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Supporting Information

Regioselective and Stereospecific Ring Opening of Aziridines by DMPU-HF

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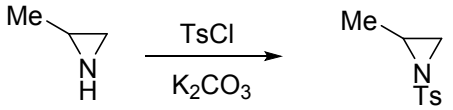
1. General

NMR spectra were recorded on 400 or 500 MHz Varian spectrometers. Chemical shifts are given in ppm. The spectra are calibrated to the residual ^{1}H and ^{13}C signals of the solvents. Multiplicities are abbreviated as follows: singlet (s), doublet (d), triplet (t), quartet (q), doublet-doublet (dd), quintet (quint), septet (sept), multiplet (m), and broad (br). Optical rotation was measured on a JASCO P-2000 digital polarimeter with a sample cell of 100 mm length and 8.0 mm aperture at 589 mm (sodium).

Unless otherwise stated, starting materials were purchased from Aldrich and/or Fluka. Solvents were purchased in HPLC quality, degassed by purging thoroughly with nitrogen and dried over activated molecular sieves of appropriate size. Alternatively, they were purged with argon and passed through alumina columns in a solvent purification system (Innovative Technology). Conversion was monitored by thin layer chromatography (TLC) using Merck TLC silica gel 60 F254. Compounds were visualized by UV-light at 254 nm and by dipping the plates in an polymoybdenic acid (PMA), p-anisaldehyde, ninhydrin solutions or an aqueous potassium permanganate solution followed by heating depending on the compounds formed. Chloramine-T trihydrate, phenyltrimethylammonium tribromide and *S*-benzyltosyl aziridine (93% ee) were purchased from Sigma-Aldrich and used without further purification unless otherwise stated.

2. Synthesis and Characterization of Aziridines

2-methyl-1-tosylaziridine **(1a)**[1]

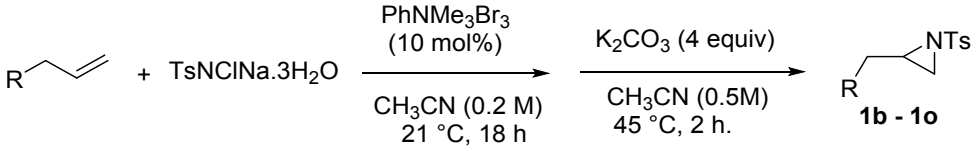


1a

2-methylaziridine (790 µL, 10 mmol) was added to a biphasic mixture of EtOAc (15mL) and 1.0 M K_2CO_3 (15 mL) at 0˚C. Under vigorous stirring, the solution of 4-methylbenzenesulfonyl chloride (1.91g, 10 mmol) in EtOAc (15mL) was added dropwise. After 1 h the reaction was allowed to reach ambient temperature and stirred for another 12 h. The phases were separated and the organic phase was washed with water, dried over Na_2SO_4 and concentrated. The crude product was subjected of 98% white solid required no further purification other than drying. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85-7.80 (m, 2H), 7.36-7.31 (m, 2H), 2.83 (dqd, *J* = 6.9, 5.6, 4.6 Hz, 1H), 2.61 (d, *J* = 7.0 Hz, 1H), 2.44 (s, 3H), 2.02 (d, *J* = 4.6 Hz, 1H), 1.25 (d, *J* = 5.6 Hz, 3H). Its spectroscopic data agree with literature data.[1]

Chiral aziridine (*S*)-**2d** was also prepared via this procedure.

Synthesis of aziridines **1b - 1o**[1]

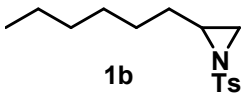


1b - 1o

General aziridination procedure. To a mixture of chloramine-T trihydrate (1.55 g, 5.5 mmol) and alkene (5.0 mmol) in CH_3CN (25 mL) at ambient temperature was added $PhNMe_3Br_3$ (188.0 mg, 0.50 mmol). The reaction was stirred vigorously for 15 h and then concentrated in vacuo. The resulting residue was dissolved in CH_2Cl_2 (5-10 mL) and filtered through a short column (silica gel, 3 x 4 cm) eluting with (150 mL of a 1:9 EtOAc/hexane mixture). After evaporation of the solvent, the residue was dissolved in CH_3CN (10 mL). After evaporation of the solvent, the residue was dissolved in CH_3CN (10 mL) and then K_2CO_3 (2.77 g, 20.0 mmol) was added, the mixture was stirred vigorously at 45°C for 2 h. After cooling to ambient temperature, the mixture was diluted with Et_2O (20 mL), filtered through a pad of Celite (washing with Et_2O) and concentrated. The crude product was subjected to silica gel column

chromatography (7:1 hexanes: EtOAc) to give aziridines product.

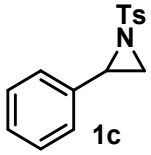
2-hexyl-1-tosylaziridine (**1b**)[2]



1b

Following the general aziridination procedure starting from1-octene (5.0 mmol, 785 µL), **1b** was isolated by column chromatography on silica gel (hexanes / EtOAc, 7:1) in 76% yield as a colorless gel to white solid. ^{1}H NMR ($CDCl_3$, 400 MHz), δ 0.85 (t, 3H, *J* = 6.8 Hz), 1.18-1.37 (m, 9H), 1.51-1.58 (m, 1H), 2.06 (d, 1H, *J* = 4.6 Hz),2.44 (s, 3H), 2.64(d, 1H, *J* = 7.0 Hz), 2.66-2.71 (m, 1H), 7.33 (d, 2H, *J* = 8.4 Hz), 7.82 (d, 2H, *J* = 8.4 Hz). Its spectroscopic data agree with literature data.[2]

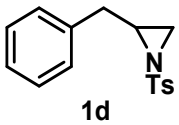
2-phenyl-1-tosylaziridine (**1c**)[2]



1c

Following the general aziridination procedure starting from styrene (5.0 mmol, 573 µL), **1c** was isolated by column chromatography on silica gel (hexanes / EtOAc, 7:1) in 62% yield as a faint yellow powder. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.38 (d, *J* = 4.6 Hz, 1H), 2.43 (s, 3H,), 2.98 (d, *J* = 7.3 Hz, 1H), 3.77 (dd, *J* = 7.3, 4.6 Hz, 1H), 7.19-7.36 (m, 7H), 7.86 (d, *J* = 8.2 Hz, 2H,). Its spectroscopic data agree with literature data.[1]

2-benzyl-1-tosylaziridine (**1d**)[1]

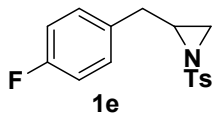


1d

Following the general aziridination procedure starting from allylbenzene (5.0 mmol, 591µL), **1d** was isolated by column chromatography on silica gel (Hex/EtOAc, 7:1) in 58% yellow solid. This compound is known. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.71–7.66 (m, 2H), 7.24 –7.19 (m, 2H), 7.18–7.12 (m, 3H),7.07–7.02 (m, 2H), 2.95 (tdd, *J* = 7.0, 5.2, 4.6 Hz, 1H), 2.81 (dd, *J* = 14.5, 5.2 Hz, 1H), 2.71 (d, *J* = 6.9 Hz, 1H), 2.69 (dd, *J* = 14.6, 7.2 Hz, 1H), 2.42 (s, 3H), 2.16 (d, *J* = 4.5 Hz, 1H). Its spectroscopic data

agree with literature data.[1]

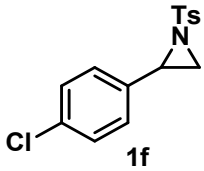
2-(4-fluorobenzyl)-1-tosylaziridine (**1e**)[1]



1e

Following the general aziridination procedure starting from 1-allyl-4-fluorobenzene (5.0 mmol, 591 μL), **1e** was isolated by column chromatography on silica gel (hexanes/EtOAc, 7:1) in 58% yellow solid. This compound is known. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.67–7.61 (m,2H), 7.20 (app d, J= 8.2 Hz,2H), 7.00–6.93(m,2H), 6.82–6.76 (m ,2H), 2.92–2.82 (m, 2H), 2.74 (d, J= 6.6 Hz, 1H), 2.56–2.48 (m, 1H), 2.43 (s, 3H), 2.16 (d, J = 4.3 Hz,1H). Its spectroscopic data agree with literature data.[1]

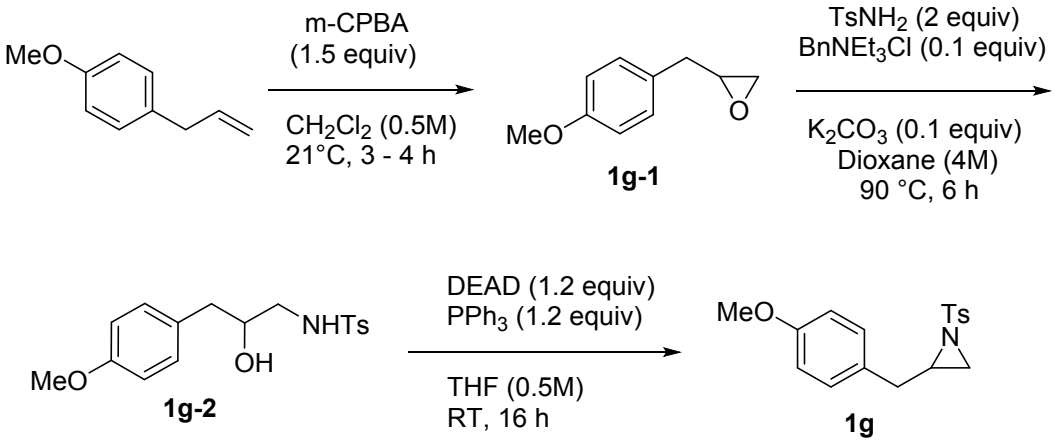
2-(4-chlorophenyl)-1-tosylaziridine (**1f**)[3]



1f

Following the general aziridination procedure starting from 1-chloro-4-vinylbenzene (5.0 mmol, 637 μL), **1f** was isolated by column chromatography on silica gel (hexanes/EtOAc, 7:1) in 58% yellow solid. This compound is known. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.86 (d, 2H, *J* = 8.3 Hz), 7.34 (2H, *J* = 8.0 Hz), 7.26 (d, 2H, *J* = 8.2), 7.14 (d, 2H, *J* = 7.8), 3.73 (m, 1H), 2.98 (m, 1H, *J* = 7.2), 2.44 (s, 3H, Ar-CH_3), 2.35 (s, *J* = 4.3 Hz). Its spectroscopic data agree with literature data.[3]

2-(4-methoxybenzyl)-1-tosylaziridine (**1g**)[1]



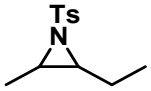
The general procedure failed for synthesis of **1g**, **1g** was synthesized using the following alternate procedure.

Synthesis of **1g-1**. A solution of 1-allyl-4-methoxybenzene (50.0 mmol, 7.410 g) in CH_2Cl_2 (75 mL) in a 250 mL round bottom flask was cooled to 0oC with an ice bath, *m*-chloroperbenzoic acid (12.1g, 50 mmol) was added portion wise over 10 minutes. The mixture was allowed to warm to ambient temperature and then stirred until TLC indicated complete consumption of the starting material (ca 4 h). If complete conversion is not obtained within 2 h, an additional portion of *m*-CPBA (ca 3g) may be added and the mixture stirred an additional 2 h. After completion, saturated aqueous $NaHCO_3$ (75mL) was slowly added and the mixture was stirred vigorously until gas evolution had ceased, after which the mixture was poured into a separatory funnel. The organic layer was separated and washed with 1M aq. Sodium sulfite, once with brine and then dried over Na_2SO_4. After removal of the solvent by rotary evaporation, the crude product was purified by chromatography on silica gel (hexanes/EtOAc 7:1) to afford the desired product **1g-1** in 92% as a colorless liquid.

Synthesis of **1g-2**. An oven-dried round bottom flask equipped with a magnetic stir bar was charged with epoxide **1g-1** (24.4 mmol, 4.00 g), 4-methylbenzenesulfonamide (48.8 mmol, 8.36 g), K_2CO_3 (2.4 mmol, 0.337 g), $BnNEt_3Cl$ (2.4 mmol, 0.556 g), and anhydrous dioxane (5.0mL). The flask was fitted with a reflux condenser and the mixture was heated to 90°C.When complete consumption of the starting material was indicated by TLC after approximately 5 h, the mixture was cooled to ambient temperature, diluted with CH_2Cl_2 (30 mL) and then filtered through a 2 cm pad of Celite, which was thoroughly washed with CH_2Cl_2 (100 mL). Purification by flash chromatography on silica gel (hexanes /EtOAc, gradient, 100 to 4:1) yielded the product as a white solid quantitatively (the product contains small amount of the $TsNH_2$).

Synthesis of **1g**. To a dry 250 mL round bottom flask containing a magnetic stir bar was added (25 mmol, 2.0 g) and PPh_3 (29.5 mmol, 7.74 g). The flask was fitted with a rubber septum, purged with argon and then THF (50.0mL) was added. The flask was cooled to 0°C with an ice bath and diethyl azodicarboxylate (DEAD) (29.5 mmol, 5.137 g, 4.65 mL) was added drop-wise over a period of 10 minutes, after which the ice bath was removed and the mixture was allowed to stir at ambient temperature for 16 h. The reaction mixture was evaporated under reduced pressure. Et_2O (200mL) was added and the reaction was stirred for 20 minutes. The solids were removed by filtration through a 3cm pad of Celite, washing with Et_2O, and the filtrate was concentrated by rotary evaporation. This crude oil so obtained was chromatographed on silica gel (hexanes / EtOAc, gradient 20:80 to 45:55), which yielded the desired aziridine as a white solid 57%. If necessary, recrystallization from hexanes/ethanol can also be carried out. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 –7.66 (m, 2H), 7.25–7.19 (m, 2H), 6.98–6.92 (m, 2H), 6.71–6.65 (m, 2H), 3.77 (s, 3H), 2.91 (tt, J = 7.1, 4.8 Hz, 1H), 2.77 (dd, *J* = 14.5, 5.1 Hz, 1H), 2.70 (d, *J* = 6.9 Hz, 1H,), 2.61 (dd, *J* = 14.5, 7.2 Hz, 1H), 2.43 (s, 3H), 2.14 (d, *J* = 4.6 Hz, 1H). Its spectroscopic data agree with literature data.[1]

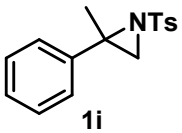
2-Ethyl-3-methyl-1-tosylaziridine (**1h**)[4]



1h

Following the general aziridination procedure starting from cyclohexene (5.0 mmol, 507µL), **1b** was isolated by column chromatography on silica gel (hexanes/EtOAc, 7:1) in 84% yield as a white solid. This compound is known. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.81 (t, *J* = 7.7 Hz, 2H), 7.28 (dd, *J* = 17.2, 9.1 Hz, 1H), 2.98 – 2.81 (m, 2H), 2.81 – 2.52 (m, 1H), 2.41 (d, *J* = 3.3 Hz, 1H), 1.18 (d, *J* = 5.9 Hz, 3H), 0.83 (t, *J* = 7.4 Hz, 3H). Its spectroscopic data agree with literature data.[4]

2-Methyl-2-phenyl-1-tosylaziridine (**1i**) [5]

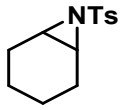


1i

Following the general aziridination procedure starting with alpha-methylstyrene (5 mmol, 655 µL), the

corresponding aziridine was isolated in 77% yield as a white solid. This compound is known (Unstable, decomposes over the bench after 24 h. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 9.29 – 8.98 (m, 2H), 7.86 (d, J = 8.3 Hz, 2H), 7.36 (d, *J* = 8.0 Hz, 2H), 7.33 – 7.26 (m, 3H), 2.95 (s, 1H), 2.51 (s, 1H), 2.42 (s, 3H), 2.04 (s, 3H). Its spectroscopic data agree with literature data.[5]

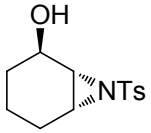
7-Tosyl-7-azabicyclo[4.1.0]heptane (**1j**)[2]



1j

Following the general aziridination procedure starting from cyclohexene (5.0 mmol, 507 µL), **1b** was isolated by column chromatography on silica gel (hexanes/EtOAc, 7:1) in 84% yield as a white solid. This compound is known. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 1.14-1.21 (m, 2H), 1.25-1.47 (m, 2H), 1.79 (dt, 4H, *J* = 1.4, 5.8 Hz), 2.44 (s, 3H), 2.97 (t, 2H, *J* = 1.4 Hz), 7.32 (d, 2H, *J* = 8.1 Hz), 7.81(d, 2H, *J* = 8.1 Hz). Its spectroscopic data agree with literature data.

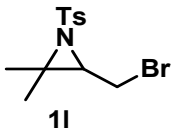
Syn-7-tosyl-7-azabicyclo[4.1.0]heptan-2-ol (**1k**)[5]



1k

Following the general aziridination procedure starting from cyclohex-2-enol (5.0 mmol, 491 µL), **1k** was isolated by column chromatography on silica gel (hexanes/EtOAc, 7:1) in 31% yield colorless oil. This compound is known. ^{1}H NMR ($CDCl_3$, 400MHz) δ 7.82 (d, J = 8.4Hz, 2H), 7.33 (d, J = 8.1Hz, 2H), 3.93 (brs, 1H), 3.18 (m, 2H), 2.43 (s, 3H) 1.80-1.15 (m, 7H). Its spectroscopic data agree with literature data.

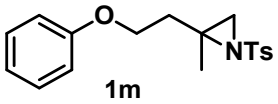
3-(Bromomethyl)-2,2-dimethyl-1-tosylaziridine (**1l**)



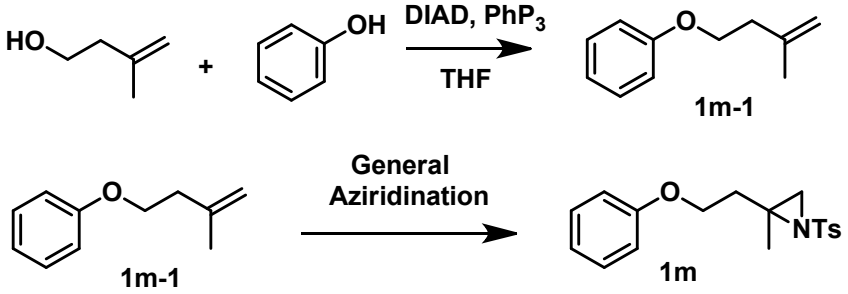
1l

Following the general aziridination procedure starting from 1-bromo-3-mthyl-2-butene (5.0 mmol, 578 µL), **1l** was isolated by column chromatography on silica gel (Hex/EtOAc, 7:1) in 76% yield as a colorless oil. ^{1}H NMR (400 MHz, cdcl$_3$) δ = 7.81 (d, *J*=8.2, 2H), 7.32 (d, *J*=8.0, 2H), 3.09 (dd, *J*=7.0, 4.5, 1H), 2.67 (d, *J* = 6.9 Hz, 3H), 2.41 (d, *J* = 7.0 Hz, 1H), 2.35 (d, *J* = 4.4 Hz, 1H), 1.59 – 1.49 (m, 6H). ^{13}C NMR (100 MHz, cdcl$_3$) δ = 144.89, 134.37, 129.77, 129.69, 128.37, 128.29, 59.75, 48.50, 31.76, 31.56, 28.85, 21.67. EI MS: m/z= 318.22 ([M] $^{+}$); ESI HRMS: calcd. for $C_{18}H_{22}NO_3S^{+}$ ([M+H]$^{+}$) 318.0158; found 318.0157.

2-Methyl-2-(2-phenoxyethyl)-1-tosylaziridine (**1m**)



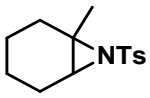
1m



Synthesis of **1m-1**. To a stirred solution of 3-methyl-3-buten-1-ol (5.8mmol) in tetrahydrofuran (15 mL) were added sequentially phenol (0.66 g), triphenylphosphine (1.92 g) and diisopropyl azodicarboxylate (1.45 g). The mixture was heated at 70° C. overnight and then was concentrated in vacuum. The residue was purified by column chromatography (SiO_2; gradient: hexane/EtOAc 100:0->70:30) to give (3-methyl-but-3-enyloxy)-benzene in 53% which agrees well with literature. ^{1}H NMR ($CDCl_3$, 400MHz) δ ^{1}H NMR (400 MHz, cdcl$_3$) δ = 7.40 – 7.16 (m, 2H), 7.03 – 6.83 (m, 3H), 4.83 (dd, *J* = 16.0 Hz, 0.7, 2H), 4.20 – 3.97 (m, 2H), 2.51 (t, *J* = 6.9 Hz, 2H), 1.81 (d, *J* = 0.4 Hz, 3H).

Synthesis of **1m**. Following the general aziridination procedure starting from alkene (**1m-1**), **1m** was isolated in 85% yield as a colorless liquid. ^{1}H NMR ($CDCl_3$, 400MHz) ^{1}H NMR (400 MHz, cdcl$_3$) δ = 7.81 (t, *J* = 16.3 Hz, 2H), 7.36 – 7.14 (m, 4H), 7.00 – 6.90 (m, 1H), 6.90 – 6.79 (m, 1H), 4.13 – 3.97 (m, 2H), 2.65 (d, *J* = 13.5 Hz, 1H), 2.45 (s, 1H), 2.41 (s, 3H), 2.29 – 2.17 (m, 1H), 2.06 (dt, *J* = 14.3 Hz, 5.8, 1H), 1.73 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 158.48, 143.92, 137.75, 129.52, 129.46, 127.35, 120.84, 114.43, 77.43, 77.11, 76.79, 64.48, 48.74, 41.38, 37.03, 21.59, 21.57, 19.12. EI: m/z= 332.1315 ([M]$^{+}$). HRMS (ESI+): calcd. for $C_{18}H_{22}NO_3S^{+}$ ([M+H]$^{+}$) 280.1338; found 332.1312.

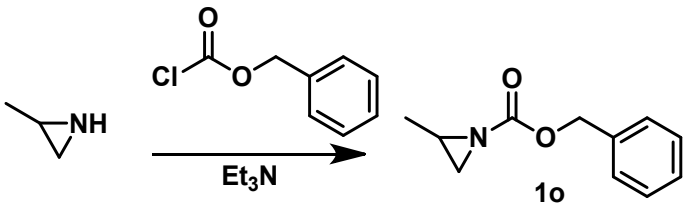
1-methyl-7-tosyl-7-azabicyclo[4.1.0]heptane (**1n**)[6]



1n

Following the general aziridination procedure starting with methylcyclohexene (5 mmol, 600 µL), the corresponding aziridine was isolated in 65% yield as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.81 (2H, d, J = 8.0Hz), 7.29 (2H, d, J = 8.0Hz), 3.04 (1H, d, J = 5.6Hz), 2.41(3H, s), 2.01 – 2.07(1H, m), 1.77 – 1.86 (1H, m), 1.70(3H, s), 1.48 – 1.59(2H, m), 1.29 – 1.44 (3H, m), 1.12 – 1.27(1H, m). Its spectroscopic data agree with literature data. [5]

Benzyl 2-methylaziridine-1-carboxylate (**1o**)[7]

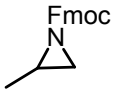


1o

2-Methyl aziridine is dissolved in CH_2Cl_2 and triethylamine under argon at 0° C. Benzylchloroformate is added and the contents of the flask are at room temperature overnight. The mixture is poured into 10% citric acid and is extracted with $CHCl_3$. The organic layer is washed with dilute aqueous $NaHCO_3$ and dried over Na_2SO_4. The solution is evaporated to yield N-Cbz-2-methyl aziridine (71% colorless oil). ^{1}H NMR (400 MHz, cdcl$_3$) δ 7.49 – 7.27 (m, 5H), 5.12 (s, 2H), 2.59 – 2.46 (m, 1H), 2.33 (d, *J* = 5.8 Hz,

1H), 1.99 – 1.92 (m, 1H), 1.27 (d, *J* = 5.5 Hz, 3H). Its spectroscopic data agree with literature data. [7]

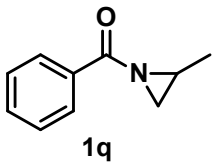
(9H-fluoren-9-yl) methyl 2-methylaziridine-1-carboxylate (**1p**)



1p

2-Methylaziridine (353 µL, 5 mmol) was added to a biphasic mixture of EtOAc (10 mL) and 4 equivalent of K_2CO_3 (2.764 g) in water (10 mL). Under vigorous stirring, the solution of fluorenylmethyloxycarbonyl chloride (1.293 g, 5 mmol) in EtOAc (10 mL) was added dropwise. The reaction was stirred for 18 h after which the phases were separated and the organic phase was washed with water and dried over Na_2SO_4, filtered and concentrated. The product a yellow oil (94%) needed no further purification. ^{1}H NMR (400 MHz, cdcl$_3$) δ 7.76 (d, *J* = 7.5 Hz, 2H), 7.62 (d, *J* = 7.3 Hz, 2H), 7.40 (t, *J* = 7.2 Hz, 2H), 7.32 (t, *J* = 7.5 Hz, 2H), 4.42 (d, *J* = 7.0 Hz, 2H), 4.24 (t, *J* = 6.7 Hz, 1H), 2.45 (s, 1H), 2.28 (d, *J* = 5.7 Hz, 1H), 1.95 (s, 1H), 1.57 (s, 1H), 1.27 (d, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.64, 141.32, 137.33, 127.76, 127.06, 125.08, 119.96, 67.97, 60.37, 46.99, 33.84, 32.59, 21.04, 17.37, 14.18. EI MS m/z= 279.13 ([M] $^+$). ESI HRMS: calcd. for $C_{18}H_{18}NO_2H^+$ ([M+H]$^+$) 280.1338; found 280.1336.

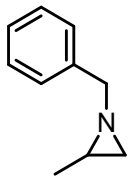
(2-Methylaziridin-1-yl)(phenyl)methanone (**1q**)[8]



1q

2-Methyl aziridine (10 mmol) is dissolved in CH_2Cl_2 and trimethylamine (2 equiv.) under argon at 0° C. Benzoylchloride (10.5 mmol) is added and the contents of the flask are at room temperature overnight. The mixture is poured into 10% citric acid and is extracted with $CHCl_3$. The organic layer is washed with dilute aqueous $NaHCO_3$ and dried over Na_2SO_4. The solution is evaporated to yield N-Benzoyl-2-methyl aziridine. (59 % colorless oil). ^{1}H NMR ($CDCl_3$, 400MHz): δ 8.03 (m, 2H), 7.55 (m, 1H), 7.46 (m, 2H), 2.58 (m, 1H), 2.55 (d, *J* = 5.6 Hz, 1H), 2.15 (d, *J* = 3.6 Hz, 1H), 1.40 (d, *J* = 5.6 Hz, 3H). Its spectroscopic data agree with literature data. [8]

1-Benzyl-2-methylaziridine (**1r**)[9]



1r

2-Methyl aziridine (10 mmol) is dissolved in CH_2Cl_2 and trimethylamine (2 equiv) under argon at 0° C. Benzylchloride (10.5 mmol) is added and the contents of the flask are at room temperature overnight. The mixture is poured into 10% citric acid and is extracted with $CHCl_3$. The organic layer is washed with dilute aqueous $NaHCO_3$ and dried over Na_2SO_4. The solution is evaporated to yield **1r** (41%, yellow oil). ^{1}H NMR ($CDC1_3$) δ 1.20 (d, *J* = 5.4 Hz, 3H), 1.37 (d, *J* = 6.3 Hz, 1H), 1.49-.54 (m, 1H), 1.57 (d, *J* = 3.6 Hz, 1H), 3.39 (d, *J* = 13.8 Hz, 1H), 3.46 (d, *J* = 13.5 Hz, 1H), 7.24-7.36 (m, 5H). Its spectroscopic data agree with literature data. [9]

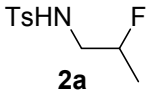
Chiral aziridines (*R*)-**1a** and (*S*)-**1c** were prepared by following a reported procedure.[1]

[1] Hsueh, N.; Clarkson, G. J.; Shipman, M. *Org. Lett.* **2015**, *17* (14), 3632–3635.

3. Hydrofluorination of Aziridines

General Procedure for the Hydrofluorination of Aziridines (General Hydrofluorination Procedure). In a 20 mL polyethylene vial charged with a magnetic stirrer is dissolved 0.5 mmol of the aziridine **1** in 1.5 mL of dichloroethane. DMPU-HF (65%) (3.6 mmol HF, 98 μL) of was then pipetted into the mixture and the reaction was heated at 55°C for 18 h. The reaction was quenched with $NaHCO_3$ and the mixture was extracted with DCM, the organic layer was washed with brine and then was dried over Na_2SO_4, concentrated under reduced pressure and chromatographed with silica gel using a mixture of hexane:EtOAc (7:1) to afford the corresponding fluorinated product.

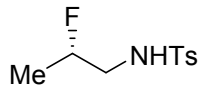
N-(2-fluoropropyl)-4-methylbenzenesulfonamide (**2a**)



2a

The product was prepared from 2-methyl-1-tosylaziridine **1a** according to the general hydrofluorination procedure in 81% yield as a yellow oil. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.74 (m, 2H), 7.30 (m, 2H), 4.97 (t, *J* = 6.5 Hz, 1H), 4.83 – 4.54 (m, 1H), 3.24 – 3.11 (m, 1H), 3.08 – 2.88 (m, 1H), 2.41 (s, 3H), 1.27 (dd, *J* = 23.9, 6.3 Hz, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 143.63 , 136.81 , 129.78 , 127.02 , 89.23 (d, *J* = 167.2 Hz), 48.11 (d, *J* = 21.5 Hz), 21.47 , 18.08 (d, *J* = 21.9 Hz). ^{19}F NMR (376 MHz, Chloroform-*d*) δ -179.90 – -180.34 (m). MS: m/z = 231.1 ([M] $^{+}$). HRMS (ESI+): calcd. For $C_{10}H_{15}FNO_2SH^{+}$ [M+H] $^{+}$ 232.0808; found 232.0806.

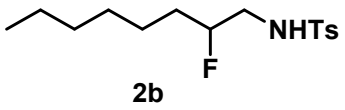
(*S*)-N-(2-fluoropropyl)-4-methylbenzenesulfonamide (**2a**)



(*S*)-**2a**, 85% *ee*

The product was prepared from (*R*)-**1a**. $[\alpha]_D^{25} = +77.7°$ (0.10 w/v% in CH_2Cl_2)

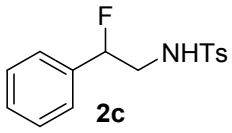
N-(2-fluorooctyl)-4-methylbenzenesulfonamide (**2b**)[10]



2b

The major product was prepared from the 1-octene-tosylaziridine according to the general hydrofluorination procedure to afford the title compound in a 65:1 ratio as determined by ^{19}F NMR) (87%, white solid). Major isomer: ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.80 – 7.67 (m, 2H), 7.35 – 7.28 (m, 2H), 4.77 (s, 1H), 4.65 – 4.30 (m, 1H), 3.31 – 3.12 (m, 1H), 3.12 – 2.85 (m, 1H), 2.43 (s, 3H), 1.74 – 1.14 (m, 10H), 0.87 (t, *J* = 6.1 Hz, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 143.62 , 136.80 , 129.78 , 127.01 , 92.67 (d, *J* = 169.9 Hz), 46.90 (d, *J* = 21.4 Hz), 32.17 (d, *J* = 19.9 Hz), 31.53 , 28.88 , 24.58 (d, *J* = 4.7 Hz), 22.48 , 21.51 , 13.99 . ^{19}F NMR (376 MHz, Chloroform-*d*) δ -186.13 – -186.51 (m, 1H). [10]

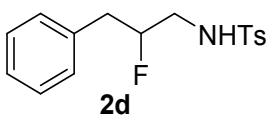
N-(2-fluoro-2-phenylethyl)-4-methylbenzenesulfonamide **(2c)[11]**



2c

The product was prepared from 2-phenyl-1-tosylaziridine according to the general procedure to afford the title compound in 79% yield, as yellow oil and the only product. ^{1}H NMR (400MHz, $CDCl_3$) δ 7.79 – 7.66 (m, 2H), 7.39 – 7.19 (m, 7H), 5.87 (dd, *J* = 7.7, 4.8 Hz, 1H), 5.47 (ddd, *J* = 48.1, 8.3, 3.0 Hz, 1H), 3.32–3.17 (m, 2H), 2.41 (s, 3H). ^{19}F NMR (376 MHz, Chloroform-*d*) δ -183.06 (ddd, *J* = 47.3, 29.7, 16.3 Hz). Its spectroscopic data agree with literature data.[11]

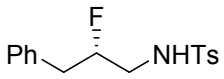
N-(2-fluoro-3-phenylpropyl)-4-methylbenzenesulfonamide **(2d)[10]**



2d

The product was prepared from 2-benzyl-1-tosylaziridine according to the general hydrofluorination procedure to afford the title compound in 79% yield, as a light yellow solid. ^{1}H NMR (400 MHz,

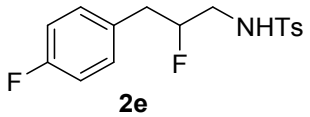
Chloroform-*d*) δ 7.78 – 7.62 (m, 2H), 7.27 (dd, *J* = 13.9, 7.8 Hz, 5H), 7.13 (d, *J* = 7.1 Hz, 2H), 4.91 – 4.52 (m, 2H), 3.22 (m, 1H), 3.13 – 3.01 (m, 1H), 3.01 – 2.78 (m, 2H), 2.42 (s, 3H).^{19}F NMR (376 MHz, Chloroform-*d*) δ -184.41 – -184.77 (m, 1F). Its spectroscopic data agree with literature data.



(*S*)-**2d**, 91% *ee*

The product was prepared from (*S*)-**1d**. $[\alpha]_D^{25} = +55.1°$ (0.17 w/v% in CH_2Cl_2)

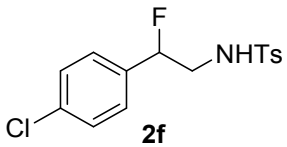
N-(2-fluoro-3-(4-fluorophenyl)propyl)-4-methylbenzenesulfonamide **(2e)**



2e

The product was prepared from 2-(4-fluorobenzyl)-1-tosylaziridine **1e** according to the general hydrofluorination procedure to afford the title compound in 74% yield, as a yellow solid. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.88 – 7.58 (m, 2H), 7.35 – 7.28 (m, 2H), 7.15 – 7.07 (m, 2H), 7.02 – 6.94 (m, 2H), 4.88 – 4.48 (m, 2H), 3.30 – 3.13 (m, 1H), 3.13 – 2.99 (m, 1H), 2.99 – 2.75 (m, 2H), 2.43 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 160.98 (d, *J* = 60.5 Hz), 143.78 , 136.59 , 131.27 , 130.76 (d, *J* = 8.0 Hz), 129.84 , 127.01 , 115.49 (d, *J* = 21.4 Hz), 92.58 (d, *J* = 174.1 Hz), 46.02 (d, *J* = 21.3 Hz), 37.64 (d, *J* = 21.0 Hz), 21.53 . ^{19}F NMR (376 MHz, Chloroform-*d*) δ -115.80 (m, 1F), -182.75 – -188.23 (m, 1F). MS: m/z = 325.09 [M] $^+$. HRMS: calcd. for $C_{16}H_{17}F_2NSO_2Na^+$ [M + Na]$^+$ 348.0840; found 348.0840, cald. for $C_{16}H_{18}FNSO_2^+$ [M + H]$^+$ 326.1021; found 326.1021.

N-(2-(4-chlorophenyl)-2-fluoroethyl)-4-methylbenzenesulfonamide **(2f)**

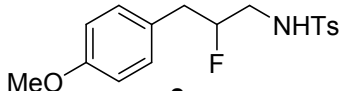


2f

The product was prepared from 2-(4-chlorophenyl)-1-tosylaziridine according to the general

hydrofluorination procedure to afford the title compound in 82% yield, as a light yellow solid. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.74 – 7.66 (m, 2H), 7.36 – 7.27 (m, 4H), 7.20 – 7.13 (m, 2H), 5.48 (ddd, *J* = 47.5, 8.1, 3.4 Hz, 1H), 4.83 (s, 1H), 3.55 – 3.13 (m, 2H), 2.43 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 143.82 , 136.75 , 129.83 , 128.91 , 128.05 , 126.98 , 126.89 , 126.82 , 92.06 (d, *J* = 174.5 Hz), 48.42 (d, *J* = 25.1 Hz), 21.53 . ^{19}F NMR (376 MHz, $CDCl_3$) δ -183.32 – -183.56 (m, 1F).

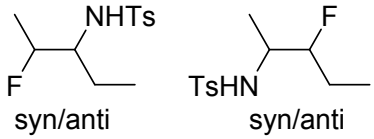
N-(2-fluoro-3-(4-methoxyphenyl)propyl)-4-methylbenzenesulfonamide (**2g**)



2g

The product was prepared from 2-(4-methoxybenzyl)-1-tosylaziridine according to the general hydrofluorination procedure to afford the title compound in 82% yield, as a white solid. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.83 – 7.64 (m, 2H), 7.34 – 7.27 (m, 2H), 7.10 – 7.00 (m, 2H), 6.87 – 6.78 (m, 2H), 4.91 – 4.41 (m, 2H), 3.79 (s, 3H), 3.36 – 3.13 (m, 1H), 3.13 – 2.99 (m, 1H), 2.99 – 2.67 (m, 2H), 2.43 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 156.82, 143.70, 130.26, 129.82, 129.69, 127.02, 126.91, 114.06, 92.82 (d, *J* = 173.3 Hz), 55.24 , 46.06 (d, *J* = 21.0 Hz), 37.64 (d, *J* = 21.0 Hz), 21.53 . ^{19}F NMR (376 MHz, Chloroform-*d*) δ -184.44 – -184.80 (m, 1F). HRMS: calcd. for $C_{17}H_{20}FNSO_3Na^+$ $[M+Na]^+$ 360.1040; found 360.1040, cald. For $C_{17}H_{21}FNSO_3^+$ $[M+H]^+$ 338.1221; found 337.1220.

N-(2-fluoropentan-3-yl)-4-methylbenzenesulfonamide (**2h**)

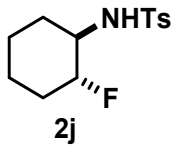


2h

The product was prepared from 2-ethyl-3-methyl-1-tosylaziridine according to the general procedure to afford regio isomers mixtures of the title compound in 94% yield, as a yellow oil. The product constitutes of four inseparable compounds (one diastereomeric pair and a regioisomeric pair), hence clear assignment of proton and ^{13}C NMR spectra is not practical. ^{19}F NMR (376 MHz, Chloroform-*d*) δ -186.12 – -186.39 (m), -187.67 – -188.05 (m), -195.90 – -195.21 (m), -197.46 – -197.74 (m). HRMS: calcd. For $C_{12}H_{18}FNSO_2Na^+$ $[M+Na]^+$ 282.0934; found 282.093, cald. for $C_{17}H_{19}FNSO_2^+$ $[M+H]^+$

260.1115; found 260.1111.

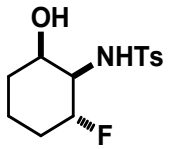
N-(2-fluorocyclohexyl)-4-methylbenzenesulfonamide (**2j**)



2j

This compound is known. The product was prepared from the cyclohexyl-tosylaziridine according to the general hydrofluorination procedure to afford the title compound, 95% yield, white solid. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.76 (m, 2H), 7.29 (m, 2H), 4.98 – 4.52 (m, 1H), 4.19 (double multiplets, $J_{C\text{-}H}$ = 48.7, 1H), 3.22 – 3.09 (m, 1H), 2.42 (s, 3H), 2.18 – 2.08 (m, 1H), 2.08 – 1.91 (m, 1H), 1.78 – 1.64 (m, 1H), 1.58 (m, 1H), 1.51 – 1.35 (m, 1H), 1.30 – 1.05 (m, 3H). ^{19}F NMR (376 MHz, $CDCl_3$, 25 °C) -178.49 (m). Its spectroscopic data agree with literature data.[11]

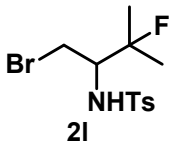
N-(2-fluoro-6-hydroxycyclohexyl)-4-methylbenzenesulfonamide **(2k)**



2k

The product was prepared from Syn-7-tosyl-7-azabicyclo[4.1.0]heptan-2-ol **1k** according to the general hydrofluorination procedure to afford the title compound in 61% yield, as a white solid. The structure of this compound is also confirmed by X-Ray crystallography. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.77 (d, *J* = 8.3 Hz, 2H), 7.31 (d, *J* = 8.2 Hz, 2H), 5.08 (d, *J* = 5.4 Hz, 1H), 4.57 (dtd, *J* = 50.0, 9.5, 4.6 Hz, 1H), 4.22 (s, 1H), 3.17 (tdd, *J* = 8.9, 5.6, 3.2 Hz, 1H), 2.43 (s, 3H), 2.20 – 1.96 (m, 2H), 1.85 – 1.33 (m, 5H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.63, 136.72, 129.65, 127.21, 90.58 (d, *J* = 176.1 Hz), 69.12 (d, *J* = 6.5 Hz), 59.68 (d, *J* = 18.1 Hz), 36.44, 26.29, 21.55, 17.44 (d, *J* = 9.8 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -186.52 (d, *J* = 48.9 Hz, 1F). MS: m/z = 287.1 $[M]^+$. HRMS: calcd. for $C_{13}H_{18}FNSO_3Na^+$ $[M+Na]^+$ 310.0884; found 310.0884, cald. for $C_{13}H_{19}FNSO_3^+$ $[M+H]^+$ 288.1064; found 288.1064.

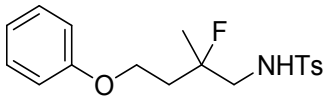
N-(1-bromo-3-fluoro-3-methylbutan-2-yl)-4-methylbenzenesulfonamide (2l)



2l

The product was prepared from 3-(bromomethyl)-2,2-dimethyl-1-tosylaziridine **1l** according to the general hydrofluorination procedure to afford the title compound in 78% yield, as a viscous colorless oil. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.89 – 7.61 (m, 2H), 7.42 – 7.21 (m, 2H), 5.06 – 4.88 (m, 1H), 4.05 – 3.83 (m, 1H), 3.62 (ddd, *J* = 14.2, 8.3, 3.6 Hz, 1H), 3.18 (ddd, *J* = 14.1, 9.4, 4.6 Hz, 1H), 2.43 (s, 3H), 1.49 (d, *J* = 18.7 Hz, 3H), 1.43 (d, *J* = 18.6 Hz, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 143.84 , 136.75 , 129.87 , 127.05 , 95.38 (d, *J* = 172.1 Hz), 58.83 (d, *J* = 26.4 Hz), 45.68 (d, *J* = 4.6 Hz), 25.94 (d, *J* = 24.0 Hz), 23.45 (d, *J* = 24.0 Hz), 21.54 . ^{19}F NMR (376 MHz, Chloroform-*d*) δ -138.14 (m, 1F). MS: m/z = 337.0 [M] $^{+}$. HRMS: calcd. for $C_{12}H_{17}FBrNSO_2Na^{+}$ [M+Na]$^{+}$ 360.0040; found 360.0037, cald. for $C_{12}H_{18}FBrNSO_2^{+}$ [M+H]$^{+}$ 338.0220; found 338.0217.

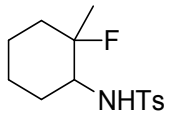
N-(2-fluoro-2-methyl-4-phenoxybutyl)-4-methylbenzenesulfonamide **(2m)**



2m

The product was prepared from 2-methyl-2-(2-phenoxyethyl)-1-tosylaziridine **1m** according to the general hydrofluorination procedure to afford the title compound in 93% yield, as a viscous colorless oil. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.85 – 7.61 (m, 2H), 7.45 – 7.19 (m, 4H), 6.96 (m, 1H), 6.87 – 6.72 (m, 2H), 4.87 (m, 1H), 4.04 (m, 2H), 3.15 (m, 2H), 2.41 (s, 3H), 2.15 (m, 2H), 1.45 (d, *J* = 22.3 Hz, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 158.09 , 143.58 , 136.78 , 129.78 , 129.52 , 126.97 , 121.12 , 114.35 , 95.49 (d, *J* = 170.5 Hz), 62.79 (d, *J* = 7.5 Hz), 50.36 (d, *J* = 25.7 Hz), 36.57 (d, *J* = 22.6 Hz), 23.06 (d, *J* = 23.5 Hz), 21.51 . ^{19}F NMR (376 MHz, Chloroform-*d*) δ -149.50 – -149.77 (m). MS: m/z = 351.13 [M] $^{+}$. HRMS: calcd. For $C_{18}H_{23}FNSO_3^{+}$ [M+H] $^{+}$ 352.1377; found 352.1375.

