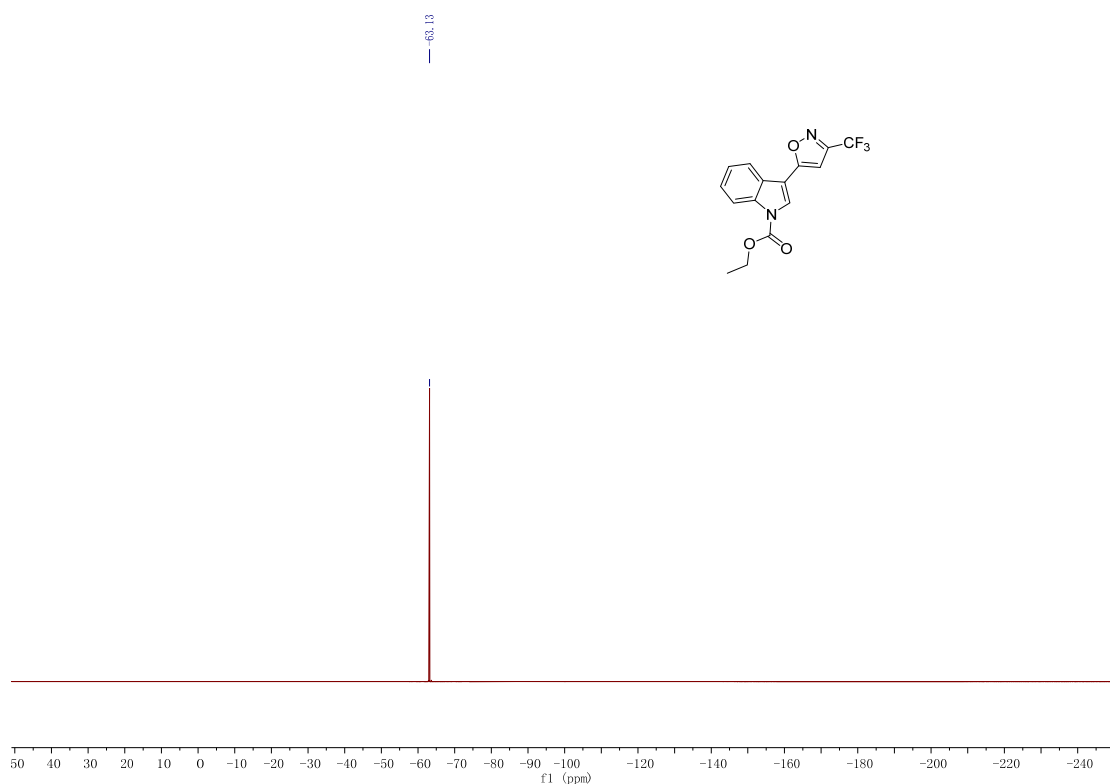
^1H NMR (CDCl₃, 400 MHz) of **9ii**



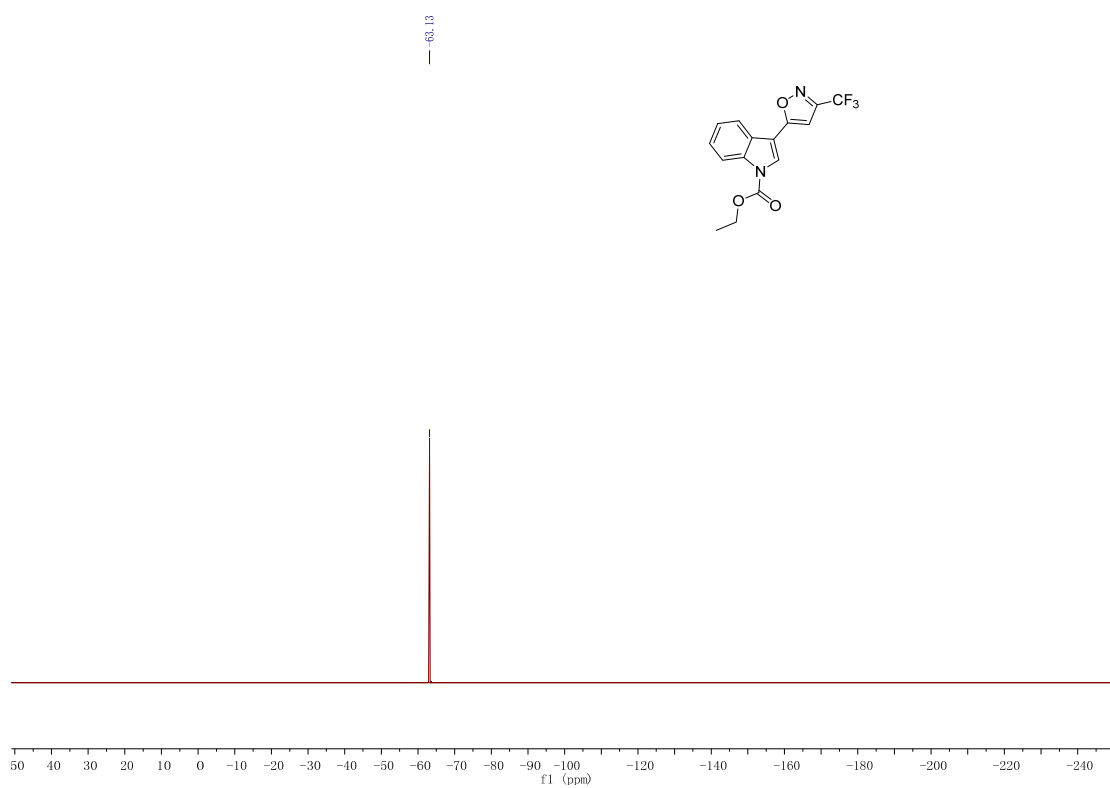
^{13}C NMR (CDCl₃, 100 MHz) of **9ii**



^{19}F NMR (CDCl₃, 376 MHz) of **9ii**



^{19}F { ^1H } NMR (CDCl₃, 376 MHz) of **9ii**



Chemical structure: Cc1cc(OC(=N1)C(F)(F)F)C=Cc2ccccc2

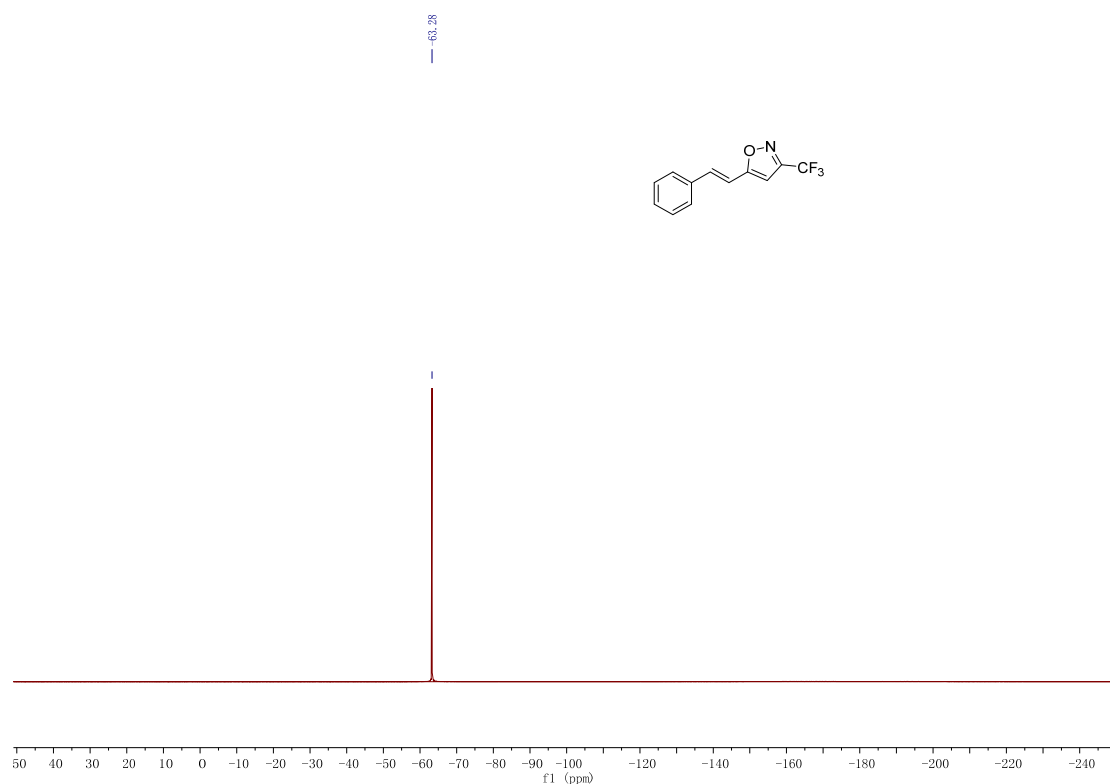
