Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information for:

Visible-light-driven selective difluoroalkylation of α-CF_3 alkenes to access CF_2-containing *gem*-difluoroalkenes and trifluoromethylalkanes

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1. General Information

Flash column chromatography was performed using silica gel from Qingdao Haiyang. Anhydrous solvents [tetrahydrofuran (THF), 2-methyltetrahydrofuran (2-MeTHF), *N,N*-dimethylformamide (DMF), benzotrifluoride ($PhCF_3$), ethyl acetate (EtOAc), acetonitrile (CH_3CN), methanol (CH_3OH), dichloromethane (DCM), methylsulfoxide (DMSO), and 1,4-dioxane] were purchased from Adamas, Energy Chemicals, or Innochem, and used as received. All commercial reagents were purchased from Bidepharm, Energy Chemical, Aladdin, and Adamas of the highest purity grade. Photosensitizers were purchased from laajoo, Adamas, Alfa, or Aldrich, and used as received.

General Analytical Information

All new compounds were characterized by NMR spectroscopy, high-resolution mass spectroscopy, and melting point (if solids). NMR spectra were recorded on a Bruker Ascend^{TM} 400 spectrometer and were calibrated using TMS or residual deuterated solvent as an internal reference (Chloroform-*d*: 7.26 ppm for ^{1}H NMR and 77.16 ppm for ^{13}C NMR, DMSO-d_6: 2.50 ppm for ^{1}H NMR and 39.52 ppm for ^{13}C NMR). Data were reported as follows: chemical shift, multiplicity (s, singlet; d, doublet; t, triplet; q, quartet; m, multiplet), coupling constants (hertz), and integration. HRMS spectra were recorded on a Waters Acquity UPLC/Xevo TQD MSMS. Melting points (Mp) were recorded on a MP450 melting point apparatus.

Experimental Set-up

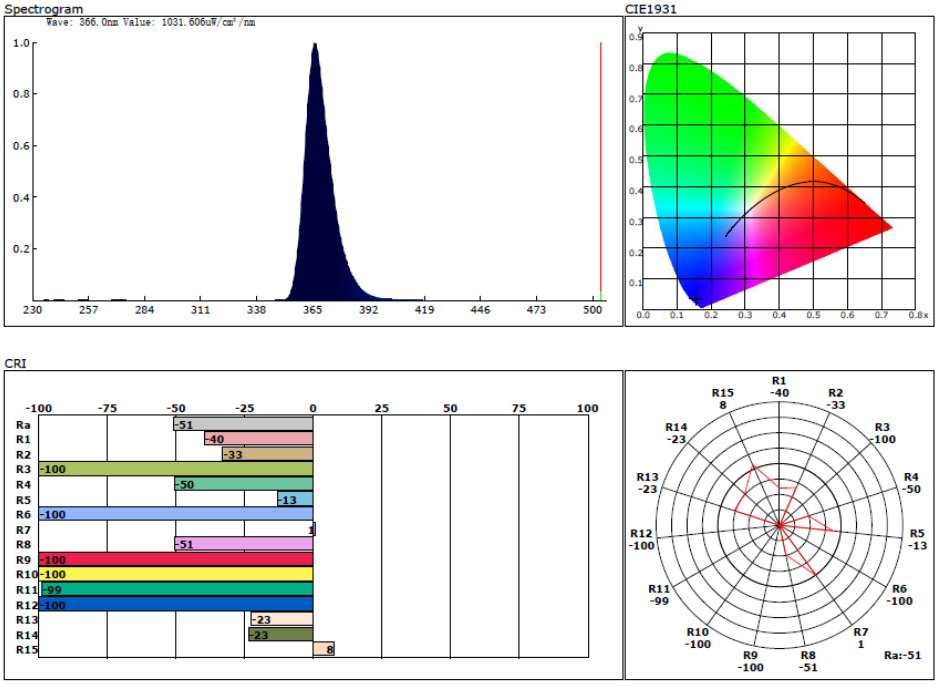


Figure S1. The emission spectra and spectral distribution of the purple LEDs

The Material of the Irradiation Vessel
Manufacturer: GeAo Chemical
Model: 24 W, purple LEDs
Broadband source: λ = 365-375 nm (λ_{max} = 366.0 nm)
Material of the irradiation vessel: borosilicate reaction tube
Distance from the light source to the irradiation vessel: 3.0 cm
Not use any filters

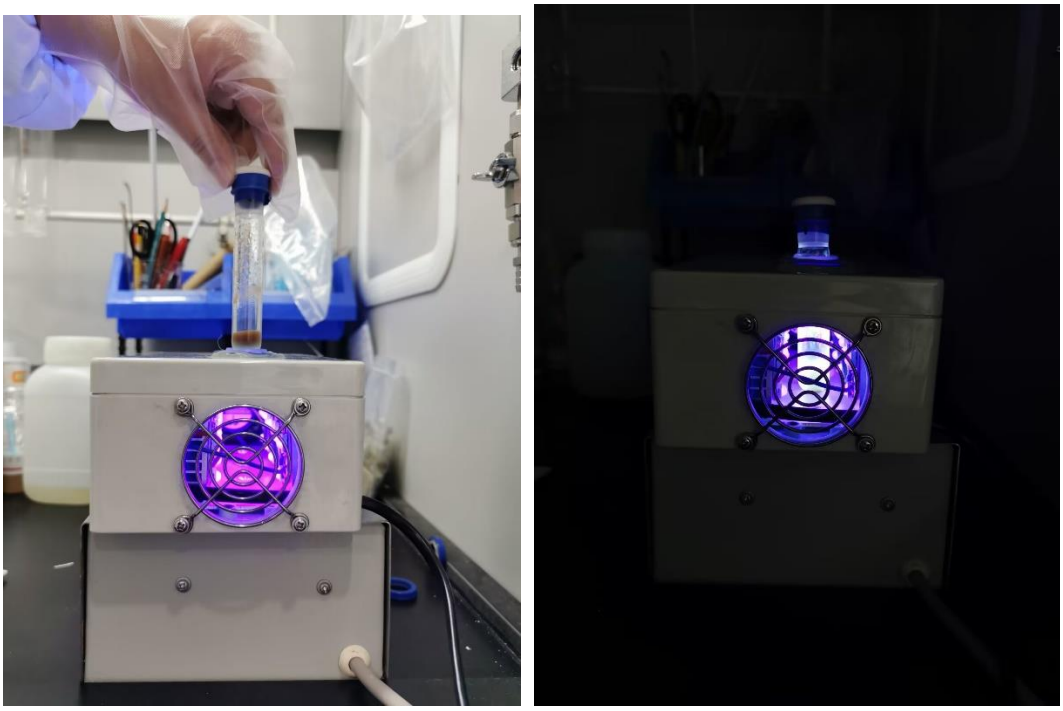
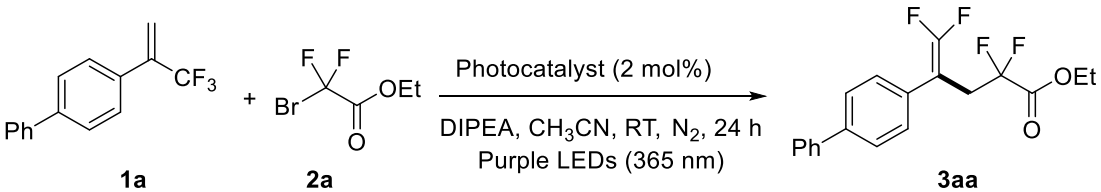


Figure S2. The set-up for the reaction

2. Reaction Optimization

Table S1. Effect of photocatalysts on this reaction[a]



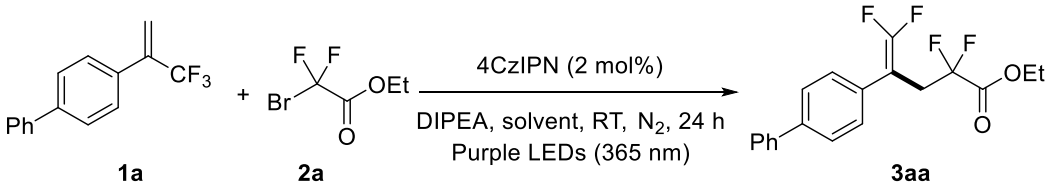
1a **2a** **3aa**

Entry	Photocatalyst	Yield (%)[b]
1	*fac*-Ir(ppy)$_3$	31
2	[Ir(dFppy)$_2$(dtbbpy)]PF$_6$	47
3	[Ir(ppy)$_2$(dtbbpy)]PF$_6$	48
4	[Ir(dFCF$_3$ppy)$_2$(dtbbpy)]PF$_6$	62

5	$[Ir(dFCF_3ppy)_2(bpy)]PF_6$	66
6	$Ru(bpy)_3(PF_6)_2$	33
7	$Ru(bpz)_3(PF_6)_2$	17
8	$Ru(phen)_3(PF_6)_2$	44
9	$[Mes\text{-}Acr\text{-}Me][BF_4]$	51
10	Rose bengal	29
11	Rhodamine 6G	63
12	Eosin Y	67
13	4CzIPN	73

[a] Reaction condition: **1a** (0.1 mmol, 1.0 equiv.), **2a** (0.2 mmol, 2.0 equiv.), photocatalyst (2 mol%), DIPEA (0.2 mmol, 2.0 equiv.), CH_3CN (1.0 mL), 24 W purple LEDs (365 nm), room temperature, nitrogen atmosphere, 24 h. [b] The yield was determined by crude ^1H NMR using CH_2Br_2 as internal standard.

Table S2. Effect of solvents on this reaction[a]

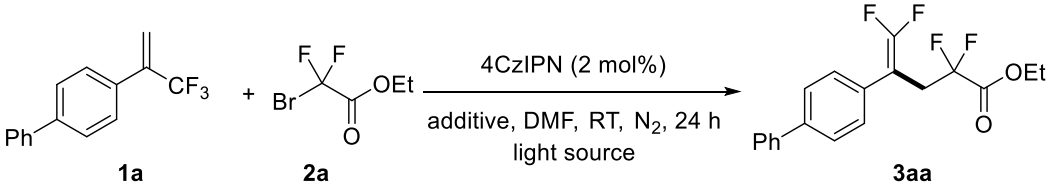


1a **2a** **3aa**

Entry	Solvent	Yield of **3aa** (%)[b]
1	THF	76
2	2-MeTHF	60
3	DCM	75
4	MeOH	0
5	EtOAc	52
6	$PhCF_3$	48
7	1,4-dioxane	64
8	DMSO	92
9	DMF	96

[a] Reaction condition: **1a** (0.1 mmol, 1.0 equiv.), **2a** (0.2 mmol, 2.0 equiv.), 4CzIPN (2 mol%), DIPEA (0.2 mmol, 2.0 equiv.), solvent (1.0 mL), 24 W purple LEDs (365 nm), room temperature, nitrogen atmosphere, 24 h. [b] The yield was determined by crude ^1H NMR using CH_2Br_2 as internal standard.

Table S3. Effect of additives and light source on this reaction[a]



1a **2a** **3aa**

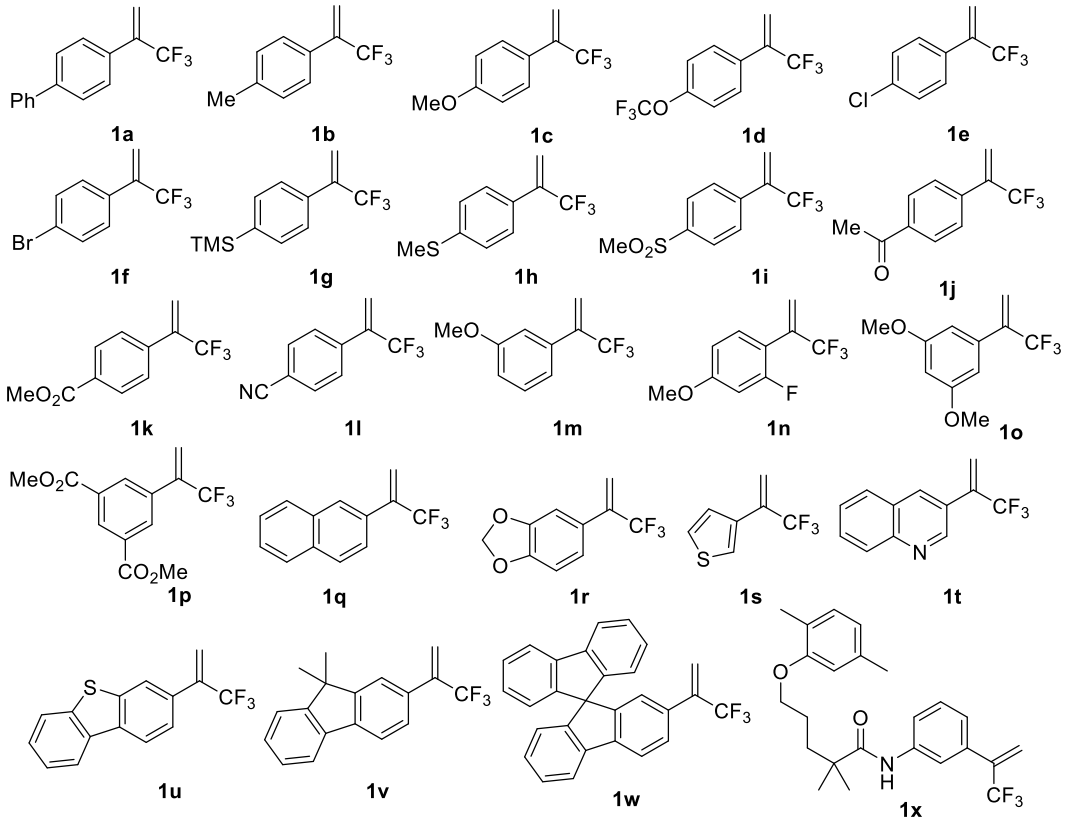
Entry	Light source	Additive	Yield of **3aa** (%)[b]
1	365 nm	TMEDA	0
2	365 nm	Et_3N	66
3	365 nm	DIPEA	96
4	365 nm	quinuclidine	34
5	365 nm	HE	54
6	400 nm	DIPEA	76
7	460 nm	DIPEA	75
8	dark conditions	DIPEA	0

[a] Reaction condition: **1a** (0.1 mmol, 1.0 equiv.), **2a** (0.2 mmol, 2.0 equiv.), 4CzIPN (2 mol%), additive (0.2 mmol, 2.0 equiv.), DMF (1.0 mL), 24 W LEDs light, room temperature, nitrogen atmosphere, 24 h. [b] The yield was determined by crude ^{1}H NMR using CH_2Br_2 as internal standard.

3. Product Synthesis and Characterization

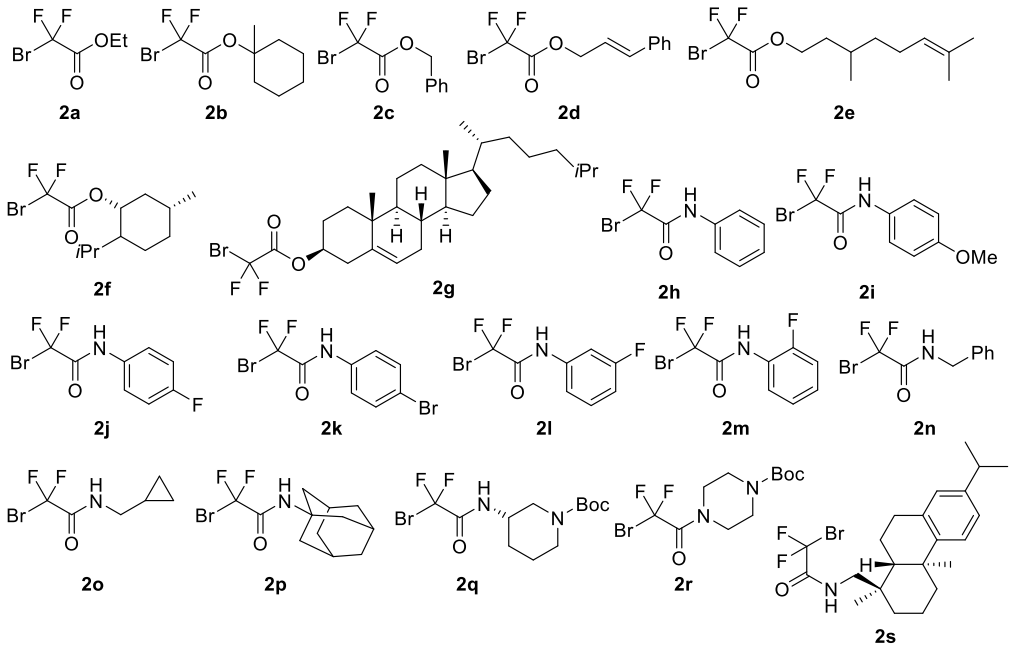
3.1 List of Substrates

List of α-trifluoromethyl styrenes



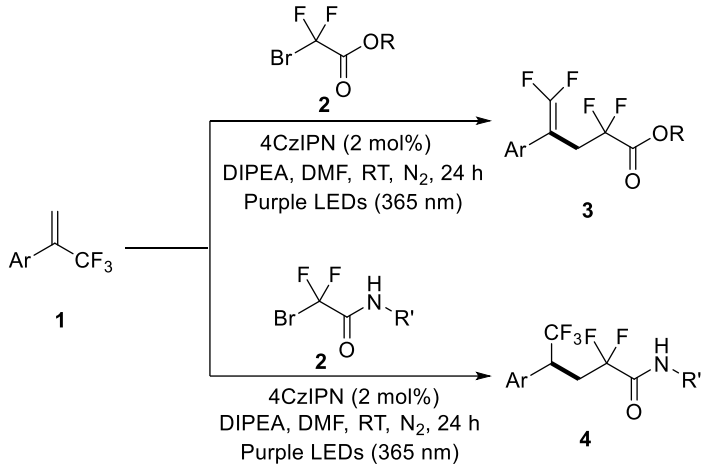
All the α-trifluoromethyl styrenes were synthesized according to the reported procedure.[1]

List of bromodifluoro precursors



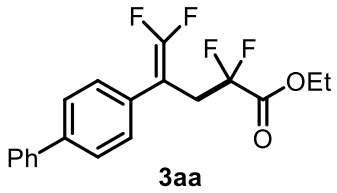
All the bromodifluoro precursors were synthesized according to the reported procedure.[2,3]

3.2 General procedure for the visible-light-promoted selective difluoroalkylation of α-CF_3 alkenes



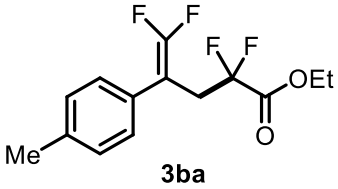
General Procedure:

To an oven-dried quartz vial, α-trifluoromethyl styrenes **1** (0.1 mmol, 1.0 equiv.) and bromodifluoro precursors **2** (0.2 mmol, 2.0 equiv.) were added sequentially. The vial was charged with a stir bar and transferred to a glovebox, where the solids were backfilled with an inert atmosphere. In the glovebox, 4CzIPN (0.002 mmol, 2 mol%) and DIPEA (0.2 mmol, 2.0 equiv.) were added into the vial, followed by DMF (1.0 mL). The vial was sealed with a rubber plug, removed from the glove box, and irradiated and stir by 24 W 365 nm LEDs at room temperature for 24 h. After removal of solvents, the crude mixture was purified by flash chromatography (petroleum ether/ethyl acetate) to afford the pure products **3aa-3xa, 3ab-3ag, 3ar, 3as, 4ah-4aq, 4ih-4lh, 4vh, 4xh.**



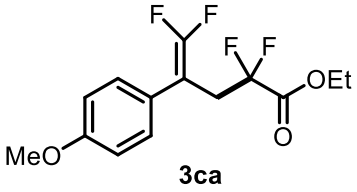
3aa

Ethyl 4-([1,1'-biphenyl]-4-yl)-2,2,5,5-tetrafluoropent-4-enoate (3aa). General Procedure was used to prepare the desired product **3aa**. Chromatographic purification on silica gel using petroleum ether/ethyl acetate (5/1) as eluent afforded **3aa** as a yellow oil (31.7 mg, 0.09 mmol, 90%). **^{1}H NMR (400 MHz, Chloroform-*d*)** δ: 7.61 – 7.54 (m, 4H), 7.47 – 7.40 (m, 2H), 7.39 – 7.32 (m, 3H), 4.03 (q, *J* = 7.2 Hz, 2H), 3.24 (tt, *J* = 15.1, 2.0, 2H), 1.19 (t, *J* = 7.2 Hz, 3H). **^{13}C NMR (101 MHz, Chloroform-*d*)** δ: 163.4 (t, *J* = 32.3 Hz), 155.4 (t, *J* = 292.6 Hz), 140.8, 140.3, 131.1 (t, *J* = 1.8 Hz),129.6, 128.8, 127.6, 127.1, 127.0, 114.5 (t, *J* = 252.7 Hz), 84.6 (t, *J* = 20.1 Hz), 63.0, 34.5 – 33.0 (m), 13.7. **^{19}F NMR (376 MHz, Chloroform-*d*)** δ: -86.18 (d, *J* = 5.5 Hz), -104.14 (d, *J* = 3.7 Hz), -104.18 (d, *J* = 3.6 Hz), -104.22 (d, *J* = 3.5 Hz). **HRMS (DART-TOF)** calculated for $C_{19}H_{18}F_4NO^+$ $[M+NH_4-H_2O]^+$ m/z 352.1319, found 352.1331.



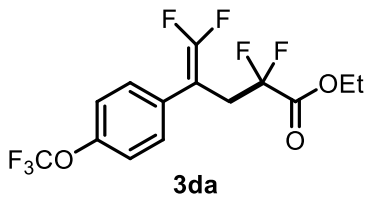
3ba

Ethyl 2,2,5,5-tetrafluoro-4-(*p*-tolyl)pent-4-enoate (3ba). General Procedure was used to prepare the desired product **3ba**. Chromatographic purification on silica gel using petroleum ether/ethyl acetate (5/1) as eluent afforded **3ba** as a yellow oil (20.0 mg, 0.069 mmol, 69%). **^{1}H NMR (400 MHz, Chloroform-*d*)** δ: 7.17 (s, 4H), 4.02 (q, *J* = 7.2 Hz, 2H), 3.18 (tt, *J* = 15.0, 2.0, 2H), 2.34 (s, 3H), 1.20 (t, *J* = 7.1 Hz, 3H). **^{13}C NMR (101 MHz, Chloroform-*d*)** δ: 162.4 (t, *J* = 32.3 Hz), 154.2 (d, *J* = 291.8, 288.3 Hz), 136.7, 128.1, 128.0 (t, *J* = 1.9 Hz), 127.3 (t, *J* = 3.0 Hz), 113.5 (t, *J* = 254.2 Hz), 83.8 – 83.3 (m), 61.9, 33.0 (t, *J* = 25.4 Hz), 20.1, 12.6. **^{19}F NMR (376 MHz, Chloroform-*d*)** δ: -87.13 (d, *J* = 7.9 Hz), -104.23 (d, *J* = 4.0 Hz), -104.27 (d, *J* = 4.1 Hz), -104.31. **HRMS (DART-TOF)** calculated for $C_{14}H_{12}F_4NaO^+$ $[M+Na-H_2O]^+$ m/z 295.0716, found 295.0710.



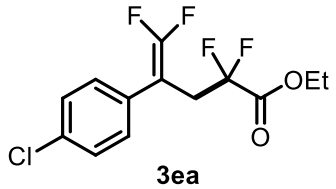
3ca

Ethyl 2,2,5,5-Tetrafluoro-4-(4-methoxyphenyl)pent-4-enoate (3ca). General Procedure was used to prepare the desired product **3ca**. Chromatographic purification on silica gel using petroleum ether/ethyl acetate (5/1) as eluent afforded **3ca** as a yellow oil (22.0 mg, 0.072 mmol, 72%). **^{1}H NMR (400 MHz, Chloroform-*d*)** δ: 7.25 – 7.18 (m, 2H), 6.92 – 6.85 (m, 2H), 4.03 (q, *J* = 7.2 Hz, 2H), 3.81 (s, 3H), 3.16 (tt, *J* = 15.0, 2.0, 2H), 1.21 (t, *J* = 7.1 Hz, 3H). **^{13}C NMR (101 MHz, Chloroform-*d*)** δ: 163.4 (t, *J* = 32.3 Hz), 159.1, 155.2 (t, *J* = 292.9 Hz), 129.7 (t, *J* = 2.8 Hz), 124.1, 113.9, 113.8 (t, *J* = 254.2 Hz), 84.8 – 84.3 (m), 62.9, 55.3, 34.1 (t, *J* = 26.1 Hz), 13.7. **^{19}F NMR (376 MHz, Chloroform-*d*)** δ: -104.24 (t, *J* = 2.9 Hz), -104.28 (t, *J* = 3.1 Hz), -104.29 – -104.35 (m). **HRMS (DART-TOF)** calculated for $C_{14}H_{14}F_4KO_3^+$ $[M+K]^+$ m/z 345.0511, found 345.0521.



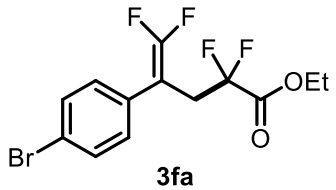
3da

Ethyl 2,2,5,5-tetrafluoro-4-(4-(trifluoromethoxy)phenyl)pent-4-enoate (3da). General Procedure was used to prepare the desired product **3da**. Chromatographic purification on silica gel using petroleum ether/ethyl acetate (5/1) as eluent afforded **3da** as a yellow oil (25.6 mg, 0.071 mmol, 71%). **^{1}H NMR (400 MHz, Chloroform-*d*)** δ: 7.37 – 7.29 (m, 2H), 7.25 – 7.18 (m, 2H), 4.06 (q, *J* = 7.2 Hz, 2H), 3.19 (tt, *J* = 15.1, 2.1, 2H), 1.21 (t, *J* = 7.2 Hz, 3H). **^{13}C NMR (101 MHz, Chloroform-*d*)** δ: 163.3 (t, *J* = 32.2 Hz), 155.4 (t, *J* = 293.0 Hz), 148.7, 130.9, 130.1 (t, *J* = 3.1 Hz), 121.0, 120.4 (q, *J* = 257.6 Hz), 114.3 (t, *J* = 253.2 Hz), 84.5 – 83.4 (m), 63.1, 34.0 (t, *J* = 25.9 Hz), 13.7. **^{19}F NMR (376 MHz, Chloroform-*d*)** δ: -85.72 (d, *J* = 4.5 Hz), -104.25 – -104.30 (m), -104.32 (d, *J* = 3.2 Hz), -104.37. **HRMS (DART-TOF)** calculated for $C_{14}H_{11}F_7KO_3^+$ $[M+K]^+$ m/z 399.0228, found 399.0224.



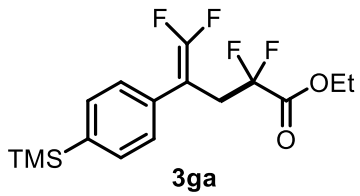
3ea

Ethyl 4-(4-chlorophenyl)-2,2,5,5-tetrafluoropent-4-enoate (3ea). General Procedure was used to prepare the desired product **3ea**. Chromatographic purification on silica gel using petroleum ether/ethyl acetate (5/1) as eluent afforded **3ea** as a yellow oil (20.5 mg, 0.066 mmol, 66%). **^{1}H NMR (400 MHz, Chloroform-*d*)** δ: 7.39 – 7.33 (m, 2H), 7.28 – 7.23 (m, 2H), 4.12 (q, *J* = 7.2 Hz, 2H), 3.20 (tt, *J* = 15.0, 2.0, 2H), 1.26 (t, *J* = 7.2 Hz, 3H). **^{13}C NMR (101 MHz, Chloroform-*d*)** δ: 163.3 (t, *J* = 32.1 Hz), 155.3 (t, *J* = 292.9 Hz), 133.9, 130.7, 129.8 (t, *J* = 3.1 Hz), 128.7, 119.5 – 105.2 (m), 89.4 – 80.3 (m), 63.1, 33.9 (t, *J* = 25.4 Hz), 13.7. **^{19}F NMR (376 MHz, Chloroform-*d*)** δ: -85.82 (d, *J* = 2.7 Hz), -104.21 (t, *J* = 3.0 Hz), -104.25 (t, *J* = 3.1 Hz), -104.29 (t, *J* = 3.1 Hz). **HRMS (DART-TOF)** calculated for $C_{13}H_{11}ClF_4KO_2^+$ $[M+K]^+$ m/z 349.0015, found 349.0002.



3fa

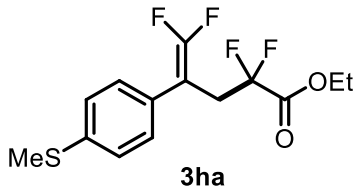
Ethyl 4-(4-bromophenyl)-2,2,5,5-tetrafluoropent-4-enoate (3fa). General Procedure was used to prepare the desired product **3fa**. Chromatographic purification on silica gel using petroleum ether/ethyl acetate (5/1) as eluent afforded **3fa** as a yellow oil (26.6 mg, 0.075 mmol, 75%). **^{1}H NMR (400 MHz, Chloroform-*d*)** δ: 7.52 – 7.46 (m, 2H), 7.20 – 7.14 (m, 2H), 4.10 (q, *J* = 7.1 Hz, 2H), 3.17 (tt, *J* = 15.1, 2.1, 2H), 1.24 (t, *J* = 7.2 Hz, 3H). **^{13}C NMR (101 MHz, Chloroform-*d*)** δ: 163.3 (t, *J* = 32.2 Hz), 155.2 (t, *J* = 293.0 Hz), 131.7, 131.2, 130.1 (t, *J* = 3.1 Hz), 122.0, 118.0 – 110.4 (m), 91.5 – 79.1 (m), 63.1, 33.8 (t, *J* = 25.5 Hz), 13.7. **^{19}F NMR (376 MHz, Chloroform-*d*)** δ: -85.69 (d, *J* = 2.9 Hz), -104.20 (t, *J* = 3.0 Hz), -104.24 (t, *J* = 3.1 Hz), -104.29 (d, *J* = 3.2 Hz). **HRMS (DART-TOF)** calculated for $C_{13}H_{11}BrF_4KO_2^+$ $[M+K]^+$ m/z 394.9490, found 394.9497.



3ga

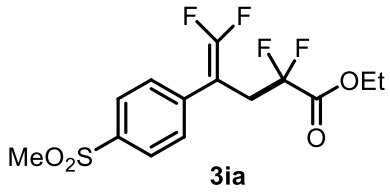
Ethyl 2,2,5,5-tetrafluoro-4-(4-(trimethylsilyl)phenyl)pent-4-enoate (3ga). General Procedure was used to prepare the desired product **3ga**. Chromatographic purification on silica gel using petroleum ether/ethyl acetate (5/1) as eluent afforded **3ga** as a yellow oil (23.0 mg, 0.066 mmol, 66%). **^{1}H NMR (400 MHz, Chloroform-*d*)** δ: 7.54 (d, *J* = 7.6 Hz, 2H),

7.32 – 7.27 (m, 2H), 3.98 (q, *J* = 7.1 Hz, 2H), 3.29 – 3.17 (m, 2H), 1.17 (t, *J* = 7.2 Hz, 3H), 0.35 – 0.25 (m, 9H). **^{13}C NMR (101 MHz, Chloroform-*d*)** δ: 64.6 (t, *J* = 32.3 Hz), 156.6 (t, *J* = 292.6 Hz), 141.6, 134.6, 133.6 (t, *J* = 2.5 Hz), 128.9 (t, *J* = 2.9 Hz), 118.9 – 112.1 (m), 86.7 – 85.2 (m), 64.1, 35.8 – 34.7 (m), 14.8, 0.0. **^{19}F NMR (376 MHz, Chloroform-*d*)** δ: -86.25 – -86.55 (m), -104.25 (d, *J* = 4.7 Hz), -104.29 (d, *J* = 4.8 Hz), -104.33 (d, *J* = 4.6 Hz). **HRMS (DART-TOF)** calculated for $C_{16}H_{21}F_4O_2Si^+$ $[M+H]^+$ m/z 349.1241, found 349.1242.



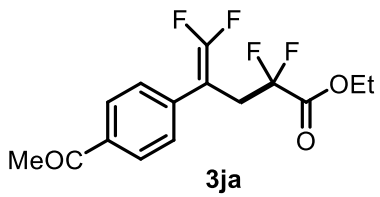
3ha

Ethyl 2,2,5,5-tetrafluoro-4-(4-(methylthio)phenyl)pent-4-enoate (3ha). General Procedure was used to prepare the desired product **3ha**. Chromatographic purification on silica gel using petroleum ether/ethyl acetate (5/1) as eluent afforded **3ha** as a yellow oil (13.2 mg, 0.041 mmol, 41%). **^{1}H NMR (400 MHz, Chloroform-*d*)** δ: 7.25 – 7.19 (m, 4H), 4.05 (q, *J* = 7.2 Hz, 2H), 3.17 (tt, *J* = 15.0, 2.0, 2H), 2.48 (s, 3H), 1.22 (t, *J* = 7.2 Hz, 3H). **^{13}C NMR (101 MHz, Chloroform-*d*)** δ: 163.4 (t, *J* = 32.2 Hz), 155.3 (t, *J* = 292.4 Hz), 138.6, 128.8 (t, *J* = 3.1 Hz), 128.6, 126.2, 114.5 (t, *J* = 252.9 Hz), 84.6 – 84.2 (m), 63.0, 33.9 (t, *J* = 25.7 Hz), 15.5, 13.7. **^{19}F NMR (376 MHz, Chloroform-*d*)** δ: -86.45 (t, *J* = 2.6 Hz), -104.23 (t, *J* = 3.1 Hz), -104.27 (t, *J* = 3.2 Hz), -104.31 (d, *J* = 2.9 Hz). **HRMS (DART-TOF)** calculated for $C_{14}H_{18}F_4NO_2S^+$ $[M+NH_4-H_2O]^+$ m/z 322.0883, found 322.0900.



3ia

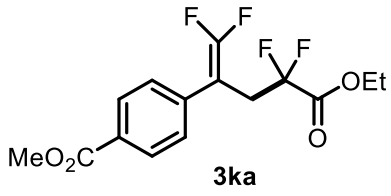
Ethyl 2,2,5,5-tetrafluoro-4-(4-(methylsulfonyl)phenyl)pent-4-enoate (3ia). General Procedure was used to prepare the desired product **3ia**. Chromatographic purification on silica gel using petroleum ether/ethyl acetate (5/1) as eluent afforded **3ia** as a yellow oil (27.6 mg, 0.078 mmol, 78%). **^{1}H NMR (400 MHz, Chloroform-*d*)** δ: 7.96 (t, *J* = 7.8 Hz, 2H), 7.54 (t, *J* = 8.4 Hz, 2H), 4.16 (q, *J* = 10.9 Hz, 2H), 3.24 (tt, *J* = 15.4, 2.0, 2H), 3.07 (d, *J* = 2.5 Hz, 3H), 1.27 (t, *J* = 7.1 Hz, 3H). **^{13}C NMR (101 MHz, Chloroform-*d*)** δ: 163.2 (t, *J* = 32.0 Hz), 155.7 (t, *J* = 294.8 Hz), 139.9, 138.3 (t, *J* = 3.8 Hz), 130.2, 129.4 (t, *J* = 3.3 Hz), 127.9, 127.7, 116.8 – 111.5 (m), 84.5 – 83.8 (m), 63.3, 44.5, 33.6 (t, *J* = 25.2 Hz), 13.8. **^{19}F NMR (376 MHz, Chloroform-*d*)** δ: -83.27 (dt, *J* = 21.0, 5.3 Hz), -83.70 (d, *J* = 23.2 Hz), -104.15 (d, *J* = 5.3 Hz), -104.19 (d, *J* = 5.2 Hz), -104.24 (d, *J* = 5.2 Hz). **HRMS (DART-TOF)** calculated for $C_{14}H_{14}F_4NaO_4S^+$ $[M+H]^+$ m/z 377.0441, found 377.0439.



3ja

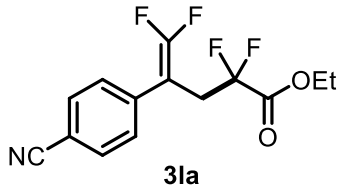
Ethyl 4-(4-acetylphenyl)-2,2,5,5-tetrafluoropent-4-enoate (3ja). General Procedure was used to prepare the desired product **3ja**. Chromatographic purification on silica gel using petroleum ether/ethyl acetate (5/1) as eluent afforded **3ja** as a yellow oil (20.0 mg, 0.063 mmol, 63%). **^{1}H NMR (400 MHz, Chloroform-*d*)** δ: 7.98 – 7.93 (m, 2H), 7.44 – 7.39 (m, 2H), 4.11 (q, *J* = 7.1 Hz, 2H), 3.23 (tt, *J* = 15.2, 2.1, 2H), 2.60 (s, 3H), 1.24 (t, *J* = 7.2 Hz, 3H). **^{13}C NMR (101 MHz, Chloroform-*d*)** δ: 197.2, 163.3 (t, *J* = 32.1 Hz), 155.5 (t, *J* = 294.1 Hz), 137.2 (t, *J* = 3.5 Hz), 136.4, 128.6 (t, *J* = 3.0 Hz), 128.5, 117.5 – 110.2 (m), 85.6 – 83.9 (m), 63.1, 34.0 – 33.2 (m), 26.5, 13.7. **^{19}F NMR (376 MHz, Chloroform-*d*)** δ: -

84.20 – -84.59 (m), -104.16 (d, *J* = 5.0 Hz), -104.20 (d, *J* = 4.9 Hz), -104.24 (d, *J* = 4.9 Hz). **HRMS (DART-TOF)** calculated for $C_{15}H_{13}F_4O_3^+$ $[M-H]^-$ m/z 317.0806, found 317.0793.



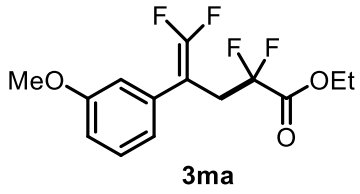
3ka

Methyl 4-(5-ethoxy-1,1,4,4-tetrafluoro-5-oxopent-1-en-2-yl)benzoate (3ka). General Procedure was used to prepare the desired product **3ka**. Chromatographic purification on silica gel using petroleum ether/ethyl acetate (5/1) as eluent afforded **3ka** as a yellow oil (19.4 mg, 0.058 mmol, 58%). **^{1}H NMR (400 MHz, Chloroform-*d*)** δ: 8.04 (dd, *J* = 8.4, 4.1 Hz, 2H), 7.42 – 7.36 (m, 2H), 4.08 (q, *J* = 7.1 Hz, 2H), 3.92 (s, 3H), 3.23 (tt, *J* = 15.2, 2.1, 2H), 1.23 (t, *J* = 7.1 Hz, 3H). **^{13}C NMR (101 MHz, Chloroform-*d*)** δ: 166.5, 163.3 (t, *J* = 31.9 Hz), 155.6 (t, *J* = 293.9 Hz), 137.0 (t, *J* = 3.3 Hz), 130.0, 129.7, 128.5 (t, *J* = 3.3 Hz), 117.7 – 109.1 (m), 85.5 – 83.7 (m), 63.1, 52.2, 33.7 (td, *J* = 25.6, 2.2 Hz), 13.7. **^{19}F NMR (376 MHz, Chloroform-*d*)** δ: -84.33 – -84.75 (m), -104.24 (d, *J* = 5.1 Hz), -104.28 (d, *J* = 4.9 Hz), -104.32 (d, *J* = 5.1 Hz). **HRMS (DART-TOF)** calculated for $C_{15}H_{15}F_4O_4^+$ $[M+H]^+$ m/z 335.0901, found 335.0899.



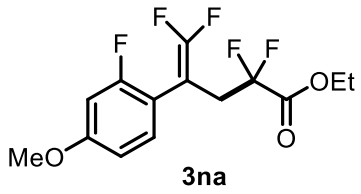
3la

Ethyl 4-(4-cyanophenyl)-2,2,5,5-tetrafluoropent-4-enoate (3la). General Procedure was used to prepare the desired product **3la**. Chromatographic purification on silica gel using petroleum ether/ethyl acetate (5/1) as eluent afforded **3la** as a yellow oil (22.3 mg, 0.074 mmol, 74%). **^{1}H NMR (400 MHz, Chloroform-*d*)** δ: 7.71 – 7.64 (m, 2H), 7.44 (d, *J* = 8.1 Hz, 2H), 4.16 (q, *J* = 7.2 Hz, 2H), 3.22 (tt, *J* = 15.4, 2.2, 2H), 1.27 (t, *J* = 7.1 Hz, 3H). **^{13}C NMR (101 MHz, Chloroform-*d*)** δ: 163.2 (t, *J* = 32.1 Hz), 155.6 (t, *J* = 294.9 Hz), 137.4 – 137.1 (m), 132.3, 129.2 (t, *J* = 3.4 Hz), 118.3, 111.7, 116.8-111.8 (m), 84.9 – 83.6 (m), 63.2, 33.8 – 33.1 (m), 13.8. **^{19}F NMR (376 MHz, Chloroform-*d*)** δ: -81.55 – -84.36 (m), -104.22 (d, *J* = 5.1 Hz), -104.26 (d, *J* = 5.1 Hz), -104.30 (d, *J* = 5.1 Hz). **HRMS (DART-TOF)** calculated for $C_{14}H_{12}F_4NO_2^+$ $[M+H]^+$ m/z 302.0799, found 302.0786.



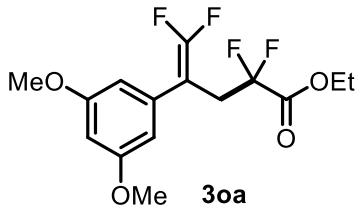
3ma

Ethyl 2,2,5,5-tetrafluoro-4-(3-methoxyphenyl)pent-4-enoate (3ma). General Procedure was used to prepare the desired product **3ma**. Chromatographic purification on silica gel using petroleum ether/ethyl acetate (5/1) as eluent afforded **3ma** as a yellow oil (19.6 mg, 0.064 mmol, 64%). **^{1}H NMR (400 MHz, Chloroform-*d*)** δ: 7.31 – 7.23 (m, 1H), 6.91 – 6.80 (m, 3H), 4.04 (q, *J* = 7.1 Hz, 2H), 3.81 (s, 3H), 3.19 (tt, *J* = 15.0, 2.0, 2H), 1.20 (t, *J* = 7.2 Hz, 3H). **^{13}C NMR (101 MHz, Chloroform-*d*)** δ: 163.4 (t, *J* = 32.3 Hz), 159.5, 155.3 (t, *J* = 292.3 Hz), 133.5 – 133.3 (m), 129.5, 120.9 (t, *J* = 3.0 Hz), 114.5-109.3 (m), 114.4 (t, *J* = 3.1 Hz), 113.3, 85.2 – 84.3 (m), 63.0, 55.3, 34.1 (t, *J* = 27.0 Hz), 13.7. **^{19}F NMR (376 MHz, Chloroform-*d*)** δ: -85.95 (d, *J* = 29.5 Hz), -86.45 (dt, *J* = 29.4, 5.4 Hz), -104.26 (d, *J* = 5.0 Hz), -104.30 (d, *J* = 5.0 Hz), -104.34 (d, *J* = 5.1 Hz). **HRMS (DART-TOF)** calculated for $C_{14}H_{14}F_4KO_3^+$ $[M+K]^+$ m/z 345.0511, found 345.0521.



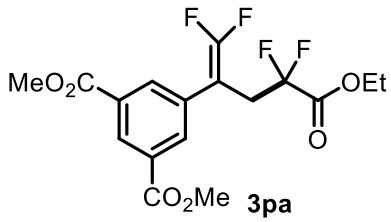
3na

Ethyl 2,2,5,5-tetrafluoro-4-(2-fluoro-4-methoxyphenyl)pent-4-enoate (3na). General Procedure was used to prepare the desired product **3na**. Chromatographic purification on silica gel using petroleum ether/ethyl acetate (5/1) as eluent afforded **3na** as a yellow oil (13.0 mg, 0.04 mmol, 40%). **^{1}H NMR (400 MHz, Chloroform-*d*)** δ: 7.15 (t, *J* = 8.6 Hz, 1H), 6.77 – 6.62 (m, 2H), 4.13 (q, *J* = 7.2 Hz, 2H), 3.82 (s, 3H), 3.18 (tt, *J* = 15.0, 2.0, 2H), 1.27 (t, *J* = 7.2 Hz, 3H). **^{13}C NMR (101 MHz, Chloroform-*d*)** δ: 163.3 (t, *J* = 32.4 Hz), 161.1 (d, *J* = 11.0 Hz), 160.9 (d, *J* = 247.7 Hz), 158.5 – 151.9 (m), 131.8 – 131.6 (m), 114.6 – 108.6 (m), 110.1 (d, *J* = 3.1 Hz), 102.0, 101.7, 80.0 – 79.0 (m), 63.0, 55.6, 33.7 (t, *J* = 25.4 Hz), 13.7. **^{19}F NMR (376 MHz, Chloroform-*d*)** δ: -84.52 (dd, *J* = 27.3, 8.4 Hz), -87.31 (dt, *J* = 27.3, 3.4 Hz), -104.32 (d, *J* = 4.0 Hz), -104.36 (d, *J* = 3.9 Hz), -104.40 (d, *J* = 3.9 Hz), -111.72 (dt, *J* = 12.7, 8.5 Hz). **HRMS (DART-TOF)** calculated for $C_{14}H_{13}F_5KO_3^+$ $[M+K]^+$ m/z 363.0416, found 363.0412.



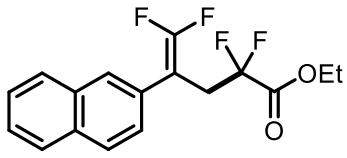
3oa

Ethyl 4-(3,5-dimethoxyphenyl)-2,2,5,5-tetrafluoropent-4-enoate (3oa). General Procedure was used to prepare the desired product **3oa**. Chromatographic purification on silica gel using petroleum ether/ethyl acetate (5/1) as eluent afforded **3oa** as a yellow oil (17.5 mg, 0.052 mmol, 52%). **^{1}H NMR (400 MHz, Chloroform-*d*)** δ: 6.43 (dd, *J* = 2.3, 1.1 Hz, 2H), 6.40 (t, *J* = 2.2 Hz, 1H), 4.07 (q, *J* = 7.2 Hz, 2H), 3.79 (s, 6H), 3.16 (tt, *J* = 15.1, 2.0, 2H), 1.22 (t, *J* = 7.2 Hz, 3H). **^{13}C NMR (101 MHz, Chloroform-*d*)** δ: 163.4 (t, *J* = 32.2 Hz), 160.7, 155.3 (t, *J* = 292.4 Hz), 134.1 – 133.8 (m), 117.8 – 110.7 (m), 106.8 (t, *J* = 3.2 Hz), 99.9, 89.4 – 78.8 (m), 63.0, 55.4, 34.1 (td, *J* = 25.8, 2.5 Hz), 13.7. **^{19}F NMR (376 MHz, Chloroform-*d*)** δ: -85.30 (d, *J* = 29.1 Hz), -86.32 (dt, *J* = 31.7, 5.5 Hz), -104.22 (d, *J* = 5.1 Hz), -104.26 (d, *J* = 5.0 Hz), -104.30 (d, *J* = 5.2 Hz). **HRMS (DART-TOF)** calculated for $C_{15}H_{17}F_4O_4^+$ $[M+H]^+$ m/z 337.1057, found 337.1045.



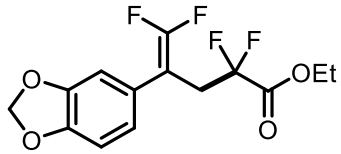
3pa

Dimethyl 5-(5-ethoxy-1,1,4,4-tetrafluoro-5-oxopent-1-en-2-yl)isophthalate (3pa). General Procedure was used to prepare the desired product **3pa**. Chromatographic purification on silica gel using petroleum ether/ethyl acetate (5/1) as eluent afforded **3pa** as a white solid (21.9 mg, 0.056 mmol, 56%); **Mp:** 87.7-88.9 °C. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ: 8.64 (t, *J* = 1.6 Hz, 1H), 8.19 (t, *J* = 1.2 Hz, 2H), 4.16 (q, *J* = 7.2 Hz, 2H), 3.98 (s, 6H), 3.27 (tt, *J* = 15.3, 2.2, 2H), 1.28 (t, *J* = 7.2 Hz, 3H). **^{13}C NMR (101 MHz, Chloroform-*d*)** δ: 165.7, 163.2 (t, *J* = 32.1 Hz), 155.6 (t, *J* = 293.8 Hz), 133.7 (t, *J* = 3.0 Hz), 133.4 (t, *J* = 3.1 Hz), 131.1, 130.1, 114.3 (t, *J* = 249.8 Hz), 63.2, 52.6, 84.0 (dd, *J* = 21.8, 19.5 Hz), 13.7. **^{19}F NMR (376 MHz, Chloroform-*d*)** δ: -84.73 – -85.01 (m), -104.07 (d, *J* = 4.3 Hz), -104.11 (d, *J* = 4.2 Hz), -104.15 (d, *J* = 4.2 Hz). **HRMS (DART-TOF)** calculated for $C_{17}H_{20}F_4NO_6^+$ $[M+NH_4]^+$ m/z 410.1221, found 410.1228.



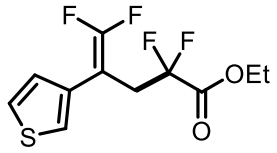
3qa

Ethyl 2,2,4,4-tetrafluoro-3-(naphthalen-2-yl)but-3-enoate (3qa). General Procedure was used to prepare the desired product **3qa**. Chromatographic purification on silica gel using petroleum ether/ethyl acetate (5/1) as eluent afforded **3qa** as a brown oil (26.7 mg, 0.082 mmol, 82%). **^{1}H NMR (400 MHz, Chloroform-*d*)** δ: 7.82 (dd, *J* = 9.1, 5.9 Hz, 3H), 7.75 (d, *J* = 1.8 Hz, 1H), 7.49 (dt, *J* = 6.2, 3.6 Hz, 2H), 7.40 (dt, *J* = 8.6, 1.7 Hz, 1H), 3.90 (q, *J* = 7.2 Hz, 2H), 3.31 (tt, *J* = 15.1, 2.0, 2H), 1.09 (t, *J* = 7.2 Hz, 3H). **^{13}C NMR (101 MHz, Chloroform-*d*)** δ: 163.4 (t, *J* = 32.2 Hz), 155.6 (t, *J* = 292.6 Hz), 133.1, 132.7, 129.5 (t, *J* = 3.1 Hz), 128.2, 128.0, 127.6, 127.9 (t, *J* = 3.1 Hz), 126.5 (2C), 126.0 (t, *J* = 3.0 Hz), 118.4 – 108.8 (m), 86.8 – 83.5 (m), 62.9, 34.1 (td, *J* = 25.8, 2.4 Hz), 13.6. **^{19}F NMR (376 MHz, Chloroform-*d*)** δ: -86.06 – -86.47 (m), -104.15 (d, *J* = 4.7 Hz), -104.19 (d, *J* = 4.8 Hz), -104.23 (d, *J* = 4.7 Hz). **HRMS (DART-TOF)** calculated for $C_{17}H_{14}F_4NaO_6^+$ $[M+Na]^+$ m/z 349.0822, found 349.0817.



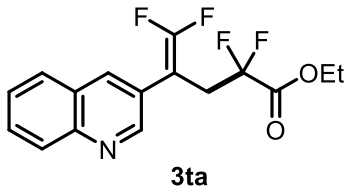
3ra

Ethyl 4-(benzo[d][1,3]dioxol-5-yl)-2,2,5,5-tetrafluoropent-4-enoate (3ra). General Procedure was used to prepare the desired product **3ra**. Chromatographic purification on silica gel using petroleum ether/ethyl acetate (5/1) as eluent afforded **3ra** as a yellow oil (23.4 mg, 0.073 mmol, 73%). **^{1}H NMR (400 MHz, Chloroform-*d*)** δ: 6.82 – 6.72 (m, 3H), 5.97 (s, 2H), 4.12 (q, *J* = 7.2 Hz, 2H), 3.13 (tt, *J* = 15.0, 2.0, 2H), 1.25 (t, *J* = 7.2 Hz, 3H). **^{13}C NMR (101 MHz, Chloroform-*d*)** δ: 163.4 (t, *J* = 32.3 Hz), 158.6 – 150.9 (m), 147.7, 147.2, 125.7 (t, *J* = 3.3 Hz), 122.3 (t, *J* = 3.1 Hz), 117.7 – 111.0 (m), 109.1 (t, *J* = 3.1 Hz), 108.3, 101.3, 84.6 (t, *J* = 20.5 Hz), 63.0, 39.7 – 31.0 (m), 13.7. **^{19}F NMR (376 MHz, Chloroform-*d*)** δ: -86.75 (d, *J* = 31.3 Hz), -87.08 – -87.34 (m), -104.19 (d, *J* = 4.8 Hz), -104.23 (d, *J* = 4.7 Hz), -104.27 (d, *J* = 4.8 Hz). **HRMS (DART-TOF)** calculated for $C_{14}H_{13}F_4O_4^+$ $[M+H]^+$ m/z 321.0744, found 321.0753.



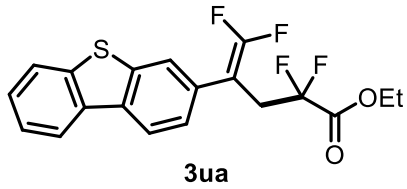
3sa

Ethyl 2,2,5,5-tetrafluoro-4-(thiophen-3-yl)pent-4-enoate (3sa). General Procedure was used to prepare the desired product **3sa**. Chromatographic purification on silica gel using petroleum ether/ethyl acetate (5/1) as eluent afforded **3sa** as a yellow oil (16.6 mg, 0.059 mmol, 59%). **^{1}H NMR (400 MHz, Chloroform-*d*)** δ: 7.33 (dd, *J* = 5.1, 3.0 Hz, 1H), 7.24 (dd, *J* = 3.0, 1.4 Hz, 1H), 7.15 (dd, *J* = 5.1, 2.2 Hz, 1H), 4.13 (q, *J* = 7.1 Hz, 2H), 3.19 (td, *J* = 15.4, 2.6 Hz, 2H), 1.28 – 1.23 (m, 3H). **^{13}C NMR (101 MHz, Chloroform-*d*)** δ: 163.3 – 161.6 (m), 157.4 – 151.6 (m), 131.2, 125.9 (d, *J* = 4.3 Hz), 124.7, 121.9 (t, *J* = 5.6 Hz), 115.9 – 110.8 (m), 84.2 – 83.5 (m), 62.1, 32.8 – 32.3 (m), 12.7. **^{19}F NMR (376 MHz, Chloroform-*d*)** δ: -82.83 (d, *J* = 28.0 Hz), -86.48 (ddq, *J* = 28.3, 6.1, 2.9 Hz), -104.36 (d, *J* = 5.8 Hz), -104.40 (d, *J* = 5.7 Hz), -104.44 (d, *J* = 6.0 Hz). **HRMS (DART-TOF)** calculated for $C_{11}H_{10}F_4KSO_2^+$ $[M+K]^+$ m/z 320.9969, found 320.9954.



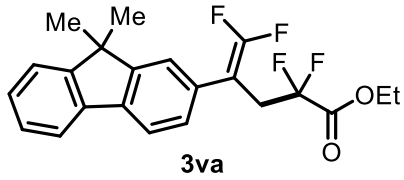
3ta

Ethyl 2,2,4,4-tetrafluoro-3-(quinolin-3-yl)but-3-enoate (3ta). General Procedure was used to prepare the desired product **3ta**. Chromatographic purification on silica gel using petroleum ether/ethyl acetate (5/1) as eluent afforded **3ta** as a pale yellow solid (21.9 mg, 0.067 mmol, 67%); **Mp:** 147.5-148.8 ºC. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ: 8.86 (d, *J* = 2.1 Hz, 1H), 8.13 – 8.06 (m, 2H), 7.82 (dd, *J* = 8.2, 1.5 Hz, 1H), 7.74 (dd, *J* = 8.3, 6.8 Hz, 1H), 7.58 (dd, *J* = 8.1, 6.9 Hz, 1H), 4.06 (q, *J* = 7.1 Hz, 2H), 3.32 (tt, *J* = 15.3, 2.1, 2H), 1.19 (t, *J* = 7.2 Hz, 3H). **^{13}C NMR (101 MHz, Chloroform-*d*)** δ: 163.3 (t, *J* = 32.0 Hz), 155.9 (t, *J* = 294.0 Hz), 149.9, 147.2, 135.5, 130.1, 129.3, 127.8, 127.4, 127.3, 125.5 (t, *J* = 3.8 Hz), 117.1 – 111.1 (m), 82.7 – 82.3 (m), 63.2, 34.1 – 33.5 (m), 13.7. **^{19}F NMR (376 MHz, Chloroform-*d*)** δ: -83.98 – -84.21 (m), -84.77 (d, *J* = 25.8 Hz), -104.06 (d, *J* = 4.9 Hz), -104.10 (d, *J* = 4.9 Hz), -104.14 (d, *J* = 4.9 Hz). **HRMS (DART-TOF)** calculated for $C_{16}H_{14}F_4NO_2^+$ $[M+H]^+$ m/z 328.0955, found 328.0957.



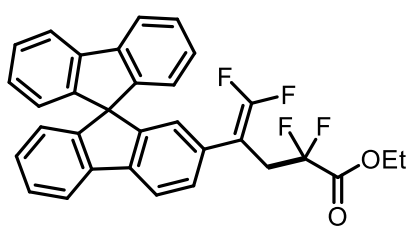
3ua

Ethyl 4-(dibenzo[*b,d*]thiophen-3-yl)-2,2,5,5-tetrafluoropent-4-enoate (3ua). General Procedure was used to prepare the desired product **3ua**. Chromatographic purification on silica gel using petroleum ether/ethyl acetate (5/1) as eluent afforded **3ua** as a yellow oil (21.4 mg, 0.056 mmol, 56%). **^{1}H NMR (400 MHz, Chloroform-*d*)** δ: 8.14 (td, *J* = 7.8, 7.0, 2.6 Hz, 2H), 7.85 (d, *J* = 5.5 Hz, 1H), 7.61 – 7.38 (m, 3H), 7.36 (dd, *J* = 7.4, 2.4 Hz, 1H), 3.99 (q, *J* = 7.2 Hz, 2H), 3.36 (td, *J* = 15.1, 2.2 Hz, 2H), 1.08 (td, *J* = 7.2, 2.6 Hz, 3H). **^{13}C NMR (101 MHz, Chloroform-*d*)** δ: 163.2 (t, *J* = 32.4 Hz), 155.4 (dd, *J* = 295.4, 292.1 Hz), 139.5, 138.9, 136.1, 135.6, 128.2, 127.1, 126.9 (d, *J* = 4.1 Hz), 124.8, 124.6, 122.8, 121.8, 121.6, 117.4 – 110.1 (m), 84.3 – 83.1 (m), 63.0, 33.0 (t, *J* = 26.6 Hz), 13.5. **^{19}F NMR (376 MHz, Chloroform-*d*)** δ: -81.57 (d, *J* = 23.8 Hz), -86.30 (d, *J* = 24.5 Hz), -104.13 (td, *J* = 15.7, 4.3 Hz). **HRMS (DART-TOF)** calculated for $C_{19}H_{14}F_4NaO_2S^+$ $[M+Na]^+$ m/z 405.0543, found 405.0542.



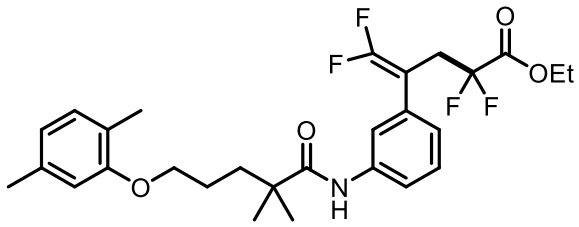
3va

Ethyl 4-(9,9-dimethyl-9*H*-fluoren-2-yl)-2,2,5,5-tetrafluoropent-4-enoate (3va). General Procedure was used to prepare the desired product **3va**. Chromatographic purification on silica gel using petroleum ether/ethyl acetate (5/1) as eluent afforded **3va** as a yellow oil (35.3 mg, 0.09 mmol, 90%). **^{1}H NMR (400 MHz, Chloroform-*d*)** δ: 7.73 – 7.66 (m, 2H), 7.46 – 7.40 (m, 1H), 7.37 – 7.30 (m, 3H), 7.25 (d, *J* = 2.1 Hz, 1H), 3.95 (q, *J* = 7.2 Hz, 2H), 3.26 (tt, *J* = 15.0, 2.0, 2H), 1.48 (s, 6H), 1.13 (t, *J* = 7.2 Hz, 3H). **^{13}C NMR (101 MHz, Chloroform-*d*)** δ: 163.4 (t, *J* = 32.2 Hz), 155.5 (t, *J* = 292.2 Hz), 153.9 (2C), 139.1, 138.5, 130.9 (t, *J* = 3.3 Hz), 127.6, 127.4 (t, *J* = 3.1 Hz), 127.1, 123.1 – 122.7 (m), 122.6, 120.2, 119.9, 118.1 – 112.0 (m), 85.3 (t, *J* = 20.1 Hz), 62.8, 46.9, 34.3 (t, *J* = 25.9 Hz), 27.1, 13.7. **^{19}F NMR (376 MHz, Chloroform-*d*)** δ: -86.26 – -86.64 (m), -104.17 (d, *J* = 5.3 Hz), -104.21 (d, *J* = 5.1 Hz), -104.25 (d, *J* = 5.2 Hz). **HRMS (DART-TOF)** calculated for $C_{22}H_{20}F_4NaO_2^+$ $[M+Na]^+$ m/z 415.1292, found 415.1299.



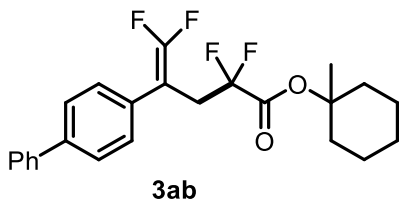
3wa

Ethyl 4-(9,9'-spirobi[fluoren]-2-yl)-2,2,5,5-tetrafluoropent-4-enoate (3wa). General Procedure was used to prepare the desired product **3wa**. Chromatographic purification on silica gel using petroleum ether/ethyl acetate (5/1) as eluent afforded **3wa** as a yellow oil (41.6 mg, 0.081 mmol, 81%). **^{1}H NMR (400 MHz, Chloroform-*d*)** δ: 7.83 (dd, *J* = 10.4, 7.7 Hz, 4H), 7.34 (dt, *J* = 24.4, 7.7 Hz, 4H), 7.11 (t, *J* = 7.5 Hz, 3H), 6.71 (t, *J* = 6.7 Hz, 3H), 6.62 (s, 1H), 3.95 (q, *J* = 7.1 Hz, 2H), 3.01 (tt, *J* = 15.0, 2.0, 2H), 1.12 (t, *J* = 7.1 Hz, 3H). **^{13}C NMR (101 MHz, Chloroform-*d*)** δ: 163.3 (t, *J* = 32.1 Hz), 159.4 – 152.3 (m), 149.1 (d, *J* = 10.9 Hz), 148.3, 141.3 (d, *J* = 72.2 Hz), 140.9, 131.7 (t, *J* = 3.4 Hz), 128.3 (t, *J* = 2.6 Hz), 128.2, 127.9 (d, *J* = 2.4 Hz), 127.8, 124.0, 123.9 (t, *J* = 2.9 Hz), 120.0 (t, *J* = 10.9 Hz), 117.0 – 110.3 (m), 85.52 – 84.4 (m), 65.9, 62.8, 34.0 (t, *J* = 25.7 Hz), 13.7. **^{19}F NMR (376 MHz, Chloroform-*d*)** δ: -85.94 (d, *J* = 29.0 Hz), -86.30 (dt, *J* = 29.1, 6.1 Hz), -104.15 (d, *J* = 5.8 Hz), -104.19 (d, *J* = 5.6 Hz), -104.23 (d, *J* = 5.9 Hz). **HRMS (DART-TOF)** calculated for $C_{32}H_{22}F_4KO_2^+$ $[M+K]^+$ m/z 553.1188, found 553.1188.



3xa

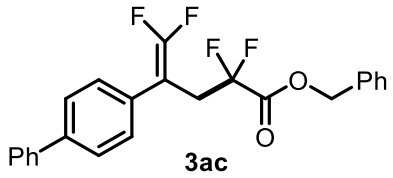
Ethyl 4-(3-(5-(2,5-dimethylphenoxy)-2,2-dimethylpentanamido)phenyl)-2,2,5,5-tetrafluoropent-4-enoate (3xa). General Procedure was used to prepare the desired product **3xa**. Chromatographic purification on silica gel using petroleum ether/ethyl acetate (5/1) as eluent afforded **3xa** as a yellow oil (39.2 mg, 0.075 mmol, 75%). **^{1}H NMR (400 MHz, Chloroform-*d*)** δ: 7.50 (d, *J* = 2.2 Hz, 1H), 7.46 (dt, *J* = 8.1, 1.5 Hz, 1H), 7.37 (s, 1H), 7.30 (t, *J* = 7.9 Hz, 1H), 7.06 – 6.96 (m, 2H), 6.66 (d, *J* = 7.4 Hz, 1H), 6.61 (d, *J* = 1.6 Hz, 1H), 4.07 (q, *J* = 7.2 Hz, 2H), 3.95 (p, *J* = 2.5 Hz, 2H), 3.18 (tt, *J* = 15.1, 2.0, 2H), 2.29 (s, 3H), 2.17 (s, 3H), 1.82 (d, *J* = 3.0 Hz, 4H), 1.34 (s, 6H), 1.22 (t, *J* = 7.2 Hz, 3H). **^{13}C NMR (101 MHz, Chloroform-*d*)** δ: 175.8, 163.4 (t, *J* = 32.2 Hz), 158.5 – 152.8 (m), 156.8, 138.2, 136.5, 133.1, 130.3, 129.1, 124.5, 123.6, 120.9, 120.0, 119.6, 115.9 – 110.0 (m), 112.3, 85.0 – 83.7 (m), 67.9, 63.0, 42.9, 37.7, 34.4 – 33.6 (m), 25.6, 25.2, 21.3, 15.8, 13.7. **^{19}F NMR (376 MHz, Chloroform-*d*)** δ: -85.92 (d, *J* = 29.1 Hz), -86.17 – -86.54 (m), -104.28 (d, *J* = 4.9 Hz), -104.32 (d, *J* = 4.8 Hz), -104.36 (d, *J* = 4.9 Hz). **HRMS (DART-TOF)** calculated for $C_{28}H_{33}F_4NNaO_4^+$ $[M+Na]^+$ m/z 546.2238, found 546.2265.



3ab

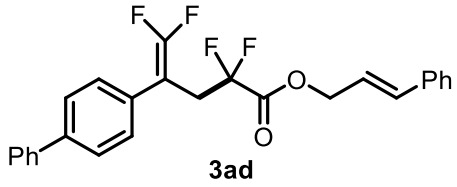
1-Methylcyclohexyl 2,2,5,5-tetrafluoro-4-(phenylcarbamoyl)pent-4-enoate (3ab). General Procedure was used to prepare the desired product **3ab**. Chromatographic purification on silica gel using petroleum ether/ethyl acetate (5/1) as eluent afforded **3ab** as a colorless oil (13.0 mg, 0.031 mmol, 31%). **^{1}H NMR (400 MHz, Chloroform-*d*)** δ: 7.63 – 7.53 (m, 4H), 7.40 (dd, *J* = 19.6, 13.3 Hz, 5H), 3.22 (td, *J* = 15.3, 2.7 Hz, 2H), 2.11 – 2.00 (m, 2H), 1.50 – 1.42 (m, 4H), 1.35 (s, 3H), 1.26 (s, 4H). **^{13}C**

NMR (101 MHz, Chloroform-*d*) δ: 162.2 (t, *J* = 31.9 Hz), 157.6 – 152.7 (m), 140.7, 140.5, 131.4, 128.9, 128.8 127.5, 127.2, 127.0, 117.4 – 111.3 (m), 86.5, 83.6 – 82.6 (m), 36.2, 34.3 – 32.9 (m), 25.1, 24.7, 21.9. **^{19}F NMR (376 MHz, Chloroform-*d*)** δ: -85.77 – -85.99 (m), -86.41 (d, *J* = 29.8 Hz), -103.23 (d, *J* = 5.6 Hz), -103.27 (d, *J* = 5.6 Hz), -103.31 (d, *J* = 5.9 Hz). **HRMS (DART-TOF)** calculated for $C_{24}H_{24}F_4NaO_2^+$ $[M+Na]^+$ m/z 443.1605, found 443.1601.



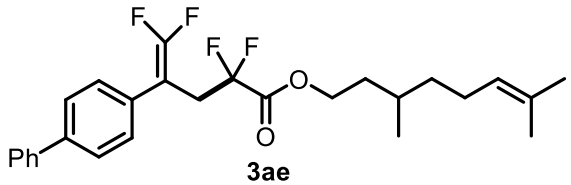
3ac

Benzyl 4-([1,1'-biphenyl]-4-yl)-2,2,5,5-tetrafluoropent-4-enoate (3ac). General Procedure was used to prepare the desired product **3ac**. Chromatographic purification on silica gel using petroleum ether/ethyl acetate (5/1) as eluent afforded **3ac** as a colorless oil (35.2 mg, 0.085 mmol, 85%). **^{1}H NMR (400 MHz, Chloroform-*d*)** δ: 7.60 – 7.53 (m, 4H), 7.44 (dd, *J* = 8.5, 6.8 Hz, 2H), 7.40 – 7.30 (m, 6H), 7.30 – 7.24 (m, 2H), 4.99 (s, 2H), 3.24 (tt, *J* = 15.1, 2.1 Hz, 2H). **^{13}C NMR (101 MHz, Chloroform-*d*)** δ: 163.8 – 162.8 (m), 158.8 – 152.1 (m), 140.7, 140.3, 134.0, 131.0, 128.9 (2C), 129.8, 128.7, 128.5, 127.6, 127.1, 127.0, 117.1 – 112.0 (m), 84.7 – 84.3 (m), 68.4, 34.0 (t, *J* = 25.7 Hz). **^{19}F NMR (376 MHz, Chloroform-*d*)** δ: -85.99 (t, *J* = 3.5 Hz), -103.89 (t, *J* = 3.3 Hz), -103.93 (t, *J* = 3.1 Hz), -103.98 (d, *J* = 3.5 Hz). **HRMS (DART-TOF)** calculated for $C_{24}H_{19}F_4O_2^+$ $[M+H]^+$ m/z 415.1316, found 415.1357.



3ad

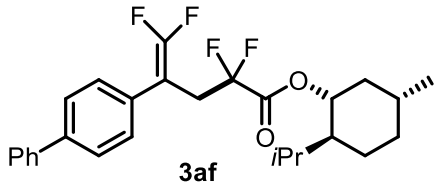
Cinnamyl 4-([1,1'-biphenyl]-4-yl)-2,2,5,5-tetrafluoropent-4-enoate (3ad). General Procedure was used to prepare the desired product **3ad**. Chromatographic purification on silica gel using petroleum ether/ethyl acetate (5/1) as eluent afforded **3ad** as a colorless oil (36.5 mg, 0.083 mmol, 83%). **^{1}H NMR (400 MHz, Chloroform-*d*)** δ: 7.61 – 7.55 (m, 4H), 7.47 – 7.41 (m, 2H), 7.40 – 7.35 (m, 3H), 7.34 – 7.26 (m, 5H), 6.58 (dt, *J* = 15.9, 1.3 Hz, 1H), 6.12 (dt, *J* = 15.9, 6.7 Hz, 1H), 4.59 (dd, *J* = 6.7, 1.3 Hz, 2H), 3.26 (tt, *J* = 15.0, 2.1 Hz, 2H). **^{13}C NMR (101 MHz, Chloroform-*d*)** δ: 163.2 (t, *J* = 32.4 Hz), 161.4 – 154.59 (m), 140.7, 140.2, 136.1, 135.6, 131.0 (t, *J* = 2.4 Hz), 128.9 (d, *J* = 3.0 Hz), 128.9, 128.6, 128.6 (t, *J* = 9.3 Hz), 128.5, 127.6, 127.1, 127.0, 126.7, 117.0 – 112.0 (m), 84.7 – 84.2 (m), 67.4, 34.01 (t, *J* = 25.5 Hz). **^{19}F NMR (376 MHz, Chloroform-*d*)** δ: -85.78 – -86.10 (m), -103.95 (d, *J* = 4.9 Hz), -103.99 (d, *J* = 4.3 Hz), -104.03 (d, *J* = 4.7 Hz). **HRMS (DART-TOF)** calculated for $C_{26}H_{20}F_4NaO_2^+$ $[M+Na]^+$ m/z 463.1292, found 463.1285.



3ae

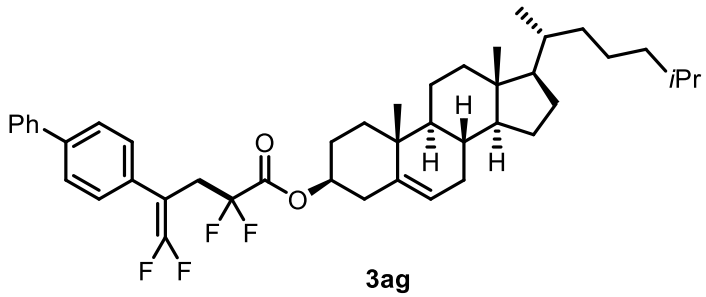
3,7-Dimethyloct-6-en-1-yl 4-([1,1'-biphenyl]-4-yl)-2,2,5,5-tetrafluoropent-4-enoate (3ae). General Procedure was used to prepare the desired product **3ae**. Chromatographic purification on silica gel using petroleum ether/ethyl acetate (5/1) as eluent afforded **3ae** as a colorless oil (25.4 mg, 0.055 mmol, 55%). **^{1}H NMR (400 MHz, Chloroform-*d*)** δ: 7.70 – 7.51 (m, 4H), 7.44 (dd, *J* = 8.3, 6.7 Hz, 2H), 7.40 – 7.32 (m, 3H), 5.04 (t, *J* = 5.5 Hz, 1H), 4.07 – 3.97 (m, 2H), 3.23 (tt, *J* = 15.1, 2.0, 2H), 1.94 (dq, *J* = 16.9, 7.5 Hz, 2H), 1.67 (d, *J* = 1.5 Hz, 3H), 1.58 (d, *J* = 1.3 Hz, 3H), 1.51 – 1.34 (m, 3H), 1.30 – 1.23 (m, 1H), 1.14 (dt, *J* = 9.3, 7.6 Hz, 1H), 0.86 (d, *J* = 6.4

Hz, 3H). **^{13}C NMR (101 MHz, Chloroform-*d*)** δ: 163.5 (t, *J* = 32.3 Hz), 155.4 (t, *J* = 292.6 Hz), 140.7, 140.3, 131.5, 128.9, 128.8, 128.8, 127.6, 127.1, 127.0, 124.3, 117.3 – 110.6 (m), 84.6 (t, *J* = 4.2 Hz), 65.5, 36.8, 33.9 (t, *J* = 25.5 Hz), 34.9, 29.3, 25.7, 25.3, 19.3, 17.6. **^{19}F NMR (376 MHz, Chloroform-*d*)** δ: -86.09 (d, *J* = 4.7 Hz), -104.13, -104.17 (d, *J* = 3.4 Hz), -104.21. **HRMS (DART-TOF)** calculated for $C_{27}H_{28}F_4NaO^+$ $[M+Na-H_2O]^+$ m/z 467.1968, found 467.1994.



3af

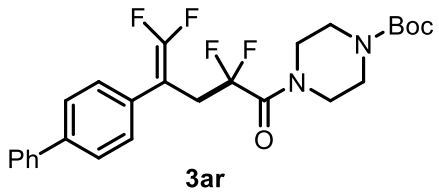
(1S,2R,5S)-2-Isopropyl-5-methylcyclohexyl 4-([1,1'-biphenyl]-4-yl)-2,2,5,5-tetrafluoropent-4-enoate (3af). General Procedure was used to prepare the desired product **3af**. Chromatographic purification on silica gel using petroleum ether/ethyl acetate (5/1) as eluent afforded **3af** as a colorless oil (29.1 mg, 0.063 mmol, 63%). **^{1}H NMR (400 MHz, Chloroform-*d*)** δ: 7.59 (d, *J* = 7.7 Hz, 4H), 7.40 (dd, *J* = 20.0, 13.5 Hz, 5H), 4.75 (td, *J* = 11.0, 4.4 Hz, 1H), 3.23 (tt, *J* = 15.5, 2.2, 2H), 1.83 (dq, *J* = 12.9, 6.7, 5.5 Hz, 2H), 1.68 (td, *J* = 12.0, 10.2, 5.6 Hz, 2H), 1.45 (t, *J* = 11.4 Hz, 2H), 1.05 (t, *J* = 12.9 Hz, 1H), 0.89 (d, *J* = 6.9 Hz, 4H), 0.84 (d, *J* = 6.5 Hz, 4H), 0.74 (d, *J* = 6.9 Hz, 3H). **^{13}C NMR (101 MHz, Chloroform-*d*)** δ: 163.2 (t, *J* = 32.0 Hz), 155.4 (t, *J* = 292.5 Hz), 140.6, 140.3, 131.4 (t, *J* = 3.6 Hz), 129.5 – 129.3 (m), 128.8, 127.5, 127.1, 127.0, 114.7 (t, *J* = 253.2 Hz), 84.7 (t, *J* = 19.8 Hz), 46.8, 40.0, 34.0, 33.7 (t, *J* = 25.1 Hz), 31.4, 26.1, 23.3, 21.9, 20.6, 16.1. **^{19}F NMR (376 MHz, Chloroform-*d*)** δ: -85.59 (dd, *J* = 29.7, 5.6 Hz), -86.12 (d, *J* = 29.0 Hz), -103.26 (td, *J* = 15.0, 5.2 Hz), -103.59 (td, *J* = 16.3, 6.3 Hz). **HRMS (DART-TOF)** calculated for $C_{27}H_{31}F_4O_2^+$ $[M+H]^+$ m/z 463.2255, found 463.2263.



3ag

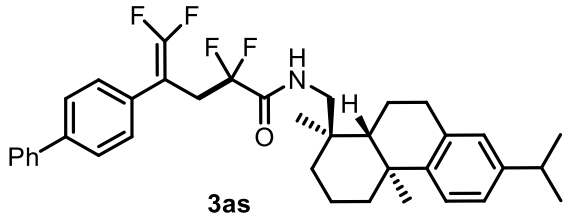
(3S,8S,9S,10R,13R,14S,17R)-10,13-Dimethyl-17-((R)-6-methylheptan-2-yl)-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1*H*-cyclopenta[*a*]phenanthren-3-yl 4-([1,1'-biphenyl]-4-yl)-2,2,5,5-tetrafluoropent-4-enoate (3ag). General Procedure was used to prepare the desired product **3ag**. Chromatographic purification on silica gel using petroleum ether/ethyl acetate (5/1) as eluent afforded **3ag** as a white solid (65.7 mg, 0.095 mmol, 95%); **Mp:** 83.9-85.2 °C. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ: 7.58 (dd, *J* = 7.9, 4.4 Hz, 4H), 7.43 (t, *J* = 7.5 Hz, 2H), 7.36 (t, *J* = 7.1 Hz, 3H), 5.28 (dd, *J* = 5.1, 2.5 Hz, 1H), 4.48 (dt, *J* = 11.5, 6.2 Hz, 1H), 3.33 – 3.06 (m, 2H), 2.23 (dd, *J* = 11.8, 2.9 Hz, 1H), 2.16 (dd, *J* = 5.2, 2.1 Hz, 1H), 2.05 – 1.64 (m, 6H), 1.63 – 1.20 (m, 9H), 1.20 – 0.98 (m, 10H), 0.94 – 0.81 (m, 13H), 0.66 (s, 3H). **^{13}C NMR (101 MHz, Chloroform-*d*)** δ: 162.9 (t, *J* = 32.1 Hz), 155.4 (t, *J* = 292.5 Hz), 140.8, 140.3, 138.7, 131.1 (t, *J* = 3.4 Hz), 128.9 (t, *J* = 3.1 Hz), 128.8, 127.5, 127.2, 127.1, 123.4, 114.5 (t, *J* = 254.0 Hz), 84.9 (t, *J* = 20.0 Hz), 56.7, 56.2, 49.9, 42.3, 39.7, 39.5, 37.4,

36.8, 36.5, 36.2, 35.8, 33.9 (t, *J* = 25.2 Hz), 31.8 (d, *J* = 2.5 Hz), 31.6, 28.2, 28.0, 27.2, 24.3, 23.9, 22.8, 22.7, 22.6, 21.0, 19.2, 18.7, 14.1, 11.8. **^{19}F NMR (376 MHz, Chloroform-*d*)** δ: -85.83 (dd, *J* = 29.0, 4.7 Hz), -86.17 (d, *J* = 29.1 Hz), -103.84 (d, *J* = 5.3 Hz), -103.88 (d, *J* = 5.4 Hz), -103.92 (d, *J* = 5.2 Hz). **HRMS (DART-TOF)** calculated for $C_{44}H_{57}F_4O_2^+$ $[M+H]^+$ m/z 693.4289, found 693.4309.



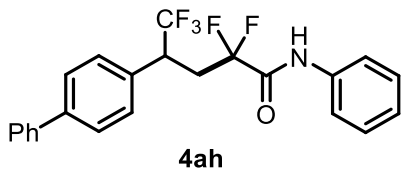
3ar

***Tert*-butyl 4-(4-([1,1'-biphenyl]-4-yl)-2,2,5,5-tetrafluoropent-4-enoyl)piperazine-1-carboxylate (3ar). General Procedure** was used to prepare the desired product **3ar**. Chromatographic purification on silica gel using petroleum ether/ethyl acetate (5/1) as eluent afforded **3ar** as a white solid (29.0 mg, 0.059 mmol, 59%); **Mp:** 95.2-96.3 °C. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ: 7.63 – 7.54 (m, 4H), 7.48 – 7.38 (m, 4H), 7.37 – 7.31 (m, 1H), 3.68 – 3.59 (m, 2H), 3.56 (d, *J* = 5.5 Hz, 2H), 3.47 – 3.29 (m, 6H), 1.45 (s, 9H). **^{13}C NMR (101 MHz, Chloroform-*d*)** δ: 162.9 – 160.1 (m), 158.3 – 152.4 (m), 154.4, 140.4, 132.2, 128.8, 128.6, 128.6, 127.5, 127.1, 127.0, 121.0 – 115.0 (m), 85.1 – 84.5 (m), 80.5, 45.6, 43.0, 33.5 (t, *J* = 22.8 Hz), 28.3. **^{19}F NMR (376 MHz, Chloroform-*d*)** δ: -86.37, -98.59 (t, *J* = 18.7 Hz). **HRMS (DART-TOF)** calculated for $C_{26}H_{28}F_4N_2NaO_3^+$ $[M+Na]^+$ m/z 515.1928, found 515.1930.



