Supporting Information

Copper-catalyzed three-component reaction of arylhydrazine hydrochloride, DABSO, and NFSI for the synthesis of arenesulfonyl fluoride

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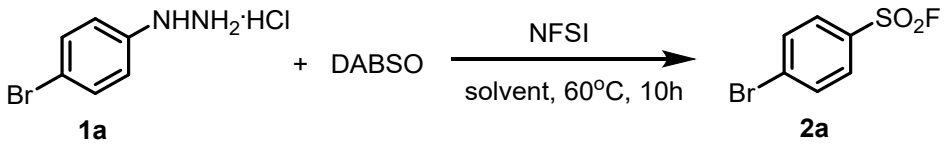
I. General information

Unless otherwise stated, all reagents were purchased from commercial source and used as received. The solvent MeCN, dichloroethane (DCE), and N, N-dimethylformamide (DMF) and so on were distilled from CaH_2. 1,4-diazabicyclo[2.2.2]octane-1,4-diium-1,4-disulfinate (DABSO) was synthesized with 1,4-diazabicyclo[2.2.2]octane(DABCO) and sulfur dioxide. ^1H, ^{19}F and ^{13}C NMR spectra were obtained on 400 MHz spectrometer. ^1H NMR and ^{13}C NMR chemical shifts were determined relative to internal $(CH_3)_4Si$ (TMS) at δ 0.0 ppm and ^{19}F NMR chemical shifts were determined relative to $CFCl_3$ at δ 0.0 ppm. Data for ^1H, ^{19}F and ^{13}C NMR were recorded as follows: chemical shift (δ, ppm), multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br = broad). Coupling constants are reported in hertz (Hz). Flash column chromatograph was carried out using 300-400 mesh silica gel at medium pressure. The NMR yield was determined by ^{19}F NMR using 1-methoxy-4-(trifluoromethoxy) benzene (^{19}F NMR: δ -58.4 ppm) as an internal standard before working up the reaction. GC-MS (EI) data were determined on an Agilent 5975C. LRMS (EI) and HRMS (EI) data were tested on a Waters Micromass GCT Premier.

II. Screening reaction conditions for fluorosulfonylation of Arylhydrazine

Table S1. Initial attempt[a]



Entry	Solvent	Yield[b] (%)	Entry	Solvent	Yield[b] (%)
1	DMF	6	2	DMAc	6
3	DMSO	n.d.	4	EtOH	11
5	MeCN	29	6	Acetone	16
7	THF	3	8	Dioxane	16
9	DCM	41	**10**	**DCE**	**45**
11	Toluene	34	12	Hexane	7

[a] Reaction conditions: **1a** (0.1 mmol, 1.0 equiv.), DABSO (0.1 mmol, 1.0 equiv.), NFSI (0.3 mmol, 3.0 equiv.), solvent (1.0 mL), Ar atmosphere, 60℃, 10 h. [b] Yields were determined by ^{19}F NMR spectroscopy using 1-methoxy-4-(trifluoromethoxy)benzene as an internal standard.

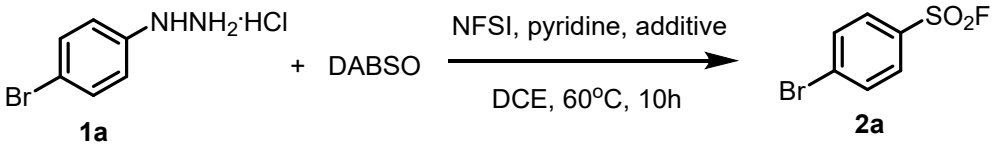
Table S2. Screening the bases[a]

Entry	Base	Yield[b] (%)
1	KF	27
2	K_2CO_3	27
3	KOH	27
4	KHF_2	36
5	K_3PO_4	19
6	Na_2CO_3	41
7	$NaHCO_3$	35

8	DBU	15
9	Et_3N	21
10	**pyridine**	**54**

[a] Reaction conditions: **1a** (0.1 mmol, 1.0 equiv.), DABSO (0.1 mmol, 1.0 equiv.), NFSI (0.3 mmol, 3.0 equiv.), base (0.2 mmol, 2.0 equiv.), DCE (1.0 mL), 60℃, Ar atmosphere, 10 h. [b] Yields were determined by ^{19}F NMR spectroscopy using 1-methoxy-4-(trifluoromethoxy)benzene as an internal standard.

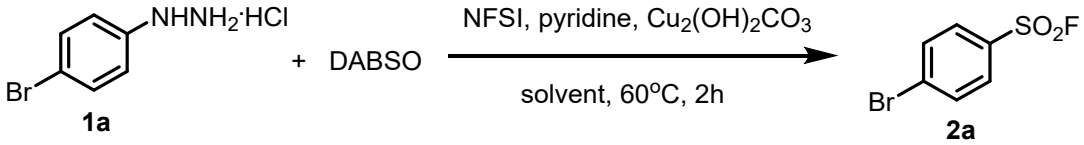
Table S3. Screening the additives[a]



Entry	Additive	Yield[b] (%)
1	DMP	45
2	$(4\text{-ClPh})_2SO$	48
3	LPO	50
4	4Å MS	50
5	TBAI	28
6	DMAP	44
7	$Pd(OAc)_2$	45
8	$AgNO_3$	38
9	$Cu(MeCN)_4BF_4$	45
10	$Cu(OH)_2$	55
11	**$Cu_2(OH)_2CO_3$**	**70**

[a] Reaction conditions: **1a** (0.2 mmol, 1.0 equiv.), DABSO (0.25 mmol, 1.25 equiv.), NFSI (0.6 mmol, 3.0 equiv.), pyridine (0.4 mmol, 2.0 equiv.), additive (0.2 mmol, 1.0 equiv.), DCE (2.0 mL), Ar atmosphere, 60℃, 10 h. [b] Yields were determined by ^{19}F NMR spectroscopy using 1-methoxy-4-(trifluoromethoxy)benzene as an internal standard.

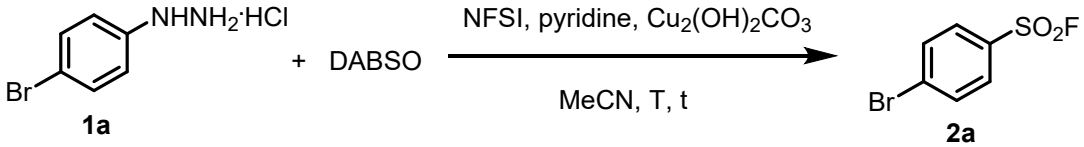
Table S4. Screening the solvents[a]



Entry	Solvent	Yield[b] (%)
1	**MeCN**	**79**
2	DCE	74
3	EtOH	26
4	EA	54
5	DMF	9
6	acetone	43
7	toluene	27

[a] Reaction conditions: **1a** (0.2 mmol, 1.0 equiv.), DABSO (0.25 mmol, 1.25 equiv.), NFSI (0.44 mmol, 2.2 equiv.), pyridine (0.4 mmol, 2.0 equiv.), $Cu_2(OH)_2CO_3$ (0.02 mmol, 0.1 equiv.), solvent (2.0 mL), Ar atmosphere, 60℃, 2 h. [b] Yields were determined by ^{19}F NMR spectroscopy using 1-methoxy-4-(trifluoromethoxy)benzene as an internal standard.

Table S5. The effect of reaction temperature and time[a]

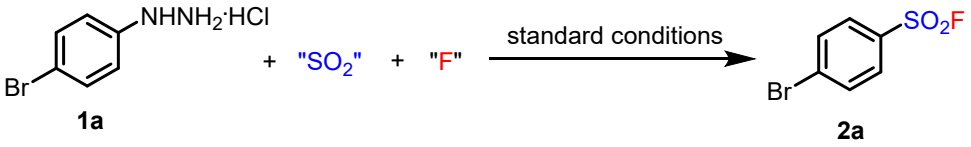


Entry	T (℃)	t (h)	Yield[b] (%)
1	60	2	77
2	60	5	74
3	60	8	72
4	60	10	73
5	60	12	75
6	20	2	60
7	**40**	**2**	**79**
8	80	2	76

[a] Reaction conditions: **1a** (0.2 mmol, 1.0 equiv.), DABSO (0.25 mmol, 1.25 equiv.), NFSI (0.44

mmol, 2.2 equiv.), pyridine (0.4 mmol, 2.0 equiv.), $Cu_2(OH)_2CO_3$ (0.02 mmol, 0.1 equiv.), MeCN (2.0 mL), Ar atmosphere, T, t. [b] Yields were determined by ^{19}F NMR spectroscopy using 1-methoxy-4-(trifluoromethoxy)benzene as an internal standard.

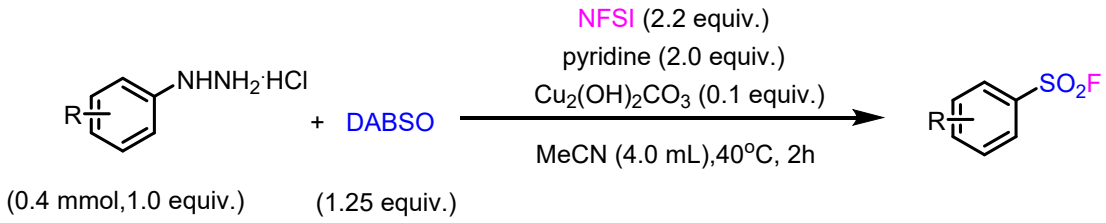
Table S6. Control experiments



Entry	Variation from the standard conditions	Yield[b] (%)
1	none	79
2	Selectfluor instead of NFSI	53
3	$Na_2S_2O_4$, $K_2S_2O_5$ instead of DABSO	<20
4	thiourea dioxide instead of DABSO	trace
5	DMF, NMP instead of MeCN	trace
6	DCE instead of MeCN	74
7	without $Cu_2(OH)_2CO_3$	54
8	$Cu_2(OH)_2CO_3$ (0.2 equiv.)	81
9	DABSO (2.5 equiv.)	79
10	air instead of Ar atmosphere	70
11	air instead of Ar atmosphere, NFSI (1.2 equiv.), $Cu_2(OH)_2CO_3$ (5 mol%)	31

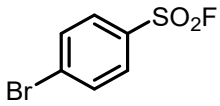
[a] Reaction conditions: **1a** (0.2 mmol, 1.0 equiv.), DABSO (0.25 mmol, 1.25 equiv.), NFSI (0.44 mmol, 2.2 equiv.), pyridine (0.4 mmol, 2.0 equiv.), $Cu_2(OH)_2CO_3$ (0.02 mmol, 0.1 equiv.), MeCN (2.0 mL), Ar atmosphere, 40℃, 2 h. [b] Yields were determined by ^{19}F NMR spectroscopy using 1-methoxy-4-(trifluoromethoxy)benzene as an internal standard.

III. General procedures for the fluorosulfonylation of arylhydrazine

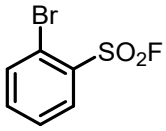


Arylhydrazine hydrochloride (0.4 mmol, 1.0 equiv.), 1,4-diazabicyclo[2.2.2] octane-1,4-diium-1,4-disulfinate (DABSO) (0.5 mmol, 1.2 equiv), N-fluorobisbenzene- sulfonamide(NFSI) (0.88 mmol, 2.2 equiv) and basic copper carbonate (0.04 mmol, 10 mol %) were added to an oven-dried sealed tube (10 mL) equipped with a magnetic rotor. The tube was then evacuated and backfilled with Ar (3 times), and anhydrous MeCN (4.0 mL) and pyridine (0.8 mmol, 2 equiv) was added via syringe under Ar atmosphere. The mixture was sealed and stirred smoothly at 40 °C for 2 hours. Yields of the desired product were measured by ^{19}F NMR spectroscopy before working-up. The reaction mixture is then filtered through 200-300 mesh silica gel and monitored by thin layer chromatography. After removal of the solvent under reduced pressure with a rotary evaporator, the crude product was purified by column chromatography on silica gel to give the desired fluorosulfonylated product.

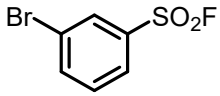
IV. Characterization data of the products



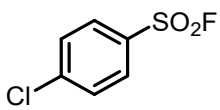
4-bromobenzenesulfonyl fluoride (2a) : Obtained as a white solid in 68% yield (65.2 mg) by silica gel flash column chromatography eluted with petroleum ether: dichloromethane = 20:3 v/v. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.88 (d, *J* = 8.7 Hz, 2H), 7.79 (d, *J* = 8.7 Hz, 2H); ^{19}F NMR (376 MHz, $CDCl_3$): δ 66.5 ppm. GC-MS (EI): m/z = 239.9 (M^+). The analytical data are consistent with literature values [1].



2-bromobenzenesulfonyl fluoride (2b) : Obtained as an off-white solid in 66% yield (63.9 mg) by silica gel flash column chromatography eluted with petroleum ether: dichloromethane = 20:3 v/v. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.15 (dd, *J* = 7.5, 2.0 Hz, 1H), 7.89 – 7.82 (m, 1H), 7.58 (td, *J* = 7.1, 6.7, 5.2 Hz, 2H); ^{19}F NMR (376 MHz, $CDCl_3$): δ 57.9 ppm. GC-MS (EI): m/z = 239.9 (M^+). The analytical data are consistent with literature values [2].

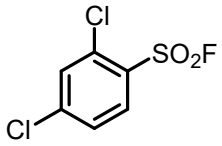


3-bromobenzenesulfonyl fluoride (2c) : Obtained as a light yellow oil in 70% yield (66.7 mg) by silica gel flash column chromatography eluted with petroleum ether: dichloromethane = 25:3 v/v. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.15 (d, *J* = 1.7 Hz, 1H), 7.94 (dd, *J* = 19.9, 8.0 Hz, 2H), 7.53 (t, *J* = 8.0 Hz, 1H); ^{19}F NMR (376 MHz, $CDCl_3$): δ 66.2 ppm. GC-MS (EI): m/z = 239.8 (M^+). The analytical data are consistent with literature values [2].

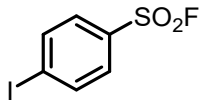


4-chlorobenzenesulfonyl fluoride (2d) : Obtained as a yellow solid in 53% yield (41.5 mg) by silica gel flash column chromatography eluted with petroleum ether: dichloromethane = 25:3 v/v. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.96 (d, *J* = 8.6 Hz, 2H),

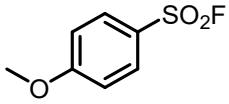
7.62 (d, J = 8.4 Hz, 2H); ^{19}F NMR (376 MHz, $CDCl_3$): δ 66.5 ppm. GC-MS (EI): m/z = 193.9 (M^+). The analytical data are consistent with literature values [1].



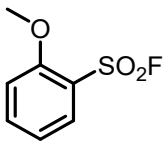
2,4-dichlorobenzenesulfonyl fluoride (2e) : Obtained as a light yellow solid in 55% yield (50.6 mg) by silica gel flash column chromatography eluted with petroleum ether: dichloromethane = 25:2 v/v. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.05 (d, J = 8.6 Hz, 1H), 7.66 (d, J = 1.9 Hz, 1H), 7.49 (dt, J = 8.6, 1.3 Hz, 1H); ^{19}F NMR (376 MHz, $CDCl_3$): δ 59.6; ^{13}C NMR (101 MHz, $CDCl_3$): δ 142.7, 134.7, 132.7, 132.7, 132.3, 127.8 ppm. Melting point: 53~55℃. HRMS (EI) m/z: $[M]^+$ Calcd for $C_6H_3Cl_2FO_2S$ 227.9215; Found 227.9213.



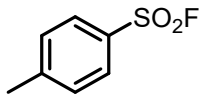
4-iodobenzenesulfonyl fluoride (2f) : Obtained as a white solid in 59% yield (67.5 mg) by silica gel flash column chromatography eluted with petroleum ether: dichloromethane = 25:3 v/v. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.01 (d, J = 8.7 Hz, 2H), 7.71 (d, J = 8.6 Hz, 2H); ^{19}F NMR (376 MHz, $CDCl_3$): δ 66.2 ppm. GC-MS (EI): m/z = 285.9 (M^+). The analytical data are consistent with literature values [3].



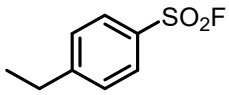
4-methoxybenzenesulfonyl fluoride (2g) : Obtained as a light yellow oil in 72% yield (55.0 mg) by silica gel flash column chromatography eluted with petroleum ether: dichloromethane = 2:1 v/v. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.94 (d, J = 9.0 Hz, 2H), 7.06 (d, J = 9.0 Hz, 2H), 3.92 (s, 3H); ^{19}F NMR (376 MHz, $CDCl_3$): δ 67.3 ppm. GC-MS (EI): m/z = 190.0 (M^+). The analytical data are consistent with literature values [1].



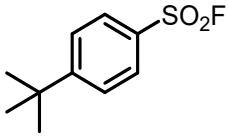
2-methoxybenzenesulfonyl fluoride (2h) : Obtained as a light yellow oil in 32% yield (24.3 mg) by silica gel flash column chromatography eluted with petroleum ether: ethyl acetate = 25:3 v/v. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.94 (dd, *J* = 8.1, 1.6 Hz, 1H), 7.74 – 7.67 (m, 1H), 7.12 (dd, *J* = 7.9, 6.0 Hz, 2H), 4.01 (s, 3H); ^{19}F NMR (376 MHz, $CDCl_3$): δ 58.5 ppm. GC-MS (EI): m/z = 190.0 (M^+). The analytical data are consistent with literature values [2].



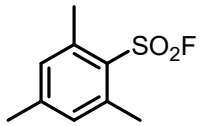
4-methylbenzenesulfonyl fluoride (2i) : Obtained as a yellow solid in 57% yield (41.4 mg) by silica gel flash column chromatography eluted with petroleum ether: dichloromethane = 10:3 v/v. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.90 (d, *J* = 8.3 Hz, 2H), 7.42 (d, *J* = 8.0 Hz, 2H), 2.49 (s, 3H); ^{19}F NMR (376 MHz, $CDCl_3$): δ 66.3 ppm. GC-MS (EI): m/z = 174.0 (M^+). The analytical data are consistent with literature values [1].



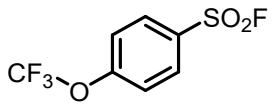
4-ethylbenzenesulfonyl fluoride (2j) : Obtained as a light yellow oil in 50% yield (38.0 mg) by silica gel flash column chromatography eluted with petroleum ether: dichloromethane = 25:3 v/v. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.92 (d, *J* = 8.3 Hz, 2H), 7.44 (d, *J* = 8.3 Hz, 2H), 2.78 (q, *J* = 7.6 Hz, 2H), 1.29 (td, *J* = 7.6, 0.7 Hz, 3H); ^{19}F NMR (376 MHz, $CDCl_3$): δ 66.9; ^{13}C NMR (101 MHz, $CDCl_3$): 153.1, 129.1, 128.6, 128.4, 29.1, 15.0 ppm. HRMS (EI) m/z: $[M]^+$ Calcd for $C_8H_9FO_2S$ 188.0307; Found 188.0305.



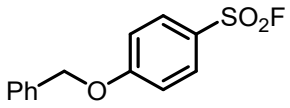
4-(tert-butyl)benzenesulfonyl fluoride (2k) : Obtained as a yellow solid in 59% yield (51.3 mg) by silica gel flash column chromatography eluted with petroleum ether: dichloromethane = 25:3 v/v. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.94 (d, *J* = 8.5 Hz, 2H), 7.63 (d, *J* = 8.2 Hz, 2H), 1.37 (s, 9H); ^{19}F NMR (376 MHz, $CDCl_3$): δ 66.2 ppm. GC-MS (EI): m/z = 216.0 (M^+). The analytical data are consistent with literature values [1].



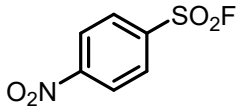
2,4,6-trimethylbenzenesulfonyl fluoride (2l) : Obtained as a white solid in 57% yield (46.5 mg) by silica gel flash column chromatography eluted with petroleum ether: dichloromethane = 10:1 v/v. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.03 (s, 2H), 2.64 (d, *J* = 1.5 Hz, 6H), 2.35 (s, 3H); ^{19}F NMR (376 MHz, $CDCl_3$): δ 68.1 ppm. GC-MS (EI): m/z = 202.0 (M^+). The analytical data are consistent with literature values [4].



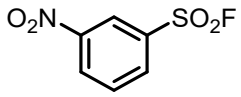
4-(trifluoromethoxy)benzenesulfonyl fluoride (2m) : Obtained as a yellow oil in 49% yield (47.9 mg) by silica gel flash column chromatography eluted with petroleum ether: dichloromethane = 10:1 v/v. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.13 – 8.06 (m, 2H), 7.46 (d, *J* = 8.5 Hz, 2H); ^{19}F NMR (376 MHz, $CDCl_3$): δ 66.6, -57.7 ppm. GC-MS (EI): m/z = 244.0 (M^+). The analytical data are consistent with literature values [5].



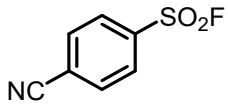
4-(benzyloxy)benzenesulfonyl fluoride (2n) : Obtained as a yellow solid in 55% yield (58.2 mg) by silica gel flash column chromatography eluted with petroleum ether: ethyl acetate = 20:1 v/v. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.97 – 7.92 (m, 2H), 7.43 (d, *J* = 4.5 Hz, 4H), 7.38 (dd, *J* = 8.4, 3.8 Hz, 1H), 7.14 (d, *J* = 8.9 Hz, 2H), 5.18 (s, 2H); ^{19}F NMR (376 MHz, $CDCl_3$): δ 67.3 ppm. GC-MS (EI): m/z = 266.0 (M^+). The analytical data are consistent with literature values [3].



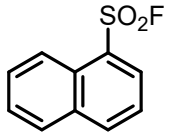
4-nitrobenzenesulfonyl fluoride (2o) : Obtained as a white solid in 51% yield (42.0 mg) by silica gel flash column chromatography eluted with petroleum ether: ethyl acetate = 100:3 v/v. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.49 (d, *J* = 8.6 Hz, 2H), 8.25 (d, *J* = 8.9 Hz, 2H); ^{19}F NMR (376 MHz, $CDCl_3$): δ 66.3 ppm. GC-MS (EI): m/z = 204.9 (M^+). The analytical data are consistent with literature values [2].



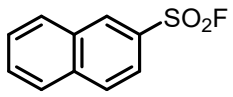
3-nitrobenzenesulfonyl fluoride (2p) : Obtained as a white solid in 71% yield (58.5 mg) by silica gel flash column chromatography eluted with petroleum ether: ethyl acetate = 20:1 v/v. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.88 (d, *J* = 1.8 Hz, 1H), 8.68 – 8.62 (m, 1H), 8.39 – 8.33 (m, 1H), 7.92 (t, *J* = 8.1 Hz, 1H); ^{19}F NMR (376 MHz, $CDCl_3$): δ 66.5 ppm. GC-MS (EI): m/z = 204.9 (M^+). The analytical data are consistent with literature values [7].



4-cyanobenzenesulfonyl fluoride (2q) : Obtained as a white solid in 67% yield (50.0 mg) by silica gel flash column chromatography eluted with petroleum ether: ethyl acetate = 100:9 v/v. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.16 (d, *J* = 8.5 Hz, 2H), 7.96 (d, *J* = 8.0 Hz, 2H); ^{19}F NMR (376 MHz, $CDCl_3$): δ 66.1 ppm. GC-MS (EI): m/z = 185.0 (M^+). The analytical data are consistent with literature values [2].

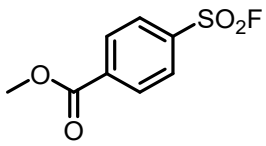


naphthalene-1-sulfonyl fluoride (2r) : Obtained as a yellow solid in 75% yield (62.7 mg) by silica gel flash column chromatography eluted with petroleum ether: dichloromethane = 25:3 v/v. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.55 (dd, *J* = 8.6, 2.8 Hz, 1H), 8.37 (d, *J* = 7.4 Hz, 1H), 8.24 (d, *J* = 8.2 Hz, 1H), 8.01 (d, *J* = 8.5 Hz, 1H), 7.83 – 7.74 (m, 1H), 7.69 (t, *J* = 7.5 Hz, 1H), 7.66 – 7.58 (m, 1H); ^{19}F NMR (376 MHz, $CDCl_3$): δ 62.5 ppm. GC-MS (EI): m/z = 210.0 (M^+). The analytical data are consistent with literature values [2].

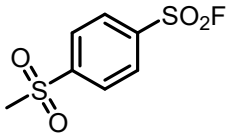


naphthalene-2-sulfonyl fluoride (2s) : Obtained as a yellow solid in 33% yield (28.1 mg) by silica gel flash column chromatography eluted with petroleum ether: dichloromethane = 5:1 v/v. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.62 (s, 1H), 8.05 (dd, *J* = 13.5, 8.5 Hz, 2H), 8.00 – 7.90 (m, 2H), 7.80 – 7.66 (m, 2H); ^{19}F NMR (376 MHz, $CDCl_3$): δ 66.3 ppm. GC-MS (EI): m/z = 210.0 (M^+). The analytical data are

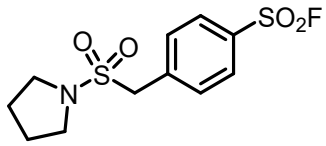
consistent with literature values [2].



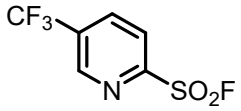
methyl 4-(fluorosulfonyl)benzoate (2t) : Obtained as a white solid in 73% yield (63.4 mg) by silica gel flash column chromatography eluted with petroleum ether: dichloromethane = 2:1 v/v. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.28 (d, J = 8.2 Hz, 2H), 8.10 (d, J = 8.5 Hz, 2H), 3.99 (s, 3H); ^{19}F NMR (376 MHz, $CDCl_3$): δ 65.8 ppm. GC-MS (EI): m/z = 218.0 (M^+). The analytical data are consistent with literature values [8].