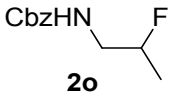
N-(2-fluoro-2-methylcyclohexyl)-4-methylbenzenesulfonamide (**2n**)



2n

The product was prepared from 1-methyl-7-tosyl-7-azabicyclo[4.1.0]heptane **1n** according to the general hydrofluorination procedure to afford the title compound in 84% yield, as a white solid. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.88 – 7.63 (m, 2H), 7.42 – 7.05 (m, 2H), 5.14 (d, *J* = 8.2 Hz, 1H), 3.52 – 3.17 (m, 1H), 2.41 (s, 3H), 1.94 – 1.05 (m, 10H), 0.86 (m, 1H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 143.31 , 137.71 , 129.55 , 127.11 , 95.36 (d, *J* = 173.5 Hz), 57.59 (d, *J* = 24.7 Hz), 35.61 (d, *J* = 20.7 Hz), 29.40 (d, *J* = 4.6 Hz), 22.07 (d, *J* = 1.5 Hz), 21.94 , 21.53 (d, *J* = 1.2 Hz), 20.81 (d, *J* = 25.1 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ = -141.11 (m, 1F). MS: m/z = 285.12 $[M]^+$. HRMS: calcd. for $C_{18}H_{23}FNSO_3^+$ $[M+H]^+$ 285.1272; found 285.1270.

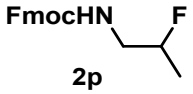
Benzyl (2-fluoropropyl)carbamate (2o)[12]



2o

This compound is known. The major product (90:1 as obtained by ^{19}F NMR) was prepared from benzyl 2-methylaziridine-1-carboxylate **1o** according to the general hydrofluorination procedure to afford the title compound in 66% yield as a yellow. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.37 (m, 5H), 5.27 – 5.16 (m, 1H), 5.12 (s, 2H), 4.90 – 4.58 (m, 1H), 3.51 (m, 1H), 3.22 (m, 1H), 1.32 (dd, *J* = 23.7, 6.4 Hz, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 156.50 , 136.39 , 128.54 , 128.17 , 128.10 , 89.73 (d, *J* = 166.6 Hz), 66.89 , 46.21 (d, *J* = 20.8 Hz), 18.05 (d, *J* = 22.0 Hz). ^{19}F NMR (376 MHz, $CDCl_3$, 25 °C) δ -179.9 (m, 1F). Its spectroscopic data agree with literature data.

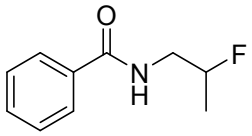
(9H-fluoren-9-yl)methyl (2-fluoropropyl)carbamate (2p)



2p

The product was prepared from (9H-fluoren-9-yl)methyl-2-methylaziridine-1-carboxylate according to the general hydrofluorination procedure to afford the title compound quantitatively as a white solid 76%. The major product was isolated almost exclusively with trace amount of the minor product. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.88 – 7.68 (m, 2H), 7.68 – 7.53 (m, 2H), 7.53 – 7.37 (m, 2H), 7.37 – 7.25 (m, 2H), 5.22 (s, 1H), 4.75 (dt, $J_{H\text{-}F}$ = 48.2, 5.8 Hz, 1H), 4.43 (d, *J* = 6. Hz, 2H), 4.23 (t, *J* = 6.5 Hz, 1H), 3.68 – 3.38 (m, 1H), 3.38 – 3.10 (m, 1H), 1.33 (dd, *J* = 23.8, 6.1 Hz, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 156.52 , 143.87 , 141.32 , 127.72 , 127.06 , 125.04 , 120.01 , 89.79 (d, *J* = 166.6 Hz), 66.85 , 47.21 , 46.19 (d, *J* = 20.6 Hz), 18.05 (d, *J* = 21.9 Hz). ^{19}F NMR (376 MHz, Chloroform-*d*) δ -179.54 – -179.87 (m, 1F). EI MS: m/z = 299.1[M] $^{+}$. HRMS (ESI+): calcd. For $C_{18}H_{17}FNSO_2Na^{+}$ [M+Na] $^{+}$ 322.1219; found 322.1218, cald. for $C_{18}H_{18}FNSO_2^{+}$ [M+H] $^{+}$ 300.1400; found 300.1399 .

N-(2-fluoropropyl)benzamide (**2q**)[11]



2q

The product was prepared from (2-methylaziridin-1-yl)(phenyl)methanone according to the general hydrofluorination procedure to afford the title compound quantitatively as a yellow oil 58%. The major product was isolated in >30:1 regioselectivity though contaminated a little with the Heine product. This compound is known. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.78–7.76 (m, 2H), 7.51–7.38 (m, 3H), 6.71 (br s, 1H), 4.92 – 4.75 (m, 1H), 3.90 – 3.79 (m, 1H), 3.44 – 3.33 (m, 1H), 1.42 – 1.35 (dd, *J* = 23.9, 6.2 Hz, 3H). 13C NMR (100 MHz, Chloroform-*d*) δ -167.67, -134.14, -131.60, -128.55, -126.96, -90.69 – -89.03 (d, *J* = 166 Hz), -45.05 – -44.85 (d, *J* = 20 Hz), -18.38 – -18.16 (d, *J* = 22 Hz) ^{19}F NMR ($CDCl_3$, 376 MHz) δ -179.16 – -179.62.1 (m, 1F). Its spectroscopic data agree with literature data.

4. Details of Computational Chemistry

The hydrogen bonding assisted pathway was taken as initial guess for the transition state calculation. In a first approach B3LYP/aug-cc-pVDZ level of theory was used and when a negative vibration mode which corresponds to the transition structure was achieved the level of theory was M062X/aug-cc-pVDZ. Many attempts to find the S_N2-like transition state that leads to non-observed product were performed, but none of them was successful.

The optimization and frequency calculations for starting materials and product was conducted in the same level of theory. For the energy barrier diagram construction the sum of energies of starting materials was taken as reference. All calculations was performed at Gaussian09.[2] The transition structure optimized showed only one imaginary frequency that corresponds to transition state displacement vectors.

Table S 1. Electronic and Free energies of optimized structures

Compound	$E_{eletronic}$/hartree	ΔE/kcal mol^{-1}	G/hartree	ΔG/kcal mol^{-1}
HF	-100.423004	0.0	-100.429909	0.0
(S)-1d	-1222.996774		-1222.745713	
TS-3	-1323.354791	40.8	-1323.097735	48.9
(S)-2d	-1323.461642	-26.3	-1323.195865	-12.7

[2] Gaussian 09, Revision E.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M. J.; Heyd, J.; Brothers, E. N.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A. P.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J.; Gaussian, Inc.: Wallingford, CT, USA, 2009.

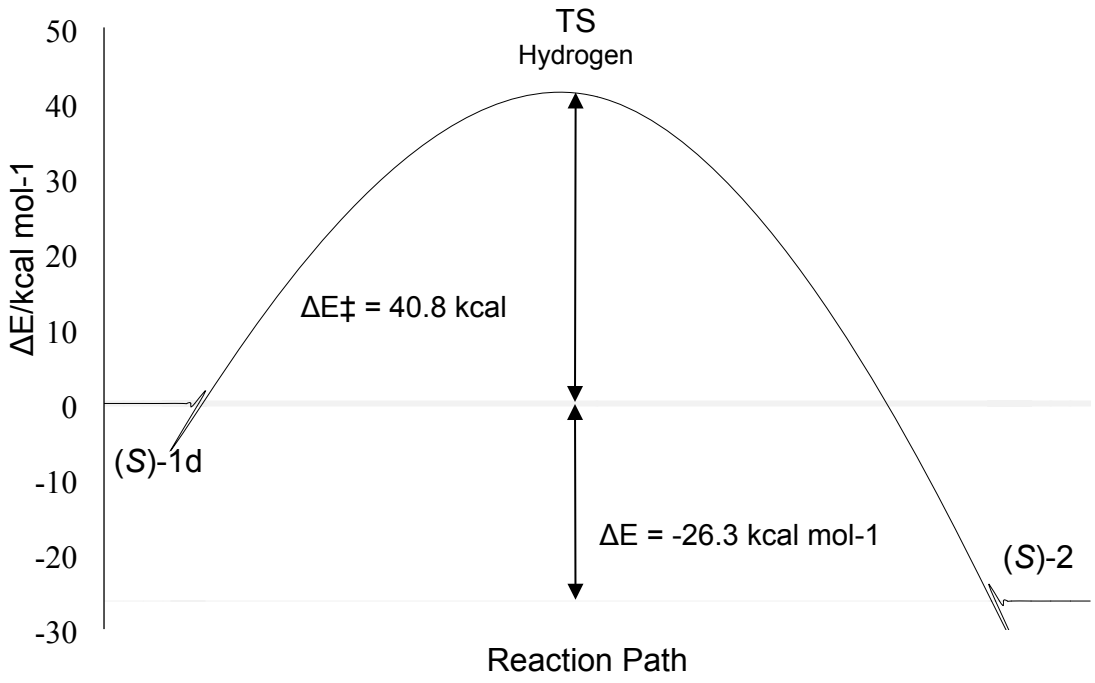


Figure S 1. Electronic energy barrier diagram for hydrogen bonding assisted pathway

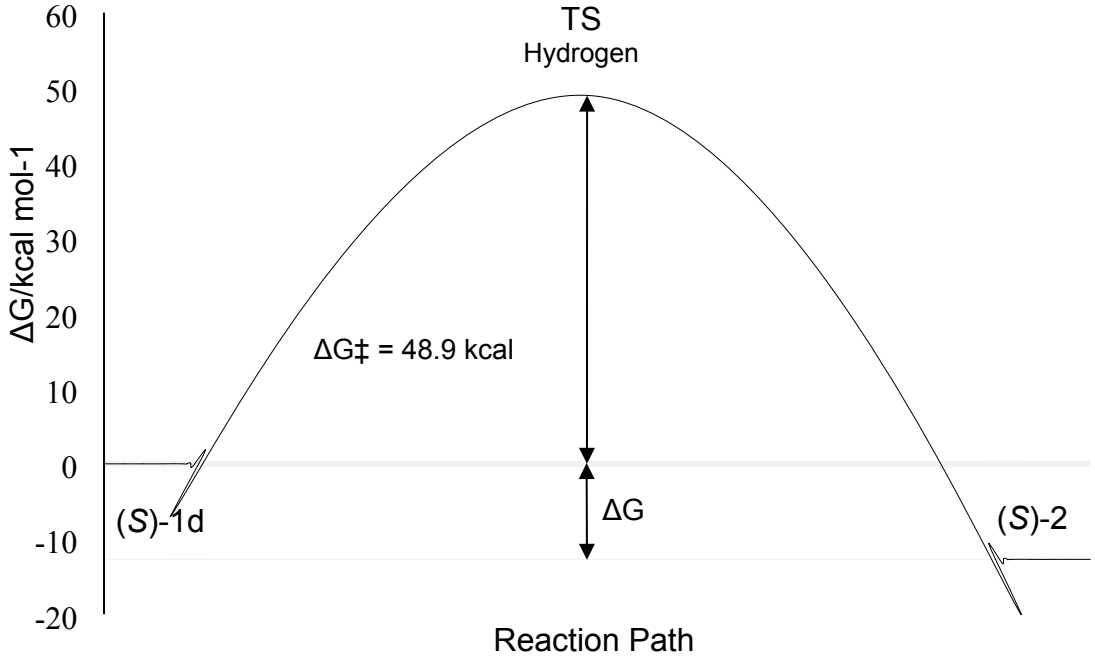


Figure S 2. Free energy barrier diagram for hydrogen bonding assisted pathway

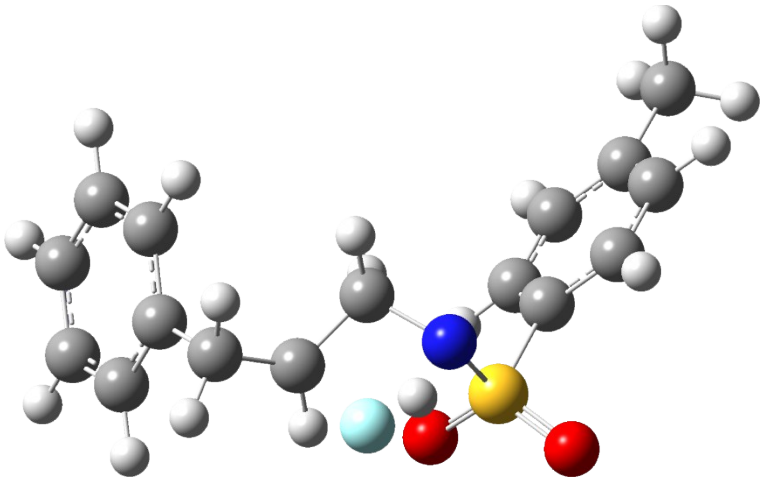


Figure S 3. Hydrogen bonding assisted transition state optimized structure

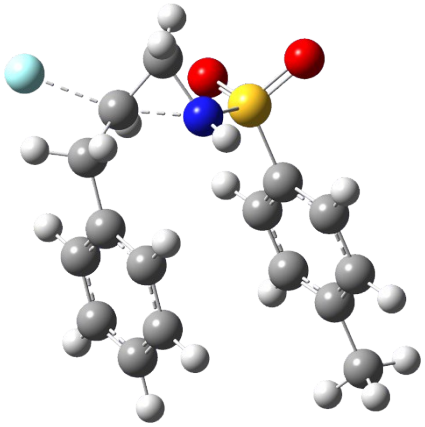


Figure S 4. One of the attempts to achieve S_N2-like transition state. Structure not optimized.

Z-matrix for optimized structures and transition state

HF-optimized structure

%mem=16000MB
opt freq M062X/aug-cc-pVDZ

OPT-HF

0 1
F 0.00000 0.00000 0.09213
H 0.00000 0.00000 -0.82917

(S)-1d-optimized structure

%mem=48000MB
opt freq M062X/aug-cc-pVDZ

OPT-Reagent-Aziridine

0 1

C	-0.93470000	1.04798900	-1.19510000
N	-0.53805000	1.10932900	0.21563000
C	-1.58343100	2.01918900	-0.27624000
C	-1.57546000	-0.25013100	-1.65397000
H	-0.22789100	1.49538900	-1.89579000
H	-1.31030100	3.06639900	-0.39919000
H	-0.78397000	-1.00901100	-1.72147000
H	-1.96300000	-0.08948100	-2.66827000
H	-2.56550100	1.80633900	0.14103000
S	0.97057900	1.84669000	0.52709000
O	0.96849900	2.20205000	1.95280000
O	1.26665900	2.87569000	-0.49362000
C	2.04241000	0.45108000	0.25108000
C	2.15509000	-0.51539000	1.24906000
C	2.73054000	0.35267000	-0.95122000
C	2.97904000	-1.61058000	1.02023000
H	1.61527000	-0.39147000	2.18645000
C	3.55360000	-0.75404000	-1.15979000
H	2.63393000	1.14092000	-1.69532000
C	3.68667000	-1.74545000	-0.18387000
H	3.08643000	-2.37348000	1.79144000
H	4.10772000	-0.84135000	-2.09387000
C	4.57545000	-2.94103000	-0.40364000
H	5.08598000	-2.88305000	-1.37039000
H	5.33468000	-3.00948000	0.38546000
H	3.98857000	-3.86800000	-0.37814000
C	-2.68595000	-0.73031100	-0.75397000
C	-4.02130000	-0.46311100	-1.06991000
C	-2.39735000	-1.40953100	0.43415000
C	-5.05049000	-0.86455100	-0.21854000
H	-4.25800000	0.06650900	-1.99357000
C	-3.42272000	-1.81176100	1.28774000
H	-1.35831000	-1.61039100	0.69393000
C	-4.75235000	-1.53981100	0.96400000

H	-6.08627000	-0.65087100	-0.47957000
H	-3.18413000	-2.33913100	2.21033000
H	-5.55367000	-1.85547100	1.63063000

TS-optimized structure

%mem=16000MB
opt=(ts,calcfc,noeigentest,tight) Int=UltraFine freq=noraman nosymm M062X/aug-cc-pVDZ

TS-Aziridine

0 1

F	-0.23145	-1.54609	-1.66941
C	-0.28844	-0.71339	0.47653
N	1.77424	-0.92111	-0.50355
C	1.10249	-1.11304	0.78497
C	-1.48285	-1.50352	0.75218
H	-0.39471	0.31093	0.11245
H	1.50328	-0.47273	1.58773
H	-1.28147	-2.57579	0.79253
H	-2.31497	-1.27008	0.08604
H	1.16544	-2.16315	1.09449
S	2.40479	0.59444	-0.65848
O	1.48240	1.62005	-0.08553
O	2.86641	0.72917	-2.05015
C	3.84220	0.58233	0.41650
C	3.87163	1.37860	1.55330
C	4.91672	-0.23978	0.07482
C	5.00523	1.34707	2.37019
H	3.02357	2.02334	1.77592
C	6.03551	-0.25718	0.89719
H	4.86758	-0.84432	-0.82957
C	6.09513	0.53421	2.05565
H	5.04190	1.97253	3.26189
H	6.88469	-0.89012	0.63799
C	7.32298	0.50106	2.92806
H	8.20934	0.81237	2.36090
H	7.21460	1.16814	3.78962
H	7.50922	-0.51483	3.29907
C	-1.68729	-0.91295	2.15413
C	-2.35038	0.31070	2.30652
C	-1.16024	-1.56285	3.27771
C	-2.51711	0.86093	3.57512

H	-2.74333	0.82544	1.42982
C	-1.33042	-1.01188	4.54373
H	-0.63337	-2.50924	3.15857
C	-2.00879	0.19980	4.69278
H	-3.04188	1.80745	3.69046
H	-0.93527	-1.52750	5.41714
H	-2.13912	0.63031	5.68433
H	0.74545	-1.28417	-1.41799

(S)-2d-optimized structure

%mem=16000MB
opt freq M062X/aug-cc-pVDZ

OPT-Product

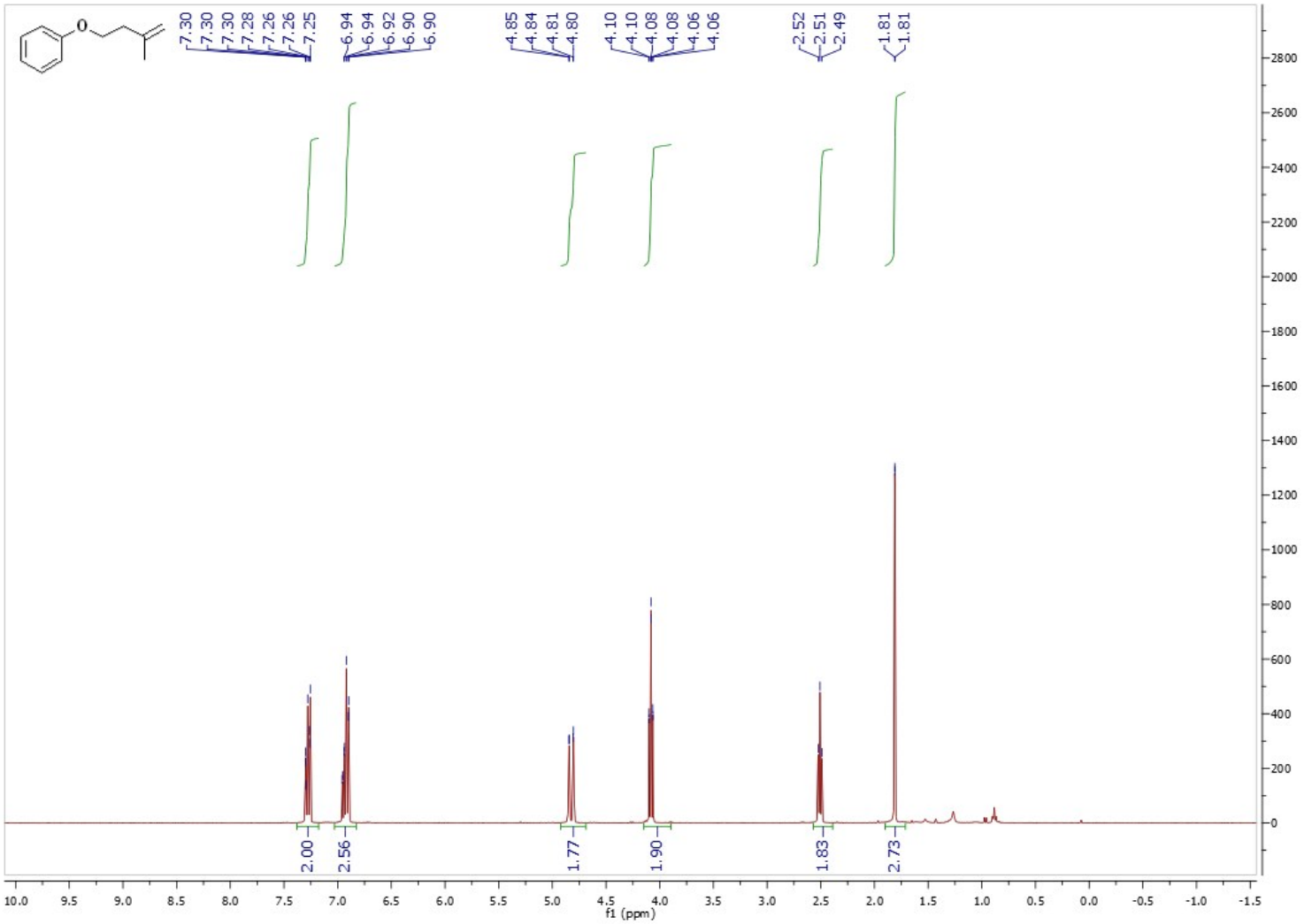
0 1

F	3.55027	-1.80767	-1.16800
C	2.63822	-0.87566	-0.64998
N	0.55106	-2.30327	-0.71161
C	1.28306	-1.16911	-1.27353
C	3.13131	0.52889	-0.97488
H	2.60645	-1.03530	0.43245
H	0.63807	-0.28645	-1.19422
H	3.12187	0.67398	-2.06362
H	4.17189	0.60786	-0.63559
H	1.43548	-1.36786	-2.34231
S	-0.19835	-2.03265	0.77968
O	0.67696	-1.27396	1.69846
O	-0.72953	-3.34665	1.17787
C	-1.52457	-0.94285	0.30058
C	-1.36715	0.42879	0.45875
C	-2.68446	-1.49948	-0.23482
C	-2.40886	1.26690	0.06018
H	-0.45004	0.82989	0.89009
C	-3.71212	-0.64680	-0.61741
H	-2.77193	-2.58050	-0.33006
C	-3.58775	0.74428	-0.47732
H	-2.29691	2.34472	0.17621
H	-4.63177	-1.06297	-1.02902
C	-4.71767	1.64508	-0.90209
H	-5.63166	1.40701	-0.34363
H	-4.47228	2.69776	-0.72867
H	-4.93842	1.51197	-1.96874

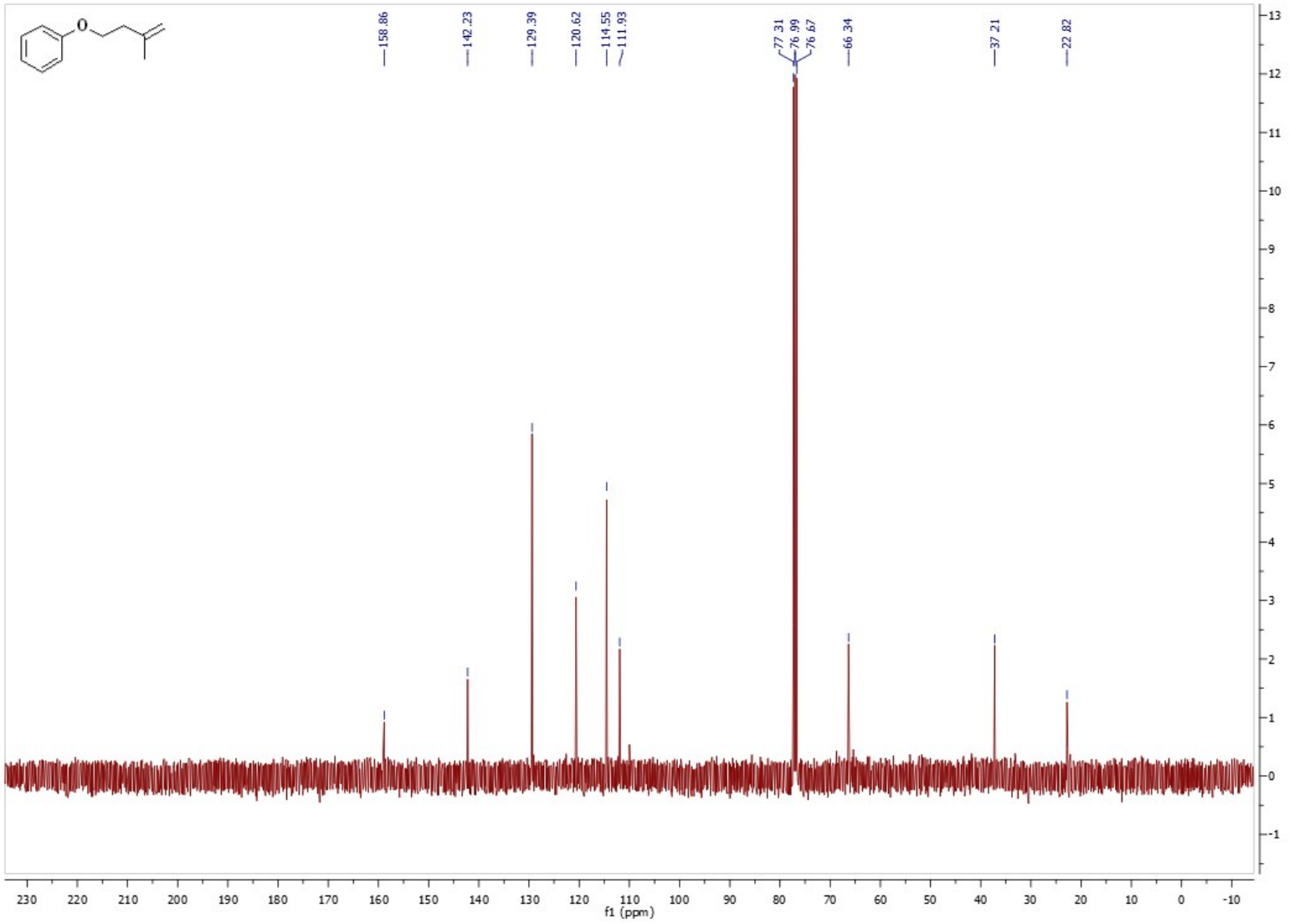
C	2.26888	1.56816	-0.29500
C	2.26629	1.67475	1.10096
C	1.42792	2.40784	-1.03162
C	1.45163	2.60433	1.74350
H	2.90057	1.01636	1.69431
C	0.61120	3.34175	-0.39280
H	1.41419	2.33280	-2.11936
C	0.62158	3.44367	0.99743
H	1.46210	2.67155	2.82988
H	-0.03203	3.99047	-0.98598
H	-0.01273	4.17281	1.49940
H	1.08643	-3.16819	-0.64502

6. Copies of NMR Spectra

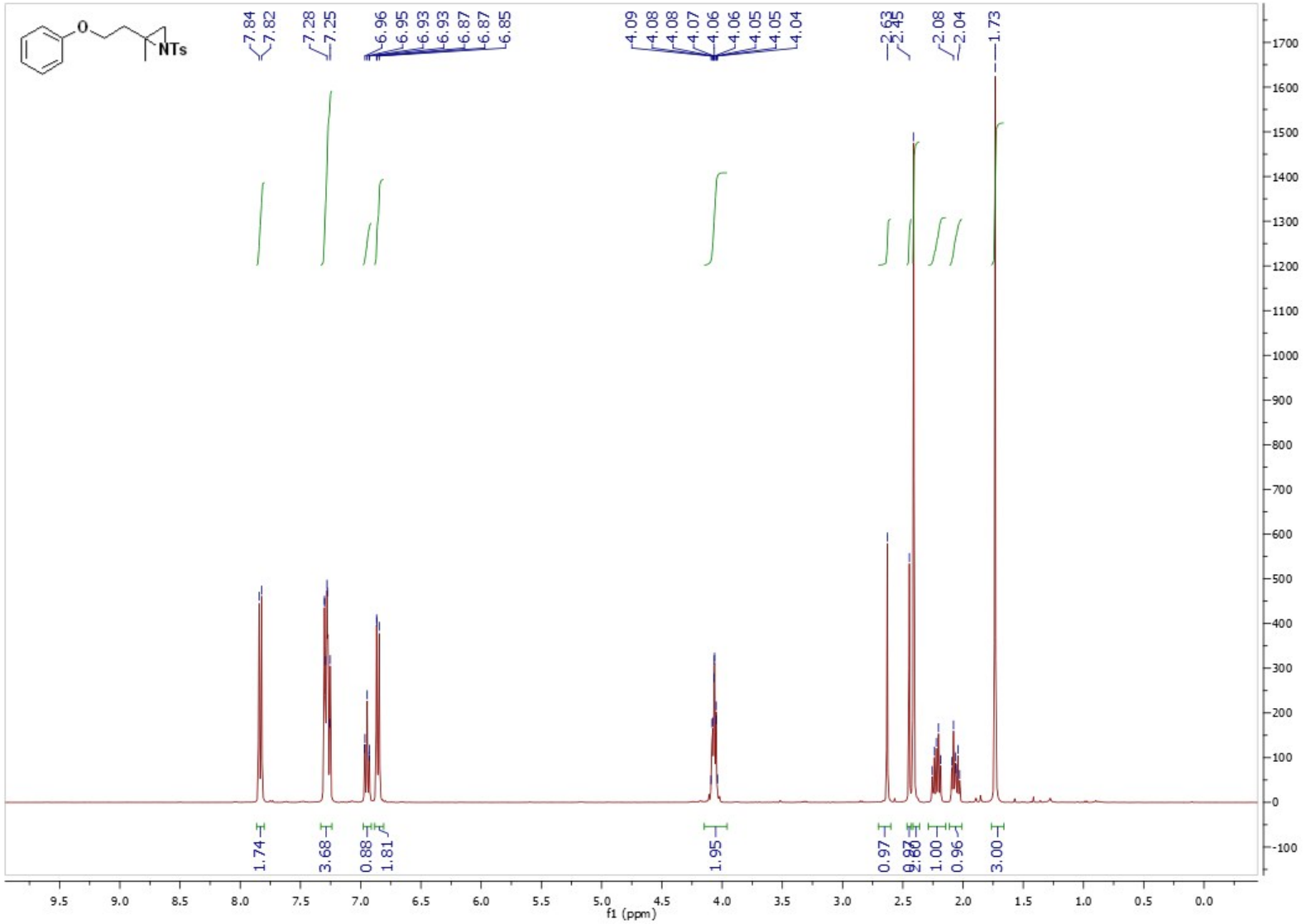
^{1}H NMR for 1n-1



^{13}C NMR for 1n-1



^{1}H NMR for 1n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4.05
4.04
2.63
2.45
2.08
2.04
1.73
1.74
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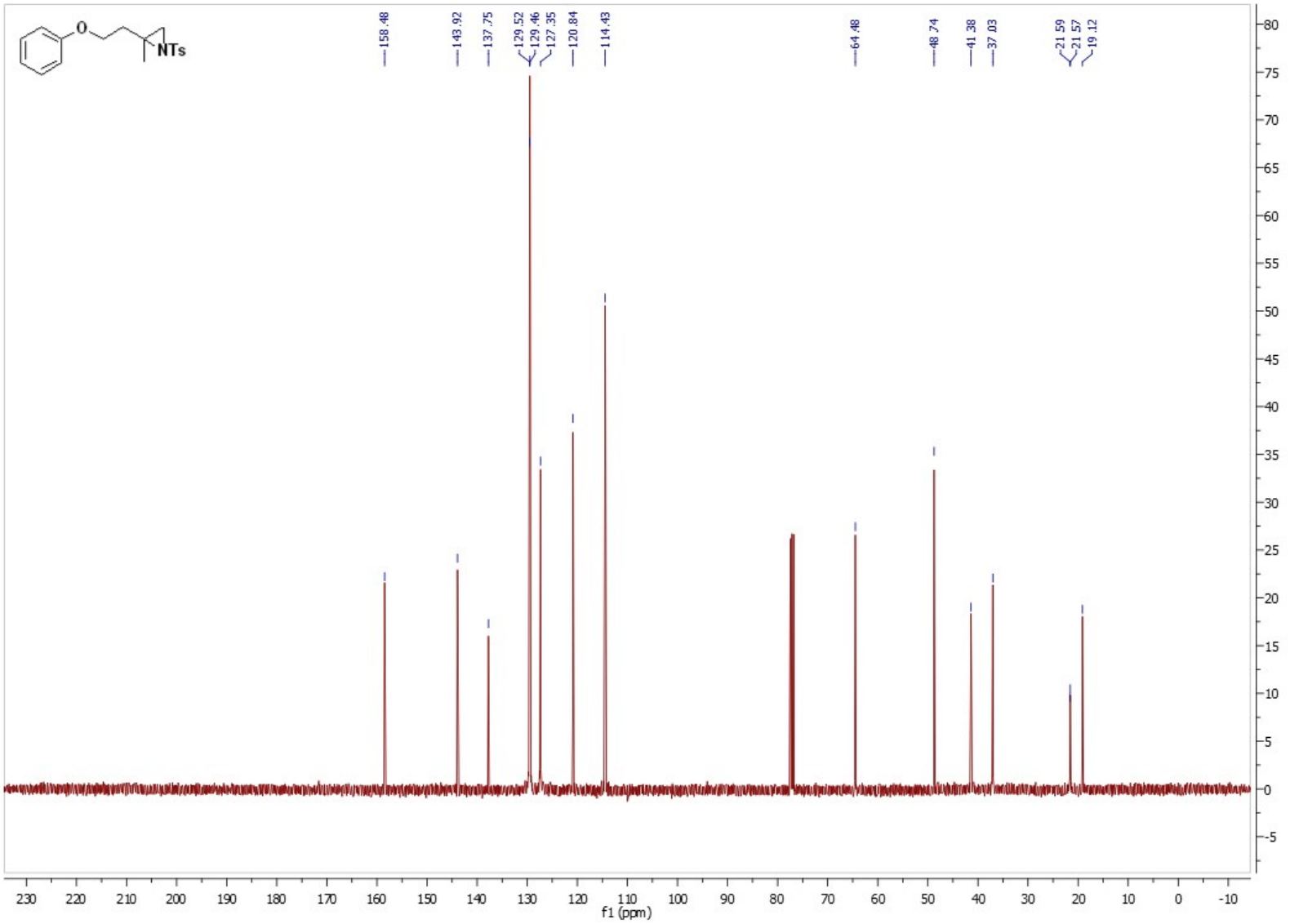
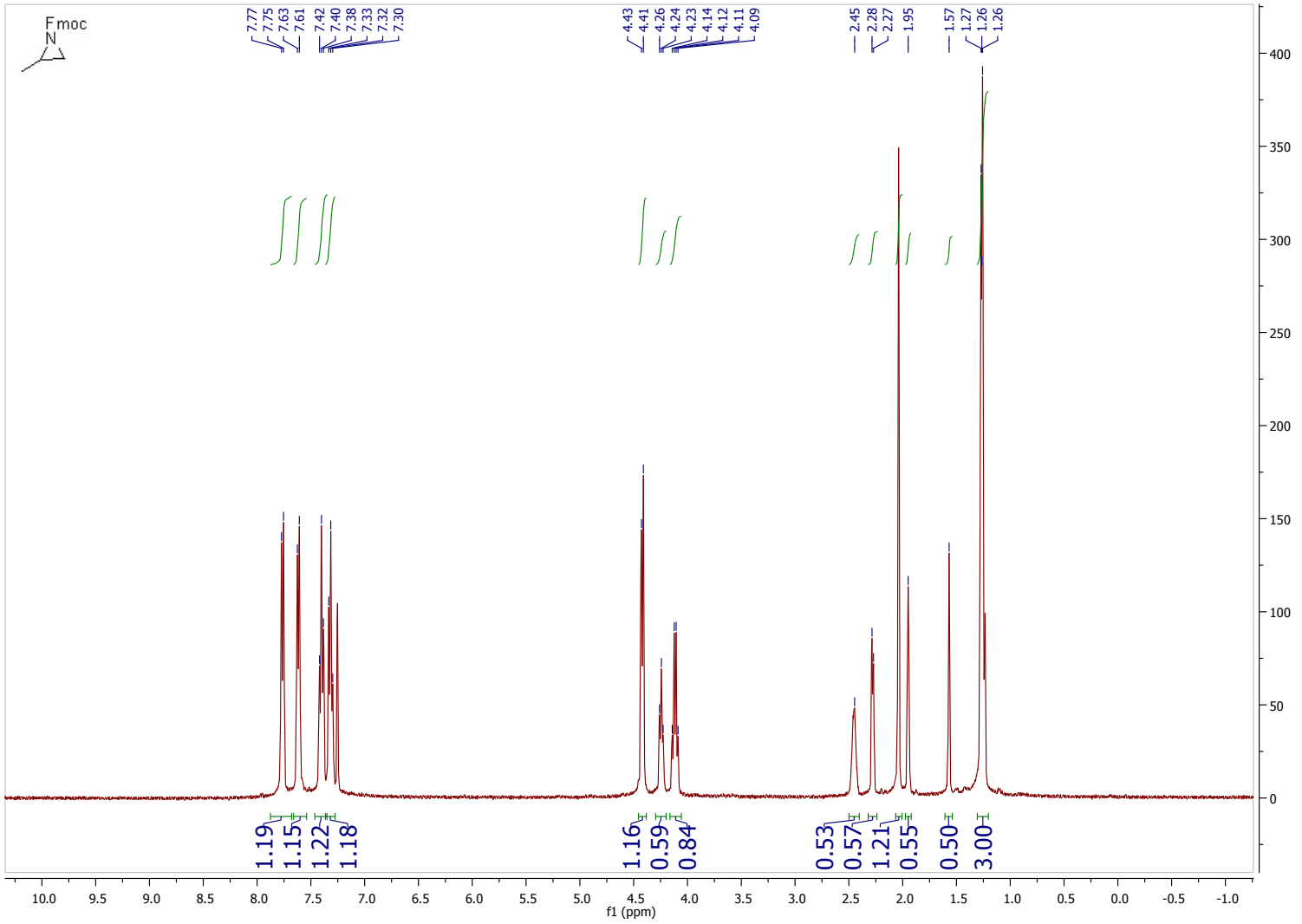
3.00
f1 (ppm)

^{13}C NMR for 1n



^{1}H NMR for 1r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4.14
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1.57
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1.26
1.19
1.15
1.22
1.18
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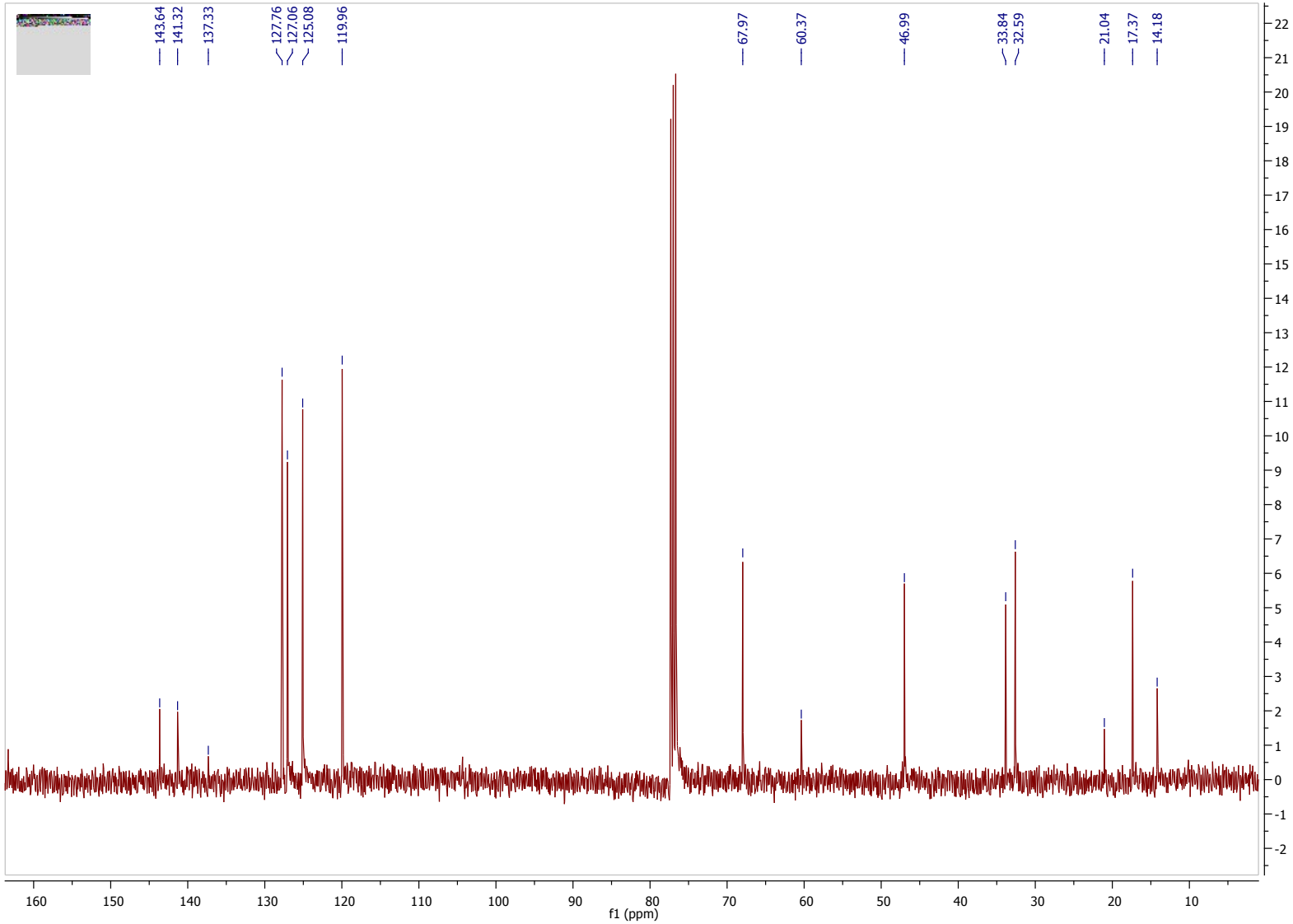
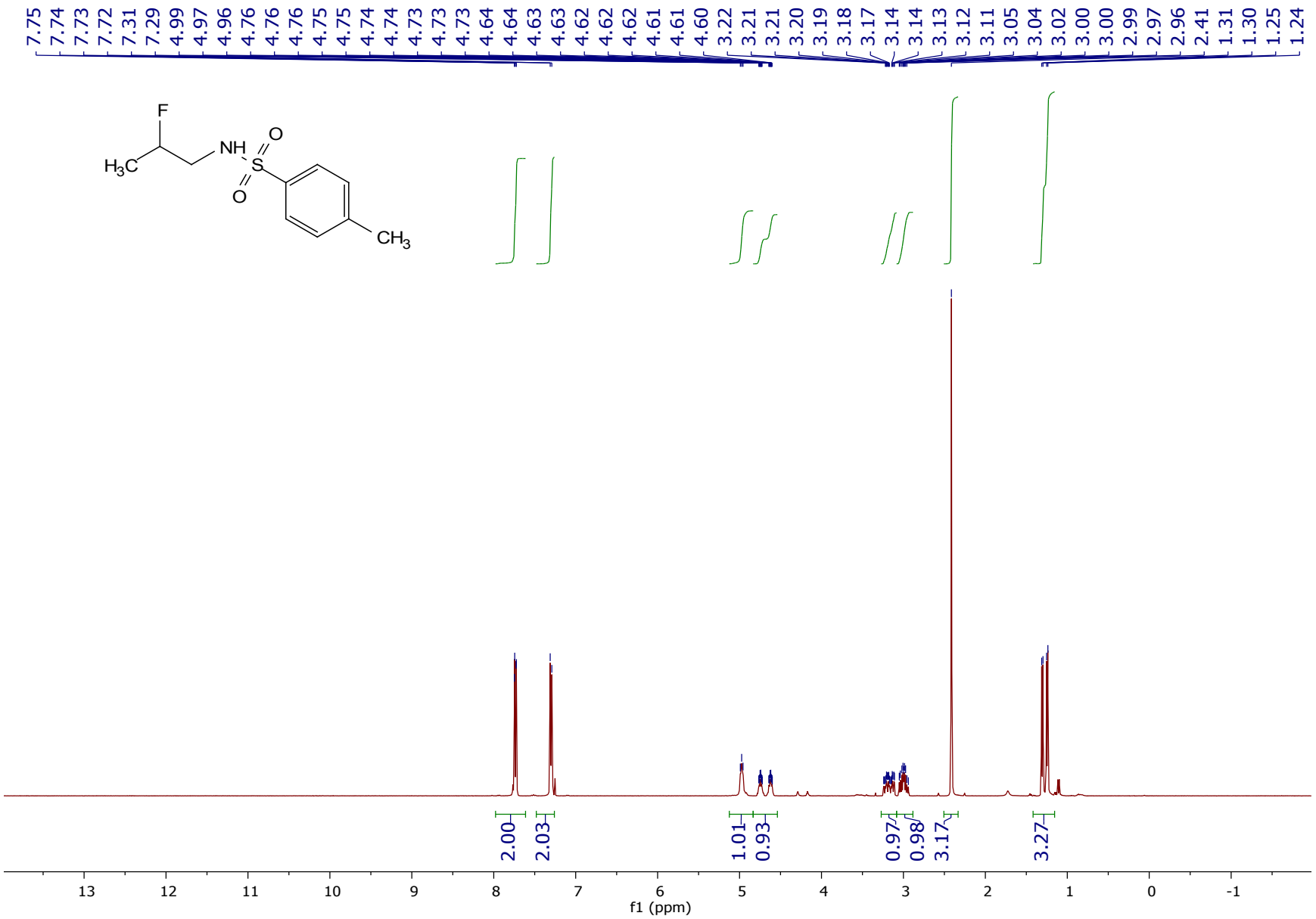
3.00
f1 (ppm)