¹H NMR spectrum (CDCl₃) showing peaks at 7.55 (d, 2H), 7.45 (d, 2H), 7.25 (m, 5H), 6.55 (s, 1H), 1.55 (s, 3H), 1.35 (s, 3H), and 0.00 (TMS). Integration values are 2.12, 4.00, 1.05, and 1.00.

Chemical structure: CN(C)(C)c1cc(OC=Cc2ccc([N+](=O)[O-])cc2)oc1

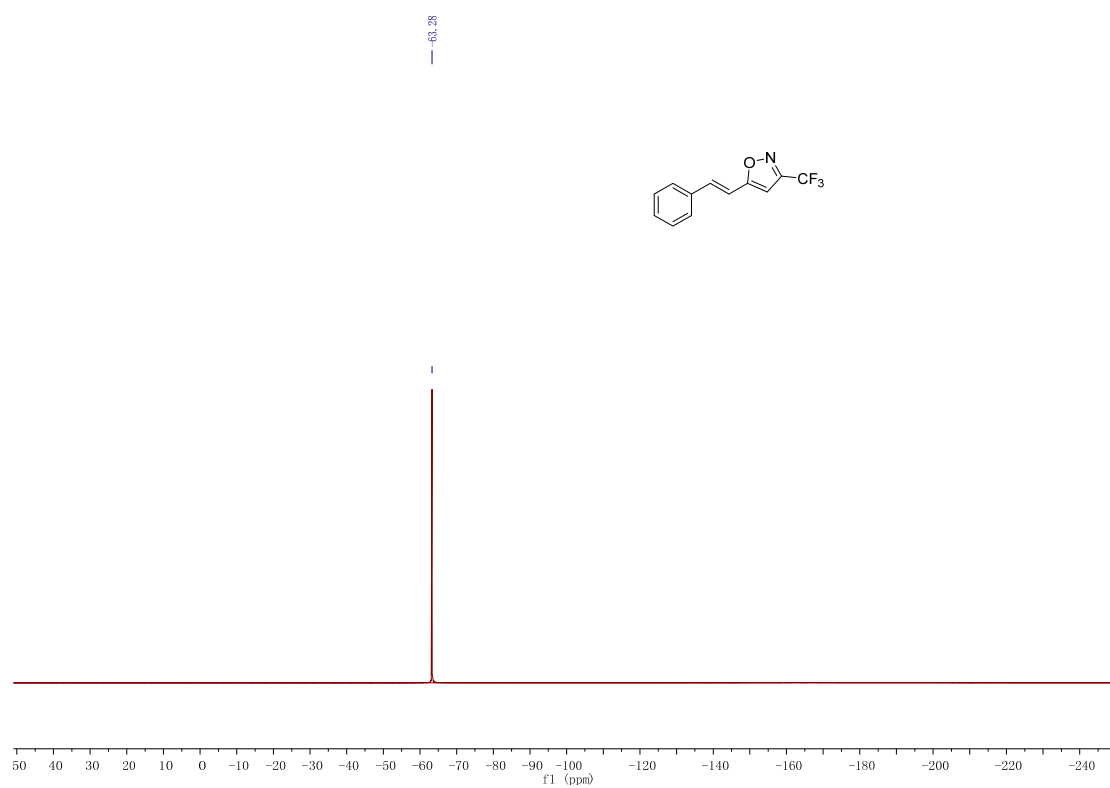
¹³C NMR peaks (ppm):

- 171.30
- 156.70, 156.32, 155.94, 155.56
- 137.48, 135.16
- 130.62, 129.74, 128.69, 128.26, 127.70, 116.00, 112.13
- 98.59
- 77.68, 77.36, 77.04