4-(methylsulfonyl)benzenesulfonyl fluoride (2u) : Obtained as a white solid in 66% yield (62.8 mg) by silica gel flash column chromatography eluted with petroleum ether: ethyl acetate = 4:1 v/v. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.24 (s, 4H), 3.13 (d, J = 0.7 Hz, 3H); ^{19}F NMR (376 MHz, $CDCl_3$): δ 66.1 ppm. GC-MS (EI): m/z = 237.9 (M^+). The analytical data are consistent with literature values [6].

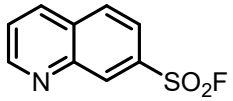


4-((pyrrolidin-1-ylsulfonyl)methyl)benzenesulfonyl fluoride (2v) : Obtained as ~~a~~ white solid in 25% yield (30.3 mg) by silica gel flash column chromatography eluted with petroleum ether: ethyl acetate = 1:1 v/v. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.03 (d, J = 8.3 Hz, 2H), 7.68 (d, J = 8.3 Hz, 2H), 4.31 (s, 2H), 3.27 (t, J = 6.6 Hz, 4H), 1.94 – 1.87 (m, 4H); ^{19}F NMR (376 MHz, $CDCl_3$): δ 66.2; ^{13}C NMR (101 MHz, $CDCl_3$): δ 131.9, 128.8, 55.7, 48.3, 25.9 ppm. Melting point: 128~130℃. HRMS (EI) m/z: $[M]^+$ Calcd for $C_{11}H_{14}FNO_4S_2$ 307.0348; Found 307.0347.



5-(trifluoromethyl)pyridine-2-sulfonyl fluoride (2w) : Obtained as a white solid in 12% yield (11.3 mg) by silica gel flash column chromatography eluted with

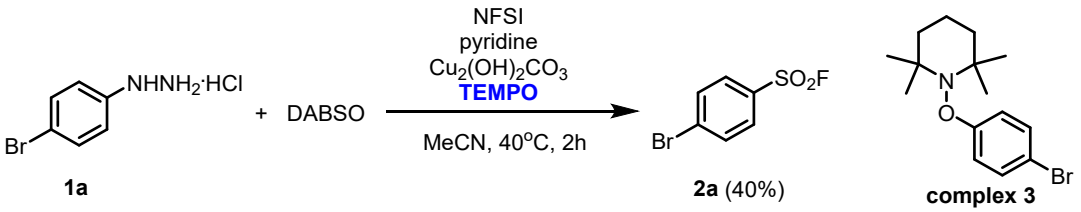
petroleum ether: dichloromethane = 1:1 v/v. ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.11 (s, 1H), 8.31 (q, *J* = 8.6 Hz, 2H); ^{19}F NMR (376 MHz, $CDCl_3$): δ 55.8, -62.8 ppm. GC-MS (EI): m/z = 228.9 (M^+). The analytical data are consistent with literature values [9].



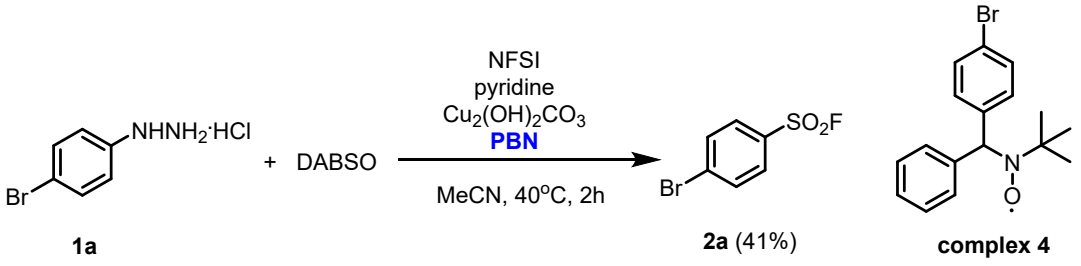
quinoline-7-sulfonyl fluoride (2x) : Obtained as a white solid in 28% yield (23.9 mg) by silica gel flash column chromatography eluted with dichloromethane: ethyl acetate = 2:1 v/v. ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.12 (d, *J* = 3.1 Hz, 1H), 8.86 (s, 1H), 8.30 (d, *J* = 8.3 Hz, 1H), 8.12 – 7.99 (m, 2H), 7.65 (dd, *J* = 8.4, 4.2 Hz, 1H); ^{19}F NMR (376 MHz, $CDCl_3$): δ 66.1; ^{13}C NMR (101 MHz, $CDCl_3$): 152.9, 146.8, 136.0, 132.2, 131.7, 130.2, 126.4, 124.6, 123.1 ppm. Melting point: 78~80℃. HRMS (EI) m/z: $[M]^+$ Calcd for $C_9H_6FNO_2S$ 211.0103; Found 211.0101.

V. Preliminary mechanistic studies and gram-scale synthesis

(a) Radical inhibition experiments



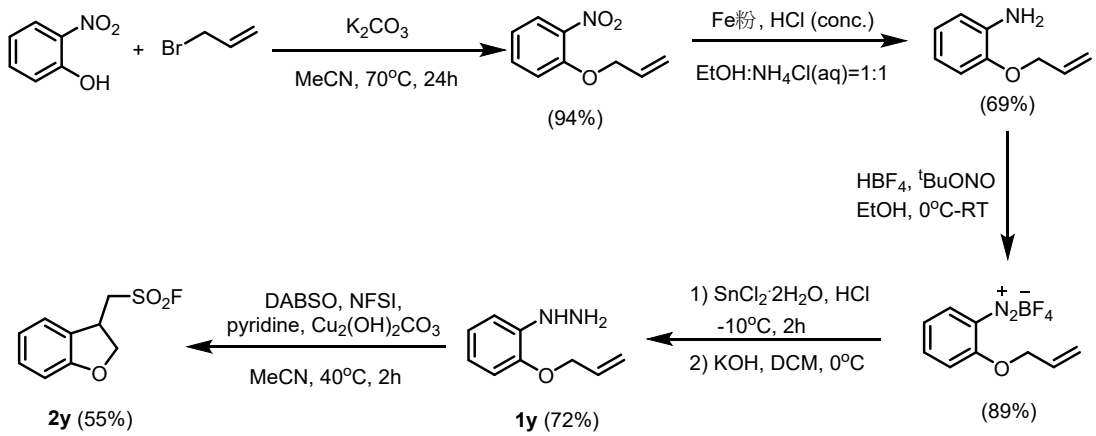
4-Bromophenylhydrazine hydrochloride (0.2 mmol, 1.0 equiv.), 1,4-diazabicyclo[2.2.2] octane-1,4-diium-1,4-disulfinate (DABSO) (0.25 mmol), N-fluorobisbenzene-sulfonamide(NFSI) (0.44 mmol) and basic copper carbonate (0.02 mmol) were added to an oven-dried sealed tube (10 mL) equipped with a magnetic rotor. The tube was then evacuated and backfilled with Ar (3 times). 2,2,6,6-Tetramethyl-1-piperidinyloxy (TEMPO, 0.4 mmol, 2.0 equiv.) was poured into the system and anhydrous MeCN (2.0 mL) and pyridine (0.4 mmol) was added via syringe under Ar atmosphere. The mixture was sealed and stirred smoothly at 40 °C for 2 hours. The yield (40%) of the desired product was measured by ^{19}F NMR spectroscopy. It can be distinguished the formation of **complex 3** from the HRMS synthesis.



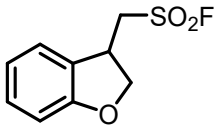
4-Bromophenylhydrazine hydrochloride (0.2 mmol, 1.0 equiv.), 1,4-diazabicyclo[2.2.2] octane-1,4-diium-1,4-disulfinate (DABSO) (0.25 mmol), N-fluorobisbenzene-sulfonamide(NFSI) (0.44 mmol), N-tert-butyl-1-phenylmethanimine oxide (0.4 mmol, 2.0 equiv.) and basic copper carbonate (0.02 mmol) were added to an oven-dried sealed tube (10 mL) equipped with a magnetic rotor. The tube was then evacuated and backfilled with, and anhydrous MeCN (2.0

mL) and pyridine (0.4 mmol) was added via syringe under Ar atmosphere. The mixture was sealed and stirred smoothly at 40 °C for 2 hours. The yield (41%) of the desired product was measured by ^{19}F NMR spectroscopy. It can be distinguished the formation of **complex 4** from the HRMS synthesis.

(b) Radical probe experiment

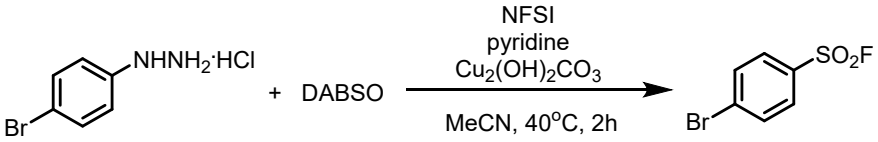


According to the previous literature[8], **1y** can be synthesized as a white solid. **1y** (0.4 mmol, 1.0 equiv.), 1,4-Diazabicyclo[2.2.2] octane-1,4-diium-1,4-disulfinate (DABSO) (0.5 mmol), N-fluorobisbenzene-sulfonamide(NFSI) (0.88 mmol) and basic copper carbonate (0.04 mmol) were added to an oven-dried sealed tube (10 mL) equipped with a magnetic rotor. The tube was then evacuated and backfilled with Ar (3 times) and anhydrous MeCN (4.0 mL) and pyridine (0.8 mmol) was added via syringe under Ar atmosphere. The mixture was sealed and stirred smoothly at 40 °C for 2 hours. Following the general procedure, the reaction mixture was purified by column chromatography to separate the products.



(2,3-dihydrobenzofuran-3-yl)methanesulfonyl fluoride (2y): Obtained as a white solid in 55% yield. ^1H NMR (400 MHz, $CDCl_3$): δ 7.23 (dt, J = 6.9, 3.5 Hz, 2H), 6.94 (t, J = 7.4 Hz, 1H), 6.87 (d, J = 8.2 Hz, 1H), 4.75 (t, J = 9.2 Hz, 1H), 4.56 (dd, J = 9.7, 5.3 Hz, 1H), 4.10 (tt, J = 9.4, 4.4 Hz, 1H), 3.76 (dt, J = 14.7, 2.8 Hz, 1H), 3.58 (ddd, J = 15.3, 10.6, 5.1 Hz, 1H); ^{19}F NMR (376 MHz, $CDCl_3$): δ 56.6 ppm. GC-MS (EI): m/z = 216.0 (M^+). The analytical data are consistent with literature values [1].

(c) Gram-scale synthesis



1a
(6.0 mmol)

2a
(1.02 g, 71%)

According to the general procedure for the fluorosulfonylation of arylhydrazine, 4-bromophenylhydrazine hydrochloride (6 mmol, 1.0 equiv.), 1,4-diazabicyclo[2.2.2] octane-1,4-diium-1,4-disulfinate (DABSO) (7.5 mmol), N-fluorobisbenzene-sulfonamide(NFSI) (13.2 mmol) and basic copper carbonate (0.6 mmol) were added to an oven-dried sealed tube (250 mL) equipped with a magnetic rotor. The tube was then evacuated and backfilled with, and anhydrous MeCN (60 mL) and pyridine (12 mmol) was added via syringe under Ar atmosphere. The mixture was sealed and stirred smoothly at 40 °C for 2 hours. The reaction mixture is then filtered through 200-300 mesh silica gel and monitored by thin layer chromatography. After removal of the solvent under reduced pressure with a rotary evaporator, the crude product was purified by column chromatography on silica gel to give the desired fluorosulfonylated product (white solid, 1.02g, 71%).

VI. References

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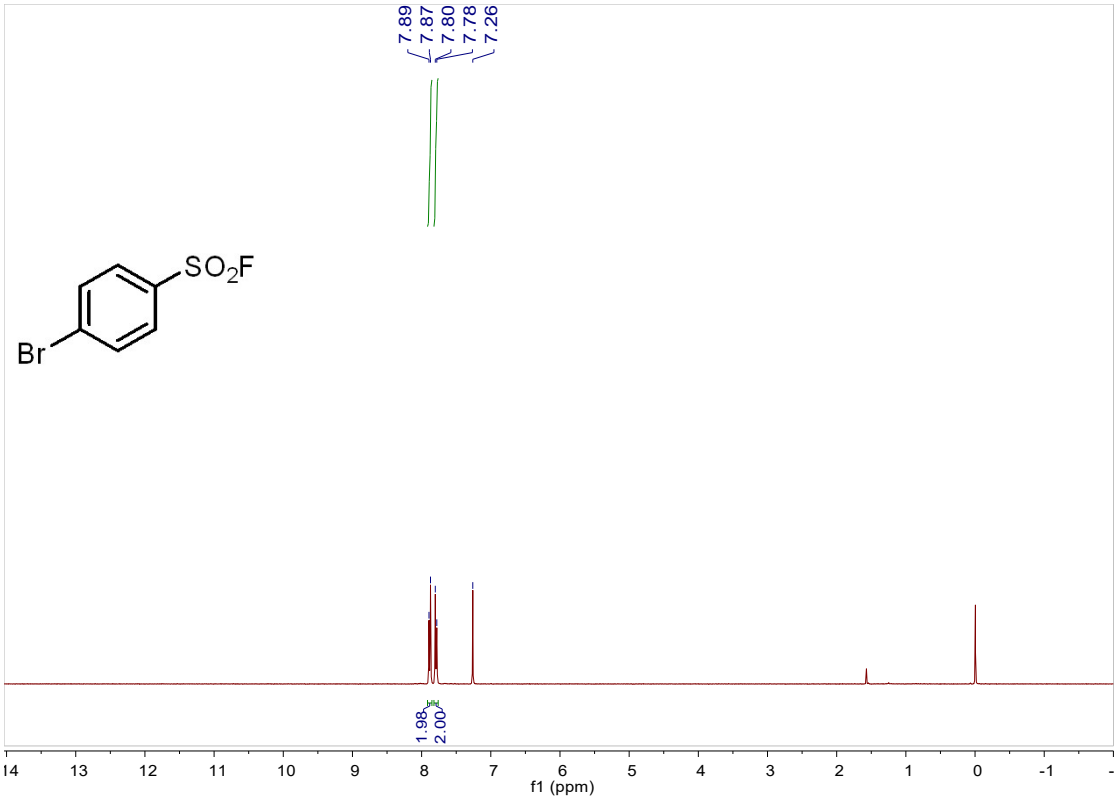
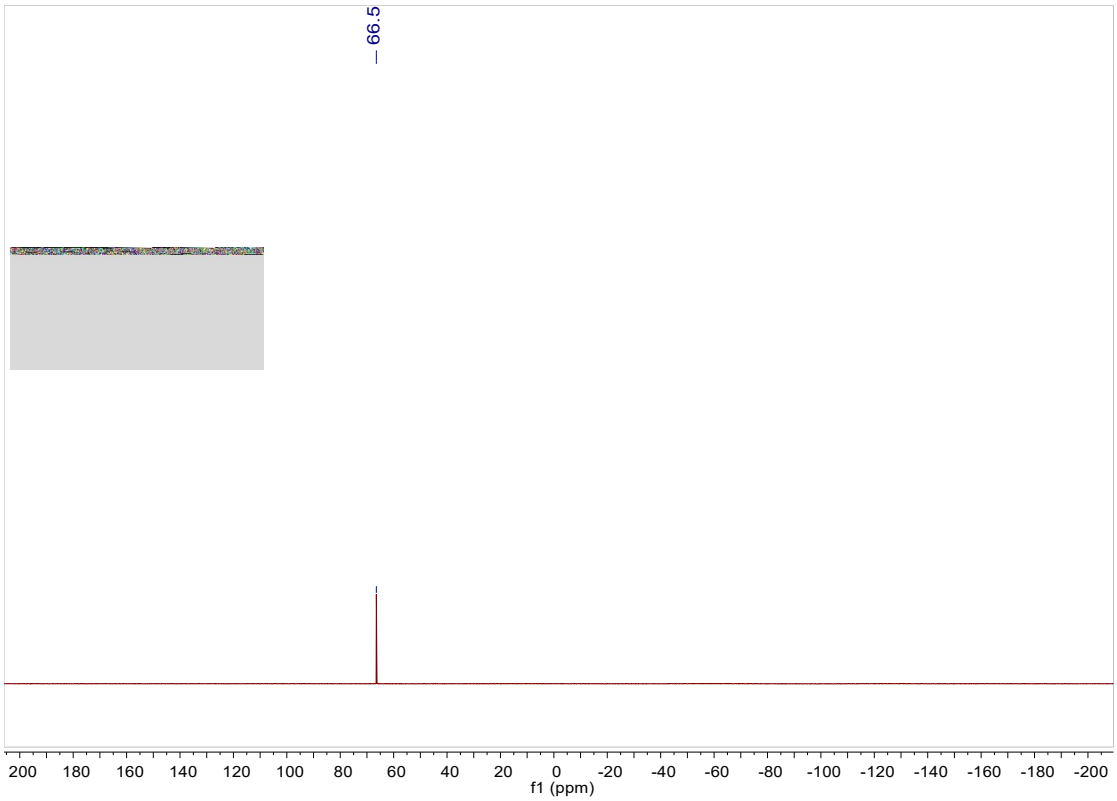
9. L. Wang and J. Cornella, *Angew. Chem. Int. Ed.,* 2020, **59,** 23510.

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

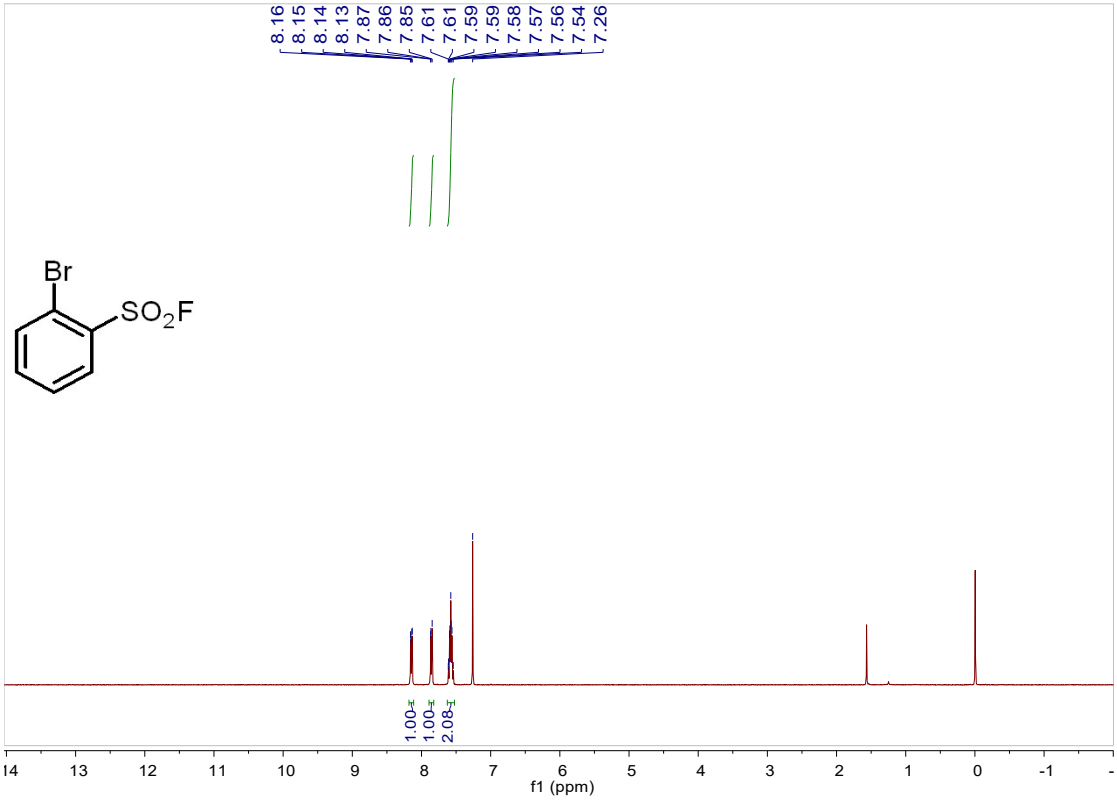
^{1}H NMR spectrum of 4-bromobenzenesulfonyl fluoride (400 MHz, $CDCl_3$)



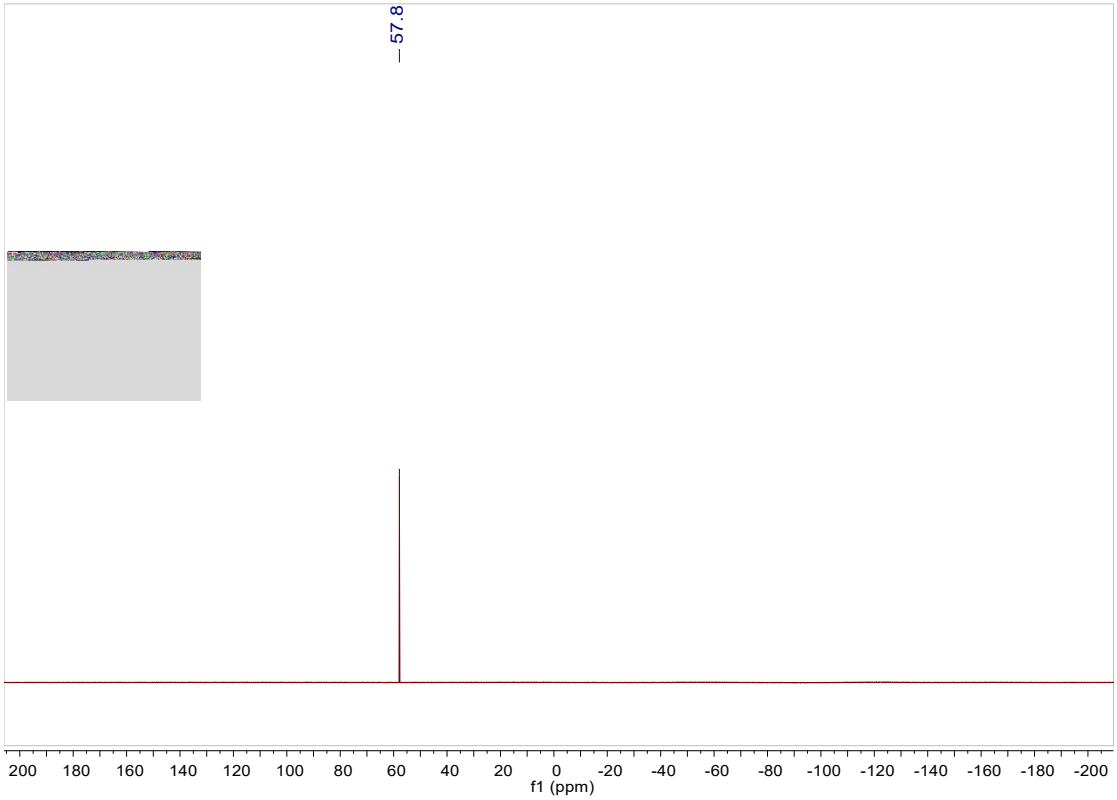
^{19}F NMR spectrum of 4-bromobenzenesulfonyl fluoride (376 MHz, $CDCl_3$)



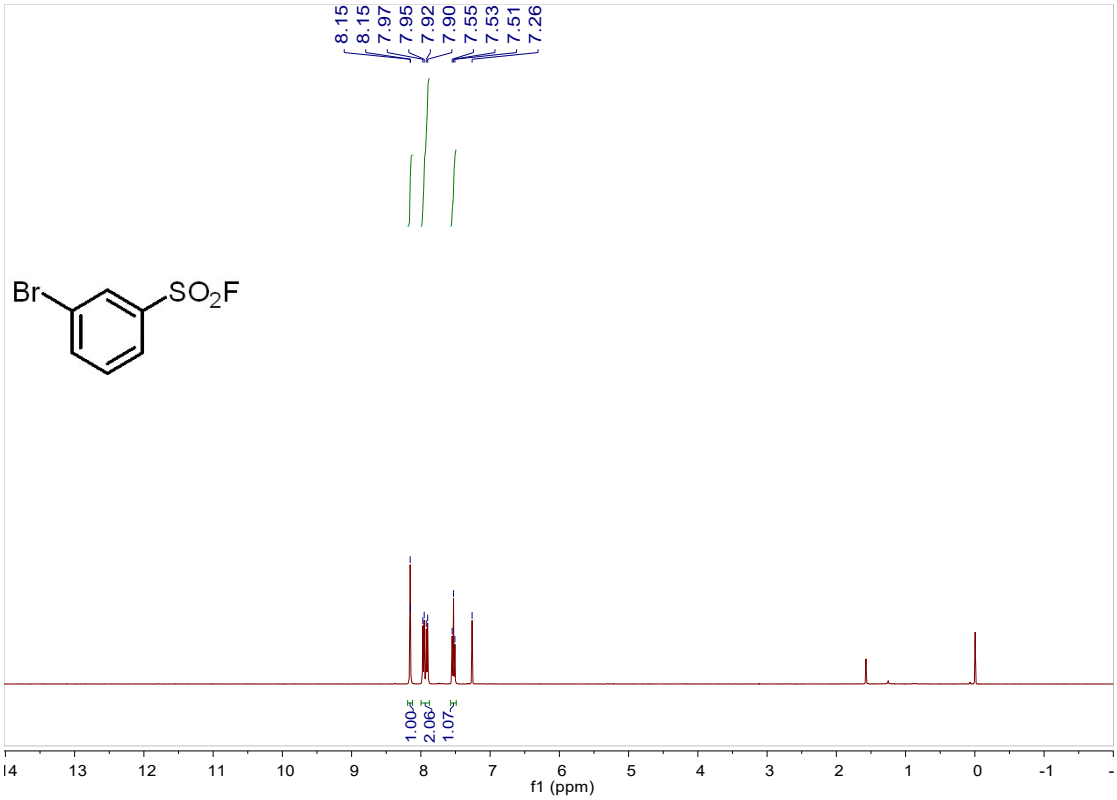
^{1}H NMR spectrum of 2-bromobenzenesulfonyl fluoride (400 MHz, $CDCl_3$)