^{13}C NMR for 1r



^{1}H NMR for 2a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F
NH
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S
O
H3C
CH3
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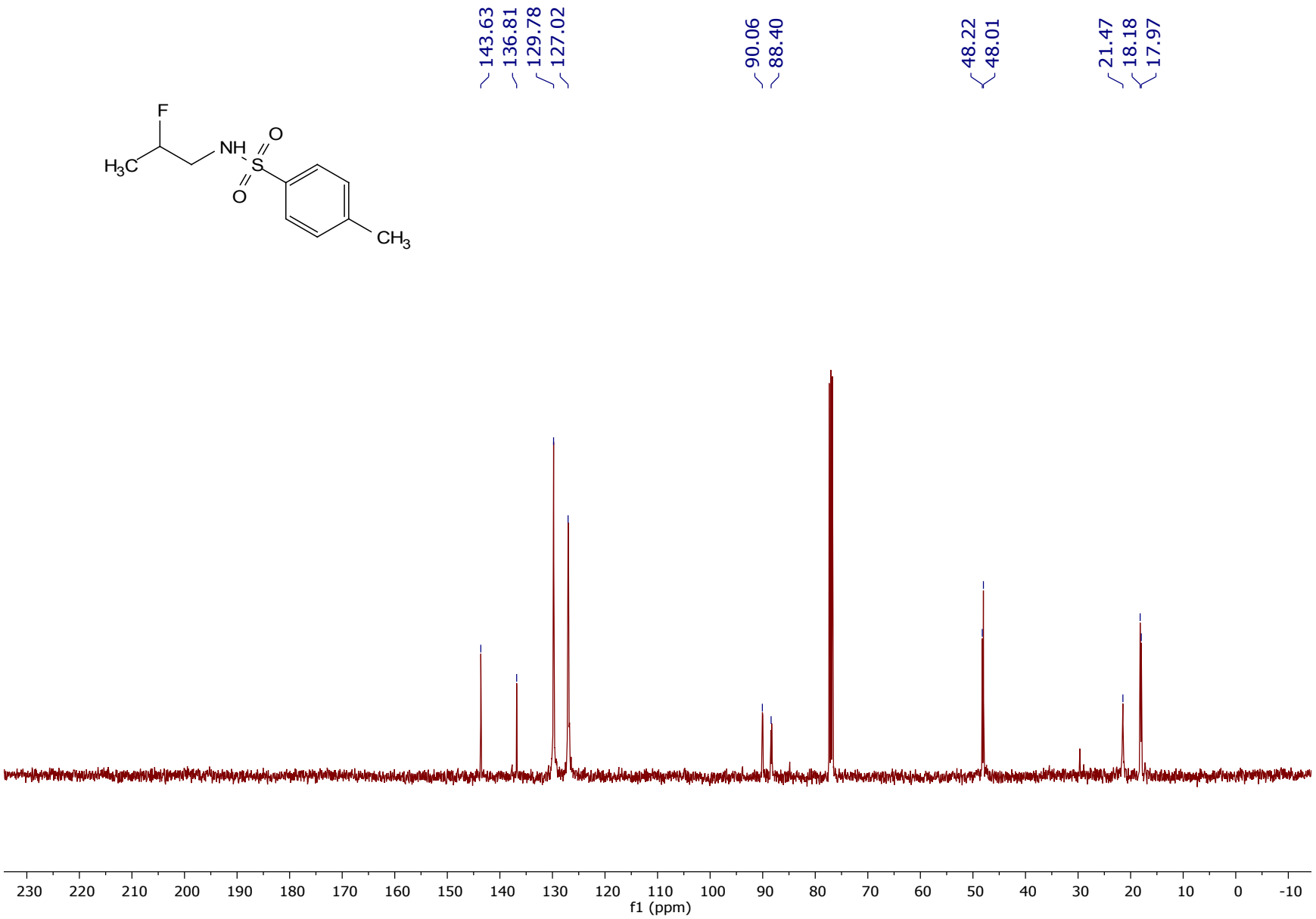
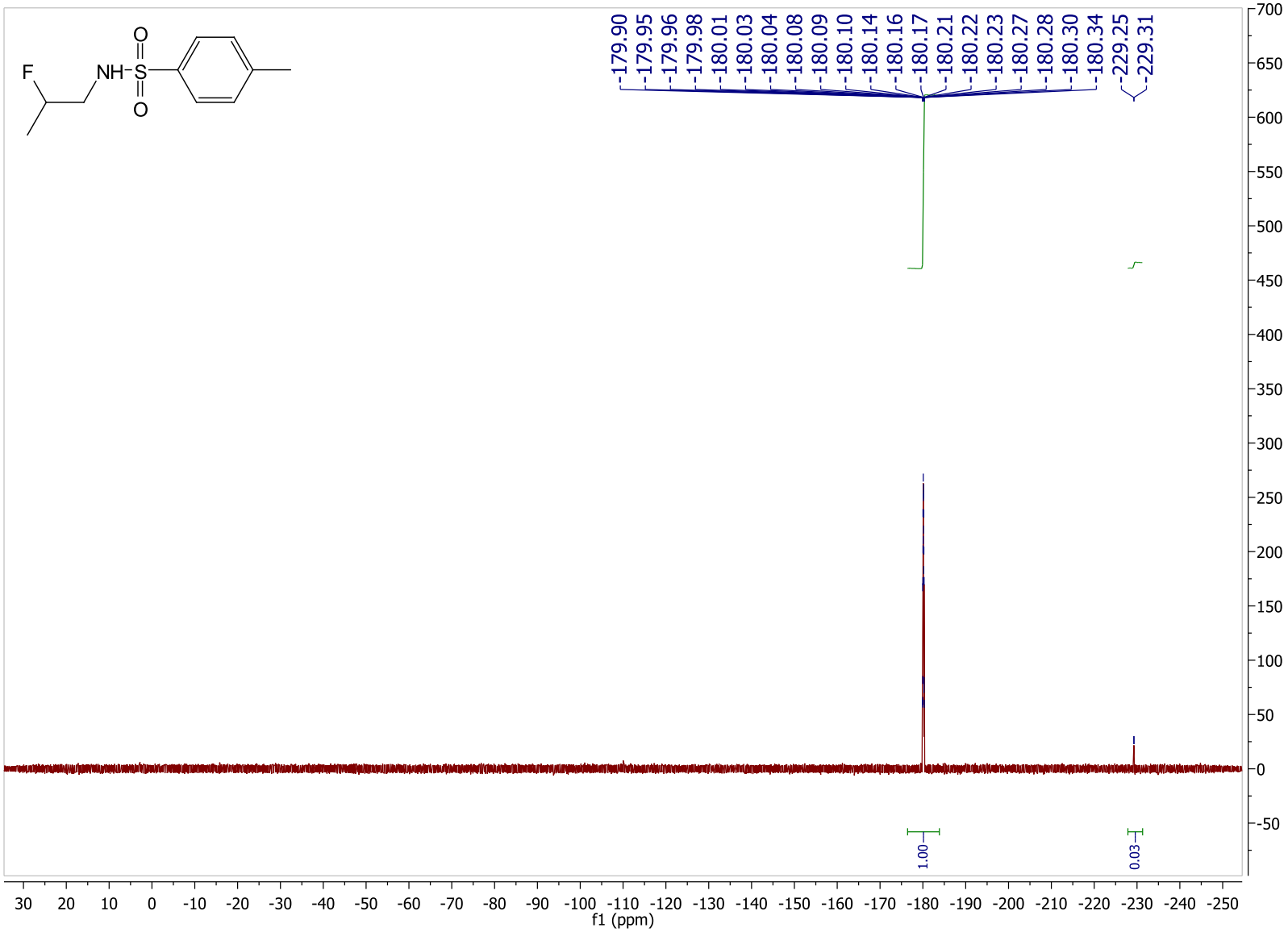
2.03
1.01
0.93
0.97
0.98
3.17
3.27
13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)

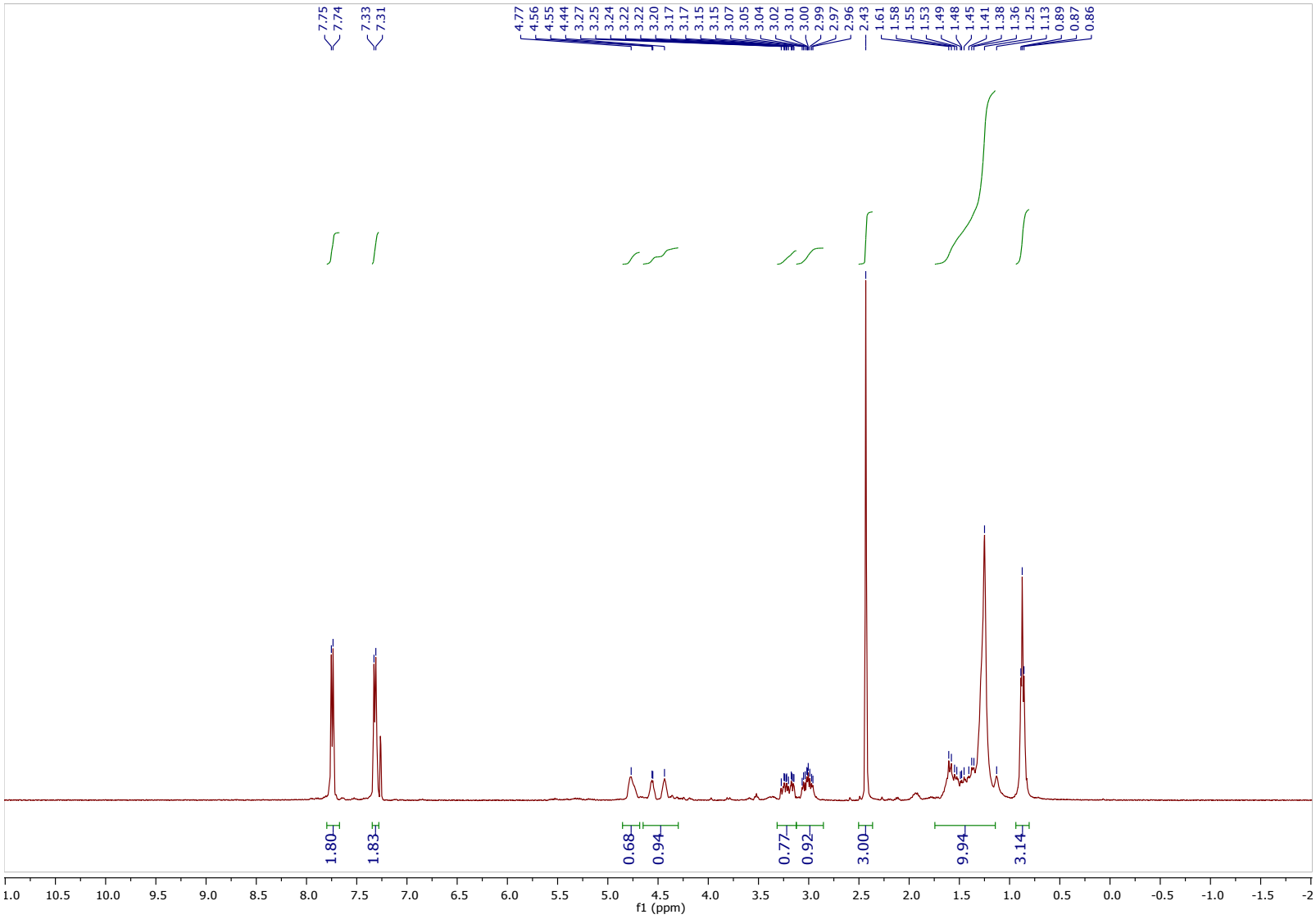
^{13}C NMR for 2a



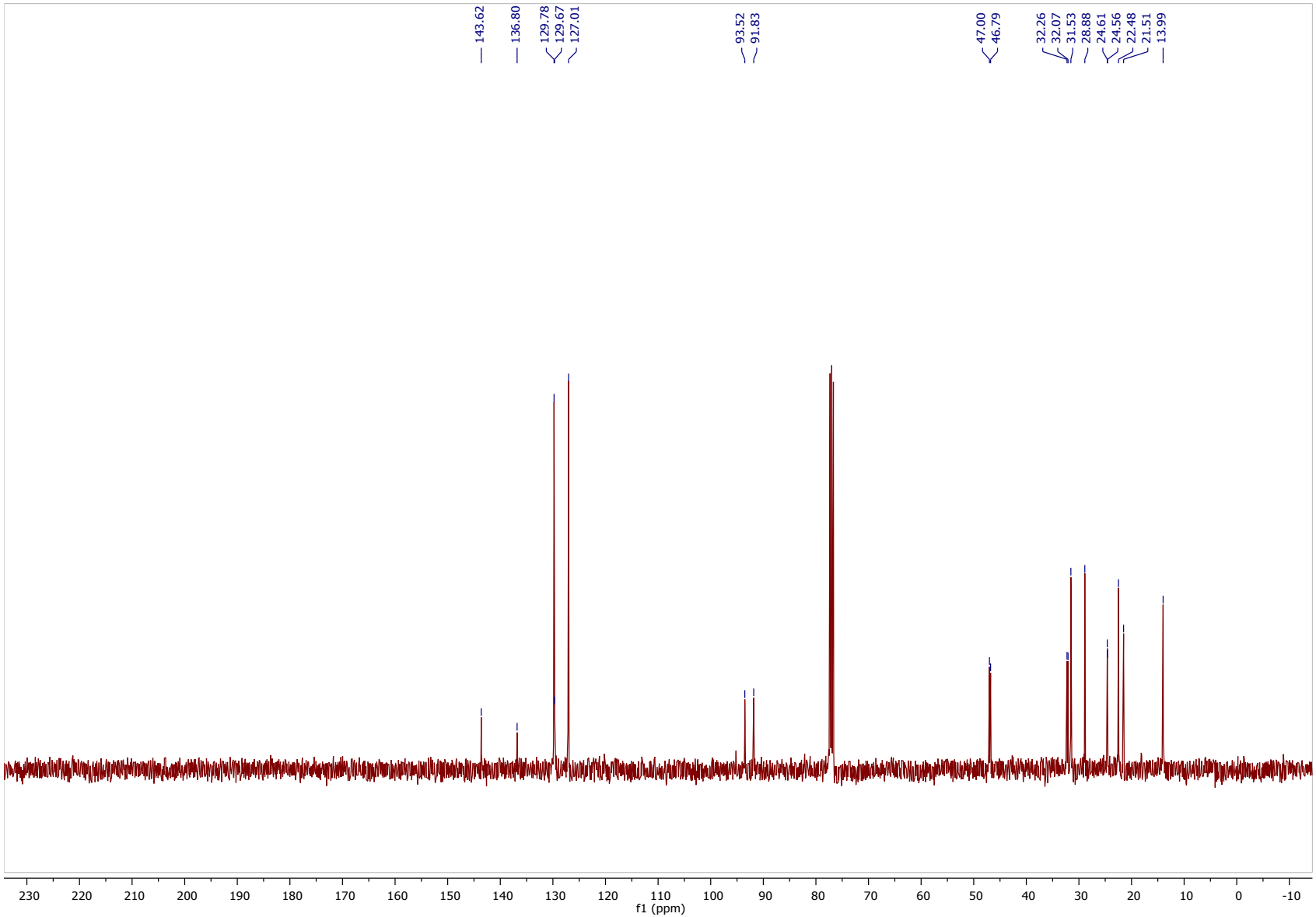
^{19}F NMR for 2a



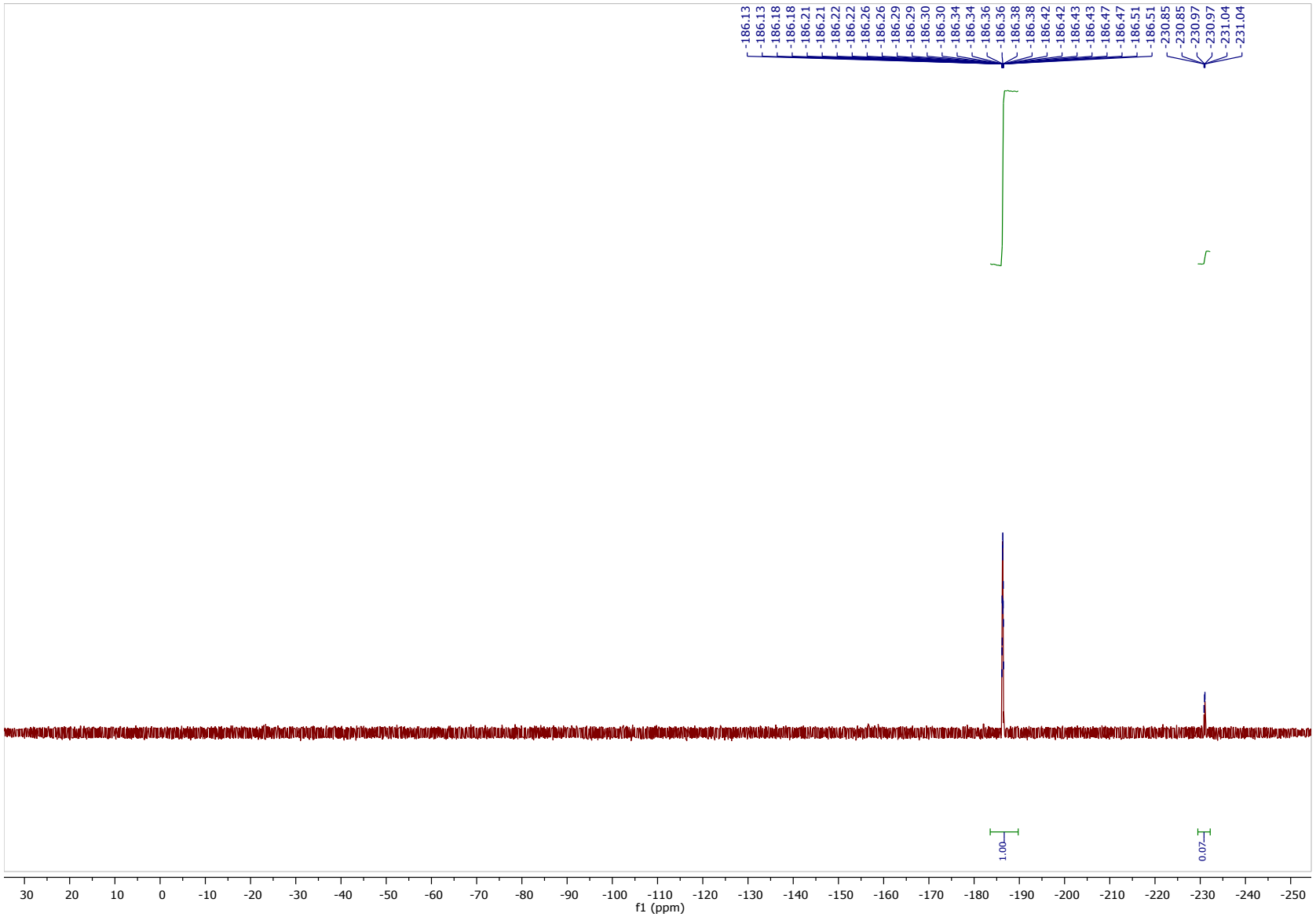
^{1}H NMR for 2b


7.75
7.74
7.33
7.31
4.77
4.56
4.55
4.44
3.27
3.25
3.24
3.22
3.22
3.20
3.17
3.17
3.15
3.15
3.07
3.05
3.04
3.02
3.01
3.00
2.99
2.97
2.96
2.43
1.61
1.58
1.55
1.53
1.49
1.48
1.45
1.41
1.38
1.36
1.25
1.13
0.89
0.87
0.86
1.80
1.83
0.68
0.94
0.77
0.92
3.00
9.94
3.14
f1 (ppm)

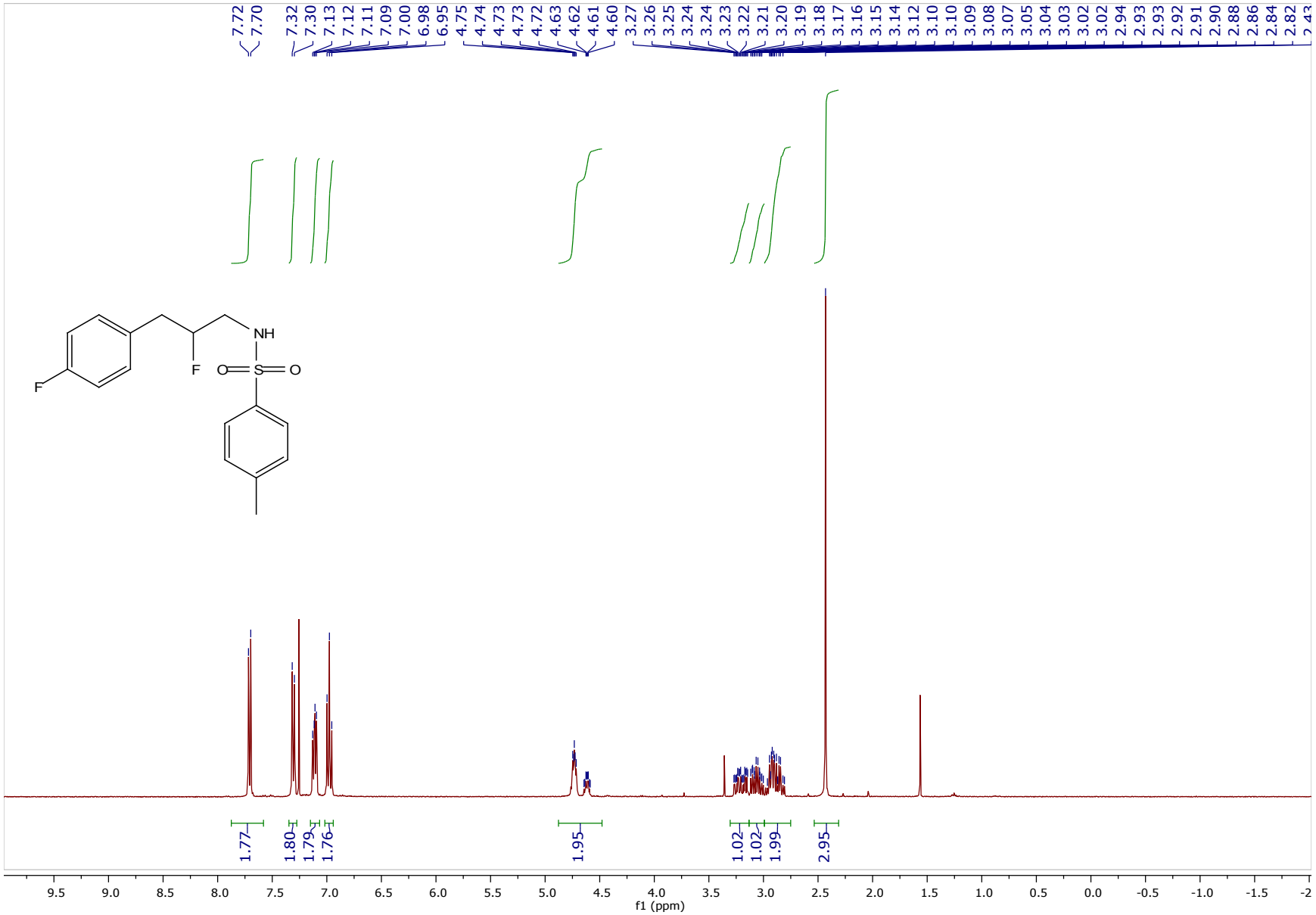
^{13}C NMR for 2b



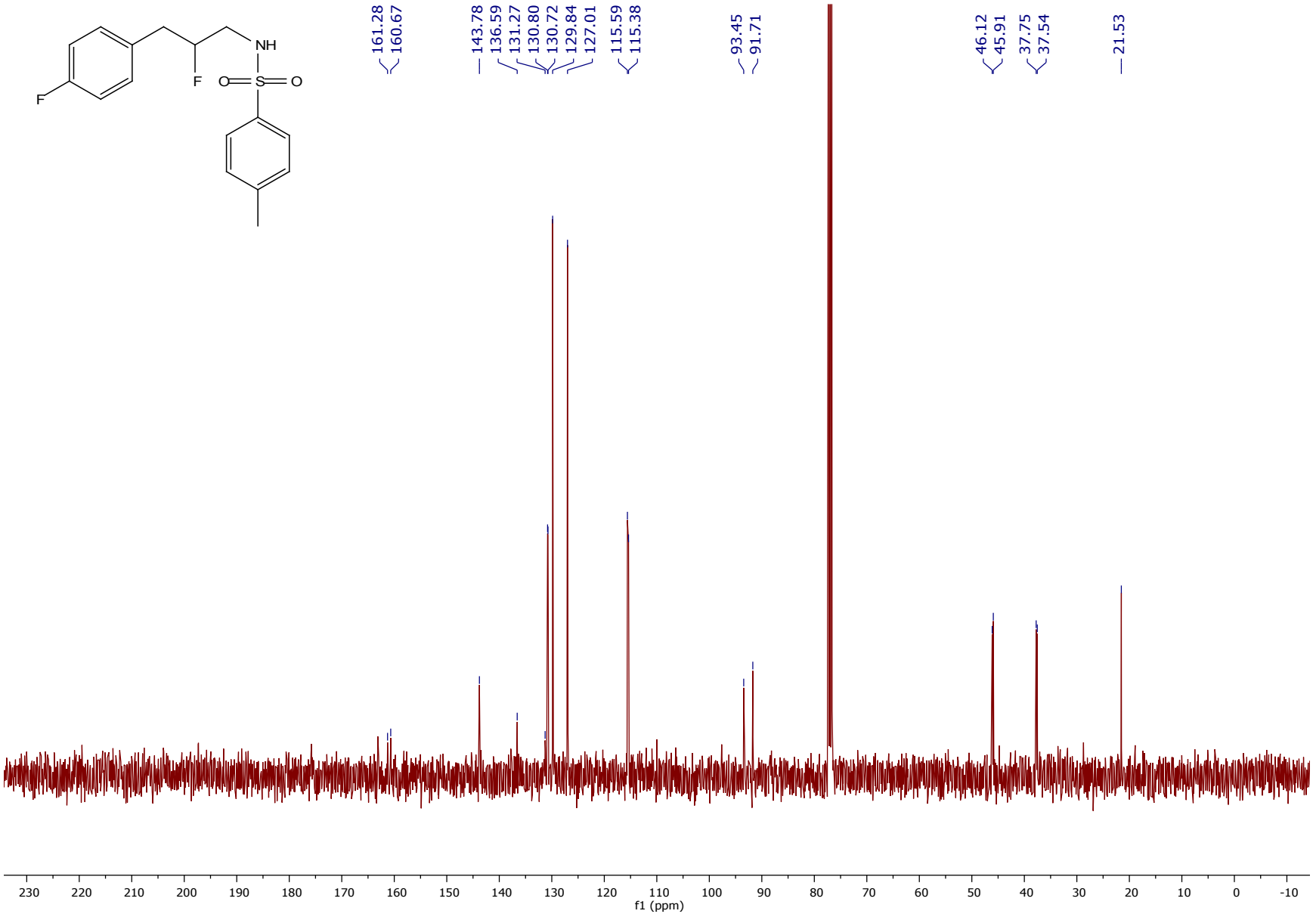
^{19}F NMR for 2b



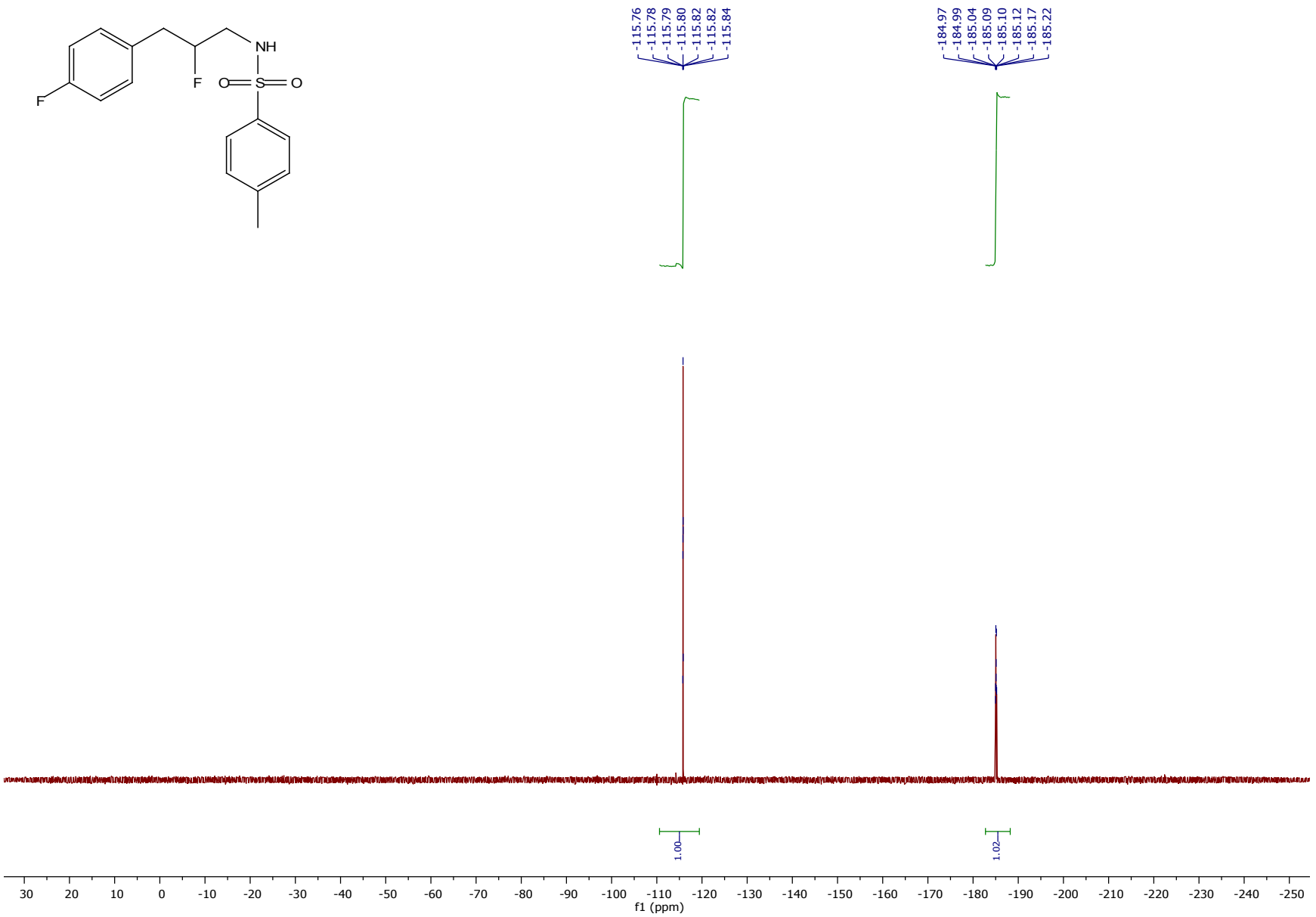
^{1}H NMR for 2e


7.72
7.70
7.32
7.30
7.13
7.12
7.11
7.09
7.00
6.98
6.95
4.75
4.74
4.73
4.73
4.72
4.63
4.62
4.61
4.60
3.27
3.26
3.25
3.24
3.24
3.23
3.22
3.21
3.20
3.19
3.18
3.17
3.16
3.15
3.14
3.12
3.10
3.10
3.09
3.08
3.07
3.05
3.04
3.03
3.02
3.02
2.94
2.93
2.93
2.92
2.91
2.90
2.88
2.86
2.84
2.82
NH
F
O
S
O
F
1.77
1.80
1.79
1.76
1.95
1.02
1.02
1.99
2.95
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
-1.5
-2
f1 (ppm)

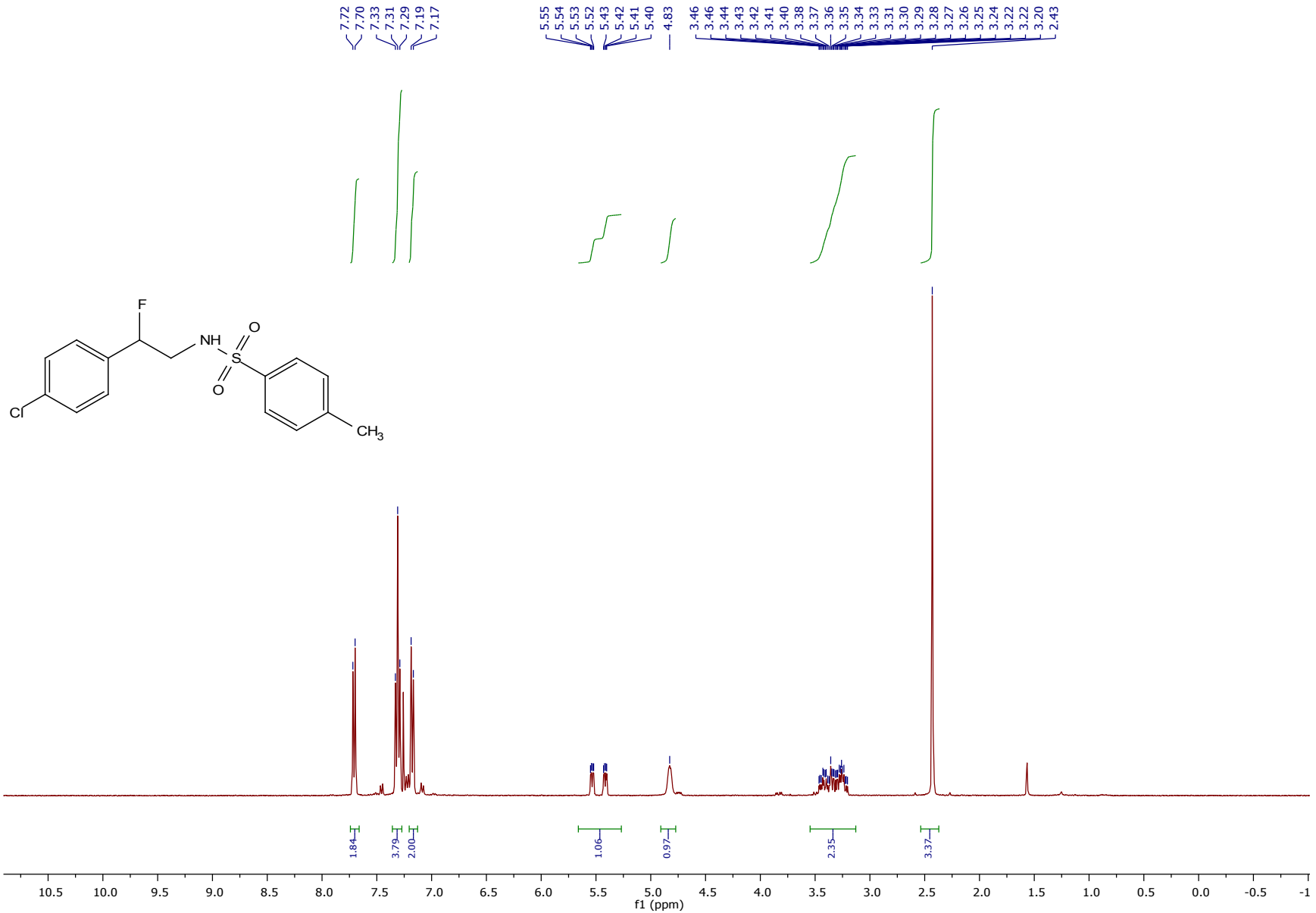
^{13}C NMR for 2e



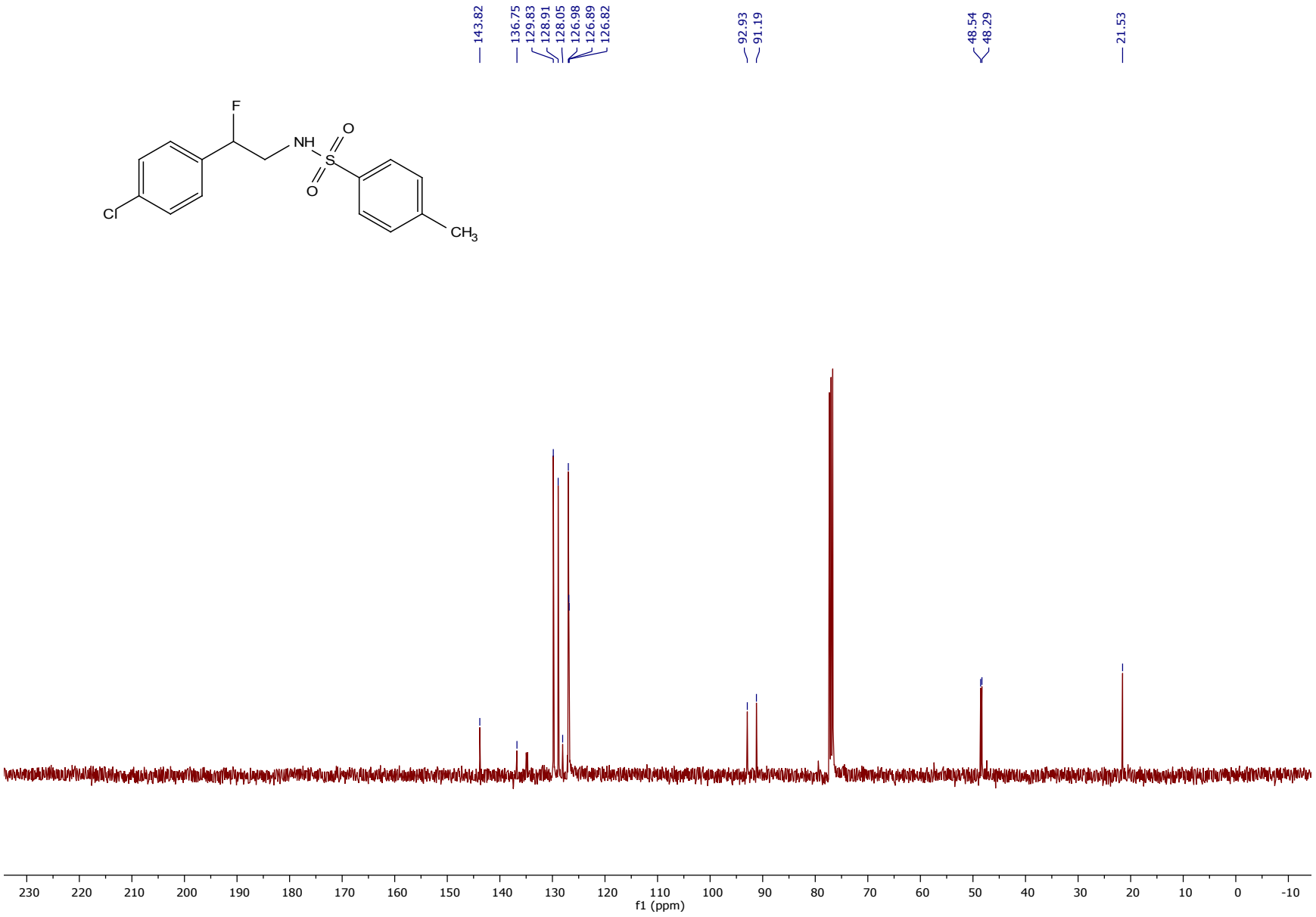
^{19}F NMR for 2e



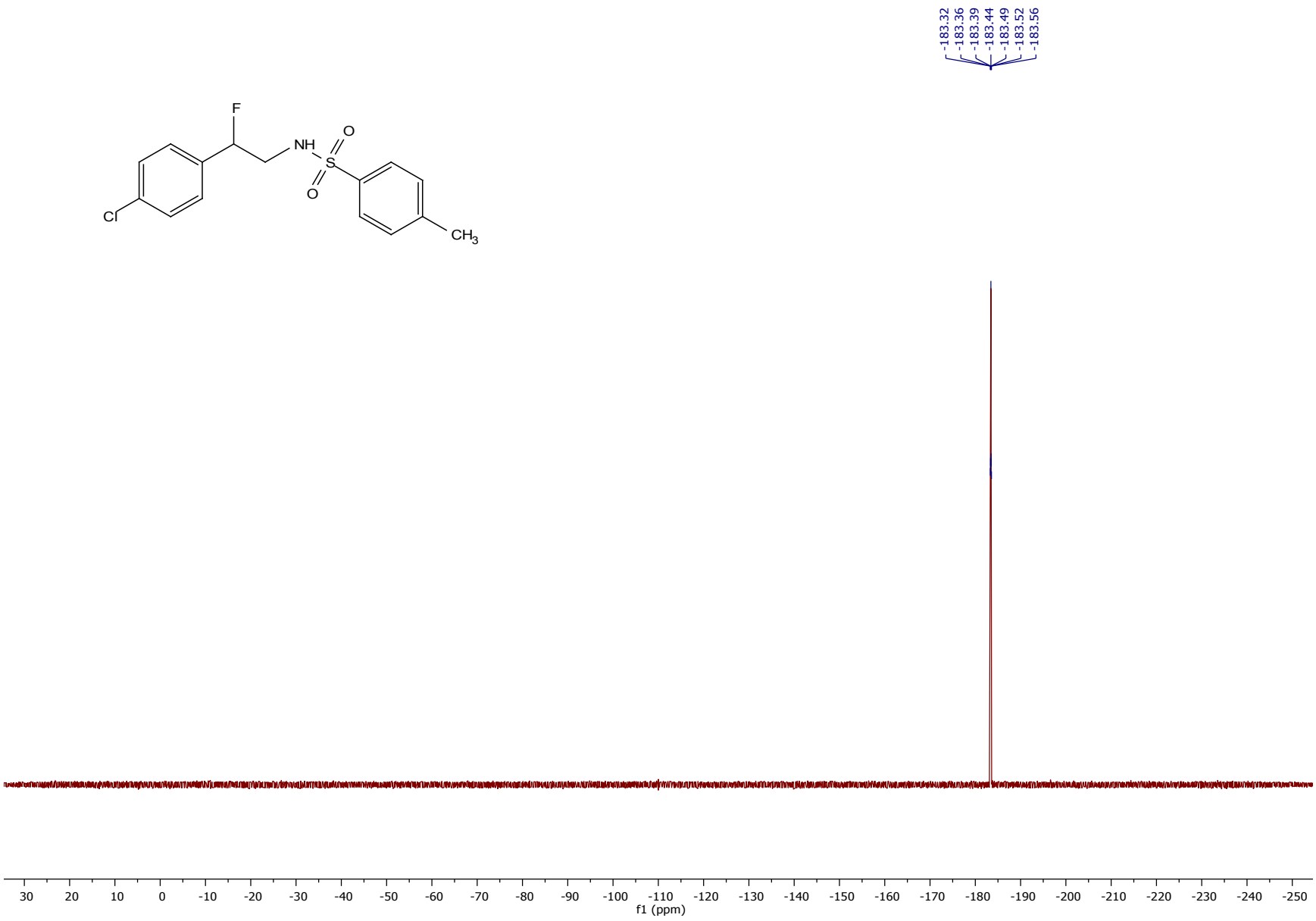
^{1}H NMR for 2f


7.72
7.70
7.33
7.31
7.29
7.19
7.17
5.55
5.54
5.53
5.52
5.43
5.42
5.41
5.40
4.83
3.46
3.46
3.44
3.43
3.42
3.41
3.40
3.38
3.37
3.36
3.35
3.34
3.33
3.31
3.30
3.29
3.28
3.27
3.26
3.25
3.24
3.22
3.22
3.20
2.43
F
NH
S
O
O
Cl
CH3
1.84
3.79
2.00
1.06
0.97
2.35
3.37
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)