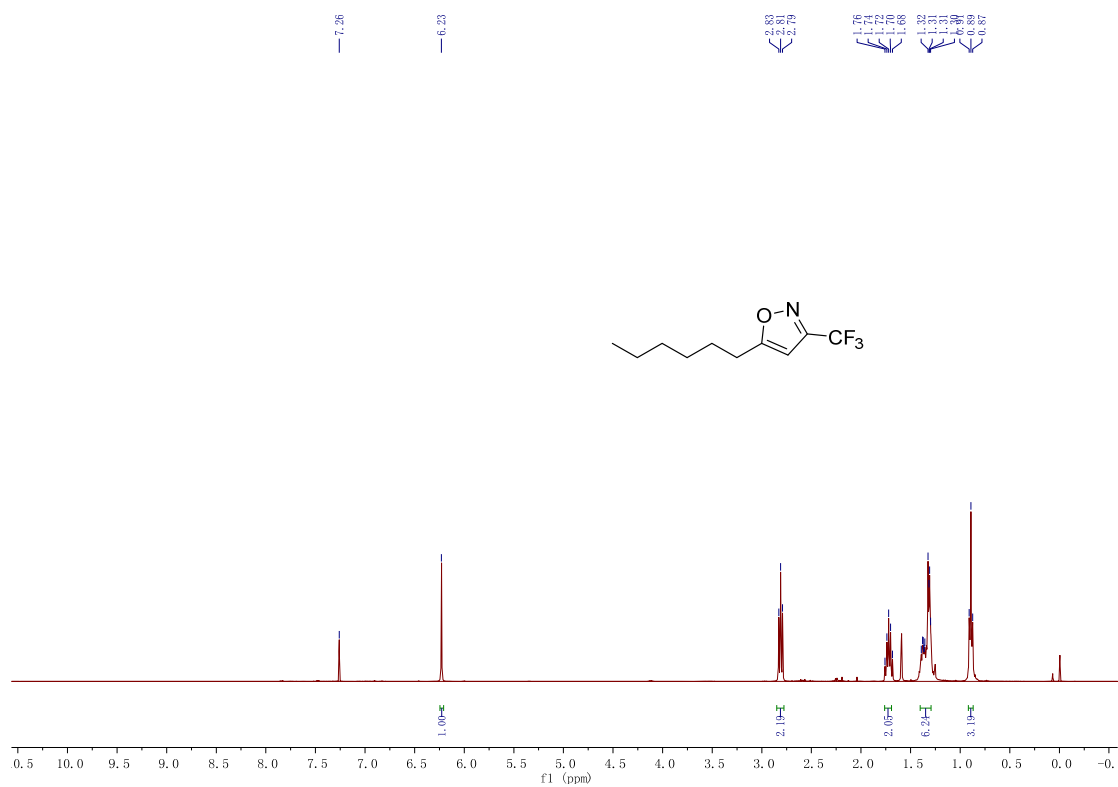
^{19}F NMR (CDCl₃, 376 MHz) of **9jj**



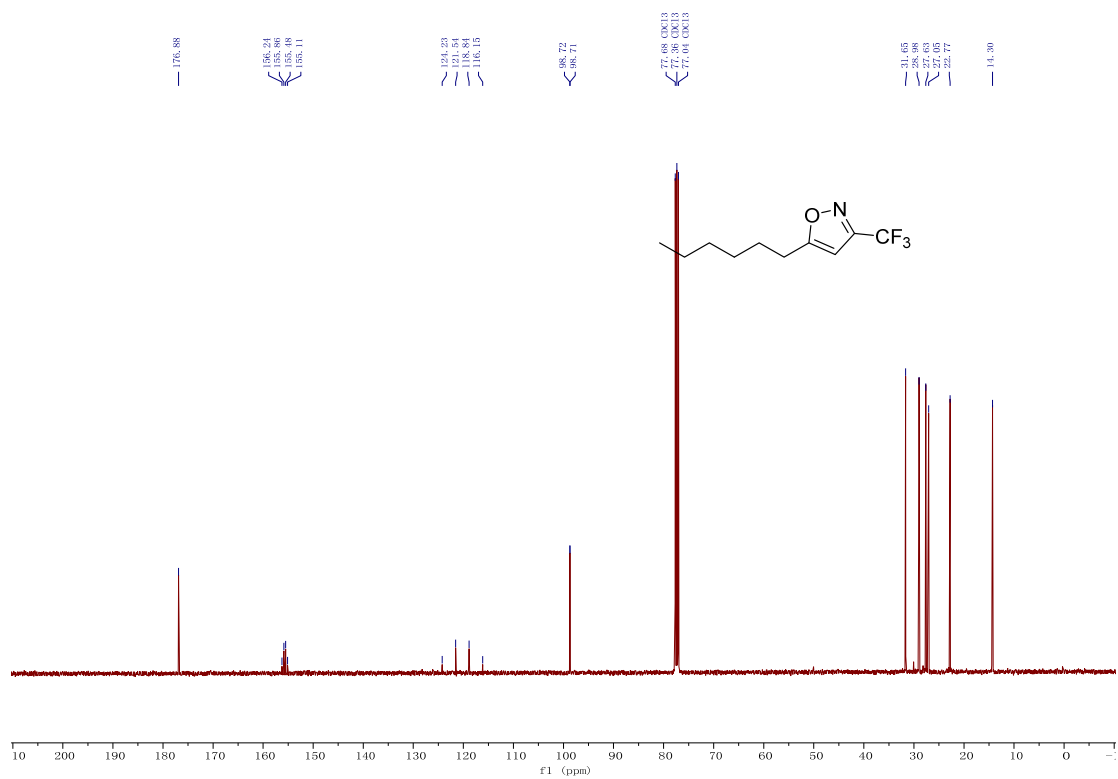
^{19}F { ^1H } NMR (CDCl₃, 376 MHz) of **9jj**