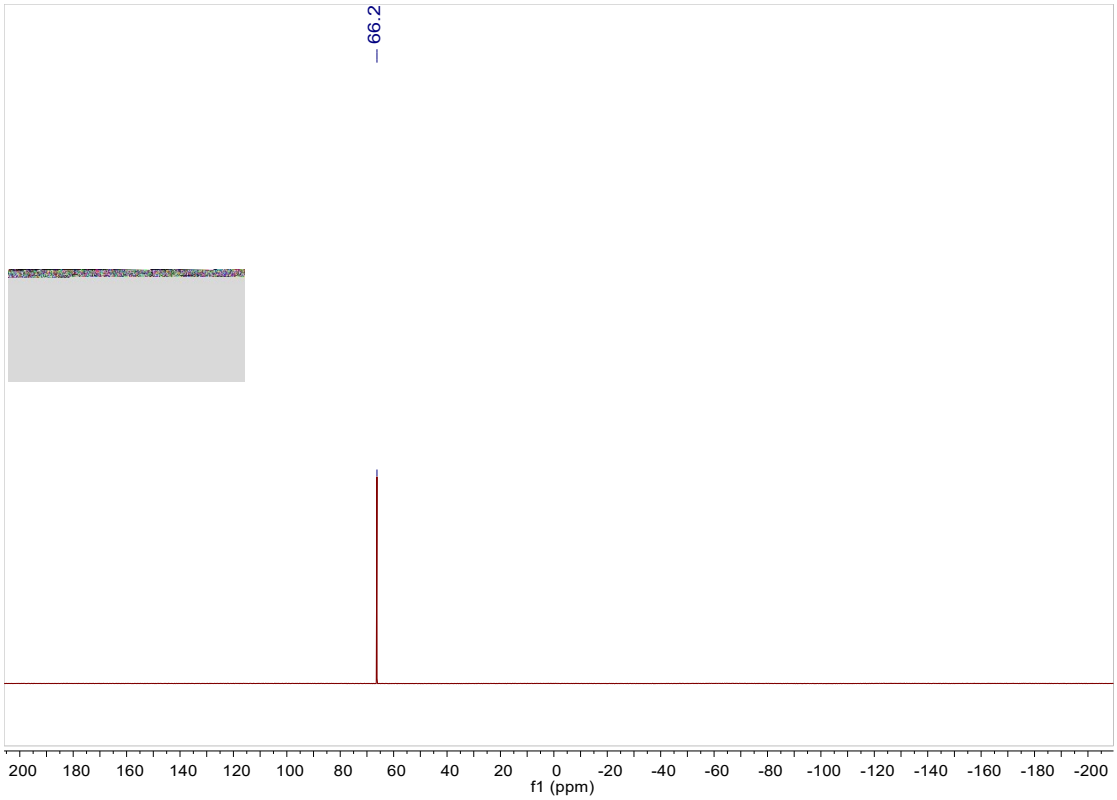
^{19}F NMR spectrum of 2-bromobenzenesulfonyl fluoride (376 MHz, $CDCl_3$)



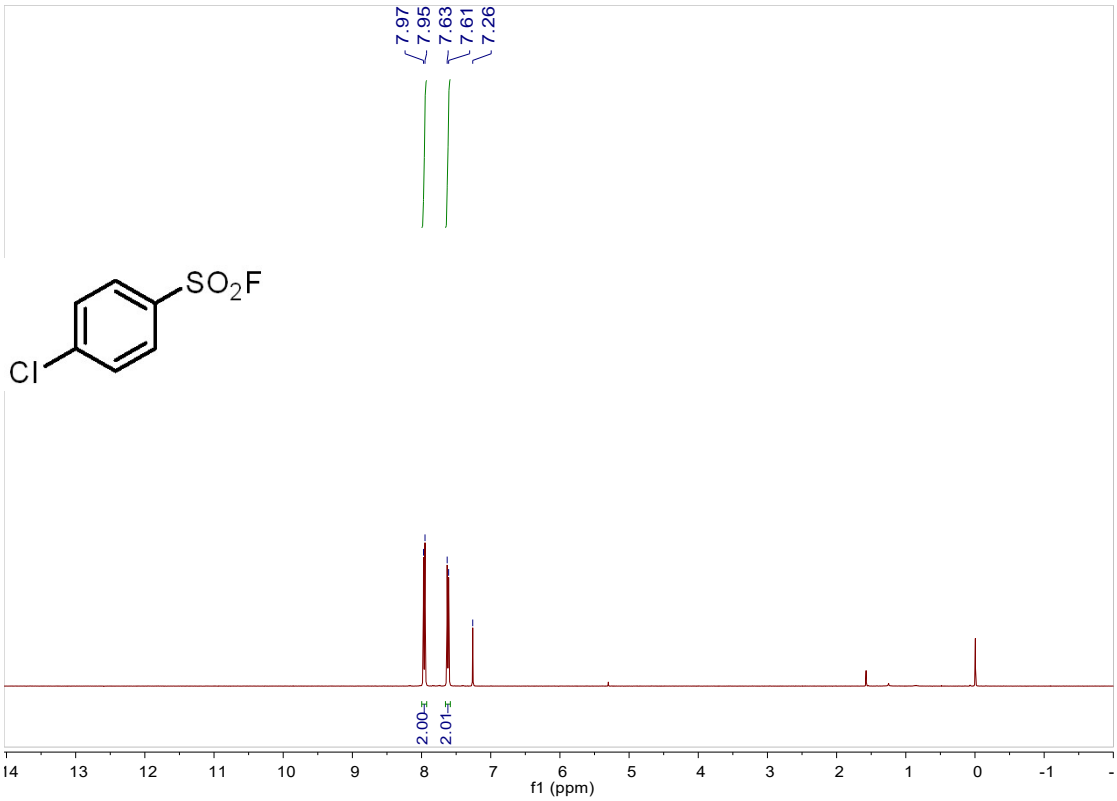
^{1}H NMR spectrum of 3-bromobenzenesulfonyl fluoride (400 MHz, $CDCl_3$)



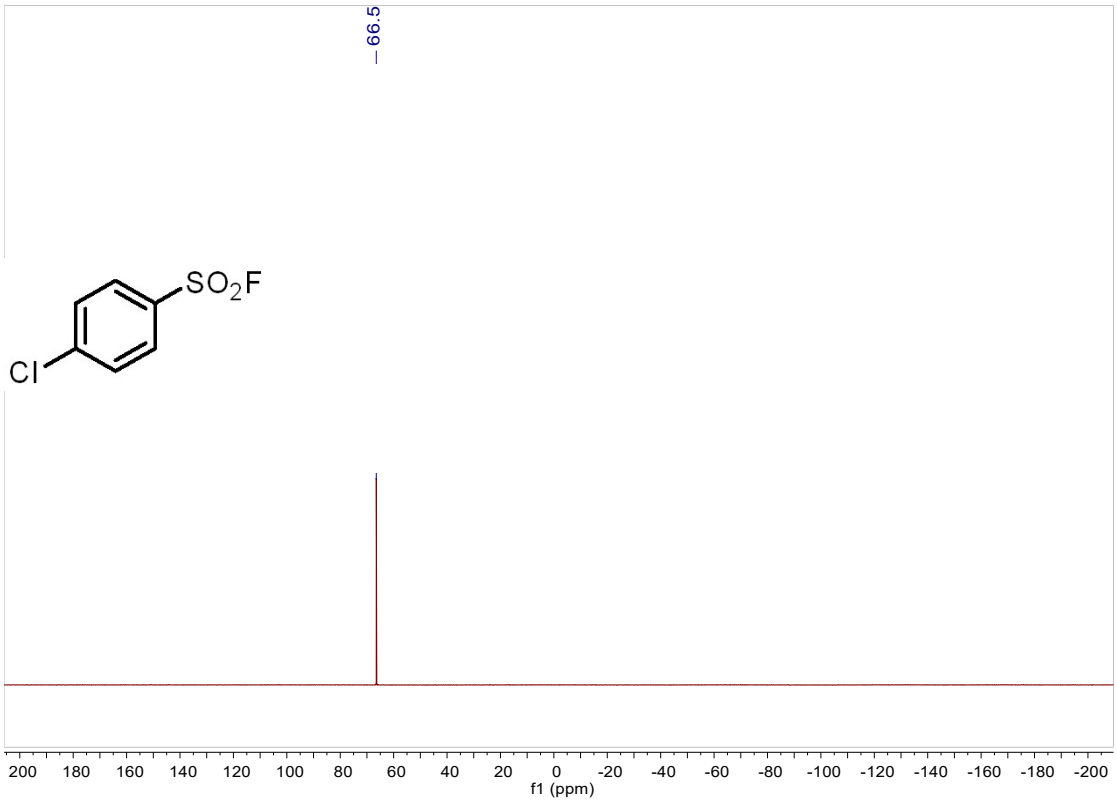
^{19}F NMR spectrum of 3-bromobenzenesulfonyl fluoride (376 MHz, $CDCl_3$)



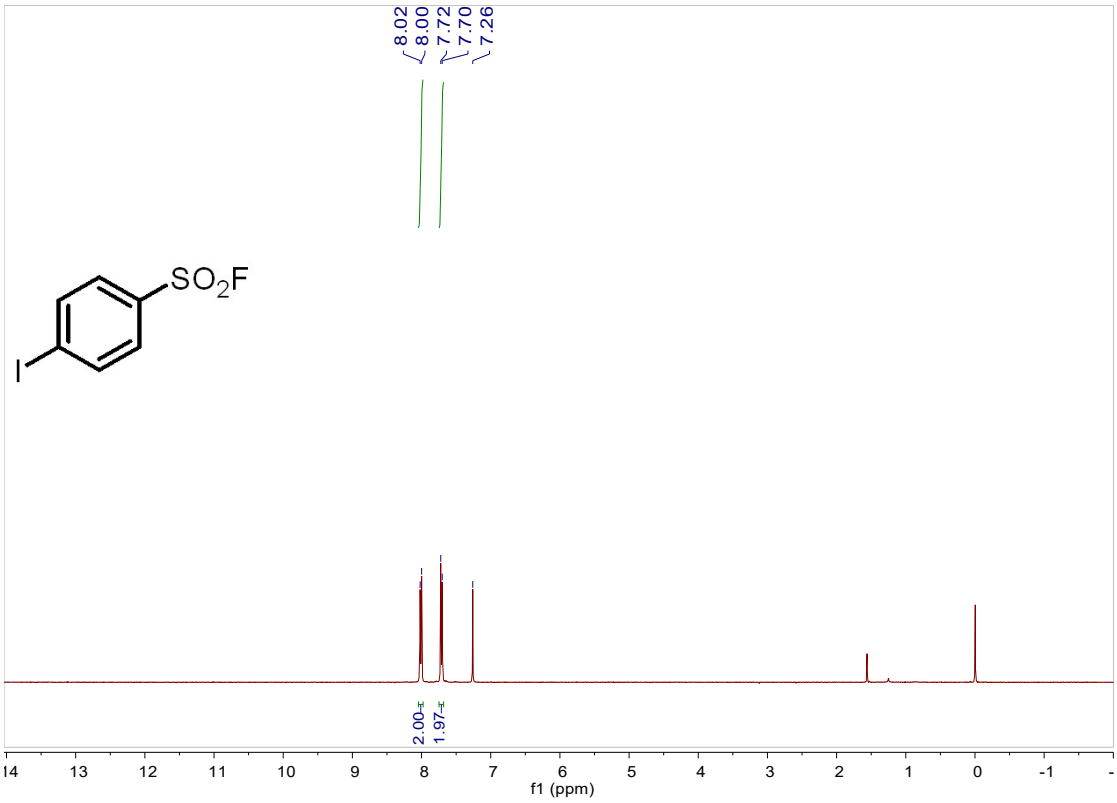
^{1}H NMR spectrum of 4-chlorobenzenesulfonyl fluoride (400 MHz, $CDCl_3$)



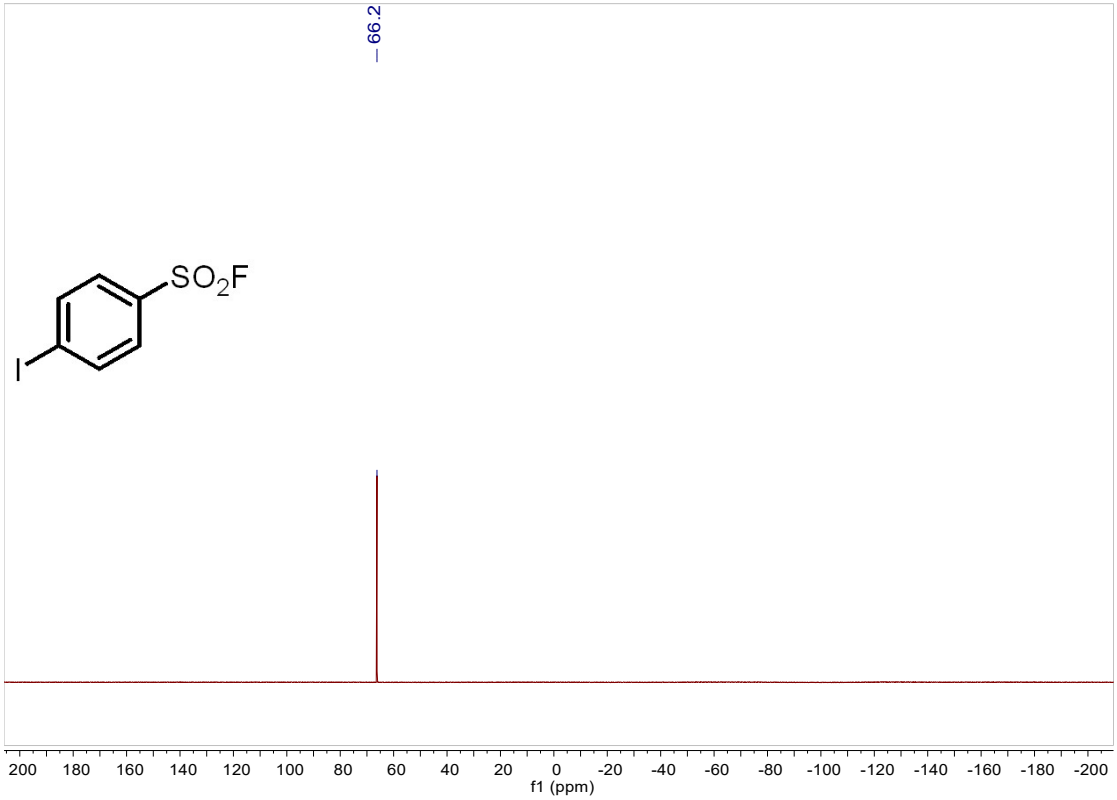
^{19}F NMR spectrum of 4-chlorobenzenesulfonyl fluoride (376 MHz, $CDCl_3$)



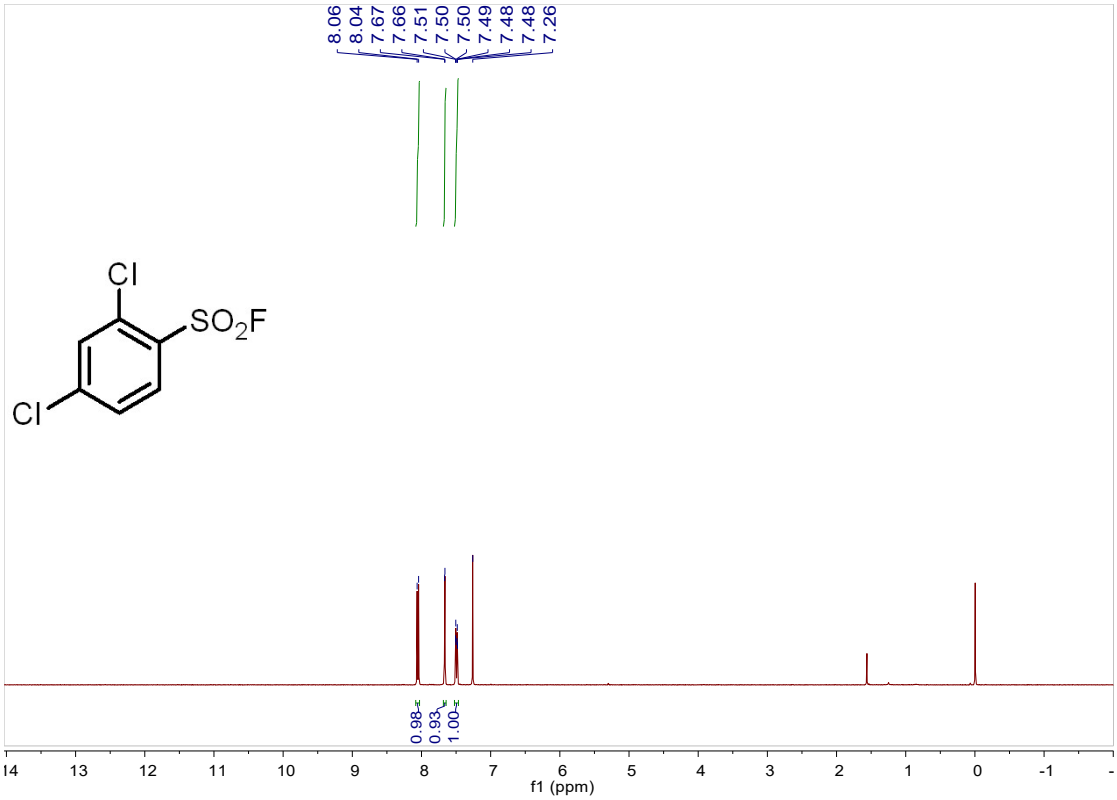
^{1}H NMR spectrum of 4-iodobenzenesulfonyl fluoride (400 MHz, $CDCl_3$)



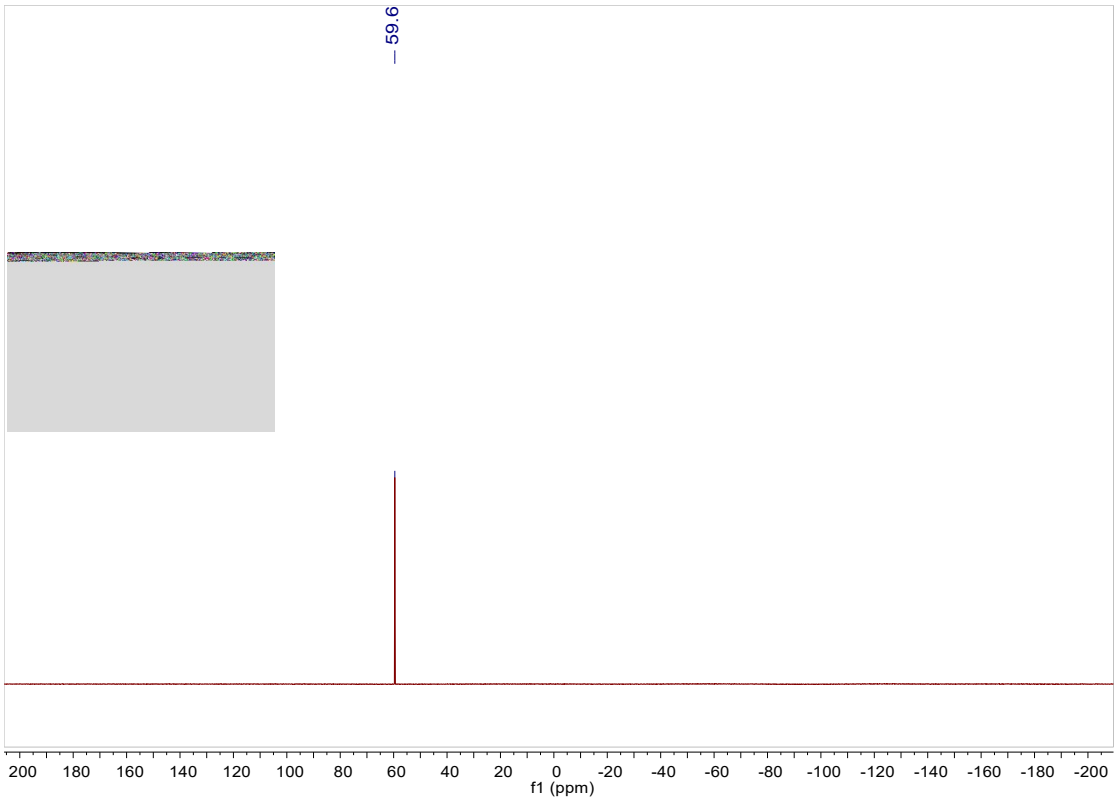
^{19}F NMR spectrum of 4-iodobenzenesulfonyl fluoride (376 MHz, $CDCl_3$)



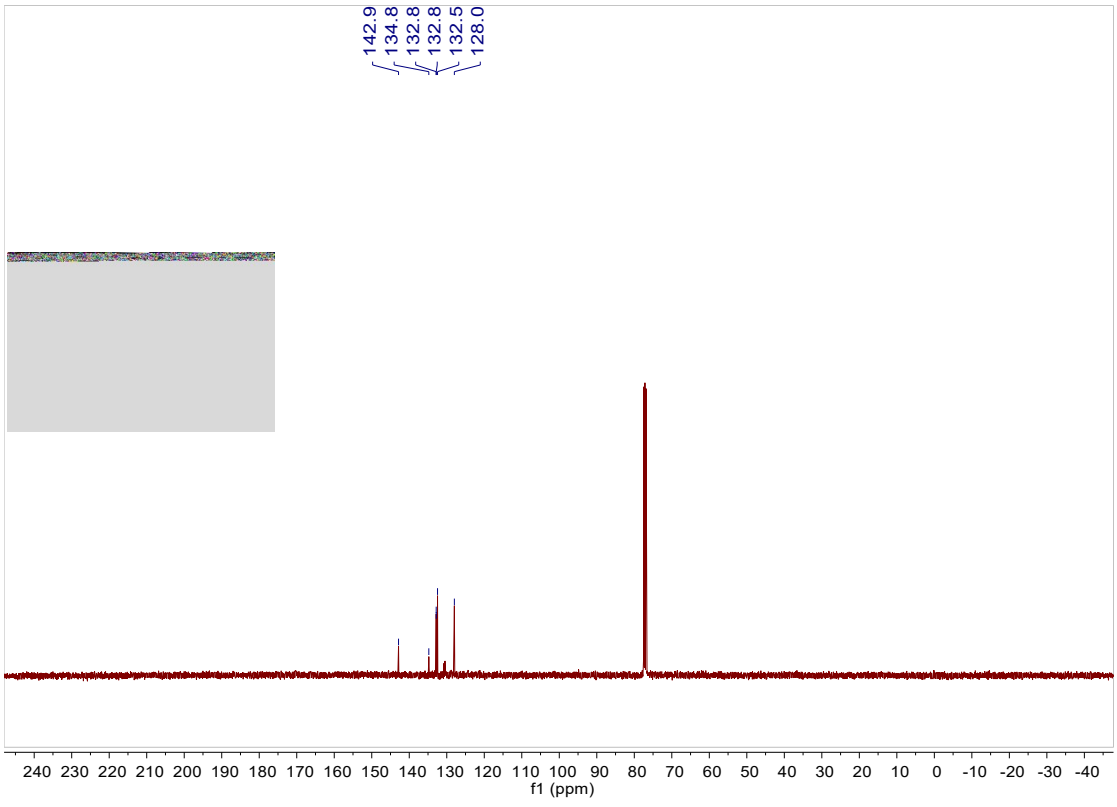
^{1}H NMR spectrum of 2,4-dichlorobenzenesulfonyl fluoride (400 MHz, $CDCl_3$)



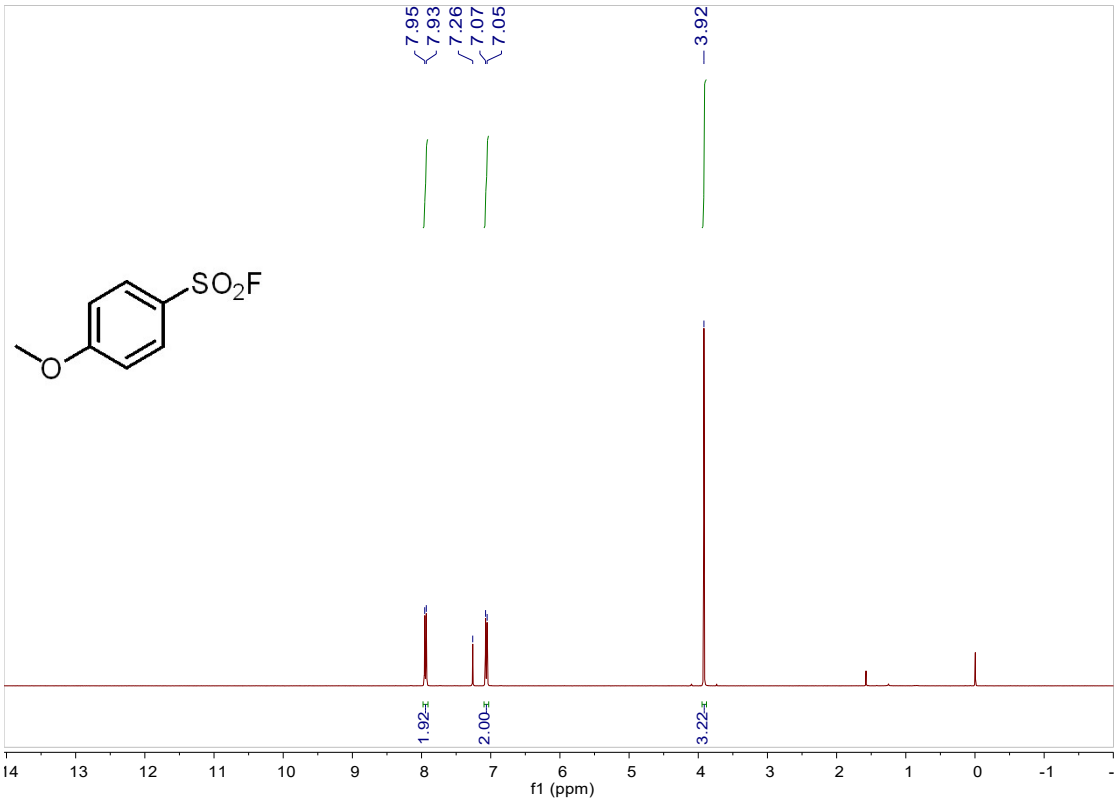
^{19}F NMR spectrum of 2,4-dichlorobenzenesulfonyl fluoride (376 MHz, $CDCl_3$)