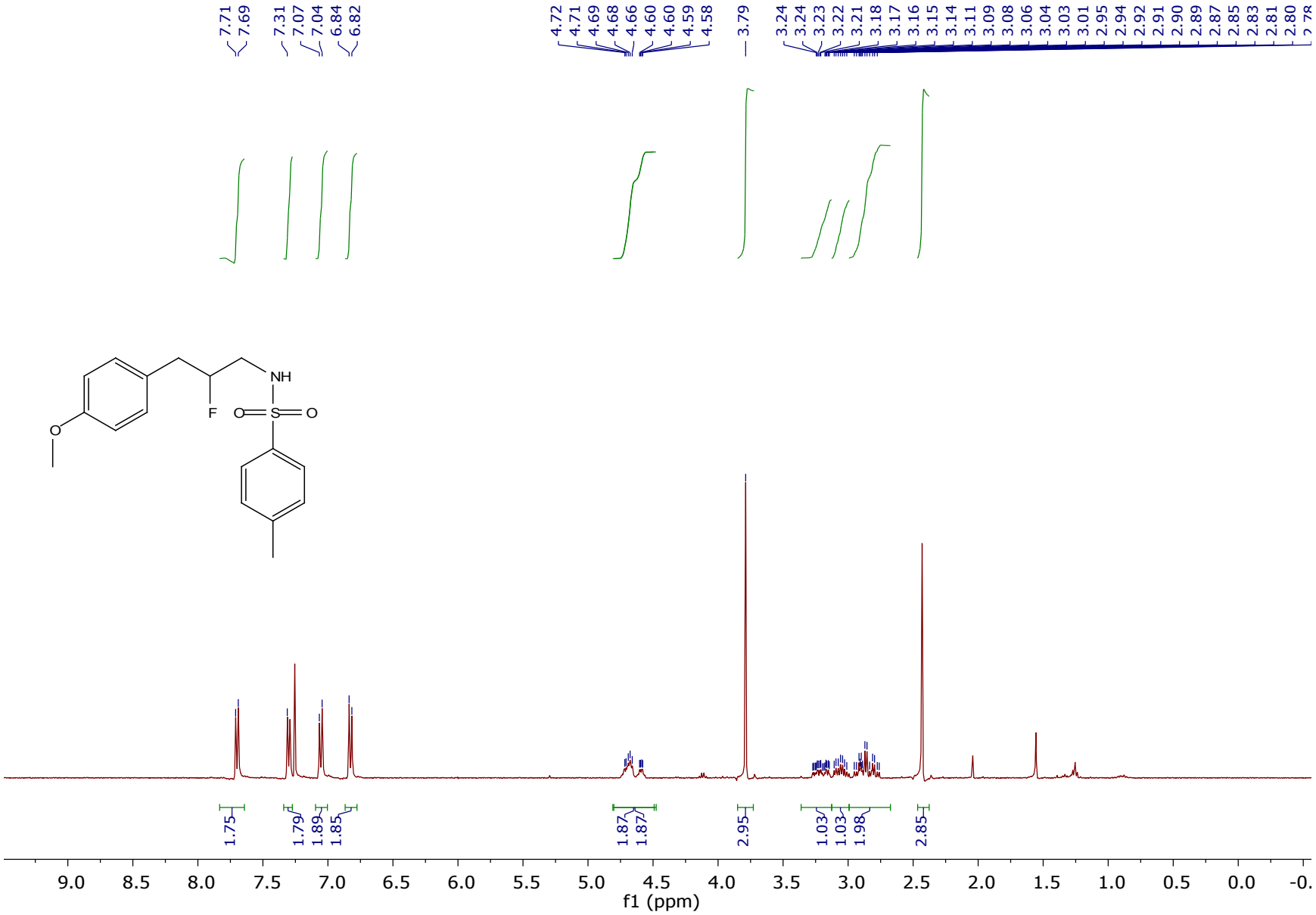
^{13}C NMR for 2f



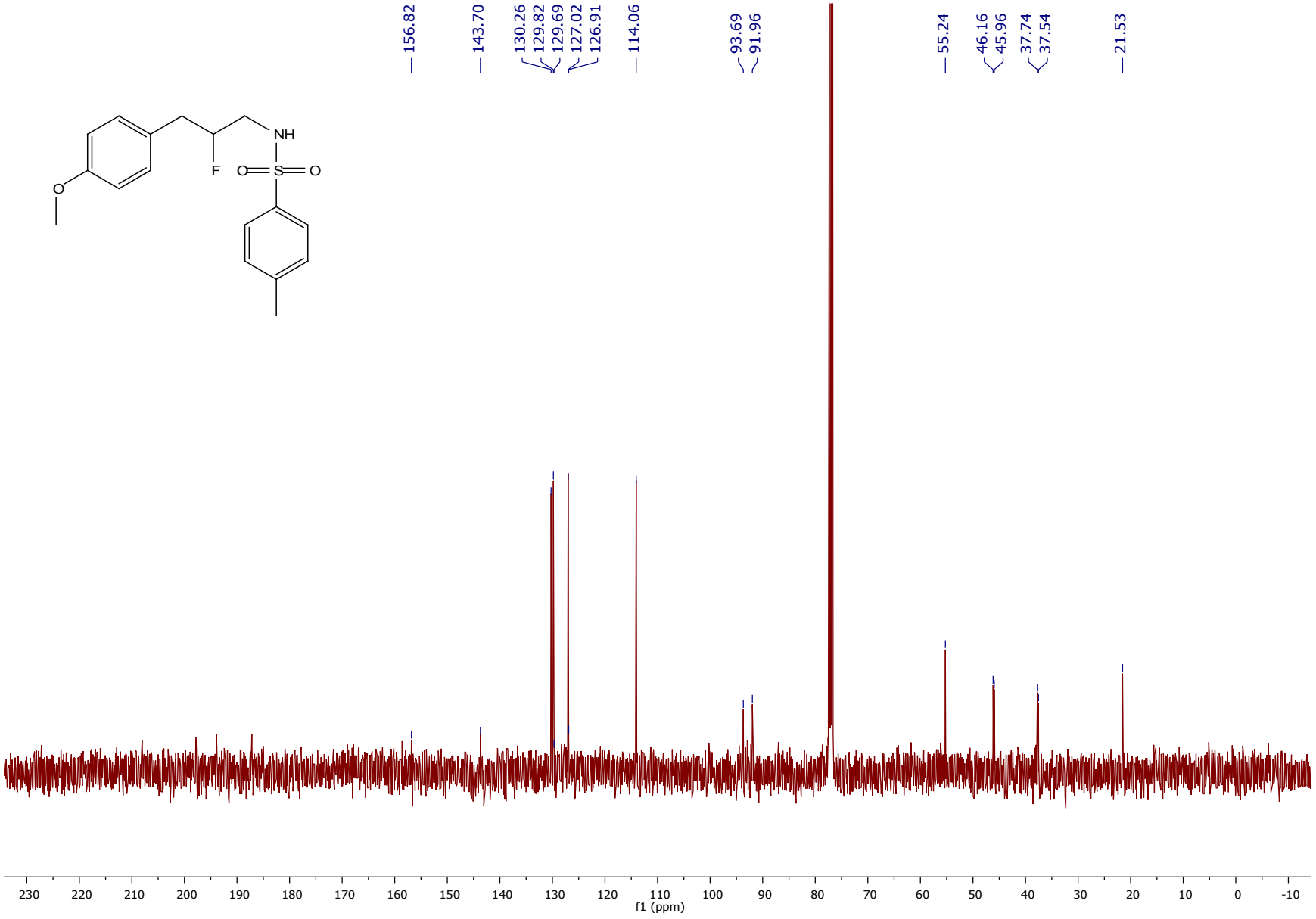
^{19}F NMR for 2f



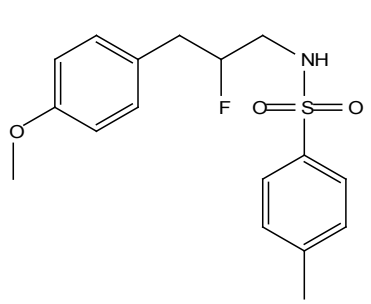
^{1}H NMR for 2g


7.71
7.69
7.31
7.07
7.04
6.84
6.82
4.72
4.71
4.69
4.68
4.66
4.60
4.60
4.59
4.58
3.79
3.24
3.24
3.23
3.22
3.21
3.18
3.17
3.16
3.15
3.14
3.11
3.09
3.08
3.06
3.04
3.03
3.01
2.95
2.94
2.92
2.91
2.90
2.89
2.87
2.85
2.83
2.81
2.80
NH
F
O
S
O
O
1.75
1.79
1.89
1.85
1.87
1.87
2.95
1.03
1.03
1.98
2.85
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

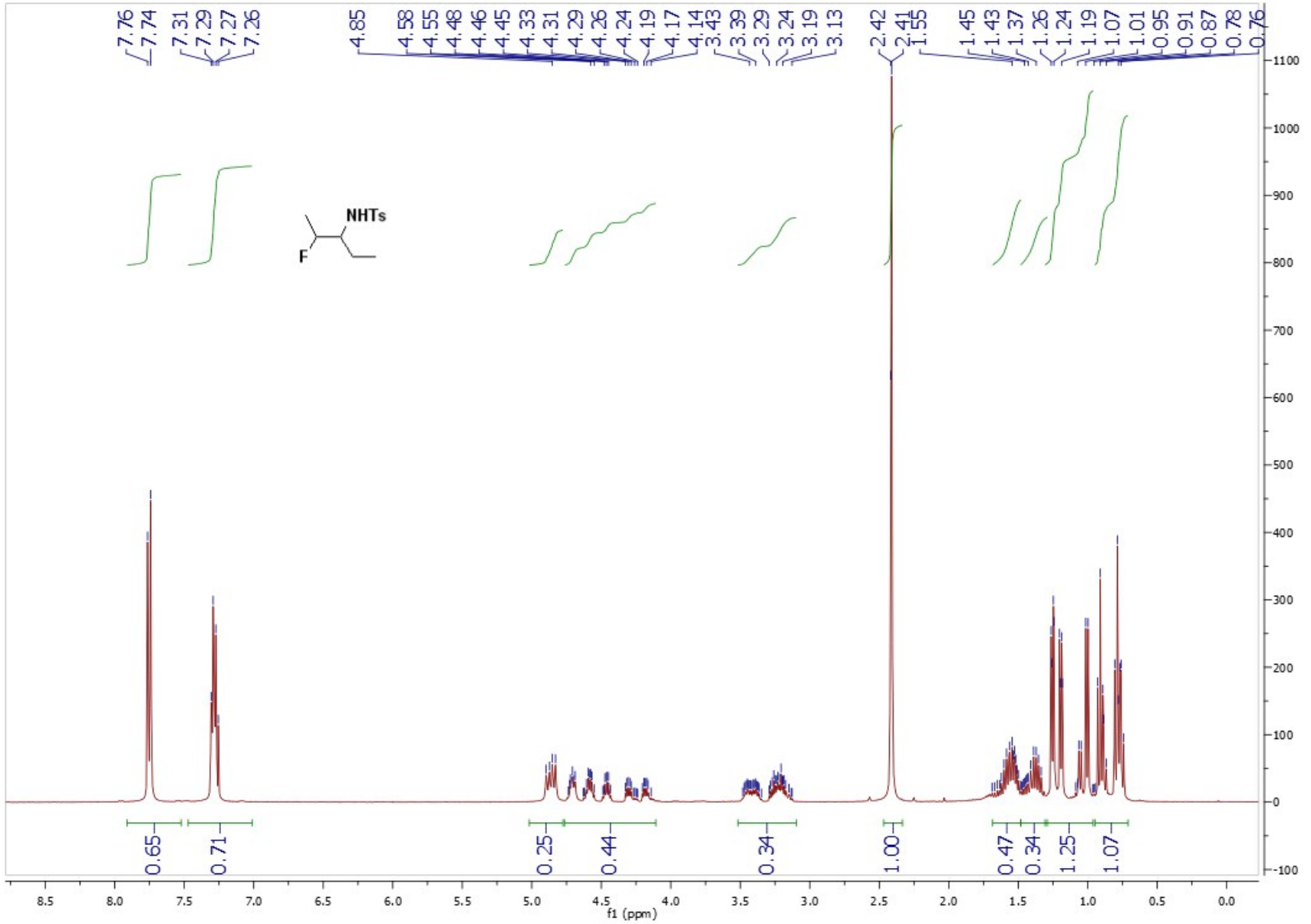
^{13}C NMR for 2g



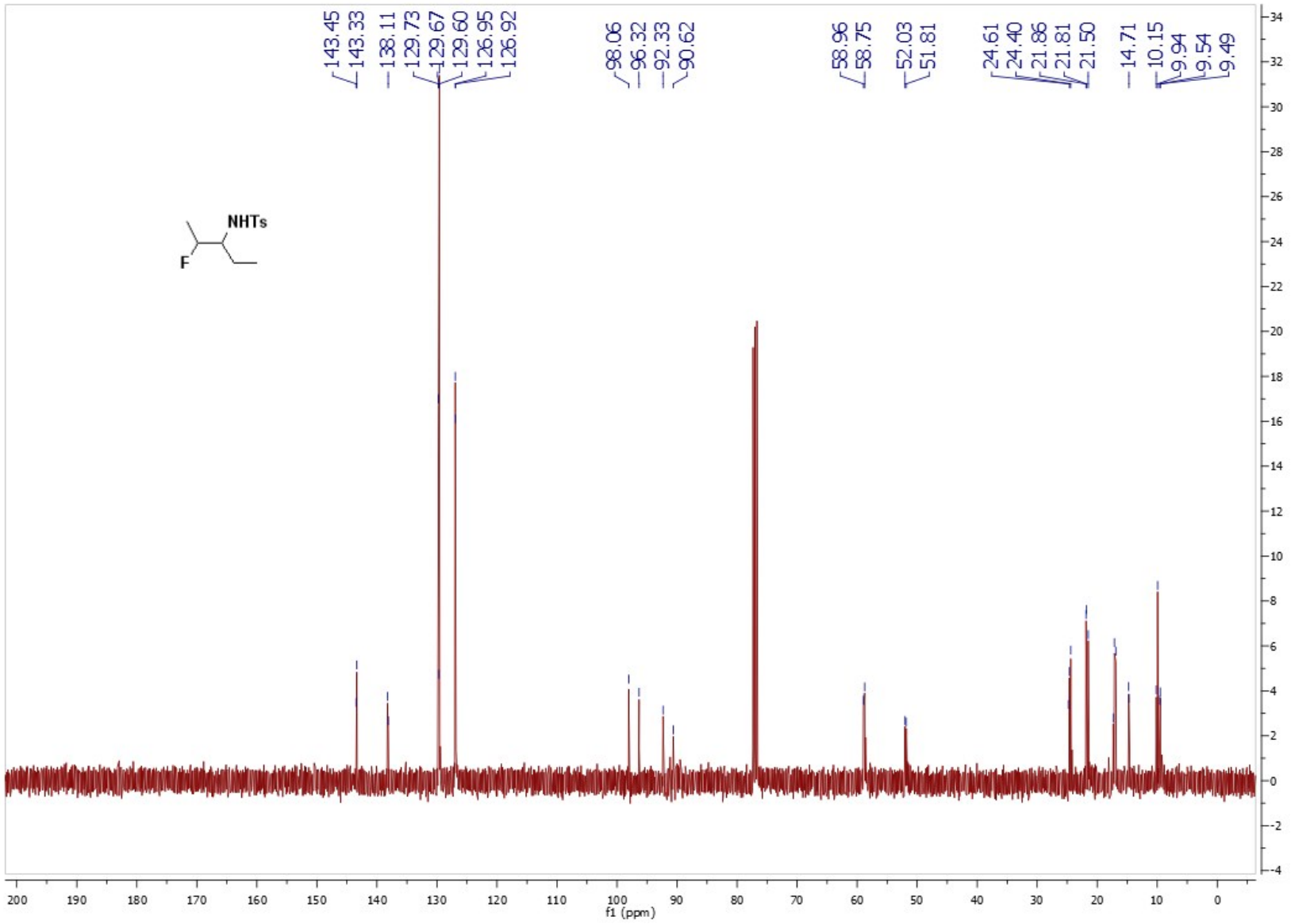
^{19}F NMR for 2g



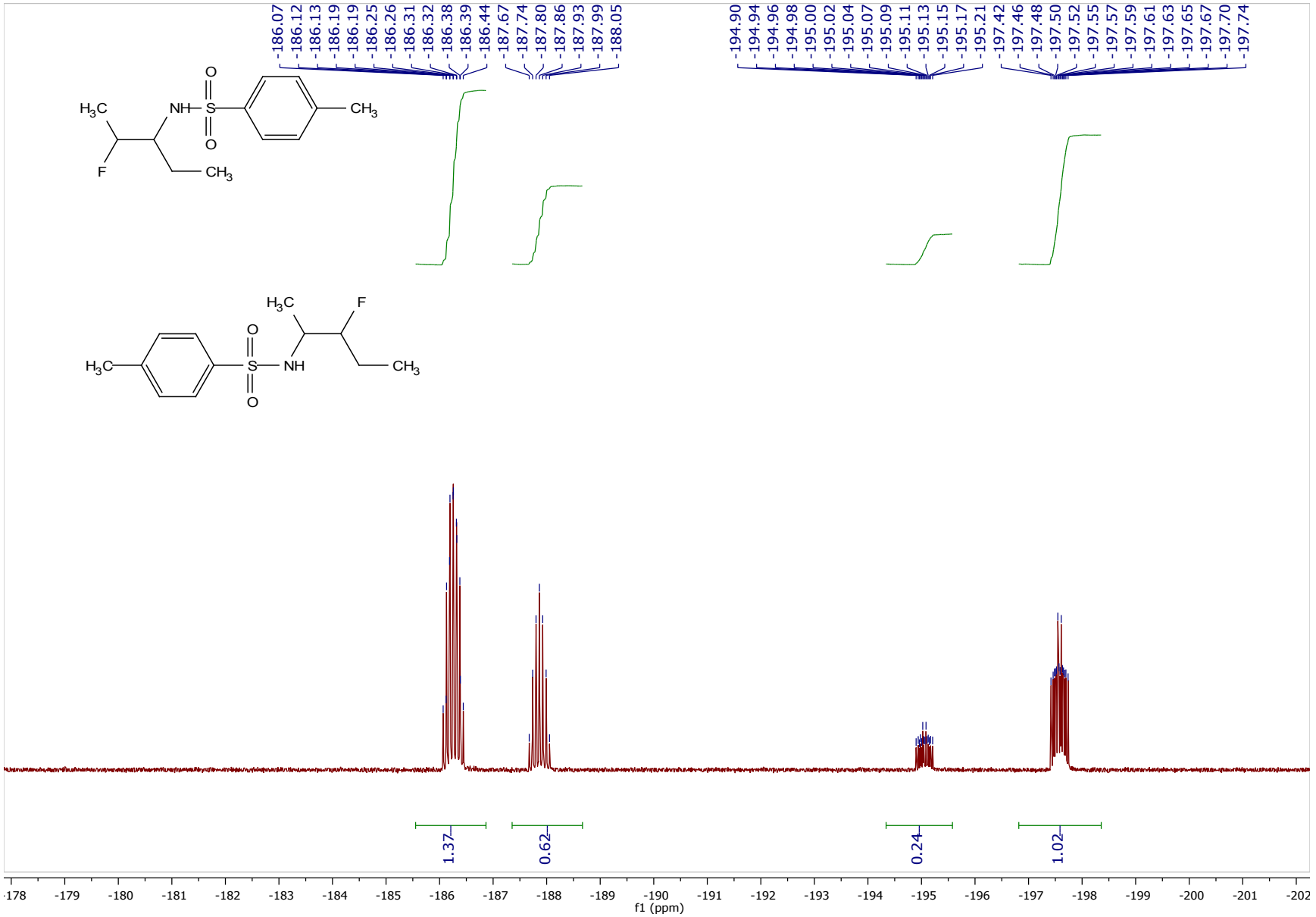
^{1}H NMR for 2h


7.76
7.74
7.31
7.29
7.27
7.26
4.85
4.58
4.55
4.48
4.46
4.45
4.33
4.31
4.29
4.26
4.24
4.19
4.17
4.14
3.43
3.39
3.29
3.24
3.19
3.13
2.42
2.41
1.55
1.45
1.43
1.37
1.26
1.24
1.19
1.07
1.01
0.95
0.91
0.87
0.78
0.76
NHTs
F
0.65
0.71
0.25
0.44
0.34
1.00
0.47
0.34
1.25
1.07
f1 (ppm)

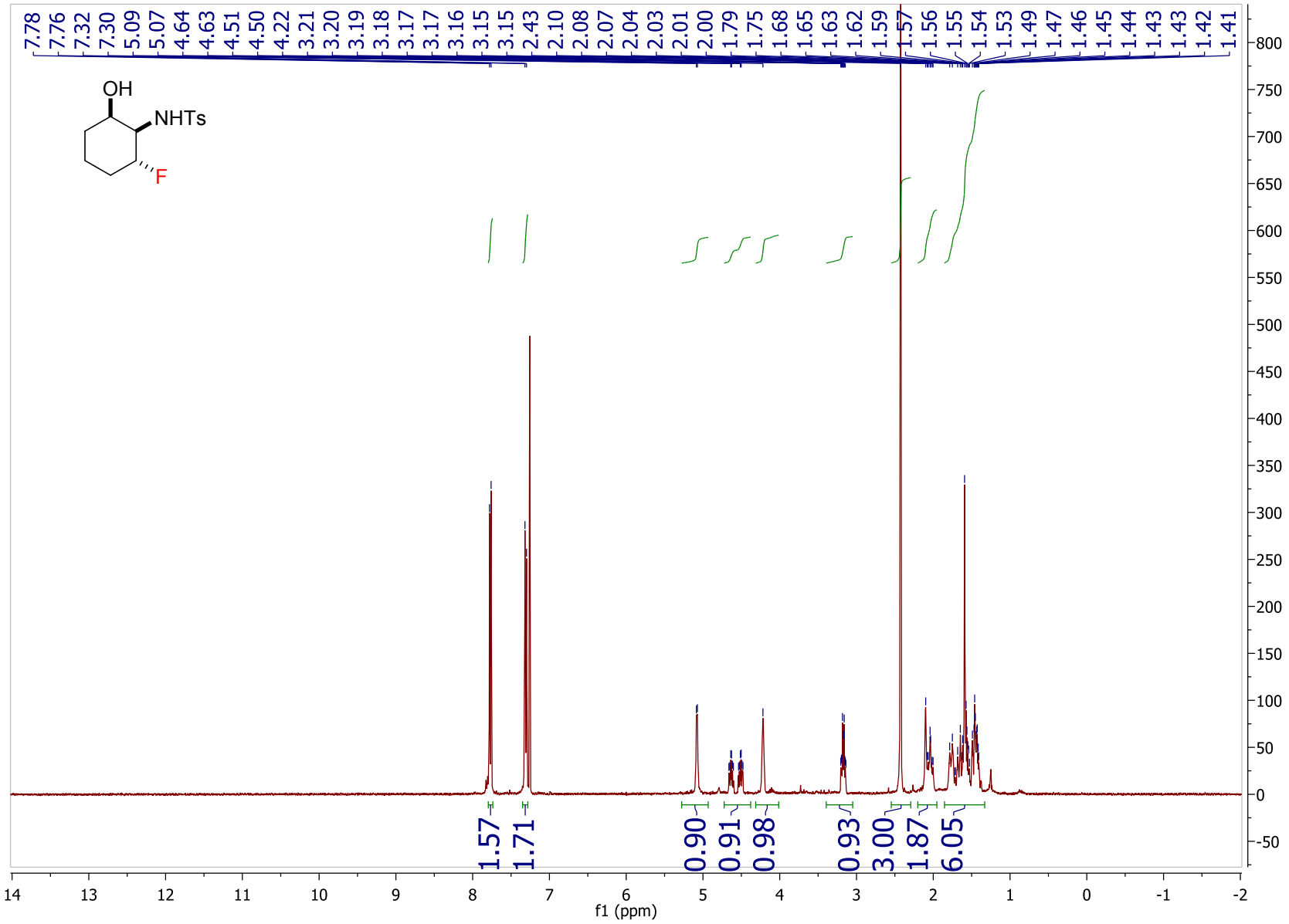
^{13}C NMR for 2h



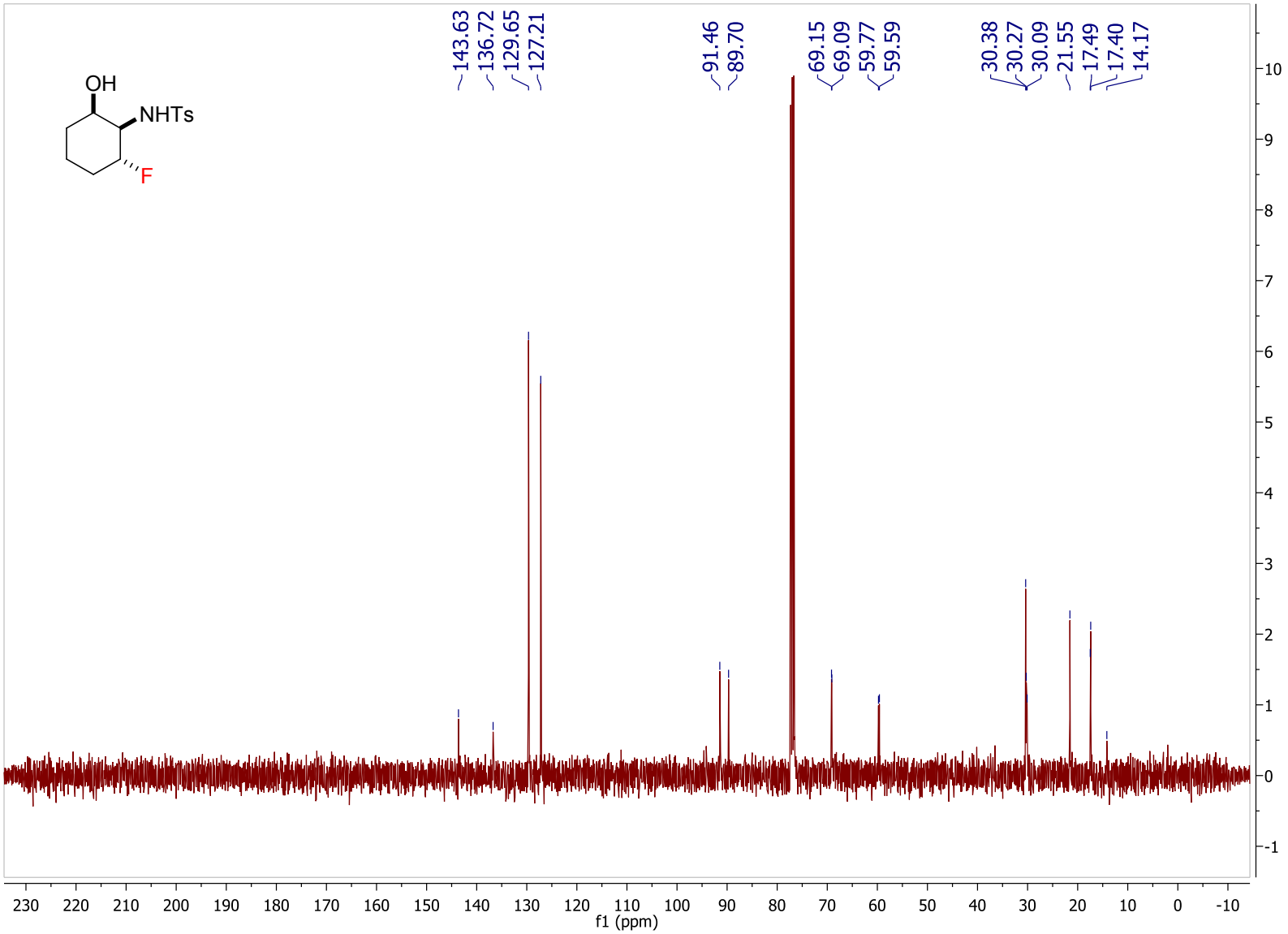
^{19}F NMR for 2h



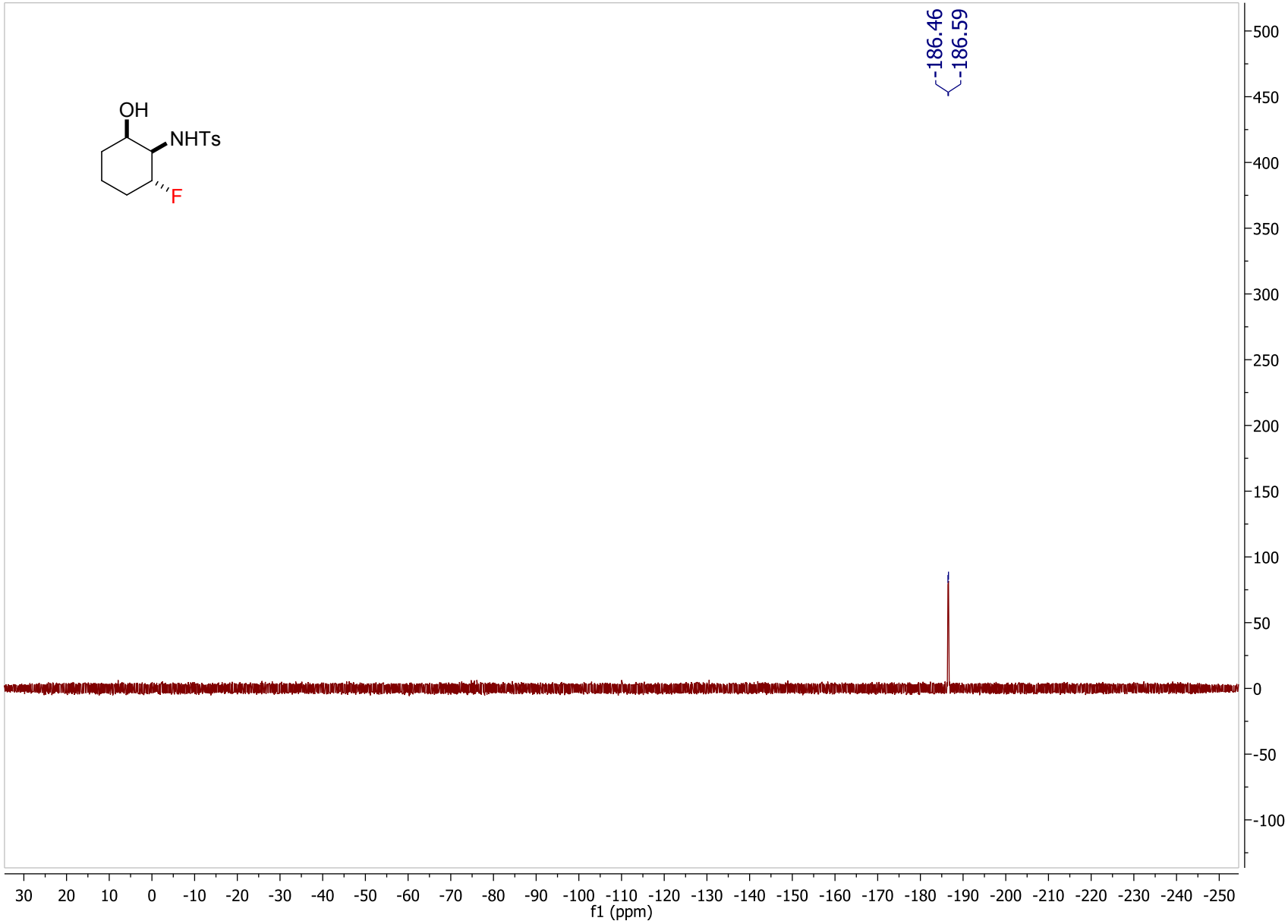
^{1}H NMR for 2l


OH
NHTs
F
7.78 7.76 7.32 7.30 5.09 5.07 4.64 4.63 4.51 4.50 4.22 3.21 3.20 3.19 3.18 3.17 3.17 3.16 3.15 3.15 2.43 2.10 2.08 2.07 2.04 2.03 2.01 2.00 1.79 1.75 1.68 1.65 1.63 1.62 1.59 1.57 1.56 1.55 1.54 1.53 1.49 1.47 1.46 1.45 1.44 1.43 1.43 1.42 1.41
1.57 1.71 0.90 0.91 0.98 0.93 3.00 1.87 6.05
f1 (ppm)

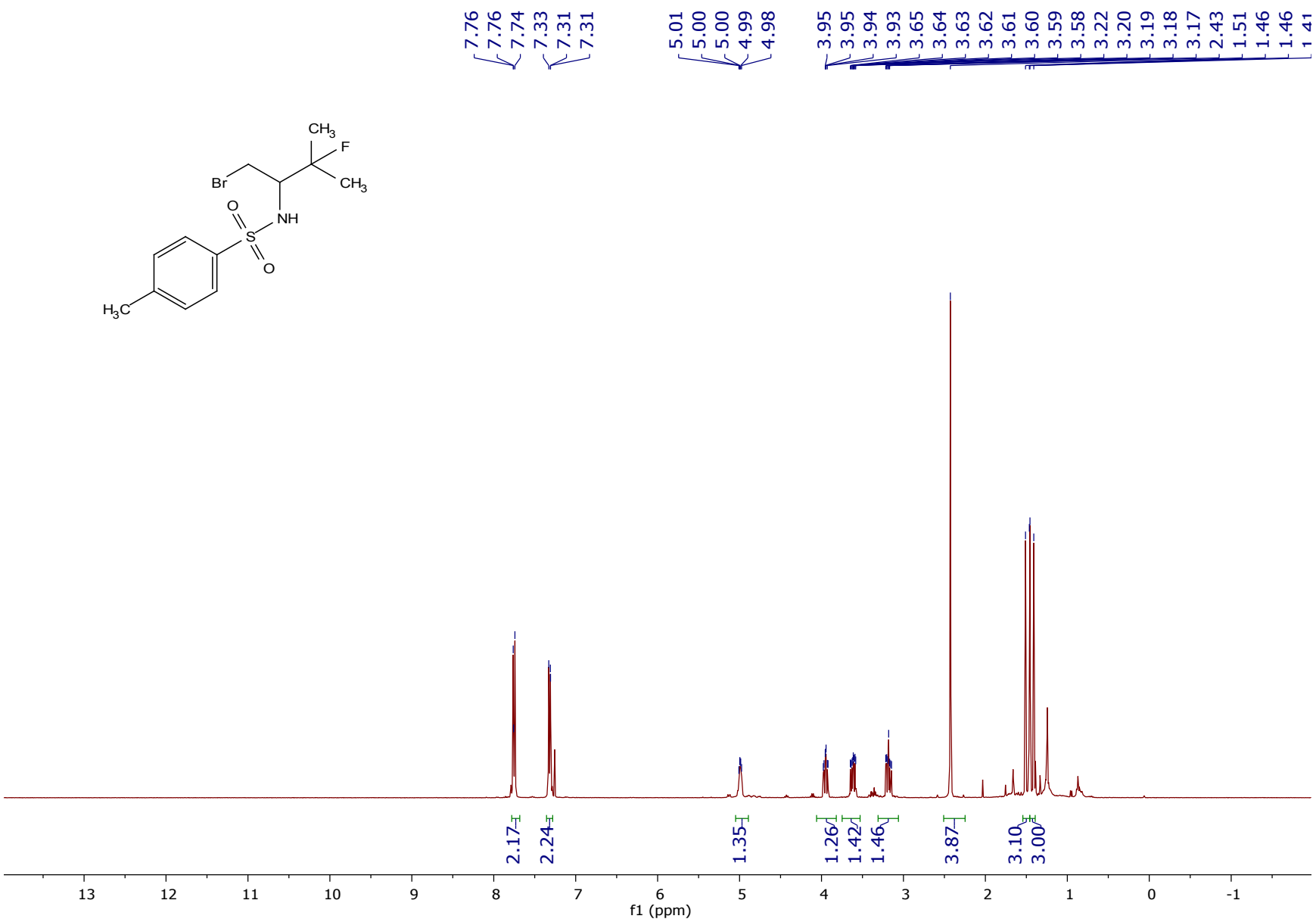
^{13}C NMR for 2l



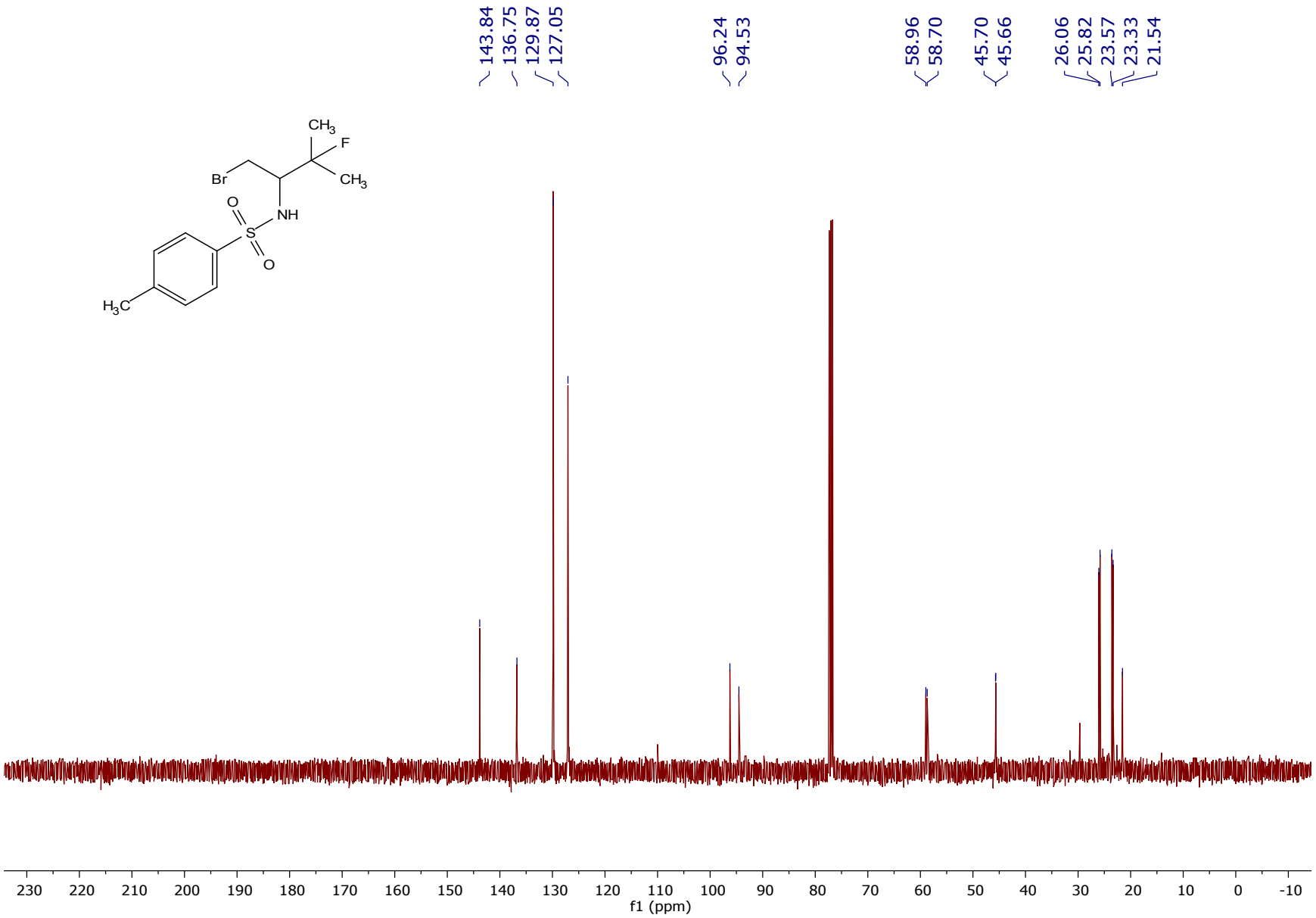
^{19}F NMR for 2l



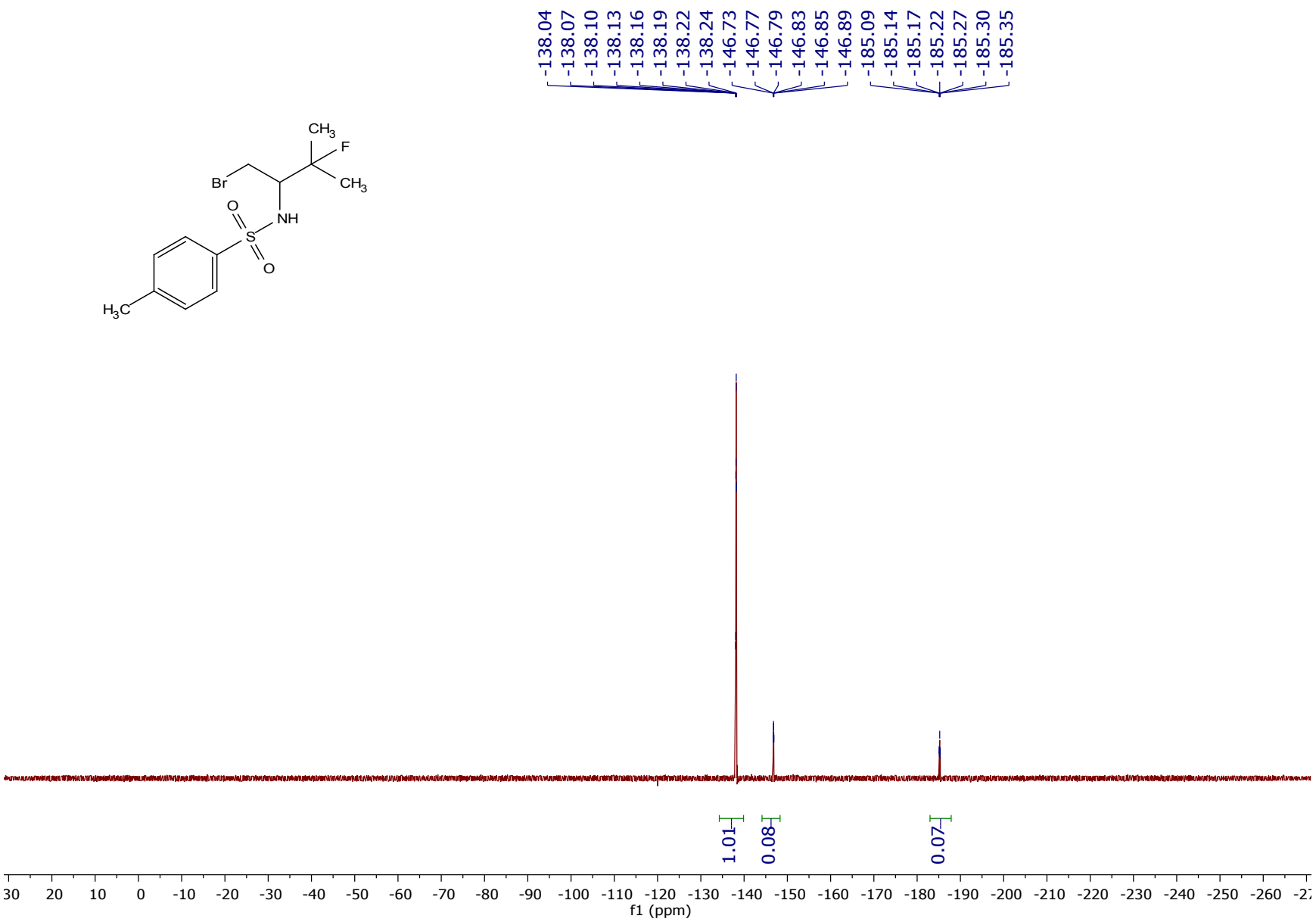
^{1}H NMR for 2m


7.76
7.76
7.74
7.33
7.31
7.31
5.01
5.00
5.00
4.99
4.98
3.95
3.95
3.94
3.93
3.65
3.64
3.63
3.62
3.61
3.60
3.59
3.58
3.22
3.20
3.19
3.18
3.17
2.43
1.51
1.46
1.46
1.41
CH3
F
Br
CH3
O
NH
S
O
H3C
2.17
2.24
1.35
1.26
1.42
1.46
3.87
3.10
3.00
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
f1 (ppm)