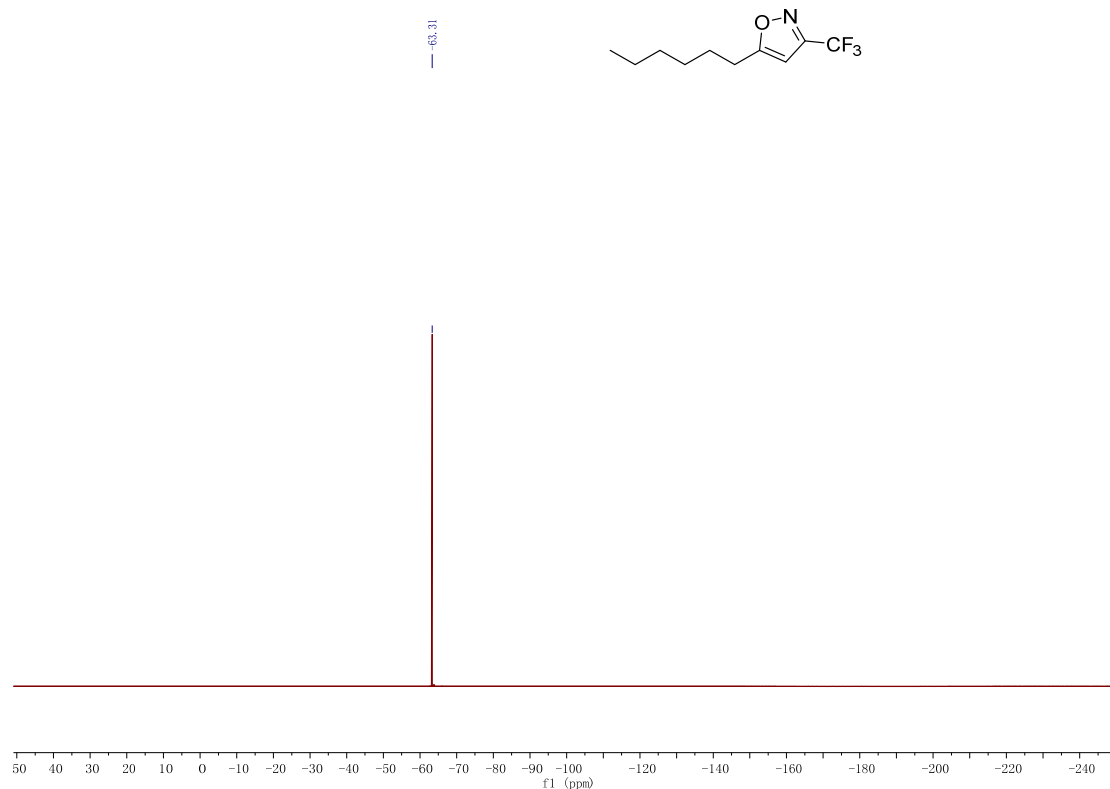
^1H NMR (CDCl₃, 400 MHz) of **9kk**



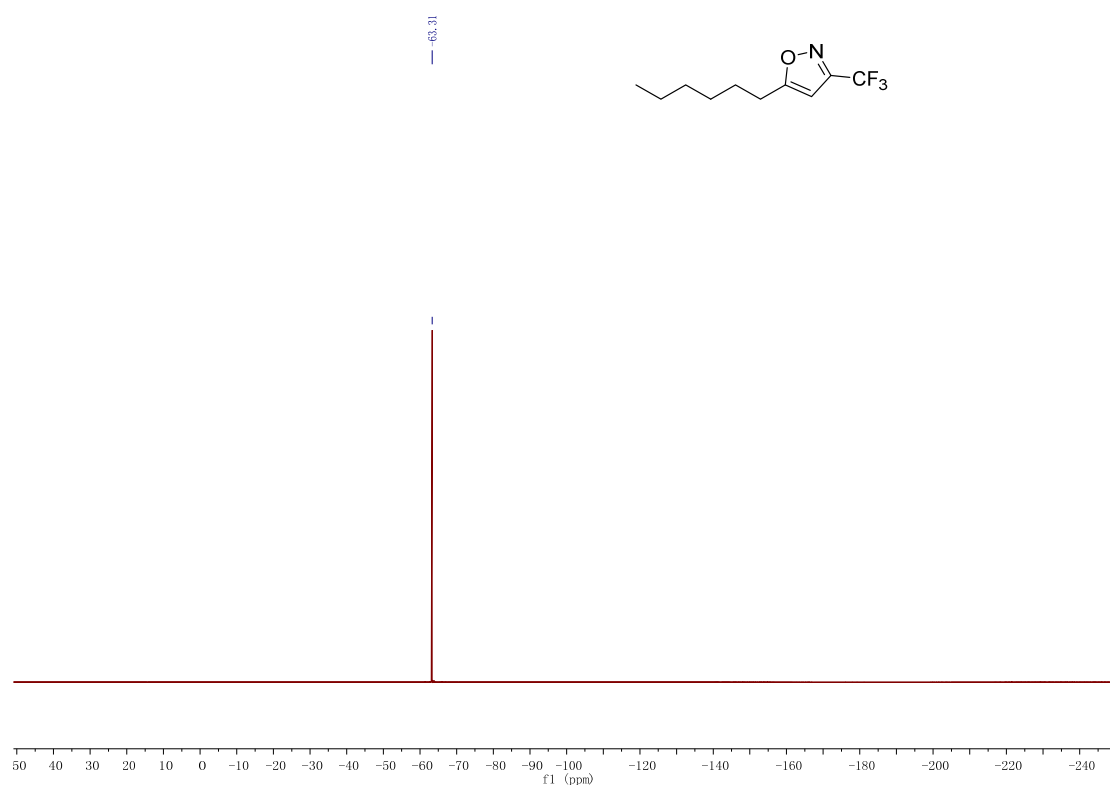
^{13}C NMR (CDCl₃, 100 MHz) of **9kk**



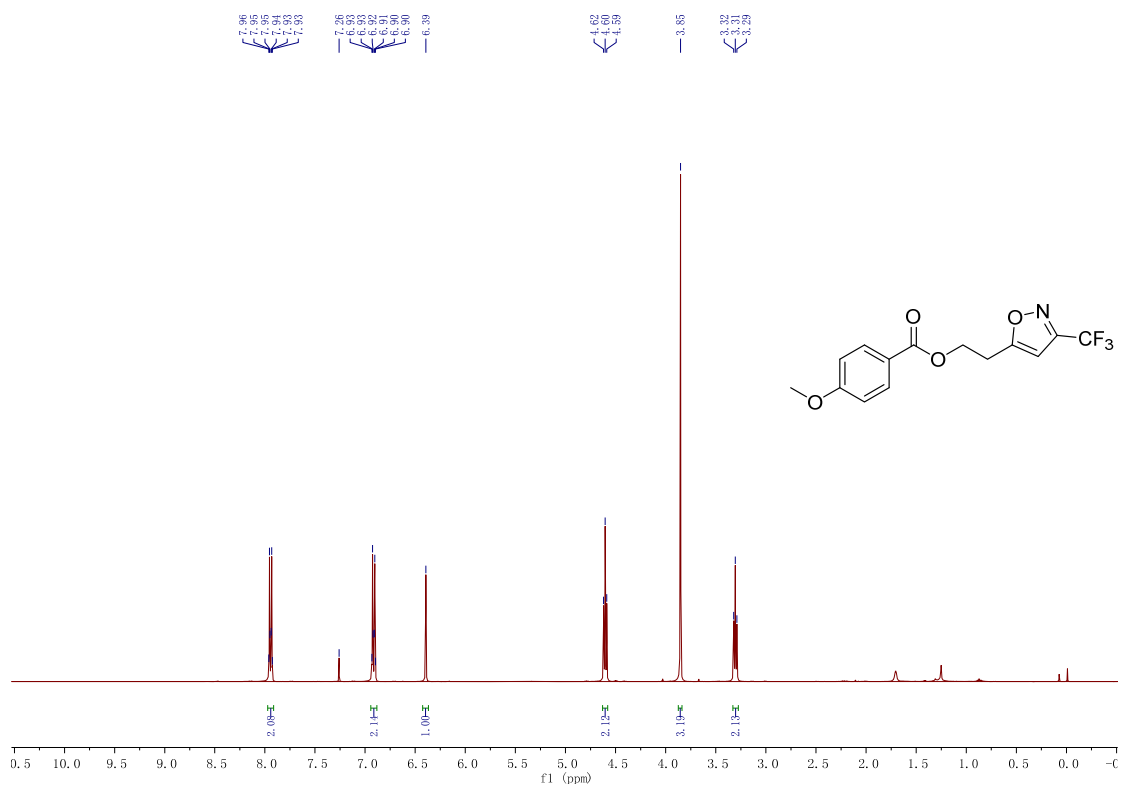
^{19}F NMR (CDCl_3 , 376 MHz) of **9kk**