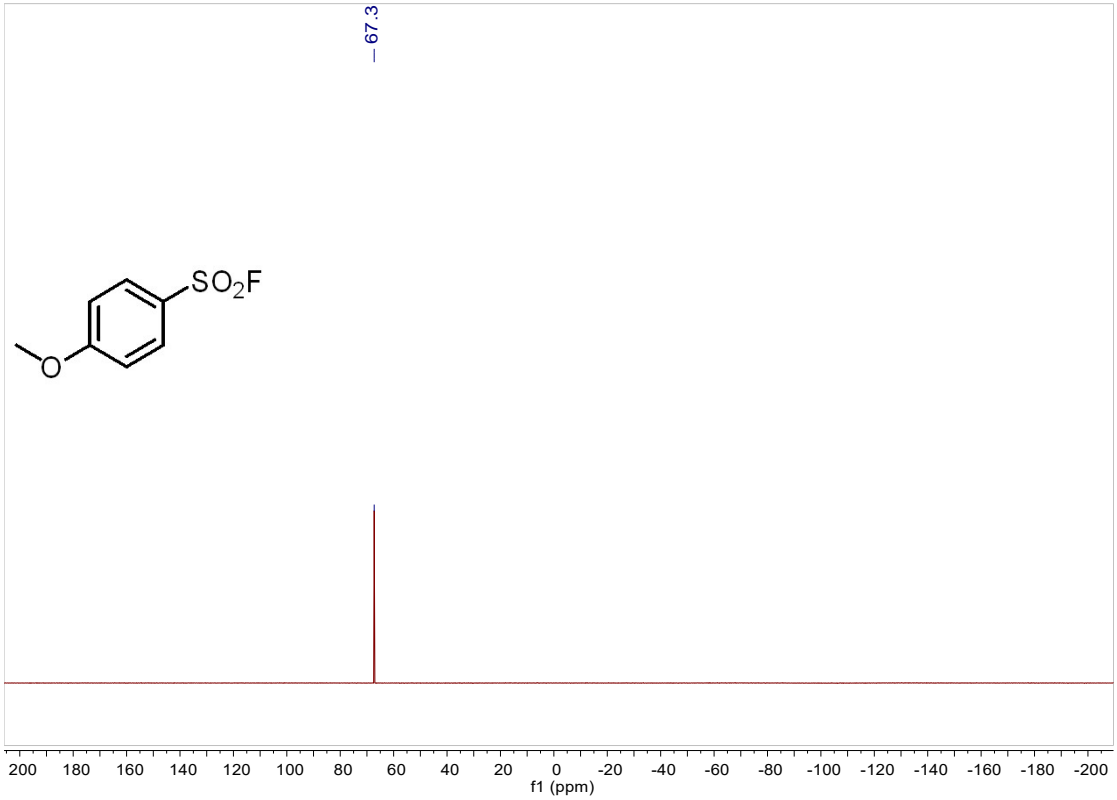
^{13}C NMR spectrum of 2,4-dichlorobenzenesulfonyl fluoride (101 MHz, $CDCl_3$)



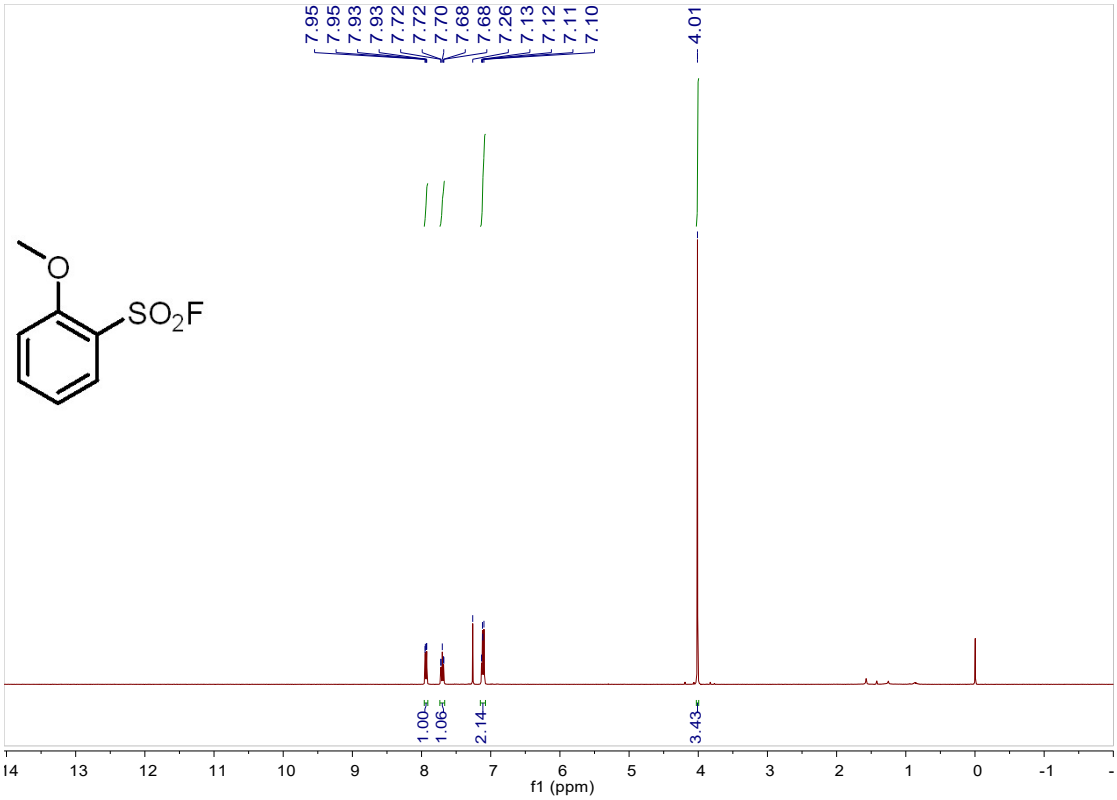
^{1}H NMR spectrum of 4-methoxybenzenesulfonyl fluoride (400 MHz, $CDCl_3$)



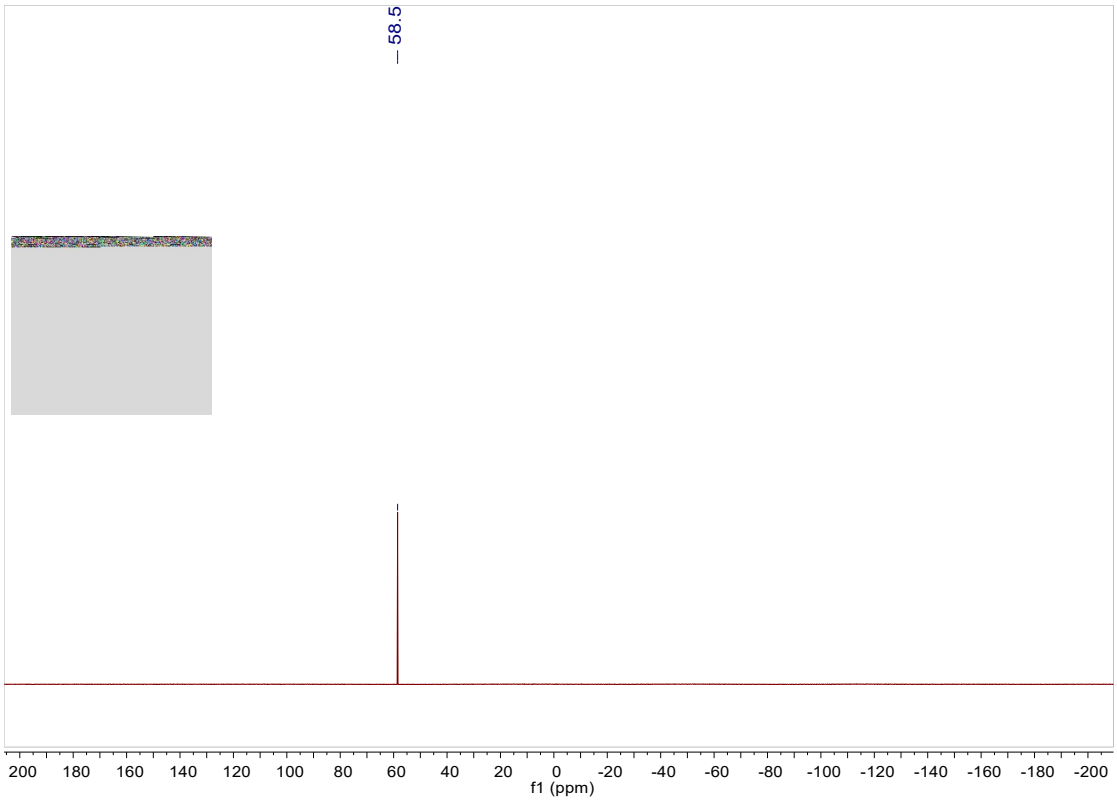
^{19}F NMR spectrum of 4-methoxybenzenesulfonyl fluoride (376 MHz, $CDCl_3$)



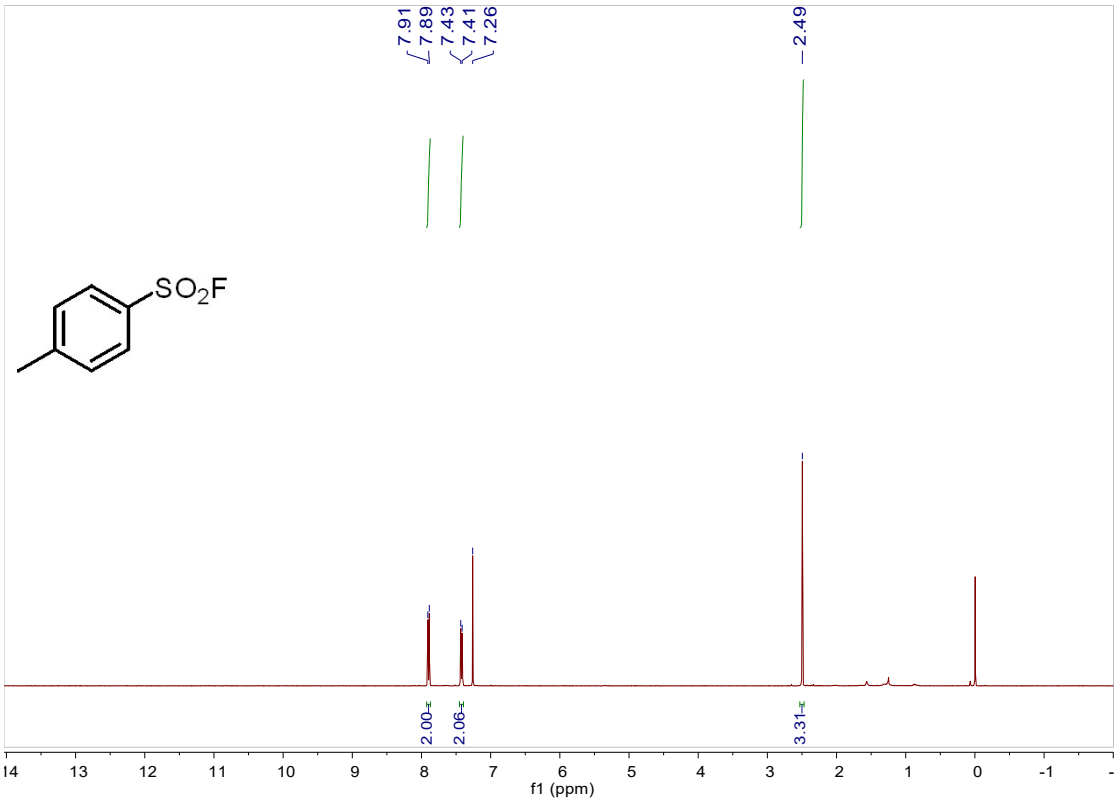
^{1}H NMR spectrum of 2-methoxybenzenesulfonyl fluoride (400 MHz, $CDCl_3$)



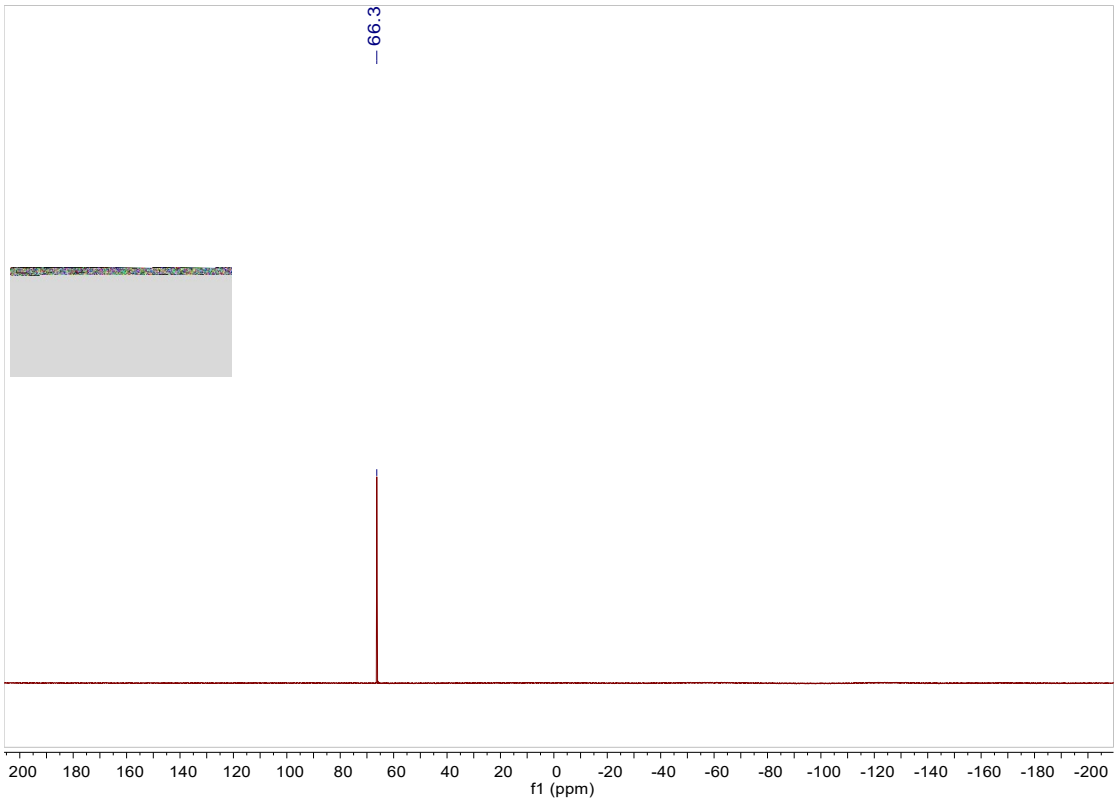
^{19}F NMR spectrum of 2-methoxybenzenesulfonyl fluoride (376 MHz, $CDCl_3$)



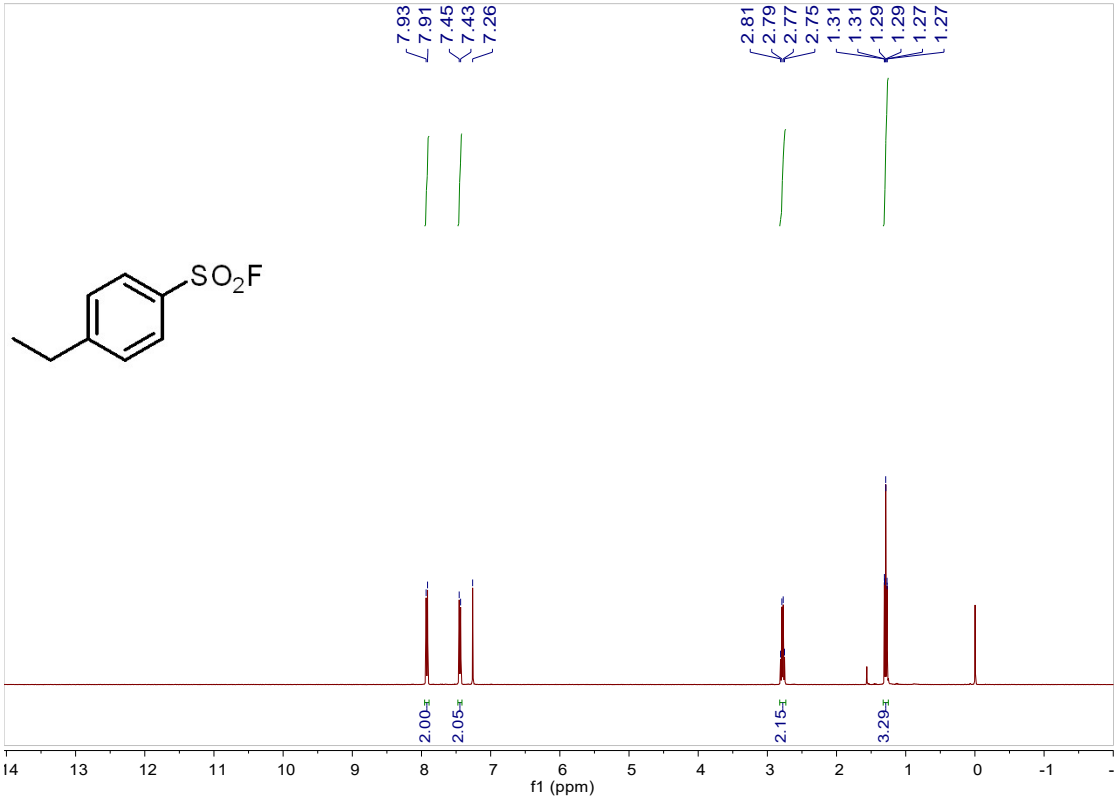
^{1}H NMR spectrum of 4-methylbenzenesulfonyl fluoride (400 MHz, $CDCl_3$)



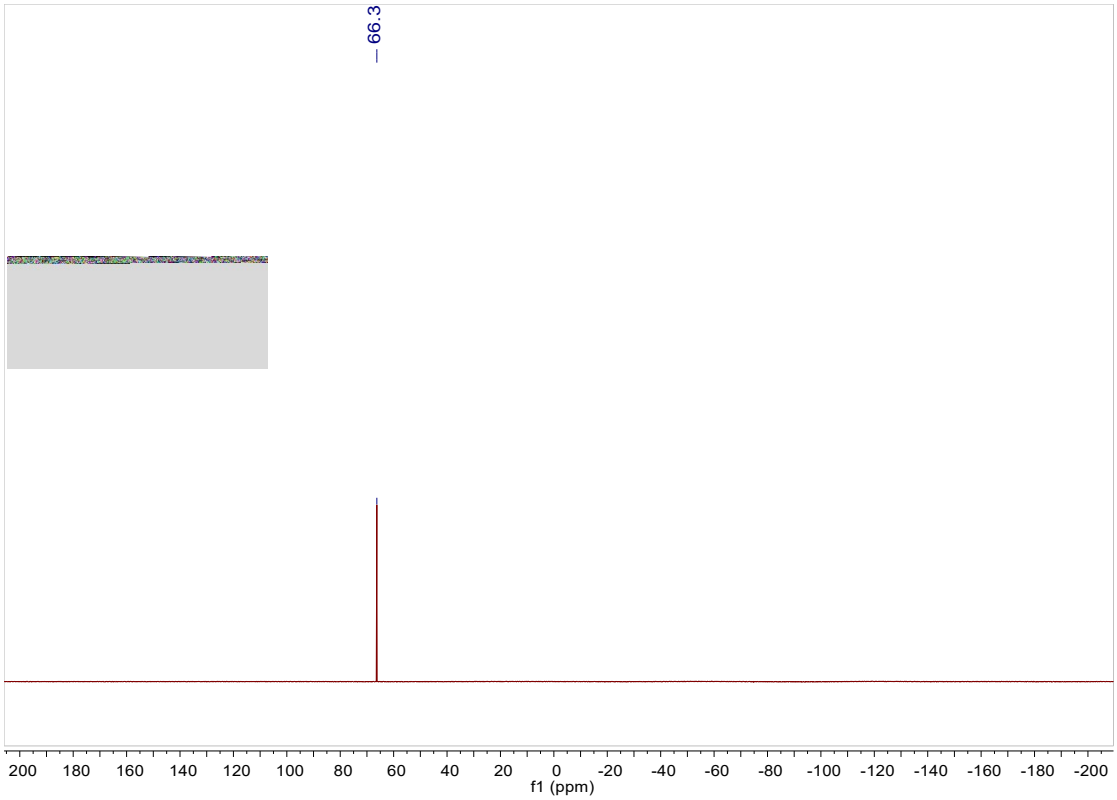
^{19}F NMR spectrum of 4-methylbenzenesulfonyl fluoride (376 MHz, $CDCl_3$)



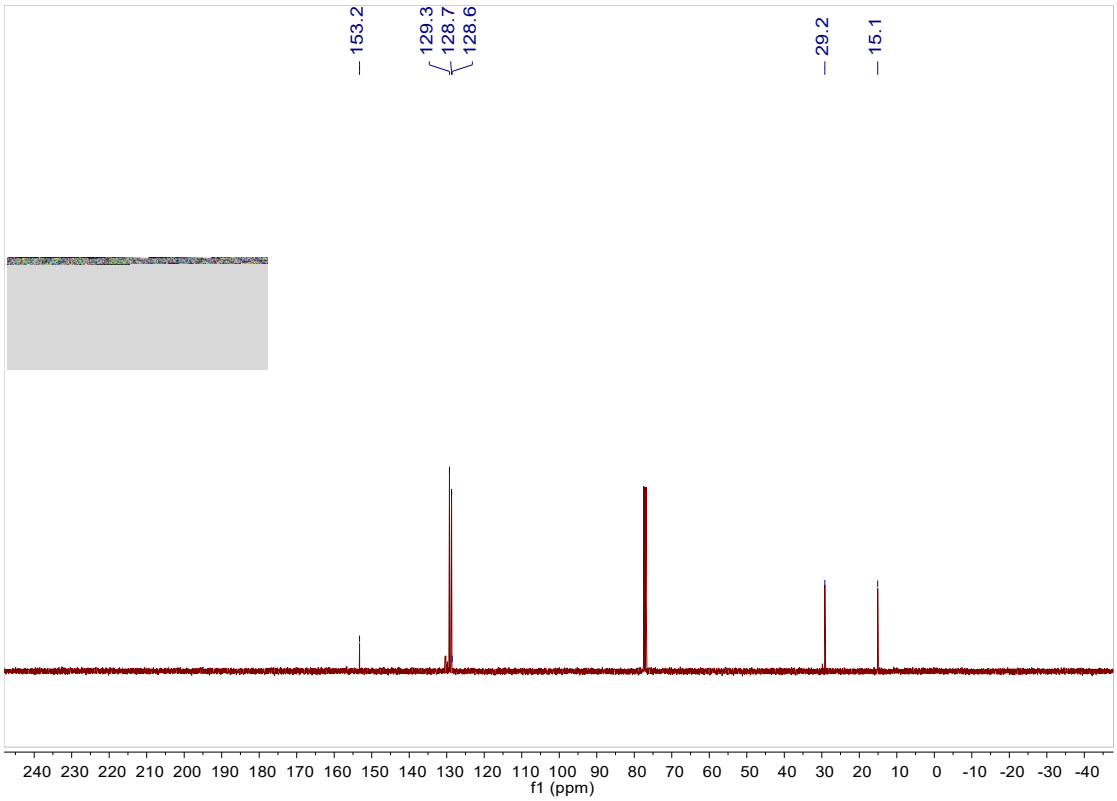
^{1}H NMR spectrum of 4-ethylbenzenesulfonyl fluoride (400 MHz, $CDCl_3$)



