Supporting Information

But-3-ene-1,3-disulfonyl Difluoride (BDF): A Highly Selective SuFEx Clickable Hub for Quick Assembly of Sultam-Containing Aliphatic Sulfonyl Fluorides

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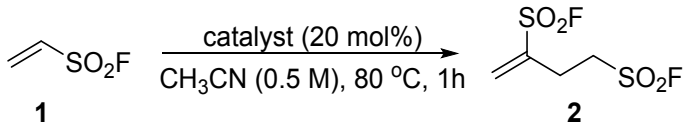
1. General considerations

All reactions were carried out under air atmosphere. Unless otherwise specified, NMR spectra were recorded in $CDCl_3$ or DMSO-d_6 on a 500 MHz (for ^1H), 471 MHz (for ^{19}F), and 126 MHz (for ^{13}C) spectrometer. All chemical shifts were reported in ppm relative to TMS (^1H NMR, 0 ppm) as internal standards. Ethenesulfonyl fluorides [1] were prepared according to literature. Melting points of the products were measured on a micro melting point apparatus (SGW X-4) and uncorrected. HRMS experiments were performed on a TOF-Q ESI or CI/EI instrument. Reagents used in the reactions were purchased from commercial sources and used without further purification.

2. Screening the optimized reaction conditions

Table 1. The reaction in the presence of different catalysts. [a]

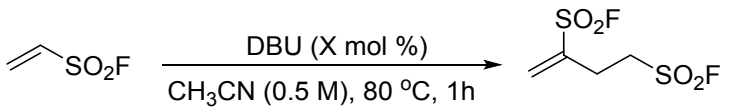


1 **2**

Entry	Catalyst (20 mol%)	Yield (**2**, %) [b]
1	NaOH	trace
2	Na_2CO_3	trace
3	$NaHCO_3$	trace
4	K_2CO_3	5
5	Et_3N	77
6	DIPEA	12
7	DABCO	79
8	**DBU**	**80**
9	DMAP	31

[a] Reaction conditions: A mixture of **1** (2 mmol, 0.165 mL), catalyst (20 mol %) and CH_3CN (0.5 M) was allowed to stir at 80 °C for 1 h under air atmosphere. [b] The yield was determined by HPLC using **2** as the external standard (t_R = 3.741 min, λ_{max} = 209.9 nm, methonal/water = 80 : 20 (v / v)).

Table 2. The reaction in the presence of different DBU loading. [a]

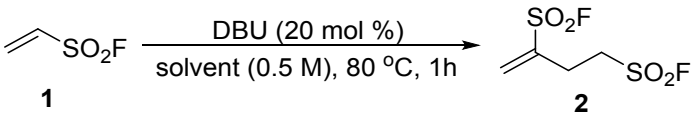


1 **2**

Entry	DBU (X mol %)	Yield (**2**, %) [b]
1	2	14
2	5	28
3	10	55
4	**20**	**80**
5	50	43
6	100	trace

[a] Reaction conditions: A mixture of **1** (2 mmol, 0.165 mL), DBU (X mol %) and CH_3CN (0.5 M) was allowed to stir at 80 °C for 1 h under air atmosphere. [b] The yield was determined by HPLC using **2** as the external standard (t_R = 3.741 min, λ_{max} = 209.9 nm, methonal/water = 80 : 20 (v / v)).

Table 3. The reaction under different solvents. [a]

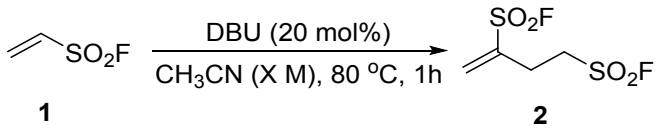


1 **2**

Entry	solvent (0.5 M)	Yield (**2**, %) [b]
1	DCM	42
2	THF	49
3	DMSO	6
4	DCE	27
5	DMF	trace
6	$CHCl_3$	52
7	**CH_3CN**	**80**
8	CH_3OH	38
9	Acetone	30
10	EA	55

[a] Reaction conditions: A mixture of **1** (2 mmol, 0.165 mL), DBU (20 mol %) and solvent (0.5 M) was allowed to stir at 80 °C for 1 h under air atmosphere. [b] The yield was determined by HPLC using **2** as the external standard (t_R = 3.741 min, λ_{max} = 209.9 nm, methonal/water = 80 : 20 (v / v)).

Table 4. The reaction in the presence of different concentration of solvents. [a]

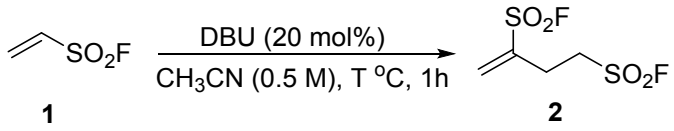


1 **2**

Entry	CH_3CN (X M)	Yield (**2**, %) [b]
1	**0.5**	**80**
2	0.8	79
3	1.0	75
4	1.5	79
5	2.0	72

[a] Reaction conditions: A mixture of **1** (2 mmol, 0.165 mL), DBU (20 mol %) and CH_3CN (X M) was allowed to stir at 80 °C for 1 h under air atmosphere. [b] The yield was determined by HPLC using **2** as the external standard (t_R = 3.741 min, λ_{max} = 209.9 nm, methonal/water = 80 : 20 (v / v)).

Table 5. The reaction under different temperatures. [a]

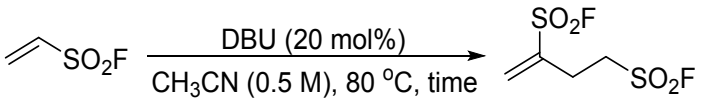


1 **2**

Entry	T °C	Yield (**2**, %) [b]
1	r.t.	29
2	50	42
3	60	54
4	**80**	**80**

[a] Reaction conditions: A mixture of **1** (2 mmol, 0.165 mL), DBU (20 mol %) and CH_3CN (0.5 M) was allowed to stir at different temperature for 1 h under air atmosphere. [b] The yield was determined by HPLC using **2** as the external standard (t_R = 3.741 min, λ_{max} = 209.9 nm, methonal/water = 80 : 20 (v / v)).

Table 6. The reaction under different times. [a]



1 **2**

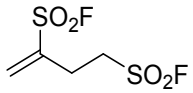
Entry	Time (h)	Yield (**2**, %) [b]
1	0.5	50
2	**1**	**80**
3	2	56
4	6	30
5	12	22

[a] Reaction conditions: A mixture of **1** (2 mmol, 0.165 mL), DBU (20 mol %) and CH_3CN (0.5 M) was allowed to stir at 80 °C for different time under air atmosphere. [b] The yield was determined by HPLC using **2** as the external standard (t_R = 3.741 min, λ_{max} = 209.9 nm, methonal/water = 80 : 20 (v / v)).

3. Procedures for the synthesis of 2

A 250 mL round-bottomed flask was charged with ethenesulfonyl fluoride (ESF) (40 mmol, 3.30 mL), DBU (8 mmol, 20 mmol %, 1.21g), and 80 mL of CH_3CN. The reaction mixture was stirred at 80 °C for 1 hour and upon completion, the reaction mixture was concentrated and purified by flash chromatography on silica gel to provide **2** as a slight yellow oil (16 mmol, 80%, 3.52g).

but-3-ene-1,3-disulfonyl difluoride (2)



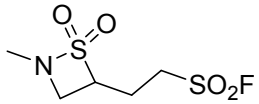
Petroleum ether / ethyl acetate = 5 : 1 (v / v) as eluent for column chromatography. Light yellow oil, 3.52 g, 80% yield. ^{1}H NMR ($CDCl_3$, 500 MHz) δ 6.66 (s, 1H), 6.28 (d, J = 5.5 Hz, 1H), 3.76-3.72 (m, 2H), 3.18 (t, J = 7.3 Hz, 2H).^{19}F NMR (471 MHz, $CDCl_3$) δ 55.71 (s, 1F), 54.58-54.57 (m, 1F). ^{13}C NMR (DMSO-d_6, 126 MHz) δ 138.1 (d, J = 21.8 Hz), 134.1 (d, J = 1.9 Hz), 47.6 (d, J = 15.4 Hz), 23.9 (s). HRMS ESI (m/z): $[M+Na]^+$ calcd for $C_4H_6F_2NaO_4S_2$: 242.9568, found: 242.9564.

4. Procedures for the synthesis of 4

A 10 mL reaction tube was charged with but-3-ene-1,3-disulfonyl difluoride (**2**) (1 mmol, 1 equiv., 220.20 mg) and primary amine (**3**, 2 mmol, 2 equiv.) were dissolved

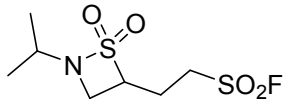
in 2 mL CH_3CN. The reaction mixture was stirred at room temperature for 5-20 minutes and upon completion, the reaction mixture was concentrated and purified by flash chromatography on silica gel to provide the product **4**.[2]

2-(2-methyl-1,1-dioxido-1,2-thiazetidin-4-yl)ethane-1-sulfonyl fluoride (4a)



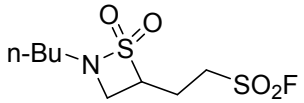
Petroleum ether / ethyl acetate = 3 : 1 (v / v) as eluent for column chromatography. white solid, 120 mg, 52% yield. ^{1}H NMR (DMSO-d_6, 500 MHz) δ 4.74-4.68 (m, 1H), 3.80-3.76 (m, 2H), 3.42-3.32 (m, 2H), 2.85 (s, 3H), 2.64-2.60 (m, 1H), 2.46-2.38 (m, 1H).^{19}F NMR (471 MHz, DMSO-d_6) δ 47.7 (s, 1F). ^{13}C NMR (DMSO-d_6, 126 MHz) δ 51.7 (d, J = 12.7 Hz), 50.2 (s), 42.7 (s), 35.5 (s), 24.8 (s). Mp 72.6-73.8 ^{o}C. HRMS ESI (m/z): [M+Na] $^+$ calcd for $C_5H_{10}FNNaO_4S_2$: 253.9927, found: 253.9924.

2-(2-isopropyl-1,1-dioxido-1,2-thiazetidin-4-yl)ethane-1-sulfonyl fluoride (4b)



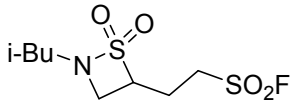
Petroleum ether / ethyl acetate = 3 : 1 (v / v) as eluent for column chromatography. white solid, 257 mg, 99% yield. ^{1}H NMR ($CDCl_3$, 500 MHz) δ 4.38-4.32 (m, 1H), 3.69-3.55 (m, 2H), 3.44-3.37 (m, 2H), 2.83 (t, J = 5.1 Hz, 1H), 2.71-2.63 (m, 1H), 2.55-2.48 (m, 1H), 1.23-1.21 (m, 6H).^{19}F NMR (471 MHz, $CDCl_3$) δ 54.5 (s, 1F). ^{13}C NMR (DMSO-d_6, 126 MHz) δ 66.0 (s), 48.4 (s), 47.1 (d, J = 15.4 Hz), 22.6 (s), 20.5 (s), 20.3 (s). Mp 99.5-101.8 ^{o}C. HRMS ESI (m/z): [M+Na] $^+$ calcd for $C_7H_{14}FNNaO_4S_2$: 282.0240, found: 282.0238.

2-(2-butyl-1,1-dioxido-1,2-thiazetidin-4-yl)ethane-1-sulfonyl fluoride (4c)



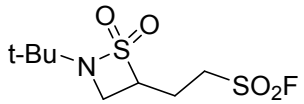
Petroleum ether / ethyl acetate = 3 : 1 (v / v) as eluent for column chromatography. white solid, 197 mg, 72% yield. ^{1}H NMR (DMSO-d_6, 500 MHz) δ 4.53-4.48 (m, 1H), 4.14-4.06 (m, 1H), 4.02-3.95 (m, 1H), 3.33 (dd, J = 7.9 Hz, J = 6.2 Hz, 1H), 2.96-2.89 (m, 3H), 2.70-2.63 (m, 1H), 2.48-2.42 (m, 1H), 2.37-2.29 (m, 1H), 1.48-1.42 (m, 2H), 1.36-1.29 (m, 2H), 0.88 (t, J = 7.3 Hz, 3H).^{19}F NMR (471 MHz, DMSO-d_6) δ 53.45-53.43 (m, 1F). ^{13}C NMR (DMSO-d_6, 126 MHz) δ 52.6 (s), 47.8 (d, J = 14.6 Hz), 47.2 (s), 47.0 (s), 27.2 (s), 22.9 (s), 19.2 (s),13.4 (s). Mp 138.6-139.4 ^{o}C. HRMS ESI (m/z): [M+Na] $^+$ calcd for $C_8H_{16}FNNaO_4S_2$: 296.0397, found: 296.0395.

2-(2-(sec-butyl)-1,1-dioxido-1,2-thiazetidin-4-yl)ethane-1-sulfonyl fluoride (4d)



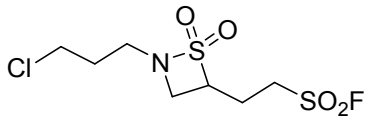
Petroleum ether / ethyl acetate = 3 : 1 (v / v) as eluent for column chromatography. white solid, 219 mg, 80% yield. ^{1}H NMR ($CDCl_3$, 500 MHz) δ 4.47-4.41 (m, 1H), 3.66-3.56 (m, 2H), 3.40 (t, J = 6.8 Hz, 1H), 2.87 (t, J = 5.0 Hz, 1H), 2.82 (d, J = 6.9 Hz, 2H), 2.70-2.63 (m, 1H), 2.55-2.48 (m, 1H), 1.82-1.76 (m, 1H), 0.95 (d, J = 6.5 Hz, 6H).^{19}F NMR (471 MHz, $CDCl_3$) δ 54.4 (s, 1F). ^{13}C NMR (DMSO-d_6, 126 MHz) δ 67.1 (s), 53.6 (s), 47.1 (d, J = 15.4 Hz), 42.8 (s), 26.9 (s), 22.8 (s), 20.2 (s). Mp 82.4-83.8 ^{o}C. HRMS ESI (m/z): [M+Na] $^+$ calcd for $C_8H_{16}FNNaO_4S_2$: 296.0397, found: 296.0395.

2-(2-(tert-butyl)-1,1-dioxido-1,2-thiazetidin-4-yl)ethane-1-sulfonyl fluoride (4e)



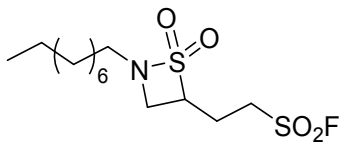
Petroleum ether / ethyl acetate = 3 : 1 (v / v) as eluent for column chromatography. white solid, 191 mg, 70% yield. ^{1}H NMR ($CDCl_3$, 500 MHz) δ 4.34-4.29 (m, 1H), 3.68-3.54 (m, 2H), 3.42 (dd, J = 7.0 Hz, J = 5.4 Hz, 1H), 2.86 (t, J = 4.8 Hz, 1H), 2.68-2.61 (m, 1H), 2.53-2.46 (m, 1H), 1.30 (s, 9H).^{19}F NMR (471 MHz, $CDCl_3$) δ 54.4 (s, 1F). ^{13}C NMR (DMSO-d_6, 126 MHz) δ 65.7 (s), 54.5 (s), 47.1 (d, J = 15.4 Hz), 36.6 (s), 26.7 (s), 22.7 (s). Mp 134.2-135.8 ^{o}C. HRMS ESI (m/z): [M+Na] $^+$ calcd for $C_8H_{16}FNNaO_4S_2$: 296.0397, found: 296.0396.

2-(2-(3-chloropropyl)-1,1-dioxido-1,2-thiazetidin-4-yl)ethane-1-sulfonyl fluoride (4f)



Petroleum ether / ethyl acetate = 3 : 1 (v / v) as eluent for column chromatography. White solid, 232 mg, 79% yield. ^{1}H NMR ($CDCl_3$, 500 MHz) δ 4.46-4.40 (m, 1H), 3.66-3.55 (m, 4H), 3.39 (dd, J = 6.1 Hz, J = 7.6 Hz, 1H), 3.16 (t, J = 6.7 Hz, 2H), 2.86 (t, J = 5.4 Hz, 1H), 2.66-2.58 (m, 1H), 2.51-2.43 (m, 1H), 2.02-1.95 (m, 2H).^{19}F NMR (471 MHz, $CDCl_3$) δ 54.2 (s, 1F). ^{13}C NMR ($CDCl_3$, 126 MHz) δ 57.3 (s), 47.6 (d, J = 18.1 Hz), 43.4 (s), 42.5 (s), 42.0 (s), 30.2 (s), 23.1 (s). Mp 118.7-119.5 ^{o}C. HRMS ESI (m/z): [M+Na] $^+$ calcd for $C_7H_{13}ClFNNaO_4S_2$: 315.9851, found: 315.9849.

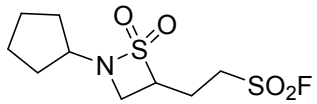
2-(2-decyl-1,1-dioxido-1,2-thiazetidin-4-yl) ethane-1-sulfonyl fluoride (4g)



Petroleum ether / ethyl acetate = 3 : 1 (v / v) as eluent for column chromatography. white solid, 236 mg, 66% yield. ^{1}H NMR (DMSO-d_6, 500 MHz) δ 4.53-4.48 (m, 1H), 4.14-4.06 (m, 1H), 4.0-3.95 (m, 1H), 2.94-2.89 (m, 3H), 2.48-2.42 (m, 1H), 2.36-2.29 (m, 1H), 1.48-1.43 (m, 2H), 1.29-1.18 (m, 15H), 0.86 (t, J = 6.8 Hz, 3H).^{19}F NMR (471 MHz, DMSO-d_6) δ 53.39-53.37 (m, 1F). ^{13}C NMR (DMSO-d_6, 126 MHz) δ 66.9

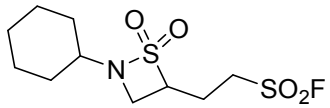
(s), 52.5 (s), 47.2 (d, J = 7.3 Hz), 45.9 (s), 31.3 (s), 28.9 (s), 28.8 (s), 28.7 (s), 28.5 (s), 25.8 (s), 25.1 (s), 22.9 (s), 22.1 (s), 13.9 (s). Mp 72.9-74.6 °C. HRMS ESI (m/z): $[M+Na]^+$ calcd for $C_{14}H_{28}FNNaO_4S_2$: 380.1336, found: 380.1334.

2-(2-cyclopentyl-1,1-dioxido-1,2-thiazetidin-4-yl) ethane-1-sulfonyl fluoride (4h)



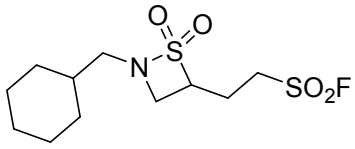
Petroleum ether / ethyl acetate = 3 : 1 (v / v) as eluent for column chromatography. white solid, 205 mg, 72% yield. ^{1}H NMR ($CDCl_3$, 500 MHz) δ 4.38-4.33 (m, 1H), 3.68-3.54 (m, 3H), 3.37 (t, J = 6.9 Hz, 1H), 2.82 (t, J = 5.4 Hz, 1H), 2.70-2.61 (m, 1H), 2.54-2.47 (m, 1H), 1.84-1.63 (m, 8H).^{19}F NMR (471 MHz, $CDCl_3$) δ 53.5 (s, 1F). ^{13}C NMR (DMSO-d_6, 126 MHz) δ 66.1 (s), 58.0 (s), 47.1 (d, J = 15.4 Hz), 40.7 (s), 30.3 (s), 30.2 (s), 23.14 (s), 23.10 (s), 22.6 (s). Mp 158.6-159.8 °C. HRMS ESI (m/z): $[M+Na]^+$ calcd for $C_9H_{16}FNNaO_4S_2$: 308.0397, found: 308.0395.

2-(2-cyclohexyl-1,1-dioxido-1,2-thiazetidin-4-yl) ethane-1-sulfonyl fluoride (4i)



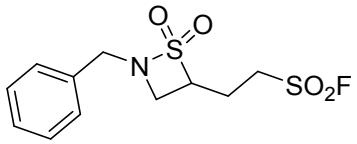
Petroleum ether / ethyl acetate = 3 : 1 (v / v) as eluent for column chromatography. white solid, 186 mg, 62% yield. ^{1}H NMR (DMSO-d_6, 500 MHz) δ 4.47-4.41 (m, 1H), 4.13-4.06 (m, 1H), 4.02-3.95 (m, 1H), 3.05 (s, 1H), 2.92 (t, J = 5.5 Hz, 1H), 2.47-2.41 (m, 1H), 2.35-2.30 (m, 1H), 1.76 (s, 2H), 1.66 (s, 2H), 1.51-1.50 (m, 1H), 1.33-1.17 (m, 5H).^{19}F NMR (471 MHz, DMSO-d_6) δ 53.44-53.43 (m, 1F). ^{13}C NMR (DMSO-d_6, 126 MHz) δ 66.0 (s), 55.2 (s), 47.1 (d, J = 5.5 Hz), 30.2 (s), 29.9 (s), 25.1 (s), 23.0 (s), 22.6 (s). Mp 172.1-173.7 °C. HRMS ESI (m/z): $[M+Na]^+$ calcd for $C_{10}H_{18}FNNaO_4S_2$: 322.0553, found: 322.0550.

2-(2-(cyclohexylmethyl)-1,1-dioxido-1,2-thiazetidin-4-yl)ethane-1-sulfonyl fluoride (4j)



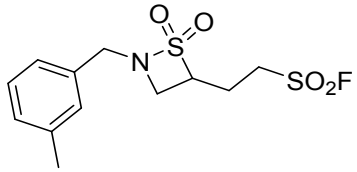
Petroleum ether / ethyl acetate = 3 : 1 (v / v) as eluent for column chromatography. white solid, 291 mg, 93% yield. ^{1}H NMR ($CDCl_3$, 500 MHz) δ 4.36-4.31 (m, 1H), 3.68-3.55 (m, 2H), 3.38-3.35 (m, 1H), 3.15-3.12 (m, 1H), 2.81 (t, J = 5.2 Hz, 1H), 2.68-2.60 (m, 1H), 2.52-2.45 (m, 1H), 1.86-1.84 (m, 2H), 1.72-1.57 (m, 4H), 1.42-1.24 (m, 6H).^{19}F NMR (471 MHz, $CDCl_3$) δ 54.3 (s, 1F). ^{13}C NMR (DMSO-d_6, 126 MHz) δ 137.1 (s), 128.69 (s), 128.66 (s), 126.8 (s), 52.7 (s), 48.4 (s), 47.8 (d, J = 14.5 Hz), 47.3 (s), 31.4 (s), 22.9 (s). Mp 110.4-112.3 °C. HRMS ESI (m/z): $[M+Na]^+$ calcd for $C_{11}H_{20}FNNaO_4S_2$: 336.0710, found: 336.0708.

2-(2-benzyl-1,1-dioxido-1,2-thiazetidin-4-yl)ethane-1-sulfonyl fluoride (4k)



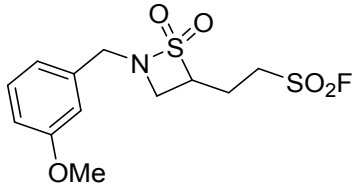
Petroleum ether / ethyl acetate = 3 : 1 (v / v) as eluent for column chromatography. white solid, 258 mg, 84% yield. ^{1}H NMR (DMSO-d_6, 500 MHz) δ 7.40-7.36 (m, 5H), 4.61-4.55 (m, 1H), 4.18 (s, 2H), 4.05-3.99 (m, 2H), 3.35-3.32 (m, 1H), 2.98 (t, J = 5.5 Hz, 1H), 2.54-2.47 (m, 1H), 2.40-2.34 (m, 1H).^{19}F NMR (471 MHz, DMSO-d_6) δ 53.45-53.43 (m, 1F). ^{13}C NMR (DMSO-d_6, 126 MHz) δ 137.4 (s), 129.0 (s), 128.2 (s), 127.3 (s), 60.8 (s), 60.4 (s), 53.9 (s), 47.3 (d, J = 15.5 Hz), 22.9 (s). Mp 70.4-72.1 ^{o}C. HRMS ESI (m/z): [M+Na] $^{+}$ calcd for $C_{11}H_{14}FNNaO_4S_2$: 330.0240, found: 330.0238.

2-(2-(3-methylbenzyl)-1,1-dioxido-1,2-thiazetidin-4-yl)ethane-1-sulfonyl fluoride (4l)



Petroleum ether / ethyl acetate = 3 : 1 (v / v) as eluent for column chromatography. white solid, 260 mg, 81% yield. ^{1}H NMR ($CDCl_3$, 500 MHz) δ 7.28-7.25 (m, 1H), 7.17-7.14 (m, 3H), 4.48-4.42 (m, 1H), 4.17 (s, 2H), 3.64-3.58 (m, 2H), 3.33 (t, J = 6.9 Hz, 1H), 2.80 (t, J = 5.3 Hz, 1H), 2.70-2.63 (m, 1H), 2.53-2.46 (m, 1H), 2.37 (s, 3H).^{19}F NMR (471 MHz, $CDCl_3$) δ 54.3 (s, 1F). ^{13}C NMR (DMSO-d_6, 126 MHz) δ 138.3 (s), 134.8 (s), 131.7 (s), 130.5 (s), 129.7 (s), 127.0 (s), 52.7 (s), 50.5 (s), 48.0 (d, J = 14.5 Hz), 47.0 (s), 22.9 (s), 20.9 (s). Mp 89.6-90.8 ^{o}C. HRMS ESI (m/z): [M+Na] $^{+}$ calcd for $C_{12}H_{16}FNNaO_4S_2$: 344.0397, found: 344.0396.

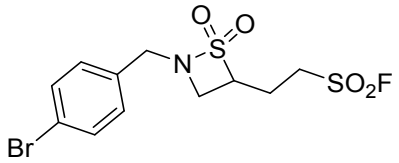
2-(2-(3-methoxybenzyl)-1,1-dioxido-1,2-thiazetidin-4-yl)ethane-1-sulfonyl fluoride (4m)



Petroleum ether / ethyl acetate = 3 : 1 (v / v) as eluent for column chromatography. white solid, 266 mg, 79% yield. ^{1}H NMR ($CDCl_3$, 500 MHz) δ 7.26 (d, J = 8.5 Hz, 2H), 6.88 (d, J = 8.4 Hz, 2H), 4.43-4.37 (m, 1H), 4.13 (s, 2H), 3.79 (s, 3H), 3.64-3.52 (m, 2H), 3.29 (t, J = 7.0 Hz, 1H), 2.76 (t, J = 5.3 Hz, 1H), 2.68-2.60 (m, 1H), 2.50-2.44 (m, 1H), .^{19}F NMR (471 MHz, $CDCl_3$) δ 54.4 (s, 1F). ^{13}C NMR ($CDCl_3$, 126 MHz) δ 159.6 (s), 130.1 (s), 125.8 (s), 114.3 (s), 67.0 (s), 55.3 (s), 49.6 (s), 47.9 (d, J

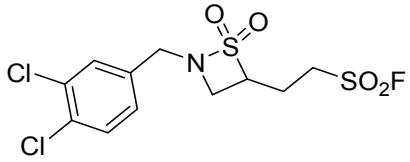
= 19.0 Hz), 41.9 (s), 23.4 (s). Mp 99.4-101.2 °C. HRMS ESI (m/z): [M+Na] $^+$ calcd for $C_{12}H_{16}FNNaO_5S_2$: 360.0346, found: 360.0344.

2-(2-(4-bromobenzyl)-1,1-dioxido-1,2-thiazetidin-4-yl)ethane-1-sulfonyl fluoride (4n)



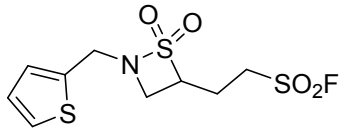
Petroleum ether / ethyl acetate = 3 : 1 (v / v) as eluent for column chromatography. white solid, 263 mg, 68% yield. ^{1}H NMR ($CDCl_3$, 500 MHz) δ 7.49 (d, J = 8.2 Hz, 2H), 7.23 (d, J = 8.2 Hz, 2H), 4.50-4.44 (m, 1H), 4.16 (s, 2H), 3.67-3.55 (m, 2H), 3.34 (t, J = 7.0 Hz, 1H), 2.81 (t, J = 5.4 Hz, 1H), 2.73-2.65 (m, 1H), 2.55-2.48 (m, 1H).^{19}F NMR (471 MHz, $CDCl_3$) δ 54.7 (s, 1F). ^{13}C NMR (DMSO-d_6, 126 MHz) δ 132.2 (s), 131.7 (s), 131.0 (s), 122.5 (s), 52.6 (s), 49.6 (s), 47.9 (d, J = 14.5 Hz), 46.9 (s), 22.9 (s). Mp 108.6-109.3 °C. HRMS ESI (m/z): [M+Na] $^+$ calcd for $C_{11}H_{13}BrFNNaO_4S_2$: 407.9346, found: 407.9342.

2-(2-(3,4-dichlorobenzyl)-1,1-dioxido-1,2-thiazetidin-4-yl)ethane-1-sulfonyl fluoride (4o)



Petroleum ether / ethyl acetate = 3 : 1 (v / v) as eluent for column chromatography. white solid, 144 mg, 38% yield. ^{1}H NMR ($CDCl_3$, 500 MHz) δ 7.46-7.44 (m, 2H), 7.21 (dd, J = 8.3 Hz, J = 1.7 Hz, 1H), 4.54-4.48 (m, 1H), 4.17 (s, 2H), 3.68-3.54 (m, 2H), 3.38 (dd, J =7.7 Hz, J = 6.1 Hz, 1H), 2.84 (t, J = 5.5 Hz, 1H), 2.75-2.68 (m, 1H), 2.60-2.51 (m, 1H).^{19}F NMR (471 MHz, $CDCl_3$) δ 54.8 (s, 1F). ^{13}C NMR ($CDCl_3$, 126 MHz) δ 134.4 (s), 133.1 (s), 132.6 (s), 131.0 (s), 130.5 (s), 127.9 (s), 67.6 (s), 49.4 (s), 48.0 (d, J = 19.1 Hz), 42.5 (s), 23.6 (s). Mp 97.9-99.9 °C. HRMS ESI (m/z): [M+Na] $^+$ calcd for $C_{11}H_{12}Cl_2FNNaO_4S_2$: 397.9461, found: 397.9458.

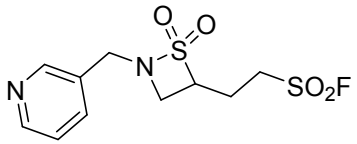
2-(1,1-dioxido-2-(thiophen-2-ylmethyl)-1,2-thiazetidin-4-yl)ethane-1-sulfonyl fluoride (4p)



Petroleum ether / ethyl acetate = 3 : 1 (v / v) as eluent for column chromatography. white solid, 273 mg, 87% yield. ^{1}H NMR (DMSO-d_6, 500 MHz) δ 7.50 (dd, J = 5.1 Hz, J = 1.1 Hz, 1H), 7.09-7.08 (m, 1H), 7.00 (dd, J = 5.0 Hz, J = 3.4 Hz, 1H), 4.60-4.54 (m, 1H), 4.37 (d, J = 1.4 Hz, 1H), 4.15-4.07 (m, 1H), 4.03-3.96 (m, 1H), 2.98 (t, J = 5.5 Hz, 1H), 2.48-2.45 (m, 1H), 2.38-2.30 (m, 1H).^{19}F NMR (471 MHz, DMSO-d_6) δ 53.46-53.43 (m, 1F). ^{13}C NMR (DMSO-d_6, 126 MHz) δ 132.5 (s), 130.9 (s),

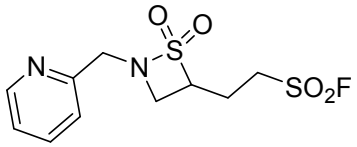
128.6 (s), 127.4 (s), 52.6 (s), 47.9 (d, J = 14.5 Hz), 46.6 (s), 44.6 (s), 22.9(s). Mp 79.3-80.8 °C. HRMS ESI (m/z): [M+Na] $^+$ calcd for $C_9H_{12}FNNaO_4S_3$: 335.9805, found: 335.9803.

2-(1,1-dioxido-2-(pyridin-3-ylmethyl)-1,2-thiazetidin-4-yl)ethane-1-sulfonyl fluoride (4q)



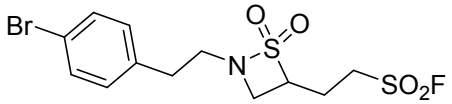
Petroleum ether / ethyl acetate = 3 : 1 (v / v) as eluent for column chromatography. white solid, 284 mg, 92% yield. ^{1}H NMR (DMSO-d_6, 500 MHz) δ 8.58 (s, 1H), 8.52 (d, J = 3.6 Hz, 1H), 7.78 (d, J = 7.6 Hz, 1H), 7.40 (dd, J = 7.7 Hz, J = 4.9 Hz, 1H), 4.63-4.58 (m, 1H), 4.23 (s, 2H), 4.14-3.98 (m, 3H), 3.03 (t, J = 5.7 Hz, 1H), 2.55-2.48 (m, 1H), 2.41-2.33 (m, 1H).^{19}F NMR (471 MHz, DMSO-d_6) δ 53.45-53.44 (m, 1F). ^{13}C NMR (DMSO-d_6, 126 MHz) δ 149.5 (s), 148.8 (s), 136.6 (s), 131.3 (s), 123.8 (s), 67.6 (s), 47.2 (s), 47.16 (d, J = 8.1 Hz), 42.1 (s), 22.8 (s). Mp 118.7-119.5 °C. HRMS ESI (m/z): [M+Na] $^+$ calcd for $C_{10}H_{13}FN_2NaO_4S_2$: 331.0193, found: 331.0190.

2-(1,1-dioxido-2-(pyridin-2-ylmethyl)-1,2-thiazetidin-4-yl)ethane-1-sulfonyl fluoride (4r)



Petroleum ether / ethyl acetate = 3 : 1 (v / v) as eluent for column chromatography. white solid, 277 mg, 90% yield. ^{1}H NMR (DMSO-d_6, 500 MHz) δ 8.53 (s, 1H), 7.81 (t, J = 7.0 Hz, 1H), 7.47 (d, J = 7.3 Hz, 1H), 7.33-7.32 (m, 1H), 4.63-4.61 (m, 1H), 4.28 (s, 2H), 4.15-4.13 (m, 1H), 4.04-4.01 (m, 1H), 3.46 (t, J = 6.5 Hz, 1H), 3.12-3.08 (m, 1H), 2.42-2.37 (m, 1H).^{19}F NMR (471 MHz, DMSO-d_6) δ 53.4 (s, 1F). ^{13}C NMR (DMSO-d_6, 126 MHz) δ 156.2 (s), 149.3 (s), 137.3 (s), 123.0 (s), 122.3 (s), 52.7 (s), 52.4 (d, J = 12.7 Hz), 48.2 (s), 44.8 (s), 24.7 (s). Mp 122.9-123.4 °C. HRMS ESI (m/z): [M+Na] $^+$ calcd for $C_{10}H_{13}FN_2NaO_4S_2$: 331.0193, found: 331.0190.

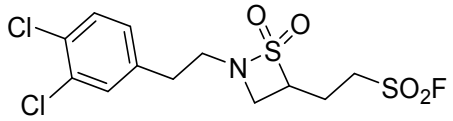
2-(2-(4-bromophenethyl)-1,1-dioxido-1,2-thiazetidin-4-yl)ethane-1-sulfonyl fluoride (4s)



Petroleum ether / ethyl acetate = 2 : 1 (v / v) as eluent for column chromatography. white solid, 288 mg, 72% yield. ^{1}H NMR ($CDCl_3$, 500 MHz) δ 7.44 (d, J = 8.1 Hz, 2H), 7.11 (d, J = 7.9 Hz, 2H), 4.45-4.40 (m, 1H), 3.65-3.53 (m, 2H), 3.32-3.25 (m, 3H), 2.85 (t, J = 7.2 Hz, 2H), 2.76 (t, J = 5.2 Hz, 1H), 2.69-2.61 (m, 1H), 2.53-2.46 (m, 1H).^{19}F NMR (471 MHz, $CDCl_3$) δ 54.6 (s, 1F). ^{13}C NMR (DMSO-d_6, 126 MHz)

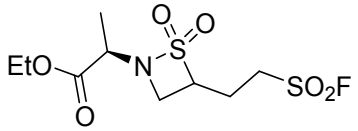
δ 138.2 (s), 131.2 (s), 131.0 (s), 119.5 (s), 67.2 (s), 47.1 (d, *J* = 15.4 Hz), 47.0 (s), 42.0 (s), 32.6 (s), 22.7 (s). Mp 95.4-97.1 °C. HRMS ESI (m/z): [M+Na] $^+$ calcd for $C_{12}H_{15}BrFNNaO_4S_2$:421.9502, found: 421.9500.

2-(2-(3,4-dichlorophenethyl)-1,1-dioxido-1,2-thiazetidin-4-yl)ethane-1-sulfonyl fluoride (4t)



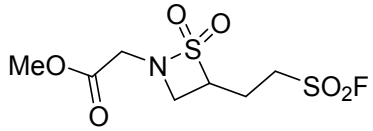
Petroleum ether / ethyl acetate = 3 : 1 (v / v) as eluent for column chromatography. white solid, 211 mg, 54% yield. ^{1}H NMR ($CDCl_3$, 500 MHz) *δ* 7.39 (d, *J* = 8.1 Hz, 1H), 7.33 (s, 1H), 7.08 (d, *J* = 7.2 Hz, 1H), 4.47-4.42 (m, 1H), 3.66-3.53 (m, 2H), 3.33 (t, *J* = 6.9 Hz, 1H), 3.27 (t, *J* = 7.3 Hz, 2H), 2.86 (t, *J* = 7.3 Hz, 2H), 2.79 (t, *J* = 5.3 Hz, 1H), 2.70-2.62 (m, 1H), 2.54-2.47 (m, 1H).^{19}F NMR (471 MHz, $CDCl_3$) *δ* 54.7 (s, 1F). ^{13}C NMR (DMSO-d_6, 126 MHz) δ 138.3 (s), 130.90 (s), 130.86 (s), 130.7 (s), 130.3 (s), 129.3 (s), 67.2 (s), 52.5 (s), 47.1 (d, *J* = 15.5 Hz), 46.7 (s). Mp 103.8-105.5 °C. HRMS ESI (m/z): [M+Na] $^+$ calcd for $C_{12}H_{14}Cl_2FNNaO_4S_2$: 411.9618, found: 411.9616.

Ethyl(2R)-2-(4-(2-(fluorosulfonyl)ethyl)-1,1-dioxido-1,2-thiazetidin-2-yl)propanoate (4u)



Petroleum ether / ethyl acetate = 3 : 1 (v / v) as eluent for column chromatography. white solid, 298 mg, 94% yield. ^{1}H NMR ($CDCl_3$, 500 MHz) *δ* 4.51-4.45 (m, 1H), 4.23-4.17 (m, 2H), 4.02-3.96 (m, 1H), 3.70-3.56 (m, 3H), 3.12 (dt, *J* = 29.2 Hz, *J* = 4.7 Hz, 1H), 2.73-2.65 (m, 1H), 2.57-2.49 (m, 1H), 1.50 (t, *J* = 6.9 Hz, 3H), 1.28 (t, *J* = 7.0 Hz, 3H).^{19}F NMR (471 MHz, $CDCl_3$) *δ* 54.35-54.31 (m, 1F). ^{13}C NMR (DMSO-d_6, 126 MHz) δ 169.2 (d, *J* = 20.9 Hz), 62.1 (s), 54.9 (d, *J* = 41.8 Hz), 52.7 (d, *J* = 27.3 Hz), 47.8 (dd, *J* = 14.5 Hz, *J* = 12.7 Hz), 45.6 (d, *J* = 40.9 Hz), 22.9 (d, *J* = 9.1 Hz), 13.9 (s), 13.8 (s). Mp 188.7-190.2 °C. HRMS ESI (m/z): [M+Na] $^+$ calcd for $C_9H_{16}FNNaO_6S_2$: 340.0295, found: 340.0293.

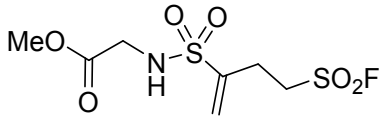
methyl 2-(4-(2-(fluorosulfonyl)ethyl)-1,1-dioxido-1,2-thiazetidin-2-yl)acetate (4v)



Petroleum ether / ethyl acetate = 3 : 1 (v / v) as eluent for column chromatography. Slight yellow solid, 130 mg, 45% yield. ^{1}H NMR (DMSO-d_6, 500 MHz) *δ* 4.66-4.60 (m, 1H), 4.15-4.07 (m, 1H), 4.03-3.97 (m, 1H), 3.93 (d, *J* = 1.2 Hz, 2H), 3.66 (s, 3H), 3.49 (dd, *J* = 8.1 Hz, *J* = 6.4 Hz, 1H), 3.11 (t, *J* = 5.8 Hz, 1H), 2.54-2.46 (m, 1H),

2.41-2.33 (m, 1H).^{19}F NMR (471 MHz, DMSO-d_6) δ 53.42-53.40 (m, 1F). ^{13}C NMR (DMSO-d_6, 126 MHz) δ 167.2 (s), 52.7 (s), 52.6 (s), 47.9 (d, J = 14.5 Hz), 47.6 (s), 47.5 (s), 22.9 (s). Mp 112.4-114.6 ^{o}C. HRMS ESI (m/z): $[M+Na]^+$ calcd for $C_7H_{12}FNNaO_6S_2$: 311.9982, found: 311.9980.

methyl ((4-(fluorosulfonyl) but-1-en-2-yl) sulfonyl) glycinate (11v)

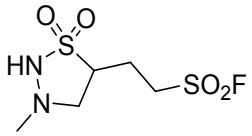


Petroleum ether / ethyl acetate = 3 : 1 (v / v) as eluent for column chromatography. Slight yellow oil, 124 mg, 43% yield. ^{1}H NMR (DMSO-d_6, 500 MHz) δ8.24 (t, J = 6.0 Hz, 1H), 6.02 (s, 1H), 5.89 (s, 1H), 4.22-4.18 (m, 2H), 3.73 (d, J = 6.1 Hz, 2H), 3.64 (s, 3H), 2.94 (t, J = 7.8 Hz, 2H).^{19}F NMR (471 MHz, DMSO-d_6) δ 53.99-53.96 (m, 1F). ^{13}C NMR (DMSO-d_6, 126 MHz) δ 169.8 (s), 143.7 (s), 124.0 (s), 51.9 (s), 48.3 (d, J = 14.6 Hz), 43.4 (s), 23.4 (s). HRMS ESI (m/z): [M+Na] $^+$ calcd for $C_7H_{12}FNNaO_6S_2$: 311.9982, found: 311.9979.

5. Procedures for the synthesis of 7, 8

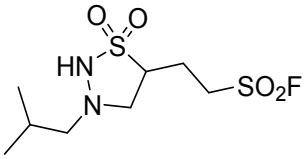
A 10 mL reaction tube was charged with alkyl hydrazine hydrochloride (**6**) (1.5 mmol, 1.5 equiv.) and Et_3N (1.5 mmol, 1.5 equiv., 151.50 mg) was dissolved in 3 mL MeCN and the mixture was stirred at room temperature for 5 minutes. Then, the mixture was added dropwise in 3 minutes into but-3-ene-1,3-disulfonyl difluoride (**2**) (1 mmol, 1 equiv., 220.20 mg) of 2 ml MeCN, Which was allowed to stir for another 30 minutes and upon completion, the reaction mixture was concentrated and purified by flash chromatography on silica gel to provide the product **7, 8**.[3]

2-(3-methyl-1,1-dioxido-1,2,3-thiadiazolidin-5-yl)ethane-1-sulfonyl fluoride (7a)



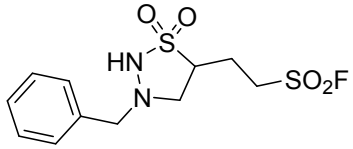
Petroleum ether / ethyl acetate = 3 : 1 (v / v) as eluent for column chromatography. White solid, 217 mg, 88% yield. ^{1}H NMR ($CDCl_3$, 500 MHz) δ 5.67 (br s, 1H), 3.78-3.70 (m, 2H), 3.67-3.56 (m, 2H), 3.23 (dd, J = 11.3 Hz, J = 8.2 Hz, 1H), 2.77 (s, 3H), 2.53-2.46 (m, 1H), 2.34-2.27 (m, 1H).^{19}F NMR (471 MHz, $CDCl_3$) δ 54.1 (s, 1F). ^{13}C NMR (DMSO-d_6, 126 MHz) δ 51.7 (d, J = 12.7 Hz), 50.2 (s), 42.7 (s), 35.5 (s), 24.8 (s). Mp 62.4-64.6 ^{o}C. HRMS ESI (m/z): [M+Na] $^+$ calcd for $C_5H_{11}FN_2NaO_4S_2$: 269.0036, found: 269.0033.

2-(3-isobutyl-1,1-dioxido-1,2,3-thiadiazolidin-5-yl)ethane-1-sulfonyl fluoride (7b)



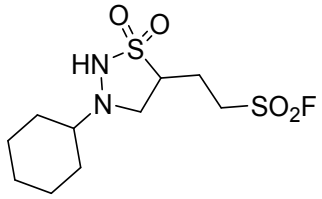
Petroleum ether / ethyl acetate = 3 : 1 (v / v) as eluent for column chromatography. White solid, 190 mg, 66% yield. ^{1}H NMR ($CDCl_3$, 500 MHz) δ 5.62 (br s, 1H), 3.80 (dd, J = 11.1 Hz, J = 7.2 Hz, 1H), 3.77-3.70 (m, 1H), 3.65-3.48 (m, 3H), 3.20 (dd, J = 11.1 Hz, J = 7.8 Hz, 1H), 3.07-3.01 (m, 1H), 2.54-2.45 (m, 1H), 2.37-2.29 (m, 1H), 1.12 (d, J = 6.3 Hz, 6H).^{19}F NMR (471 MHz, $CDCl_3$) δ 54.2 (s, 1F). ^{13}C NMR (DMSO-d_6, 126 MHz) δ 57.4 (s), 55.1 (s), 54.8 (s), 47.4 (d, J = 15.5 Hz), 22.5 (s), 20.7 (s), 20.6 (s). Mp 95.6-97.3 ^{o}C. HRMS ESI (m/z): $[M+Na]^+$ calcd for $C_8H_{17}FN_2NaO_4S_2$: 311.0506, found: 311.0503.

2-(3-benzyl-1,1-dioxido-1,2,3-thiadiazolidin-5-yl)ethane-1-sulfonyl fluoride (7c)



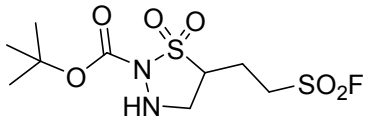
Petroleum ether / ethyl acetate = 3 : 1 (v / v) as eluent for column chromatography. White solid, 235 mg, 73% yield. ^{1}H NMR (DMSO-d_6, 500 MHz) δ 8.18(s, 1H), 7.36-7.27 (m, 5H), 4.17-4.09 (m, 1H), 4.06-3.97 (m, 3H), 3.75-3.71 (m, 1H), 3.67-3.61 (m, 1H), 3.31 (dd, J = 11.6 Hz, J = 7.0 Hz, 1H), 2.36-2.29 (m, 1H), 2.14-2.07 (m, 1H).^{19}F NMR (471 MHz, DMSO-d_6) δ 53.16-53.13 (m, 1F). ^{13}C NMR (DMSO-d_6, 126 MHz) δ 137.4 (s), 129.0 (s), 128.2 (s), 127.3 (s), 60.8 (s), 60.4 (s), 53.9 (s), 47.3 (d, J = 15.5 Hz), 22.9 (s). Mp 118.7-120.2 ^{o}C. HRMS ESI (m/z): $[M+Na]^+$ calcd for $C_{11}H_{15}FN_2NaO_4S_2$: 345.0349, found: 345.0347.

2-(3-cyclohexyl-1,1-dioxido-1,2,3-thiadiazolidin-5-yl)ethane-1-sulfonyl fluoride (7d)



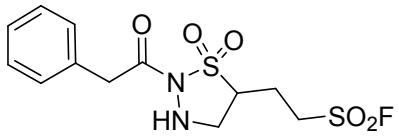
Petroleum ether / ethyl acetate = 3 : 1 (v / v) as eluent for column chromatography. White solid, 239 mg, 76% yield. ^{1}H NMR (DMSO-d_6, 500 MHz) δ 4.16-4.08 (m, 1H), 4.02-3.87 (m, 2H), 3.72 (dd, J = 11.5 Hz, J = 7.2 Hz, 1H), 3.51-3.46 (m, 2H), 3.23 (dd, J = 11.5 Hz, J = 7.0 Hz, 1H), 2.62-2.58 (m, 1H), 2.32-2.22 (m, 1H), 2.11-1.52 (m, 9H). ^{19}F NMR (471 MHz, DMSO-d_6) δ 53.08-53.05 (m, 1F). ^{13}C NMR (DMSO-d_6, 126 MHz) δ 62.3 (s), 57.1 (s), 54.4 (s), 47.4 (d, J = 14.5 Hz), 30.4 (s), 30.2 (s), 25.6 (s), 23.8 (s), 22.5 (s). Mp 120.3-122.5 ^{o}C. HRMS ESI (m/z): $[M+Na]^+$ calcd for $C_{10}H_{19}FN_2NaO_4S_2$: 337.0662, found: 337.0658.

tert-butyl 5-(2-(fluorosulfonyl)ethyl)-1,2,3-thiadiazolidine-2-carboxylate 1,1-dioxide (8e)



Petroleum ether / ethyl acetate = 3 : 1 (v / v) as eluent for column chromatography. White solid, 200 mg, 60% yield. ^{1}H NMR ($CDCl_3$, 500 MHz) δ 6.40 (br s, 1H), 3.82-3.71 (m, 3H), 3.55 (dd, J = 13.6 Hz, J = 4.3 Hz, 1H), 3.18 (dd, J = 13.4 Hz, J = 8.0 Hz, 1H), 2.73-2.66 (m, 1H), 2.61-2.54 (m, 1H), 1.44 (s, 9H).^{19}F NMR (471 MHz, $CDCl_3$) δ 53.7 (s, 1F). ^{13}C NMR ($CDCl_3$, 126 MHz) δ 157.2 (s), 81.6 (s), 58.9 (d, J = 12.7 Hz), 50.2 (s), 28.2 (s), 22.0 (s). Mp 98.5-100.9 ^{o}C. HRMS ESI (m/z): [M+Na] $^{+}$ calcd for $C_9H_{17}FN_2NaO_6S_2$: 355.0404, found: 355.0401.

2-(1,1-dioxido-2-(2-phenylacetyl)-1,2,3-thiadiazolidin-5-yl)ethane-1-sulfonyl fluoride (8f)



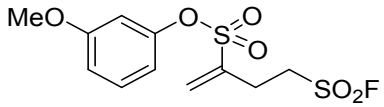
Petroleum ether / ethyl acetate = 3 : 1 (v / v) as eluent for column chromatography. White solid, 312 mg, 89% yield. ^{1}H NMR (DMSO-d_6, 500 MHz) δ 7.33 (t, J = 7.4 Hz, 2H), 7.28-7.23 (m, 3H), 4.17-4.10 (m, 1H), 4.05-3.97 (m, 1H), 3.82 (s, 2H), 3.74-3.69 (m, 1H), 3.68-3.62 (m, 1H), 3.34-3.29 (m, 1H), 2.36-2.29 (m, 1H), 2.27-2.20 (m, 1H).^{19}F NMR (471 MHz, DMSO-d_6) δ 53.40-53.39 (m, 1F). ^{13}C NMR (DMSO-d_6, 126 MHz) δ 169.5 (s), 134.0 (s), 129.7 (s), 128.6 (s), 127.1 (s), 57.6 (s), 49.7 (s), 47.2 (d, J = 15.5 Hz), 40.9 (s), 21.5 (s). Mp 118.7-120.3 ^{o}C. HRMS ESI (m/z): [M+Na] $^{+}$ calcd for $C_{12}H_{15}FN_2NaO_5S_2$: 373.0299, found: 373.0296.

6. Procedures for the synthesis of 11

Method A: a 10 mL reaction tube was charged with but-3-ene-1,3-disulfonyl difluoride (**2**) (1 mmol, 1 equiv., 220.20 mg), phenol (**10a-10e**, 1 mmol, 1 equiv.) and Cs_2CO_3 (1 mmol, 1 equiv., 325. 32 mg) were dissolved in 5 mL CH_3CN. The reaction mixture was stirred at room temperature for 1-2 hours and upon completion, the reaction mixture was washed by Aqueous solution of sodium carbonate and concentrated and purified by flash chromatography on silica gel to provide the product **11a-11d**.[3]

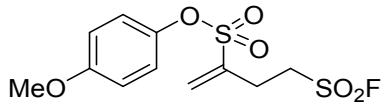
Method B: a 10 mL reaction tube was charged with but-3-ene-1,3-disulfonyl difluoride (**2**) (1 mmol, 1 equiv., 220.20 mg), secondary amines (**10f-10k**, 1.5 mmol, 1.5 equiv.) were dissolved in 5 mL DCM. The reaction mixture was stirred at room temperature for 1-2 hours and upon completion, the reaction mixture was concentrated and purified by flash chromatography on silica gel to provide the product **11e-11j**.[3]

3-methoxyphenyl 4-(fluorosulfonyl)but-1-ene-2-sulfonate (11a)



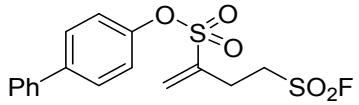
Petroleum ether / ethyl acetate = 3 : 1 (v / v) as eluent for column chromatography. Slight yellow oil, 208 mg, 64% yield (Method A). ^{1}H NMR ($CDCl_3$, 500 MHz) δ 7.39 (t, J = 8.2 Hz, 1H), 6.87 (dd, J = 8.6 Hz, J = 2.0 Hz, 1H), 6.79-6.76 (m, 2H), 6.34 (d, J = 1.2 Hz, 1H), 6.07 (d, J = 1.1 Hz, 1H), 3.81-3.79 (m, 5H), 3.18 (t, J = 7.4 Hz, 1H). ^{19}F NMR (471 MHz, $CDCl_3$) δ 54.95-54.94 (m, 1F). ^{13}C NMR ($CDCl_3$, 126 MHz) δ 160.9 (s), 150.1 (s), 140.5 (s), 131.1 (s), 130.5 (s), 113.8 (s), 113.4 (s), 108.1 (s), 55.7 (s), 49.3 (d, J = 18.2 Hz), 25.9 (s). HRMS ESI (m/z): $[M+H]^+$ calcd for $C_9H_8O_3ClFS$: 248.9783, found: 248.9779.

4-methoxyphenyl 4-(fluorosulfonyl) but-1-ene-2-sulfonate (11b)



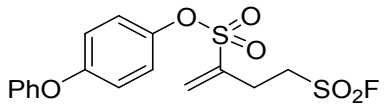
Petroleum ether / ethyl acetate = 3 : 1 (v / v) as eluent for column chromatography. Slight yellow oil, 220 mg, 68% yield (Method A). ^{1}H NMR (DMSO-d_6, 500 MHz) δ 7.24-7.21 (m, 2H), 7.00-6.96 (m, 2H), 6.33 (s, 1H), 6.19 (s, 1H), 4.35-4.31 (m, 2H), 3.76 (s, 3H), 3.12-3.09 (m, 2H). ^{19}F NMR (471 MHz, DMSO-d_6) δ 54.47-54.46 (m, 1F). ^{13}C NMR (DMSO-d_6, 126 MHz) δ 158.2 (s), 142.3 (s), 139.4 (s), 130.8 (s), 123.2 (s), 114.9 (s), 55.5 (s), 47.8 (d, J = 14.5 Hz), 24.1 (s). HRMS ESI (m/z): $[M+Na]^+$ calcd for $C_{11}H_{13}FNaO_6S_2$: 347.0030, found: 347.0020.

[1,1'-biphenyl]-4-yl 4-(fluorosulfonyl) but-1-ene-2-sulfonate (11c)



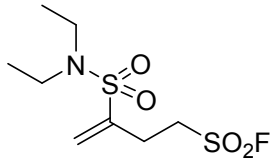
Petroleum ether / ethyl acetate = 5 : 1 (v / v) as eluent for column chromatography. White solid, 193 mg, 52% yield (Method A). ^{1}H NMR (DMSO-d_6, 500 MHz) δ 7.76-7.74 (m, 2H), 7.68-7.66 (m, 2H), 7.50-7.46 (m, 2H), 7.40-7.38 (m, 3H), 6.38 (d, J = 1.4 Hz, 1H), 6.27 (d, J = 0.8 Hz, 1H), 4.39-4.35 (m, 2H), 3.13 (t, J = 7.5 Hz, 2H). ^{19}F NMR (471 MHz, DMSO-d_6) δ 54.74-54.72 (m, 1F). ^{13}C NMR (DMSO-d_6, 126 MHz) δ 148.4 (s), 139.6 (s), 139.5 (s), 138.8 (s), 131.0 (s), 129.0 (s), 128.4 (s), 127.9 (s), 126.8 (s), 122.6 (s), 47.8 (d, J = 15.5 Hz), 24.1 (s). Mp 61.5-63.0 ^{o}C HRMS ESI (m/z): $[M+Na]^+$ calcd for $C_{16}H_{15}FNaO_5S_2$: 393.0237, found: 393.0237.

4-phenoxyphenyl 4-(fluorosulfonyl) but-1-ene-2-sulfonate (11d)



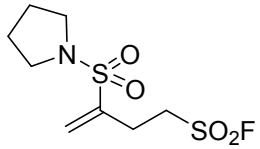
Petroleum ether / ethyl acetate = 2 : 1 (v / v) as eluent for column chromatography. Slight yellow oil, 155 mg, 40% yield (Method A). ^{1}H NMR ($CDCl_3$, 500 MHz) δ 7.41-7.38 (m, 2H), 7.20-7.16 (m, 3H), 7.05-7.01 (m, 4H), 6.35 (d, J = 1.2 Hz, 1H), 6.10 (d, J = 1.1 Hz, 1H), 3.85-3.81 (m, 2H), 3.22-3.19 (m, 2H). ^{19}F NMR (471 MHz, $CDCl_3$) δ 54.99-54.97 (m, 1F). ^{13}C NMR ($CDCl_3$, 126 MHz) δ 156.7 (s), 156.4 (s), 144.1 (s), 140.3 (s), 131.1 (s), 130.1 (s), 124.2 (s), 123.3 (s), 119.53 (s), 119.48 (s), 49.2 (d, J = 18.2 Hz), 25.8 (s). HRMS ESI (m/z): $[M+Na]^+$ calcd for $C_{16}H_{15}FNaO_6S_2$: 409.0186, found: 409.0183.

3-(N, N-diethylsulfamoyl) but-3-ene-1-sulfonyl fluoride (11e)



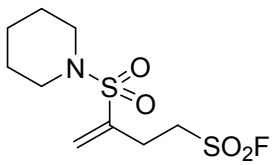
Petroleum ether / ethyl acetate = 3 : 1 (v / v) as eluent for column chromatography. Yellow oil, 197 mg, 72% yield (Method B). ^{1}H NMR ($CDCl_3$, 500 MHz) δ 6.15 (s, 1H), 5.77 (s, 1H), 3.78-3.74 (m, 2H), 3.30 (q, J = 7.1 Hz, 1H), 2.94 (t, J = 7.9 Hz, 2H), 1.22 (t, J = 7.1 Hz, 1H).^{19}F NMR (471 MHz, $CDCl_3$) δ 54.03-54.02 (m, 1F). ^{13}C NMR ($CDCl_3$, 126 MHz) δ 144.2 (s), 125.2 (s), 49.9 (d, J = 17.3 Hz), 41.9 (s), 25.5 (s), 14.5 (s). HRMS ESI (m/z): $[M+Na]^+$ calcd for $C_8H_{16}FNNaO_4S_2$: 296.0397, found: 296.0395.

3-(pyrrolidin-1-ylsulfonyl) but-3-ene-1-sulfonyl fluoride (11f)



Petroleum ether / ethyl acetate = 3 : 1 (v / v) as eluent for column chromatography. Yellow oil, 212 mg, 78% yield (Method B). ^{1}H NMR ($CDCl_3$, 500 MHz) δ 6.15 (s, 1H), 5.81 (s, 1H), 3.79-3.75 (m, 2H), 3.36-3.33 (m, 4H), 2.97 (t, J = 7.7 Hz, 2H), 1.97-1.95 (m, 4H).^{19}F NMR (471 MHz, $CDCl_3$) δ 54.25-54.24 (m, 1F). ^{13}C NMR ($CDCl_3$, 126 MHz) δ 143.1 (s), 125.7 (s), 140.9 (s), 49.8 (d, J = 17.3 Hz), 48.0 (s), 26.0 (s). Mp 92.4-94.6 ^{o}C. HRMS ESI (m/z): $[M+Na]^+$ calcd for $C_8H_{14}FNNaO_4S_2$: 294.0240, found: 294.0238.

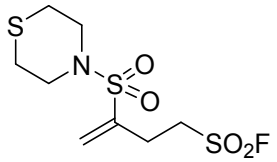
3-(piperidin-1-ylsulfonyl) but-3-ene-1-sulfonyl fluoride (11g)



Petroleum ether / ethyl acetate = 3 : 1 (v / v) as eluent for column chromatography. Yellow oil, 191 mg, 67% yield (Method B). ^{1}H NMR ($CDCl_3$, 500 MHz) δ 6.15 (s, 1H), 5.83 (s, 1H), 3.76-3.72 (m, 2H), 3.21-3.19 (m, 4H), 3.43-3.38 (m, 1H), 2.93 (t, J = 7.7 Hz, 2H), 1.64-1.58 (m, 6H).^{19}F NMR (471 MHz, $CDCl_3$) δ 54.18-54.17 (m, 1F). ^{13}C NMR ($CDCl_3$, 126 MHz) δ 143.0 (s), 126.4 (s), 49.8 (d, J = 17.3 Hz), 46.5 (s),

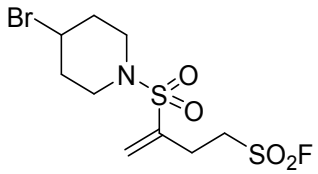
26.0 (s), 25.7 (s), 23.8 (s). Mp 83.8-85.0 °C. HRMS ESI (m/z): $[M+Na]^+$ calcd for $C_9H_{16}FNNaO_4S_2$: 308.0397, found: 308.0394.

3-(thiomorpholinosulfonyl) but-3-ene-1-sulfonyl fluoride (11h)



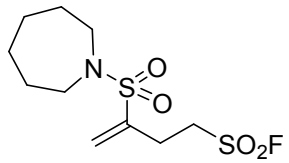
Petroleum ether / ethyl acetate = 3 : 1 (v / v) as eluent for column chromatography. Slight yellow oil, 209 mg, 69% yield (Method B). ^{1}H NMR ($CDCl_3$, 500 MHz) δ 6.16 (s, 1H), 5.85 (d, J = 0.9 Hz, 1H), 3.75-3.71 (m, 2H), 3.55-3.53 (m, 4H), 2.93-2.90 (m, 2H), 2.71-2.69 (m, 4H). ^{19}F NMR (471 MHz, $CDCl_3$) δ 54.47-54.46 (m, 1F). ^{13}C NMR ($CDCl_3$, 126 MHz) δ 142.9 (s), 126.5 (s), 49.5 (d, J = 17.2 Hz), 47.6 (s), 27.6 (s), 25.6 (s). HRMS ESI (m/z): $[M+Na]^+$ calcd for $C_8H_{14}FNNaO_4S_3$: 325.9961, found: 325.9958.

3-((4-bromopiperidin-1-yl)sulfonyl)but-3-ene-1-sulfonyl fluoride (11i)



Petroleum ether / ethyl acetate = 3 : 1 (v / v) as eluent for column chromatography. Slight yellow oil, 269 mg, 74% yield (Method B). ^{1}H NMR ($CDCl_3$, 500 MHz) δ 6.15 (s, 1H), 5.86 (d, J = 0.9 Hz, 1H), 4.42-4.38 (m, 1H), 3.75-3.71 (m, 2H), 3.43-3.38 (m, 2H), 3.32-3.27 (m, 2H), 2.94-2.90 (m, 2H), 2.20-2.14 (m, 2H), 2.06-2.00 (m, 2H).^{19}F NMR (471 MHz, $CDCl_3$) δ 54.44-54.43 (m, 1F). ^{13}C NMR ($CDCl_3$, 126 MHz) δ 142.6 (s), 126.8 (s), 49.5 (d, J = 17.3 Hz), 47.9 (s), 43.1 (s), 34.9 (s), 25.7 (s). HRMS ESI (m/z): $[M+H]^+$ calcd for $C_9H_8O_3ClFS$: 248.9783, found: 248.9779.

3-(azepan-1-ylsulfonyl) but-3-ene-1-sulfonyl fluoride (11j)



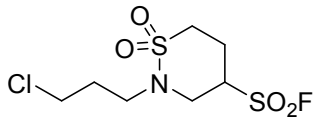
Petroleum ether / ethyl acetate = 3 : 1 (v / v) as eluent for column chromatography. Yellow oil, 135 mg, 45% yield (Method B). ^{1}H NMR ($CDCl_3$, 500 MHz) δ 6.08 (s, 1H), 5.76 (s, 1H), 3.78-3.74 (m, 2H), 3.33 (t, J = 6.0 Hz, 4H), 2.93 (t, J = 7.9 Hz, 2H), 1.82-1.72 (m, 4H), 1.66-1.65 (m, 4H).^{19}F NMR (471 MHz, $CDCl_3$) δ 54.13-54.12 (m, 1F). ^{13}C NMR ($CDCl_3$, 126 MHz) δ 133.5 (s), 124.9 (s), 48.8 (d, J = 18.2 Hz), 29.7

(s), 26.9 (s), 25.6 (s). HRMS ESI (m/z): $[M+Na]^+$ calcd for $C_{10}H_{18}FNNaO_4S_2$: 322.0553, found: 322.0555.