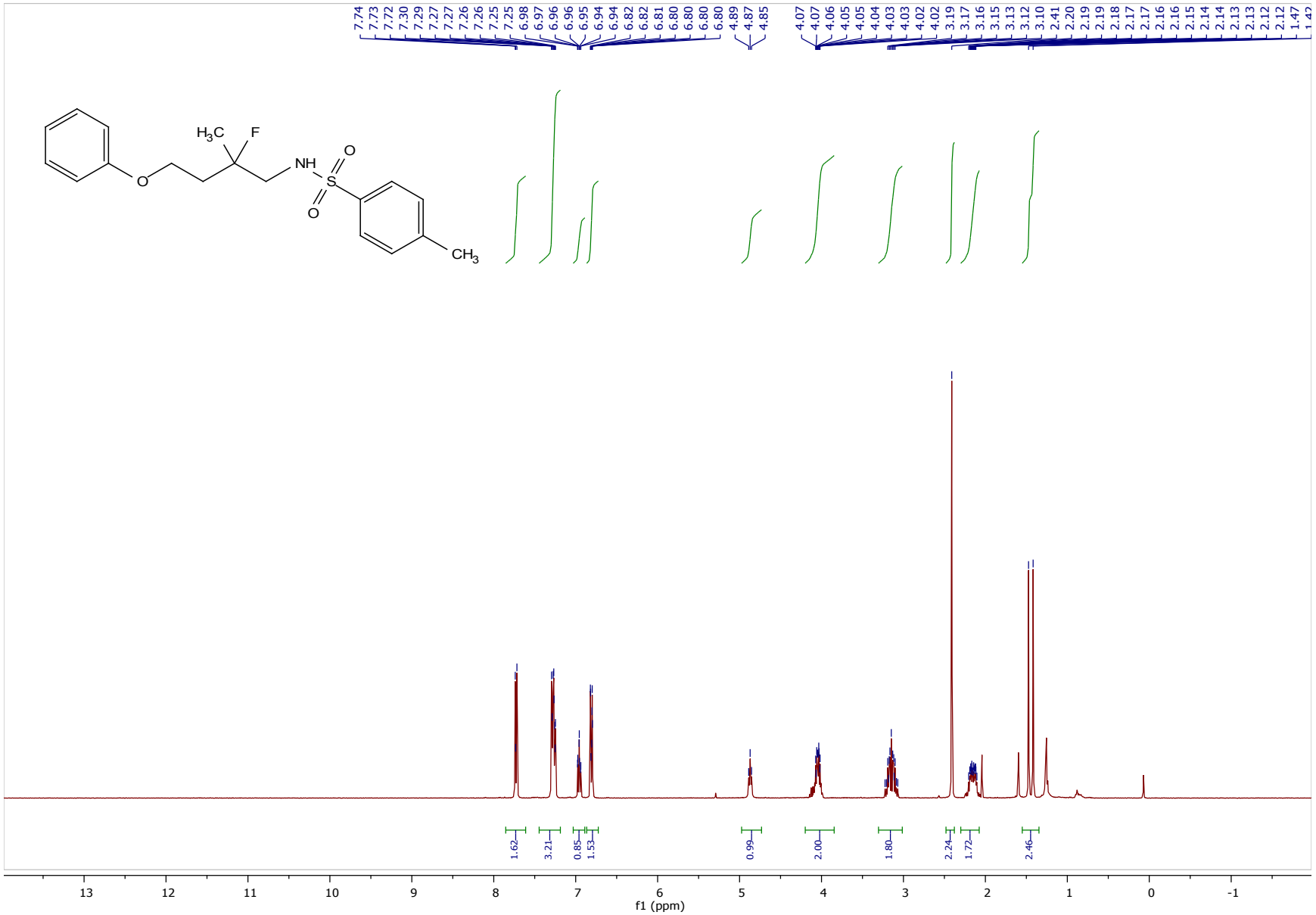
^{13}C NMR for 2m



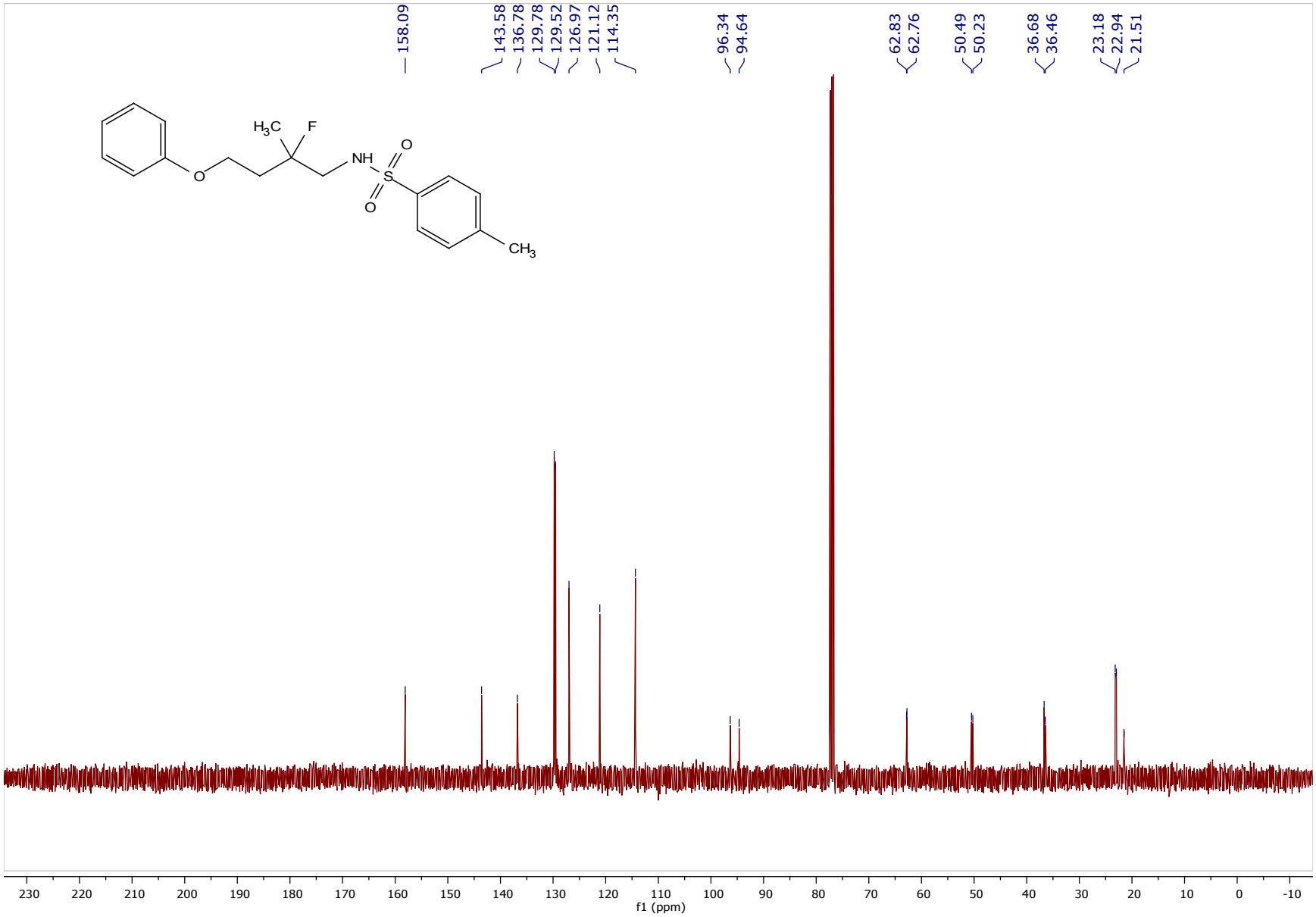
^{19}F NMR for 2m



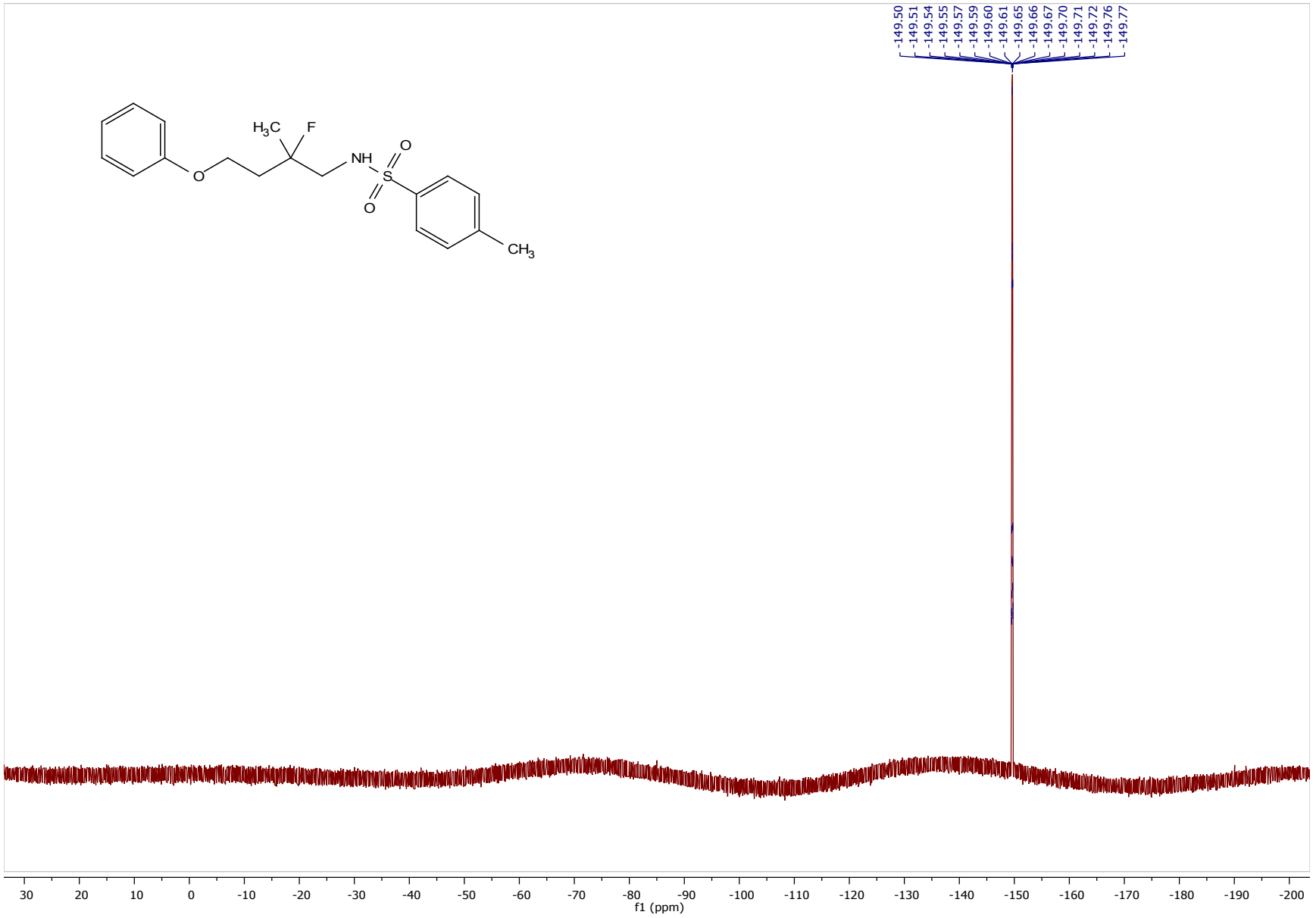
^{1}H NMR for 2n


7.74 7.73 7.72 7.30 7.29 7.27 7.27 7.26 7.26 7.25 7.25 6.98 6.97 6.96 6.96 6.95 6.94 6.94 6.82 6.82 6.81 6.80 6.80 6.80 6.80 4.89 4.87 4.85
4.07 4.07 4.06 4.05 4.05 4.04 4.03 4.03 4.02 4.02 3.19 3.17 3.16 3.15 3.13 3.12 3.10 2.41 2.20 2.19 2.19 2.18 2.17 2.17 2.16 2.16 2.15 2.14 2.14 2.13 2.13 2.12 2.12 1.47
H3C
F
NH
O
S
O
O
CH3
1.62
3.21
0.85
1.53
0.99
2.00
1.80
2.24
1.72
2.46
13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)

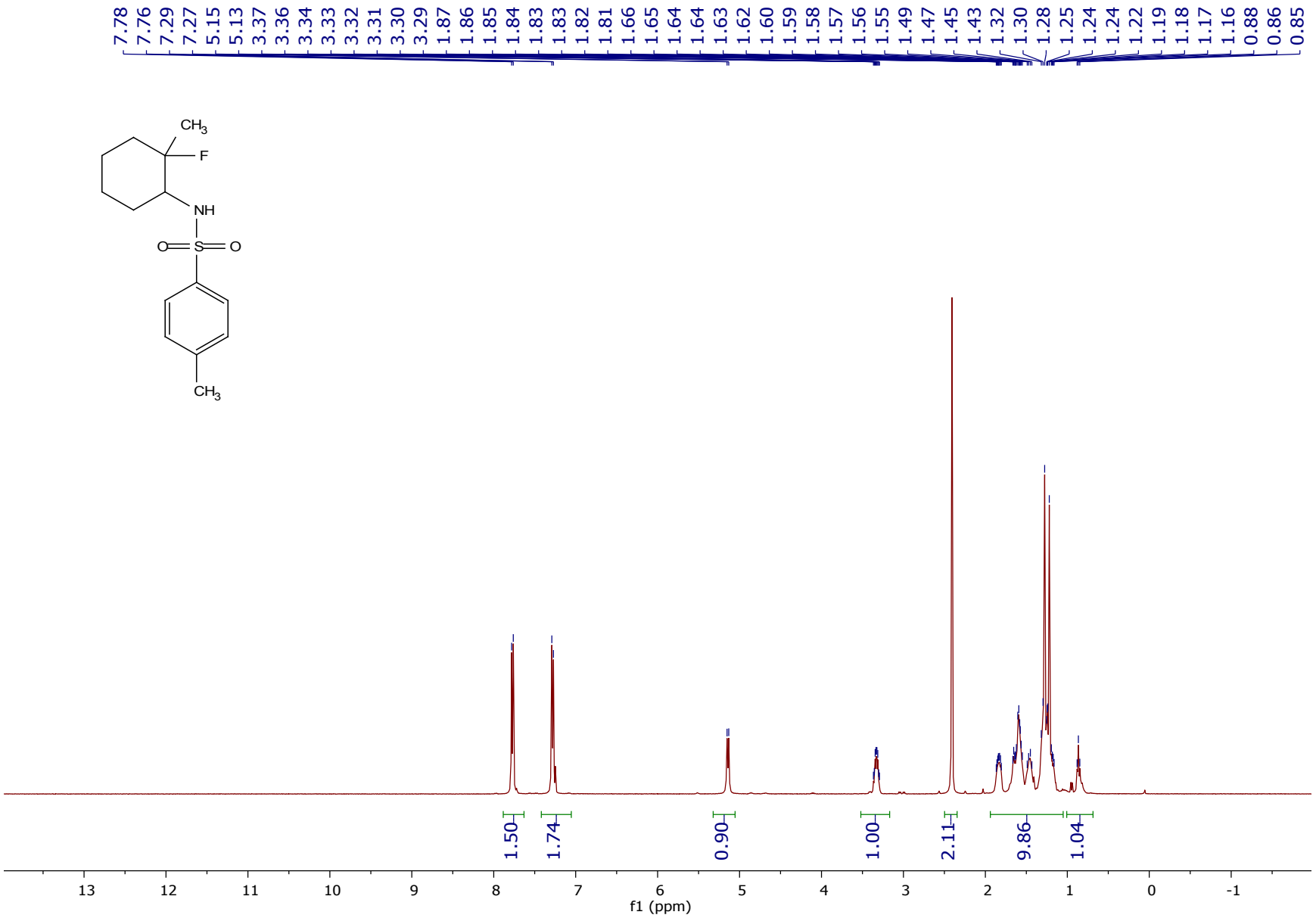
^{13}C NMR for 2n



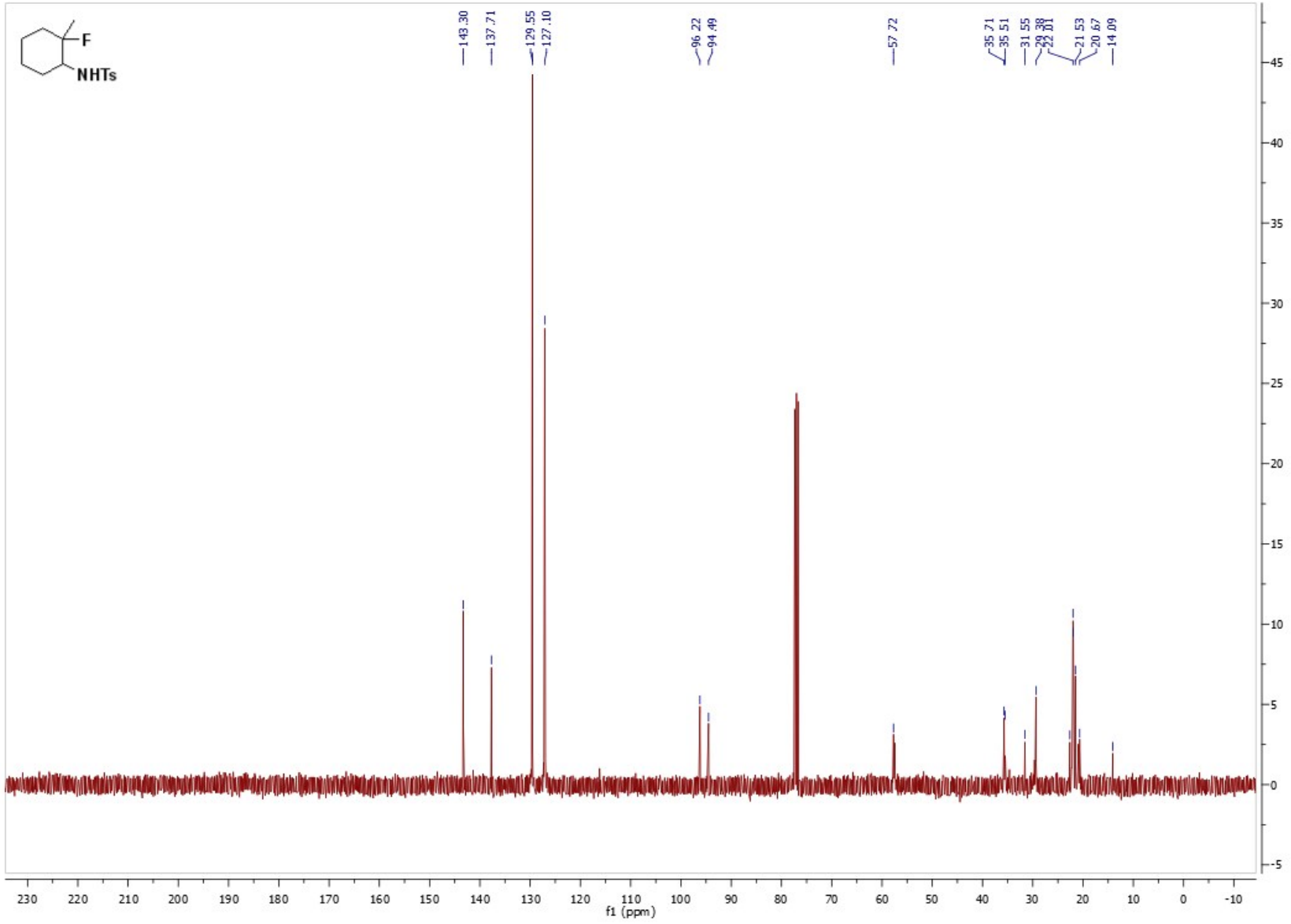
^{19}F NMR for 2m



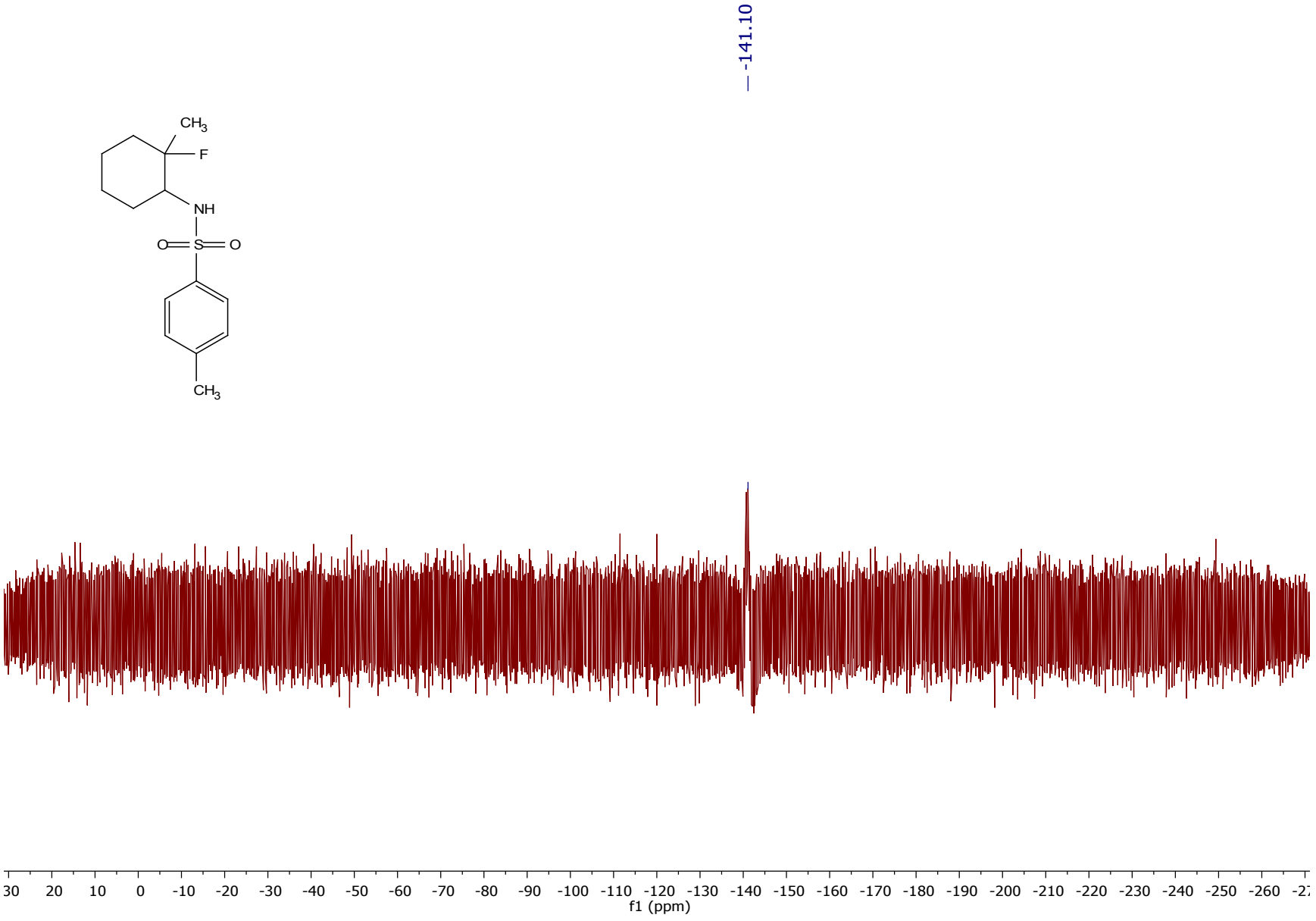
^{1}H NMR for 2n


7.78
7.76
7.29
7.27
5.15
5.13
3.37
3.36
3.34
3.33
3.32
3.31
3.30
3.29
1.87
1.86
1.85
1.84
1.83
1.83
1.82
1.81
1.66
1.65
1.64
1.64
1.63
1.62
1.60
1.59
1.58
1.57
1.56
1.55
1.49
1.47
1.45
1.43
1.32
1.30
1.28
1.25
1.24
1.24
1.22
1.19
1.18
1.17
1.16
0.88
0.86
0.85
CH3
F
NH
O
S
O
CH3
1.50
1.74
0.90
1.00
2.11
9.86
1.04
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
f1 (ppm)

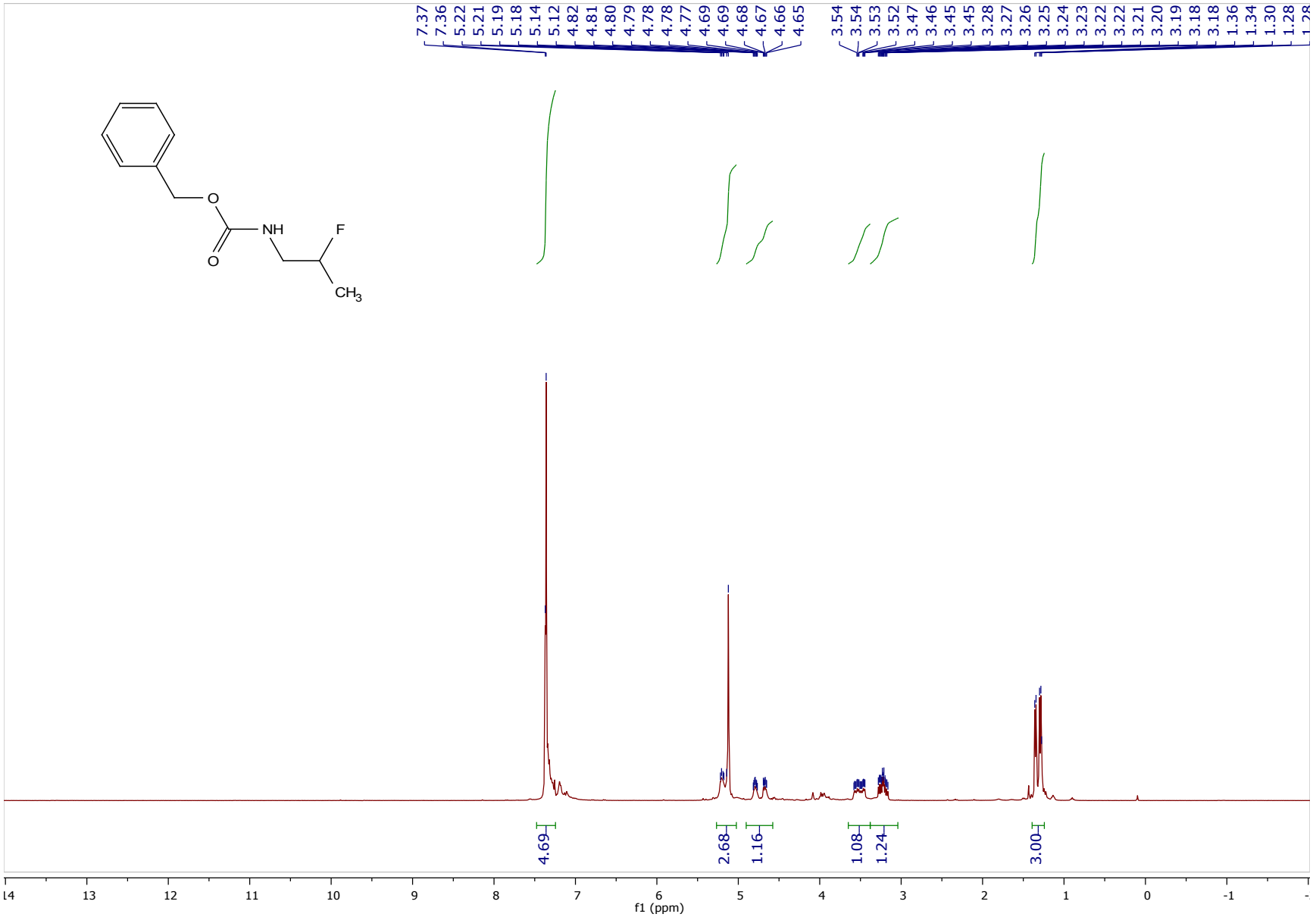
^{13}C NMR for 2n



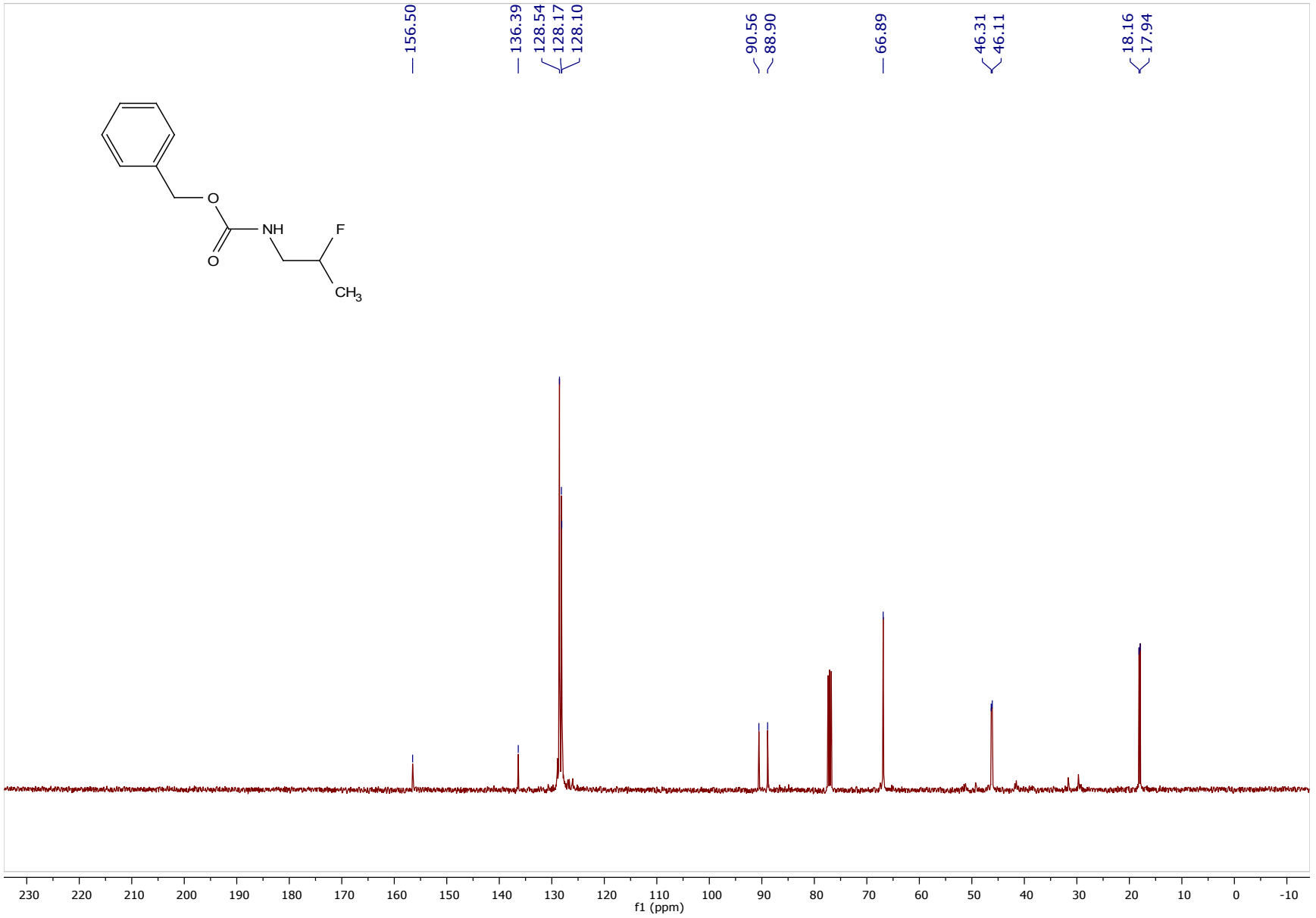
^{19}F NMR of 2n


-141.10
CH3
F
NH
O
S
O
CH3
30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220 -230 -240 -250 -260
f1 (ppm)

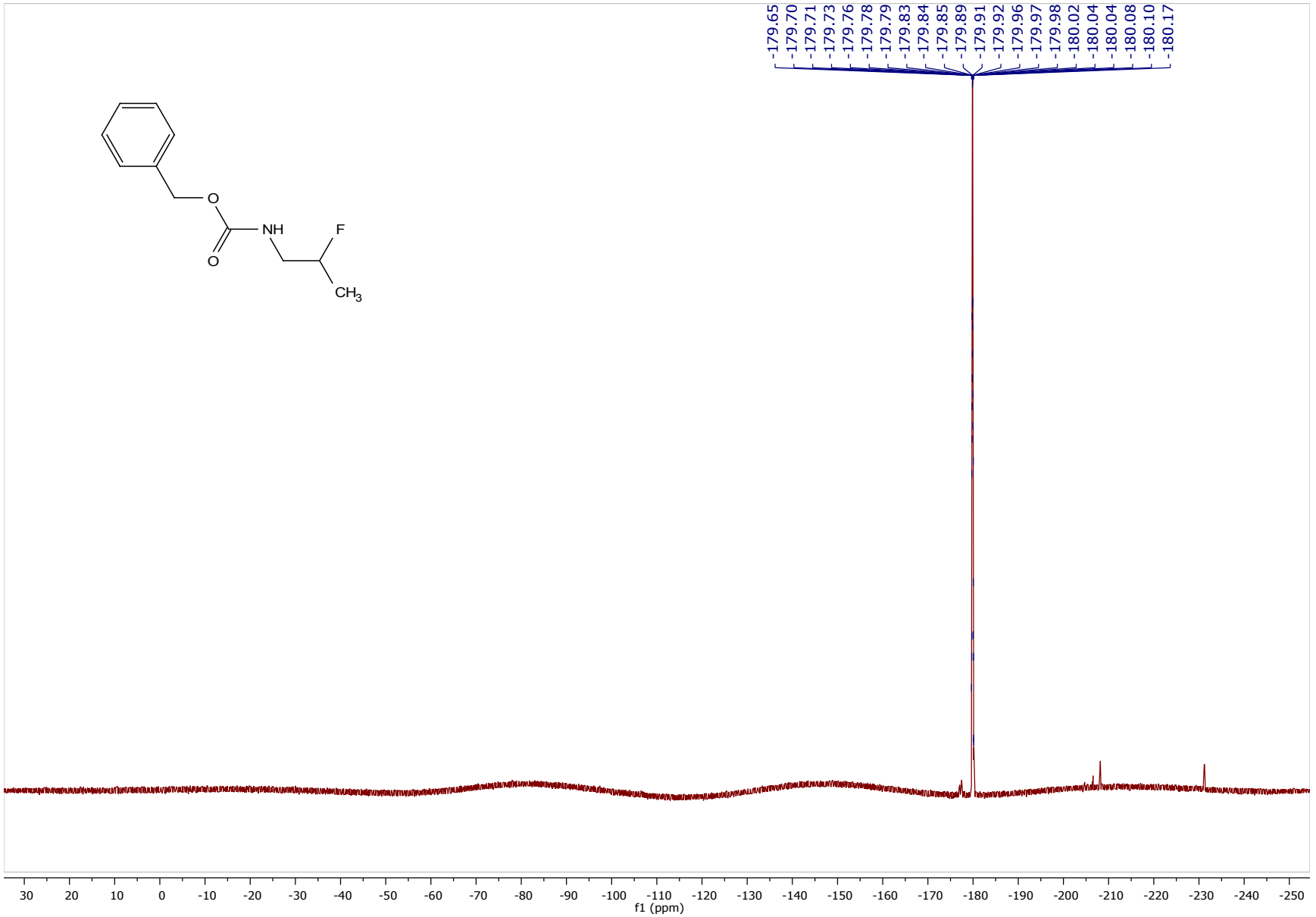
^{1}H NMR of 2o


7.37
7.36
5.22
5.21
5.19
5.18
5.14
5.12
4.82
4.81
4.80
4.79
4.78
4.78
4.77
4.69
4.69
4.68
4.67
4.66
4.65
3.54
3.54
3.53
3.52
3.47
3.46
3.45
3.45
3.28
3.27
3.26
3.25
3.24
3.23
3.22
3.22
3.21
3.20
3.19
3.18
3.18
1.36
1.34
1.30
1.28
O
NH
F
O
CH3
4.69
2.68
1.16
1.08
1.24
3.00
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
f1 (ppm)

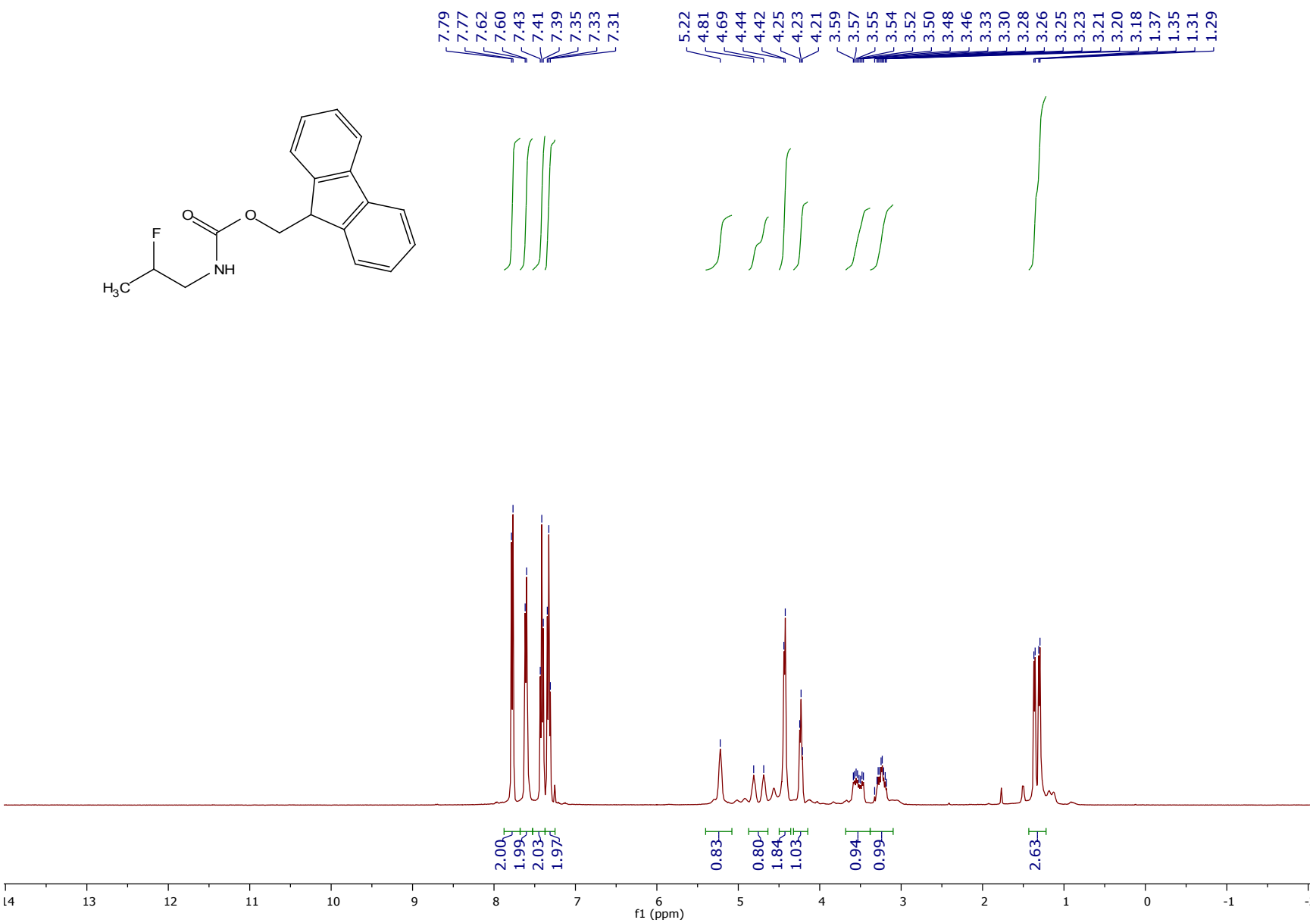
^{13}C NMR of 2o


156.50
136.39
128.54
128.17
128.10
90.56
88.90
66.89
46.31
46.11
18.16
17.94
O
NH
F
O
CH3
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

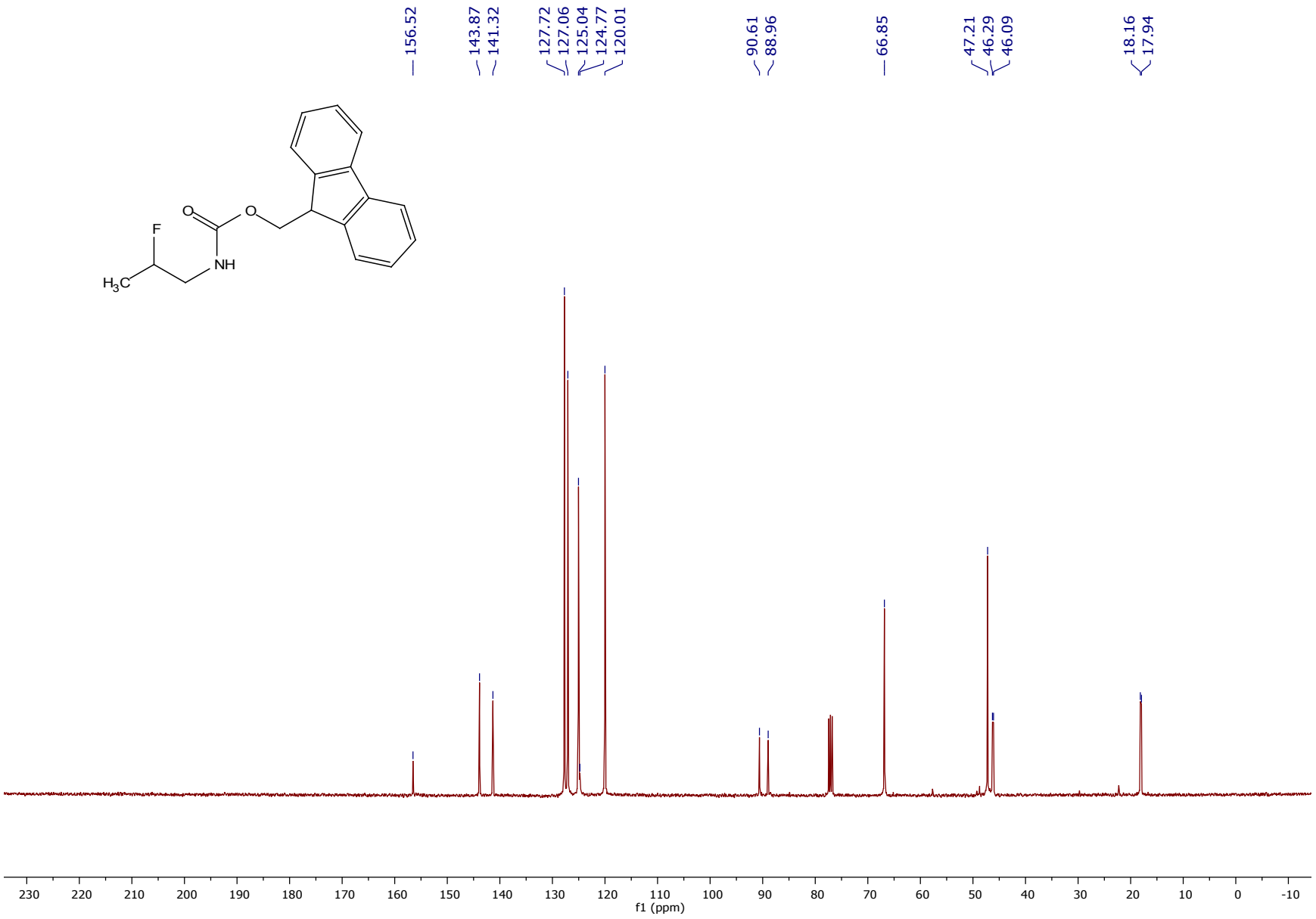
^{19}F NMR of 2o


-179.65
-179.70
-179.71
-179.73
-179.76
-179.78
-179.79
-179.83
-179.84
-179.85
-179.89
-179.91
-179.92
-179.96
-179.97
-179.98
-180.02
-180.04
-180.04
-180.08
-180.10
-180.17
O
NH
F
O
CH3
30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220 -230 -240 -250
f1 (ppm)

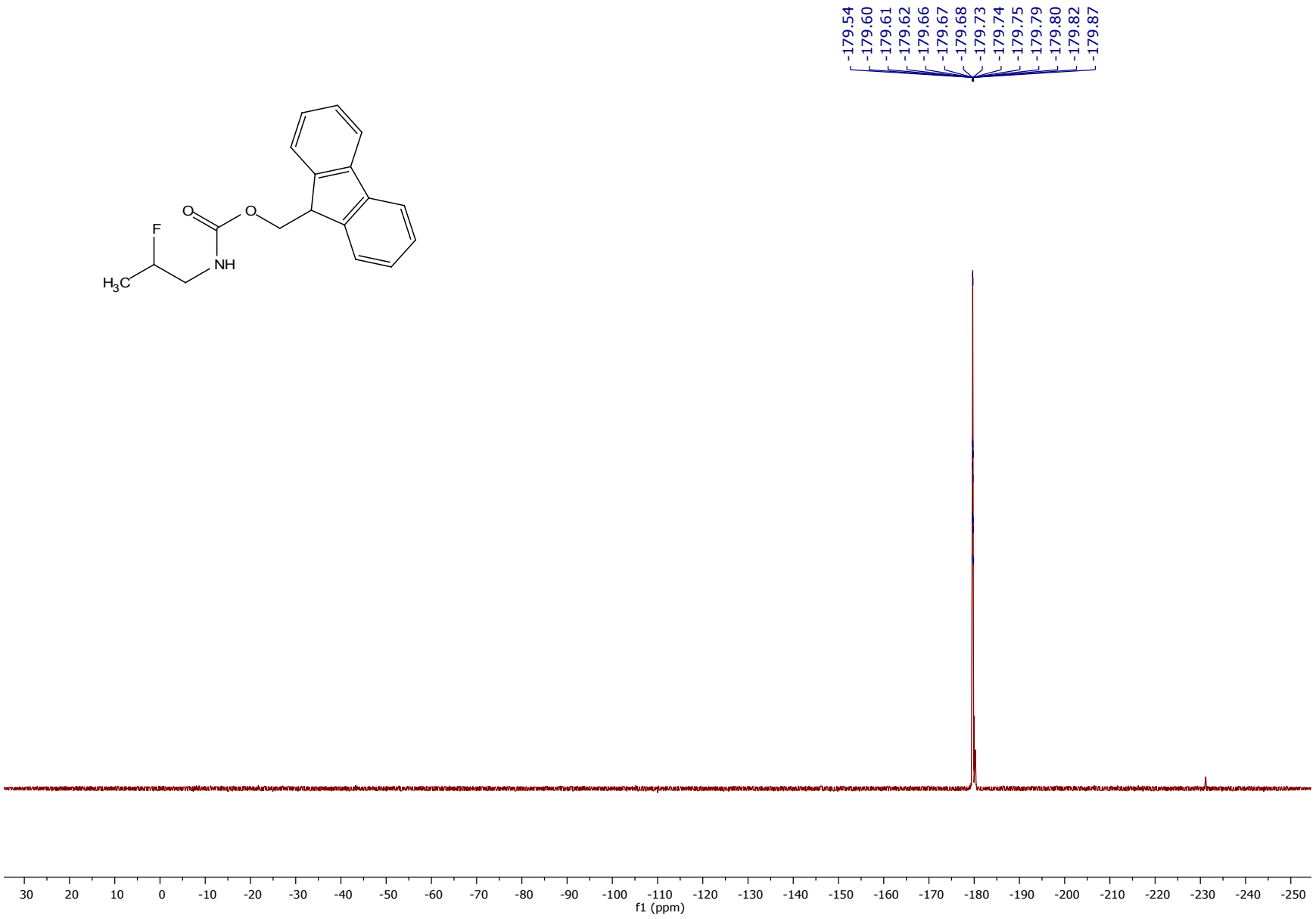
^{1}H NMR for 2p


7.79
7.77
7.62
7.60
7.43
7.41
7.39
7.35
7.33
7.31
5.22
4.81
4.69
4.44
4.42
4.25
4.23
4.21
3.59
3.57
3.55
3.54
3.52
3.50
3.48
3.46
3.33
3.30
3.28
3.26
3.25
3.23
3.21
3.20
3.18
1.37
1.35
1.31
1.29
O
O
F
NH
H3C
2.00
1.99
2.03
1.97
0.83
0.80
1.84
1.03
0.94
0.99
2.63
f1 (ppm)

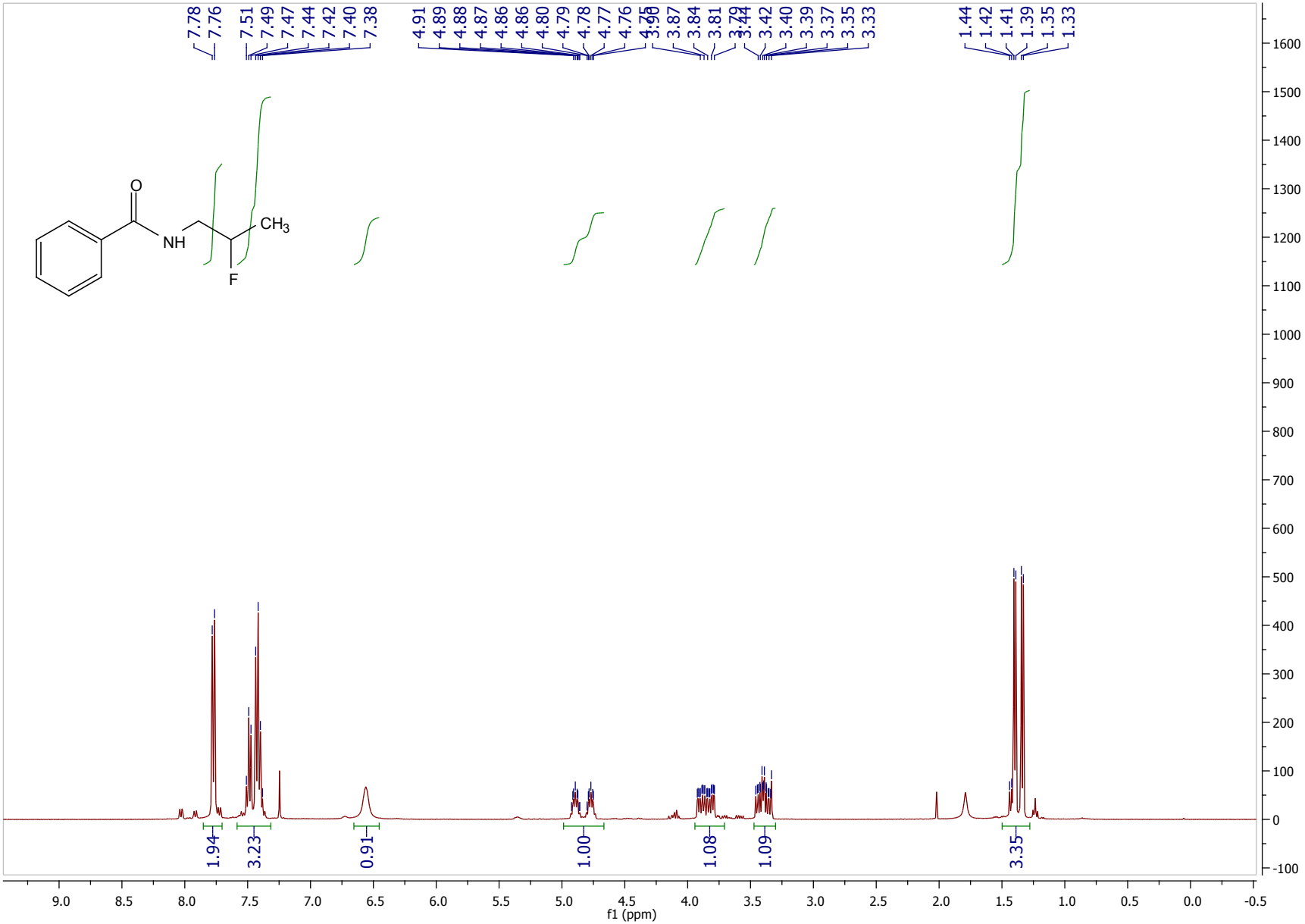
^{13}C NMR for 2p



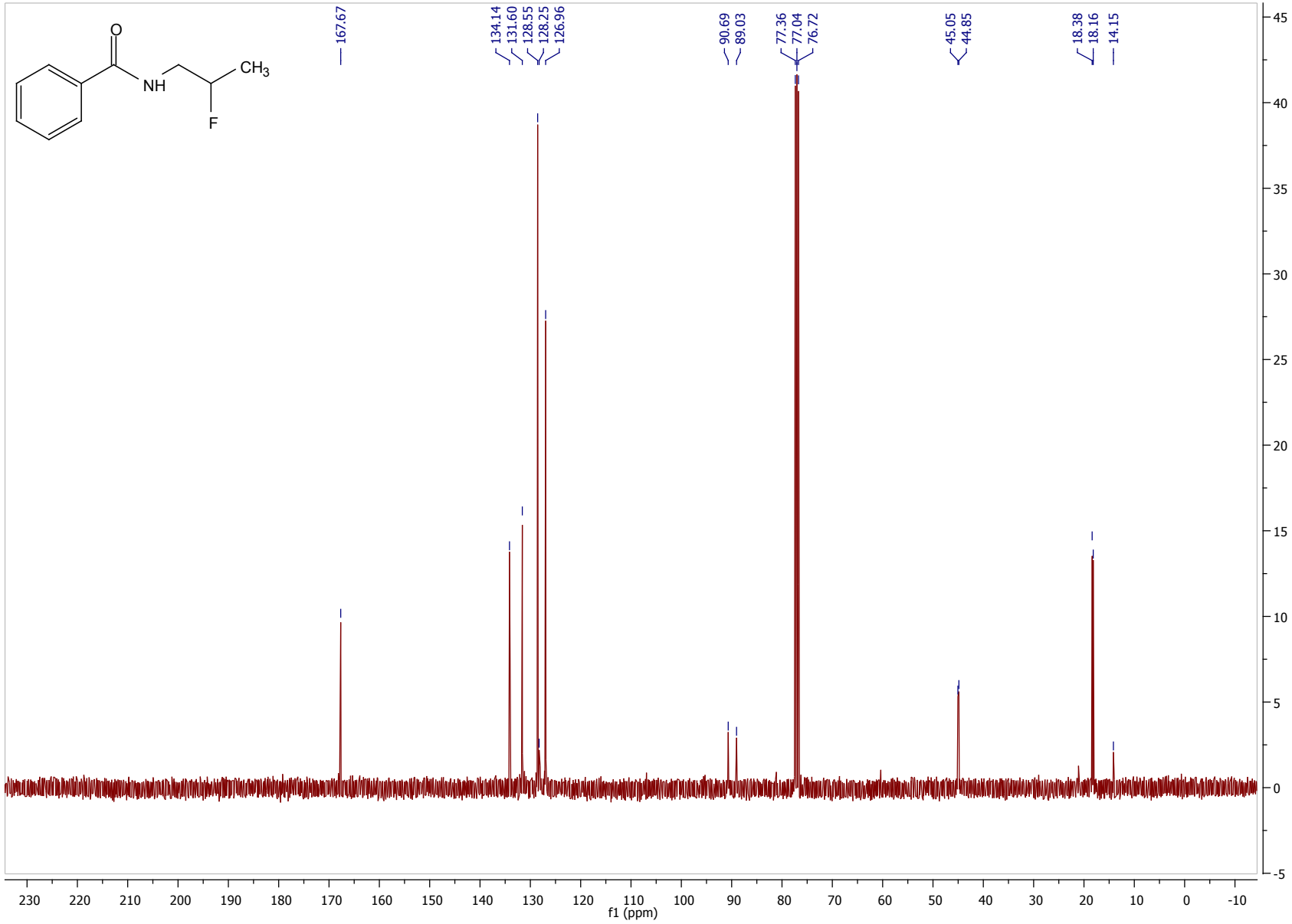
^{19}F NMR for 2p



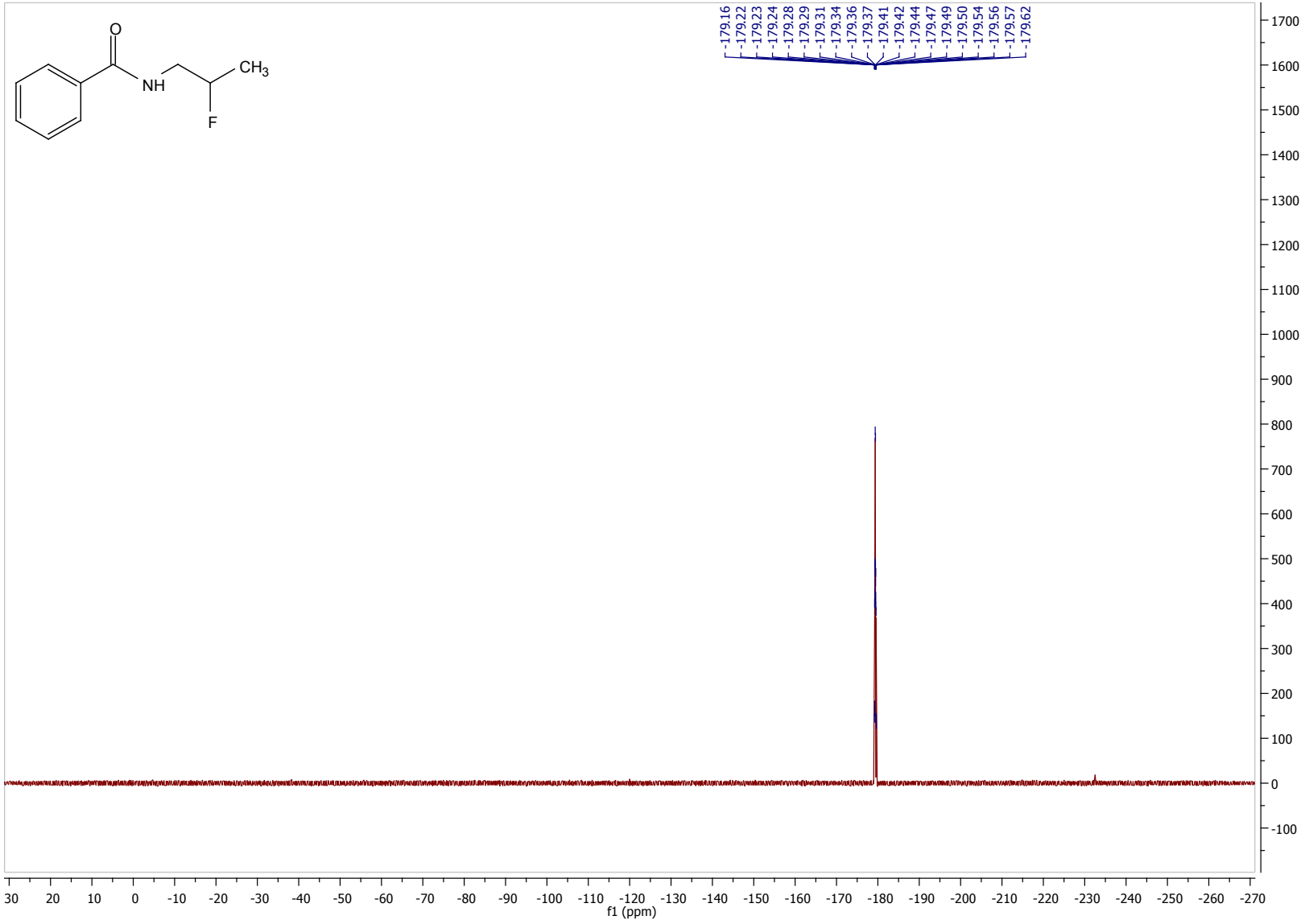
^{1}H NMR for 2q


7.78
7.76
7.51
7.49
7.47
7.44
7.42
7.40
7.38
4.91
4.89
4.88
4.87
4.86
4.86
4.80
4.79
4.78
4.77
4.76
3.87
3.84
3.81
3.42
3.40
3.39
3.37
3.35
3.33
1.44
1.42
1.41
1.39
1.35
1.33
O
NH
CH3
F
1.94
3.23
0.91
1.00
1.08
1.09
3.35
f1 (ppm)

^{13}C NMR for 2q

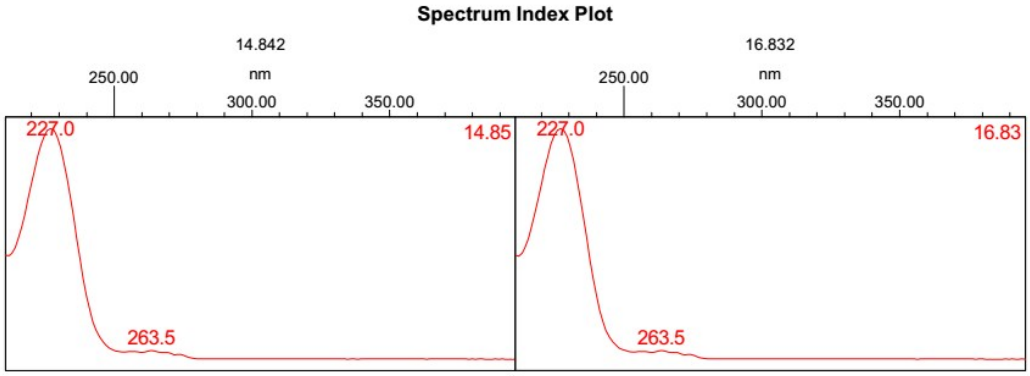


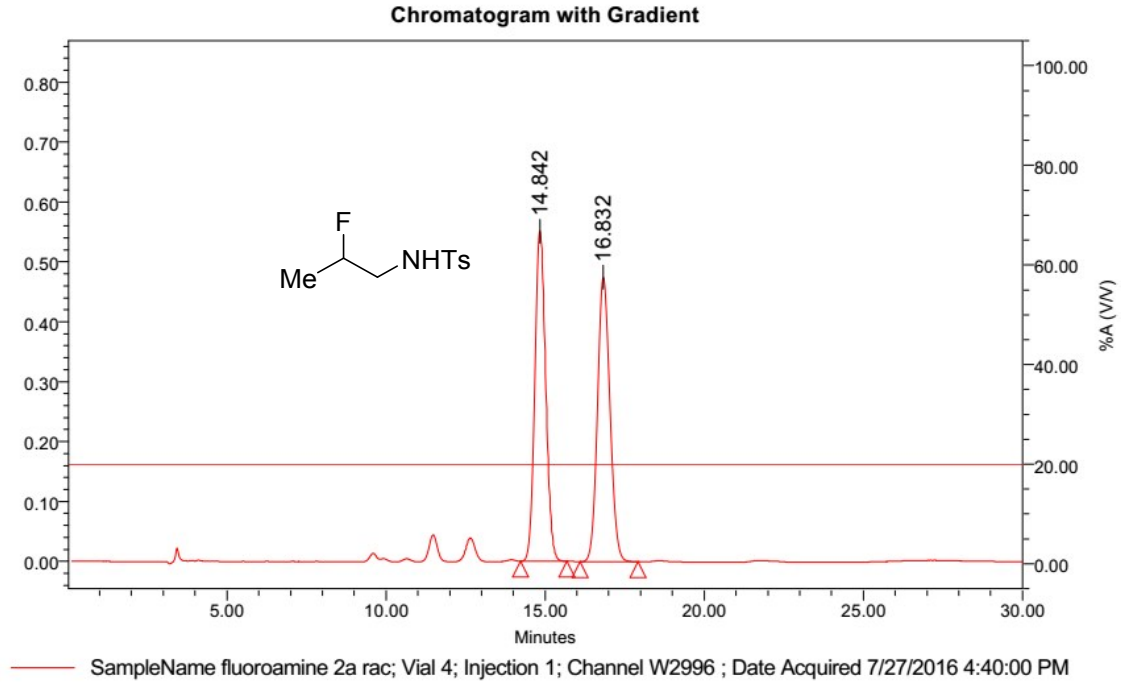
^{19}F NMR for 2q



7. HPLC Traces

HPLC traces for ***rac*-1a**



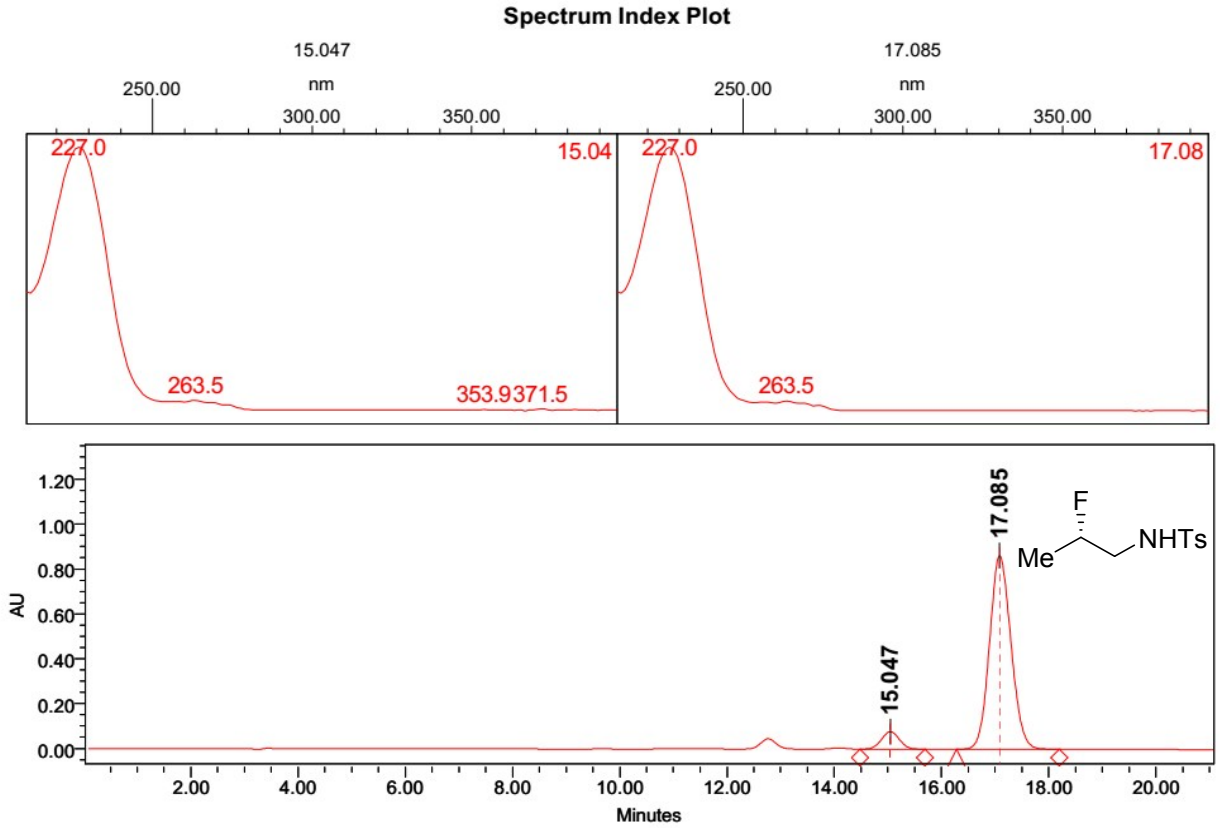


Peak Results

	Retention time (min)	Height	Width (sec)	Area	% Area	Peak Type	Processed Channel Descr.
1	14.842	551965	86.955	12954070	49.83	Unknown	PDA 214.0 nm
2	16.832	475511	108.945	13044909	50.17	Unknown	PDA 214.0 nm

Chromatography conditions: Waters 600 HPLC pump, Waters 2996 PDA detector, CHIRALPAK®IC column (5 μm, 4.6 mm I.D. × 250 mm L), 20% isopropanol/80% hexane, 1 m L/min, λ= 214 nm

HPLC traces for **(*S*)-1a**



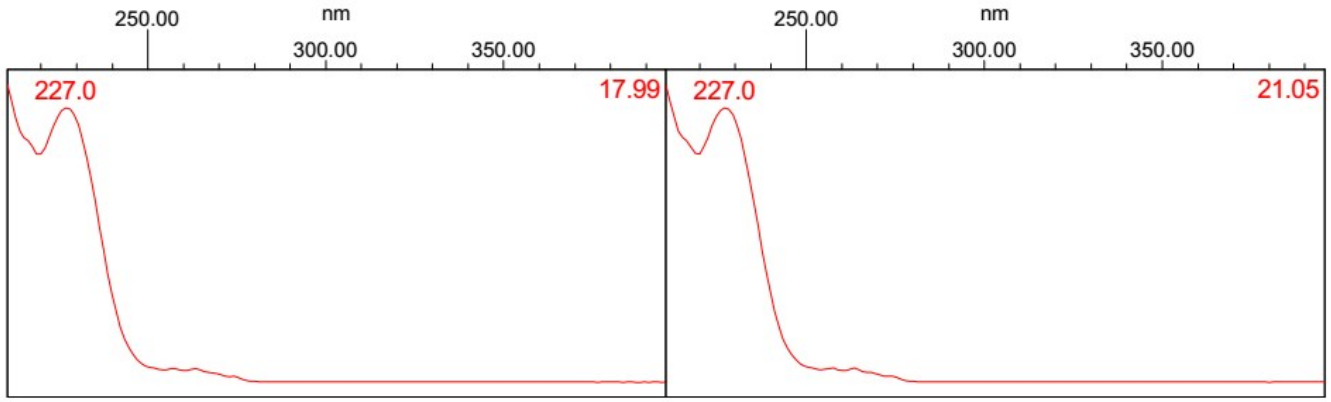
SampleName ZL654; Vial 1; Injection 1; Date Acquired 8/4/2016 3:12:33 PM

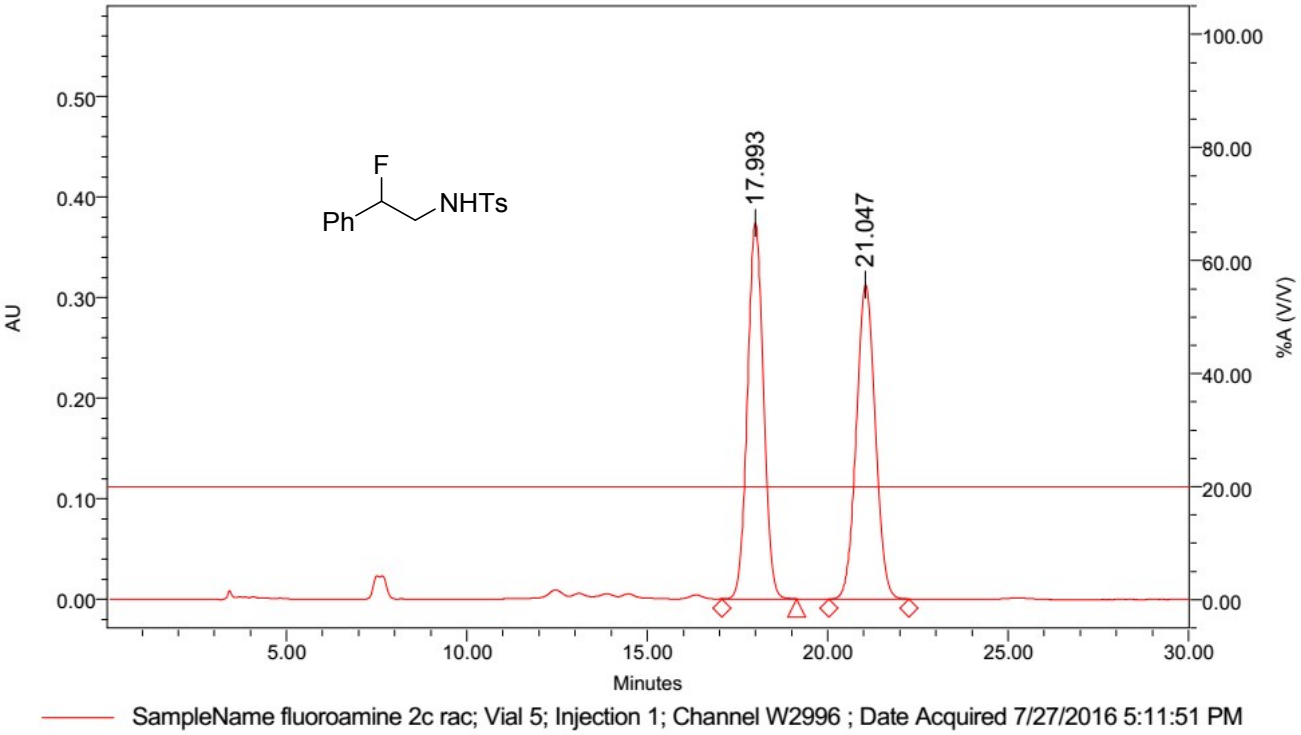
Peak Results

	Retention time (min)	Height	Width (sec)	Area	% Area	Processed Channel Descr.
1	15.047	78393	72.980	1862127	7.18	PDA 227.0 nm
2	17.085	864127	114.970	24077050	92.82	PDA 227.0 nm

Chromatography conditions: Waters 600 HPLC pump, Waters 2996 PDA detector, CHIRALPAK®IC column (5 μm, 4.6 mm I.D. × 250 mm L), 20% isopropanol/80% hexane, 1 m L/min, λ= 214 nm

HPLC Traces for ***rac*-2c**



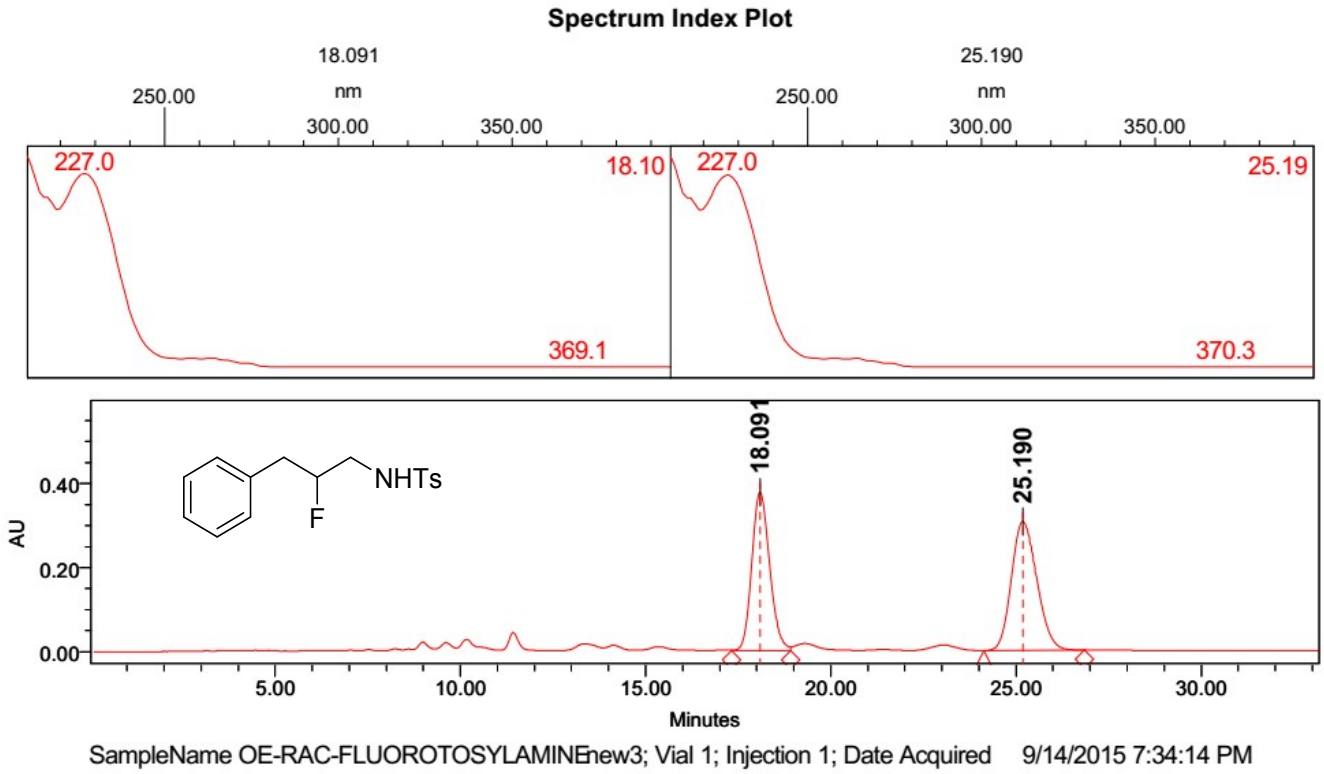


Peak Results

	Retention time (min)	Height	Width (sec)	Area	% Area	Peak Type	Processed Channel Descr.
1	17.993	374387	123.935	11415266	49.89	Unknown	PDA 227.0 nm
2	21.047	312683	132.930	11463394	50.11	Unknown	PDA 227.0 nm

Chromatography conditions: Waters 600 HPLC pump, Waters 2996 PDA detector, CHIRALPAK®IC column (5 μm, 4.6 mm I.D. × 250 mm L), 20% isopropanol/80% hexane, 1 m L/min, λ= 227 nm

HPLC Traces for ***rac*-2d**



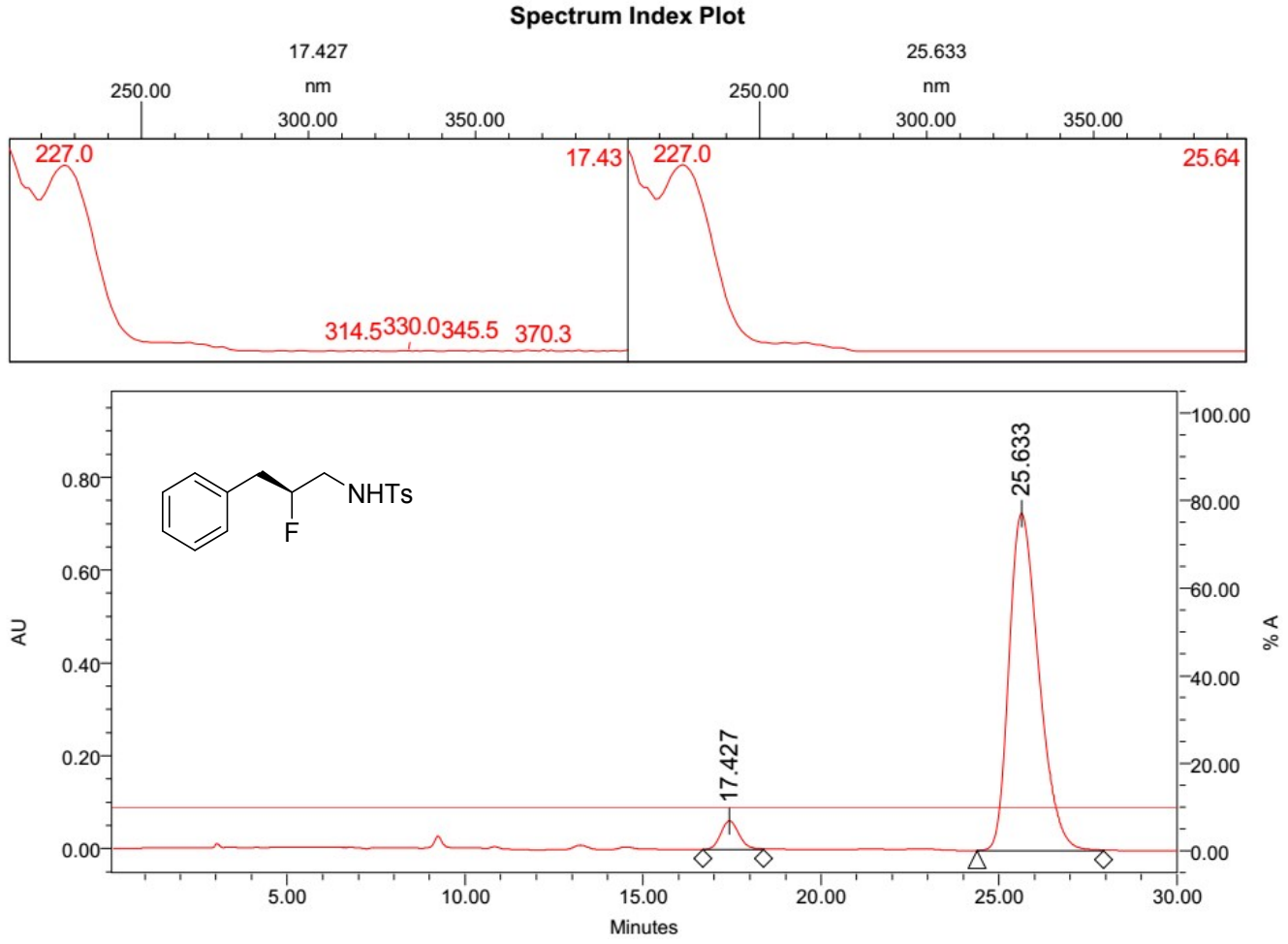
SampleName OE-RAC-FLUOROTOSYLAMINEnew3; Vial 1; Injection 1; Date Acquired 9/14/2015 7:34:14 PM

Peak Results

	Retention time (min)	Peak Type	Width (sec)	Height	Area	% Area	Processed Channel Descr.
1	18.091	Unknown	94.960	376461	12701597	46.54	PDA 227.0 nm
2	25.190	Unknown	162.935	306614	14589820	53.46	PDA 227.0 nm

Chromatography conditions: Waters 600 HPLC pump, Waters 2996 PDA detector, CHIRALCEL®OD-H column (5 μm, 4.6 mm I.D. × 250 mm L), 10% isopropanol/90% hexane, 1 mL/min, λ = 214 nm

HPLC Traces for **(*S*)-2d**



Peak Results

	Retention time (min)	Peak Type	Width (sec)	Height	Area	% Area	Processed Channel Descr.
1	17.428	Unknown	124.945	55380	1999027	4.95	PDA 214.0 nm
2	25.634	Unknown	200.920	656651	38417580	95.05	PDA 214.0 nm

Chromatography conditions: Waters 600 HPLC pump, Waters 2996 PDA detector, CHIRALCEL®OD-H column (5 μm, 4.6 mm I.D. × 250 mm L), 10% isopropanol/90% hexane, 1 mL/min, λ = 214 nm

8. X-Ray Crystallography Data of 2k (CCDC 1490050)

Table 1. Crystal data and structure refinement for gbh33rta.

Identification code	gbh33rta	
Empirical formula	C26 H36 F2 N2 O6 S2	
Formula weight	574.69	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 6.3281(4) Å	α= 105.544(6)°.
	b = 12.8693(9) Å	β= 93.657(5)°.
	c = 17.8671(10) Å	γ = 100.435(5)°.
Volume	1368.94(15) $Å^3$	
Z	2	
Density (calculated)	1.394 Mg/m^3	
Absorption coefficient	0.252 mm^{-1}	
F(000)	608	
Crystal color, habit	colorless plate	
Crystal size	0.40 x 0.11 x 0.05 mm^3	
Theta range for data collection	3.37 to 25.68°.	
Index ranges	-7<=h<=7, -15<=k<=15, -21<=l<=21	
Reflections collected	18222	
Independent reflections	5177 [R(int) = 0.0359]	
Completeness to theta = 25.68°	99.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.000 and 0.976	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5177 / 0 / 476	
Goodness-of-fit on F^2	1.030	
Final R indices [I>2sigma(I)]	R1 = 0.0396, wR2 = 0.0729	
R indices (all data)	R1 = 0.0601, wR2 = 0.0811	
Largest diff. peak and hole	0.281 and -0.289 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for gbh33rta. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
S(1)	6164(1)	5000(1)	2554(1)	41(1)
O(1)	7080(3)	5209(1)	3345(1)	57(1)
O(2)	3897(2)	4976(1)	2404(1)	55(1)
O(3)	6900(2)	7955(1)	2058(1)	45(1)
F(1)	9965(2)	5459(1)	965(1)	66(1)
N(1)	7477(3)	5932(1)	2226(1)	40(1)
C(1)	6862(3)	6075(2)	1461(1)	37(1)
C(2)	5566(3)	6984(2)	1533(1)	39(1)
C(3)	5008(4)	7157(2)	745(2)	52(1)
C(4)	7014(5)	7393(2)	347(2)	58(1)
C(5)	8279(5)	6478(2)	271(2)	57(1)
C(6)	8850(4)	6329(2)	1057(1)	42(1)
C(7)	6582(3)	3708(2)	1999(1)	37(1)
C(8)	8568(4)	3609(2)	1740(2)	50(1)
C(9)	8870(4)	2588(2)	1323(2)	55(1)
C(10)	7241(4)	1661(2)	1161(1)	52(1)
C(11)	5278(4)	1776(2)	1436(1)	53(1)
C(12)	4941(4)	2791(2)	1850(1)	44(1)
C(13)	7626(5)	551(2)	707(2)	86(1)
S(2)	2583(1)	9681(1)	2453(1)	41(1)
O(4)	4826(2)	9663(1)	2604(1)	55(1)
O(5)	1651(3)	9482(1)	1664(1)	55(1)
O(6)	1795(2)	6746(1)	2964(1)	44(1)
F(2)	-1399(2)	9256(1)	3991(1)	69(1)
N(2)	1211(3)	8761(1)	2777(1)	45(1)
C(14)	1756(3)	8628(2)	3549(1)	41(1)
C(15)	3068(3)	7729(2)	3500(1)	39(1)
C(16)	3548(4)	7567(2)	4297(1)	49(1)
C(17)	1489(4)	7326(2)	4667(2)	53(1)
C(18)	218(5)	8230(2)	4722(2)	58(1)
C(19)	-278(4)	8375(2)	3928(1)	45(1)
C(20)	2292(3)	10999(2)	2996(1)	36(1)
C(21)	4018(4)	11723(2)	3483(1)	46(1)
C(22)	3822(4)	12783(2)	3854(1)	51(1)
C(23)	1925(4)	13136(2)	3749(1)	48(1)
C(24)	202(4)	12392(2)	3268(1)	50(1)
C(25)	356(4)	11329(2)	2893(1)	45(1)
C(26)	1764(7)	14308(2)	4136(3)	76(1)

Table 3. Bond lengths [Å] and angles [°] for gbh33rta.

S(1)-O(1)	1.4282(16)
S(1)-O(2)	1.4357(15)
S(1)-N(1)	1.5977(18)
S(1)-C(7)	1.7684(19)
O(3)-C(2)	1.429(2)
O(3)-H(30)	0.80(2)
F(1)-C(6)	1.407(2)
N(1)-C(1)	1.465(3)
N(1)-H(1N)	0.82(2)
C(1)-C(6)	1.518(3)
C(1)-C(2)	1.529(3)
C(1)-H(1)	0.93(2)
C(2)-C(3)	1.513(3)
C(2)-H(2)	0.985(19)
C(3)-C(4)	1.517(4)
C(3)-H(3A)	0.94(2)
C(3)-H(3B)	0.97(2)
C(4)-C(5)	1.522(4)
C(4)-H(4A)	0.96(2)
C(4)-H(4B)	0.93(3)
C(5)-C(6)	1.499(3)
C(5)-H(5A)	0.97(2)
C(5)-H(5B)	0.94(2)
C(6)-H(6)	0.941(19)
C(7)-C(12)	1.376(3)
C(7)-C(8)	1.382(3)
C(8)-C(9)	1.379(3)
C(8)-H(8)	0.90(2)
C(9)-C(10)	1.379(3)
C(9)-H(9)	0.95(2)
C(10)-C(11)	1.383(3)
C(10)-C(13)	1.513(3)
C(11)-C(12)	1.380(3)
C(11)-H(11)	0.94(3)
C(12)-H(12)	0.92(2)
C(13)-H(13A)	0.9600
C(13)-H(13B)	0.9600
C(13)-H(13C)	0.9600
S(2)-O(5)	1.4312(16)
S(2)-O(4)	1.4333(15)
S(2)-N(2)	1.5965(19)
S(2)-C(20)	1.7624(19)
O(6)-C(15)	1.431(2)
O(6)-H(6O)	0.80(3)
F(2)-C(19)	1.426(2)
N(2)-C(14)	1.462(3)
N(2)-H(2N)	0.82(2)
C(14)-C(19)	1.516(3)
C(14)-C(15)	1.529(3)
C(14)-H(14)	0.93(2)
C(15)-C(16)	1.514(3)
C(15)-H(15)	0.967(19)
C(16)-C(17)	1.518(3)
C(16)-H(16A)	1.00(2)

C(16)-H(16B)	0.99(2)
C(17)-C(18)	1.516(4)
C(17)-H(17A)	0.97(2)
C(17)-H(17B)	0.97(3)
C(18)-C(19)	1.501(3)
C(18)-H(18A)	0.98(2)
C(18)-H(18B)	0.91(3)
C(19)-H(19)	0.989(19)
C(20)-C(21)	1.377(3)
C(20)-C(25)	1.384(3)
C(21)-C(22)	1.379(3)
C(21)-H(21)	0.91(2)
C(22)-C(23)	1.378(3)
C(22)-H(22)	0.94(2)
C(23)-C(24)	1.380(3)
C(23)-C(26)	1.506(3)
C(24)-C(25)	1.377(3)
C(24)-H(24)	0.93(2)
C(25)-H(25)	0.90(2)
C(26)-H(26A)	0.89(4)
C(26)-H(26B)	0.91(4)
C(26)-H(26C)	0.87(3)

O(1)-S(1)-O(2)	118.43(10)
O(1)-S(1)-N(1)	106.66(10)
O(2)-S(1)-N(1)	108.10(10)
O(1)-S(1)-C(7)	108.98(10)
O(2)-S(1)-C(7)	106.18(9)
N(1)-S(1)-C(7)	108.15(9)
C(2)-O(3)-H(30)	109.4(17)
C(1)-N(1)-S(1)	123.19(15)
C(1)-N(1)-H(1N)	119.9(15)
S(1)-N(1)-H(1N)	113.5(15)
N(1)-C(1)-C(6)	110.62(17)
N(1)-C(1)-C(2)	111.53(16)
C(6)-C(1)-C(2)	110.02(17)
N(1)-C(1)-H(1)	108.6(12)
C(6)-C(1)-H(1)	108.5(12)
C(2)-C(1)-H(1)	107.5(12)
O(3)-C(2)-C(3)	111.22(18)
O(3)-C(2)-C(1)	105.99(16)
C(3)-C(2)-C(1)	111.27(18)
O(3)-C(2)-H(2)	108.9(11)
C(3)-C(2)-H(2)	111.3(11)
C(1)-C(2)-H(2)	108.0(11)
C(2)-C(3)-C(4)	111.6(2)
C(2)-C(3)-H(3A)	107.8(13)
C(4)-C(3)-H(3A)	112.7(13)
C(2)-C(3)-H(3B)	110.3(14)
C(4)-C(3)-H(3B)	109.5(14)
H(3A)-C(3)-H(3B)	104.7(18)
C(3)-C(4)-C(5)	110.7(2)
C(3)-C(4)-H(4A)	110.2(14)
C(5)-C(4)-H(4A)	109.0(14)
C(3)-C(4)-H(4B)	109.4(15)
C(5)-C(4)-H(4B)	109.1(14)

H(4A)-C(4)-H(4B)	108(2)
C(6)-C(5)-C(4)	110.5(2)
C(6)-C(5)-H(5A)	107.3(15)
C(4)-C(5)-H(5A)	108.8(14)
C(6)-C(5)-H(5B)	107.8(16)
C(4)-C(5)-H(5B)	111.4(15)
H(5A)-C(5)-H(5B)	111(2)
F(1)-C(6)-C(5)	109.11(17)
F(1)-C(6)-C(1)	109.07(17)
C(5)-C(6)-C(1)	112.1(2)
F(1)-C(6)-H(6)	105.2(12)
C(5)-C(6)-H(6)	112.4(12)
C(1)-C(6)-H(6)	108.7(12)
C(12)-C(7)-C(8)	120.1(2)
C(12)-C(7)-S(1)	119.55(16)
C(8)-C(7)-S(1)	120.35(16)
C(9)-C(8)-C(7)	119.3(2)
C(9)-C(8)-H(8)	121.7(14)
C(7)-C(8)-H(8)	119.0(14)
C(10)-C(9)-C(8)	121.6(2)
C(10)-C(9)-H(9)	120.8(15)
C(8)-C(9)-H(9)	117.6(15)
C(9)-C(10)-C(11)	118.1(2)
C(9)-C(10)-C(13)	120.4(2)
C(11)-C(10)-C(13)	121.5(2)
C(12)-C(11)-C(10)	121.1(2)
C(12)-C(11)-H(11)	119.5(15)
C(10)-C(11)-H(11)	119.4(15)
C(7)-C(12)-C(11)	119.8(2)
C(7)-C(12)-H(12)	121.3(14)
C(11)-C(12)-H(12)	118.8(14)
C(10)-C(13)-H(13A)	109.5
C(10)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(10)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
O(5)-S(2)-O(4)	119.15(10)
O(5)-S(2)-N(2)	106.02(10)
O(4)-S(2)-N(2)	107.78(10)
O(5)-S(2)-C(20)	108.31(9)
O(4)-S(2)-C(20)	105.56(9)
N(2)-S(2)-C(20)	109.86(10)
C(15)-O(6)-H(6O)	108.7(18)
C(14)-N(2)-S(2)	123.10(15)
C(14)-N(2)-H(2N)	118.7(16)
S(2)-N(2)-H(2N)	113.7(16)
N(2)-C(14)-C(19)	110.46(18)
N(2)-C(14)-C(15)	111.40(17)
C(19)-C(14)-C(15)	110.50(17)
N(2)-C(14)-H(14)	109.5(12)
C(19)-C(14)-H(14)	108.2(12)
C(15)-C(14)-H(14)	106.7(12)
O(6)-C(15)-C(16)	111.22(18)
O(6)-C(15)-C(14)	106.45(16)
C(16)-C(15)-C(14)	110.96(18)

O(6)-C(15)-H(15)	108.6(11)
C(16)-C(15)-H(15)	110.7(12)
C(14)-C(15)-H(15)	108.8(11)
C(15)-C(16)-C(17)	111.4(2)
C(15)-C(16)-H(16A)	108.5(13)
C(17)-C(16)-H(16A)	108.7(13)
C(15)-C(16)-H(16B)	108.2(13)
C(17)-C(16)-H(16B)	112.9(13)
H(16A)-C(16)-H(16B)	107.0(18)
C(18)-C(17)-C(16)	111.0(2)
C(18)-C(17)-H(17A)	109.3(13)
C(16)-C(17)-H(17A)	109.9(13)
C(18)-C(17)-H(17B)	109.4(14)
C(16)-C(17)-H(17B)	109.3(14)
H(17A)-C(17)-H(17B)	108.0(19)
C(19)-C(18)-C(17)	110.4(2)
C(19)-C(18)-H(18A)	109.0(15)
C(17)-C(18)-H(18A)	111.5(14)
C(19)-C(18)-H(18B)	107.0(17)
C(17)-C(18)-H(18B)	109.9(16)
H(18A)-C(18)-H(18B)	109(2)
F(2)-C(19)-C(18)	109.82(17)
F(2)-C(19)-C(14)	108.56(18)
C(18)-C(19)-C(14)	112.0(2)
F(2)-C(19)-H(19)	103.6(11)
C(18)-C(19)-H(19)	111.9(11)
C(14)-C(19)-H(19)	110.6(11)
C(21)-C(20)-C(25)	120.01(19)
C(21)-C(20)-S(2)	120.26(15)
C(25)-C(20)-S(2)	119.60(16)
C(20)-C(21)-C(22)	119.7(2)
C(20)-C(21)-H(21)	119.7(14)
C(22)-C(21)-H(21)	120.6(14)
C(23)-C(22)-C(21)	121.4(2)
C(23)-C(22)-H(22)	120.8(15)
C(21)-C(22)-H(22)	117.9(15)
C(22)-C(23)-C(24)	118.0(2)
C(22)-C(23)-C(26)	120.6(3)
C(24)-C(23)-C(26)	121.3(3)
C(25)-C(24)-C(23)	121.7(2)
C(25)-C(24)-H(24)	119.0(14)
C(23)-C(24)-H(24)	119.3(14)
C(24)-C(25)-C(20)	119.2(2)
C(24)-C(25)-H(25)	120.5(14)
C(20)-C(25)-H(25)	120.2(14)
C(23)-C(26)-H(26A)	110(2)
C(23)-C(26)-H(26B)	110(2)
H(26A)-C(26)-H(26B)	101(3)
C(23)-C(26)-H(26C)	111(2)
H(26A)-C(26)-H(26C)	120(3)
H(26B)-C(26)-H(26C)	104(3)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for gbh33rta. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
S(1)	40(1)	37(1)	47(1)	14(1)	11(1)	10(1)
O(1)	73(1)	57(1)	41(1)	16(1)	10(1)	8(1)
O(2)	38(1)	46(1)	85(1)	17(1)	18(1)	14(1)
O(3)	42(1)	38(1)	53(1)	2(1)	5(1)	17(1)
F(1)	84(1)	65(1)	68(1)	23(1)	32(1)	49(1)
N(1)	37(1)	37(1)	44(1)	14(1)	-1(1)	3(1)
C(1)	42(1)	30(1)	36(1)	6(1)	0(1)	4(1)
C(2)	32(1)	39(1)	45(1)	10(1)	4(1)	8(1)
C(3)	54(1)	57(2)	51(2)	18(1)	0(1)	22(1)
C(4)	76(2)	67(2)	46(2)	28(1)	12(1)	29(2)
C(5)	74(2)	61(2)	44(2)	15(1)	18(1)	26(2)
C(6)	49(1)	36(1)	45(1)	9(1)	13(1)	19(1)
C(7)	38(1)	36(1)	43(1)	16(1)	7(1)	12(1)
C(8)	43(1)	41(1)	70(2)	21(1)	11(1)	12(1)
C(9)	56(2)	57(2)	64(2)	25(1)	17(1)	30(1)
C(10)	70(2)	44(1)	46(1)	15(1)	0(1)	24(1)
C(11)	62(2)	39(1)	56(2)	16(1)	0(1)	3(1)
C(12)	43(1)	46(1)	48(1)	19(1)	9(1)	7(1)
C(13)	113(2)	58(2)	82(2)	1(2)	-3(2)	44(2)
S(2)	43(1)	32(1)	49(1)	11(1)	8(1)	10(1)
O(4)	41(1)	39(1)	85(1)	11(1)	14(1)	16(1)
O(5)	72(1)	47(1)	43(1)	12(1)	7(1)	9(1)
O(6)	40(1)	37(1)	51(1)	5(1)	6(1)	14(1)
F(2)	77(1)	57(1)	73(1)	5(1)	10(1)	35(1)
N(2)	43(1)	37(1)	54(1)	17(1)	-6(1)	0(1)
C(14)	45(1)	32(1)	42(1)	7(1)	-4(1)	3(1)
C(15)	33(1)	41(1)	44(1)	13(1)	5(1)	5(1)
C(16)	44(1)	54(1)	51(2)	19(1)	1(1)	10(1)
C(17)	59(2)	61(2)	44(2)	21(1)	7(1)	14(1)
C(18)	64(2)	64(2)	46(2)	8(1)	15(1)	20(1)
C(19)	49(1)	36(1)	48(1)	2(1)	7(1)	18(1)
C(20)	38(1)	33(1)	41(1)	15(1)	9(1)	10(1)
C(21)	42(1)	43(1)	54(1)	14(1)	3(1)	14(1)
C(22)	57(2)	39(1)	51(1)	6(1)	2(1)	7(1)
C(23)	66(2)	40(1)	48(1)	18(1)	24(1)	21(1)
C(24)	50(1)	55(1)	60(2)	27(1)	18(1)	28(1)
C(25)	40(1)	45(1)	53(1)	16(1)	4(1)	11(1)
C(26)	100(3)	46(2)	88(3)	15(2)	37(2)	30(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for gbh33rta.

	x	y	z	U(eq)
H(30)	6190(40)	8410(20)	2193(14)	58(8)
H(1N)	8730(30)	6169(17)	2436(12)	43(6)
H(1)	5980(30)	5420(16)	1150(11)	39(5)
H(2)	4250(30)	6777(15)	1772(11)	36(5)
H(3A)	4220(30)	7726(18)	823(12)	48(6)
H(3B)	4000(40)	6510(20)	408(14)	59(7)
H(4A)	7930(40)	8080(20)	641(14)	54(7)
H(4B)	6610(40)	7446(19)	-148(15)	60(7)
H(5A)	7370(40)	5790(20)	-47(14)	65(8)
H(5B)	9580(40)	6640(20)	56(14)	65(7)
H(6)	9810(30)	6948(16)	1392(11)	34(5)
H(8)	9620(30)	4214(19)	1842(13)	51(6)
H(9)	10230(40)	2550(20)	1136(14)	69(8)
H(11)	4150(40)	1150(20)	1336(14)	71(8)
H(12)	3620(40)	2836(18)	2034(13)	56(7)
H(13A)	7655	523	165	128
H(13B)	6482	-21	755	128
H(13C)	8986	446	912	128
H(6O)	2530(40)	6300(20)	2856(15)	68(9)
H(2N)	-50(40)	8549(18)	2573(13)	47(7)
H(14)	2610(30)	9276(16)	3867(11)	38(5)
H(15)	4390(30)	7932(15)	3286(11)	36(5)
H(16A)	4500(40)	8259(19)	4644(13)	57(7)
H(16B)	4390(40)	6975(19)	4237(13)	58(7)
H(17A)	590(30)	6626(18)	4359(13)	49(6)
H(17B)	1860(40)	7267(19)	5186(15)	62(7)
H(18A)	-1150(40)	8067(19)	4943(14)	65(7)
H(18B)	1030(40)	8890(20)	5029(15)	71(8)
H(19)	-1310(30)	7729(16)	3578(11)	33(5)
H(21)	5280(40)	11495(18)	3562(13)	55(7)
H(22)	5040(40)	13270(20)	4174(14)	68(8)
H(24)	-1100(40)	12612(18)	3196(13)	58(7)
H(25)	-770(40)	10863(18)	2565(13)	53(7)
H(26A)	2920(60)	14780(30)	4080(20)	138(16)
H(26B)	1910(60)	14440(30)	4660(20)	130(16)
H(26C)	470(60)	14410(30)	4020(20)	113(14)

Table 6. Torsion angles [°] for gbh33rta.

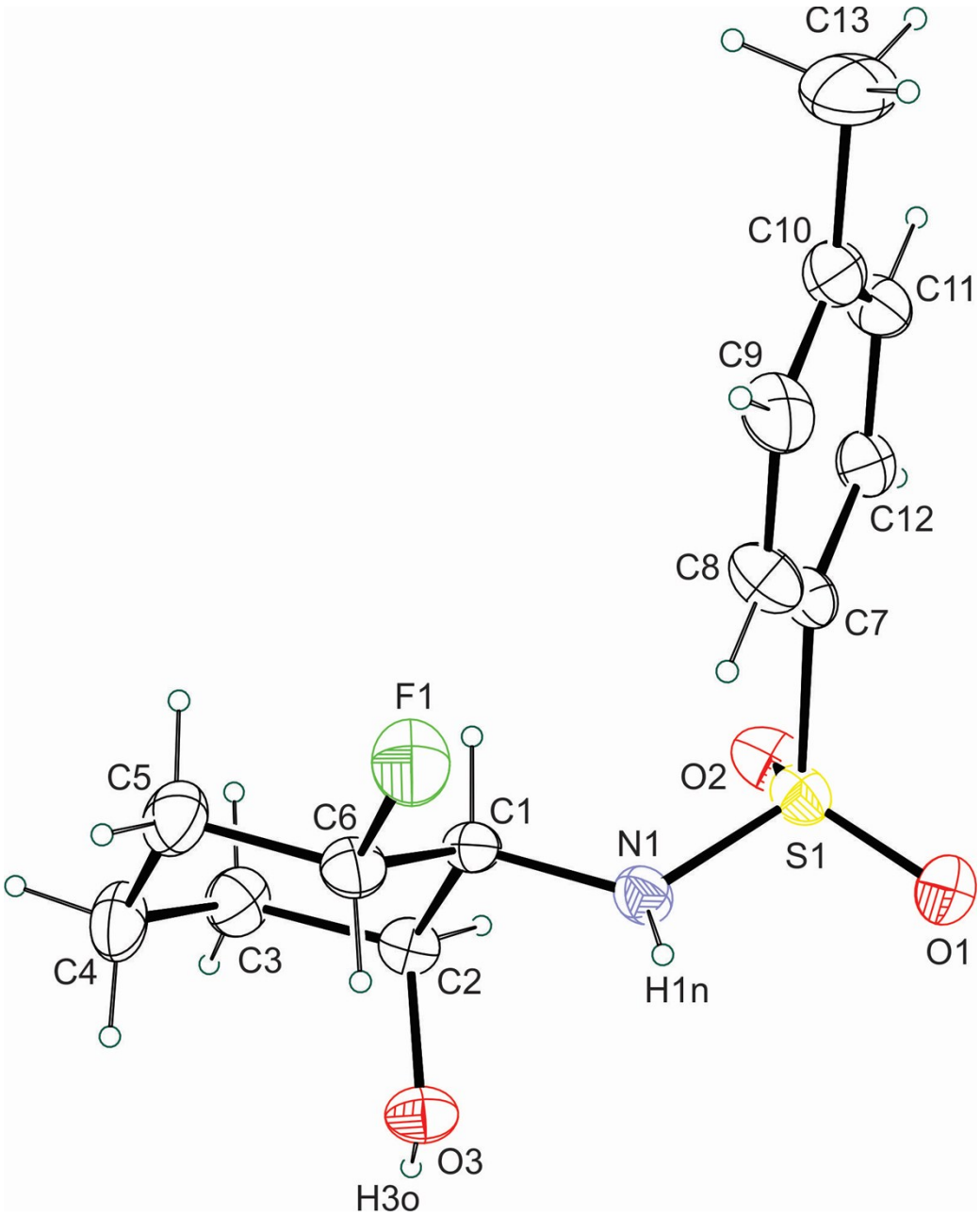
O(1)-S(1)-N(1)-C(1)	-172.83(15)
O(2)-S(1)-N(1)-C(1)	-44.46(18)
C(7)-S(1)-N(1)-C(1)	70.09(18)
S(1)-N(1)-C(1)-C(6)	-139.26(16)
S(1)-N(1)-C(1)-C(2)	97.95(18)
N(1)-C(1)-C(2)-O(3)	56.8(2)
C(6)-C(1)-C(2)-O(3)	-66.3(2)
N(1)-C(1)-C(2)-C(3)	177.86(18)
C(6)-C(1)-C(2)-C(3)	54.7(2)
O(3)-C(2)-C(3)-C(4)	62.7(3)
C(1)-C(2)-C(3)-C(4)	-55.3(3)
C(2)-C(3)-C(4)-C(5)	55.7(3)
C(3)-C(4)-C(5)-C(6)	-56.4(3)
C(4)-C(5)-C(6)-F(1)	178.4(2)
C(4)-C(5)-C(6)-C(1)	57.5(3)
N(1)-C(1)-C(6)-F(1)	59.0(2)
C(2)-C(1)-C(6)-F(1)	-177.36(17)
N(1)-C(1)-C(6)-C(5)	179.89(18)
C(2)-C(1)-C(6)-C(5)	-56.4(2)
O(1)-S(1)-C(7)-C(12)	98.40(19)
O(2)-S(1)-C(7)-C(12)	-30.2(2)
N(1)-S(1)-C(7)-C(12)	-146.03(18)
O(1)-S(1)-C(7)-C(8)	-79.1(2)
O(2)-S(1)-C(7)-C(8)	152.28(18)
N(1)-S(1)-C(7)-C(8)	36.5(2)
C(12)-C(7)-C(8)-C(9)	1.1(3)
S(1)-C(7)-C(8)-C(9)	178.58(18)
C(7)-C(8)-C(9)-C(10)	-0.4(4)
C(8)-C(9)-C(10)-C(11)	-0.6(4)
C(8)-C(9)-C(10)-C(13)	-179.5(2)
C(9)-C(10)-C(11)-C(12)	1.0(4)
C(13)-C(10)-C(11)-C(12)	179.9(2)
C(8)-C(7)-C(12)-C(11)	-0.7(3)
S(1)-C(7)-C(12)-C(11)	-178.23(17)
C(10)-C(11)-C(12)-C(7)	-0.4(4)
O(5)-S(2)-N(2)-C(14)	175.19(16)
O(4)-S(2)-N(2)-C(14)	46.56(19)
C(20)-S(2)-N(2)-C(14)	-67.99(19)
S(2)-N(2)-C(14)-C(19)	140.00(16)
S(2)-N(2)-C(14)-C(15)	-96.79(19)
N(2)-C(14)-C(15)-O(6)	-56.6(2)
C(19)-C(14)-C(15)-O(6)	66.6(2)
N(2)-C(14)-C(15)-C(16)	-177.77(18)
C(19)-C(14)-C(15)-C(16)	-54.6(2)
O(6)-C(15)-C(16)-C(17)	-63.2(3)
C(14)-C(15)-C(16)-C(17)	55.1(3)
C(15)-C(16)-C(17)-C(18)	-56.2(3)
C(16)-C(17)-C(18)-C(19)	56.5(3)
C(17)-C(18)-C(19)-F(2)	-177.8(2)
C(17)-C(18)-C(19)-C(14)	-57.1(3)
N(2)-C(14)-C(19)-F(2)	-58.7(2)
C(15)-C(14)-C(19)-F(2)	177.56(16)
N(2)-C(14)-C(19)-C(18)	179.85(18)
C(15)-C(14)-C(19)-C(18)	56.1(2)

O(5)-S(2)-C(20)-C(21)	-133.23(17)
O(4)-S(2)-C(20)-C(21)	-4.6(2)
N(2)-S(2)-C(20)-C(21)	111.39(18)
O(5)-S(2)-C(20)-C(25)	42.8(2)
O(4)-S(2)-C(20)-C(25)	171.47(17)
N(2)-S(2)-C(20)-C(25)	-72.57(19)
C(25)-C(20)-C(21)-C(22)	-1.4(3)
S(2)-C(20)-C(21)-C(22)	174.63(18)
C(20)-C(21)-C(22)-C(23)	0.1(4)
C(21)-C(22)-C(23)-C(24)	1.0(3)
C(21)-C(22)-C(23)-C(26)	-177.9(3)
C(22)-C(23)-C(24)-C(25)	-0.8(3)
C(26)-C(23)-C(24)-C(25)	178.0(3)
C(23)-C(24)-C(25)-C(20)	-0.4(3)
C(21)-C(20)-C(25)-C(24)	1.5(3)
S(2)-C(20)-C(25)-C(24)	-174.50(17)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for gbh33rta [Å and °].

D-H	d(D-H)	d(H..A)	<DHA	d(D..A)	A
O3-H30	0.804	1.952	172.07	2.751	O4
O3-H30	0.804	3.025	165.36	3.808	S2
N1-H1N	0.821	2.019	179.34	2.840	O6 [x+1, y, z]
O6-H6O	0.800	2.042	168.09	2.829	O2
N2-H2N	0.819	2.007	177.28	2.825	O3 [x-1, y, z]



X-ray crystallography of **2k**. Thermal ellipsoids are shown at 50% probability

9. X-Ray Crystallography Data of 2n (CCDC 1490051)

Table 1. Crystal data and structure refinement for gbh34ltc.

Identification code	gbh34ltc	
Empirical formula	C14 H20 F N O2 S	
Formula weight	285.37	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P $2_1/c$	
Unit cell dimensions	a = 7.9327(2) Å	α= 90°.
	b = 9.5312(2) Å	β= 100.885(2)°.
	c = 19.6547(5) Å	γ = 90°.
Volume	1459.33(6) $Å^3$	
Z	4	
Density (calculated)	1.299 Mg/m^3	
Absorption coefficient	0.231 mm^{-1}	
F(000)	608	
Crystal size	0.38 x 0.25 x 0.18 mm^3	
Theta range for data collection	3.38 to 28.05°.	
Index ranges	-10<=h<=10, -12<=k<=12, -25<=l<=26	
Reflections collected	17380	
Independent reflections	3544 [R(int) = 0.0298]	
Completeness to theta = 28.05°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00 and 0.88	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3544 / 0 / 252	
Goodness-of-fit on F^2	1.052	
Final R indices [I>2σ (I)]	R1 = 0.0367, wR2 = 0.0902	
R indices (all data)	R1 = 0.0432, wR2 = 0.0943	
Largest diff. peak and hole	0.376 and -0.309 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for gbh34ltc. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
S(1)	6836(1)	8249(1)	5361(1)	20(1)
F(1)	9950(1)	10046(1)	7518(1)	33(1)
O(1)	8469(1)	7562(1)	5479(1)	27(1)
O(2)	6150(1)	8804(1)	4684(1)	25(1)
N(1)	6965(2)	9573(1)	5883(1)	21(1)
C(1)	5328(2)	7058(1)	5578(1)	20(1)
C(2)	3607(2)	7461(2)	5467(1)	25(1)
C(3)	2404(2)	6517(2)	5615(1)	27(1)
C(4)	2877(2)	5178(2)	5865(1)	26(1)
C(5)	4601(2)	4811(2)	5980(1)	28(1)
C(6)	5836(2)	5745(2)	5839(1)	25(1)
C(7)	1524(2)	4162(2)	6002(1)	36(1)
C(8)	7703(2)	9383(2)	6627(1)	23(1)
C(9)	6340(2)	9566(2)	7080(1)	29(1)
C(10)	5738(2)	11079(2)	7103(1)	31(1)
C(11)	7240(2)	12078(2)	7318(1)	30(1)
C(12)	8559(2)	11918(2)	6849(1)	28(1)
C(13)	9194(2)	10422(2)	6825(1)	25(1)
C(14)	10586(2)	10250(2)	6402(1)	32(1)

Table 3. Bond lengths [Å] and angles [°] for gbh34ltc.

S(1)-O(1)	1.4304(10)
S(1)-O(2)	1.4402(10)
S(1)-N(1)	1.6179(12)
S(1)-C(1)	1.7588(14)
F(1)-C(13)	1.4251(16)
N(1)-C(8)	1.4791(17)
N(1)-H(1N)	0.821(19)
C(1)-C(6)	1.3833(19)
C(1)-C(2)	1.3955(19)
C(2)-C(3)	1.381(2)
C(2)-H(2)	0.980(19)
C(3)-C(4)	1.393(2)
C(3)-H(3)	0.947(19)
C(4)-C(5)	1.388(2)
C(4)-C(7)	1.507(2)
C(5)-C(6)	1.390(2)
C(5)-H(5)	0.96(2)
C(6)-H(6)	0.953(18)
C(7)-H(7A)	0.96(2)
C(7)-H(7B)	0.99(3)
C(7)-H(7C)	0.96(2)
C(8)-C(9)	1.535(2)
C(8)-C(13)	1.535(2)
C(8)-H(8)	0.988(17)
C(9)-C(10)	1.523(2)
C(9)-H(9A)	0.994(19)
C(9)-H(9B)	1.00(2)
C(10)-C(11)	1.521(2)
C(10)-H(10A)	0.967(19)
C(10)-H(10B)	0.99(2)
C(11)-C(12)	1.526(2)
C(11)-H(11A)	0.99(2)
C(11)-H(11B)	0.988(19)
C(12)-C(13)	1.516(2)
C(12)-H(12A)	1.00(2)
C(12)-H(12B)	0.996(15)
C(13)-C(14)	1.512(2)
C(14)-H(14A)	0.962(19)
C(14)-H(14B)	1.01(2)
C(14)-H(14C)	0.98(2)
O(1)-S(1)-O(2)	119.33(6)
O(1)-S(1)-N(1)	107.92(6)
O(2)-S(1)-N(1)	105.52(6)

O(1)-S(1)-C(1)	107.57(6)
O(2)-S(1)-C(1)	107.80(6)
N(1)-S(1)-C(1)	108.30(6)
C(8)-N(1)-S(1)	119.81(10)
C(8)-N(1)-H(1N)	117.4(13)
S(1)-N(1)-H(1N)	110.9(13)
C(6)-C(1)-C(2)	120.98(13)
C(6)-C(1)-S(1)	120.65(11)
C(2)-C(1)-S(1)	118.36(11)
C(3)-C(2)-C(1)	118.84(14)
C(3)-C(2)-H(2)	120.3(11)
C(1)-C(2)-H(2)	120.8(11)
C(2)-C(3)-C(4)	121.34(14)
C(2)-C(3)-H(3)	120.5(12)
C(4)-C(3)-H(3)	118.2(12)
C(5)-C(4)-C(3)	118.66(14)
C(5)-C(4)-C(7)	121.44(15)
C(3)-C(4)-C(7)	119.89(15)
C(4)-C(5)-C(6)	121.07(14)
C(4)-C(5)-H(5)	119.6(12)
C(6)-C(5)-H(5)	119.3(12)
C(1)-C(6)-C(5)	119.09(13)
C(1)-C(6)-H(6)	121.2(11)
C(5)-C(6)-H(6)	119.7(11)
C(4)-C(7)-H(7A)	109.5(13)
C(4)-C(7)-H(7B)	111.9(15)
H(7A)-C(7)-H(7B)	105(2)
C(4)-C(7)-H(7C)	109.4(14)
H(7A)-C(7)-H(7C)	111.0(19)
H(7B)-C(7)-H(7C)	110(2)
N(1)-C(8)-C(9)	111.60(12)
N(1)-C(8)-C(13)	108.31(11)
C(9)-C(8)-C(13)	111.92(12)
N(1)-C(8)-H(8)	107.0(10)
C(9)-C(8)-H(8)	110.0(10)
C(13)-C(8)-H(8)	107.9(10)
C(10)-C(9)-C(8)	112.58(12)
C(10)-C(9)-H(9A)	111.4(11)
C(8)-C(9)-H(9A)	107.7(11)
C(10)-C(9)-H(9B)	111.9(11)
C(8)-C(9)-H(9B)	106.0(11)
H(9A)-C(9)-H(9B)	106.9(15)
C(11)-C(10)-C(9)	111.58(14)
C(11)-C(10)-H(10A)	108.1(12)
C(9)-C(10)-H(10A)	109.7(11)
C(11)-C(10)-H(10B)	110.5(12)

C(9)-C(10)-H(10B)	109.1(12)
H(10A)-C(10)-H(10B)	107.8(16)
C(10)-C(11)-C(12)	111.12(13)
C(10)-C(11)-H(11A)	109.4(11)
C(12)-C(11)-H(11A)	108.9(11)
C(10)-C(11)-H(11B)	111.3(11)
C(12)-C(11)-H(11B)	109.3(11)
H(11A)-C(11)-H(11B)	106.7(16)
C(13)-C(12)-C(11)	112.48(13)
C(13)-C(12)-H(12A)	109.3(11)
C(11)-C(12)-H(12A)	112.6(11)
C(13)-C(12)-H(12B)	111.3(9)
C(11)-C(12)-H(12B)	108.7(8)
H(12A)-C(12)-H(12B)	102.0(14)
F(1)-C(13)-C(14)	106.23(12)
F(1)-C(13)-C(12)	106.79(12)
C(14)-C(13)-C(12)	113.59(13)
F(1)-C(13)-C(8)	104.21(11)
C(14)-C(13)-C(8)	113.47(13)
C(12)-C(13)-C(8)	111.70(12)
C(13)-C(14)-H(14A)	107.7(11)
C(13)-C(14)-H(14B)	109.1(11)
H(14A)-C(14)-H(14B)	110.3(15)
C(13)-C(14)-H(14C)	110.2(11)
H(14A)-C(14)-H(14C)	107.6(16)
H(14B)-C(14)-H(14C)	111.7(16)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for gbh34ltc. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
S(1)	19(1)	20(1)	21(1)	0(1)	4(1)	3(1)
F(1)	36(1)	35(1)	25(1)	4(1)	-6(1)	1(1)
O(1)	20(1)	29(1)	33(1)	-2(1)	5(1)	5(1)
O(2)	28(1)	26(1)	20(1)	1(1)	5(1)	4(1)
N(1)	22(1)	19(1)	21(1)	1(1)	1(1)	2(1)
C(1)	21(1)	19(1)	19(1)	-2(1)	2(1)	1(1)
C(2)	23(1)	23(1)	28(1)	0(1)	3(1)	3(1)
C(3)	22(1)	31(1)	30(1)	-5(1)	5(1)	0(1)
C(4)	33(1)	27(1)	18(1)	-6(1)	6(1)	-8(1)
C(5)	37(1)	20(1)	25(1)	2(1)	4(1)	1(1)
C(6)	26(1)	22(1)	25(1)	1(1)	2(1)	5(1)
C(7)	45(1)	37(1)	27(1)	-8(1)	13(1)	-17(1)
C(8)	26(1)	21(1)	22(1)	3(1)	2(1)	-1(1)
C(9)	31(1)	33(1)	22(1)	3(1)	7(1)	-7(1)
C(10)	32(1)	39(1)	23(1)	-2(1)	8(1)	0(1)
C(11)	36(1)	29(1)	26(1)	-3(1)	5(1)	3(1)
C(12)	33(1)	24(1)	27(1)	0(1)	5(1)	-4(1)
C(13)	26(1)	26(1)	21(1)	3(1)	0(1)	-2(1)
C(14)	25(1)	34(1)	38(1)	-1(1)	7(1)	-3(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for gbh34ltc.

	x	y	z	U(eq)
H(1N)	6120(20)	10080(20)	5785(9)	30(5)
H(2)	3250(20)	8390(20)	5282(9)	31(5)
H(3)	1230(20)	6770(20)	5546(9)	32(5)
H(5)	4940(20)	3890(20)	6149(10)	36(5)
H(6)	7010(20)	5465(19)	5913(9)	30(5)
H(7A)	960(30)	4540(20)	6351(12)	49(6)
H(7B)	2030(30)	3270(30)	6193(13)	68(7)
H(7C)	720(30)	3990(20)	5579(12)	56(6)
H(8)	8180(20)	8424(19)	6681(8)	23(4)
H(9A)	5370(20)	8930(20)	6897(9)	33(5)
H(9B)	6870(20)	9210(20)	7551(10)	37(5)
H(10A)	5130(20)	11360(20)	6650(10)	35(5)
H(10B)	4930(30)	11150(20)	7427(10)	39(5)
H(11A)	7800(20)	11880(20)	7801(11)	38(5)
H(11B)	6850(20)	13060(20)	7307(9)	31(5)
H(12A)	9570(30)	12560(20)	6983(10)	39(5)
H(12B)	8043(18)	12264(15)	6378(8)	10(3)
H(14A)	10130(20)	10570(20)	5939(10)	32(5)
H(14B)	10910(20)	9230(20)	6395(10)	38(5)
H(14C)	11580(20)	10840(20)	6591(10)	37(5)

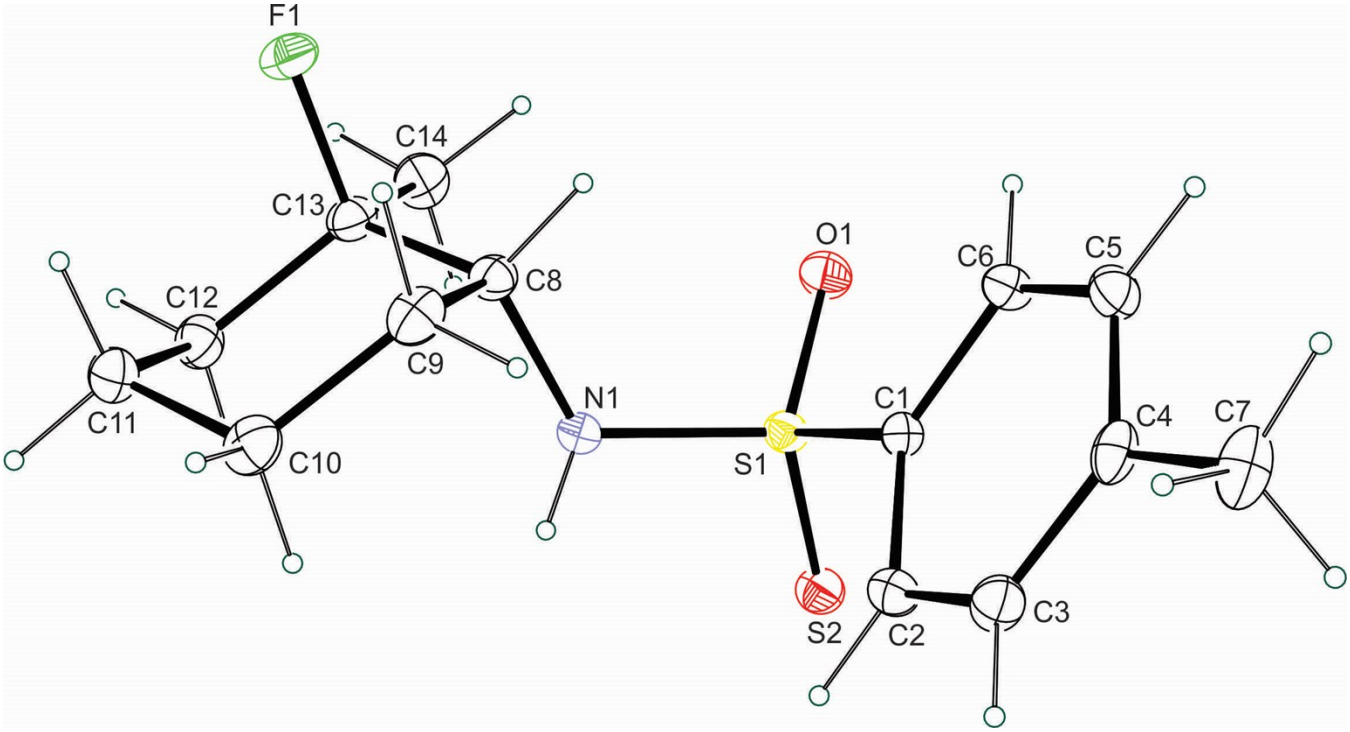
Table 6. Torsion angles [°] for gbh34ltc.

O(1)-S(1)-N(1)-C(8)	-48.59(12)
O(2)-S(1)-N(1)-C(8)	-177.20(10)
C(1)-S(1)-N(1)-C(8)	67.58(12)
O(1)-S(1)-C(1)-C(6)	2.42(13)
O(2)-S(1)-C(1)-C(6)	132.31(12)
N(1)-S(1)-C(1)-C(6)	-113.98(12)
O(1)-S(1)-C(1)-C(2)	-176.24(11)
O(2)-S(1)-C(1)-C(2)	-46.35(13)
N(1)-S(1)-C(1)-C(2)	67.36(12)
C(6)-C(1)-C(2)-C(3)	-0.7(2)
S(1)-C(1)-C(2)-C(3)	178.00(11)
C(1)-C(2)-C(3)-C(4)	-0.6(2)
C(2)-C(3)-C(4)-C(5)	1.5(2)
C(2)-C(3)-C(4)-C(7)	-178.24(14)
C(3)-C(4)-C(5)-C(6)	-1.1(2)
C(7)-C(4)-C(5)-C(6)	178.65(14)
C(2)-C(1)-C(6)-C(5)	1.0(2)
S(1)-C(1)-C(6)-C(5)	-177.58(11)
C(4)-C(5)-C(6)-C(1)	-0.2(2)
S(1)-N(1)-C(8)-C(9)	-112.30(12)
S(1)-N(1)-C(8)-C(13)	124.06(11)
N(1)-C(8)-C(9)-C(10)	-69.88(16)
C(13)-C(8)-C(9)-C(10)	51.69(17)
C(8)-C(9)-C(10)-C(11)	-53.52(17)
C(9)-C(10)-C(11)-C(12)	54.81(17)
C(10)-C(11)-C(12)-C(13)	-55.56(18)
C(11)-C(12)-C(13)-F(1)	-59.49(16)
C(11)-C(12)-C(13)-C(14)	-176.26(13)
C(11)-C(12)-C(13)-C(8)	53.84(17)
N(1)-C(8)-C(13)-F(1)	-173.08(11)
C(9)-C(8)-C(13)-F(1)	63.47(15)
N(1)-C(8)-C(13)-C(14)	-57.98(16)
C(9)-C(8)-C(13)-C(14)	178.57(13)
N(1)-C(8)-C(13)-C(12)	71.99(15)
C(9)-C(8)-C(13)-C(12)	-51.46(16)

Symmetry transformations used to generate equivalent atoms:

Table 7. Intermolecular Hydrogen bonds for gbh34ltc [Å and °].

D-H	d(D-H)	d(H..A)	<DHA	d(D..A)	A
N1-H1N	0.821	2.142	167.93	2.950	O2 [-x+1, -y+2, -z+1]



X-ray crystallography of **2n**. Thermal ellipsoids are shown at 50% probability

10.X-Ray Crystallography Data of (*S*)-1a

Table 1. Crystal data and structure refinement for gbh38ltd.

Identification code	gbh38ltd	
Empirical formula	C10 H14 F N O2 S	
Formula weight	231.28	
Temperature	100(4) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21	
Unit cell dimensions	a = 8.2803(3) Å	α= 90°.
	b = 5.19337(16) Å	β= 104.425(4)°.
	c = 13.1224(6) Å	γ = 90°.
Volume	546.51(4) $Å^3$	
Z	2	
Density (calculated)	1.405 Mg/m^3	
Absorption coefficient	0.290 mm^{-1}	
F(000)	244	
Crystal color, habit	colorless needle	
Crystal size	0.48 x 0.06 x 0.05 mm^3	
Theta range for data collection	3.32 to 27.54°.	
Index ranges	-10<=h<=10, -6<=k<=6, -17<=l<=17	
Reflections collected	11615	
Independent reflections	2456 [R(int) = 0.043]	
Completeness to theta = 27.54°	99.1 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.000 and 0.741	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2456 / 1 / 168	
Goodness-of-fit on F^2	1.043	
Final R indices [I>2sigma(I)]	R1 = 0.0330, wR2 = 0.0680	
R indices (all data)	R1 = 0.0358, wR2 = 0.0693	
Absolute structure parameter	0.00(7)	
Largest diff. peak and hole	0.351 and -0.234 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3)for gbh38ltd. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
S(1)	7352(1)	4917(1)	7535(1)	21(1)
F(1)	11532(1)	43(3)	9290(1)	30(1)
O(1)	7757(2)	7571(3)	7800(1)	27(1)
O(2)	5782(2)	3885(3)	7620(1)	26(1)
N(1)	8784(2)	3186(3)	8294(1)	22(1)
C(1)	7463(2)	4496(3)	6218(1)	20(1)
C(2)	8320(2)	6260(4)	5748(2)	23(1)
C(3)	8304(2)	5991(4)	4696(2)	24(1)
C(4)	7438(2)	3970(4)	4097(2)	22(1)
C(5)	6644(2)	2174(4)	4594(2)	22(1)
C(6)	6646(2)	2413(4)	5641(2)	21(1)
C(7)	7313(3)	3780(4)	2932(2)	29(1)
C(8)	10531(3)	3982(5)	8495(2)	24(1)
C(9)	11541(2)	2742(4)	9484(2)	24(1)
C(10)	13315(2)	3658(5)	9796(2)	33(1)

Table 3. Bond lengths [Å] and angles [°] for gbh38ltd.

S(1)-O(2)	1.4366(14)
S(1)-O(1)	1.4403(15)
S(1)-N(1)	1.6179(16)
S(1)-C(1)	1.7672(19)
F(1)-C(9)	1.424(2)
N(1)-C(8)	1.464(3)
N(1)-H(1N)	0.87(2)
C(1)-C(2)	1.393(3)
C(1)-C(6)	1.395(3)
C(2)-C(3)	1.385(3)
C(2)-H(2)	0.97(2)
C(3)-C(4)	1.398(3)
C(3)-H(3)	0.92(2)
C(4)-C(5)	1.394(3)
C(4)-C(7)	1.509(3)
C(5)-C(6)	1.380(3)
C(5)-H(5)	0.93(2)
C(6)-H(6)	0.92(2)
C(7)-H(7A)	0.9600
C(7)-H(7B)	0.9600
C(7)-H(7C)	0.9600
C(8)-C(9)	1.503(3)
C(8)-H(8A)	0.94(3)
C(8)-H(8B)	0.97(2)
C(9)-C(10)	1.501(3)
C(9)-H(9)	0.99(2)
C(10)-H(10A)	0.9600
C(10)-H(10B)	0.9600
C(10)-H(10C)	0.9600

O(2)-S(1)-O(1)	119.91(9)
O(2)-S(1)-N(1)	106.46(9)
O(1)-S(1)-N(1)	107.00(9)
O(2)-S(1)-C(1)	107.37(8)
O(1)-S(1)-C(1)	106.82(9)
N(1)-S(1)-C(1)	108.95(9)
C(8)-N(1)-S(1)	119.57(14)
C(8)-N(1)-H(1N)	114.6(14)
S(1)-N(1)-H(1N)	111.1(14)
C(2)-C(1)-C(6)	120.15(18)
C(2)-C(1)-S(1)	120.48(14)
C(6)-C(1)-S(1)	119.35(15)
C(3)-C(2)-C(1)	119.67(18)

C(3)-C(2)-H(2)	119.9(14)
C(1)-C(2)-H(2)	120.3(13)
C(2)-C(3)-C(4)	120.87(19)
C(2)-C(3)-H(3)	118.8(14)
C(4)-C(3)-H(3)	120.3(14)
C(5)-C(4)-C(3)	118.37(19)
C(5)-C(4)-C(7)	120.60(18)
C(3)-C(4)-C(7)	121.00(19)
C(6)-C(5)-C(4)	121.50(19)
C(6)-C(5)-H(5)	119.0(12)
C(4)-C(5)-H(5)	119.4(12)
C(5)-C(6)-C(1)	119.35(19)
C(5)-C(6)-H(6)	118.3(13)
C(1)-C(6)-H(6)	122.3(13)
C(4)-C(7)-H(7A)	109.5
C(4)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	109.5
C(4)-C(7)-H(7C)	109.5
H(7A)-C(7)-H(7C)	109.5
H(7B)-C(7)-H(7C)	109.5
N(1)-C(8)-C(9)	110.31(18)
N(1)-C(8)-H(8A)	110.1(14)
C(9)-C(8)-H(8A)	106.5(14)
N(1)-C(8)-H(8B)	111.6(13)
C(9)-C(8)-H(8B)	108.3(13)
H(8A)-C(8)-H(8B)	110(2)
F(1)-C(9)-C(10)	108.78(17)
F(1)-C(9)-C(8)	106.84(16)
C(10)-C(9)-C(8)	113.33(18)
F(1)-C(9)-H(9)	106.3(12)
C(10)-C(9)-H(9)	109.5(11)
C(8)-C(9)-H(9)	111.7(11)
C(9)-C(10)-H(10A)	109.5
C(9)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(9)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for gbh38ltd. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
S(1)	23(1)	16(1)	22(1)	-1(1)	3(1)	1(1)
F(1)	36(1)	18(1)	35(1)	4(1)	4(1)	2(1)
O(1)	34(1)	19(1)	26(1)	-2(1)	5(1)	3(1)
O(2)	23(1)	28(1)	28(1)	-1(1)	7(1)	0(1)
N(1)	23(1)	15(1)	24(1)	2(1)	0(1)	-2(1)
C(1)	18(1)	17(1)	22(1)	2(1)	1(1)	4(1)
C(2)	20(1)	16(1)	30(1)	-1(1)	2(1)	-1(1)
C(3)	22(1)	19(1)	32(1)	4(1)	8(1)	0(1)
C(4)	18(1)	22(1)	27(1)	1(1)	4(1)	6(1)
C(5)	19(1)	17(1)	28(1)	-3(1)	1(1)	1(1)
C(6)	19(1)	15(1)	29(1)	0(1)	5(1)	0(1)
C(7)	30(1)	29(1)	28(1)	-2(1)	8(1)	3(1)
C(8)	24(1)	18(1)	29(1)	0(1)	5(1)	-2(1)
C(9)	27(1)	21(1)	25(1)	-1(1)	7(1)	0(1)
C(10)	24(1)	33(1)	39(1)	0(1)	3(1)	1(1)

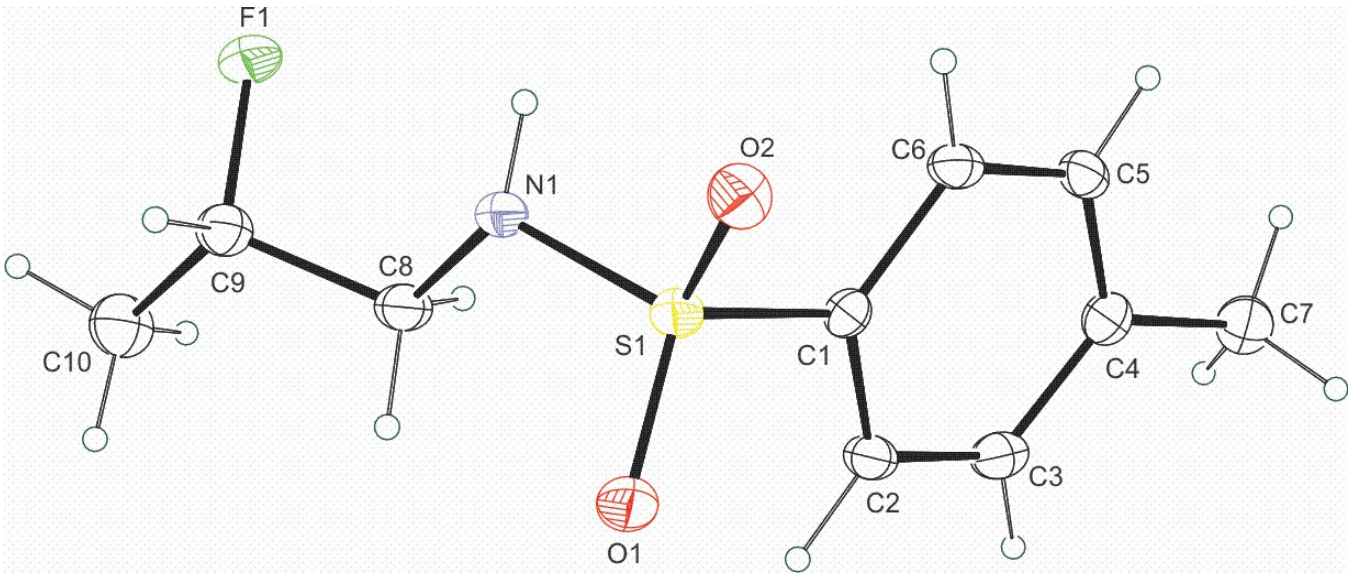
Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for gbh38ltd.

	x	y	z	U(eq)
H(1N)	8610(20)	1550(50)	8162(16)	20(6)
H(2)	8880(30)	7730(50)	6146(17)	27(6)
H(3)	8840(30)	7210(40)	4387(18)	30(6)
H(5)	6160(20)	730(40)	4226(15)	13(5)
H(6)	6090(20)	1180(50)	5934(16)	22(5)
H(7A)	8377	4168	2801	43
H(7B)	6497	4984	2561	43
H(7C)	6987	2065	2694	43
H(8A)	10620(30)	5780(50)	8606(18)	28
H(8B)	11010(30)	3500(40)	7919(18)	28
H(9)	11020(20)	2980(40)	10078(16)	18(5)
H(10A)	13818	3429	9218	49
H(10B)	13923	2683	10390	49
H(10C)	13339	5450	9980	49

Table 6. Torsion angles [°] for gbh38ltd.

O(2)-S(1)-N(1)-C(8)	-171.39(16)
O(1)-S(1)-N(1)-C(8)	-42.04(19)
C(1)-S(1)-N(1)-C(8)	73.11(18)
O(2)-S(1)-C(1)-C(2)	148.22(15)
O(1)-S(1)-C(1)-C(2)	18.40(17)
N(1)-S(1)-C(1)-C(2)	-96.87(16)
O(2)-S(1)-C(1)-C(6)	-30.05(16)
O(1)-S(1)-C(1)-C(6)	-159.87(14)
N(1)-S(1)-C(1)-C(6)	84.86(16)
C(6)-C(1)-C(2)-C(3)	2.4(3)
S(1)-C(1)-C(2)-C(3)	-175.84(14)
C(1)-C(2)-C(3)-C(4)	0.0(3)
C(2)-C(3)-C(4)-C(5)	-2.4(3)
C(2)-C(3)-C(4)-C(7)	175.52(18)
C(3)-C(4)-C(5)-C(6)	2.5(3)
C(7)-C(4)-C(5)-C(6)	-175.43(18)
C(4)-C(5)-C(6)-C(1)	-0.2(3)
C(2)-C(1)-C(6)-C(5)	-2.3(3)
S(1)-C(1)-C(6)-C(5)	175.95(14)
S(1)-N(1)-C(8)-C(9)	159.39(15)
N(1)-C(8)-C(9)-F(1)	65.6(2)
N(1)-C(8)-C(9)-C(10)	-174.66(19)

Symmetry transformations used to generate equivalent atoms:



X-ray crystallography of **(*S*)-1a**. Thermal ellipsoids are shown at 50% probability

11.X-Ray Crystallography Data of (*S*)-1d (CCDC 1490053)

Table 1. Crystal data and structure refinement for gbh36lta.

Identification code	gbh36lta	
Empirical formula	C16 H17 N O2 S	
Formula weight	287.37	
Temperature	100.5(6) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P\ 2_1$	
Unit cell dimensions	a = 7.3082(2) Å	α= 90°.
	b = 12.6670(4) Å	β= 102.802(3)°.
	c = 7.9739(3) Å	γ = 90°.
Volume	719.82(4) $Å^3$	
Z	2	
Density (calculated)	1.326 Mg/m^3	
Absorption coefficient	0.225 mm^{-1}	
F(000)	304	
Crystal color, habit	colorless plate	
Crystal size	0.38 x 0.28 x 0.10 mm^3	
Theta range for data collection	3.28 to 28.16°.	
Index ranges	-9<=h<=9, -16<=k<=16, -10<=l<=10	
Reflections collected	17424	
Independent reflections	3518 [R(int) = 0.034]	
Completeness to theta = 28.16°	99.8 %	
Absorption correction	multi-scan	
Max. and min. transmission	1.000 and 0.928	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3518 / 1 / 238	
Goodness-of-fit on F^2	1.019	
Final R indices [I>2σ(I)]	R1 = 0.025, wR2 = 0.058	
R indices (all data)	R1 = 0.026, wR2 = 0.058	
Absolute structure parameter	-0.03(4)	
Largest diff. peak and hole	0.291 and -0.195 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3)for gbh36lta. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
S(1)	11061(1)	3397(1)	3463(1)	19(1)
O(1)	11424(2)	2535(1)	4661(1)	29(1)
O(2)	12605(1)	4069(1)	3308(1)	25(1)
N(1)	9300(2)	4075(1)	3949(1)	18(1)
C(1)	9981(2)	2935(1)	1406(2)	17(1)
C(2)	8764(2)	2079(1)	1242(2)	21(1)
C(3)	7874(2)	1746(1)	-386(2)	22(1)
C(4)	8166(2)	2257(1)	-1853(2)	20(1)
C(5)	9432(2)	3096(1)	-1645(2)	20(1)
C(6)	10337(2)	3445(1)	-23(2)	18(1)
C(7)	7100(2)	1951(1)	-3623(2)	27(1)
C(8)	9856(2)	5001(1)	5117(2)	22(1)
C(9)	9055(2)	5177(1)	3275(2)	18(1)
C(10)	7047(2)	5512(1)	2622(2)	22(1)
C(11)	6351(2)	5249(1)	741(2)	19(1)
C(12)	6710(2)	5936(1)	-509(2)	23(1)
C(13)	6107(2)	5702(1)	-2247(2)	26(1)
C(14)	5135(2)	4774(1)	-2748(2)	26(1)
C(15)	4775(2)	4086(1)	-1510(2)	26(1)
C(16)	5385(2)	4315(1)	226(2)	22(1)

Table 3. Bond lengths [Å] and angles [°] for gbh36lta.

S(1)-O(1)	1.4361(11)
S(1)-O(2)	1.4409(11)
S(1)-N(1)	1.6633(11)
S(1)-C(1)	1.7552(13)
N(1)-C(9)	1.4917(17)
N(1)-C(8)	1.4968(18)
C(1)-C(6)	1.3840(18)
C(1)-C(2)	1.3897(18)
C(2)-C(3)	1.383(2)
C(2)-H(2)	0.989(18)
C(3)-C(4)	1.395(2)
C(3)-H(3)	0.924(19)
C(4)-C(5)	1.3940(18)
C(4)-C(7)	1.5044(19)
C(5)-C(6)	1.3882(17)
C(5)-H(5)	0.930(17)
C(6)-H(6)	0.946(16)
C(7)-H(7A)	0.9600
C(7)-H(7B)	0.9600
C(7)-H(7C)	0.9600
C(8)-C(9)	1.4724(19)
C(8)-H(8A)	0.930(18)
C(8)-H(8B)	0.921(17)
C(9)-C(10)	1.5056(18)
C(9)-H(9)	0.923(15)
C(10)-C(11)	1.5103(18)
C(10)-H(10A)	0.963(17)
C(10)-H(10B)	0.958(18)
C(11)-C(12)	1.391(2)
C(11)-C(16)	1.3924(19)
C(12)-C(13)	1.390(2)
C(12)-H(12)	0.968(18)
C(13)-C(14)	1.385(2)
C(13)-H(13)	0.98(2)
C(14)-C(15)	1.386(2)
C(14)-H(14)	0.926(17)
C(15)-C(16)	1.387(2)
C(15)-H(15)	0.97(2)
C(16)-H(16)	0.970(18)

O(1)-S(1)-O(2)	118.27(7)
O(1)-S(1)-N(1)	106.04(6)
O(2)-S(1)-N(1)	112.07(6)
O(1)-S(1)-C(1)	110.29(7)

O(2)-S(1)-C(1)	108.37(6)
N(1)-S(1)-C(1)	100.32(6)
C(9)-N(1)-C(8)	59.03(8)
C(9)-N(1)-S(1)	115.89(9)
C(8)-N(1)-S(1)	115.62(9)
C(6)-C(1)-C(2)	121.31(12)
C(6)-C(1)-S(1)	119.09(10)
C(2)-C(1)-S(1)	119.59(10)
C(3)-C(2)-C(1)	118.99(12)
C(3)-C(2)-H(2)	120.5(10)
C(1)-C(2)-H(2)	120.4(10)
C(2)-C(3)-C(4)	121.19(13)
C(2)-C(3)-H(3)	118.9(11)
C(4)-C(3)-H(3)	119.9(11)
C(5)-C(4)-C(3)	118.39(12)
C(5)-C(4)-C(7)	120.03(13)
C(3)-C(4)-C(7)	121.54(13)
C(6)-C(5)-C(4)	121.31(13)
C(6)-C(5)-H(5)	119.7(11)
C(4)-C(5)-H(5)	119.0(11)
C(1)-C(6)-C(5)	118.77(13)
C(1)-C(6)-H(6)	119.7(9)
C(5)-C(6)-H(6)	121.5(9)
C(4)-C(7)-H(7A)	109.5
C(4)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	109.5
C(4)-C(7)-H(7C)	109.5
H(7A)-C(7)-H(7C)	109.5
H(7B)-C(7)-H(7C)	109.5
C(9)-C(8)-N(1)	60.31(8)
C(9)-C(8)-H(8A)	119.8(11)
N(1)-C(8)-H(8A)	114.0(11)
C(9)-C(8)-H(8B)	119.5(11)
N(1)-C(8)-H(8B)	117.0(11)
H(8A)-C(8)-H(8B)	114.7(15)
C(8)-C(9)-N(1)	60.66(9)
C(8)-C(9)-C(10)	121.96(12)
N(1)-C(9)-C(10)	114.73(11)
C(8)-C(9)-H(9)	117.6(9)
N(1)-C(9)-H(9)	115.6(10)
C(10)-C(9)-H(9)	114.8(9)
C(9)-C(10)-C(11)	111.67(11)
C(9)-C(10)-H(10A)	107.6(9)
C(11)-C(10)-H(10A)	111.6(9)
C(9)-C(10)-H(10B)	109.1(10)
C(11)-C(10)-H(10B)	108.6(10)

H(10A)-C(10)-H(10B)	108.1(14)
C(12)-C(11)-C(16)	118.90(13)
C(12)-C(11)-C(10)	119.93(13)
C(16)-C(11)-C(10)	121.15(12)
C(13)-C(12)-C(11)	120.89(13)
C(13)-C(12)-H(12)	119.8(10)
C(11)-C(12)-H(12)	119.2(10)
C(14)-C(13)-C(12)	119.83(14)
C(14)-C(13)-H(13)	119.7(12)
C(12)-C(13)-H(13)	120.5(12)
C(13)-C(14)-C(15)	119.60(14)
C(13)-C(14)-H(14)	119.7(11)
C(15)-C(14)-H(14)	120.7(11)
C(14)-C(15)-C(16)	120.65(14)
C(14)-C(15)-H(15)	120.6(11)
C(16)-C(15)-H(15)	118.8(11)
C(15)-C(16)-C(11)	120.12(13)
C(15)-C(16)-H(16)	121.5(10)
C(11)-C(16)-H(16)	118.4(10)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for gbh36lta. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
S(1)	19(1)	22(1)	15(1)	-1(1)	3(1)	4(1)
O(1)	37(1)	30(1)	19(1)	4(1)	5(1)	12(1)
O(2)	17(1)	36(1)	22(1)	-8(1)	2(1)	-1(1)
N(1)	21(1)	18(1)	17(1)	0(1)	6(1)	3(1)
C(1)	18(1)	17(1)	15(1)	-2(1)	4(1)	3(1)
C(2)	22(1)	20(1)	23(1)	3(1)	10(1)	-1(1)
C(3)	19(1)	18(1)	31(1)	-1(1)	9(1)	-4(1)
C(4)	16(1)	21(1)	22(1)	-4(1)	4(1)	2(1)
C(5)	23(1)	21(1)	18(1)	2(1)	6(1)	-1(1)
C(6)	19(1)	17(1)	20(1)	0(1)	6(1)	-1(1)
C(7)	24(1)	29(1)	25(1)	-7(1)	1(1)	-1(1)
C(8)	25(1)	22(1)	18(1)	-3(1)	5(1)	3(1)
C(9)	20(1)	17(1)	18(1)	0(1)	4(1)	0(1)
C(10)	22(1)	23(1)	21(1)	-2(1)	5(1)	5(1)
C(11)	13(1)	22(1)	22(1)	0(1)	4(1)	4(1)
C(12)	18(1)	22(1)	28(1)	2(1)	4(1)	0(1)
C(13)	23(1)	32(1)	23(1)	8(1)	5(1)	3(1)
C(14)	18(1)	39(1)	20(1)	-2(1)	-1(1)	4(1)
C(15)	16(1)	27(1)	32(1)	-7(1)	3(1)	-2(1)
C(16)	18(1)	22(1)	29(1)	3(1)	8(1)	2(1)

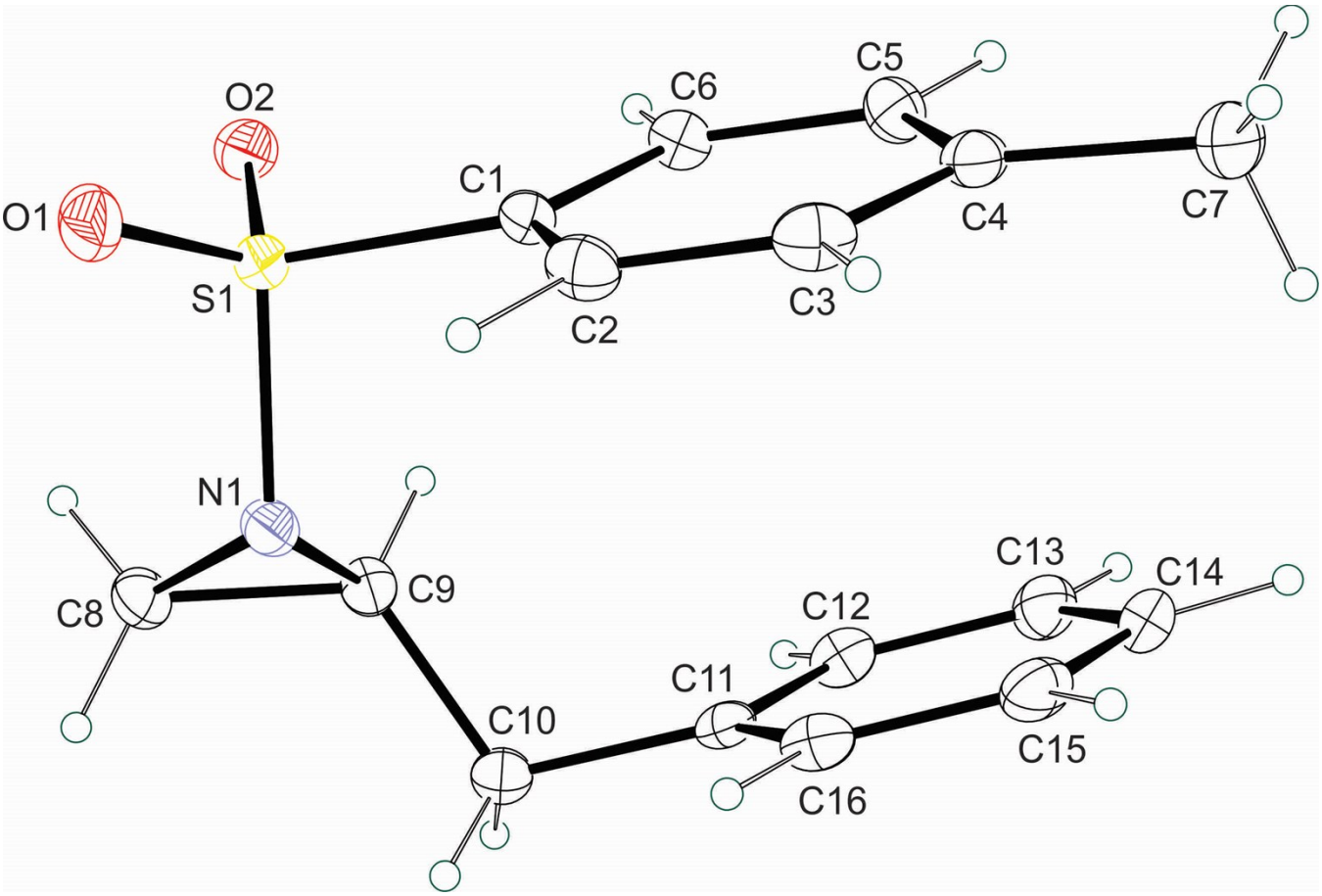
Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for gbh36lta.

	x	y	z	U(eq)
H(2)	8490(20)	1738(15)	2270(20)	24(4)
H(3)	7060(20)	1181(15)	-490(20)	25(5)
H(5)	9690(20)	3414(15)	-2620(20)	25(4)
H(6)	11200(20)	4013(13)	122(19)	17(4)
H(7A)	6807	1211	-3641	40
H(7B)	7853	2094	-4442	40
H(7C)	5958	2351	-3916	40
H(8A)	9110(30)	5097(14)	5910(20)	26(4)
H(8B)	11120(20)	5105(13)	5550(20)	24(4)
H(9)	9860(20)	5381(12)	2596(19)	11(3)
H(10A)	6310(20)	5170(13)	3320(20)	18(4)
H(10B)	6950(20)	6259(14)	2770(20)	23(4)
H(12)	7330(20)	6601(14)	-160(20)	27(4)
H(13)	6340(30)	6196(16)	-3120(30)	38(5)
H(14)	4780(20)	4607(13)	-3910(20)	23(4)
H(15)	4090(30)	3439(18)	-1840(20)	40(5)
H(16)	5150(20)	3838(14)	1110(20)	28(4)

Table 6. Torsion angles [°] for gbh36lta.

O(1)-S(1)-N(1)-C(9)	161.44(9)
O(2)-S(1)-N(1)-C(9)	31.03(11)
C(1)-S(1)-N(1)-C(9)	-83.77(10)
O(1)-S(1)-N(1)-C(8)	95.12(10)
O(2)-S(1)-N(1)-C(8)	-35.30(11)
C(1)-S(1)-N(1)-C(8)	-150.10(10)
O(1)-S(1)-C(1)-C(6)	-147.78(10)
O(2)-S(1)-C(1)-C(6)	-16.87(12)
N(1)-S(1)-C(1)-C(6)	100.70(11)
O(1)-S(1)-C(1)-C(2)	33.38(12)
O(2)-S(1)-C(1)-C(2)	164.29(10)
N(1)-S(1)-C(1)-C(2)	-78.14(11)
C(6)-C(1)-C(2)-C(3)	-1.01(19)
S(1)-C(1)-C(2)-C(3)	177.81(11)
C(1)-C(2)-C(3)-C(4)	-0.5(2)
C(2)-C(3)-C(4)-C(5)	2.1(2)
C(2)-C(3)-C(4)-C(7)	-175.53(13)
C(3)-C(4)-C(5)-C(6)	-2.31(19)
C(7)-C(4)-C(5)-C(6)	175.37(13)
C(2)-C(1)-C(6)-C(5)	0.82(19)
S(1)-C(1)-C(6)-C(5)	-178.01(10)
C(4)-C(5)-C(6)-C(1)	0.88(19)
S(1)-N(1)-C(8)-C(9)	106.08(10)
N(1)-C(8)-C(9)-C(10)	102.41(14)
S(1)-N(1)-C(9)-C(8)	-105.62(11)
C(8)-N(1)-C(9)-C(10)	-114.18(13)
S(1)-N(1)-C(9)-C(10)	140.20(10)
C(8)-C(9)-C(10)-C(11)	-158.53(13)
N(1)-C(9)-C(10)-C(11)	-88.93(14)
C(9)-C(10)-C(11)-C(12)	-84.00(16)
C(9)-C(10)-C(11)-C(16)	94.55(15)
C(16)-C(11)-C(12)-C(13)	0.5(2)
C(10)-C(11)-C(12)-C(13)	179.04(13)
C(11)-C(12)-C(13)-C(14)	0.0(2)
C(12)-C(13)-C(14)-C(15)	-0.1(2)
C(13)-C(14)-C(15)-C(16)	-0.3(2)
C(14)-C(15)-C(16)-C(11)	0.8(2)
C(12)-C(11)-C(16)-C(15)	-0.82(19)
C(10)-C(11)-C(16)-C(15)	-179.39(12)

Symmetry transformations used to generate equivalent atoms:



X-ray crystallography of **(*S*)-1d**. Thermal ellipsoids are shown at 50% probability

12.X-Ray Crystallography Data of (*S*)-2d (CCDC 1490052)

Table 1. Crystal data and structure refinement for gbh35lta.

Identification code	gbh35lta	
Empirical formula	C16 H18 F N O2 S	
Formula weight	307.37	
Temperature	99.9(1) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P 2_1 2_1 2_1	
Unit cell dimensions	a = 8.2947(3) Å	α= 90°.
	b = 9.5293(2) Å	β= 90°.
	c = 18.8749(4) Å	γ = 90°.
Volume	1491.92(7) $Å^3$	
Z	4	
Density (calculated)	1.368 Mg/m^3	
Absorption coefficient	0.231 mm^{-1}	
F(000)	648	
Crystal color, habit	colorless prism	
Crystal size	0.30 x 0.18 x 0.15 mm^3	
Theta range for data collection	3.26 to 28.06°.	
Index ranges	-10<=h<=10, -12<=k<=12, -24<=l<=24	
Reflections collected	16718	
Independent reflections	3614 [R(int) = 0.046]	
Completeness to theta = 28.06°	99.8 %	
Absorption correction	multi-scan	
Max. and min. transmission	1.000 and 0.845	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3614 / 0 / 248	
Goodness-of-fit on F^2	1.032	
Final R indices [I>2sigma(I)]	R1 = 0.0341, wR2 = 0.0733	
R indices (all data)	R1 = 0.0379, wR2 = 0.0752	
Absolute structure parameter	-0.04(6)	
Largest diff. peak and hole	0.376 and -0.320 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for gbh35lta. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
S(1)	4248(1)	5944(1)	2400(1)	17(1)
F(1)	8675(1)	5418(1)	3467(1)	25(1)
O(1)	4153(2)	7312(1)	2720(1)	22(1)
O(2)	3118(2)	4889(1)	2618(1)	22(1)
N(1)	6013(2)	5327(2)	2545(1)	19(1)
C(1)	4047(2)	6189(2)	1476(1)	16(1)
C(2)	3096(2)	7292(2)	1234(1)	19(1)
C(3)	2836(3)	7433(2)	509(1)	22(1)
C(4)	3522(2)	6500(2)	28(1)	21(1)
C(5)	4477(2)	5416(2)	283(1)	20(1)
C(6)	4741(2)	5248(2)	1007(1)	20(1)
C(7)	3214(3)	6680(2)	-756(1)	29(1)
C(8)	7444(2)	6184(2)	2411(1)	19(1)
C(9)	8236(2)	6643(2)	3092(1)	18(1)
C(10)	9741(2)	7518(2)	2981(1)	21(1)
C(11)	10404(2)	8068(2)	3675(1)	19(1)
C(12)	11608(2)	7355(2)	4036(1)	22(1)
C(13)	12140(3)	7816(2)	4694(1)	25(1)
C(14)	11471(2)	9000(2)	4997(1)	25(1)
C(15)	10293(2)	9737(2)	4637(1)	24(1)
C(16)	9764(2)	9276(2)	3980(1)	22(1)

Table 3. Bond lengths [Å] and angles [°] for gbh35lta.

S(1)-O(2)	1.4345(13)
S(1)-O(1)	1.4388(12)
S(1)-N(1)	1.6012(15)
S(1)-C(1)	1.7683(16)
F(1)-C(9)	1.413(2)
N(1)-C(8)	1.463(2)
N(1)-H(1N)	0.815(19)
C(1)-C(6)	1.386(2)
C(1)-C(2)	1.391(2)
C(2)-C(3)	1.392(2)
C(2)-H(2)	0.94(2)
C(3)-C(4)	1.392(3)
C(3)-H(3)	0.94(2)
C(4)-C(5)	1.388(3)
C(4)-C(7)	1.513(3)
C(5)-C(6)	1.392(3)
C(5)-H(5)	0.96(2)
C(6)-H(6)	0.95(2)
C(7)-H(7C)	0.9600
C(7)-H(7A)	0.9600
C(7)-H(7B)	0.9600
C(8)-C(9)	1.508(2)
C(8)-H(8A)	0.97(2)
C(8)-H(8B)	0.94(2)
C(9)-C(10)	1.516(3)
C(9)-H(9)	1.03(2)
C(10)-C(11)	1.515(2)
C(10)-H(10A)	0.94(2)
C(10)-H(10B)	0.95(2)
C(11)-C(12)	1.386(3)
C(11)-C(16)	1.392(3)
C(12)-C(13)	1.391(3)
C(12)-H(12)	0.93(2)
C(13)-C(14)	1.381(3)
C(13)-H(13)	0.95(2)
C(14)-C(15)	1.383(3)
C(14)-H(14)	0.98(2)
C(15)-C(16)	1.387(3)
C(15)-H(15)	0.92(2)
C(16)-H(16)	0.93(2)
O(2)-S(1)-O(1)	118.60(8)
O(2)-S(1)-N(1)	106.96(8)
O(1)-S(1)-N(1)	108.12(8)

O(2)-S(1)-C(1)	108.31(8)
O(1)-S(1)-C(1)	106.75(7)
N(1)-S(1)-C(1)	107.67(8)
C(8)-N(1)-S(1)	120.50(12)
C(8)-N(1)-H(1N)	119.8(14)
S(1)-N(1)-H(1N)	112.7(14)
C(6)-C(1)-C(2)	120.97(15)
C(6)-C(1)-S(1)	120.39(13)
C(2)-C(1)-S(1)	118.51(13)
C(1)-C(2)-C(3)	118.91(17)
C(1)-C(2)-H(2)	119.2(12)
C(3)-C(2)-H(2)	121.9(12)
C(4)-C(3)-C(2)	121.05(18)
C(4)-C(3)-H(3)	121.3(12)
C(2)-C(3)-H(3)	117.6(12)
C(5)-C(4)-C(3)	118.88(17)
C(5)-C(4)-C(7)	121.34(17)
C(3)-C(4)-C(7)	119.78(17)
C(4)-C(5)-C(6)	121.01(17)
C(4)-C(5)-H(5)	122.0(13)
C(6)-C(5)-H(5)	117.0(13)
C(1)-C(6)-C(5)	119.17(17)
C(1)-C(6)-H(6)	121.6(12)
C(5)-C(6)-H(6)	119.1(12)
C(4)-C(7)-H(7C)	109.5
C(4)-C(7)-H(7A)	109.5
H(7C)-C(7)-H(7A)	109.5
C(4)-C(7)-H(7B)	109.5
H(7C)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	109.5
N(1)-C(8)-C(9)	111.60(15)
N(1)-C(8)-H(8A)	109.4(13)
C(9)-C(8)-H(8A)	107.3(12)
N(1)-C(8)-H(8B)	108.0(13)
C(9)-C(8)-H(8B)	112.2(13)
H(8A)-C(8)-H(8B)	108.4(18)
F(1)-C(9)-C(8)	107.36(14)
F(1)-C(9)-C(10)	108.17(14)
C(8)-C(9)-C(10)	113.60(15)
F(1)-C(9)-H(9)	106.2(11)
C(8)-C(9)-H(9)	109.9(12)
C(10)-C(9)-H(9)	111.3(12)
C(11)-C(10)-C(9)	111.67(15)
C(11)-C(10)-H(10A)	110.8(12)
C(9)-C(10)-H(10A)	106.4(13)
C(11)-C(10)-H(10B)	111.1(12)

C(9)-C(10)-H(10B)	106.8(12)
H(10A)-C(10)-H(10B)	109.9(17)
C(12)-C(11)-C(16)	118.54(17)
C(12)-C(11)-C(10)	121.11(17)
C(16)-C(11)-C(10)	120.29(17)
C(11)-C(12)-C(13)	120.82(18)
C(11)-C(12)-H(12)	120.1(14)
C(13)-C(12)-H(12)	119.0(14)
C(14)-C(13)-C(12)	120.06(19)
C(14)-C(13)-H(13)	123.0(14)
C(12)-C(13)-H(13)	116.9(14)
C(13)-C(14)-C(15)	119.70(18)
C(13)-C(14)-H(14)	119.3(13)
C(15)-C(14)-H(14)	121.0(13)
C(14)-C(15)-C(16)	120.17(19)
C(14)-C(15)-H(15)	120.0(14)
C(16)-C(15)-H(15)	119.8(14)
C(15)-C(16)-C(11)	120.68(18)
C(15)-C(16)-H(16)	119.1(14)
C(11)-C(16)-H(16)	120.1(14)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for gbh35lta. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
S(1)	18(1)	15(1)	17(1)	0(1)	0(1)	-1(1)
F(1)	26(1)	24(1)	26(1)	8(1)	-5(1)	-2(1)
O(1)	26(1)	18(1)	21(1)	0(1)	1(1)	0(1)
O(2)	23(1)	21(1)	24(1)	1(1)	2(1)	-4(1)
N(1)	19(1)	15(1)	22(1)	0(1)	-4(1)	0(1)
C(1)	14(1)	17(1)	17(1)	1(1)	-2(1)	-4(1)
C(2)	20(1)	14(1)	23(1)	-1(1)	0(1)	0(1)
C(3)	22(1)	18(1)	25(1)	4(1)	-5(1)	0(1)
C(4)	19(1)	22(1)	21(1)	2(1)	-2(1)	-6(1)
C(5)	18(1)	22(1)	22(1)	-6(1)	2(1)	-1(1)
C(6)	17(1)	18(1)	24(1)	0(1)	-3(1)	0(1)
C(7)	35(1)	29(1)	22(1)	1(1)	-6(1)	-1(1)
C(8)	18(1)	22(1)	18(1)	2(1)	1(1)	0(1)
C(9)	17(1)	18(1)	20(1)	2(1)	0(1)	0(1)
C(10)	18(1)	24(1)	21(1)	3(1)	1(1)	0(1)
C(11)	14(1)	20(1)	23(1)	4(1)	2(1)	-5(1)
C(12)	20(1)	18(1)	28(1)	4(1)	0(1)	0(1)
C(13)	22(1)	23(1)	31(1)	8(1)	-5(1)	-2(1)
C(14)	24(1)	25(1)	25(1)	2(1)	-4(1)	-9(1)
C(15)	20(1)	21(1)	31(1)	-3(1)	2(1)	-2(1)
C(16)	15(1)	22(1)	30(1)	3(1)	-2(1)	0(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for gbh35lta.

	x	y	z	U(eq)
H(1N)	6060(20)	4480(20)	2495(10)	16(5)
H(2)	2660(20)	7920(20)	1562(10)	15(5)
H(3)	2200(30)	8190(20)	356(10)	16(5)
H(5)	4980(30)	4740(20)	-28(12)	26(6)
H(6)	5360(20)	4480(20)	1166(10)	19(5)
H(7C)	4030	6193	-1020	43
H(7A)	3241	7660	-874	43
H(7B)	2174	6302	-873	43
H(8A)	7130(30)	7020(20)	2157(11)	23
H(8B)	8140(30)	5660(20)	2124(11)	23
H(9)	7410(30)	7160(20)	3406(11)	22
H(10A)	9440(20)	8260(20)	2682(11)	21(5)
H(10B)	10510(30)	6930(20)	2747(11)	21(5)
H(12)	12050(30)	6540(20)	3846(12)	32(6)
H(13)	12980(30)	7290(20)	4911(12)	30(6)
H(14)	11870(30)	9320(20)	5461(11)	22(5)
H(15)	9830(30)	10510(20)	4841(12)	30(6)
H(16)	8940(30)	9760(20)	3753(12)	30(6)

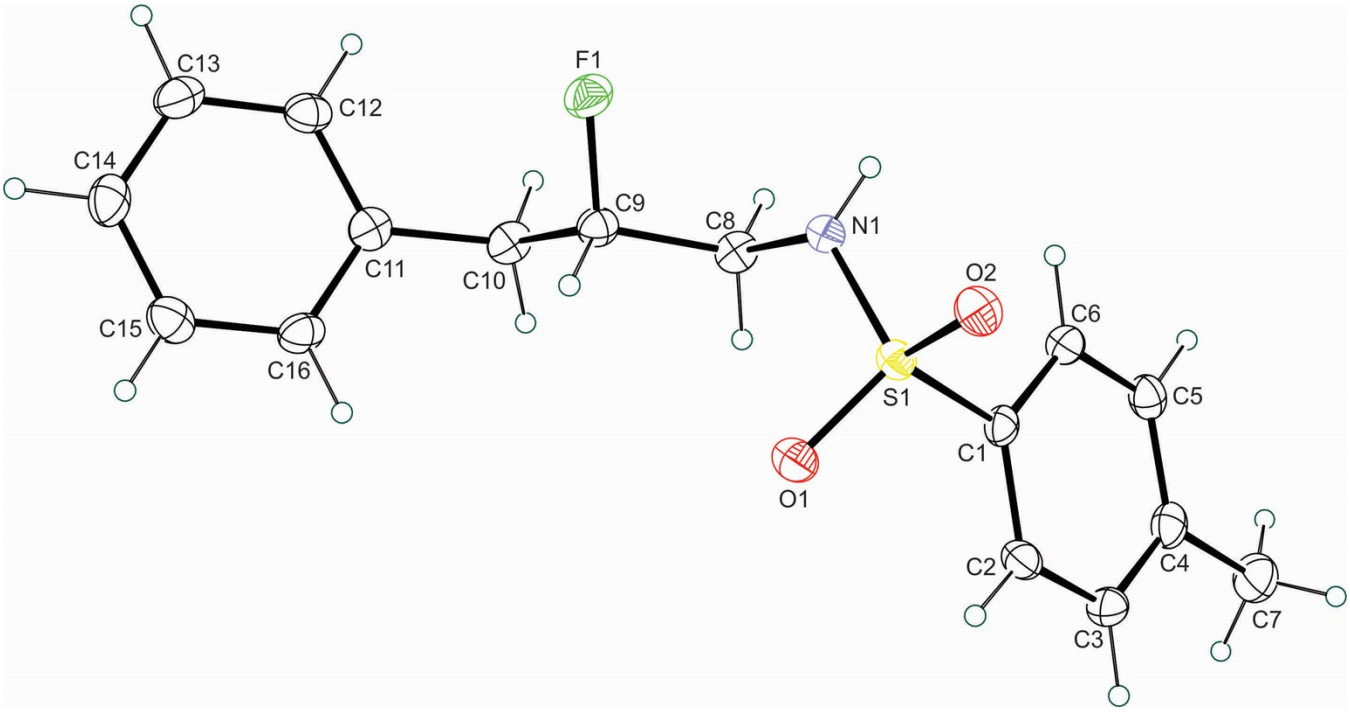
Table 6. Torsion angles [°] for gbh35lta.

O(2)-S(1)-N(1)-C(8)	-176.88(13)
O(1)-S(1)-N(1)-C(8)	-48.10(15)
C(1)-S(1)-N(1)-C(8)	66.90(14)
O(2)-S(1)-C(1)-C(6)	-78.93(16)
O(1)-S(1)-C(1)-C(6)	152.30(15)
N(1)-S(1)-C(1)-C(6)	36.41(16)
O(2)-S(1)-C(1)-C(2)	97.04(15)
O(1)-S(1)-C(1)-C(2)	-31.74(16)
N(1)-S(1)-C(1)-C(2)	-147.63(14)
C(6)-C(1)-C(2)-C(3)	0.5(3)
S(1)-C(1)-C(2)-C(3)	-175.41(15)
C(1)-C(2)-C(3)-C(4)	-0.6(3)
C(2)-C(3)-C(4)-C(5)	0.1(3)
C(2)-C(3)-C(4)-C(7)	179.89(18)
C(3)-C(4)-C(5)-C(6)	0.5(3)
C(7)-C(4)-C(5)-C(6)	-179.32(18)
C(2)-C(1)-C(6)-C(5)	0.0(3)
S(1)-C(1)-C(6)-C(5)	175.89(14)
C(4)-C(5)-C(6)-C(1)	-0.5(3)
S(1)-N(1)-C(8)-C(9)	108.21(15)
N(1)-C(8)-C(9)-F(1)	59.62(18)
N(1)-C(8)-C(9)-C(10)	179.17(15)
F(1)-C(9)-C(10)-C(11)	-66.22(19)
C(8)-C(9)-C(10)-C(11)	174.69(15)
C(9)-C(10)-C(11)-C(12)	94.7(2)
C(9)-C(10)-C(11)-C(16)	-82.6(2)
C(16)-C(11)-C(12)-C(13)	1.5(3)
C(10)-C(11)-C(12)-C(13)	-175.91(18)
C(11)-C(12)-C(13)-C(14)	-0.1(3)
C(12)-C(13)-C(14)-C(15)	-1.2(3)
C(13)-C(14)-C(15)-C(16)	1.2(3)
C(14)-C(15)-C(16)-C(11)	0.2(3)
C(12)-C(11)-C(16)-C(15)	-1.5(3)
C(10)-C(11)-C(16)-C(15)	175.90(17)

Symmetry transformations used to generate equivalent atoms:

Table 7. Intermolecular Hydrogen bonds for gbh35lta [Å and °].

D-H	d(D-H)	d(H..A)	<DHA	d(D..A)	A
N1-H1N	0.815	2.111	171.41	2.920	O1 [-x+1, y-1/2, -z+1/2]



X-ray crystallography of **(*S*)-2d**. Thermal ellipsoids are shown at 50% probability

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