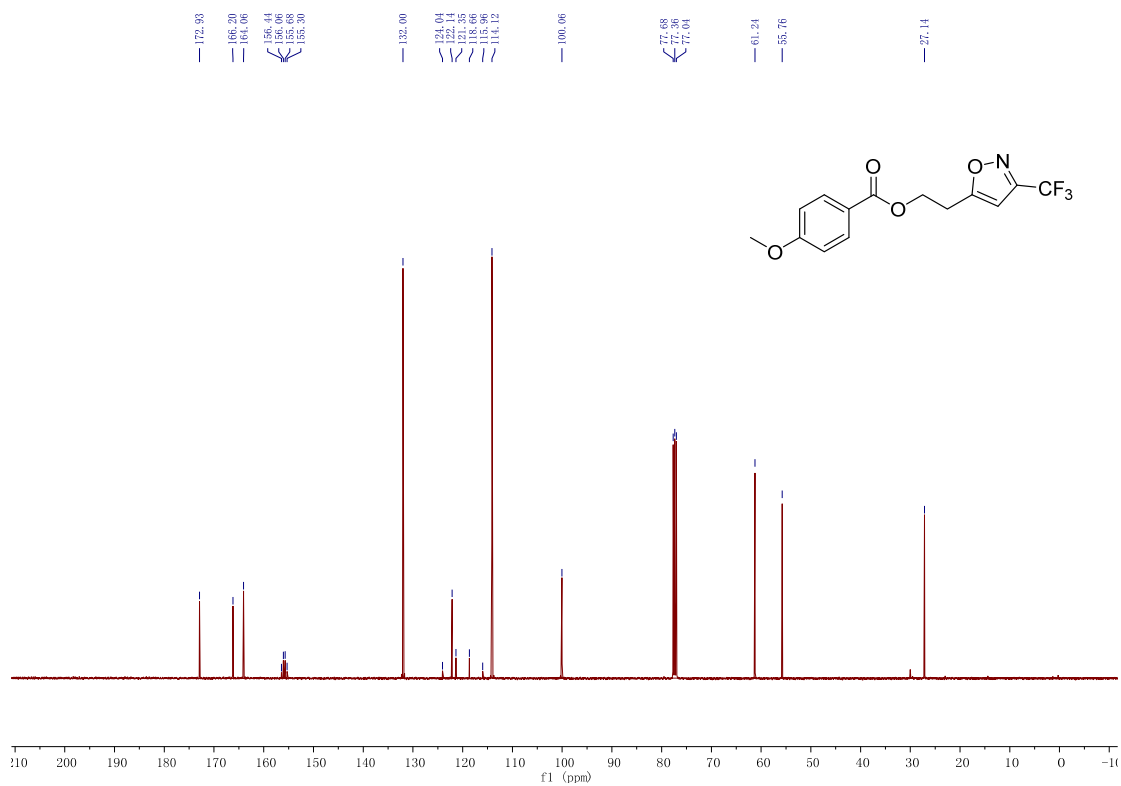
^{19}F { ^1H } NMR (CDCl_3 , 376 MHz) of **9kk**