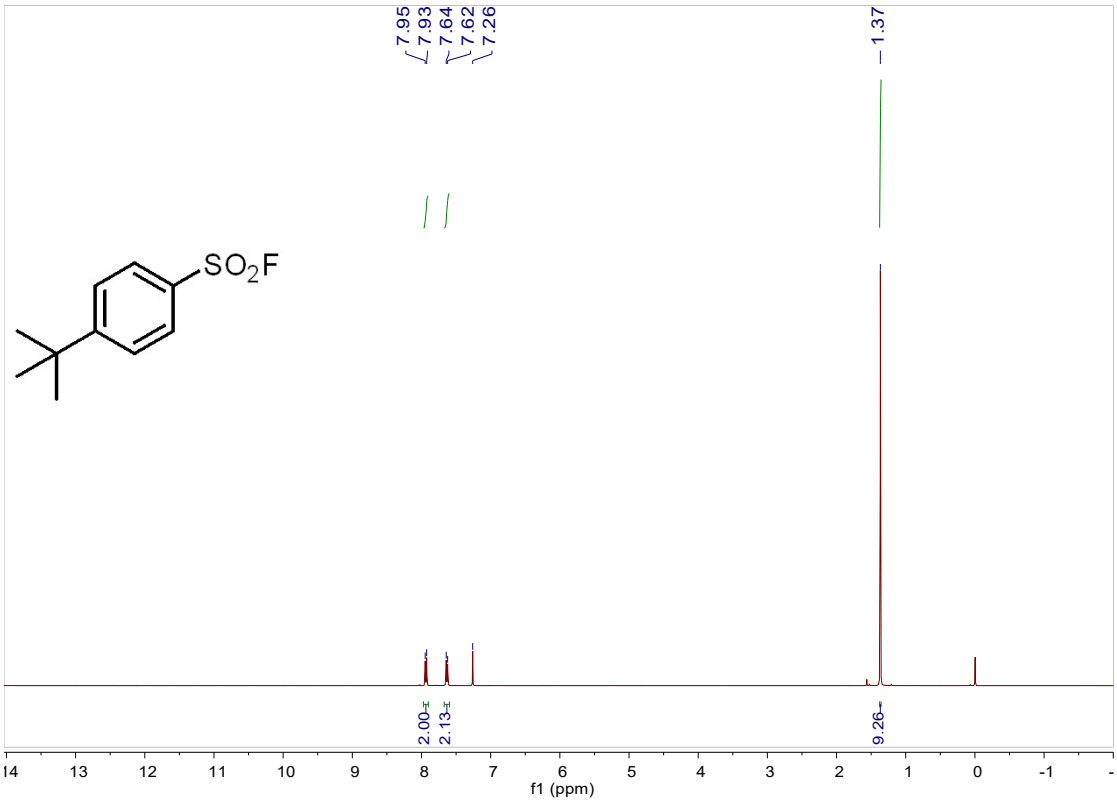
^{19}F NMR spectrum of 4-ethylbenzenesulfonyl fluoride (376 MHz, $CDCl_3$)



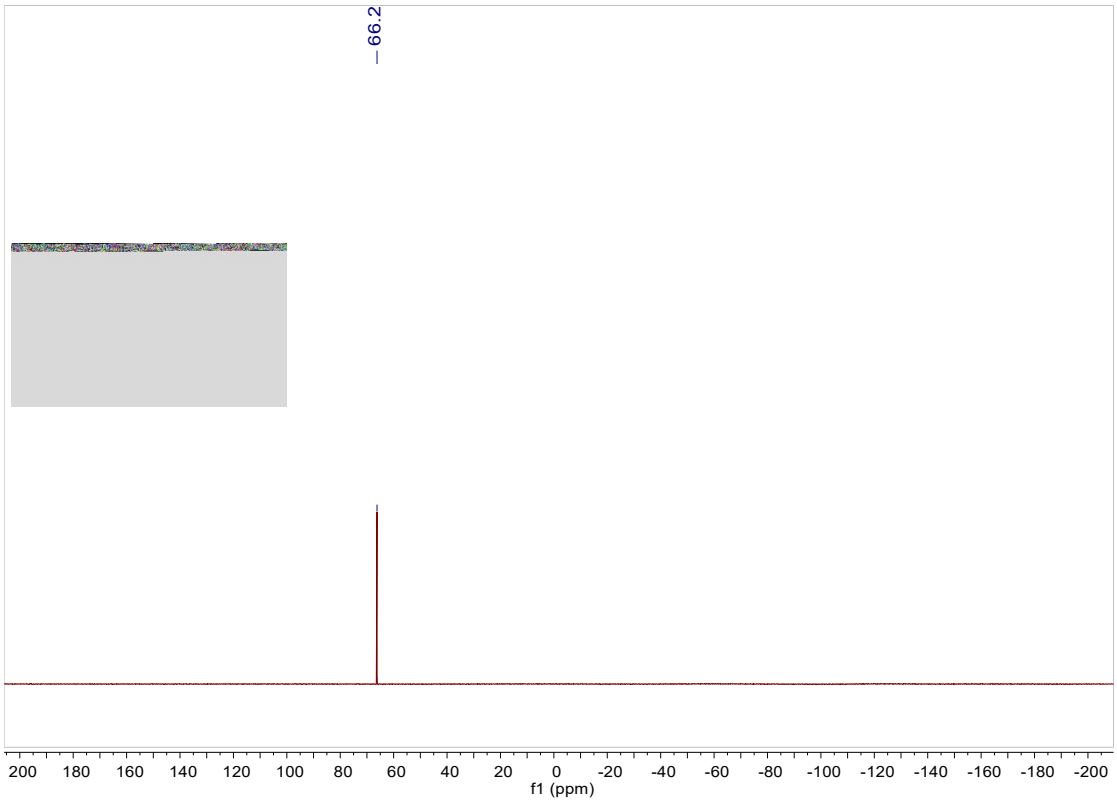
^{13}C NMR spectrum of 4-ethylbenzenesulfonyl fluoride (101 MHz, $CDCl_3$)



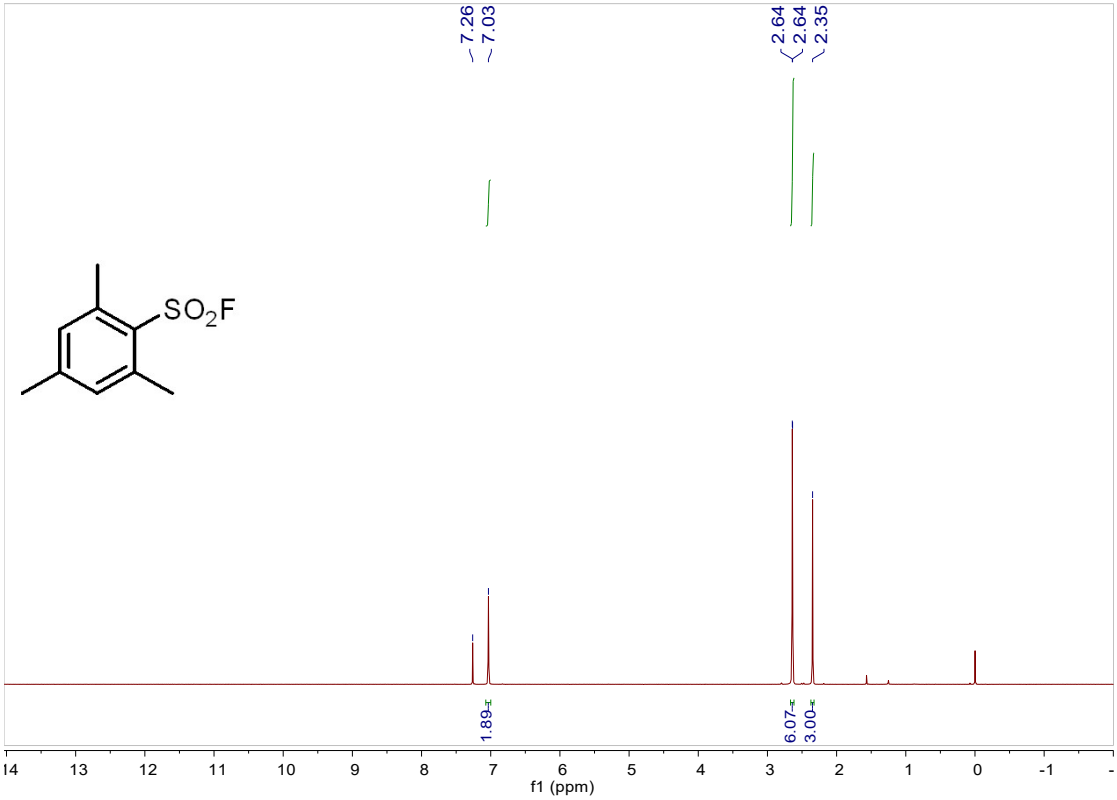
^{1}H NMR spectrum of 4-(tert-butyl)benzenesulfonyl fluoride (400 MHz, $CDCl_3$)



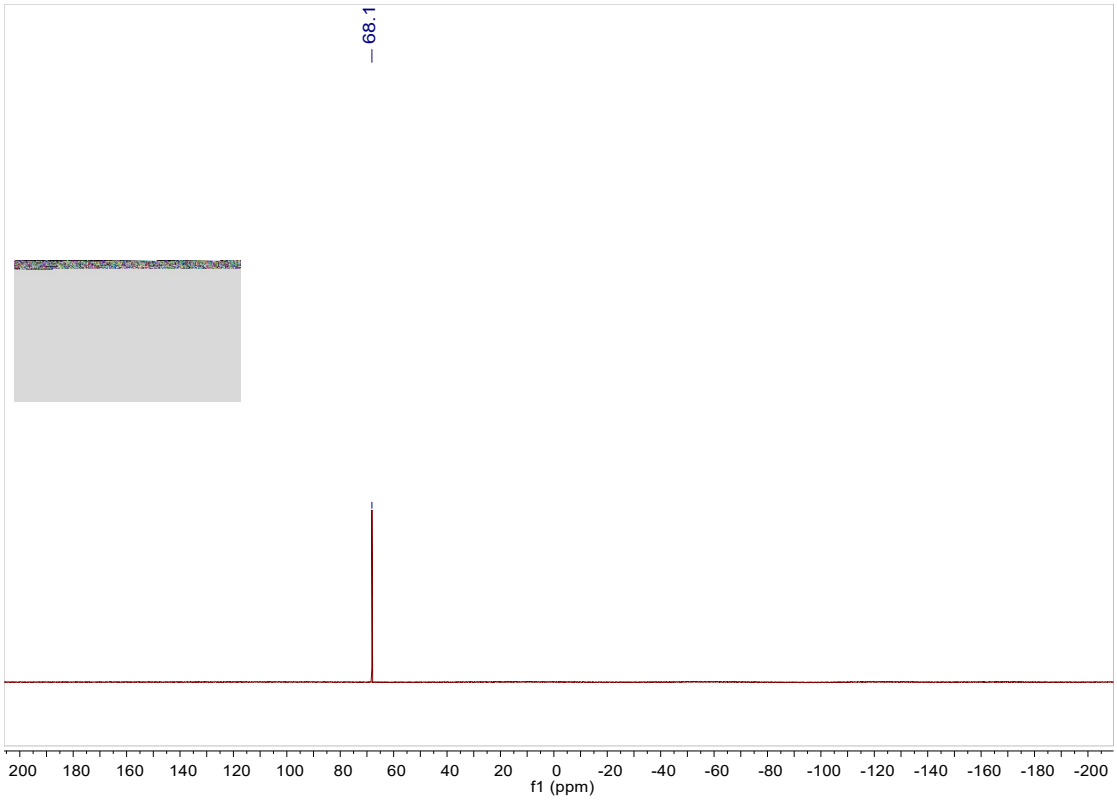
^{19}F NMR spectrum of 4-(tert-butyl)benzenesulfonyl fluoride (376 MHz, $CDCl_3$)



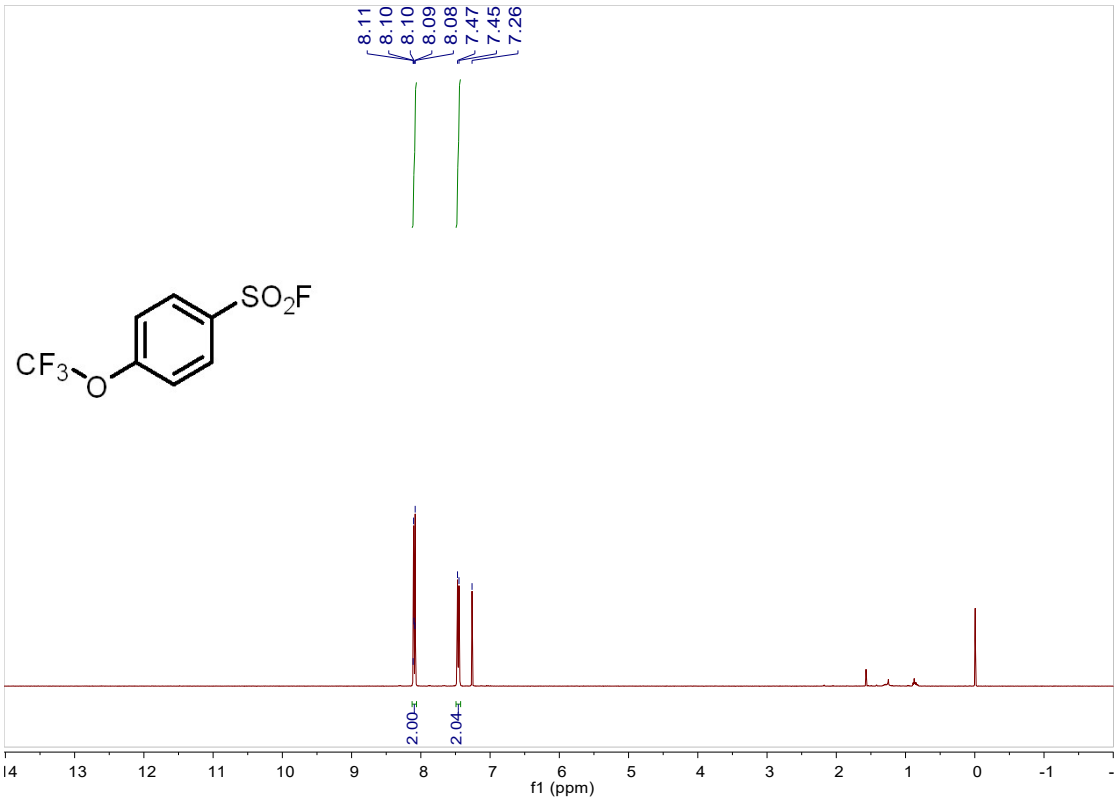
^{1}H NMR spectrum of 2,4,6-trimethylbenzenesulfonyl fluoride (400 MHz, $CDCl_3$)



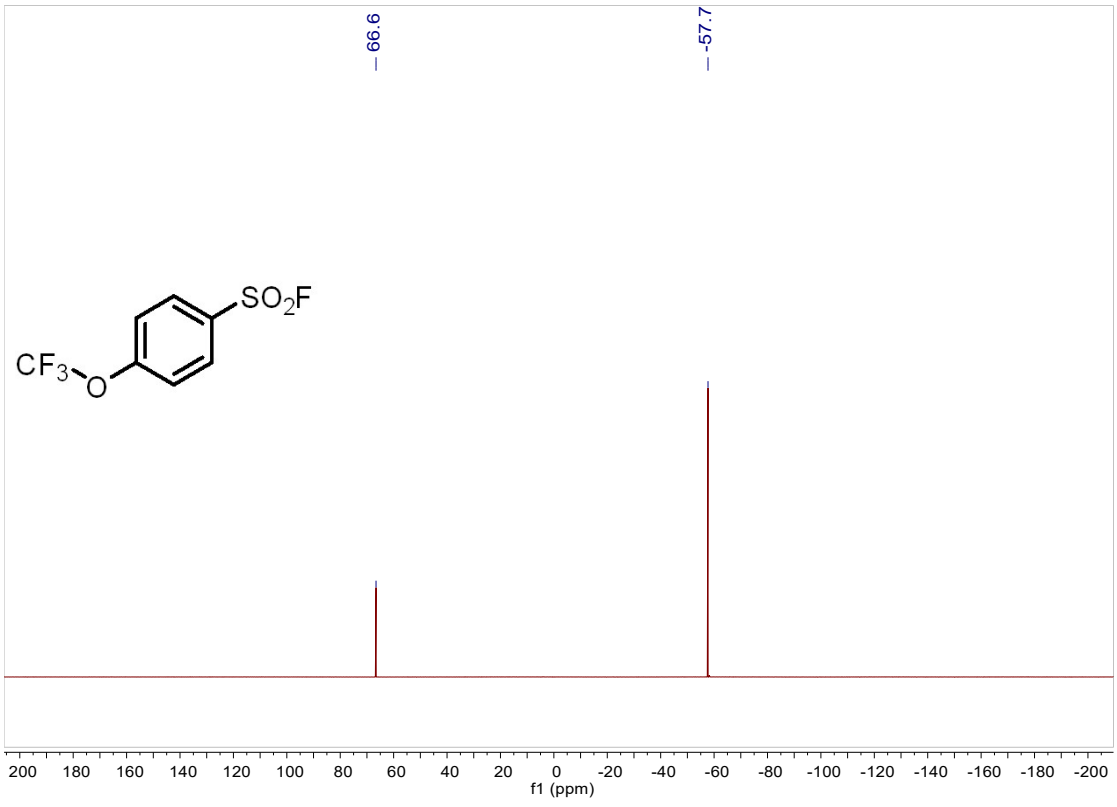
^{19}F NMR spectrum of 2,4,6-trimethylbenzenesulfonyl fluoride (376 MHz, $CDCl_3$)



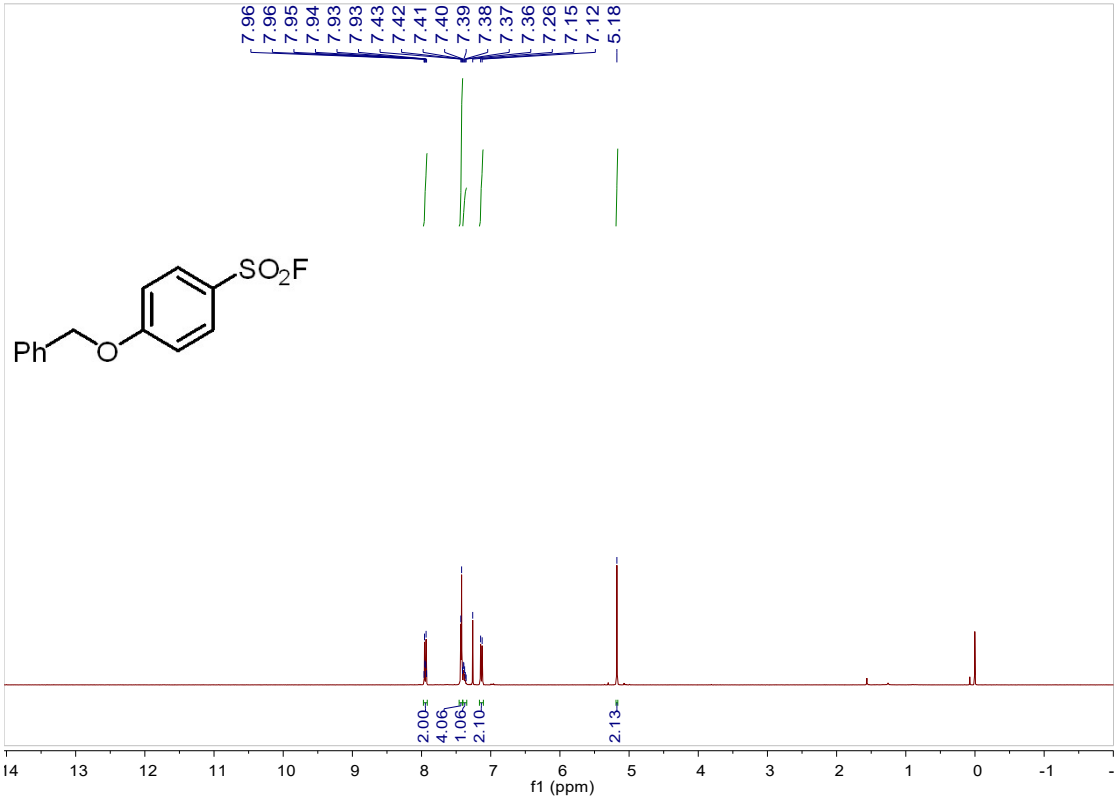
^{1}H NMR spectrum of 4-(trifluoromethoxy)benzenesulfonyl fluoride (400 MHz, $CDCl_3$)



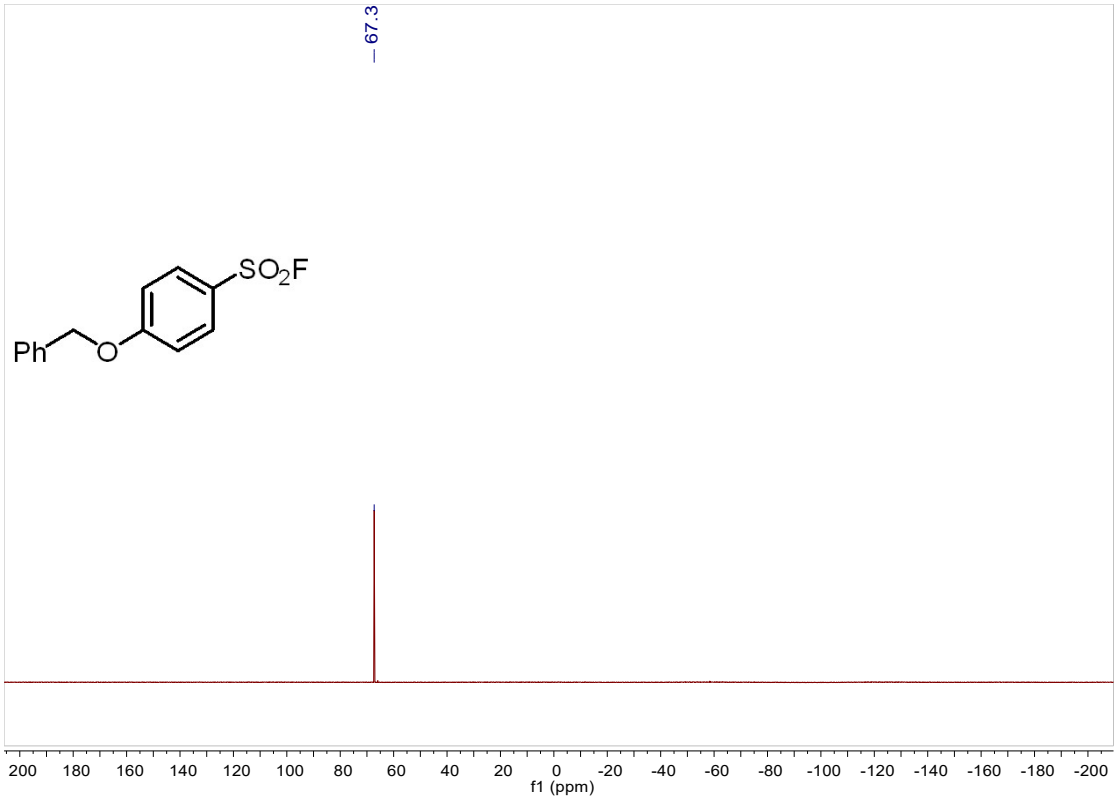
^{19}F NMR spectrum of 4-(trifluoromethoxy)benzenesulfonyl fluoride (376 MHz, $CDCl_3$)



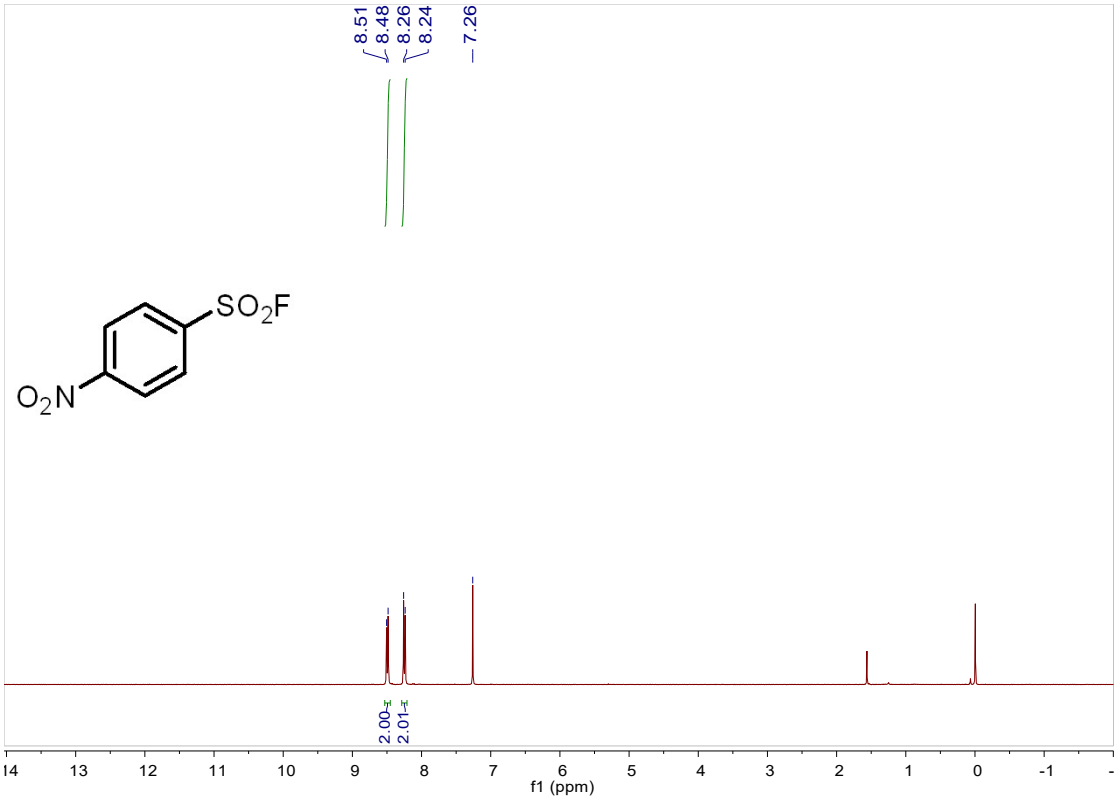
^{1}H NMR spectrum of 4-(benzyloxy)benzenesulfonyl fluoride (400 MHz, $CDCl_3$)



