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Supporting Information

Fluoroalkylated Hypervalent Sulfur Fluorides: Radical Addition of Arylchlorotetrafluoro-λ^6-sulfanes to Tetrafluoroethylene

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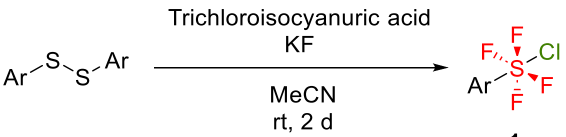
1. Experimental Section

1.1. General Information

All reactions were carried out using oven-dried glassware and anhydrous solvents, under Ar or N_2 atmosphere unless noted otherwise. ^{1}H, ^{13}C, and ^{19}F NMR spectra were recorded on a JEOL JNM-ECZ400 spectrometer (^{1}H NMR: 400 MHz, ^{13}C NMR: 101 MHz, ^{19}F NMR: 376 MHz) at ambient temperature. ^{1}H and ^{13}C NMR chemical shifts were respectively referenced to tetramethylsilane (δ = 0.00 ppm) and residual solvent (δ = 77.16 ppm for $CDCl_3$; δ = 39.52 ppm for DMSO-d_6). For ^{19}F NMR, chemical shift values were not calibrated by an internal reference. High-resolution mass (HRMS) spectra were measured on a JEOL JMS-T100LP spectrometer in the electron spray ionization time-of-flight (ESI-TOF) mode. GC–MS analyses were performed using a Shimadzu GCMS-QP2020 gas chromatograph mass spectrometer equipped with an HP-5 capillary column (0.320 i.d.; 0.25 µm df; 30 m; Agilent Technologies) with helium as the carrier gas using Chemical Ionization (CI) with the following method: 40 °C for 5 min then 10 °C/min until 240 °C. Elemental analyses were performed on a Elementar Vario MICRO Cube analyzer (the ratio of elements was calculated on a Microsoft Excel spreadsheet). A single crystal X-ray diffraction measurement was made on XtaLAB mini II diffractometer using graphite monochromated Mo-Kα radiation. Liquid chromatographic analyses were performed by HPLC system (Shimadzu Scientific Instruments) comprising a UV-Vis detector (SPD-M40), a pump (LC-20AD), and an automatic injector (SIL-20AC). The wavelength of the UV-Vis detector was set at 254 nm and a reverse phase column (Shim-pack Scepter C18-120, 5 µm, Shimadzu Scientific Instruments) was used. The mobile phase (methanol/water, 75/25) are pumped through the column at a flow rate of 1 mL/min. The column temperature was maintained at 40 °C using a column oven (CTO-20AC, Shimadzu Scientific Instruments). Tetrafluoroethylene (TFE) was received from AGC Inc. All other materials were purchased from Kanto Chemical Co., Inc., FUJIFILM Wako Pure Chemical Corporation, Tokyo Chemical Industry Co., Ltd., and Sigma–Aldrich Japan, and used as received. Column chromatography was performed using Silica Gel 60 N (spherical, neutral; Kanto Chemical Co., Inc.). Analytical thin layer chromatography (TLC) was performed on a glass plates pre-coated with silica-gel (Merck Kieselgel 60 F254, layer thickness 0.25 nm). The corresponding disulfide starting materials for compounds **1a**, **1c**, **1d**, **1e**, **1f**, **1k**, **1l**, **1o**, and **1p** are commercially available. The corresponding disulfide starting materials for compounds **1b**,[1] **1g**,[1] **1h**,[2] **1i**,[3] **1j**,[1] **1m**,[1] **1n**,[1] and **1q**[1] were synthesized according to literature procedure. For hydrophobicity measurements, PhC_4F_9 and PhC_3F_7 were synthesized according to the literature procedure and consistent with previously reported characterization.[4–6]

1.2. Preparation of Arylchlorotetrafluoro-λ^6-sulfanes 1

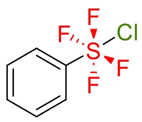
General Procedure



1

Reaction was performed according to the literature procedure.[3,7] To a solution of the disulfide substrate (4.0 mmol) and potassium fluoride (4.65 g, 80 mmol, 20 equiv.) in CH_3CN (50 mL) in a round-bottom flask under Ar atmosphere was added trichloroisocyanuric acid (11.1 g, 48 mmol, 12 equiv.). The reaction mixture was stirred vigorously at ambient temperature for 2 d. Upon reaction completion, the yield was determined by ^{19}F NMR analysis using trifluorotoluene as an internal standard. Subsequently, the crude reaction mixture was filtered through glass filter under N_2 and concentrated in vacuo. Then, the crude reaction mixture was diluted with dry 19:1 hexane:CH_2Cl_2, filtered, and concentrated in vacuo. The crude material was carried forward immidiately without further purification.

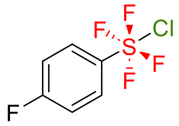
Chlorotetrafluoro(phenyl)-λ^6-sulfane (1a)



The reaction was run according to the general procedure, and the product is consistent with previously reported characterization data.[8] ^{19}F NMR yield: 64%.

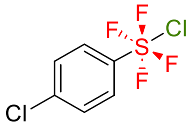
^{19}F NMR (376 MHz, CH_3CN) δ 136.6 (s, 4F).

Chlorotetrafluoro(4-fluorophenyl)-λ⁶-sulfane (1b)



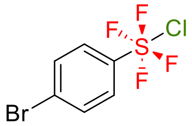
The reaction was run according to the general procedure, and the product is consistent with previously reported characterization data.[8] ^{19}F NMR yield: 57%.
^{19}F NMR (376 MHz, CH_3CN) δ 137.6 (s, 4F), −108.3 (s, 1F).

Chloro(4-chlorophenyl)tetrafluoro-λ⁶-sulfane (1c)



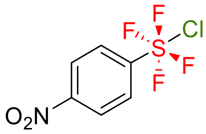
The reaction was run according to the general procedure, and the product is consistent with previously reported characterization data.[8] ^{19}F NMR yield: 79%.
^{19}F NMR (376 MHz, CH_3CN) δ 136.7 (s, 4F).

(4-Bromophenyl)chlorotetrafluoro-λ⁶-sulfane (1d)



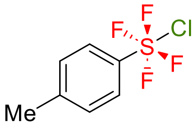
The reaction was run according to the general procedure, and the product is consistent with previously reported characterization data.[8] ^{19}F NMR yield: 73%.
^{19}F NMR (376 MHz, CH_3CN) δ 136.6 (s, 4F).

Chlorotetrafluoro(4-nitrophenyl)-λ⁶-sulfane (1e)



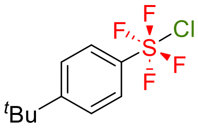
The reaction was run according to the general procedure, and the product is consistent with previously reported characterization data.[8] ^{19}F NMR yield: 83%.
^{19}F NMR (376 MHz, CH_3CN) δ 135.0 (s, 4F).

Chlorotetrafluoro(*p*-tolyl)-λ⁶-sulfane (1f)



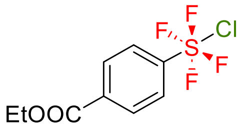
The reaction was run according to the general procedure, and the product is consistent with previously reported characterization data.[8] ^{19}F NMR yield: 68%.
^{19}F NMR (376 MHz, CH_3CN) δ 137.6 (s, 4F).

(4-(*tert*-Butyl)phenyl)chlorotetrafluoro-λ⁶-sulfane (1g)



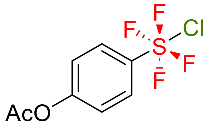
The reaction was run according to the general procedure, and the product is consistent with previously reported characterization data.[8] ^{19}F NMR yield: 55%.
^{19}F NMR (376 MHz, CH_3CN) δ 137.6 (s, 4F).

Ethyl 4-(chlorotetrafluoro-λ⁶-sulfanyl)benzoate (1h)



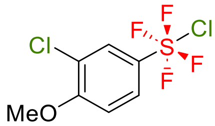
The reaction was run according to the general procedure, and the product was converted to the stable compound **2i** to obtain complete characterization data. ^{19}F NMR yield: 69%.
^{19}F NMR (376 MHz, CH_3CN) δ 135.6 (s, 4F).

4-(Chlorotetrafluoro-λ^6-sulfanyl)phenyl acetate (1i)



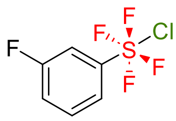
The reaction was run according to the general procedure, and the product is consistent with previously reported characterization data.[3] ^{19}F NMR yield: 68%.
^{19}F NMR (376 MHz, CH_3CN) δ 137.4 (s, 4F).

Chloro(3-chloro-4-methoxyphenyl)tetrafluoro-λ^6-sulfane (1j)



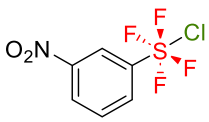
To a solution of bis(4-methoxyphenyl) disulfide (1.11 g, 4.0 mmol, 1.0 equiv.) and potassium fluoride (7.44 g, 128 mmol, 32 equiv.) in CH_3CN (50 mL) in a round-bottom flask under Ar atmosphere were added trichloroisocyanuric acid (16.7 g, 72 mmol, 18 equiv.) and trifluoroacetic acid (31 µL, 0.40 mmol, 10 mol%). The reaction mixture was stirred vigorously at ambient temperature for 24 h. Upon reaction completion, the yield was determined by ^{19}F NMR analysis using trifluorotoluene as an internal standard. Subsequently, the crude reaction mixture was filtered through glass filter under N_2 and concentrated in vacuo. Then, the crude reaction mixture was diluted with dry 19:1 hexane:CH_2Cl_2, filtered, and concentrated in vacuo. The crude material was analyzed by ^{1}H, ^{19}F NMR using 1,4-bis(trifluoromethyl)benzene and converted to the stable compound **2j** to obtain complete characterization data. ^{19}F NMR yield: 33%.
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.77 (m, 1H), 7.63 (dd, J = 9.0, 2.6 Hz, 1H), 6.92 (d, J = 8.9 Hz, 1H), 3.95 (s, 3H); ^{19}F NMR (376 MHz, $CDCl_3$) δ 139.1 (s, 4F); ^{19}F NMR (376 MHz, CH_3CN) δ 138.6 (s, 4F).

Chlorotetrafluoro(3-fluorophenyl)-λ^6-sulfane (1k)



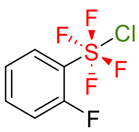
The reaction was run according to the general procedure, and the product is consistent with previously reported characterization data.[9] ^{19}F NMR yield: 63%.
^{19}F NMR (376 MHz, CH_3CN) δ 136.1 (s, 4F), −111.3 (s, 1F).

Chlorotetrafluoro(3-nitrophenyl)-λ^6-sulfane (1l)



The reaction was run according to the general procedure, and the product is consistent with previously reported characterization data.[9] ^{19}F NMR yield: 65%.
^{19}F NMR (376 MHz, CH_3CN) δ 135.3 (s, 4F).

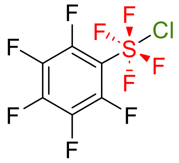
Chlorotetrafluoro(2-fluorophenyl)-λ^6-sulfane (1m)



The reaction was run according to the general procedure, and the product is consistent with previously reported characterization data.[8] ^{19}F NMR yield: 61%.

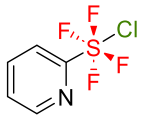
^{19}F NMR (376 MHz, CH_3CN) δ 140.3 (d, J = 23.1 Hz, 4F), −110.0 (m, 1F).

Chlorotetrafluoro(perfluorophenyl)-λ^6-sulfane (1n)



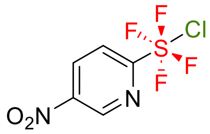
The reaction was run according to the general procedure, and the product is consistent with previously reported characterization data.[8] ^{19}F NMR yield: 62% (*trans*:*cis* 1.3:1).
trans-isomer: ^{19}F NMR (376 MHz, CH_3CN) δ 143.2 (m, 4F); *cis*-isomer: ^{19}F NMR (376 MHz, CH_3CN) δ 153.0 (q, J = 159.9 Hz, 1F), 123.2–122.3 (m, 2F), 79.7–78.7 (m, 1F).
Fluorine atoms on the aromatic ring could not be identified due to contamination of other side-products.

2-(Chlorotetrafluoro-λ^6-sulfanyl)pyridine (1o)



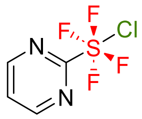
The reaction was run according to the general procedure, and the product is consistent with previously reported characterization data.[10] ^{19}F NMR yield: 80%.
^{19}F NMR (376 MHz, CH_3CN) δ 124.0 (s, 4F).

2-(Chlorotetrafluoro-λ^6-sulfanyl)-5-nitropyridine (1p)



The reaction was run according to the general procedure, and the product is consistent with previously reported characterization data.[10] ^{19}F NMR yield: 85%.
^{19}F NMR (376 MHz, CH_3CN) δ 123.5 (s, 4F).

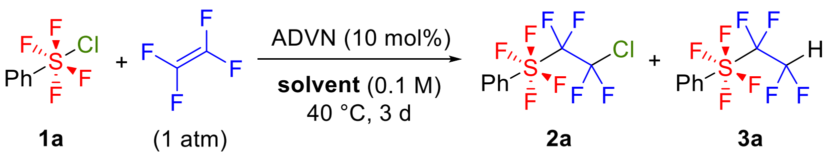
2-(Chlorotetrafluoro-λ^6-sulfanyl)pyrimidine (1q)



The reaction was run according to the general procedure, and the product is consistent with previously reported characterization data.[11] ^{19}F NMR yield: 71%.
^{19}F NMR (376 MHz, CH_3CN) δ 118.0 (s, 4F).

1.3. Optimization

Table S1. Effect of solvents on addition of **1a** to tetrafluoroethylene.

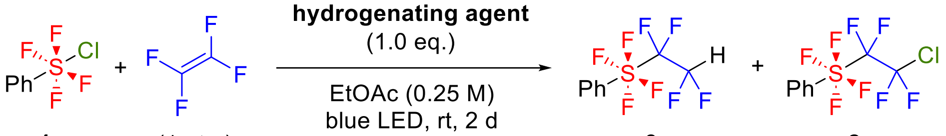


Entry	Solvent	Yield [%][a]	
		2a	**3a**
1	MeCN	8	n.d.
2	hexane	2	5
3	THF	8	38

4	CH_2ClCH_2Cl	59	n.d.
5	EtOAc	69	n.d.

[a] Determined by ^{19}F NMR analysis of the crude mixture relative to an internal standard (1,4-bis(trifluoromethyl)benzene).

Table S2. Effect of hydrogenating agents on addition of **1a** to tetrafluoroethylene.



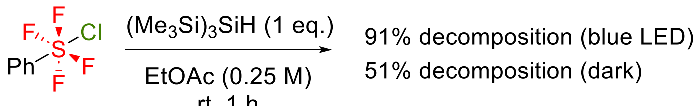
1a (1 atm) **3a** **2a**

Entry	Hydrogenating agent	Yield [%][a]	
		3a	**2a**
1[b]	-	0	49
2	$(Me_3Si)_3SiH$	0	2
3	Et_3SiH	8	12
4	Bu_3SnH	0	1

[a] Determined by ^{19}F NMR analysis relative to an internal standard (1,4-bis(trifluoromethyl)benzene). [b] Reaction time: 3 d.

Reductive decomposition of 1a

Control experiments were performed in order to examine the stability of **1a** in the presence of a reductant $(Me_3Si)_3SiH$. **1a** (0.25 M in EtOAc, 0.10 mmol, 1.0 equiv.) and $(Me_3Si)_3SiH$ (24.9 mg, 0.10 mmol, 1.0 equiv.) were engaged and the reaction mixture was irradiated by blue LED (or in the dark) at rt for 1 h. The decomposition ratio was determined by ^{19}F NMR analysis using 1,4-bis(trifluoromethyl)benzene as an internal standard.

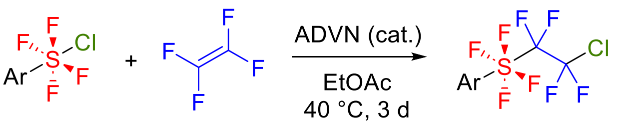


1a

Scheme S1. Reductive decomposition of **1a**. 1,4-Bis(trifluoromethyl)benzene was used as an internal standard.

1.4. Radical Addition Reaction of Arylchlorotetrafluoro-λ^6-sulfanes 1 to Tetrafluoroethylene

General Procedure

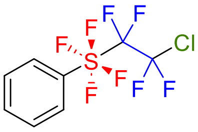


1 (1.0 atm) **2**

An oven-dried microwave vial (30 mL) was charged with a solution of **1** (1.0 equiv.) in EtOAc (0.25 M). To this mixture, ADVN (10 mol%) was added. The reaction vial was cooled to 0 °C, charged with tetrafluoroethylene (1.0 atm) by bubbling, and sealed. The reaction mixture was stirred at 40 °C on the oil bath for 3 d. Upon reaction completion, the yield was determined by ^{19}F NMR analysis using an internal standard (1,4-bis(trifluoromethyl)benzene). The insoluble solid was removed by filtration, and the filtrate was evaporated under reduced pressure. The crude product was purified via flash silica-gel column chromatography (EtOAc/hexane) to afford the desired products.

*Since hexacoordinated sulfur fluorides are generally difficult to ionize, HRMS (ESI(+), ESI(−), APCI(+), and APCI(−)) data were not available for **2a–q**.*[12]

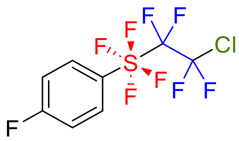
(2-Chloro-1,1,2,2-tetrafluoroethyl)tetrafluoro(phenyl)-λ^6-sulfane (2a)



1a (0.25 M in EtOAc, 0.60 mmol, 1.0 equiv.), ADVN (14.9 mg, 0.060 mmol, 10 mol%), tetrafluoroethylene (1.0 atm) were engaged in the general procedure. The yield (88%) was determined by ^{19}F NMR analysis using 1,4-bis(trifluoromethyl)benzene as an internal standard. Purification by silica-gel column chromatography (5% EtOAc/hexane) gave the compound (149 mg, 77% yield) as a colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79 (d, *J* = 8.2 Hz, 2H), 7.52–7.45 (m, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 155.9 (quint, $J_{C\text{-}F}$ = 19.7 Hz), 131.6, 128.8, 124.2 (quint, $J_{C\text{-}F}$ = 5.1 Hz), 122.4 (tt, $J_{C\text{-}F}$ = 303.4, 34.7 Hz), 121.4 (tquint, $J_{C\text{-}F}$ = 312.1, 38.5 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ 48.3–48.2 (m, 4F), −67.3–−67.4 (m, 2F), −90.2–−90.3 (m, 2F); MS (CI) *m*/*z* (%): 320 (100), 322 (36) $[M]^{\bullet+}$.

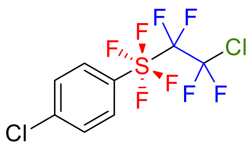
(2-Chloro-1,1,2,2-tetrafluoroethyl)tetrafluoro(4-fluorophenyl)-λ^6-sulfane (2b)



1b (0.25 M in EtOAc, 0.40 mmol, 1.0 equiv.), ADVN (9.9 mg, 0.040 mmol, 10 mol%), tetrafluoroethylene (1.0 atm) were engaged in the general procedure. The yield (72%) was determined by ^{19}F NMR analysis using 1,4-bis(trifluoromethyl)benzene as an internal standard. Purification by silica-gel column chromatography (5% EtOAc/hexane) gave the compound (70.8 mg, 54% yield) as a colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81–7.76 (m, 2H), 7.12 (dd (apparent t), *J* = 8.5 Hz, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.8 (d, $J_{C\text{-}F}$ = 253.0 Hz), 151.4 (quintd, $J_{C\text{-}F}$ = 21.1, 2.9 Hz), 128.6–128.4 (m), 124.2 (tt, $J_{C\text{-}F}$ = 303.4, 35.0 Hz), 121.4 (tquint, $J_{C\text{-}F}$ = 311.5, 38.6 Hz), 115.8 (d, $J_{C\text{-}F}$ = 23.0 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ 49.7–49.5 (m, 4F), −67.4–−67.5 (m, 2F), −90.1–−90.3 (m, 2F), −107.2 (s, 1F); MS (CI) *m*/*z* (%): 338 (100), 340 (32) $[M]^{\bullet+}$.

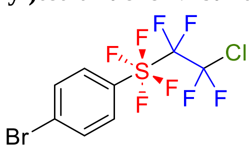
(2-Chloro-1,1,2,2-tetrafluoroethyl)(4-chlorophenyl)tetrafluoro-λ^6-sulfane (2c)



1c (0.25 M in EtOAc, 1.0 mmol, 1.0 equiv.), ADVN (24.8 mg, 0.10 mmol, 10 mol%), tetrafluoroethylene (1.0 atm) were engaged in the general procedure. The yield (82%) was determined by ^{19}F NMR analysis using 1,4-bis(trifluoromethyl)benzene as an internal standard. Purification by silica-gel column chromatography (5% EtOAc/hexane) gave the compound (236 mg, 67% yield) as a colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 (d, *J* = 8.7 Hz, 2H), 7.39 (d, *J* = 9.1 Hz, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 153.9 (quint, $J_{C\text{-}F}$ = 21.1 Hz), 137.9, 129.0, 127.5 (quint, $J_{C\text{-}F}$ = 5.1 Hz), 122.4 (tt, $J_{C\text{-}F}$ = 303.2, 35.2 Hz), 121.4 (tquint, $J_{C\text{-}F}$ = 311.9, 38.2 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ 49.0–48.9 (m, 4F), −67.5–−67.6 (m, 2F), −90.2–−90.3 (m, 2F); MS (CI) *m*/*z* (%): 354 (100), 356 (63), 358 (13) $[M]^{\bullet+}$.

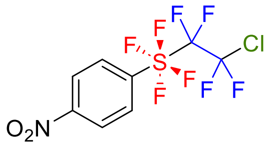
(4-Bromophenyl)(2-chloro-1,1,2,2-tetrafluoroethyl)tetrafluoro-λ^6-sulfane (2d)



1d (0.25 M in EtOAc, 1.0 mmol, 1.0 equiv.), ADVN (24.8 mg, 0.10 mmol, 10 mol%), tetrafluoroethylene (1.0 atm) were engaged in the general procedure. The yield (85%) was determined by ^{19}F NMR analysis using 1,4-bis(trifluoromethyl)benzene as an internal standard. Purification by silica-gel column chromatography (5% EtOAc/hexane) gave the compound (271 mg, 68% yield) as a colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (d, *J* = 8.7 Hz, 2H), 7.56 (d, *J* = 8.7 Hz, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 154.5 (quint, $J_{C\text{-}F}$ = 21.2 Hz), 132.0, 127.7 (quint, $J_{C\text{-}F}$ = 5.0 Hz), 126.1, 122.3 (tt, $J_{C\text{-}F}$ = 303.8, 35.5 Hz), 121.4 (tquint, $J_{C\text{-}F}$ = 311.5, 38.3 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ 48.9–48.7 (m, 4F), −67.5–−67.6 (m, 2F), −90.1–−90.3 (m, 2F); MS (CI) *m*/*z* (%): 398 (77), 400 (100), 402 (28) $[M]^{\bullet+}$.

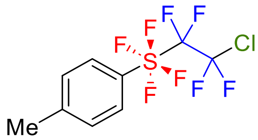
(2-Chloro-1,1,2,2-tetrafluoroethyl)tetrafluoro(4-nitrophenyl)-λ⁶-sulfane (2e)



1e (0.25 M in EtOAc, 0.40 mmol, 1.0 equiv.), ADVN (9.9 mg, 0.040 mmol, 10 mol%), tetrafluoroethylene (1.0 atm) were engaged in the general procedure. The yield (80%) was determined by ^{19}F NMR analysis using 1,4-bis(trifluoromethyl)benzene as an internal standard. Purification by silica-gel column chromatography (10% EtOAc/hexane) gave the compound (88.6 mg, 61% yield) as a colorless solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.33 (d, J = 8.7 Hz, 2H), 8.00 (d, J = 9.2 Hz, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.4 (quint, $J_{C\text{-}F}$ = 22.2 Hz), 149.2, 127.7 (quint, $J_{C\text{-}F}$ = 4.8 Hz), 124.2, 122.1 (tt, $J_{C\text{-}F}$ = 303.4, 34.7 Hz), 121.3 (tquint, $J_{C\text{-}F}$ = 312.1, 37.6 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ 48.7–48.5 (m, 4F), −67.5–−67.6 (m, 2F), −90.0–−90.2 (m, 2F); MS (CI) m/z (%): 366 (100), 368 (31) $[M+H]^+$; Elemental analysis calcd (%) for $C_8H_4ClF_8N_2O_2S$: C 26.28, H 1.10, N 3.83, found: C 26.57, H 1.34, N 3.95.

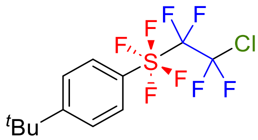
(2-Chloro-1,1,2,2-tetrafluoroethyl)tetrafluoro(*p*-tolyl)-λ⁶-sulfane (2f)



1f (0.25 M in EtOAc, 1.0 mmol, 1.0 equiv.), AIBN (16.4 mg, 0.10 mmol, 10 mol%), tetrafluoroethylene (1.0 atm) were engaged in the general procedure. Reaction temperature was 60 °C. The yield (69%) was determined by ^{19}F NMR analysis using 1,4-bis(trifluoromethyl)benzene as an internal standard. Purification by silica-gel column chromatography (5% EtOAc/hexane) gave the compound (225 mg, 67% yield) as a colorless solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 (d, J = 8.7 Hz, 2H), 7.24 (d, J = 8.2 Hz, 2H), 2.40 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 153.4 (quint, $J_{C\text{-}F}$ = 19.3 Hz), 142.1, 129.3, 125.9 (quint, $J_{C\text{-}F}$ = 4.8 Hz), 122.4 (tt, $J_{C\text{-}F}$ = 303.4, 35.2 Hz), 121.4 (tquint, $J_{C\text{-}F}$ = 311.6, 38.5 Hz), 21.2; ^{19}F NMR (376 MHz, $CDCl_3$) δ 48.9–48.8 (m, 4F), −67.3 (m, 2F), −90.1–−90.3 (m, 2F); MS (CI) m/z (%): 334 (100), 336 (35) $[M]^{\bullet+}$; Elemental analysis calcd (%) for $C_9H_7ClF_8S$: C 32.30, H 2.11, found: C 32.60, H 2.32.

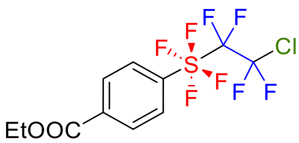
(4-(*tert*-Butyl)phenyl)(2-chloro-1,1,2,2-tetrafluoroethyl)tetrafluoro-λ⁶-sulfane (2g)



1g (0.25 M in EtOAc, 1.0 mmol, 1.0 equiv.), ADVN (24.8 mg, 0.10 mmol, 10 mol%), tetrafluoroethylene (1.0 atm) were engaged in the general procedure. The yield (87%) was determined by ^{19}F NMR analysis using 1,4-bis(trifluoromethyl)benzene as an internal standard. Purification by silica-gel column chromatography (5% EtOAc/hexane) gave the compound (132 mg, 70% yield) as a colorless solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 (d, J = 9.2 Hz, 2H), 7.45 (d, J = 8.2 Hz, 2H), 1.33 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 155.2, 153.3 (quint, $J_{C\text{-}F}$ = 19.3 Hz), 125.8–125.6 (m, overlapped), 122.4 (tt, $J_{C\text{-}F}$ = 304.4, 35.2 Hz), 121.4 (tquint, $J_{C\text{-}F}$ = 311.6, 38.8 Hz), 35.1, 31.2; ^{19}F NMR (376 MHz, $CDCl_3$) δ 48.9–48.8 (m, 4F), −67.3 (m, 2F), −90.1–−90.3 (m, 2F); MS (CI) m/z (%): 376 (100), 378 (31) $[M]^{\bullet+}$; Elemental analysis calcd (%) for $C_{12}H_{13}ClF_8S$: C 38.26, H 3.48, found: C 38.48, H 3.65.

Ethyl 4-((2-chloro-1,1,2,2-tetrafluoroethyl)tetrafluoro-λ⁶-sulfanyl)benzoate (2h)

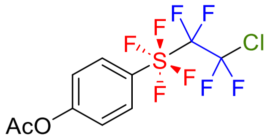


1h (0.25 M in EtOAc, 0.50 mmol, 1.0 equiv.), ADVN (12.4 mg, 0.050 mmol, 10 mol%), tetrafluoroethylene (1.0 atm) were engaged in the general procedure. The yield (82%) was determined by ^{19}F NMR analysis using 1,4-bis(trifluoromethyl)benzene as an internal standard. Purification by silica-gel column chromatography (10% EtOAc/hexane) gave the compound (146 mg, 74% yield) as a colorless solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13 (d, J = 8.2 Hz, 2H), 7.86 (d, J = 8.2 Hz, 2H), 4.42 (q, J = 7.0 Hz, 2H), 1.42 (t, J = 7.1 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.0, 158.6 (quint, $J_{C\text{-}F}$ = 20.7 Hz), 133.4, 130.1, 126.2 (quint, $J_{C\text{-}F}$ = 4.8 Hz), 122.4 (tt,

J_{C-F} = 302.5, 34.7 Hz), 121.3 (tquint, J_{C-F} = 312.1, 38.5 Hz), 61.8, 14.4; ^{19}F NMR (376 MHz, $CDCl_3$) δ 48.2–48.1 (m, 4F), −67.4–−67.5 (m, 2F), −90.1–−90.3 (m, 2F); MS (CI) *m/z* (%): 393 (100), 395 (31) $[M+H]^+$; Elemental analysis calcd (%) for $C_{11}H_9ClF_8O_2S$: C 33.65, H 2.31, found: C 33.61, H 2.51.

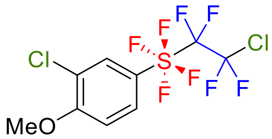
4-((2-Chloro-1,1,2,2-tetrafluoroethyl)tetrafluoro-λ^6-sulfanyl)phenyl acetate (2i)



1i (0.25 M in EtOAc, 0.60 mmol, 1.0 equiv.), ADVN (14.9 mg, 0.060 mmol, 10 mol%), tetrafluoroethylene (1.0 atm) were engaged in the general procedure. The yield (87%) was determined by ^{19}F NMR analysis using 1,4-bis(trifluoromethyl)benzene as an internal standard. Purification by silica-gel column chromatography (10% EtOAc/hexane) gave the compound (164 mg, 72% yield) as a colorless solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 (d, *J* = 9.2 Hz, 2H), 7.20 (d, *J* = 8.7 Hz, 2H), 2.32 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.9, 152.7 (quint, J_{C-F} = 20.6 Hz), 152.5, 127.6 (quint, J_{C-F} = 4.8 Hz), 122.3 (tt, J_{C-F} = 303.4, 35.0 Hz), 121.9, 121.3 (tquint, J_{C-F} = 311.5, 38.3 Hz), 21.2; ^{19}F NMR (376 MHz, $CDCl_3$) δ 49.3–49.2 (m, 4F), −67.4 (m, 2F), −90.1–−90.3 (m, 2F); MS (CI) *m/z* (%): 379 (100), 381 (37) $[M+H]^+$; Elemental analysis calcd (%) for $C_{10}H_7ClF_8O_2S$: C 31.72, H 1.86, found: C 32.06, H 2.11.

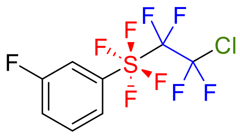
(2-Chloro-1,1,2,2-tetrafluoroethyl)(3-chloro-4-methoxyphenyl)tetrafluoro-λ^6-sulfane (2j)



1j (0.25 M in EtOAc, 0.20 mmol, 1.0 equiv.), ADVN (14.9 mg, 0.060 mmol, 30 mol%), tetrafluoroethylene (1.0 atm) were engaged in the general procedure. The yield (79%) was determined by ^{19}F NMR analysis using 1,4-bis(trifluoromethyl)benzene as an internal standard. Purification by silica-gel column chromatography (5% EtOAc/hexane) and HPLC (70–99% MeCN/H_2O) gave the compound (29.9 mg, 39% yield) as a colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82 (d, *J* = 2.7 Hz, 1H), 7.67 (dd, *J* = 9.2, 2.7 Hz, 1H), 6.94 (d, *J* = 9.2 Hz, 1H), 3.96 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.1, 148.1 (quint, J_{C-F} = 21.6 Hz), 128.2 (quint, J_{C-F} = 5.1 Hz), 125.9 (quint, J_{C-F} = 5.1 Hz), 122.4, 122.3 (tt, J_{C-F} = 303.4, 36.1 Hz), 121.3 (tquint, J_{C-F} = 311.6, 38.4 Hz), 110.9, 56.6; ^{19}F NMR (376 MHz, $CDCl_3$) δ 50.2–50.0 (m, 4F), −67.3–−67.5 (m, 2F), −90.1–−90.2 (m, 2F); MS (CI) *m/z* (%): 384 (100), 386 (65), 388 (15) $[M]^{•+}$.

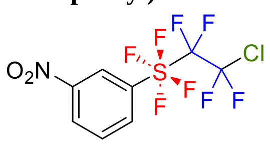
(2-Chloro-1,1,2,2-tetrafluoroethyl)tetrafluoro(3-fluorophenyl)-λ^6-sulfane (2k)



1k (0.25 M in EtOAc, 1.0 mmol, 1.0 equiv.), ADVN (24.8 mg, 0.10 mmol, 10 mol%), tetrafluoroethylene (1.0 atm) were engaged in the general procedure. The yield (81%) was determined by ^{19}F NMR analysis using 1,4-bis(trifluoromethyl)benzene as an internal standard. Purification by silica-gel column chromatography (5% EtOAc/hexane) gave the compound (262 mg, 77% yield) as a colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 (dd, *J* = 8.2, 1.8 Hz, 1H), 7.52 (dt, *J* = 4.6, 2.3 Hz, 1H), 7.47–7.41 (m, 1H), 7.22 (td, *J* = 8.0, 2.3 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.8 (d, J_{C-F} = 250.5 Hz), 151.4 (quintd, J_{C-F} = 21.4, 7.7 Hz), 130.1 (d, J_{C-F} = 7.7 Hz), 122.3 (tt, J_{C-F} = 303.9, 35.2 Hz), 121.9–121.8 (m), 121.3 (tquint, J_{C-F} = 311.6, 38.1 Hz), 118.9 (d, J_{C-F} = 21.2 Hz), 114.3 (dquint, J_{C-F} = 26.0, 5.1 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ 48.7–48.5 (m, 4F), −67.4–−67.5 (m, 2F), −90.2–−90.4 (m, 2F), −109.8 (s, 1F); MS (CI) *m/z* (%): 338 (100), 340 (37) $[M]^{•+}$.

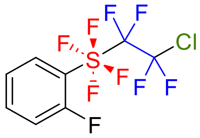
(2-Chloro-1,1,2,2-tetrafluoroethyl)tetrafluoro(3-nitrophenyl)-λ^6-sulfane (2l)



1l (0.25 M in EtOAc, 1.0 mmol, 1.0 equiv.), ADVN (24.8 mg, 0.10 mmol, 10 mol%), tetrafluoroethylene (1.0 atm) were engaged in the general procedure. The yield (70%) was determined by ^{19}F NMR analysis using 1,4-bis(trifluoromethyl)benzene

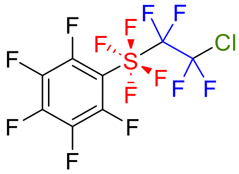
as an internal standard. Purification by silica-gel column chromatography (10% EtOAc/hexane) gave the compound (246 mg, 67% yield) as a colorless oil.
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.68 (t, J = 2.1 Hz, 1H), 8.41 (d, J = 8.2 Hz, 1H), 8.14 (d, J = 8.2 Hz, 1H), 7.73 (t, J = 8.2 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 155.7 (quint, J_{C-F} = 23.0 Hz), 148.0, 131.8 (quint, J_{C-F} = 4.8 Hz), 130.1, 126.4, 122.1 (tt, J_{C-F} = 303.4, 34.5 Hz), 121.9 (quint, J_{C-F} = 5.3 Hz), 121.3 (tquint, J_{C-F} = 311.5, 37.4 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ 48.9–48.7 (m, 4F), −67.6 (m, 2F), −90.1–−90.3 (m, 2F); MS (CI) m/z (%): 366 (100), 368 (37) $[M+H]^+$.

(2-Chloro-1,1,2,2-tetrafluoroethyl)tetrafluoro(2-fluorophenyl)-λ⁶-sulfane (2m)



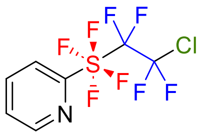
1m (0.25 M in EtOAc, 0.50 mmol, 1.0 equiv.), ADVN (12.4 mg, 0.050 mmol, 10 mol%), tetrafluoroethylene (1.0 atm) were engaged in the general procedure. The yield (77%) was determined by ^{19}F NMR analysis using 1,4-bis(trifluoromethyl)benzene as an internal standard. Purification by silica-gel column chromatography (5% EtOAc/hexane) gave the compound (118 mg, 70% yield) as a colorless oil.
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80–7.76 (m, 1H), 7.50 (dd, J = 12.4, 7.6 Hz, 1H), 7.24–7.17 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 155.9 (d, J_{C-F} = 260.6 Hz), 151.4 (quintd, J_{C-F} = 21.6, 11.1 Hz), 133.7 (d, J_{C-F} = 9.2 Hz), 128.6 (quint, J_{C-F} = 5.3 Hz), 124.1 (d, J_{C-F} = 3.9 Hz), 122.3 (tt, J_{C-F} = 303.4, 34.7 Hz), 121.2 (tquint, J_{C-F} = 311.4, 37.9 Hz), 118.1 (d, J_{C-F} = 11.8 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ 53.1–52.9 (m, 4F), −67.4–−67.5 (m, 2F), −90.8–−90.9 (m, 2F), −107.2–−107.5 (m, 1F); MS (CI) m/z (%): 338 (100), 340 (35) $[M]^{\bullet+}$.

(2-Chloro-1,1,2,2-tetrafluoroethyl)tetrafluoro(perfluorophenyl)-λ⁶-sulfane (2n)



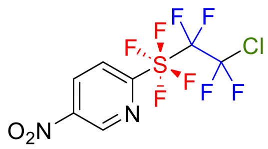
1n (0.50 M in EtOAc, 0.90 mmol, a mixture of *cis*/*trans* isomer (39/61), 1.0 equiv.), ADVN (22.4 mg, 0.090 mmol, 10 mol%), tetrafluoroethylene (1.0 atm) were engaged in the general procedure. The yield (44%) was determined by ^{19}F NMR analysis using 1,4-bis(trifluoromethyl)benzene as an internal standard. Purification by silica-gel column chromatography (5% EtOAc/hexane) gave the compound (119 mg, 32% yield) as a colorless oil.
^{13}C NMR (101 MHz, $CDCl_3$) δ 145.1–142.1 (m, overlapped), 139.4–136.5 (m), 128.8–128.0 (m), 121.9 (tt, J_{C-F} = 303.4, 34.7 Hz), 120.9 (tquint, J_{C-F} = 311.4, 36.0 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ 59.4–59.1 (m, 4F), −67.8–−67.9 (m, 2F), −91.3–−91.5 (m, 2F), −132.1–−132.5 (m, 2F), −146.6–−146.7 (m, 1F), −158.7–−158.9 (m, 2F); MS (CI) m/z (%): 410 (100), 412 (33) $[M]^{\bullet+}$.

2-((2-Chloro-1,1,2,2-tetrafluoroethyl)tetrafluoro-λ⁶-sulfanyl)pyridine (2o)



1o (0.25 M in EtOAc, 1.0 mmol, 1.0 equiv.), ADVN (24.8 mg, 0.10 mmol, 10 mol%), tetrafluoroethylene (1.0 atm) were engaged in the general procedure. The yield (73%) was determined by ^{19}F NMR analysis using 1,4-bis(trifluoromethyl)benzene as an internal standard. Purification by silica-gel column chromatography (10% EtOAc/hexane) gave the compound (220 mg, 68% yield) as a colorless oil.
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.58 (d, J = 4.6 Hz, 1H), 7.93 (t, J = 7.6 Hz, 1H), 7.78 (d, J = 8.2 Hz, 1H), 7.50 (dd, J = 7.3, 4.8 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.8 (quint, J_{C-F} = 25.4 Hz), 148.1, 139.0, 127.0, 122.3 (tt, J_{C-F} = 303.7, 35.4 Hz), 121.5 (quint, J_{C-F} = 4.3 Hz), 121.1 (tquint, J_{C-F} = 311.2, 37.6 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ 38.1–38.0 (m, 4F), −67.4 (m, 2F), −90.5–−90.7 (m, 2F); MS (CI) m/z (%): 322 (100), 324 (39) $[M+H]^+$.

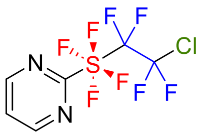
2-((2-Chloro-1,1,2,2-tetrafluoroethyl)tetrafluoro-λ⁶-sulfanyl)-5-nitropyridine (2p)



1p (0.25 M in EtOAc, 0.70 mmol, 1.0 equiv.), ADVN (17.4 mg, 0.070 mmol, 10 mol%), tetrafluoroethylene (1.0 atm) were engaged in the general procedure. The yield (53%) was determined by ^{19}F NMR analysis using 1,4-bis(trifluoromethyl)benzene as an internal standard. Purification by silica-gel column chromatography (10% EtOAc/hexane) gave the compound (113 mg, 44% yield) as a colorless solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.39 (d, J = 2.7 Hz, 1H), 8.73 (dd, J = 8.9, 2.5 Hz, 1H), 8.03 (d, J = 8.9 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.1 (quint, $J_{C\text{-}F}$ = 27.7 Hz), 145.4, 143.9, 134.3, 122.5 (m), 122.0 (tt, $J_{C\text{-}F}$ = 303.7, 35.2 Hz), 121.0 (tquint, $J_{C\text{-}F}$ = 312.1, 36.1 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ 39.2–39.1 (m, 4F), −67.6–−67.7 (m, 2F), −90.5–−90.6 (m, 2F); MS (CI) m/z (%): 367 (100), 369 (33) $[M+H]^+$; Elemental analysis calcd (%) for $C_7H_3ClF_8N_2O_2S$: C 22.93, H 0.82, N 7.64, found: C 23.39, H 1.17, N 7.48.

2-((2-Chloro-1,1,2,2-tetrafluoroethyl)tetrafluoro-λ^6-sulfanyl)pyrimidine (2q)

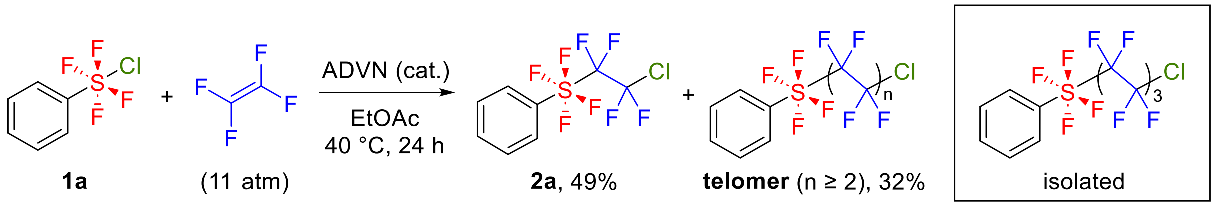


1q (0.50 M in EtOAc, 1.0 mmol, 1.0 equiv.), ADVN (24.8 mg, 0.10 mmol, 10 mol%), tetrafluoroethylene (1.0 atm) were engaged in the general procedure. The yield (93%) was determined by ^{19}F NMR analysis using 1,4-bis(trifluoromethyl)benzene as an internal standard. Purification by silica-gel column chromatography (50% EtOAc/hexane) gave the compound (291 mg, 90% yield) as a colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.93 (d, J = 5.0 Hz, 2H), 7.57 (t, J = 4.6 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.2 (quint, $J_{C\text{-}F}$ = 30.4 Hz), 158.9, 123.7, 122.2 (tt, $J_{C\text{-}F}$ = 303.4, 35.0 Hz), 120.8 (tquint, $J_{C\text{-}F}$ = 310.5, 36.9 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ 33.7–33.6 (m, 4F), −67.5–−67.6 (m, 2F), −91.0–−91.2 (m, 2F); MS (CI) m/z (%): 323 (100), 325 (35) $[M+H]^+$.

1.5. Telomerization Reaction

Experimental procedure



To a solution of **1a** (1.0 mmol, 1.0 equiv.) in EtOAc (0.25 M) was added ADVN (24.8 mg, 0.10 mmol, 10 mol%). After several freeze–degas–thaw cycles on a vacuum line, tetrafluoroethylene (11 atm) was charged to the solution. The reaction mixture was then stirred at 40 °C on the oil bath for 24 h. Upon reaction completion, the atmosphere of the vial was vented carefully and the yield was determined by ^{19}F NMR analysis using 1,4-bis(trifluoromethyl)benzene as an internal standard. The insoluble solid was removed by filtration, and the filtrate was evaporated under reduced pressure. The crude product was subjected to flash silica-gel column chromatography (5% EtOAc/hexane) to afford the mixture of **2a** and **telomer**. Further purification by HPLC (80% MeOH/H_2O) gave the trimer (19.0 mg, 4% yield) as a colorless solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80 (d, J = 8.0 Hz, 2H), 7.53–7.45 (m, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 155.7 (quint, $J_{C\text{-}F}$ = 19.1 Hz), 131.7, 128.9, 126.1 (quint, $J_{C\text{-}F}$ = 5.1 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ 47.4–47.2 (m, 4F), −67.9 (t, J = 13.4 Hz, 2F), −90.4–−90.7 (m, 2F), −119.9 (m, 2F), −120.8–−120.9 (m, 4F), −121.5 (m, 2F); MS (CI) m/z (%): 520 (100), 522 (31) $[M]^{\bullet+}$.

Fluorinated carbons could not be observed because of low intensity. HRMS (ESI(+), ESI(−), APCI(+), and APCI(−)) data were not available due to the difficult ionization of hexacoordinated sulfur fluorides.[12]

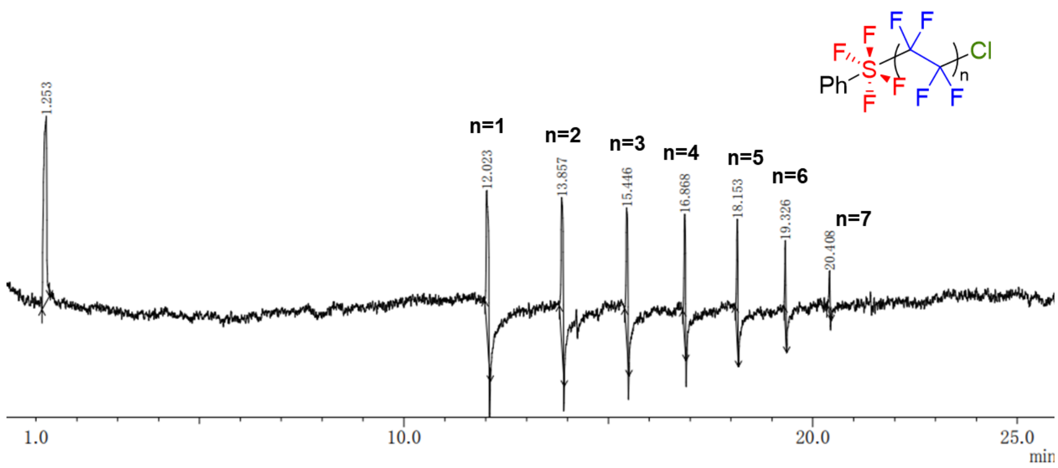
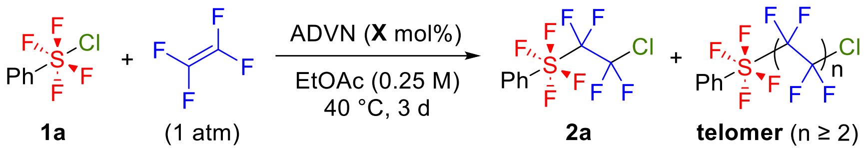


Figure S1. GC spectrum of the mixture of **2a** (n = 1) and **telomer** (n ≥ 2). The parent MS of **telomer** (n = 6, 7) could not be detected.

Table S3. Effect of an amount of the radical initiator on telomerization selectivity.

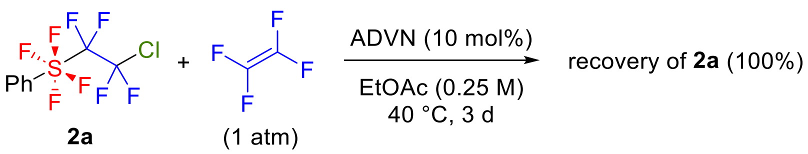


Entry	X	Yield [%][a]	
		2a	**telomer**
1	10	88	4
2	50	67	2
3[b]	50	63	2
4	100	65	2
5[b]	100	65	2

[a] Determined by ^{19}F NMR analysis of the crude mixture relative to an internal standard (1,4-bis(trifluoromethyl)benzene). [b] Reaction time: 20 h.

Telomerization experiment from 2a

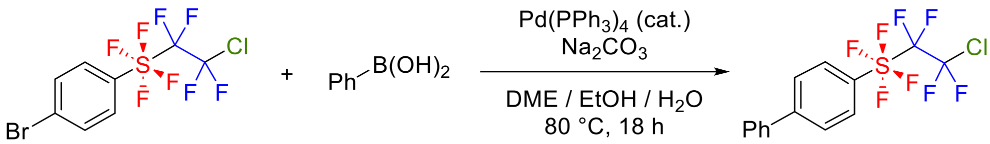
A control experiment was performed in order to confirm whether **2a** is still active or not. The reaction was carried out according to the general procedure of single addition reactions. **2a** (0.25 M in EtOAc, 0.10 mmol, 1.0 equiv.), ADVN (2.5 mg, 0.010 mmol, 10 mol%), tetrafluoroethylene (1.0 atm) were engaged and the reaction mixture was stirred at 40 °C on the oil bath for 3 d, but no change was observed in ^{19}F NMR analysis. This control experiment showed that this condition is effective only for the activation of S–Cl bond.



Scheme S2. An attempt of an addition reaction from **2a**. Tribromofluoromethane was used as an internal standard.

1.6. Transformation of Compounds 2

[1,1'-Biphenyl]-4-yl(2-chloro-1,1,2,2-tetrafluoroethyl)tetrafluoro-λ^6-sulfane (2r)

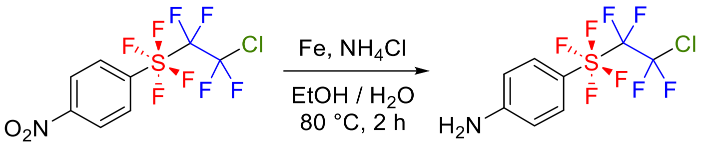


2d **2r**, 92%

A vial was charged with $Pd(PPh_3)_4$ (17.2 mg, 0.015 mmol, 3 mol%), **2d** (199 mg, 0.50 mmol, 1.0 equiv.) and 1,2-dimethoxyethane (1.0 mL). The mixture was stirred at ambient temperature for 10 minutes. To this mixture, a solution of phenylboronic acid (67.1 mg, 0.55 mmol, 1.1 equiv.) in EtOH (0.50 mL) and a solution of Na_2CO_3 (106 mg, 1.0 mmol, 2.0 equiv.) in H_2O (0.50 mL) were added. The reaction mixture was stirred at 80 °C for 18 h. Upon reaction completion, the reaction mixture was filtered over short pad of celite and the crude was extracted into EtOAc. The combined organic layers were washed with brine, dried over Na_2SO_4, filtered, and concentrated *in vacuo*. Purification by silica-gel column chromatography (5% EtOAc/hexane) gave the compound (182 mg, 92% yield) as a colorless solid.

^1H NMR (400 MHz, $CDCl_3$) δ 7.84–7.81 (m, 2H), 7.61 (d, J = 8.0 Hz, 2H), 7.57–7.55 (m, 2H), 7.47–7.38 (m, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 154.7 (quint, $J_{C\text{-}F}$ = 19.2 Hz), 144.6, 139.2, 129.2, 128.6, 127.4, 127.3, 126.5, 122.4 (tt, $J_{C\text{-}F}$ = 303.4, 36.9 Hz), 121.4 (tquint, $J_{C\text{-}F}$ = 312.0, 37.4 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ 49.0–48.8 (m, 4F), −67.3 (m, 2F), −90.0–−90.2 (m, 2F) ; MS (CI) *m/z* (%): 396 (100), 398 (39) $[M]^{\bullet+}$; Elemental analysis calcd (%) for $C_{14}H_9ClF_8S$: C 42.39, H 2.29, found: C 42.59, H 2.49.

4-((2-Chloro-1,1,2,2-tetrafluoroethyl)tetrafluoro-λ^6-sulfanyl)aniline (2s)

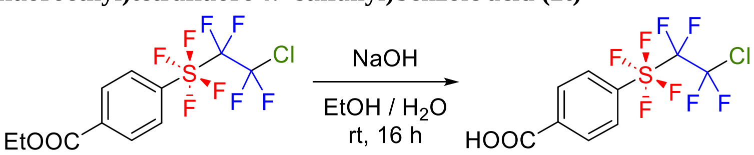


2e **2s**, 99%

A suspension of iron (280 mg, 5.0 mmol, 10 equiv.) and **2e** (199 mg, 0.50 mmol, 1.0 equiv.) in EtOH (7.5 mL) was heated at 80 °C. To this mixture, an aqueous solution of NH_4Cl (2.0 M, 2.5 mL) was added. The resulting suspension was stirred at 80 °C for 2 h. Upon reaction completion, the reaction mixture was basified with a saturated aqueous solution of Na_2CO_3, filtered through a short pad of celite, and extracted into CH_2Cl_2. The combined organic layers were washed with brine, dried over Na_2SO_4, filtered, and concentrated *in vacuo*. Purification by silica-gel column chromatography (20% EtOAc/hexane) gave the compound (167 mg, 99% yield) as a pale-yellow oil.

^1H NMR (400 MHz, $CDCl_3$) δ 7.53 (d, J = 9.2 Hz, 2H), 6.56 (d, J = 9.2 Hz, 2H), 3.95 (s, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 149.1, 146.3 (quint, $J_{C\text{-}F}$ = 19.9 Hz), 127.5 (quint, $J_{C\text{-}F}$ = 4.8 Hz), 122.5 (tt, $J_{C\text{-}F}$ = 303.4, 35.5 Hz), 121.5 (tquint, $J_{C\text{-}F}$ = 311.5, 39.1 Hz), 113.4; ^{19}F NMR (376 MHz, $CDCl_3$) δ 50.2–50.1 (m, 4F), −67.2–−67.3 (m, 2F), −90.0–−90.2 (m, 2F); HRMS (ESI-TOF): *m/z* calcd for $C_8H_7ClF_8NS$ $[M+H]^+$: 335.9860; found: 335.9846.

4-((2-Chloro-1,1,2,2-tetrafluoroethyl)tetrafluoro-λ^6-sulfanyl)benzoic acid (2t)

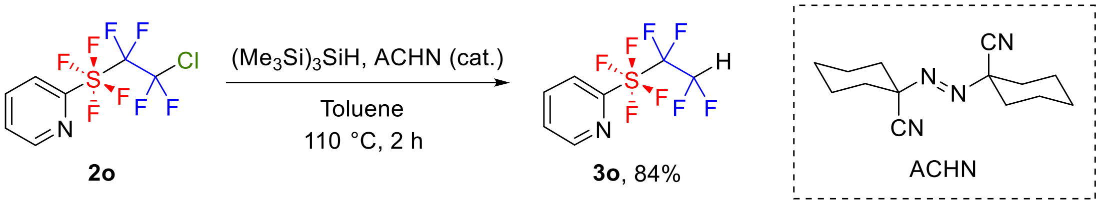


2h **2t**, 82%

A vial was charged with **2h** (39.3 mg, 0.10 mmol, 1.0 equiv.) and EtOH (1.0 mL). To this mixture, an aqueous solution of NaOH (2.0 M, 0.25 mL) was added. The reaction mixture was stirred at ambient temperature for 16 h. Upon reaction completion, the reaction mixture was acidified with an aqueous solution of 1N HCl, and extracted into EtOAc. The combined organic layers were washed with brine, dried over Na_2SO_4, filtered, and concentrated *in vacuo*. Purification by recrystallization (hexane) gave the compound (29.9 mg, 82% yield) as a colorless solid.

^1H NMR (400 MHz, DMSO-d_6) δ 8.13 (d, J = 8.7 Hz, 2H), 8.05 (d, J = 9.0 Hz, 2H); ^{13}C NMR (101 MHz, DMSO-d_6) δ 165.7, 157.4 (quint, $J_{C\text{-}F}$ = 18.8 Hz), 134.3, 130.4, 126.1 (quint, $J_{C\text{-}F}$ = 4.8 Hz), 121.6 (tt, $J_{C\text{-}F}$ = 301.5, 34.9 Hz), 120.8 (tquint, $J_{C\text{-}F}$ = 310.4, 38.3 Hz); ^{19}F NMR (376 MHz, DMSO-d_6) δ 48.6–48.4 (m, 4F), −67.8 (m, 2F), −90.2–−90.4 (m, 2F); MS (CI) *m/z* (%): 365 (100), 367 (38) $[M+H]^+$; Elemental analysis calcd (%) for $C_9H_5ClF_8O_2S$: C 29.65, H 1.38, found: C 29.30, H 1.66.