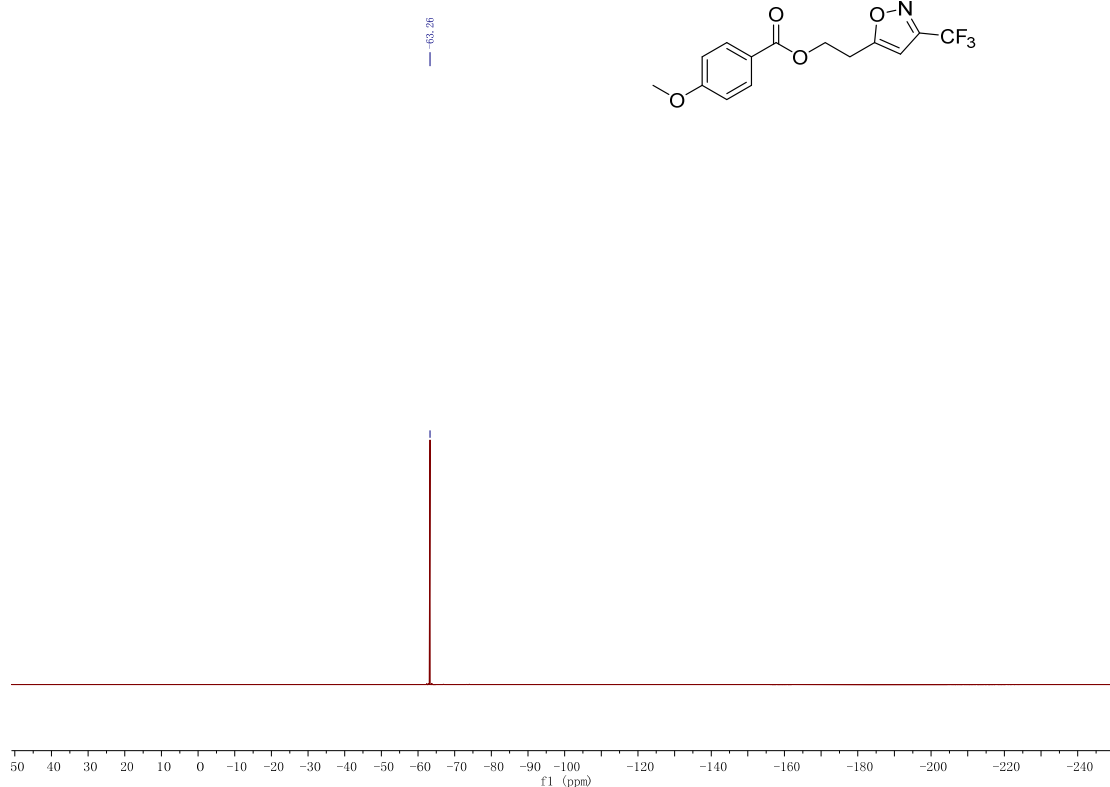
¹H NMR (CDCl₃, 400 MHz) of 9II



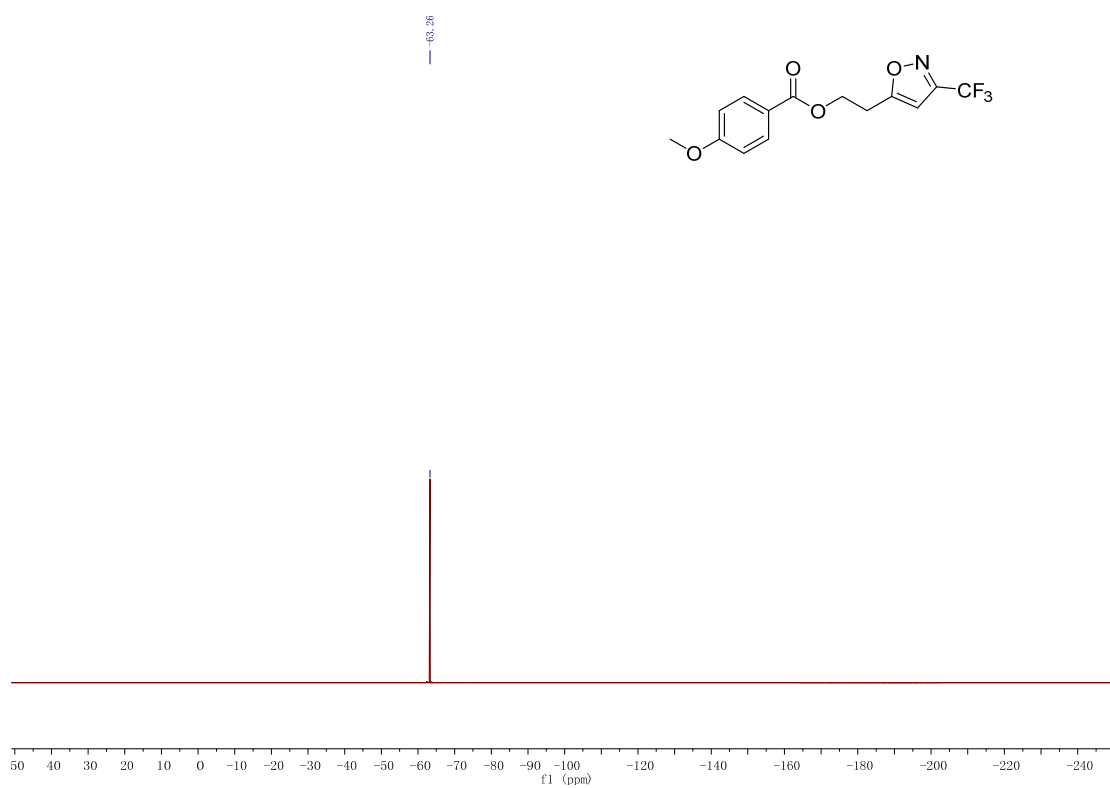
¹³C NMR (CDCl₃, 100 MHz) of 9II



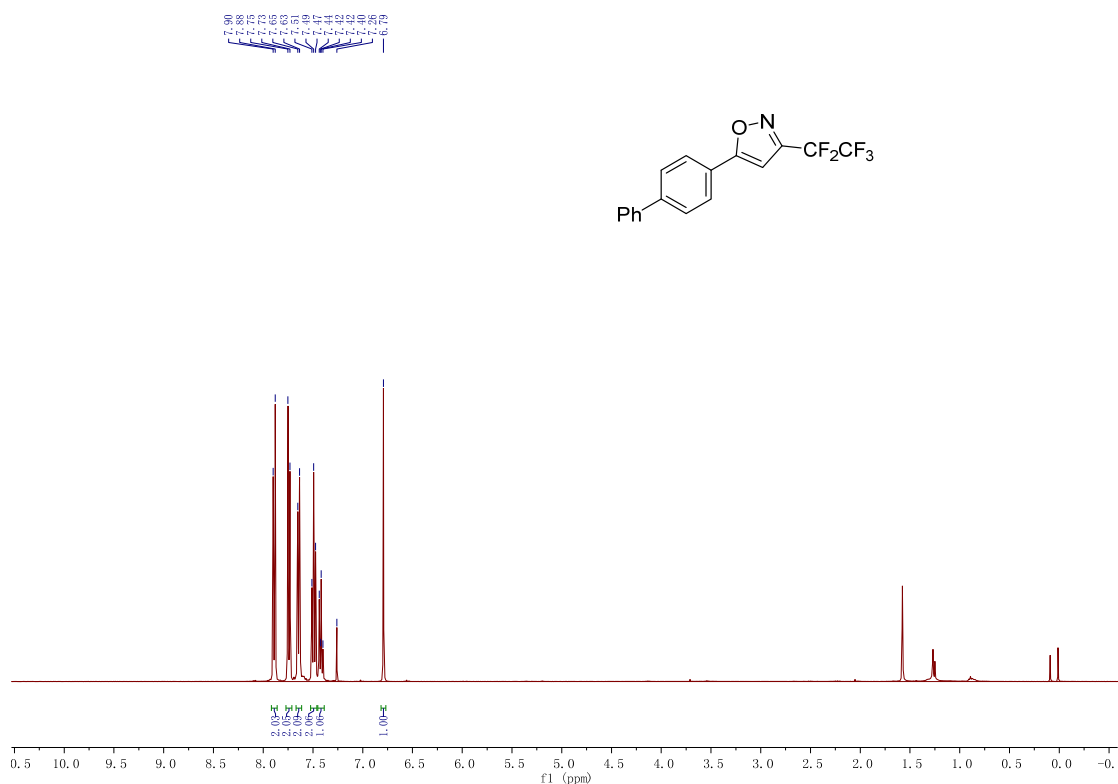
^{19}F NMR (CDCl₃, 376 MHz) of **9II**



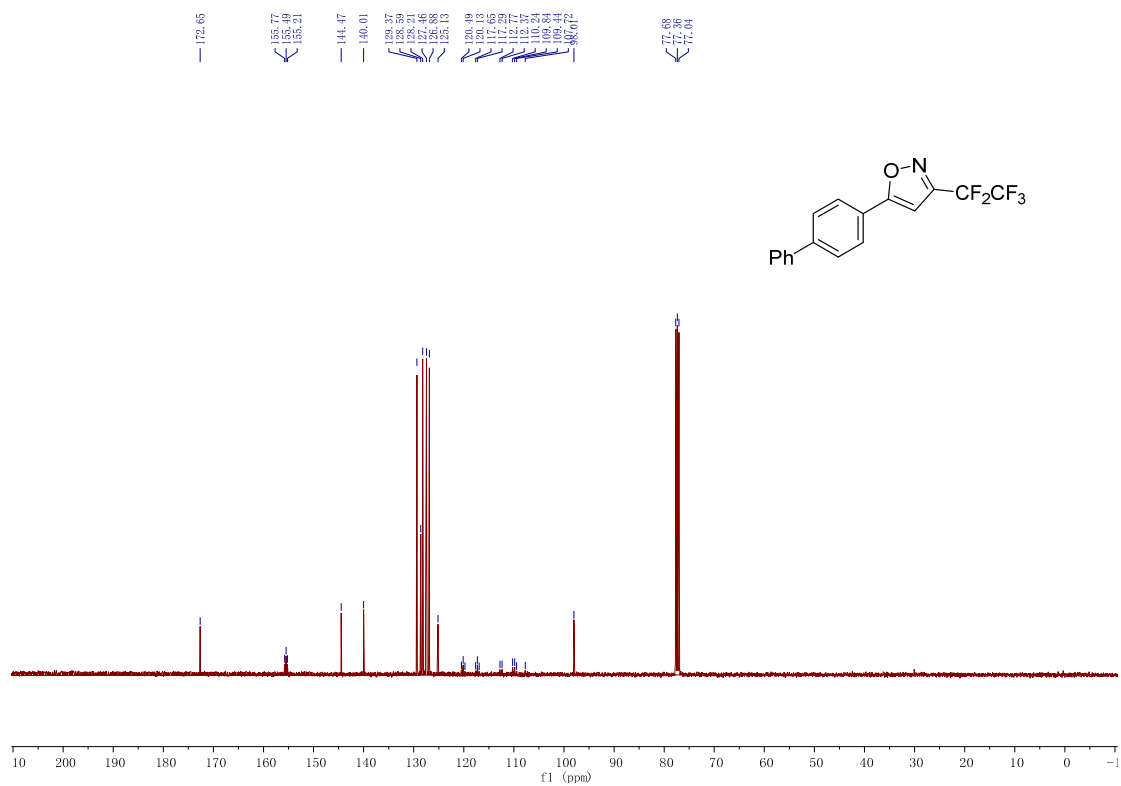
^{19}F { ^1H } NMR (CDCl₃, 376 MHz) of **9II**