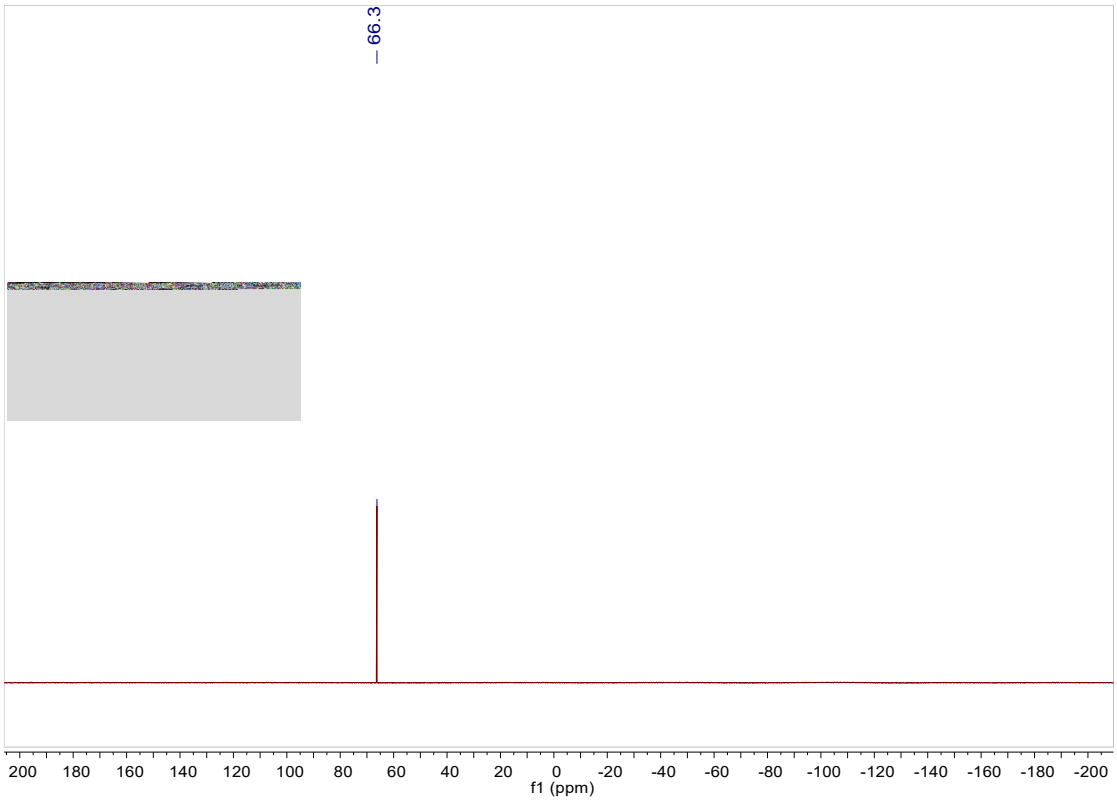
^{19}F NMR spectrum of 4-(benzyloxy)benzenesulfonyl fluoride (376 MHz, $CDCl_3$)



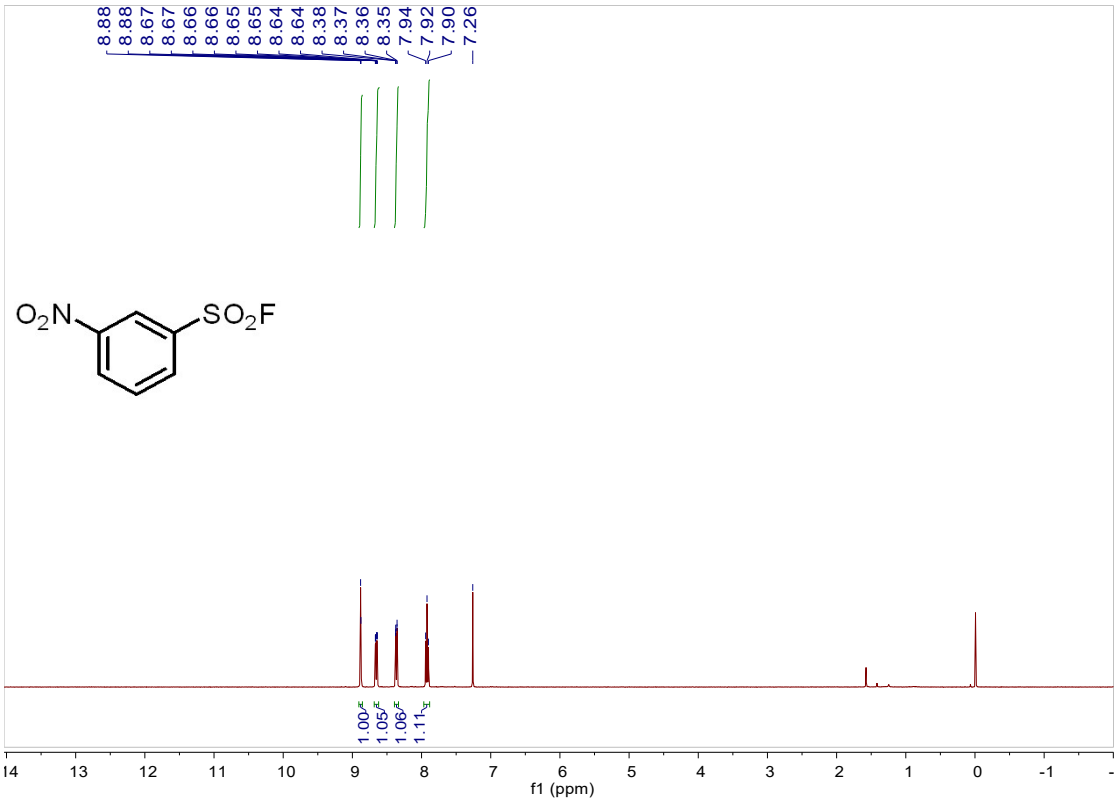
^{1}H NMR spectrum of 4-nitrobenzenesulfonyl fluoride (400 MHz, $CDCl_3$)



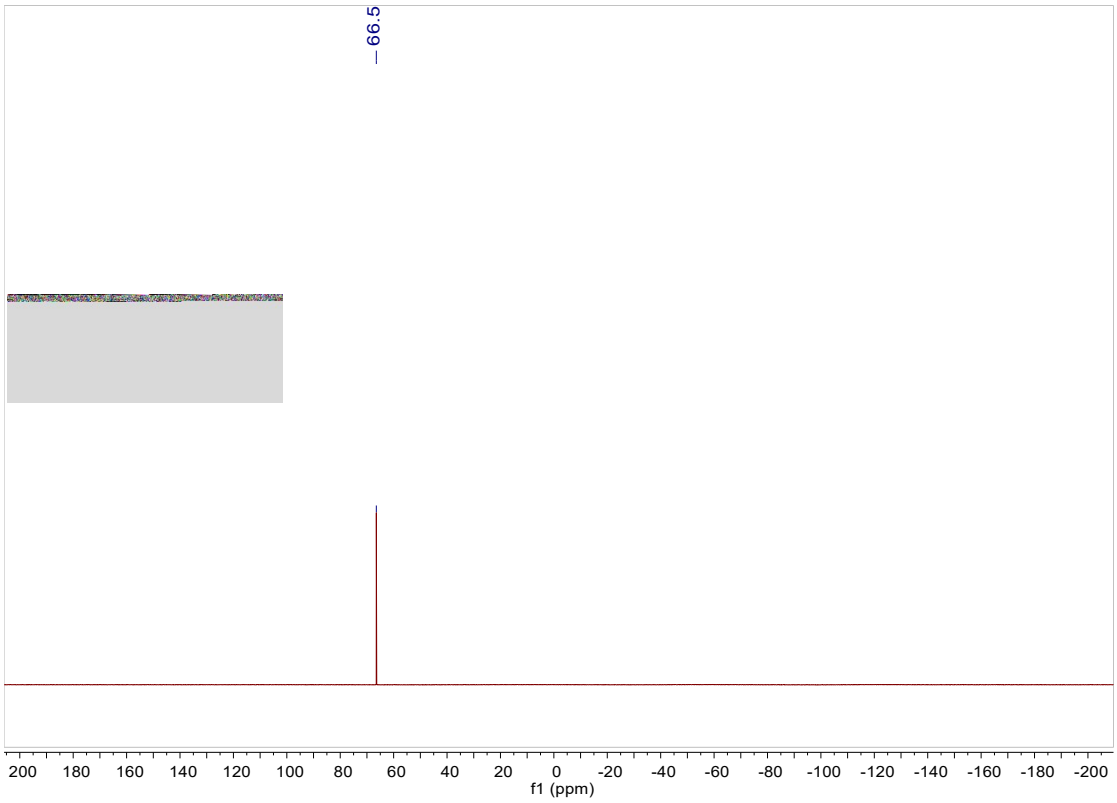
^{19}F NMR spectrum of 4-nitrobenzenesulfonyl fluoride (376 MHz, $CDCl_3$)



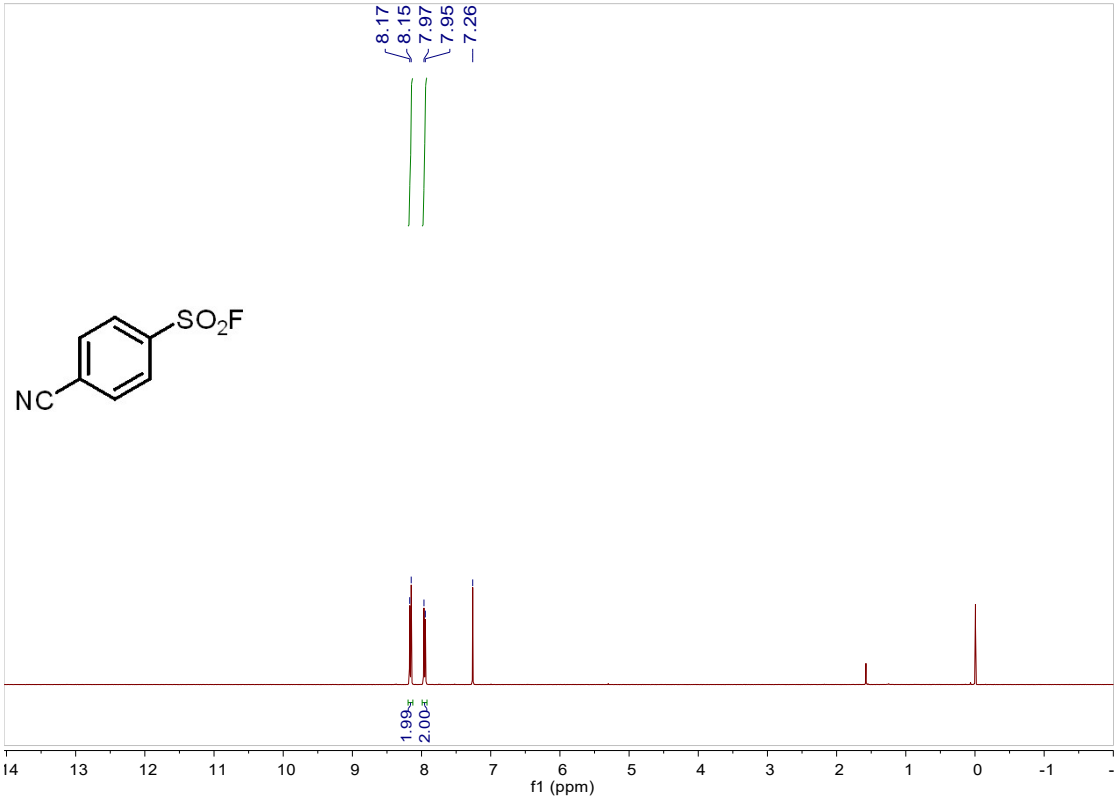
^{1}H NMR spectrum of 3-nitrobenzenesulfonyl fluoride (400 MHz, $CDCl_3$)



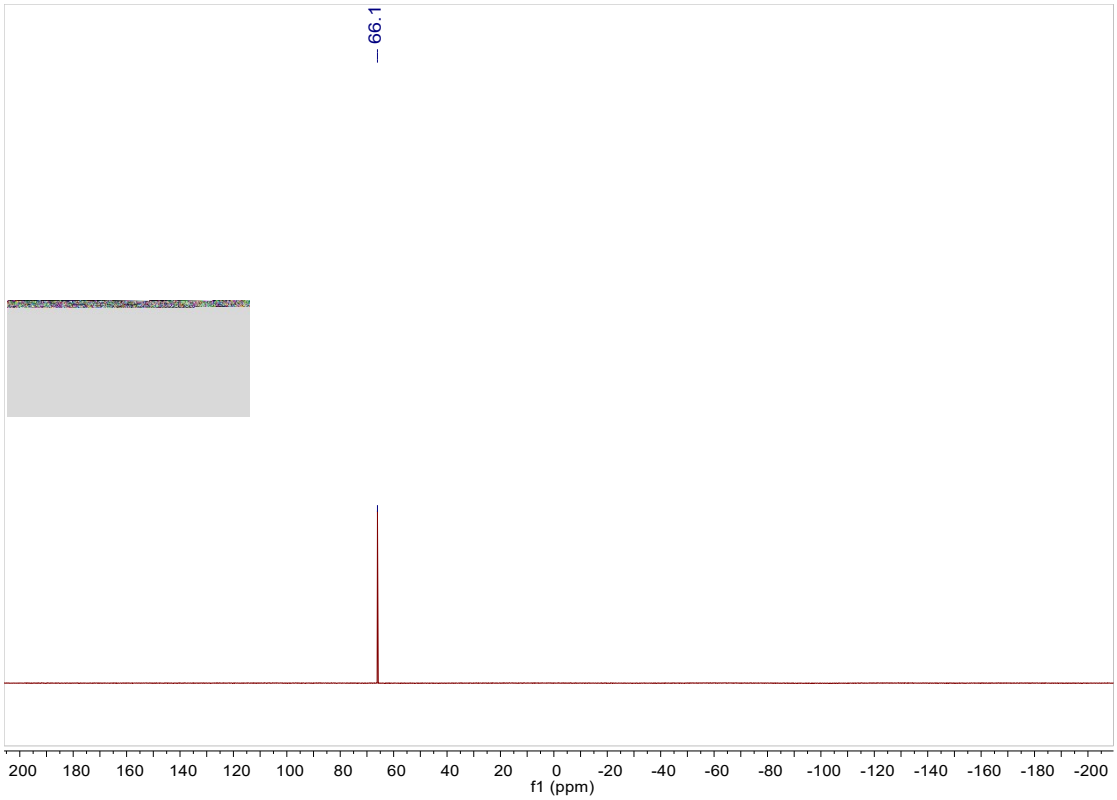
^{19}F NMR spectrum of 3-nitrobenzenesulfonyl fluoride (376 MHz, $CDCl_3$)



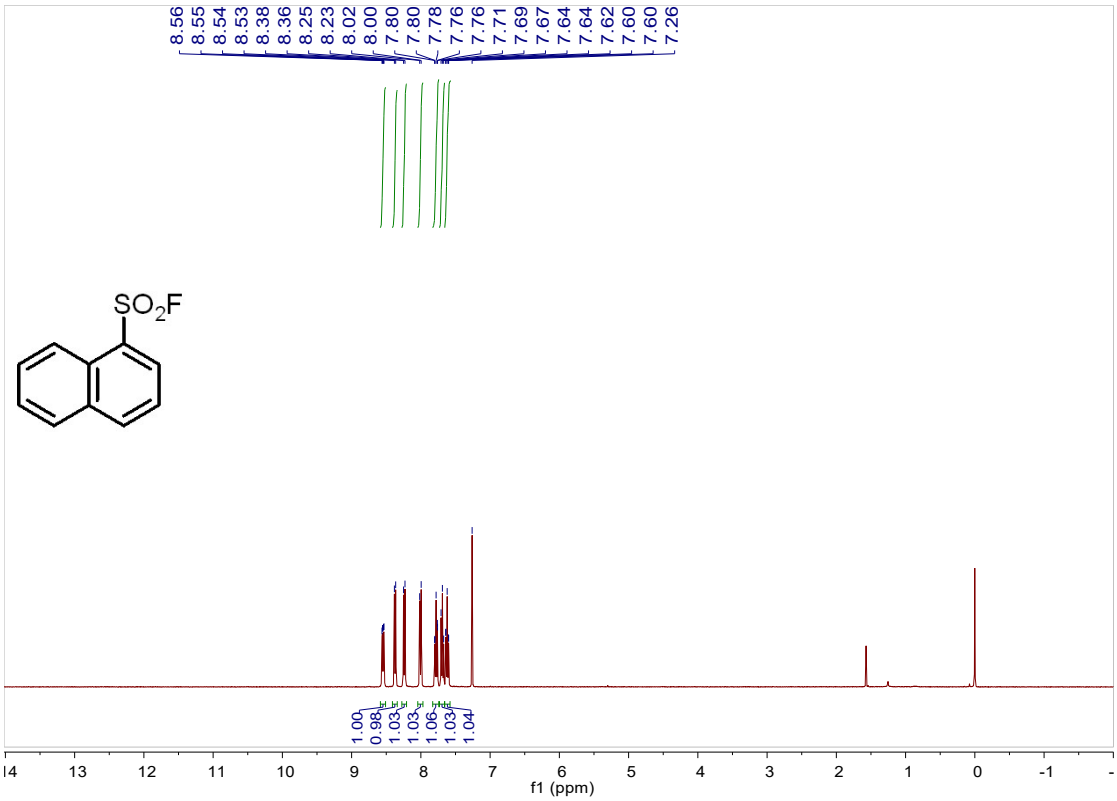
^{1}H NMR spectrum of 4-cyanobenzenesulfonyl fluoride (400 MHz, $CDCl_3$)



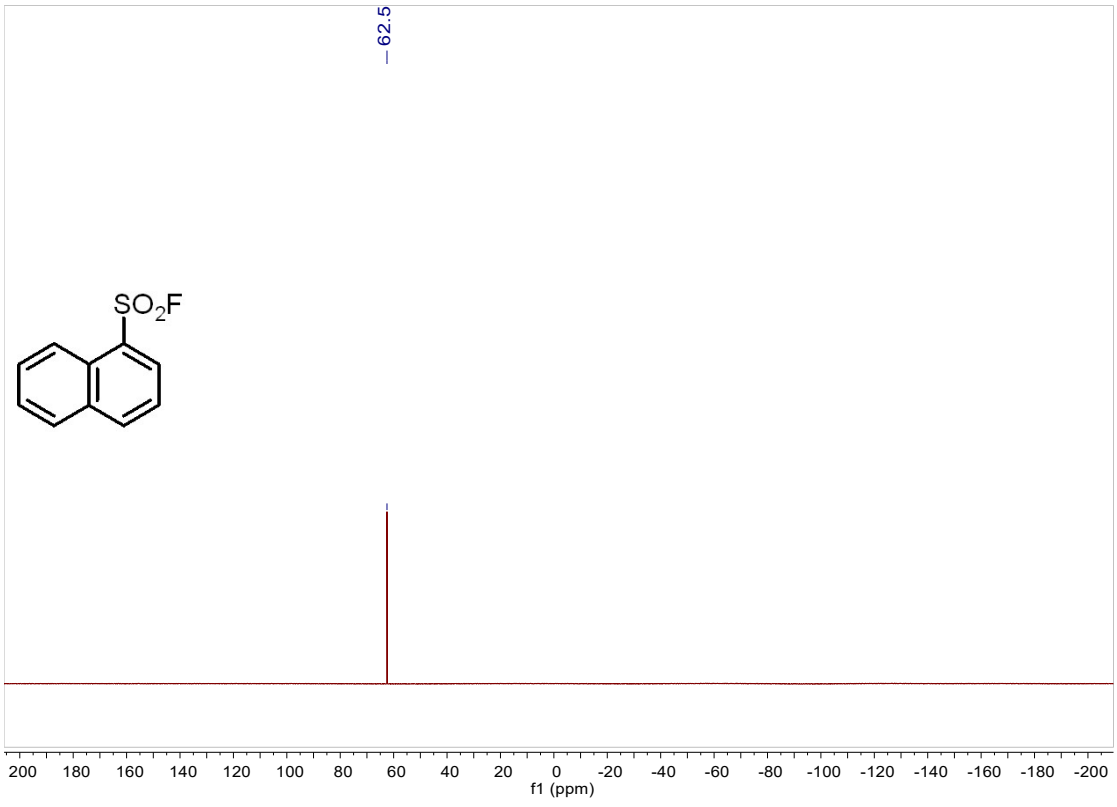
^{19}F NMR spectrum of 4-cyanobenzenesulfonyl fluoride (376 MHz, $CDCl_3$)



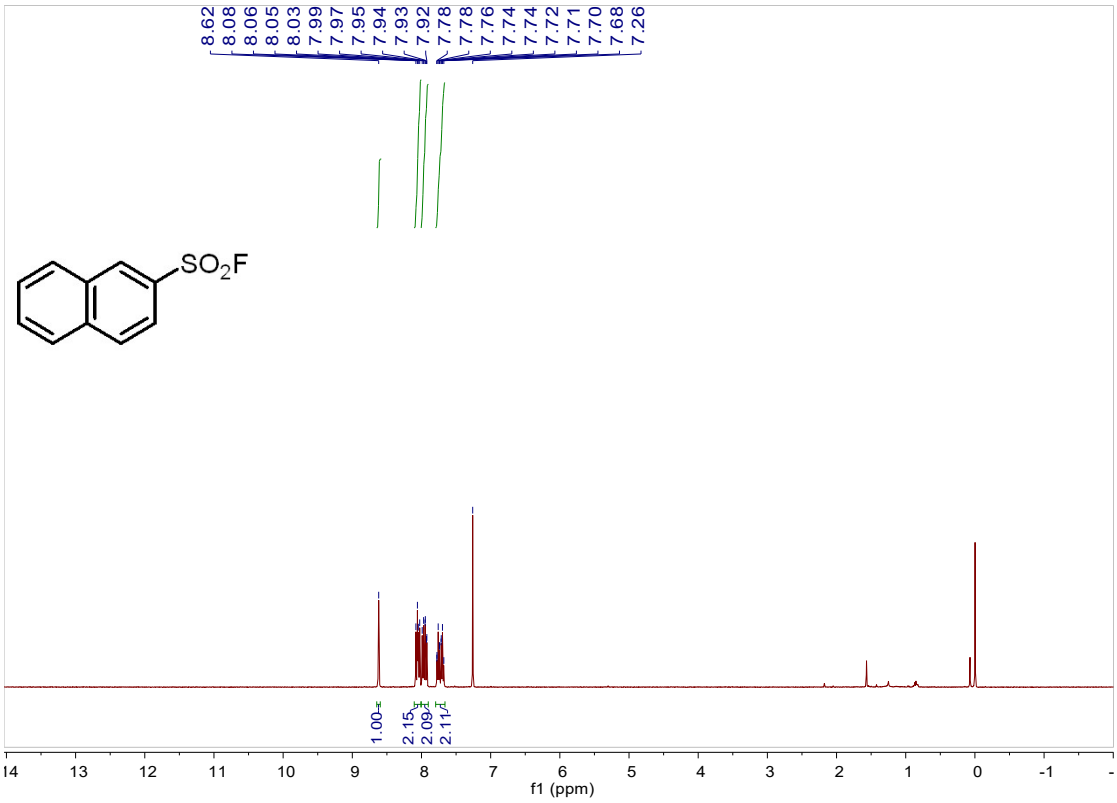
^{1}H NMR spectrum of naphthalene-1-sulfonyl fluoride (400 MHz, $CDCl_3$)



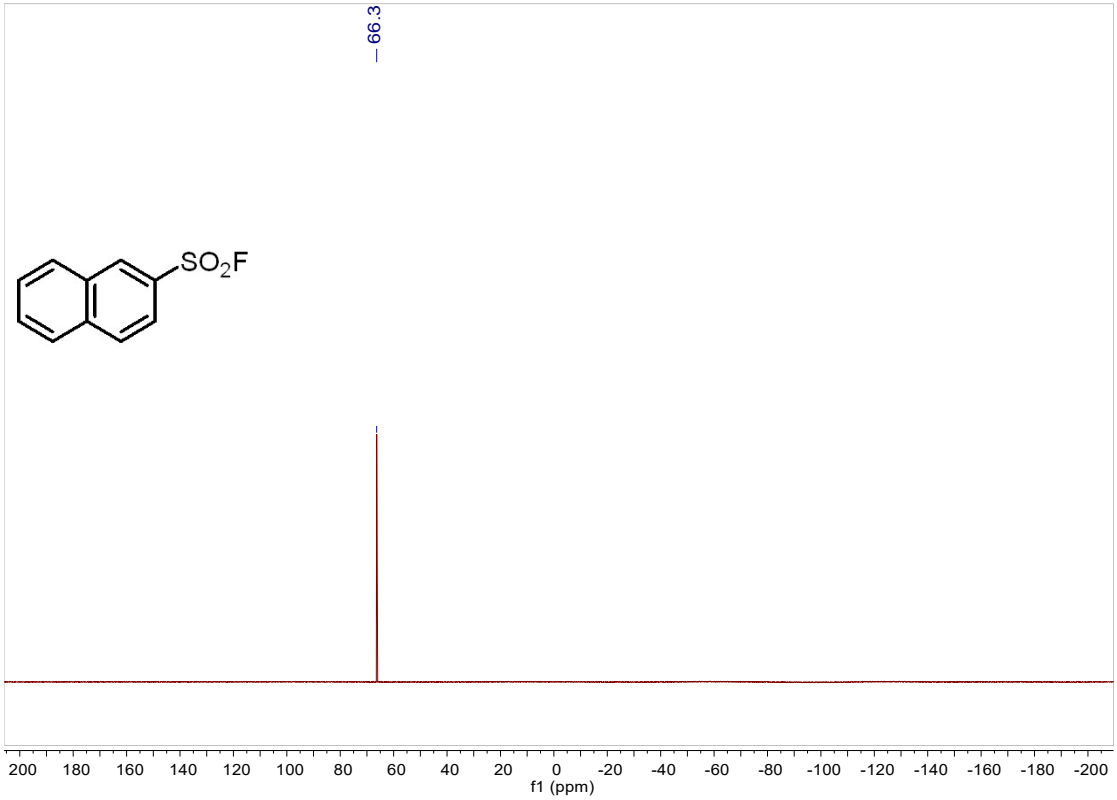
^{19}F NMR spectrum of naphthalene-1-sulfonyl fluoride (376 MHz, $CDCl_3$)