2-(Tetrafluoro(1,1,2,2-tetrafluoroethyl)-λ^6-sulfanyl)pyridine (3o)



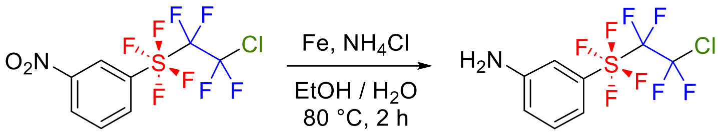
2o → **3o**, 84%

A vial was charged with **2o** (129 mg, 0.40 mmol, 1.0 equiv.) and toluene (2.0 mL). To this mixture, ACHN (19.5 mg, 0.080 mmol, 20 mol%) and $(Me_3Si)_3SiH$ (497 mg, 2.0 mmol, 5.0 equiv.) were added. The reaction mixture was stirred at 110 °C on the oil bath for 2 h. Upon reaction completion, the crude mixture was concentrated *in vacuo*. Purification by silica-gel column chromatography (50% EtOAc/hexane) gave the compound (96.5 mg, 84% yield) as a colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.58 (dd, J = 4.6, 1.4 Hz, 1H), 7.96-7.91 (m, 1H), 7.78 (d, J = 8.2 Hz, 1H), 7.50 (dd, J = 7.5, 4.8 Hz, 1H), 6.22 (tt, $J_{H\text{-}F}$ = 52.0, 5.6 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 167.0 (quint, $J_{C\text{-}F}$ = 25.9 Hz), 148.1, 139.0, 127.0, 122.9 (tquint, $J_{C\text{-}F}$ = 307.8, 34.7 Hz), 121.5 (quint, $J_{C\text{-}F}$ = 4.3 Hz), 108.3 (ttquint, $J_{C\text{-}F}$ = 256.0, 28.2, 4.2 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ 33.3–33.2 (m, 4F), −97.7–−97.9 (m, 2F), −133.6–−133.8 (m, 2F); MS (CI) m/z (%): 288 (100) $[M+H]^+$. *HRMS (ESI(+), ESI(−), APCI(+), and APCI(−)) data were not available due to the difficult ionization of hexacoordinated sulfur fluorides.*[12]

1.7. Synthesis of an Analog of Bioactive Molecules

3-((2-Chloro-1,1,2,2-tetrafluoroethyl)tetrafluoro-λ^6-sulfanyl)aniline (2u)

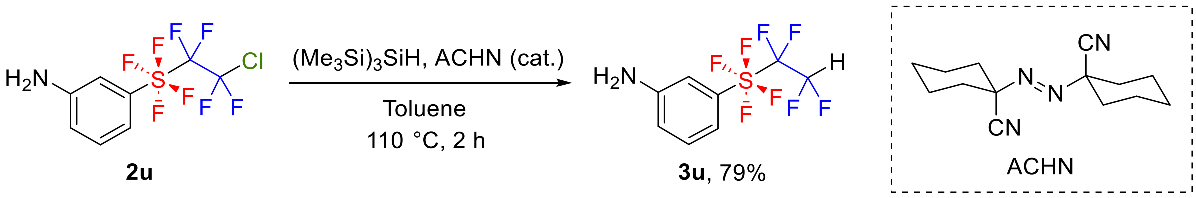


2l → **2u**, 90%

A suspension of iron (558 mg, 10.0 mmol, 10 equiv.) and **2l** (366 mg, 1.0 mmol, 1.0 equiv.) in EtOH (15 mL) was heated at 80 °C. To this mixture, an aqueous solution of NH_4Cl (2.0 M, 5.0 mL) was added. The resulting suspension was stirred at 80 °C for 2 h. Upon reaction completion, the reaction mixture was basified with a saturated aqueous solution of Na_2CO_3, filtered through a short pad of celite, and extracted into CH_2Cl_2. The combined organic layers were washed with brine, dried over Na_2SO_4, filtered, and concentrated *in vacuo*. Purification by silica-gel column chromatography (20% EtOAc/hexane) gave the compound (302 mg, 90% yield) as a pale-yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.20 (t, J = 8.1 Hz, 1H), 7.14 (ddd, J = 8.2, 2.1, 1.1 Hz, 1H), 7.07 (t, J = 2.1 Hz, 1H), 6.76 (d, J = 7.6 Hz, 1H), 3.82 (s, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 156.7 (quint, $J_{C\text{-}F}$ = 19.1 Hz), 146.8, 129.4, 122.4 (tt, $J_{C\text{-}F}$ = 303.4, 35.2 Hz), 121.3 (tquint, $J_{C\text{-}F}$ = 311.4, 38.8 Hz), 117.8, 115.8 (quint, $J_{C\text{-}F}$ = 5.2 Hz), 112.3 (quint, $J_{C\text{-}F}$ = 5.2 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ 48.1–47.9 (m, 4F), −67.3–−67.4 (m, 2F), −90.2–−90.4 (m, 2F); HRMS (ESI-TOF): m/z calcd for $C_8H_7ClF_8NS$ $[M+H]^+$: 335.9860; found: 335.9828.

3-(Tetrafluoro(1,1,2,2-tetrafluoroethyl)-λ^6-sulfanyl)aniline (3u)

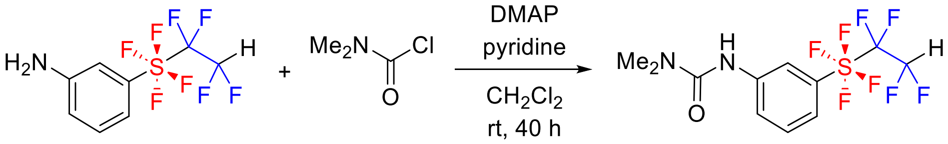


2u → **3u**, 79%

A vial was charged with **2u** (168 mg, 0.50 mmol, 1.0 equiv.) and toluene (2.5 mL). To this mixture, ACHN (24.4 mg, 0.10 mmol, 20 mol%) and $(Me_3Si)_3SiH$ (622 mg, 2.5 mmol, 5.0 equiv.) were added. The reaction mixture was stirred at 110 °C on the oil bath for 2 h. Upon reaction completion, the crude mixture was concentrated *in vacuo*. Purification by silica-gel column chromatography (33% EtOAc/hexane) gave the compound (119 mg, 79% yield) as a colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.18 (t, J = 8.0 Hz, 1H), 7.12 (dd, J = 8.2, 0.9 Hz, 1H), 7.06–7.05 (m, 1H), 6.74 (d, J = 7.6 Hz, 1H), 6.15 (tt, $J_{H\text{-}F}$ = 52.0, 5.5 Hz, 1H), 3.82 (s, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.1 (quint, $J_{C\text{-}F}$ = 19.5 Hz), 146.8, 129.4, 123.1 (tquintt, $J_{C\text{-}F}$ = 308.0, 37.1, 25.5 Hz), 117.7, 115.7 (quint, $J_{C\text{-}F}$ = 5.3 Hz), 112.2 (quint, $J_{C\text{-}F}$ = 5.2 Hz), 108.3 (ttquint, $J_{C\text{-}F}$ = 255.5, 28.2, 4.2 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ 43.1–43.0 (m, 4F), −97.4–−97.6 (m, 2F), −133.5–−133.8 (m, 2F); HRMS (ESI-TOF): m/z calcd for $C_8H_8F_8NS$ $[M+H]^+$: 302.0250; found: 302.0233.

1,1-Dimethyl-3-(3-(tetrafluoro(1,1,2,2-tetrafluoroethyl)-λ[6]-sulfanyl)phenyl)urea (3v)



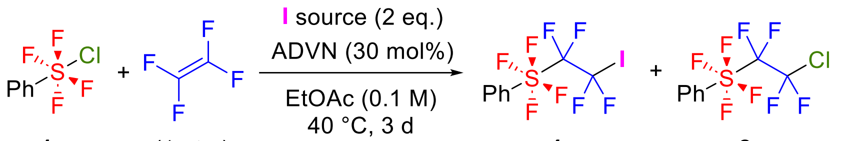
3u **3v**, 98%

A vial was charged with **3u** (30.1 mg, 0.10 mmol, 1.0 equiv.) and CH_2Cl_2 (0.2 mL). To this mixture, DMAP (12.2 mg, 0.10 mmol, 1 equiv.), dimethylcarbamoyl chloride (43.0 mg, 0.40 mmol, 4 equiv.), and pyridine (32 μL, 0.40 mmol, 4 equiv.) were added. The reaction mixture was stirred at room temperature for 40 h. Upon reaction completion, the reaction mixture was acidified with an aqueous solution of 2N HCl, and extracted into CH_2Cl_2. The combined organic layers were washed with brine, dried over Na_2SO_4, filtered, and concentrated *in vacuo*. Purification by silica-gel column chromatography (50% EtOAc/hexane) gave the compound (36.4 mg, 98% yield) as a colorless solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 (t, J = 2.1 Hz, 1H), 7.57 (d, J = 8.0 Hz, 1H), 7.42 (ddd, J = 8.2, 2.1, 1.0 Hz, 1H), 7.35 (t, J = 8.2 Hz, 1H), 6.44 (s, 1H), 6.16 (tt, J_{H-F} = 52.1, 5.7 Hz, 1H), 3.05 (s, 6H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 156.2 (quint, J_{C-F} = 20.1 Hz), 155.5, 139.8, 128.8, 123.1 (tt, J_{C-F} = 308.3, 36.6 Hz), 122.9, 120.1 (quint, J_{C-F} = 5.1 Hz), 117.5 (quint, J_{C-F} = 5.3 Hz), 108.3 (ttquint, J_{C-F} = 255.5, 28.2, 4.3 Hz), 36.5; ^{19}F NMR (376 MHz, $CDCl_3$) δ 43.5–43.4 (m, 4F), −97.3–−97.6 (m, 2F), −133.5–−133.7 (m, 2F); HRMS (ESI-TOF): m/z calcd for $C_{11}H_{13}F_8N_2OS$ $[M+H]^+$: 373.0621; found: 373.0614.

1.8. Synthesis of Tetrafluoro(perfluoroethyl)(phenyl)-λ[6]-sulfane

Table S4. Effect of iodinating agents on addition of **1a** to tetrafluoroethylene.

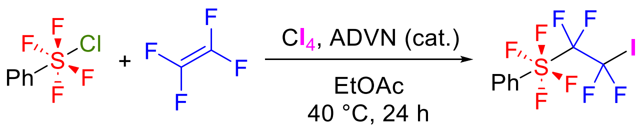


1a (1 atm) **4** **2a**

Entry	I source	Yield [%][a] 4	2a
1	1,3-Diiodo-5,5-dimethylhydantoin	43	9
2[b]	1,3-Diiodo-5,5-dimethylhydantoin	59	10
3	*N*-Iodosuccinimide	41	20
4	*N*-Iodophthalimide	44	23
5	I_2	27	24
6	Carbon tetraiodide	69	n.d.
7[c]	Carbon tetraiodide	65 (63[d])	n.d.

[a] Determined by ^{19}F NMR analysis relative to an internal standard (1,4-bis(trifluoromethyl)benzene). [b] 60 °C. [c] 24 h. [d] Isolated yield.

Tetrafluoro(1,1,2,2-tetrafluoro-2-iodoethyl)(phenyl)-λ[6]-sulfane (4)

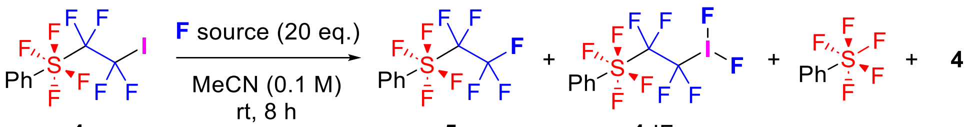


1a (1 atm) **4**

An oven-dried microwave vial was charged with a solution of **1a** (0.50 mmol, 1.0 equiv.) in EtOAc (5.0 mL). To this mixture, ADVN (37.3 mg, 0.15 mmol, 30 mol%) and carbon tetraiodide (520 mg, 1.0 mmol, 2.0 equiv.) were added. The reaction vial was cooled to 0 °C, charged with tetrafluoroethylene (1.0 atm) by bubbling, and sealed. The reaction mixture was stirred at 40 °C on the oil bath for 24 h. Upon reaction completion, the crude mixture was cooled down, poured onto water, and extracted into EtOAc. The combined organic layers were washed with a saturated aqueous solution of $Na_2S_2O_3$ and brine, dried over

Na_2SO_4, filtered, and concentrated *in vacuo*. Purification by silica-gel column chromatography (hexane) gave the compound (130 mg, 63% yield) as a colorless oil.
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79–7.76 (m, 2H), 7.51–7.42 (m, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 156.1 (quint, $J_{C\text{-}F}$ = 19.6 Hz), 131.6, 128.8, 126.1 (quint, $J_{C\text{-}F}$ = 5.1 Hz), 121.0 (tquint, $J_{C\text{-}F}$ = 308.7, 37.8 Hz), 93.5 (tt, $J_{C\text{-}F}$ = 324.4, 41.9 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ 50.0–49.8 (m, 4F), −57.2–−57.3 (m, 2F), −83.5–−83.7 (m, 2F); MS (CI) *m/z* (%): 285 (51) $[M{-}I]^+$, 393 (100) $[M{-}F]^+$.
HRMS (ESI(+), ESI(−), APCI(+), and APCI(−)) data were not available due to the difficult ionization of hexacoordinated sulfur fluorides.[12]

Table S5. Investigation of reaction conditions for fluorodeiodination of **4**.

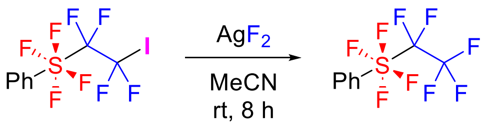


4 **5** **4**-IF_2

Entry	F source	Yield [%][a]			
		5	**4**-IF_2	$PhSF_5$	**4**
1	AgF_2	54 (53[b])	0	31	3
2[c]	AgF_2[d]	<1	0	<1	82
3[c]	AgF	0	0	0	72
4	XeF_2	7	15	5	23
5	XeF_2[d]	0	41	0	12
6[c,e]	AgF_2	0	0	0	0[f]

[a] Determined by ^{19}F NMR analysis relative to an internal standard (1,4-bis(trifluoromethyl)benzene). [b] Isolated yield. [c] Reaction time: 2 d. [d] 3 eq. of **F** source were added. [e] **2a** ($PhSF_4CF_2CF_2Cl$) was used instead of **4**. [f] 97% of **2a** was recovered.

Tetrafluoro(perfluoroethyl)(phenyl)-λ^6-sulfane (5)

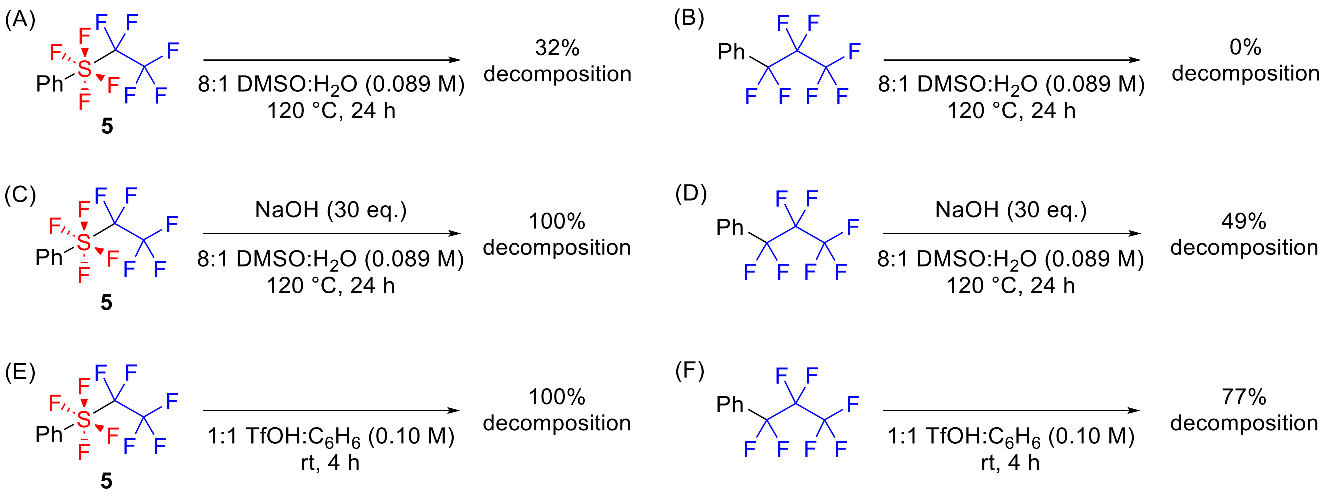


4 **5**

To a solution of **4** (0.40 mmol, 1.0 equiv.) in MeCN (4.0 mL) was added AgF_2 (1.17 g, 8.0 mmol, 20 equiv.). The reaction mixture was stirred at ambient temperature for 8 h. Upon reaction completion, the crude mixture was poured onto water, and extracted into Et_2O. The combined organic layers were washed with brine, dried over Na_2SO_4, filtered, and concentrated *in vacuo*. Purification by silica-gel column chromatography (pentane) gave the compound (64.2 mg, 53% yield) as a colorless oil.
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80–7.77 (m, 2H), 7.53–7.44 (m, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 155.6 (quint, $J_{C\text{-}F}$ = 19.6 Hz), 131.7, 128.9, 126.0 (quint, $J_{C\text{-}F}$ = 4.8 Hz), 119.7 (tquint, $J_{C\text{-}F}$ = 310.1, 40.7 Hz), 117.8 (qt, $J_{C\text{-}F}$ = 287.5, 33.6 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ 46.2–46.1 (m, 4F), −79.9–−80.0 (m, 3F), −95.6–−95.7 (m, 2F); MS (CI) *m/z* (%): 304 (100) $[M]^{\bullet+}$.
HRMS (ESI(+), ESI(−), APCI(+), and APCI(−)) data were not available due to the difficult ionization of hexacoordinated sulfur fluorides.[12]

1.9. Decomposition of 5 and $PhCF_2CF_2CF_3$

Degradation experiments were performed according to the previously reported conditions.[13,14] The decomposition ratio was determined by ^{19}F NMR analysis using trifluorotoluene or 4,4'-difluorobiphenyl as an internal standard.



Scheme S3. Decomposition reactions. (A and B) High temperature conditions without acids and bases. (C and D) Basic defluorination conditions.[13] (E and F) Protolytic defluorination conditions.[14]

1.10. X-ray Crystallographic Data

CCDC 2282789 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge via www.ccdc.cam.ac.uk/data_request/cif, or by emailing data_request@ccdc.cam.ac.uk, or by contacting The Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK; fax: +44 1223 336033.

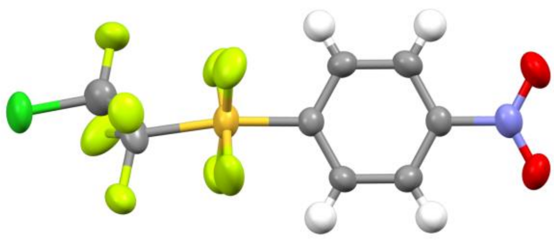


Figure S2. Molecular structure of **2e** with thermal ellipsoids at 50% probability.

Table S6. Crystallographic data and structure refinement details of **2e**.

	2e	
Formula	$C_8H_4ClF_8NO_2S$	
Formula weight	365.63	
Temperature	170 K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P\ 2_1/c$	
Unit cell dimensions	a = 8.9467(4) Å	α = 90 °
	b = 10.7344(4) Å	β = 101.742(4) °
	c = 12.9509(5) Å	γ = 90 °
Volume	1217.74(9) Å^3	
Z	4	
Density (calculated)	1.994 g/cm^3	
F(000)	720.0	

Crystal size	0.53 × 0.31 × 0.28 mm^3
Absorption coefficient	0.592 mm^{-1}
Absorption correction type	Multi-scan
Reflections collected	2487
Index ranges	$-11 \leq h \leq 11$, $-13 \leq k \leq 13$, $-16 \leq l \leq 16$
Theta range for data collection	2.325 to 26.366°
Independent reflections	2091
R_{int}	0.0146
Completeness to theta = 25.242°	1.000
Max. and min. transmission	1.00000 and 0.96086
Data / restraints / parameters	2487 / 24 / 254
Goodness-of-fit on F^2	1.057
R_1, wR_2 [I>2σ(I)]	0.0541, 0.1321
R_1, wR_2 (all data)	0.0639, 0.1402
Largest diff. peak and hole	0.862 and −0.715 e/$Å^3$

1.11. Determination of Hydrophobic Constants

All measurements were performed at least twice and the average value is shown. Calibration and determination of P_{OW} were performed according to guidelines.[15] Chlorobenzene, naphthalene, biphenyl, dibenzyl, fluoranthene and triphenylamine were chosen as standards.

Table S7. HPLC measurement for calibration.

	Retention time (t) [min]	k[a]	log k	log P_{OW}[b]
Thiourea	1.5865 (= t_0)			
Chlorobenzene	4.5905	1.893	0.277	2.89
Naphthalene	5.7745	2.640	0.422	3.30
Biphenyl	7.9890	4.036	0.606	4.01
Dibenzyl	12.0935	6.623	0.821	4.79
Fluoranthene	14.1615	7.926	0.899	5.16
Triphenylamine	21.6435	12.642	1.102	5.74

[a] $k = (t - t_0) / t_0$. [b] From ref. 16.

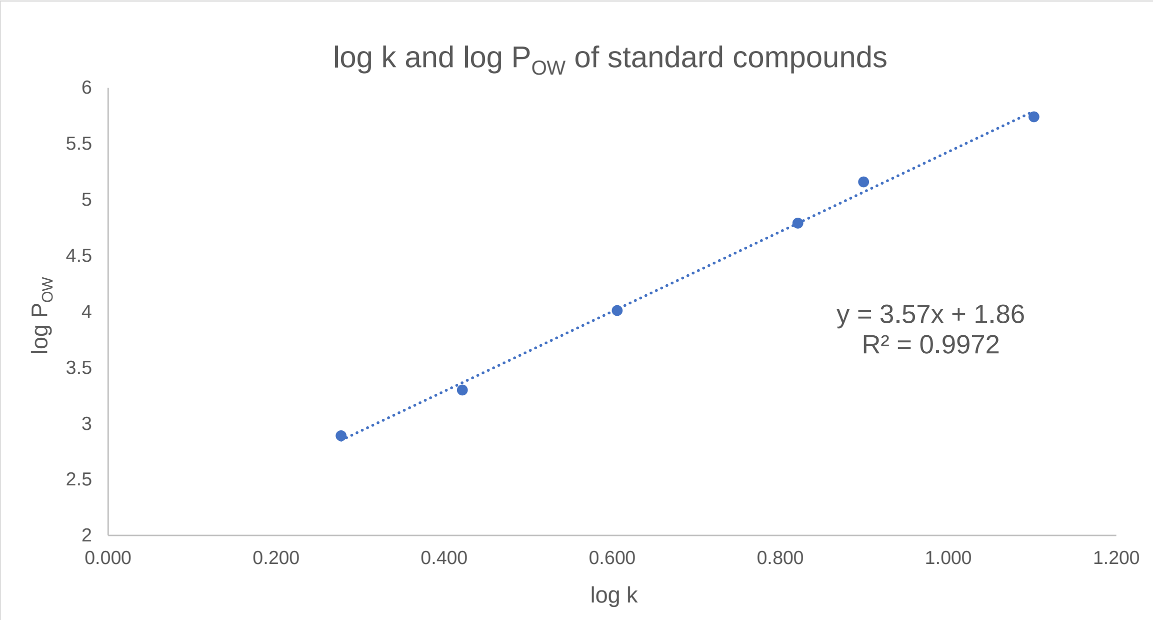


Figure S3. Calibration graph.

Table S8. HPLC measurement of test substances.

	Retention time (t) [min]	k[a]	log k	log P_{OW}	$\pi_{Ph}(R)$
2a	11.0155	5.943	0.774	4.62	2.49
5	9.9510	5.272	0.722	4.44	2.31
PhC_4F_9	11.8000	6.438	0.809	4.75	2.62
PhC_3F_7	8.1030	4.107	0.614	4.05	1.92

[a] $k = (t - t_0) / t_0$.

1.12. Determination of the Hammett Substituent Parameters

A sample of fluorobenzene, **2b** and **2k** in CD_3CN (ca. 0.02 M) were prepared containing α,α,α-trifluorotoluene (δ = −63.10 ppm). From the differences in chemical shifts (i.e. $\delta_H^{m\text{-}X}$ and $\delta_H^{p\text{-}X}$), the Hammett substituent parameters σ_I, σ_R^0, σ_m^0, and σ_p^0 were calculated using the method of Taft according to Eq. 1–4 *vide infra*.[17,18]

$$\delta_H^{m\text{-}X} = -7.10\sigma_I + 0.60 \quad (1)$$

$$\sigma_R^0 = -0.0339(\delta_H^{p\text{-}X} - \delta_H^{m\text{-}X}) \quad (2)$$

$$\sigma_m^0 = \sigma_I + 0.50\sigma_R^0 \quad (3)$$

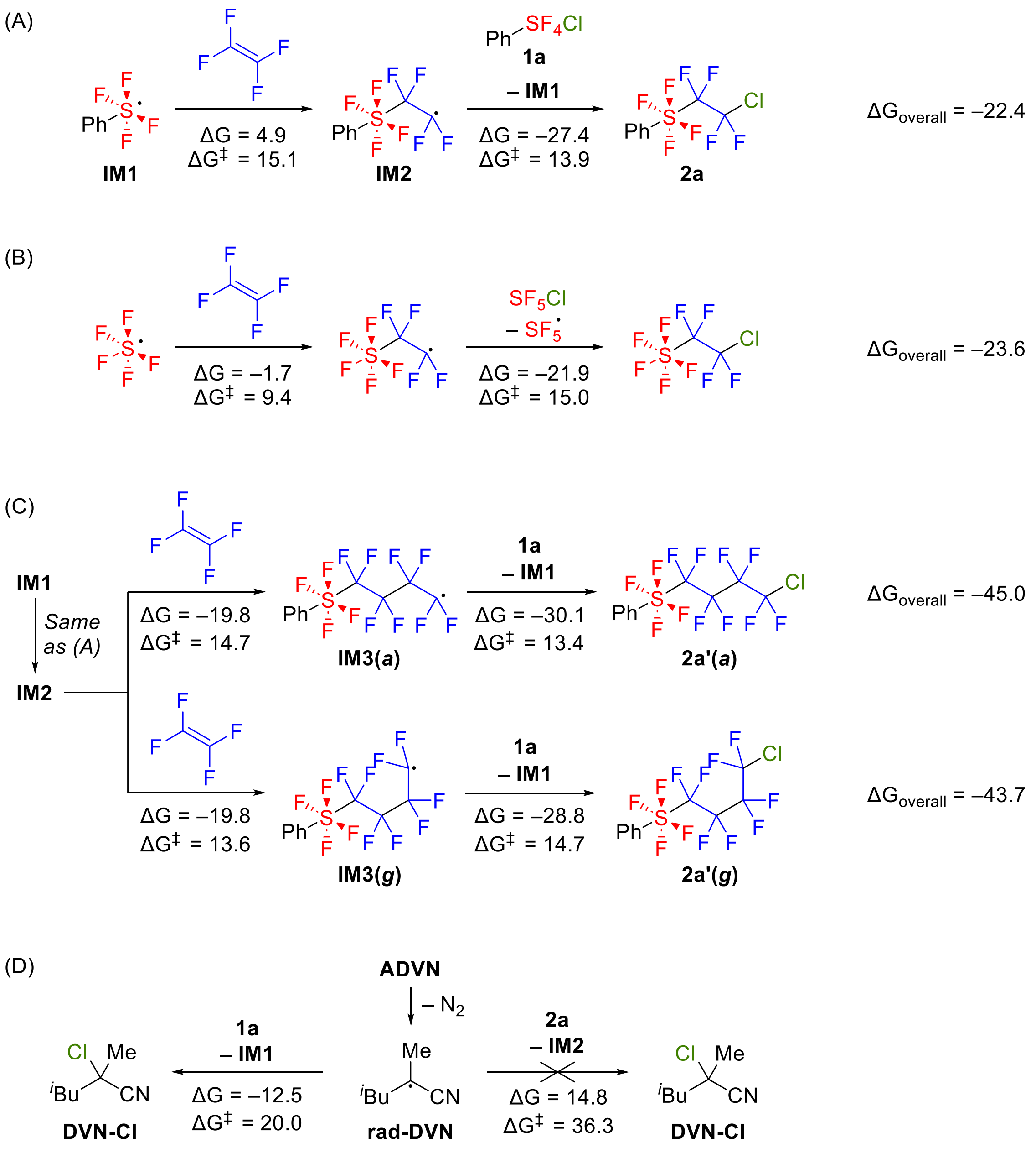
$$\sigma_p^0 = \sigma_I + \sigma_R^0 \quad (4)$$

2. Theoretical Calculations

2.1. General Information

All geometries and harmonic vibrational frequencies were calculated using density functional theory (DFT) in Gaussian9. [19] Calculations were carried out with the M06-2X/Def2TZVPP level of theory, and the added SMD solvation model for EtOAc.[20,21] Electronic energies and energy corrections were obtained using a standard state of 1 atm pressure and 298 K temperature.

2.2. Potential Energy Surface



Scheme S4. Free energy change and free energy of activation (in kcal mol^{-1}). (A) Addition reaction of **1a** to form **2a**. (B) Addition reaction of SF_5Cl to form $SF_5CF_2CF_2Cl$. (C) Addition reaction of **1a** to form **2a'**. (D) Initiation with ADVN.

2.3. Energies for All Reported Structures

	Sum of electronic and zero-point energies (a.u.)	Sum of electronic and thermal free energies (a.u.)
TFE	−475.543195	−475.571588
1a	−1489.258385	−1489.294602
2a	−1964.858608	−1964.901941
SF_5Cl	−1357.562363	−1357.591660
$SF_5CF_2CF_2Cl$	−1833.162565	−1833.200843
2a'(*a*)	−2440.457895	−2440.509446
2a'(*g*)	−2440.456859	−2440.507404
DVN-Cl	−788.716150	−788.752261
IM1	−1029.039094	−1029.075078
IM2	−1504.595781	−1504.638832
SF_5 radical	−897.334464	−897.363056
$SF_5CF_2CF_2$ radical	−1372.899770	−1372.937389
IM3(*a*)	−1980.191854	−1980.241921
IM3(*g*)	−1980.191911	−1980.241985
rad-DVN	−328.475956	−328.512785
TS TFE+IM1	−1504.578335	−1504.622679
TS 1a+IM2	−2993.850194	−2993.911335
TS TFE+SF_5	−1372.879675	−1372.919708
TS SF_5Cl+$SF_5CF_2CF_2$	−2730.454917	−2730.505131
TS TFE+IM2(*a*)	−1980.135413	−1980.187072
TS TFE+IM2(*g*)	−1980.136377	−1980.188791
TS 1a+IM3(*a*)	−3469.446575	−3469.515103
TS 1a+IM3(*g*)	−3469.445321	−3469.513094
TS 1a+DVN	−1817.722404	−1817.775549
TS 2a+DVN	−2293.296285	−2293.356853

2.4. Cartesian Coordinates of All Reported Structures

TFE

C	0.00000000	0.65718300	0.00000000
C	0.00000000	-0.65718300	0.00000000
F	1.09482500	-1.37977600	0.00000000
F	-1.09482500	-1.37977600	0.00000000
F	-1.09482500	1.37977600	0.00000000
F	1.09482500	1.37977600	0.00000000

1a

C	3.00234700	-1.20293600	-0.00000100
C	1.61516200	-1.21138800	0.00000500
C	0.94254800	0.00000200	-0.00000200
C	1.61516500	1.21138800	-0.00000100

C	3.00235100	1.20293200	0.00000300
C	3.69445300	-0.00000200	0.00000100
H	3.53907400	-2.14173500	-0.00000300
H	1.07590400	-2.14762000	0.00000300
H	1.07591100	2.14762300	-0.00000100
H	3.53907900	2.14173100	0.00000500
H	4.77626100	-0.00000500	0.00000100
S	-0.85869400	0.00000300	-0.00000500
F	-0.92128200	1.12916000	1.12936700
F	-0.92128300	-1.12912500	1.12939600
F	-0.92129400	1.12913300	-1.12940500
F	-0.92128500	-1.12916200	-1.12937000
Cl	-2.96076400	-0.00000500	0.00000900

2a

C	-4.32329600	-0.89520700	-0.48710800
C	-2.94888100	-1.05846500	-0.39543600
C	-2.17577500	0.02302900	-0.00551500
C	-2.73450600	1.25536000	0.29136900
C	-4.11069400	1.40180100	0.19492700
C	-4.90351300	0.33056700	-0.19224400
H	-4.93741700	-1.73259400	-0.78920200
H	-2.49613500	-2.01268400	-0.62298200
H	-2.11834800	2.08996100	0.59274100
H	-4.55946600	2.35883700	0.42396400
H	-5.97613600	0.45218500	-0.26492400
S	-0.38908200	-0.18258700	0.12093600
F	-0.33563800	0.62090300	1.51381700
F	-0.11499200	1.19700600	-0.65973700
F	-0.55805800	-1.58028000	0.91481500
F	-0.32193400	-0.96521800	-1.28452300
C	1.49443100	-0.50553700	0.30469800
C	2.44202800	0.54340700	-0.33679900
Cl	4.11473800	0.05128900	-0.07645400
F	1.77116500	-0.57552100	1.60231300
F	1.75414200	-1.68775400	-0.24479900
F	2.25122600	1.73430600	0.22174600
F	2.21225500	0.62589700	-1.64343300

SF_5Cl

S	0.00000000	0.00000000	-0.25794600
F	0.00000000	1.56986600	-0.27730700
F	-1.56986600	0.00000000	-0.27730700
F	0.00000000	-1.56986600	-0.27730700
F	1.56986600	0.00000000	-0.27730700
F	0.00000000	0.00000000	-1.82202100
Cl	0.00000000	0.00000000	1.79461000

$SF_5CF_2CF_2Cl$

F	-1.40068700	-0.07317600	-1.57470800
F	-1.86681500	1.45034500	-0.00003400
F	-1.40071700	-0.07311800	1.57470300

F	-0.94530600	-1.56647700	0.00003000
F	-2.88391600	-0.50801500	-0.00000800
S	-1.38904200	-0.05438400	-0.00000200
C	0.39987300	0.59878300	-0.00000100
C	1.51091200	-0.48548000	0.00000800
F	0.54122300	1.35607500	1.07921900
F	0.54122600	1.35606100	-1.07923100
F	1.39448100	-1.24532900	1.08393000
F	1.39447700	-1.24535100	-1.08389800
Cl	3.08201600	0.30183500	-0.00000300

2a’(*a*)

C	5.56478000	-0.50769400	0.88137400
C	4.22250800	-0.80531000	0.69695800
C	3.41646600	0.12741200	0.06484000
C	3.91153000	1.34073200	-0.38466500
C	5.25624300	1.62279800	-0.19226200
C	6.08092900	0.70233500	0.43894200
H	6.20481100	-1.22756400	1.37304400
H	3.82150400	-1.74705200	1.04255800
H	3.26898900	2.05669600	-0.87610600
H	5.65437600	2.56643400	-0.53973500
H	7.12871700	0.92772200	0.58653700
S	1.67005000	-0.24775000	-0.17850100
F	1.69755800	0.30902300	-1.68588600
F	1.22265600	1.21499400	0.32110900
F	2.00975900	-1.73317700	-0.71598900
F	1.52450600	-0.79913900	1.32926400
C	-0.16614400	-0.75312200	-0.43564700
C	-1.23667200	0.23898100	0.09964700
F	-0.35862400	-0.92809900	-1.73807600
F	-0.35697800	-1.92093200	0.17784700
F	-1.20741600	1.35283100	-0.64032400
F	-0.99034100	0.54021600	1.37775000
C	-2.67753800	-0.37344400	0.04972600
C	-3.79229700	0.70777400	0.12604800
F	-2.85684500	-1.06373100	-1.08063600
F	-2.81068900	-1.20133700	1.08912100
F	-3.80484300	1.41272700	-1.00155500
F	-3.53448500	1.53411500	1.13895100
Cl	-5.35802100	-0.05131900	0.35622200

2a’(*g*)

C	-5.47120100	-1.12962200	-0.35808800
C	-4.09061000	-1.21492600	-0.25302900
C	-3.36940300	-0.05530200	-0.01957800
C	-3.98562200	1.17867200	0.11051500
C	-5.36706900	1.24634000	0.00308000
C	-6.10842900	0.09669700	-0.23046000
H	-6.04459900	-2.02791200	-0.54232800
H	-3.59429000	-2.16912400	-0.35452200
H	-3.41045100	2.07448700	0.29424500

H	-5.85972900	2.20374400	0.10457600
H	-7.18550500	0.15652500	-0.31347100
S	-1.57436900	-0.15466400	0.11315100
F	-1.55377000	0.85681500	1.36592700
F	-1.37201900	1.09046200	-0.88440500
F	-1.66609400	-1.42331900	1.10927900
F	-1.47391000	-1.14341900	-1.14954000
C	0.32569300	-0.32836900	0.34322100
C	1.20382500	0.77153600	-0.30352200
F	0.57776800	-0.34130200	1.65050500
F	0.68582800	-1.50367800	-0.16644600
F	0.79415900	1.97741400	0.11060700
F	1.09926600	0.69278000	-1.63257500
C	2.73062900	0.73459000	0.06081100
C	3.49703500	-0.59769300	-0.14895900
F	3.28921400	1.67086500	-0.71661000
F	2.87621800	1.09399700	1.33884500
F	3.20294500	-1.10128200	-1.34570000
F	3.12170400	-1.46802200	0.78619800
Cl	5.22727100	-0.32861400	-0.02456600

DVN-Cl

C	2.88202500	-1.08378200	-0.55391900
H	3.81228200	-0.58659600	-0.83059300
H	2.61843600	-1.78036400	-1.35126100
H	3.06784500	-1.66223800	0.35448900
C	1.77551600	-0.05928800	-0.31759900
H	1.65150800	0.52326200	-1.23514600
C	0.46875400	-0.82486800	-0.07336000
H	0.58859500	-1.51545200	0.76583700
H	0.26842700	-1.42307800	-0.96202900
C	2.17578200	0.89579800	0.80228700
H	1.50960500	1.75623800	0.87486700
H	2.18885700	0.38331700	1.76779900
H	3.17909800	1.28234100	0.61669000
C	-0.79069600	0.00954800	0.22381000
C	-0.84200700	1.20164200	-0.63346200
N	-0.85314200	2.14388300	-1.28566800
Cl	-2.24580900	-0.98222000	-0.23215600
C	-0.95916200	0.40185900	1.68767900
H	-0.97132700	-0.50523700	2.28978400
H	-0.13211500	1.02980100	2.00928700
H	-1.89174200	0.94311800	1.83398600

IM1

C	-2.47051500	-1.20456800	-0.00000100
C	-1.08392500	-1.21448600	-0.00000100
C	-0.41709400	0.00000000	-0.00000100
C	-1.08392500	1.21448700	-0.00000200
C	-2.47051400	1.20456800	0.00000000
C	-3.16065900	0.00000000	0.00000100
H	-3.00885000	-2.14228600	-0.00000100

H	-0.53991200	-2.14803500	0.00000000
H	-0.53991100	2.14803500	-0.00000100
H	-3.00885000	2.14228600	0.00000000
H	-4.24248500	0.00000100	0.00000100
S	1.36072900	0.00000000	0.00000000
F	1.49133600	-1.15607400	1.15306900
F	1.49133700	-1.15607800	-1.15306400
F	1.49133600	1.15607800	1.15306600
F	1.49133900	1.15607400	-1.15306900

IM2

C	-3.62679200	1.40496400	0.19587400
C	-4.42215900	0.33314200	-0.18446800
C	-3.84436700	-0.89484500	-0.47488600
C	-2.46995900	-1.05969200	-0.38550800
C	-1.69446500	0.02222600	-0.00169900
C	-2.25065600	1.25674700	0.29050200
H	-4.07360100	2.36379700	0.42130600
H	-5.49476900	0.45602400	-0.25519800
H	-4.46034800	-1.73274600	-0.77175200
H	-2.01870700	-2.01542600	-0.60946100
H	-1.63227400	2.09119500	0.58737700
S	0.09152500	-0.18820500	0.12588300
F	0.15077600	-0.97326900	-1.28558600
F	-0.07716800	-1.58661600	0.92443300
F	0.14034300	0.62427500	1.51950600
F	0.37018700	1.20010200	-0.66375800
C	1.99051900	-0.47339000	0.28142500
C	2.85404700	0.56024800	-0.38476800
F	2.25518700	-1.66319700	-0.25373100
F	2.28722800	-0.51326200	1.57739500
F	2.79468800	0.60162300	-1.69149100
F	2.85634700	1.74945900	0.16154000

SF_5 radical

S	0.00000000	0.00000000	0.20370300
F	0.00000000	1.59593100	0.24313100
F	-1.59593100	0.00000000	0.24313100
F	0.00000000	-1.59593100	0.24313100
F	1.59593100	0.00000000	0.24313100
F	0.00000000	0.00000000	-1.33466100

$SF_5CF_2CF_2$ radical

F	-0.98911300	-0.08146900	-1.58092600
F	-1.67085900	1.22543000	0.11087800
F	-0.87956500	-0.29281400	1.56775000
F	-0.20225500	-1.56887900	-0.12548100
F	-2.30369900	-0.88878900	-0.00634600
S	-0.92156600	-0.16113400	-0.00611300
C	0.75210100	0.76775400	0.01185500
C	1.96956700	-0.11451900	0.00646800
F	0.75729000	1.51686900	1.10903300

F	0.77208500	1.55603500	-1.05616200
F	2.14924700	-0.84003900	1.07918800
F	2.19076300	-0.77537200	-1.09928200

IM3(*a*)

C	-5.17866800	-0.42487600	-0.66299600
C	-3.83685300	-0.76432300	-0.57199500
C	-2.95290700	0.15943200	-0.03852200
C	-3.36919200	1.40531700	0.40161300
C	-4.71443100	1.72962400	0.30243000
C	-5.61702100	0.81788800	-0.22717400
H	-5.87961900	-1.13778300	-1.07549200
H	-3.49395200	-1.73069200	-0.91169400
H	-2.66579000	2.11322800	0.81555900
H	-5.05317200	2.69826400	0.64378100
H	-6.66523700	1.07591500	-0.29918800
S	-1.20790200	-0.27598500	0.08832300
F	-1.11845700	0.30001800	1.59010800
F	-0.74359500	1.16049500	-0.46843100
F	-1.56572000	-1.74866600	0.65320700
F	-1.18185300	-0.84258700	-1.41806600
C	0.62022700	-0.84326400	0.27455500
C	1.70869000	0.19942400	-0.09472900
F	0.79374900	-1.20360200	1.54304200
F	0.78783600	-1.91777000	-0.49106500
F	1.56749500	1.28213900	0.68112800
F	1.58168400	0.54055900	-1.38341900
C	3.17034900	-0.31104900	0.09528900
C	4.22552400	0.72341300	-0.24186300
F	3.34831900	-0.67008900	1.37354900
F	3.36732900	-1.37088300	-0.70071000
F	4.28811400	1.75324000	0.56655800
F	4.29175200	1.07795600	-1.50209900

IM3(*g*)

C	-5.01523800	-1.09729700	-0.36855400
C	-3.63578000	-1.19004800	-0.25447900
C	-2.90966500	-0.03304800	-0.02339100
C	-3.51928200	1.20543900	0.09512300
C	-4.89959500	1.28044400	-0.02142900
C	-5.64612500	0.13352300	-0.25231800
H	-5.59322600	-1.99389300	-0.55057300
H	-3.14392000	-2.14826400	-0.34685100
H	-2.93916700	2.09920300	0.27733600
H	-5.38766100	2.24182900	0.07132400
H	-6.72303100	0.19905100	-0.34195300
S	-1.11654100	-0.14131800	0.12483800
F	-1.10223600	0.86770100	1.37958900
F	-0.89808300	1.10725600	-0.86517800
F	-1.22200900	-1.41096600	1.11812900
F	-1.00817400	-1.12753700	-1.13954100
C	0.77640700	-0.32001100	0.36666000

C	1.67153600	0.75048800	-0.30028300
F	1.02397900	-0.31435900	1.67465300
F	1.14571000	-1.50701400	-0.11812200
F	1.31321600	1.97338500	0.10580500
F	1.55025900	0.65988300	-1.62921300
C	3.19215300	0.60028800	0.04314400
C	3.85614800	-0.73957200	-0.18666000
F	3.81529400	1.50246500	-0.73601100
F	3.37234300	0.93830300	1.32554400
F	3.71680100	-1.24069000	-1.39083500
F	3.67382500	-1.63487900	0.75367200

rad-DVN

C	2.67767100	-0.31805600	-0.63444700
H	3.45535900	0.43758400	-0.51546700
H	2.64528000	-0.60898400	-1.68576100
H	2.97082700	-1.19454200	-0.05051600
C	1.32960000	0.21063700	-0.16024200
H	1.05950500	1.07308100	-0.77709300
C	0.25694800	-0.86441800	-0.34544100
H	0.48283600	-1.72076700	0.29908100
H	0.29622500	-1.24498100	-1.37514800
C	-1.14881400	-0.43701900	-0.06717700
C	-2.16759100	-1.44331800	0.34248000
H	-1.87598400	-1.90059700	1.29243900
H	-3.15870300	-1.00933500	0.45018000
H	-2.21384500	-2.25049900	-0.39518400
C	1.40935900	0.65880900	1.29533000
H	0.46074100	1.06425500	1.65144300
H	1.67759700	-0.18598300	1.93565700
H	2.16973700	1.43058400	1.42251500
C	-1.53148500	0.88833900	-0.28141700
N	-1.84624300	1.99147700	-0.44952200

TS TFE+IM1: Imaginary frequency = −403.63 cm^{-1}

S	0.00343300	-0.15168600	0.10090600
F	-0.07818700	-0.98956300	-1.31992400
F	-0.25023700	1.25890100	-0.73278200
F	-0.07175100	0.69259400	1.51735000
F	0.11741400	-1.57314100	0.94013900
C	-2.39381100	-0.49745100	0.30642800
C	-2.84533400	0.58472400	-0.39259800
F	-2.46875100	-0.51027800	1.61389200
F	-2.45242600	-1.69221800	-0.22741100
F	-2.93559900	0.57858300	-1.68299800
F	-2.95975900	1.75416300	0.14887900
C	1.78304500	0.01940100	-0.00390900
C	2.53990000	-1.08031000	-0.37430800
C	2.35958700	1.24387600	0.29138300
C	3.91806800	-0.94306500	-0.44883000
H	2.06845900	-2.02587100	-0.59948800
C	3.73910400	1.36414600	0.21218500

H	1.75120200	2.08908400	0.57823600
C	4.51651400	0.27470200	-0.15625500
H	4.52119500	-1.79362500	-0.73602200
H	4.20334700	2.31412200	0.43970300
H	5.59212500	0.37576000	-0.21581600

TS 1a+IM2: Imaginary frequency = −361.48 cm^{-1}

C	-7.25092200	0.70171600	0.80200800
C	-7.94301500	-0.17246500	-0.02430000
C	-7.25083300	-1.05771100	-0.83885200
C	-5.86387300	-1.07481700	-0.83330100
C	-5.19279700	-0.19448600	-0.00049200
C	-5.86384700	0.69694900	0.82032200
H	-7.78739700	1.39320100	1.43735000
H	-9.02473700	-0.16383900	-0.03360700
H	-7.78725900	-1.74039600	-1.48370200
H	-5.32333400	-1.76245600	-1.46726800
H	-5.32371300	1.37673800	1.46295700
S	-3.39138700	-0.20817800	0.01052200
F	-3.32885000	-0.23003900	-1.60099100
F	-3.34380600	-1.82360400	0.05623600
F	-3.34421600	-0.14051500	1.62069100
F	-3.31769500	1.40916900	-0.03403800
C	-1.46509800	-0.29517000	0.01963200
F	-1.09044200	-1.01016700	-1.03445500
F	-1.09503100	-0.93198800	1.12417600
F	-0.92424400	1.79675100	1.03128100
C	-0.76884200	1.05208000	-0.02827500
F	-0.92571500	1.72027800	-1.13727900
Cl	1.48917300	0.52636000	-0.01068200
S	3.68583700	0.13646700	-0.00239000
F	3.56216200	-0.07502700	1.58855500
F	3.88621300	1.71692800	0.22678900
F	3.33241800	-1.41579300	-0.23283000
F	3.65526400	0.37694600	-1.59349000
C	5.45254600	-0.17666800	0.00522300
C	5.94115100	-1.25464400	0.72544400
C	6.28675600	0.66887600	-0.70814400
C	7.30852900	-1.48767400	0.72690400
H	5.27649800	-1.90343900	1.27748300
C	7.65154100	0.42176500	-0.69642200
H	5.88768200	1.50552300	-1.26344100
C	8.16160500	-0.65271500	0.01879500
H	7.70303000	-2.32575300	1.28517600
H	8.31315400	1.07349000	-1.25060300
H	9.22698800	-0.84046500	0.02405900

TS TFE+SF_5: Imaginary frequency = −240.49 cm^{-1}

S	-1.06009100	-0.11198800	0.00000100
F	-1.06921000	-0.12307200	-1.61654500
F	-0.60300700	-1.66740000	0.00002000
F	-1.06922700	-0.12303500	1.61654600

F	-1.54415000	1.43256200	-0.00002000
C	1.28290200	0.81947200	-0.00000100
C	1.90309600	-0.38584300	0.00000100
F	1.16229600	1.51946900	1.09385900
F	1.16229300	1.51946300	-1.09386500
F	2.13310800	-1.04208300	-1.08789900
F	2.13311200	-1.04207700	1.08790500
F	-2.54460800	-0.56382500	-0.00000100

TS SF_5Cl+$SF_5CF_2CF_2$: Imaginary frequency = -364.90 cm^{-1}

S	3.33282100	-0.15309800	-0.01388400
F	3.40842200	-0.15567800	1.55942000
F	3.48151600	-1.72333400	-0.03888400
F	3.28364200	-0.11321300	-1.58874700
F	3.20625200	1.42474700	0.01314100
C	1.43436500	-0.38216600	0.04595100
F	1.14336800	-1.03691100	1.15947600
F	1.09823000	-1.11962700	-1.00212700
F	0.77350000	1.60295700	-1.09097200
C	0.65189800	0.92314800	0.01193500
F	0.77460400	1.66168600	1.07591900
Cl	-1.51412600	0.28426600	0.02661700
S	-3.68335100	-0.12745600	-0.00753100
F	-3.97797500	1.40694000	0.22148100
F	-3.67030000	-0.35840500	1.55500400
F	-3.70321900	0.10203300	-1.57001000
F	-3.39740400	-1.66360400	-0.23690800
F	4.88453700	-0.01423200	-0.07439700
F	-5.21283400	-0.41219900	-0.03319300

TS TFE+IM2(*a*): Imaginary frequency = -574.22 cm^{-1}

C	-5.24770000	-0.68389300	-0.55444500
C	-3.88828400	-0.92588900	-0.42136200
C	-3.06347700	0.11442200	-0.02533600
C	-3.55651100	1.38198500	0.23730000
C	-4.91856500	1.60739900	0.09967600
C	-5.76248300	0.57836700	-0.29380000
H	-5.90152500	-1.48859600	-0.86191400
H	-3.48600900	-1.90856000	-0.62089600
H	-2.90035300	2.18313300	0.54452500
H	-5.31626700	2.59266700	0.30199300
H	-6.82379700	0.76079300	-0.39818400
S	-1.29684600	-0.19572200	0.15994200
F	-1.24342200	0.63119500	1.54399300
F	-0.91447100	1.16167600	-0.63471100
F	-1.57415300	-1.56898700	0.97434700
F	-1.24254700	-1.00543700	-1.23848900
C	0.57595000	-0.60151300	0.37267000
C	1.53981500	0.32632200	-0.33116200
F	0.84151200	-0.59293800	1.67562000
F	0.76321900	-1.83667100	-0.09220400
F	1.58850100	1.54355800	0.17669300

F	1.40754600	0.35690300	-1.64181100
C	3.66401300	-0.52056600	-0.10826000
C	4.34344500	0.64008500	-0.01946900
F	3.46349800	-1.26756700	0.95583800
F	3.62752000	-1.20076000	-1.23263000
F	4.50260300	1.27262900	1.10795900
F	4.67577800	1.33882200	-1.06788000

TS TFE+IM2(*g*): Imaginary frequency = −607.94 cm^{-1}

C	-5.10975200	-1.14199200	-0.37557200
C	-3.73023900	-1.21660600	-0.24938900
C	-3.01969900	-0.04934300	-0.02141900
C	-3.64577400	1.18194700	0.08246000
C	-5.02588000	1.23934400	-0.04678300
C	-5.75653400	0.08184400	-0.27520400
H	-5.67469900	-2.04662900	-0.55484100
H	-3.22598900	-2.16861700	-0.33001400
H	-3.07832200	2.08352400	0.26101200
H	-5.52604800	2.19494000	0.03295800
H	-6.83254700	0.13355500	-0.37557500
S	-1.22542800	-0.13508000	0.13549500
F	-1.23792400	0.85310100	1.41324200
F	-1.02313200	1.14911100	-0.82902100
F	-1.31759000	-1.42849400	1.10562100
F	-1.10691700	-1.09256900	-1.15809300
C	0.68265600	-0.26879000	0.35095300
C	1.50452800	0.80069100	-0.32794300
F	0.93959600	-0.23940300	1.65721900
F	1.06219000	-1.45523400	-0.12469700
F	1.29972800	2.02043500	0.12763400
F	1.46735500	0.76194000	-1.64489800
C	3.72284600	0.50083200	0.11896400
C	3.98566800	-0.78797900	-0.17485300
F	4.02336800	1.45922900	-0.73384500
F	3.67201400	0.91584500	1.36592200
F	4.16909200	-1.20320300	-1.39615700
F	3.86305700	-1.74911100	0.69610000

TS 1a+ IM3(*a*): Imaginary frequency = −362.91 cm^{-1}

C	-8.41599900	-1.17681800	-0.48774400
C	-7.03434000	-1.29547500	-0.44876900
C	-6.29400600	-0.25723500	0.09247600
C	-6.89222400	0.88822100	0.59172200
C	-8.27490000	0.99097300	0.54531100
C	-9.03526300	-0.03780900	0.00764500
H	-9.00505900	-1.98035300	-0.90841600
H	-6.55277700	-2.18222300	-0.83472100
H	-6.30007200	1.68879900	1.01053900
H	-8.75322800	1.88019700	0.93266000
H	-10.11315100	0.04861800	-0.02588800
S	-4.49749800	-0.39853900	0.14658300
F	-4.43909600	0.16480700	1.65340000

F	-4.30394900	1.10337900	-0.39827700
F	-4.58381800	-1.91604200	0.69716700
F	-4.43696400	-0.93276200	-1.37078600
C	-2.59437100	-0.66206500	0.24583600
C	-1.71479400	0.54225300	-0.18356100
F	-2.30012400	-0.97442800	1.50404700
F	-2.29201100	-1.70289900	-0.52412500
F	-1.97661000	1.58643500	0.61192000
F	-1.97962900	0.85654600	-1.45705600
C	-0.18062200	0.26564600	-0.09329600
C	0.66471000	1.47512200	-0.49237800
F	0.13613100	-0.05830700	1.16358400
F	0.12953700	-0.74207300	-0.91452100
F	0.58190000	2.49575700	0.31832300
F	0.55497200	1.83446500	-1.74321000
Cl	2.85706800	0.74062000	-0.27343200
S	4.98360400	0.11465900	-0.05642000
F	4.82459400	0.40524500	1.51777800
F	5.37898000	1.65605300	-0.29607800
F	4.99344100	-0.13126600	-1.64613300
F	4.43715700	-1.38132800	0.16768000
C	6.69675200	-0.38812200	0.12115100
C	7.13368200	-1.53040900	-0.52977200
C	7.54282600	0.37887500	0.90620000
C	8.45976300	-1.91084600	-0.38607100
H	6.46124500	-2.11764100	-1.13831200
C	8.86572200	-0.01562200	1.03964700
H	7.18480300	1.26749500	1.40603700
C	9.32375200	-1.15671000	0.39587300
H	8.81341700	-2.80073000	-0.88875100
H	9.53548800	0.57480100	1.64989200
H	10.35675600	-1.45951200	0.50365700

TS 1a+ IM3(*g*): Imaginary frequency = −369.52 cm^{-1}

C	8.40446700	-1.04971800	0.25500400
C	7.02122700	-1.15222200	0.23626400
C	6.27744300	-0.03362500	-0.10355500
C	6.87315100	1.17586600	-0.42147000
C	8.25751900	1.26153100	-0.39680600
C	9.02150900	0.15281300	-0.06008900
H	8.99633100	-1.91578300	0.51827200
H	6.53978400	-2.08746200	0.48288300
H	6.27929400	2.03928100	-0.68394100
H	8.73545100	2.20031200	-0.64148000
H	10.10067900	0.22654800	-0.04273700
S	4.47934100	-0.15468500	-0.12479000
F	4.38525200	0.62141500	-1.53252600
F	4.31310800	1.24667200	0.64576900
F	4.52818900	-1.57758400	-0.88599500
F	4.45281100	-0.90641300	1.29483100
C	2.57537000	-0.35782000	-0.21981500
C	1.71975900	0.83528200	0.26888800

F	2.24964600	-0.60947400	-1.48622300
F	2.23668600	-1.41902700	0.51397900
F	2.07136700	1.95590400	-0.36932800
F	1.89269100	0.98762000	1.58549100
C	0.17944000	0.66711900	0.01245900
C	-0.47849400	-0.62487700	0.48320100
F	-0.39423800	1.68903700	0.66233400
F	-0.05083000	0.79423200	-1.29699400
F	-0.29576200	-0.90247800	1.74715400
F	-0.26239200	-1.65820700	-0.28703100
Cl	-2.75818400	-0.27322900	0.25640500
S	-4.97124600	-0.10707000	0.04675400
F	-5.06518100	-1.53883000	0.77416500
F	-4.81156900	-0.84403000	-1.37395100
F	-4.72013500	1.31277600	-0.66558900
F	-4.97362700	0.61915700	1.48235600
C	-6.75277100	0.02337800	-0.12022300
C	-7.37076300	1.22314800	0.19338800
C	-7.46840500	-1.07939300	-0.55797000
C	-8.74851400	1.31490200	0.06230500
H	-6.79710400	2.07358100	0.53270700
C	-8.84542300	-0.97087100	-0.68353000
H	-6.96942300	-2.00736900	-0.79728400
C	-9.48401500	0.22209400	-0.37476500
H	-9.24400800	2.24542400	0.30336400
H	-9.41606100	-1.82464400	-1.02277800
H	-10.55848000	0.30052500	-0.47501600

TS 1a+DVN: Imaginary frequency = −482.38 cm^{-1}

C	-3.23679000	2.68997900	1.07978300
H	-3.24871100	3.62886400	0.52465200
H	-2.23940600	2.55570500	1.50230600
H	-3.94742800	2.77916300	1.90576900
C	-3.61242600	1.52178000	0.17576000
H	-2.84487100	1.43165800	-0.59817100
C	-3.62797600	0.21973500	0.98689900
H	-4.63078700	0.05660400	1.40685400
H	-2.95356600	0.28058500	1.84401900
C	-3.26455300	-1.03449400	0.24915100
C	-3.27152300	-2.32412700	1.00467900
H	-4.31286800	-2.61219200	1.18503600
H	-2.78669500	-3.12403500	0.44933700
H	-2.78241400	-2.19201900	1.96841700
C	-4.95915200	1.77587300	-0.49566200
H	-5.27277200	0.93971500	-1.12141500
H	-5.73035100	1.93877500	0.26156400
H	-4.91424300	2.66467100	-1.12641200
C	-3.59095800	-1.12372600	-1.13916600
N	-3.84908600	-1.20835300	-2.25754800
C	5.22161000	-0.46050900	0.64211600
C	3.86300800	-0.74009500	0.65337500
C	3.00463100	0.09970700	-0.03768700

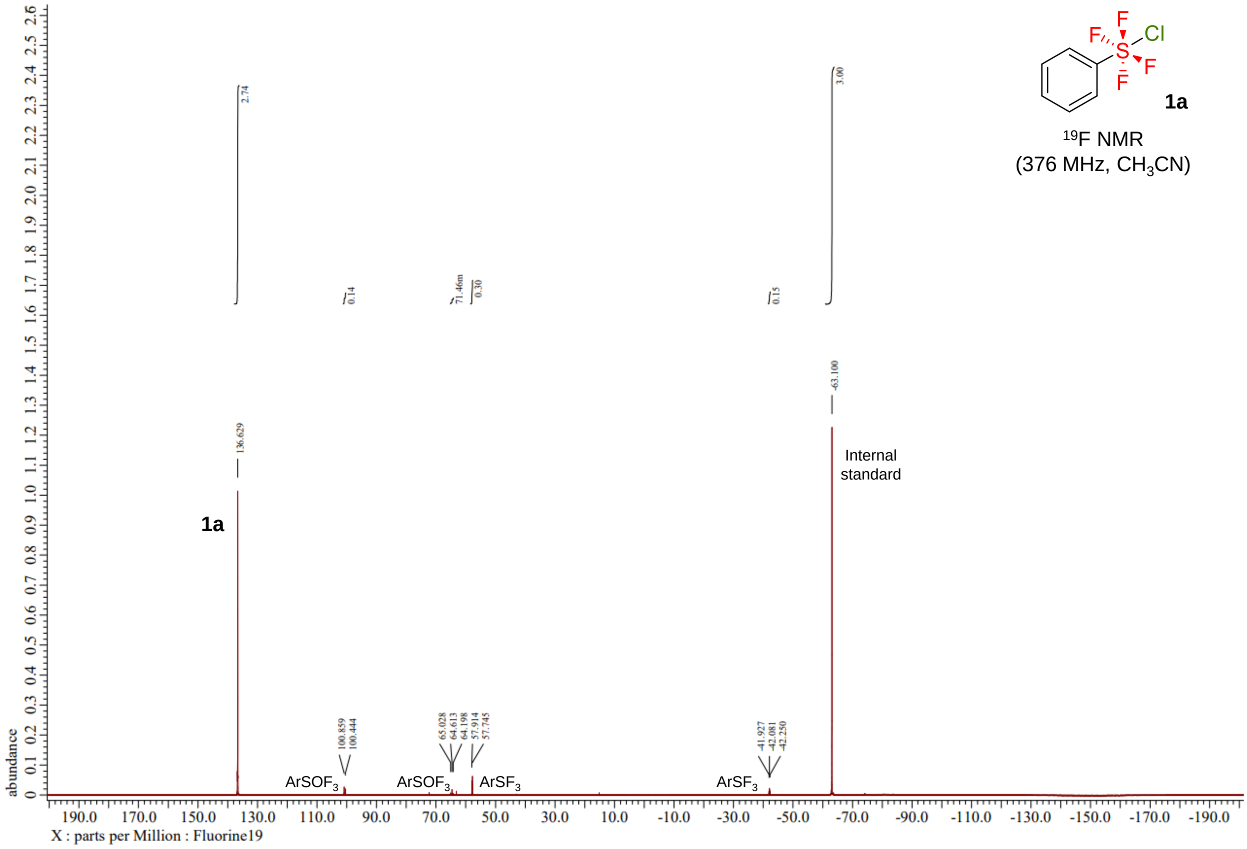
C	3.46550700	1.20408200	-0.73579100
C	4.82704500	1.47029700	-0.73725600
C	5.70329000	0.64133200	-0.05077500
H	5.90109500	-1.10911100	1.17814600
H	3.48663000	-1.59841600	1.19083700
H	2.78265500	1.84773500	-1.27112900
H	5.19835100	2.32989300	-1.27860000
H	6.76397500	0.85441700	-0.05602400
S	1.24450200	-0.25671800	-0.02969200
F	0.86226500	1.29732700	0.24016200
F	1.24011700	-0.53151400	1.57065600
F	1.11648000	-0.00897500	-1.62668200
F	1.49347100	-1.83763200	-0.29507800
Cl	-0.99872400	-0.70693500	-0.01537400

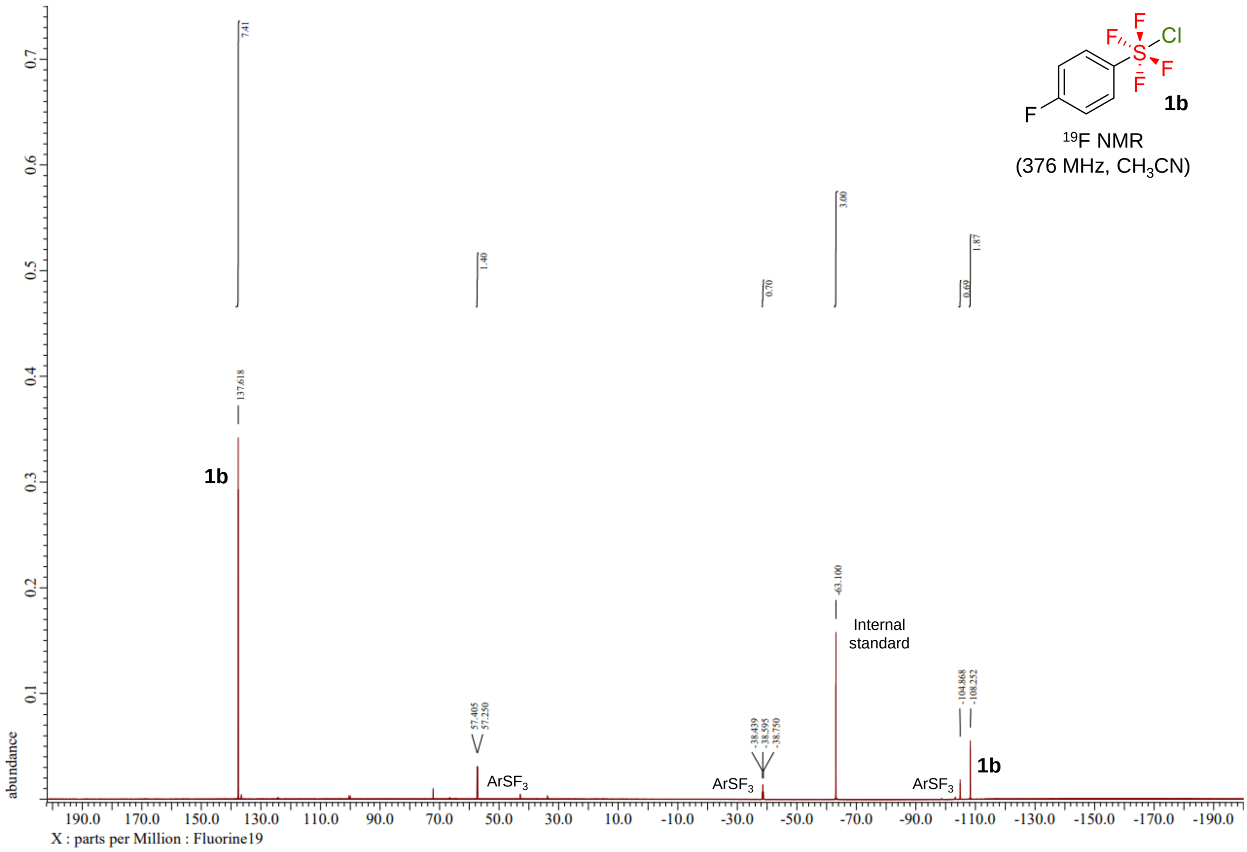
TS 2a+DVN: Imaginary frequency = −520.27 cm^{-1}

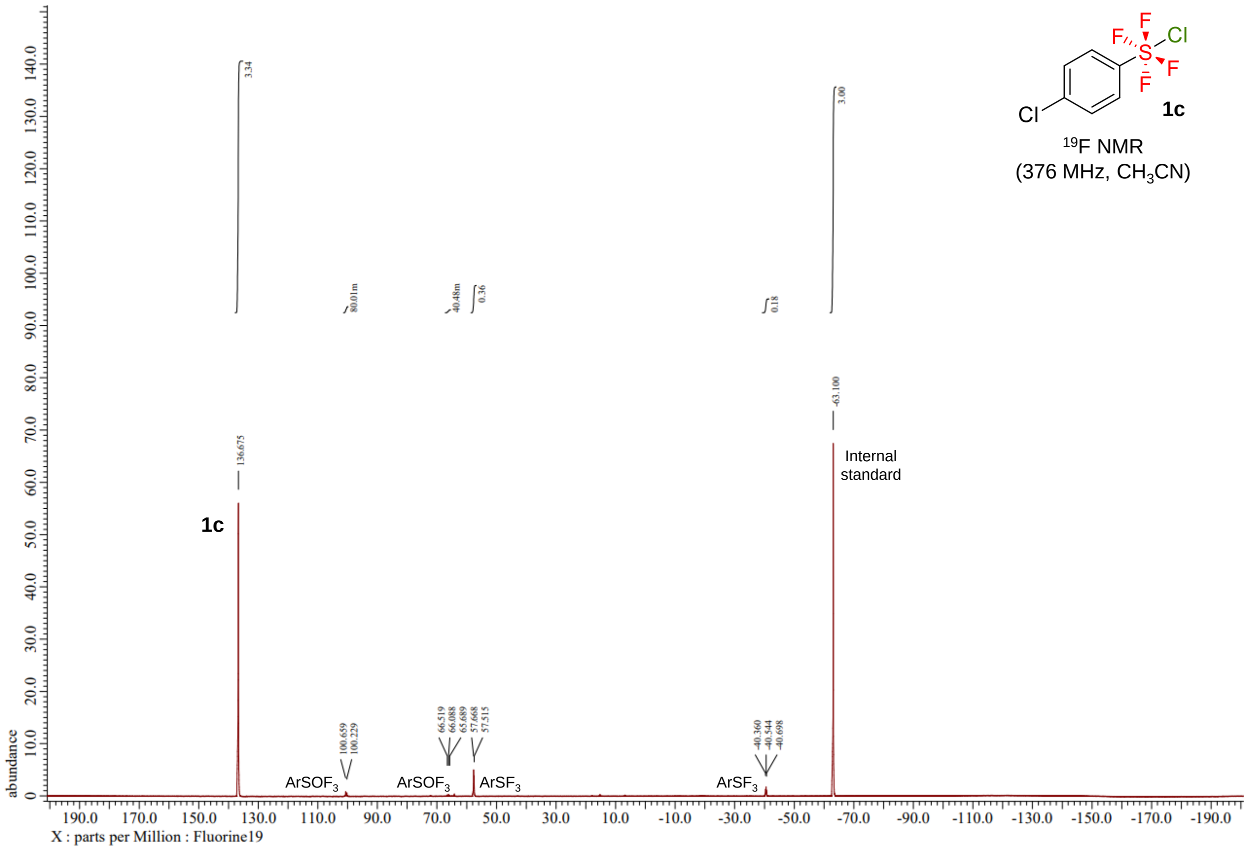
C	3.98641300	3.02972300	0.05100700
H	3.99422400	3.69326100	0.91690200
H	2.95273000	2.91180300	-0.27888500
H	4.54406600	3.51878200	-0.75211400
C	4.61259000	1.68258600	0.39331300
H	3.99181400	1.20588200	1.15744800
C	4.62741100	0.77956500	-0.84833000
H	5.58541600	0.88700000	-1.37234300
H	3.85388000	1.07840600	-1.55895700
C	4.42748300	-0.69875300	-0.60730000
C	4.50368400	-1.57816100	-1.82658200
H	5.53022100	-1.56687300	-2.20255400
H	4.22842000	-2.60578800	-1.59881900
H	3.84542400	-1.18572200	-2.60013800
C	6.01709100	1.87774200	0.95837000
H	6.51106500	0.92991000	1.17408900
H	6.63564800	2.42556400	0.24285000
H	5.98405500	2.45425100	1.88380800
C	5.10242000	-1.24991700	0.54444600
N	5.63351000	-1.70546700	1.45544200
C	-6.03032000	1.54024900	0.00000200
C	-4.65611400	1.42918800	-0.15324900
C	-4.06534100	0.18947800	0.03056500
C	-4.80533500	-0.93415100	0.36083700
C	-6.17846500	-0.80594700	0.51036900
C	-6.79023700	0.42677300	0.33068400
H	-6.50312900	2.50275700	-0.14072600
H	-4.06499700	2.29566800	-0.41215400
H	-4.32919500	-1.89344100	0.50195900
H	-6.76667400	-1.67584600	0.76924100
H	-7.86159100	0.52050800	0.44938000
S	-2.27930500	0.03425600	-0.16150100
F	-2.43777900	-1.30848200	-1.04294400
F	-2.15578100	-0.87941200	1.16617600
F	-2.29154200	0.94017000	-1.50309300
F	-2.01691200	1.34314700	0.74404400

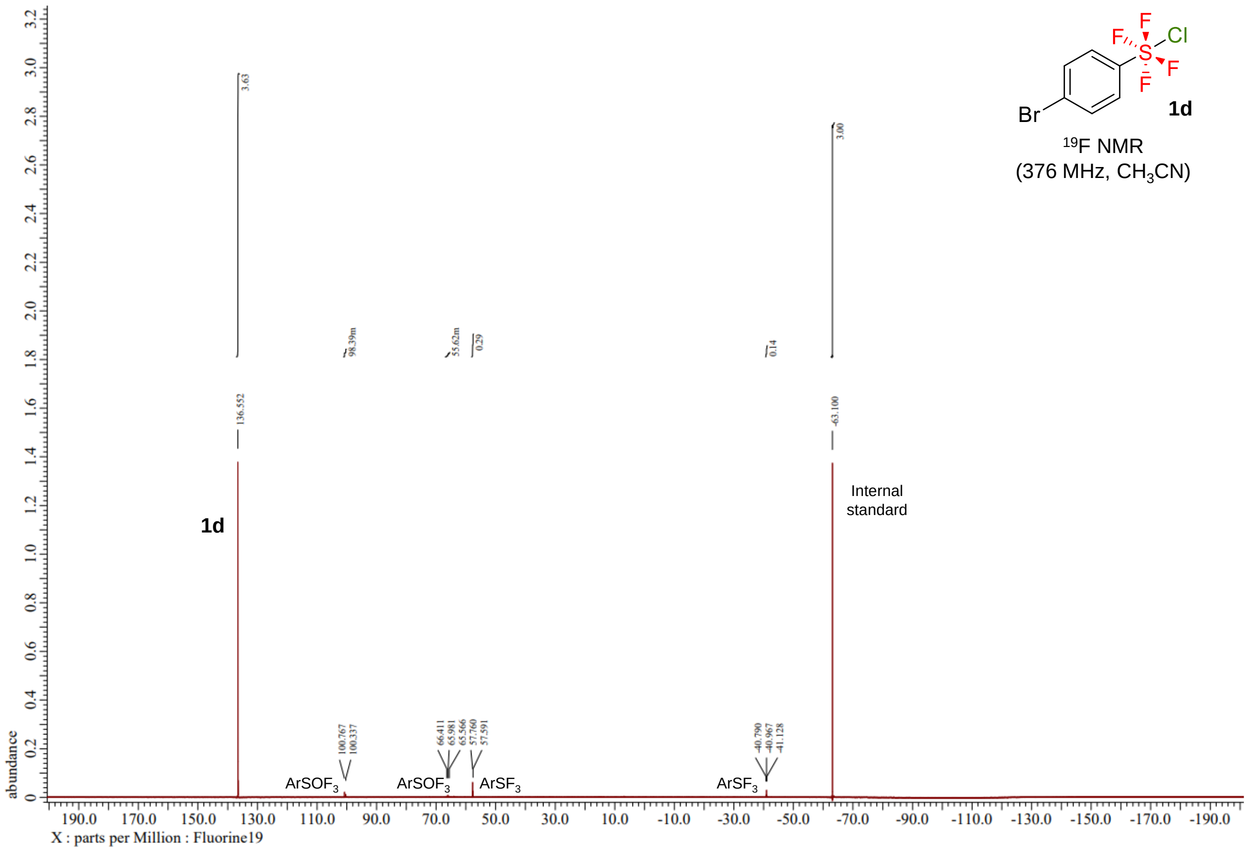
C	-0.37548800	-0.08638400	-0.43655700
C	0.38632300	-0.92228900	0.58277000
Cl	2.43713000	-0.84580800	-0.00761800
F	-0.18058900	-0.60317400	-1.64549400
F	0.10869700	1.15192400	-0.42218300
F	0.05542700	-2.19392400	0.57115000
F	0.35170300	-0.42863000	1.79949300

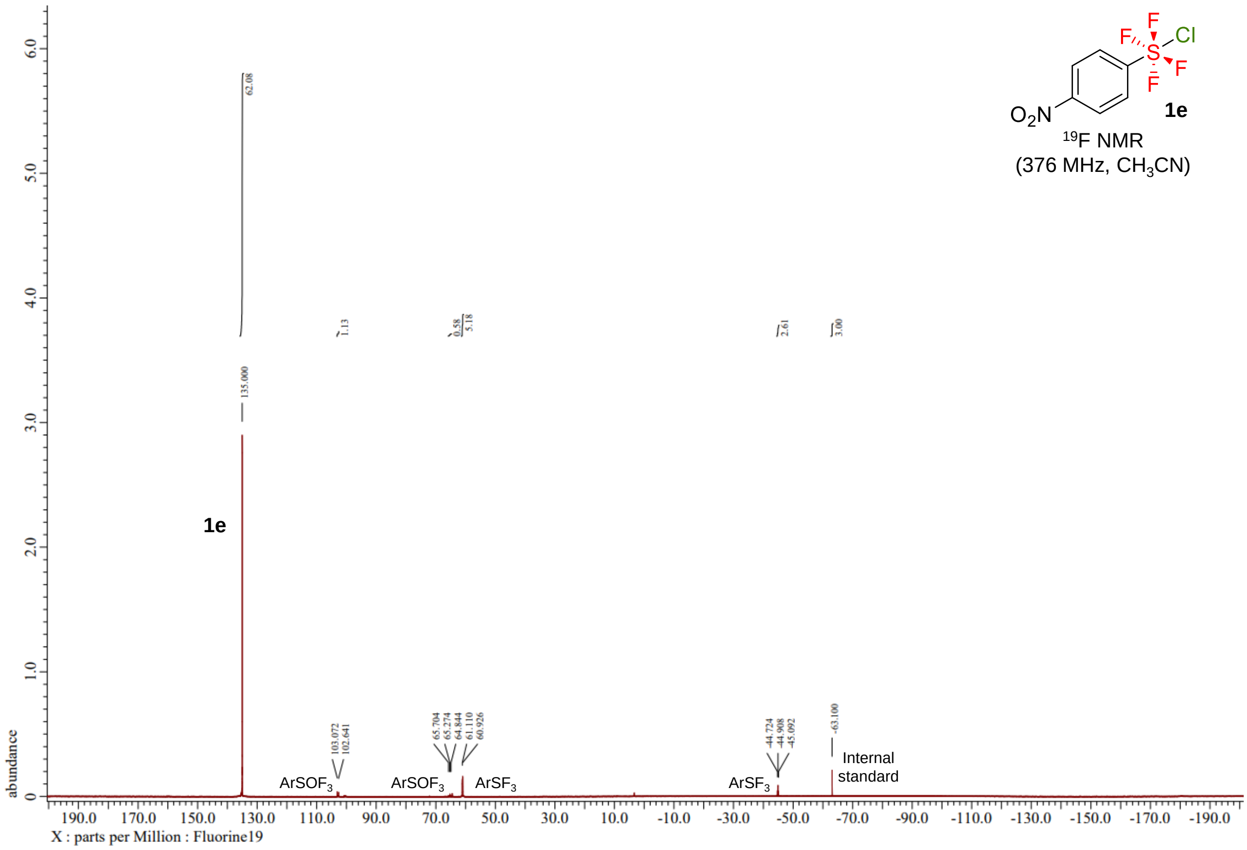
3. NMR spectra

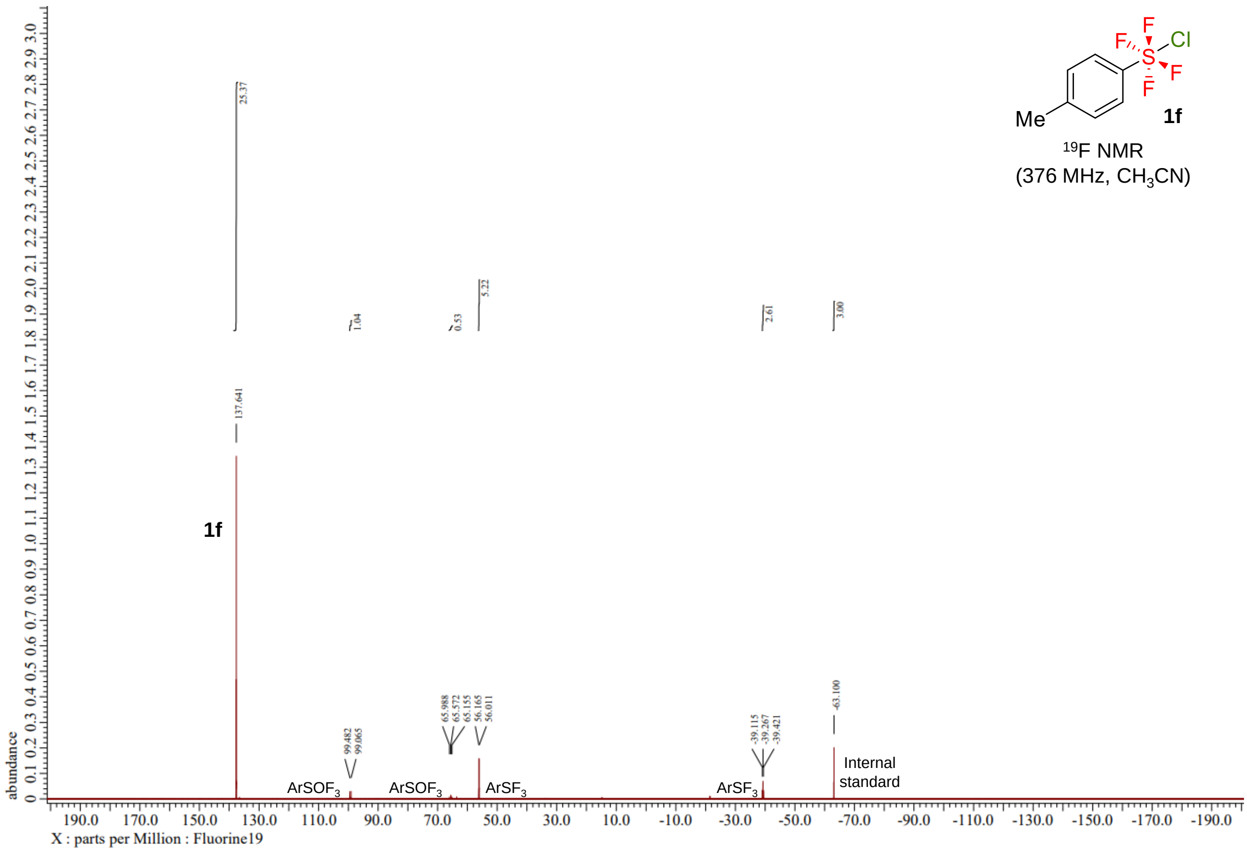


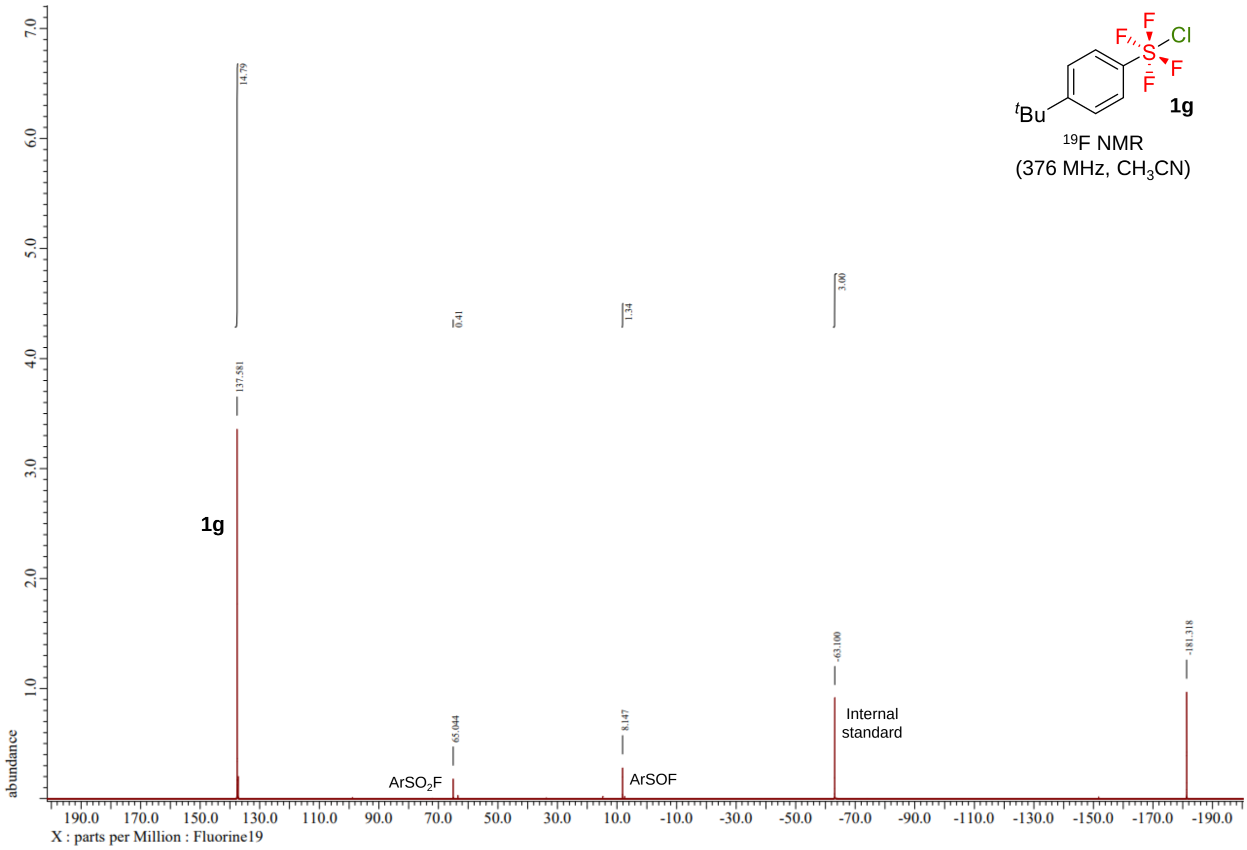


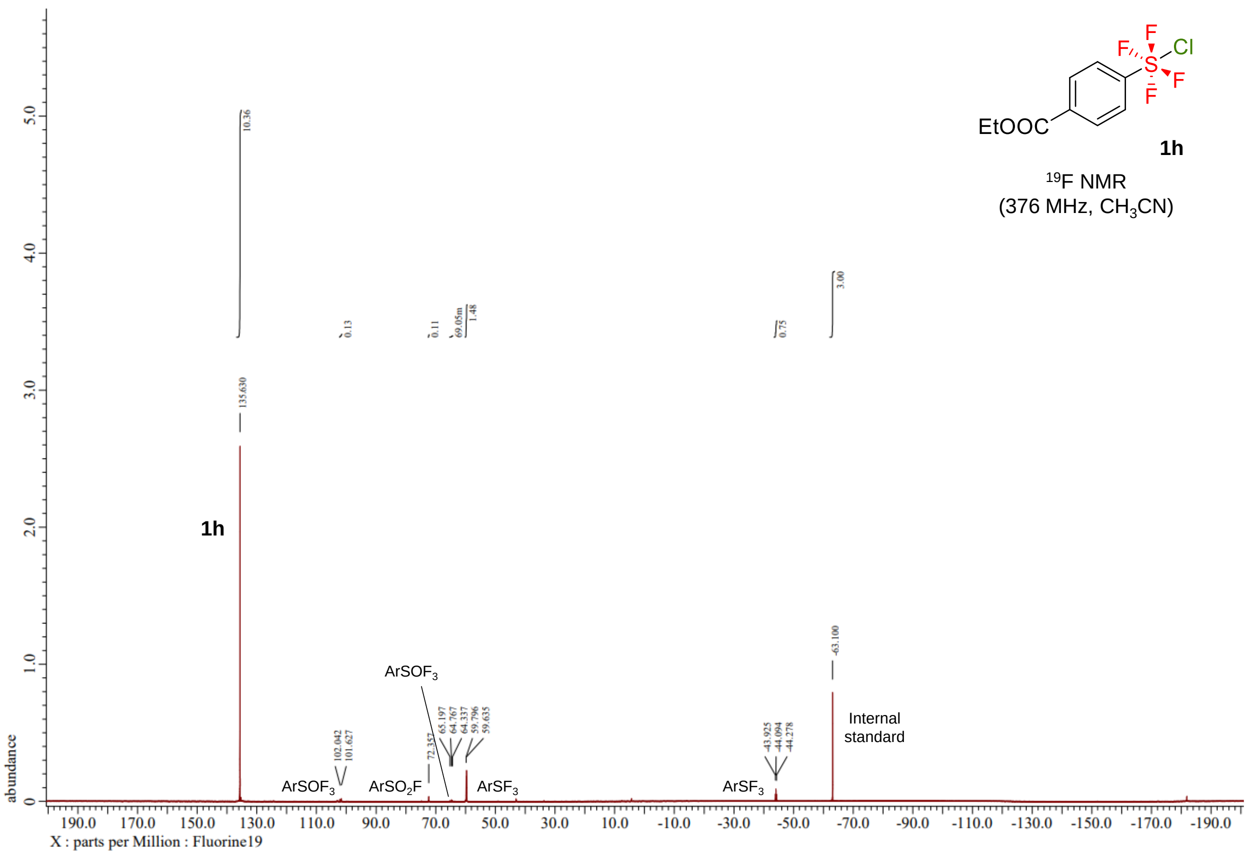

1c
19F NMR
(376 MHz, CH3CN)
Internal standard
ArSOF3
ArSOF3
ArSF3
ArSF3
abundance
X : parts per Million : Fluorine19

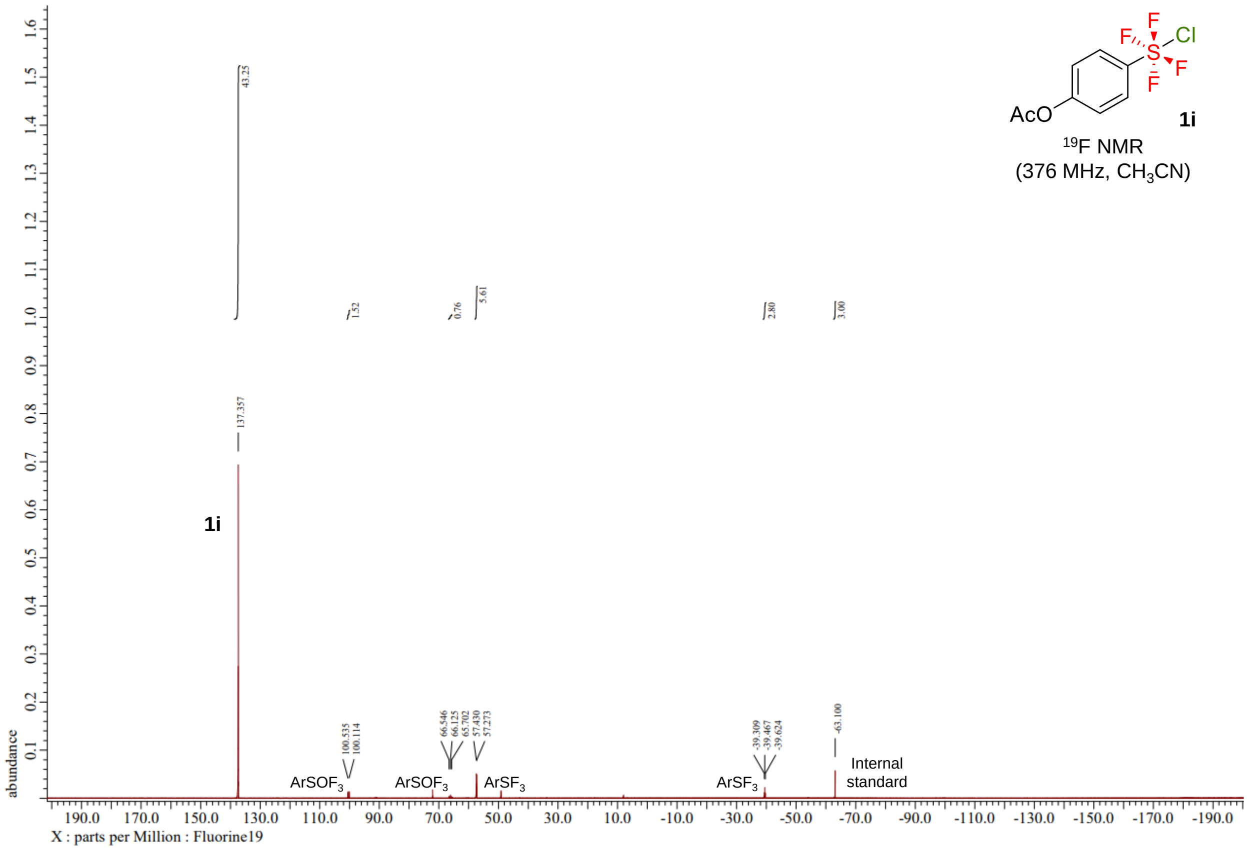

1d
19F NMR
(376 MHz, CH3CN)
Internal standard
ArSOF3
ArSOF3
ArSF3
ArSF3
abundance
X : parts per Million : Fluorine19

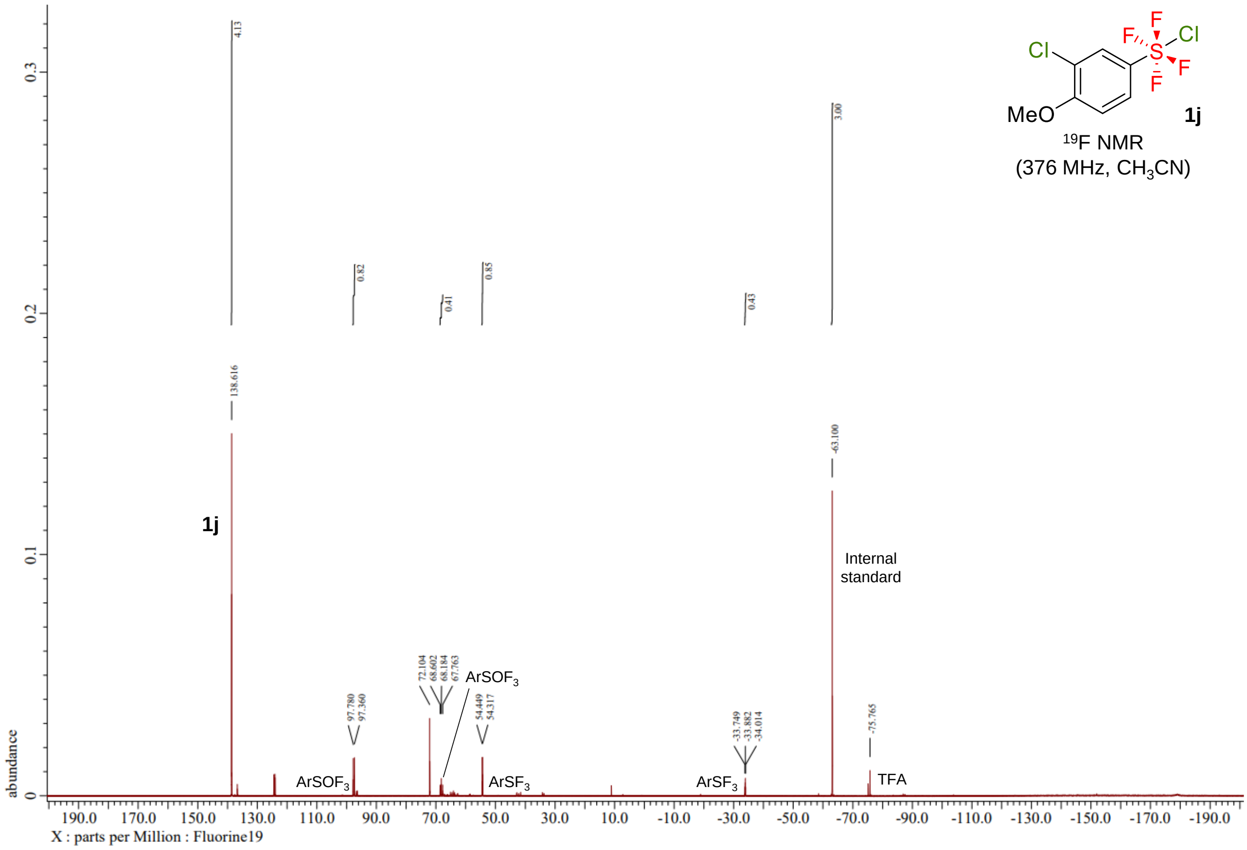

1e
^{19}F NMR
(376 MHz, CH_3CN)
ArSOF$_3$
ArSOF$_3$
ArSF$_3$
ArSF$_3$
Internal standard
abundance
X : parts per Million : Fluorine19

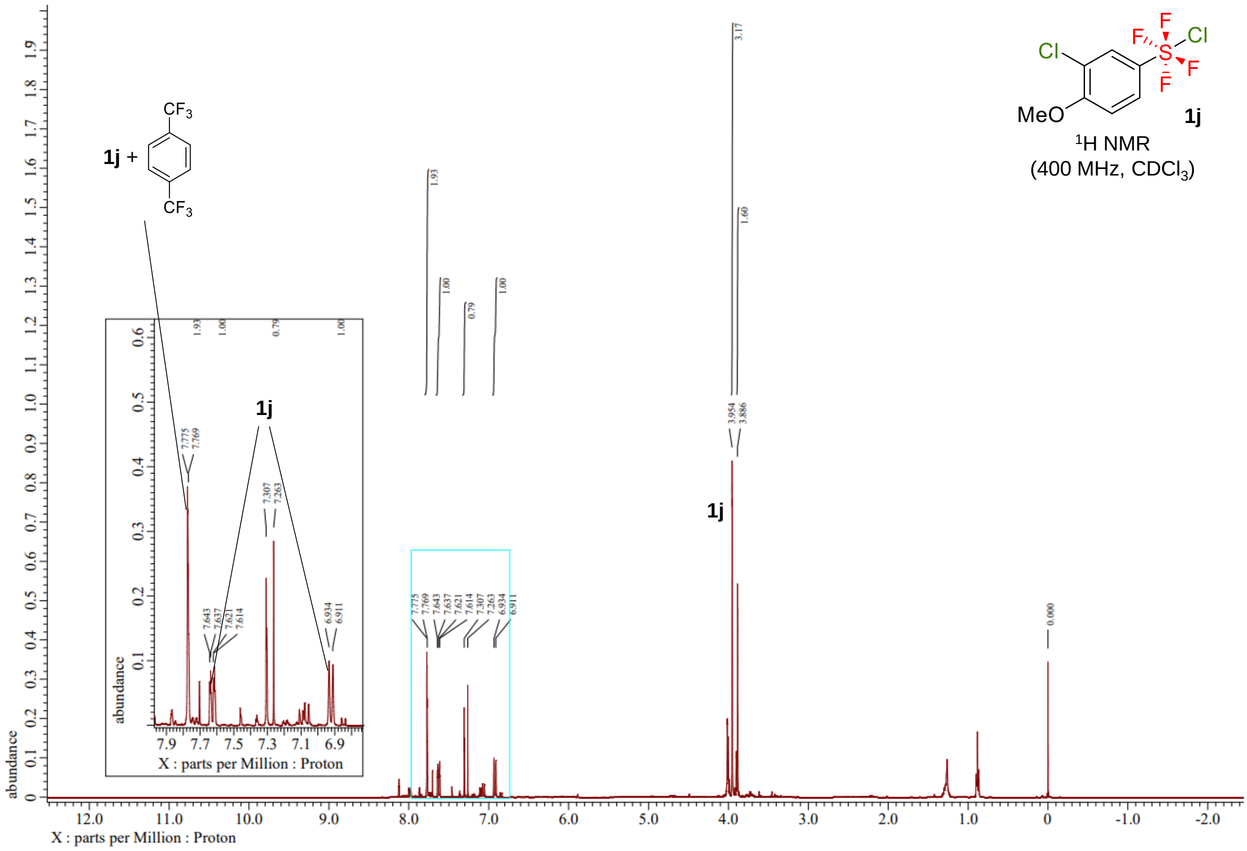

1f
^{19}F NMR
(376 MHz, CH_3CN)
Me
ArSOF$_3$
ArSOF$_3$
ArSF$_3$
ArSF$_3$
Internal standard
abundance
X : parts per Million : Fluorine19


1g
19F NMR
(376 MHz, CH3CN)
Internal standard
ArSO2F
ArSOF
abundance
X : parts per Million : Fluorine19

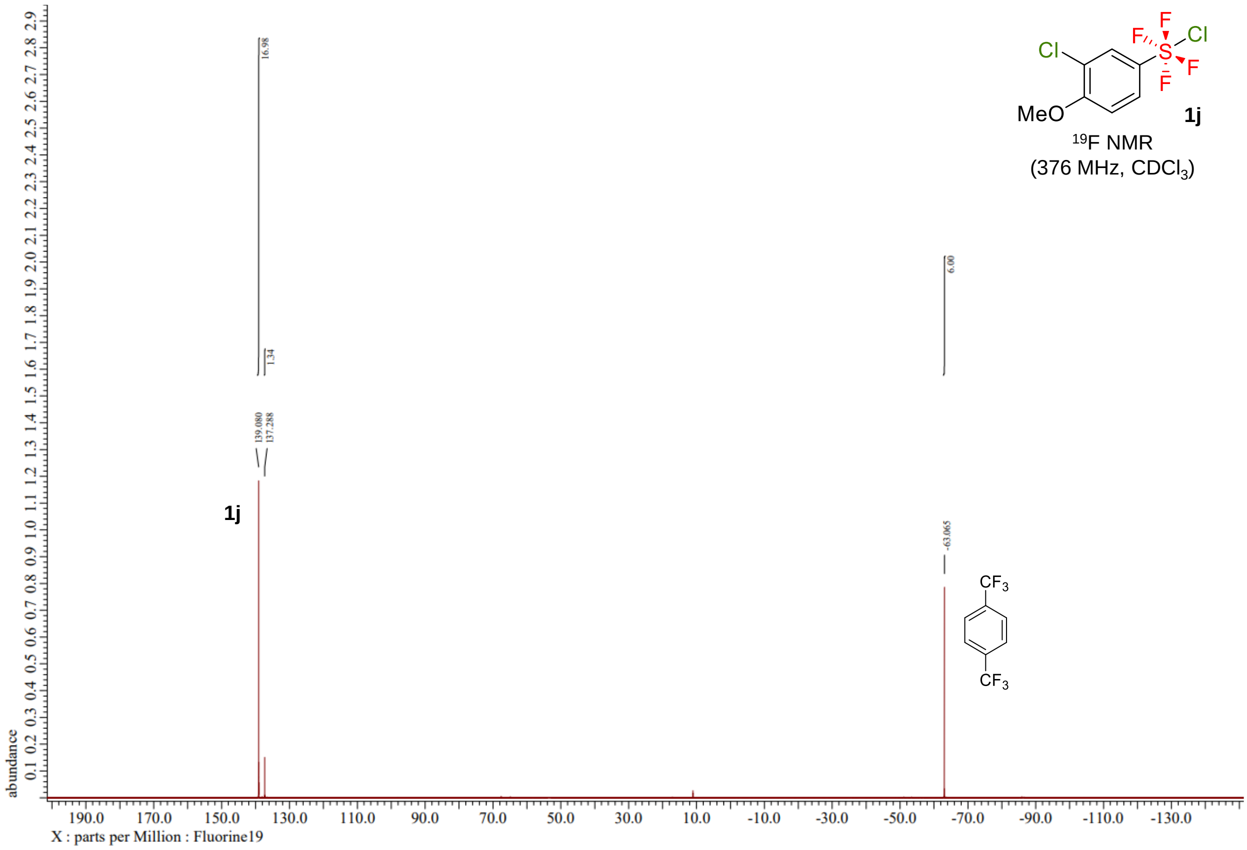

EtOOC
1h
19F NMR
(376 MHz, CH3CN)
ArSOF3
ArSO2F
ArSF3
Internal standard
abundance
X : parts per Million : Fluorine19


AcO
1i
^{19}F NMR
(376 MHz, CH_3CN)
1i
ArSOF3
ArSOF3
ArSF3
ArSF3
Internal standard
X : parts per Million : Fluorine19
abundance

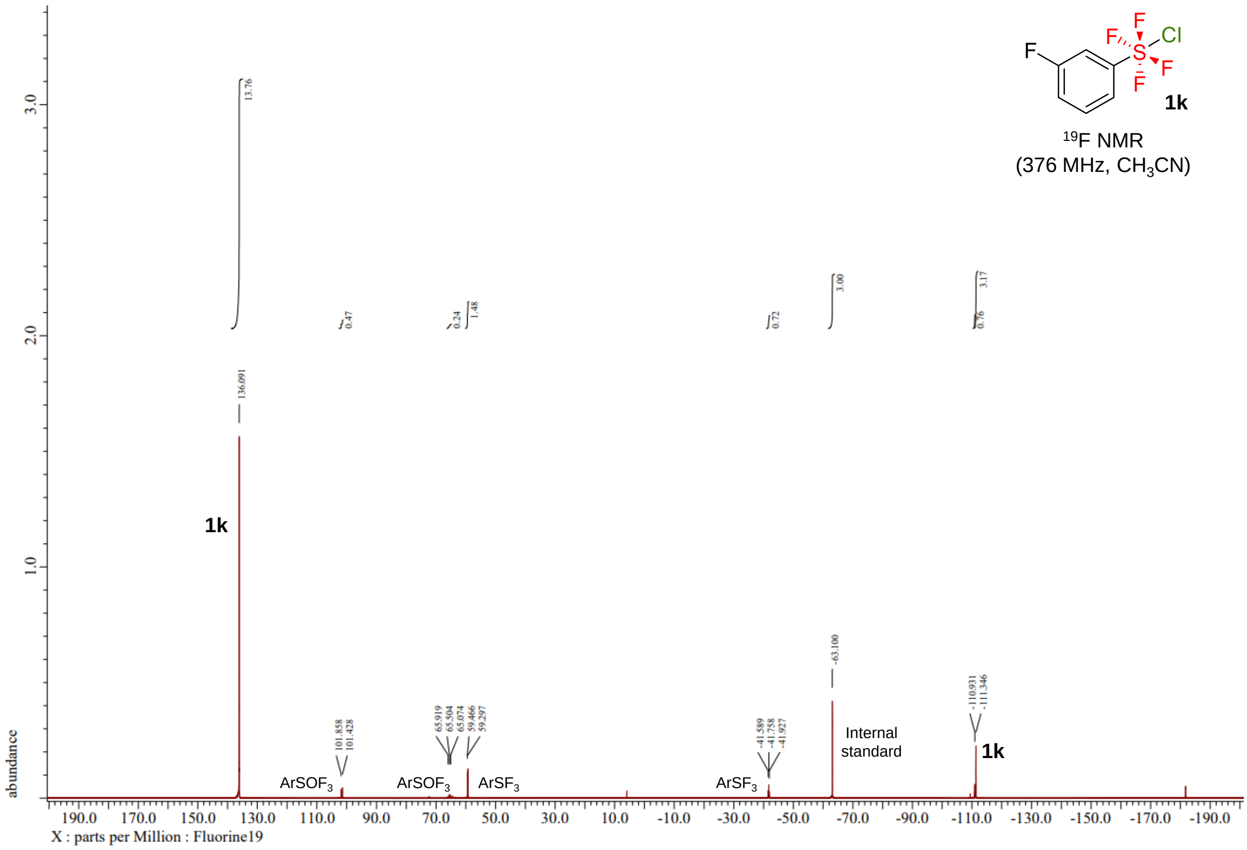

Cl
MeO
1j
^{19}F NMR
(376 MHz, CH_3CN)
1j
Internal standard
ArSOF3
ArSOF3
ArSF3
ArSF3
TFA
X : parts per Million : Fluorine19
abundance

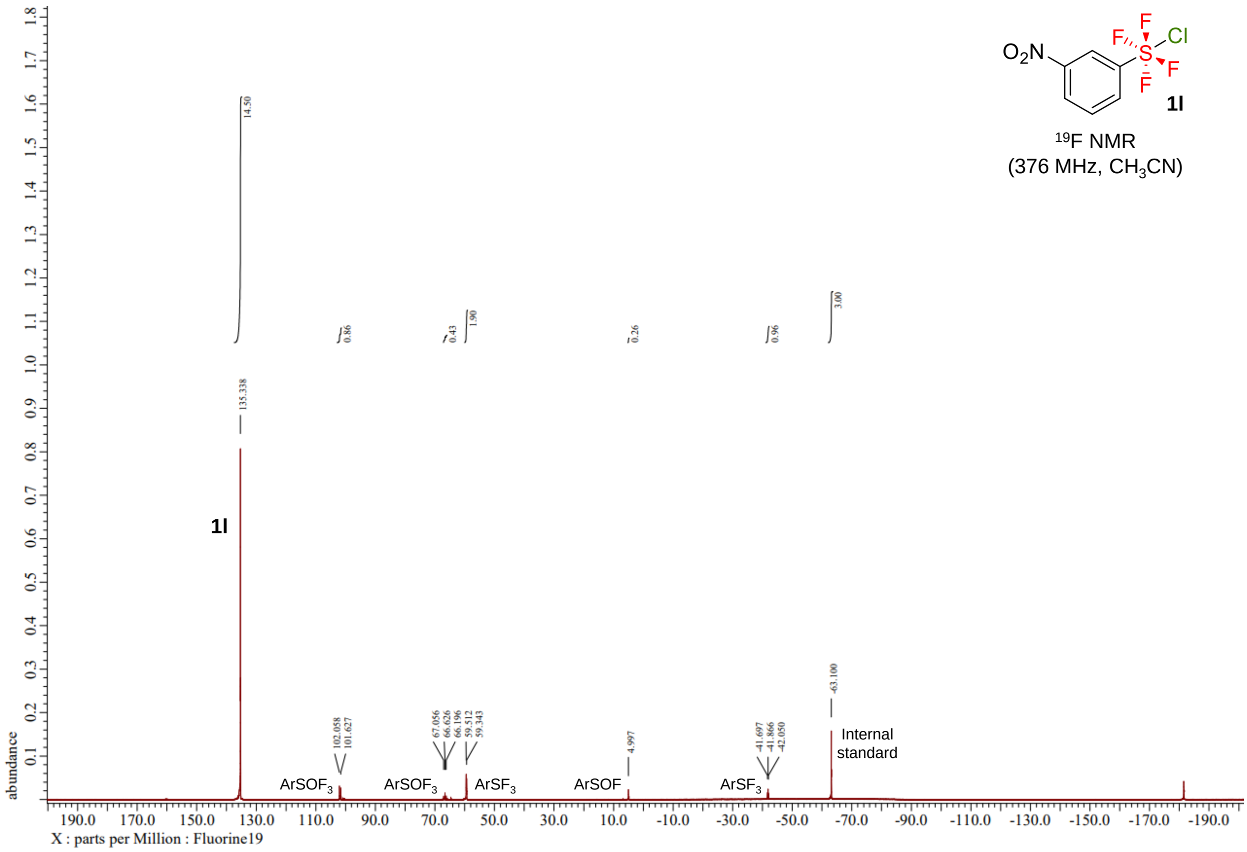


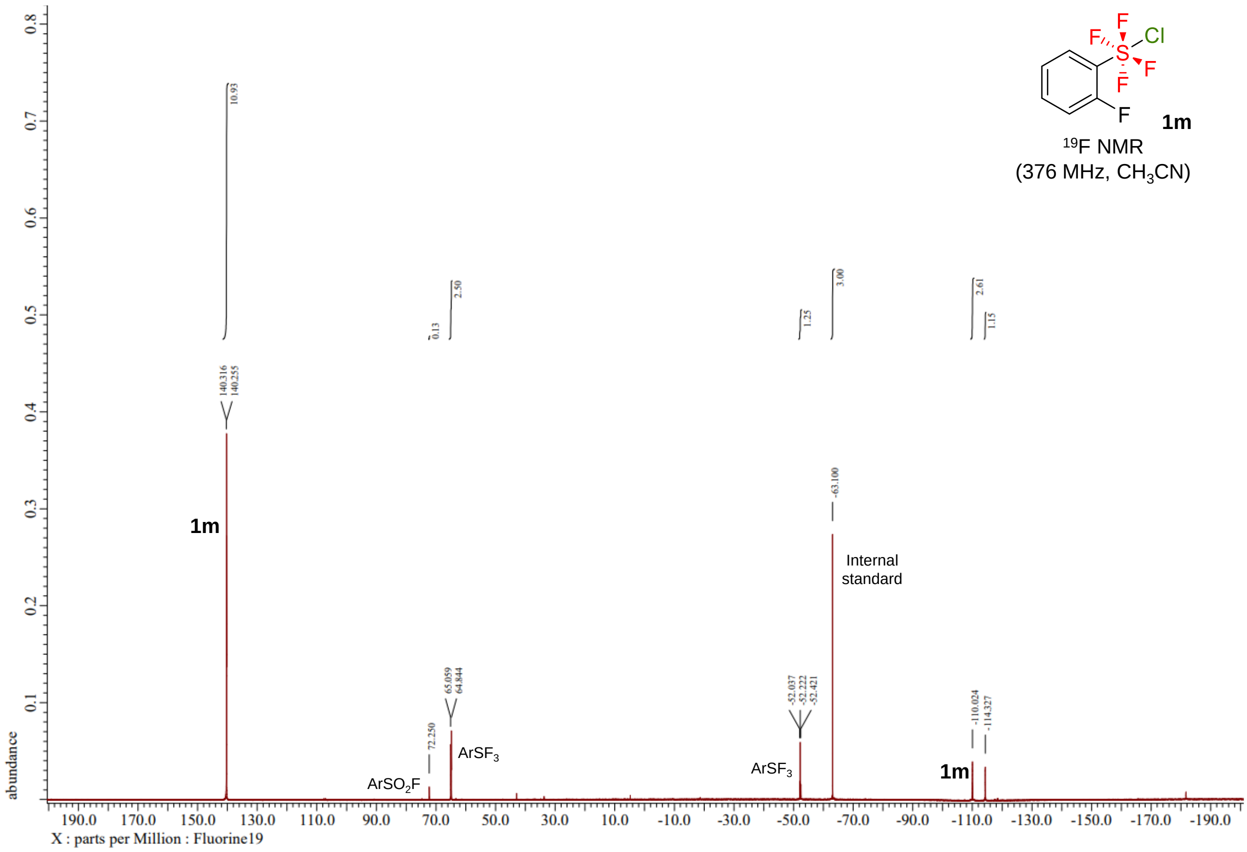
1j +
CF3
CF3
1j
1H NMR
(400 MHz, CDCl3)
X : parts per Million : Proton
abundance

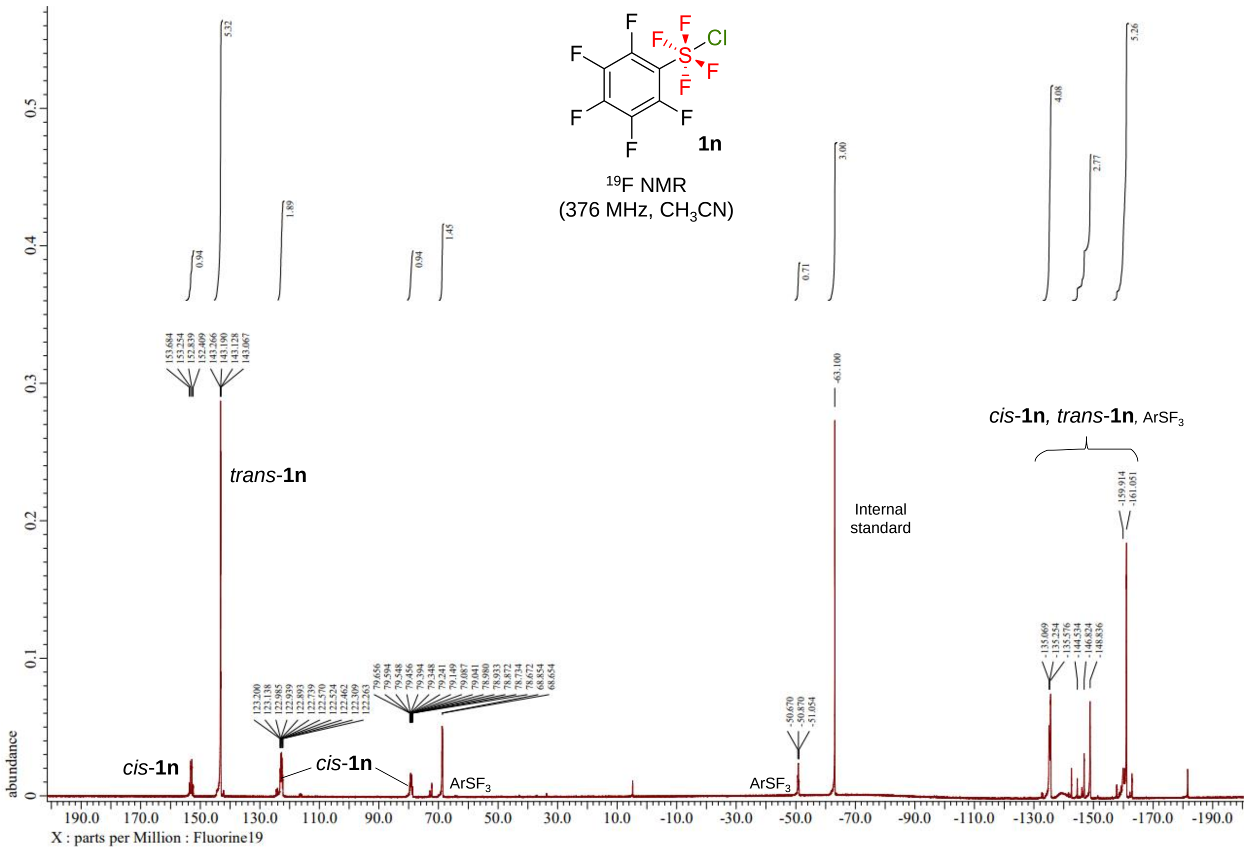


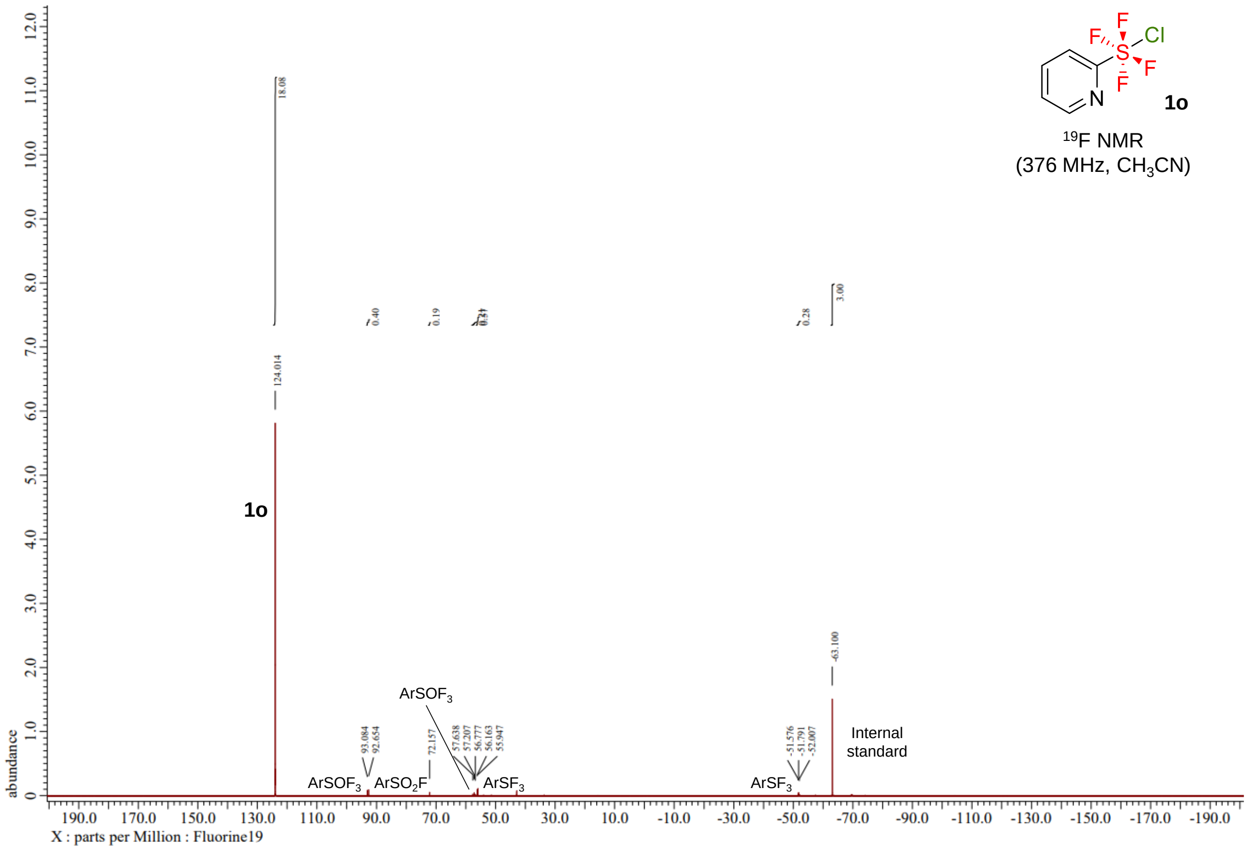
1j
19F NMR
(376 MHz, CDCl3)
CF3
CF3
X : parts per Million : Fluorine19
abundance

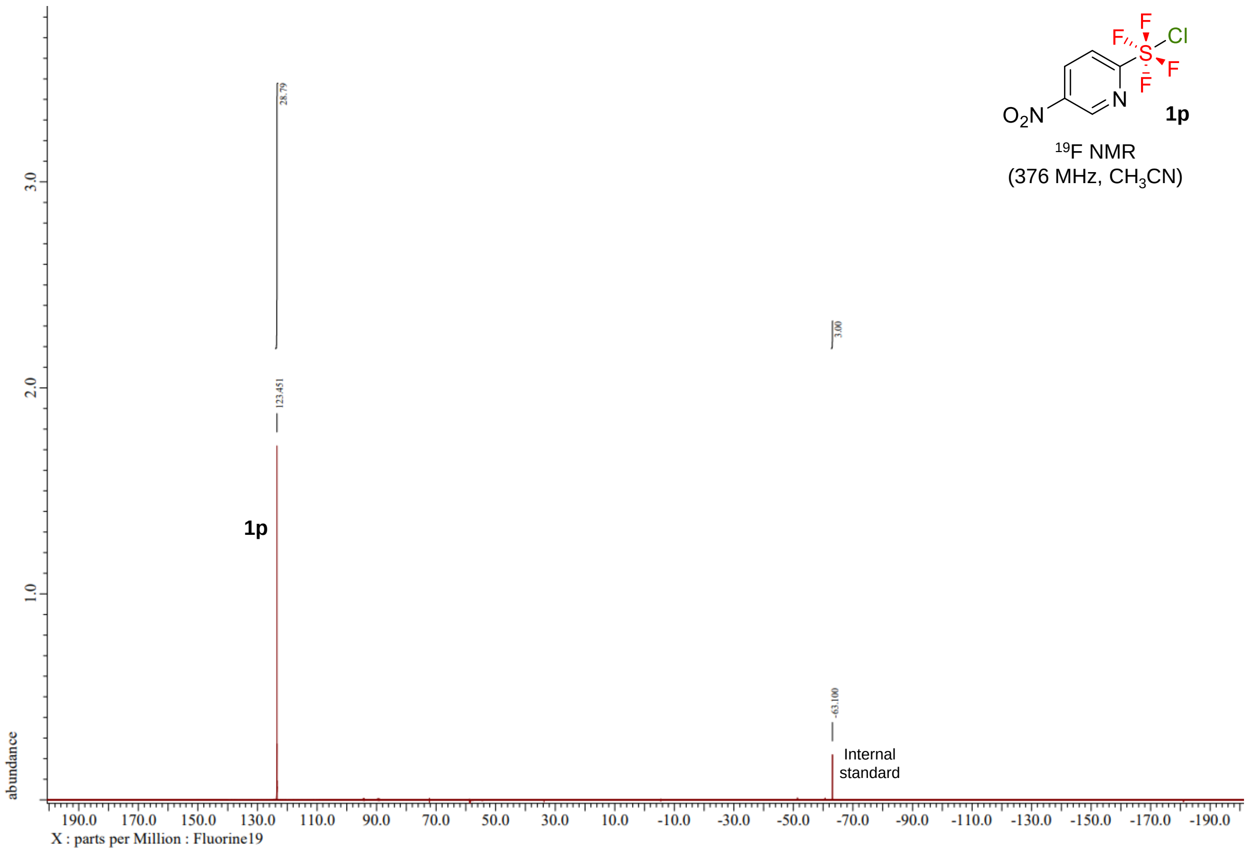

F
F
Cl
F
S
F
F
1k
^{19}F NMR
(376 MHz, CH_3CN)
1k
ArSOF$_3$
ArSOF$_3$
ArSF$_3$
ArSF$_3$
Internal standard
1k
abundance
X : parts per Million : Fluorine19

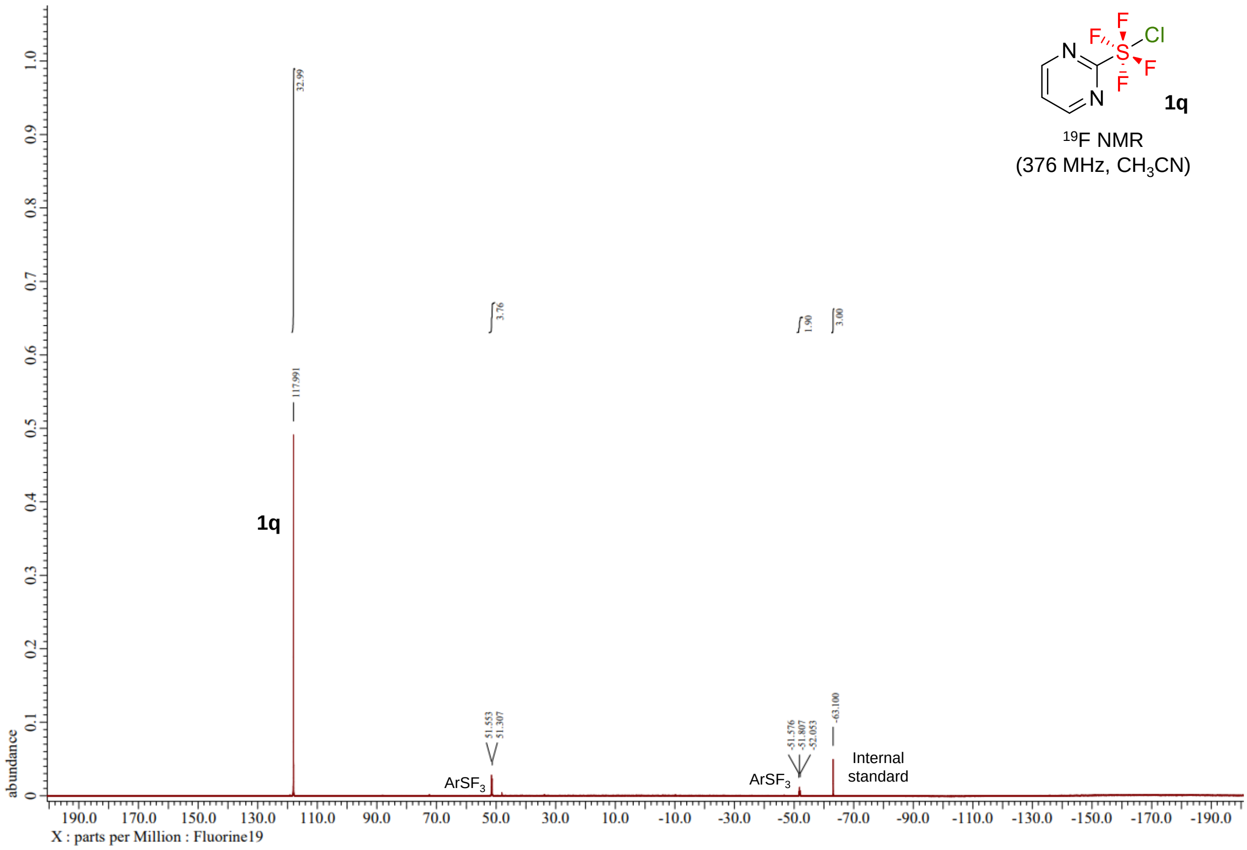

O_2N
F
Cl
F
S
F
F
1l
^{19}F NMR
(376 MHz, CH_3CN)
1l
ArSOF$_3$
ArSOF$_3$
ArSF$_3$
ArSOF
ArSF$_3$
Internal standard
abundance
X : parts per Million : Fluorine19

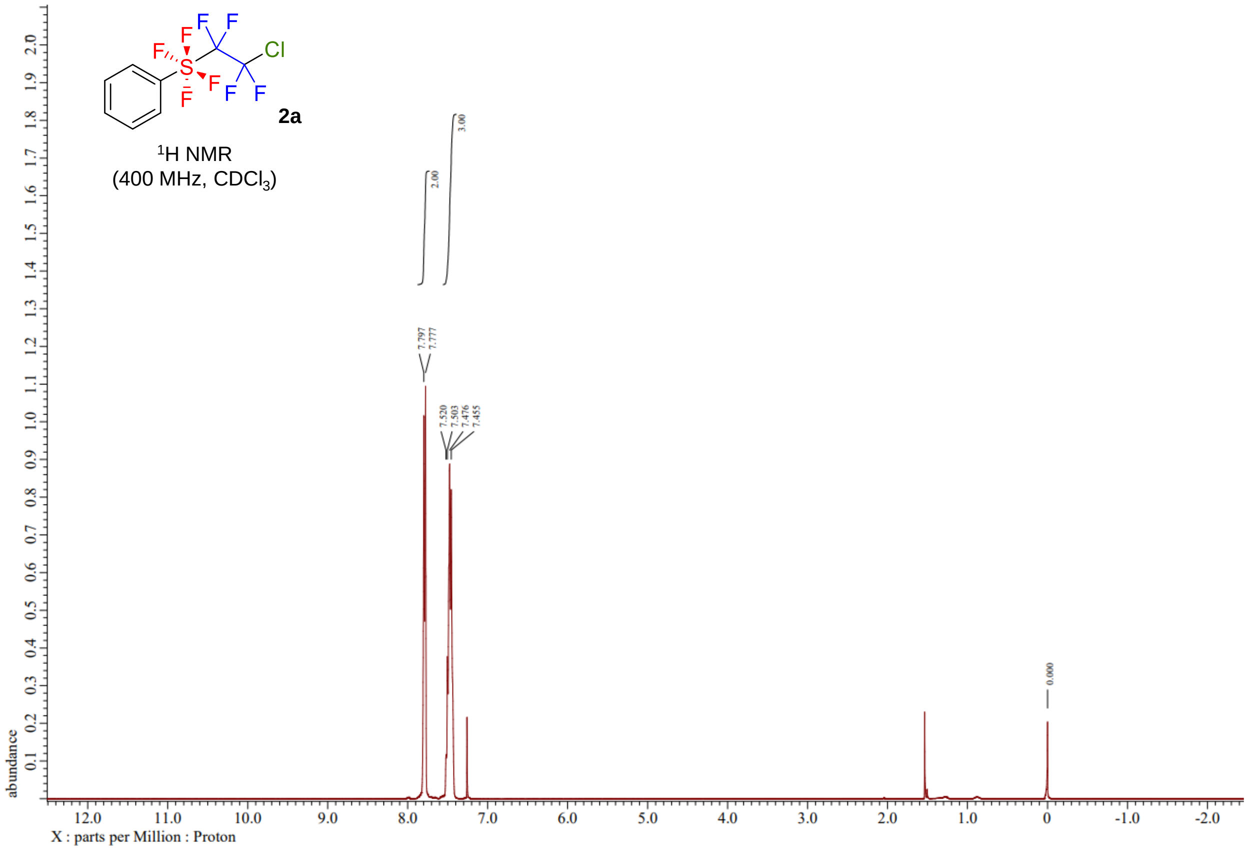

1m
^{19}F NMR
(376 MHz, CH_3CN)
1m
Internal standard
$ArSO_2F$
$ArSF_3$
$ArSF_3$
1m
abundance
X : parts per Million : Fluorine19

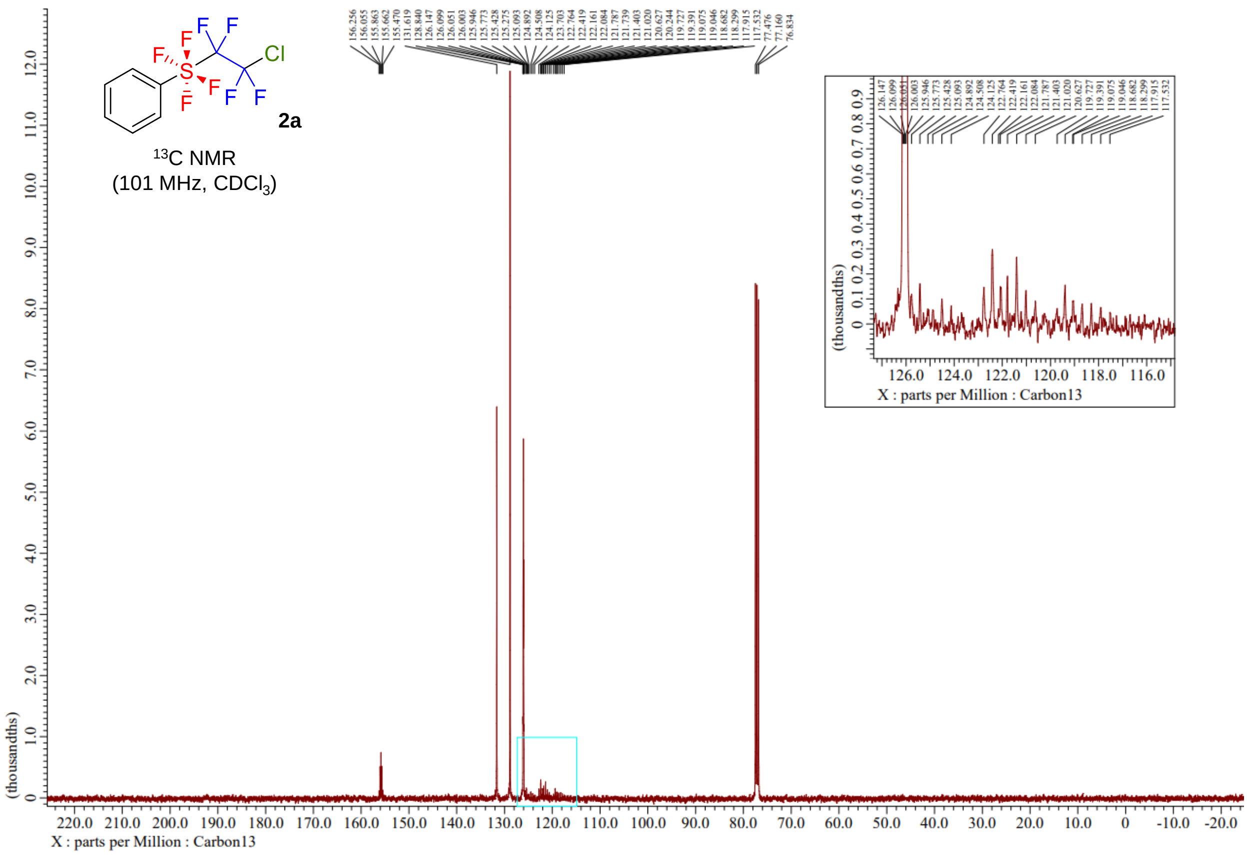

1n
^{19}F NMR
(376 MHz, CH_3CN)
trans-**1n**
cis-**1n**
cis-**1n**
$ArSF_3$
$ArSF_3$
Internal standard
cis-**1n**, *trans*-**1n**, $ArSF_3$
abundance
X : parts per Million : Fluorine19

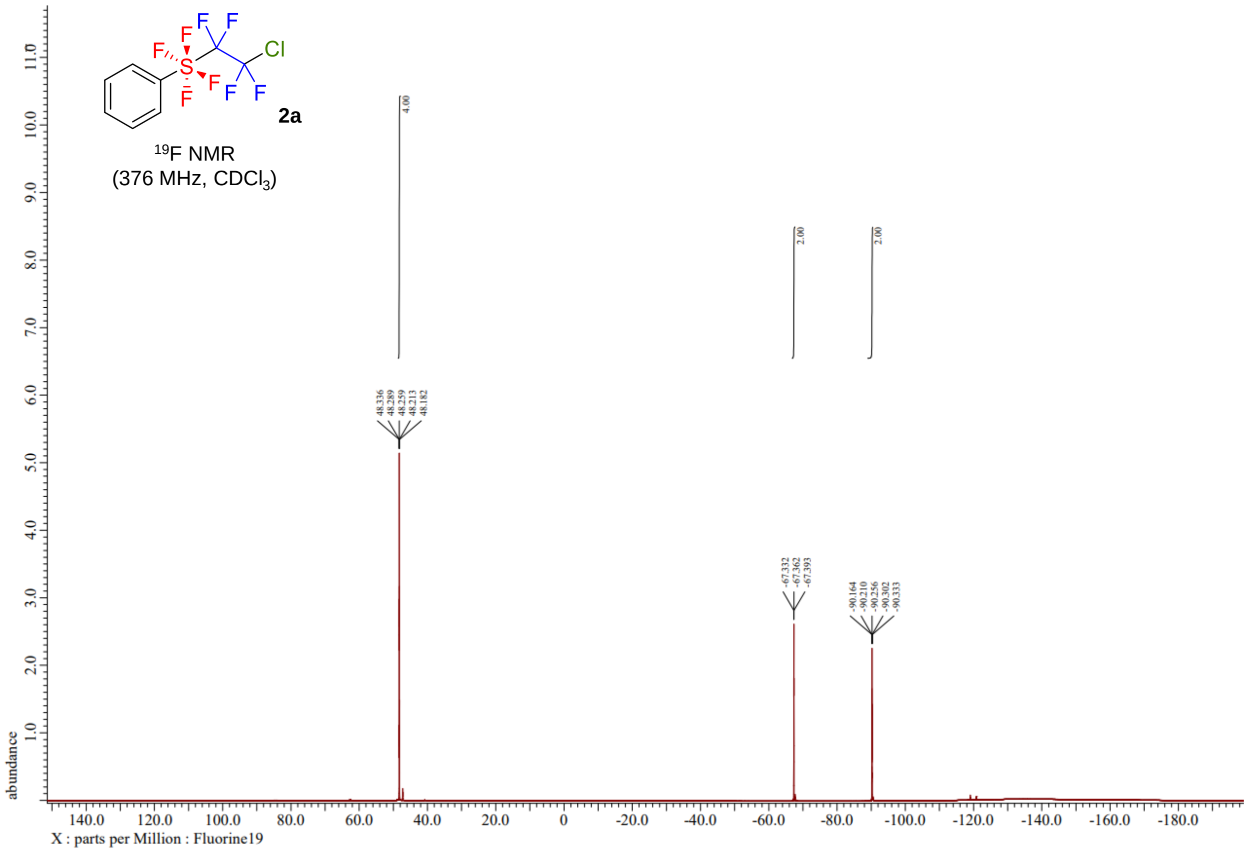

1o
19F NMR
(376 MHz, CH3CN)
ArSOF3
ArSOF3
ArSO2F
ArSF3
ArSF3
Internal
standard
abundance
X : parts per Million : Fluorine19

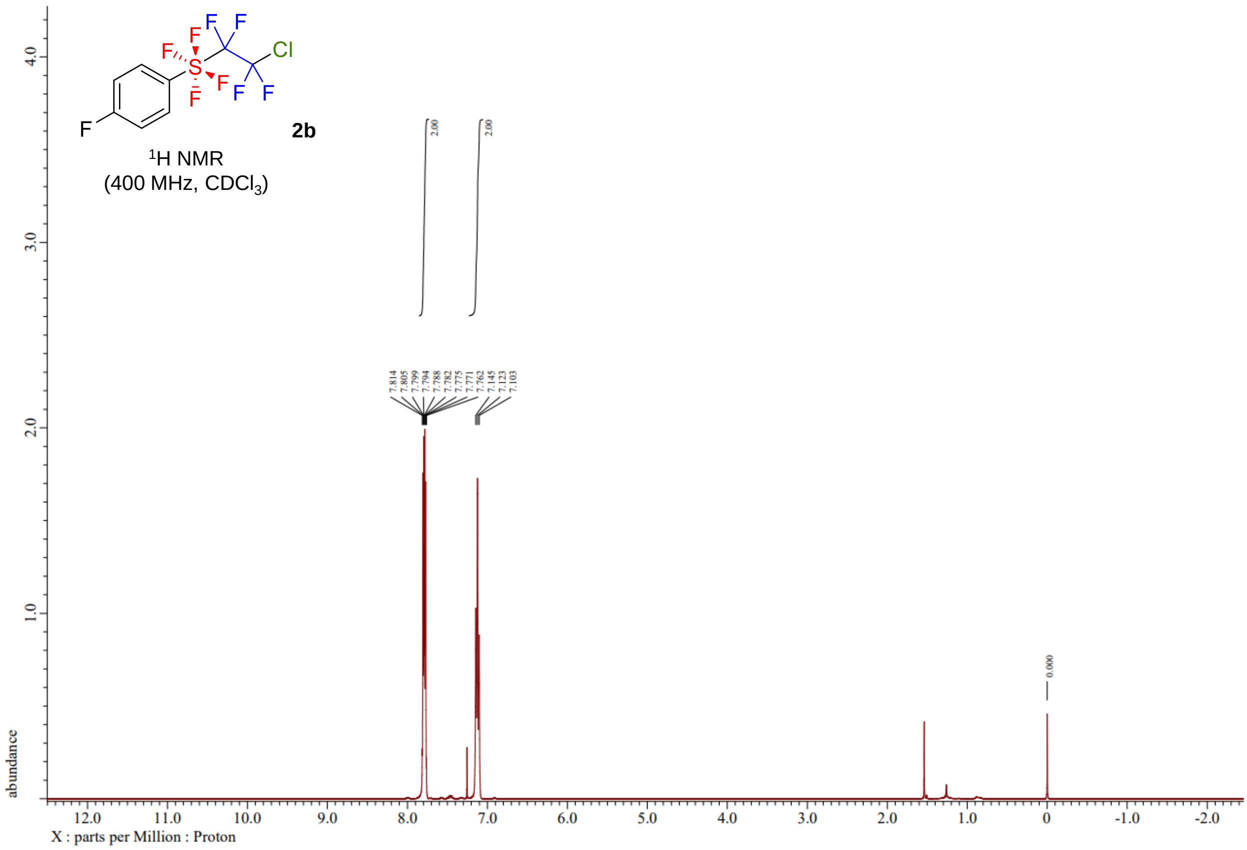

1p
19F NMR
(376 MHz, CH3CN)
Internal
standard
abundance
X : parts per Million : Fluorine19

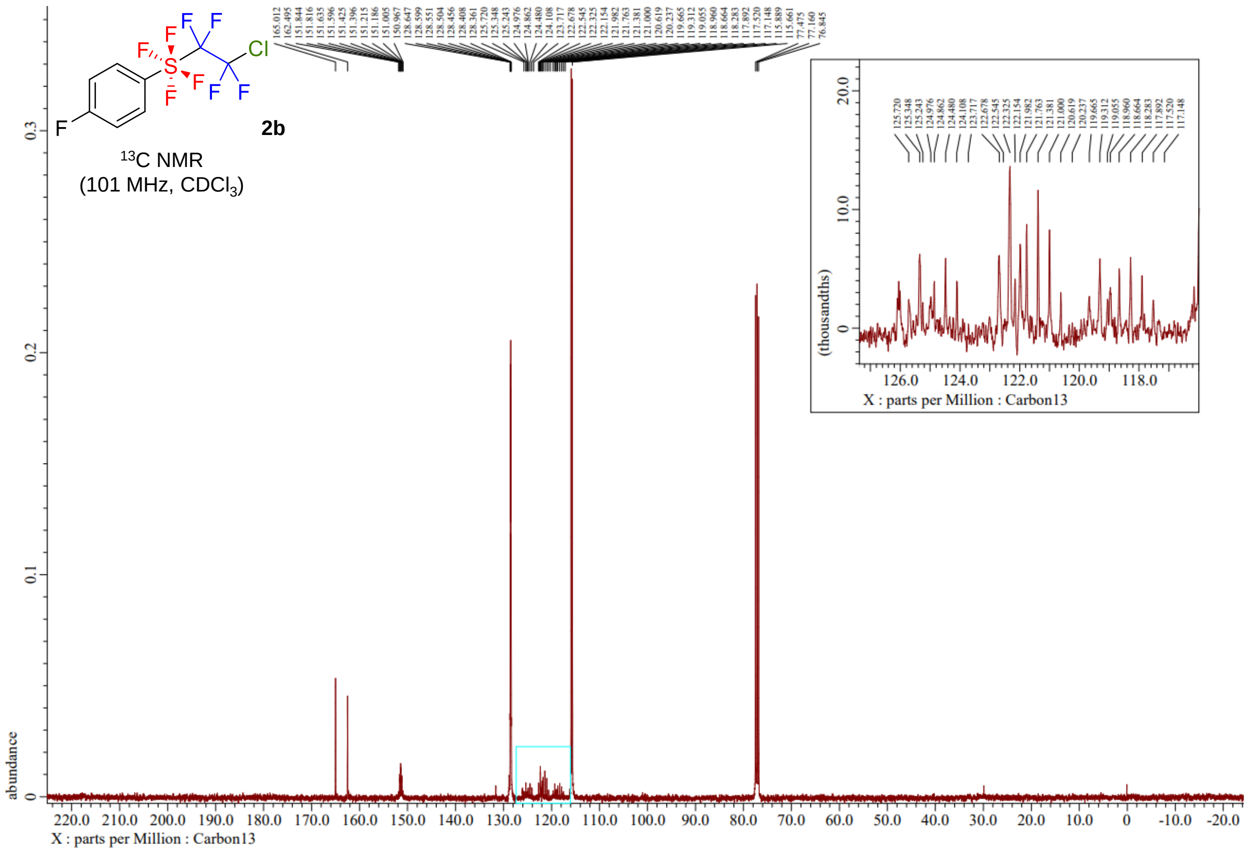

1q
19F NMR
(376 MHz, CH3CN)
32.99
3.76
1.90
3.00
117.991
51.553
51.307
-51.576
-51.807
-52.053
-63.100
ArSF3
ArSF3
Internal standard
abundance
X : parts per Million : Fluorine19

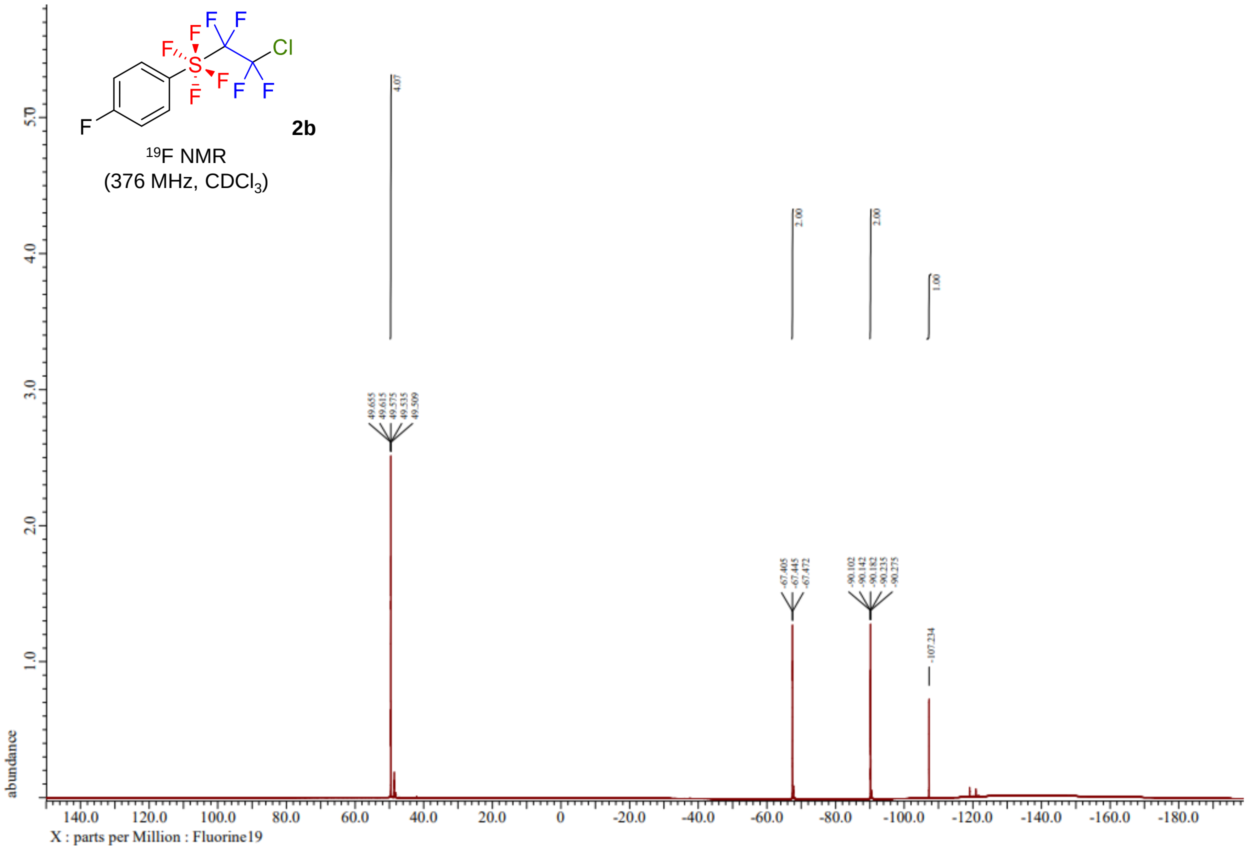

2a
1H NMR
(400 MHz, CDCl3)
X : parts per Million : Proton
abundance

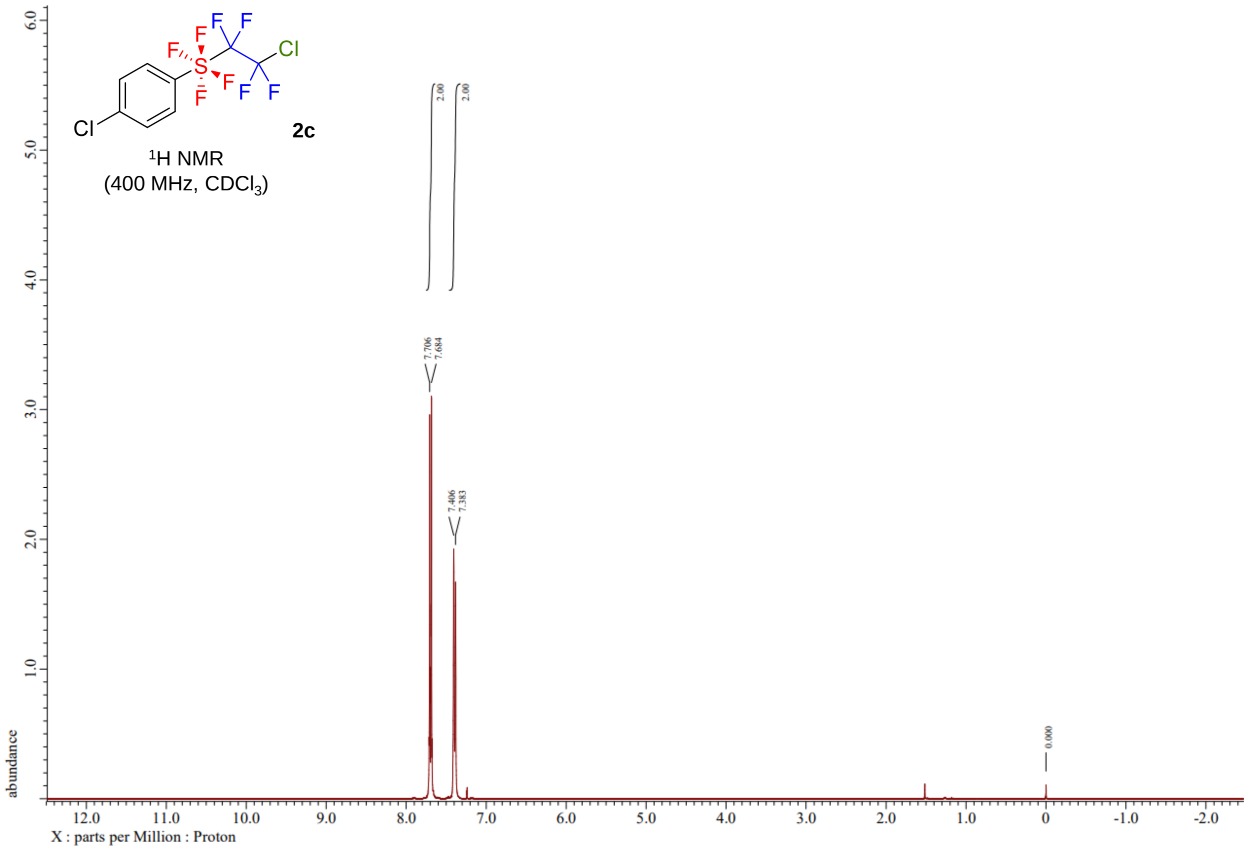

2a
13C NMR
(101 MHz, CDCl3)
X : parts per Million : Carbon13
(thousandths)

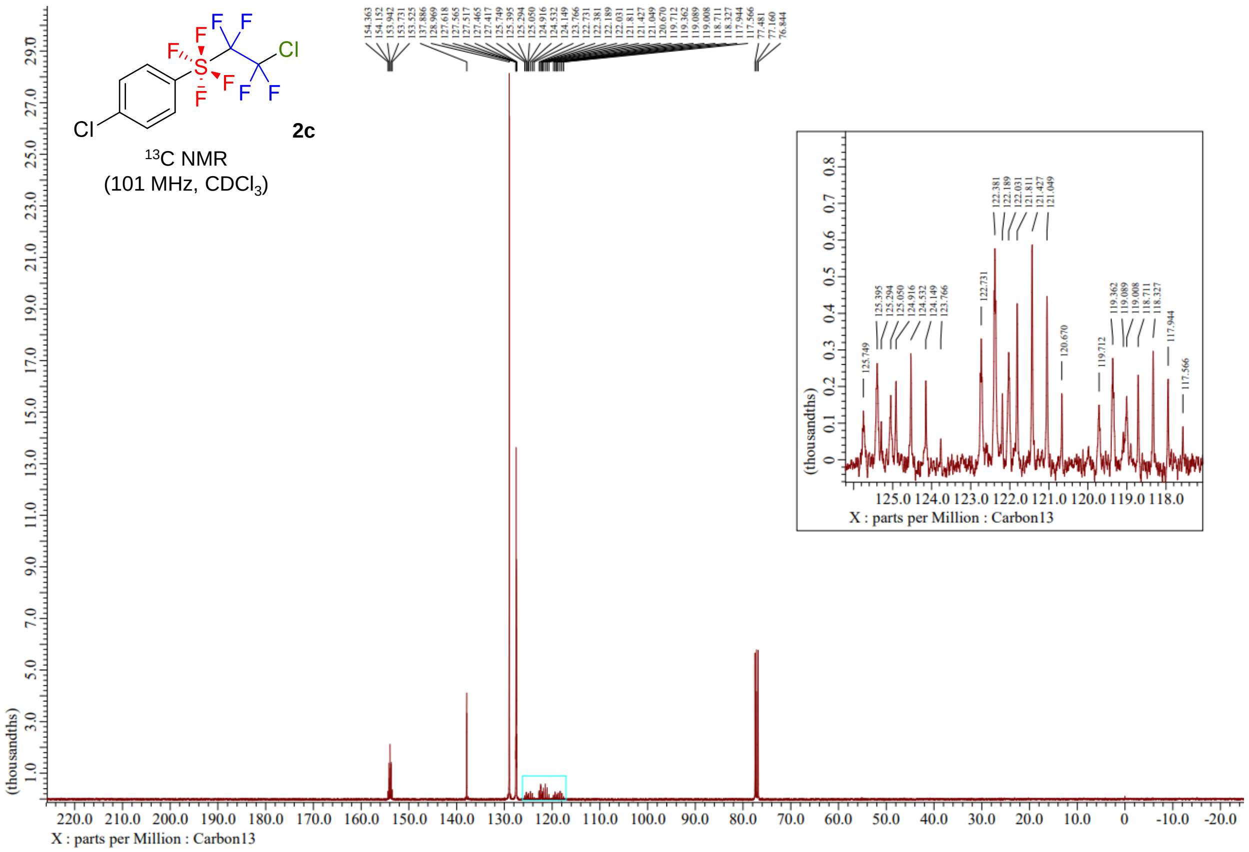

2a
^{19}F NMR
(376 MHz, $CDCl_3$)
4.00
2.00
2.00
48.336
48.289
48.259
48.213
48.182
-67.332
-67.362
-67.393
-90.164
-90.210
-90.256
-90.302
-90.333
abundance
X : parts per Million : Fluorine19

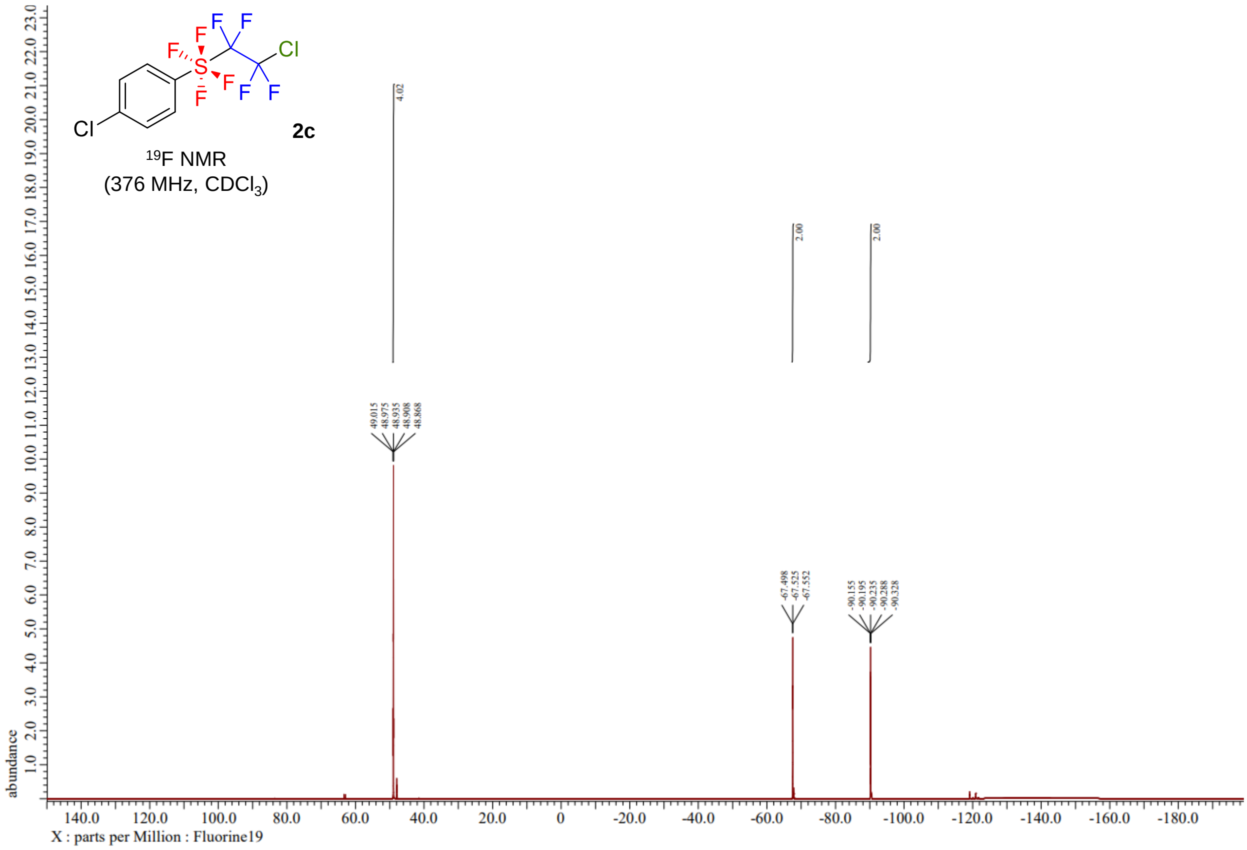

2b
^{1}H NMR
(400 MHz, $CDCl_3$)
2.00
2.00
7.814
7.805
7.799
7.794
7.788
7.782
7.775
7.771
7.762
7.145
7.123
7.103
0.000
abundance
X : parts per Million : Proton

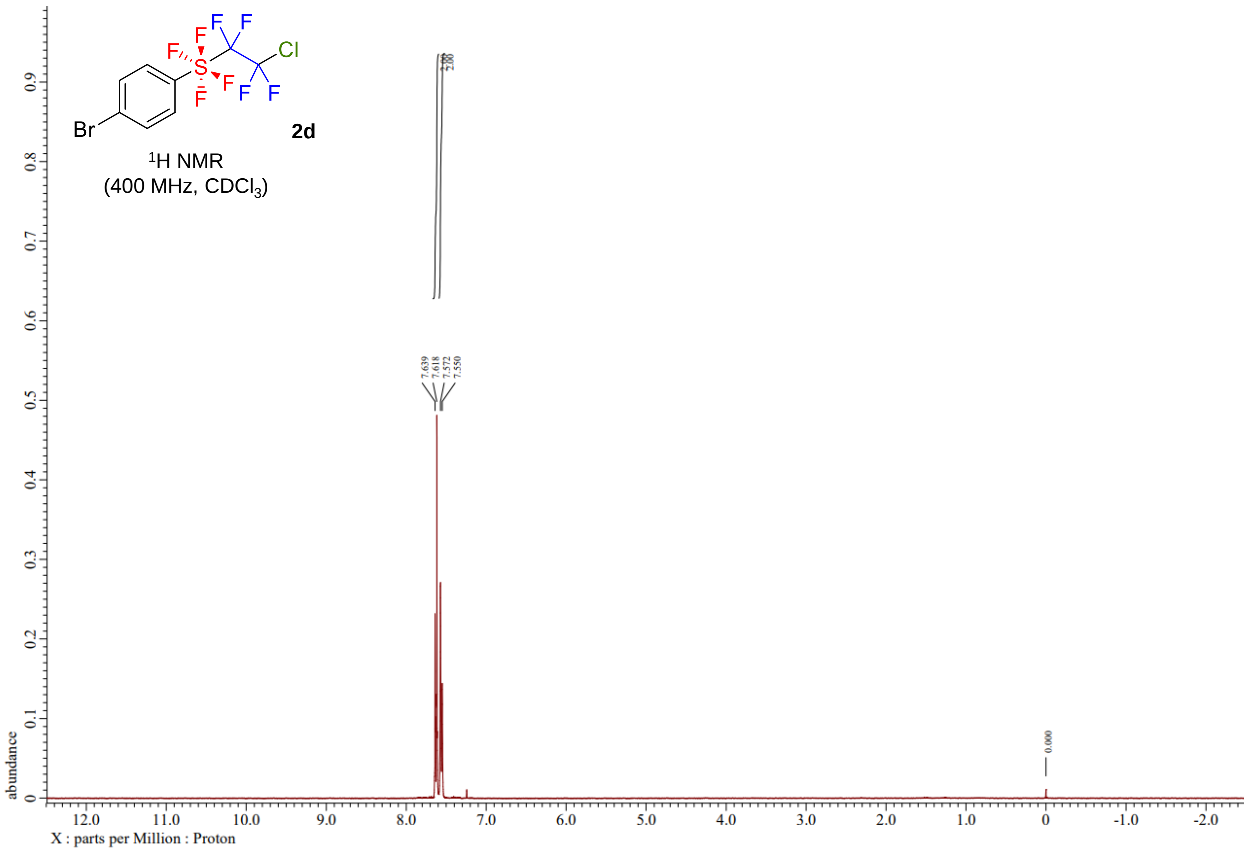

2b
^{13}C NMR
(101 MHz, $CDCl_3$)
X : parts per Million : Carbon13
abundance
X : parts per Million : Carbon13
(thousandths)

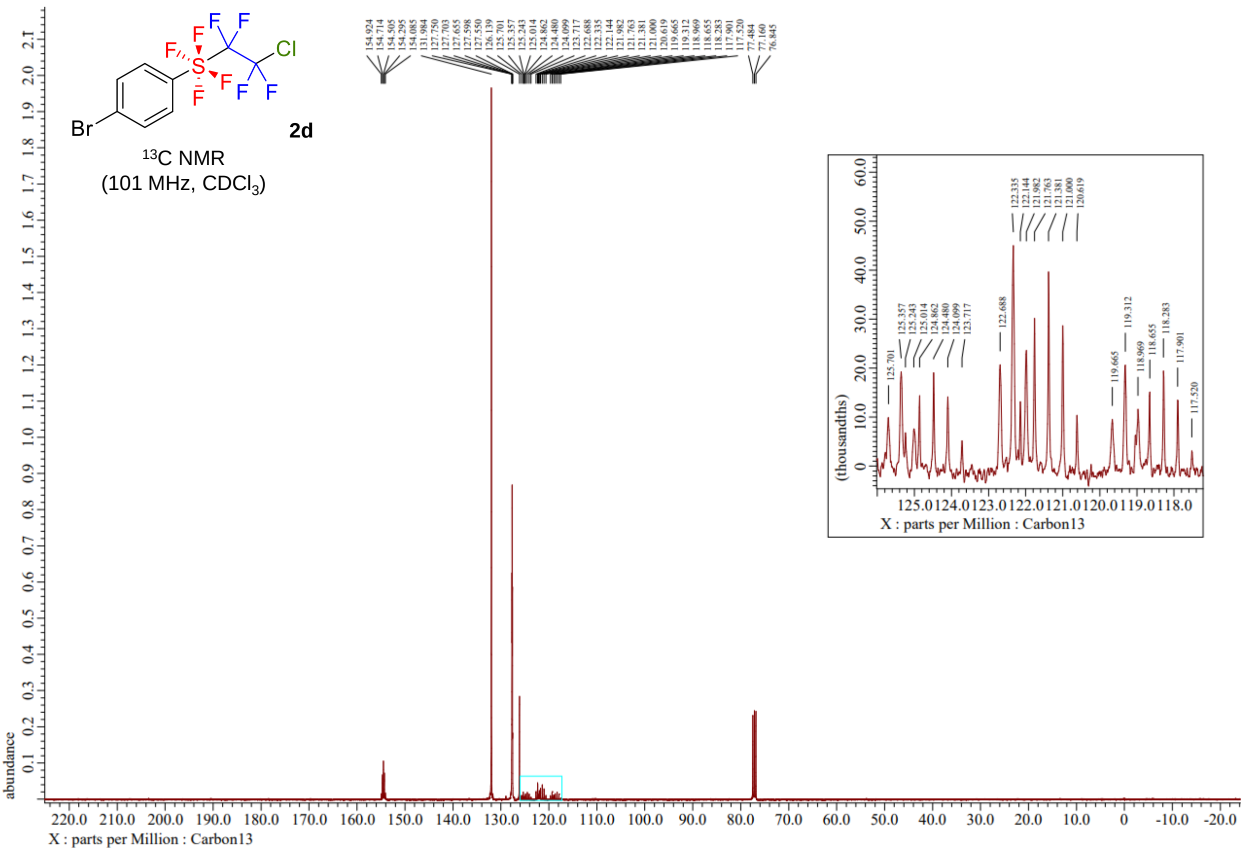

2b
^{19}F NMR
(376 MHz, $CDCl_3$)
X : parts per Million : Fluorine19
abundance

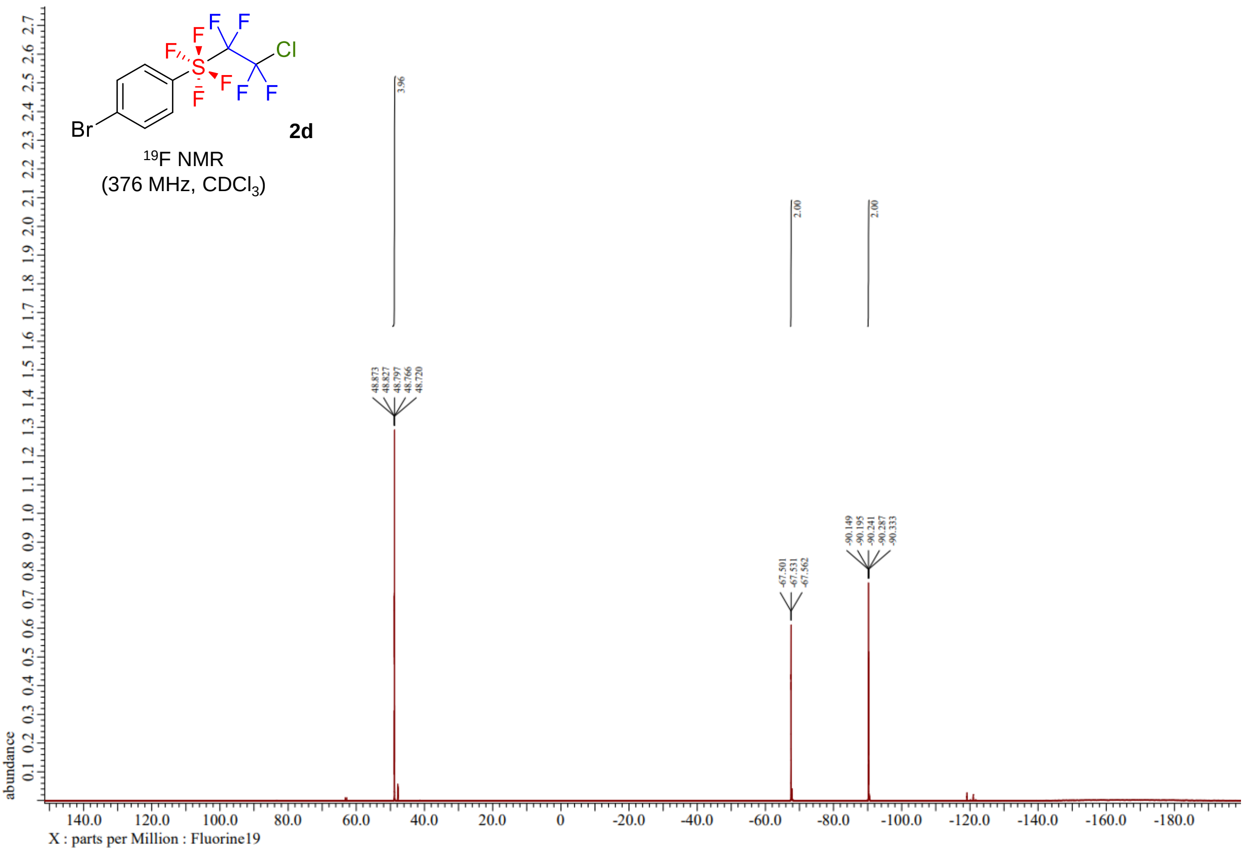

2c
^{1}H NMR
(400 MHz, CDCl$_3$)
X : parts per Million : Proton
abundance

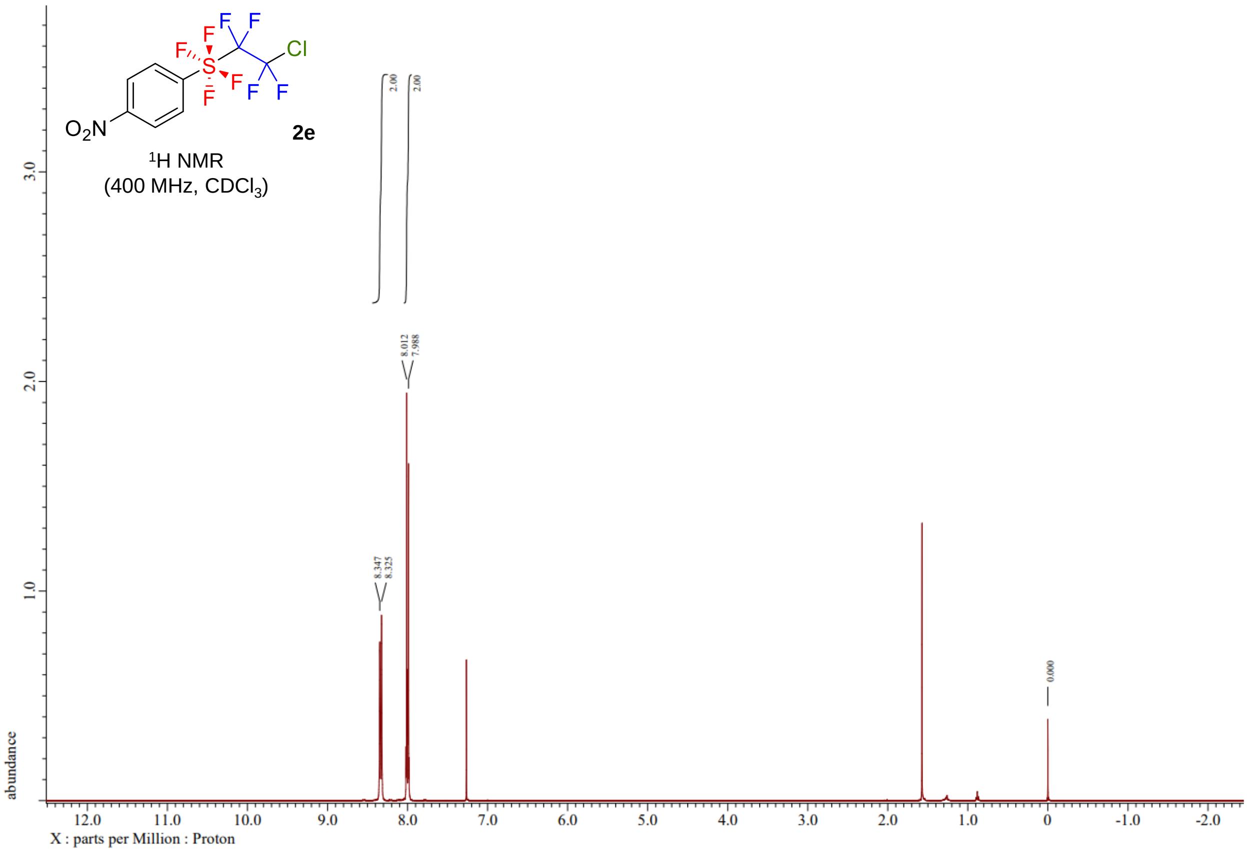

2c
^{13}C NMR
(101 MHz, CDCl$_3$)
X : parts per Million : Carbon13
(thousandths)


Cl
2c
19F NMR
(376 MHz, CDCl3)
X : parts per Million : Fluorine19
abundance

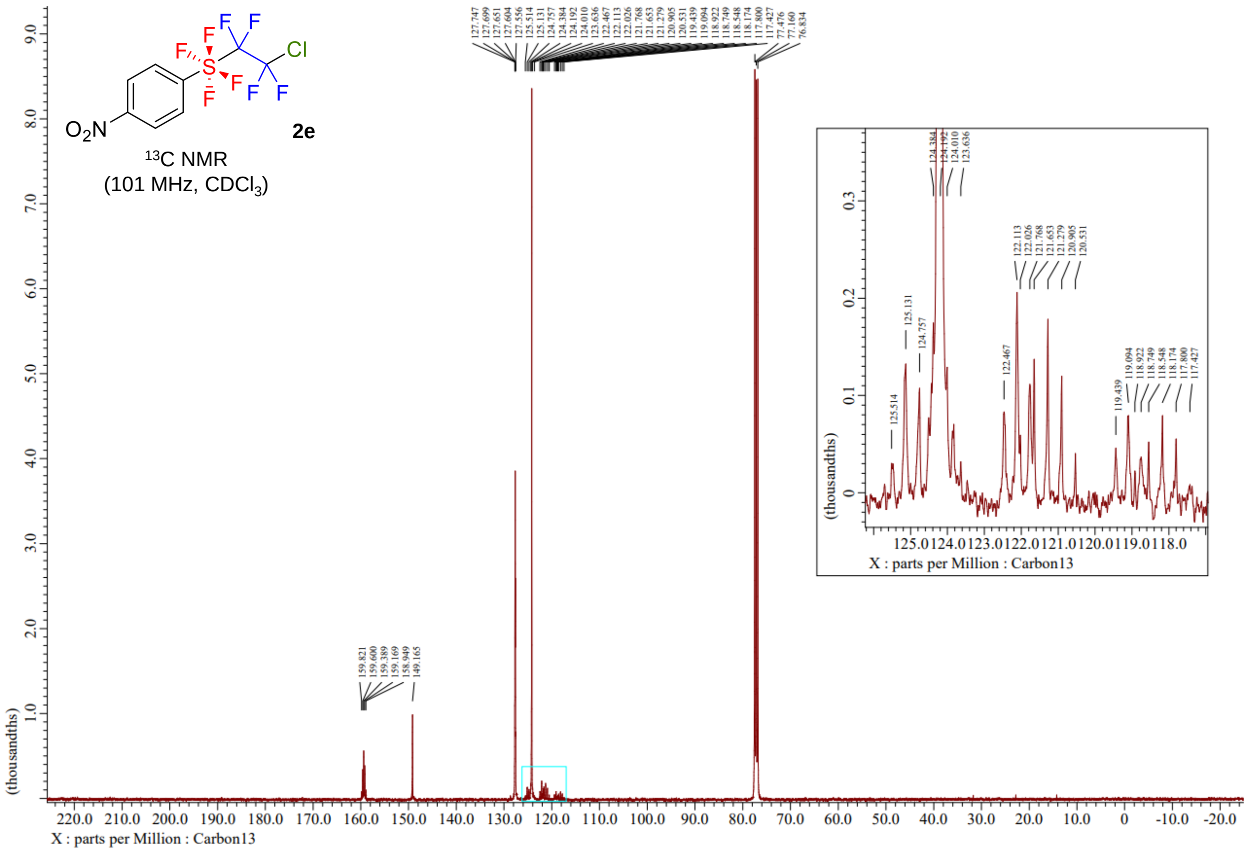

Br
2d
1H NMR
(400 MHz, CDCl3)
X : parts per Million : Proton
abundance


2d
^{13}C NMR
(101 MHz, $CDCl_3$)
abundance
X : parts per Million : Carbon13
X : parts per Million : Carbon13
(thousandths)

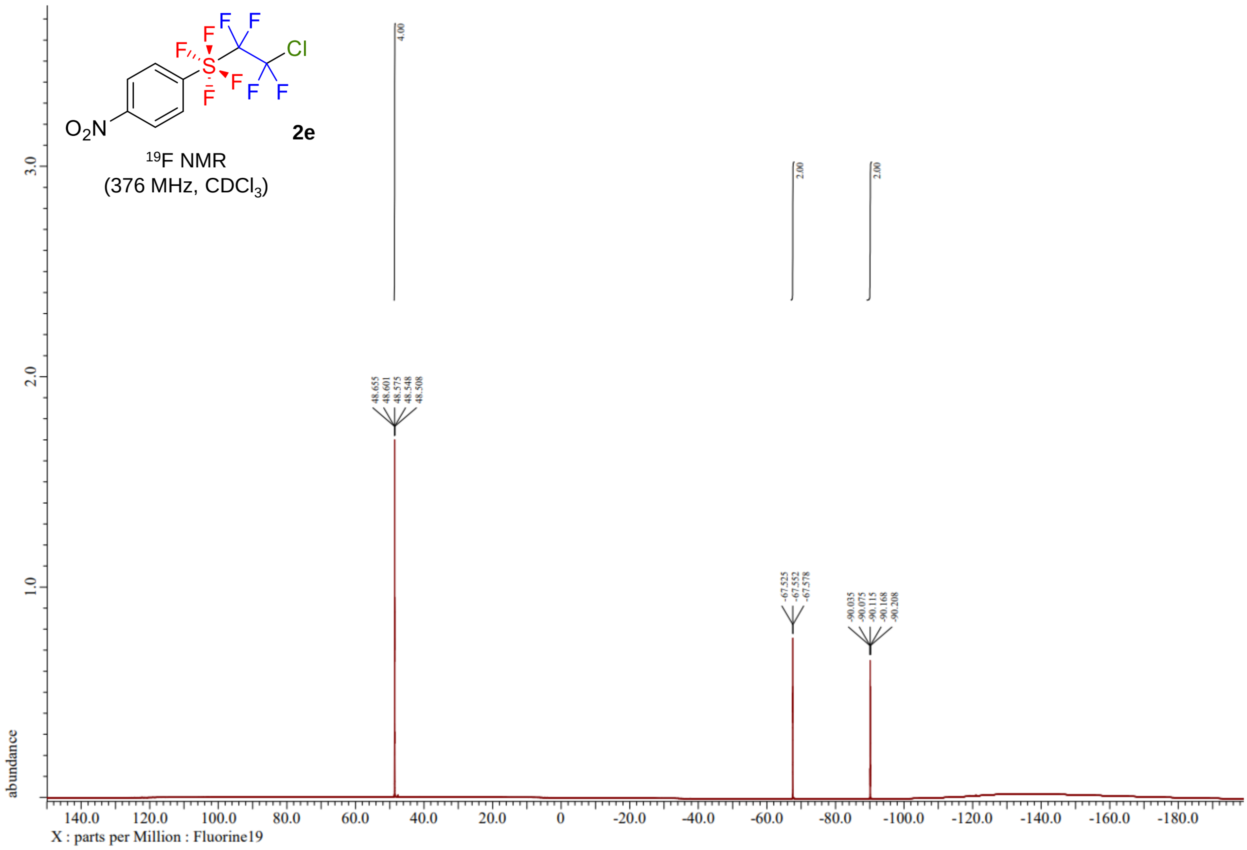

2d
^{19}F NMR
(376 MHz, $CDCl_3$)
abundance
X : parts per Million : Fluorine19
3.96
2.00
2.00



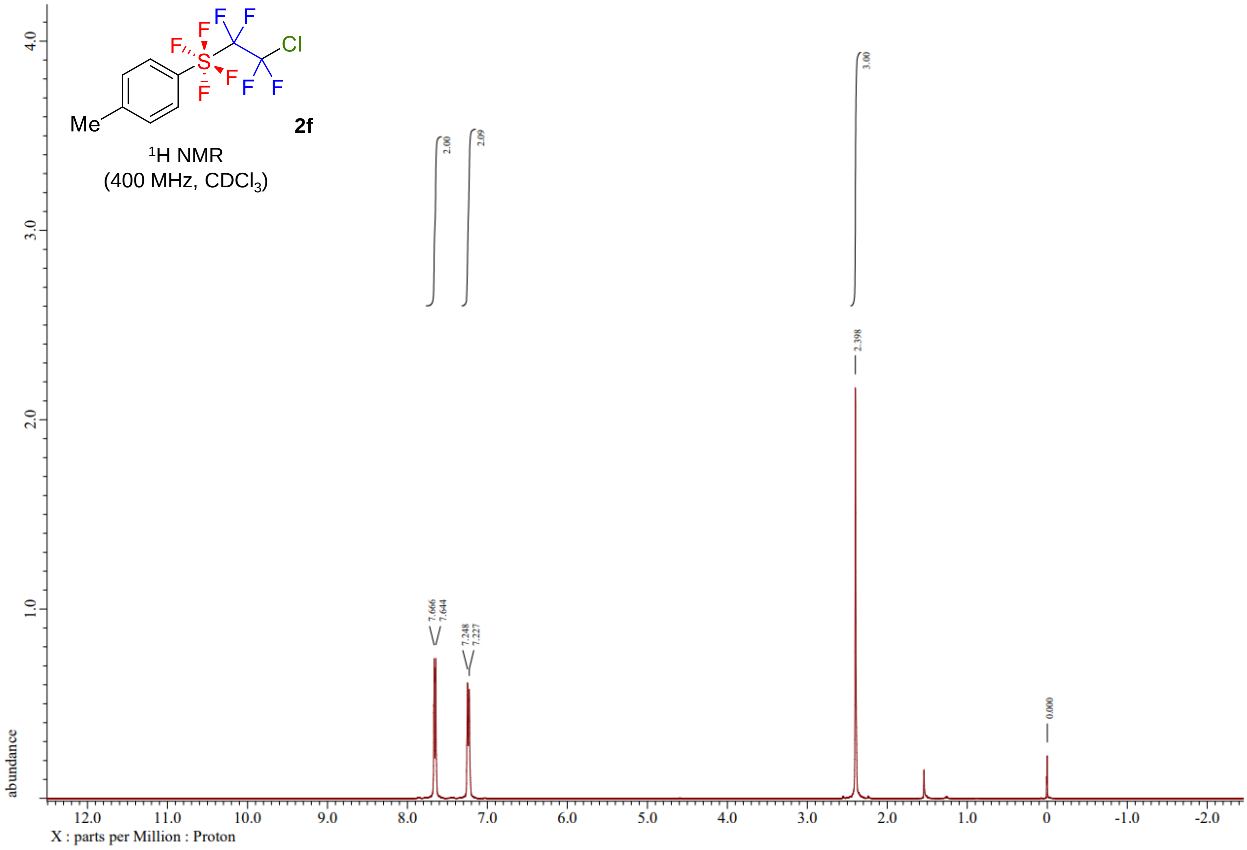
2e
^{1}H NMR
(400 MHz, CDCl$_3$)
abundance
X : parts per Million : Proton



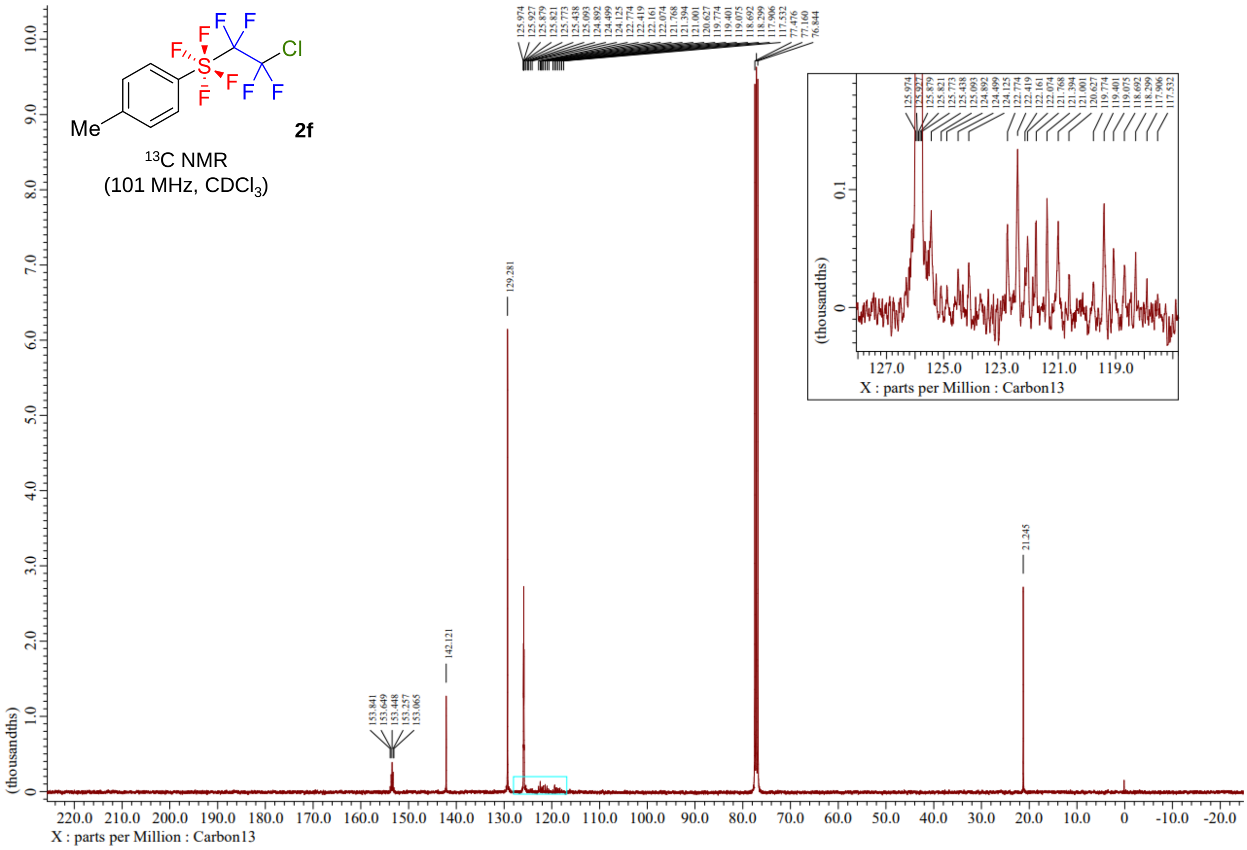
2e
^{13}C NMR
(101 MHz, CDCl$_3$)
(thousandths)
X : parts per Million : Carbon13

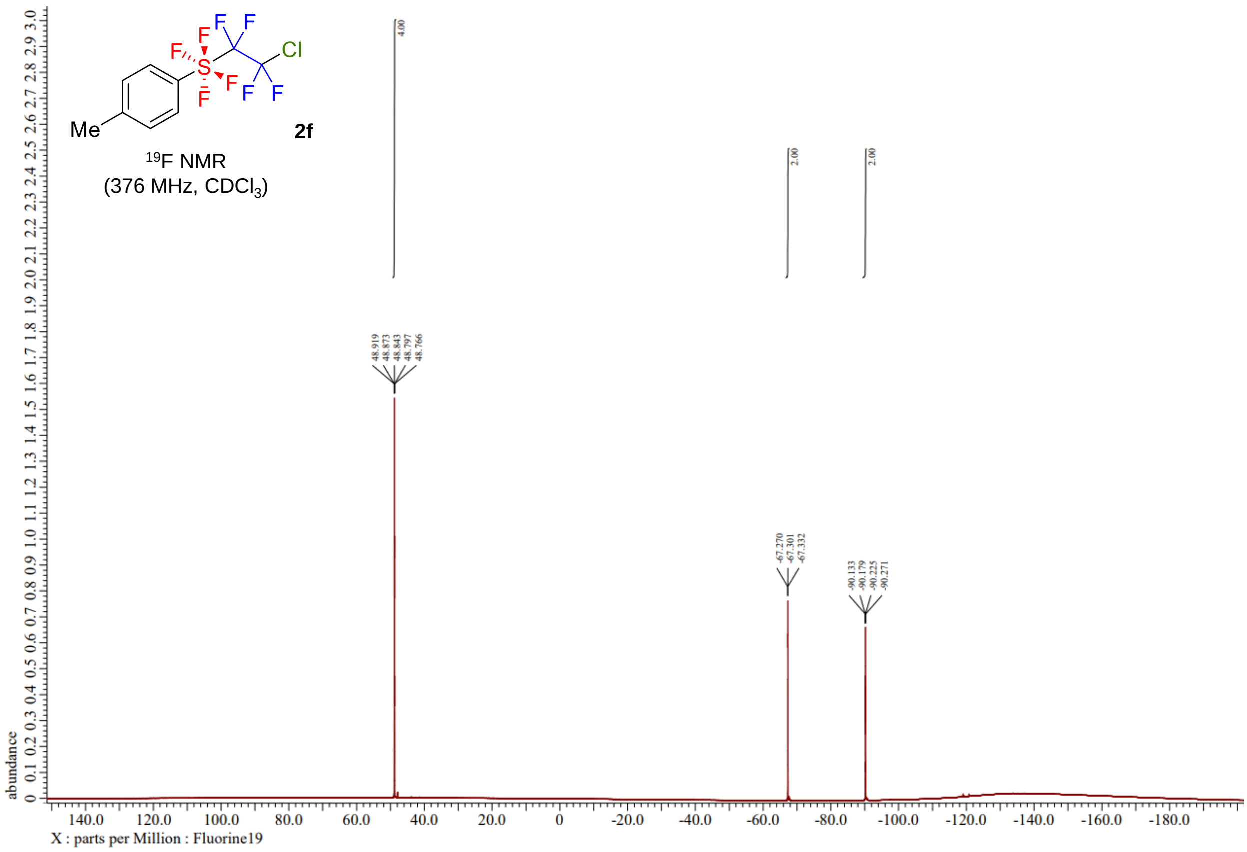


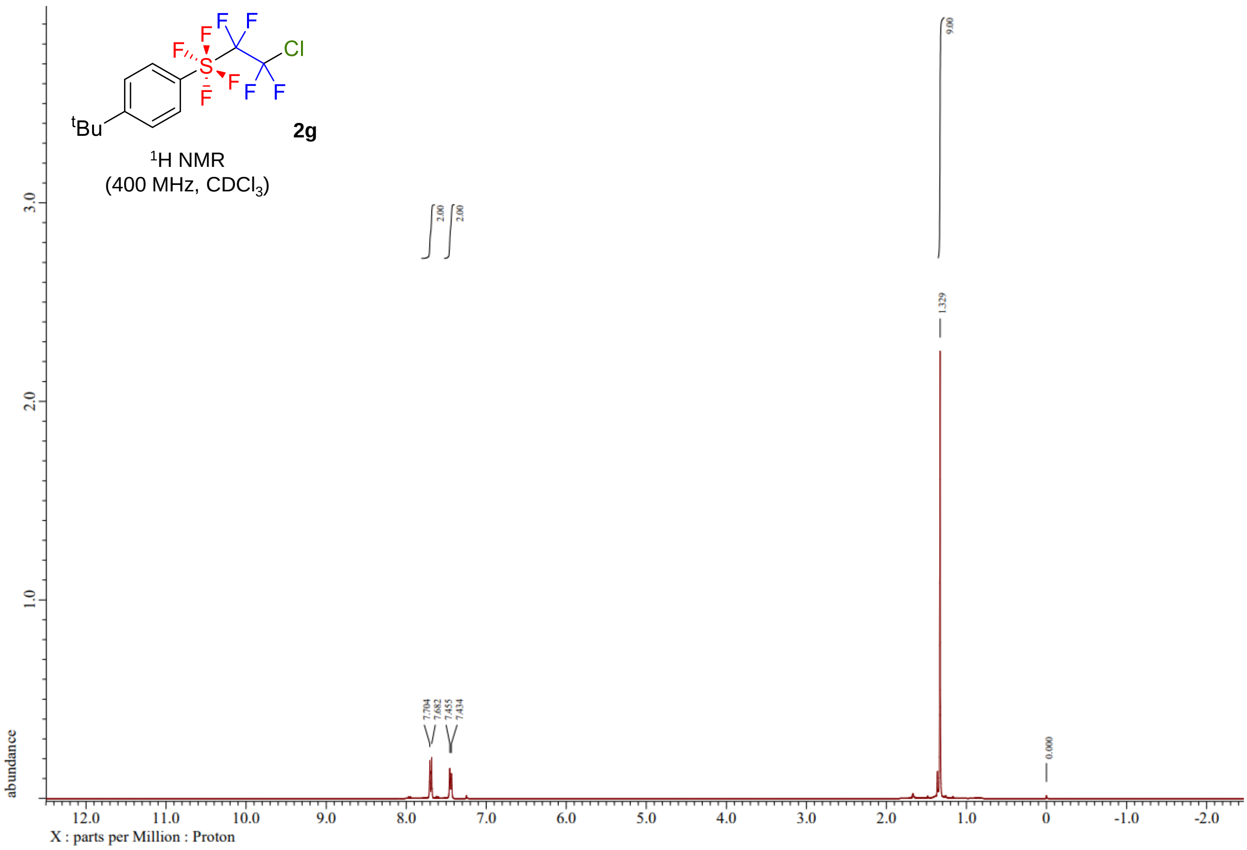
O2N
2e
19F NMR
(376 MHz, CDCl3)
48.655
48.601
48.575
48.548
48.508
-67.525
-67.552
-67.578
-90.035
-90.075
-90.115
-90.168
-90.208
4.00
2.00
2.00
abundance
X : parts per Million : Fluorine19



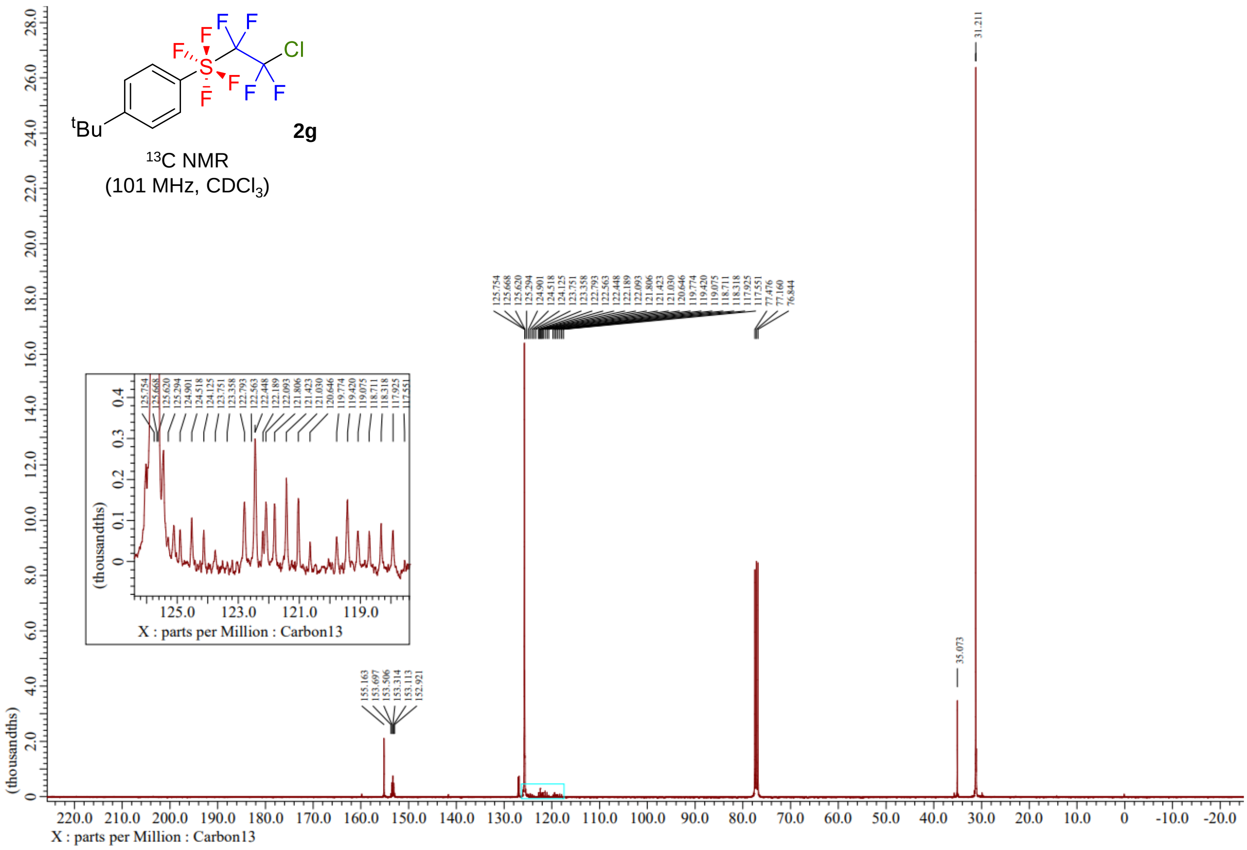
Me
2f
1H NMR
(400 MHz, CDCl3)
7.666
7.644
7.248
7.227
2.398
0.000
2.00
2.09
3.00
abundance
X : parts per Million : Proton


Me
2f
13C NMR
(101 MHz, CDCl3)
X : parts per Million : Carbon13
X : parts per Million : Carbon13

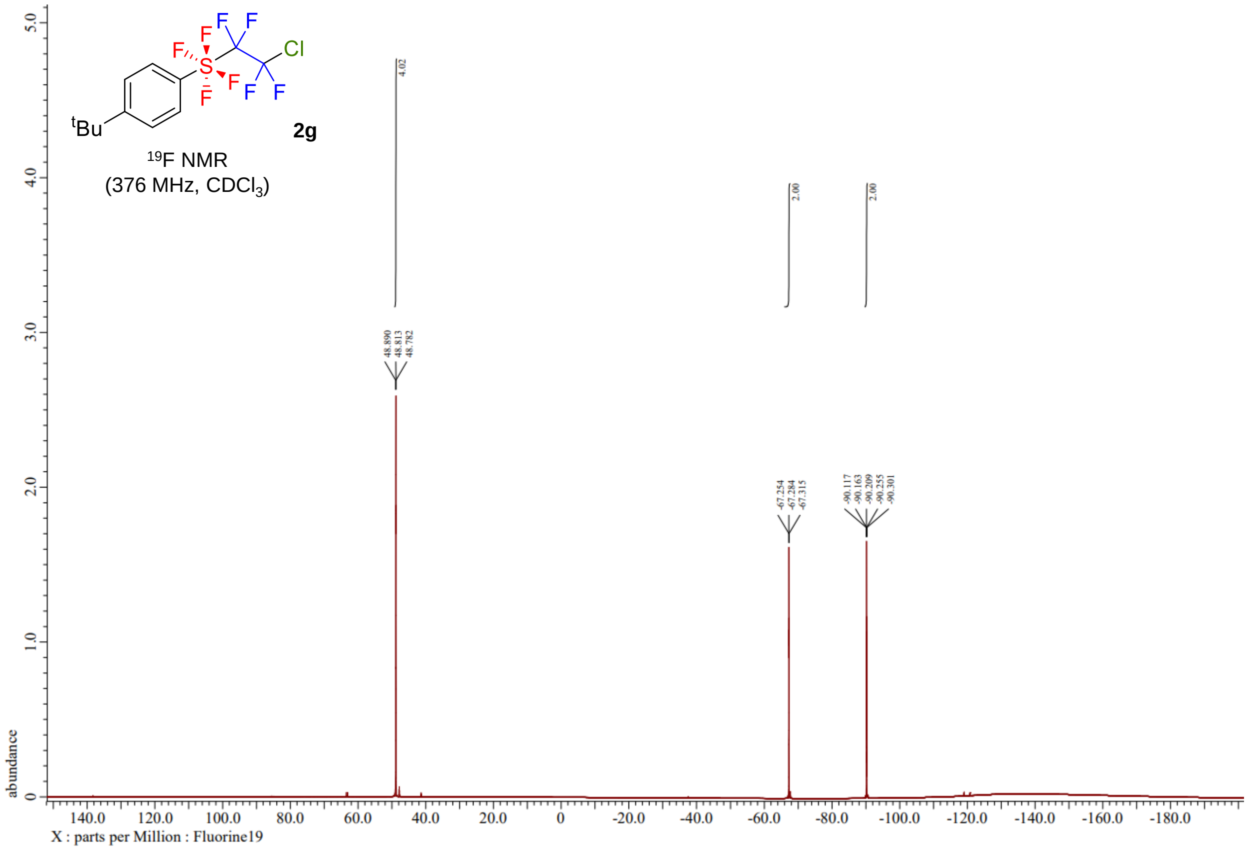

Me
2f
19F NMR
(376 MHz, CDCl3)
X : parts per Million : Fluorine19



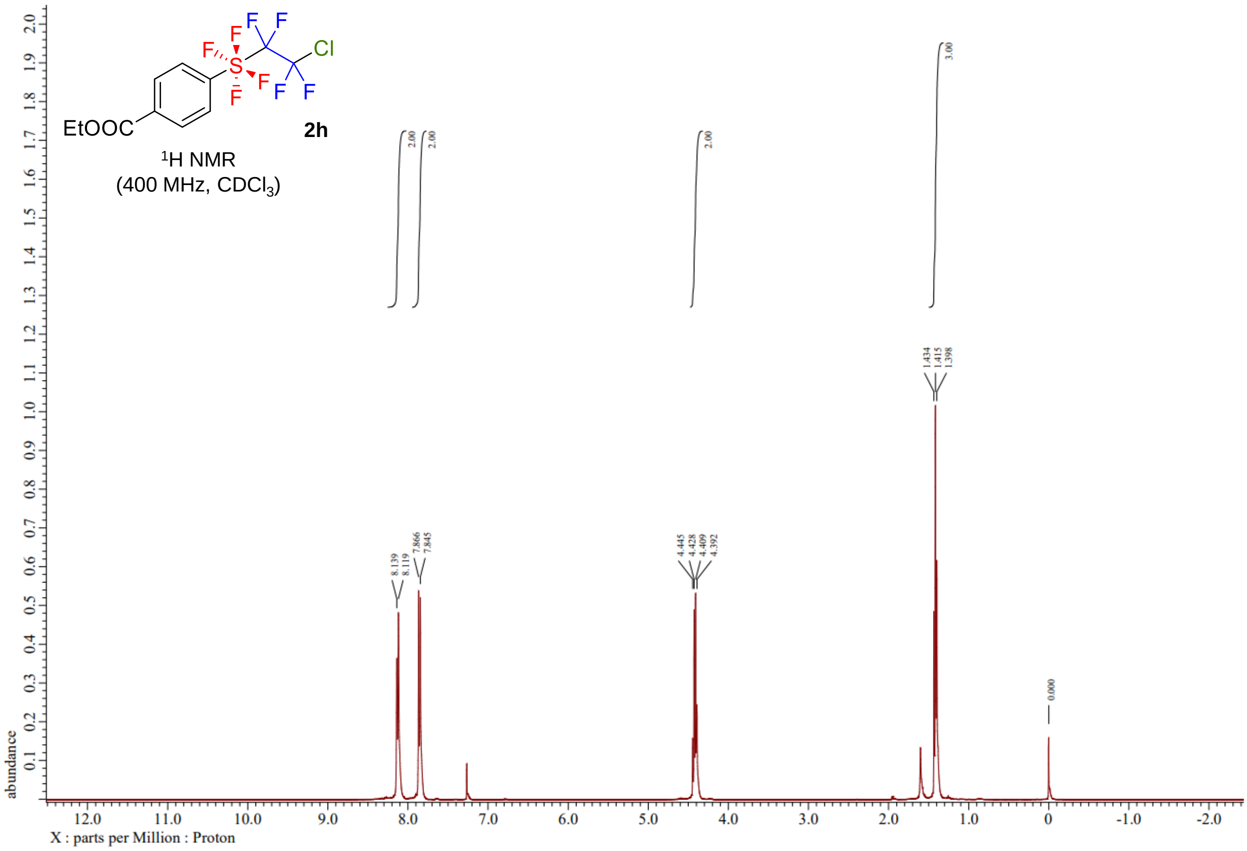
tBu
2g
1H NMR
(400 MHz, CDCl3)
7.704
7.682
7.455
7.434
1.329
0.000
2.00
2.00
9.00
abundance
X : parts per Million : Proton



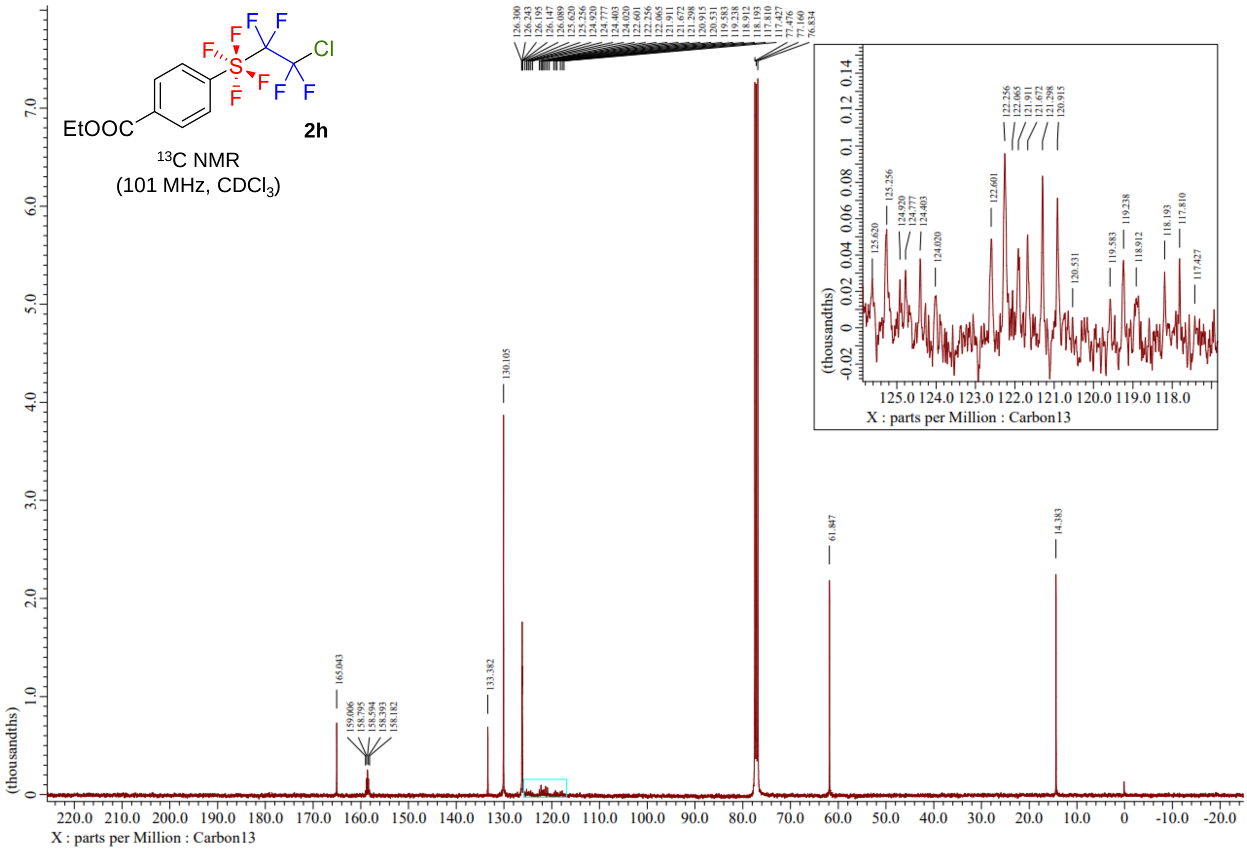
tBu
2g
13C NMR
(101 MHz, CDCl3)
155.163
153.697
153.506
153.314
153.113
152.921
35.073
31.211
77.476
77.160
76.844
(thousandths)
X : parts per Million : Carbon13

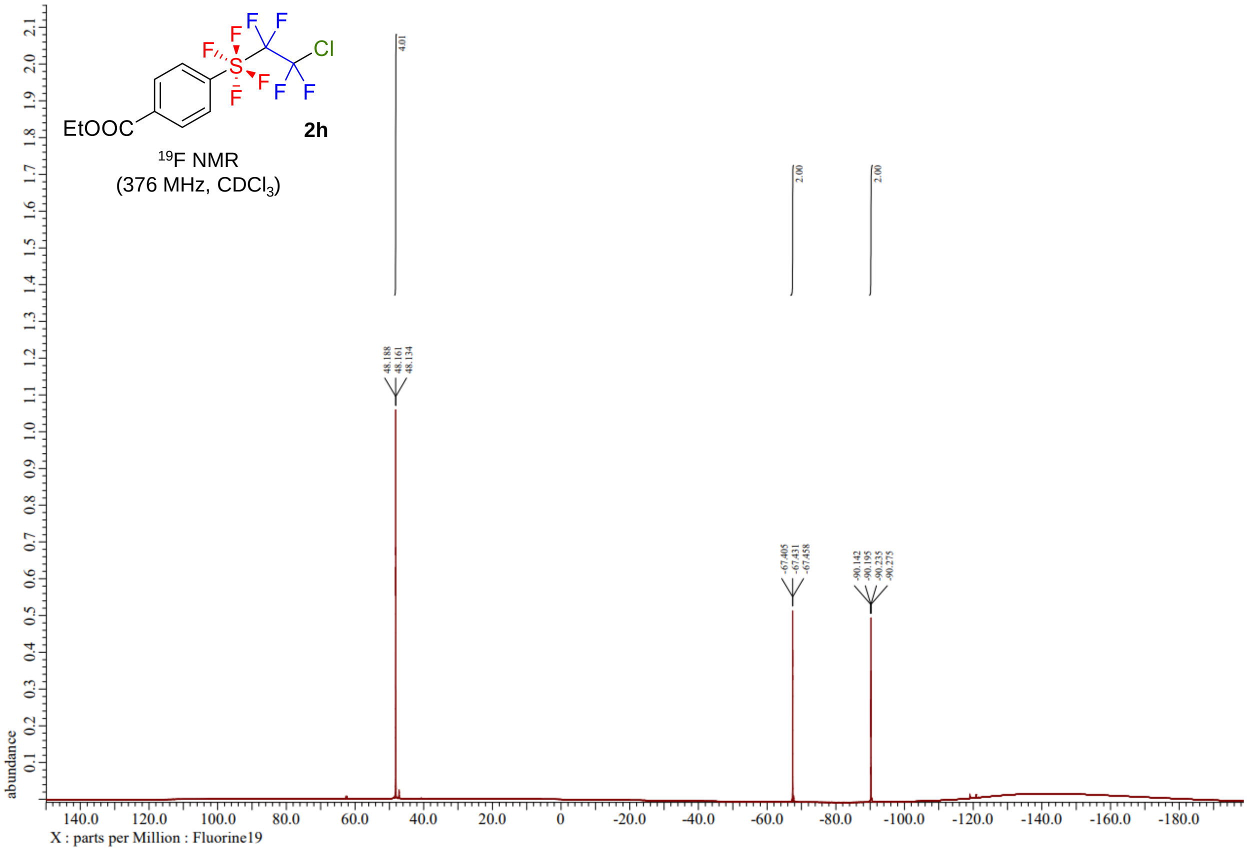


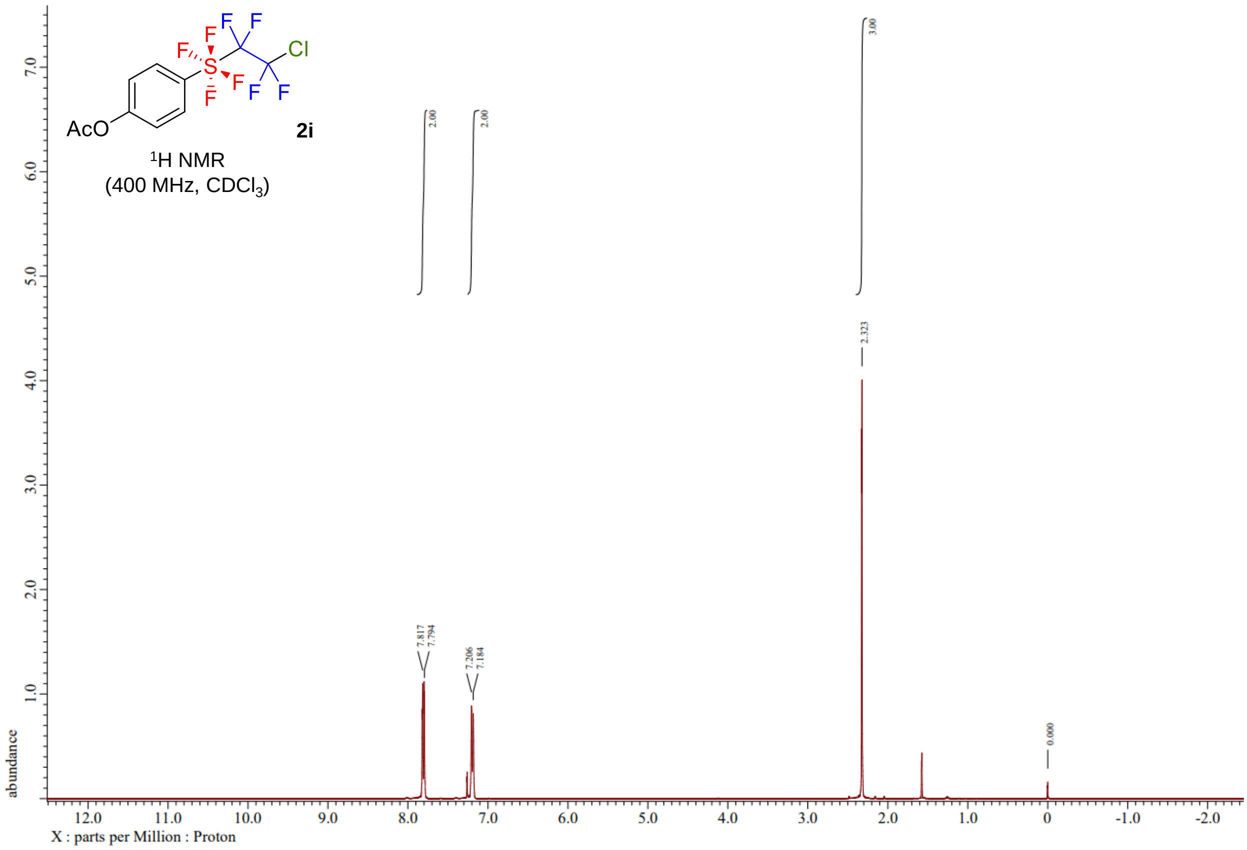
tBu
2g
19F NMR
(376 MHz, CDCl3)
4.02
2.00
2.00
48.890
48.813
48.782
-67.254
-67.284
-67.315
-90.117
-90.163
-90.209
-90.255
-90.301
abundance
X : parts per Million : Fluorine19

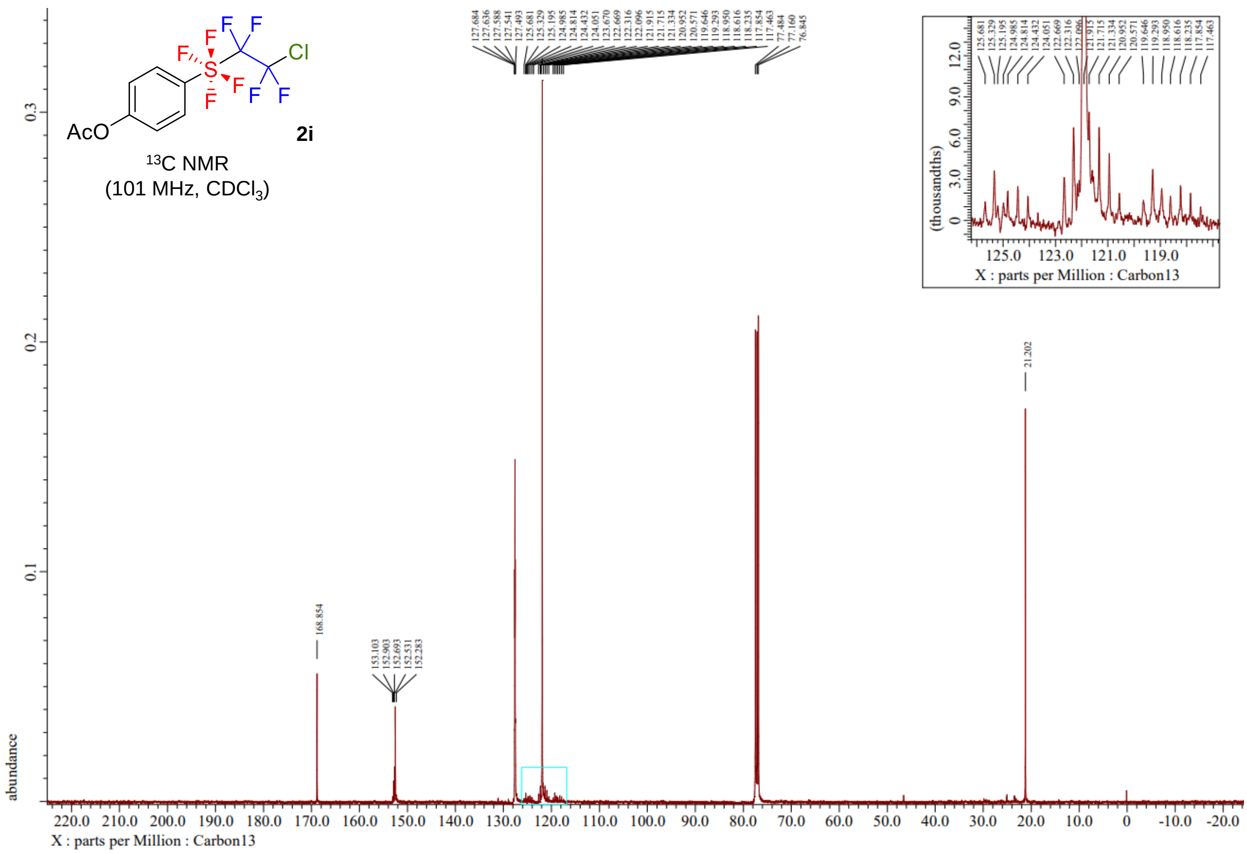


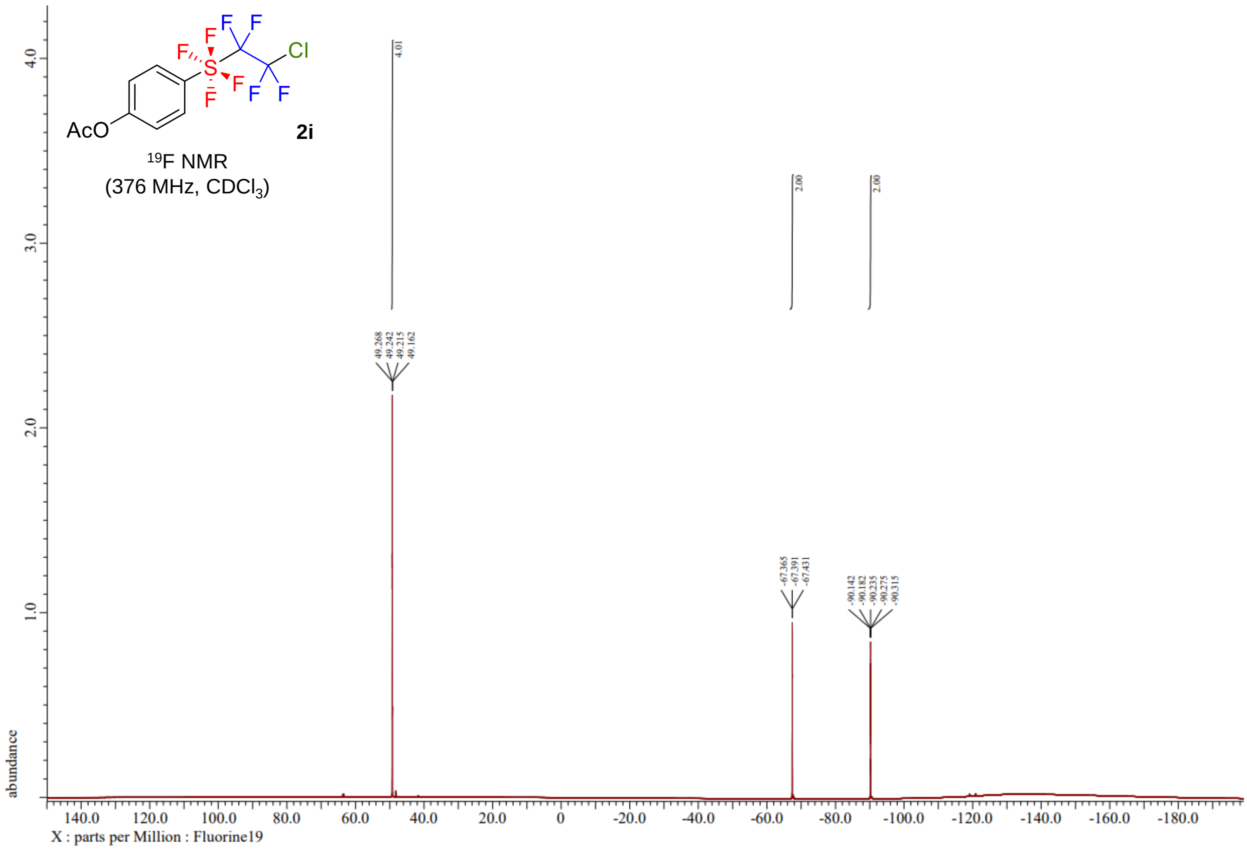
EtOOC
2h
1H NMR
(400 MHz, CDCl3)
2.00
2.00
2.00
3.00
8.139
8.119
7.866
7.845
4.445
4.428
4.409
4.392
1.434
1.415
1.398
0.000
abundance
X : parts per Million : Proton

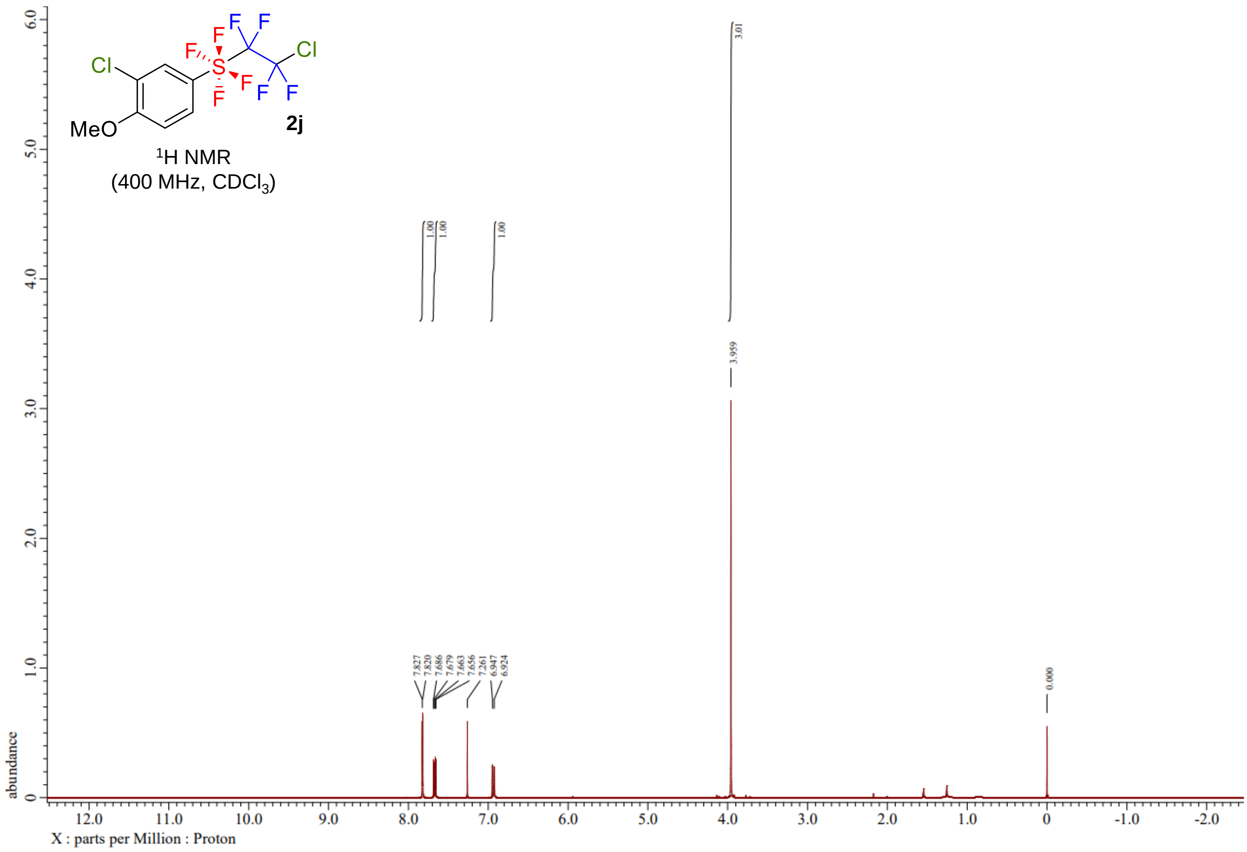

EtOOC
2h
^{13}C NMR
(101 MHz, $CDCl_3$)
X : parts per Million : Carbon13
(thousandths)

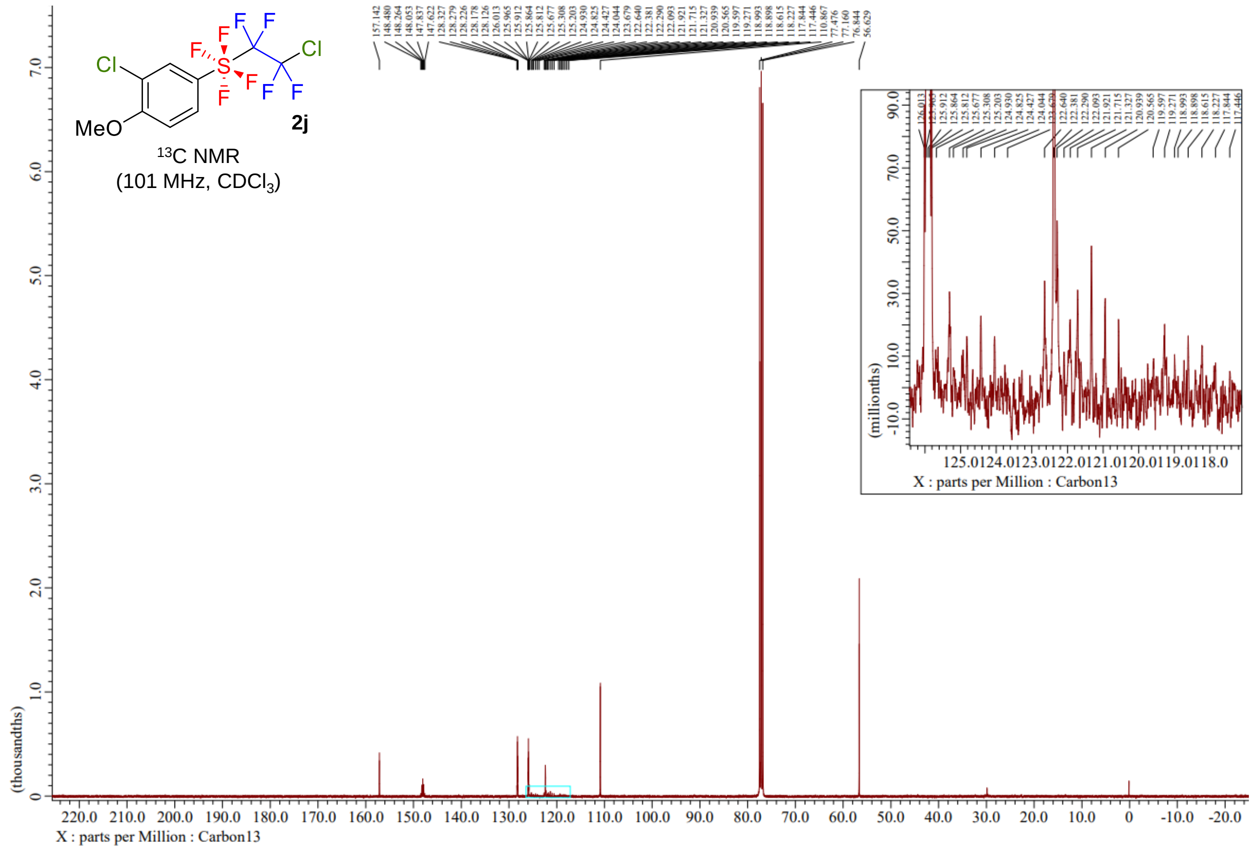

EtOOC
2h
^{19}F NMR
(376 MHz, $CDCl_3$)
X : parts per Million : Fluorine19
abundance


AcO
2i
1H NMR
(400 MHz, CDCl3)
7.817
7.794
7.206
7.184
2.323
0.000
2.00
2.00
3.00
abundance
X : parts per Million : Proton

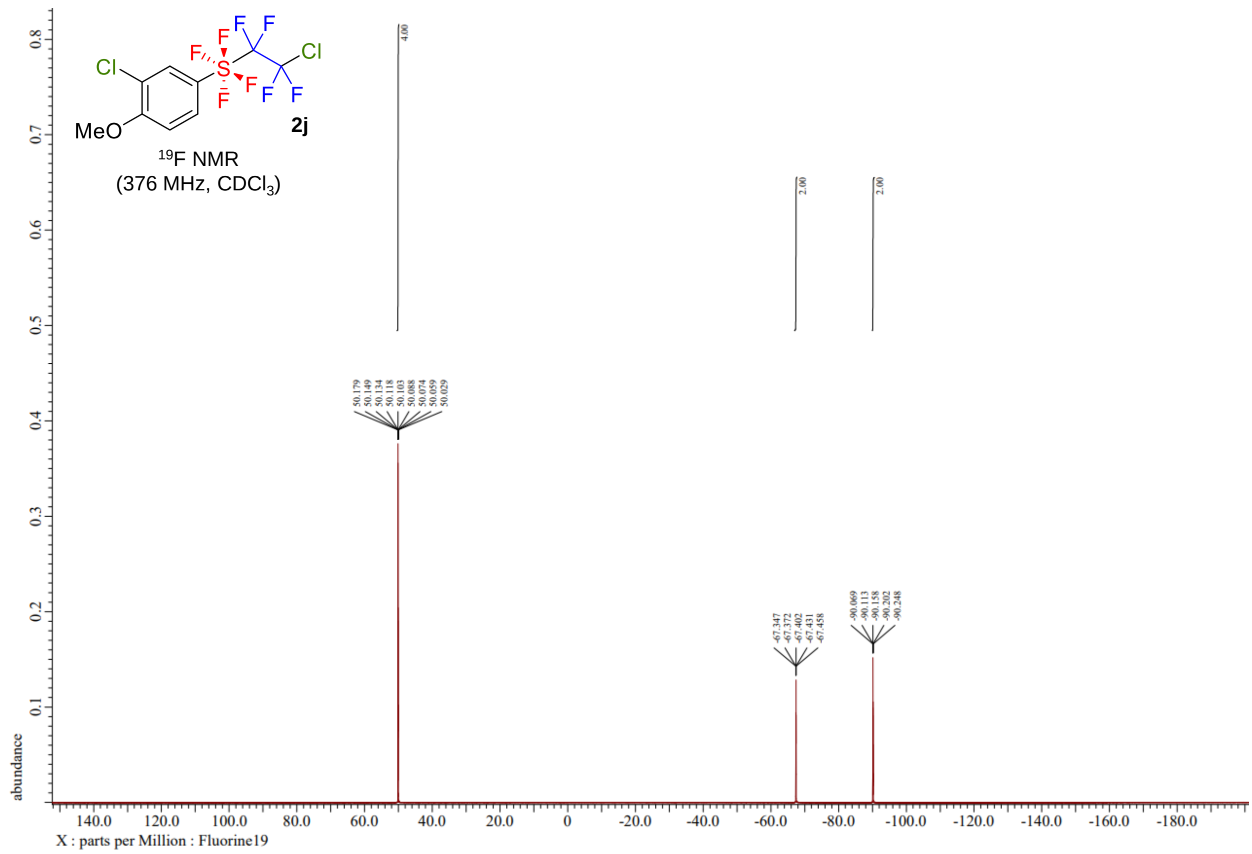

AcO
2i
13C NMR
(101 MHz, CDCl3)
168.854
153.103
152.903
152.693
152.531
152.283
127.684
127.636
127.588
127.541
127.493
125.681
125.329
125.195
124.985
124.814
124.432
124.051
123.670
122.669
122.316
122.096
121.915
121.715
121.334
120.952
120.571
119.646
119.293
118.950
118.616
118.235
117.854
117.463
77.484
77.160
76.845
21.202
abundance
X : parts per Million : Carbon13
(thousandths)
X : parts per Million : Carbon13


AcO
2i
19F NMR
(376 MHz, CDCl3)
4.01
2.00
2.00
49.268
49.242
49.215
49.162
-67.365
-67.391
-67.431
-90.142
-90.182
-90.235
-90.275
-90.315
abundance
X : parts per Million : Fluorine19

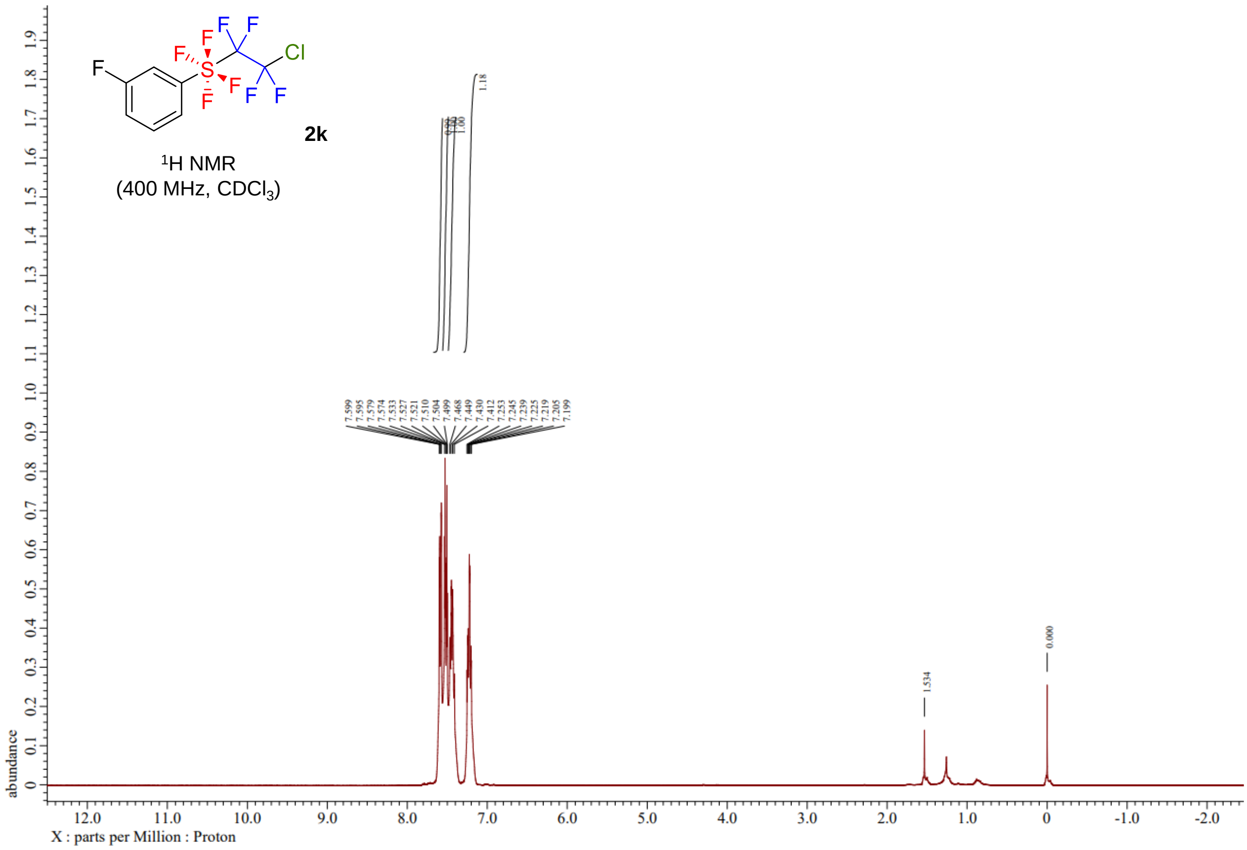

Cl
MeO
2j
1H NMR
(400 MHz, CDCl3)
1.00
1.00
1.00
3.01
3.959
7.827
7.820
7.686
7.679
7.663
7.656
7.261
6.947
6.924
0.000
abundance
X : parts per Million : Proton

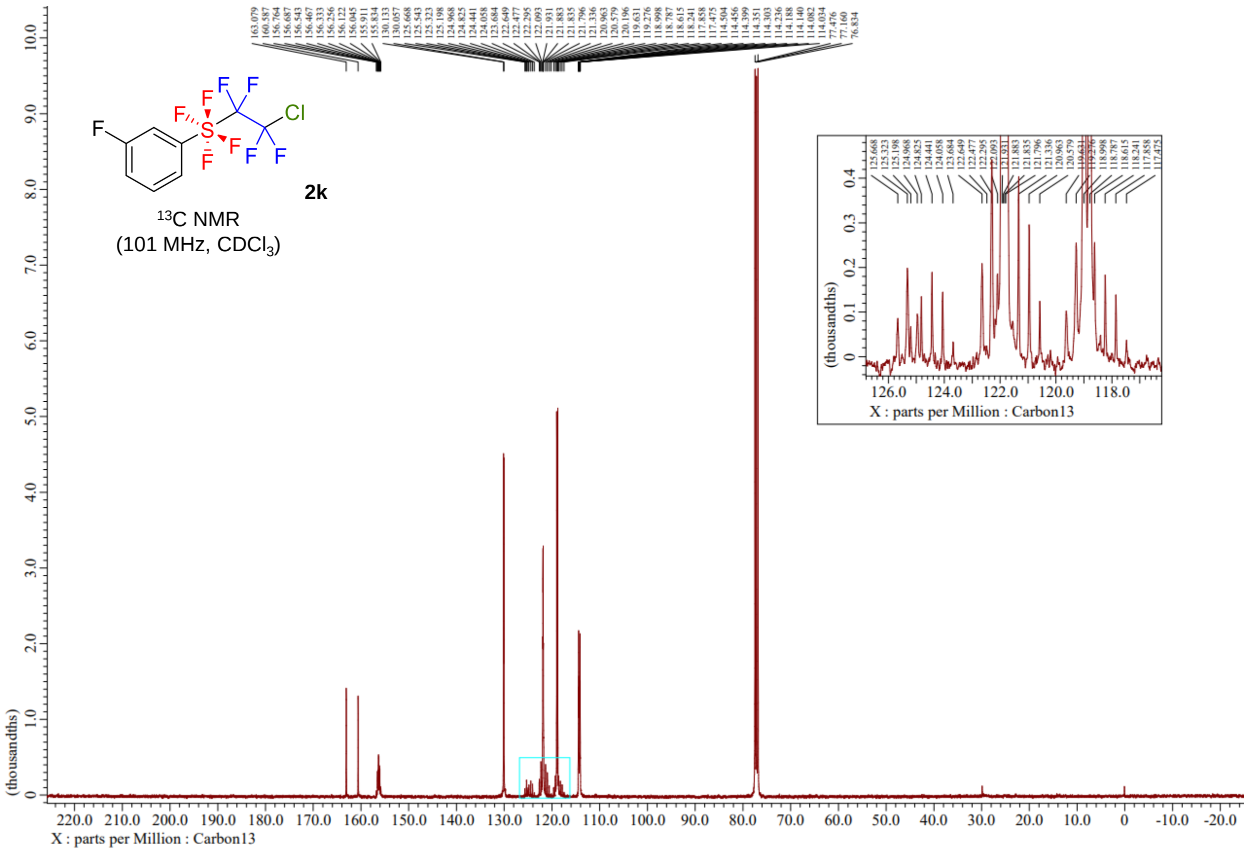


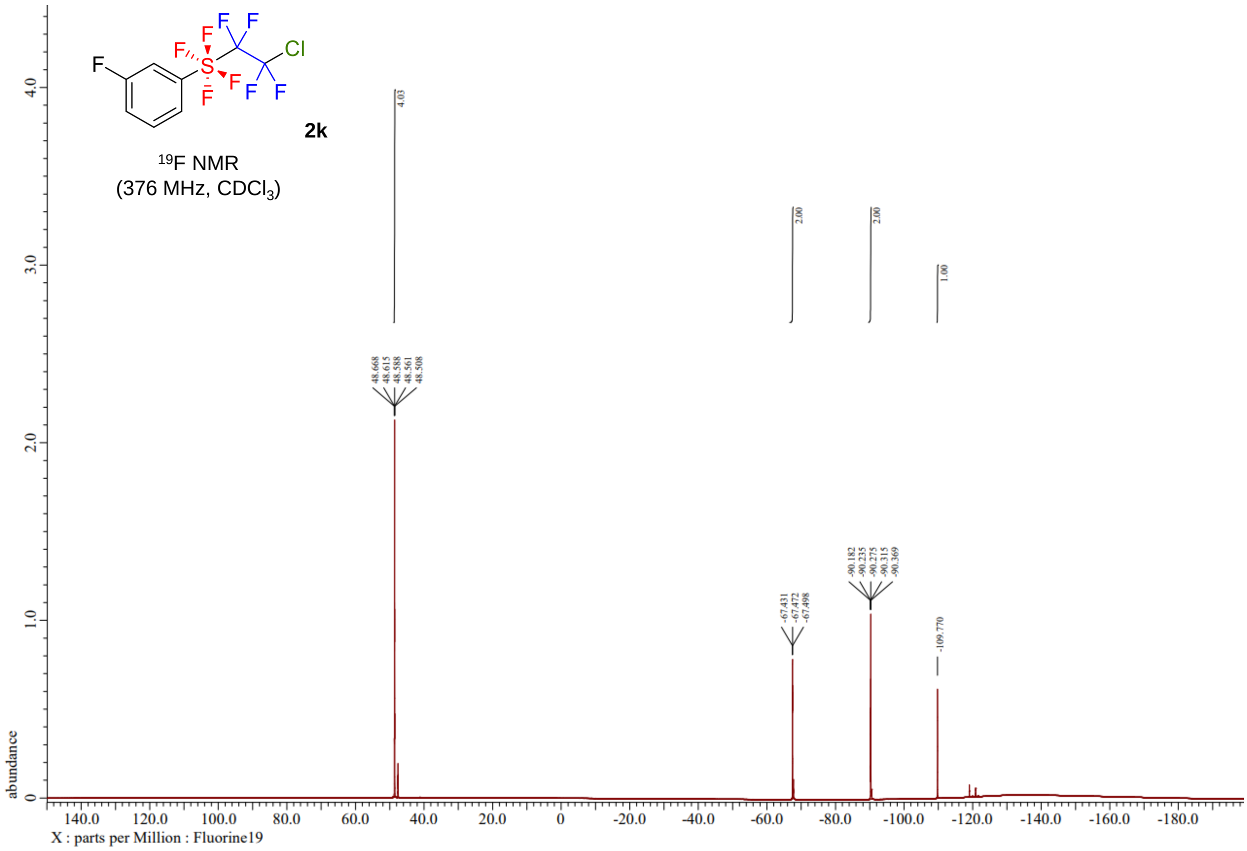
2j
13C NMR
(101 MHz, CDCl3)
X : parts per Million : Carbon13

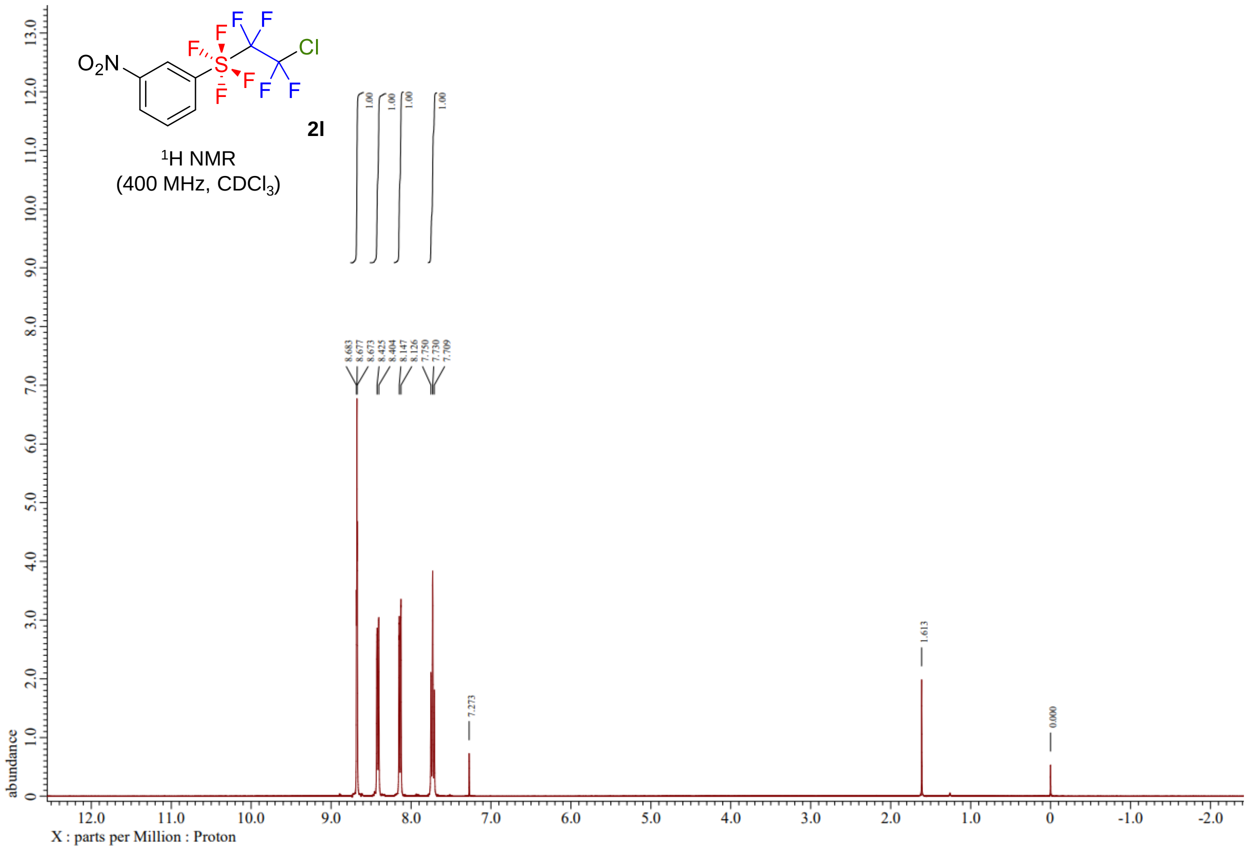


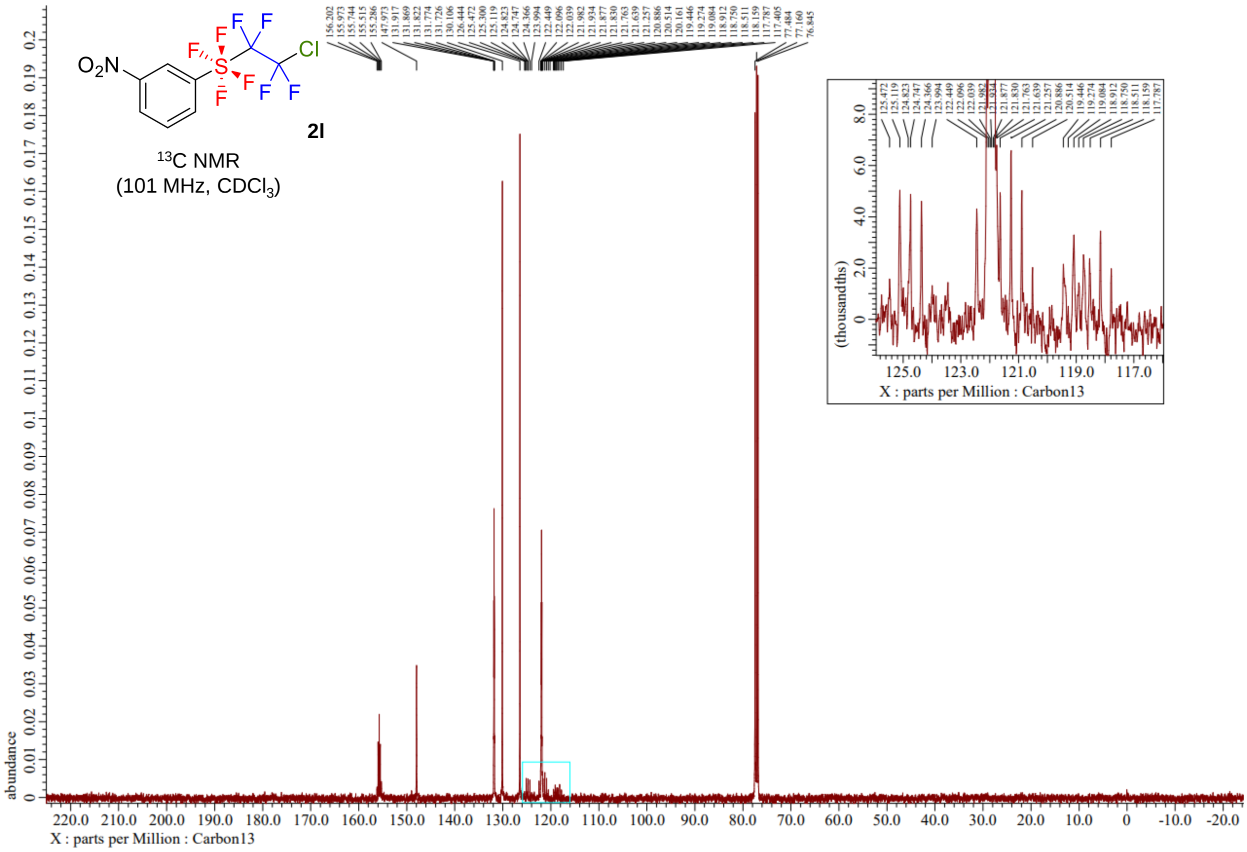
2j
19F NMR
(376 MHz, CDCl3)
X : parts per Million : Fluorine19


2k
^{1}H NMR
(400 MHz, $CDCl_3$)
abundance
X : parts per Million : Proton

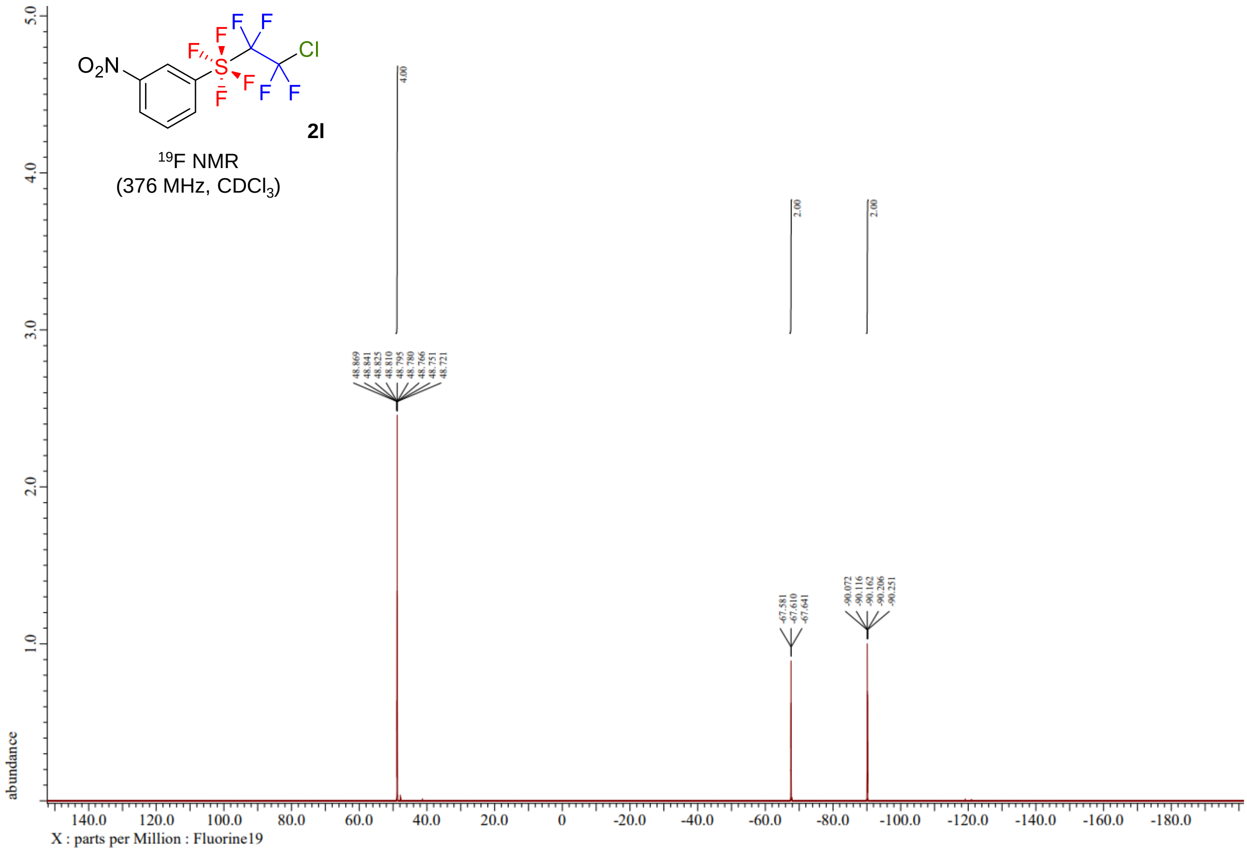

2k
^{13}C NMR
(101 MHz, $CDCl_3$)
(thousandths)
X : parts per Million : Carbon13


2k
^{19}F NMR
(376 MHz, CDCl$_3$)
abundance
X : parts per Million : Fluorine19

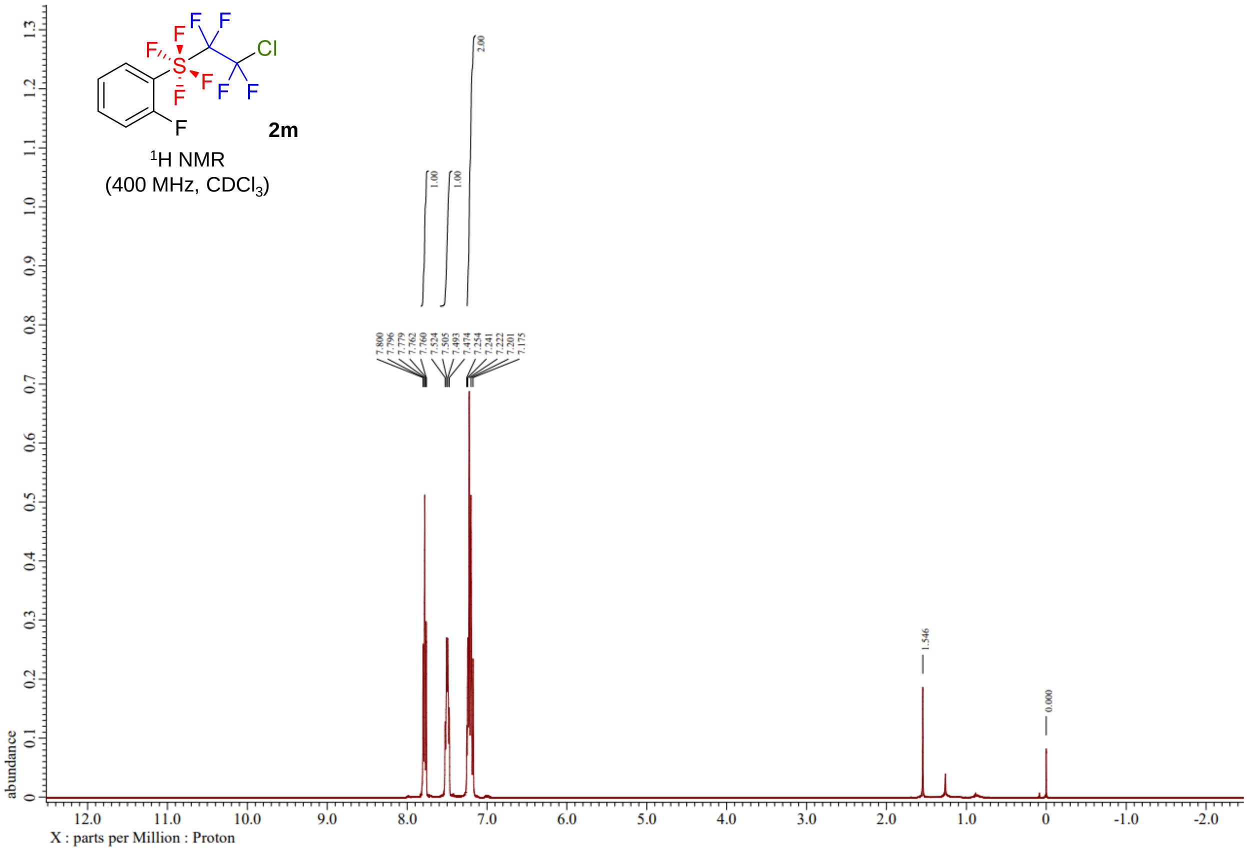

2l
^{1}H NMR
(400 MHz, CDCl$_3$)
abundance
X : parts per Million : Proton

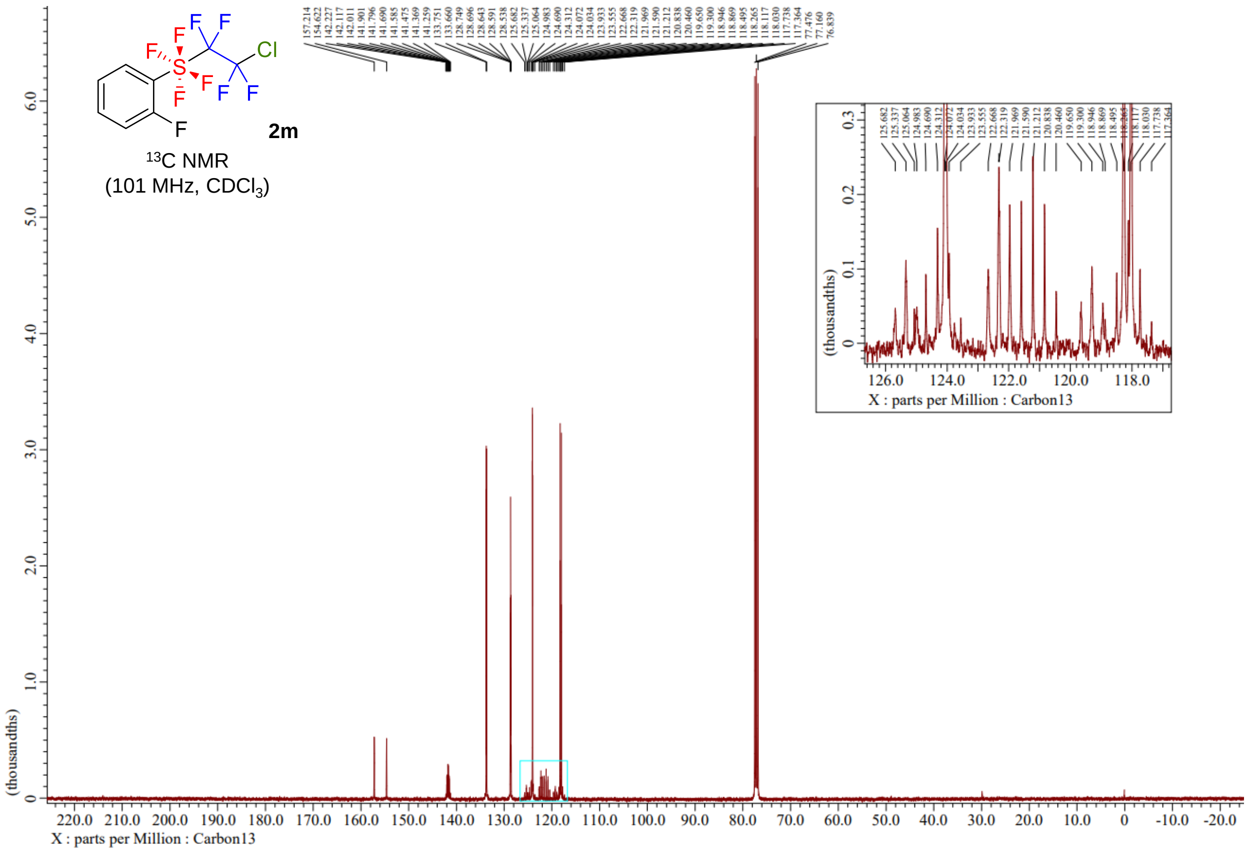


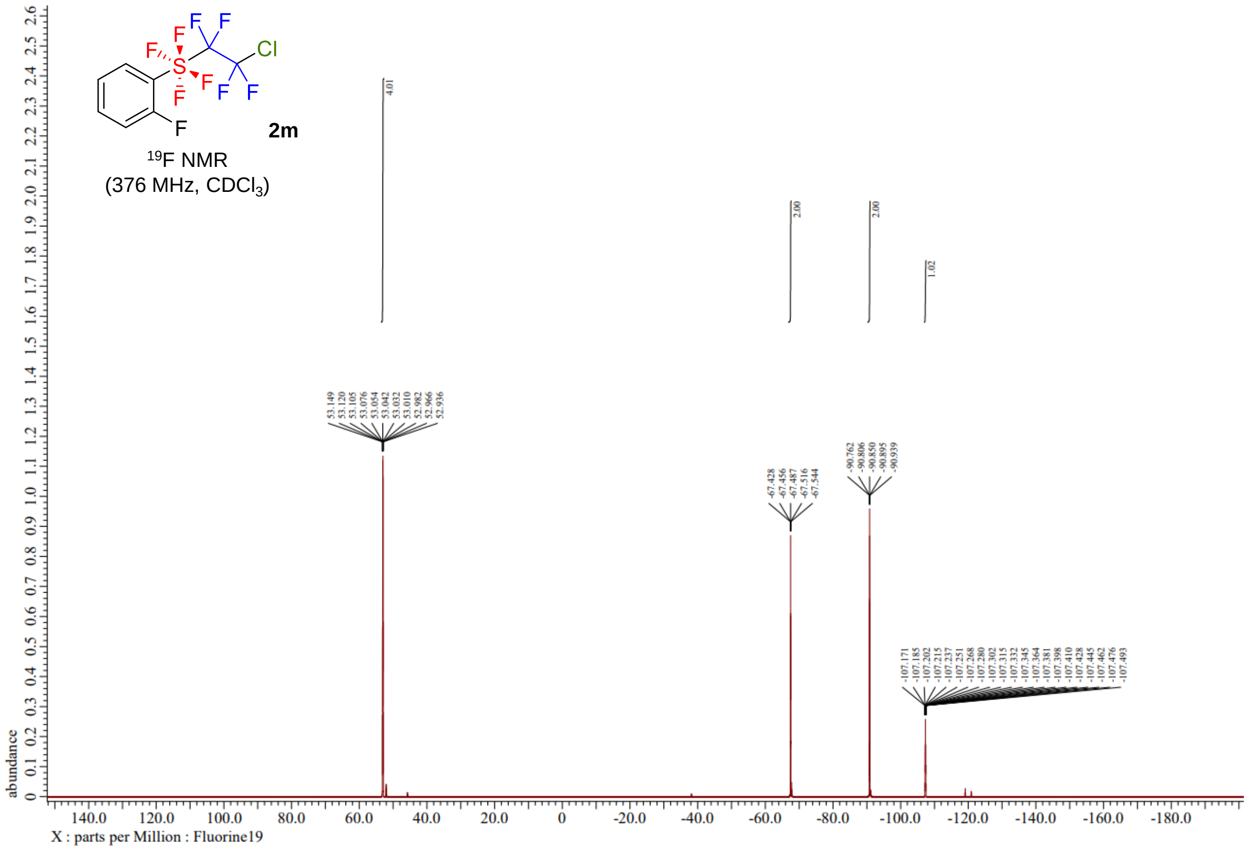
O2N
F
Cl
2l
13C NMR
(101 MHz, CDCl3)
(thousandths)
X : parts per Million : Carbon13
abundance
X : parts per Million : Carbon13

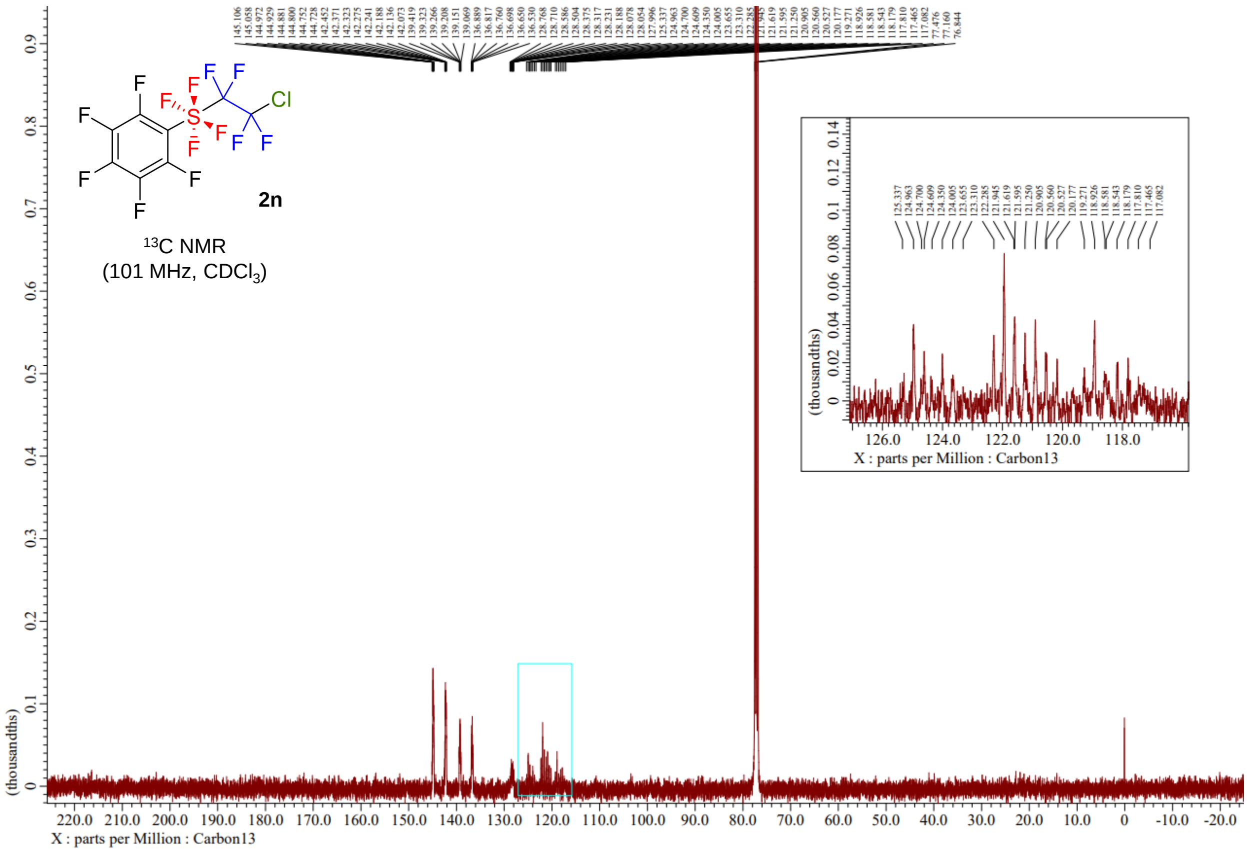


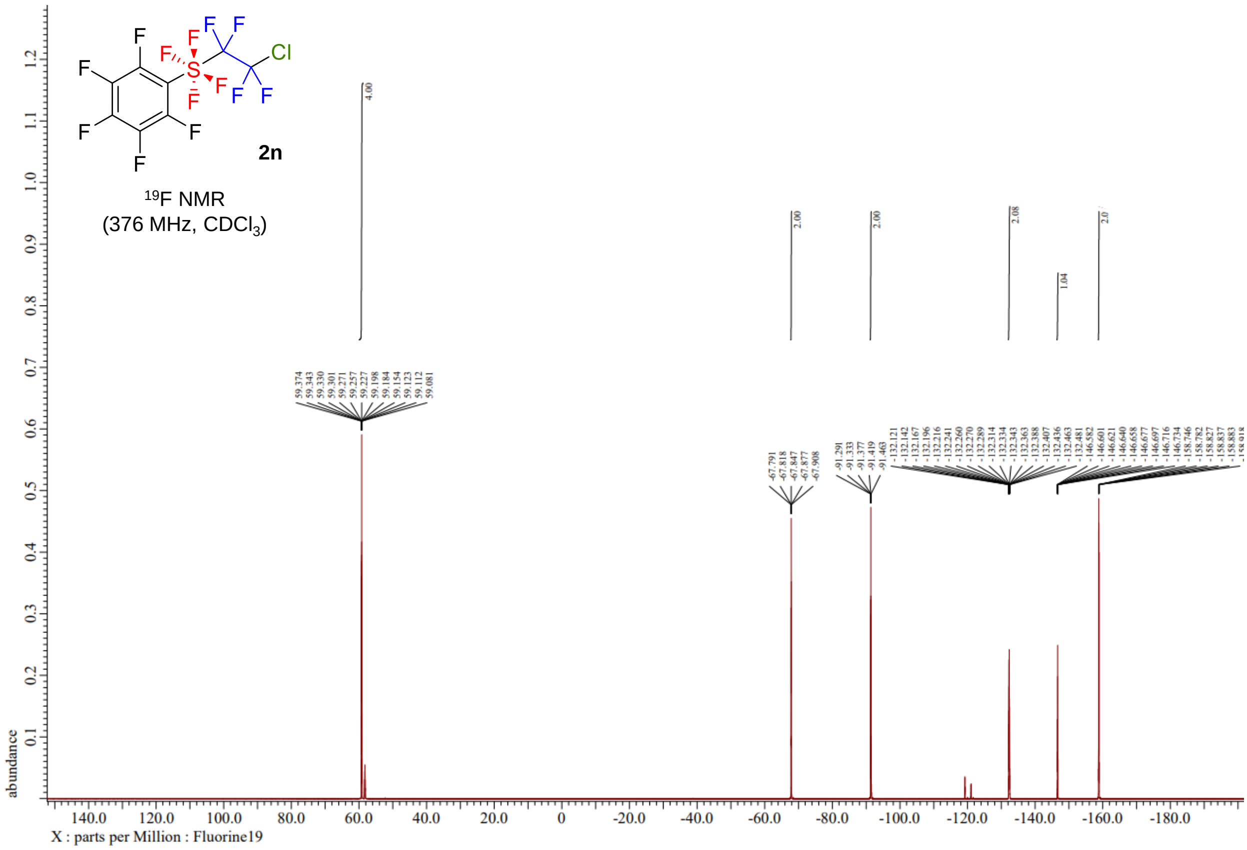
O2N
F
Cl
2l
19F NMR
(376 MHz, CDCl3)
4.00
2.00
2.00
abundance
X : parts per Million : Fluorine19

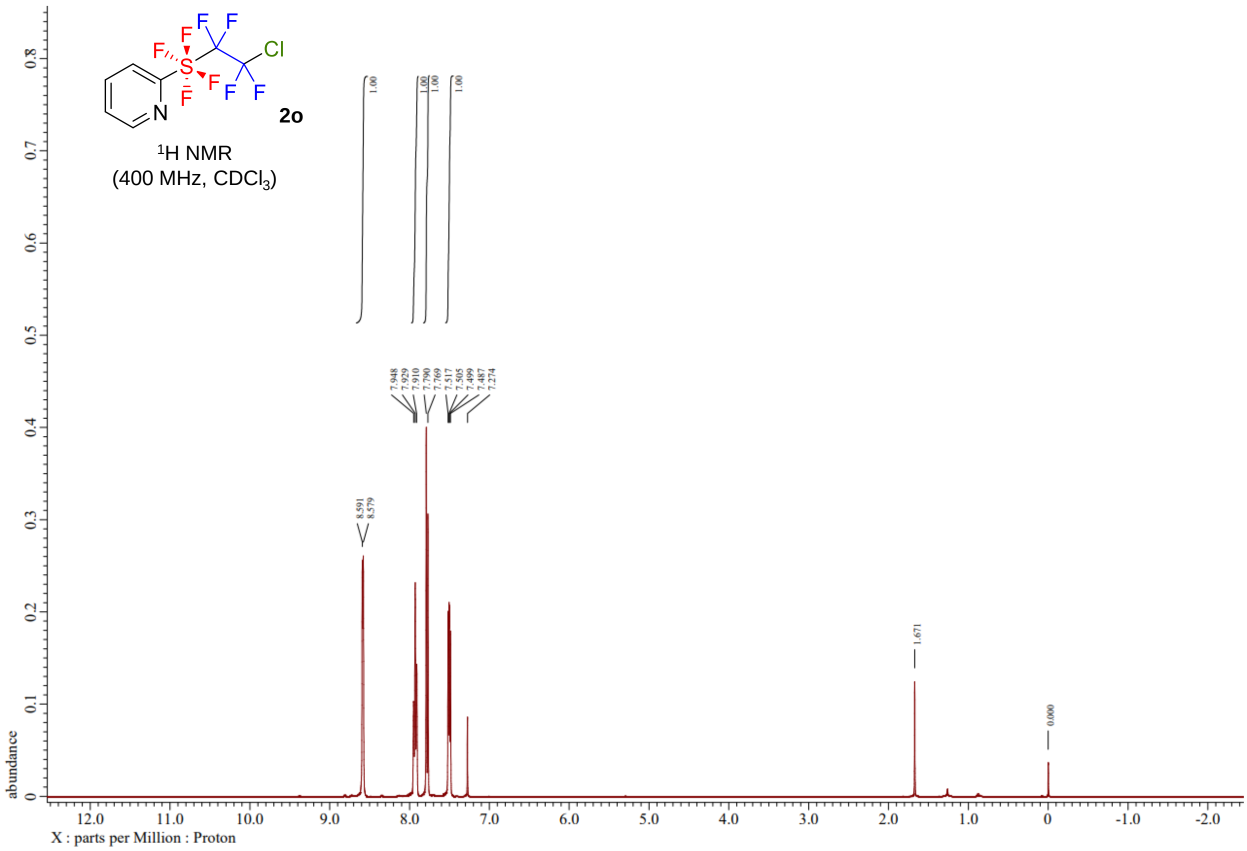


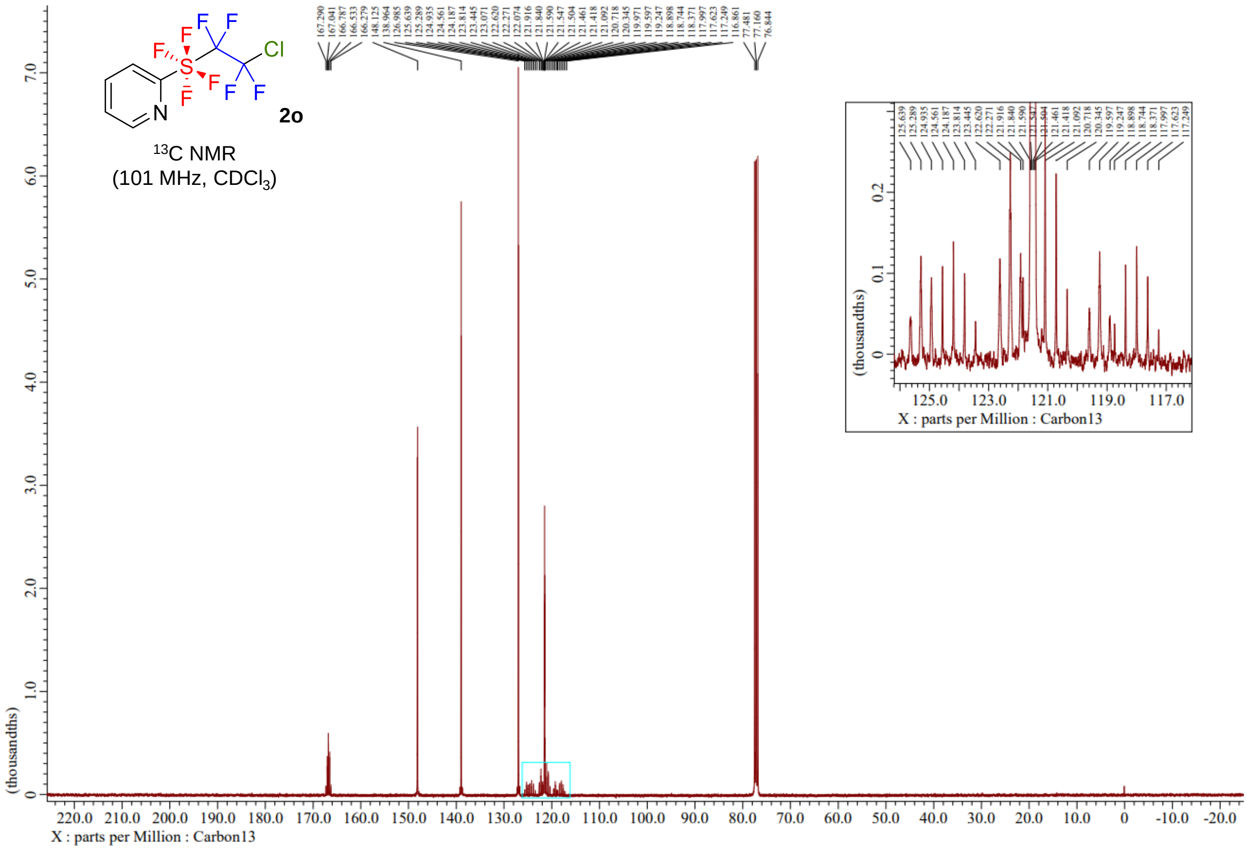



2m
19F NMR
(376 MHz, CDCl3)
X : parts per Million : Fluorine19
abundance

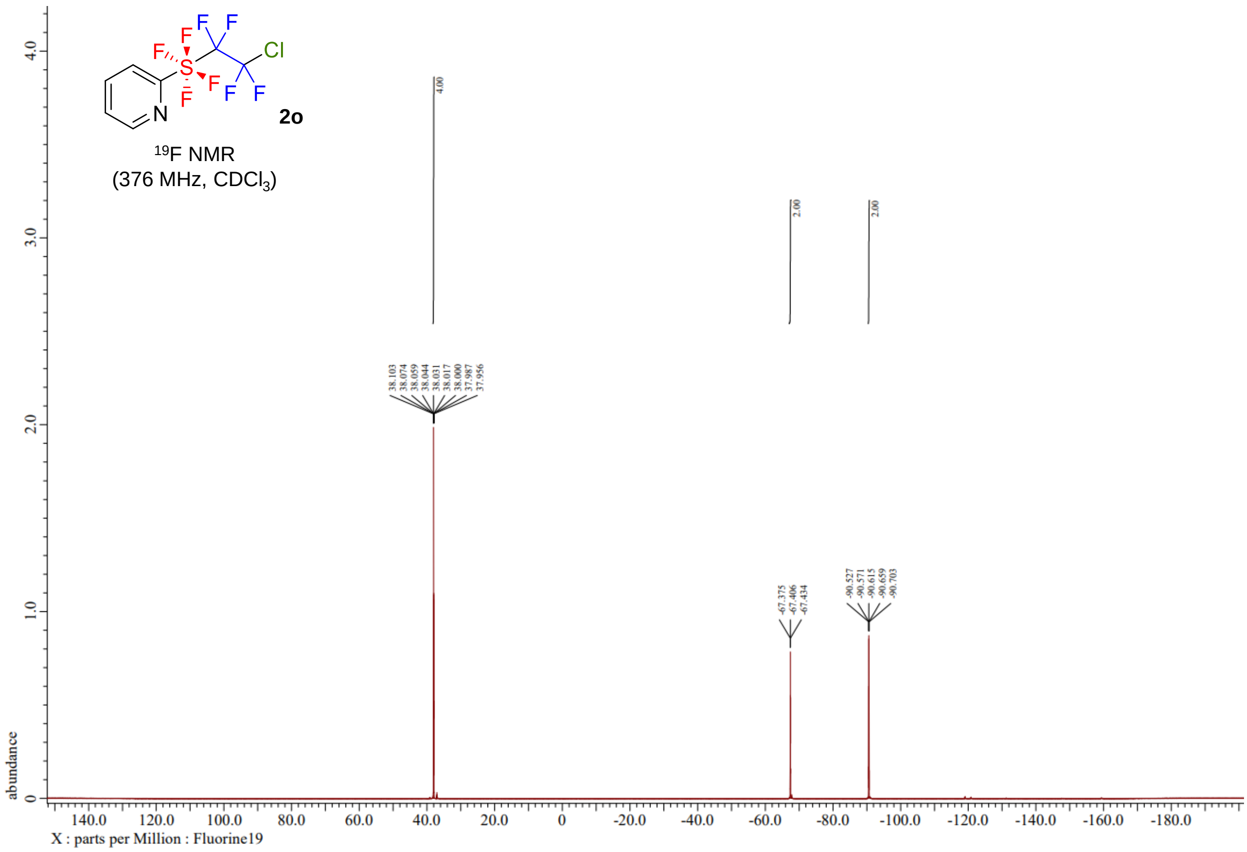

2n
13C NMR
(101 MHz, CDCl3)
X : parts per Million : Carbon13
(thousandths)


2n
^{19}F NMR
(376 MHz, $CDCl_3$)
X : parts per Million : Fluorine19
abundance

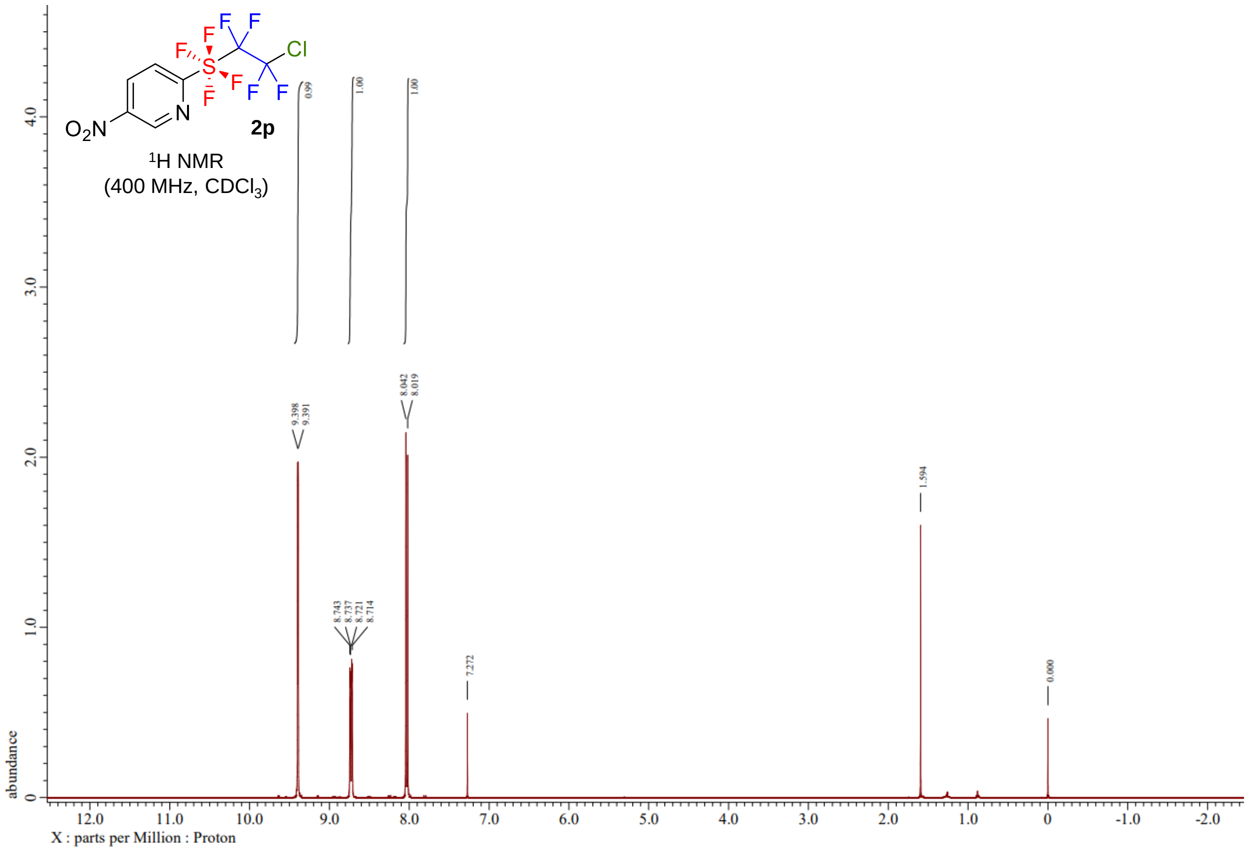

2o
^{1}H NMR
(400 MHz, $CDCl_3$)
X : parts per Million : Proton
abundance

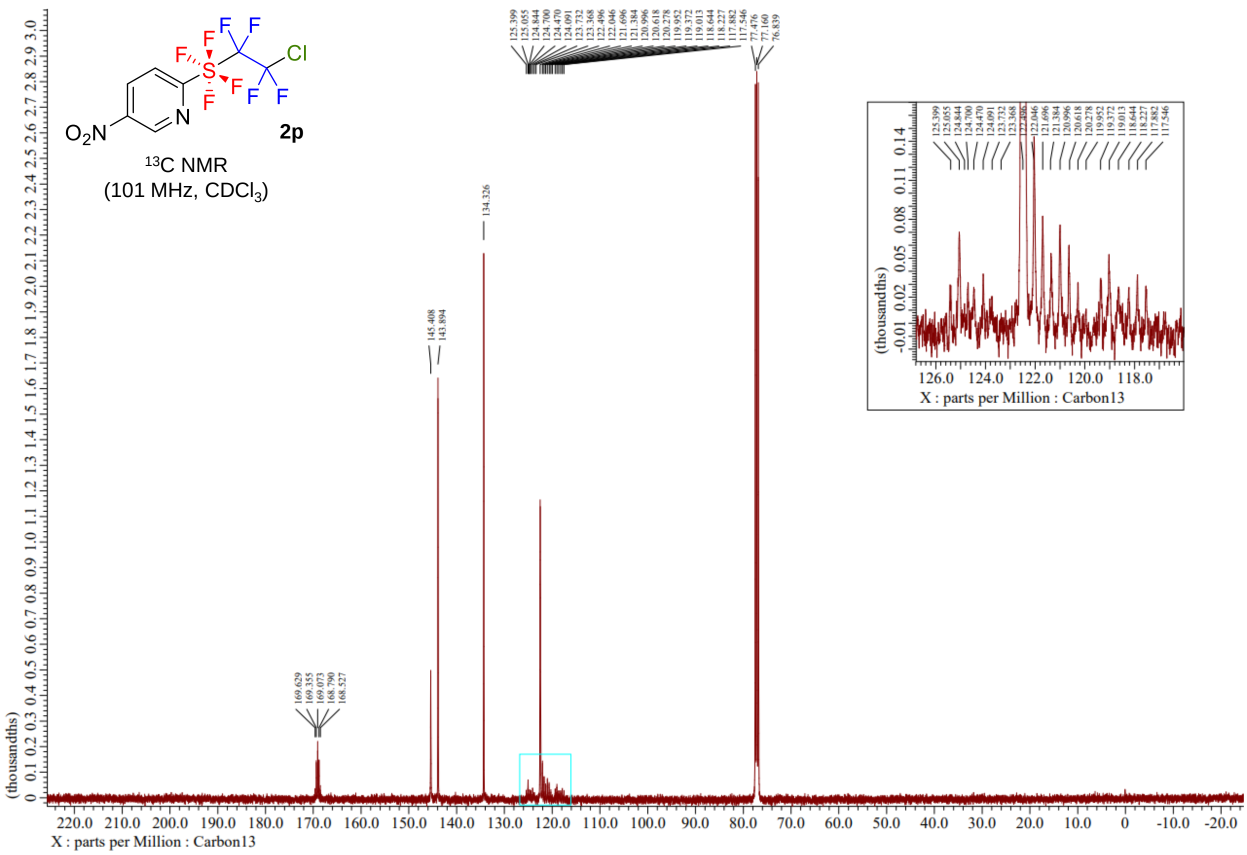


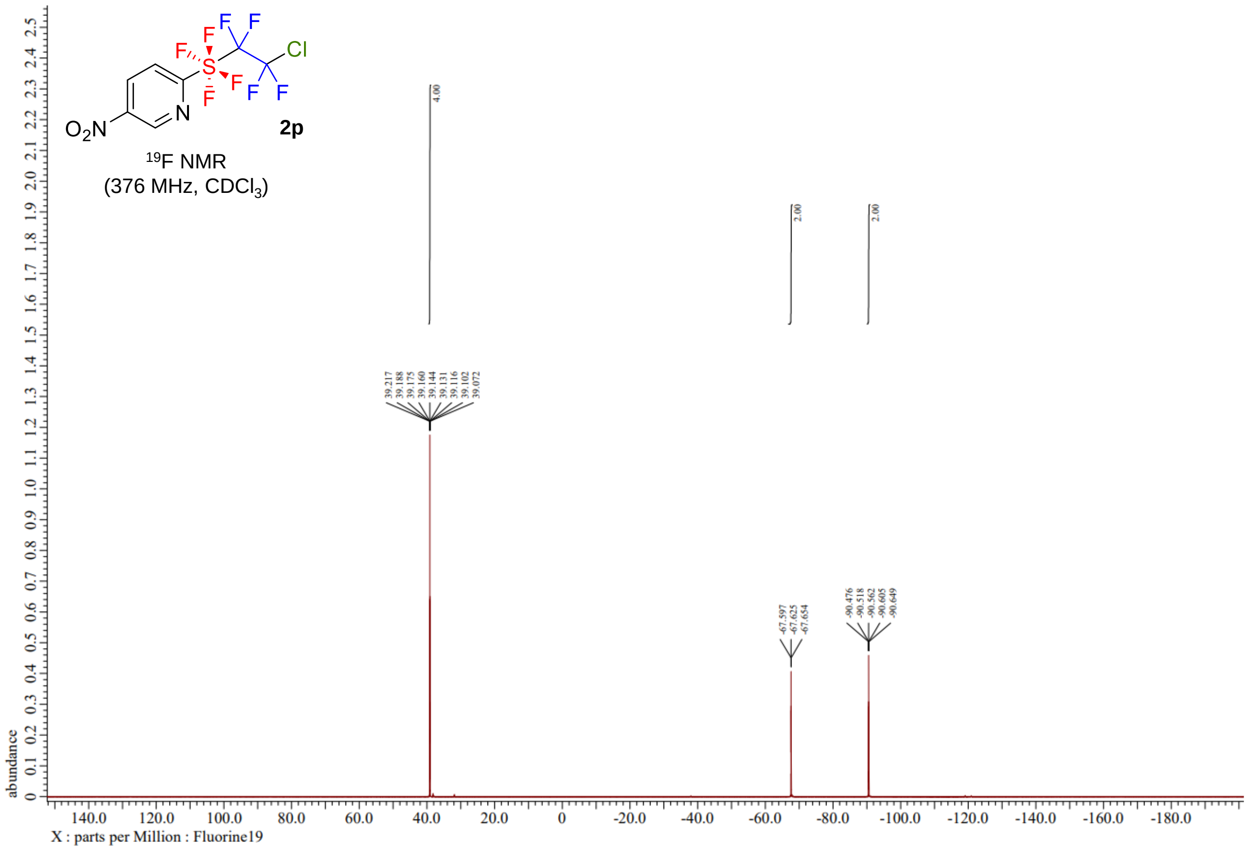
2o
^{13}C NMR
(101 MHz, $CDCl_3$)
X : parts per Million : Carbon13
(thousandths)



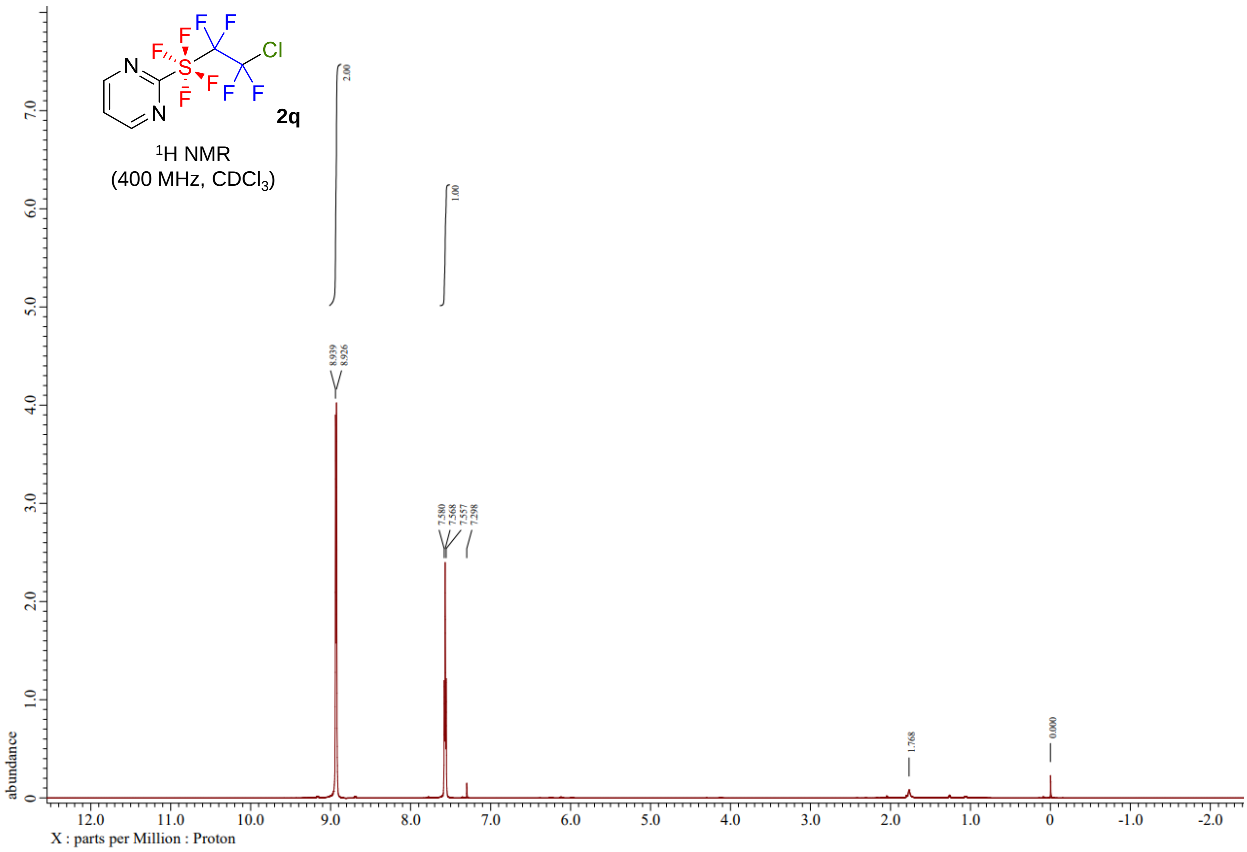
2o
^{19}F NMR
(376 MHz, $CDCl_3$)
X : parts per Million : Fluorine19
abundance


2p
^{1}H NMR
(400 MHz, $CDCl_3$)
X : parts per Million : Proton
abundance

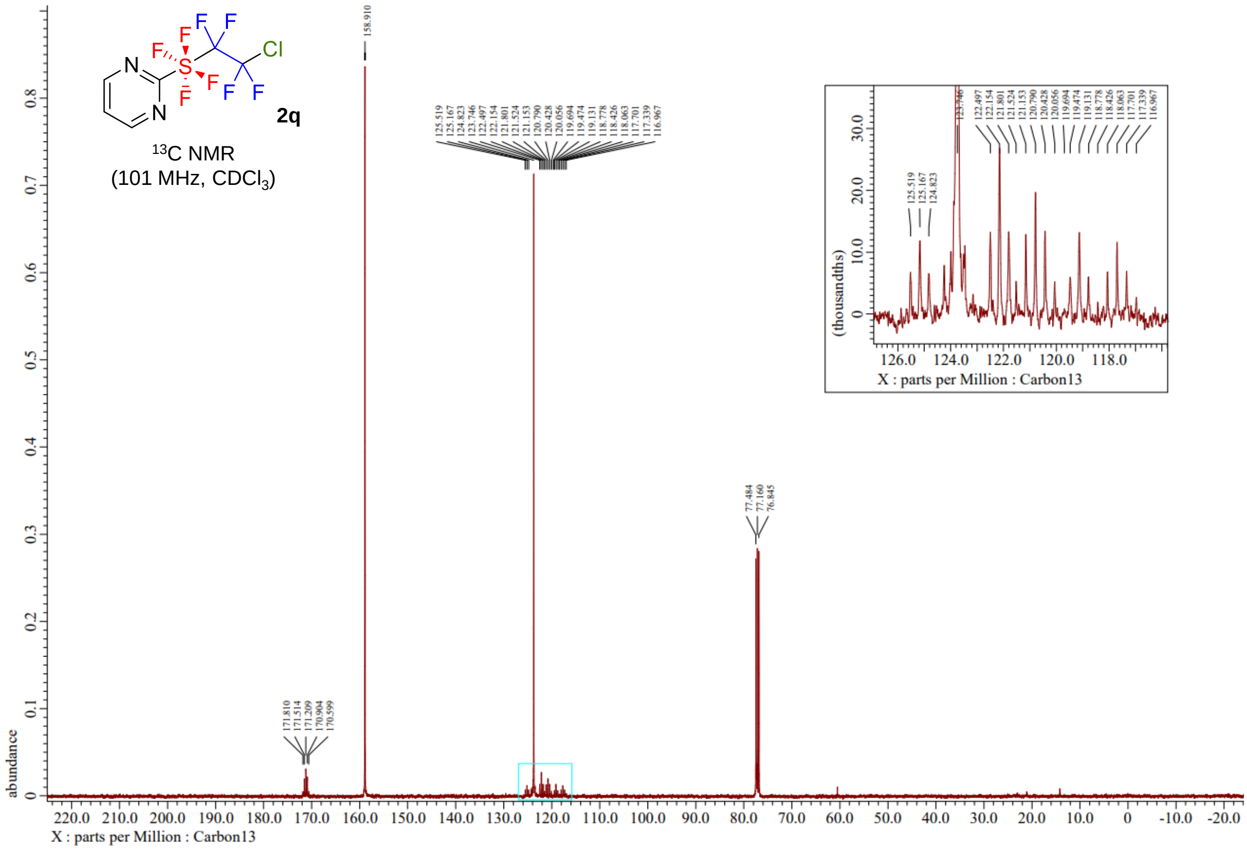

2p
^{13}C NMR
(101 MHz, $CDCl_3$)
X : parts per Million : Carbon13
(thousandths)

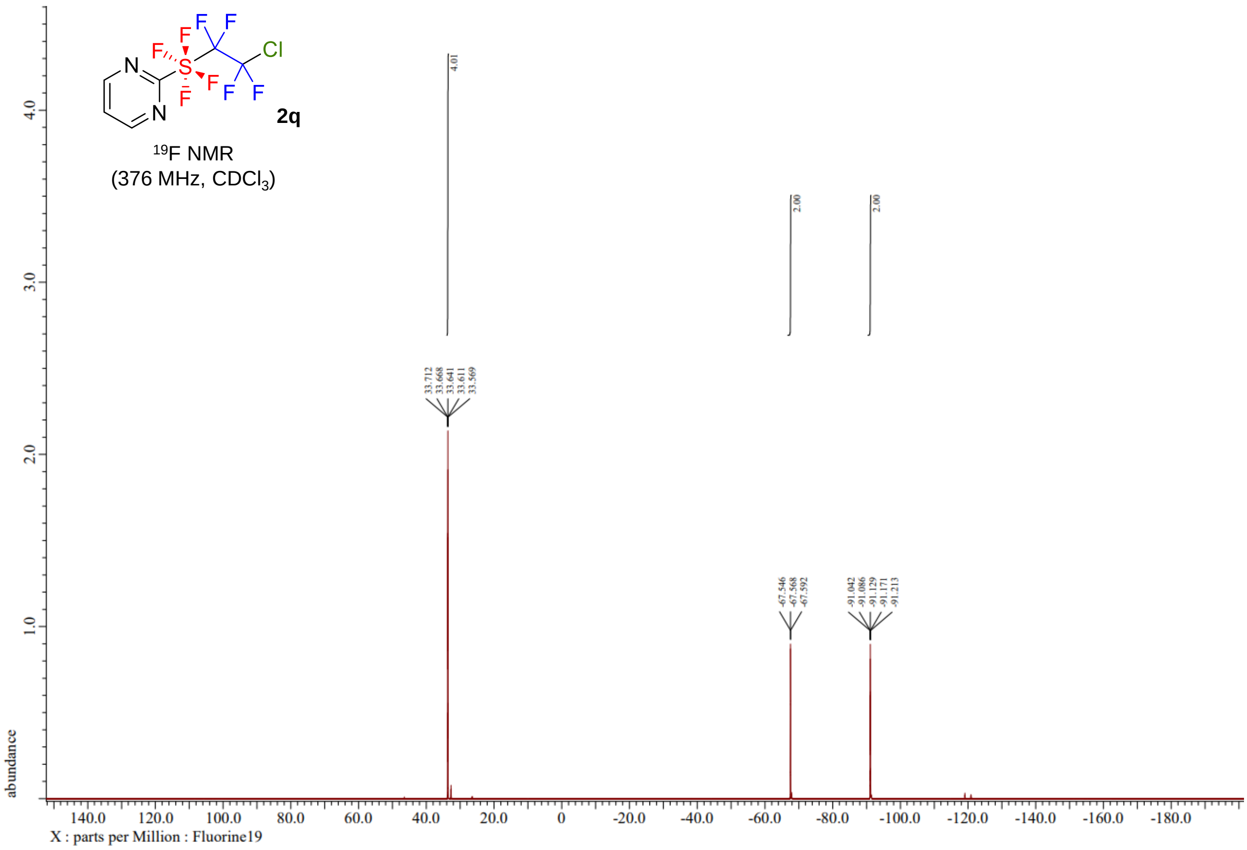


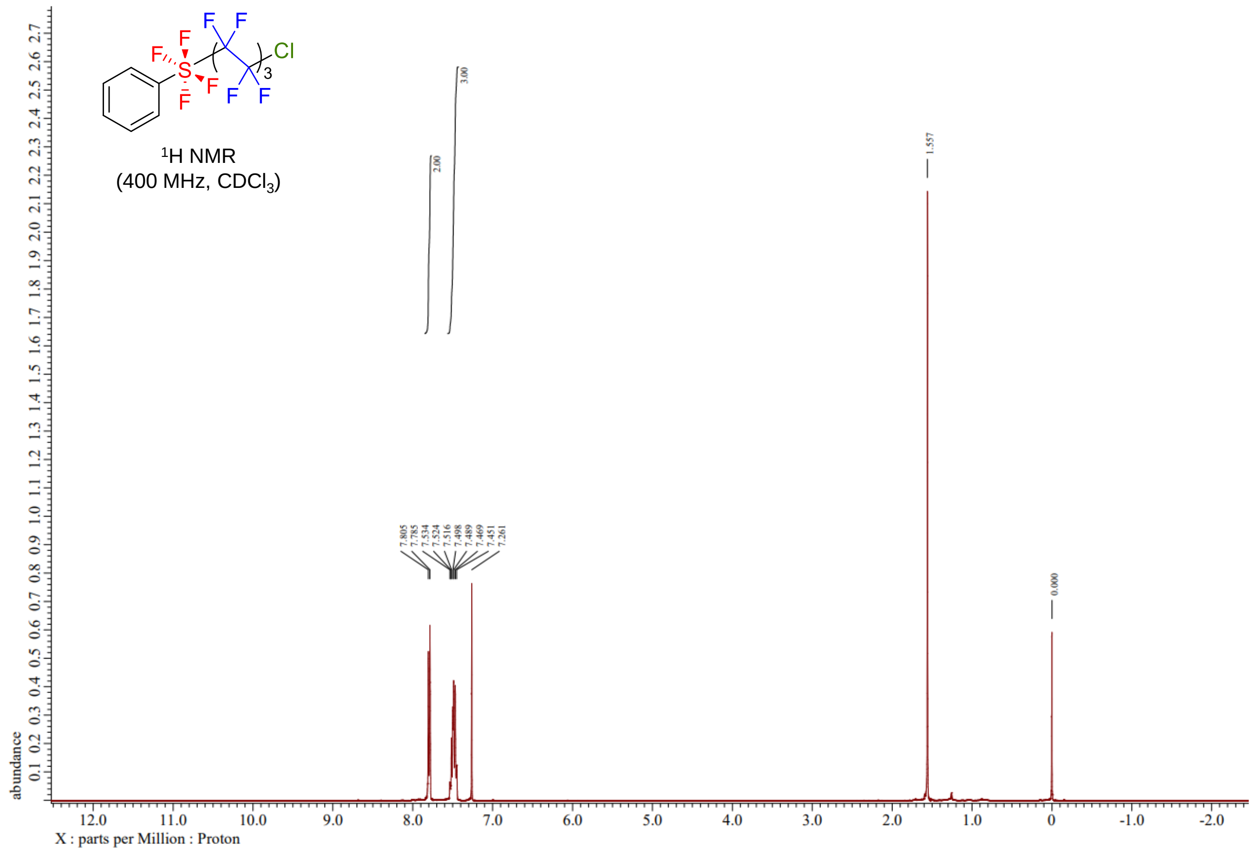
2p
^{19}F NMR
(376 MHz, $CDCl_3$)
X : parts per Million : Fluorine19
abundance



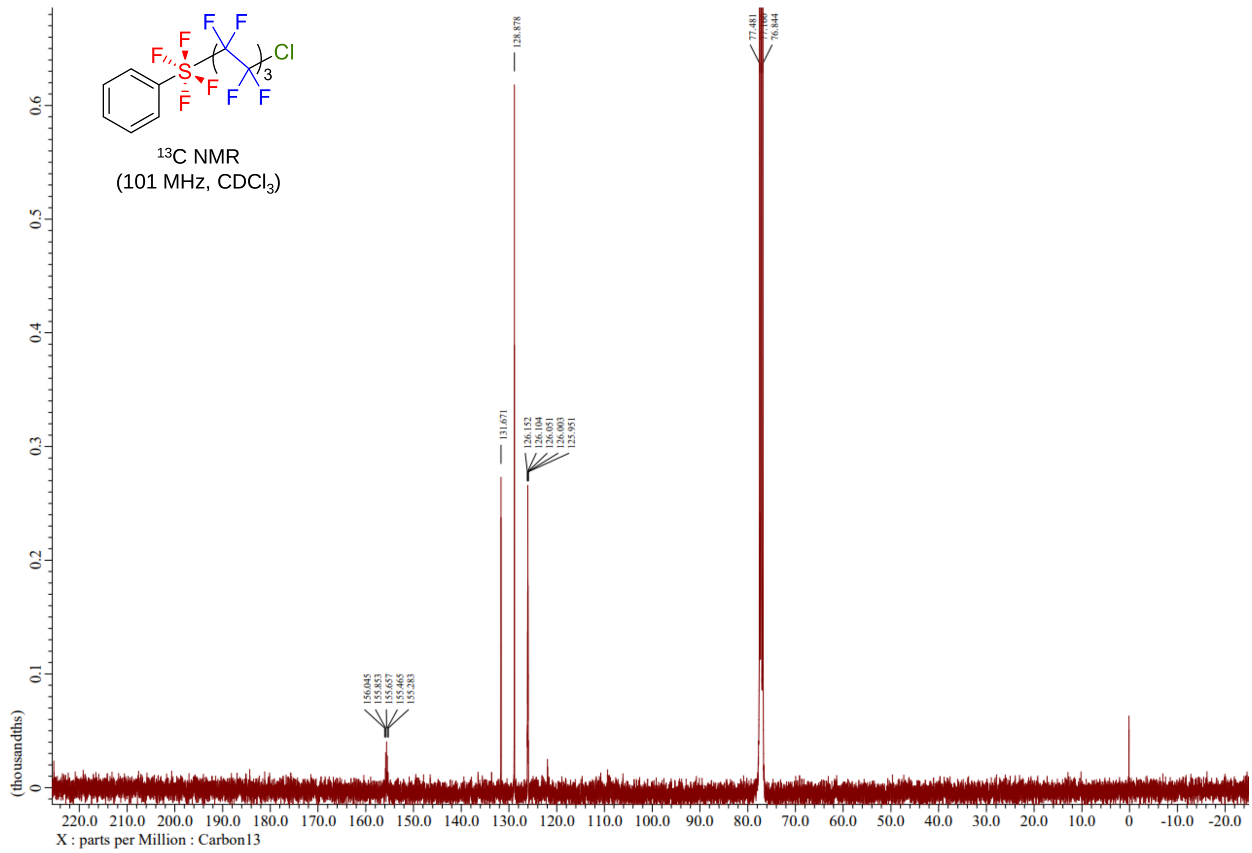
2q
^{1}H NMR
(400 MHz, $CDCl_3$)
X : parts per Million : Proton
abundance



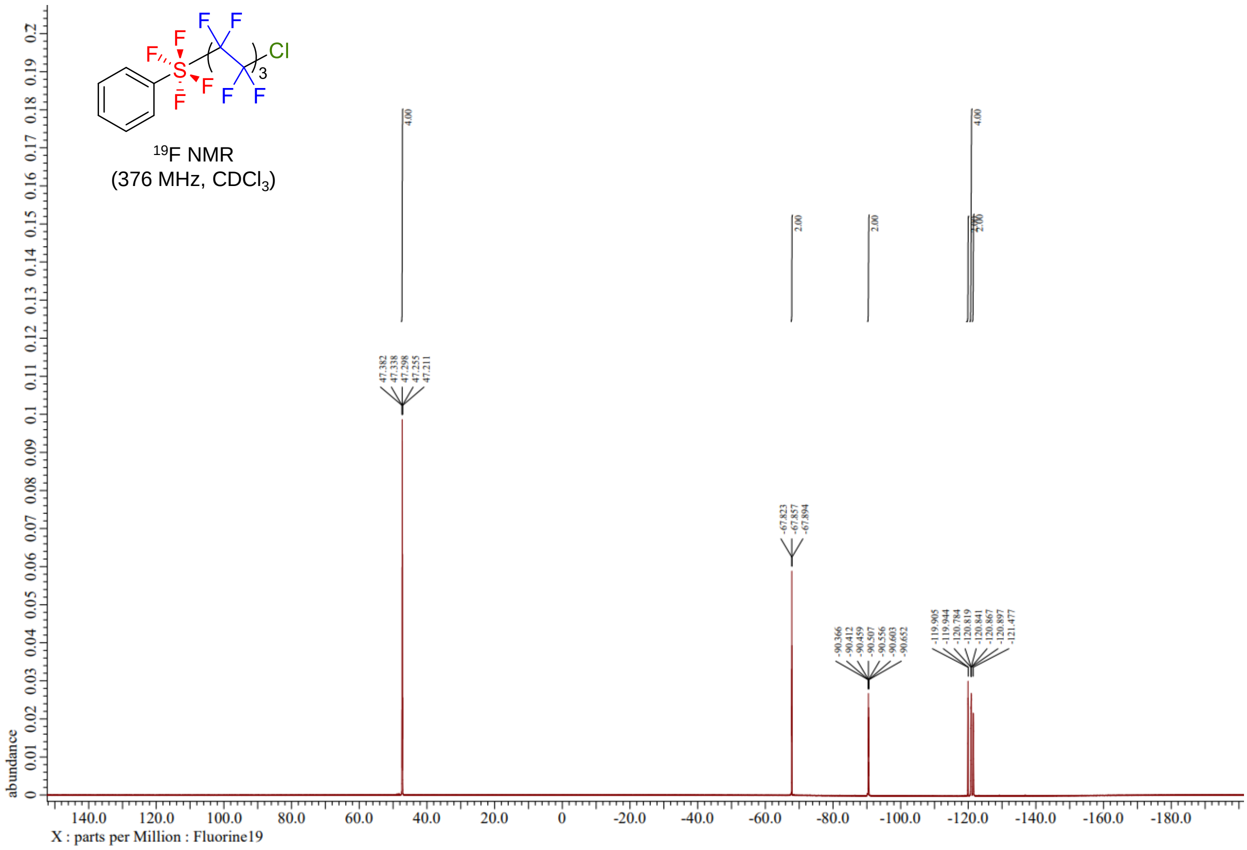


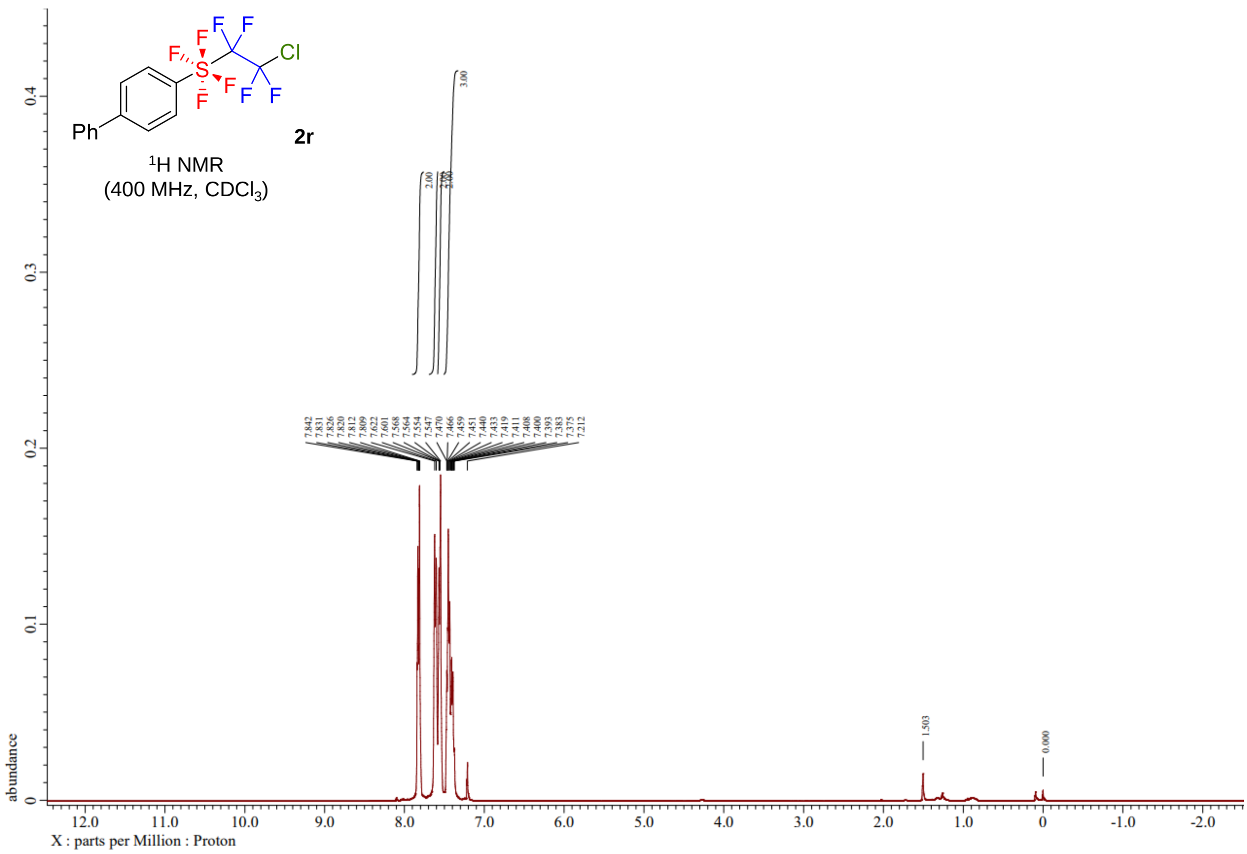


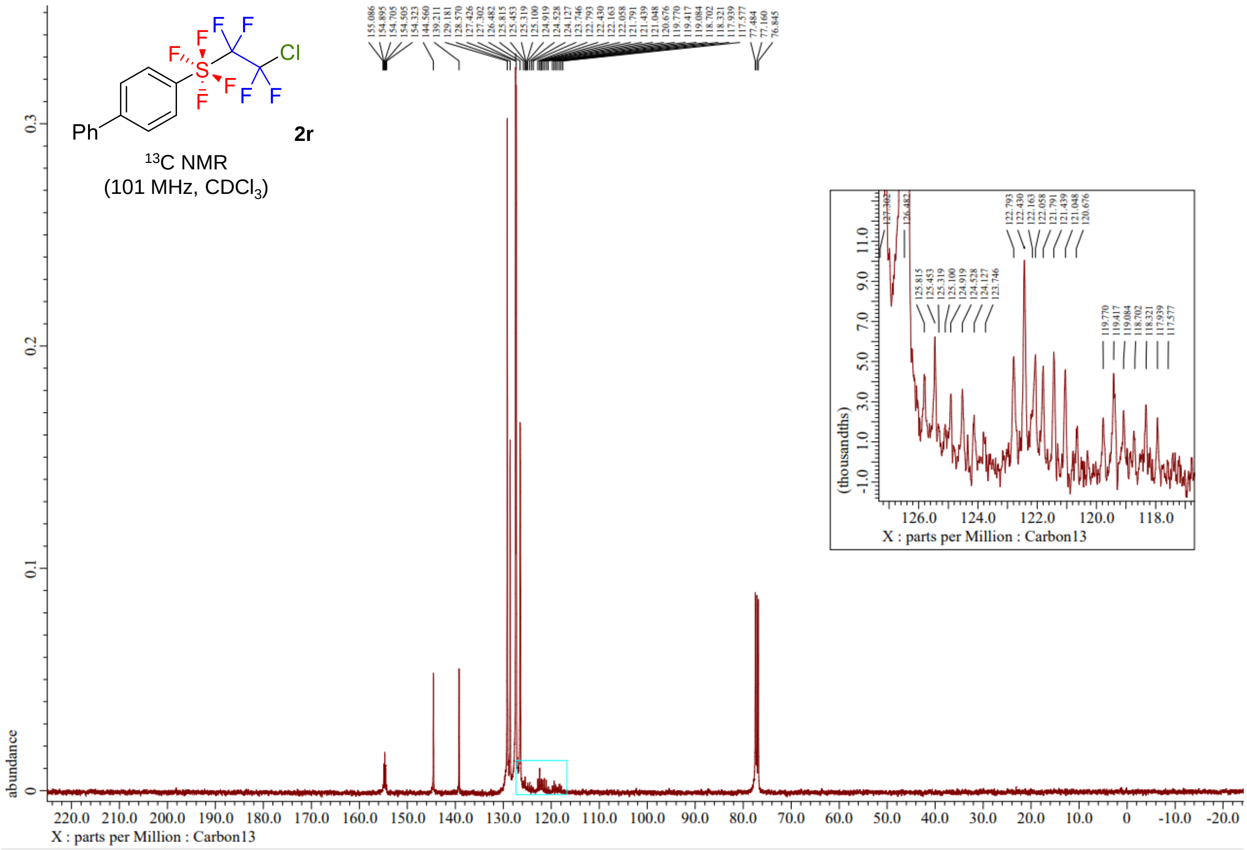
F
F
F
F
S
F
Cl
3
F
F
F
F
^{1}H NMR
(400 MHz, CDCl$_3$)
2.00
3.00
1.557
7.805
7.785
7.534
7.524
7.516
7.498
7.489
7.469
7.451
7.261
0.000
abundance
X : parts per Million : Proton



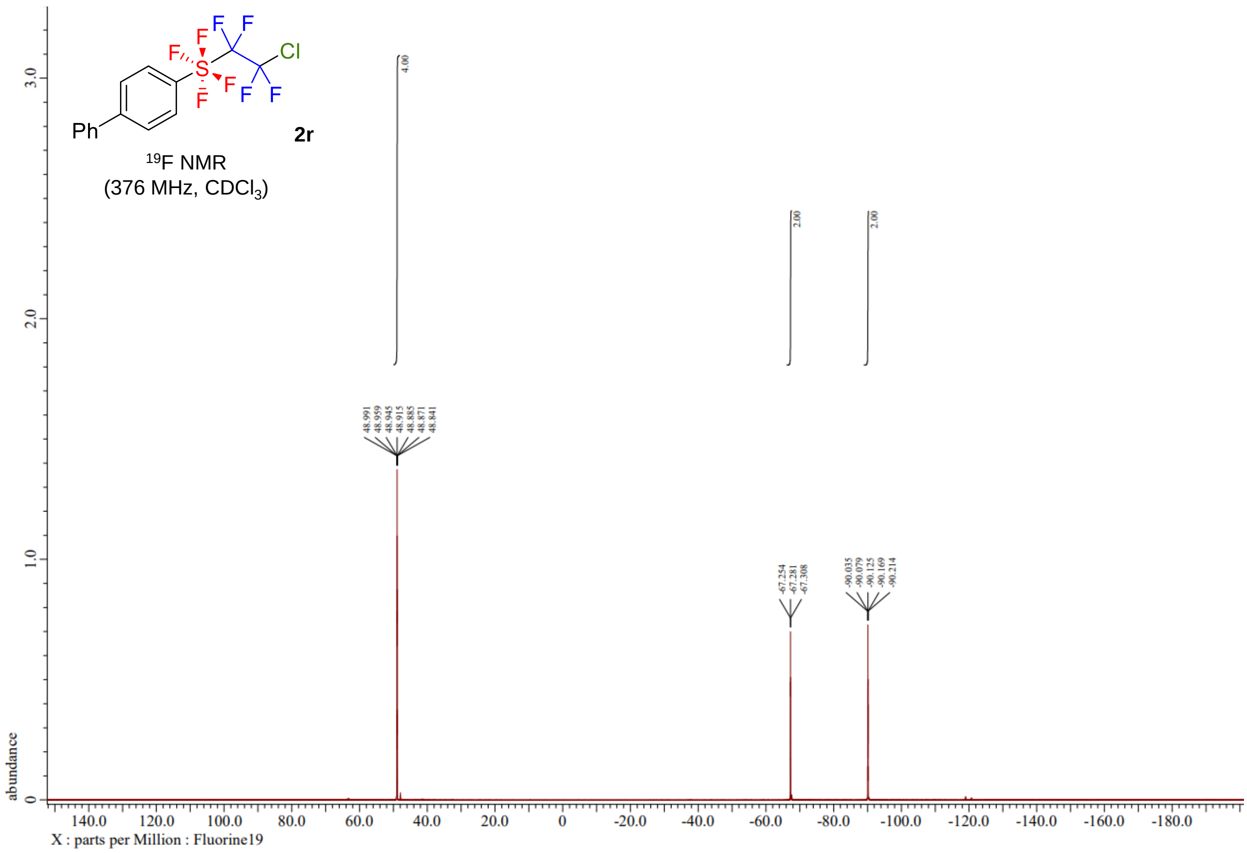
^{13}C NMR
(101 MHz, CDCl$_3$)
128.878
77.481
76.844
131.671
126.152
126.104
126.051
126.003
125.951
156.045
155.853
155.657
155.465
155.283
(thousandths)
X : parts per Million : Carbon13



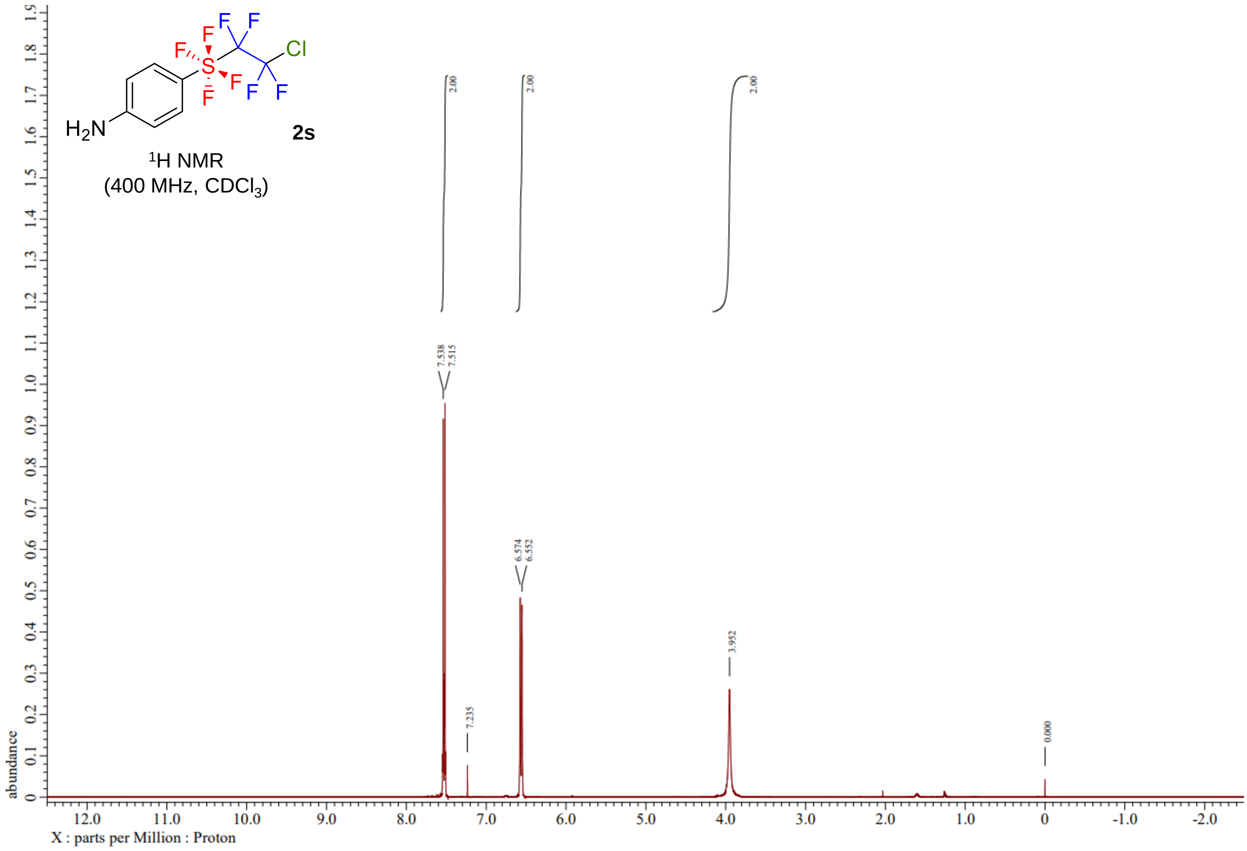


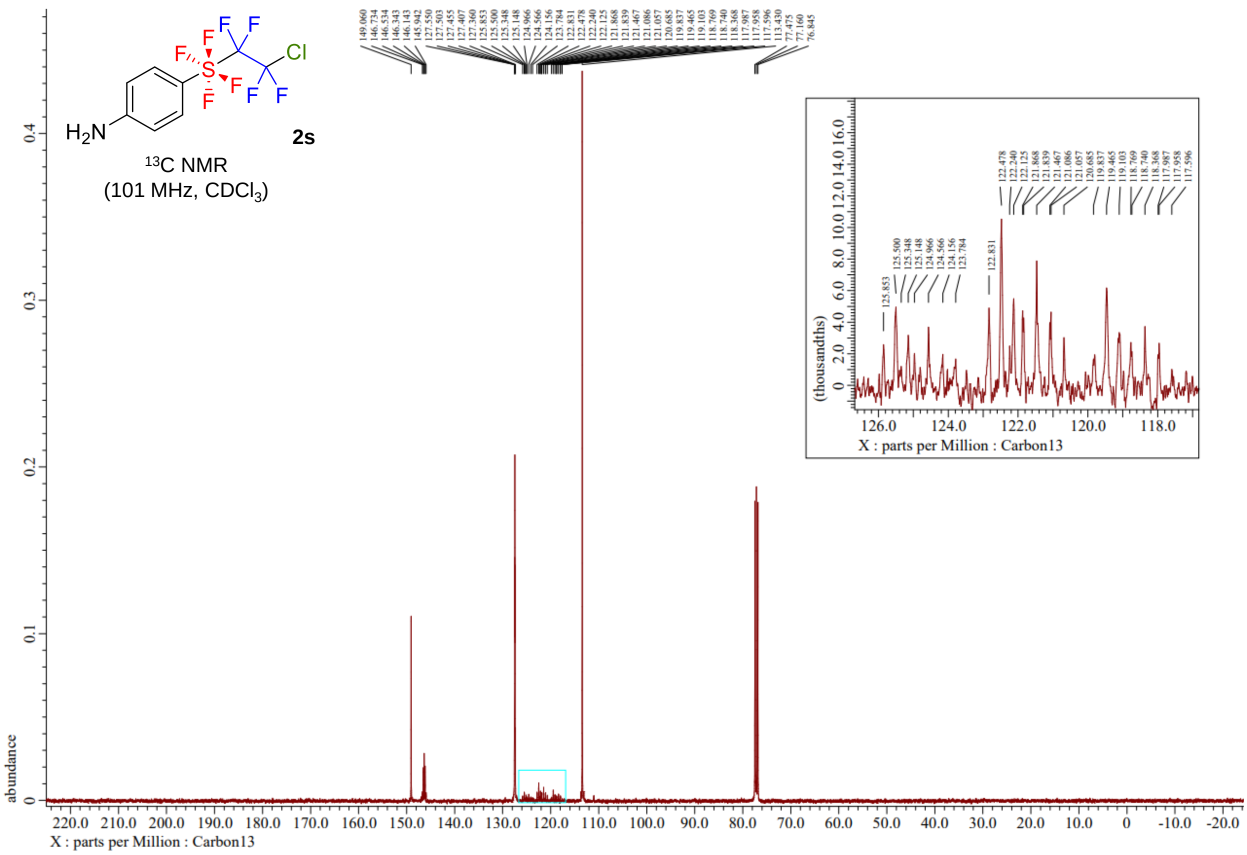


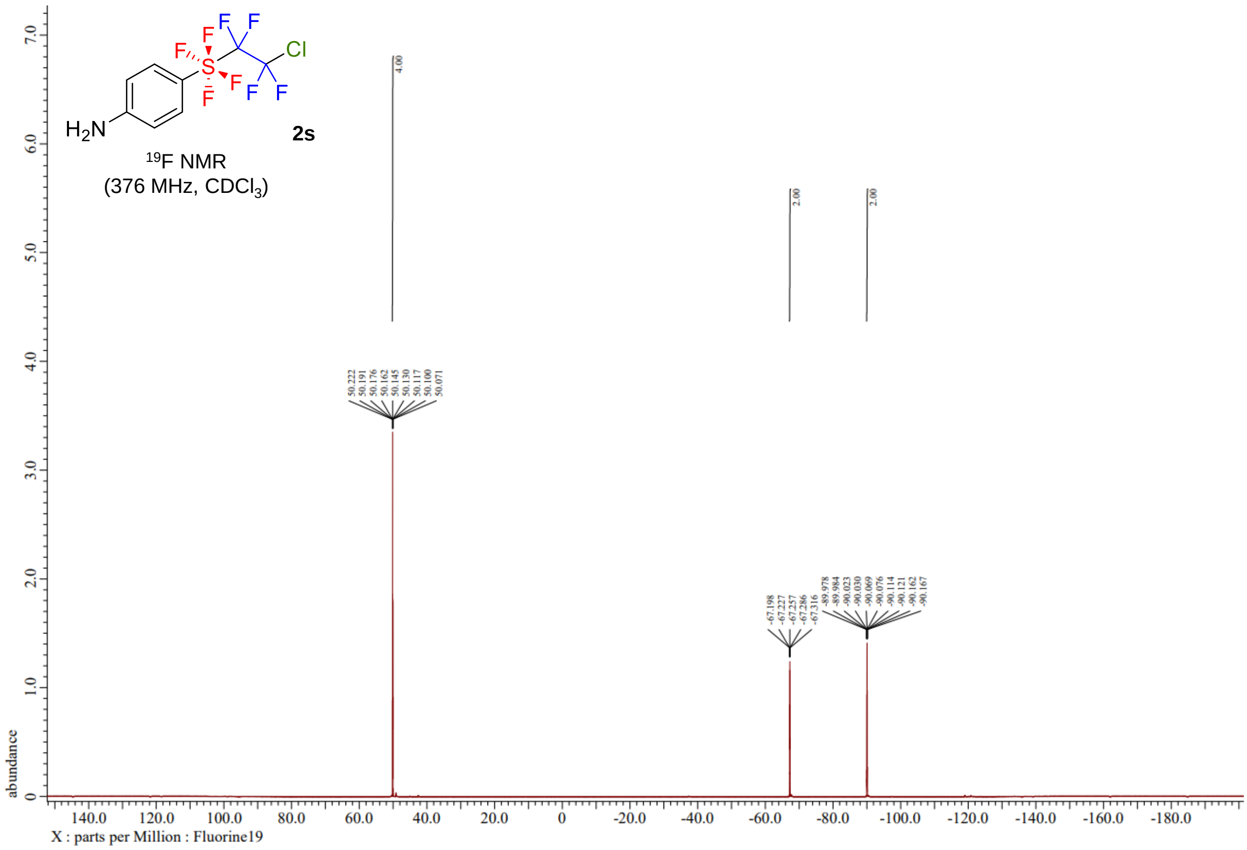
Ph
2r
^{13}C NMR
(101 MHz, $CDCl_3$)
abundance
X : parts per Million : Carbon13
X : parts per Million : Carbon13

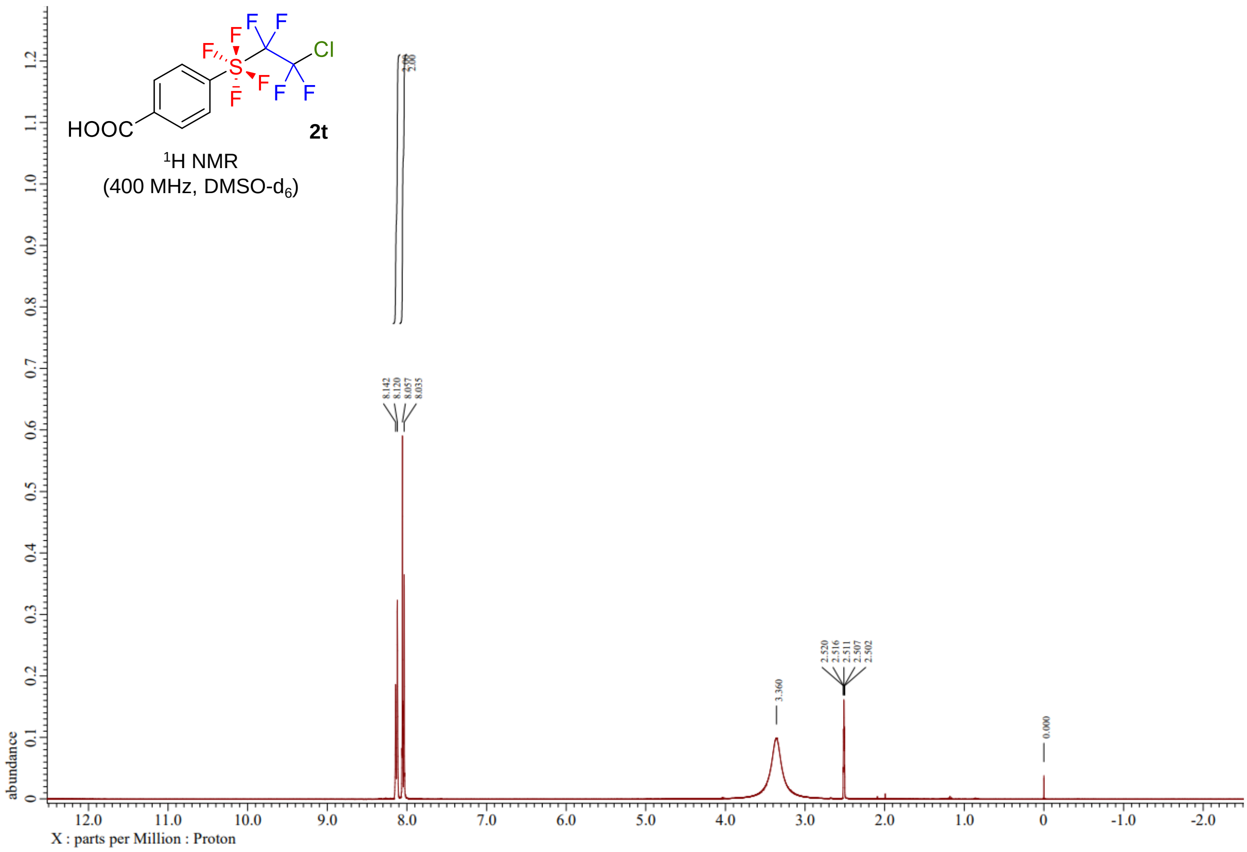


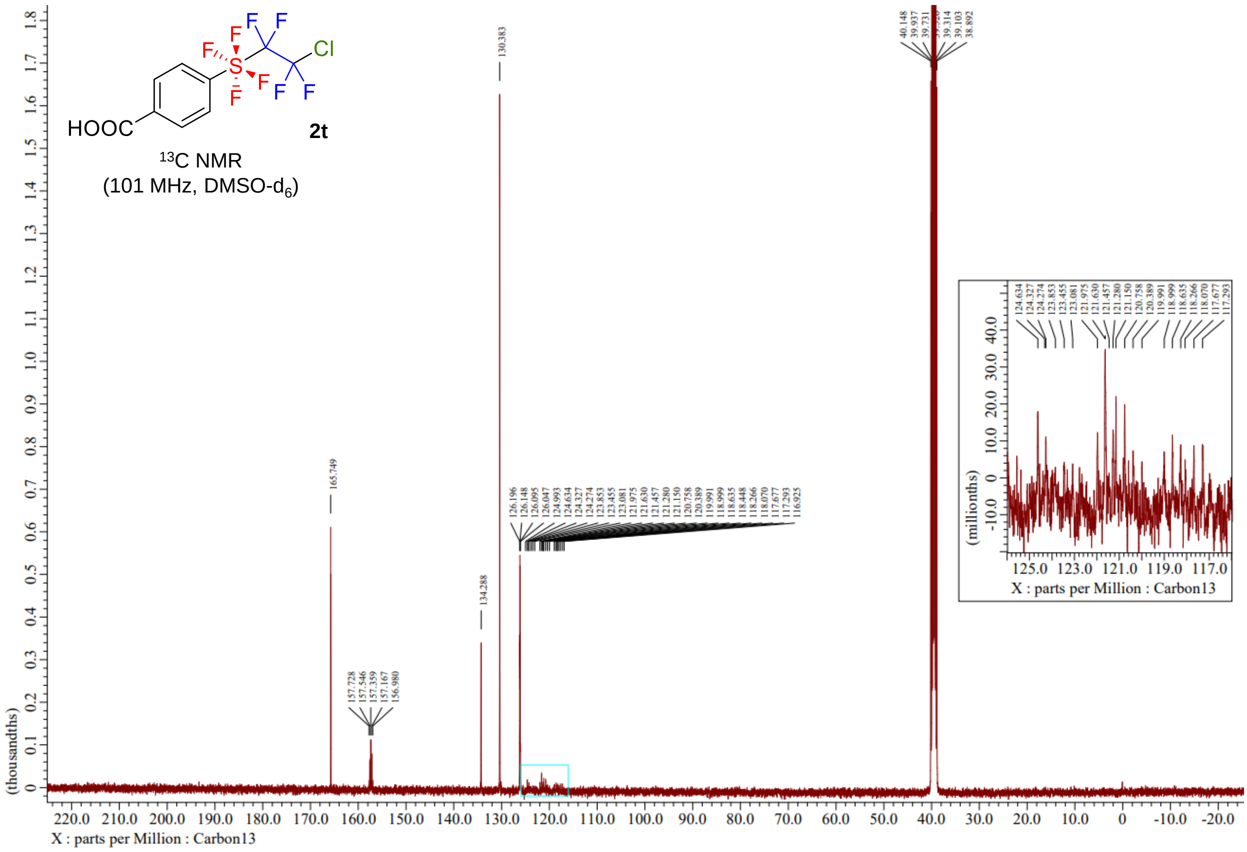
Ph
2r
^{19}F NMR
(376 MHz, $CDCl_3$)
abundance
X : parts per Million : Fluorine19

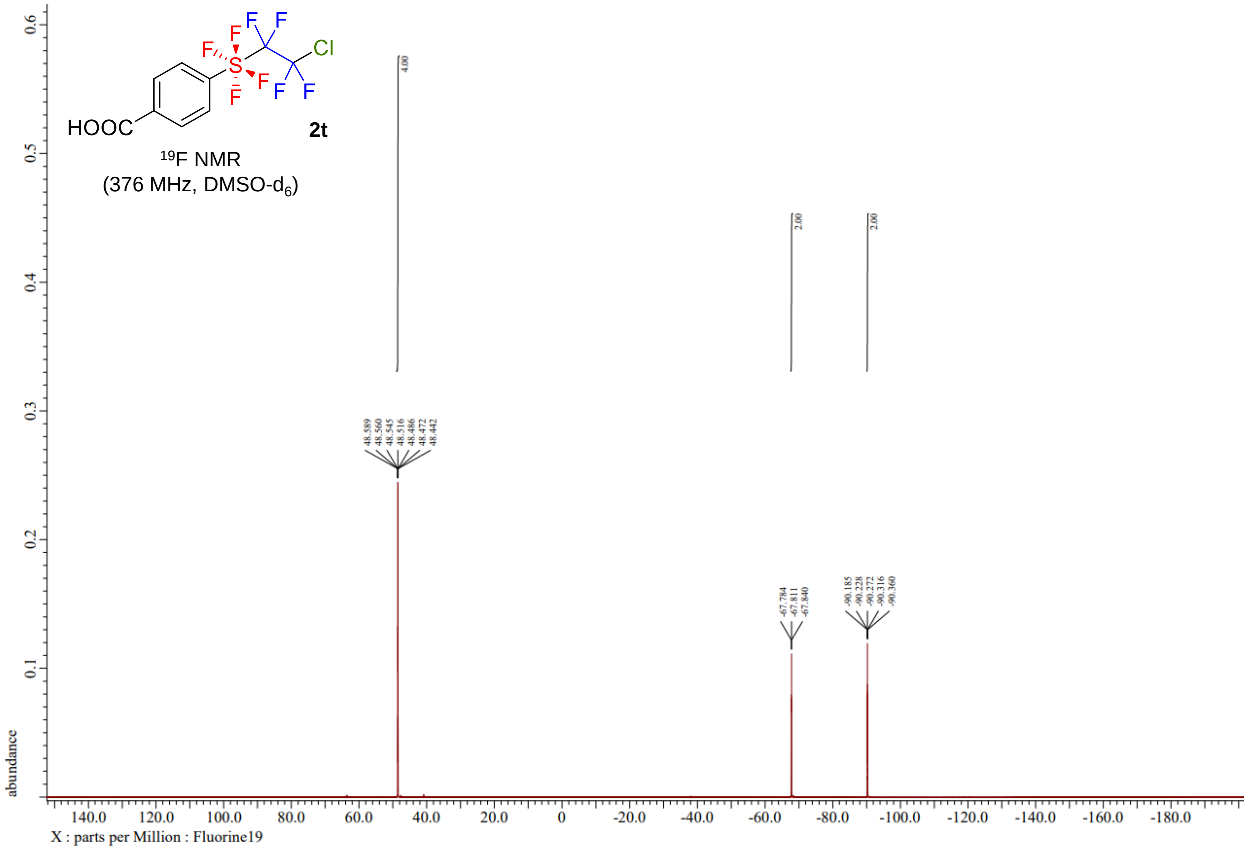

H2N
2s
1H NMR
(400 MHz, CDCl3)
7.538
7.515
7.235
6.574
6.552
3.952
0.000
2.00
2.00
2.00
abundance
X : parts per Million : Proton

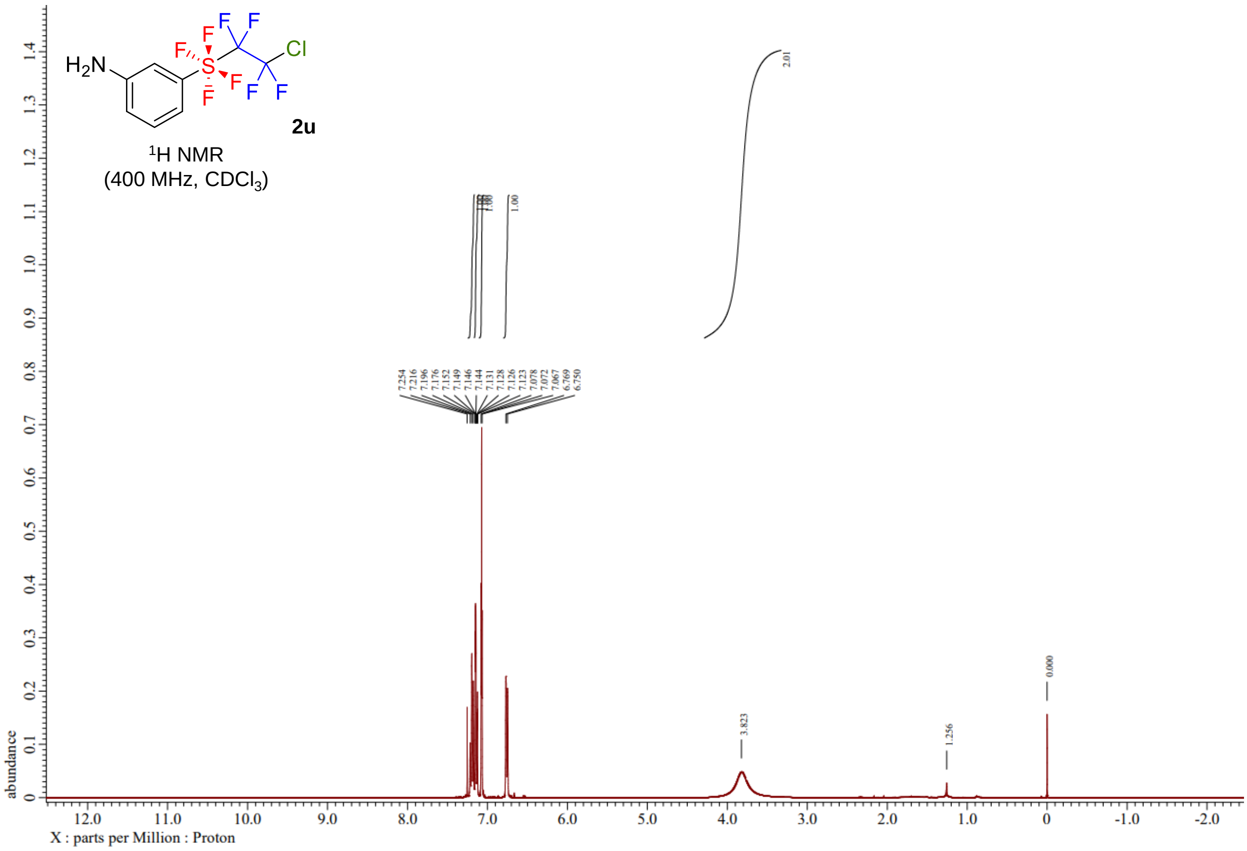

H2N
2s
13C NMR
(101 MHz, CDCl3)
abundance
X : parts per Million : Carbon13
(thousandths)
X : parts per Million : Carbon13

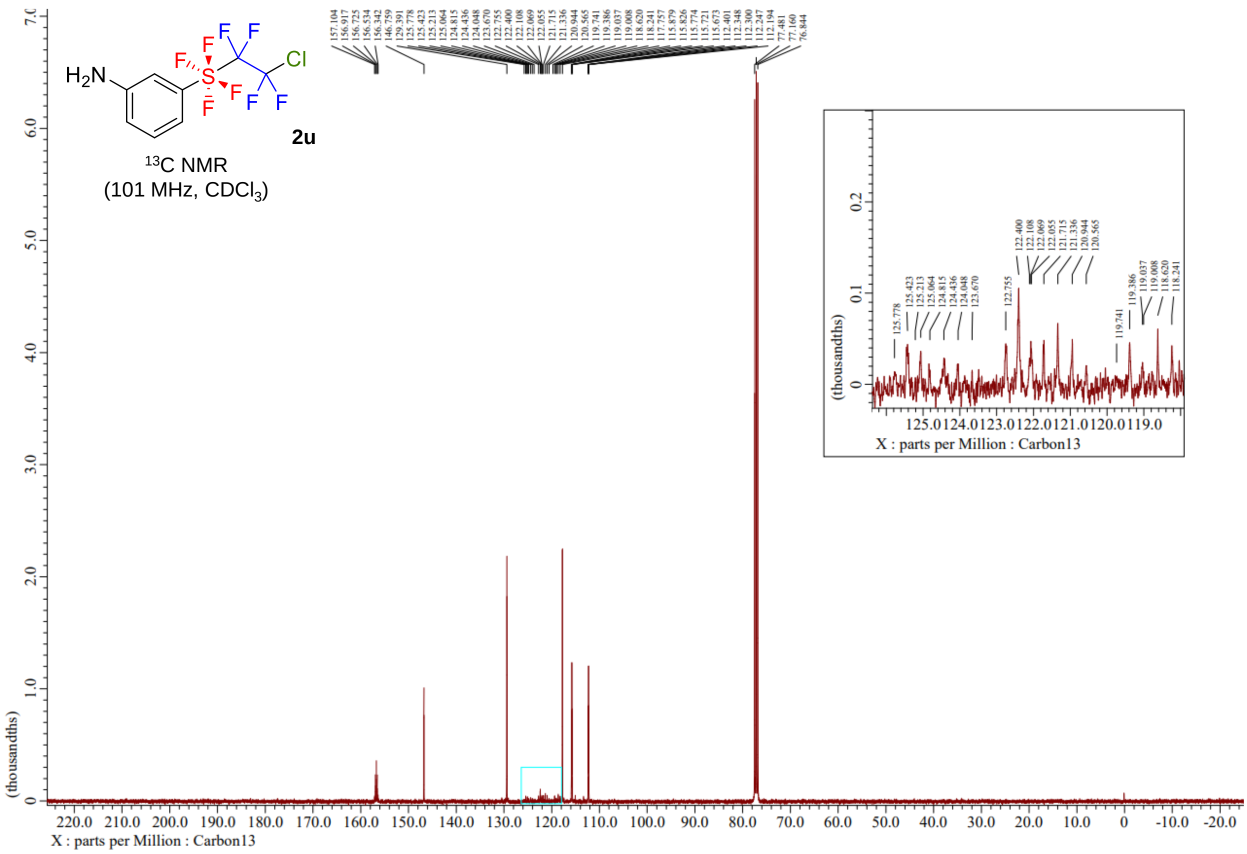

H2N
2s
19F NMR
(376 MHz, CDCl3)
abundance
X : parts per Million : Fluorine19

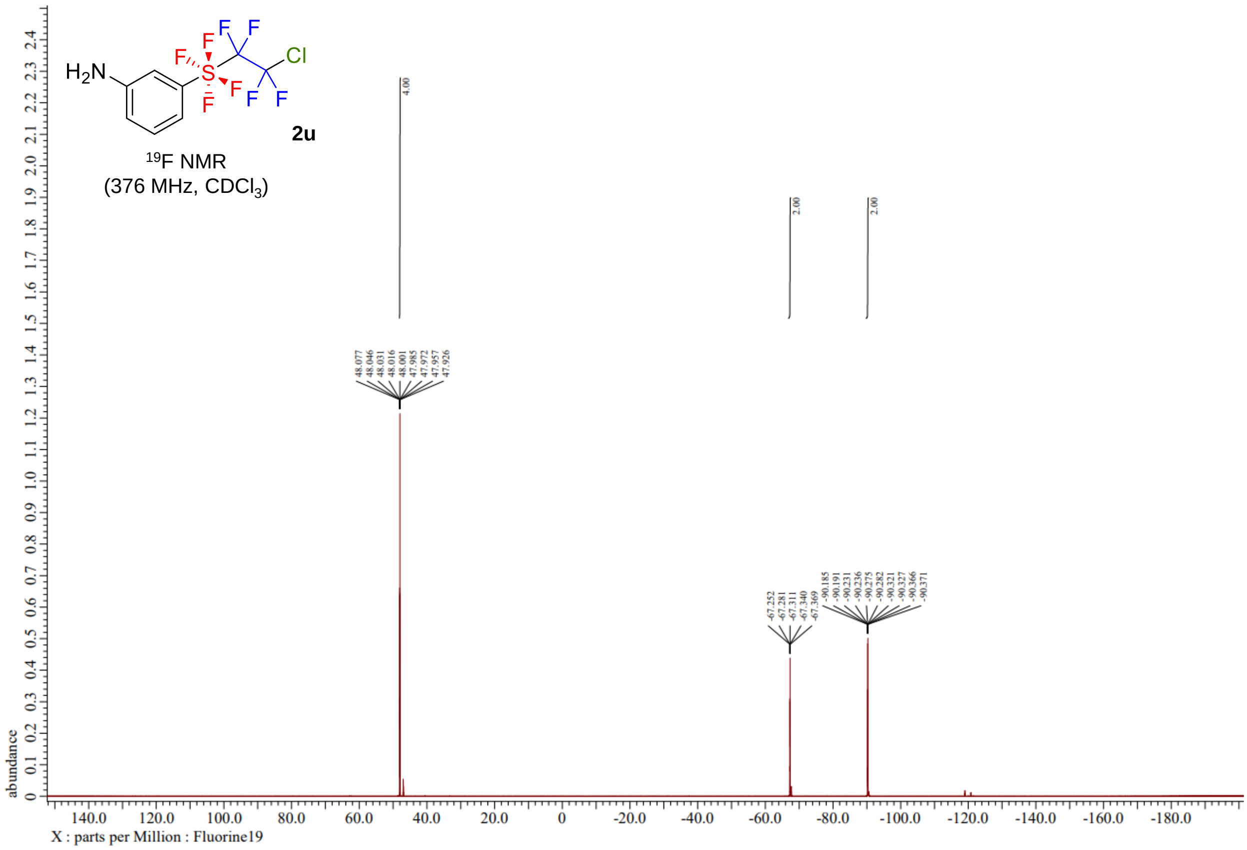

HOOC
2t
1H NMR
(400 MHz, DMSO-d6)
abundance
X : parts per Million : Proton

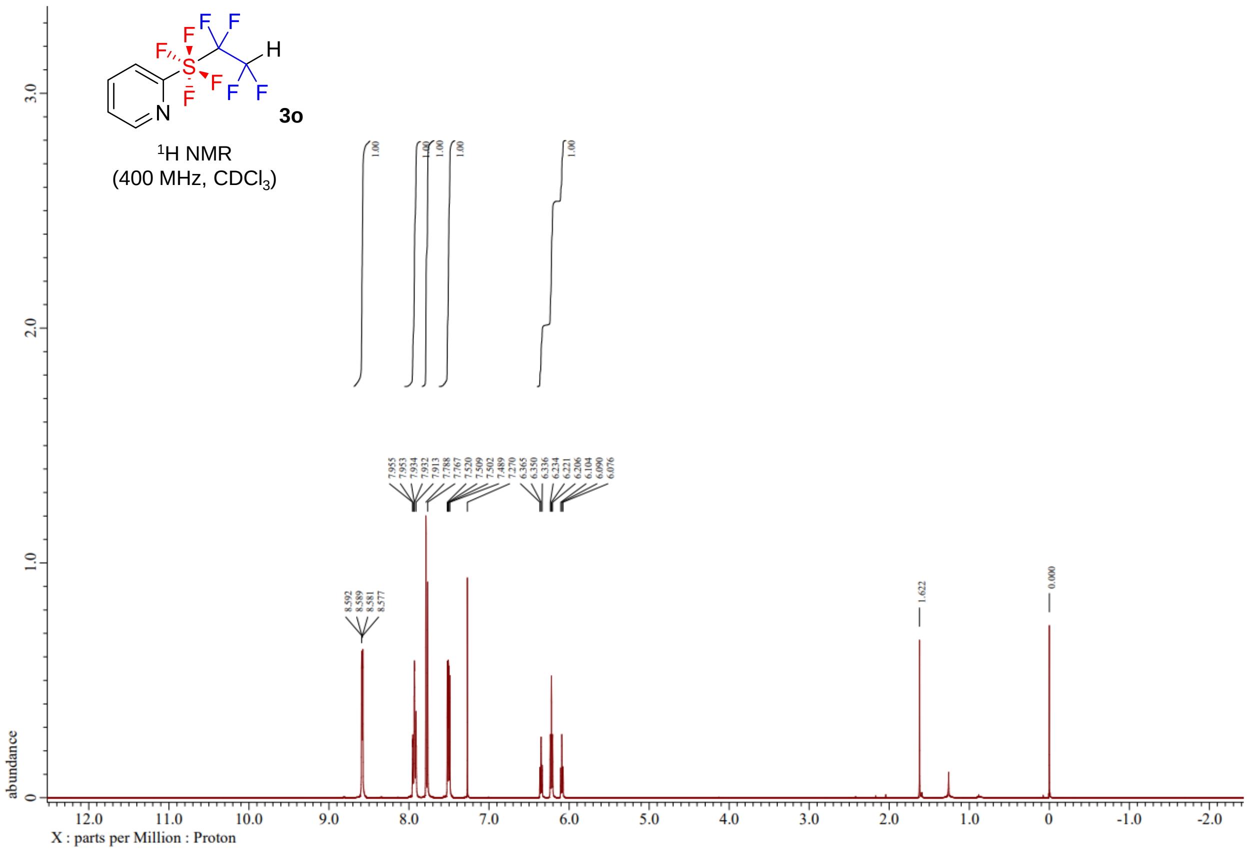

HOOC
2t
13C NMR
(101 MHz, DMSO-d6)
X : parts per Million : Carbon13
(thousandths)
165.749
157.728
157.546
157.359
157.167
156.980
134.288
130.383
40.148
39.937
39.731
39.314
39.103
38.892
X : parts per Million : Carbon13
(millionths)

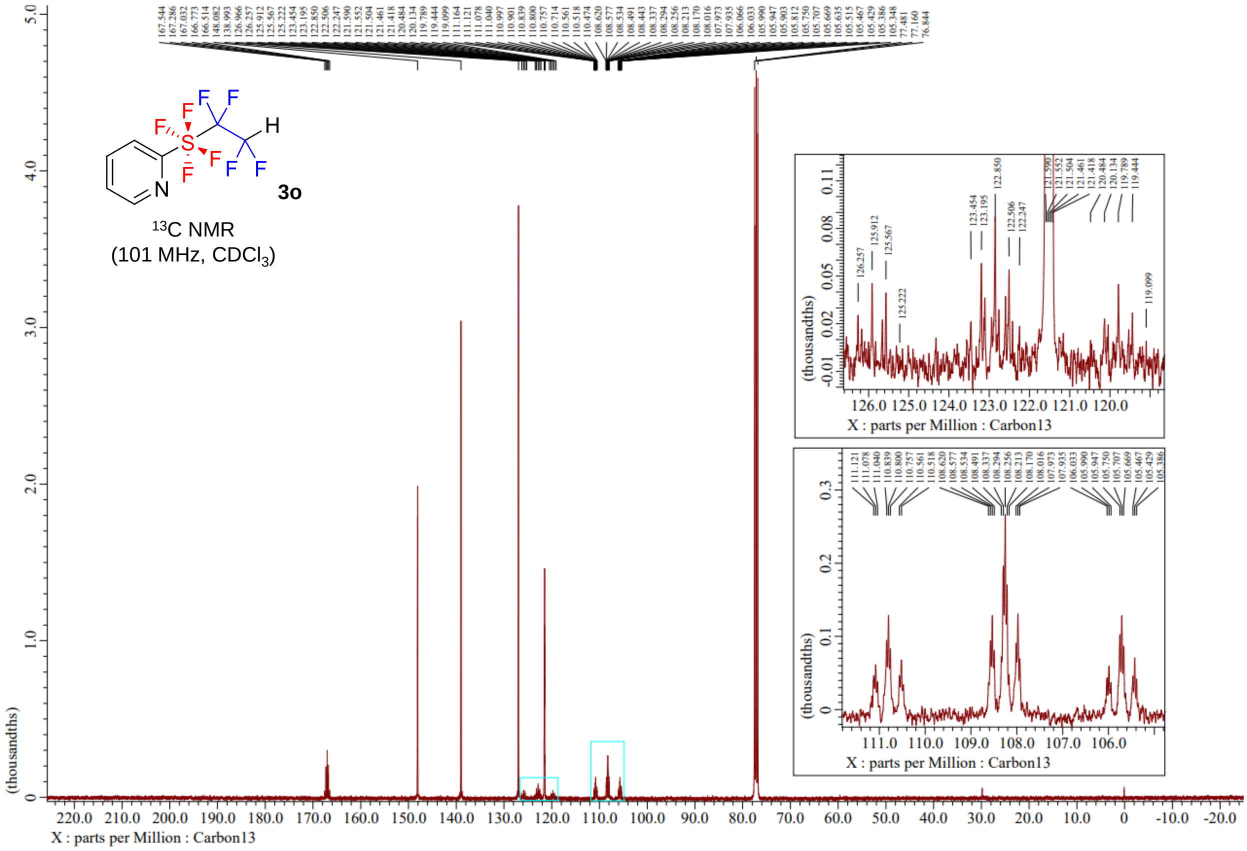

HOOC
2t
19F NMR
(376 MHz, DMSO-d6)
abundance
4.00
2.00
2.00
48.589
48.560
48.545
48.516
48.486
48.472
48.442
-67.784
-67.811
-67.840
-90.185
-90.228
-90.272
-90.316
-90.360
X : parts per Million : Fluorine19

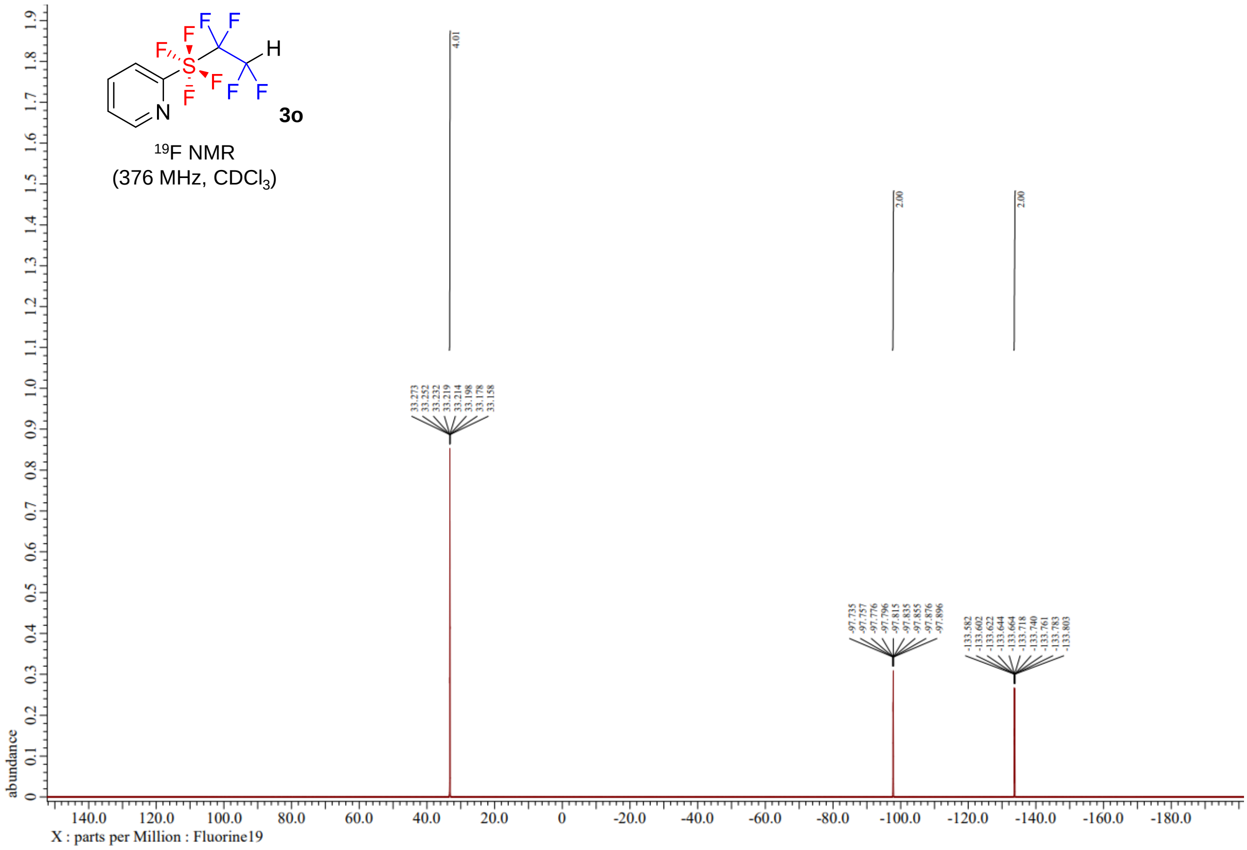

2u
^{1}H NMR
(400 MHz, $CDCl_3$)
abundance
X : parts per Million : Proton

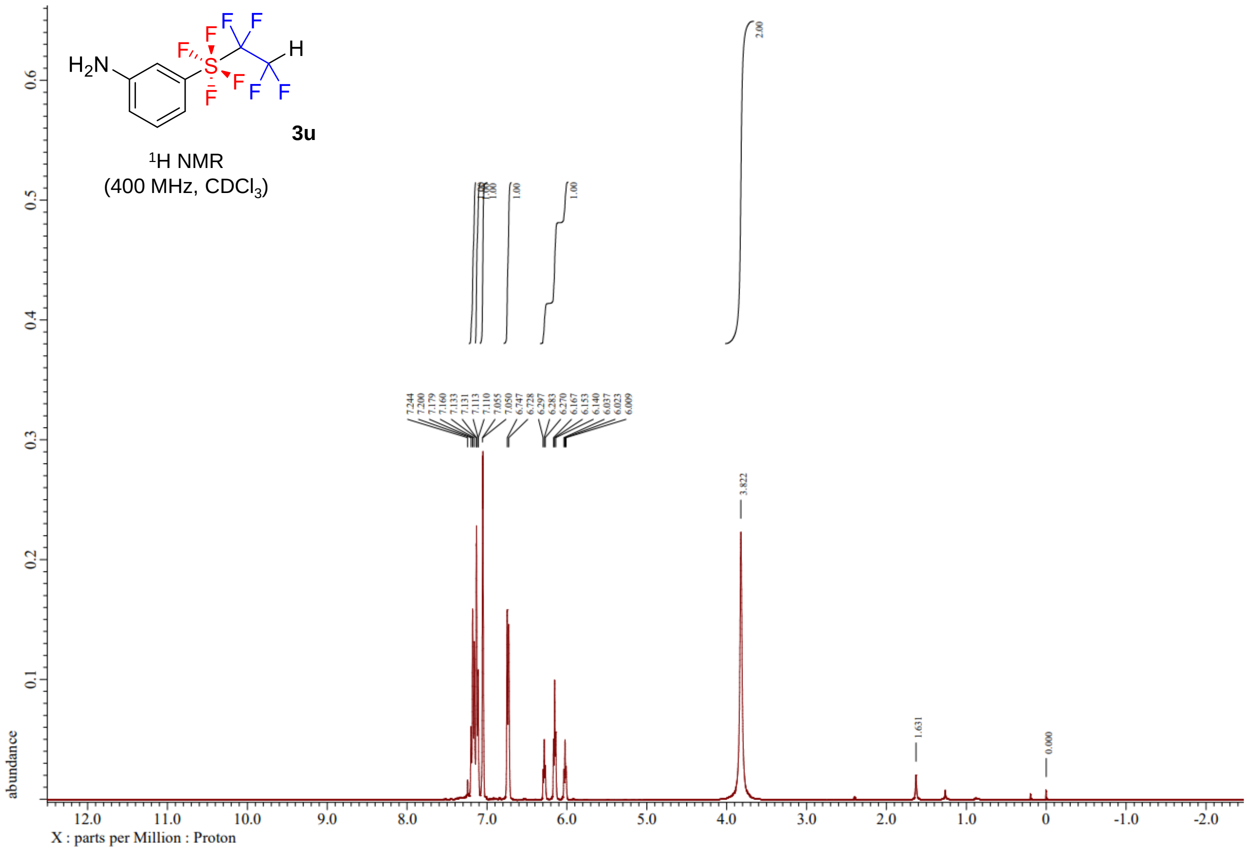

2u
^{13}C NMR
(101 MHz, $CDCl_3$)
(thousandths)
X : parts per Million : Carbon13

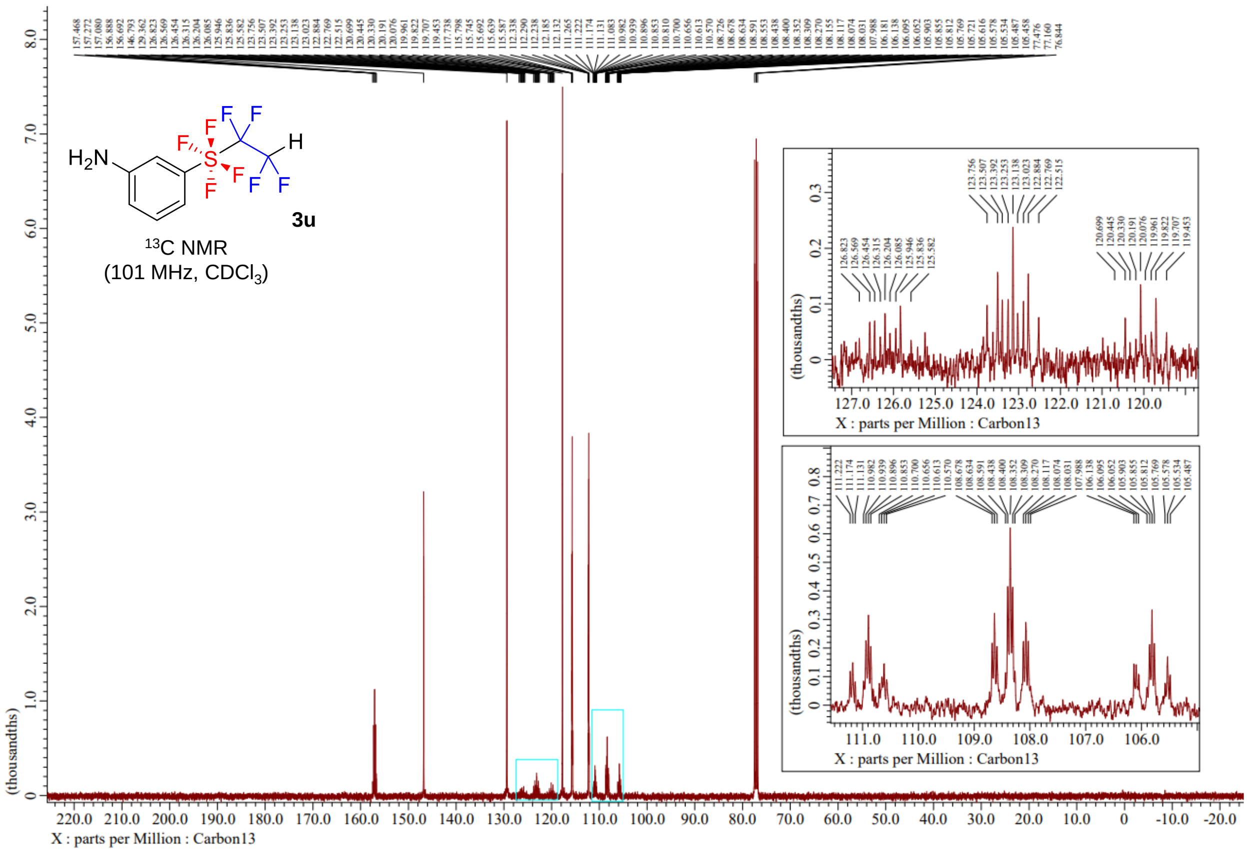

2u
19F NMR
(376 MHz, CDCl3)
X : parts per Million : Fluorine19
abundance

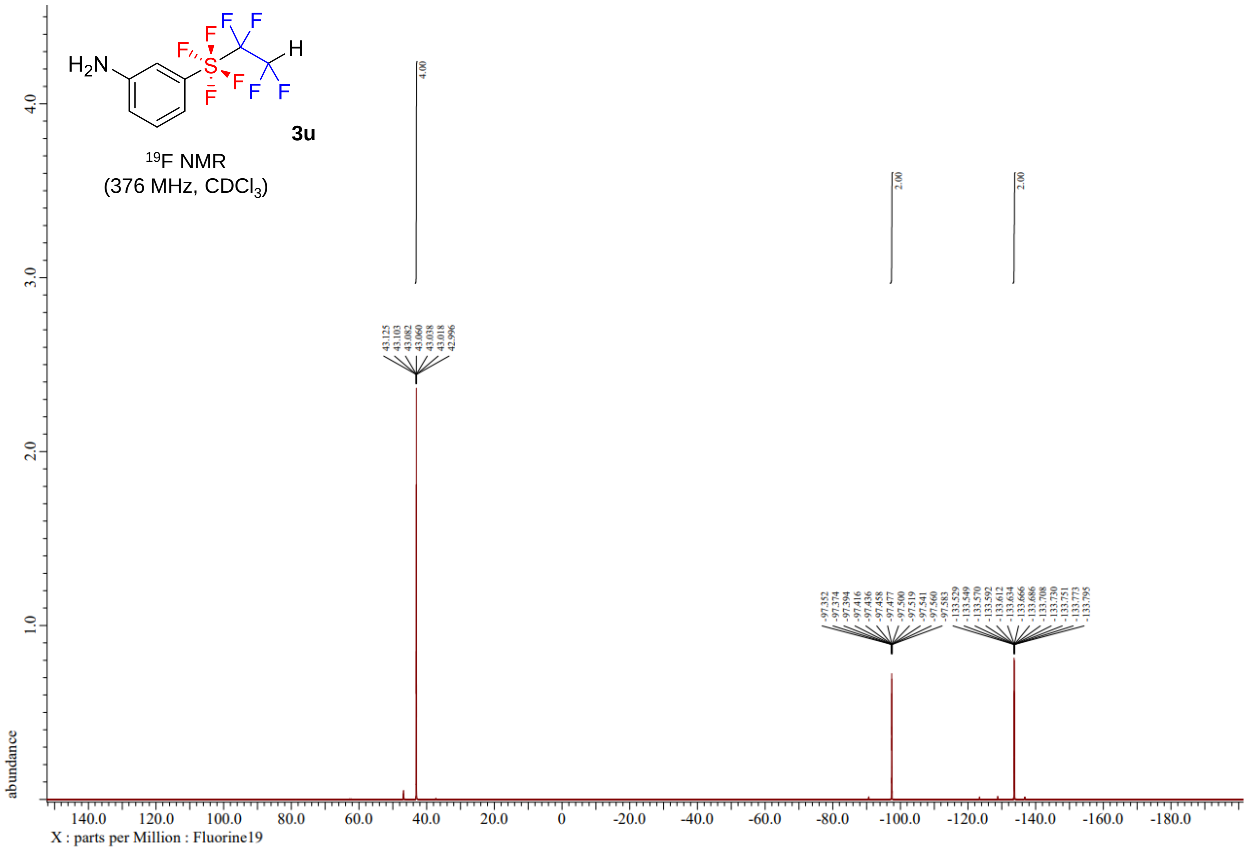

3o
1H NMR
(400 MHz, CDCl3)
X : parts per Million : Proton
abundance

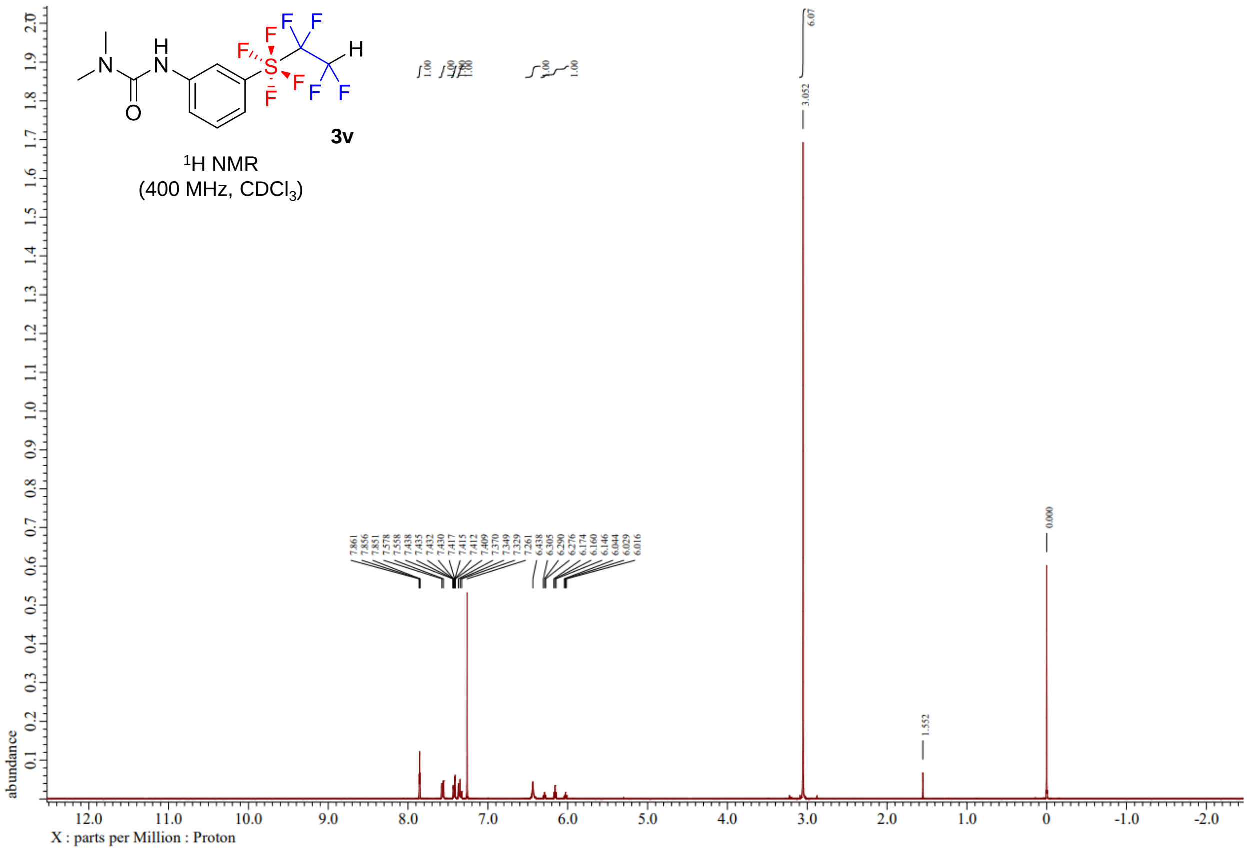

3o
^{13}C NMR
(101 MHz, $CDCl_3$)
X : parts per Million : Carbon13

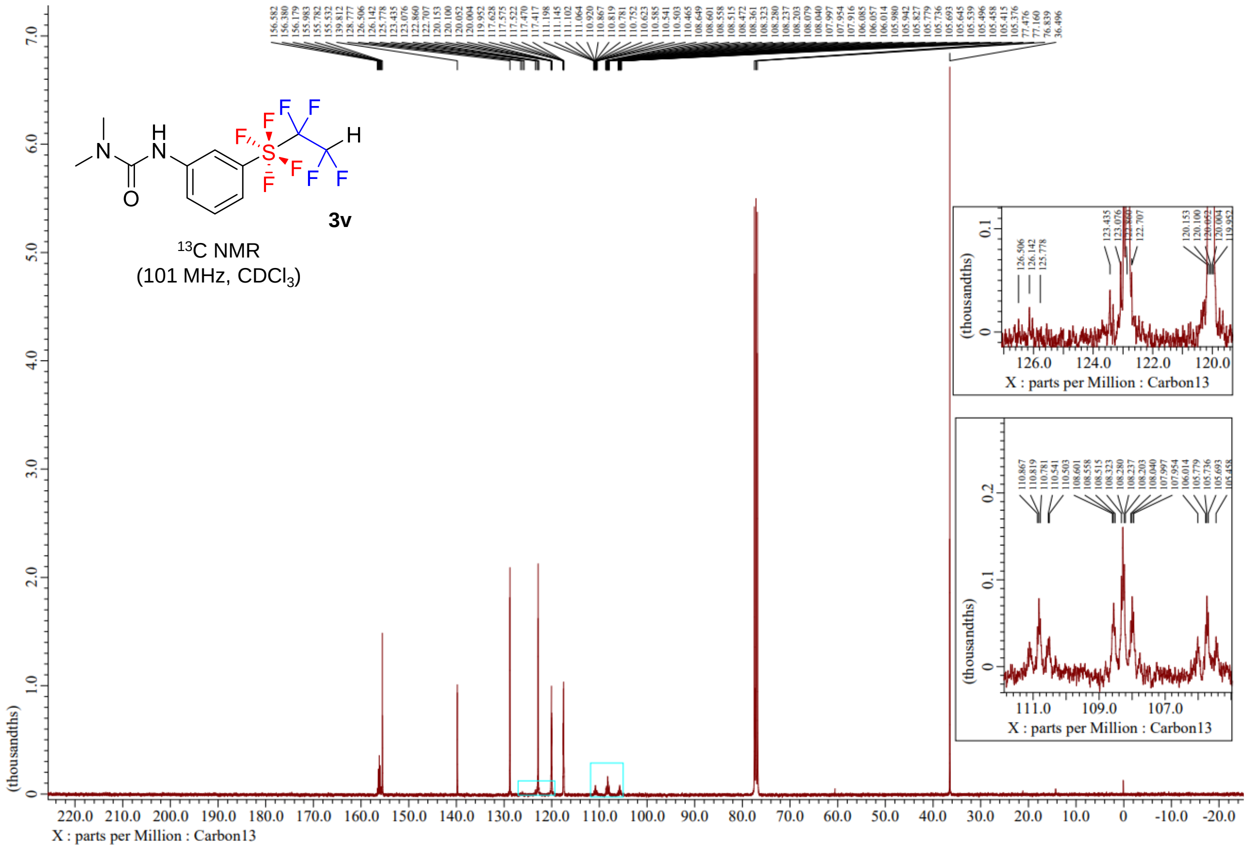

3o
^{19}F NMR
(376 MHz, $CDCl_3$)
X : parts per Million : Fluorine19

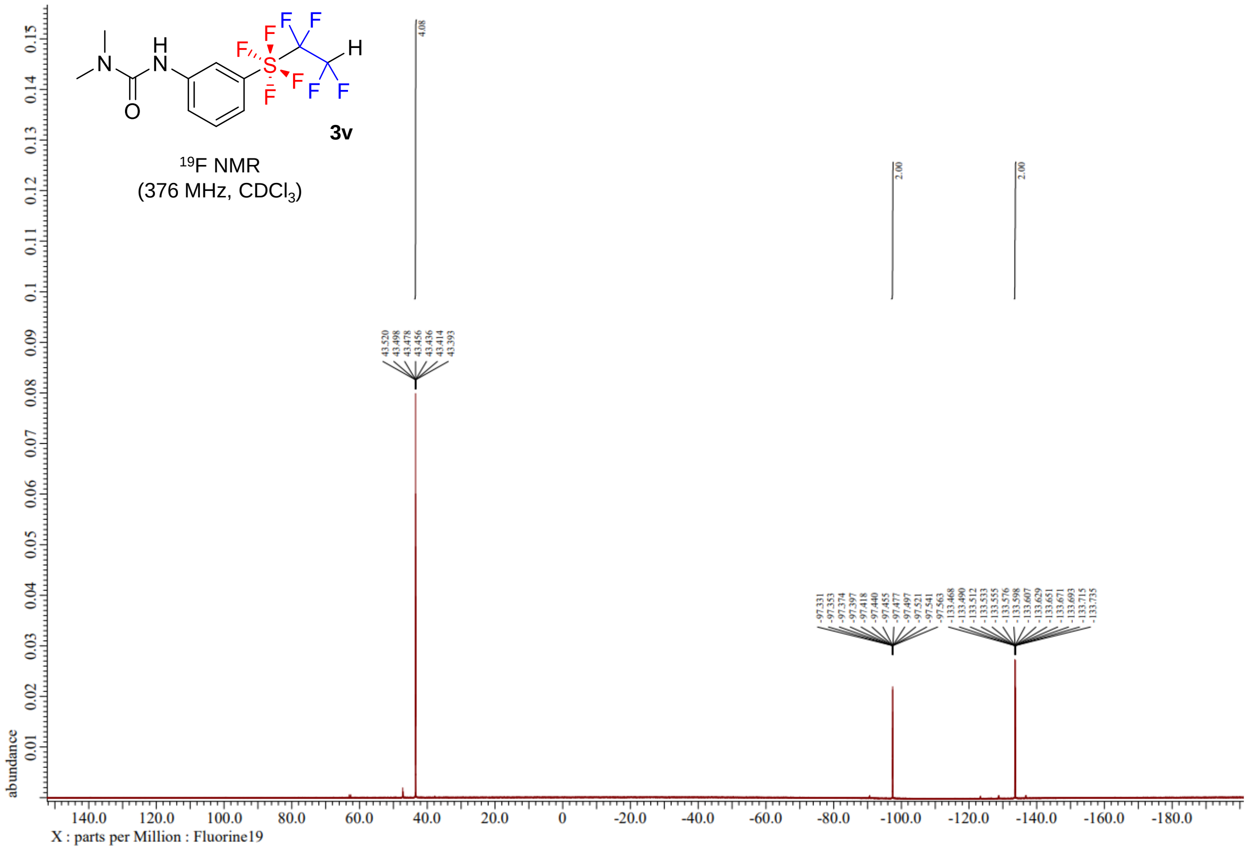

3u
1H NMR
(400 MHz, CDCl3)
abundance
X : parts per Million : Proton

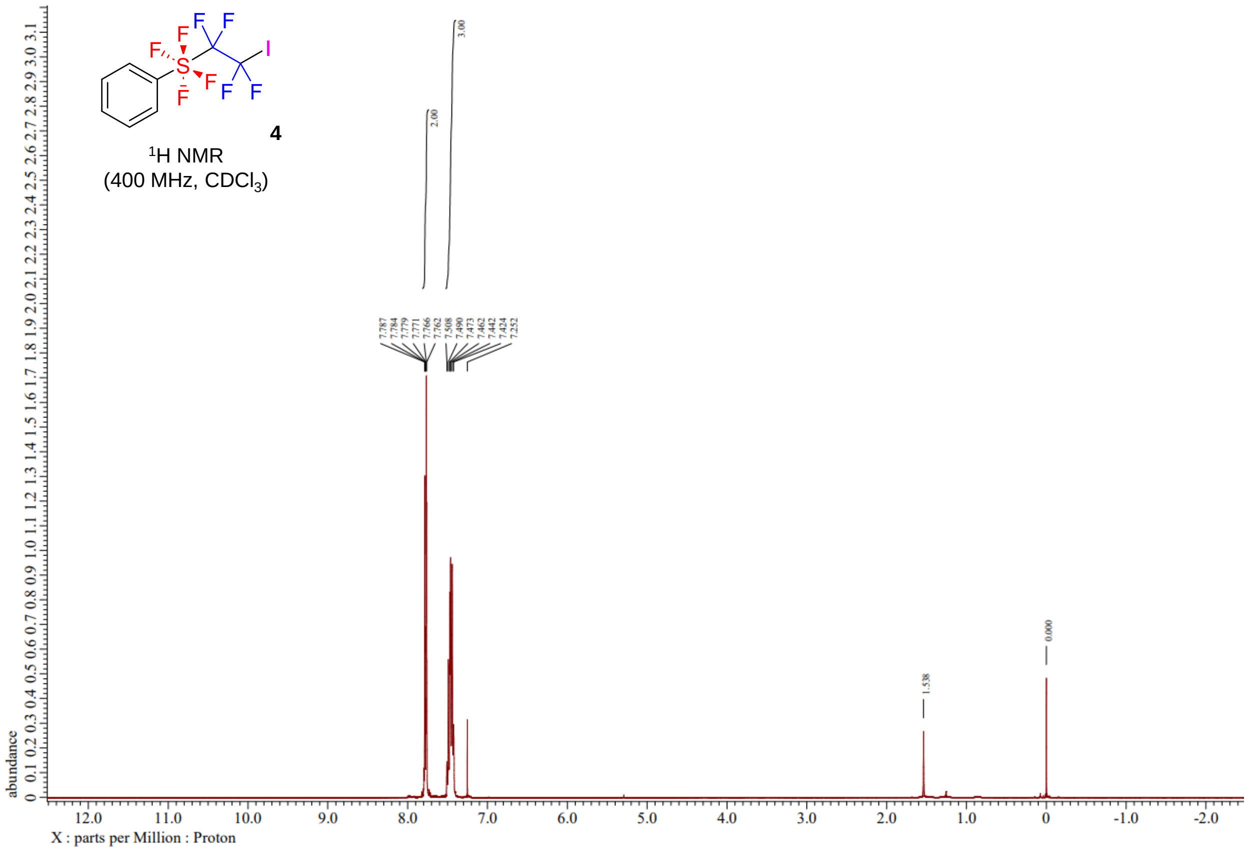

3u
13C NMR
(101 MHz, CDCl3)
(thousandths)
X : parts per Million : Carbon13

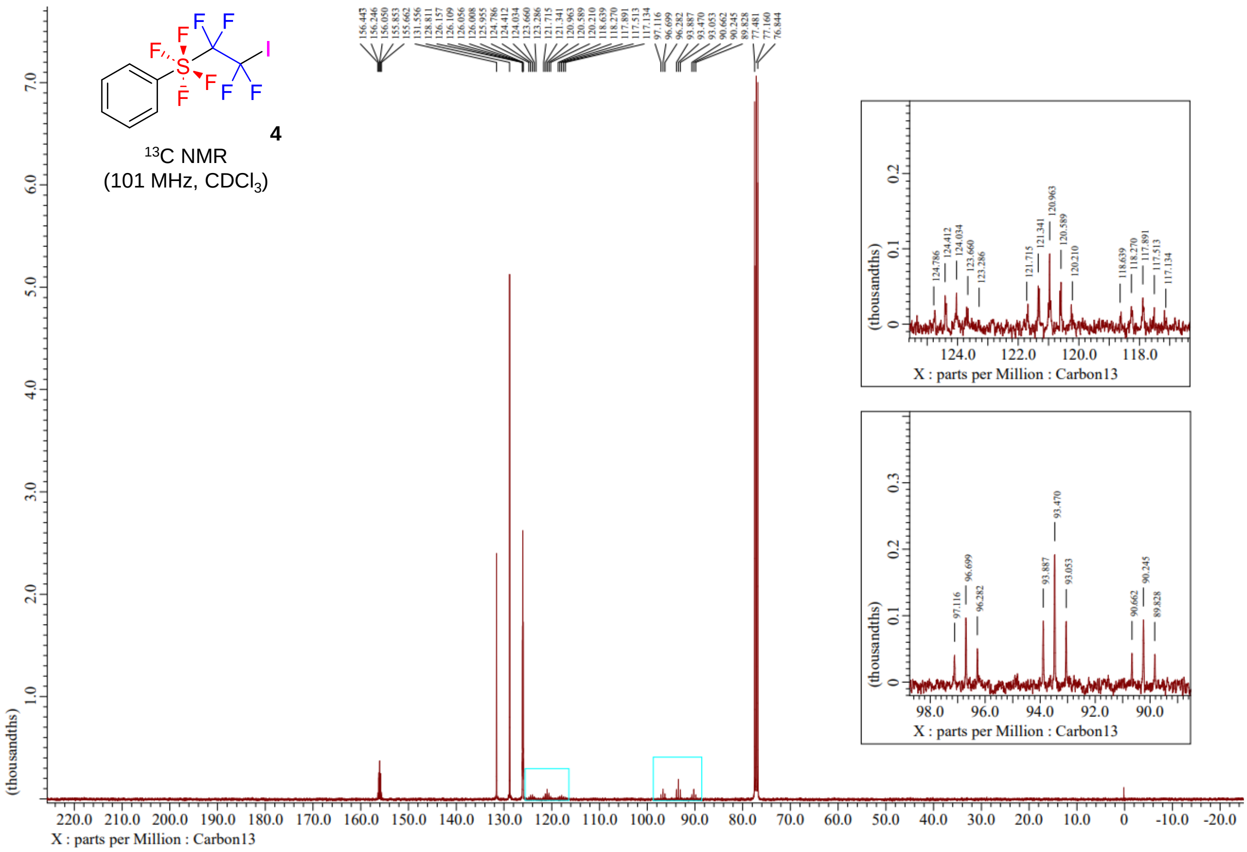

3u
^{19}F NMR
(376 MHz, $CDCl_3$)
abundance
X : parts per Million : Fluorine19

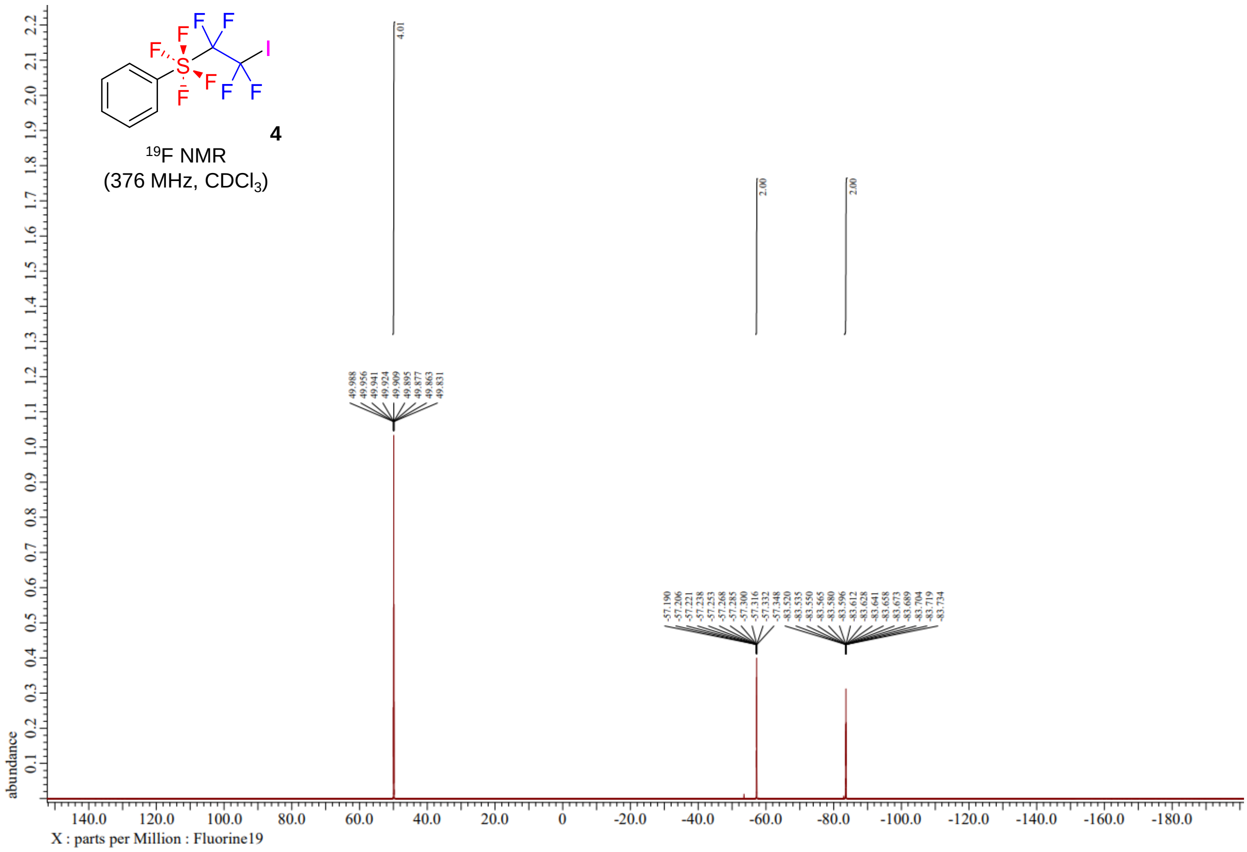

3v
^{1}H NMR
(400 MHz, $CDCl_3$)
abundance
X : parts per Million : Proton


3v
13C NMR
(101 MHz, CDCl3)
X : parts per Million : Carbon13
(thousandths)

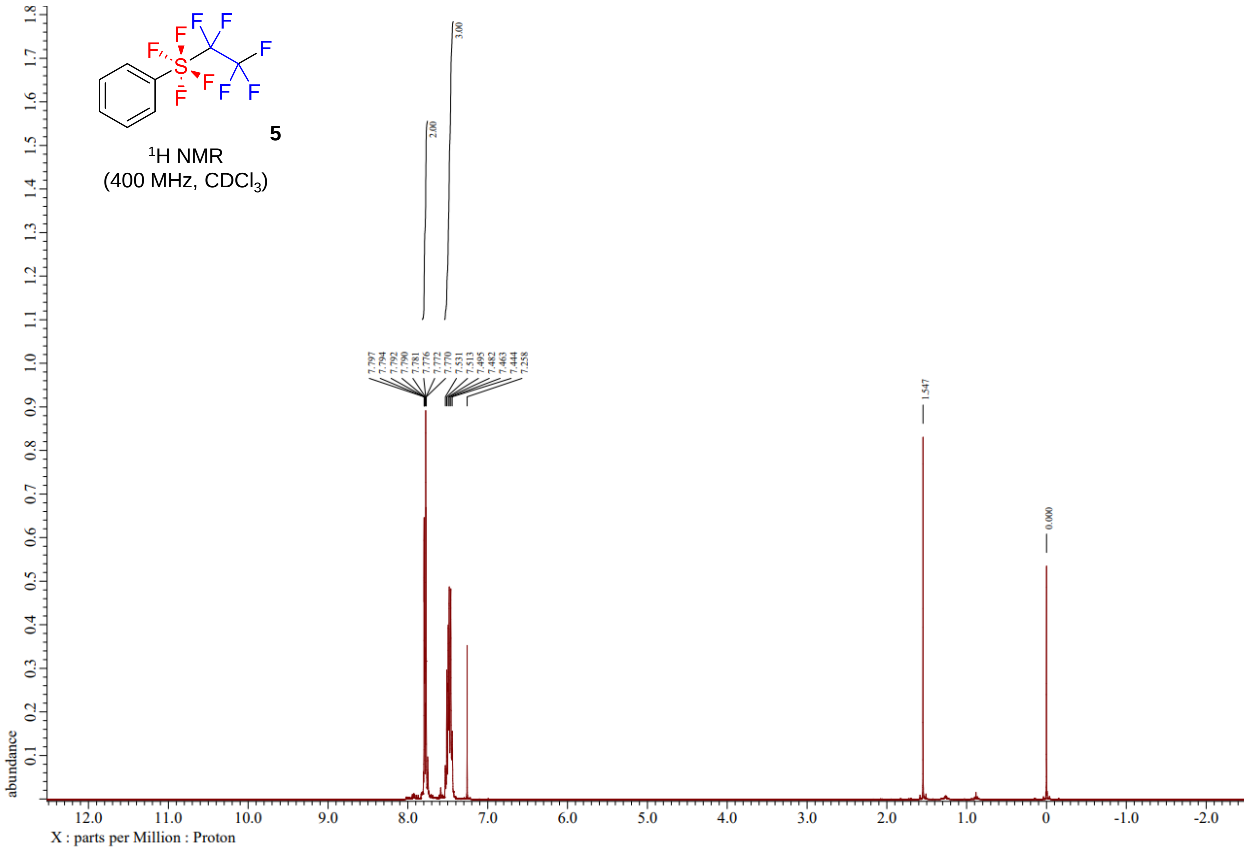

3v
19F NMR
(376 MHz, CDCl3)
X : parts per Million : Fluorine19
abundance


4
¹H NMR
(400 MHz, CDCl3)
abundance
X : parts per Million : Proton

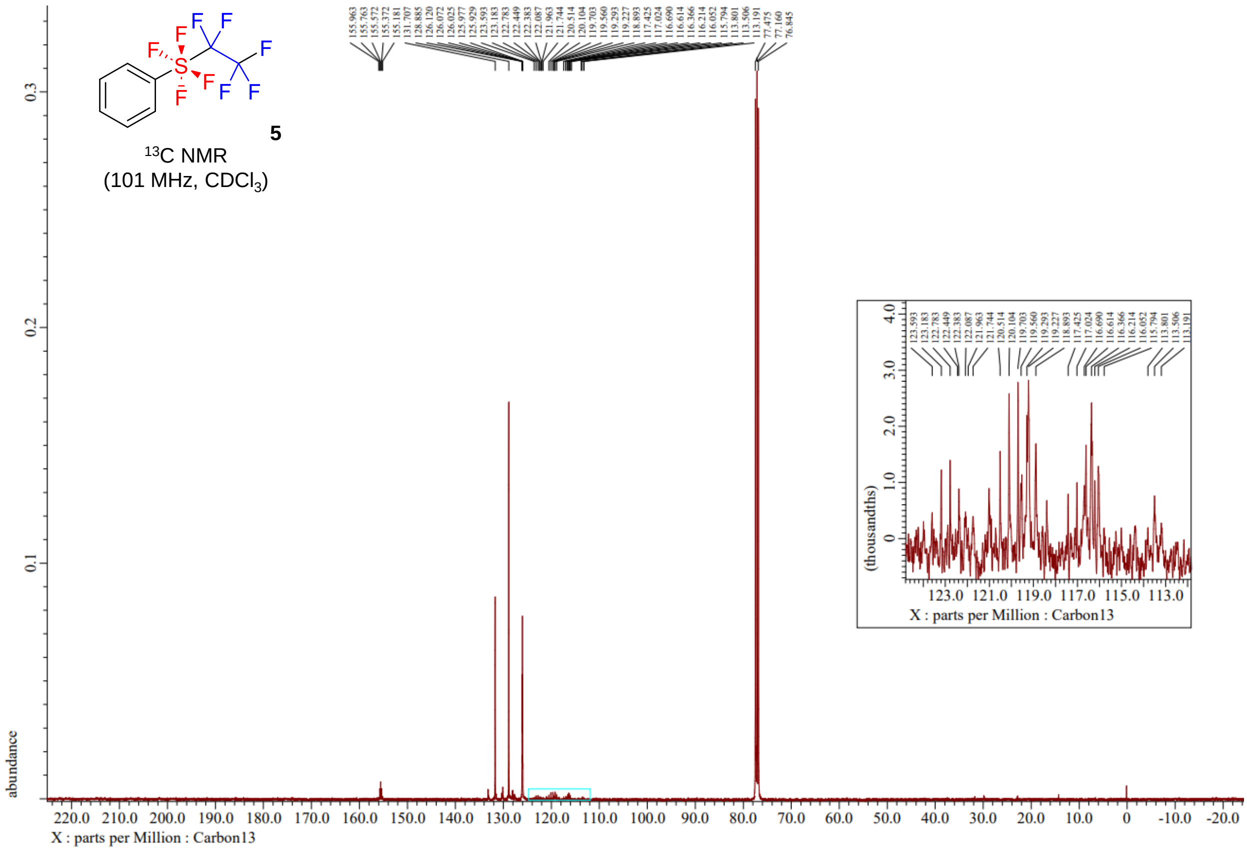

4
¹³C NMR
(101 MHz, CDCl3)
(thousandths)
X : parts per Million : Carbon13

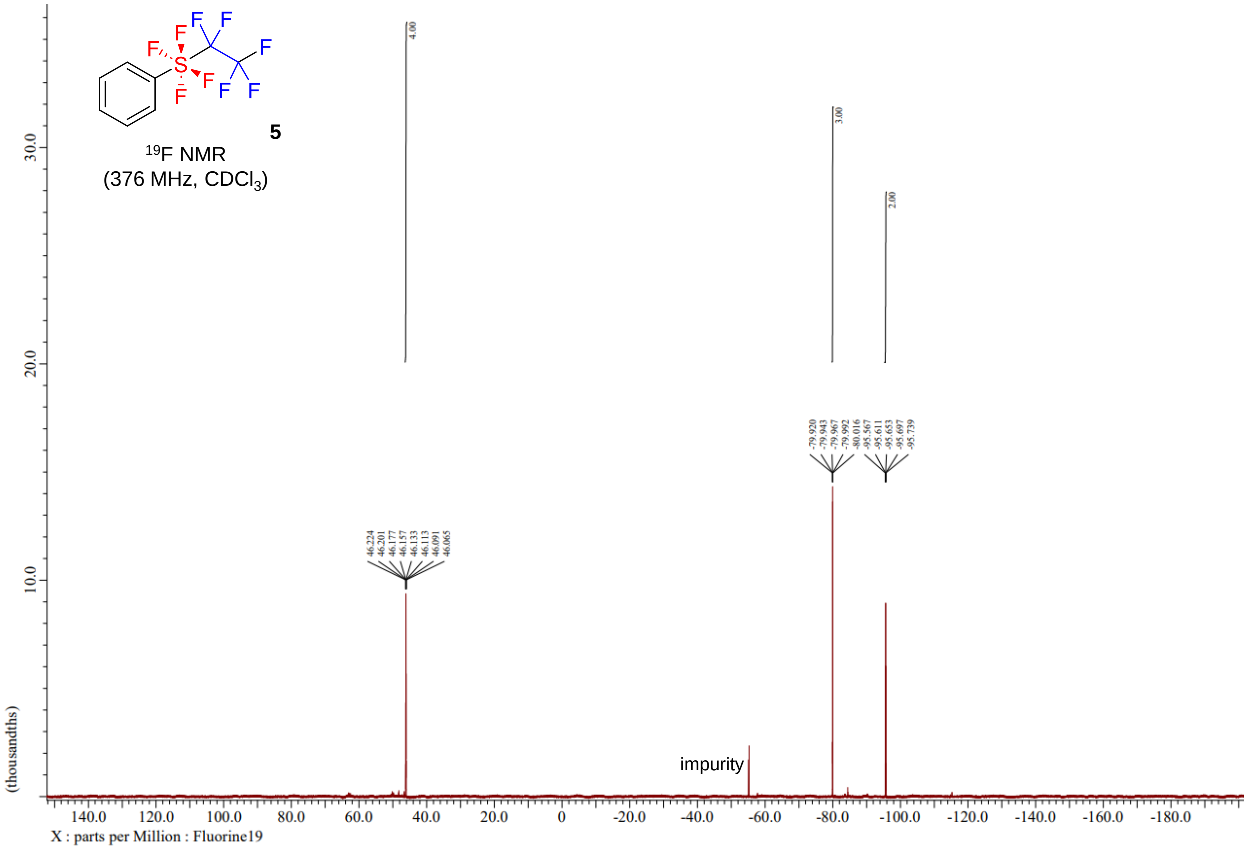


4
^{19}F NMR
(376 MHz, CDCl$_3$)
X : parts per Million : Fluorine19
abundance



5
^{1}H NMR
(400 MHz, CDCl$_3$)
X : parts per Million : Proton
abundance


5
^{13}C NMR
(101 MHz, $CDCl_3$)
abundance
X : parts per Million : Carbon13
(thousandths)
X : parts per Million : Carbon13


5
^{19}F NMR
(376 MHz, $CDCl_3$)
(thousandths)
impurity
X : parts per Million : Fluorine19

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