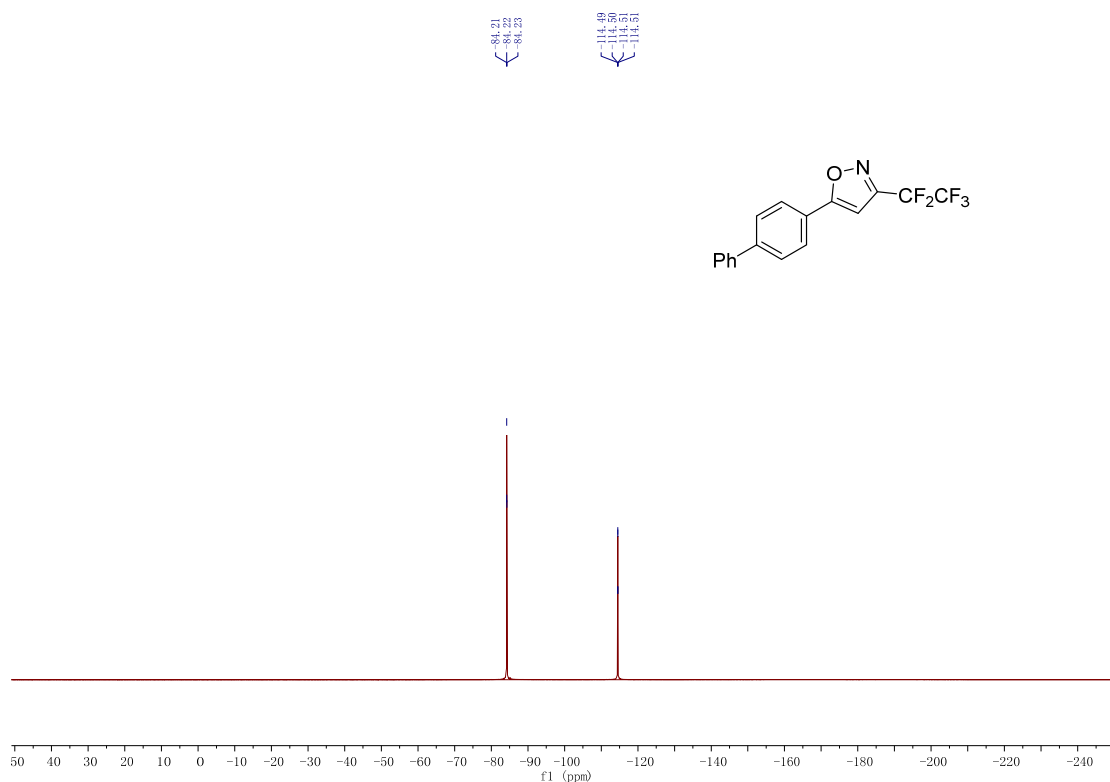
^1H NMR (CDCl₃, 400 MHz) of **10**



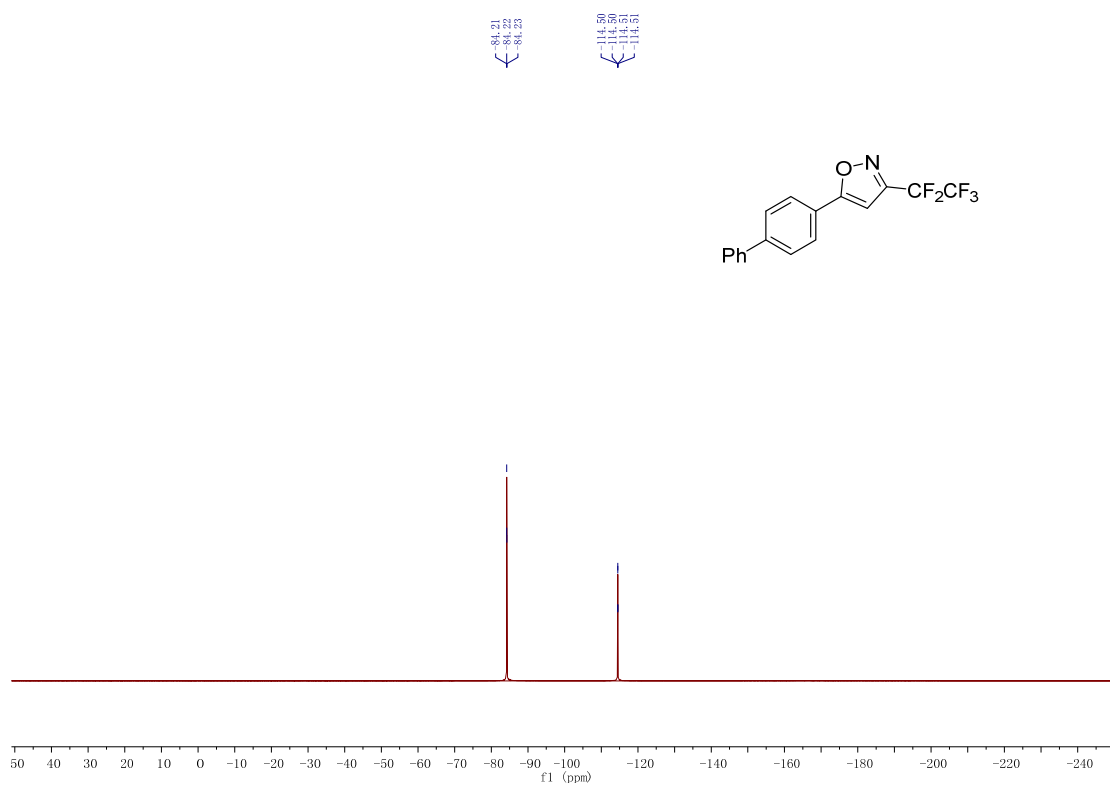
^{13}C NMR (CDCl₃, 100 MHz) of **10**



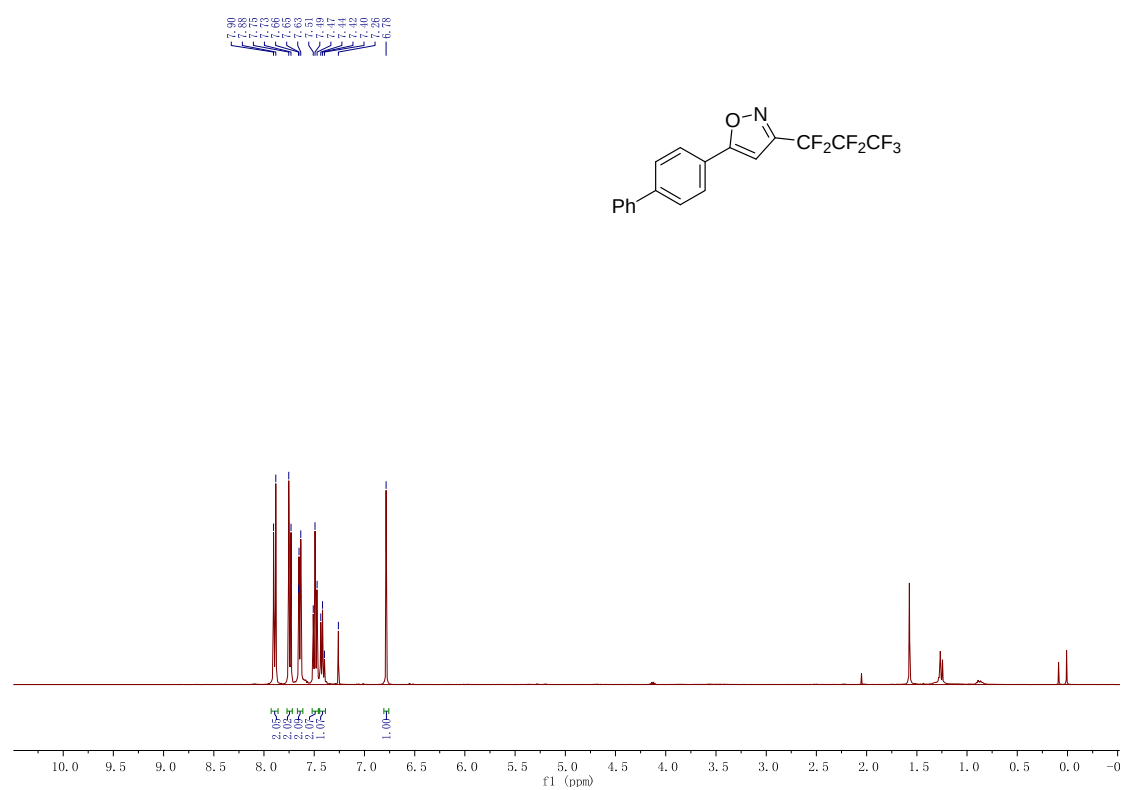
^{19}F NMR (CDCl₃, 376 MHz) of **10**



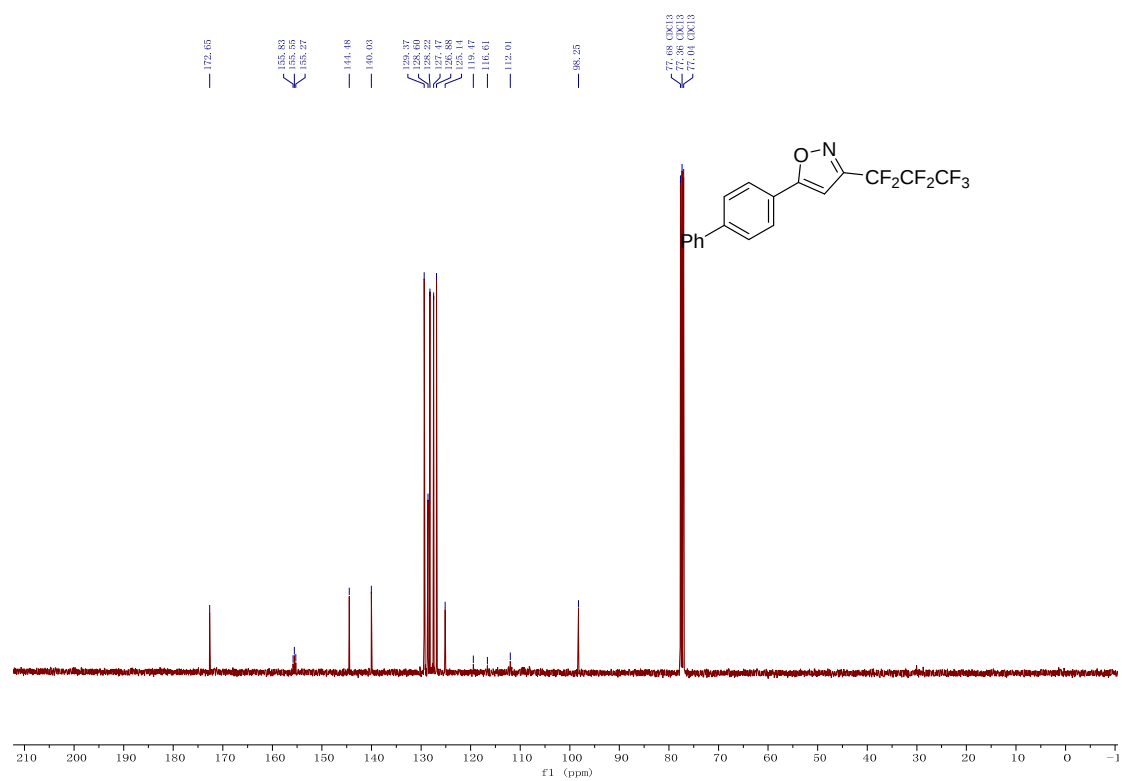
^{19}F { ^1H } NMR (CDCl₃, 376 MHz) of **10**



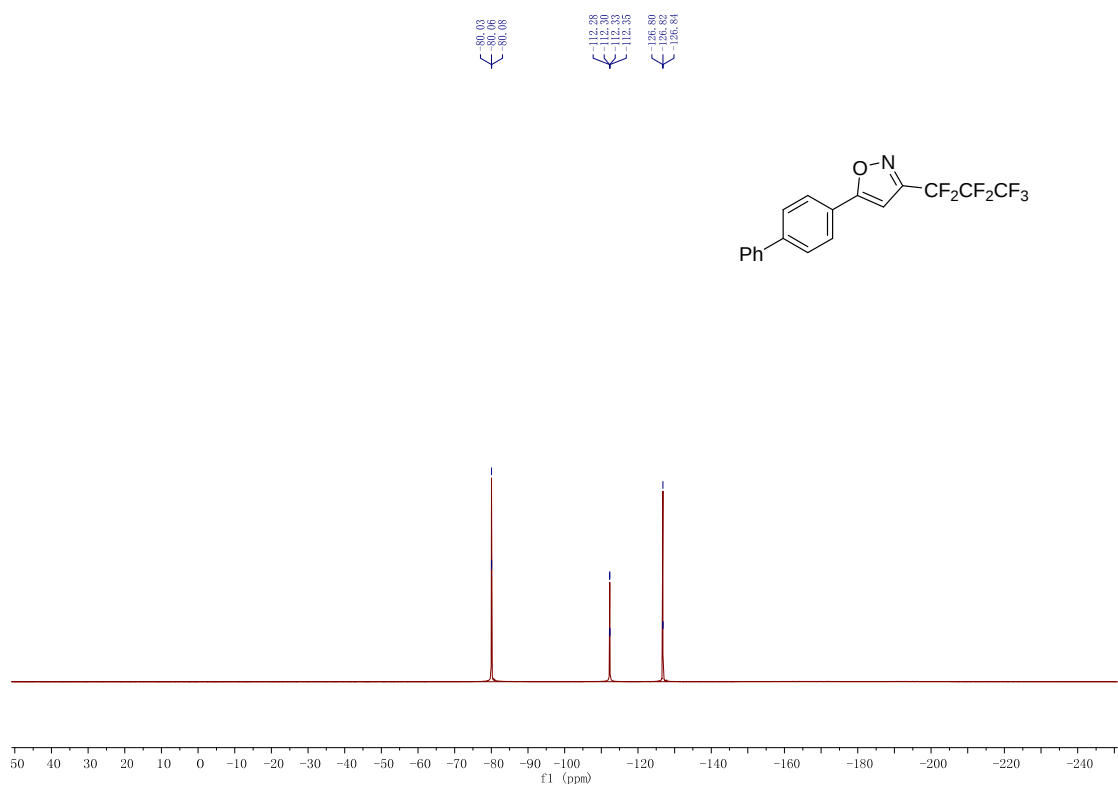
^1H NMR (CDCl₃, 400 MHz) of **11**



^{13}C NMR (CDCl₃, 100 MHz) of **11**



^{19}F NMR (CDCl₃, 376 MHz) of **11**



^{19}F { ^1H } NMR (CDCl₃, 376 MHz) of **11**