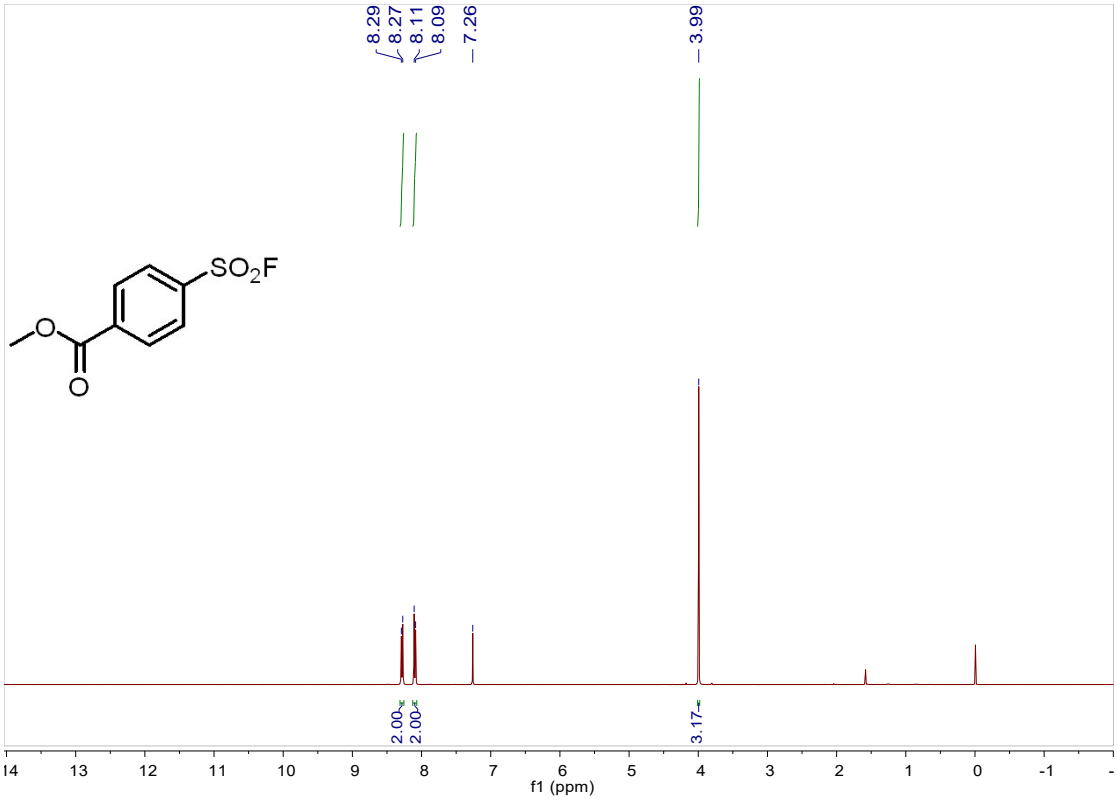
^{1}H NMR spectrum of naphthalene-2-sulfonyl fluoride (400 MHz, $CDCl_3$)



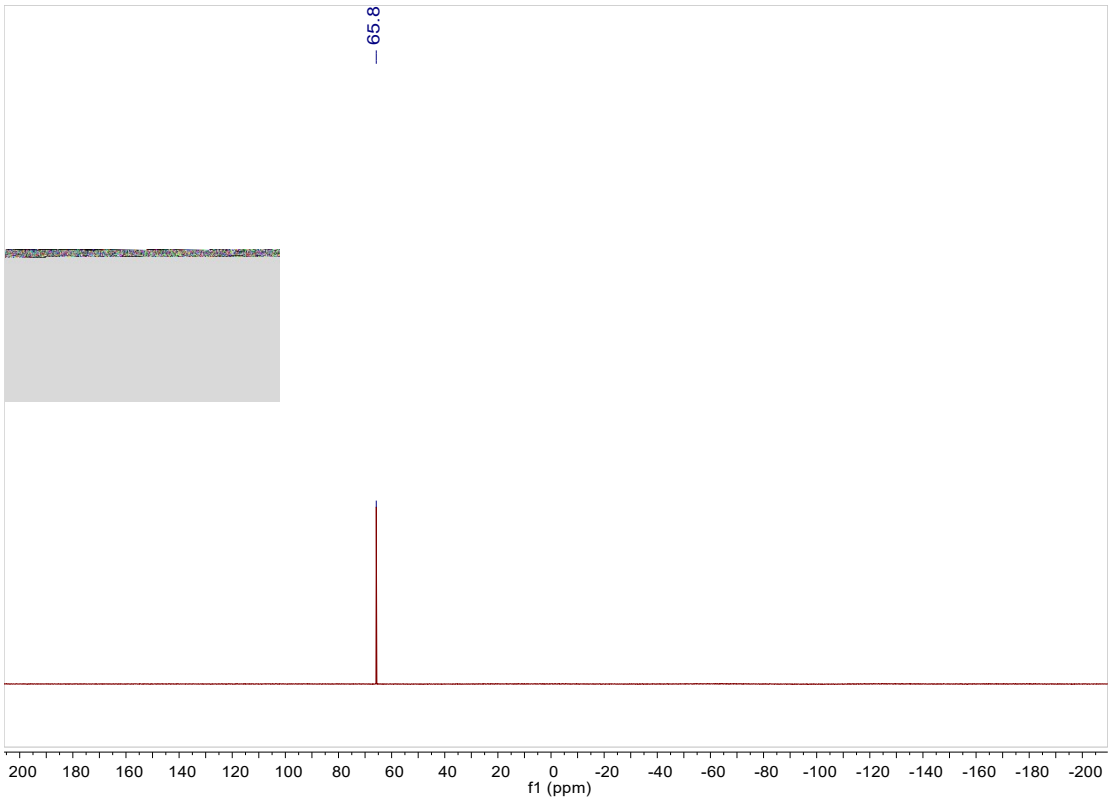
^{19}F NMR spectrum of naphthalene-2-sulfonyl fluoride (376 MHz, $CDCl_3$)



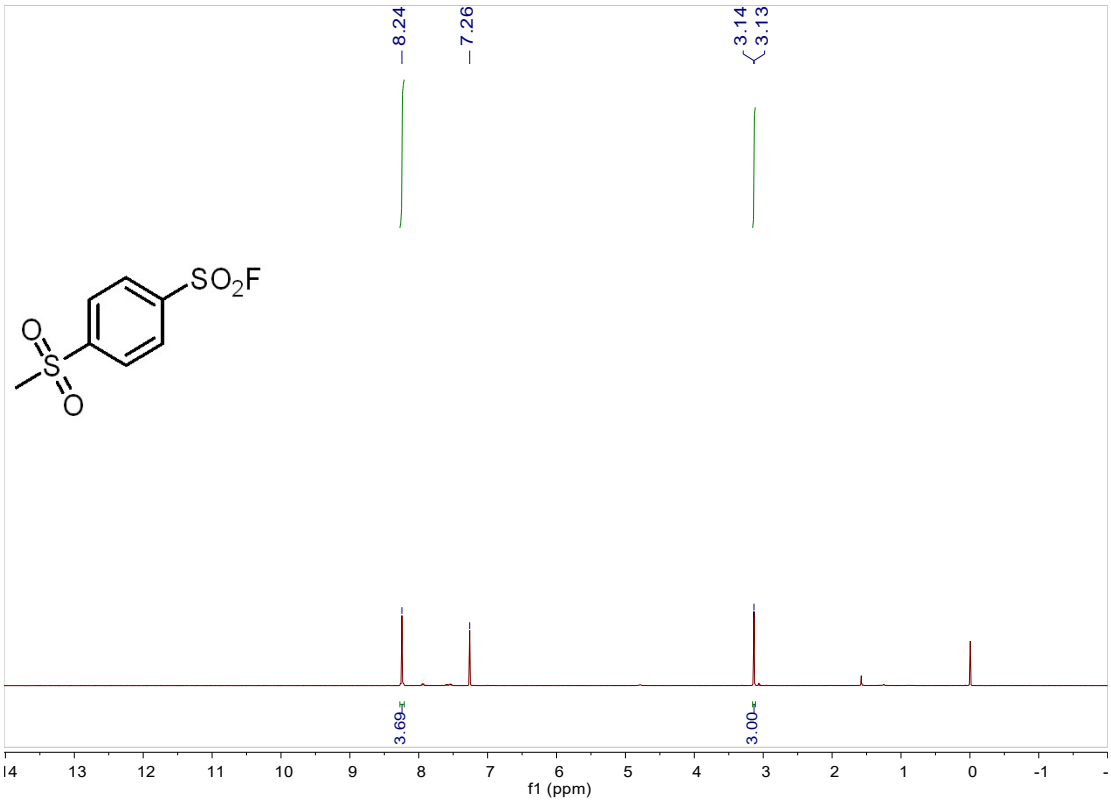
^{1}H NMR spectrum of methyl 4-(fluorosulfonyl)benzoate (400 MHz, $CDCl_3$)



^{19}F NMR spectrum of methyl 4-(fluorosulfonyl)benzoate (376 MHz, $CDCl_3$)

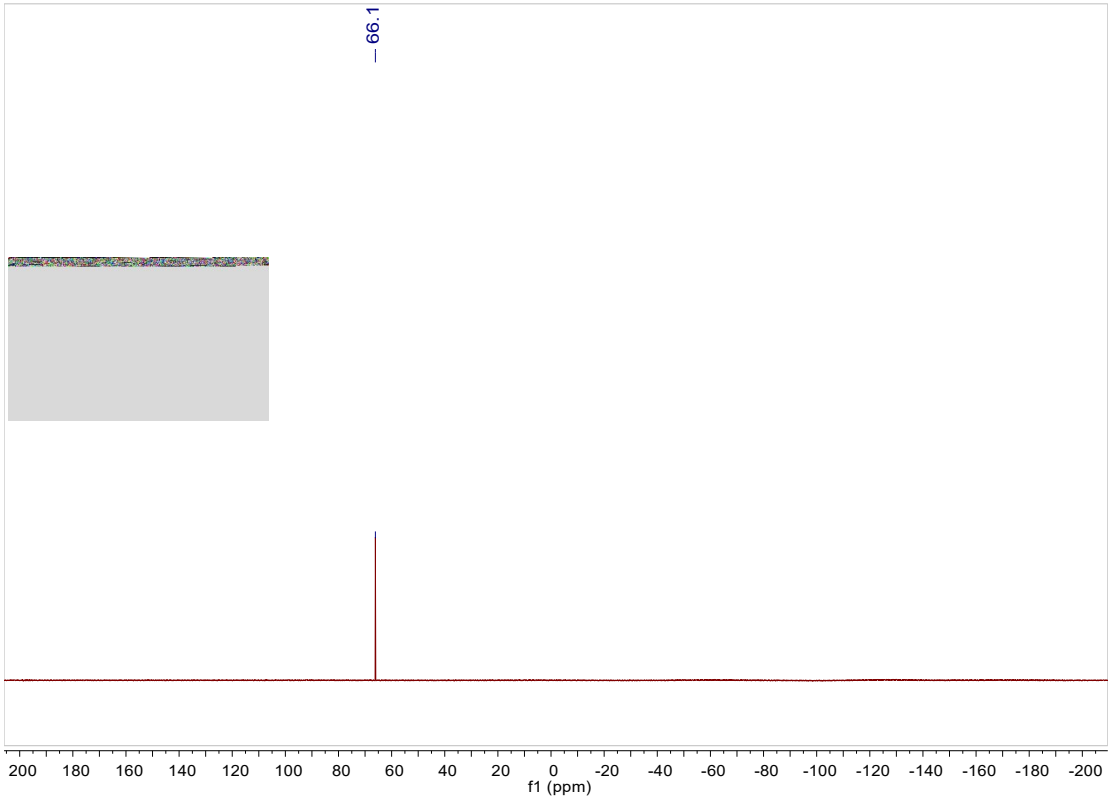


^{1}H NMR spectrum of 4-(methylsulfonyl)benzenesulfonyl fluoride (400 MHz, $CDCl_3$)

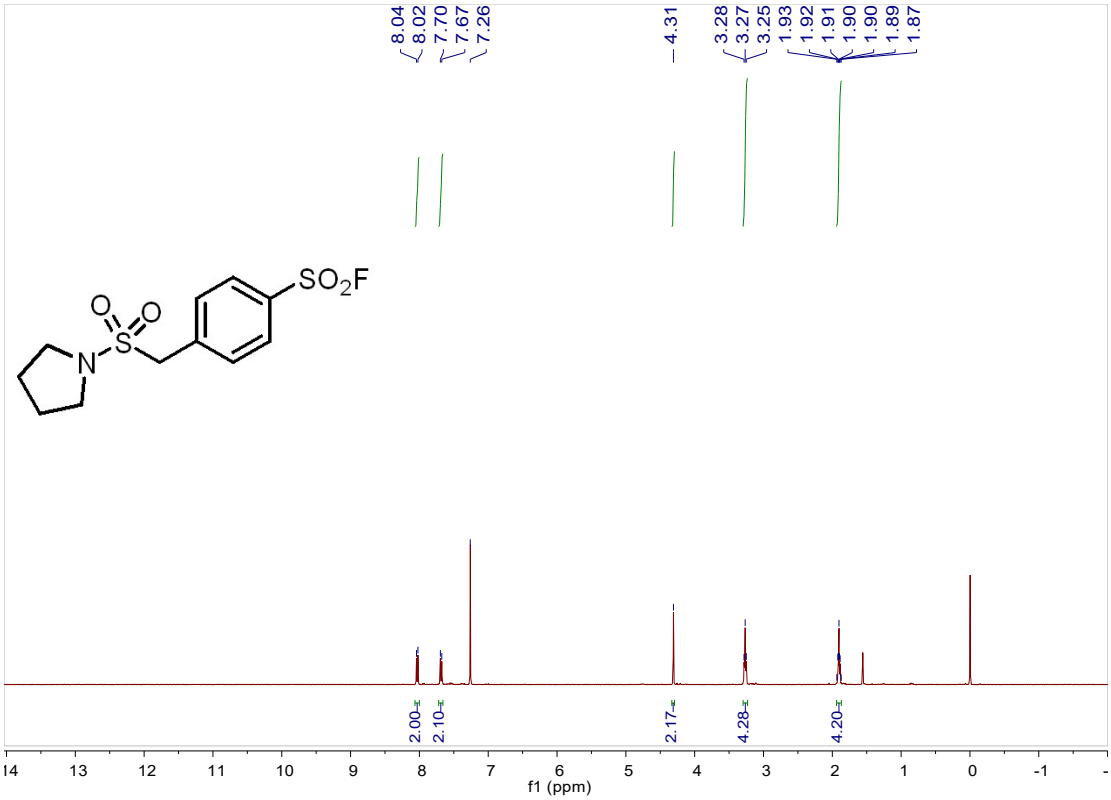


^{19}F NMR spectrum of 4-(methylsulfonyl)benzenesulfonyl fluoride (376 MHz,

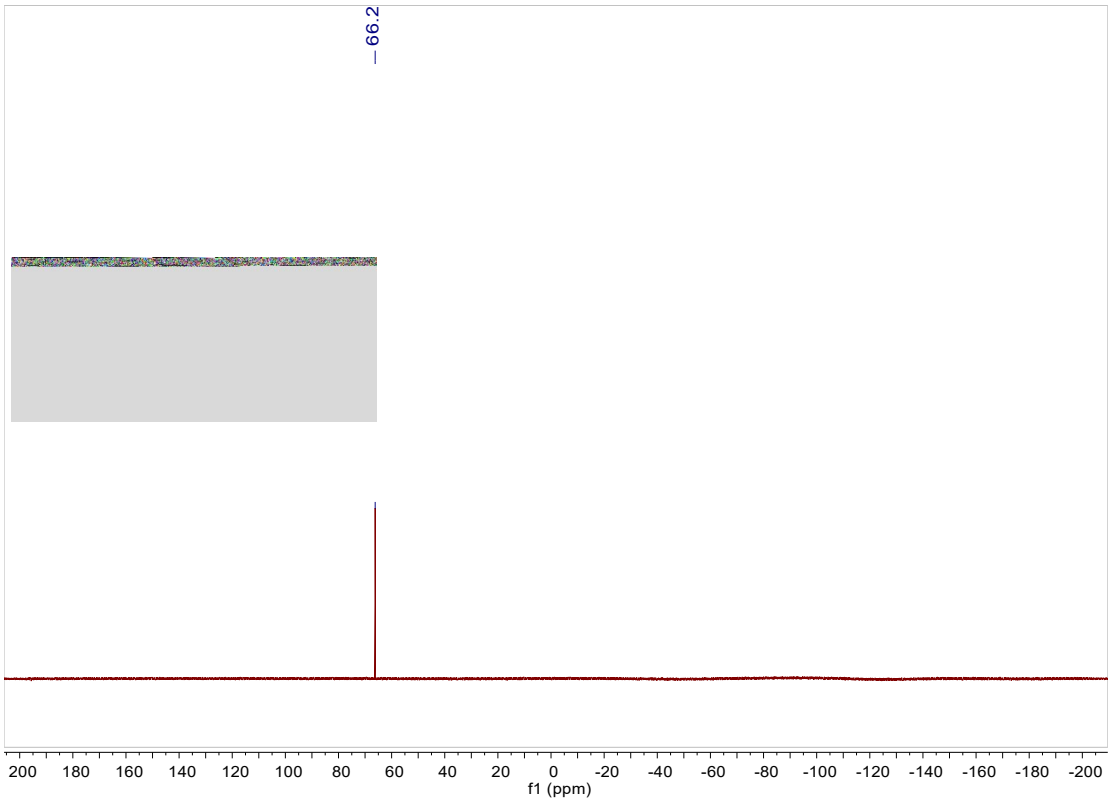
$CDCl_3$)



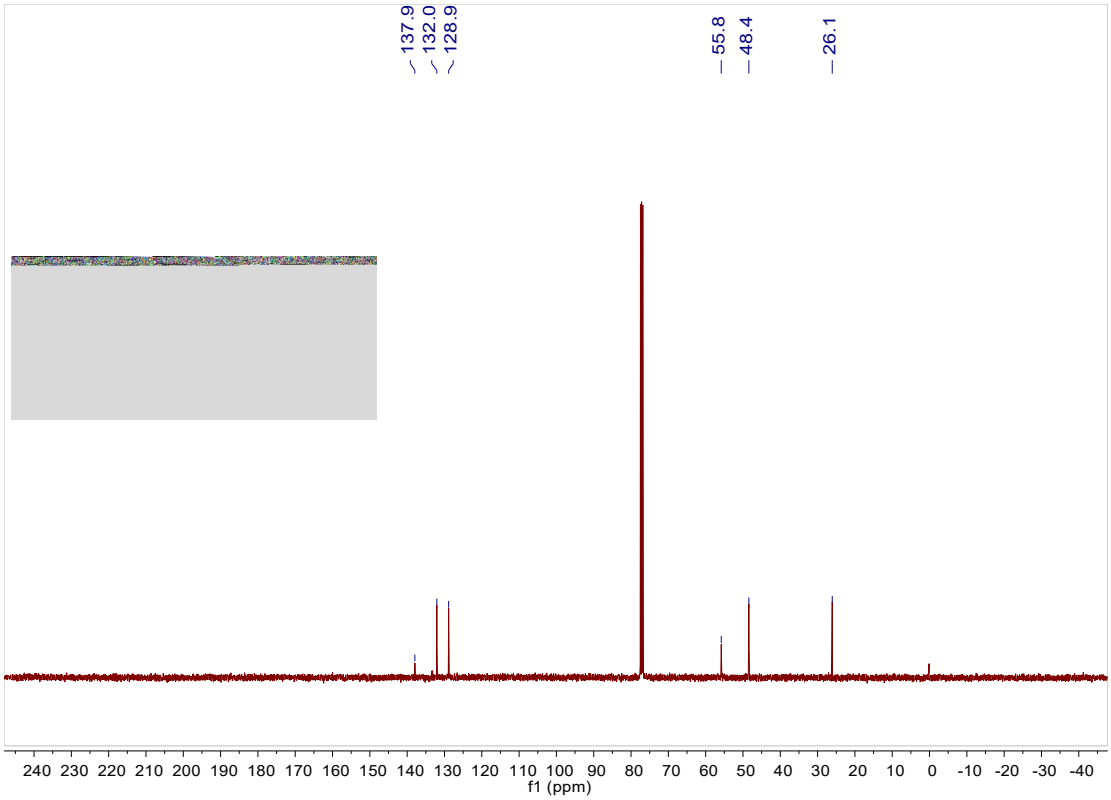
^1H NMR spectrum of 4-((pyrrolidin-1-ylsulfonyl)methyl)benzenesulfonyl fluoride (400 MHz, $CDCl_3$)



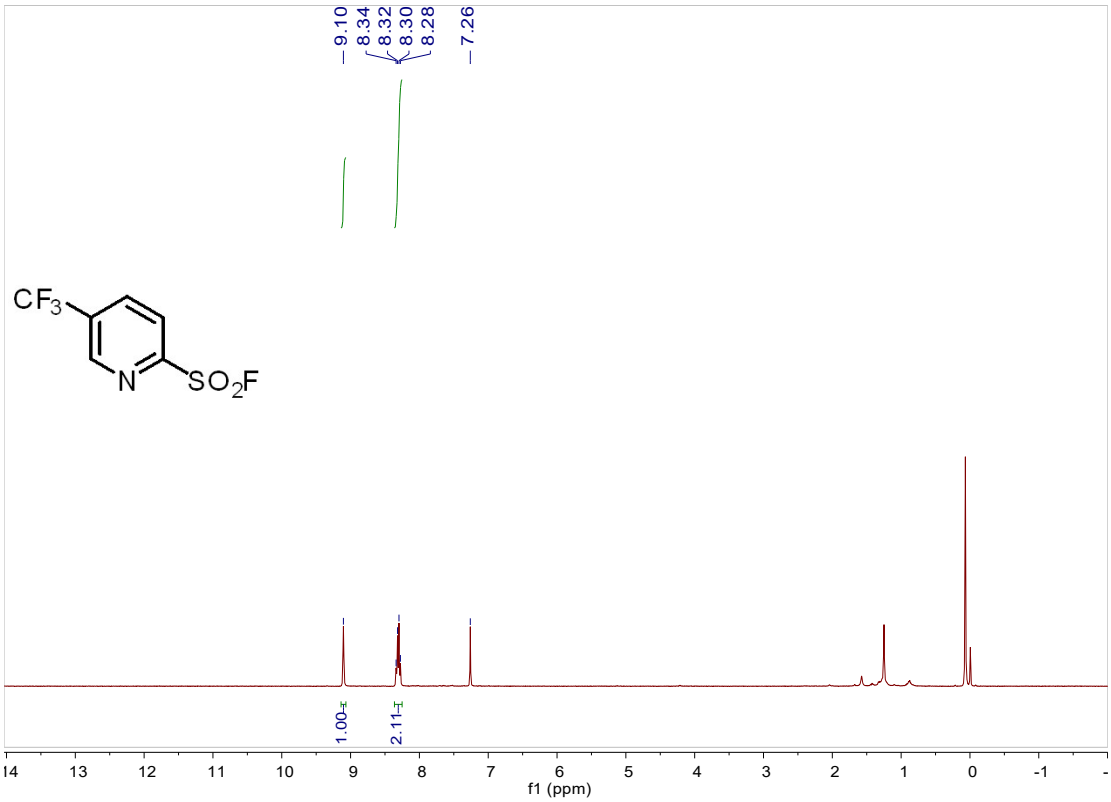
^{19}F NMR spectrum of 4-((pyrrolidin-1-ylsulfonyl)methyl)benzenesulfonyl fluoride (376 MHz, $CDCl_3$)



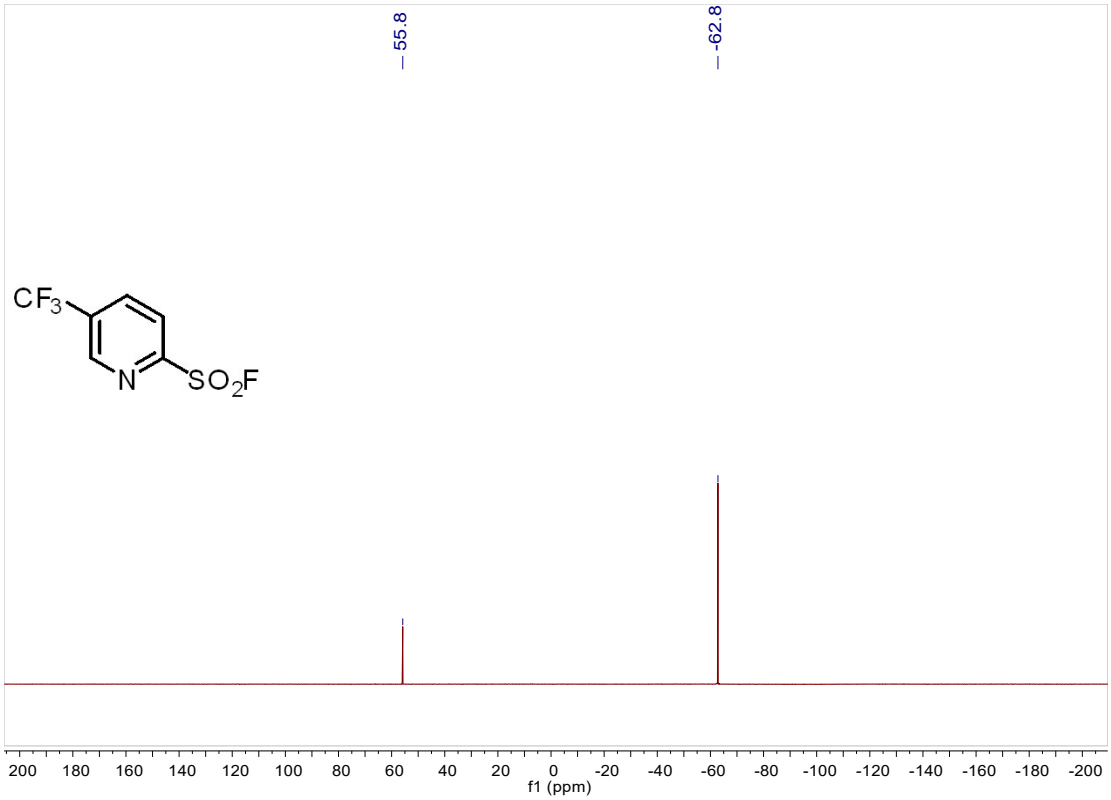
^{13}C NMR spectrum of 4-((pyrrolidin-1-ylsulfonyl)methyl)benzenesulfonyl fluoride (101 MHz, $CDCl_3$)