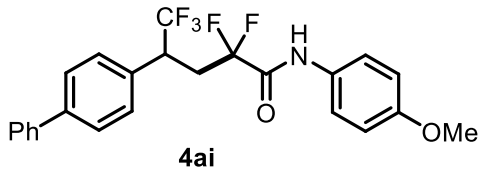
3as

4-([1,1'-Biphenyl]-4-yl)-2,2,5,5-tetrafluoro-*N*-(((1R,4aS,10aR)-7-isopropyl-1,4a-dimethyl-1,2,3,4,4a,9,10,10a-octahydrophenanthren-1-yl)methyl)pent-4-enamide (3as). General Procedure was used to prepare the desired product **3as**. Chromatographic purification on silica gel using petroleum ether/ethyl acetate (5/1) as eluent afforded **3as** as a yellow oil (35.5 mg, 0.06 mmol, 60%). **^{1}H NMR (400 MHz, Chloroform-*d*)** δ: 7.62 – 7.51 (m, 4H), 7.43 (dd, *J* = 8.4, 6.8 Hz, 2H), 7.41 – 7.29 (m, 3H), 7.15 (d, *J* = 8.2 Hz, 1H), 6.99 (dd, *J* = 8.1, 2.0 Hz, 1H), 6.91 – 6.82 (m, 1H), 6.16 (s, 1H), 3.28 (t, *J* = 16.3 Hz, 2H), 3.07 (t, *J* = 6.7 Hz, 2H), 2.94 – 2.70 (m, 3H), 2.28 (d, *J* = 12.8 Hz, 1H), 1.85 – 1.50 (m, 4H), 1.46 – 1.24 (m, 4H), 1.22 (s, 3H), 1.20 (d, *J* = 2.4 Hz, 6H), 0.90 (s, 3H). **^{13}C NMR (101 MHz, Chloroform-*d*)** δ: 163.7 (t, *J* = 28.0 Hz), 158.6 – 152.2 (m), 146.8, 145.7, 140.5, 140.3, 134.5, 131.2, 128.8, 128.6 (t, *J* = 3.1 Hz), 127.5, 127.1, 127.0, 126.9, 124.2, 123.9, 120.3 – 115.8 (m), 85.1 – 84.6 (m), 50.1, 45.9, 38.2, 37.5, 37.2, 36.1, 33.4, 33.0 – 32.3 (m), 30.1, 25.3, 24.0, 19.0, 18.5, 18.4. **^{19}F NMR (376 MHz, Chloroform-*d*)** δ: -85.58 – -85.95 (m), -86.21 (d, *J* = 29.3 Hz), -103.89 (td, *J* = 17.3, 4.5 Hz), -104.01 – -104.18 (m). **HRMS (DART-TOF)** calculated for $C_{37}H_{41}F_4KNO^+$ $[M+K]^+$ m/z 630.2756, found 630.2688.



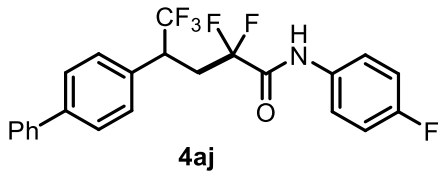
4ah

4-([1,1'-Biphenyl]-4-yl)-2,2,5,5,5-pentafluoro-*N*-phenylpentanamide (4ah). General Procedure was used to prepare the desired product **4ah**. Chromatographic purification on silica gel using petroleum ether/ethyl acetate (5/1) as eluent afforded **4ah** as a white solid (21.8 mg, 0.052 mmol, 52%); **Mp:** 129.3-130.6 °C. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ: 7.66 (s, 1H), 7.52 (d, *J* = 8.3 Hz, 2H), 7.48 – 7.31 (m, 9H), 7.31 – 7.24 (m, 2H), 7.19 – 7.08 (m, 1H), 3.81 – 3.66 (m, 1H), 3.14 – 2.82 (m, 2H). **^{13}C NMR (101 MHz, Chloroform-*d*)** δ: 160.8 (t, *J* = 27.9 Hz), 141.8, 140.2, 135.5, 131.6, 129.6, 129.1, 128.7, 127.6, 127.5, 127.1, 126.1 (q, *J* = 286.8 Hz), 125.7, 120.1, 116.7 (t, *J* = 254.7 Hz), 44.4 (q, *J* = 27.7 Hz), 33.5 (t, *J* = 23.9 Hz). **^{19}F NMR (376 MHz, Chloroform-*d*)** δ: -70.24 (d, *J* = 9.2 Hz), -100.52 (t, *J* = 15.4 Hz), -101.21 (t, *J* = 15.5 Hz), -105.32 (t, *J* = 16.7 Hz), -106.01 (t, *J* = 16.7 Hz). **HRMS (DART-TOF)** calculated for $C_{23}H_{18}F_5NNaO^+$ $[M+Na]^+$ m/z 442.1201, found 442.1199.



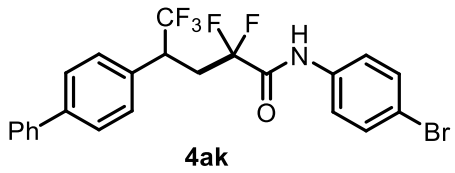
4ai

4-([1,1'-Biphenyl]-4-yl)-2,2,5,5,5-pentafluoro-*N*-(4-methoxyphenyl)pentanamide (4ai). General Procedure was used to prepare the desired product **4ai**. Chromatographic purification on silica gel using petroleum ether/ethyl acetate (5/1) as eluent afforded **4ai** as a yellow solid (17.1 mg, 0.038 mmol, 38%); **Mp:** 119.1-120.6 °C. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ: 7.60 – 7.51 (m, 3H), 7.52 – 7.46 (m, 2H), 7.47 – 7.35 (m, 5H), 7.25 (d, *J* = 8.9 Hz, 2H), 6.84 – 6.79 (m, 2H), 3.79 – 3.74 (m, 4H), 3.12 – 2.86 (m, 2H). **^{13}C NMR (101 MHz, Chloroform-*d*)** δ: 160.6 (t, *J* = 27.9 Hz), 157.3, 141.8, 140.2, 131.6, 129.6, 128.7, 128.5, 127.6, 127.4, 127.1, 126.1 (d, *J* = 287.0 Hz), 121.8, 114.5 (t, *J* = 233.9 Hz), 114.3, 55.4, 45.5 – 43.3 (m), 33.5 (t, *J* = 24.4 Hz). **^{19}F NMR (376 MHz, Chloroform-*d*)** δ: -70.27 (d, *J* = 9.1 Hz), -100.19 (t, *J* = 15.2 Hz), -100.87 (t, *J* = 15.1 Hz), -105.68 (t, *J* = 16.7 Hz), -106.36 (td, *J* = 16.6, 3.9 Hz). **HRMS (DART-TOF)** calculated for $C_{24}H_{20}F_5NNaO_2^+$ $[M+Na]^+$ m/z 472.1306, found 472.1315.



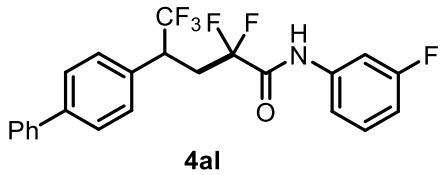
4aj

4-([1,1'-Biphenyl]-4-yl)-2,2,5,5,5-pentafluoro-*N*-(4-fluorophenyl)pentanamide (4aj). General Procedure was used to prepare the desired product **4aj**. Chromatographic purification on silica gel using petroleum ether/ethyl acetate (5/1) as eluent afforded **4aj** as a white solid (24.5 mg, 0.056 mmol, 56%); **Mp:** 137.3-138.6 °C. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ: 7.62 (s, 1H), 7.55 – 7.49 (m, 2H), 7.47 – 7.32 (m, 7H), 7.31 – 7.26 (m, 2H), 6.99 – 6.90 (m, 2H), 3.81 – 3.66 (m, 1H), 3.12 – 2.82 (m, 2H). **^{13}C NMR (101 MHz, Chloroform-*d*)** δ: 160.8 (t, *J* = 27.8 Hz), 160.1 (d, *J* = 245.8 Hz), 141.9, 140.0, 131.5, 131.5 (d, *J* = 2.9 Hz), 129.6, 128.8, 127.7, 127.4, 127.0, 126.1 (q, *J* = 294.4 Hz), 122.0 (d, *J* = 8.1 Hz), 116.7 (d, *J* = 256.9 Hz), 115.9 (d, *J* = 22.8 Hz), 44.9 – 44.1 (m), 33.7 – 33.2 (m). **^{19}F NMR (376 MHz, Chloroform-*d*)** δ: -70.27, -99.24 – -102.25 (m), -106.33 (dd, *J* = 258.7, 16.7 Hz), -115.80 (d, *J* = 8.1 Hz). **HRMS (DART-TOF)** calculated for $C_{23}H_{17}F_6NNaO^+$ $[M+Na]^+$ m/z 460.1107, found 460.1116.



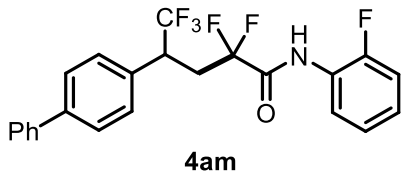
4ak

4-([1,1'-Biphenyl]-4-yl)-*N*-(4-bromophenyl)-2,2,5,5,5-pentafluoropentanamide (4ak). General Procedure was used to prepare the desired product **4ak**. Chromatographic purification on silica gel using petroleum ether/ethyl acetate (5/1) as eluent afforded **4ak** as a white solid (45.7 mg, 0.092 mmol, 92%); **Mp:** 101.3-102.3 °C. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ: 7.62 (s, 1H), 7.55 – 7.49 (m, 2H), 7.48 – 7.34 (m, 9H), 7.27 – 7.22 (m, 2H), 3.84 – 3.66 (m, 1H), 3.18 – 2.80 (m, 2H). **^{13}C NMR (101 MHz, Chloroform-*d*)** δ: 161.7 – 160.0 (m), 141.9, 140.0, 134.6, 132.2, 131.2, 129.6, 128.8, 127.7, 127.4, 127.0, 126.0 (q, *J* = 280.5 Hz), 121.5, 118.6, 116.6 (t, *J* = 257.4 Hz), 44.6 – 44.2 (m), 33.7 – 33.2 (m). **^{19}F NMR (376 MHz, Chloroform-*d*)** δ: -70.29 (d, *J* = 9.0 Hz), -99.43 (t, *J* = 14.8 Hz), -100.12 (t, *J* = 14.7 Hz), -106.46 (dd, *J* = 18.5, 15.2 Hz), -107.01 – -107.27 (m). **HRMS (DART-TOF)** calculated for $C_{23}H_{17}F_5NNaO^+$ $[M+Na]^+$ m/z 520.0306, found 520.0304.



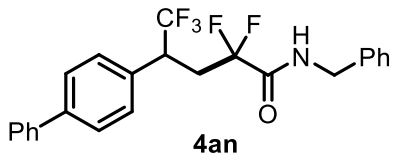
4al

4-([1,1'-Biphenyl]-4-yl)-2,2,5,5,5-pentafluoro-*N*-(3-fluorophenyl)pentanamide (4al). General Procedure was used to prepare the desired product **4al**. Chromatographic purification on silica gel using petroleum ether/ethyl acetate (5/1) as eluent afforded **4al** as a white solid (35.0 mg, 0.08 mmol, 80%); **Mp:** 119.2-121.0 °C. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ: 7.68 (s, 1H), 7.57 – 7.51 (m, 2H), 7.50 – 7.29 (m, 8H), 7.23 (td, *J* = 8.2, 6.3 Hz, 1H), 7.05 – 6.97 (m, 1H), 6.85 (td, *J* = 8.3, 2.5 Hz, 1H), 3.82 – 3.66 (m, 1H), 3.14 – 2.84 (m, 2H). **^{13}C NMR (101 MHz, Chloroform-*d*)** δ: 162.8 (d, *J* = 246.3 Hz), 161.0 (t, *J* = 28.2 Hz), 141.9, 140.0, 137.0 (d, *J* = 10.7 Hz), 131.4 (d, *J* = 2.0 Hz), 130.3 (d, *J* = 9.2 Hz), 129.6, 128.7, 127.6, 127.5, 127.0, 126.0 (q, *J* = 280.0 Hz), 116.6 (t, *J* = 257.0 Hz), 115.4 (d, *J* = 3.1 Hz), 112.5 (d, *J* = 21.3 Hz), 107.7 (d, *J* = 26.5 Hz), 45.3 – 43.1 (m), 33.5 (t, *J* = 23.8 Hz). **^{19}F NMR (376 MHz, Chloroform-*d*)** δ: -70.27, -100.43 (dd, *J* = 259.4, 15.3 Hz), -104.16 – -109.56 (m), -110.62 (d, *J* = 6.7 Hz). **HRMS (DART-TOF)** calculated for $C_{23}H_{17}F_6NNaO^+$ $[M+Na]^+$ m/z 460.1107, found 460.1112.



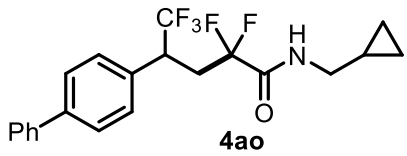
4am

4-([1,1'-Biphenyl]-4-yl)-2,2,5,5,5-pentafluoro-*N*-(2-fluorophenyl)pentanamide (4am). General Procedure was used to prepare the desired product **4am**. Chromatographic purification on silica gel using petroleum ether/ethyl acetate (5/1) as eluent afforded **4am** as a pale yellow solid (40.6 mg, 0.093 mmol, 93%); **Mp:** 118.1-19.3 °C. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ: 8.03 (dd, *J* = 10.3, 5.5 Hz, 1H), 7.90 (s, 1H), 7.53 – 7.45 (m, 2H), 7.44 – 7.28 (m, 7H), 7.09 – 6.97 (m, 3H), 3.85 – 3.65 (m, 1H), 3.13 – 2.82 (m, 2H). **^{13}C NMR (101 MHz, Chloroform-*d*)** δ: 160.9 (t, *J* = 28.4 Hz), 152.5 (d, *J* = 244.9 Hz), 141.8, 140.1, 131.3 – 131.2 (m), 129.56, 128.7, 127.5, 127.4, 127.2 (q, *J* = 258.8 Hz), 127.1, 125.8 (d, *J* = 7.7 Hz), 124.7 (d, *J* = 3.8 Hz), 124.2 (d, *J* = 10.2 Hz), 121.5. 115.0 (d, *J* = 18.9 Hz), 44.8 – 43.6 (m), 33.5 (t, *J* = 23.9 Hz). **^{19}F NMR (376 MHz, Chloroform-*d*)** δ: -70.27 (d, *J* = 9.0 Hz), -100.27 (d, *J* = 259.3 Hz), -103.88 – -110.84 (m), -130.66 (d, *J* = 3.3 Hz). **HRMS (DART-TOF)** calculated for $C_{23}H_{17}F_6NNaO^+$ $[M+Na]^+$ m/z 460.1107, found 460.1128.



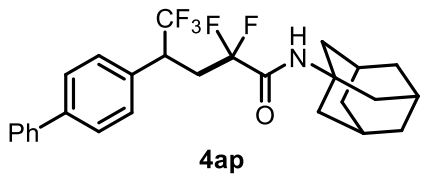
4an

4-([1,1'-Biphenyl]-4-yl)-*N*-benzyl-2,2,5,5,5-pentafluoropentanamide (4an). General Procedure was used to prepare the desired product **4an**. Chromatographic purification on silica gel using petroleum ether/ethyl acetate (5/1) as eluent afforded **4an** as a pale yellow solid (29.4 mg, 0.068 mmol, 68%); **Mp:** 87.6-89.3 °C. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ: 7.58 (dt, *J* = 8.3, 1.8 Hz, 4H), 7.44 (t, *J* = 7.7 Hz, 2H), 7.39 – 7.27 (m, 6H), 7.18 (dd, *J* = 7.5, 2.1 Hz, 2H), 6.35 (s, 1H), 4.41 (dd, *J* = 14.6, 6.1 Hz, 1H), 4.19 (dd, *J* = 14.6, 5.4 Hz, 1H), 3.71 (td, *J* = 9.3, 4.6 Hz, 1H), 2.99 – 2.81 (m, 2H). **^{13}C NMR (101 MHz, Chloroform-*d*)** δ: 163.1 (t, *J* = 28.5 Hz), 141.6, 140.2, 136.4, 132.1, 129.6, 128.9, 128.9, 128.1, 127.9, 127.6, 127.3, 127.1, 126.1 (q, *J* = 277.0 Hz), 116.7 (t, *J* = 254.3 Hz), 44.4 – 44.0 (m), 43.6, 33.9 – 32.9 (m). **^{19}F NMR (376 MHz, Chloroform-*d*)** δ: -70.29 (d, *J* = 9.1 Hz), -102.15 (t, *J* = 16.5 Hz), -102.84 (t, *J* = 16.4 Hz), -104.76 (t, *J* = 16.2 Hz), -105.45 (t, *J* = 16.1 Hz). **HRMS (DART-TOF)** calculated for $C_{24}H_{20}F_5NNaO^+$ $[M+Na]^+$ m/z 456.1357, found 456.1359.



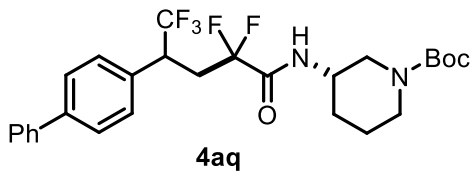
4ao

4-([1,1'-Biphenyl]-4-yl)-*N*-(cyclopropylmethyl)-2,2,5,5,5-pentafluoropentanamide (4ao). General Procedure was used to prepare the desired product **4ao**. Chromatographic purification on silica gel using petroleum ether/ethyl acetate (5/1) as eluent afforded **4ao** as a white solid (32.9 mg, 0.083 mmol, 83%); **Mp:** 95-96 °C. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ: 7.57 (dd, *J* = 7.8, 4.4 Hz, 4H), 7.44 (dd, *J* = 8.4, 6.7 Hz, 2H), 7.37 (t, *J* = 7.3 Hz, 3H), 6.21 (s, 1H), 3.72 (td, *J* = 9.4, 4.0 Hz, 1H), 3.15 – 2.95 (m, 1H), 2.97 – 2.74 (m, 3H), 0.99 – 0.70 (m, 1H), 0.56 – 0.34 (m, 2H), 0.15 (d, *J* = 4.8 Hz, 2H). **^{13}C NMR (101 MHz, Chloroform-*d*)** δ: 163.0 (t, *J* = 28.0 Hz), 141.6, 140.2, 132.1 (d, *J* = 2.2 Hz), 129.6, 128.8, 127.6, 127.3, 127.0, 126.1 (q, *J* = 279.6 Hz), 119.9 – 112.5 (m), 44.5, 44.4 – 43.9 (m), 33.5 (t, *J* = 24.4 Hz), 10.1, 3.5, 3.5. **^{19}F NMR (376 MHz, Chloroform-*d*)** δ: -70.28 (d, *J* = 9.2 Hz), -102.08 (t, *J* = 16.2 Hz), -102.77 (t, *J* = 16.2 Hz), -105.37 (t, *J* = 16.3 Hz), -106.05 (t, *J* = 16.3 Hz). **HRMS (DART-TOF)** calculated for $C_{21}H_{20}F_5NNaO^+$ $[M+Na]^+$ m/z 420.1357, found 420.1357.



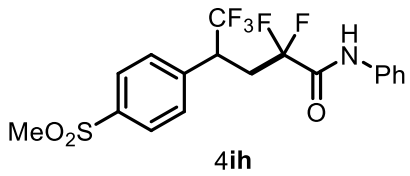
4ap

4-([1,1'-Biphenyl]-4-yl)-*N*-((3s,5s,7s)-adamantan-1-yl)-2,2,5,5,5-pentafluoropentanamide (4ap). General Procedure was used to prepare the desired product **4ap**. Chromatographic purification on silica gel using petroleum ether/ethyl acetate (5/1) as eluent afforded **4ap** as a colorless oil (30.1 mg, 0.063 mmol, 63%). **^{1}H NMR (400 MHz, Chloroform-*d*)** δ: 7.64 – 7.53 (m, 4H), 7.48 – 7.32 (m, 5H), 5.79 (s, 1H), 3.70 (pd, *J* = 9.4, 3.7 Hz, 1H), 2.98 – 2.71 (m, 2H), 2.09 – 1.99 (m, 3H), 1.87 (s, 6H), 1.63 (d, *J* = 3.1 Hz, 6H). **^{13}C NMR (101 MHz, Chloroform-*d*)** δ: 161.8 (t, *J* = 27.0 Hz), 141.6, 140.4, 132.3, 129.6, 128.8, 127.6, 127.4, 127.1, 52.6, 126.2 (q, *J* = 286.2 Hz), 120.9 – 112.2 (m), 44.8 – 44.2 (m), 41.1, 36.1, 33.3 (t, *J* = 24.3 Hz), 29.3. **^{19}F NMR (376 MHz, Chloroform-*d*)** δ: -70.27 (d, *J* = 9.1 Hz), -101.04 (t, *J* = 16.2 Hz), -101.73 (t, *J* = 16.3 Hz), -104.13 (t, *J* = 15.9 Hz), -104.81 (t, *J* = 15.9 Hz). **HRMS (DART-TOF)** calculated for $C_{27}H_{28}F_5NKO^+$ $[M+K]^+$ m/z 516.1723, found 516.1724.



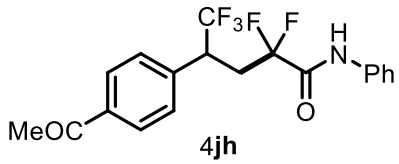
4aq

***Tert*-Butyl (3S)-3-((3-([1,1'-biphenyl]-4-yl)-1,1,4,4,4-pentafluorobutyl)amino)piperidine-1-carboxylate (4aq). General Procedure** was used to prepare the desired product **4aq**. Chromatographic purification on silica gel using petroleum ether/ethyl acetate (5/1) as eluent afforded **4aq** as a white solid (41.5 mg, 0.079 mmol, 79%); **Mp:** 115.3-116.5 °C. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ: 7.58 (dt, *J* = 8.5, 4.3 Hz, 4H), 7.41 (dt, *J* = 26.1, 7.7 Hz, 5H), 6.42 (s, 1H), 3.97 (t, *J* = 3.7 Hz, 1H), 3.82 – 3.50 (m, 2H), 3.52 – 3.29 (m, 3H), 3.28 – 3.11 (m, 1H), 2.99 – 2.66 (m, 1H), 1.75 – 1.49 (m, 4H), 1.43 (s, 9H). **^{13}C NMR (101 MHz, Chloroform-*d*)** δ: 197.3, 161.7 (t, *J* = 27.8 Hz), 138.5 (d, *J* = 1.9 Hz), 137.3, 136.3, 129.5, 128.6, 128.5, 125.8 (q, *J* = 280.0 Hz), 116.4 (t, *J* = 254.7 Hz), 50.9, 45.2 – 43.3 (m), 34.6, 34.6, 33.4 (t, *J* = 23.9 Hz), 27.8, 26.6, 24.0, 23.9. **^{19}F NMR (376 MHz, Chloroform-*d*)** δ: -70.30 (t, *J* = 11.1 Hz), -99.46 – -110.55 (m). **HRMS (DART-TOF)** calculated for $C_{27}H_{32}F_5N_2O_3^+$ $[M+K]^+$ m/z 527.2328, found 527.2331.



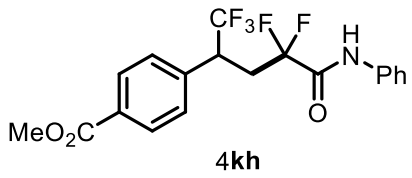
4ih

4-(1,1,1,4,4-Pentafluoro-5-oxo-5-(phenylamino)pentan-2-yl)phenyl methanesulfinate (4ih). General Procedure was used to prepare the desired product **4ih**. Chromatographic purification on silica gel using petroleum ether/ethyl acetate (5/1) as eluent afforded **4ih** as a yellow oil (21.9 mg, 0.052 mmol, 52%). **^{1}H NMR (400 MHz, Chloroform-*d*)** δ: 7.91 (d, *J* = 8.1 Hz, 2H), 7.81 (s, 1H), 7.56 (d, *J* = 8.1 Hz, 2H), 7.42 (d, *J* = 7.5 Hz, 2H), 7.34 (t, *J* = 7.9 Hz, 2H), 7.23 – 7.14 (m, 1H), 3.98 – 3.78 (m, 1H), 3.10 – 2.84 (m, 5H). **^{13}C NMR (101 MHz, Chloroform-*d*)** δ: 160.5 (t, *J* = 27.8 Hz), 141.1, 139.2, 135.5, 130.3, 129.3, 127.8, 126.0, 125.6 (q, *J* = 280.2 Hz), 120.1, 116.3 (t, *J* = 256.2 Hz), 45.3 – 44.1 (m), 44.3, 33.4 (t, *J* = 23.4 Hz). **^{19}F NMR (376 MHz, Chloroform-*d*)** δ: -69.85 (d, *J* = 8.9 Hz), -101.63 (t, *J* = 15.9 Hz), -102.32 (t, *J* = 15.9 Hz), -104.17 (t, *J* = 16.5 Hz), -104.86 (t, *J* = 16.5 Hz). **HRMS (DART-TOF)** calculated for $C_{18}H_{16}F_5KNO_3^+$ $[M+K]^+$ m/z 460.0403, found 460.0402.



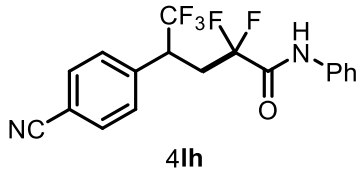
4jh

4-(4-Acetylphenyl)-2,2,5,5,5-pentafluoro-N-phenylpentanamide (4jh). General Procedure was used to prepare the desired product **4jh**. Chromatographic purification on silica gel using petroleum ether/ethyl acetate (5/1) as eluent afforded **4jh** as a white solid (29.6 mg, 0.077 mmol, 77%); **Mp:** 123.5-124.6 °C. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ: 7.89 (d, *J* = 8.4 Hz, 2H), 7.74 (s, 1H), 7.43 (d, *J* = 8.1 Hz, 2H), 7.39 – 7.34 (m, 2H), 7.31 (t, *J* = 7.9 Hz, 2H), 7.21 – 7.12 (m, 1H), 3.80 (td, *J* = 9.4, 3.8 Hz, 1H), 3.29 – 2.59 (m, 2H), 2.50 (s, 3H). **^{13}C NMR (101 MHz, Chloroform-*d*)** δ: 197.3, 160.7 (t, *J* = 27.9 Hz), 137.9 (d, *J* = 1.9 Hz), 137.3, 135.5, 129.5, 129.2, 128.7, 125.8, 125.7 (q, *J* = 280.0 Hz), 120.1, 119.2 – 113.4 (m), 45.7 – 43.2 (m), 33.4 (t, *J* = 24.0 Hz), 26.5. **^{19}F NMR (376 MHz, Chloroform-*d*)** δ: -69.98 (d, *J* = 9.1 Hz), -101.29 (t, *J* = 15.7 Hz), -101.98 (t, *J* = 15.6 Hz), -104.90 (dd, *J* = 18.1, 15.0 Hz), -105.49 – -105.67 (m). **HRMS (DART-TOF)** calculated for $C_{19}H_{17}F_5NO_2^+$ $[M+H]^+$ m/z 386.1174, found 386.1191.



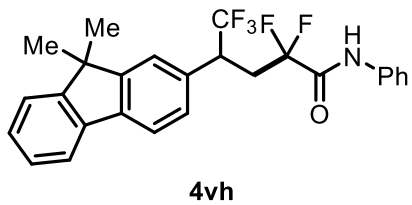
4kh

Methyl 4-(1,1,1,4,4-pentafluoro-5-oxo-5-(phenylamino)pentan-2-yl)benzoate (4kh). General Procedure was used to prepare the desired product **4kh**. Chromatographic purification on silica gel using petroleum ether/ethyl acetate (5/1) as eluent afforded **4kh** as a pale yellow solid (31.3 mg, 0.078 mmol, 78%); **Mp:** 111.7-112.7 °C. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ: 8.01 (d, *J* = 8.2 Hz, 2H), 7.73 (s, 1H), 7.47 – 7.39 (m, 4H), 7.34 (dd, *J* = 8.7, 7.1 Hz, 2H), 7.23 – 7.16 (m,1H), 3.91 (s, 3H), 3.87 – 3.75 (m, 1H), 2.96 (td, *J* = 16.1, 7.3 Hz, 2H). **^{13}C NMR (101 MHz, Chloroform-*d*)** δ: 165.3, 159.7 (t, *J* = 27.9 Hz), 136.9 (d, *J* = 2.0 Hz), 134.4, 129.6, 129.0, 128.2, 128.2, 124.8, 124.7 (q, *J* = 279.8 Hz), 119.1, 118.4 – 111.9 (m), 51.2, 43.5 (q, *J* = 28.5 Hz), 32.4 (t, *J* = 24.3 Hz). **^{19}F NMR (376 MHz, Chloroform-*d*)** δ: -69.99 (d, *J* = 9.0 Hz), -101.88 (t, *J* = 16.2 Hz), -102.57 (t, *J* = 16.2 Hz), -104.27 (t, *J* = 16.4 Hz), -104.96 (t, *J* = 16.4 Hz). **HRMS (DART-TOF)** calculated for $C_{19}H_{16}F_5NNaO_3^+$ $[M+Na]^+$ m/z 424.0943, found 424.0944.



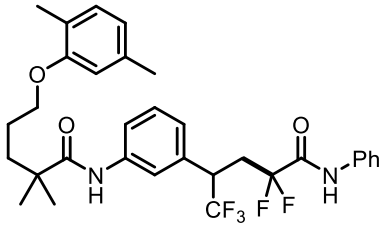
4lh

4-(4-Cyanophenyl)-2,2,5,5,5-pentafluoro-*N*-phenylpentanamide (4lh). General Procedure was used to prepare the desired product **4lh**. Chromatographic purification on silica gel using petroleum ether/ethyl acetate (5/1) as eluent afforded **4lh** as a yellow oil (18.8 mg, 0.051 mmol, 51%). **^{1}H NMR (400 MHz, Chloroform-*d*)** δ: 7.80 (s, 1H), 7.68 – 7.61 (m, 2H), 7.49 (d, *J* = 8.1 Hz, 2H), 7.45 – 7.41 (m, 2H), 7.38 (dd, *J* = 8.8, 7.1 Hz, 2H), 7.26 – 7.20 (m, 1H), 3.85 (dd, *J* = 11.2, 7.2 Hz, 1H), 3.04 – 2.85 (m, 2H). **^{13}C NMR (101 MHz, Chloroform-*d*)** δ: 160.5 (t, *J* = 27.8 Hz), 138.3 (d, *J* = 1.9 Hz), 135.4, 132.5, 130.0, 129.3, 126.1, 125.5 (q, *J* = 280.0 Hz), 120.1, 118.0, 119.3 – 113.3 (m), 113.0, 45.0 – 44.2 (m), 33.4 (t, *J* = 23.8 Hz). **^{19}F NMR (376 MHz, Chloroform-*d*)** δ: -69.92 (d, *J* = 8.9 Hz), -102.16 (d, *J* = 15.8 Hz), -102.83 (t, *J* = 16.1 Hz), -103.92 (t, *J* = 16.5 Hz), -104.63 (d, *J* = 16.5 Hz). **HRMS (DART-TOF)** calculated for $C_{18}H_{14}F_5N_2O^+$ $[M+H]^+$ m/z 369.1021, found 369.1029.



4vh

4-(9,9-Dimethyl-9H-fluoren-2-yl)-2,2,5,5,5-pentafluoro-*N*-phenylpentanamide (4vh). General Procedure was used to prepare the desired product **4vh**. Chromatographic purification on silica gel using petroleum ether/ethyl acetate (5/1) as eluent afforded **4vh** as a white solid (26.2 mg, 0.057 mmol, 57%); **Mp:** 92.4-93.8 °C. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ: 7.70 – 7.56 (m, 3H), 7.41 – 7.36 (m, 1H), 7.35 (s, 1H), 7.33 – 7.25 (m, 5H), 7.19 (t, *J* = 7.9 Hz, 2H), 7.11 – 7.02 (m, 1H), 3.89 – 3.64 (m, 1H), 3.22 – 2.74 (m, 2H), 1.41 (s, 3H), 1.38 (s, 3H). **^{13}C NMR (101 MHz, Chloroform-*d*)** δ: 160.9 (t, *J* = 28.0 Hz), 154.2, 153.8, 140.1, 138.3, 135.4, 131.5, 129.0, 128.1, 127.6, 127.0, 125.7, 123.4, 122.6, 120.2, 120.2, 126.1 (q, *J* = 279.8 Hz), 120.1, 119.5 – 113.9 (m), 46.9, 44.8 (d, *J* = 28.3 Hz), 33.7 (t, *J* = 23.5 Hz), 27.0, 26.9. **^{19}F NMR (376 MHz, Chloroform-*d*)** δ: -70.23 (d, *J* = 9.1 Hz), -100.93 (dd, *J* = 258.4, 15.7 Hz), -105.31 (dd, *J* = 258.4, 16.5 Hz). **HRMS (DART-TOF)** calculated for $C_{26}H_{22}F_5KNO^+$ $[M+K]^+$ m/z 498.1253, found 498.1252.

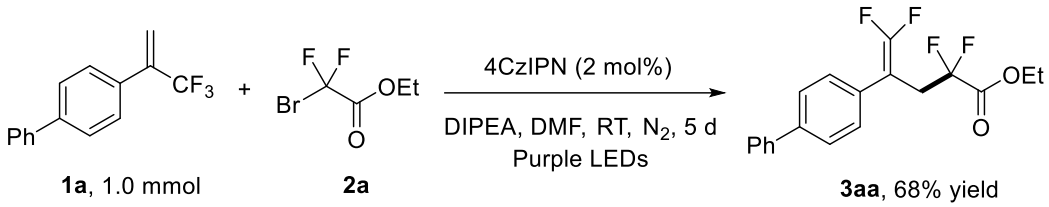


4xh

4-(3-(5-(2,5-Dimethylphenoxy)-2,2-dimethylpentanamido)phenyl)-2,2,5,5,5-pentafluoro-*N*-phenylpentanamide (4xh). General Procedure was used to prepare the desired product **4xh**. Chromatographic purification on silica gel using petroleum ether/ethyl acetate (5/1) as eluent afforded **4xh** as a yellow solid (15.3 mg, 0.026 mmol, 26%); **Mp:** 113.6-114.6 °C. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ: 7.85 (s, 1H), 7.56 (s, 1H), 7.42 – 7.35 (m, 2H), 7.32 – 7.28 (m, 2H), 7.28 – 7.24 (m, 3H), 7.18 – 7.07 (m, 2H), 7.00 (d, *J* = 7.5 Hz, 1H), 6.66 (d, *J* = 7.5 Hz, 1H), 6.61 (s, 1H), 3.94 (t, *J* = 2.9 Hz, 2H), 3.67 (td, *J* = 9.7, 3.6 Hz, 1H), 3.08 – 2.73 (m, 2H), 2.29 (s, 3H), 2.16 (s, 3H), 1.80 (s, 4H), 1.31 (s, 6H). **^{13}C NMR (101 MHz, Chloroform-*d*)** δ: 175.9, 161.0 (t, *J* = 27.9 Hz), 156.8, 138.1, 136.6, 135.7, 133.6, 130.4, 129.4, 128.9, 125.9 (q, *J* = 279.7 Hz), 125.6, 124.8, 123.5, 121.8, 121.0, 120.6, 120.3, 119.3 – 113.4 (m), 112.2, 67.9, 44.7 (d, *J* = 28.2 Hz), 42.8, 37.6, 33.6 (t, *J* = 23.7 Hz), 25.6, 25.5, 25.1, 21.4, 15.8. **^{19}F NMR (376 MHz, Chloroform-*d*)** δ: -69.99 (d, *J* = 9.0 Hz), -100.35 (t, *J* = 15.2 Hz), -101.04 (t, *J* = 15.3 Hz), -105.59 (t, *J* = 16.4 Hz), -106.28 (t, *J* = 16.5 Hz). **HRMS (DART-TOF)** calculated for $C_{32}H_{35}F_5N_2NaO_3^+$ $[M+Na]^+$ m/z 613.2460, found 613.2468.

4. Scale-Up and Transformation of Product 3aa

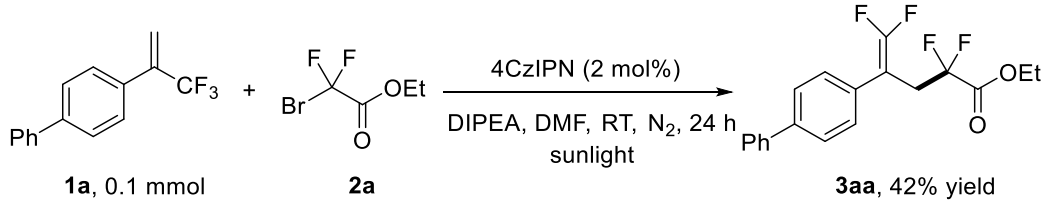
4.1 Gram-scale synthesis



1a, 1.0 mmol **2a** **3aa**, 68% yield

A mixture of 4CzIPN (0.02 mmol, 2 mol%), α-trifluoromethyl styrene **1a** (1.0 mmol, 1.0 equiv.), bromodifluoroacetate **2a** (2.0 mmol, 2.0 equiv.), DIPEA (2.0 mmol, 2.0 equiv.) and DMF (5 mL) was degassed by three cycles of freeze-pump-thaw. The mixture was irradiated by 24 W 365 nm LEDs at room temperature for 5 days. After removal of solvents, the crude mixture was purified by flash chromatography (petroleum ether/ethyl acetate) to afford the pure product **3aa** (0.24 g, 0.68 mmol, 68%).

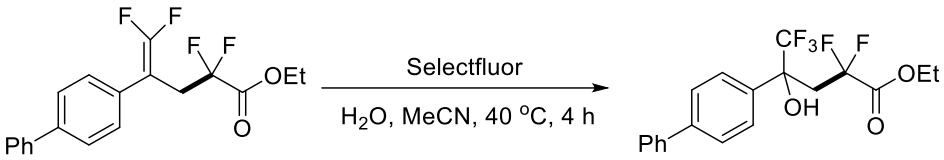
4.2 Sunlight driven experiment



1a, 0.1 mmol **2a** **3aa**, 42% yield

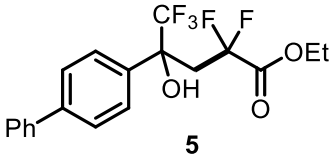
A mixture of 4CzIPN (0.002 mmol, 2 mol%), α-trifluoromethyl styrene **1a** (0.1 mmol, 1.0 equiv.), bromodifluoroacetate **2a** (0.2 mmol, 2.0 equiv.), DIPEA (0.2 mmol, 2.0 equiv.) and DMF (1 mL) was degassed by three cycles of freeze-pump-thaw. The resulting mixture was stirred upon sunlight irradiation under nitrogen atmosphere for 24 h (as an on/off visible light irradiation experiment, the reaction solution was kept in dark place at night). After completion of the reaction, the crude mixture was purified by flash chromatography (petroleum ether/ethyl acetate) to afford the product **3aa** (14.8 mg, 0.042 mmol, 42% yield).

4.3 Synthetic applications



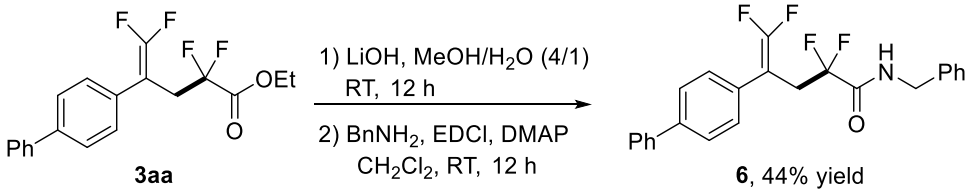
3aa **5**, 65% yield

To a 10 mL Schlenk flask was added *gem*-difluoroalkene **3aa** (35.2 mg, 0.1 mmol, 1.0 equiv.), and Selectfluor (46.0 mg, 0.13 mmol, 1.3 equiv.). Then H_2O (0.80 mmol, 14.4 μL) and CH_3CN (1 mL) was added by syringe. The reaction mixture was stirred at 40 ℃ for 4 h. After cooling to room temperature, the solvent was removed under vacuum, and the crude mixture was purified by flash chromatography (petroleum ether/ethyl acetate) to afford the product **5**.



5

Ethyl 4-([1,1'-biphenyl]-4-yl)-2,2,5,5,5-pentafluoro-4-hydroxypentanoate (5). Chromatographic purification on silica gel using petroleum ether/ethyl acetate (5/1) as eluent afforded **5** as a white solid (25.2 mg, 0.065 mmol, 65% yield); **Mp:** 115.3-116.5 °C. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ 7.68 – 7.54 (m, 6H), 7.45 (t, *J* = 7.5 Hz, 2H), 7.36 (t, *J* = 7.3 Hz, 1H), 4.09 (m, 2H), 3.27 (s, 1H), 3.10 (m, 2H), 1.25 (t, *J* = 7.1 Hz, 3H). **^{13}C NMR (101 MHz, Chloroform-*d*)** δ 163.8 (t, *J* = 31.8 Hz), 141.9, 140.1, 133.8, 128.9, 127.7, 127.5 (q, *J* = 285.9 Hz), 127.1, 127.0, 126.7, 114.4 (dd, *J* = 250.6, 250.7 Hz), 74.9 (dd, *J* = 34.0, 4.6 Hz), 63.4, 39.5 (t, *J* = 23.5 Hz), 13.7. **^{19}F NMR (376 MHz, Chloroform-*d*)** δ -80.94, -97.29 (d, *J* = 13.8 Hz), -97.99 (dd, *J* = 16.6, 11.5 Hz), -99.63 (dd, *J* = 17.8, 11.3 Hz), -100.35 (dd, *J* = 16.9, 12.3 Hz). **HRMS (DART-TOF)** calculated for $C_{19}H_{17}F_5NaO_3^+$ $[M+Na]^+$ m/z 411.0990, found 411.0981.

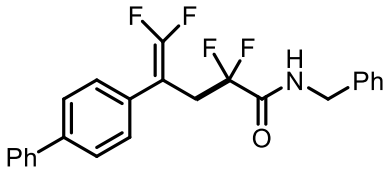


3aa **6**, 44% yield

The *gem*-difluoroalkene **3aa** (35.2 mg, 0.1 mmol, 1.0 equiv.) was dissolved in a 4:1 mixture of MeOH and water, and lithium hydroxide monohydrate was added (5 equiv.). When full conversion was observed, the resulting mixture was diluted with water and

washed with ethyl acetate. The organic layer was discarded. The aqueous layer was acidified with 2 M HCl solution and extracted with ethyl acetate (×3). The combined organic layers were dried over anhydrous Na_2SO_4. The solvent was removed in vacuo, and the resulting acid was used in the next step without further purification.

To a flame-dried round-bottom flask, EDC-HCl (1-(3-dimethylaminopropyl)-3-ethylcarbodiimide hydrochloride, 1.3 equiv.) and DMAP (1.4 equiv.) were added. The mixture was degassed and flushed with nitrogen. Dry DCM (2 mL) was added, and the mixture was cooled to 0 ℃ in an ice bath. The above the resulting acid (0.1 mmol, 1.0 equiv.) was added, and the mixture was stirred for five minutes before the benzylamine (0.12 mmol, 1.2 equiv.) was added. The ice bath was then removed and the reaction allowed to stir overnight at room temperature. The reaction was quenched with 1 M HCl and the organics were separated. The aqueous layer was then extracted with DCM twice. The organic layers were combined, dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The crude mixture was purified by flash chromatography (petroleum ether/ethyl acetate) to afford the product **6**.

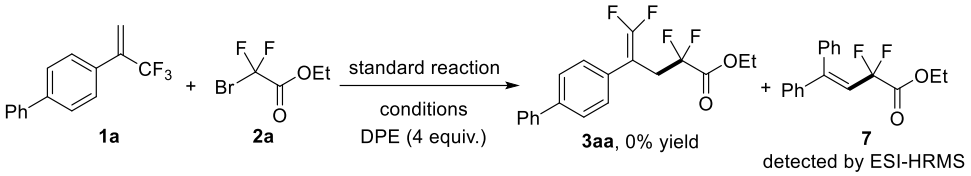


6

4-([1,1'-Biphenyl]-4-yl)-*N*-benzyl-2,2,5,5-tetrafluoropent-4-enamide (6). Chromatographic purification on silica gel using petroleum ether/ethyl acetate (5/1) as eluent afforded **6** as a white solid (18.2 mg, 0.044 mmol, 44% yield); **Mp:** 89.2-90.2 °C. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ: 7.61 – 7.51 (m, 4H), 7.44 (t, *J* = 7.6 Hz, 2H), 7.40 – 7.27 (m, 6H), 7.23 – 7.16 (m, 2H), 6.45 (s, 1H), 4.33 (d, *J* = 5.8 Hz, 2H), 3.32 (t, *J* = 16.1 Hz, 2H). **^{13}C NMR (101 MHz, Chloroform-*d*)** δ: 163.3 (t, *J* = 28.3 Hz), 155.3 (t, *J* = 292.8 Hz), 140.6, 140.3, 136.5, 131.2 (t, *J* = 3.5 Hz), 128.9, 128.8, 128.7, 128.1, 127.9, 127.5, 127.1, 127.0, 120.4 – 114.0 (m), 85.0 – 84.6 (m), 43.6, 33.1 – 32.6 (m). **^{19}F NMR (376 MHz, Chloroform-*d*)** δ: -85.74 (d, *J* = 29.8 Hz), -86.13 (d, *J* = 29.2 Hz), -104.55 (dd, *J* = 16.1, 5.2 Hz). **HRMS (DART-TOF)** calculated for $C_{24}H_{19}F_4NNaO^+$ $[M+Na]^+$ m/z 436.1295, found 436.1322.

5. Mechanistic Experiments

5.1 Radical Inhibition Experiment



To an oven-dried quartz vial, α-trifluoromethyl styrene **1a** (0.1 mmol, 1.0 equiv.) and bromodifluoroacetate **2a** (0.2 mmol, 2.0 equiv.) were added sequentially. The vial was charged with a stir bar and transferred to a glovebox, where the solids were backfilled with an inert atmosphere. In the glovebox, 4CzIPN (0.002 mmol, 2 mol%), ethene-1,1-diyldibenzene (DPE, 4.0 equiv.), and DIPEA (0.2 mmol, 2.0 equiv.) were added into the vial, followed by DMF (1.0 mL). The vial was sealed with a rubber plug, removed from the glove box, and irradiated and stir by 24 W 365 nm LEDs at room temperature for 24 h. **HRMS (DART-TOF)**: compound **7** calculated for $C_{18}H_{17}F_2O_2^+$ $[M+H]^+$ m/z 303.1191, found 303.1194.

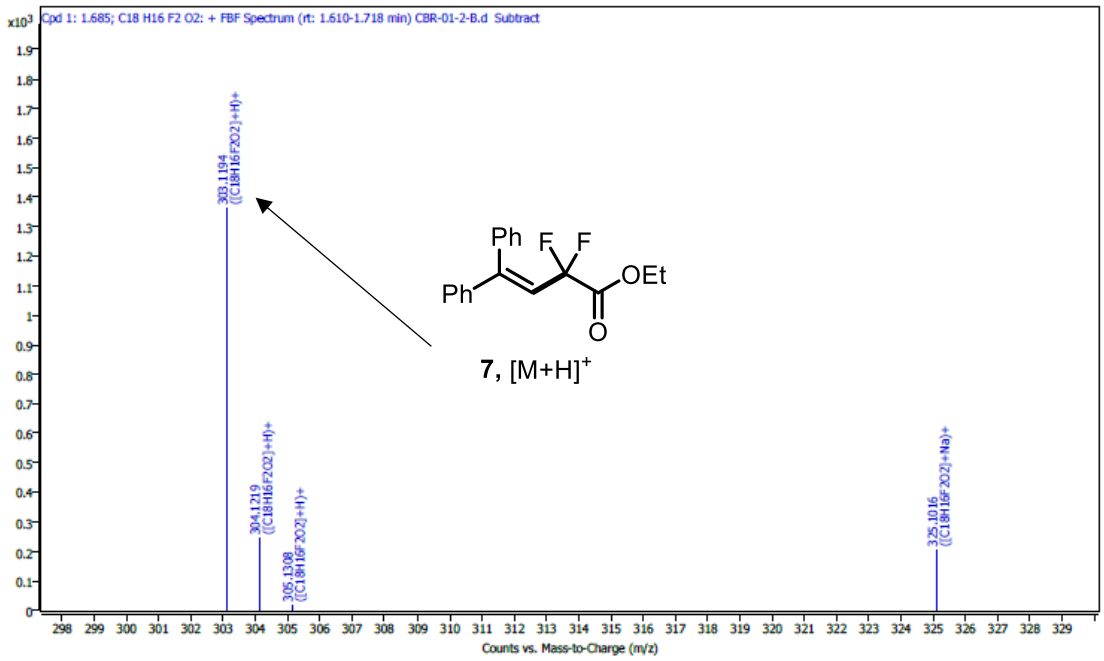
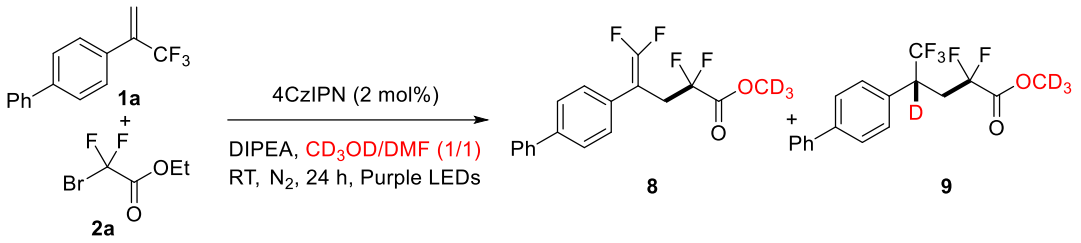
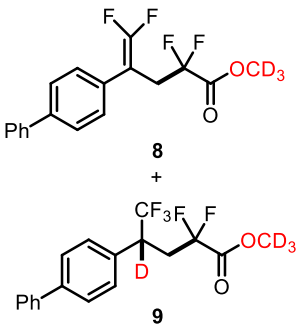


Figure S3 α-trifluoromethyl styrene **1a** and bromodifluoroacetate **2a** under standard conditions with ethene-1,1-diyldibenzene (4.0 equiv.)

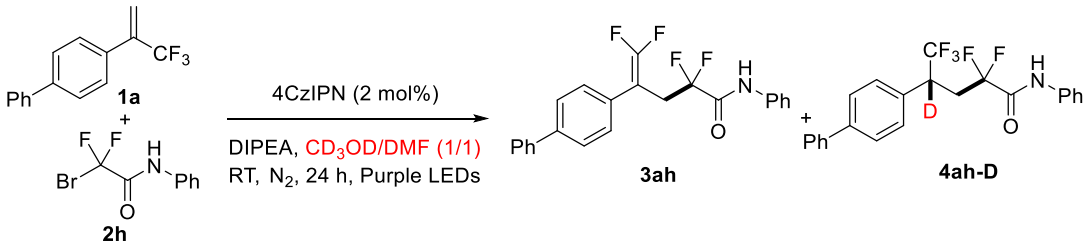
5.2 Control experiments



Procedure: To an oven-dried quartz vial, α-trifluoromethyl styrene **1a** (0.1 mmol, 1.0 equiv.) and bromodifluoroacetate **2a** (0.2 mmol, 2.0 equiv.) were added. The vial was charged with a stir bar and transferred to a glovebox, where the solids were backfilled with an inert atmosphere. In the glovebox, 4CzIPN (0.002 mmol, 2 mol%) and DIPEA (0.2 mmol, 2.0 equiv.) were added into the vial, followed by CD_3OD (0.5 mL) and DMF (0.5 mL). The vial was sealed with a rubber plug, removed from the glove box, and irradiated and stir by 24 W 365 nm LEDs at room temperature for 24 h.

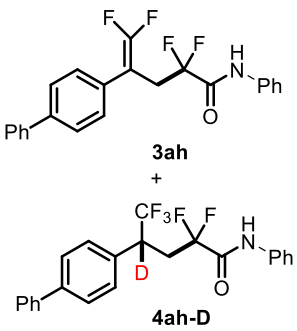


Methyl-*d*$_3$ 4-([1,1'-biphenyl]-4-yl)-2,2,5,5-tetrafluoropent-4-enoate (8) and methyl-*d*$_3$ 4-([1,1'-biphenyl]-4-yl)-2,2,5,5,5-pentafluoropentanoate-4-*d* (9). Chromatographic purification on silica gel using petroleum ether/ethyl acetate (5/1) as eluent afforded **8** and **9** as a yellow oil (0.086 mmol, 86%, **8**:**9** = 1.6:1, products **8** and **9** were inseparable). **^{1}H NMR (8, 400 MHz, Chloroform-*d*)** δ: 7.63 – 7.55 (m, 4H), 7.44 (t, *J* = 7.5 Hz, 2H), 7.40 – 7.33 (m, 3H), 3.32 – 3.16 (m, 2H). **^{19}F NMR (8, 376 MHz, Chloroform-*d*)** δ: -86.02 – -86.44 (m), -104.37 (td, *J* = 14.9, 4.8 Hz). **HRMS (8, DART-TOF)** calculated for $C_{18}H_{12}D_3F_4O_2^+$ $[M+H]^+$ m/z 342.1191, found 342.1200. **^{1}H NMR (9, 400 MHz, Chloroform-*d*)** δ: 7.63 – 7.55 (m, 4H), 7.44 (t, *J* = 7.5 Hz, 2H), 7.40 – 7.33 (m, 3H), 2.91 – 2.72 (m, 2H). **^{19}F NMR (9, 376 MHz, Chloroform-*d*)** δ -70.47, -101.47 (t, *J* = 13.2 Hz), -102.17 (t, *J* = 13.1 Hz), -106.21 – -106.86 (m), -107.14 (t, *J* = 17.4 Hz). **HRMS (9, DART-TOF)** calculated for $C_{18}H_{12}D_4F_5O_2^+$ $[M+H]^+$ m/z 363.1316, found 363.1325.

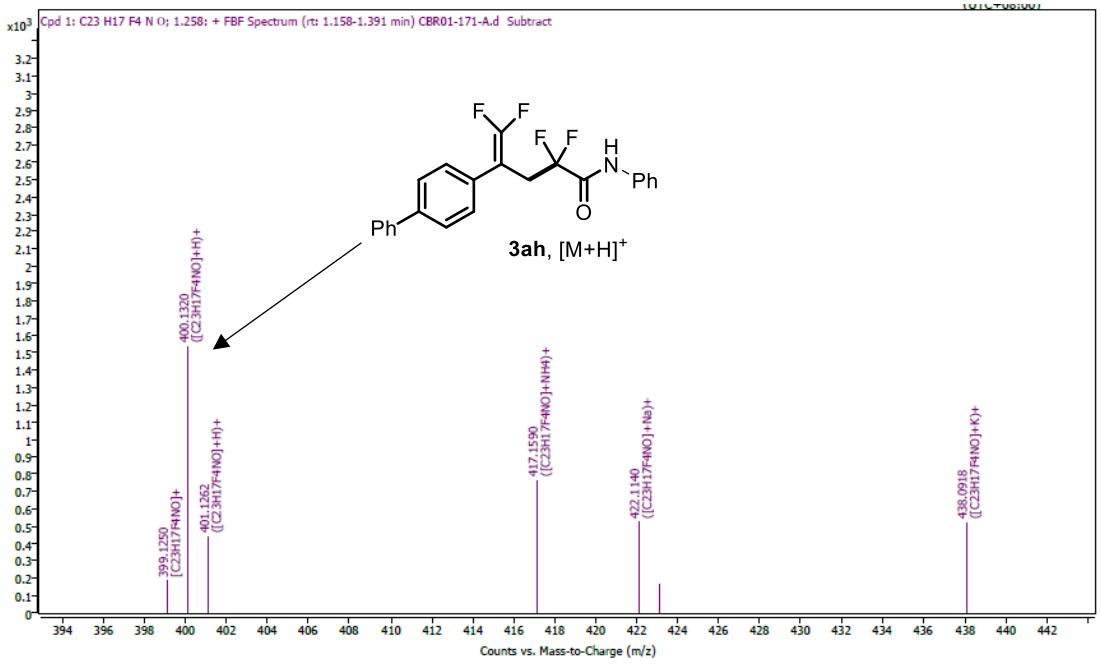


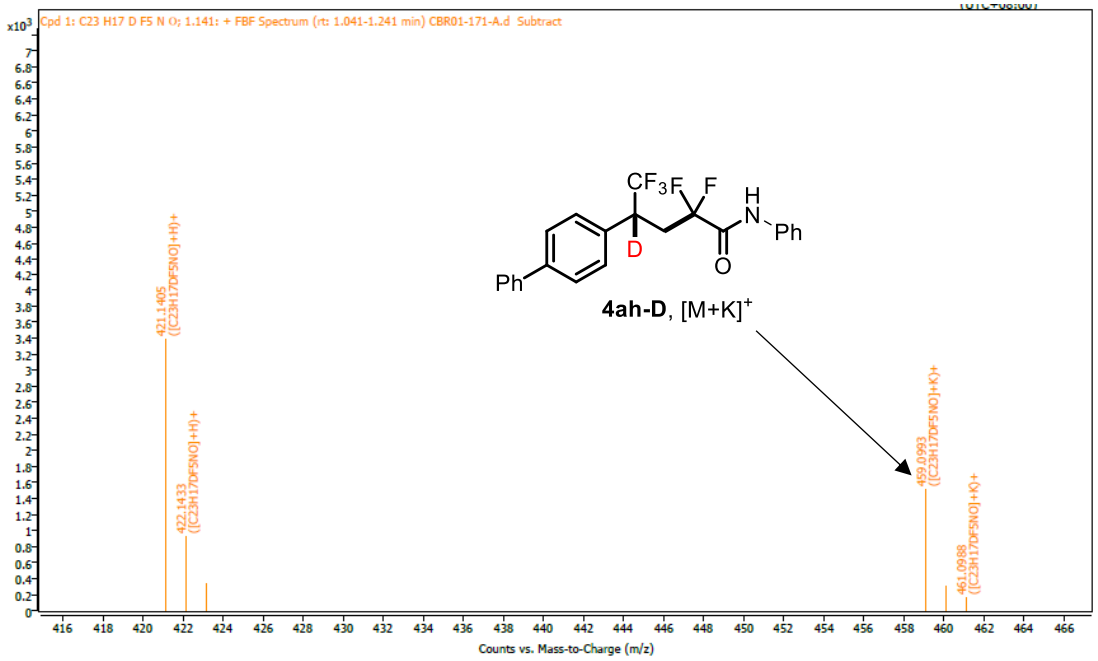
Procedure: To an oven-dried quartz vial, α-trifluoromethyl styrene **1a** (0.1 mmol, 1.0 equiv.) and bromodifluoroacetamide **2h** (0.2 mmol, 2.0 equiv.) were added. The vial was charged with a stir bar and transferred to a glovebox, where the solids were backfilled with an inert atmosphere. In the glovebox, 4CzIPN (0.002 mmol, 2 mol%) and DIPEA (0.2 mmol, 2.0 equiv.) were added into the vial, followed by CD_3OD (0.5 mL) and DMF (0.5 mL). The vial was sealed with a rubber plug, removed from the

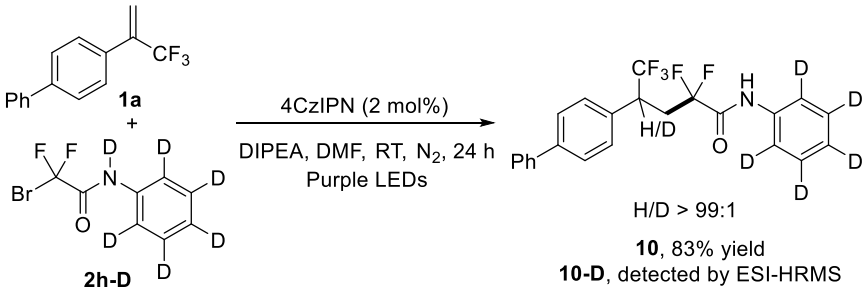
glove box, and irradiated and stir by 24 W 365 nm LEDs at room temperature for 24 h.



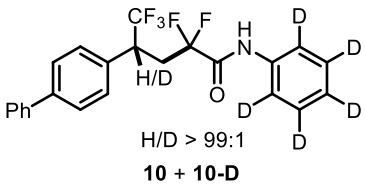
4-([1,1'-biphenyl]-4-yl)-2,2,5,5-tetrafluoro-*N*-phenylpent-4-enamide (3ah) and 4-([1,1'-biphenyl]-4-yl)-2,2,5,5,5-pentafluoro-*N*-phenylpentanamide-4-*d* (4ah-D). Chromatographic purification on silica gel using petroleum ether/ethyl acetate (5/1) as eluent afforded **3ah** and **4ah-D** as a yellow oil (0.05 mmol, 50%, **3ah**:**4ah-D** = 1:1.9, products **3ah** and **4ah-D** were inseparable). **^{1}H NMR (3ah, 400 MHz, Chloroform-*d*)** δ: 7.78 (s, 1H), 7.61 – 7.48 (m, 3H), 7.48 – 7.26 (m, 10H), 7.19 – 7.07 (m, 1H), 3.46 – 3.28 (m, 2H). **^{19}F NMR (3ah, 376 MHz, Chloroform-*d*)** δ: -85.19 – -87.27 (m), -104.37 (td, *J* = 16.0, 3.8 Hz). **HRMS (3ah, DART-TOF)** calculated for $C_{23}H_{18}F_4NO^+$ $[M+H]^+$ m/z 400.1319, found 400.1320. **^{1}H NMR (4ah-D, 400 MHz, Chloroform-*d*)** δ: 7.67 (s, 1H), 7.61 – 7.49 (m, 3H), 7.48 – 7.26 (m, 10H), 7.19 – 7.04 (m, 1H), 3.18 – 2.45 (m, 2H). **^{19}F NMR (4ah-D, 376 MHz, Chloroform-*d*)** δ -70.34, -100.49 (t, *J* = 15.4 Hz), -101.18 (t, *J* = 15.5 Hz), -105.41 (t, *J* = 16.5 Hz), -106.10 (dd, *J* = 18.5, 14.8 Hz). **HRMS (4ah-D, DART-TOF)** calculated for $C_{23}H_{17}DF_5KNO^+$ $[M+H]^+$ m/z 459.1003, found 459.0993.



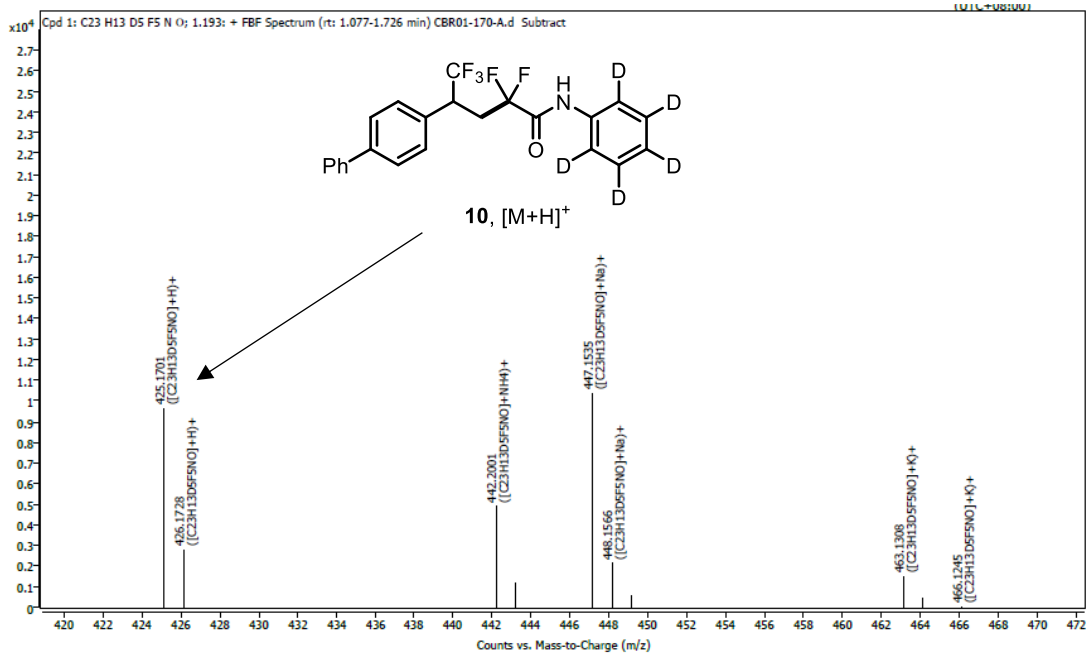


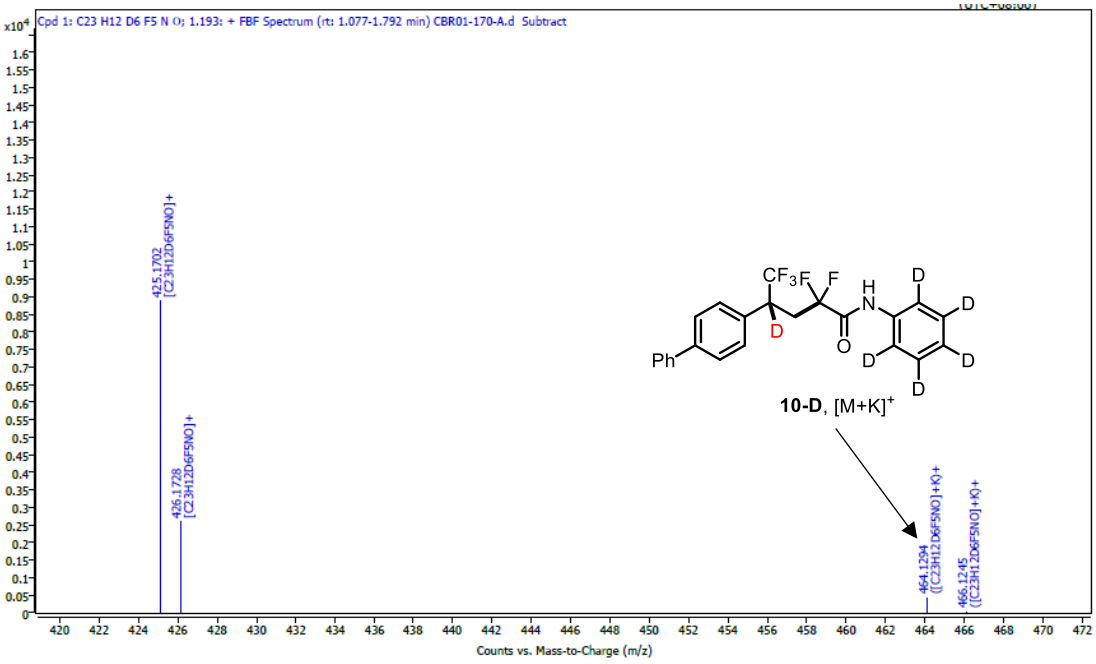


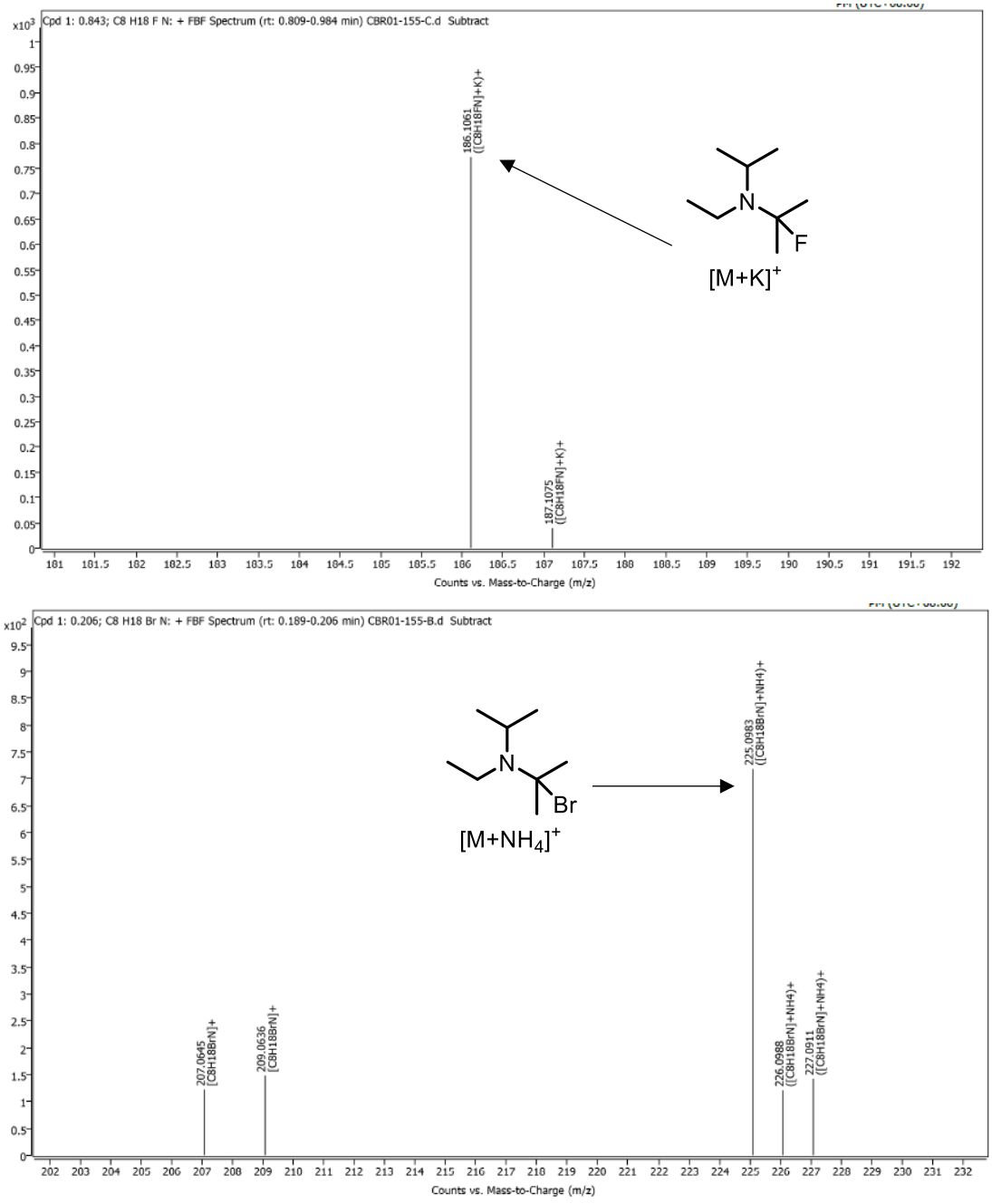
Procedure: To an oven-dried quartz vial, α-trifluoromethyl styrene **1a** (0.1 mmol, 1.0 equiv.) and deuterated bromodifluoroacetamide **2h-D** (0.2 mmol, 2.0 equiv.) were added. The vial was charged with a stir bar and transferred to a glovebox, where the solids were backfilled with an inert atmosphere. In the glovebox, 4CzIPN (0.002 mmol, 2 mol%) and DIPEA (0.2 mmol, 2.0 equiv.) were added into the vial, followed by and DMF (1.0 mL). The vial was sealed with a rubber plug, removed from the glove box, and irradiated and stir by 24 W 365 nm LEDs at room temperature for 24 h.



4-([1,1'-biphenyl]-4-yl)-2,2,5,5,5-pentafluoro-*N*-(phenyl-*d*5)pentanamide (10) and 4-([1,1'-biphenyl]-4-yl)-2,2,5,5,5-pentafluoro-*N*-(phenyl-*d*5)pentanamide-4-*d* (10-D). Chromatographic purification on silica gel using petroleum ether/ethyl acetate (5/1) as eluent afforded **10** and **10-D** as a yellow oil (0.083 mmol, 83%, products **10** and **10-D** were inseparable). **^{1}H NMR (10, 400 MHz, Chloroform-*d*)** δ: 7.66 (s, 1H), 7.52 (d, *J* = 7.9 Hz, 2H), 7.49 – 7.30 (m, 7H), 3.75 (td, *J* = 10.4, 9.9, 3.3 Hz, 1H), 3.12 – 2.84 (m, 2H). **^{19}F NMR (10, 376 MHz, Chloroform-*d*)** δ: -70.25, -100.54 (t, *J* = 15.5 Hz), -101.22 (t, *J* = 15.5 Hz), -105.38 (t, *J* = 16.7 Hz), -106.07 (t, *J* = 16.6 Hz). **HRMS (10, DART-TOF)** calculated for $C_{23}H_{14}D_5F_5NO^+$ $[M+H]^+$ m/z 425.1695, found 425.1701. **HRMS (10-D, DART-TOF)** calculated for $C_{23}H_{12}D_6F_5KNO^+$ $[M+K]^+$ m/z 464.1317, found 464.1294.

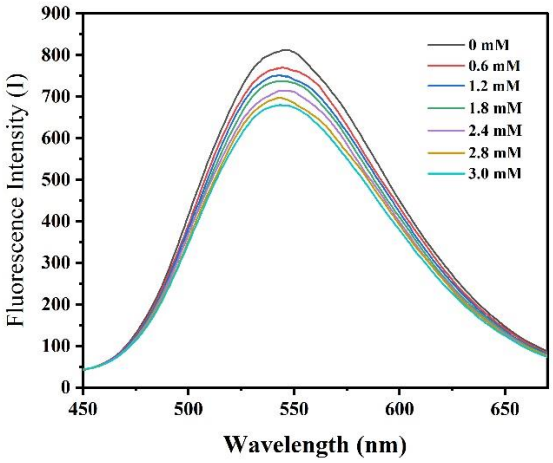

Cpd 1: C23 H13 D5 F5 N O; 1.193: + FBF Spectrum (rt: 1.077-1.726 min) CBR01-170-A.d Subtract
CF3
F
F
H
N
O
D
Ph
10, [M+H]+
425.1701 ([C23H13D5F5NO]+H)+
426.1728 ([C23H13D5F5NO]+H)+
442.2001 ([C23H13D5F5NO]+NH4)+
447.1535 ([C23H13D5F5NO]+Na)+
448.1566 ([C23H13D5F5NO]+Na)+
463.1308 ([C23H13D5F5NO]+K)+
466.1245 ([C23H13D5F5NO]+K)+
Counts vs. Mass-to-Charge (m/z)


Cpd 1: C23 H12 D6 F5 N O; 1.193: + FBF Spectrum (rt: 1.077-1.792 min) CBR01-170-A.d Subtract
CF3
F
F
H
N
O
D
Ph
10-D, [M+K]+
425.1702 [C23H12D6F5NO]+
426.1728 [C23H12D6F5NO]+
464.1294 ([C23H12D6F5NO]+K)+
466.1245 ([C23H12D6F5NO]+K)+
Counts vs. Mass-to-Charge (m/z)

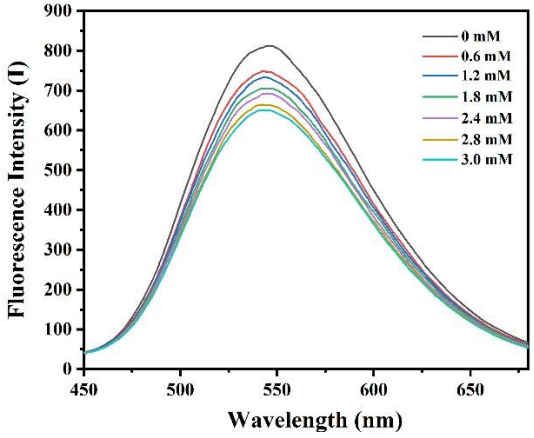


5.3 Stern-Volmer fluorescence quenching experiments

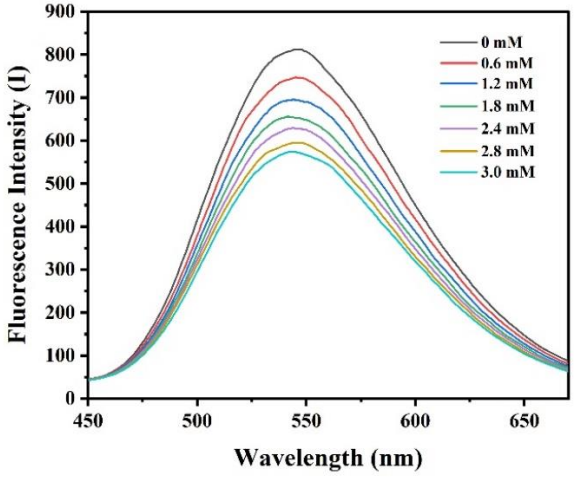
All fluorescence measurements were recorded by an Agilent Cary Eclipse fluorescence spectrophotometer. Stern-Volmer fluorescence quenching experiments were run with freshly prepared solutions of 1.5 μM 4CzIPN, in degassed dry DMF at room temperature. The solutions were irradiated at 360 nm and fluorescence was measured from 450 nm to 670 nm. Control experiments showed that the excited state 4CzIPN* was mainly quenched by **DIPEA**.



(a)

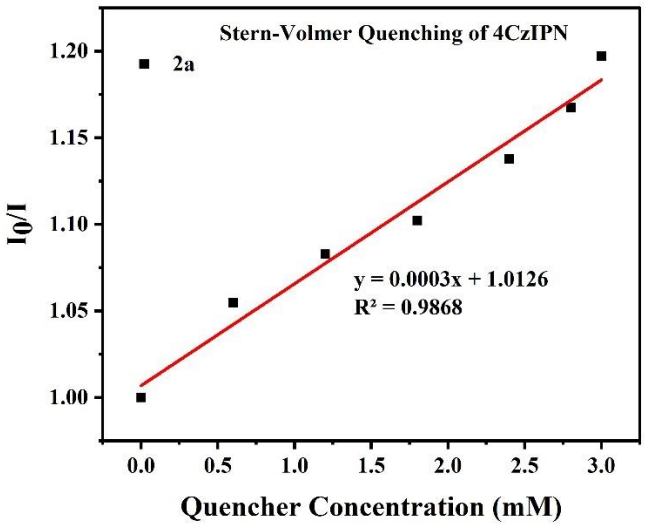


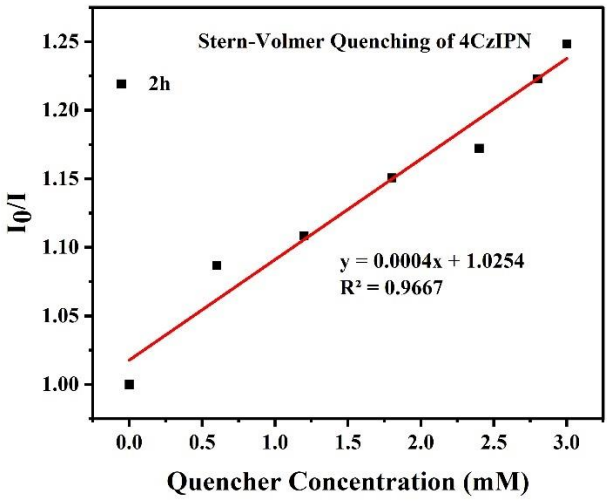
(b)



(c)

Figure S4 The fluorescence emission spectra of excited 4CzIPN* with different concentration of $BrCF_2COOEt$ **2a**, $BrCF_2CONHPh$ **2h**, or DIPEA in DMF (excitation wavelength: 360 nm). (a) $BrCF_2COOEt$ **2a** (b) $BrCF_2CONHPh$ **2h** (c) DIPEA





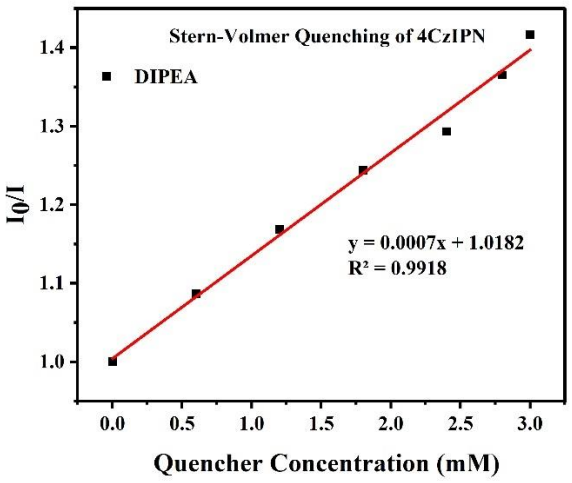


Figure S5 Stern-Volmer fluorescence quenching plot

6. X-Ray Structure of Product 4jh

X-ray crystallography of **4jh**

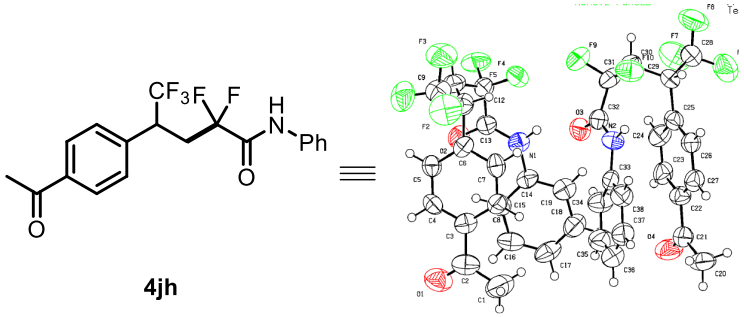


Figure S6. ORTEP diagram (50% probability) of **4jh**

A single crystal of **4jh** was obtained *via* evaporation of its hexanes/dichloromethane solvent mixture. A suitable crystal of **4jh** was selected and analyzed by an Agilent Gemini X-ray Single Crystal Diffractometer. Using Olex2[4], the structure was solved with the ShelXT[5] structure solution program using Direct Methods and refined with the ShelXL[6] refinement package using Least Squares minimization. Details of the crystal, data collection, and structure refinement parameters for crystallographic analysis of **4jh** are summarized in **Table S4**. Crystallographic data (CCDC 2213890) for **4jh** can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Table S4. Parameters for crystallographic analysis of **4jh**

Identification code	0417JFC2_0m_5
Empirical formula	C19 H16 F5 N O2
Formula weight	385.33
Temperature	296(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	a = 8.161(2) Å α= 79.398(7)°
	b = 10.353(3) Å β= 85.889(7)°
	c = 20.984(6) Å γ = 89.958(7)°
Volume	1738.0(8) $Å^3$
Z	4
Density (calculated)	1.473 Mg/m^3
Absorption coefficient	0.131 mm^{-1}
F(000)	792
Crystal size	0.200 x 0.200 x 0.200 mm^3
Theta range for data collection	0.990 to 25.000°.
Index ranges	-9<=h<=9, -12<=k<=12, 0<=l<=24
Reflections collected	6011

Independent reflections	6011 [R(int) = 0]
Completeness to theta = 25.000°	99.1 %
Absorption correction	Semi-empirical from equivalents
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6011 / 0 / 442
Goodness-of-fit on F^2	0.989
Final R indices [I>2sigma(I)]	R1 = 0.0717, wR2 = 0.1962
R indices (all data)	R1 = 0.1723, wR2 = 0.2571
Extinction coefficient	n/a
Largest diff. peak and hole	0.322 and -0.320 e.$Å^{-3}$

7. DFT Computational Study

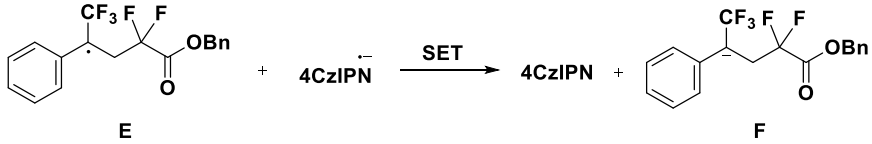
7.1 Computational Methods

All the species are fully optimized at the ωB97X-D/6-31++G(d,p) level[7, 8]. Frequency analyses are performed at the same level to confirm that the characteristics of the structures are minima (without imaginary frequencies) or transition states (only one imaginary frequency). Calculations of the intrinsic reaction coordinates (IRC)[9-10] are calculated to ensure that the transition states indeed have connected two minima. The solvent N,N-Dimethylformamide(DMF) was evaluated by single-point energy calculation with SMD solvation model[11], using ωB97X-D functional method on the basis sets of 6-311++G(d, p). The single-point energies are added to the Gibbs free energy correction to obtain the Gibbs free energy (ΔG). All these calculations are performed with Gaussian 16 program[12].

7.2 Modified Marcus theory

The activation free energies of the outer-sphere single electron transfer reactions were calculated using modified Marcus theory[13]. According to the Marcus equation, the solvent reorganization energy λ_0 may be calculated from equation (1):

$$\lambda_0 = (332\text{kcal/mol})\left(\frac{1}{2a_1}+\frac{1}{2a_2}-\frac{1}{R}\right)\left(\frac{1}{\varepsilon_{op}}-\frac{1}{\varepsilon}\right) \quad (1)$$



E F (2)

a_1 and a_2 are the radii of **E** and 4CzIPN$^{\bullet-}$, R = a_1 + a_2, ε_{op} is the optical dielectric constat (ε_{op} =2.05), ε is the static dielectric constant for the DMF solvent (ε =37.2). We estimate the inner reorganization energy for the reactants $\lambda_i = 0$. Thus, the total reorganization energy $\lambda = \lambda_i + \lambda_0$. According to Marcus theory, ΔG_r is the reaction energy, and $\Delta G_0^{\neq}$ is the intrinsic barrier.

$$\Delta G^{\neq}_{ET'} = \Delta G_0^{\neq}\left(1+\frac{\Delta G_r}{4\Delta G_0^{\neq}}\right)^2 \qquad \Delta G_0^{\neq} = \frac{\lambda}{4} \quad (3)$$

For eq2, ΔG_r = -11.8 kcal mol^{-1}, $\Delta G_0^{\neq}$ = 2.0 kcal mol^{-1}, the activation barrier for ET with respect to mixture is $\Delta G^{\neq}_{ET'}$ = 0.4 kcal mol^{-1}, according to eq.3.

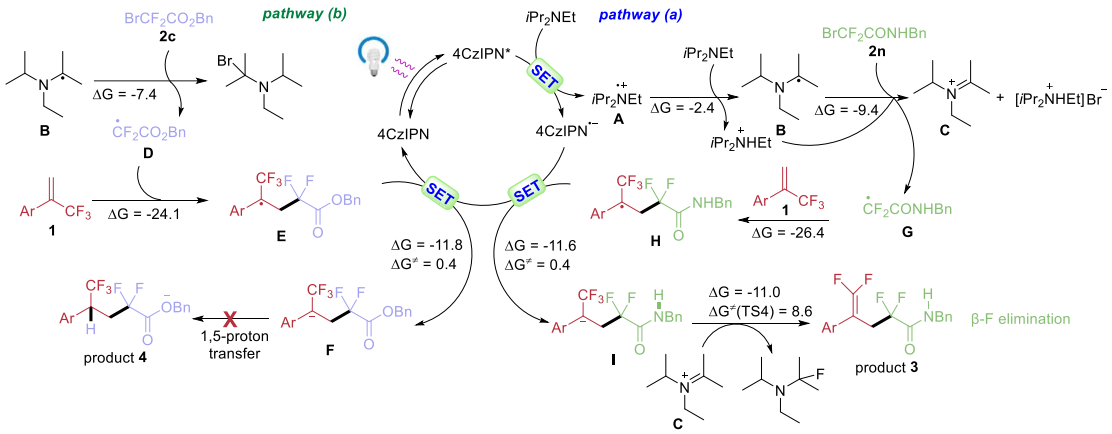
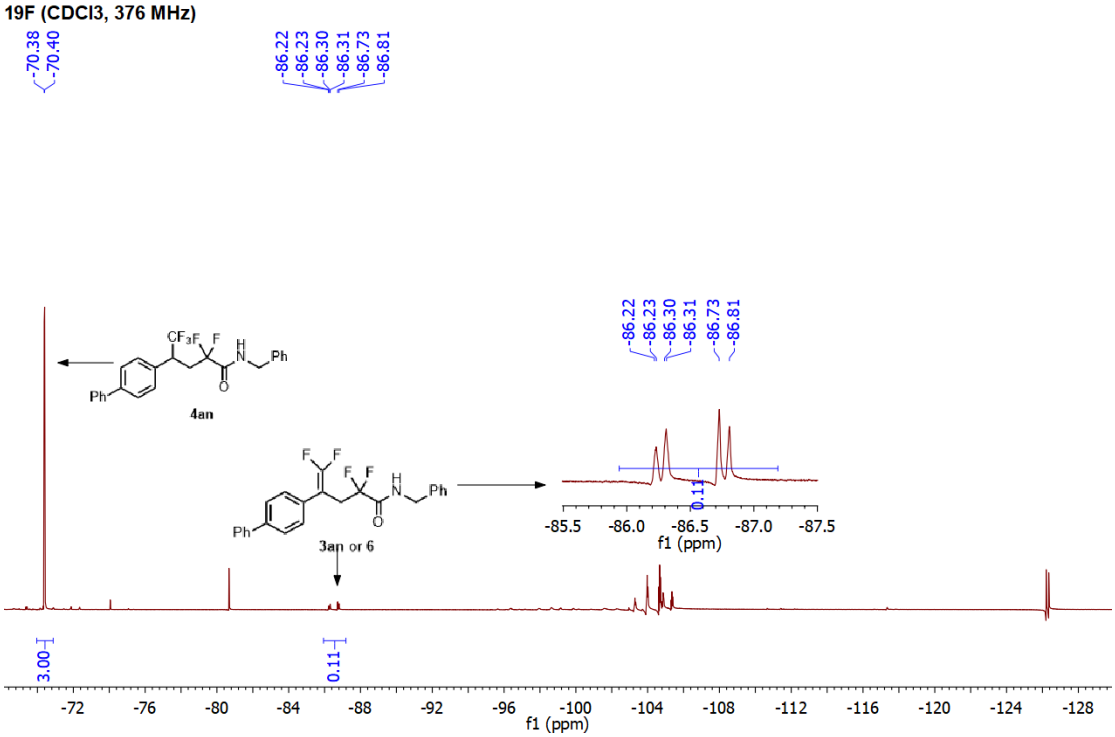


Figure S7. Two possible mechanism pathways for the allylic defluorinative difluoroalkylation and hydrodifluoroalkylation.



Note: For the substrate bromodifluoroacetamide **2n**, the hydrodifluoroalkylation product **4an** (major, 70%) and the defluorinative difluoroalkylated product **3an** (or **6**, minor, 4%) were observed by the crude ^{19}F NMR. The results suggest that two pathways of β-F elimination or protonation can occur toward the bromodifluoroacetamides.

Cartesian coordinates together with the electronic energies (hartree) for all the complexes calculated in this study

***i*Pr$_2$NEt**

E = -370.967334

N	-0.01156300	-0.02782300	-0.49577800
C	0.51300600	1.19291600	-1.07749600

C	0.35463000	2.49244900	-0.27160300
H	0.03532600	1.34084500	-2.05691800
H	1.57585400	1.03484200	-1.28974700
H	0.81467000	3.32498700	-0.81535900
H	-0.70105400	2.74160000	-0.12343100
H	0.82750300	2.42420300	0.71170300
C	-1.43609400	-0.04518000	-0.18268900
C	-1.78845500	0.28281800	1.27930900
C	-2.07851500	-1.37236100	-0.60500600
H	-1.88247200	0.73701800	-0.81026800
H	-1.36004600	1.23975600	1.58886100
H	-2.87472100	0.33504500	1.40951000
H	-1.41364200	-0.49190600	1.95786200
H	-1.87181200	-1.57331900	-1.65948300
H	-1.68816500	-2.21040600	-0.01664000
H	-3.16329000	-1.34458800	-0.45597500
C	0.88224300	-0.86048700	0.30278100
C	1.64720500	-0.12441700	1.41588900
C	1.85444300	-1.63771700	-0.59345600
H	0.24513200	-1.60536700	0.79263400
H	0.96481800	0.40946400	2.08286400
H	2.22425100	-0.83671900	2.01526900
H	2.35428300	0.60012500	0.99660600
H	1.30020100	-2.21085800	-1.34130300
H	2.53661600	-0.96181900	-1.12117300
H	2.46671500	-2.32627000	-0.00093900

A

E = -370.714290

N	-0.00219300	0.10666600	-0.26129300
C	0.58491200	1.18347600	-1.03678500
C	0.46955900	2.53303300	-0.30850100
H	0.04373100	1.22451100	-1.98953300
H	1.62859800	0.94528100	-1.23981200
H	0.91869600	3.29896900	-0.94371400
H	-0.57085700	2.81103800	-0.12743800
H	1.00617900	2.51251800	0.64180500
C	-1.45903600	0.06361400	-0.11493000
C	-1.85262900	0.23240000	1.35937800

C	-2.01301700	-1.22618600	-0.73755600
H	-1.83917100	0.91691800	-0.68253800
H	-1.43199200	1.14716600	1.78320200
H	-2.94150600	0.30089000	1.41261300
H	-1.54209100	-0.62031500	1.96809600
H	-1.71923800	-1.32244900	-1.78548400
H	-1.69278100	-2.11643500	-0.19059400
H	-3.10338400	-1.18022000	-0.69312400
C	0.84277700	-0.91050500	0.36596500
C	1.83605000	-0.25735200	1.33578800
C	1.53615000	-1.75580700	-0.71465500
H	0.17015400	-1.55607600	0.93290000
H	1.32094700	0.33053700	2.09894500
H	2.39208500	-1.05302300	1.83652200
H	2.55852500	0.37810500	0.81709800
H	0.81331700	-2.18975000	-1.40884200
H	2.27280900	-1.17814200	-1.27804500
H	2.06273600	-2.57223500	-0.21522800

***i*Pr$_2$N$^+$HEt**

E = -371.366559

N	-0.02274200	0.24936300	0.27872000
C	0.11338400	1.57491500	-0.42827200
C	-0.77520200	2.65433300	0.16866900
H	-0.09878100	1.40596400	-1.48451500
H	1.16014600	1.86754300	-0.33676400
H	-0.53539800	3.60284500	-0.31669300
H	-1.84024000	2.47362600	0.01222200
H	-0.59019000	2.78243000	1.24025900
C	-1.37971600	-0.42550000	0.06250400
C	-1.66643300	-1.37325100	1.22200800
C	-1.49616300	-1.09754200	-1.29709900
H	-2.09374000	0.39894300	0.11175800
H	-1.58871100	-0.87087100	2.19189800
H	-2.69165100	-1.73788200	1.12938600
H	-1.01114300	-2.24845800	1.22353700
H	-1.28747800	-0.41674700	-2.12571600
H	-0.85037000	-1.97527300	-1.38095300
H	-2.52697700	-1.43919000	-1.41428300

C	1.19339400	-0.67212800	0.09918100
C	2.21302800	-0.33610800	1.18151800
C	1.79204300	-0.61448000	-1.30150200
H	0.80639400	-1.67632000	0.27986500
H	1.80207300	-0.47449400	2.18697200
H	3.07170900	-1.00394300	1.08630700
H	2.58616200	0.68890500	1.08693600
H	1.05329400	-0.75962700	-2.09031500
H	2.32827500	0.31950000	-1.48517800
H	2.51959700	-1.42531300	-1.38309800
H	-0.01979100	0.48138400	1.27530100

B

E = -370.315050

N	0.06089800	0.08658900	-0.02714400
C	-0.06532000	1.35285200	0.69679800
C	0.17326400	2.57861100	-0.18289000
H	0.62141200	1.35691200	1.55031000
H	-1.06689100	1.41682300	1.13341300
H	0.07784700	3.49782300	0.40573300
H	1.17261800	2.55452700	-0.62572800
H	-0.55332200	2.61499400	-0.99955700
C	1.26439500	-0.62602800	0.11931900
C	-1.18656500	-0.65851700	-0.23049100
C	-2.23601100	0.18581300	-0.95712600
C	-1.74132800	-1.26121200	1.06820500
H	-0.94458700	-1.48178700	-0.90557000
H	-1.82929900	0.58409700	-1.89078700
H	-3.10540300	-0.43500500	-1.19477900
H	-2.59118100	1.02478700	-0.34980600
H	-0.97671800	-1.86232100	1.56906400
H	-2.06630600	-0.48049500	1.76453600
H	-2.60553500	-1.89992300	0.85817400
C	1.35309200	-1.99901000	-0.48175900
C	2.53681900	0.17359400	0.07521200
H	0.61025100	-2.69916100	-0.08515400
H	1.24115800	-1.98930400	-1.58187400
H	2.33762200	-2.42258000	-0.26666600
H	3.38085300	-0.44949600	0.38364900

H	2.75271100	0.53701000	-0.94689600
H	2.52840900	1.05035600	0.72833600

2c

E = -3268.868811

C	-2.10668700	-0.41896000	-0.11463700
C	-0.83584700	-1.28781700	-0.20545000
F	-2.88522500	-0.62993800	-1.17794400
F	-2.81729800	-0.69901500	0.99013300
O	-0.45463900	-1.77333200	-1.23482000
O	-0.25039900	-1.34641800	0.98154500
C	1.11740900	-1.81780700	0.99432900
H	1.19231900	-2.73199700	0.40170000
H	1.29858800	-2.04659100	2.04541700
C	2.04185900	-0.74415700	0.48129100
C	1.96250500	0.54984100	1.00385300
C	2.98101200	-1.02753300	-0.50874600
C	2.81133700	1.54707100	0.53653700
H	1.23081200	0.77524100	1.77401500
C	3.83885400	-0.03084500	-0.97026200
H	3.02795600	-2.02459000	-0.93745700
C	3.75789000	1.25607900	-0.44550300
H	2.73786900	2.55198700	0.94033500
H	4.56442900	-0.25949600	-1.74427100
H	4.42202300	2.03415600	-0.80829000
Br	-1.56917100	1.44184700	-0.07381200

C

E = -370.150295

N	0.07914100	0.01746900	0.12553600
C	-0.01398600	1.38710600	0.69910200
C	0.26374700	2.48186800	-0.32478100
H	0.66373000	1.44575400	1.55147700
H	-1.02139200	1.48893200	1.10000000
H	0.19236700	3.45320100	0.17006900
H	1.26348600	2.39719100	-0.75728800
H	-0.46400400	2.46343100	-1.13763900
C	1.21926700	-0.57519900	-0.05590200
C	-1.22569400	-0.66129600	-0.16996200

C	-2.13158400	0.21366700	-1.03166600
C	-1.87594300	-1.10457800	1.13998400
H	-0.98248200	-1.54703900	-0.75278300
H	-1.63904300	0.51169400	-1.96044300
H	-3.01442400	-0.37296700	-1.29587400
H	-2.48175400	1.10705900	-0.50853500
H	-1.20435100	-1.73695100	1.72705800
H	-2.18298900	-0.25544300	1.75650000
H	-2.77286100	-1.68419600	0.90992200
C	1.30668000	-1.96959900	-0.60518900
C	2.52729800	0.06505800	0.27229700
H	0.72629300	-2.67600900	-0.00548200
H	0.93461500	-2.00855600	-1.63399400
H	2.34500400	-2.29973300	-0.61200600
H	3.04052600	-0.56665400	1.00574900
H	3.14839700	0.05449400	-0.62988000
H	2.47618700	1.08133800	0.65110300

[*i*Pr$_2$N$^+$HEt]Br$^-$

E = -2943.335065

N	1.15517600	-0.11601000	-0.37363300
C	0.56236100	0.55850900	-1.59249800
C	1.34126400	1.78189400	-2.04432100
H	-0.47762300	0.78187500	-1.32468900
H	0.57104200	-0.18304300	-2.38916200
H	0.87824300	2.13990400	-2.96702000
H	1.30535000	2.60528400	-1.32774700
H	2.38985300	1.55284000	-2.26877800
C	1.20387500	0.86909000	0.82462500
C	2.64836000	1.33313900	0.98807900
C	0.62206900	0.36437100	2.13940200
H	0.56017100	1.69157600	0.50814100
H	3.07139700	1.73574200	0.06341000
H	2.69154600	2.12314400	1.74125300
H	3.28497500	0.51104200	1.33671800
H	-0.44173600	0.13809100	2.03137400
H	1.16853400	-0.47989500	2.56614100
H	0.70196100	1.19632700	2.84554600
C	0.57403500	-1.50162200	-0.05755500

C	1.68737500	-2.34423200	0.55693500
C	-0.03953600	-2.19513600	-1.26463900
H	-0.24194400	-1.31402500	0.63842200
H	2.20353800	-1.84001100	1.37736900
H	1.26113800	-3.26730900	0.95599900
H	2.43202700	-2.62338300	-0.19979400
H	-0.91927500	-1.65713500	-1.62223600
H	0.67907300	-2.36140100	-2.07597200
H	-0.38200100	-3.17643600	-0.92460700
H	2.13241400	-0.29714300	-0.61340800
Br	-2.35867800	0.29542700	0.19898000

D

E = -697.062846

C	-2.72706200	0.05982300	-0.57722500
C	-1.66218000	-0.30017100	0.35019400
F	-3.65779300	-0.81636000	-0.86936000
F	-3.12222600	1.30236200	-0.74766300
O	-1.44811600	-1.44929600	0.67955200
O	-0.96262100	0.77825400	0.71797400
C	0.22075500	0.53523100	1.51739900
H	0.01425600	-0.27967400	2.21393800
H	0.35479300	1.46600400	2.06948600
C	1.41322600	0.23448500	0.64931300
C	2.14857200	1.28028800	0.08514700
C	1.78598600	-1.08526800	0.38308000
C	3.24022600	1.01307400	-0.73570300
H	1.86275500	2.30883400	0.28958100
C	2.87961800	-1.35384100	-0.43664300
H	1.20764500	-1.89914900	0.80965000
C	3.60721000	-0.30616200	-0.99694700
H	3.80614600	1.83217300	-1.16810300
H	3.16243000	-2.38214400	-0.63833500
H	4.45993200	-0.51649500	-1.63491400

1

E = -646.526858

C	-3.35116500	-0.38166500	-0.10303700
C	-2.44025700	-1.31087400	0.39428400

H	-2.77712300	-2.30026100	0.68693900
C	-1.09500300	-0.97901500	0.52356900
H	-0.40025500	-1.71007300	0.92101700
C	-0.64191200	0.29468500	0.15911400
C	-1.56259200	1.21757600	-0.35116100
H	-1.21539100	2.19560800	-0.67027000
C	-2.90775200	0.88448100	-0.47684900
H	-3.60663700	1.61150800	-0.87822000
C	1.84056600	-0.26552300	-0.16375800
C	0.78122500	0.70183900	0.31241900
C	1.15297400	1.87631800	0.82383800
F	1.93064200	-1.35034300	0.64189200
F	1.57270200	-0.72330900	-1.40114200
F	3.06766400	0.28287700	-0.20224900
H	-4.39911700	-0.64515500	-0.20454900
H	2.19448900	2.16697000	0.89097400
H	0.40844800	2.57144700	1.19708600

E

E = -1343.654865

C	2.09229000	2.62901000	-1.35271000
C	1.24116100	3.21667900	-0.41516000
H	1.52008300	4.15117700	0.06145700
C	0.03917800	2.61905400	-0.07981100
H	-0.59342400	3.10498600	0.65110700
C	-0.37529900	1.40329700	-0.69309400
C	0.51851200	0.82041700	-1.63211300
H	0.27942100	-0.12305400	-2.10676100
C	1.72431800	1.42221100	-1.94759600
H	2.38698700	0.93986900	-2.65831000
C	-2.54770800	1.42850500	0.61608500
C	-1.63819300	0.79781000	-0.40392800
C	-2.17650400	-0.39734100	-1.13945000
H	-3.25910200	-0.30999400	-1.26278200
H	-1.74211000	-0.47290500	-2.13782900
C	-1.96046600	-1.74980200	-0.45534100
C	-0.48657800	-2.20349400	-0.41859200
F	-1.98526100	1.48247500	1.84631300
F	-2.87720300	2.70581400	0.29456500

F	-3.70997000	0.76962000	0.74901000
F	-2.63749900	-2.69846500	-1.17011700
F	-2.48549700	-1.74704800	0.79443400
O	0.12795200	-2.41509500	-1.43582300
H	3.03690400	3.09892200	-1.60638300
O	-0.02278200	-2.31080200	0.81450100
C	1.36705500	-2.67928800	0.95042600
H	1.61056500	-3.44318000	0.20905400
H	1.41797500	-3.11217300	1.95102500
C	2.27695700	-1.48520500	0.82584400
C	2.01525000	-0.32100900	1.55385900
C	3.41441800	-1.55073000	0.02308200
C	2.89293400	0.75479800	1.49106300
H	1.11855600	-0.25658400	2.16376400
C	4.30042900	-0.47600200	-0.03115400
H	3.60793400	-2.44395000	-0.56455500
C	4.04251500	0.67541700	0.70616900
H	2.67726000	1.65864800	2.05127200
H	5.18665400	-0.53797300	-0.65503400
H	4.72818700	1.51586100	0.66122600

F

E = -1343.728806

C	-1.60408600	3.18820500	1.61435300
C	-0.83074900	3.57988700	0.51751800
H	-1.03044900	4.53141600	0.02710600
C	0.19672900	2.78638600	0.02951500
H	0.76457000	3.14905000	-0.81888100
C	0.53735400	1.52985100	0.61810500
C	-0.27432200	1.15767500	1.72940700
H	-0.12988600	0.19282000	2.20356500
C	-1.30191500	1.96084700	2.20532800
H	-1.89253000	1.60420000	3.04676500
C	2.40206700	1.14801900	-0.99006600
C	1.59440000	0.69186900	0.12955700
C	2.19828400	-0.37879000	0.99897700
H	3.29614600	-0.34821200	0.99638200
H	1.89130100	-0.24827000	2.04294800
C	1.87524100	-1.83223200	0.65829800

C	0.37573000	-2.18184100	0.63696800
F	1.70496300	1.39938000	-2.15715900
F	3.09781600	2.35718500	-0.81284000
F	3.38515400	0.27623900	-1.34089800
F	2.43590500	-2.65866100	1.61685300
F	2.44146300	-2.21298100	-0.52040500
O	-0.28182800	-2.27084100	1.64523800
H	-2.41275400	3.81051700	1.98643600
O	-0.08049400	-2.38846500	-0.59776600
C	-1.46550600	-2.71695000	-0.72485800
H	-1.75479100	-3.38705500	0.09047400
H	-1.52186400	-3.25861600	-1.67294600
C	-2.36576000	-1.50378400	-0.75038200
C	-1.86313500	-0.22070300	-0.95283000
C	-3.74073300	-1.68796100	-0.58098700
C	-2.72985100	0.87090800	-0.96916800
H	-0.79367300	-0.05968000	-1.05929800
C	-4.60696900	-0.59946800	-0.61706000
H	-4.13477800	-2.68720700	-0.40515000
C	-4.09938000	0.68595100	-0.80762600
H	-2.31407600	1.86746300	-1.07303200
H	-5.67359800	-0.75224200	-0.47637400
H	-4.76715400	1.54258800	-0.80804200

3

E = -1243.835332

C	-3.24227700	1.57179000	1.59764300
C	-2.86597000	2.49257700	0.62290100
H	-3.57183600	3.24174600	0.27776700
C	-1.57872100	2.47062600	0.09673400
H	-1.29649600	3.21102500	-0.64370300
C	-0.64374600	1.51953900	0.52673500
C	-1.03102500	0.60443000	1.51284900
H	-0.33830300	-0.15188600	1.86616500
C	-2.31780400	0.63081000	2.04038100
H	-2.59718400	-0.09774500	2.79467400
C	0.99549500	1.77040300	-1.28885100
C	0.74623300	1.51177700	-0.00683000
C	1.90872600	1.27915800	0.94142800

H	2.64783800	2.08313400	0.86581800
H	1.53109200	1.28041800	1.96556500
C	2.69936500	-0.02049300	0.77081400
C	1.81995500	-1.28004800	0.64056200
F	3.48688500	-0.18117400	1.87264500
F	3.53931600	0.05995000	-0.29591400
O	1.32362800	-1.81626000	1.60062900
H	-4.24548300	1.59166900	2.01173900
O	1.65675800	-1.63157100	-0.62528300
C	0.71636200	-2.70300500	-0.88267900
H	0.88462200	-3.50618900	-0.16235100
H	0.98985900	-3.04305400	-1.88235900
C	-0.70244300	-2.20236500	-0.83144200
C	-1.11769100	-1.19982400	-1.71093100
C	-1.60869700	-2.71980600	0.09360300
C	-2.41832900	-0.71102600	-1.65726600
H	-0.41415700	-0.78997900	-2.43018300
C	-2.91862200	-2.24815000	0.13219400
H	-1.28256400	-3.48175800	0.79569100
C	-3.32261700	-1.23941900	-0.73805300
H	-2.72430000	0.08451500	-2.32863800
H	-3.61761700	-2.65478800	0.85633500
H	-4.33630200	-0.85464200	-0.69210100
F	0.08618800	1.96365100	-2.23241800
F	2.20078700	1.88072200	-1.81719400

4CzIPN

E = -2481.099289

C	-0.49212900	0.00000000	0.00000200
C	0.21938100	-1.14187200	-0.42590200
C	1.62511300	-1.11817000	-0.45522500
C	2.33326400	-0.00028200	-0.00008400
C	1.62536400	1.11774400	0.45511300
C	0.21963700	1.14172700	0.42586700
C	4.54825500	-0.79471300	0.81253400
C	4.54832800	0.79391900	-0.81271200
C	4.18031700	-1.71391800	1.79036500
C	5.89381300	-0.50692700	0.51959200
C	4.18047400	1.71312900	-1.79057200

C	5.89386000	0.50614500	-0.51964200
C	5.20182200	-2.36591000	2.47068500
H	3.13851300	-1.91450100	2.01916600
C	6.90250600	-1.17192800	1.21740300
C	5.20203800	2.36514200	-2.47078200
H	3.13868900	1.91369000	-2.01948100
C	6.90261400	1.17115900	-1.21735200
C	6.54953800	-2.10168200	2.18774500
H	4.94901600	-3.09233800	3.23617800
H	7.94669800	-0.96364100	1.00626500
C	6.54972900	2.10092200	-2.18771600
H	4.94930000	3.09157300	-3.23629400
H	7.94678700	0.96288100	-1.00611600
H	7.32313800	-2.62802400	2.73665000
H	7.32337700	2.62727800	-2.73654100
C	-1.48281900	2.36450000	1.78250600
C	-0.41349700	3.52408400	0.14400500
C	-1.85166200	1.42396600	2.73747600
C	-2.12422900	3.60941700	1.67550300
C	0.41243700	3.91964500	-0.90400700
C	-1.44425800	4.34778700	0.62855200
C	-2.93050300	1.72993600	3.55693800
H	-1.32911700	0.47978700	2.83847500
C	-3.19744600	3.90482200	2.51637200
C	0.18972400	5.17397800	-1.46091400
H	1.20854500	3.28515200	-1.27833000
C	-1.64962600	5.60314000	0.05784400
C	-3.60312400	2.95509100	3.44569100
H	-3.25453300	1.00315500	4.29462200
H	-3.70609600	4.86105500	2.44438100
C	-0.82936400	6.01090600	-0.98691800
H	0.82545100	5.51083200	-2.27332000
H	-2.44509700	6.24691400	0.41998200
H	-4.44215400	3.16530000	4.10058100
H	-0.97546000	6.98564800	-1.44026900
C	-0.41428600	-3.52408300	-0.14398500
C	-1.48340500	-2.36426900	-1.78245600
C	0.41161100	-3.91983300	0.90398200
C	-1.44530500	-4.34752200	-0.62843100

C	-1.85205000	-1.42367300	-2.73744100
C	-2.12514400	-3.60900700	-1.67536600
C	0.18859100	-5.17408200	1.46095400
H	1.20791300	-3.28554000	1.27823500
C	-1.65098000	-5.60279600	-0.05766200
C	-2.93102900	-1.72937800	-3.55682000
H	-1.32925100	-0.47964200	-2.83850800
C	-3.19849700	-3.90415100	-2.51615200
C	-0.83076000	-6.01074800	0.98706100
H	0.82427900	-5.51107800	2.27333200
H	-2.44665100	-6.24636700	-0.41972300
C	-3.60397800	-2.95434400	-3.44547900
H	-3.25490900	-1.00253700	-4.29450900
H	-3.70740400	-4.86024200	-2.44409000
H	-0.97709200	-6.98543300	1.44045900
H	-4.44311000	-3.16434800	-4.10030300
C	-2.71376600	-0.85369600	0.74735300
C	-2.71360700	0.85414100	-0.74732600
C	-2.35613900	-1.82518500	1.67663200
C	-4.05825000	-0.54669600	0.47511500
C	-2.35579500	1.82560800	-1.67655700
C	-4.05814800	0.54731000	-0.47517900
C	-3.37877900	-2.52801300	2.30102200
H	-1.31997600	-2.03828600	1.91237200
C	-5.07129200	-1.25836400	1.11743100
C	-3.37830500	2.52856600	-2.30101400
H	-1.31958800	2.03859700	-1.91221100
C	-5.07105700	1.25910800	-1.11756100
C	-4.72523400	-2.25459900	2.02195700
H	-3.12356400	-3.30416700	3.01527000
H	-6.11379100	-1.03271000	0.91546600
C	-4.72481400	2.25530700	-2.02205600
H	-3.12294500	3.30469800	-3.01523400
H	-6.11359800	1.03358200	-0.91566900
H	-5.50182900	-2.82174600	2.52440600
H	-5.50130400	2.82255100	-2.52455700
N	-0.44324400	2.30364300	0.84252200
N	3.73355400	-0.00041800	-0.00014800
N	-0.44374700	-2.30365500	-0.84254600

N	-1.89440900	0.00015800	0.00002900
C	2.34698000	2.21379700	1.03428500
C	2.34647800	-2.21437200	-1.03442900
N	2.93643400	3.08696100	1.51561400
N	2.93572600	-3.08766300	-1.51578100

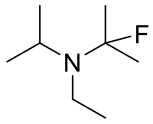
4CzIPN$^{\bullet-}$

E = -2481.165023

C	-0.50996200	-0.00040800	-0.00013400
C	0.17558200	-1.14754000	-0.41573200
C	1.62907100	-1.12190500	-0.47873500
C	2.30851300	0.00080300	0.00015600
C	1.62801900	1.12291300	0.47889600
C	0.17453300	1.14733700	0.41562900
C	4.53510900	-0.76401500	0.82805800
C	4.53460800	0.76763900	-0.82727300
C	4.16601600	-1.66567500	1.82467200
C	5.88603700	-0.48793000	0.53362900
C	4.16493200	1.66898300	-1.82395700
C	5.88571800	0.49277700	-0.53252600
C	5.18361100	-2.29944700	2.52441300
H	3.12118700	-1.86500000	2.03660800
C	6.89189400	-1.13697500	1.25184100
C	5.18211500	2.30369100	-2.52344700
H	3.11997000	1.86735800	-2.03613900
C	6.89115300	1.14274100	-1.25049700
C	6.53539700	-2.04159200	2.24402600
H	4.92644500	-3.01167400	3.30261100
H	7.93753200	-0.93558500	1.03723400
C	6.53406900	2.04705200	-2.24275000
H	4.92448500	3.01569500	-3.30169600
H	7.93692300	0.94229800	-1.03564700
H	7.30655000	-2.55597600	2.80907500
H	7.30488800	2.56214100	-2.80761200
C	-1.45190700	2.48525300	1.77112100
C	-0.48068700	3.51350500	0.02140900
C	-1.80585700	1.58812300	2.77703800
C	-2.05907500	3.75324900	1.66271800

C	0.30438700	3.82945700	-1.08710600
C	-1.43075700	4.41638000	0.53944400
C	-2.80881400	1.96764400	3.65738000
H	-1.32090700	0.62257500	2.85964000
C	-3.06116300	4.11840200	2.56384700
C	0.11439400	5.07111800	-1.67830100
H	1.04099200	3.12915000	-1.46627500
C	-1.60510000	5.65927400	-0.07082700
C	-3.43756100	3.21948100	3.55371600
H	-3.11453200	1.27652600	4.43700000
H	-3.54047300	5.09037400	2.48783000
C	-0.83211200	5.98113800	-1.17976400
H	0.71721100	5.34499400	-2.53909300
H	-2.33905900	6.36187200	0.31374600
H	-4.22238000	3.48453300	4.25556100
H	-0.95517200	6.94509000	-1.66398600
C	-0.47736300	-3.51442600	-0.02201000
C	-1.44919100	-2.48693000	-1.77183000
C	0.30761600	-3.82965500	1.08678300
C	-1.42594700	-4.41844500	-0.54078300
C	-1.80395200	-1.58994200	-2.77759200
C	-2.05463700	-3.75581500	-1.66414400
C	0.11910900	-5.07179700	1.67744300
H	1.04307600	-3.12846400	1.46653500
C	-1.59881200	-5.66180400	0.06896900
C	-2.80590700	-1.97061200	-3.65858100
H	-1.32032400	-0.62368500	-2.85965100
C	-3.05574000	-4.12209700	-2.56591100
C	-0.82586800	-5.98298000	1.17813700
H	0.72191900	-5.34513000	2.53841000
H	-2.33160300	-6.36530000	-0.31619100
C	-3.43290700	-3.22338800	-3.55567800
H	-3.11220600	-1.27968000	-4.43813900
H	-3.53370100	-5.09477700	-2.49046200
H	-0.94778700	-6.94728000	1.66195200
H	-4.21697000	-3.48933200	-4.25803000
C	-2.74394400	-0.79201900	0.80228800
C	-2.74441200	0.79030700	-0.80200900
C	-2.38281400	-1.70739500	1.78892300

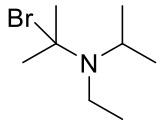
C	-4.09415400	-0.50959800	0.51484000
C	-2.38384900	1.70558200	-1.78894400
C	-4.09445100	0.50844600	-0.51325900
C	-3.40083000	-2.36591500	2.46370900
H	-1.34258300	-1.90571200	2.01800500
C	-5.10296800	-1.17798300	1.21021100
C	-3.40222400	2.36472300	-2.46256900
H	-1.34374000	1.90350600	-2.01895100
C	-5.10365700	1.17741600	-1.20750600
C	-4.75156200	-2.10989100	2.17837800
H	-3.14059900	-3.09798900	3.22209000
H	-6.14727900	-0.96898300	0.99644400
C	-4.75278600	2.10931900	-2.17587200
H	-3.14241500	3.09683100	-3.22106000
H	-6.14785000	0.96891800	-0.99267700
H	-5.52488900	-2.64380200	2.72205100
H	-5.52640900	2.64372400	-2.71863700
N	-0.50724000	2.33635000	0.76192100
N	3.72497300	0.00141100	0.00026600
N	-0.50515600	-2.33709700	-0.76218600
N	-1.93019600	-0.00105500	-0.00030000
C	2.34190300	2.19371300	1.07209800
C	2.34397800	-2.19199700	-1.07196000
N	2.91941200	3.08526900	1.55197500
N	2.92234000	-3.08301400	-1.55181900



E = -470.199353

N	-0.14072300	0.17760300	-0.16126800
C	-0.51947400	1.28375000	0.72730500
C	-0.79988100	2.58903400	-0.01505600
H	0.25717800	1.43429000	1.48283000
H	-1.40839900	0.99796600	1.29825700
H	-1.07848200	3.37925400	0.69088500
H	0.08018700	2.92183000	-0.57220400
H	-1.61757500	2.46302500	-0.72994400
C	1.22949000	-0.19895700	-0.12376000

C	-1.16088900	-0.87109900	-0.32566000
C	-2.46985600	-0.28067900	-0.85529800
C	-1.39717300	-1.72202300	0.93038400
H	-0.79790200	-1.53368800	-1.11412700
H	-2.29075600	0.29969500	-1.76470100
H	-3.16764300	-1.08975400	-1.09159400
H	-2.96033000	0.36811800	-0.12222000
H	-0.46693000	-2.17924500	1.27531700
H	-1.79557000	-1.11830600	1.75275600
H	-2.12239700	-2.51511000	0.71933000
C	1.58155400	-1.36808500	-1.03554900
C	2.16632400	0.97761100	-0.38193500
H	1.11370500	-2.29525000	-0.70059100
H	1.27915100	-1.15810800	-2.06508300
H	2.66263900	-1.51736600	-1.01217100
H	3.20177500	0.64724800	-0.27678600
H	2.01168800	1.35460300	-1.39629700
H	2.00222800	1.79272200	0.32431700
F	1.58910100	-0.66138400	1.21203500



E = -2942.142375

N	0.87647700	0.21069800	0.24902500
C	1.17751400	0.99780900	-0.95198600
C	2.07108500	2.20930500	-0.70016600
H	0.23367100	1.30312700	-1.41404900
H	1.65152200	0.34102200	-1.68713700
H	2.22853200	2.75607900	-1.63571700
H	1.61960900	2.89406600	0.02220300
H	3.04813600	1.90959800	-0.31273500
C	-0.38123100	0.37956900	0.81124100
C	1.57840300	-1.08138500	0.37108100
C	3.09033600	-0.89356400	0.22950000
C	1.04963000	-2.16559000	-0.57599100
H	1.41813700	-1.42085000	1.39606800
H	3.45367900	-0.12527200	0.91756500

H	3.59252300	-1.83484900	0.47020300
H	3.38569100	-0.61789800	-0.78768300
H	0.01737100	-2.43383600	-0.34096600
H	1.06964400	-1.82894300	-1.61745300
H	1.67192700	-3.06263000	-0.49606900
C	-0.68536900	-0.48286900	2.02484200
C	-0.77079400	1.83256000	1.04539400
H	-0.68153900	-1.54713500	1.78850000
H	0.04753500	-0.28129100	2.81528500
H	-1.67826900	-0.23234500	2.39892000
H	-1.79023700	1.88484300	1.42884300
H	-0.08473300	2.26049500	1.78592300
H	-0.72761900	2.43171400	0.13595500
Br	-1.92538200	-0.24702300	-0.57526600

2n

E = -3249.021248

C	-2.12645000	-0.53168200	0.43198700
C	-0.96227200	-1.14638400	-0.38211600
F	-3.22098200	-1.29019800	0.31482200
F	-1.82988300	-0.44690700	1.75391100
O	-1.14832200	-1.48751200	-1.53248000
C	1.44636700	-1.60703000	-0.32950500
H	1.22830200	-1.74238700	-1.39281400
H	1.77181200	-2.57580100	0.06414300
C	2.53088300	-0.57003800	-0.12857400
C	2.23885900	0.79491300	-0.19534200
C	3.84904600	-0.97193600	0.09128400
C	3.25083500	1.73945500	-0.04860500
H	1.21533200	1.12121300	-0.35978000
C	4.86360100	-0.02758100	0.23337600
H	4.08574000	-2.03125400	0.15208400
C	4.56658800	1.33108800	0.16284400
H	3.01172700	2.79680000	-0.10366100
H	5.88436100	-0.35451900	0.40465500
H	5.35467100	2.06848400	0.27714700
N	0.19775500	-1.21514700	0.29944000
H	0.21664800	-0.90921200	1.26128700
Br	-2.49866500	1.24576900	-0.22200000

G

E = -677.211765

C	-2.83684800	-0.10085600	-0.61173700
C	-1.79772700	-0.15948400	0.44387900
F	-3.94424900	-0.78553600	-0.44628600
F	-3.06008800	1.05512700	-1.23880200
O	-1.77034000	-1.09400600	1.23226100
C	0.28759200	0.86863600	1.24704900
H	0.05617900	0.25271600	2.11871600
H	0.45443800	1.89304700	1.59182000
C	1.51412000	0.34343400	0.53239100
C	2.54037100	1.20464600	0.14439400
C	1.61837800	-1.01962200	0.23453500
C	3.65678900	0.71715600	-0.53485000
H	2.47155800	2.26470500	0.37718100
C	2.72971200	-1.50674900	-0.44553700
H	0.82371500	-1.69439800	0.54172800
C	3.75182100	-0.63914000	-0.83213000
H	4.44998100	1.39722200	-0.82953100
H	2.80244000	-2.56636600	-0.66993700
H	4.61979700	-1.02143700	-1.36006100
N	-0.90047500	0.86038300	0.40287100
H	-0.95827400	1.52943600	-0.35027300

H

E = -1323.809027

C	-2.07696600	2.49419100	1.41421900
C	-1.24249100	3.12856600	0.49165200
H	-1.55018900	4.06361600	0.03410900
C	-0.02324300	2.57513900	0.14463100
H	0.59358800	3.09588400	-0.57577000
C	0.42706000	1.35865800	0.73173000
C	-0.44564300	0.73247400	1.66252200
H	-0.17812900	-0.21312500	2.11746200
C	-1.67129700	1.28899000	1.98629600
H	-2.31918500	0.77112700	2.68551500
C	2.57637600	1.44545500	-0.61212700
C	1.70059700	0.78786900	0.41909000

C	2.26864800	-0.42030100	1.11070900
H	3.35379000	-0.32988700	1.20283800
H	1.86314700	-0.52503400	2.11877600
C	2.02399800	-1.75160600	0.39990600
C	0.55223000	-2.21240500	0.42465600
F	1.99008900	1.48659600	-1.83513600
F	2.88092500	2.72920400	-0.29766200
F	3.75159700	0.81437000	-0.77115700
F	2.76824000	-2.71450700	1.00935500
F	2.46819200	-1.68351800	-0.90005700
O	0.02193300	-2.45573100	1.49711900
H	-3.03781400	2.92697700	1.67256000
C	-1.46080200	-2.61774400	-0.89323500
H	-1.69901700	-3.33829800	-0.10740600
H	-1.59888100	-3.11761500	-1.85699300
C	-2.38671900	-1.42085400	-0.79511000
C	-2.10304800	-0.23437900	-1.47577900
C	-3.56848000	-1.51398000	-0.06120300
C	-2.99724400	0.82973300	-1.44193700
H	-1.17350100	-0.13216500	-2.02954700
C	-4.46646600	-0.44832300	-0.02508200
H	-3.78755800	-2.42453900	0.49014300
C	-4.18547300	0.72332000	-0.72136100
H	-2.76056200	1.74736000	-1.97055800
H	-5.38291600	-0.53481000	0.55053800
H	-4.88234800	1.55527300	-0.69435600
N	-0.05192000	-2.28434200	-0.77475700
H	0.48992500	-2.06665300	-1.59652100

I

E = -1323.888775

C	-2.04585100	2.75601800	1.30334800
C	-1.11819800	3.35131900	0.44561100
H	-1.30248000	4.35225900	0.05964100
C	0.05199100	2.70156000	0.07765800
H	0.74481600	3.21898700	-0.57533500
C	0.37581900	1.40044700	0.55342900
C	-0.60713300	0.80717800	1.39227700
H	-0.47439100	-0.21022900	1.74693400

C	-1.77015600	1.46987600	1.76228600
H	-2.48610200	0.95312000	2.39683600
C	2.62254500	1.38500200	-0.55148500
C	1.59025700	0.69290600	0.20830600
C	2.07103000	-0.41316000	1.12420000
H	3.14436800	-0.32857800	1.33225000
H	1.56913700	-0.34973300	2.09702000
C	1.90175900	-1.87015500	0.67063300
C	0.56056600	-2.30480700	0.02286100
F	2.21176200	1.85660900	-1.78212500
F	3.17509000	2.53408700	0.03055200
F	3.70970600	0.61021400	-0.80889900
F	2.13802500	-2.68563700	1.74444200
F	2.88071700	-2.18704700	-0.25351600
O	-0.03037500	-3.31988000	0.37463100
H	-2.96124300	3.26838800	1.58522900
C	-1.01613700	-1.71422500	-1.74714900
H	-1.15160000	-2.79500700	-1.84600600
H	-0.85516600	-1.29751500	-2.74635600
C	-2.25130800	-1.09409400	-1.12812100
C	-2.65099300	0.19509000	-1.48323400
C	-2.98986000	-1.79470700	-0.17128300
C	-3.77961100	0.77173200	-0.90838100
H	-2.05772000	0.76393700	-2.19459900
C	-4.12078000	-1.21990900	0.40405300
H	-2.65441300	-2.78275500	0.13142700
C	-4.52247000	0.06158100	0.03127000
H	-4.06049100	1.78589700	-1.17391400
H	-4.68535300	-1.77187500	1.15057100
H	-5.39762300	0.51450400	0.48867300
N	0.19556600	-1.49201600	-0.98380100
H	0.65578200	-0.56219100	-0.97458000

J

E = -1323.900115

C	2.28246100	2.60232400	-1.75476600
C	1.39822800	3.38434700	-1.01989300
H	1.57935800	4.44903400	-0.89854400
C	0.27016500	2.81238200	-0.43047100

H	-0.39484500	3.45280400	0.13567100
C	0.00648300	1.44675800	-0.56700800
C	0.90277700	0.66729200	-1.31129400
H	0.72680200	-0.40053000	-1.43585100
C	2.02529000	1.24023800	-1.89647800
H	2.70882700	0.60648800	-2.45295200
C	-2.06084500	1.60411200	0.92932900
C	-1.18562800	0.72425800	0.05933100
C	-2.04121800	-0.03676700	-0.98941100
H	-3.04671900	0.38598700	-1.07439600
H	-1.56692400	0.03808200	-1.96897500
C	-2.18357900	-1.52953200	-0.69426400
C	-0.81470900	-2.23161000	-0.53131900
F	-1.36866100	2.17829800	1.94412700
F	-2.64992700	2.62381600	0.24717300
F	-3.06307800	0.91740700	1.50251100
F	-2.87991800	-2.08203800	-1.75118300
F	-2.99962100	-1.70022100	0.39466300
O	-0.17423800	-2.40694000	-1.60353400
H	3.16406900	3.04697900	-2.20839100
C	0.87728100	-2.95712500	0.86841900
H	1.13908700	-3.66659700	0.06966100
H	0.92202000	-3.49725800	1.82493600
C	1.93012500	-1.86233700	0.89826400
C	1.78810500	-0.77668600	1.77052500
C	3.04427800	-1.89155000	0.05770900
C	2.72696200	0.24984100	1.79890600
H	0.91124500	-0.73647200	2.41138600
C	3.99583900	-0.87191300	0.09025600
H	3.14711900	-2.71053200	-0.64949400
C	3.83963300	0.20510300	0.95884800
H	2.58251300	1.09557200	2.46567800
H	4.84846700	-0.90727000	-0.58351900
H	4.56415400	1.01457200	0.96602300
N	-0.46732800	-2.42828200	0.71698700
H	-0.77902900	-0.02752600	0.75242700

4

E = -1324.461786

C	-4.53316400	-0.90876200	1.13447100
C	-4.45094400	0.38003700	0.61089000
H	-5.34275500	0.99357400	0.53143800
C	-3.22586900	0.88742200	0.18786100
H	-3.17760500	1.89177200	-0.22172300
C	-2.06939300	0.10828500	0.27968700
C	-2.15839300	-1.18107600	0.80407300
H	-1.26310500	-1.79201400	0.87735200
C	-3.38341200	-1.68781400	1.23088600
H	-3.43710800	-2.69227300	1.63902200
C	-0.66572700	0.83973200	-1.66541100
C	-0.71238700	0.64361200	-0.15061400
C	-0.36282700	1.91051700	0.66059600
H	-0.93754200	2.77475700	0.31680600
H	-0.64811700	1.70922100	1.69559700
C	1.09947700	2.32383400	0.72276800
C	2.01703900	1.13613900	1.07520600
F	-1.17927000	-0.21817600	-2.31515900
F	-1.34876400	1.92828800	-2.07284100
F	0.59977900	0.98510100	-2.12306700
F	1.23669700	3.28158800	1.68039900
F	1.50210700	2.90801900	-0.45476100
O	1.93485400	0.62504800	2.18005300
H	-5.48879900	-1.30189700	1.46646500
C	3.42759500	-0.62458500	0.15377800
H	3.92981300	-0.69953700	1.12068700
H	4.18873500	-0.67067800	-0.62868900
C	2.41711900	-1.74292800	-0.00707600
C	1.88927000	-2.03764200	-1.26759400
C	1.95547800	-2.45012200	1.10436800
C	0.91462700	-3.01964800	-1.41660700
H	2.23342300	-1.48661200	-2.13930400
C	0.98938800	-3.44424300	0.95578700
H	2.34049900	-2.20484200	2.08928500
C	0.46582300	-3.72898800	-0.30328200
H	0.50483200	-3.22980000	-2.39912700
H	0.63967200	-3.98897500	1.82742200
H	-0.29314300	-4.49653600	-0.41799400
N	2.79457500	0.68722600	0.06998400

H	2.70603800	1.13624100	-0.82932700
H	0.02715800	-0.13937200	0.05192200

product **3**

E = -1223.987898

C	-3.17022200	1.67300800	1.59423000
C	-2.74059500	2.62198400	0.66997800
H	-3.40679000	3.41924600	0.35498600
C	-1.44942700	2.56450700	0.15592200
H	-1.12455900	3.32565300	-0.54524300
C	-0.56588300	1.54978400	0.54746300
C	-1.00406600	0.60790900	1.48564900
H	-0.35026800	-0.19548600	1.80741800
C	-2.29492200	0.67032400	2.00025300
H	-2.61646700	-0.08014300	2.71517400
C	1.07710600	1.80269500	-1.25733200
C	0.82567700	1.50377900	0.01573200
C	1.98337500	1.20094000	0.95224500
H	2.75121100	1.97899400	0.89410400
H	1.61024900	1.18436700	1.97808200
C	2.71377600	-0.12488300	0.73935200
C	1.78434600	-1.35316500	0.68728200
F	3.59892500	-0.29399700	1.75751600
F	3.46437000	-0.07636900	-0.41412100
O	1.24173700	-1.74533500	1.70786400
H	-4.17689600	1.71868100	1.99794500
C	0.54474500	-2.86030100	-0.77838600
H	0.60760300	-3.62251300	0.00200100
H	0.76812800	-3.34068700	-1.73499800
C	-0.84175200	-2.24675300	-0.79702400
C	-1.13085700	-1.18424000	-1.65598200
C	-1.84146300	-2.72404100	0.04895900
C	-2.39361000	-0.60186100	-1.66442300
H	-0.35844700	-0.79344100	-2.31383200
C	-3.11281100	-2.15366400	0.03198500
H	-1.61885000	-3.53392700	0.73813600
C	-3.38990200	-1.08932800	-0.82100200
H	-2.59623800	0.23802900	-2.32088000
H	-3.88104200	-2.52977200	0.70057600

H	-4.37276600	-0.62934400	-0.81856300
N	1.58835800	-1.87320300	-0.53903700
H	2.08828200	-1.46871000	-1.31512500
F	0.17054800	2.05338900	-2.19100500
F	2.28430700	1.90186400	-1.79226200

TS1

E = -1714.005237

C	-0.32542200	3.27508900	0.52372800
C	0.24851000	2.85603800	-0.67565200
H	0.66147600	3.59055200	-1.36392400
C	0.30936700	1.51023200	-1.01572200
H	0.79462000	1.23395700	-1.94234400
C	-0.20521700	0.50158400	-0.16629000
C	-0.82638700	0.95688900	1.02054500
H	-1.29824200	0.25427600	1.69739300
C	-0.87545600	2.30462200	1.35817800
H	-1.37299600	2.59564200	2.27909300
C	0.64144600	-1.36179600	-1.56651300
C	-0.02685600	-0.92303200	-0.42903900
C	-0.24057900	-1.94716200	0.65770600
H	0.50668600	-2.74574000	0.60734800
H	-0.15841800	-1.50175300	1.65641800
C	-1.56723800	-2.70659600	0.64345400
C	-2.81597100	-1.83071300	0.84795400
F	-1.55607300	-3.60937300	1.68058500
F	-1.69387800	-3.43666300	-0.49483300
O	-3.08262100	-1.34488900	1.92124600
H	-0.37566100	4.32809900	0.78248600
O	-3.51228200	-1.68067900	-0.26833700
C	-4.66410600	-0.81617100	-0.19568200
H	-5.20425400	-1.01306300	0.73327200
H	-5.27240000	-1.13289300	-1.04499600
C	-4.28560200	0.63737800	-0.30684400
C	-3.45484500	1.07040100	-1.34327700
C	-4.78326600	1.56565100	0.60592600
C	-3.14029100	2.41798300	-1.47073500
H	-3.03255600	0.34582700	-2.03374500
C	-4.47624200	2.91843100	0.47259600

H	-5.40419300	1.22806900	1.43133500
C	-3.65604900	3.34538500	-0.56738600
H	-2.47473200	2.74167300	-2.26377300
H	-4.86661300	3.63423800	1.18964100
H	-3.40064200	4.39602900	-0.66407100
F	0.45018800	-0.77088900	-2.75172300
F	0.76410200	-2.67578300	-1.76075600
N	3.81869300	0.30993900	0.54970100
C	2.69022500	0.76817900	1.39225400
C	3.00298600	0.78056000	2.88145200
H	1.83567300	0.13685300	1.15804800
H	2.40799300	1.76218200	1.04317400
H	2.10392300	1.09164500	3.41970700
H	3.29074500	-0.21031300	3.24449700
H	3.80614100	1.47990000	3.12532900
C	3.98725300	-0.94944400	0.27977800
C	4.59874200	1.36247500	-0.15899400
C	5.04474400	2.46607600	0.79627500
C	3.80342300	1.88867500	-1.35244400
H	5.50121900	0.87463400	-0.52480800
H	5.62331600	2.06593500	1.63355700
H	5.68410200	3.15870400	0.24277700
H	4.20253600	3.04200900	1.18882300
H	3.40195900	1.06148800	-1.94415900
H	2.96181200	2.50270500	-1.02326100
H	4.45842100	2.50645200	-1.97346900
C	5.03575300	-1.41045700	-0.68871900
C	3.26138600	-2.03719300	0.99654000
H	4.91433500	-0.91523700	-1.65269900
H	6.04028500	-1.21590700	-0.29699500
H	4.92884800	-2.48227300	-0.84975900
H	2.82799800	-2.69329900	0.23932500
H	4.00139800	-2.61394400	1.56434600
H	2.47726500	-1.70461500	1.67008500
F	2.34416100	-1.02122100	-1.52153600

TS2

E = -1323.880332

C	1.74433000	2.81071200	-2.28186600

C	0.67473100	2.02511400	-2.70640500
H	0.50666500	1.85661700	-3.76694100
C	-0.18019200	1.43078000	-1.78347300
H	-0.97696400	0.79633700	-2.15954500
C	-0.01013000	1.59696700	-0.39231500
C	1.07252200	2.40296300	0.01233700
H	1.26000200	2.56641800	1.06627800
C	1.92869800	2.99249600	-0.91176800
H	2.75238600	3.60410400	-0.55137400
C	-0.70988600	1.09518400	1.98211700
C	-0.88764100	0.84162200	0.53458600
C	-2.36332900	0.74223200	0.12116600
H	-3.03831900	1.08916800	0.91079200
H	-2.55854100	1.37067900	-0.75305300
C	-2.84527300	-0.66877900	-0.25250900
C	-1.84905100	-1.52863900	-1.07556800
F	0.54874300	0.83340800	2.42923000
F	-0.95389900	2.39509900	2.39782000
F	-1.53817000	0.34135000	2.74358500
F	-4.02567300	-0.54290400	-0.93716300
F	-3.16466400	-1.36346500	0.89896700
O	-2.19132900	-2.06279400	-2.13742100
H	2.41721100	3.27020000	-3.00012900
C	0.44112200	-2.16301800	-1.19320700
H	0.50405200	-1.77176300	-2.22020300
H	0.27187000	-3.24532500	-1.28323400
C	1.73818500	-1.90080100	-0.46172100
C	2.16204800	-2.75026800	0.56349100
C	2.50934900	-0.77427500	-0.75700800
C	3.32912800	-2.48542200	1.27590300
H	1.55771600	-3.61902300	0.81249700
C	3.67430400	-0.50095400	-0.04385300
H	2.18015300	-0.08955400	-1.53405600
C	4.09047100	-1.35710500	0.97329400
H	3.63957900	-3.15415300	2.07422500
H	4.24600300	0.39255000	-0.27782400
H	4.99595700	-1.14203800	1.53406100
N	-0.65736500	-1.54122000	-0.48212700
H	-0.53893100	-0.45754700	0.21161400

TS3

E = -1695.422090

C	-2.73823000	3.26235800	-0.91016400
C	-3.36938100	2.28207000	-1.67409500
H	-3.79588600	2.53399200	-2.63965500
C	-3.43674900	0.97127100	-1.21607700
H	-3.90457800	0.21519400	-1.83672800
C	-2.88048400	0.62341400	0.01681600
C	-2.25944600	1.61284100	0.77772200
H	-1.81812400	1.35296300	1.73605200
C	-2.18122800	2.92529200	0.31930200
H	-1.66875500	3.67437400	0.91430600
C	-4.33749900	-1.17335600	0.99430500
C	-2.92854600	-0.80199400	0.54295000
C	-2.40083900	-1.87980900	-0.42164900
H	-2.66067900	-2.87202200	-0.04302000
H	-2.82971400	-1.76525500	-1.41802800
C	-0.89119500	-1.87023300	-0.58065000
C	-0.34775700	-0.64062600	-1.34411200
F	-4.84618200	-0.26448900	1.84408800
F	-5.20346100	-1.29015300	-0.03248300
F	-4.34795000	-2.36017300	1.64502200
F	-0.53540300	-3.01123500	-1.26857400
F	-0.31628900	-2.02131700	0.67067100
O	-0.95161100	-0.40290000	-2.39765200
H	-2.67330000	4.28229600	-1.27621900
C	0.78249900	1.38136300	-1.39351600
H	-0.18685500	1.69201100	-1.80569000
H	1.46615600	1.36368100	-2.25769000
C	1.24602700	2.43471500	-0.41066400
C	1.09361500	2.27499500	0.96667300
C	1.82232900	3.61743200	-0.88132000
C	1.51952800	3.26135800	1.85412200
H	0.63164300	1.36515400	1.33219700
C	2.24581800	4.60965100	-0.00104100
H	1.94949400	3.75810100	-1.95252600
C	2.10112300	4.43342300	1.37475000
H	1.39168800	3.11635600	2.92340000

H	2.69449000	5.51958100	-0.38850500
H	2.43509600	5.20284100	2.06399400
N	0.63820800	0.06662100	-0.78271700
H	1.89869400	-0.53254100	-0.36975200
H	-2.33600000	-0.84654400	1.46285600
N	2.82611200	-1.13343900	0.10444100
C	2.42717300	-0.95457200	1.53978900
C	2.75873100	-2.03836400	2.55563900
H	1.34509400	-0.82419200	1.51285800
H	2.84491700	0.00625700	1.84945200
H	2.37868300	-1.70194800	3.52484000
H	2.25289300	-2.97842600	2.32325400
H	3.82809000	-2.22495800	2.66732800
C	2.61740300	-2.51383900	-0.47480400
C	3.68649700	-3.55381300	-0.13400200
C	2.47118300	-2.43062300	-1.99890900
H	1.66441100	-2.83878200	-0.05598500
H	3.84940600	-3.68484300	0.93485900
H	3.35461100	-4.51433500	-0.53825200
H	4.64409800	-3.31935200	-0.60887300
H	1.80869900	-1.62465400	-2.31605900
H	3.44006200	-2.30187800	-2.49213900
H	2.04155200	-3.36781700	-2.35953700
C	4.17659300	-0.55640200	-0.24241900
C	5.26120700	-0.83069100	0.80174800
C	4.09130800	0.93539900	-0.53456200
H	4.46927600	-1.05474500	-1.16887200
H	5.37037000	-1.88962100	1.03667300
H	6.21667500	-0.47942100	0.40251500
H	5.07658400	-0.28252100	1.73028200
H	3.43058200	1.13797400	-1.37737500
H	3.73126300	1.50575000	0.32608500
H	5.08747600	1.30700900	-0.79039600

TS4

E = -1694.161416

C	-0.09748300	2.67076500	1.71874000
C	0.19690400	2.66215800	0.35454700
H	0.40409000	3.59720200	-0.16074100

C	0.22728500	1.47851700	-0.37136200
H	0.46483000	1.53062500	-1.42374200
C	-0.03984900	0.22204600	0.23118400
C	-0.35301900	0.26121200	1.61167600
H	-0.60664400	-0.64741400	2.14482900
C	-0.37783000	1.45239300	2.33311100
H	-0.63414400	1.41865700	3.38840800
C	0.56671000	-1.13122100	-1.75456700
C	0.03562300	-1.04716100	-0.48279100
C	-0.16022700	-2.36430500	0.22876700
H	0.41979200	-3.15588600	-0.25398400
H	0.16386700	-2.33361300	1.27531800
C	-1.59445800	-2.88893000	0.24479500
C	-2.56324200	-2.05270000	1.10255800
F	-1.59495100	-4.16166500	0.73990300
F	-2.07837300	-2.97866300	-1.03950800
O	-2.53288100	-2.14594000	2.32211200
H	-0.13153300	3.60005400	2.27814400
C	-4.21531000	-0.24821600	1.08690000
H	-3.72421500	0.03287300	2.02381500
H	-5.16514100	-0.72828800	1.34918500
C	-4.45471500	0.96114300	0.21644900
C	-3.40156900	1.83886300	-0.05692300
C	-5.70992700	1.21317800	-0.33765200
C	-3.60084500	2.94706900	-0.87227200
H	-2.42208600	1.64747900	0.36897600
C	-5.91389600	2.32736900	-1.15158100
H	-6.53426600	0.53489700	-0.13229400
C	-4.85906200	3.19522400	-1.42127800
H	-2.77046800	3.61621700	-1.07609300
H	-6.89548800	2.51340200	-1.57641000
H	-5.01579200	4.06107200	-2.05728100
F	0.41391600	-0.16470400	-2.66090000
F	0.57577900	-2.30114300	-2.38254900
N	3.99022300	0.47220700	0.28725000
C	3.18075500	1.15338700	1.32244400
C	3.81977900	1.08534900	2.70217900
H	2.17839500	0.73036400	1.32040000
H	3.05945400	2.18814400	1.00889000

H	3.17711300	1.61318000	3.41147200
H	3.92486100	0.05383000	3.04907200
H	4.80707800	1.55506900	2.71383000
C	3.97194500	-0.81903100	0.13813000
C	4.69326300	1.35950500	-0.67875300
C	5.59021300	2.36665500	0.03577300
C	3.66407300	1.99727900	-1.61253000
H	5.33347200	0.71710700	-1.27922600
H	6.31157000	1.86748700	0.68937100
H	6.14698800	2.93114900	-0.71660900
H	5.01936800	3.08689400	0.62846800
H	3.02959300	1.21894900	-2.04633600
H	3.02990600	2.71712100	-1.08649200
H	4.19041600	2.52989000	-2.40973500
C	4.88295300	-1.51225500	-0.83192400
C	3.16276600	-1.70887400	1.02017500
H	4.58695100	-1.26460200	-1.85295600
H	5.92749700	-1.23644500	-0.65653300
H	4.78144400	-2.59067000	-0.71425300
H	2.69769800	-2.45645300	0.37611000
H	3.83918700	-2.22627400	1.71106600
H	2.38373300	-1.20270300	1.58547900
F	2.36599800	-0.94591800	-1.70566100
N	-3.34372100	-1.20149100	0.41548600
H	-3.28633900	-1.19448900	-0.59253600

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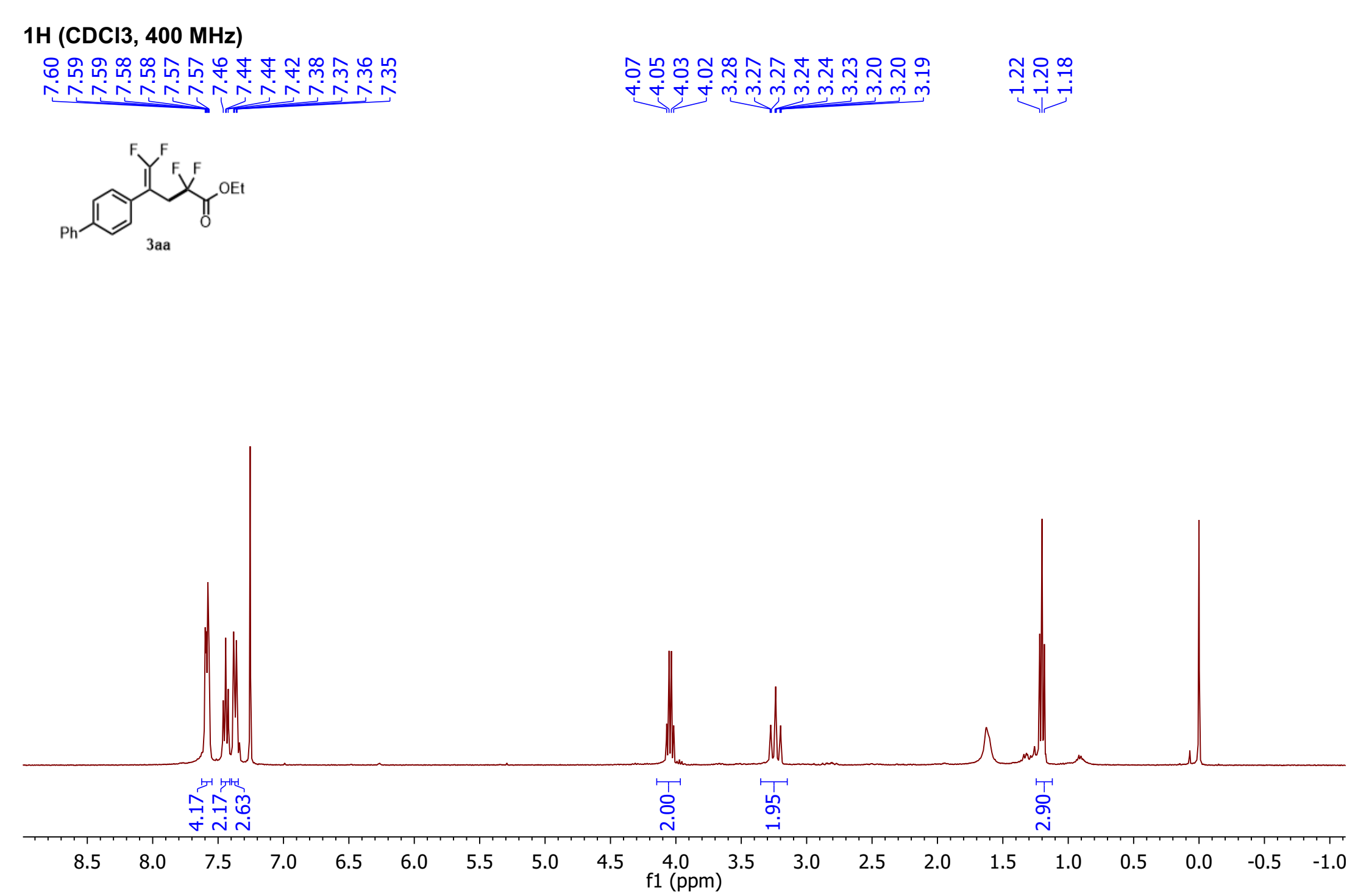
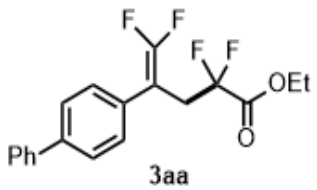
1H (CDCl3, 400 MHz)



^{1}H NMR Spectrum of **3aa**

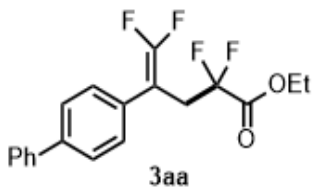
13C (CDCl3, 101 MHz)



3aa

^{13}C NMR Spectrum of **3aa**

19F (CDCl3, 376 MHz)



3aa

^{19}F NMR Spectrum of **3aa**

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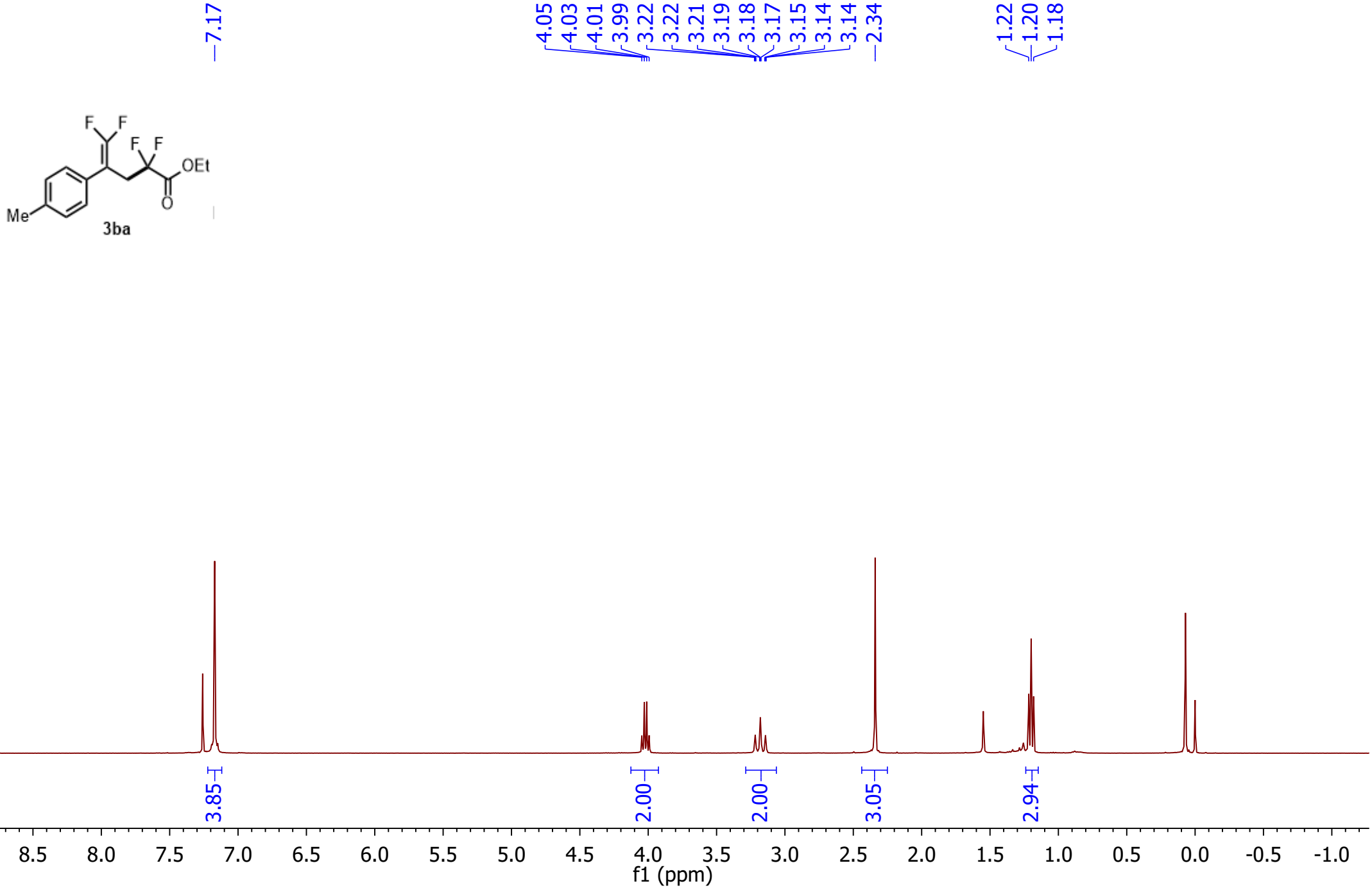
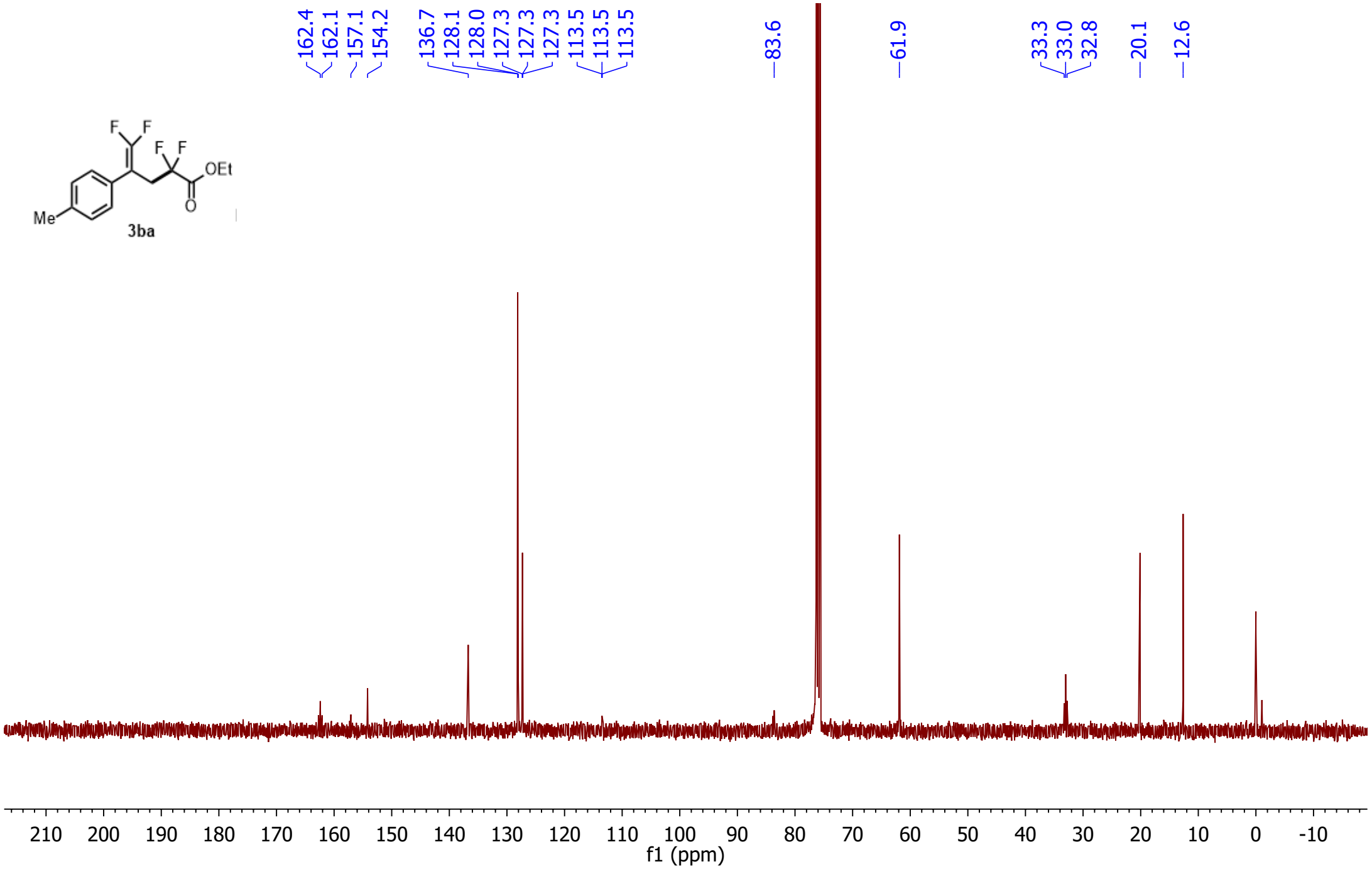
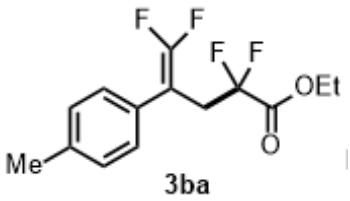


^{1}H NMR Spectrum of **3ba**



^{13}C NMR Spectrum of **3ba**

19F (CDCl3, 400 MHz)



3ba

^{19}F NMR Spectrum of **3ba**

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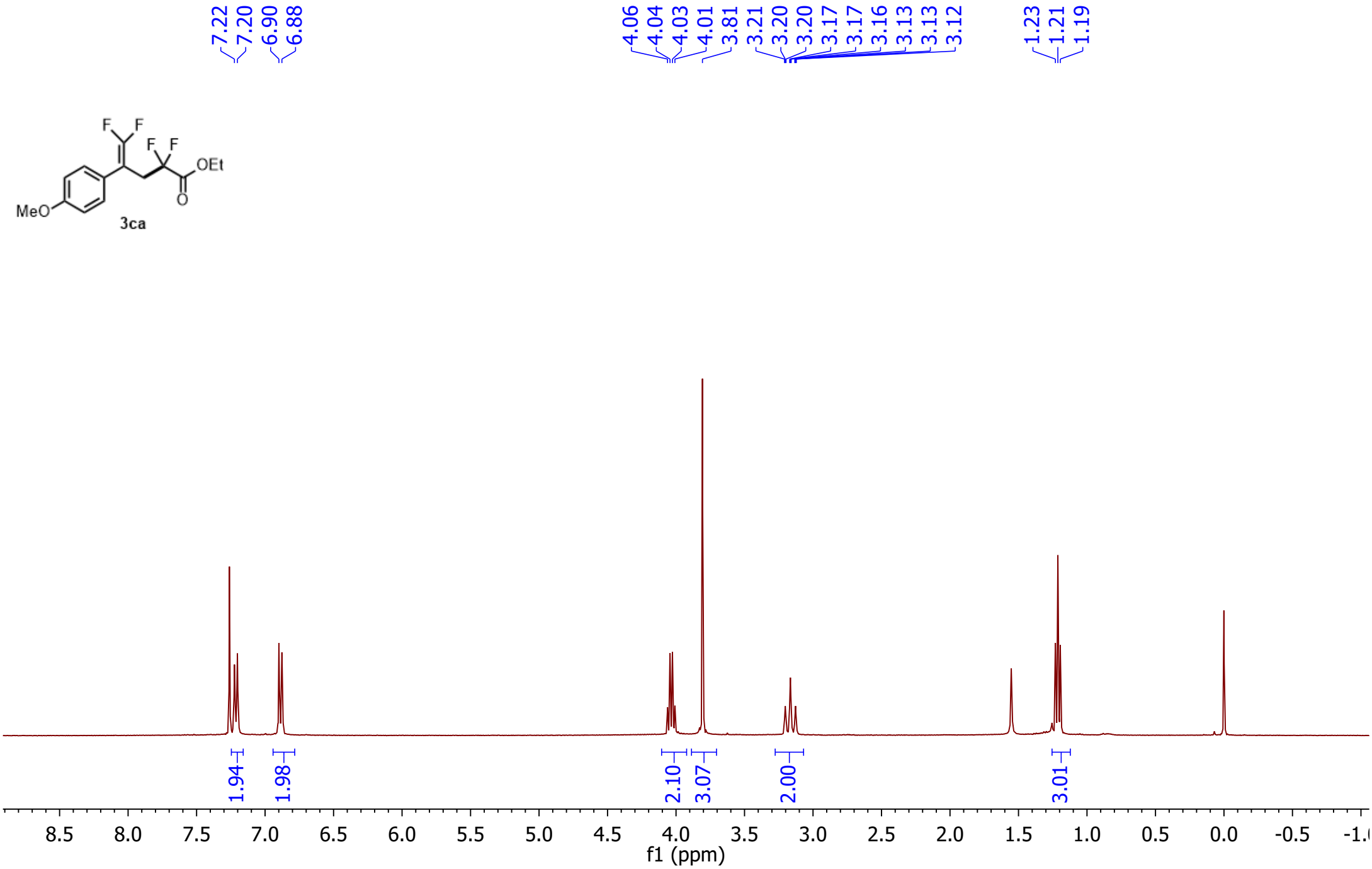
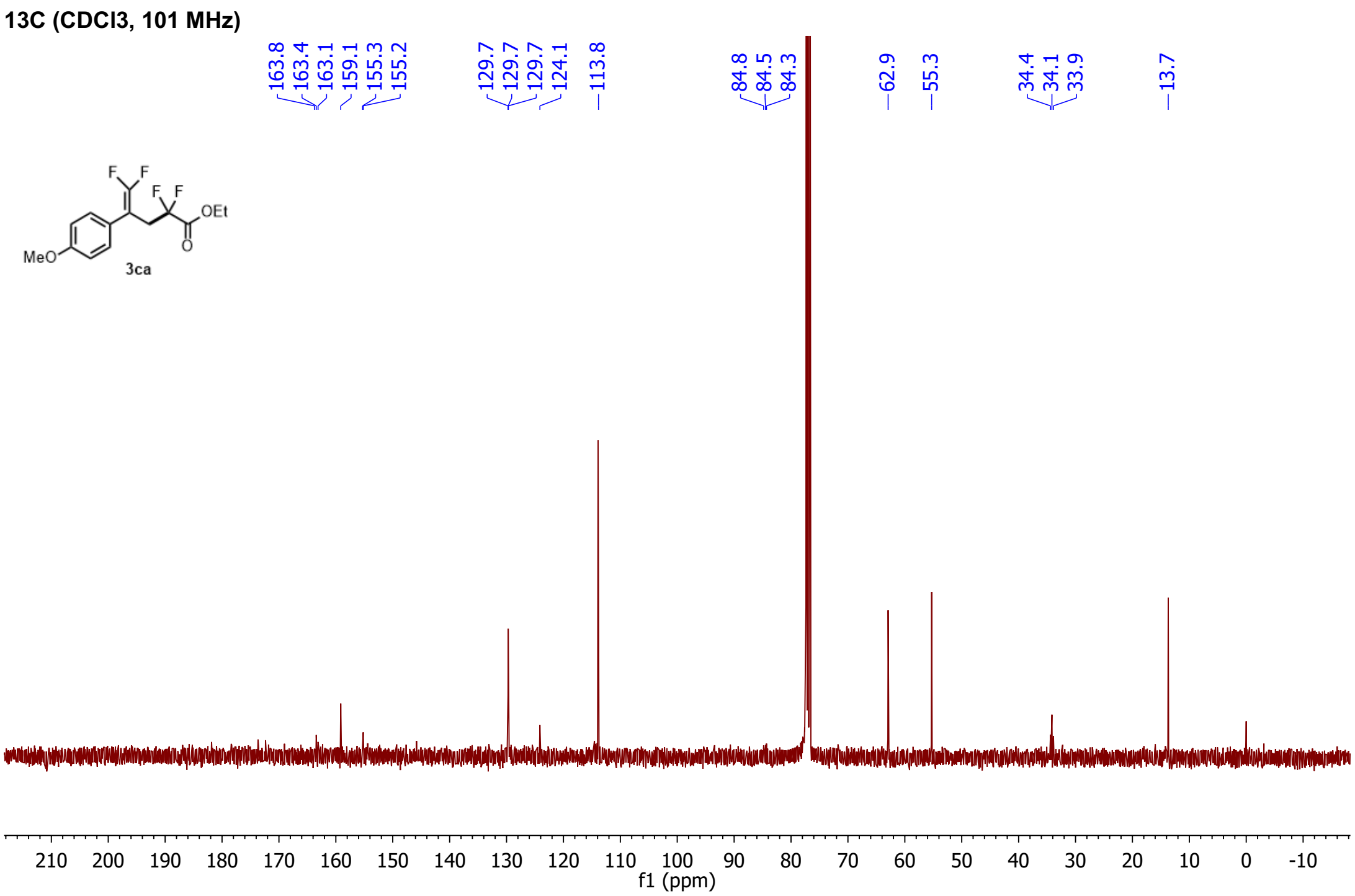
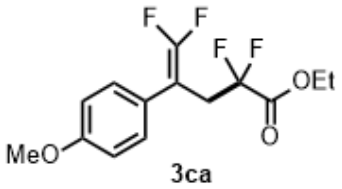


^{1}H NMR Spectrum of **3ca**



^{13}C NMR Spectrum of **3ca**

19F (CDCl3, 376 MHz)



3ca

^{19}F NMR Spectrum of **3ca**

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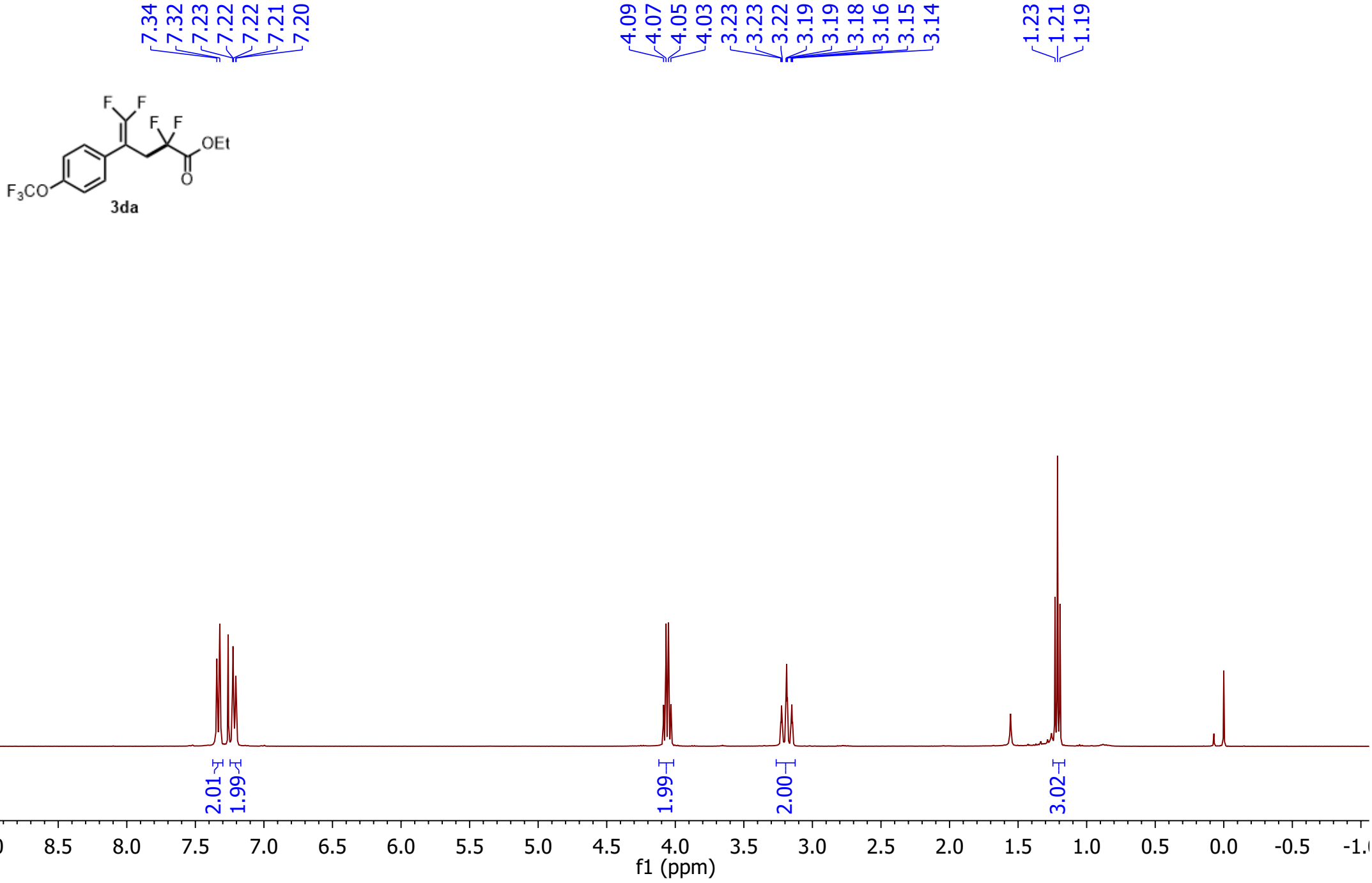
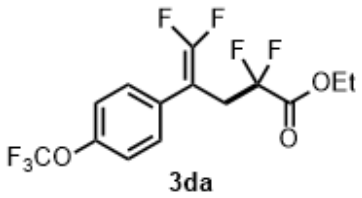


^{1}H NMR Spectrum of **3da**

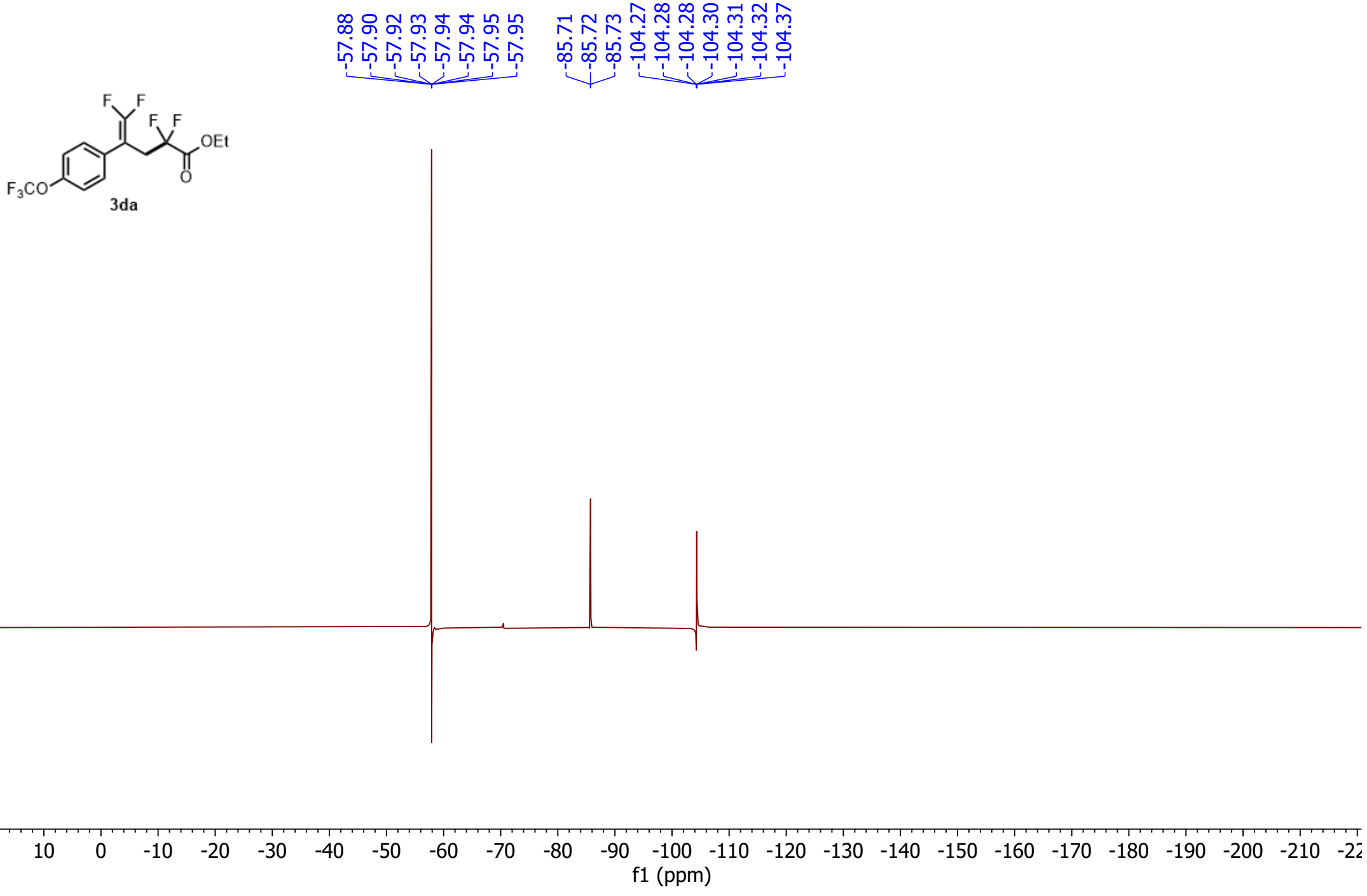
13C (CDCl3, 101 MHz)



3da

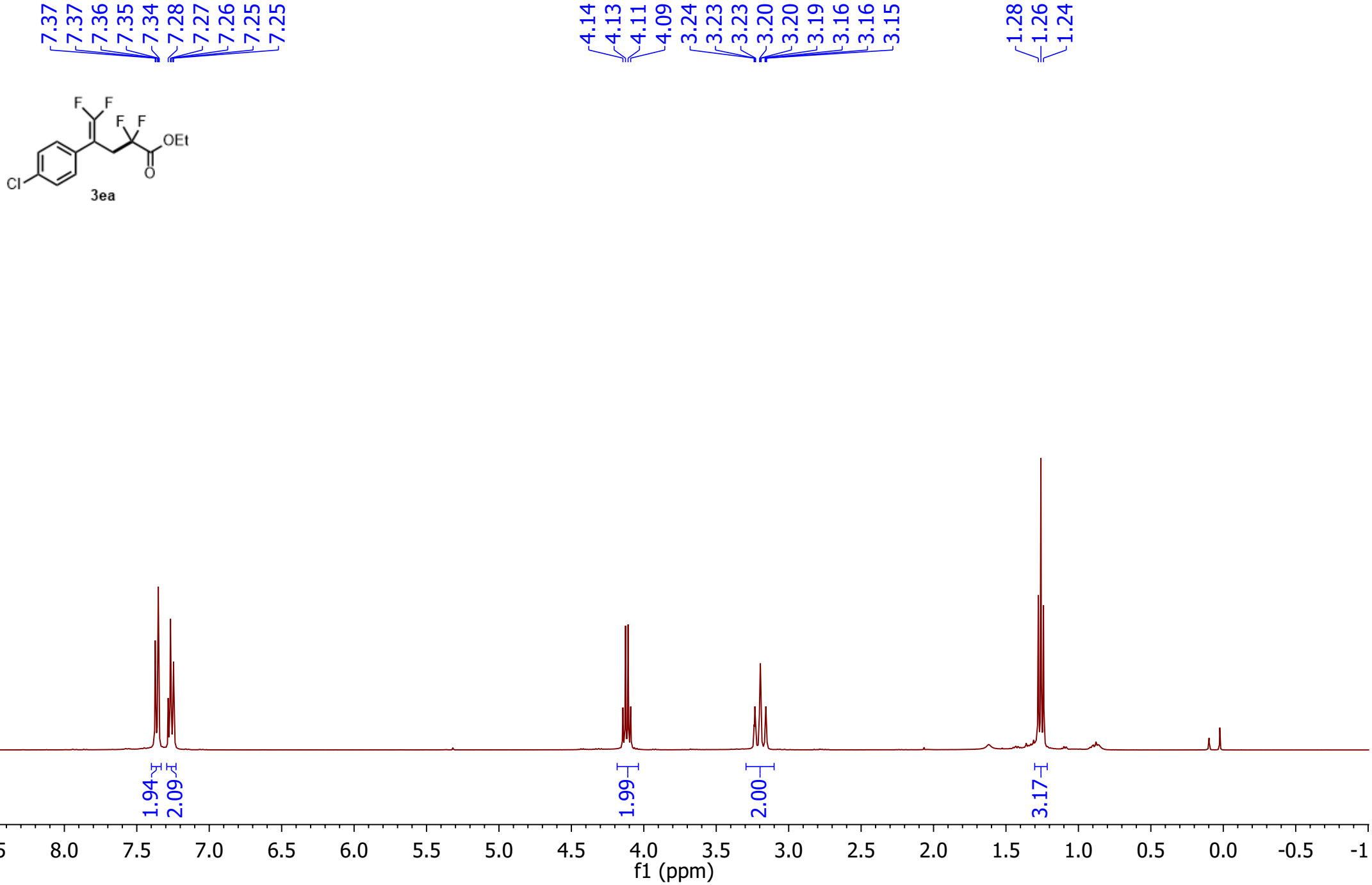
^{13}C NMR Spectrum of **3da**

19F (CDCl3, 376 MHz)



^{19}F NMR Spectrum of **3da**

1H (CDCl3, 400 MHz)



^{1}H NMR Spectrum of **3ea**

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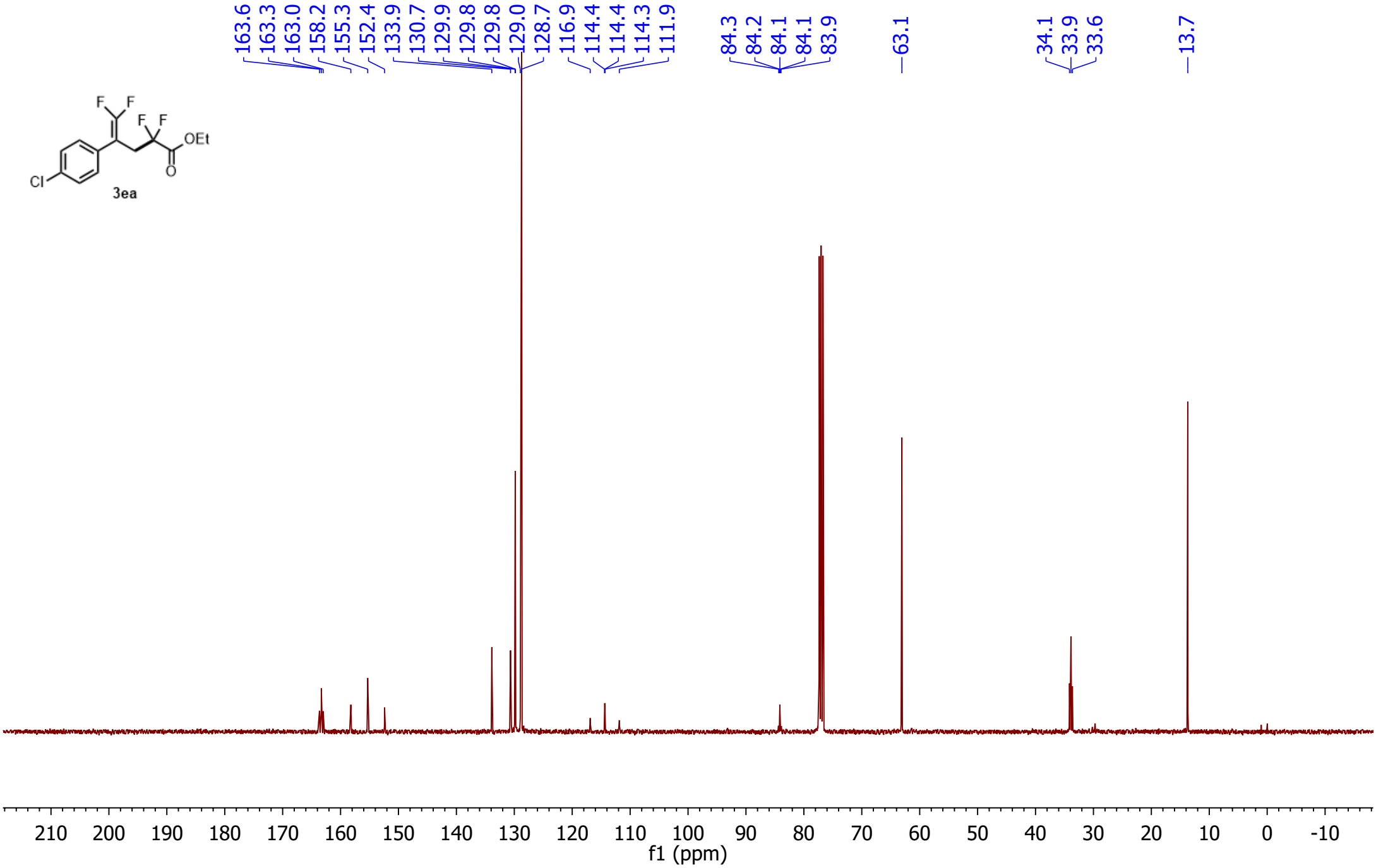

^{13}C NMR Spectrum of **3ea**

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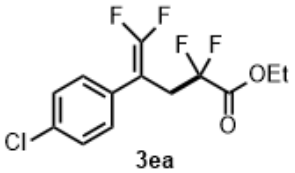

3ea

^{19}F NMR Spectrum of **3ea**

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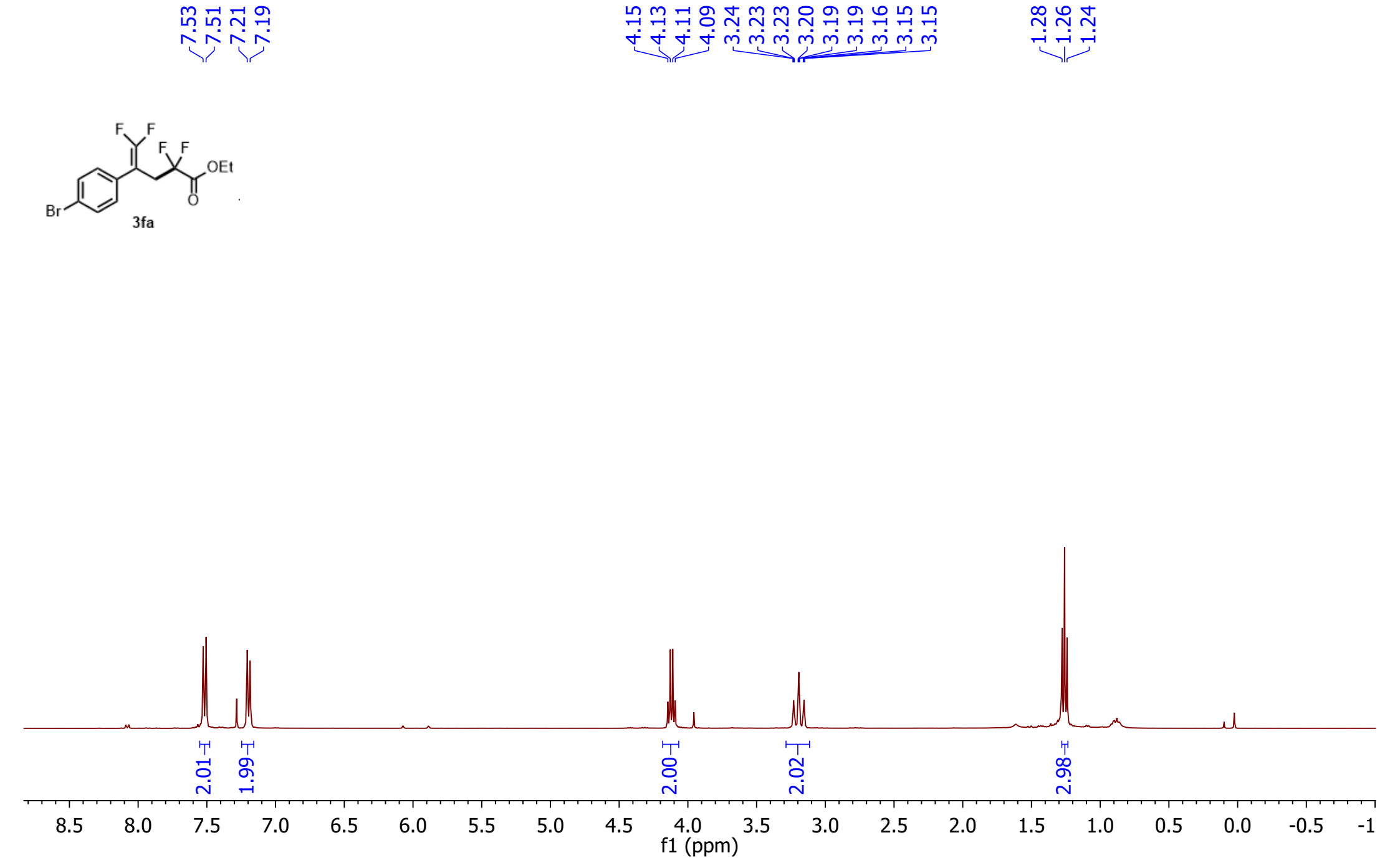
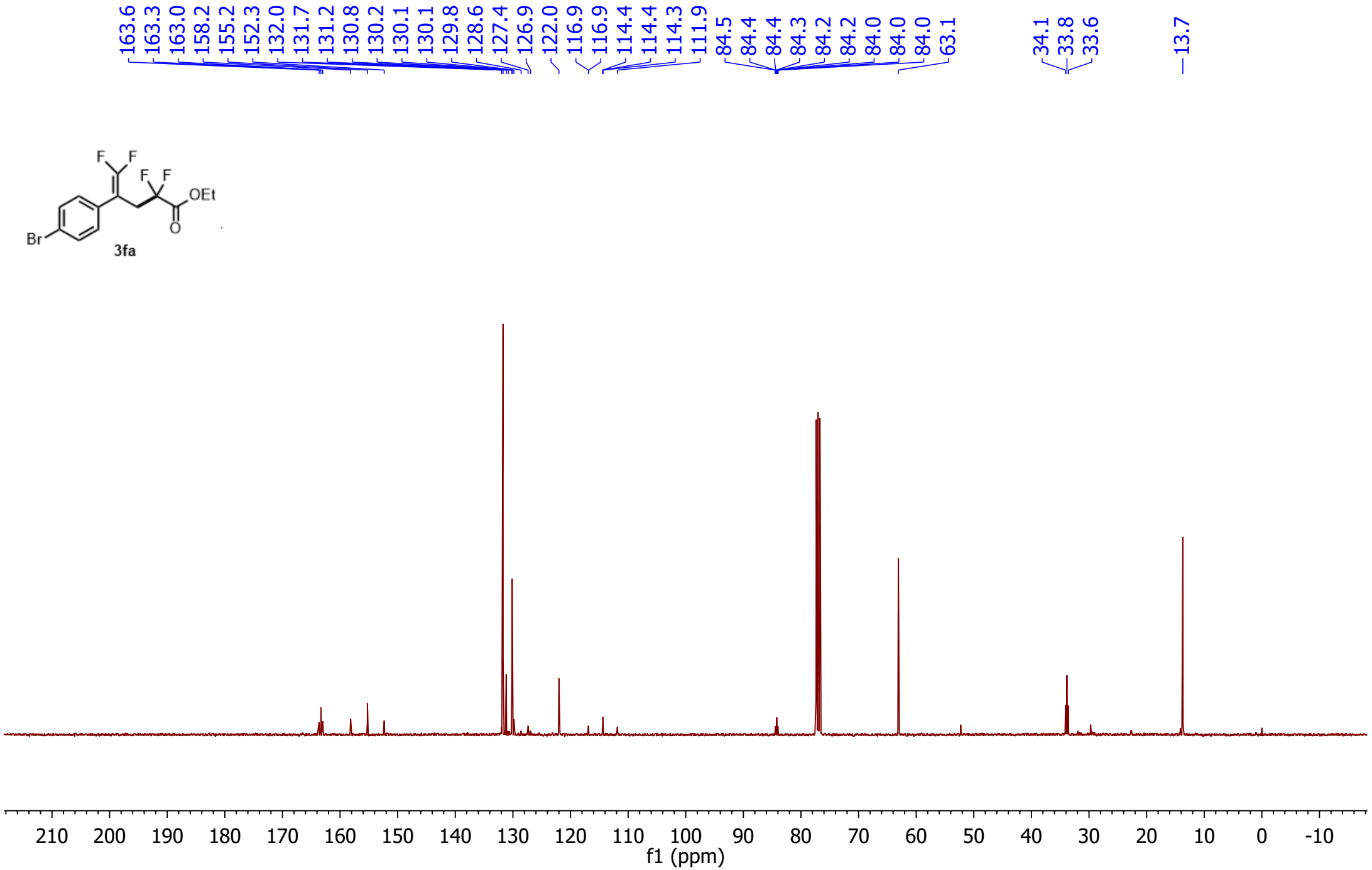


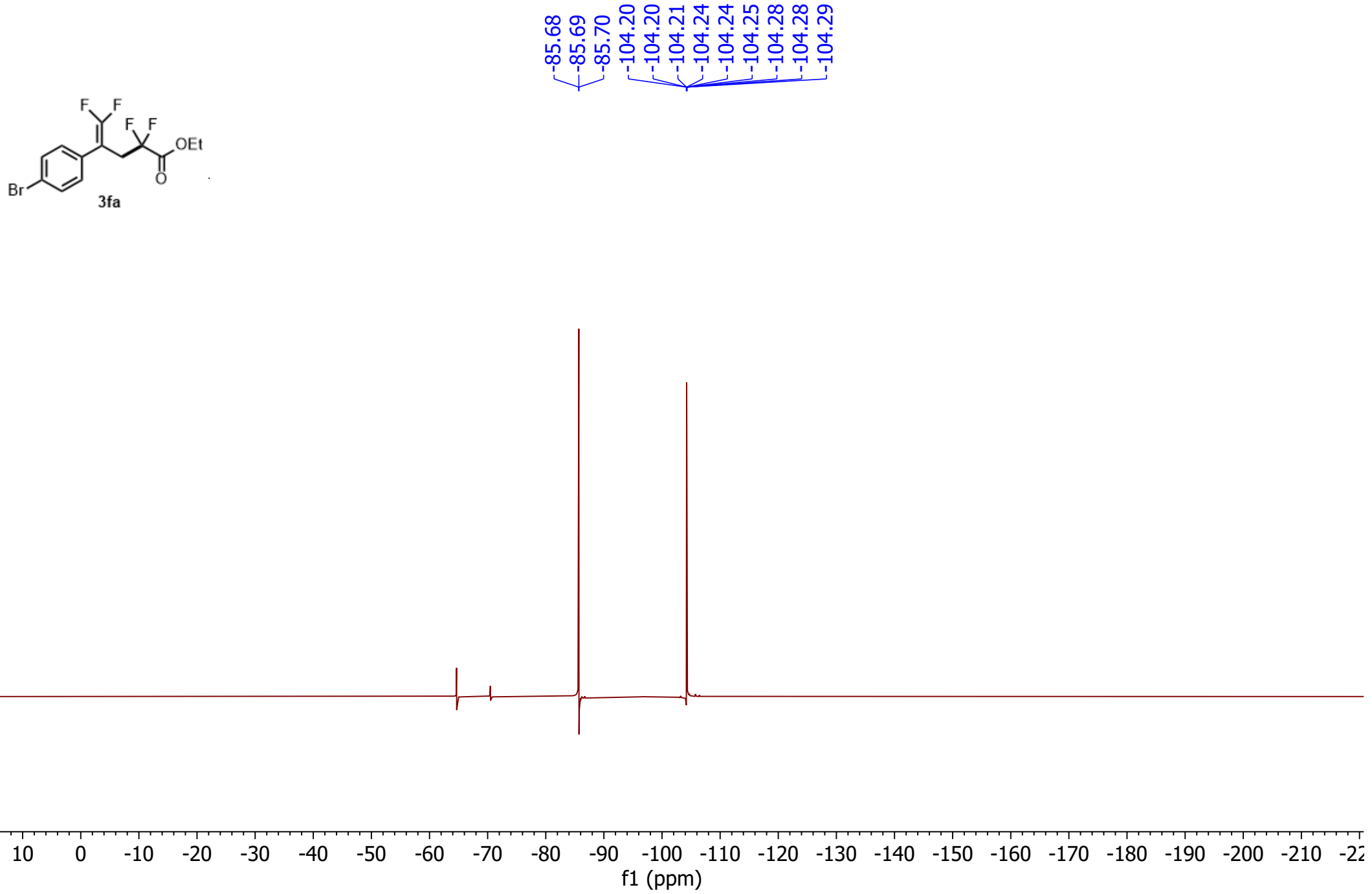
^{1}H NMR Spectrum of **3fa**

13C (CDCl3, 101 MHz)



^{13}C NMR Spectrum of **3fa**

19F (CDCl3, 376 MHz)



^{19}F NMR Spectrum of **3fa**

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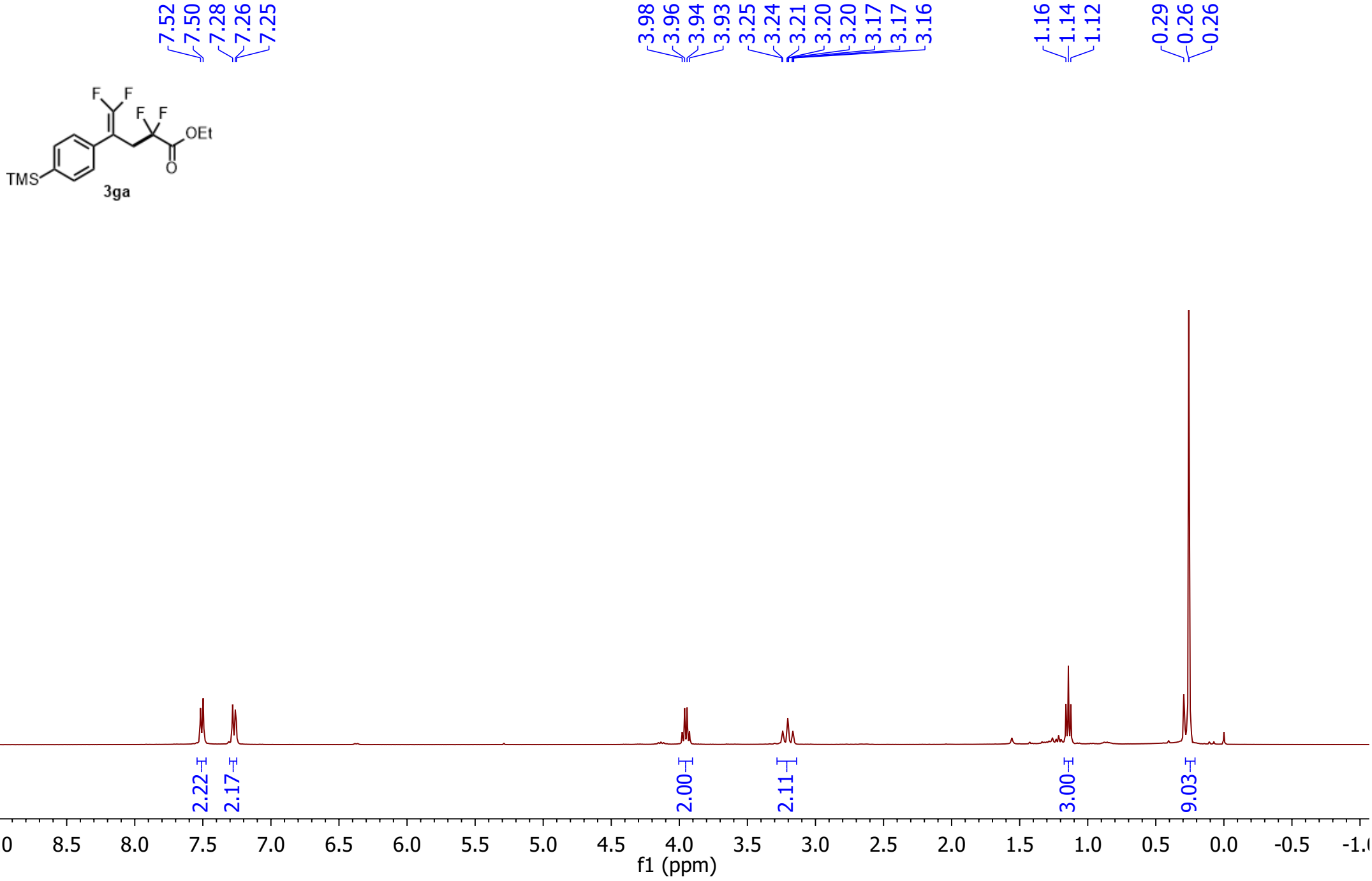
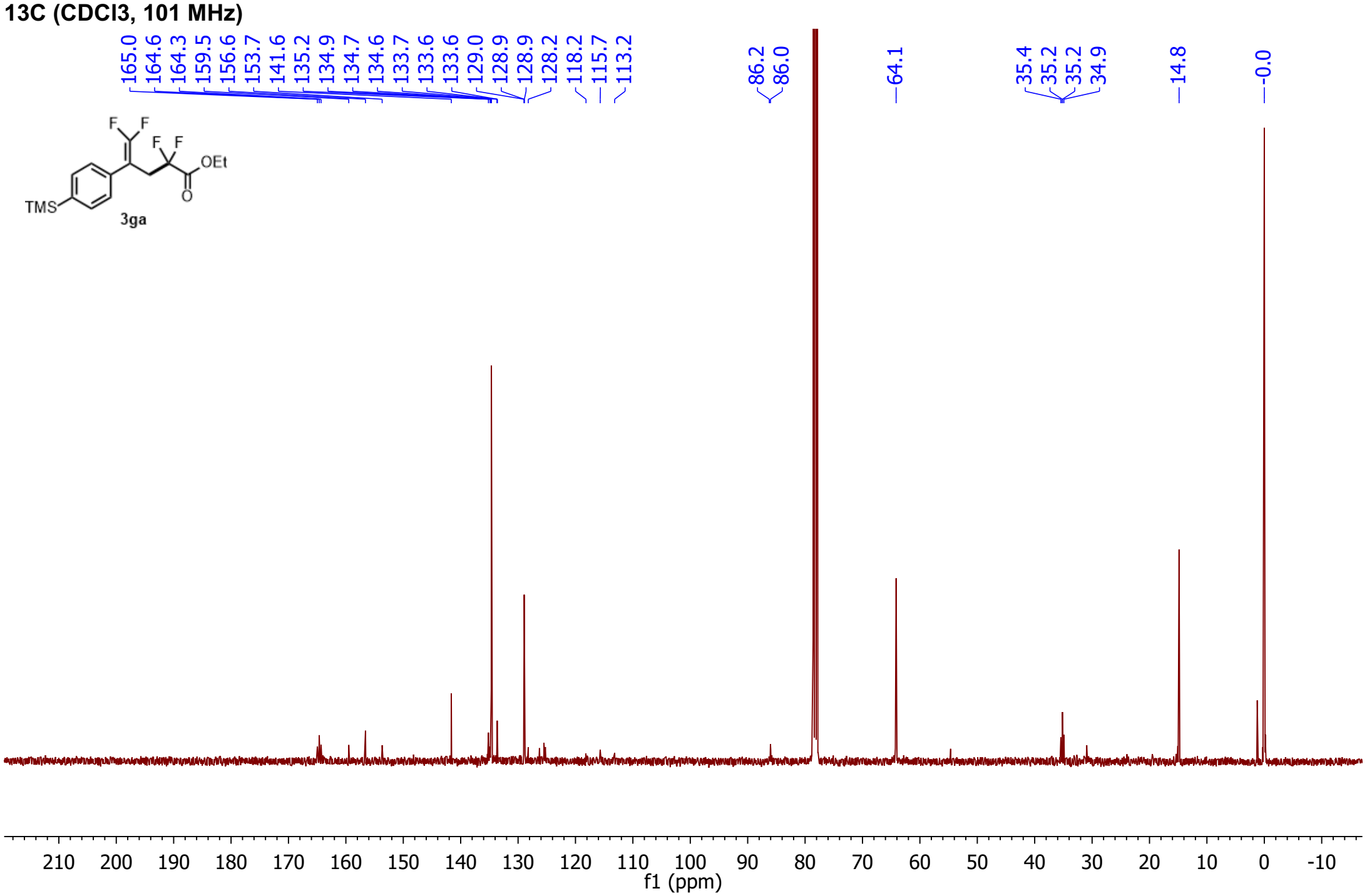
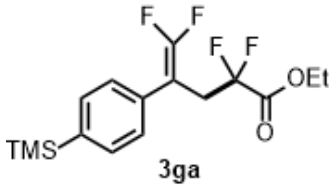


^{1}H NMR Spectrum of **3ga**



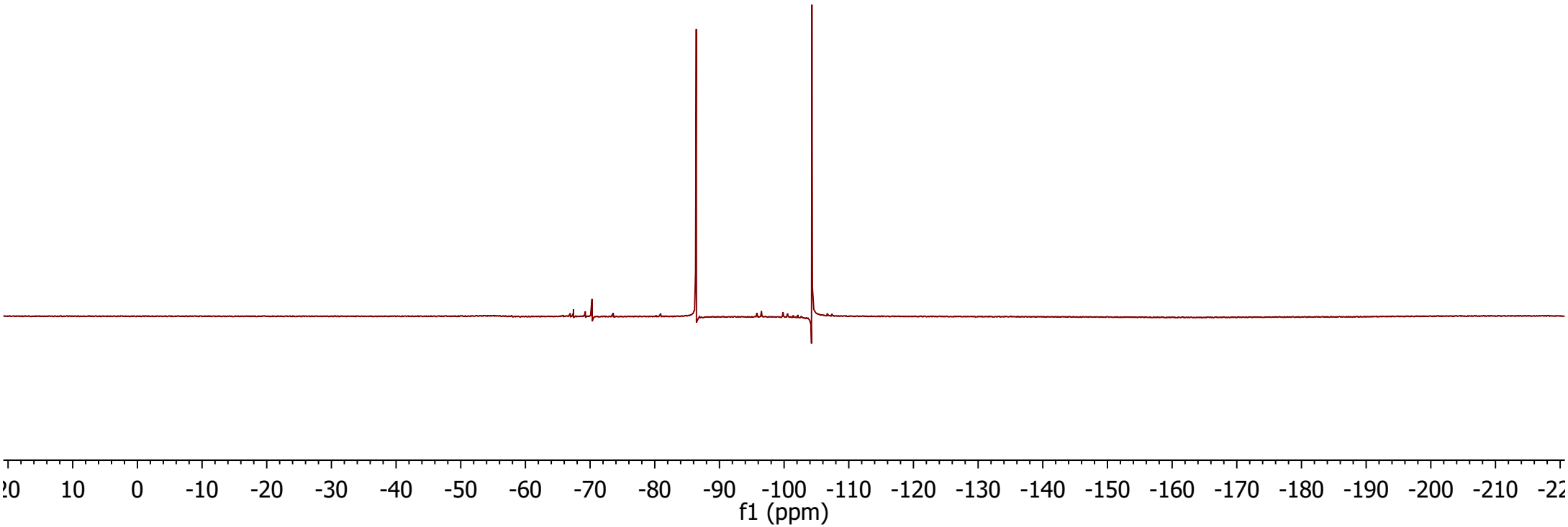
^{13}C NMR Spectrum of **3ga**

19F (CDCl3, 376 MHz)



3ga

-86.30
-86.31
-86.37
-86.38
-86.39
-86.39
-86.42
-86.50
-104.25
-104.26
-104.29
-104.30
-104.33
-104.34



^{19}F NMR Spectrum of **3ga**

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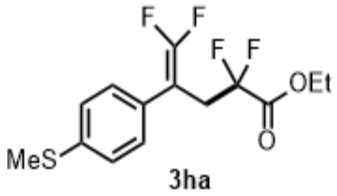
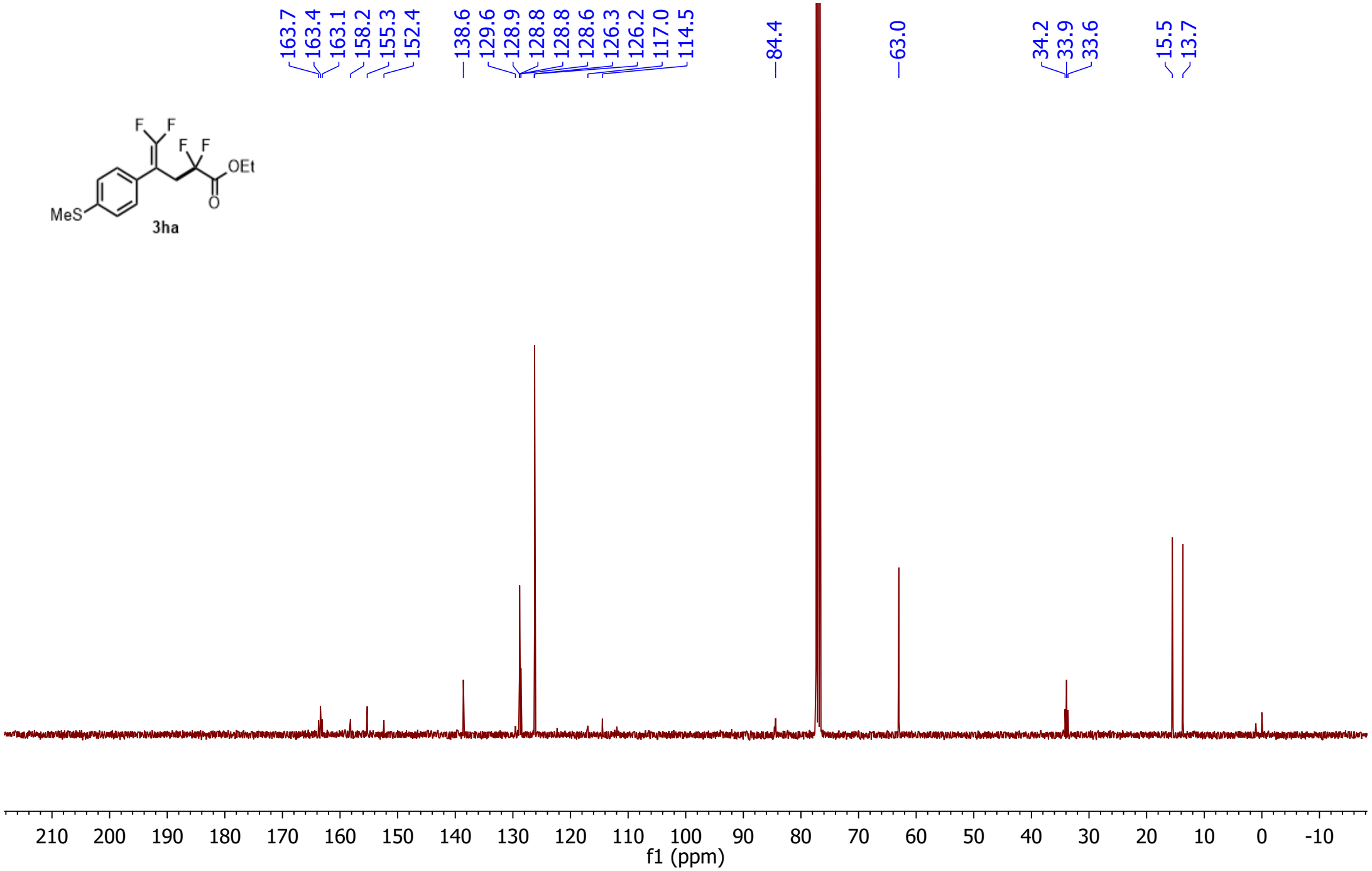


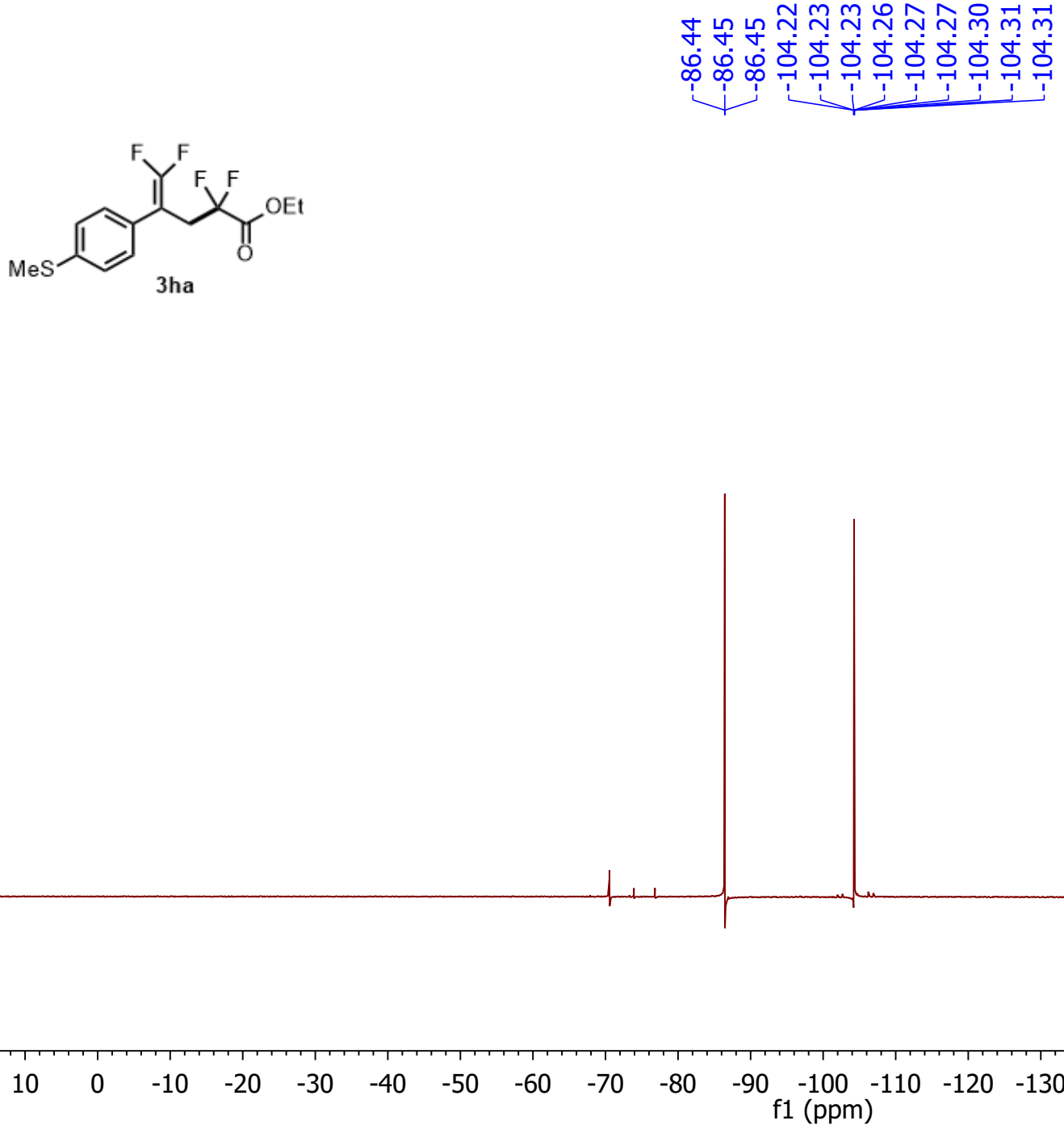
3ha

^{1}H NMR Spectrum of **3ha**



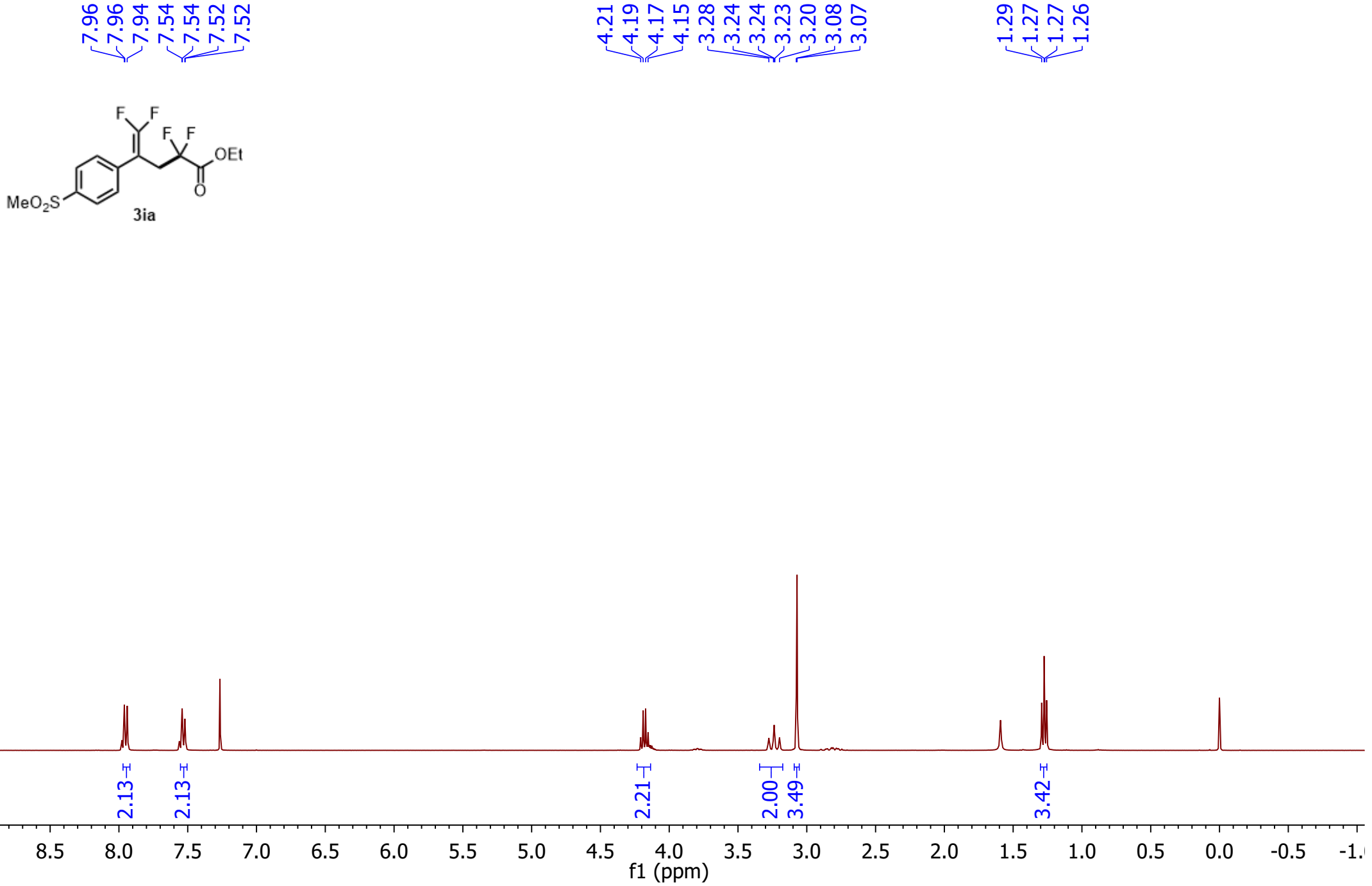
^{13}C NMR Spectrum of **3ha**

19F (CDCl3, 376 MHz)



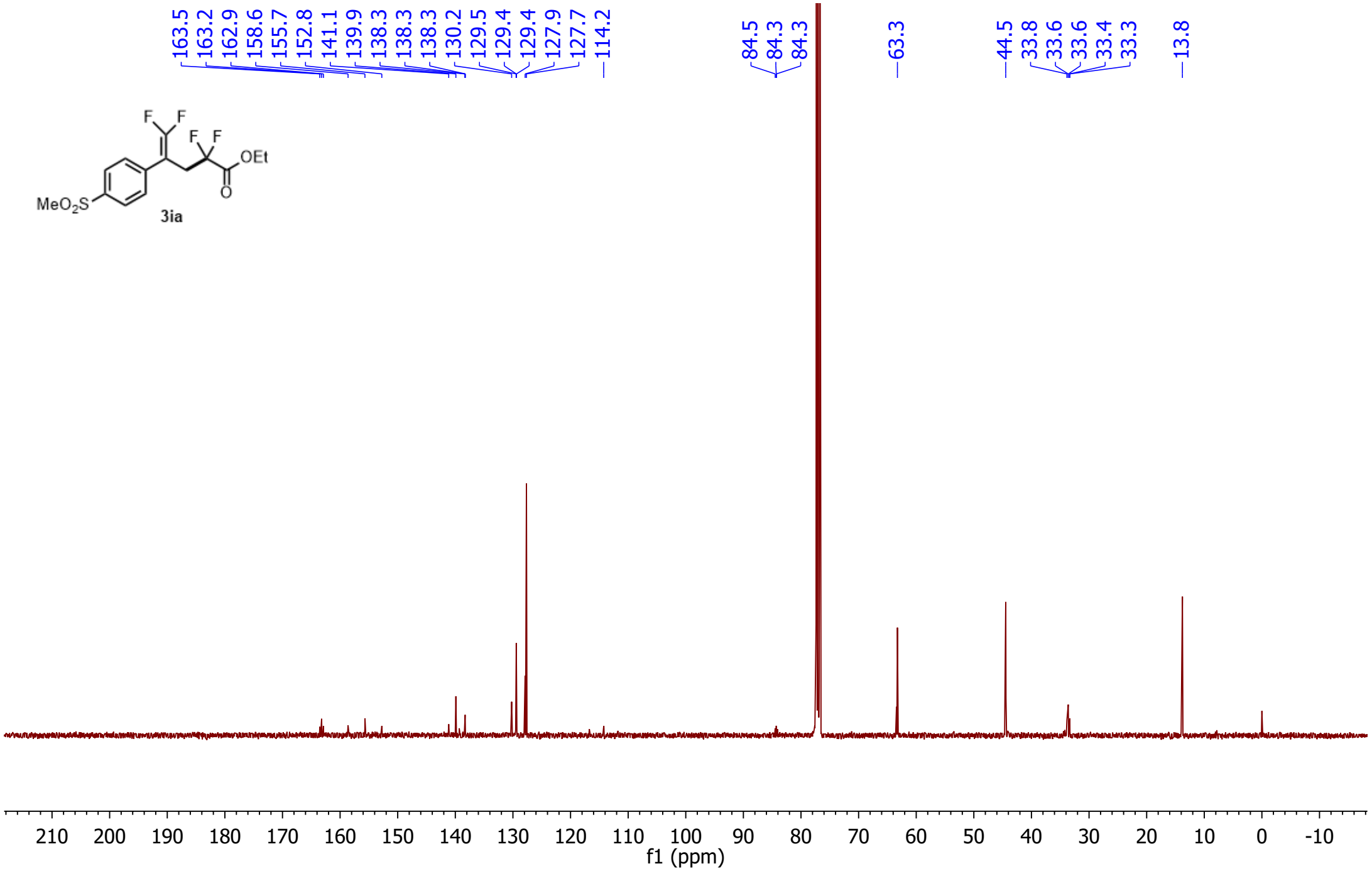
^{19}F NMR Spectrum of **3ha**

1H (CDCl3, 400 MHz)



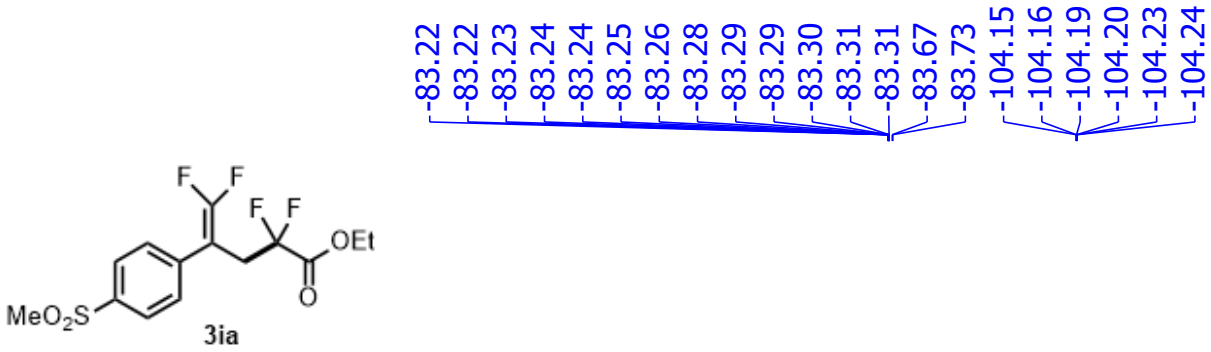
^{1}H NMR Spectrum of **3ia**

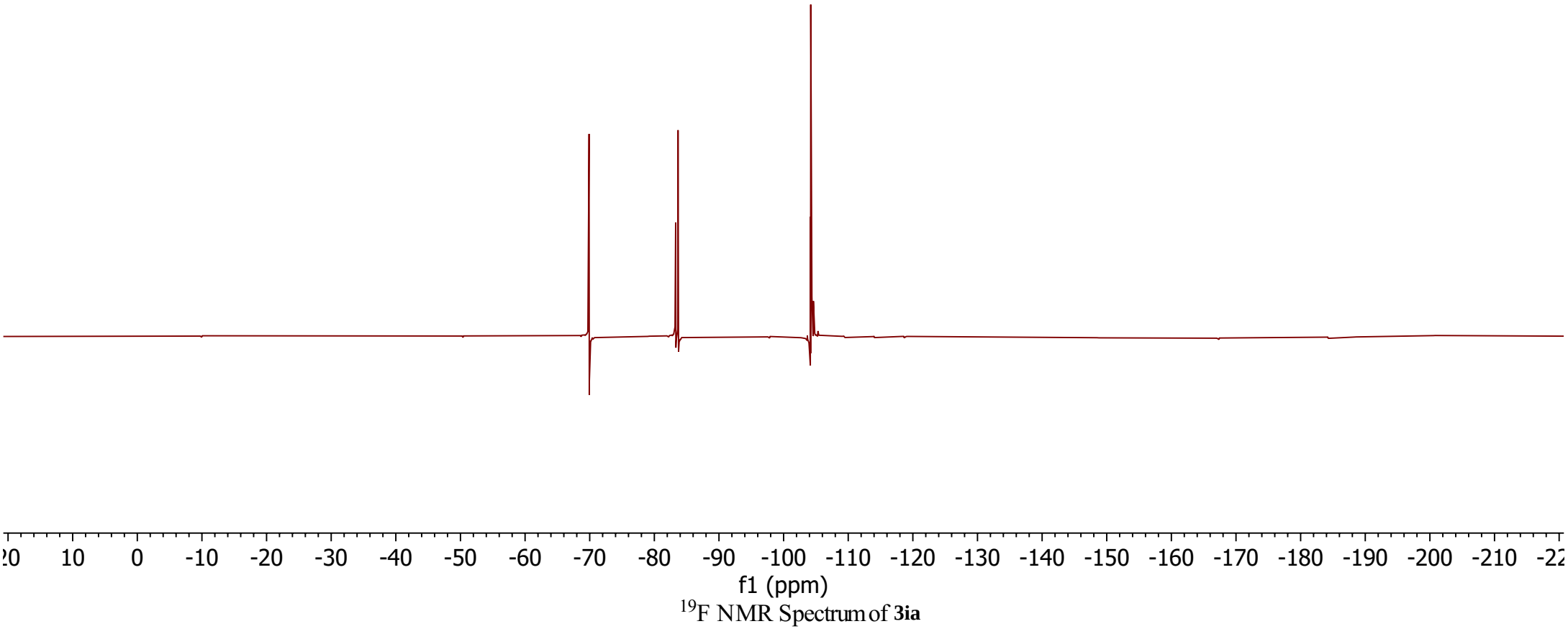
13C (CDCl3, 101 MHz)



^{13}C NMR Spectrum of **3ia**

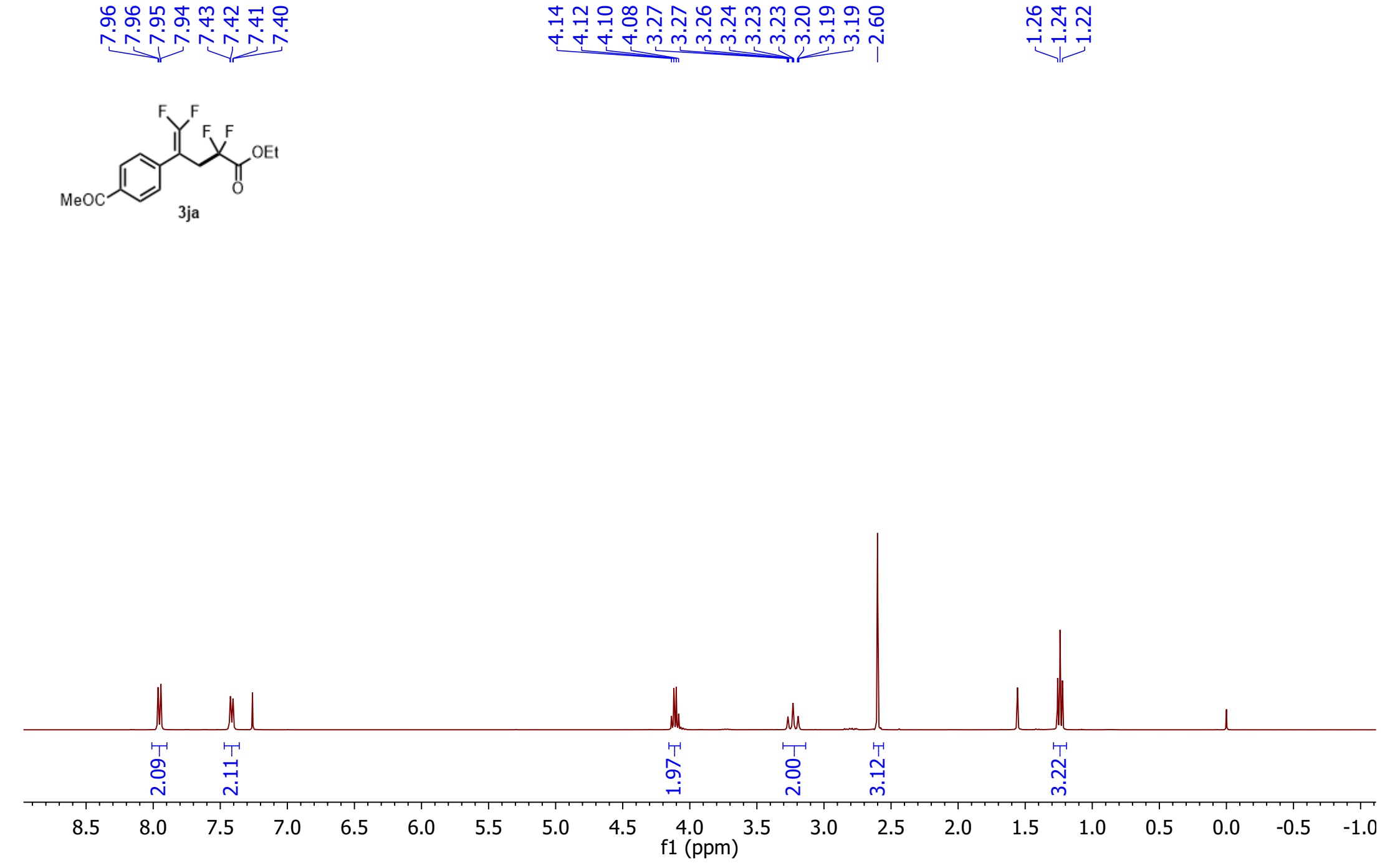
19F (CDCl3, 376 MHz)



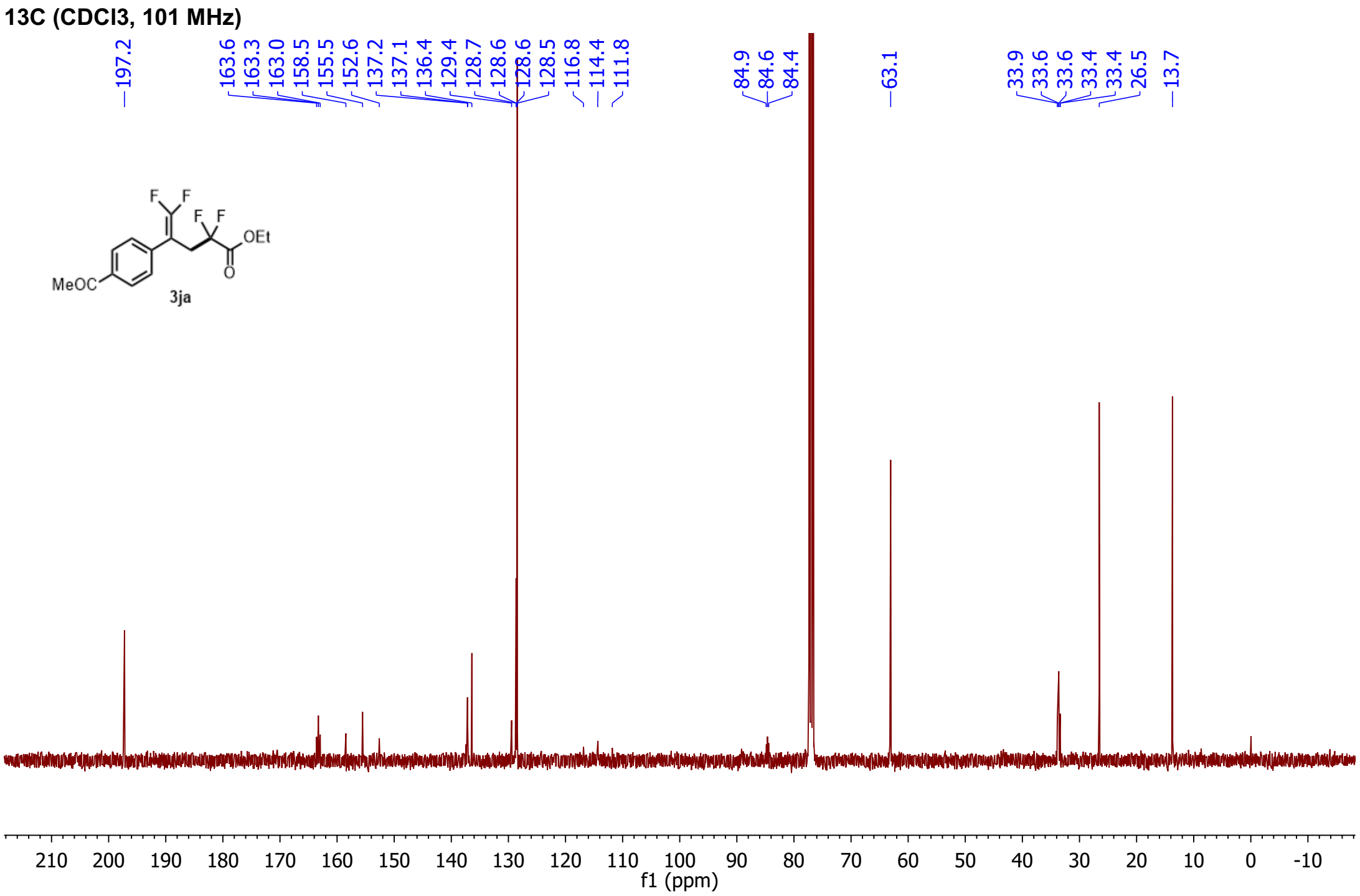


^{19}F NMR Spectrum of **3ia**

1H (CDCl3, 400 MHz)



^{1}H NMR Spectrum of **3ja**



^{13}C NMR Spectrum of **3ja**

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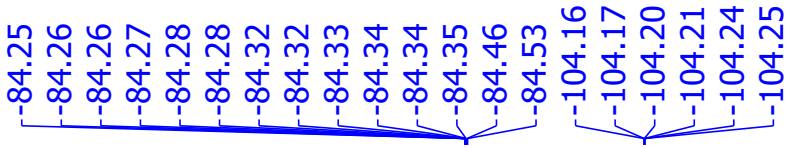
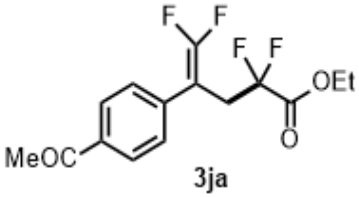
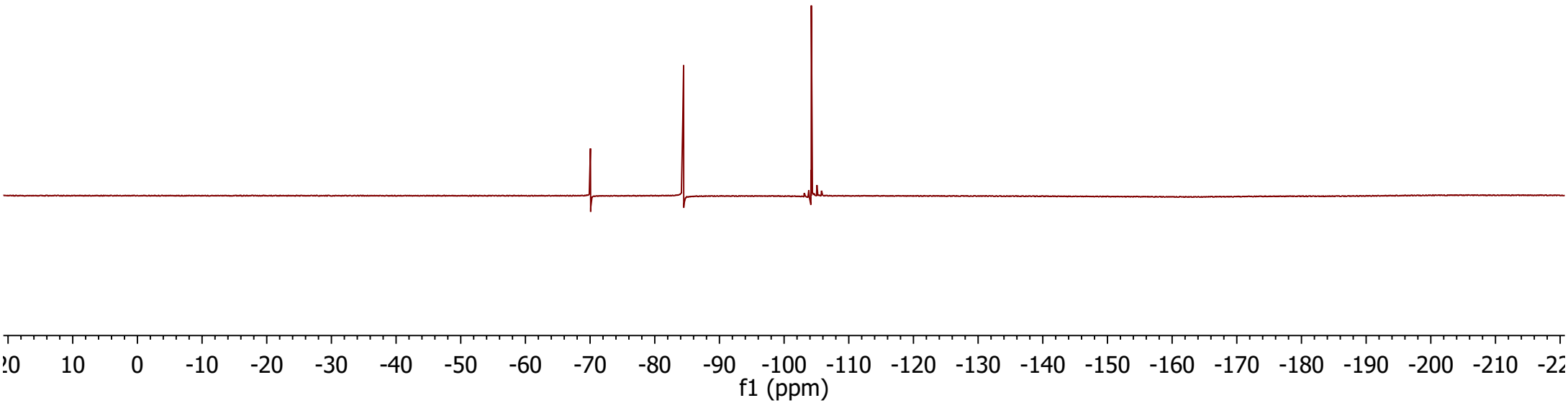


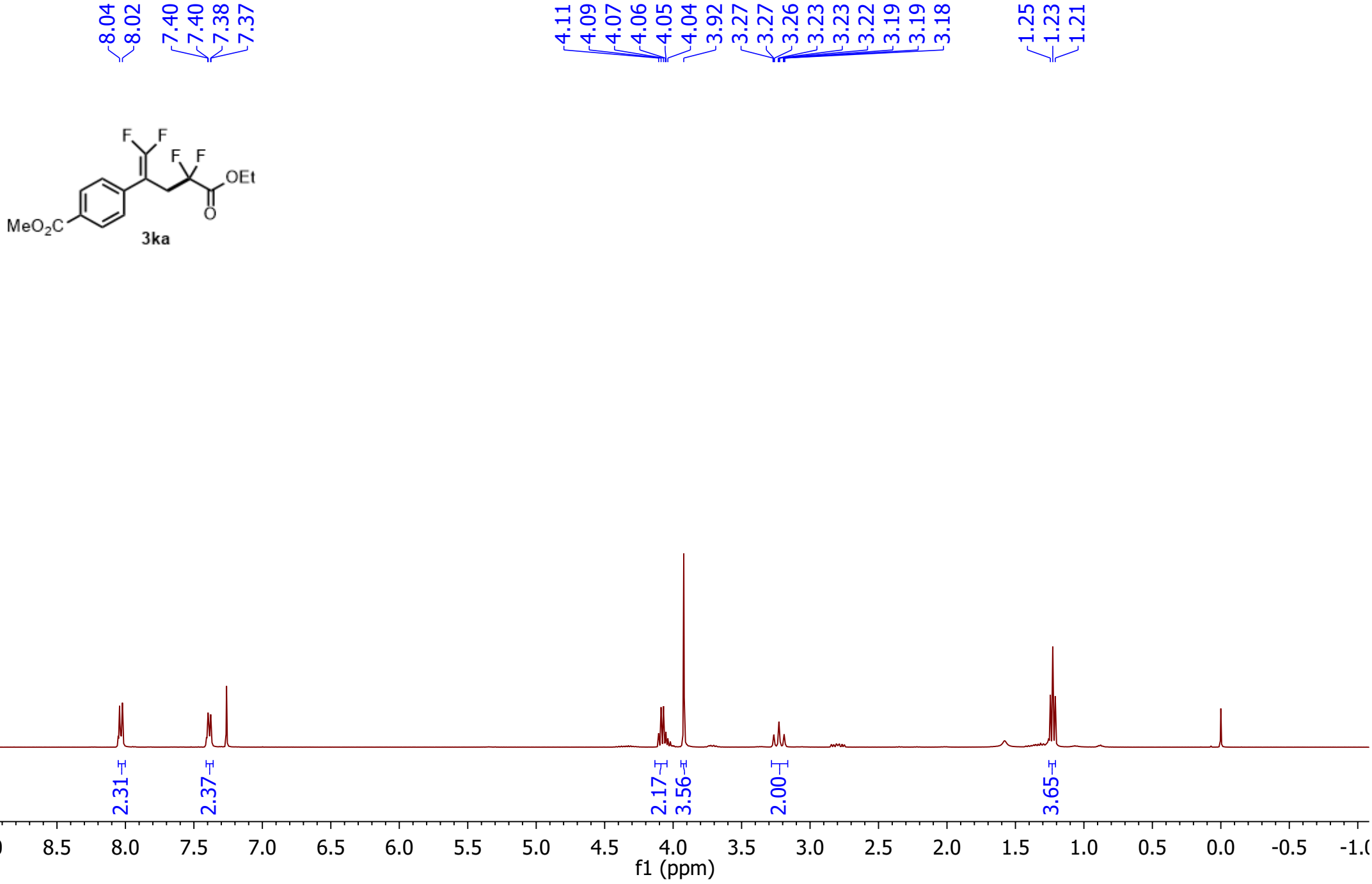


3ja



^{19}F NMR Spectrum of **3ja**

1H (CDCl3, 400 MHz)



[1]H NMR Spectrum of **3ka**

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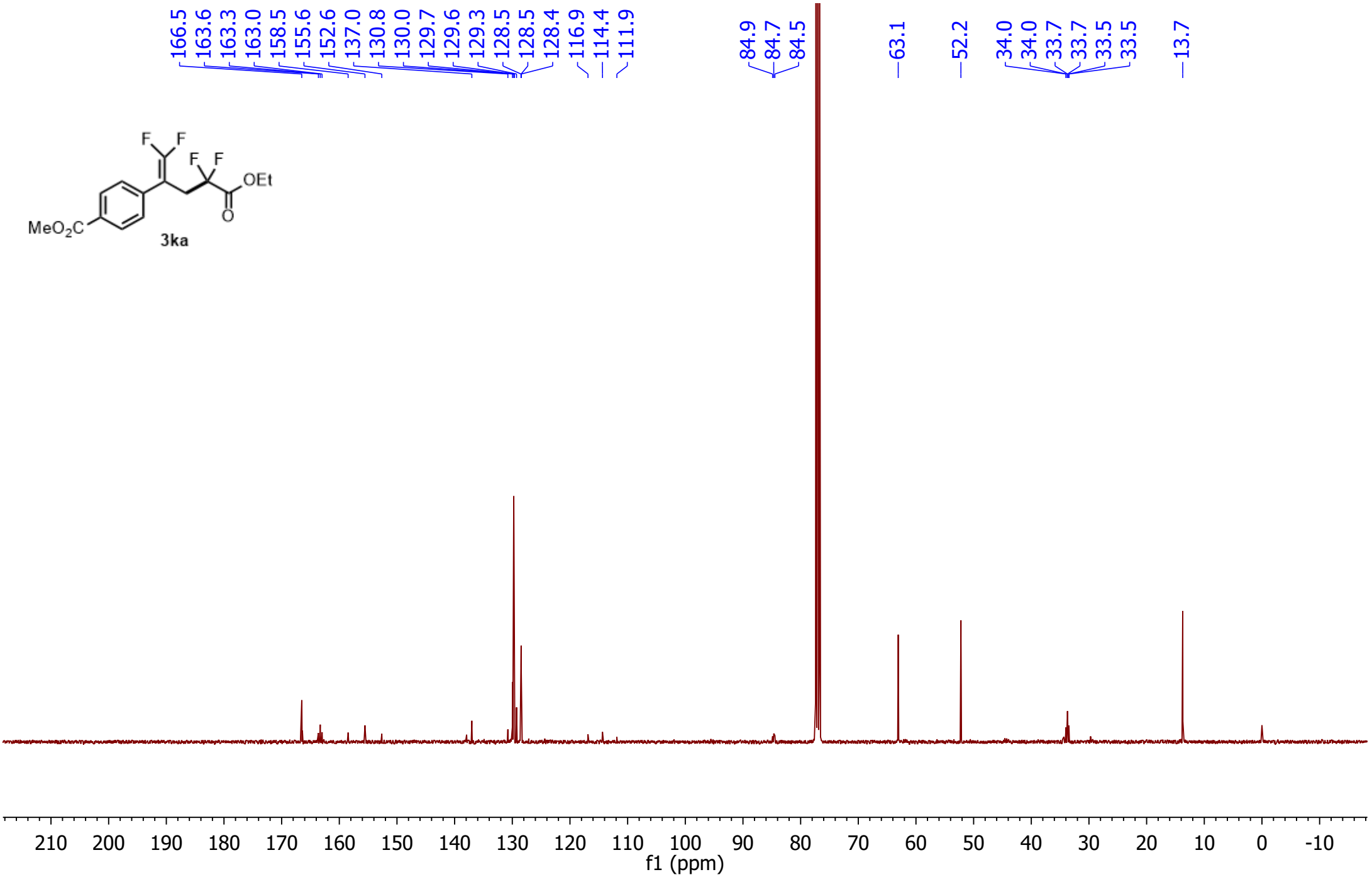
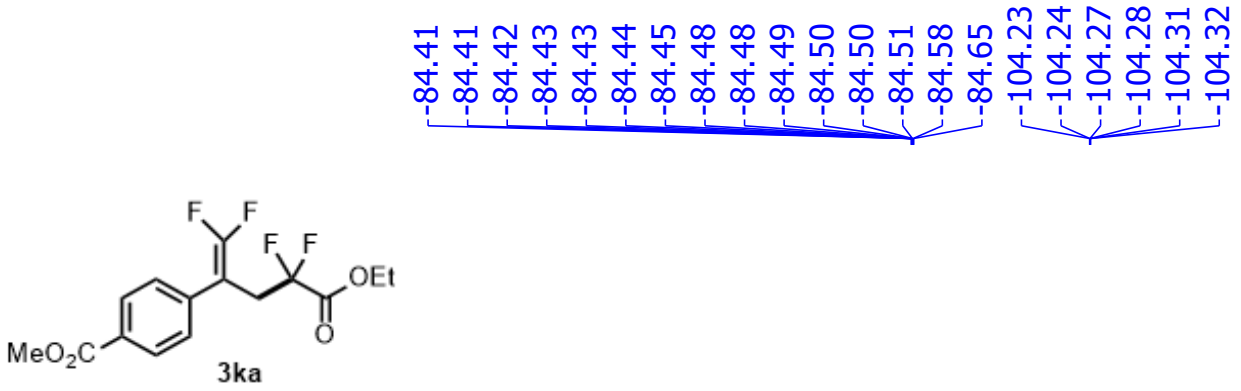


^{13}C NMR Spectrum of **3ka**

19F (CDCl3, 376 MHz)



^{19}F NMR Spectrum of **3ka**

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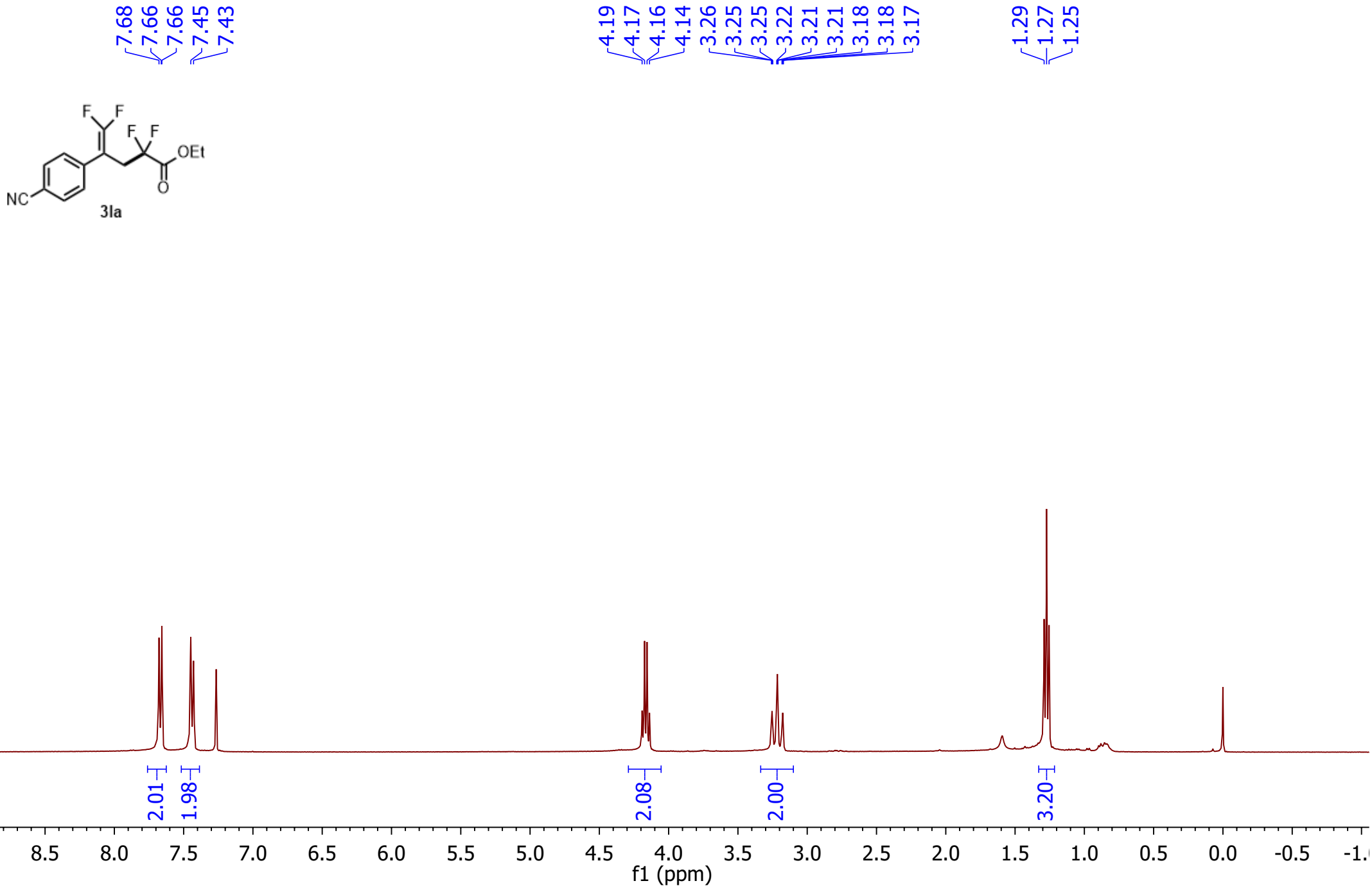

^{1}H NMR Spectrum of **3la**

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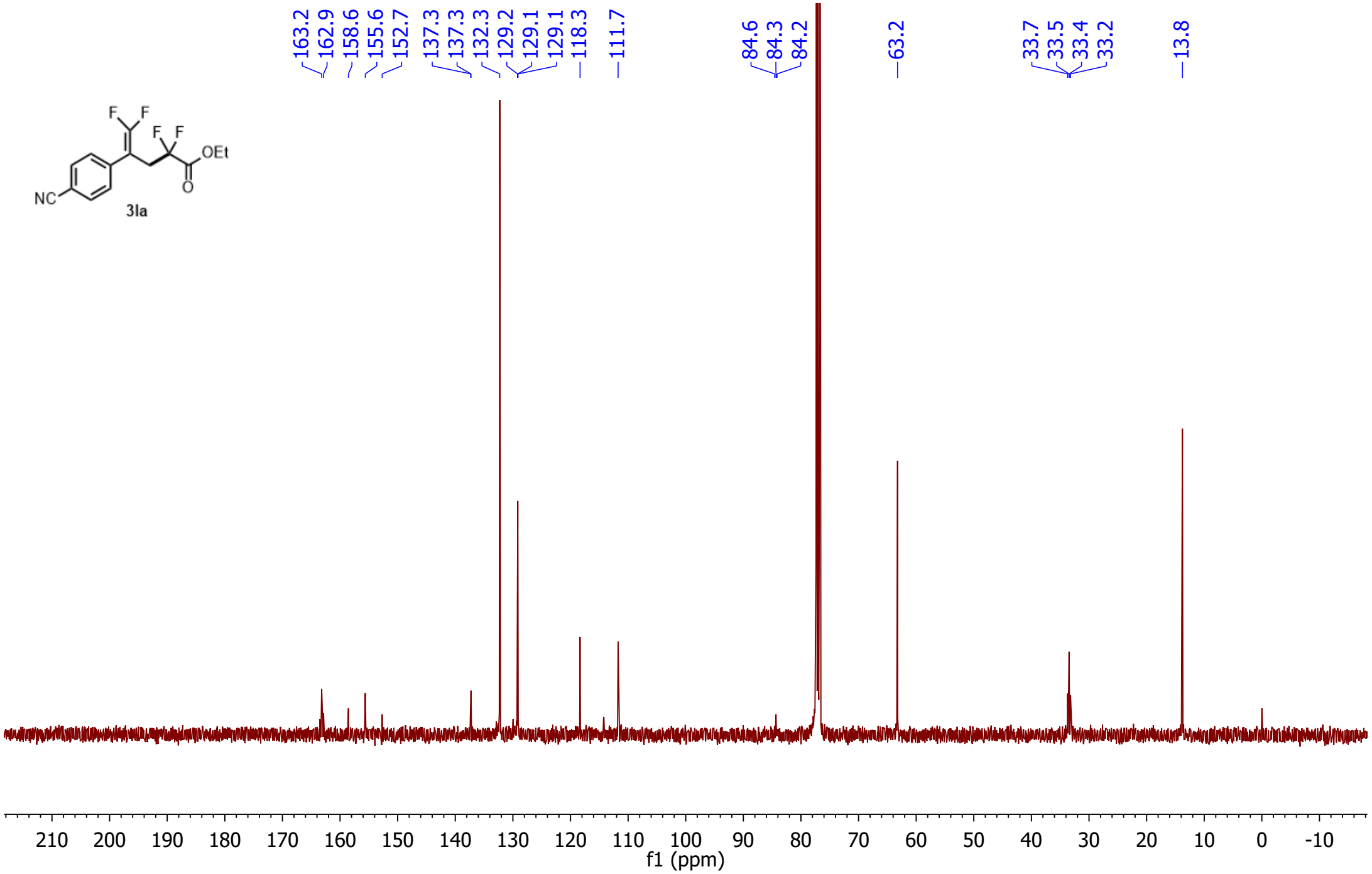

^{13}C NMR Spectrum of **3la**

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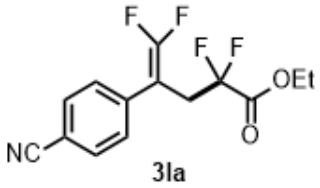

3la

^{19}F NMR Spectrum of **3la**

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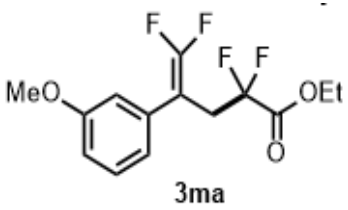

3ma

^{1}H NMR Spectrum of **3ma**

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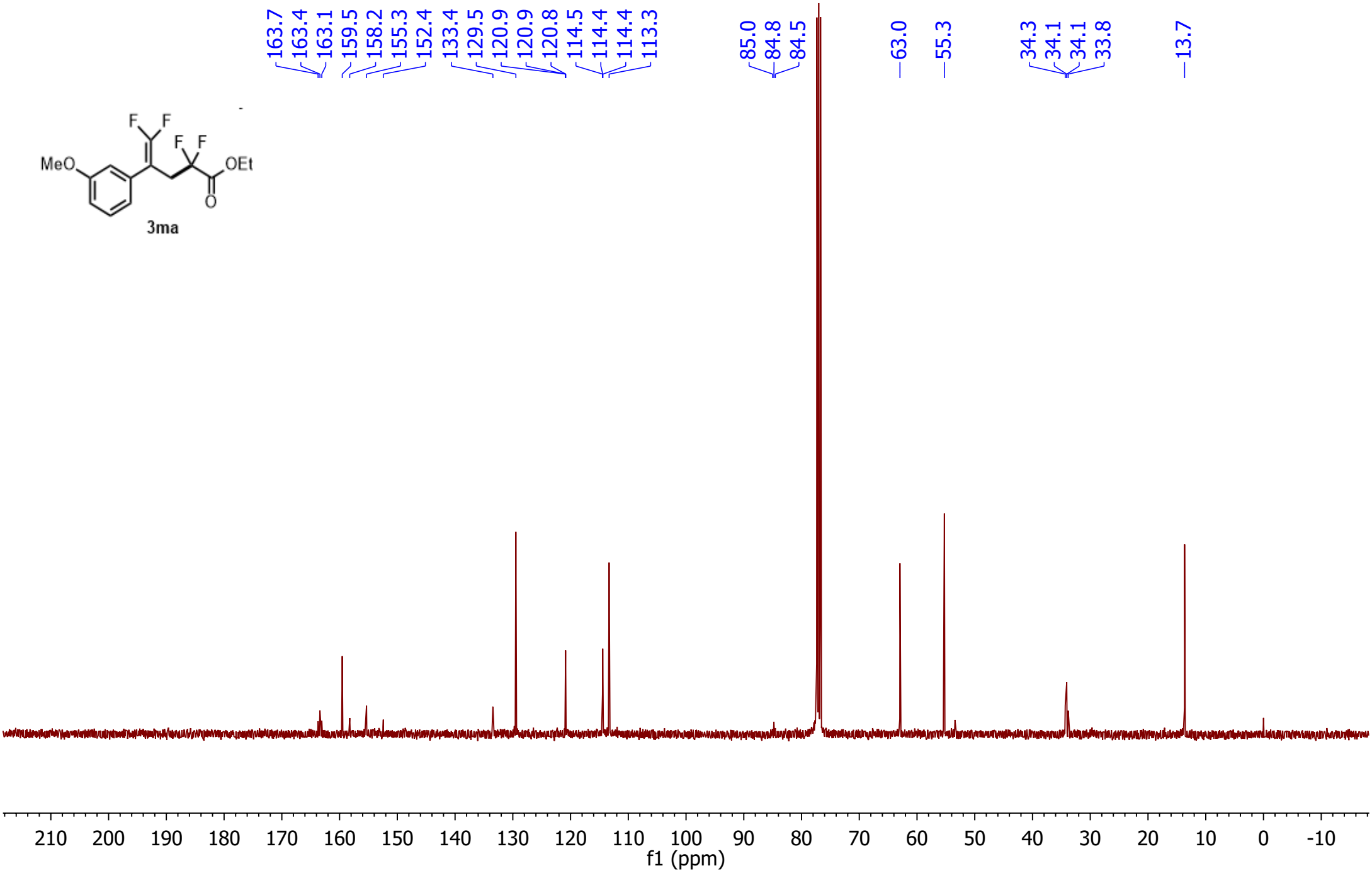
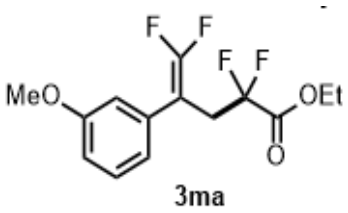


^{13}C NMR Spectrum of **3ma**

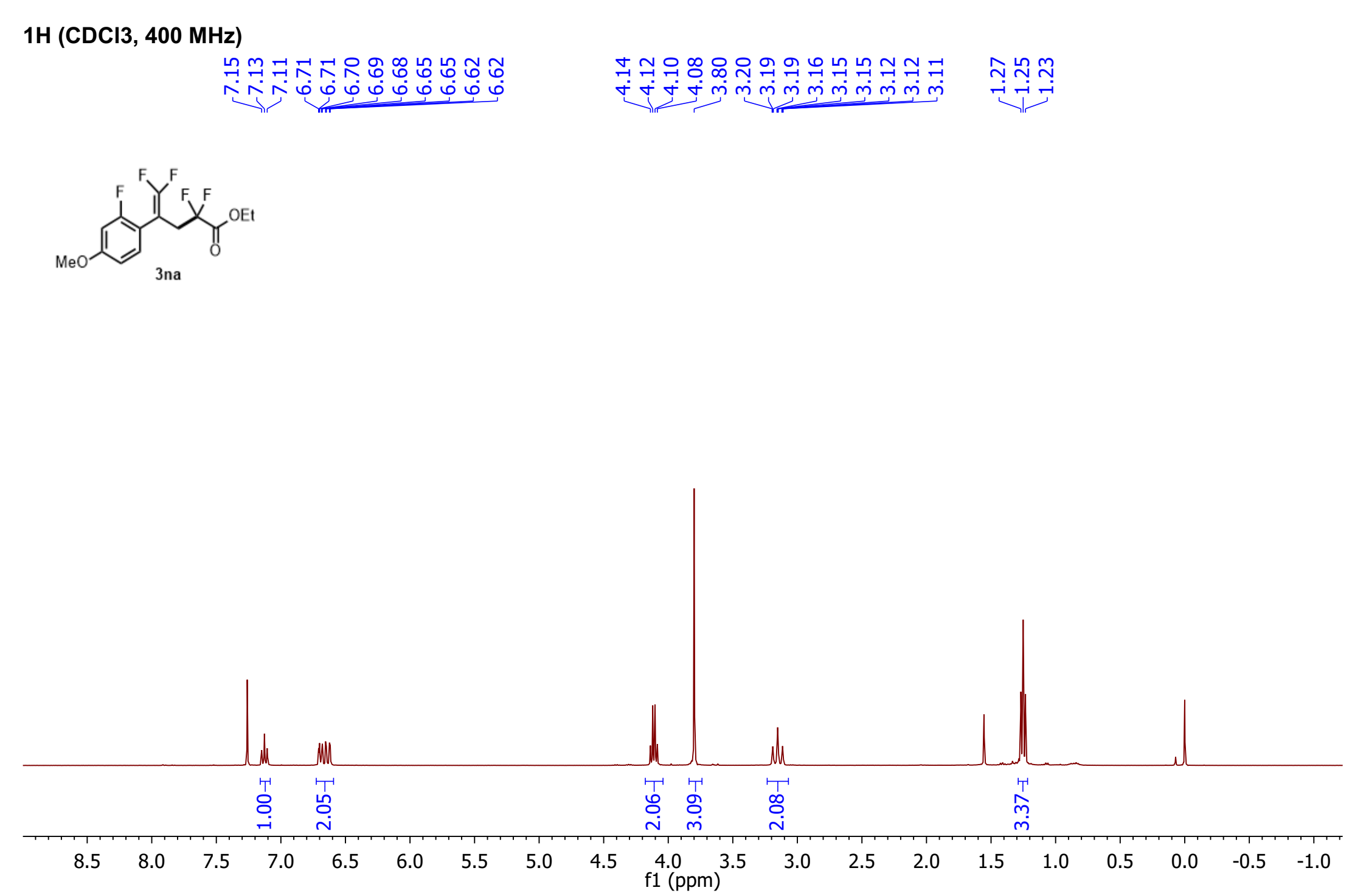
19F (CDCl3, 376 MHz)



3ma

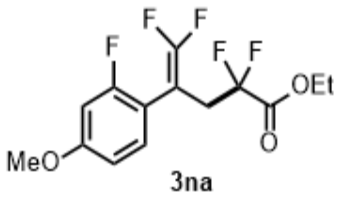
^{19}F NMR Spectrum of **3ma**

1H (CDCl3, 400 MHz)



^{1}H NMR Spectrum of **3na**

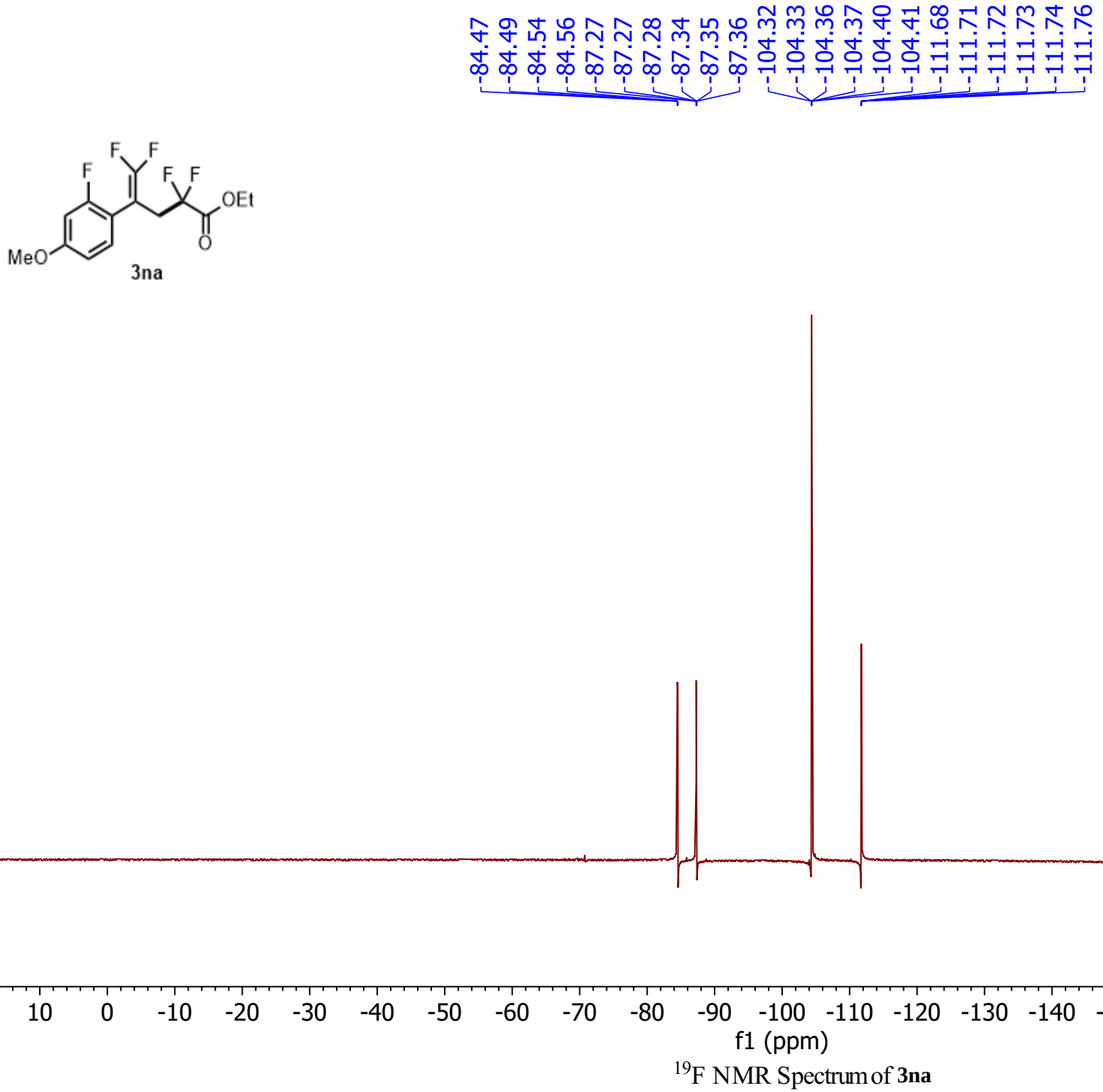
13C (CDCl3, 101 MHz)



3na

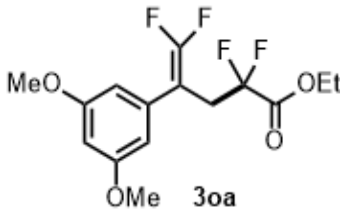
^{13}C NMR Spectrum of **3na**

19F (CDCl3, 376 MHz)



^{19}F NMR Spectrum of **3na**

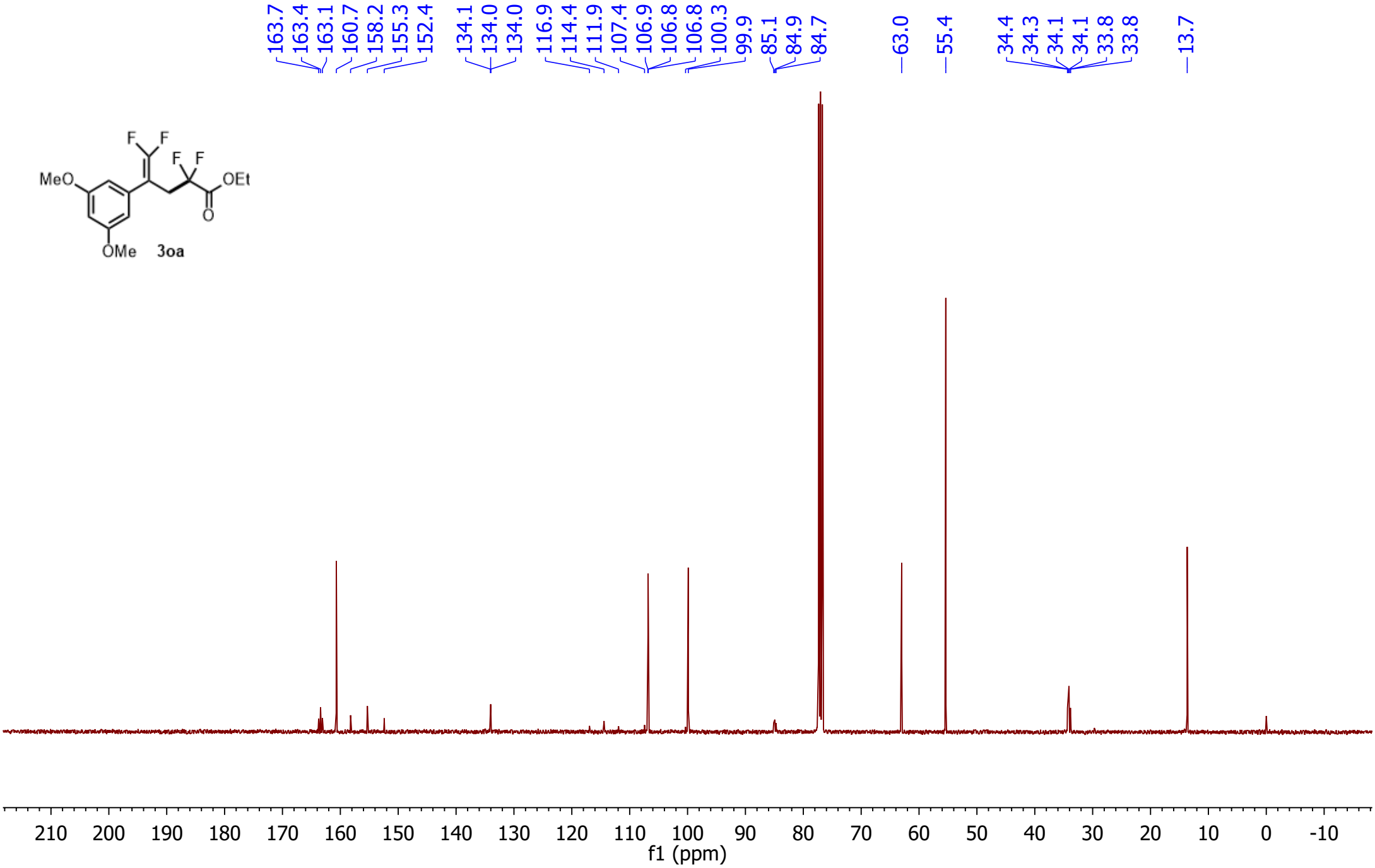
1H (CDCl3, 400 MHz)



3oa

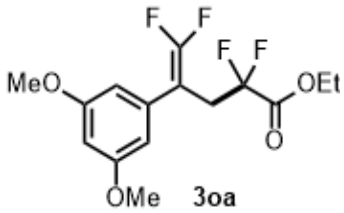
^{1}H NMR Spectrum of **3oa**

13C (CDCl3, 101 MHz)



^{13}C NMR Spectrum of **3oa**

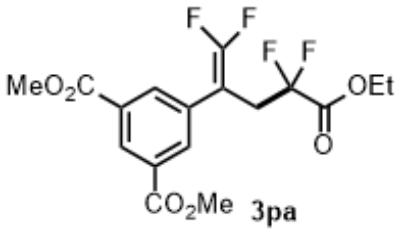
19F (CDCl3, 376 MHz)



3oa

^{19}F NMR Spectrum of **3oa**

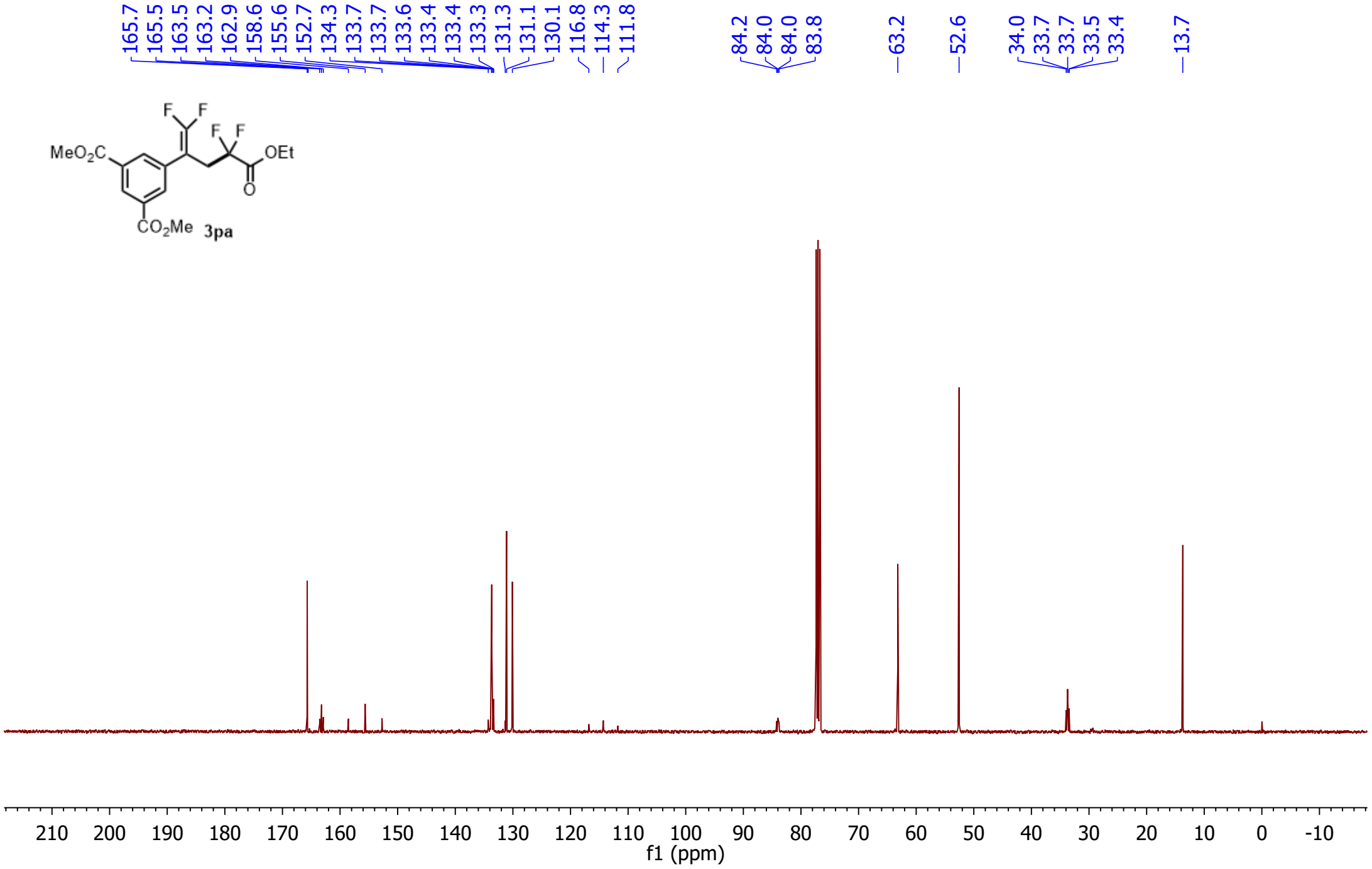
1H (CDCl3, 400 MHz)



3pa

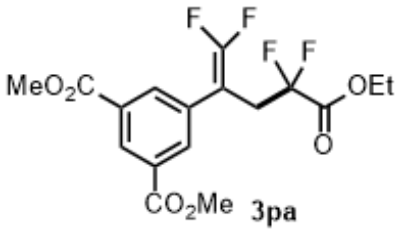
[1]H NMR Spectrum of **3pa**

13C (CDCl3, 101 MHz)



^{13}C NMR Spectrum of **3pa**

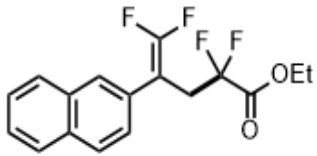
19F (CDCl3, 376 MHz)



3pa

^{19}F NMR Spectrum of **3pa**

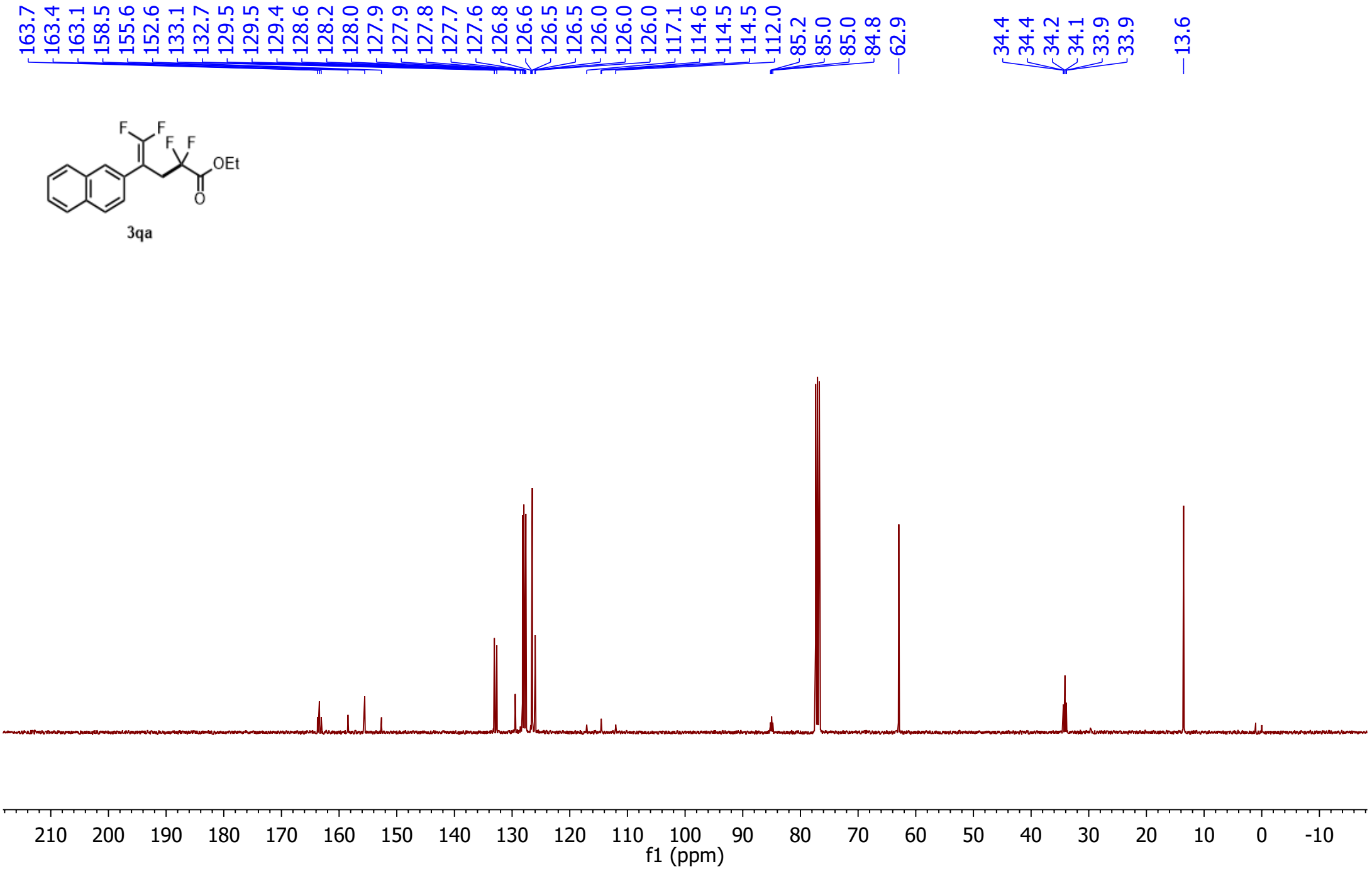
1H (CDCl3, 400 MHz)



3qa

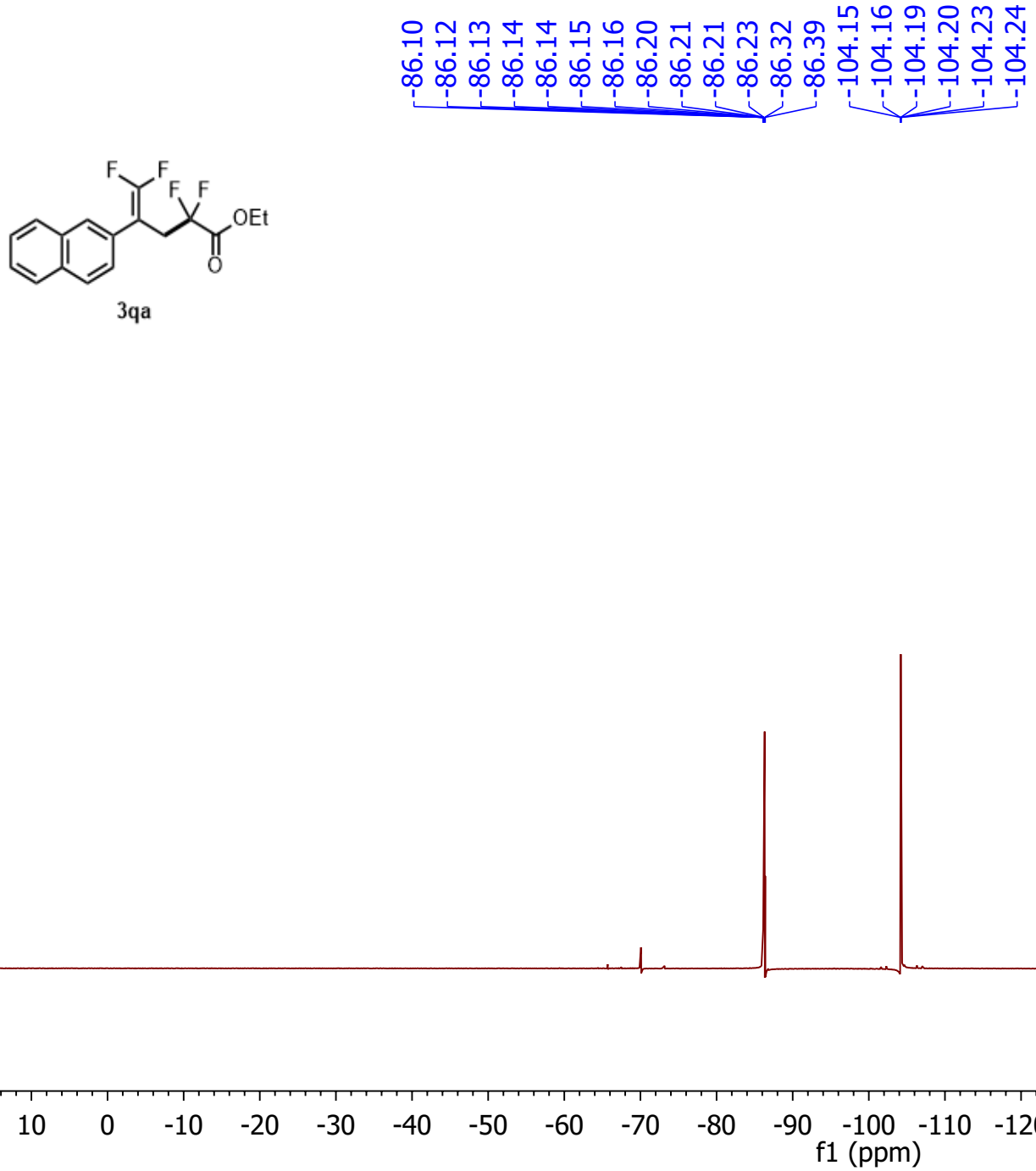
^{1}H NMR Spectrum of **3qa**

13C (CDCl3, 101 MHz)



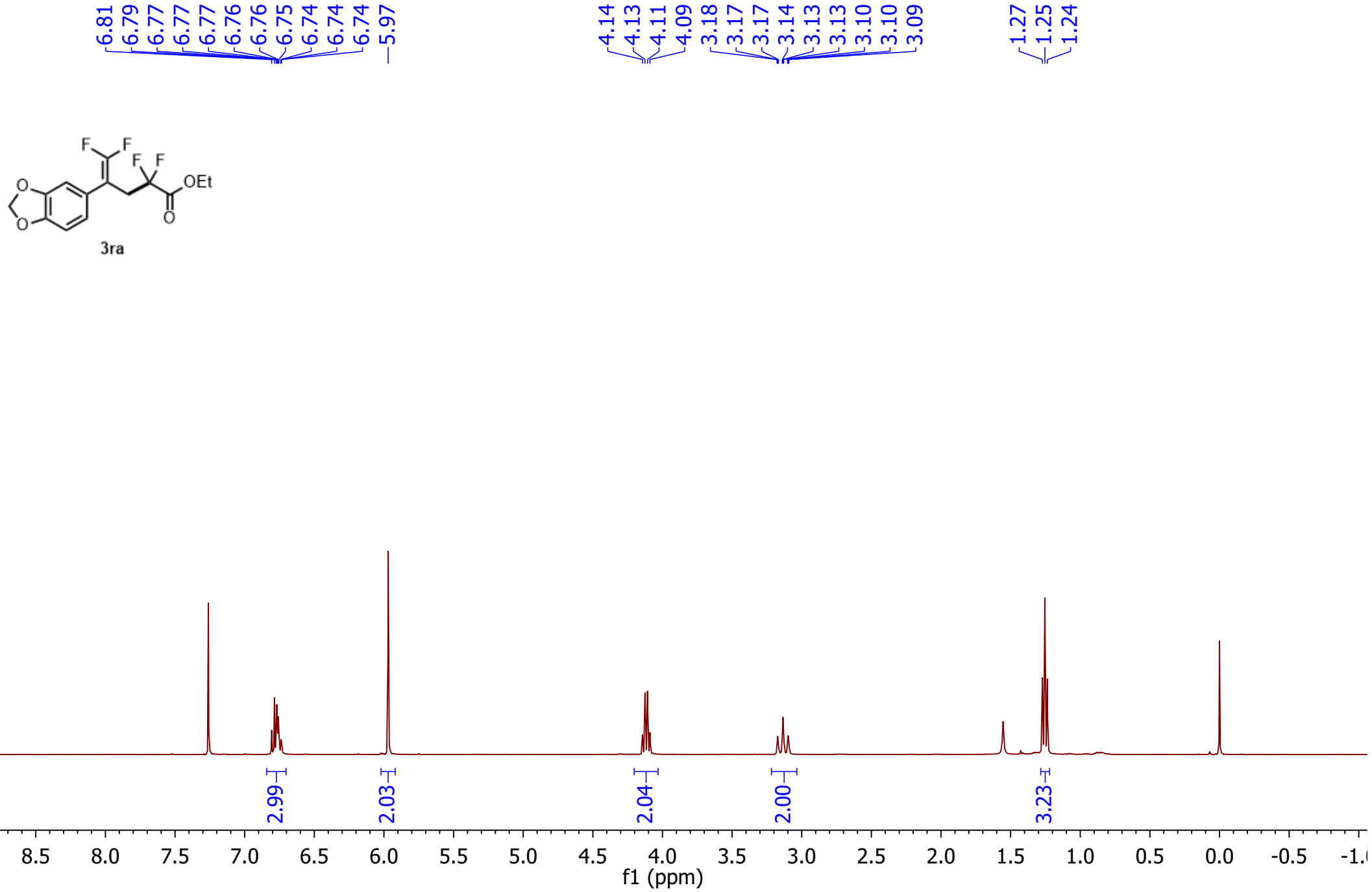
^{13}C NMR Spectrum of **3qa**

19F (CDCl3, 376 MHz)



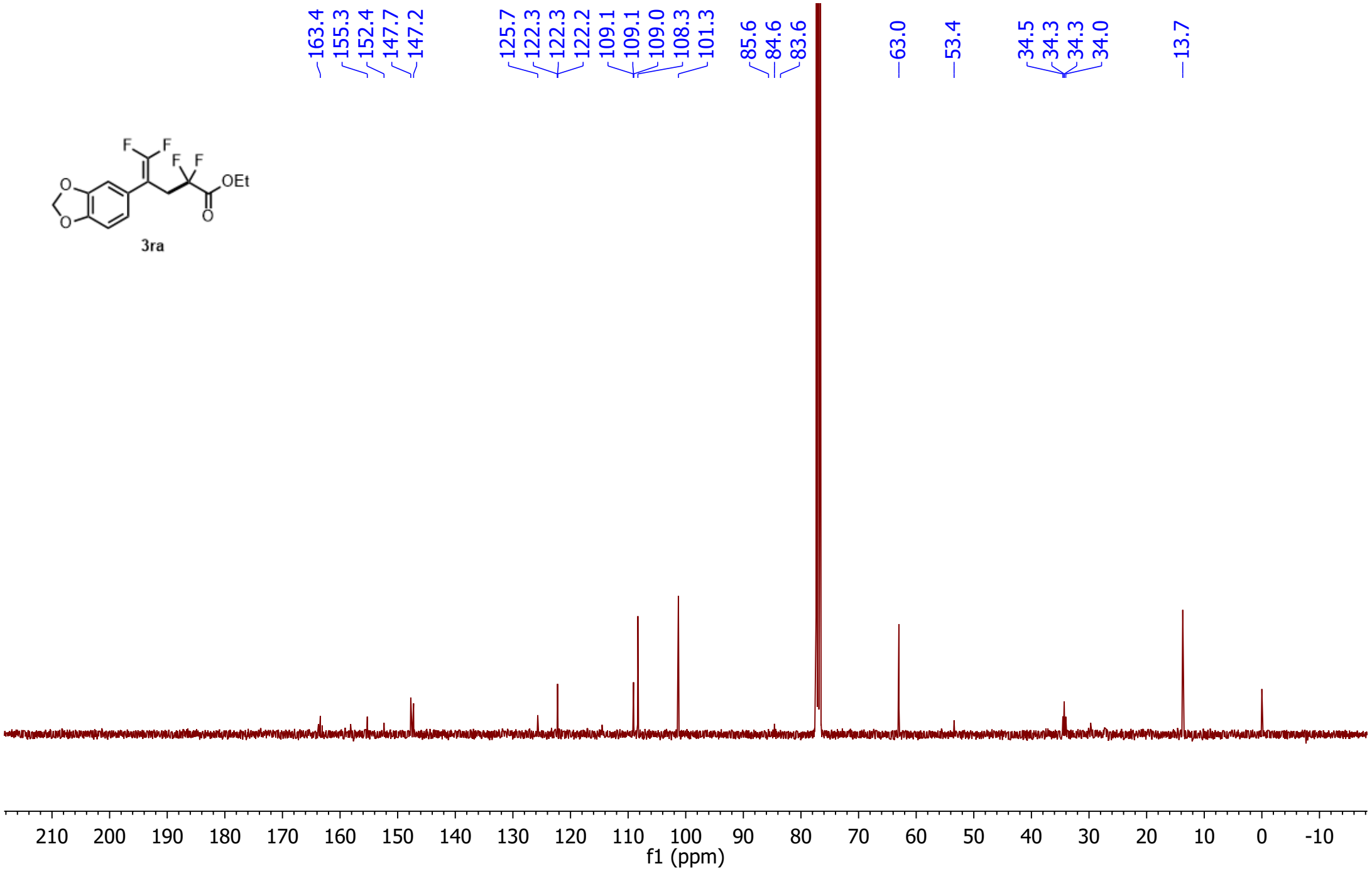
^{19}F NMR Spectrum of **3qa**

1H (CDCl3, 400 MHz)



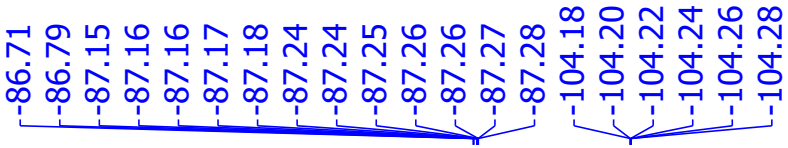
^{1}H NMR Spectrum of **3ra**

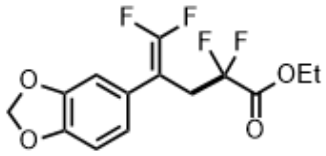
13C (CDCl3, 101 MHz)



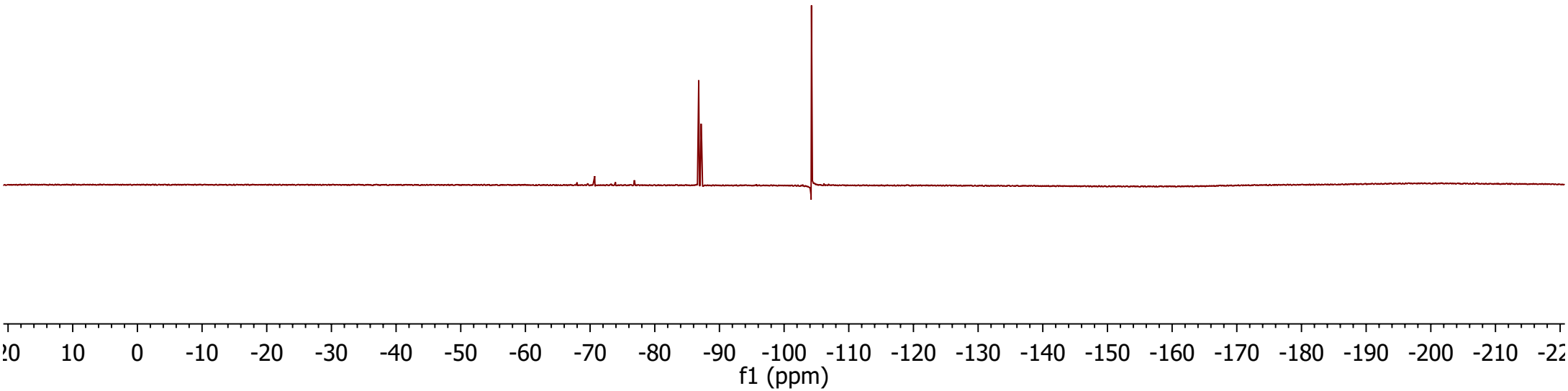
^{13}C NMR Spectrum of **3ra**

19F (CDCl3, 376 MHz)



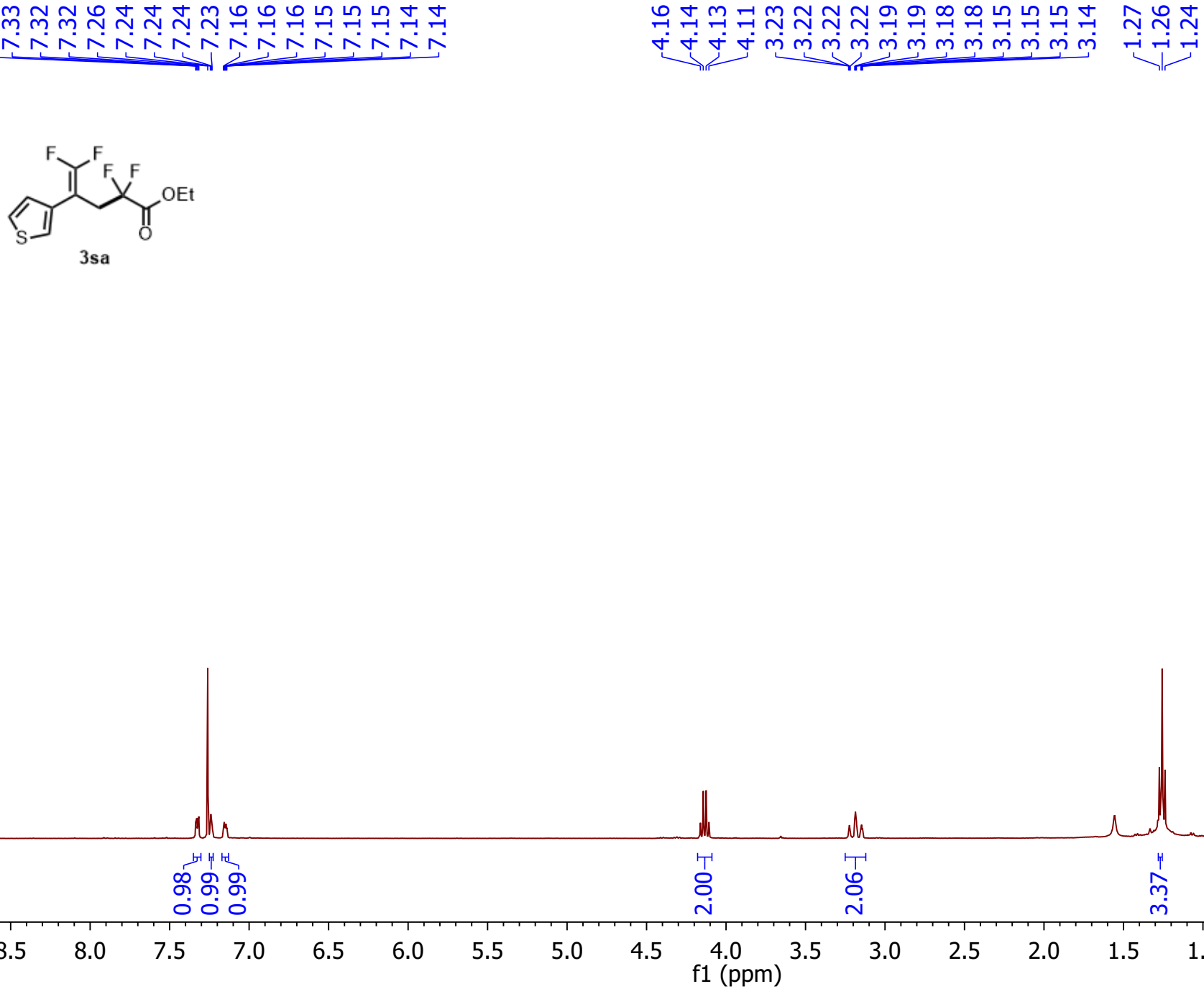


3ra



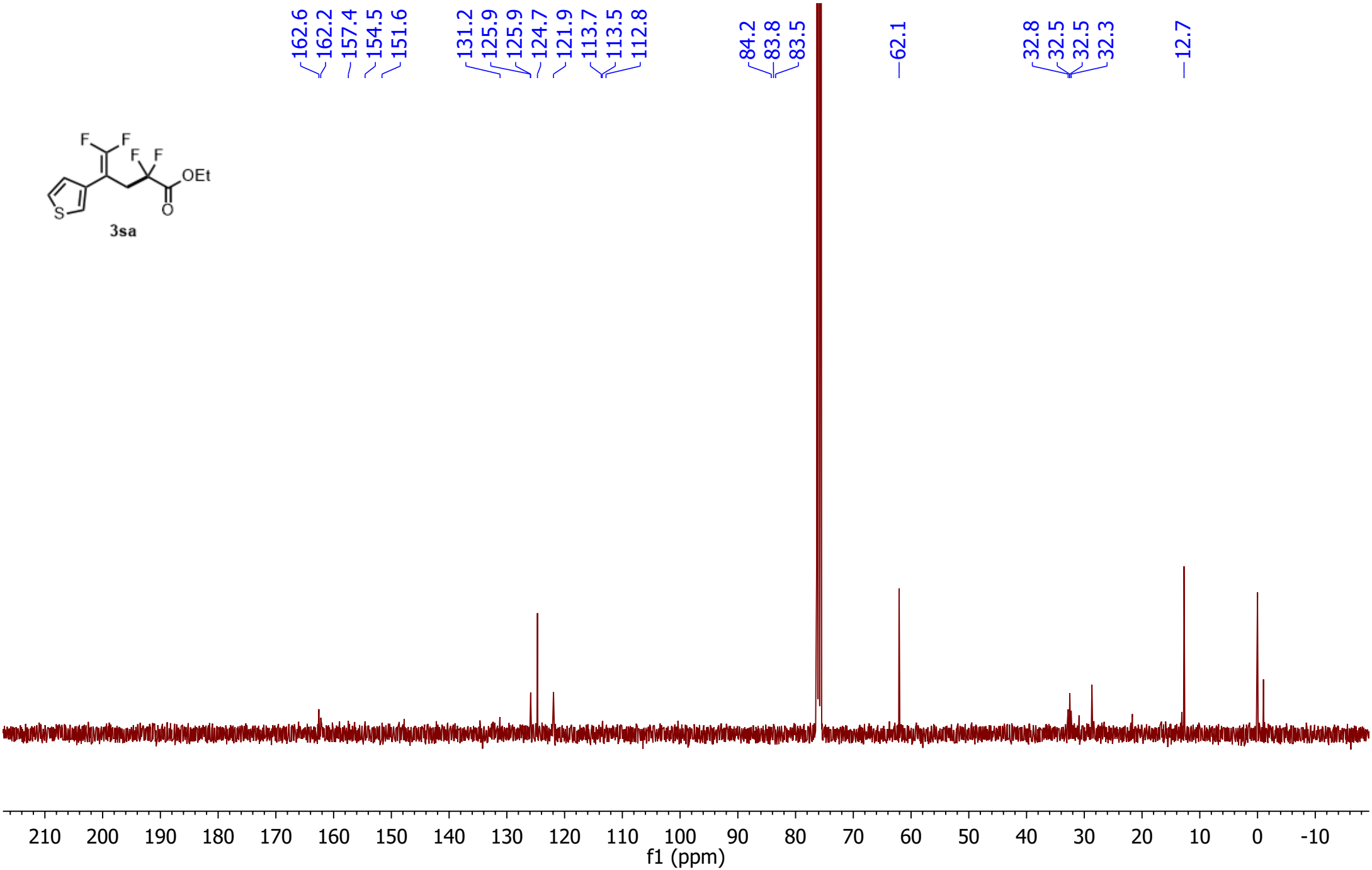
^{19}F NMR Spectrum of **3ra**

1H (CDCl3, 400 MHz)



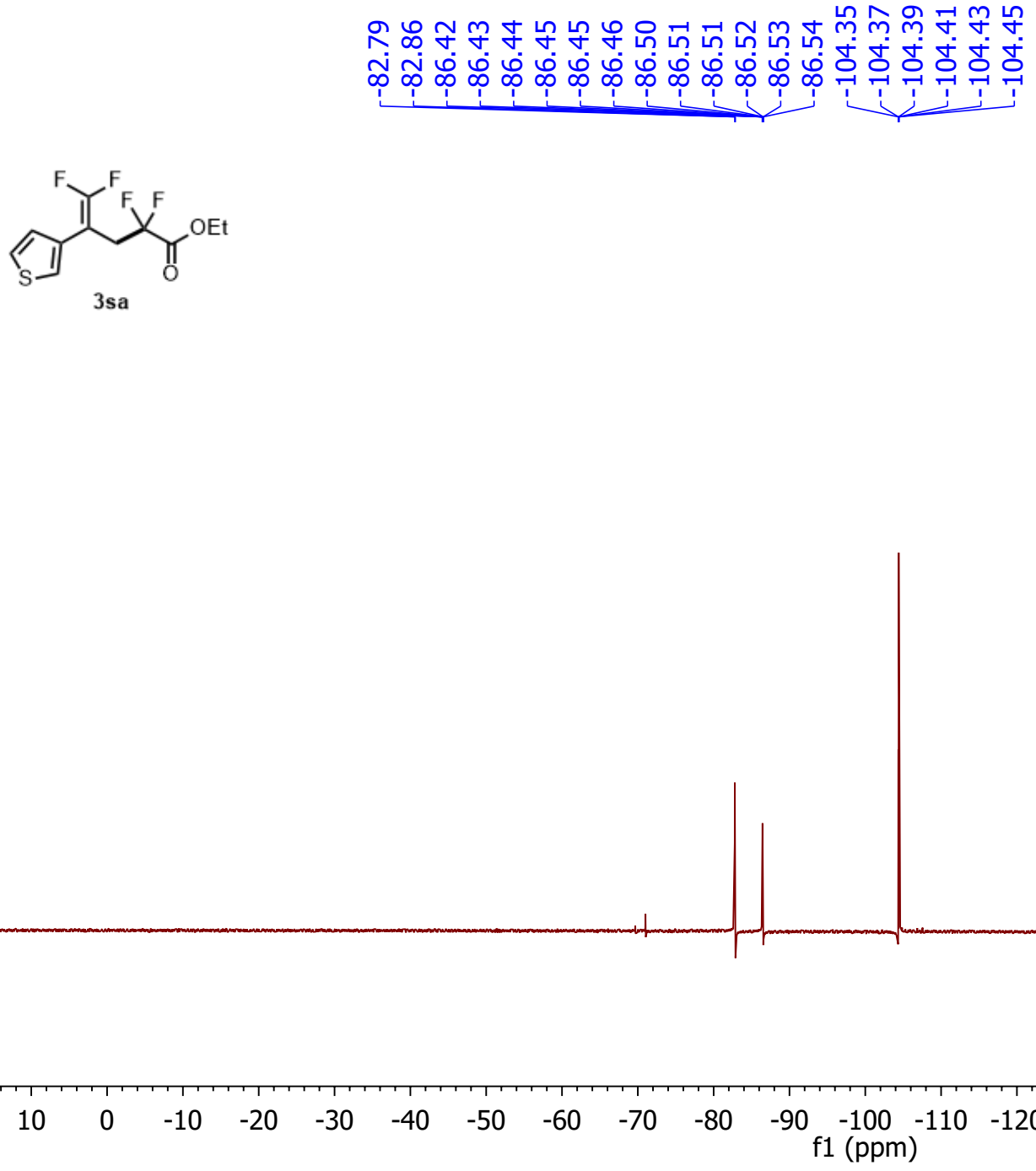
^{1}H NMR Spectrum of **3sa**

13C (CDCl3, 101 MHz)



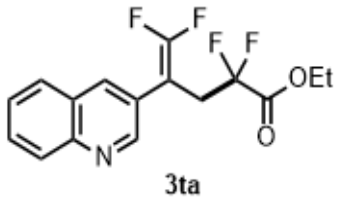
^{13}C NMR Spectrum of **3sa**

19F (CDCl3, 376 MHz)

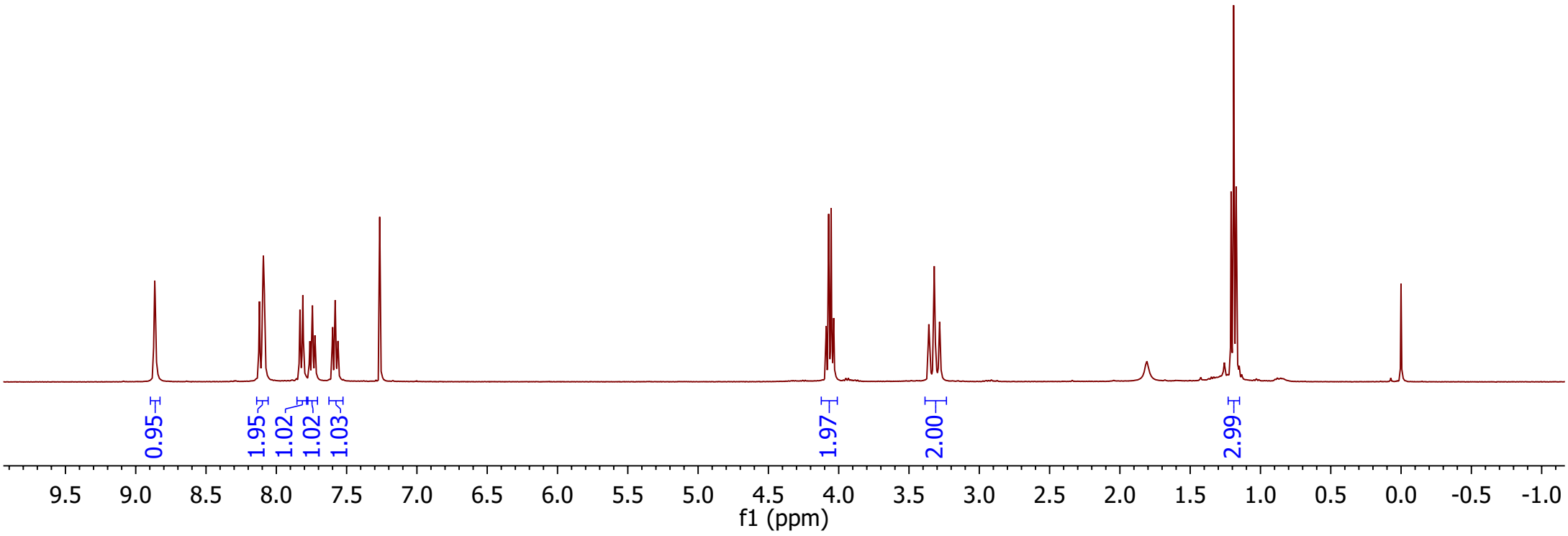


^{19}F NMR Spectrum of **3sa**

1H (CDCl3, 400 MHz)

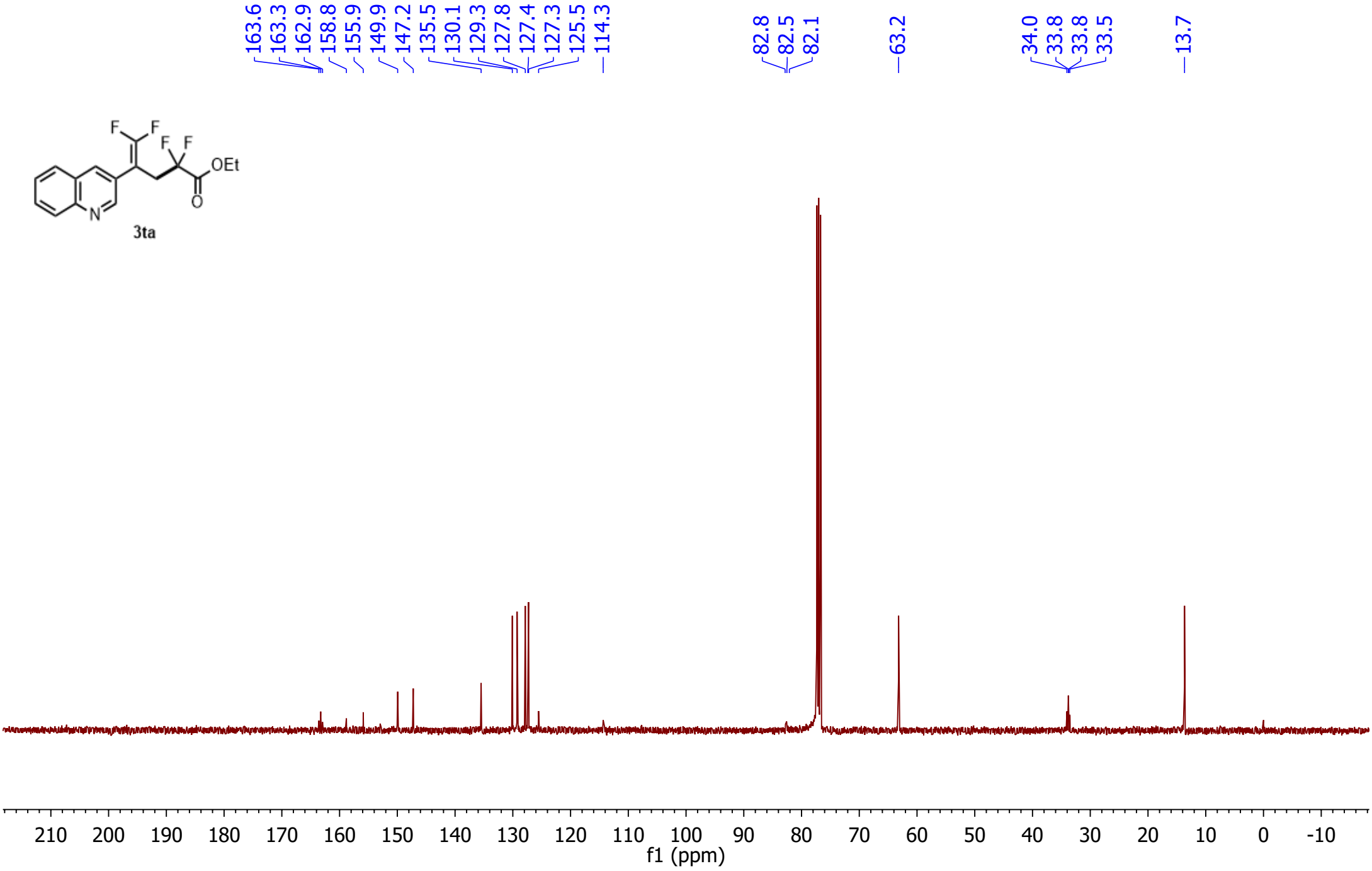


3ta



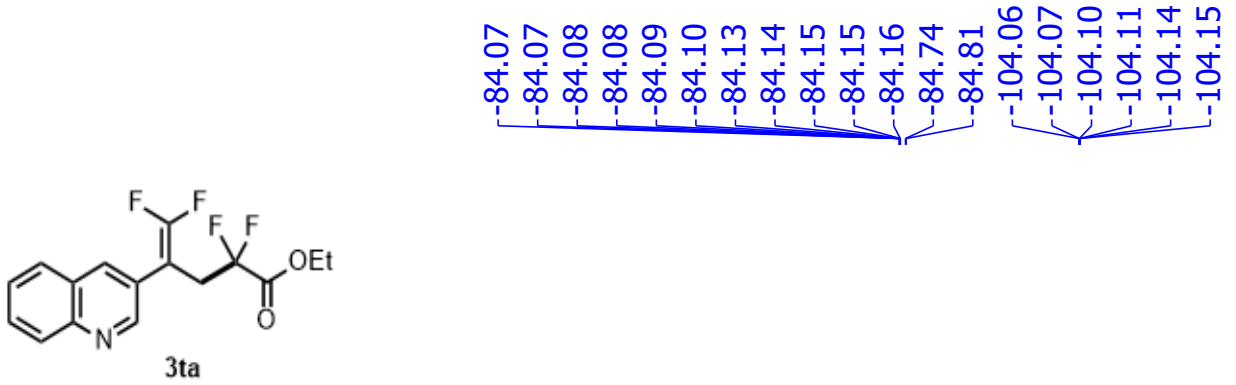
^{1}H NMR Spectrum of **3ta**

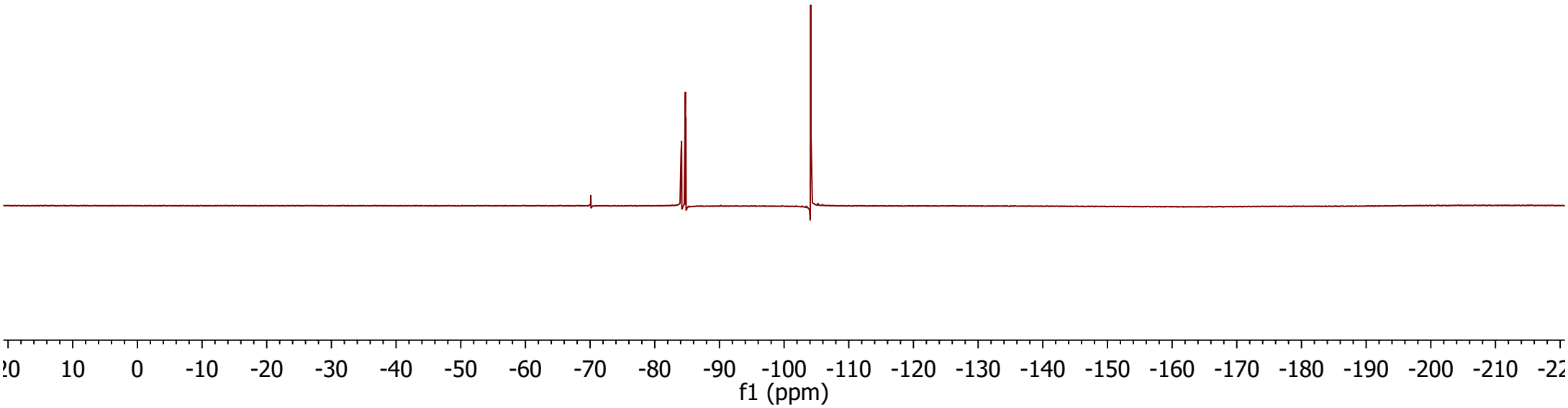
13C (CDCl3, 101 MHz)



^{13}C NMR Spectrum of **3ta**

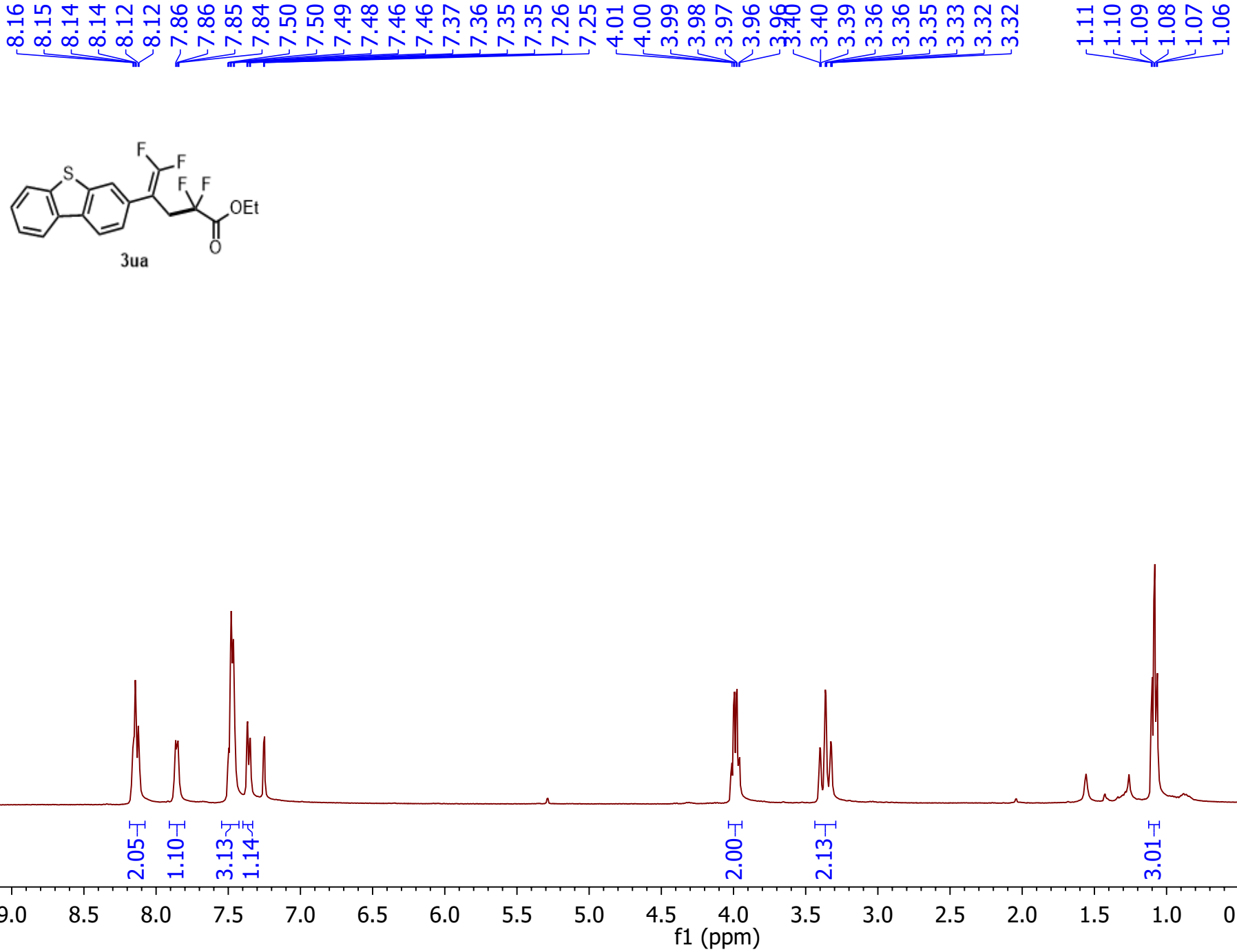
19F (CDCl3, 376 MHz)





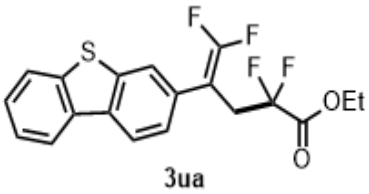
^{19}F NMR Spectrum of **3ta**

1H (CDCl3, 400 MHz)



^{1}H NMR Spectrum of **3ua**

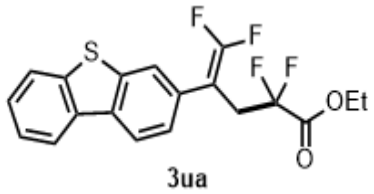
13C (CDCl3, 101 MHz)



3ua

^{13}C NMR Spectrum of **3ua**

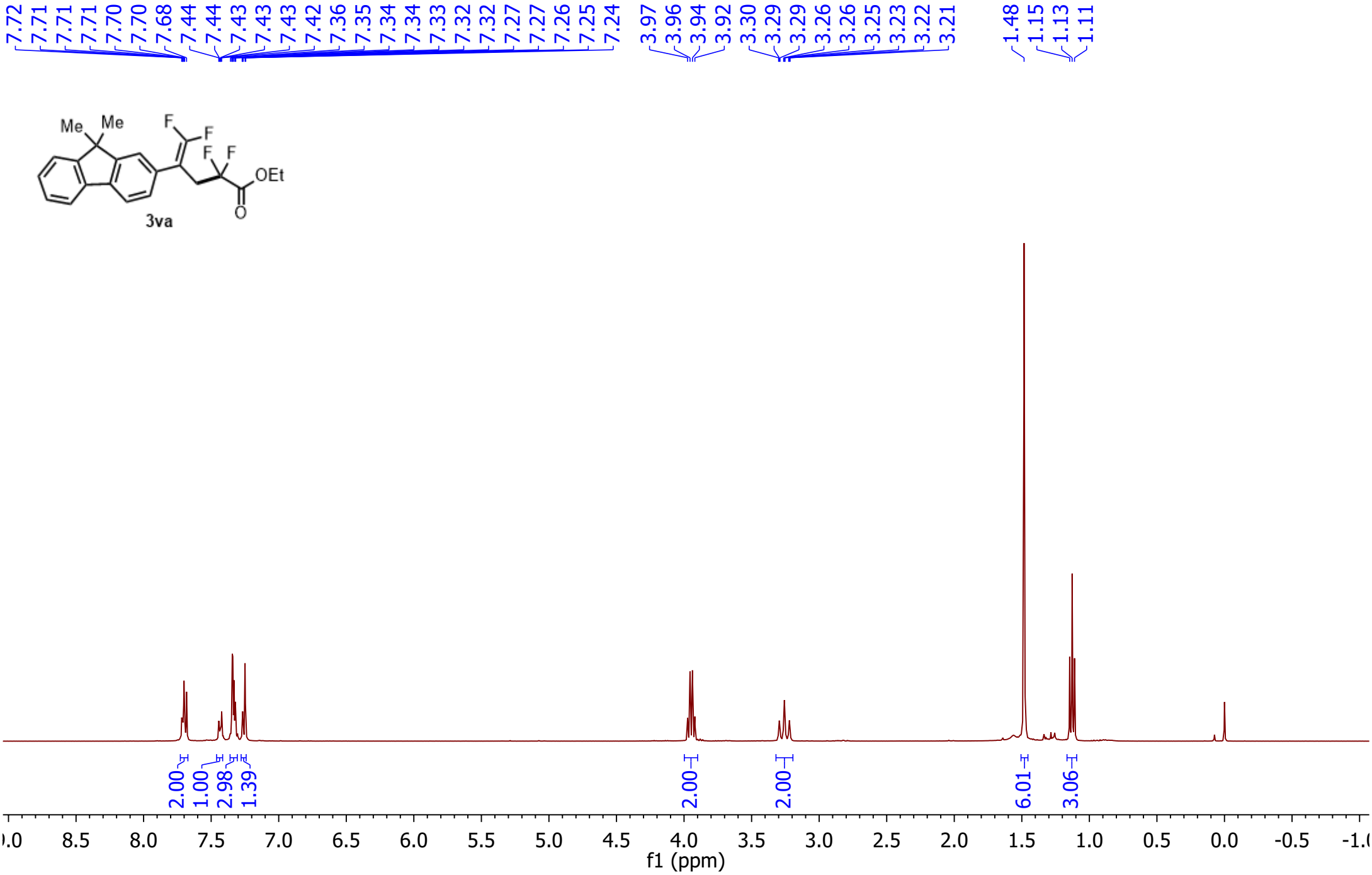
19F (CDCl3, 376 MHz)



3ua

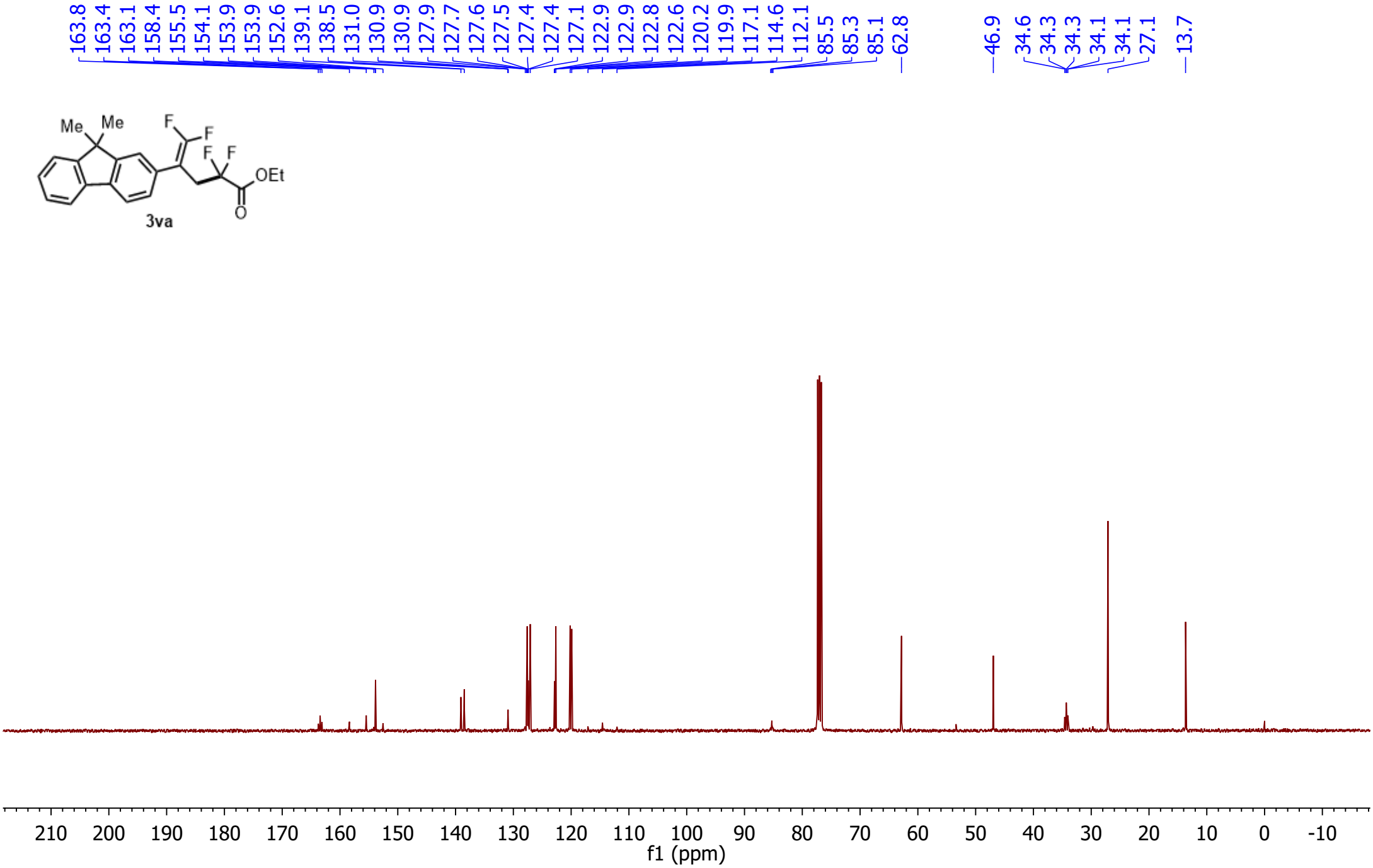
^{19}F NMR Spectrum of **3ua**

1H (CDCl3, 400 MHz)



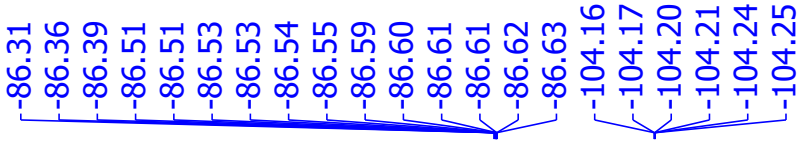
^{1}H NMR Spectrum of **3va**

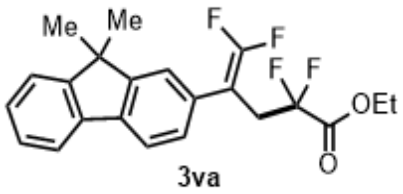
13C (CDCl3, 101 MHz)



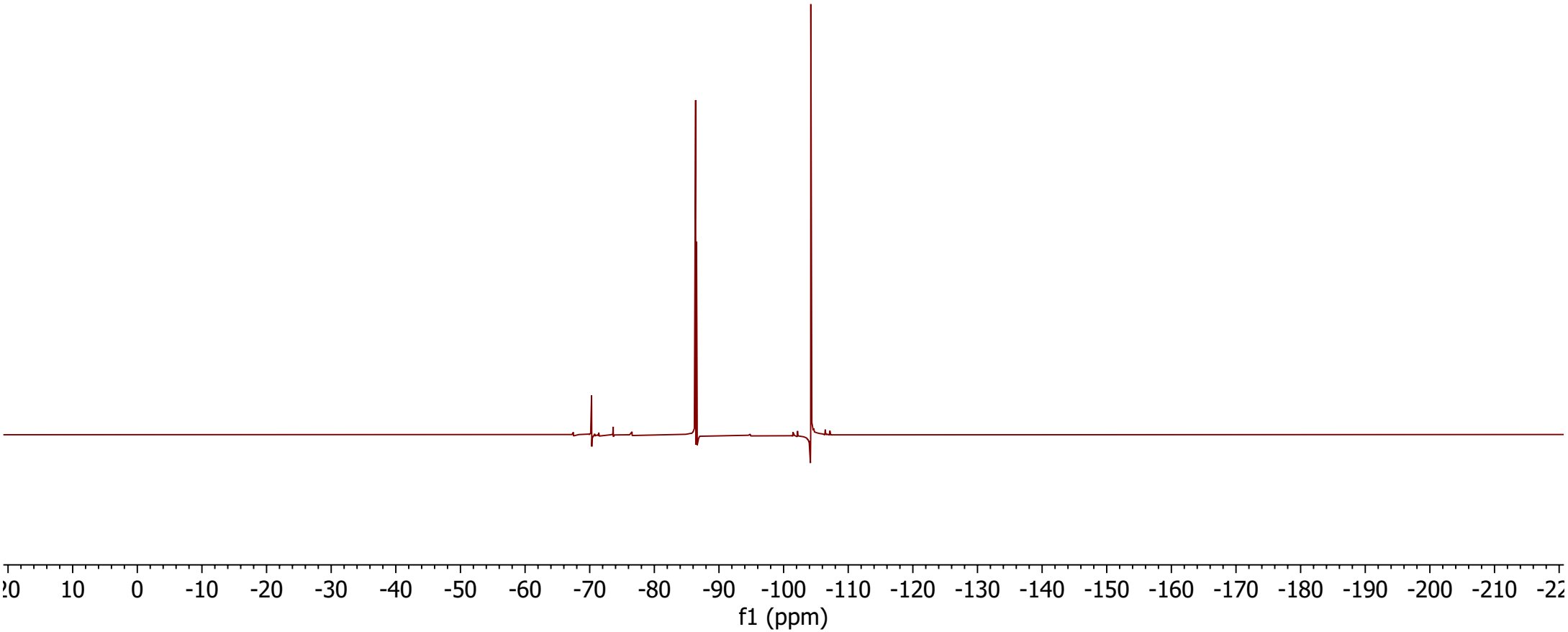
^{13}C NMR Spectrum of **3va**

19F (CDCl3, 376 MHz)



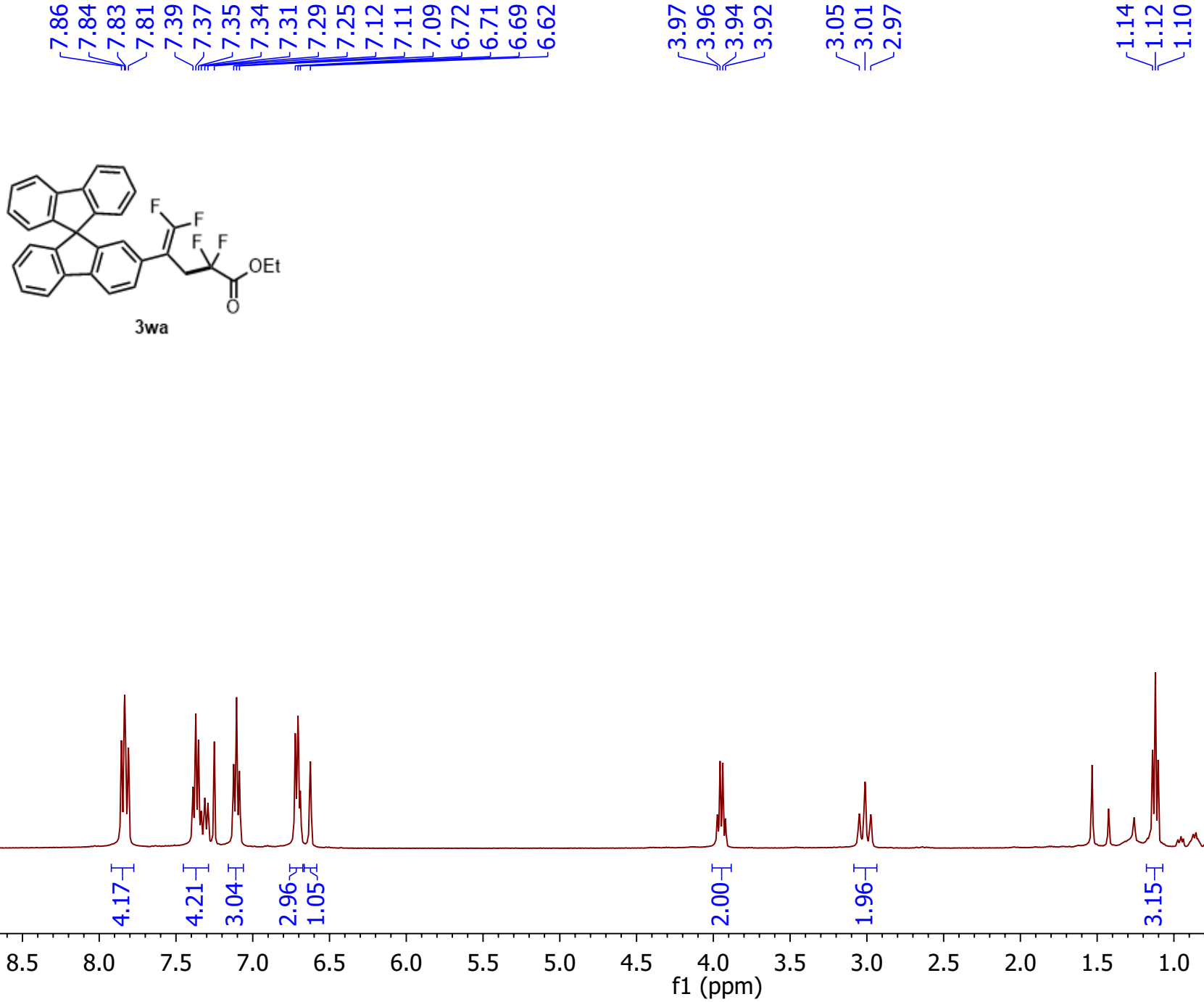


3va



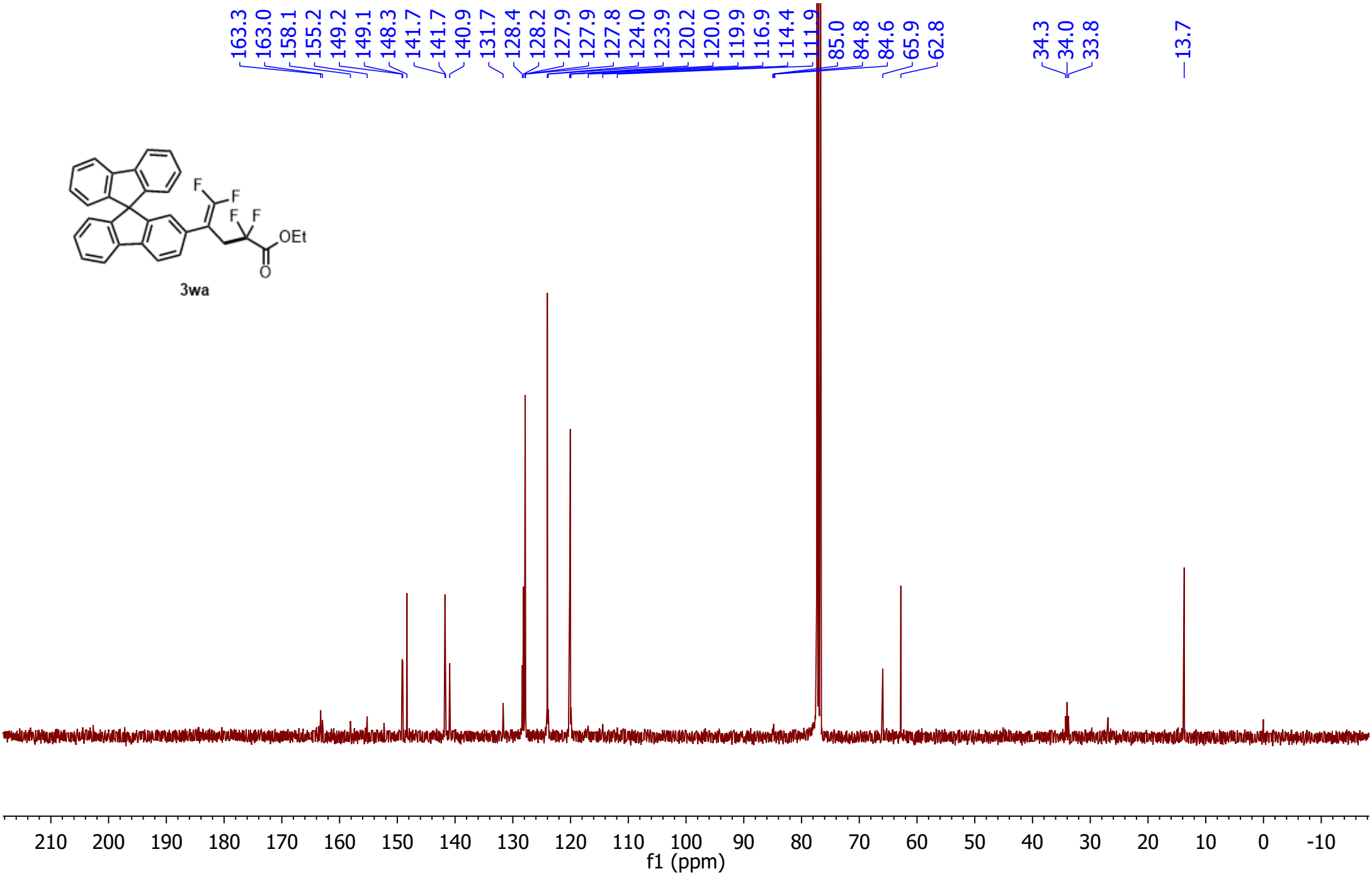
^{19}F NMR Spectrum of **3va**

1H (CDCl3, 400 MHz)



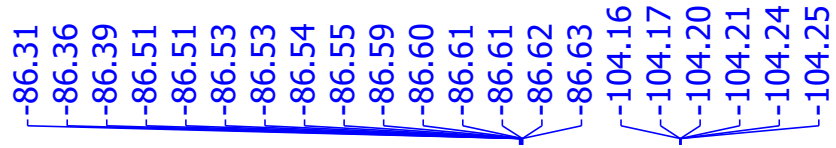
^{1}H NMR Spectrum of **3wa**

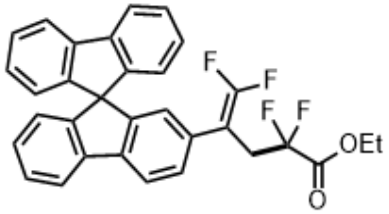
13C (CDCl3, 101 MHz)



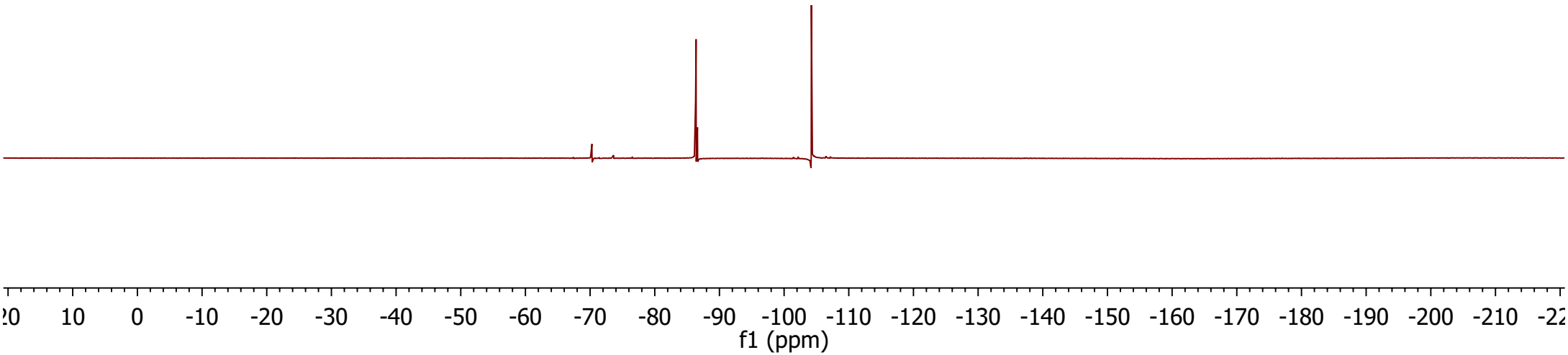
^{13}C NMR Spectrum of **3wa**

19F (CDCl3, 376 MHz)



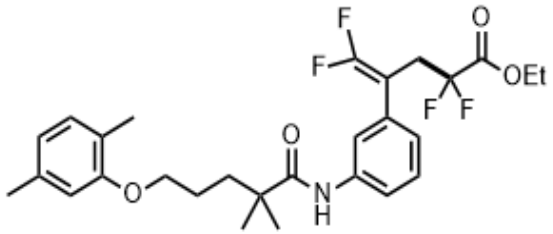


3wa



^{19}F NMR Spectrum of **3wa**

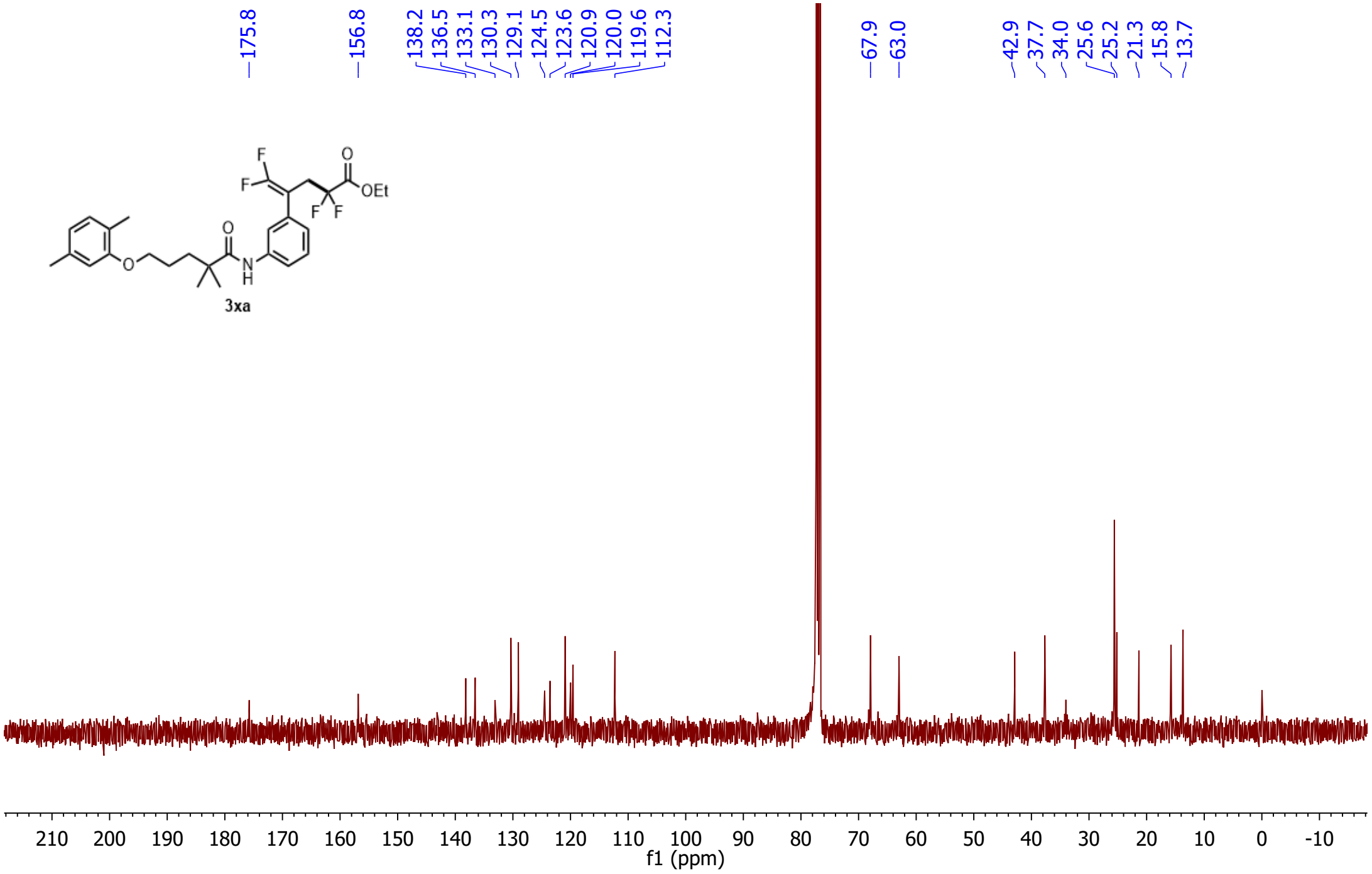
1H (CDCl3, 400 MHz)



3xa

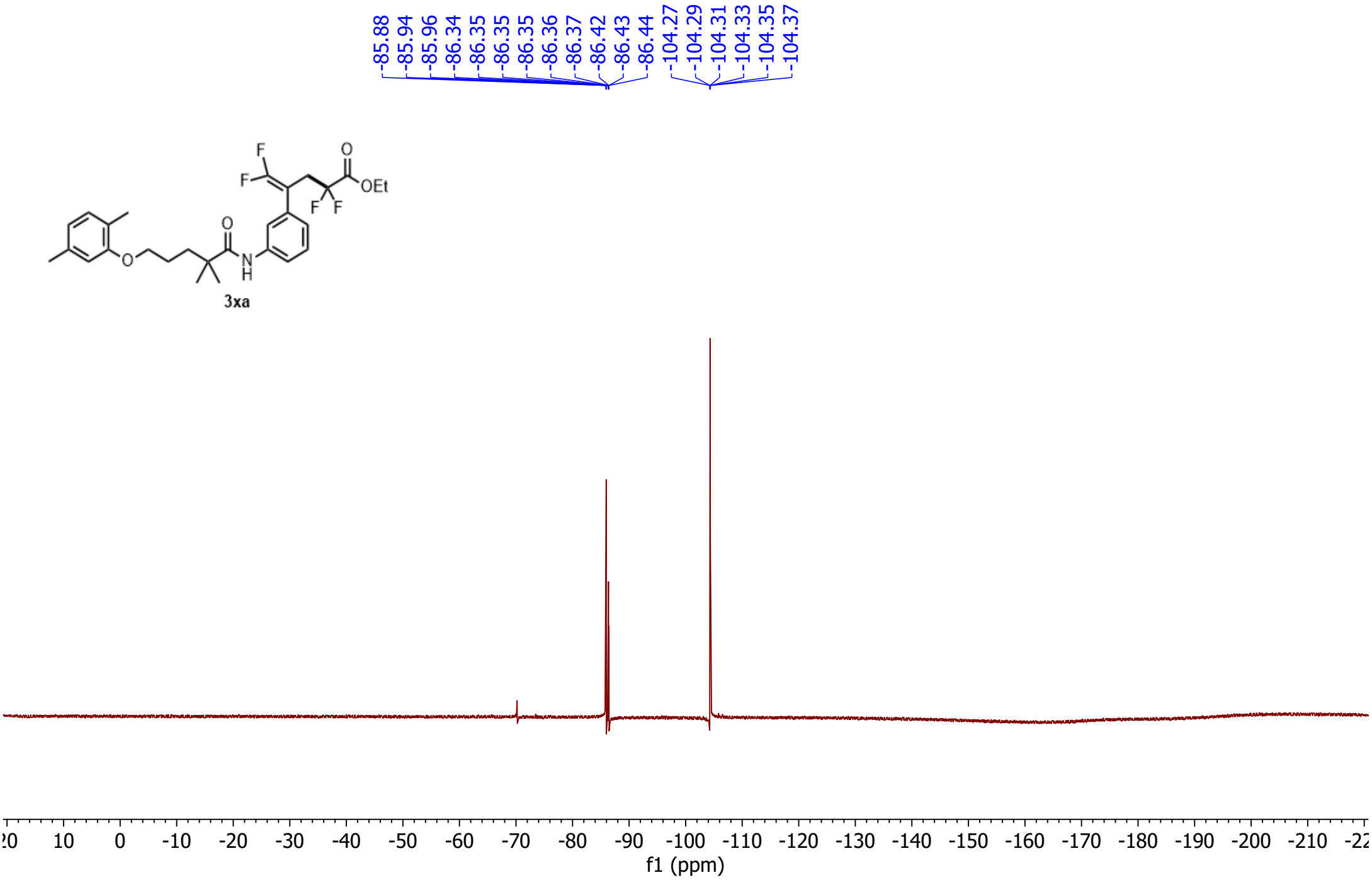
^{1}H NMR Spectrum of **3xa**

13C (CDCl3, 101 MHz)



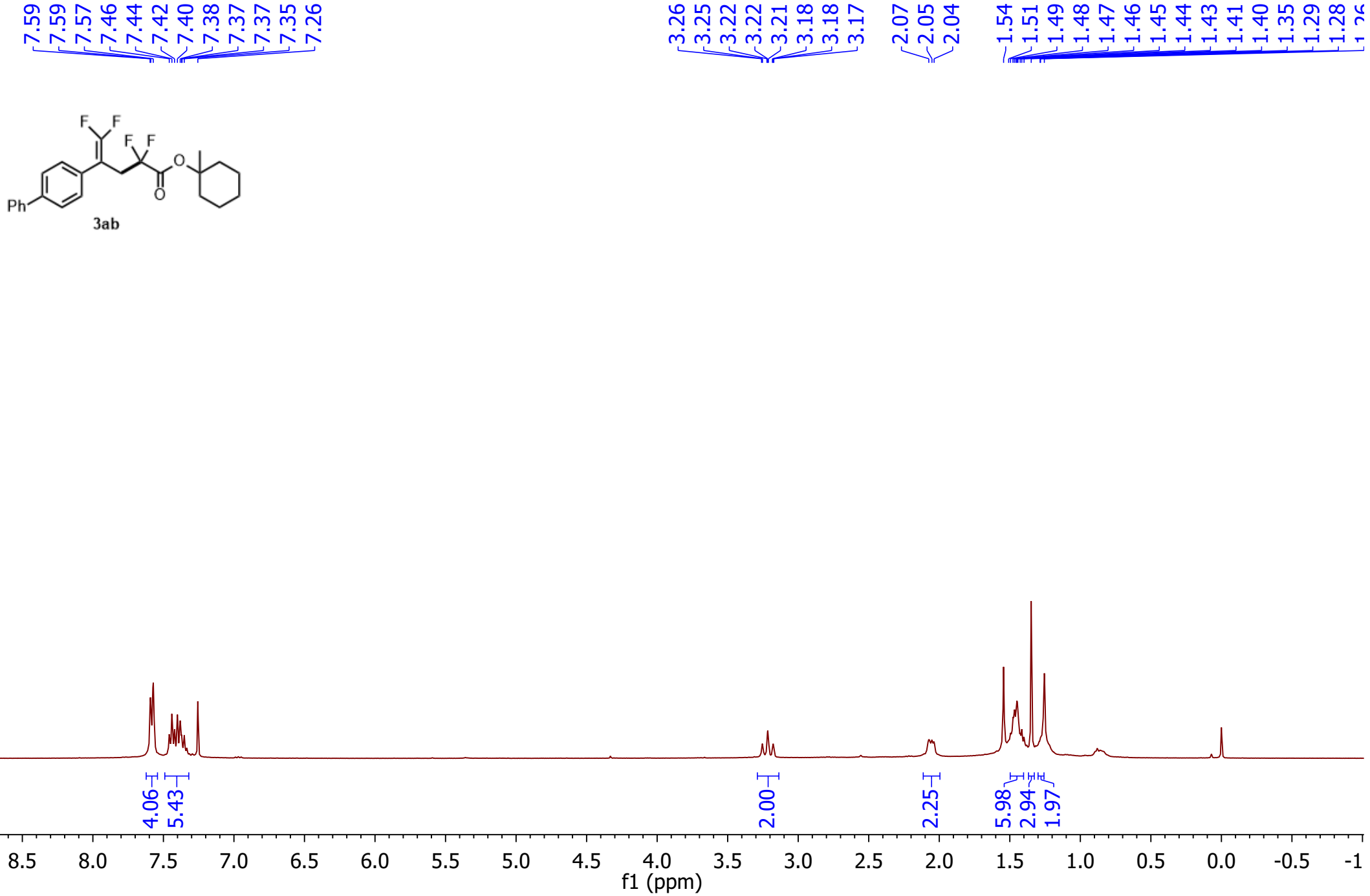
^{13}C NMR Spectrum of **3xa**

19F (CDCl3, 376 MHz)



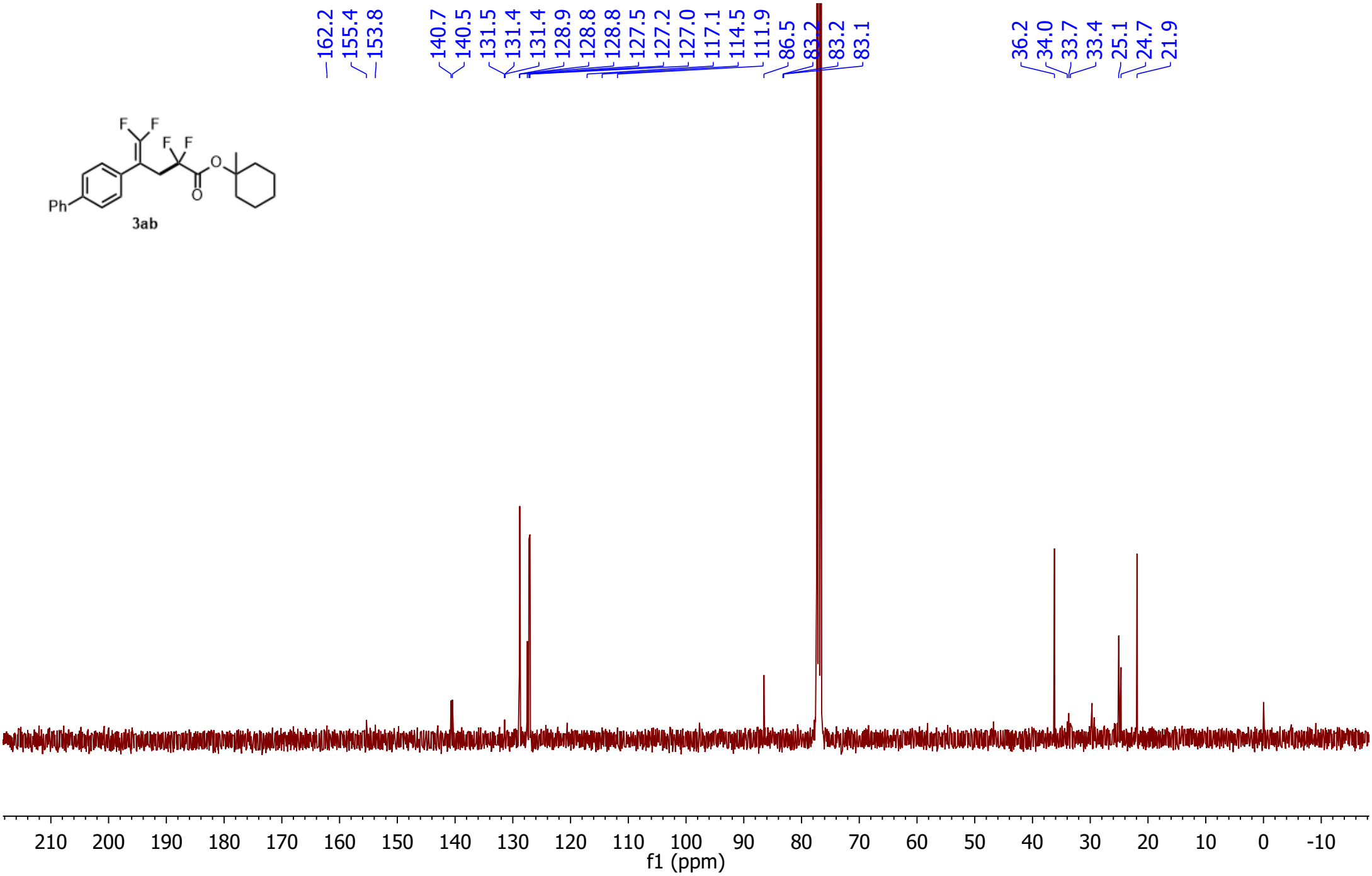
^{19}F NMR Spectrum of **3xa**

1H (CDCl3, 400 MHz)



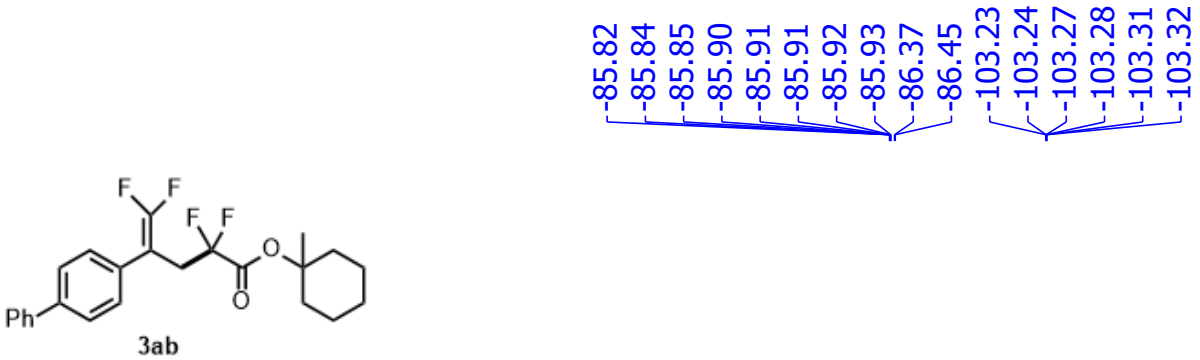
^{1}H NMR Spectrum of **3ab**

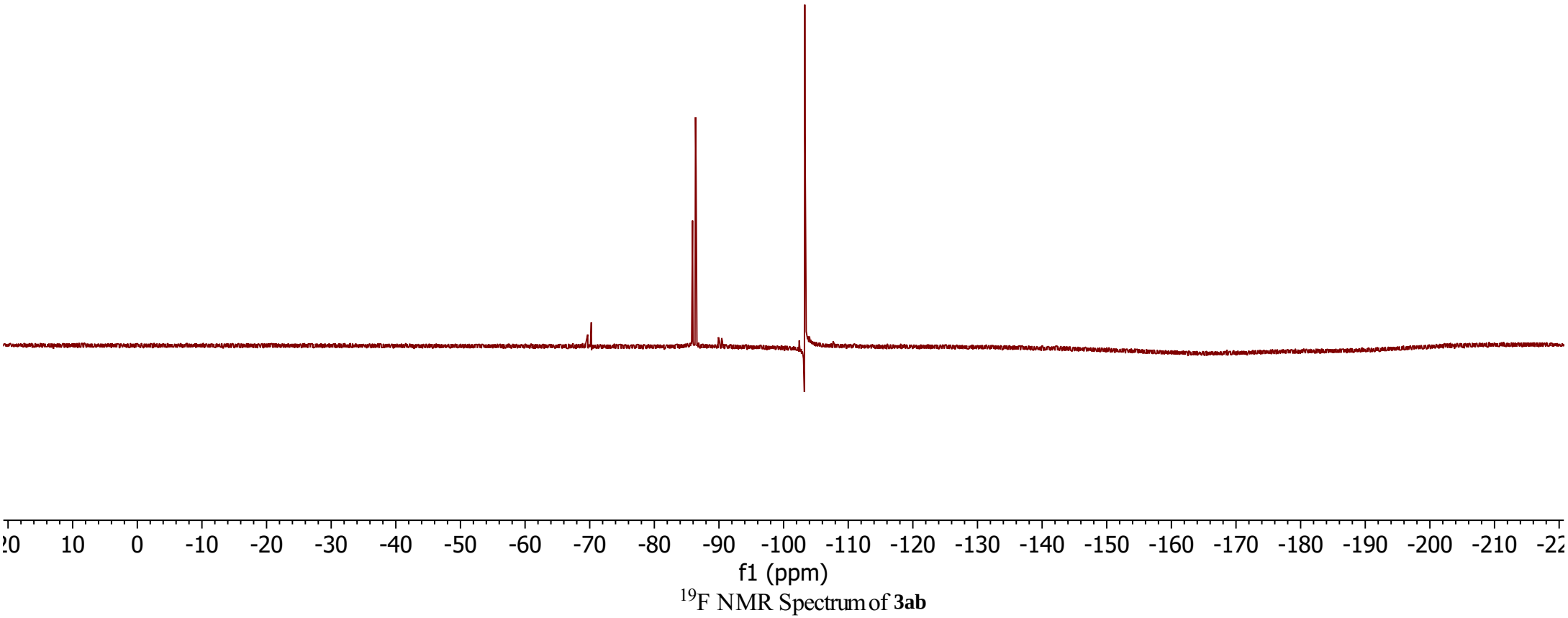
13C (CDCl3, 101 MHz)



^{13}C NMR Spectrum of **3ab**

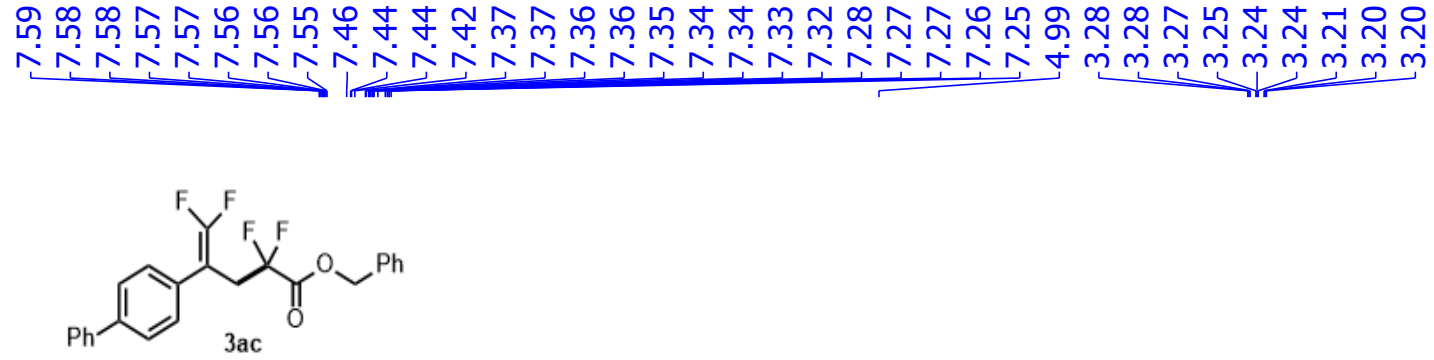
19F (CDCl3, 376 MHz)



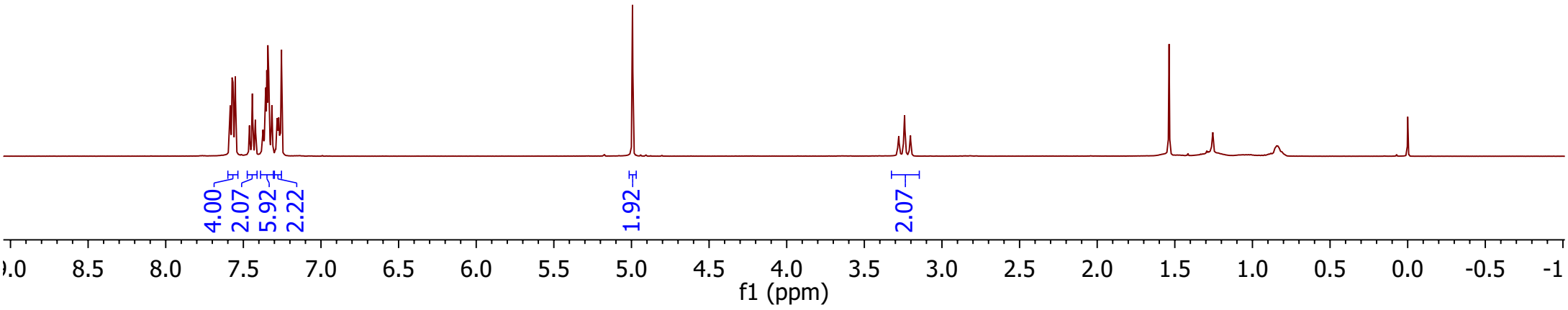


^{19}F NMR Spectrum of **3ab**

1H (CDCl3, 400 MHz)

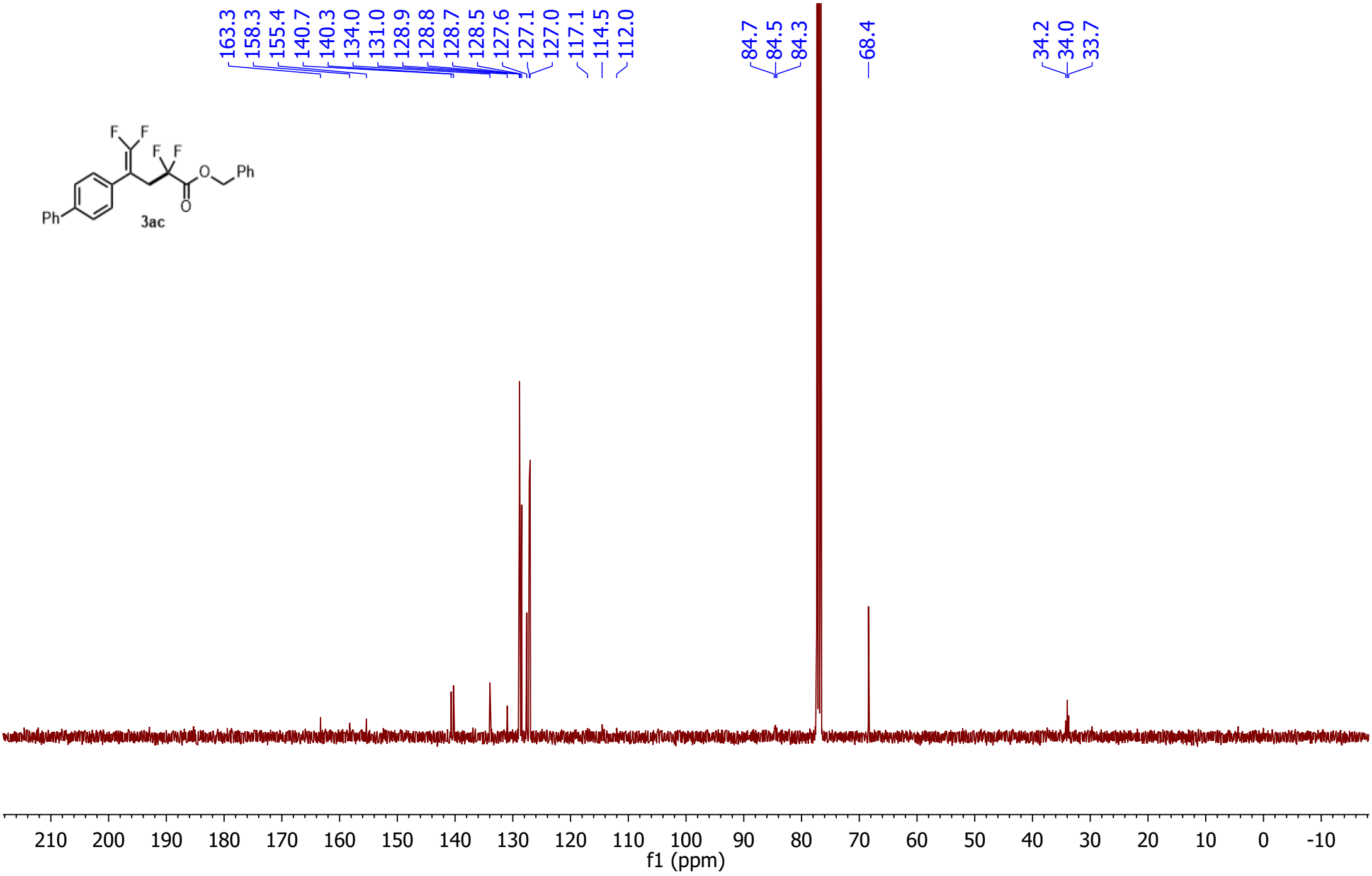


3ac



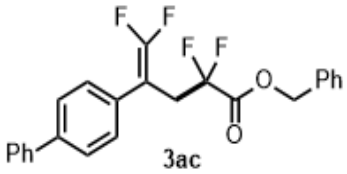
^{1}H NMR Spectrum of **3ac**

13C (CDCl3, 101 MHz)



^{13}C NMR Spectrum of **3ac**

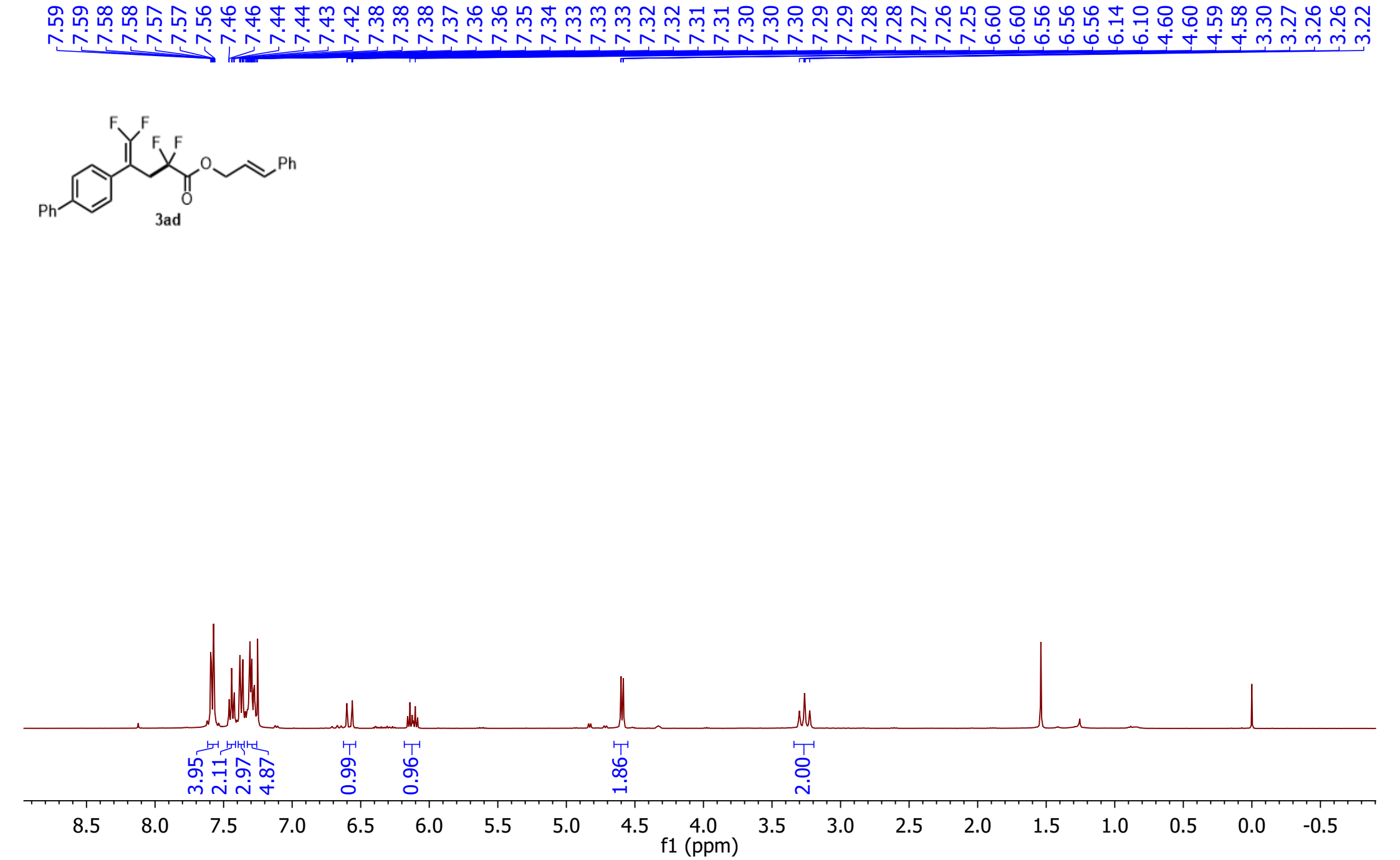
19F (CDCl3, 376 MHz)



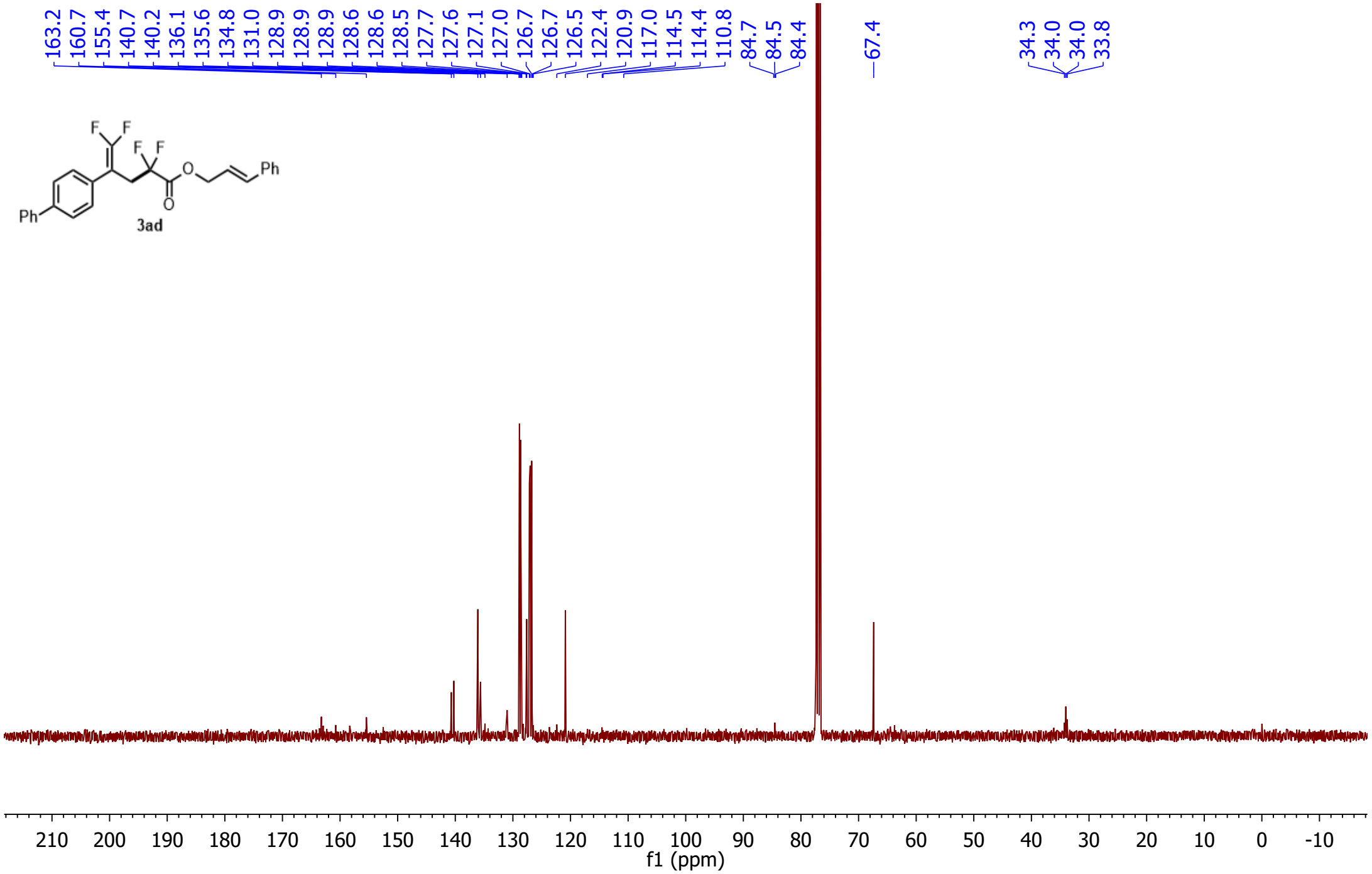
3ac

^{19}F NMR Spectrum of **3ac**

1H (CDCl3, 400 MHz)

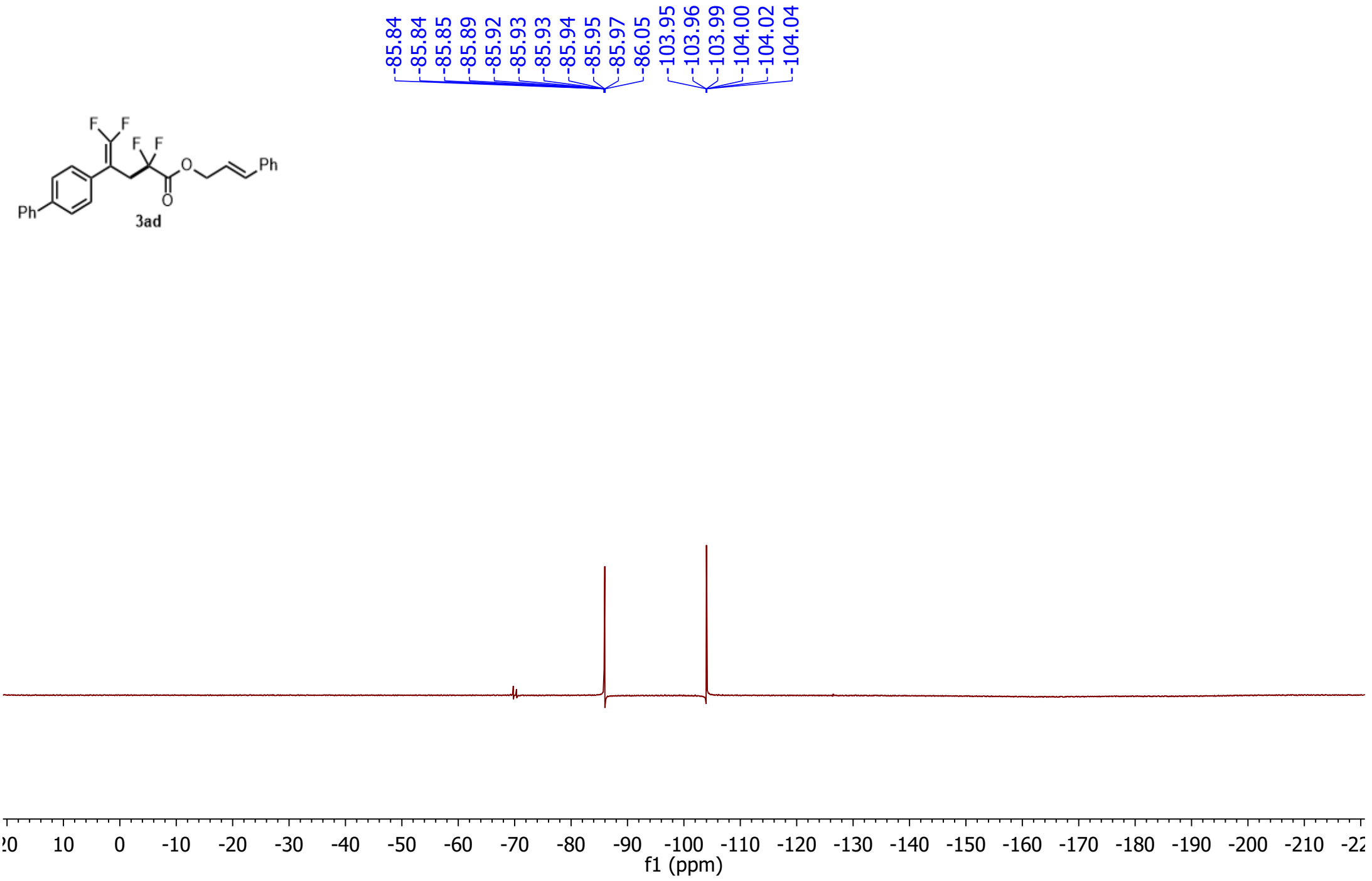


^{1}H NMR Spectrum of **3ad**



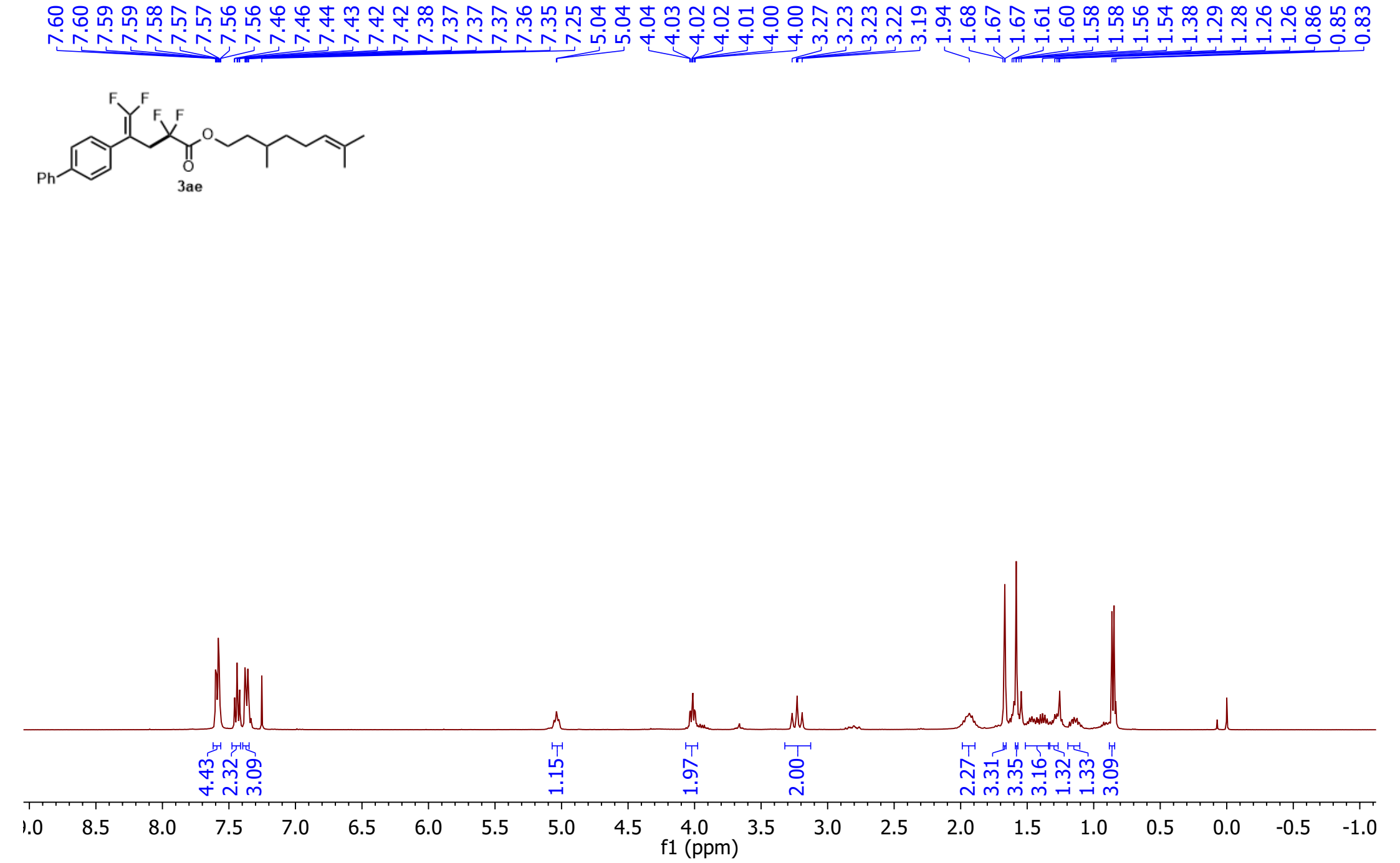
^{13}C NMR Spectrum of **3ad**

19F (CDCl3, 376 MHz)



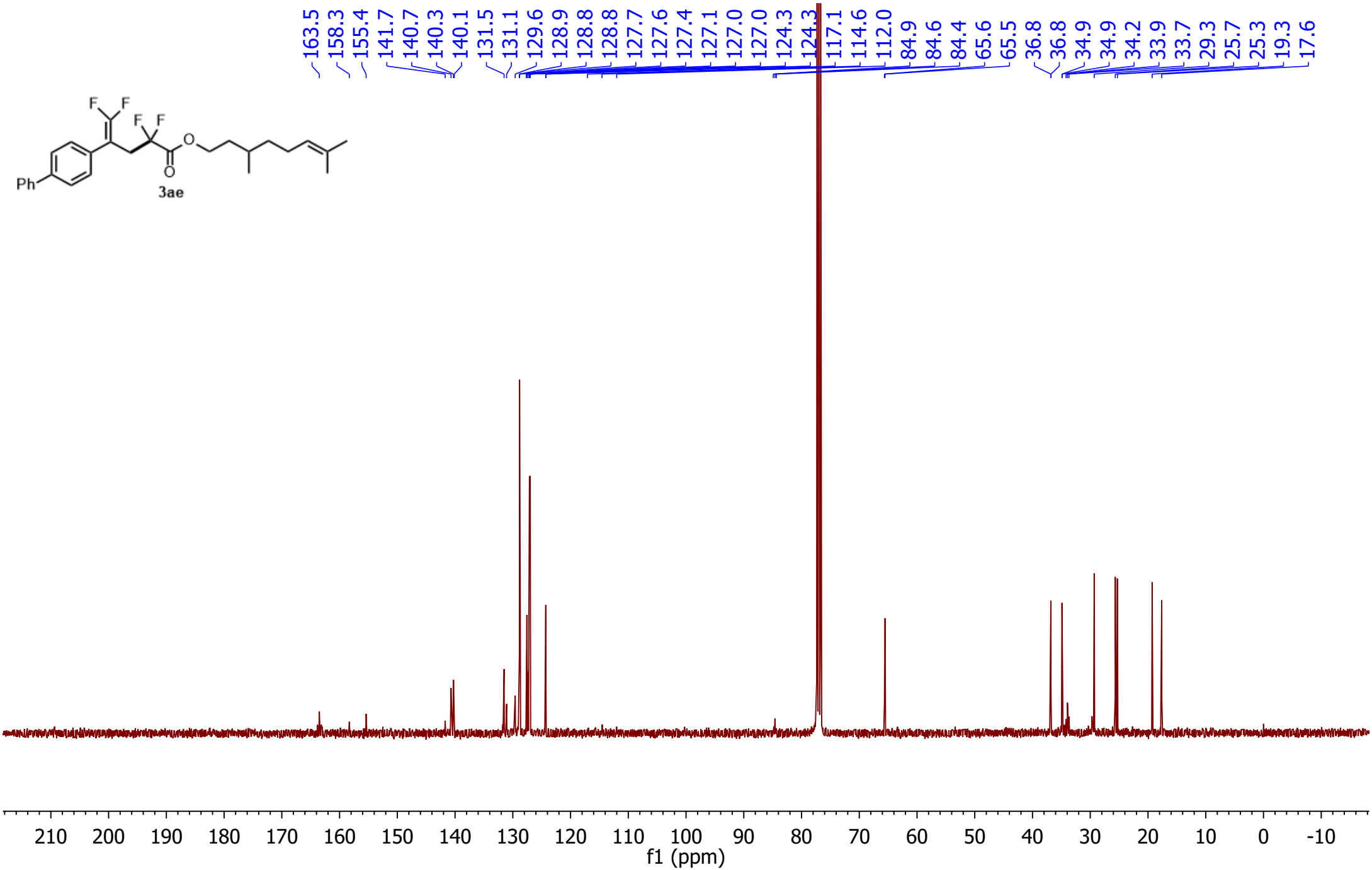
^{19}F NMR Spectrum of **3ad**

1H (CDCl3, 400 MHz)



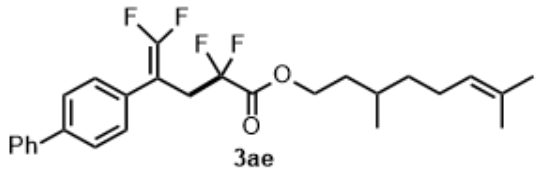
^{1}H NMR Spectrum of **3ae**

13C (CDCl3, 101 MHz)



^{13}C NMR Spectrum of **3ae**

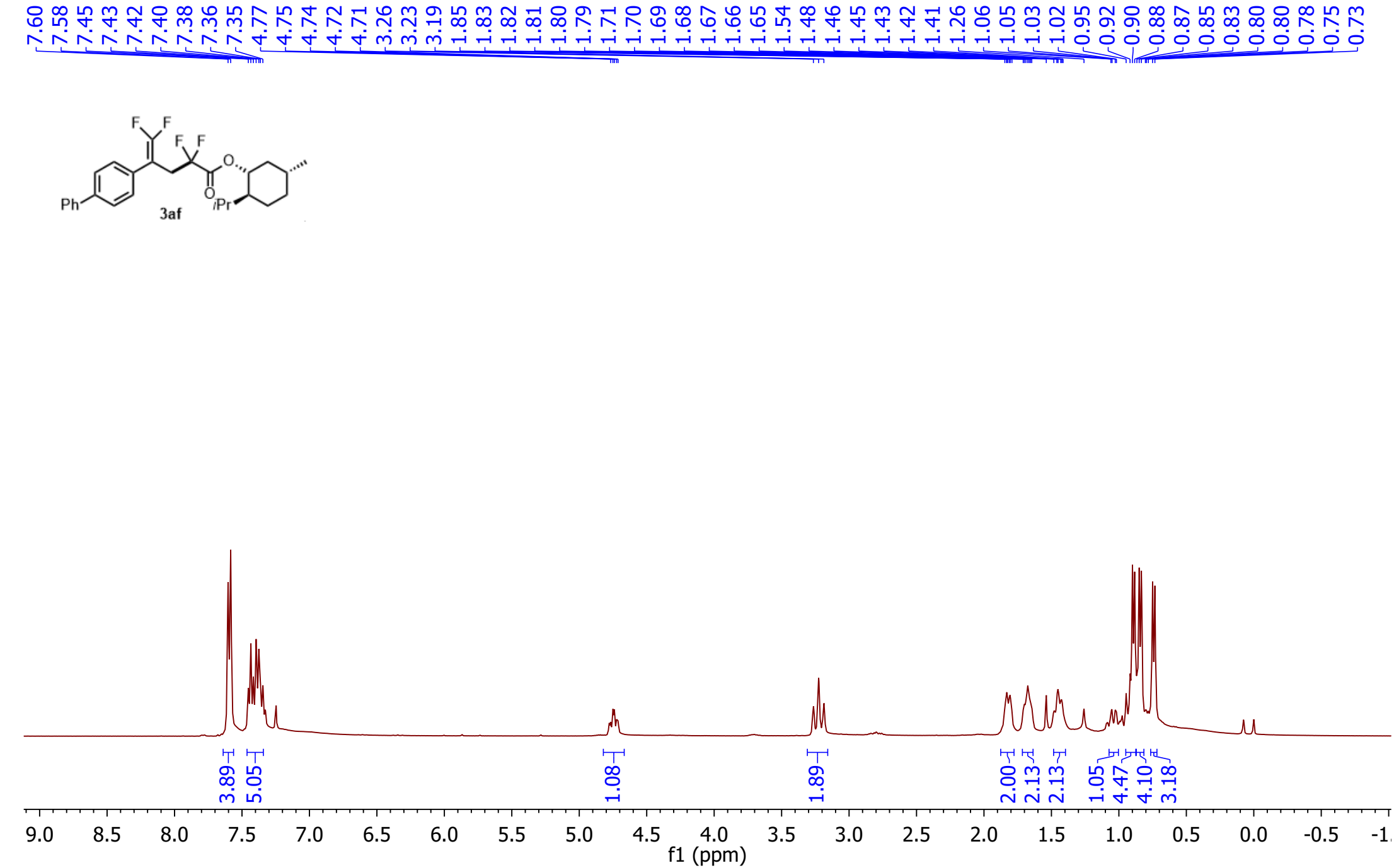
19F (CDCl3, 376 MHz)



3ae

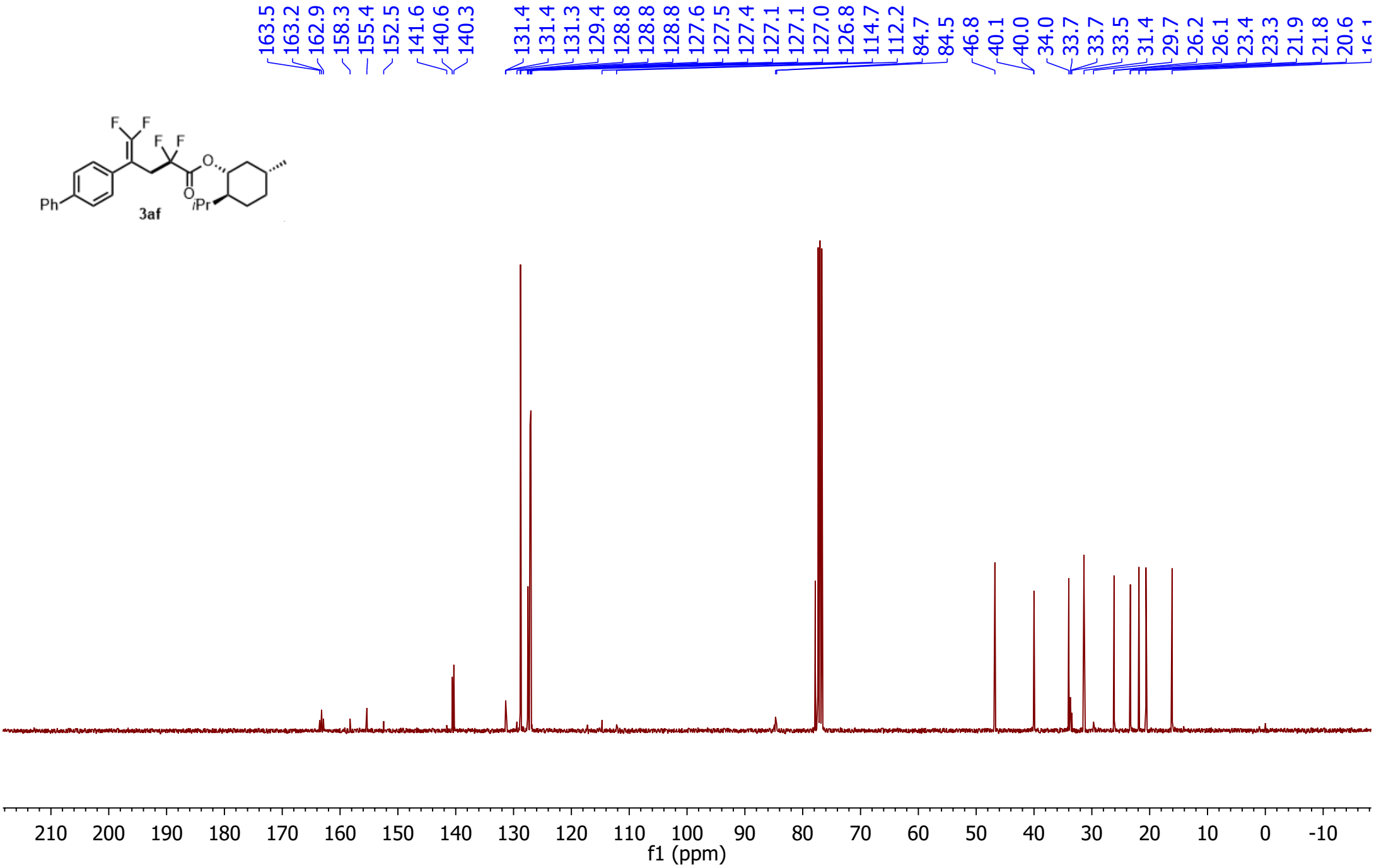
^{19}F NMR Spectrum of **3ae**

1H (CDCl3, 400 MHz)



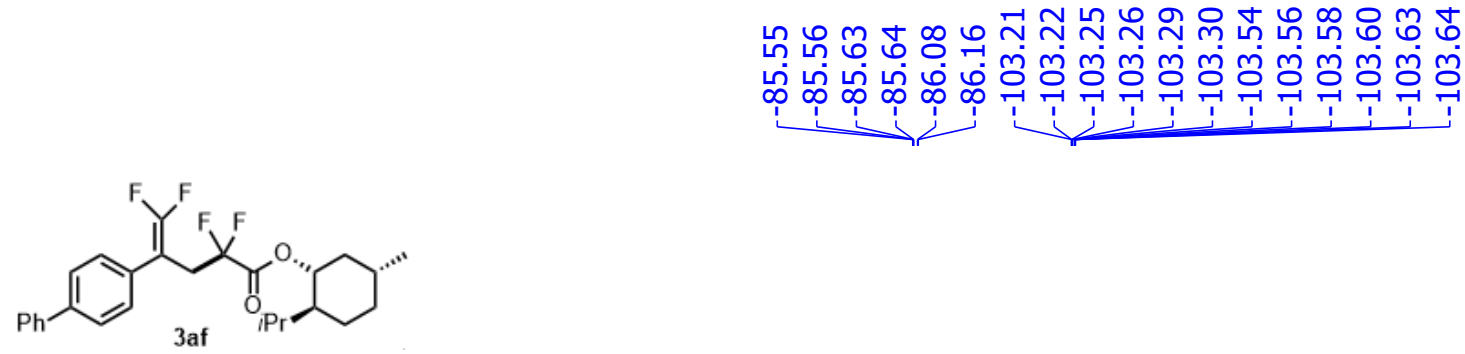
^{1}H NMR Spectrum of **3af**

13C (CDCl3, 101 MHz)



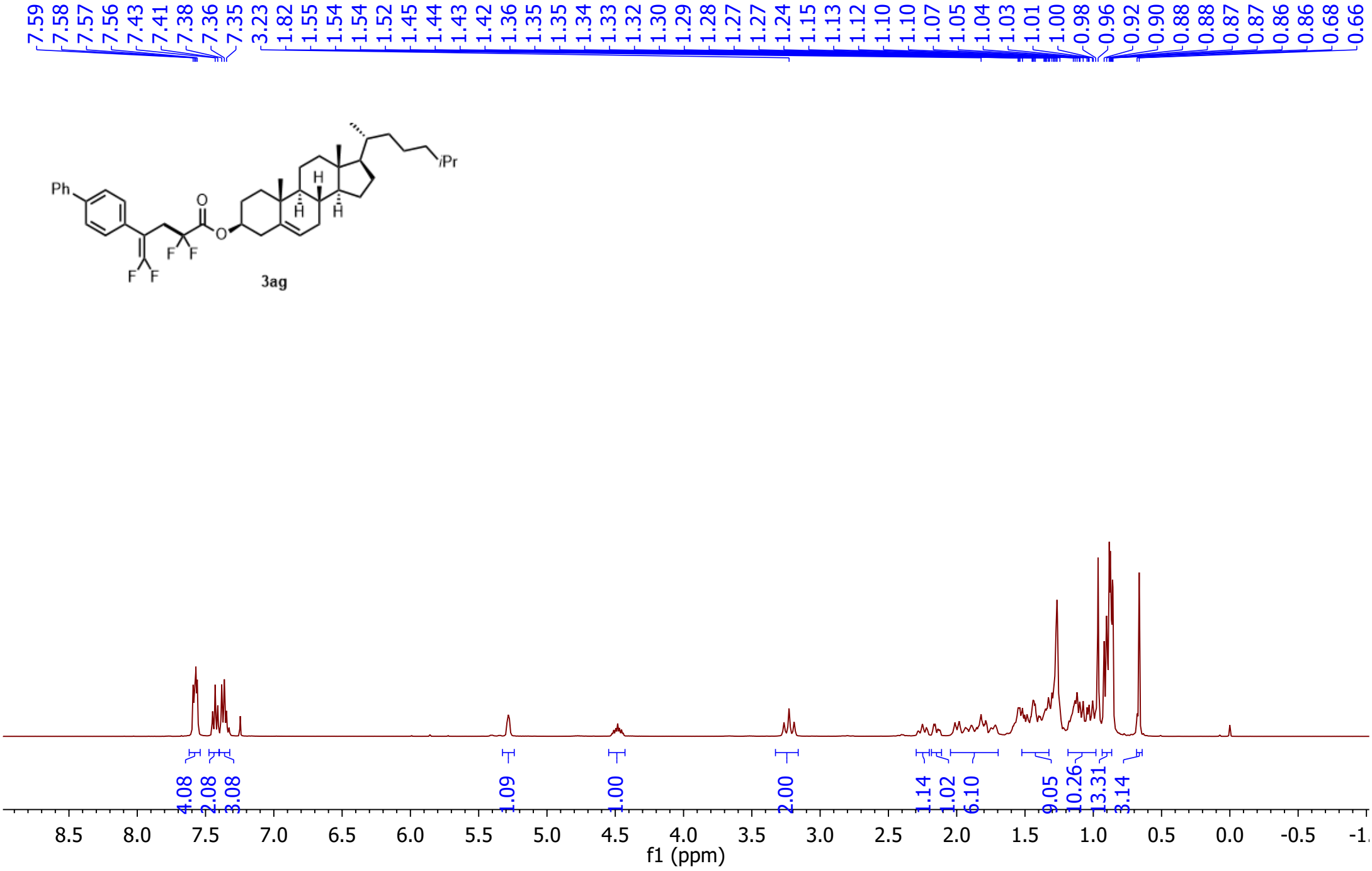
^{13}C NMR Spectrum of **3af**

19F (CDCl3, 376 MHz)



^{19}F NMR Spectrum of **3af**

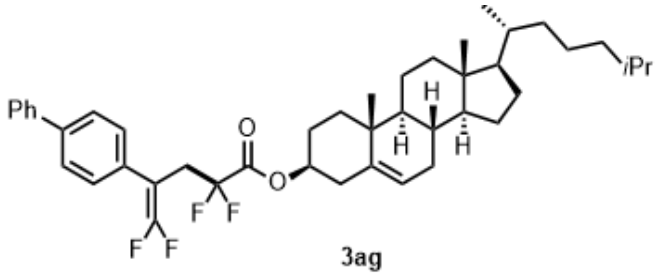
1H (CDCl3, 400 MHz)



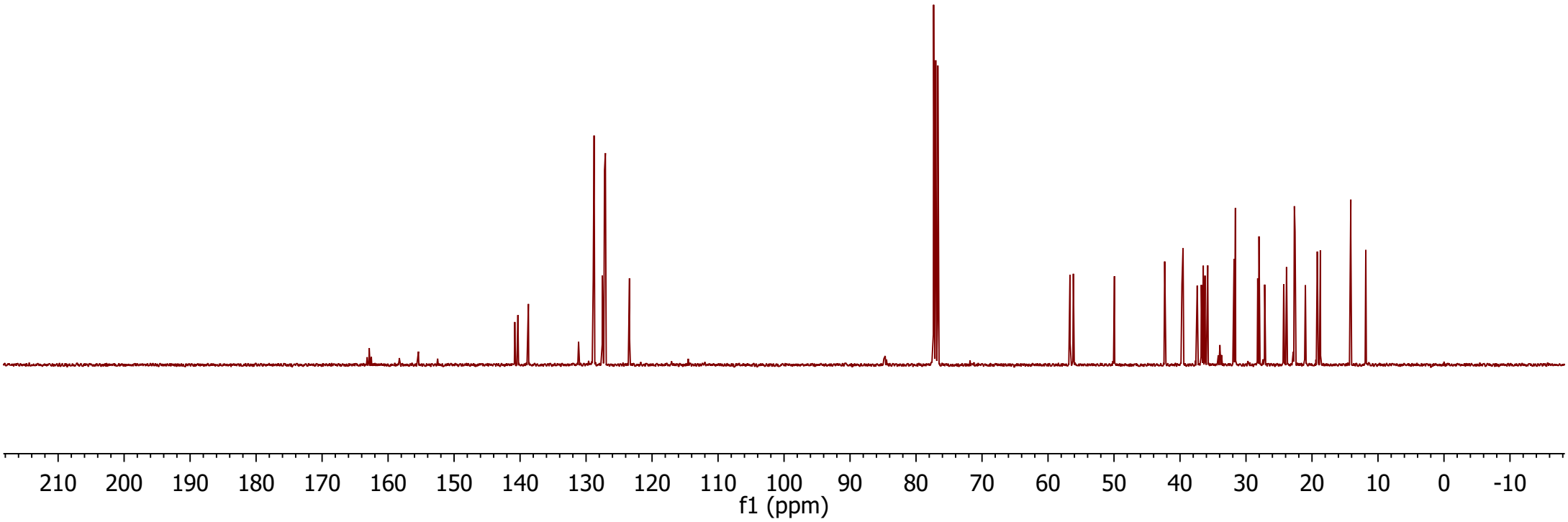
^{1}H NMR Spectrum of **3ag**

13C (CDCl3, 101 MHz)

162.9 155.4 140.8 140.3 138.7 131.2 131.1 131.1 128.9 128.9 128.9 128.8 127.5 127.2 127.1 127.1 123.4 84.7 77.3 56.7 56.2 56.2 49.9 42.3 39.7 39.5 37.4 36.8 36.5 36.2 35.8 34.2 34.0 33.9 33.7 31.8 31.8 31.6 28.2 28.0 27.2 24.3 23.9 22.8 22.7 22.7 22.6 21.1 21.0 19.3 19.2 18.7 14.1 11.8

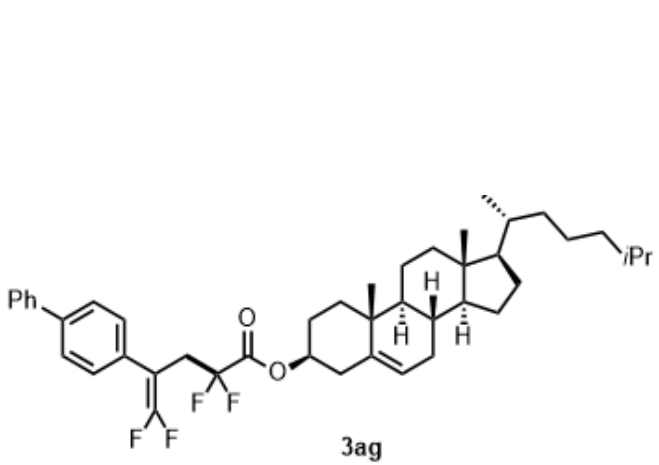


3ag



^{13}C NMR Spectrum of **3ag**

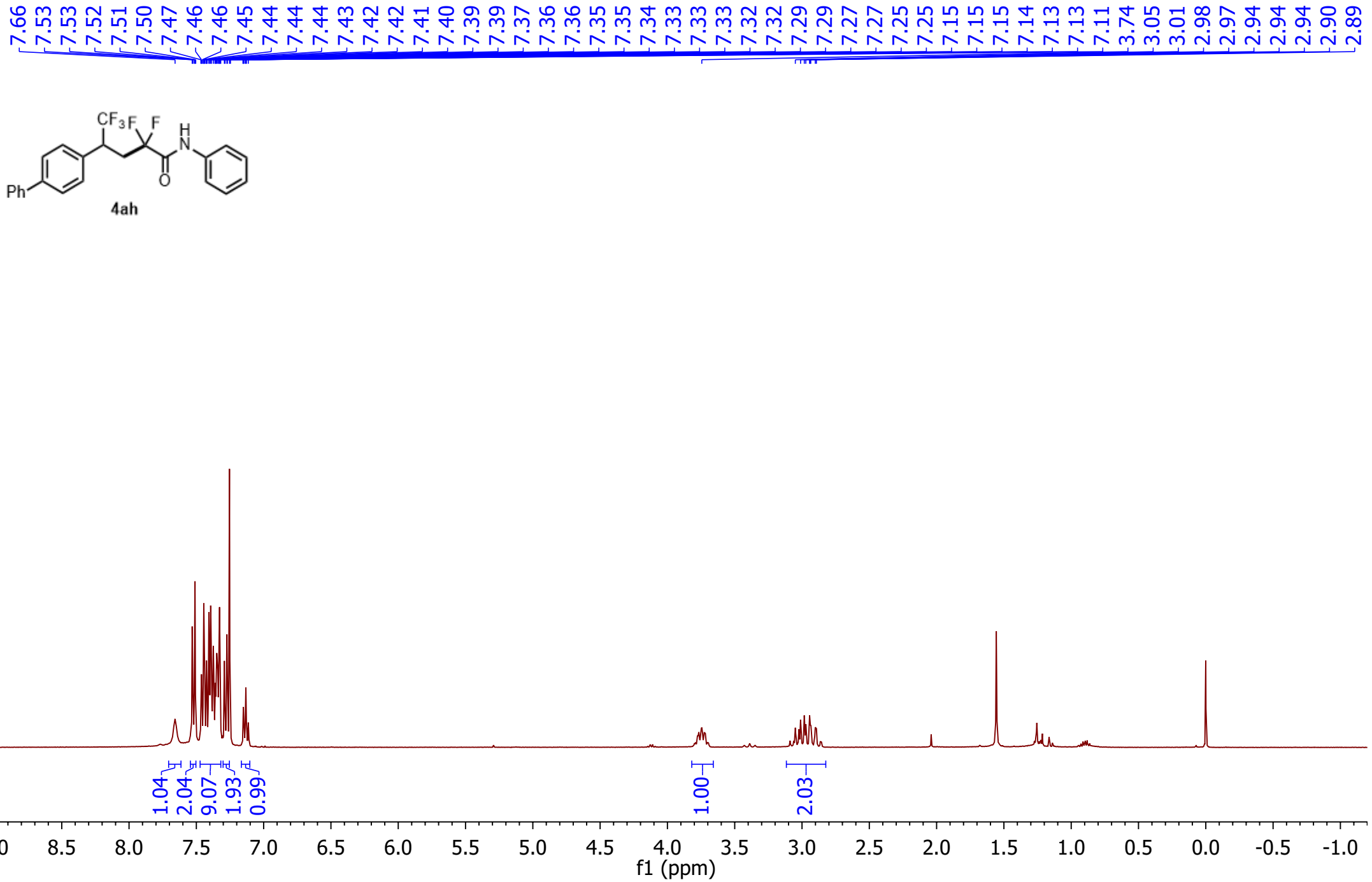
19F (CDCl3, 376 MHz)



3ag

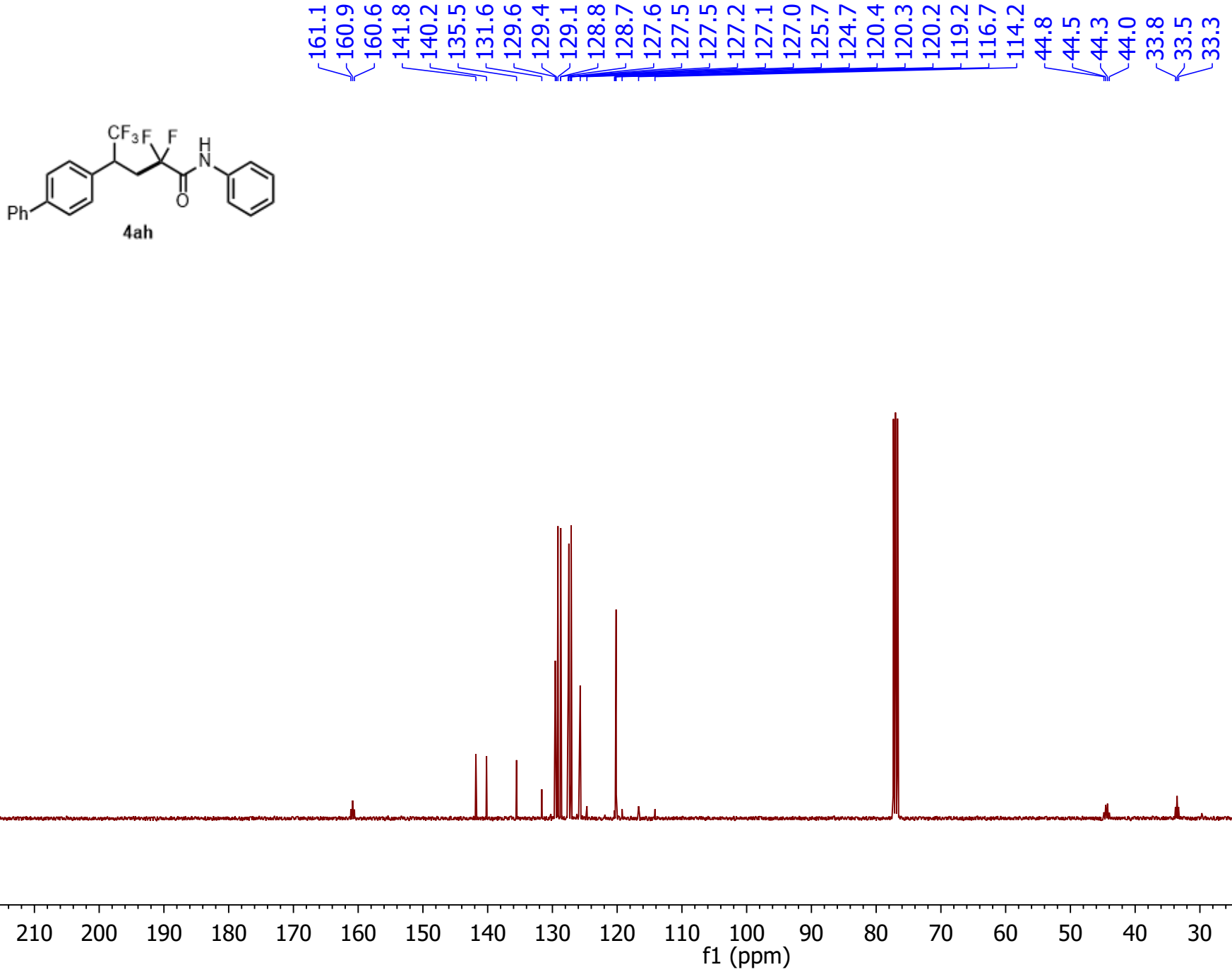
^{19}F NMR Spectrum of **3ag**

1H (CDCl3, 400 MHz)



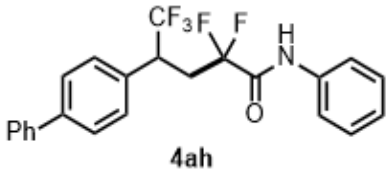
^{1}H NMR Spectrum of **4ah**

13C (CDCl3, 101 MHz)

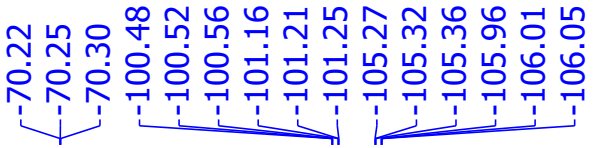


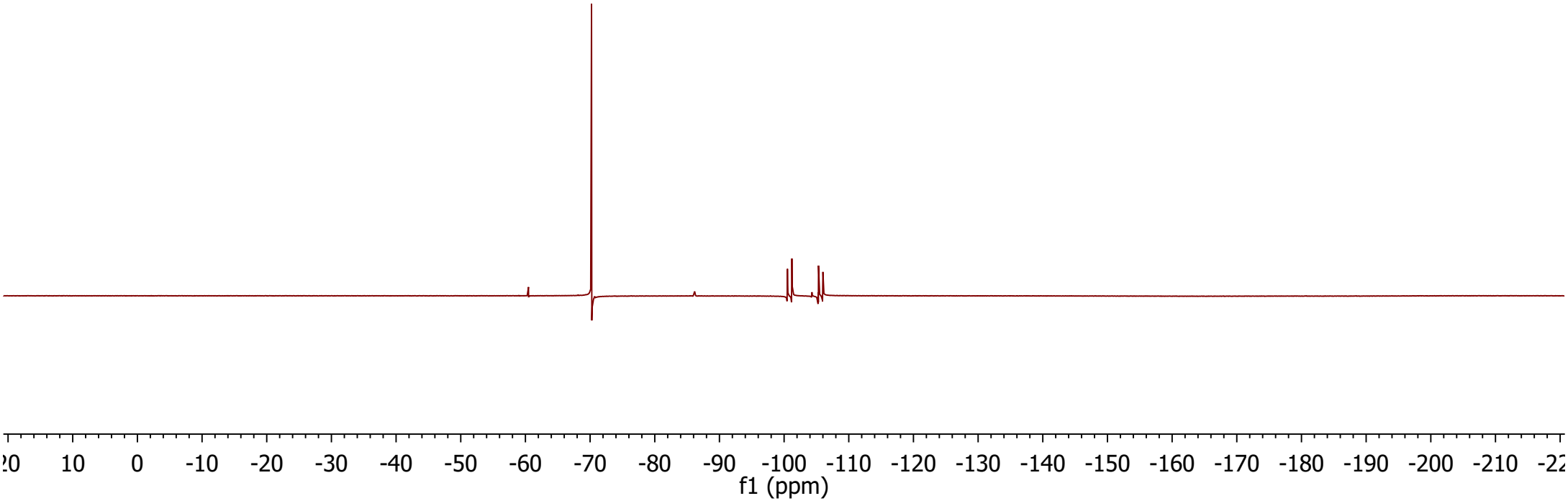
^{13}C NMR Spectrum of **4ah**

19F (CDCl3, 376 MHz)



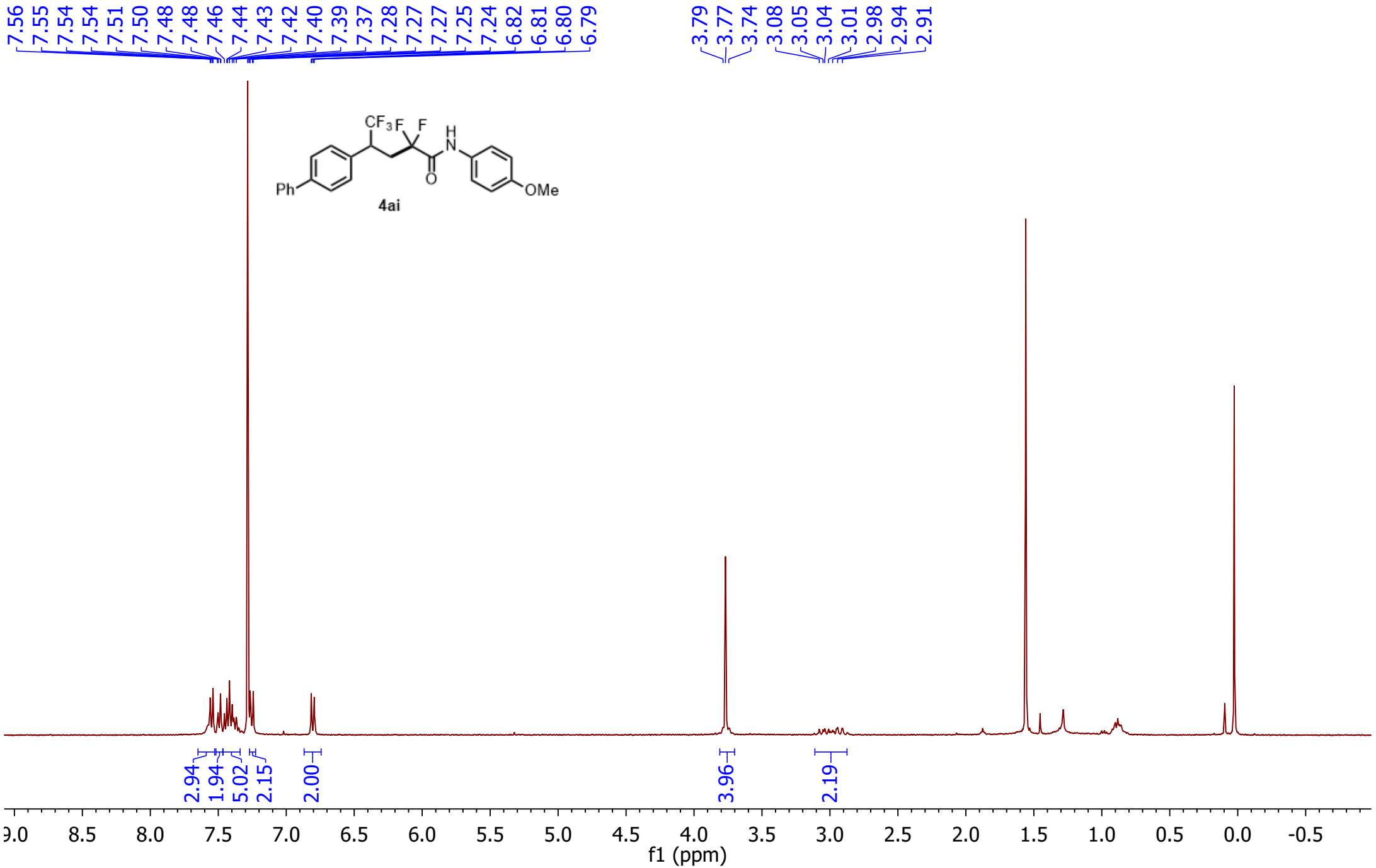
4ah





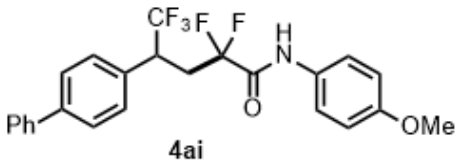
^{19}F NMR Spectrum of **4ah**

1H (CDCl3, 400 MHz)



^{1}H NMR Spectrum of **4ai**

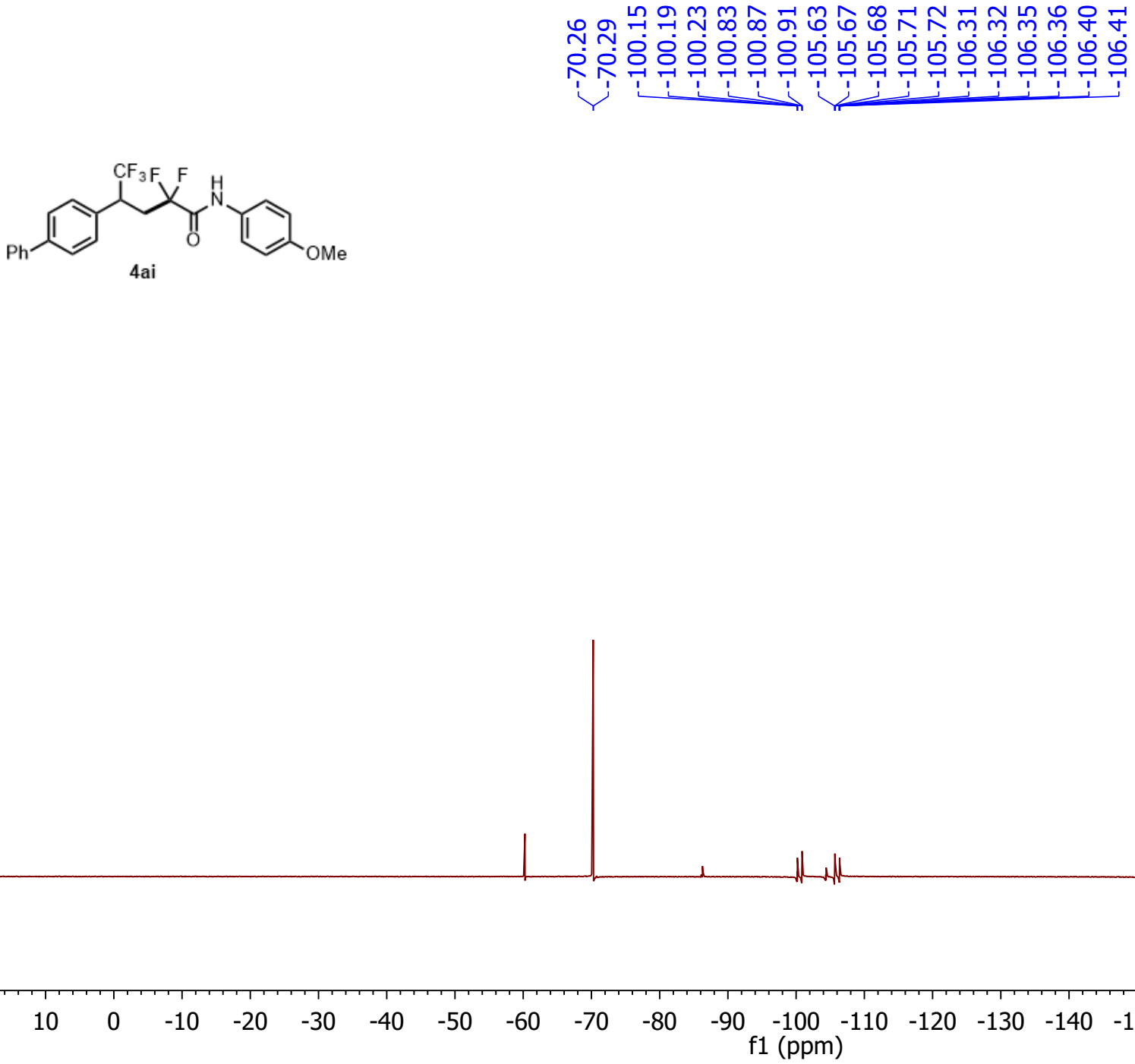
13C (CDCl3, 101 MHz)



4ai

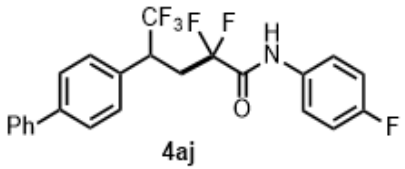
^{13}C NMR Spectrum of **4ai**

19F (CDCl3, 376 MHz)



^{19}F NMR Spectrum of **4ai**

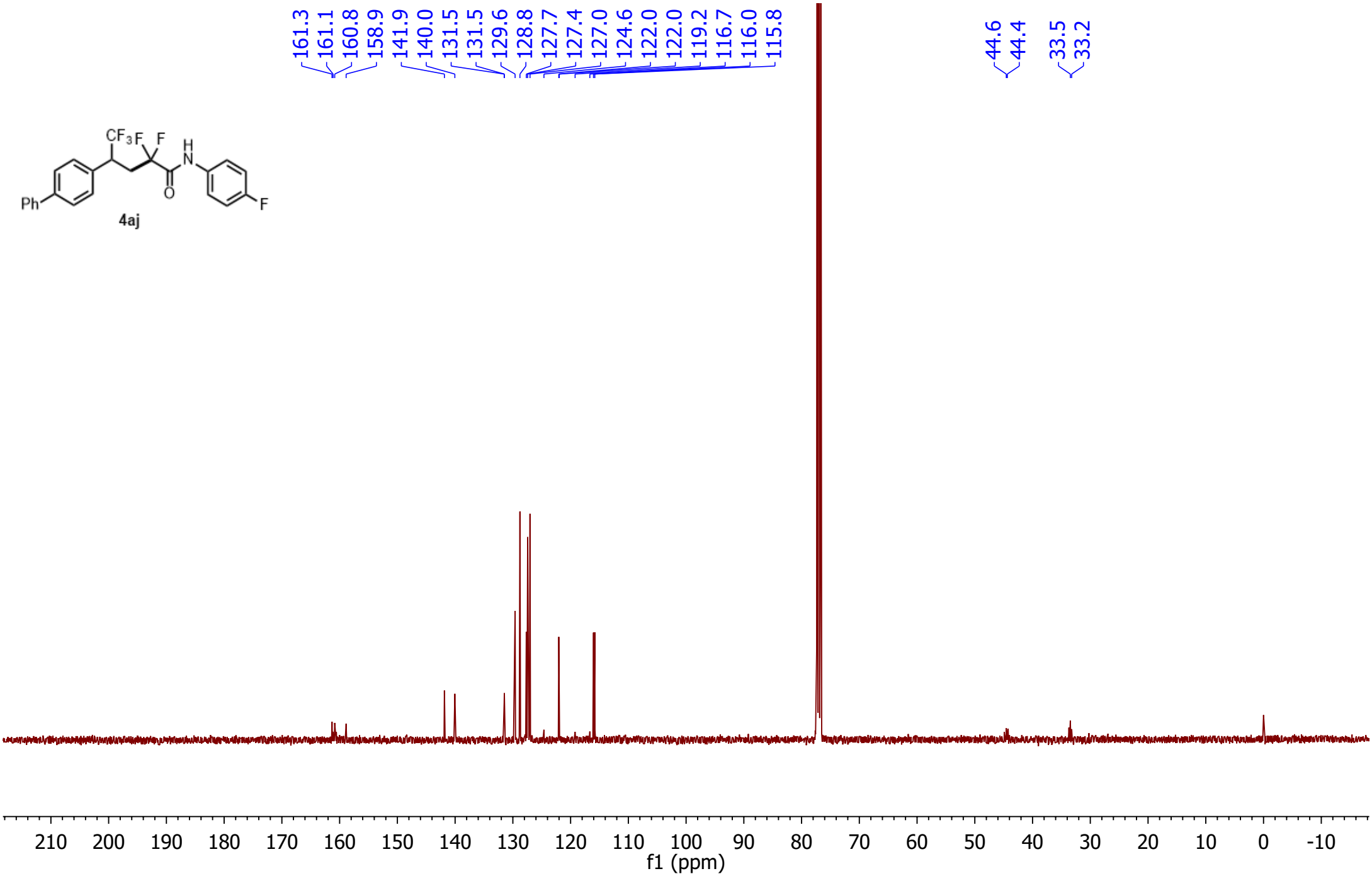
1H (CDCl3, 400 MHz)



4aj

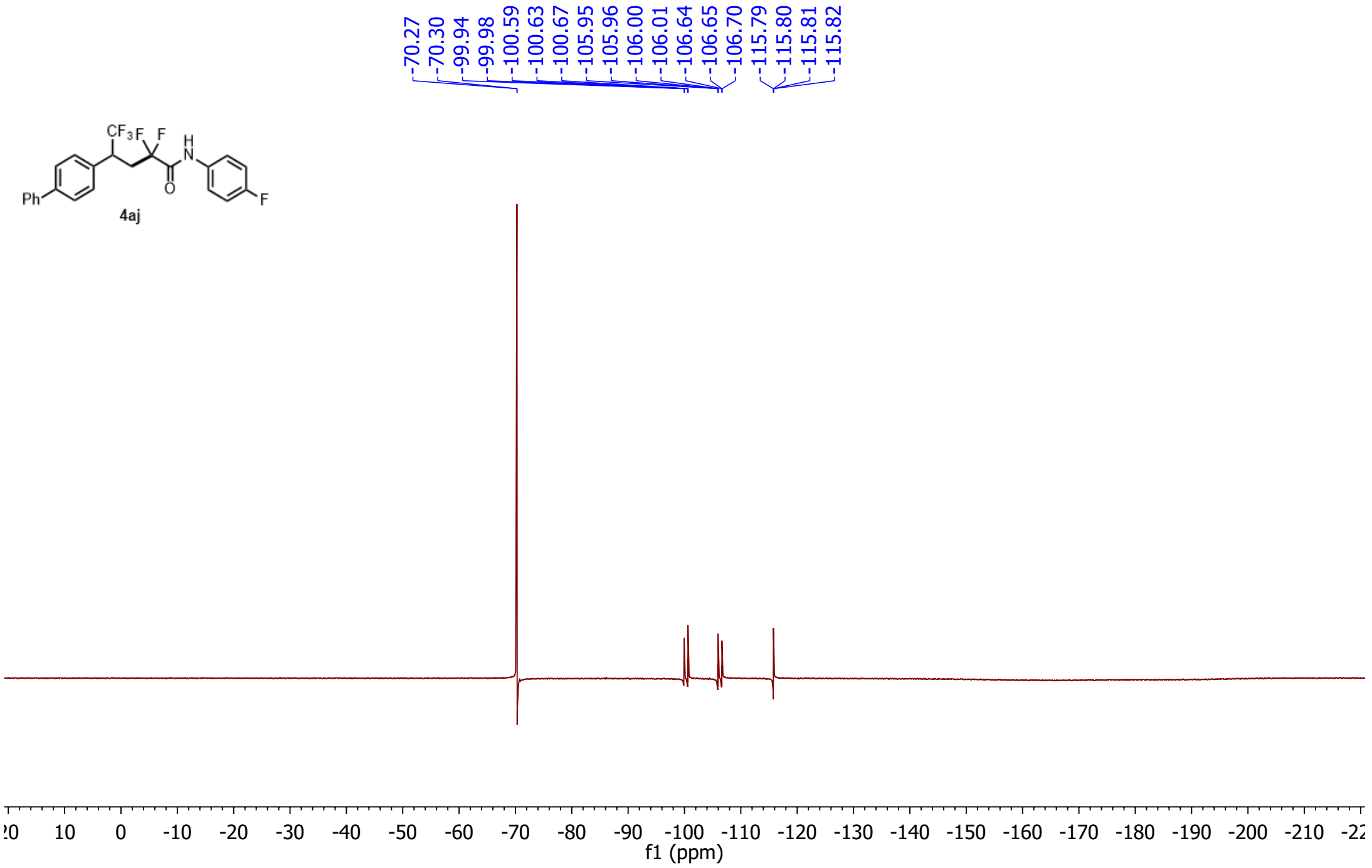
^{1}H NMR Spectrum of **4aj**

13C (CDCl3, 101 MHz)



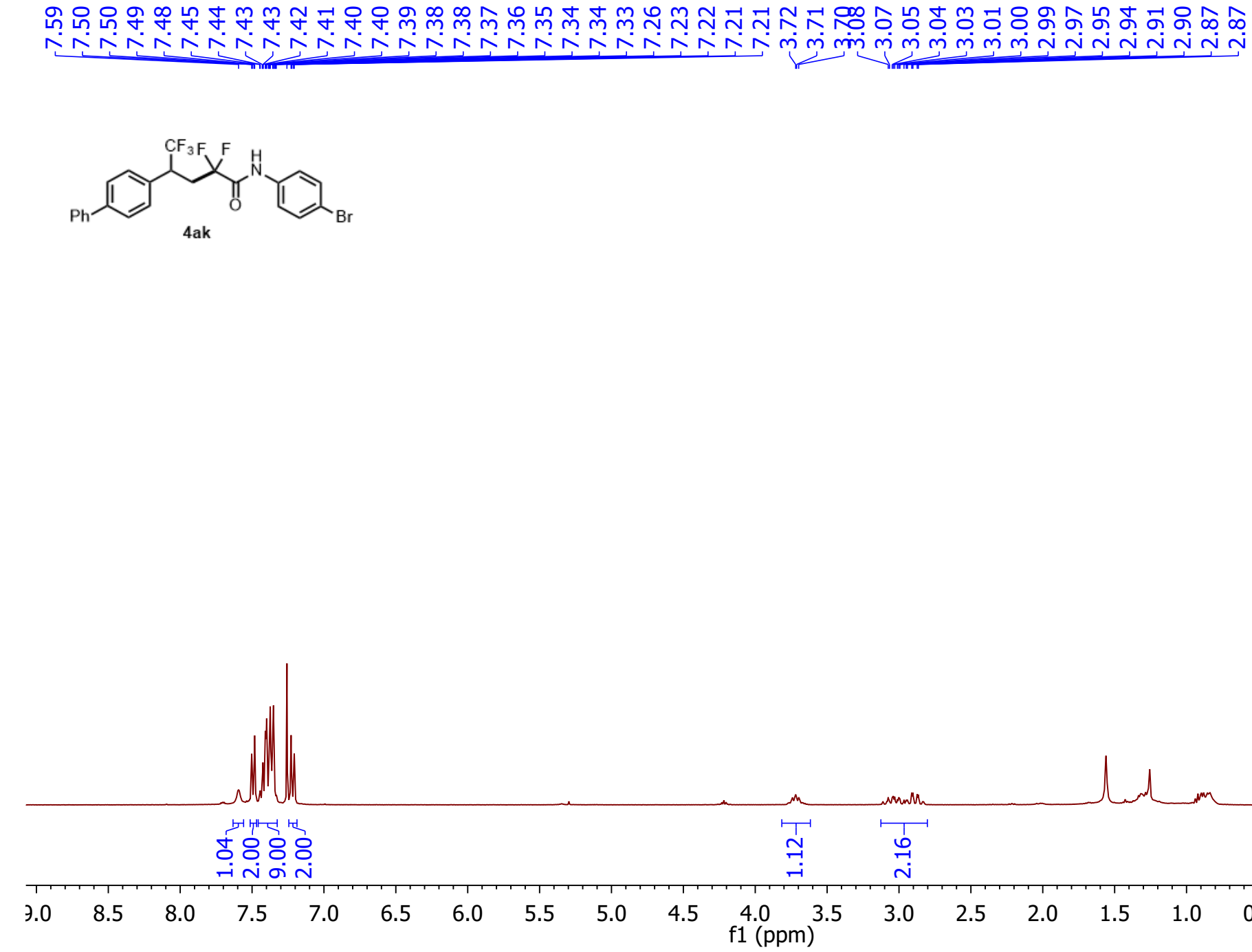
^{13}C NMR Spectrum of **4aj**

19F (CDCl3, 376 MHz)



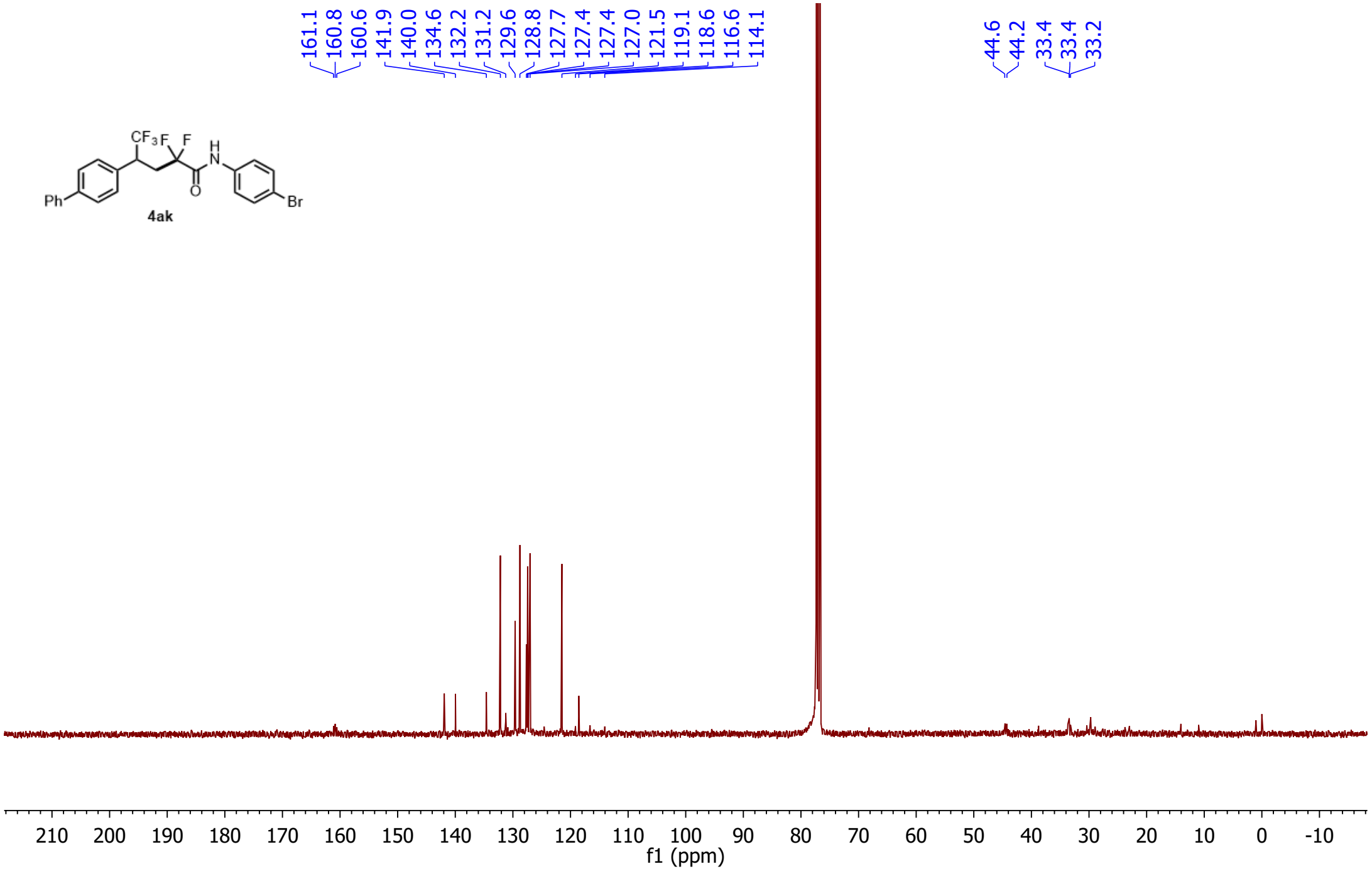
^{19}F NMR Spectrum of **4aj**

1H (CDCl3, 400 MHz)



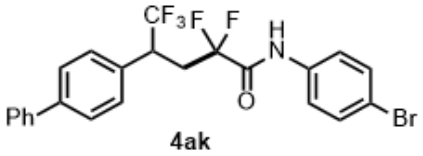
^{1}H NMR Spectrum of **4ak**

13C (CDCl3, 101 MHz)



^{13}C NMR Spectrum of **4ak**

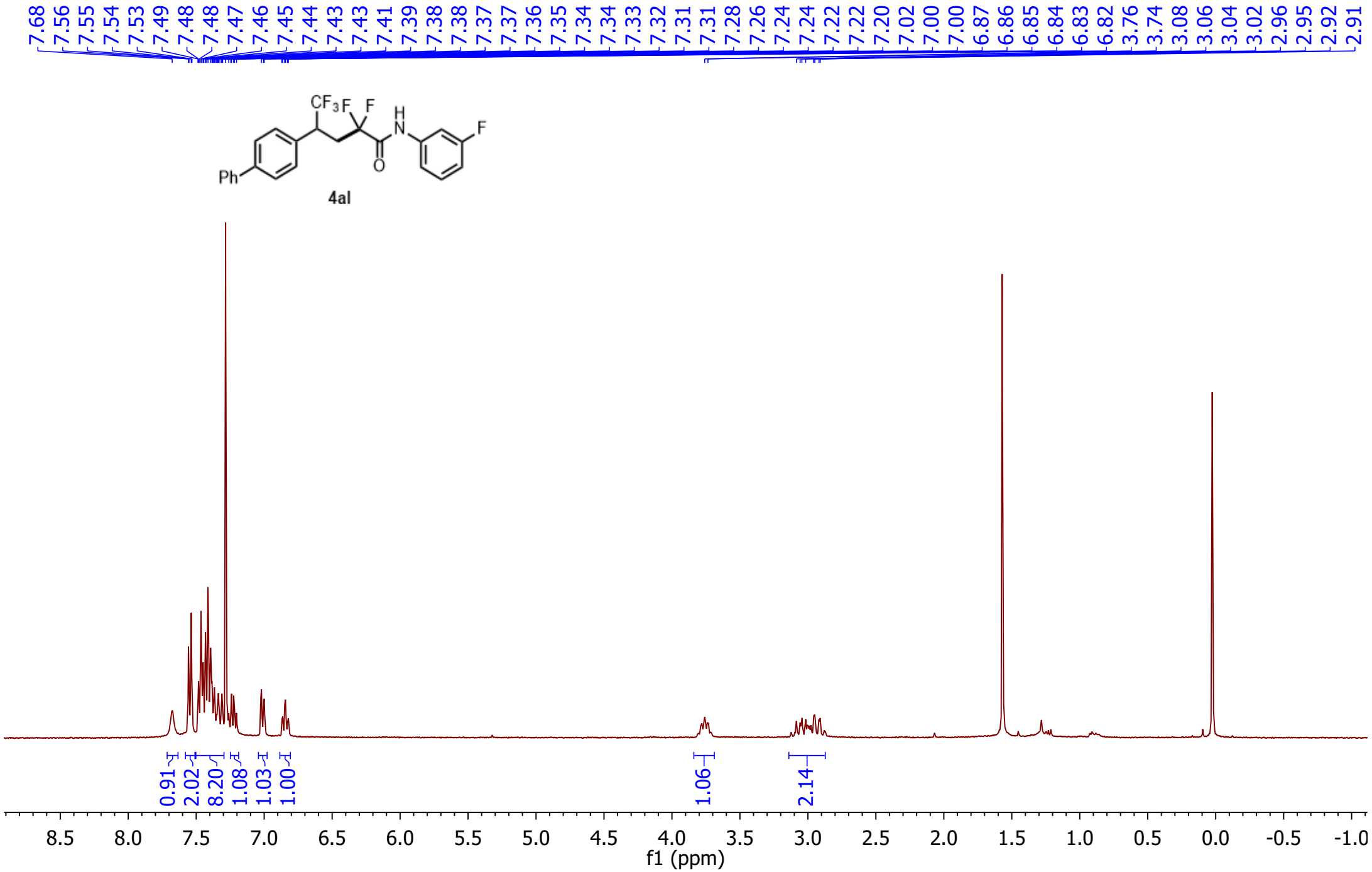
19F (CDCl3, 376 MHz)



4ak

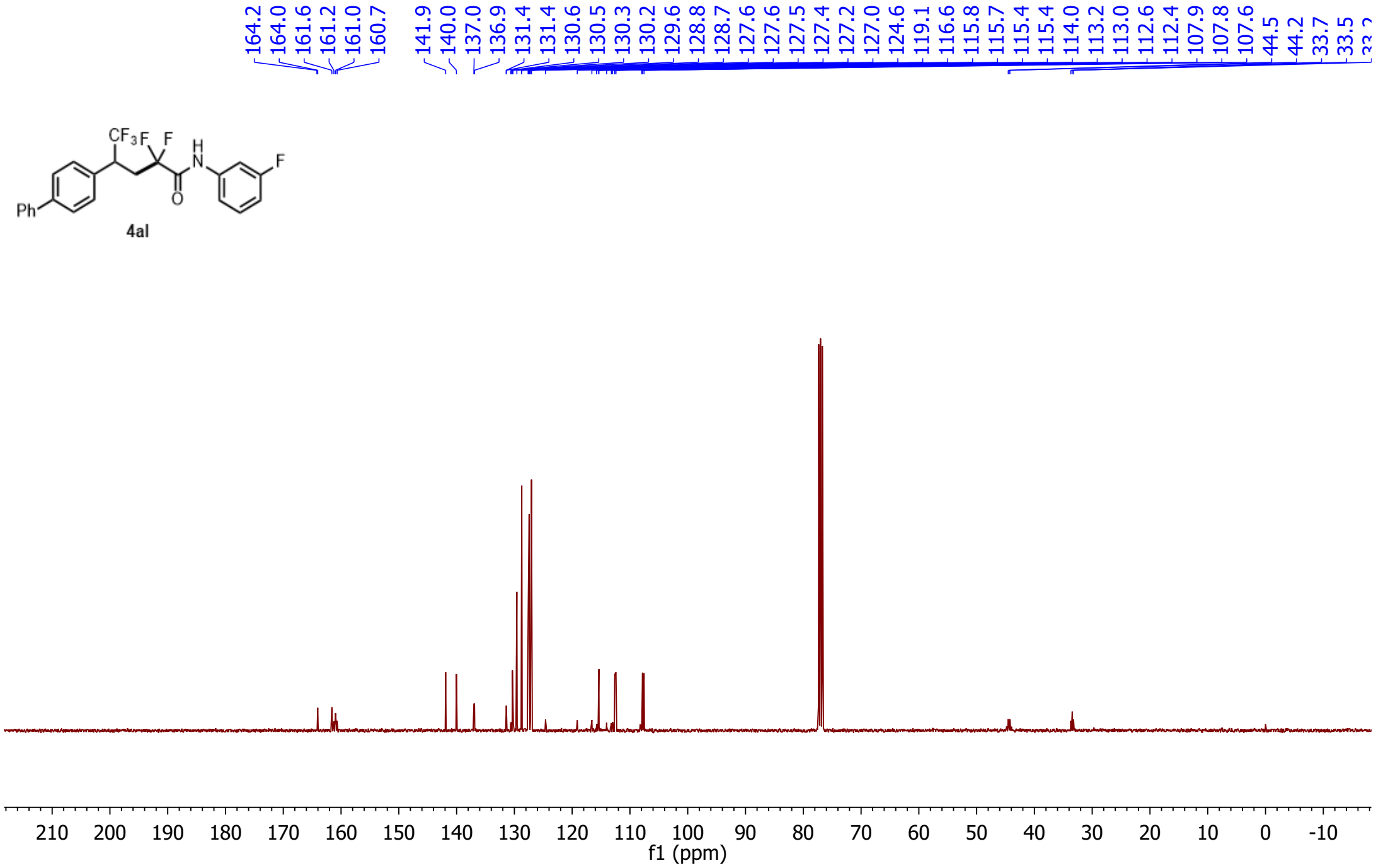
^{19}F NMR Spectrum of **4ak**

1H (CDCl3, 400 MHz)



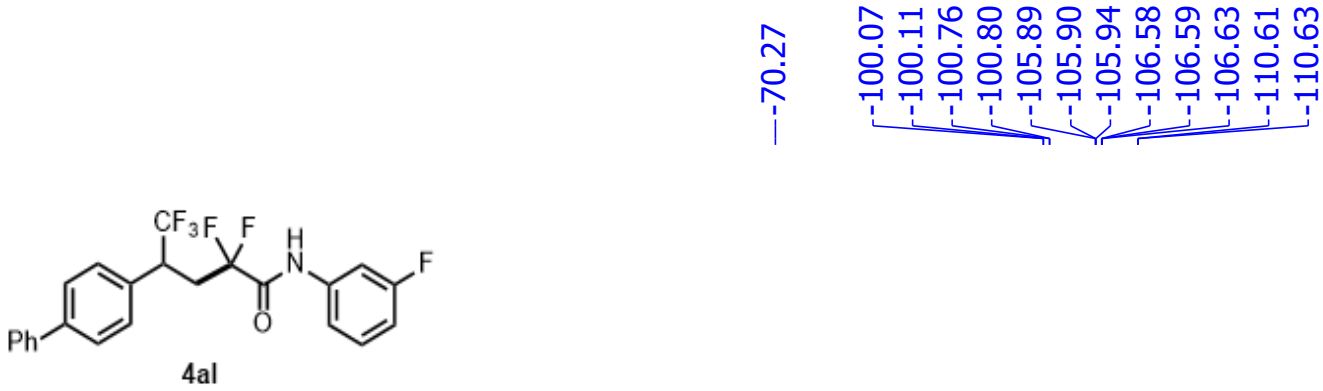
^{1}H NMR Spectrum of **4al**

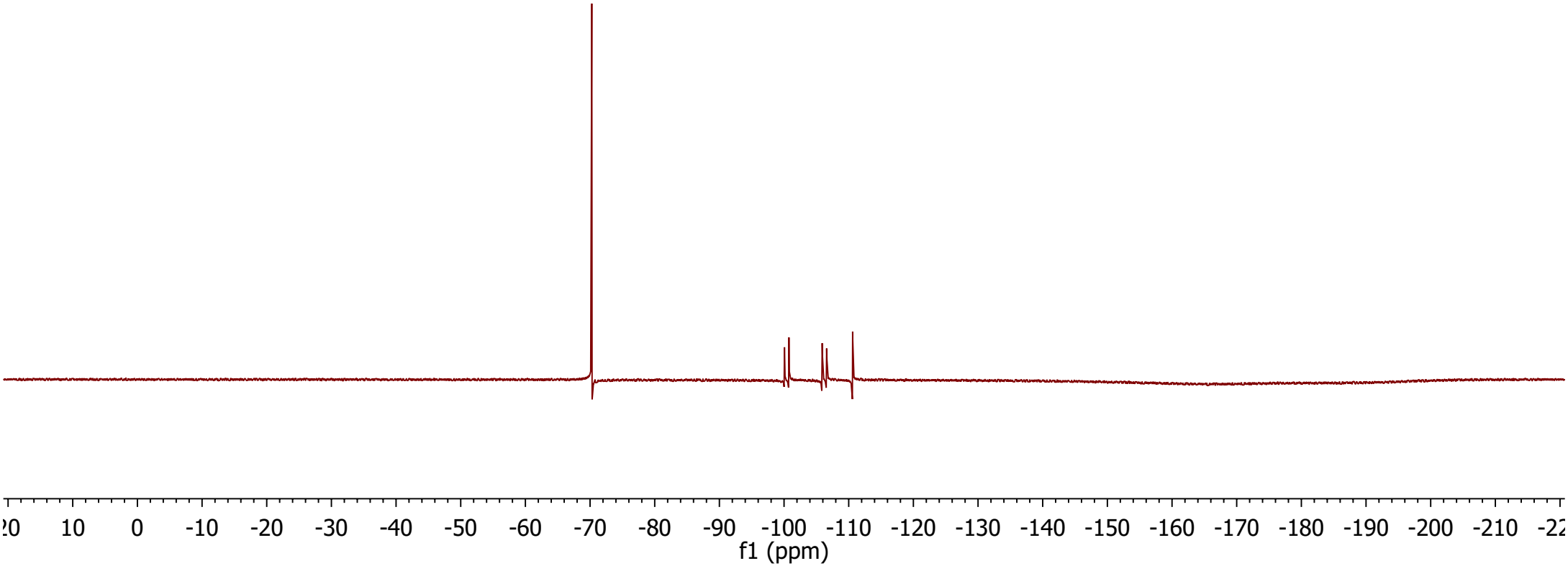
13C (CDCl3, 101 MHz)



^{13}C NMR Spectrum of **4al**

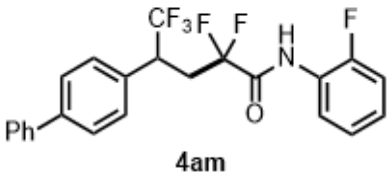
19F (CDCl3, 376 MHz)





^{19}F NMR Spectrum of **4al**

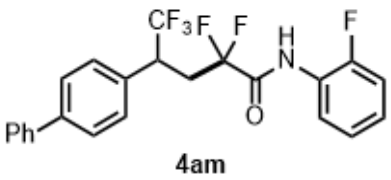
1H (CDCl3, 400 MHz)



4am

^{1}H NMR Spectrum of **4am**

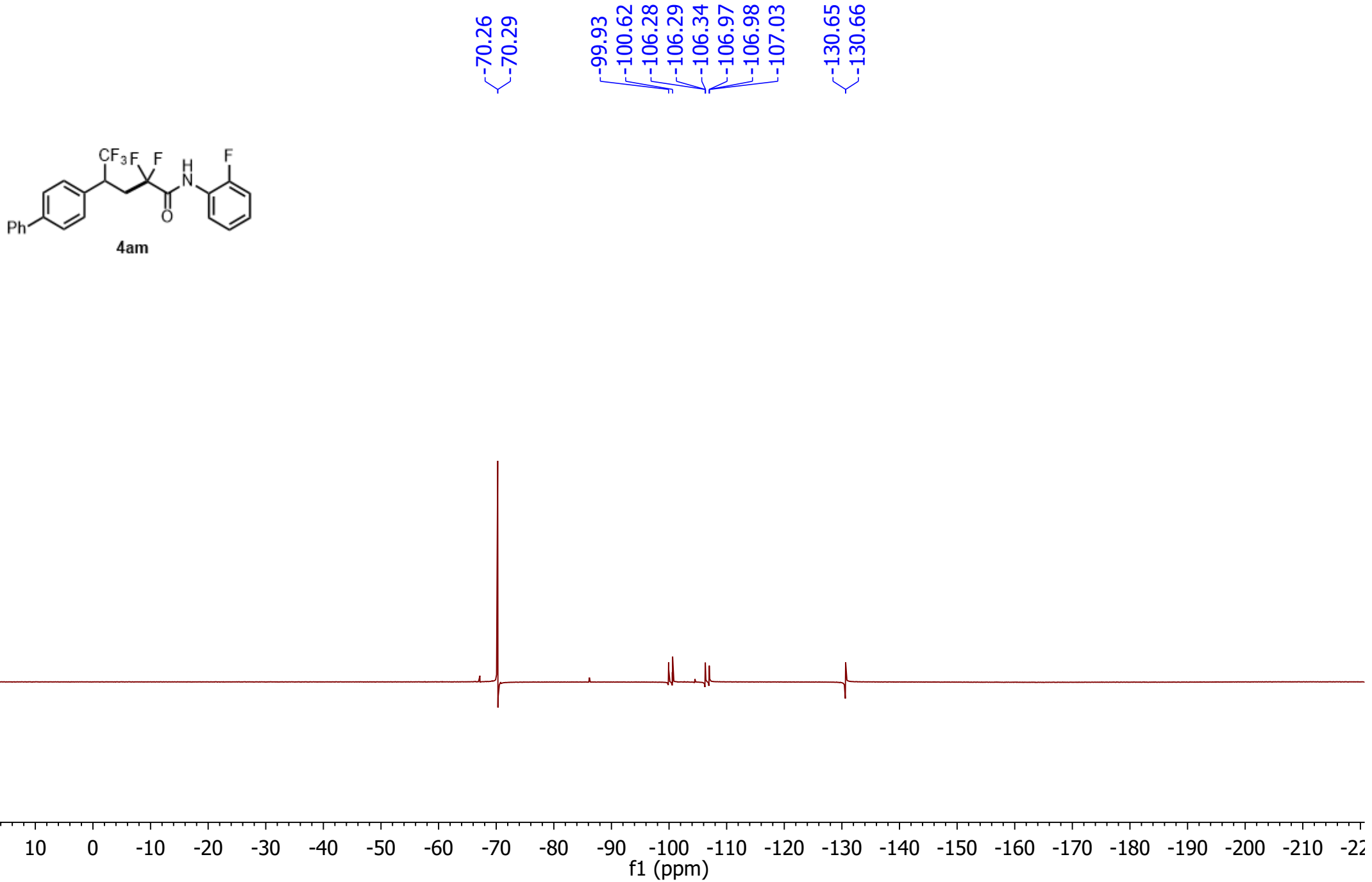
13C (CDCl3, 101 MHz)



4am

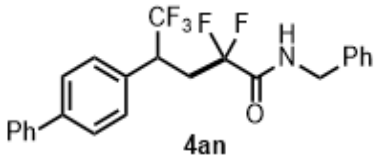
^{13}C NMR Spectrum of **4am**

19F (CDCl3, 376 MHz)



^{19}F NMR Spectrum of **4am**

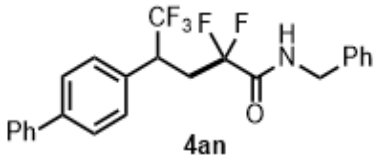
1H (CDCl3, 400 MHz)



4an

^{1}H NMR Spectrum of **4an**

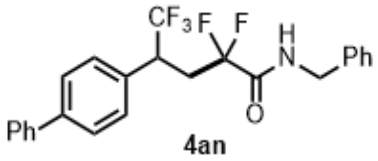
13C (CDCl3, 101 MHz)



4an

^{13}C NMR Spectrum of **4an**

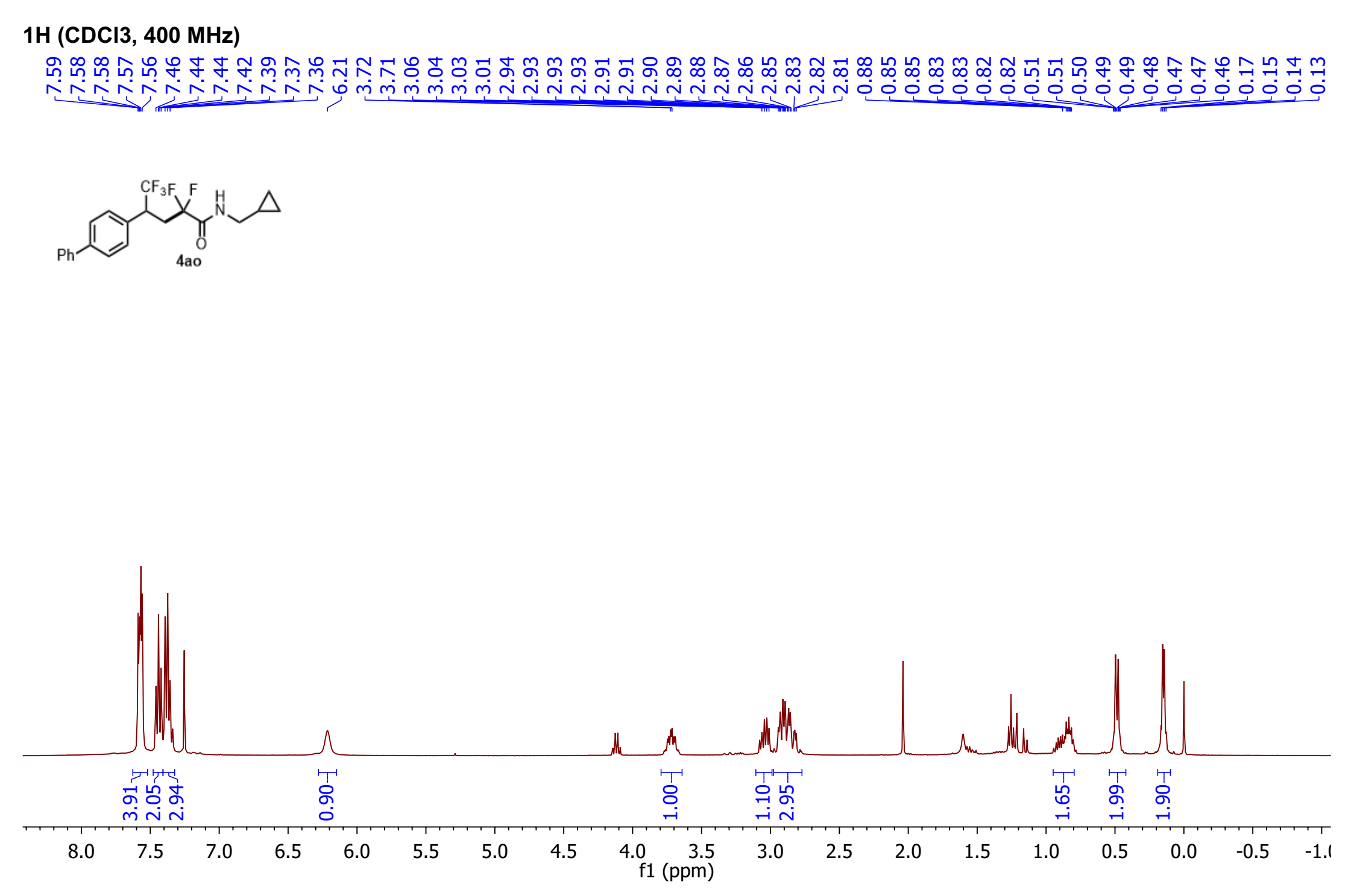
19F (CDCl3, 376 MHz)



4an

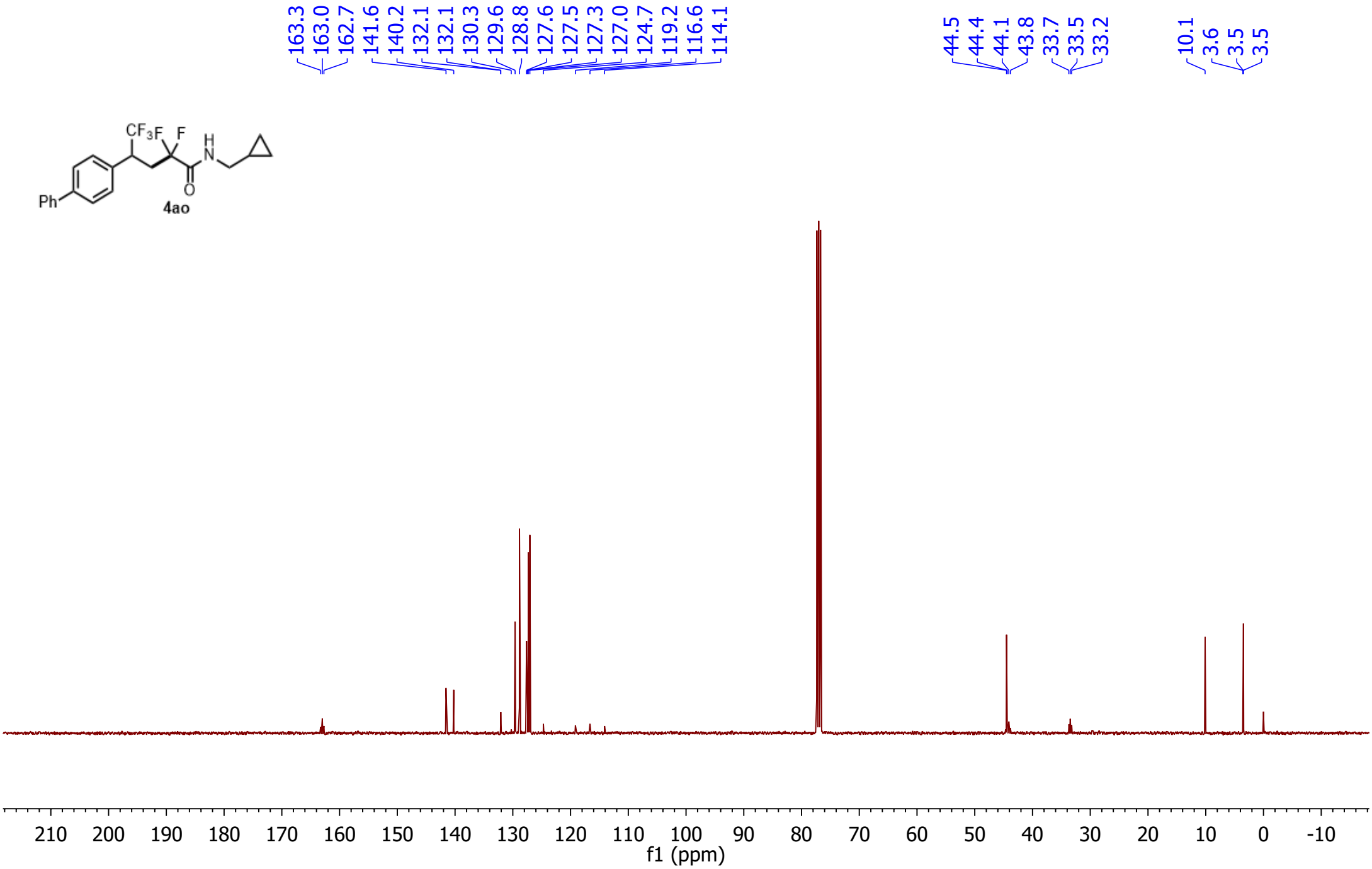
^{19}F NMR Spectrum of **4an**

1H (CDCl3, 400 MHz)



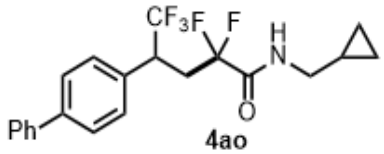
^{1}H NMR Spectrum of **4ao**

13C (CDCl3, 101 MHz)



^{13}C NMR Spectrum of **4ao**

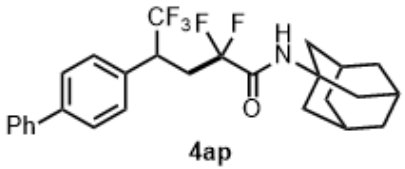
19F (CDCl3, 376 MHz)



4ao

^{19}F NMR Spectrum of **4ao**

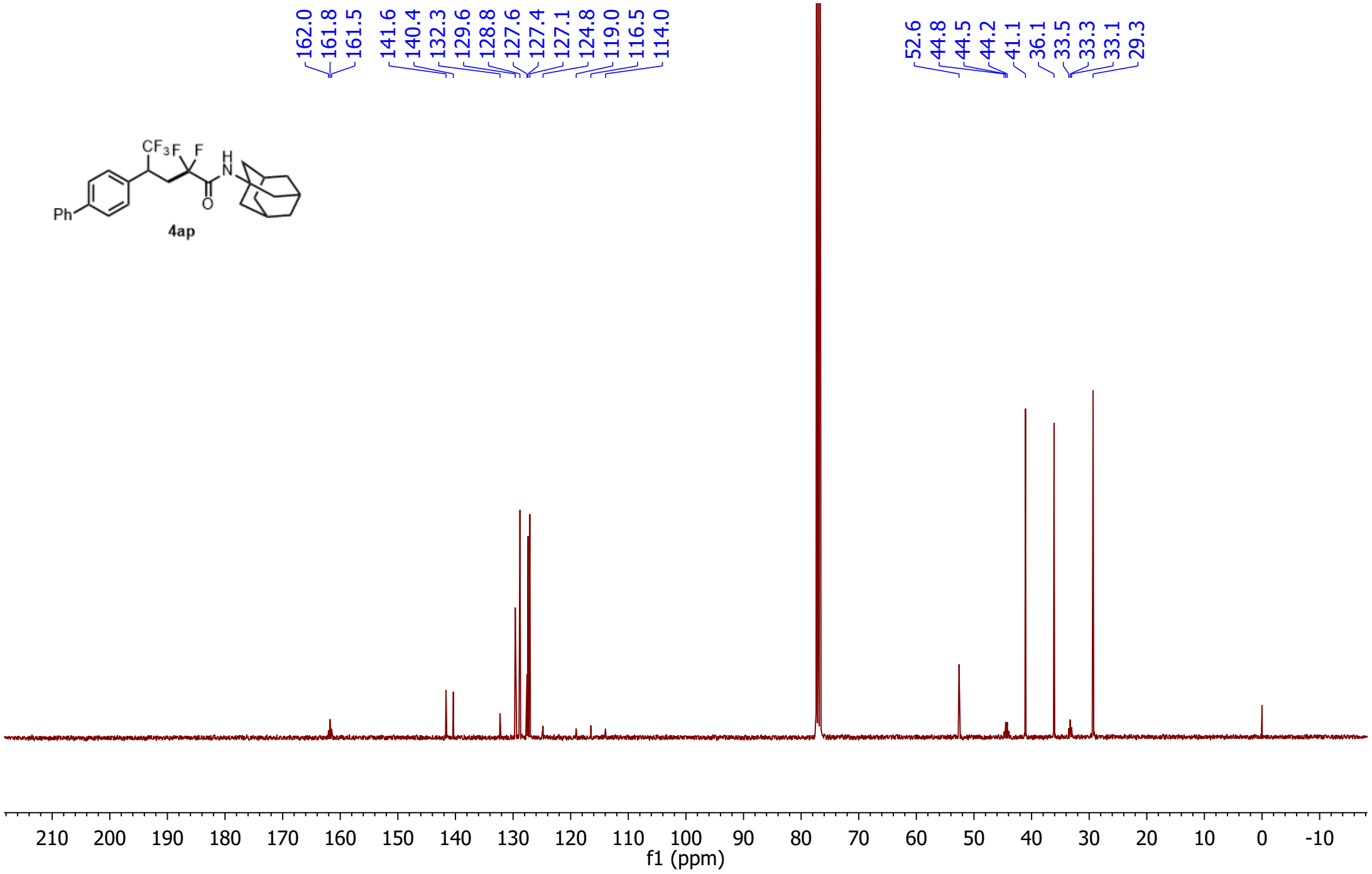
1H (CDCl3, 400 MHz)



4ap

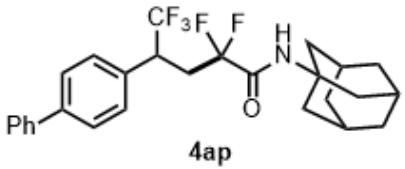
^{1}H NMR Spectrum of **4ap**

13C (CDCl3, 101 MHz)



^{13}C NMR Spectrum of **4ap**

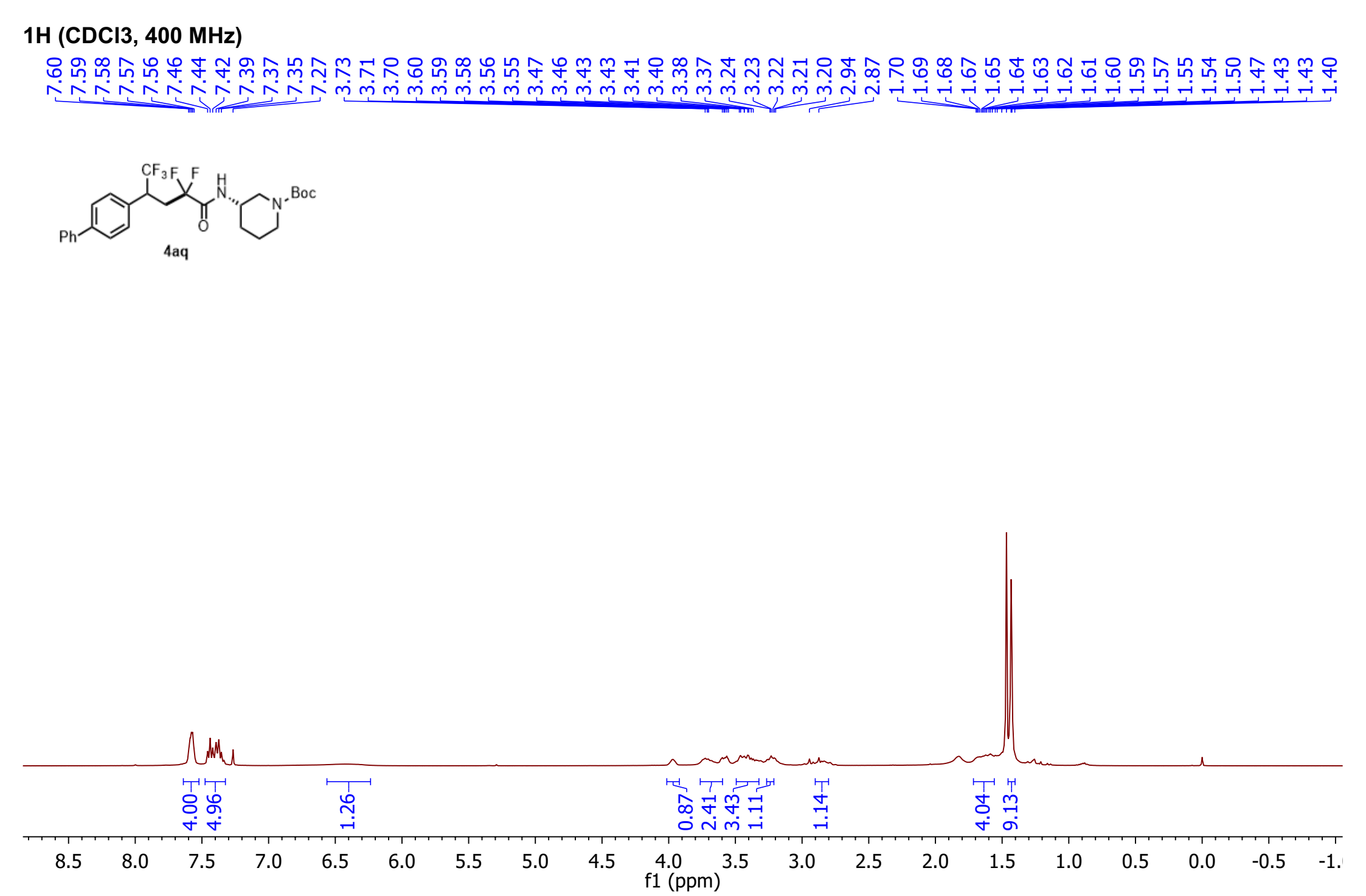
19F (CDCl3, 376 MHz)



4ap

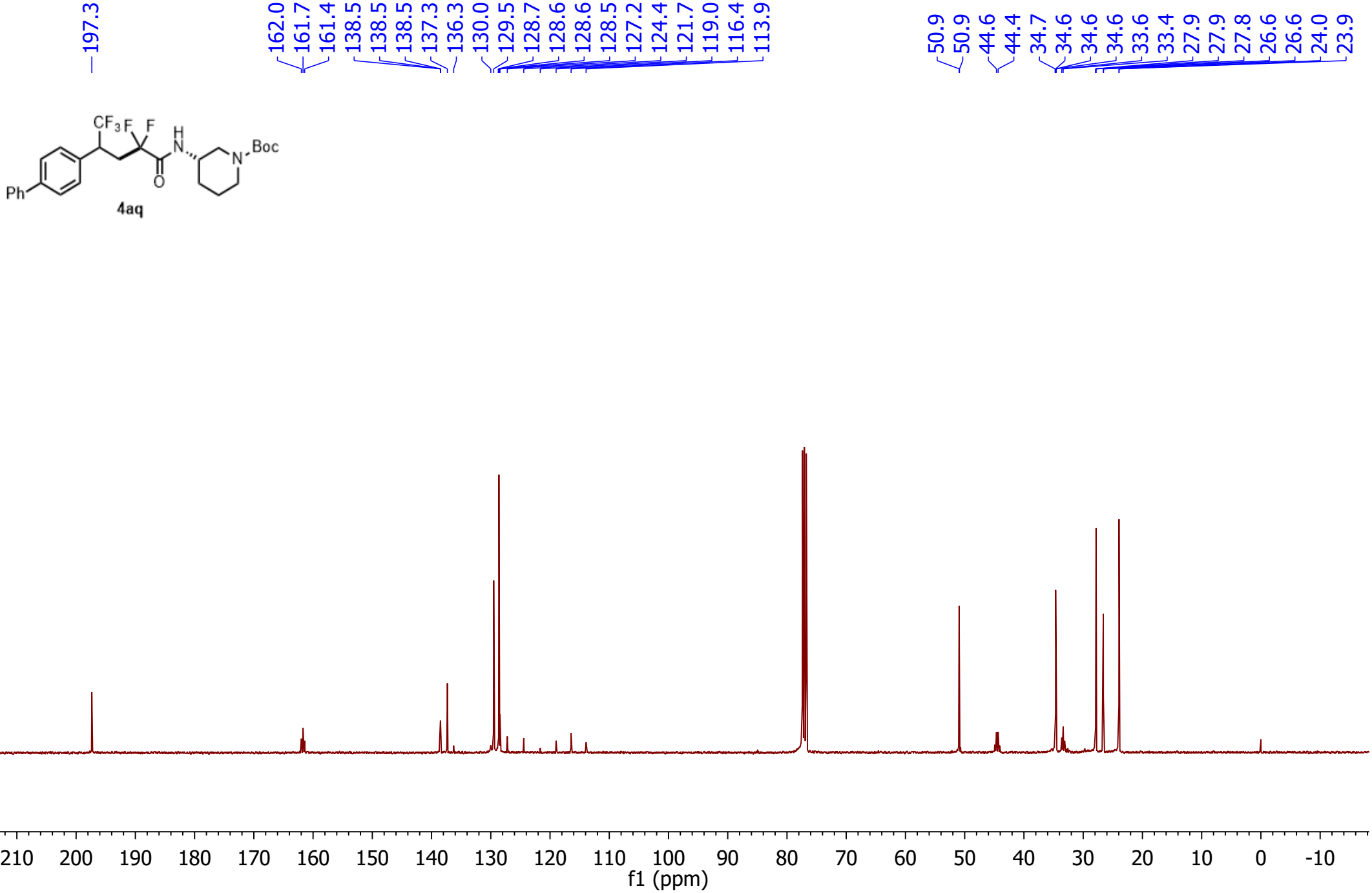
^{19}F NMR Spectrum of **4ap**

1H (CDCl3, 400 MHz)



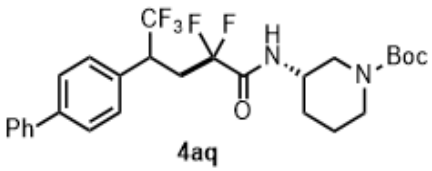
^{1}H NMR Spectrum of **4aq**

13C (CDCl3, 101 MHz)



^{13}C NMR Spectrum of **4aq**

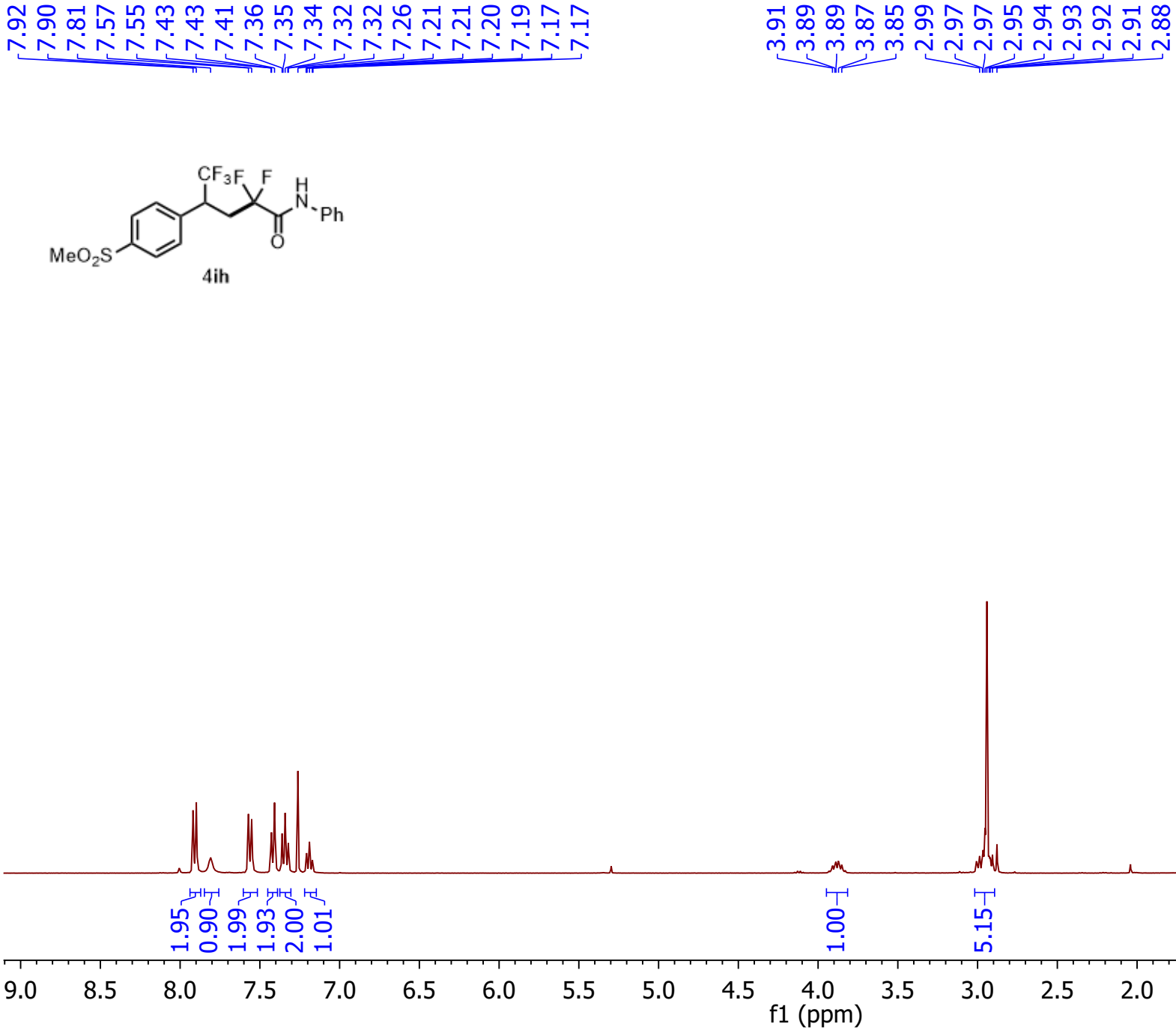
19F (CDCl3, 376 MHz)



4aq

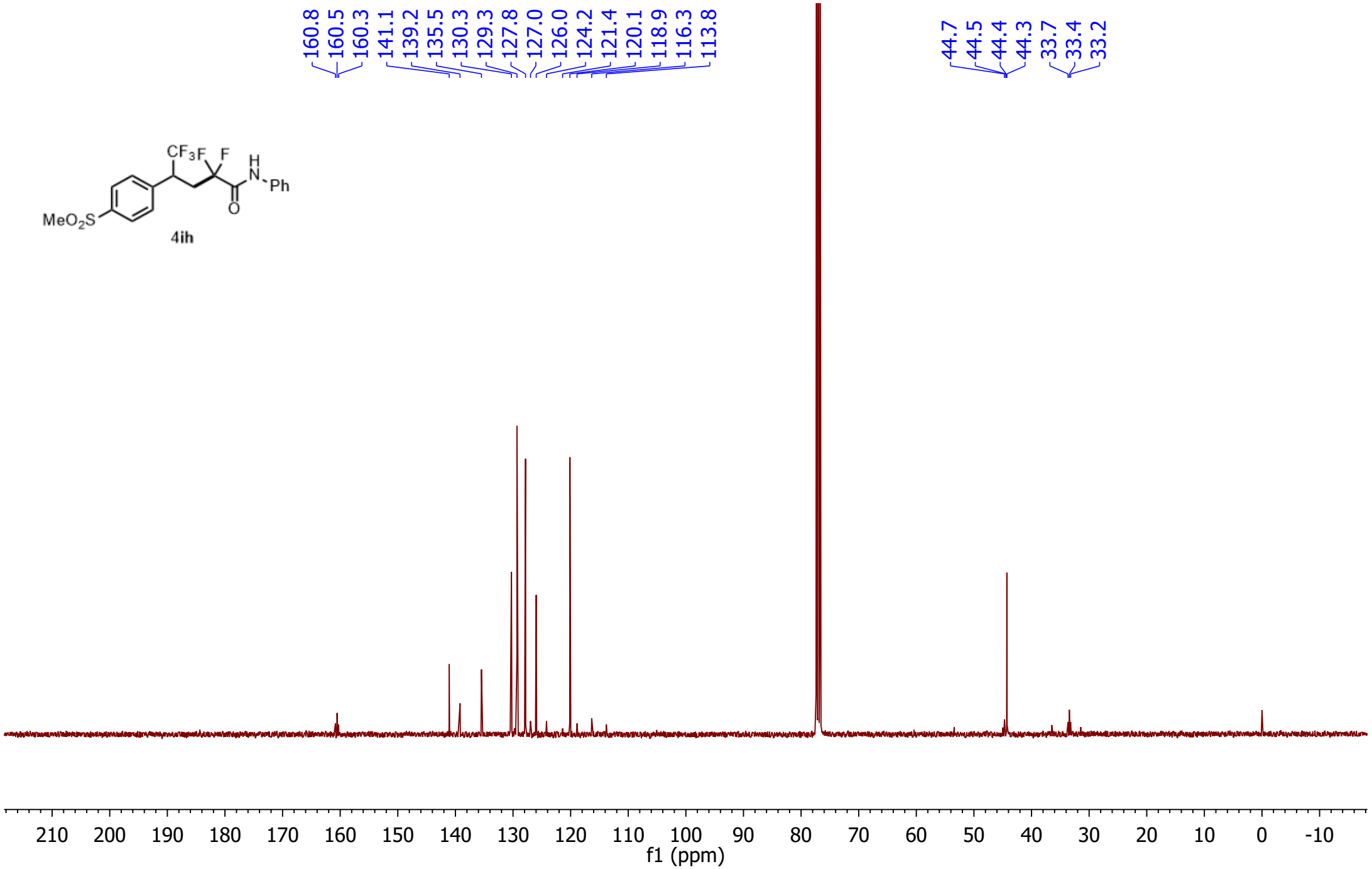
^{19}F NMR Spectrum of **4aq**

1H (CDCl3, 400 MHz)



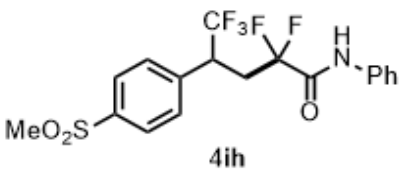
^{1}H NMR Spectrum of **4ih**

13C (CDCl3, 101 MHz)



^{13}C NMR Spectrum of **4ih**

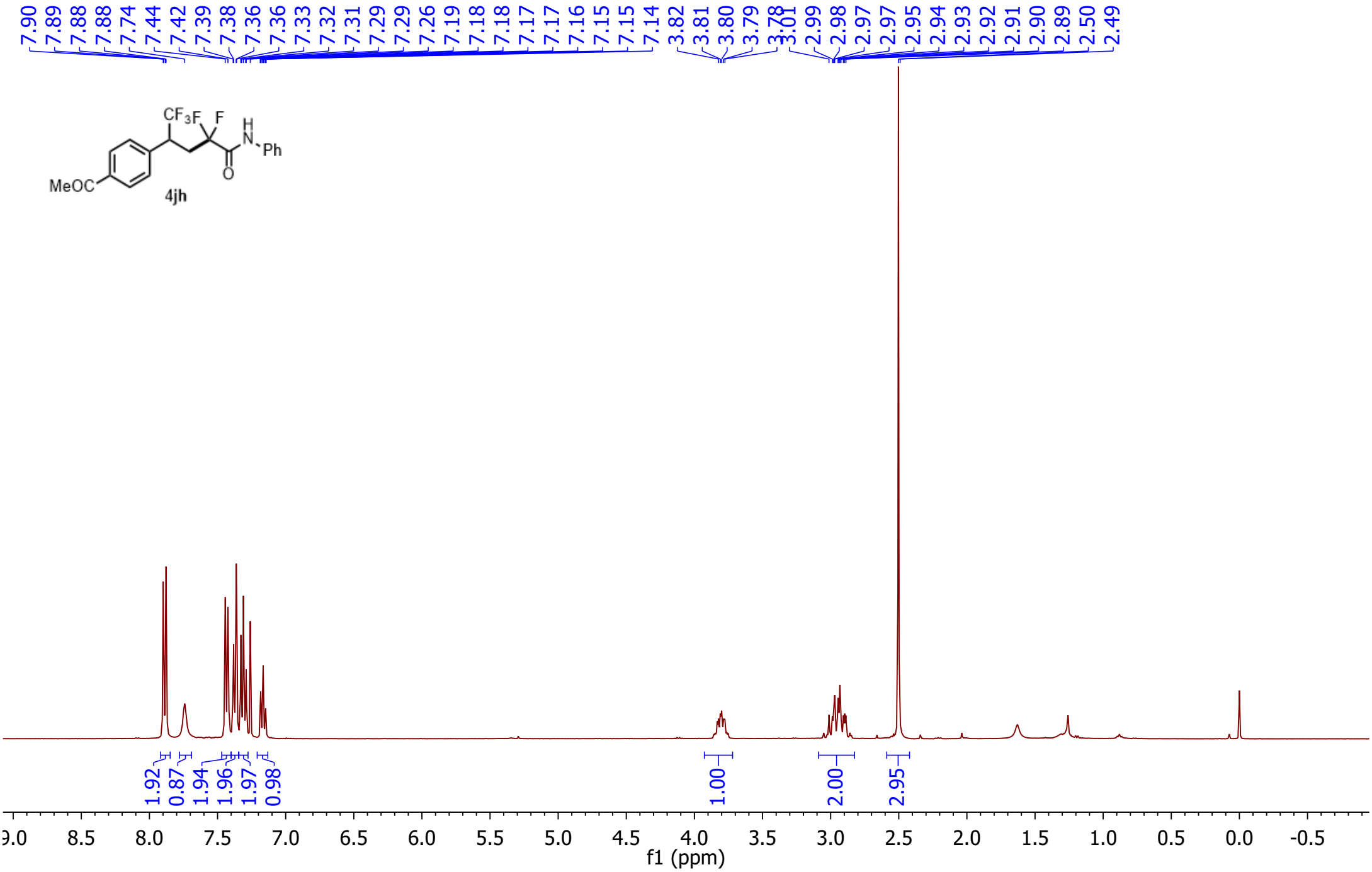
19F (CDCl3, 376 MHz)



4ih

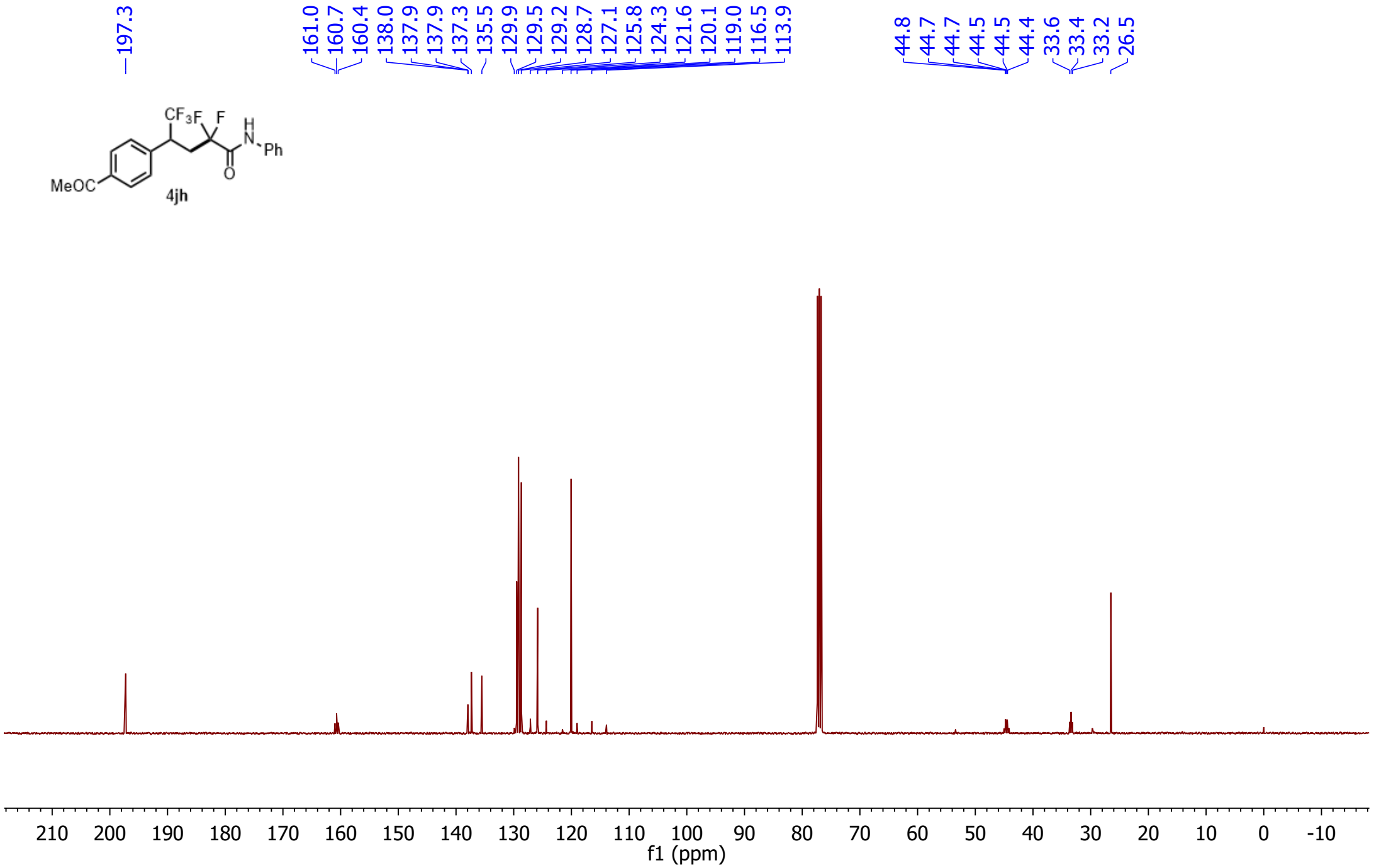
^{19}F NMR Spectrum of **4ih**

1H (CDCl3, 400 MHz)



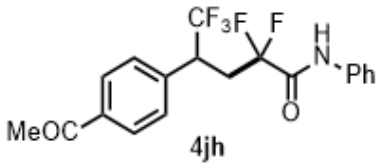
^{1}H NMR Spectrum of **4jh**

13C (CDCl3, 101 MHz)



^{13}C NMR Spectrum of **4jh**

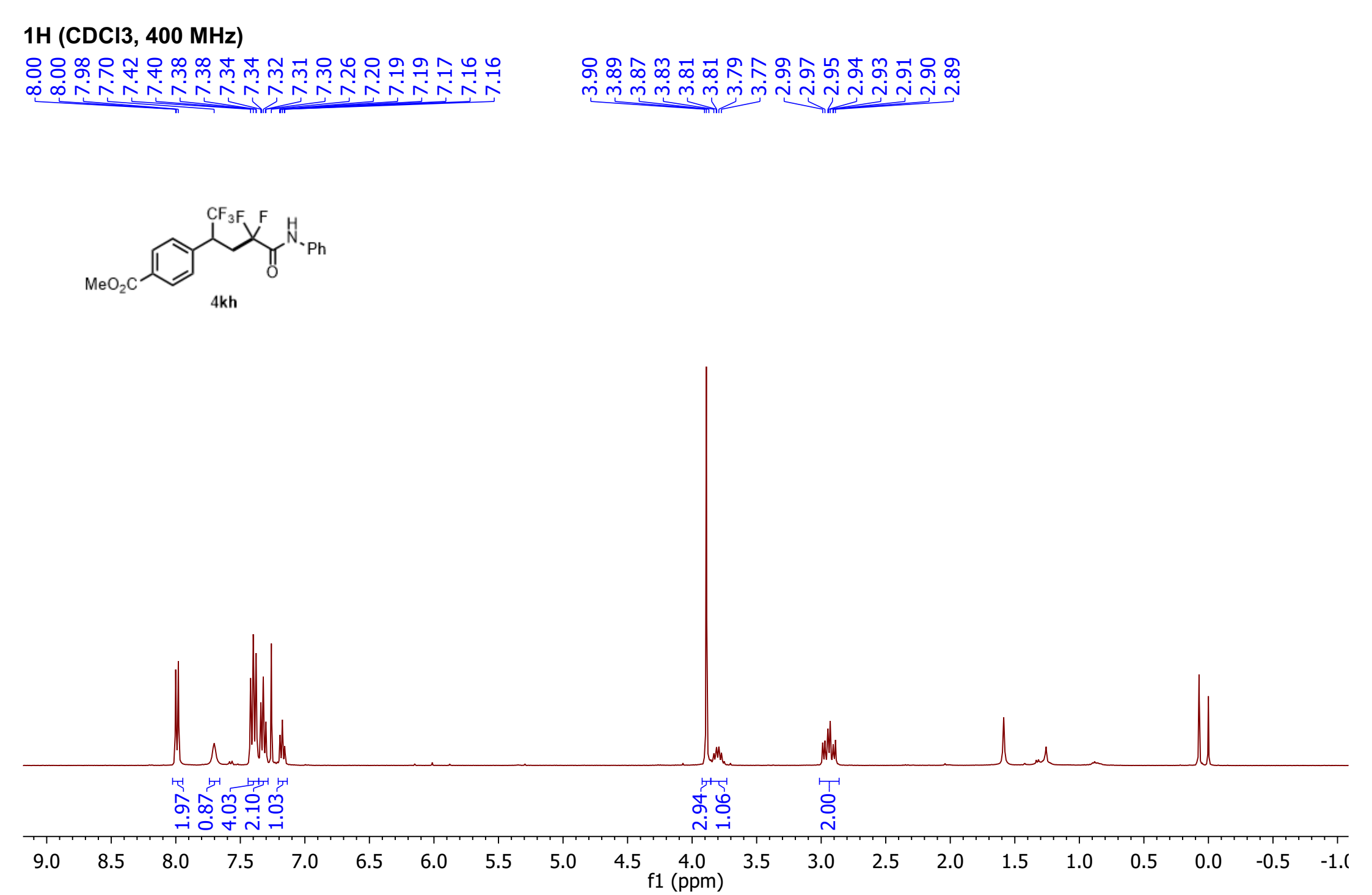
19F (CDCl3, 376 MHz)



4jh

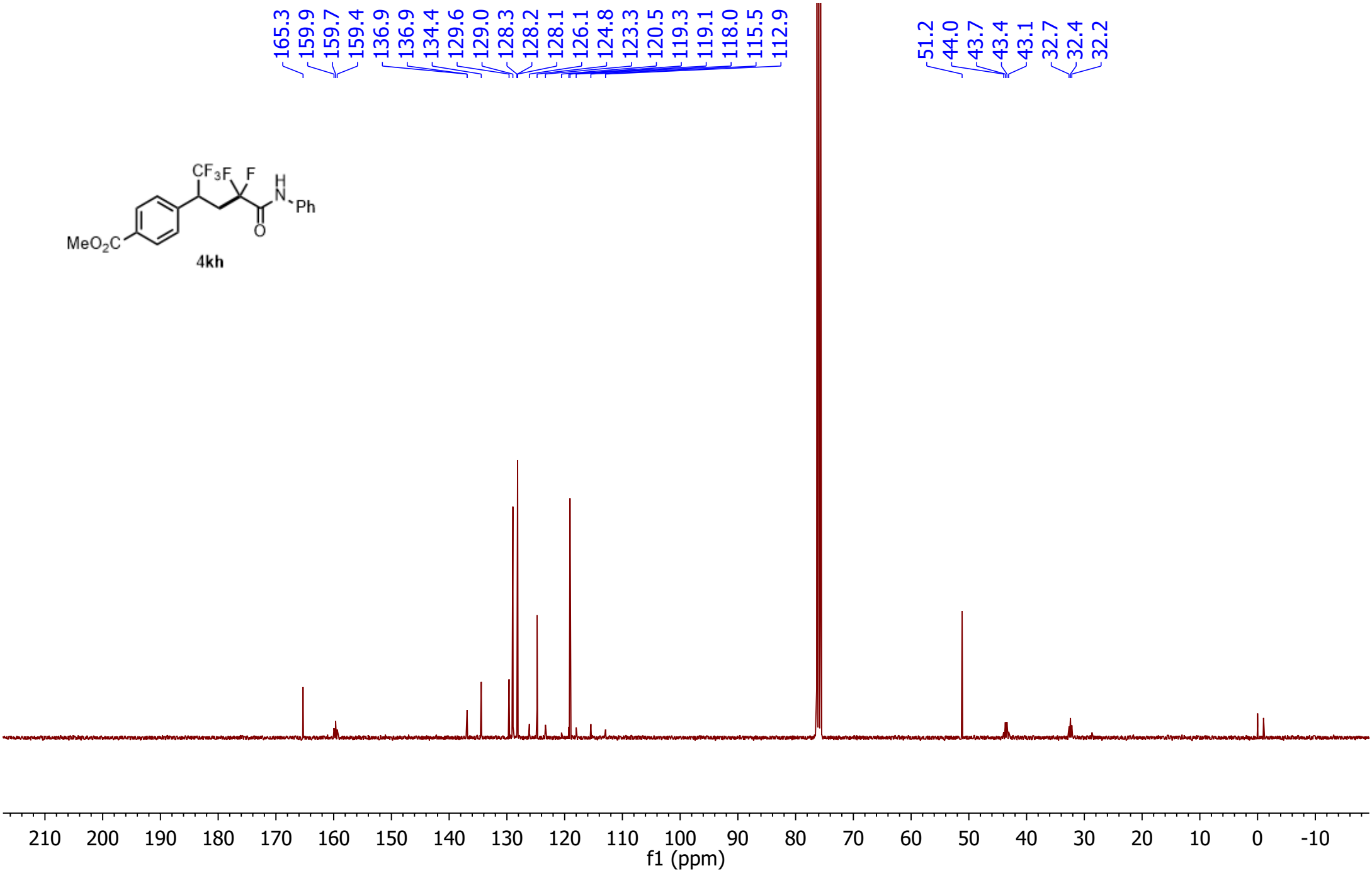
^{19}F NMR Spectrum of **4jh**

1H (CDCl3, 400 MHz)



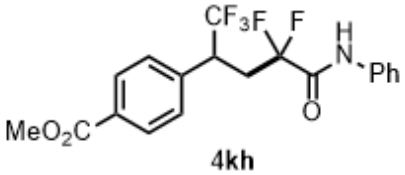
^{1}H NMR Spectrum of **4kh**

13C (CDCl3, 101 MHz)



^{13}C NMR Spectrum of **4kh**

19F (CDCl3, 376 MHz)

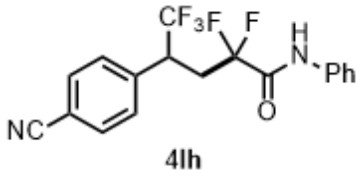


4kh

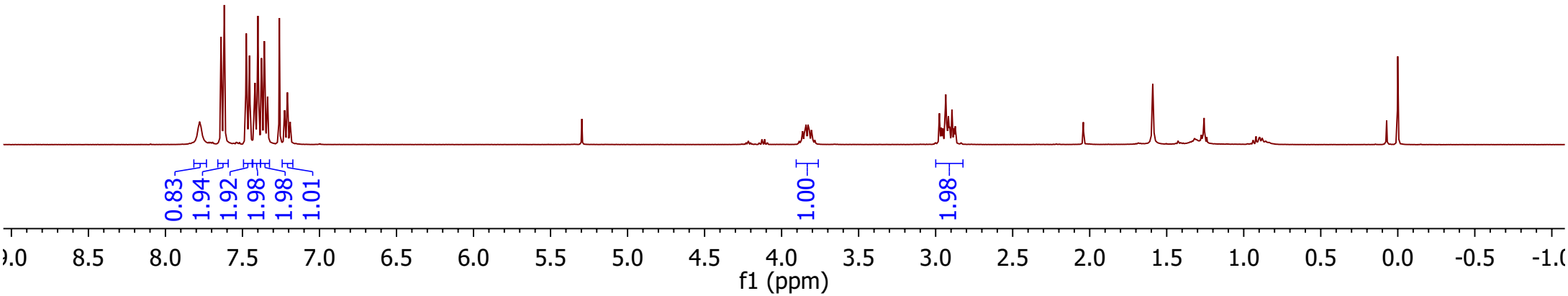
^{19}F NMR Spectrum of **4kh**

1H (CDCl3, 400 MHz)

7.78 7.64 7.63 7.62 7.62 7.48 7.45 7.42 7.42 7.41 7.40 7.40 7.39 7.38 7.37 7.36 7.35 7.34 7.34 7.26 7.23 7.23 7.22 7.21 7.21 7.20 7.19 7.19 7.19 3.86 3.85 3.84 3.83 3.82 3.82 3.81 2.98 2.96 2.95 2.94 2.93 2.93 2.92 2.91 2.89 2.88 2.87

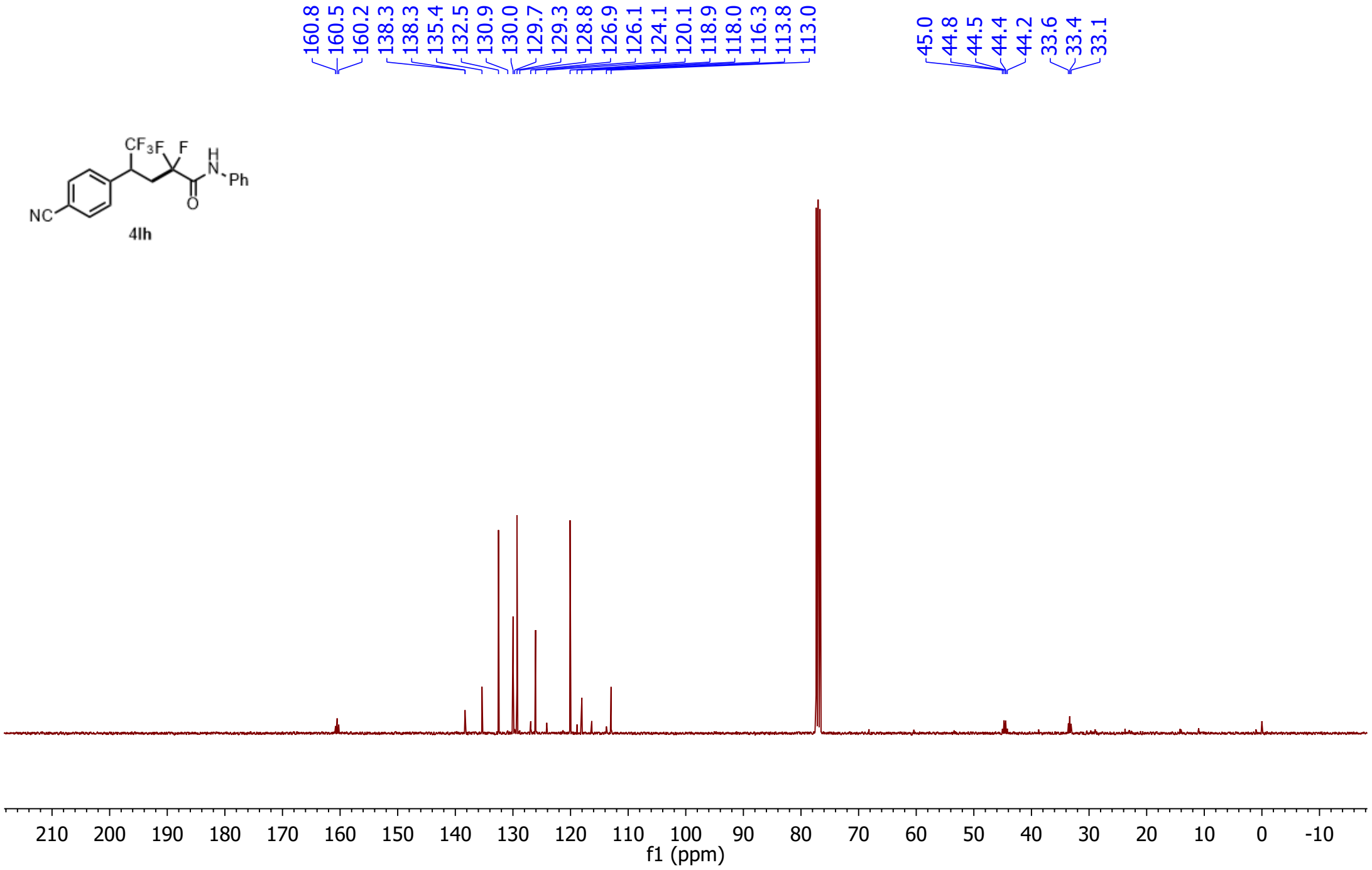


4lh



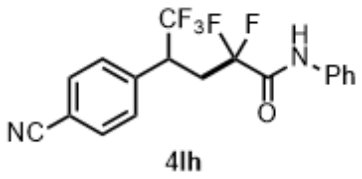
^{1}H NMR Spectrum of **4lh**

13C (CDCl3, 101 MHz)



^{13}C NMR Spectrum of **4lh**

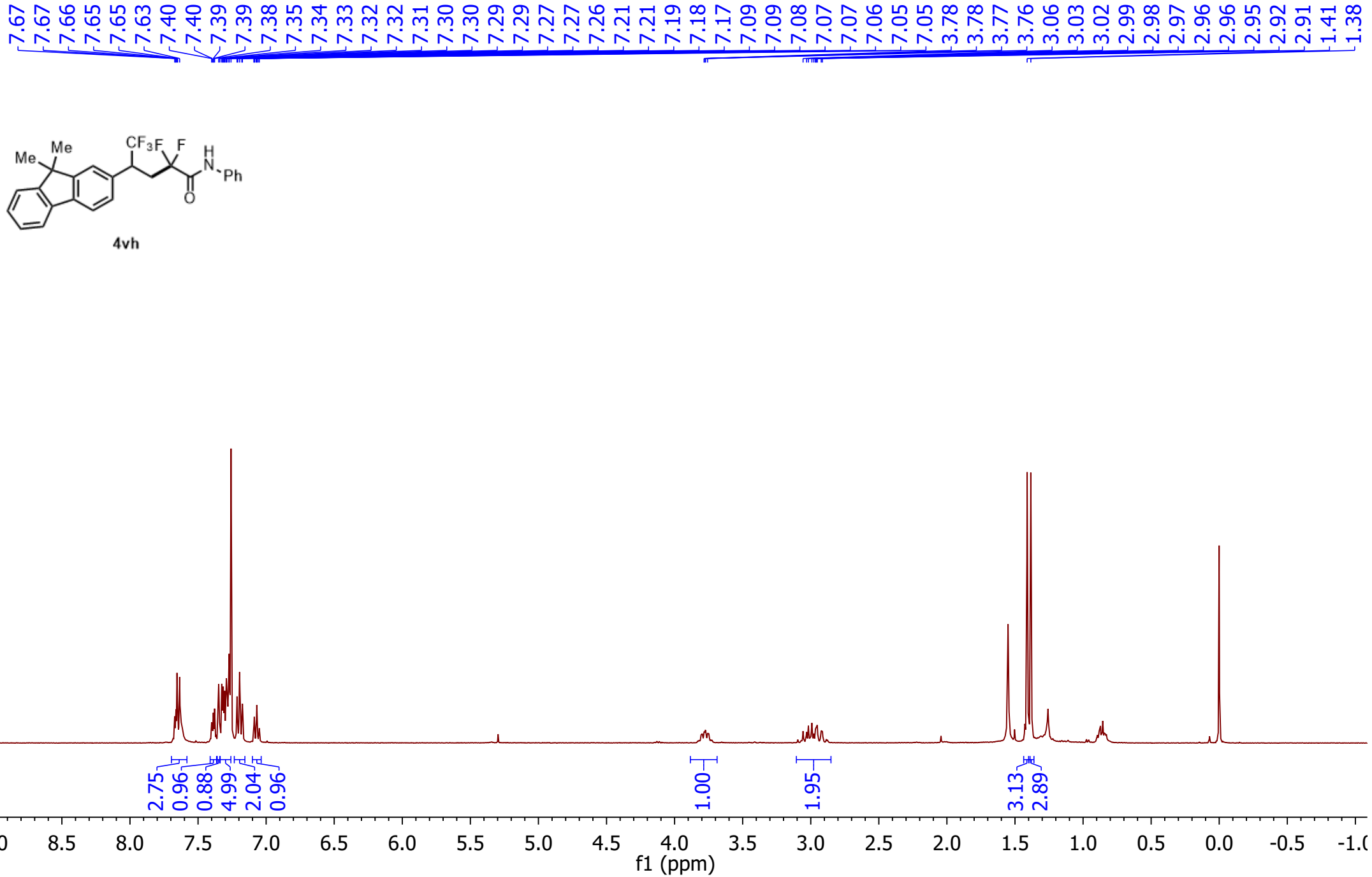
19F (CDCl3, 376 MHz)



4llh

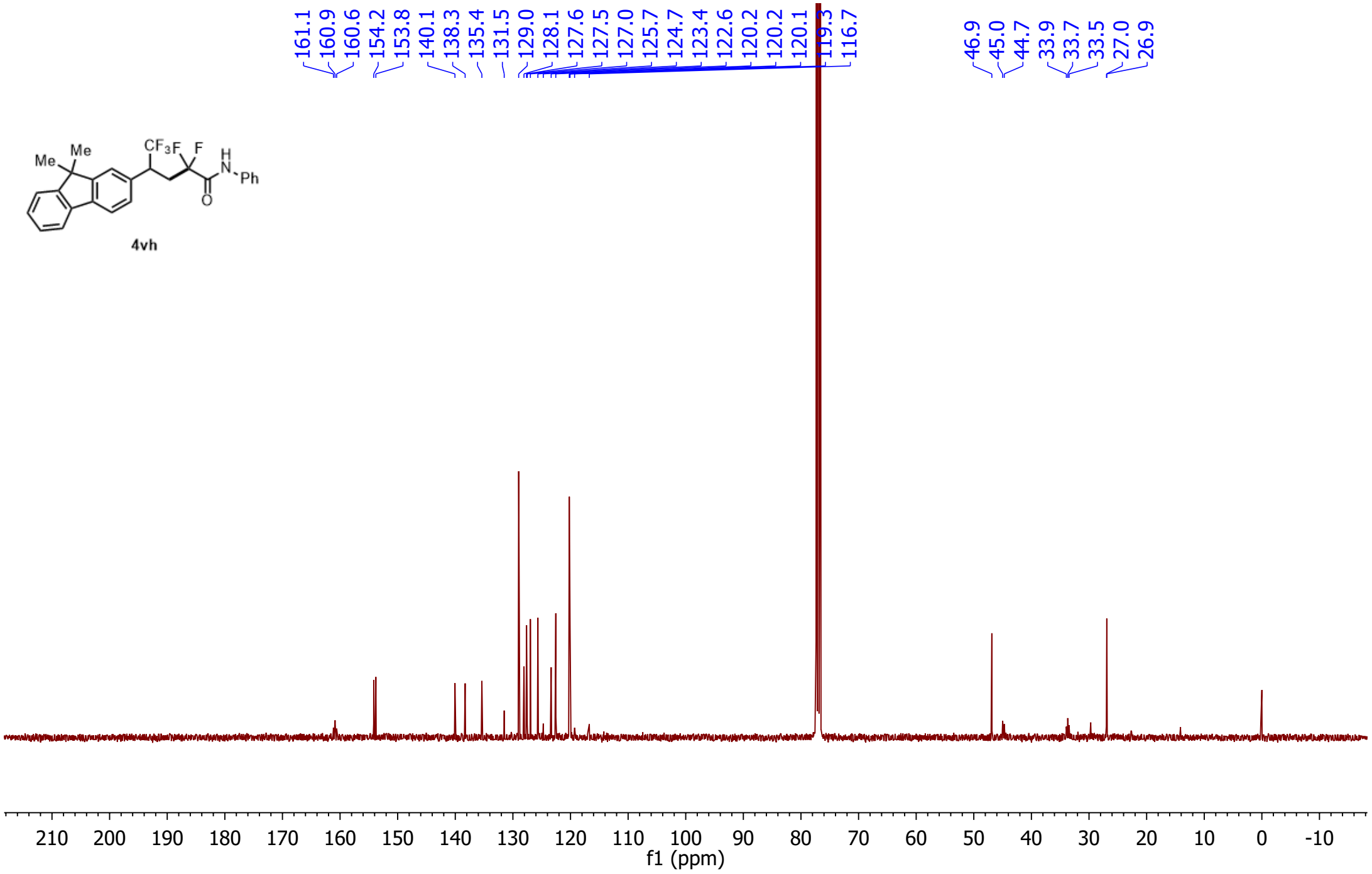
^{19}F NMR Spectrum of **4llh**

1H (CDCl3, 400 MHz)



^{1}H NMR Spectrum of **4vh**

13C (CDCl3, 101 MHz)

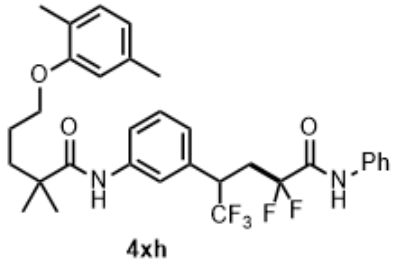


^{13}C NMR Spectrum of **4vh**

19F (CDCl3, 376 MHz)

^{19}F NMR Spectrum of **4vh**

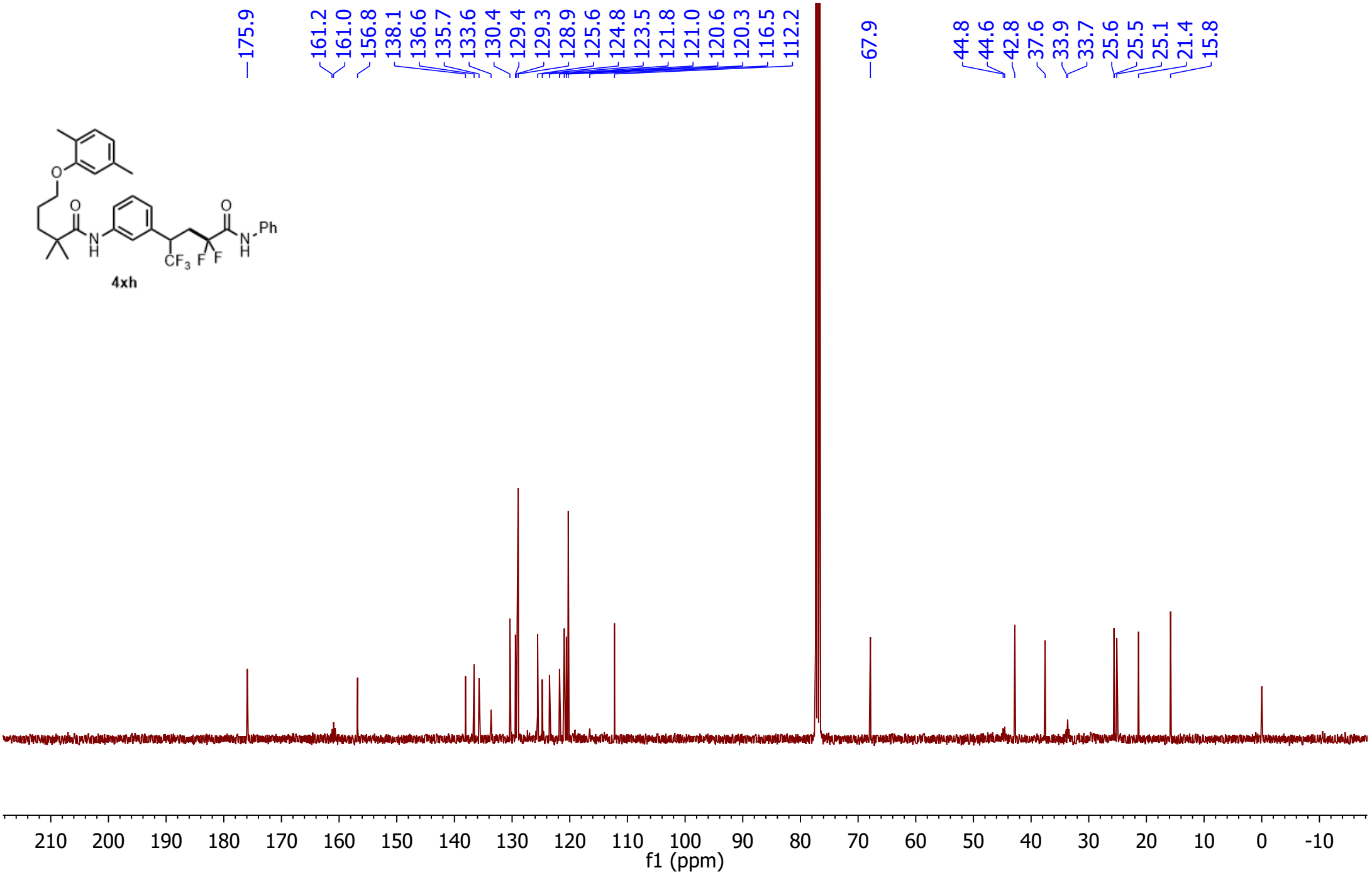
1H (CDCl3, 400 MHz)



4xh

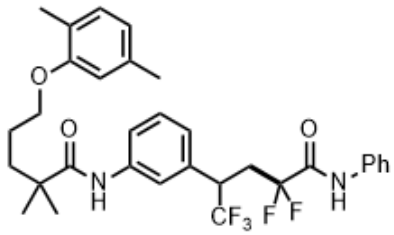
^{1}H NMR Spectrum of **4xh**

13C (CDCl3, 101 MHz)



^{13}C NMR Spectrum of **4xh**

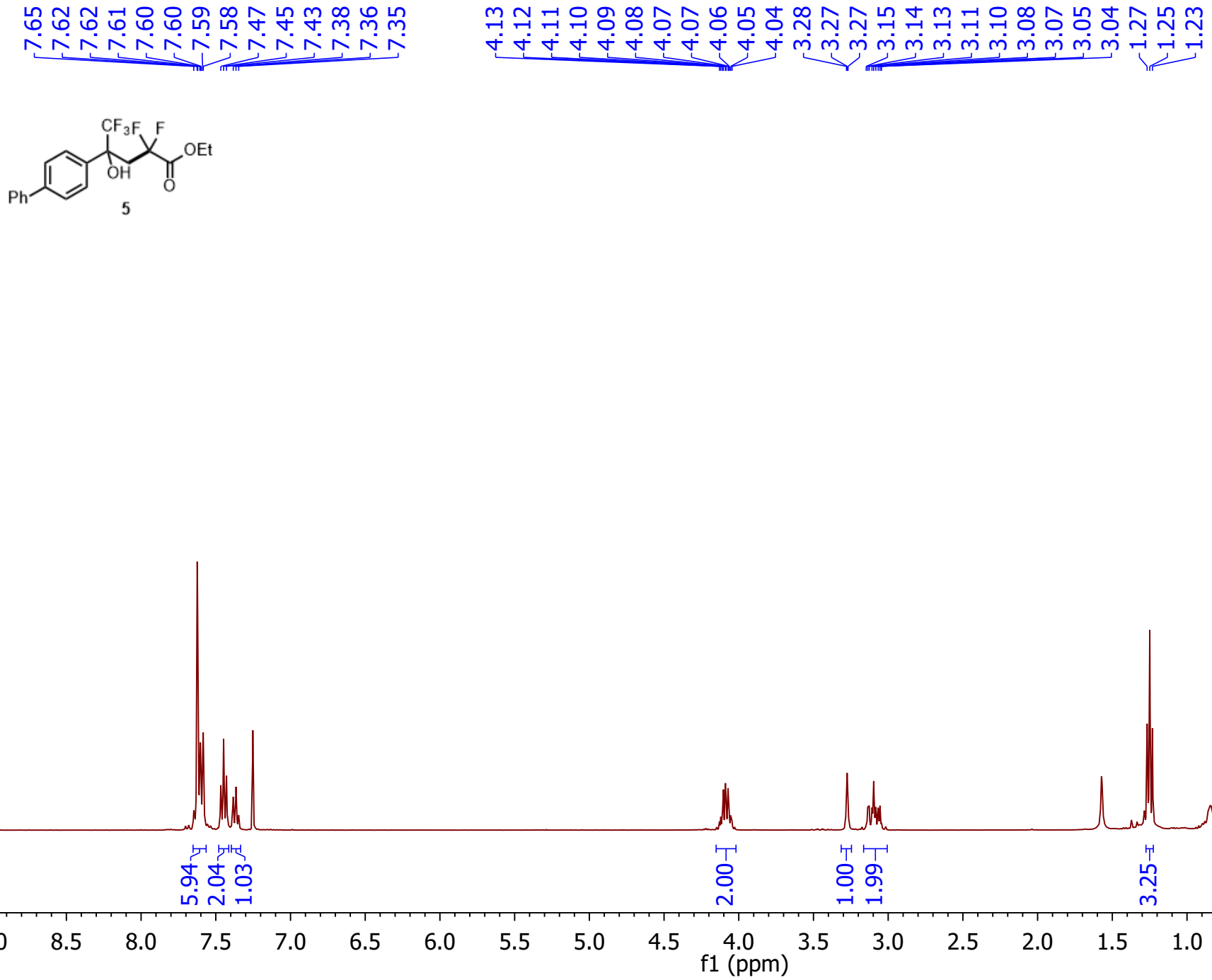
19F (CDCl3, 376 MHz)



4xh

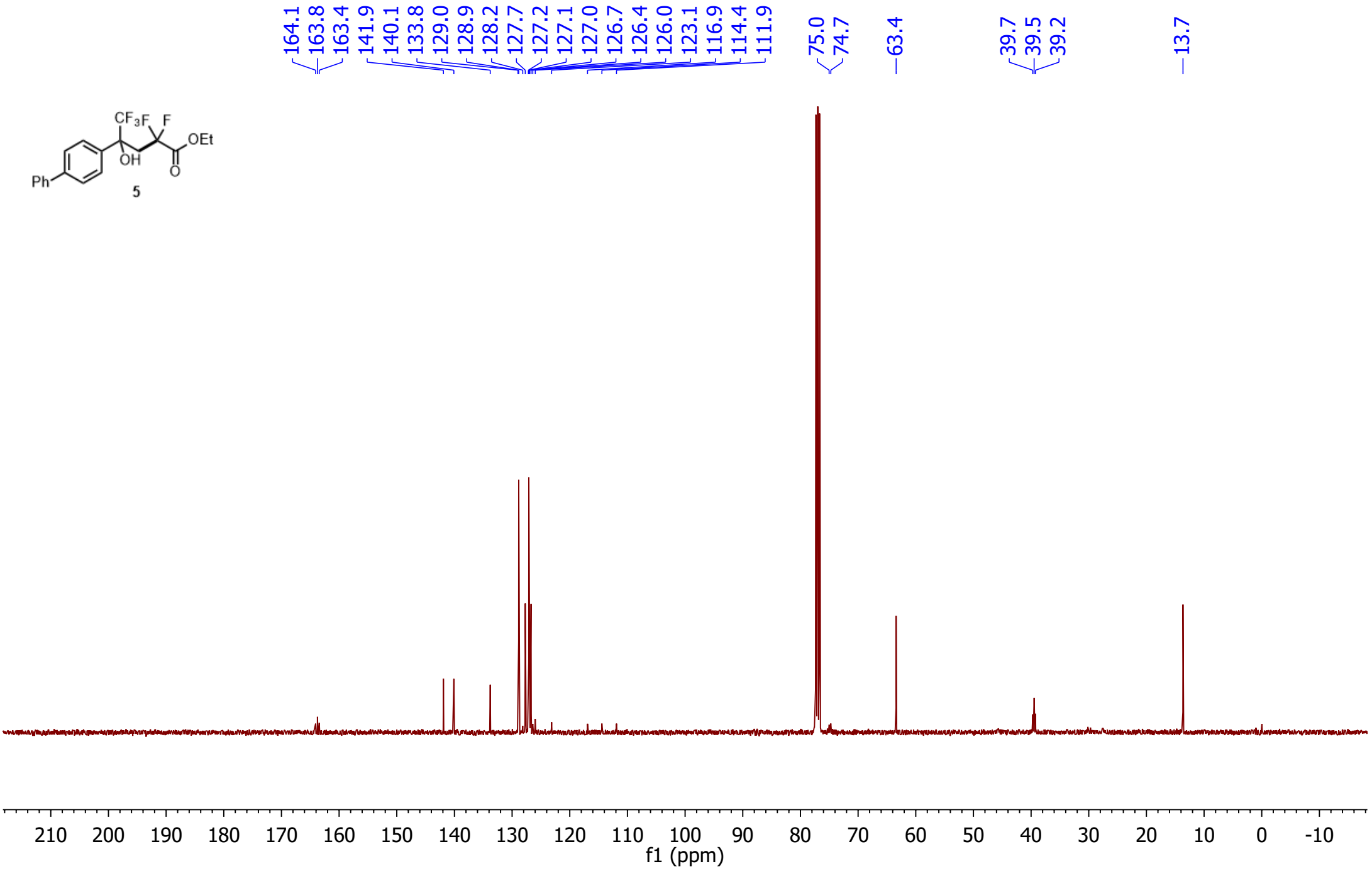
^{19}F NMR Spectrum of **4xh**

1H (CDCl3, 400 MHz)



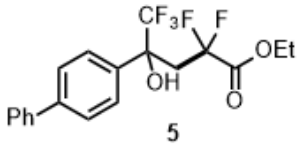
^{1}H NMR Spectrum of **5**

13C (CDCl3, 101 MHz)



^{13}C NMR Spectrum of **5**

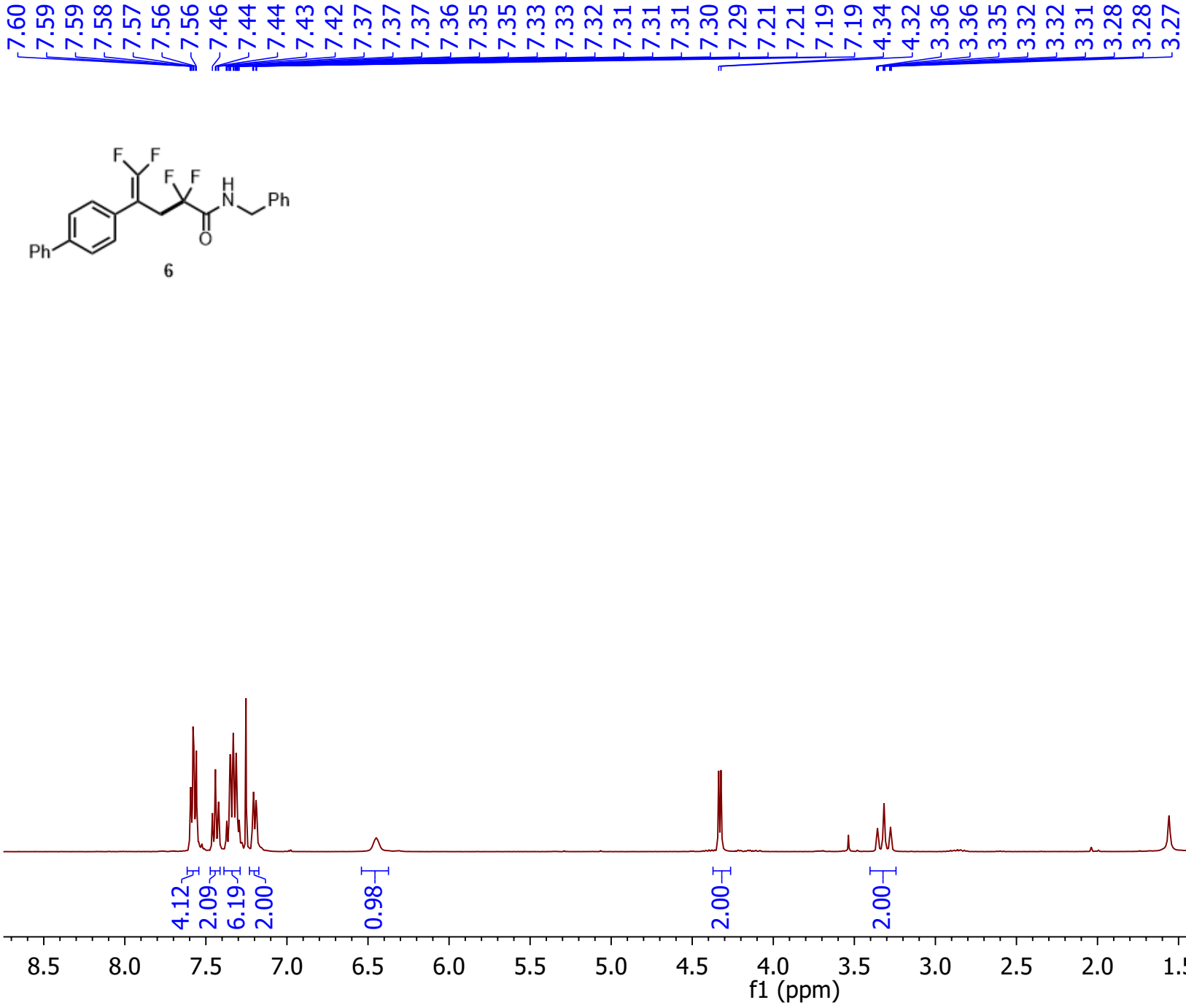
19F (CDCl3, 376 MHz)



5

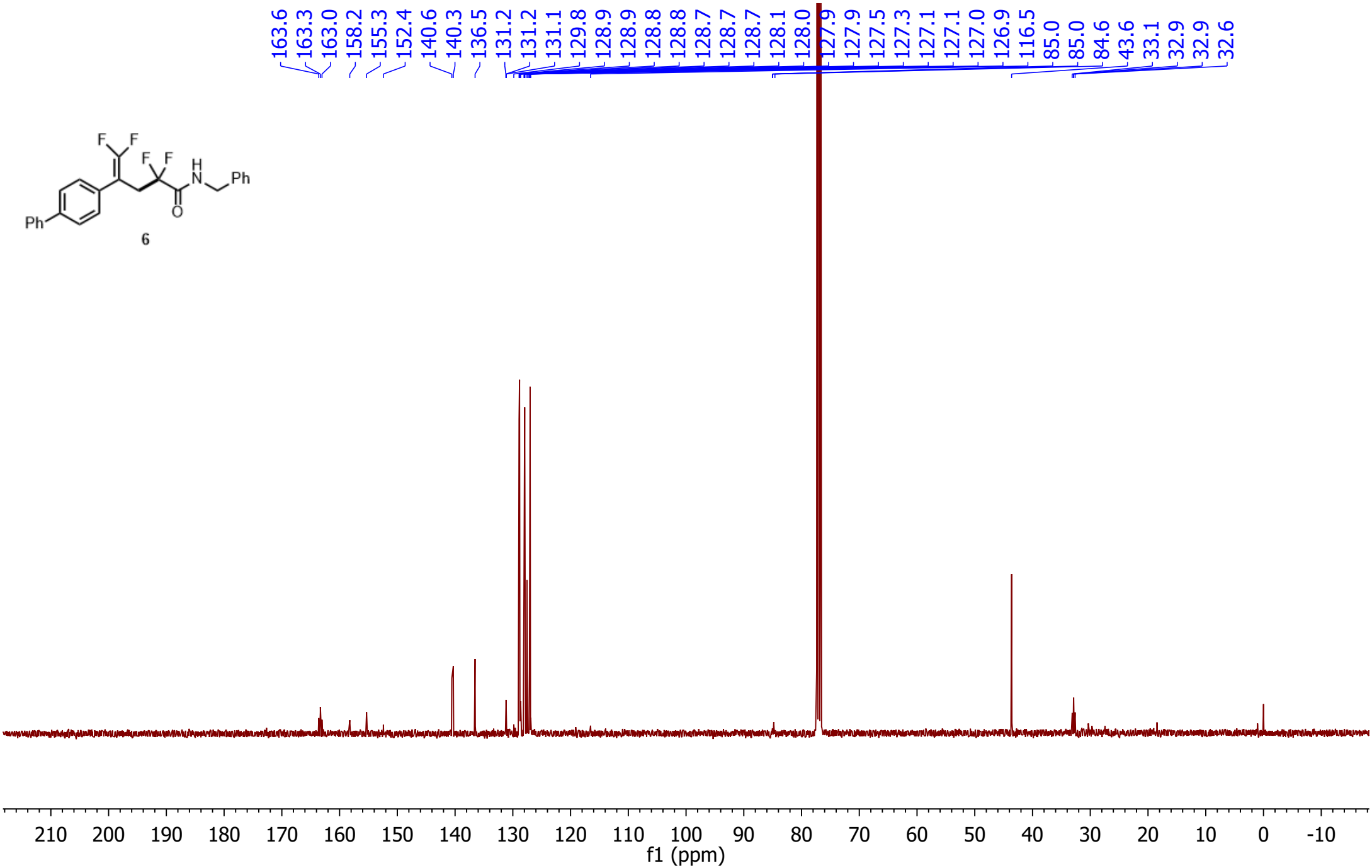
^{19}F NMR Spectrum of **5**

1H (CDCl3, 400 MHz)



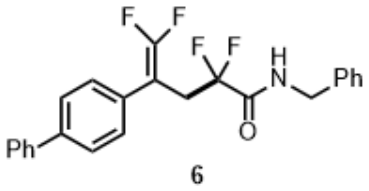
^{1}H NMR Spectrum of **6**

13C (CDCl3, 101 MHz)



^{13}C NMR Spectrum of **6**

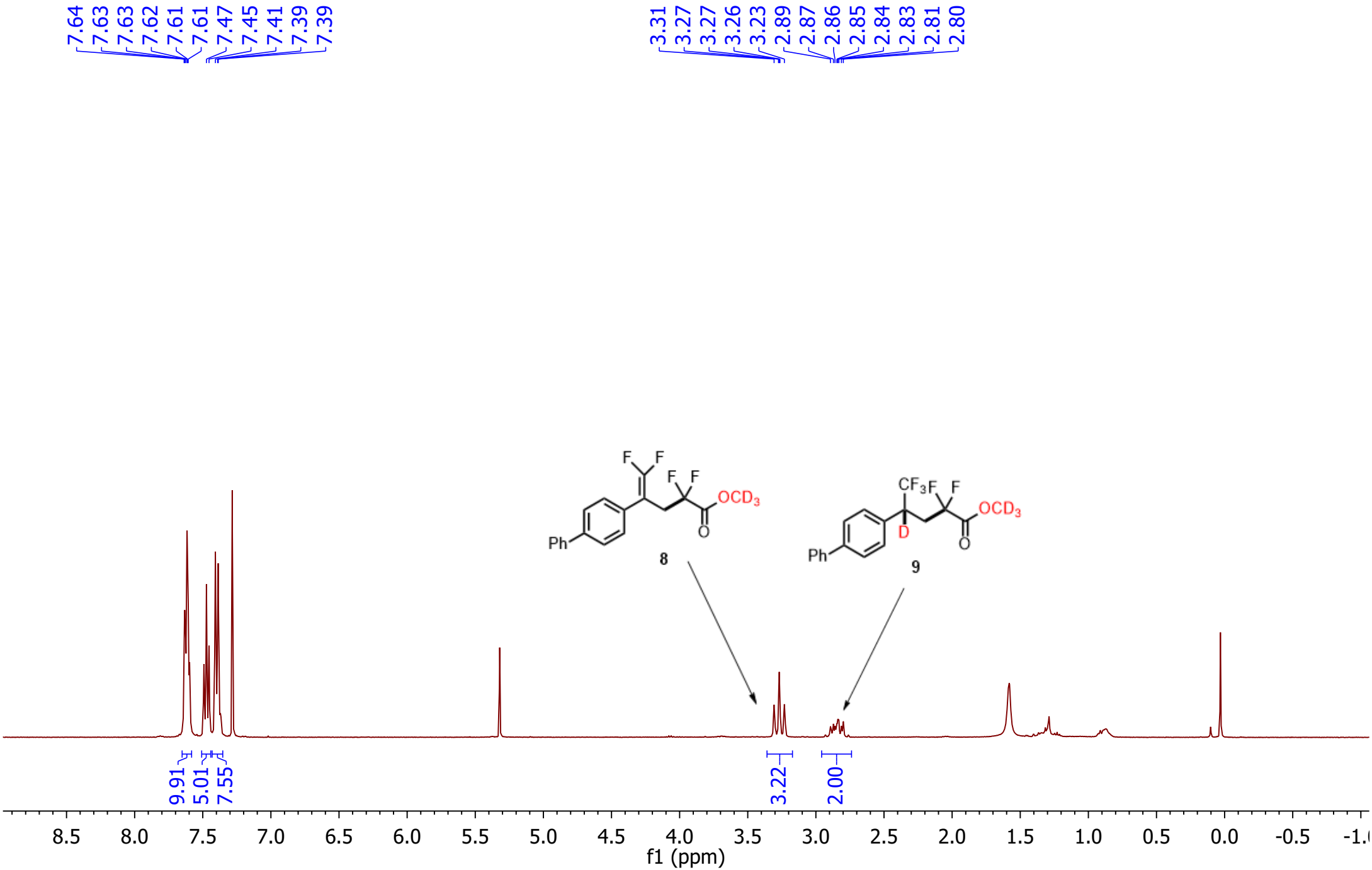
19F (CDCl3, 376 MHz)



6

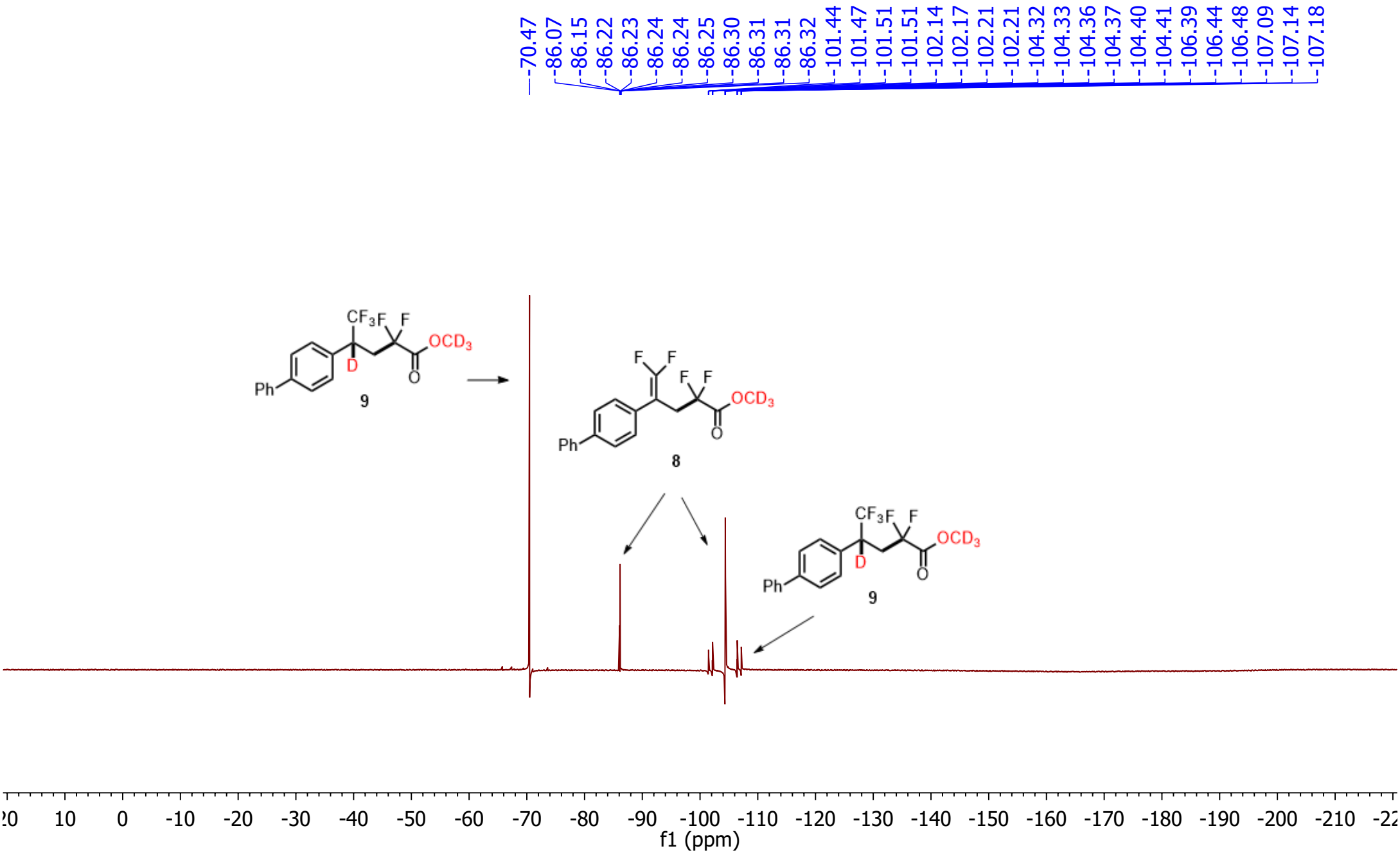
^{19}F NMR Spectrum of **6**

1H (CDCl3, 400 MHz)

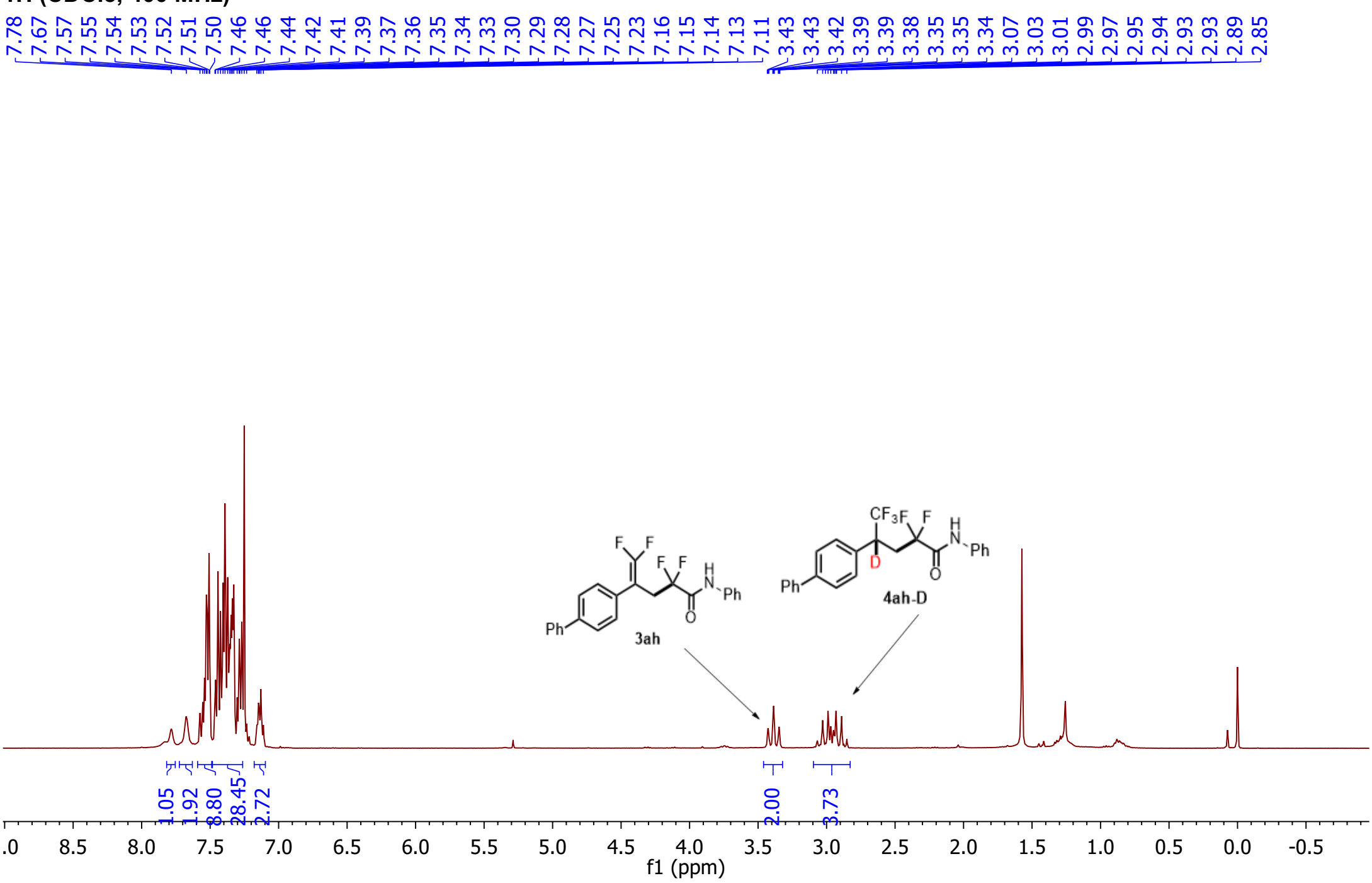


^{1}H NMR Spectrum of **8+9**

19F (CDCl3, 376 MHz)

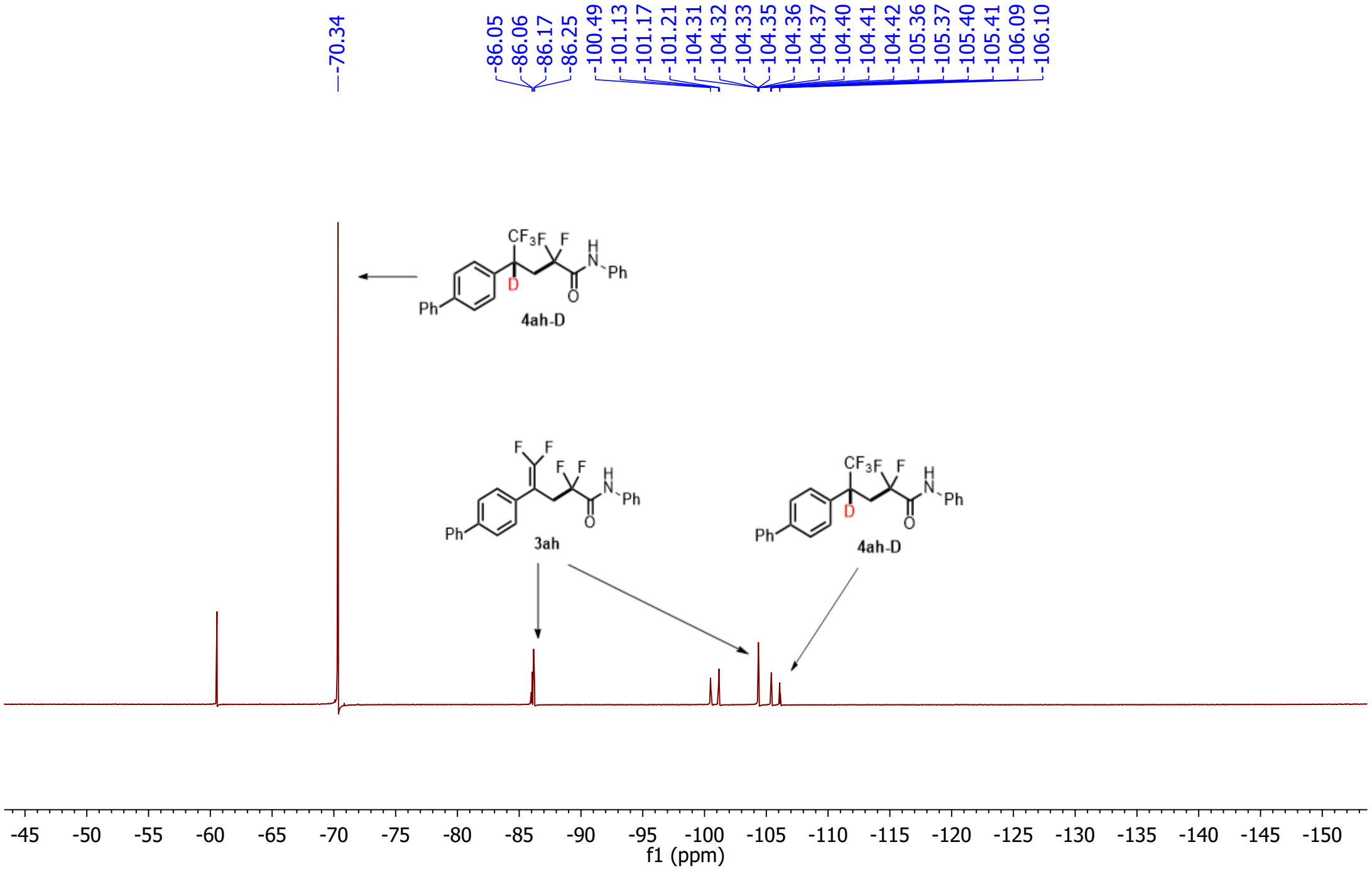


^{19}F NMR Spectrum of **8+9**



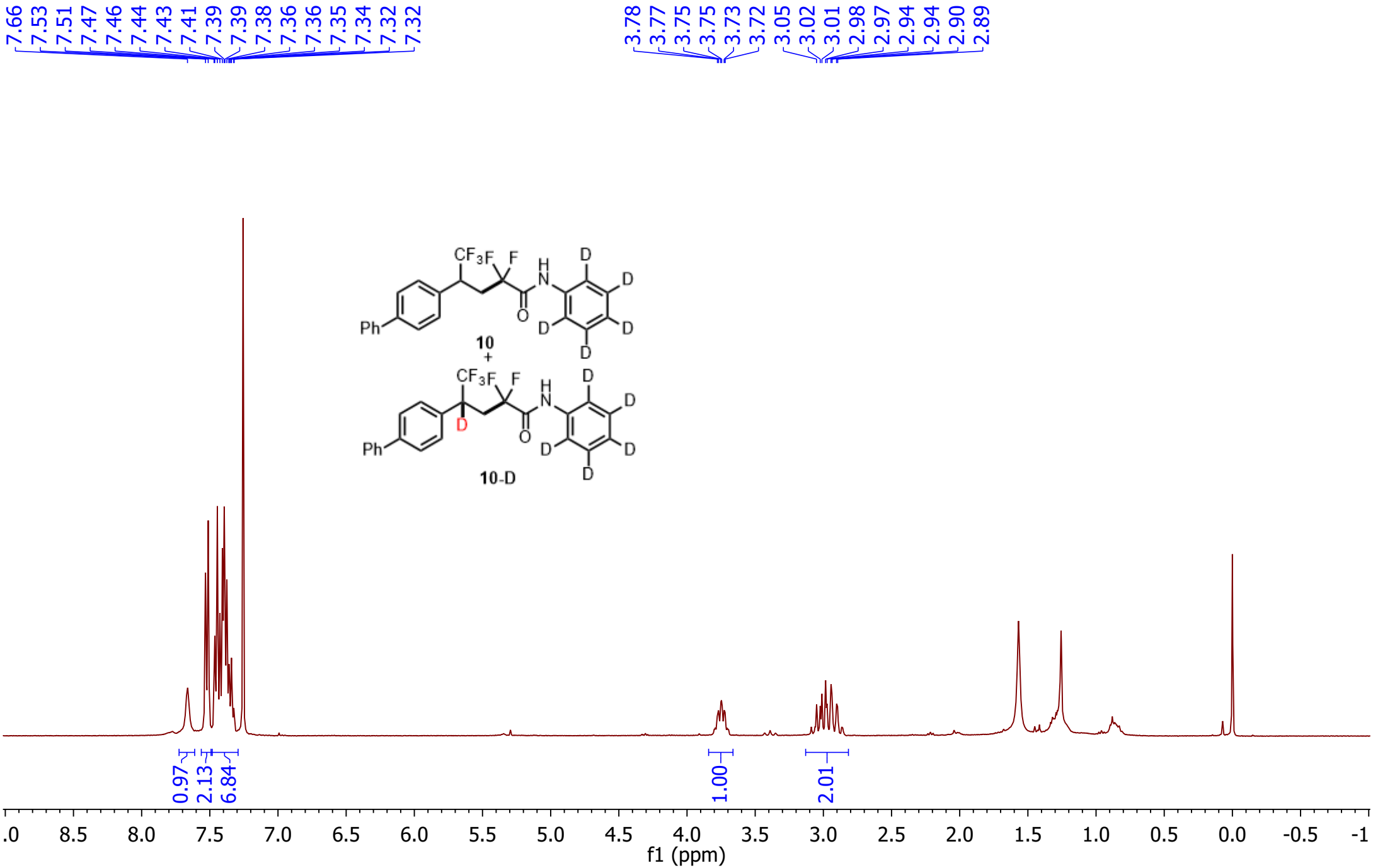
^{1}H NMR Spectrum of **3ah+4ah-D**

19F (CDCl3, 376 MHz)



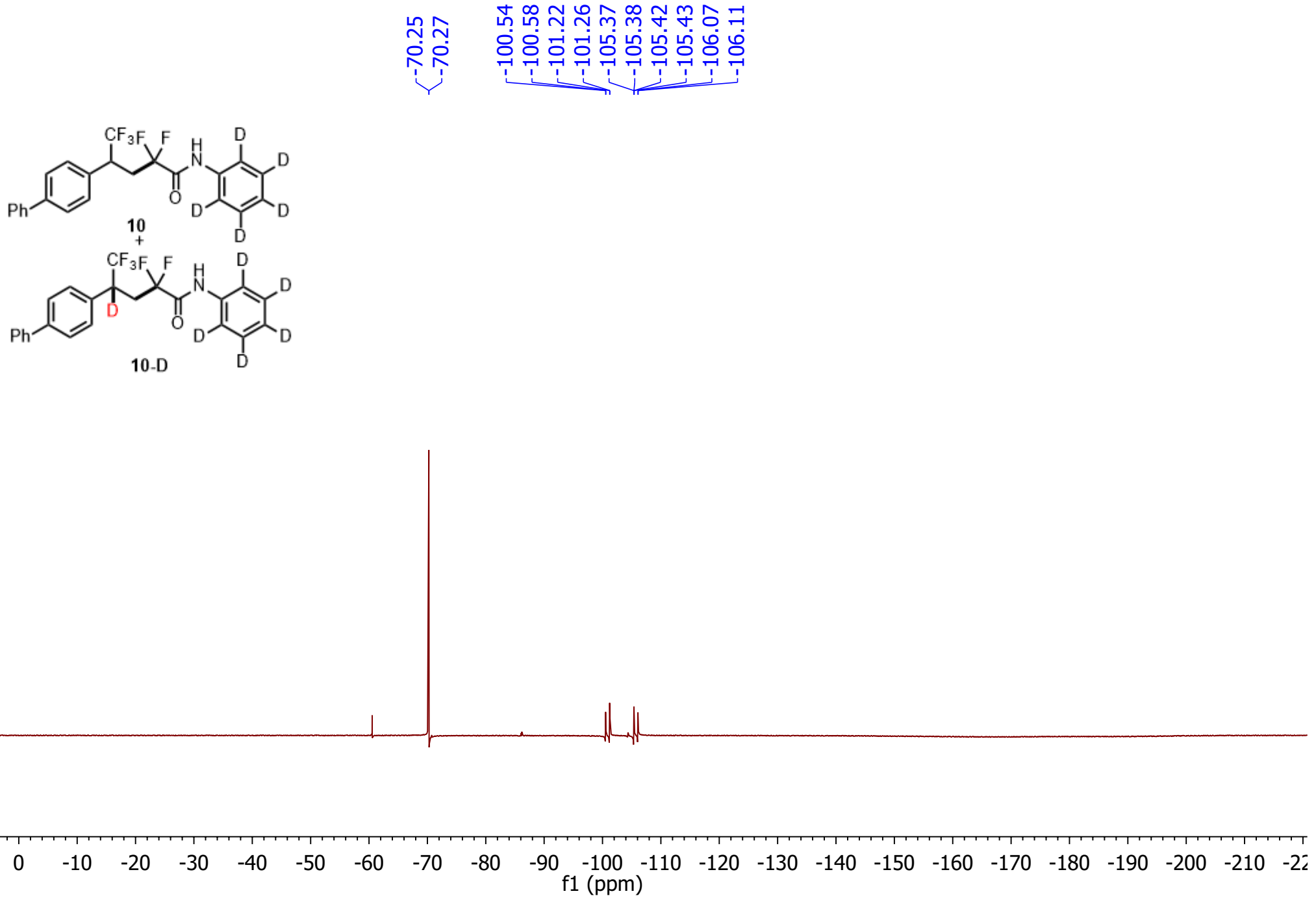
^{19}F NMR Spectrum of **3ah+4ah-D**

1H (CDCl3, 400 MHz)



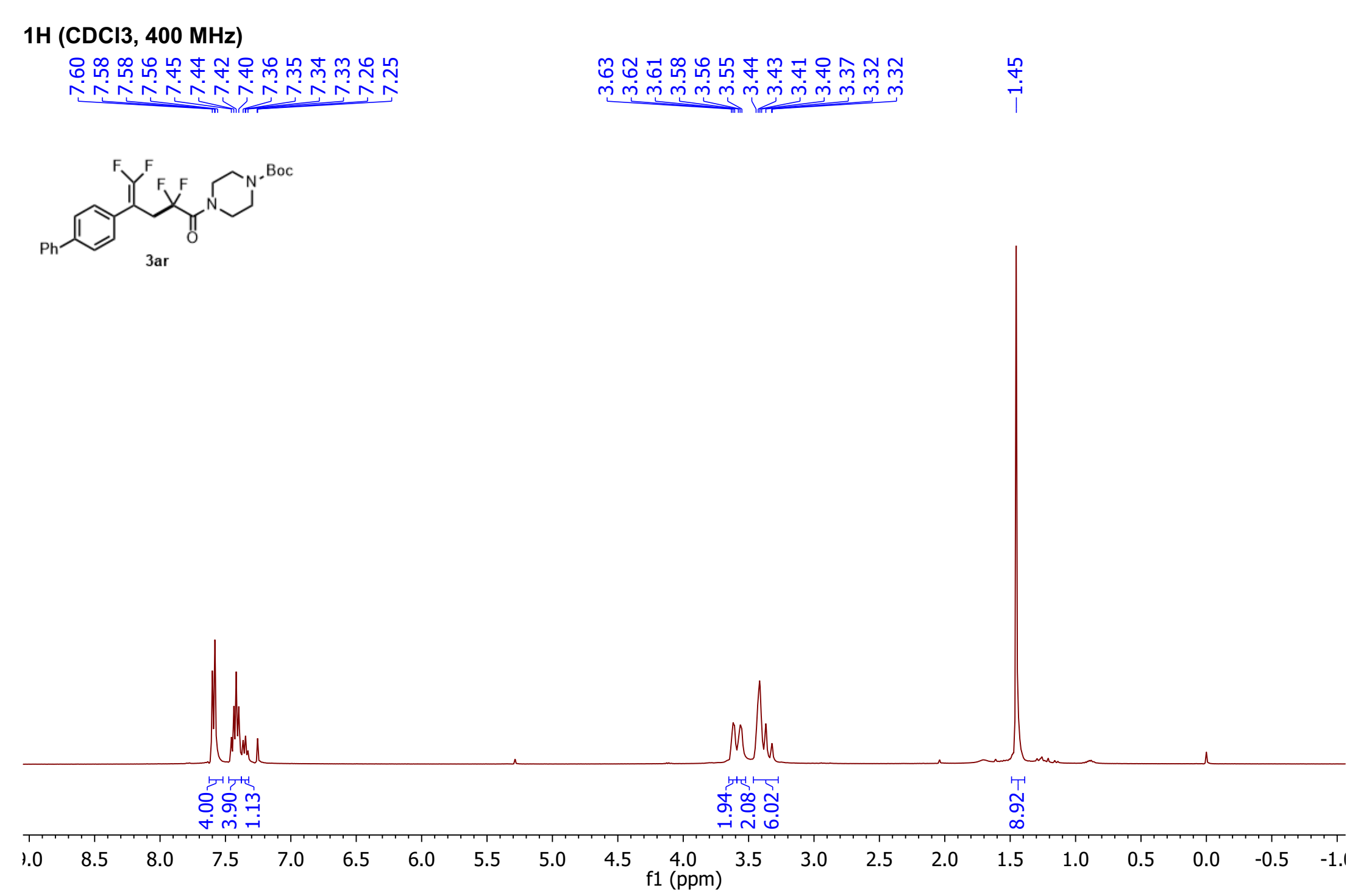
[1]H NMR Spectrum of **10+10-D**

19F (CDCl3, 376 MHz)



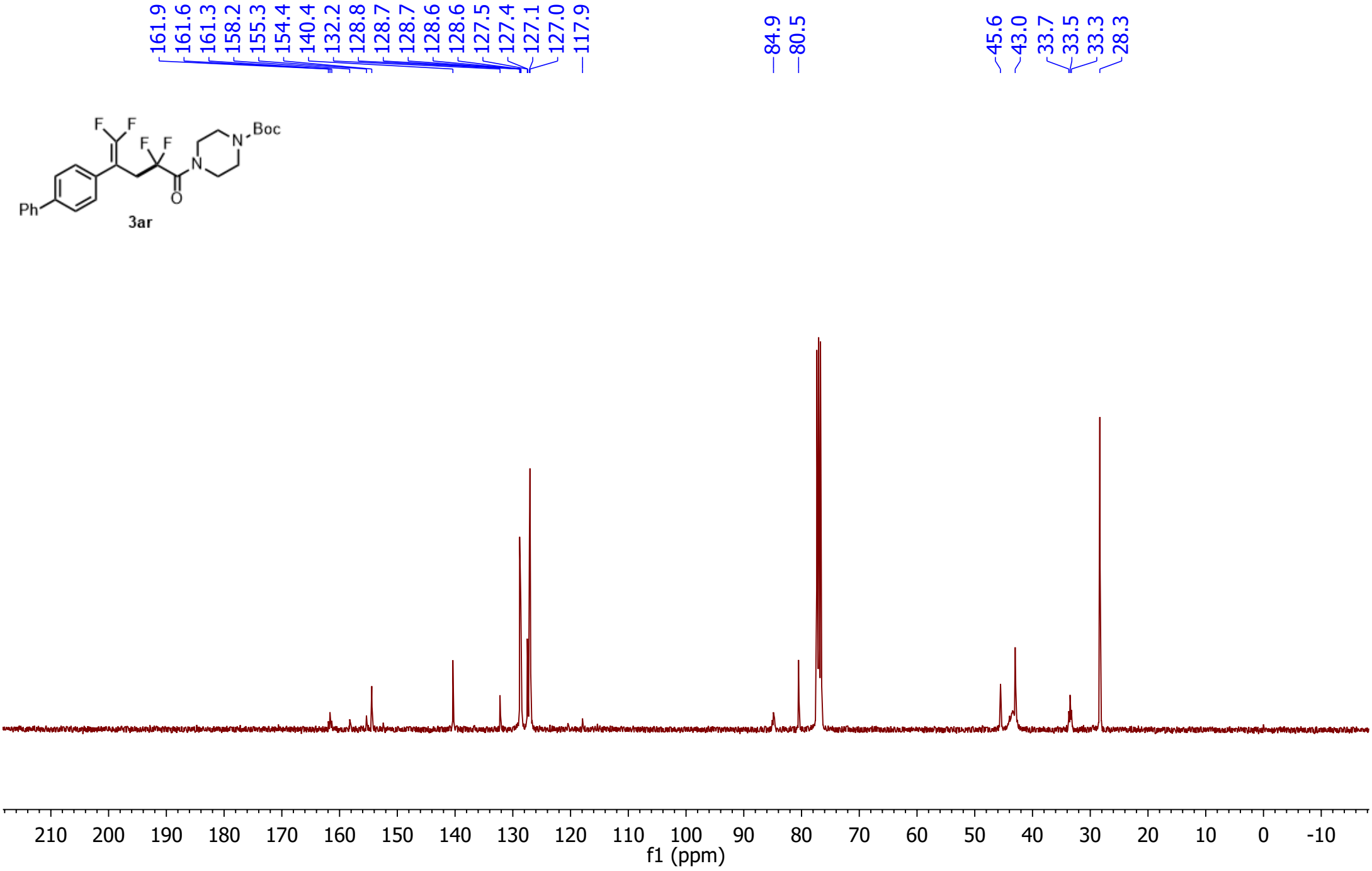
^{19}F NMR Spectrum of **10+10-D**

1H (CDCl3, 400 MHz)



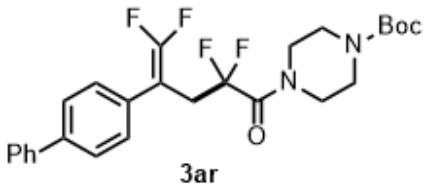
^{1}H NMR Spectrum of **3ar**

13C (CDCl3, 101 MHz)



^{13}C NMR Spectrum of **3ar**

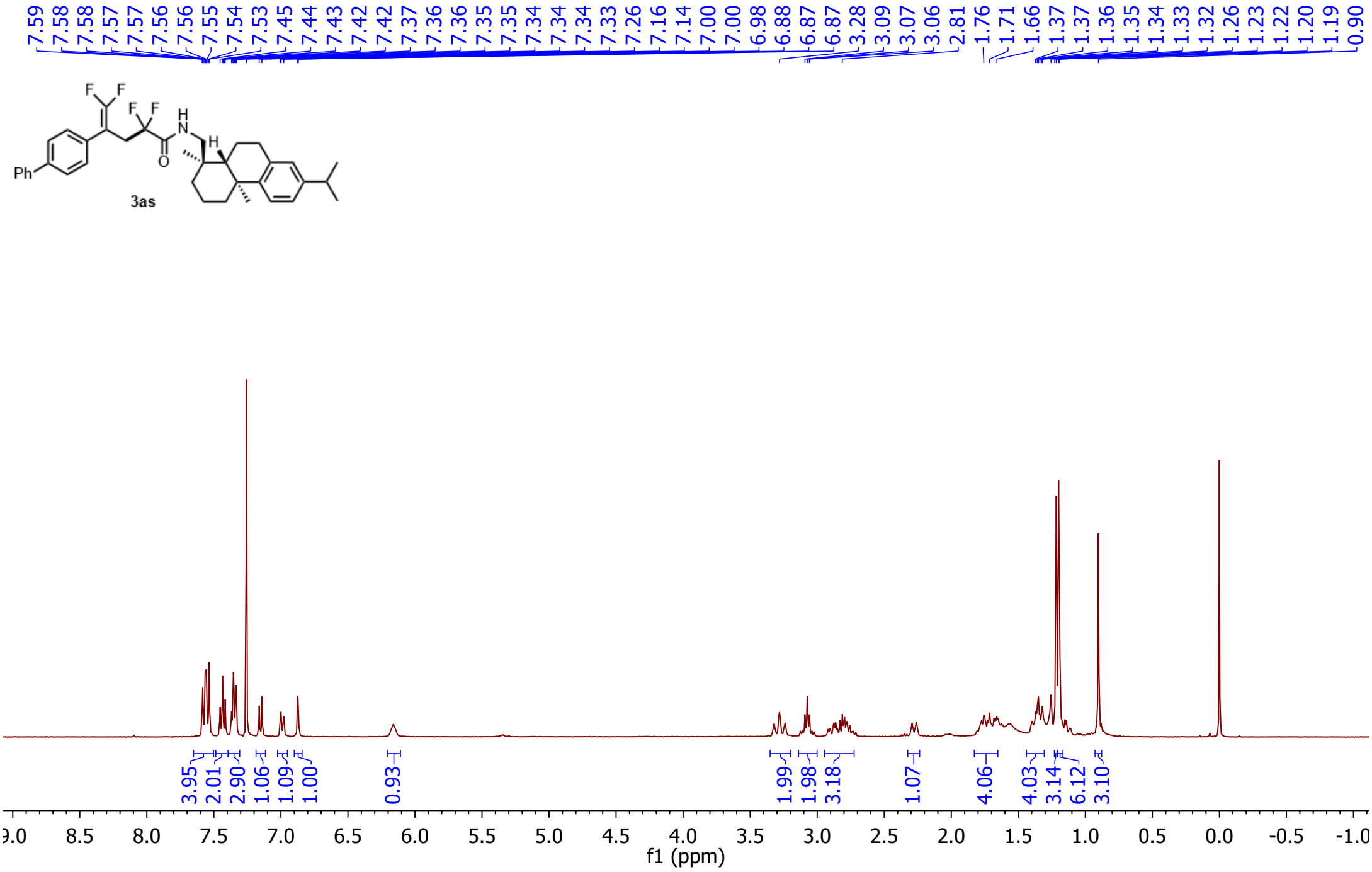
19F (CDCl3, 376 MHz)



3ar

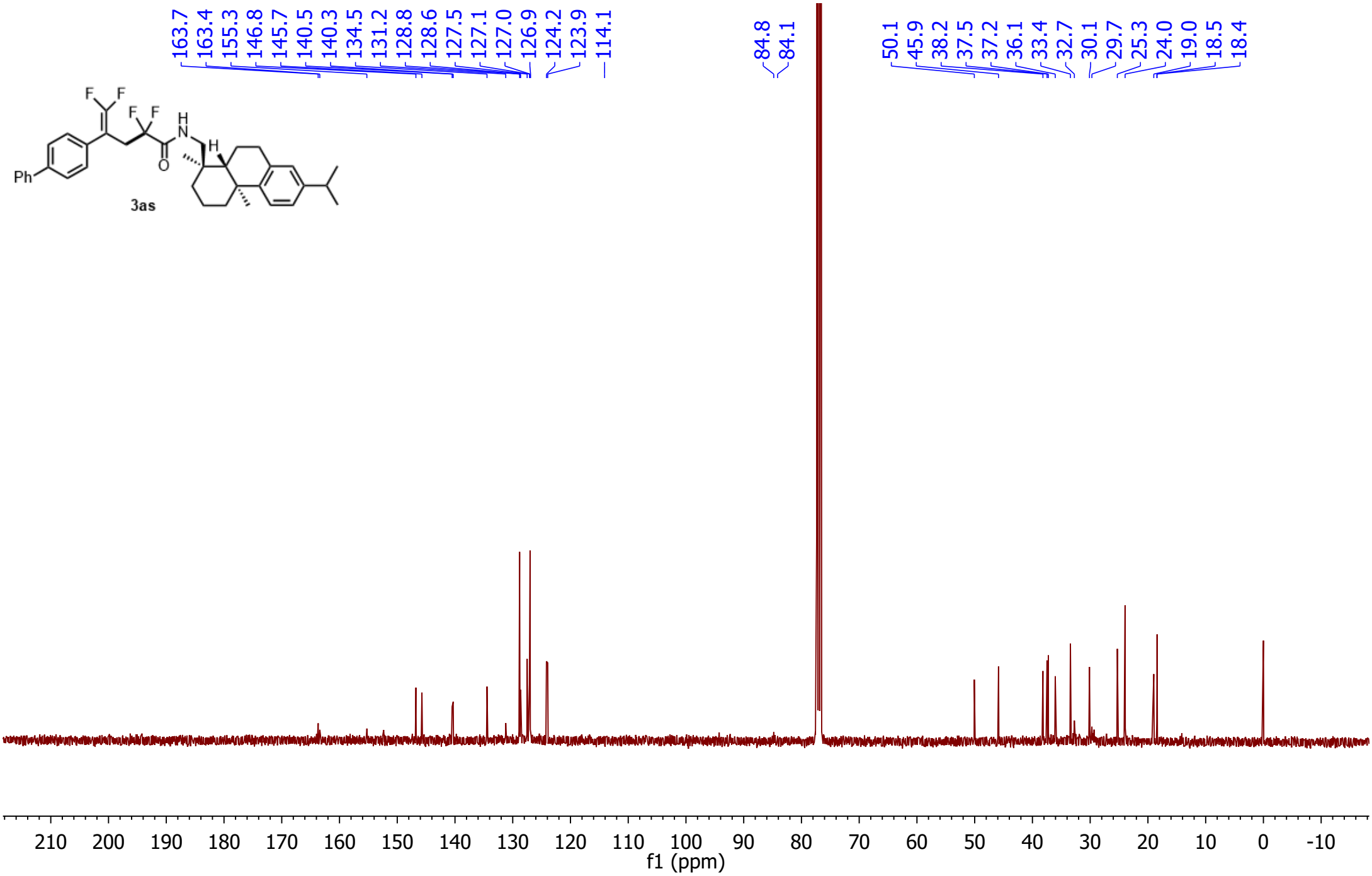
^{19}F NMR Spectrum of **3ar**

1H (CDCl3, 400 MHz)



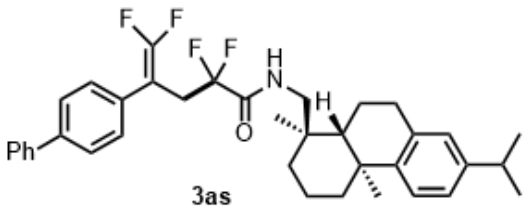
^{1}H NMR Spectrum of **3as**

13C (CDCl3, 101 MHz)

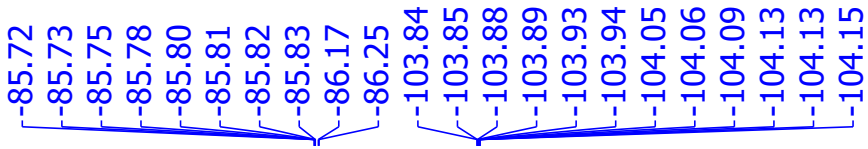


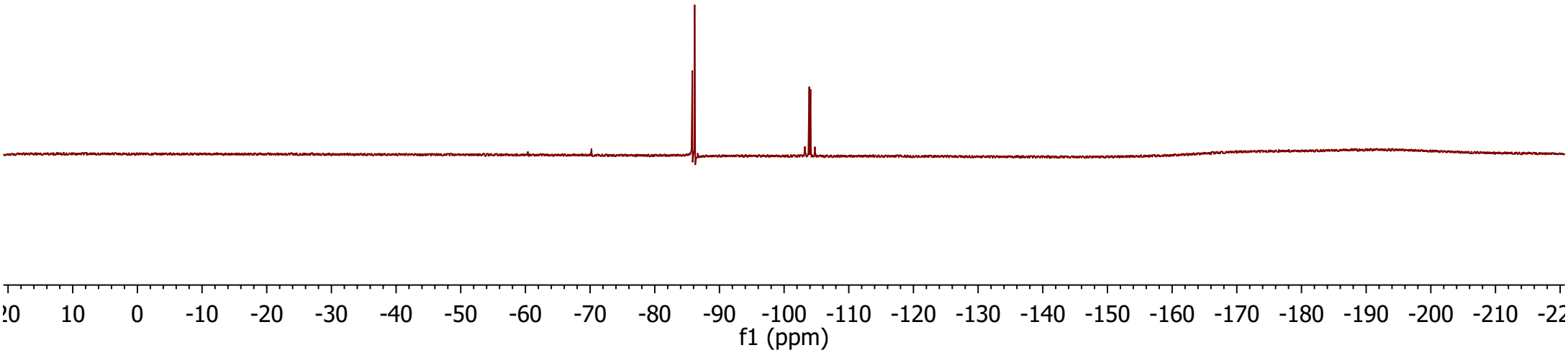
^{13}C NMR Spectrum of **3as**

19F (CDCl3, 376 MHz)



3as





^{19}F NMR Spectrum of **3as**