7. Procedures for the synthesis of 14

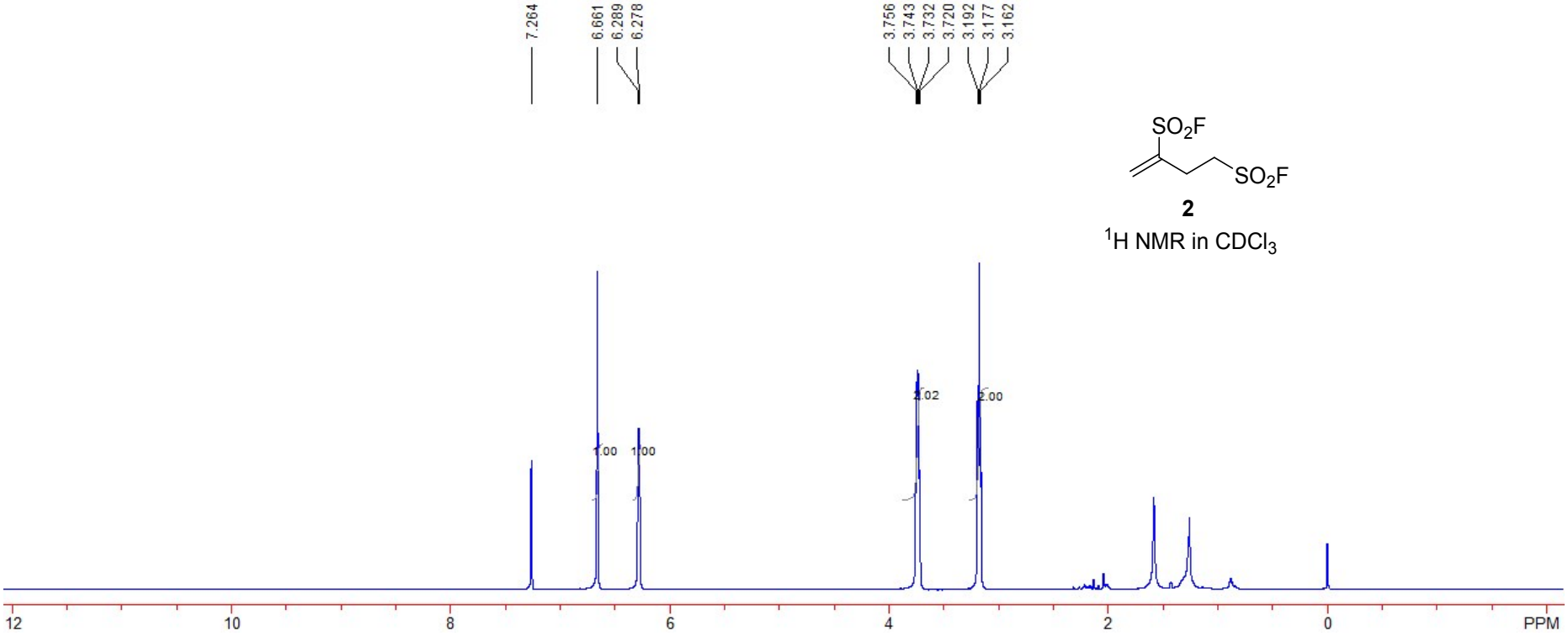
A 10 mL reaction tube was charged with but-3-ene-1,3-disulfonyl difluoride (**2**) (1 mmol, 1 equiv., 220.20 mg), azetidine hydrochloride (**10k**, 1 mmol, 1 equiv., 93.55 mg) and Cs_2CO_3 (1 mmol, 1 equiv., 325. 32 mg) were dissolved in 5 mL CH_3CN. The reaction mixture was stirred at room temperature for 1-2 hours and upon completion, the reaction mixture was washed by Aqueous solution of sodium carbonate and concentrated and purified by flash chromatography on silica gel to provide the product **14**.[3]

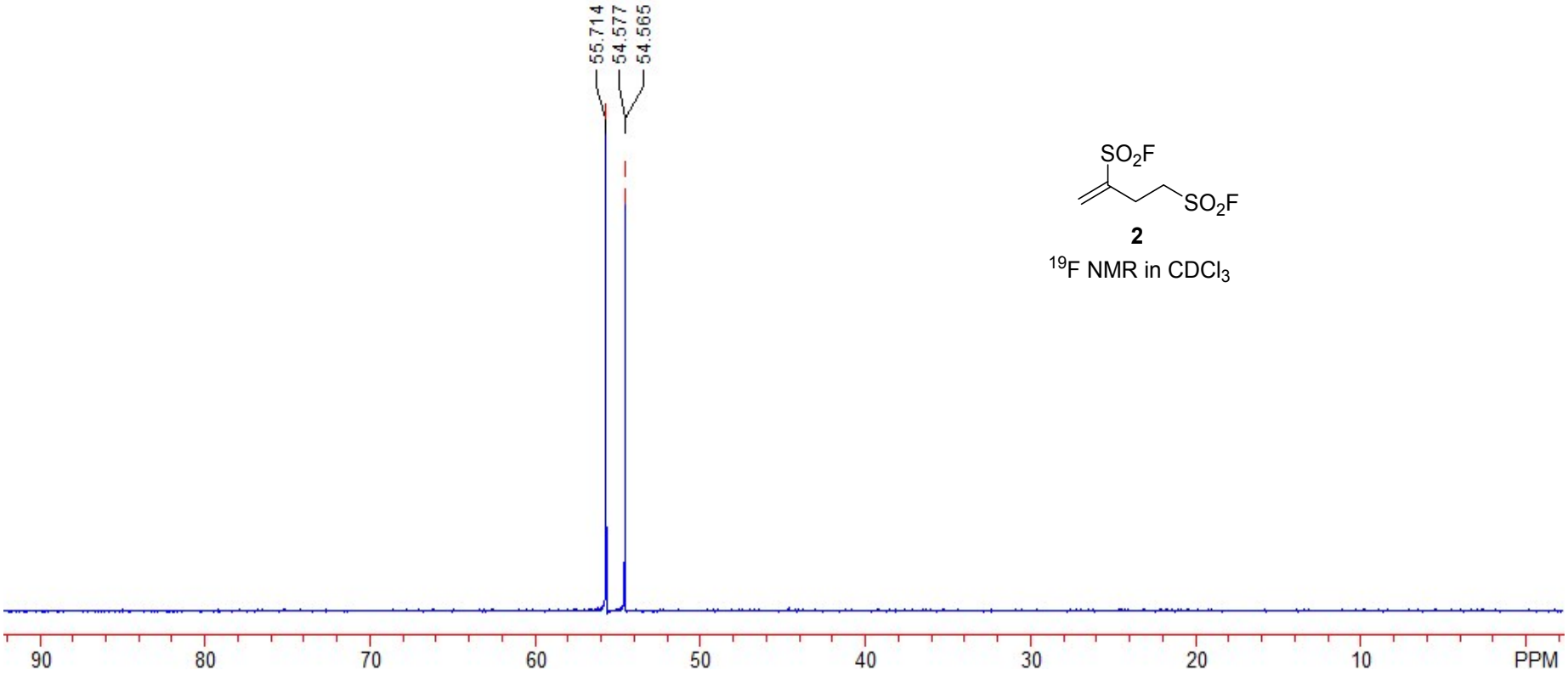
2-(3-chloropropyl)-1,2-thiazinane-4-sulfonyl fluoride 1,1-dioxide (14)



Petroleum ether / ethyl acetate = 3 : 1 (v / v) as eluent for column chromatography. White solid, 163 mg, 63% yield(Method A). ^{1}H NMR ($CDCl_3$, 500 MHz) δ 4.03 (dd, J = 14.3 Hz, J = 8.5 Hz, 1H), 3.85-3.82 (m, 1H), 3.68-3.59 (m, 3H), 3.54-3.50 (m, 1H), 3.43-3.38 (m, 1H), 3.32-3.27 (m, 1H), 3.13-3.08 (m, 1H), 2.81-2.77 (m, 2H), 2.10-2.05 (m, 2H).^{19}F NMR (471 MHz, $CDCl_3$) δ 49.2 (s, 1F). ^{13}C NMR ($CDCl_3$, 126 MHz) δ 54.6 (d, J = 14.5 Hz), 49.5 (s), 46.3 (s), 45.6 (s), 41.6 (s), 31.9 (s), 24.8 (s). Mp 120.3-122.5 ^{o}C. HRMS ESI (m/z): $[M+Na]^+$ calcd for $C_7H_{13}ClFNNaO_4S_2$: 315.9851, found: 315.9849.

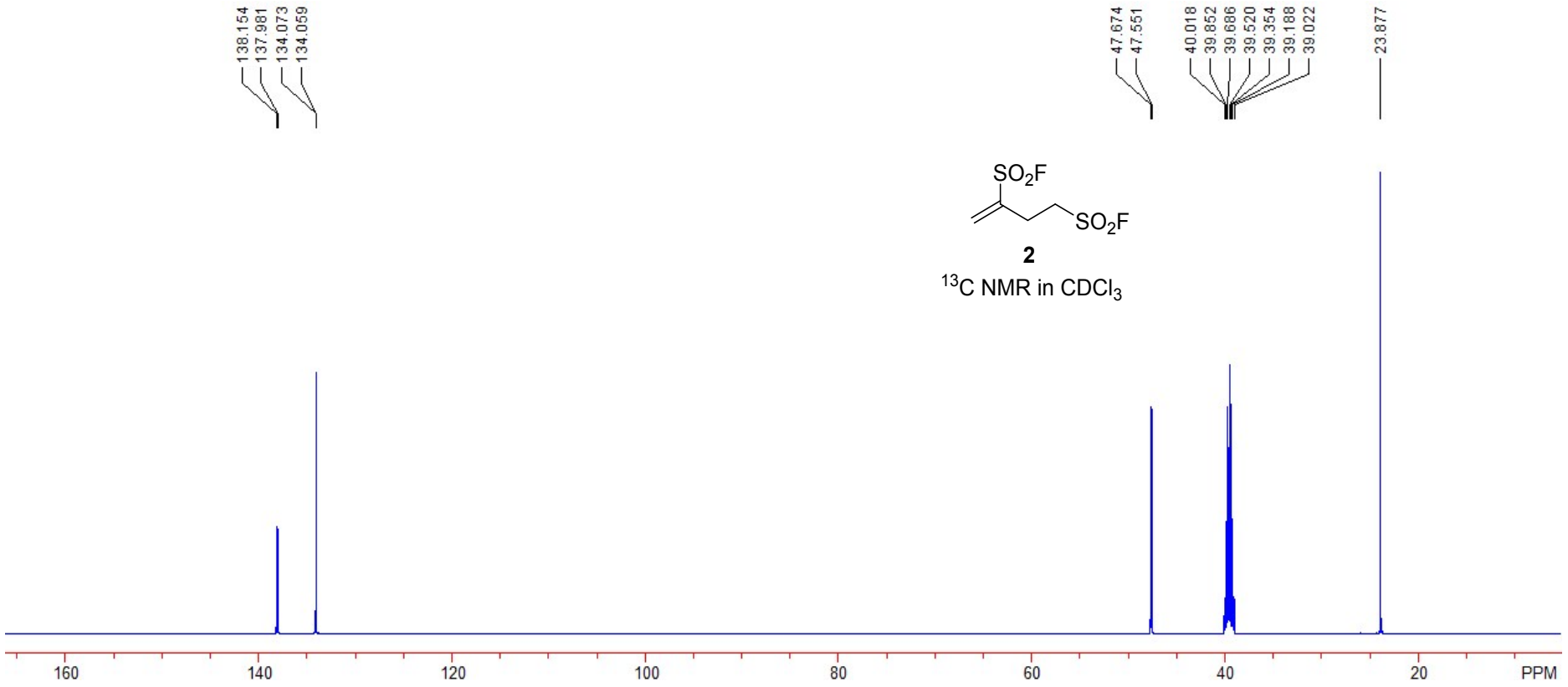
8. NMR spectra

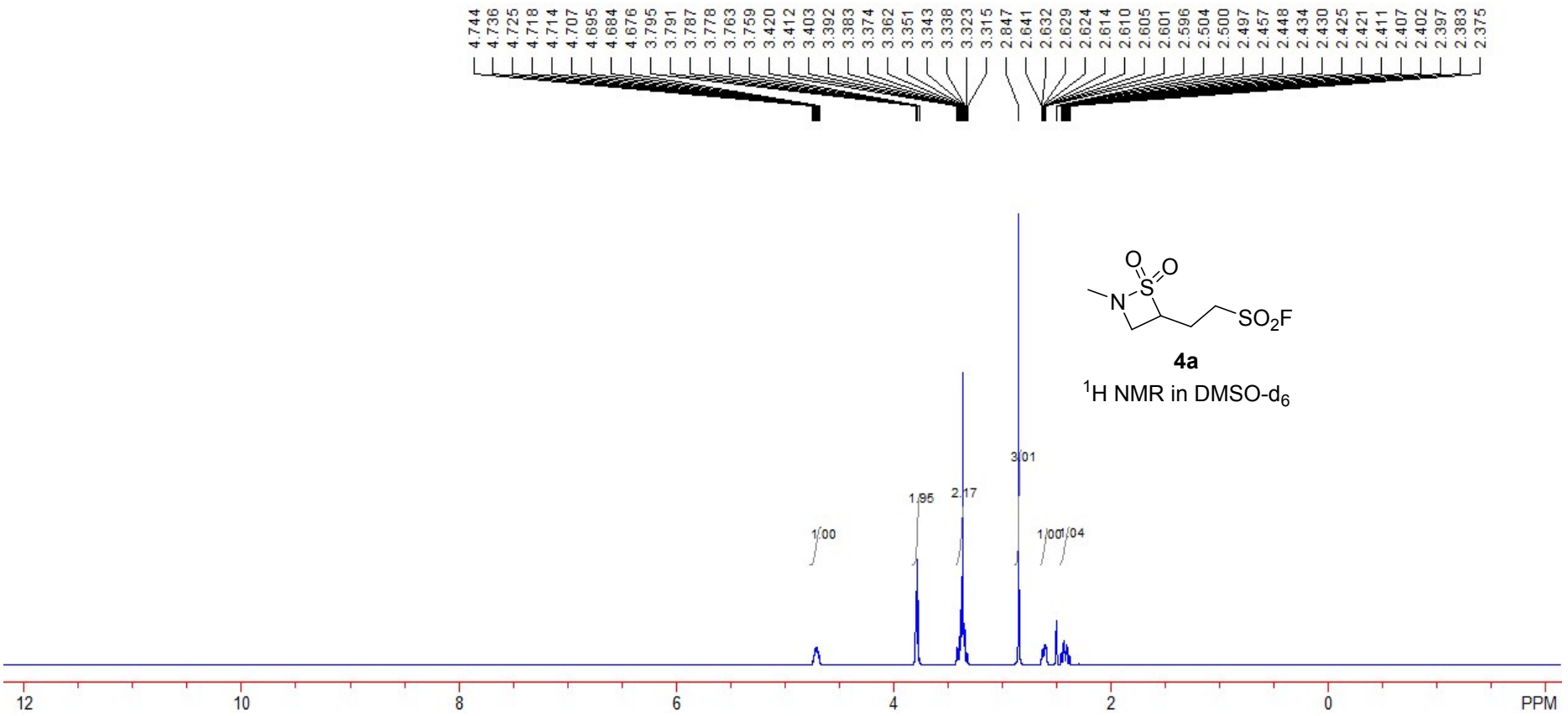


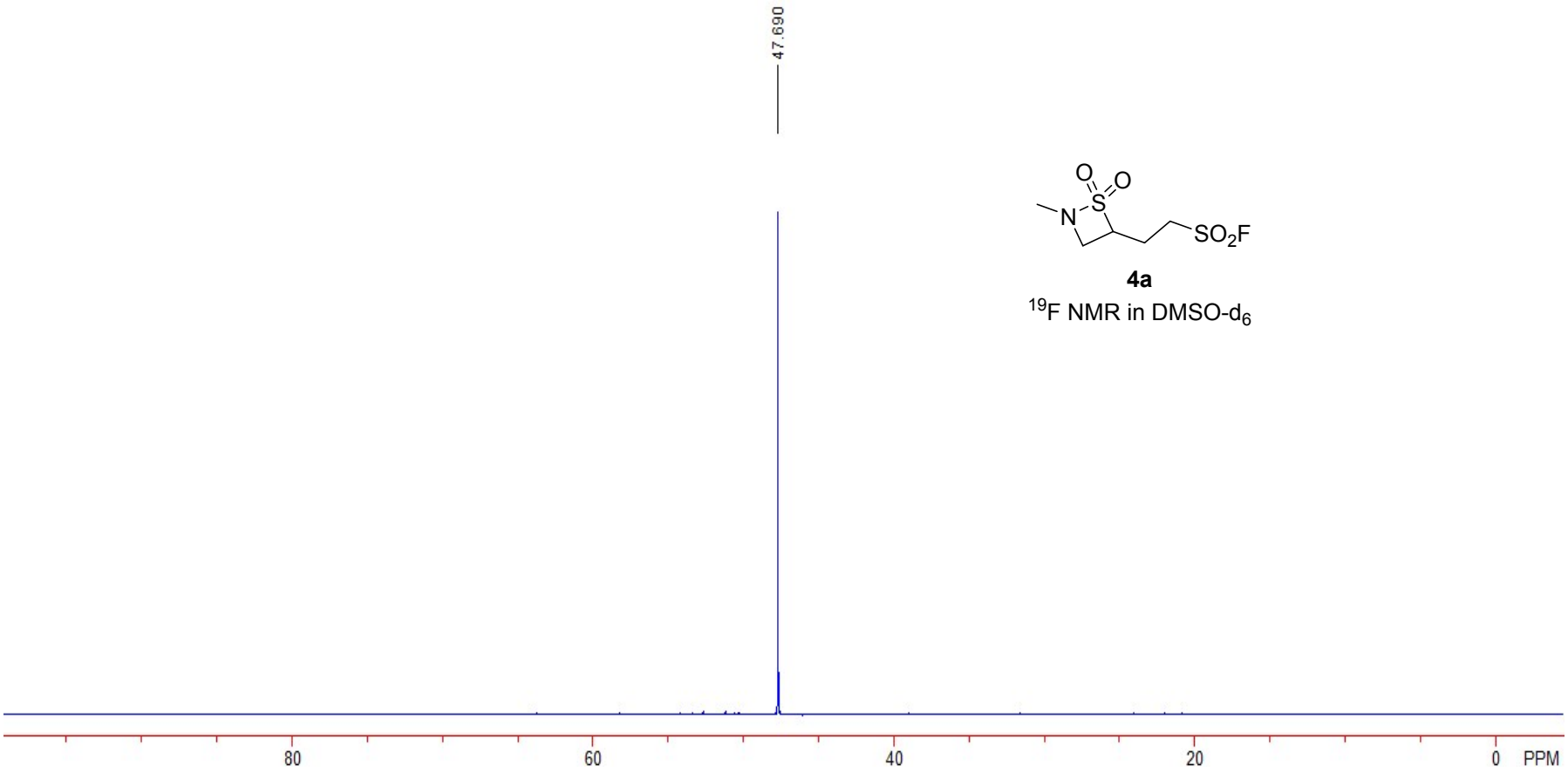


2

^{19}F NMR in $CDCl_3$

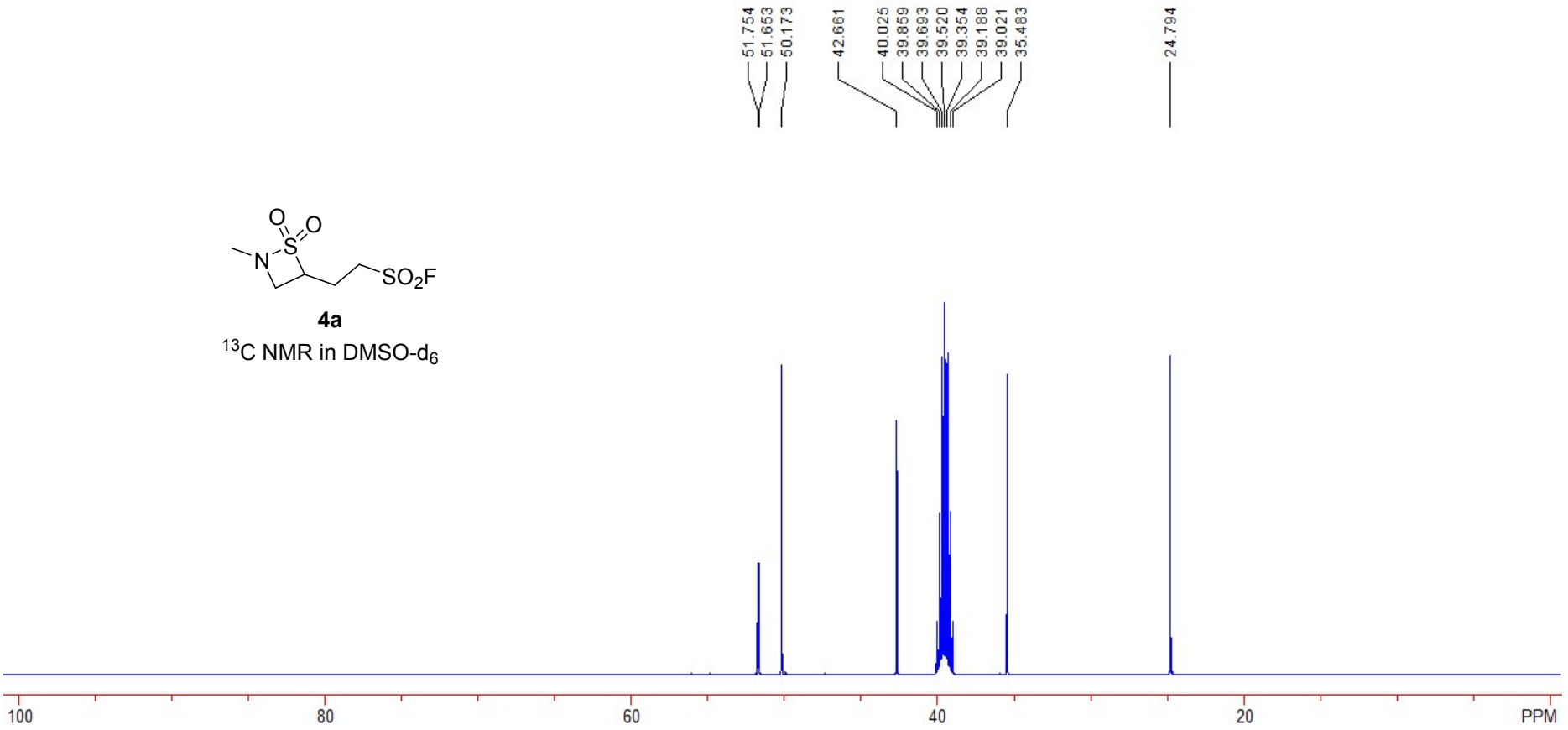

138.154
137.981
134.073
134.059
47.674
47.551
40.018
39.852
39.686
39.520
39.354
39.188
39.022
23.877
SO2F
SO2F
2
13C NMR in CDCl3
160
140
120
100
80
60
40
20
PPM


4.744
4.736
4.725
4.718
4.714
4.707
4.695
4.684
4.676
3.795
3.791
3.787
3.778
3.763
3.759
3.420
3.412
3.403
3.392
3.383
3.374
3.362
3.351
3.343
3.338
3.323
3.315
2.847
2.641
2.632
2.629
2.624
2.614
2.610
2.605
2.601
2.596
2.504
2.500
2.497
2.457
2.448
2.434
2.430
2.425
2.421
2.411
2.407
2.402
2.397
2.383
2.375
O
O
S
N
SO2F
4a
1H NMR in DMSO-d6
3.01
2.17
1.95
1.00
1.00
1.04
12
10
8
6
4
2
0
PPM



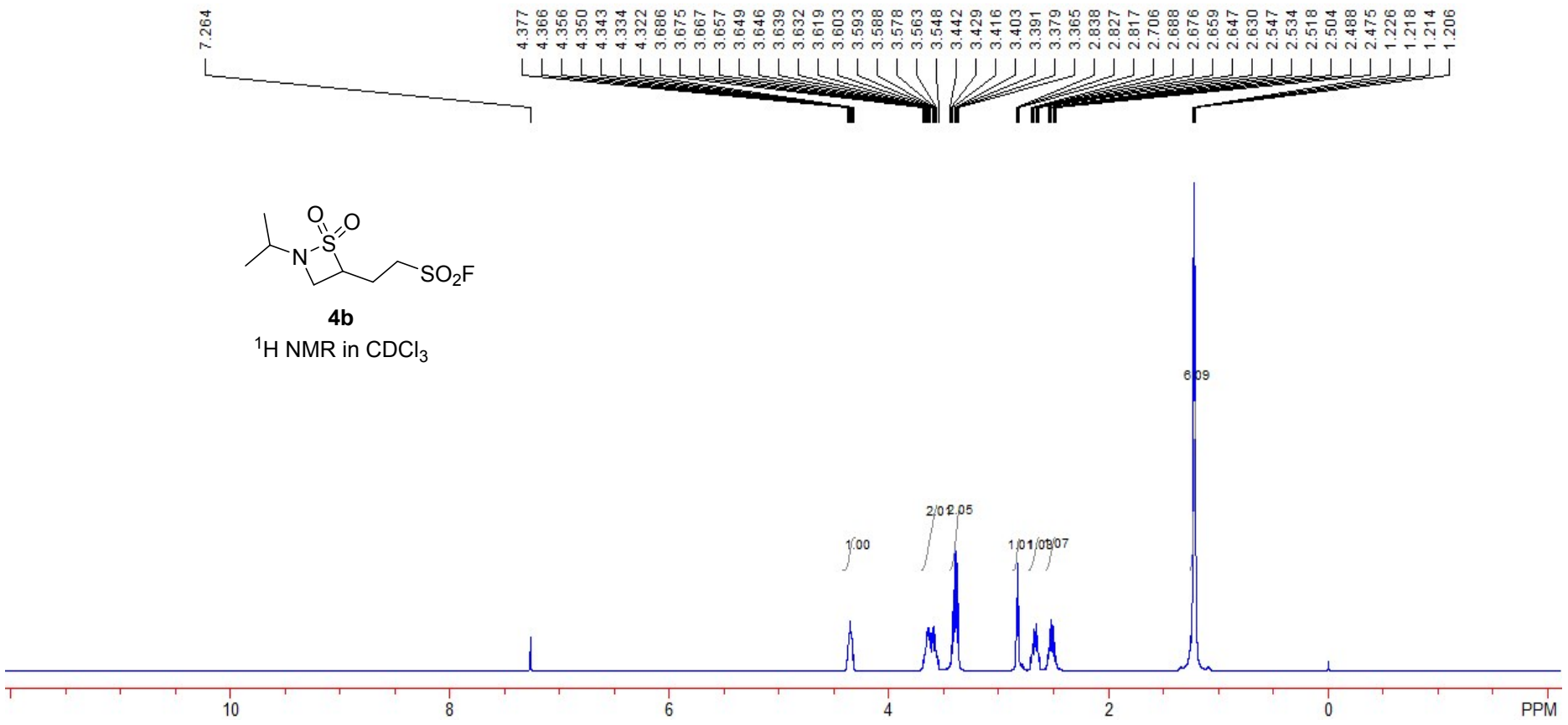
4a

^{19}F NMR in DMSO-d_6



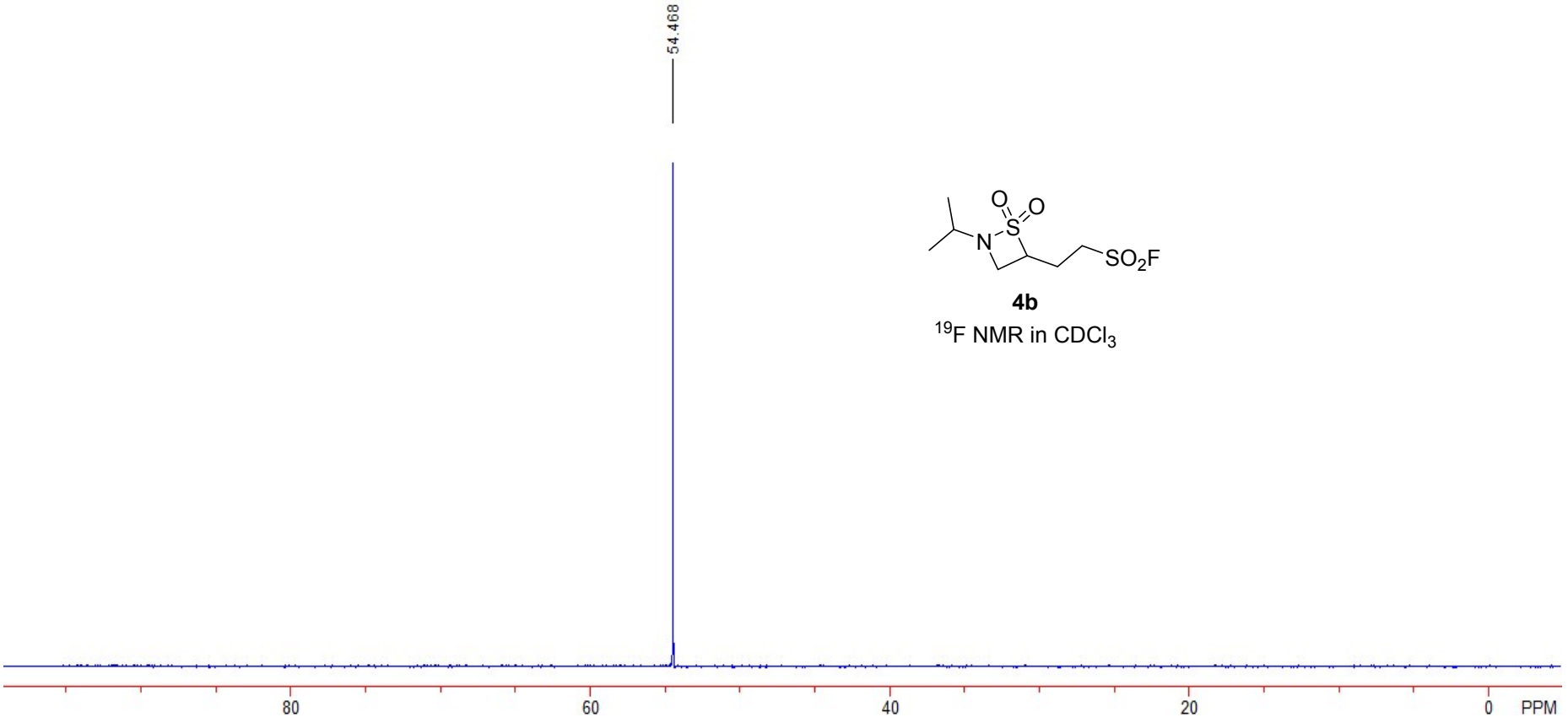
4a

^{13}C NMR in DMSO-d_6



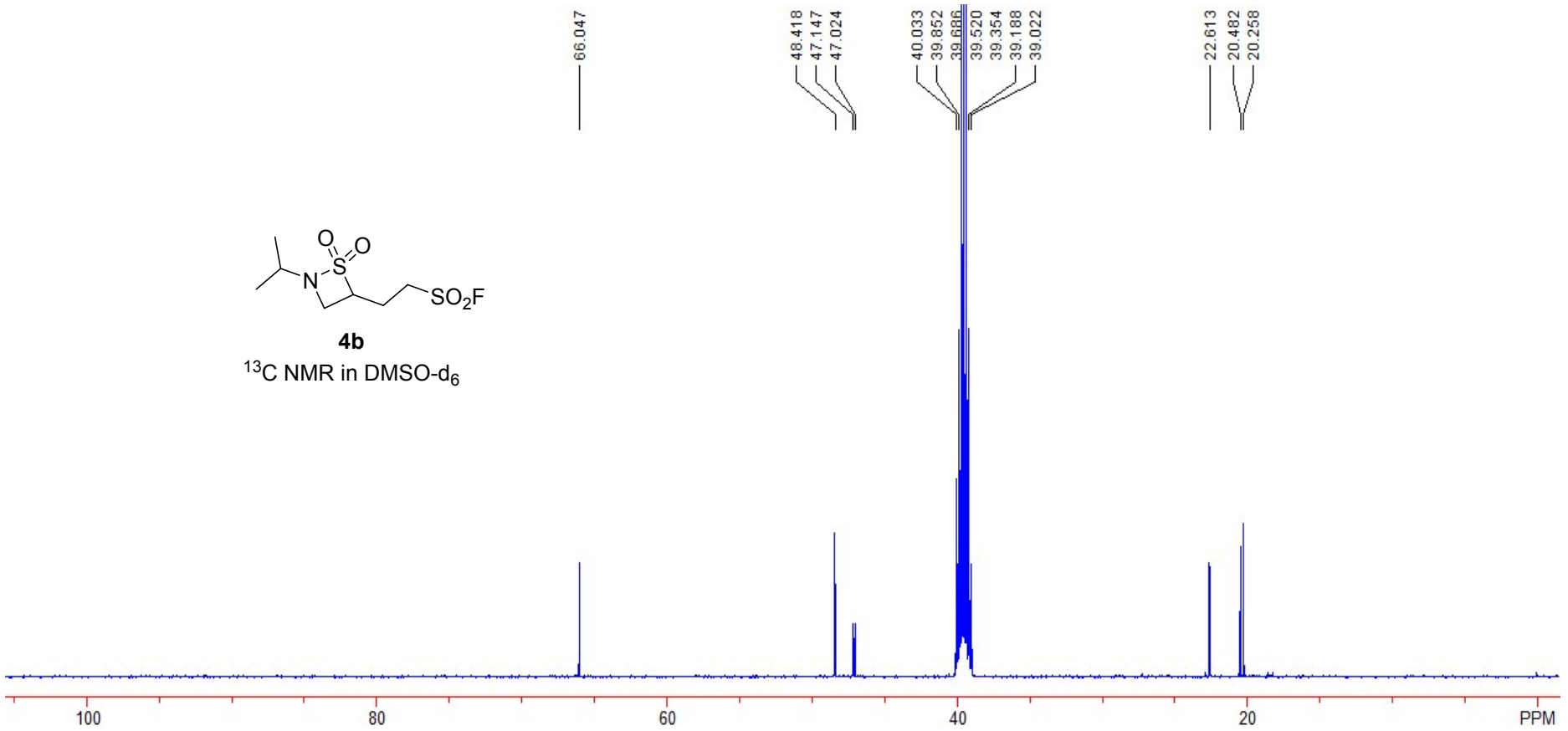
4b

^{1}H NMR in $CDCl_3$



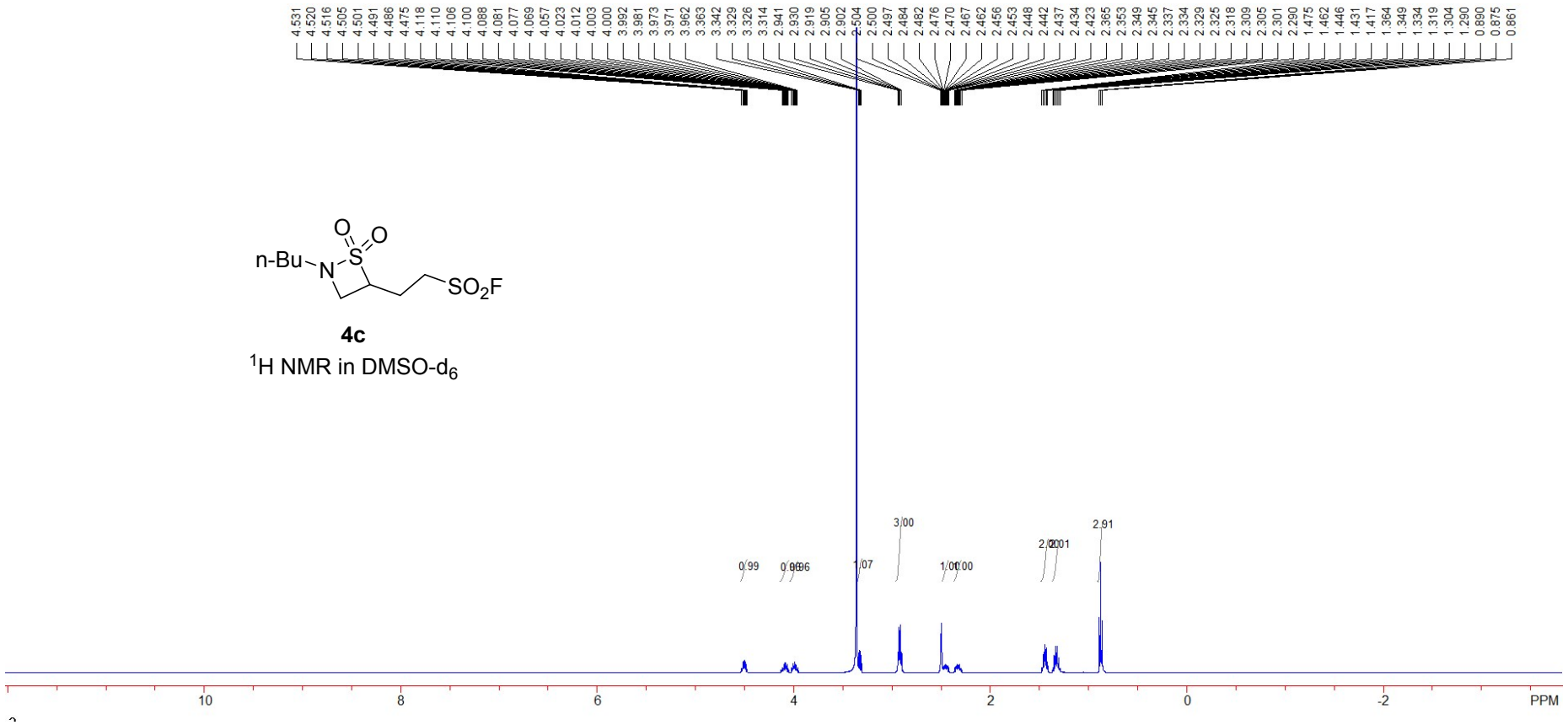
4b

^{19}F NMR in $CDCl_3$



4b

^{13}C NMR in DMSO-d_6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4.501
4.491
4.486
4.475
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4.106
4.100
4.088
4.081
4.077
4.069
4.057
4.023
4.012
4.003
4.000
3.992
3.981
3.973
3.971
3.962
3.363
3.342
3.329
3.326
3.314
2.941
2.930
2.919
2.905
2.902
2.504
2.500
2.497
2.484
2.482
2.476
2.470
2.467
2.462
2.456
2.453
2.448
2.442
2.437
2.434
2.423
2.365
2.353
2.349
2.345
2.337
2.334
2.329
2.325
2.318
2.309
2.305
2.301
2.290
1.475
1.462
1.446
1.431
1.417
1.364
1.349
1.334
1.319
1.304
1.290
0.890
0.875
0.861
n-Bu
N
S
O
O
SO2F
4c
1H NMR in DMSO-d6
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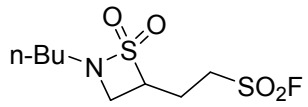
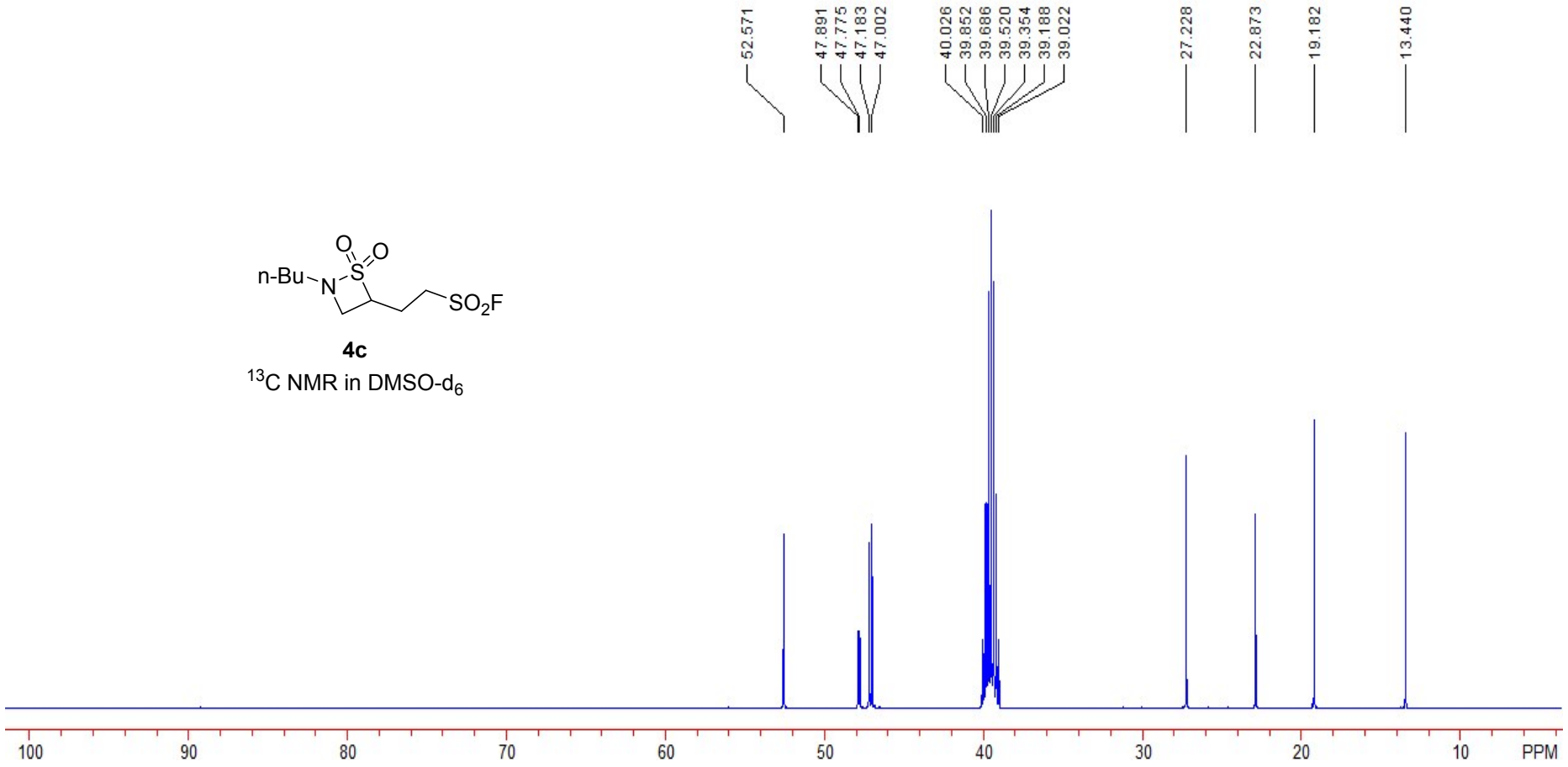
3.00
1.00
2.01
2.91
10
8
6
4
2
0
-2
PPM



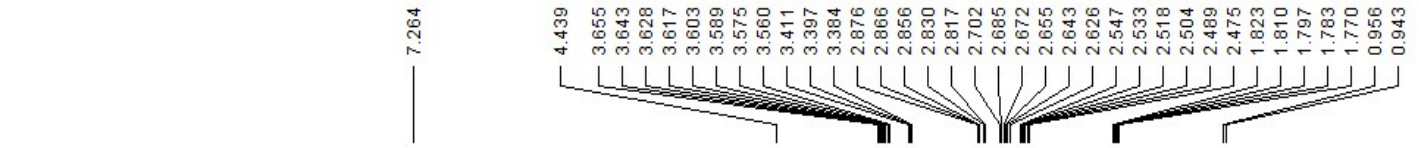
4c

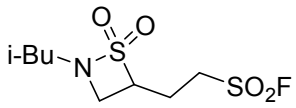
^{19}F NMR in DMSO-d_6



4c

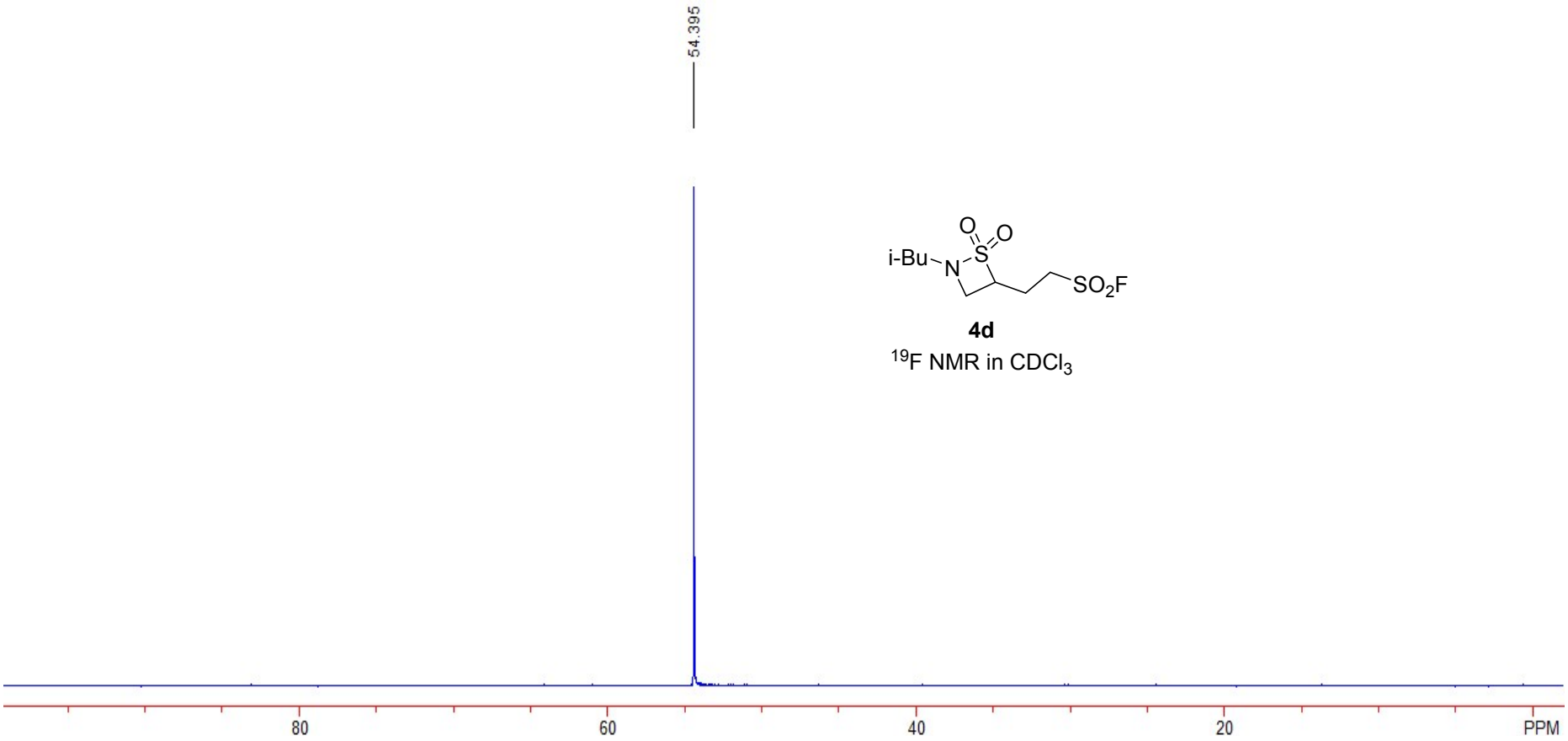
^{13}C NMR in DMSO-d_6





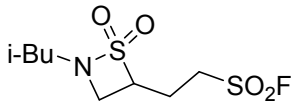
4d

^{1}H NMR in $CDCl_3$



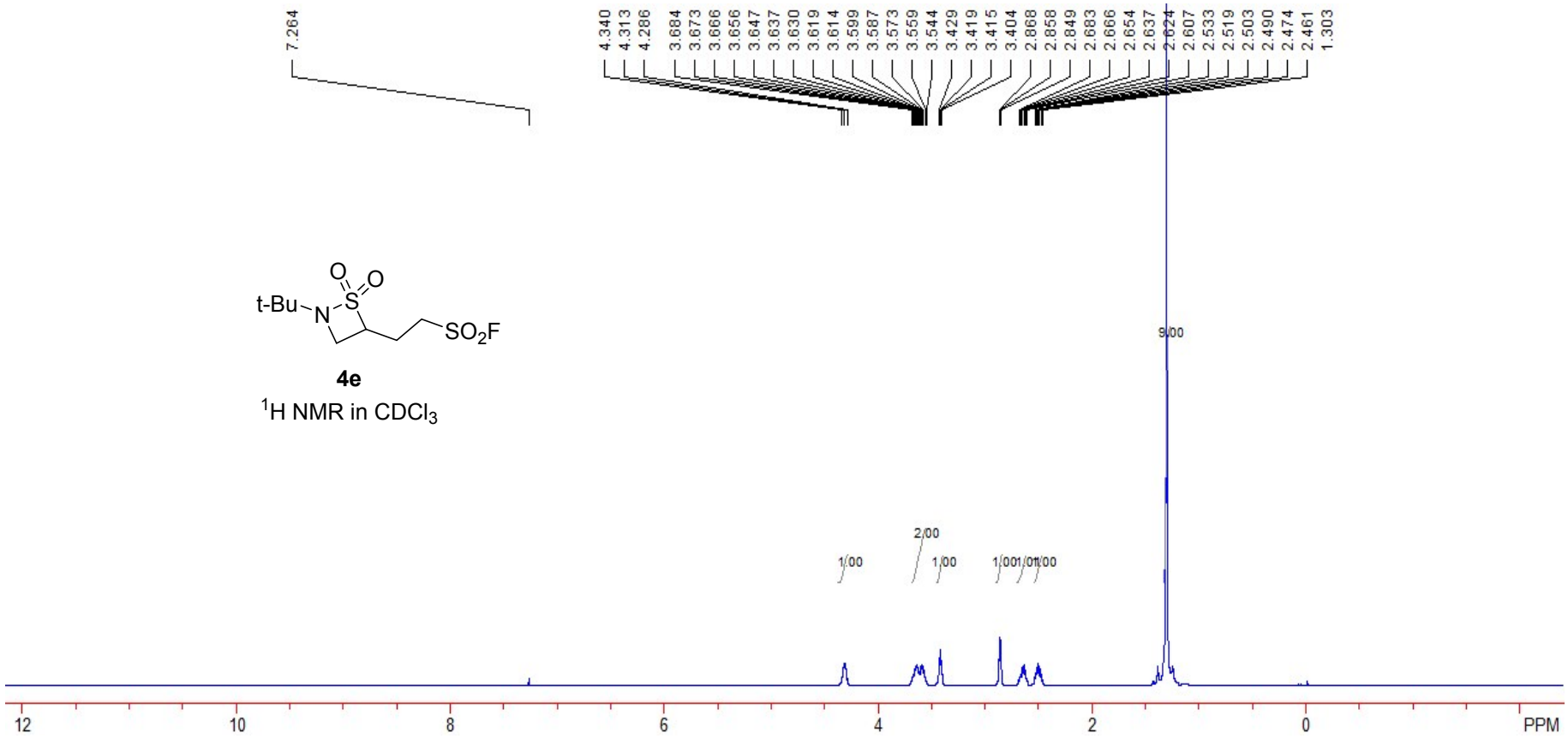
4d

^{19}F NMR in $CDCl_3$



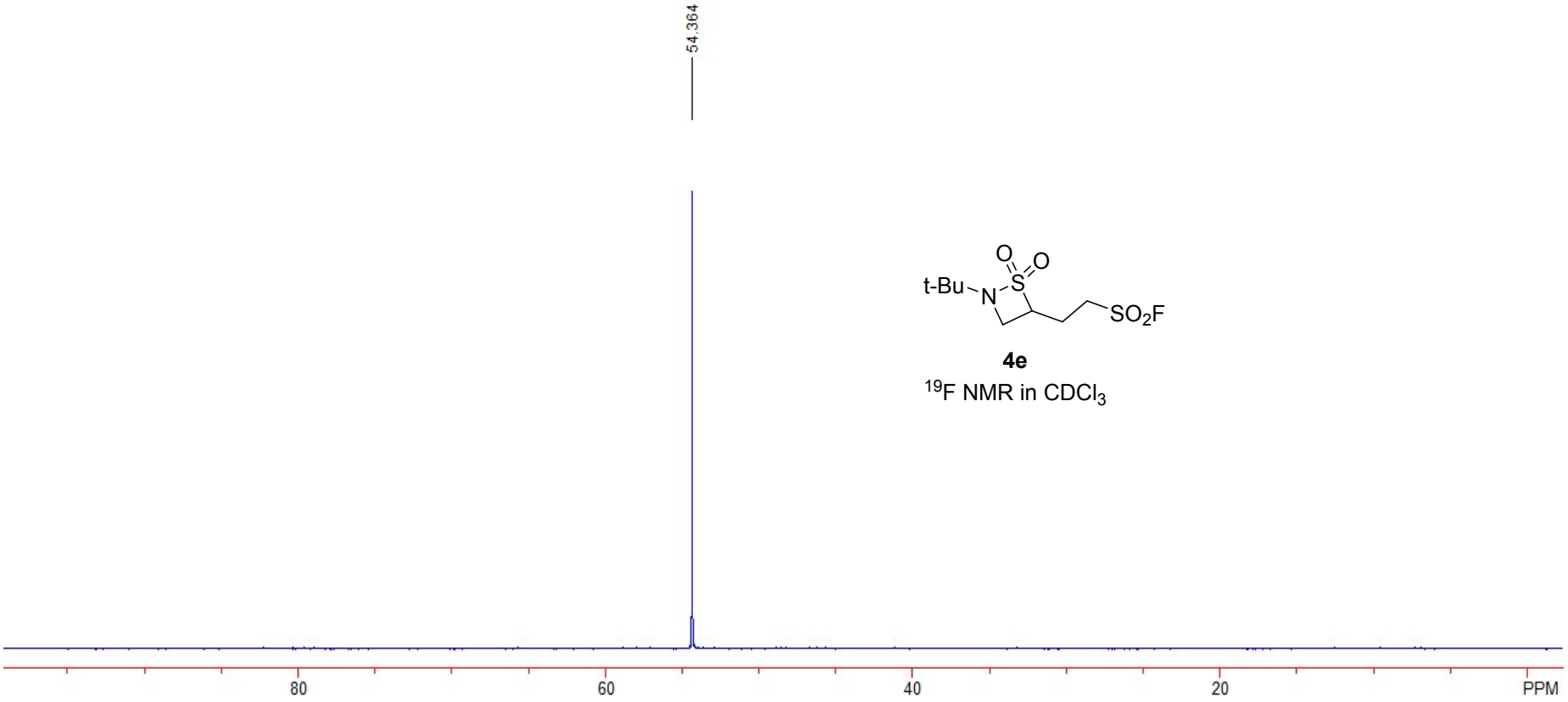
4d

^{13}C NMR in DMSO-d_6



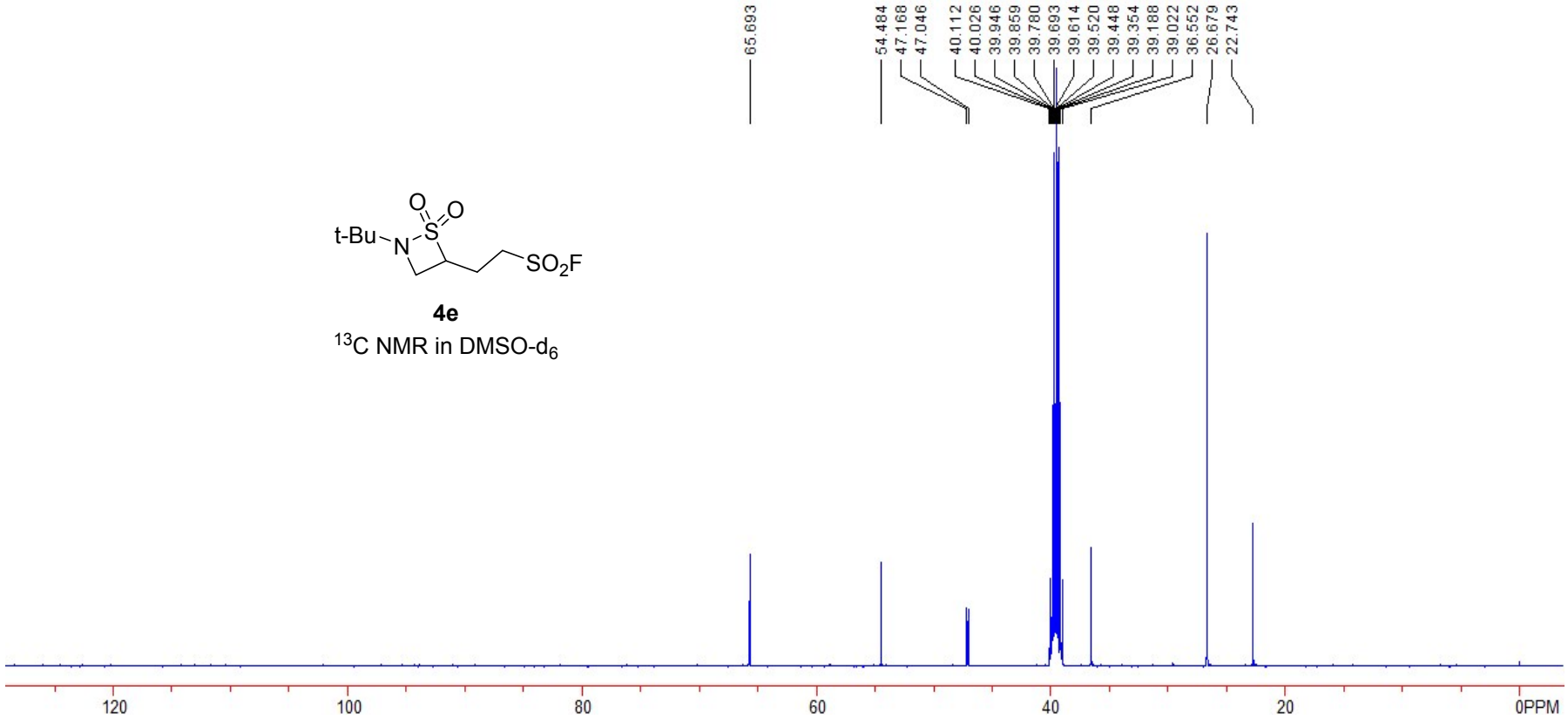
4e

^{1}H NMR in $CDCl_3$



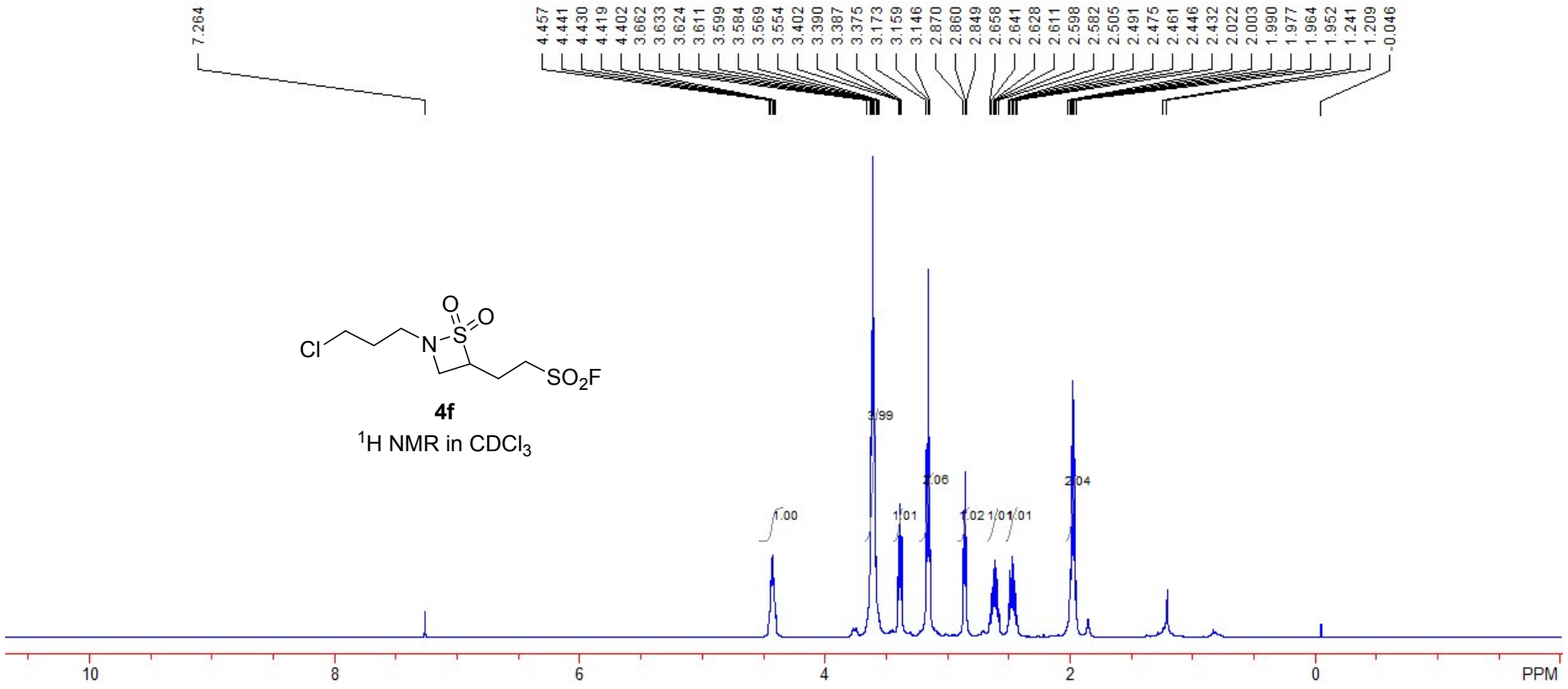
4e

^{19}F NMR in $CDCl_3$



4e

^{13}C NMR in DMSO-d_6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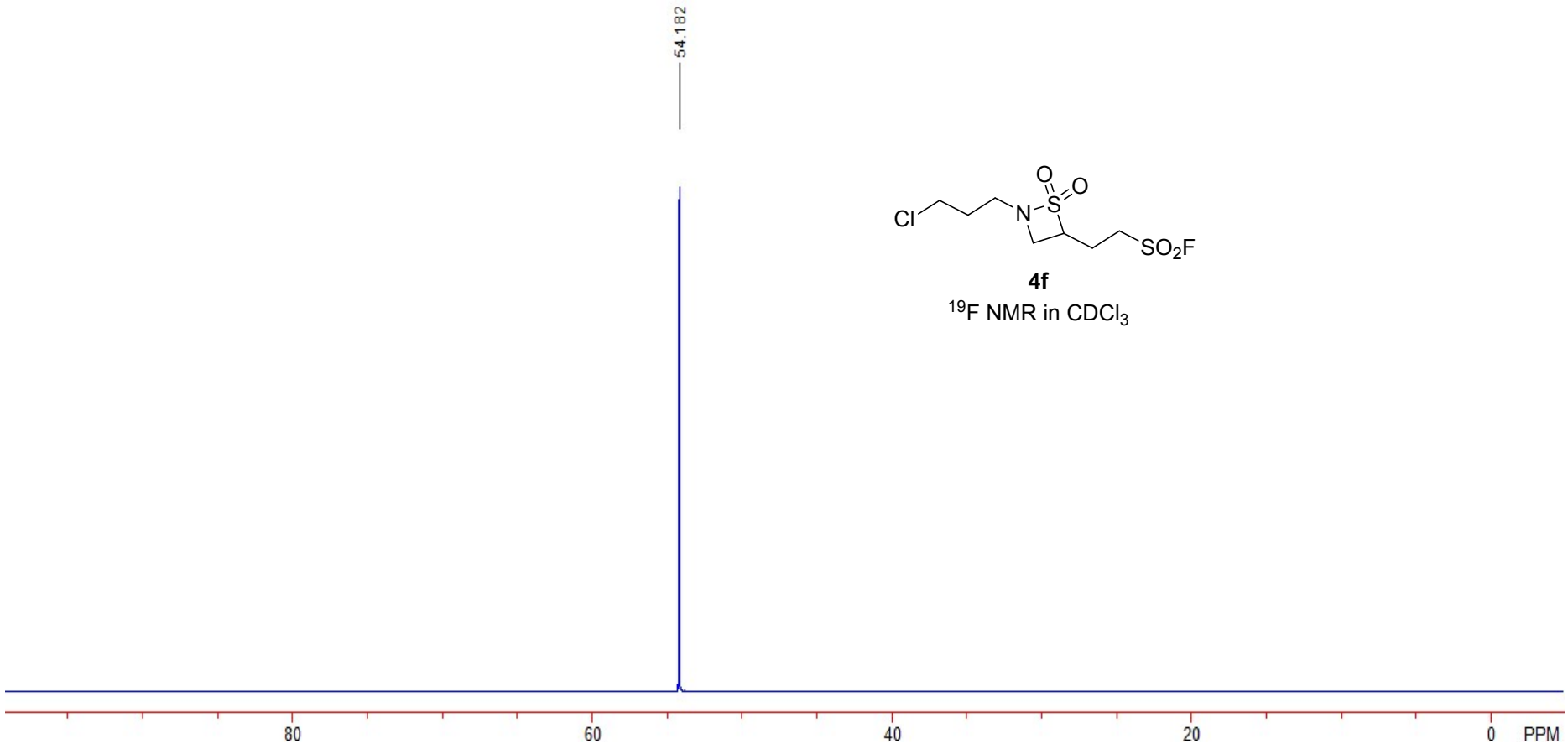
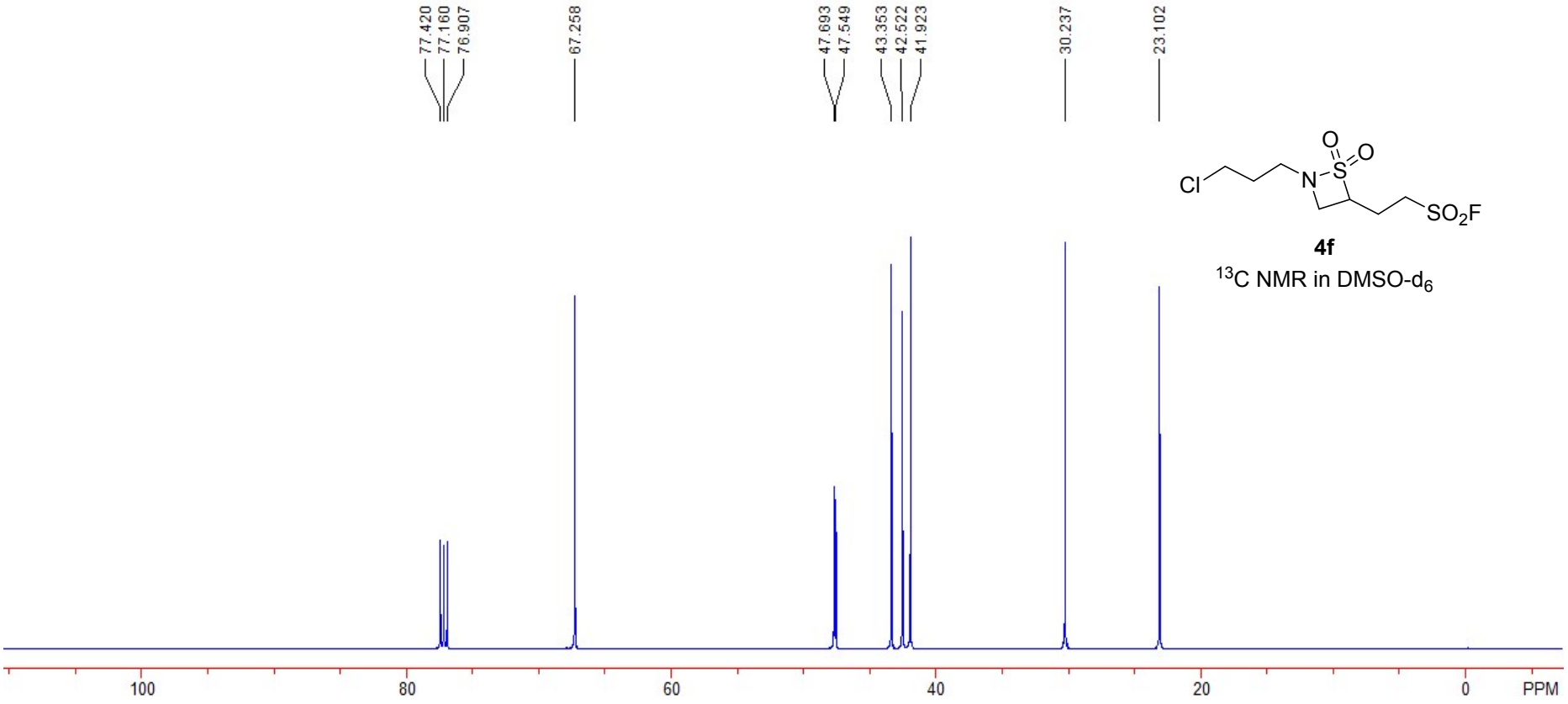
4.441
4.430
4.419
4.402
3.662
3.633
3.624
3.611
3.599
3.584
3.569
3.554
3.402
3.390
3.387
3.375
3.173
3.159
3.146
2.870
2.860
2.849
2.658
2.641
2.628
2.611
2.598
2.582
2.505
2.491
2.475
2.461
2.446
2.432
2.022
2.003
1.990
1.977
1.964
1.952
1.241
1.209
-0.046
Cl
N
S
O
O
SO2F
4f
1H NMR in CDCl3
1.00
3.99
1.01
2.06
1.02
1.01
1.01
2.04
10
8
6
4
2
0
PPM



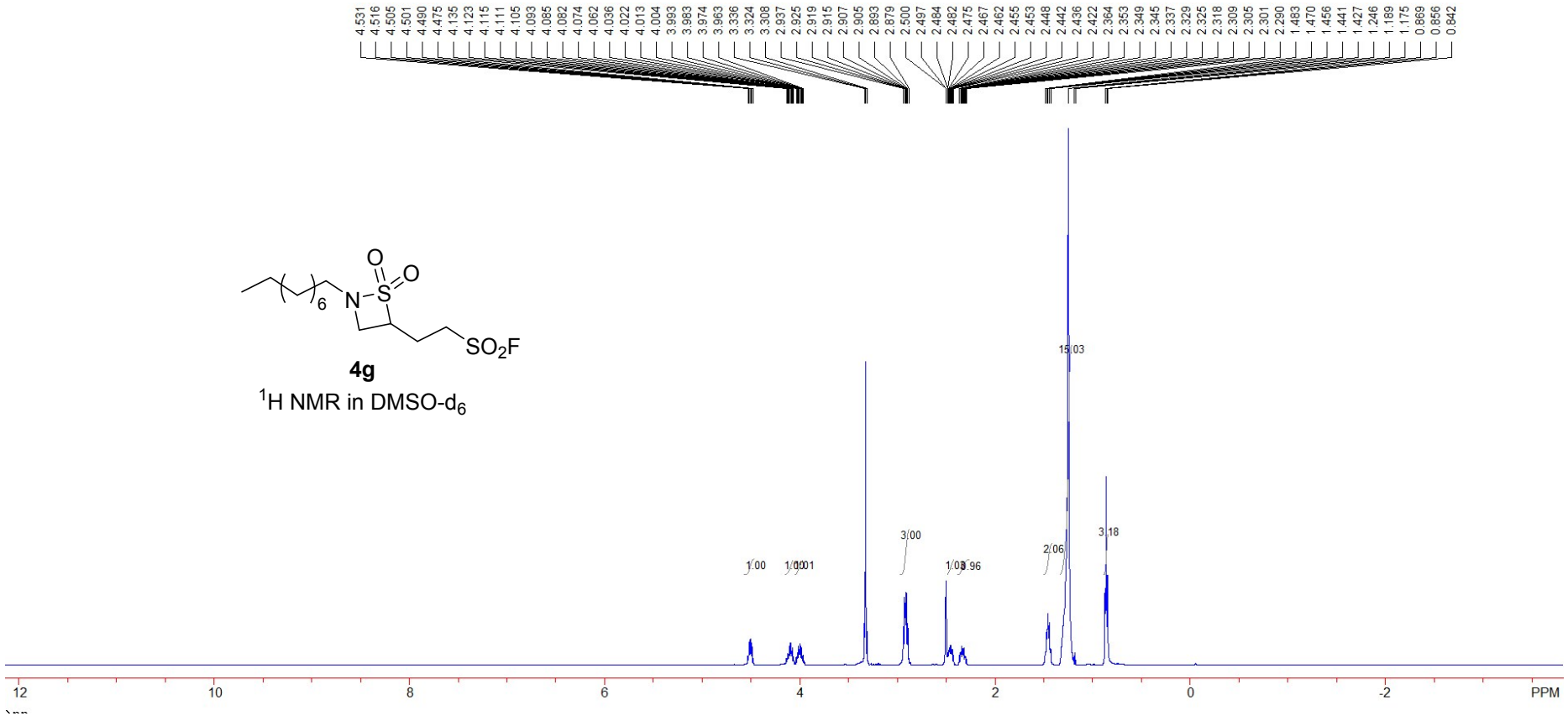
4f

^{19}F NMR in $CDCl_3$



4f

^{13}C NMR in DMSO-d_6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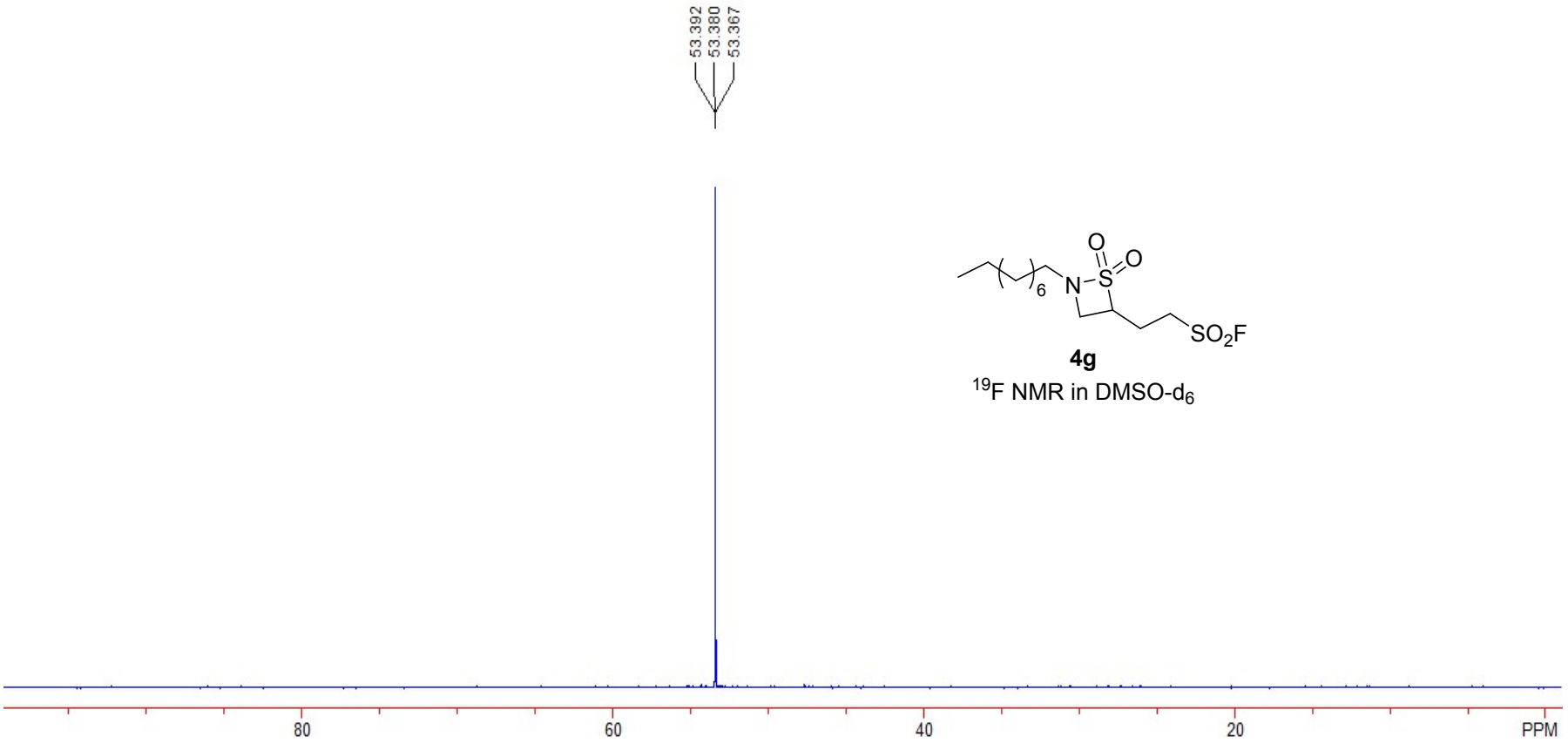
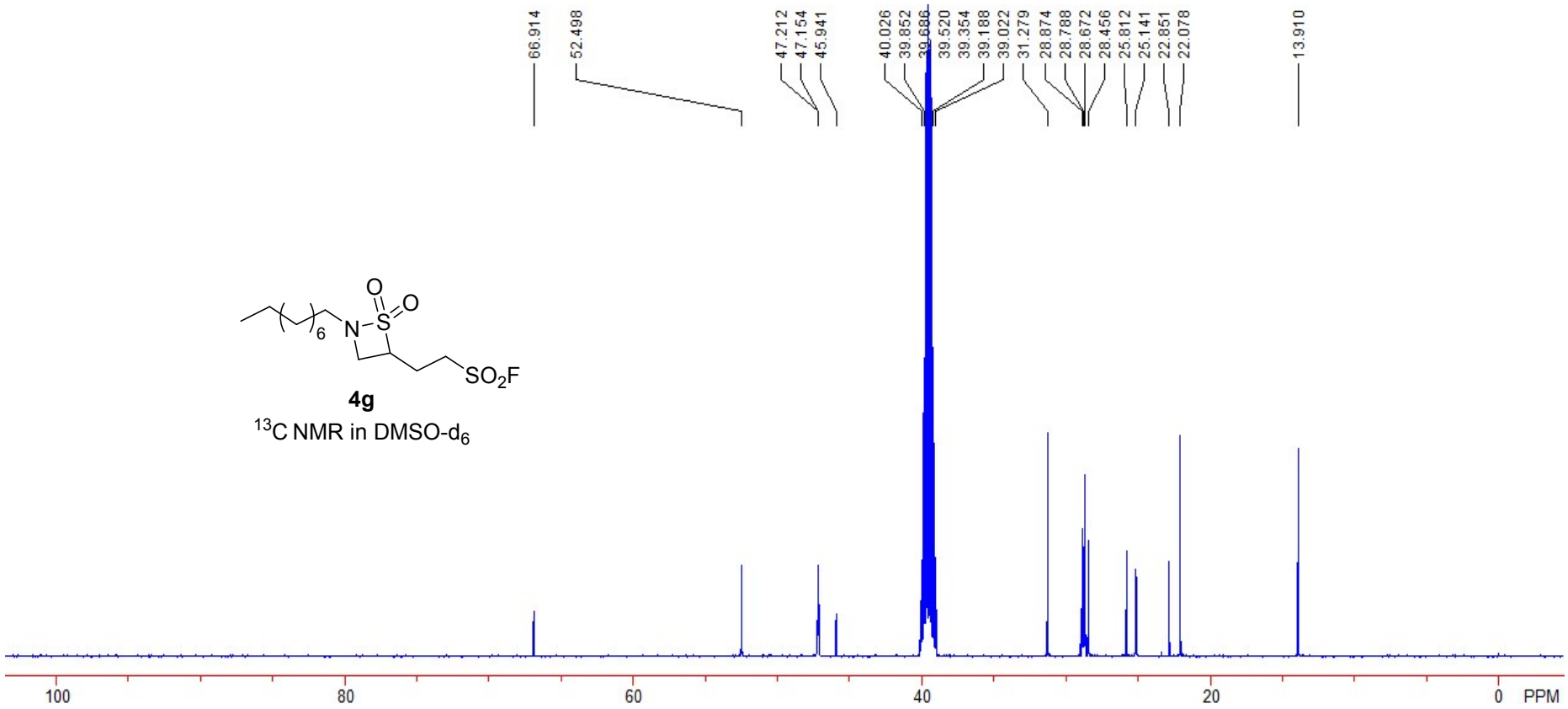
O
O
O
N
S
6
SO2F
4g
1H NMR in DMSO-d6
1.00
1.00
1.01
3.00
1.03
0.96
2.06
15.03
3.18
12
10
8
6
4
2
0
-2
PPM



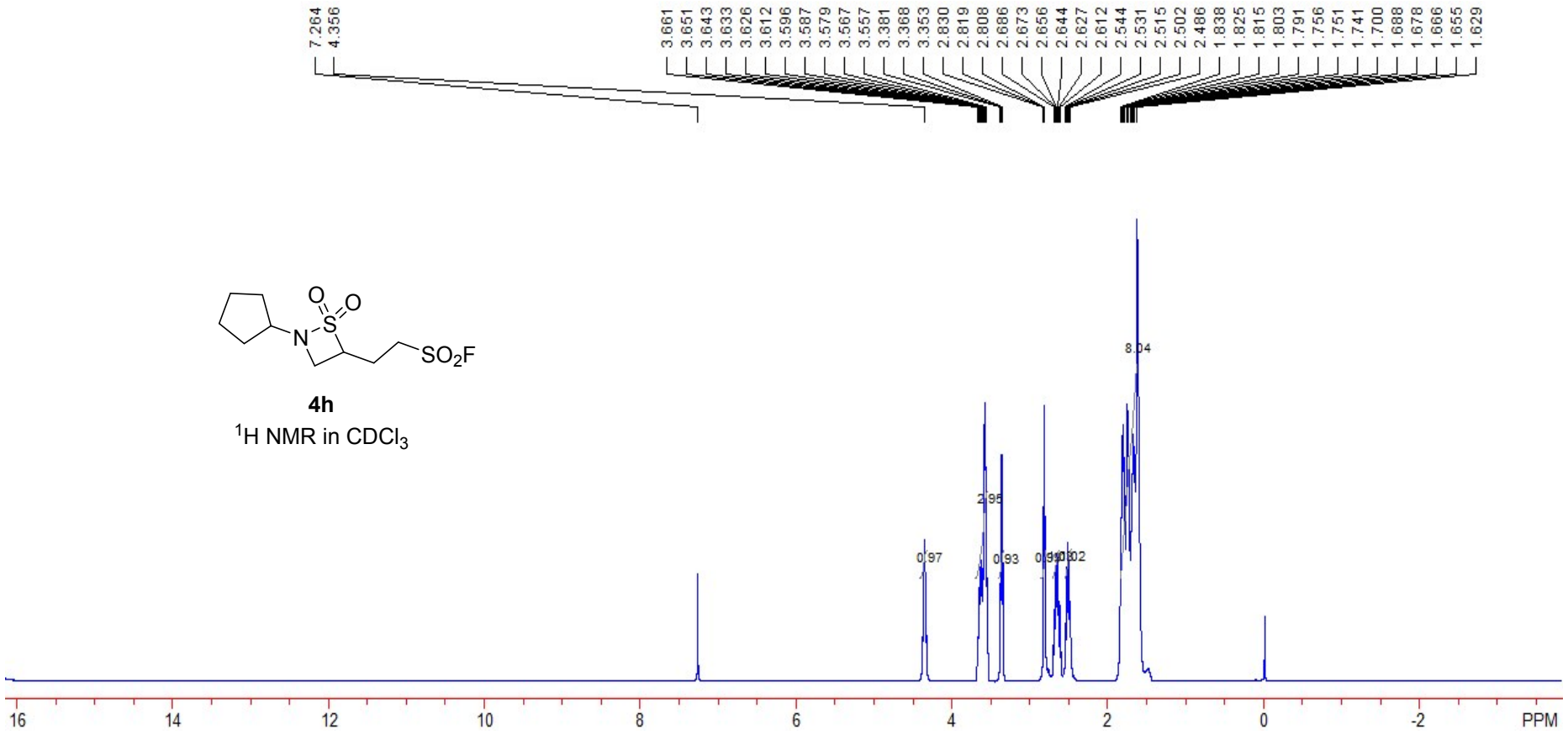
4g

^{19}F NMR in DMSO-d_6



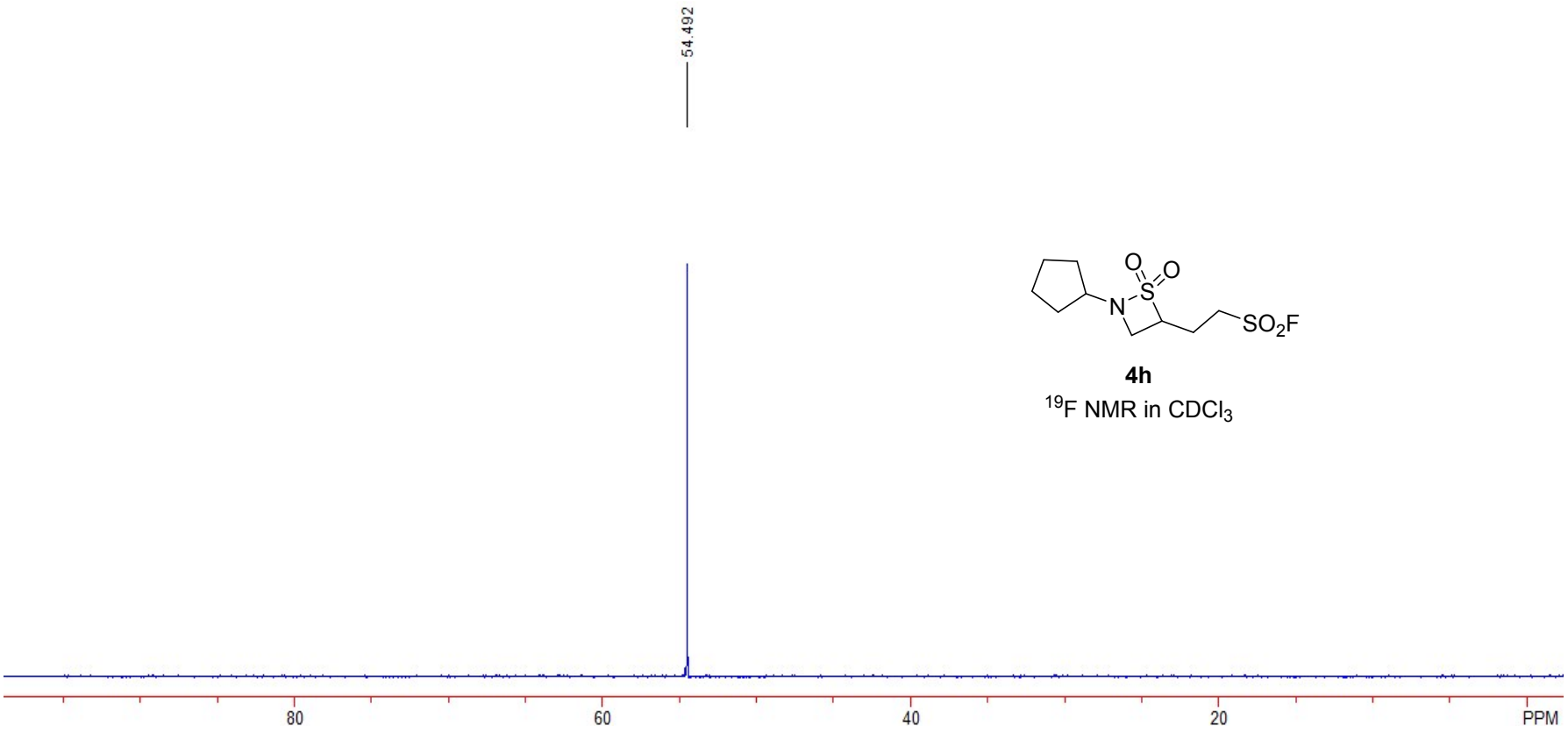
4g

^{13}C NMR in DMSO-d_6



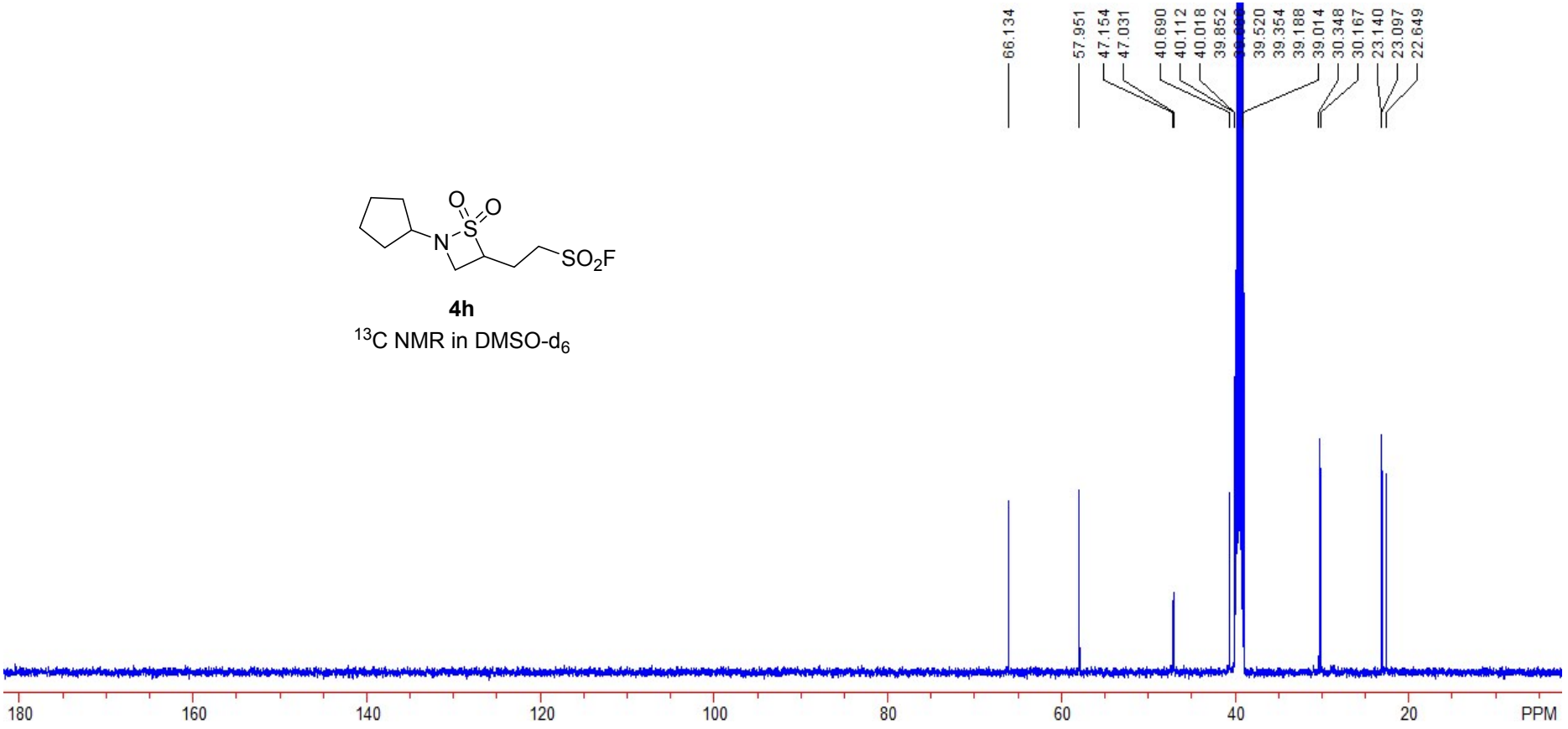
4h

^{1}H NMR in $CDCl_3$



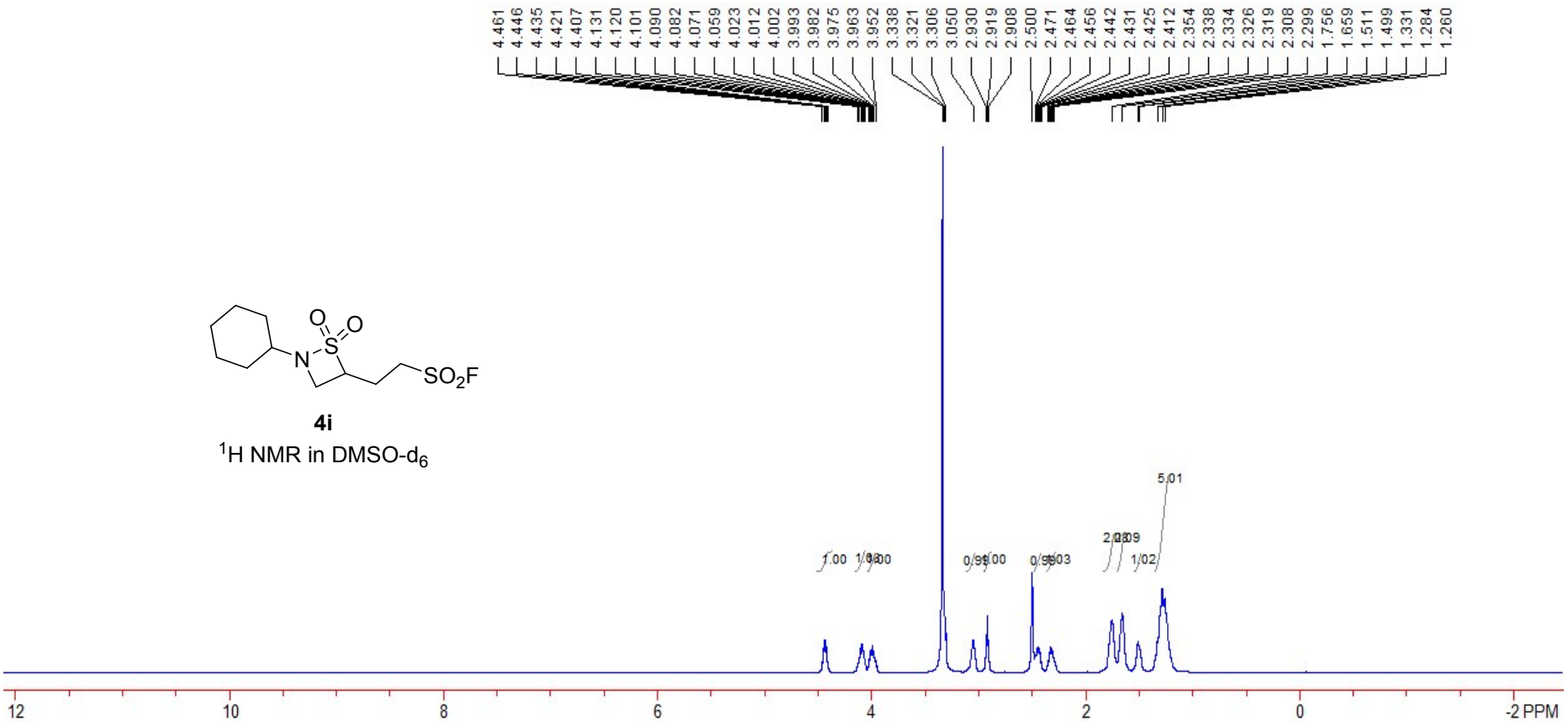
4h

^{19}F NMR in $CDCl_3$



4h

^{13}C NMR in DMSO-d_6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4.446
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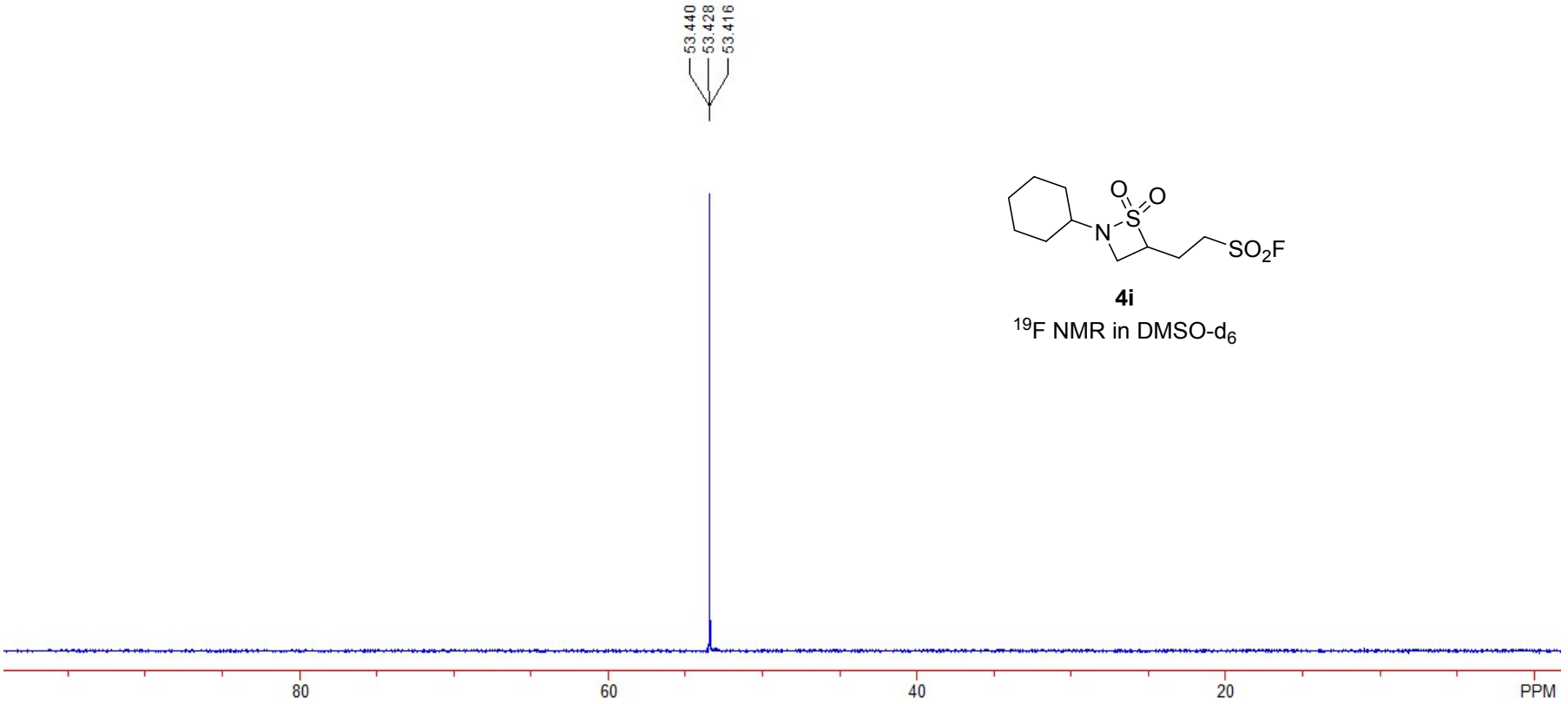
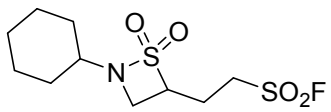
4.421
4.407
4.131
4.120
4.101
4.090
4.082
4.071
4.059
4.023
4.012
4.002
3.993
3.982
3.975
3.963
3.952
3.338
3.321
3.306
3.050
2.930
2.919
2.908
2.500
2.471
2.464
2.456
2.442
2.431
2.425
2.412
2.354
2.338
2.334
2.326
2.319
2.308
2.299
1.756
1.659
1.511
1.499
1.331
1.284
1.260
O
O
S
N
SO2F
4i
1H NMR in DMSO-d6
5.01
1.02
12
10
8
6
4
2
0
-2 PPM



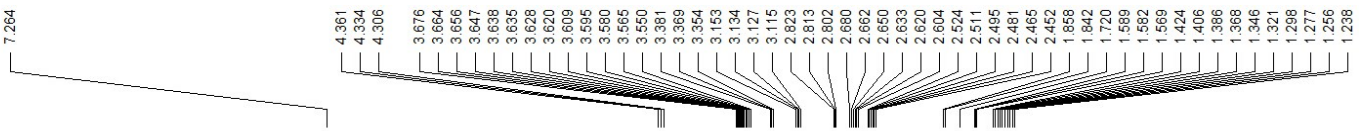
4i

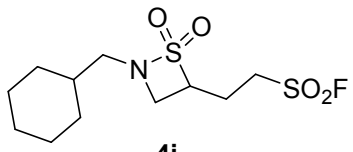
^{19}F NMR in DMSO-d_6



4i

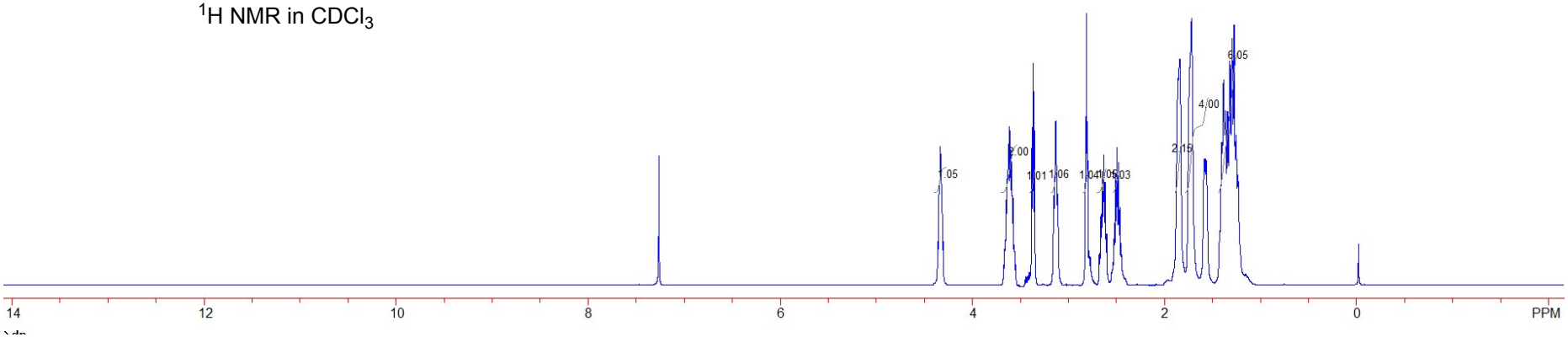
^{13}C NMR in DMSO-d_6

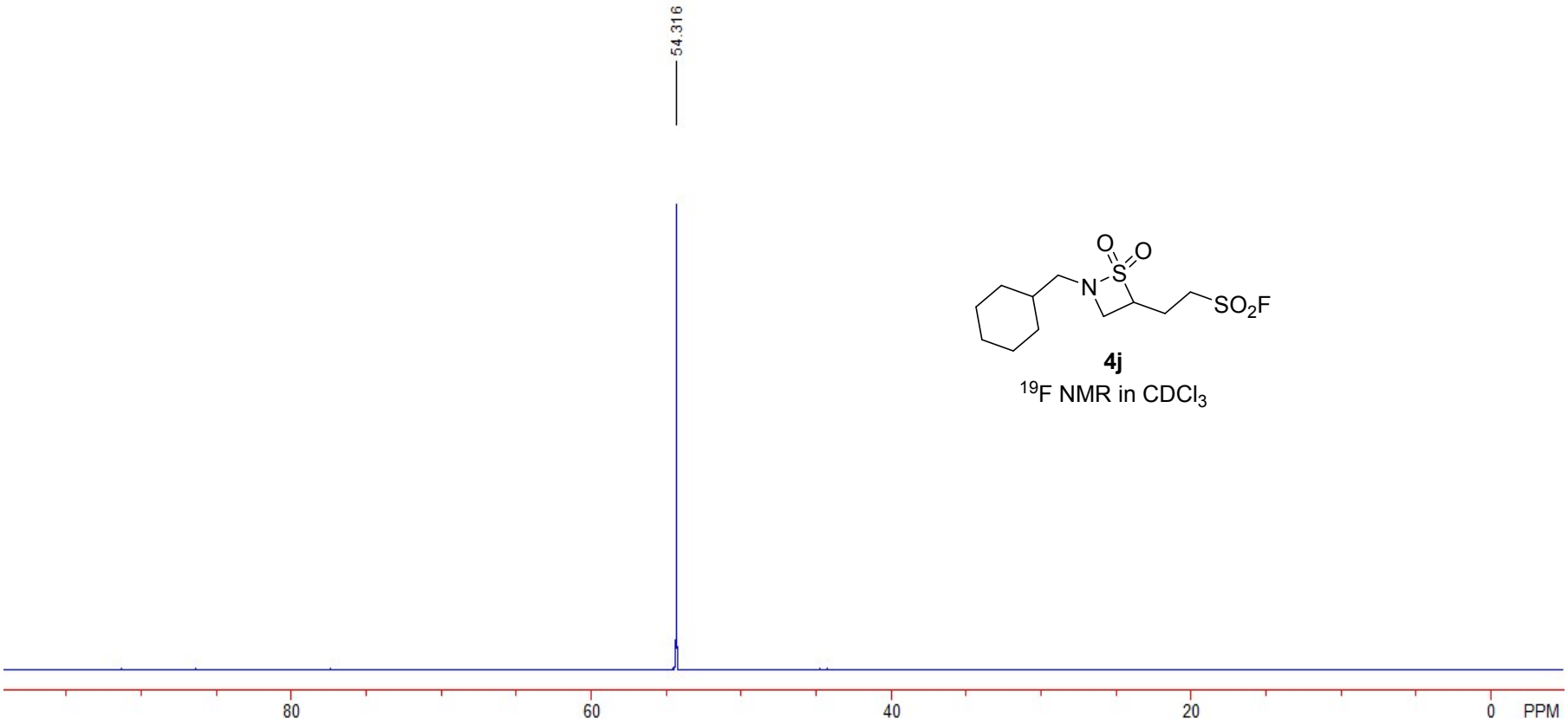




4j

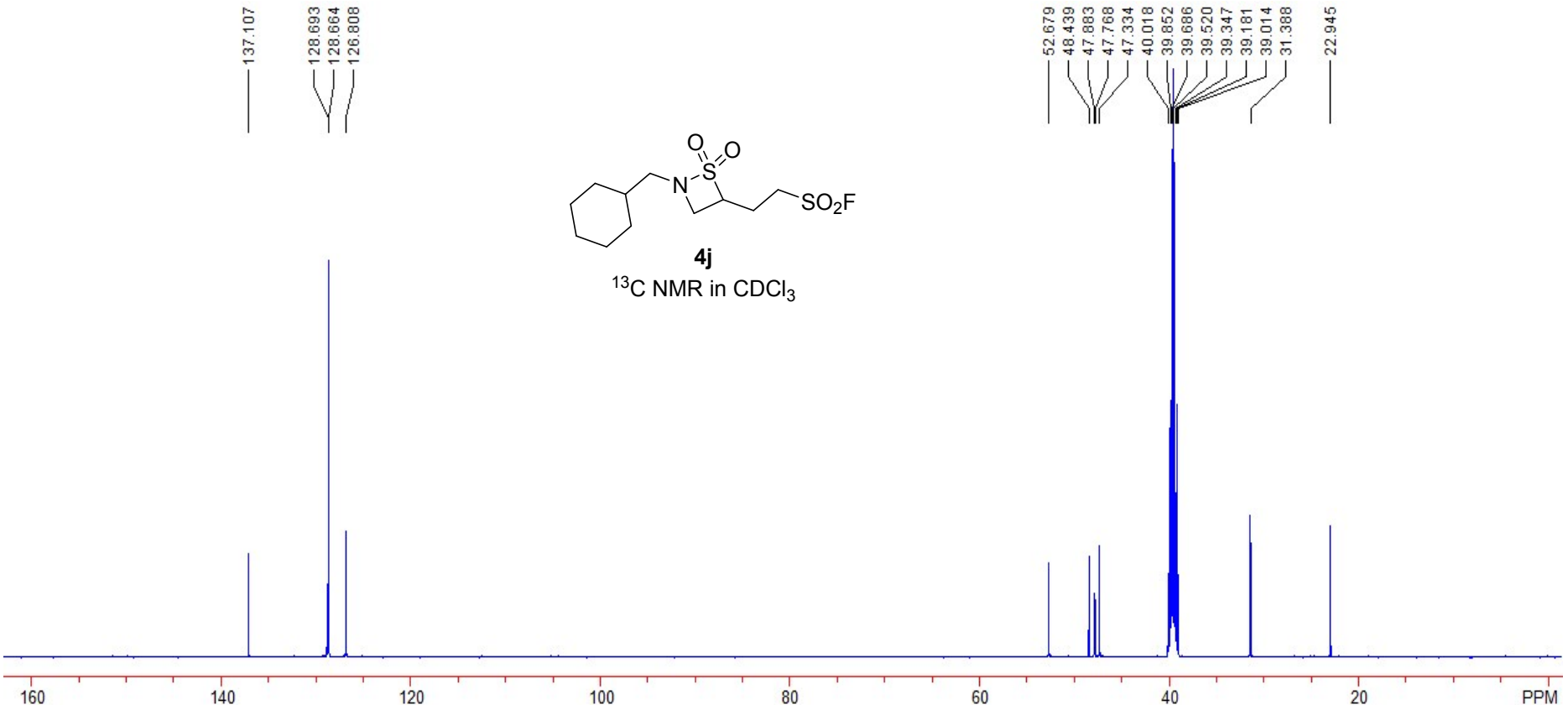
^{1}H NMR in $CDCl_3$





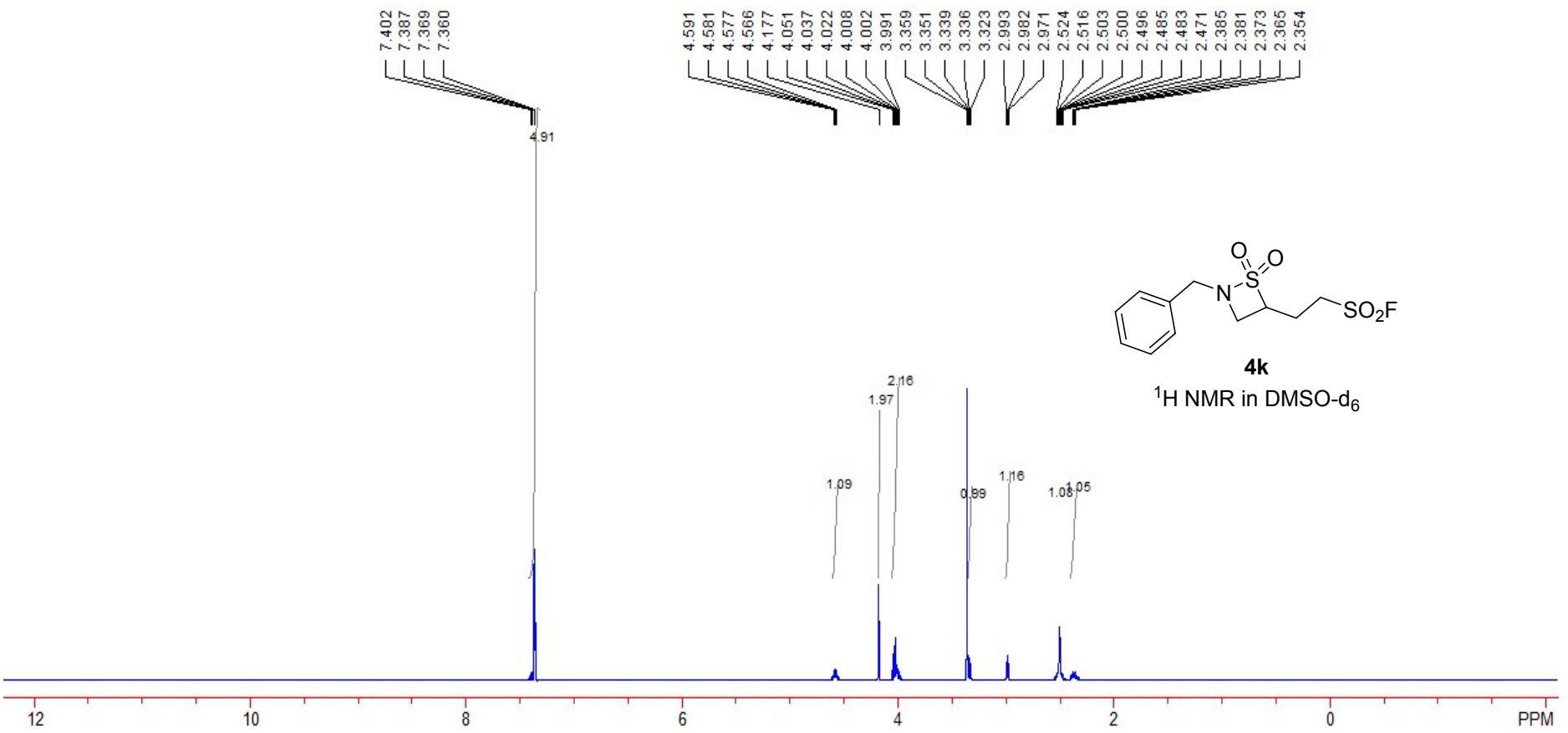
4j

^{19}F NMR in $CDCl_3$



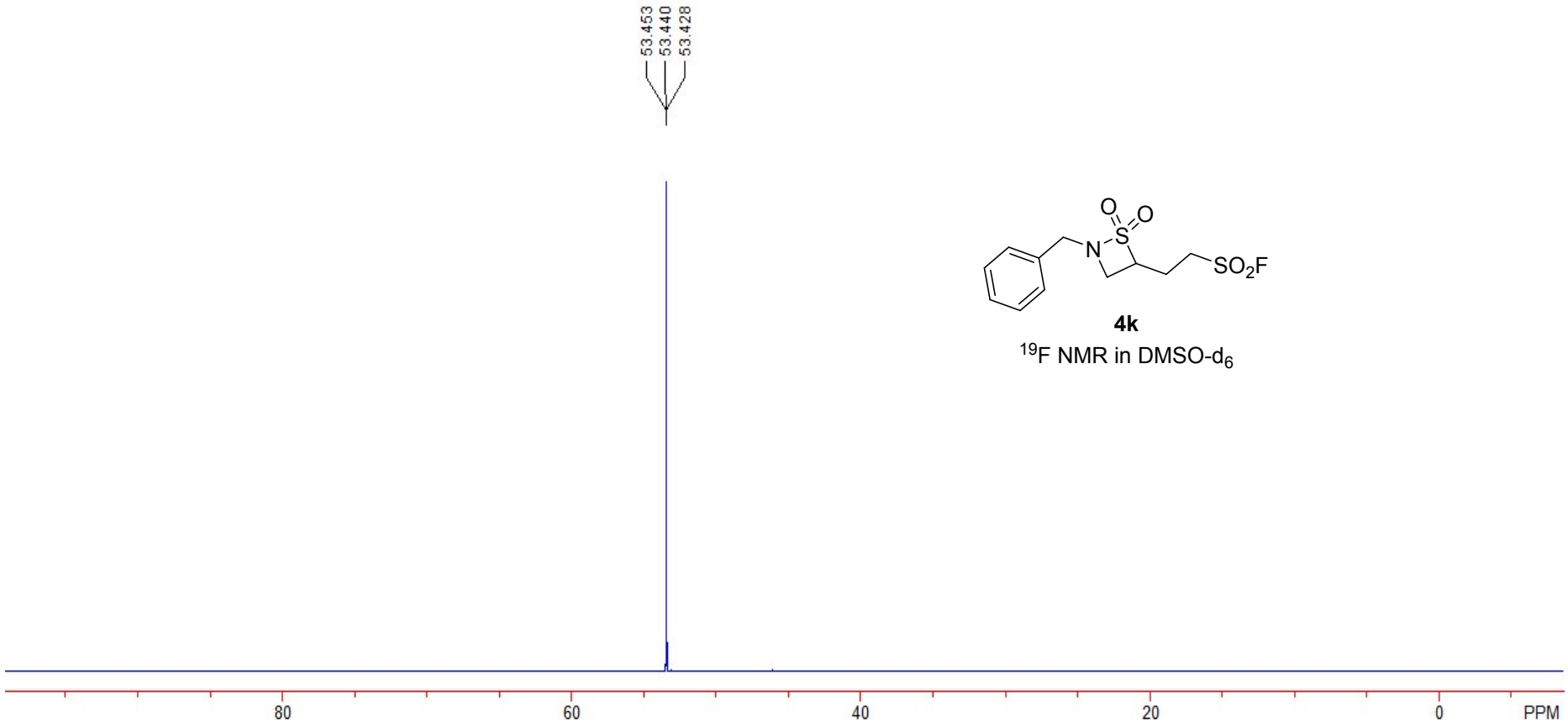
4j

^{13}C NMR in $CDCl_3$



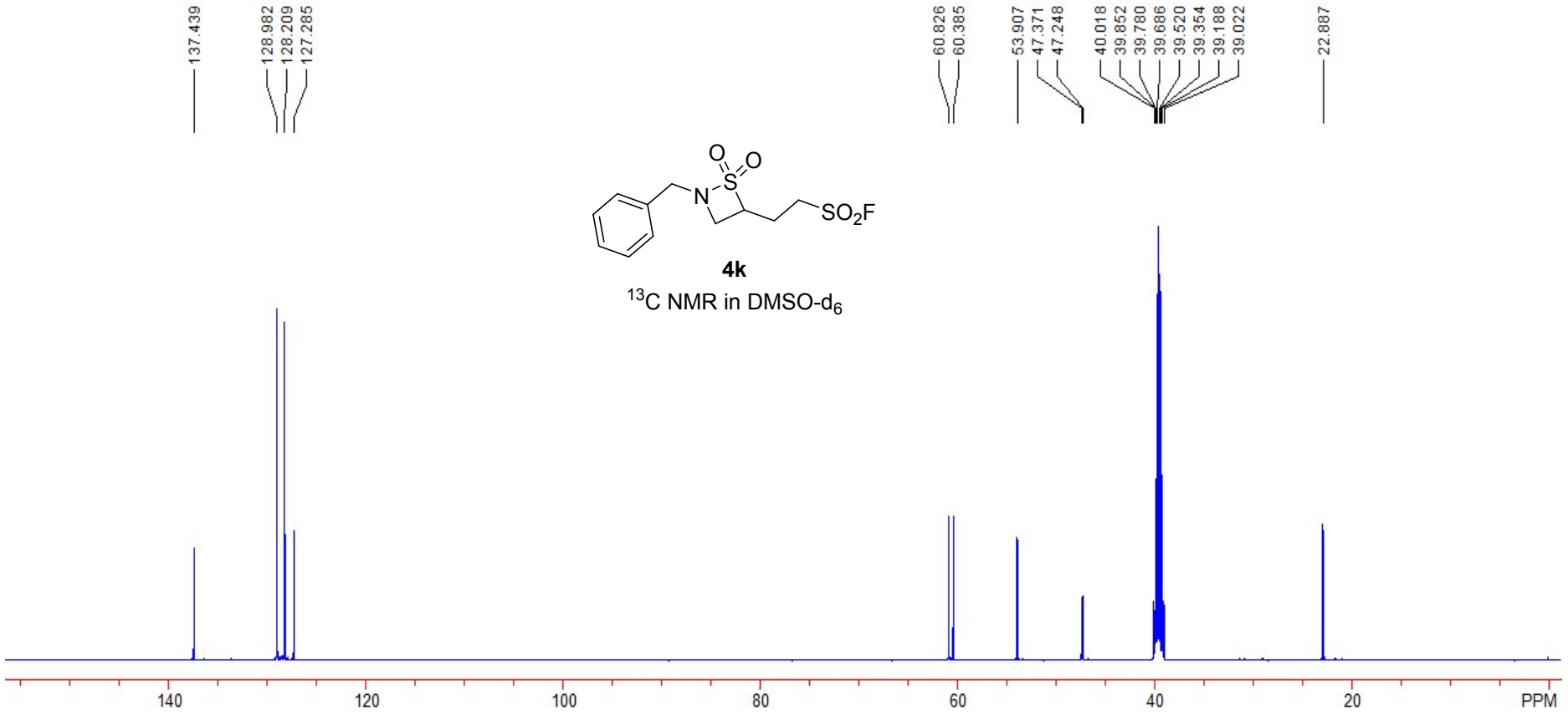
4k

^{1}H NMR in DMSO-d_6



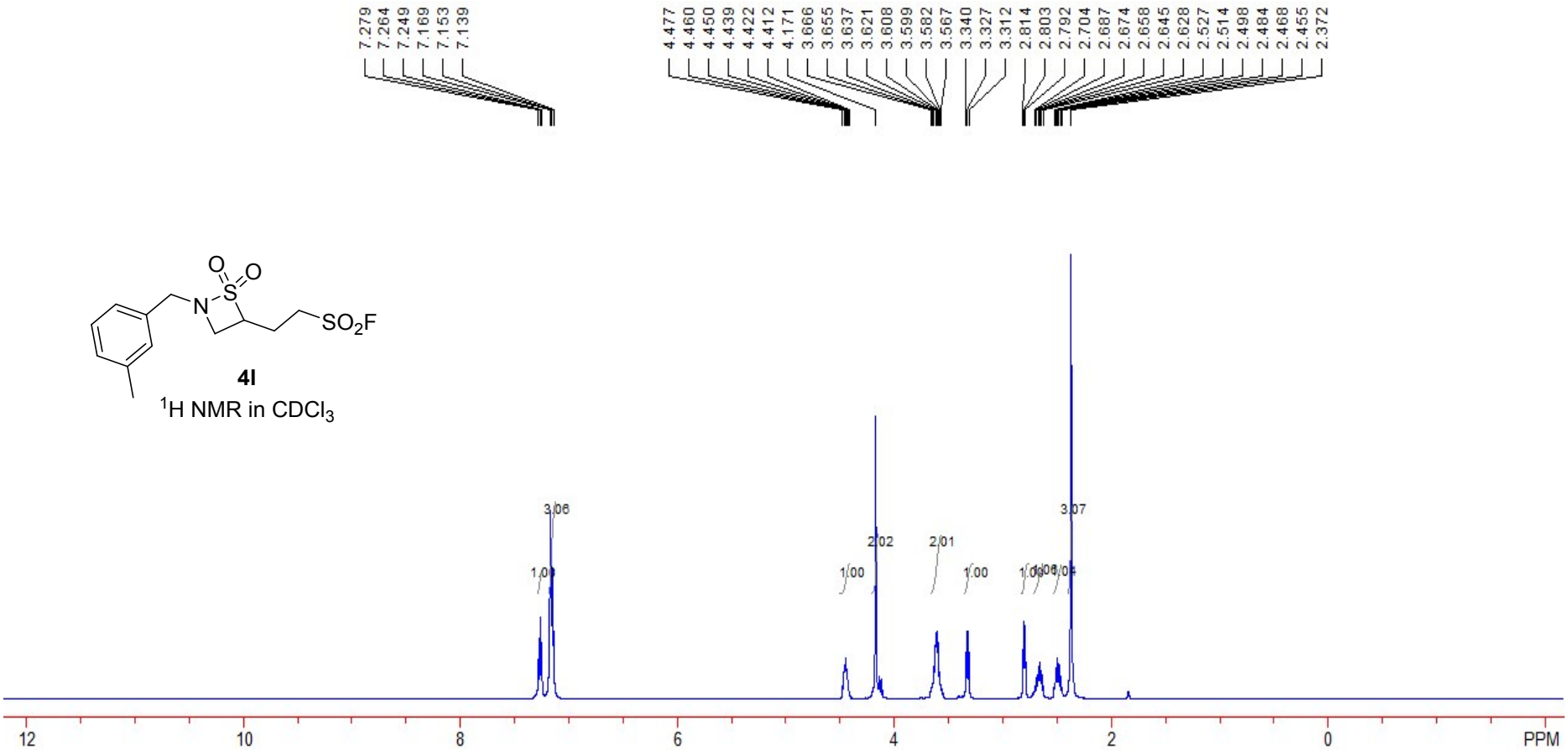
4k

^{19}F NMR in DMSO-d_6



4k

^{13}C NMR in DMSO-d_6


7.279
7.264
7.249
7.169
7.153
7.139
4.477
4.460
4.450
4.439
4.422
4.412
4.171
3.666
3.655
3.637
3.621
3.608
3.599
3.582
3.567
3.340
3.327
3.312
2.814
2.803
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2.704
2.687
2.674
2.658
2.645
2.628
2.527
2.514
2.498
2.484
2.468
2.455
2.372
O
O
S
N
SO2F
4l
1H NMR in CDCl3
3.06
2.02
2.01
3.07
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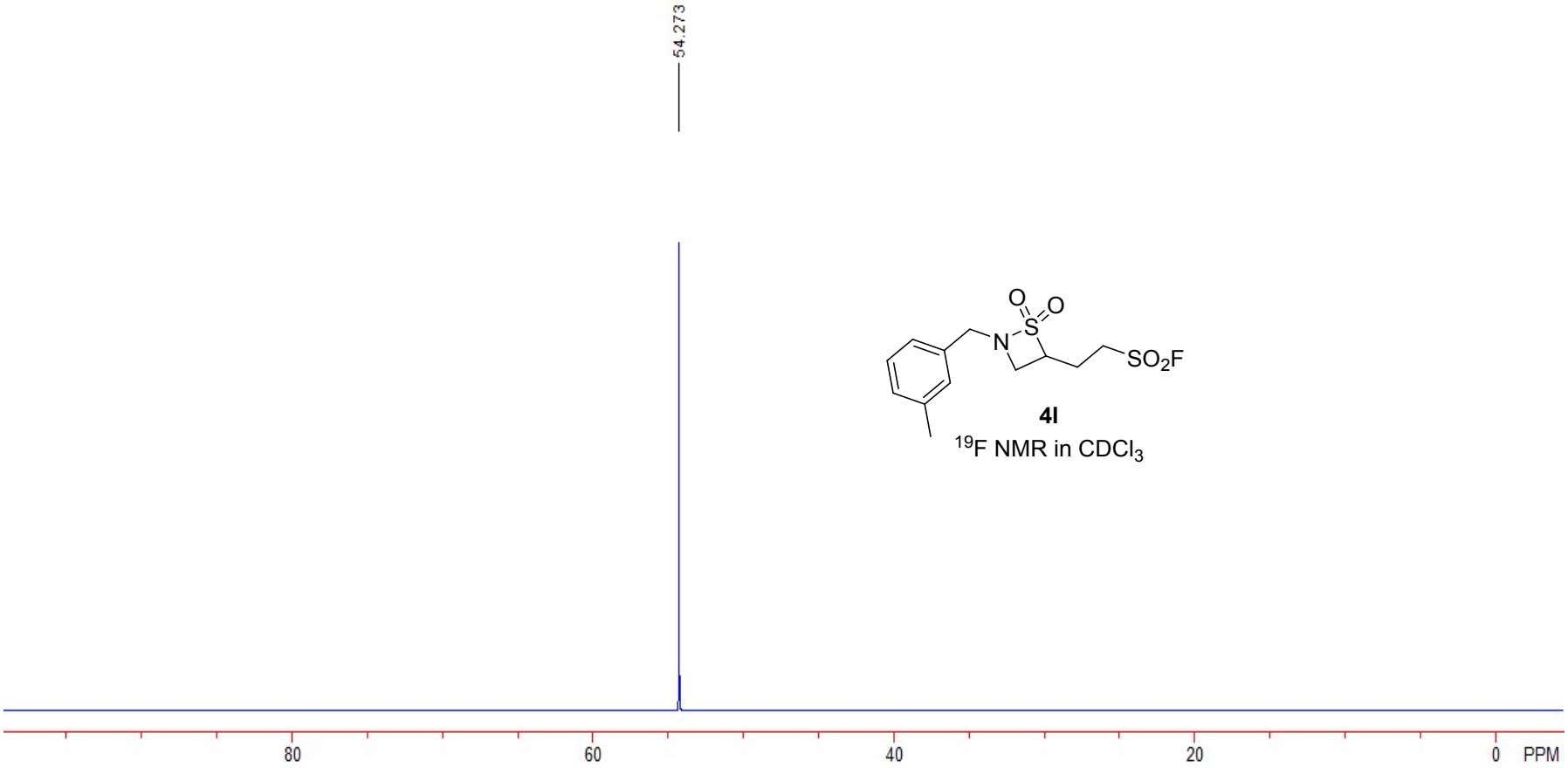
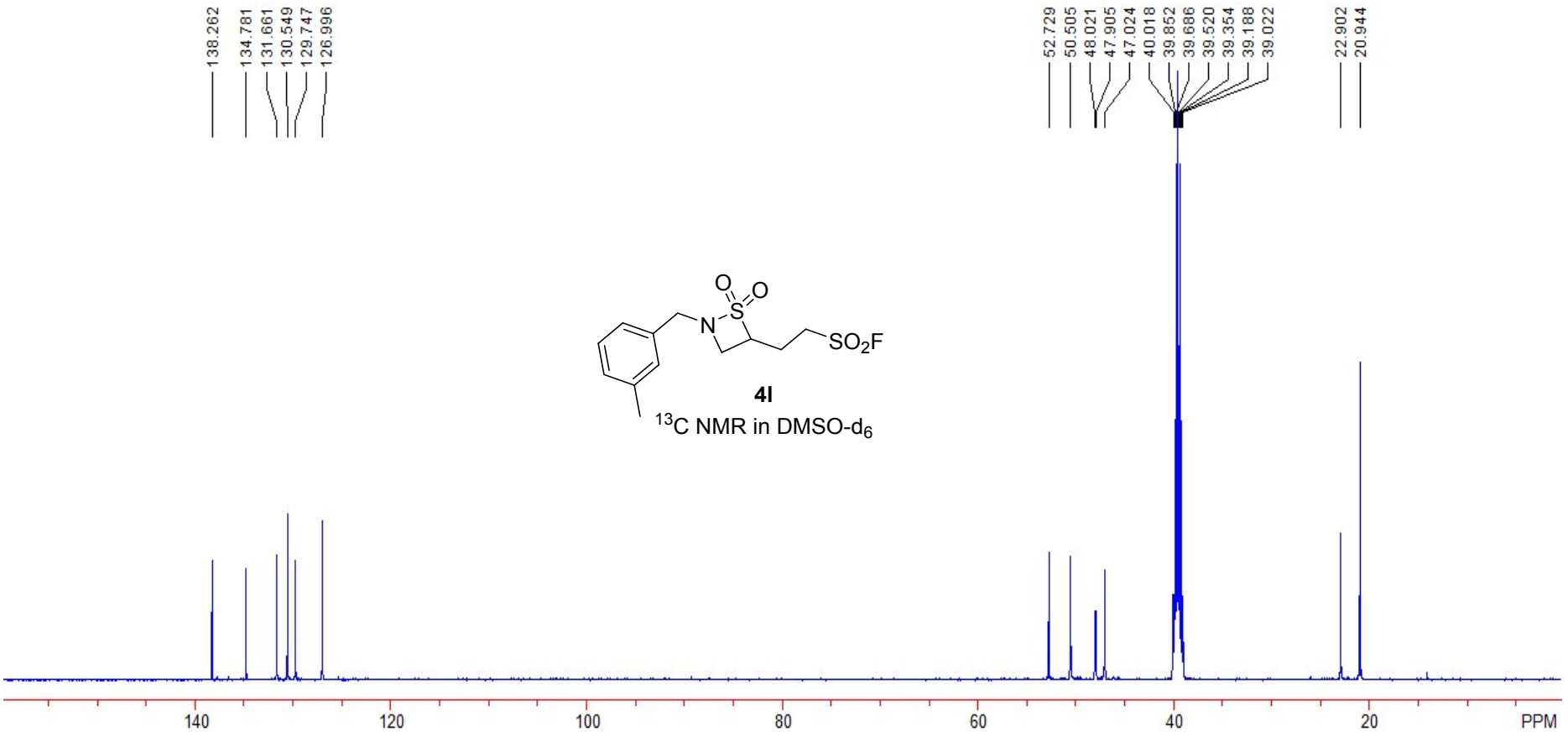
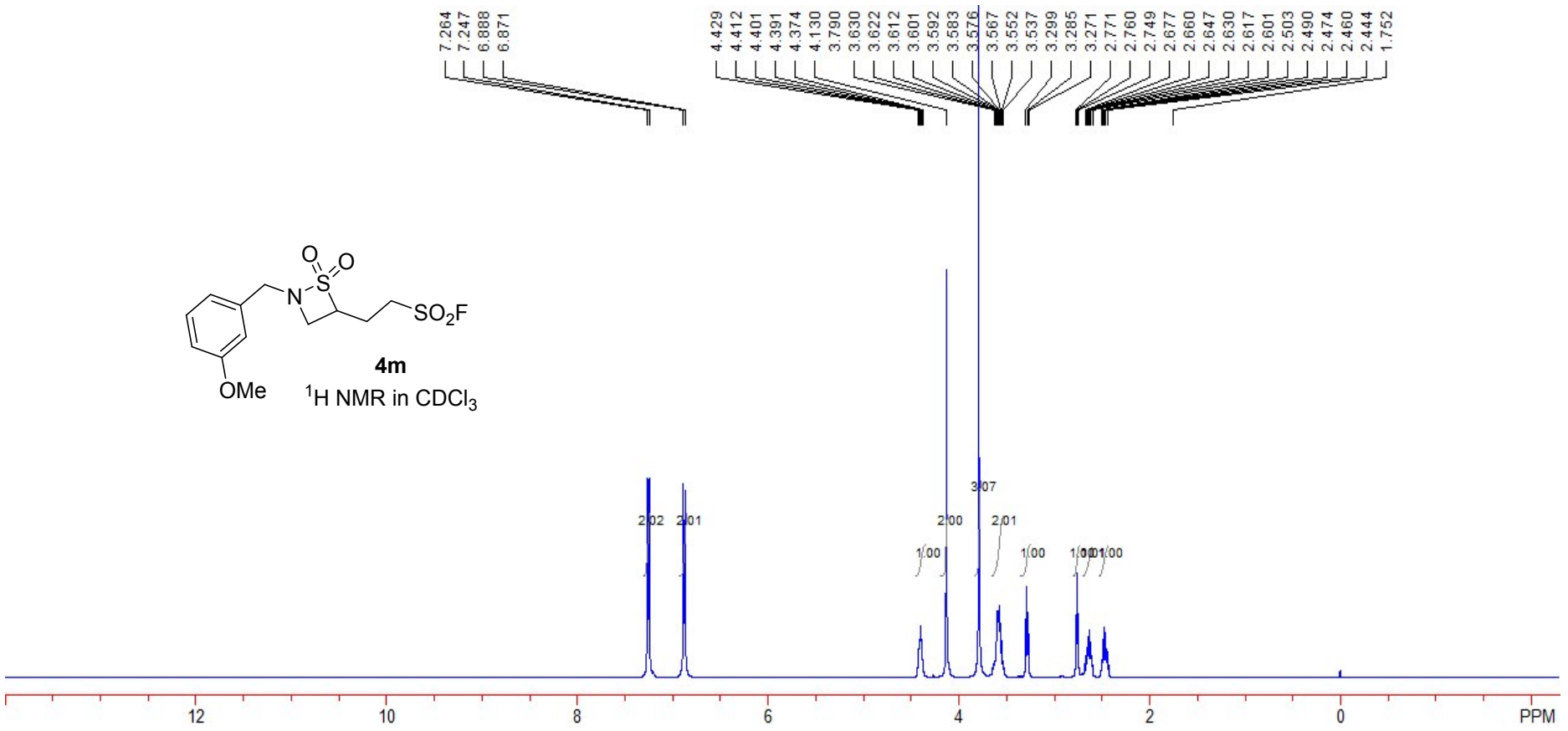
1.00
1.00
12
10
8
6
4
2
0
PPM

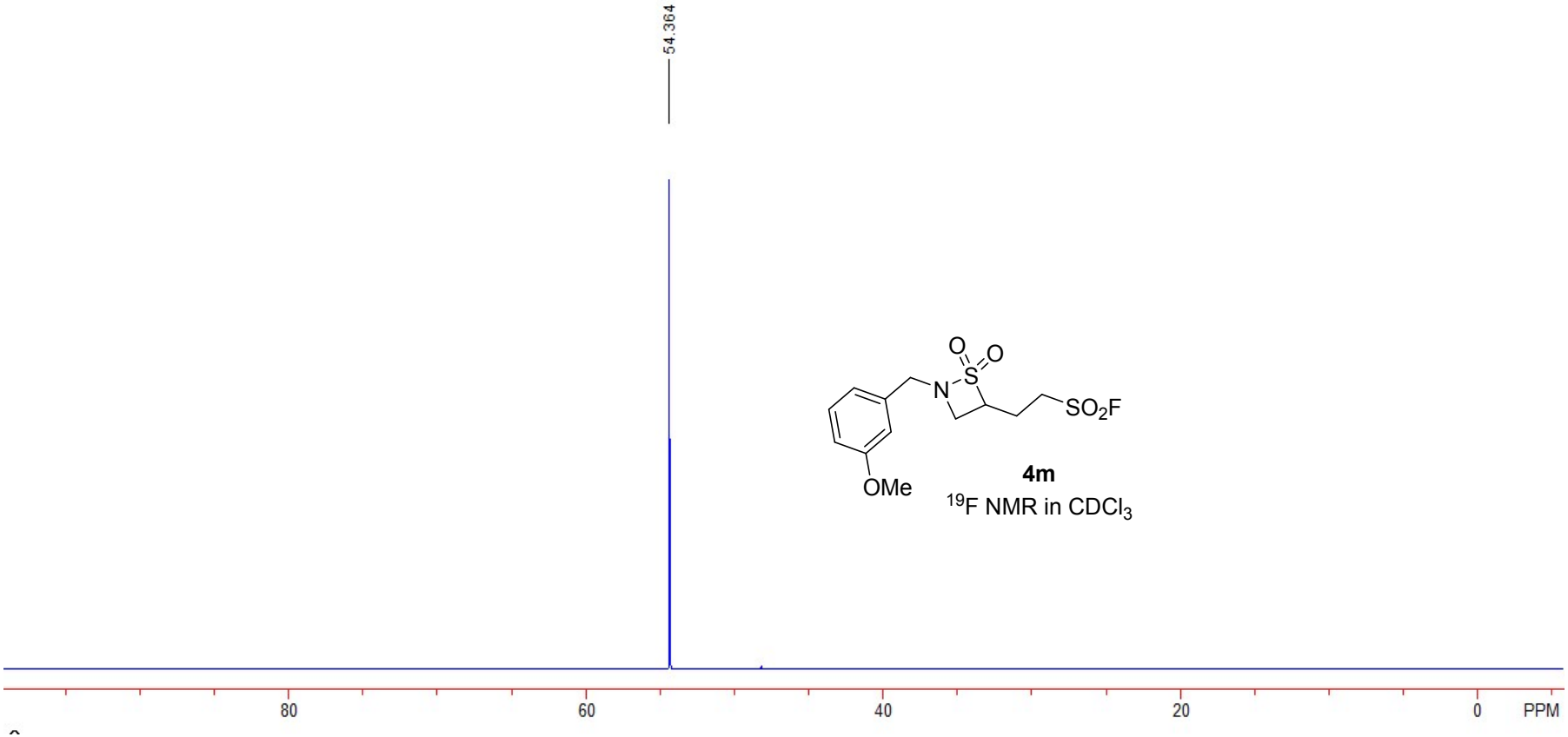


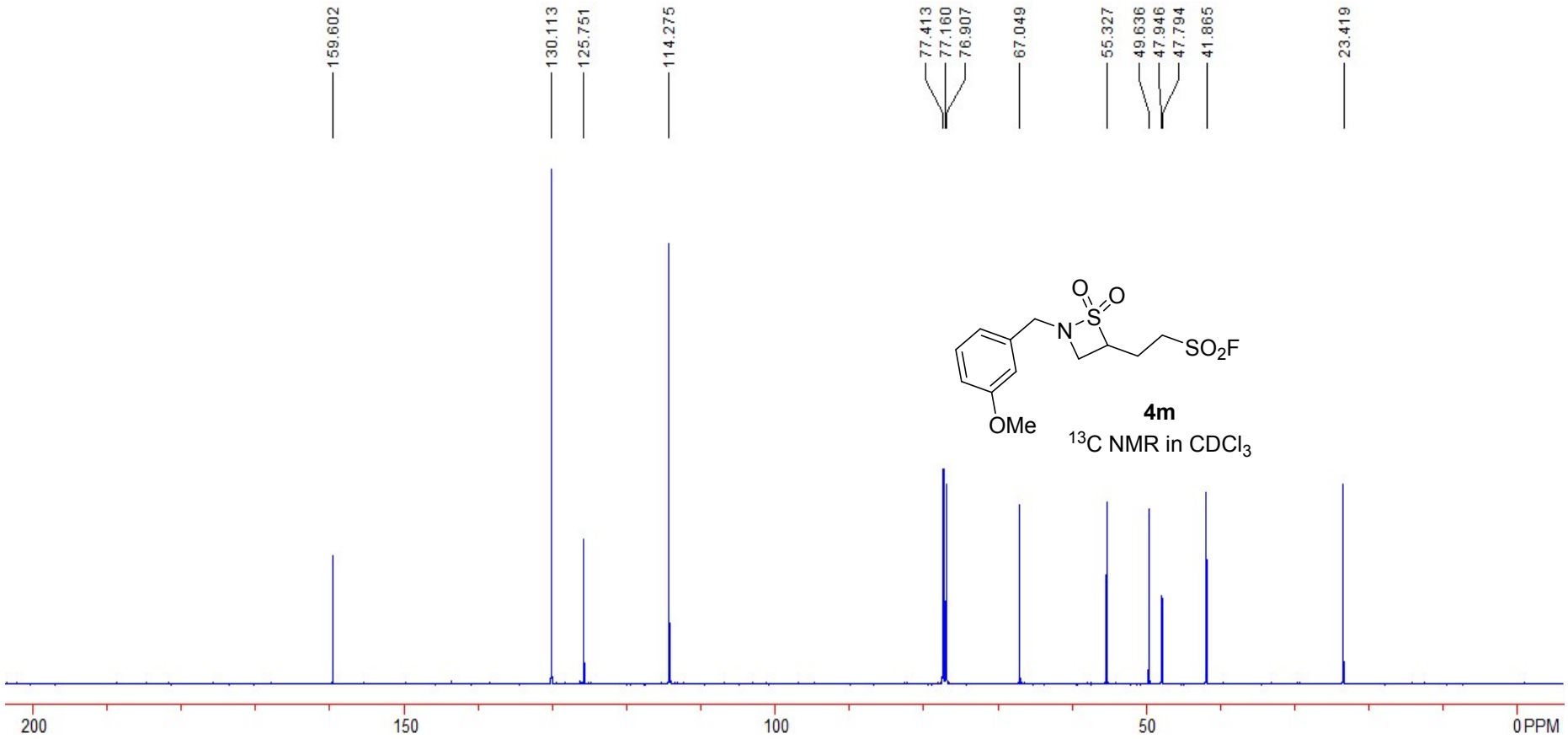
4l

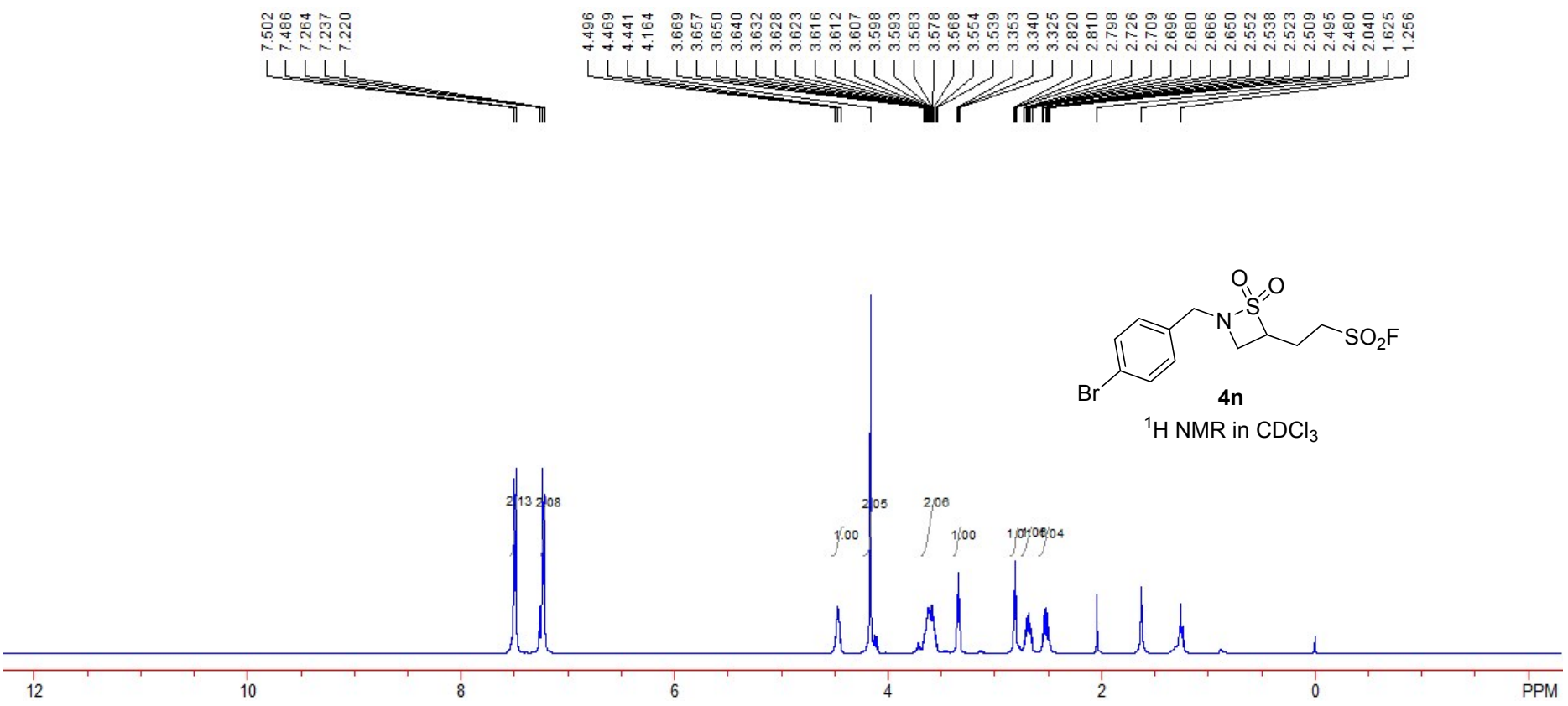
^{19}F NMR in $CDCl_3$


138.262
134.781
131.661
130.549
129.747
126.996
52.729
50.505
48.021
47.905
47.024
40.018
39.852
39.686
39.520
39.354
39.188
39.022
22.902
20.944
O
O
S
N
SO2F
4l
13C NMR in DMSO-d6
140
120
100
80
60
40
20
PPM


7.264
7.247
6.888
6.871
4.429
4.412
4.401
4.391
4.374
4.130
3.790
3.630
3.622
3.612
3.601
3.592
3.583
3.576
3.567
3.552
3.537
3.299
3.285
3.271
2.771
2.760
2.749
2.677
2.660
2.647
2.630
2.617
2.601
2.503
2.490
2.474
2.460
2.444
1.752
O
O
S
N
SO2F
OMe
4m
1H NMR in CDCl3
2.02
2.01
3.07
2.00
2.01
1.00
1.00
1.00
1.00
1.00
12
10
8
6
4
2
0
PPM


54.364
O
O
S
N
SO2F
OMe
4m
19F NMR in CDCl3
80
60
40
20
0
PPM


159.602
130.113
125.751
114.275
77.413
77.160
76.907
67.049
55.327
49.636
47.946
47.794
41.865
23.419
O
O
N
S
SO2F
OMe
4m
13C NMR in CDCl3
200
150
100
50
0 PPM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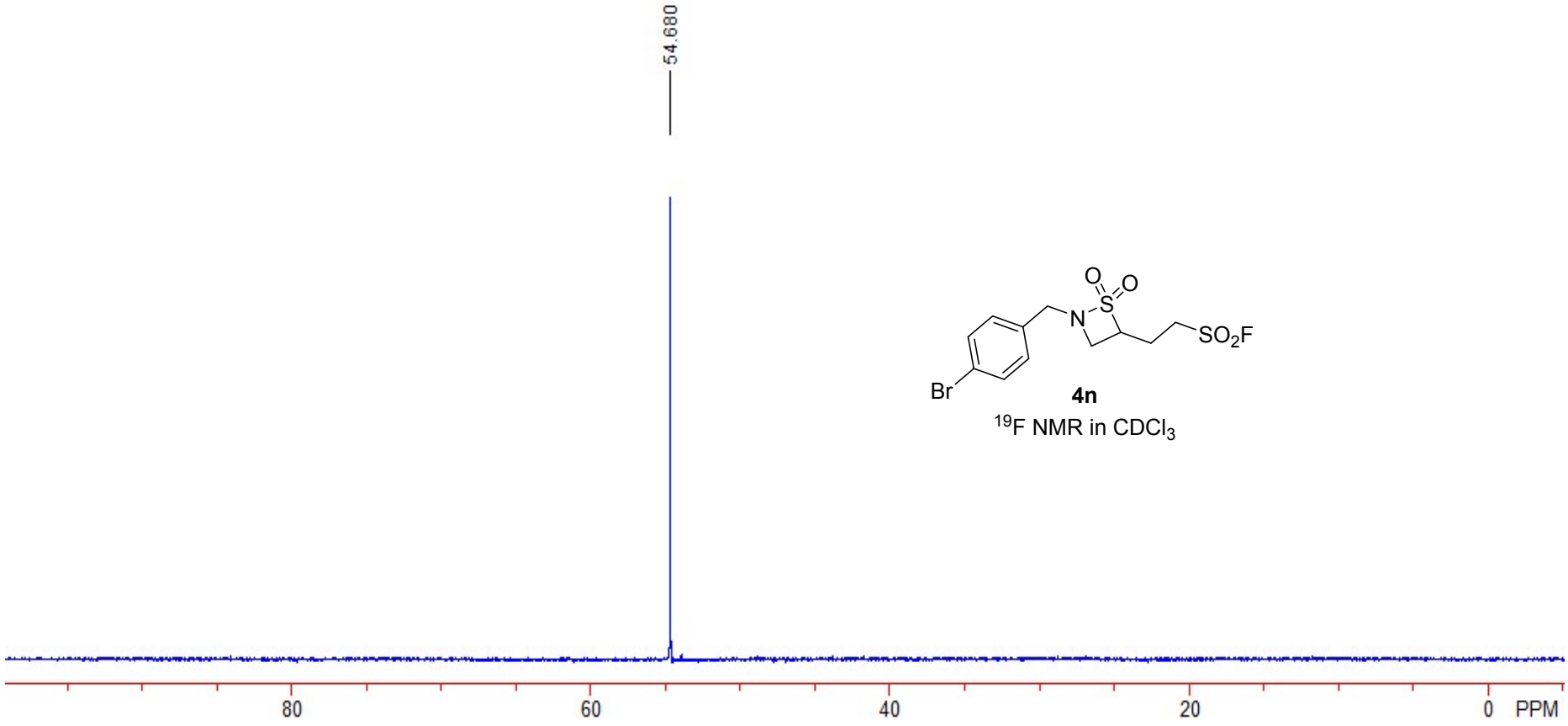
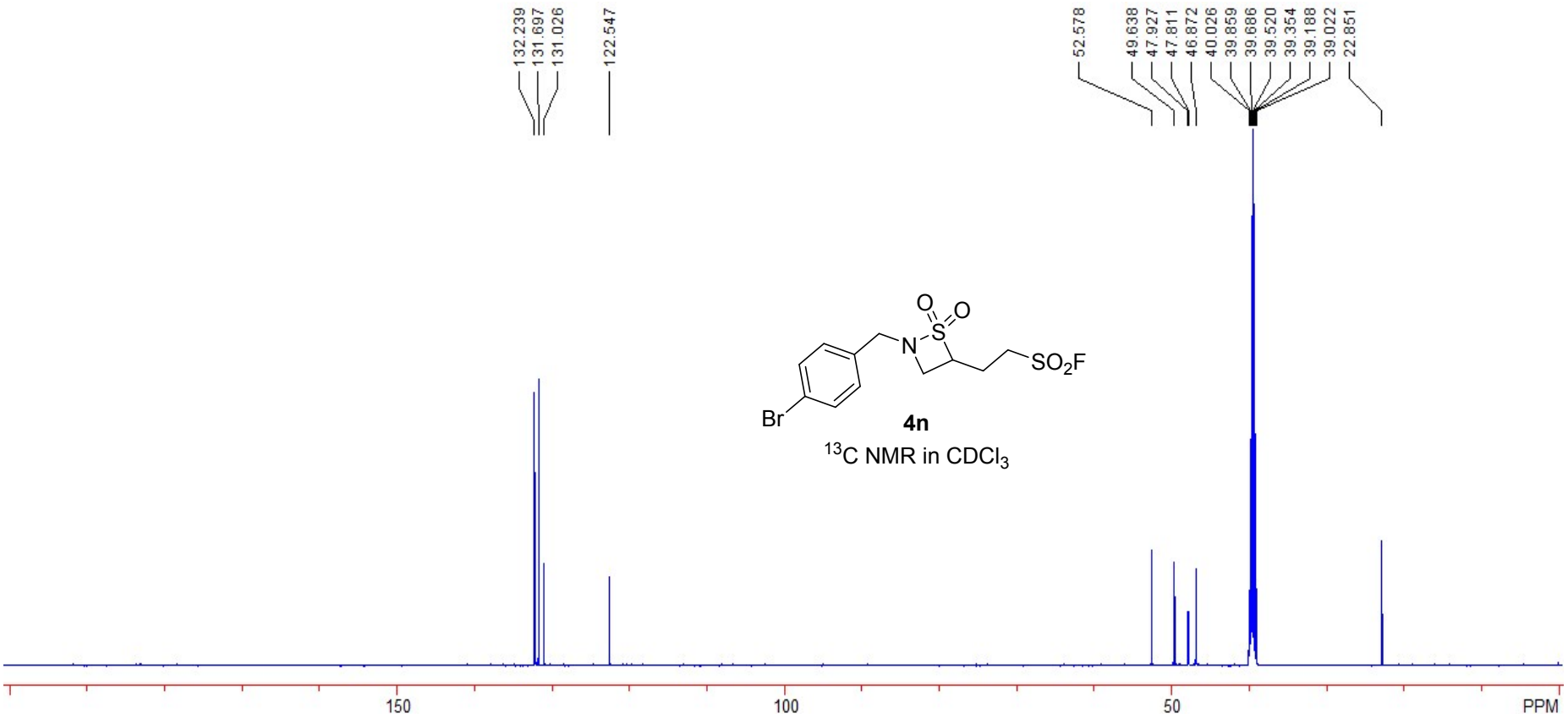
7.486
7.264
7.237
7.220
4.496
4.469
4.441
4.164
3.669
3.657
3.650
3.640
3.632
3.628
3.623
3.616
3.612
3.607
3.598
3.593
3.583
3.578
3.568
3.554
3.539
3.353
3.340
3.325
2.820
2.810
2.798
2.726
2.709
2.696
2.680
2.666
2.650
2.552
2.538
2.523
2.509
2.495
2.480
2.040
1.625
1.256
O
O
S
N
SO2F
Br
4n
1H NMR in CDCl3
2.13
2.08
2.05
2.06
1.00
1.00
1.01
1.06
1.04
12
10
8
6
4
2
0
PPM



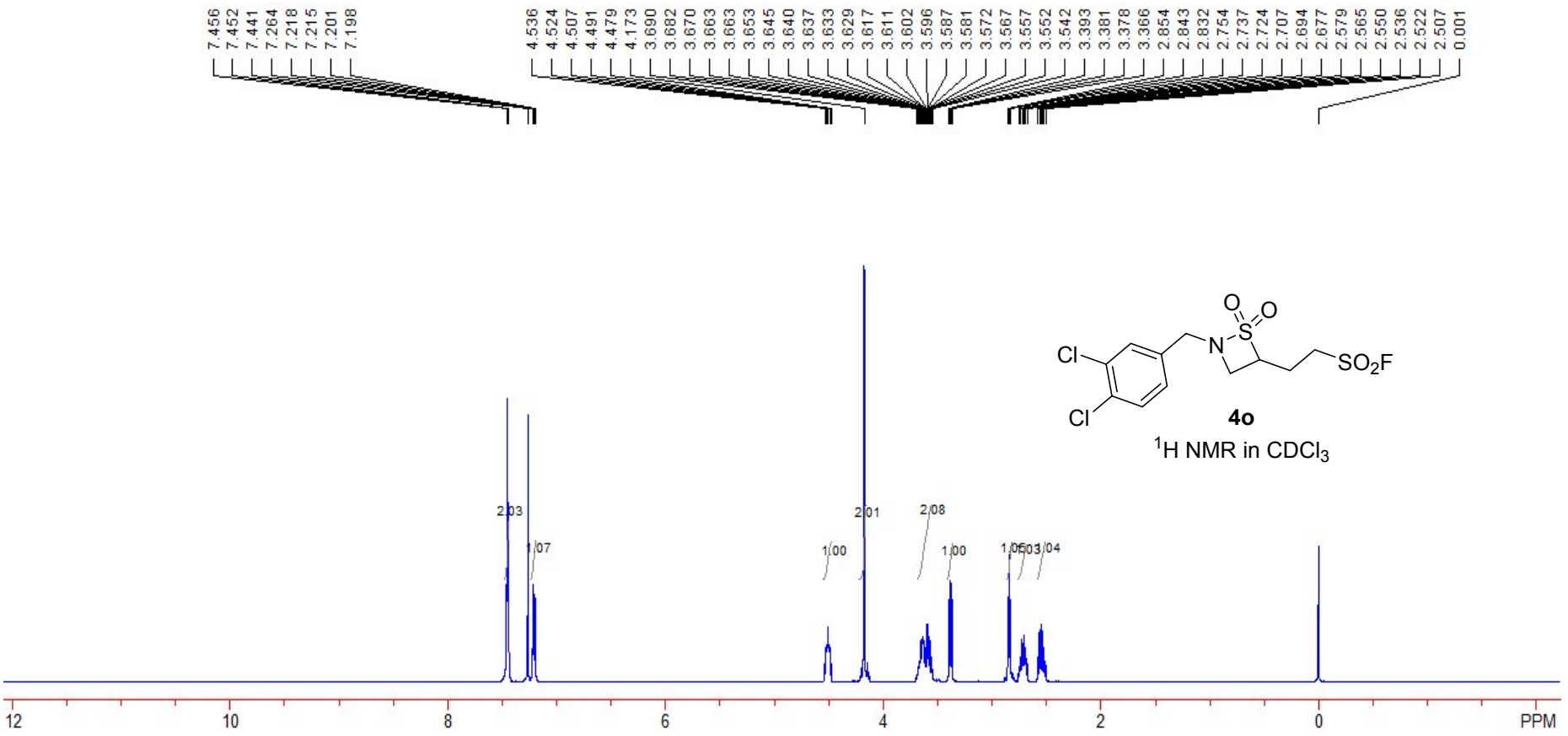
4n

^{19}F NMR in $CDCl_3$



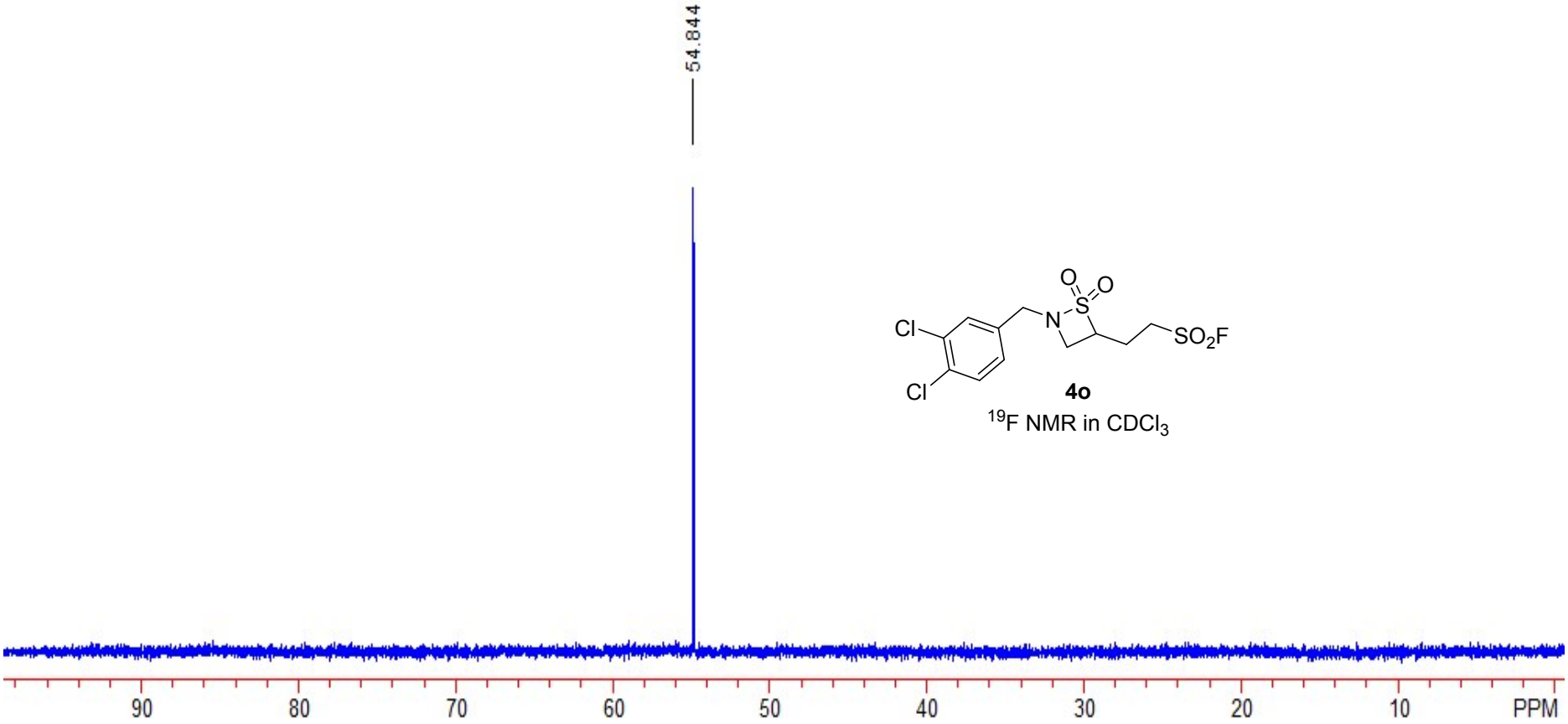
4n

^{13}C NMR in $CDCl_3$



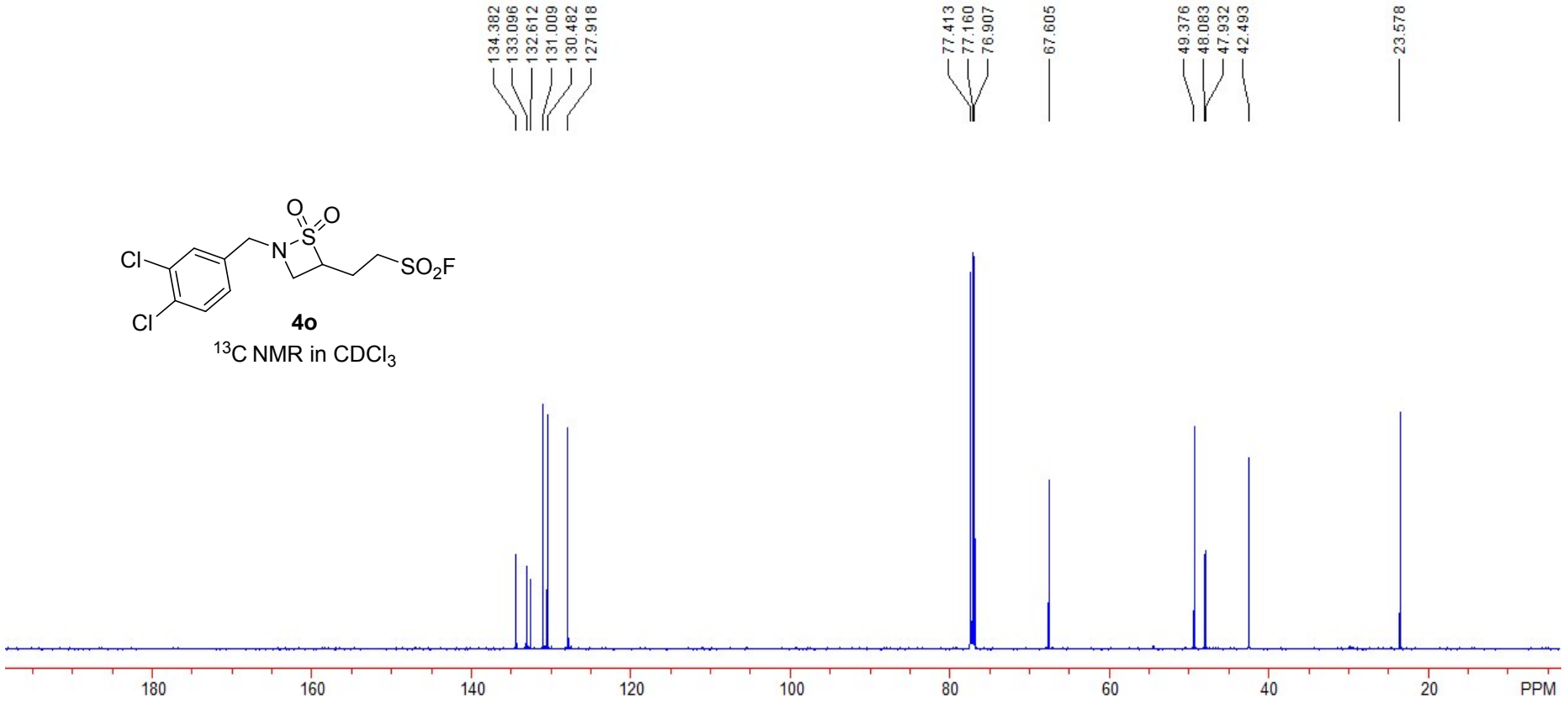
4o

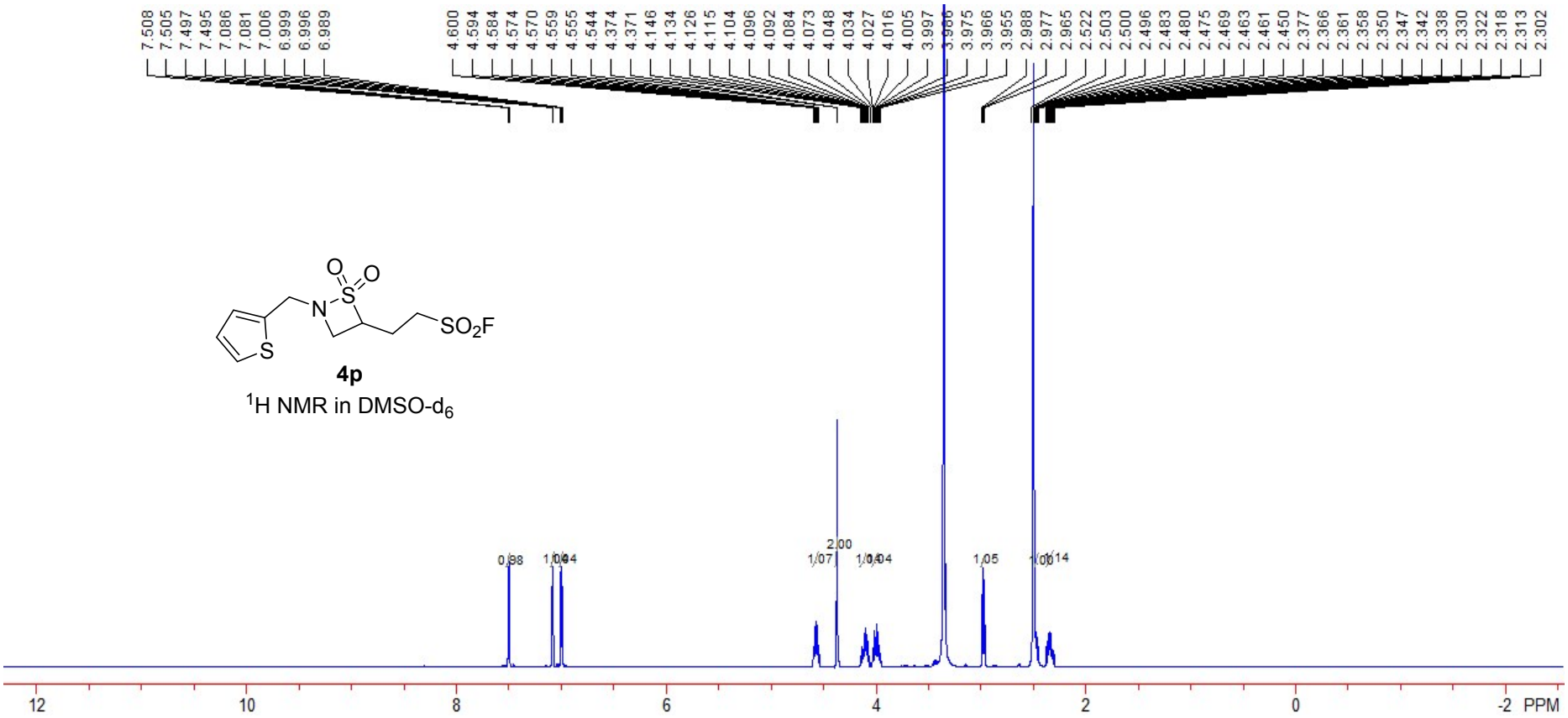
^{1}H NMR in $CDCl_3$



4o

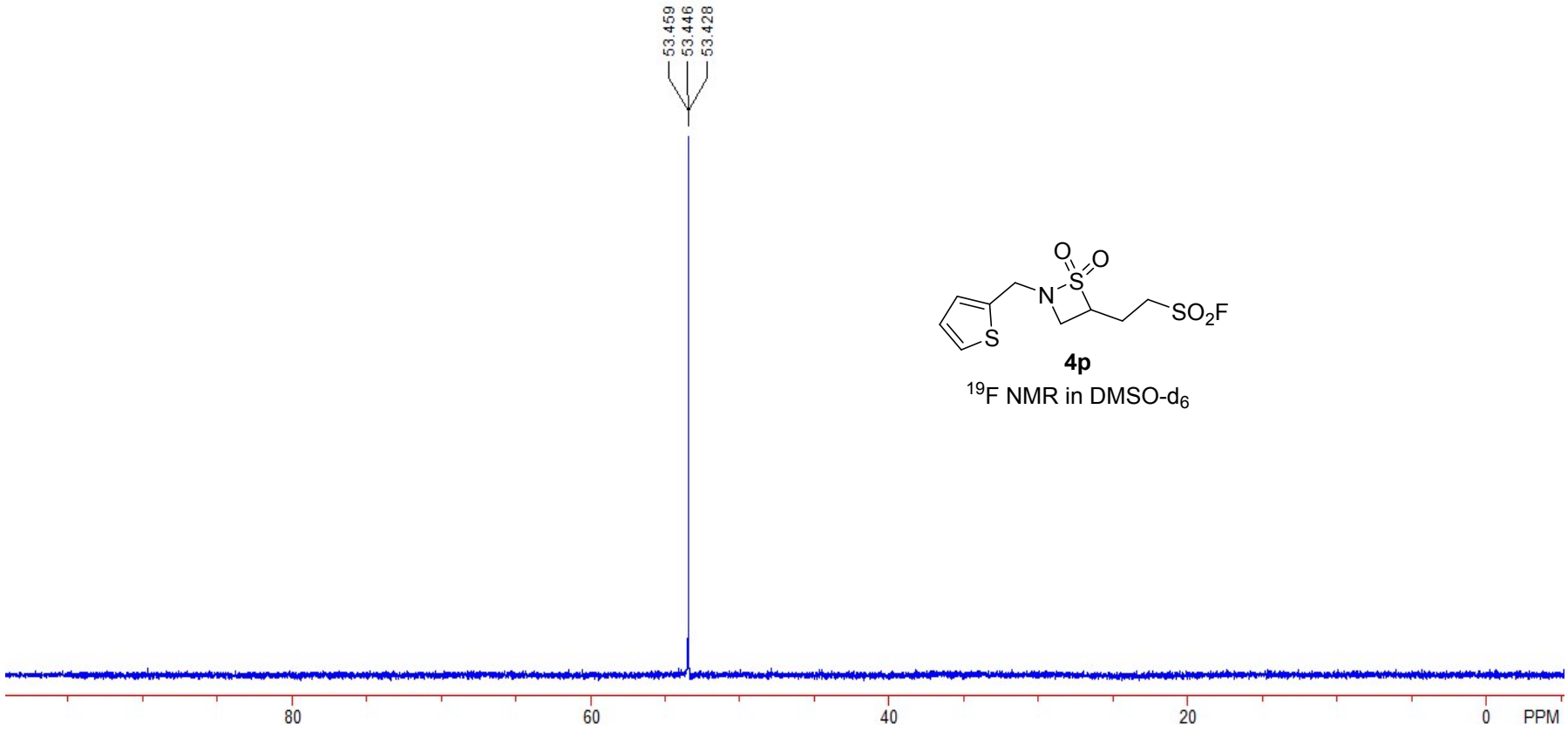
^{19}F NMR in $CDCl_3$


134.382
133.096
132.612
131.009
130.482
127.918
77.413
77.160
76.907
67.605
49.376
48.083
47.932
42.493
23.578
O
O
S
N
Cl
Cl
SO2F
4o
13C NMR in CDCl3
180
160
140
120
100
80
60
40
20
PPM



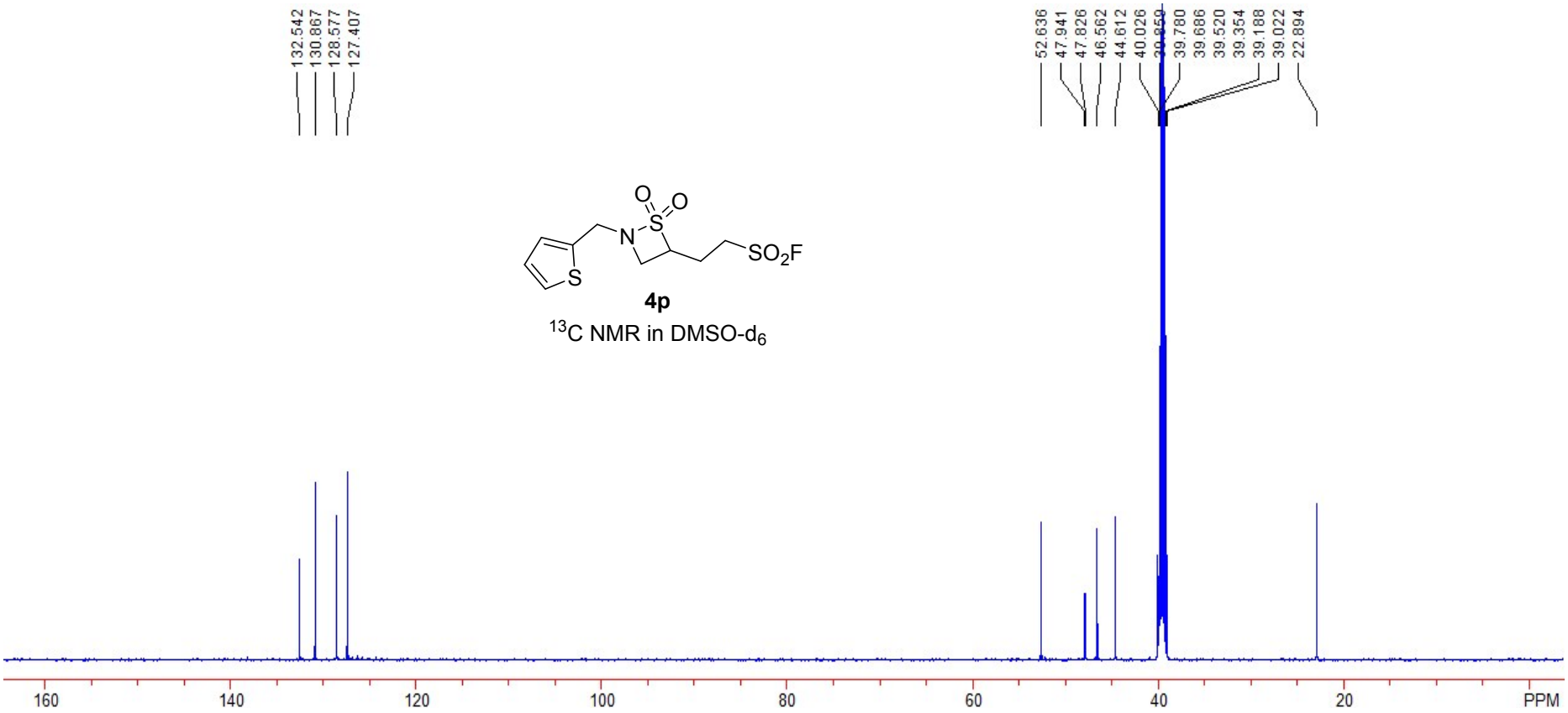
4p

^{1}H NMR in DMSO-d_6



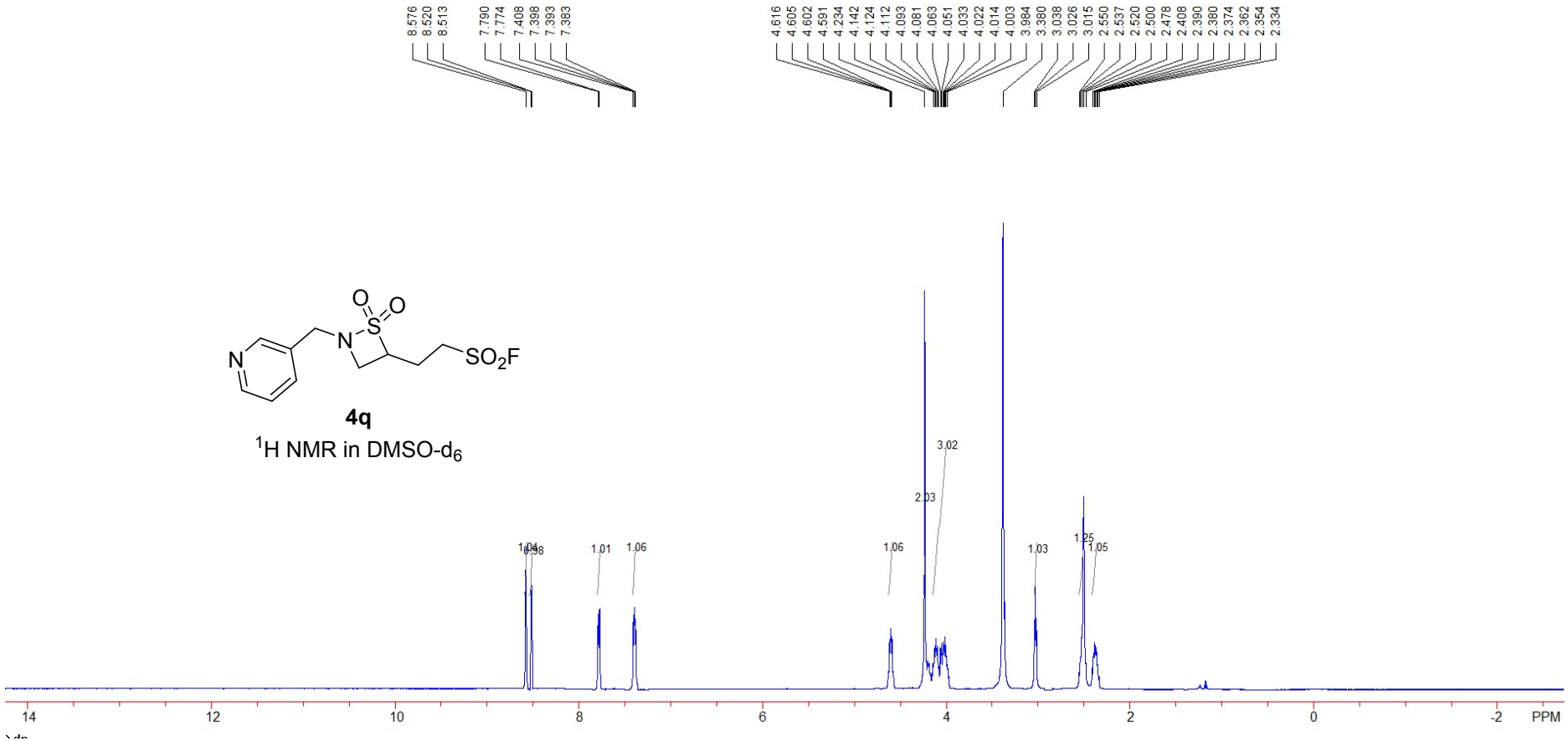
4p

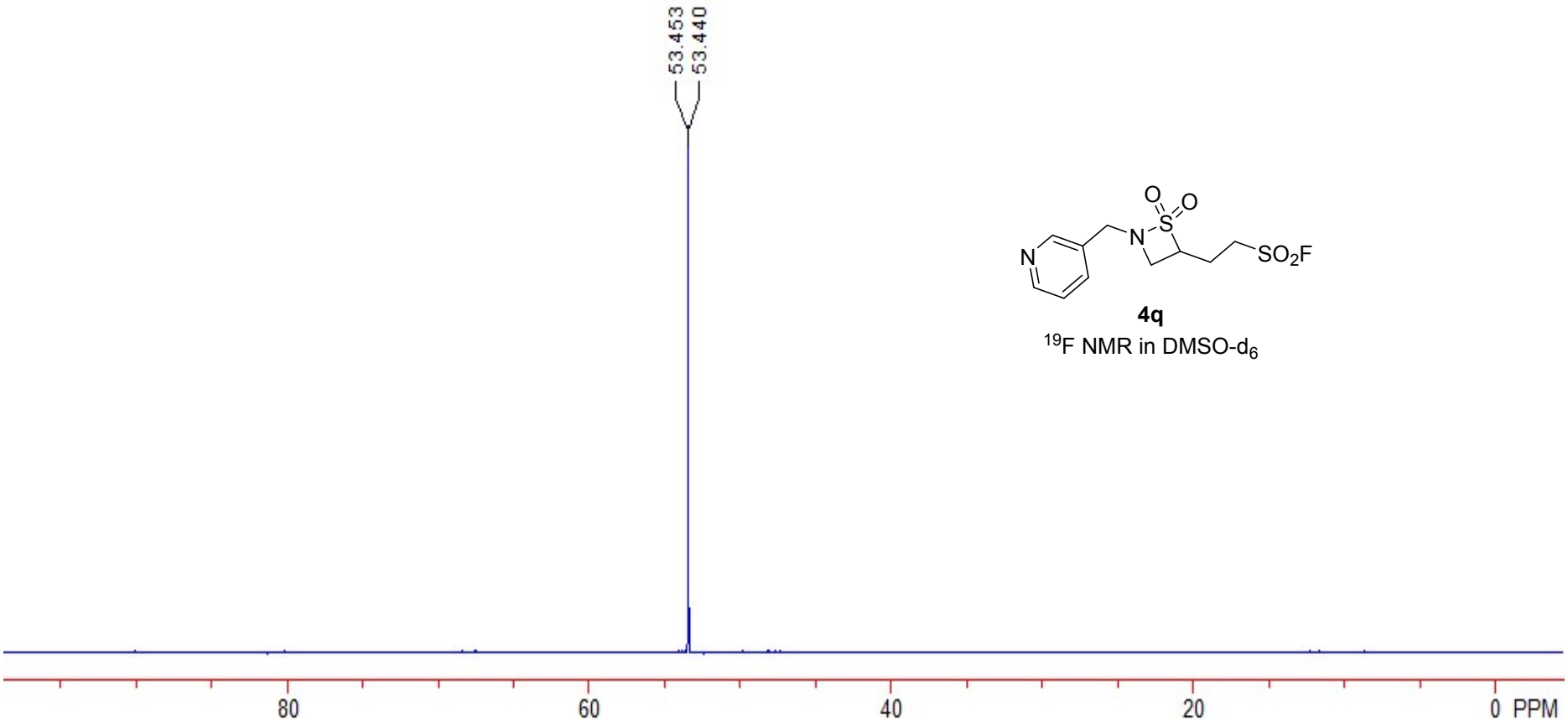
^{19}F NMR in DMSO-d_6



4p

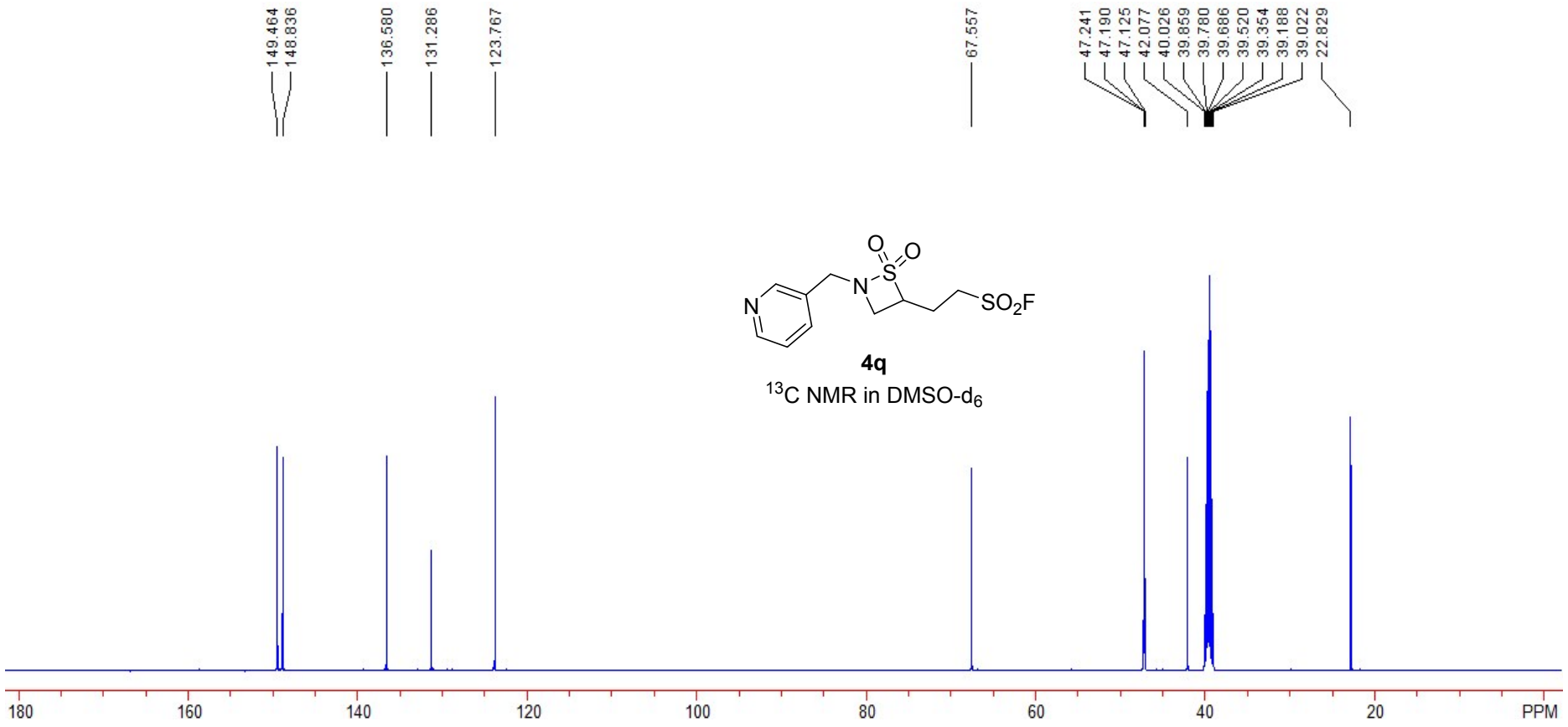
^{13}C NMR in DMSO-d_6

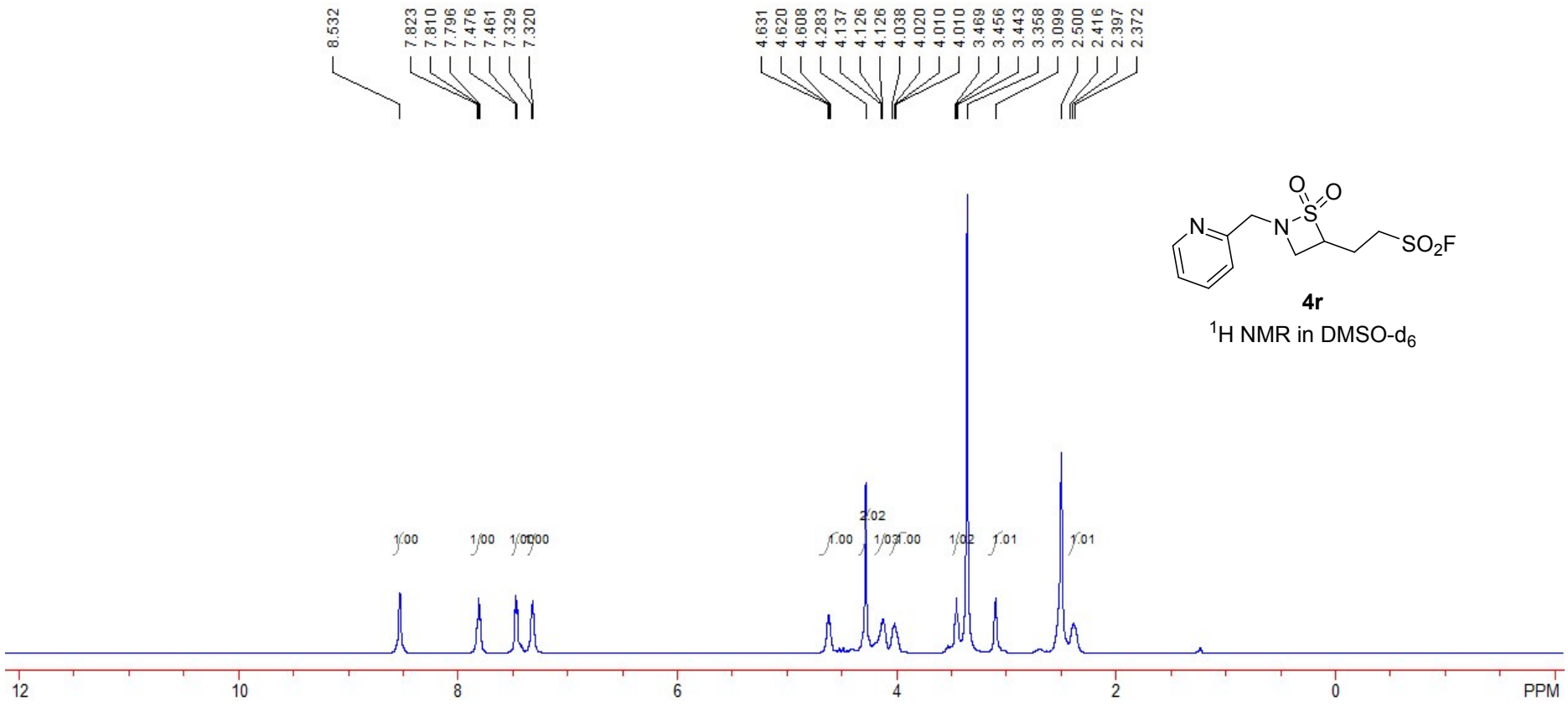

8.576
8.520
8.513
7.790
7.774
7.408
7.398
7.393
7.383
4.616
4.605
4.602
4.591
4.234
4.142
4.124
4.112
4.093
4.081
4.063
4.051
4.033
4.022
4.014
4.003
3.984
3.380
3.038
3.026
3.015
2.550
2.537
2.520
2.500
2.478
2.408
2.390
2.380
2.374
2.362
2.354
2.334
O
O
S
N
N
SO2F
4q
1H NMR in DMSO-d6
1.04
0.98
1.01
1.06
1.06
3.02
2.03
1.03
1.25
1.05
14
12
10
8
6
4
2
0
-2
PPM



4q

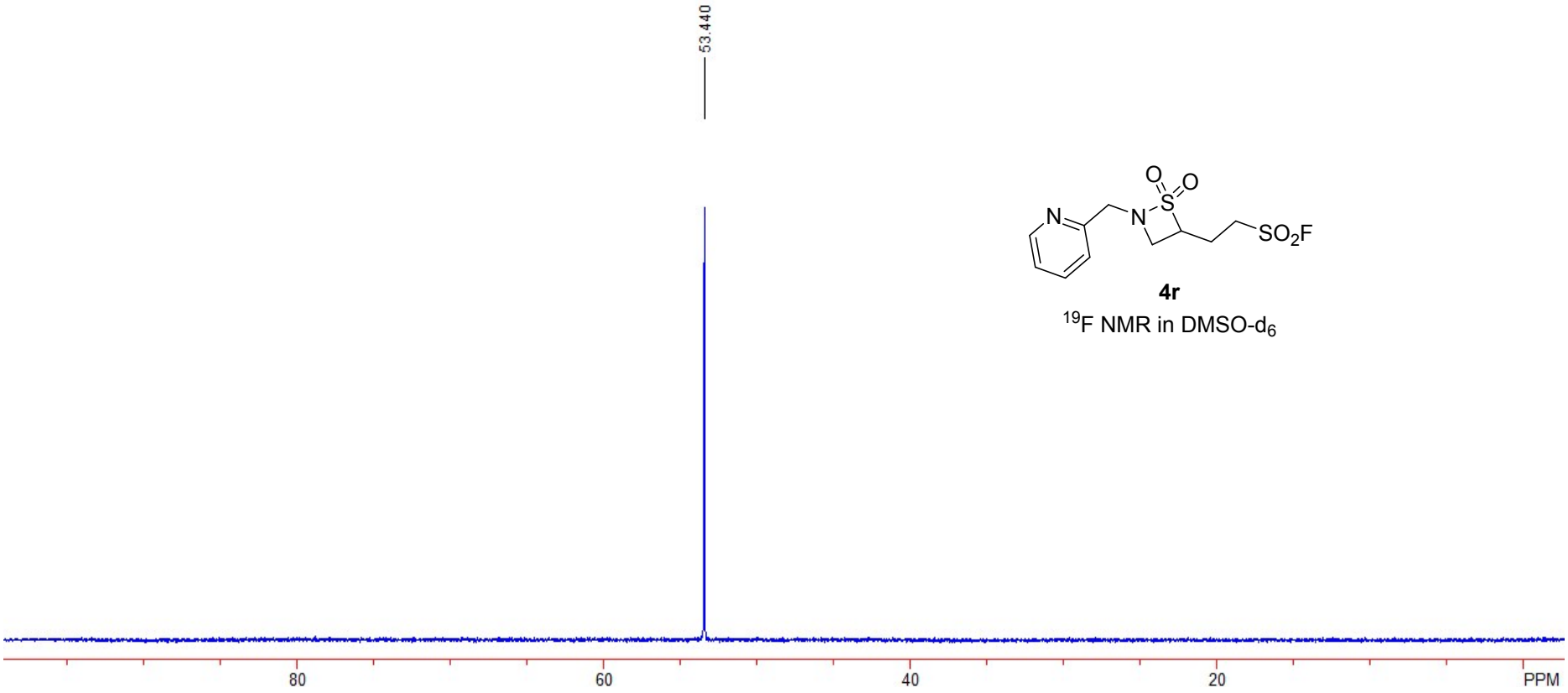
^{19}F NMR in DMSO-d_6


149.464
148.836
136.580
131.286
123.767
67.557
47.241
47.190
47.125
42.077
40.026
39.859
39.780
39.686
39.520
39.354
39.188
39.022
22.829
O
O
S
N
N
SO2F
4q
13C NMR in DMSO-d6
180
160
140
120
100
80
60
40
20
PPM



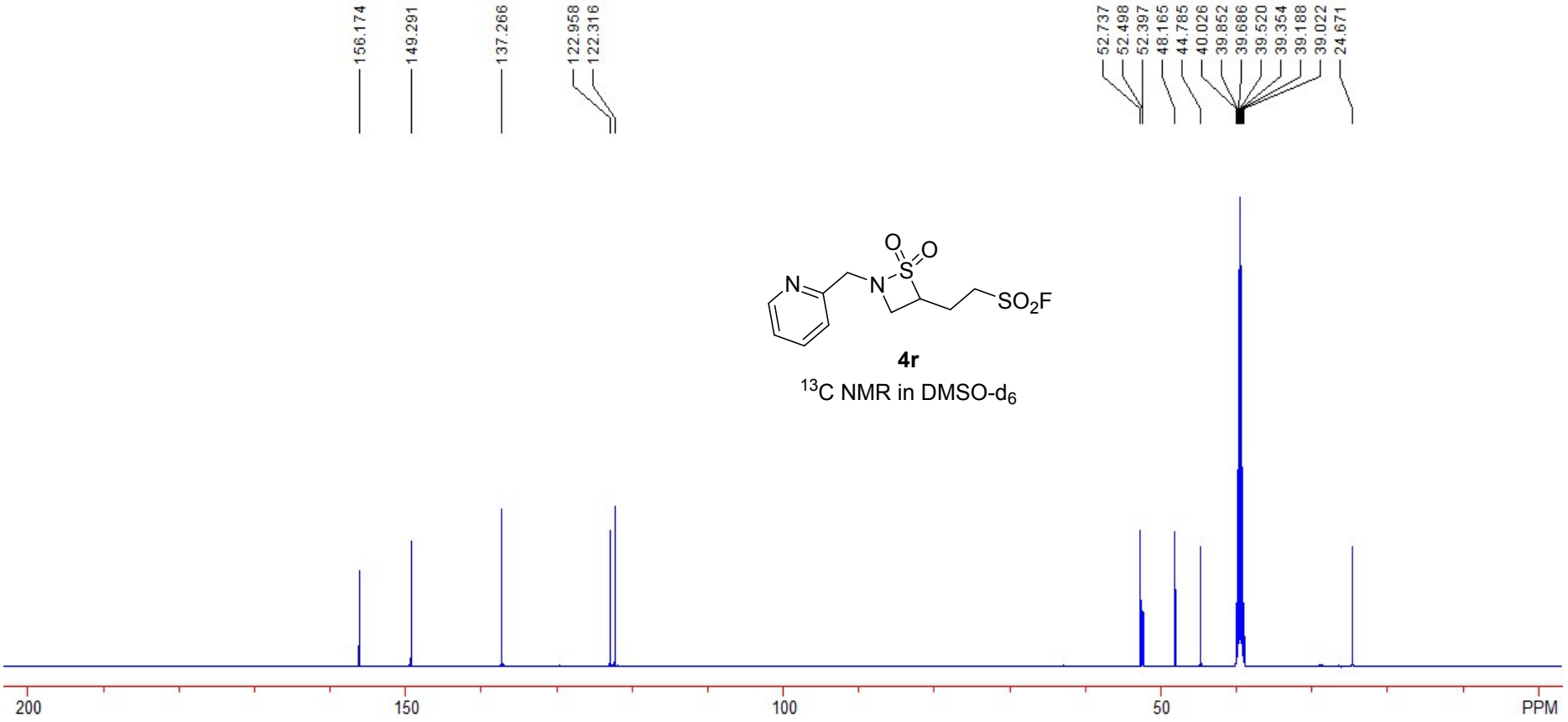
4r

^{1}H NMR in DMSO-d_6



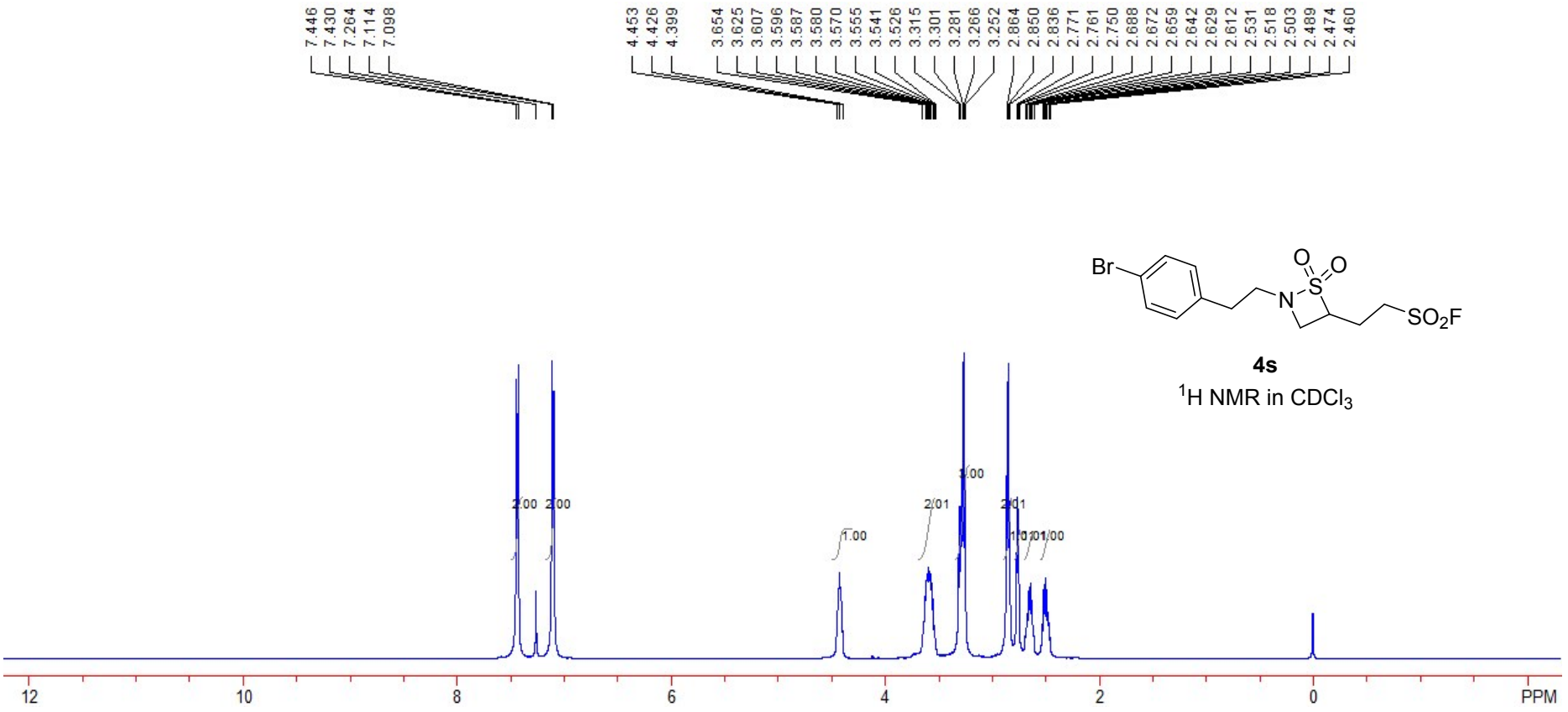
4r

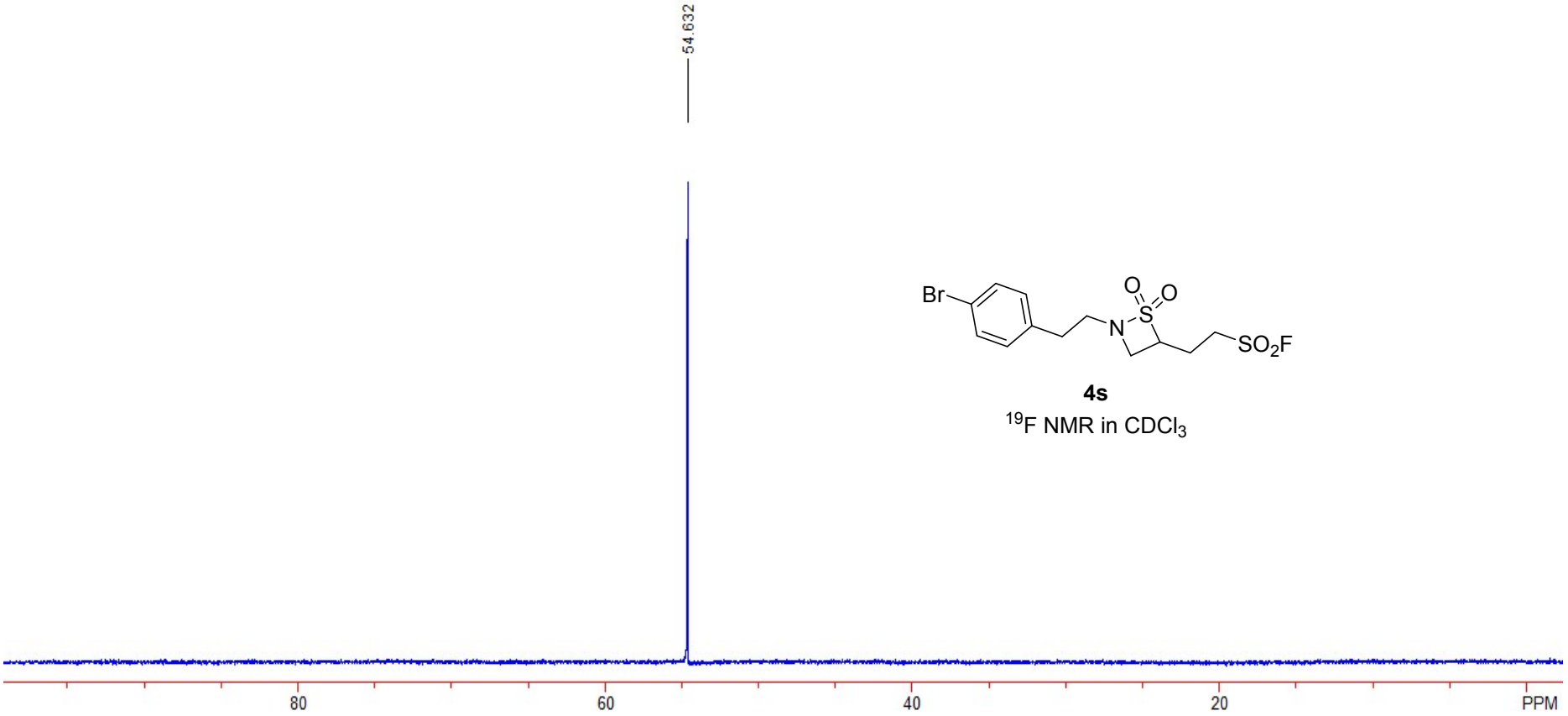
^{19}F NMR in DMSO-d_6



4r

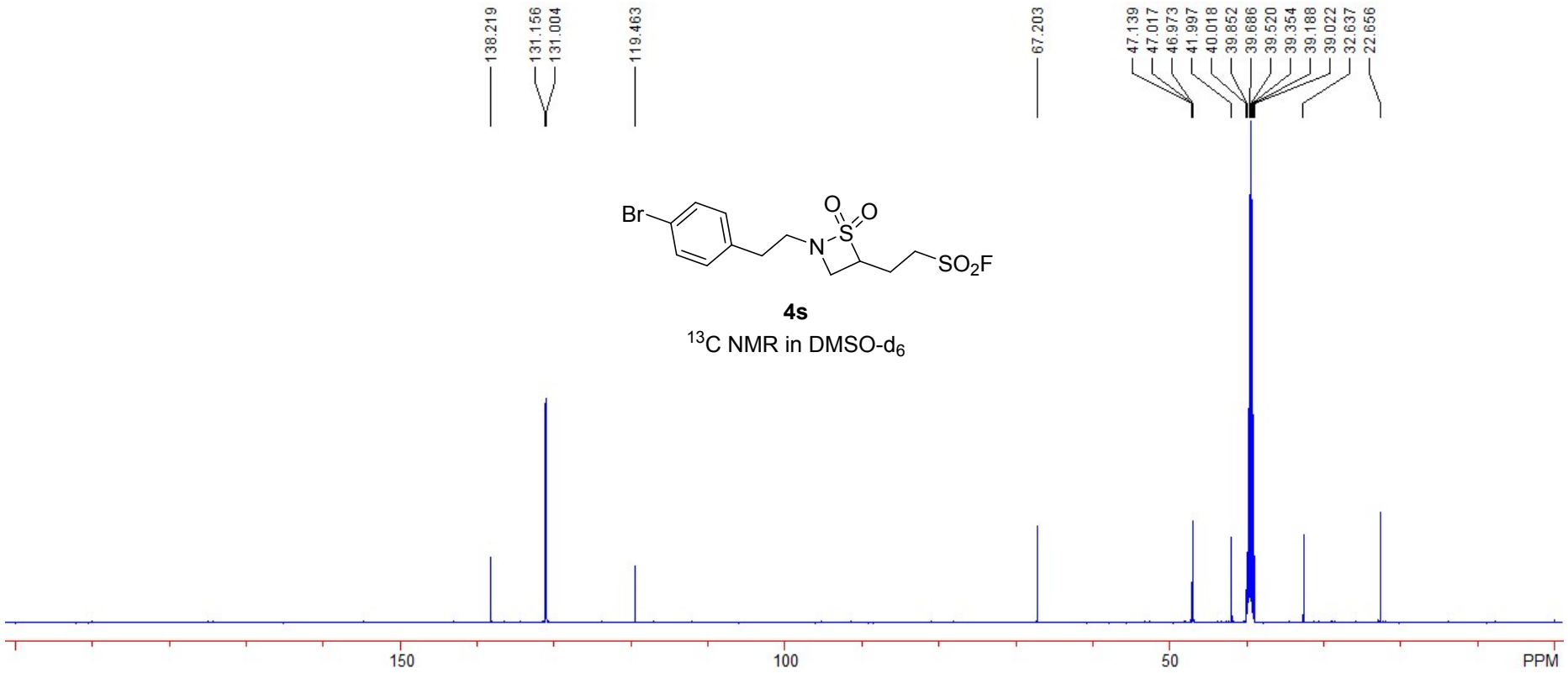
^{13}C NMR in DMSO-d_6


7.446
7.430
7.264
7.114
7.098
4.453
4.426
4.399
3.654
3.625
3.607
3.596
3.587
3.580
3.570
3.555
3.541
3.526
3.315
3.301
3.281
3.266
3.252
2.864
2.850
2.836
2.771
2.761
2.750
2.688
2.672
2.659
2.642
2.629
2.612
2.531
2.518
2.503
2.489
2.474
2.460
Br
O
O
S
N
SO2F
4s
1H NMR in CDCl3
2.00
2.00
1.00
2.01
3.00
2.01
1.01
1.01
1.00
12
10
8
6
4
2
0
PPM



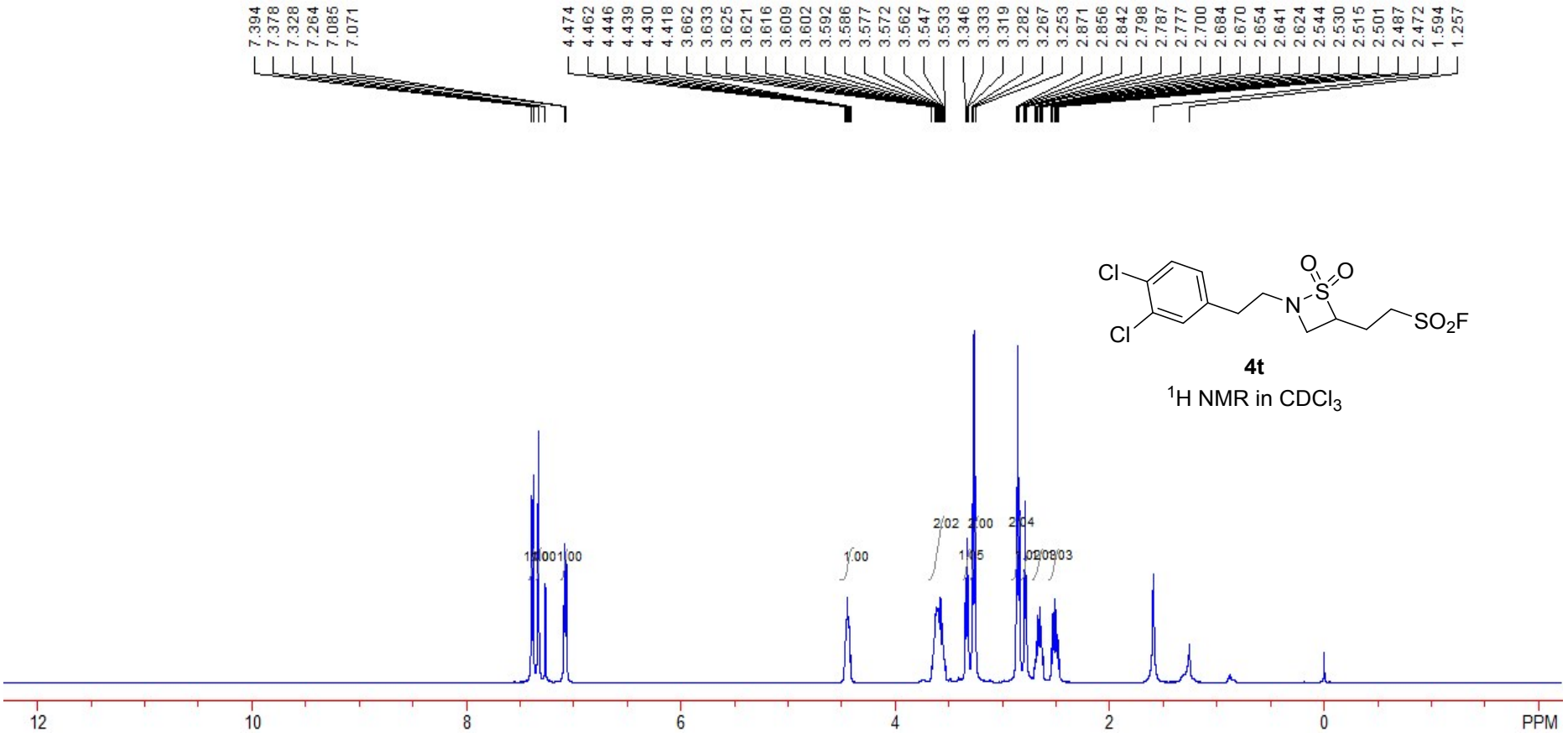
4s

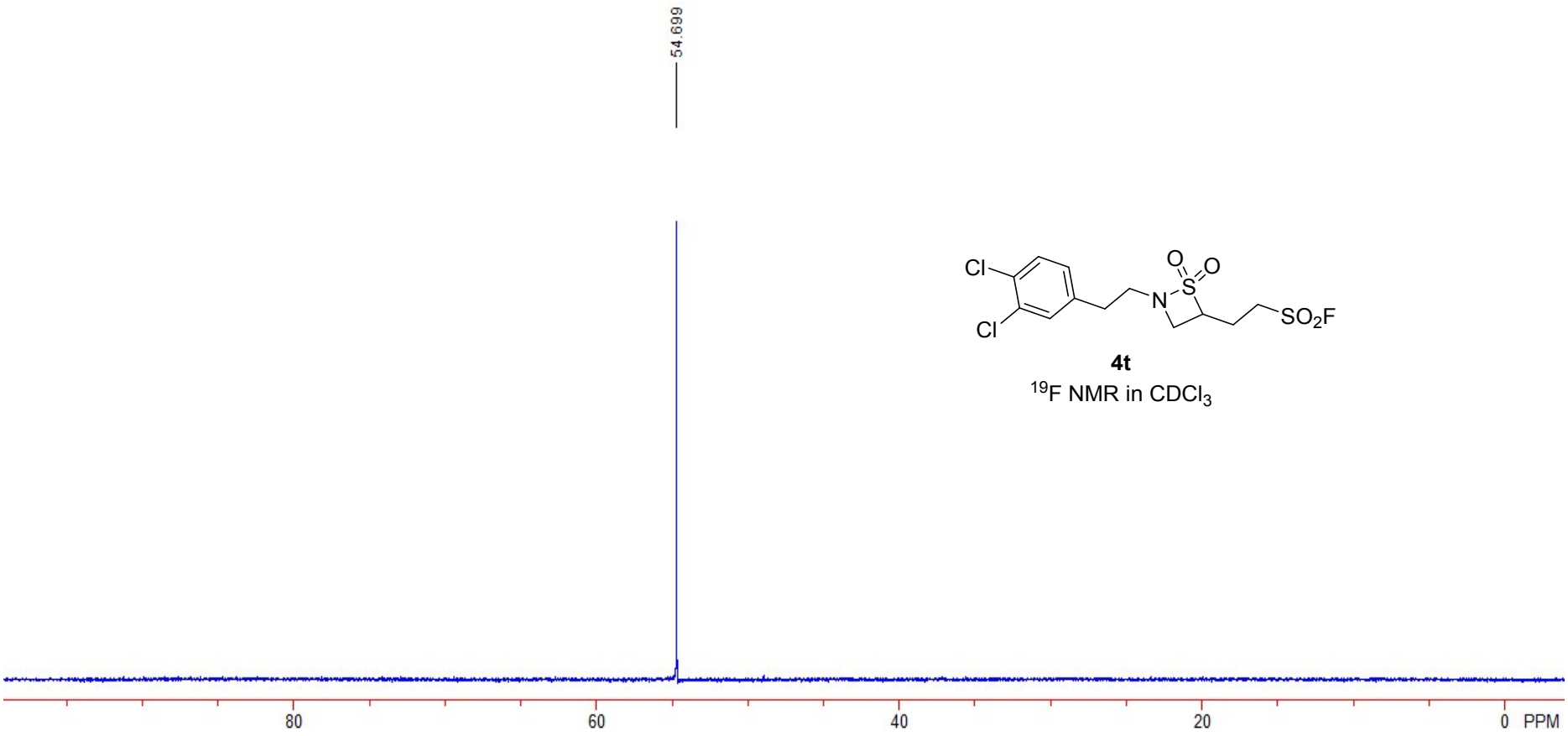
^{19}F NMR in $CDCl_3$



4s

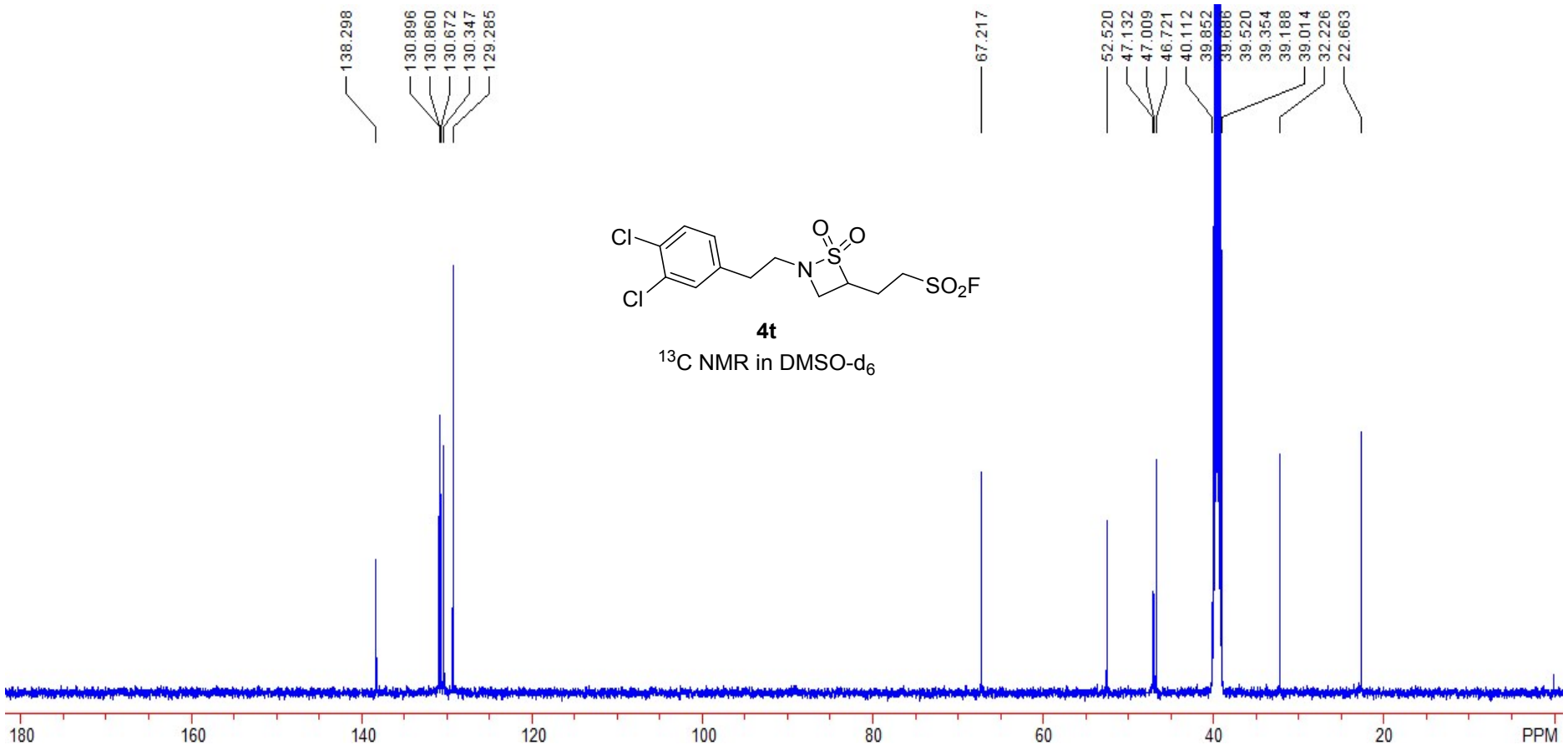
^{13}C NMR in DMSO-d_6


7.394
7.378
7.328
7.264
7.085
7.071
4.474
4.462
4.446
4.439
4.430
4.418
3.662
3.633
3.625
3.621
3.616
3.609
3.602
3.592
3.586
3.577
3.572
3.562
3.547
3.533
3.346
3.333
3.319
3.282
3.267
3.253
2.871
2.856
2.842
2.798
2.787
2.777
2.700
2.684
2.670
2.654
2.641
2.624
2.544
2.530
2.515
2.501
2.487
2.472
1.594
1.257
Cl
Cl
O
O
S
N
SO2F
4t
1H NMR in CDCl3
1.00
2.02
2.00
2.04
1.05
12
10
8
6
4
2
0
PPM



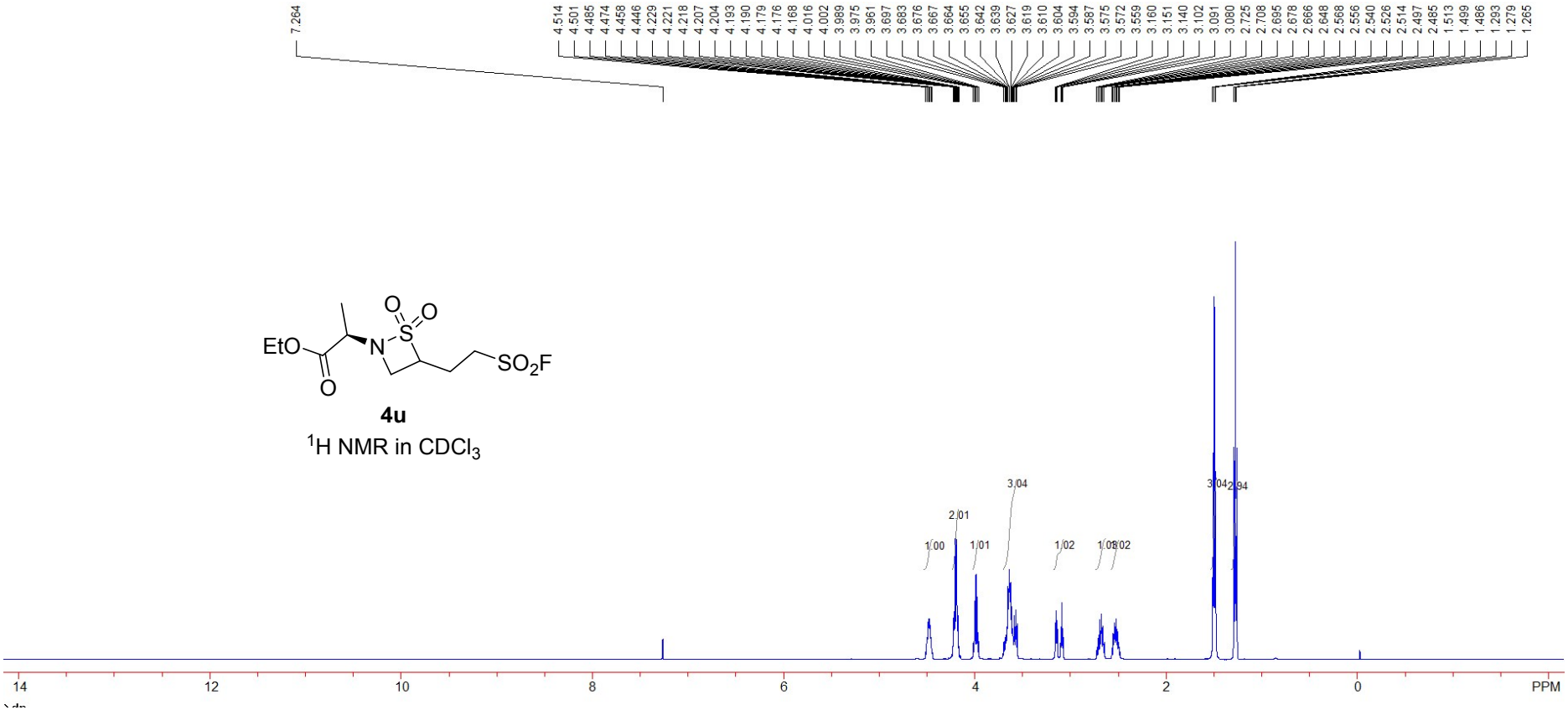
4t

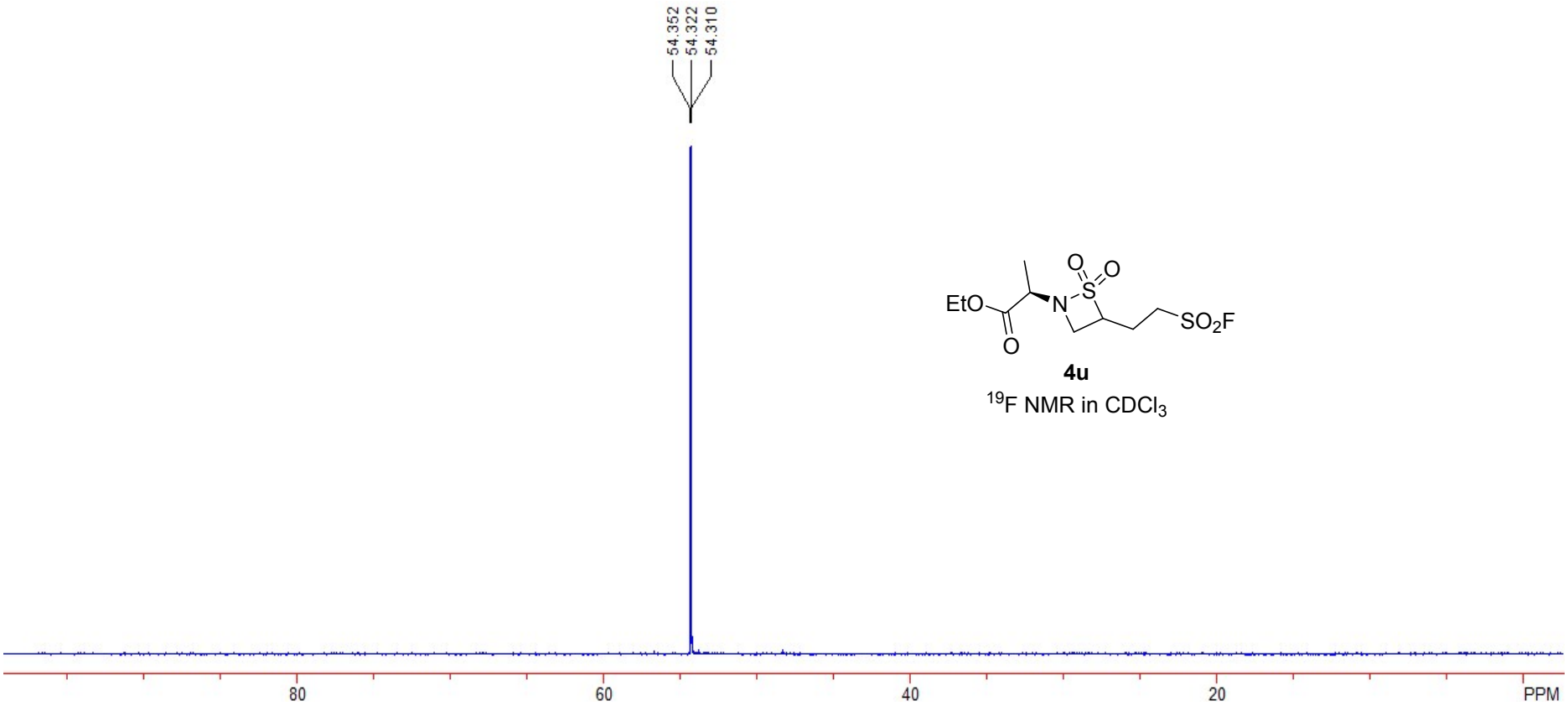
^{19}F NMR in $CDCl_3$



4t

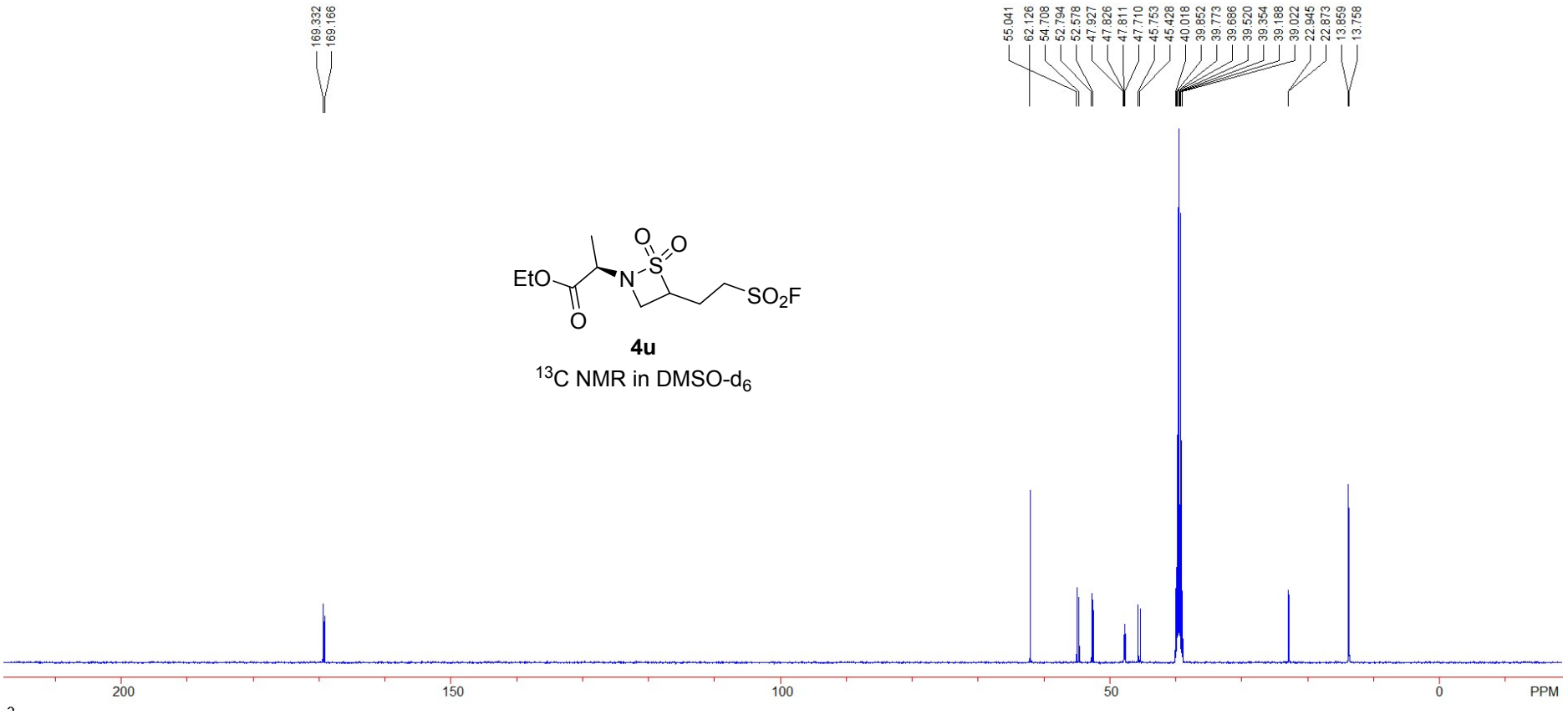
^{13}C NMR in DMSO-d_6


7.264
4.514
4.501
4.485
4.474
4.458
4.446
4.229
4.221
4.218
4.207
4.204
4.193
4.190
4.179
4.176
4.168
4.016
4.002
3.989
3.975
3.961
3.697
3.683
3.676
3.667
3.664
3.655
3.642
3.639
3.627
3.619
3.610
3.604
3.594
3.587
3.575
3.572
3.559
3.160
3.151
3.140
3.102
3.091
3.080
2.725
2.708
2.695
2.678
2.666
2.648
2.568
2.556
2.540
2.526
2.514
2.497
2.485
1.513
1.499
1.486
1.293
1.279
1.265
EtO
O
O
O
N
S
SO2F
4u
1H NMR in CDCl3
1.00
2.01
1.01
3.04
1.02
1.08
1.02
3.04
2.94
14
12
10
8
6
4
2
0
PPM



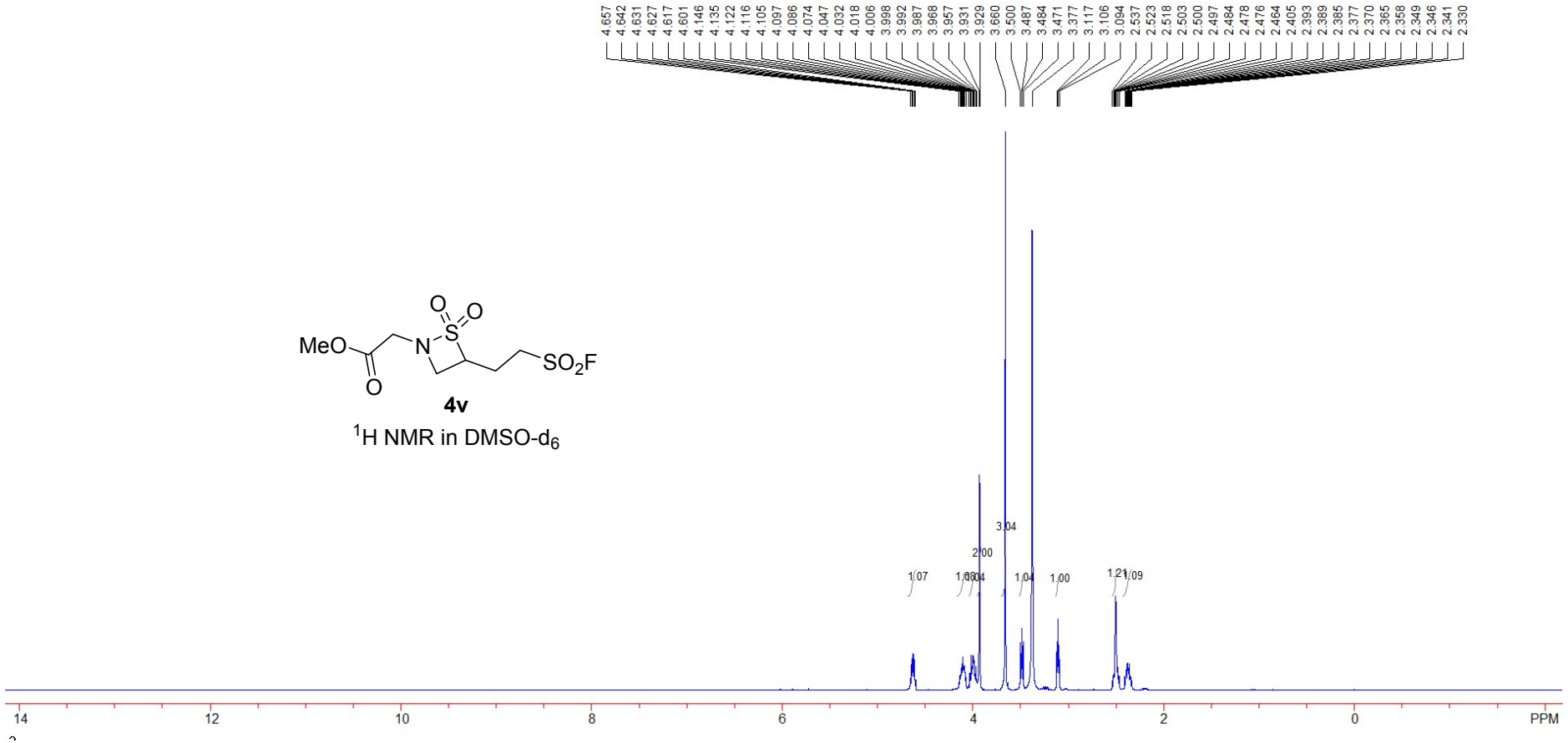
4u

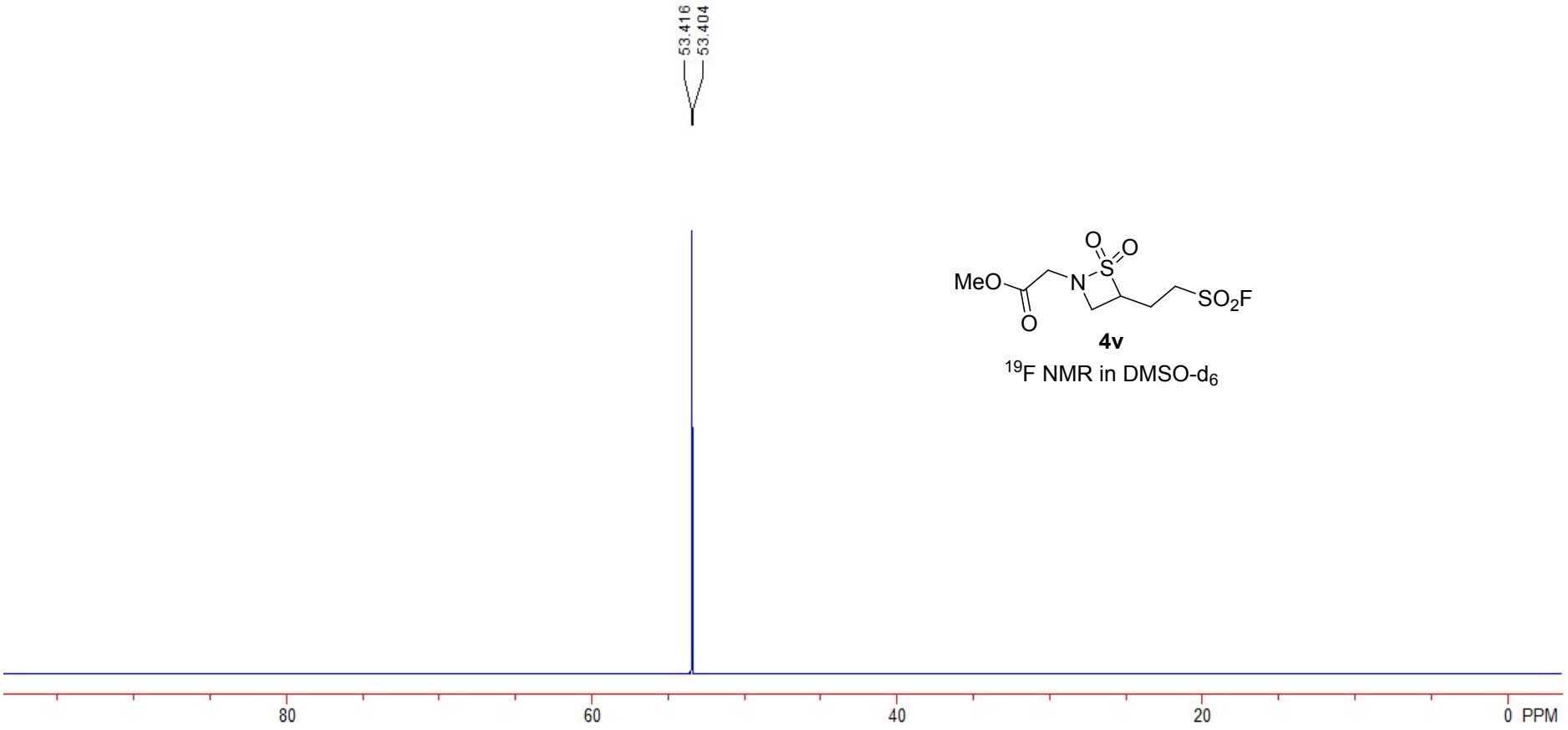
^{19}F NMR in $CDCl_3$



4u

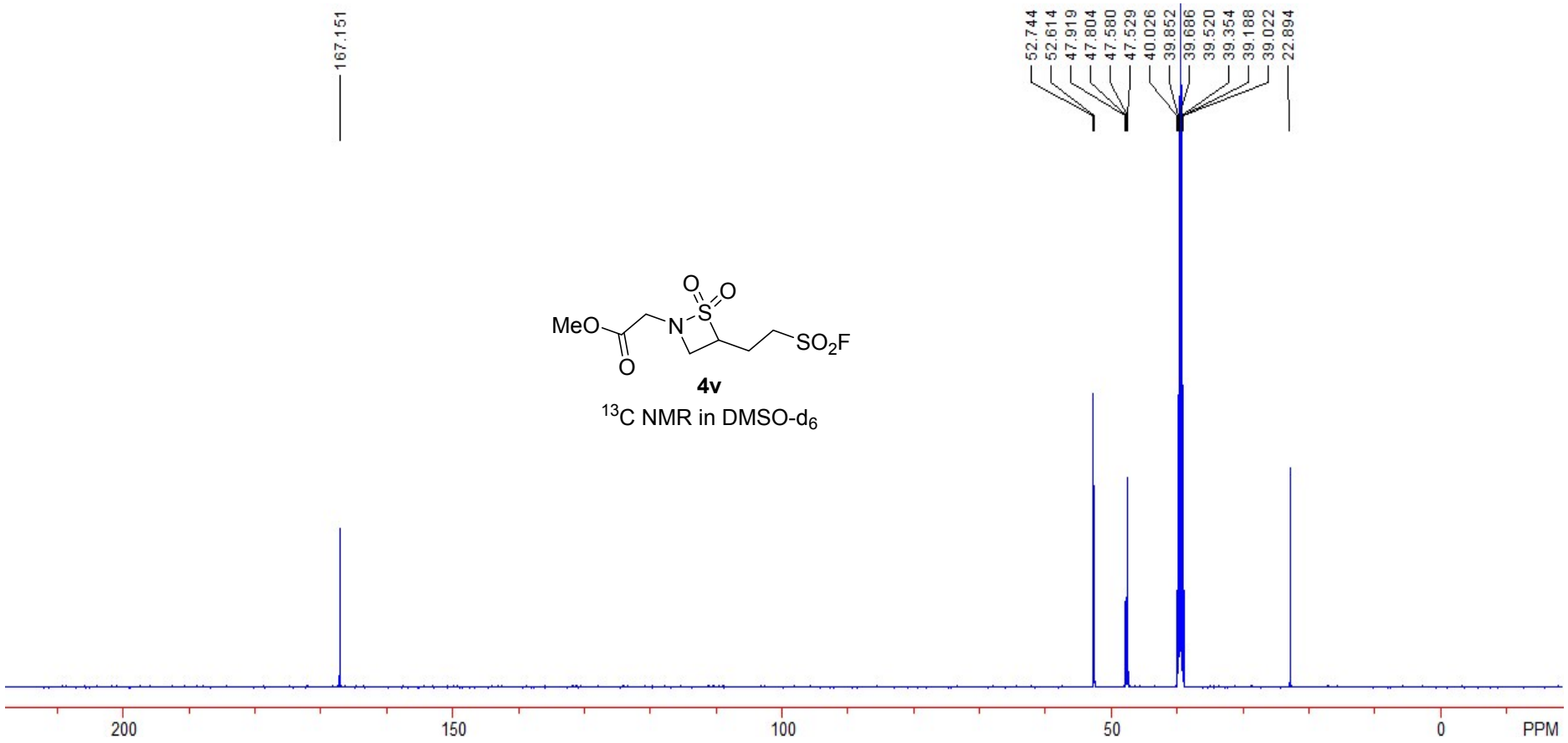
^{13}C NMR in DMSO-d_6


4.657
4.642
4.631
4.627
4.617
4.601
4.146
4.135
4.122
4.116
4.105
4.097
4.086
4.074
4.047
4.032
4.018
4.006
3.998
3.992
3.987
3.968
3.957
3.931
3.929
3.660
3.500
3.487
3.484
3.471
3.377
3.117
3.106
3.094
2.537
2.523
2.518
2.503
2.500
2.497
2.484
2.478
2.476
2.464
2.405
2.393
2.389
2.385
2.377
2.370
2.365
2.358
2.349
2.346
2.341
2.330
MeO
O
O
N
S
O
O
SO2F
4v
1H NMR in DMSO-d6
3.04
2.00
1.07
1.00
1.04
1.00
1.21
1.09
14
12
10
8
6
4
2
0
PPM



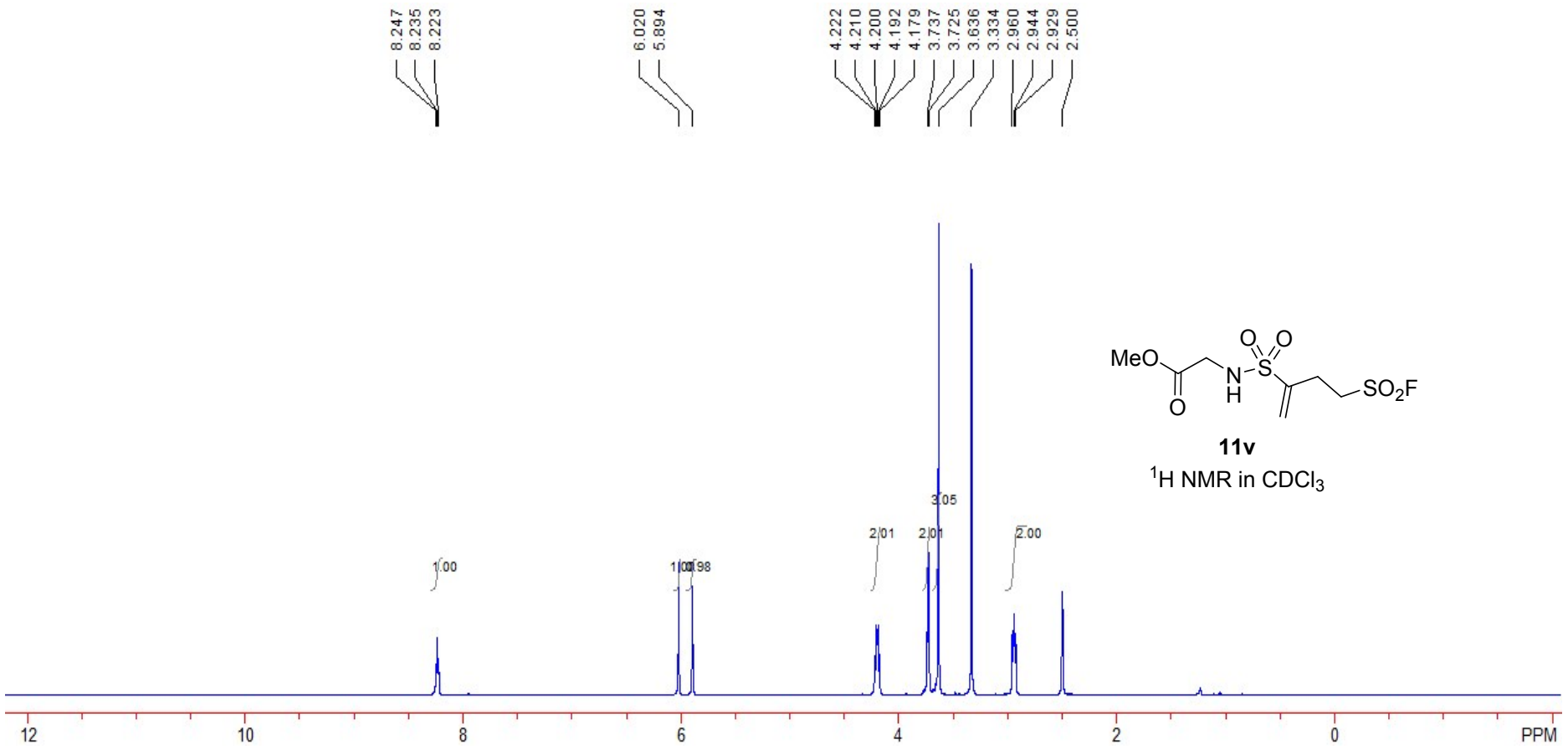
4v

^{19}F NMR in DMSO-d_6



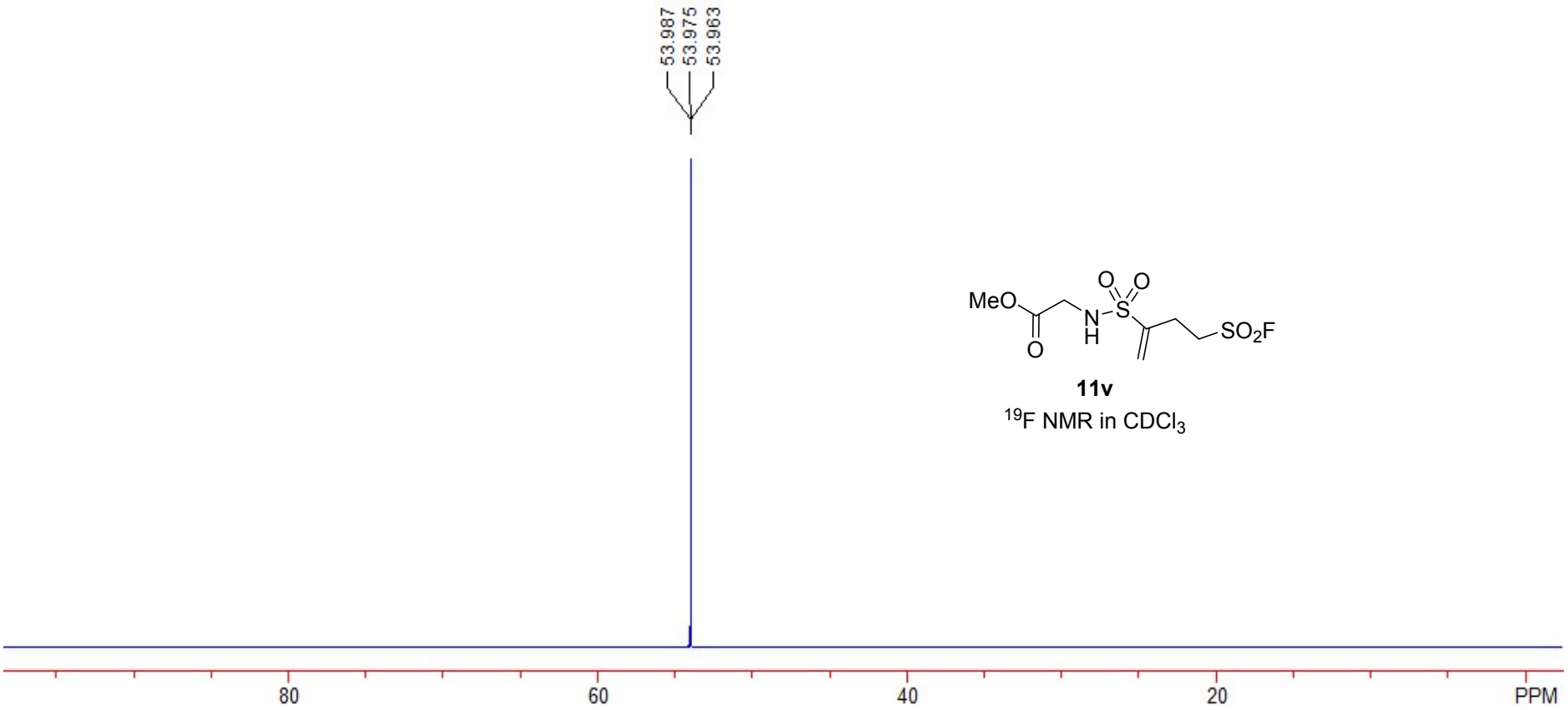
4v

^{13}C NMR in DMSO-d_6



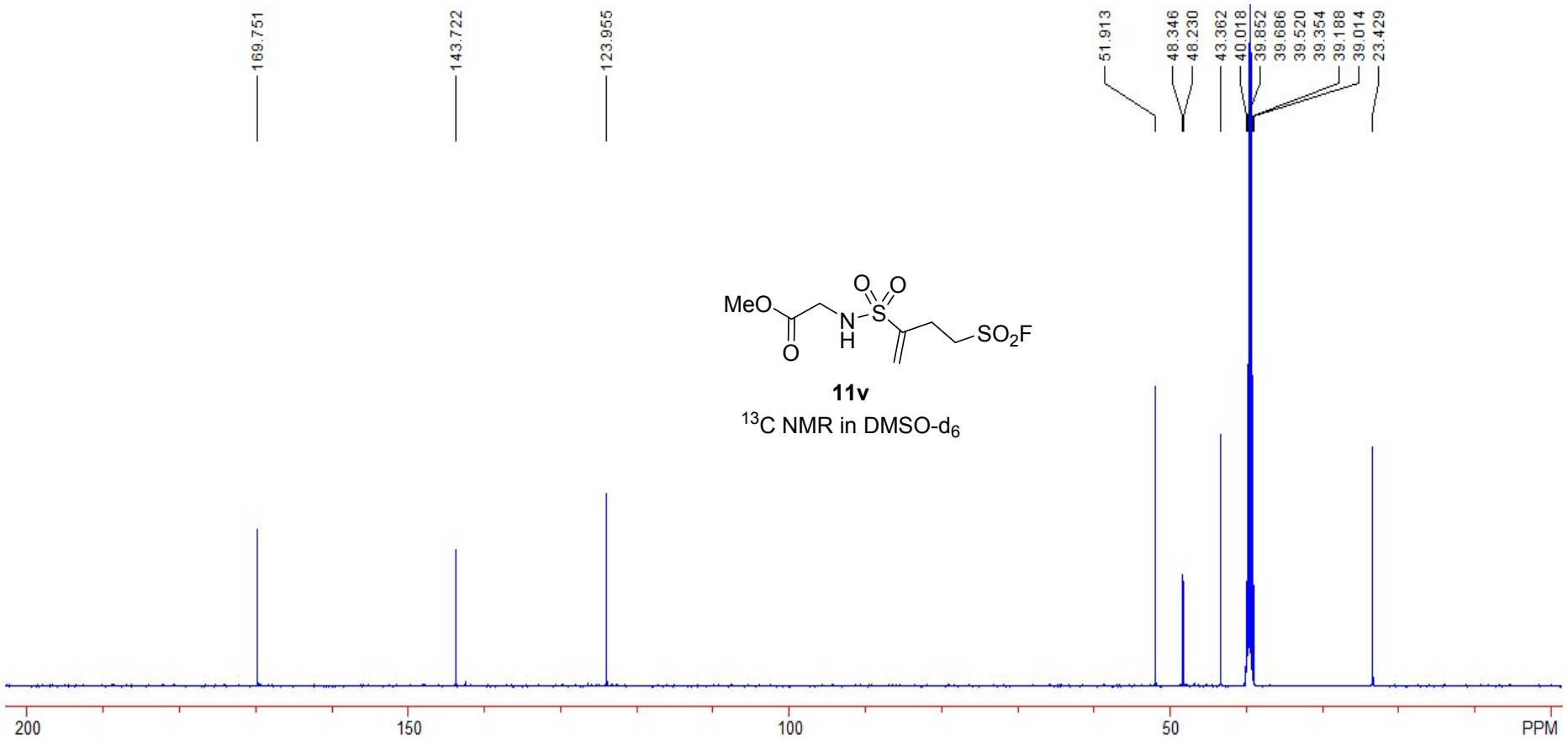
11v

^{1}H NMR in $CDCl_3$



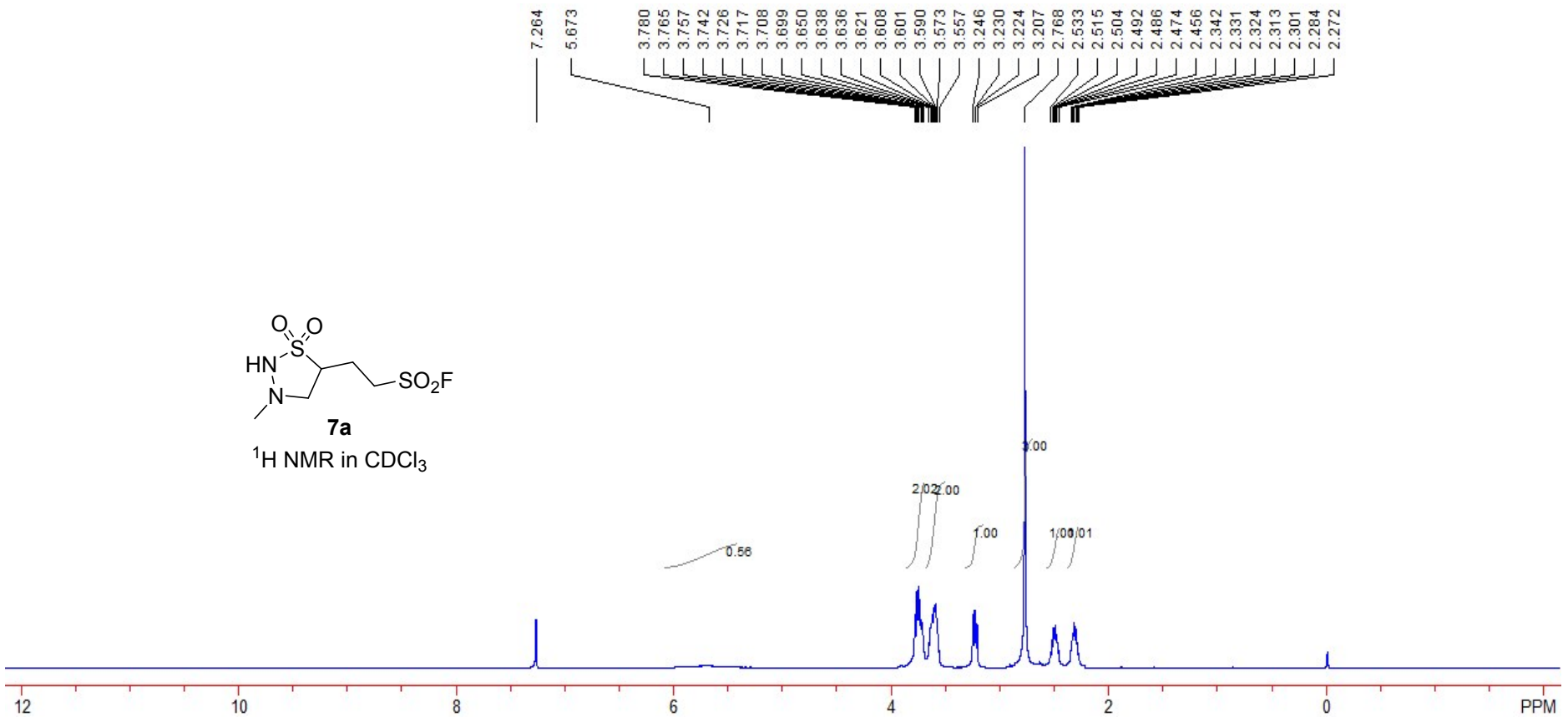
11v

^{19}F NMR in $CDCl_3$



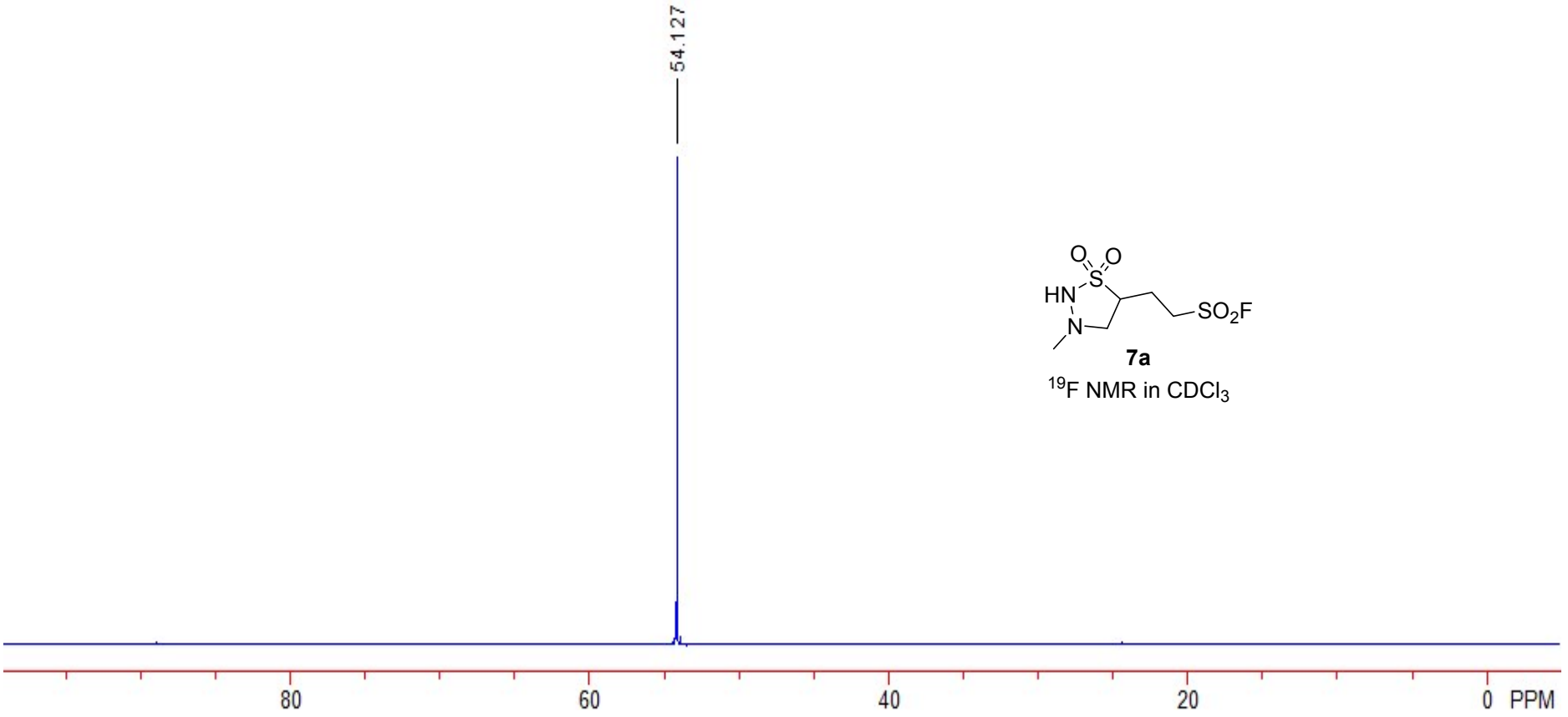
11v

^{13}C NMR in DMSO-d_6



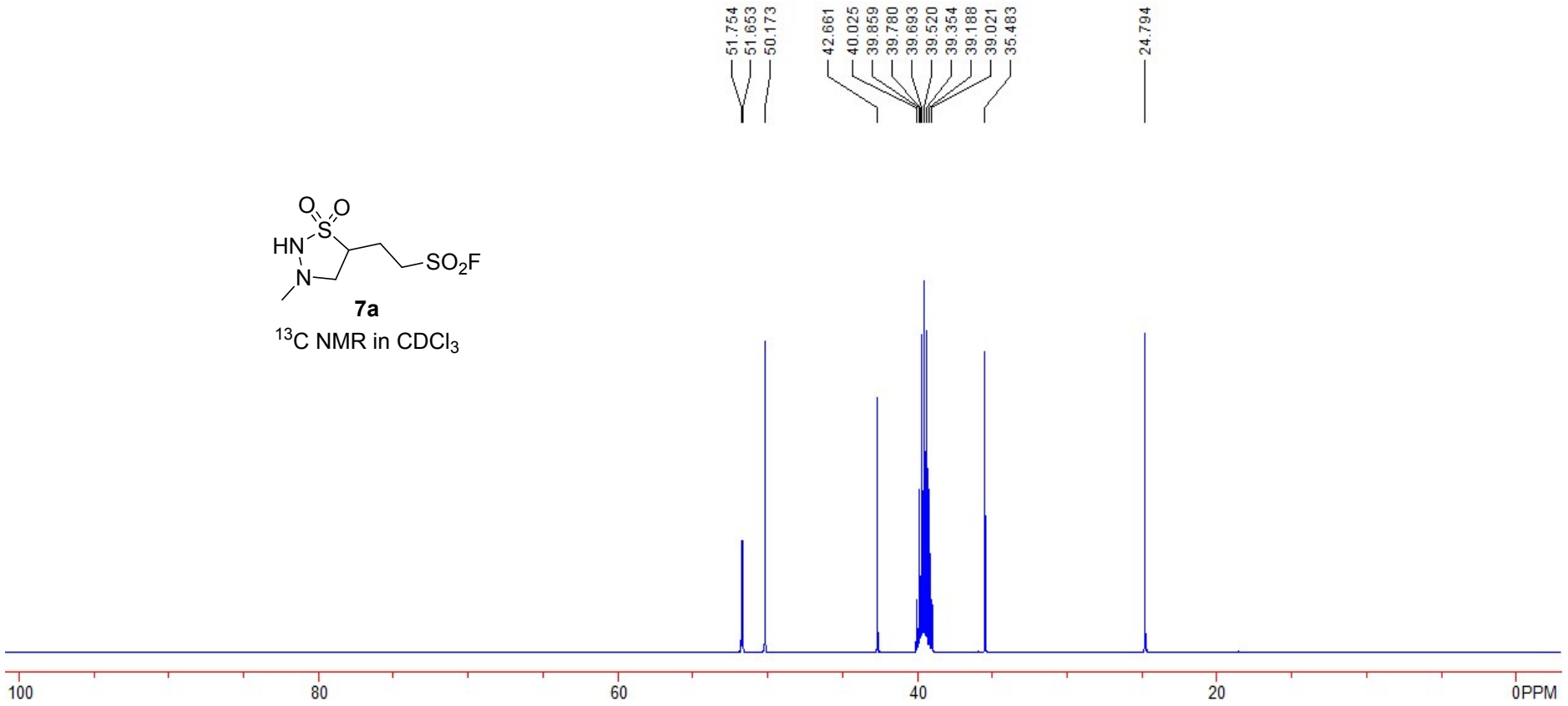
7a

^{1}H NMR in $CDCl_3$



7a

^{19}F NMR in $CDCl_3$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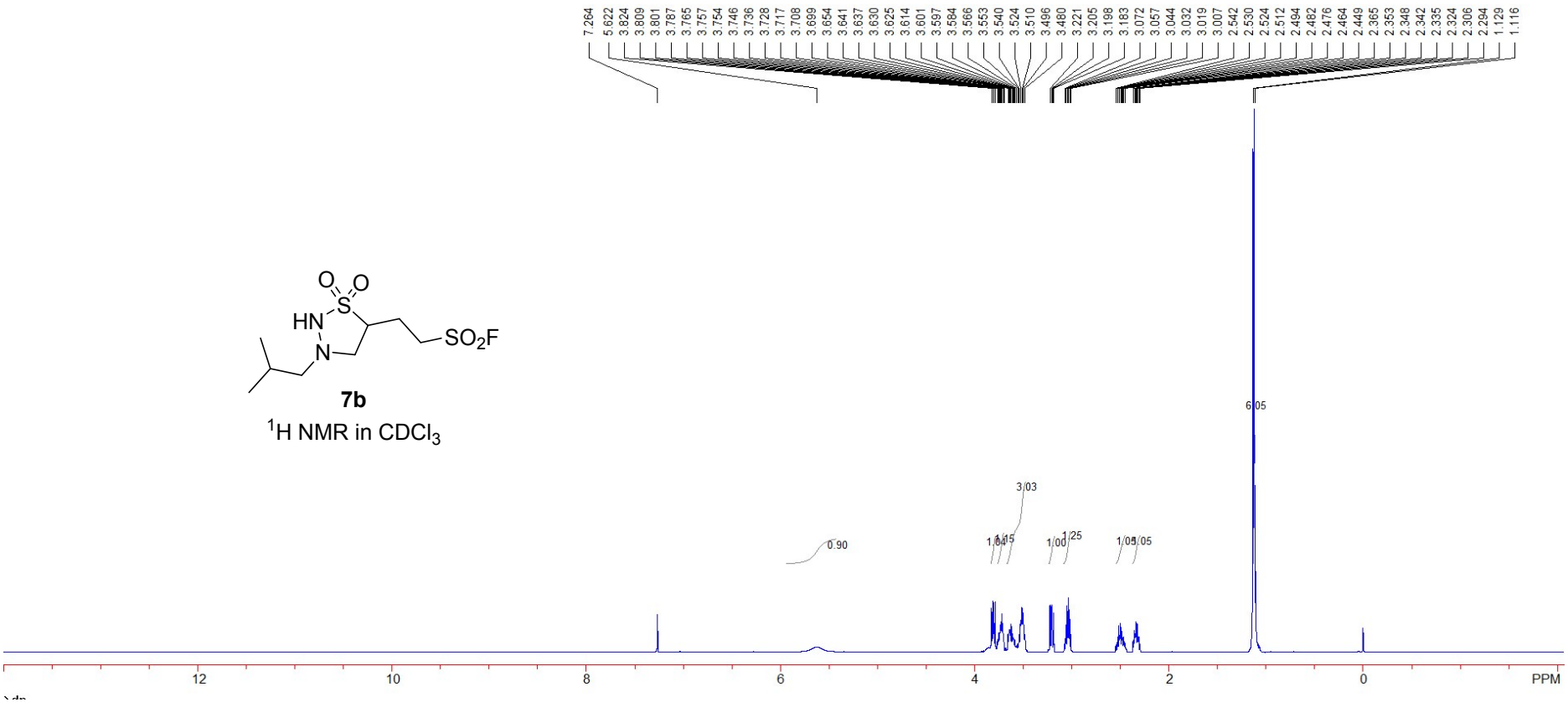
51.653
50.173
42.661
40.025
39.859
39.780
39.693
39.520
39.354
39.188
39.021
35.483
24.794
O
O
S
HN
N
SO2F
7a
13C NMR in CDCl3
100
80
60
40
20
0PPM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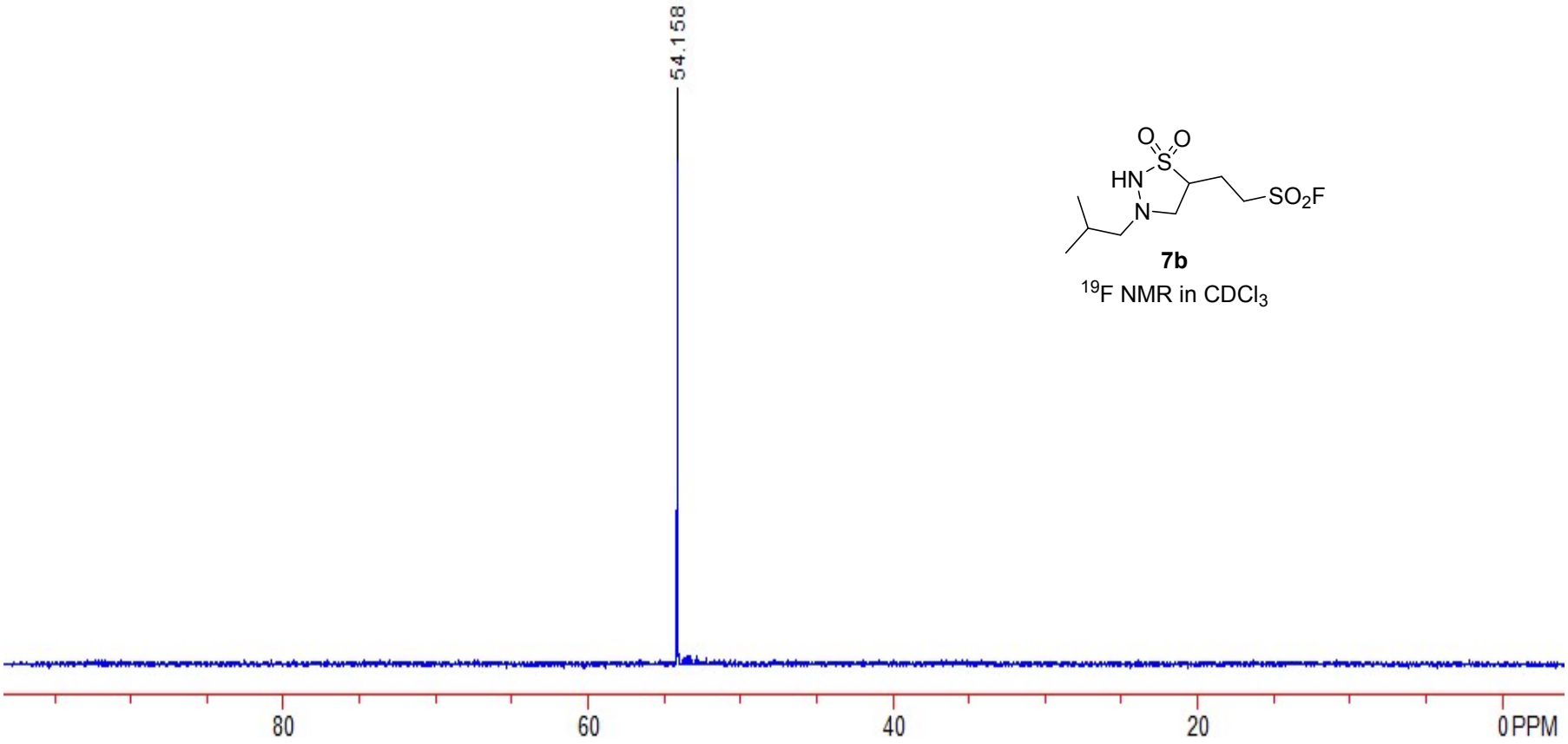
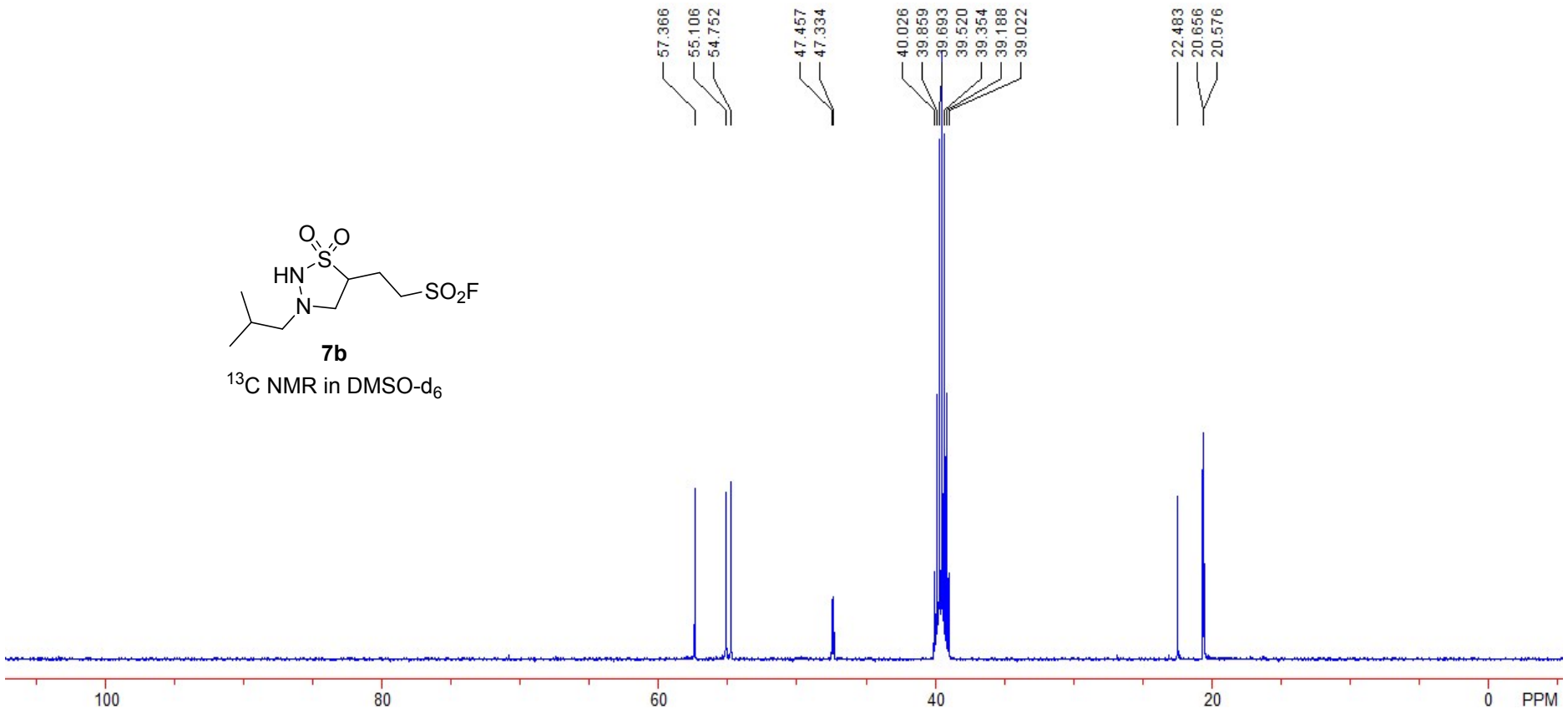
5.622
3.824
3.809
3.801
3.787
3.765
3.757
3.754
3.746
3.736
3.728
3.717
3.708
3.699
3.654
3.641
3.637
3.630
3.625
3.614
3.601
3.597
3.584
3.566
3.553
3.540
3.524
3.510
3.496
3.480
3.221
3.205
3.198
3.183
3.072
3.057
3.044
3.032
3.019
3.007
2.542
2.530
2.524
2.512
2.494
2.482
2.476
2.464
2.449
2.365
2.353
2.348
2.342
2.335
2.324
2.306
2.294
1.129
1.116
O
O
S
HN
N
SO2F
7b
1H NMR in CDCl3
6.05
3.03
0.90
1.00
1.25
1.05
1.05
12
10
8
6
4
2
0
PPM



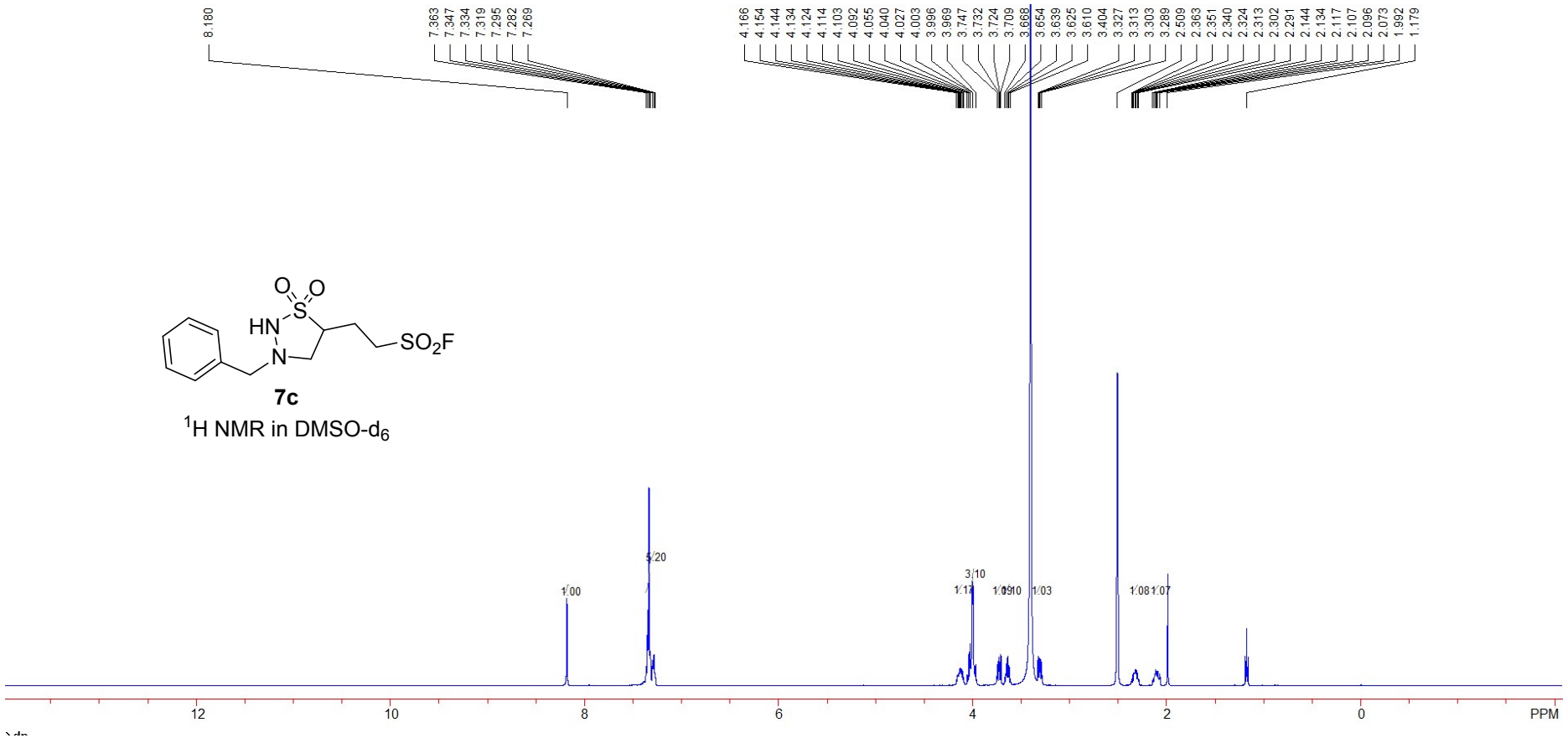
7b

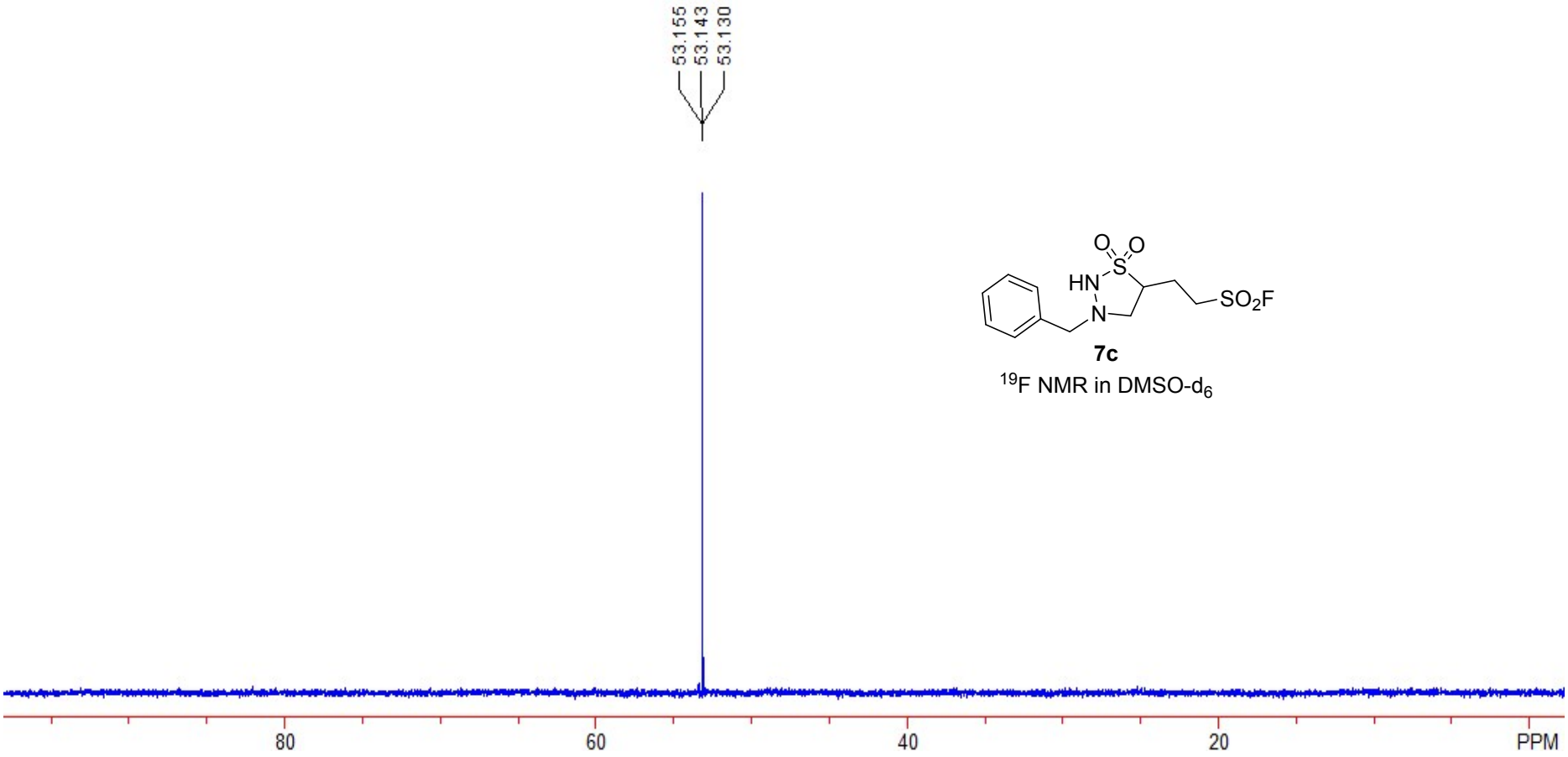
^{19}F NMR in $CDCl_3$



7b

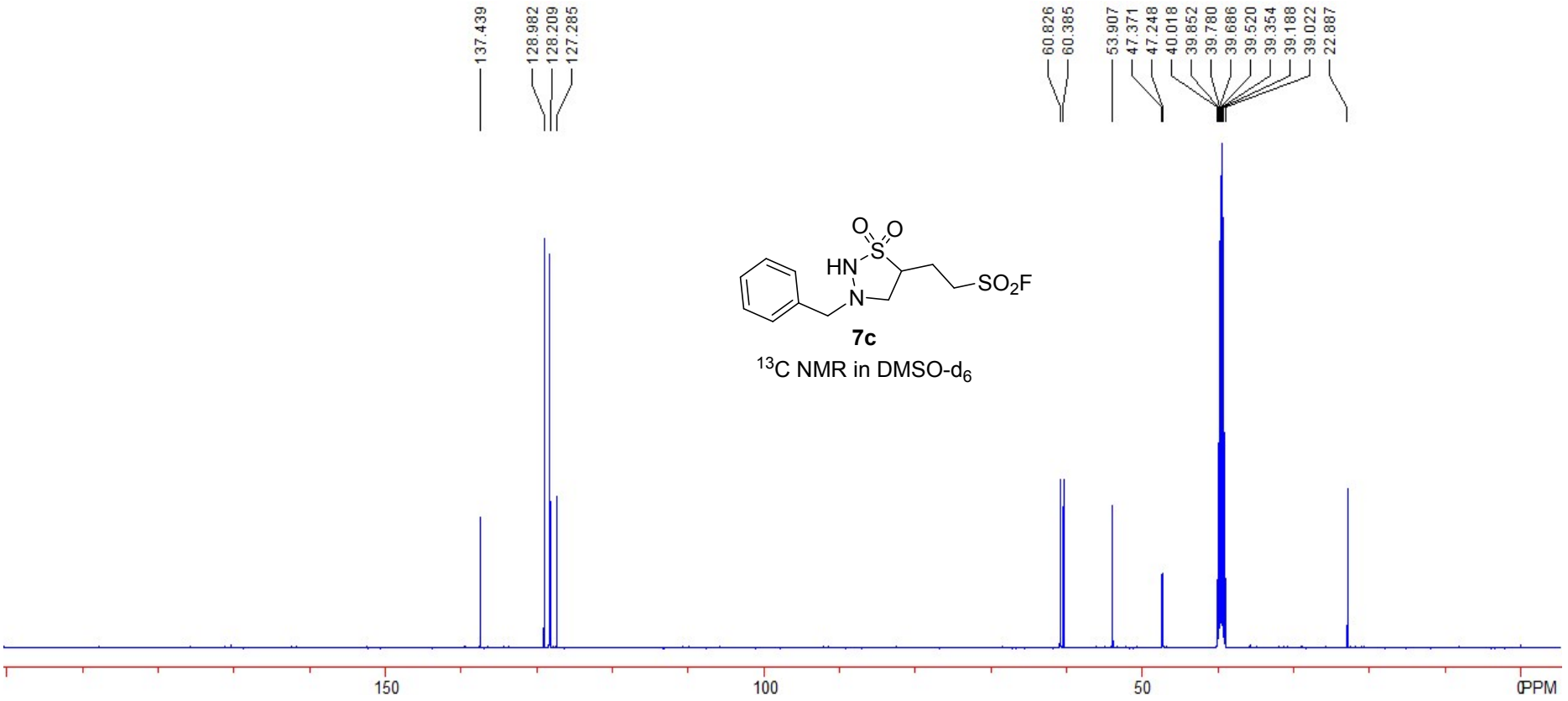
^{13}C NMR in DMSO-d_6


8.180
7.363
7.347
7.334
7.319
7.295
7.282
7.269
4.166
4.154
4.144
4.134
4.124
4.114
4.103
4.092
4.055
4.040
4.027
4.003
3.996
3.969
3.747
3.732
3.724
3.709
3.668
3.654
3.639
3.625
3.610
3.404
3.327
3.313
3.303
3.289
2.509
2.363
2.351
2.340
2.324
2.313
2.302
2.291
2.144
2.134
2.117
2.107
2.096
2.073
1.992
1.179
HN
S
O
O
N
SO2F
7c
1H NMR in DMSO-d6
1.00
5.20
3.10
1.03
1.08
1.07
12
10
8
6
4
2
0
PPM



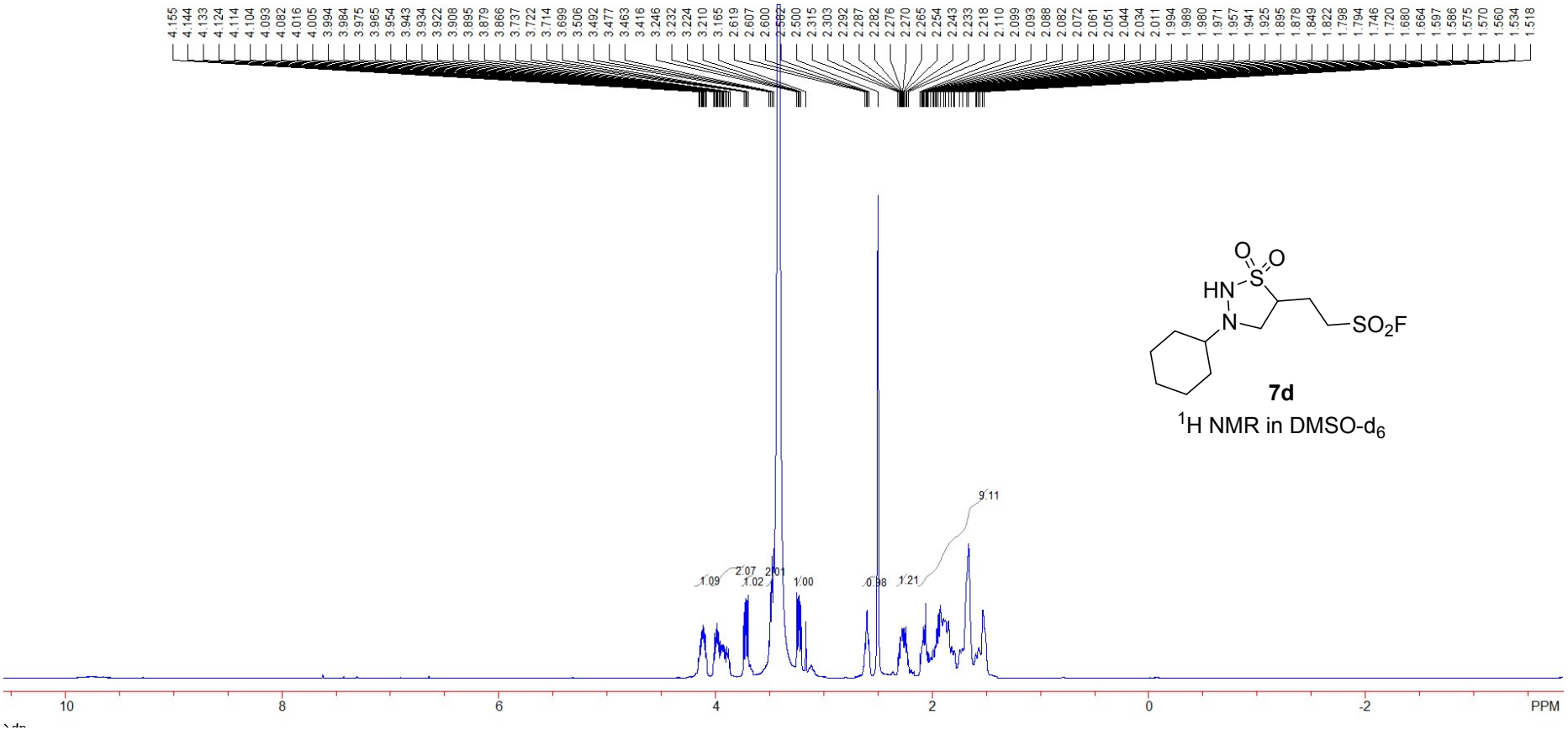
7c

^{19}F NMR in DMSO-d_6



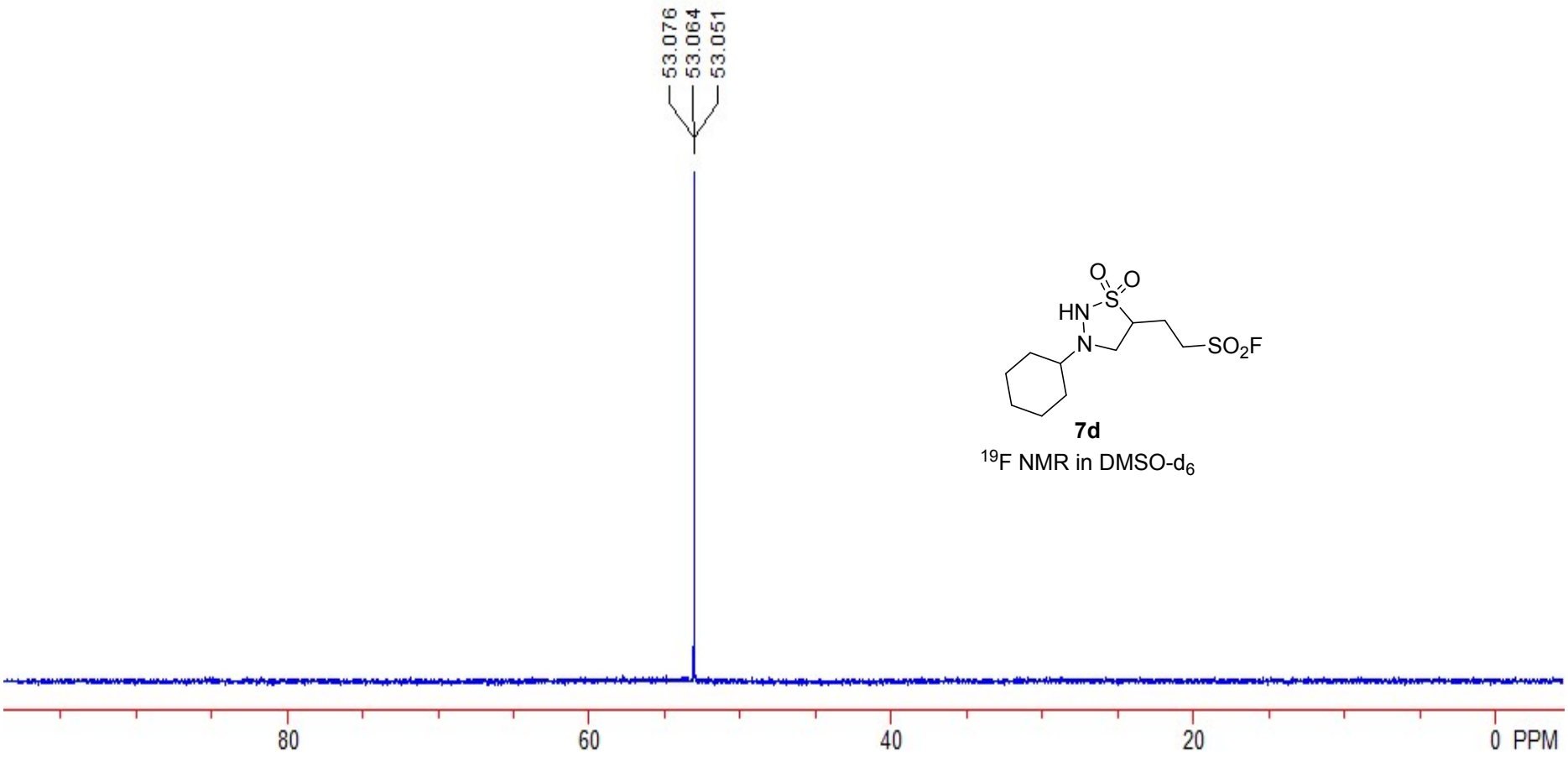
7c

^{13}C NMR in DMSO-d_6



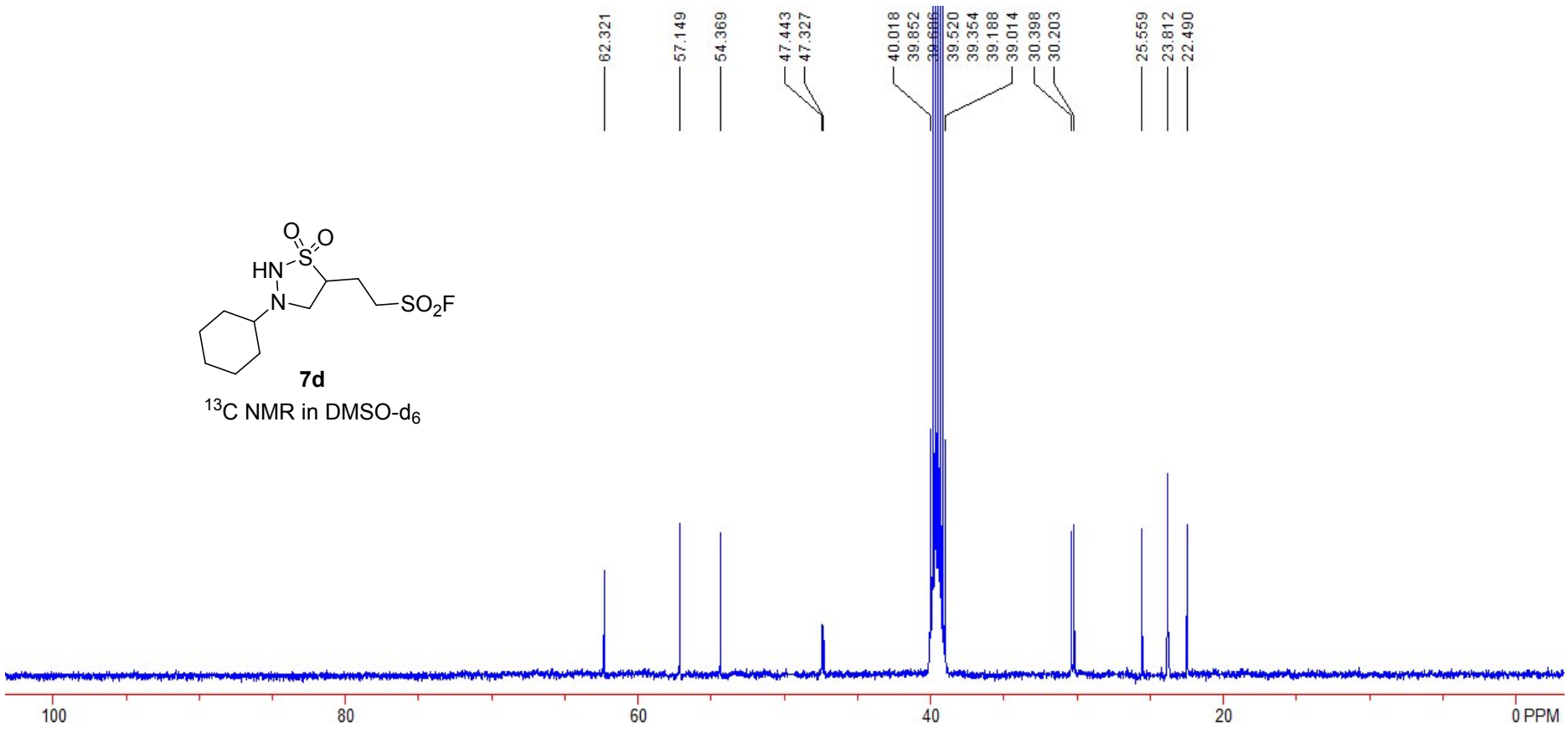
7d

^{1}H NMR in DMSO-d_6



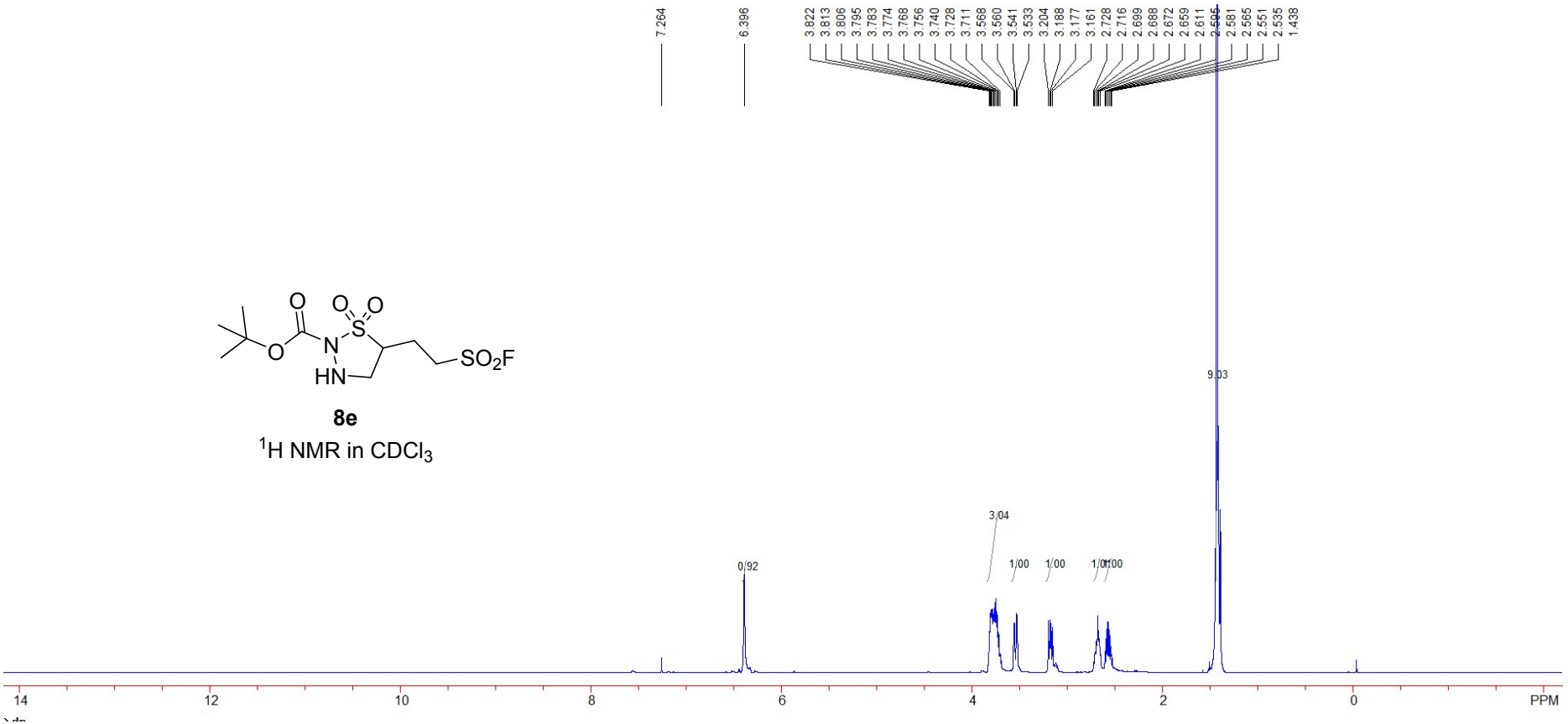
7d

^{19}F NMR in DMSO-d_6



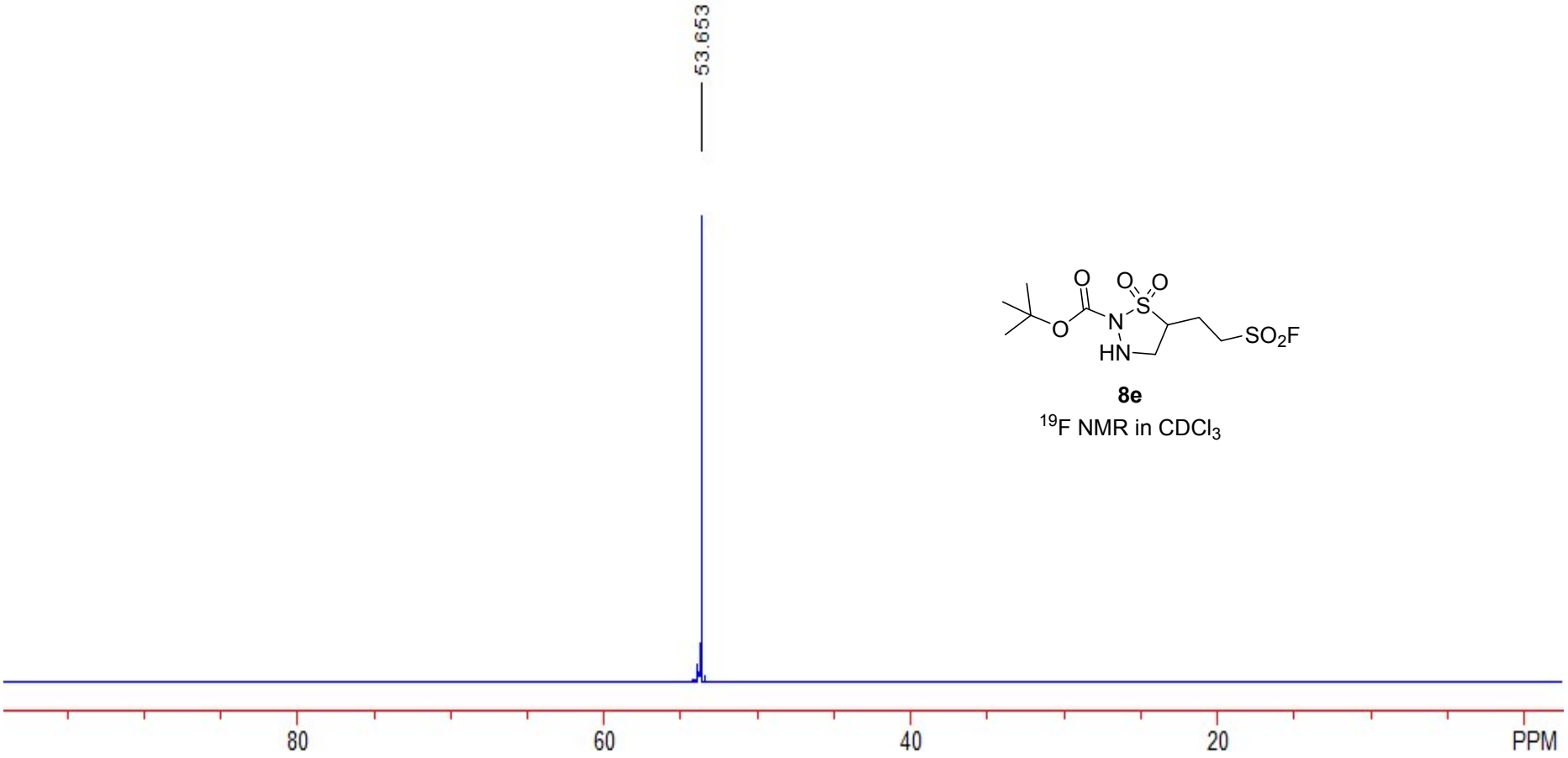
7d

^{13}C NMR in DMSO-d_6



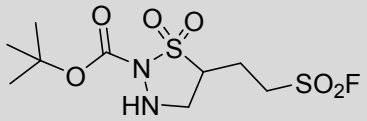
8e

^{1}H NMR in $CDCl_3$



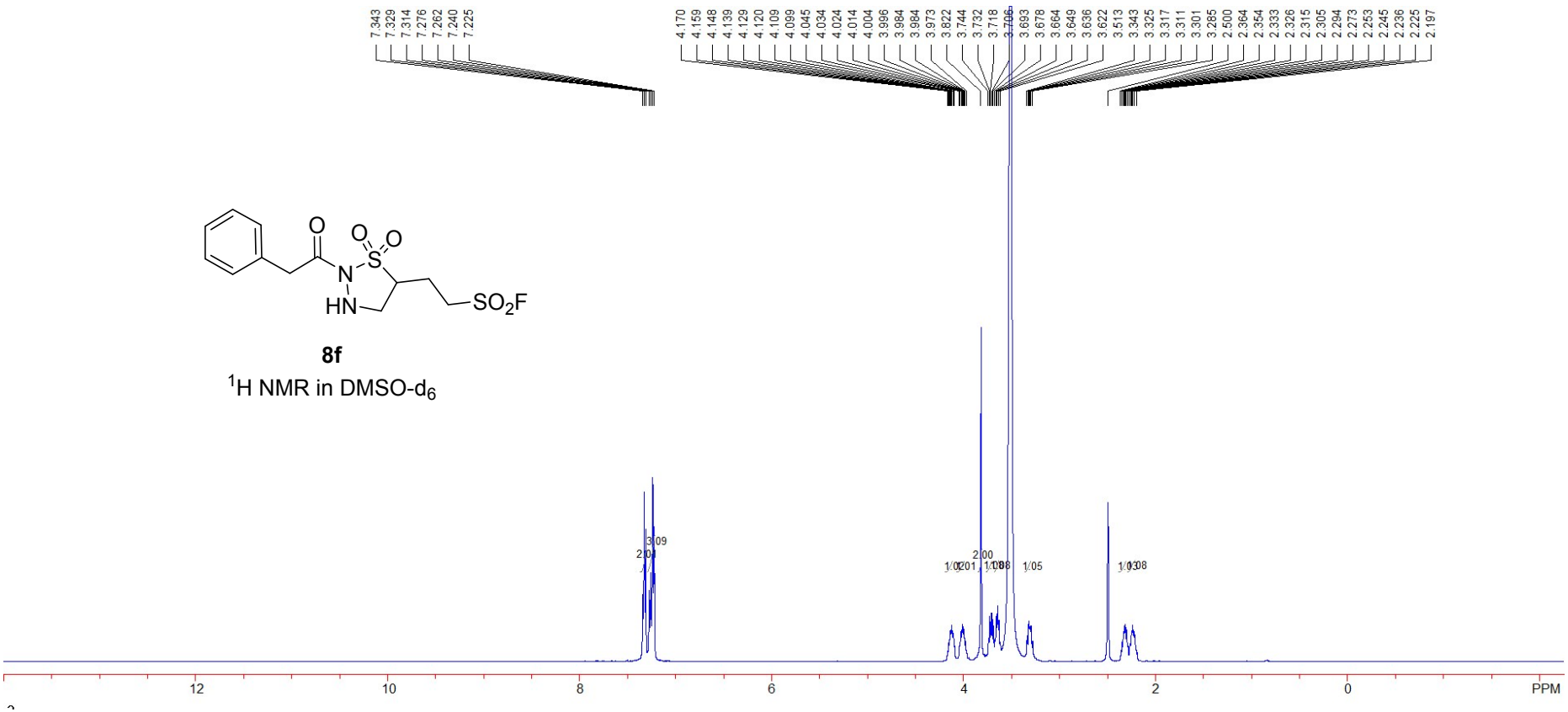
8e

^{19}F NMR in $CDCl_3$



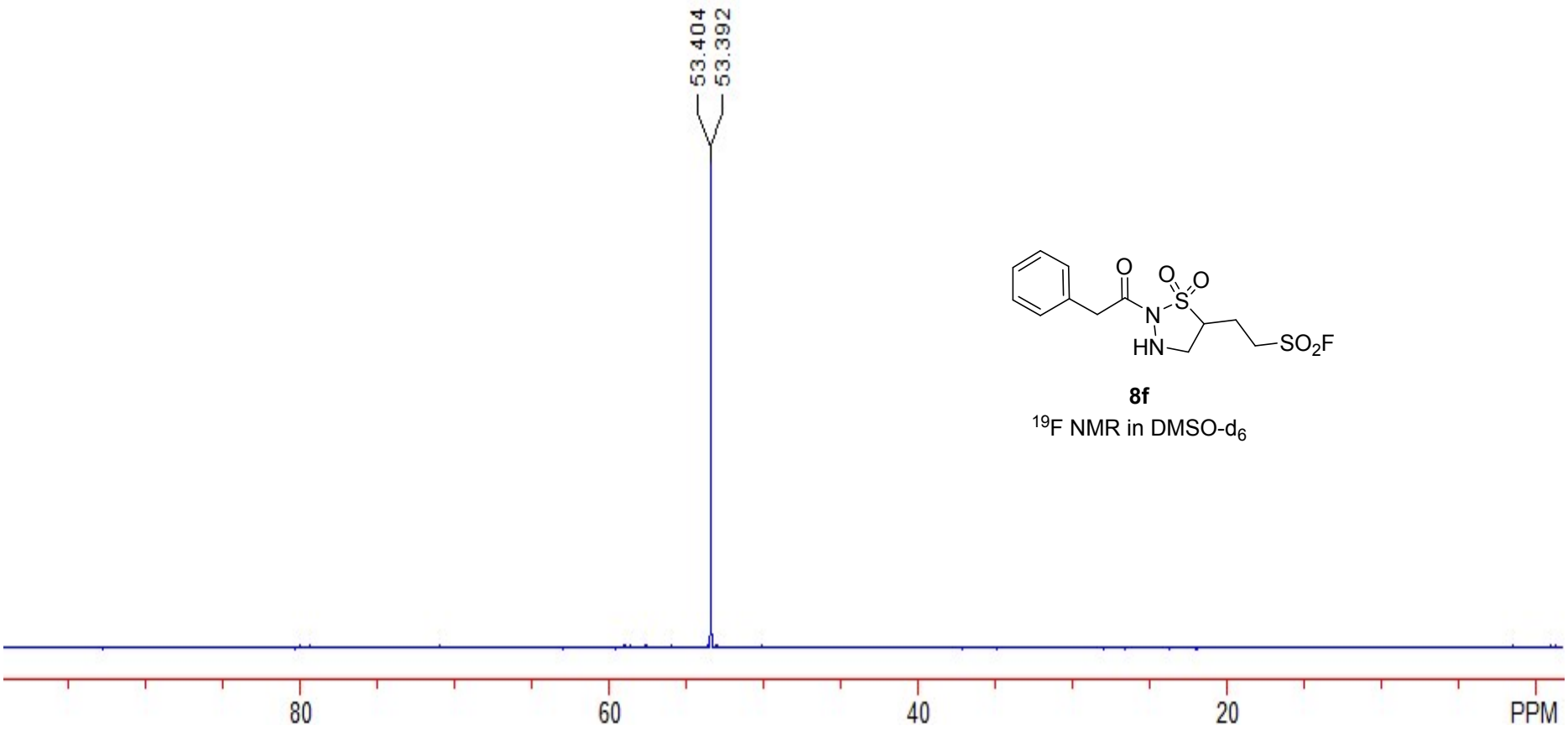
8e

^{13}C NMR in $CDCl_3$



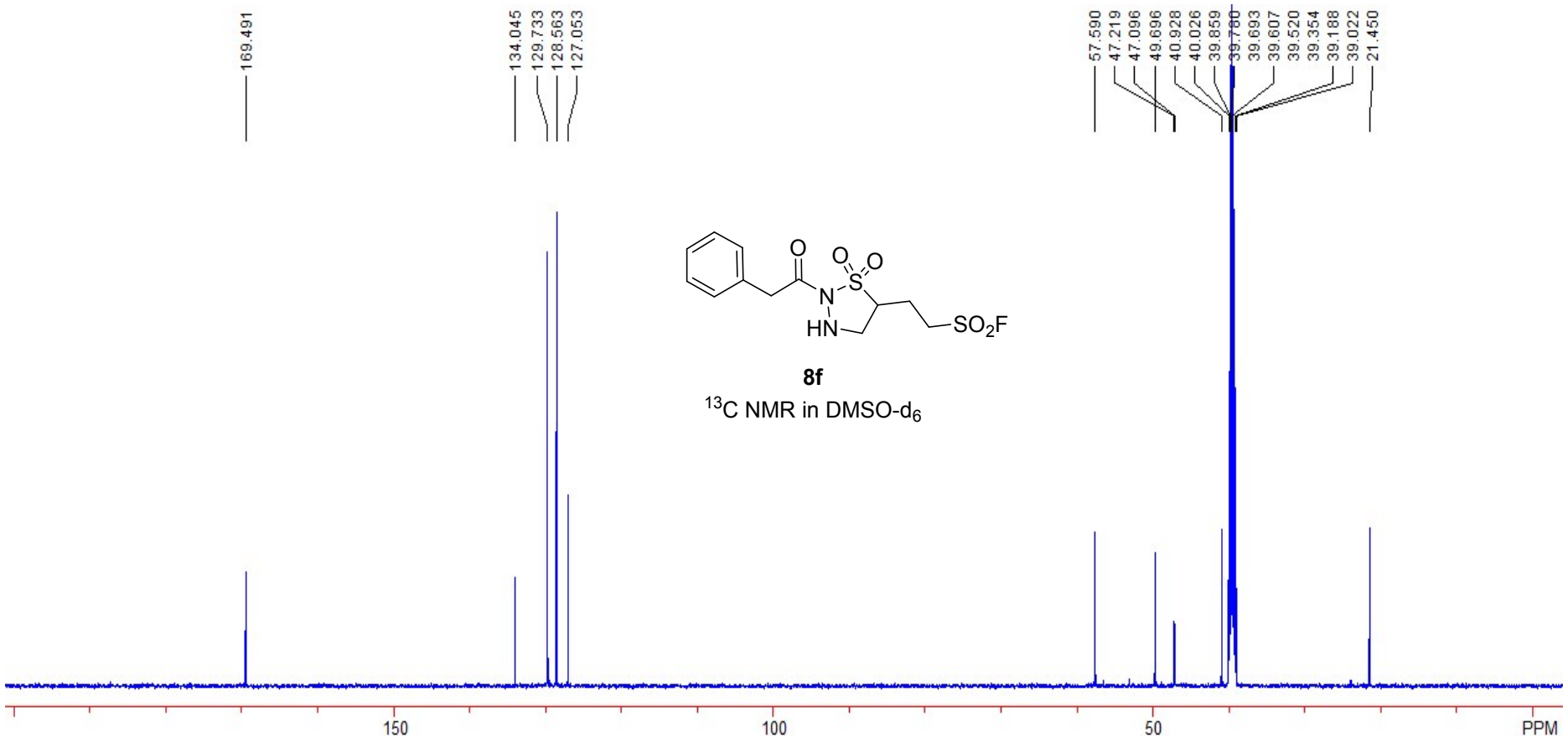
8f

^{1}H NMR in DMSO-d_6



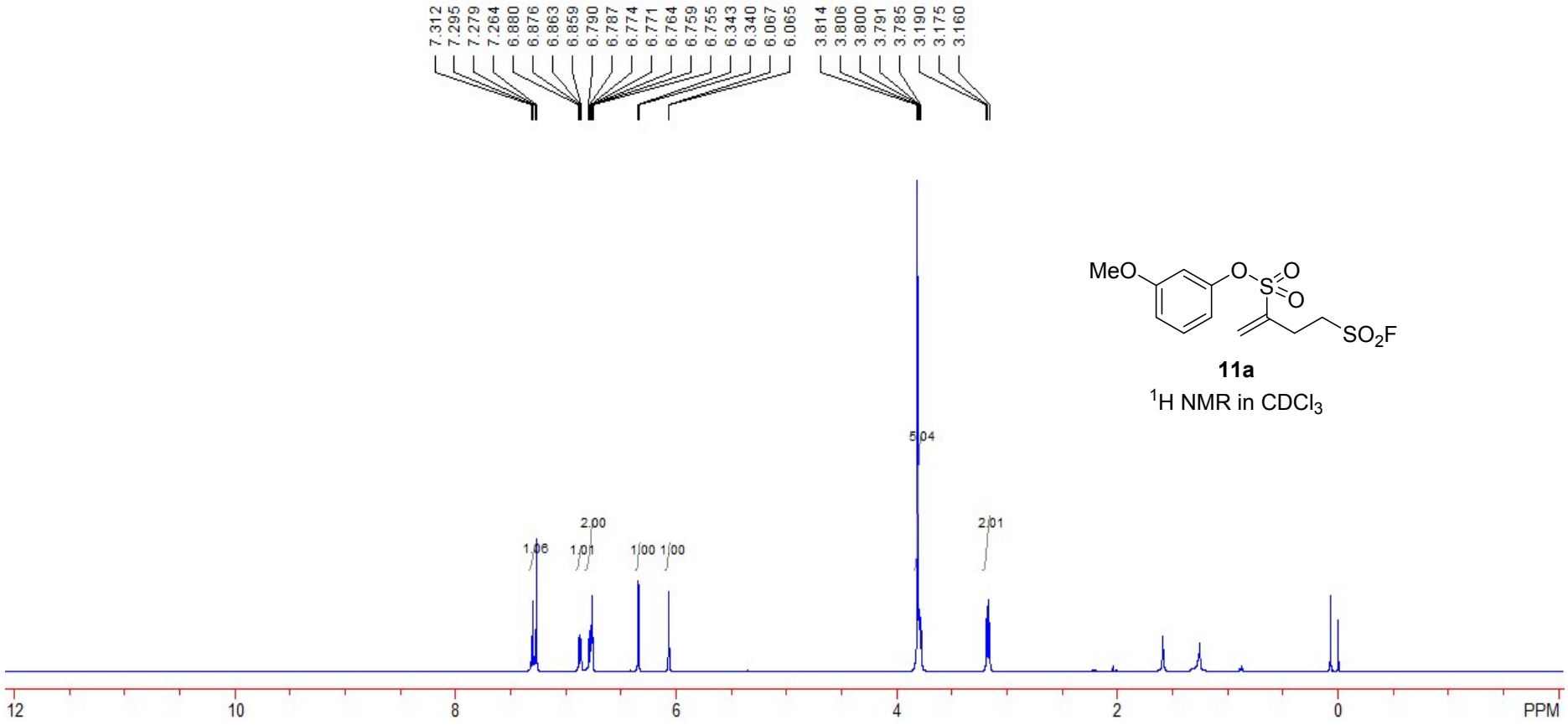
8f

^{19}F NMR in DMSO-d_6



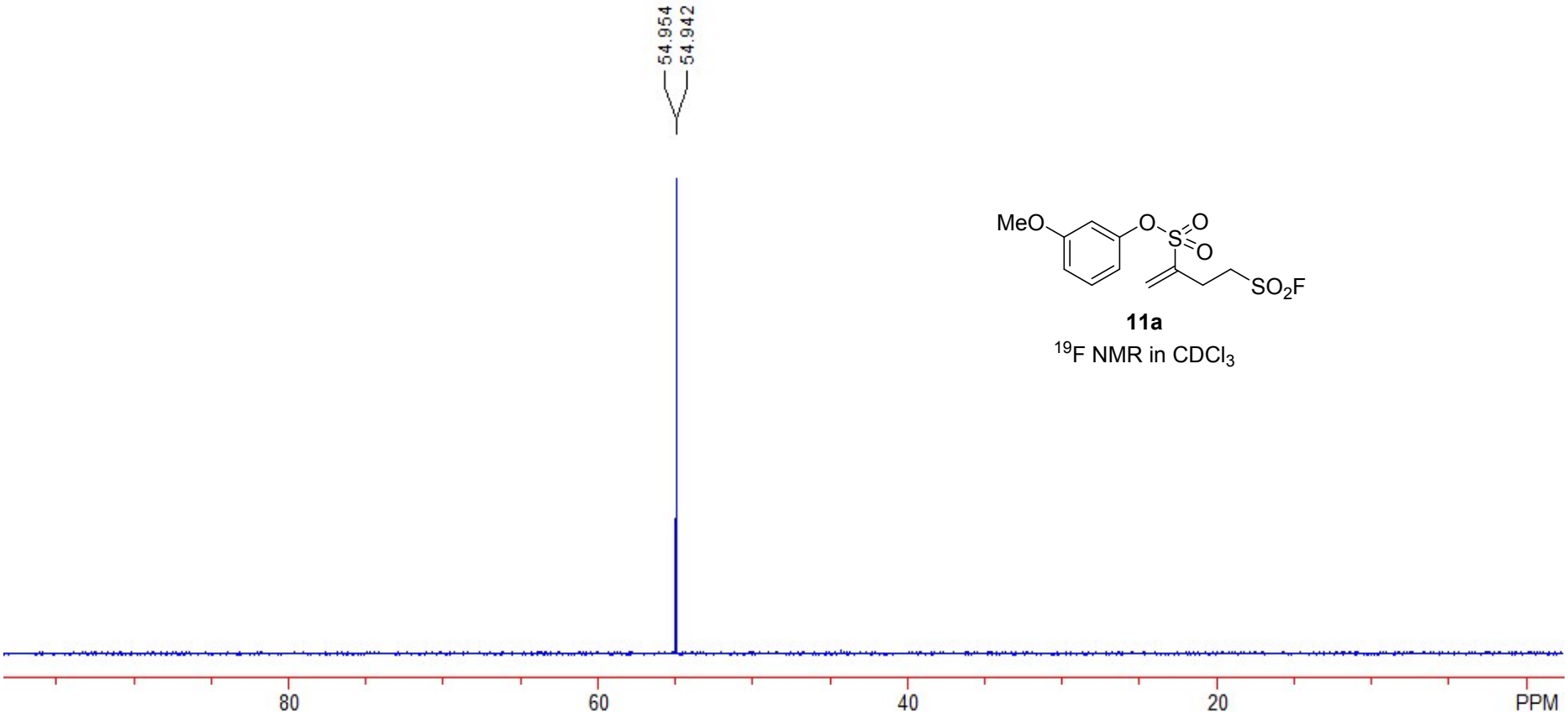
8f

^{13}C NMR in DMSO-d_6



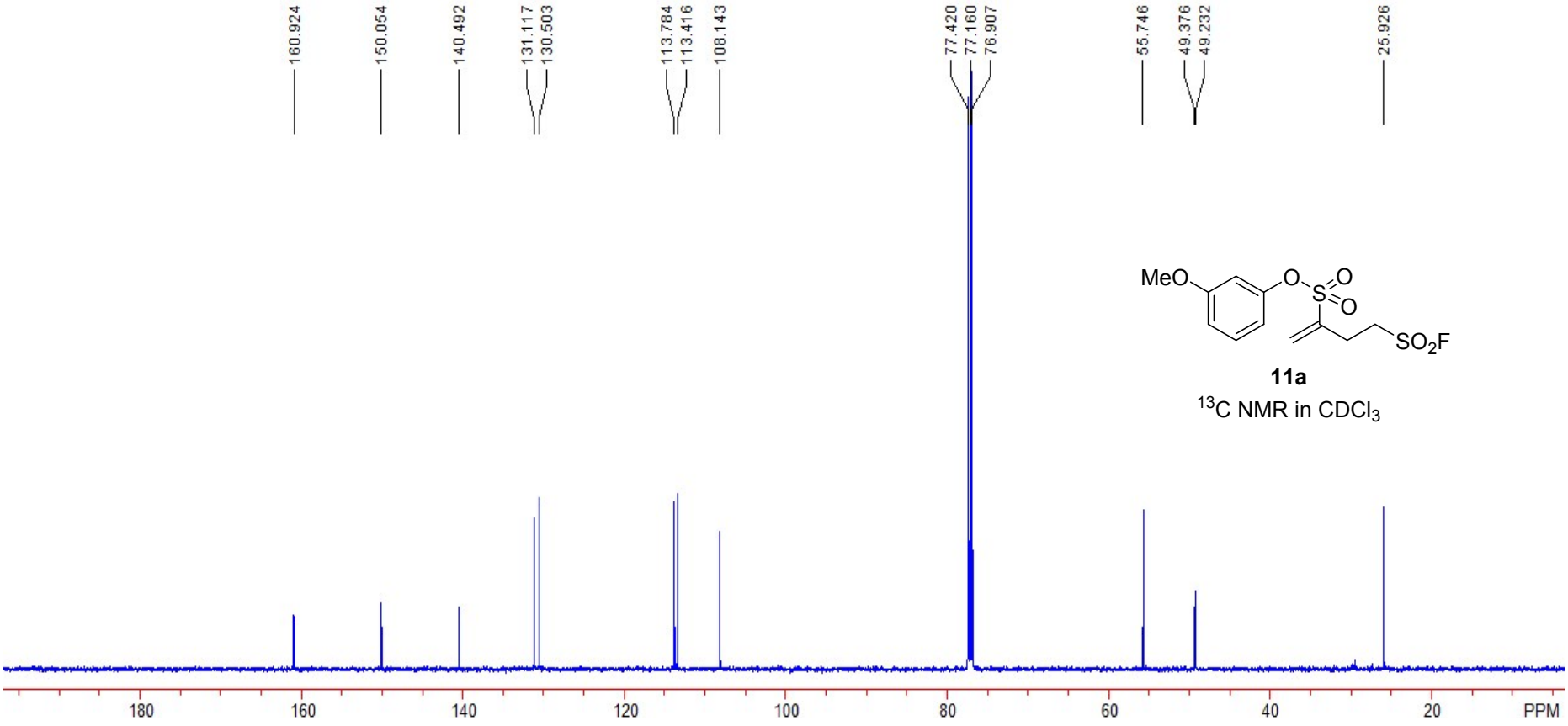
11a

^{1}H NMR in $CDCl_3$



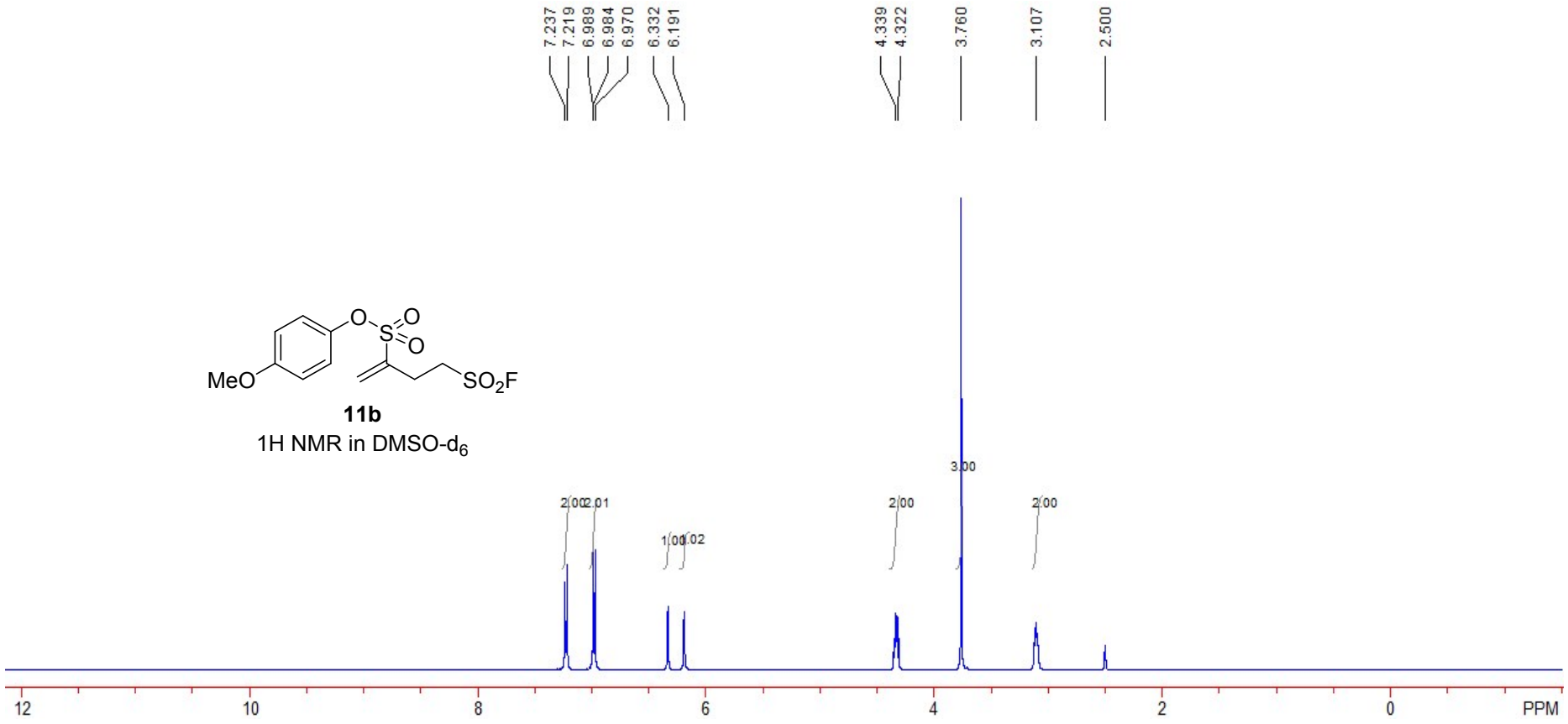
11a

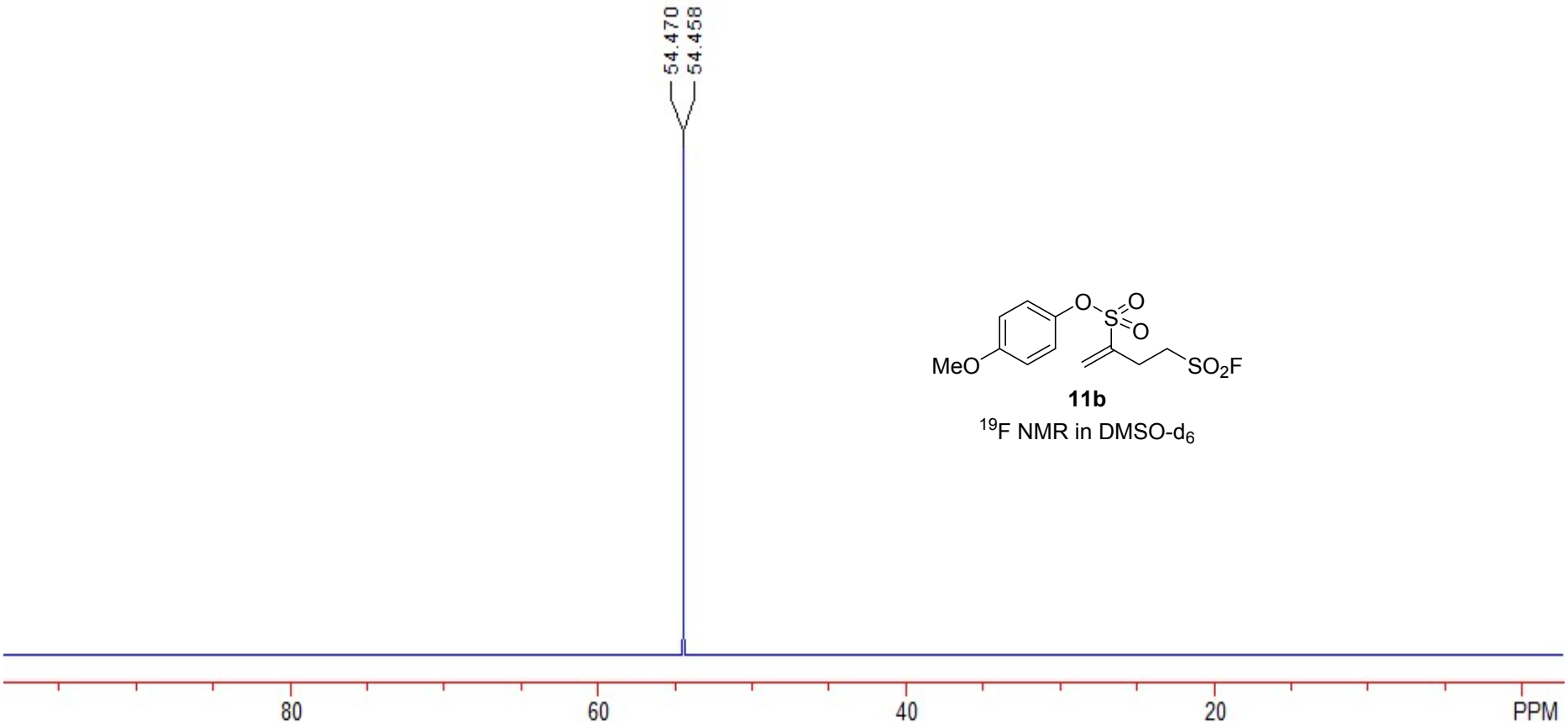
^{19}F NMR in $CDCl_3$



11a

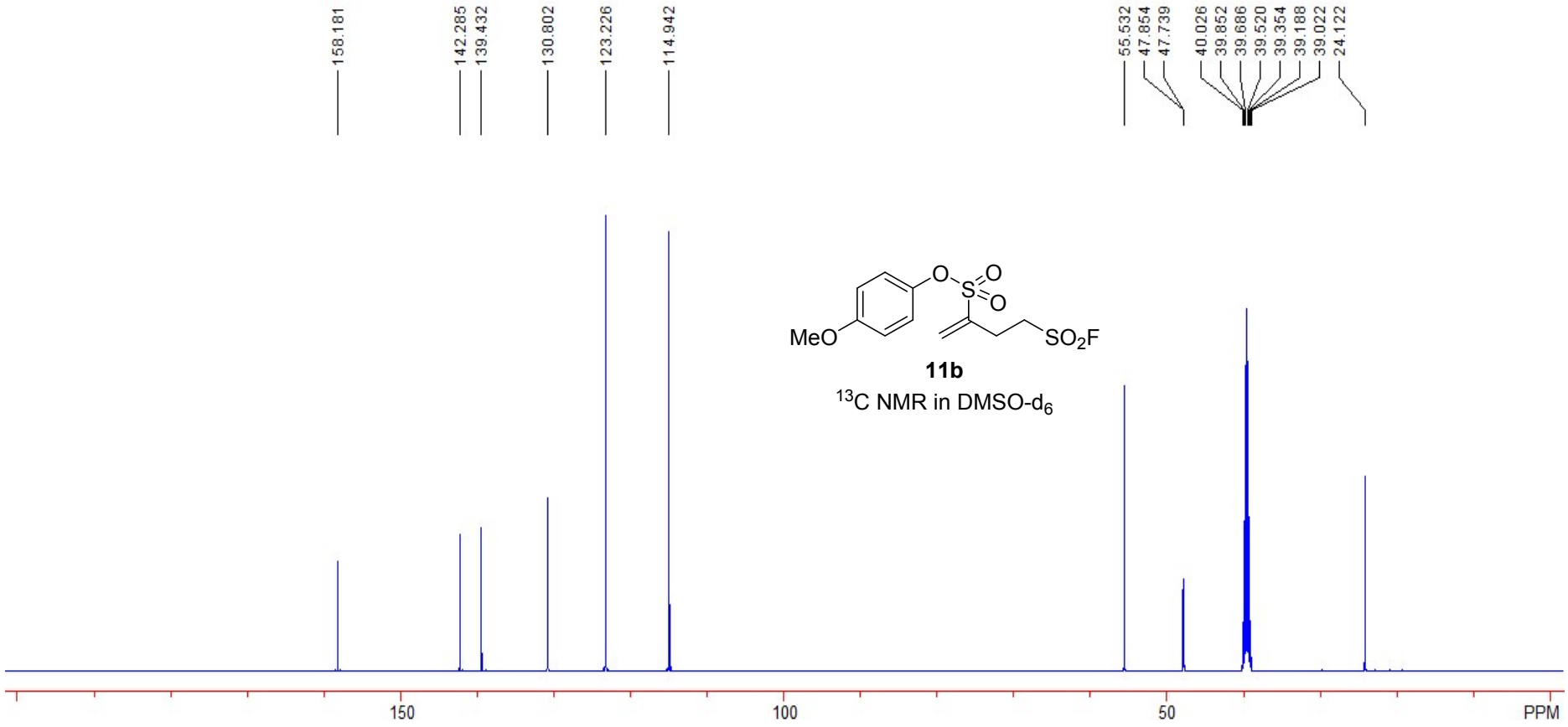
^{13}C NMR in $CDCl_3$


7.237
7.219
6.989
6.984
6.970
6.332
6.191
4.339
4.322
3.760
3.107
2.500
MeO
O
S
O
O
SO2F
11b
1H NMR in DMSO-d6
2.00
2.01
1.00
1.02
2.00
3.00
2.00
12
10
8
6
4
2
0
PPM



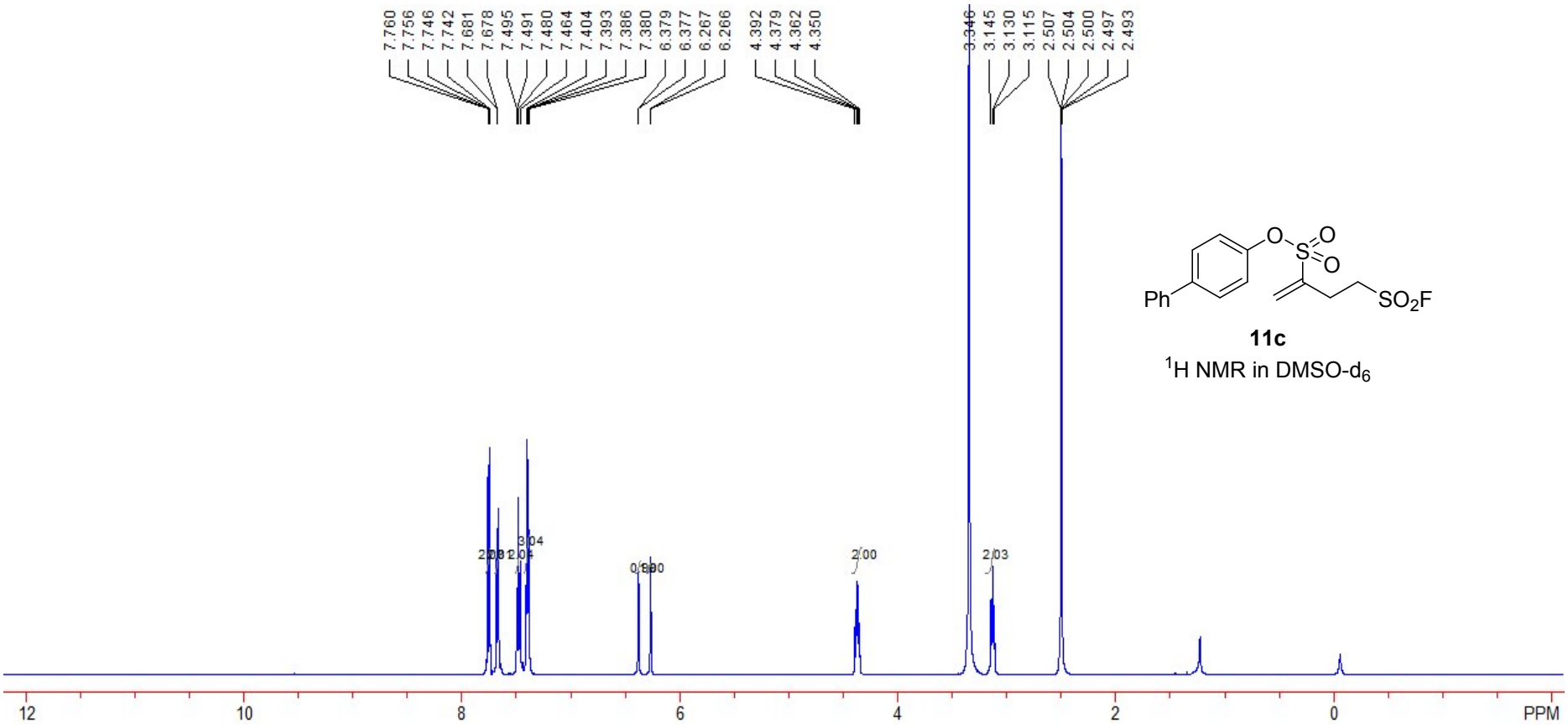
11b

^{19}F NMR in DMSO-d_6



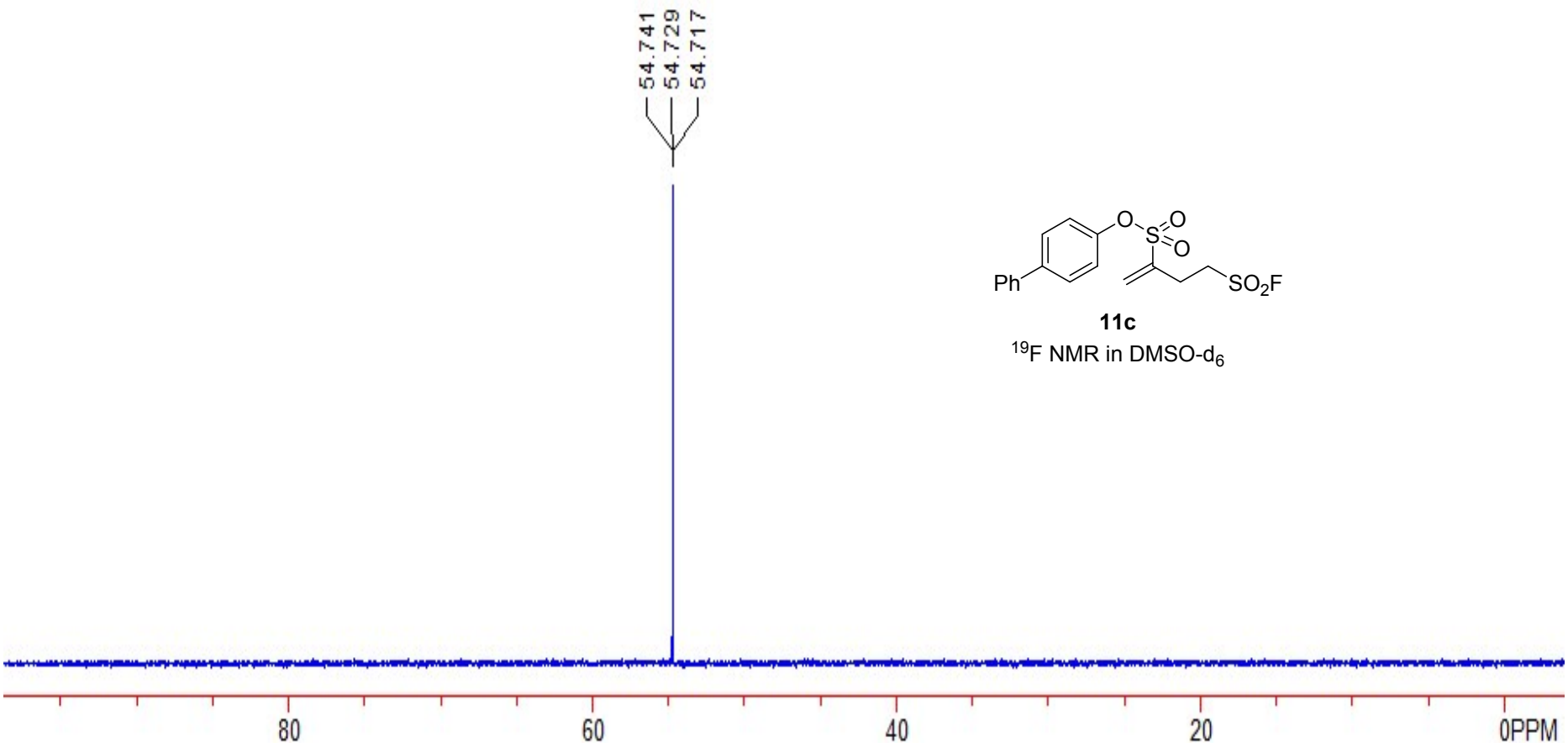
11b

^{13}C NMR in DMSO-d_6



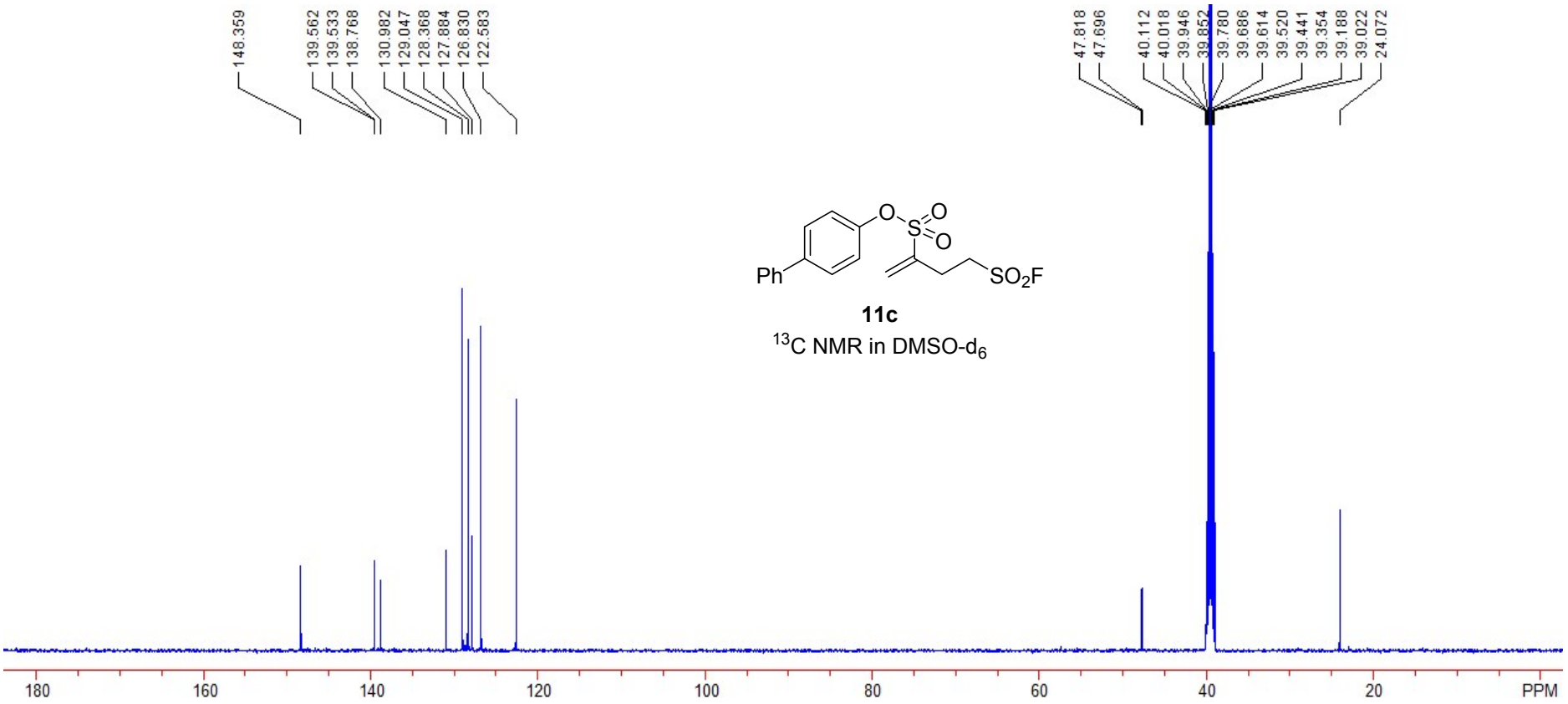
11c

^{1}H NMR in DMSO-d_6



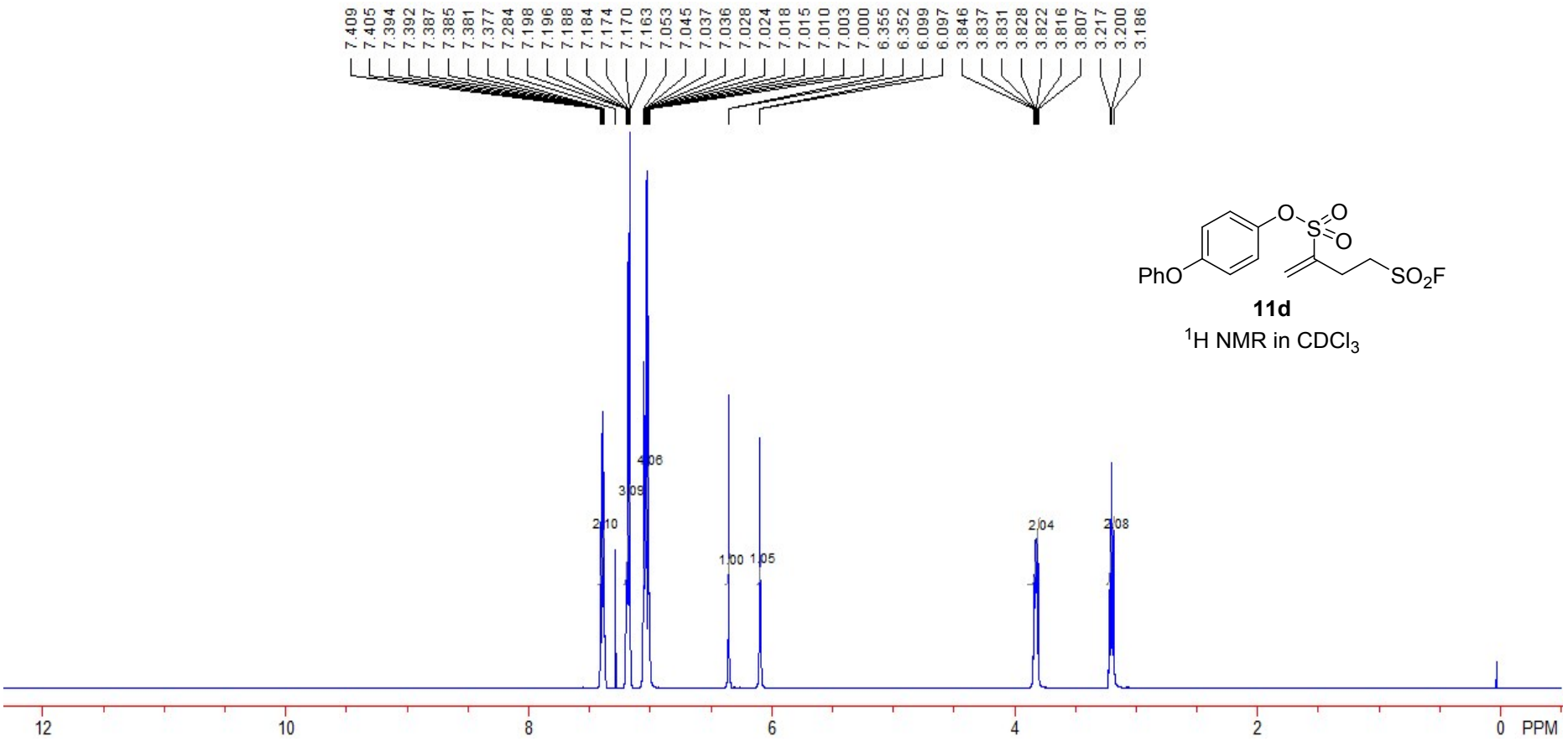
11c

^{19}F NMR in DMSO-d_6



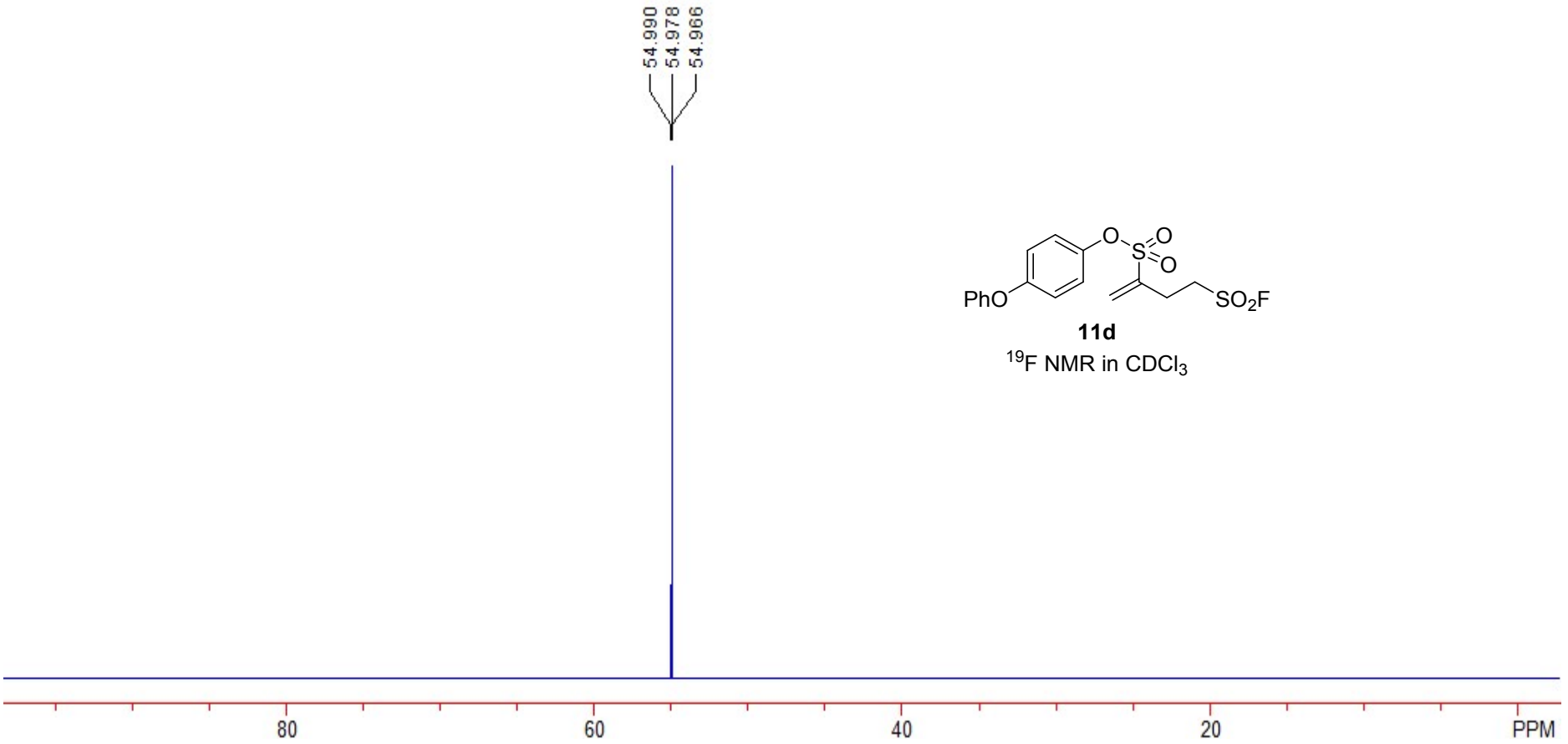
11c

^{13}C NMR in DMSO-d_6



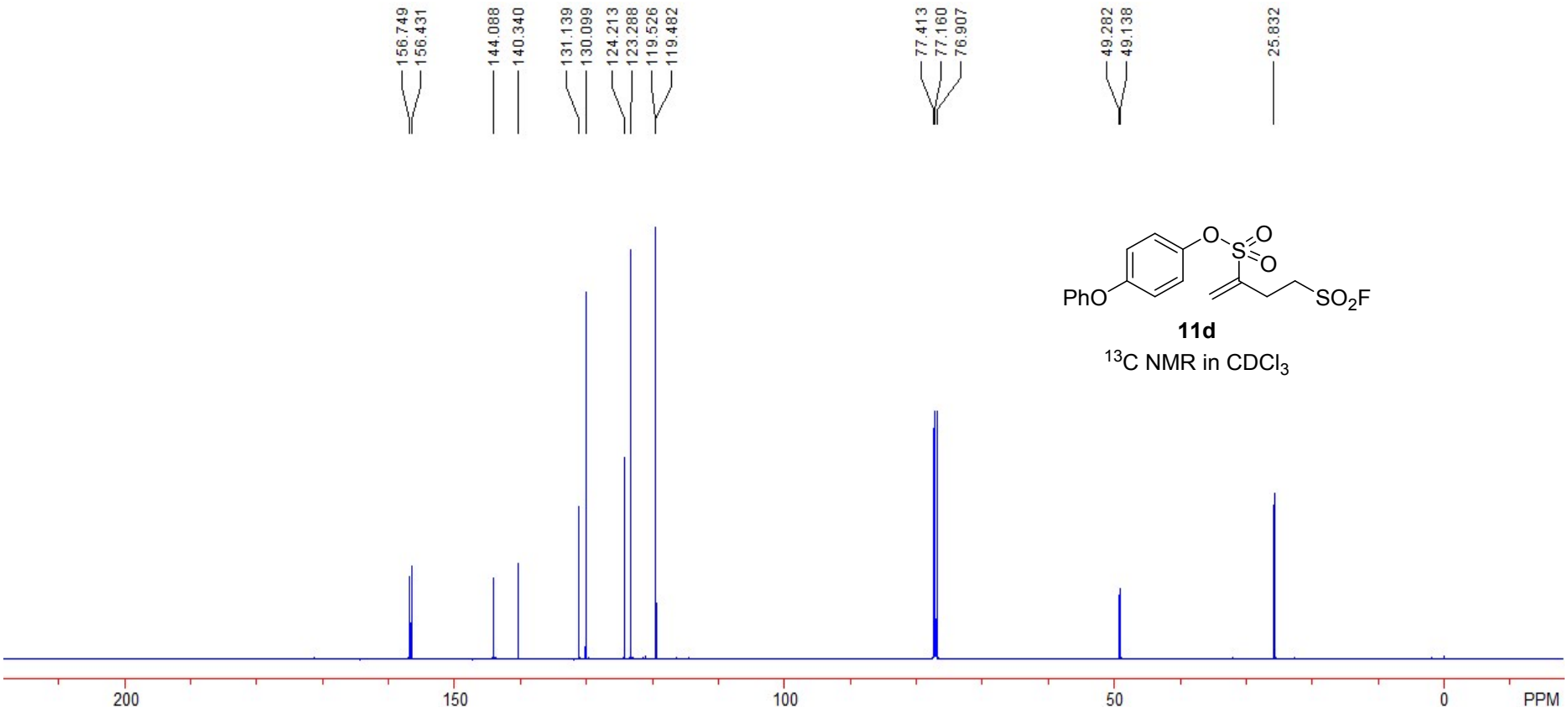
11d

^{1}H NMR in $CDCl_3$



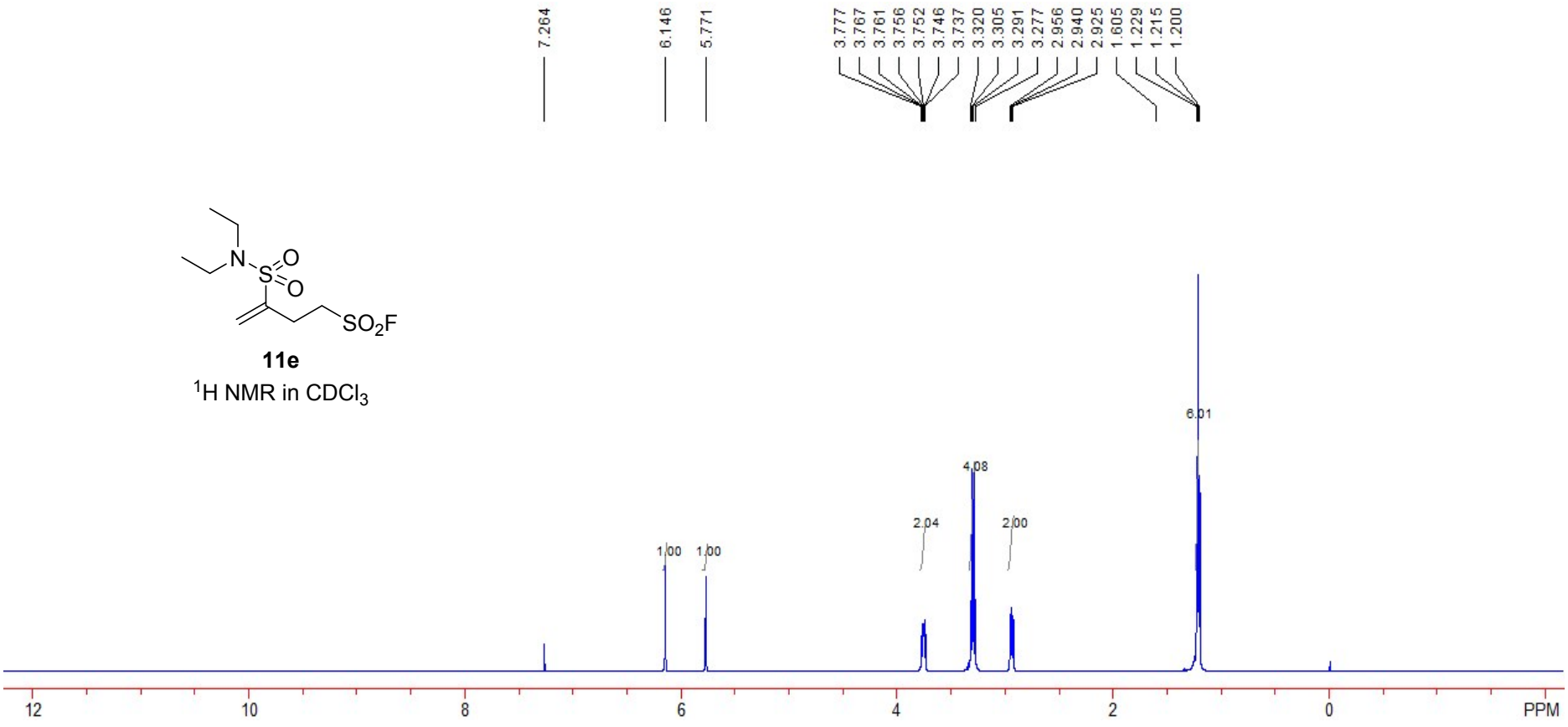
11d

^{19}F NMR in $CDCl_3$



11d

^{13}C NMR in $CDCl_3$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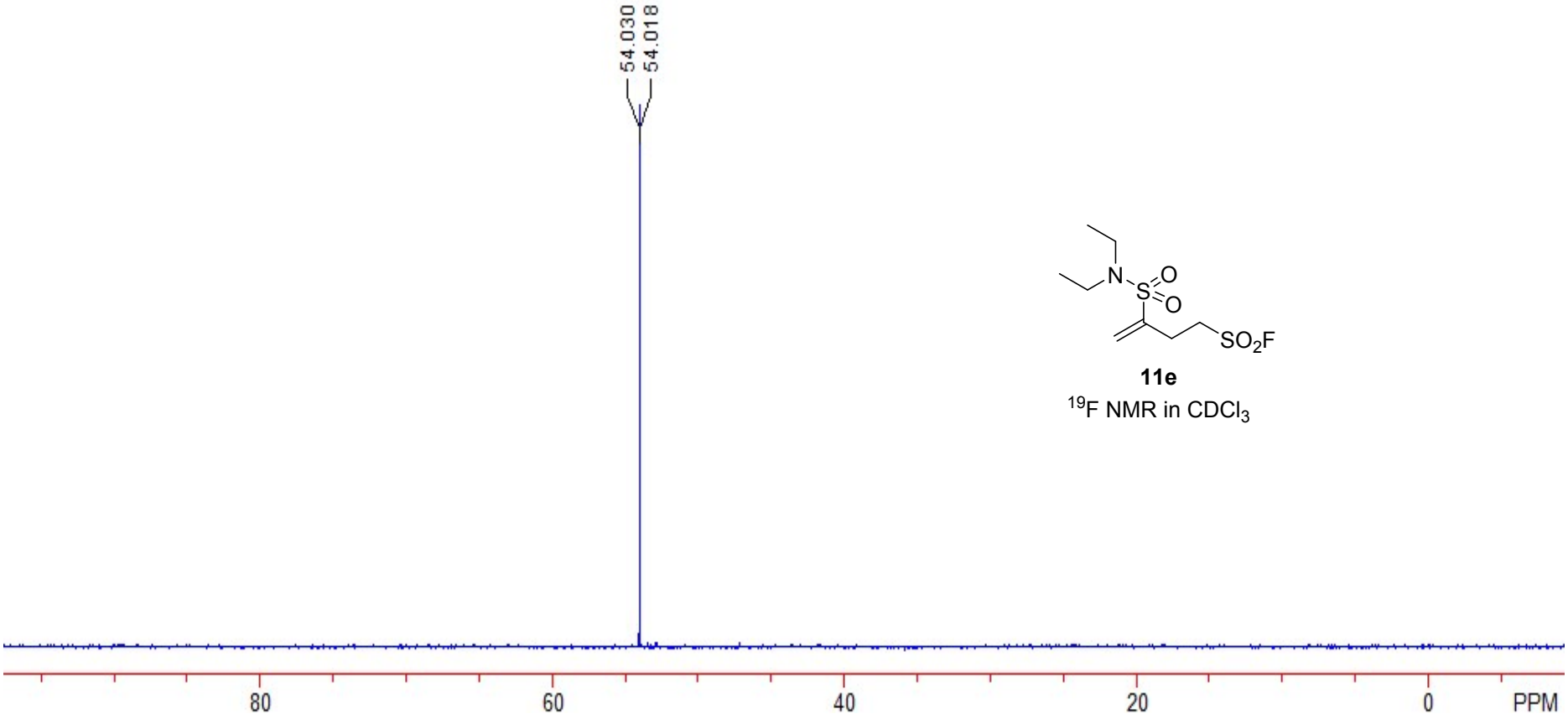
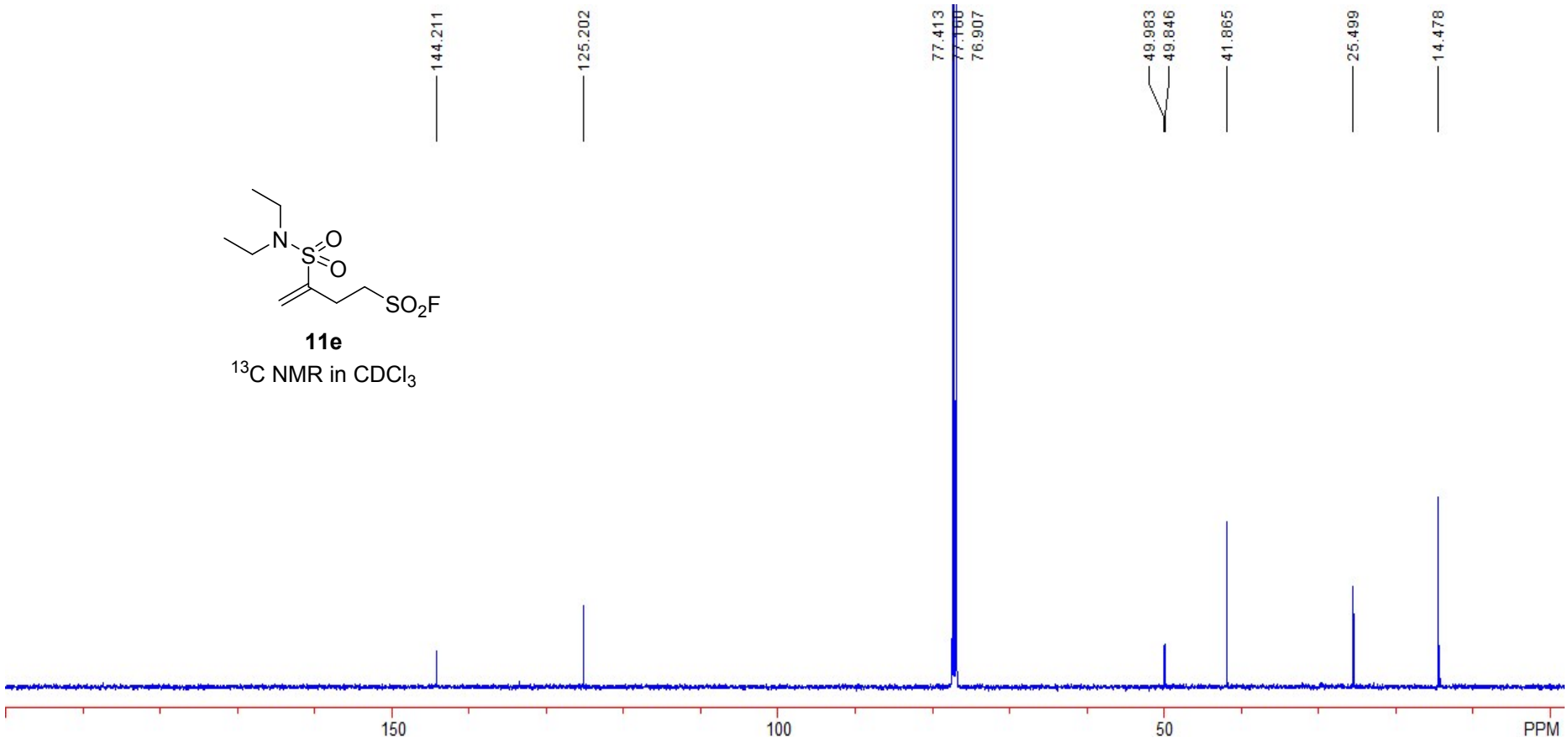
6.146
5.771
3.777
3.767
3.761
3.756
3.752
3.746
3.737
3.320
3.305
3.291
3.277
2.956
2.940
2.925
1.605
1.229
1.215
1.200
N
S
O
O
SO2F
11e
1H NMR in CDCl3
6.01
4.08
2.04
2.00
1.00
1.00
12
10
8
6
4
2
0
PPM



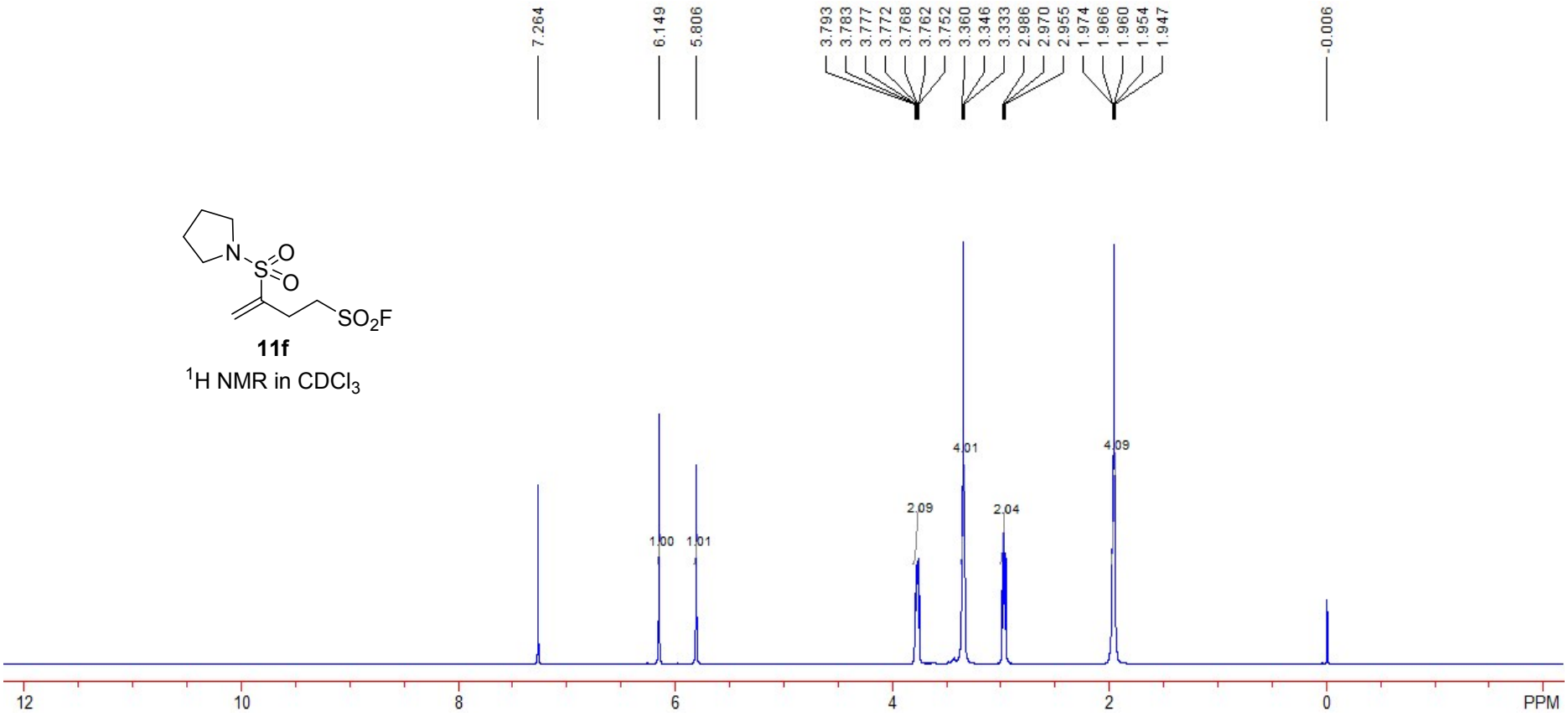
11e

^{19}F NMR in $CDCl_3$



11e

^{13}C NMR in $CDCl_3$


7.264
6.149
5.806
3.793
3.783
3.777
3.772
3.768
3.762
3.752
3.360
3.346
3.333
2.986
2.970
2.955
1.974
1.966
1.960
1.954
1.947
-0.006
N
S
O
O
SO2F
11f
1H NMR in CDCl3
1.00
1.01
2.09
4.01
2.04
4.09
12
10
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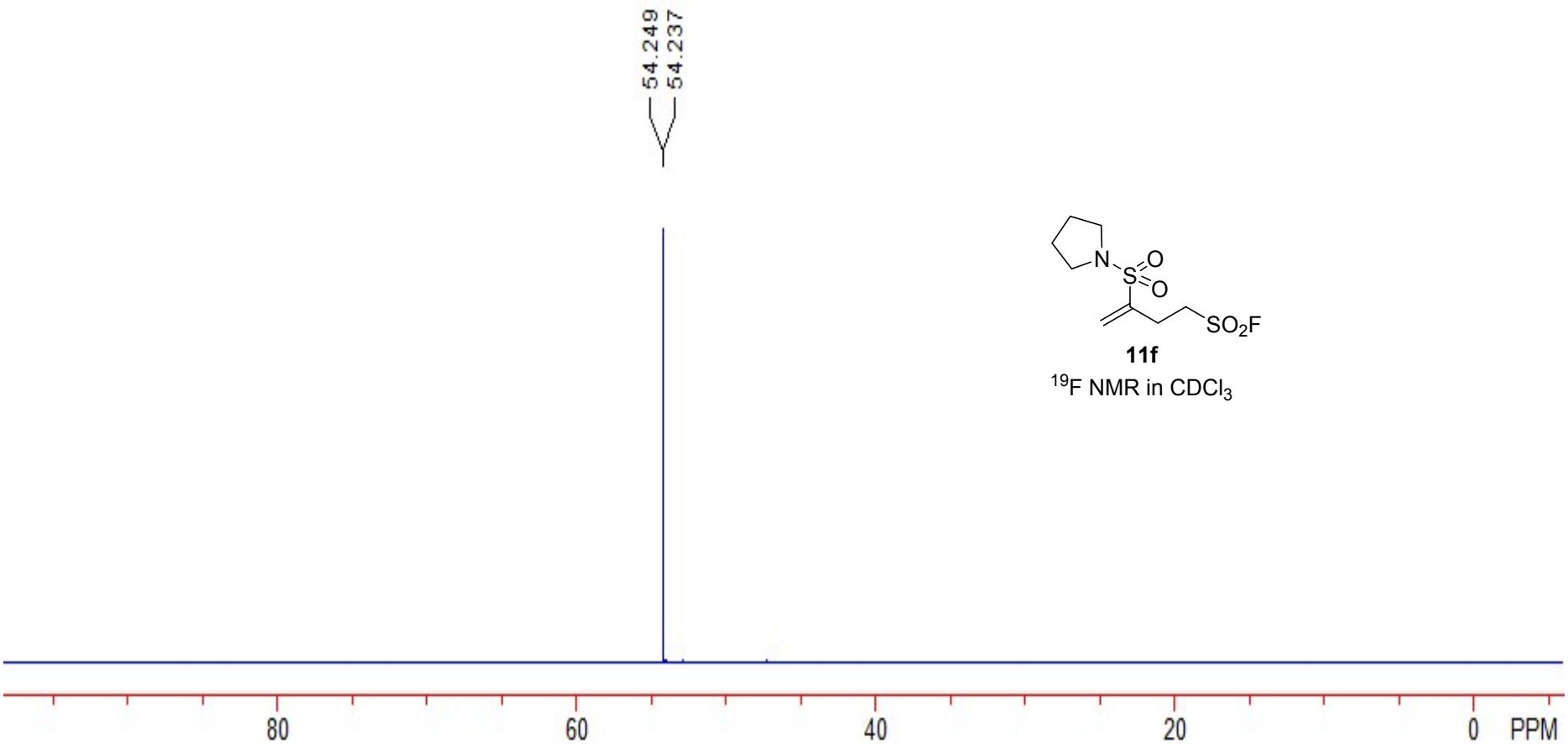
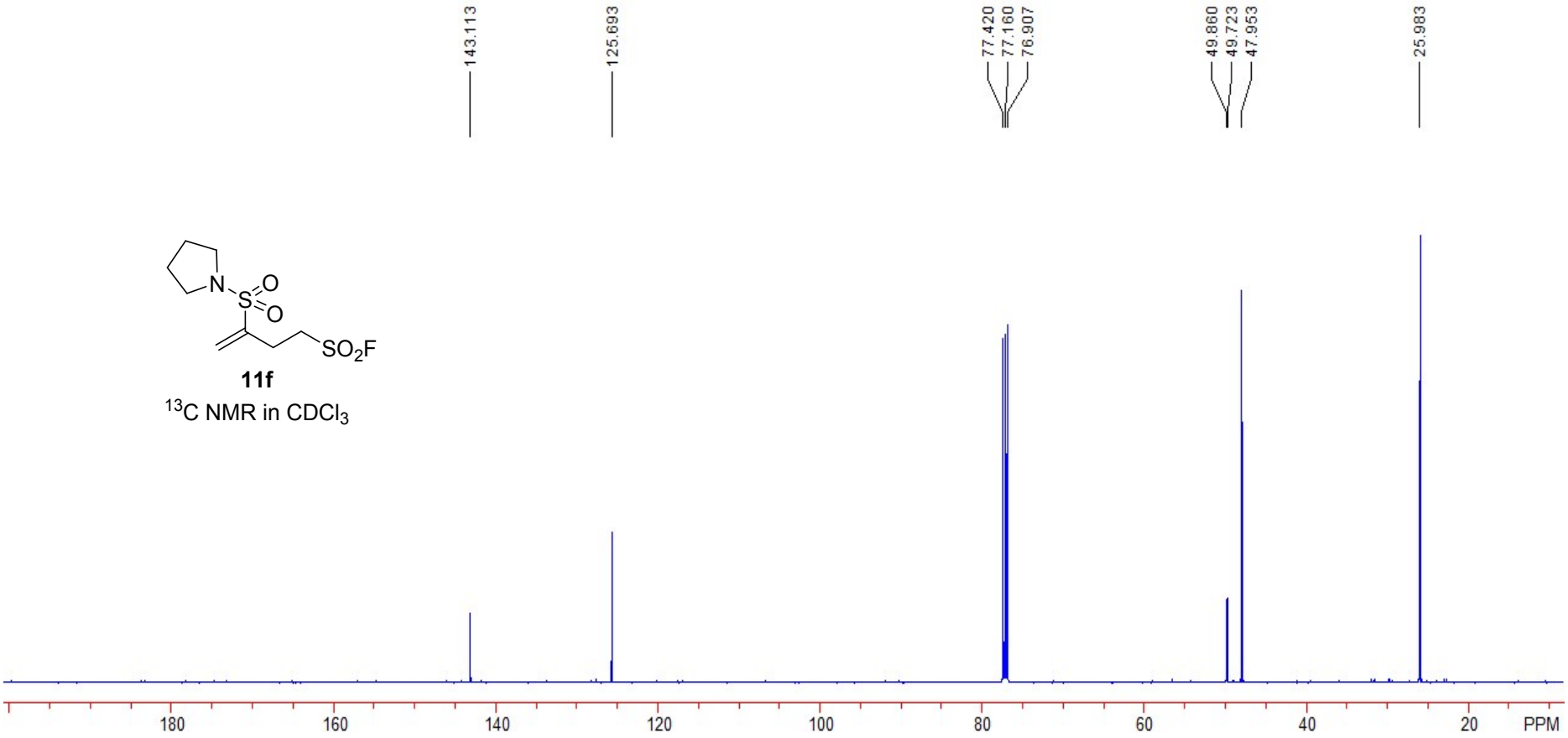


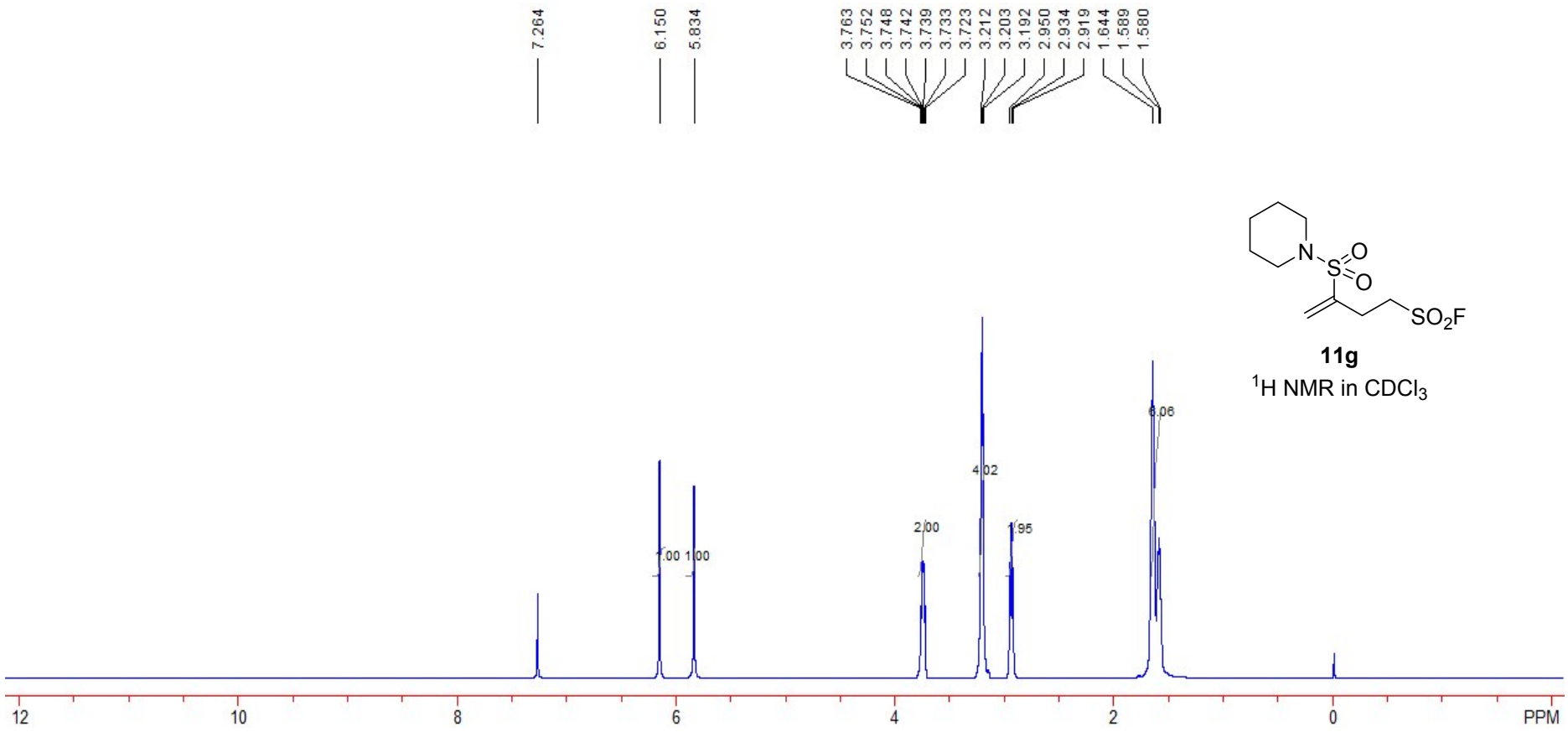
11f

^{19}F NMR in $CDCl_3$



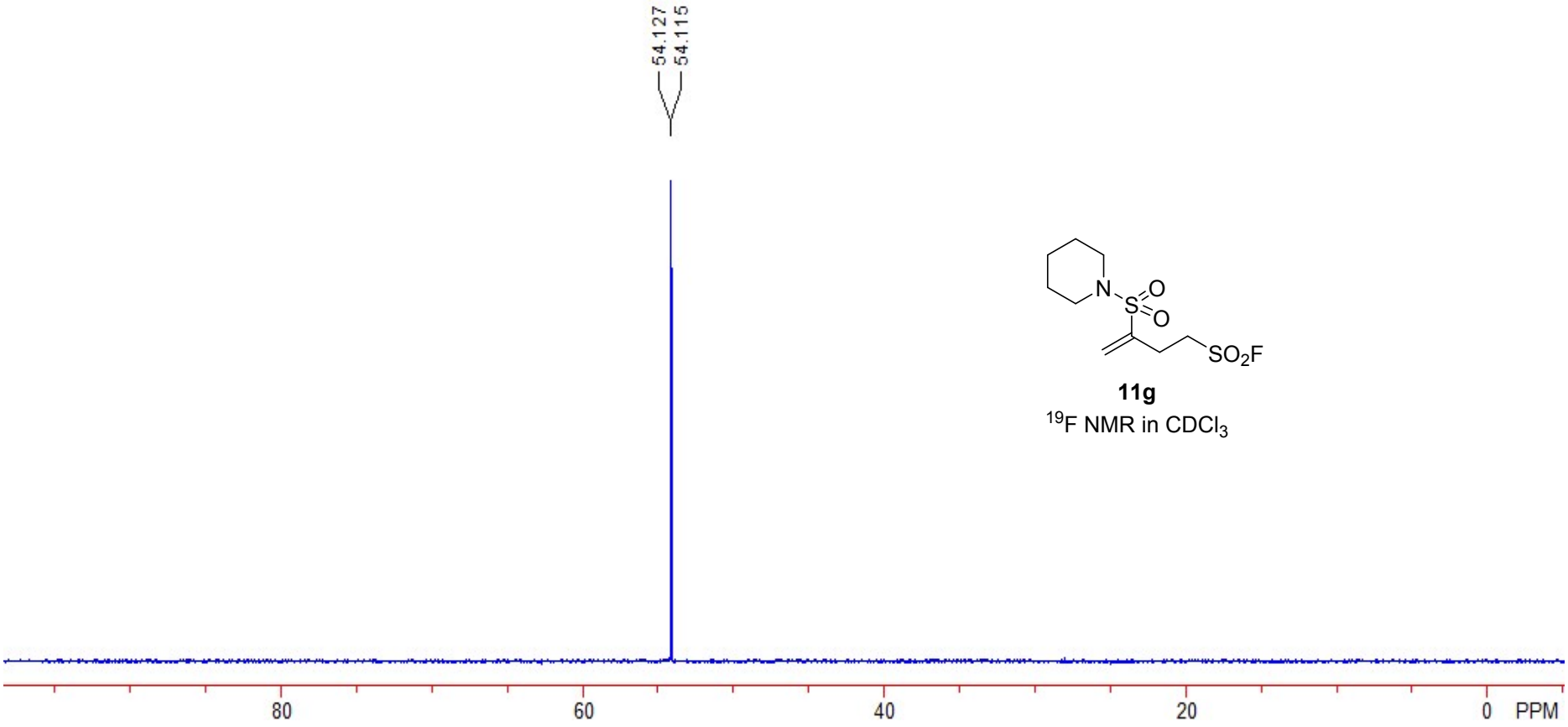
11f

^{13}C NMR in $CDCl_3$



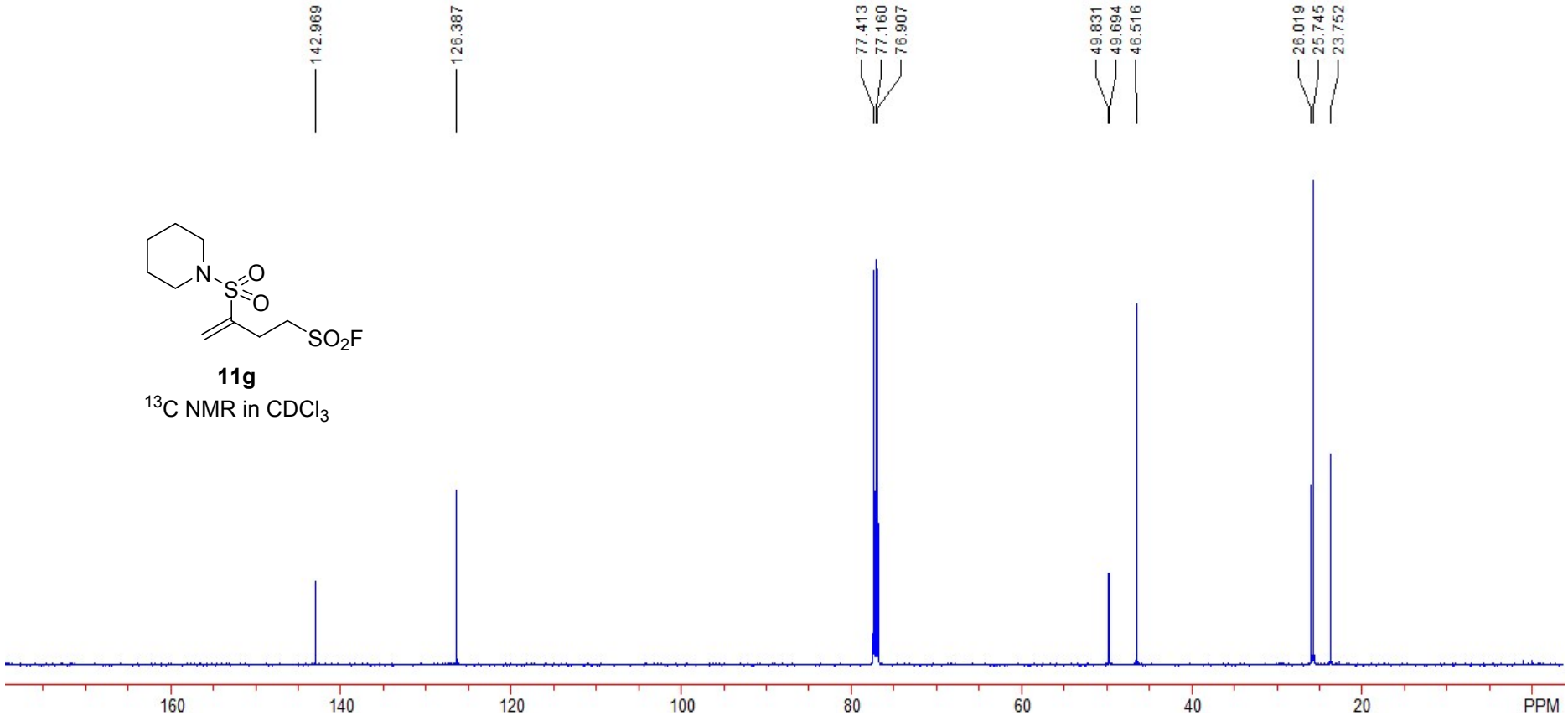
11g

^{1}H NMR in $CDCl_3$



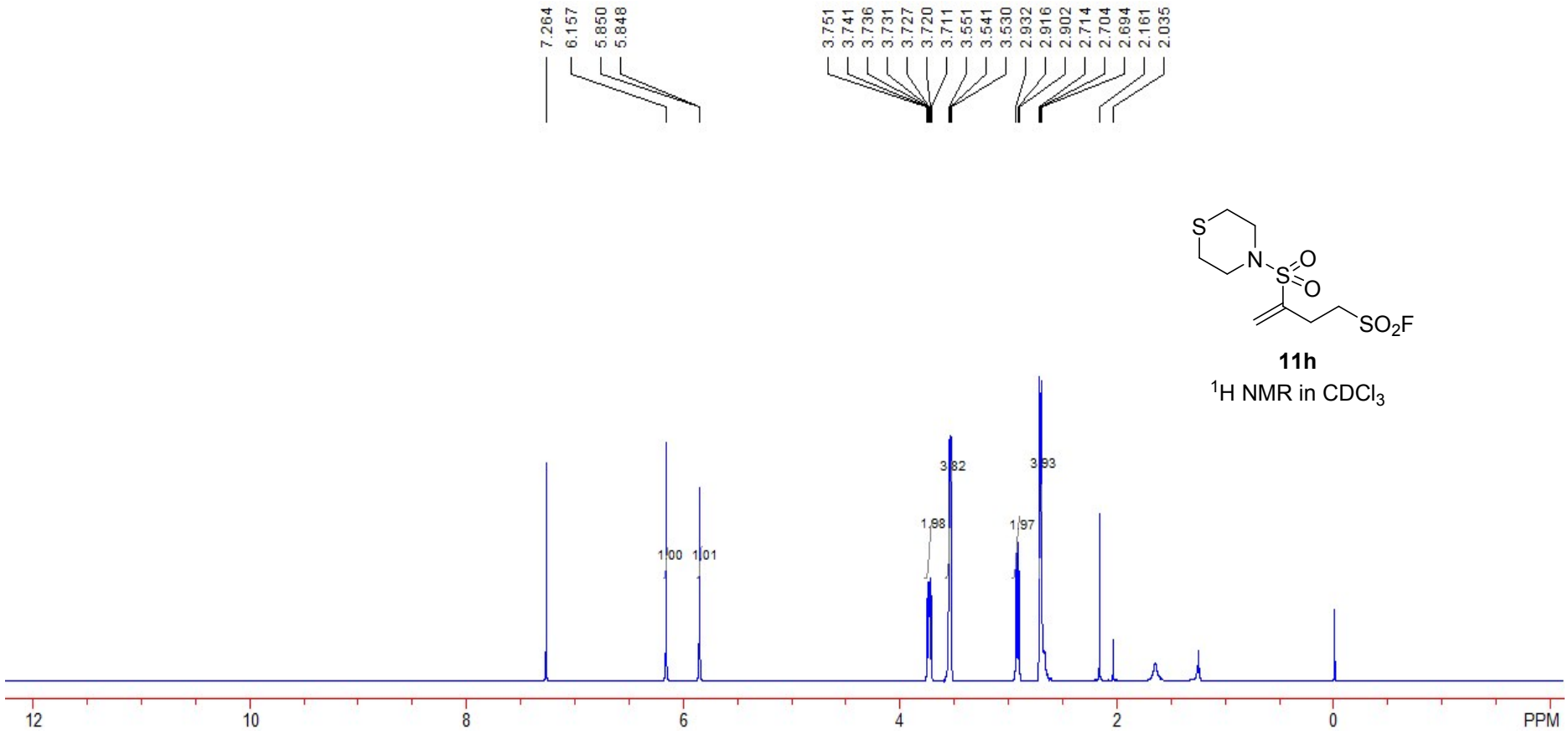
11g

^{19}F NMR in $CDCl_3$



11g

^{13}C NMR in $CDCl_3$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3.551
3.541
3.530
2.932
2.916
2.902
2.714
2.704
2.694
2.161
2.035
S
N
S
O
O
SO2F
11h
1H NMR in CDCl3
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12
10
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4
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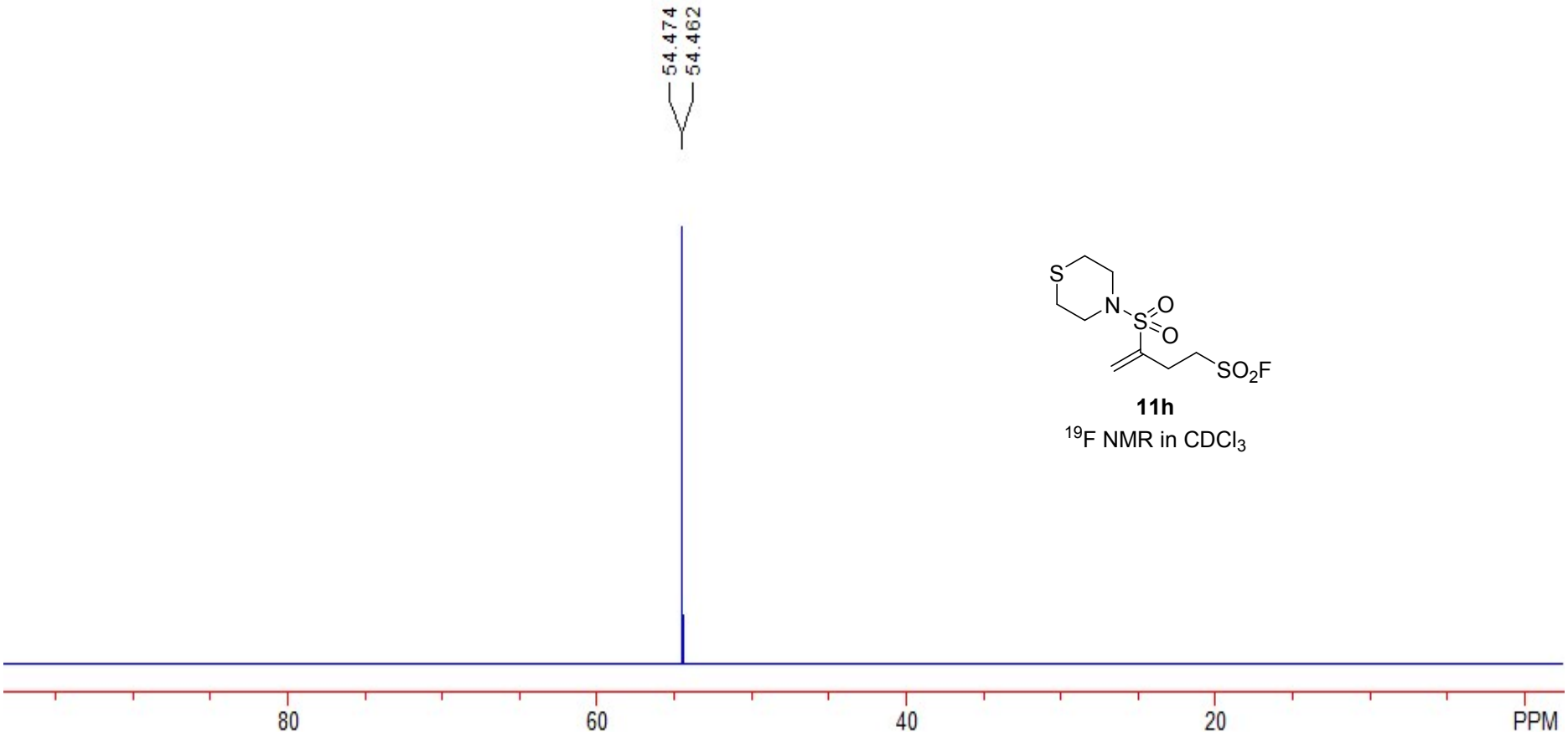
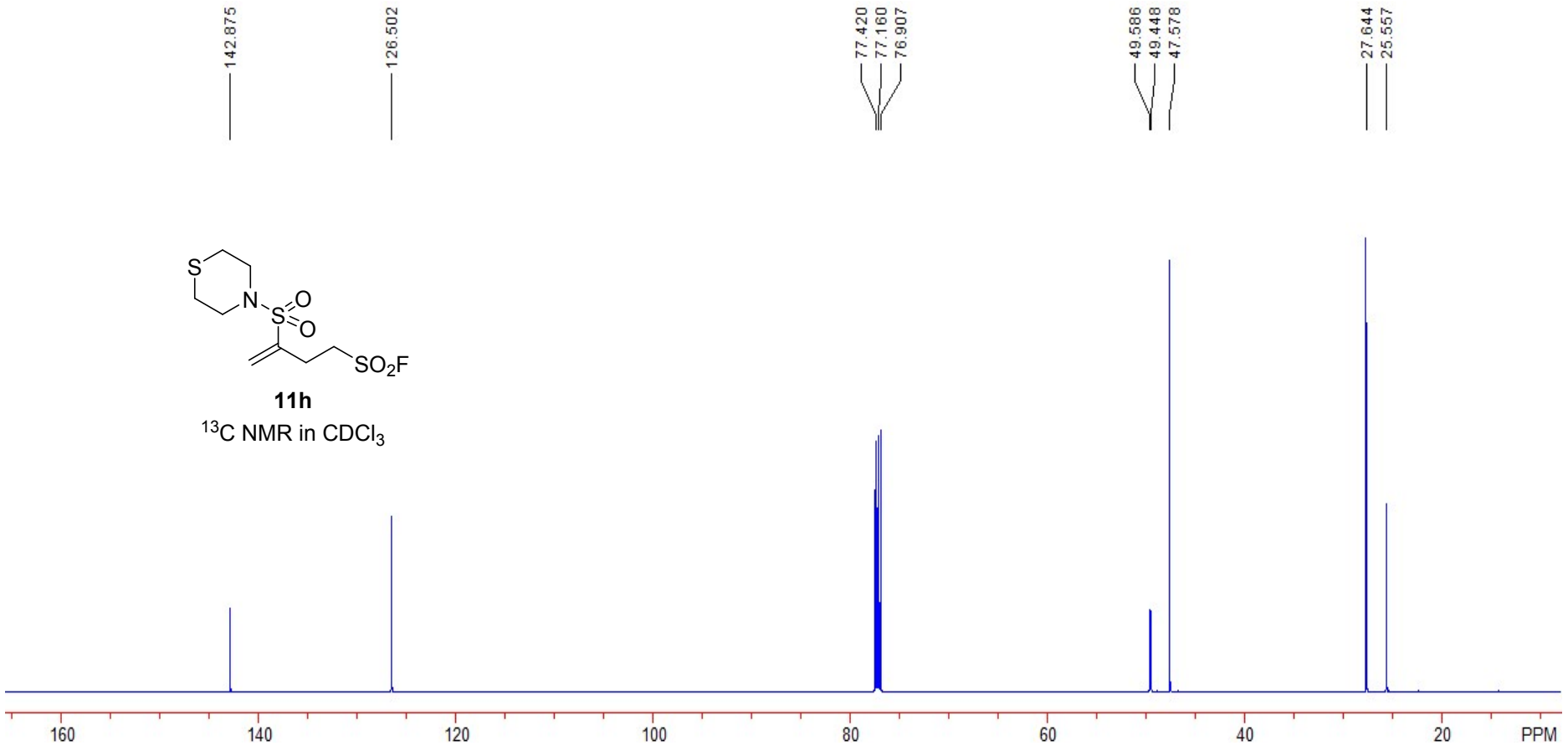
0
PPM



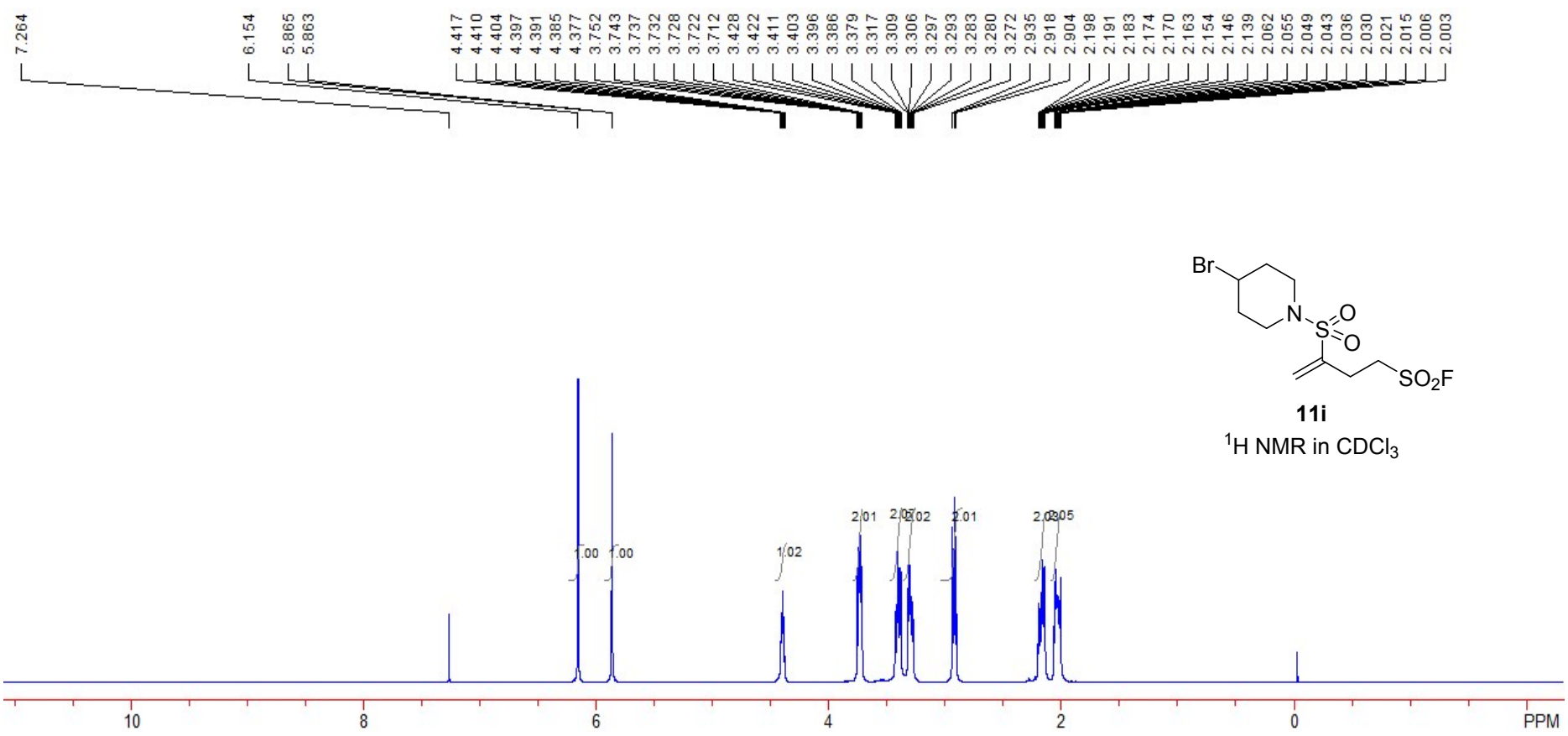
11h

^{19}F NMR in $CDCl_3$



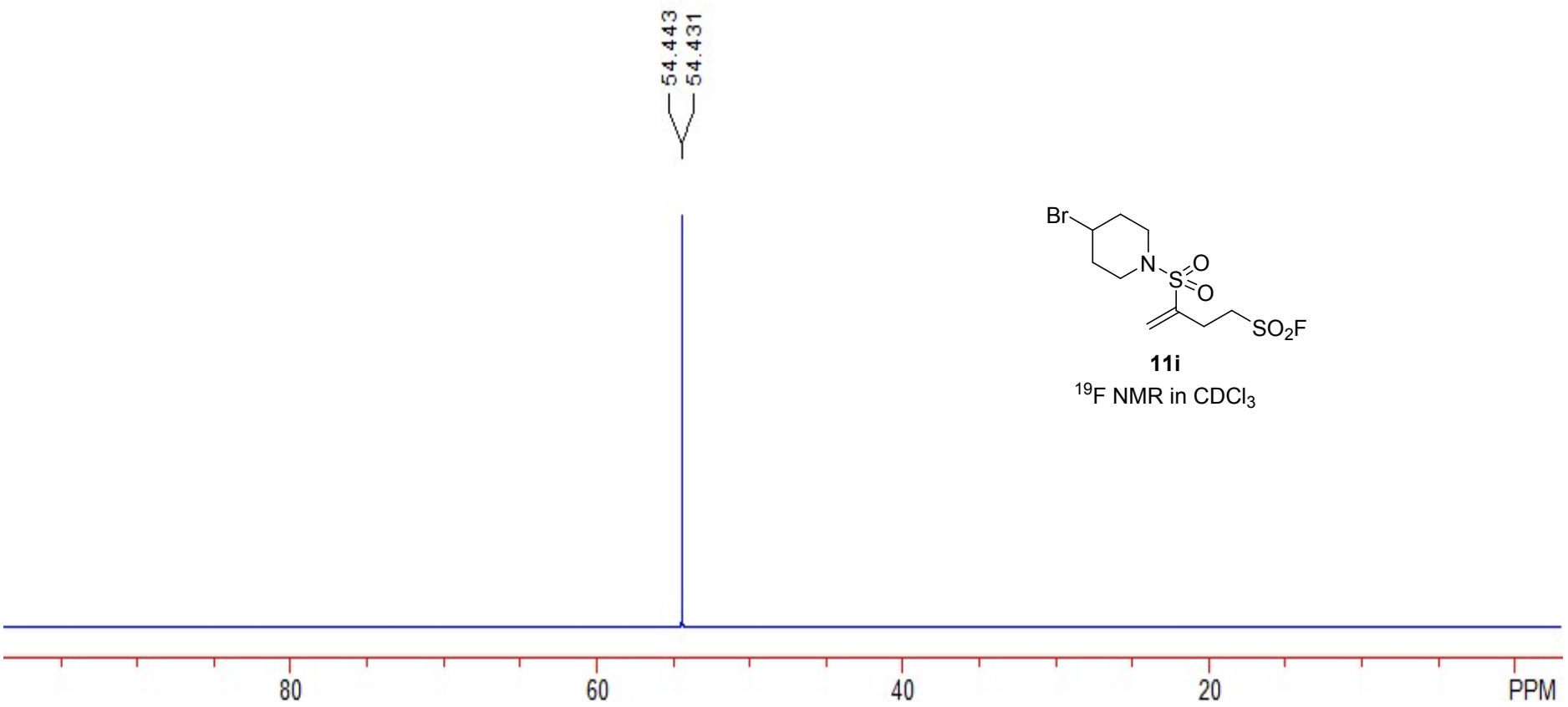
11h

^{13}C NMR in $CDCl_3$



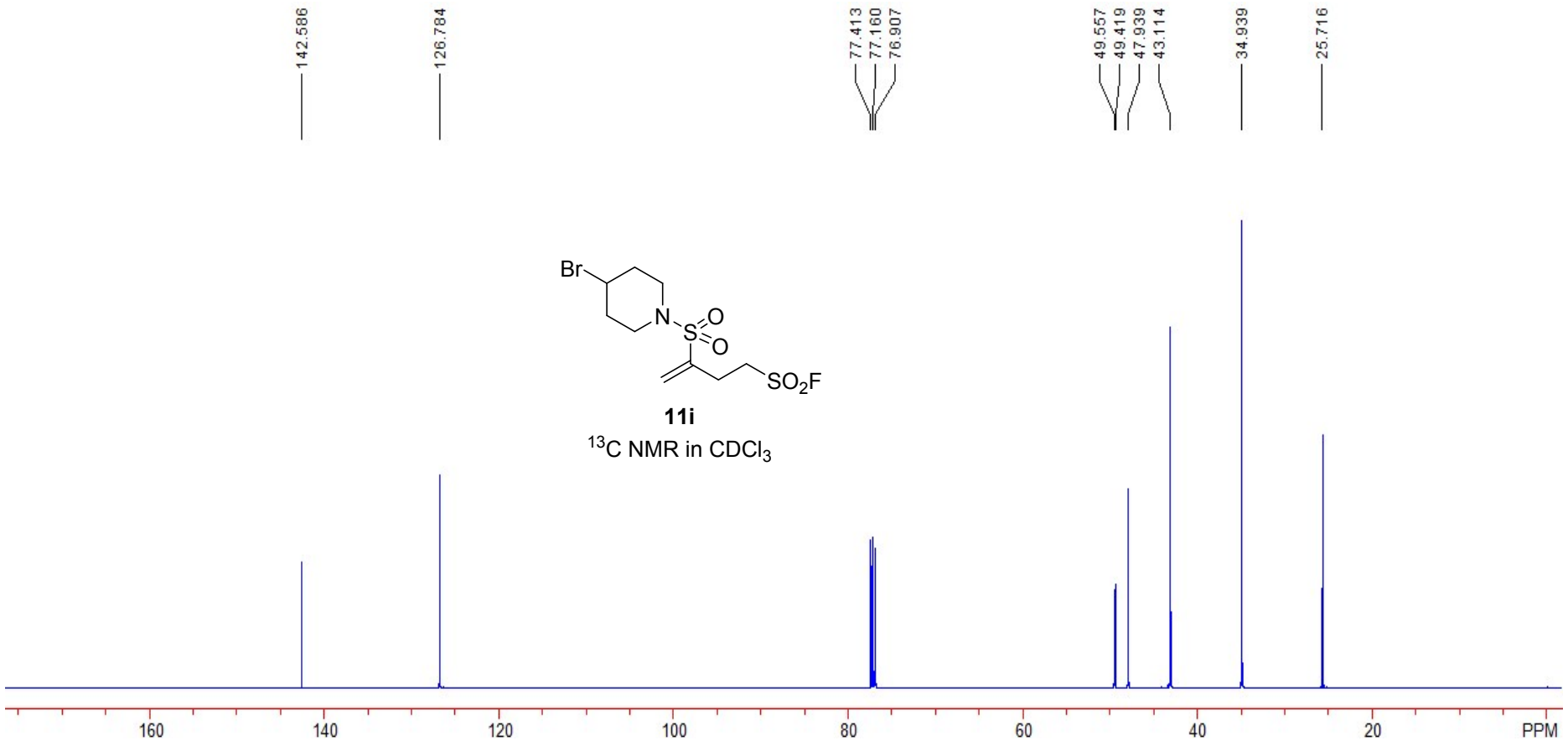
11i

^{1}H NMR in $CDCl_3$



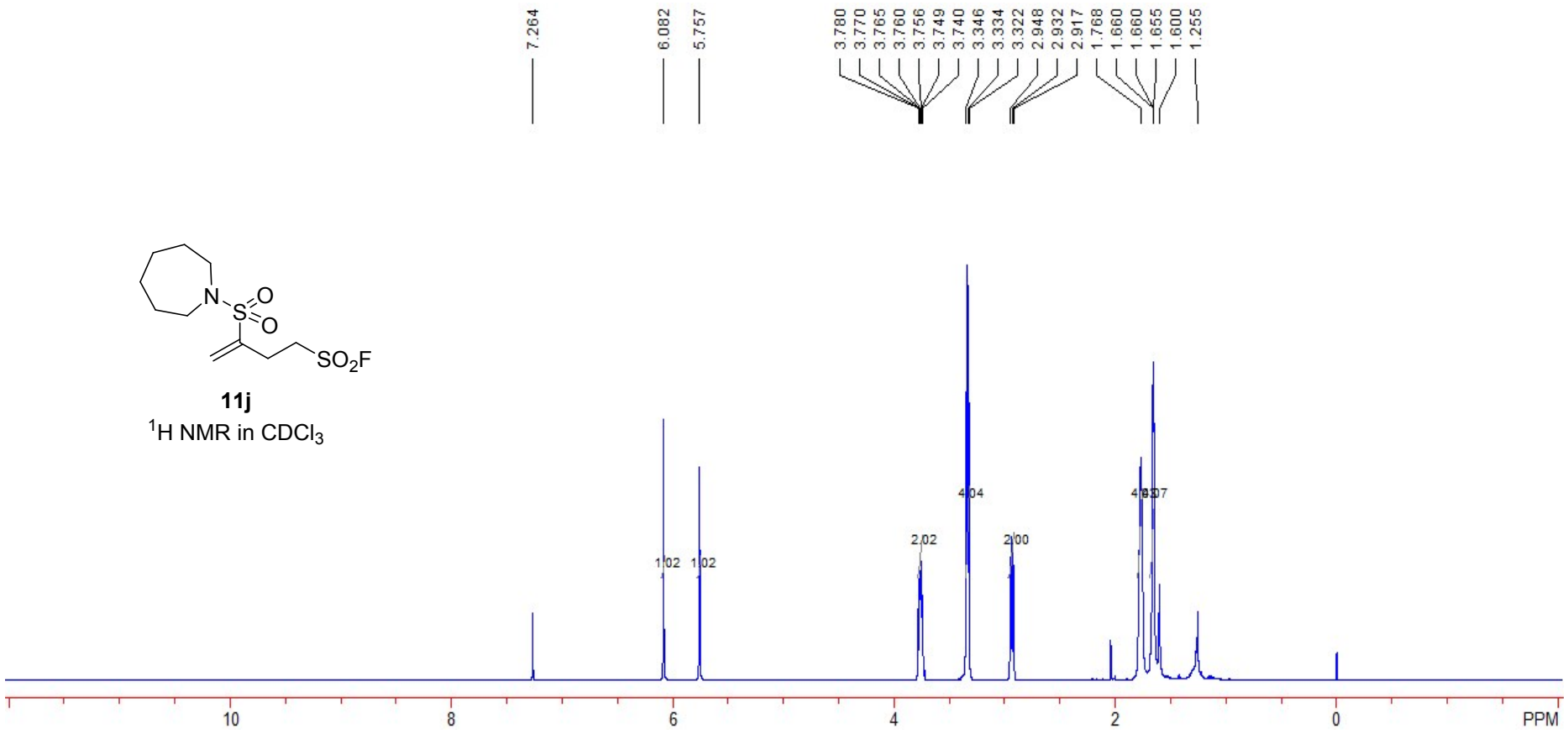
11i

^{19}F NMR in $CDCl_3$



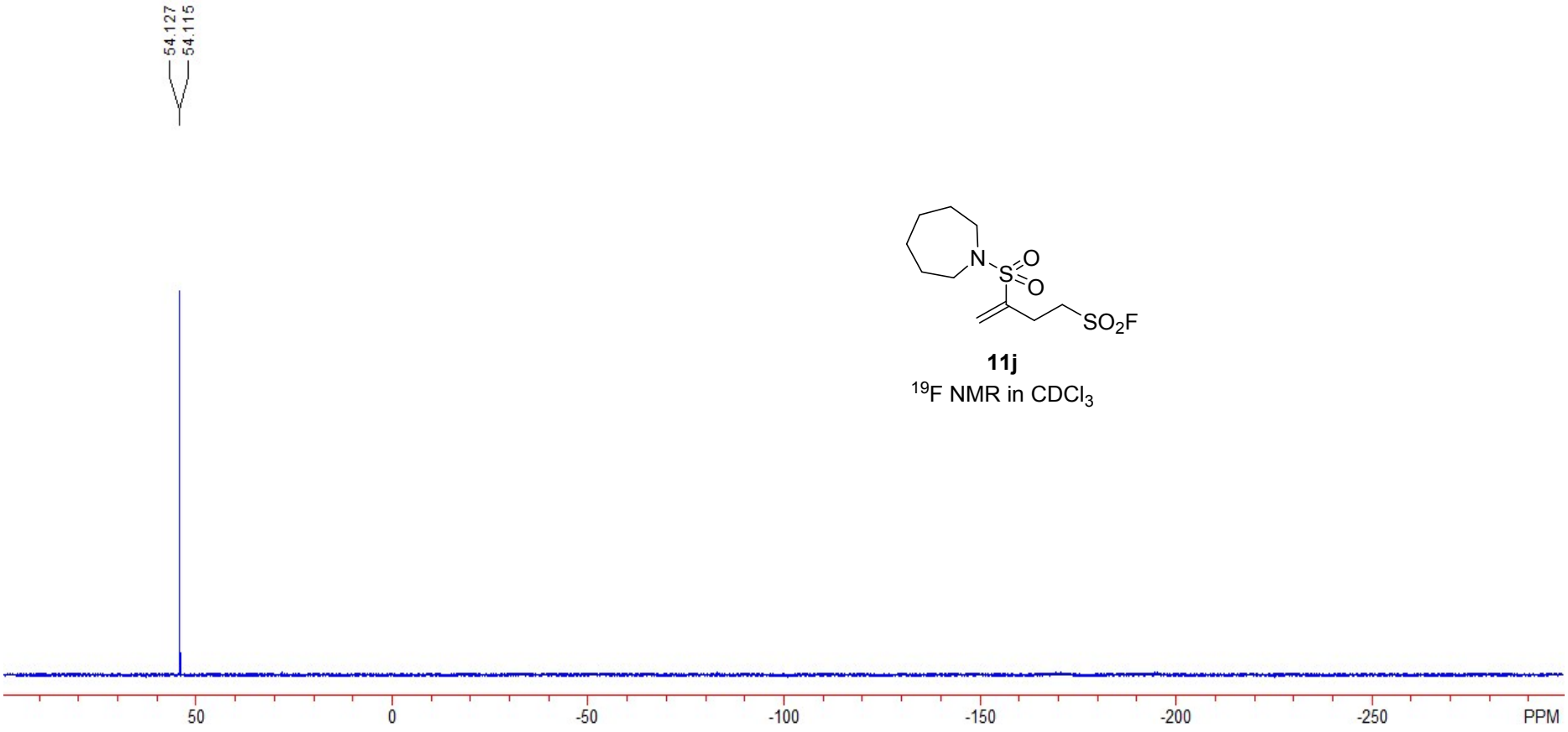
11i

^{13}C NMR in $CDCl_3$



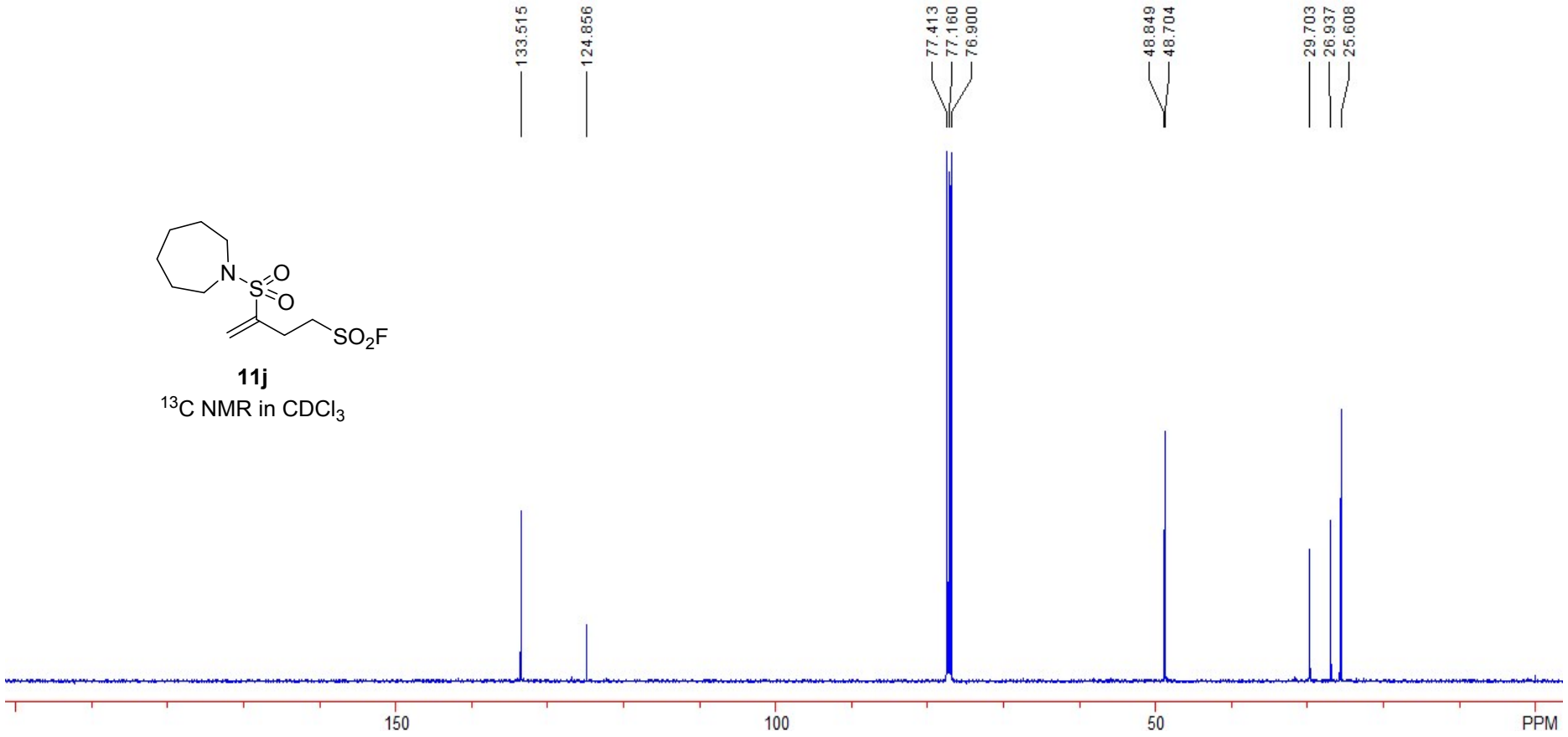
11j

^{1}H NMR in $CDCl_3$



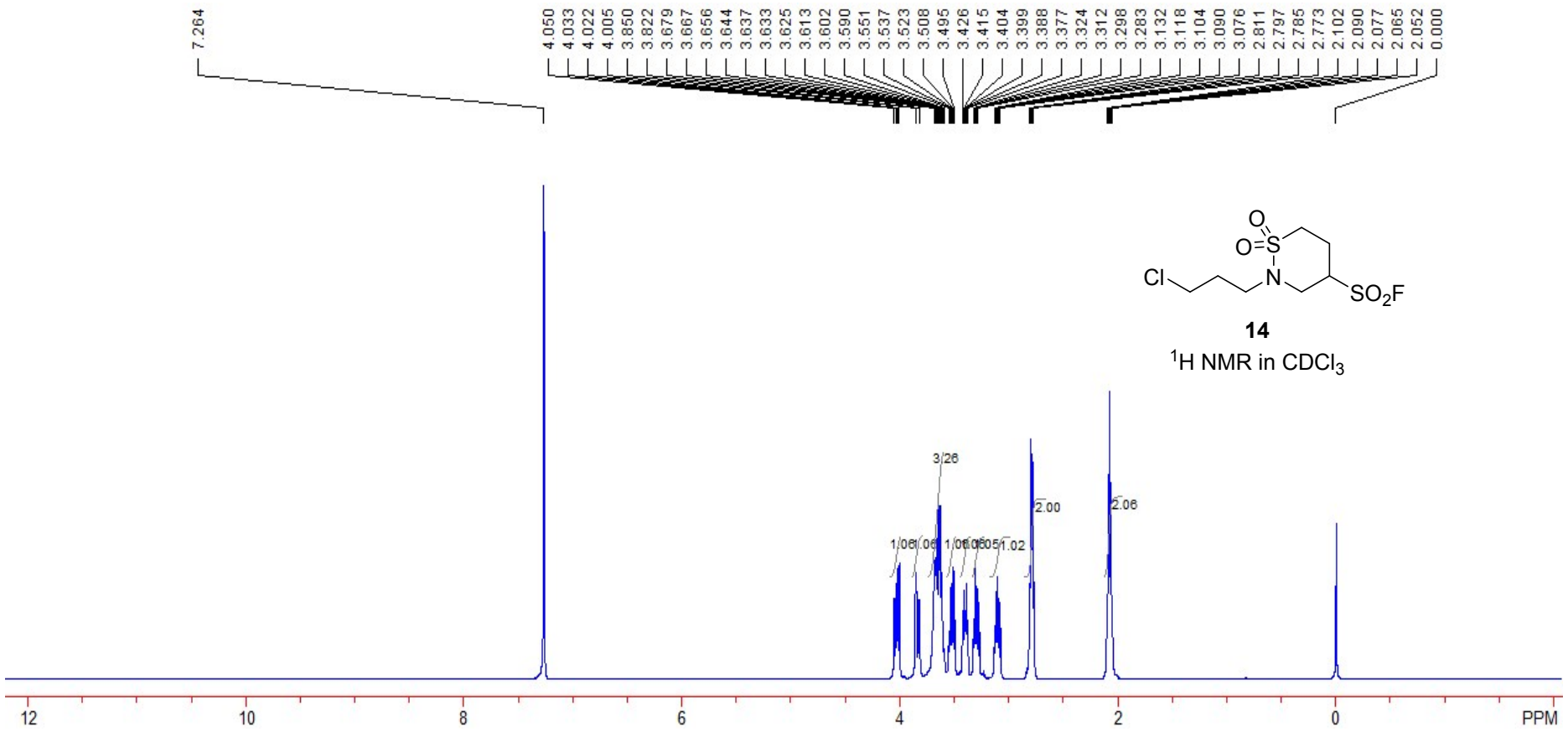
11j

^{19}F NMR in $CDCl_3$



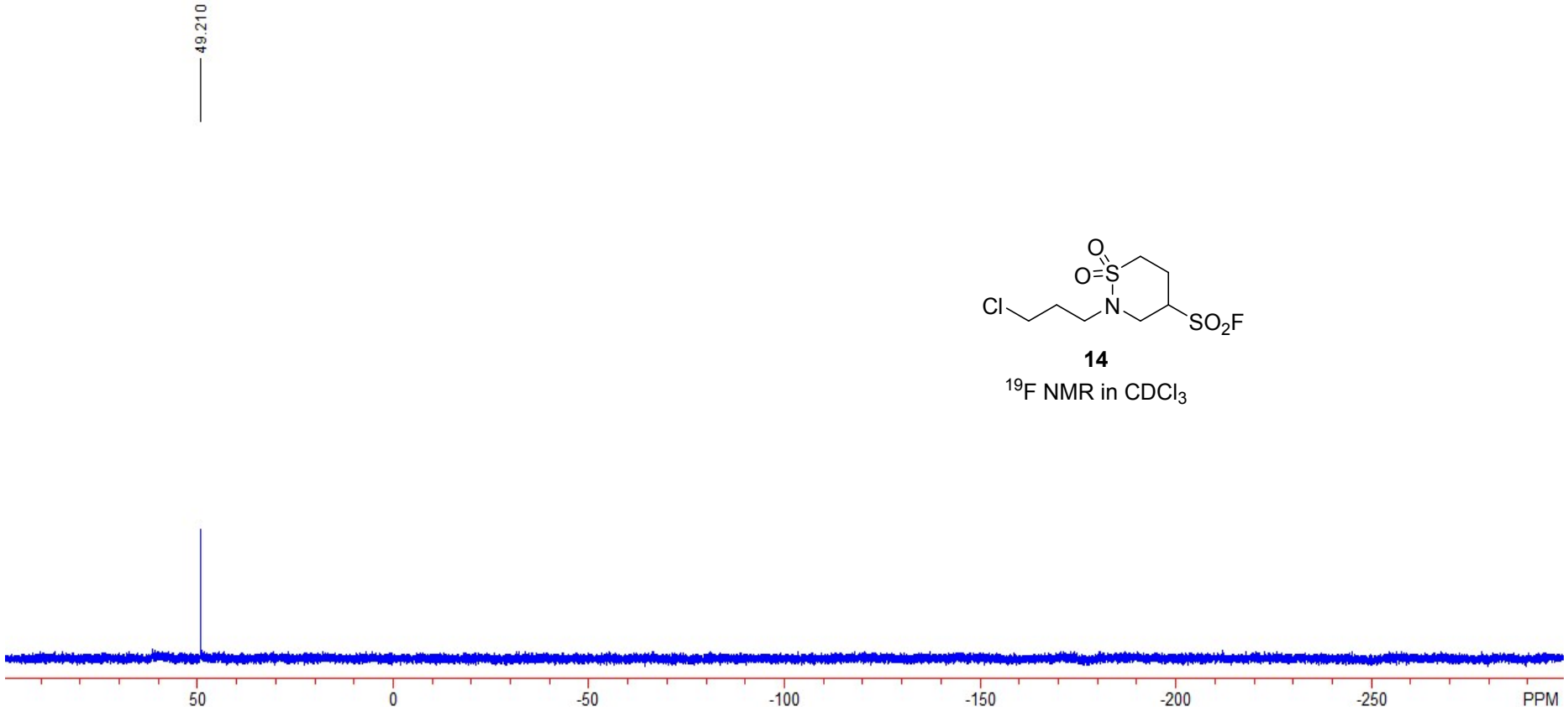
11j

^{13}C NMR in $CDCl_3$



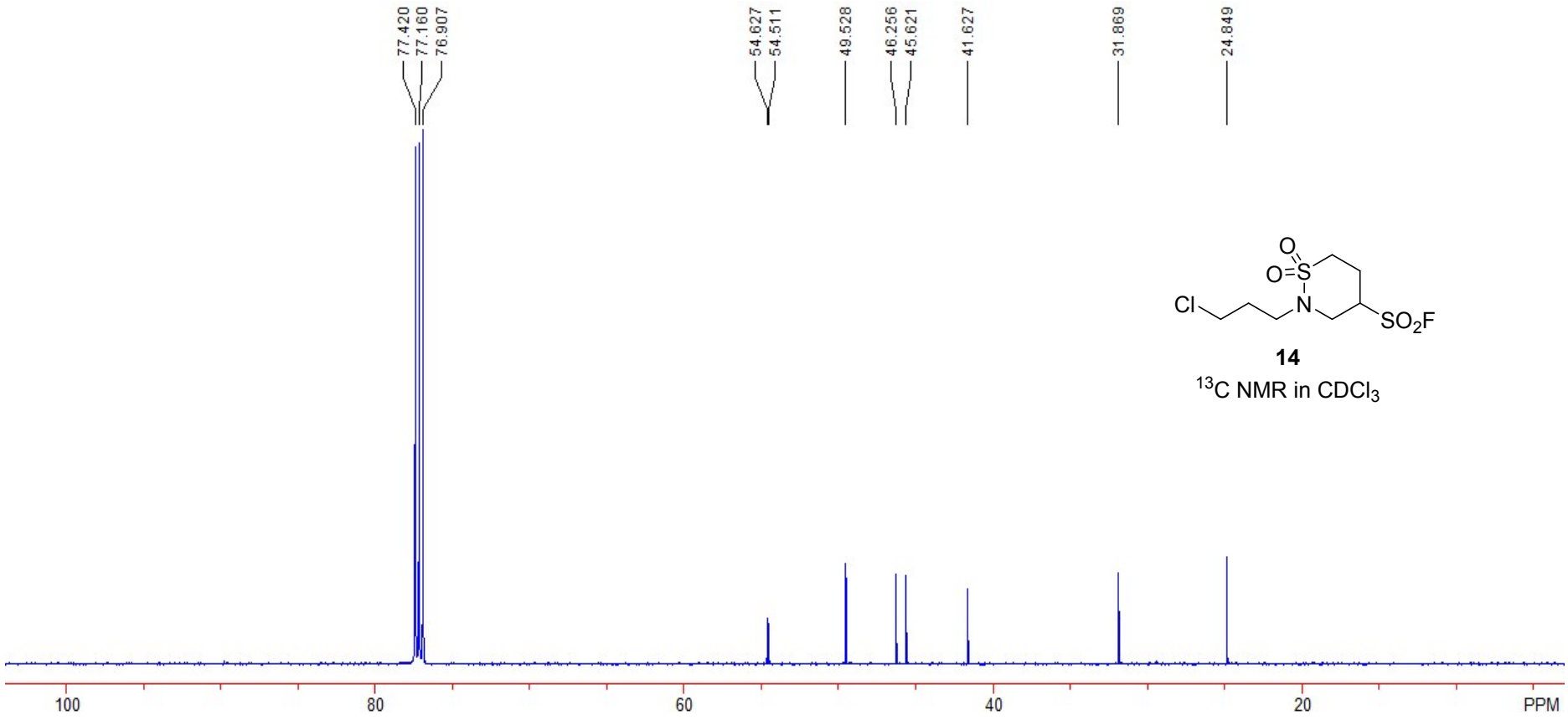
14

^{1}H NMR in $CDCl_3$



14

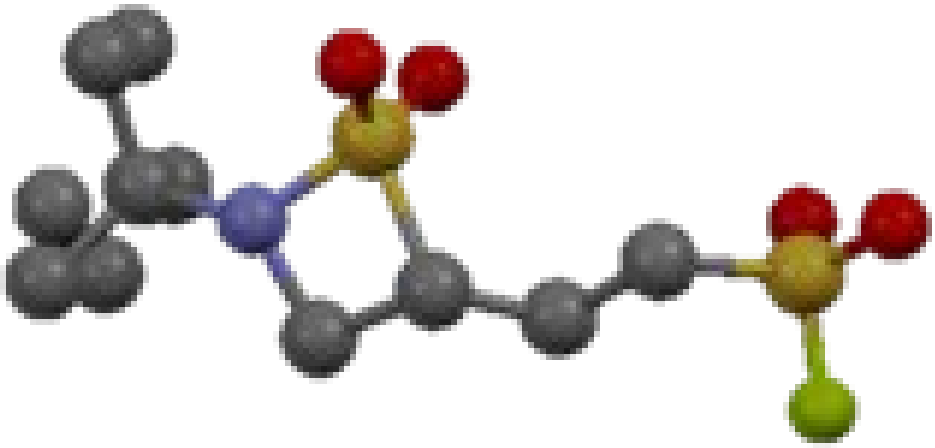
^{19}F NMR in $CDCl_3$



14

^{13}C NMR in $CDCl_3$

9. Data of crystal structures for 4e (hide hydrogens)



The purified compound **4e** about 100 mg is dissolved in diethyl ether and placed in a dark cabinet to slowly evaporate. After several days, a colorless bulk crystal is obtained. The X-ray crystal-structure determinations were obtained on a Bruker Smart-1000 CDCC diffractometer (graphite-monochromated Mo Kα radiation, λ=0.71073 nm) at 298(2) K. The crystal structure has been deposited at the Cambridge Crystallographic Data Centre (CCDC 1953896).

The ellipsoid contour probability level in the caption is 50 %.

Table 7. Crystal data and structure refinement for 190914d.

Identification code	190914d
Empirical formula	C8 H16 F N O4 S2
Formula weight	273.34
Temperature	298(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/c
Unit cell dimensions	a = 12.6609(11) A alpha = 90 deg.
	b = 10.4865(9) A beta = 97.188(2) deg.
	c = 9.8417(8) A gamma = 90 deg.

Volume	1296.40(19) A^3
Z, Calculated density	4, 1.400 Mg/m^3
Absorption coefficient	0.422 mm^-1
F(000)	576
Crystal size	0.45 x 0.40 x 0.32 mm
Theta range for data collection	2.53 to 25.02 deg.
Limiting indices	-13<=h<=15, -12<=k<=12, -9<=l<=11
Reflections collected / unique	6247 / 2287 [R(int) = 0.0347]
Completeness to theta = 25.02	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.8768 and 0.8329
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2287 / 24 / 155
Goodness-of-fit on F^2	1.071
Final R indices [I>2sigma(I)]	R1 = 0.0483, wR2 = 0.1216
R indices (all data)	R1 = 0.0774, wR2 = 0.1404
Largest diff. peak and hole	0.427 and -0.199 e.A^-3

Table 8. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 190914d. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
F(1)	2906(3)	3103(3)	4377(3)	108(1)
N(1)	7515(2)	3653(3)	2132(3)	61(1)

O(1)	6238(2)	4237(2)	31(2)	67(1)
O(2)	6197(2)	5530(2)	2045(3)	70(1)
O(3)	2001(2)	4187(4)	2483(3)	105(1)
O(4)	3329(3)	5255(3)	3991(3)	89(1)
S(1)	6408(1)	4326(1)	1481(1)	45(1)
S(2)	2984(1)	4108(1)	3324(1)	65(1)
C(1)	7027(3)	2860(3)	3121(4)	53(1)
C(2)	5878(3)	3028(3)	2397(3)	49(1)
C(3)	5018(3)	3353(3)	3256(3)	52(1)
C(4)	3954(2)	3521(3)	2379(3)	50(1)
C(5)	8608(3)	4148(4)	2305(4)	63(1)
C(6)	9339(5)	3006(7)	2497(9)	116(2)
C(7)	8776(5)	4883(7)	1019(6)	93(2)
C(8)	8742(5)	5054(7)	3521(6)	100(2)
C(6')	9010(30)	3140(40)	1320(50)	116(2)
C(7')	8710(30)	5470(40)	1580(40)	93(2)
C(8')	9240(30)	4000(40)	3720(30)	100(2)

Table 9. Bond lengths [A] and angles [deg] for 190914d.

F(1)-S(2)	1.490(3)
N(1)-C(5)	1.468(4)
N(1)-C(1)	1.474(4)
N(1)-S(1)	1.627(3)
O(1)-S(1)	1.419(2)
O(2)-S(1)	1.418(2)
O(3)-S(2)	1.408(3)

O(4)-S(2)	1.413(3)
S(1)-C(2)	1.808(3)
S(2)-C(4)	1.743(3)
C(1)-C(2)	1.548(4)
C(1)-H(1A)	0.9700
C(1)-H(1B)	0.9700
C(2)-C(3)	1.498(5)
C(2)-H(2)	0.9800
C(3)-C(4)	1.517(4)
C(3)-H(3A)	0.9700
C(3)-H(3B)	0.9700
C(4)-H(4A)	0.9700
C(4)-H(4B)	0.9700
C(5)-C(6)	1.511(7)
C(5)-C(7)	1.519(7)
C(5)-C(8)	1.521(7)
C(5)-C(8')	1.53(3)
C(5)-C(6')	1.56(4)
C(5)-C(7')	1.58(4)
C(6)-H(6A)	0.9600
C(6)-H(6B)	0.9600
C(6)-H(6C)	0.9600
C(7)-H(7A)	0.9600
C(7)-H(7B)	0.9600
C(7)-H(7C)	0.9600
C(8)-H(8A)	0.9600
C(8)-H(8B)	0.9600
C(8)-H(8C)	0.9600

C(6')-H(6'1)	0.9600
C(6')-H(6'2)	0.9600
C(6')-H(6'3)	0.9600
C(7')-H(7'1)	0.9600
C(7')-H(7'2)	0.9600
C(7')-H(7'3)	0.9600
C(8')-H(8'1)	0.9600
C(8')-H(8'2)	0.9600
C(8')-H(8'3)	0.9600
C(5)-N(1)-C(1)	126.2(3)
C(5)-N(1)-S(1)	130.2(3)
C(1)-N(1)-S(1)	95.4(2)
O(2)-S(1)-O(1)	116.09(16)
O(2)-S(1)-N(1)	115.27(17)
O(1)-S(1)-N(1)	112.47(16)
O(2)-S(1)-C(2)	112.08(16)
O(1)-S(1)-C(2)	115.65(15)
N(1)-S(1)-C(2)	80.34(15)
O(3)-S(2)-O(4)	115.0(2)
O(3)-S(2)-F(1)	108.7(2)
O(4)-S(2)-F(1)	108.82(18)
O(3)-S(2)-C(4)	109.68(18)
O(4)-S(2)-C(4)	110.53(18)
F(1)-S(2)-C(4)	103.50(16)
N(1)-C(1)-C(2)	94.5(2)
N(1)-C(1)-H(1A)	112.8
C(2)-C(1)-H(1A)	112.8
N(1)-C(1)-H(1B)	112.8

C(2)-C(1)-H(1B)	112.8
H(1A)-C(1)-H(1B)	110.3
C(3)-C(2)-C(1)	118.3(3)
C(3)-C(2)-S(1)	116.8(2)
C(1)-C(2)-S(1)	85.96(19)
C(3)-C(2)-H(2)	111.2
C(1)-C(2)-H(2)	111.2
S(1)-C(2)-H(2)	111.2
C(2)-C(3)-C(4)	111.2(3)
C(2)-C(3)-H(3A)	109.4
C(4)-C(3)-H(3A)	109.4
C(2)-C(3)-H(3B)	109.4
C(4)-C(3)-H(3B)	109.4
H(3A)-C(3)-H(3B)	108.0
C(3)-C(4)-S(2)	111.9(2)
C(3)-C(4)-H(4A)	109.2
S(2)-C(4)-H(4A)	109.2
C(3)-C(4)-H(4B)	109.2
S(2)-C(4)-H(4B)	109.2
H(4A)-C(4)-H(4B)	107.9
N(1)-C(5)-C(6)	106.8(4)
N(1)-C(5)-C(7)	108.1(3)
C(6)-C(5)-C(7)	111.0(5)
N(1)-C(5)-C(8)	108.8(4)
C(6)-C(5)-C(8)	113.0(5)
C(7)-C(5)-C(8)	109.0(4)
N(1)-C(5)-C(8')	116.5(13)
C(6)-C(5)-C(8')	64.3(17)

C(7)-C(5)-C(8')	134.5(13)
C(8)-C(5)-C(8')	49.3(17)
N(1)-C(5)-C(6')	93.8(14)
C(6)-C(5)-C(6')	45.3(16)
C(7)-C(5)-C(6')	74.9(16)
C(8)-C(5)-C(6')	153.8(15)
C(8')-C(5)-C(6')	109(2)
N(1)-C(5)-C(7')	113.0(15)
C(6)-C(5)-C(7')	132.1(15)
C(7)-C(5)-C(7')	31.3(14)
C(8)-C(5)-C(7')	78.4(15)
C(8')-C(5)-C(7')	116(2)
C(6')-C(5)-C(7')	105(2)
C(5)-C(6)-H(6A)	109.5
C(5)-C(6)-H(6B)	109.5
H(6A)-C(6)-H(6B)	109.5
C(5)-C(6)-H(6C)	109.5
H(6A)-C(6)-H(6C)	109.5
H(6B)-C(6)-H(6C)	109.5
C(5)-C(7)-H(7A)	109.5
C(5)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	109.5
C(5)-C(7)-H(7C)	109.5
H(7A)-C(7)-H(7C)	109.5
H(7B)-C(7)-H(7C)	109.5
C(5)-C(8)-H(8A)	109.5
C(5)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5

C(5)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
C(5)-C(6')-H(6'1)	109.5
C(5)-C(6')-H(6'2)	109.5
H(6'1)-C(6')-H(6'2)	109.5
C(5)-C(6')-H(6'3)	109.5
H(6'1)-C(6')-H(6'3)	109.5
H(6'2)-C(6')-H(6'3)	109.5
C(5)-C(7')-H(7'1)	109.5
C(5)-C(7')-H(7'2)	109.5
H(7'1)-C(7')-H(7'2)	109.5
C(5)-C(7')-H(7'3)	109.5
H(7'1)-C(7')-H(7'3)	109.5
H(7'2)-C(7')-H(7'3)	109.5
C(5)-C(8')-H(8'1)	109.5
C(5)-C(8')-H(8'2)	109.5
H(8'1)-C(8')-H(8'2)	109.5
C(5)-C(8')-H(8'3)	109.5
H(8'1)-C(8')-H(8'3)	109.5
H(8'2)-C(8')-H(8'3)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 10. Anisotropic displacement parameters (A^2 x 10^3) for 190914d.

The anisotropic displacement factor exponent takes the form:

-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
F(1)	140(3)	90(2)	106(2)	26(2)	60(2)	6(2)
N(1)	41(2)	73(2)	69(2)	23(2)	5(1)	1(1)
O(1)	72(2)	81(2)	48(1)	3(1)	5(1)	-7(1)
O(2)	72(2)	47(1)	92(2)	-7(1)	13(2)	1(1)
O(3)	51(2)	160(3)	102(2)	-4(2)	3(2)	12(2)
O(4)	105(2)	62(2)	102(2)	-17(2)	24(2)	0(2)
S(1)	44(1)	43(1)	46(1)	3(1)	5(1)	1(1)
S(2)	59(1)	70(1)	67(1)	-2(1)	13(1)	-2(1)
C(1)	48(2)	53(2)	57(2)	12(2)	4(2)	7(2)
C(2)	54(2)	40(2)	51(2)	4(1)	4(2)	0(2)
C(3)	49(2)	59(2)	47(2)	6(2)	5(2)	-3(2)
C(4)	48(2)	53(2)	48(2)	7(2)	3(2)	-6(2)
C(5)	41(2)	79(3)	67(2)	2(2)	5(2)	-9(2)
C(6)	51(3)	131(5)	167(7)	20(5)	15(4)	19(3)
C(7)	74(3)	124(5)	85(4)	7(3)	25(3)	-29(4)
C(8)	84(4)	130(5)	84(4)	-14(4)	-1(3)	-45(4)
C(6')	51(3)	131(5)	167(7)	20(5)	15(4)	19(3)
C(7')	74(3)	124(5)	85(4)	7(3)	25(3)	-29(4)
C(8')	84(4)	130(5)	84(4)	-14(4)	-1(3)	-45(4)

Table 11. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for 190914d.

	x	y	z	U(eq)

H(1A)	7124	3210	4041	64
H(1B)	7266	1981	3133	64
H(2)	5669	2309	1786	59
H(3A)	5204	4135	3756	62
H(3B)	4962	2679	3917	62
H(4A)	3723	2706	1981	60
H(4B)	4037	4105	1636	60
H(6A)	10066	3289	2625	175
H(6B)	9224	2471	1701	175
H(6C)	9192	2533	3287	175
H(7A)	8259	5555	872	140
H(7B)	8697	4317	247	140
H(7C)	9479	5244	1126	140
H(8A)	8615	4602	4334	150
H(8B)	8242	5742	3360	150
H(8C)	9453	5390	3637	150
H(6'1)	9776	3153	1417	175
H(6'2)	8733	3333	395	175
H(6'3)	8775	2305	1557	175
H(7'1)	8489	6144	2141	140
H(7'2)	8273	5477	708	140
H(7'3)	9441	5611	1436	140
H(8'1)	8819	4318	4401	150
H(8'2)	9886	4482	3765	150
H(8'3)	9399	3120	3895	150

Table 12. Torsion angles [deg] for 190914d.

C(5)-N(1)-S(1)-O(2)	-53.1(4)
C(1)-N(1)-S(1)-O(2)	95.7(2)
C(5)-N(1)-S(1)-O(1)	83.1(4)
C(1)-N(1)-S(1)-O(1)	-128.1(2)
C(5)-N(1)-S(1)-C(2)	-163.0(4)
C(1)-N(1)-S(1)-C(2)	-14.2(2)
C(5)-N(1)-C(1)-C(2)	167.2(3)
S(1)-N(1)-C(1)-C(2)	16.5(2)
N(1)-C(1)-C(2)-C(3)	-133.1(3)
N(1)-C(1)-C(2)-S(1)	-14.8(2)
O(2)-S(1)-C(2)-C(3)	19.8(3)
O(1)-S(1)-C(2)-C(3)	-116.4(3)
N(1)-S(1)-C(2)-C(3)	133.3(3)
O(2)-S(1)-C(2)-C(1)	-100.0(2)
O(1)-S(1)-C(2)-C(1)	123.9(2)
N(1)-S(1)-C(2)-C(1)	13.5(2)
C(1)-C(2)-C(3)-C(4)	178.3(3)
S(1)-C(2)-C(3)-C(4)	77.8(3)
C(2)-C(3)-C(4)-S(2)	-171.9(2)
O(3)-S(2)-C(4)-C(3)	-177.1(3)
O(4)-S(2)-C(4)-C(3)	55.1(3)
F(1)-S(2)-C(4)-C(3)	-61.3(3)
C(1)-N(1)-C(5)-C(6)	58.9(6)
S(1)-N(1)-C(5)-C(6)	-160.8(4)
C(1)-N(1)-C(5)-C(7)	178.4(4)
S(1)-N(1)-C(5)-C(7)	-41.3(5)

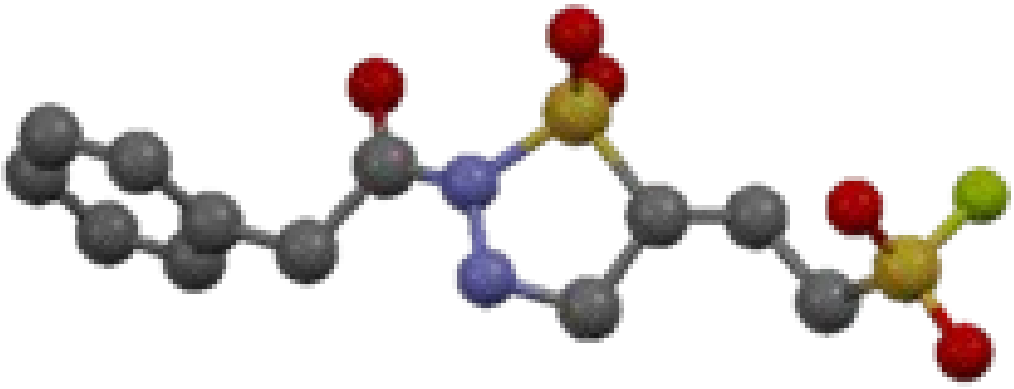
C(1)-N(1)-C(5)-C(8)	-63.4(5)
S(1)-N(1)-C(5)-C(8)	77.0(5)
C(1)-N(1)-C(5)-C(8')	-10(2)
S(1)-N(1)-C(5)-C(8')	130(2)
C(1)-N(1)-C(5)-C(6')	103.1(17)
S(1)-N(1)-C(5)-C(6')	-116.6(17)
C(1)-N(1)-C(5)-C(7')	-148.5(17)
S(1)-N(1)-C(5)-C(7')	-8.1(17)

Symmetry transformations used to generate equivalent atoms:

Table 13. Hydrogen bonds for 190914d [A and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)

10. Data of crystal structures for 8f (hide hydrogens)



The purified compound **8f** about 100 mg is dissolved in diethyl ether and placed in a dark cabinet to slowly evaporate. After several days, a colorless bulk crystal is obtained. The X-ray crystal-structure determinations were obtained on a Bruker Smart-1000 CDCC diffractometer (graphite-monochromated Mo Kα radiation, λ=0.71073 nm) at 298(2) K. The crystal structure has been deposited at the Cambridge Crystallographic Data Centre (CCDC 1951376).

The ellipsoid contour probability level in the caption is 50 %.

Table 14. Crystal data and structure refinement for 190831a.

Identification code	190831a
Empirical formula	C12 H15 F N2 O5 S2
Formula weight	350.38
Temperature	298(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/c
Unit cell dimensions	a = 14.0641(12) A alpha = 90 deg.
	b = 9.2583(8) A beta = 102.973(3) deg.
	c = 12.1126(11) A gamma = 90 deg.
Volume	1536.9(2) A^3

Z, Calculated density	4, 1.514 Mg/m^3
Absorption coefficient	0.381 mm^-1
F(000)	728
Crystal size	0.48 x 0.40 x 0.11 mm
Theta range for data collection	2.65 to 25.02 deg.
Limiting indices	-16<=h<=16, -11<=k<=10, -14<=l<=13
Reflections collected / unique	7407 / 2694 [R(int) = 0.0511]
Completeness to theta = 25.02	99.4 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9593 and 0.8382
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2694 / 0 / 199
Goodness-of-fit on F^2	1.095
Final R indices [I>2sigma(I)]	R1 = 0.0561, wR2 = 0.1493
R indices (all data)	R1 = 0.0954, wR2 = 0.1842
Largest diff. peak and hole	0.488 and -0.426 e.A^-3

Table 15. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 190831a. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
F(1)	1199(2)	7361(4)	4309(3)	110(1)
N(1)	5793(2)	6596(3)	3582(3)	43(1)
N(2)	5926(2)	7442(4)	4581(3)	47(1)

O(1)	6289(2)	5941(3)	2024(3)	50(1)
O(2)	4245(2)	6345(3)	2005(2)	56(1)
O(3)	4579(2)	4516(3)	3476(3)	59(1)
O(4)	1824(3)	8647(5)	6008(4)	109(2)
O(5)	2565(3)	6377(4)	5596(4)	101(1)
S(1)	4633(1)	5986(1)	3149(1)	37(1)
S(2)	2121(1)	7720(2)	5236(1)	71(1)
C(1)	6449(3)	6619(4)	2893(3)	41(1)
C(2)	7361(3)	7508(5)	3335(4)	57(1)
C(3)	8096(3)	7354(5)	2631(4)	50(1)
C(4)	8693(4)	6158(6)	2715(5)	74(2)
C(5)	9370(4)	6047(9)	2040(7)	101(2)
C(6)	9439(5)	7124(12)	1292(7)	112(3)
C(7)	8868(5)	8296(9)	1216(6)	102(2)
C(8)	8201(4)	8425(6)	1872(5)	73(1)
C(9)	5010(3)	8196(4)	4521(4)	45(1)
C(10)	4180(3)	7122(4)	4135(4)	46(1)
C(11)	3200(3)	7727(5)	3603(4)	54(1)
C(12)	2787(3)	8651(5)	4430(4)	53(1)

Table 16. Bond lengths [A] and angles [deg] for 190831a.

F(1)-S(2)	1.549(4)
N(1)-C(1)	1.376(5)
N(1)-N(2)	1.418(4)
N(1)-S(1)	1.695(3)
N(2)-C(9)	1.453(5)

N(2)-H(2)	0.9000
O(1)-C(1)	1.203(4)
O(2)-S(1)	1.410(3)
O(3)-S(1)	1.424(3)
O(4)-S(2)	1.401(4)
O(5)-S(2)	1.416(4)
S(1)-C(10)	1.811(4)
S(2)-C(12)	1.728(4)
C(1)-C(2)	1.517(6)
C(2)-C(3)	1.488(6)
C(2)-H(2C)	0.9700
C(2)-H(2D)	0.9700
C(3)-C(4)	1.379(6)
C(3)-C(8)	1.383(7)
C(4)-C(5)	1.391(9)
C(4)-H(4)	0.9300
C(5)-C(6)	1.365(10)
C(5)-H(5)	0.9300
C(6)-C(7)	1.341(11)
C(6)-H(6)	0.9300
C(7)-C(8)	1.363(8)
C(7)-H(7)	0.9300
C(8)-H(8)	0.9300
C(9)-C(10)	1.525(5)
C(9)-H(9A)	0.9700
C(9)-H(9B)	0.9700
C(10)-C(11)	1.493(6)
C(10)-H(10)	0.9800

C(11)-C(12)	1.527(6)
C(11)-H(11A)	0.9700
C(11)-H(11B)	0.9700
C(12)-H(12A)	0.9700
C(12)-H(12B)	0.9700
C(1)-N(1)-N(2)	122.1(3)
C(1)-N(1)-S(1)	123.2(3)
N(2)-N(1)-S(1)	112.4(2)
N(1)-N(2)-C(9)	106.1(3)
N(1)-N(2)-H(2)	110.1
C(9)-N(2)-H(2)	110.1
O(2)-S(1)-O(3)	117.75(19)
O(2)-S(1)-N(1)	111.04(16)
O(3)-S(1)-N(1)	109.86(18)
O(2)-S(1)-C(10)	113.26(19)
O(3)-S(1)-C(10)	108.86(19)
N(1)-S(1)-C(10)	93.39(17)
O(4)-S(2)-O(5)	120.6(3)
O(4)-S(2)-F(1)	106.8(2)
O(5)-S(2)-F(1)	105.9(3)
O(4)-S(2)-C(12)	110.7(2)
O(5)-S(2)-C(12)	110.7(2)
F(1)-S(2)-C(12)	99.8(2)
O(1)-C(1)-N(1)	120.2(3)
O(1)-C(1)-C(2)	124.7(4)
N(1)-C(1)-C(2)	115.0(3)
C(3)-C(2)-C(1)	112.7(4)
C(3)-C(2)-H(2C)	109.0

C(1)-C(2)-H(2C)	109.0
C(3)-C(2)-H(2D)	109.0
C(1)-C(2)-H(2D)	109.0
H(2C)-C(2)-H(2D)	107.8
C(4)-C(3)-C(8)	118.1(5)
C(4)-C(3)-C(2)	121.6(4)
C(8)-C(3)-C(2)	120.3(4)
C(3)-C(4)-C(5)	120.1(6)
C(3)-C(4)-H(4)	120.0
C(5)-C(4)-H(4)	120.0
C(6)-C(5)-C(4)	119.8(6)
C(6)-C(5)-H(5)	120.1
C(4)-C(5)-H(5)	120.1
C(7)-C(6)-C(5)	120.4(6)
C(7)-C(6)-H(6)	119.8
C(5)-C(6)-H(6)	119.8
C(6)-C(7)-C(8)	120.7(7)
C(6)-C(7)-H(7)	119.6
C(8)-C(7)-H(7)	119.6
C(7)-C(8)-C(3)	121.0(6)
C(7)-C(8)-H(8)	119.5
C(3)-C(8)-H(8)	119.5
N(2)-C(9)-C(10)	108.1(3)
N(2)-C(9)-H(9A)	110.1
C(10)-C(9)-H(9A)	110.1
N(2)-C(9)-H(9B)	110.1
C(10)-C(9)-H(9B)	110.1
H(9A)-C(9)-H(9B)	108.4

C(11)-C(10)-C(9)	117.2(3)
C(11)-C(10)-S(1)	111.1(3)
C(9)-C(10)-S(1)	102.9(3)
C(11)-C(10)-H(10)	108.4
C(9)-C(10)-H(10)	108.4
S(1)-C(10)-H(10)	108.4
C(10)-C(11)-C(12)	112.1(4)
C(10)-C(11)-H(11A)	109.2
C(12)-C(11)-H(11A)	109.2
C(10)-C(11)-H(11B)	109.2
C(12)-C(11)-H(11B)	109.2
H(11A)-C(11)-H(11B)	107.9
C(11)-C(12)-S(2)	115.2(3)
C(11)-C(12)-H(12A)	108.5
S(2)-C(12)-H(12A)	108.5
C(11)-C(12)-H(12B)	108.5
S(2)-C(12)-H(12B)	108.5
H(12A)-C(12)-H(12B)	107.5

Symmetry transformations used to generate equivalent atoms:

Table 17. Anisotropic displacement parameters (A^2 x 10^3) for 190831a.

The anisotropic displacement factor exponent takes the form:

-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
F(1)	62(2)	171(4)	95(3)	-21(2)	10(2)	-32(2)

N(1)	43(2)	50(2)	36(2)	-12(2)	12(1)	-6(1)
N(2)	50(2)	64(2)	27(2)	-6(2)	11(2)	-4(2)
O(1)	49(2)	56(2)	47(2)	-17(2)	16(1)	-4(1)
O(2)	52(2)	77(2)	36(2)	3(2)	6(1)	-2(1)
O(3)	75(2)	37(2)	64(2)	2(1)	19(2)	-9(1)
O(4)	84(3)	175(4)	84(3)	-28(3)	55(2)	-5(3)
O(5)	122(3)	91(3)	97(3)	30(2)	38(3)	-22(3)
S(1)	45(1)	34(1)	35(1)	-4(1)	12(1)	-3(1)
S(2)	60(1)	103(1)	55(1)	-3(1)	23(1)	-16(1)
C(1)	45(2)	41(2)	37(2)	-2(2)	11(2)	1(2)
C(2)	51(3)	70(3)	52(3)	-19(2)	15(2)	-14(2)
C(3)	38(2)	65(3)	45(3)	-8(2)	8(2)	-7(2)
C(4)	60(3)	84(4)	74(4)	-1(3)	6(3)	7(3)
C(5)	51(3)	144(6)	107(6)	-40(5)	16(3)	19(3)
C(6)	63(4)	201(9)	83(5)	-43(6)	38(4)	-32(5)
C(7)	87(4)	152(6)	77(5)	-5(4)	39(4)	-43(5)
C(8)	65(3)	83(3)	73(4)	3(3)	18(3)	-10(3)
C(9)	54(2)	42(2)	41(2)	-12(2)	15(2)	-3(2)
C(10)	54(2)	46(2)	38(2)	-7(2)	9(2)	3(2)
C(11)	57(3)	61(3)	44(3)	-8(2)	14(2)	-2(2)
C(12)	50(2)	56(2)	56(3)	-3(2)	20(2)	7(2)

Table 18. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for 190831a.

	x	y	z	U(eq)

H(2)	6060	6869	5196	56
H(2C)	7180	8517	3355	68
H(2D)	7652	7210	4105	68
H(4)	8643	5424	3224	89
H(5)	9774	5242	2097	121
H(6)	9885	7045	833	135
H(7)	8927	9028	710	123
H(8)	7812	9246	1808	88
H(9A)	4948	8991	3989	54
H(9B)	4988	8583	5259	54
H(10)	4118	6533	4787	55
H(11A)	2753	6939	3334	64
H(11B)	3252	8310	2954	64
H(12A)	2373	9391	4003	63
H(12B)	3325	9135	4937	63

Table 19. Torsion angles [deg] for 190831a.

C(1)-N(1)-N(2)-C(9)	130.0(4)
S(1)-N(1)-N(2)-C(9)	-33.3(4)
C(1)-N(1)-S(1)-O(2)	-36.1(4)
N(2)-N(1)-S(1)-O(2)	127.0(3)
C(1)-N(1)-S(1)-O(3)	96.0(3)
N(2)-N(1)-S(1)-O(3)	-101.0(3)
C(1)-N(1)-S(1)-C(10)	-152.6(3)
N(2)-N(1)-S(1)-C(10)	10.5(3)
N(2)-N(1)-C(1)-O(1)	-176.4(4)

S(1)-N(1)-C(1)-O(1)	-15.0(5)
N(2)-N(1)-C(1)-C(2)	5.1(5)
S(1)-N(1)-C(1)-C(2)	166.6(3)
O(1)-C(1)-C(2)-C(3)	-5.3(6)
N(1)-C(1)-C(2)-C(3)	173.1(4)
C(1)-C(2)-C(3)-C(4)	-78.2(6)
C(1)-C(2)-C(3)-C(8)	102.1(5)
C(8)-C(3)-C(4)-C(5)	-0.6(8)
C(2)-C(3)-C(4)-C(5)	179.7(5)
C(3)-C(4)-C(5)-C(6)	-0.2(9)
C(4)-C(5)-C(6)-C(7)	0.9(11)
C(5)-C(6)-C(7)-C(8)	-0.8(11)
C(6)-C(7)-C(8)-C(3)	-0.1(10)
C(4)-C(3)-C(8)-C(7)	0.7(8)
C(2)-C(3)-C(8)-C(7)	-179.6(5)
N(1)-N(2)-C(9)-C(10)	44.3(4)
N(2)-C(9)-C(10)-C(11)	-157.7(4)
N(2)-C(9)-C(10)-S(1)	-35.4(4)
O(2)-S(1)-C(10)-C(11)	25.9(4)
O(3)-S(1)-C(10)-C(11)	-107.2(3)
N(1)-S(1)-C(10)-C(11)	140.5(3)
O(2)-S(1)-C(10)-C(9)	-100.3(3)
O(3)-S(1)-C(10)-C(9)	126.6(3)
N(1)-S(1)-C(10)-C(9)	14.3(3)
C(9)-C(10)-C(11)-C(12)	-64.0(5)
S(1)-C(10)-C(11)-C(12)	178.2(3)
C(10)-C(11)-C(12)-S(2)	-88.2(4)
O(4)-S(2)-C(12)-C(11)	176.6(3)

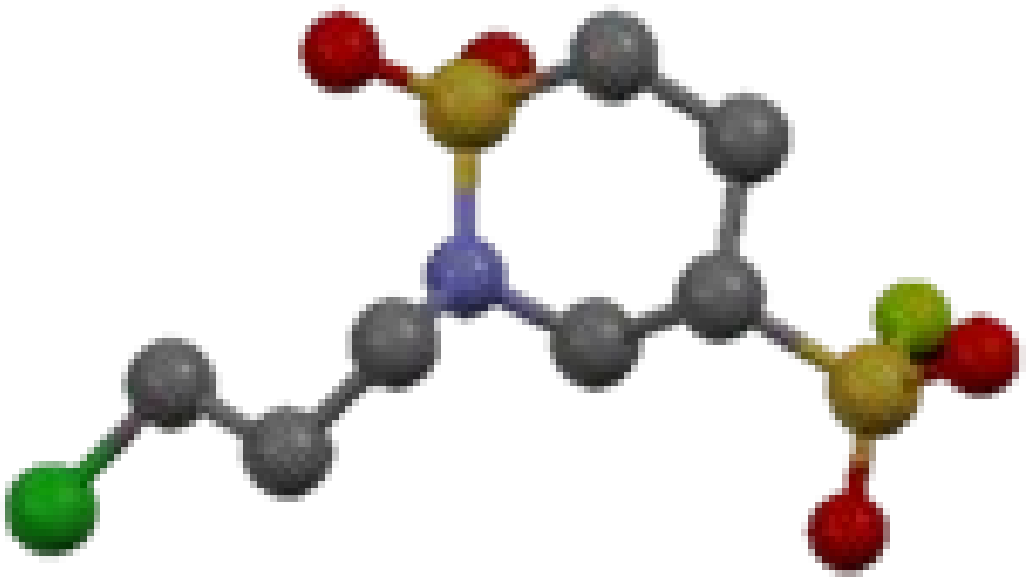
O(5)-S(2)-C(12)-C(11)	40.1(4)
F(1)-S(2)-C(12)-C(11)	-71.2(4)

Symmetry transformations used to generate equivalent atoms:

Table 20. Hydrogen bonds for 190831a [A and deg.].

D-H	d(D-H)	d(H..A)	<DHA	d(D..A)	A
N2-H2	0.900	2.384	146.57	3.174	O3 [-x+1, -y+1, -z+1]

11. Data of crystal structures for 14 ((hide hydrogens)



The purified compound **14** about 100 mg is dissolved in diethyl ether and placed in a dark cabinet to slowly evaporate. After several days, a colorless bulk crystal is obtained. The X-ray crystal-structure determinations were obtained on a Bruker Smart-1000 CDCC diffractometer (graphite-monochromated Mo Kα radiation, λ=0.71073 nm) at 298(2) K. The crystal structure has been deposited at the Cambridge Crystallographic Data Centre (CCDC 1940975).

The ellipsoid contour probability level in the caption is 50 %.

Table 21. Crystal data and structure refinement for 190612f.

Identification code	190612f
Empirical formula	C7 H13 Cl F N O4 S2
Formula weight	293.75
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/c
Unit cell dimensions	a = 14.829(12) A alpha = 90 deg.
	b = 5.526(5) A beta = 127.47(4) deg.

	c = 18.143(11) A gamma = 90 deg.
Volume	1180.0(16) A^3
Z, Calculated density	4, 1.654 Mg/m^3
Absorption coefficient	0.689 mm^-1
F(000)	608
Crystal size	0.23 x 0.11 x 0.04 mm
Theta range for data collection	2.25 to 25.02 deg.
Limiting indices	-17<=h<=14, -6<=k<=6, 0<=l<=21
Reflections collected / unique	2082 / 2082 [R(int) = 0.0000]
Completeness to theta = 25.02	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9730 and 0.8577
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2082 / 0 / 146
Goodness-of-fit on F^2	1.089
Final R indices [I>2sigma(I)]	R1 = 0.0779, wR2 = 0.1805
R indices (all data)	R1 = 0.1001, wR2 = 0.1930
Largest diff. peak and hole	0.737 and -0.476 e.A^-3

Table 22. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 190612f. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Cl(1)	1403(2)	6549(4)	1196(2)	88(1)
F(1)	5556(4)	3662(12)	6892(4)	125(2)

N(1)	2380(4)	4236(9)	4004(3)	47(1)
O(1)	2158(4)	7439(7)	4799(3)	67(1)
O(2)	486(4)	5288(9)	3548(4)	74(2)
O(3)	5285(6)	-464(15)	6862(5)	129(3)
O(4)	5796(5)	1317(12)	5958(4)	96(2)
S(1)	1646(2)	5249(2)	4330(1)	51(1)
S(2)	5191(2)	1457(4)	6318(1)	69(1)
C(1)	1881(6)	3128(12)	5139(5)	57(2)
C(2)	3170(6)	2753(14)	5889(5)	62(2)
C(3)	3737(5)	2045(11)	5454(4)	50(2)
C(4)	3582(5)	3908(12)	4763(4)	50(2)
C(5)	1862(6)	2425(11)	3257(4)	53(2)
C(6)	1941(6)	3236(11)	2500(5)	57(2)
C(7)	1250(8)	5446(13)	2027(6)	74(2)

Table 23. Bond lengths [A] and angles [deg] for 190612f.

Cl(1)-C(7)	1.764(7)
F(1)-S(2)	1.476(6)
N(1)-C(4)	1.455(8)
N(1)-C(5)	1.470(8)
N(1)-S(1)	1.622(5)
O(1)-S(1)	1.407(5)
O(2)-S(1)	1.414(5)
O(3)-S(2)	1.398(6)
O(4)-S(2)	1.396(6)
S(1)-C(1)	1.740(6)
S(2)-C(3)	1.761(7)

C(1)-C(2)	1.544(9)
C(1)-H(1A)	0.9700
C(1)-H(1B)	0.9700
C(2)-C(3)	1.513(9)
C(2)-H(2A)	0.9700
C(2)-H(2B)	0.9700
C(3)-C(4)	1.527(8)
C(3)-H(3)	0.9800
C(4)-H(4A)	0.9700
C(4)-H(4B)	0.9700
C(5)-C(6)	1.516(9)
C(5)-H(5A)	0.9700
C(5)-H(5B)	0.9700
C(6)-C(7)	1.486(9)
C(6)-H(6A)	0.9700
C(6)-H(6B)	0.9700
C(7)-H(7A)	0.9700
C(7)-H(7B)	0.9700
C(4)-N(1)-C(5)	116.1(5)
C(4)-N(1)-S(1)	113.9(4)
C(5)-N(1)-S(1)	118.7(4)
O(1)-S(1)-O(2)	118.3(3)
O(1)-S(1)-N(1)	106.4(3)
O(2)-S(1)-N(1)	108.5(3)
O(1)-S(1)-C(1)	108.1(3)
O(2)-S(1)-C(1)	110.7(3)
N(1)-S(1)-C(1)	103.9(3)
O(4)-S(2)-O(3)	118.2(5)

O(4)-S(2)-F(1)	108.2(4)
O(3)-S(2)-F(1)	107.0(5)
O(4)-S(2)-C(3)	112.4(4)
O(3)-S(2)-C(3)	108.1(4)
F(1)-S(2)-C(3)	101.6(3)
C(2)-C(1)-S(1)	109.8(4)
C(2)-C(1)-H(1A)	109.7
S(1)-C(1)-H(1A)	109.7
C(2)-C(1)-H(1B)	109.7
S(1)-C(1)-H(1B)	109.7
H(1A)-C(1)-H(1B)	108.2
C(3)-C(2)-C(1)	111.0(5)
C(3)-C(2)-H(2A)	109.4
C(1)-C(2)-H(2A)	109.4
C(3)-C(2)-H(2B)	109.4
C(1)-C(2)-H(2B)	109.4
H(2A)-C(2)-H(2B)	108.0
C(2)-C(3)-C(4)	113.5(5)
C(2)-C(3)-S(2)	110.6(4)
C(4)-C(3)-S(2)	110.3(4)
C(2)-C(3)-H(3)	107.4
C(4)-C(3)-H(3)	107.4
S(2)-C(3)-H(3)	107.4
N(1)-C(4)-C(3)	110.3(5)
N(1)-C(4)-H(4A)	109.6
C(3)-C(4)-H(4A)	109.6
N(1)-C(4)-H(4B)	109.6
C(3)-C(4)-H(4B)	109.6

H(4A)-C(4)-H(4B)	108.1
N(1)-C(5)-C(6)	110.4(5)
N(1)-C(5)-H(5A)	109.6
C(6)-C(5)-H(5A)	109.6
N(1)-C(5)-H(5B)	109.6
C(6)-C(5)-H(5B)	109.6
H(5A)-C(5)-H(5B)	108.1
C(7)-C(6)-C(5)	111.1(5)
C(7)-C(6)-H(6A)	109.4
C(5)-C(6)-H(6A)	109.4
C(7)-C(6)-H(6B)	109.4
C(5)-C(6)-H(6B)	109.4
H(6A)-C(6)-H(6B)	108.0
C(6)-C(7)-Cl(1)	112.1(5)
C(6)-C(7)-H(7A)	109.2
Cl(1)-C(7)-H(7A)	109.2
C(6)-C(7)-H(7B)	109.2
Cl(1)-C(7)-H(7B)	109.2
H(7A)-C(7)-H(7B)	107.9

Symmetry transformations used to generate equivalent atoms:

Table 24. Anisotropic displacement parameters (A^2 x 10^3) for 190612f.

The anisotropic displacement factor exponent takes the form:

-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Cl(1)	127(2)	85(1)	83(2)	17(1)	79(2)	18(1)
F(1)	60(3)	165(5)	101(4)	-50(4)	24(3)	-10(3)
N(1)	41(3)	50(3)	51(3)	-2(3)	28(3)	-3(3)
O(1)	80(3)	41(2)	93(4)	-10(2)	61(3)	-9(2)
O(2)	54(3)	83(3)	79(4)	20(3)	39(3)	21(3)
O(3)	71(5)	158(6)	112(5)	85(5)	32(4)	15(4)
O(4)	66(4)	127(5)	89(4)	24(4)	45(3)	27(4)
S(1)	52(1)	44(1)	64(1)	3(1)	37(1)	3(1)
S(2)	49(1)	80(1)	64(1)	13(1)	27(1)	5(1)
C(1)	56(4)	59(4)	64(4)	7(3)	42(4)	-1(3)
C(2)	62(5)	73(5)	53(4)	2(4)	36(4)	-9(4)
C(3)	46(4)	47(3)	45(3)	3(3)	21(3)	-6(3)
C(4)	46(4)	54(4)	51(4)	-1(3)	30(3)	1(3)
C(5)	52(4)	52(3)	52(4)	-6(3)	30(3)	-6(3)
C(6)	52(4)	64(4)	54(4)	-10(3)	33(3)	-2(3)
C(7)	89(6)	74(4)	78(5)	16(4)	60(5)	20(5)

Table 25. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for 190612f.

	x	y	z	U(eq)
H(1A)	1543	3687	5428	68
H(1B)	1527	1604	4830	68
H(2A)	3508	4237	6240	75
H(2B)	3296	1496	6315	75
H(3)	3385	534	5112	60
H(4A)	3910	5440	5077	60
H(4B)	3974	3368	4518	60
H(5A)	1070	2200	2997	64
H(5B)	2248	887	3508	64
H(6A)	2729	3566	2770	68
H(6B)	1676	1947	2049	68
H(7A)	1480	6694	2486	88
H(7B)	456	5080	1723	88

Table 26. Torsion angles [deg] for 190612f.

C(4)-N(1)-S(1)-O(1)	56.8(5)
C(5)-N(1)-S(1)-O(1)	-160.8(4)
C(4)-N(1)-S(1)-O(2)	-175.0(4)
C(5)-N(1)-S(1)-O(2)	-32.6(5)
C(4)-N(1)-S(1)-C(1)	-57.2(5)
C(5)-N(1)-S(1)-C(1)	85.2(5)
O(1)-S(1)-C(1)-C(2)	-60.0(5)
O(2)-S(1)-C(1)-C(2)	169.0(5)
N(1)-S(1)-C(1)-C(2)	52.7(6)
S(1)-C(1)-C(2)-C(3)	-55.5(7)
C(1)-C(2)-C(3)-C(4)	58.8(7)
C(1)-C(2)-C(3)-S(2)	-176.7(5)
O(4)-S(2)-C(3)-C(2)	-166.9(5)
O(3)-S(2)-C(3)-C(2)	60.9(6)
F(1)-S(2)-C(3)-C(2)	-51.5(6)
O(4)-S(2)-C(3)-C(4)	-40.5(6)
O(3)-S(2)-C(3)-C(4)	-172.7(5)
F(1)-S(2)-C(3)-C(4)	74.9(5)
C(5)-N(1)-C(4)-C(3)	-81.7(6)
S(1)-N(1)-C(4)-C(3)	61.7(6)
C(2)-C(3)-C(4)-N(1)	-60.3(7)
S(2)-C(3)-C(4)-N(1)	175.0(4)
C(4)-N(1)-C(5)-C(6)	-91.0(6)
S(1)-N(1)-C(5)-C(6)	127.4(5)
N(1)-C(5)-C(6)-C(7)	-65.6(7)
C(5)-C(6)-C(7)-Cl(1)	176.0(5)

Symmetry transformations used to generate equivalent atoms:

Table 27. Hydrogen bonds for 190612f [A and deg.].

D-H...A	(D-H)	d(H...A)	d(D...A)	<(DHA)

12. Reference

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