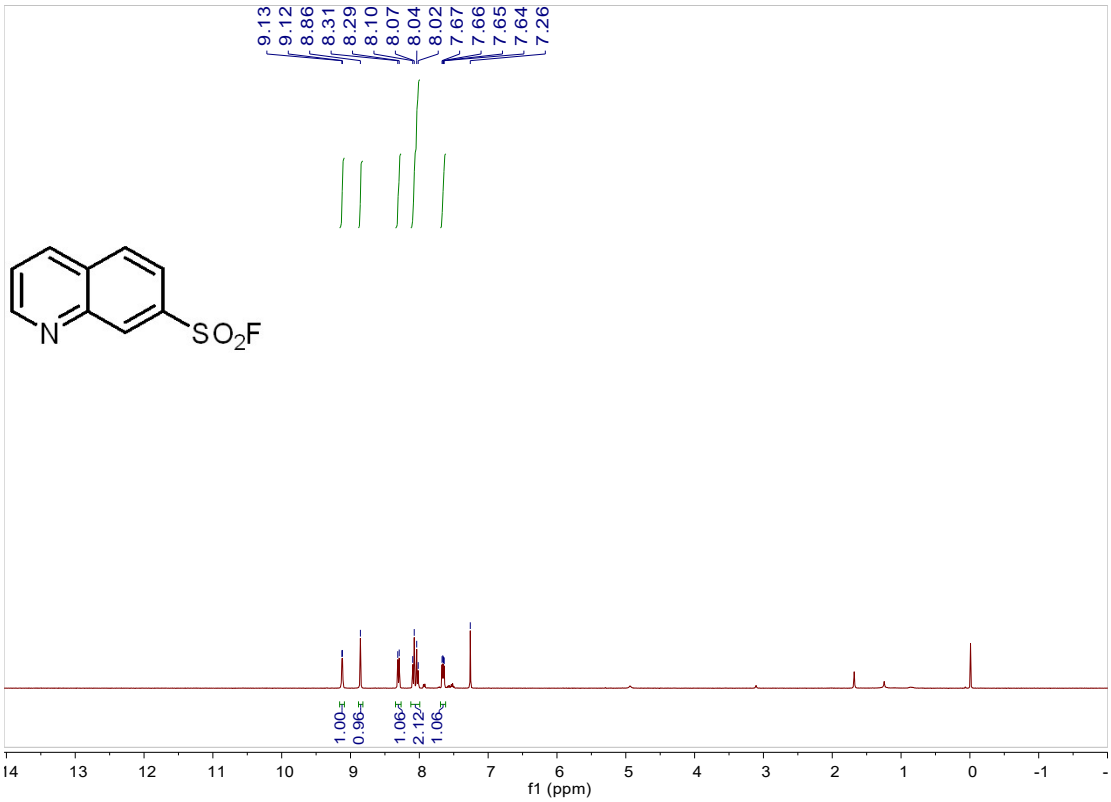
^{1}H NMR spectrum of 5-(trifluoromethyl)pyridine-2-sulfonyl fluoride (400 MHz, $CDCl_3$)



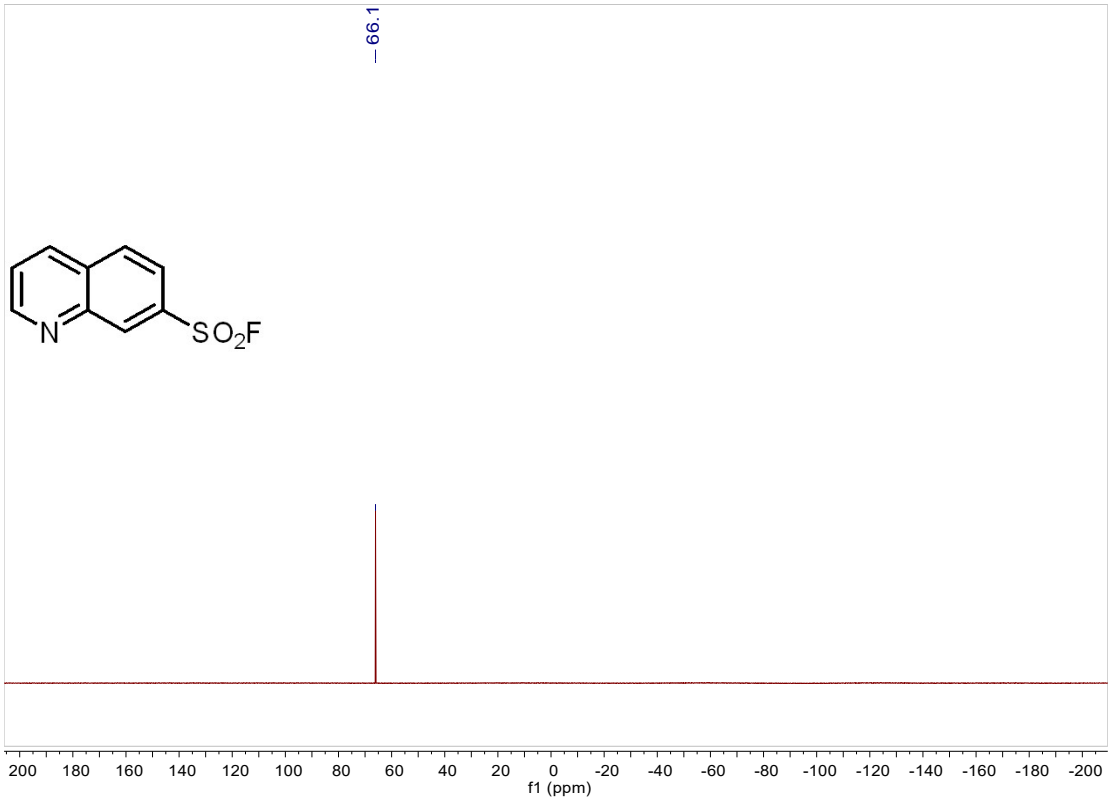
^{19}F NMR spectrum of 5-(trifluoromethyl)pyridine-2-sulfonyl fluoride (376 MHz, $CDCl_3$)



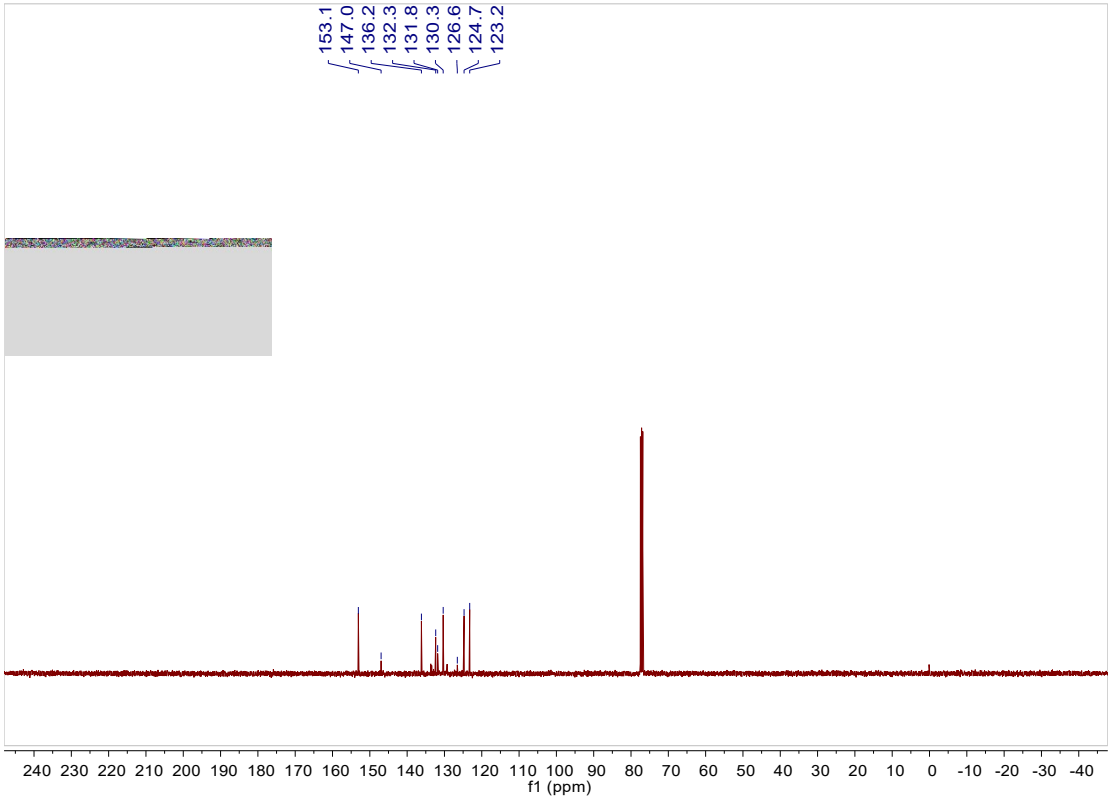
^{1}H NMR spectrum of quinoline-7-sulfonyl fluoride (400 MHz, $CDCl_3$)



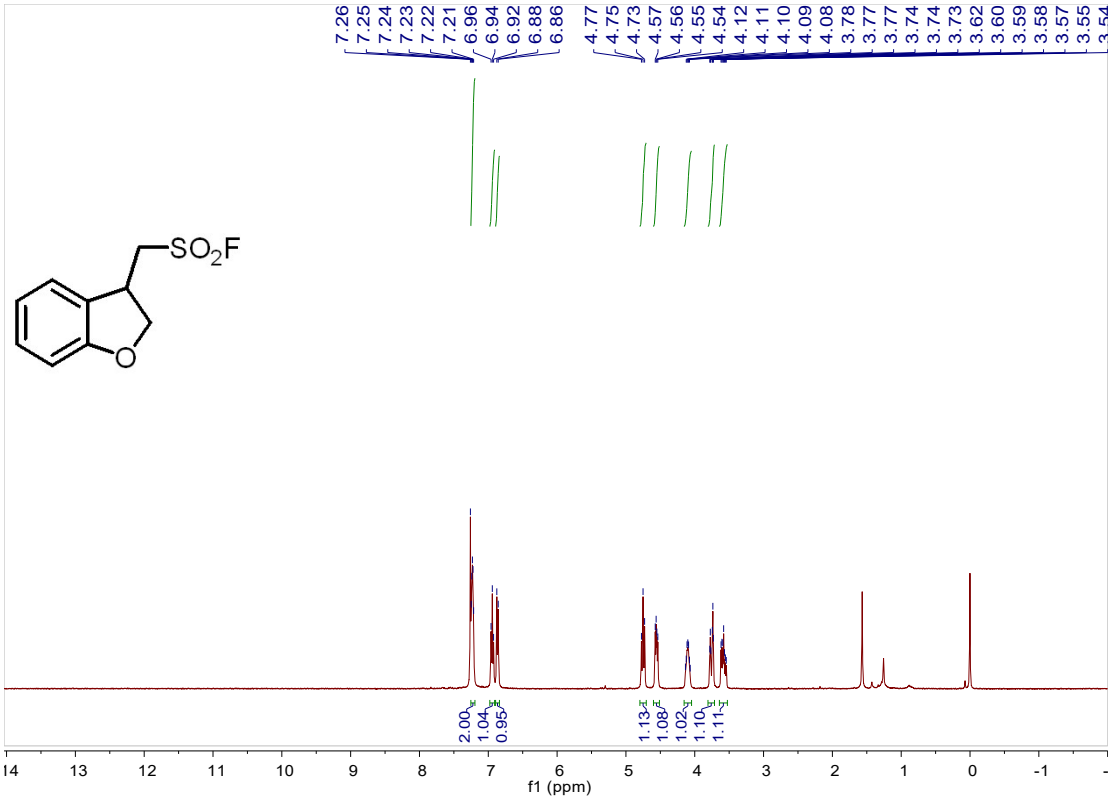
^{19}F NMR spectrum of quinoline-7-sulfonyl fluoride (376 MHz, $CDCl_3$)



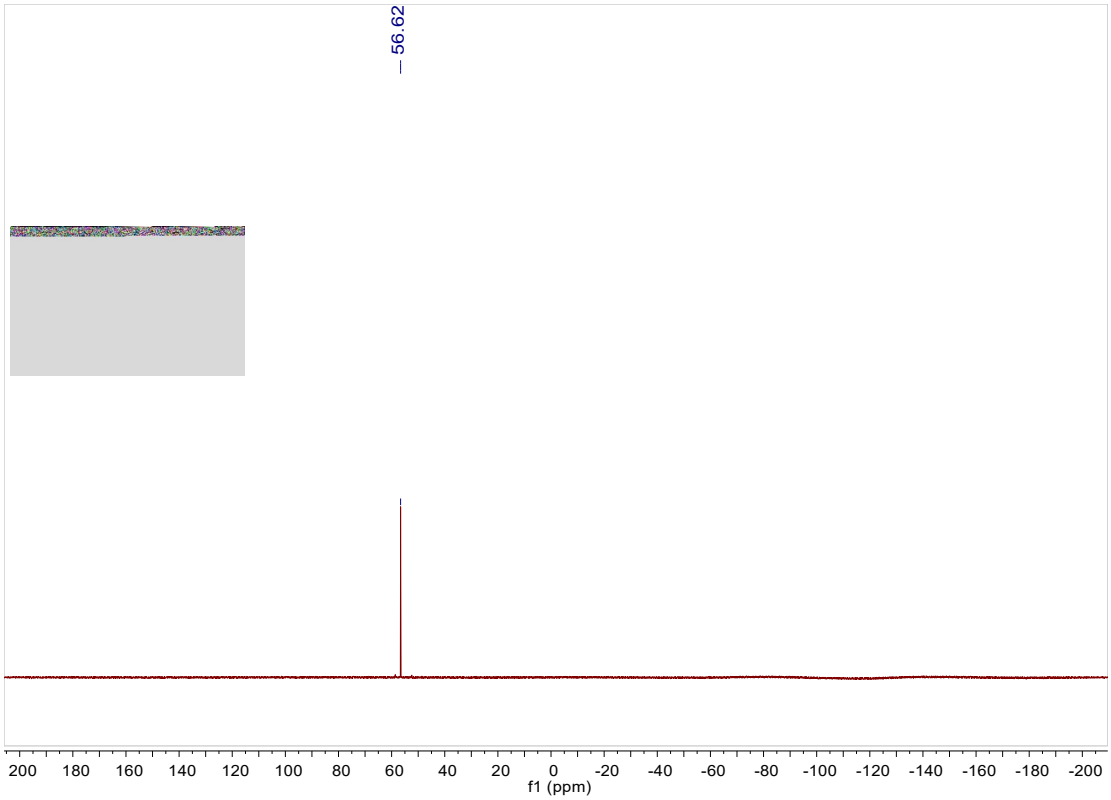
^{13}C NMR spectrum of quinoline-7-sulfonyl fluoride (101 MHz, $CDCl_3$)



^{1}H NMR spectrum of (2,3-dihydrobenzofuran-3-yl)methanesulfonyl fluoride (400 MHz, $CDCl_3$)



^{19}F NMR spectrum of (2,3-dihydrobenzofuran-3-yl)methanesulfonyl fluoride (376 MHz, $CDCl_3$)



VIII. Single crystal structure data of 2,4-dichlorobenzenesulfonyl fluoride (2e)

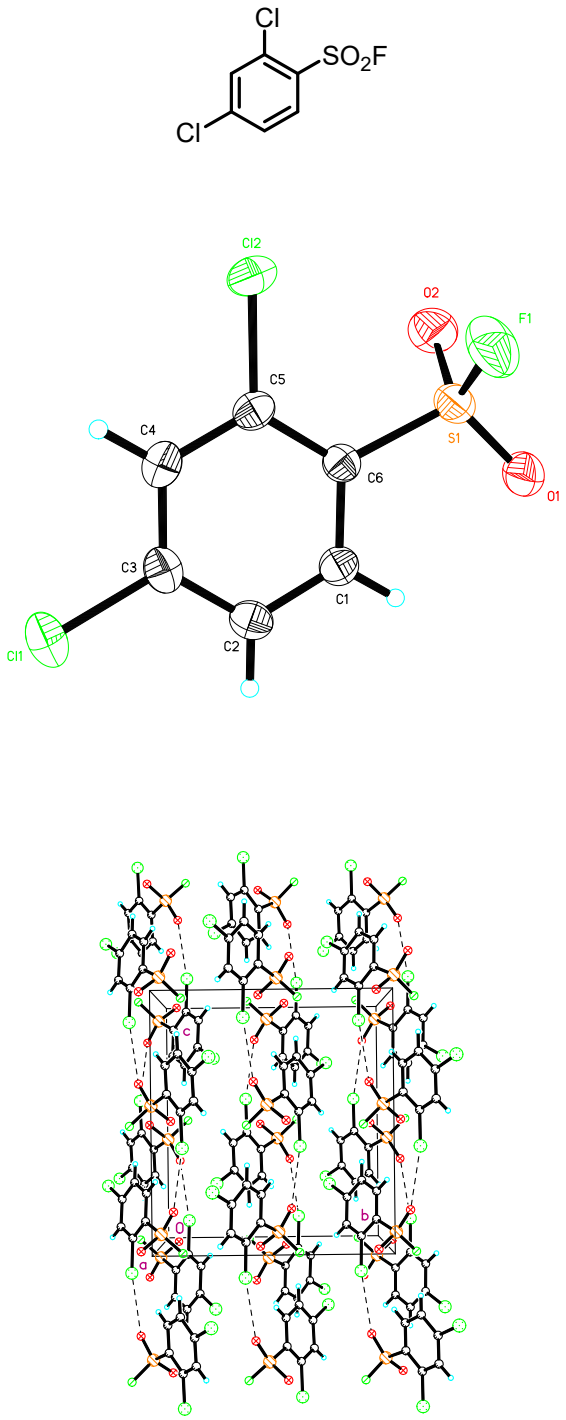


Figure S1. Single crystal structure data of 2,4-dichlorobenzenesulfonyl fluoride (2e)

Table S7. Crystal data and structure refinement for **2e**

Compound	**2e**
Solvent system for crystal growth	petroleum ether / CH_2Cl_2
Identification code	d8v21377
Empirical formula	$C_6H_3Cl_2FO_2S$
Formula weight	229.04
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	P b c a
Unit cell dimensions	a = 12.038(4) Å α= 90°
	b = 11.289(3) Å β= 90°
	c = 12.334(3) Å γ= 90°
Volume	1676.2(8) $Å^3$
Z	8
Density (calculated)	1.815 Mg/m^3
Absorption coefficient	0.991 mm^{-1}
F(000)	912
Crystal size	0.170 x 0.140 x 0.110 mm^3
Theta range for data collection	2.974 to 25.983°.
Index ranges	-14<=h<=14, -13<=k<=13, -14<=l<=15
Reflections collected	13355
Independent reflections	1630 [R(int) = 0.0357]
Completeness to theta = 25.242°	98.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7456 and 0.5595
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1630 / 1 / 110
Goodness-of-fit on F^2	1.057
Final R indices [I>2sigma(I)]	R1 = 0.0343, wR2 = 0.0863
R indices (all data)	R1 = 0.0390, wR2 = 0.0906
Extinction coefficient	0.062(4)
Largest diff. peak and hole	0.289 and -0.276 $e.Å^{-3}$

Table S8. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for d8v21377. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cl(1)	6238(1)	2554(1)	2569(1)	74(1)
Cl(2)	3756(1)	3803(1)	5965(1)	66(1)
S(1)	2102(1)	5220(1)	4318(1)	58(1)
F(1)	2542(2)	6114(2)	5108(2)	92(1)
O(1)	1601(2)	5790(2)	3435(2)	77(1)
O(2)	1414(2)	4426(2)	4929(2)	80(1)
C(1)	3516(2)	4494(2)	2781(2)	49(1)
C(2)	4423(2)	3906(2)	2370(2)	52(1)
C(3)	5090(2)	3286(2)	3074(2)	50(1)
C(4)	4880(2)	3242(2)	4175(2)	51(1)
C(5)	3976(2)	3841(2)	4582(2)	46(1)
C(6)	3287(2)	4463(2)	3882(2)	44(1)

Table S9. Bond lengths [Å] and angles [°] for d8v21377.

Cl(1)-C(3)	1.726(2)
Cl(2)-C(5)	1.726(2)
S(1)-O(1)	1.4019(19)
S(1)-O(2)	1.435(2)
S(1)-F(1)	1.4987(18)
S(1)-C(6)	1.748(2)
C(1)-C(2)	1.375(3)
C(1)-C(6)	1.386(3)
C(1)-H(1)	0.9300
C(2)-C(3)	1.374(3)
C(2)-H(2)	0.9300
C(3)-C(4)	1.382(3)
C(4)-C(5)	1.377(3)
C(4)-H(4)	0.9300
C(5)-C(6)	1.388(3)
O(1)-S(1)-O(2)	116.48(14)
O(1)-S(1)-F(1)	110.35(13)
O(2)-S(1)-F(1)	106.48(13)
O(1)-S(1)-C(6)	109.65(11)
O(2)-S(1)-C(6)	109.17(12)
F(1)-S(1)-C(6)	103.93(11)
C(2)-C(1)-C(6)	120.4(2)
C(2)-C(1)-H(1)	119.8
C(6)-C(1)-H(1)	119.8
C(3)-C(2)-C(1)	118.5(2)
C(3)-C(2)-H(2)	120.7
C(1)-C(2)-H(2)	120.7
C(2)-C(3)-C(4)	122.2(2)
C(2)-C(3)-Cl(1)	118.94(19)
C(4)-C(3)-Cl(1)	118.89(18)
C(5)-C(4)-C(3)	119.0(2)
C(5)-C(4)-H(4)	120.5
C(3)-C(4)-H(4)	120.5
C(4)-C(5)-C(6)	119.6(2)
C(4)-C(5)-Cl(2)	118.01(17)

C(6)-C(5)-Cl(2)	122.39(18)
C(1)-C(6)-C(5)	120.2(2)
C(1)-C(6)-S(1)	116.85(17)
C(5)-C(6)-S(1)	122.91(17)

Symmetry transformations used to generate equivalent atoms:

Table S10. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for d8v21377. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cl(1)	57(1)	71(1)	93(1)	-10(1)	10(1)	14(1)
Cl(2)	75(1)	77(1)	44(1)	11(1)	-2(1)	4(1)
S(1)	55(1)	71(1)	49(1)	-5(1)	2(1)	13(1)
F(1)	96(1)	90(1)	92(1)	-39(1)	-12(1)	18(1)
O(1)	74(1)	98(1)	60(1)	3(1)	-2(1)	38(1)
O(2)	55(1)	104(2)	79(1)	10(1)	15(1)	3(1)
C(1)	50(1)	53(1)	44(1)	-1(1)	-4(1)	3(1)
C(2)	55(1)	56(1)	45(1)	-6(1)	3(1)	-2(1)
C(3)	43(1)	42(1)	64(1)	-8(1)	1(1)	-2(1)
C(4)	49(1)	45(1)	60(1)	6(1)	-8(1)	-2(1)
C(5)	50(1)	45(1)	44(1)	4(1)	-4(1)	-6(1)
C(6)	44(1)	44(1)	44(1)	-2(1)	0(1)	-1(1)

Table S11. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for d8v21377.

	x	y	z	U(eq)
H(1)	3053	4916	2317	59
H(2)	4582	3928	1632	63
H(4)	5343	2813	4633	62

Table S12. Torsion angles [°] for d8v21377.

C(6)-C(1)-C(2)-C(3)	0.3(3)
C(1)-C(2)-C(3)-C(4)	-0.4(3)
C(1)-C(2)-C(3)-Cl(1)	-179.43(17)
C(2)-C(3)-C(4)-C(5)	-0.2(3)
Cl(1)-C(3)-C(4)-C(5)	178.88(16)
C(3)-C(4)-C(5)-C(6)	0.8(3)
C(3)-C(4)-C(5)-Cl(2)	-178.33(17)
C(2)-C(1)-C(6)-C(5)	0.3(3)
C(2)-C(1)-C(6)-S(1)	-178.97(17)
C(4)-C(5)-C(6)-C(1)	-0.9(3)
Cl(2)-C(5)-C(6)-C(1)	178.21(17)
C(4)-C(5)-C(6)-S(1)	178.36(17)
Cl(2)-C(5)-C(6)-S(1)	-2.5(3)
O(1)-S(1)-C(6)-C(1)	-2.6(2)
O(2)-S(1)-C(6)-C(1)	126.14(19)
F(1)-S(1)-C(6)-C(1)	-120.55(19)
O(1)-S(1)-C(6)-C(5)	178.16(19)
O(2)-S(1)-C(6)-C(5)	-53.1(2)
F(1)-S(1)-C(6)-C(5)	60.2(2)

Symmetry transformations used to generate equivalent atoms: