Electronic Supplementary Material (ESI) for ChemComm.

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General procedures and methods

^{1}H, ^{13}C, ^{19}F and 2D NMR spectra were recorded either on a Bruker Avance III 400 or Bruker Avance 500. Chemical shifts are reported in parts per million (ppm). For ^{1}H and ^{13}C NMR, the residual solvent peak was used as an internal reference ($CDCl_3$, 7.26ppm for ^{1}H and 77.00 for ^{13}C). For ^{19}F NMR, perfluorobenzene was used as the reference (-164.90ppm), if not stated no reference is used the default value of perfluorobenzene without calibration is -161.78ppm. MestReNova 8.14 was used to process the NMR data. Low resolution mass spectra were obtained on a Finnigan/MAT LCQ spectrometer in ESI mode and a Finnigan/MAT 95XL-T mass spectrometer in FAB mode. All high resolution mass spectra were obtained on a Finnigan/MAT 95XL-T spectrometer. Analytical thin layer chromatography (TLC) was performed with Merck pre-coated TLC plates, silica gel 60F-254, layer thickness 0.25 mm. Visualization of TLC *via* 2,4-dinitrophenylhydrazine = 2,4-DNPH, fluorescence quenching, Ceric Ammonium Molybdate (CAM) and iodine stain. Flash chromatography separations were performed on Merck 60 (0.040 - 0.063mm) mesh silica gel. Reagents and solvents were commercial grade and were used as supplied without further purification, unless otherwise stated. Gas chromatography-Mass Spectrometry (GC-MS) analysis was performed using a Shimadzu GC-2010 plus with a mass sensitive detector (GCMS-QP2010SE). Ionization mode is electron ionization. The column used was a 30m Restek Rtx-5ms(Film: 0.25µm Length: 30m in length and Internal Diameter: 0.25mm).

Conformation sampling was performed with Macromodel. Density Functional Theory calculations were performed with Gaussian 09 A2 on the high performance computing clusters of the National University of Singapore.

Experimental details and results

Procedure

For all substrates unless specified: 2mmol (708mg) of Selectfluor® (M.W=354.26) and 8.4mg of photocatalyst: anthracene-9,10-dione (0.04mmol, M.W=208.2160) and magnetic stir bar was added to a 2-necked Schlenk flask. The air in the Schlenk flask was replaced with purified N_2 (H_2O and O_2<2ppm). 1.5 equivalents of substrate (3mmol, which is degassed by freeze-pump-thaw if the sample is liquid) were added under N_2 via a gas tight syringe. 8mL of acetonitrile (degassed by bubbling purified N_2 for about 15 minutes) was added under N_2 via a gas tight syringe. The Schlenk flask was sealed with a glass stopper. The reaction was stirred with irradiation from an 11W fluorescent lamp (except in Table 1 where LED bulb was used) for 24 hours (exact reaction time can be found in the table with experimental details under the name of each product).

Purification: 30mL of diethyl ether (inhibitor free) was added to the reaction mixture after the reaction. Instant precipitation of unreacted Selectfluor® and salt derived from Selectfluor® was observed. The mixture was filtered into a RBF. The residue was rinsed with 3x10mL of diethyl ether (inhibitor free). Solvent was then removed by a rotary evaporator. The crude product was subjected to column chromatography.

For **11,** 2 mmol of adipic acid and 3 mmol of Selectfluor® was used.

For **13**, 5 mmol of butyramide and 7.5 mmol of Selectfluor® were used in Figure 1 and 25 mmol of butyramide and 37.5mmol of Selectfluor®.

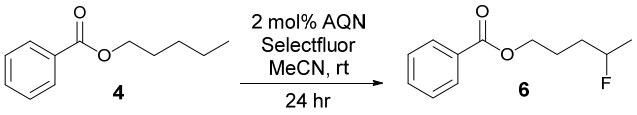
For **15**, 4 mmol of substrate and 2 mmol of Selectfluor® were used and 2-Cl-AQN (2-chloroanthracene-9,10-dione) was used as the photocatalyst instead.

For **17**, 2 mmol of substrate and 3 mmol of Selectfluor® were used.

Note: A glovebox was used in some cases; however, this is out of convenience and is not essential. The reaction works as long as the solvent (MeCN) is rigorously degassed and the reaction is conducted under dioxygen free N2 or Argon.

Survey of reaction conditions

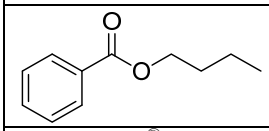
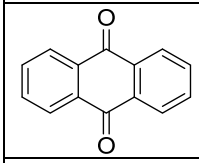
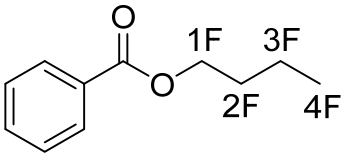
Table 1 Survey of reaction conditions

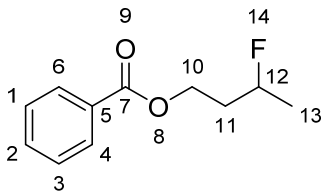


Entry	PC[a]	Light source	Substrate: Selectfluor	Yield[b] (%)
1	AQN	No Light	1.5:1	0
2	-		1.5:1	0
3	AQN(1 atm of O_2)		1.5:1	0
4	AQN	OSRAM	1.5:1	65
5	$Ru(bpy)_3Cl_2$	11W	1.5:1	0
6	Rose Bengal	fluorescence	1.5:1	0
7	AQN		1:1	56
8	AQN		1:1.5	61
9[c]	AQN	Philip 10W LED	1.5:1	54
10[d]	AQN	OSRAM 11W fluorescence	1.5:1	54

Entries 1-9: 0.1 mmol scale. [a] PC = photocatalyst, [b](GC-MS yield based on internal standard calibration – biphenyl - for entry 1-9) [c] 10W Philips LED was used, [d] 2.0 mmol scale, isolated yield.

3-fluorobutyl benzoate

	M.W (mg/mmol)	Amount added	Amount added/mmol
	178.2310	540mg	3.03
Selectfluor®	354.26	727mg	2.05
	208.2160	8.6mg	0.0413
MeCN	-	8mL	-
Reaction Time	26 hours		
Column Chromatography Details	2cm(column outer diameter) X 20cm (SiO_2 length) Crude is dissolved in minimal DCM and separation was performed with gradient elution. Gradient Elution: *n*-Hexane to 49:1(*n*-Hexane:Et_2O) Total 3-fluorobutyl benzoate obtained = 155.7mg(0.793mmol) Yield (based on limiting reagent) = 0.793/2.05 X100 =39%		
	R_f (3-fluorobutyl benzoate) = 0.14 (15:1, *n*-Hexane,Et_2O); stain CAM blue R_f (starting material) = 0.34 (15:1, *n*-Hexane,Et_2O); weak CAM stain		
Ratio from ^{19}F NMR		F position	^{19}F Integration Ratio
		1F	1.33
		2F	5.25
		3F	1.00
		4F	Not detected



^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.06 – 8.02 (m, 2H), 7.59 – 7.54 (m, 1H), 7.44 (d, *J* = 7.7 Hz, 2H), 4.89 (dtdd, *J* = 48.8, 6.2, 4.0, 2.1 Hz, 1H), 4.51 – 4.42 (m, 2H), 2.15 – 1.96 (m, 2H), 1.42 (dd, *J* = 23.9, 6.2 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 166.46, 132.99, 130.17, 129.56, 128.38, 88.52, 87.21, 61.14, 61.10, 36.18, 36.01, 21.22, 21.04.

^{13}C NMR (126 MHz, Chloroform-*d*) δ 166.46 , 132.99 , 130.17 , 129.56 , 128.38 , 87.86 (d, *J* = 165.5 Hz), 61.12 (d, *J* = 5.4 Hz), 36.10 (d, *J* = 21.0 Hz), 21.13 (d, *J* = 22.5 Hz).

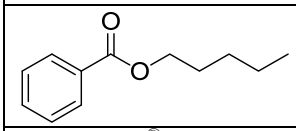
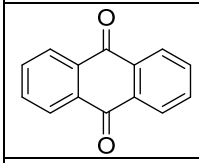
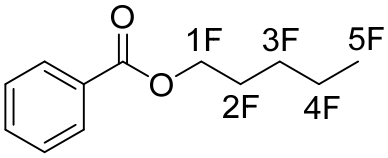
^{19}F NMR (376 MHz, Chloroform-*d*) δ -175.53 (ddqd, *J* = 48.1, 29.5, 23.9, 16.2 Hz).

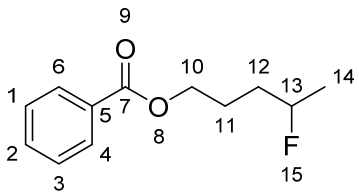
Refer to chemdraw above for label	^{13}C Assignment	^{19}F Assignment	^{1}H Assignment
1,3	128.38	-	7.44 (d, *J* = 7.7 Hz, 2H)
2	132.99	-	7.59 – 7.53 (m, 1H)
4,6	129.56	-	8.06 – 8.02 (m, 2H)
5	130.17	-	-
7	166.46	-	-
10	61.14, 61.10	-	4.51 – 4.42 (m, 2H)
11	36.18, 36.01	-	2.15 – 1.96 (m, 2H)
12	88.52, 87.21 (d, *J* = 165.5 Hz)	-	4.89 (dtdd, *J* = 48.8, 6.2, 4.0, 2.1 Hz, 1H)
13	21.22, 21.04	-	1.42 (dd, *J* = 23.9, 6.2 Hz, 3H)
14	-	-175.53	-

HRMS (ESI-TOF) $[M-H]^+$ calculated for $C_{11}H_{14}FO_2^+$ 197.0972, found 197.0977.

Appearance: Colorless to yellow liquid

4-fluoropentyl benzoate

	M.W (mg/mmol)	Amount added	Amount added/mmol
	192.2580	580mg	3.01
Selectfluor®	354.26	718mg	2.03
	208.2160	8.4mg	0.0403mmol
MeCN	-	8mL	-
Reaction Time	26 hours		
Column Chromatography Details	2cm(column outer diameter) X 20cm (SiO_2 length) Crude is dissolved in minimal DCM and separation was performed with gradient elution. Gradient Elution: *n*-Hexane to 49:1(*n*-Hexane:Et_2O) Total 4-fluoropentyl benzoate obtained = 228.8mg(1.09mmol) Yield (based on limiting reagent) = 1.09/2.03 X100 = 54%		
	R_f (4-fluoropentyl benzoate) = 0.17 (15:1, *n*-Hexane,Et_2O); stain CAM blue R_f (starting material) = 0.28 (15:1, *n*-Hexane,Et_2O); weak CAM stain		
Ratio from ^{19}F NMR		F position	^{19}F Integration Ratio
		1F	1.36
		2F	1.00
		3F	2.81
		4F	13.66
		5F	Not detected



^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.07 – 8.02 (m, 2H), 7.56 (ddt, *J* = 7.9, 7.0, 1.4 Hz, 1H), 7.48 – 7.42 (m, 2H), 4.82 – 4.64 (m, 1H), 4.41 – 4.31 (m, 2H), 2.02 – 1.64 (m, 4H), 1.36 (dd, *J* = 23.9, 6.2 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 166.58, 132.92, 130.31, 129.54, 128.37, 91.08, 89.77, 64.60, 33.58, 33.41, 24.60, 24.56, 21.11, 20.93.

^{13}C NMR (126 MHz, Chloroform-*d*) δ 166.58 , 132.92 , 130.31 , 129.54 , 128.37 , 90.43 (d, *J* = 165.2 Hz), 64.60 , 33.50 (d, *J* = 21.1 Hz), 24.58 (d, *J* = 4.6 Hz), 21.02 (d, *J* = 22.7 Hz).

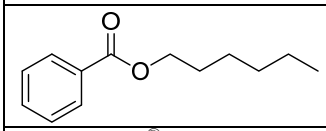
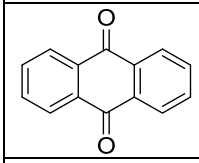
^{19}F NMR (376 MHz, $CDCl_3$) δ -173.47.

Refer to chemdraw above for label	^{13}C Assignment	^{19}F Assignment	^{1}H Assignment
1,3	128.37	-	7.48 – 7.42 (m, 2H)
2	132.92	-	7.56 (ddt, *J* = 7.9, 7.0, 1.4 Hz, 1H)
4,6	129.54	-	8.07 – 8.02 (m, 2H)
5	130.31	-	-
7	166.58	-	-
10	64.60	-	4.41 – 4.31 (m, 2H)
11	24.60, 24.56	-	2.02 – 1.64 (m, 4H)
12	33.58, 33.41	-	
13	91.08, 89.77	-	4.82 – 4.64 (m, 1H)
14	21.11, 20.93	-	1.36 (dd, *J* = 23.9, 6.2 Hz, 3H)
15	-	-173.47.	-

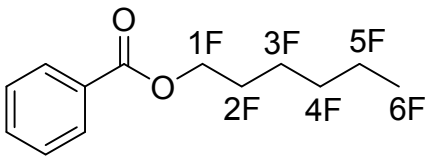
HRMS (ESI-TOF) $[M-H]^+$ calculated for $C_{12}H_{16}FO_2^+$ 211.1129, found 211.1137

Appearance: Colorless to yellow liquid

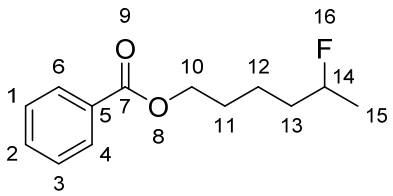
5-fluorohexyl benzoate

	M.W (mg/mmol)	Amount added	Amount added/mmol
	206.2850	636mg	3.08
Selectfluor®	354.26	710mg	2.00
	208.2160	8.4mg	0.0403
MeCN	-	8mL	-
Reaction Time	24 hours		
Column Chromatography Details	2cm(column outer diameter) X 22cm (SiO_2 length) Crude is dissolved in minimal DCM and separation was performed with gradient elution. Gradient Elution: *n*-Hexane to 49:1(*n*-Hexane:Et_2O) Total 5-fluorohexyl benzoate obtained = 209.3mg(0.93mmol) Yield (based on limiting reagent) = 0.93/2.00 X100 = 47%		
	R_f (5-fluorohexyl benzoate) = 0.30 (15:1, *n*-Hexane,Et_2O, develop the same TLC plate twice); stain CAM blue R_f (starting material) = 0.57 (15:1, *n*-Hexane,Et_2O,develop the same TLC plate twice); weak CAM stain		

Ratio from ^{19}F NMR



F position	^{19}F Integration Ratio
1F	1.18
2F	1.00
3F	2.41
4F	7.30
5F	19.52
6F	0.15



^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.06 – 8.03 (m, 2H), 7.58 – 7.53 (m, 1H), 7.47 – 7.42 (m, 2H), 4.68 (ddtd, *J* = 48.8, 7.8, 3.9, 1.7 Hz, 1H), 4.34 (t, *J* = 6.5 Hz, 2H), 1.85 – 1.77 (m, 2H), 1.77 – 1.48 (m, 4H), 1.33 (dd, *J* = 23.9, 6.2 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 166.64, 132.86, 130.40, 129.54, 128.35, 91.38, 90.07, 64.77, 36.60, 36.43, 28.57, 21.77, 21.73, 21.10, 20.92.

^{13}C NMR (126 MHz, Chloroform-*d*) δ 166.64, 132.86 , 130.40 , 129.54 , 128.35 , 90.12 – 90.01 (m), 90.73 (d, *J* = 164.8 Hz), 64.77 , 36.51 (d, *J* = 20.8 Hz), 28.57 , 21.75 (d, *J* = 4.9 Hz), 21.01 (d, *J* = 22.8 Hz), 91.50 – 91.30 (m).

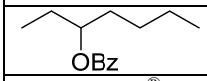
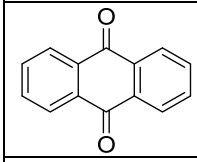
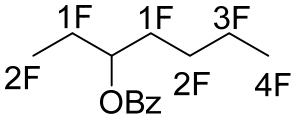
^{19}F NMR (376 MHz, $CDCl_3$) δ -172.97

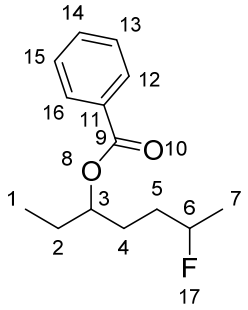
Refer to chemdraw above for label	^{13}C Assignment	^{19}F Assignment	^{1}H Assignment
1,3	128.35	-	7.47 – 7.42 (m, 2H)
2	132.86	-	7.58 – 7.53 (m, 1H)
4,6	129.54	-	8.06 – 8.03 (m, 2H)
5	130.40	-	-
7	166.64	-	-
10	64.77	-	4.34 (t, *J* = 6.5 Hz, 2H)
11	28.57	-	1.85 – 1.77 (m, 2H)
12	21.77, 21.73 (d, *J* = 4.9 Hz)	-	1.77 – 1.48 (m, 4H)
13	36.60, 36.43 (d, *J* = 20.8 Hz)	-	
14	91.38, 90.07 (d, *J* = 164.8 Hz)	-	4.68 (ddtd, *J* = 48.8, 7.8, 3.9, 1.7 Hz, 1H)
15	21.10, 20.92. (d, *J* = 22.8 Hz)	-	1.33 (dd, *J* = 23.9, 6.2 Hz, 3H)
16	-	-172.97	-

HRMS (ESI-TOF) $[M-H]^+$ calculated for $C_{12}H_{16}FO_2^+$ 211.1129, found 211.1137

Appearance: Colorless to yellow liquid

6-fluoroheptan-3-yl benzoate

	M.W (mg/mmol)	Amount added	Amount added/mmol
	220.3120	662mg	3.00
Selectfluor®	354.26	720mg	2.03
	208.2160	8.6mg	0.0413
MeCN	-	8mL	-
Reaction Time	24 hours		
Column Chromatography Details	2cm(column outer diameter) X 22cm (SiO_2 length) Crude is dissolved in minimal DCM and separation was performed with gradient elution. Gradient Elution: 99:1(*n*-Hexane:DCM) to 60:1(*n*-Hexane:Et_2O) to 49:1(*n*-Hexane:Et_2O) Total 6-fluoroheptan-3-yl benzoate obtained = 245.5mg(1.03mmol) Yield (based on limiting reagent) = 1.03/2.03 X100 =51%		
	R_f (6-fluoroheptan-3-yl benzoate) = 0.42 (15:1, *n*-Hexane,Et_2O, develop the same TLC plate twice); stain CAM blue R_f (starting material) = 0.63 (15:1, *n*-Hexane:Et_2O, develop the same TLC plate twice); weak CAM stain		
Ratio from ^{19}F NMR		Confident assignment of 19F chemical shift is difficult as the two diastereomers gave many peaks.	



Inseparable Diastereomer (*cis*- and *trans*-)

^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.09 – 8.02 (m, 2H), 7.59 – 7.52 (m, 1H), 7.49 – 7.41 (m, 2H), 5.11 (ddtd, *J* = 19.8, 7.7, 6.1, 4.0 Hz, 1H), 4.78 – 4.56 (m, 1H), 1.93 – 1.55 (m, 6H), 1.31 (ddd, *J* = 23.9, 6.2, 1.0 Hz, 3H), 0.96 (t, *J* = 7.4 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 166.37, 166.34, 132.83, 130.61, 130.59, 129.55, 128.34, 91.50, 91.10, 90.18, 89.79, 75.88, 75.43, 33.07, 32.91, 32.71, 32.54, 29.44, 29.40, 29.20, 29.17, 27.20, 27.18, 21.11, 21.10, 20.93, 20.91, 9.65, 9.60.

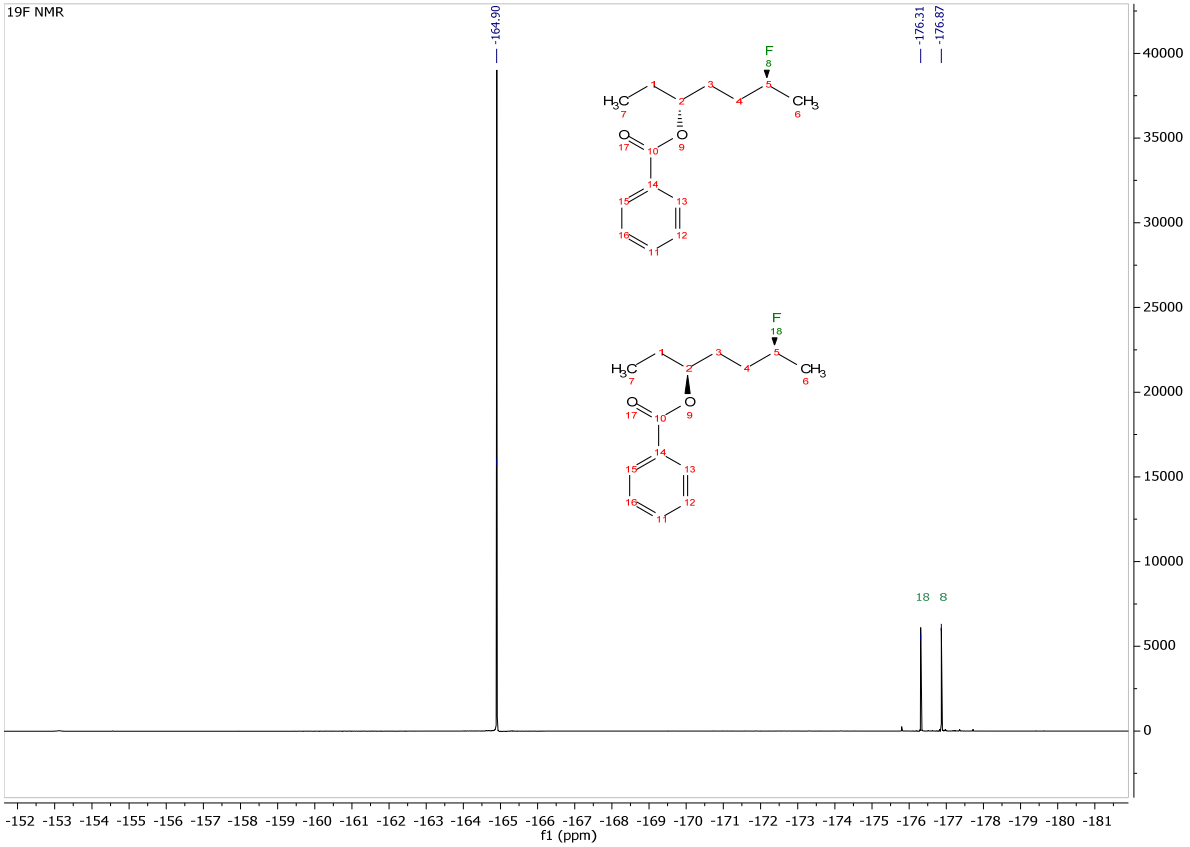
^{19}F NMR (376 MHz, Chloroform-*d*) δ -173.19, -173.75.

Refer to chemdraw above for label	^{13}C Assignment	^{19}F Assignment	^{1}H Assignment
1	9.65, 9.60	-	0.96 (t, *J* = 7.4 Hz, 3H)
2	27.20, 27.18	-	1.93 – 1.55 (m, 2H)
3	75.88, 75.43	-	5.11 (ddtd, *J* = 19.8, 7.7, 6.1, 4.0 Hz, 1H)
4	29.44, 29.40, 29.20, 29.17	-	1.93 – 1.55 (m, 4H)
5	33.07, 32.91, 32.71, 32.54	-	
6	91.50, 91.10, 90.18, 89.79	-	4.78 – 4.56 (m, 1H)
7	21.11, 21.10, 20.93, 20.91	-	1.31 (ddd, *J* = 23.9, 6.2, 1.0 Hz, 3H),
9	166.37, 166.34	-	-
11	130.61, 130.59	-	-
12,16	129.55	-	8.09 – 8.02 (m, 2H)
13,15	128.34	-	7.49 – 7.41 (m, 2H)
14	132.83	-	7.59 – 7.52 (m, 1H)
17	-	-173.19 , -173.75	-

HRMS (ESI-TOF) $[M-H]^+$ calculated for $C_{14}H_{20}FO_2^+$ 239.1444, found 239.1448.

Appearance: Colorless to yellow liquid

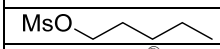
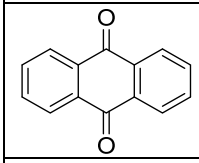
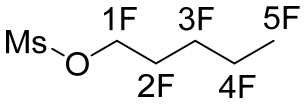
Determination of diastereomers

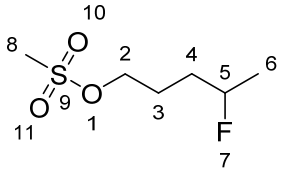


Assignment based on DFT calculated NMR shielding tensor corrected with least-square linear regression model.

See Section: “19F NMR chemical shifts”

4-fluoropentyl methanesulfonate

	M.W (mg/mmol)	Amount added	Amount added/mmol
	166.2350	499mg	3.00
Selectfluor®	354.26	706mg	1.99
	208.2160	8.4mg	0.0403
MeCN	-	8mL	-
Reaction Time	24 hours		
Column Chromatography Details	2cm(column outer diameter) X 20.5cm (SiO_2 length) Crude is dissolved in minimal DCM and separation was performed with gradient elution. Gradient Elution: *n*-Hexane to 9:1(*n*-HexaneMixture*) to 5:1(*n*-Hexane:Mixture*) *[Mixture=Ethyl Acetate:Et_2O(7:3)] Total 4-fluoropentyl methanesulfonate obtained= 219.5mg(1.19mmol) Yield (based on limiting reagent) = 1.19/2.00 X100 = 60%		
	R_f (4-fluoropentyl methanesulfonate) = 0.08 (5:1, *n*-Hexane:Ethyl Acetate) R_f (starting material) = 0.16 (5:1, *n*-Hexane:Ethyl Acetate)		
Ratio from ^{19}F NMR		F position	^{19}F Integration Ratio
		1F	negligible
		2F	1.1
		3F	
		4F	5.07
		5F	0



^{1}H NMR (500 MHz, Chloroform-*d*) δ 4.69 (dddd, *J* = 48.9, 7.9, 6.1, 4.4 Hz, 1H), 4.32 – 4.22 (m, 2H), 3.01 (s, 3H), 1.99 – 1.79 (m, 2H), 1.79 – 1.61 (m, 2H), 1.35 (dd, *J* = 23.8, 6.2 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 90.85, 89.54, 69.66, 69.62, 37.40, 32.86, 32.69, 25.11, 25.08, 21.07, 20.89.

^{13}C NMR (126 MHz, Chloroform-*d*) δ 90.20 (d, *J* = 165.4 Hz), 69.62 , 37.40 , 32.77 (d, *J* = 21.1 Hz), 25.09 (d, *J* = 4.1 Hz), 20.98 (d, *J* = 22.7 Hz).

^{19}F NMR (376 MHz, $CDCl_3$) δ -174.10.

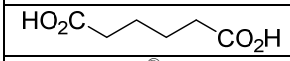
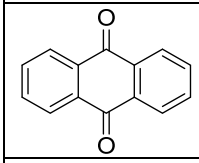
Refer to chemdraw above for label	^{13}C Assignment	^{19}F Assignment	^{1}H Assignment
2	69.66, 69.62	-	4.32 – 4.22 (m, 2H)
3		-	1.99 – 1.79 (m, 2H)
4	32.86, 32.69 (d, *J* = 21.1 Hz)	-	1.79 – 1.61 (m, 2H)
5	90.85, 89.54 (d, *J* = 165.4 Hz)	-	4.69 (dddd, *J* = 48.9, 7.9, 6.1, 4.4 Hz, 1H)
6	21.07, 20.89 (d, *J* = 22.7 Hz).	-	1.35 (dd, *J* = 23.8, 6.2 Hz, 3H).
7	-	-174.10	-
8	37.40	-	3.01 (s, 3H)

HRMS (ESI-TOF) $[M\text{-}Na]^+$ calculated for $C_6H_{13}FO_3SNa^+$ 207.0462, found 207.0473

Appearance: Colorless to yellow liquid.

Adipic acid fluorination

(*Performed by Chin Kek Foo)

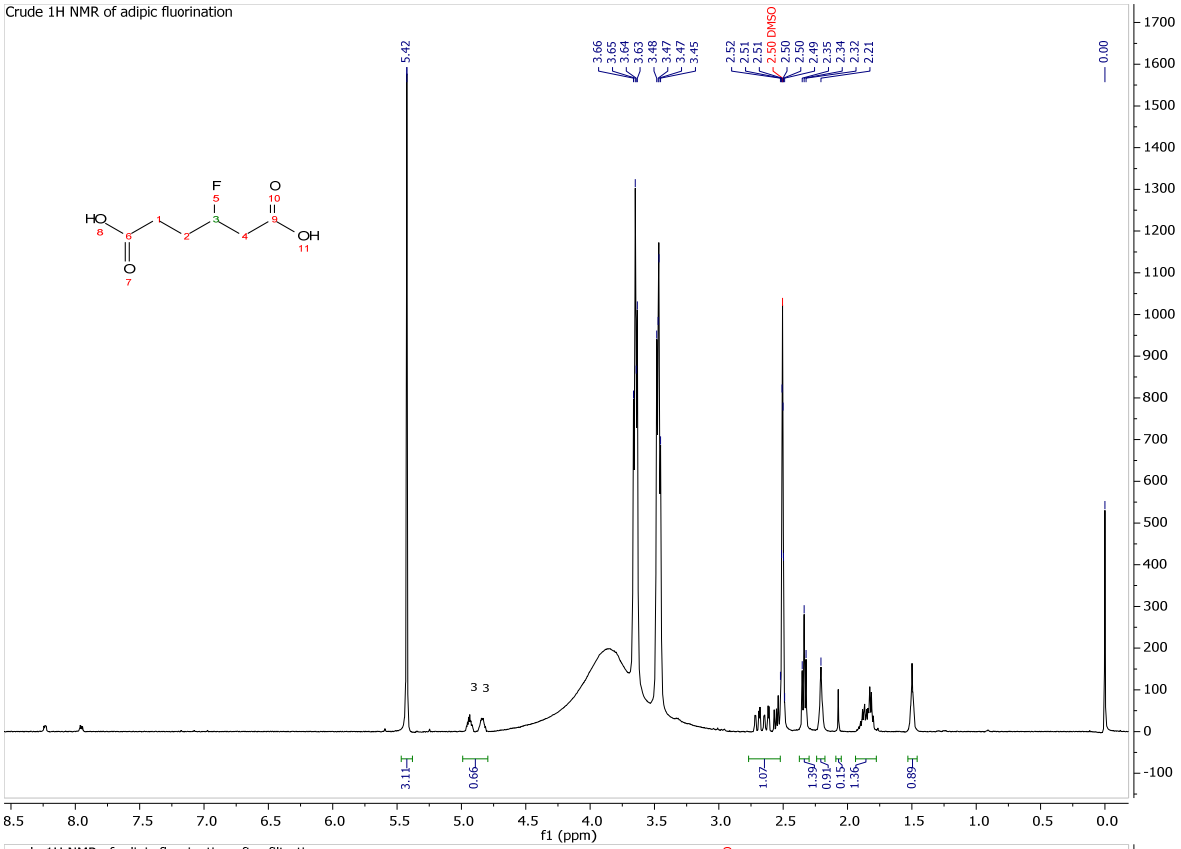
	M.W (mg/mmol)	Amount added	Amount added/mmol
	146.1420	295.1mg	2.02
Selectfluor®	354.26	1.0688g	3.02
	208.2160	11.2mg	0.0538
MeCN	-	8mL	-

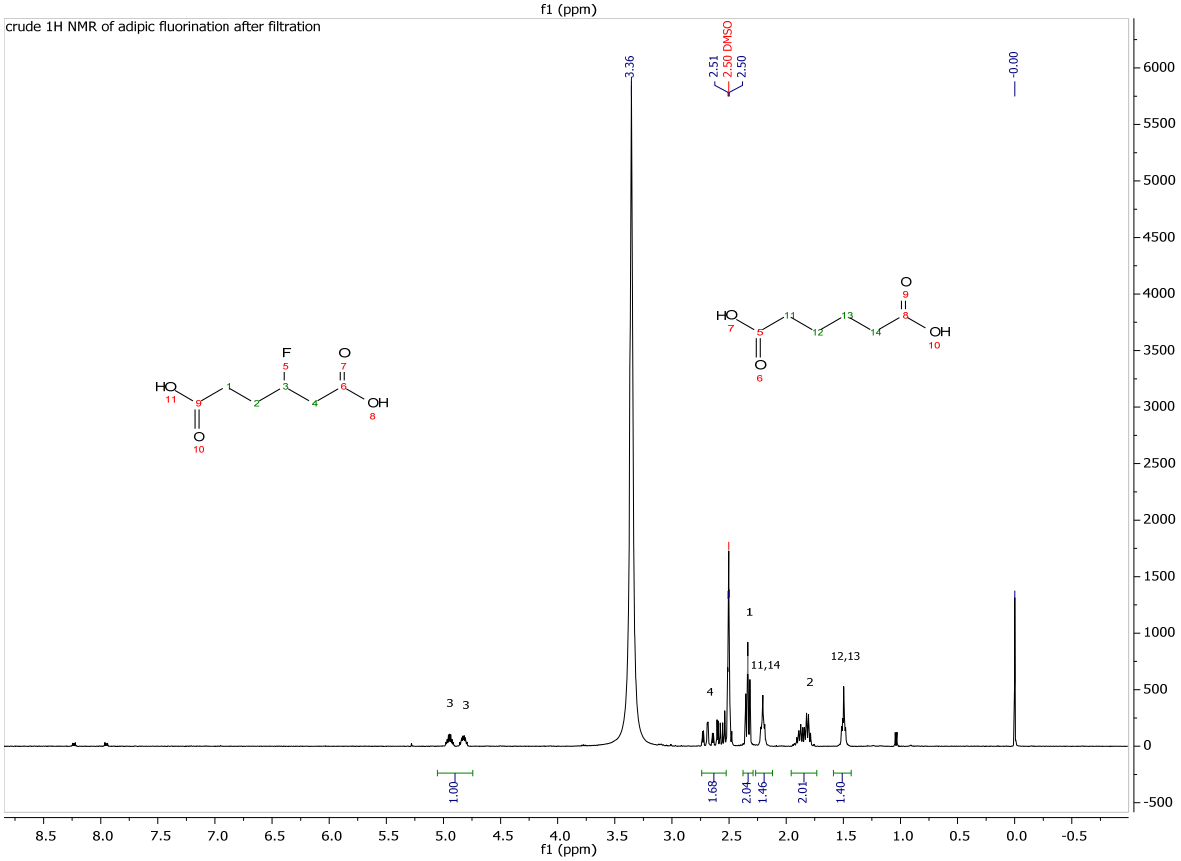
Fluorinated adipic acid was converted to ester to facilitate purification.

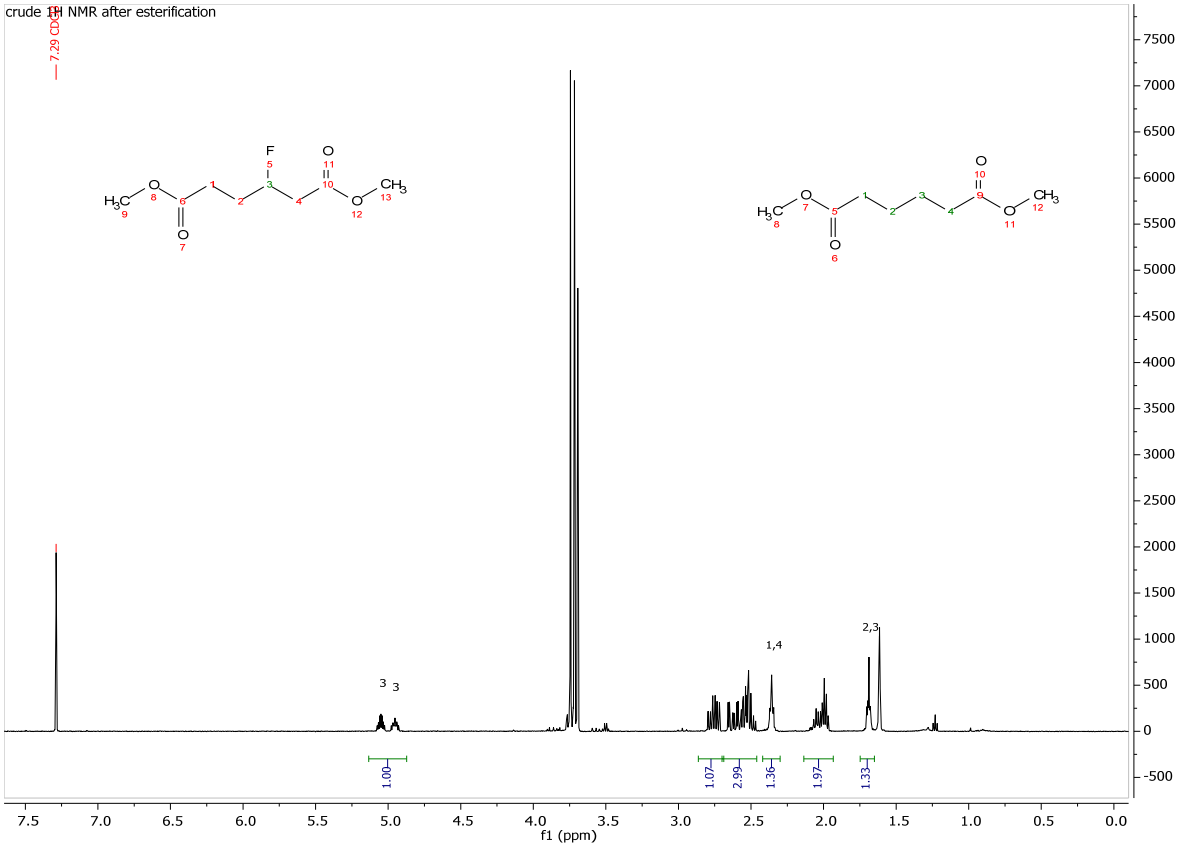
Under air atmosphere, adipic acid, Selectfluor, catalyst was weight into a Flame-dried 50mL RBF. It was then transferred into glovebox and MeCN was added. The reaction mixture was irradiated with 11W Fluorescent lamp in glovebox for 2 days. The reaction mixture was removed from glovebox and the solvent was removed *in vacuo*. (Check ^{1}H NMR (in DMSO-d6), pdt: SM =4: 1). 20mL of Isopropyl Alcohol (IPA) was added into the crude and the crude was stirred for 5mins. The solid was filtered off (obtained: 960.8mg) through normal filtration and washed with IPA. The solvent of the filtrate was removed *in vacuo* and dried under high vacuum for 12 hours. (Check ^{1}H NMR (in dmso-d6), pdt:SM= 3: 1). The pale yellow solid obtained was then dissolved in 25mL of Methanol, 4 drops of conc. H_2SO_4 was added. The reaction mixture was stirred at reflux (oil bath temperature: 75°C) for 18 hours. The solvent was removed *in vacuo* and Et_2O (BHT-free) and deionized water was added. Sat. aq $NaHCO_3$ (10mL) was then added. The mixture was extracted twice with 15mL of Et_2O (BHT-free), dried over anhydrous Na_2SO_4, the solvent was removed *in vacuo*. (check 1H NMR (in $CDCl_3$), pdt :SM: 2.8:1). The crude was purified by column chromatography.

Column Chromatography details:
2cm (column outer diameter) X 24cm (SiO_2 length)
Crude is dissolved in minimal DCM and separation was performed with gradient elution.
Gradient Elution: *n*-Hexane to 15:1(*n*-Hexane:Et_2O) to 4:1(*n*-Hexane:Solvent)

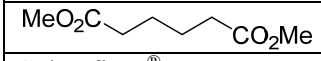
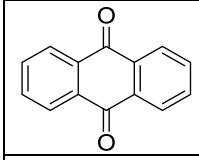
Isolated product: 191.5 mg (Yield: 55% based on 2mmol scale of Starting material), pale yellow liquid

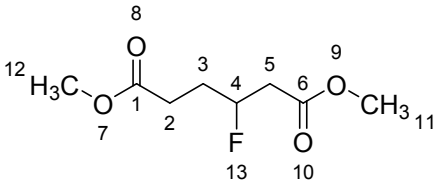

Crude 1H NMR of adipic fluorination
5.42
3.66
3.65
3.64
3.63
3.48
3.47
3.47
3.45
2.52
2.51
2.51
2.50 DMSO
2.50
2.50
2.49
2.35
2.34
2.32
2.21
0.00
3 3
3.11
0.66
1.07
1.39
0.91
0.15
1.36
0.89
f1 (ppm)


crude 1H NMR of adipic fluorination after filtration
3.36
2.51
2.50 DMSO
2.50
-0.00
3 3
1
11,14
12,13
4
2
1.00
1.68
2.04
1.46
2.01
1.40
f1 (ppm)


crude 1H NMR after esterification
7.29 CDCl3
3
3
1,4
2,3
1.00
1.07
2.99
1.36
1.97
1.33
f1 (ppm)

dimethyl 3-fluorohexanedioate

	M.W (mg/mmol)	Amount added	Amount added/mmol
	174.1960	548mg	3.15
Selectfluor®	354.26	708mg	2.00
	208.2160	8.4mg	0.0403
MeCN	-	8mL	-
Reaction Time	28 hours		
Column Chromatography Details	2cm(column outer diameter) X 22cm (SiO_2 length) Crude is dissolved in minimal DCM and separation was performed with gradient elution. Gradient Elution: *n*-Hexane to 19:1(*n*-Hexane:Mixture) to 5:1(*n*-Hexane:Mixture) *[Mixture=Ethyl Acetate:Et_2O(1:4)] Total dimethyl 3-fluorohexanedioate obtained = 203.9mg(1.06mmol) Yield (based on limiting reagent) = 1.06/2.00 X100 = 53%		
	R_f (dimethyl 3-fluorohexanedioate) = 0.13 (4:1, *n*-Hexane,Et_2O); stain $KMnO_4$ R_f (starting material) = 0.17 (4:1, *n*-Hexane:Et_2O); stain $KMnO_4$		



^{1}H NMR (500 MHz, Chloroform-*d*) δ 5.09 – 4.85 (m, 1H), 3.71 (s, 3H), 3.68 (s, 3H), 2.72 (dddd, *J* = 15.8, 15.0, 8.1, 0.7 Hz, 1H), 2.66 – 2.39 (m, 3H), 1.89-2.08 (s, 2H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 173.10, 170.18, 170.13 , 89.93, 88.57, 77.25, 76.99, 76.74, 51.93, 51.74, 40.13, 39.94, 30.03, 29.86, 29.39, 29.35.

^{13}C NMR (126 MHz, Chloroform-*d*) δ 173.10 , 170.15 (d, *J* = 6.3 Hz), 89.25 (d, *J* = 170.7 Hz), 51.84 (d, *J* = 24.6 Hz), 40.04 (d, *J* = 23.8 Hz), 29.95 (d, *J* = 20.9 Hz), 29.37 (d, *J* = 4.0 Hz).

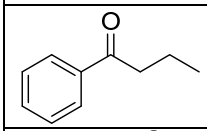
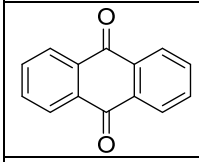
^{19}F NMR (376 MHz, $CDCl_3$) δ -182.61.

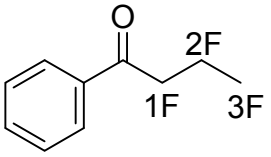
Refer to chemdraw above for label	^{13}C Assignment	^{19}F Assignment	^{1}H Assignment
1	173.10	-	N/A
2	29.37 (d, *J* = 4.0 Hz)	-	2.66 – 2.39 (m, 2H)
3	29.95 (d, *J* = 20.9 Hz)	-	1.89-2.08 (s, 2H)
4	89.25 (d, *J* = 170.7 Hz)	-	5.09 – 4.85 (m, 1H)
5	40.04 (d, *J* = 23.8 Hz)	-	2.72 (dddd, J = 15.8, 15.0, 8.1, 0.7 Hz, 1H) and 2.66 – 2.39 (m, 1H)
6	170.15 (d, *J* = 6.3 Hz)	-	N/A
11	51.93	-	3.71 (s, 3H)
12	51.74	-	3.68 (s, 3H)
13	-	-182.61	-

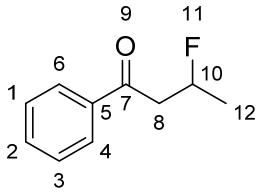
HRMS (ESI-TOF) $[M\text{-}Na]^+$ calculated for $C_8H_{14}FO_4^+$ 193.0871, found 193.0880

Appearance: Colorless to pale yellow liquid

3-fluoro-1-phenylbutan-1-one

	M.W (mg/mmol)	Amount added	Amount added/mmol
	148.2050	450mg	3.04
Selectfluor®	354.26	755mg	2.13
	208.2160	8.4mg	0.0403
MeCN	-	8mL	-
Reaction Time	24 hours		
Column Chromatography Details	2cm(column outer diameter) X 18cm (SiO_2 length) Crude is dissolved in minimal DCM and separation was performed with gradient elution. Gradient Elution: *n*-Hexane to 30:1(*n*-Hexane:Et_2O) to 20:1(*n*-Hexane:Et_2O) Total 3-fluoro-1-phenylbutan-1-one obtained = 239.2mg(1.44mmol) Yield (based on limiting reagent) = 1.44/2.13 X100 = 68%		
	R_f (3-fluoro-1-phenylbutan-1-one) = 0.16 (15:1, *n*-Hexane,Et_2O); strong fluorescence quenching R_f (starting material) = 0.28 (15:1, *n*-Hexane:Et_2O); strong fluorescence quenching		

Ratio from ^{19}F NMR		F position	^{19}F Integration Ratio
		1F	1.00
		2F	41.07
		3F	1.07



^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.98 – 7.94 (m, 2H), 7.61 – 7.56 (m, 1H), 7.48 (t, *J* = 7.7 Hz, 2H), 5.41 – 5.22 (m, 1H), 3.51 (ddd, *J* = 16.5, 15.0, 6.7 Hz, 1H), 3.19 – 3.03 (m, 1H), 1.46 (d, *J* = 6.2 Hz, 3H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 196.88 (d, *J* = 6.7 Hz), 136.81 (d, *J* = 1.5 Hz), 133.42 , 128.69 , 128.17 , 87.21 (d, *J* = 165.4 Hz), 45.39 (d, *J* = 23.0 Hz), 21.20 (d, *J* = 22.3 Hz).

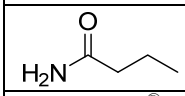
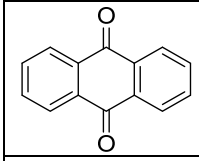
^{19}F NMR (377 MHz, Chloroform-*d*) δ -172.65 (dpd, *J* = 47.9, 24.0, 15.0 Hz).

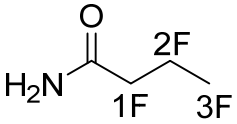
Refer to chemdraw above for label	^{13}C Assignment	^{19}F Assignment	^{1}H Assignment
1,3	128.69	-	7.48 (t, *J* = 7.7 Hz, 2H)
2	133.42	-	7.61 – 7.56 (m, 1H)
4,6	128.17	-	7.98 – 7.94 (m, 2H)
5	136.81 (d, *J* = 1.5 Hz)	-	-
7	196.88 (d, *J* = 6.7 Hz)	-	-
8	45.39 (d, *J* = 23.0 Hz)	-	3.51 (ddd, *J* = 16.5, 15.0, 6.7 Hz, 1H), 3.19 – 3.03 (m, 1H)
10	87.21 (d, *J* = 165.4 Hz)	-	5.41 – 5.22 (m, 1H)
11	-	-172.65 (dpd, *J* = 47.9, 24.0, 15.0 Hz).	-
12	21.20 (d, *J* = 22.3 Hz)	-	1.46 (d, *J* = 6.2 Hz, 3H)

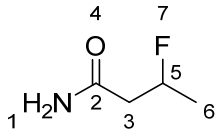
HRMS (ESI-TOF) $[M-H]^{+}$ calculated for $C_{10}H_{12}FO^{+}$ 167.0867, found 167.0870

Appearance: Colorless to pale yellow liquid

3-fluorobutanamide

	M.W (mg/mmol)	Amount added	Amount added/mmol
	87.1220	2.178g	25.0
Selectfluor®	354.26	13.285g	37.5
	208.2160	104.1mg	0.5
MeCN	-	150mL	-
Reaction Time	49 hours		
Purification Procedure	Rotavap carefully to remove MeCN. 25mL of IPA(isopropyl alcohol) was added to the RBF with crude product. Filter into a 50mL RBF. Another 19mL of IPA was added to the RBF with crude product. 2.2g of crude product was obtained after preliminary removal of IPA by rotary evaporator, followed by 16 hours of high-vacuum. Recrystallization: 40mL of n-Hexane and 5mL of IPA was added to the 50mL RBF. Stir and heat at about 55 degree Celsius. Hot filtration was performed. Wash the reside with about 3mL of hot 10:3 (n-Hexane:IPA). Cool to room temperature and then transferred to a 4 degree Celsius fridge. 903mg Another 100mg of 3-fluorobutanamide could be obtained from the residue.		

Ratio from ^{19}F NMR		F position	^{19}F Integration Ratio
		1F	1.00
		2F	14.75
		3F	Not detected



^{1}H NMR (500 MHz, Chloroform-*d*) δ 5.76 (broad singlet, 2H), 5.08 (dddd, *J* = 48.2, 8.1, 6.0, 3.6 Hz, 1H), 2.77 – 2.34 (m, 2H), 1.42 (ddd, *J* = 24.0, 6.3, 1.5 Hz, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 171.84 , 87.82 (d, *J* = 165.9 Hz), 43.46 (d, *J* = 21.8 Hz), 20.76 (d, *J* = 22.4 Hz).

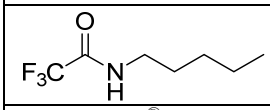
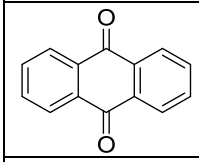
^{19}F NMR (377 MHz, $CDCl_3$) δ -175.31. [reference (C_6F_6 = -164.90)]

Refer to chemdraw above for label	^{13}C Assignment	^{19}F Assignment	^{1}H Assignment
1	N/A	-	δ 5.76 (two broad singlet, 2H),
2	171.84	-	
3	43.46 (d, *J* = 21.8 Hz)	-	5.08 (dddd, *J* = 48.2, 8.1, 6.0, 3.6 Hz, 1H)
5	87.82 (d, *J* = 165.9 Hz)	-	2.77 – 2.34 (m, 2H)
6	20.76 (d, *J* = 22.4 Hz)	-	1.42 (ddd, *J* = 24.0, 6.3, 1.5 Hz, 3H
7	-	-175.31	-

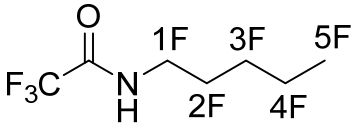
HRMS (ESI-TOF) $[M\text{-}Na]^+$ calculated for $C_4H_8FNNaO^+$ 128.0488, found 128.0483

Appearance: White crystalline solid

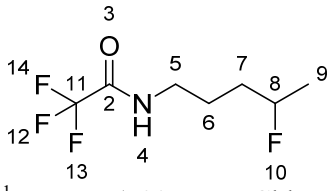
2,2,2-trifluoro-N-(4-fluoropentyl)acetamide

	M.W (mg/mmol)	Amount added	Amount added/mmol
	183.1742	551mg	3.00
Selectfluor®	354.26	708mg	2.00
	208.2160	9.0mg	0.0432
MeCN	-	8mL	-
Reaction Time	26 hours		
Column Chromatography Details	2cm(column outer diameter) X 22cm (SiO_2 length) Crude is dissolved in minimal DCM and separation was performed with gradient elution. Gradient Elution: *n*-Hexane to 12:1(*n*-Hexane:Et_2O) to 4.5:1(*n*-Hexane:Et_2O) Total 2,2,2-trifluoro-N-(4-fluoropentyl)acetamide = 159.0mg(0.79mmol) Yield (based on limiting reagent) =0.79/2.00 X100 = 40%		
	R_f (2,2,2-trifluoro-N-(4-fluoropentyl)acetamide) = 0.09 (5:1, *n*-Hexane,Et_2O);stain $KMnO_4$ R_f (starting material) = 0.19 (5:1, *n*-Hexane:Et_2O); stain $KMnO_4$		

Ratio from ^{19}F NMR



F position	^{19}F Integration Ratio
1F	Not detected
2F	1.00
3F	4.41
4F	18.78
5F	0.59



^{1}H NMR (500 MHz, Chloroform-*d*) δ 6.42 (s, 1H), 4.79 – 4.60 (m, 1H), 3.41 (q, *J* = 6.6 Hz, 2H), 1.79 – 1.57 (m, 4H), 1.34 (dd, *J* = 24.0, 6.2 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 157.72, 157.43, 157.13, 156.84, 119.27, 116.98, 114.69, 112.40, 91.18, 89.86, 39.64, 33.90, 33.74, 24.84, 24.81, 21.05, 20.87.

^{13}C NMR (126 MHz, Chloroform-*d*) δ 157.28 (d, *J* = 36.9 Hz), 115.83 (q, *J* = 287.9 Hz), 90.52 (d, *J* = 164.9 Hz), 39.64, 33.82 (d, *J* = 20.9 Hz), 24.82 (d, *J* = 3.6 Hz), 20.96 (d, *J* = 22.8 Hz).

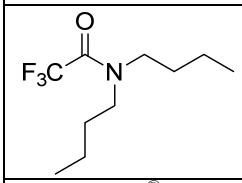
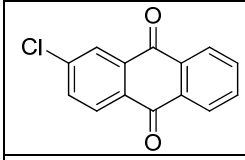
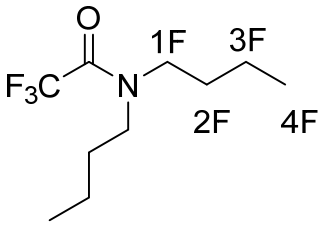
^{19}F NMR (376 MHz, Chloroform-*d*) δ -76.05 , -173.25 (ddqd, *J* = 47.9, 29.4, 23.9, 17.7 Hz).

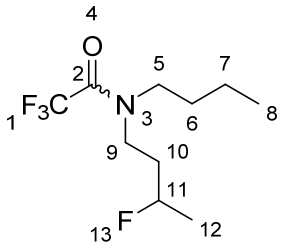
Refer to chemdraw above for label	^{13}C Assignment	^{19}F Assignment	^{1}H Assignment
2	157.28 (d, *J* = 36.9 Hz)	-	-
4	-	-	6.42 (s, 1H)
5	39.64	-	3.41 (q, *J* = 6.6 Hz, 2H)
6	24.82 (d, *J* = 3.6 Hz)	-	1.79 – 1.57 (m, 2H)
7	33.82 (d, *J* = 20.9 Hz)	-	1.79 – 1.57 (m, 2H)
8	90.52 (d, *J* = 164.9 Hz)	-	4.79 – 4.60 (m, 1H)
9	20.96 (d, *J* = 22.8 Hz)	-	1.34 (dd, *J* = 24.0, 6.2 Hz, 3H)
10	-	-173.25	-
11	115.83 (q, *J* = 287.9 Hz)	-	-
12,13,14	-	-76.05	-

HRMS (ESI-TOF) $[M\text{-}Na]^+$ calculated for $C_7H_{12}F_4NO+^+$ 202.0850, found 202.0851

Appearance:

N-butyl-2,2,2-trifluoro-N-(3-fluorobutyl)acetamide

	M.W (mg/mmol)	Amount added	Amount added/mmol
	225.2552	904mg	4.00
Selectfluor®	354.26	708mg	2.00
	242.6572	10.7mg	0.0441
MeCN	-	8mL	-
Reaction Time	42 hours		
Column Chromatography Details	2cm(column outer diameter) X 21.5cm (SiO_2 length) Crude is dissolved in minimal DCM and separation was performed with gradient elution. Gradient Elution: 49:1(*n*-Hexane:DCM)to 36:1(*n*-Hexane:Mixture*) to 20:1(*n*-Hexane:Mixture*) *[Mixture= Et_2O:Ethyl Acetate(4:1)] Total N-butyl-2,2,2-trifluoro-N-(3-fluorobutyl)acetamide obtained = 170.4mg(0.70mmol) Yield (based on limiting reagent) = 0.74/2.00 X100 = 37%		
	R_f (N-butyl-2,2,2-trifluoro-N-(3-fluorobutyl)acetamide) = 0.28 (5:1, *n*-Hexane,Et_2O); stain $KMnO_4$ R_f (starting material) = 0.47 (5:1, *n*-Hexane:Et_2O); stain $KMnO_4$		
Ratio from ^{19}F NMR			Confident assignment of 19F chemical shift is difficult.



mixture of cis- and trans- diastereomer

^{1}H NMR (500 MHz, Chloroform-*d*) δ 4.70 (ddtd, *J* = 49.0, 9.2, 6.2, 3.0 Hz, 1H), 3.64 – 3.44 (m, 2H), 3.44 – 3.28 (m, 2H), 2.06 – 1.77 (m, 2H), 1.59 (m, 2H), 1.43 – 1.27 (m, 5H), 0.95 (m, 3H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 157.30 – 156.28 (m), 120.33 – 112.45 (m), 89.61 – 87.45 (m), 48.37 – 46.82 (m), 44.27 – 43.68 (m), 89.00 – 87.42 (m), 36.56 – 33.74 (m), 31.23 – 28.64 (m), 21.36 – 20.61 (m), 19.89 (d, *J* = 29.4 Hz), 13.67 (d, *J* = 15.3 Hz), 89.60 – 87.92 (m).

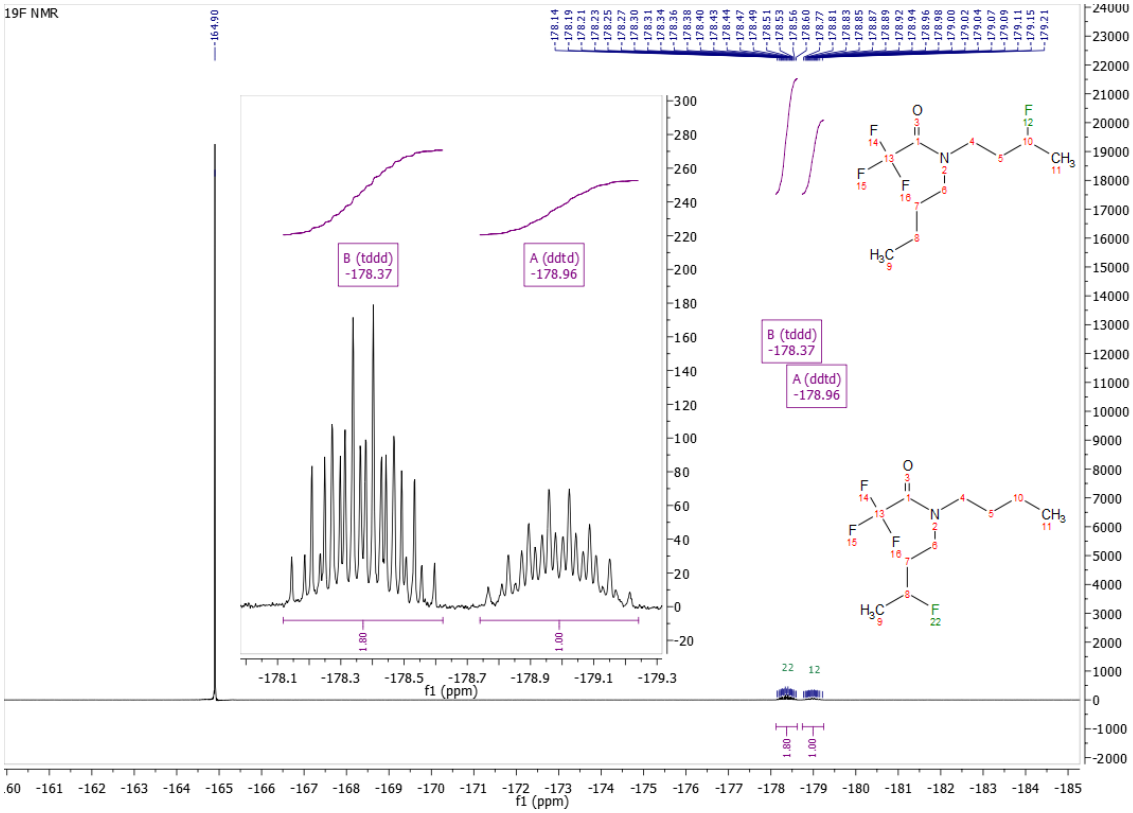
^{19}F NMR (376 MHz, Chloroform-*d*) δ -69.12 , -69.15 , -175.32 , -175.91 .

Refer to chemdraw above for label	^{13}C Assignment	^{19}F Assignment	^{1}H Assignment
1	120.33 – 112.45 (m)	-69.12 , -69.15	-
2	157.30 – 156.28 (m)	-	-
5	48.37 – 46.82 (m)	-	3.44 – 3.28 (m, 2H)
6	31.23 – 28.64 (m)	-	1.59 (m, 2H)
7	20.07 – 19.71 (m)	-	1.43 – 1.27 (m, 2H)
8	13.80 – 13.55 (m)	-	0.95 (m, 3H)
9	44.27 – 43.68 (m) (d, *J* = 4.1 Hz)	-	3.64 – 3.44 (m, 2H)
10	36.56 – 33.74 (m) (d, 20.6 Hz)	-	2.06 – 1.77 (m, 2H)
11	89.00 – 87.42 (m) (d, *J* = 165.2 Hz) (d, *J* = 166.2 Hz)	-	4.70 (ddtd, *J* = 49.0, 9.2, 6.2, 3.0 Hz, 1H)
12	21.36 – 20.61 (m) (d, *J* = 9.6 Hz)	-	1.43 – 1.27 (m, 3H)
13	-	-175.32 , -175.91	-

HRMS (ESI-TOF) $[M-Na]^+$ calculated for $C_{10}H_{18}F_4NO^+$ 244.1320, found 244.1322

Appearance: Pale Yellow Liquid

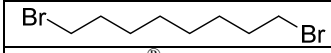
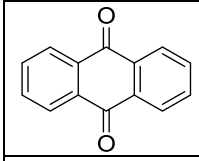
Determination of conformation isomers

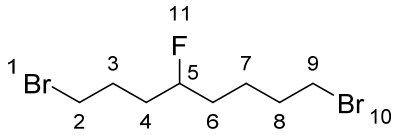


Assignment based on DFT calculated NMR shielding tensor corrected with least-square linear regression model.

See Section: “19F NMR chemical shifts”

1,8-dibromo-4-fluorooctane

	M.W (mg/mmol)	Amount added	Amount added/mmol
	272.0240	816mg	3.00
Selectfluor®	354.26	716mg	2.02
	208.2160	8.7mg	0.0418
MeCN	-	8mL	-
Reaction Time	48 hours		
Column Chromatography Details	2cm(column outer diameter) X 23.4cm (SiO_2 length) Crude is dissolved in minimal DCM and separation was performed with gradient elution. Gradient Elution: *n*-Hexane to 99:1(*n*-Pentane:DCM) to 99:1(*n*-Pentane:Et_2O) Total 1,8-dibromo-3-fluorooctane obtained = 74.8mg(0.26mmol) Total 1,8-dibromo-4-fluorooctane obtained = 181.9mg(0.63mmol) Yield (based on limiting reagent) = 0.89/2.02 X100 = 44%		
	R_f (1,8-dibromo-4-fluorooctane) = 0.19 (99:1, *n*-pentane,DCM, develop the same TLC plate twice); stain CAM blue R_f (1,8-dibromo-3-fluorooctane) = 0.27 (99:1, *n*-pentane,DCM, develop the same TLC plate twice); stain CAM blue R_f (starting material) = 0.53 (99:1, *n*-pentane,DCM, develop the same TLC plate twice); stain CAM blue		



^{1}H NMR (500 MHz, Chloroform-*d*) δ 4.51 (dtt, *J* = 49.5, 7.9, 4.1 Hz, 1H), 3.53 – 3.39 (m, 4H), 2.12 – 1.85 (m, 4H), 1.81 – 1.49 (m, 6H).

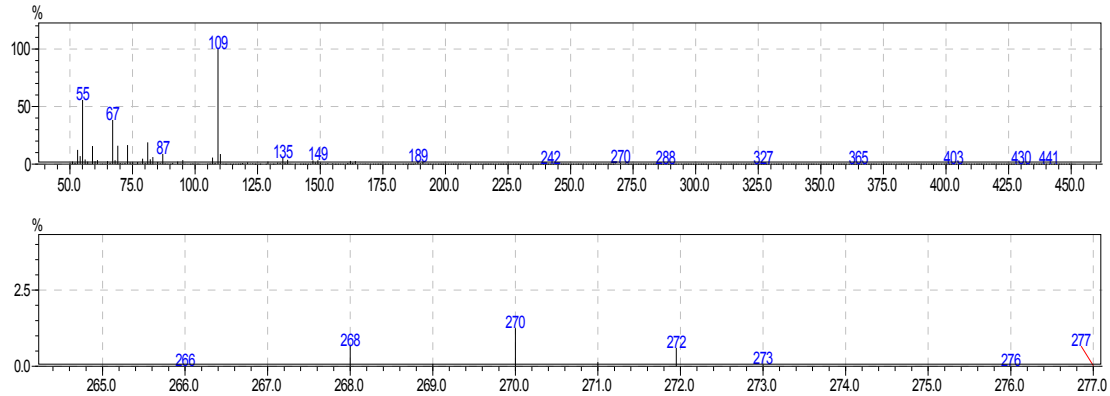
^{13}C NMR (126 MHz, $CDCl_3$) δ 93.92, 92.58, 34.32, 34.15, 33.70, 33.53, 33.45, 33.39, 32.42, 28.40, 28.37, 23.80, 23.77.

^{13}C NMR (126 MHz, Chloroform-*d*) δ 93.25 (d, *J* = 168.7 Hz), 34.23 (d, *J* = 21.0 Hz), 33.61 (d, *J* = 21.0 Hz), 33.45 , 33.39 , 32.42 , 28.38 (d, *J* = 3.8 Hz), 23.79 (d, *J* = 4.5 Hz).

^{19}F NMR (376 MHz, Chloroform-*d*) δ -181.54 (dddd, *J* = 57.4, 49.8, 24.3, 15.1 Hz).

Refer to chemdraw above for label	^{13}C Assignment	^{19}F Assignment	^{1}H Assignment
2	33.45	-	3.53 – 3.39 (m, 2H)
3	28.40, 28.37 (d, *J* = 3.8 Hz)	-	2.12 – 1.85 (m, 2H)
4	33.70, 33.53 (d, *J* = 21.0 Hz)	-	1.81 – 1.49 (m, 2H)
5	93.92, 92.58 (d, *J* = 168.7 Hz),	-	4.51 (dtt, *J* = 49.5, 7.9, 4.1 Hz, 1H)
6	34.32, 34.15 (d, *J* = 21.0 Hz)	-	1.81 – 1.49 (m, 2H)
7	23.80, 23.77 (d, *J* = 4.5 Hz)	-	1.81 – 1.49 (m, 2H)
8	32.42	-	2.12 – 1.85 (m, 2H)
9	33.39	-	3.53 – 3.39 (m, 2H)
11	-	-181.54	-

LRMS (EI) $[M\text{-}HF]^+$ calculated for $C_8H_{14}Br_2$ 269.9 (100.0%), 267.9 (51.4%), 271.9 (48.6%), found 270(100%) 267.95 (53%) 272(48%)

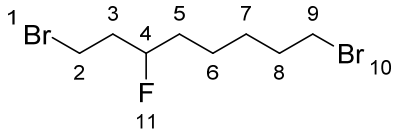


Appearance: Colorless liquid

Reference: *Angew. Chem. Int. Ed.* **2012**, *51*, 10580-10583.

1,8-dibromo-3-fluorooctane

Refer to 1,8-dibromo-4-fluorooctane



^{1}H NMR (500 MHz, Chloroform-*d*) δ 4.76 – 4.59 (m, 1H), 3.51 (dd, *J* = 8.0, 5.4 Hz, 2H), 3.41 (t, *J* = 6.7 Hz, 2H), 2.26 – 1.94 (m, 2H), 1.88 (p, *J* = 6.9 Hz, 2H), 1.77 – 1.57 (m, 2H), 1.54 – 1.38 (m, 4H).

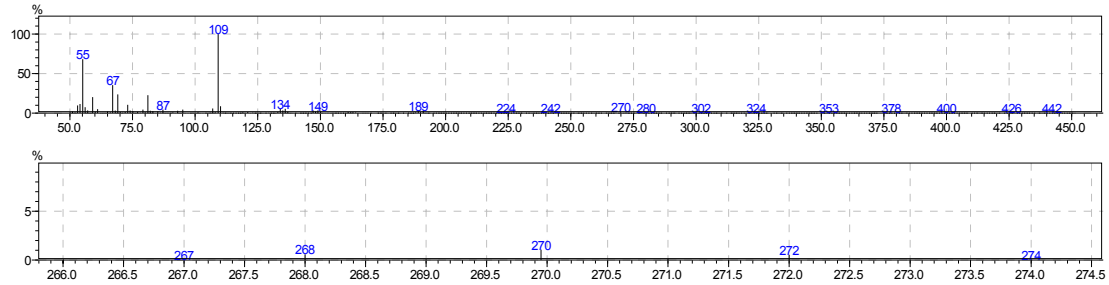
^{13}C NMR (101 MHz, $CDCl_3$) δ 92.55, 90.87, 38.40, 38.19, 34.77, 34.57, 33.62, 32.56, 28.75, 28.71, 27.89, 24.22, 24.17.

^{13}C NMR (101 MHz, Chloroform-*d*) δ 91.71 (d, *J* = 169.0 Hz), 38.30 (d, *J* = 21.2 Hz), 34.67 (d, *J* = 20.5 Hz), 33.62 , 32.56 , 28.73 (d, *J* = 4.5 Hz), 27.89 , 24.19 (d, *J* = 4.3 Hz).

^{19}F NMR (376 MHz, Chloroform-*d*) δ -185.05 (dtt, *J* = 48.7, 31.2, 16.1 Hz).

Refer to chemdraw above for label	^{13}C Assignment	^{19}F Assignment	^{1}H Assignment
2	28.75, 28.71 (d, *J* = 4.5 Hz)	-	3.51 (dd, *J* = 8.0, 5.4 Hz, 2H)
3	38.40, 38.19 (d, *J* = 21.2 Hz)	-	2.26 – 1.94 (m, 2H)
4	92.55, 90.87 (d, *J* = 169.0 Hz)	-	δ 4.76 – 4.59 (m, 1H)
5	34.77, 34.57 (d, *J* = 20.5 Hz)	-	1.77 – 1.57 (m, 2H)
6	24.22, 24.17 (d, *J* = 4.3 Hz)	-	1.54 – 1.38 (m, 4H)
7	28.79	-	
8	32.56	-	1.88 (p, *J* = 6.9 Hz, 2H)
9	33.62	-	3.41 (t, *J* = 6.7 Hz, 2H)
11	-	-181.05	-

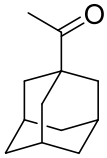
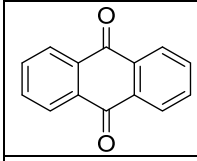
LRMS (EI) $[M-HF]^+$ calculated for $C_8H_{14}Br_2$ 269.9 (100.0%), 267.9 (51.4%), 271.9 (48.6%), found 270(100%) 267.95 (55%) 272(51%)

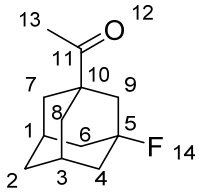


Appearance: Colorless liquid

Reference: *Angew. Chem. Int. Ed.* **2012**, *51*, 10580-10583.

1-((1r,3s,5R,7S)-3-fluoroadamantan-1-yl)ethan-1-one

	M.W (mg/mmol)	Amount added	Amount added/mmol
	178.2750	533.4	2.99
Selectfluor®	354.26	709.8mg	2.00
	208.2160	8.4mg	0.0399
MeCN	-	8mL	-
Reaction Time	24 hours		
Column Chromatography Details	2cm(column outer diameter) X 17cm (SiO_2 length) Crude is dissolved in minimal DCM and separation was performed with gradient elution. Gradient Elution: *n*-Hexane to 20:1(*n*-Hexane:Ethyl Acetate) to 20:1(*n*-Hexane:Et_2O) Total 1-((1r,3s,5R,7S)-3-fluoroadamantan-1-yl)ethan-1-one obtained = 235.0mg(1.20mmol) Yield (based on limiting reagent) = 1.20/2.00 X100 = 60%		
	R_f (1-((1r,3s,5R,7S)-3-fluoroadamantan-1-yl)ethan-1-one) = 0.41 (5:1, *n*-Hexane:Ethyl Acetate, develop the same TLC plate twice); stain 2,4-DNPH R_f (starting material) = 0.60 (5:1, *n*-Hexane:Ethyl Acetate, develop the same TLC plate twice); stain 2,4-DNPH		



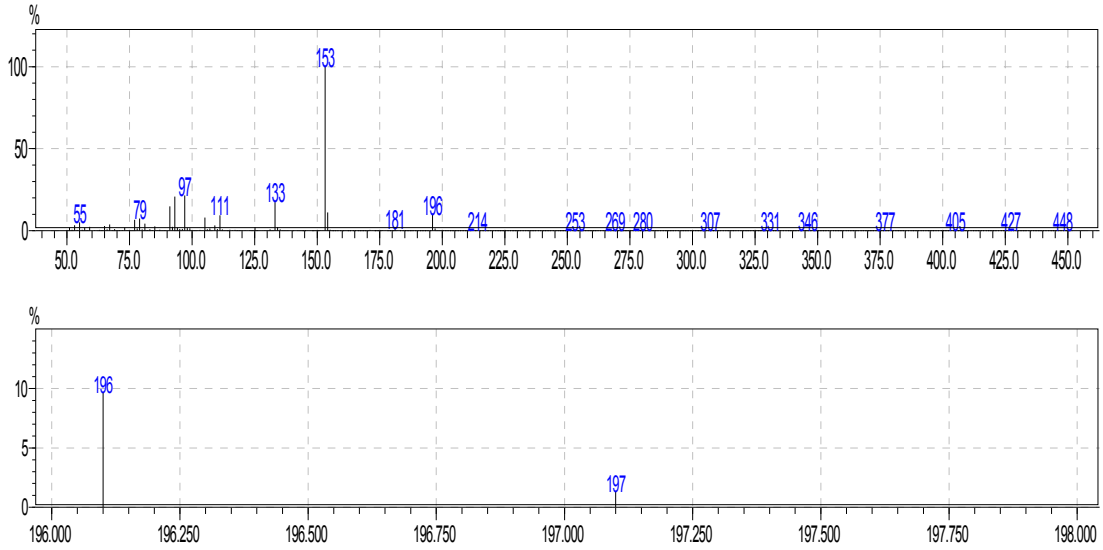
^{1}H NMR (400 MHz, Chloroform-*d*) δ 2.43 – 2.32 (m, 2H), 2.12 (s, 3H), 1.96 – 1.92 (m, 2H), 1.91 – 1.84 (m, 4H), 1.78 – 1.66 (m, 4H), 1.66 – 1.59 (m, 2H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 211.31 , 92.43 (d, *J* = 184.2 Hz), 50.82 (d, *J* = 9.1 Hz), 43.20 (d, *J* = 19.5 Hz), 41.87 (d, *J* = 17.5 Hz), 37.02 (d, *J* = 2.0 Hz), 34.89 (d, *J* = 2.0 Hz), 30.90 (d, *J* = 9.9 Hz), 24.55 .

^{19}F NMR (377 MHz, $CDCl_3$) δ -135.31 [reference (C_6F_6 = -164.92)]

Refer to chemdraw above for label	^{13}C Assignment	^{19}F Assignment	^{1}H Assignment
1,3	30.90 (d, *J* = 9.9 Hz)	-	2.43 – 2.32 (m, 2H)
2	34.89 (d, *J* = 2.0 Hz)	-	1.66 – 1.59 (m, 2H).
4,6	41.87 (d, *J* = 17.5 Hz)	-	1.91 – 1.84 (m, 4H)
5	92.43 (d, *J* = 184.2 Hz)	-	-
7,8	37.02 (d, *J* = 2.0 Hz)	-	1.78 – 1.66 (m, 4H)
9	50.82 (d, *J* = 9.1 Hz)	-	1.96 – 1.92 (m, 2H)
10	50.82 (d, *J* = 9.1 Hz)	-	-
11	211.31	-	-
13	24.55	-	2.12 (s, 3H),
14	-	-135.31	-

LRMS (EI) $[M]^+$ calculated for $C_{12}H_{17}FO$ 196.1 (100.0%), 197.1 (13.0%), found 196.1(100%), 197.1(13.7%)

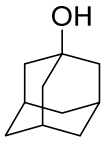
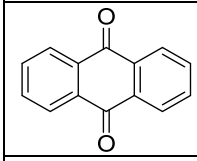


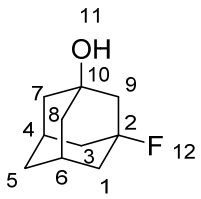
Appearance: White Solid

Reference: *Russ. J. Org. Chem.* **2003**, *39*, 739-741.

(1r,3s,5R,7S)-3-fluoroadamantan-1-ol

(*Performed by Chin Kek Foo)

	M.W (mg/mmol)	Amount added	Amount added/mmol
	152.2370	461.4mg	3.03
Selectfluor®	354.26	710mg	2.00
	208.2160	8.9mg	0.0427
MeCN	-	8mL	-
Reaction Time	24 hours		
Column Chromatography Details	4cm(column outer diameter) X 19cm (SiO_2 length) Crude is dissolved in minimal DCM and separation was performed with gradient elution. Gradient Elution: 15:1 (*n*-Hexane:Ethyl Acetate), then 10:1 (*n*-Hexane:Ethyl Acetate), and finally 6:1 (*n*-Hexane:Ethyl Acetate) Total (1r,3s,5R,7S)-3-fluoroadamantan-1-ol obtained = 231mg(1.36mmol) Yield (based on limiting reagent) = 1.36/2.00 X 100 = 68%		
	R_f ((1r,3s,5R,7S)-3-fluoroadamantan-1-ol) = 0.25 (4:1, *n*-Hexane,Ethyl Acetate); Hanneson's stain R_f (starting material) 0.33 (4:1, *n*-Hexane,Ethyl Acetate); Hanneson's stain		



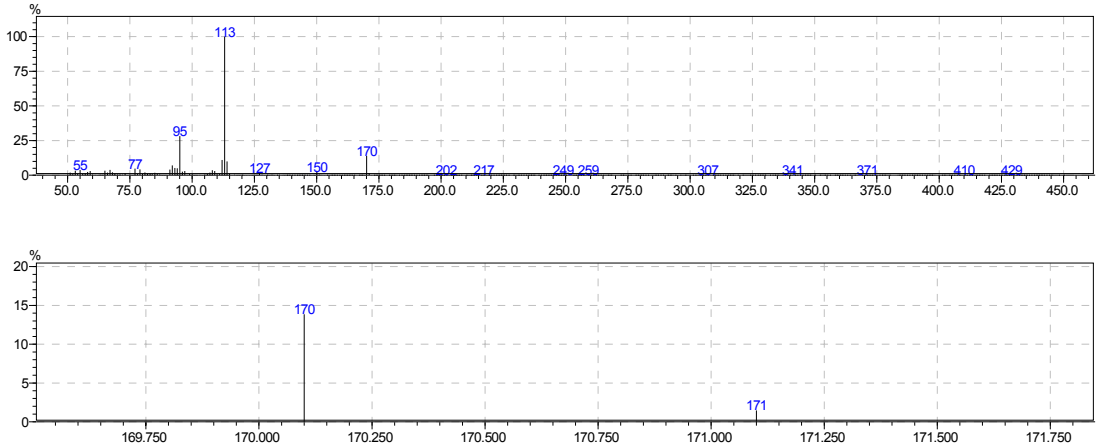
^{1}H NMR (400 MHz, Chloroform-*d*) δ 2.37 (dt, *J* = 5.9, 3.3 Hz, 2H), 1.90 (d, *J* = 5.7 Hz, 2H), 1.82 (dd, *J* = 5.6, 3.1 Hz, 4H), 1.73 – 1.61 (m, 4H), 1.55 (s, 1H), 1.50 (t, *J* = 3.3 Hz, 2H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 93.30 (d, *J* = 185.7 Hz), 71.03 (d, *J* = 11.9 Hz), 50.43 (d, *J* = 17.2 Hz), 43.79 (d, *J* = 1.6 Hz), 41.36 (d, *J* = 17.5 Hz), 34.41 (d, *J* = 2.1 Hz), 31.39 (d, *J* = 10.3 Hz).

^{19}F NMR (376 MHz, $CDCl_3$) δ -133.19.

Refer to chemdraw above for label	^{13}C Assignment	^{19}F Assignment	^{1}H Assignment
1,3	41.36 (d, *J* = 17.5 Hz)	-	1.82 (dd, *J* = 5.6, 3.1 Hz, 4H)
2	93.30 (d, *J* = 185.7 Hz)	-	-
4,6	31.39 (d, *J* = 10.3 Hz)	-	2.37 (dt, *J* = 5.9, 3.3 Hz, 2H)
5	34.41 (d, *J* = 2.1 Hz)	-	1.50 (t, *J* = 3.3 Hz, 2H)
7,8	43.79 (d, *J* = 1.6 Hz)	-	1.73 – 1.61 (m, 4H)
9	50.43 (d, *J* = 17.2 Hz)	-	1.90 (d, *J* = 5.7 Hz, 2H)
10	71.03 (d, *J* = 11.9 Hz)	-	-
11	-	-	1.55 (s, 1H) Indistinguishable with residual H_2O peak
12	-	-133.19.	-

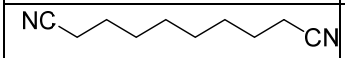
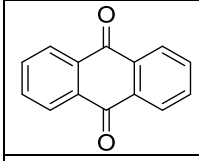
LRMS (EI) $[M]^+$ calculated for $C_{10}H_{15}FO$ 170.1 (100.0%), 171.1 (10.8%), found 170.1(100%), 197.1(10.6%)

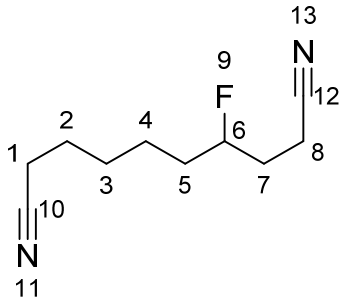


Appearance: White Solid

Reference: *Org. Lett.* **2013**, *15*, 2160-2163.

4-fluorodecanedinitrile

	M.W (mg/mmol)	Amount added	Amount added/mmol
	164.2520	329mg	2.00
Selectfluor®	354.26	1062.8mg	3.00
	208.2160	8.6mg	0.0394
MeCN	-	8mL	-
Reaction Time	48 hours		
Column Chromatography Details	2cm(column outer diameter) X 19.5cm (SiO_2 length) Crude is dissolved in minimal DCM and separation was performed with gradient elution. Gradient Elution: *n*-Hexane to 19:1(*n*-HexaneMixture*) to 2:1(*n*-Hexane:Mixture*) to 3:1(*n*-Hexane:Ethyl Acetate) *[Mixture=Et_2O:Ethyl Acetate(1:1)] Total 4-fluorodecanedinitrile obtained = 30.0(0.16mmol) Total 5-fluorodecanedinitrile obtained = 119.8(0.66mmol) Yield (based on limiting reagent) = 0.82/2.00 X100 = 41%		
	R_f (4- and 5-fluorodecanedinitrile) = 0.34 (1:1, *n*-Hexane,Ethyl Acetate); stain CAM white on heating with hair dryer R_f (starting material) = 0.44 (15:1, *n*-Hexane,Ethyl Acetate); stain CAM white on heating with hair dryer		



^{1}H NMR (500 MHz, Chloroform-*d*) δ 4.66 – 4.50 (m, 1H), 2.51 (ddd, *J* = 8.5, 6.6, 2.1 Hz, 2H), 2.36 (t, *J* = 7.1 Hz, 2H), 1.99 – 1.83 (m, 2H), 1.77 – 1.61 (m, 4H), 1.61 – 1.37 (m, 4H)*Overlap with H_2O peak.

^{13}C NMR (126 MHz, Chloroform-*d*) δ 119.55 , 119.00 , 91.74 (d, *J* = 170.7 Hz), 34.47 (d, *J* = 20.6 Hz), 31.03 (d, *J* = 21.5 Hz), 28.35 , 25.21 , 24.27 (d, *J* = 4.2 Hz), 17.09 , 13.41 (d, *J* = 4.9 Hz).

^{19}F NMR (377 MHz, $CDCl_3$) δ -184.94

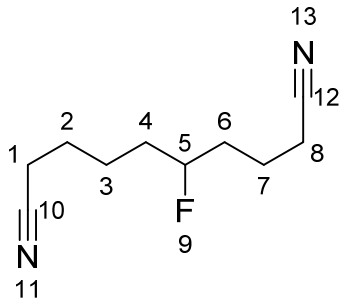
Refer to chemdraw above for label	^{13}C Assignment	^{19}F Assignment	^{1}H Assignment
1	17.09	-	2.36 (t, *J* = 7.1 Hz, 2H)
2	25.21	-	1.77 – 1.61 (m, 2H)
3	28.35	-	1.61 – 1.37 (m, 2H)*
4	24.27 (d, *J* = 4.2 Hz)	-	1.61 – 1.37 (m, 2H)*
5	34.47 (d, *J* = 20.6 Hz)	-	1.77 – 1.61 (m, 2H)
6	91.74 (d, *J* = 170.7 Hz)	-	4.68 – 4.49 (m, 1H)
7	31.03 (d, *J* = 21.5 Hz)	-	1.99 – 1.83 (m, 2H)
8	13.41 (d, *J* = 4.9 Hz)	-	2.51 (ddd, *J* = 8.5, 6.6, 2.1 Hz, 2H)
9	-	-184.94	-
10	119.55	-	-
12	119.00	-	-

HRMS (ESI-TOF) $[M-H]^+$ calculated for $C_8H_{14}FO_4^+$ 193.0871, found 193.0880

Appearance: Colorless Liquid

5-fluorodecanedinitrile

Refer to 4-fluorodecanedinitrile



^{1}H NMR (500 MHz, Chloroform-*d*) δ 4.51 (dtt, *J* = 46.1, 8.1, 3.4 Hz, 1H), 2.41 (td, *J* = 6.8, 3.2 Hz, 2H), 2.37 (t, *J* = 6.9 Hz, 2H), 1.97 – 1.36 (m, 10H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 119.39 , 119.25 , 92.91 (d, *J* = 169.5 Hz), 34.27 (d, *J* = 21.1 Hz), 33.85 (d, *J* = 21.2 Hz), 25.14 , 24.33 (d, *J* = 4.1 Hz), 21.37 (d, *J* = 3.8 Hz), 17.11 , 17.02 .

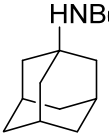
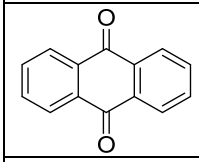
^{19}F NMR (377 MHz, $CDCl_3$) δ -182.49

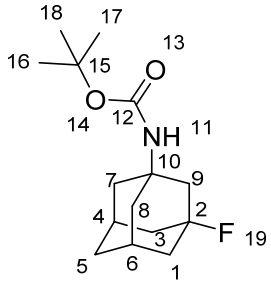
Refer to chemdraw above for label	^{13}C Assignment	^{19}F Assignment	^{1}H Assignment
1	17.02	-	2.37 (t, *J* = 6.9 Hz, 2H)
2	25.14	-	1.97 – 1.36 (m, 2H)
3	24.33 (d, *J* = 4.1 Hz)	-	1.97 – 1.36 (m, 2H)
4	34.27 (d, *J* = 21.1 Hz)	-	1.97 – 1.36 (m, 2H)
5	92.91 (d, *J* = 169.5 Hz)	-	4.51 (dtt, *J* = 46.1, 8.1, 3.4 Hz, 1H)
6	33.85 (d, *J* = 21.2 Hz)	-	1.97 – 1.36 (m, 2H)
7	21.37 (d, *J* = 3.8 Hz)	-	1.97 – 1.36 (m, 2H)
8	17.11	-	2.41 (td, *J* = 6.8, 3.2 Hz, 2H)
9	-	-182.49	-
10	119.39	-	-
12	119.25	-	-

HRMS (ESI-TOF) $[M-H]^+$ calculated for $C_8H_{14}FO_4^+$ 193.0871, found 193.0880

Appearance: Colorless liquid

tert-butyl ((1r,3s,5R,7S)-3-fluoroadamantan-1-yl)carbamate

	M.W (mg/mmol)	Amount added	Amount added/mmol
	251.3700	470.2mg	1.87
Selectfluor®	354.26	725.8mg	2.05
	208.2160	8.4mg	0.0403
MeCN	-	8mL	-
Reaction Time	24 hours		
Column Chromatography Details	2cm(column outer diameter) X 19.7cm (SiO_2 length) Crude is dissolved in minimal DCM and separation was performed with gradient elution. Gradient Elution: *n*-Hexane to 25:1(*n*-HexaneMixture*) to 20:1(*n*-Hexane:Mixture*) to 9:1(*n*-Hexane:Ethyl Acetate) *[Mixture= Et_2O:Ethyl Acetate(1:3)] Total tert-butyl ((1r,3s,5R,7S)-3-fluoroadamantan-1-yl)carbamateobtained = 238.9mg(0.89mmol) Yield (based on limiting reagent) = 0.89/2.02 X100 = 44%		
	R_f (tert-butyl ((1r,3s,5R,7S)-3-fluoroadamantan-1-yl)carbamate) = 0.27 (5:1, *n*-Hexane:Ethyl Acetate); stain $KMnO_4$ R_f (starting material) = 0.45 (5:1, *n*-Hexane:Ethyl Acetate); stain $KMnO_4$		



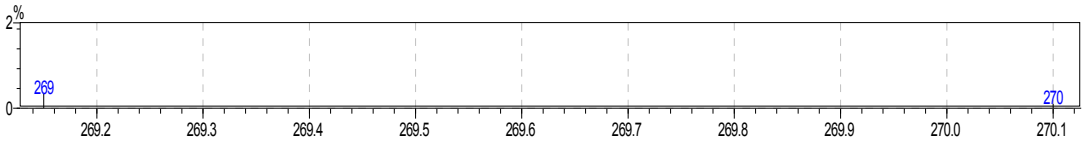
^{1}H NMR (400 MHz, Chloroform-*d*) δ 4.46 (s, 1H), 2.32 (dt, *J* = 5.4, 3.0 Hz, 2H), 2.09 (d, *J* = 6.0 Hz, 2H), 1.95 – 1.74 (m, 8H), 1.60 – 1.48 (m, 2H), 1.43 (s, 9H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 154.14, 92.47 (d, *J* = 184.5 Hz), 79.18, 53.67 (d, *J* = 12.1 Hz), 46.81 (d, *J* = 18.4 Hz), 41.67 (d, *J* = 17.5 Hz), 40.49, 34.73 (d, *J* = 2.0 Hz), 30.97 (d, *J* = 10.3 Hz), 28.43

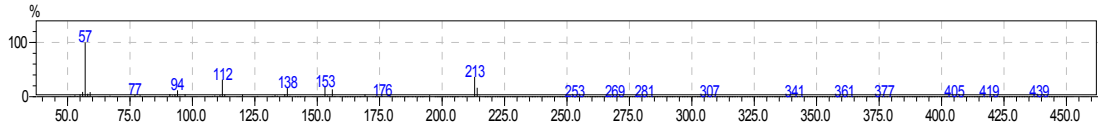
^{19}F NMR (376 MHz, $CDCl_3$) δ -132.66.

Refer to chemdraw above for label	^{13}C Assignment	^{19}F Assignment	^{1}H Assignment
1,3	41.67 (d, *J* = 17.5 Hz)	-	1.86 (m, 4H)
2	92.47 (d, *J* = 184.5 Hz)	-	-
4,6	30.97 (d, *J* = 10.3 Hz)	-	2.32 (dt, *J* = 5.4, 3.0 Hz, 2H)
5	34.73 (d, *J* = 2.0 Hz)	-	1.54 (m, 2H)
7,8	40.49	-	1.86 (m, 4H)
9	46.81 (d, *J* = 18.4 Hz)	-	2.09 (d, *J* = 6.0 Hz, 2H)
10	53.67 (d, *J* = 12.1 Hz)	-	-
11	-	-	4.46 (s, 1H)
12	154.14	-	-
15	79.18	-	-
16,17,18	28.43	-	1.43 (s, 9H)
19	-	-132.66	-

LRMS (EI) $[M]^+$ calculated for $C_{15}H_{24}FNO_2$ 269.2, found 269.2



LRMS (EI) $[M\text{-}C_4H_8]^+$ calculated for $C_{11}H_{16}FNO_2$ 213.1, found 213.1

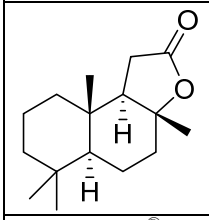
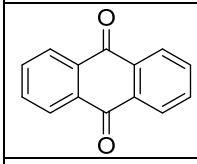


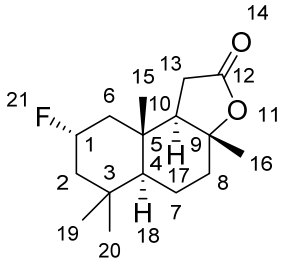
Appearance: White solid

HRMS (ESI-TOF) $[M\text{-}Na]^+$ calculated for $C_{15}H_{25}NFO_2^+$ 270.1864, found 270.1869

Fluorinated (+)-Sclareolide

(3aR,5aS,8S,9aS,9bR)-8-fluoro-3a,6,6,9a-tetramethyldecahydronaphtho[2,1-b]furan-2(1H)-one

	M.W (mg/mmol)	Amount added	Amount added/mmol
	250.3820	751.4mg	3.00
Selectfluor®	354.26	720mg	2.03
	208.2160	8.6mg	0.0413
MeCN	-	8mL	-
Reaction Time	26 hours		
Column Chromatography Details	2cm(column outer diameter) X 21.5cm (SiO_2 length) Crude is dissolved in minimal DCM and separation was performed with gradient elution. Gradient Elution: 49:1(*n*-Hexane:DCM) to 15:1(*n*-HexaneMixture*) to 15:1(*n*-Hexane:Ethyl Acetate) to 5:1(*n*-Hexane:Ethyl Acetate) *[Mixture=Ethyl Acetate:Et_2O(1:1)] Total Fluorinated (+)-Sclareolide obtained = 414.5mg(1.54mmol) Yield (based on limiting reagent) = 1.54/2.00 X100 = 77%		
	R_f (3-F and 2-F (+)-Sclareolide) = 0.22 (15:1, *n*-Hexane:Ethyl Acetate, develop the same TLC plate twice); stain CAM blue R_f (starting material) = 0.44 (15:1, *n*-Hexane:Ethyl Acetate, develop the same TLC plate twice); stain CAM blue		



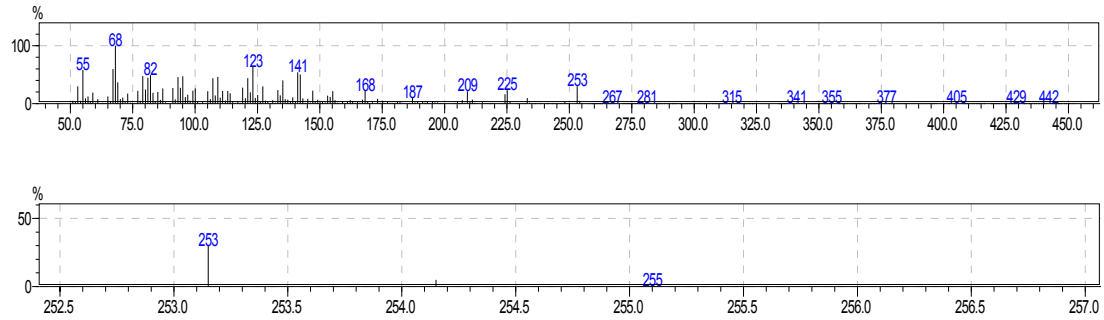
^{1}H NMR (400 MHz, Chloroform-*d*) δ 4.84 (dtt, *J* = 48.0, 11.3, 4.7 Hz, 1H), 2.46 (dd, *J* = 16.2, 14.7 Hz, 1H), 2.28 (dd, *J* = 16.2, 6.5 Hz, 1H), 2.11 (dt, *J* = 12.0, 3.3 Hz, 1H), 2.08 – 1.95 (m, 3H), 1.92 (dq, *J* = 14.2, 3.3 Hz, 1H), 1.71 (td, *J* = 12.5, 4.2 Hz, 1H), 1.44 – 1.30 (m, 5H), 1.24 – 1.10 (m, 2H), 1.00 (s, 3H), 0.96 (s, 3H), 0.90 (s, 3H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 176.07 , 87.61 (d, *J* = 167.9 Hz), 85.81 , 58.79 , 56.05 (d, *J* = 2.2 Hz), 47.87 (d, *J* = 16.0 Hz), 45.25 (d, *J* = 17.4 Hz), 38.37 , 37.47 (d, *J* = 11.8 Hz), 35.00 (d, *J* = 12.1 Hz), 33.23 , 28.68 , 21.80 , 21.62 , 20.12 (d, *J* = 1.5 Hz), 16.13 .

^{19}F NMR (376 MHz, Chloroform-*d*) δ -179.87 (dtt, *J* = 48.1, 11.2, 5.6 Hz).

Refer to chemdraw above for label	^{13}C Assignment	^{19}F Assignment	^{1}H Assignment
1	87.61 (d, *J* = 167.9 Hz)	-	4.84 (dtt, *J* = 48.0, 11.3, 4.7 Hz, 1H)
2	47.87 (d, *J* = 16.0 Hz)	-	1.44 – 1.30 (m, 1H) 2.08 – 1.95 (m, 1H)
3	35.00 (d, *J* = 12.1 Hz)	-	-
4(H18)	56.05 (d, *J* = 2.2 Hz)	-	1.24 – 1.10 (m, 1H)
5	37.47 (d, *J* = 11.8 Hz)	-	-
6	45.25 (d, *J* = 17.4 Hz)	-	1.24 – 1.10 (m, 1H) 2.08 – 1.95 (m, 1H)
7	20.12 (d, *J* = 1.5 Hz)	-	1.44 – 1.30 (m, 1H) 1.92 (dq, *J* = 14.2, 3.3 Hz, 1H)
8	38.37	-	1.71 (td, *J* = 12.5, 4.2 Hz, 1H) 2.11 (dt, *J* = 12.0, 3.3 Hz, 1H)
9	85.81	-	-
10(H17)	58.79	-	2.08 – 1.95 (m, 1H)
12	176.07	-	
13	28.68	-	2.46 (dd, *J* = 16.2, 14.7 Hz, 1H), 2.28 (dd, *J* = 16.2, 6.5 Hz, 1H)
15	16.13	-	0.96 (s, 3H)
16	21.62	-	1.44 – 1.30 (m, 3H)
19	33.23	-	1.00 (s, 3H)
20	21.80	-	0.90 (s, 3H)
21	-	-179.87 (dtt, *J* = 48.1, 11.2, 5.6 Hz)	-

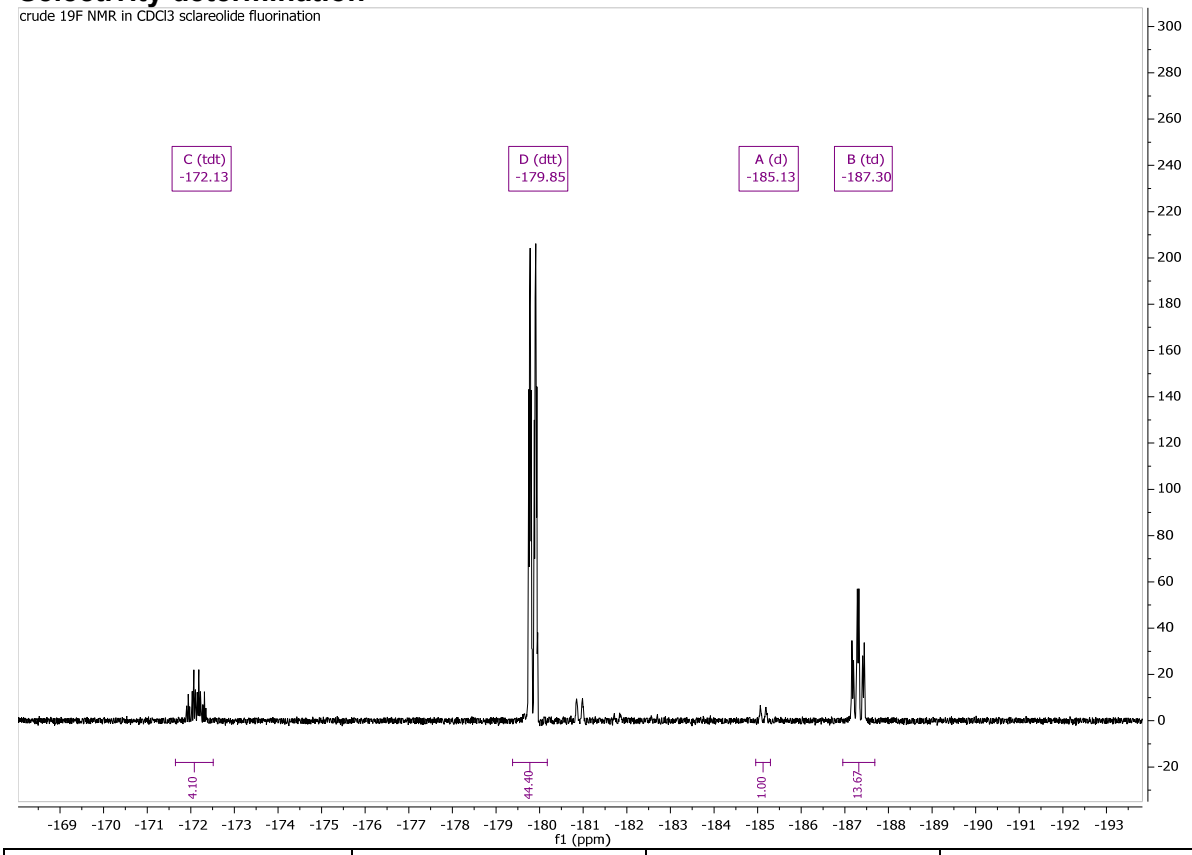
LRMS (EI) $[M\text{-}CH_3]^+$ calculated for $C_{15}H_{22}FO_2^+$ 253.1599 (100.0%), 254.1632 (16.2%), 255.1666 (1.2%), found 253.15(100%), 254.10(16.5%), 255.10(2.2%)

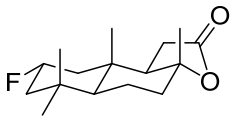
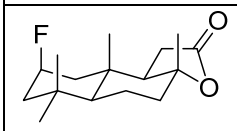
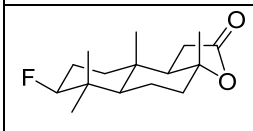
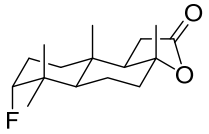


Appearance: white solid

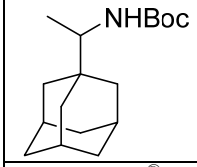
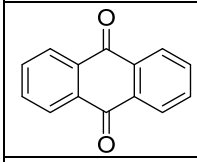
Reference: *Science* **2012**, *337*, 1322-1325.

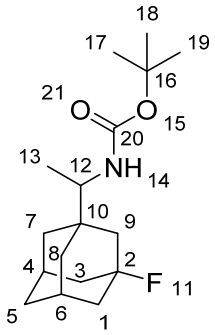
Selectivity determination



	Calculated 19F NMR shielding tensor	Predicted 19F NMR chemical shift from linear regression model (see Calculated 19F NMR chemical shifts)/ppm	Experimental 19F chemical shift(reference to C_6F_6 at -164/)/ppm
	374.144	-180.65	-179.85
	363.9657	-170.98	-172.13
	379.0884	-185.35	-185.13
	382.9581	-189.03	-187.30

tert-butyl (1-((1r,3s,5R,7S)-3-fluoroadamantan-1-yl)ethyl)carbamate

	M.W (mg/mmol)	Amount added	Amount added/mmol
	279.4240	839.4mg	3.00
Selectfluor®	354.26	776mg	2.19
	208.2160	8.4mg	0.0403
MeCN	-	8mL	-
Reaction Time	25 hours		
Column Chromatography Details	2cm(column outer diameter) X 22.7cm (SiO_2 length) Crude is dissolved in minimal DCM and separation was performed with gradient elution. Gradient Elution: *n*-Hexane to 50:1:1(*n*-Hexane:Et_2O:Ethyl Acetate) to 30:1:1(*n*-Hexane:Et_2O:Ethyl Acetate) Total tert-butyl (1-((1r,3s,5R,7S)-3-fluoroadamantan-1-yl)ethyl)carbamate obtained = 350.4mg(1.18mmol) Yield (based on limiting reagent) = 1.18/2.07 X100 =57%		
	R_f (tert-butyl (1-((1r,3s,5R,7S)-3-fluoroadamantan-1-yl)ethyl)carbamate) = 0.25 (5:1, *n*-Hexane:Ethyl Acetate); stain $KMnO_4$ R_f (starting material) = 0.31 (5:1, *n*-Hexane:Ethyl Acetate); stain $KMnO_4$		



^{1}H NMR (500 MHz, Chloroform-*d*) δ 4.39 – 4.07 (m, 1H), 3.54 – 3.30 (m, 1H), 2.34 – 2.26 (m, 2H), 1.89 – 1.76 (m, 4H), 1.71 – 1.50 (m, 4H), 1.44 (m, 13H), 1.04 (d, *J* = 6.9 Hz, 3H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 155.67 , 93.18 (d, *J* = 183.1 Hz), 79.12 , 53.53 , 43.22 (d, *J* = 17.7 Hz), 42.23 (d, *J* = 18.1 Hz), 41.28 (d, *J* = 9.1 Hz), 37.00 (d, *J* = 20.1 Hz), 35.30 (d, *J* = 2.0 Hz), 30.98 (dd, *J* = 9.8, 6.3 Hz), 28.44 , 15.23 .

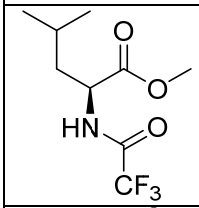
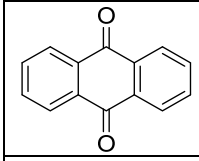
^{19}F NMR (376 MHz, $CDCl_3$) δ -130.93.

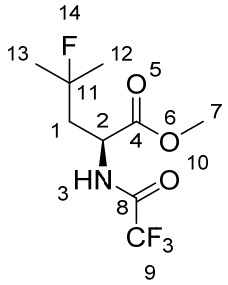
Refer to chemdraw above for label	^{13}C Assignment	^{19}F Assignment	^{1}H Assignment
1,3	42.23 (d, *J* = 18.1 Hz)	-	1.89 – 1.76 (m, 4H)
2	93.18 (d, *J* = 183.1 Hz)	-	-
4,6	30.98 (dd, *J* = 9.8, 6.3 Hz)	-	2.34 – 2.26 (m, 2H)
5	35.30 (d, *J* = 2.0 Hz)	-	1.71 – 1.50 (m, 2H)
7,8	37.00 (d, *J* = 20.1 Hz)	-	1.44 (m, 4H)
9	43.22 (d, *J* = 17.7 Hz)	-	1.71 – 1.50 (m, 2H)
10	41.28 (d, *J* = 9.1 Hz)	-	-
11	-	-130.93	-
12	53.53	-	3.54 – 3.30 (m, 1H)
13	15.23	-	1.04 (d, *J* = 6.9 Hz, 3H)
14	-	-	4.39 – 4.07 (m, 1H)
16	79.12	-	-
17,18,19	28.44	-	1.44 (m, 9H)
20	155.67	-	-

HRMS (ESI-TOF) $[M\text{-}Na]^+$ calculated for $C_{17}H_{28}FNNaO_2$ 320.2002, found 320.1999.

Appearance: White solid

methyl (S)-4-fluoro-4-methyl-2-(2,2,2-trifluoroacetamido)pentanoate

	M.W (mg/mmol)	Amount added	Amount added/mmol
	241.2102	723mg	2.997
Selectfluor®	354.26	715mg	2.02
	208.2160	8.3mg	0.0399
MeCN	-	8mL	-
Reaction Time	52 hours		
Column Chromatography Details	2cm(column outer diameter) X 21.5cm (SiO_2 length) Crude is dissolved in minimal DCM and separation was performed with gradient elution. Gradient Elution: *n*-Hexane to 38:1:1(*n*-Hexane:Et_2O:Ethyl Acetate) to 10:1:1(*n*-Hexane:Et_2O:Ethyl Acetate) Total methyl (S)-4-fluoro-4-methyl-2-(2,2,2-trifluoroacetamido)pentanoate obtained = 176.5mg(0.68mmol) Yield (based on limiting reagent) = 0.68/2.00 X100 = 34%		
	R_f (methyl (S)-4-fluoro-4-methyl-2-(2,2,2-trifluoroacetamido)pentanoate) = 0.19 (2:1, *n*-Hexane:Et_2O); stain $KMnO_4$ R_f (starting material) = 0.28 (2:1, *n*-Hexane:Et_2O); stain $KMnO_4$		



^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.26 (s, 1H), 7.01 (s, 1H), 4.71 (td, *J* = 7.7, 4.9 Hz, 1H), 3.79 (s, 3H), 2.29 – 2.12 (m, 2H), 1.43 (d, *J* = 21.6 Hz, 6H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 170.78 , 156.85 (d, *J* = 37.8 Hz), 115.57 (q, *J* = 287.4 Hz), 95.27 (d, *J* = 165.6 Hz), 52.99, 50.09,41.42 (d, *J* = 21.1 Hz), 26.84 (dd, *J* = 161.9, 24.5 Hz).

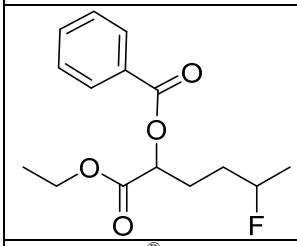
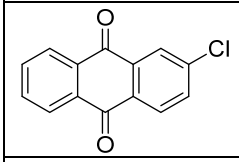
^{19}F NMR (376 MHz, $CDCl_3$) δ -76.12, -137.88.

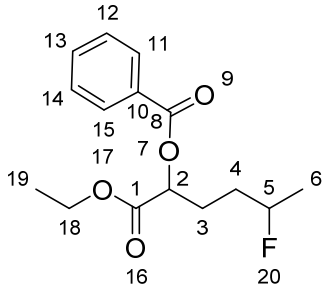
Refer to chemdraw above for label	^{13}C Assignment	^{19}F Assignment	^{1}H Assignment
1	41.42 (d, *J* = 21.1 Hz)	-	2.29 – 2.12 (m, 2H)
2	50.09	-	4.71 (td, *J* = 7.7, 4.9 Hz, 1H)
3	-	-	7.01 (s, 1H)
4	170.78	-	-
7	52.99	-	3.79 (s, 3H)
8	156.85	-	-
9	115.57	-76.12	-
11	95.27	-	-
12	26.84 (dd, *J* = 161.9, 24.5 Hz).	-	1.43 (d, *J* = 21.6 Hz, 6H)
13			
14	-	-137.88.	-

HRMS (ESI-TOF) $[M-H]^+$ calculated for $C_9H_{13}F_4NO_3Na^+$ 260.0905, found 260.0911

Appearance: Colorless to light yellow liquid

1-ethoxy-5-fluoro-1-oxohexan-2-yl benzoate

	M.W (mg/mmol)	Amount added	Amount added/mmol
	282.3114	807mg	2.859
Selectfluor®	354.26	711mg	2.01
	242.6580	9.5mg	0.0392
MeCN	-	8mL	-
Reaction Time	27 hours		
Column Chromatography Details	2cm(column outer diameter) X 21.5cm (SiO_2 length) Crude is dissolved in minimal DCM and separation was performed with gradient elution. Gradient Elution: *n*-Hexane to 36:1(*n*-Hexane:Mixture) to 10:1(*n*-Hexane:Mixture) *[Mixture= Et_2O:Ethyl Acetate(4:1)] Total 1-ethoxy-5-fluoro-1-oxohexan-2-yl benzoate obtained = 340.6mg(1.21mmol) Yield (based on limiting reagent) = 1.21/2.00 X100 = 61%		
	R_f (6-fluoroheptan-3-yl benzoate) = 0.19 (5:1, *n*-Hexane:Et_2O); stain CAM blue R_f (starting material) = 0.34 (5:1, *n*-Hexane:Et_2O); weak CAM stain		



inseparable *cis*- *trans*- diastereomer

^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.11 – 8.06 (m, 2H), 7.63 – 7.56 (m, 1H), 7.46 (t, *J* = 7.8 Hz, 2H), 5.26 (ddd, *J* = 12.5, 8.0, 4.5 Hz, 1H), 4.83 – 4.63 (m, 1H), 4.24 (q, *J* = 7.1 Hz, 2H), 2.27 – 2.00 (m, 2H), 1.89 – 1.71 (m, 2H), 1.37 (dd, *J* = 23.8, 6.2 Hz, 3H), 1.28 (t, *J* = 7.1 Hz, 3H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 169.89, 165.98, 133.36, 129.83 , 129.41 , 128.44 , 90.09 (d, *J* = 165.8 Hz), 72.94 – 71.84 (m), 61.47 , 32.54 (m), 27.01 (d, *J* = 4.6 Hz), 20.97 (dd, *J* = 22.6 Hz), 14.13 .

^{19}F NMR (376 MHz, Chloroform-*d*) δ -174.12 , -174.49 .

Refer to chemdraw above for label	^{13}C Assignment	^{19}F Assignment	^{1}H Assignment
1	169.89	-	-
2	72.38	-	5.26 (ddd, *J* = 12.5, 8.0, 4.5 Hz, 1H)
3	27.01 (d, *J* = 4.6 Hz),	-	2.27 – 2.00 (m, 2H)
4	32.54	-	1.89 – 1.71 (m, 2H)
5	90.09 (d, *J* = 165.8 Hz)	-	4.83 – 4.63 (m, 1H)
6	20.97 (dd, *J* = 22.6 Hz)	-	1.37 (dd, *J* = 23.8, 6.2 Hz, 3H)
8	165.98	-	-
10	129.41	-	-
11,15	129.83	-	8.11 – 8.06 (m, 2H)
12,14	128.44	-	7.46 (t, *J* = 7.8 Hz, 2H)
13	133.36	-	7.63 – 7.56 (m, 1H)
18	61.47	-	4.24 (q, *J* = 7.1 Hz, 2H)
19	14.13	-	1.28 (t, *J* = 7.1 Hz, 3H)
20	-	-174.12 , -174.49	-

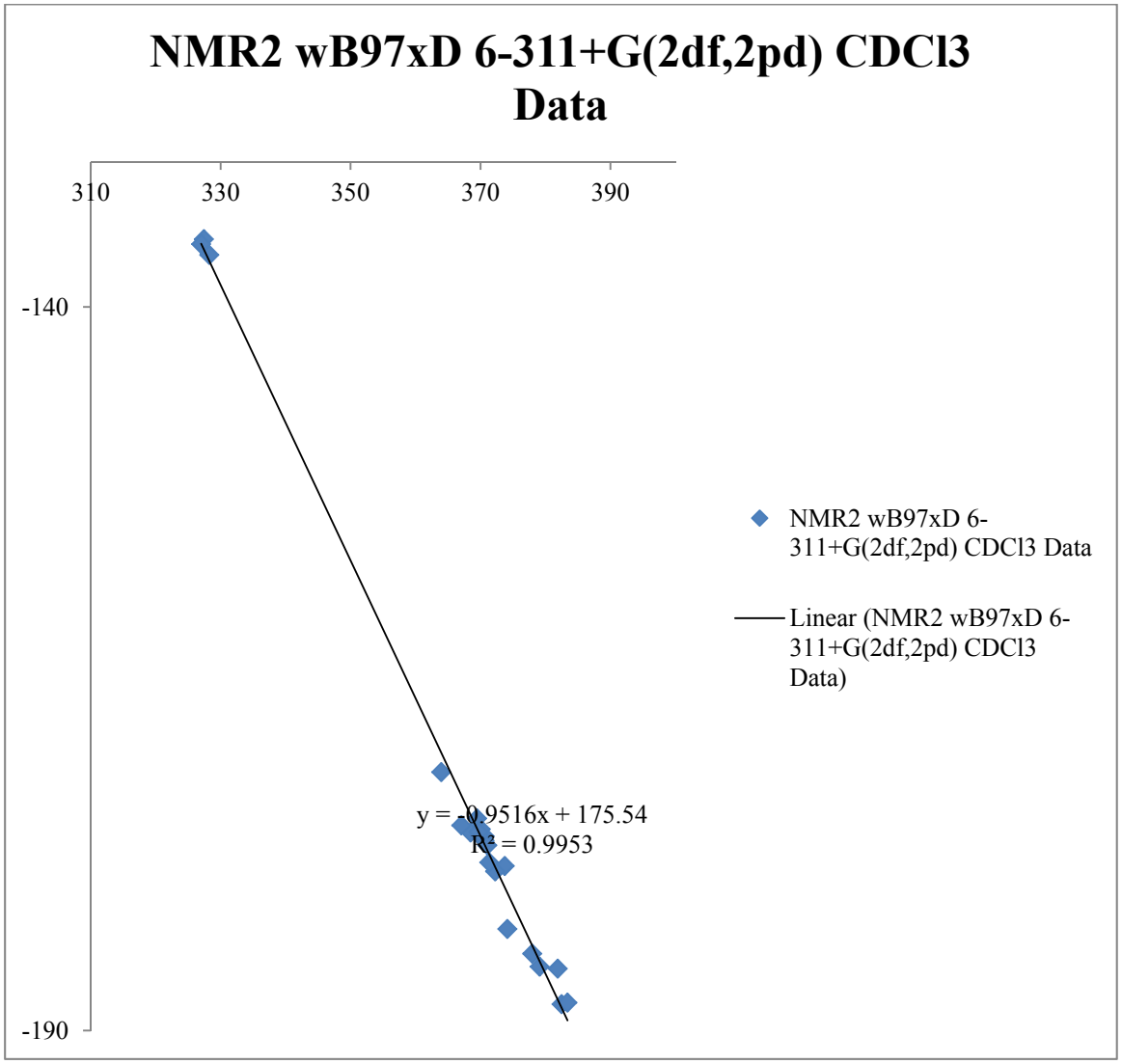
HRMS (ESI-TOF) $[M-H]^+$ calculated for $C_8H_{14}FO_4^+$ 193.0871, found 193.0880

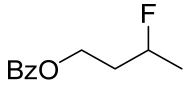
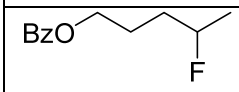
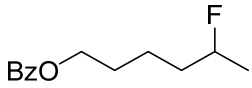
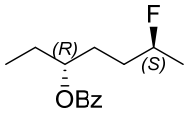
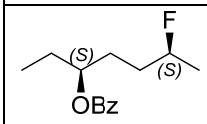
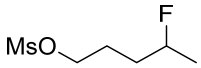
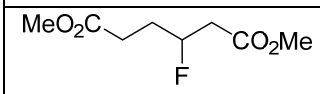
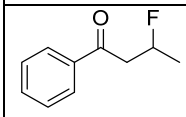
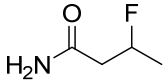
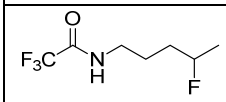
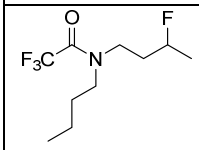
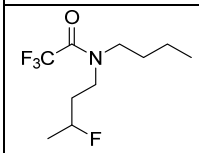
Appearance: Colorless liquid

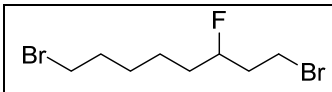
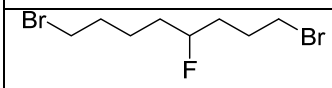
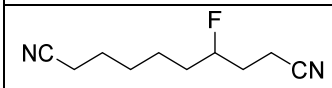
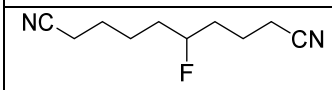
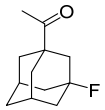
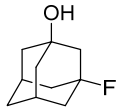
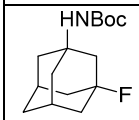
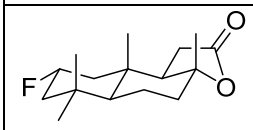
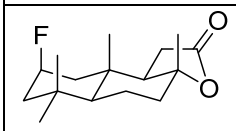
Calculated 19F NMR chemical shifts

Conformation samplings were performed with MacroModel. A maximum of 12 conformations were included in geometry optimization via density functional theory using Gaussian 09 A2. Geometry optimizations were performed at SMD($CHCl_3$)-wB97xD/6-311+G(d,p). Frequency calculations on the optimized geometries were performed to ensure that there is no imaginary frequency. NMR calculations were then performed on the optimized geometries at wB97xD/6-311+G(2df,2pd).

A least square linear regression was performed to model the experimental chemical shifts as a function of the calculated NMR shielding Tensor.

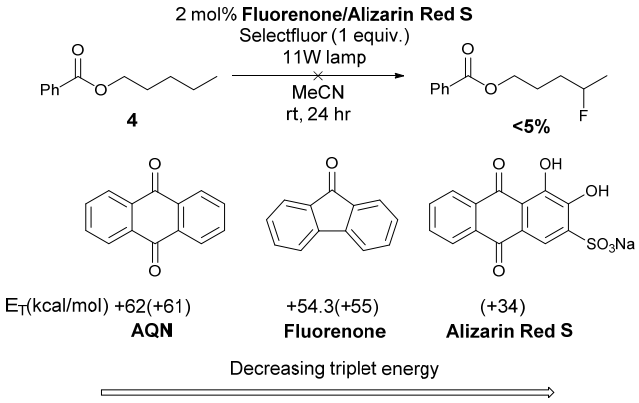


	Calculated NMR shielding Tensor	Predicted from regression model/ppm	Experimental (reference to C_6F_6 at -164.90)/ppm
	373.7307	-180.10	-178.62
	370.6451	-177.17	-176.56
	370.0535	-176.60	-176.08
	370.6228	-177.14	-176.87
	368.4722	-175.10	-176.31
	371.0508	-177.55	-177.19
	381.8872	-187.86	-185.71
	367.0430	-173.74	-175.82
	369.4833	-176.06	-175.33
	369.6864	-176.25	-176.26
	372.2576	-178.70	-178.99
	371.3615	-177.85	-178.37

	382.4705	-188.42	-188.17
	377.9543	-184.12	-184.68
	383.3830	-189.29	-188.06
	379.1003	-185.21	-185.58
	327.4145	-136.03	-135.31
	326.2822	-134.95	-136.4
	327.0042	-135.64	-135.66
	374.1440	-180.50	-182.97
	363.9657	-170.81	-175.25

Mechanism Study

Further discussion on reaction mechanisms

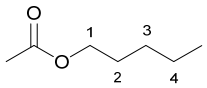


Scheme. 3 Experiments with relevant photocatalysts. E_T of AQN and fluorenone are taken from Zalesskaya.[38] Numbers in parentheses are calculated E_T.

In a related work by Chen and co-workers on benzylic fluorination which used fluorenone as the photocatalyst, they proposed that triplet fluorenone is the hydrogen abstractor. However, when fluorenone was used for **4**, insignificant amount of product was observed (Scheme 3). This suggests that a different mechanism is in operation. The reactivity for the photo-fluorination of **4** correlates with the triplet energy (E_T) of the photocatalysts (Scheme 3), the singlet-triplet gap of **1** (Scheme 1) is 61.4 kcal/mol, thus triplet-triplet energy transfer is feasible between AQN and **1** but not between **1** and fluorenone or alizarin red S salt.

The selectivity observed for this photo-fluorination resembles that of other reactions using cationic *N*-radicals.[20] Density functional theory (DFT) was used to predict the selectivity of hydrogen abstraction for triplet AQN and cationic *N*-radical derived from Selectfluor II® **30**, which was chosen to simplify calculation as multiple conformations exist for **2**. Experimentally, similar selectivity was observed for Selectfluor® and Selectfluor II®. The calculated result shows that cationic *N*-radical derived from **30** has selectivity that is consistent with the experimentally observed results (Table 2). In the case of ^{3}AQN, the hydrogen abstraction is predicted to proceed with selectivity for C2 and C3 hydrogens.

Table 2 Probing the hydrogen abstracting species using DFT

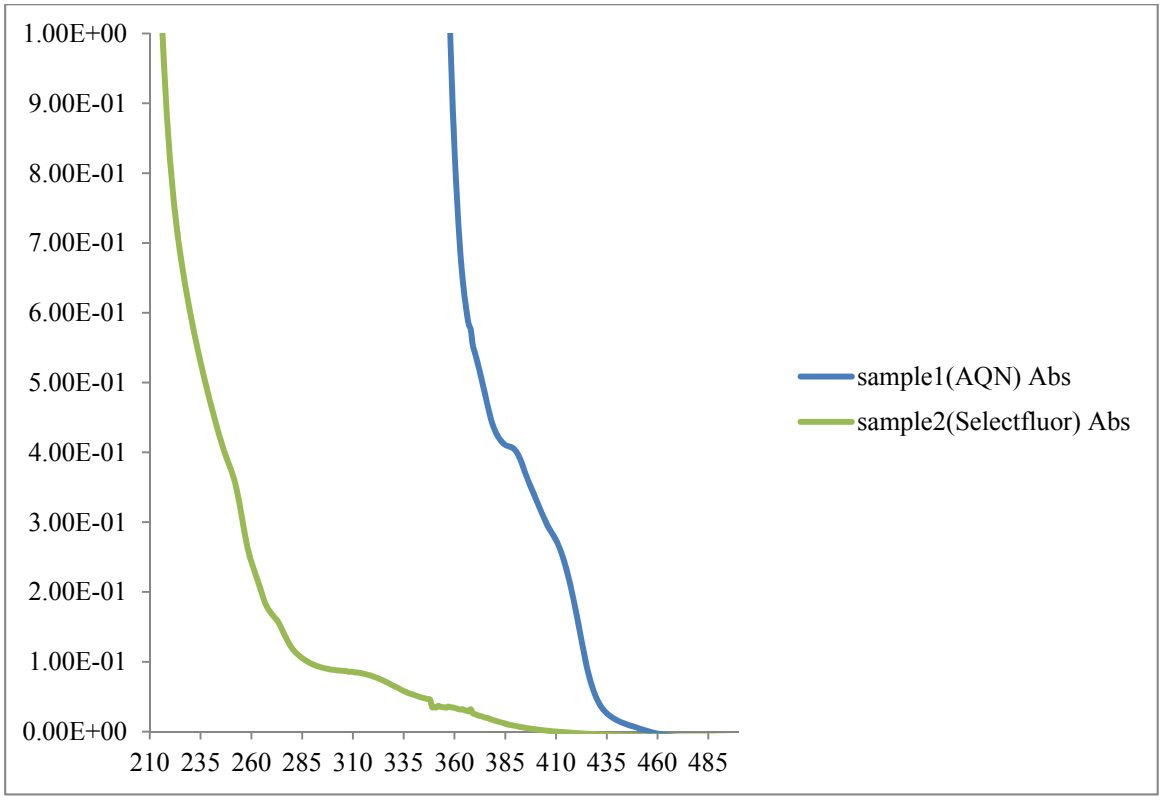


25

H-abstractor	Selectivity (%)			
	1	2	3	4
^{3}AQN	10	21	58	11
 **30**	1.7	1.3	12	85
Experimental result[a]	7	7	13	73

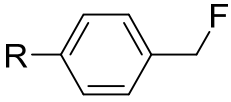
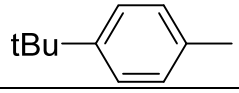
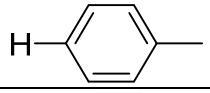
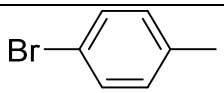
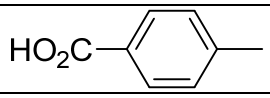
SMD(MeCN)-wB97xD/6-31+G(d,p).[40] [a] Determined from crude ^{19}F NMR

UV-visible spectra of anthraquinone



Hammett equation

0.15 mmol of substrates (various para substituted toluenes and toluene). 1mL of CD_3CN was added in a glovebox. 0.1 mmol of Selectfluor© was added. The sample vials were screwed tight and removed from the glovebox. The reaction mixtures were irradiated with a 11W lamps at room temperature for 24 hours. For workup and analysis, after filtration through a short plug of Celite, 7uL of hexafluorobenzene was added to the reaction mixture and transferred into a NMR tube, extra 0.2 mL of CD3CN. ^{19}F NMR were then recorded.

Substrate for Hammett equation	 19F NMR chemical shift/ppm	σ	σ+
	-204.2	-0.15	-0.26
	-206.4	0	0
	-208.3	0.26	0.15
	-212.7	0.44	0.42

^{19}F Chemical shift is referenced to perfluorobenzene at -164.90ppm

Justification for experimental methodologies to obtain ρ

A general rate equation is given below (the photocatalyst is omitted):

$$rate = k[\mathrm{RH}]^{x}[selectfluor]^{y} - (1)$$

In the Hammett plot, we are interested in the relative rate constants ki/kH

$$\frac{rate_i}{rate_H} = \frac{k_i[\mathrm{R}_i\mathrm{H}]^{x}[selectfluor]^{y}}{k_H[R_HH]^{x}[selectfluor]^{y}} - (2)$$

[selectfluor]y is the same as the reaction is one-pot (toluene and its para-substituted derivatives are added to the same reaction mixture). Therefore the equation can be reduced to:

$$\frac{rate_i}{rate_H} = \frac{k_i[\mathrm{R}_i\mathrm{H}]^{x}}{k_H[R_HH]^{x}} - (3)$$

From equation 3, ratei/rateH is the product of the ki/kh and [RiH]/ [RHH]. Therefore, measuring the rate is not sufficient to obtain ki/kH for the Hammett plot, unless [RHH]/[RiH] and x are known.

$$\frac{k_i}{k_H} = \frac{rate_i}{rate_H}\left(\frac{[R_HH]}{[R_iH]}\right)^{x} - (4)$$

ki/kH can also be expressed in ratio of products [Pi]/[PH]. This could be determined conveniently from 19F NMR and was the method used in our work.

The rate can be expressed as the change(increase) in product concentration with time:

$$rate = \frac{d[p_i]}{dt} = k_i[\mathrm{R}_i\mathrm{H}]^{\mathrm{x}}[selectfluor]^{y} - (5)$$

This differential equation can be expressed as:

$$\int_0^t d[p_i] = k_i \int_0^t [\mathrm{R}_i\mathrm{H}]^{\mathrm{x}}[selectfluor]^{y}\ dt - (6)$$

As [Pi] at time = 0 is 0 (there is no product initially), the left hand side becomes [pi]t which is the concentration of the fluorinated product at any point of time, t.

$$[p_i]_t = k_i \int_0^t [\mathrm{R}_i\mathrm{H}]^{\mathrm{x}}[selectfluor]^{y}\ dt - (7)$$

$$k_i = \frac{[p_i]_t}{\int_0^t [\mathrm{R}_i\mathrm{H}]^{\mathrm{x}}[selectfluor]^{y}\ dt} - (8)$$

For the Hammett plot, we require ki/kH, therefore we require: (Let the integrands = c)

$$\frac{k_i}{k_H} = \frac{[p_i]_t}{[p_H]_t}\left(\frac{\int_0^t [\mathrm{R}_H\mathrm{H}]^{\mathrm{x}}[selectfluor]^{y}\ dt}{\int_0^t [\mathrm{R}_i\mathrm{H}]^{\mathrm{x}}[selectfluor]^{y}\ dt}\right) - (9)$$

$$\frac{k_i}{k_H} = \frac{[p_i]_t}{[p_H]_t}c - (10)$$

At any point of time, the ratio of the rate constants is equal to ratio of fluorinated product times a constant c.

$$log\frac{k_i}{k_H} = \log\left(\frac{[p_i]_t}{[p_H]_t}c_i\right) - (10)$$

$$log\frac{k_i}{k_H} = \log\left(\frac{[p_i]_t}{[p_H]_t}\right) + \log c_i - (11)$$

$$\log\left(\frac{[p_i]_t}{[p_H]_t}\right) = log\frac{k_i}{k_H} - \log c_i - (12)$$

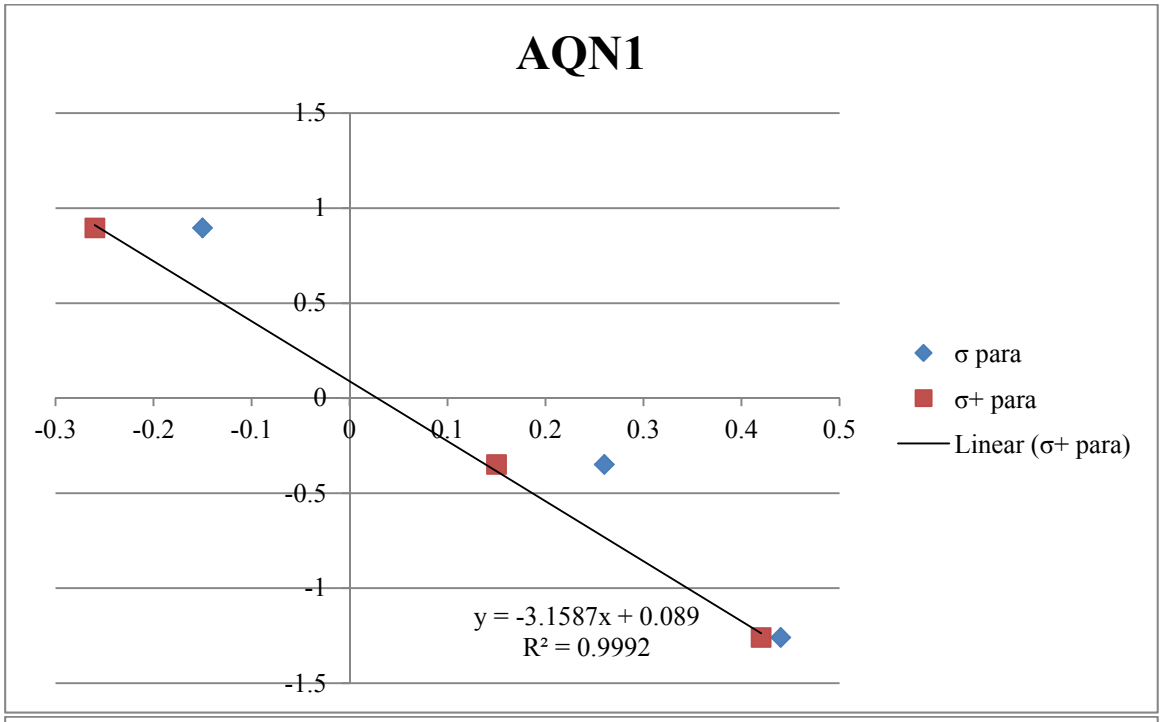
If log (ki/KH) is used for the Hammett plot, we should get a straight line through the origin, because the Hammett equation is log(ki/kH) = ρσ. However, if we used log([pi]t/[pH]t) which is the ratio of the fluorinated product from 19F NMR, we would not expect a straight line through the origin. The intercept is an estimate of log ci for each toluene derivative.

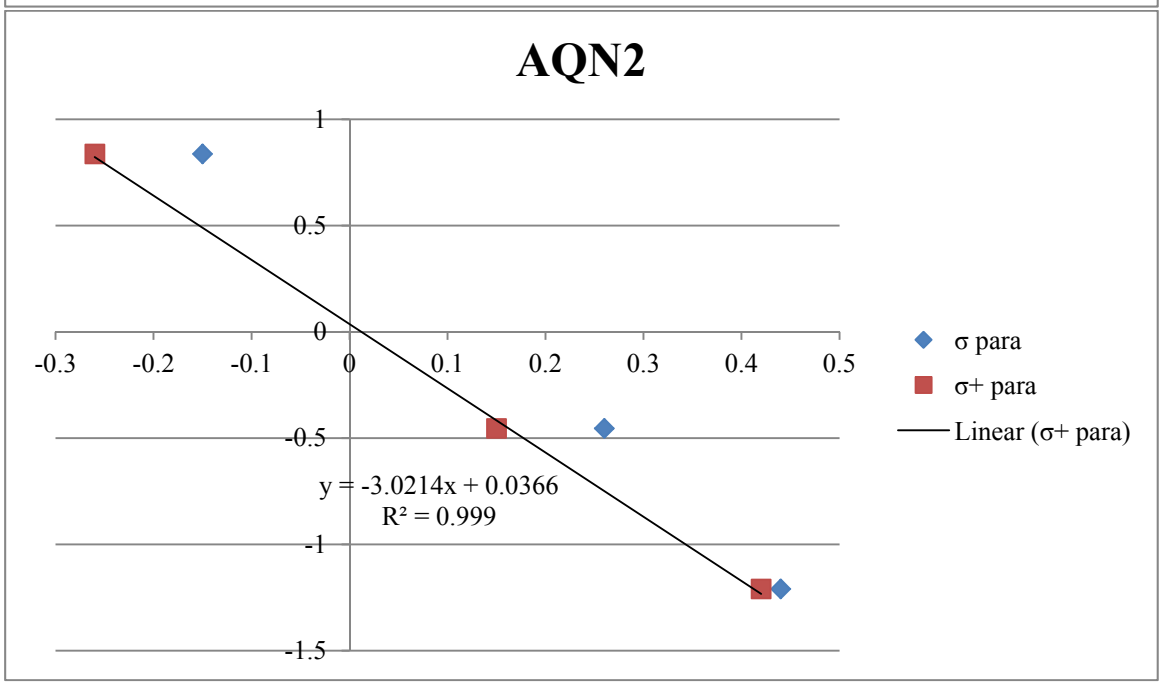
$$log\frac{k_i}{k_H} = \rho\sigma - (13)$$

$$\log\left(\frac{[p_i]_t}{[p_H]_t}\right) + \log c = \rho\sigma - (14)$$

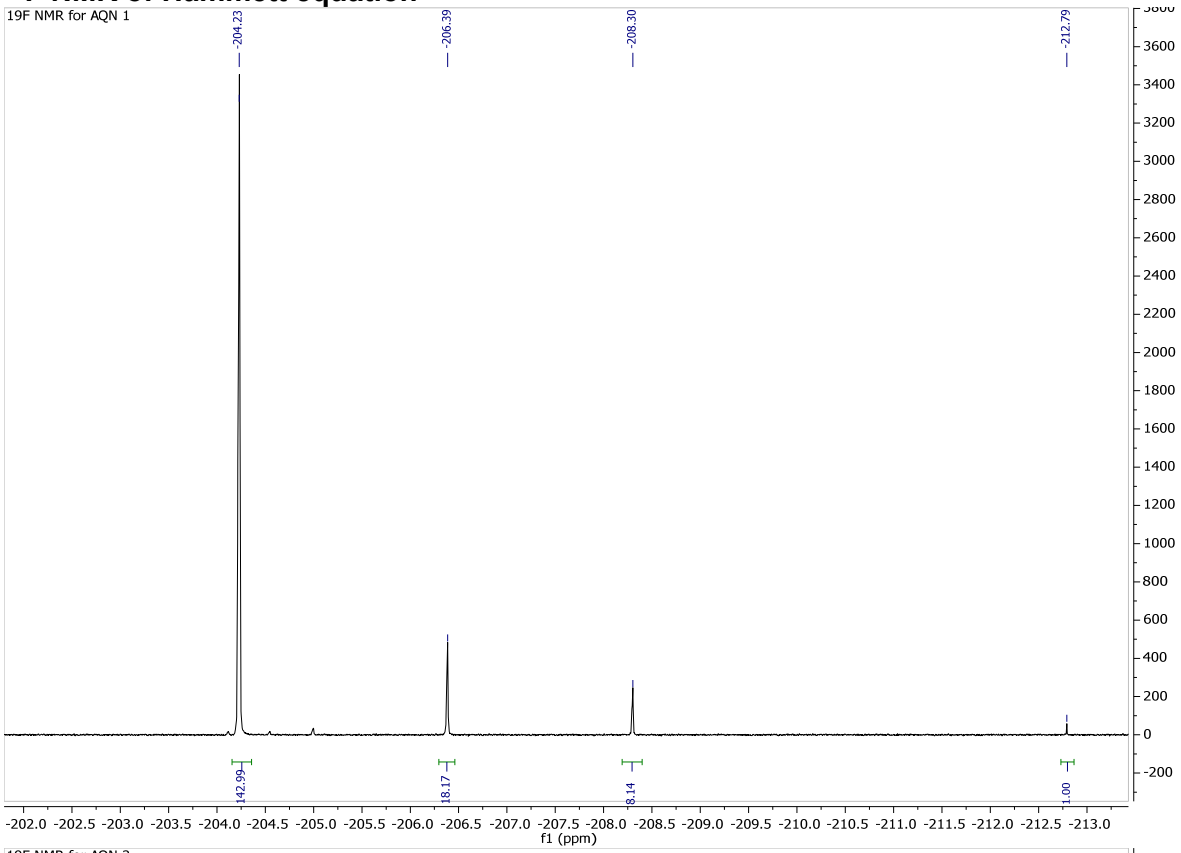
$$\log\left(\frac{[p_i]_t}{[p_H]_t}\right) = \rho\sigma - \log c\ \ (15)$$

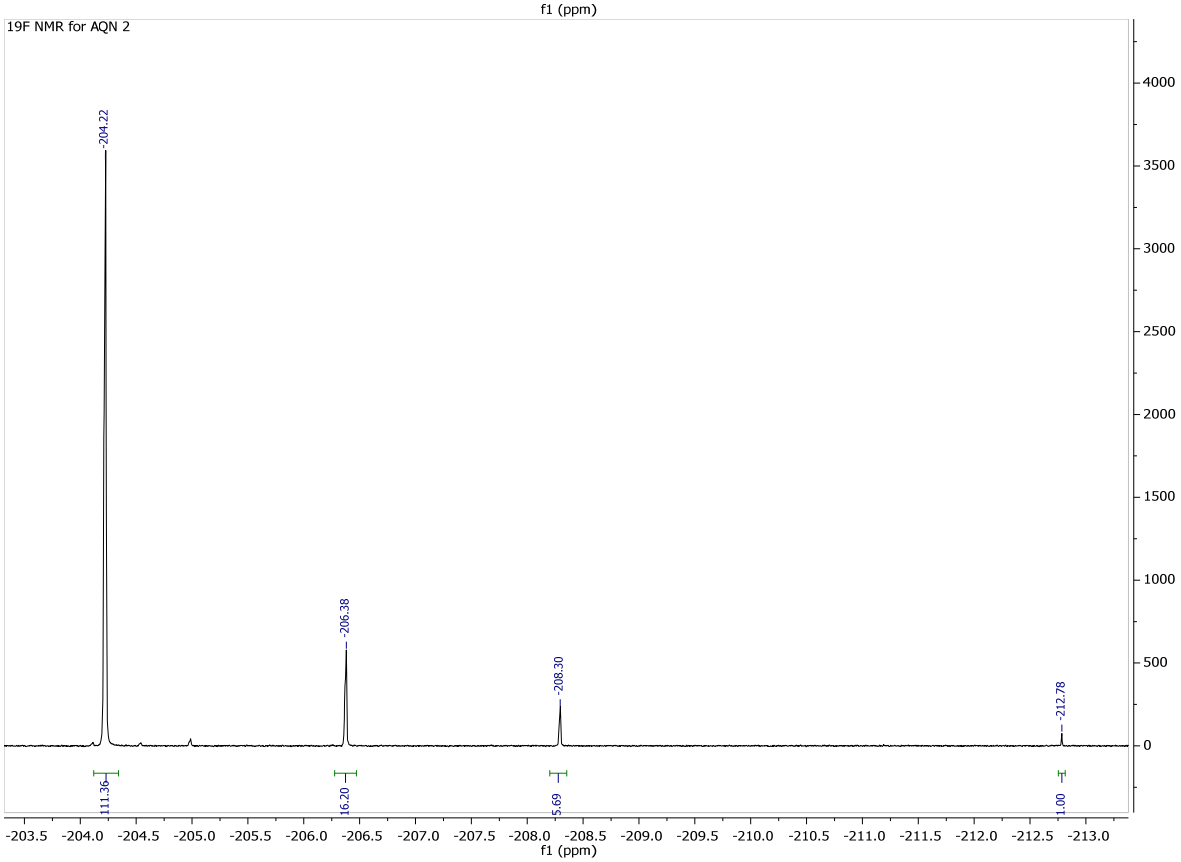
Results of Hammett equation



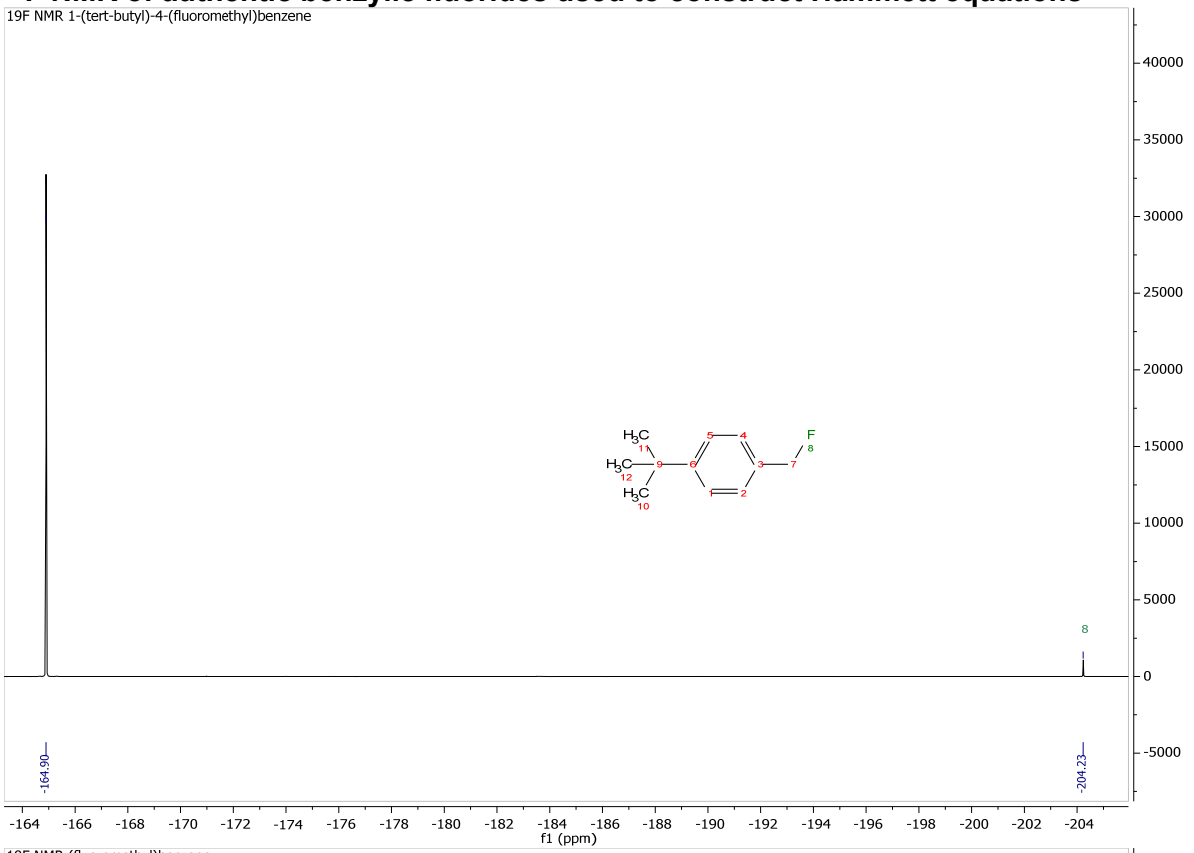


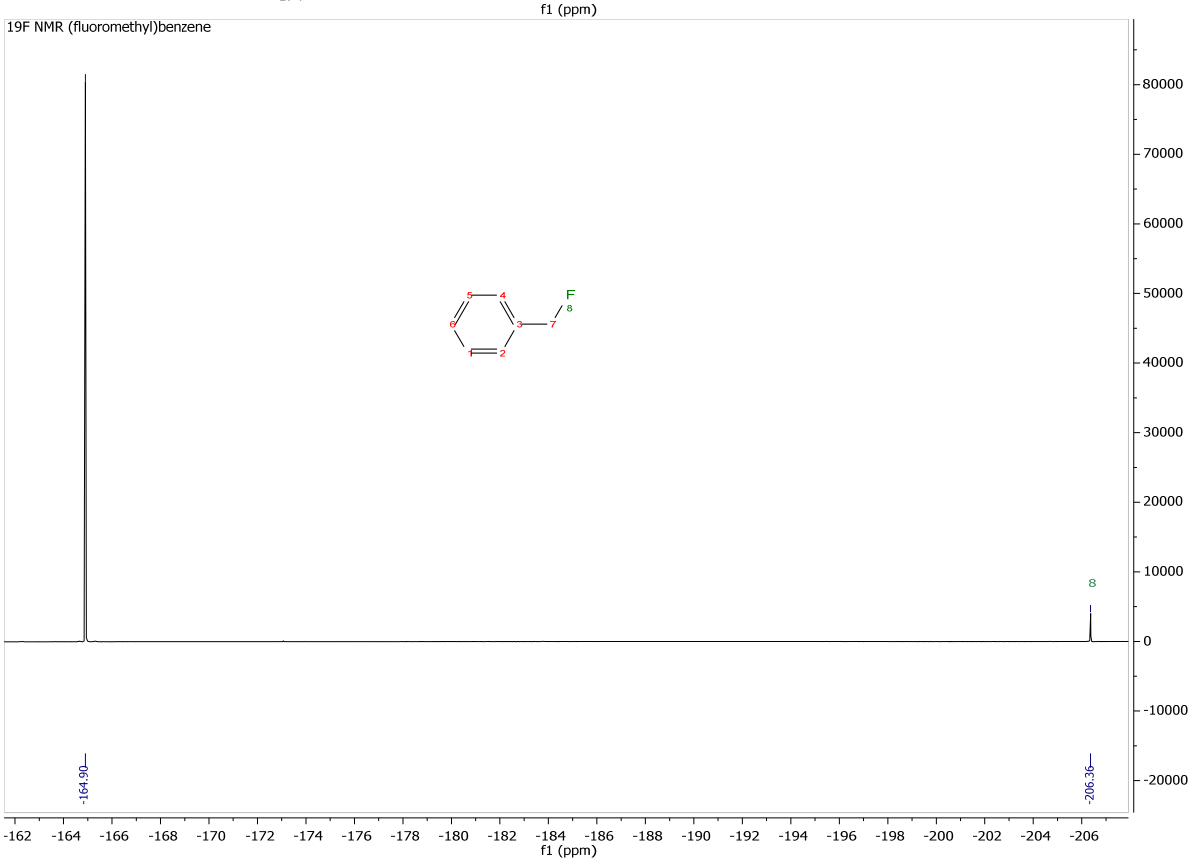
^{19}F NMR of Hammett equation

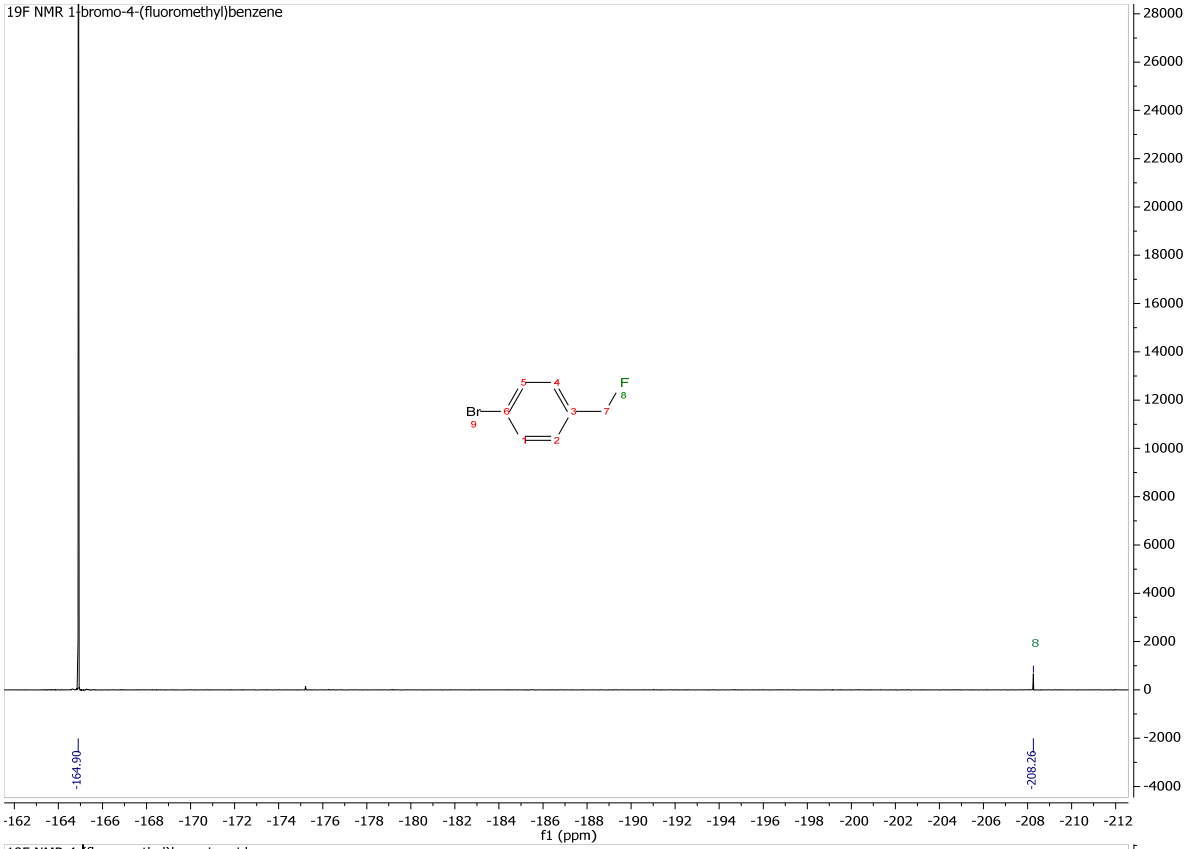


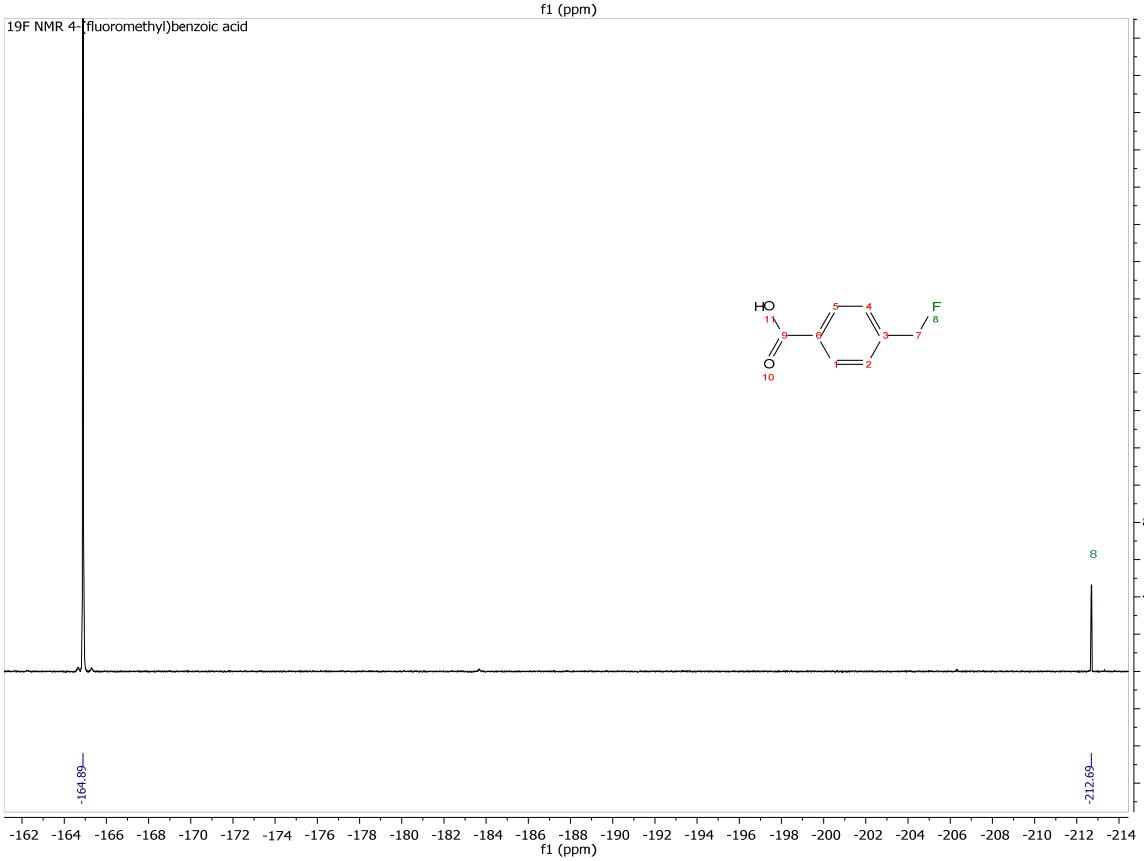


^{19}F NMR of authentic benzylic fluorides used to construct Hammett equations





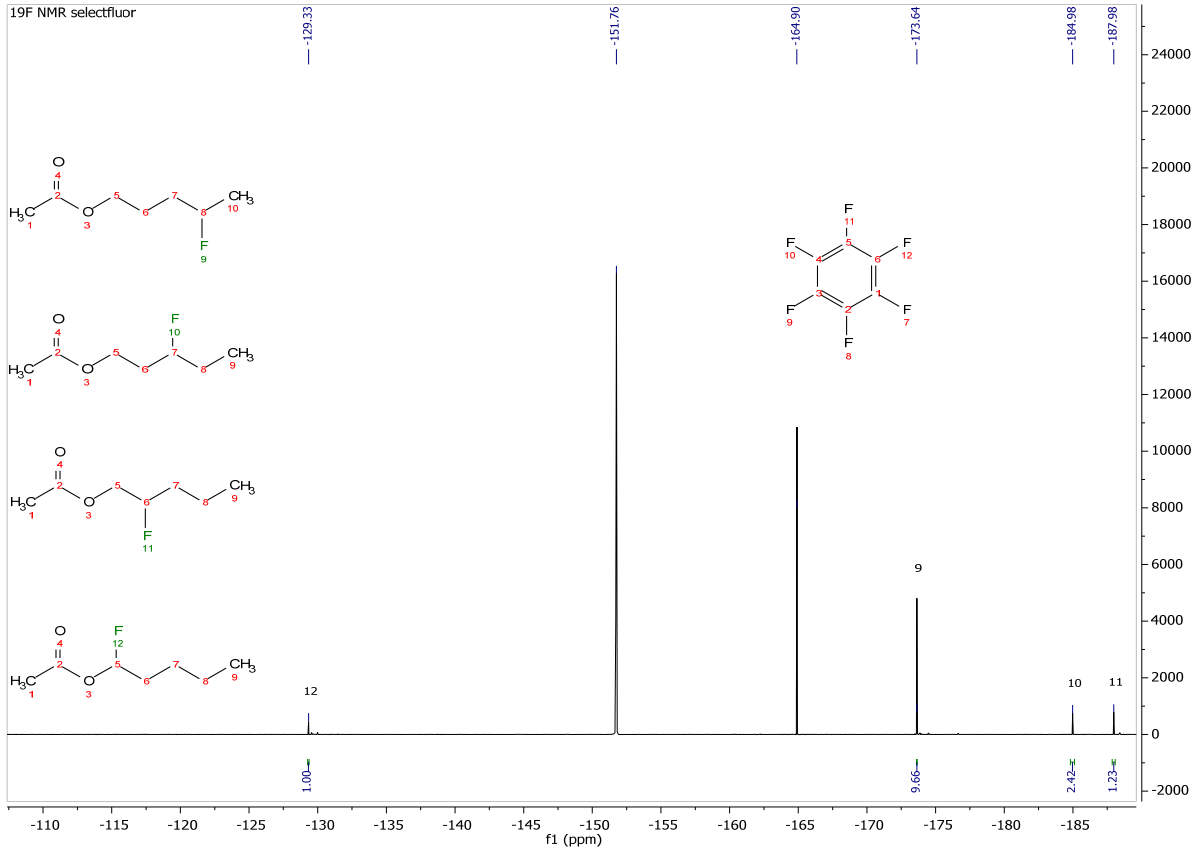

19F NMR 1-bromo-4-(fluoromethyl)benzene
-164.90
-208.26
f1 (ppm)

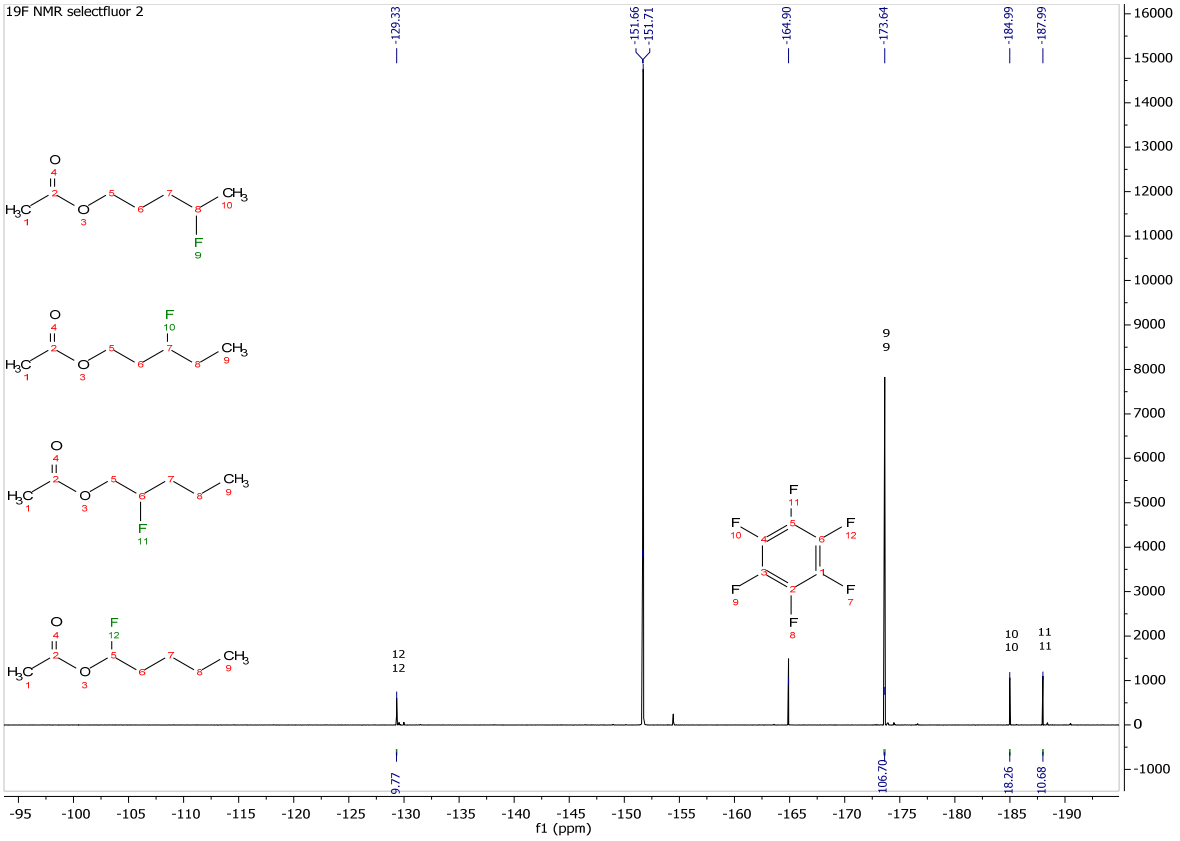

19F NMR 4-(fluoromethyl)benzoic acid
-164.89
-212.69
f1 (ppm)

Selectivity of H abstraction by different species

Experimental: 0.02mmol of AQN, 1 mmol of Selectfluor or Selectfluor 2 and a small magnetic stir bar were added to a 4mL sample vial. The sample vial was transferred into a MBraun Glovebox. 0.15mmol of pentyl acetate (degassed by freeze-pump-thaw prior to use) was added , followed by 0.6mL of CD_3CN (deuteriated acetonitrile which was dried with CaH_2 and degassed by freeze-pump-thaw). The sample vial was capped tightly and removed from the glovebox. It was stirred and irradiated with 11W lamps for 24 hours. After 24 hours, the reaction mixture was filtered through a short plug of cotton and celite into a NMR tube. 1uL of perfluorobenzene was added to the NMR tube. NMR analysis was performed.

	Integration ratio from ^{1}H-decoupled ^{19}F NMR	
	Selectfluor®	Selectfluor 2®
1F	1.00	1.00
2F	1.23	1.07
3F	2.42	2.53
4F	9.66	10.67

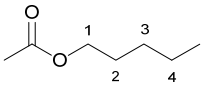




Calculated selectivity of H abstraction by Selectfluor II cation and AQN

Density functional theory (DFT) was used to predict the selectivity of hydrogen abstraction for triplet AQN and cationic *N*-radical derived from Selectfluor II® **30**, which was chosen to simplify calculation as multiple conformations exist for **2**. Experimentally, similar selectivity was observed for Selectfluor® and Selectfluor II®. The calculated result shows that cationic *N*-radical derived from **30** has selectivity that is consistent with the experimentally observed results. In the case of ^{3}AQN, the hydrogen abstraction is predicted to proceed with selectivity for C2 and C3 hydrogens.

Probing the hydrogen abstracting species using DFT



25

H-abstractor	Selectivity (%)			
	1	2	3	4
^{3}AQN	10	21	58	11
 **30**	1.7	1.3	12	85
Experimental result[a]	7	7	13	73

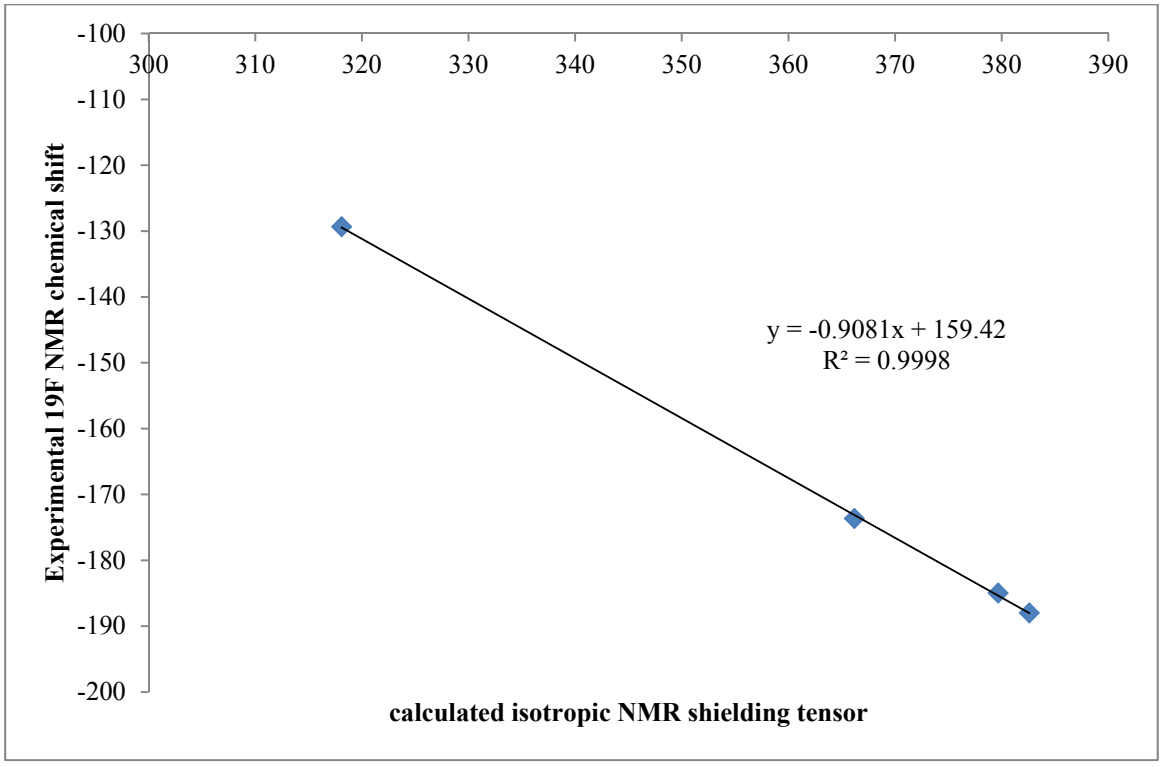
SMD(MeCN)-wB97xD/6-31+G(d,p).[40] [a] Determined from crude ^{19}F NMR

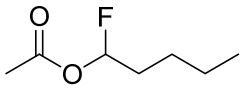
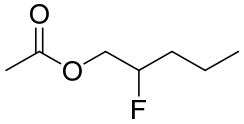
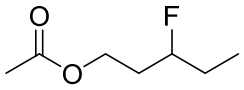
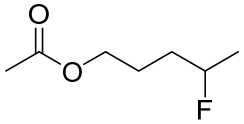
Assignment of 19F NMR to various regioisomers of fluoropentyl acetate

Assignment of 19F NMR to various regioisomers of fluoropentyl acetate was performed by DFT calculations. Macromodel was used to generate structures of 1-,2-,3-, and 4-fluoropentyl acetate. 10 conformations for each regioisomer were optimized at SMD(MeCN)-wB97xD/6-311+G(d,p) using default convergence criteria and integration grid as implemented in Gaussian 09 A2. Frequency calculations were performed to ensure that there is no imaginary frequency for all the conformers. NMR calculations were performed on all the optimized conformers at wB97xD/6-311+G(2df,2pd). A boltzmann distribution was used to calculate the contribution of each conformer to the final 19F NMR shielding tensor (i.e the 19F NMR shielding tensor is a weighted average and the weights are derived for the Boltzmann distribution using the relative Gibbs free energy of each conformer). A least square linear regression was performed.

y = chemical shift with reference to C_6F_6 at -164.90ppm

x = calculated NMR isotropic shielding tensor at the level of theory given above



	Calculated isotropic NMR shielding tensor	Experimental chemical shift/ppm	Predicted chemical shift using linear regression model/ppm
	318.093	-129.33	-129.44
	382.5983	-187.99	-188.02
	379.667	-184.99	-185.36
	366.192	-173.64	-173.12

Calculating the relative $\Delta G^{\ddagger}$ for hydrogen abstraction by triplet AQN and selectfluor 2

Transition state structures were optimized at SMD(MeCN)-wB97xD/6-31+G(d,p) using tight convergence criteria and ultrafine integration grid as implemented in Gaussian 09 A2. Frequency calculations were performed to ensure that there is only one imaginary frequency for all transition state structures. IRC calculations were performed to locate the reactant and product which the transition state structures connect. Stability of wavefunction was checked in all cases by using the stable keyword in Gaussian 09 A2.

Calculations relevant to Triplet-Triplet energy transfer

Transition state structures were optimized at SMD(MeCN)-M06-2X/6-311+G(d,p) using default convergence criteria and integration grid as implemented in Gaussian 09 A2. Frequency calculations were performed to ensure that there is only one imaginary frequency for all transition state structures. IRC calculations were performed to locate the reactant and product which the transition state structures connect. Stability of wavefunction was checked in all cases by using the stable keyword in Gaussian 09 A2.

OPT-M062X-6-311+Gdp-selectfluorodication.out

2 1

C	1.739694	1.274112	-0.171732
C	0.283600	1.635904	0.150646
H	2.426769	1.732935	0.536362
H	2.020936	1.495902	-1.199691
H	0.159530	1.978934	1.176565
H	-0.081269	2.385840	-0.548766
C	1.261003	-0.632941	1.306552
H	1.572019	-1.661850	1.476718
H	1.663020	0.033378	2.067562
C	-0.264481	-0.532563	1.152458
H	-0.704638	-1.500741	0.923413
H	-0.710170	-0.111154	2.052046
C	-0.202321	-0.286392	-1.294320
H	-0.937320	-1.059758	-1.504085
H	-0.223565	0.478576	-2.070121
C	1.187518	-0.917729	-1.137318
H	1.152626	-1.973400	-0.873437
H	1.798939	-0.750269	-2.021984
N	1.849984	-0.206886	-0.000685
C	-1.999833	0.847590	-0.002173
H	-2.157197	1.440582	0.895773
H	-2.156867	1.427199	-0.908380
Cl	-3.132073	-0.513384	0.006196
N	-0.571014	0.393868	0.000034
F	3.179488	-0.542274	-0.001564

Zero-point correction = 0.225394
Thermal correction to Energy = 0.234612
Thermal correction to Enthalpy = 0.235557
Thermal correction to Gibbs Free Energy = 0.191065
Sum of electronic and zero-point Energies = -944.015654
Sum of electronic and thermal Energies = -944.006435
Sum of electronic and thermal Enthalpies = -944.005491
Sum of electronic and thermal Free Energies = -944.049983
Number of imaginary frequencies/frequency = 0

OPT2-M062X-6-311+Gdp-selectfluorodicationtripletC2.out

2 3

C	1.648924	1.295711	-0.160003
C	0.157928	1.656286	0.132894
H	2.296791	1.765150	0.579356
H	1.937044	1.554462	-1.176456
H	0.019644	2.015140	1.151154
H	-0.204818	2.381968	-0.592678
C	1.215988	-0.610151	1.281409
H	1.518410	-1.645829	1.430544
H	1.601871	0.041622	2.061886
C	-0.340643	-0.523097	1.160720
H	-0.768957	-1.499897	0.947503
H	-0.770300	-0.090020	2.062482
C	-0.291203	-0.295327	-1.297617
H	-0.992566	-1.104454	-1.486509
H	-0.342507	0.458999	-2.081673
C	1.151130	-0.871396	-1.135944
H	1.139570	-1.933956	-0.904202
H	1.739286	-0.655485	-2.026944
N	1.675404	-0.140425	-0.005225
F	4.390753	-0.437141	0.077203
C	-2.105035	0.811780	-0.000868
H	-2.274396	1.395646	0.900643
H	-2.275897	1.393899	-0.902814
Cl	-3.211416	-0.570981	0.000152
N	-0.665988	0.388124	-0.002940

Zero-point correction = 0.220137
Thermal correction to Energy = 0.23103
Thermal correction to Enthalpy = 0.231974
Thermal correction to Gibbs Free Energy = 0.180556
Sum of electronic and zero-point Energies = -943.917839
Sum of electronic and thermal Energies = -943.906945
Sum of electronic and thermal Enthalpies = -943.906001
Sum of electronic and thermal Free Energies = -943.957419
Number of imaginary frequencies/frequency = 0

OPT-M062X-6-311+Gdp_9-fluorenone.out

0 1

C	-3.017967	-1.390880	0.000149
C	-3.457360	-0.068266	0.000142
C	-2.536298	0.982988	0.000086
C	-1.190448	0.665517	0.000036
C	-0.742883	-0.663353	0.000039
C	-1.653880	-1.706232	0.000099
H	-3.747378	-2.193179	0.000195
H	-4.519964	0.144143	0.000180
H	-2.864135	2.016953	0.000081
H	-1.326773	-2.739986	0.000104
C	0.000000	1.574503	-0.000022
C	1.190448	0.665517	-0.000056
C	2.536298	0.982988	-0.000110
C	3.457360	-0.068266	-0.000136
C	3.017967	-1.390880	-0.000111
C	1.653880	-1.706232	-0.000056
C	0.742883	-0.663353	-0.000026
H	2.864135	2.016953	-0.000130
H	4.519964	0.144143	-0.000176
H	3.747378	-2.193179	-0.000133
H	1.326773	-2.739986	-0.000036
O	0.000000	2.782479	-0.000038

Zero-point correction = 0.170236
Thermal correction to Energy = 0.179838
Thermal correction to Enthalpy = 0.180782
Thermal correction to Gibbs Free Energy = 0.135012
Sum of electronic and zero-point Energies = -575.191734
Sum of electronic and thermal Energies = -575.182132
Sum of electronic and thermal Enthalpies = -575.181188
Sum of electronic and thermal Free Energies = -575.226958
Number of imaginary frequencies/frequency = 0

OPT-M062X-6-311+Gdp_9-fluorenoneTriplet.out

0 3

C	-2.974423	-1.431753	0.000151
C	-3.411237	-0.061016	0.000139
C	-2.517190	0.992968	0.000085
C	-1.152922	0.704283	0.000036
C	-0.696717	-0.681880	0.000038
C	-1.647818	-1.746515	0.000103
H	-3.723631	-2.214317	0.000201
H	-4.476550	0.139862	0.000176
H	-2.864789	2.019788	0.000080
H	-1.312132	-2.777425	0.000111
C	0.000000	1.598951	-0.000023
C	1.152922	0.704283	-0.000058
C	2.517191	0.992968	-0.000108
C	3.411237	-0.061016	-0.000132
C	2.974422	-1.431755	-0.000110
C	1.647817	-1.746516	-0.000059
C	0.696717	-0.681881	-0.000026
H	2.864790	2.019788	-0.000127
H	4.476550	0.139861	-0.000168
H	3.723631	-2.214318	-0.000135
H	1.312131	-2.777425	-0.000041
O	0.000001	2.844683	-0.000040

Zero-point correction = 0.166885
Thermal correction to Energy = 0.176896
Thermal correction to Enthalpy = 0.177841
Thermal correction to Gibbs Free Energy = 0.130287
Sum of electronic and zero-point Energies = -575.104367
Sum of electronic and thermal Energies = -575.094356
Sum of electronic and thermal Enthalpies = -575.093412
Sum of electronic and thermal Free Energies = -575.140965
Number of imaginary frequencies/frequency = 0

OPT-M062X-6-311+Gdp_AlizarinRedSC4.out

0 1

C	5.750538	0.281713	-0.000043
C	4.622646	1.092069	-0.000032
C	3.353338	0.515411	-0.000024
C	3.215381	-0.879362	-0.000027
C	4.351685	-1.685095	-0.000037
C	5.614695	-1.105748	-0.000046
C	2.162432	1.397178	-0.000011
C	1.869483	-1.524920	-0.000018
C	0.676658	-0.632763	-0.000006
C	0.826556	0.767032	-0.000001
C	-0.308452	1.579373	0.000011
C	-1.588004	0.997235	0.000019
C	-1.715086	-0.383161	0.000012
C	-0.586482	-1.198410	0.000000
H	6.737130	0.729681	-0.000050
H	4.714650	2.171331	-0.000030
H	4.233644	-2.761944	-0.000039
H	6.496566	-1.735676	-0.000054
H	-0.702387	-2.274958	-0.000005
O	1.751350	-2.732109	-0.000020
O	2.278741	2.618127	-0.000008
O	-0.288710	2.920490	0.000016
H	0.649654	3.208818	0.000008
O	-2.672556	1.809536	0.000032
H	-2.378601	2.736191	0.000036
S	-3.355891	-1.113815	0.000017
O	-3.161085	-2.558643	-0.000002
O	-4.019761	-0.563515	1.208745
O	-4.019779	-0.563487	-1.208687
Na	-4.952211	1.180100	0.000044

Zero-point correction = 0.193812
Thermal correction to Energy = 0.212928
Thermal correction to Enthalpy = 0.213872
Thermal correction to Gibbs Free Energy = 0.145844
Sum of electronic and zero-point Energies = -1624.529782
Sum of electronic and thermal Energies = -1624.510666
Sum of electronic and thermal Enthalpies = -1624.509722
Sum of electronic and thermal Free Energies = -1624.57775
Number of imaginary frequencies/frequency = 0

0 3

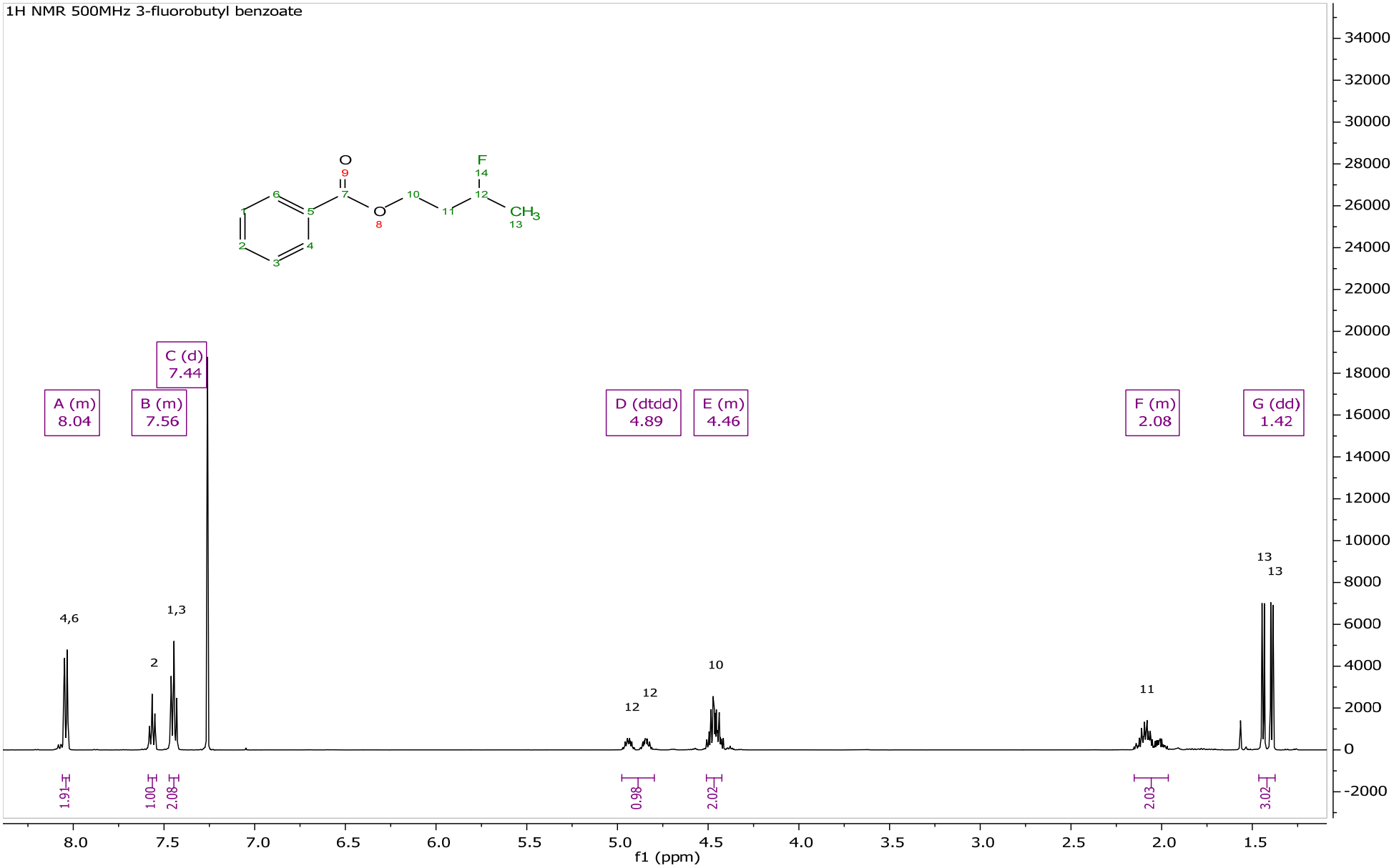
C	5.741446	0.229236	-0.000176
C	4.639937	1.056718	-0.000222
C	3.340672	0.503539	-0.000142
C	3.183268	-0.902223	-0.000013
C	4.319999	-1.723455	0.000028
C	5.584049	-1.167752	-0.000051
C	2.187061	1.344228	-0.000189
C	1.849012	-1.514002	0.000080
C	0.702268	-0.598754	0.000033
C	0.883579	0.780482	-0.000099
C	-0.293085	1.644874	-0.000146
C	-1.591069	1.021227	-0.000034
C	-1.735442	-0.389625	0.000105
C	-0.624314	-1.169860	0.000132
H	6.736758	0.657905	-0.000237
H	4.760110	2.132699	-0.000317
H	4.182968	-2.798192	0.000124
H	6.458235	-1.808191	-0.000019
H	-0.715785	-2.249539	0.000232
O	1.679957	-2.736081	0.000195
O	2.378643	2.658905	-0.000317
O	-0.237506	2.896571	-0.000280
H	1.504922	3.106268	-0.000340
O	-2.645925	1.826461	-0.000075
H	-2.321484	2.751088	-0.000191
S	-3.378974	-1.103662	0.000210
O	-3.199851	-2.548976	0.000344
O	-4.032166	-0.539070	1.208003
O	-4.032216	-0.539299	-1.207663
Na	-4.995809	1.184607	-0.000010

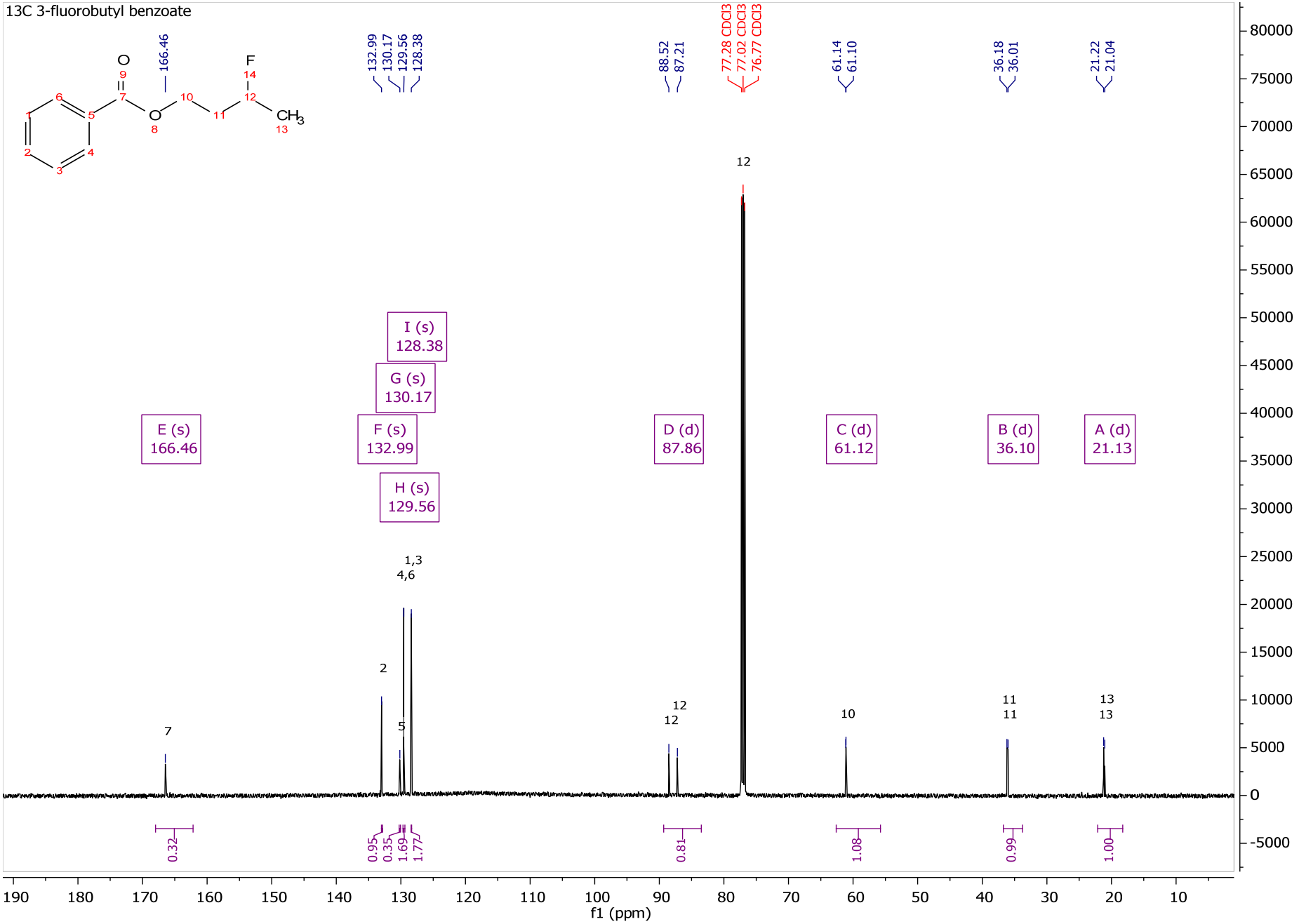
Zero-point correction = 0.192396
Thermal correction to Energy = 0.211393
Thermal correction to Enthalpy = 0.212338
Thermal correction to Gibbs Free Energy = 0.143938
Sum of electronic and zero-point Energies = -1624.471029
Sum of electronic and thermal Energies = -1624.452032
Sum of electronic and thermal Enthalpies = -1624.451088
Sum of electronic and thermal Free Energies = -1624.519487
Number of imaginary frequencies/frequency = 0

OPT-M062X-6-311+Gdp_AlizarinRed_triplet_C4.out

NMR spectra of reported compounds

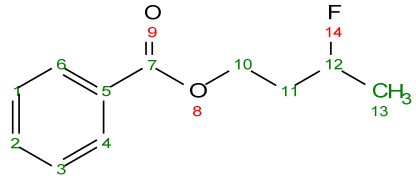
NMR Spectra of 3-fluorobutyl benzoate

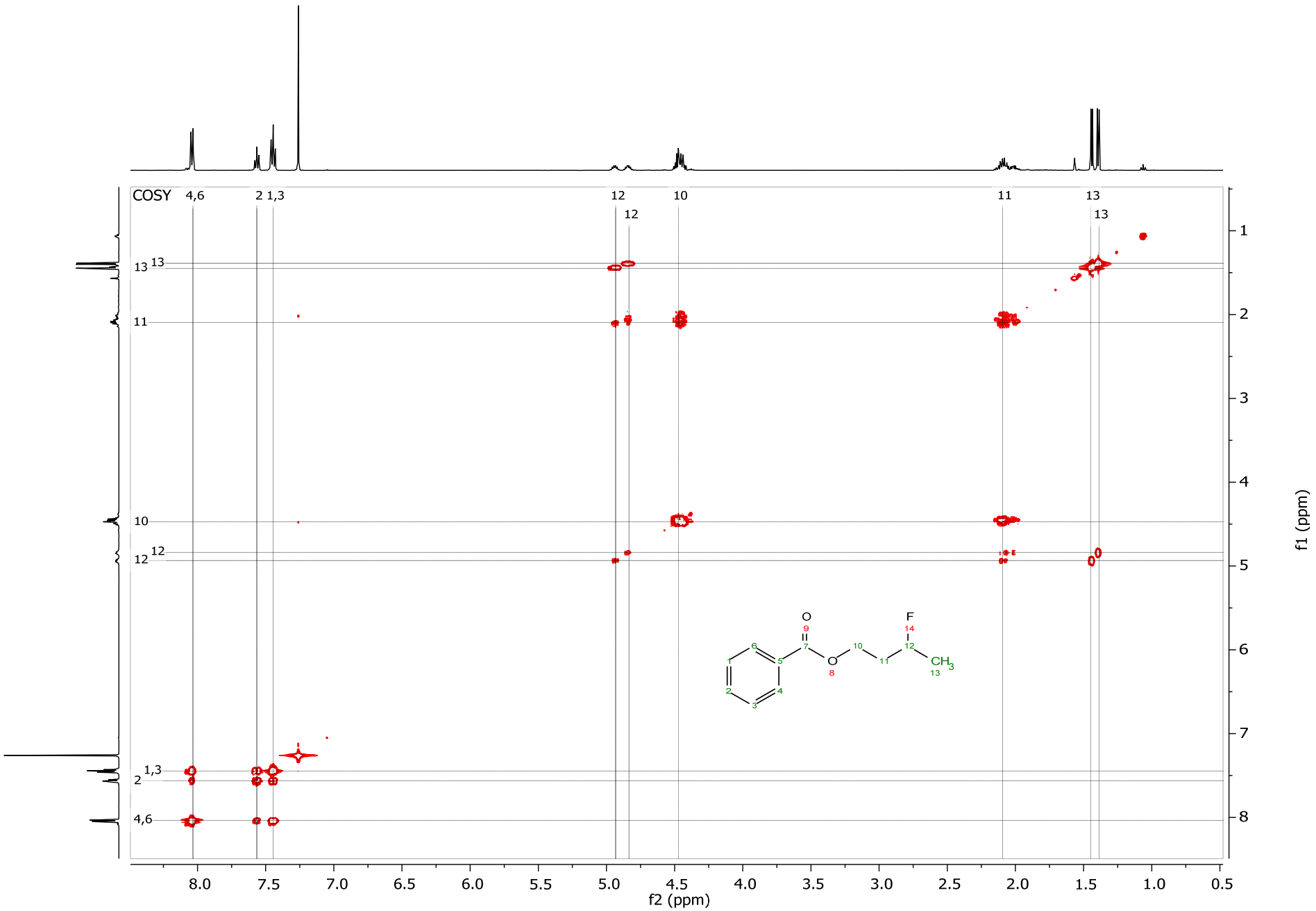


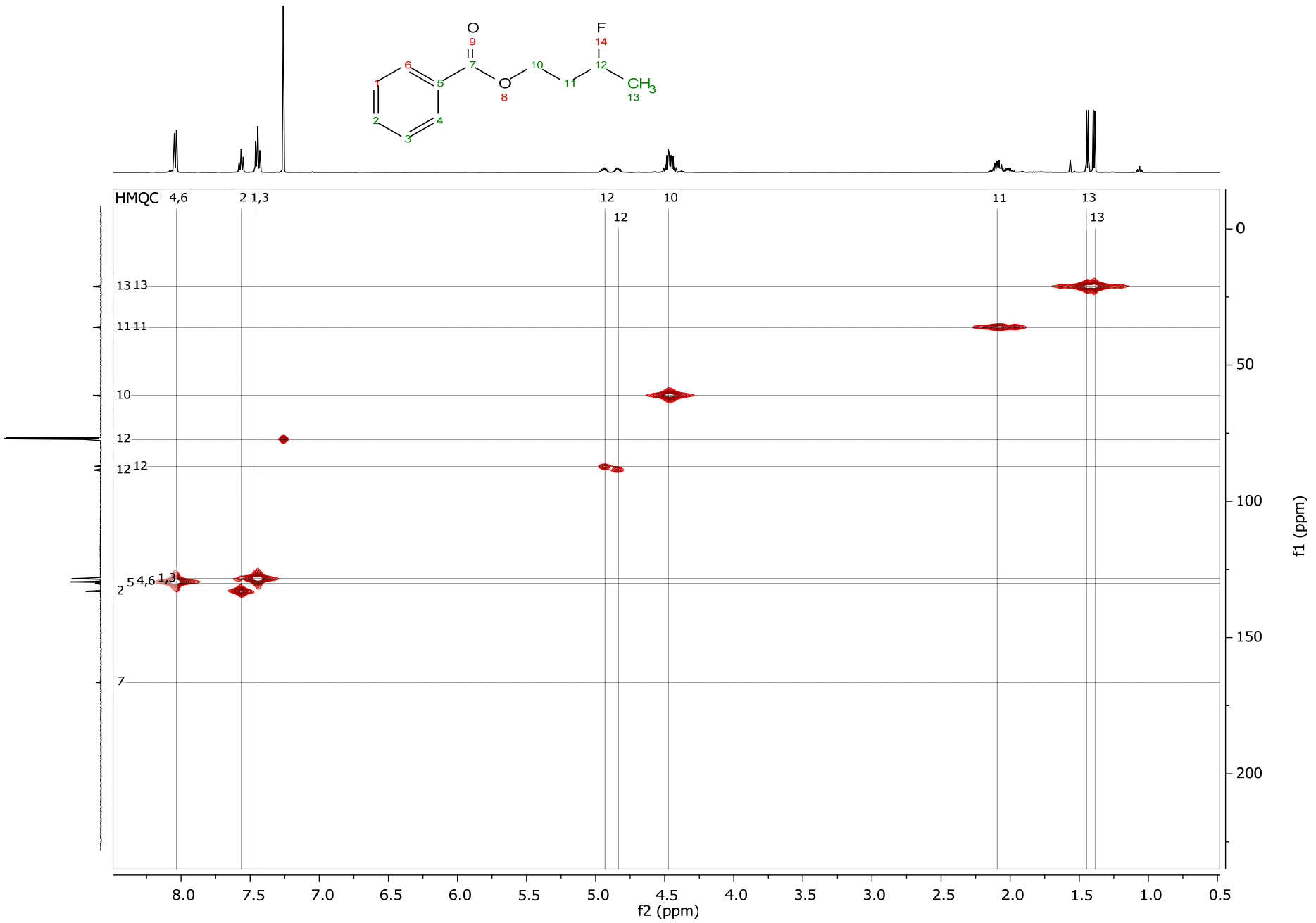

13C 3-fluorobutyl benzoate
O
F
CH3
166.46
132.99
130.17
129.56
128.38
88.52
87.21
77.28 CDCl3
77.02 CDCl3
76.77 CDCl3
61.14
61.10
36.18
36.01
21.22
21.04
I (s) 128.38
G (s) 130.17
E (s) 166.46
F (s) 132.99
H (s) 129.56
D (d) 87.86
C (d) 61.12
B (d) 36.10
A (d) 21.13
1,3 4,6
2
5
7
12
12
12
10
11 11
13 13
0.32
0.95
0.35
1.69
1.77
0.81
1.08
0.99
1.00
f1 (ppm)

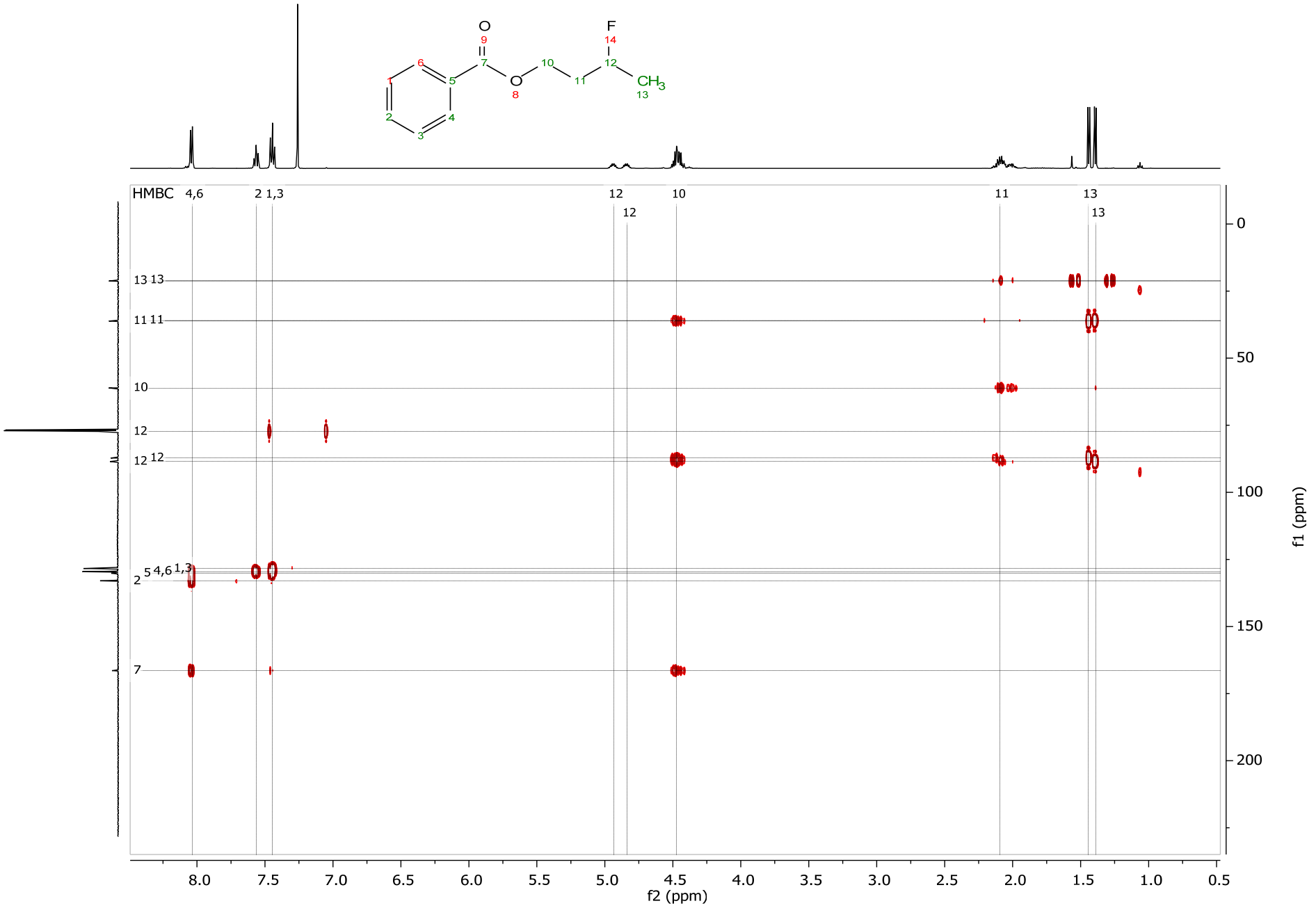
1H NMR 500MHz 3-fluorobutyl benzoate

^{19}F NMR (376 MHz, Chloroform-*d*) δ -175.53 (ddqd, *J* = 48.1, 29.5, 23.9, 16.2 Hz).

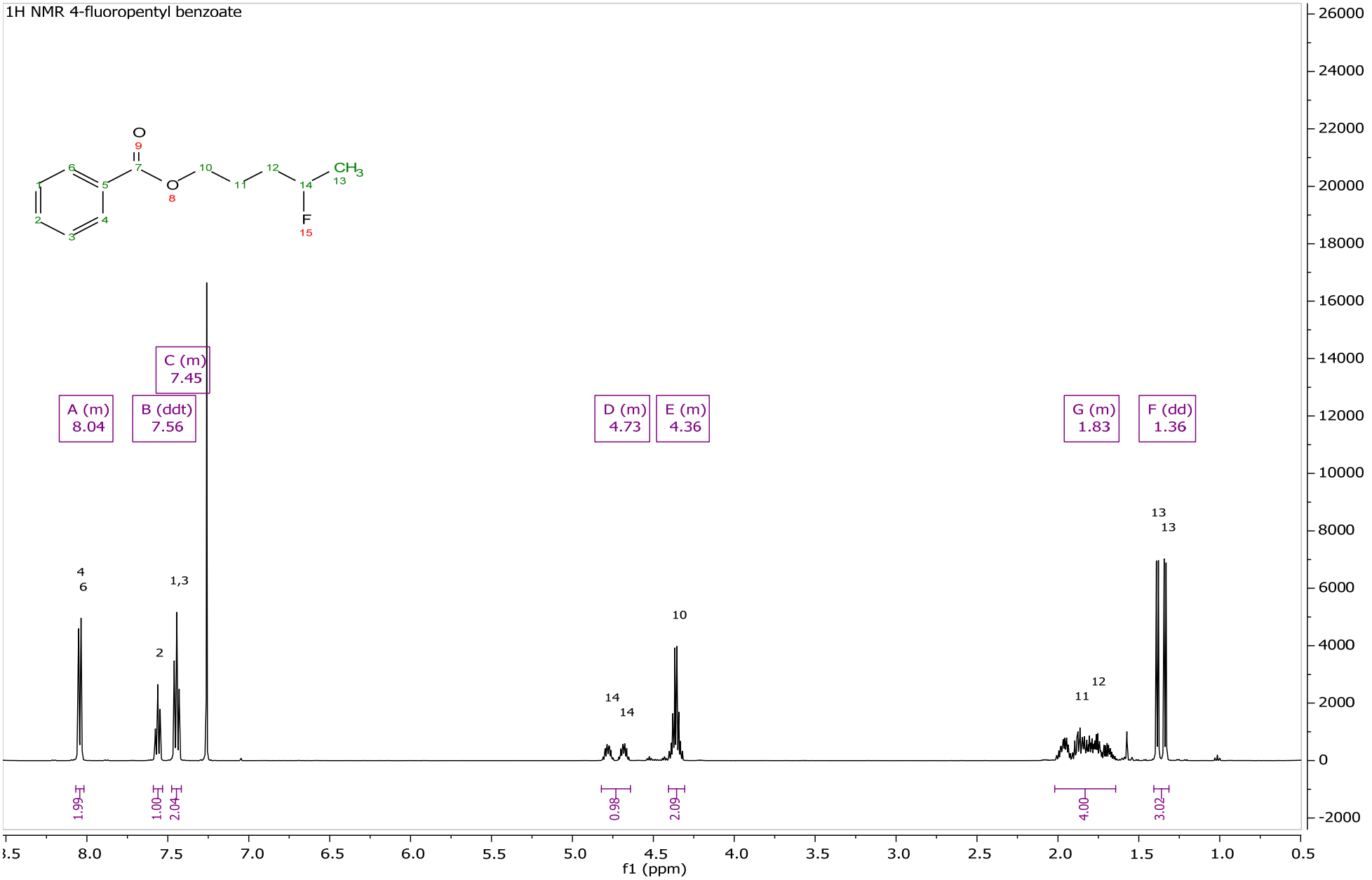


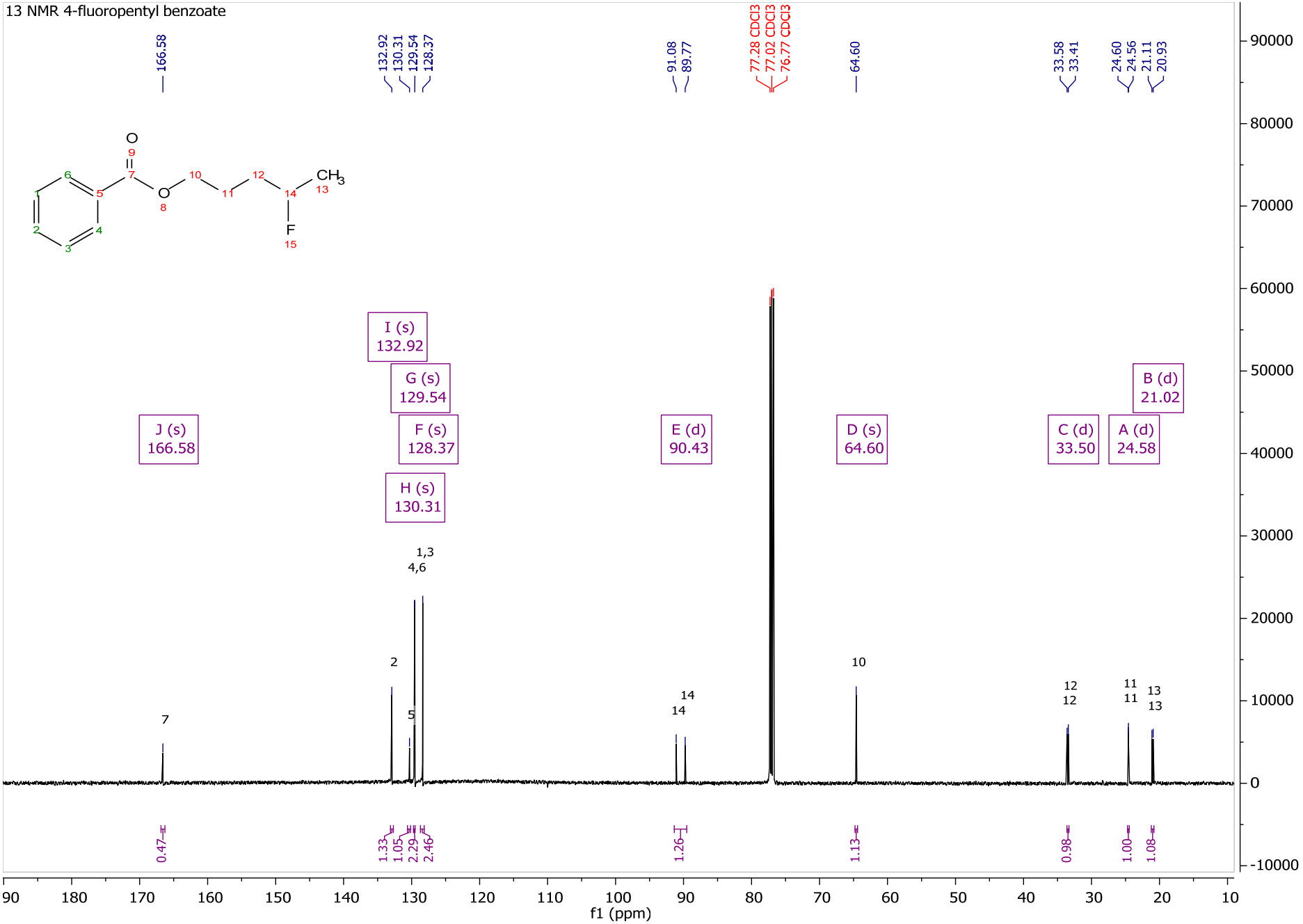

COSY
4,6
2 1,3
12
10
11
13
f2 (ppm)
f1 (ppm)
O
F
CH3


HMQC
4,6
2
1,3
12
12
10
11
13
13
f2 (ppm)
f1 (ppm)

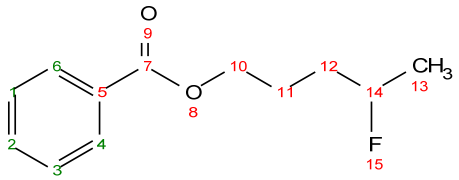

HMBC
f2 (ppm)
f1 (ppm)

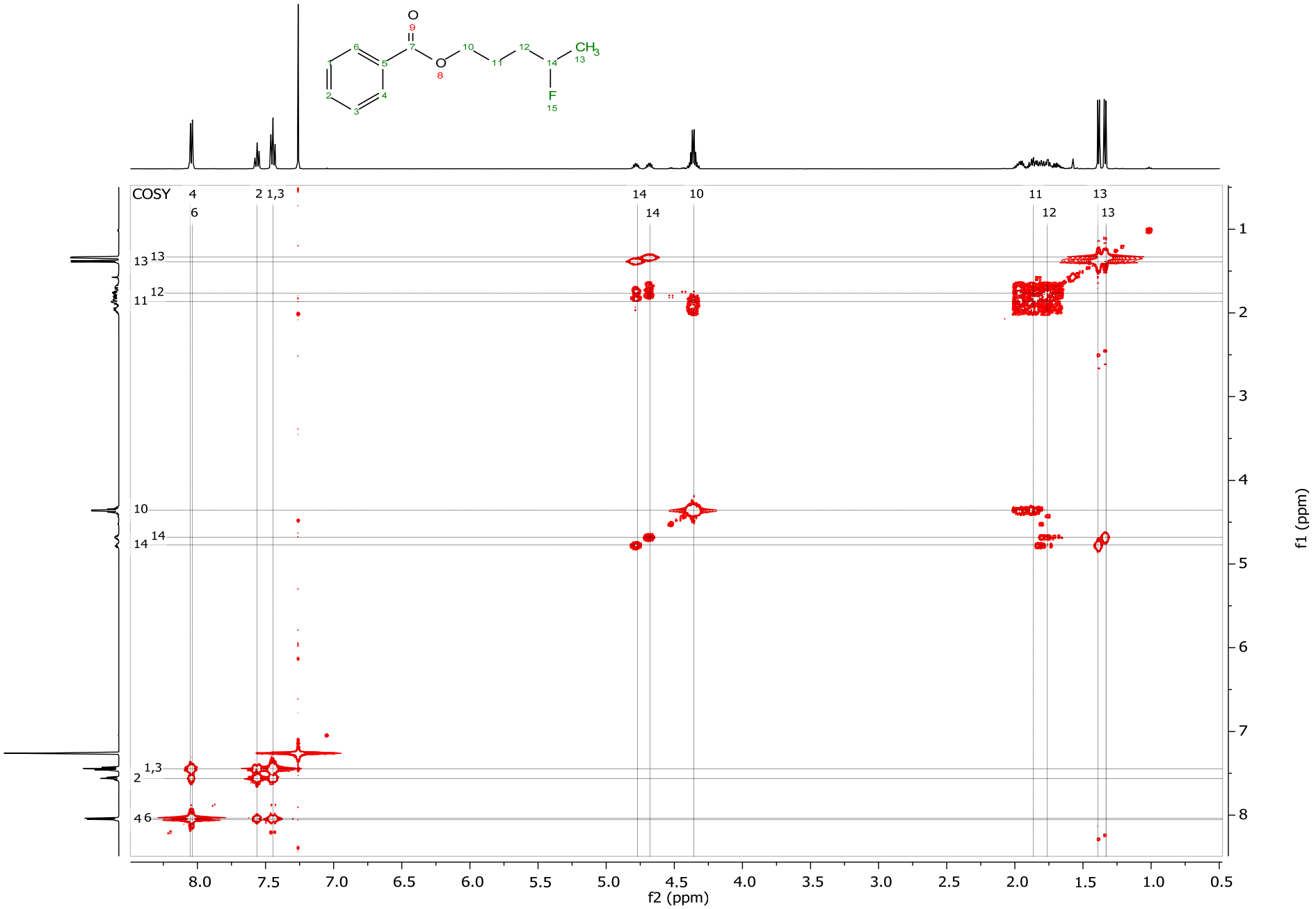
NMR Spectra of 4-fluoropentyl benzoate

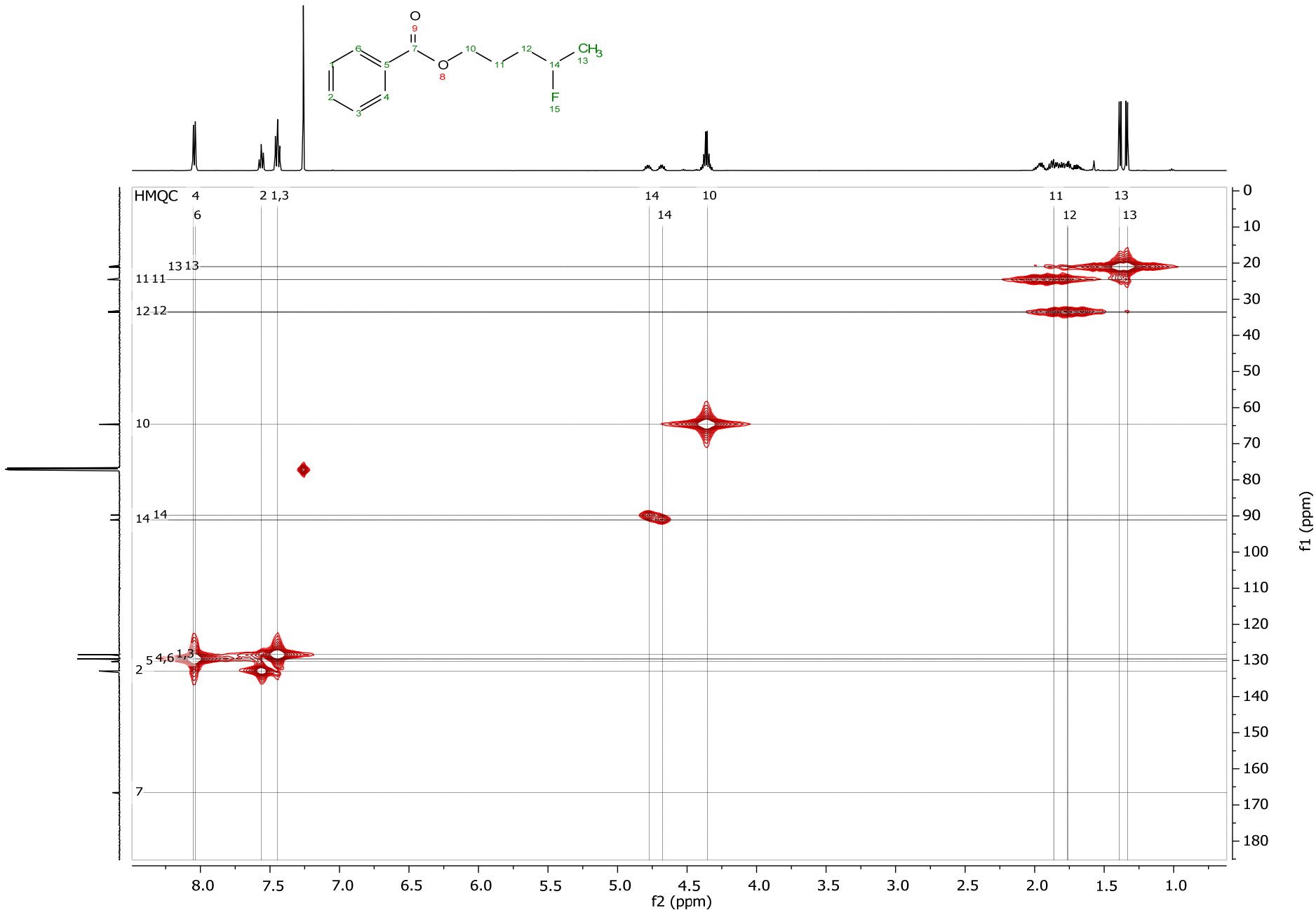


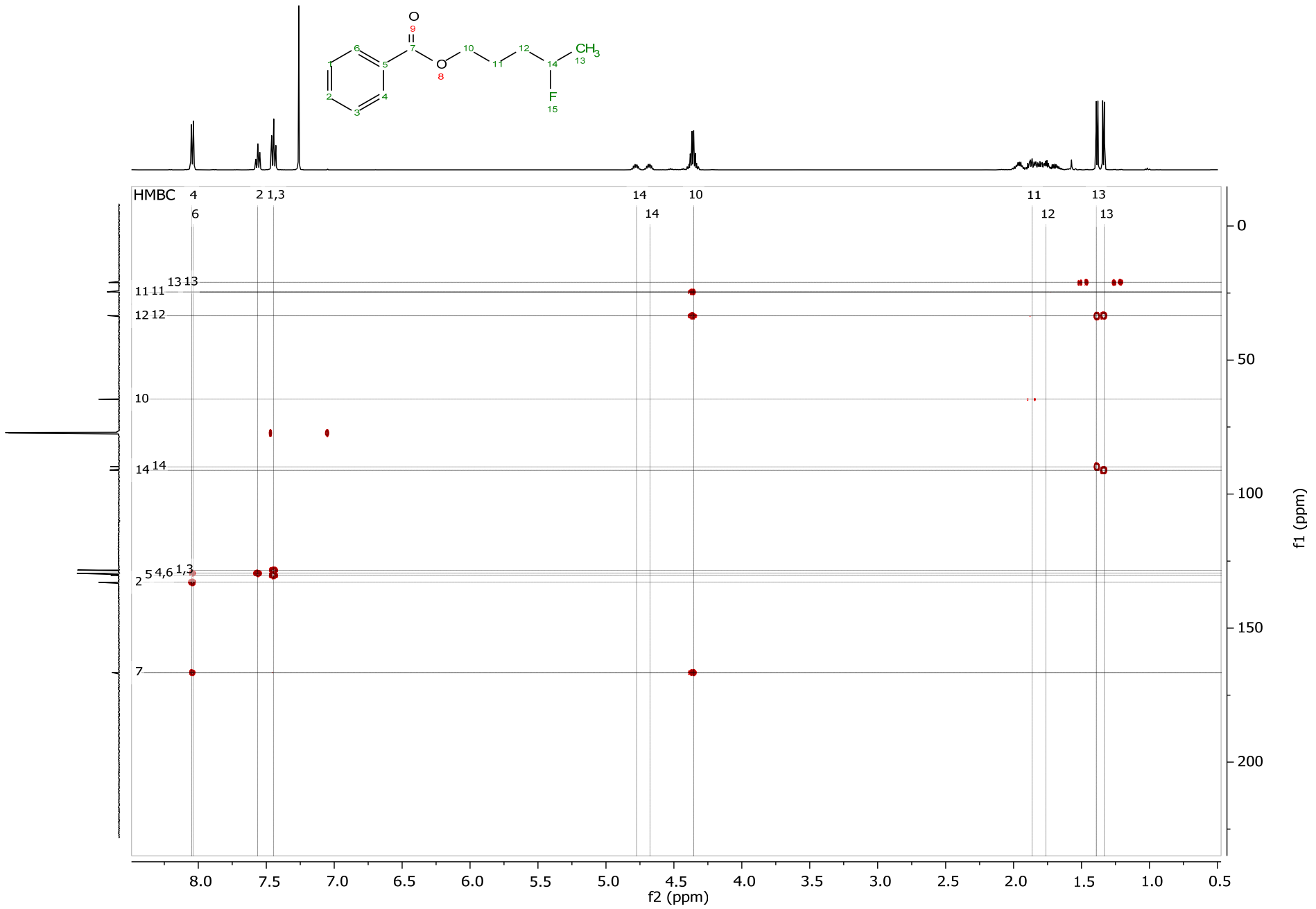

13 NMR 4-fluoropentyl benzoate
166.58
132.92
130.31
129.54
128.37
91.08
89.77
77.28 CDCl3
77.02 CDCl3
76.77 CDCl3
64.60
33.58
33.41
24.60
24.56
21.11
20.93
I (s) 132.92
G (s) 129.54
F (s) 128.37
H (s) 130.31
J (s) 166.58
E (d) 90.43
D (s) 64.60
C (d) 33.50
A (d) 24.58
B (d) 21.02
1,3
4,6
2
5
7
14
14
10
12
12
11
11
13
13
0.47
1.33
1.05
2.29
2.46
1.26
1.13
0.98
1.00
1.08
f1 (ppm)

19F NMR (376 MHz, $CDCl_3$) δ -173.47.

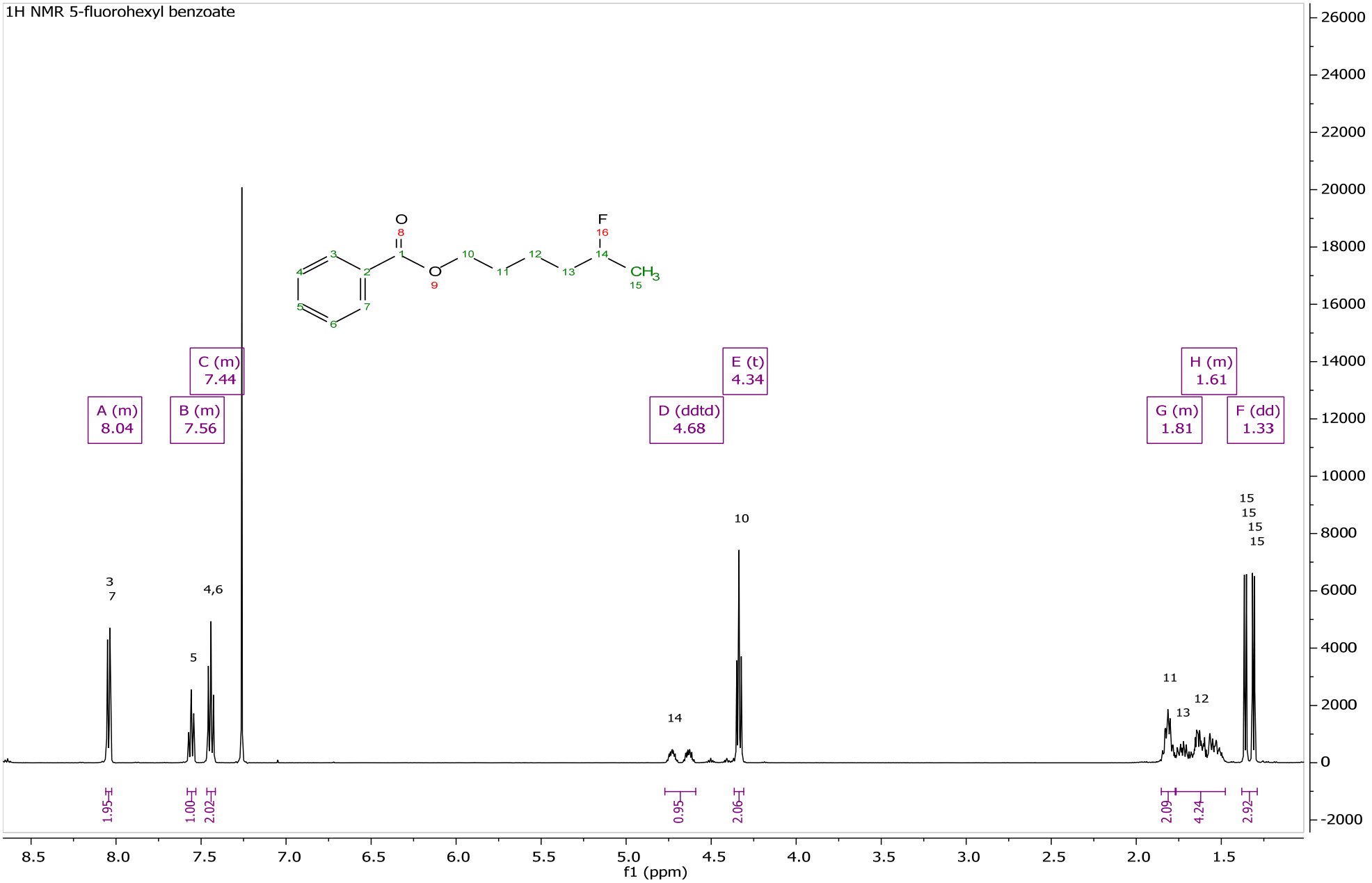


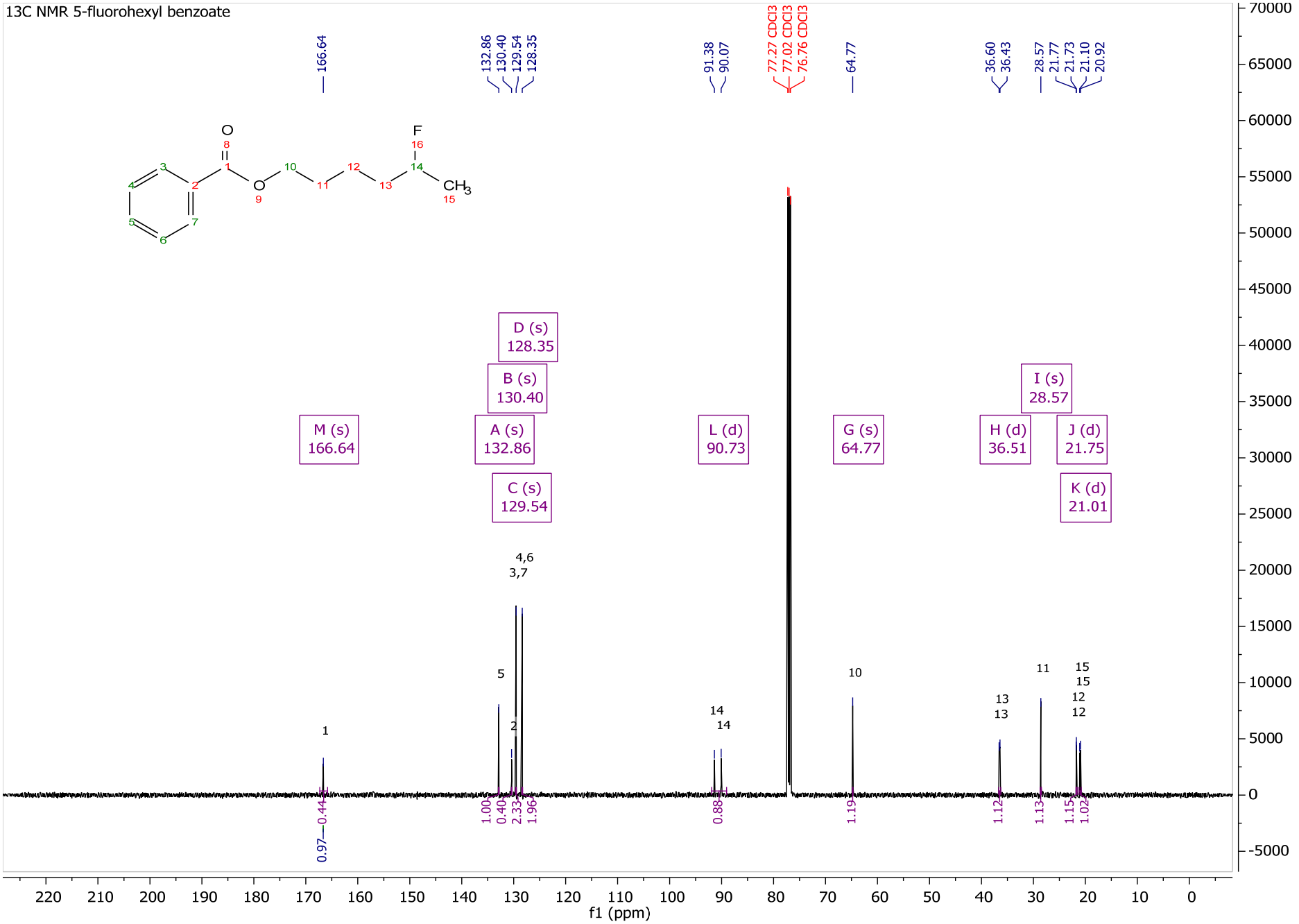

COSY
f2 (ppm)
f1 (ppm)

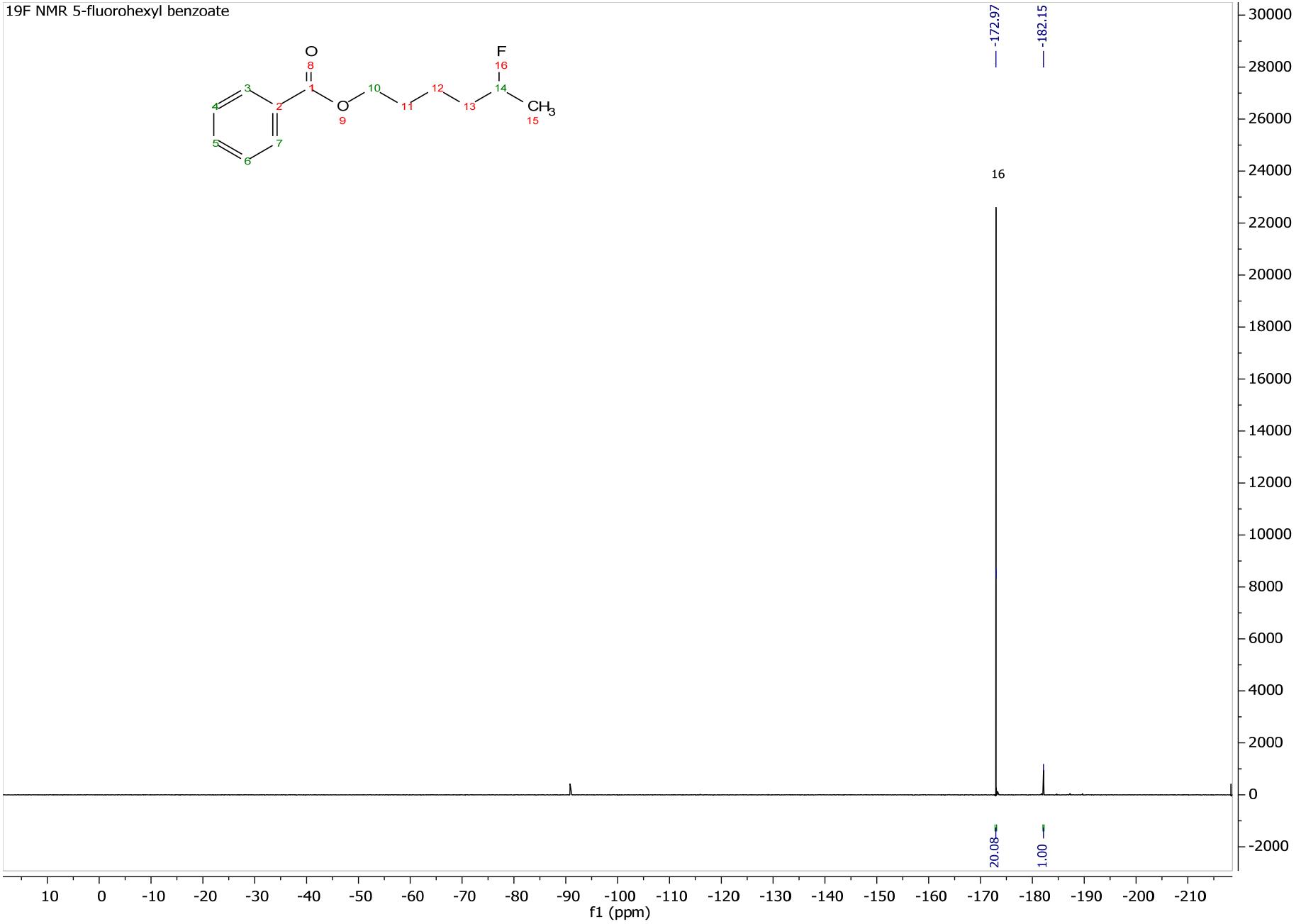

HMQC
f2 (ppm)
f1 (ppm)

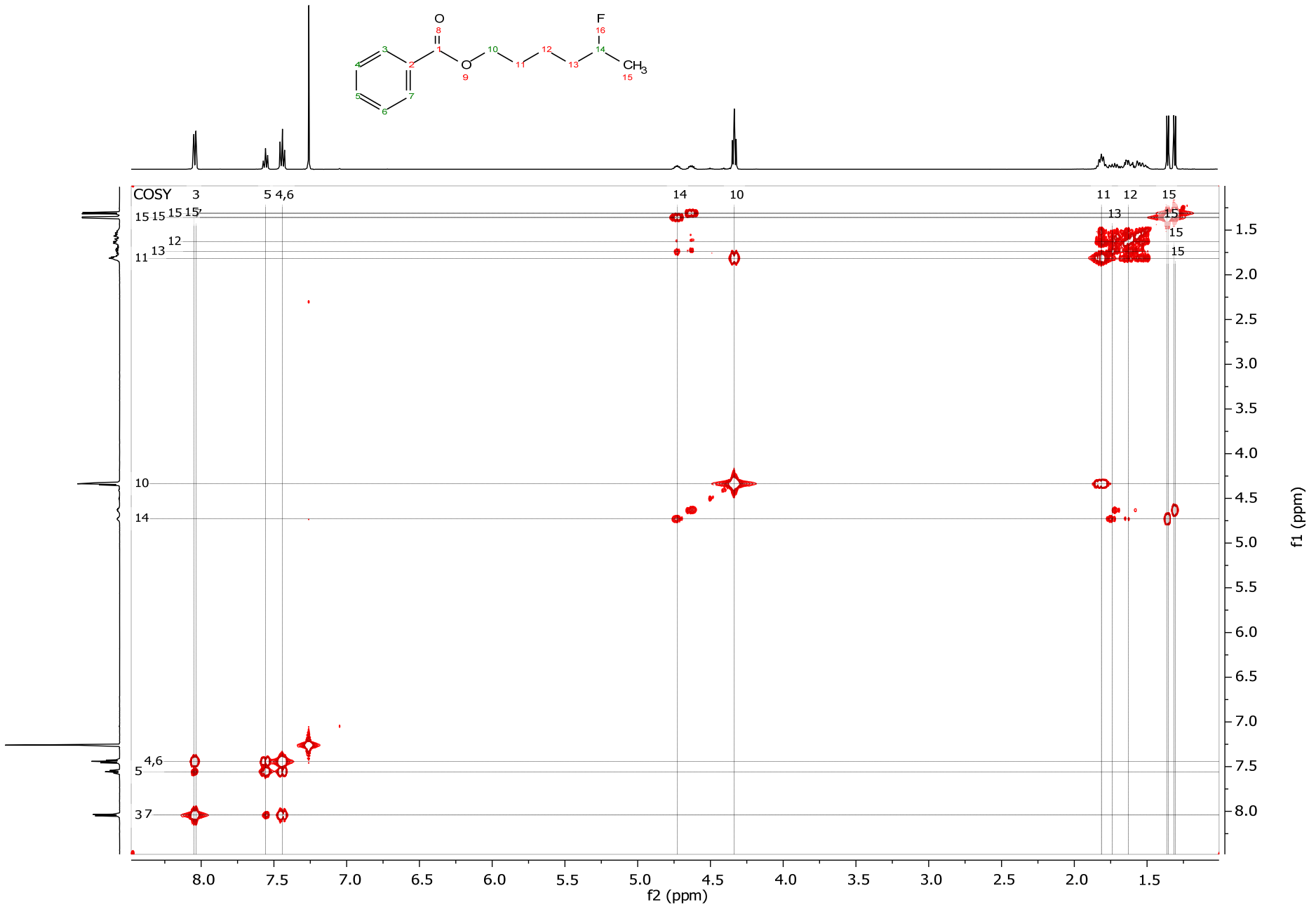

HMBC
f2 (ppm)
f1 (ppm)

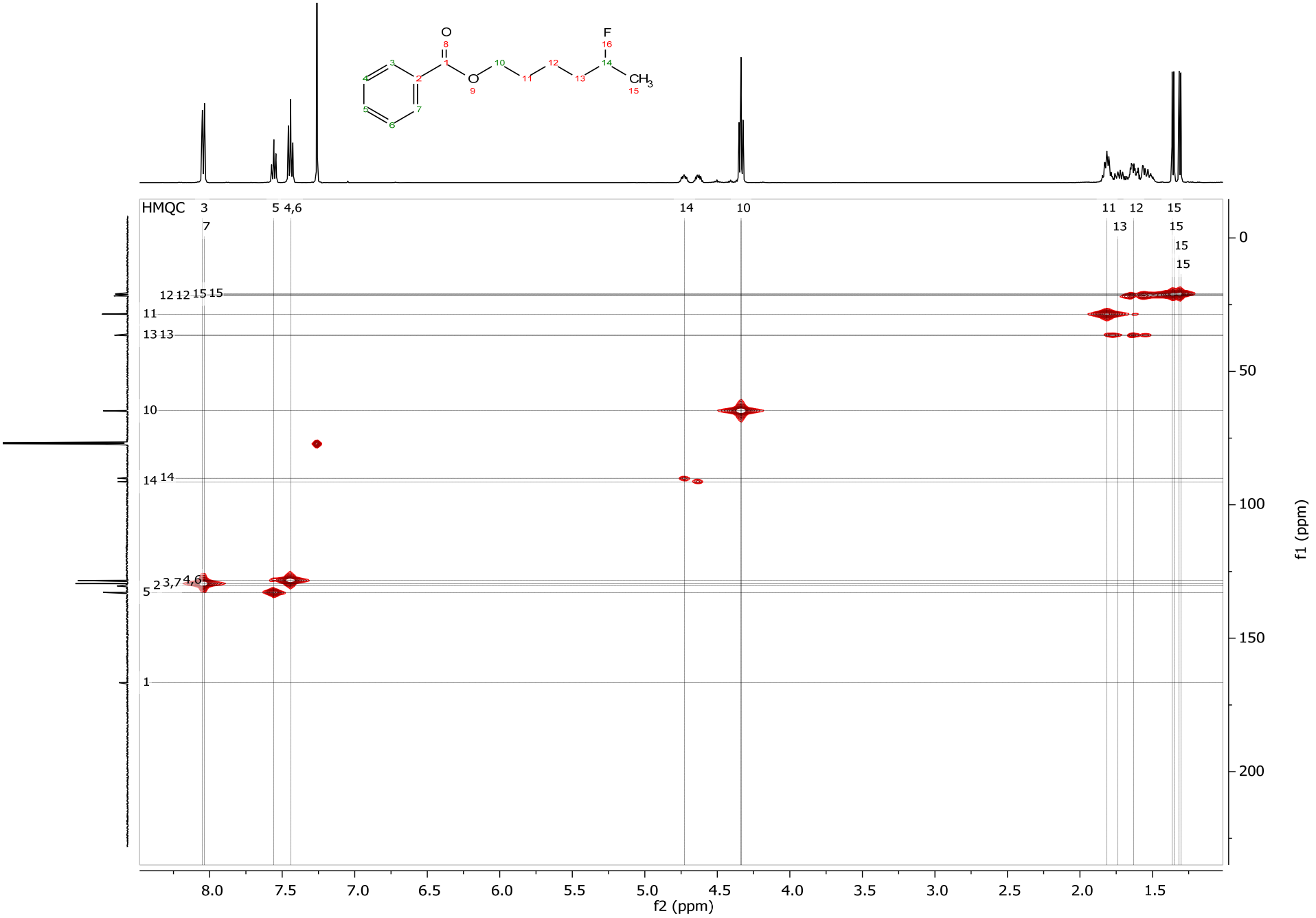
NMR Spectra of 5-fluorohexyl benzoate

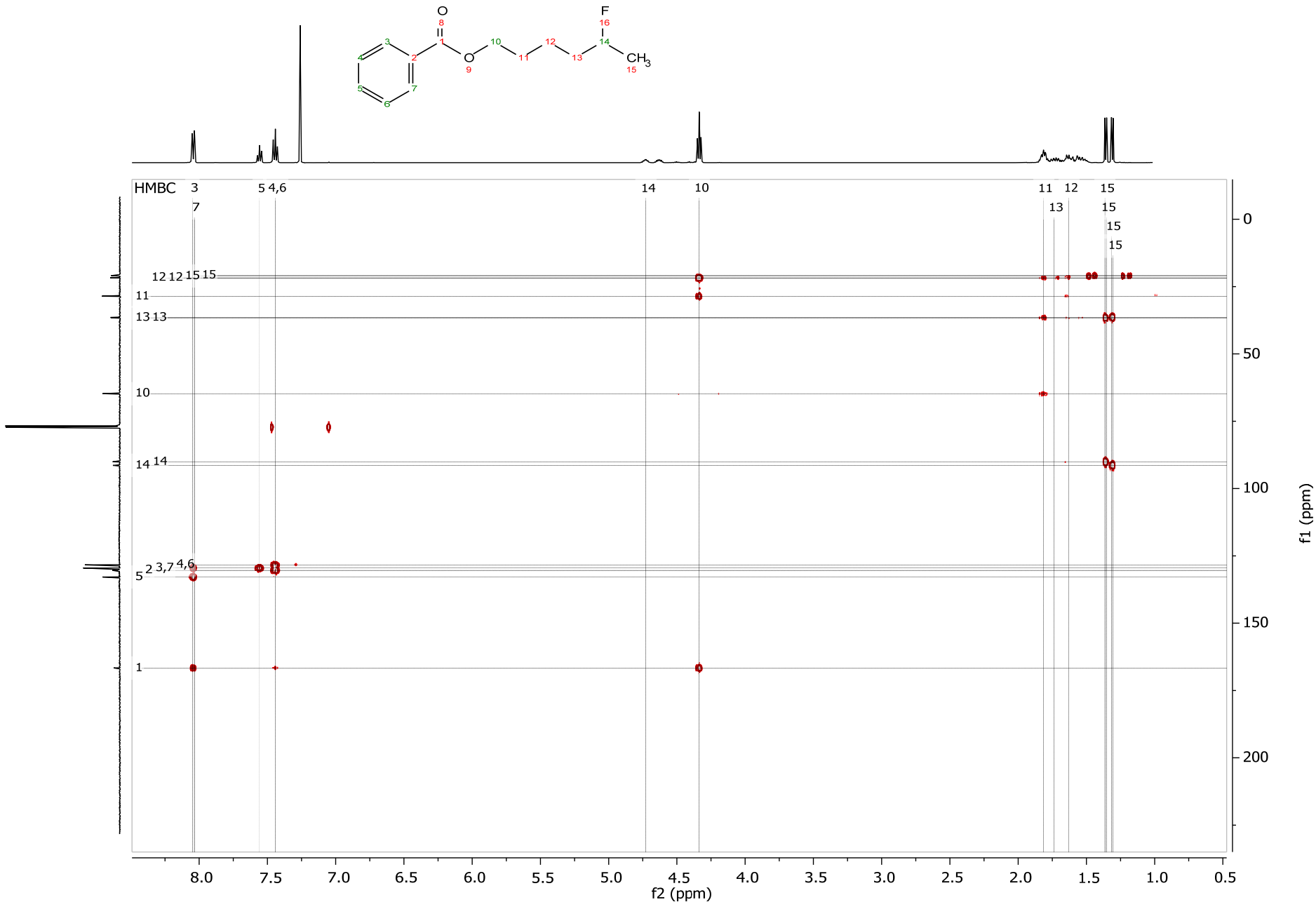



13C NMR 5-fluorohexyl benzoate
166.64
132.86
130.40
129.54
128.35
91.38
90.07
77.27 CDCl3
77.02 CDCl3
76.76 CDCl3
64.77
36.60
36.43
28.57
21.77
21.73
21.10
20.92
M (s) 166.64
A (s) 132.86
B (s) 130.40
C (s) 129.54
D (s) 128.35
L (d) 90.73
G (s) 64.77
H (d) 36.51
I (s) 28.57
J (d) 21.75
K (d) 21.01
f1 (ppm)

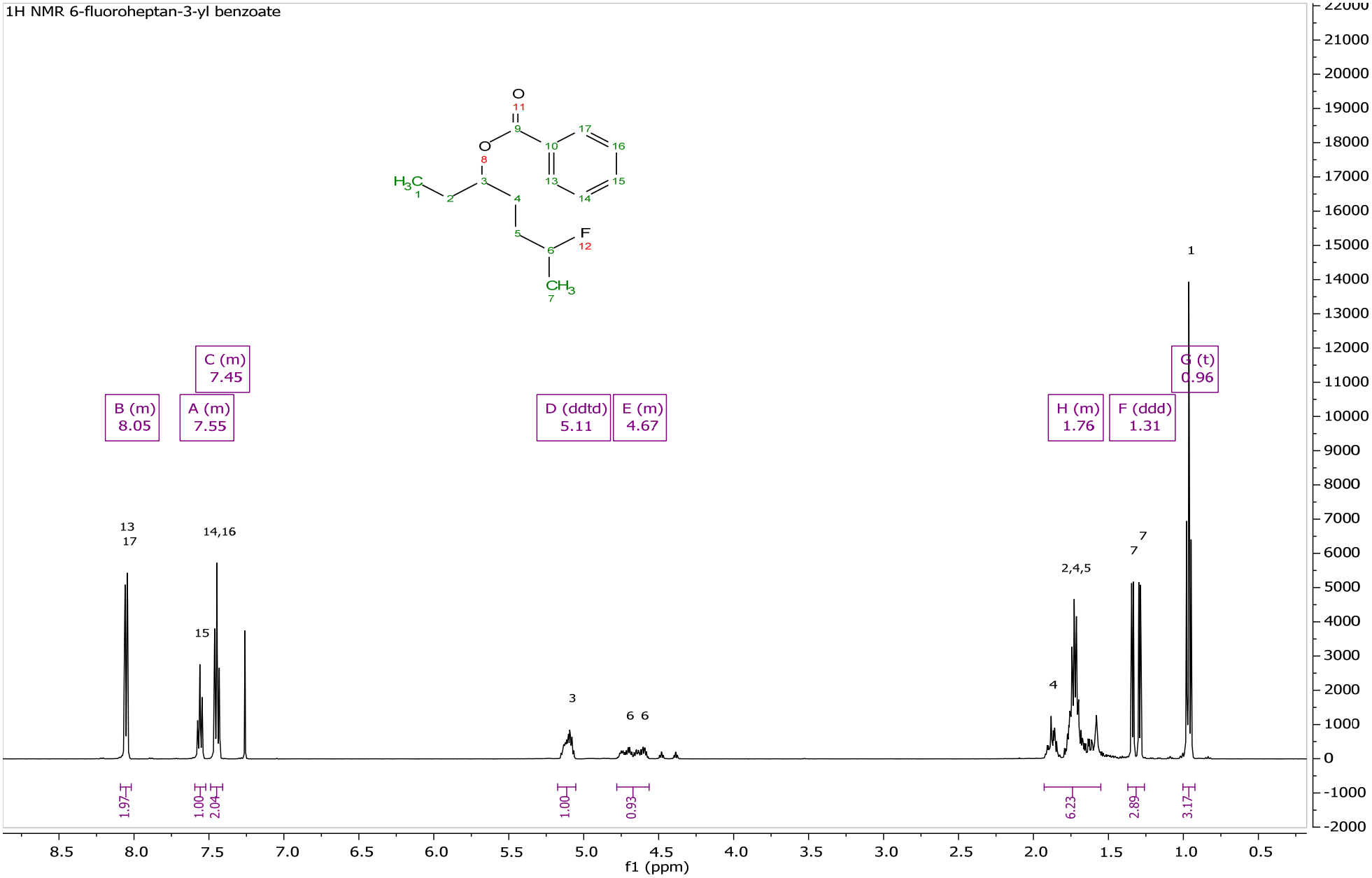

19F NMR 5-fluorohexyl benzoate
O
8
F
16
3
1
10
12
14
4
2
O
11
13
CH3
9
15
5
7
6
-172.97
-182.15
16
30000
28000
26000
24000
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
-2000
20.08
1.00
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

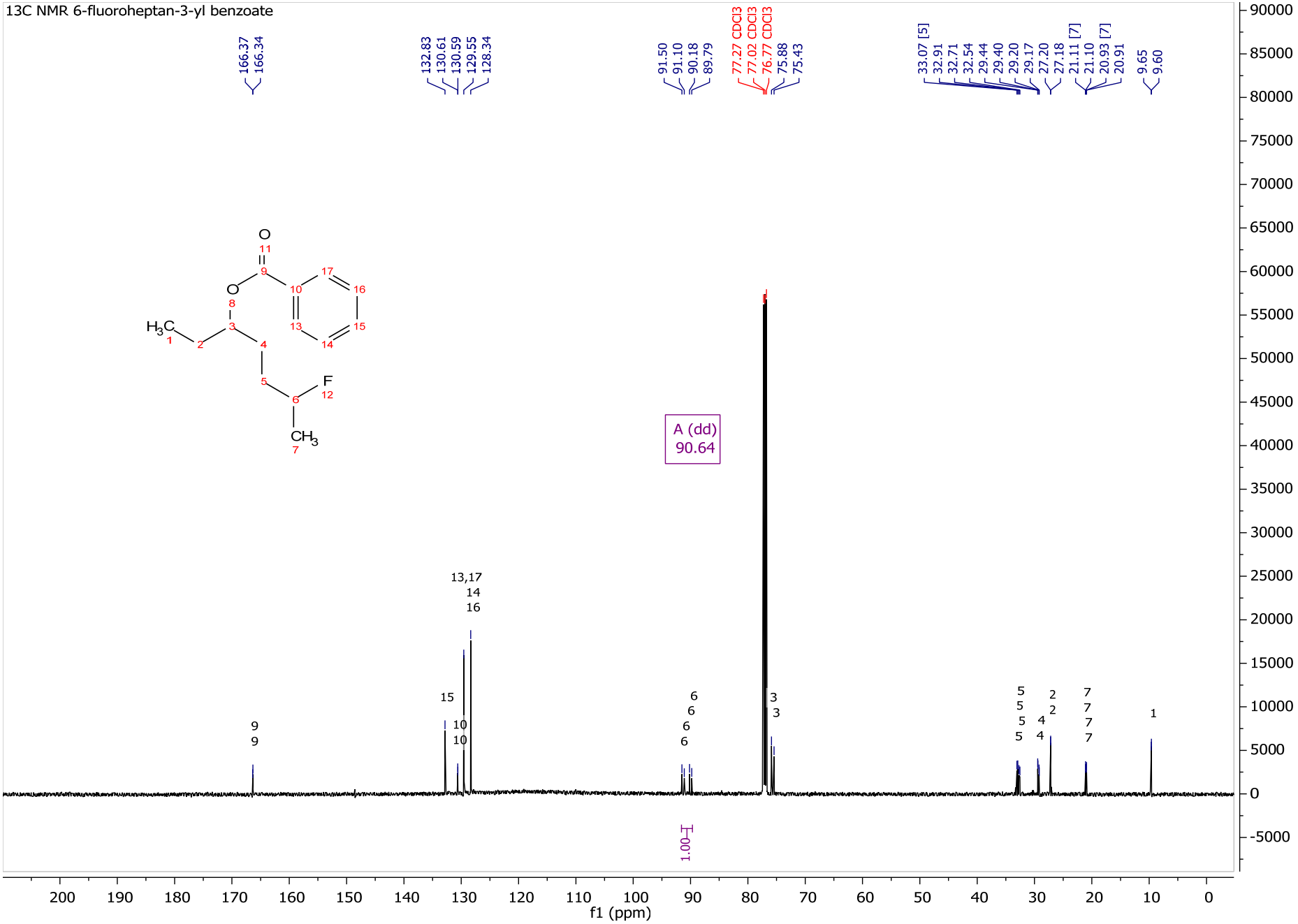

COSY
f2 (ppm)
f1 (ppm)

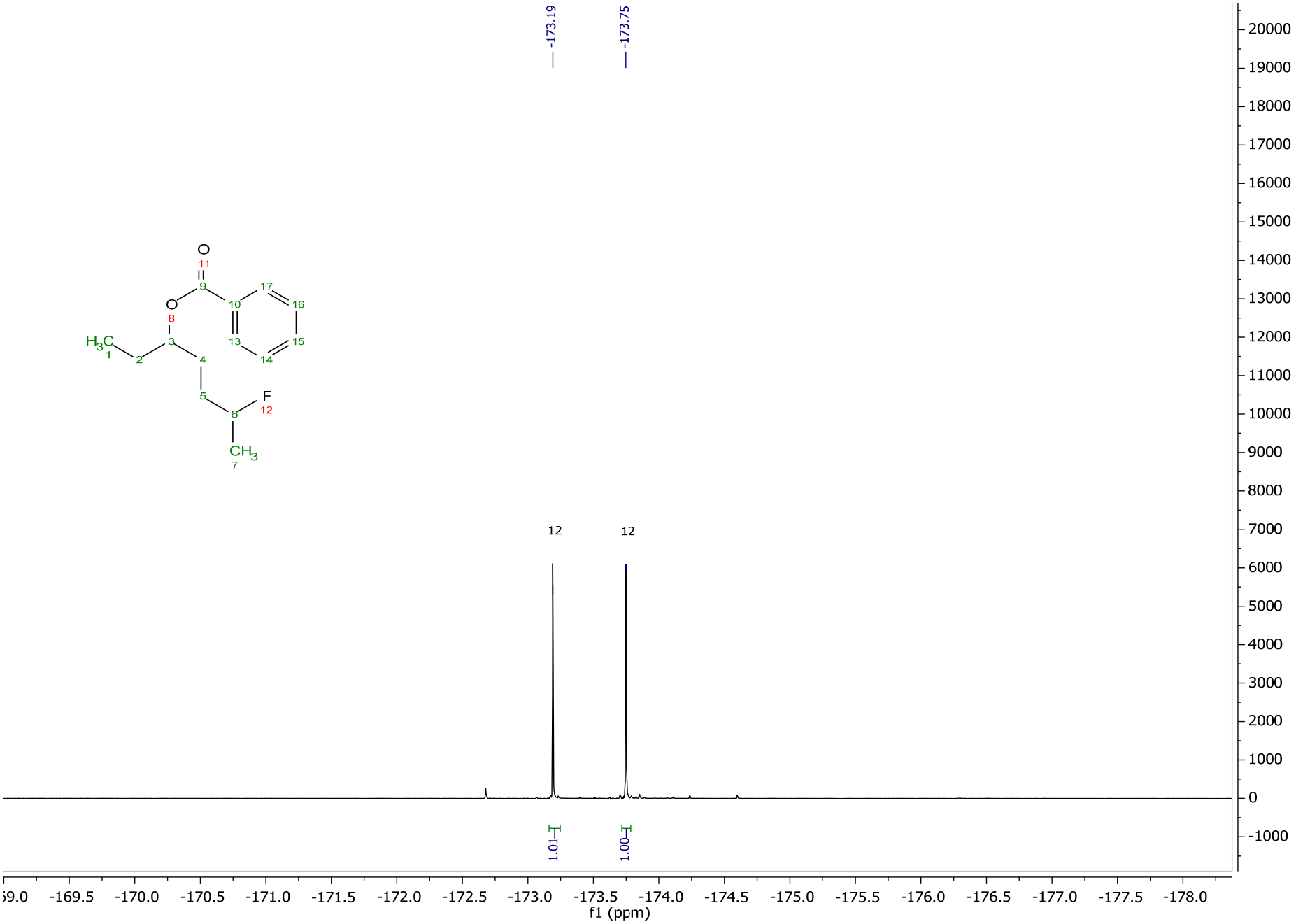

HMQC
f2 (ppm)
f1 (ppm)

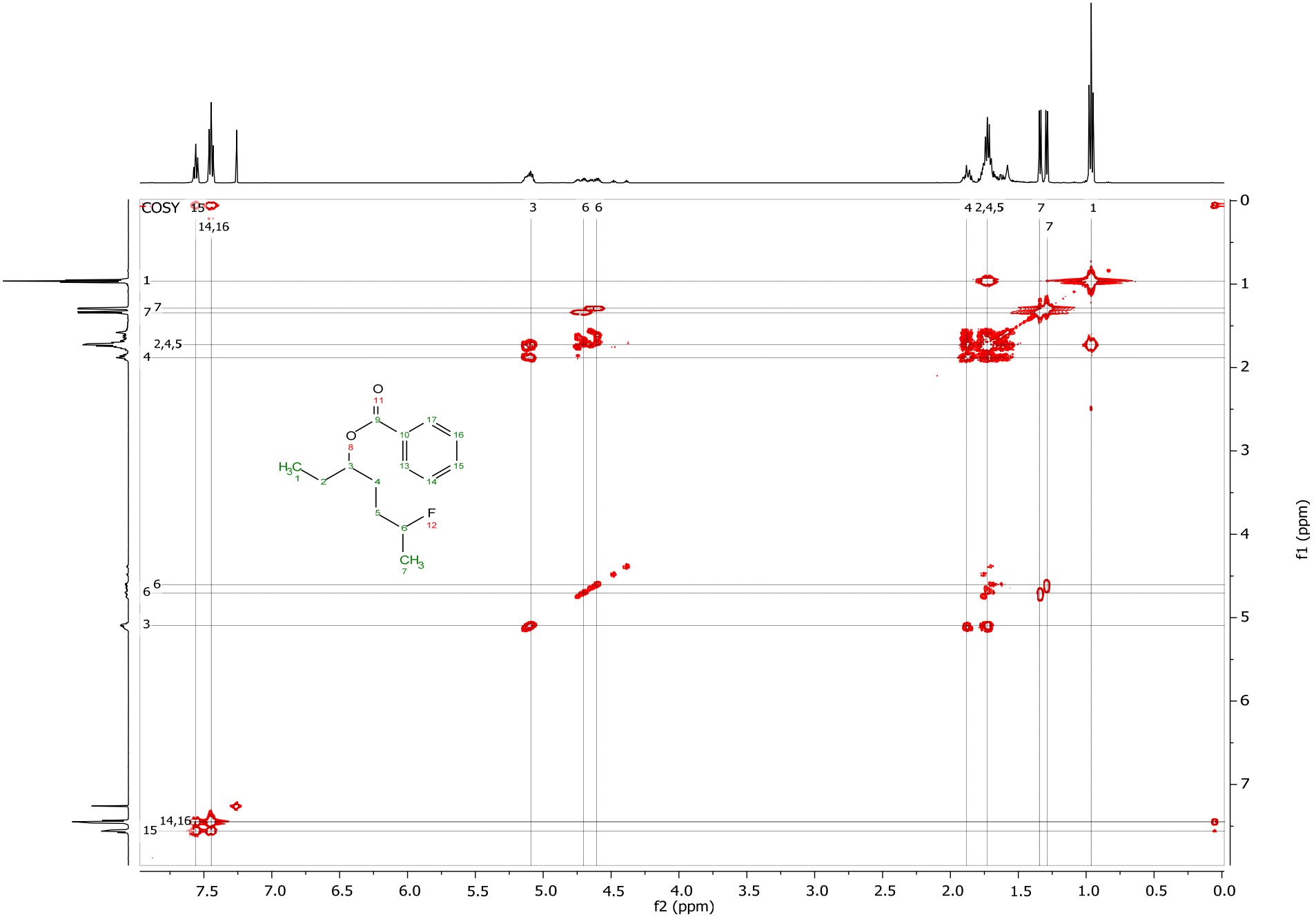

HMBC
f2 (ppm)
f1 (ppm)

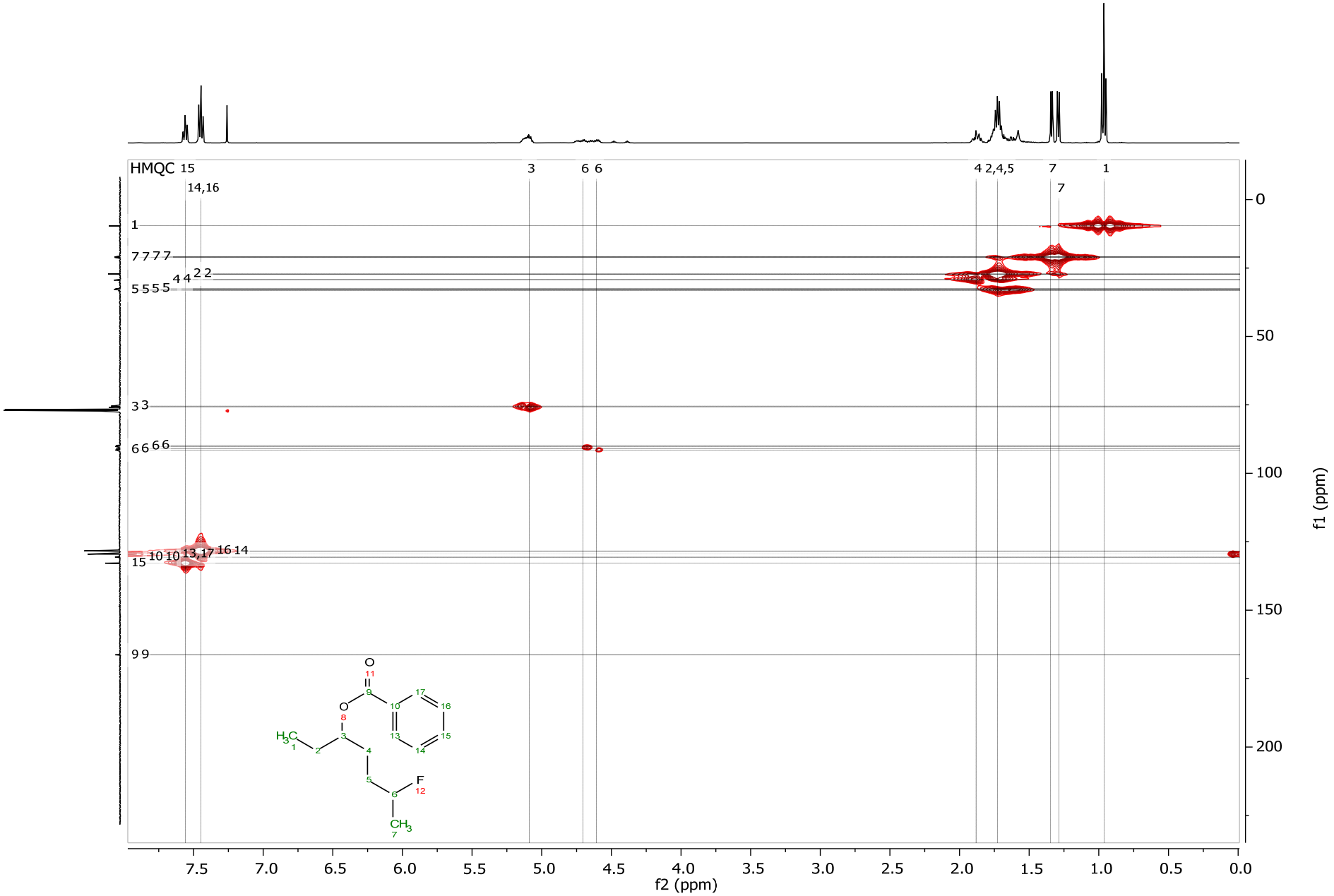
NMR Spectra of 6-fluoroheptan-3-yl benzoate

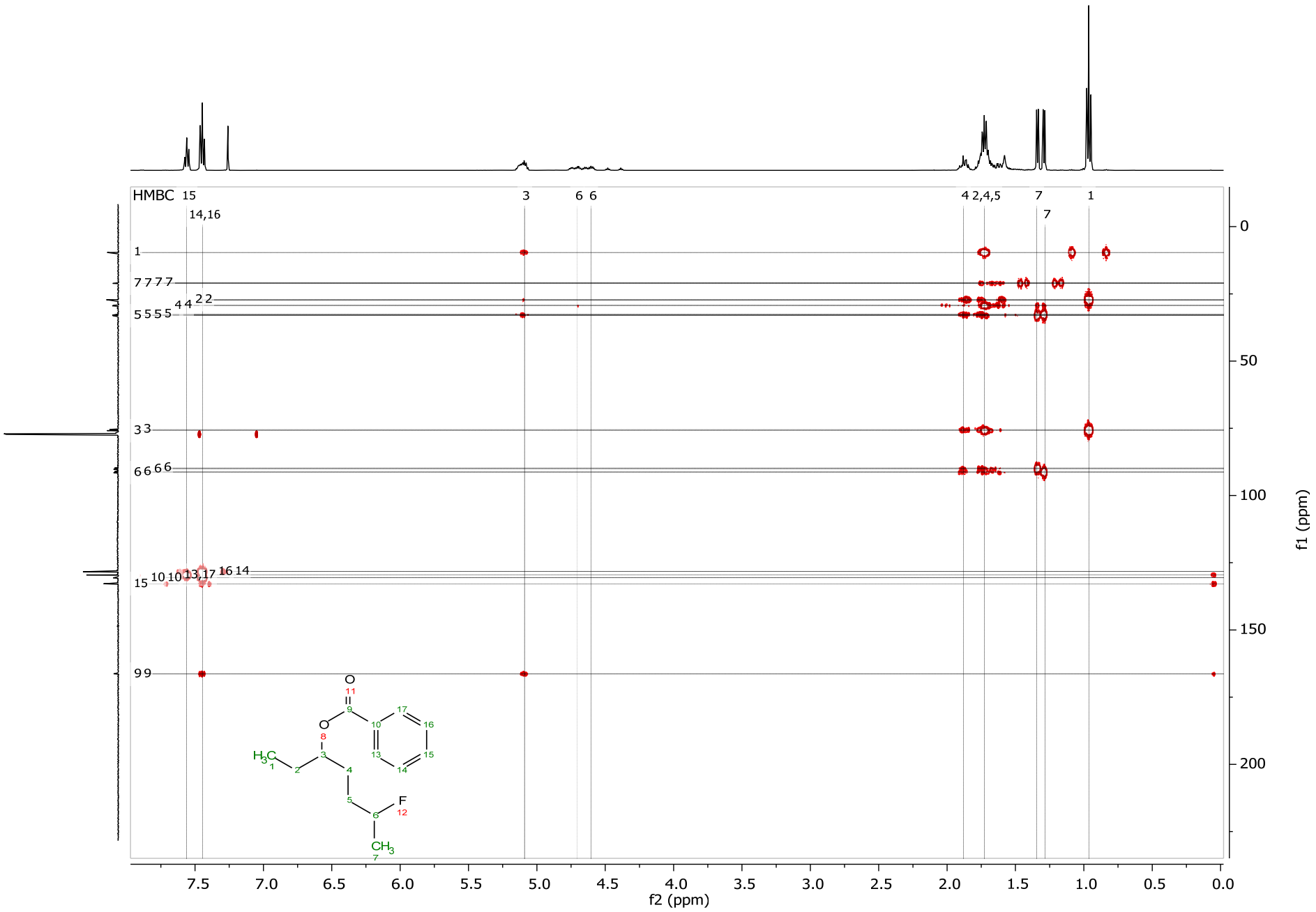



13C NMR 6-fluoroheptan-3-yl benzoate
166.37
166.34
132.83
130.61
130.59
129.55
128.34
91.50
91.10
90.18
89.79
77.27 CDCl3
77.02 CDCl3
76.77 CDCl3
75.88
75.43
33.07 [5]
32.91
32.71
32.54
29.44
29.40
29.20
29.17
27.20
27.18
21.11 [7]
21.10
20.93 [7]
20.91
9.65
9.60
A (dd)
90.64
1.00
f1 (ppm)

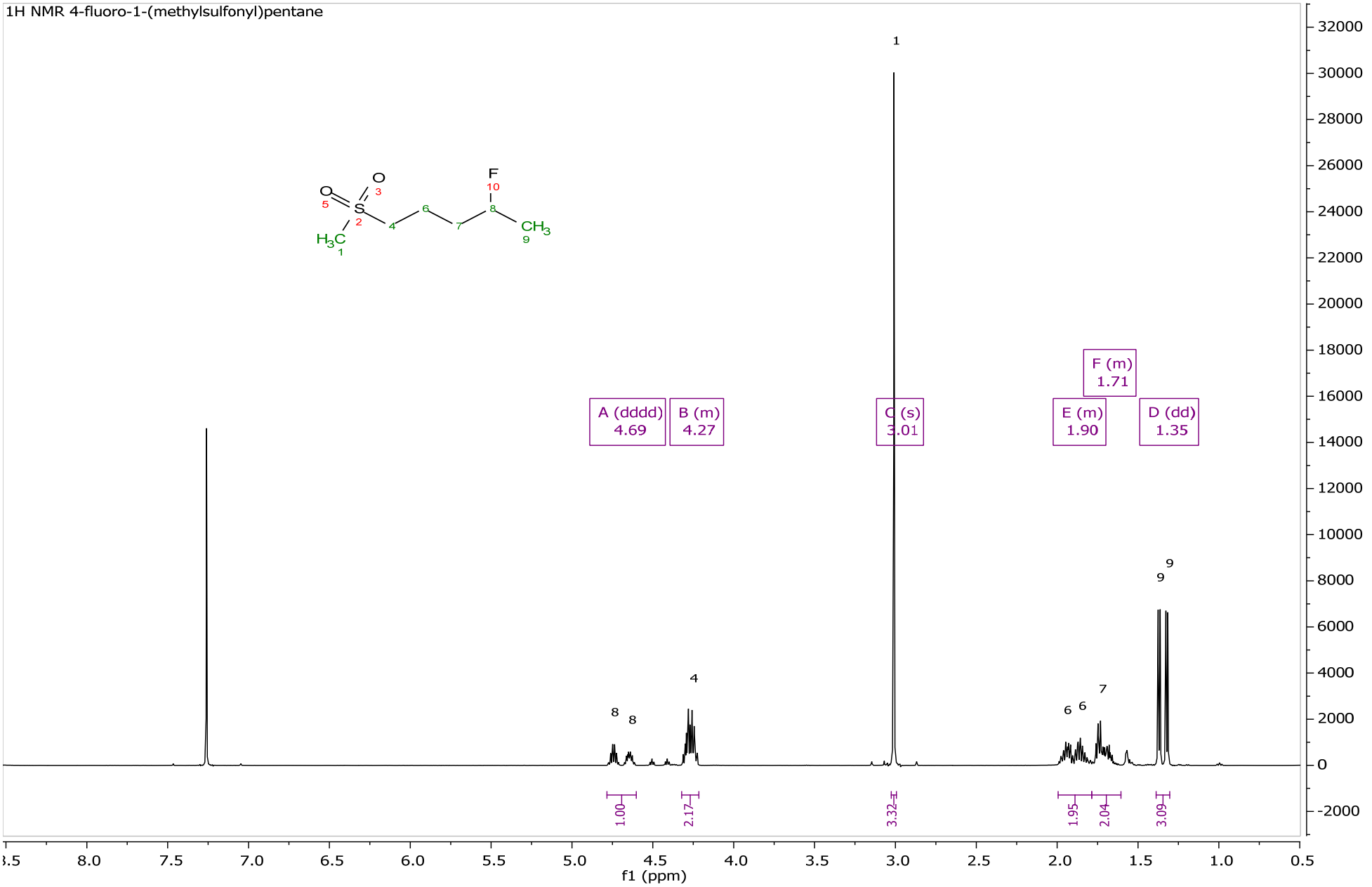

-173.19
-173.75
12
12
1.01
1.00
f1 (ppm)

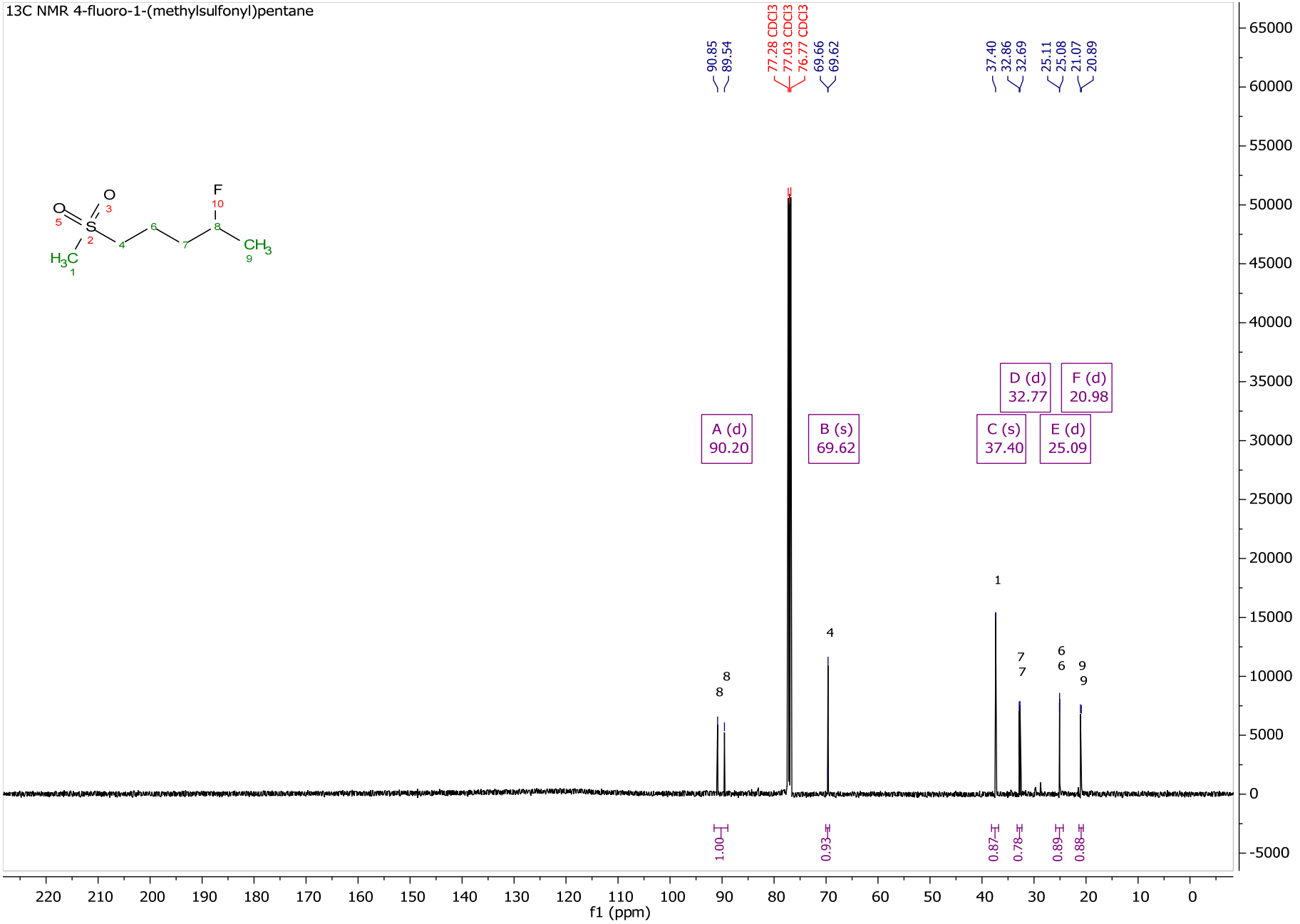

COSY
15
14,16
3
6 6
4 2,4,5
7
7
1
1
7 7
2,4,5
4
6 6
3
14,16
15
O
11
9
O
8
10
17
16
13
15
14
H3C
1
2
3
4
5
6
F
12
CH3
7
f2 (ppm)
f1 (ppm)

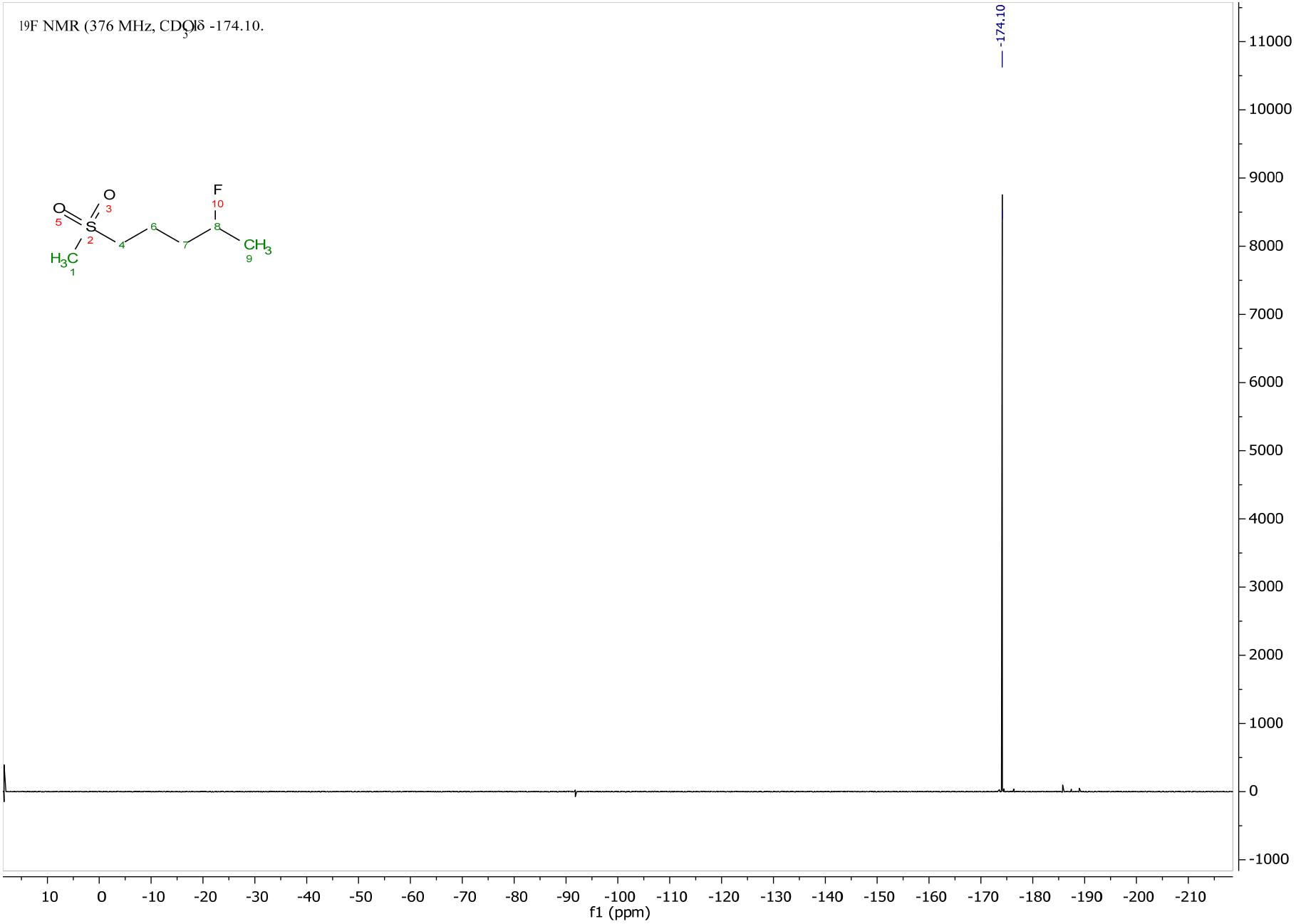

HMQC
f2 (ppm)
f1 (ppm)

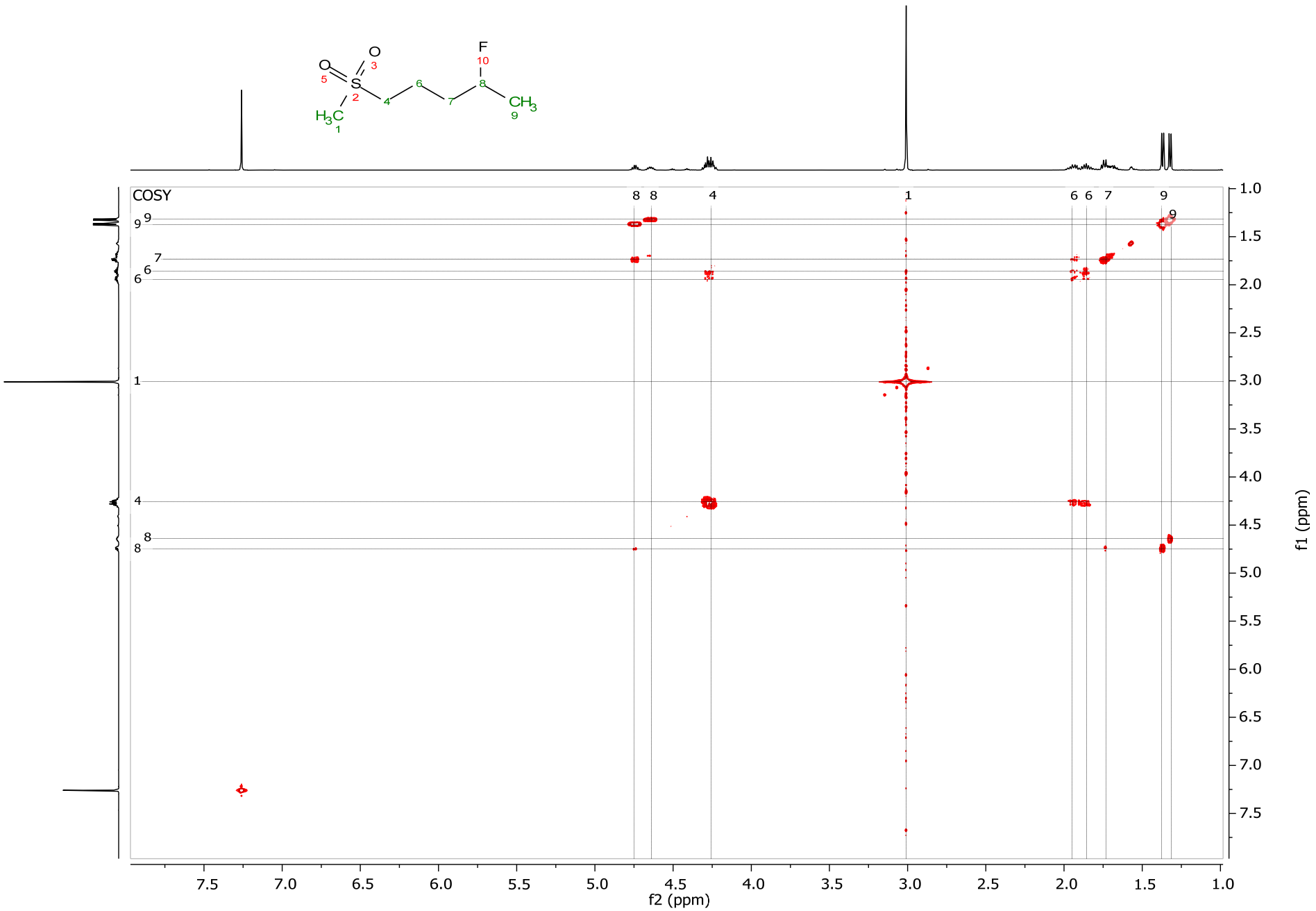

HMBC
f2 (ppm)
f1 (ppm)

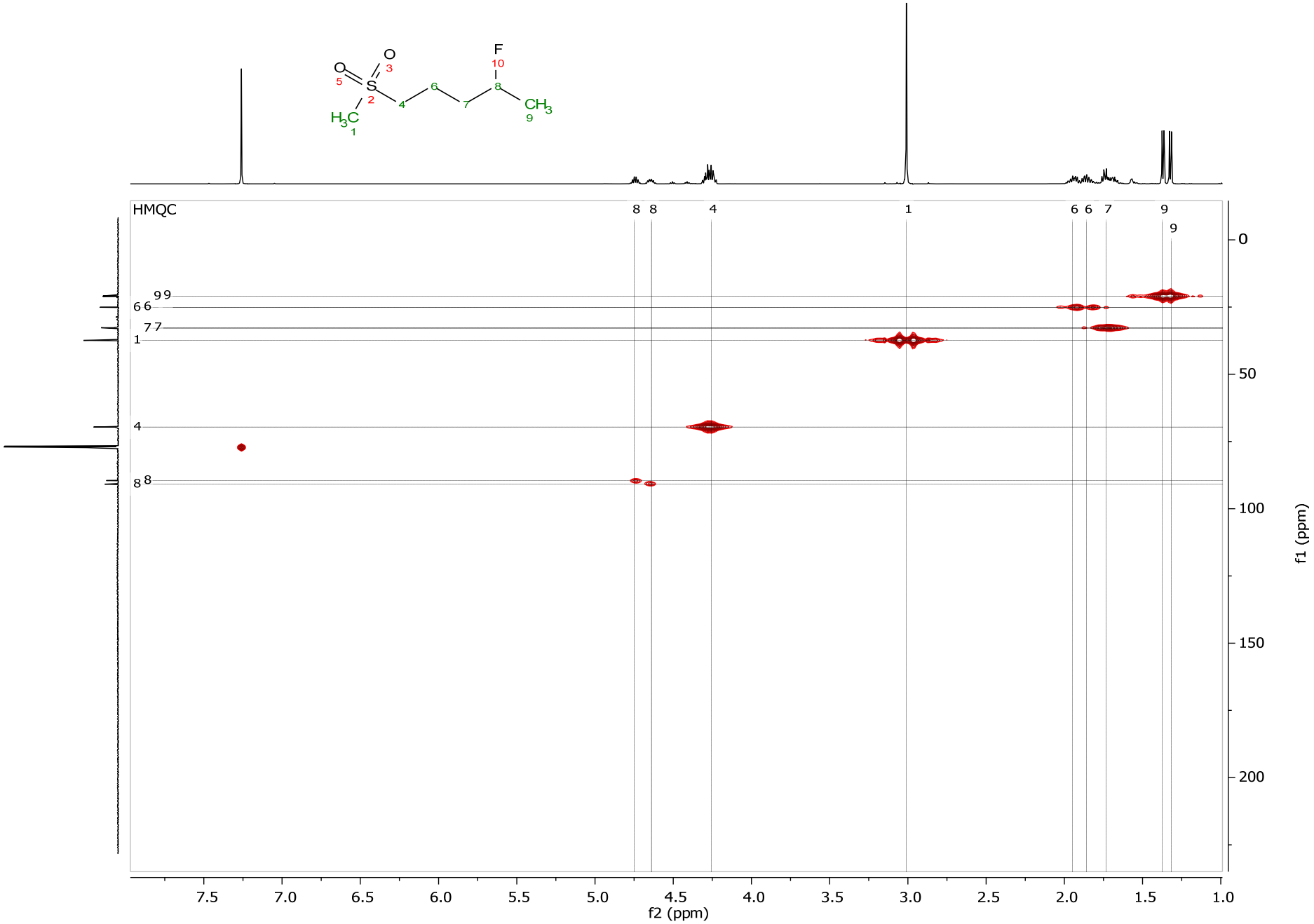
NMR Spectra of 4-fluoropentyl methanesulfonate

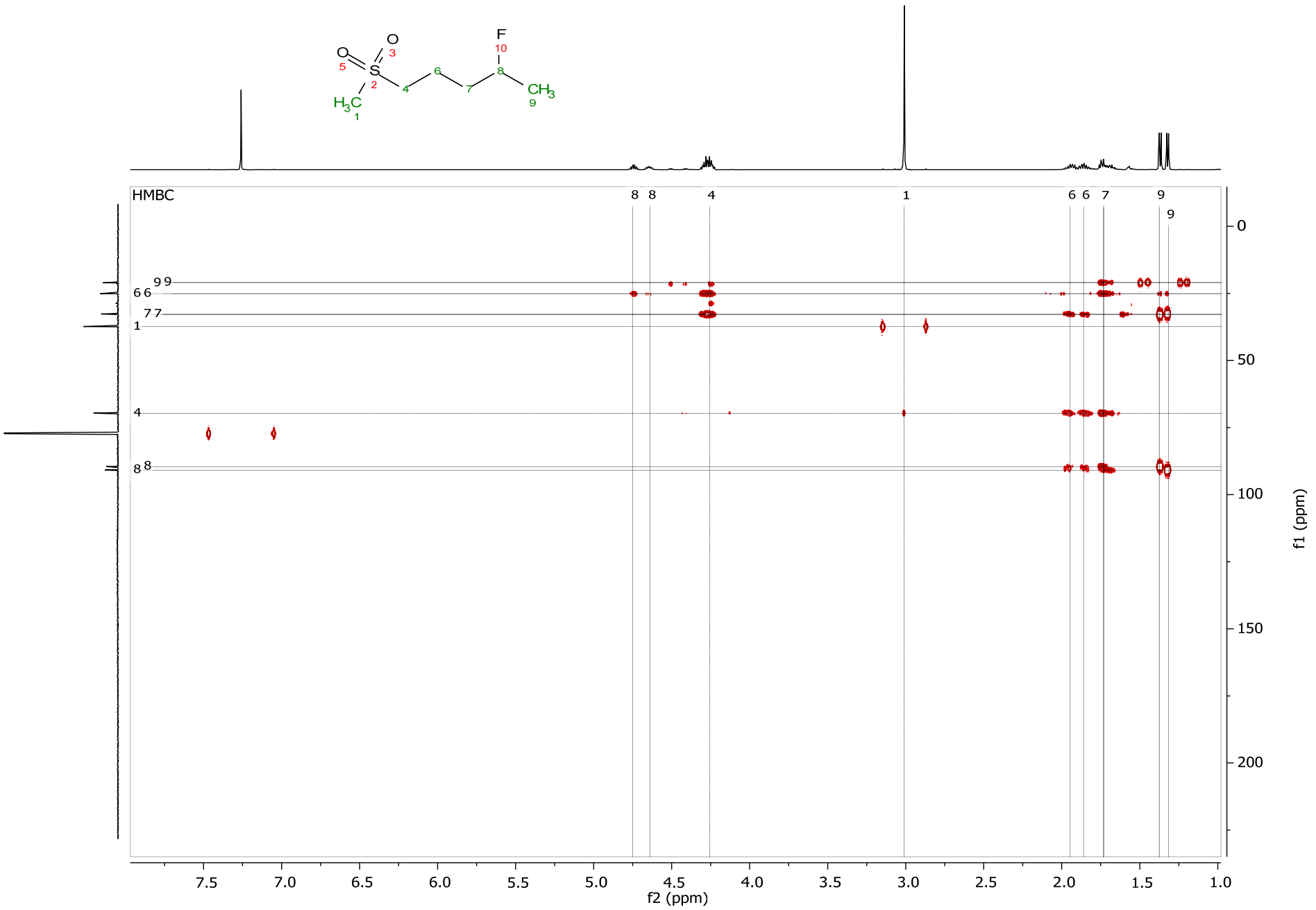



13C NMR 4-fluoro-1-(methylsulfonyl)pentane
90.85
89.54
77.28 CDCl3
77.03 CDCl3
76.77 CDCl3
69.66
69.62
37.40
32.86
32.69
25.11
25.08
21.07
20.89
A (d)
90.20
B (s)
69.62
C (s)
37.40
D (d)
32.77
E (d)
25.09
F (d)
20.98
1.00
0.93
0.87
0.78
0.89
0.88
f1 (ppm)

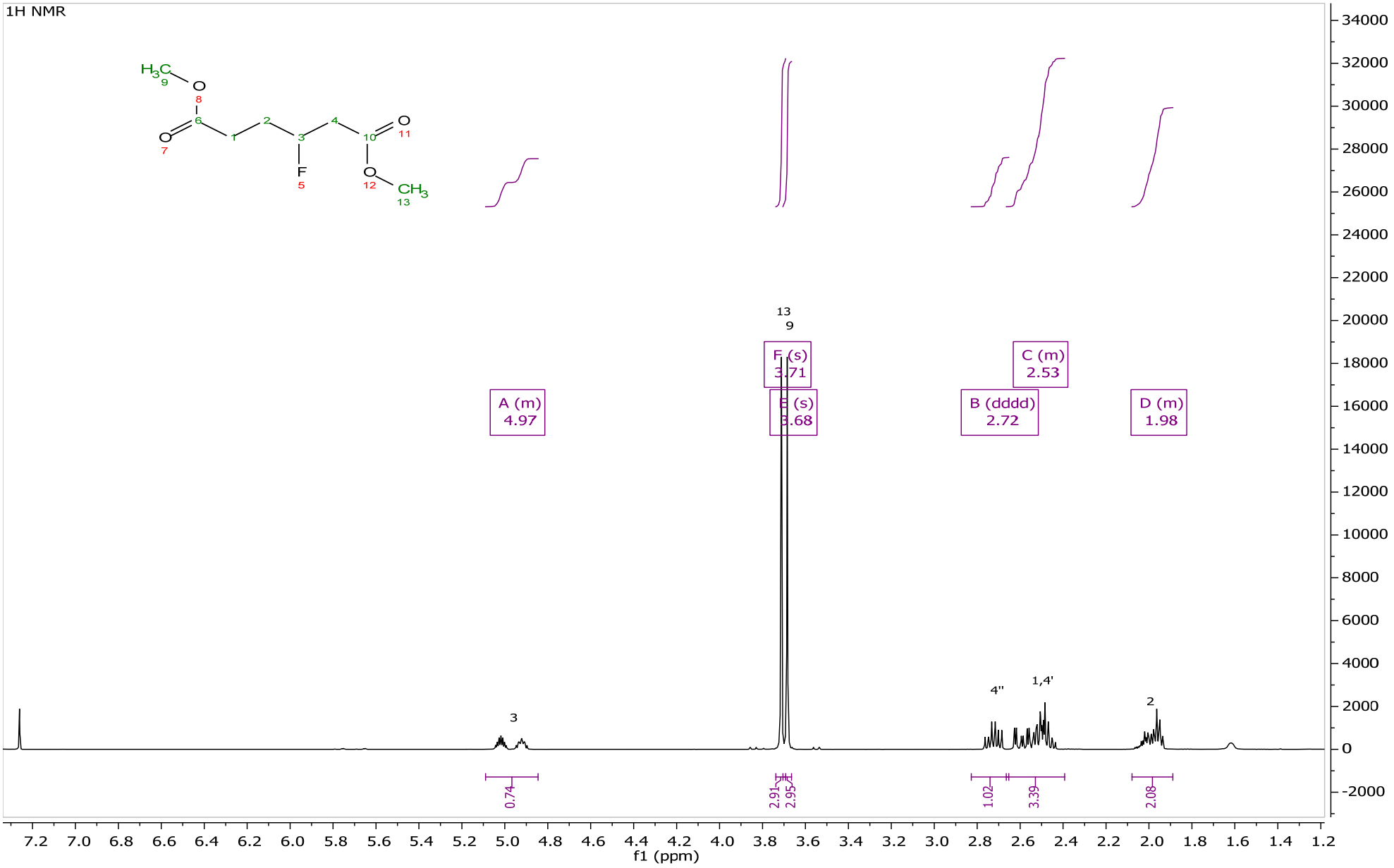

19F NMR (376 MHz, CDCl3) δ -174.10.
-174.10
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

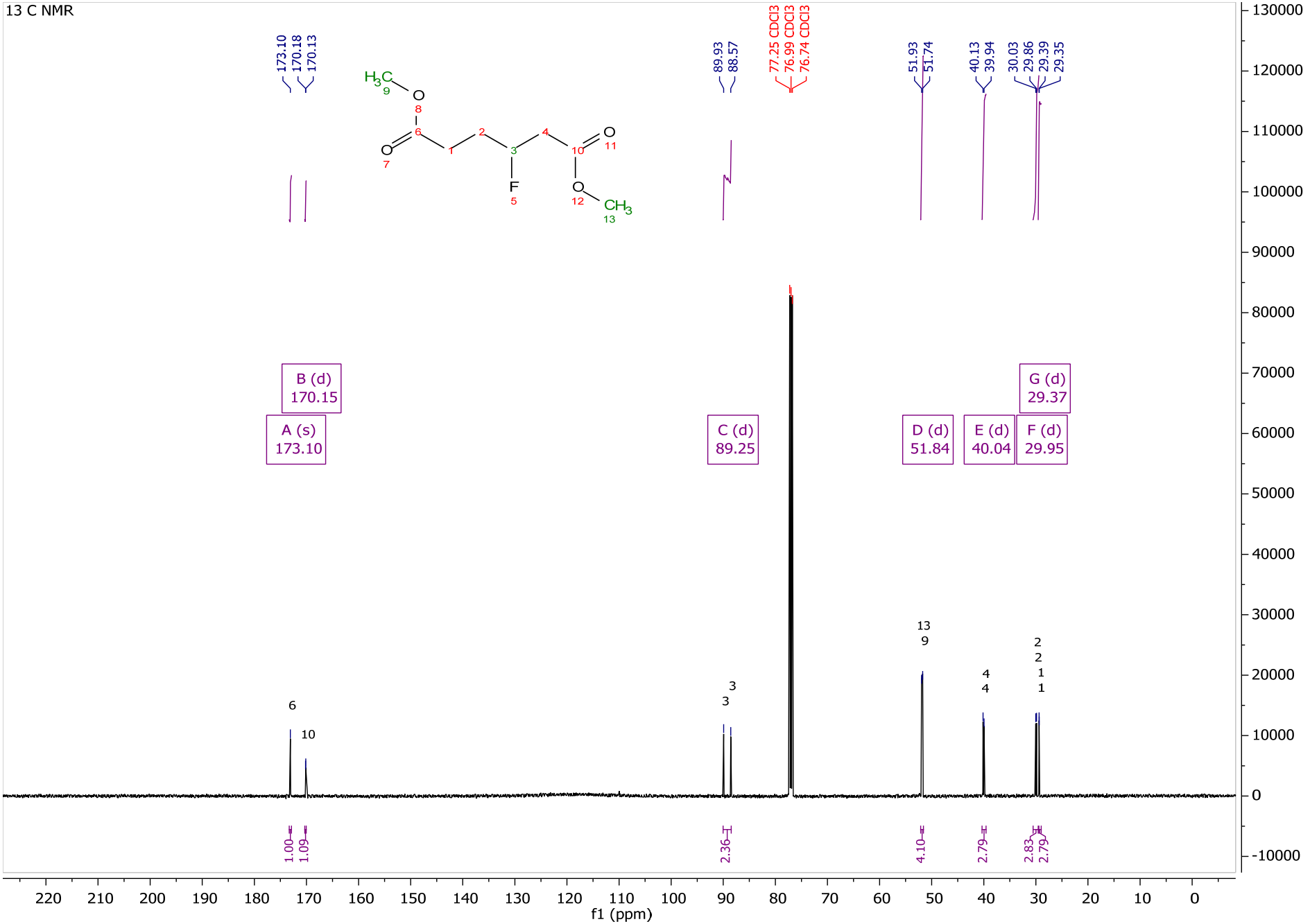

COSY
f2 (ppm)
f1 (ppm)

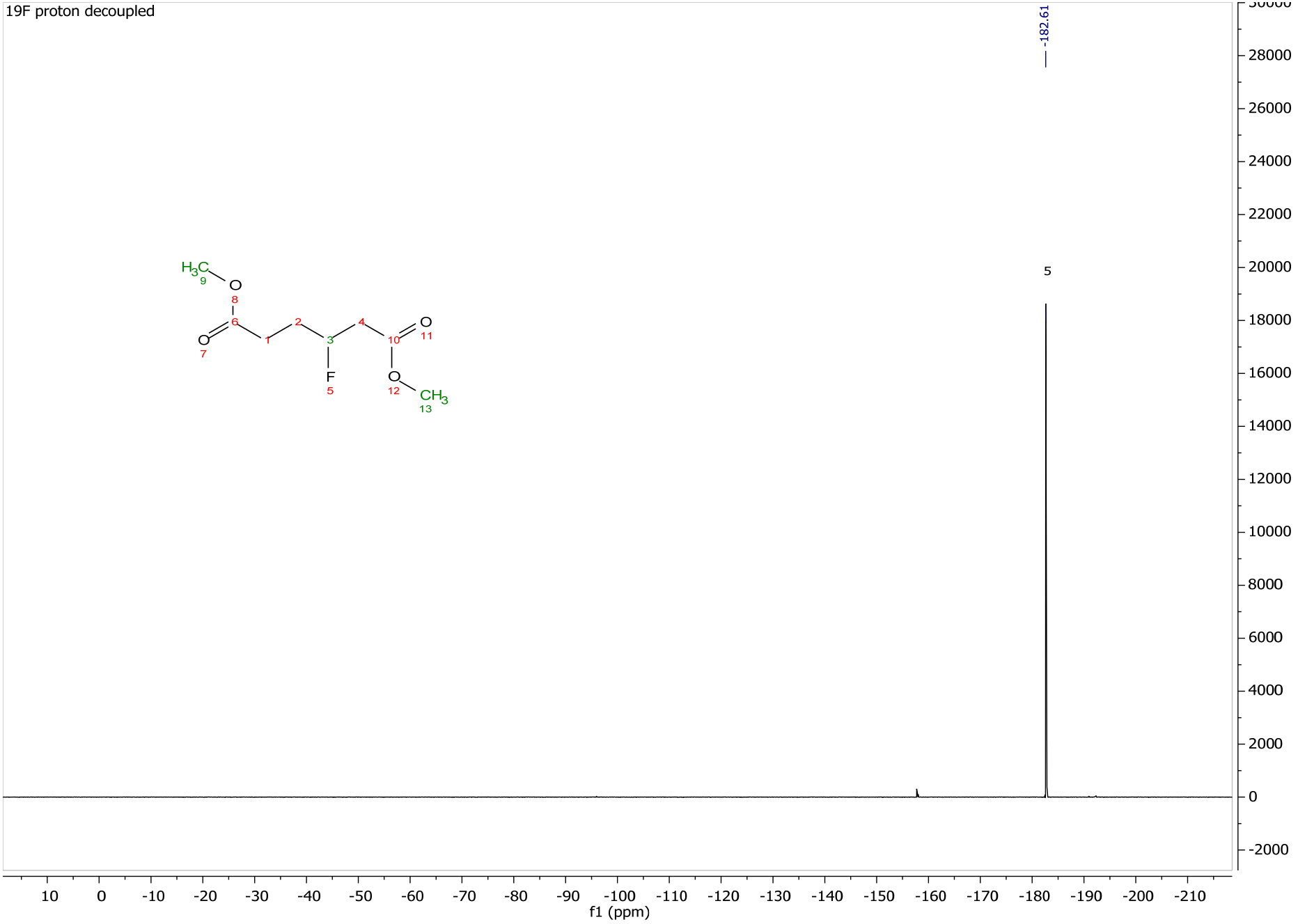

HMQC
f2 (ppm)
f1 (ppm)

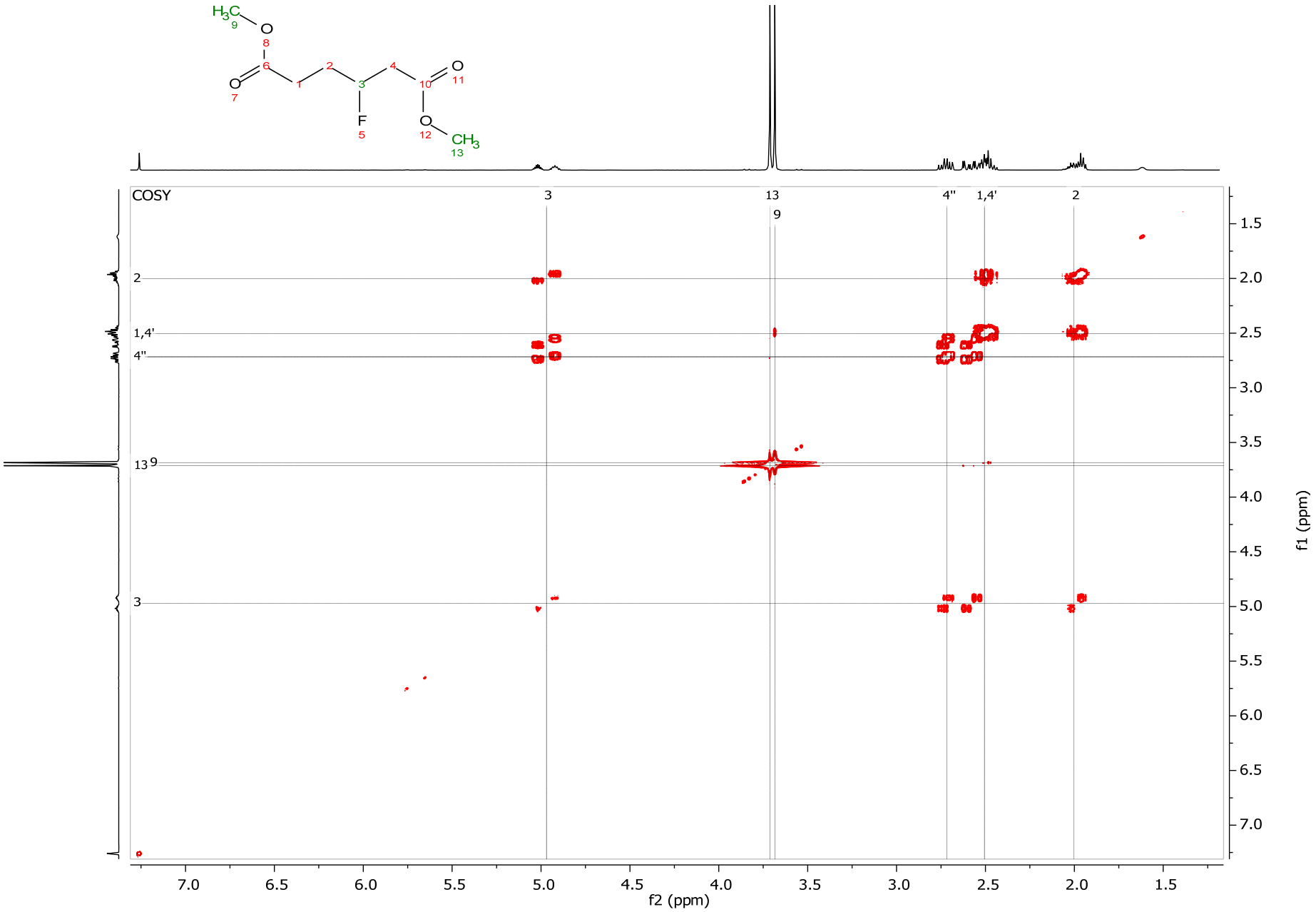

HMBC
f2 (ppm)
f1 (ppm)

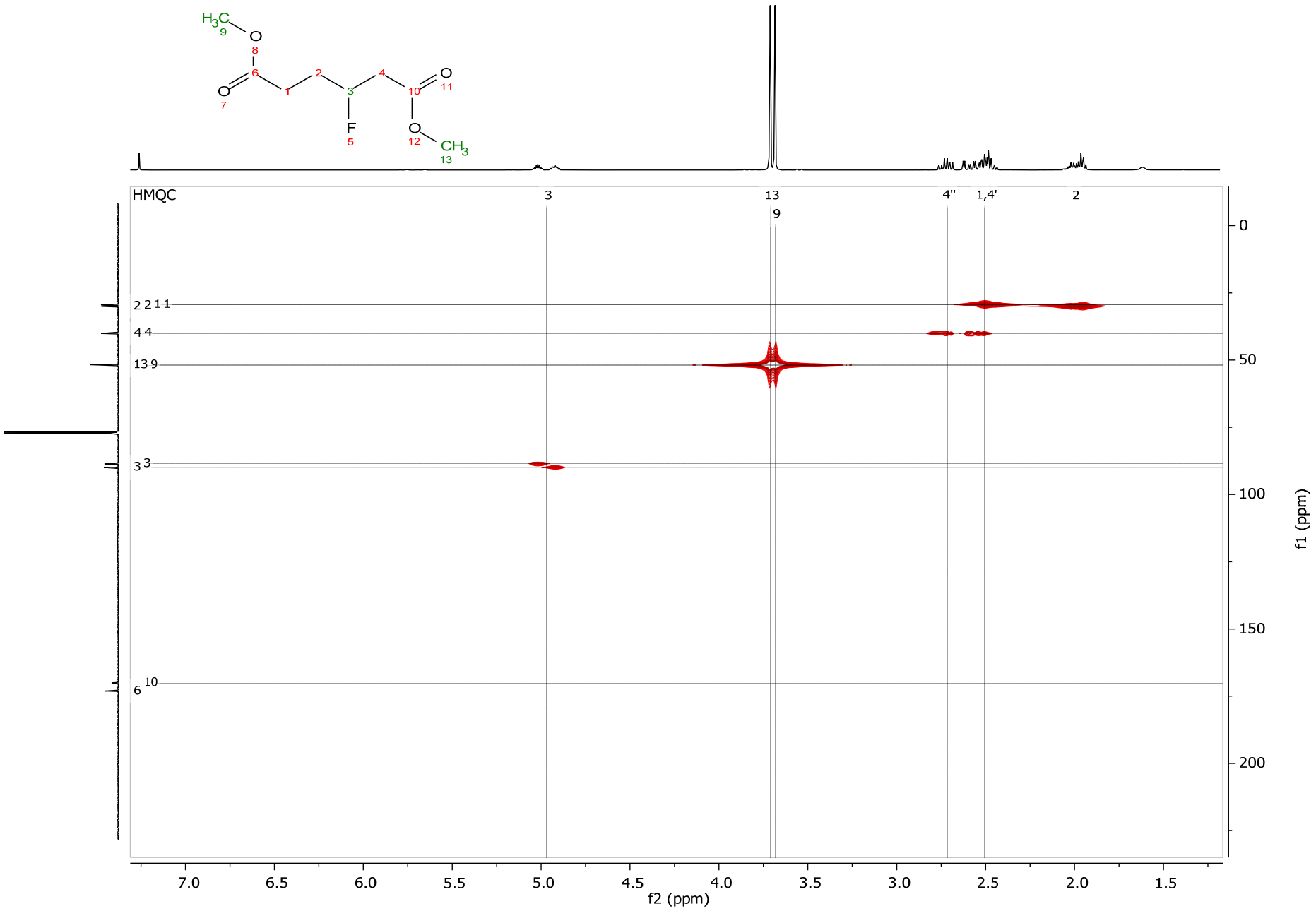
NMR Spectra of dimethyl 3-fluorohexanedioate

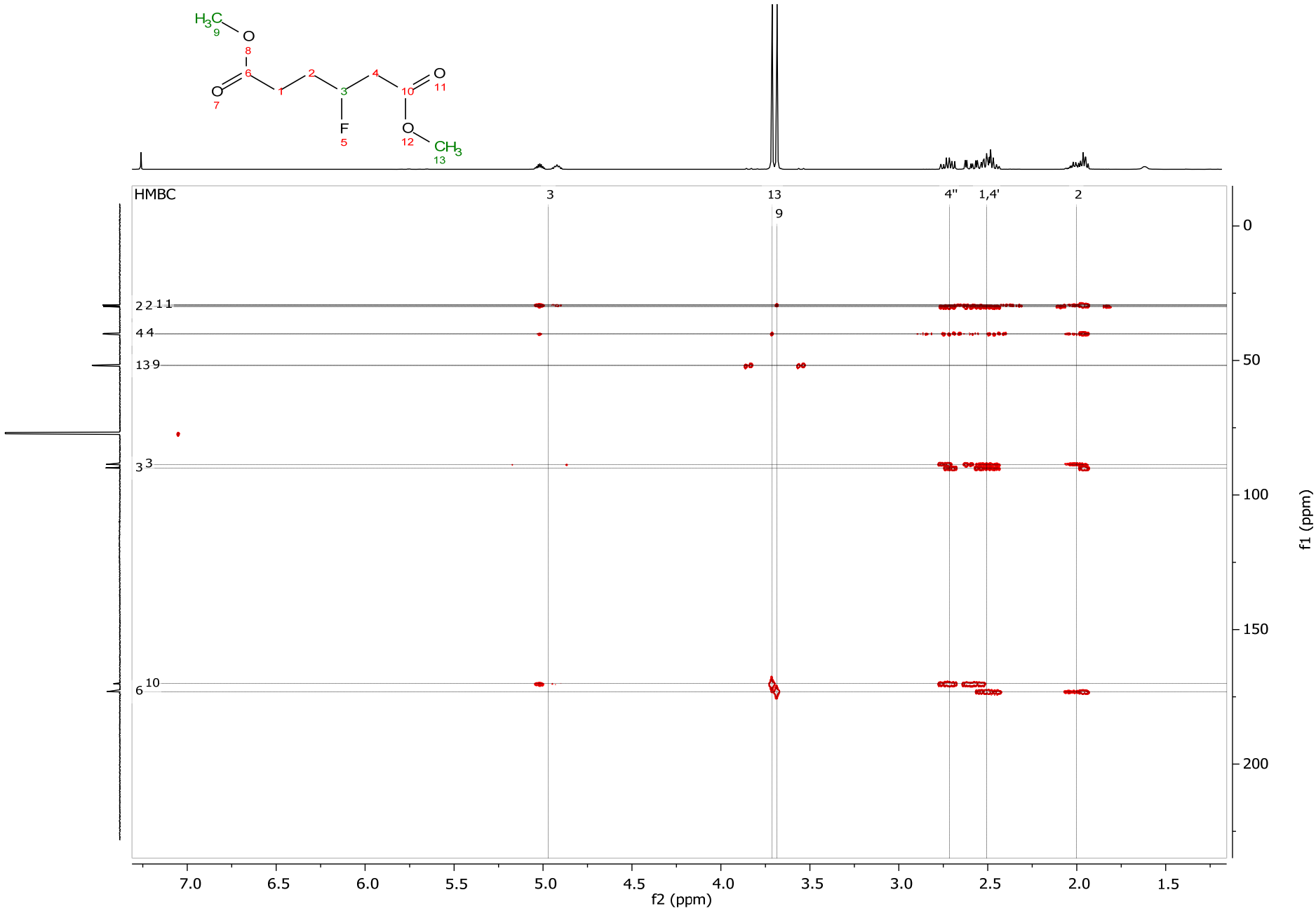



13 C NMR
173.10
170.18
170.13
89.93
88.57
77.25 CDCl3
76.99 CDCl3
76.74 CDCl3
51.93
51.74
40.13
39.94
30.03
29.86
29.39
29.35
B (d)
170.15
A (s)
173.10
C (d)
89.25
D (d)
51.84
E (d)
40.04
G (d)
29.37
F (d)
29.95
f1 (ppm)

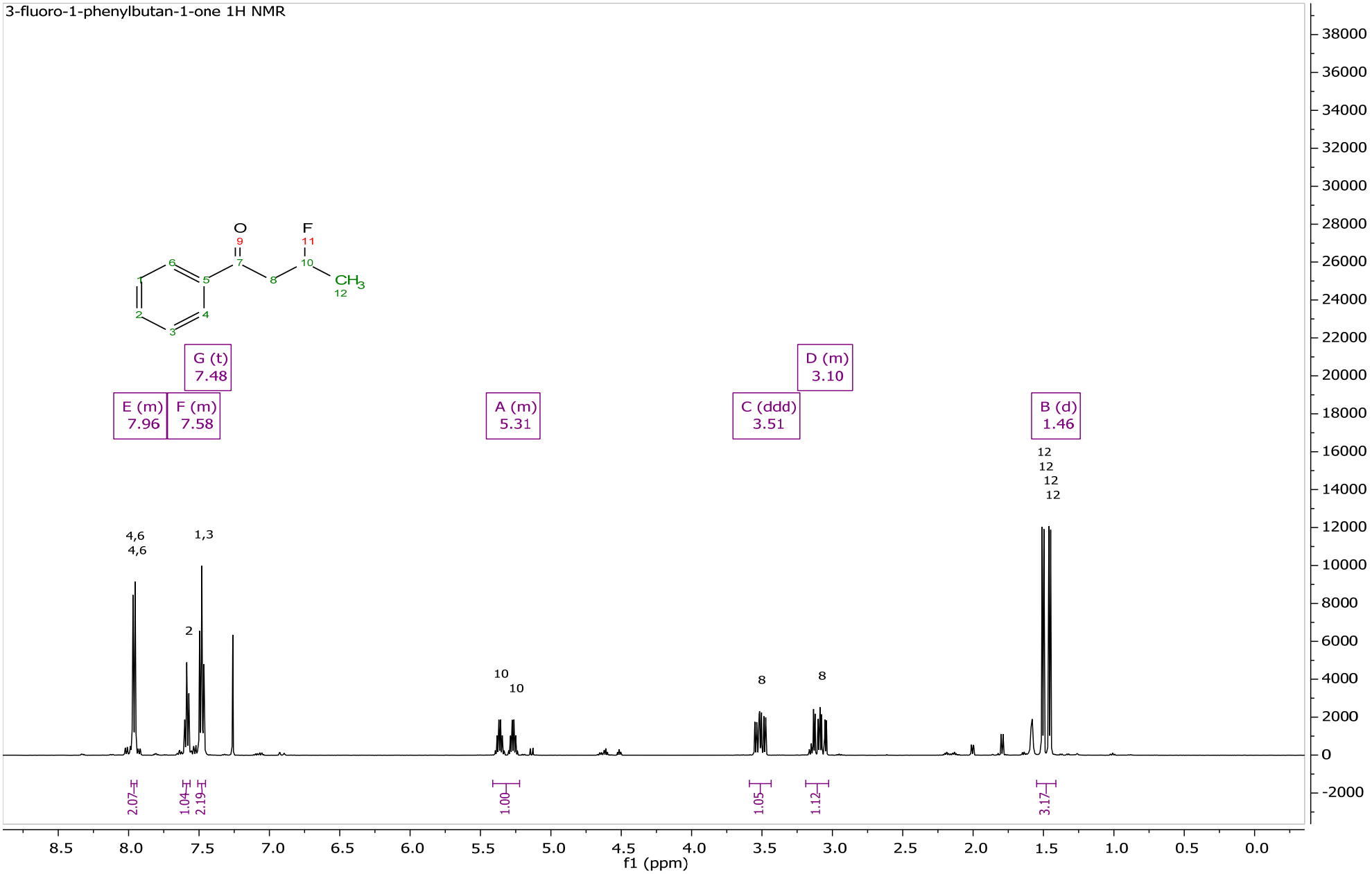

19F proton decoupled
-182.61
5
H3C
9
O
8
6
2
4
O
11
O
7
1
3
10
F
5
O
12
CH3
13
30000
28000
26000
24000
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
-2000
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

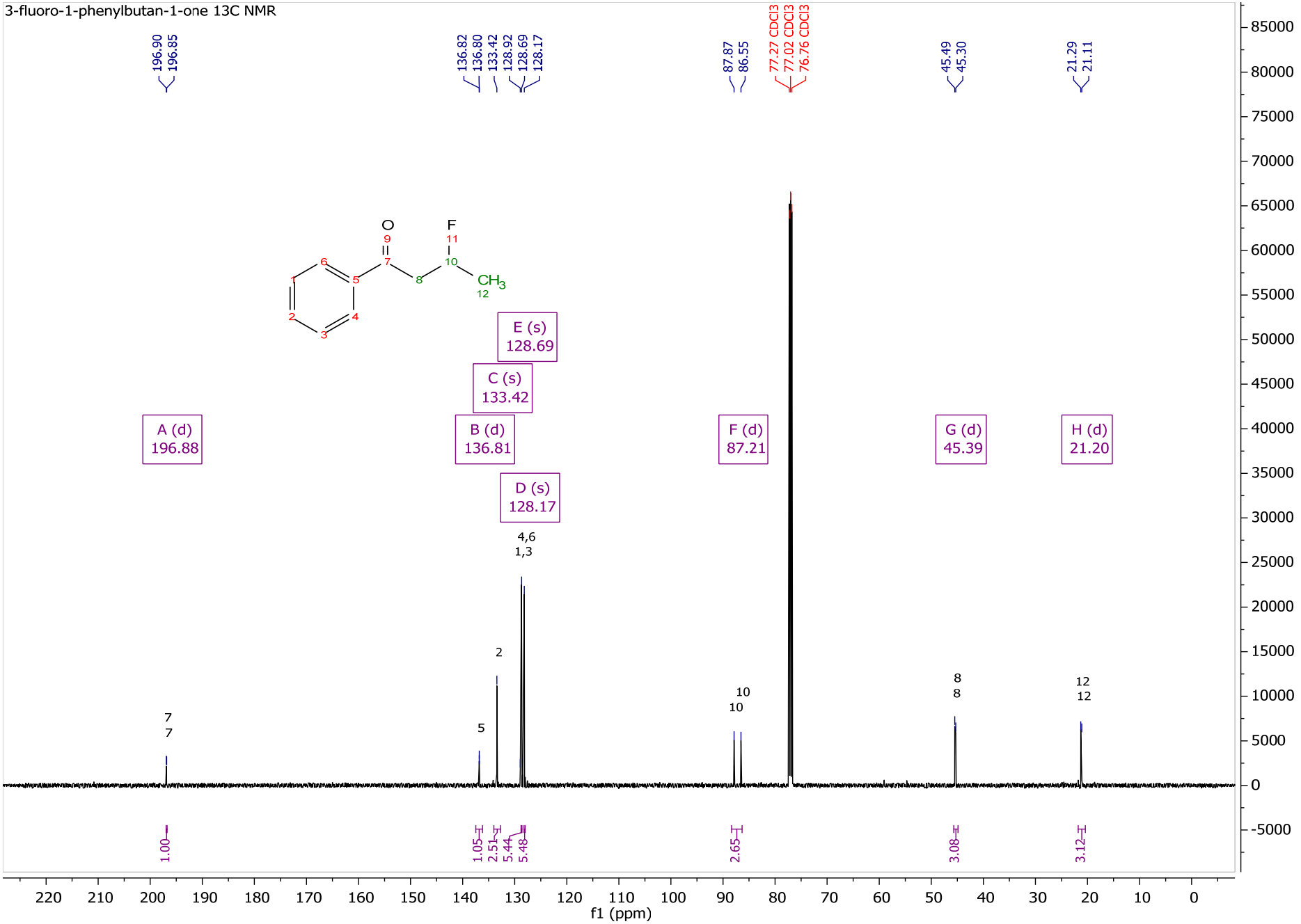

COSY
f2 (ppm)
f1 (ppm)

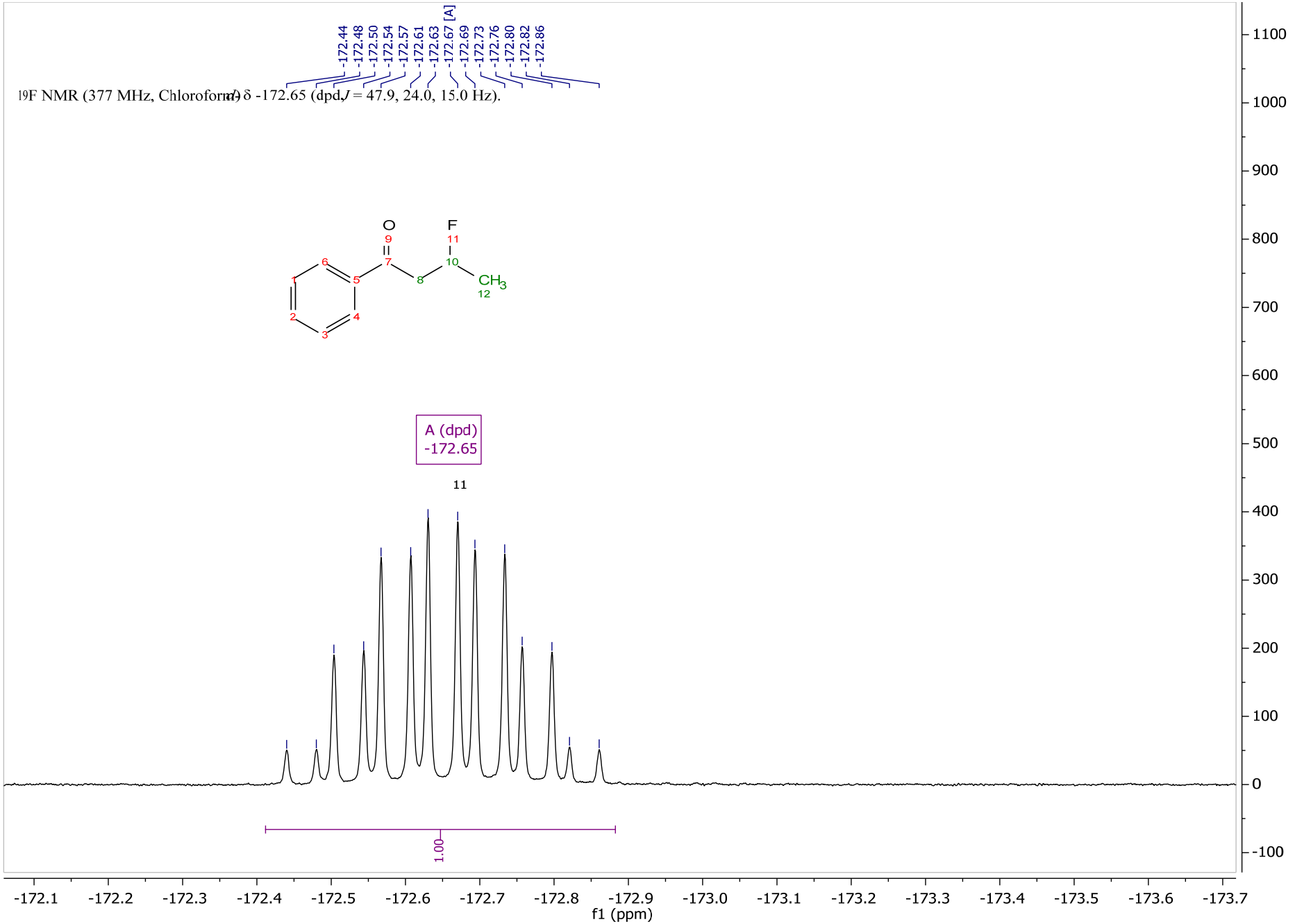

HMQC
3
13
9
4''
1,4'
2
2 2 1 1
4 4
13 9
3 3
6 10
0
50
100
150
200
f1 (ppm)
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
f2 (ppm)


HMBC
3
13
9
4''
1,4'
2
f2 (ppm)
f1 (ppm)

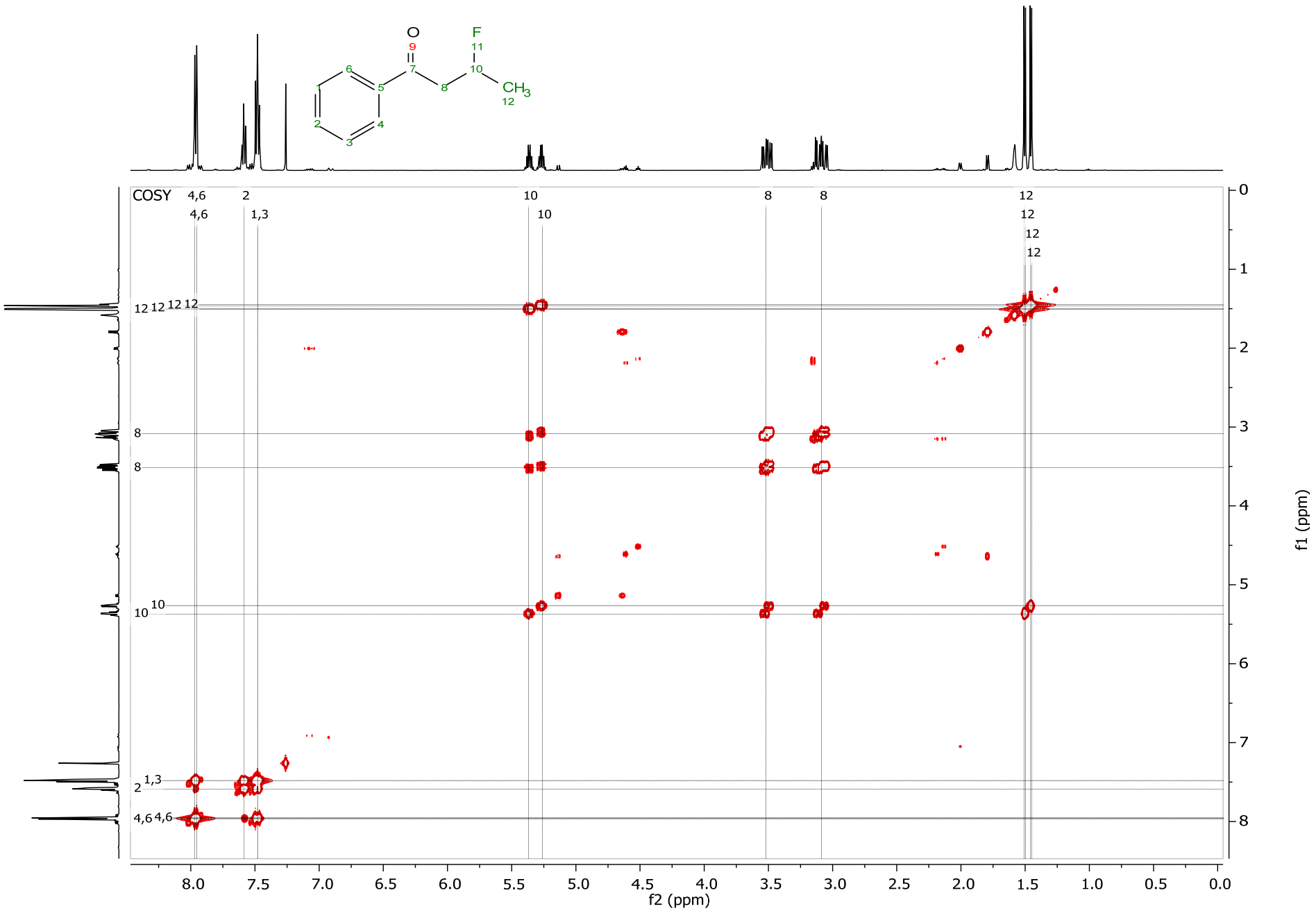
NMR Spectra of 3-fluoro-1-phenylbutan-1-one

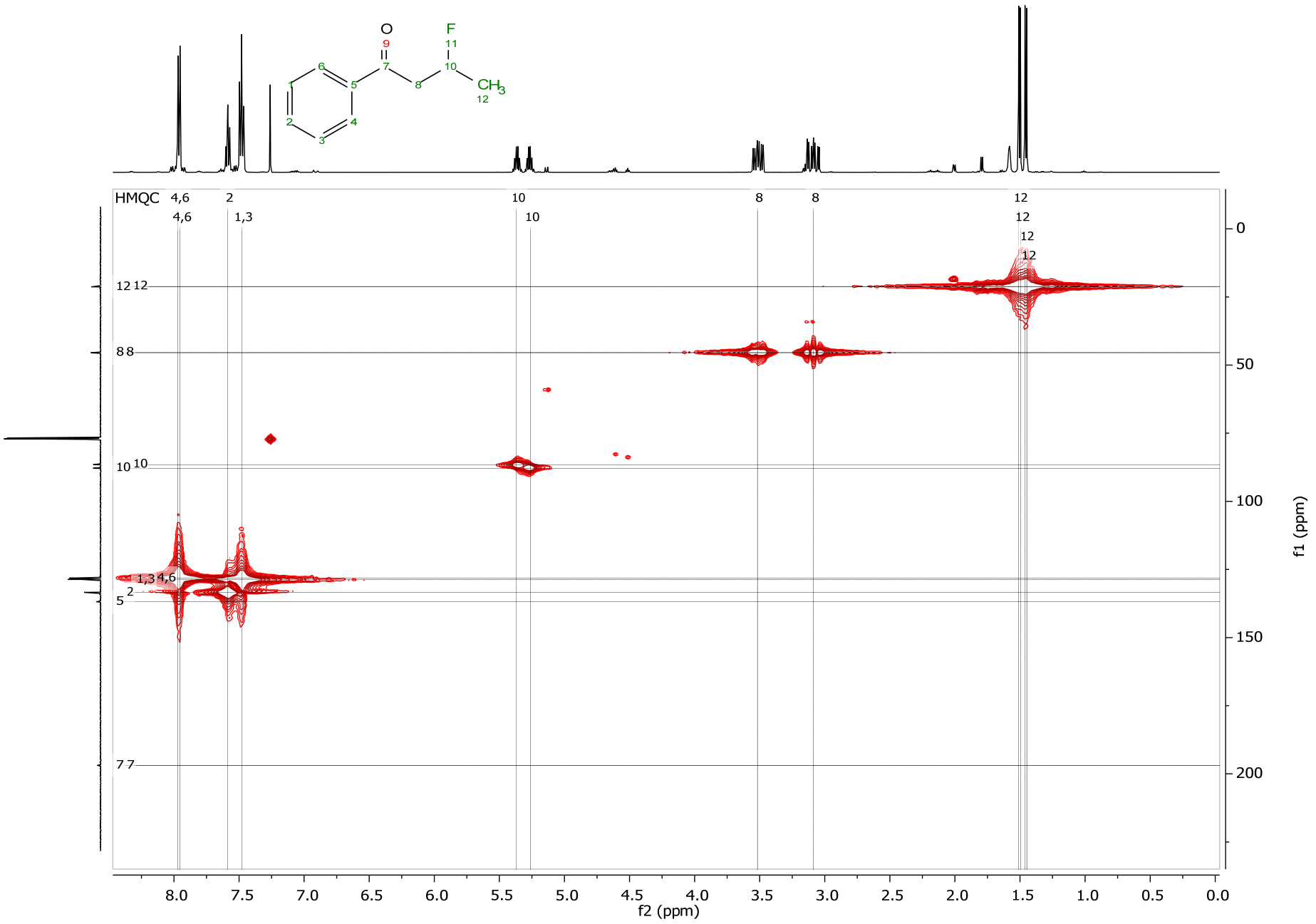


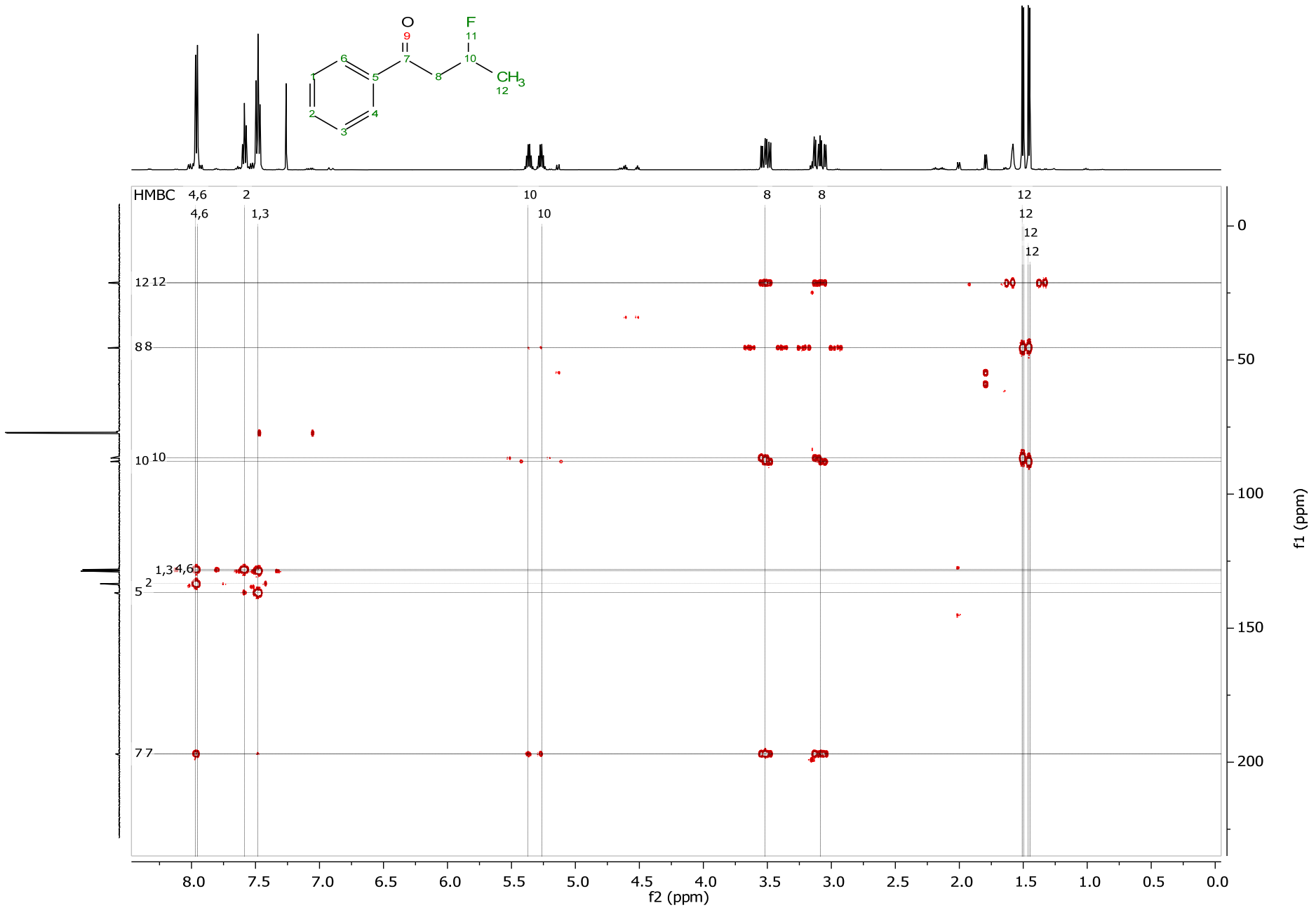

3-fluoro-1-phenylbutan-1-one 13C NMR
196.90
196.85
136.82
136.80
133.42
128.92
128.69
128.17
87.87
86.55
77.27 CDCl3
77.02 CDCl3
76.76 CDCl3
45.49
45.30
21.29
21.11
A (d)
196.88
B (d)
136.81
C (s)
133.42
D (s)
128.17
E (s)
128.69
F (d)
87.21
G (d)
45.39
H (d)
21.20
4,6
1,3
f1 (ppm)



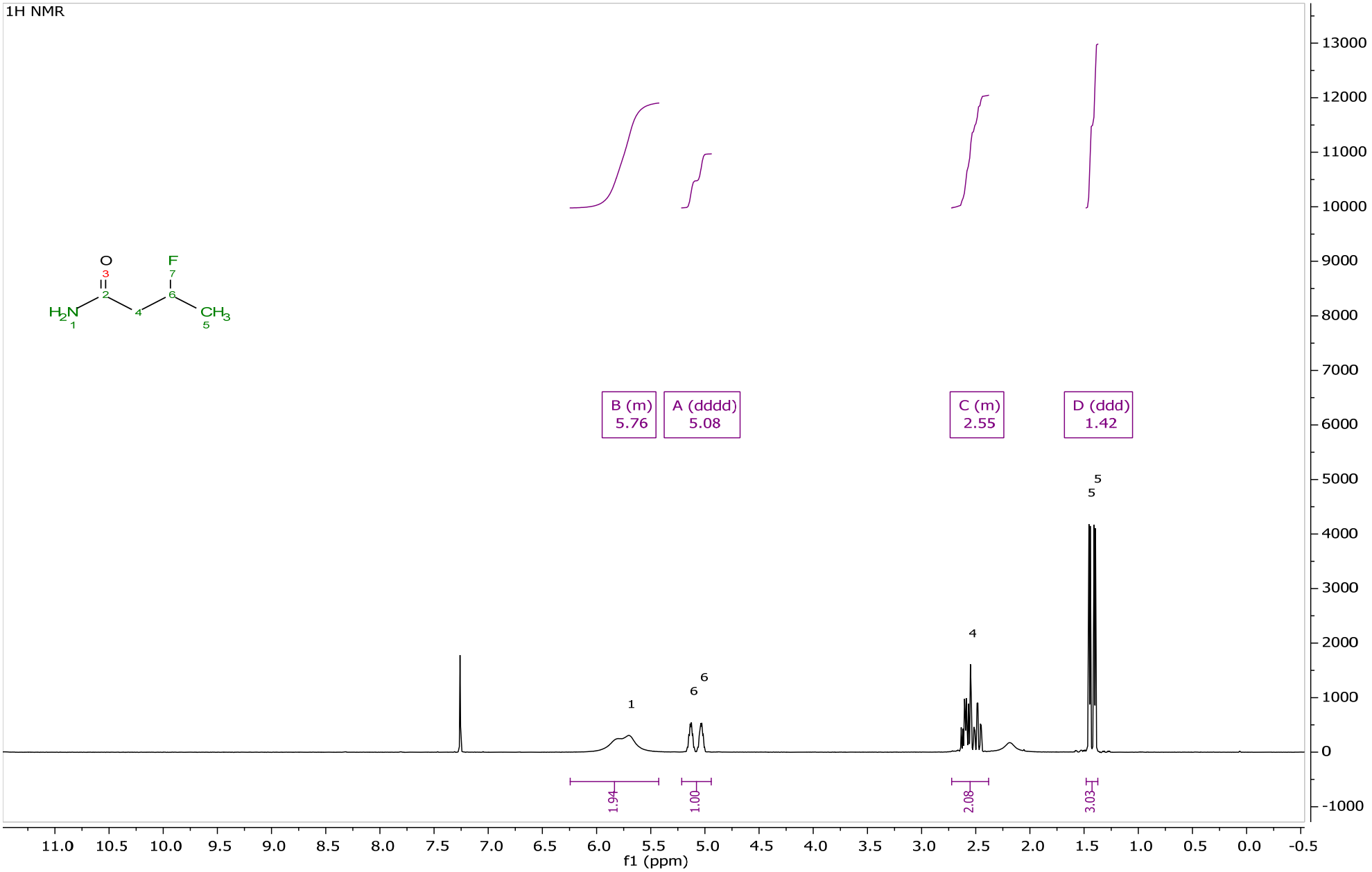
^{19}F NMR (377 MHz, Chloroform-*d*) δ -172.65 (dpd, *J* = 47.9, 24.0, 15.0 Hz).

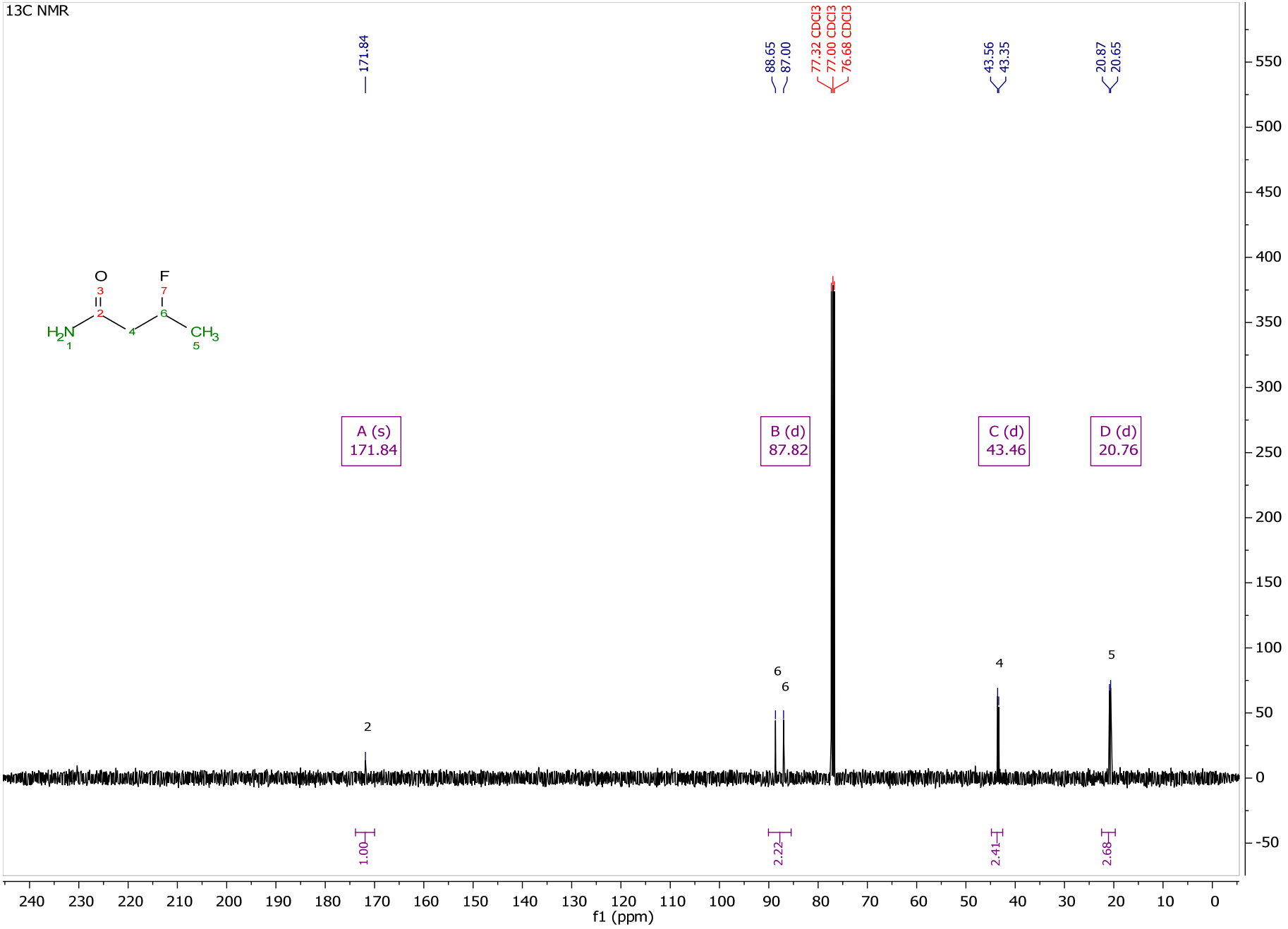

COSY
O
9
F
11
6
7
10
1
5
8
CH3
12
2
4
3
4,6
4,6
2
1,3
10
10
8
8
12
12
12
12
12 12 12 12
8
8
10 10
2 1,3
4,6 4,6
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f2 (ppm)
0
1
2
3
4
5
6
7
8
f1 (ppm)

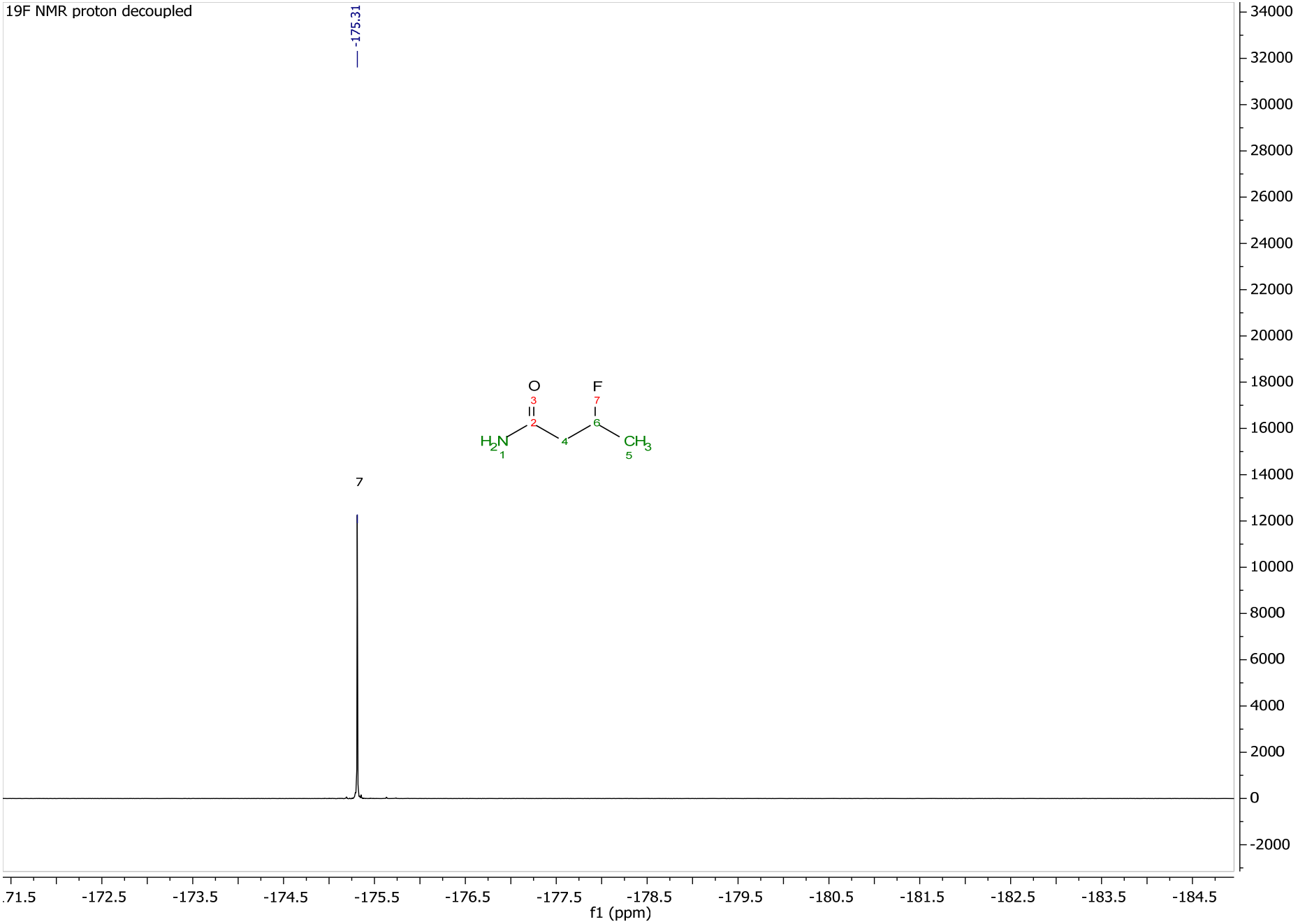

HMQC
f2 (ppm)
f1 (ppm)

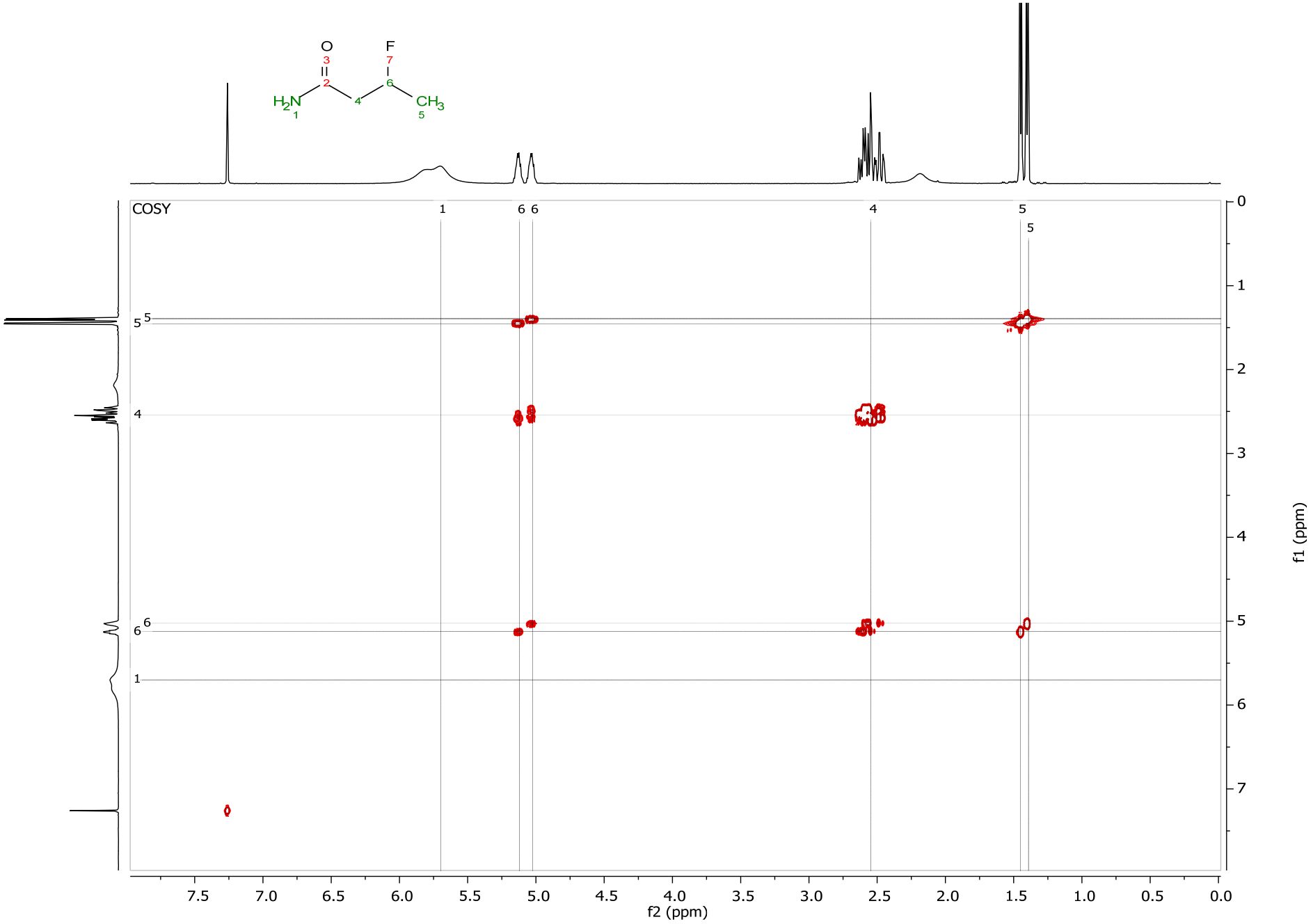

HMBC
f2 (ppm)
f1 (ppm)

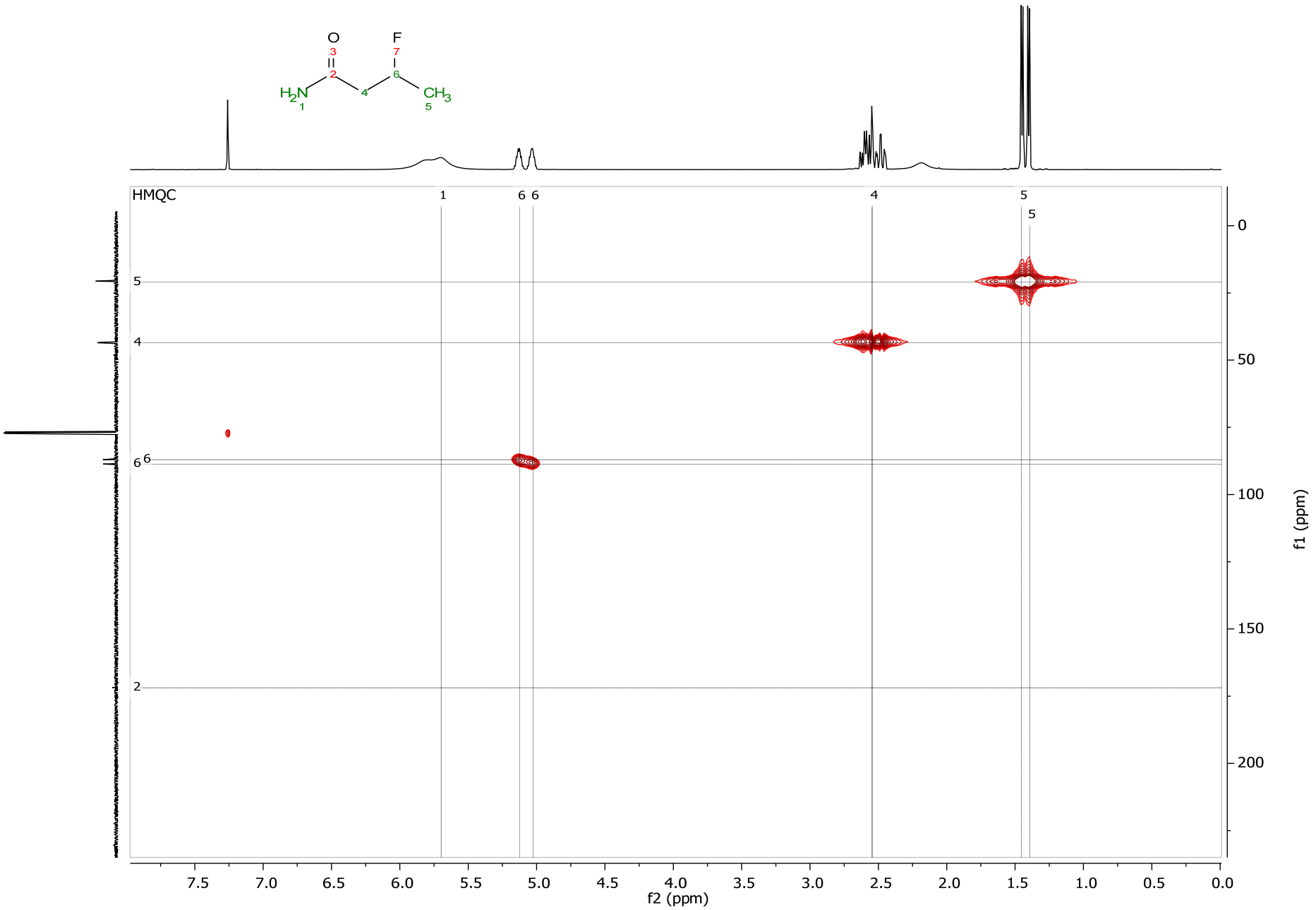
NMR Spectra of 3-fluorobutanamide

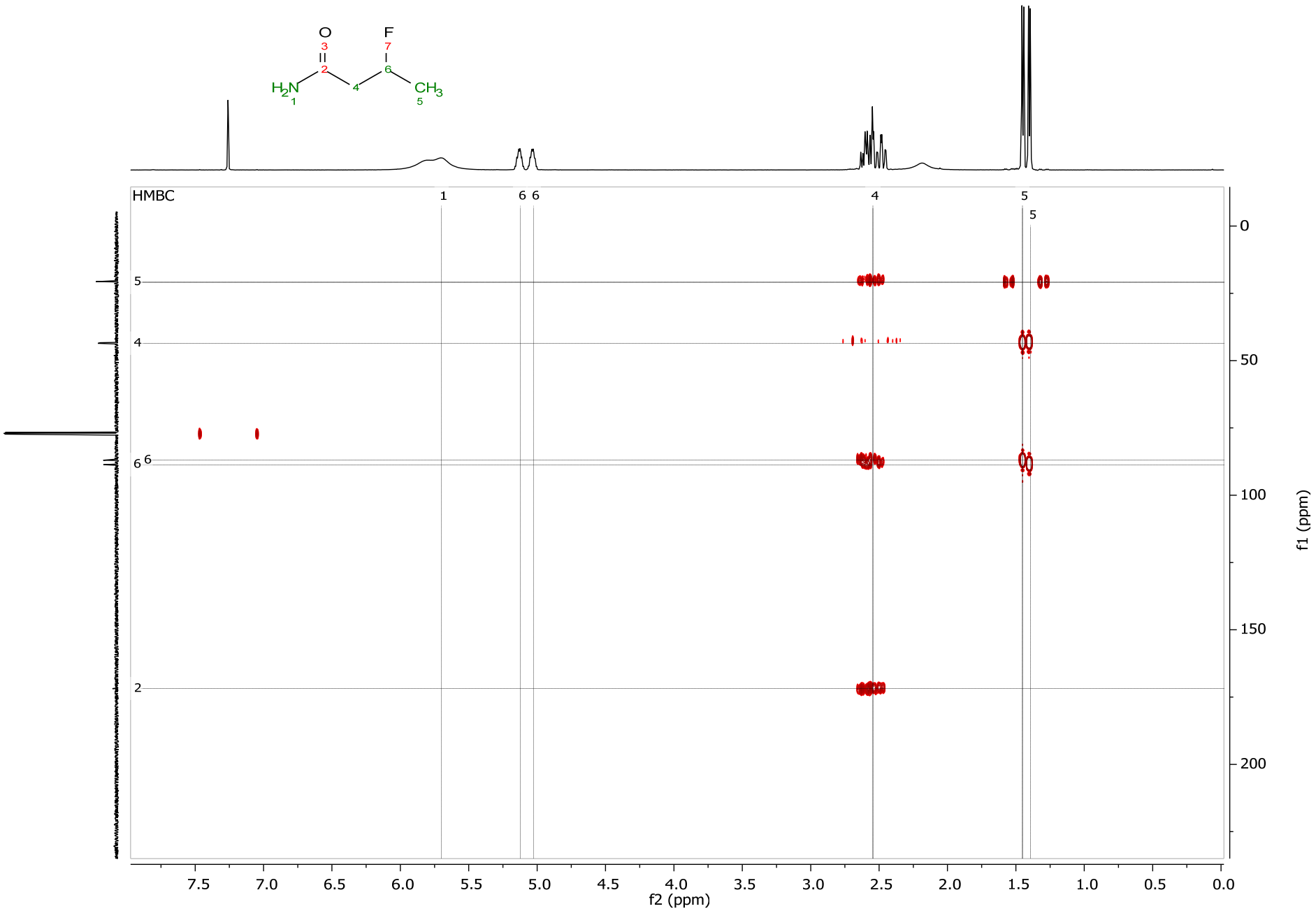



13C NMR
171.84
88.65
87.00
77.32 CDCl3
77.00 CDCl3
76.68 CDCl3
43.56
43.35
20.87
20.65
O
F
H2N
CH3
A (s)
171.84
B (d)
87.82
C (d)
43.46
D (d)
20.76
2
6
6
4
5
1.00
2.22
2.41
2.68
f1 (ppm)

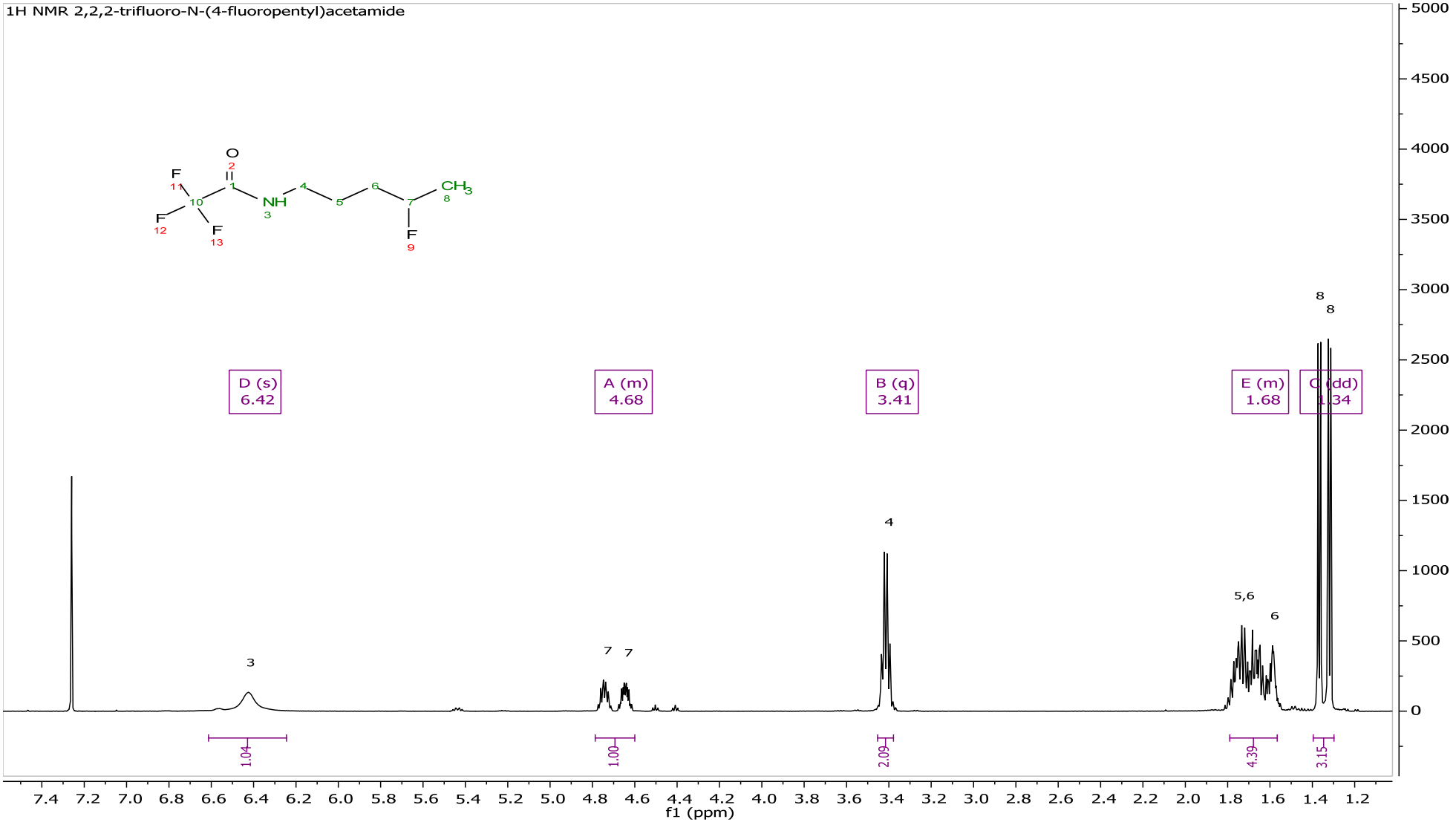

19F NMR proton decoupled
-175.31
O
F
H2N
CH3
7
34000
32000
30000
28000
26000
24000
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
-2000
.71.5
-172.5
-173.5
-174.5
-175.5
-176.5
-177.5
-178.5
-179.5
-180.5
-181.5
-182.5
-183.5
-184.5
f1 (ppm)

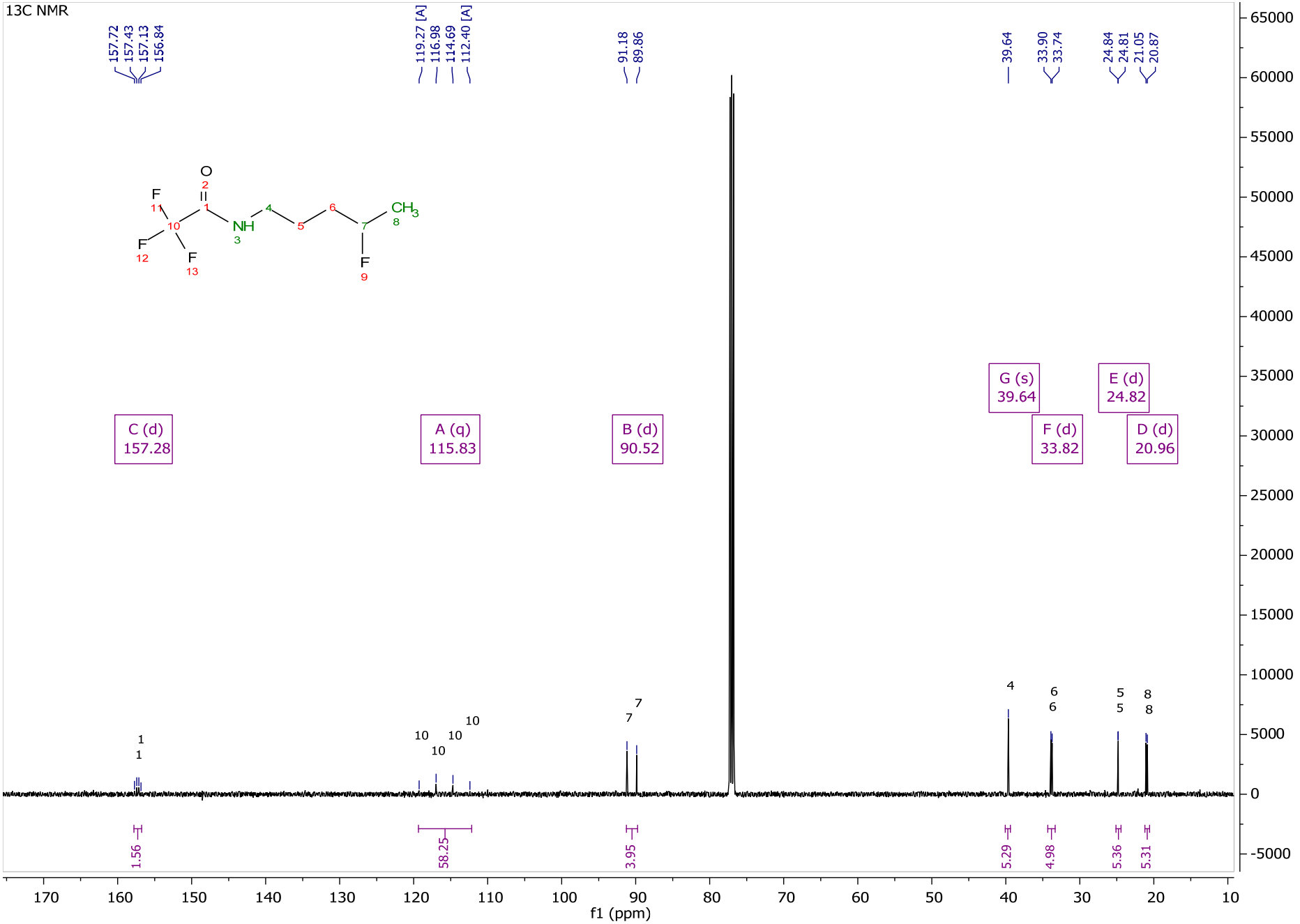

COSY
O
F
H2N
CH3
f2 (ppm)
f1 (ppm)

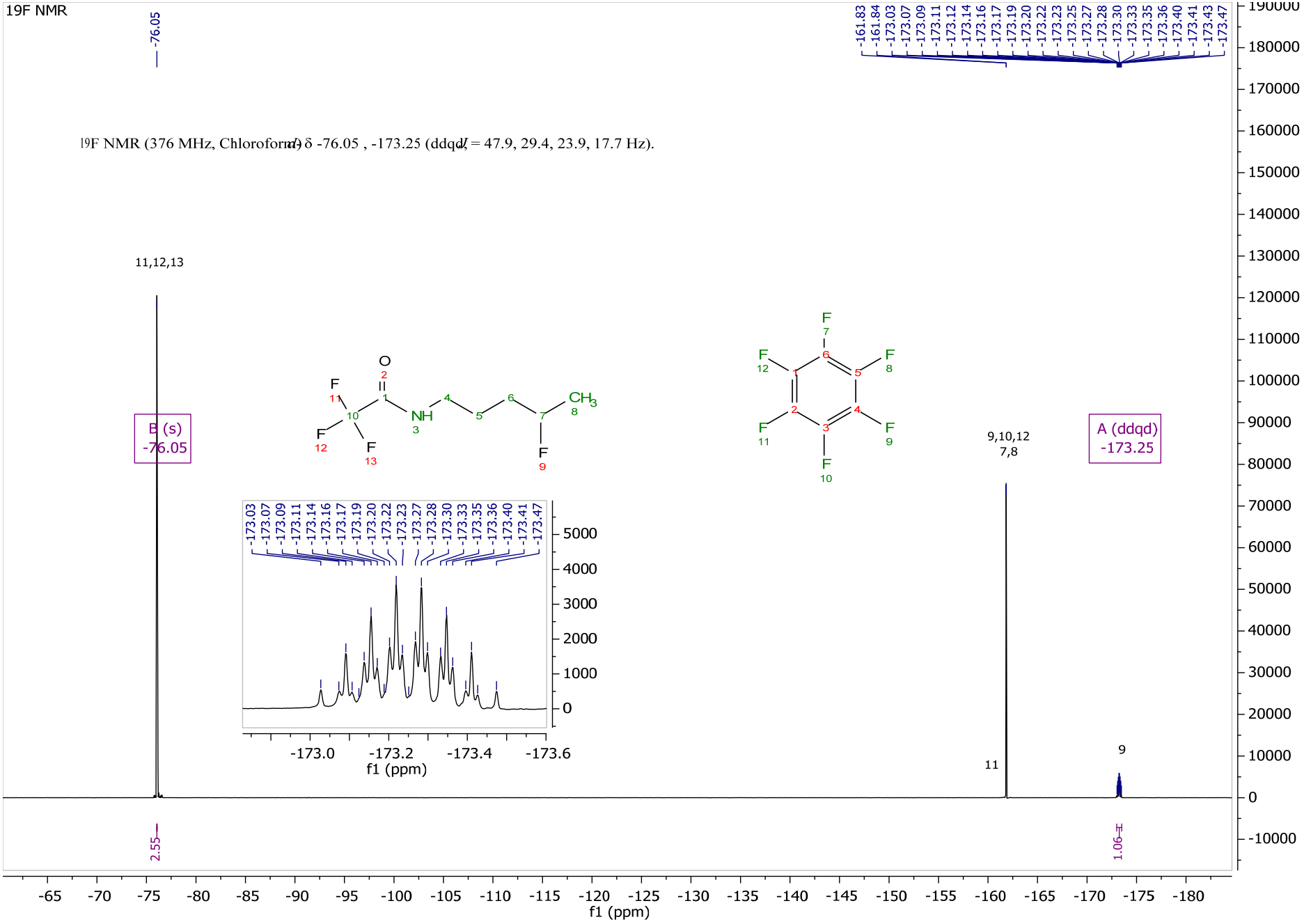

O
F
3
7
2
6
4
H_2N
1
CH_3
5
HMQC
1
6 6
4
5
5
0
50
100
150
200
f1 (ppm)
5
4
6 6
2
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f2 (ppm)

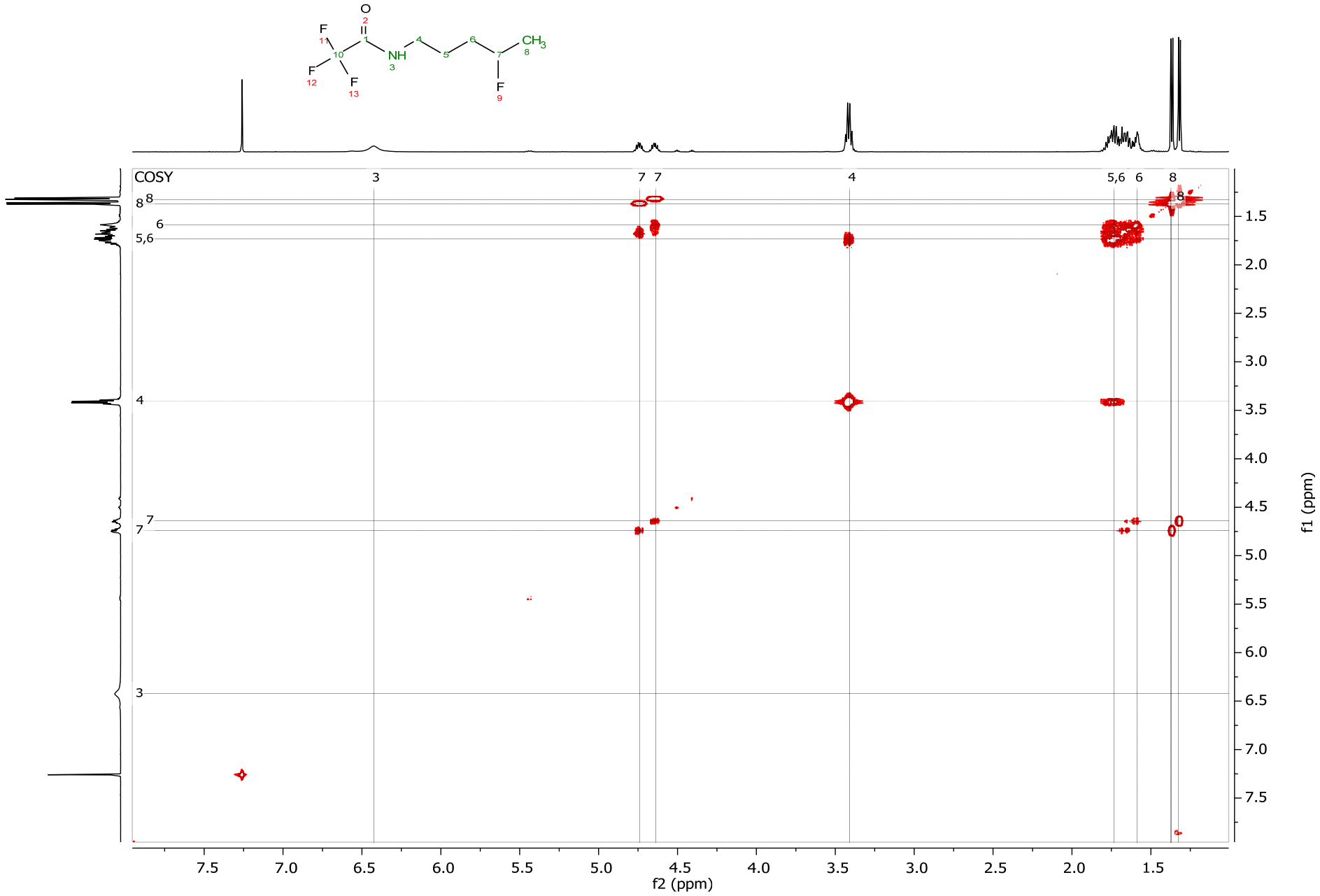

HMBC
O
F
H2N
CH3
1
6 6
4
5
5
5
4
6 6
2
0
50
100
150
200
f1 (ppm)
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f2 (ppm)

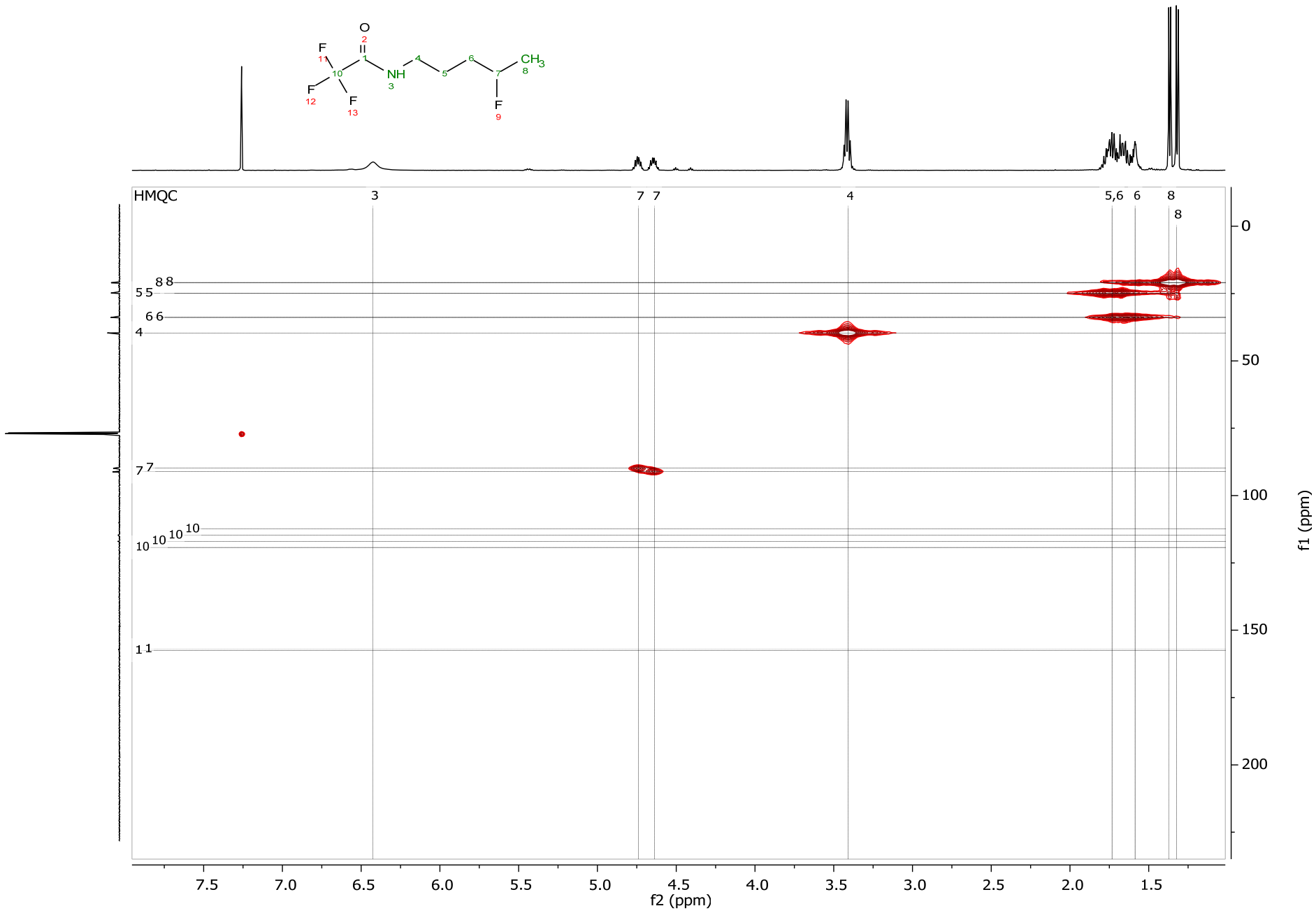
NMR Spectra of 2,2,2-trifluoro-N-(4-fluoropentyl)acetamide

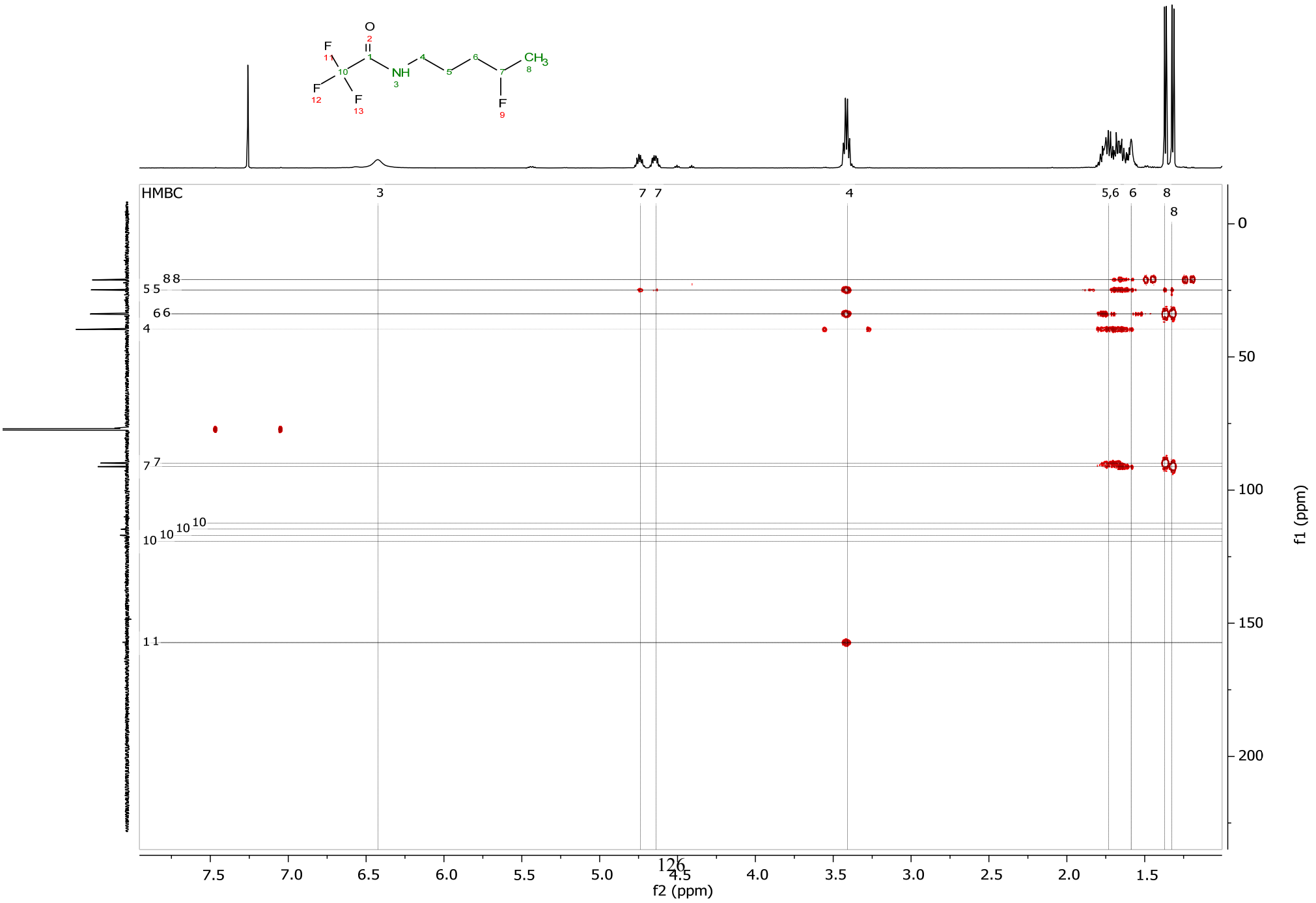



13C NMR
157.72
157.43
157.13
156.84
119.27 [A]
116.98
114.69
112.40 [A]
91.18
89.86
39.64
33.90
33.74
24.84
24.81
21.05
20.87
C (d)
157.28
A (q)
115.83
B (d)
90.52
G (s)
39.64
F (d)
33.82
E (d)
24.82
D (d)
20.96
1.56
58.25
3.95
5.29
4.98
5.36
5.31
f1 (ppm)

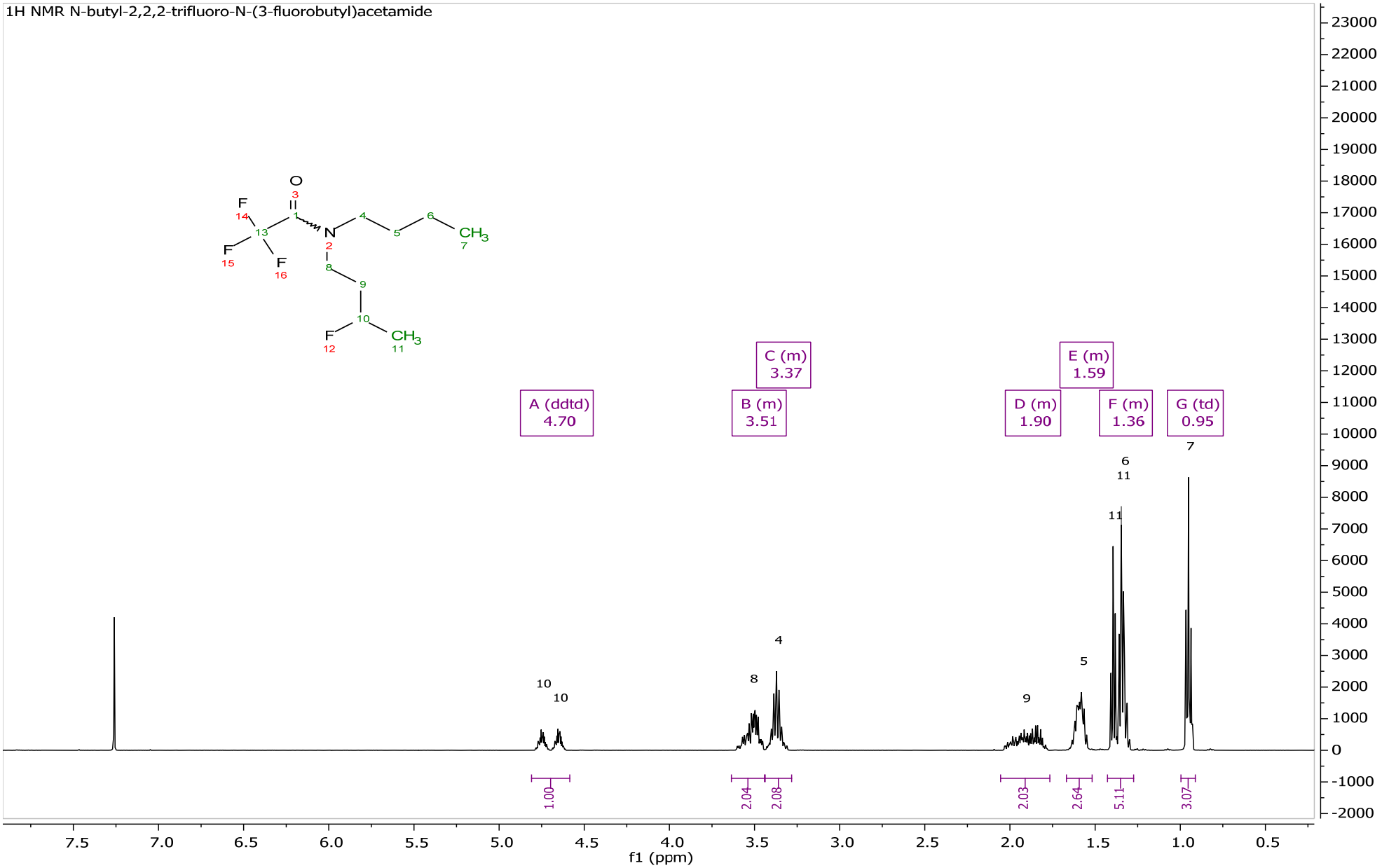

19F NMR
-76.05
-161.83
-161.84
-173.03
-173.07
-173.09
-173.11
-173.12
-173.14
-173.16
-173.17
-173.19
-173.20
-173.22
-173.23
-173.25
-173.27
-173.28
-173.30
-173.33
-173.35
-173.36
-173.40
-173.41
-173.43
-173.47
19F NMR (376 MHz, Chloroform-d) δ -76.05 , -173.25 (ddqd, J = 47.9, 29.4, 23.9, 17.7 Hz).
11,12,13
B (s)
-76.05
A (ddqd)
-173.25
9,10,12
7,8
11
9
2.55
1.06
f1 (ppm)

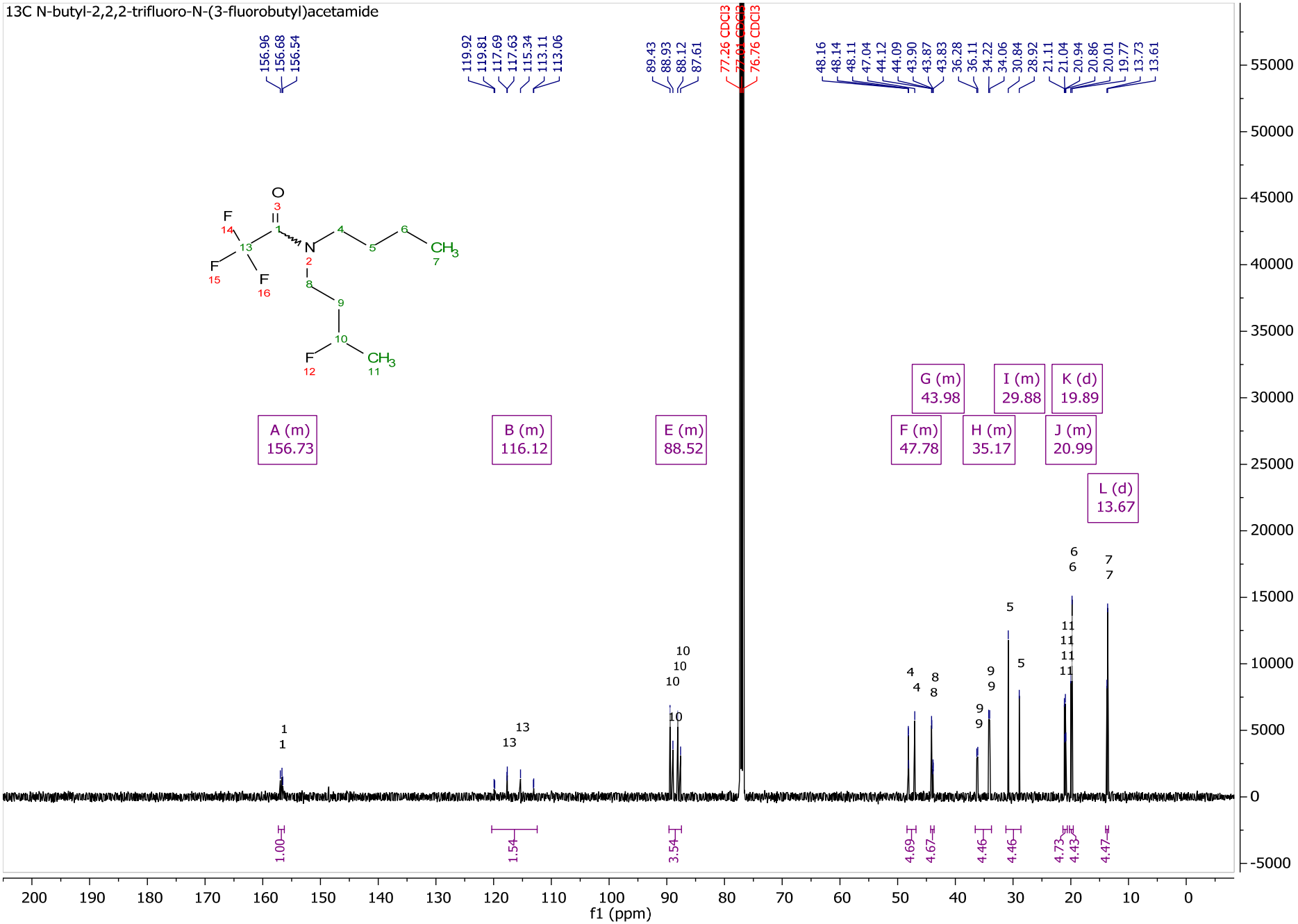

COSY
f2 (ppm)
f1 (ppm)

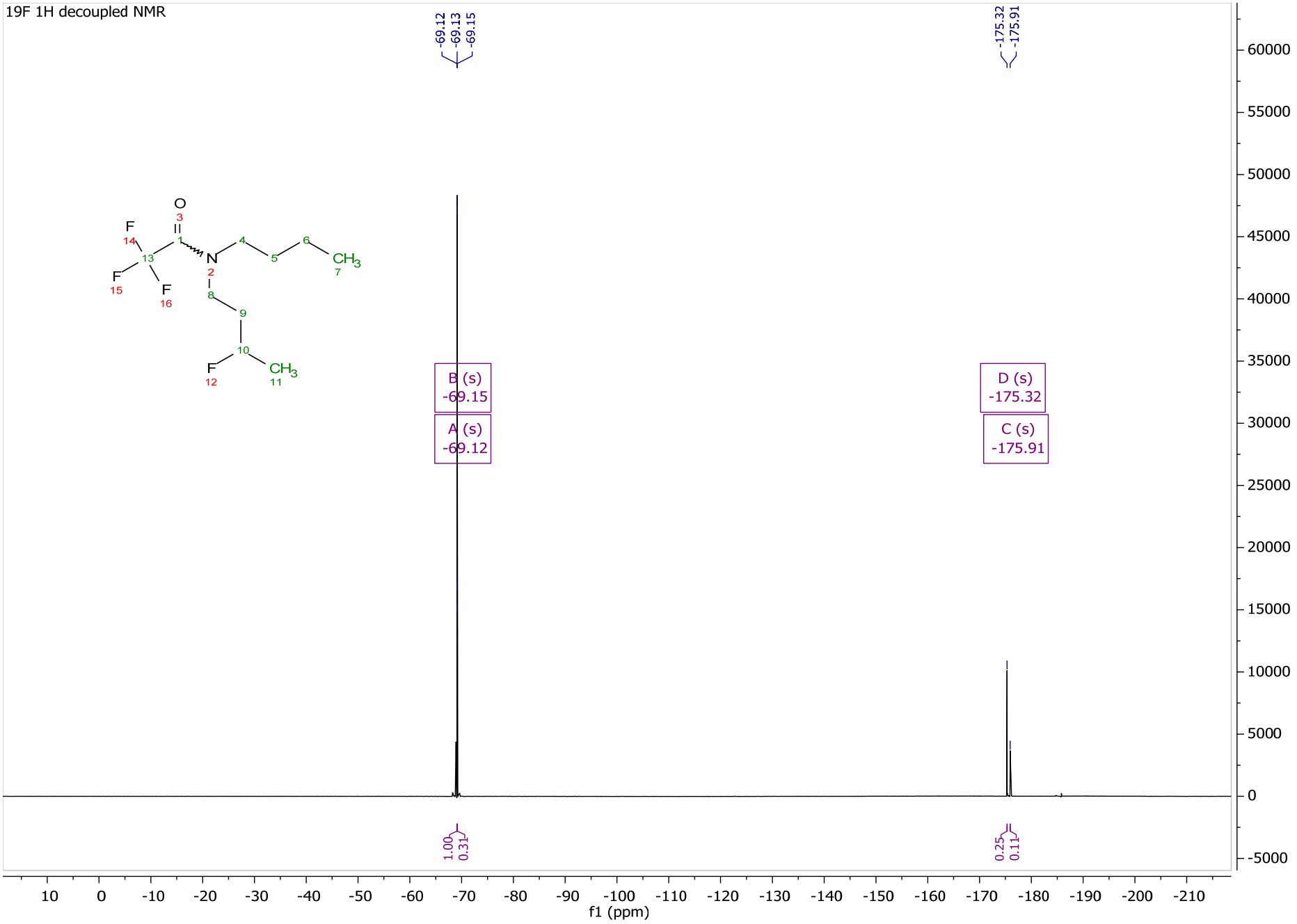

HMQC
f2 (ppm)
f1 (ppm)

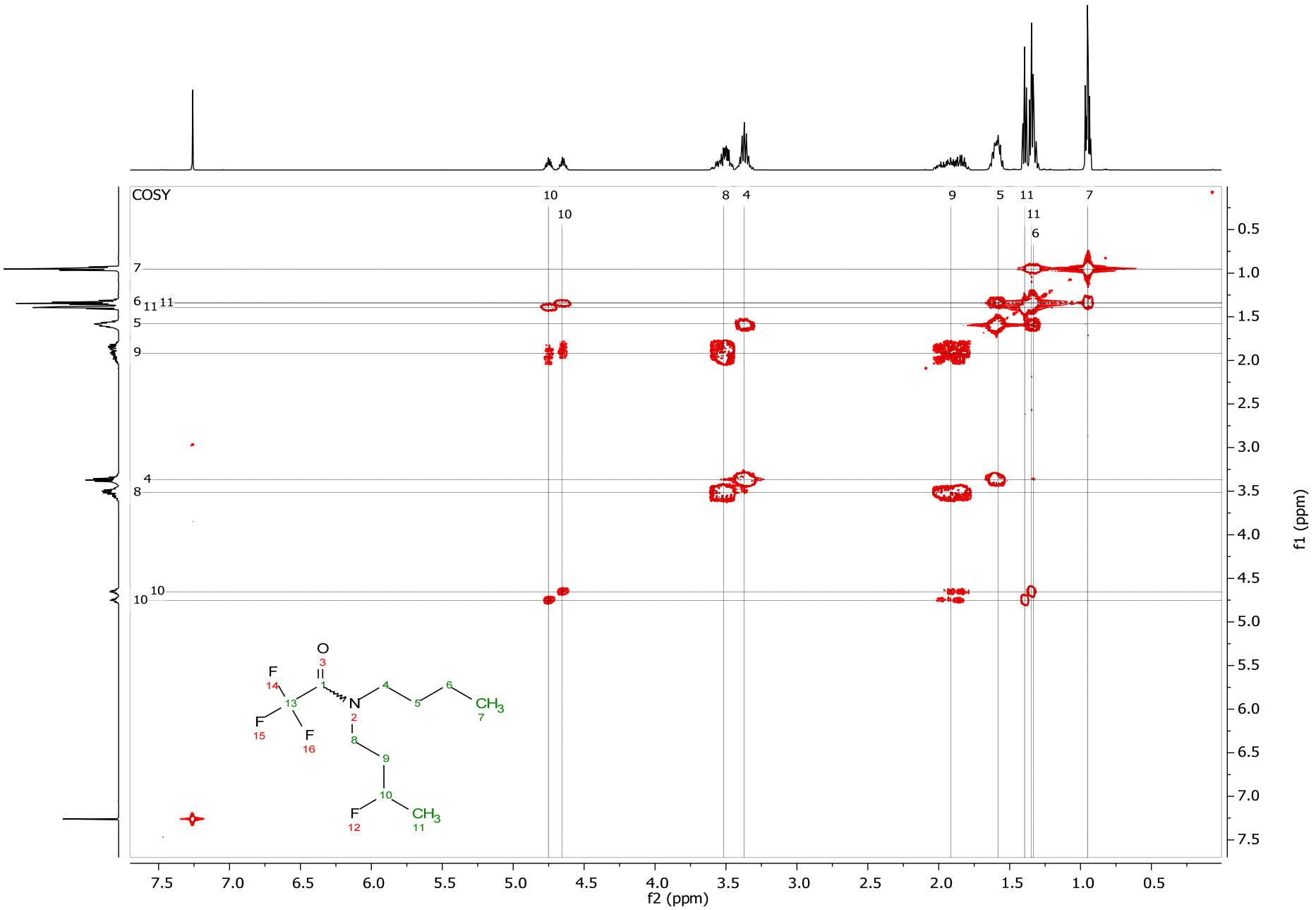

HMBC
f2 (ppm)
f1 (ppm)

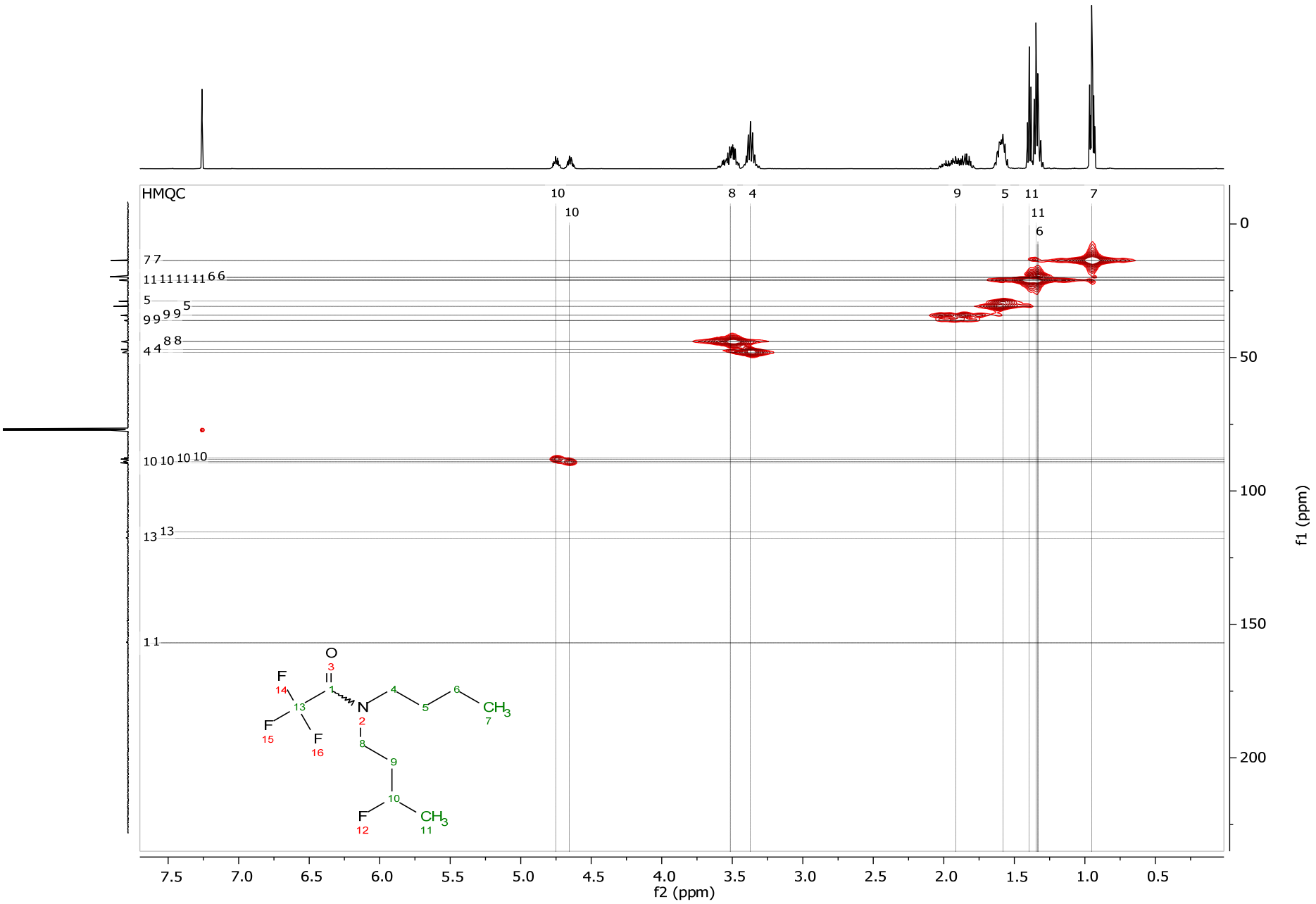
NMR Spectra of N-butyl-2,2,2-trifluoro-N-(3-fluorobutyl)acetamide

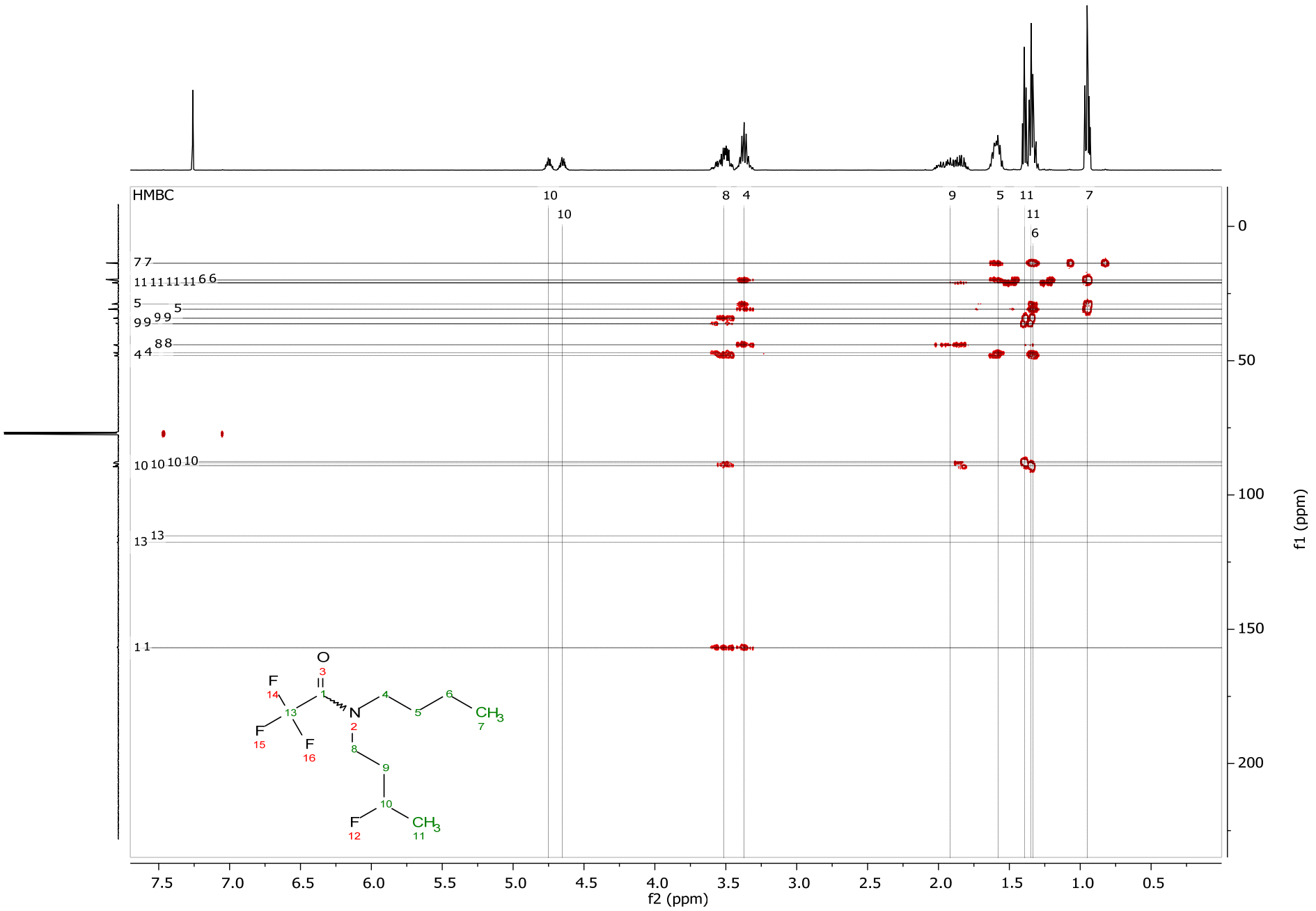



13C N-butyl-2,2,2-trifluoro-N-(3-fluorobutyl)acetamide
156.96
156.68
156.54
119.92
119.81
117.69
117.63
115.34
113.11
113.06
89.43
88.93
88.12
87.61
77.26 CDCl3
77.01 CDCl3
76.76 CDCl3
48.16
48.14
48.11
47.04
44.12
44.09
43.90
43.87
43.83
36.28
36.11
34.22
34.06
30.84
28.92
21.11
21.04
20.94
20.86
20.01
19.77
13.73
13.61
A (m) 156.73
B (m) 116.12
E (m) 88.52
F (m) 47.78
G (m) 43.98
H (m) 35.17
I (m) 29.88
J (m) 20.99
K (d) 19.89
L (d) 13.67
1.00
1.54
3.54
4.69
4.67
4.46
4.46
4.73
4.43
4.47
f1 (ppm)

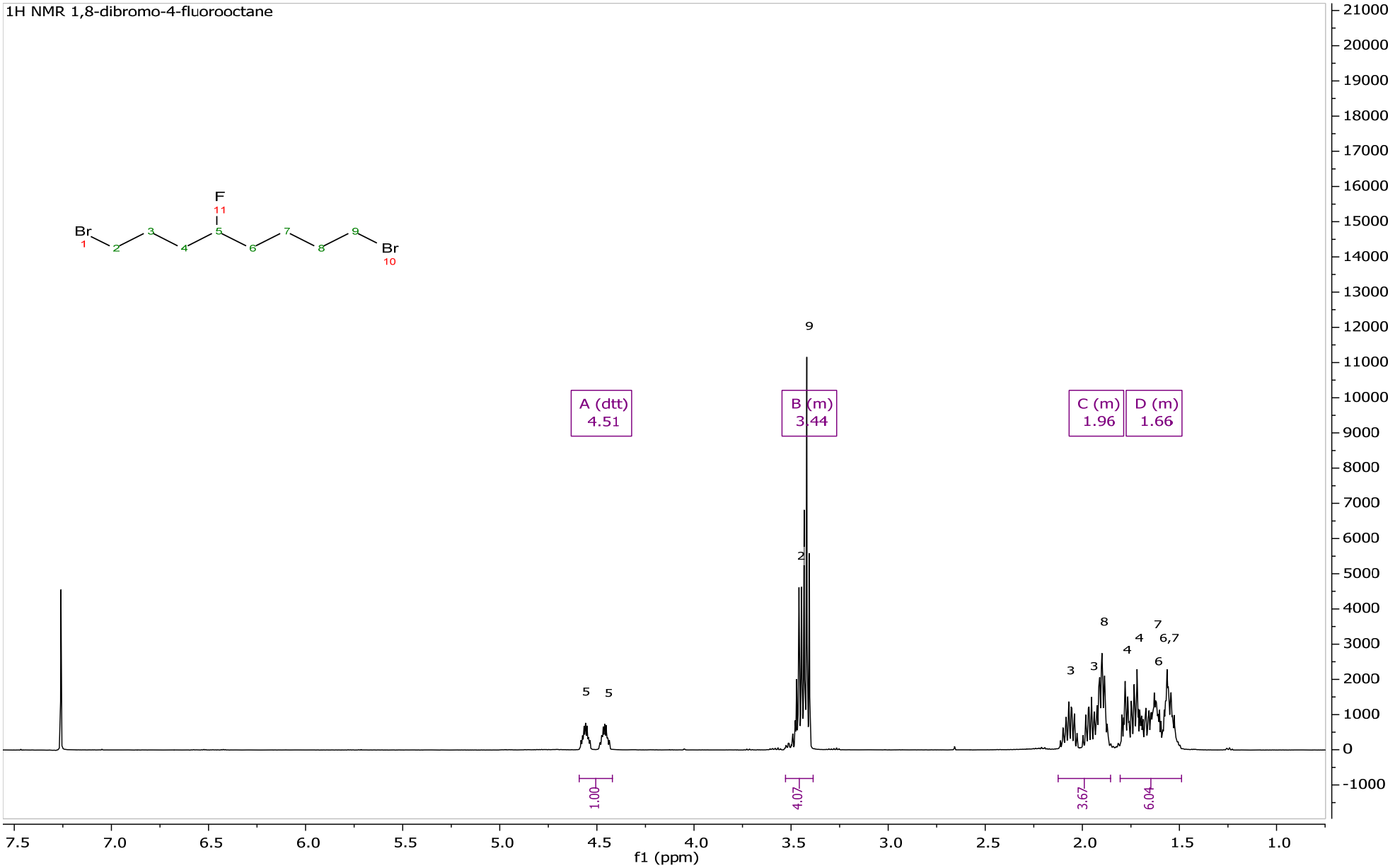

19F 1H decoupled NMR
-69.12
-69.13
-69.15
-175.32
-175.91
B (s)
-69.15
A (s)
-69.12
D (s)
-175.32
C (s)
-175.91
1.00
0.31
0.25
0.11
f1 (ppm)

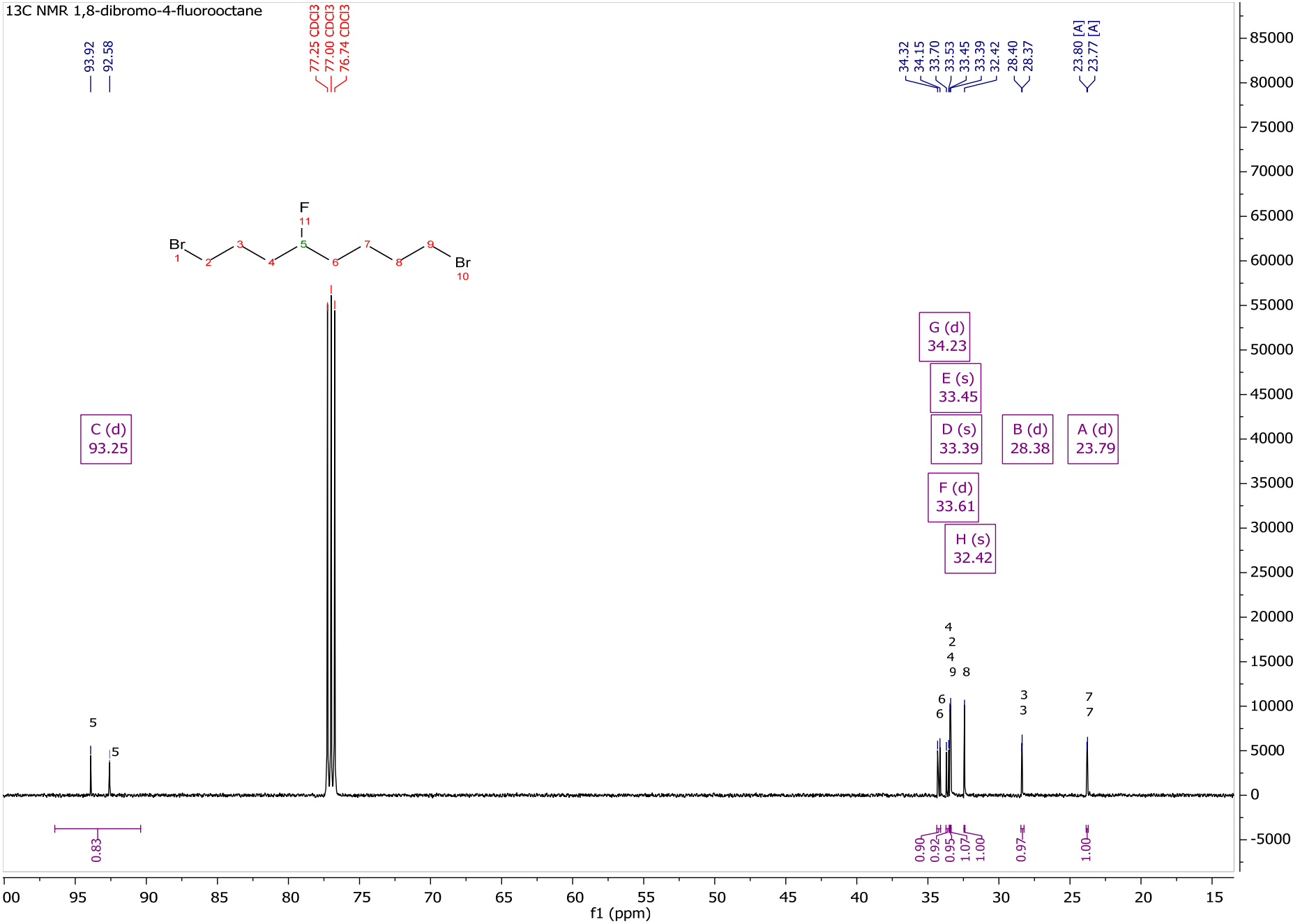

COSY
f2 (ppm)
f1 (ppm)
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
O
F
N
CH3

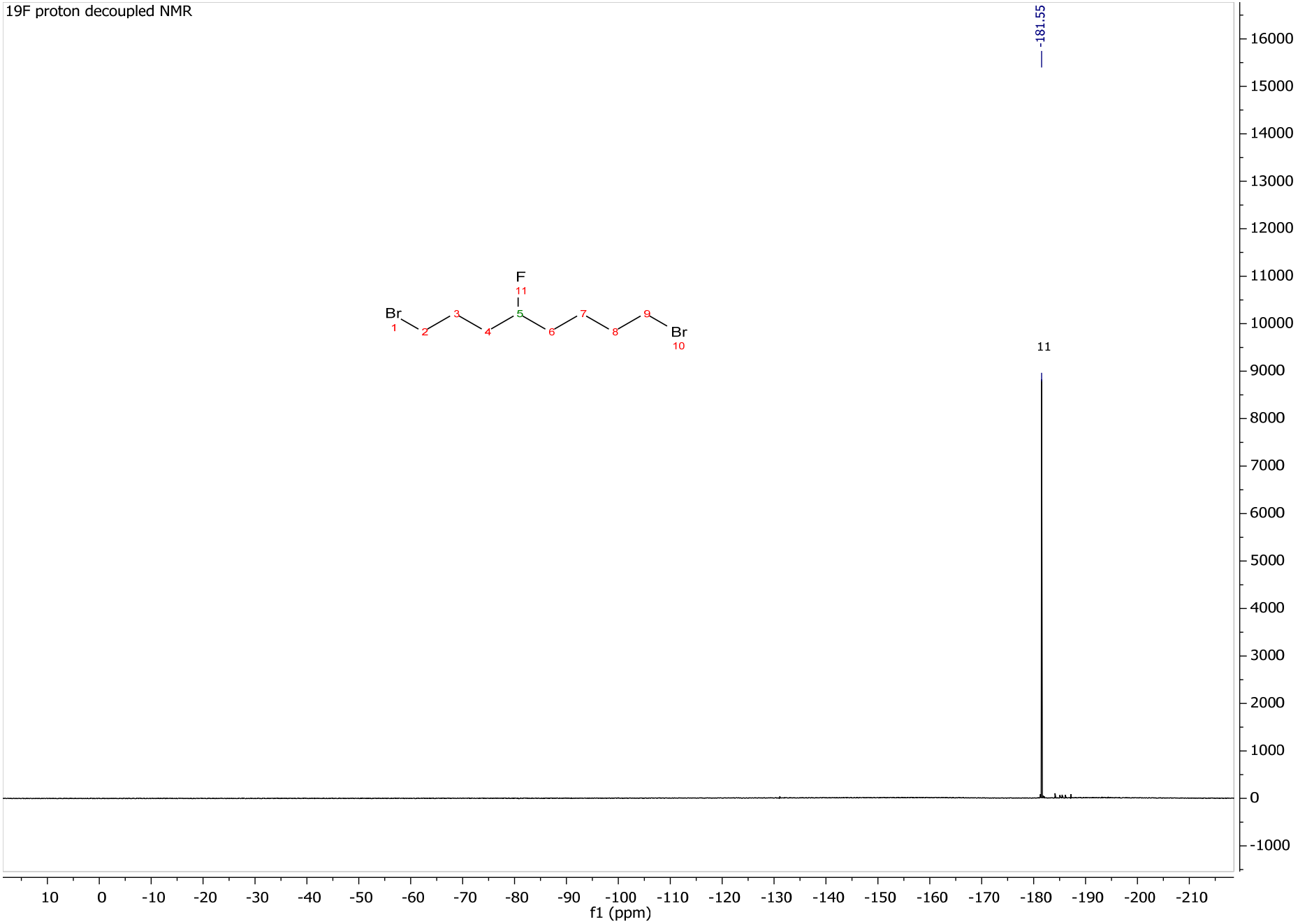

HMQC
f2 (ppm)
f1 (ppm)
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0
50
100
150
200
O
F
N
CH3

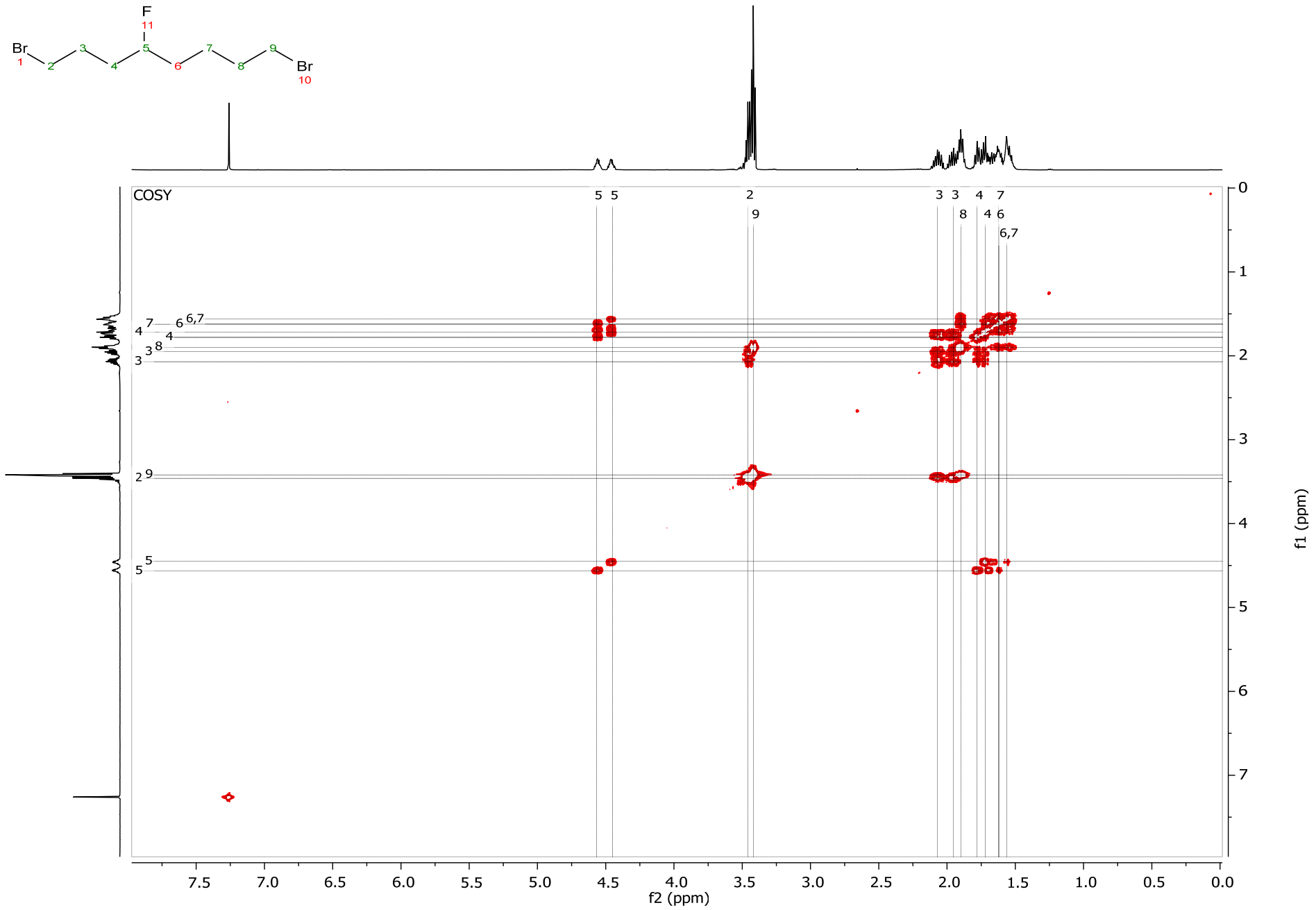

HMBC
f2 (ppm)
f1 (ppm)
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0
50
100
150
200
O
F
N
CH3

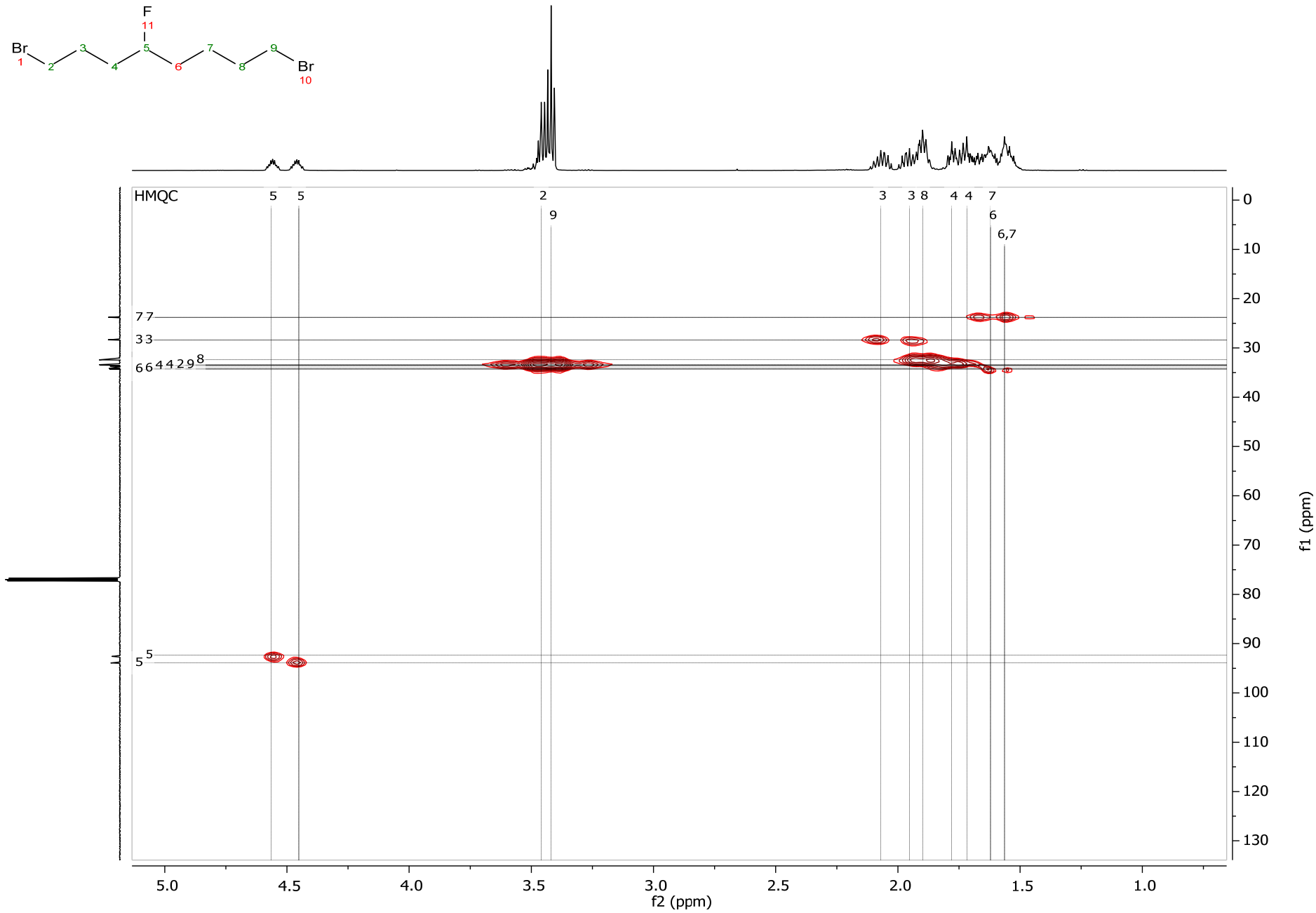
NMR Spectra of 1,8-dibromo-4-fluorooctane

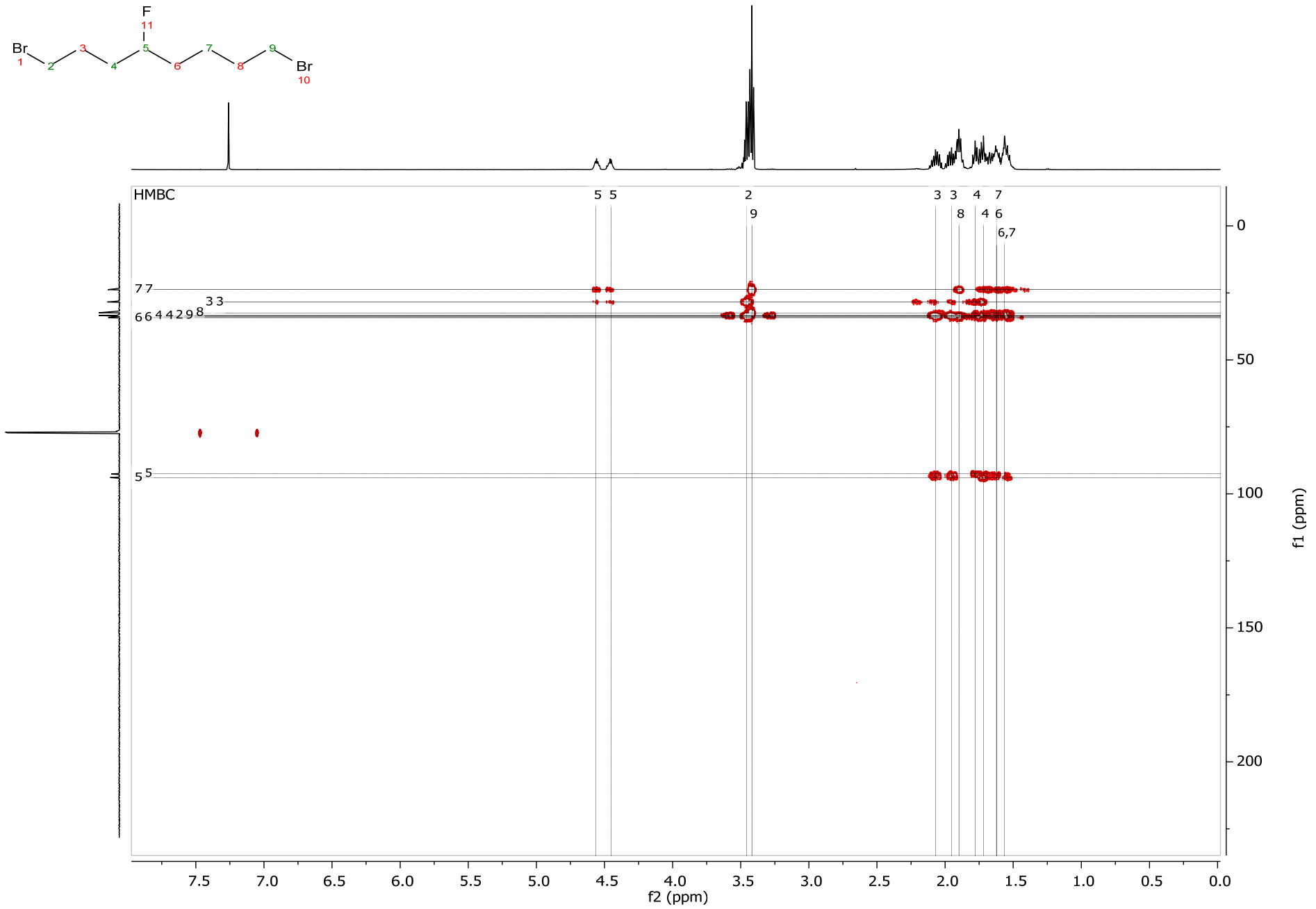



13C NMR 1,8-dibromo-4-fluorooctane
93.92
92.58
77.25 CDCl3
77.00 CDCl3
76.74 CDCl3
34.32
34.15
33.70
33.53
33.45
33.39
32.42
28.40
28.37
23.80 [A]
23.77 [A]
F
11
Br
1
2
3
4
5
6
7
8
9
Br
10
C (d)
93.25
G (d)
34.23
E (s)
33.45
D (s)
33.39
B (d)
28.38
A (d)
23.79
F (d)
33.61
H (s)
32.42
f1 (ppm)

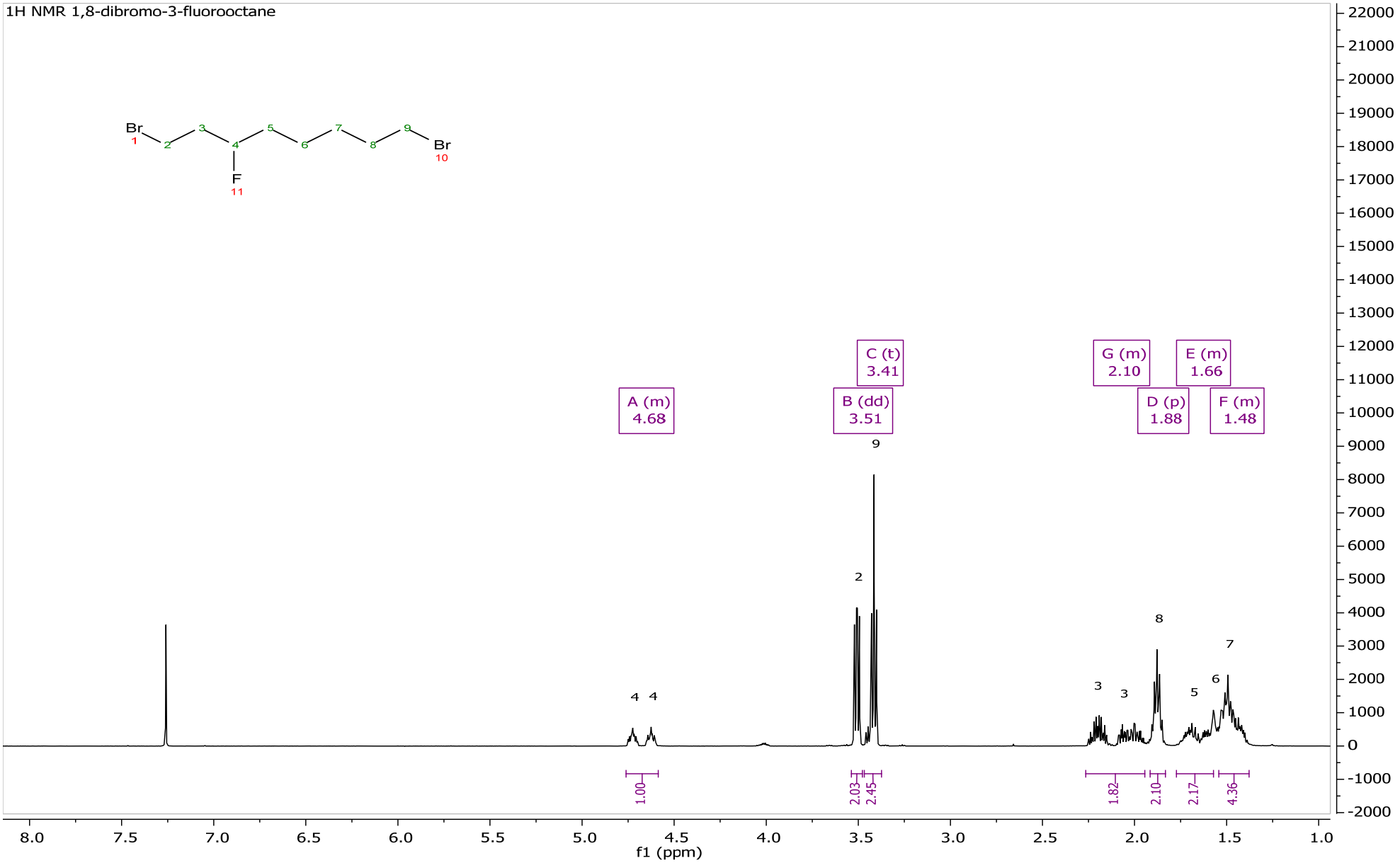

19F proton decoupled NMR
-181.55
11
F
11
Br
1
2
3
4
5
6
7
8
9
Br
10
16000
15000
14000
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

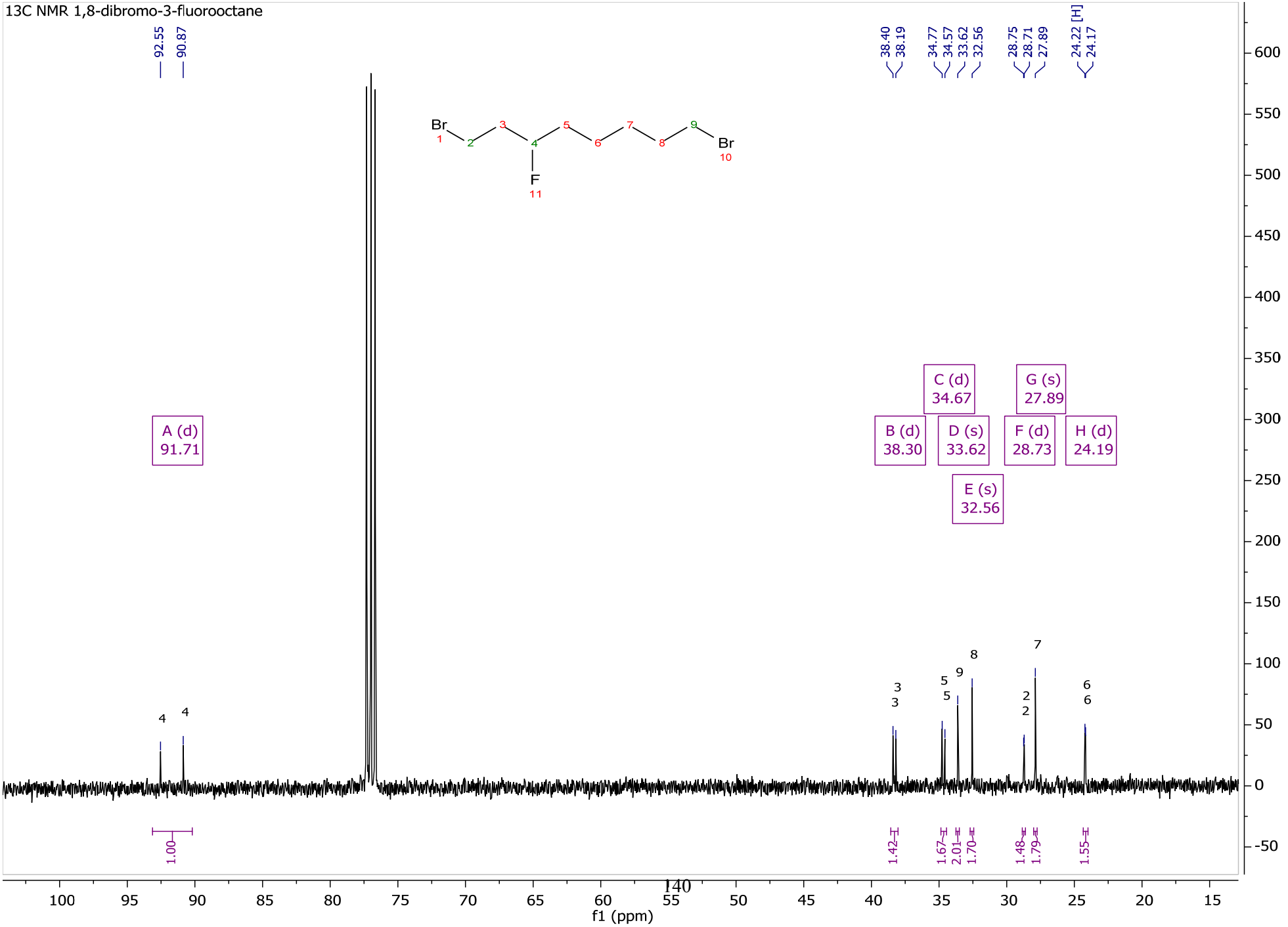

F
11
Br
1
2
3
4
5
6
7
8
9
Br
10
COSY
f2 (ppm)
f1 (ppm)

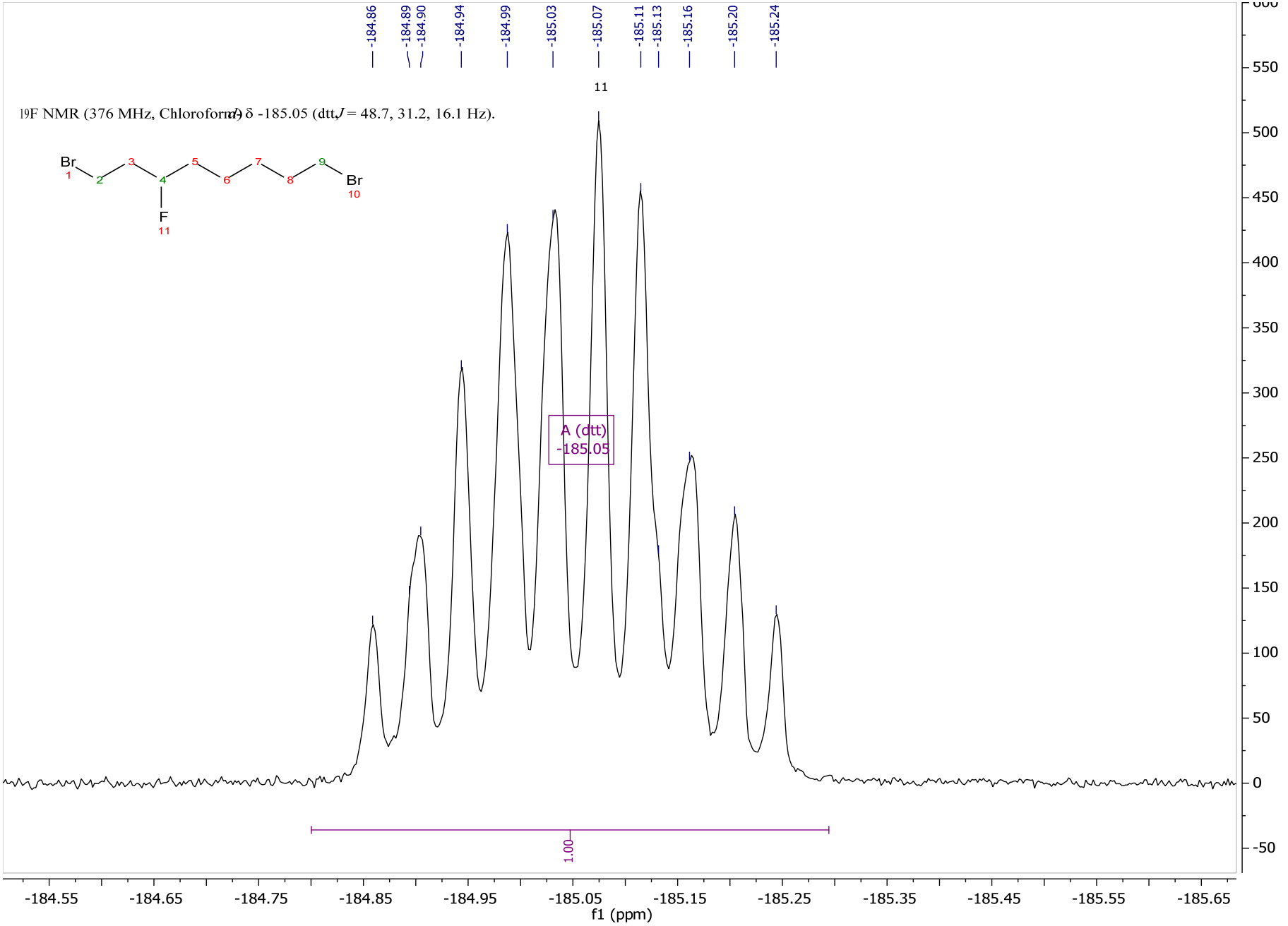

F
11
Br
1
2
3
4
5
6
7
8
9
Br
10
HMQC
f2 (ppm)
f1 (ppm)

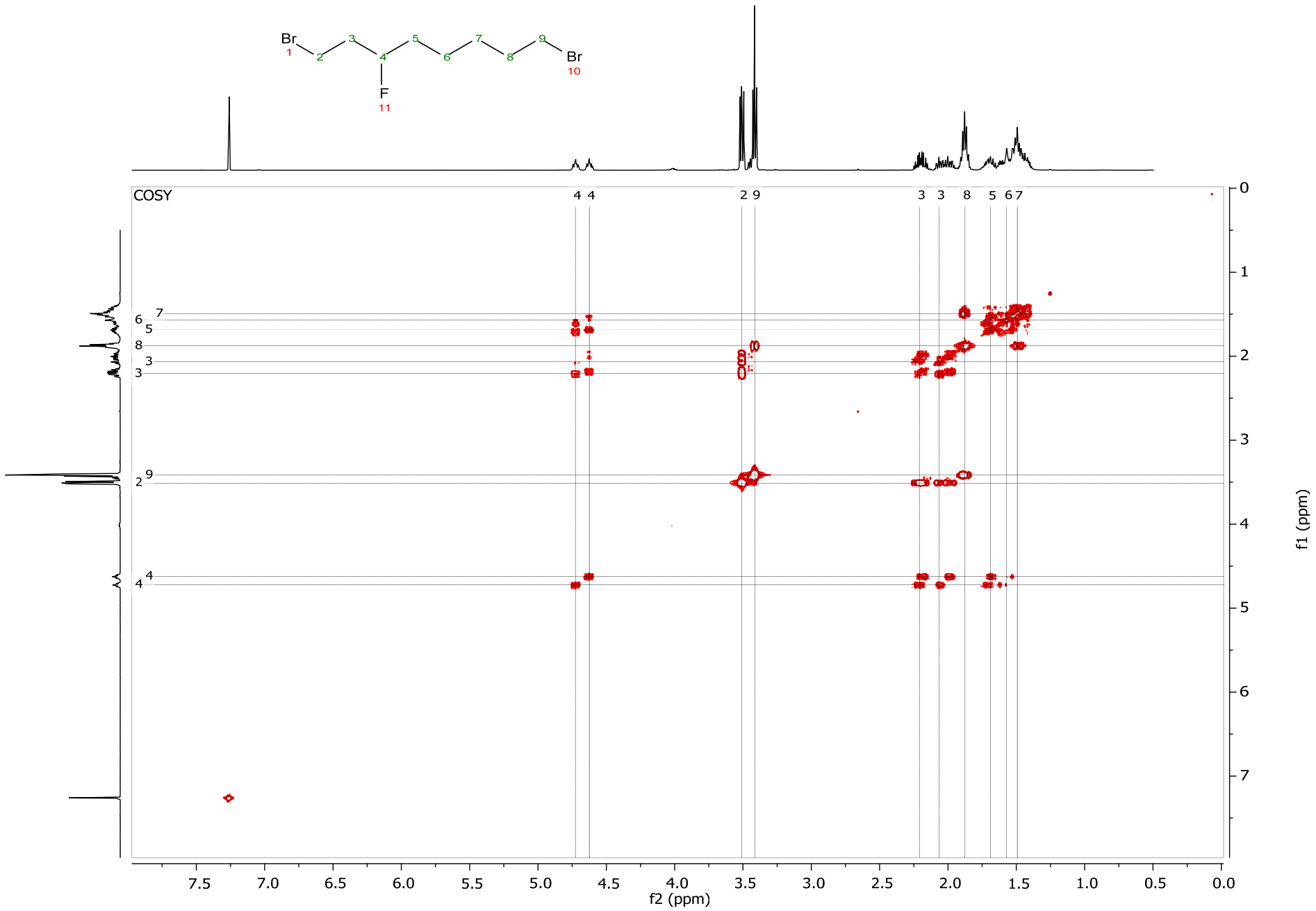

F
11
Br
1
2
3
4
5
6
7
8
9
Br
10
HMBC
5 5
2
9
3 3
8
4 4
7
6
6,7
7 7
3 3
6 6 4 4 2 9 8
5 5
0
50
100
150
200
f1 (ppm)
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f2 (ppm)

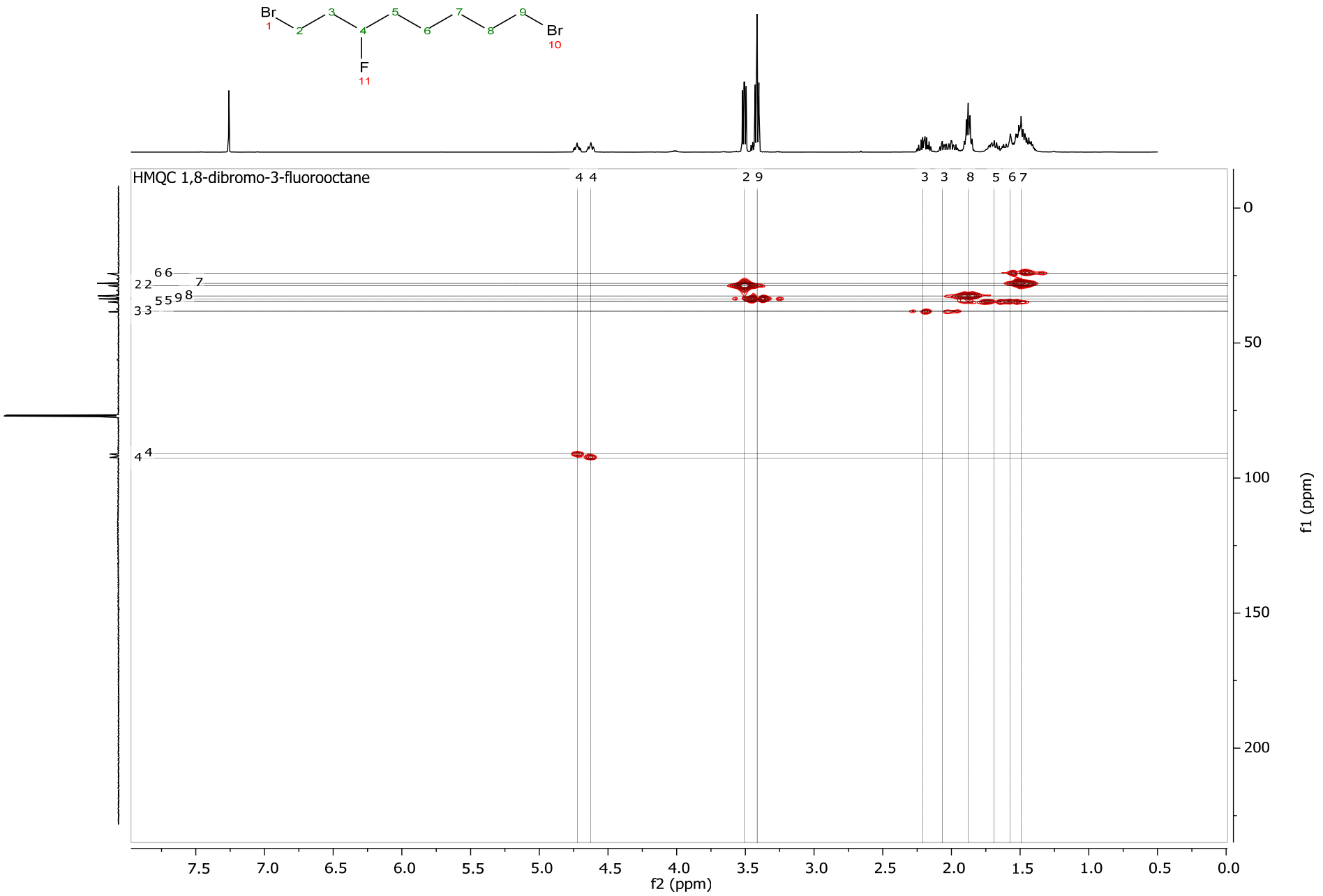
NMR Spectra of 1,8-dibromo-3-fluorooctane

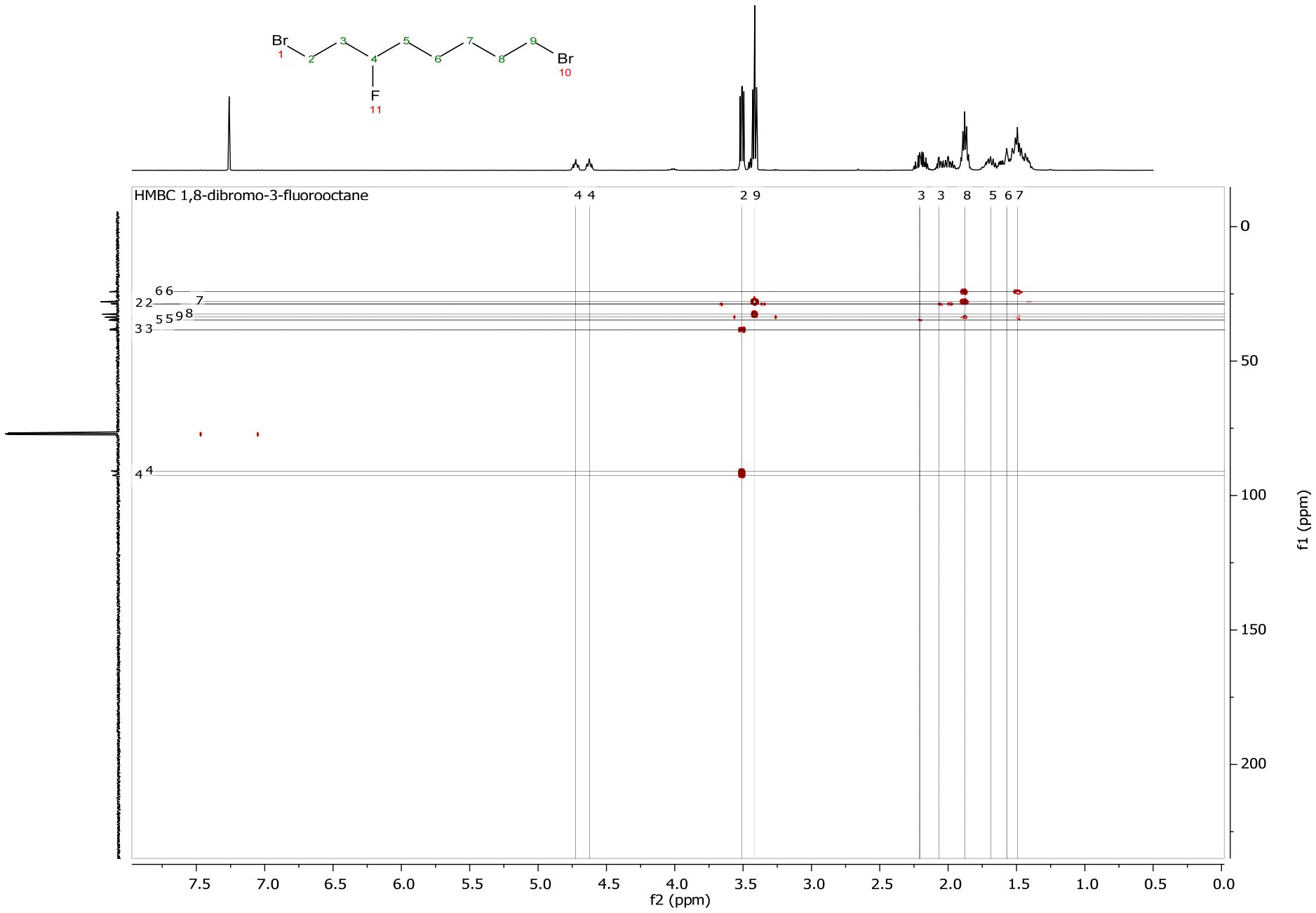



13C NMR 1,8-dibromo-3-fluorooctane
92.55
90.87
38.40
38.19
34.77
34.57
33.62
32.56
28.75
28.71
27.89
24.22 [H]
24.17
Br
1
2
3
4
5
6
7
8
9
Br
10
F
11
A (d)
91.71
C (d)
34.67
G (s)
27.89
B (d)
38.30
D (s)
33.62
F (d)
28.73
H (d)
24.19
E (s)
32.56
4
4
3
3
5
5
9
8
2
2
7
6
6
1.00
1.42
1.67
2.01
1.70
1.48
1.79
1.55
f1 (ppm)

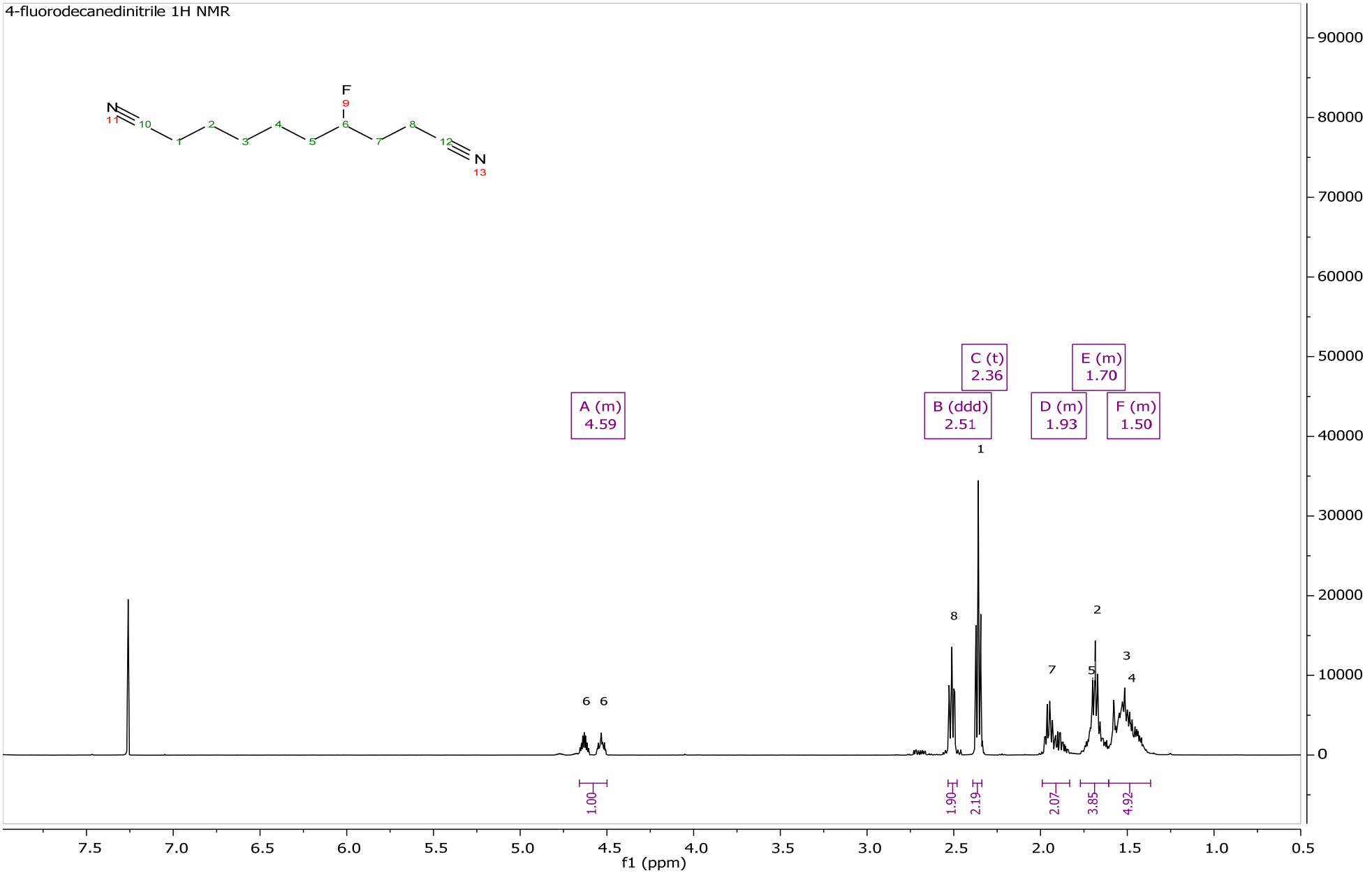

-184.86
-184.89
-184.90
-184.94
-184.99
-185.03
-185.07
-185.11
-185.13
-185.16
-185.20
-185.24
11
19F NMR (376 MHz, Chloroform-d) δ -185.05 (dtt, J = 48.7, 31.2, 16.1 Hz).
Br
1
2
3
4
5
6
7
8
9
Br
10
F
11
A (dtt)
-185.05
1.00
-184.55
-184.65
-184.75
-184.85
-184.95
-185.05
-185.15
-185.25
-185.35
-185.45
-185.55
-185.65
f1 (ppm)
550
500
450
400
350
300
250
200
150
100
50
0
-50

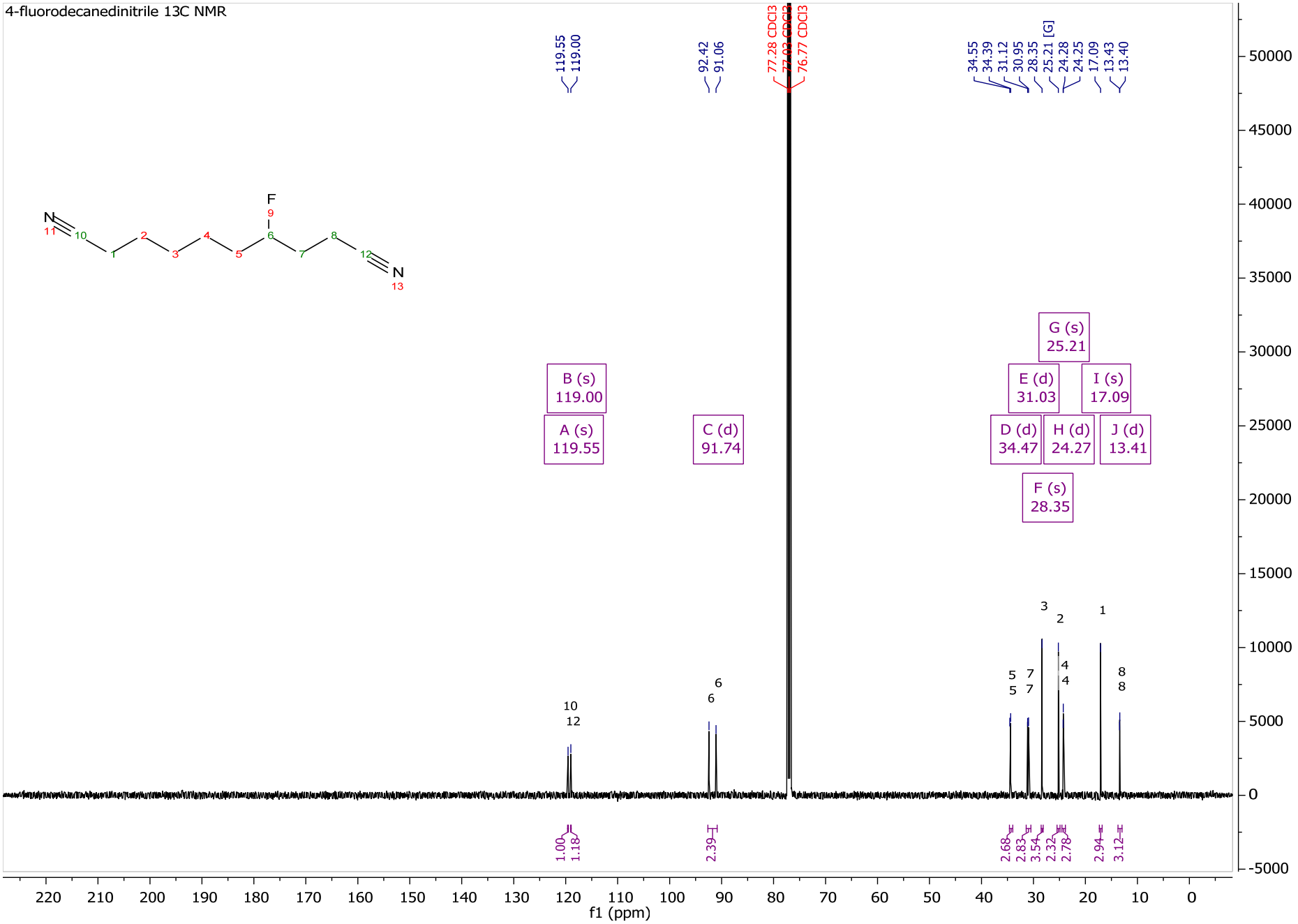

Br
1
2
3
4
5
6
7
8
9
Br
10
F
11
COSY
4 4
2 9
3 3
8
5
6 7
f2 (ppm)
f1 (ppm)

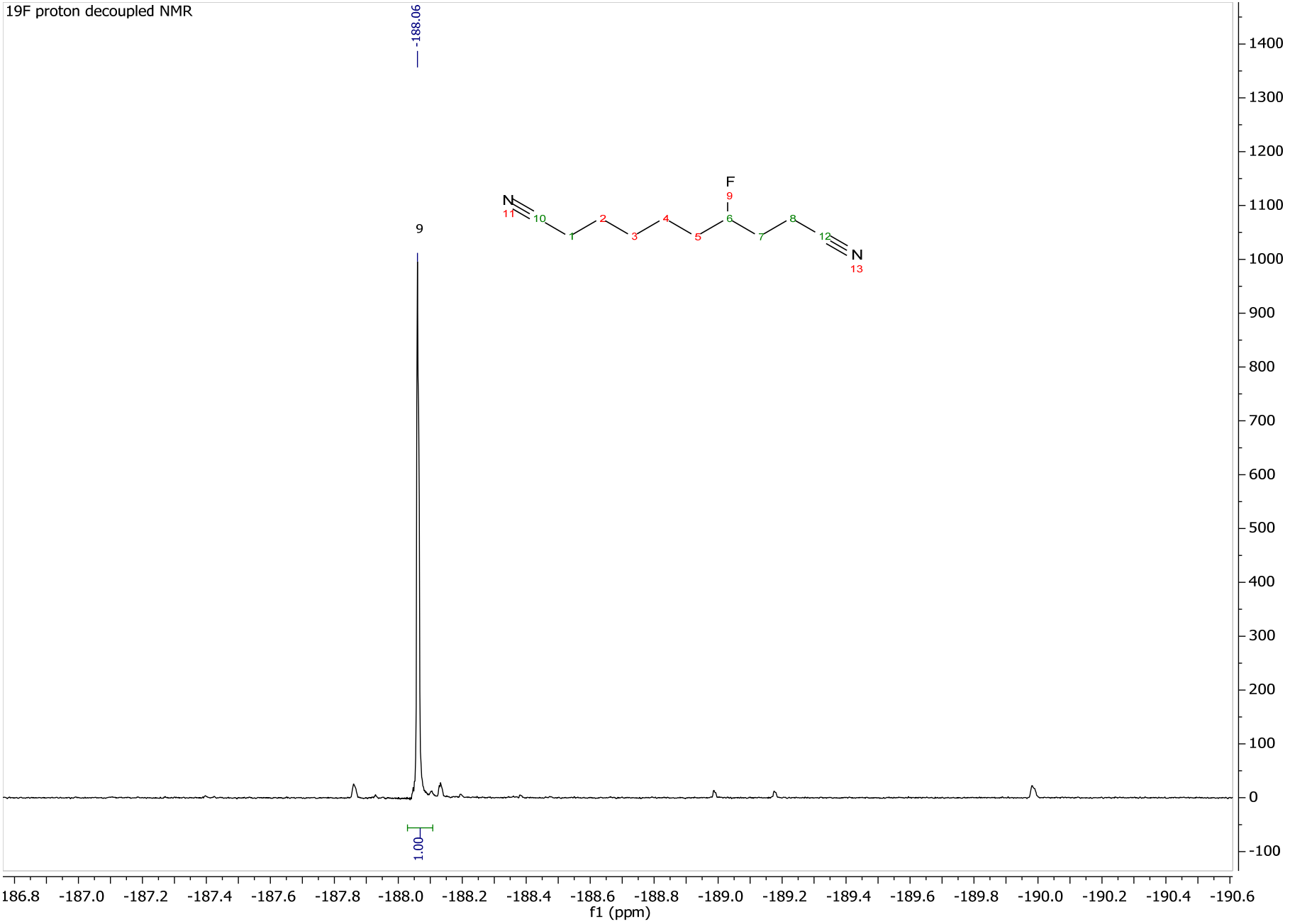

Br
1
2
3
4
5
6
7
8
9
Br
10
F
11
HMQC 1,8-dibromo-3-fluorooctane
4 4
2 9
3 3
8
5
6 7
2 2
6 6
7
3 3
5 5 9 8
4 4
0
50
100
150
200
f1 (ppm)
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f2 (ppm)

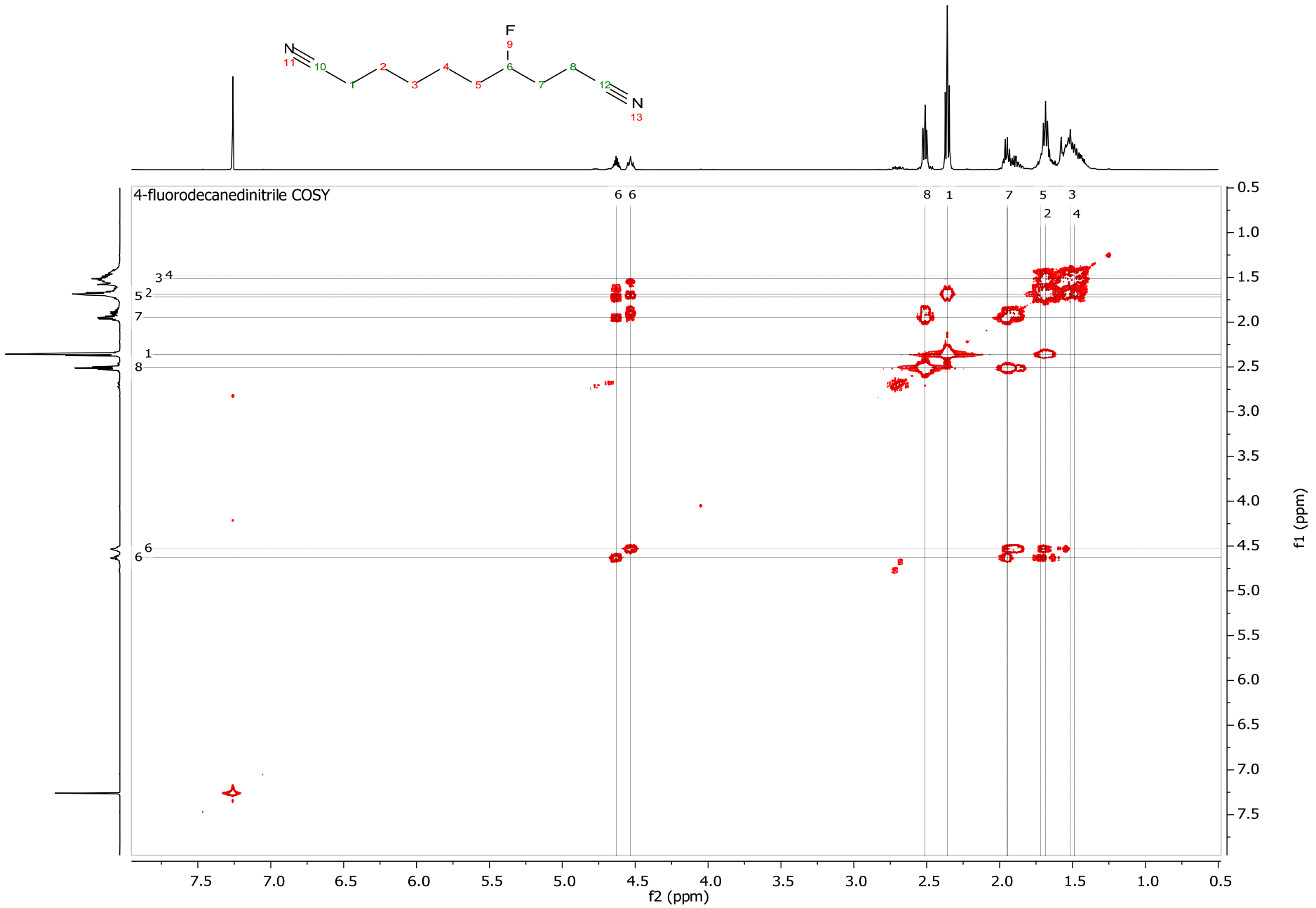

HMBC 1,8-dibromo-3-fluorooctane
Br
1
2
3
4
5
6
7
8
9
Br
10
F
11
f2 (ppm)
f1 (ppm)

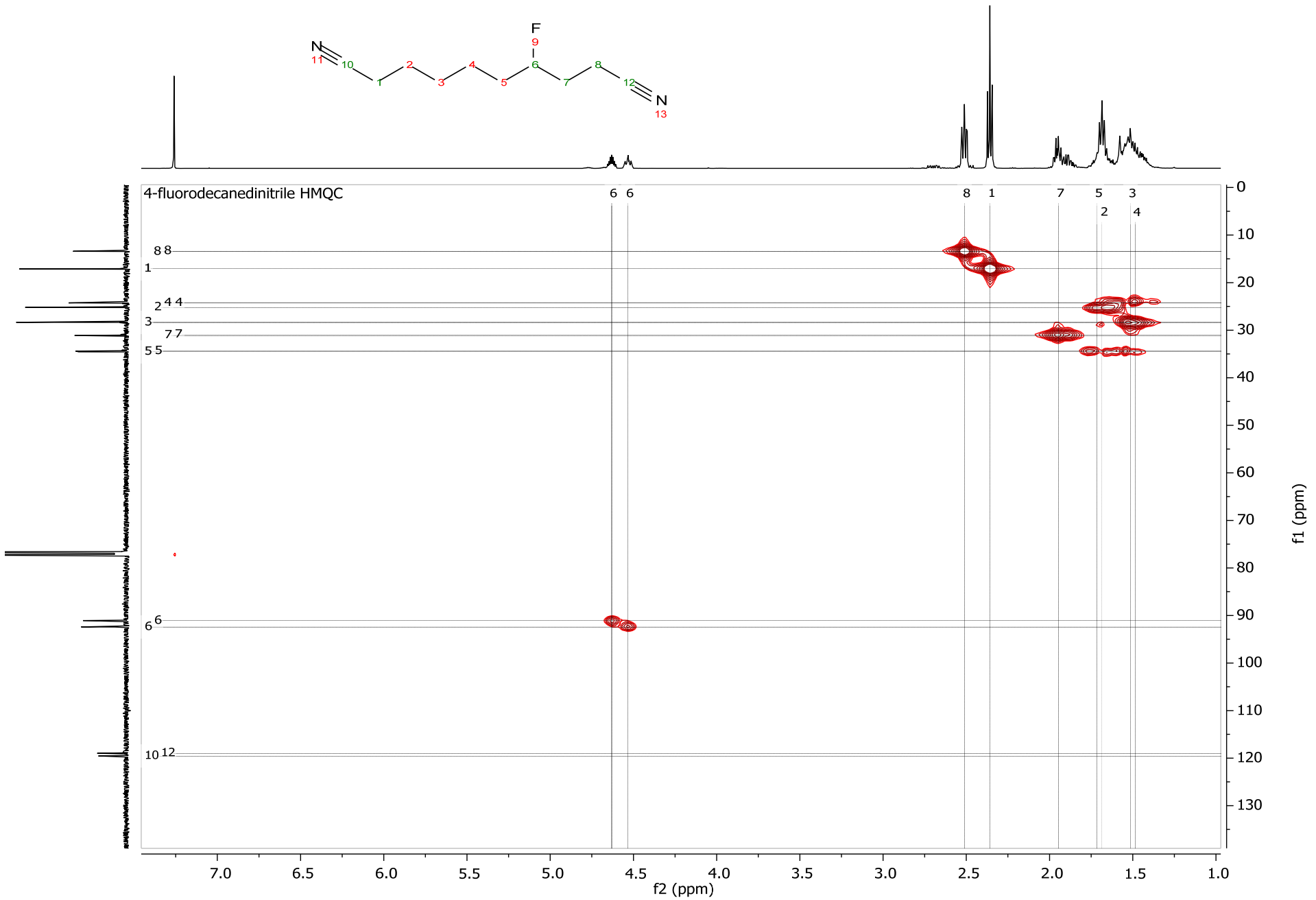
NMR Spectra of 4-fluorodecanedinitrile

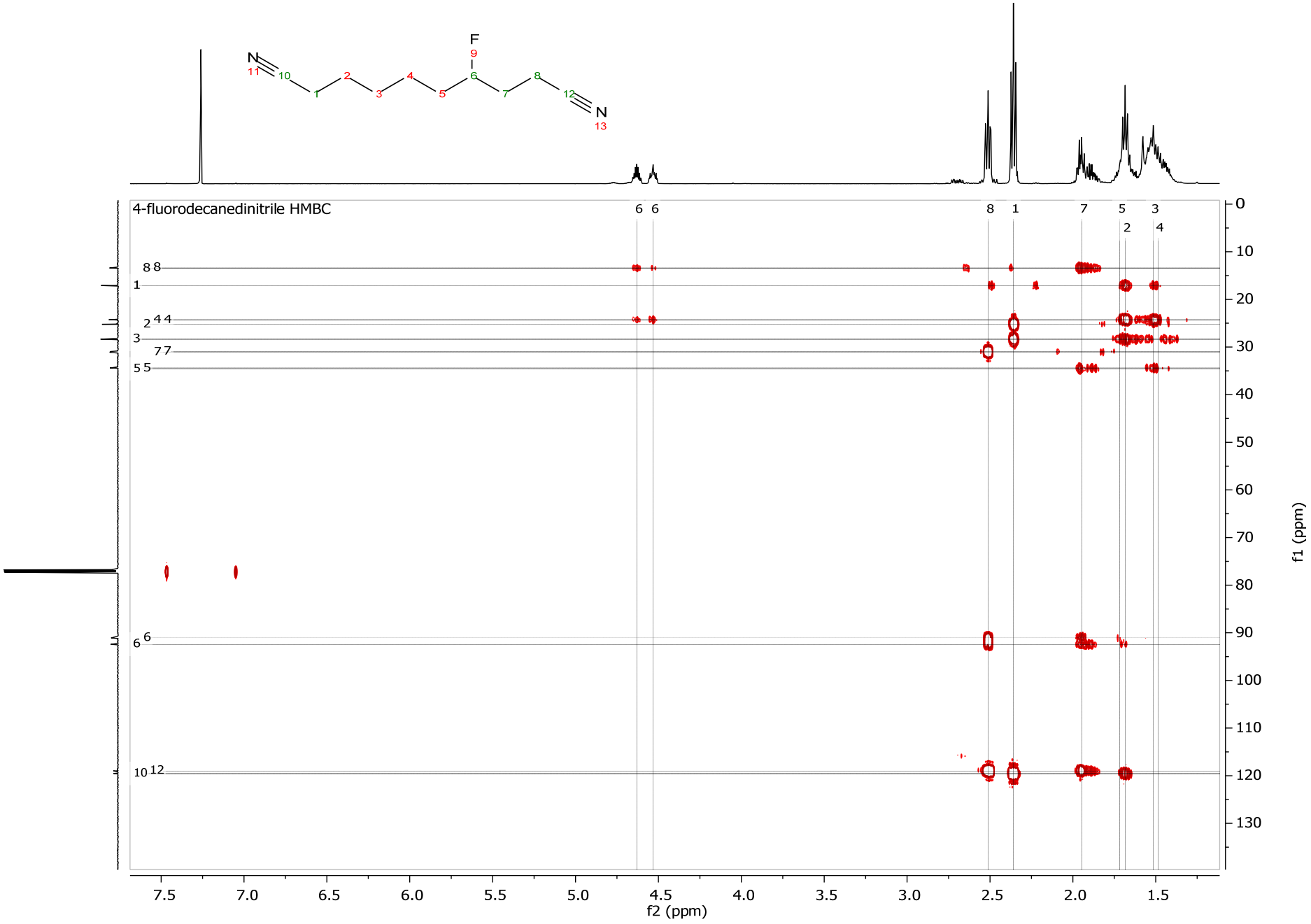



4-fluorodecanedinitrile 13C NMR
119.55
119.00
92.42
91.06
77.28 CDCl3
77.03 CDCl3
76.77 CDCl3
34.55
34.39
31.12
30.95
28.35
25.21 [G]
24.28
24.25
17.09
13.43
13.40
B (s) 119.00
A (s) 119.55
C (d) 91.74
G (s) 25.21
E (d) 31.03
I (s) 17.09
D (d) 34.47
H (d) 24.27
J (d) 13.41
F (s) 28.35
f1 (ppm)

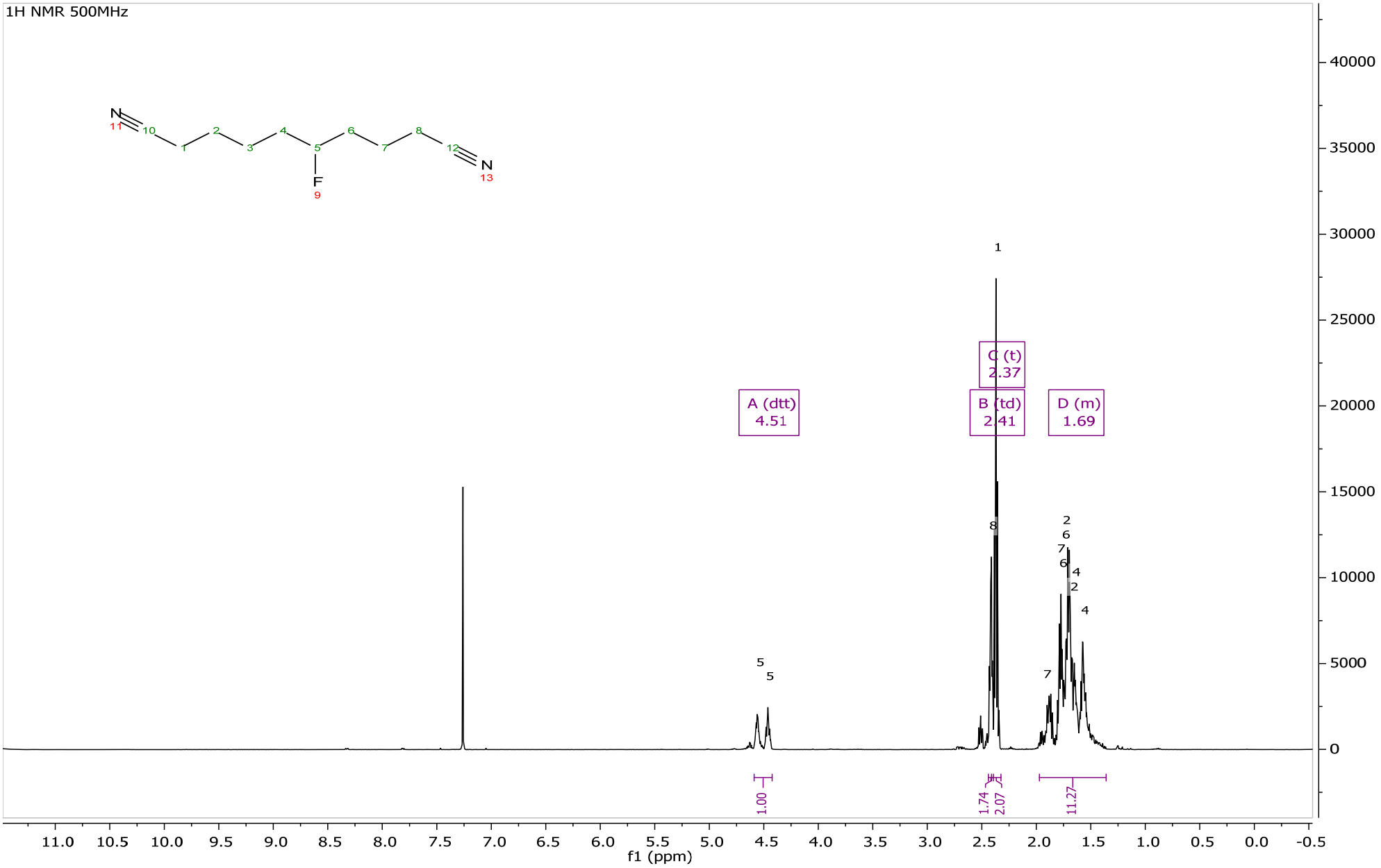

19F proton decoupled NMR
-188.06
9
1.00
F
9
N
11
10
1
2
3
4
5
6
7
8
12
N
13
1400
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
-100
186.8
-187.0
-187.2
-187.4
-187.6
-187.8
-188.0
-188.2
-188.4
-188.6
-188.8
-189.0
-189.2
-189.4
-189.6
-189.8
-190.0
-190.2
-190.4
-190.6
f1 (ppm)

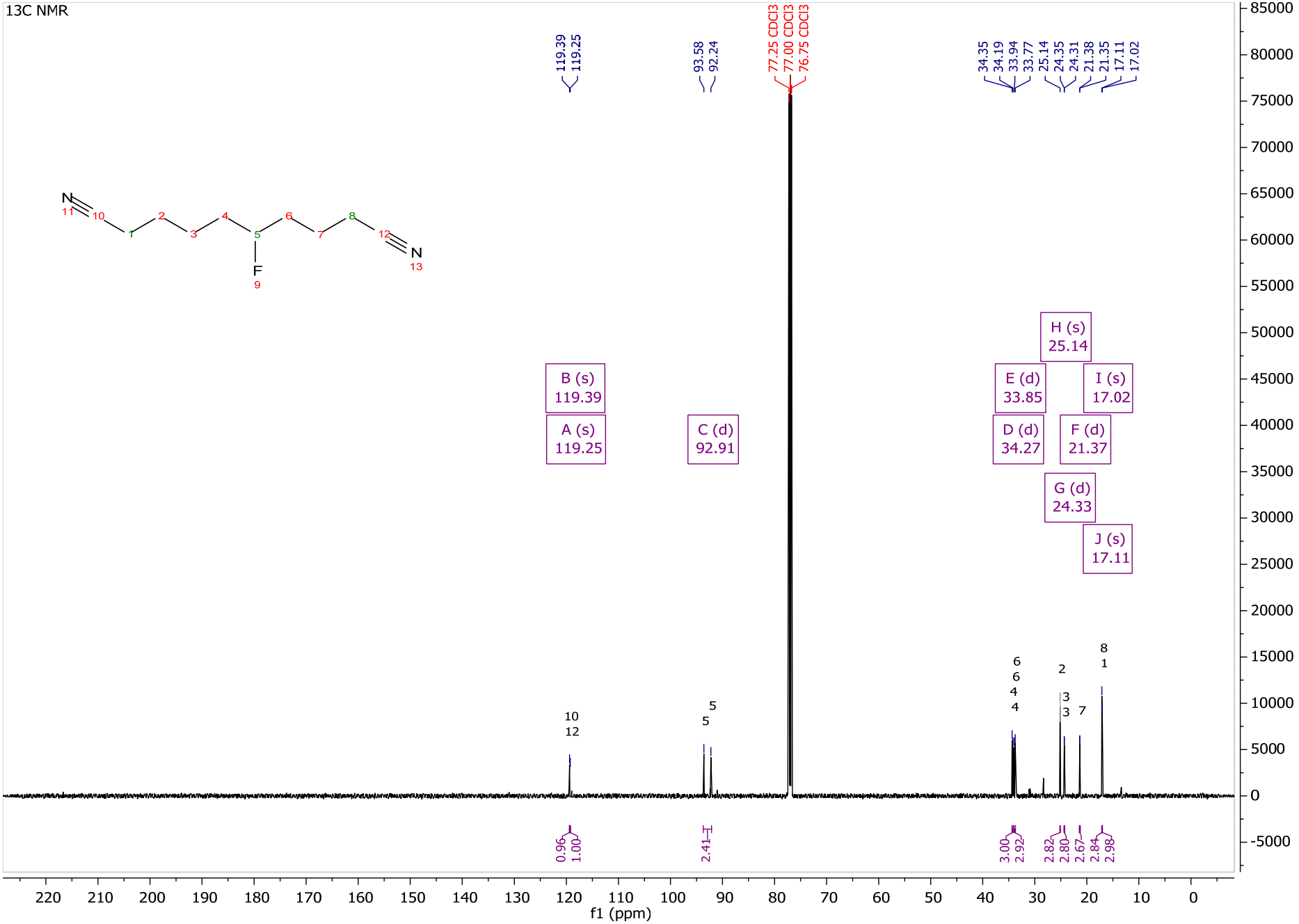

4-fluorodecanedinitrile COSY
F
9
N
11
10
1
2
3
4
5
6
7
8
12
N
13
f2 (ppm)
f1 (ppm)

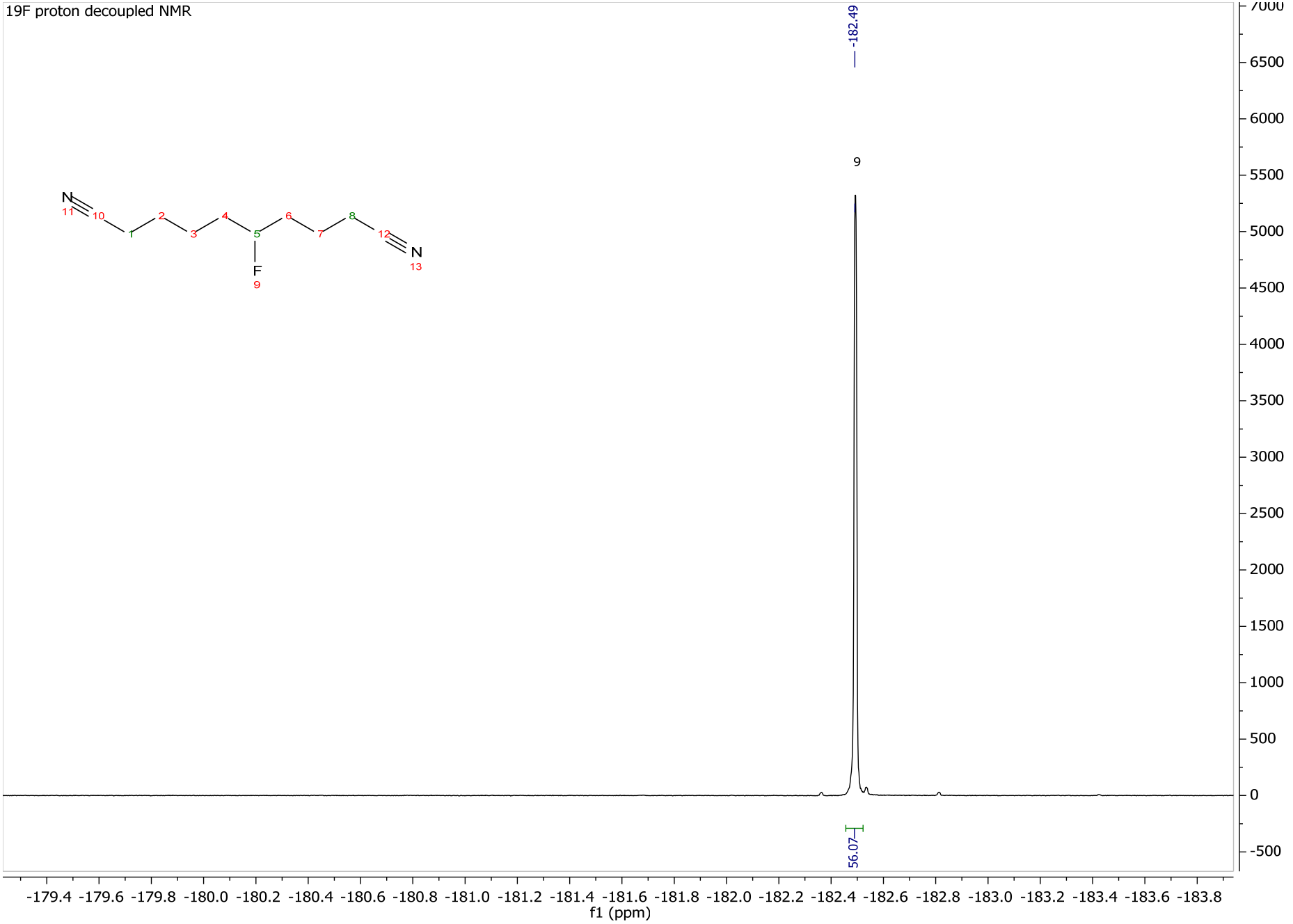

4-fluorodecanedinitrile HMQC
F
9
N
11
10
1
2
3
4
5
6
7
8
12
N
13
f2 (ppm)
f1 (ppm)

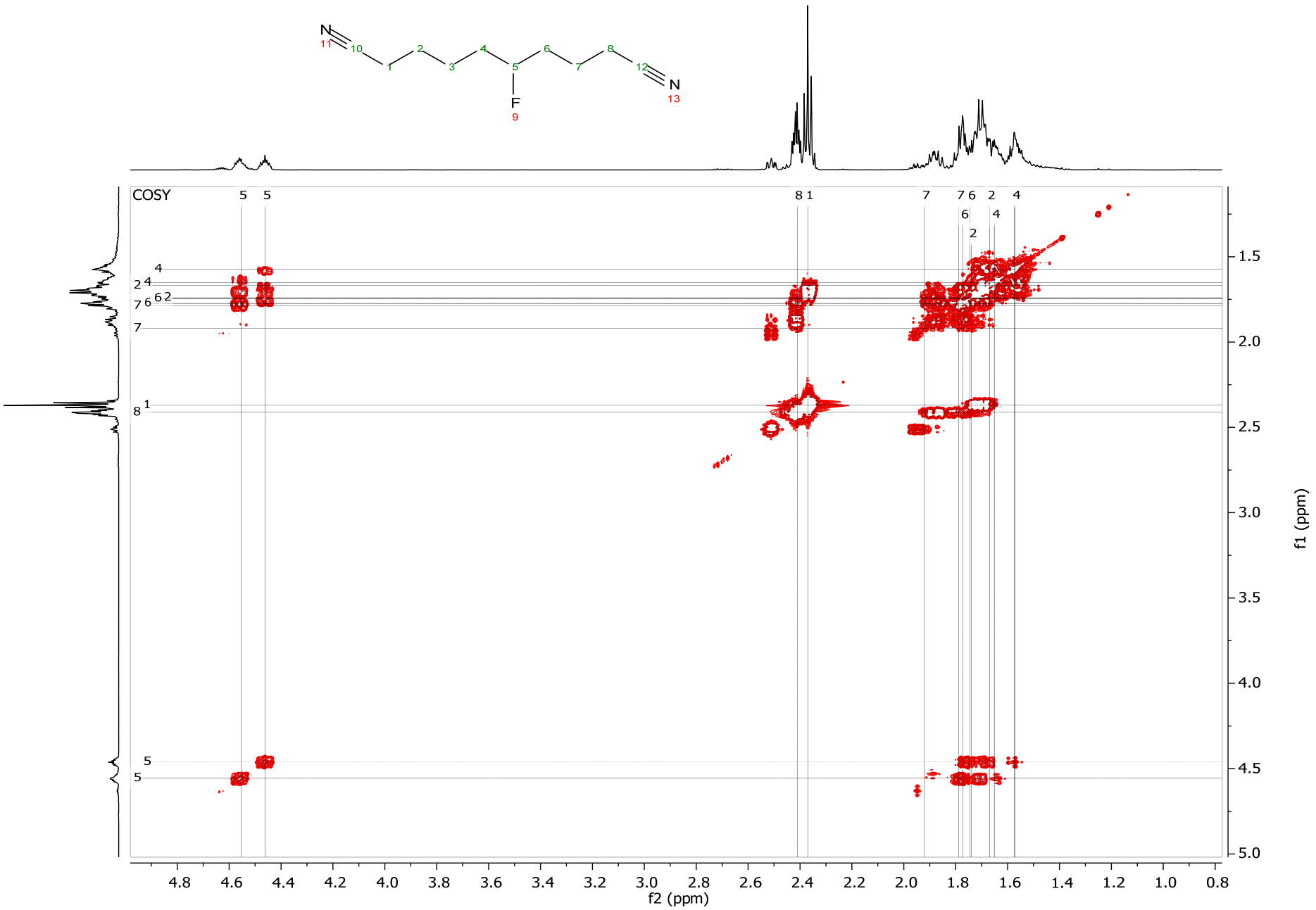

4-fluorodecanedinitrile HMBC
F
N
N
f2 (ppm)
f1 (ppm)

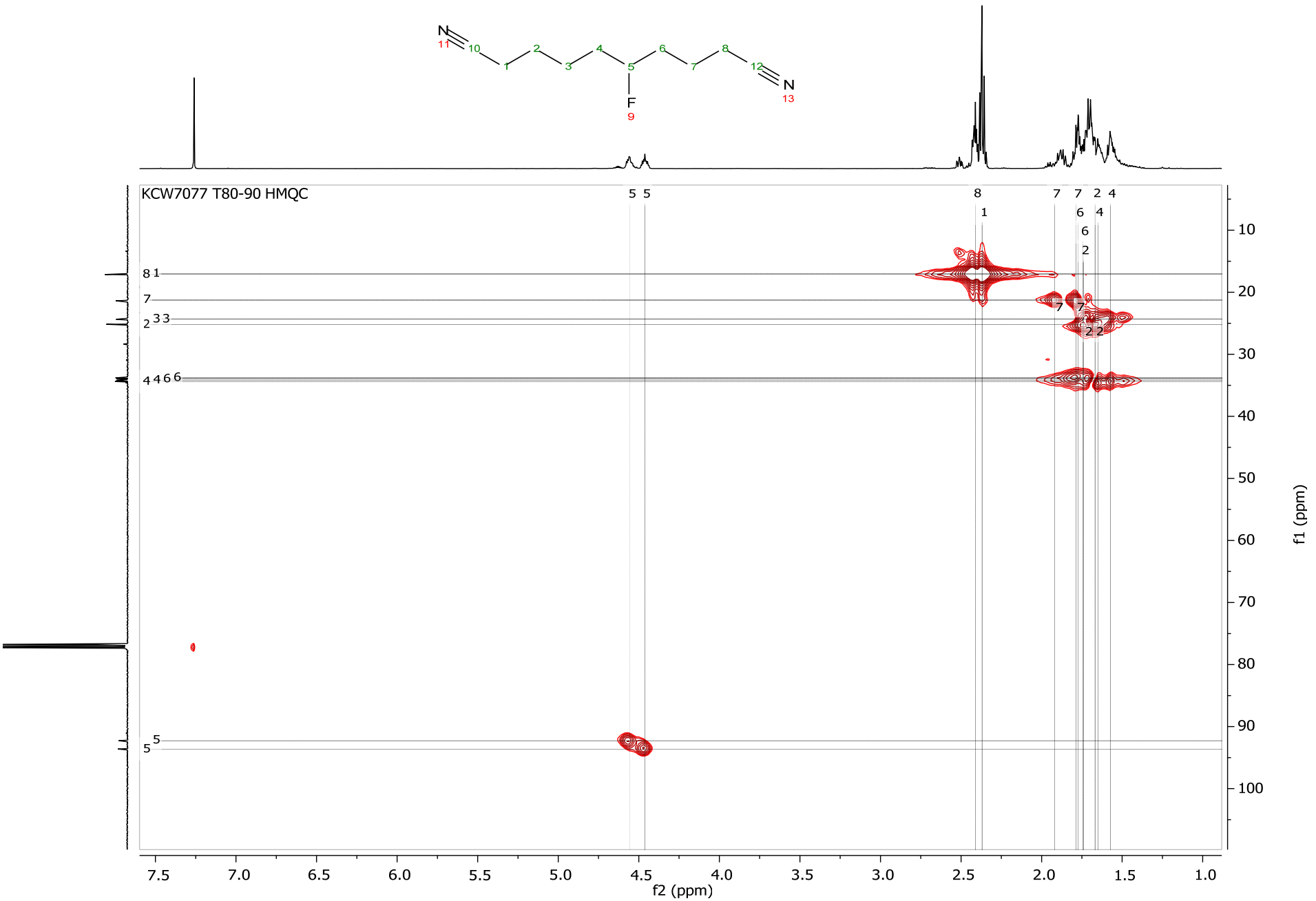
NMR Spectra of 5-fluorodecanedinitrile

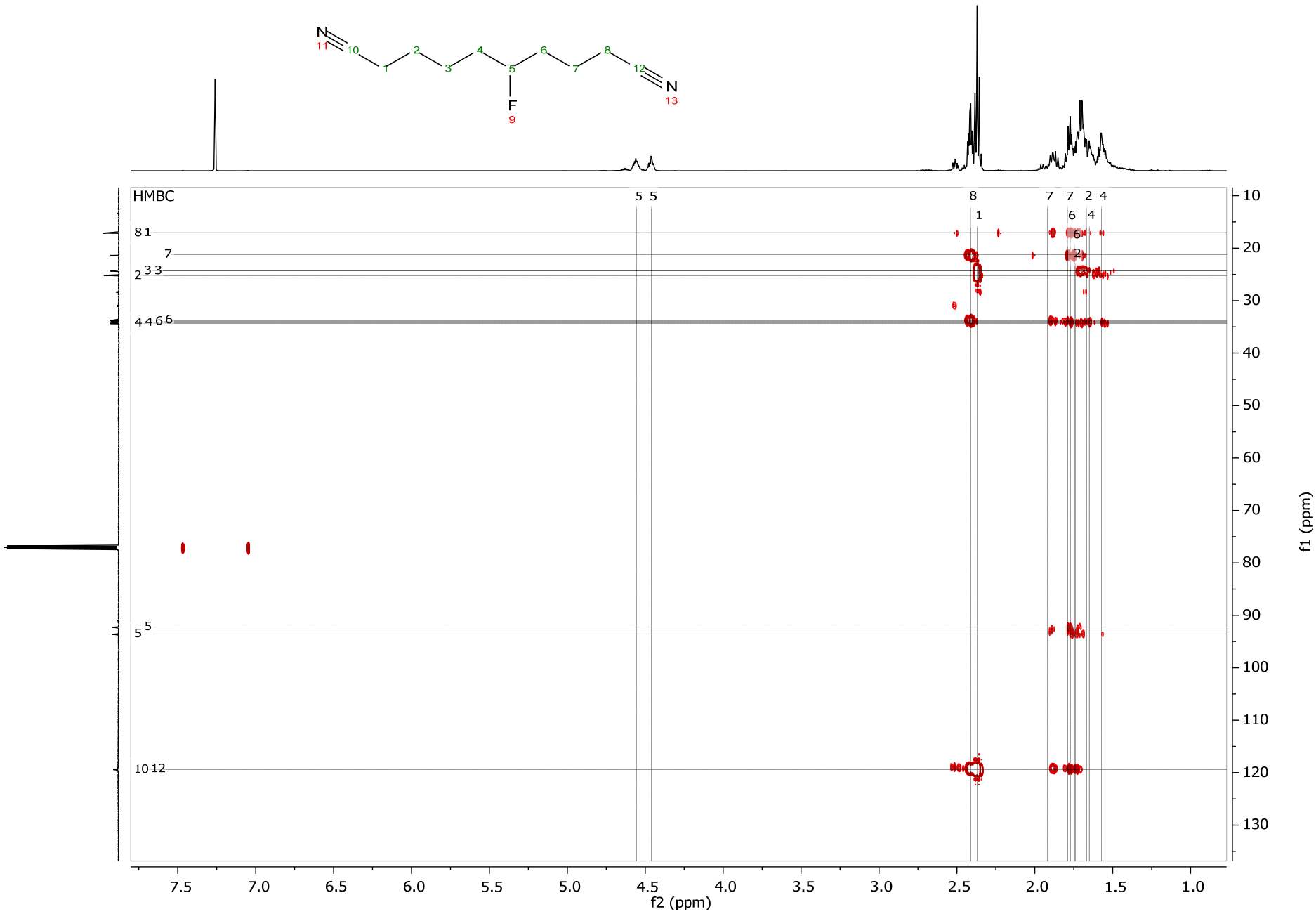



13C NMR
119.39
119.25
93.58
92.24
77.25 CDCl3
77.00 CDCl3
76.75 CDCl3
34.35
34.19
33.94
33.77
25.14
24.35
24.31
21.38
21.35
17.11
17.02
B (s)
119.39
A (s)
119.25
C (d)
92.91
H (s)
25.14
E (d)
33.85
I (s)
17.02
D (d)
34.27
F (d)
21.37
G (d)
24.33
J (s)
17.11
f1 (ppm)

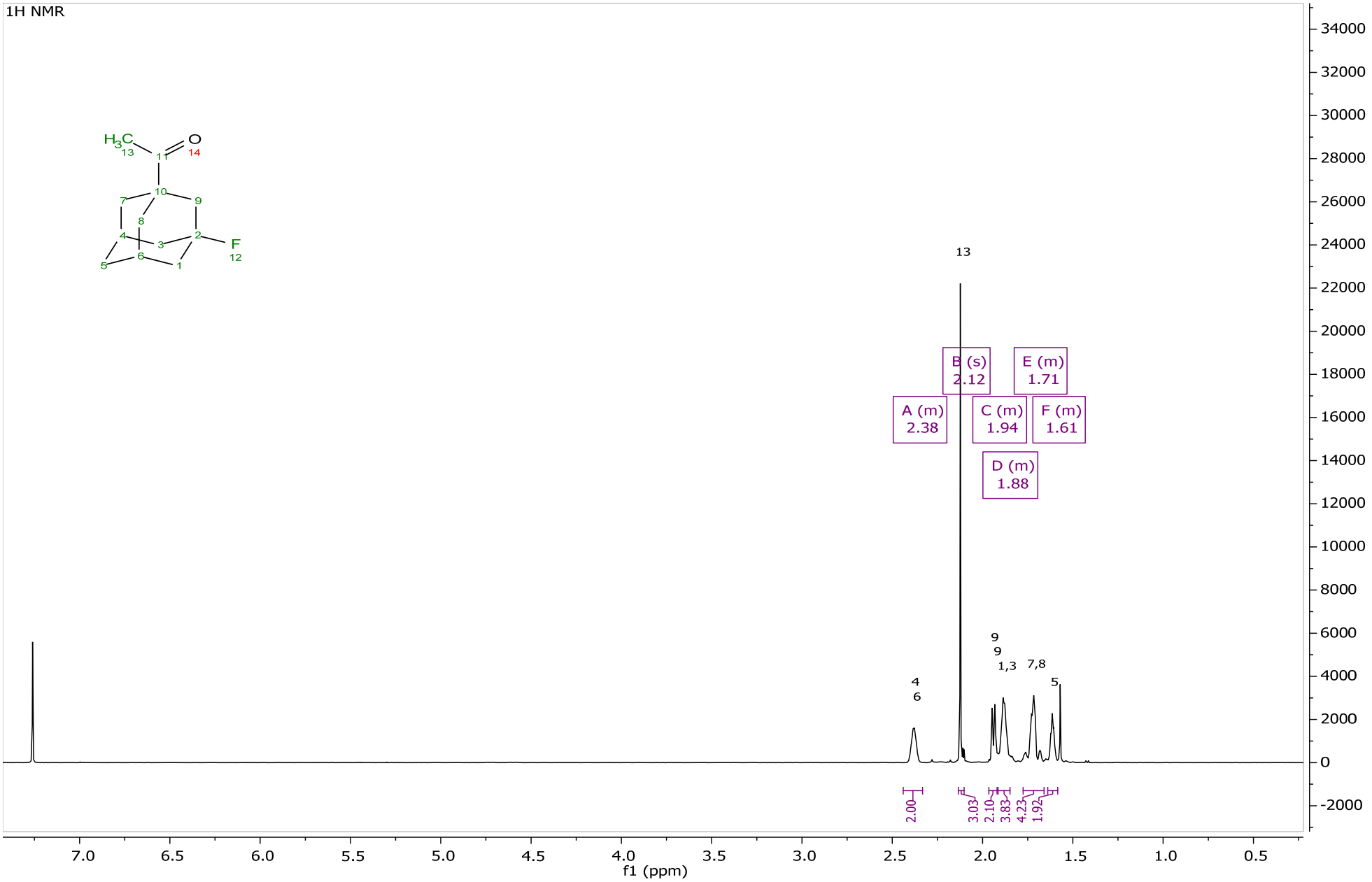

19F proton decoupled NMR
-182.49
9
56.07
f1 (ppm)

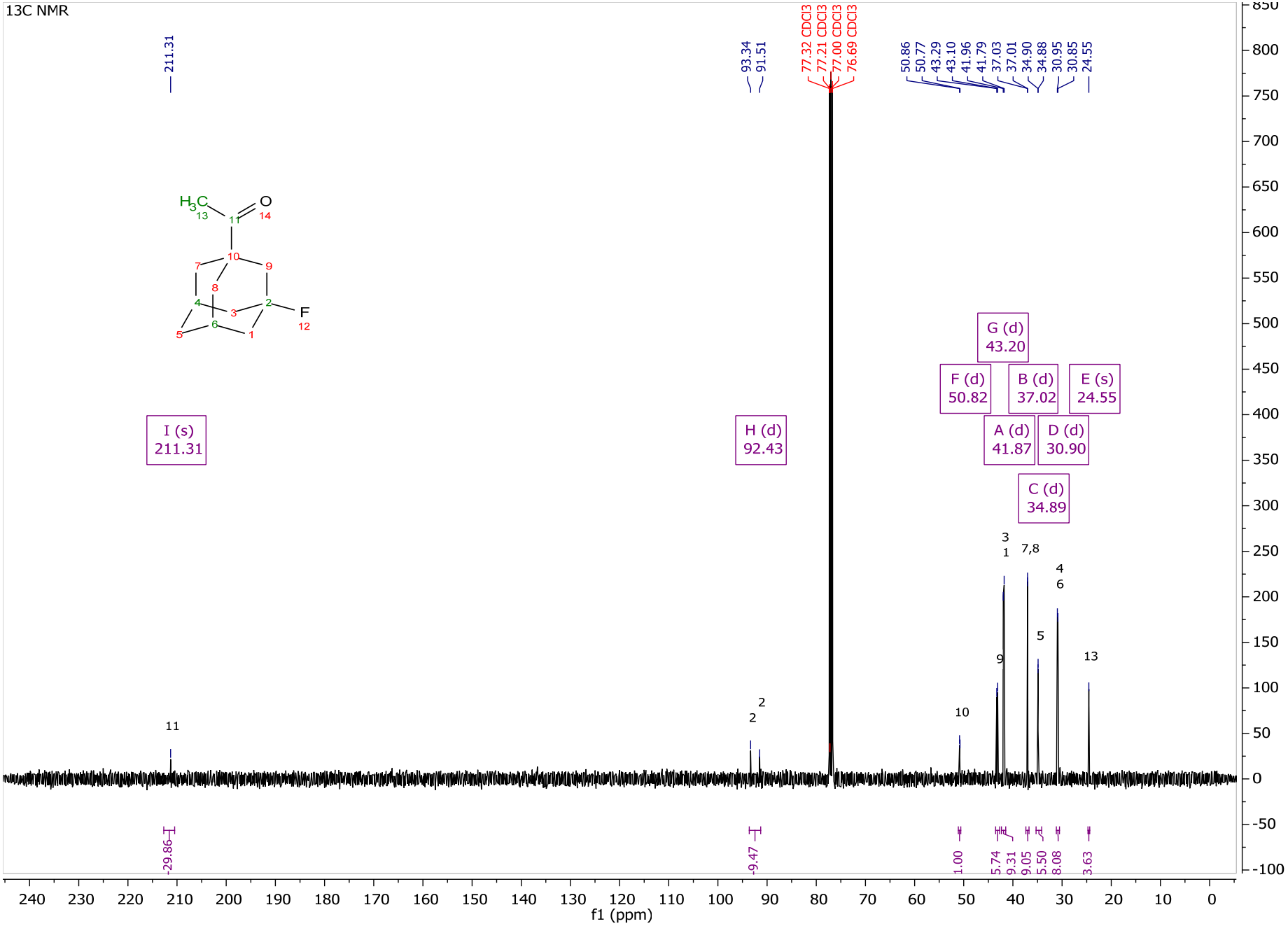

COSY
f2 (ppm)
f1 (ppm)
4.8
4.6
4.4
4.2
4.0
3.8
3.6
3.4
3.2
3.0
2.8
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.8
1.5
2.0
2.5
3.0
3.5
4.0
4.5
5.0
N
11
10
1
2
3
4
5
6
7
8
12
N
13
F
9

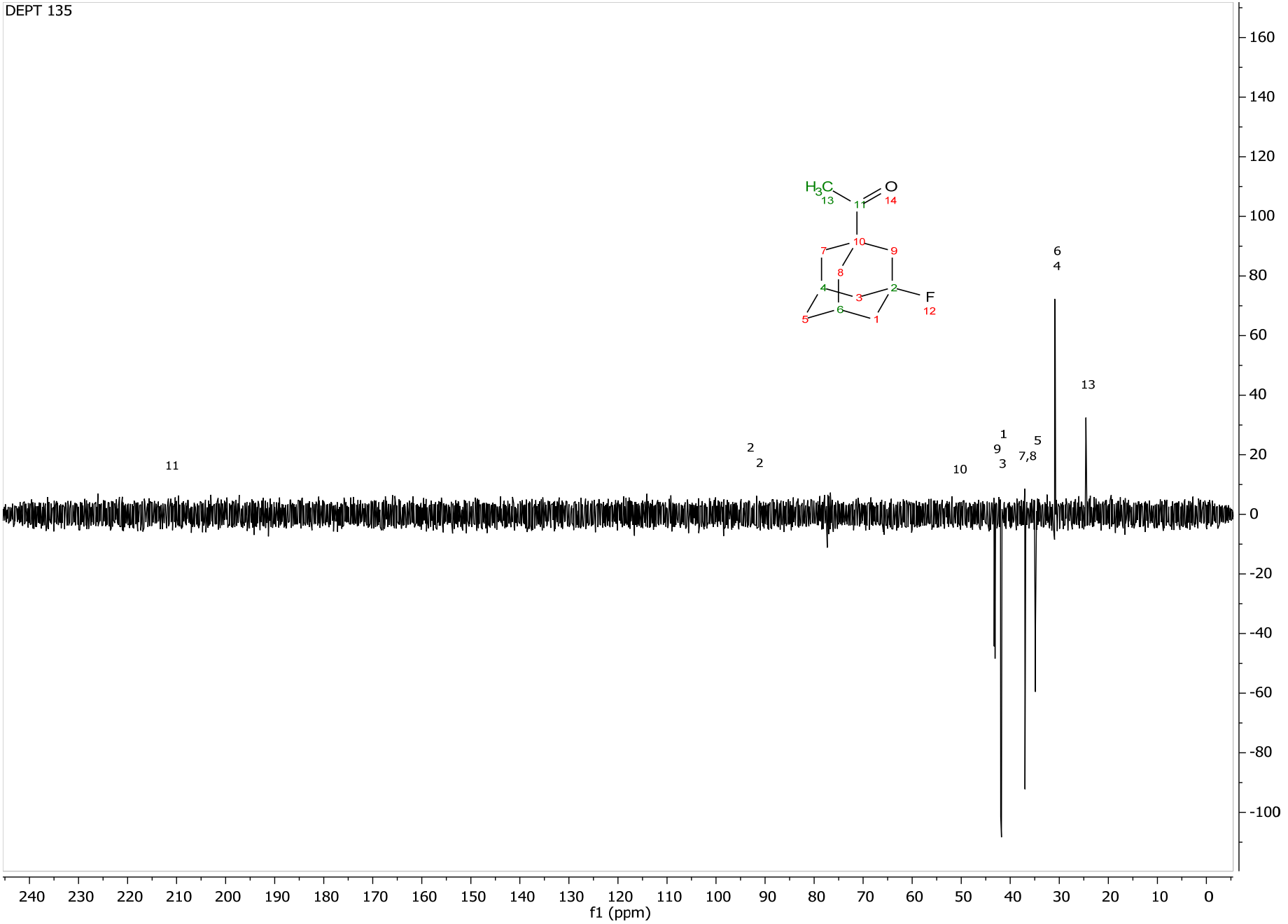

KCW7077 T80-90 HMQC
f2 (ppm)
f1 (ppm)

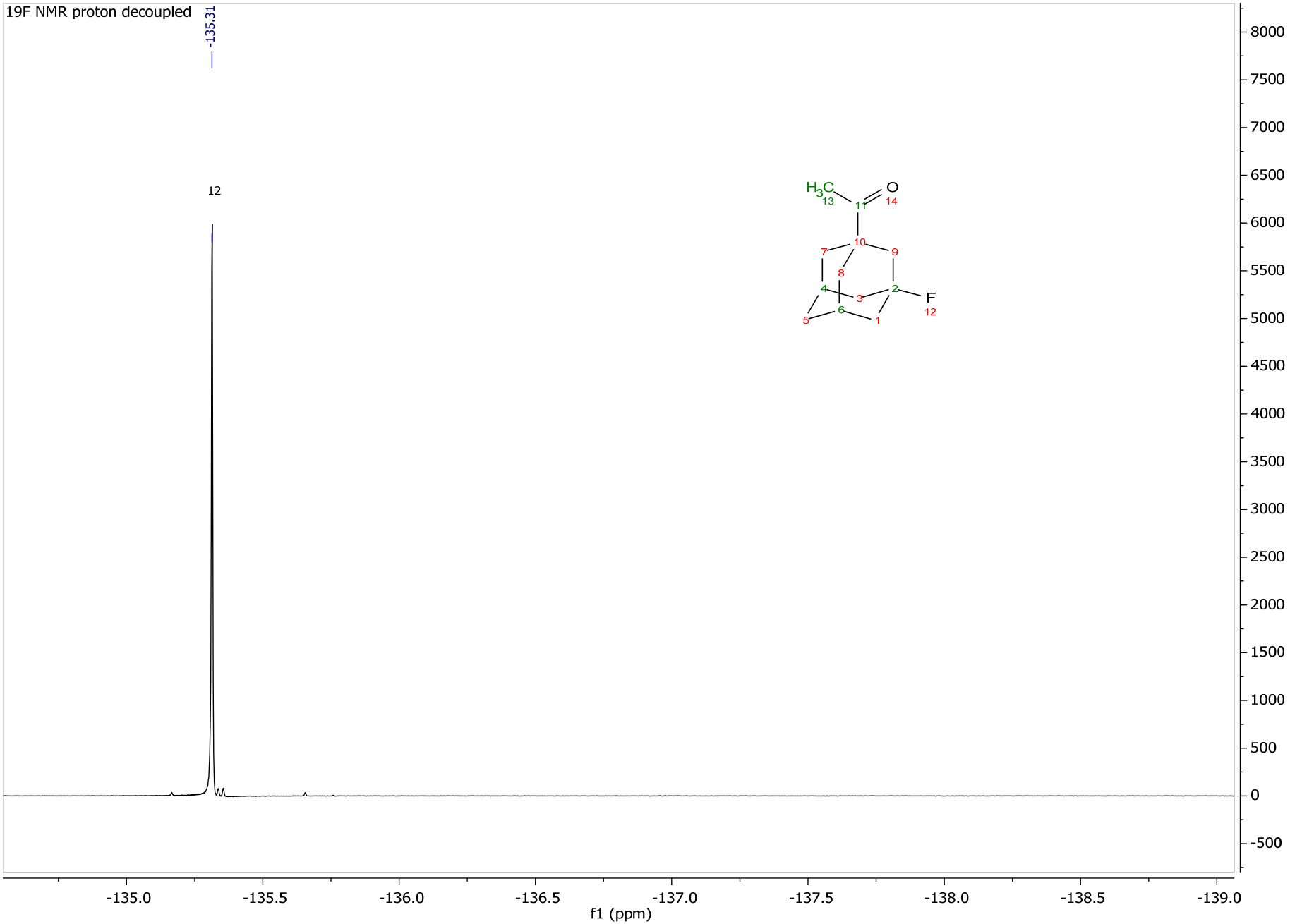

HMBC
f2 (ppm)
f1 (ppm)

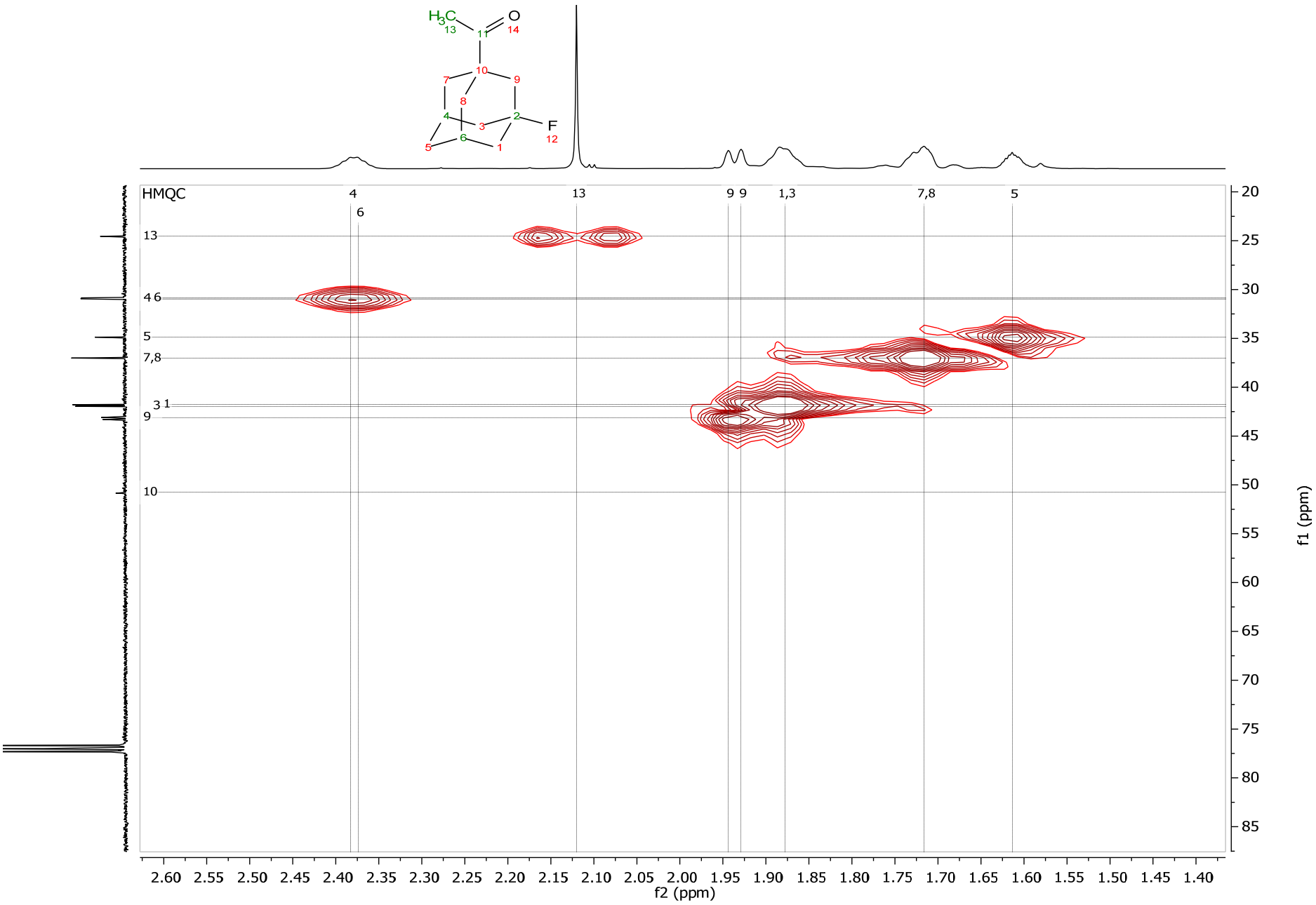
NMR Spectra of 1-((1r,3s,5R,7S)-3-fluoroadamantan-1-yl)ethan-1-one



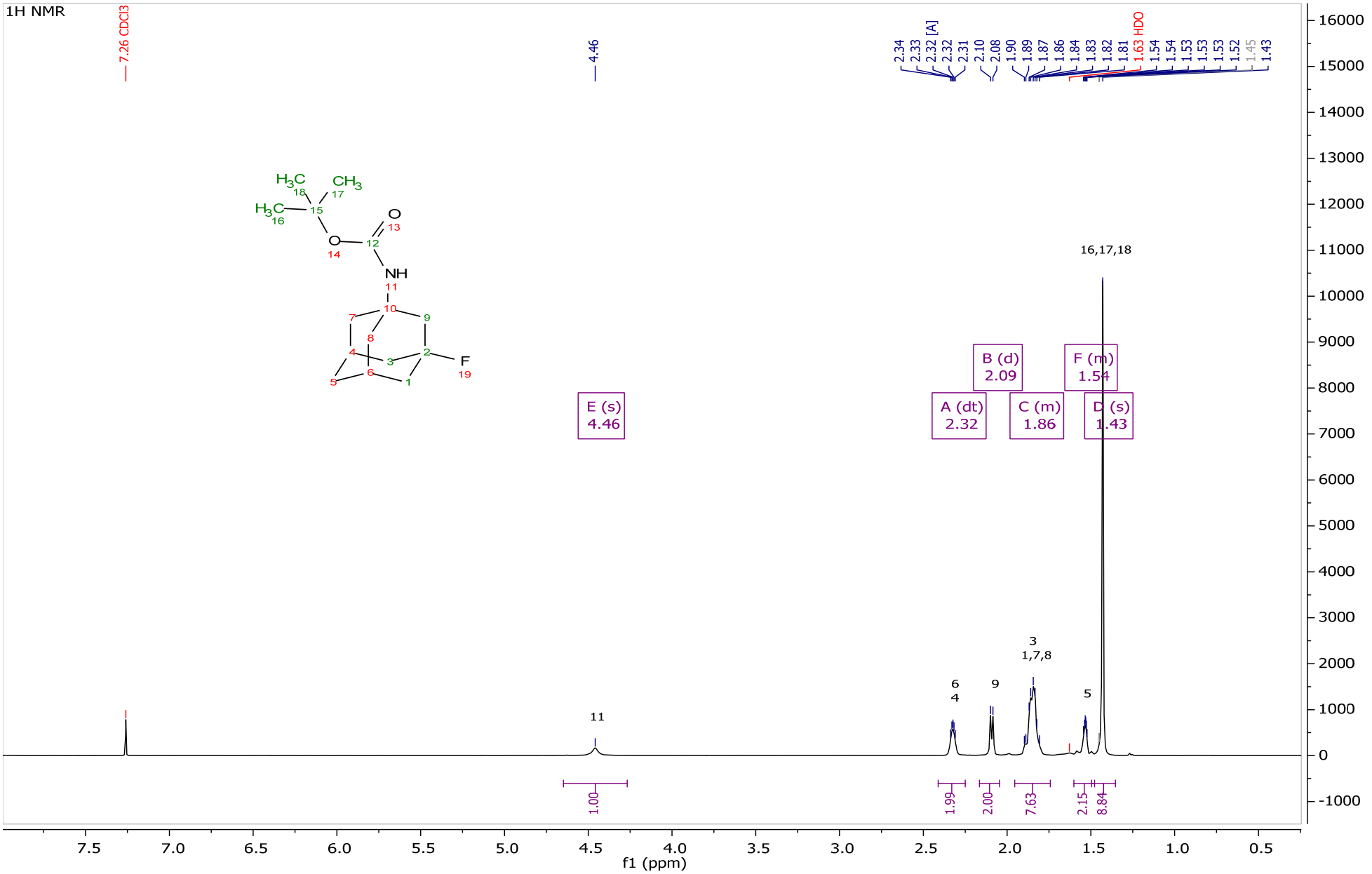

13C NMR
211.31
93.34
91.51
77.32 CDCl3
77.21 CDCl3
77.00 CDCl3
76.69 CDCl3
50.86
50.77
43.29
43.10
41.96
41.79
37.03
37.01
34.90
34.88
30.95
30.85
24.55
I (s)
211.31
H (d)
92.43
G (d)
43.20
F (d)
50.82
B (d)
37.02
E (s)
24.55
A (d)
41.87
D (d)
30.90
C (d)
34.89
f1 (ppm)

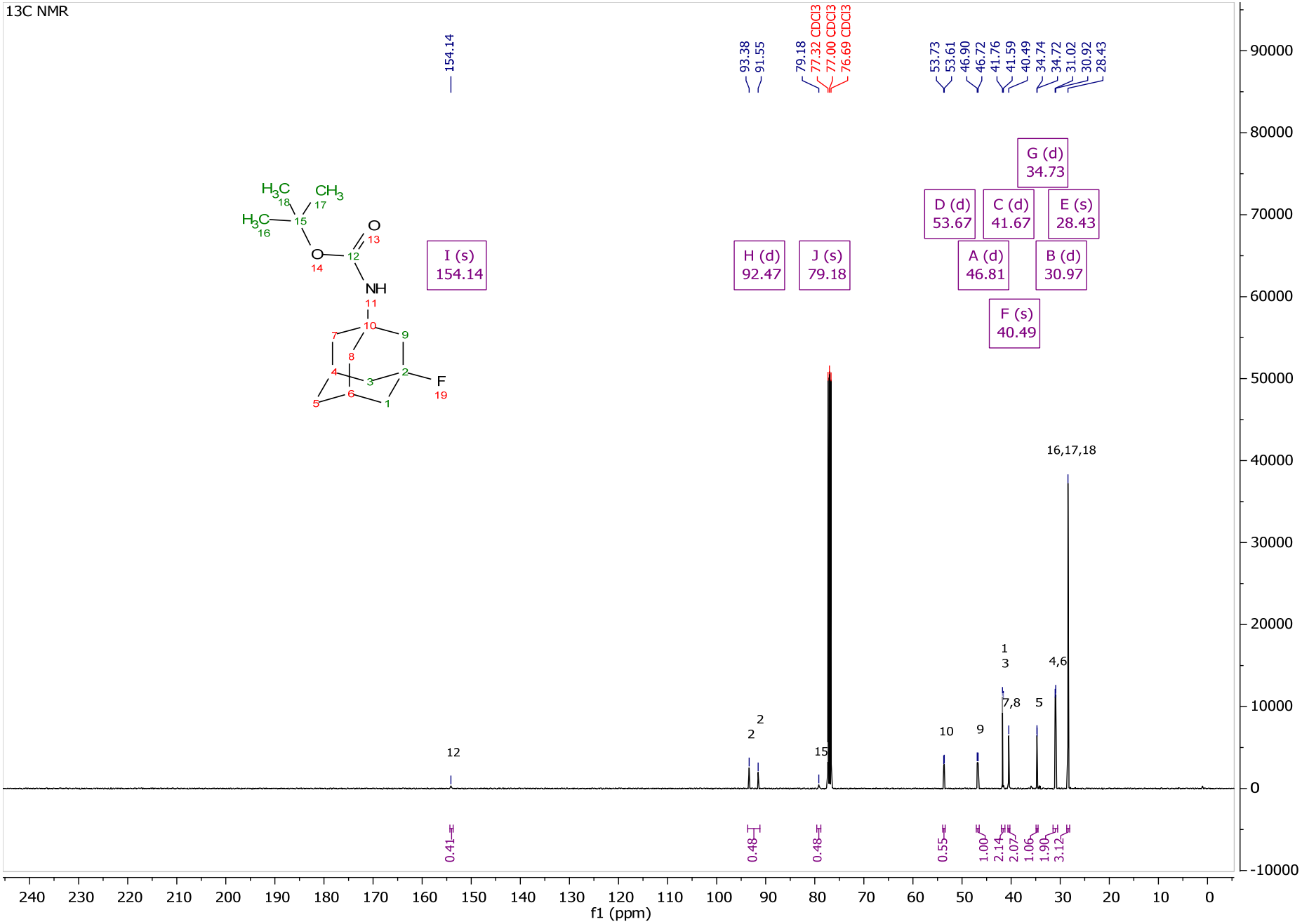

DEPT 135
H3C
13
11
O
14
10
7
9
8
4
3
2
F
12
5
6
1
11
2
2
10
1
9
3
7,8
5
6
4
13
160
140
120
100
80
60
40
20
0
-20
-40
-60
-80
-100
240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

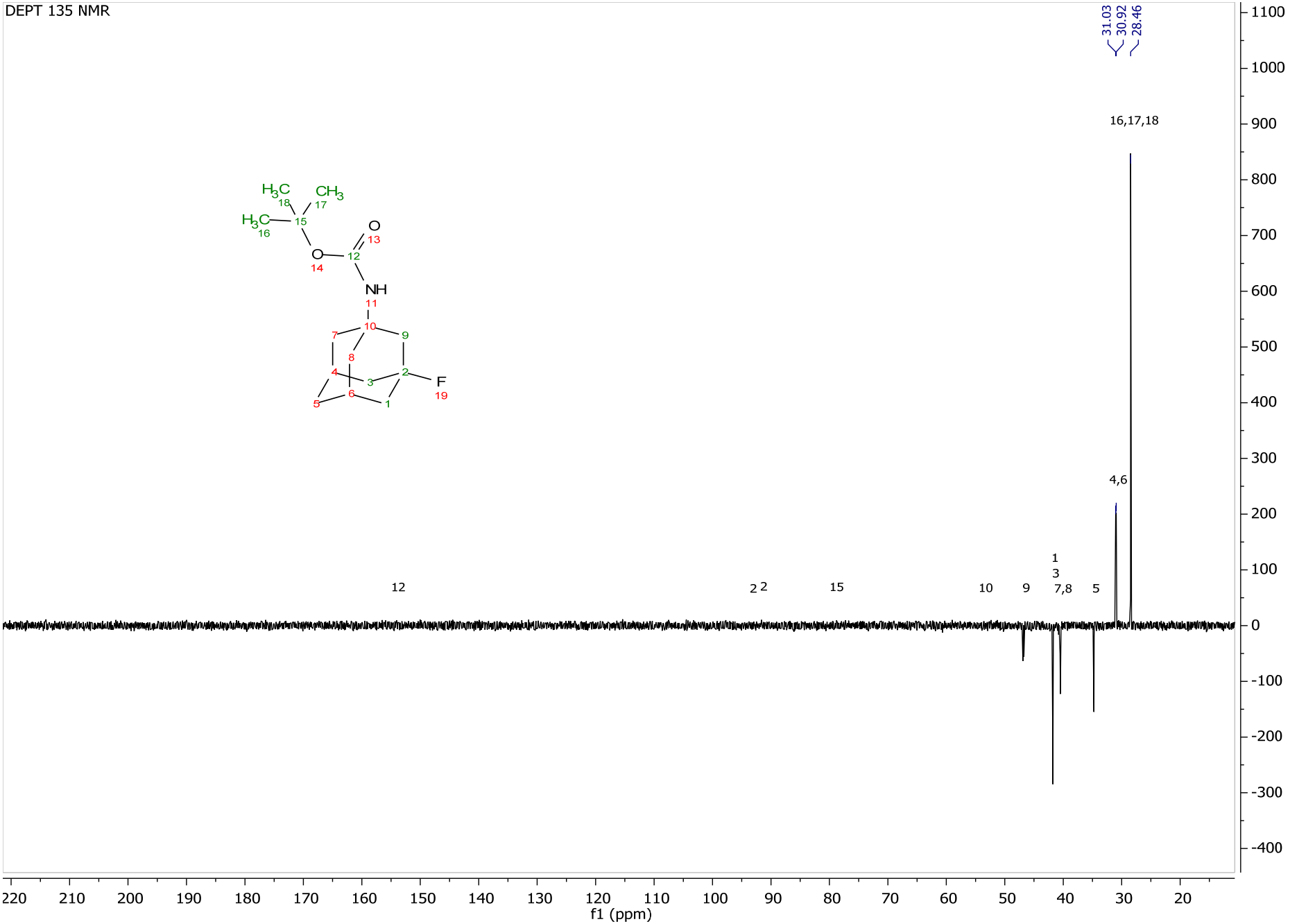

19F NMR proton decoupled
-135.31
12
H3C
13
11
O
14
10
7
9
8
4
2
3
F
12
5
6
1
8000
7500
7000
6500
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
-135.0
-135.5
-136.0
-136.5
-137.0
-137.5
-138.0
-138.5
-139.0
f1 (ppm)

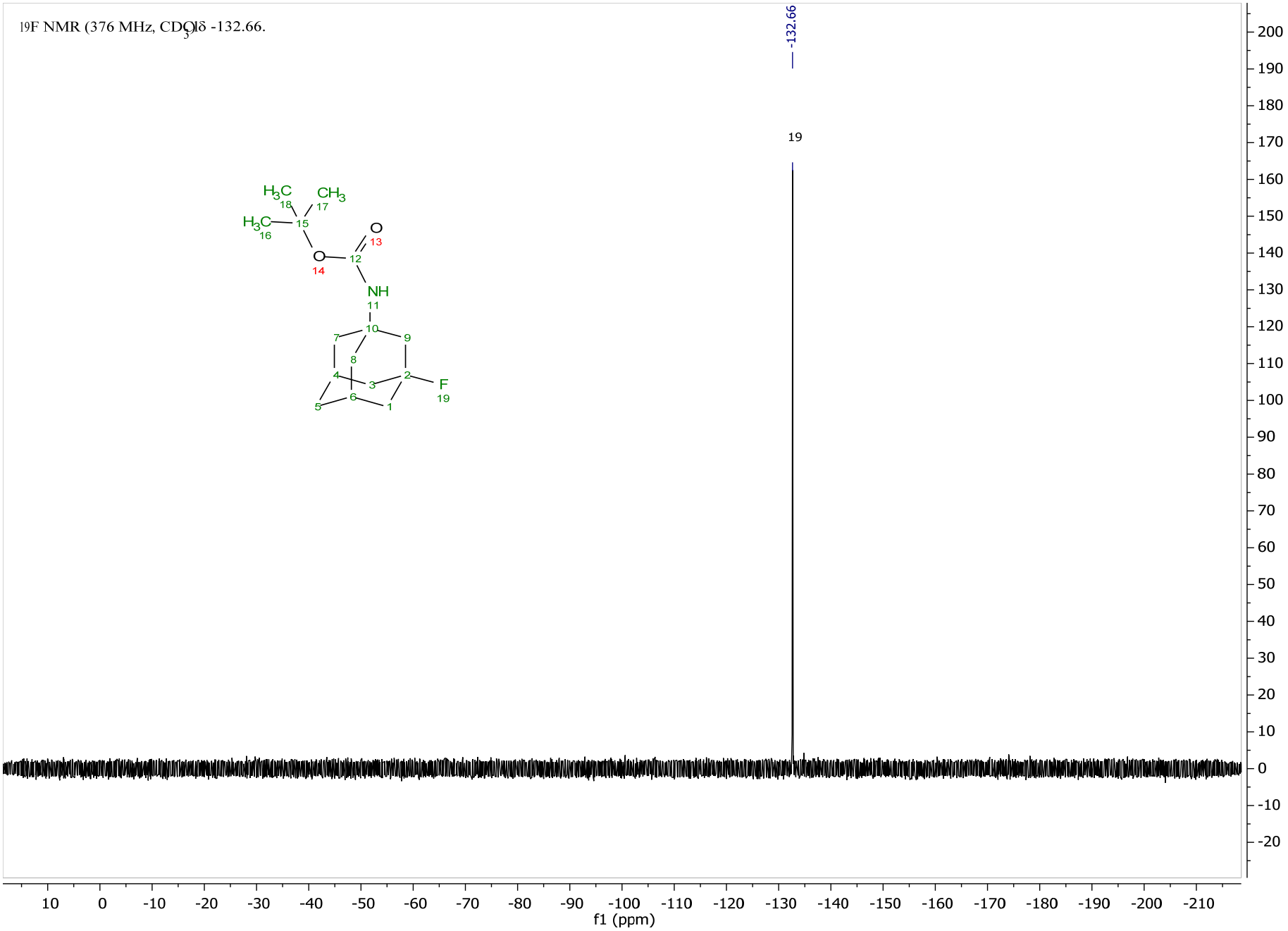

HMQC
f2 (ppm)
f1 (ppm)

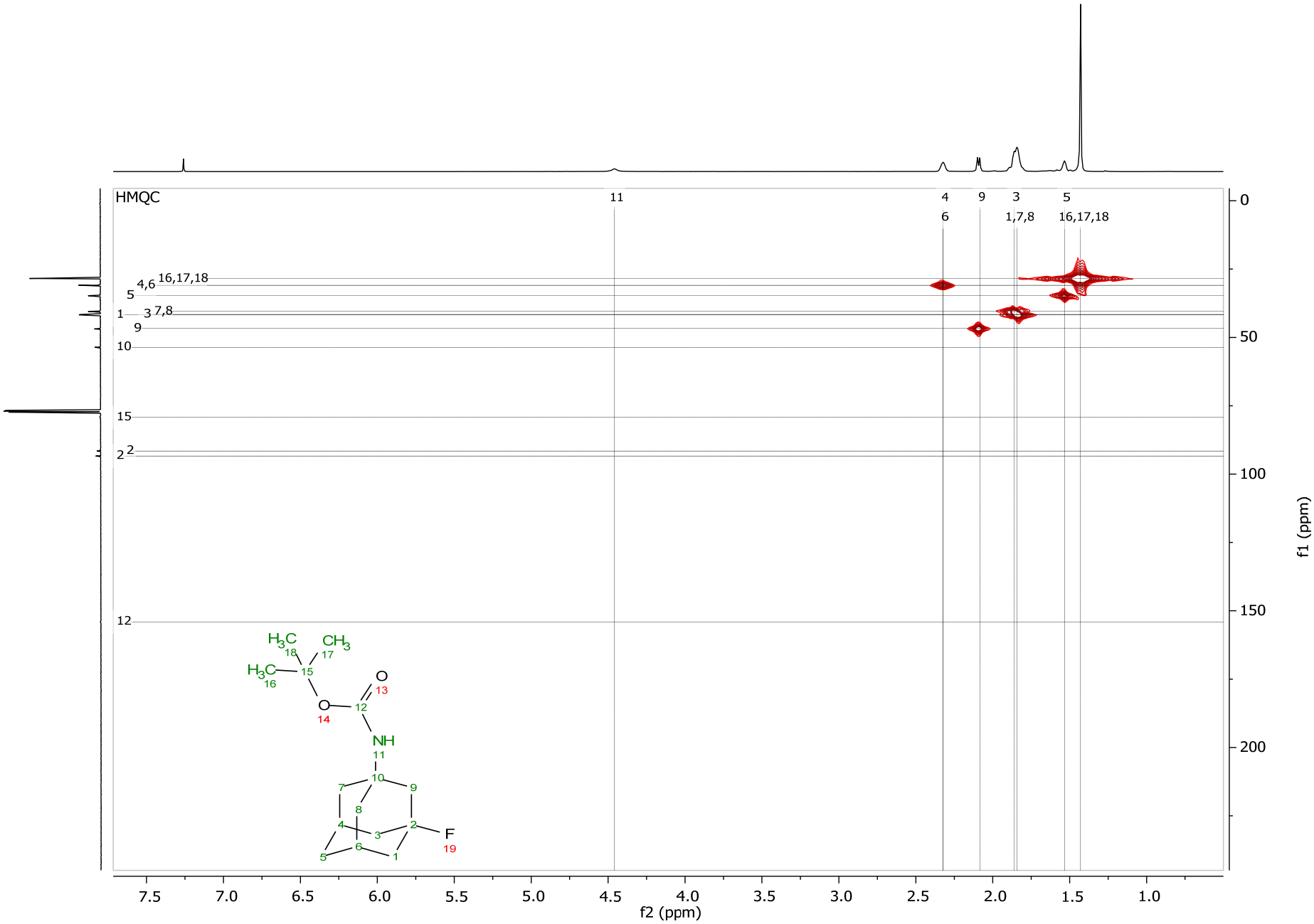
NMR Spectra of tert-butyl ((1r,3s,5R,7S)-3-fluoroadamantan-1-yl)carbamate

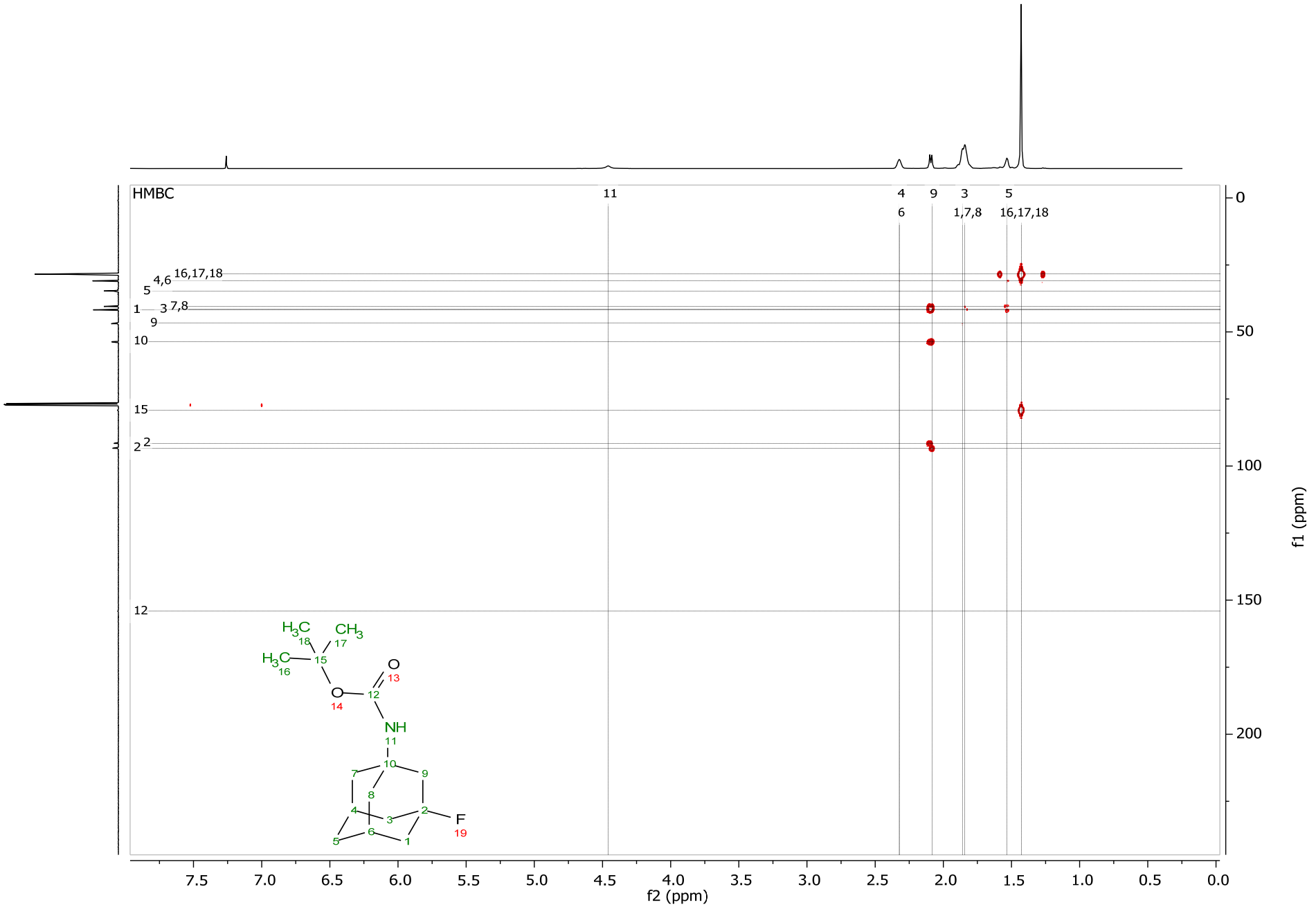



13C NMR
154.14
93.38
91.55
79.18
77.32 CDCl3
77.00 CDCl3
76.69 CDCl3
53.73
53.61
46.90
46.72
41.76
41.59
40.49
34.74
34.72
31.02
30.92
28.43
I (s) 154.14
H (d) 92.47
J (s) 79.18
G (d) 34.73
D (d) 53.67
C (d) 41.67
E (s) 28.43
A (d) 46.81
B (d) 30.97
F (s) 40.49
16,17,18
4,6
1
3
7,8
5
10
9
2
2
12
15
0.41
0.48
0.48
0.55
1.00
2.14
2.07
1.06
1.90
3.12
f1 (ppm)

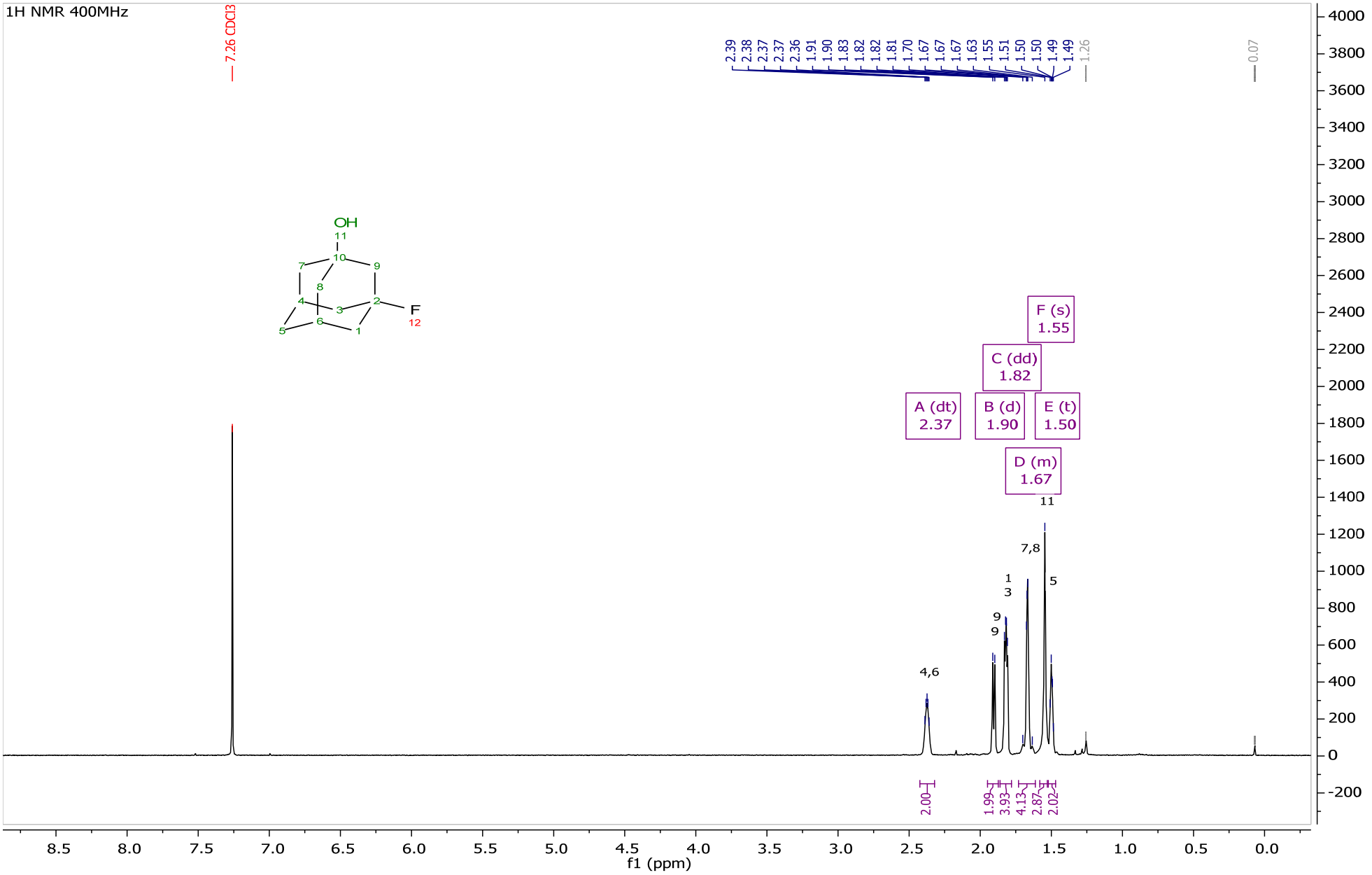

DEPT 135 NMR
31.03
30.92
28.46
16,17,18
4,6
12
2
2
15
10
9
1
3
7,8
5
f1 (ppm)

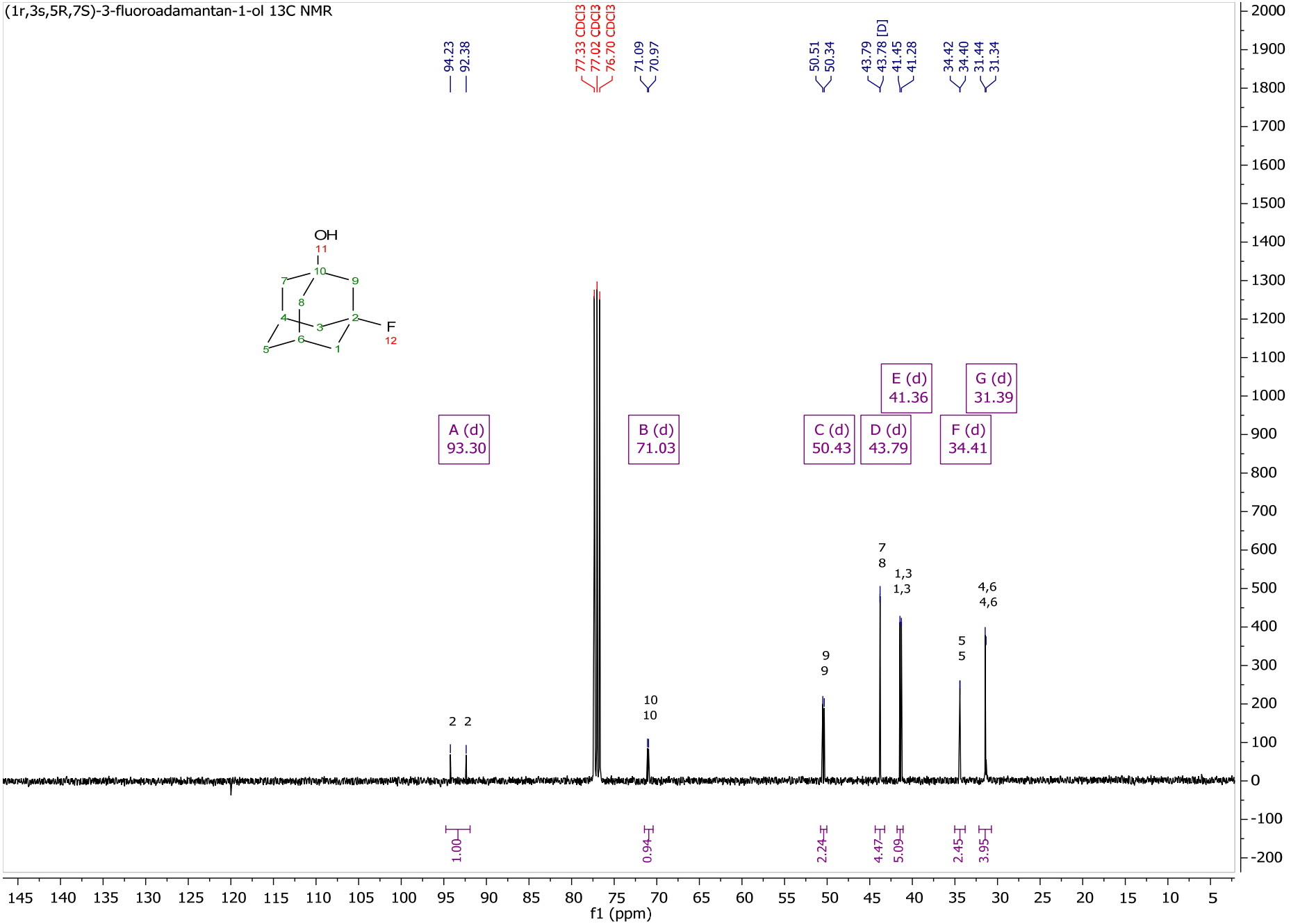

19F NMR (376 MHz, CDCl3) δ -132.66.
-132.66
19
H3C
CH3
18
17
H3C
16
15
O
13
O
14
12
NH
11
10
7
9
8
4
3
2
F
19
5
6
1
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
-20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

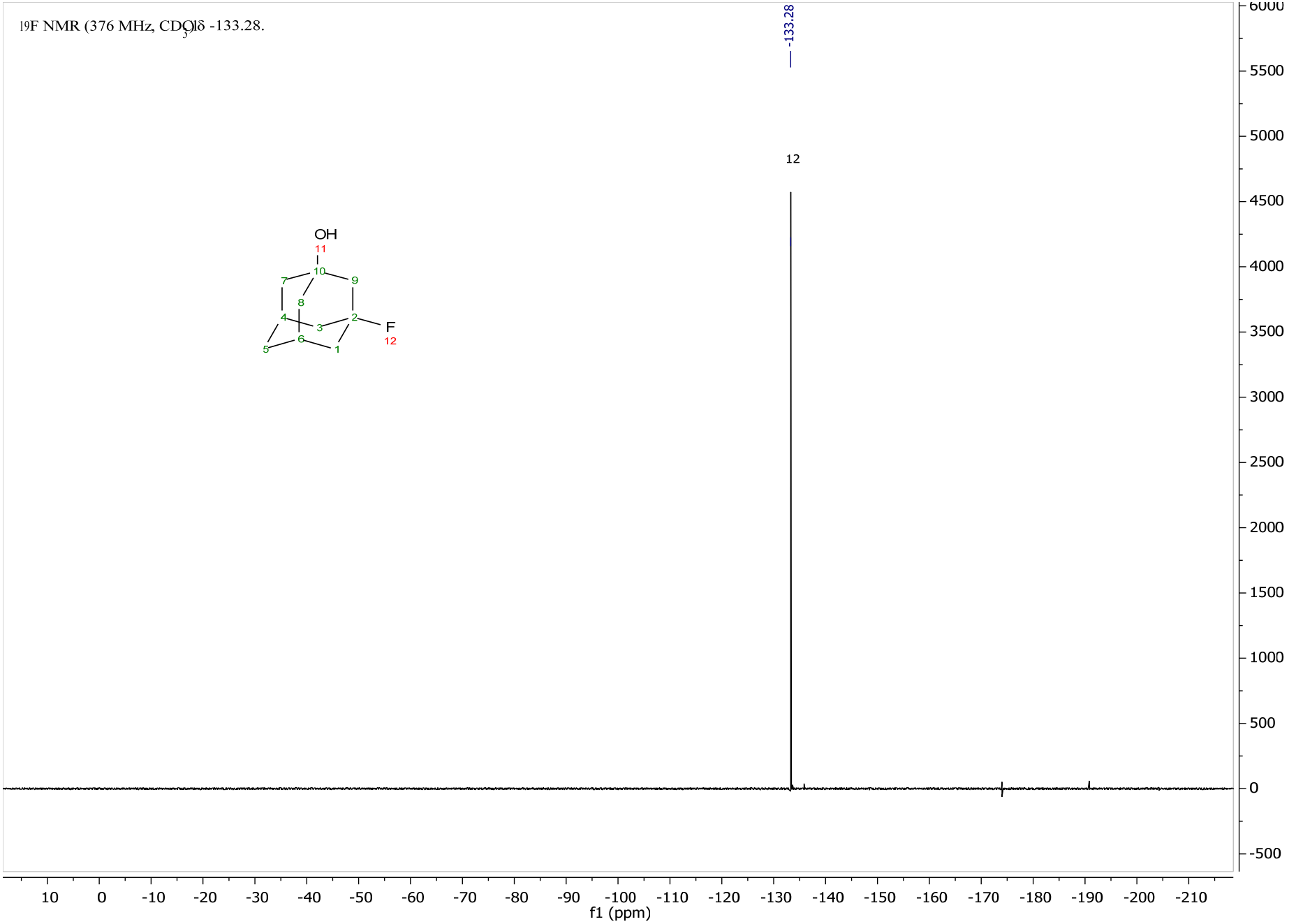

HMQC
11
4
6
9
3
1,7,8
5
16,17,18
4,6
16,17,18
5
1
3
7,8
9
10
15
2
2
12
0
50
100
150
200
f1 (ppm)
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
f2 (ppm)
H3C
18
CH3
17
H3C
16
15
O
13
O
12
14
NH
11
10
7
9
8
4
3
2
F
19
5
6
1

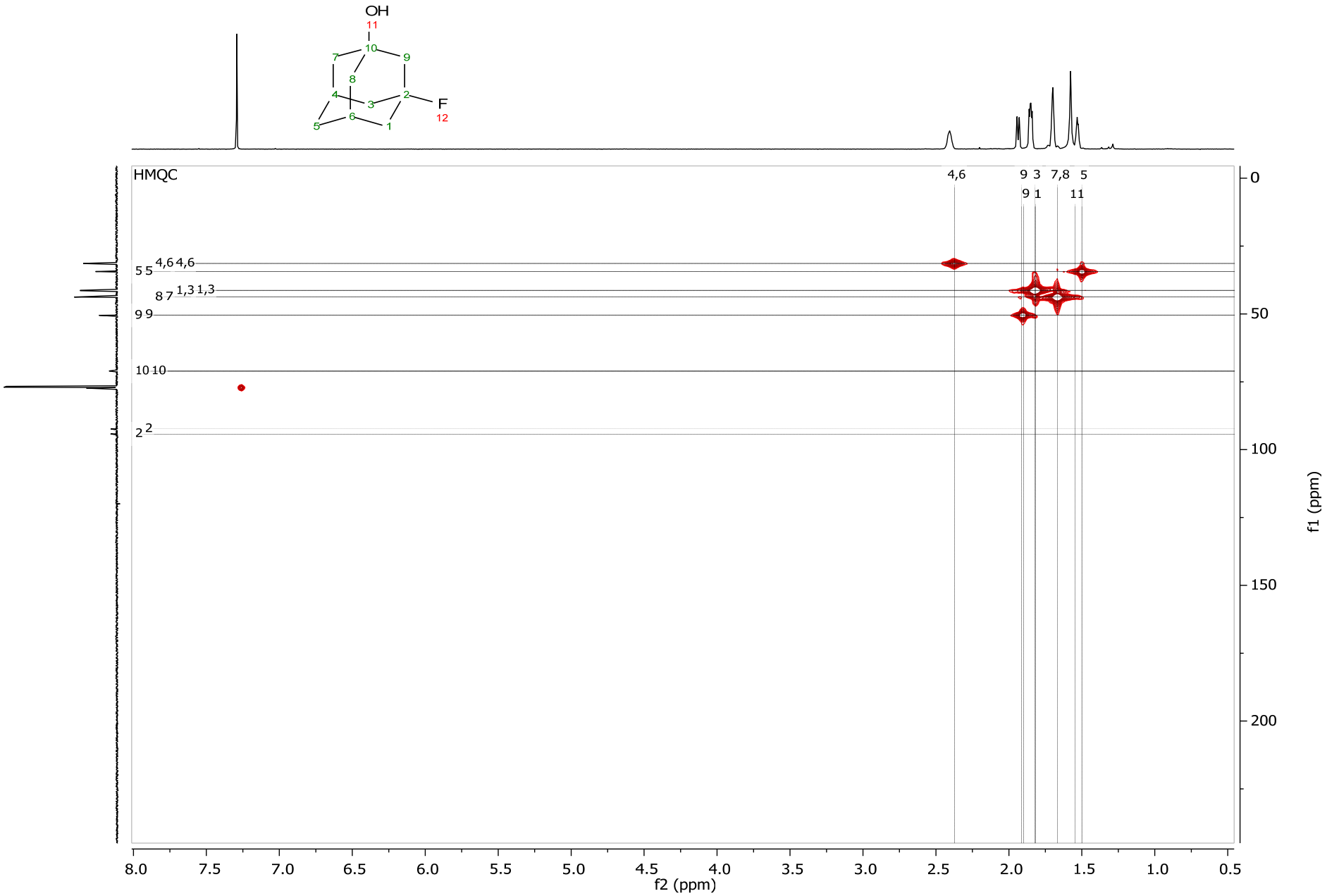

HMBC
11
4
6
9
3
1,7,8
5
16,17,18
4,6
16,17,18
5
1
3
7,8
9
10
15
2
2
12
H3C
18
CH3
17
H3C
16
15
O
13
O
14
12
NH
11
10
9
7
8
4
3
2
F
19
5
6
1
0
50
100
150
200
f1 (ppm)
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f2 (ppm)

NMR Spectra of (1r,3s,5R,7S)-3-fluoroadamantan-1-ol

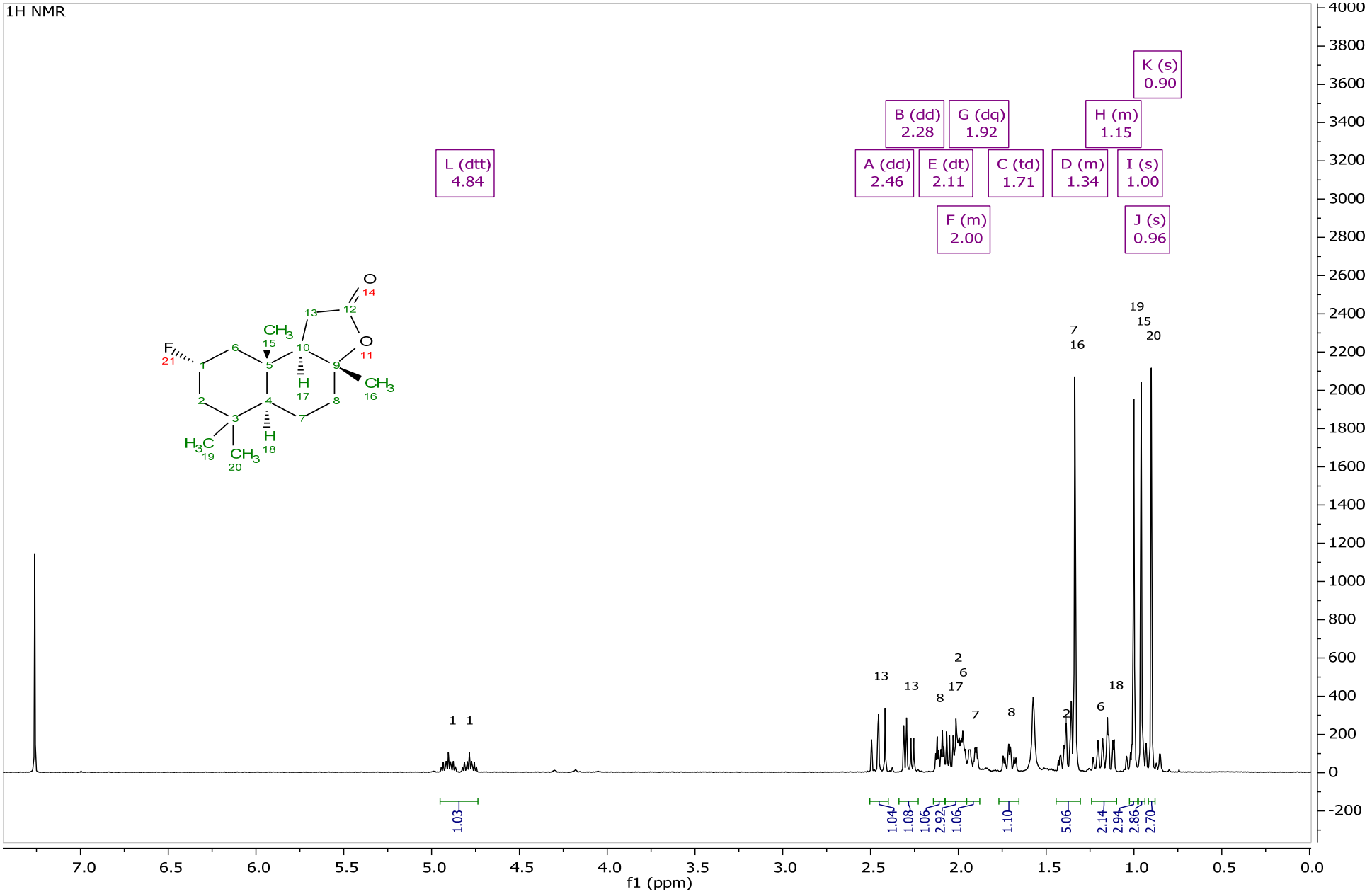


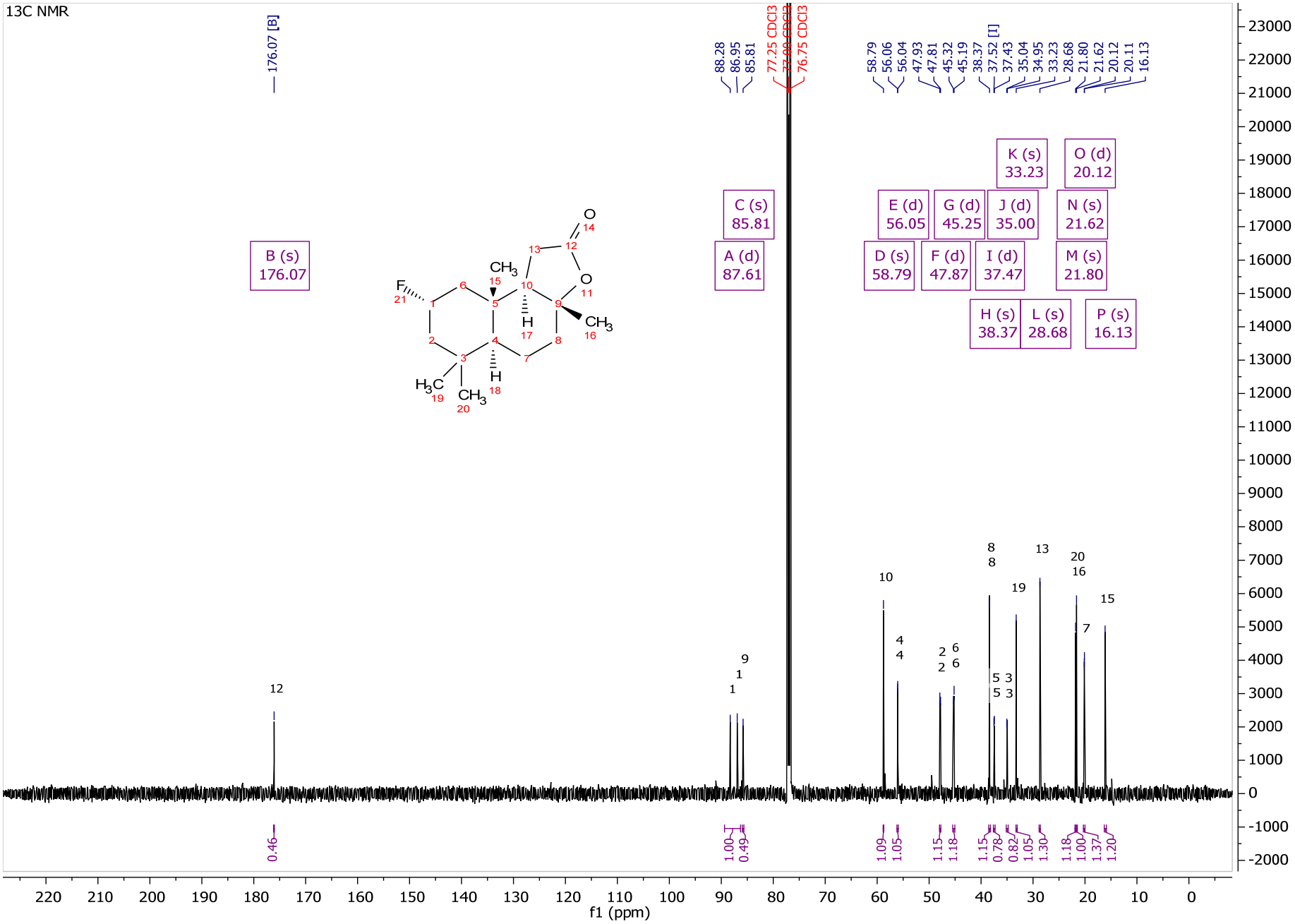

(1r,3s,5R,7S)-3-fluoroadamantan-1-ol 13C NMR
94.23
92.38
77.33 CDCl3
77.02 CDCl3
76.70 CDCl3
71.09
70.97
50.51
50.34
43.79
43.78 [D]
41.45
41.28
34.42
34.40
31.44
31.34
OH
11
F
12
A (d)
93.30
B (d)
71.03
C (d)
50.43
D (d)
43.79
E (d)
41.36
F (d)
34.41
G (d)
31.39
2 2
10
10
9
9
7
8
1,3
1,3
5
5
4,6
4,6
1.00
0.94
2.24
4.47
5.09
2.45
3.95
f1 (ppm)

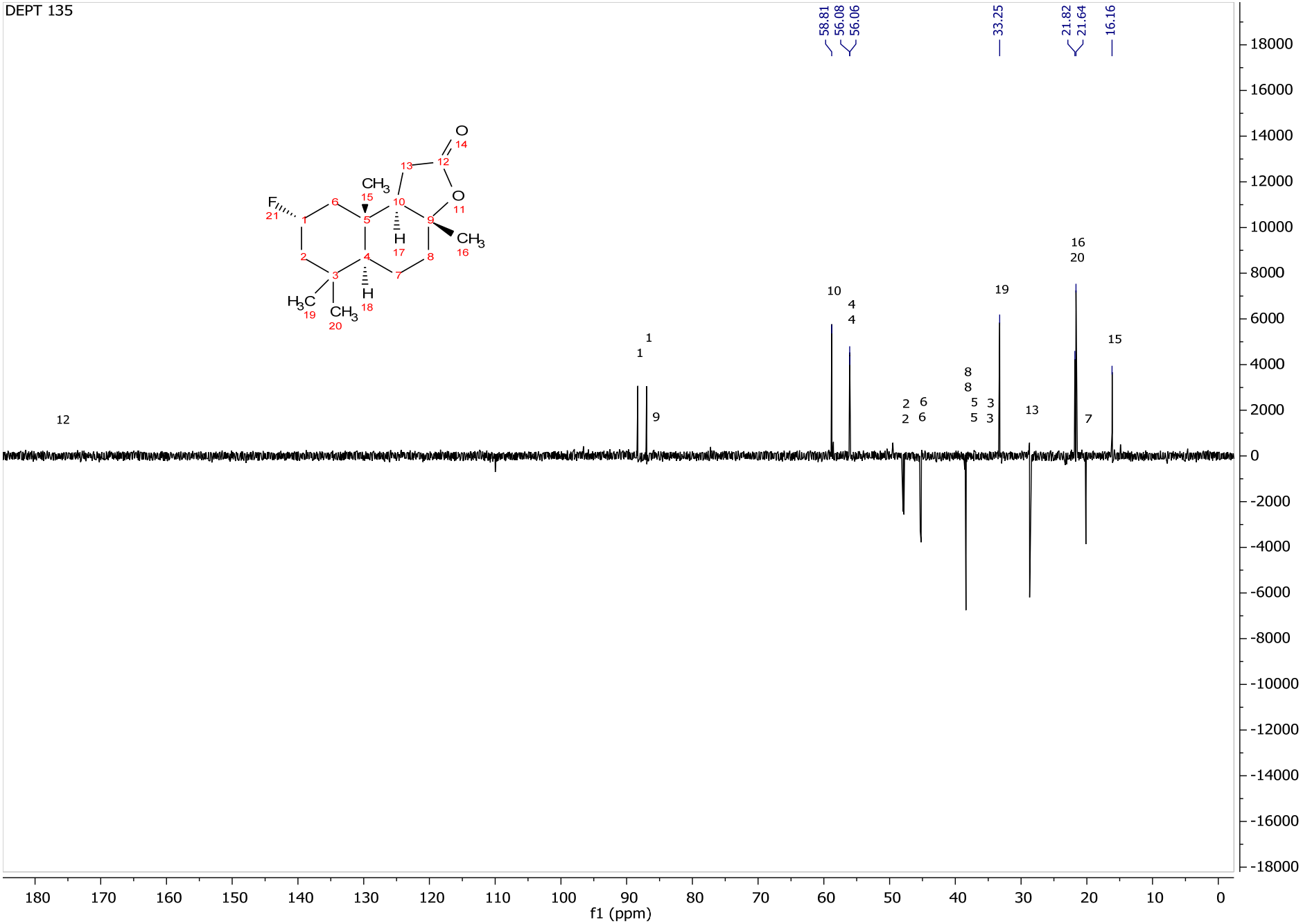

19F NMR (376 MHz, CDCl3) δ -133.28.
-133.28
12
OH
11
10
9
7
8
4
3
2
F
12
6
5
1
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

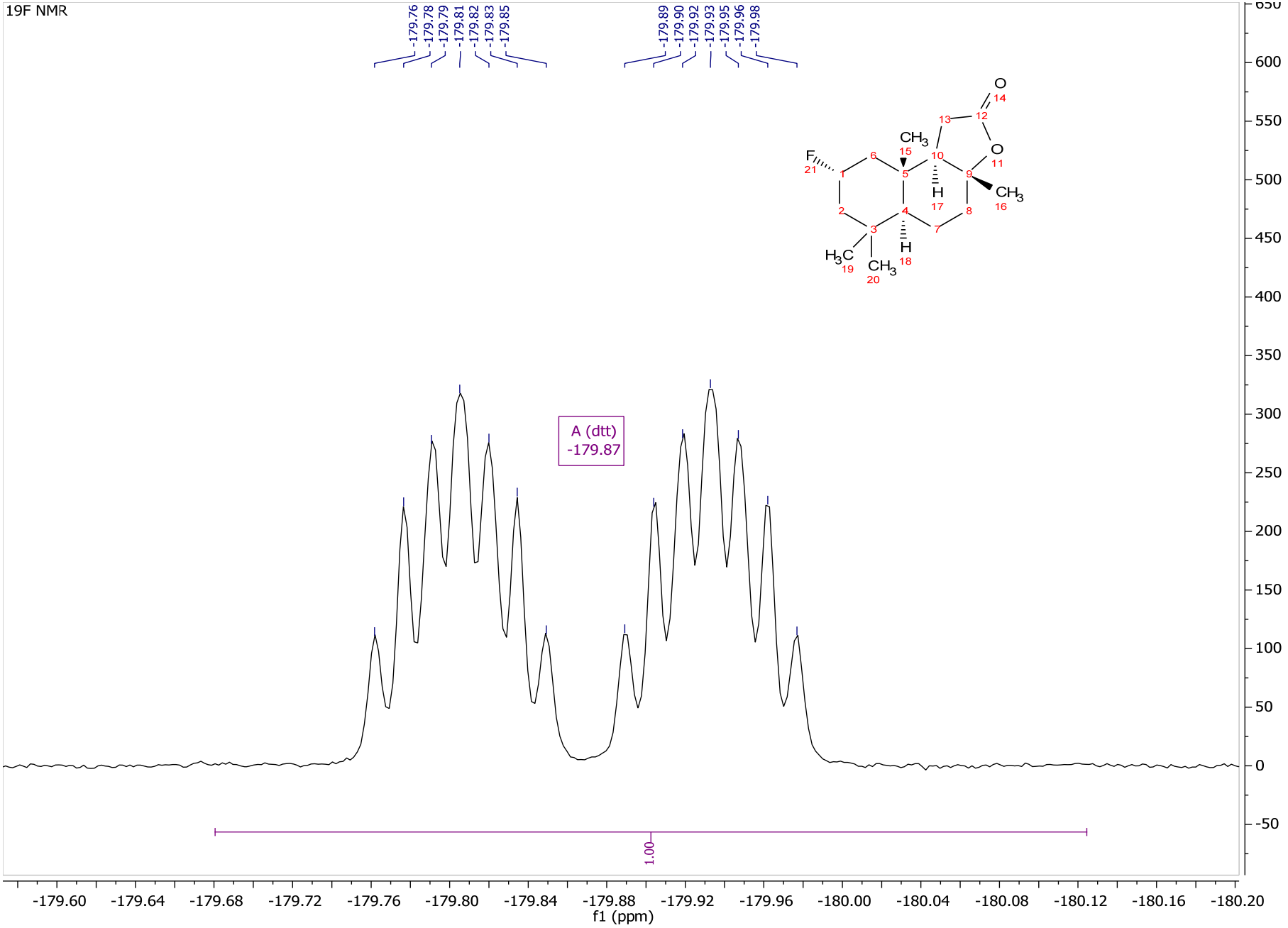

OH
11
10
7
9
8
4
2
3
F
12
5
6
1
HMQC
4,6
9 3
9 1
7,8
5
11
5 5
4,6 4,6
8 7
1,3 1,3
9 9
10 10
2 2
0
50
100
150
200
f1 (ppm)
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f2 (ppm)

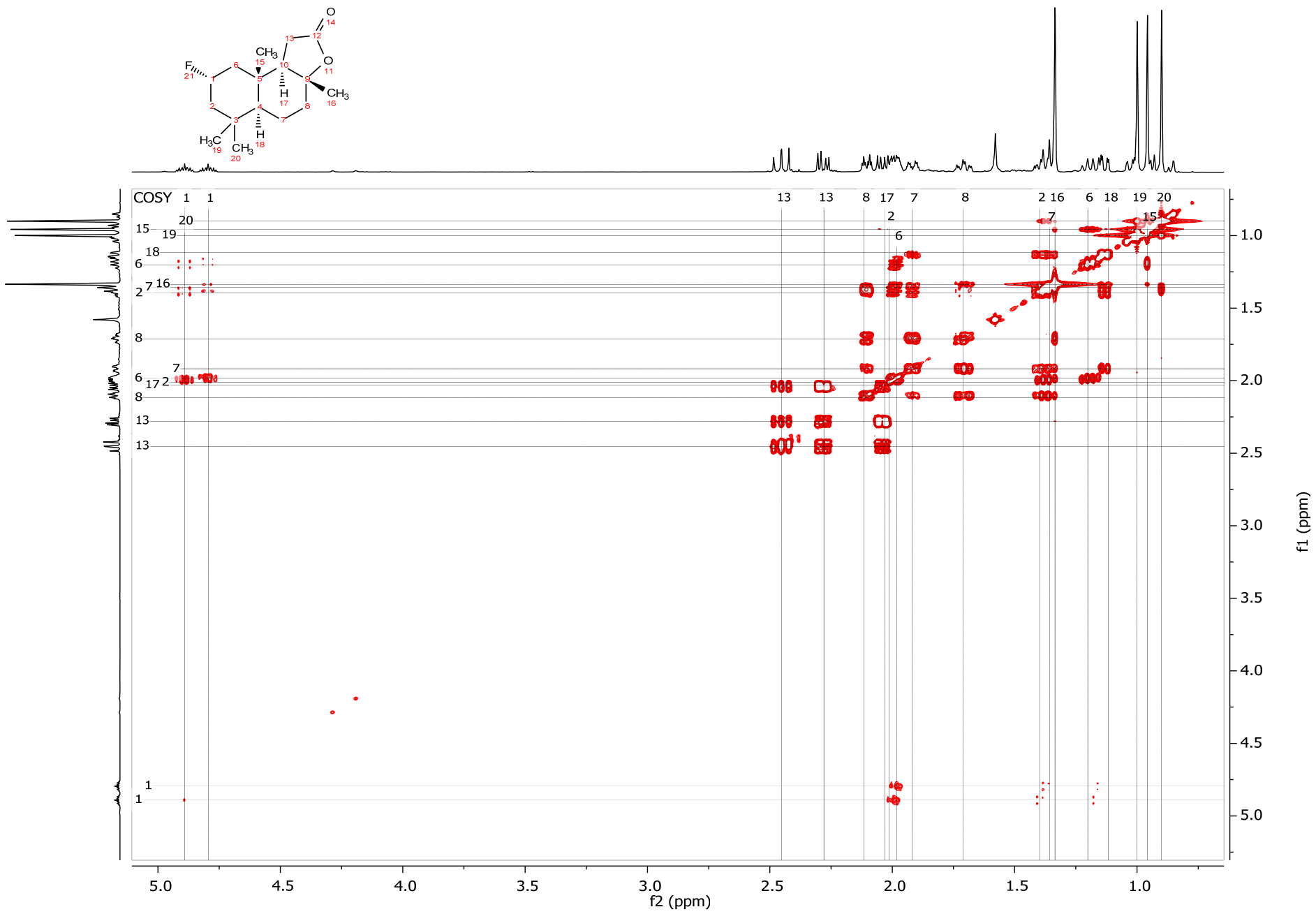
NMR Spectra of Fluorinated (+)-Sclareolide

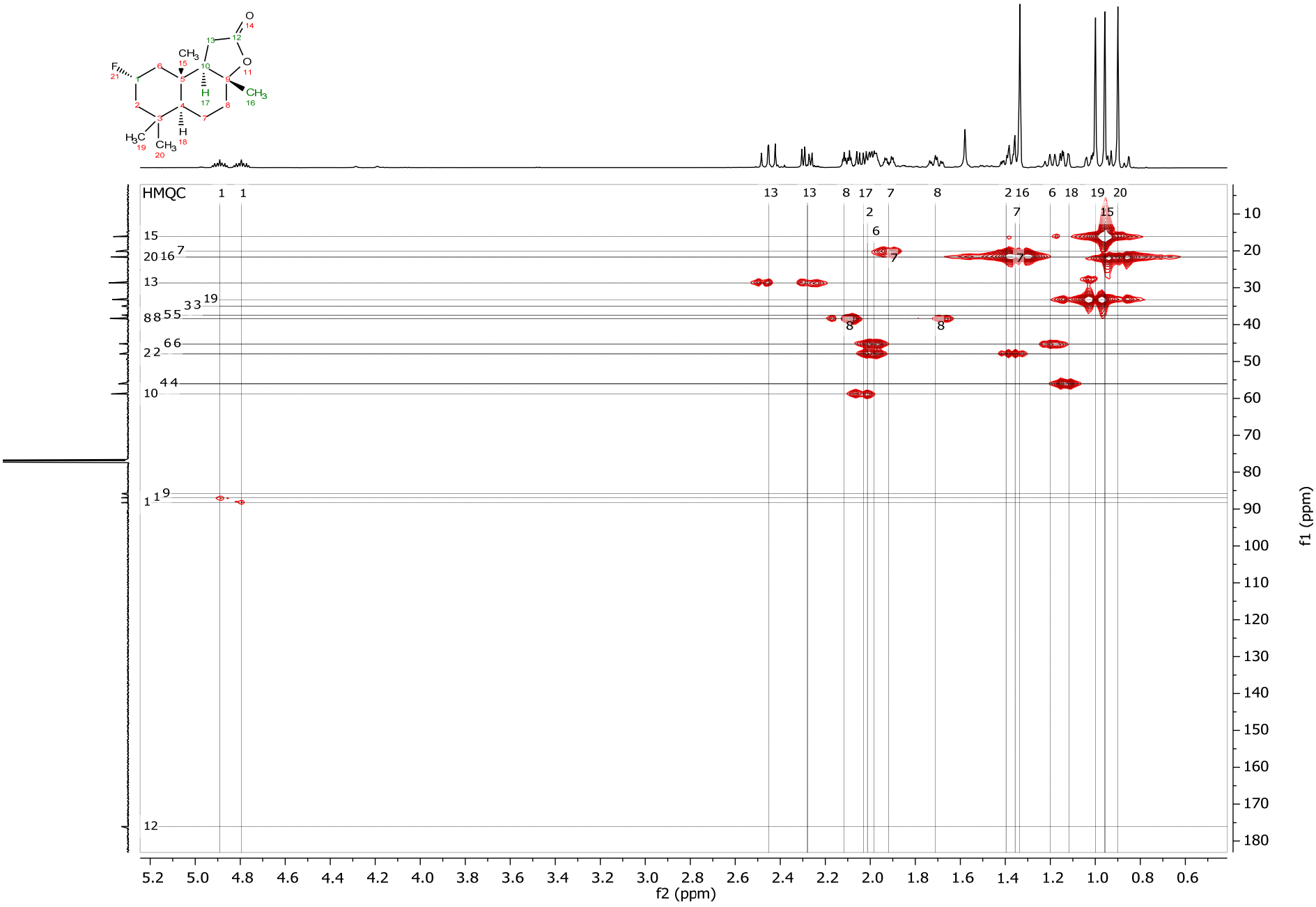


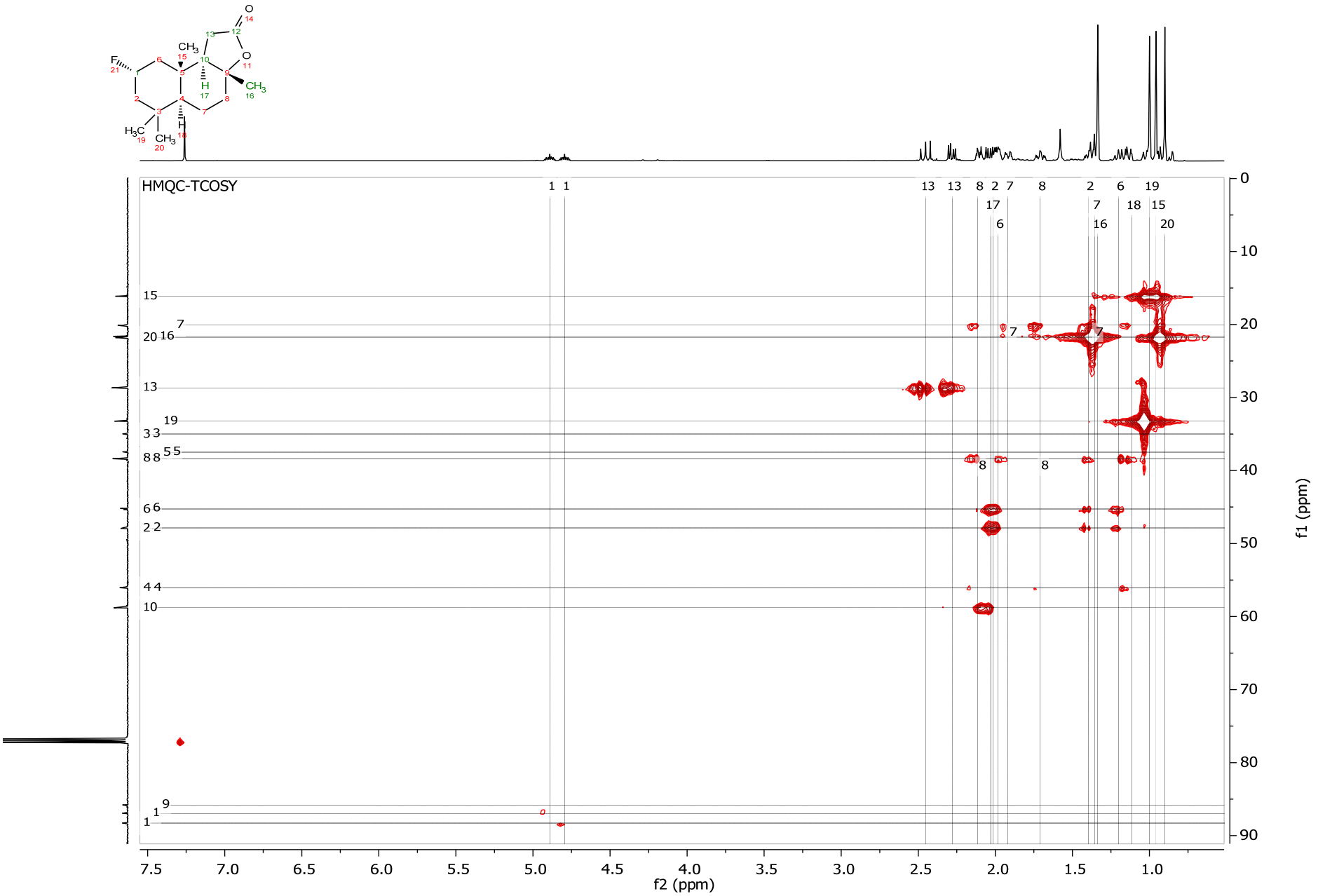

13C NMR
f1 (ppm)
B (s) 176.07
C (s) 85.81
A (d) 87.61
K (s) 33.23
O (d) 20.12
E (d) 56.05
G (d) 45.25
J (d) 35.00
N (s) 21.62
D (s) 58.79
F (d) 47.87
I (d) 37.47
M (s) 21.80
H (s) 38.37
L (s) 28.68
P (s) 16.13

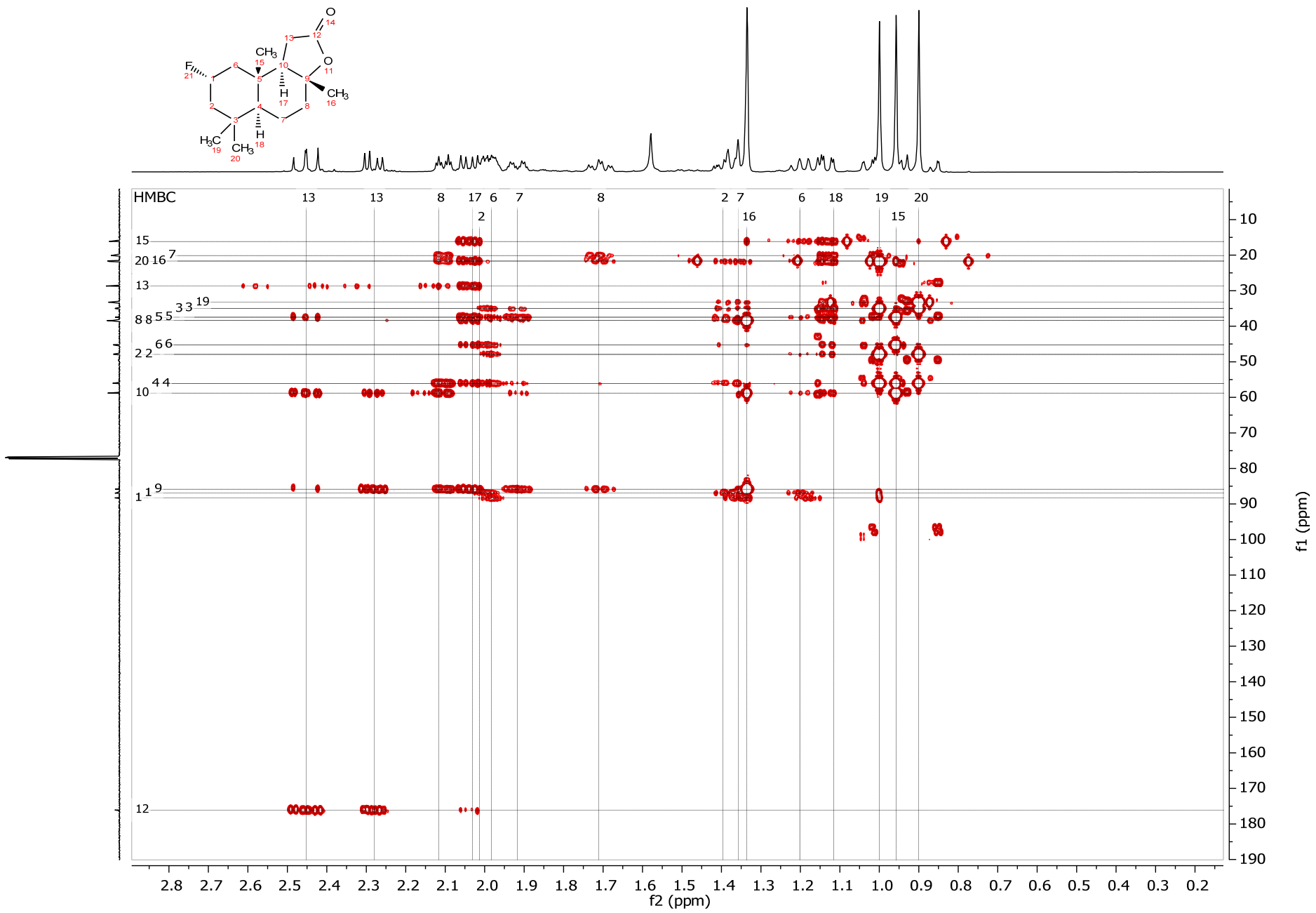

DEPT 135
58.81
56.08
56.06
33.25
21.82
21.64
16.16
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
-2000
-4000
-6000
-8000
-10000
-12000
-14000
-16000
-18000
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

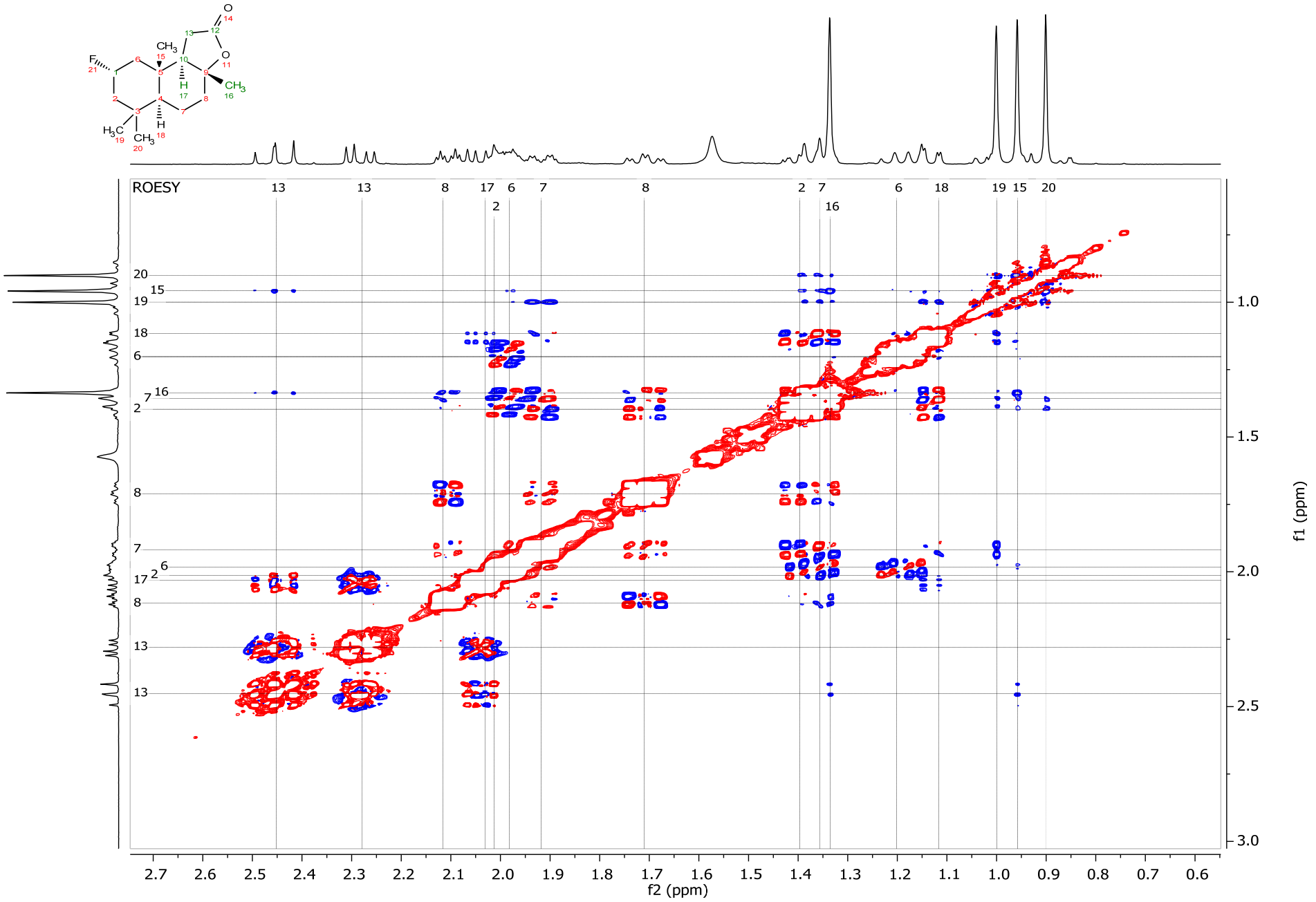

19F NMR
-179.76
-179.78
-179.79
-179.81
-179.82
-179.83
-179.85
-179.89
-179.90
-179.92
-179.93
-179.95
-179.96
-179.98
A (dtt)
-179.87
1.00
f1 (ppm)


COSY
f2 (ppm)
f1 (ppm)
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0

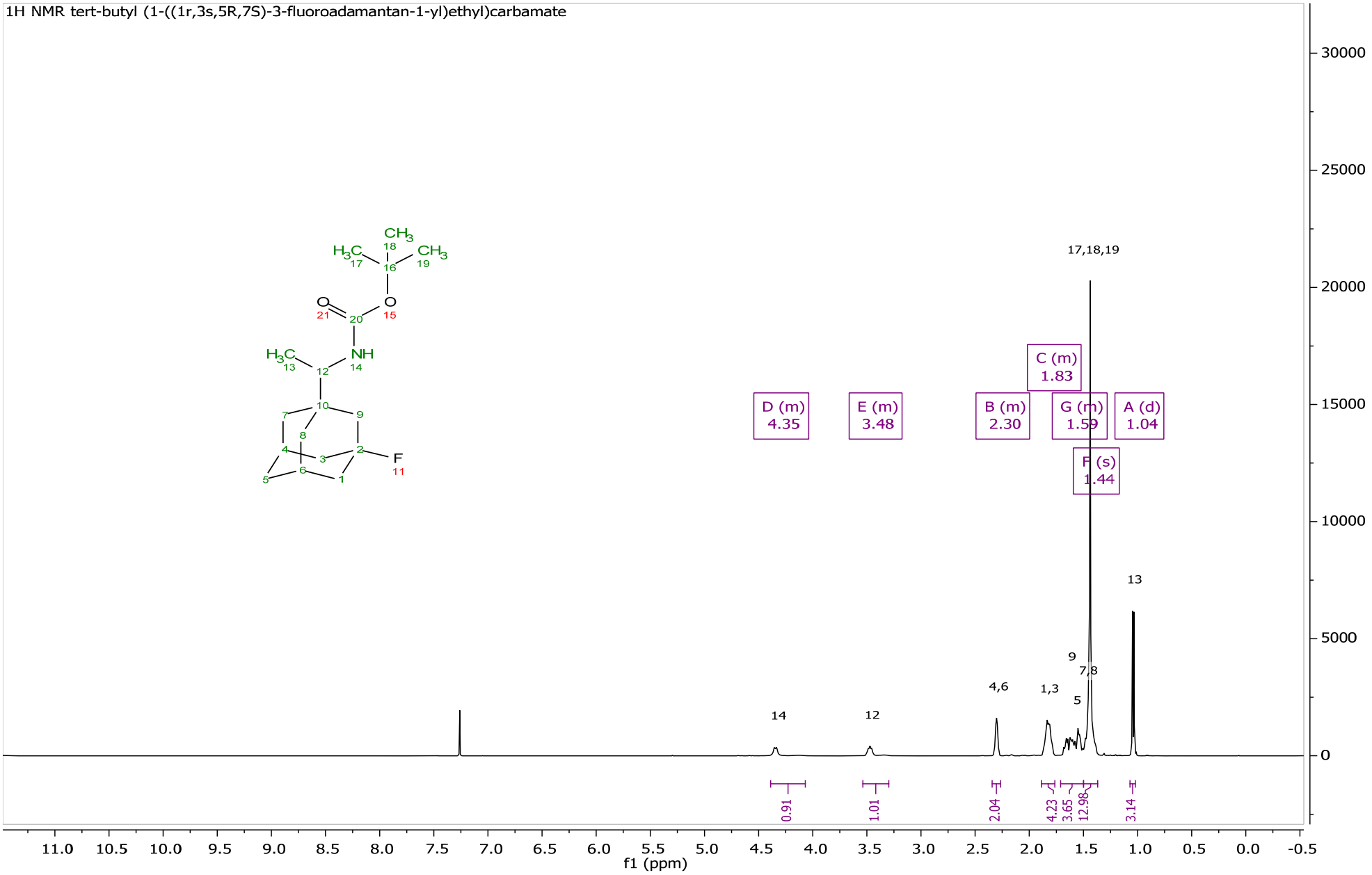

HMQC
f2 (ppm)
f1 (ppm)

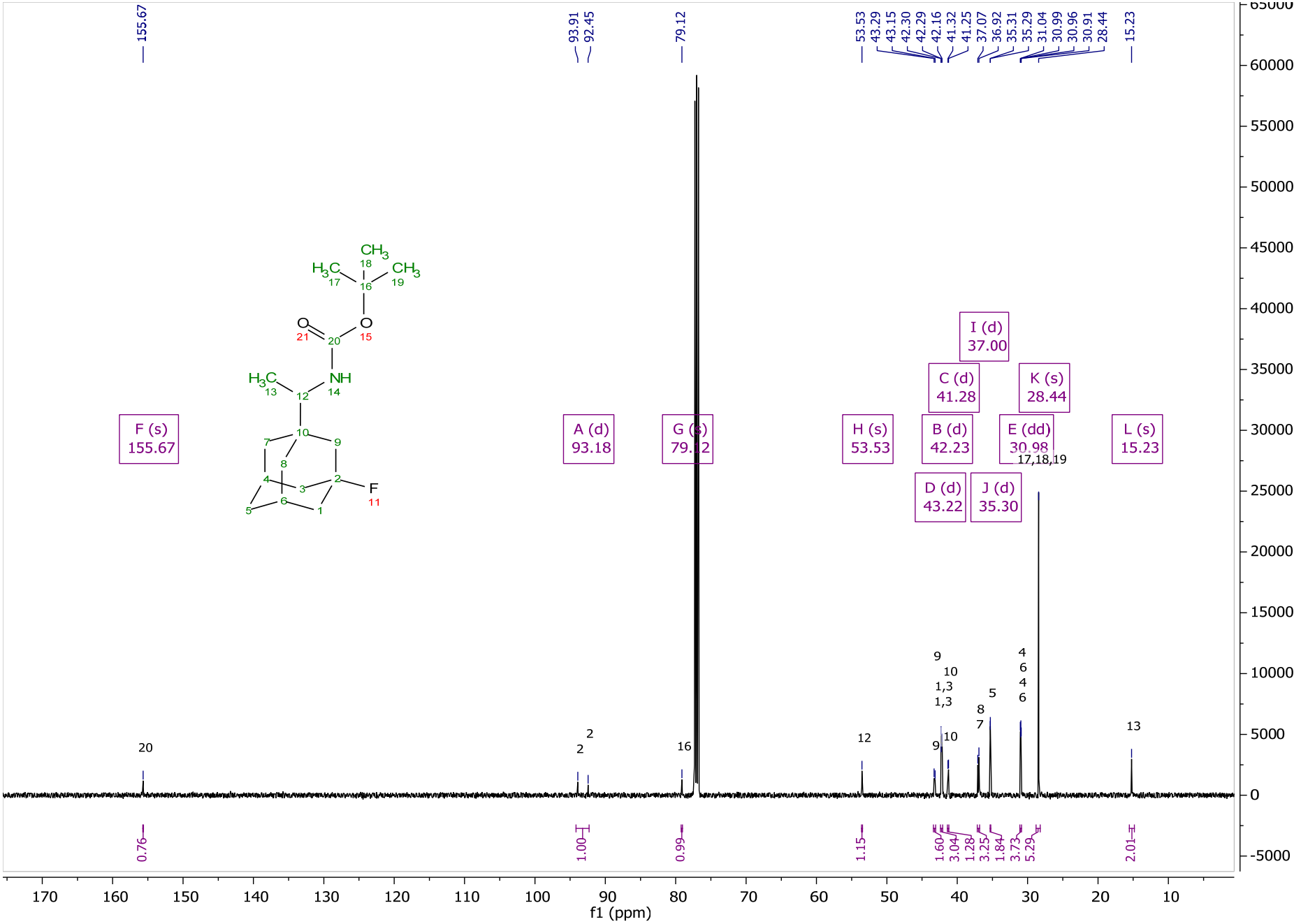

HMQC-TCOSY
f2 (ppm)
f1 (ppm)


HMBC
f2 (ppm)
f1 (ppm)

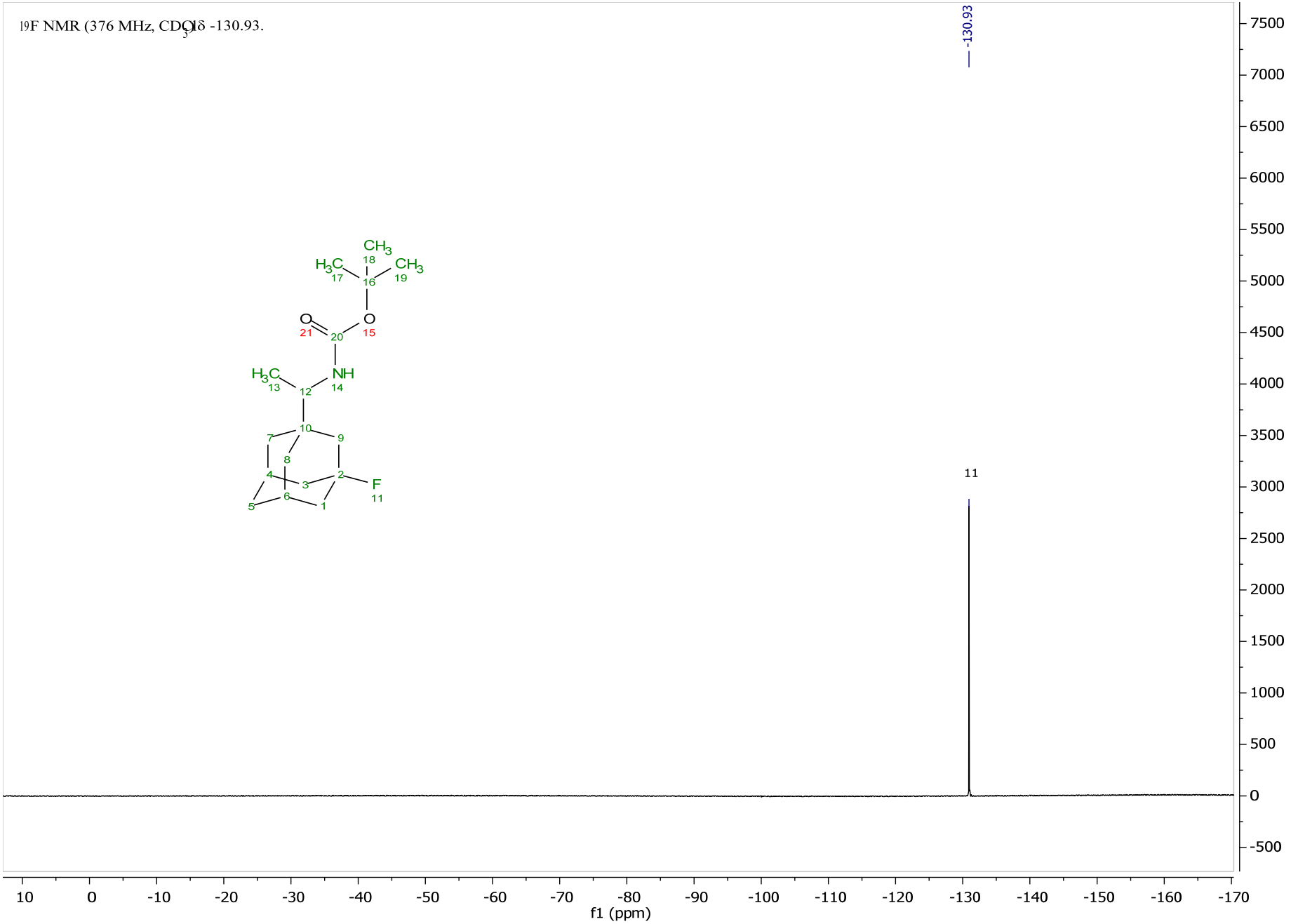

ROESY
f2 (ppm)
f1 (ppm)

NMR Spectra of tert-butyl (1-((1r,3s,5R,7S)-3-fluoroadamantan-1-yl)ethyl)carbamate

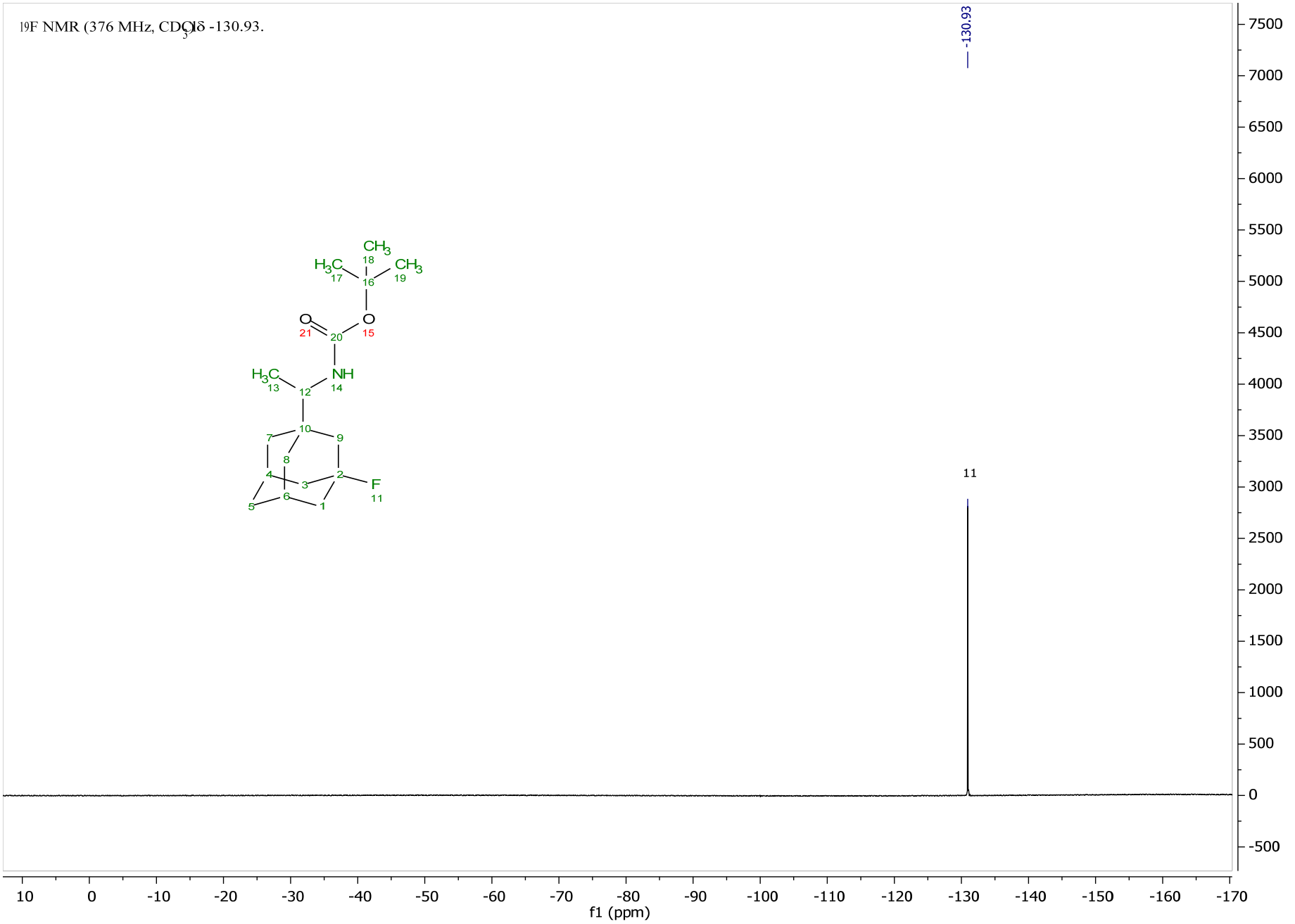


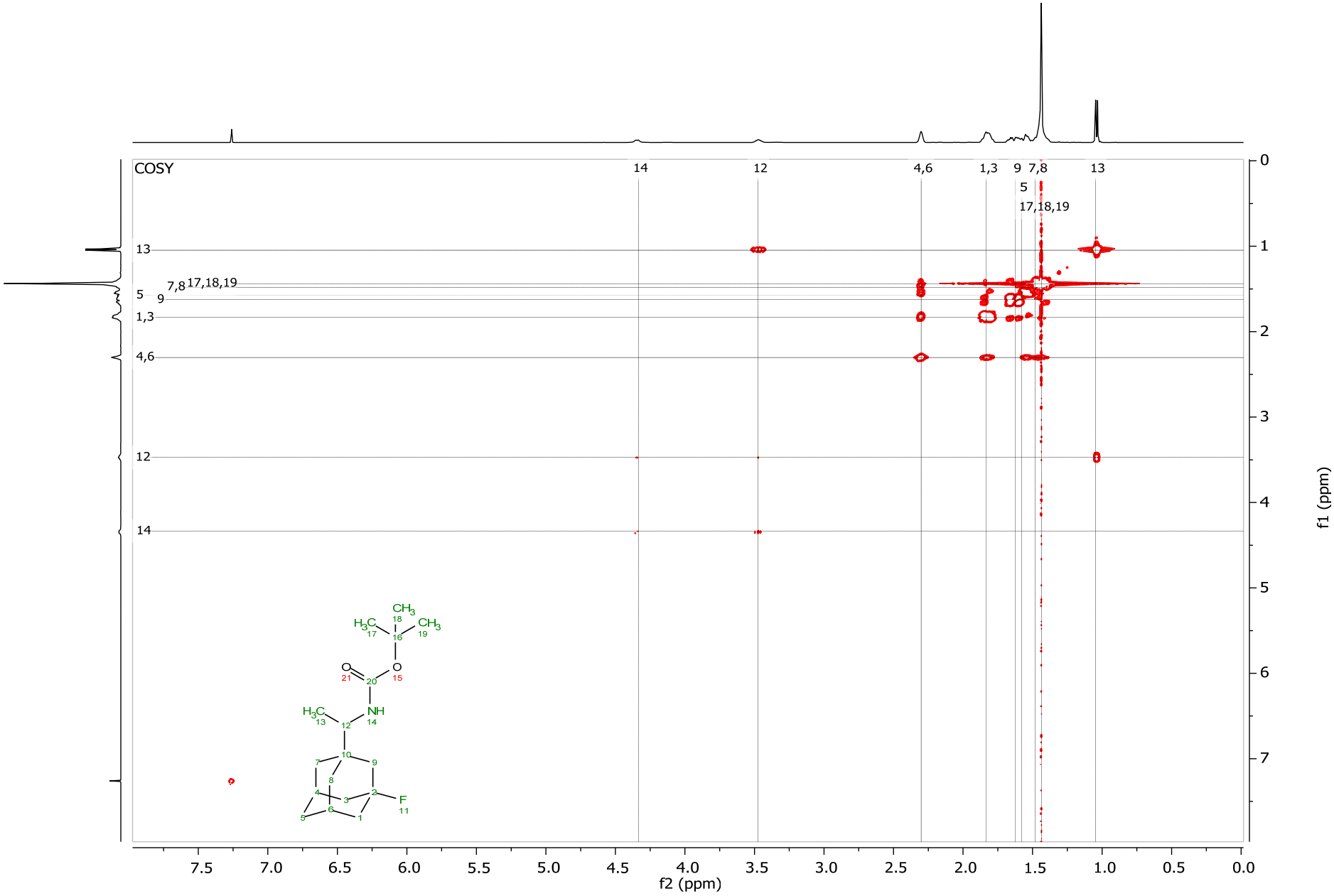

155.67
93.91
92.45
79.12
53.53
43.29
43.15
42.30
42.29
42.16
41.32
41.25
37.07
36.92
35.31
35.29
31.04
30.99
30.96
30.91
28.44
15.23
F (s)
155.67
A (d)
93.18
G (s)
79.12
H (s)
53.53
I (d)
37.00
C (d)
41.28
B (d)
42.23
K (s)
28.44
E (dd)
30.98
L (s)
15.23
D (d)
43.22
J (d)
35.30
17,18,19
f1 (ppm)

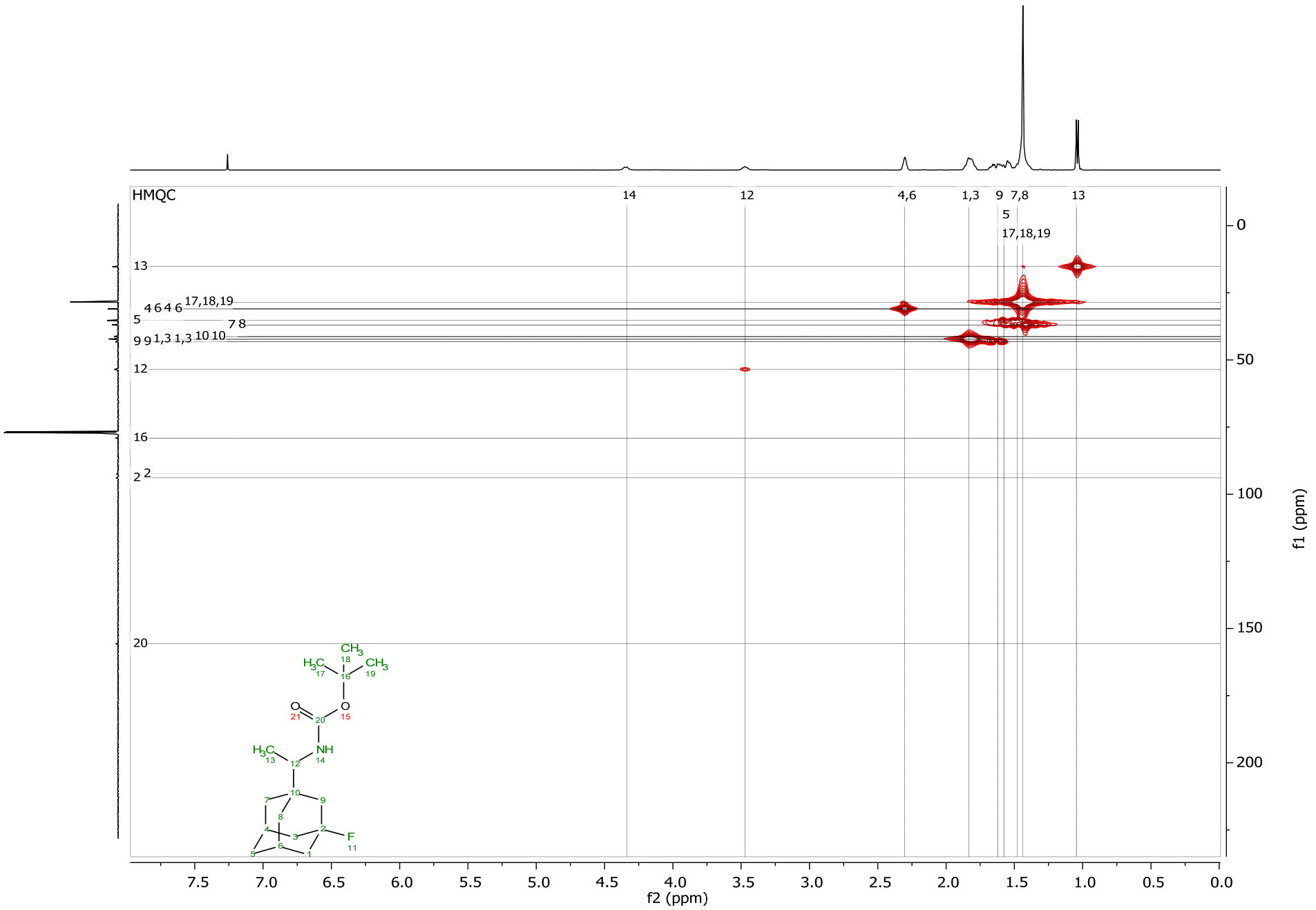
^{19}F NMR (376 MHz, $CDCl_3$) δ -130.93.

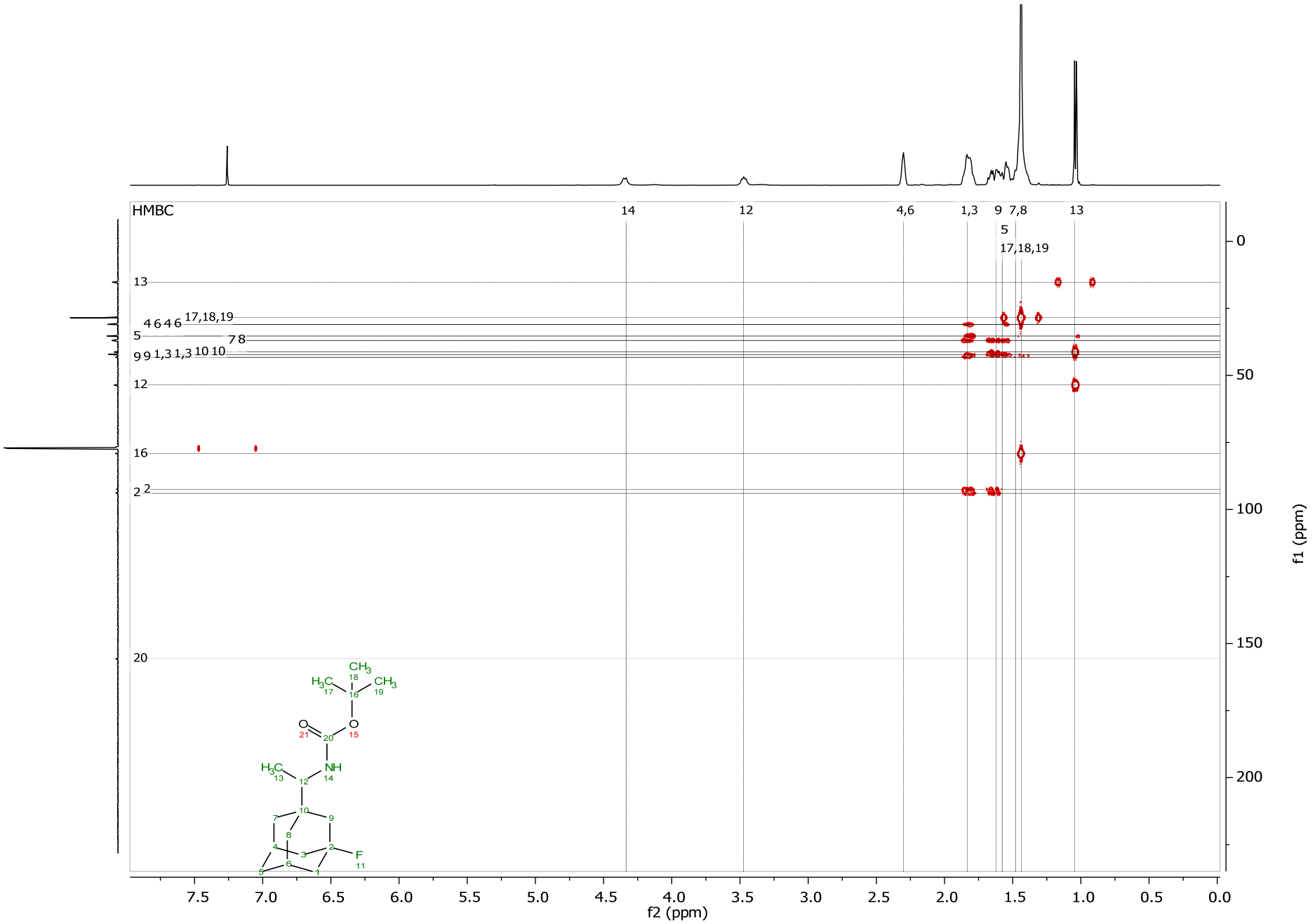


^{19}F NMR (376 MHz, $CDCl_3$) δ -130.93.

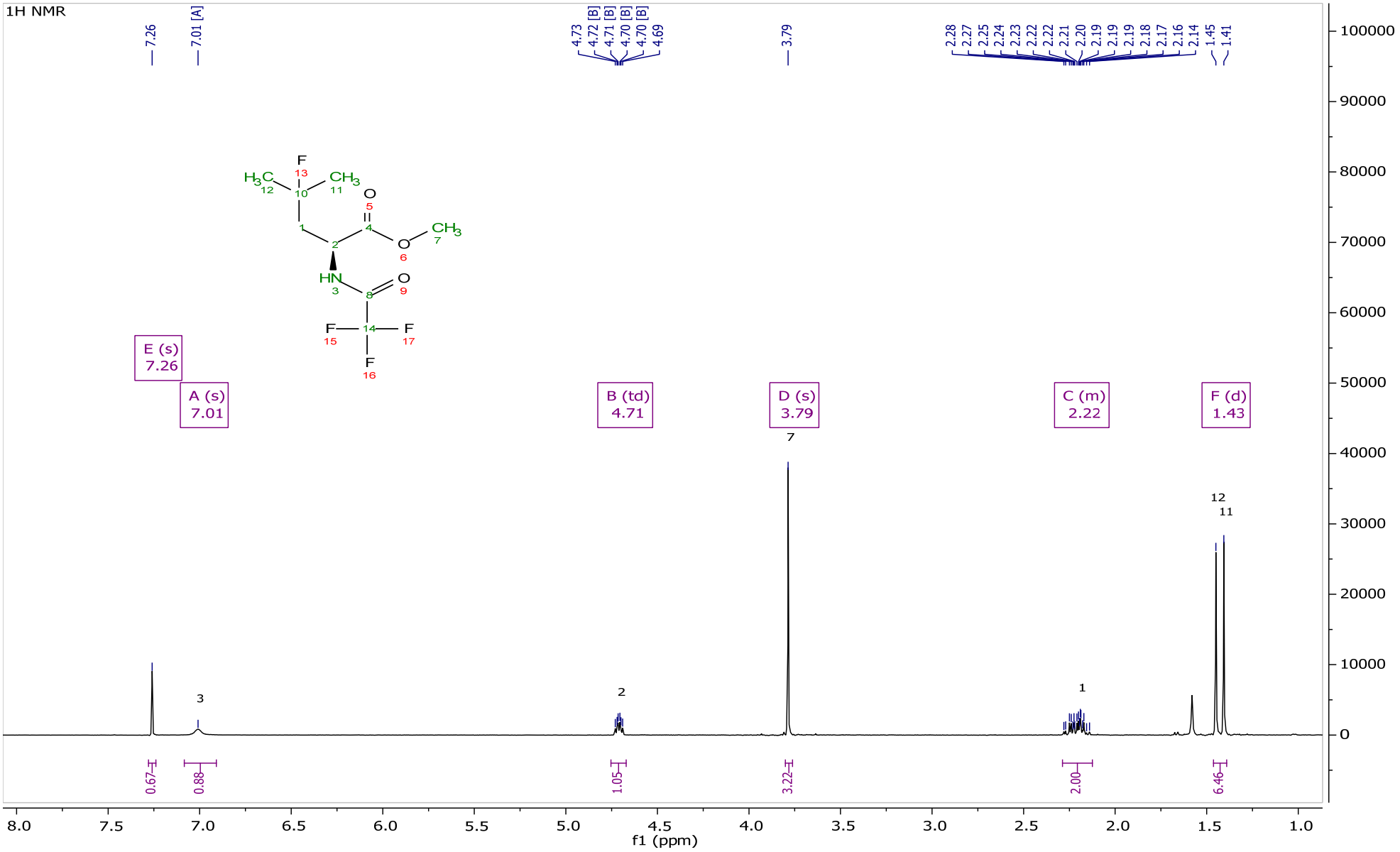


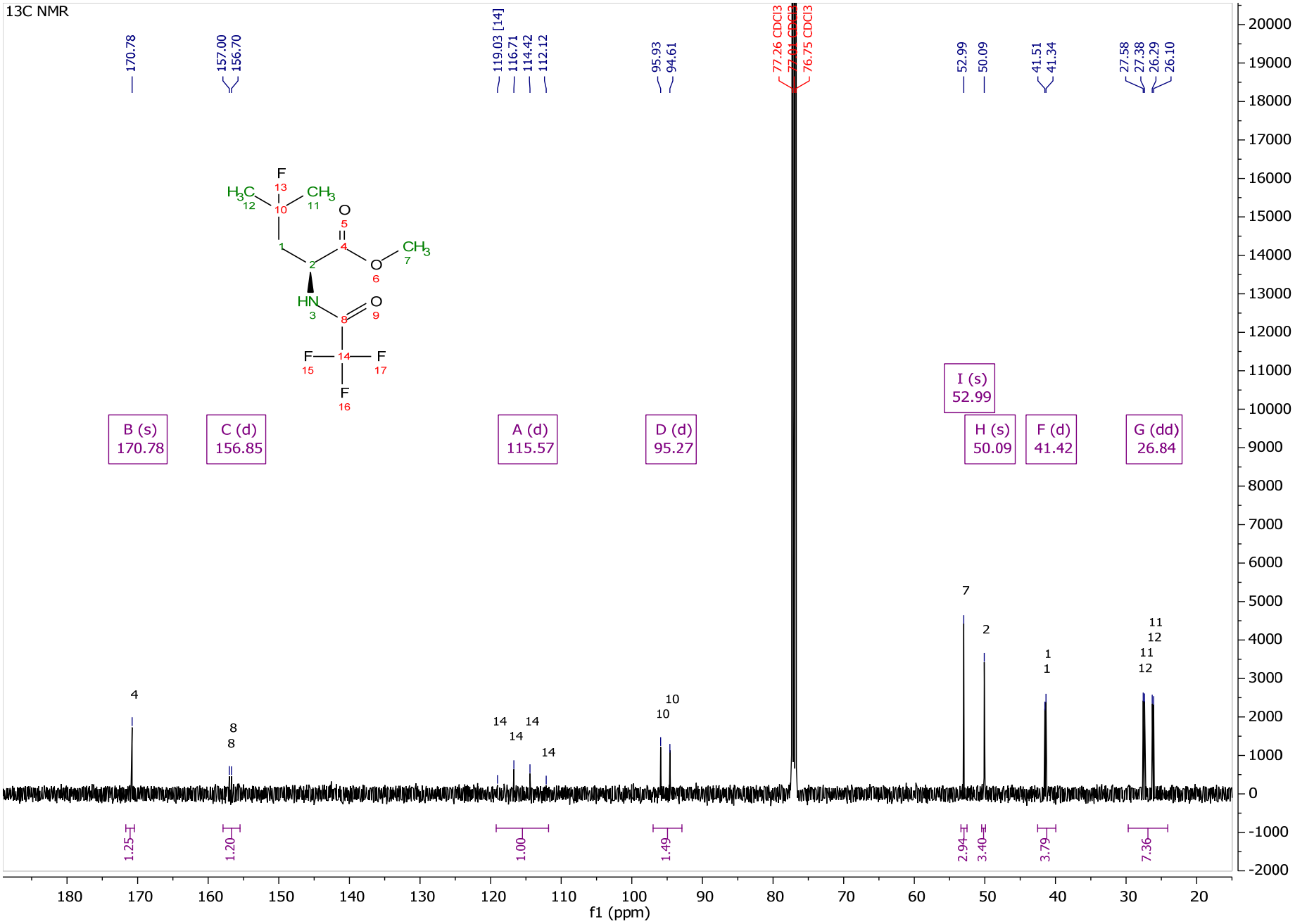

COSY
14
12
4,6
1,3
9
7,8
13
5
17,18,19
13
5
9
7,8
17,18,19
1,3
4,6
12
14
f2 (ppm)
f1 (ppm)

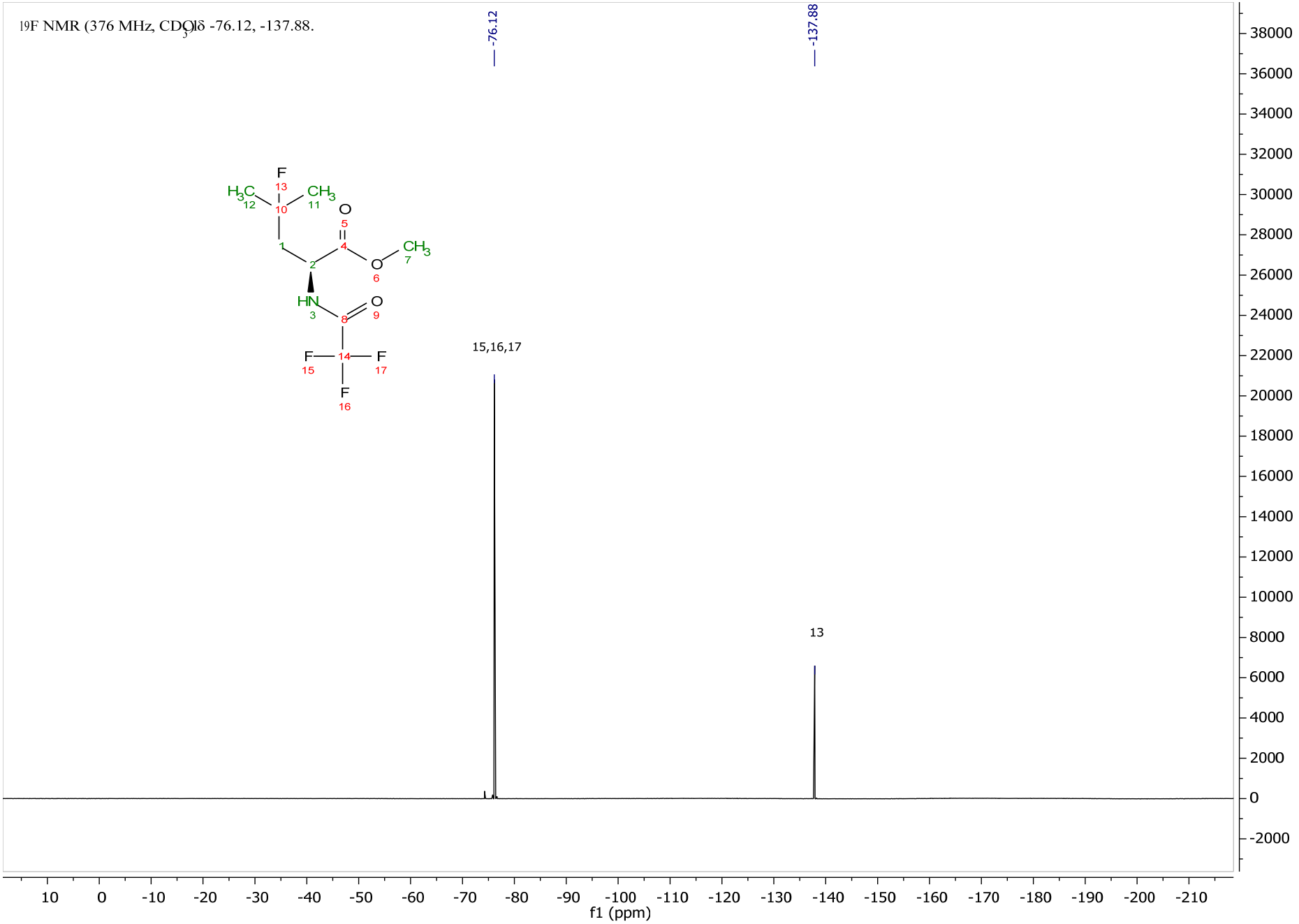

HMQC
14
12
4,6
1,3
9
7,8
13
5
17,18,19
f2 (ppm)
f1 (ppm)

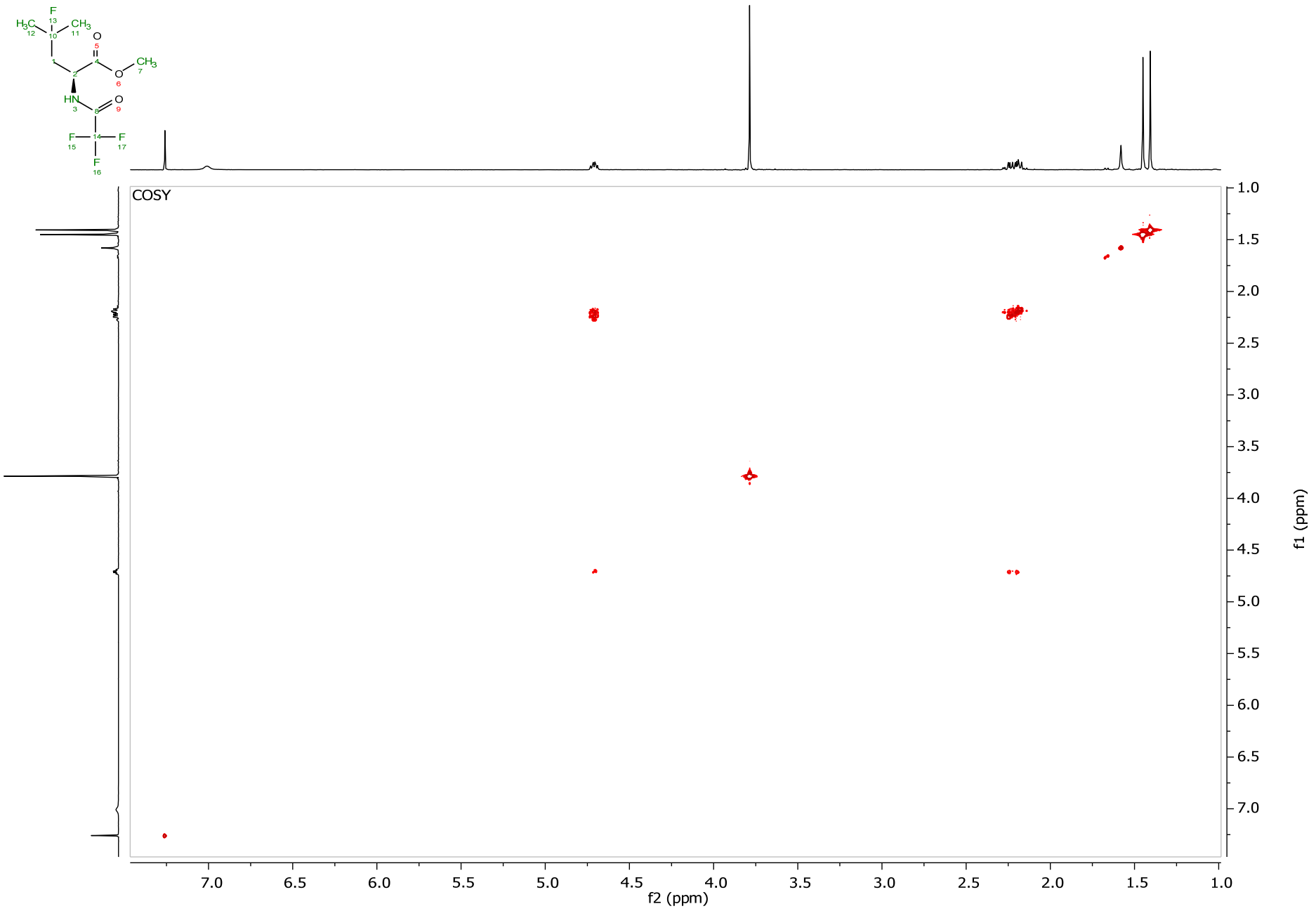

HMBC
14
12
4,6
1,3
9
7,8
13
5
17,18,19
13
4 6 4 6 17,18,19
5
7 8
9 9 1,3 1,3 10 10
12
16
2 2
20
0
50
100
150
200
f1 (ppm)
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f2 (ppm)

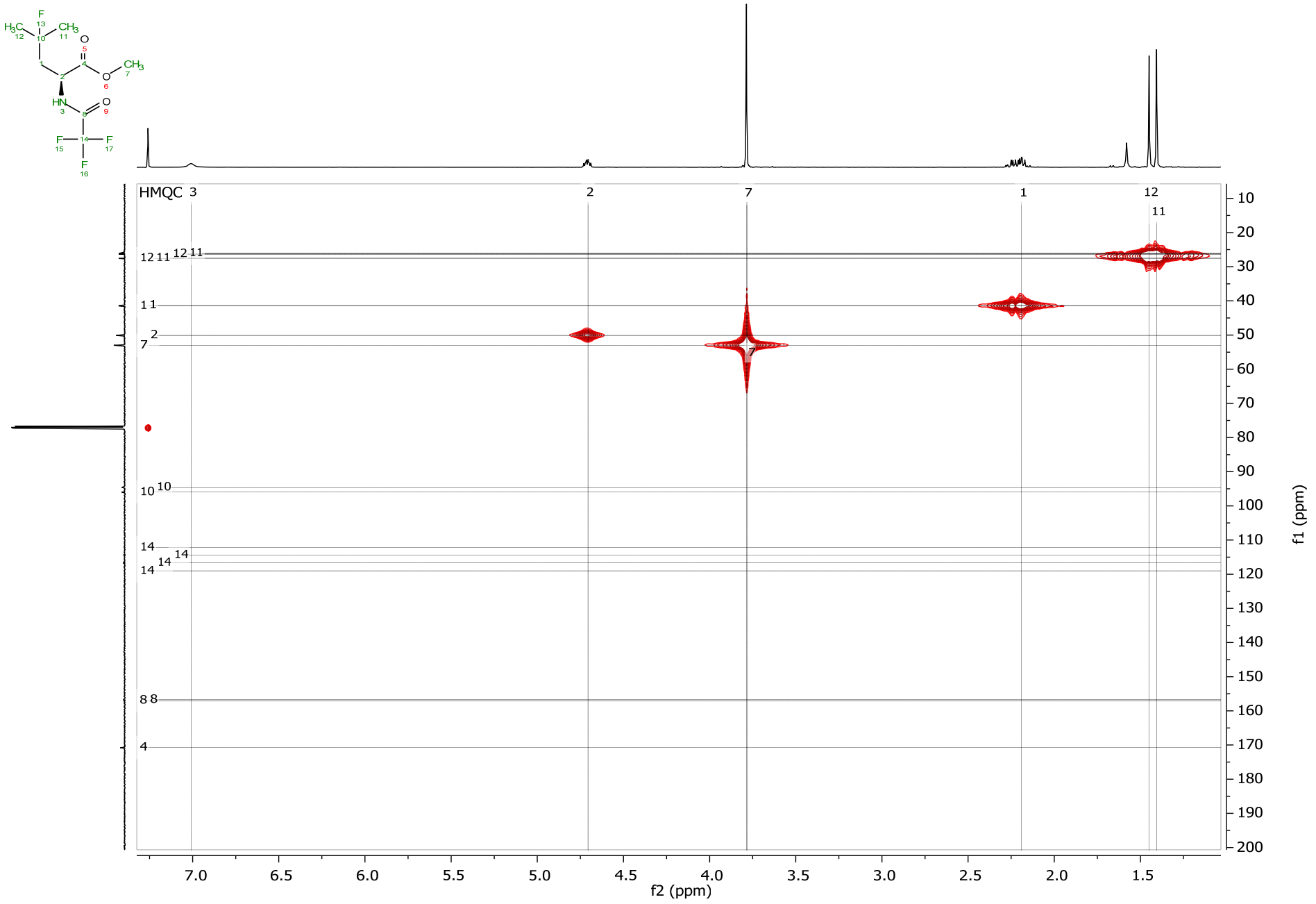
NMR Spectra of methyl (S)-4-fluoro-4-methyl-2-(2,2,2-trifluoroacetamido)pentanoate

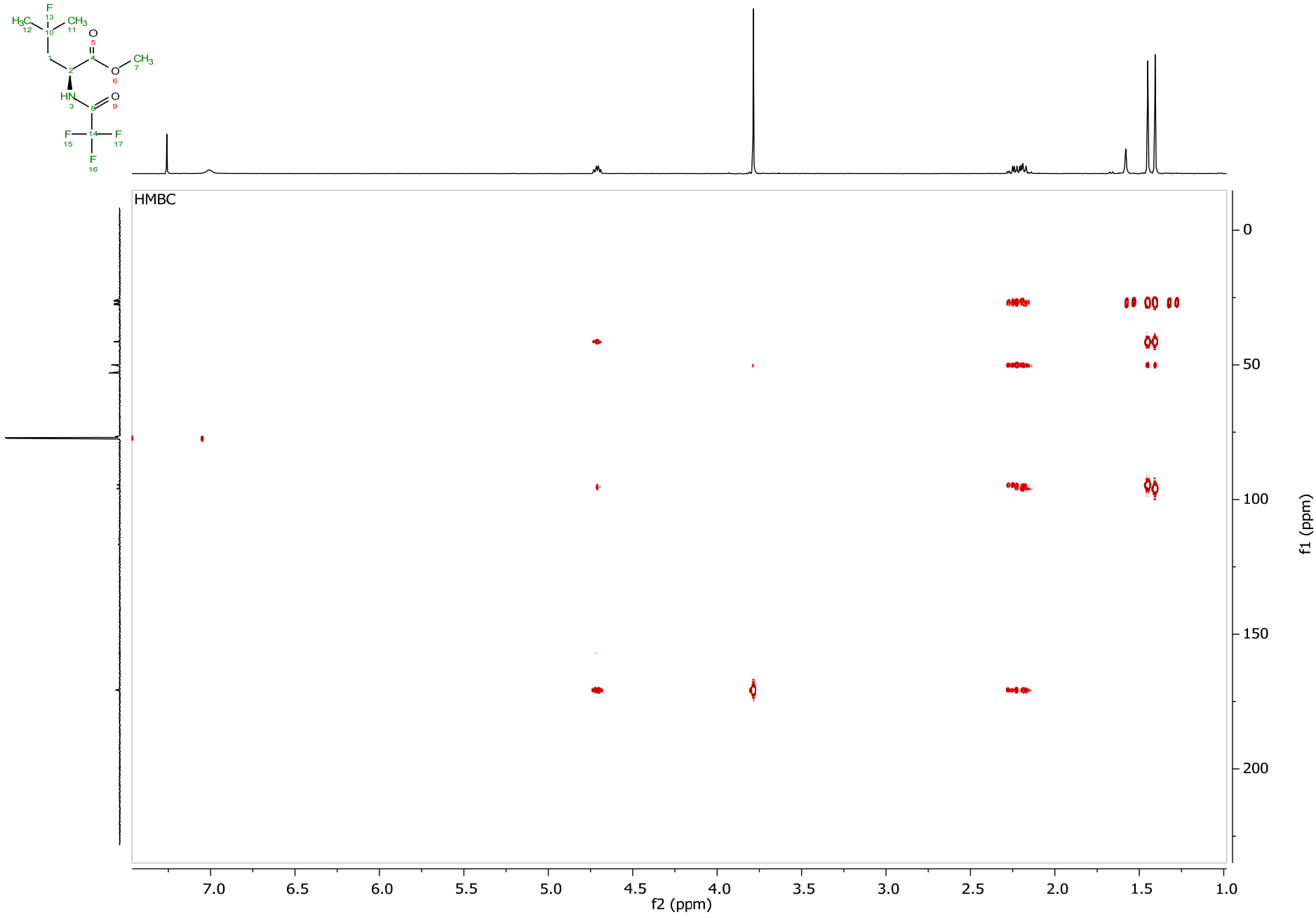



13C NMR
170.78
157.00
156.70
119.03 [14]
116.71
114.42
112.12
95.93
94.61
77.26 CDCl3
77.01 CDCl3
76.75 CDCl3
52.99
50.09
41.51
41.34
27.58
27.38
26.29
26.10
B (s) 170.78
C (d) 156.85
A (d) 115.57
D (d) 95.27
I (s) 52.99
H (s) 50.09
F (d) 41.42
G (dd) 26.84
1.25
1.20
1.00
1.49
2.94
3.40
3.79
7.36
f1 (ppm)

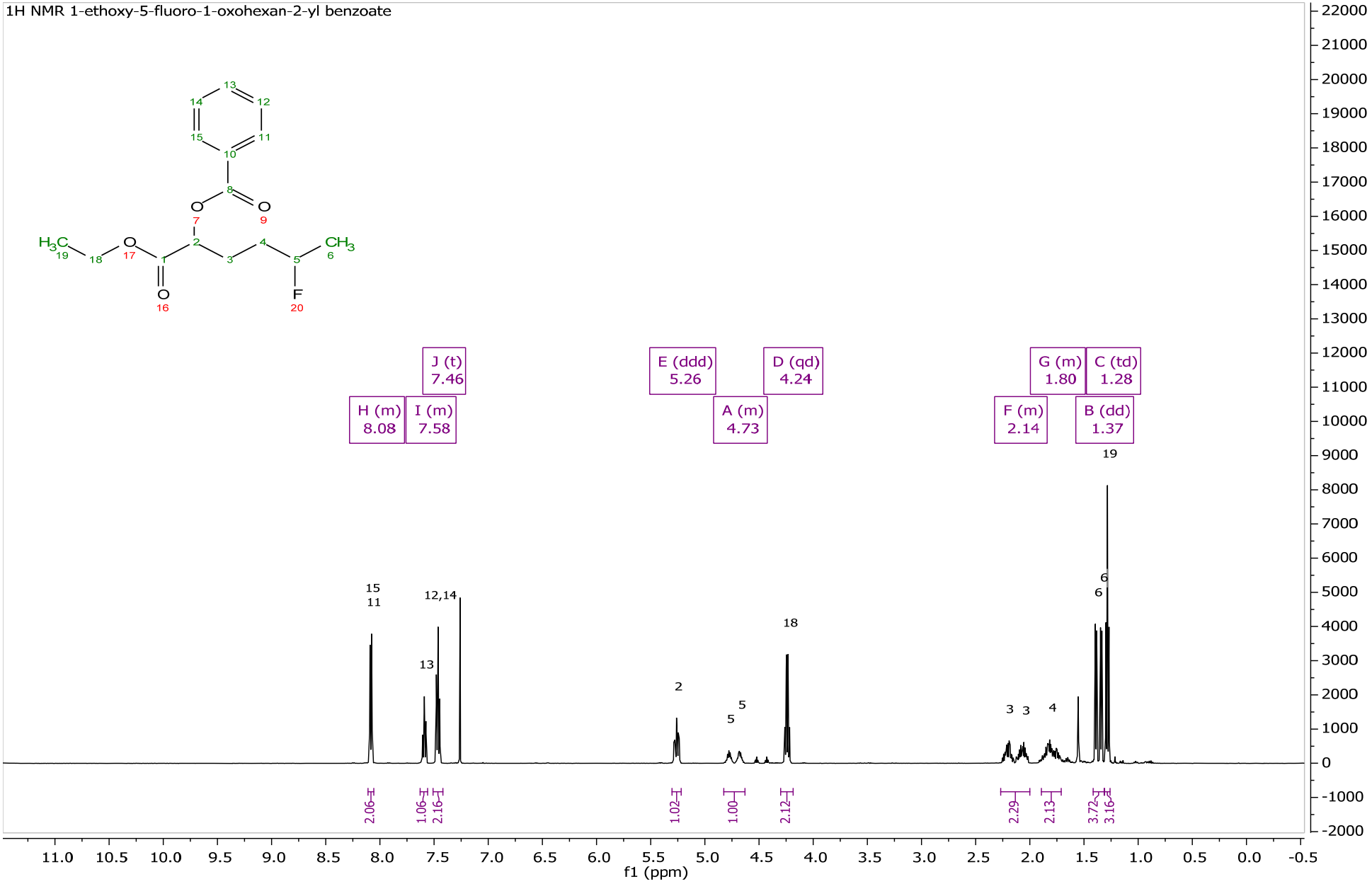

19F NMR (376 MHz, CDCl3) δ -76.12, -137.88.
-76.12
-137.88
15,16,17
13
f1 (ppm)

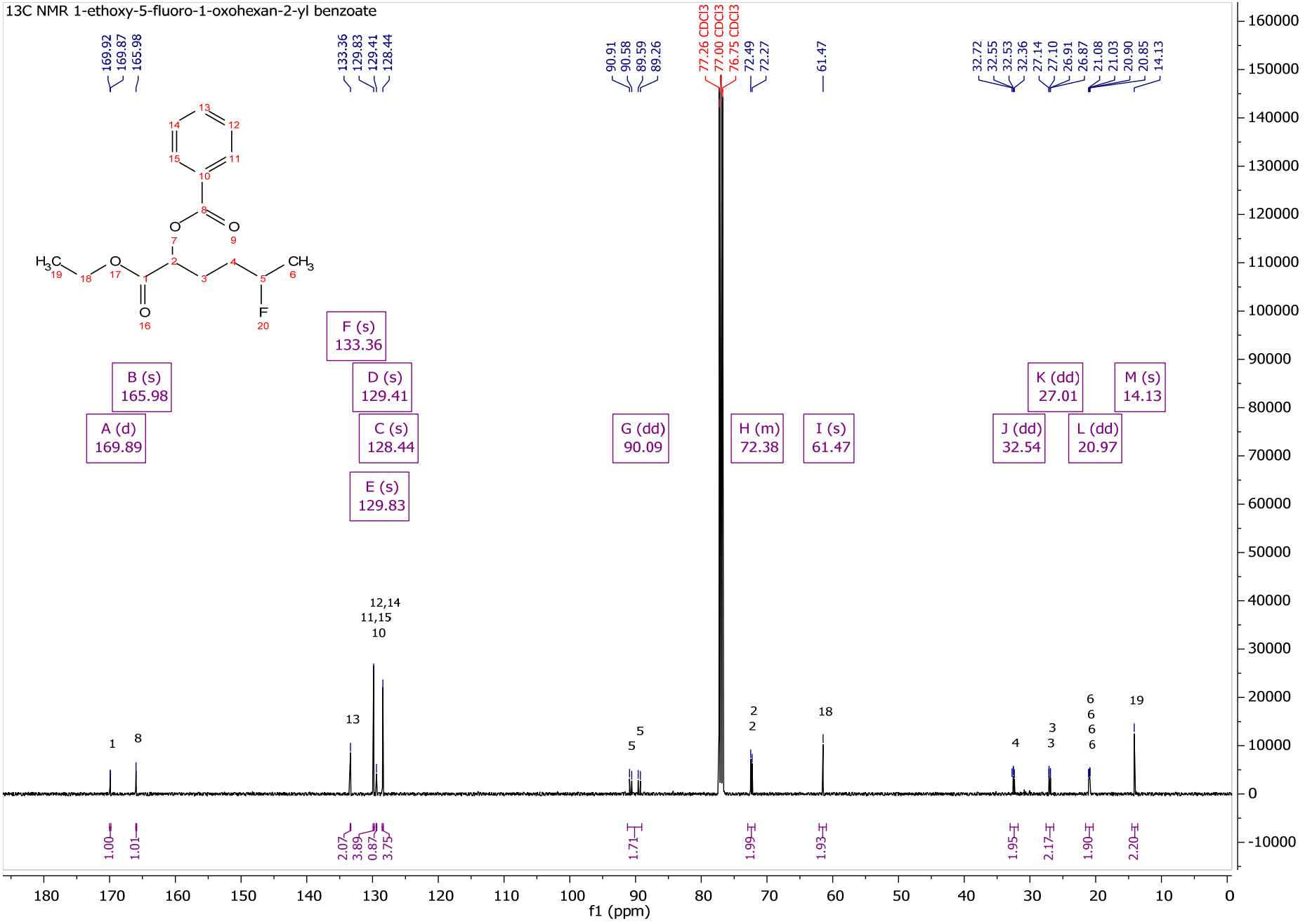

COSY
f2 (ppm)
f1 (ppm)
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0

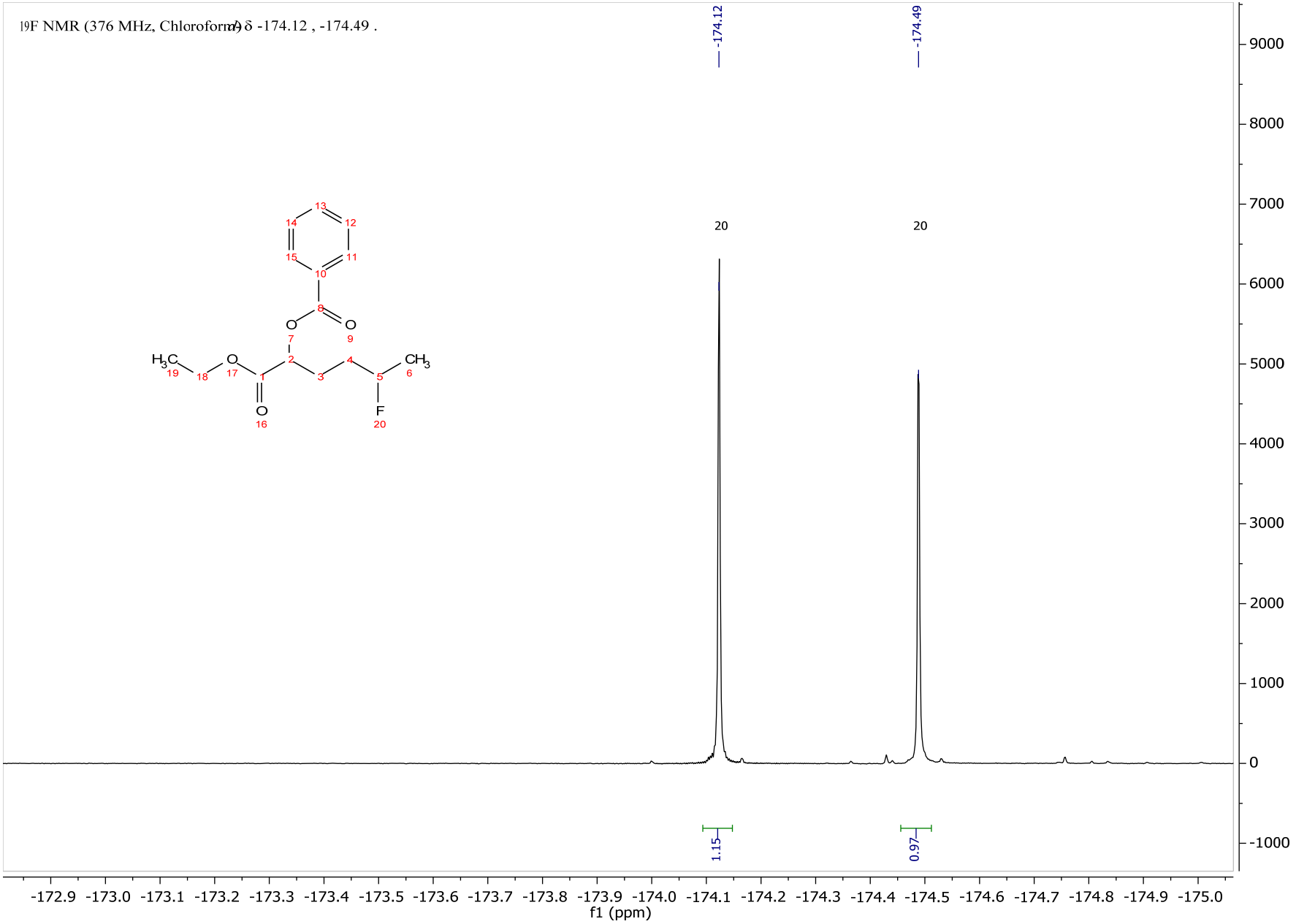

HMQC
f2 (ppm)
f1 (ppm)

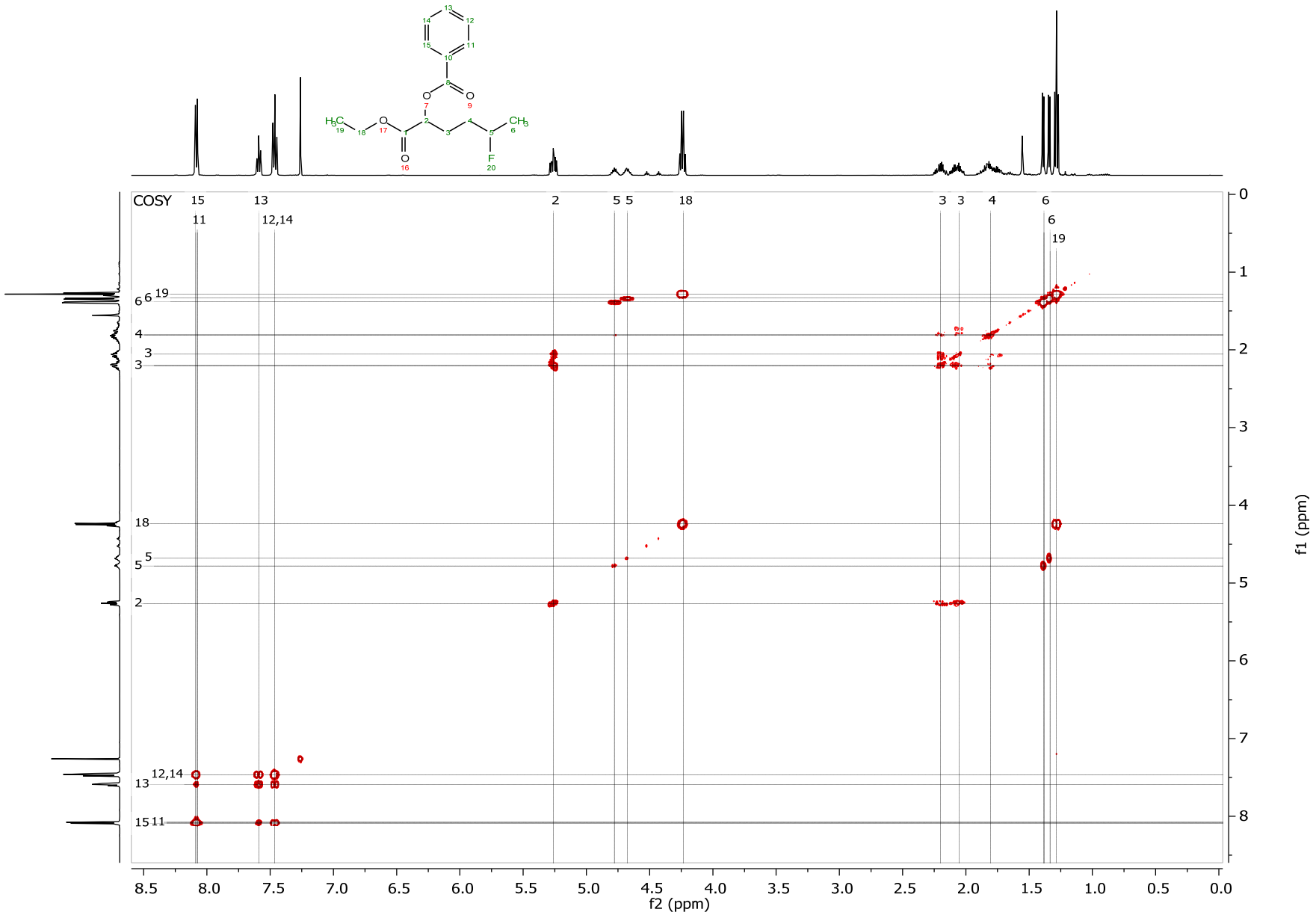

HMBC
f2 (ppm)
f1 (ppm)
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0
50
100
150
200

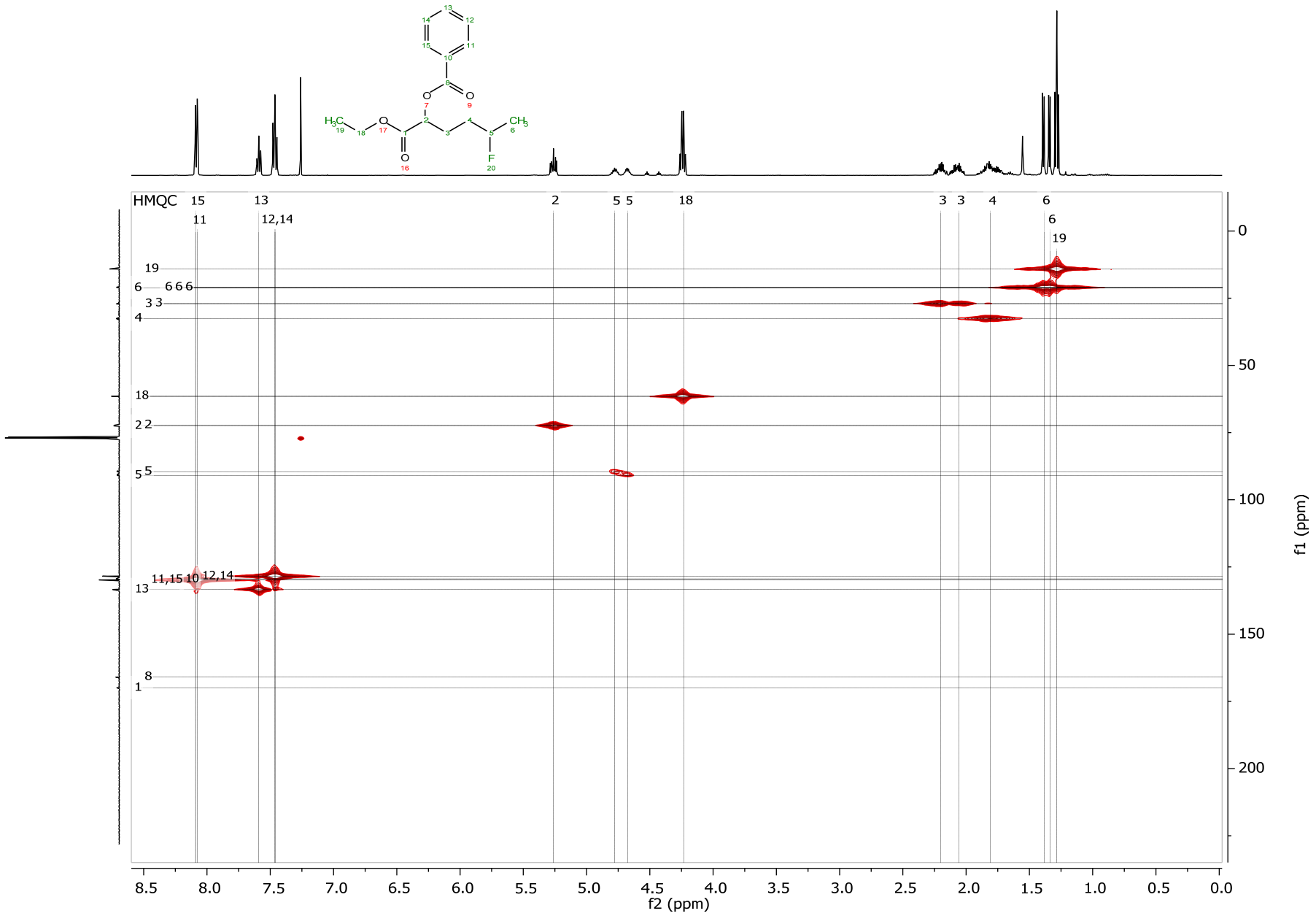
NMR Spectra of methyl 1-ethoxy-5-fluoro-1-oxohexan-2-yl benzoate

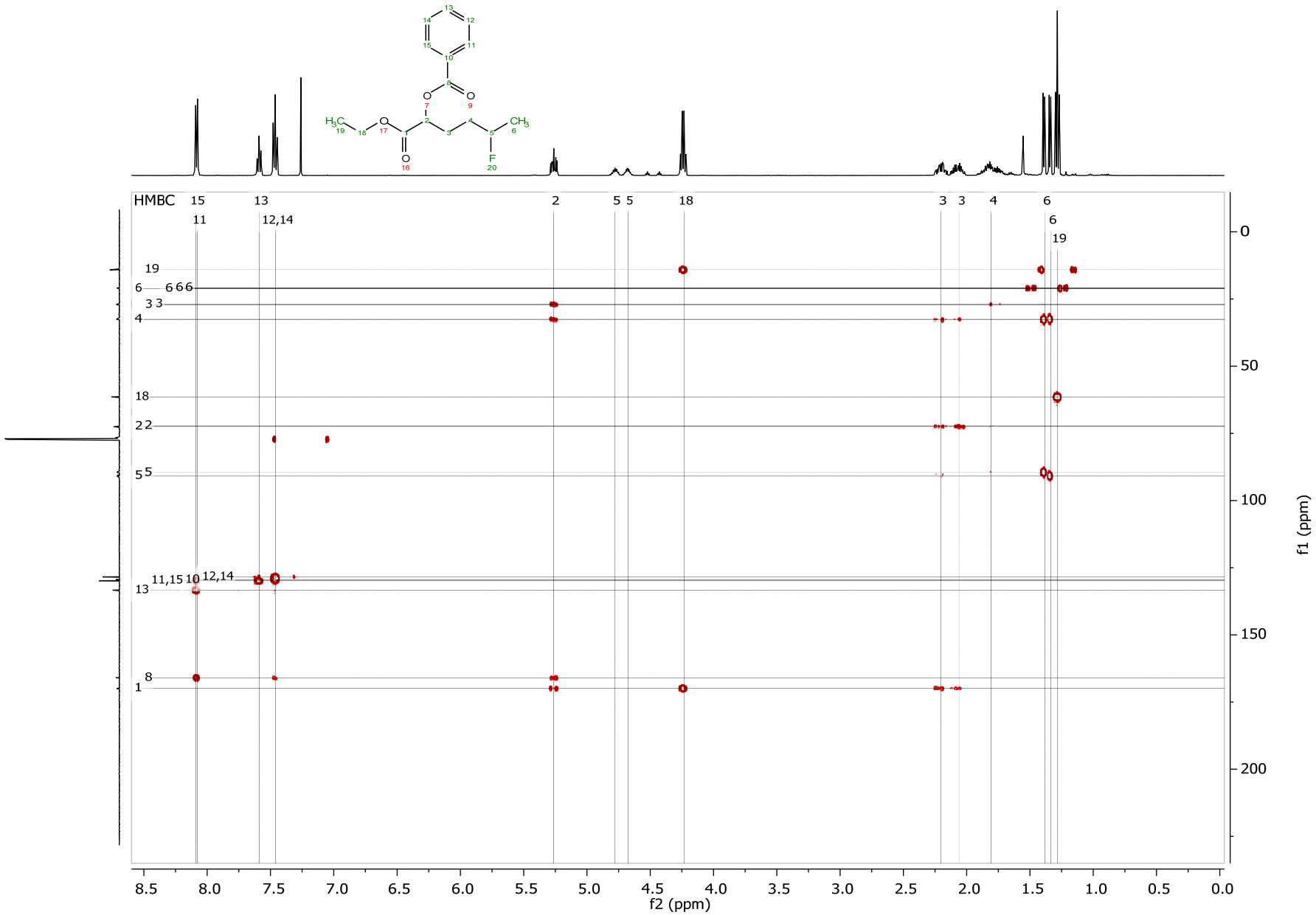



13C NMR 1-ethoxy-5-fluoro-1-oxohexan-2-yl benzoate
169.92
169.87
165.98
133.36
129.83
129.41
128.44
90.91
90.58
89.59
89.26
77.26 CDCl3
77.00 CDCl3
76.75 CDCl3
72.49
72.27
61.47
32.72
32.55
32.53
32.36
27.14
27.10
26.91
26.87
21.08
21.03
20.90
20.85
14.13
F (s)
133.36
B (s)
165.98
D (s)
129.41
K (dd)
27.01
M (s)
14.13
A (d)
169.89
C (s)
128.44
G (dd)
90.09
H (m)
72.38
I (s)
61.47
J (dd)
32.54
L (dd)
20.97
E (s)
129.83
12,14
11,15
10
f1 (ppm)


19F NMR (376 MHz, Chloroform-d) δ -174.12 , -174.49 .
-174.12
-174.49
20
20
1.15
0.97
f1 (ppm)

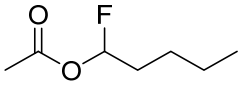

COSY
f2 (ppm)
f1 (ppm)


HMQC
f2 (ppm)
f1 (ppm)


HMBC
f2 (ppm)
f1 (ppm)

Cartesian Coordinates and thermochemical data

Result for Table 3: relevant to ^{19}F NMR calculation of fluoropentyl acetate



OPT-wB97xD-6-311+Gdp_1-fluoropentyl_acetateC_1.out

0 1

C	-2.730022	-0.053503	-0.252885
O	-2.841384	0.947986	-0.908860
C	-0.401047	0.299148	-0.008552
H	-0.473900	0.778494	-0.984917
C	0.825410	-0.556919	0.153993
H	0.734259	-1.378174	-0.564294
C	2.121776	0.209569	-0.095816
H	2.076116	0.687328	-1.082140
C	3.350343	-0.694806	-0.027471
H	3.387326	-1.178511	0.955718
H	3.246701	-1.498344	-0.766133
H	2.222944	1.014082	0.640659
F	-0.394813	1.332481	0.934698
H	0.817353	-0.993229	1.158334
O	-1.538993	-0.480244	0.245791
C	4.651813	0.060802	-0.273899
H	4.653745	0.528668	-1.263825
H	4.793832	0.852724	0.468890
H	5.516058	-0.607381	-0.218735
C	-3.831867	-0.982318	0.138213
H	-4.747723	-0.711102	-0.383366
H	-3.990694	-0.906043	1.217434
H	-3.558112	-2.014610	-0.086847

Zero-point correction	=	0.196052
Thermal correction to Energy	=	0.207943
Thermal correction to Enthalpy	=	0.208888
Thermal correction to Gibbs Free Energy	=	0.15709
Sum of electronic and zero-point Energies	=	-524.704754
Sum of electronic and thermal Energies	=	-524.692863
Sum of electronic and thermal Enthalpies	=	-524.691918
Sum of electronic and thermal Free Energies	=	-524.743716
Number of imaginary frequencies/frequency	=	0

OPT-wB97xD-6-311+Gdp_1-fluoropentyl_acetateC_2.out

0 1

C	2.246629	-0.552207	0.149311
O	2.535970	-0.298142	1.291809
C	0.613594	1.170587	0.125620
H	1.290567	1.661613	0.823634
C	-0.671750	0.722238	0.774409
H	-1.126046	1.605284	1.235306
C	-1.659731	0.040967	-0.169540
H	-1.931424	0.728917	-0.977597
C	-2.926804	-0.408980	0.555140
H	-2.654026	-1.102574	1.359287
H	-3.394146	0.457977	1.037154
H	-1.183558	-0.827126	-0.638114
F	0.352049	2.072173	-0.895489
H	-0.394679	0.046459	1.590792
O	1.282558	0.105779	-0.526794
C	-3.930911	-1.076503	-0.379012
H	-4.827349	-1.394884	0.160971
H	-4.245122	-0.390529	-1.172498
H	-3.496861	-1.961375	-0.856166
C	2.865444	-1.614286	-0.701020
H	3.269442	-1.170772	-1.613675
H	2.100419	-2.338422	-0.990944
H	3.657294	-2.116126	-0.148320

Zero-point correction	=	0.196294
Thermal correction to Energy	=	0.208233
Thermal correction to Enthalpy	=	0.209178
Thermal correction to Gibbs Free Energy	=	0.156512
Sum of electronic and zero-point Energies	=	-524.701842
Sum of electronic and thermal Energies	=	-524.689903
Sum of electronic and thermal Enthalpies	=	-524.688959
Sum of electronic and thermal Free Energies	=	-524.741624
Number of imaginary frequencies/frequency	=	0

OPT-wB97xD-6-311+Gdp_1-fluoropentyl_acetateC_3.out

0 1

C	2.643635	0.135127	-0.177604
O	2.933035	-0.968118	-0.558092
C	0.351032	-0.449154	-0.035672
H	0.579338	-1.139039	-0.848120
C	-0.968721	0.256834	-0.189702
H	-0.896980	0.871820	-1.093120
C	-2.144988	-0.711187	-0.312524
H	-1.924720	-1.441455	-1.099410
C	-3.466282	-0.010871	-0.636787
H	-3.364791	0.524816	-1.588282
H	-4.233857	-0.776267	-0.792705
H	-2.253965	-1.274527	0.620710
F	0.350315	-1.213655	1.136549
H	-1.095205	0.933311	0.660740
O	1.366144	0.508433	0.101801
C	-3.938597	0.955811	0.446534
H	-4.918398	1.373785	0.198361
H	-4.027420	0.447207	1.412657
H	-3.247146	1.793805	0.573870
C	3.589312	1.264878	0.065964
H	3.615362	1.479489	1.137804
H	3.242810	2.164394	-0.446383
H	4.586355	0.994407	-0.275989

Zero-point correction	=	0.196368
Thermal correction to Energy	=	0.208187
Thermal correction to Enthalpy	=	0.209131
Thermal correction to Gibbs Free Energy	=	0.157328
Sum of electronic and zero-point Energies	=	-524.703858
Sum of electronic and thermal Energies	=	-524.692039
Sum of electronic and thermal Enthalpies	=	-524.691095
Sum of electronic and thermal Free Energies	=	-524.742898
Number of imaginary frequencies/frequency	=	0

OPT-wB97xD-6-311+Gdp_1-fluoropentyl_acetateC_4.out

0 1

C	-2.516546	0.364652	-0.178437
O	-2.339934	1.519834	0.104538
C	-0.237223	-0.139567	0.220925
H	-0.067034	0.883418	-0.111172
C	0.765314	-1.139188	-0.294209
H	0.487312	-2.123858	0.093920
C	2.213391	-0.810773	0.071785
H	2.319970	-0.772270	1.161706
C	2.741796	0.486210	-0.540915
H	2.165832	1.339834	-0.167140
H	2.588190	0.458141	-1.626380
H	2.838106	-1.643885	-0.267787
F	-0.200387	-0.106960	1.618964
H	0.651934	-1.170699	-1.382684
O	-1.522401	-0.562735	-0.149286
C	4.219541	0.712018	-0.237409
H	4.581312	1.640666	-0.688102
H	4.393523	0.774771	0.841883
H	4.831354	-0.108635	-0.626382
C	-3.807391	-0.257640	-0.598879
H	-4.096961	-1.017667	0.130913
H	-3.683080	-0.752462	-1.564474
H	-4.581578	0.504221	-0.664154

Zero-point correction	=	0.196402
Thermal correction to Energy	=	0.208203
Thermal correction to Enthalpy	=	0.209147

Thermal correction to Gibbs Free Energy = 0.157393
Sum of electronic and zero-point Energies = -524.704075
Sum of electronic and thermal Energies = -524.692274
Sum of electronic and thermal Enthalpies = -524.69133
Sum of electronic and thermal Free Energies = -524.743084
Number of imaginary frequencies/frequency = 0

OPT-wB97xD-6-311+Gdp_1-fluoropentyl_acetateC_5.out

0 1

C	1.885076	-0.763306	0.130377
O	2.068839	-0.700377	1.316905
C	0.370082	1.057793	0.205338
H	0.195338	0.714157	1.223368
C	-0.877082	1.466793	-0.534440
H	-0.576685	1.893411	-1.496314
C	-1.865364	0.318980	-0.750825
H	-2.726095	0.721969	-1.295064
C	-2.358009	-0.349955	0.532896
H	-1.521491	-0.837000	1.047136
H	-2.740443	0.415729	1.218521
H	-1.411938	-0.435284	-1.403312
F	1.224680	2.160698	0.311957
H	-1.347906	2.263208	0.049888
O	1.049730	0.079743	-0.533369
C	-3.442842	-1.387154	0.261496
H	-3.077166	-2.168074	-0.413518
H	-3.772516	-1.871337	1.185134
H	-4.319206	-0.926930	-0.206589
C	2.511228	-1.735334	-0.814265
H	3.122518	-1.190340	-1.538058
H	1.734467	-2.268231	-1.366881
H	3.131926	-2.439390	-0.263669

Zero-point correction = 0.196415
Thermal correction to Energy = 0.208218
Thermal correction to Enthalpy = 0.209162
Thermal correction to Gibbs Free Energy = 0.157079
Sum of electronic and zero-point Energies = -524.704593
Sum of electronic and thermal Energies = -524.69279
Sum of electronic and thermal Enthalpies = -524.691846
Sum of electronic and thermal Free Energies = -524.74393
Number of imaginary frequencies/frequency = 0

OPT-wB97xD-6-311+Gdp_1-fluoropentyl_acetateC_6.out

0 1

C	-2.640861	-0.157887	0.192961
O	-2.579200	-1.152064	0.866735
C	-0.277758	-0.009200	0.091355
H	-0.309912	-0.495513	1.066442
C	0.737447	1.100797	0.006561
H	0.335781	1.919815	0.610144
C	2.128060	0.732135	0.528492
H	2.681966	1.667128	0.666657
C	2.953046	-0.188733	-0.370974
H	2.464406	-1.162931	-0.463033
H	2.990206	0.238464	-1.380139
H	2.031861	0.283216	1.524992
F	0.002749	-1.014691	-0.838399
H	0.786849	1.453213	-1.029357
O	-1.539502	0.507633	-0.244357
C	4.371509	-0.380542	0.156872
H	4.896096	0.577762	0.232800
H	4.361509	-0.833373	1.153904
H	4.957815	-1.031479	-0.498170
C	-3.888323	0.510756	-0.283937
H	-4.755781	0.061161	0.195375
H	-3.965227	0.385212	-1.367486
H	-3.849404	1.581037	-0.073549

Zero-point correction = 0.196203
Thermal correction to Energy = 0.20804
Thermal correction to Enthalpy = 0.208984
Thermal correction to Gibbs Free Energy = 0.157071
Sum of electronic and zero-point Energies = -524.702761
Sum of electronic and thermal Energies = -524.690924
Sum of electronic and thermal Enthalpies = -524.689979
Sum of electronic and thermal Free Energies = -524.741893
Number of imaginary frequencies/frequency = 0

OPT-wB97xD-6-311+Gdp_1-fluoropentyl_acetateC_7.out

0 1

C	2.382390	-0.360555	0.186862
O	2.749134	0.277329	1.137694
C	0.344904	0.847290	0.084853
H	0.476071	0.944157	1.162618
C	-1.074381	0.567895	-0.328841
H	-1.664164	1.442551	-0.042040
C	-1.630175	-0.695272	0.328568
H	-0.969754	-1.537988	0.101136
C	-3.048852	-1.039715	-0.129774
H	-3.337779	-1.990108	0.331135
H	-3.043750	-1.209602	-1.213124
H	-1.619728	-0.568539	1.418182
F	0.765164	2.059317	-0.473140
H	-1.110136	0.481862	-1.420357
O	1.186472	-0.151247	-0.425722
C	-4.090967	0.020789	0.216430
H	-3.907140	0.961772	-0.310205
H	-5.095685	-0.315193	-0.055972
H	-4.089814	0.233559	1.291085
C	3.129778	-1.467073	-0.481324
H	2.540882	-2.386339	-0.435878
H	4.089204	-1.616117	0.010054
H	3.284281	-1.222683	-1.534796

Zero-point correction = 0.196501
Thermal correction to Energy = 0.208224
Thermal correction to Enthalpy = 0.209168
Thermal correction to Gibbs Free Energy = 0.157447
Sum of electronic and zero-point Energies = -524.704094
Sum of electronic and thermal Energies = -524.692371
Sum of electronic and thermal Enthalpies = -524.691427
Sum of electronic and thermal Free Energies = -524.743148
Number of imaginary frequencies/frequency = 0

OPT-wB97xD-6-311+Gdp_1-fluoropentyl_acetateC_8.out

0 1

C	-2.321715	0.386709	0.081293
O	-2.174778	0.946556	1.135245
C	-0.079986	-0.377438	0.109710
H	0.109954	0.534655	0.674153
C	0.975648	-0.700757	-0.913929
H	0.672317	-1.608561	-1.444268
C	2.375535	-0.882661	-0.320775
H	2.389667	-1.783671	0.300552
C	2.900007	0.301788	0.497990
H	3.921735	0.066488	0.813730
H	2.317406	0.406942	1.420363
H	3.061449	-1.071425	-1.153653
F	-0.166268	-1.408408	1.051697
H	0.969003	0.115857	-1.641684
O	-1.323901	-0.302372	-0.534264
C	2.900304	1.627515	-0.258886
H	3.438678	1.537566	-1.208616
H	1.884564	1.966784	-0.483765
H	3.385417	2.412778	0.327826
C	-3.581295	0.323497	-0.718244
H	-4.303697	1.038743	-0.329432
H	-3.993625	-0.686630	-0.639397
H	-3.378013	0.520765	-1.771877

Zero-point correction = 0.196907
Thermal correction to Energy = 0.208406
Thermal correction to Enthalpy = 0.20935
Thermal correction to Gibbs Free Energy = 0.158622
Sum of electronic and zero-point Energies = -524.703433
Sum of electronic and thermal Energies = -524.691933
Sum of electronic and thermal Enthalpies = -524.690989
Sum of electronic and thermal Free Energies = -524.741717
Number of imaginary frequencies/frequency = 0

OPT-wB97xD-6-311+Gdp_1-fluoropentyl_acetateC_9.out

0 1

C	2.284861	-0.493774	0.133336
O	2.847826	0.203410	0.935012

C	0.413107	0.963393	0.081918
H	0.690406	1.185695	1.112407
C	-1.070566	0.826250	-0.128874
H	-1.519445	1.802189	0.080192
C	-1.684219	-0.233838	0.786152
H	-1.233910	-1.209008	0.569195
C	-3.204728	-0.341602	0.654859
H	-3.658871	0.629723	0.883845
H	-3.566584	-1.040326	1.416522
H	-1.431020	0.006452	1.825094
F	0.903368	2.017752	-0.695119
H	-1.246554	0.596110	-1.183819
O	1.051634	-0.204313	-0.360314
C	-3.674885	-0.814728	-0.718921
H	-4.759028	-0.959464	-0.732957
H	-3.429437	-0.093497	-1.503886
H	-3.206350	-1.768750	-0.983530
C	2.809090	-1.757589	-0.465717
H	3.007067	-1.588401	-1.527805
H	2.062314	-2.549971	-0.387990
H	3.729464	-2.051969	0.034703

Zero-point correction	=	0.196773
Thermal correction to Energy	=	0.208443
Thermal correction to Enthalpy	=	0.209387
Thermal correction to Gibbs Free Energy	=	0.158061
Sum of electronic and zero-point Energies	=	-524.703893
Sum of electronic and thermal Energies	=	-524.692224
Sum of electronic and thermal Enthalpies	=	-524.69128
Sum of electronic and thermal Free Energies	=	-524.742606
Number of imaginary frequencies/frequency	=	0

OPT-wB97xD-6-311+Gdp_1-fluoropentyl_acetateC_10.out

0 1

C	2.388604	0.427815	-0.093204
O	3.061540	-0.414394	-0.625926
C	0.429598	-0.868627	-0.392706
H	0.928284	-1.220257	-1.294930
C	-1.041206	-0.615235	-0.594521
H	-1.474958	-1.538048	-0.993720
C	-1.793272	-0.176441	0.661409
H	-1.669562	-0.939018	1.436689
C	-3.287772	0.043851	0.415056
H	-3.728787	-0.879722	0.020986
H	-3.772584	0.229666	1.379199
H	-1.351358	0.747031	1.051301
F	0.624165	-1.862895	0.572308
H	-1.116621	0.138148	-1.384279
O	1.047673	0.296958	0.085126
C	-3.597863	1.202908	-0.529923
H	-4.676869	1.359478	-0.617773
H	-3.153891	2.134536	-0.162767
H	-3.210491	1.024032	-1.537241
C	2.869430	1.732505	0.451761
H	3.939466	1.834164	0.282029
H	2.655995	1.782240	1.522146
H	2.335072	2.552637	-0.033255

Zero-point correction	=	0.196715
Thermal correction to Energy	=	0.208437
Thermal correction to Enthalpy	=	0.209381
Thermal correction to Gibbs Free Energy	=	0.157784
Sum of electronic and zero-point Energies	=	-524.703016
Sum of electronic and thermal Energies	=	-524.691295
Sum of electronic and thermal Enthalpies	=	-524.69035
Sum of electronic and thermal Free Energies	=	-524.741948
Number of imaginary frequencies/frequency	=	0

OPT-wB97xD-6-311+Gdp_2-fluoropentyl_acetateC_1.out

0 1

C	2.550870	-0.421479	-0.071611
O	2.146634	-1.550551	-0.218616
C	0.544454	0.186635	1.040840
H	0.336813	0.900192	1.838670
H	0.558836	-0.823675	1.451646
C	-0.515179	0.284899	-0.032345
H	-0.212514	-0.259182	-0.930717
C	-1.869255	-0.182793	0.456367
H	-1.755072	-1.224736	0.776567
C	-2.967935	-0.092914	-0.600486
H	-3.080955	0.945907	-0.925571
H	-2.664335	-0.668832	-1.482308
H	-2.148262	0.396683	1.344726
F	-0.605370	1.645361	-0.428198
O	1.845239	0.535655	0.549595
C	-4.304728	-0.612875	-0.081950
H	-5.079584	-0.549852	-0.851101
H	-4.225742	-1.659937	0.228465
H	-4.643149	-0.033521	0.783236
C	3.870857	0.099984	-0.547693
H	3.702380	0.832672	-1.341397
H	4.476863	-0.718348	-0.932037
H	4.393558	0.604803	0.267041

Zero-point correction	=	0.196349
Thermal correction to Energy	=	0.208294
Thermal correction to Enthalpy	=	0.209238
Thermal correction to Gibbs Free Energy	=	0.156731
Sum of electronic and zero-point Energies	=	-524.698979
Sum of electronic and thermal Energies	=	-524.687034
Sum of electronic and thermal Enthalpies	=	-524.68609
Sum of electronic and thermal Free Energies	=	-524.738597
Number of imaginary frequencies/frequency	=	0

OPT-wB97xD-6-311+Gdp_2-fluoropentyl_acetateC_2.out

0 1

C	-2.571701	0.331464	-0.093422
O	-3.213146	-0.314572	-0.888087
C	-0.668737	-1.002874	-0.525199
H	-1.172032	-1.938712	-0.272300
H	-0.747231	-0.841694	-1.603279
C	0.787827	-1.068074	-0.142936
H	1.249008	-1.862729	-0.736858
C	1.552182	0.229749	-0.293734
H	1.373496	0.594651	-1.312111
C	3.053532	0.080932	-0.057429
H	3.227077	-0.316082	0.947835
H	3.455402	-0.657085	-0.761251
H	1.130852	0.973840	0.389797
F	0.875519	-1.499085	1.207756
O	-1.284964	0.082752	0.177397
C	3.796676	1.403007	-0.217096
H	4.869862	1.276244	-0.049226
H	3.660822	1.814265	-1.222820
H	3.432441	2.146875	0.499008
C	-3.080948	1.493534	0.702232
H	-4.139758	1.646113	0.501628
H	-2.522041	2.393321	0.433093
H	-2.925679	1.310889	1.767699

Zero-point correction	=	0.19674
Thermal correction to Energy	=	0.20849
Thermal correction to Enthalpy	=	0.209434
Thermal correction to Gibbs Free Energy	=	0.157967
Sum of electronic and zero-point Energies	=	-524.698631
Sum of electronic and thermal Energies	=	-524.686881
Sum of electronic and thermal Enthalpies	=	-524.685937
Sum of electronic and thermal Free Energies	=	-524.737404
Number of imaginary frequencies/frequency	=	0

OPT-wB97xD-6-311+Gdp_2-fluoropentyl_acetateC_3.out

0 1

C	2.398863	-0.310632	-0.155427
O	2.592032	0.505077	-1.023900
C	0.680217	1.036653	0.785182
H	0.368859	1.205409	1.816533
H	1.272403	1.882821	0.435481
C	-0.533274	0.838583	-0.112692
H	-0.217711	0.619393	-1.136352
C	-1.515027	-0.192387	0.392283
H	-0.960048	-1.125455	0.542800
C	-2.686810	-0.441971	-0.554793
H	-3.223235	0.496621	-0.727319
H	-2.297673	-0.766250	-1.526792
H	-1.878342	0.124872	1.377368
F	-1.172626	2.102436	-0.165831

O	1.479567	-0.150994	0.812370
C	-3.653997	-1.488840	-0.012521
H	-4.078478	-1.172513	0.945773
H	-4.482631	-1.658112	-0.705901
H	-3.149132	-2.447470	0.145756
C	3.111647	-1.618822	-0.013700
H	2.446188	-2.414859	-0.360457
H	3.356765	-1.816377	1.030581
H	4.014161	-1.618158	-0.622748

Zero-point correction	=	0.196535
Thermal correction to Energy	=	0.208376
Thermal correction to Enthalpy	=	0.209321
Thermal correction to Gibbs Free Energy	=	0.157451
Sum of electronic and zero-point Energies	=	-524.696674
Sum of electronic and thermal Energies	=	-524.684833
Sum of electronic and thermal Enthalpies	=	-524.683888
Sum of electronic and thermal Free Energies	=	-524.735758
Number of imaginary frequencies/frequency	=	0

OPT-wB97xD-6-311+Gdp_2-fluoropentyl_acetateC_4.out

0 1

C	-2.645638	-0.452575	-0.019980
O	-2.514008	-1.645421	-0.162128
C	-0.305205	-0.216602	0.192701
H	-0.238372	-0.946620	1.003395
H	-0.124478	-0.722691	-0.757769
C	0.697122	0.884951	0.422277
H	0.364928	1.525208	1.242890
C	2.107233	0.390554	0.680317
H	2.750526	1.271956	0.774285
C	2.676635	-0.557062	-0.376051
H	2.096932	-1.485880	-0.394630
H	2.575646	-0.102564	-1.367185
H	2.105640	-0.100027	1.660266
F	0.702813	1.717483	-0.728701
O	-1.611438	0.374221	0.177645
C	4.142605	-0.884960	-0.110993
H	4.536006	-1.574948	-0.862788
H	4.757897	0.020450	-0.131634
H	4.269837	-1.352765	0.870900
C	-3.945293	0.290936	-0.036632
H	-4.093115	0.793184	0.922381
H	-4.765031	-0.401121	-0.220362
H	-3.922916	1.056609	-0.815418

Zero-point correction	=	0.196955
Thermal correction to Energy	=	0.20868
Thermal correction to Enthalpy	=	0.209624
Thermal correction to Gibbs Free Energy	=	0.158227
Sum of electronic and zero-point Energies	=	-524.698279
Sum of electronic and thermal Energies	=	-524.686554
Sum of electronic and thermal Enthalpies	=	-524.68561
Sum of electronic and thermal Free Energies	=	-524.737008
Number of imaginary frequencies/frequency	=	0

OPT-wB97xD-6-311+Gdp_2-fluoropentyl_acetateC_5.out

0 1

C	-2.484311	0.220515	-0.232973
O	-2.212674	1.309855	-0.679653
C	-0.538503	0.253845	1.126646
H	-0.710774	1.326866	1.217012
H	-0.322672	-0.164398	2.110097
C	0.617317	-0.003904	0.184752
H	0.339515	0.241685	-0.843744
C	1.873153	0.734601	0.603737
H	1.577434	1.767043	0.818037
C	2.996114	0.757885	-0.436505
H	2.604033	1.177319	-1.370426
H	3.759657	1.458136	-0.082426
H	2.231837	0.306147	1.547259
F	0.858047	-1.403090	0.187613
O	-1.736995	-0.401835	0.691025
C	3.654272	-0.591287	-0.715574
H	4.026488	-1.045280	0.208781
H	2.958026	-1.296264	-1.175625
H	4.503731	-0.470010	-1.394268
C	-3.662161	-0.613029	-0.632119
H	-3.305831	-1.475253	-1.202695
H	-4.339110	-0.025667	-1.249785
H	-4.182699	-0.988423	0.250508

Zero-point correction	=	0.196599
Thermal correction to Energy	=	0.208438
Thermal correction to Enthalpy	=	0.209382
Thermal correction to Gibbs Free Energy	=	0.157207
Sum of electronic and zero-point Energies	=	-524.696655
Sum of electronic and thermal Energies	=	-524.684816
Sum of electronic and thermal Enthalpies	=	-524.683872
Sum of electronic and thermal Free Energies	=	-524.736047
Number of imaginary frequencies/frequency	=	0

OPT-wB97xD-6-311+Gdp_2-fluoropentyl_acetateC_6.out

0 1

C	2.109709	-0.516520	0.037342
O	1.496540	-1.537404	-0.166782
C	0.161150	0.523441	0.911642
H	-0.077553	-0.454809	1.330493
H	0.017626	1.289554	1.674452
C	-0.720958	0.801628	-0.282815
H	-0.464425	0.139296	-1.111822
C	-2.203838	0.750052	0.038053
H	-2.416278	1.500823	0.806823
C	-2.713569	-0.619798	0.500266
H	-2.284424	-0.866116	1.476964
H	-3.792971	-0.531526	0.656649
H	-2.740383	1.050205	-0.867936
F	-0.426012	2.111668	-0.744091
O	1.554127	0.579304	0.575260
C	-2.433887	-1.752441	-0.484802
H	-2.912705	-2.678598	-0.155122
H	-2.820877	-1.511537	-1.480553
H	-1.362355	-1.951473	-0.579960
C	3.558508	-0.293926	-0.267531
H	3.651129	0.483323	-1.030323
H	4.008350	-1.216287	-0.630102
H	4.080958	0.052317	0.626509

Zero-point correction	=	0.197104
Thermal correction to Energy	=	0.20878
Thermal correction to Enthalpy	=	0.209725
Thermal correction to Gibbs Free Energy	=	0.158243
Sum of electronic and zero-point Energies	=	-524.697483
Sum of electronic and thermal Energies	=	-524.685806
Sum of electronic and thermal Enthalpies	=	-524.684862
Sum of electronic and thermal Free Energies	=	-524.736344
Number of imaginary frequencies/frequency	=	0

OPT-wB97xD-6-311+Gdp_2-fluoropentyl_acetateC_7.out

0 1

C	2.263978	-0.361905	-0.132446
O	2.125821	-1.093771	-1.082911
C	0.521355	1.085265	-0.892533
H	0.627932	2.150116	-1.100365
H	0.661304	0.521061	-1.815342
C	-0.856174	0.802594	-0.338867
H	-1.577541	1.051612	-1.121614
C	-1.061468	-0.605254	0.180645
H	-0.829555	-1.288848	-0.643834
C	-2.471777	-0.890215	0.702073
H	-2.472278	-1.898416	1.127908
H	-2.701883	-0.208549	1.527259
H	-0.329738	-0.798032	0.972293
F	-1.106228	1.717791	0.718916
O	1.550251	0.759762	0.051556
C	-3.559640	-0.794988	-0.364472
H	-3.334451	-1.448967	-1.213701
H	-4.528542	-1.097541	0.042601
H	-3.670645	0.223805	-0.747465
C	3.223868	-0.581877	0.995613
H	3.946205	-1.349256	0.723369
H	2.661199	-0.913025	1.873322
H	3.734608	0.346277	1.256085

Zero-point correction	=	0.196788
Thermal correction to Energy	=	0.208565

Thermal correction to Enthalpy = 0.209509
Thermal correction to Gibbs Free Energy = 0.157807
Sum of electronic and zero-point Energies = -524.697802
Sum of electronic and thermal Energies = -524.686025
Sum of electronic and thermal Enthalpies = -524.685081
Sum of electronic and thermal Free Energies = -524.736783
Number of imaginary frequencies/frequency = 0

OPT-wB97xD-6-311+Gdp_2-fluoropentyl_acetateC_8.out

0 1

C	2.797219	0.089820	0.029932
O	3.096346	1.194404	-0.358759
C	0.508403	0.653115	-0.114719
H	0.599491	0.975165	-1.155254
H	0.616704	1.521729	0.538418
C	-0.830556	0.004717	0.129619
H	-0.862094	-0.429540	1.132888
C	-1.984356	0.965147	-0.096229
H	-1.693139	1.934450	0.321461
C	-3.309160	0.537288	0.539247
H	-3.168981	0.459954	1.623760
H	-4.034249	1.341921	0.379015
H	-2.101820	1.110347	-1.176277
F	-0.947211	-1.092211	-0.763057
O	1.528656	-0.306111	0.189254
C	-3.888670	-0.771002	0.007490
H	-4.866637	-0.967018	0.456634
H	-4.020115	-0.732176	-1.078720
H	-3.241225	-1.621613	0.235221
C	3.760839	-0.992655	0.407047
H	3.694539	-1.172014	1.483485
H	4.775564	-0.692946	0.151389
H	3.504528	-1.923275	-0.102795

Zero-point correction = 0.19646
Thermal correction to Energy = 0.208331
Thermal correction to Enthalpy = 0.209275
Thermal correction to Gibbs Free Energy = 0.157182
Sum of electronic and zero-point Energies = -524.697097
Sum of electronic and thermal Energies = -524.685226
Sum of electronic and thermal Enthalpies = -524.684282
Sum of electronic and thermal Free Energies = -524.736375
Number of imaginary frequencies/frequency = 0

OPT-wB97xD-6-311+Gdp_2-fluoropentyl_acetateC_9.out

0 1

C	2.255593	0.229927	0.179468
O	2.239993	-0.163242	1.320611
C	0.557356	-1.321591	-0.424604
H	0.368007	-1.874759	-1.345207
H	1.011037	-1.981114	0.316015
C	-0.736404	-0.730144	0.118902
H	-0.527362	-0.133621	1.009620
C	-1.530690	0.044288	-0.908349
H	-0.867417	0.819211	-1.309510
C	-2.809218	0.694078	-0.374788
H	-3.333135	1.146129	-1.222874
H	-3.477065	-0.077634	0.022289
H	-1.766598	-0.633566	-1.736466
F	-1.504517	-1.834558	0.564020
O	1.467127	-0.275876	-0.784212
C	-2.562551	1.761793	0.688356
H	-1.865399	2.523445	0.323099
H	-3.495696	2.263658	0.959192
H	-2.142106	1.337190	1.604756
C	3.141719	1.309389	-0.359238
H	2.549268	2.043623	-0.908572
H	3.861553	0.872041	-1.056155
H	3.673775	1.792930	0.457953

Zero-point correction = 0.196823
Thermal correction to Energy = 0.208589
Thermal correction to Enthalpy = 0.209533
Thermal correction to Gibbs Free Energy = 0.157508
Sum of electronic and zero-point Energies = -524.696036
Sum of electronic and thermal Energies = -524.68427
Sum of electronic and thermal Enthalpies = -524.683325
Sum of electronic and thermal Free Energies = -524.73535
Number of imaginary frequencies/frequency = 0

OPT-wB97xD-6-311+Gdp_2-fluoropentyl_acetateC_10.out

0 1

C	-2.471712	-0.390669	-0.101796
O	-2.491109	-1.144572	-1.046128
C	-0.182411	0.048868	-0.489392
H	-0.329294	0.387890	-1.518225
H	0.045754	-1.018971	-0.497301
C	0.939458	0.807858	0.168033
H	0.969981	0.584998	1.236636
C	2.289788	0.591913	-0.491311
H	2.219275	0.917099	-1.534733
C	2.814686	-0.846943	-0.434147
H	2.183114	-1.499283	-1.046019
H	3.801685	-0.852977	-0.906523
H	3.000736	1.256729	0.010047
F	0.639496	2.192855	0.081960
O	-1.374068	0.276472	0.274108
C	2.927481	-1.416766	0.977873
H	3.412851	-2.396367	0.960973
H	3.522504	-0.759557	1.620753
H	1.946773	-1.545050	1.445977
C	-3.630461	-0.093063	0.799069
H	-3.448517	-0.549579	1.775931
H	-4.543689	-0.506060	0.374375
H	-3.736194	0.983032	0.946660

Zero-point correction = 0.197239
Thermal correction to Energy = 0.208833
Thermal correction to Enthalpy = 0.209777
Thermal correction to Gibbs Free Energy = 0.15884
Sum of electronic and zero-point Energies = -524.69769
Sum of electronic and thermal Energies = -524.686096
Sum of electronic and thermal Enthalpies = -524.685152
Sum of electronic and thermal Free Energies = -524.736089
Number of imaginary frequencies/frequency = 0

OPT-wB97xD-6-311+Gdp_3-fluoropentyl_acetateC_1.out

0 1

C	-2.740213	-0.271231	-0.132685
O	-2.399588	-1.133505	-0.908687
C	-0.659611	0.853220	-0.398332
H	-0.708259	0.534239	-1.441357
H	-0.404775	1.911293	-0.359838
C	0.333592	0.013779	0.387956
H	0.359646	0.343220	1.431659
H	0.017916	-1.033161	0.373508
C	1.730329	0.078736	-0.193653
H	1.716673	-0.156644	-1.262840
C	2.734174	-0.792776	0.530815
H	2.753971	-0.504392	1.587651
H	2.353971	-1.818648	0.487206
F	2.174232	1.433744	-0.123584
C	-4.046399	-0.231891	0.600060
H	-4.712148	-1.003229	0.216736
H	-3.863131	-0.406628	1.663681
H	-4.511890	0.750171	0.497816
C	4.135038	-0.734291	-0.067911
H	4.560726	0.269695	0.005975
H	4.805751	-1.418883	0.457617
H	4.122028	-1.020649	-1.124318
O	-1.972915	0.778086	0.186345

Zero-point correction = 0.196162
Thermal correction to Energy = 0.208189
Thermal correction to Enthalpy = 0.209133
Thermal correction to Gibbs Free Energy = 0.155854
Sum of electronic and zero-point Energies = -524.701104
Sum of electronic and thermal Energies = -524.689077
Sum of electronic and thermal Enthalpies = -524.688133
Sum of electronic and thermal Free Energies = -524.741412
Number of imaginary frequencies/frequency = 0

OPT-wB97xD-6-311+Gdp_3-fluoropentyl_acetateC_2.out

0 1

C	-2.653779	0.216953	0.088825

O	-3.224880	-0.713488	0.608967
C	-0.749758	-1.144216	-0.300621
H	-0.749050	-1.465515	0.742799
H	-1.301312	-1.880006	-0.889623
C	0.655990	-0.973898	-0.835606
H	1.130628	-1.959755	-0.872669
H	0.614295	-0.594281	-1.860918
C	1.523051	-0.038798	-0.016515
H	1.027498	0.924679	0.133694
C	2.910195	0.161285	-0.588873
H	3.391785	-0.816931	-0.698271
H	2.782137	0.568174	-1.597450
F	1.648580	-0.595011	1.291775
C	-3.226028	1.588383	-0.104382
H	-4.172479	1.673994	0.426399
H	-2.524742	2.345363	0.251836
H	-3.391671	1.761014	-1.171238
C	3.781573	1.098267	0.240716
H	3.308671	2.079440	0.349452
H	3.958736	0.695745	1.241298
H	4.753715	1.244452	-0.237114
O	-1.414232	0.129845	-0.402146

Zero-point correction	=	0.196941
Thermal correction to Energy	=	0.208588
Thermal correction to Enthalpy	=	0.209532
Thermal correction to Gibbs Free Energy	=	0.158334
Sum of electronic and zero-point Energies	=	-524.701748
Sum of electronic and thermal Energies	=	-524.690101
Sum of electronic and thermal Enthalpies	=	-524.689157
Sum of electronic and thermal Free Energies	=	-524.740355
Number of imaginary frequencies/frequency	=	0

OPT-wB97xD-6-311+Gdp_3-fluoropentyl_acetateC_3.out

0 1

C	2.425805	0.293689	0.105105
O	2.652126	-0.074000	1.234329
C	0.778452	-1.405757	-0.167952
H	0.447596	-1.952747	-1.049961
H	1.440996	-2.043779	0.417984
C	-0.401100	-0.948356	0.672249
H	-0.915670	-1.839490	1.047501
H	-0.041603	-0.391719	1.541995
C	-1.392408	-0.074996	-0.068915
H	-0.894182	0.788060	-0.520169
C	-2.560971	0.372918	0.782900
H	-3.069858	-0.514720	1.174894
H	-2.142161	0.904484	1.643811
F	-1.899936	-0.823611	-1.172830
C	3.101603	1.439126	-0.585394
H	3.592959	1.083681	-1.494030
H	2.356869	2.182786	-0.878152
H	3.835134	1.892408	0.078858
C	-3.544109	1.275336	0.045375
H	-4.341562	1.604776	0.716545
H	-3.041904	2.167249	-0.342412
H	-4.010176	0.756874	-0.796602
O	1.527793	-0.293140	-0.694956

Zero-point correction	=	0.196775
Thermal correction to Energy	=	0.208563
Thermal correction to Enthalpy	=	0.209507
Thermal correction to Gibbs Free Energy	=	0.15771
Sum of electronic and zero-point Energies	=	-524.701361
Sum of electronic and thermal Energies	=	-524.689573
Sum of electronic and thermal Enthalpies	=	-524.688628
Sum of electronic and thermal Free Energies	=	-524.740426
Number of imaginary frequencies/frequency	=	0

OPT-wB97xD-6-311+Gdp_3-fluoropentyl_acetateC_5.out

0 1

C	2.881424	-0.032846	0.088375
O	3.107409	1.002207	0.671193
C	0.552806	0.380552	0.226647
H	0.571072	0.481802	1.315200
H	0.678924	1.369580	-0.217441
C	-0.723763	-0.287562	-0.241754
H	-0.712074	-0.405915	-1.330188
H	-0.787928	-1.285188	0.201986
C	-1.961505	0.485213	0.163373
H	-1.964620	0.672964	1.241774
C	-3.272404	-0.142400	-0.269583
H	-4.068754	0.575254	-0.050864
H	-3.252113	-0.290734	-1.354582
F	-1.887939	1.776822	-0.438272
C	3.916511	-0.996029	-0.407593
H	3.811552	-1.947556	0.119517
H	3.768730	-1.186630	-1.472686
H	4.912255	-0.590810	-0.236938
C	-3.566193	-1.461785	0.440259
H	-3.528995	-1.340601	1.527416
H	-4.565090	-1.818154	0.177519
H	-2.852752	-2.241461	0.161724
O	1.645090	-0.459058	-0.188234

Zero-point correction	=	0.196676
Thermal correction to Energy	=	0.208587
Thermal correction to Enthalpy	=	0.209531
Thermal correction to Gibbs Free Energy	=	0.157343
Sum of electronic and zero-point Energies	=	-524.700802
Sum of electronic and thermal Energies	=	-524.688891
Sum of electronic and thermal Enthalpies	=	-524.687947
Sum of electronic and thermal Free Energies	=	-524.740135
Number of imaginary frequencies/frequency	=	0

OPT-wB97xD-6-311+Gdp_3-fluoropentyl_acetateC_6.out

0 1

C	-2.634996	0.332549	-0.040290
O	-2.238983	1.461958	0.130975
C	-0.445448	-0.391336	-0.626538
H	-0.103952	-1.162672	-1.316265
H	-0.342271	0.583969	-1.103019
C	0.302319	-0.464381	0.695923
H	-0.022350	0.347412	1.353249
H	0.058929	-1.407387	1.194272
C	1.810521	-0.368669	0.560596
H	2.263368	-0.429319	1.553988
C	2.330896	0.847831	-0.178480
H	1.983572	0.815371	-1.216159
H	1.870399	1.727562	0.283874
F	2.268392	-1.535695	-0.123048
C	-4.047505	-0.129028	0.150139
H	-4.679900	0.712565	0.426910
H	-4.418334	-0.586577	-0.769659
H	-4.078591	-0.887889	0.935779
C	3.850126	0.970759	-0.136635
H	4.210526	1.030482	0.895159
H	4.332165	0.113680	-0.614535
H	4.179120	1.872380	-0.659644
O	-1.843978	-0.673792	-0.431575

Zero-point correction	=	0.197168
Thermal correction to Energy	=	0.208874
Thermal correction to Enthalpy	=	0.209818
Thermal correction to Gibbs Free Energy	=	0.158231
Sum of electronic and zero-point Energies	=	-524.699451
Sum of electronic and thermal Energies	=	-524.687745
Sum of electronic and thermal Enthalpies	=	-524.686801
Sum of electronic and thermal Free Energies	=	-524.738387
Number of imaginary frequencies/frequency	=	0

OPT-wB97xD-6-311+Gdp_3-fluoropentyl_acetateC_7.out

0 1

C	2.802125	0.310116	0.090564
O	2.674708	1.375450	0.648367
C	0.449725	0.040251	0.038910
H	0.353326	0.169377	1.119395
H	0.326524	1.013177	-0.440642
C	-0.537004	-0.981464	-0.492406
H	-0.463543	-1.033402	-1.583135
H	-0.284768	-1.971056	-0.100645
C	-1.982383	-0.682304	-0.139499
H	-2.625570	-1.443379	-0.589477
C	-2.476849	0.703925	-0.500062
H	-1.911838	1.447294	0.071669

H	-2.239823	0.867470	-1.556901
F	-2.136906	-0.856535	1.269244
C	4.106949	-0.301708	-0.319818
H	4.927723	0.196778	0.193396
H	4.119430	-1.371422	-0.106617
H	4.230798	-0.171496	-1.398876
C	-3.972274	0.887987	-0.265557
H	-4.554119	0.178828	-0.862630
H	-4.230410	0.736926	0.786076
H	-4.285357	1.897649	-0.543824
O	1.766298	-0.459043	-0.258839

Zero-point correction	=	0.196772
Thermal correction to Energy	=	0.208571
Thermal correction to Enthalpy	=	0.209516
Thermal correction to Gibbs Free Energy	=	0.158111
Sum of electronic and zero-point Energies	=	-524.700294
Sum of electronic and thermal Energies	=	-524.688495
Sum of electronic and thermal Enthalpies	=	-524.687551
Sum of electronic and thermal Free Energies	=	-524.738955
Number of imaginary frequencies/frequency	=	0

OPT-wB97xD-6-311+Gdp_3-fluoropentyl_acetateC_8.out

0 1

C	-2.694116	0.012097	-0.015278
O	-3.157142	-1.054631	0.316411
C	-0.572868	-0.993849	-0.344414
H	-0.607370	-1.431900	0.655065
H	-0.954010	-1.727714	-1.057614
C	0.830499	-0.566255	-0.717417
H	1.448494	-1.466876	-0.776336
H	0.826308	-0.108631	-1.711824
C	1.453243	0.418203	0.252893
H	0.778934	1.259732	0.427561
C	2.822954	0.934331	-0.146004
H	2.683411	1.549661	-1.041399
H	3.167703	1.608720	0.644171
F	1.566711	-0.230699	1.520027
C	-3.447345	1.306298	-0.069265
H	-3.047720	1.990041	0.684427
H	-3.320284	1.777048	-1.046232
H	-4.503764	1.129547	0.125009
C	3.870958	-0.143895	-0.407924
H	4.845097	0.315902	-0.593074
H	3.977475	-0.812850	0.450608
H	3.621125	-0.751324	-1.281986
O	-1.417327	0.172549	-0.375681

Zero-point correction	=	0.197023
Thermal correction to Energy	=	0.208712
Thermal correction to Enthalpy	=	0.209657
Thermal correction to Gibbs Free Energy	=	0.158029
Sum of electronic and zero-point Energies	=	-524.700938
Sum of electronic and thermal Energies	=	-524.689248
Sum of electronic and thermal Enthalpies	=	-524.688304
Sum of electronic and thermal Free Energies	=	-524.739932
Number of imaginary frequencies/frequency	=	0

OPT-wB97xD-6-311+Gdp_3-fluoropentyl_acetateC_9.out

0 1

C	-2.530900	0.230064	-0.023522
O	-3.007045	0.091432	-1.126180
C	-0.630067	-1.031991	-0.669584
H	-1.212073	-1.914234	-0.944520
H	-0.508980	-0.411783	-1.559804
C	0.700153	-1.445467	-0.074798
H	0.523840	-2.088793	0.792020
H	1.230690	-2.037696	-0.827468
C	1.577583	-0.281690	0.354769
H	1.082716	0.312187	1.127839
C	2.066298	0.609233	-0.767311
H	2.583640	-0.009089	-1.509443
H	1.184655	1.029487	-1.261836
F	2.714648	-0.852178	0.999677
C	-3.166104	0.973847	1.111562
H	-4.076838	1.463010	0.771066
H	-3.405697	0.271603	1.914295
H	-2.470195	1.713773	1.512244
C	2.966347	1.743362	-0.288100
H	3.255112	2.386126	-1.123671
H	2.451424	2.364754	0.451415
H	3.881539	1.360555	0.170335
O	-1.349397	-0.285737	0.330223

Zero-point correction	=	0.196819
Thermal correction to Energy	=	0.208597
Thermal correction to Enthalpy	=	0.209541
Thermal correction to Gibbs Free Energy	=	0.157551
Sum of electronic and zero-point Energies	=	-524.700841
Sum of electronic and thermal Energies	=	-524.689064
Sum of electronic and thermal Enthalpies	=	-524.688119
Sum of electronic and thermal Free Energies	=	-524.740109
Number of imaginary frequencies/frequency	=	0

OPT-wB97xD-6-311+Gdp_3-fluoropentyl_acetateC_10.out

0 1

C	-2.656823	-0.001561	0.029137
O	-3.225049	-1.001386	-0.347167
C	-0.598468	-1.169097	0.082888
H	-0.984991	-1.936585	0.757522
H	-0.742692	-1.509781	-0.946039
C	0.863653	-0.901694	0.369434
H	0.988126	-0.511888	1.383855
H	1.369635	-1.872465	0.337562
C	1.564689	0.009103	-0.623094
H	1.205265	-0.187806	-1.637213
C	3.080785	-0.070179	-0.594443
H	3.466171	0.656446	-1.316687
H	3.358780	-1.060930	-0.969710
F	1.191875	1.358100	-0.354359
C	-3.306588	1.330092	0.255834
H	-3.075339	1.697946	1.257522
H	-2.913393	2.052675	-0.463968
H	-4.384300	1.241935	0.130748
C	3.708788	0.167895	0.775956
H	4.799063	0.165611	0.697956
H	3.406286	1.134162	1.188945
H	3.425967	-0.609076	1.491233
O	-1.347661	0.042575	0.285072

Zero-point correction	=	0.196609
Thermal correction to Energy	=	0.208494
Thermal correction to Enthalpy	=	0.209438
Thermal correction to Gibbs Free Energy	=	0.156556
Sum of electronic and zero-point Energies	=	-524.69914
Sum of electronic and thermal Energies	=	-524.687255
Sum of electronic and thermal Enthalpies	=	-524.68631
Sum of electronic and thermal Free Energies	=	-524.739193
Number of imaginary frequencies/frequency	=	0

OPT-wB97xD-6-311+Gdp_4-fluoropentyl_acetateC_1.out

0 1

C	3.132460	-0.120265	-0.049034
O	3.321369	-1.270417	-0.372852
C	0.790254	-0.474883	-0.092460
H	0.816789	-0.860764	-1.115048
H	0.875672	-1.318450	0.597953
C	-0.469749	0.322148	0.166399
H	-0.431021	0.738735	1.178535
H	-0.516231	1.160219	-0.534840
C	-1.710042	-0.556325	0.021157
H	-1.766362	-0.981753	-0.987627
C	-3.003858	0.172407	0.316007
H	-2.949744	0.667735	1.289531
H	-1.649606	-1.397906	0.720352
O	1.913995	0.403440	0.107626
C	-4.235232	-0.694958	0.221293
H	-5.138234	-0.104584	0.392764
H	-4.301424	-1.171263	-0.760993
H	-4.189083	-1.476647	0.984100
F	-3.144272	1.234876	-0.628254
C	4.206722	0.881386	0.249720
H	4.229920	1.064153	1.327827
H	3.998435	1.831032	-0.245856
H	5.173097	0.494368	-0.069089

Zero-point correction = 0.196549
Thermal correction to Energy = 0.208432
Thermal correction to Enthalpy = 0.209376
Thermal correction to Gibbs Free Energy = 0.157393
Sum of electronic and zero-point Energies = -524.702767
Sum of electronic and thermal Energies = -524.690885
Sum of electronic and thermal Enthalpies = -524.689941
Sum of electronic and thermal Free Energies = -524.741924
Number of imaginary frequencies/frequency = 0

OPT-wB97xD-6-311+Gdp_4-fluoropentyl_acetateC_2.out

0 1

C	-2.872646	0.144016	-0.071949
O	-3.453479	-0.741257	-0.657066
C	-0.878436	-1.143657	-0.056735
H	-1.380071	-1.990051	0.417397
H	-0.912652	-1.282408	-1.140929
C	0.543770	-1.003876	0.439687
H	0.532507	-0.832465	1.521723
H	1.038533	-1.965512	0.273329
C	1.315901	0.111803	-0.259867
H	1.371465	-0.083318	-1.337473
C	2.716783	0.309440	0.277514
H	2.693707	0.455324	1.361294
H	0.789012	1.062864	-0.132039
O	-1.587756	0.065464	0.281743
C	3.484875	1.418496	-0.398893
H	4.496569	1.492892	0.006436
H	3.543489	1.246739	-1.477325
H	2.977656	2.371537	-0.226803
F	3.447308	-0.904033	0.086201
C	-3.476834	1.451703	0.341901
H	-2.987416	2.266037	-0.198567
H	-3.316527	1.617712	1.409211
H	-4.542640	1.455743	0.120589

Zero-point correction = 0.19691
Thermal correction to Energy = 0.208591
Thermal correction to Enthalpy = 0.209535
Thermal correction to Gibbs Free Energy = 0.158077
Sum of electronic and zero-point Energies = -524.702953
Sum of electronic and thermal Energies = -524.691272
Sum of electronic and thermal Enthalpies = -524.690328
Sum of electronic and thermal Free Energies = -524.741786
Number of imaginary frequencies/frequency = 0

OPT-wB97xD-6-311+Gdp_4-fluoropentyl_acetateC_3.out

0 1

C	-2.477249	-0.285079	0.082117
O	-2.658336	0.093825	1.216202
C	-0.963378	1.508785	-0.330169
H	-0.759335	2.075436	-1.239952
H	-1.612258	2.098816	0.318326
C	0.324186	1.131273	0.378798
H	0.780445	2.061196	0.736726
H	0.088091	0.532112	1.262613
C	1.308808	0.391493	-0.522910
H	0.859475	-0.527556	-0.914596
C	2.611115	0.037504	0.163123
H	3.043835	0.917613	0.647482
H	1.556953	1.019272	-1.386572
O	-1.683055	0.345344	-0.789484
C	3.620477	-0.629373	-0.739010
H	4.511290	-0.918508	-0.176518
H	3.192315	-1.517653	-1.212044
H	3.924482	0.069016	-1.523118
F	2.319416	-0.863526	1.233474
C	-3.094586	-1.506921	-0.528155
H	-3.549330	-1.264832	-1.490477
H	-3.842094	-1.921238	0.146186
H	-2.313718	-2.251386	-0.705833

Zero-point correction = 0.196647
Thermal correction to Energy = 0.208529
Thermal correction to Enthalpy = 0.209473
Thermal correction to Gibbs Free Energy = 0.156246
Sum of electronic and zero-point Energies = -524.702386
Sum of electronic and thermal Energies = -524.690504
Sum of electronic and thermal Enthalpies = -524.68956
Sum of electronic and thermal Free Energies = -524.742787
Number of imaginary frequencies/frequency = 0

OPT-wB97xD-6-311+Gdp_4-fluoropentyl_acetateC_4.out

0 1

C	3.040324	-0.021005	-0.000695
O	3.339968	-1.172961	-0.216158
C	0.741533	-0.581652	-0.115694
H	0.877229	-1.056885	-1.090884
H	0.835785	-1.348314	0.658193
C	-0.593202	0.127056	-0.030290
H	-0.683507	0.611806	0.946517
H	-0.628501	0.909689	-0.793356
C	-1.737775	-0.864996	-0.232526
H	-1.688243	-1.292741	-1.240325
C	-3.128108	-0.281680	-0.062959
H	-3.870126	-1.065267	-0.233953
H	-1.636111	-1.700871	0.468129
O	1.775680	0.402230	0.073918
C	-3.442228	0.934043	-0.902076
H	-3.298896	0.695564	-1.959624
H	-4.480528	1.240023	-0.756023
H	-2.789790	1.772229	-0.645831
F	-3.293678	0.085935	1.308403
C	4.011042	1.100639	0.213014
H	3.836510	1.563826	1.186859
H	3.864280	1.867048	-0.551916
H	5.030303	0.721898	0.161867

Zero-point correction = 0.197055
Thermal correction to Energy = 0.208803
Thermal correction to Enthalpy = 0.209747
Thermal correction to Gibbs Free Energy = 0.158073
Sum of electronic and zero-point Energies = -524.701704
Sum of electronic and thermal Energies = -524.689956
Sum of electronic and thermal Enthalpies = -524.689012
Sum of electronic and thermal Free Energies = -524.740687
Number of imaginary frequencies/frequency = 0

OPT-wB97xD-6-311+Gdp_4-fluoropentyl_acetateC_5.out

0 1

C	-2.856981	0.324571	0.028142
O	-2.736840	1.512044	-0.169257
C	-0.532953	0.019900	-0.308234
H	-0.571938	0.484795	-1.297473
H	-0.297691	0.791793	0.427506
C	0.464158	-1.120678	-0.276896
H	0.516563	-1.533912	0.734532
H	0.104508	-1.918012	-0.933750
C	1.856852	-0.698284	-0.748126
H	2.508055	-1.577719	-0.785518
C	2.534712	0.362023	0.097767
H	1.919064	1.261417	0.177543
H	1.796594	-0.303913	-1.768855
O	-1.829023	-0.527751	0.000367
C	3.924185	0.716527	-0.372281
H	3.867439	1.161421	-1.369263
H	4.385374	1.443368	0.300230
H	4.555807	-0.174914	-0.424944
F	2.636863	-0.132532	1.433721
C	-4.152253	-0.377756	0.301105
H	-4.037727	-1.110815	1.100929
H	-4.457456	-0.912125	-0.603360
H	-4.919771	0.349243	0.561183

Zero-point correction = 0.196617
Thermal correction to Energy = 0.208472
Thermal correction to Enthalpy = 0.209417
Thermal correction to Gibbs Free Energy = 0.156565
Sum of electronic and zero-point Energies = -524.70209
Sum of electronic and thermal Energies = -524.690235
Sum of electronic and thermal Enthalpies = -524.689291
Sum of electronic and thermal Free Energies = -524.742143
Number of imaginary frequencies/frequency = 0

OPT-wB97xD-6-311+Gdp_4-fluoropentyl_acetateC_6.out

0 1

C	2.779242	0.229670	0.144987
O	2.394173	0.929233	1.053026
C	0.820244	-1.115390	0.287853
H	0.661274	-2.176278	0.091506
H	0.890396	-0.959538	1.366234
C	-0.289593	-0.277565	-0.321607
H	-0.074745	0.780814	-0.153330
H	-0.309931	-0.445248	-1.403854
C	-1.641693	-0.648987	0.287066
H	-1.803453	-1.727225	0.183113
C	-2.798637	0.066254	-0.383694
H	-2.836511	-0.182994	-1.447929
H	-1.651055	-0.413993	1.357461
O	2.094024	-0.822111	-0.317334
C	-2.835746	1.561312	-0.181301
H	-3.748642	1.981958	-0.609185
H	-2.790161	1.808682	0.883327
H	-1.984274	2.027859	-0.682921
F	-4.000780	-0.473280	0.167022
C	4.067018	0.411514	-0.599909
H	4.663218	-0.501594	-0.538971
H	4.623485	1.247089	-0.179415
H	3.856832	0.602164	-1.655131

Zero-point correction	=	0.196802
Thermal correction to Energy	=	0.208695
Thermal correction to Enthalpy	=	0.209639
Thermal correction to Gibbs Free Energy	=	0.156914
Sum of electronic and zero-point Energies	=	-524.701828
Sum of electronic and thermal Energies	=	-524.689935
Sum of electronic and thermal Enthalpies	=	-524.688991
Sum of electronic and thermal Free Energies	=	-524.741715
Number of imaginary frequencies/frequency	=	0

OPT-wB97xD-6-311+Gdp_4-fluoropentyl_acetateC_7.out

0 1

C	2.779376	0.229681	0.144920
O	2.394462	0.929362	1.052931
C	0.820209	-1.115175	0.288011
H	0.661198	-2.176085	0.091805
H	0.890423	-0.959191	1.366370
C	-0.289653	-0.277426	-0.321509
H	-0.074899	0.780977	-0.153242
H	-0.309923	-0.445130	-1.403756
C	-1.641756	-0.648950	0.287100
H	-1.803434	-1.727201	0.183134
C	-2.798717	0.066211	-0.383717
H	-2.836558	-0.183051	-1.447951
H	-1.651193	-0.413954	1.357496
O	2.093966	-0.822028	-0.317301
C	-2.835936	1.561264	-0.181312
H	-3.748819	1.981866	-0.609270
H	-2.790453	1.808623	0.883325
H	-1.984446	2.027868	-0.682852
F	-4.000856	-0.473404	0.166959
C	4.067193	0.411201	-0.599993
H	4.663366	-0.501894	-0.538543
H	4.623646	1.246966	-0.179854
H	3.857082	0.601341	-1.655319

Zero-point correction	=	0.196801
Thermal correction to Energy	=	0.208694
Thermal correction to Enthalpy	=	0.209638
Thermal correction to Gibbs Free Energy	=	0.15691
Sum of electronic and zero-point Energies	=	-524.701829
Sum of electronic and thermal Energies	=	-524.689935
Sum of electronic and thermal Enthalpies	=	-524.688991
Sum of electronic and thermal Free Energies	=	-524.741719
Number of imaginary frequencies/frequency	=	0

OPT-wB97xD-6-311+Gdp_4-fluoropentyl_acetateC_8.out

0 1

C	-2.030152	-0.425965	-0.231269
O	-1.369386	-1.057200	-1.023733
C	-0.673476	1.532941	-0.516928
H	-0.374444	1.004194	-1.422026
H	-1.052859	2.516959	-0.793938
C	0.464816	1.667821	0.479150
H	1.228082	2.300725	0.015162
H	0.098595	2.210686	1.355669
C	1.085954	0.347470	0.937044
H	1.790407	0.541522	1.752842
C	1.814851	-0.426345	-0.143005
H	1.180336	-0.576685	-1.018551
H	0.312832	-0.310994	1.348170
O	-1.795760	0.851965	0.083827
C	2.384771	-1.740325	0.333034
H	2.952558	-2.226973	-0.463454
H	3.036889	-1.590957	1.198408
H	1.568288	-2.406380	0.624787
F	2.901470	0.379648	-0.607015
C	-3.214421	-0.956652	0.518821
H	-3.051398	-0.843861	1.592957
H	-3.370557	-2.006181	0.276364
H	-4.104849	-0.380695	0.254907

Zero-point correction	=	0.197035
Thermal correction to Energy	=	0.20862
Thermal correction to Enthalpy	=	0.209565
Thermal correction to Gibbs Free Energy	=	0.158464
Sum of electronic and zero-point Energies	=	-524.702246
Sum of electronic and thermal Energies	=	-524.690661
Sum of electronic and thermal Enthalpies	=	-524.689717
Sum of electronic and thermal Free Energies	=	-524.740817
Number of imaginary frequencies/frequency	=	0

OPT-wB97xD-6-311+Gdp_4-fluoropentyl_acetateC_9.out

0 1

C	2.855016	0.046287	-0.040196
O	3.408733	-1.029049	-0.063573
C	0.771762	-1.010823	0.377508
H	0.874176	-1.649696	-0.504184
H	1.171044	-1.543824	1.243085
C	-0.668483	-0.605913	0.601757
H	-1.223396	-1.518967	0.839899
H	-0.722588	0.040828	1.482673
C	-1.288273	0.079936	-0.614384
H	-0.787193	1.034818	-0.802957
C	-2.771741	0.373063	-0.497747
H	-3.119308	0.852397	-1.415929
H	-1.131865	-0.537832	-1.505682
O	1.545093	0.189246	0.174081
C	-3.189438	1.181228	0.707948
H	-4.261746	1.387338	0.677085
H	-2.959629	0.656497	1.638211
H	-2.655778	2.135744	0.708298
F	-3.471522	-0.872932	-0.447765
C	3.523607	1.371203	-0.250479
H	3.307384	2.038479	0.586401
H	3.128541	1.835631	-1.157606
H	4.598749	1.233515	-0.349908

Zero-point correction	=	0.196837
Thermal correction to Energy	=	0.208603
Thermal correction to Enthalpy	=	0.209547
Thermal correction to Gibbs Free Energy	=	0.157277
Sum of electronic and zero-point Energies	=	-524.702213
Sum of electronic and thermal Energies	=	-524.690448
Sum of electronic and thermal Enthalpies	=	-524.689504
Sum of electronic and thermal Free Energies	=	-524.741774
Number of imaginary frequencies/frequency	=	0

OPT-wB97xD-6-311+Gdp_4-fluoropentyl_acetateC_10.out

0 1

C	2.873060	0.109210	-0.059051
O	3.445017	-0.790278	-0.630987
C	0.862750	-1.150432	-0.045620
H	0.912532	-1.305072	-1.126901
H	1.342452	-1.997982	0.448813
C	-0.566013	-0.985325	0.424532
H	-1.065460	-1.946410	0.267810
H	-0.569998	-0.795783	1.503675
C	-1.312995	0.126646	-0.311689
H	-0.744162	1.058280	-0.242423
C	-2.695252	0.377166	0.258026

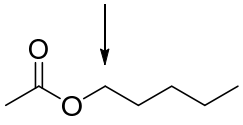
H	-2.625715	0.694441	1.302460
H	-1.407074	-0.128416	-1.373696
O	1.585120	0.051221	0.288466
C	-3.671381	-0.764064	0.110797
H	-4.665808	-0.461177	0.446970
H	-3.729298	-1.095705	-0.930038
H	-3.352144	-1.608339	0.727155
F	-3.237179	1.501859	-0.436155
C	3.492189	1.413462	0.342695
H	3.017490	2.227253	-0.211495
H	4.559334	1.399719	0.128338
H	3.327227	1.594942	1.406750

Zero-point correction = 0.196757
Thermal correction to Energy = 0.208518
Thermal correction to Enthalpy = 0.209462
Thermal correction to Gibbs Free Energy = 0.157549
Sum of electronic and zero-point Energies = -524.702548
Sum of electronic and thermal Energies = -524.690787
Sum of electronic and thermal Enthalpies = -524.689843
Sum of electronic and thermal Free Energies = -524.741756
Number of imaginary frequencies/frequency = 0

	Calculated ^{19}F NMR shielding tensor
OPT-wB97xD-6-311+Gdp_1-fluoropentyl_acetateC_1.out	319.3401
OPT-wB97xD-6-311+Gdp_1-fluoropentyl_acetateC_2.out	339.4513
OPT-wB97xD-6-311+Gdp_1-fluoropentyl_acetateC_3.out	318.9424
OPT-wB97xD-6-311+Gdp_1-fluoropentyl_acetateC_4.out	323.2767
OPT-wB97xD-6-311+Gdp_1-fluoropentyl_acetateC_5.out	317.2136
OPT-wB97xD-6-311+Gdp_1-fluoropentyl_acetateC_6.out	312.1463
OPT-wB97xD-6-311+Gdp_1-fluoropentyl_acetateC_7.out	310.743
OPT-wB97xD-6-311+Gdp_1-fluoropentyl_acetateC_8.out	325.1141
OPT-wB97xD-6-311+Gdp_1-fluoropentyl_acetateC_9.out	310.809
OPT-wB97xD-6-311+Gdp_1-fluoropentyl_acetateC_10.out	323.3469
OPT-wB97xD-6-311+Gdp_2-fluoropentyl_acetateC_1.out	384.8514
OPT-wB97xD-6-311+Gdp_2-fluoropentyl_acetateC_2.out	380.9586
OPT-wB97xD-6-311+Gdp_2-fluoropentyl_acetateC_3.out	385.3947
OPT-wB97xD-6-311+Gdp_2-fluoropentyl_acetateC_4.out	381.4407
OPT-wB97xD-6-311+Gdp_2-fluoropentyl_acetateC_5.out	376.8295
OPT-wB97xD-6-311+Gdp_2-fluoropentyl_acetateC_6.out	381.3531
OPT-wB97xD-6-311+Gdp_2-fluoropentyl_acetateC_7.out	383.319
OPT-wB97xD-6-311+Gdp_2-fluoropentyl_acetateC_8.out	370.7863
OPT-wB97xD-6-311+Gdp_2-fluoropentyl_acetateC_9.out	390.3925
OPT-wB97xD-6-311+Gdp_2-fluoropentyl_acetateC_10.out	376.2743
OPT-wB97xD-6-311+Gdp_3-fluoropentyl_acetateC_1.out	380.4089
OPT-wB97xD-6-311+Gdp_3-fluoropentyl_acetateC_2.out	385.8247
OPT-wB97xD-6-311+Gdp_3-fluoropentyl_acetateC_3.out	384.5472
OPT-wB97xD-6-311+Gdp_3-fluoropentyl_acetateC_5.out	363.1581
OPT-wB97xD-6-311+Gdp_3-fluoropentyl_acetateC_6.out	380.6008
OPT-wB97xD-6-311+Gdp_3-fluoropentyl_acetateC_7.out	379.1147
OPT-wB97xD-6-311+Gdp_3-fluoropentyl_acetateC_8.out	388.3087
OPT-wB97xD-6-311+Gdp_3-fluoropentyl_acetateC_9.out	377.0816
OPT-wB97xD-6-311+Gdp_3-fluoropentyl_acetateC_10.out	374.293
OPT-wB97xD-6-311+Gdp_4-fluoropentyl_acetateC_1.out	367.5754
OPT-wB97xD-6-311+Gdp_4-fluoropentyl_acetateC_2.out	369.6171
OPT-wB97xD-6-311+Gdp_4-fluoropentyl_acetateC_3.out	368.0343
OPT-wB97xD-6-311+Gdp_4-fluoropentyl_acetateC_4.out	369.9261
OPT-wB97xD-6-311+Gdp_4-fluoropentyl_acetateC_5.out	374.4415
OPT-wB97xD-6-311+Gdp_4-fluoropentyl_acetateC_6.out	354.8459
OPT-wB97xD-6-311+Gdp_4-fluoropentyl_acetateC_7.out	354.8414
OPT-wB97xD-6-311+Gdp_4-fluoropentyl_acetateC_8.out	375.6764
OPT-wB97xD-6-311+Gdp_4-fluoropentyl_acetateC_9.out	370.9556
OPT-wB97xD-6-311+Gdp_4-fluoropentyl_acetateC_10.out	355.2946

Result for Table 3: relevant to selectfluor 2 abstracting H from pentyl acetate

Transition State for abstracting C1



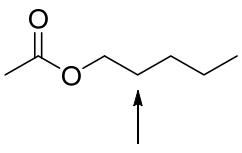
TS-TUF-wB97xD-6-31+Gdp-Selectfluor2-ModelSubstrateA1.out

2 2

H	0.731413	0.412778	0.286383
C	1.849515	0.784251	0.259425
H	2.092526	0.922429	1.317861
C	2.667206	-0.259862	-0.453600
H	3.698769	0.111979	-0.517341
H	2.299929	-0.372265	-1.480794
C	2.636268	-1.603499	0.273585
H	3.003463	-1.472306	1.299763
H	1.598786	-1.952456	0.352722
C	3.469567	-2.671513	-0.433729
H	3.106038	-2.787776	-1.462906
H	4.509832	-2.329219	-0.506061
O	1.867599	1.995602	-0.446447
C	1.401426	3.105522	0.184358
O	0.919596	3.059595	1.294325
C	1.564586	4.321644	-0.667065
H	2.625349	4.478216	-0.883465
H	1.047661	4.177342	-1.620026
H	1.158972	5.190717	-0.150893
C	3.421826	-4.019405	0.281416
H	4.022719	-4.769740	-0.242684
H	3.807875	-3.936466	1.303998
H	2.394216	-4.396563	0.342248
C	-1.116691	-0.760148	1.349400
C	-0.839718	-0.846784	-1.067454
C	-1.550282	1.218515	0.002787
C	-2.515090	-1.373648	1.087312
H	-0.377901	-1.543697	1.514198
H	-1.125159	-0.065922	2.188677
H	-0.372370	-0.315033	-1.896220
H	-0.314062	-1.780169	-0.870996
C	-2.345239	-1.083708	-1.341072
C	-3.038492	0.795912	0.070608
H	-1.303218	1.681133	-0.952815
H	-1.305261	1.889275	0.824864
H	-2.455669	-2.437074	0.855566
H	-3.176376	-1.211939	1.937631
H	-2.714130	-0.469629	-2.162205
H	-2.541214	-2.136027	-1.543691
H	-3.613632	1.266167	-0.725928
H	-3.482164	1.026006	1.039093
N	-0.773355	-0.016392	0.136458
C	-4.552071	-1.110058	-0.263379
H	-4.940620	-0.674057	-1.183286
H	-4.589131	-2.198133	-0.309489
H	-5.108303	-0.744542	0.599300
N	-3.125609	-0.696168	-0.112470

Zero-point correction	=	0.432174
Thermal correction to Energy	=	0.451919
Thermal correction to Enthalpy	=	0.452863
Thermal correction to Gibbs Free Energy	=	0.382577
Sum of electronic and zero-point Energies	=	-809.95471
Sum of electronic and thermal Energies	=	-809.934965
Sum of electronic and thermal Enthalpies	=	-809.93402
Sum of electronic and thermal Free Energies	=	-810.004307
Number of imaginary frequencies/frequency	=	1

Transition State for abstracting C2



TS-TUF-wB97xD-6-31+Gdp-Selectfluor2-ModelSubstrateA2.out

2 2

H	-0.591462	0.765512	0.431161
C	-1.654286	1.290319	0.401423
H	-1.904098	1.369087	1.465611
C	-1.459700	2.630733	-0.271438
H	-2.450682	3.091445	-0.397278
H	-1.062266	2.481439	-1.284219
C	-0.554299	3.577275	0.516379
H	-1.003803	3.767731	1.498571
H	0.409262	3.086994	0.703323
C	-0.320228	4.897483	-0.212165
H	0.167041	4.731370	-1.179946
H	-1.266526	5.417896	-0.398867
C	-3.225664	-1.928795	-0.128339
C	1.533808	0.278028	1.437123
C	1.360135	0.701696	-0.955925
C	0.475650	-1.361053	-0.015837
C	2.964486	-0.229064	1.132106
H	1.542386	1.342013	1.669546
H	1.065320	-0.280966	2.246085
H	0.647929	0.677233	-1.780996
H	1.602191	1.731434	-0.696592
C	2.625423	-0.121953	-1.296182
C	1.849917	-2.075314	-0.034905
H	-0.044079	-1.459873	-0.968831
H	-0.144512	-1.738641	0.795785
H	3.661400	0.592859	0.970117
H	3.328141	-0.876190	1.929488
H	2.476923	-0.754011	-2.171206
H	3.485787	0.529270	-1.446116
H	1.935366	-2.736149	-0.896716
H	2.029518	-2.634113	0.883794
N	0.756798	0.059380	0.214522
C	4.257465	-1.697685	-0.352900
H	4.232967	-2.211169	-1.313667
H	5.028406	-0.927234	-0.348621
H	4.421757	-2.407471	0.457263
N	2.935192	-1.036673	-0.139663
H	0.318809	5.564742	0.374966
C	-2.557460	0.338029	-0.334750
H	-2.161383	0.092342	-1.324767
H	-3.551417	0.783101	-0.463114
O	-2.671011	-0.854624	0.455939
C	-3.260047	-3.101585	0.803681
H	-3.798346	-2.835664	1.717536
H	-3.748326	-3.945990	0.318458
H	-2.239473	-3.377785	1.085316
O	-3.634232	-1.918730	-1.272154

Zero-point correction	=	0.432681
Thermal correction to Energy	=	0.452097
Thermal correction to Enthalpy	=	0.453041
Thermal correction to Gibbs Free Energy	=	0.384113
Sum of electronic and zero-point Energies	=	-809.955258
Sum of electronic and thermal Energies	=	-809.935842
Sum of electronic and thermal Enthalpies	=	-809.934898
Sum of electronic and thermal Free Energies	=	-810.003826
Number of imaginary frequencies/frequency	=	1

TS-TUF-wB97xD-6-31+Gdp-Selectfluor2-ModelSubstrateA2b.out

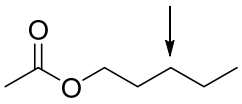
2 2

H	-0.660210	0.485820	0.028986
C	-1.798628	0.786482	-0.053530
H	-2.163605	0.588860	0.960390
C	-1.855397	2.250089	-0.433338
H	-2.916138	2.518292	-0.550548
H	-1.390461	2.393633	-1.417600
C	-1.209280	3.180549	0.592328
H	-1.664095	3.005320	1.575086
H	-0.145960	2.931032	0.688040
C	-1.353454	4.651330	0.210669
H	-0.887391	4.853331	-0.760574
H	-2.409058	4.937478	0.141194
C	-3.153882	-2.016709	0.174919
C	1.333397	0.327572	1.371983
C	1.474544	0.895537	-0.993226
C	0.873717	-1.363667	-0.309214
C	2.868334	0.151089	1.291393
H	1.077279	1.345513	1.661727
H	0.874508	-0.385771	2.055575
H	0.920376	0.813835	-1.928183
H	1.476588	1.927004	-0.643563
C	2.909451	0.335874	-1.152251
C	2.342800	-1.802313	-0.093660
H	0.558243	-1.489737	-1.344021
H	0.205997	-1.907923	0.357135
H	3.387140	1.108955	1.262421
H	3.237291	-0.447760	2.123040
H	3.018085	-0.260701	-2.057781

H	3.643203	1.141486	-1.144585
H	2.700736	-2.389923	-0.938149
H	2.469465	-2.363191	0.832316
N	0.826259	0.063297	0.022992
C	4.648072	-0.956590	0.011057
H	4.884526	-1.396962	-0.957190
H	5.242766	-0.058950	0.179060
H	4.810671	-1.678086	0.811269
N	3.205554	-0.572141	0.013273
H	-0.878209	5.301105	0.952450
C	-2.401672	-0.141306	-1.081490
H	-1.884703	-0.056956	-2.039552
H	-3.458876	0.103006	-1.228784
O	-2.267542	-1.520131	-0.706037
C	-2.879254	-3.459491	0.471650
H	-1.823102	-3.605730	0.712058
H	-3.502862	-3.792547	1.300727
H	-3.105695	-4.058215	-0.416178
O	-4.061420	-1.358743	0.641992

Zero-point correction	=	0.432226
Thermal correction to Energy	=	0.451824
Thermal correction to Enthalpy	=	0.452769
Thermal correction to Gibbs Free Energy	=	0.382657
Sum of electronic and zero-point Energies	=	-809.954546
Sum of electronic and thermal Energies	=	-809.934947
Sum of electronic and thermal Enthalpies	=	-809.934003
Sum of electronic and thermal Free Energies	=	-810.004114
Number of imaginary frequencies/frequency	=	1

Transition State for abstracting C3



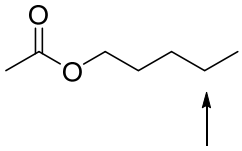
TS-TUF-wB97xD-6-31+Gdp-Selectfluor2-ModelSubstrateA3.out

2 2

H	0.121450	1.319512	0.363519
C	-0.749510	2.103827	0.212849
H	-1.015494	2.339907	1.251319
C	-0.147890	3.292717	-0.508614
H	-0.965430	4.004844	-0.688662
H	0.205623	2.981218	-1.499702
C	0.968778	3.982066	0.267760
H	0.610833	4.330130	1.242802
H	1.810055	3.304014	0.442443
C	2.166363	0.382860	1.361928
C	1.927848	0.589070	-1.052119
C	0.622381	-1.062173	0.164552
C	3.395205	-0.508831	1.050322
H	2.466637	1.423510	1.470779
H	1.635257	0.048974	2.252304
H	1.173959	0.671234	-1.835291
H	2.446737	1.538937	-0.928258
C	2.908904	-0.569191	-1.354626
C	1.762779	-2.109688	0.164720
H	0.017591	-1.116018	-0.740552
H	-0.002554	-1.183338	1.048074
H	4.264032	0.081847	0.759526
H	3.642577	-1.141945	1.901487
H	2.533583	-1.227901	-2.137695
H	3.891798	-0.186314	-1.626705
H	1.610815	-2.853562	-0.616134
H	1.862529	-2.600001	1.132759
N	1.270486	0.250983	0.211159
C	4.153228	-2.411182	-0.309709
H	3.927974	-2.989927	-1.205397
H	5.095429	-1.876437	-0.425492
H	4.185149	-3.058650	0.566269
N	3.065111	-1.407617	-0.112864
C	-1.855312	1.382448	-0.535718
H	-1.427181	0.797671	-1.359350
H	-2.516882	2.130392	-0.991160
C	-4.344185	-1.175649	0.159424
H	1.346618	4.849043	-0.282289
C	-2.663797	0.479323	0.374968
H	-3.233211	1.062541	1.104963
H	-2.025849	-0.221356	0.919776
O	-3.577783	-0.262769	-0.451368
C	-5.251990	-1.874174	-0.808336
H	-5.822823	-2.644511	-0.290713
H	-5.936909	-1.149701	-1.258611
H	-4.665732	-2.324090	-1.614151
O	-4.290038	-1.389997	1.355327

Zero-point correction	=	0.432809
Thermal correction to Energy	=	0.452384
Thermal correction to Enthalpy	=	0.453328
Thermal correction to Gibbs Free Energy	=	0.382441
Sum of electronic and zero-point Energies	=	-809.955761
Sum of electronic and thermal Energies	=	-809.936186
Sum of electronic and thermal Enthalpies	=	-809.935242
Sum of electronic and thermal Free Energies	=	-810.006129
Number of imaginary frequencies/frequency	=	1

Transition State for abstracting C4



TS-TUF-wB97xD-6-31+Gdp-Selectfluor2-ModelSubstrateA4.out

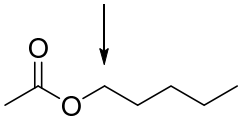
2 2

H	-0.625987	1.511937	-0.478478
C	0.059088	2.448308	-0.489724
H	0.217064	2.608517	-1.562881
C	-0.720366	3.576852	0.150219
H	-0.142236	4.507034	0.086849
H	-0.913310	3.376372	1.209335
C	-2.925974	0.853342	-1.015463
C	-2.035452	0.418084	1.204752
C	-1.256158	-0.887063	-0.692149
C	-4.109492	-0.052961	-0.590502
H	-3.132925	1.896447	-0.776236
H	-2.688129	0.747103	-2.072882
H	-1.095001	0.286119	1.739689
H	-2.490001	1.373811	1.464187
C	-2.994026	-0.770043	1.475031
C	-2.459133	-1.864485	-0.655598
H	-0.462214	-1.199186	-0.015323
H	-0.873568	-0.780806	-1.706710
H	-4.797191	0.460505	0.081375
H	-4.645641	-0.424601	-1.462784
H	-2.474848	-1.618720	1.919761
H	-3.823759	-0.461724	2.109461
H	-2.179731	-2.803736	-0.178900
H	-2.863559	-2.052325	-1.650099
N	-1.779077	0.398340	-0.232826
C	-4.647944	-2.236900	0.402110
H	-4.241644	-3.043704	1.011514
H	-5.463881	-1.736321	0.922500
H	-4.984535	-2.617708	-0.561624
N	-3.562523	-1.240042	0.160243
C	1.336169	2.055796	0.227926
H	1.098838	1.776867	1.262971
H	1.973968	2.949730	0.287887
C	2.097958	0.925568	-0.462326
H	2.370470	1.229026	-1.479727
H	1.456508	0.041057	-0.543840
C	5.097637	-1.040864	0.149201
H	-1.676051	3.745247	-0.355178
C	3.350320	0.556263	0.306906
H	3.111269	0.223446	1.321713
H	4.045007	1.399590	0.372558
O	3.992359	-0.523374	-0.399166
O	5.565552	-0.643539	1.199547
C	5.672406	-2.140297	-0.694098
H	4.898681	-2.868788	-0.948915
H	6.053864	-1.717103	-1.628486
H	6.486261	-2.630464	-0.160400

Zero-point correction =	0.432481	
Thermal correction to Energy =	0.452418	
Thermal correction to Enthalpy =	0.453362	
Thermal correction to Gibbs Free Energy =		0.380981
Sum of electronic and zero-point Energies =		-809.956508
Sum of electronic and thermal Energies =		-809.936571
Sum of electronic and thermal Enthalpies =		-809.935626
Sum of electronic and thermal Free Energies =		-810.008007
Number of imaginary frequencies/frequency =		1

Result for Table 3: relevant to triplet AQN abstracting H from pentyl acetate

Transition State for abstracting C1



TS-TUF-wB97xD-6-31+Gdp-AQN-ModelSubstrateA1.out

0 3

C	-3.922535	-2.488690	-1.333656
C	-4.014473	-1.190167	-0.865049
C	-2.869580	-0.389070	-0.731701
C	-1.603215	-0.927717	-1.072878
C	-1.522204	-2.265130	-1.530967
C	-2.665879	-3.025844	-1.665739
C	-2.995868	0.975844	-0.198713
C	-0.423054	-0.127585	-0.908775
C	-0.507389	1.245015	-0.512025
C	-1.766539	1.780892	-0.128744
C	-1.849013	3.118844	0.287500
H	-2.818382	3.505278	0.584631
C	-0.728108	3.928899	0.306604
C	0.508964	3.415720	-0.121684
C	0.621684	2.101193	-0.525810
H	-4.816826	-3.094802	-1.437548
H	-4.974568	-0.766661	-0.588464
H	-0.554353	-2.689794	-1.774916
H	-2.592296	-4.047947	-2.024089
H	-0.806016	4.961764	0.630619
H	1.383373	4.058772	-0.145137
H	1.577824	1.736359	-0.884099
O	-4.091710	1.432081	0.160338
O	0.728962	-0.733167	-1.169162
H	1.817835	-0.291083	-0.247385
C	2.690381	-0.303874	0.540204
H	2.845988	0.745257	0.812482
C	2.264159	-1.195012	1.676136
H	3.085268	-1.223904	2.406022
H	2.124672	-2.216859	1.304010
C	0.984395	-0.694680	2.346171
H	1.116296	0.349924	2.658306
H	0.163722	-0.703005	1.618017
C	0.576973	-1.539698	3.552441
H	0.476663	-2.587243	3.240118
H	1.376849	-1.511594	4.303586
O	3.809973	-0.838643	-0.117328
C	4.345806	-0.105696	-1.124030
O	3.859856	0.944008	-1.484973
C	5.566615	-0.758891	-1.687202
H	6.351751	-0.774591	-0.925038
H	5.346304	-1.793485	-1.962346
H	5.912630	-0.203993	-2.558414
C	-0.733542	-1.065125	4.176536
H	-1.012498	-1.681723	5.037301
H	-0.653390	-0.027167	4.519926
H	-1.552971	-1.113083	3.449694

Zero-point correction =	0.380623	
Thermal correction to Energy =	0.404327	
Thermal correction to Enthalpy =	0.405271	
Thermal correction to Gibbs Free Energy =		0.322349
Sum of electronic and zero-point Energies =		-1113.673892
Sum of electronic and thermal Energies =		-1113.650188
Sum of electronic and thermal Enthalpies =		-1113.649244
Sum of electronic and thermal Free Energies =		-1113.732165
Number of imaginary frequencies/frequency =		1

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0 3

C	4.102528	2.978773	0.185354
C	4.186045	1.616172	-0.039386
C	3.032813	0.854037	-0.284227
C	1.766801	1.493566	-0.286881
C	1.695481	2.884810	-0.033963
C	2.846847	3.612587	0.188526
C	3.152453	-0.597506	-0.489156
C	0.579993	0.717701	-0.503897
C	0.658682	-0.667696	-0.848355
C	1.916591	-1.328885	-0.806986
C	1.988507	-2.693725	-1.123005
H	2.956526	-3.181958	-1.078918
C	0.857862	-3.398345	-1.497846
C	-0.378284	-2.735157	-1.591921
C	-0.478918	-1.396700	-1.275362
H	5.002905	3.556924	0.367437
H	5.145798	1.109904	-0.028609
H	0.728334	3.375475	-0.014909
H	2.780643	4.680132	0.374656
H	0.928171	-4.454138	-1.739301
H	-1.260389	-3.275923	-1.920395
H	-1.432869	-0.893056	-1.381842
O	4.247844	-1.175009	-0.416826
O	-0.577419	1.360631	-0.398683
H	-1.595987	0.515312	0.317857
C	-2.290538	-0.001709	1.117872
H	-2.286956	0.736244	1.927648
C	-3.638067	-0.266846	0.498956
H	-4.295498	-0.659969	1.286908
H	-3.539694	-1.051960	-0.259979
C	-4.251030	0.990400	-0.115858
H	-4.301506	1.783466	0.641887
H	-3.596755	1.359740	-0.916573
C	-5.648124	0.740360	-0.683621
H	-5.595913	-0.068871	-1.423540
H	-6.306577	0.386903	0.120279
O	-1.687940	-1.205805	1.502977
C	-0.540643	-1.150586	2.228612
O	-0.073427	-0.106513	2.623563
C	0.038591	-2.514451	2.420184
H	-0.722622	-3.206116	2.789513
H	0.386169	-2.885754	1.449568
H	0.876685	-2.466849	3.114487
C	-6.251585	1.984923	-1.329801
H	-7.251561	1.781897	-1.727097
H	-6.339498	2.801989	-0.604352
H	-5.627881	2.339843	-2.158420

Zero-point correction =	0.380463	
Thermal correction to Energy =	0.403941	
Thermal correction to Enthalpy =	0.404885	
Thermal correction to Gibbs Free Energy =		0.324598
Sum of electronic and zero-point Energies =		-1113.674594
Sum of electronic and thermal Energies =		-1113.651116
Sum of electronic and thermal Enthalpies =		-1113.650172
Sum of electronic and thermal Free Energies =		-1113.730458
Number of imaginary frequencies/frequency =		1

TS-TUF-wB97xD-6-31+Gdp-AQN-ModelSubstrateA1c.out

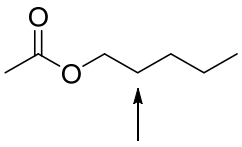
0 3

C	4.104226	2.976709	0.184058
C	4.186814	1.614025	-0.040519
C	3.033034	0.852602	-0.284994
C	1.767430	1.492940	-0.287417
C	1.697064	2.884260	-0.034670
C	2.848953	3.611330	0.187430
C	3.151707	-0.599025	-0.489869
C	0.580070	0.717803	-0.504059
C	0.657803	-0.667676	-0.848415
C	1.915296	-1.329664	-0.807249
C	1.986236	-2.694634	-1.122929
H	2.953935	-3.183507	-1.078898
C	0.855027	-3.398619	-1.497251

C	-0.380704	-2.734637	-1.591222
C	-0.480372	-1.396031	-1.275006
H	5.005018	3.554332	0.365766
H	5.146247	1.107145	-0.029954
H	0.730240	3.375561	-0.015531
H	2.783479	4.678963	0.373318
H	0.924570	-4.454553	-1.738313
H	-1.263251	-3.274938	-1.919272
H	-1.434024	-0.891803	-1.381389
O	4.246767	-1.177202	-0.417863
O	-0.576923	1.361419	-0.398508
H	-1.595734	0.516612	0.318236
C	-2.290094	-0.000081	1.118668
H	-2.286417	0.738336	1.928021
C	-3.637721	-0.265802	0.500215
H	-4.295107	-0.657828	1.288751
H	-3.539496	-1.051922	-0.257695
C	-4.250654	0.990661	-0.116222
H	-4.300888	1.784813	0.640400
H	-3.596507	1.358770	-0.917610
C	-5.647890	0.739907	-0.683330
H	-5.595885	-0.070441	-1.422043
H	-6.306197	0.387690	0.121233
O	-1.687266	-1.203902	1.504275
C	-0.539859	-1.148234	2.229696
O	-0.072689	-0.103939	2.624101
C	0.039490	-2.511960	2.421923
H	-0.721373	-3.203126	2.792920
H	0.385894	-2.884343	1.451310
H	0.878365	-2.463692	3.115238
C	-6.251427	1.983505	-1.331295
H	-7.251499	1.779870	-1.728041
H	-6.339155	2.801702	-0.607108
H	-5.627915	2.337080	-2.160634

Zero-point correction	=	0.380461
Thermal correction to Energy	=	0.403942
Thermal correction to Enthalpy	=	0.404886
Thermal correction to Gibbs Free Energy	=	0.324579
Sum of electronic and zero-point Energies	=	-1113.674595
Sum of electronic and thermal Energies	=	-1113.651114
Sum of electronic and thermal Enthalpies	=	-1113.65017
Sum of electronic and thermal Free Energies	=	-1113.730477
Number of imaginary frequencies/frequency	=	1

Transition State for abstracting C2



TS-TUF-wB97xD-6-31+Gdp-AQN-ModelSubstrateA2.out

0 3

C	4.649683	1.487435	-1.521272
C	4.506638	0.295016	-0.833913
C	3.234842	-0.200220	-0.507284
C	2.084738	0.540421	-0.880402
C	2.247835	1.768918	-1.566215
C	3.510163	2.226768	-1.885345
C	3.116442	-1.454650	0.250726
C	0.779819	0.057254	-0.528361
C	0.607779	-1.200956	0.131837
C	1.756107	-1.933791	0.540121
C	1.594206	-3.165453	1.193757
H	2.484671	-3.703120	1.502499
C	0.335550	-3.689775	1.424798
C	-0.800239	-2.992743	0.976395
C	-0.670815	-1.775534	0.340191
H	5.639188	1.856338	-1.771790
H	5.376335	-0.278927	-0.531067
H	1.373606	2.352187	-1.834262
H	3.622602	3.167962	-2.414524
H	0.224993	-4.643163	1.931445
H	-1.789364	-3.416761	1.120500
H	-1.560177	-1.274807	-0.021787
O	4.118520	-2.086597	0.617296
O	-0.234586	0.829011	-0.902019
H	-1.343476	0.839561	0.087608
C	-2.183739	1.198862	0.826561
H	-2.159999	0.464864	1.639949
C	-1.766890	2.583452	1.271325
H	-2.568063	2.995307	1.903565
H	-1.691547	3.244190	0.397794
C	-3.468921	1.140840	0.043856
H	-4.307550	1.480942	0.663342
H	-3.423840	1.765443	-0.852999
C	-0.450804	2.591515	2.050244
H	-0.551811	1.945608	2.931247
H	0.339843	2.153354	1.428489
C	-0.036813	3.995174	2.483718
H	0.906952	3.975411	3.038156
H	0.098102	4.650340	1.615459
H	-0.796307	4.448774	3.130931
O	-3.680527	-0.229455	-0.332075
C	-4.731778	-0.501724	-1.119178
O	-5.502906	0.352995	-1.507543
C	-4.813485	-1.964996	-1.434342
H	-3.879304	-2.300296	-1.893324
H	-4.953555	-2.532538	-0.509714
H	-5.647199	-2.153177	-2.110083

Zero-point correction	=	0.380321
Thermal correction to Energy	=	0.404136
Thermal correction to Enthalpy	=	0.40508
Thermal correction to Gibbs Free Energy	=	0.322363
Sum of electronic and zero-point Energies	=	-1113.673089
Sum of electronic and thermal Energies	=	-1113.649274
Sum of electronic and thermal Enthalpies	=	-1113.64833
Sum of electronic and thermal Free Energies	=	-1113.731047
Number of imaginary frequencies/frequency	=	1

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0 3

C	-3.842763	-3.193505	-0.403349
C	-4.127442	-1.840434	-0.445817
C	-3.096986	-0.887500	-0.476758
C	-1.748204	-1.322338	-0.452469
C	-1.472641	-2.710098	-0.390062
C	-2.504961	-3.626053	-0.374528
C	-3.432832	0.543676	-0.496951
C	-0.686004	-0.354593	-0.452509
C	-0.960431	1.044300	-0.586591
C	-2.310096	1.490902	-0.575252
C	-2.585494	2.863557	-0.679603
H	-3.622685	3.181536	-0.659933
C	-1.565460	3.786908	-0.816595
C	-0.232357	3.344679	-0.878773
C	0.067122	2.002442	-0.768933
H	-4.648929	-3.920067	-0.385355
H	-5.153988	-1.488959	-0.454534
H	-0.443769	-3.051136	-0.353707
H	-2.280356	-4.687436	-0.333518
H	-1.792828	4.845210	-0.895373
H	0.570255	4.061176	-1.023793
H	1.098419	1.684892	-0.853267
O	-4.609778	0.933378	-0.464553
O	0.538079	-0.856491	-0.355733
H	1.495630	0.007057	0.367049
C	2.328305	0.323573	1.143259
H	2.447044	1.402334	0.996351
C	1.794841	-0.033456	2.513821
H	2.580025	0.200697	3.248782
H	1.628296	-1.116790	2.573657
C	3.553780	-0.447411	0.732722
H	4.375200	-0.247019	1.431189
H	3.366778	-1.525693	0.722785
C	0.513842	0.711768	2.889973
H	0.683590	1.792073	2.800648
H	-0.277597	0.458693	2.174357
C	0.041550	0.377295	4.302381
H	-0.879143	0.915611	4.549271
H	-0.159836	-0.695202	4.405374
H	0.798981	0.648688	5.046657
O	3.930492	-0.012716	-0.582391

C	5.003719	-0.598561	-1.131226
O	5.654448	-1.450913	-0.558749
C	5.278157	-0.070166	-2.507156
H	4.410717	-0.243414	-3.150173
H	5.451524	1.008765	-2.462900
H	6.152867	-0.566985	-2.925673

Zero-point correction = 0.380372
Thermal correction to Energy = 0.404182
Thermal correction to Enthalpy = 0.405126
Thermal correction to Gibbs Free Energy = 0.322315
Sum of electronic and zero-point Energies = -1113.67272
Sum of electronic and thermal Energies = -1113.64891
Sum of electronic and thermal Enthalpies = -1113.647965
Sum of electronic and thermal Free Energies = -1113.730777
Number of imaginary frequencies/frequency = 1

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0 3

C	0.883648	3.674039	0.036167
C	-0.430685	3.254924	0.143975
C	-0.809161	1.961428	-0.246395
C	0.177217	1.064042	-0.736855
C	1.509889	1.525472	-0.878593
C	1.853517	2.804975	-0.496045
C	-2.224350	1.568325	-0.172477
C	-0.198044	-0.262513	-1.107534
C	-1.573252	-0.656594	-1.152611
C	-2.574036	0.236375	-0.690109
C	-3.912731	-0.184080	-0.672286
H	-4.664409	0.503644	-0.298776
C	-4.266435	-1.447548	-1.111861
C	-3.274706	-2.334039	-1.569682
C	-1.948665	-1.952529	-1.582461
H	1.162922	4.676909	0.343064
H	-1.196008	3.923013	0.525196
H	2.260123	0.875310	-1.315107
H	2.878371	3.143175	-0.614089
H	-5.306232	-1.758305	-1.095753
H	-3.551931	-3.328781	-1.904744
H	-1.183852	-2.646397	-1.914004
O	-3.086472	2.330641	0.290770
O	0.703423	-1.183987	-1.446563
H	1.789428	-1.156381	-0.460301
C	2.413825	-1.389154	0.527703
H	2.405429	-2.485391	0.500252
C	3.801559	-0.805125	0.386806
H	4.393652	-1.145848	1.249839
H	3.754796	0.288926	0.457707
C	1.622512	-0.841384	1.685371
H	2.133359	-1.072026	2.628973
H	1.508742	0.244120	1.618888
C	4.507094	-1.216627	-0.905275
H	4.567112	-2.311206	-0.950616
H	3.899160	-0.900357	-1.762692
C	5.904998	-0.615234	-1.021832
H	6.394355	-0.929068	-1.949406
H	5.862455	0.480112	-1.018901
H	6.540137	-0.927514	-0.184956
O	0.331094	-1.465941	1.687417
C	-0.644495	-0.867662	2.386855
O	-0.469351	0.144701	3.036274
C	-1.937670	-1.621609	2.297120
H	-2.058192	-2.094922	1.321036
H	-1.929053	-2.407484	3.060476
H	-2.770084	-0.947728	2.500833

Zero-point correction = 0.380326
Thermal correction to Energy = 0.403636
Thermal correction to Enthalpy = 0.40458
Thermal correction to Gibbs Free Energy = 0.324472
Sum of electronic and zero-point Energies = -1113.676857
Sum of electronic and thermal Energies = -1113.653547
Sum of electronic and thermal Enthalpies = -1113.652603
Sum of electronic and thermal Free Energies = -1113.732711
Number of imaginary frequencies/frequency = 1

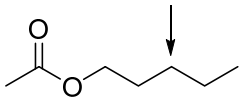
TS-TUF-wB97xD-6-31+Gdp-AQN-ModelSubstrateA2d.out

0 3

C	4.054434	-1.489606	-1.284008
C	3.907093	-0.251372	-0.683553
C	2.643749	0.348045	-0.569214
C	1.505314	-0.331774	-1.072686
C	1.669715	-1.606982	-1.667035
C	2.925213	-2.169279	-1.774965
C	2.511055	1.635255	0.128786
C	0.203827	0.244385	-0.912831
C	0.032023	1.535169	-0.322322
C	1.160110	2.210126	0.218121
C	0.991101	3.471746	0.810766
H	1.863794	3.967028	1.223586
C	-0.252081	4.075792	0.856673
C	-1.362334	3.430949	0.281783
C	-1.226098	2.187108	-0.298022
H	5.037921	-1.941284	-1.366268
H	4.766311	0.274421	-0.280180
H	0.799330	-2.145147	-2.026252
H	3.038877	-3.147242	-2.232383
H	-0.368553	5.051142	1.318293
H	-2.333457	3.916255	0.286202
H	-2.087967	1.716402	-0.756342
O	3.495659	2.213605	0.614096
O	-0.815479	-0.474720	-1.376454
H	-1.944998	-0.415692	-0.419859
C	-2.601207	-0.767141	0.497651
H	-2.563526	0.083521	1.187141
C	-3.991803	-1.044431	-0.029148
H	-4.606421	-1.390977	0.815764
H	-3.958387	-1.871321	-0.750022
C	-1.868791	-1.968972	1.031590
H	-2.427797	-2.426623	1.857119
H	-1.720048	-2.724675	0.255893
C	-4.650506	0.179235	-0.666350
H	-4.652718	1.004290	0.056988
H	-4.043437	0.509632	-1.518896
C	-6.076640	-0.102197	-1.132062
H	-6.524394	0.784105	-1.593097
H	-6.095892	-0.910858	-1.871710
H	-6.713517	-0.401259	-0.291606
O	-0.596909	-1.521599	1.525408
C	0.392265	-2.420177	1.612655
O	0.248691	-3.596722	1.340245
C	1.677529	-1.808861	2.085899
H	2.457959	-2.018140	1.348866
H	1.590304	-0.732560	2.234318
H	1.967115	-2.287642	3.025720

Zero-point correction = 0.380535
Thermal correction to Energy = 0.404015
Thermal correction to Enthalpy = 0.404959
Thermal correction to Gibbs Free Energy = 0.324978
Sum of electronic and zero-point Energies = -1113.675929
Sum of electronic and thermal Energies = -1113.652449
Sum of electronic and thermal Enthalpies = -1113.651505
Sum of electronic and thermal Free Energies = -1113.731486
Number of imaginary frequencies/frequency = 1

Transition State for abstracting C3



TS-TUF-wB97xD-6-31+Gdp-AQN-ModelSubstrateA3.out

0 3

C	-4.680127	-2.446748	-1.152583
C	-4.713851	-1.090380	-0.882494
C	-3.535047	-0.381514	-0.601747
C	-2.297124	-1.072207	-0.587444
C	-2.280782	-2.464402	-0.846116
C	-3.453431	-3.134101	-1.131395
C	-3.607851	1.054128	-0.292472
C	-1.087847	-0.361091	-0.276448
C	-1.092585	1.057792	-0.083087
C	-2.333779	1.750764	-0.058015

C	-2.346145	3.139420	0.147582
H	-3.305620	3.645440	0.171851
C	-1.168633	3.848293	0.299286
C	0.062822	3.174636	0.219462
C	0.103340	1.808964	0.029352
H	-5.598405	-2.981777	-1.372959
H	-5.653833	-0.548248	-0.879900
H	-1.340710	-3.004690	-0.817766
H	-3.427245	-4.200229	-1.334559
H	-1.193070	4.921666	0.457731
H	0.991871	3.730964	0.296633
H	1.063731	1.318529	-0.063169
O	-4.692740	1.653313	-0.248475
O	0.011252	-1.099692	-0.224373
H	1.018555	-0.616498	0.818012
C	1.754340	-0.612347	1.726619
H	1.771903	0.436880	2.046136
C	1.118382	-1.511000	2.767782
H	1.814459	-1.579043	3.616472
H	1.022765	-2.526669	2.364743
C	3.095955	-1.072116	1.190073
H	3.807099	-1.107560	2.026607
H	3.012388	-2.089371	0.790716
C	3.627401	-0.138719	0.119777
H	3.733281	0.882480	0.498697
H	2.969872	-0.119971	-0.755108
C	-0.236378	-1.005139	3.255785
H	-0.633753	-1.650911	4.044869
H	-0.155358	0.010543	3.658745
H	-0.969651	-0.986024	2.441910
O	4.921023	-0.628077	-0.278722
C	5.571945	0.069155	-1.217655
O	5.112621	1.067878	-1.738456
C	6.916267	-0.524571	-1.517819
H	7.567450	-0.399865	-0.647171
H	6.825543	-1.595295	-1.717000
H	7.360245	-0.020643	-2.375939

Zero-point correction	=	0.380919
Thermal correction to Energy	=	0.404695
Thermal correction to Enthalpy	=	0.405639
Thermal correction to Gibbs Free Energy	=	0.323163
Sum of electronic and zero-point Energies	=	-1113.674223
Sum of electronic and thermal Energies	=	-1113.650448
Sum of electronic and thermal Enthalpies	=	-1113.649503
Sum of electronic and thermal Free Energies	=	-1113.73198
Number of imaginary frequencies/frequency	=	1

TS-TUF-wB97xD-6-31+Gdp-AQN-ModelSubstrateA3b.out

0 3

C	0.880407	3.709173	-0.575192
C	2.106487	3.070801	-0.520310
C	2.189715	1.672335	-0.432357
C	0.995212	0.904965	-0.372578
C	-0.248898	1.574073	-0.472244
C	-0.302574	2.948747	-0.570421
C	3.511520	1.027238	-0.455945
C	1.078487	-0.518224	-0.259808
C	2.337115	-1.197274	-0.385178
C	3.534202	-0.443355	-0.481810
C	4.763712	-1.115883	-0.565375
H	5.671126	-0.524120	-0.627913
C	4.819004	-2.498231	-0.566019
C	3.632384	-3.246470	-0.464505
C	2.411161	-2.611129	-0.365843
H	0.831101	4.791182	-0.644167
H	3.029683	3.639824	-0.557235
H	-1.167040	1.000071	-0.505740
H	-1.265765	3.442763	-0.653103
H	5.775988	-3.005255	-0.637577
H	3.676007	-4.331244	-0.456653
H	1.500858	-3.193599	-0.272974
O	4.558446	1.692005	-0.473523
O	0.016617	-1.289676	-0.064534
H	-0.975838	-0.651274	0.875688
C	-1.654479	-0.448557	1.820535
H	-1.766188	-1.475628	2.192009
C	-0.866536	0.421424	2.778088
H	-1.518321	0.618707	3.642349
H	-0.674078	1.395785	2.312759
C	-2.975532	0.131317	1.354924
H	-3.656131	0.147467	2.217046
H	-2.844162	1.169139	1.028023
C	-3.595830	-0.689225	0.241566
H	-3.745325	-1.728776	0.548689
H	-2.970838	-0.678411	-0.657353
C	0.439134	-0.203878	3.259255
H	0.931290	0.444636	3.990478
H	0.260230	-1.174483	3.734848
H	1.139033	-0.359627	2.431401
O	-4.871830	-0.102024	-0.070821
C	-5.593489	-0.694882	-1.029856
O	-5.219060	-1.690496	-1.619770
C	-6.881956	0.029484	-1.283804
H	-7.388096	0.257328	-0.342711
H	-6.665298	0.977559	-1.786553
H	-7.527092	-0.575213	-1.920865

Zero-point correction	=	0.380442
Thermal correction to Energy	=	0.404071
Thermal correction to Enthalpy	=	0.405015
Thermal correction to Gibbs Free Energy	=	0.322485
Sum of electronic and zero-point Energies	=	-1113.674828
Sum of electronic and thermal Energies	=	-1113.651199
Sum of electronic and thermal Enthalpies	=	-1113.650255
Sum of electronic and thermal Free Energies	=	-1113.732785
Number of imaginary frequencies/frequency	=	1

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0 3

C	0.059536	-3.119792	-2.671693
C	1.198562	-2.416893	-2.323376
C	1.268175	-1.707034	-1.114619
C	0.140312	-1.685583	-0.250130
C	-1.001063	-2.446799	-0.604418
C	-1.037727	-3.146515	-1.792758
C	2.525767	-1.035862	-0.751113
C	0.208805	-0.941100	0.970646
C	1.440093	-0.349195	1.412136
C	2.580993	-0.394589	0.571481
C	3.771389	0.215106	0.997080
H	4.632122	0.180842	0.337256
C	3.845762	0.848743	2.224842
C	2.712375	0.900780	3.055780
C	1.525031	0.321353	2.656407
H	0.019655	-3.665428	-3.608975
H	2.067804	-2.410412	-2.972787
H	-1.844454	-2.506952	0.072869
H	-1.918718	-3.729489	-2.042934
H	4.774191	1.311627	2.543705
H	2.767692	1.406038	4.015027
H	0.650316	0.378244	3.295364
O	3.501428	-1.028002	-1.516140
O	-0.835008	-0.773061	1.772711
H	-2.124022	-0.570316	0.977726
C	-3.085179	-0.085513	0.520356
H	-3.211062	-0.605121	-0.437279
C	-4.199595	-0.409664	1.494866
H	-5.122768	0.046555	1.109052
H	-3.994360	0.071851	2.458733
C	-2.776793	1.386459	0.331893
H	-3.676571	1.876678	-0.064356
H	-2.552268	1.852087	1.298514
C	-1.623016	1.606474	-0.627706
H	-1.816249	1.140516	-1.599442
H	-0.687334	1.203716	-0.231710
C	-4.407255	-1.909318	1.685554
H	-5.235638	-2.106373	2.372975
H	-4.636109	-2.399565	0.732821
H	-3.508874	-2.380539	2.100180
O	-1.471125	3.025728	-0.810286
C	-0.424262	3.431914	-1.539362
O	0.378732	2.661804	-2.030780
C	-0.388688	4.925404	-1.672897
H	0.521173	5.229999	-2.189327
H	-1.261574	5.258934	-2.242333
H	-0.434498	5.395103	-0.686925

Zero-point correction = 0.380979
Thermal correction to Energy = 0.404741
Thermal correction to Enthalpy = 0.405686
Thermal correction to Gibbs Free Energy = 0.322819
Sum of electronic and zero-point Energies = -1113.67486
Sum of electronic and thermal Energies = -1113.651098
Sum of electronic and thermal Enthalpies = -1113.650153
Sum of electronic and thermal Free Energies = -1113.73302
Number of imaginary frequencies/frequency = 1

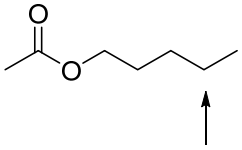
TS-TUF-wB97xD-6-31+Gdp-AQN-ModelSubstrateA3d.out

0 3

C	0.396109	-2.343099	-3.258093
C	1.463495	-1.628608	-2.745661
C	1.479870	-1.215627	-1.404248
C	0.369252	-1.511557	-0.568051
C	-0.694061	-2.282350	-1.099455
C	-0.678361	-2.686256	-2.418574
C	2.670297	-0.525133	-0.884065
C	0.378363	-1.061088	0.791070
C	1.547245	-0.455549	1.365211
C	2.676729	-0.195203	0.549087
C	3.804886	0.419683	1.114518
H	4.657640	0.620084	0.474079
C	3.829223	0.765744	2.453888
C	2.705661	0.515901	3.261996
C	1.578600	-0.076207	2.729165
H	0.396554	-2.656053	-4.297248
H	2.317125	-1.382379	-3.368502
H	-1.516709	-2.584671	-0.462921
H	-1.499396	-3.282025	-2.805206
H	4.710137	1.235683	2.879431
H	2.720665	0.795683	4.310817
H	0.710312	-0.253692	3.354520
O	3.631907	-0.249003	-1.616592
O	-0.659144	-1.194336	1.605958
H	-1.993711	-1.011975	0.888603
C	-3.046102	-0.576828	0.617521
H	-3.240337	-0.960441	-0.391496
C	-3.991710	-1.164763	1.645120
H	-4.996214	-0.767576	1.439419
H	-3.714236	-0.805038	2.643402
C	-2.902845	0.931693	0.639538
H	-3.891799	1.374275	0.458140
H	-2.576530	1.262718	1.632282
C	-1.931430	1.427482	-0.413977
H	-2.239841	1.121557	-1.418539
H	-0.918326	1.056523	-0.235771
C	-4.024545	-2.690338	1.622191
H	-4.736770	-3.078761	2.356684
H	-4.321247	-3.062849	0.635436
H	-3.038902	-3.106858	1.858475
O	-1.912180	2.864856	-0.344673
C	-1.059382	3.496837	-1.160393
O	-0.335882	2.911462	-1.943561
C	-1.111752	4.983887	-0.972383
H	-2.138143	5.342466	-1.087008
H	-0.781256	5.235757	0.039778
H	-0.463861	5.472006	-1.699874

Zero-point correction = 0.380823
Thermal correction to Energy = 0.404616
Thermal correction to Enthalpy = 0.40556
Thermal correction to Gibbs Free Energy = 0.322769
Sum of electronic and zero-point Energies = -1113.674923
Sum of electronic and thermal Energies = -1113.65113
Sum of electronic and thermal Enthalpies = -1113.650186
Sum of electronic and thermal Free Energies = -1113.732977
Number of imaginary frequencies/frequency = 1

Transition State for abstracting C4



TS-TUF-wB97xD-6-31+Gdp-AQN-ModelSubstrateA4a.out

0 3

C	3.364730	3.914419	0.142202
C	4.092785	2.739316	0.090681
C	3.452107	1.500196	-0.067137
C	2.038362	1.457590	-0.161175
C	1.305235	2.667031	-0.089040
C	1.961903	3.872786	0.051841
C	4.253049	0.267685	-0.097586
C	1.370835	0.191812	-0.292885
C	2.112679	-1.023220	-0.447438
C	3.528559	-0.992536	-0.321680
C	4.260000	-2.183416	-0.454901
H	5.338677	-2.137119	-0.347010
C	3.627020	-3.381440	-0.730675
C	2.231819	-3.406797	-0.904708
C	1.487422	-2.253642	-0.768767
H	3.873504	4.866004	0.258922
H	5.174732	2.752590	0.172294
H	0.222176	2.641880	-0.143414
H	1.389282	4.793870	0.099525
H	4.204735	-4.294607	-0.831680
H	1.733396	-4.337955	-1.155867
H	0.417545	-2.292824	-0.933456
O	5.485329	0.291925	0.041036
O	0.047686	0.241452	-0.302538
H	-0.609883	-0.990557	0.350872
C	-1.143610	-1.621596	1.173605
H	-1.323128	-2.586288	0.684151
C	-0.184709	-1.735165	2.338352
H	-0.650525	-2.314990	3.145346
H	0.738795	-2.246394	2.051693
H	0.070813	-0.748882	2.740117
C	-2.432713	-0.878637	1.462723
H	-2.944256	-1.402488	2.283989
H	-2.197653	0.126764	1.835802
C	-3.361054	-0.790482	0.251952
H	-3.600547	-1.799723	-0.103046
H	-2.856055	-0.264240	-0.566511
C	-4.645269	-0.064102	0.597297
H	-5.193357	-0.578640	1.392707
H	-4.449702	0.963672	0.918770
O	-5.463445	-0.033747	-0.588834
C	-6.664337	0.546334	-0.488394
O	-7.081798	1.033947	0.545286
C	-7.405127	0.516779	-1.792778
H	-6.852369	1.090666	-2.542482
H	-7.487415	-0.511803	-2.154387
H	-8.399059	0.944959	-1.664859

Zero-point correction = 0.38088
Thermal correction to Energy = 0.404686
Thermal correction to Enthalpy = 0.405631
Thermal correction to Gibbs Free Energy = 0.32272
Sum of electronic and zero-point Energies = -1113.673707
Sum of electronic and thermal Energies = -1113.649901
Sum of electronic and thermal Enthalpies = -1113.648957
Sum of electronic and thermal Free Energies = -1113.731867
Number of imaginary frequencies/frequency = 1

TS-TUF-wB97xD-6-31+Gdp-AQN-ModelSubstrateA4b.out

0 3

C	3.589621	-0.699330	-1.804966
C	3.213083	0.394437	-1.046265
C	1.858744	0.721808	-0.876193
C	0.867605	-0.097327	-1.472932
C	1.267144	-1.227298	-2.226394
C	2.606765	-1.511899	-2.397534
C	1.490558	1.878457	-0.047177
C	-0.521112	0.202882	-1.262640
C	-0.923766	1.399806	-0.589936
C	0.060201	2.205029	0.044098
C	-0.334345	3.360026	0.737325
H	0.432072	3.953485	1.224899
C	-1.662629	3.741910	0.785637
C	-2.630878	2.980844	0.106586
C	-2.272201	1.833521	-0.569936

H	4.640720	-0.936977	-1.934078
H	3.957926	1.020513	-0.566005
H	0.513956	-1.870802	-2.668361
H	2.901240	-2.376244	-2.984641
H	-1.954116	4.637264	1.325239
H	-3.668174	3.300937	0.104714
H	-3.026554	1.279491	-1.114721
O	2.349754	2.558922	0.534448
O	-1.384566	-0.679010	-1.749172
H	-2.617345	-0.873410	-0.843421
C	-3.501933	-1.275717	-0.195506
H	-3.952964	-0.362417	0.208050
C	-4.424973	-2.000099	-1.150365
H	-5.282531	-2.408513	-0.600016
H	-4.811115	-1.327362	-1.921610
H	-3.913872	-2.836562	-1.638786
C	-2.904924	-2.126542	0.911148
H	-3.733912	-2.413482	1.571545
H	-2.521331	-3.063524	0.486320
C	-1.804882	-1.416001	1.722472
H	-1.974362	-1.534735	2.796943
H	-1.821399	-0.340425	1.512826
C	-0.435661	-1.971902	1.375757
H	-0.310150	-2.984333	1.770713
H	-0.276408	-2.007921	0.293850
O	0.559794	-1.110255	1.957760
C	1.835558	-1.501729	1.856288
O	2.168513	-2.547937	1.332120
C	2.773173	-0.521223	2.495946
H	2.530232	0.501377	2.199214
H	2.668852	-0.589346	3.583813
H	3.800392	-0.758692	2.219792

Zero-point correction	=	0.381723
Thermal correction to Energy	=	0.404852
Thermal correction to Enthalpy	=	0.405796
Thermal correction to Gibbs Free Energy	=	0.327542
Sum of electronic and zero-point Energies	=	-1113.675969
Sum of electronic and thermal Energies	=	-1113.65284
Sum of electronic and thermal Enthalpies	=	-1113.651896
Sum of electronic and thermal Free Energies	=	-1113.73015
Number of imaginary frequencies/frequency	=	1

TS-TUF-wB97xD-6-31+Gdp-AQN-ModelSubstrateA4c.out

0 3

C	-4.008087	-1.979865	-1.205168
C	-2.746121	-2.535326	-1.097511
C	-1.745863	-1.912997	-0.333932
C	-2.031713	-0.686445	0.324673
C	-3.338679	-0.147376	0.225130
C	-4.304383	-0.783900	-0.526404
C	-0.432202	-2.563086	-0.206724
C	-1.010061	-0.052228	1.099585
C	0.268537	-0.670910	1.295709
C	0.561272	-1.899531	0.650571
C	1.840788	-2.458932	0.789259
H	2.055380	-3.388850	0.272861
C	2.810902	-1.833779	1.552652
C	2.520817	-0.616473	2.193939
C	1.274589	-0.038042	2.065362
H	-4.772107	-2.471311	-1.799021
H	-2.506346	-3.468452	-1.596754
H	-3.591869	0.761557	0.759006
H	-5.301928	-0.359947	-0.586738
H	3.797899	-2.275262	1.647012
H	3.286187	-0.119242	2.781519
H	1.064501	0.913254	2.542117
O	-0.175547	-3.625924	-0.792521
O	-1.185569	1.129728	1.679279
H	-1.885178	2.082093	0.698849
C	-1.962459	2.954405	-0.079359
H	-2.471337	2.488996	-0.931830
C	-2.787651	4.041837	0.571654
H	-2.916956	4.877453	-0.128193
H	-3.782082	3.679126	0.847608
H	-2.295005	4.429719	1.469471
C	-0.519033	3.306786	-0.382786
H	-0.498959	4.245849	-0.953204
H	-0.008315	3.519114	0.566291
C	0.218468	2.201033	-1.148296
H	0.052417	2.307308	-2.225678
H	-0.180498	1.222654	-0.863306
C	1.703177	2.195301	-0.845237
H	2.212340	3.078094	-1.245252
H	1.880012	2.150843	0.233407
O	2.261357	1.012949	-1.450280
C	3.518566	0.693406	-1.127457
O	4.216013	1.380860	-0.404985
C	3.956731	-0.580034	-1.789075
H	3.152526	-1.318558	-1.789546
H	4.218436	-0.361674	-2.830003
H	4.835278	-0.976717	-1.280082

Zero-point correction	=	0.381051
Thermal correction to Energy	=	0.40451
Thermal correction to Enthalpy	=	0.405454
Thermal correction to Gibbs Free Energy	=	0.325183
Sum of electronic and zero-point Energies	=	-1113.675758
Sum of electronic and thermal Energies	=	-1113.6523
Sum of electronic and thermal Enthalpies	=	-1113.651355
Sum of electronic and thermal Free Energies	=	-1113.731626
Number of imaginary frequencies/frequency	=	1

TS-TUF-wB97xD-6-31+Gdp-AQN-ModelSubstrateA4d.out

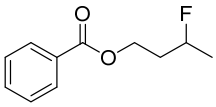
0 3

C	-1.838512	-1.690619	1.664787
C	-0.808876	-2.246978	0.927432
C	0.355023	-1.514958	0.646090
C	0.460378	-0.170275	1.095910
C	-0.585942	0.365783	1.883919
C	-1.710789	-0.382415	2.162386
C	1.462511	-2.173328	-0.062807
C	1.639774	0.582772	0.795583
C	2.776487	-0.041200	0.182141
C	2.698236	-1.394970	-0.235582
C	3.808658	-1.986445	-0.858357
H	3.728906	-3.019305	-1.181414
C	4.975741	-1.270942	-1.059349
C	5.051757	0.073809	-0.653315
C	3.970706	0.684514	-0.051136
H	-2.734693	-2.266880	1.871907
H	-0.877054	-3.266008	0.561209
H	-0.501202	1.371782	2.279538
H	-2.504534	0.047687	2.765173
H	5.828469	-1.742856	-1.536988
H	5.963801	0.638367	-0.821142
H	4.028588	1.726367	0.244880
O	1.366552	-3.338260	-0.478996
O	1.772347	1.865406	1.104657
H	0.510287	2.656279	0.815542
C	-0.080785	3.424537	0.135896
H	-0.744032	3.923272	0.852634
C	0.993314	4.340781	-0.401642
H	0.528261	5.148579	-0.981678
H	1.574708	4.798178	0.403833
H	1.676945	3.802280	-1.066380
C	-0.828229	2.612513	-0.908278
H	-0.937103	3.227896	-1.811456
H	-0.199468	1.763345	-1.212133
C	-2.204450	2.118217	-0.444564
H	-2.969715	2.867499	-0.674658
H	-2.206924	1.978938	0.639797
C	-2.557968	0.798009	-1.096669
H	-2.631313	0.887544	-2.185347
H	-1.808874	0.035384	-0.860332
O	-3.829848	0.373525	-0.571264
C	-4.261587	-0.839192	-0.931569
O	-3.669264	-1.548334	-1.723326
C	-5.534625	-1.207329	-0.228665
H	-5.314905	-1.397428	0.826907
H	-6.254488	-0.386777	-0.276929
H	-5.958899	-2.106543	-0.674787

Zero-point correction	=	0.380993
Thermal correction to Energy	=	0.404392
Thermal correction to Enthalpy	=	0.405336
Thermal correction to Gibbs Free Energy	=	0.325531
Sum of electronic and zero-point Energies	=	-1113.673049

Sum of electronic and thermal Energies = -1113.64965
Sum of electronic and thermal Enthalpies = -1113.648706
Sum of electronic and thermal Free Energies = -1113.728511
Number of imaginary frequencies/frequency = 1

Result for "Calculated 19F NMR chemical shifts"



3F-butyl_benzoate

OPT-wB97xD-6-311+Gdp_3F-butyl_benzoateC_1.out

0 1

C	3.707640	-1.445058	0.418978
C	2.384203	-1.173991	0.097254
C	1.980045	0.142019	-0.132538
C	2.906179	1.180879	-0.034452
C	4.228059	0.905793	0.286585
C	4.629618	-0.407375	0.513514
H	4.019597	-2.468154	0.596338
H	1.663869	-1.979014	0.023686
H	2.581535	2.199245	-0.213371
H	4.946782	1.714301	0.359025
H	5.663335	-0.621666	0.762178
C	0.571939	0.483206	-0.482017
O	0.177168	1.609964	-0.676435
O	-0.209194	-0.596707	-0.563531
C	-1.598983	-0.392589	-0.874451
H	-1.925828	-1.339565	-1.300967
H	-1.688158	0.391266	-1.629351
C	-2.386707	-0.047849	0.379059
H	-1.979091	0.863390	0.826096
H	-2.290509	-0.854539	1.112952
C	-3.853664	0.199260	0.091284
H	-3.968680	0.965633	-0.681243
C	-4.663899	0.548488	1.316033
H	-4.580255	-0.236250	2.072997
H	-4.297946	1.485212	1.744547
H	-5.716592	0.679080	1.056332
F	-4.399825	-0.984633	-0.476110

Zero-point correction = 0.222875
Thermal correction to Energy = 0.236058
Thermal correction to Enthalpy = 0.237002
Thermal correction to Gibbs Free Energy = 0.181366
Sum of electronic and zero-point Energies = -677.077004
Sum of electronic and thermal Energies = -677.063821
Sum of electronic and thermal Enthalpies = -677.062876
Sum of electronic and thermal Free Energies = -677.118513
Number of imaginary frequencies/frequency = 0
Number of imaginary frequencies/frequency = 1

OPT-wB97xD-6-311+Gdp_3F-butyl_benzoateC_2.out

0 1

C	4.476390	-0.403221	-0.037862
C	3.224570	-0.998552	-0.106511
C	2.072850	-0.214811	-0.029091
C	2.181894	1.168742	0.120229
C	3.436293	1.760347	0.191016
C	4.583154	0.976207	0.112558
H	5.369762	-1.014363	-0.099872
H	3.127729	-2.071673	-0.222297
H	1.287983	1.776579	0.183669
H	3.520114	2.834548	0.311388
H	5.561263	1.441213	0.169785
C	0.750352	-0.899165	-0.097816
O	0.609948	-2.097530	-0.178995
O	-0.272273	-0.043618	-0.059325
C	-1.594573	-0.607904	-0.082203
H	-1.746028	-1.181839	0.834294
H	-1.680729	-1.286117	-0.934792
C	-2.568691	0.547243	-0.191640
H	-2.368207	1.101787	-1.113892
H	-2.434515	1.236500	0.648025
C	-4.011245	0.083409	-0.229607
H	-4.149889	-0.678883	-1.002446
C	-5.008808	1.203451	-0.398402
H	-4.887111	1.953596	0.387897
H	-4.862478	1.687874	-1.367397
H	-6.028412	0.814148	-0.360516
F	-4.296000	-0.575407	0.996519

Zero-point correction = 0.22229
Thermal correction to Energy = 0.235669
Thermal correction to Enthalpy = 0.236613
Thermal correction to Gibbs Free Energy = 0.180351
Sum of electronic and zero-point Energies = -677.07741
Sum of electronic and thermal Energies = -677.06403
Sum of electronic and thermal Enthalpies = -677.063086
Sum of electronic and thermal Free Energies = -677.119348
Number of imaginary frequencies/frequency = 0

OPT-wB97xD-6-311+Gdp_3F-butyl_benzoateC_3.out

0 1

C	-3.965324	0.191027	0.758031
C	-2.767478	0.874829	0.605364
C	-1.705519	0.281002	-0.077269
C	-1.848461	-1.003442	-0.605171
C	-3.048498	-1.685012	-0.448595
C	-4.106715	-1.089067	0.230361
H	-4.789894	0.656210	1.286264
H	-2.644249	1.871341	1.013158
H	-1.023760	-1.465462	-1.133600
H	-3.158902	-2.682021	-0.860149
H	-5.043509	-1.622609	0.349403
C	-0.438772	1.054937	-0.212953
O	-0.260311	2.148914	0.271263
O	0.479376	0.408054	-0.933671
C	1.766272	1.034554	-1.098278
H	1.628379	2.103190	-1.265529
H	2.175860	0.579611	-1.999222
C	2.663445	0.787319	0.102076
H	2.226831	1.250680	0.991441
H	3.623386	1.281306	-0.082849
C	2.905757	-0.679565	0.398483
H	1.956507	-1.209801	0.512508
C	3.798928	-0.919261	1.591568
H	4.760085	-0.413060	1.465142
H	3.318971	-0.531744	2.494206
H	3.976493	-1.987723	1.731174
F	3.524386	-1.263287	-0.740488

Zero-point correction = 0.222907
Thermal correction to Energy = 0.23607
Thermal correction to Enthalpy = 0.237014
Thermal correction to Gibbs Free Energy = 0.180357
Sum of electronic and zero-point Energies = -677.078037
Sum of electronic and thermal Energies = -677.064875
Sum of electronic and thermal Enthalpies = -677.063931
Sum of electronic and thermal Free Energies = -677.120588
Number of imaginary frequencies/frequency = 0

OPT-wB97xD-6-311+Gdp_3F-butyl_benzoateC_4.out

0 1

C	2.725943	-1.894794	0.261630
C	1.614492	-1.062098	0.235247
C	1.776634	0.303959	-0.000357
C	3.052152	0.828534	-0.209860
C	4.160339	-0.006861	-0.179374
C	3.997566	-1.368818	0.056034
H	2.598388	-2.956172	0.442079
H	0.623200	-1.469011	0.390959
H	3.166280	1.890336	-0.394122
H	5.150663	0.404349	-0.339179
H	4.863101	-2.022160	0.078373
C	0.614303	1.236027	-0.041460
O	0.694059	2.409847	-0.325710
O	-0.531867	0.634679	0.272298
C	-1.716602	1.446315	0.256206
H	-1.835763	1.882714	-0.739473

H	-1.591686	2.261543	0.972845
C	-2.908416	0.590044	0.629731
H	-3.753889	1.273032	0.763600
H	-2.739811	0.098987	1.593580
C	-3.323623	-0.446560	-0.398838
H	-3.293989	-0.016489	-1.404776
C	-4.675797	-1.060940	-0.121048
H	-4.706206	-1.493770	0.882883
H	-5.454018	-0.296717	-0.193643
H	-4.895934	-1.844002	-0.849667
F	-2.369979	-1.495300	-0.411514

Zero-point correction =	0.222442	
Thermal correction to Energy =	0.23567	
Thermal correction to Enthalpy =	0.236614	
Thermal correction to Gibbs Free Energy =		0.180607
Sum of electronic and zero-point Energies =		-677.076306
Sum of electronic and thermal Energies =		-677.063078
Sum of electronic and thermal Enthalpies =		-677.062134
Sum of electronic and thermal Free Energies =		-677.118141
Number of imaginary frequencies/frequency =		0

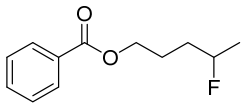
OPT-wB97xD-6-311+Gdp_3F-butyl_benzoateC_5.out

0 1

C	-4.237539	0.848986	0.258522
C	-2.896252	1.175474	0.114321
C	-1.949077	0.170096	-0.081688
C	-2.352370	-1.165380	-0.130139
C	-3.694874	-1.488210	0.018864
C	-4.637611	-0.483332	0.211750
H	-4.971854	1.632608	0.407400
H	-2.571777	2.208851	0.152204
H	-1.617387	-1.945765	-0.282325
H	-4.005706	-2.526310	-0.017467
H	-5.685646	-0.737857	0.326888
C	-0.520278	0.567117	-0.231719
O	-0.118098	1.702602	-0.121320
O	0.269766	-0.471719	-0.512442
C	1.678167	-0.217429	-0.663892
H	1.811639	0.728817	-1.188955
H	2.036744	-1.032592	-1.291699
C	2.366360	-0.219422	0.692189
H	2.095951	-1.132666	1.230296
H	2.015589	0.630073	1.285701
C	3.880499	-0.136071	0.613836
H	4.287856	-0.137750	1.627549
C	4.433499	1.029546	-0.174262
H	4.151868	0.966104	-1.228169
H	4.043463	1.966300	0.233084
H	5.523236	1.051497	-0.107781
F	4.361060	-1.334068	0.017408

Zero-point correction =	0.222804	
Thermal correction to Energy =	0.235987	
Thermal correction to Enthalpy =	0.236932	
Thermal correction to Gibbs Free Energy =		0.181057
Sum of electronic and zero-point Energies =		-677.076023
Sum of electronic and thermal Energies =		-677.06284
Sum of electronic and thermal Enthalpies =		-677.061895
Sum of electronic and thermal Free Energies =		-677.11777
Number of imaginary frequencies/frequency =		0

	Calculated 19F NMR Shielding Tensor
OPT-wB97xD-6-311+Gdp_3F-butyl_benzoateC_1.out	371.2104
OPT-wB97xD-6-311+Gdp_3F-butyl_benzoateC_2.out	369.3232
OPT-wB97xD-6-311+Gdp_3F-butyl_benzoateC_3.out	376.0112
OPT-wB97xD-6-311+Gdp_3F-butyl_benzoateC_4.out	364.3046
OPT-wB97xD-6-311+Gdp_3F-butyl_benzoateC_5.out	371.5643



4F-pentyl_benzoate

C2 omitted due to presence of 1 imaginary frequency

OPT-wB97xD-6-311+Gdp_4F-pentyl_benzoateC_1.out

0 1

C	-3.803876	1.879952	0.131977
C	-2.606552	1.177006	0.098972
C	-2.620407	-0.214572	-0.010433
C	-3.836461	-0.893980	-0.084860
C	-5.030835	-0.187827	-0.051620
C	-5.015176	1.199648	0.057275
H	-3.791346	2.960736	0.217642
H	-1.662754	1.704558	0.157963
H	-3.834661	-1.974296	-0.171323
H	-5.974555	-0.718150	-0.111225
H	-5.948964	1.750793	0.083358
C	-1.363073	-1.015036	-0.052296
O	-1.329069	-2.219666	-0.159268
O	-0.271025	-0.256884	0.039432
C	1.000415	-0.928118	-0.007461
H	1.091473	-1.443933	-0.967535
H	1.036486	-1.675684	0.789458
C	2.075919	0.123153	0.161956
H	1.946536	0.618386	1.130246
H	1.959295	0.883934	-0.614669
C	3.467700	-0.499223	0.077224
H	3.574150	-1.280109	0.839161
C	4.588721	0.496788	0.296969
H	4.452010	1.020948	1.247970
F	4.492381	1.505480	-0.699780
C	5.970103	-0.107051	0.210615
H	6.114796	-0.604246	-0.752465
H	6.735542	0.662990	0.329352
H	6.101179	-0.846085	1.005719
H	3.611267	-0.981210	-0.896829

Zero-point correction =	0.251355	
Thermal correction to Energy =	0.265969	
Thermal correction to Enthalpy =	0.266913	
Thermal correction to Gibbs Free Energy =		0.207402
Sum of electronic and zero-point Energies =		-716.363366
Sum of electronic and thermal Energies =		-716.348752
Sum of electronic and thermal Enthalpies =		-716.347808
Sum of electronic and thermal Free Energies =		-716.407318
Number of imaginary frequencies/frequency =		0

OPT-wB97xD-6-311+Gdp_4F-pentyl_benzoateC_3.out

0 1

C	-3.087843	1.996520	-0.536703
C	-2.064608	1.059900	-0.470572
C	-2.322902	-0.219345	0.024274
C	-3.608083	-0.551299	0.453566
C	-4.627860	0.387944	0.387333
C	-4.368670	1.662408	-0.107684
H	-2.886271	2.988828	-0.924309
H	-1.067655	1.317757	-0.805592
H	-3.797484	-1.547002	0.837197
H	-5.625511	0.126505	0.721854
H	-5.165041	2.396935	-0.158918
C	-1.260338	-1.262324	0.108723
O	-1.448785	-2.391501	0.499765
O	-0.073332	-0.816041	-0.298893
C	1.025545	-1.748278	-0.280318
H	0.802215	-2.563197	-0.972676
H	1.119784	-2.165114	0.725985
C	2.274105	-1.000161	-0.691110
H	2.129244	-0.574578	-1.690236
H	3.079497	-1.736023	-0.770912
C	2.667240	0.096116	0.295909
H	1.851598	0.820170	0.392398
C	3.905463	0.864214	-0.116385
H	3.786077	1.266850	-1.127204

F	4.989201	-0.052878	-0.210022
C	4.304209	1.954592	0.848955
H	4.446782	1.547948	1.853937
H	5.230349	2.435065	0.526107
H	3.520282	2.715551	0.889341
H	2.832721	-0.335174	1.290308

Zero-point correction = 0.25109
Thermal correction to Energy = 0.265656
Thermal correction to Enthalpy = 0.2666
Thermal correction to Gibbs Free Energy = 0.206892
Sum of electronic and zero-point Energies = -716.364429
Sum of electronic and thermal Energies = -716.349863
Sum of electronic and thermal Enthalpies = -716.348919
Sum of electronic and thermal Free Energies = -716.408627
Number of imaginary frequencies/frequency = 0

OPT-wB97xD-6-311+Gdp_4F-pentyl_benzoateC_4.out

0 1

C	-4.228962	0.414000	-1.023557
C	-3.117036	-0.416655	-1.007565
C	-2.145265	-0.264153	-0.018301
C	-2.294937	0.723644	0.956569
C	-3.408798	1.553008	0.937152
C	-4.375777	1.399094	-0.051470
H	-4.982156	0.293848	-1.794082
H	-2.991753	-1.187225	-1.759247
H	-1.541123	0.840373	1.725086
H	-3.522349	2.320103	1.694904
H	-5.244255	2.048728	-0.065108
C	-0.964422	-1.174857	-0.043045
O	-0.791164	-2.032326	-0.878418
O	-0.120148	-0.939848	0.961952
C	1.092152	-1.719567	1.019975
H	0.858311	-2.762323	0.800397
H	1.408843	-1.635687	2.060572
C	2.157584	-1.184761	0.080683
H	1.843152	-1.335963	-0.956420
H	3.052928	-1.794619	0.235534
C	2.481279	0.287448	0.321902
H	1.589000	0.896799	0.143153
C	3.577379	0.817800	-0.578512
H	3.346396	0.608728	-1.627645
F	4.767419	0.085004	-0.309570
C	3.882426	2.283142	-0.378945
H	4.719163	2.592358	-1.009273
H	3.009058	2.881770	-0.651908
H	4.130521	2.487919	0.666246
H	2.774245	0.448677	1.366322

Zero-point correction = 0.251377
Thermal correction to Energy = 0.265816
Thermal correction to Enthalpy = 0.26676
Thermal correction to Gibbs Free Energy = 0.20781
Sum of electronic and zero-point Energies = -716.363828
Sum of electronic and thermal Energies = -716.349389
Sum of electronic and thermal Enthalpies = -716.348445
Sum of electronic and thermal Free Energies = -716.407395
Number of imaginary frequencies/frequency = 0

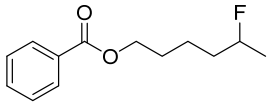
OPT-wB97xD-6-311+Gdp_4F-pentyl_benzoateC_5.out

0 1

C	-2.872354	-2.113346	-0.304331
C	-1.903586	-1.118794	-0.271525
C	-2.266090	0.195422	0.028021
C	-3.599942	0.505046	0.294353
C	-4.565494	-0.491145	0.258214
C	-4.202371	-1.801121	-0.040358
H	-2.589623	-3.134020	-0.536385
H	-0.868254	-1.358472	-0.479495
H	-3.868804	1.529307	0.524840
H	-5.602034	-0.247518	0.462402
H	-4.957414	-2.579262	-0.068007
C	-1.265422	1.299861	0.071243
O	-1.531953	2.445514	0.355016
O	-0.037590	0.890064	-0.242338
C	1.005246	1.883832	-0.251128
H	1.053450	2.353085	0.735486
H	0.750143	2.650315	-0.986256
C	2.301889	1.189701	-0.604902
H	3.067382	1.967118	-0.706887
H	2.198415	0.712767	-1.583624
C	2.743290	0.167718	0.439825
H	2.834061	0.657239	1.416647
C	4.080612	-0.472839	0.130239
H	4.842627	0.294891	-0.037660
F	3.969248	-1.159549	-1.110488
C	4.543835	-1.466844	1.167887
H	3.794257	-2.249449	1.314806
H	5.484831	-1.930503	0.864052
H	4.705053	-0.958133	2.122127
H	1.991340	-0.620993	0.545693

Zero-point correction = 0.251165
Thermal correction to Energy = 0.265759
Thermal correction to Enthalpy = 0.266704
Thermal correction to Gibbs Free Energy = 0.207007
Sum of electronic and zero-point Energies = -716.364134
Sum of electronic and thermal Energies = -716.34954
Sum of electronic and thermal Enthalpies = -716.348596
Sum of electronic and thermal Free Energies = -716.408292
Number of imaginary frequencies/frequency = 0

	Calculated 19F NMR Shielding Tensor
OPT-wB97xD-6-311+Gdp_4F-pentyl_benzoateC_1.out	370.9888
OPT-wB97xD-6-311+Gdp_4F-pentyl_benzoateC_3.out	371.1784
OPT-wB97xD-6-311+Gdp_4F-pentyl_benzoateC_4.out	370.803
OPT-wB97xD-6-311+Gdp_4F-pentyl_benzoateC_5.out	369.7011



5F-hexyl_benzoate

OPT-wB97xD-6-311+Gdp_5F-hexyl_benzoateC_1.out

0 1

C	4.404189	1.901444	0.258567
C	3.206060	1.199696	0.230588
C	3.212106	-0.177825	0.005522
C	4.420931	-0.844182	-0.195264
C	5.615789	-0.138257	-0.173384
C	5.608260	1.234631	0.055125
H	4.398263	2.970478	0.439531
H	2.266758	1.715474	0.386748
H	4.413416	-1.913993	-0.368625
H	6.553833	-0.657933	-0.333016
H	6.542824	1.784693	0.076017
C	1.952838	-0.976135	-0.021706
O	1.916708	-2.183438	-0.090039
O	0.863541	-0.210917	0.032407
C	-0.412768	-0.876877	0.028961
H	-0.515837	-1.439025	0.961572
H	-0.442977	-1.583846	-0.803701
C	-1.481131	0.186712	-0.103439
H	-1.324344	0.732568	-1.040305
H	-1.375277	0.907894	0.714248
C	-2.883457	-0.417649	-0.080817
H	-2.980631	-1.153841	-0.888161
C	-3.967508	0.645877	-0.234419
H	-3.820858	1.186670	-1.176704
C	-5.377225	0.091286	-0.250494
H	-5.473594	-0.685844	-1.015470
H	-3.033353	-0.958777	0.858858
C	-6.449705	1.141469	-0.417017
H	-6.340642	1.630416	-1.388812
H	-7.442500	0.688556	-0.370521
H	-6.371457	1.902086	0.364944

F	-5.610600	-0.575213	0.984361
H	-3.890501	1.385045	0.571859

Zero-point correction	=	0.280161
Thermal correction to Energy	=	0.296094
Thermal correction to Enthalpy	=	0.297039
Thermal correction to Gibbs Free Energy	=	0.234442
Sum of electronic and zero-point Energies	=	-755.648438
Sum of electronic and thermal Energies	=	-755.632505
Sum of electronic and thermal Enthalpies	=	-755.63156
Sum of electronic and thermal Free Energies	=	-755.694157
Number of imaginary frequencies/frequency	=	0

OPT-wB97xD-6-311+Gdp_5F-hexyl_benzoateC_2.out

0 1

C	4.764356	-1.429233	0.632974
C	3.468833	-1.165657	0.208032
C	3.083832	0.144959	-0.078900
C	4.002429	1.185315	0.062681
C	5.297375	0.917529	0.484736
C	5.679297	-0.390079	0.770099
H	5.060431	-2.448225	0.855648
H	2.755114	-1.972535	0.099231
H	3.693634	2.199565	-0.162034
H	6.010624	1.727350	0.589589
H	6.691590	-0.599074	1.098707
C	1.705359	0.476078	-0.542463
O	1.316888	1.601344	-0.757486
O	0.951979	-0.611998	-0.706878
C	-0.401982	-0.434027	-1.164745
H	-0.642728	-1.374717	-1.662060
H	-0.427297	0.373080	-1.899530
C	-1.354212	-0.167651	-0.013575
H	-1.070670	0.764440	0.485543
H	-1.260002	-0.975588	0.720364
C	-2.796852	-0.078655	-0.506776
H	-2.884163	0.736219	-1.235719
C	-3.789679	0.152535	0.629206
H	-3.539106	1.080233	1.156809
C	-5.227702	0.271475	0.167569
H	-5.318969	1.043515	-0.603072
H	-3.058288	-1.001915	-1.034541
C	-6.218457	0.508466	1.282128
H	-6.013253	1.468661	1.763152
H	-7.238109	0.534457	0.891232
H	-6.149058	-0.279604	2.037185
F	-5.590377	-0.941993	-0.481657
H	-3.722872	-0.659021	1.363524

Zero-point correction	=	0.280211
Thermal correction to Energy	=	0.29603
Thermal correction to Enthalpy	=	0.296975
Thermal correction to Gibbs Free Energy	=	0.234873
Sum of electronic and zero-point Energies	=	-755.648166
Sum of electronic and thermal Energies	=	-755.632347
Sum of electronic and thermal Enthalpies	=	-755.631403
Sum of electronic and thermal Free Energies	=	-755.693505
Number of imaginary frequencies/frequency	=	0

OPT-wB97xD-6-311+Gdp_5F-hexyl_benzoateC_3.out

0 1

C	4.786623	-0.986135	-0.335442
C	3.986069	0.143637	-0.434015
C	2.652354	0.092958	-0.028399
C	2.124646	-1.095950	0.478167
C	2.928746	-2.224178	0.575158
C	4.258813	-2.170555	0.170070
H	5.822839	-0.942629	-0.651392
H	4.386092	1.071186	-0.826413
H	1.088915	-1.136320	0.791507
H	2.516180	-3.146291	0.968794
H	4.884239	-3.053349	0.247204
C	1.828099	1.329782	-0.151347
O	2.238093	2.377315	-0.597404
O	0.582783	1.155559	0.285260
C	-0.312629	2.281420	0.207422
H	-0.356007	2.625494	-0.829757
H	0.087758	3.089995	0.823305
C	-1.667312	1.821623	0.701172
H	-2.316345	2.703782	0.742584
H	-1.566082	1.454335	1.728709
C	-2.300921	0.748316	-0.181332
H	-2.442215	1.149911	-1.192564
C	-3.640249	0.261823	0.365072
H	-4.337069	1.104292	0.449985
C	-4.308307	-0.788785	-0.498498
H	-4.401048	-0.433691	-1.529680
H	-1.614888	-0.098352	-0.271327
C	-5.642415	-1.263723	0.025725
H	-6.046852	-2.054069	-0.610592
H	-5.543308	-1.646608	1.045308
H	-6.354902	-0.434307	0.033755
F	-3.447136	-1.918939	-0.573244
H	-3.511190	-0.147313	1.374401

Zero-point correction	=	0.279363
Thermal correction to Energy	=	0.29529
Thermal correction to Enthalpy	=	0.296235
Thermal correction to Gibbs Free Energy	=	0.233645
Sum of electronic and zero-point Energies	=	-755.649714
Sum of electronic and thermal Energies	=	-755.633786
Sum of electronic and thermal Enthalpies	=	-755.632842
Sum of electronic and thermal Free Energies	=	-755.695432
Number of imaginary frequencies/frequency	=	0

OPT-wB97xD-6-311+Gdp_5F-hexyl_benzoateC_4.out

0 1

C	-3.458986	-1.818893	-1.039254
C	-2.524392	-0.792609	-0.999307
C	-2.537523	0.120180	0.056428
C	-3.490568	-0.001250	1.068089
C	-4.423849	-1.027773	1.024141
C	-4.408732	-1.937039	-0.029385
H	-3.445698	-2.528910	-1.858577
H	-1.782843	-0.700011	-1.782718
H	-3.493040	0.714832	1.881515
H	-5.165521	-1.117635	1.809884
H	-5.139381	-2.737934	-0.063376
C	-1.549657	1.234647	0.143724
O	-1.519452	2.042180	1.044163
O	-0.705468	1.242640	-0.887347
C	0.337879	2.238421	-0.901741
H	-0.084232	3.200972	-0.608458
H	0.639723	2.284878	-1.949076
C	1.506560	1.853490	-0.012882
H	1.188883	1.870868	1.034363
H	2.262233	2.639996	-0.125875
C	2.116028	0.496030	-0.355398
H	1.358769	-0.286889	-0.234555
C	3.320529	0.170430	0.523621
H	3.025429	0.204460	1.579247
C	3.916400	-1.198515	0.269386
H	3.145510	-1.971553	0.349097
H	2.414762	0.483905	-1.409170
C	5.099444	-1.529768	1.147568
H	5.878280	-0.768036	1.051267
H	4.782618	-1.569994	2.193322
H	5.519371	-2.502017	0.880623
F	4.352337	-1.251687	-1.084672
H	4.104664	0.925570	0.390084

Zero-point correction	=	0.279813
Thermal correction to Energy	=	0.295632
Thermal correction to Enthalpy	=	0.296576
Thermal correction to Gibbs Free Energy	=	0.234124
Sum of electronic and zero-point Energies	=	-755.649065
Sum of electronic and thermal Energies	=	-755.633246
Sum of electronic and thermal Enthalpies	=	-755.632302
Sum of electronic and thermal Free Energies	=	-755.694754
Number of imaginary frequencies/frequency	=	0

OPT-wB97xD-6-311+Gdp_5F-hexyl_benzoateC_5.out

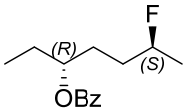
0 1

C	4.474609	-1.795637	-0.052014
C	3.233835	-1.172865	-0.014962
C	3.155740	0.220282	0.017789

C	4.324438	0.982309	0.011237
C	5.562512	0.356304	-0.028448
C	5.638507	-1.033001	-0.059431
H	4.534136	-2.878037	-0.075036
H	2.326437	-1.763818	-0.008805
H	4.251312	2.063314	0.037888
H	6.469231	0.950779	-0.034777
H	6.606062	-1.522118	-0.089267
C	1.848324	0.935906	0.065702
O	1.736644	2.138137	0.142445
O	0.807858	0.105202	0.014458
C	-0.504864	0.694145	0.061970
H	-0.592236	1.427428	-0.744101
H	-0.622251	1.216083	1.015781
C	-1.515508	-0.422130	-0.088767
H	-1.365281	-1.155558	0.710687
H	-1.340784	-0.937563	-1.039696
C	-2.946201	0.110732	-0.041751
H	-3.115643	0.620508	0.912776
C	-3.973667	-1.006504	-0.211833
H	-3.781624	-1.797631	0.521403
C	-5.424493	-0.582926	-0.067043
H	-6.069415	-1.453916	-0.211039
H	-3.075599	0.861687	-0.828814
C	-5.872501	0.552422	-0.958194
H	-6.939099	0.744489	-0.822769
H	-5.323632	1.470675	-0.737318
H	-5.700931	0.289849	-2.006028
F	-5.639649	-0.183475	1.282201
H	-3.864243	-1.465838	-1.201460

Zero-point correction	=	0.280023
Thermal correction to Energy	=	0.295889
Thermal correction to Enthalpy	=	0.296833
Thermal correction to Gibbs Free Energy	=	0.234305
Sum of electronic and zero-point Energies	=	-755.647945
Sum of electronic and thermal Energies	=	-755.63208
Sum of electronic and thermal Enthalpies	=	-755.631136
Sum of electronic and thermal Free Energies	=	-755.693663
Number of imaginary frequencies/frequency	=	0

	Calculated 19F NMR Shielding Tensor
OPT-wB97xD-6-311+Gdp_5F-hexyl_benzoateC_1.out	370.9721
OPT-wB97xD-6-311+Gdp_5F-hexyl_benzoateC_2.out	370.3785
OPT-wB97xD-6-311+Gdp_5F-hexyl_benzoateC_3.out	369.3206
OPT-wB97xD-6-311+Gdp_5F-hexyl_benzoateC_4.out	370.233
OPT-wB97xD-6-311+Gdp_5F-hexyl_benzoateC_5.out	372.4307



6F-(S,R)-heptan-2-yl-benzoate

OPT-wB97xD-6-311+Gdp_6F-(S,R)-heptan-2-yl-benzoateC_1.out

0 1

C	0.325717	2.244045	0.072475
H	0.333668	2.443291	-1.002140
C	-0.137208	3.474119	0.830482
H	-0.178697	3.271488	1.904617
H	0.563162	4.296204	0.660840
H	-1.125275	3.793467	0.492835
C	1.683847	1.734306	0.525334
H	1.623052	1.476993	1.589846
H	2.394634	2.564092	0.441280
C	2.187667	0.536249	-0.275159
H	1.446861	-0.266760	-0.233076
H	2.288894	0.818615	-1.330343
C	3.526779	0.018979	0.243072
H	4.280256	0.813785	0.188376
H	3.438992	-0.262085	1.299504
C	4.066836	-1.168101	-0.528198
H	4.115943	-0.941086	-1.597865
C	5.398406	-1.674707	-0.026947
H	5.340522	-1.925346	1.036025
H	5.708516	-2.562195	-0.583095
H	6.161841	-0.903229	-0.159707
O	-0.604632	1.155850	0.308422
F	3.130241	-2.233513	-0.419884
C	-1.690896	1.059415	-0.454141
O	-1.981775	1.851516	-1.321915
C	-2.504543	-0.146472	-0.120437
C	-2.062726	-1.095787	0.802271
C	-3.728561	-0.322428	-0.766015
C	-2.841689	-2.212689	1.074271
H	-1.111290	-0.960936	1.300845
C	-4.506713	-1.438121	-0.488295
H	-4.060694	0.419001	-1.483301
C	-4.063410	-2.384281	0.431046
H	-2.493967	-2.950770	1.788234
H	-5.458588	-1.571334	-0.990069
H	-4.669778	-3.257670	0.645540

Zero-point correction	=	0.307463
Thermal correction to Energy	=	0.324839
Thermal correction to Enthalpy	=	0.325783
Thermal correction to Gibbs Free Energy	=	0.259727
Sum of electronic and zero-point Energies	=	-794.940218
Sum of electronic and thermal Energies	=	-794.922842
Sum of electronic and thermal Enthalpies	=	-794.921898
Sum of electronic and thermal Free Energies	=	-794.987954
Number of imaginary frequencies/frequency	=	0

OPT-wB97xD-6-311+Gdp_6F-(S,R)-heptan-2-yl-benzoateC_2.out

0 1

C	-0.796456	2.171839	0.111740
H	-1.115942	1.866173	1.109106
C	-0.382219	3.630187	0.134679
H	-0.006755	3.941694	-0.844251
H	-1.242980	4.254362	0.389785
H	0.395970	3.801603	0.882029
C	-1.878663	1.864953	-0.913153
H	-1.574864	2.273140	-1.883571
H	-2.777422	2.412288	-0.607235
C	-2.202161	0.378184	-1.070187
H	-2.996615	0.276163	-1.814966
H	-1.325887	-0.140455	-1.473741
C	-2.633247	-0.306401	0.225609
H	-1.830256	-0.257192	0.969449
H	-3.501031	0.204068	0.661410
C	-2.967541	-1.773205	0.049796
H	-2.140816	-2.293276	-0.444604
C	-3.352867	-2.476586	1.329129
H	-4.201565	-1.977184	1.804930
H	-3.618913	-3.517571	1.132808
H	-2.510226	-2.464905	2.025855
O	0.352493	1.360144	-0.245731
F	-4.063830	-1.880818	-0.851556
C	1.100660	0.844079	0.726251
O	0.915097	1.046622	1.905333
C	2.189892	-0.028759	0.198352
C	2.347468	-0.266443	-1.167956
C	3.060057	-0.623880	1.111980
C	3.368647	-1.096167	-1.612628
H	1.672159	0.195999	-1.876868
C	4.079706	-1.452154	0.663918
H	2.927611	-0.432346	2.170305
C	4.234472	-1.688809	-0.698705
H	3.490046	-1.280461	-2.674146
H	4.754551	-1.912501	1.376769
H	5.030195	-2.337391	-1.048822

Zero-point correction	=	0.30775
Thermal correction to Energy	=	0.324983
Thermal correction to Enthalpy	=	0.325927
Thermal correction to Gibbs Free Energy	=	0.259976
Sum of electronic and zero-point Energies	=	-794.940511
Sum of electronic and thermal Energies	=	-794.923278
Sum of electronic and thermal Enthalpies	=	-794.922333
Sum of electronic and thermal Free Energies	=	-794.988285

Number of imaginary frequencies/frequency = 0

OPT-wB97xD-6-311+Gdp_6F-(S,R)-heptan-2-yl-benzoateC_3.out

0 1

C	-0.386830	-0.861496	0.370730
H	-0.457178	-1.534693	-0.486538
C	-0.454814	-1.656578	1.661570
H	-0.389250	-0.990771	2.527375
H	-1.396847	-2.206918	1.717004
H	0.358929	-2.383227	1.709910
C	-1.426814	0.241598	0.249598
H	-1.224886	0.795501	-0.673558
H	-1.303036	0.945731	1.081261
C	-2.859478	-0.286871	0.220330
H	-2.950694	-1.051704	-0.558170
H	-3.097957	-0.774912	1.171733
C	-3.875283	0.823779	-0.034524
H	-3.777196	1.597241	0.736449
H	-3.677517	1.308340	-0.998021
C	-5.314616	0.351509	-0.015942
H	-5.528831	-0.182479	0.915453
C	-6.327900	1.446472	-0.249392
H	-6.133401	1.958288	-1.196109
H	-7.339964	1.036248	-0.271917
H	-6.273912	2.180727	0.558931
O	0.901122	-0.193459	0.301684
F	-5.480005	-0.617973	-1.043779
C	1.935756	-0.862301	-0.204747
O	1.863208	-1.987041	-0.645669
C	3.198807	-0.067846	-0.170814
C	3.258834	1.202313	0.404430
C	4.347423	-0.634495	-0.723693
C	4.461565	1.896840	0.425439
H	2.367475	1.641103	0.835026
C	5.546822	0.063566	-0.703441
H	4.289407	-1.621639	-1.166992
C	5.605285	1.329197	-0.127492
H	4.507151	2.881839	0.876208
H	6.436918	-0.379885	-1.135339
H	6.543651	1.872846	-0.109134

Zero-point correction = 0.308026
Thermal correction to Energy = 0.325222
Thermal correction to Enthalpy = 0.326166
Thermal correction to Gibbs Free Energy = 0.26138
Sum of electronic and zero-point Energies = -794.938656
Sum of electronic and thermal Energies = -794.92146
Sum of electronic and thermal Enthalpies = -794.920516
Sum of electronic and thermal Free Energies = -794.985302
Number of imaginary frequencies/frequency = 0

OPT-wB97xD-6-311+Gdp_6F-(S,R)-heptan-2-yl-benzoateC_4.out

0 1

C	-0.510871	2.144095	-0.103994
H	-0.618027	2.273523	0.975655
C	-0.052956	3.440772	-0.744472
H	0.097382	3.305389	-1.819423
H	-0.812224	4.213133	-0.596006
H	0.880066	3.790533	-0.298133
C	-1.800619	1.602710	-0.695849
H	-1.656442	1.440679	-1.771261
H	-2.561446	2.384432	-0.593077
C	-2.286951	0.317907	-0.031063
H	-1.511796	-0.447967	-0.124573
H	-2.429843	0.495547	1.040515
C	-3.592522	-0.181948	-0.645162
H	-4.349315	0.609221	-0.603519
H	-3.439771	-0.410289	-1.706973
C	-4.179683	-1.424181	0.001087
H	-5.113527	-1.686160	-0.503764
C	-3.265671	-2.626088	0.064120
H	-2.946503	-2.897646	-0.946207
H	-2.376785	-2.418877	0.664088
H	-3.787452	-3.480946	0.499806
O	0.495814	1.120864	-0.324051
F	-4.559615	-1.097960	1.333340
C	1.524033	1.045102	0.517615
O	1.684132	1.788426	1.459159
C	2.458039	-0.065894	0.169869
C	2.178462	-0.971181	-0.855052
C	3.638481	-0.189435	0.902528
C	3.075489	-1.992175	-1.140940
H	1.261517	-0.874526	-1.422827
C	4.535571	-1.207515	0.610099
H	3.845075	0.519117	1.696087
C	4.254308	-2.110109	-0.411177
H	2.854862	-2.696897	-1.934866
H	5.455228	-1.297643	1.177183
H	4.955305	-2.905665	-0.639287

Zero-point correction = 0.307589
Thermal correction to Energy = 0.324939
Thermal correction to Enthalpy = 0.325883
Thermal correction to Gibbs Free Energy = 0.25967
Sum of electronic and zero-point Energies = -794.939429
Sum of electronic and thermal Energies = -794.922079
Sum of electronic and thermal Enthalpies = -794.921135
Sum of electronic and thermal Free Energies = -794.987347
Number of imaginary frequencies/frequency = 0

OPT-wB97xD-6-311+Gdp_6F-(S,R)-heptan-2-yl-benzoateC_5.out

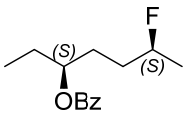
0 1

C	0.325721	2.249880	0.106992
H	-0.093445	3.021982	-0.540944
C	0.703130	2.845785	1.448056
H	1.028435	2.076177	2.152007
H	1.519435	3.560889	1.316849
H	-0.148303	3.373082	1.884391
C	1.467282	1.554610	-0.629607
H	2.217630	2.318456	-0.863772
H	1.084354	1.191448	-1.589113
C	2.118903	0.403073	0.133579
H	2.592014	0.777814	1.045611
H	1.349019	-0.312050	0.445241
C	3.162721	-0.321036	-0.712842
H	2.691966	-0.714215	-1.621551
H	3.943061	0.378199	-1.037044
C	3.820914	-1.488274	-0.006550
H	3.062524	-2.171321	0.389043
C	4.824358	-2.236558	-0.851485
H	5.307771	-3.024240	-0.269185
H	4.317773	-2.702358	-1.701180
H	5.590932	-1.557284	-1.234743
O	-0.729465	1.289620	0.383165
F	4.503244	-0.991055	1.139308
C	-1.606492	1.007581	-0.577392
O	-1.617720	1.541245	-1.663843
C	-2.579221	-0.045075	-0.161253
C	-3.561172	-0.435184	-1.071926
C	-2.520123	-0.646190	1.096987
C	-4.478951	-1.417846	-0.727314
H	-3.596978	0.038478	-2.045961
C	-3.440358	-1.628626	1.438534
H	-1.757267	-0.343684	1.803334
C	-4.418651	-2.015766	0.527997
H	-5.240495	-1.718757	-1.437872
H	-3.392771	-2.094835	2.416196
H	-5.135721	-2.783448	0.797690

Zero-point correction = 0.307607
Thermal correction to Energy = 0.324966
Thermal correction to Enthalpy = 0.32591
Thermal correction to Gibbs Free Energy = 0.25941
Sum of electronic and zero-point Energies = -794.939414
Sum of electronic and thermal Energies = -794.922056
Sum of electronic and thermal Enthalpies = -794.921112
Sum of electronic and thermal Free Energies = -794.987611
Number of imaginary frequencies/frequency = 0

	Calculated 19F NMR Shielding Tensor
OPT-wB97xD-6-311+Gdp_6F-(S,R)-heptan-2-yl-benzoateC_4.out	369.7974
OPT-wB97xD-6-311+Gdp_6F-(S,R)-heptan-2-yl-benzoateC_4.out	370.9717

OPT-wB97xD-6-311+Gdp_6F-(S,R)-heptan-2-yl-benzoateC_4.out	369.0566
OPT-wB97xD-6-311+Gdp_6F-(S,R)-heptan-2-yl-benzoateC_4.out	372.1343
OPT-wB97xD-6-311+Gdp_6F-(S,R)-heptan-2-yl-benzoateC_4.out	370.0903



6F-(S,S)-heptan-2-yl-benzoate

OPT-wB97xD-6-311+Gdp_6F-(S,S)-heptan-2-yl-benzoateC_1.out

0 1

C	-0.321688	2.122831	-0.126994
H	-0.393646	2.300532	0.948764
C	0.149106	3.378225	-0.837084
H	0.264947	3.192620	-1.908856
H	-0.587144	4.174953	-0.702158
H	1.102808	3.723810	-0.433203
C	-1.641055	1.591261	-0.660547
H	-1.525000	1.369237	-1.728620
H	-2.375508	2.400809	-0.584534
C	-2.154633	0.360962	0.082209
H	-1.411704	-0.441546	0.020050
H	-2.271571	0.600459	1.144279
C	-3.483395	-0.138170	-0.478531
H	-4.248429	0.644207	-0.404121
H	-3.368869	-0.368700	-1.544402
C	-4.002521	-1.389706	0.198792
C	-5.302105	-1.906270	-0.370718
H	-5.650358	-2.777161	0.188966
H	-6.073375	-1.131652	-0.338540
H	-5.154376	-2.205234	-1.411987
O	0.649766	1.063410	-0.331398
C	1.706452	0.996976	0.475032
O	1.924319	1.779988	1.371637
C	2.590683	-0.160453	0.148303
C	3.782817	-0.305104	0.857881
C	2.251799	-1.089505	-0.836579
C	4.631218	-1.369029	0.582963
H	4.036644	0.421544	1.620738
C	3.100480	-2.155212	-1.105608
H	1.325937	-0.976735	-1.386474
C	4.290432	-2.295144	-0.398291
H	5.559424	-1.476573	1.132874
H	2.833012	-2.877529	-1.868634
H	4.953250	-3.126562	-0.612424
H	-3.237144	-2.172179	0.191931
F	-4.217458	-1.096829	1.574386

Zero-point correction = 0.307422
Thermal correction to Energy = 0.324811
Thermal correction to Enthalpy = 0.325756
Thermal correction to Gibbs Free Energy = 0.259632
Sum of electronic and zero-point Energies = -794.940206
Sum of electronic and thermal Energies = -794.922817
Sum of electronic and thermal Enthalpies = -794.921873
Sum of electronic and thermal Free Energies = -794.987996
Number of imaginary frequencies/frequency = 0

OPT-wB97xD-6-311+Gdp_6F-(S,S)-heptan-2-yl-benzoateC_2.out

0 1

C	-0.352110	1.123092	0.672998
H	-0.384401	0.884886	1.738993
C	-0.619979	2.597717	0.453798
H	0.138542	3.201344	0.957320
H	-0.613560	2.840922	-0.612864
H	-1.594749	2.869210	0.864360
C	-1.282406	0.192151	-0.096119
H	-0.952370	-0.838296	0.071090
H	-1.173609	0.398085	-1.167480
C	-2.748179	0.326177	0.312329
H	-2.836046	0.241756	1.402664
H	-3.123294	1.316494	0.039465
C	-3.622377	-0.739244	-0.344913
H	-3.496477	-0.714596	-1.434019
H	-3.305704	-1.734122	-0.011178
C	-5.097565	-0.599562	-0.029860
C	-5.959742	-1.694594	-0.610736
H	-5.700709	-2.651138	-0.148838
H	-7.016332	-1.497474	-0.416418
H	-5.806951	-1.778242	-1.690288
O	1.006529	0.897694	0.211831
C	1.711440	-0.093143	0.753801
O	1.300778	-0.813149	1.636024
C	3.071553	-0.213708	0.150487
C	3.913926	-1.225423	0.611640
C	3.509093	0.650151	-0.854763
C	5.183381	-1.374529	0.069802
H	3.564614	-1.891153	1.392182
C	4.780381	0.499342	-1.393013
H	2.854518	1.435034	-1.212250
C	5.617440	-0.512423	-0.932890
H	5.835415	-2.162889	0.428849
H	5.118346	1.172722	-2.172678
H	6.608535	-0.630024	-1.357545
H	-5.253934	-0.515036	1.050116
F	-5.549937	0.640015	-0.564409

Zero-point correction = 0.30732
Thermal correction to Energy = 0.324796
Thermal correction to Enthalpy = 0.325741
Thermal correction to Gibbs Free Energy = 0.258574
Sum of electronic and zero-point Energies = -794.939551
Sum of electronic and thermal Energies = -794.922075
Sum of electronic and thermal Enthalpies = -794.921131
Sum of electronic and thermal Free Energies = -794.988297
Number of imaginary frequencies/frequency = 0

OPT-wB97xD-6-311+Gdp_6F-(S,S)-heptan-2-yl-benzoateC_3.out

0 1

C	-1.010362	2.151233	0.065382
H	-1.345330	1.833688	1.054017
C	-0.639689	3.621362	0.099670
H	-0.251466	3.945112	-0.870309
H	-1.523882	4.219813	0.335656
H	0.116180	3.814426	0.864325
C	-2.061259	1.817555	-0.983398
H	-1.751118	2.240699	-1.945355
H	-2.981609	2.336134	-0.691004
C	-2.334995	0.322221	-1.153733
H	-3.130011	0.199969	-1.898035
H	-1.445321	-0.162032	-1.564604
C	-2.743127	-0.385807	0.136813
H	-1.935331	-0.348608	0.876193
H	-3.606950	0.120869	0.584645
C	-3.126967	-1.837601	-0.065475
C	-3.529365	-2.551085	1.203203
H	-3.744485	-3.603133	1.003103
H	-2.733450	-2.488932	1.950687
H	-4.430426	-2.090370	1.617497
O	0.168637	1.373762	-0.265600
C	0.925225	0.910536	0.727081
O	0.711051	1.127116	1.898847
C	2.066915	0.087158	0.233562
C	2.241059	-0.195235	-1.121940
C	2.973327	-0.411158	1.169365
C	3.316677	-0.971350	-1.533721
H	1.535202	0.188854	-1.847579
C	4.047856	-1.185220	0.754093
H	2.825837	-0.187777	2.219444
C	4.220197	-1.465591	-0.598114
H	3.450112	-1.191548	-2.586950
H	4.751210	-1.569629	1.484173
H	5.058868	-2.071839	-0.923132
H	-3.909915	-1.924424	-0.825753
F	-2.006508	-2.523376	-0.611080

Zero-point correction = 0.308064
Thermal correction to Energy = 0.325183
Thermal correction to Enthalpy = 0.326127
Thermal correction to Gibbs Free Energy = 0.260991

Sum of electronic and zero-point Energies = -794.939822
Sum of electronic and thermal Energies = -794.922703
Sum of electronic and thermal Enthalpies = -794.921759
Sum of electronic and thermal Free Energies = -794.986895
Number of imaginary frequencies/frequency = 0

OPT-wB97xD-6-311+Gdp_6F-(S,S)-heptan-2-yl-benzoateC_4.out

0 1

C	-0.418524	2.402707	0.091488
H	-0.475448	2.487629	1.177781
C	-0.091123	3.746698	-0.526356
H	0.841069	4.144118	-0.117881
H	0.009651	3.662415	-1.612170
H	-0.891055	4.458595	-0.307057
C	-1.696864	1.782890	-0.453481
H	-1.600405	1.674537	-1.540680
H	-2.509685	2.495545	-0.274839
C	-2.043666	0.436403	0.176433
H	-1.218305	-0.264039	0.012755
H	-2.145102	0.557919	1.261536
C	-3.332627	-0.150103	-0.397423
H	-4.142342	0.581130	-0.300883
H	-3.205957	-0.357560	-1.466404
C	-3.764874	-1.426333	0.299385
C	-2.827609	-2.598650	0.131925
H	-1.881707	-2.401207	0.642505
H	-3.263629	-3.499684	0.569349
H	-2.620701	-2.781378	-0.926628
O	0.678937	1.506568	-0.227614
C	1.285255	0.831723	0.747617
O	1.035418	0.959781	1.924737
C	2.313621	-0.112890	0.219770
C	3.072247	-0.842509	1.135224
C	2.518337	-0.289110	-1.149528
C	4.029947	-1.740758	0.685182
H	2.903993	-0.698341	2.196015
C	3.476251	-1.190007	-1.596150
H	1.928032	0.277228	-1.858793
C	4.231997	-1.915656	-0.680610
H	4.618829	-2.305907	1.398839
H	3.633272	-1.327082	-2.660121
H	4.979065	-2.619098	-1.031766
H	-3.954896	-1.235004	1.359988
F	-5.025969	-1.798560	-0.244375

Zero-point correction = 0.307869
Thermal correction to Energy = 0.32515
Thermal correction to Enthalpy = 0.326094
Thermal correction to Gibbs Free Energy = 0.260137
Sum of electronic and zero-point Energies = -794.939726
Sum of electronic and thermal Energies = -794.922444
Sum of electronic and thermal Enthalpies = -794.9215
Sum of electronic and thermal Free Energies = -794.987458
Number of imaginary frequencies/frequency = 0

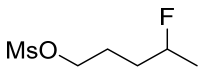
OPT-wB97xD-6-311+Gdp_6F-(S,S)-heptan-2-yl-benzoateC_5.out

0 1

C	0.519119	2.054601	0.216657
H	0.363106	2.538967	-0.750036
C	0.311362	3.054083	1.338515
H	0.423229	2.569276	2.312583
H	1.053324	3.853381	1.262700
H	-0.681734	3.504692	1.279784
C	1.879150	1.378050	0.246088
H	1.988302	0.854682	1.202489
H	2.638255	2.168644	0.227268
C	2.100201	0.423800	-0.926338
H	1.376686	-0.394615	-0.875731
H	1.897882	0.959325	-1.860878
C	3.515802	-0.148633	-1.005866
H	3.624433	-0.730802	-1.927631
H	4.244322	0.669298	-1.061734
C	3.921235	-1.029026	0.160671
C	5.304352	-1.620076	0.022934
H	6.049921	-0.820145	0.025541
H	5.523206	-2.292797	0.855193
H	5.396285	-2.174899	-0.915040
O	-0.465478	0.994838	0.337292
C	-1.641127	1.145809	-0.268016
O	-1.952646	2.126907	-0.905215
C	-2.532317	-0.036457	-0.081826
C	-2.139953	-1.150206	0.662455
C	-3.790755	-0.010496	-0.683178
C	-3.005590	-2.227571	0.802727
H	-1.161819	-1.172159	1.126448
C	-4.652022	-1.089602	-0.542500
H	-4.082940	0.859751	-1.259084
C	-4.260113	-2.198675	0.201480
H	-2.699629	-3.092547	1.380498
H	-5.628495	-1.066525	-1.012932
H	-4.933607	-3.041652	0.311956
H	3.826756	-0.495845	1.110737
F	2.994605	-2.104843	0.249825

Zero-point correction = 0.308044
Thermal correction to Energy = 0.325208
Thermal correction to Enthalpy = 0.326152
Thermal correction to Gibbs Free Energy = 0.260606
Sum of electronic and zero-point Energies = -794.939248
Sum of electronic and thermal Energies = -794.922084
Sum of electronic and thermal Enthalpies = -794.92114
Sum of electronic and thermal Free Energies = -794.986685
Number of imaginary frequencies/frequency = 0

	Calculated 19F NMR Shielding Tensor
OPT-wB97xD-6-311+Gdp_6F--(S,S)-heptan-2-yl-benzoateC_1.out	370.3056
OPT-wB97xD-6-311+Gdp_6F--(S,S)-heptan-2-yl-benzoateC_2.out	369.9304
OPT-wB97xD-6-311+Gdp_6F--(S,S)-heptan-2-yl-benzoateC_3.out	370.7498
OPT-wB97xD-6-311+Gdp_6F--(S,S)-heptan-2-yl-benzoateC_4.out	357.4477
OPT-wB97xD-6-311+Gdp_6F--(S,S)-heptan-2-yl-benzoateC_5.out	375.2346



4-fluoropentyl methanesulfonate

OPT-wB97xD-6-311+Gdp_4-fluoropentyl methanesulfonateC1.out

0 1

O	1.222442	0.473685	-0.110463
C	0.109522	-0.407229	0.204265
H	0.122726	-0.607783	1.278360
H	0.233515	-1.347341	-0.341137
C	-1.155637	0.305901	-0.215695
H	-1.120106	0.493933	-1.293370
H	-1.207544	1.273593	0.290014
C	-2.384736	-0.533308	0.128468
H	-2.303278	-1.520374	-0.340825
C	-3.685640	0.081563	-0.346465
H	-3.635856	0.297906	-1.418033
F	-3.835873	1.347647	0.281424
C	-4.907044	-0.744466	-0.021635
H	-4.972592	-0.933039	1.053418
H	-5.815344	-0.232714	-0.346957
H	-4.851417	-1.705416	-0.540141
H	-2.446815	-0.696483	1.210384
S	2.699504	-0.149560	0.005144
O	2.866587	-0.736649	1.321803
O	2.955765	-0.989614	-1.149118
C	3.616804	1.356630	-0.120769
H	4.671114	1.080549	-0.075322
H	3.387074	1.827856	-1.075306
H	3.351350	1.999524	0.717015

Zero-point correction = 0.197652
Thermal correction to Energy = 0.210721
Thermal correction to Enthalpy = 0.211666

Thermal correction to Gibbs Free Energy = 0.156535
Sum of electronic and zero-point Energies = -959.940037
Sum of electronic and thermal Energies = -959.926968
Sum of electronic and thermal Enthalpies = -959.926024
Sum of electronic and thermal Free Energies = -959.981154
Number of imaginary frequencies/frequency = 0

OPT-wB97xD-6-311+Gdp_4-fluoropentyl methanesulfonateC2.out

0 1

O	-1.383416	0.241467	-0.894429
C	-0.160035	-0.549367	-0.889208
H	0.056147	-0.721601	-1.944023
H	-0.350900	-1.518123	-0.418521
C	0.959313	0.204483	-0.201854
H	0.690821	0.378457	0.844224
H	1.075006	1.179487	-0.682296
C	2.268665	-0.577076	-0.281900
H	2.145338	-1.559601	0.187806
C	3.422439	0.113265	0.417297
H	3.156175	0.346833	1.452617
F	3.631537	1.373343	-0.206338
C	4.721232	-0.654233	0.357707
H	5.001372	-0.858494	-0.679444
H	5.524660	-0.091588	0.838030
H	4.610324	-1.607591	0.881245
H	2.546228	-0.753500	-1.327815
S	-2.495842	-0.100345	0.211933
O	-3.128639	-1.362792	-0.119497
O	-1.918383	0.035304	1.536753
C	-3.597339	1.240973	-0.124416
H	-3.073115	2.179092	0.050700
H	-3.942651	1.160743	-1.154182
H	-4.431913	1.131212	0.569410

Zero-point correction = 0.197751
Thermal correction to Energy = 0.210764
Thermal correction to Enthalpy = 0.211708
Thermal correction to Gibbs Free Energy = 0.156675
Sum of electronic and zero-point Energies = -959.939227
Sum of electronic and thermal Energies = -959.926214
Sum of electronic and thermal Enthalpies = -959.92527
Sum of electronic and thermal Free Energies = -959.980302
Number of imaginary frequencies/frequency = 0

OPT-wB97xD-6-311+Gdp_4-fluoropentyl methanesulfonateC3.out

0 1

O	-1.025540	-0.264896	-0.573890
C	-0.247170	-1.345515	0.020522
H	-0.675780	-2.290099	-0.317860
H	-0.321232	-1.282633	1.110037
C	1.184778	-1.181720	-0.431476
H	1.229166	-1.228631	-1.524867
H	1.734731	-2.048067	-0.051654
C	1.823198	0.109129	0.073577
H	1.282747	0.971767	-0.328488
C	3.277485	0.258149	-0.321428
H	3.396510	0.139148	-1.402837
F	4.006383	-0.822333	0.249069
C	3.912406	1.544841	0.149281
H	3.801848	1.658631	1.231120
H	4.975099	1.564874	-0.102084
H	3.429119	2.395363	-0.339126
H	1.746383	0.165682	1.165794
S	-2.389333	0.142785	0.168140
O	-3.264272	-1.012919	0.231109
O	-2.072338	0.820216	1.411229
C	-2.984645	1.305394	-1.023166
H	-2.256526	2.109498	-1.120579
H	-3.141428	0.790136	-1.969480
H	-3.927867	1.689886	-0.633280

Zero-point correction = 0.197412
Thermal correction to Energy = 0.210372
Thermal correction to Enthalpy = 0.211317
Thermal correction to Gibbs Free Energy = 0.156079
Sum of electronic and zero-point Energies = -959.94122
Sum of electronic and thermal Energies = -959.928259
Sum of electronic and thermal Enthalpies = -959.927315
Sum of electronic and thermal Free Energies = -959.982552
Number of imaginary frequencies/frequency = 0

OPT-wB97xD-6-311+Gdp_4-fluoropentyl methanesulfonateC4.out

0 1

O	-1.220724	-0.419603	0.948877
C	-0.339511	-1.538391	0.640587
H	-0.923807	-2.309720	0.135241
H	-0.055895	-1.899784	1.629244
C	0.874931	-1.136770	-0.171641
H	0.570088	-0.840375	-1.181066
H	1.483134	-2.040499	-0.280832
C	1.692908	-0.024146	0.477072
H	1.079702	0.877697	0.569072
C	2.928914	0.351848	-0.312423
H	2.666665	0.576503	-1.350709
F	3.776778	-0.789468	-0.384294
C	3.724459	1.481777	0.296314
H	4.639094	1.660141	-0.273432
H	3.129990	2.399380	0.284625
H	3.991263	1.254271	1.332285
H	1.995404	-0.314518	1.490457
S	-2.086189	0.236594	-0.235452
O	-1.334996	1.321682	-0.836664
O	-2.579948	-0.816890	-1.102889
C	-3.402921	0.897058	0.743296
H	-3.918710	0.074721	1.236593
H	-2.985324	1.596816	1.466140
H	-4.070915	1.415299	0.054442

Zero-point correction = 0.197629
Thermal correction to Energy = 0.210479
Thermal correction to Enthalpy = 0.211423
Thermal correction to Gibbs Free Energy = 0.156498
Sum of electronic and zero-point Energies = -959.941196
Sum of electronic and thermal Energies = -959.928346
Sum of electronic and thermal Enthalpies = -959.927401
Sum of electronic and thermal Free Energies = -959.982326
Number of imaginary frequencies/frequency = 0

OPT-wB97xD-6-311+Gdp_4-fluoropentyl methanesulfonateC5.out

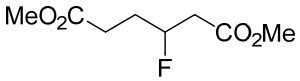
0 1

O	-0.921190	-0.242113	0.390310
C	-0.280634	-1.350385	-0.303403
H	-0.425884	-1.224442	-1.380325
H	-0.754842	-2.277314	0.024410
C	1.186697	-1.315986	0.058119
H	1.646406	-2.201819	-0.394377
H	1.292850	-1.419475	1.141315
C	1.891952	-0.054418	-0.431732
H	1.771474	0.035943	-1.517446
C	3.377420	-0.038360	-0.135373
H	3.855277	-0.945733	-0.518050
F	3.549950	-0.096516	1.275314
C	4.089569	1.194326	-0.638671
H	3.630947	2.099173	-0.230516
H	5.144609	1.172866	-0.356633
H	4.028065	1.236353	-1.729492
H	1.435144	0.834338	0.014930
S	-2.397904	0.171892	-0.082747
O	-2.332530	0.734263	-1.418849
O	-3.302811	-0.940148	0.138891
C	-2.682983	1.449534	1.106130
H	-2.638304	1.015507	2.103656
H	-1.929452	2.224613	0.973608
H	-3.679240	1.844089	0.901808

Zero-point correction = 0.197563
Thermal correction to Energy = 0.210575
Thermal correction to Enthalpy = 0.21152
Thermal correction to Gibbs Free Energy = 0.15596
Sum of electronic and zero-point Energies = -959.940919
Sum of electronic and thermal Energies = -959.927906
Sum of electronic and thermal Enthalpies = -959.926962
Sum of electronic and thermal Free Energies = -959.982522
Number of imaginary frequencies/frequency = 0

	Calculated

	19F NMR Shielding Tensor
OPT-wB97xD-6-311+Gdp_1-pentyl_methanesulfonateC1.out	370.8073
OPT-wB97xD-6-311+Gdp_1-pentyl_methanesulfonateC2.out	371.0255
OPT-wB97xD-6-311+Gdp_1-pentyl_methanesulfonateC3.out	370.7318
OPT-wB97xD-6-311+Gdp_1-pentyl_methanesulfonateC4.out	372.3754
OPT-wB97xD-6-311+Gdp_1-pentyl_methanesulfonateC5.out	370.3634



dimethyl 3-fluorohexanedioate

OPT-wB97xD-6-311+Gdp_dimethyl_3-fluorohexanedioate3C_1.out

0 1

C	1.707912	0.569178	0.376605
C	0.359715	0.334296	-0.289308
H	2.061049	1.589720	0.202774
H	1.633003	0.450381	1.462497
C	-0.698224	1.308315	0.184387
H	0.450708	0.416756	-1.376600
H	0.010805	-0.679146	-0.071818
C	-2.072693	1.051718	-0.407829
H	-0.752629	1.336123	1.275032
H	-2.715977	1.915585	-0.210428
H	-2.016027	0.928258	-1.491723
C	-2.751359	-0.145526	0.206468
C	2.777267	-0.369801	-0.113999
O	-2.470513	-0.632606	1.275462
O	2.629483	-1.234796	-0.943379
O	3.944547	-0.127309	0.490254
O	-3.736518	-0.594812	-0.569725
F	-0.315927	2.612009	-0.214929
C	-4.493176	-1.703155	-0.064551
H	-3.845414	-2.566468	0.095513
H	-4.986744	-1.434649	0.870980
H	-5.233396	-1.924613	-0.830410
C	5.052488	-0.946022	0.099392
H	5.263199	-0.823182	-0.964485
H	5.897095	-0.597960	0.690944
H	4.850097	-1.996727	0.314206

Zero-point correction	=	0.212524
Thermal correction to Energy	=	0.22713
Thermal correction to Enthalpy	=	0.228074
Thermal correction to Gibbs Free Energy	=	0.168664
Sum of electronic and zero-point Energies	=	-713.237572
Sum of electronic and thermal Energies	=	-713.222966
Sum of electronic and thermal Enthalpies	=	-713.222022
Sum of electronic and thermal Free Energies	=	-713.281433
Number of imaginary frequencies/frequency	=	0

OPT-wB97xD-6-311+Gdp_dimethyl_3-fluorohexanedioate3C_2.out

0 1

C	1.887451	-0.495723	0.011564
C	0.725254	0.477245	-0.135062
H	1.821432	-1.040041	0.959036
H	1.875142	-1.252383	-0.778396
C	-0.618136	-0.220689	-0.107834
H	0.756866	1.230743	0.656889
H	0.805077	1.008778	-1.088216
C	-1.784252	0.735769	-0.244060
H	-0.674611	-1.003661	-0.868384
H	-1.792208	1.453950	0.577541
H	-1.668201	1.296939	-1.177700
C	-3.108569	0.017819	-0.333573
C	3.228342	0.188279	-0.007159
O	-3.291772	-1.009941	-0.939572
O	3.410181	1.380512	0.056157
O	4.223247	-0.699980	-0.087076
O	-4.071232	0.673652	0.313104
F	-0.757289	-0.888181	1.134311
C	-5.385656	0.104209	0.249485
H	-6.016045	0.756683	0.850196
H	-5.741528	0.078958	-0.781918
H	-5.384986	-0.905011	0.663879
C	5.555392	-0.174175	-0.064208
H	6.212684	-1.036417	-0.157934
H	5.713382	0.512310	-0.897870
H	5.746261	0.342437	0.878266

Zero-point correction	=	0.212538
Thermal correction to Energy	=	0.227321
Thermal correction to Enthalpy	=	0.228265
Thermal correction to Gibbs Free Energy	=	0.167967
Sum of electronic and zero-point Energies	=	-713.237793
Sum of electronic and thermal Energies	=	-713.223009
Sum of electronic and thermal Enthalpies	=	-713.222065
Sum of electronic and thermal Free Energies	=	-713.282363
Number of imaginary frequencies/frequency	=	0

OPT-wB97xD-6-311+Gdp_dimethyl_3-fluorohexanedioate3C_3.out

0 1

C	2.091328	1.309635	0.170979
C	0.726931	1.490059	-0.482980
H	2.753499	2.134914	-0.111457
H	2.019758	1.333668	1.260345
C	-0.317117	0.514706	0.023862
H	0.372524	2.509312	-0.302761
H	0.814876	1.359493	-1.564878
C	-1.665730	0.699928	-0.636938
H	0.018105	-0.519679	-0.076002
H	-2.049334	1.706342	-0.459016
H	-1.544325	0.575924	-1.718661
C	-2.675961	-0.329488	-0.194090
C	2.794166	0.042189	-0.245748
O	-2.422407	-1.481801	0.057665
O	2.519748	-0.624130	-1.215468
O	3.799684	-0.250422	0.581747
O	-3.906370	0.182136	-0.147796
F	-0.489195	0.728122	1.415102
C	-4.962710	-0.721109	0.203693
H	-4.794722	-1.139009	1.197465
H	-5.873402	-0.125403	0.194723
H	-5.033380	-1.528351	-0.527375
C	4.582041	-1.406299	0.258407
H	5.344280	-1.467632	1.032604
H	3.962663	-2.304963	0.268169
H	5.049295	-1.291709	-0.721366

Zero-point correction	=	0.212648
Thermal correction to Energy	=	0.227174
Thermal correction to Enthalpy	=	0.228119
Thermal correction to Gibbs Free Energy	=	0.168583
Sum of electronic and zero-point Energies	=	-713.238257
Sum of electronic and thermal Energies	=	-713.22373
Sum of electronic and thermal Enthalpies	=	-713.222786
Sum of electronic and thermal Free Energies	=	-713.282322
Number of imaginary frequencies/frequency	=	0

OPT-wB97xD-6-311+Gdp_dimethyl_3-fluorohexanedioate3C_4.out

0 1

C	-1.687897	0.725260	1.125300
C	-0.168251	0.784520	1.026876
H	-1.985498	0.568725	2.167747
H	-2.147569	1.664632	0.812186
C	0.336954	1.218047	-0.335622
H	0.216329	1.483837	1.775264
H	0.254542	-0.199172	1.251729
C	1.856090	1.248252	-0.438667
H	-0.082254	0.601305	-1.133898
H	2.131494	1.722596	-1.384547
H	2.283009	1.825434	0.382569
C	2.424284	-0.148904	-0.459716
C	-2.297245	-0.408699	0.339449
O	2.103749	-1.000262	-1.252898

O	-1.716309	-1.408486	-0.008835
O	-3.591693	-0.191564	0.093988
O	3.329586	-0.338860	0.500542
F	-0.118937	2.533780	-0.582004
C	3.925756	-1.641495	0.565807
H	3.166540	-2.397269	0.773725
H	4.433093	-1.877548	-0.370932
H	4.645058	-1.594184	1.380984
C	-4.291599	-1.224142	-0.610935
H	-5.310162	-0.858935	-0.727319
H	-3.838300	-1.394001	-1.589028
H	-4.287063	-2.153097	-0.037767

Zero-point correction =	0.213184	
Thermal correction to Energy =	0.227551	
Thermal correction to Enthalpy =	0.228495	
Thermal correction to Gibbs Free Energy =		0.169492
Sum of electronic and zero-point Energies =		-713.236286
Sum of electronic and thermal Energies =		-713.221919
Sum of electronic and thermal Enthalpies =		-713.220975
Sum of electronic and thermal Free Energies =		-713.279978
Number of imaginary frequencies/frequency =		0

OPT-wB97xD-6-311+Gdp_dimethyl_3-fluorohexanedioate3C_5.out

0 1

C	1.646822	-1.037300	0.899846
C	0.124039	-1.078662	0.925515
H	2.039115	-1.120820	1.918856
H	2.063334	-1.879598	0.343704
C	-0.504944	-1.194131	-0.449450
H	-0.206052	-1.928331	1.530345
H	-0.259089	-0.172449	1.403774
C	-2.028478	-1.230051	-0.422403
H	-0.152846	-0.405185	-1.117189
H	-2.393817	-1.399943	-1.438723
H	-2.373285	-2.042150	0.218802
C	-2.623510	0.059254	0.086798
C	2.204889	0.245549	0.337750
O	-3.342946	0.156273	1.050875
O	1.595113	1.281356	0.216800
O	3.492364	0.112469	0.010202
O	-2.254741	1.095906	-0.666043
F	-0.080683	-2.410458	-1.034195
C	-2.712952	2.389471	-0.253314
H	-2.346993	2.619268	0.748604
H	-2.297916	3.090562	-0.974455
H	-3.803289	2.432926	-0.267999
C	4.152387	1.285080	-0.481504
H	3.672288	1.641048	-1.394531
H	4.140520	2.074603	0.271909
H	5.176348	0.980889	-0.689462

Zero-point correction =	0.212941	
Thermal correction to Energy =	0.227432	
Thermal correction to Enthalpy =	0.228376	
Thermal correction to Gibbs Free Energy =		0.169222
Sum of electronic and zero-point Energies =		-713.237254
Sum of electronic and thermal Energies =		-713.222762
Sum of electronic and thermal Enthalpies =		-713.221818
Sum of electronic and thermal Free Energies =		-713.280972
Number of imaginary frequencies/frequency =		0

OPT-wB97xD-6-311+Gdp_dimethyl_3-fluorohexanedioate3C_6.out

0 1

C	-2.022558	-1.328090	0.230428
C	-0.687366	-1.632648	-0.438169
H	-2.746759	-2.115314	-0.003319
H	-1.931110	-1.309209	1.318531
C	0.428180	-0.702351	-0.006276
H	-0.395370	-2.661735	-0.209036
H	-0.790359	-1.554435	-1.523739
C	1.746972	-0.999169	-0.696059
H	0.149735	0.343753	-0.146294
H	2.026795	-2.043811	-0.552568
H	1.621496	-0.815645	-1.767743
C	2.880399	-0.135215	-0.200148
C	-2.638825	-0.030998	-0.229525
O	3.934688	-0.552406	0.211687
O	-2.321358	0.582561	-1.220899
O	-3.617319	0.360232	0.589682
O	2.582362	1.162559	-0.281799
F	0.628438	-0.859463	1.388665
C	3.570178	2.082183	0.198842
H	4.497032	1.983160	-0.368378
H	3.142425	3.072169	0.053425
H	3.767092	1.908497	1.258020
C	-4.305427	1.566179	0.235468
H	-3.609337	2.405677	0.197868
H	-4.800500	1.455083	-0.730880
H	-5.043392	1.724061	1.019408

Zero-point correction =	0.213088	
Thermal correction to Energy =	0.227495	
Thermal correction to Enthalpy =	0.228439	
Thermal correction to Gibbs Free Energy =		0.169606
Sum of electronic and zero-point Energies =		-713.237565
Sum of electronic and thermal Energies =		-713.223158
Sum of electronic and thermal Enthalpies =		-713.222214
Sum of electronic and thermal Free Energies =		-713.281047
Number of imaginary frequencies/frequency =		0

OPT-wB97xD-6-311+Gdp_dimethyl_3-fluorohexanedioate3C_7.out

0 1

C	-2.091001	0.973217	0.939024
C	-0.563852	1.034148	1.043586
H	-2.514769	0.835882	1.938155
H	-2.493923	1.898165	0.526004
C	0.122468	1.333876	-0.274640
H	-0.280646	1.808986	1.762147
H	-0.182218	0.082361	1.422150
C	1.637799	1.277454	-0.202969
H	-0.238818	0.680877	-1.073003
H	2.058067	1.757043	-1.092754
H	2.013934	1.824244	0.665561
C	2.166192	-0.133672	-0.176332
C	-2.576500	-0.165053	0.076201
O	1.531276	-1.122989	-0.451404
O	-3.286997	-0.051518	-0.894277
O	-2.124063	-1.341652	0.516518
O	3.454423	-0.157389	0.165962
F	-0.225099	2.647882	-0.665352
C	4.091962	-1.441646	0.171532
H	3.640380	-2.088797	0.925440
H	4.015948	-1.912368	-0.809806
H	5.134191	-1.248495	0.416800
C	-2.469124	-2.496086	-0.256018
H	-3.551721	-2.632511	-0.283967
H	-2.082616	-2.403944	-1.272505
H	-1.996690	-3.337429	0.247251

Zero-point correction =	0.21331	
Thermal correction to Energy =	0.227649	
Thermal correction to Enthalpy =	0.228593	
Thermal correction to Gibbs Free Energy =		0.170334
Sum of electronic and zero-point Energies =		-713.235909
Sum of electronic and thermal Energies =		-713.22157
Sum of electronic and thermal Enthalpies =		-713.220626
Sum of electronic and thermal Free Energies =		-713.278885
Number of imaginary frequencies/frequency =		0

OPT-wB97xD-6-311+Gdp_dimethyl_3-fluorohexanedioate3C_8.out

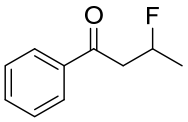
0 1

C	-1.542584	0.615578	-0.422773
C	-0.218730	0.481091	0.316717
H	-1.913696	1.643069	-0.392385
H	-1.422521	0.364683	-1.482788
C	0.886533	1.296603	-0.320359
H	-0.330435	0.783953	1.362328
H	0.093933	-0.567600	0.321414
C	2.220433	1.193679	0.405053
H	0.999865	1.046168	-1.377409
H	2.937596	1.866534	-0.076007
H	2.109154	1.502663	1.445305
C	2.824139	-0.187930	0.392268
C	-2.616064	-0.284717	0.129430
O	3.366884	-0.707414	1.335718

O	-2.461688	-1.119249	0.988142
O	-3.790392	-0.055553	-0.465758
O	2.713095	-0.769240	-0.804515
F	0.517260	2.662286	-0.289568
C	3.269385	-2.084264	-0.933116
H	4.344245	-2.063464	-0.746402
H	2.787860	-2.772390	-0.236459
H	3.070943	-2.385941	-1.959519
C	-4.893832	-0.863779	-0.040637
H	-4.692095	-1.920047	-0.227040
H	-5.094702	-0.710137	1.021071
H	-5.744368	-0.533970	-0.634187

Zero-point correction	=	0.212889
Thermal correction to Energy	=	0.227418
Thermal correction to Enthalpy	=	0.228362
Thermal correction to Gibbs Free Energy	=	0.169403
Sum of electronic and zero-point Energies	=	-713.236504
Sum of electronic and thermal Energies	=	-713.221974
Sum of electronic and thermal Enthalpies	=	-713.22103
Sum of electronic and thermal Free Energies	=	-713.279989
Number of imaginary frequencies/frequency	=	0

	Calculated 19F NMR Shielding Tensor
OPT-wB97xD-6-311+Gdp_dimethyl_3-fluorohexanedioate3C_1.out	383.3872
OPT-wB97xD-6-311+Gdp_dimethyl_3-fluorohexanedioate3C_2.out	379.1371
OPT-wB97xD-6-311+Gdp_dimethyl_3-fluorohexanedioate3C_3.out	383.8858
OPT-wB97xD-6-311+Gdp_dimethyl_3-fluorohexanedioate3C_4.out	381.4387
OPT-wB97xD-6-311+Gdp_dimethyl_3-fluorohexanedioate3C_5.out	381.42
OPT-wB97xD-6-311+Gdp_dimethyl_3-fluorohexanedioate3C_6.out	384.3019
OPT-wB97xD-6-311+Gdp_dimethyl_3-fluorohexanedioate3C_7.out	384.8558
OPT-wB97xD-6-311+Gdp_dimethyl_3-fluorohexanedioate3C_8.out	378.7403



3-fluoro-1-phenylbutan-1-one

C1 omitted due to presence of 1 imaginary frequency

OPT-wB97xD-6-311+Gdp_3-fluoro-1-phenylbutan-1-oneC2.out

0 1

C	3.374035	-0.832855	0.136712
C	2.036306	-1.159011	-0.028950
C	1.070142	-0.153831	-0.123698
C	1.466556	1.183798	-0.054503
C	2.808564	1.510004	0.099573
C	3.762179	0.503210	0.199362
H	4.117188	-1.618417	0.215887
H	1.723950	-2.195424	-0.083876
H	0.734364	1.979084	-0.126115
H	3.108094	2.551015	0.146262
H	4.808702	0.757818	0.327215
C	-0.362157	-0.551421	-0.306219
O	-0.656188	-1.700125	-0.563619
C	-1.426120	0.524235	-0.179151
C	-2.841183	-0.011902	-0.132614
H	-1.325818	1.193257	-1.041984
H	-1.238325	1.134061	0.709774
C	-3.895474	1.061615	-0.265558
H	-2.979970	-0.794685	-0.880487
H	-4.891753	0.628462	-0.154191
H	-3.762155	1.839712	0.491442
H	-3.831199	1.522595	-1.254782
F	-3.018963	-0.648837	1.121121

Zero-point correction	=	0.188253
Thermal correction to Energy	=	0.199315
Thermal correction to Enthalpy	=	0.200259
Thermal correction to Gibbs Free Energy	=	0.150137
Sum of electronic and zero-point Energies	=	-562.561088
Sum of electronic and thermal Energies	=	-562.550026
Sum of electronic and thermal Enthalpies	=	-562.549082
Sum of electronic and thermal Free Energies	=	-562.599204
Number of imaginary frequencies/frequency	=	0

OPT-wB97xD-6-311+Gdp_3-fluoro-1-phenylbutan-1-oneC3.out

0 1

C	-3.307853	0.512814	0.223966
C	-2.063138	1.114861	0.128276
C	-0.926394	0.351396	-0.157942
C	-1.058089	-1.027595	-0.337223
C	-2.304934	-1.631735	-0.227926
C	-3.430010	-0.863638	0.048309
H	-4.184836	1.112952	0.439508
H	-1.954078	2.183447	0.272475
H	-0.190772	-1.643198	-0.540775
H	-2.397111	-2.704116	-0.357640
H	-4.402563	-1.336727	0.129334
C	0.393781	1.047241	-0.227682
O	0.516426	2.184352	0.184941
C	1.606445	0.344644	-0.814905
C	2.607369	-0.041863	0.263735
H	2.093602	1.069175	-1.473012
H	1.348650	-0.531499	-1.411250
C	3.869505	-0.666192	-0.278366
H	2.834317	0.823181	0.891709
H	4.527298	-0.964268	0.540937
H	3.639690	-1.545818	-0.885939
H	4.402717	0.058135	-0.899328
F	1.981289	-0.981742	1.121444

Zero-point correction	=	0.188598
Thermal correction to Energy	=	0.199637
Thermal correction to Enthalpy	=	0.200581
Thermal correction to Gibbs Free Energy	=	0.150238
Sum of electronic and zero-point Energies	=	-562.560003
Sum of electronic and thermal Energies	=	-562.548964
Sum of electronic and thermal Enthalpies	=	-562.54802
Sum of electronic and thermal Free Energies	=	-562.598363
Number of imaginary frequencies/frequency	=	0

OPT-wB97xD-6-311+Gdp_3-fluoro-1-phenylbutan-1-oneC4.out

0 1

C	3.282836	0.536586	0.291188
C	2.030888	1.123552	0.195596
C	0.914976	0.360072	-0.164072
C	1.077634	-1.003547	-0.420256
C	2.330933	-1.593938	-0.310109
C	3.434277	-0.825346	0.041594
H	4.142965	1.138138	0.563196
H	1.900597	2.180585	0.395795
H	0.230156	-1.620586	-0.692272
H	2.445328	-2.654926	-0.501162
H	4.412443	-1.286680	0.122151
C	-0.415653	1.040308	-0.226384
O	-0.554892	2.163063	0.218933
C	-1.616955	0.337945	-0.835181
C	-2.617440	-0.061246	0.245528
H	-1.345710	-0.537581	-1.425255
H	-2.097640	1.062960	-1.496172
C	-2.139213	-1.143902	1.182057
H	-2.935039	0.824338	0.800713
H	-2.929212	-1.409874	1.887303
H	-1.842523	-2.037894	0.626893
H	-1.277980	-0.789592	1.755625
F	-3.773105	-0.532922	-0.420894

Zero-point correction	=	0.188904

Thermal correction to Energy	=	0.199798
Thermal correction to Enthalpy	=	0.200742
Thermal correction to Gibbs Free Energy	=	0.151225
Sum of electronic and zero-point Energies	=	-562.559439
Sum of electronic and thermal Energies	=	-562.548545
Sum of electronic and thermal Enthalpies	=	-562.547601
Sum of electronic and thermal Free Energies	=	-562.597118
Number of imaginary frequencies/frequency	=	0

OPT-wB97xD-6-311+Gdp_3-fluoro-1-phenylbutan-1-oneC5.out

0 1

C	-3.156381	0.539955	0.525264
C	-1.928574	1.109439	0.225730
C	-0.883096	0.321850	-0.266622
C	-1.090677	-1.047292	-0.453925
C	-2.323108	-1.616502	-0.156456
C	-3.355544	-0.824958	0.333529
H	-3.960379	1.158766	0.907728
H	-1.762221	2.170565	0.369356
H	-0.301691	-1.680545	-0.842432
H	-2.477258	-2.678427	-0.310257
H	-4.316400	-1.271522	0.564838
C	0.420405	0.987928	-0.578570
O	0.517946	2.198614	-0.545623
C	1.630595	0.138134	-0.917524
C	2.204014	-0.577534	0.303727
H	2.392072	0.803480	-1.328628
H	1.371381	-0.606554	-1.674136
C	2.702628	0.345479	1.388075
H	1.487514	-1.296418	0.708097
H	3.184364	-0.230422	2.180987
H	3.415580	1.071084	0.987860
H	1.863610	0.891148	1.828265
F	3.293144	-1.353229	-0.160674

Zero-point correction	=	0.18891
Thermal correction to Energy	=	0.199815
Thermal correction to Enthalpy	=	0.200759
Thermal correction to Gibbs Free Energy	=	0.151033
Sum of electronic and zero-point Energies	=	-562.56004
Sum of electronic and thermal Energies	=	-562.549135
Sum of electronic and thermal Enthalpies	=	-562.548191
Sum of electronic and thermal Free Energies	=	-562.597917
Number of imaginary frequencies/frequency	=	0

OPT-wB97xD-6-311+Gdp_3-fluoro-1-phenylbutan-1-oneC6.out

0 1

C	2.982603	0.700232	0.597978
C	1.722229	1.202546	0.316608
C	0.745339	0.386566	-0.264845
C	1.056879	-0.942661	-0.560361
C	2.321976	-1.444982	-0.279171
C	3.284586	-0.626410	0.299312
H	3.731472	1.340497	1.050761
H	1.476625	2.233155	0.544072
H	0.317681	-1.599787	-0.999282
H	2.552919	-2.478901	-0.509326
H	4.270629	-1.021511	0.518750
C	-0.596174	0.985889	-0.545009
O	-0.798280	2.166176	-0.329779
C	-1.726512	0.130137	-1.090312
C	-2.518832	-0.632891	-0.028417
H	-1.375006	-0.577671	-1.843531
H	-2.424510	0.816078	-1.575353
C	-2.919146	0.170983	1.185356
H	-3.398030	-1.064736	-0.512282
H	-3.502914	1.042430	0.878636
H	-3.531189	-0.439658	1.852220
H	-2.041588	0.520862	1.734672
F	-1.756393	-1.741846	0.412452

Zero-point correction	=	0.188878
Thermal correction to Energy	=	0.199745
Thermal correction to Enthalpy	=	0.200689
Thermal correction to Gibbs Free Energy	=	0.151092
Sum of electronic and zero-point Energies	=	-562.558854
Sum of electronic and thermal Energies	=	-562.547987
Sum of electronic and thermal Enthalpies	=	-562.547042
Sum of electronic and thermal Free Energies	=	-562.59664
Number of imaginary frequencies/frequency	=	0

OPT-wB97xD-6-311+Gdp_3-fluoro-1-phenylbutan-1-oneC7.out

0 1

C	3.108678	0.436412	0.627569
C	1.900121	1.054123	0.343649
C	0.867747	0.340759	-0.272268
C	1.069505	-1.002004	-0.601659
C	2.284871	-1.617087	-0.326829
C	3.303654	-0.900527	0.290954
H	3.901426	0.995897	1.111457
H	1.739818	2.095678	0.596621
H	0.289250	-1.576337	-1.087571
H	2.435726	-2.657027	-0.593505
H	4.250171	-1.383070	0.508663
C	-0.413628	1.057115	-0.568508
O	-0.457698	2.270315	-0.555284
C	-1.663814	0.254101	-0.872524
C	-2.160770	-0.566151	0.310382
H	-1.476045	-0.429135	-1.706582
H	-2.440649	0.957315	-1.179022
C	-3.455805	-1.288400	0.027963
H	-1.396284	-1.264082	0.658850
H	-3.302651	-2.027613	-0.762986
H	-3.802130	-1.810441	0.922416
H	-4.228211	-0.585780	-0.295148
F	-2.372466	0.323559	1.390746

Zero-point correction	=	0.188357
Thermal correction to Energy	=	0.199414
Thermal correction to Enthalpy	=	0.200358
Thermal correction to Gibbs Free Energy	=	0.15
Sum of electronic and zero-point Energies	=	-562.560197
Sum of electronic and thermal Energies	=	-562.54914
Sum of electronic and thermal Enthalpies	=	-562.548195
Sum of electronic and thermal Free Energies	=	-562.598553
Number of imaginary frequencies/frequency	=	0

OPT-wB97xD-6-311+Gdp_3-fluoro-1-phenylbutan-1-oneC8.out

0 1

C	-3.243876	1.050400	-0.002316
C	-1.867416	1.214146	-0.037178
C	-1.019740	0.102779	-0.017179
C	-1.577176	-1.177464	0.035748
C	-2.957053	-1.340903	0.067125
C	-3.791375	-0.228807	0.049297
H	-3.892725	1.919060	-0.015966
H	-1.429841	2.204570	-0.080203
H	-0.945862	-2.058050	0.048439
H	-3.381228	-2.337876	0.105323
H	-4.867759	-0.358818	0.075615
C	0.462403	0.344097	-0.055972
O	0.892408	1.471880	-0.175435
C	1.373191	-0.863680	0.058787
C	2.871695	-0.613529	0.053600
H	1.128898	-1.548924	-0.759768
H	1.120432	-1.399907	0.980710
C	3.407021	0.309595	1.124702
H	3.366513	-1.586310	0.127716
H	4.496203	0.362561	1.059826
H	2.991510	1.311706	1.026281
H	3.144593	-0.087873	2.109497
F	3.242663	-0.108332	-1.214853

Zero-point correction	=	0.188327
Thermal correction to Energy	=	0.199401
Thermal correction to Enthalpy	=	0.200345
Thermal correction to Gibbs Free Energy	=	0.15007
Sum of electronic and zero-point Energies	=	-562.557744
Sum of electronic and thermal Energies	=	-562.54667
Sum of electronic and thermal Enthalpies	=	-562.545726
Sum of electronic and thermal Free Energies	=	-562.596001
Number of imaginary frequencies/frequency	=	0

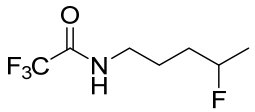
OPT-wB97xD-6-311+Gdp_3-fluoro-1-phenylbutan-1-oneC9.out

0 1

C	2.456856	-1.295115	0.522737
C	1.173782	-0.833870	0.792060
C	0.742606	0.392391	0.281029
C	1.616442	1.145575	-0.509251
C	2.891841	0.679369	-0.787890
C	3.315362	-0.541807	-0.269751
H	2.785805	-2.243499	0.932460
H	0.520043	-1.436757	1.410414
H	1.277835	2.095546	-0.905702
H	3.557969	1.267464	-1.409175
H	4.314689	-0.905266	-0.483352
C	-0.622209	0.950943	0.547405
O	-0.854992	2.122066	0.325032
C	-1.726324	0.056437	1.081519
C	-2.494380	-0.707549	0.002394
H	-2.432275	0.701188	1.607791
H	-1.342680	-0.675422	1.795809
C	-1.699593	-1.666971	-0.852274
H	-3.318834	-1.232869	0.491149
H	-2.367214	-2.173084	-1.552848
H	-0.921189	-1.153408	-1.420519
H	-1.227578	-2.424730	-0.222030
F	-3.103659	0.236434	-0.854679

Zero-point correction	=	0.188896
Thermal correction to Energy	=	0.199828
Thermal correction to Enthalpy	=	0.200772
Thermal correction to Gibbs Free Energy	=	0.150369
Sum of electronic and zero-point Energies	=	-562.557372
Sum of electronic and thermal Energies	=	-562.54644
Sum of electronic and thermal Enthalpies	=	-562.545496
Sum of electronic and thermal Free Energies	=	-562.595899
Number of imaginary frequencies/frequency	=	0

	Calculated 19F NMR Shielding Tensor
OPT-wB97xD-6-311+Gdp_2-fluoro-1-phenylbutan-1-oneC2.out	367.9361
OPT-wB97xD-6-311+Gdp_2-fluoro-1-phenylbutan-1-oneC3.out	366.948
OPT-wB97xD-6-311+Gdp_2-fluoro-1-phenylbutan-1-oneC4.out	361.3133
OPT-wB97xD-6-311+Gdp_2-fluoro-1-phenylbutan-1-oneC5.out	362.4823
OPT-wB97xD-6-311+Gdp_2-fluoro-1-phenylbutan-1-oneC6.out	361.2477
OPT-wB97xD-6-311+Gdp_2-fluoro-1-phenylbutan-1-oneC7.out	369.3003
OPT-wB97xD-6-311+Gdp_2-fluoro-1-phenylbutan-1-oneC8.out	372.477
OPT-wB97xD-6-311+Gdp_2-fluoro-1-phenylbutan-1-oneC9.out	367.3605



2,2,2-trifluoro-N-(4-fluoropentyl)acetamide

C2 omitted due to presence of 1 imaginary frequency
C5 omitted as it is identical to C6 (within limits of convergence criteria and integration grid)

OPT-wB97xD-6-311+Gdp_4-fluoropentylacetamideC1.out

0 1

C	0.621193	1.811289	-0.707178
C	1.688195	1.790477	0.388699
H	0.033348	2.726289	-0.631714
C	2.817859	0.771819	0.219105
H	2.140296	2.786548	0.413868
C	2.437041	-0.695022	0.286642
H	3.546404	0.942519	1.018053
H	1.658031	-0.867670	1.034199
C	3.607039	-1.623173	0.498534
H	3.286610	-2.665868	0.441759
H	4.383763	-1.446183	-0.251123
C	-1.449821	0.745885	0.041410
O	-1.923545	1.705980	0.622606
N	-0.306130	0.688920	-0.633816
H	0.003734	-0.194447	-1.016025
C	-2.263353	-0.572426	0.057767
F	-2.512851	-0.944194	1.319346
F	-1.645653	-1.597715	-0.547583
F	-3.443252	-0.396782	-0.551269
H	4.035156	-1.450392	1.489202
H	1.083700	1.788519	-1.696186
H	1.198494	1.645448	1.358015
H	3.348110	0.942071	-0.725468
F	1.831167	-1.066888	-0.963669

Zero-point correction	=	0.186916
Thermal correction to Energy	=	0.200458
Thermal correction to Enthalpy	=	0.201402
Thermal correction to Gibbs Free Energy	=	0.144887
Sum of electronic and zero-point Energies	=	-802.585132
Sum of electronic and thermal Energies	=	-802.57159
Sum of electronic and thermal Enthalpies	=	-802.570646
Sum of electronic and thermal Free Energies	=	-802.627161
Number of imaginary frequencies/frequency	=	0

OPT-wB97xD-6-311+Gdp_4-fluoropentylacetamideC3.out

0 1

C	-0.304262	-1.704201	0.751773
C	-1.493048	-1.246928	-0.090102
H	-0.609137	-1.875653	1.785626
C	-2.126751	0.040639	0.428466
H	-1.170032	-1.109937	-1.127562
C	-3.295151	0.522540	-0.404437
H	-1.384078	0.846121	0.428966
H	-3.010957	0.598768	-1.457916
C	-3.905337	1.814211	0.082627
H	-4.214885	1.726665	1.127950
H	-3.166625	2.616472	0.006019
C	1.662939	-0.608111	-0.196438
O	1.736568	-1.290288	-1.201900
N	0.776043	-0.723570	0.789043
H	0.805125	-0.069645	1.557474
C	2.706882	0.521851	-0.017337
F	2.591523	1.186228	1.142628
F	2.587737	1.418088	-1.005689
F	3.945889	0.021603	-0.073910
H	-4.771391	2.088056	-0.524358
H	0.100113	-2.638479	0.358588
H	-2.228707	-2.056224	-0.086463
H	-2.459966	-0.089223	1.465333
F	-4.312475	-0.480323	-0.370703

Zero-point correction	=	0.186477
Thermal correction to Energy	=	0.200297
Thermal correction to Enthalpy	=	0.201241
Thermal correction to Gibbs Free Energy	=	0.14314
Sum of electronic and zero-point Energies	=	-802.586559
Sum of electronic and thermal Energies	=	-802.572739
Sum of electronic and thermal Enthalpies	=	-802.571794
Sum of electronic and thermal Free Energies	=	-802.629895
Number of imaginary frequencies/frequency	=	0

OPT-wB97xD-6-311+Gdp_4-fluoropentylacetamideC4.out

0 1

C	0.259936	2.058898	-0.180731
C	1.643132	1.549335	0.213508
H	0.089551	3.051093	0.241176
C	1.980694	0.196072	-0.405721
H	2.375279	2.296404	-0.110998
C	3.375137	-0.293832	-0.077883
H	1.910269	0.265668	-1.496905
H	4.120297	0.464069	-0.335567
C	3.719795	-1.623929	-0.701760
H	2.988973	-2.385360	-0.415359
H	3.713520	-1.528614	-1.790795
C	-1.493656	0.370079	-0.502004
O	-1.376086	0.234815	-1.706094
N	-0.808201	1.186998	0.294835
H	-0.999786	1.178563	1.287217

C	-2.558800	-0.500460	0.210042
F	-2.666229	-0.261954	1.525511
F	-2.262237	-1.798157	0.060386
F	-3.762846	-0.296414	-0.335765
H	4.715592	-1.950730	-0.393122
H	0.167215	2.130190	-1.265180
H	1.706373	1.492081	1.304846
H	1.260666	-0.565901	-0.086243
F	3.475835	-0.440358	1.340216

Zero-point correction = 0.186259
Thermal correction to Energy = 0.200091
Thermal correction to Enthalpy = 0.201035
Thermal correction to Gibbs Free Energy = 0.143072
Sum of electronic and zero-point Energies = -802.586838
Sum of electronic and thermal Energies = -802.573006
Sum of electronic and thermal Enthalpies = -802.572062
Sum of electronic and thermal Free Energies = -802.630025
Number of imaginary frequencies/frequency = 0

OPT-wB97xD-6-311+Gdp_4-fluoropentylacetamideC6.out

0 1

C	0.401939	0.729070	-0.241036
C	1.580083	-0.150257	0.147504
H	0.365636	1.624520	0.384657
C	2.904888	0.585009	-0.027862
H	1.467644	-0.463816	1.191202
C	4.112289	-0.247122	0.348403
H	2.916808	1.480273	0.603863
H	3.986806	-0.680670	1.344594
C	5.425033	0.489249	0.243270
H	5.553212	0.917425	-0.754893
H	5.445328	1.301087	0.975023
C	-2.031152	0.610339	-0.085928
O	-2.237197	1.804032	-0.210641
N	-0.850089	0.000170	-0.074732
H	-0.809975	-1.006861	0.005318
C	-3.258957	-0.320740	0.066098
F	-4.032836	0.090826	1.076057
F	-2.940522	-1.602782	0.298588
F	-3.999659	-0.287392	-1.049988
H	6.260915	-0.181352	0.455387
H	0.493929	1.056026	-1.282165
H	1.572086	-1.055805	-0.468062
H	3.022028	0.923244	-1.063938
F	4.169577	-1.369630	-0.534150

Zero-point correction = 0.186136
Thermal correction to Energy = 0.200214
Thermal correction to Enthalpy = 0.201158
Thermal correction to Gibbs Free Energy = 0.141716
Sum of electronic and zero-point Energies = -802.585643
Sum of electronic and thermal Energies = -802.571564
Sum of electronic and thermal Enthalpies = -802.57062
Sum of electronic and thermal Free Energies = -802.630062
Number of imaginary frequencies/frequency = 0

OPT-wB97xD-6-311+Gdp_4-fluoropentylacetamideC7.out

0 1

C	0.264670	1.914699	-0.582644
C	1.508860	1.417474	0.149639
H	-0.180465	2.755374	-0.048323
C	2.206972	0.271871	-0.577711
H	2.196696	2.263792	0.249897
C	3.467667	-0.207724	0.109864
H	2.488738	0.594058	-1.586994
H	4.142552	0.629967	0.307577
C	4.184716	-1.315961	-0.621441
H	3.512899	-2.160684	-0.798504
H	4.539992	-0.945961	-1.586962
C	-1.620299	0.591042	0.238761
O	-1.736744	1.148896	1.314314
N	-0.753713	0.879812	-0.729078
H	-0.743333	0.313346	-1.564815
C	-2.573183	-0.592259	-0.062785
F	-2.431761	-1.101121	-1.296138
F	-3.847686	-0.209513	0.071284
F	-2.356643	-1.587002	0.807985
H	5.049396	-1.660200	-0.049513
H	0.519722	2.251001	-1.589304
H	1.229788	1.108869	1.161241
H	1.528793	-0.581672	-0.691421
F	3.108173	-0.701541	1.401763

Zero-point correction = 0.186346
Thermal correction to Energy = 0.200156
Thermal correction to Enthalpy = 0.201101
Thermal correction to Gibbs Free Energy = 0.143181
Sum of electronic and zero-point Energies = -802.586406
Sum of electronic and thermal Energies = -802.572595
Sum of electronic and thermal Enthalpies = -802.571651
Sum of electronic and thermal Free Energies = -802.629571
Number of imaginary frequencies/frequency = 0

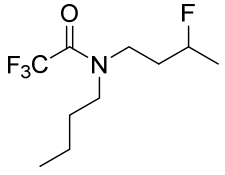
OPT-wB97xD-6-311+Gdp_4-fluoropentylacetamideC8.out

0 1

C	0.677015	2.008810	-0.053603
C	2.058623	1.677875	-0.606480
H	0.706122	2.114502	1.033440
C	2.844552	0.613269	0.163676
H	1.966539	1.395858	-1.660767
C	2.199842	-0.755438	0.270198
H	3.016232	0.960294	1.188884
H	1.250643	-0.704479	0.807626
C	3.097111	-1.802871	0.881600
H	3.332235	-1.524025	1.912356
H	2.599480	-2.775178	0.897696
C	-1.367400	0.727546	0.363086
O	-1.714601	1.322229	1.367985
N	-0.291340	0.965534	-0.379142
H	-0.126152	0.410007	-1.207648
C	-2.239360	-0.464106	-0.103942
F	-2.228257	-1.427661	0.827303
F	-1.831438	-1.015015	-1.256819
F	-3.508814	-0.077439	-0.269560
H	4.033251	-1.887195	0.322463
H	0.325324	2.957501	-0.469657
H	2.642307	2.601916	-0.589467
H	3.829520	0.497160	-0.301669
F	1.852774	-1.192491	-1.046521

Zero-point correction = 0.186831
Thermal correction to Energy = 0.200479
Thermal correction to Enthalpy = 0.201424
Thermal correction to Gibbs Free Energy = 0.144056
Sum of electronic and zero-point Energies = -802.585139
Sum of electronic and thermal Energies = -802.57149
Sum of electronic and thermal Enthalpies = -802.570546
Sum of electronic and thermal Free Energies = -802.627914
Number of imaginary frequencies/frequency = 0

	Calculated 19F NMR Shielding Tensor
OPT-wB97xD-6-311+Gdp_4-fluoropentylacetamideC1.out	360.383
OPT-wB97xD-6-311+Gdp_4-fluoropentylacetamideC3.out	370.8653
OPT-wB97xD-6-311+Gdp_4-fluoropentylacetamideC4.out	371.1051
OPT-wB97xD-6-311+Gdp_4-fluoropentylacetamideC6.out	370.3646
OPT-wB97xD-6-311+Gdp_4-fluoropentylacetamideC7.out	369.3023
OPT-wB97xD-6-311+Gdp_4-fluoropentylacetamideC8.out	372.6515



N-butyl-2,2,2-trifluoro-N-(3-fluorobutyl)acetamide

OPT-wB97xD-6-311+Gdp_3-trans-fluorobutylacetamideC1.out

0 1

C	-0.692408	-0.484674	0.440816
C	-1.751088	-1.057763	-0.498779
H	-1.153573	0.166875	1.180696
C	-2.775320	-1.902656	0.231177
H	-2.276261	-0.240087	-0.999962
C	-3.866699	-2.443330	-0.660208
H	-3.200751	-1.353118	1.076372
H	-4.455069	-1.616023	-1.065455
H	-3.441021	-3.008870	-1.493470
C	0.488097	1.549830	-0.429339
O	1.394070	2.111349	-1.018050
N	0.367286	0.222532	-0.281776
C	-0.600601	2.452956	0.222550
F	-0.412718	3.719634	-0.124064
F	-0.546598	2.391508	1.566118
F	-1.850565	2.119756	-0.145649
H	-0.207263	-1.288061	0.999070
H	-1.280965	-1.669585	-1.275441
H	-4.535736	-3.094173	-0.093315
C	1.444057	-0.613044	-0.824780
H	1.010692	-1.586426	-1.065627
H	1.797320	-0.164524	-1.754057
C	2.593896	-0.771840	0.165301
H	3.022050	0.214408	0.372830
H	2.200761	-1.159399	1.112859
C	3.680262	-1.707403	-0.358704
H	4.050299	-1.330454	-1.319361
H	3.243936	-2.693596	-0.556859
C	4.846318	-1.850815	0.614381
H	4.507850	-2.238561	1.580772
H	5.604679	-2.537491	0.227721
H	5.330020	-0.885226	0.792983
F	-2.094521	-3.007761	0.812769

Zero-point correction	=	0.272671
Thermal correction to Energy	=	0.290329
Thermal correction to Enthalpy	=	0.291274
Thermal correction to Gibbs Free Energy	=	0.225014
Sum of electronic and zero-point Energies	=	-920.426038
Sum of electronic and thermal Energies	=	-920.40838
Sum of electronic and thermal Enthalpies	=	-920.407436
Sum of electronic and thermal Free Energies	=	-920.473695
Number of imaginary frequencies/frequency	=	0

OPT-wB97xD-6-311+Gdp_3-trans-fluorobutylacetamideC2.out

0 1

C	-0.692288	-0.484863	0.440835
C	-1.750902	-1.057938	-0.498850
H	-1.153510	0.166616	1.180740
C	-2.775421	-1.902514	0.231066
H	-2.275843	-0.240249	-1.000255
C	-3.866658	-2.443258	-0.660448
H	-3.200976	-1.352689	1.076015
H	-3.440870	-3.009231	-1.493362
H	-4.536050	-3.093711	-0.093526
C	0.488055	1.549759	-0.429252
O	1.393996	2.111370	-1.017926
N	0.367396	0.222451	-0.281663
C	-0.600790	2.452786	0.222536
F	-0.546875	2.391404	1.566110
F	-1.850694	2.119431	-0.145735
F	-0.413027	3.719468	-0.124121
H	-0.207130	-1.288257	0.999066
H	-1.280748	-1.669955	-1.275340
H	-4.454686	-1.615952	-1.066200
C	1.444229	-0.613017	-0.824706
H	1.010931	-1.586416	-1.065605
H	1.797455	-0.164415	-1.753958
C	2.594090	-0.771764	0.165355
H	3.022047	0.214534	0.373050
H	2.201036	-1.159558	1.112849
C	3.680650	-1.707013	-0.358811
H	4.050724	-1.329720	-1.319318
H	3.244504	-2.693217	-0.557307
C	4.846627	-1.850531	0.614352
H	4.508137	-2.238730	1.580552
H	5.605197	-2.536873	0.227512
H	5.330080	-0.884899	0.793394
F	-2.094914	-3.007558	0.813111

Zero-point correction	=	0.272668
Thermal correction to Energy	=	0.290328
Thermal correction to Enthalpy	=	0.291272
Thermal correction to Gibbs Free Energy	=	0.225003
Sum of electronic and zero-point Energies	=	-920.426041
Sum of electronic and thermal Energies	=	-920.408381
Sum of electronic and thermal Enthalpies	=	-920.407437
Sum of electronic and thermal Free Energies	=	-920.473706
Number of imaginary frequencies/frequency	=	0

OPT-wB97xD-6-311+Gdp_3-trans-fluorobutylacetamideC3.out

0 1

C	0.574852	-0.614884	0.417380
C	1.518899	-1.336200	-0.541888
H	0.047516	-1.340060	1.044117
C	2.481368	-2.254760	0.182710
H	0.943670	-1.949876	-1.242369
C	3.430620	-2.990635	-0.731169
H	1.932943	-2.957835	0.817753
H	4.008011	-2.288298	-1.338221
H	4.119574	-3.608183	-0.151106
C	-0.468914	1.495666	-0.441323
O	-1.355862	2.123268	-0.990527
N	-0.448562	0.163336	-0.283326
C	0.732134	2.308866	0.126678
F	0.760920	2.273028	1.471532
F	0.630970	3.582487	-0.232836
F	1.918555	1.861185	-0.316630
H	1.139150	0.019590	1.095355
H	2.084089	-0.608423	-1.131024
H	2.864303	-3.644867	-1.399518
C	-1.602547	-0.588775	-0.785122
H	-1.961962	-0.105168	-1.694195
H	-1.248086	-1.586011	-1.056851
C	-2.722391	-0.686008	0.246454
H	-2.326178	-1.126810	1.169139
H	-3.065530	0.323940	0.494542
C	-3.895775	-1.522418	-0.257579
H	-3.540679	-2.527191	-0.516937
H	-4.283116	-1.080902	-1.183139
C	-5.021999	-1.629950	0.765012
H	-5.421470	-0.642518	1.016772
H	-5.848372	-2.235671	0.382754
H	-4.669680	-2.093246	1.692325
F	3.251241	-1.468186	1.080288

Zero-point correction	=	0.272666
Thermal correction to Energy	=	0.290335
Thermal correction to Enthalpy	=	0.291279
Thermal correction to Gibbs Free Energy	=	0.225154
Sum of electronic and zero-point Energies	=	-920.425295
Sum of electronic and thermal Energies	=	-920.407626
Sum of electronic and thermal Enthalpies	=	-920.406682
Sum of electronic and thermal Free Energies	=	-920.472807
Number of imaginary frequencies/frequency	=	0

OPT-wB97xD-6-311+Gdp_3-trans-fluorobutylacetamideC4.out

0 1

C	-0.804245	0.575626	-0.798257
C	-0.614969	1.668323	0.250747
H	-1.819319	0.188265	-0.750967
C	-1.658194	2.761890	0.138232
H	-0.691215	1.229989	1.250302
C	-1.504919	3.855385	1.166999
H	-2.665614	2.335928	0.170492
H	-0.511941	4.308624	1.103868
H	-2.258850	4.631515	1.018534
C	-0.101418	-1.759520	-0.229466
O	0.707682	-2.668101	-0.179404
N	0.162227	-0.516268	-0.658253
C	-1.550813	-2.073195	0.246600
F	-1.977819	-1.211164	1.187782

F	-1.604762	-3.289326	0.774099
F	-2.435679	-2.036312	-0.766386
H	-0.677852	0.988497	-1.801419
H	0.378469	2.119154	0.161459
H	-1.635716	3.438275	2.168960
C	1.549512	-0.231184	-1.046847
H	1.899974	-1.040277	-1.692837
H	1.526960	0.683455	-1.643617
C	2.495157	-0.065546	0.140213
H	2.112771	0.714281	0.807360
H	2.518410	-0.996693	0.714065
C	3.908580	0.294477	-0.310146
H	3.879825	1.228147	-0.884687
H	4.279352	-0.479354	-0.992398
C	4.873769	0.446410	0.861017
H	4.955272	-0.487767	1.425786
H	5.876499	0.716922	0.518400
H	4.536046	1.225008	1.552913
F	-1.543393	3.349993	-1.150802

Zero-point correction	=	0.272606
Thermal correction to Energy	=	0.290338
Thermal correction to Enthalpy	=	0.291283
Thermal correction to Gibbs Free Energy	=	0.224731
Sum of electronic and zero-point Energies	=	-920.425485
Sum of electronic and thermal Energies	=	-920.407753
Sum of electronic and thermal Enthalpies	=	-920.406808
Sum of electronic and thermal Free Energies	=	-920.47336
Number of imaginary frequencies/frequency	=	0

OPT-wB97xD-6-311+Gdp_3-trans-fluorobutylacetamideC5.out

0 1

C	0.704690	-0.397004	-0.279082
C	2.002624	-0.356336	0.525065
H	0.782625	0.243330	-1.156016
C	3.198721	-0.794705	-0.295157
H	2.184592	0.663201	0.875159
C	4.514670	-0.692736	0.436256
H	3.238439	-0.247161	-1.241932
H	4.482217	-1.251476	1.375480
H	5.326631	-1.082561	-0.181294
C	-1.027903	1.190163	0.585105
O	-1.955457	1.495931	1.312342
N	-0.462475	-0.024734	0.524818
C	-0.481070	2.294121	-0.368897
F	0.837385	2.512276	-0.212341
F	-1.098934	3.445221	-0.137706
F	-0.687634	1.980043	-1.660940
H	0.525377	-1.405550	-0.653347
H	1.926052	-0.997165	1.409753
H	4.728938	0.355278	0.661709
C	-1.033760	-1.066377	1.391420
H	-0.274643	-1.844630	1.492978
H	-1.207253	-0.636967	2.379715
C	-2.328611	-1.659412	0.840326
H	-2.683928	-2.395928	1.570304
H	-3.090803	-0.875429	0.792067
C	-2.183554	-2.324745	-0.526648
H	-1.414656	-3.105154	-0.473581
H	-1.831547	-1.587948	-1.257506
C	-3.494398	-2.929594	-1.019323
H	-3.864178	-3.689877	-0.323571
H	-4.269321	-2.162143	-1.114236
H	-3.371417	-3.403389	-1.997296
F	3.000893	-2.154317	-0.662928

Zero-point correction	=	0.273027
Thermal correction to Energy	=	0.290464
Thermal correction to Enthalpy	=	0.291408
Thermal correction to Gibbs Free Energy	=	0.226431
Sum of electronic and zero-point Energies	=	-920.425943
Sum of electronic and thermal Energies	=	-920.408506
Sum of electronic and thermal Enthalpies	=	-920.407562
Sum of electronic and thermal Free Energies	=	-920.472539
Number of imaginary frequencies/frequency	=	0

OPT-wB97xD-6-311+Gdp_3-trans-fluorobutylacetamideC6.out

0 1

C	-0.745986	0.512025	0.943545
C	-0.671393	1.708320	-0.001890
H	-0.637662	0.845555	1.980123
C	-1.783422	2.706843	0.248764
H	0.278605	2.234354	0.132261
C	-1.734567	3.914509	-0.655752
H	-1.797040	3.010104	1.300475
H	-1.756537	3.611815	-1.706090
H	-2.581627	4.574815	-0.458676
C	0.135923	-1.700189	0.171428
O	1.023379	-2.518114	0.010444
N	0.305541	-0.475798	0.694970
C	-1.300033	-2.114835	-0.265154
F	-1.832223	-1.251033	-1.146061
F	-2.140759	-2.202311	0.781457
F	-1.271640	-3.307486	-0.847457
H	-1.724291	0.046611	0.870029
H	-0.717392	1.367022	-1.040825
H	-0.813697	4.475170	-0.474311
C	1.677117	-0.106769	1.066885
H	1.602810	0.725951	1.770440
H	2.125202	-0.950441	1.597495
C	2.551239	0.277179	-0.124688
H	2.560983	-0.548357	-0.842444
H	2.116524	1.142175	-0.636452
C	3.981547	0.598968	0.300949
H	4.418297	-0.279768	0.789187
H	3.970300	1.398706	1.051546
C	4.856298	1.015356	-0.877030
H	4.464958	1.917341	-1.358731
H	5.881544	1.224730	-0.559287
H	4.895573	0.225261	-1.633494
F	-3.023457	2.048165	0.037402

Zero-point correction	=	0.272828
Thermal correction to Energy	=	0.290506
Thermal correction to Enthalpy	=	0.29145
Thermal correction to Gibbs Free Energy	=	0.22408
Sum of electronic and zero-point Energies	=	-920.424733
Sum of electronic and thermal Energies	=	-920.407055
Sum of electronic and thermal Enthalpies	=	-920.406111
Sum of electronic and thermal Free Energies	=	-920.473482
Number of imaginary frequencies/frequency	=	0

OPT-wB97xD-6-311+Gdp_3-trans-fluorobutylacetamideC7.out

0 1

C	-0.594863	0.711227	0.198504
C	-1.385252	1.425233	-0.896876
H	0.005850	1.430650	0.759819
C	-2.218613	2.588418	-0.389259
H	-0.701395	1.804469	-1.661506
C	-3.199817	2.262614	0.713165
H	-2.735467	3.050880	-1.233556
H	-3.891304	1.486875	0.372860
H	-2.691179	1.903743	1.611044
C	0.155386	-1.611656	-0.368469
O	0.960950	-2.422393	-0.788300
N	0.333664	-0.282289	-0.347054
C	-1.183338	-2.172320	0.197883
F	-2.267022	-1.599574	-0.355676
F	-1.268902	-1.993935	1.529387
F	-1.266827	-3.476223	-0.032379
H	-1.261837	0.244711	0.918705
H	-2.057391	0.717929	-1.390404
H	-3.781378	3.148458	0.976838
C	1.617854	0.228417	-0.837497
H	1.954099	-0.413811	-1.652223
H	1.440229	1.224477	-1.249932
C	2.673474	0.291539	0.261976
H	2.310379	0.928436	1.077287
H	2.817424	-0.711615	0.677319
C	4.003934	0.831274	-0.256663
H	3.844267	1.815955	-0.712197
H	4.370591	0.175203	-1.054455
C	5.058198	0.942256	0.839808
H	6.006536	1.315293	0.443005
H	4.733757	1.628276	1.628893
H	5.248241	-0.031615	1.302123
F	-1.330189	3.586938	0.097194

Zero-point correction =	0.272959	
Thermal correction to Energy =	0.290564	
Thermal correction to Enthalpy =	0.291509	
Thermal correction to Gibbs Free Energy =	0.225799	
Sum of electronic and zero-point Energies =	-920.425254	
Sum of electronic and thermal Energies =	-920.407649	
Sum of electronic and thermal Enthalpies =	-920.406704	
Sum of electronic and thermal Free Energies =	-920.472414	
Number of imaginary frequencies/frequency =	0	

OPT-wB97xD-6-311+Gdp_3-trans-fluorobutylacetamideC8.out

0 1			
C	0.272249	0.543080	1.061890
C	0.105352	2.045017	0.849677
H	1.314948	0.348217	1.291356
C	0.894201	2.602327	-0.318862
H	-0.947394	2.307684	0.715288
C	0.669630	4.076800	-0.552183
H	0.695922	2.031908	-1.231189
H	-0.372804	4.252314	-0.831371
H	0.887569	4.649948	0.353353
C	0.512964	-1.349189	-0.555398
O	0.130496	-2.075115	-1.454251
N	-0.132304	-0.257118	-0.104232
C	1.861341	-1.737110	0.124264
F	1.705222	-1.985327	1.438186
F	2.798525	-0.784827	-0.003674
F	2.345203	-2.843008	-0.428307
H	-0.315328	0.231855	1.930133
H	0.434802	2.544546	1.766116
H	1.306363	4.438189	-1.362339
C	-1.457543	0.005486	-0.676416
H	-1.535755	1.070649	-0.904123
H	-1.515147	-0.530866	-1.621768
C	-2.593786	-0.429596	0.244329
H	-2.467397	-1.492095	0.481457
H	-2.540562	0.118381	1.192322
C	-3.961363	-0.201212	-0.394810
H	-4.011671	-0.745737	-1.344565
H	-4.074721	0.861715	-0.639381
C	-5.110547	-0.641097	0.506170
H	-5.038396	-1.707962	0.740599
H	-5.104975	-0.090692	1.452616
H	-6.078598	-0.470863	0.026845
F	2.272194	2.401665	-0.048838

Zero-point correction =	0.273294	
Thermal correction to Energy =	0.290732	
Thermal correction to Enthalpy =	0.291676	
Thermal correction to Gibbs Free Energy =	0.226412	
Sum of electronic and zero-point Energies =	-920.423195	
Sum of electronic and thermal Energies =	-920.405757	
Sum of electronic and thermal Enthalpies =	-920.404813	
Sum of electronic and thermal Free Energies =	-920.470077	
Number of imaginary frequencies/frequency =	0	

	Calculated 19F NMR Shielding Tensor
OPT-wB97xD-6-311+Gdp_3-trans-fluorobutylacetamideC1.out	370.6751
OPT-wB97xD-6-311+Gdp_3-trans-fluorobutylacetamideC2.out	371.4078
OPT-wB97xD-6-311+Gdp_3-trans-fluorobutylacetamideC3.out	371.4101
OPT-wB97xD-6-311+Gdp_3-trans-fluorobutylacetamideC4.out	371.2371
OPT-wB97xD-6-311+Gdp_3-trans-fluorobutylacetamideC5.out	371.4333
OPT-wB97xD-6-311+Gdp_3-trans-fluorobutylacetamideC6.out	371.6496
OPT-wB97xD-6-311+Gdp_3-trans-fluorobutylacetamideC7.out	372.8353
OPT-wB97xD-6-311+Gdp_3-trans-fluorobutylacetamideC8.out	374.9402

OPT-wB97xD-6-311+Gdp_3-cis-fluorobutylacetamideC1.out

0 1			
C	-1.278706	0.185424	-0.682372
C	-2.386769	-0.239110	0.277947
H	-1.426359	-0.275284	-1.660115
C	-3.762452	0.175035	-0.200726
H	-2.378613	-1.328047	0.381801
C	-4.885883	-0.271969	0.702463
H	-3.930798	-0.164989	-1.226998
H	-4.929987	-1.364134	0.722312
H	-4.730353	0.089028	1.722714
C	0.456059	-1.441053	-0.430568
O	-0.177727	-2.275760	-1.051954
N	0.044221	-0.190416	-0.179617
C	1.843783	-1.875125	0.126297
F	1.831110	-1.949654	1.470529
F	2.835179	-1.038732	-0.222896
F	2.162829	-3.078438	-0.333683
H	-1.281545	1.267193	-0.816644
H	-2.211176	0.190836	1.270292
H	-5.844034	0.102635	0.335812
C	0.758929	0.832233	0.591811
H	0.014213	1.320485	1.227514
H	1.473358	0.364020	1.266928
C	1.455940	1.863050	-0.290345
H	2.210139	1.358143	-0.902103
H	0.729887	2.305494	-0.981665
C	2.110168	2.967294	0.536379
H	2.818579	2.520222	1.243679
H	1.344596	3.470087	1.139122
C	2.834417	3.994417	-0.327681
H	3.635914	3.525891	-0.907583
H	2.146456	4.470542	-1.033716
H	3.282549	4.782223	0.284042
F	-3.793947	1.596099	-0.270801

Zero-point correction =	0.272084	
Thermal correction to Energy =	0.289967	
Thermal correction to Enthalpy =	0.290911	
Thermal correction to Gibbs Free Energy =	0.223469	
Sum of electronic and zero-point Energies =	-920.427034	
Sum of electronic and thermal Energies =	-920.409152	
Sum of electronic and thermal Enthalpies =	-920.408208	
Sum of electronic and thermal Free Energies =	-920.47565	
Number of imaginary frequencies/frequency =	0	

OPT-wB97xD-6-311+Gdp_3-cis-fluorobutylacetamideC2.out

0 1			
C	-1.146362	-0.619961	-0.955734
C	-2.015826	-0.628813	0.301052
H	-1.230410	-1.579421	-1.471686
C	-3.470446	-0.921129	-0.000063
H	-1.657312	-1.403730	0.983985
C	-4.354488	-0.923527	1.223424
H	-3.568760	-1.859900	-0.553430
H	-4.043818	-1.722725	1.901469
H	-4.280942	0.030192	1.753304
C	0.963352	-1.395280	-0.148810
O	0.511587	-2.506592	0.063944
N	0.269214	-0.370437	-0.665663
C	2.462628	-1.159108	0.199736
F	3.202840	-0.919120	-0.897980
F	2.968473	-2.235712	0.788244
F	2.636446	-0.125053	1.041771
H	-1.473789	0.160918	-1.642517
H	-1.943114	0.331312	0.820282
H	-5.396640	-1.096146	0.946128
C	0.780886	0.976299	-0.942511
H	1.868193	0.972022	-0.928733
H	0.489641	1.224725	-1.967463
C	0.256179	2.030222	0.027601
H	-0.830219	2.123061	-0.077793
H	0.454010	1.700261	1.053283
C	0.905654	3.391296	-0.211110
H	0.739408	3.696359	-1.251018
H	1.990320	3.299053	-0.082450
C	0.368973	4.465930	0.728435
H	0.854995	5.428932	0.548668

H	-0.708238	4.605941	0.593320
H	0.542284	4.196980	1.775397
F	-3.950659	0.084595	-0.885899

Zero-point correction	=	0.272797
Thermal correction to Energy	=	0.290364
Thermal correction to Enthalpy	=	0.291309
Thermal correction to Gibbs Free Energy	=	0.225818
Sum of electronic and zero-point Energies	=	-920.426254
Sum of electronic and thermal Energies	=	-920.408686
Sum of electronic and thermal Enthalpies	=	-920.407742
Sum of electronic and thermal Free Energies	=	-920.473233
Number of imaginary frequencies/frequency	=	0

OPT-wB97xD-6-311+Gdp_3-cis-fluorobutylacetamideC3.out

0 1

C	1.257981	0.433440	-0.602241
C	2.351819	0.211124	0.439819
H	1.123471	1.500277	-0.793734
C	3.665130	0.870320	0.072481
H	2.030107	0.631173	1.399078
C	4.756796	0.660019	1.094125
H	3.517356	1.937547	-0.121774
H	4.472381	1.127732	2.040517
H	4.922971	-0.406349	1.268541
C	-0.272952	-1.394515	-0.380709
O	0.478964	-2.156202	-0.960570
N	-0.029104	-0.096299	-0.144997
C	-1.615871	-1.984675	0.142758
F	-1.638888	-2.031977	1.488425
F	-1.770986	-3.226234	-0.298916
F	-2.690109	-1.282749	-0.255199
H	1.518711	-0.047285	-1.543934
H	2.512529	-0.861390	0.585186
H	5.690926	1.113423	0.755630
C	-0.893440	0.835494	0.586077
H	-1.564743	0.287707	1.244910
H	-0.242620	1.423342	1.240991
C	-1.691072	1.758762	-0.330193
H	-1.007336	2.325312	-0.972231
H	-2.318243	1.151669	-0.990424
C	-2.563756	2.724814	0.467247
H	-1.929852	3.328130	1.128020
H	-3.233277	2.149856	1.117748
C	-3.389144	3.643865	-0.427306
H	-4.016784	4.314627	0.165911
H	-2.745106	4.262112	-1.061088
H	-4.046212	3.064818	-1.083940
F	4.106071	0.326417	-1.162335

Zero-point correction	=	0.273218
Thermal correction to Energy	=	0.290671
Thermal correction to Enthalpy	=	0.291615
Thermal correction to Gibbs Free Energy	=	0.226315
Sum of electronic and zero-point Energies	=	-920.424781
Sum of electronic and thermal Energies	=	-920.407328
Sum of electronic and thermal Enthalpies	=	-920.406384
Sum of electronic and thermal Free Energies	=	-920.471684
Number of imaginary frequencies/frequency	=	0

OPT-wB97xD-6-311+Gdp_3-cis-fluorobutylacetamideC4.out

0 1

C	0.790492	-1.239666	1.260903
C	1.904284	-1.904410	0.451399
H	0.084258	-2.002426	1.595943
C	2.975239	-0.967288	-0.079207
H	2.388842	-2.630159	1.112417
C	4.204476	-1.684495	-0.584799
H	3.239213	-0.215082	0.668070
H	4.904110	-0.974458	-1.031018
H	4.709008	-2.184930	0.245991
C	0.370469	1.056328	0.697131
O	1.237085	1.463400	1.450217
N	0.032927	-0.229570	0.518343
C	-0.396112	2.128090	-0.134690
F	-0.116428	2.030833	-1.445671
F	-0.042172	3.346600	0.256316
F	-1.731341	2.040222	0.001301
H	1.207001	-0.762484	2.147271
H	1.495357	-2.472656	-0.390745
H	3.934874	-2.435364	-1.332901
C	-0.995833	-0.734994	-0.395467
H	-1.167853	-0.019295	-1.197042
H	-0.583733	-1.626696	-0.875201
C	-2.307511	-1.072349	0.308207
H	-2.123382	-1.801431	1.105133
H	-2.699661	-0.169774	0.786622
C	-3.342543	-1.631764	-0.665417
H	-2.948379	-2.541896	-1.132701
H	-3.500758	-0.909829	-1.475137
C	-4.675870	-1.939160	0.008375
H	-5.104411	-1.039463	0.461267
H	-5.402371	-2.328329	-0.710517
H	-4.557766	-2.686706	0.799608
F	2.427267	-0.235542	-1.168148

Zero-point correction	=	0.273047
Thermal correction to Energy	=	0.290417
Thermal correction to Enthalpy	=	0.291361
Thermal correction to Gibbs Free Energy	=	0.226812
Sum of electronic and zero-point Energies	=	-920.42473
Sum of electronic and thermal Energies	=	-920.407361
Sum of electronic and thermal Enthalpies	=	-920.406416
Sum of electronic and thermal Free Energies	=	-920.470965
Number of imaginary frequencies/frequency	=	0

OPT-wB97xD-6-311+Gdp_3-cis-fluorobutylacetamideC5.out

0 1

C	1.395515	0.062200	-0.428118
C	2.357868	-0.362147	0.680250
H	1.473086	1.134725	-0.611199
C	3.793284	0.074973	0.455335
H	2.018296	0.052503	1.634766
C	4.409234	-0.347880	-0.858164
H	4.406978	-0.268680	1.291539
H	3.884823	0.097225	-1.707104
H	5.457920	-0.046401	-0.902297
C	-0.447511	-1.458713	-0.316979
O	0.198086	-2.347802	-0.843466
N	0.006612	-0.223781	-0.060372
C	-1.910024	-1.795334	0.099075
F	-2.807036	-0.916238	-0.377437
F	-2.044585	-1.826270	1.438248
F	-2.250225	-2.993169	-0.360285
H	1.617222	-0.456438	-1.360276
H	2.347242	-1.451962	0.777191
H	4.359325	-1.435934	-0.953936
C	-0.724352	0.858052	0.608047
H	-1.527440	0.449056	1.218539
H	-0.022384	1.326608	1.304487
C	-1.273991	1.897339	-0.363914
H	-0.455008	2.312828	-0.961409
H	-1.961404	1.408738	-1.061489
C	-1.994191	3.027057	0.368504
H	-1.302703	3.499094	1.076307
H	-2.811487	2.606465	0.966022
C	-2.547771	4.080758	-0.584667
H	-1.745619	4.541206	-1.170268
H	-3.263025	3.640684	-1.286845
H	-3.062405	4.877677	-0.040569
F	3.835983	1.496083	0.521770

Zero-point correction	=	0.271748
Thermal correction to Energy	=	0.289754
Thermal correction to Enthalpy	=	0.290698
Thermal correction to Gibbs Free Energy	=	0.222712
Sum of electronic and zero-point Energies	=	-920.426597
Sum of electronic and thermal Energies	=	-920.408591
Sum of electronic and thermal Enthalpies	=	-920.407647
Sum of electronic and thermal Free Energies	=	-920.475633
Number of imaginary frequencies/frequency	=	0

OPT-wB97xD-6-311+Gdp_3-cis-fluorobutylacetamideC6.out

0 1

C	1.395565	0.062079	-0.428128
C	2.357941	-0.362284	0.680213

H	1.473156	1.134601	-0.611220
C	3.793345	0.074890	0.455311
H	2.018357	0.052323	1.634744
C	4.409295	-0.347855	-0.858221
H	4.407062	-0.268787	1.291487
H	5.457963	-0.046310	-0.902355
H	4.359452	-1.435904	-0.954070
C	-0.447573	-1.458728	-0.316957
O	0.197935	-2.347870	-0.843462
N	0.006668	-0.223846	-0.060316
C	-1.910127	-1.795197	0.099083
F	-2.807039	-0.915976	-0.377393
F	-2.044692	-1.826172	1.438255
F	-2.250467	-2.992973	-0.360327
H	1.617222	-0.456570	-1.360292
H	2.347343	-1.452103	0.777115
H	3.884844	0.097270	-1.707128
C	-0.724214	0.858053	0.608084
H	-1.527217	0.449121	1.218730
H	-0.022148	1.326666	1.304386
C	-1.273970	1.897243	-0.363912
H	-0.455062	2.312658	-0.961562
H	-1.961496	1.408572	-1.061326
C	-1.994042	3.027053	0.368496
H	-1.302438	3.499151	1.076145
H	-2.811260	2.606532	0.966171
C	-2.547739	4.080665	-0.584704
H	-3.062219	4.877688	-0.040611
H	-1.745670	4.540994	-1.170512
H	-3.263159	3.640554	-1.286692
F	3.836003	1.496001	0.521832

Zero-point correction	=	0.271751
Thermal correction to Energy	=	0.289756
Thermal correction to Enthalpy	=	0.2907
Thermal correction to Gibbs Free Energy	=	0.222716
Sum of electronic and zero-point Energies	=	-920.426595
Sum of electronic and thermal Energies	=	-920.40859
Sum of electronic and thermal Enthalpies	=	-920.407646
Sum of electronic and thermal Free Energies	=	-920.47563
Number of imaginary frequencies/frequency	=	0

OPT-wB97xD-6-311+Gdp_3-cis-fluorobutylacetamideC7.out

0 1

C	0.971063	-0.816057	0.910180
C	1.892912	-0.554914	-0.280166
H	0.918731	-1.889653	1.106299
C	3.259804	-1.178520	-0.094231
H	1.450751	-0.987178	-1.181869
C	4.201590	-0.944621	-1.250131
H	3.166578	-2.247124	0.121707
H	4.327090	0.125230	-1.437971
H	5.179344	-1.385976	-1.045447
C	-1.195137	-1.097491	-0.042802
O	-0.852008	-2.134493	-0.583255
N	-0.394239	-0.322783	0.703921
C	-2.680087	-0.665625	-0.222607
F	-2.798600	0.539961	-0.804717
F	-3.334442	-0.616330	0.952284
F	-3.318192	-1.539195	-0.991600
H	1.356116	-0.330752	1.807290
H	2.011000	0.519443	-0.449472
H	3.797897	-1.411267	-2.152590
C	-0.763618	0.917017	1.400648
H	-1.821943	1.118593	1.258737
H	-0.611356	0.744977	2.470239
C	0.048542	2.127457	0.946449
H	-0.239869	2.964487	1.592022
H	1.113644	1.952382	1.136638
C	-0.165186	2.510486	-0.515482
H	-1.219002	2.764044	-0.672240
H	0.041104	1.646091	-1.155976
C	0.714914	3.679600	-0.944432
H	0.550505	3.933423	-1.995252
H	0.504567	4.573458	-0.348257
H	1.776665	3.441789	-0.820404
F	3.847361	-0.613384	1.072986

Zero-point correction	=	0.273349
Thermal correction to Energy	=	0.290698
Thermal correction to Enthalpy	=	0.291642
Thermal correction to Gibbs Free Energy	=	0.227175
Sum of electronic and zero-point Energies	=	-920.426525
Sum of electronic and thermal Energies	=	-920.409176
Sum of electronic and thermal Enthalpies	=	-920.408232
Sum of electronic and thermal Free Energies	=	-920.472699
Number of imaginary frequencies/frequency	=	0

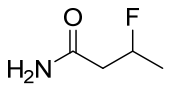
OPT-wB97xD-6-311+Gdp_3-cis-fluorobutylacetamideC8.out

0 1

C	0.873952	-1.208045	-0.980892
C	1.946553	-1.779483	-0.055297
H	1.329315	-0.737891	-1.850932
C	3.050882	-0.806767	0.309273
H	1.487399	-2.139711	0.870847
C	4.020775	-1.349366	1.332274
H	2.640124	0.150874	0.641044
H	3.506042	-1.507898	2.283726
H	4.443018	-2.302096	1.000478
C	0.249881	1.082718	-0.554984
O	1.110163	1.526348	-1.291292
N	0.020119	-0.219180	-0.312214
C	-0.629779	2.122180	0.205113
F	-0.412038	2.066814	1.533232
F	-1.947138	1.948891	0.005121
F	-0.330208	3.351341	-0.193552
H	0.229360	-2.014543	-1.334997
H	2.399887	-2.649884	-0.541327
H	4.834583	-0.640531	1.499423
C	-1.075842	-0.758552	0.500609
H	-0.678709	-1.623101	1.039265
H	-1.365746	-0.037886	1.262989
C	-2.290218	-1.171705	-0.327480
H	-2.649813	-0.306723	-0.893081
H	-1.996819	-1.931874	-1.059647
C	-3.412986	-1.717504	0.551395
H	-3.702845	-0.954020	1.282658
H	-3.042623	-2.574740	1.126035
C	-4.635936	-2.136958	-0.257993
H	-5.050710	-1.288844	-0.811760
H	-4.379807	-2.915816	-0.983389
H	-5.424392	-2.529970	0.389858
F	3.780040	-0.514931	-0.871186

Zero-point correction	=	0.272484
Thermal correction to Energy	=	0.290125
Thermal correction to Enthalpy	=	0.291069
Thermal correction to Gibbs Free Energy	=	0.224928
Sum of electronic and zero-point Energies	=	-920.425111
Sum of electronic and thermal Energies	=	-920.40747
Sum of electronic and thermal Enthalpies	=	-920.406525
Sum of electronic and thermal Free Energies	=	-920.472667
Number of imaginary frequencies/frequency	=	0

	Calculated 19F NMR Shielding Tensor
OPT-wB97xD-6-311+Gdp_3-cis-fluorobutylacetamideC1.out	371.349
OPT-wB97xD-6-311+Gdp_3-cis-fluorobutylacetamideC2.out	372.6538
OPT-wB97xD-6-311+Gdp_3-cis-fluorobutylacetamideC3.out	371.2022
OPT-wB97xD-6-311+Gdp_3-cis-fluorobutylacetamideC4.out	367.7689
OPT-wB97xD-6-311+Gdp_3-cis-fluorobutylacetamideC5.out	372.7979
OPT-wB97xD-6-311+Gdp_3-cis-fluorobutylacetamideC6.out	372.7962
OPT-wB97xD-6-311+Gdp_3-cis-fluorobutylacetamideC7.out	372.7639
OPT-wB97xD-6-311+Gdp_3-cis-fluorobutylacetamideC8.out	368.605



3-fluorobutanamide

OPT-wB97xD-6-311+Gdp_3-fluorobutanamideC1.out

0 1

C	-1.428624	-0.208999	0.031146
O	-2.364327	-0.986273	-0.104511
N	-1.575931	1.127393	-0.089863
H	-2.493308	1.502929	-0.274665
H	-0.809729	1.761832	0.071729
C	-0.033963	-0.711010	0.369768
H	0.104363	-0.632039	1.454112
H	-0.012752	-1.772583	0.117895
C	1.129735	-0.022584	-0.322503
H	0.929448	0.111422	-1.388542
C	2.449450	-0.719974	-0.103297
H	2.426198	-1.703969	-0.578326
H	3.262881	-0.144011	-0.549054
H	2.646997	-0.852131	0.963858
F	1.243606	1.300264	0.199715

Zero-point correction	=	0.124139
Thermal correction to Energy	=	0.132006
Thermal correction to Enthalpy	=	0.13295
Thermal correction to Gibbs Free Energy	=	0.091641
Sum of electronic and zero-point Energies	=	-386.977259
Sum of electronic and thermal Energies	=	-386.969392
Sum of electronic and thermal Enthalpies	=	-386.968448
Sum of electronic and thermal Free Energies	=	-387.009757
Number of imaginary frequencies/frequency	=	0

OPT-wB97xD-6-311+Gdp_3-fluorobutanamideC2.out

0 1

C	1.262387	-0.030501	0.104695
O	2.155509	-0.849465	-0.064882
N	1.261632	1.177230	-0.500393
H	1.994543	1.398989	-1.156663
H	0.484794	1.811526	-0.403088
C	0.090905	-0.301950	1.035553
H	0.228687	-1.302857	1.447037
H	0.122227	0.408678	1.867062
C	-1.286005	-0.236486	0.389184
H	-2.032975	-0.537108	1.126405
C	-1.436196	-1.034928	-0.882626
H	-1.241838	-2.090462	-0.675183
H	-2.451036	-0.940911	-1.274216
H	-0.731084	-0.698413	-1.647160
F	-1.581706	1.125429	0.095197

Zero-point correction	=	0.12427
Thermal correction to Energy	=	0.132122
Thermal correction to Enthalpy	=	0.133066
Thermal correction to Gibbs Free Energy	=	0.091667
Sum of electronic and zero-point Energies	=	-386.977262
Sum of electronic and thermal Energies	=	-386.96941
Sum of electronic and thermal Enthalpies	=	-386.968466
Sum of electronic and thermal Free Energies	=	-387.009865
Number of imaginary frequencies/frequency	=	0

OPT-wB97xD-6-311+Gdp_3-fluorobutanamideC3.out

0 1

C	-1.334722	-0.189968	0.095967
O	-1.558331	-0.267609	1.296186
N	-2.237315	0.299516	-0.780026
H	-3.144035	0.586155	-0.442895
H	-2.047843	0.352403	-1.767081
C	-0.016846	-0.653735	-0.498316
H	0.004553	-1.744298	-0.415107
H	0.066009	-0.390942	-1.556339
C	1.166561	-0.082151	0.267217
H	1.092555	-0.347829	1.323099
C	1.356739	1.405225	0.093649
H	0.498707	1.939224	0.511238
H	2.252384	1.739769	0.621129
H	1.449324	1.663621	-0.965058
F	2.325088	-0.736674	-0.218821

Zero-point correction	=	0.123841
Thermal correction to Energy	=	0.131928
Thermal correction to Enthalpy	=	0.132872
Thermal correction to Gibbs Free Energy	=	0.090171
Sum of electronic and zero-point Energies	=	-386.977393
Sum of electronic and thermal Energies	=	-386.969306
Sum of electronic and thermal Enthalpies	=	-386.968362
Sum of electronic and thermal Free Energies	=	-387.011063
Number of imaginary frequencies/frequency	=	0

OPT-wB97xD-6-311+Gdp_3-fluorobutanamideC4.out

0 1

C	-1.355978	-0.008282	-0.200533
O	-1.890019	1.032266	-0.554076
N	-1.908602	-0.833965	0.717455
H	-2.811103	-0.607838	1.106817
H	-1.496305	-1.723828	0.945570
C	-0.002976	-0.450911	-0.731384
H	-0.022925	-1.521338	-0.953750
H	0.195479	0.097675	-1.653334
C	1.115306	-0.184403	0.271488
H	0.941242	-0.737523	1.198585
C	1.366713	1.275145	0.558983
H	0.492637	1.716506	1.044914
H	2.222527	1.386746	1.228116
H	1.559532	1.823388	-0.366786
F	2.295655	-0.738162	-0.281225

Zero-point correction	=	0.124107
Thermal correction to Energy	=	0.13215
Thermal correction to Enthalpy	=	0.133094
Thermal correction to Gibbs Free Energy	=	0.090985
Sum of electronic and zero-point Energies	=	-386.975957
Sum of electronic and thermal Energies	=	-386.967915
Sum of electronic and thermal Enthalpies	=	-386.96697
Sum of electronic and thermal Free Energies	=	-387.00908
Number of imaginary frequencies/frequency	=	0

OPT-wB97xD-6-311+Gdp_3-fluorobutanamideC5.out

0 1

C	-1.342508	-0.241737	0.074906
O	-1.653475	-1.068700	-0.770935
N	-2.171662	0.748007	0.466618
H	-3.068877	0.844829	0.015717
H	-1.871364	1.469577	1.100781
C	0.010448	-0.288596	0.763400
H	0.112159	0.488431	1.525866
H	0.084387	-1.260761	1.259116
C	1.149146	-0.179760	-0.233233
H	1.009576	-0.899740	-1.042494
C	2.516448	-0.315835	0.390739
H	2.628600	-1.315232	0.819336
H	3.294091	-0.178001	-0.363581
H	2.657872	0.422157	1.185165
F	1.064642	1.099762	-0.841515

Zero-point correction	=	0.124232
Thermal correction to Energy	=	0.132148
Thermal correction to Enthalpy	=	0.133093
Thermal correction to Gibbs Free Energy	=	0.091557
Sum of electronic and zero-point Energies	=	-386.977712
Sum of electronic and thermal Energies	=	-386.969795
Sum of electronic and thermal Enthalpies	=	-386.968851
Sum of electronic and thermal Free Energies	=	-387.010386
Number of imaginary frequencies/frequency	=	0

OPT-wB97xD-6-311+Gdp_3-fluorobutanamideC6.out

0 1

C	-1.371397	-0.049607	-0.223913
O	-2.068677	-1.049295	-0.305323
N	-1.791269	1.074718	0.399401
H	-2.698302	1.082885	0.839911
H	-1.220429	1.901438	0.461872

C	0.018178	0.010568	-0.837135
H	0.193103	-0.941002	-1.341732
H	0.041293	0.805637	-1.589619
C	1.134127	0.272305	0.161158
H	0.992010	1.228346	0.673567
C	2.510570	0.202928	-0.455991
H	2.616515	0.983674	-1.214008
H	3.278384	0.356060	0.305182
H	2.670389	-0.768038	-0.931838
F	1.051830	-0.710536	1.175414

Zero-point correction	=	0.124196
Thermal correction to Energy	=	0.132188
Thermal correction to Enthalpy	=	0.133132
Thermal correction to Gibbs Free Energy	=	0.091382
Sum of electronic and zero-point Energies	=	-386.975315
Sum of electronic and thermal Energies	=	-386.967323
Sum of electronic and thermal Enthalpies	=	-386.966379
Sum of electronic and thermal Free Energies	=	-387.008129
Number of imaginary frequencies/frequency	=	0

OPT-wB97xD-6-311+Gdp_3-fluorobutanamideC7.out

0 1

C	-1.233237	-0.151514	0.089642
O	-1.695730	-1.151342	-0.438231
N	-1.743627	1.082509	-0.131303
H	-2.499581	1.191118	-0.790092
H	-1.347889	1.906852	0.289002
C	-0.051328	-0.214345	1.043094
H	-0.140529	0.560331	1.810757
H	-0.079787	-1.185558	1.538954
C	1.313323	-0.045624	0.380305
H	2.076714	-0.131746	1.157908
C	1.514781	1.226322	-0.410551
H	1.364722	2.095705	0.235757
H	2.533529	1.265631	-0.801472
H	0.817477	1.287720	-1.249350
F	1.531704	-1.138436	-0.486827

Zero-point correction	=	0.124317
Thermal correction to Energy	=	0.132225
Thermal correction to Enthalpy	=	0.133169
Thermal correction to Gibbs Free Energy	=	0.091209
Sum of electronic and zero-point Energies	=	-386.973902
Sum of electronic and thermal Energies	=	-386.965995
Sum of electronic and thermal Enthalpies	=	-386.965051
Sum of electronic and thermal Free Energies	=	-387.00701
Number of imaginary frequencies/frequency	=	0

OPT-wB97xD-6-311+Gdp_3-fluorobutanamideC8.out

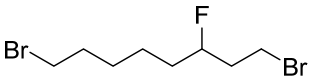
0 1

C	-1.233235	-0.151514	0.089643
O	-1.695727	-1.151343	-0.438230
N	-1.743626	1.082508	-0.131305
H	-1.347896	1.906851	0.289006
H	-2.499581	1.191115	-0.790092
C	-0.051327	-0.214344	1.043096
H	-0.140528	0.560334	1.810757
H	-0.079786	-1.185556	1.538957
C	1.313323	-0.045623	0.380305
H	2.076716	-0.131744	1.157906
C	1.514778	1.226323	-0.410552
H	1.364731	2.095705	0.235760
H	2.533522	1.265627	-0.801485
H	0.817462	1.287724	-1.249341
F	1.531703	-1.138435	-0.486827

Zero-point correction	=	0.124317
Thermal correction to Energy	=	0.132225
Thermal correction to Enthalpy	=	0.133169
Thermal correction to Gibbs Free Energy	=	0.091208
Sum of electronic and zero-point Energies	=	-386.973903
Sum of electronic and thermal Energies	=	-386.965995
Sum of electronic and thermal Enthalpies	=	-386.965051
Sum of electronic and thermal Free Energies	=	-387.007012
Number of imaginary frequencies/frequency	=	0

	Calculated

	19F NMR Shielding Tensor
OPT-wB97xD-6-311+Gdp_3-fluorobutanamideC1.out	367.6728
OPT-wB97xD-6-311+Gdp_3-fluorobutanamideC2.out	368.4321
OPT-wB97xD-6-311+Gdp_3-fluorobutanamideC3.out	371.4468
OPT-wB97xD-6-311+Gdp_3-fluorobutanamideC4.out	361.2021
OPT-wB97xD-6-311+Gdp_3-fluorobutanamideC5.out	369.2269
OPT-wB97xD-6-311+Gdp_3-fluorobutanamideC6.out	368.0803
OPT-wB97xD-6-311+Gdp_3-fluorobutanamideC7.out	368.5821
OPT-wB97xD-6-311+Gdp_3-fluorobutanamideC8.out	368.5821



1,8-dibromo-3-fluorooctane

C9 omitted due to presence of 1 imaginary frequency

OPT-wB97xD-6-311+Gdp_18dibromooctane3FC1.out

0 1

C	-4.466824	-0.784541	0.284035
C	-3.298647	0.103408	-0.094789
H	-4.475318	-1.714758	-0.282701
H	-4.479225	-1.011634	1.349255
C	-1.966704	-0.588184	0.202088
H	-3.355009	0.351875	-1.159423
H	-3.355554	1.045038	0.460329
C	-0.766422	0.280119	-0.168261
H	-1.915242	-0.840310	1.268297
H	-1.915805	-1.536415	-0.347234
H	-0.813204	0.530002	-1.235380
H	-0.821678	1.226757	0.378870
C	0.564093	-0.405347	0.131362
C	1.772771	0.436561	-0.221311
H	0.635417	-1.339646	-0.437226
C	3.094425	-0.263445	0.043878
H	1.715656	0.779061	-1.260162
C	4.276905	0.605983	-0.339504
H	3.146498	-0.535174	1.102343
H	3.105500	-1.189812	-0.537686
H	4.274332	0.851077	-1.400760
H	4.318739	1.522182	0.244714
Br	5.981318	-0.307892	-0.010516
Br	-6.198591	0.069176	-0.087083
F	1.739809	1.620215	0.561636
H	0.623599	-0.672458	1.193018

Zero-point correction	=	0.221462
Thermal correction to Energy	=	0.235341
Thermal correction to Enthalpy	=	0.236285
Thermal correction to Gibbs Free Energy	=	0.176596
Sum of electronic and zero-point Energies	=	-5561.895295
Sum of electronic and thermal Energies	=	-5561.881416
Sum of electronic and thermal Enthalpies	=	-5561.880472
Sum of electronic and thermal Free Energies	=	-5561.940161
Number of imaginary frequencies/frequency	=	0

OPT-wB97xD-6-311+Gdp_18dibromooctane3FC2.out

0 1

C	-4.304206	0.425534	-0.609724
C	-2.899191	0.558245	-0.056620
H	-4.908937	1.307872	-0.404341
H	-4.305583	0.228817	-1.681129
C	-2.170554	1.734078	-0.714405
H	-2.941067	0.712960	1.026561
H	-2.352721	-0.373078	-0.230035
C	-0.781683	1.998421	-0.129760
H	-2.082889	1.552439	-1.792827
H	-2.776373	2.639736	-0.598508

H	-0.375140	2.905560	-0.591543
H	-0.872021	2.207208	0.941268
C	0.204173	0.851175	-0.347108
C	1.618793	1.186305	0.077098
H	0.235998	0.592431	-1.412254
C	2.609454	0.061878	-0.171843
H	1.956172	2.110821	-0.404023
C	4.016184	0.456074	0.236577
H	2.286023	-0.828629	0.375141
H	2.582293	-0.174458	-1.239615
H	4.370038	1.326932	-0.313521
H	4.095944	0.644800	1.304547
Br	5.307371	-0.971466	-0.143680
Br	-5.281999	-1.076465	0.198397
F	1.617381	1.471282	1.467605
H	-0.114012	-0.047609	0.191440

Zero-point correction	=	0.221889
Thermal correction to Energy	=	0.235635
Thermal correction to Enthalpy	=	0.236579
Thermal correction to Gibbs Free Energy	=	0.177006
Sum of electronic and zero-point Energies	=	-5561.894215
Sum of electronic and thermal Energies	=	-5561.880469
Sum of electronic and thermal Enthalpies	=	-5561.879525
Sum of electronic and thermal Free Energies	=	-5561.939098
Number of imaginary frequencies/frequency	=	0

OPT-wB97xD-6-311+Gdp_18dibromooctane3FC3.out

0 1

C	4.248491	0.519021	-0.344524
C	2.850357	0.101806	0.065414
H	4.331373	0.672149	-1.419629
H	4.575263	1.419671	0.173286
C	1.830964	1.182513	-0.299021
H	2.585029	-0.837143	-0.430686
H	2.821827	-0.082374	1.144295
C	0.413306	0.812857	0.132500
H	2.116192	2.130263	0.172889
H	1.849136	1.353128	-1.382222
H	0.143473	-0.149745	-0.314847
H	0.393856	0.670144	1.220221
C	-0.608367	1.879081	-0.262132
C	-1.978128	1.653425	0.348698
H	-0.707640	1.925437	-1.352325
C	-2.693059	0.409663	-0.150211
H	-1.910151	1.645374	1.441799
C	-4.056069	0.247805	0.496092
H	-2.788417	0.464978	-1.239080
H	-2.068523	-0.456177	0.086305
H	-3.984743	0.168632	1.580010
H	-4.735330	1.055304	0.234157
Br	-4.943258	-1.398509	-0.098315
Br	5.589955	-0.849597	0.092839
F	-2.782634	2.778510	0.031414
H	-0.256983	2.860458	0.073881

Zero-point correction	=	0.221643
Thermal correction to Energy	=	0.235507
Thermal correction to Enthalpy	=	0.236452
Thermal correction to Gibbs Free Energy	=	0.176354
Sum of electronic and zero-point Energies	=	-5561.894624
Sum of electronic and thermal Energies	=	-5561.88076
Sum of electronic and thermal Enthalpies	=	-5561.879816
Sum of electronic and thermal Free Energies	=	-5561.939913
Number of imaginary frequencies/frequency	=	0

OPT-wB97xD-6-311+Gdp_18dibromooctane3FC4.out

0 1

C	3.850699	-0.737591	-0.216948
C	3.097244	0.571505	-0.095077
H	3.540697	-1.460014	0.536757
H	3.743150	-1.181620	-1.205825
C	1.601383	0.368590	-0.344994
H	3.492726	1.294525	-0.815412
H	3.249607	0.993654	0.903455
C	0.811639	1.665182	-0.166544
H	1.450194	-0.016538	-1.361476
H	1.222989	-0.396771	0.342130
H	0.865374	1.981445	0.880314
H	1.289633	2.457862	-0.752452
C	-0.651549	1.577043	-0.602752
C	-1.478505	0.549388	0.144204
H	-0.703320	1.321619	-1.667533
C	-2.935869	0.532011	-0.283931
H	-1.044479	-0.450751	0.049513
C	-3.728002	-0.524749	0.462335
H	-3.371452	1.522586	-0.122455
H	-2.962666	0.328706	-1.358500
H	-3.323100	-1.523455	0.304340
H	-3.784062	-0.320218	1.528924
Br	-5.588070	-0.600545	-0.157092
Br	5.785187	-0.506206	0.044808
F	-1.426340	0.846802	1.530815
H	-1.129579	2.555767	-0.486907

Zero-point correction	=	0.221981
Thermal correction to Energy	=	0.235752
Thermal correction to Enthalpy	=	0.236696
Thermal correction to Gibbs Free Energy	=	0.177024
Sum of electronic and zero-point Energies	=	-5561.894285
Sum of electronic and thermal Energies	=	-5561.880514
Sum of electronic and thermal Enthalpies	=	-5561.87957
Sum of electronic and thermal Free Energies	=	-5561.939242
Number of imaginary frequencies/frequency	=	0

OPT-wB97xD-6-311+Gdp_18dibromooctane3FC5.out

0 1

C	3.653052	0.144375	0.354286
C	3.134035	0.748709	-0.937166
H	3.801158	0.900785	1.124399
H	3.007750	-0.641418	0.741304
C	1.816135	1.502872	-0.728715
H	2.996001	-0.039720	-1.684562
H	3.880579	1.442216	-1.334626
C	0.642605	0.624155	-0.298131
H	1.965708	2.298819	0.011552
H	1.562290	2.002438	-1.670514
H	0.524943	-0.200690	-1.012126
H	0.846619	0.170103	0.676227
C	-0.663253	1.410873	-0.216466
C	-1.845187	0.580429	0.237844
H	-0.907540	1.823117	-1.202315
C	-3.152868	1.347257	0.249755
H	-1.930433	-0.329207	-0.364117
C	-4.345838	0.574921	0.777252
H	-3.034562	2.228707	0.891807
H	-3.352647	1.710819	-0.762322
H	-4.154065	0.143931	1.757375
H	-5.231754	1.204349	0.824192
Br	-4.850013	-0.940179	-0.373363
Br	5.407386	-0.709365	0.112231
F	-1.595886	0.128498	1.560581
H	-0.551235	2.261760	0.466184

Zero-point correction	=	0.221559
Thermal correction to Energy	=	0.235281
Thermal correction to Enthalpy	=	0.236225
Thermal correction to Gibbs Free Energy	=	0.17632
Sum of electronic and zero-point Energies	=	-5561.895062
Sum of electronic and thermal Energies	=	-5561.88134
Sum of electronic and thermal Enthalpies	=	-5561.880396
Sum of electronic and thermal Free Energies	=	-5561.940302
Number of imaginary frequencies/frequency	=	0

OPT-wB97xD-6-311+Gdp_18dibromooctane3FC6.out

0 1

C	3.259101	-0.622404	-0.336409
C	2.633005	0.736510	-0.094921
H	2.796022	-1.399297	0.270403
H	3.217515	-0.911756	-1.385657
C	1.148538	0.725415	-0.465229
H	3.156357	1.495337	-0.685450
H	2.745892	1.011007	0.958732
C	0.480038	2.075701	-0.208562
H	1.035746	0.458946	-1.523735
H	0.644732	-0.058134	0.111669

H	0.549803	2.319343	0.856652
H	1.034676	2.856077	-0.741061
C	-0.981660	2.144344	-0.654671
C	-1.906949	1.178807	0.058730
H	-1.050633	1.926070	-1.726925
C	-3.355745	1.308433	-0.367508
H	-1.565748	0.147238	-0.060572
C	-4.316693	0.380191	0.348706
H	-3.688945	2.333529	-0.164851
H	-3.417832	1.157468	-1.448972
H	-4.222795	0.449817	1.430217
H	-5.346467	0.579338	0.060798
Br	-4.015383	-1.515480	-0.088188
Br	5.166319	-0.655671	0.139610
F	-1.840507	1.433612	1.453343
H	-1.364327	3.160815	-0.511936

Zero-point correction	=	0.221719
Thermal correction to Energy	=	0.235432
Thermal correction to Enthalpy	=	0.236376
Thermal correction to Gibbs Free Energy	=	0.176347
Sum of electronic and zero-point Energies	=	-5561.895266
Sum of electronic and thermal Energies	=	-5561.881553
Sum of electronic and thermal Enthalpies	=	-5561.880609
Sum of electronic and thermal Free Energies	=	-5561.940638
Number of imaginary frequencies/frequency	=	0

OPT-wB97xD-6-311+Gdp_18dibromooctane3FC7.out

0 1

C	-4.138387	0.688841	-0.159566
C	-2.645643	0.455618	-0.275526
H	-4.389538	1.319086	0.692571
H	-4.556976	1.125474	-1.065284
C	-1.905215	1.782925	-0.467033
H	-2.439662	-0.206039	-1.123569
H	-2.289107	-0.051701	0.625255
C	-0.409986	1.617558	-0.745152
H	-2.357713	2.327303	-1.303369
H	-2.043453	2.407804	0.423732
H	-0.273425	1.036547	-1.665668
H	0.022295	2.604827	-0.931766
C	0.355845	0.945326	0.393081
C	1.848474	0.866493	0.149696
H	0.002151	-0.081437	0.534140
C	2.604408	0.171335	1.264953
H	2.052605	0.392861	-0.815456
C	4.105352	0.088911	1.069812
H	2.432895	0.722838	2.197463
H	2.183780	-0.828786	1.402051
H	4.544861	1.059189	0.848584
H	4.591545	-0.337714	1.943993
Br	4.620101	-1.080187	-0.427155
Br	-5.129191	-0.986300	0.118748
F	2.363394	2.184139	0.034915
H	0.178249	1.477504	1.335752

Zero-point correction	=	0.221883
Thermal correction to Energy	=	0.235569
Thermal correction to Enthalpy	=	0.236513
Thermal correction to Gibbs Free Energy	=	0.176594
Sum of electronic and zero-point Energies	=	-5561.89492
Sum of electronic and thermal Energies	=	-5561.881234
Sum of electronic and thermal Enthalpies	=	-5561.880289
Sum of electronic and thermal Free Energies	=	-5561.940209
Number of imaginary frequencies/frequency	=	0

OPT-wB97xD-6-311+Gdp_18dibromooctane3FC8.out

0 1

C	-4.274486	0.691305	-0.667837
C	-3.720981	1.569303	0.438344
H	-5.220809	1.074583	-1.044260
H	-3.581639	0.578064	-1.499620
C	-2.389635	1.123046	1.042159
H	-4.470501	1.673208	1.228585
H	-3.597783	2.564125	-0.010283
C	-1.259391	0.990743	0.023611
H	-2.102671	1.855371	1.804581
H	-2.525078	0.169500	1.565009
H	-1.495720	0.200680	-0.698938
H	-1.171399	1.922709	-0.545376
C	0.079530	0.667317	0.681972
C	1.210851	0.490283	-0.308900
H	-0.006363	-0.265061	1.251559
C	2.538328	0.139709	0.340682
H	0.944611	-0.253776	-1.067168
C	3.632337	-0.052422	-0.692912
H	2.812012	0.928156	1.047884
H	2.395377	-0.783685	0.909285
H	3.391654	-0.849278	-1.395009
H	3.844208	0.862823	-1.240640
Br	5.330437	-0.574118	0.140044
Br	-4.669639	-1.145802	-0.072085
F	1.378007	1.705587	-1.024543
H	0.354805	1.453806	1.394002

Zero-point correction	=	0.221797
Thermal correction to Energy	=	0.235527
Thermal correction to Enthalpy	=	0.236471
Thermal correction to Gibbs Free Energy	=	0.17614
Sum of electronic and zero-point Energies	=	-5561.89502
Sum of electronic and thermal Energies	=	-5561.88129
Sum of electronic and thermal Enthalpies	=	-5561.880346
Sum of electronic and thermal Free Energies	=	-5561.940677
Number of imaginary frequencies/frequency	=	0

OPT-wB97xD-6-311+Gdp_18dibromooctane3FC10.out

0 1

C	4.103569	-1.444665	0.141332
C	2.697010	-1.142153	-0.333599
H	4.135445	-1.666852	1.207547
H	4.548270	-2.268878	-0.412528
C	1.964144	-0.070327	0.466683
H	2.147495	-2.089703	-0.255824
H	2.712682	-0.877889	-1.396158
C	0.512180	0.095351	0.024446
H	1.995675	-0.329993	1.532791
H	2.484583	0.887854	0.362947
H	0.484198	0.351491	-1.040557
H	-0.005969	-0.864166	0.132064
C	-0.212674	1.173314	0.827591
C	-1.621508	1.494695	0.363588
H	0.363548	2.104562	0.802423
C	-2.559092	0.301187	0.287269
H	-2.047827	2.270466	1.007139
C	-3.976013	0.727912	-0.046646
H	-2.192311	-0.405994	-0.460969
H	-2.537029	-0.201855	1.258644
H	-4.379427	1.415846	0.695025
H	-4.048483	1.177335	-1.034440
Br	-5.202754	-0.802445	-0.070782
Br	5.349541	0.061981	-0.109584
F	-1.551827	2.080622	-0.927834
H	-0.277642	0.876543	1.881203

Zero-point correction	=	0.22143
Thermal correction to Energy	=	0.235261
Thermal correction to Enthalpy	=	0.236206
Thermal correction to Gibbs Free Energy	=	0.175565
Sum of electronic and zero-point Energies	=	-5561.894573
Sum of electronic and thermal Energies	=	-5561.880742
Sum of electronic and thermal Enthalpies	=	-5561.879798
Sum of electronic and thermal Free Energies	=	-5561.940439
Number of imaginary frequencies/frequency	=	0

OPT-wB97xD-6-311+Gdp_18dibromooctane3FC11.out

0 1

C	3.940124	0.335370	-0.659449
C	3.056103	1.469141	-0.180511
H	3.800184	0.130248	-1.720227
H	4.992488	0.533194	-0.465939
C	1.576000	1.310938	-0.514117
H	3.442643	2.374638	-0.666797
H	3.188416	1.614374	0.896859
C	0.755724	2.531099	-0.098931
H	1.463253	1.144552	-1.593383

H	1.193216	0.414554	-0.017163
H	0.836483	2.673978	0.983811
H	1.187590	3.426201	-0.560635
C	-0.719904	2.460758	-0.495514
C	-1.502438	1.341461	0.162323
H	-0.804675	2.319602	-1.579459
C	-2.972131	1.344798	-0.209211
H	-1.054173	0.367421	-0.050159
C	-3.794014	0.240422	0.425316
H	-3.409319	2.297015	0.114642
H	-3.060667	1.304394	-1.298496
H	-3.650490	0.189343	1.502616
H	-4.852316	0.360950	0.205621
Br	-3.325933	-1.545608	-0.256638
Br	3.572233	-1.374187	0.250689
F	-1.413175	1.491912	1.570803
H	-1.211328	3.411243	-0.259745

Zero-point correction	=	0.222304
Thermal correction to Energy	=	0.235784
Thermal correction to Enthalpy	=	0.236728
Thermal correction to Gibbs Free Energy	=	0.177536
Sum of electronic and zero-point Energies	=	-5561.894537
Sum of electronic and thermal Energies	=	-5561.881057
Sum of electronic and thermal Enthalpies	=	-5561.880113
Sum of electronic and thermal Free Energies	=	-5561.939305
Number of imaginary frequencies/frequency	=	0

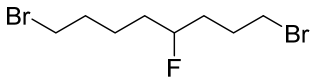
OPT-wB97xD-6-311+Gdp_18dibromooctane3FC12.out

0 1

C	3.952391	-0.576608	0.350633
C	3.119641	0.601859	-0.111976
H	3.938038	-0.687903	1.433925
H	3.632970	-1.509753	-0.111044
C	1.654512	0.424299	0.290821
H	3.513535	1.525645	0.323892
H	3.194825	0.700425	-1.199972
C	0.781838	1.573717	-0.213890
H	1.280078	-0.526742	-0.100001
H	1.578702	0.361491	1.382926
H	1.239058	2.522550	0.088710
H	0.780172	1.571673	-1.311140
C	-0.662802	1.569418	0.289585
C	-1.508385	0.390577	-0.154642
H	-1.159079	2.475230	-0.074372
C	-2.993300	0.590722	0.101845
H	-1.328599	0.159105	-1.210326
C	-3.801980	-0.621790	-0.319488
H	-3.148912	0.804428	1.163731
H	-3.314116	1.468802	-0.465442
H	-3.677560	-0.843048	-1.378542
H	-3.556382	-1.503693	0.267110
Br	-5.724564	-0.332388	-0.058859
Br	5.849570	-0.379592	-0.129541
F	-1.101106	-0.769798	0.555851
H	-0.689464	1.616128	1.384542

Zero-point correction	=	0.221742
Thermal correction to Energy	=	0.235557
Thermal correction to Enthalpy	=	0.236501
Thermal correction to Gibbs Free Energy	=	0.17686
Sum of electronic and zero-point Energies	=	-5561.893336
Sum of electronic and thermal Energies	=	-5561.879521
Sum of electronic and thermal Enthalpies	=	-5561.878577
Sum of electronic and thermal Free Energies	=	-5561.938218
Number of imaginary frequencies/frequency	=	0

	Calculated 19F NMR Shielding Tensor
OPT-wB97xD-6-311+Gdp_18dibromooctane3FC1.out	378.8709
OPT-wB97xD-6-311+Gdp_18dibromooctane3FC2.out	378.8101
OPT-wB97xD-6-311+Gdp_18dibromooctane3FC3.out	366.7975
OPT-wB97xD-6-311+Gdp_18dibromooctane3FC4.out	386.383
OPT-wB97xD-6-311+Gdp_18dibromooctane3FC5.out	384.9724
OPT-wB97xD-6-311+Gdp_18dibromooctane3FC6.out	391.5733
OPT-wB97xD-6-311+Gdp_18dibromooctane3FC7.out	385.8482
OPT-wB97xD-6-311+Gdp_18dibromooctane3FC8.out	379.1623
OPT-wB97xD-6-311+Gdp_18dibromooctane3FC10.out	380.7723
OPT-wB97xD-6-311+Gdp_18dibromooctane3FC11.out	390.4874
OPT-wB97xD-6-311+Gdp_18dibromooctane3FC12.out	371.2837



1,8-dibromo-4-fluorooctane

OPT-wB97xD-6-311+Gdp_18dibromooctane4FC1.out

0 1

C	4.408991	0.641672	-0.346423
C	3.235035	-0.236749	0.037095
H	4.416793	0.872752	-1.410827
H	4.428574	1.569467	0.223737
C	1.909658	0.472002	-0.247492
H	3.279835	-1.177690	-0.520690
H	3.295743	-0.487706	1.100797
C	0.707935	-0.387022	0.139101
H	1.874997	1.417254	0.303294
H	1.847257	0.722723	-1.313325
H	0.728170	-1.326249	-0.425293
H	0.758748	-0.651434	1.201807
C	-0.624968	0.279601	-0.131814
C	-1.823142	-0.579398	0.220655
H	-0.684989	0.613847	-1.173334
C	-3.158581	0.095870	-0.096900
H	-1.736104	-1.515057	-0.342810
H	-1.768057	-0.837155	1.284505
C	-4.313452	-0.815520	0.267559
H	-3.239940	1.034606	0.456236
H	-3.201275	0.339397	-1.163218
H	-4.297086	-1.746650	-0.297668
H	-4.334305	-1.041203	1.332910
Br	-6.053752	0.006307	-0.127686
Br	6.134206	-0.229949	0.010926
F	-0.692568	1.468648	0.642199

Zero-point correction	=	0.221605
Thermal correction to Energy	=	0.23547
Thermal correction to Enthalpy	=	0.236414
Thermal correction to Gibbs Free Energy	=	0.176756
Sum of electronic and zero-point Energies	=	-5561.896008
Sum of electronic and thermal Energies	=	-5561.882143
Sum of electronic and thermal Enthalpies	=	-5561.881199
Sum of electronic and thermal Free Energies	=	-5561.940857
Number of imaginary frequencies/frequency	=	0

OPT-wB97xD-6-311+Gdp_18dibromooctane4FC2.out

0 1

C	-4.268632	-1.349182	0.319534
C	-2.884296	-1.386554	-0.295840
H	-4.910416	-2.130335	-0.082638
H	-4.236025	-1.431734	1.405433
C	-1.893034	-0.394100	0.304095
H	-2.956890	-1.242535	-1.379029
H	-2.513248	-2.408380	-0.141073
C	-0.502271	-0.530579	-0.309499
H	-2.257730	0.625847	0.155414
H	-1.830291	-0.554198	1.387661
H	-0.123231	-1.546633	-0.149883
H	-0.550665	-0.374536	-1.393645
C	0.515336	0.428286	0.273705
C	1.905974	0.269747	-0.304853
H	0.541812	0.342830	1.365656
C	2.926439	1.223484	0.308388
H	2.214593	-0.766694	-0.135148

H	1.856143	0.417503	-1.390085
C	4.309709	1.127542	-0.300766
H	2.598865	2.257114	0.149954
H	2.984314	1.072664	1.391386
H	4.286677	1.226523	-1.385391
H	4.985336	1.871813	0.115291
Br	5.190076	-0.602331	0.045361
Br	-5.230930	0.331171	-0.046523
F	0.076144	1.755496	0.017574

Zero-point correction =	0.221575	
Thermal correction to Energy =	0.235209	
Thermal correction to Enthalpy =	0.236153	
Thermal correction to Gibbs Free Energy =		0.176443
Sum of electronic and zero-point Energies =		-5561.896193
Sum of electronic and thermal Energies =		-5561.882559
Sum of electronic and thermal Enthalpies =		-5561.881615
Sum of electronic and thermal Free Energies =		-5561.941325
Number of imaginary frequencies/frequency =		0

OPT-wB97xD-6-311+Gdp_18dibromooctane4FC3.out

0 1

C	-4.248579	0.549909	0.237006
C	-2.802280	0.536437	-0.215404
H	-4.341585	0.742211	1.304902
H	-4.844324	1.276182	-0.314140
C	-2.141076	1.892446	0.048753
H	-2.267445	-0.257196	0.314098
H	-2.753133	0.304856	-1.284816
C	-0.730496	2.008306	-0.532943
H	-2.755356	2.684690	-0.392779
H	-2.111299	2.084080	1.126085
H	-0.765859	1.839708	-1.615392
H	-0.353181	3.025213	-0.380759
C	0.277846	1.033632	0.044159
C	1.670159	1.187144	-0.534926
H	-0.061412	-0.000463	-0.069344
C	2.671605	0.183791	0.040912
H	1.588237	1.049578	-1.618999
H	2.015398	2.213150	-0.364143
C	4.023057	0.342627	-0.626781
H	2.770534	0.337042	1.118178
H	2.299412	-0.834155	-0.112301
H	3.976060	0.144868	-1.696980
H	4.447196	1.331956	-0.461424
Br	5.349713	-0.920966	0.081372
Br	-5.130273	-1.181292	-0.062239
F	0.350551	1.247952	1.445946

Zero-point correction =	0.221986	
Thermal correction to Energy =	0.23574	
Thermal correction to Enthalpy =	0.236684	
Thermal correction to Gibbs Free Energy =		0.176914
Sum of electronic and zero-point Energies =		-5561.895261
Sum of electronic and thermal Energies =		-5561.881507
Sum of electronic and thermal Enthalpies =		-5561.880563
Sum of electronic and thermal Free Energies =		-5561.940333
Number of imaginary frequencies/frequency =		0

OPT-wB97xD-6-311+Gdp_18dibromooctane4FC4.out

0 1

C	-4.067577	0.274994	0.524676
C	-2.718550	0.075082	-0.136613
H	-4.017760	0.130358	1.603059
H	-4.486200	1.257349	0.311540
C	-1.701351	1.089361	0.389855
H	-2.359938	-0.941387	0.055352
H	-2.818904	0.184374	-1.221092
C	-0.327915	0.903791	-0.251463
H	-2.062963	2.104486	0.198393
H	-1.607811	0.984829	1.477497
H	0.030964	-0.110861	-0.048165
H	-0.398559	1.006334	-1.340880
C	0.714583	1.875754	0.260016
C	2.099145	1.709175	-0.341041
H	0.769848	1.839517	1.353474
C	2.764658	0.388759	0.059739
H	2.026459	1.782693	-1.431586
H	2.712063	2.548785	0.002987
C	4.221937	0.386679	-0.358703
H	2.693569	0.250203	1.143531
H	2.250059	-0.453599	-0.409936
H	4.338006	0.502128	-1.435283
H	4.794025	1.160898	0.150278
Br	5.112444	-1.305470	0.089216
Br	-5.406930	-1.014463	-0.113479
F	0.281617	3.192220	-0.048752

Zero-point correction =	0.221848	
Thermal correction to Energy =	0.235681	
Thermal correction to Enthalpy =	0.236625	
Thermal correction to Gibbs Free Energy =		0.176401
Sum of electronic and zero-point Energies =		-5561.895274
Sum of electronic and thermal Energies =		-5561.881441
Sum of electronic and thermal Enthalpies =		-5561.880496
Sum of electronic and thermal Free Energies =		-5561.940721
Number of imaginary frequencies/frequency =		0

OPT-wB97xD-6-311+Gdp_18dibromooctane4FC5.out

0 1

C	3.752732	0.016898	-0.726726
C	2.645181	0.134690	0.301073
H	3.536916	-0.745084	-1.474216
H	3.949069	0.965218	-1.225072
C	1.328225	0.534148	-0.367113
H	2.918275	0.880497	1.054123
H	2.520127	-0.820827	0.820393
C	0.193311	0.676886	0.644614
H	1.461036	1.479272	-0.902990
H	1.053777	-0.219872	-1.114437
H	0.076491	-0.261012	1.199542
H	0.432511	1.455806	1.377562
C	-1.145857	0.990840	0.010401
C	-2.280554	1.112389	1.007863
H	-1.372978	0.247369	-0.760816
C	-3.633740	1.479220	0.398204
H	-2.357089	0.157687	1.538071
H	-2.012033	1.867875	1.752910
C	-4.157646	0.544986	-0.675366
H	-4.373605	1.565969	1.198697
H	-3.564587	2.466376	-0.072775
H	-5.127964	0.872716	-1.042482
H	-3.476767	0.447863	-1.519056
Br	-4.450420	-1.293804	-0.029563
Br	5.463690	-0.515188	0.081544
F	-1.037507	2.223834	-0.689611

Zero-point correction =	0.221959	
Thermal correction to Energy =	0.235656	
Thermal correction to Enthalpy =	0.2366	
Thermal correction to Gibbs Free Energy =		0.176545
Sum of electronic and zero-point Energies =		-5561.896136
Sum of electronic and thermal Energies =		-5561.882438
Sum of electronic and thermal Enthalpies =		-5561.881494
Sum of electronic and thermal Free Energies =		-5561.94155
Number of imaginary frequencies/frequency =		0

OPT-wB97xD-6-311+Gdp_18dibromooctane4FC6.out

0 1

C	-3.625935	0.158420	-0.359887
C	-3.029295	0.457838	1.002600
H	-3.855535	1.069258	-0.912056
H	-2.988500	-0.479968	-0.968268
C	-1.731265	1.266119	0.897447
H	-2.838116	-0.479584	1.535464
H	-3.753374	1.023979	1.595236
C	-0.583974	0.510862	0.227134
H	-1.923695	2.201361	0.361794
H	-1.425543	1.545939	1.911614
H	-0.441244	-0.454335	0.727111
H	-0.810435	0.296099	-0.823118
C	0.736903	1.249807	0.285225
C	1.895623	0.483840	-0.317693
H	0.966553	1.543551	1.315433
C	3.222967	1.230471	-0.228989
H	1.967449	-0.469298	0.216372

H	1.664002	0.250054	-1.363501
C	4.395535	0.485107	-0.832752
H	3.146702	2.175025	-0.779214
H	3.442783	1.489241	0.811917
H	4.186366	0.139911	-1.844644
H	5.298697	1.091511	-0.838297
Br	4.879963	-1.134892	0.181132
Br	-5.327182	-0.815540	-0.214441
F	0.592580	2.474175	-0.424281

Zero-point correction	=	0.221973
Thermal correction to Energy	=	0.235623
Thermal correction to Enthalpy	=	0.236567
Thermal correction to Gibbs Free Energy	=	0.176787
Sum of electronic and zero-point Energies	=	-5561.895446
Sum of electronic and thermal Energies	=	-5561.881796
Sum of electronic and thermal Enthalpies	=	-5561.880851
Sum of electronic and thermal Free Energies	=	-5561.940632
Number of imaginary frequencies/frequency	=	0

OPT-wB97xD-6-311+Gdp_18dibromooctane4FC7.out

0 1

C	-3.875178	-0.303519	0.419722
C	-3.386193	1.034966	-0.101236
H	-3.326504	-1.144260	0.000006
H	-3.837203	-0.354637	1.507455
C	-1.962488	1.352102	0.369215
H	-4.058158	1.824583	0.245948
H	-3.422286	1.039510	-1.195669
C	-0.909299	0.366360	-0.135503
H	-1.709986	2.357385	0.020670
H	-1.936627	1.384351	1.465398
H	-1.071610	-0.624203	0.302910
H	-0.989113	0.252099	-1.223413
C	0.509237	0.772889	0.208763
C	1.556750	-0.221954	-0.249895
H	0.606270	0.963842	1.283065
C	2.982179	0.192762	0.120420
H	1.318968	-1.186152	0.212982
H	1.465900	-0.353196	-1.334143
C	3.975239	-0.847743	-0.356940
H	3.213356	1.160093	-0.331837
H	3.061009	0.310945	1.205742
H	3.808284	-1.818247	0.108550
H	3.959134	-0.960960	-1.440077
Br	5.825203	-0.365456	0.093109
Br	-5.752302	-0.637410	-0.057279
F	0.780619	2.019329	-0.414321

Zero-point correction	=	0.221411
Thermal correction to Energy	=	0.235412
Thermal correction to Enthalpy	=	0.236356
Thermal correction to Gibbs Free Energy	=	0.175316
Sum of electronic and zero-point Energies	=	-5561.895257
Sum of electronic and thermal Energies	=	-5561.881257
Sum of electronic and thermal Enthalpies	=	-5561.880313
Sum of electronic and thermal Free Energies	=	-5561.941353
Number of imaginary frequencies/frequency	=	0

OPT-wB97xD-6-311+Gdp_18dibromooctane4FC8.out

0 1

C	-4.450456	0.331686	0.661416
C	-3.477997	1.339393	0.082282
H	-4.292352	0.174032	1.727709
H	-5.484244	0.623291	0.488700
C	-2.010527	1.051970	0.385686
H	-3.632725	1.424805	-0.998375
H	-3.754009	2.309893	0.514351
C	-1.084232	2.093592	-0.240221
H	-1.863446	1.029617	1.472850
H	-1.754543	0.056178	0.012406
H	-1.146999	2.039250	-1.333075
H	-1.408010	3.098010	0.053059
C	0.366936	1.937002	0.173191
C	1.023421	0.646514	-0.275176
H	0.473876	2.061992	1.256045
C	2.504741	0.565305	0.099714
H	0.481392	-0.181636	0.193726
H	0.895875	0.541926	-1.358907
C	3.083908	-0.769268	-0.326229
H	3.053035	1.377910	-0.382386
H	2.618522	0.690631	1.181089
H	2.602173	-1.606542	0.177299
H	3.023925	-0.915458	-1.403863
Br	4.991850	-0.919899	0.118260
Br	-4.286337	-1.454096	-0.157599
F	1.084423	3.020975	-0.398634

Zero-point correction	=	0.22189
Thermal correction to Energy	=	0.235559
Thermal correction to Enthalpy	=	0.236503
Thermal correction to Gibbs Free Energy	=	0.1771
Sum of electronic and zero-point Energies	=	-5561.895255
Sum of electronic and thermal Energies	=	-5561.881587
Sum of electronic and thermal Enthalpies	=	-5561.880642
Sum of electronic and thermal Free Energies	=	-5561.940046
Number of imaginary frequencies/frequency	=	0

OPT-wB97xD-6-311+Gdp_18dibromooctane4FC9.out

0 1

C	-4.166526	0.700988	-0.078085
C	-2.877716	-0.055523	0.173041
H	-4.373332	1.430808	0.703372
H	-4.165351	1.200705	-1.045607
C	-1.679286	0.895055	0.195940
H	-2.943858	-0.589524	1.126356
H	-2.735608	-0.807213	-0.610086
C	-0.364790	0.146366	0.405102
H	-1.633892	1.450861	-0.746099
H	-1.810316	1.634691	0.995104
H	-0.408169	-0.424492	1.340417
H	-0.221364	-0.576604	-0.404685
C	0.843587	1.057293	0.489450
C	2.166339	0.370439	0.782452
H	0.671439	1.837955	1.237021
C	2.555948	-0.718837	-0.213726
H	2.941408	1.141629	0.812336
H	2.101755	-0.052627	1.791679
C	3.892982	-1.372377	0.073468
H	1.821084	-1.532031	-0.185749
H	2.549193	-0.321381	-1.232462
H	3.960232	-1.741071	1.096546
H	4.093789	-2.188098	-0.618011
Br	5.420901	-0.146297	-0.136807
Br	-5.728912	-0.492074	-0.106484
F	0.967794	1.748773	-0.745645

Zero-point correction	=	0.222067
Thermal correction to Energy	=	0.235742
Thermal correction to Enthalpy	=	0.236686
Thermal correction to Gibbs Free Energy	=	0.177242
Sum of electronic and zero-point Energies	=	-5561.894563
Sum of electronic and thermal Energies	=	-5561.880887
Sum of electronic and thermal Enthalpies	=	-5561.879943
Sum of electronic and thermal Free Energies	=	-5561.939387
Number of imaginary frequencies/frequency	=	0

OPT-wB97xD-6-311+Gdp_18dibromooctane4FC10.out

0 1

C	3.719150	-0.098299	1.157009
C	3.424927	1.336878	0.763597
H	4.601497	-0.160218	1.790768
H	2.884532	-0.577132	1.666205
C	2.203039	1.557004	-0.127133
H	4.309019	1.769245	0.285988
H	3.284471	1.878517	1.708415
C	0.898223	1.042841	0.477924
H	2.113141	2.630057	-0.316660
H	2.364649	1.080329	-1.100211
H	0.928094	-0.047335	0.582471
H	0.756502	1.457354	1.483683
C	-0.322078	1.369838	-0.358340
C	-1.618792	0.840599	0.218253
H	-0.185777	1.019127	-1.387186
C	-2.833925	1.142845	-0.652977
H	-1.505684	-0.241085	0.340654

H	-1.758483	1.265104	1.219607
C	-4.154910	0.710090	-0.051560
H	-2.913777	2.225457	-0.803619
H	-2.710357	0.693939	-1.643899
H	-4.298732	1.110997	0.951130
H	-4.995168	0.999162	-0.679222
Br	-4.316224	-1.244858	0.142483
Br	4.118743	-1.257215	-0.385704
F	-0.428432	2.784253	-0.460670

Zero-point correction = 0.222274
Thermal correction to Energy = 0.235691
Thermal correction to Enthalpy = 0.236635
Thermal correction to Gibbs Free Energy = 0.177547
Sum of electronic and zero-point Energies = -5561.895834
Sum of electronic and thermal Energies = -5561.882418
Sum of electronic and thermal Enthalpies = -5561.881474
Sum of electronic and thermal Free Energies = -5561.940561
Number of imaginary frequencies/frequency = 0

OPT-wB97xD-6-311+Gdp_18dibromooctane4FC11.out

0 1

C	4.100337	-0.090475	1.236232
C	2.615782	-0.387416	1.178654
H	4.298391	0.964178	1.424067
H	4.603103	-0.692686	1.990223
C	1.824792	0.492848	0.216258
H	2.456710	-1.446026	0.946939
H	2.241018	-0.232127	2.198990
C	0.322707	0.232337	0.297648
H	2.025760	1.545903	0.440794
H	2.165945	0.317821	-0.809746
H	0.114499	-0.818637	0.063897
H	-0.032728	0.408049	1.318664
C	-0.483500	1.081177	-0.664808
C	-1.968077	0.773899	-0.728609
H	-0.057034	1.014405	-1.670245
C	-2.694251	0.861978	0.611487
H	-2.425469	1.470323	-1.439967
H	-2.077021	-0.227687	-1.157216
C	-4.203221	0.791269	0.499628
H	-2.342398	0.089128	1.300469
H	-2.474107	1.828767	1.079859
H	-4.684210	0.936233	1.464546
H	-4.595207	1.515721	-0.213507
Br	-4.848741	-0.960980	-0.130329
Br	5.038958	-0.502242	-0.447427
F	-0.329138	2.445078	-0.288363

Zero-point correction = 0.222139
Thermal correction to Energy = 0.235676
Thermal correction to Enthalpy = 0.23662
Thermal correction to Gibbs Free Energy = 0.177274
Sum of electronic and zero-point Energies = -5561.895318
Sum of electronic and thermal Energies = -5561.881781
Sum of electronic and thermal Enthalpies = -5561.880837
Sum of electronic and thermal Free Energies = -5561.940183
Number of imaginary frequencies/frequency = 0

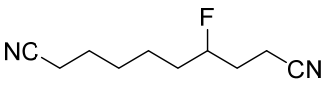
OPT-wB97xD-6-311+Gdp_18dibromooctane4FC12.out

0 1

C	-3.903177	0.344240	0.638894
C	-3.000865	1.432046	0.092643
H	-3.733018	0.166881	1.700179
H	-4.954187	0.573030	0.475144
C	-1.515776	1.232688	0.380166
H	-3.166448	1.547735	-0.983631
H	-3.338778	2.364907	0.562278
C	-0.675548	2.398796	-0.139346
H	-1.367912	1.122919	1.461854
H	-1.182652	0.298013	-0.079768
H	-0.746264	2.454308	-1.231722
H	-1.071108	3.339254	0.259024
C	0.787376	2.313363	0.252718
C	1.548013	1.152546	-0.352783
H	0.892714	2.308168	1.343069
C	3.027344	1.148209	0.020730
H	1.077914	0.229408	-0.000190
H	1.430933	1.177755	-1.442839
C	3.811282	-0.011765	-0.557529
H	3.502484	2.056597	-0.365565
H	3.144122	1.170523	1.109173
H	3.669719	-0.107290	-1.633380
H	4.873503	0.073831	-0.338954
Br	3.277755	-1.754699	0.192763
Br	-3.625098	-1.403095	-0.229351
F	1.406009	3.520668	-0.174119

Zero-point correction = 0.221919
Thermal correction to Energy = 0.235562
Thermal correction to Enthalpy = 0.236506
Thermal correction to Gibbs Free Energy = 0.176648
Sum of electronic and zero-point Energies = -5561.895743
Sum of electronic and thermal Energies = -5561.8821
Sum of electronic and thermal Enthalpies = -5561.881156
Sum of electronic and thermal Free Energies = -5561.941014
Number of imaginary frequencies/frequency = 0

	Calculated 19F NMR Shielding Tensor
OPT-wB97xD-6-311+Gdp_18dibromooctane4FC1.out	378.4044
OPT-wB97xD-6-311+Gdp_18dibromooctane4FC2.out	378.5977
OPT-wB97xD-6-311+Gdp_18dibromooctane4FC3.out	384.5066
OPT-wB97xD-6-311+Gdp_18dibromooctane4FC4.out	365.735
OPT-wB97xD-6-311+Gdp_18dibromooctane4FC5.out	386.249
OPT-wB97xD-6-311+Gdp_18dibromooctane4FC6.out	378.0946
OPT-wB97xD-6-311+Gdp_18dibromooctane4FC7.out	380.0917
OPT-wB97xD-6-311+Gdp_18dibromooctane4FC8.out	366.247
OPT-wB97xD-6-311+Gdp_18dibromooctane4FC9.out	382.108
OPT-wB97xD-6-311+Gdp_18dibromooctane4FC10.out	379.5742
OPT-wB97xD-6-311+Gdp_18dibromooctane4FC11.out	380.1517
OPT-wB97xD-6-311+Gdp_18dibromooctane4FC12.out	366.2091



4-fluorodecanedinitrile

C3 omitted due to presence of 1 imaginary frequency

OPT-wB97xD-6-311+Gdp_18diCNoctane3FC_1.out

0 1

C	-4.558417	-0.725380	0.244429
C	-3.341569	0.129501	-0.136257
H	-4.546296	-1.677064	-0.295121
H	-4.547788	-0.957023	1.313557
C	-2.033391	-0.588131	0.181693
H	-3.387635	0.365649	-1.204013
H	-3.385501	1.079748	0.404711
C	-0.807958	0.247443	-0.178656
H	-2.003744	-0.833962	1.250344
H	-1.999932	-1.541597	-0.360105
H	-0.837480	0.495675	-1.246824
H	-0.843670	1.196767	0.365644
C	0.502209	-0.470870	0.134236
C	1.732932	0.341161	-0.210340
H	0.554725	-1.407347	-0.432742
C	3.033990	-0.395548	0.036096
H	1.683301	0.699969	-1.244082
C	4.254086	0.464145	-0.319595

H	3.030679	-1.302536	-0.574546
H	3.084467	-0.702804	1.084627
H	4.208916	0.785258	-1.364347
H	4.286174	1.364183	0.298911
F	1.736955	1.513988	0.588931
H	0.546626	-0.737784	1.196659
C	5.505453	-0.257199	-0.127726
N	6.486198	-0.839709	0.023630
C	-5.821284	-0.061072	-0.054052
N	-6.810731	0.474378	-0.296776

Zero-point correction	=	0.23797
Thermal correction to Energy	=	0.252721
Thermal correction to Enthalpy	=	0.253665
Thermal correction to Gibbs Free Energy	=	0.194043
Sum of electronic and zero-point Energies	=	-599.190792
Sum of electronic and thermal Energies	=	-599.176041
Sum of electronic and thermal Enthalpies	=	-599.175097
Sum of electronic and thermal Free Energies	=	-599.234719
Number of imaginary frequencies/frequency	=	0

OPT-wB97xD-6-311+Gdp_18diCNoctane3FC_2.out

0 1

C	-4.439172	-0.297467	-0.513930
C	-3.135741	0.221485	0.109168
H	-4.434027	-0.149532	-1.597940
H	-4.554914	-1.369873	-0.331482
C	-1.918487	-0.493419	-0.469564
H	-3.054335	1.298371	-0.068328
H	-3.172192	0.076205	1.193133
C	-0.607696	-0.000416	0.137532
H	-2.016013	-1.572567	-0.298183
H	-1.894947	-0.349484	-1.556993
H	-0.506083	1.077460	-0.037665
H	-0.635453	-0.141591	1.222847
C	0.608289	-0.720347	-0.439959
C	1.926436	-0.234271	0.125182
H	0.644014	-0.570135	-1.525197
C	3.132418	-0.929692	-0.475340
H	2.009972	0.852745	0.020307
C	4.474603	-0.452775	0.096346
H	3.050369	-2.005178	-0.295784
H	3.115340	-0.773305	-1.557398
H	4.505645	-0.588894	1.180009
H	5.293935	-1.036441	-0.329750
F	1.938347	-0.476477	1.523458
H	0.527402	-1.800225	-0.268256
C	4.737998	0.953831	-0.189214
N	4.930448	2.063470	-0.425776
C	-5.619059	0.372647	0.019058
N	-6.542071	0.911285	0.446331

Zero-point correction	=	0.238397
Thermal correction to Energy	=	0.253
Thermal correction to Enthalpy	=	0.253945
Thermal correction to Gibbs Free Energy	=	0.194697
Sum of electronic and zero-point Energies	=	-599.19091
Sum of electronic and thermal Energies	=	-599.176306
Sum of electronic and thermal Enthalpies	=	-599.175362
Sum of electronic and thermal Free Energies	=	-599.23461
Number of imaginary frequencies/frequency	=	0

OPT-wB97xD-6-311+Gdp_18diCNoctane3FC_4.out

0 1

C	-4.543428	0.959341	-0.195973
C	-3.141692	1.082834	0.418758
H	-5.256029	1.595130	0.335745
H	-4.536355	1.280175	-1.241957
C	-2.075940	0.291012	-0.332608
H	-2.883160	2.146131	0.418581
H	-3.177964	0.764115	1.465304
C	-0.688459	0.448370	0.283318
H	-2.345639	-0.772101	-0.343105
H	-2.052504	0.618124	-1.379822
H	-0.410550	1.509608	0.293657
H	-0.716662	0.120623	1.327626
C	0.376589	-0.343872	-0.470664
C	1.767227	-0.192866	0.108761
H	0.418429	-0.007260	-1.513021
C	2.825814	-0.966553	-0.651998
H	2.035512	0.866156	0.188981
C	4.239972	-0.818101	-0.074301
H	2.566164	-2.028659	-0.642185
H	2.815118	-0.634928	-1.693815
H	4.262578	-1.111179	0.978026
H	4.935340	-1.468414	-0.610204
F	1.757012	-0.674897	1.443913
H	0.116234	-1.408771	-0.488754
C	4.745653	0.547176	-0.173284
N	5.130978	1.627790	-0.263631
C	-5.057964	-0.405929	-0.154695
N	-5.455300	-1.485382	-0.112676

Zero-point correction	=	0.237807
Thermal correction to Energy	=	0.252499
Thermal correction to Enthalpy	=	0.253443
Thermal correction to Gibbs Free Energy	=	0.19319
Sum of electronic and zero-point Energies	=	-599.191768
Sum of electronic and thermal Energies	=	-599.177076
Sum of electronic and thermal Enthalpies	=	-599.176131
Sum of electronic and thermal Free Energies	=	-599.236384
Number of imaginary frequencies/frequency	=	0

OPT-wB97xD-6-311+Gdp_18diCNoctane3FC_5.out

0 1

C	-3.569805	0.906483	-0.269198
C	-2.838208	-0.416554	-0.002996
H	-3.103569	1.724479	0.287730
H	-3.521260	1.166570	-1.330697
C	-1.371431	-0.333389	-0.414627
H	-2.912865	-0.660669	1.061248
H	-3.335846	-1.221725	-0.552661
C	-0.620175	-1.636767	-0.149135
H	-1.304954	-0.086612	-1.481928
H	-0.897665	0.492597	0.127923
H	-0.640307	-1.859231	0.922869
H	-1.146116	-2.459623	-0.645550
C	0.827256	-1.634432	-0.644492
C	1.726588	-0.618755	0.031643
H	0.847700	-1.421762	-1.719739
C	3.161540	-0.672770	-0.453685
H	1.325390	0.393923	-0.073364
C	4.088482	0.337993	0.235674
H	3.563598	-1.674339	-0.278782
H	3.165216	-0.500514	-1.533532
H	4.087474	0.188450	1.317982
H	5.115629	0.205181	-0.111596
F	1.728333	-0.875235	1.427568
H	1.266543	-2.628628	-0.508231
C	3.705615	1.721298	-0.028189
N	3.388913	2.805452	-0.248759
C	-4.975914	0.852304	0.111642
N	-6.084292	0.792626	0.415959

Zero-point correction	=	0.2383
Thermal correction to Energy	=	0.252983
Thermal correction to Enthalpy	=	0.253927
Thermal correction to Gibbs Free Energy	=	0.193359
Sum of electronic and zero-point Energies	=	-599.190755
Sum of electronic and thermal Energies	=	-599.176072
Sum of electronic and thermal Enthalpies	=	-599.175127
Sum of electronic and thermal Free Energies	=	-599.235696
Number of imaginary frequencies/frequency	=	0

OPT-wB97xD-6-311+Gdp_18diCNoctane3FC_6.out

0 1

C	-4.364792	-0.018674	-0.318135
C	-2.901669	-0.031281	0.146510
H	-4.428794	-0.186035	-1.397399
H	-4.931242	-0.818087	0.168401
C	-2.220121	-1.350792	-0.210207
H	-2.376509	0.809443	-0.315600
H	-2.866819	0.124680	1.229855
C	-0.811744	-1.494124	0.367414
H	-2.834664	-2.180783	0.156422
H	-2.177071	-1.454116	-1.301520

H	-0.861307	-1.456783	1.462792
H	-0.426604	-2.483550	0.104526
C	0.165943	-0.428995	-0.128256
C	1.595492	-0.679488	0.303964
H	-0.120213	0.556882	0.253037
C	2.551739	0.422345	-0.106027
H	1.650146	-0.852547	1.384206
C	3.993203	0.121321	0.324797
H	2.214356	1.351408	0.361279
H	2.504454	0.561039	-1.189912
H	4.048424	-0.038961	1.405544
H	4.362297	-0.785318	-0.160052
F	2.040685	-1.889972	-0.288305
H	0.139096	-0.367988	-1.223012
C	4.901629	1.210072	-0.010917
N	5.609480	2.077037	-0.278052
C	-5.032068	1.243593	-0.023268
N	-5.541963	2.246763	0.218185

Zero-point correction	=	0.238282
Thermal correction to Energy	=	0.252954
Thermal correction to Enthalpy	=	0.253899
Thermal correction to Gibbs Free Energy	=	0.194051
Sum of electronic and zero-point Energies	=	-599.189875
Sum of electronic and thermal Energies	=	-599.175202
Sum of electronic and thermal Enthalpies	=	-599.174258
Sum of electronic and thermal Free Energies	=	-599.234106
Number of imaginary frequencies/frequency	=	0

OPT-wB97xD-6-311+Gdp_18diCNoctane3FC_7.out

0 1

C	3.945464	-0.203293	-0.643833
C	3.459250	0.749704	0.460086
H	3.336429	-1.109849	-0.684417
H	3.877366	0.280211	-1.623258
C	2.045062	1.268522	0.203735
H	3.498975	0.232851	1.424207
H	4.150220	1.594863	0.522033
C	0.960922	0.192564	0.241861
H	1.818828	2.024905	0.963144
H	2.017333	1.784934	-0.763989
H	1.132029	-0.550166	-0.546296
H	1.016577	-0.342006	1.196103
C	-0.436119	0.782771	0.064417
C	-1.539116	-0.254057	0.045329
H	-0.485964	1.329022	-0.884809
C	-2.919512	0.337314	-0.159655
H	-1.334370	-1.022928	-0.707700
C	-4.011296	-0.740625	-0.161698
H	-3.119828	1.071365	0.625935
H	-2.922396	0.866949	-1.116135
H	-3.822715	-1.482841	-0.942835
H	-4.034278	-1.268467	0.794529
F	-1.537495	-0.941321	1.286663
H	-0.646183	1.506896	0.860000
C	-5.334361	-0.174977	-0.392185
N	-6.373183	0.284222	-0.576573
C	5.329653	-0.614195	-0.445654
N	6.424004	-0.927968	-0.276414

Zero-point correction	=	0.238459
Thermal correction to Energy	=	0.253088
Thermal correction to Enthalpy	=	0.254032
Thermal correction to Gibbs Free Energy	=	0.194398
Sum of electronic and zero-point Energies	=	-599.189695
Sum of electronic and thermal Energies	=	-599.175066
Sum of electronic and thermal Enthalpies	=	-599.174121
Sum of electronic and thermal Free Energies	=	-599.233756
Number of imaginary frequencies/frequency	=	0

OPT-wB97xD-6-311+Gdp_18diCNoctane3FC_8.out

0 1

C	-4.414166	-0.082341	-0.741627
C	-2.935307	-0.497098	-0.721477
H	-4.778607	0.003600	-1.768584
H	-5.032991	-0.830031	-0.236436
C	-2.393225	-0.718883	0.689211
H	-2.851100	-1.424809	-1.295766
H	-2.349455	0.259855	-1.250399
C	-0.948040	-1.218442	0.724076
H	-2.467383	0.212737	1.263877
H	-3.031732	-1.449479	1.198675
H	-0.861041	-2.126830	0.117826
H	-0.702052	-1.504769	1.752802
C	0.071368	-0.182871	0.251003
C	1.503554	-0.665301	0.346424
H	-0.017606	0.722000	0.863025
C	2.526218	0.411332	0.045300
H	1.698066	-1.113251	1.326866
C	3.961275	-0.130161	0.092691
H	2.322748	0.847588	-0.936833
H	2.406316	1.202641	0.790325
H	4.168806	-0.592424	1.062291
H	4.111628	-0.893869	-0.673938
F	1.683587	-1.722344	-0.584067
H	-0.116386	0.114853	-0.785864
C	4.947140	0.921121	-0.122461
N	5.714164	1.761657	-0.293422
C	-4.645879	1.200868	-0.085367
N	-4.812610	2.216049	0.430866

Zero-point correction	=	0.238189
Thermal correction to Energy	=	0.25287
Thermal correction to Enthalpy	=	0.253815
Thermal correction to Gibbs Free Energy	=	0.193289
Sum of electronic and zero-point Energies	=	-599.190179
Sum of electronic and thermal Energies	=	-599.175497
Sum of electronic and thermal Enthalpies	=	-599.174553
Sum of electronic and thermal Free Energies	=	-599.235079
Number of imaginary frequencies/frequency	=	0

OPT-wB97xD-6-311+Gdp_18diCNoctane3FC_9.out

0 1

C	4.368635	-0.438176	-0.419591
C	3.030672	0.168908	0.024571
H	4.526148	-1.412204	0.052771
H	4.382370	-0.595060	-1.502193
C	1.855625	-0.727020	-0.355285
H	3.047160	0.322779	1.107912
H	2.911825	1.153907	-0.437679
C	0.514712	-0.148816	0.089894
H	1.847467	-0.876211	-1.442192
H	1.992175	-1.717593	0.095481
H	0.516018	-0.026975	1.178638
H	0.399740	0.852338	-0.340337
C	-0.660712	-1.031559	-0.326042
C	-2.017399	-0.598695	0.197894
H	-0.490978	-2.060230	0.009308
C	-2.393409	0.838690	-0.106177
H	-2.783366	-1.286192	-0.173950
C	-3.822710	1.205047	0.317712
H	-1.708780	1.510295	0.416740
H	-2.268122	1.011010	-1.178946
H	-3.975239	1.002639	1.380847
H	-4.001767	2.270972	0.158785
F	-2.031693	-0.756613	1.609502
H	-0.733027	-1.069207	-1.419352
C	-4.836528	0.469632	-0.431236
N	-5.621556	-0.116685	-1.034806
C	5.503763	0.410445	-0.078460
N	6.388372	1.093616	0.196086

Zero-point correction	=	0.238706
Thermal correction to Energy	=	0.253257
Thermal correction to Enthalpy	=	0.254202
Thermal correction to Gibbs Free Energy	=	0.194933
Sum of electronic and zero-point Energies	=	-599.189999
Sum of electronic and thermal Energies	=	-599.175448
Sum of electronic and thermal Enthalpies	=	-599.174504
Sum of electronic and thermal Free Energies	=	-599.233772
Number of imaginary frequencies/frequency	=	0

OPT-wB97xD-6-311+Gdp_18diCNoctane3FC_10.out

0 1

C	-4.382798	-1.148546	0.403867
C	-2.908742	-1.243507	-0.015424

H	-4.915888	-2.070597	0.157719
H	-4.469268	-1.000262	1.484392
C	-2.077846	-0.033987	0.401641
H	-2.499925	-2.148494	0.443911
H	-2.851164	-1.383083	-1.099650
C	-0.621122	-0.146237	-0.041446
H	-2.511422	0.879115	-0.023108
H	-2.121970	0.077345	1.492045
H	-0.202249	-1.086630	0.333679
H	-0.581366	-0.199316	-1.136702
C	0.222113	1.031621	0.447624
C	1.599142	1.094039	-0.183859
H	0.333998	0.987595	1.536807
C	2.498893	-0.079434	0.147546
H	1.516837	1.218454	-1.268911
C	3.895639	0.079522	-0.468378
H	2.576705	-0.185142	1.233718
H	2.032258	-0.987985	-0.241266
H	3.827540	0.209089	-1.552499
H	4.399914	0.959768	-0.063356
F	2.231457	2.275438	0.281557
H	-0.290394	1.970074	0.212404
C	4.739106	-1.079997	-0.208341
N	5.394337	-2.002555	0.000595
C	-5.083305	-0.047910	-0.251014
N	-5.624794	0.820805	-0.777236

Zero-point correction	=	0.238697
Thermal correction to Energy	=	0.25327
Thermal correction to Enthalpy	=	0.254214
Thermal correction to Gibbs Free Energy	=	0.194751
Sum of electronic and zero-point Energies	=	-599.189935
Sum of electronic and thermal Energies	=	-599.175361
Sum of electronic and thermal Enthalpies	=	-599.174417
Sum of electronic and thermal Free Energies	=	-599.233881
Number of imaginary frequencies/frequency	=	0

OPT-wB97xD-6-311+Gdp_18diCNoctane3FC_11.out

0 1

C	-4.277153	1.295671	0.060783
C	-2.814230	1.162976	-0.386606
H	-4.334151	1.570525	1.118418
H	-4.786637	2.078180	-0.507368
C	-2.022426	0.136756	0.418151
H	-2.783438	0.909268	-1.450914
H	-2.355209	2.150745	-0.280966
C	-0.558761	0.061404	-0.009236
H	-2.081016	0.389178	1.484642
H	-2.481917	-0.852643	0.306148
H	-0.503584	-0.196726	-1.072510
H	-0.102404	1.051653	0.099602
C	0.224291	-0.965835	0.806426
C	1.655608	-1.197260	0.359175
H	-0.290046	-1.932261	0.777458
C	2.514722	0.049955	0.287095
H	2.124590	-1.941751	1.009944
C	3.973468	-0.284361	-0.052612
H	2.109771	0.734447	-0.462221
H	2.465491	0.553676	1.256572
H	4.403523	-0.953587	0.698214
H	4.037564	-0.790010	-1.019291
F	1.639238	-1.789241	-0.930786
H	0.257883	-0.662490	1.859566
C	4.805328	0.910368	-0.118091
N	5.448652	1.863122	-0.167489
C	-5.035064	0.060493	-0.113246
N	-5.624116	-0.918271	-0.254118

Zero-point correction	=	0.238439
Thermal correction to Energy	=	0.253039
Thermal correction to Enthalpy	=	0.253983
Thermal correction to Gibbs Free Energy	=	0.19433
Sum of electronic and zero-point Energies	=	-599.189995
Sum of electronic and thermal Energies	=	-599.175396
Sum of electronic and thermal Enthalpies	=	-599.174451
Sum of electronic and thermal Free Energies	=	-599.234104
Number of imaginary frequencies/frequency	=	0

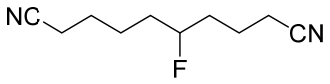
OPT-wB97xD-6-311+Gdp_18diCNoctane3FC_12.out

0 1

C	4.540508	-0.588303	0.165812
C	3.089910	-0.782592	0.630775
H	5.239895	-1.030654	0.879934
H	4.705582	-1.076496	-0.799500
C	2.058605	-0.263619	-0.366385
H	2.942770	-1.854801	0.791351
H	2.954558	-0.292903	1.600394
C	0.624164	-0.483755	0.107140
H	2.220998	0.806922	-0.541532
H	2.205233	-0.763647	-1.331683
H	0.455991	-1.553255	0.275730
H	0.488959	0.014440	1.073732
C	-0.398730	0.040366	-0.899570
C	-1.848436	-0.261467	-0.569653
H	-0.192411	-0.380765	-1.889430
C	-2.307300	0.203554	0.798916
H	-2.492500	0.151799	-1.351765
C	-3.801906	-0.032599	1.059026
H	-1.748048	-0.329341	1.571266
H	-2.075496	1.267662	0.900284
H	-4.056114	-1.086062	0.917146
H	-4.051143	0.227918	2.090432
F	-2.044642	-1.667562	-0.633183
H	-0.305151	1.127927	-0.999111
C	-4.656945	0.760552	0.181835
N	-5.316100	1.395714	-0.515600
C	4.896631	0.819610	0.017647
N	5.163192	1.934120	-0.090379

Zero-point correction	=	0.238937
Thermal correction to Energy	=	0.253369
Thermal correction to Enthalpy	=	0.254313
Thermal correction to Gibbs Free Energy	=	0.195183
Sum of electronic and zero-point Energies	=	-599.190178
Sum of electronic and thermal Energies	=	-599.175746
Sum of electronic and thermal Enthalpies	=	-599.174802
Sum of electronic and thermal Free Energies	=	-599.233931
Number of imaginary frequencies/frequency	=	0

	Calculated 19F NMR Shielding Tensor
OPT-wB97xD-6-311+Gdp_18diCNoctane4FC_1.out	378.8497
OPT-wB97xD-6-311+Gdp_18diCNoctane4FC_2.out	379.4767
OPT-wB97xD-6-311+Gdp_18diCNoctane4FC_4.out	379.3055
OPT-wB97xD-6-311+Gdp_18diCNoctane4FC_5.out	379.4378
OPT-wB97xD-6-311+Gdp_18diCNoctane4FC_6.out	378.852
OPT-wB97xD-6-311+Gdp_18diCNoctane4FC_7.out	378.3463
OPT-wB97xD-6-311+Gdp_18diCNoctane4FC_8.out	378.2275
OPT-wB97xD-6-311+Gdp_18diCNoctane4FC_9.out	378.7216
OPT-wB97xD-6-311+Gdp_18diCNoctane4FC_10.out	380.0504
OPT-wB97xD-6-311+Gdp_18diCNoctane4FC_11.out	365.2879
OPT-wB97xD-6-311+Gdp_18diCNoctane4FC_12.out	380.0286



5-fluorodecanedinitrile

OPT-wB97xD-6-311+Gdp_18diCNoctane4FC_1.out

0 1

C	4.456721	0.545224	-0.321840
C	3.247429	-0.325663	0.045611
H	4.425786	0.821124	-1.380043
H	4.453540	1.473940	0.256304
C	1.935877	0.401493	-0.233546

H	3.287754	-1.258506	-0.525528
H	3.306500	-0.594779	1.104784
C	0.719217	-0.449656	0.119869
H	1.908664	1.335056	0.337556
H	1.889202	0.677585	-1.294094
H	0.732490	-1.375080	-0.467182
H	0.753801	-0.741058	1.176220
C	-0.601080	0.242239	-0.149420
C	-1.815306	-0.608734	0.163061
H	-0.641972	0.607857	-1.181220
C	-3.134544	0.088275	-0.155993
H	-1.733381	-1.531921	-0.421438
C	-4.328732	-0.810833	0.190963
H	-3.210955	1.021920	0.405987
H	-3.171061	0.344983	-1.219234
H	-4.282678	-1.751357	-0.366201
H	-4.324877	-1.062450	1.255568
C	-5.606576	-0.177599	-0.111387
N	-6.608728	0.331758	-0.357473
C	5.725052	-0.129868	-0.075829
N	6.718715	-0.676069	0.121343
F	-0.663328	1.409680	0.657939
H	-1.781117	-0.893534	1.221024

Zero-point correction	=	0.237742
Thermal correction to Energy	=	0.25261
Thermal correction to Enthalpy	=	0.253554
Thermal correction to Gibbs Free Energy	=	0.193209
Sum of electronic and zero-point Energies	=	-599.191558
Sum of electronic and thermal Energies	=	-599.17669
Sum of electronic and thermal Enthalpies	=	-599.175745
Sum of electronic and thermal Free Energies	=	-599.236091
Number of imaginary frequencies/frequency	=	0

OPT-wB97xD-6-311+Gdp_18diCNoctane4FC_2.out

0 1

C	4.310398	-0.208283	0.433482
C	3.007816	0.358419	-0.147743
H	4.288990	-0.181834	1.526995
H	4.443402	-1.252622	0.136402
C	1.796819	-0.442732	0.320532
H	2.903319	1.405735	0.152592
H	3.065210	0.342249	-1.240459
C	0.491045	0.103201	-0.250548
H	1.917238	-1.490528	0.026944
H	1.748623	-0.424570	1.416223
H	0.374063	1.154790	0.034710
H	0.512807	0.070657	-1.346182
C	-0.739204	-0.634339	0.235205
C	-2.040276	-0.078745	-0.306210
H	-0.760833	-0.666344	1.330102
C	-3.272023	-0.805169	0.226241
H	-2.083175	0.981161	-0.031739
C	-4.586877	-0.248757	-0.337458
H	-3.225930	-1.862777	-0.042381
H	-3.295444	-0.750061	1.319122
H	-4.594237	-0.305890	-1.429915
H	-5.438083	-0.830111	0.025389
C	-4.812353	1.144254	0.036338
N	-4.973726	2.242058	0.342157
C	5.486660	0.531636	-0.006923
N	6.406796	1.123276	-0.364521
F	-0.635934	-1.993098	-0.170841
H	-2.016059	-0.126218	-1.401183

Zero-point correction	=	0.237906
Thermal correction to Energy	=	0.252707
Thermal correction to Enthalpy	=	0.253652
Thermal correction to Gibbs Free Energy	=	0.19302
Sum of electronic and zero-point Energies	=	-599.192114
Sum of electronic and thermal Energies	=	-599.177313
Sum of electronic and thermal Enthalpies	=	-599.176369
Sum of electronic and thermal Free Energies	=	-599.237001
Number of imaginary frequencies/frequency	=	0

OPT-wB97xD-6-311+Gdp_18diCNoctane4FC_3.out

0 1

C	4.676222	-0.482560	0.253148
C	3.344717	-1.000344	-0.309773
H	4.669846	-0.511968	1.346807
H	5.508334	-1.104838	-0.085807
C	2.131781	-0.232499	0.206585
H	3.377946	-0.963387	-1.403488
H	3.262588	-2.054460	-0.028401
C	0.821847	-0.782929	-0.350572
H	2.114381	-0.278252	1.300338
H	2.221195	0.826327	-0.063959
H	0.835039	-0.725382	-1.445101
H	0.709523	-1.841266	-0.087080
C	-0.402507	-0.030111	0.128130
C	-1.705127	-0.552048	-0.443490
H	-0.295892	1.041683	-0.070409
C	-2.926248	0.235896	0.021682
H	-1.627580	-0.504067	-1.535457
C	-4.211845	-0.332474	-0.593868
H	-3.002484	0.199646	1.110781
H	-2.821229	1.287550	-0.261781
H	-4.172587	-0.286371	-1.686256
H	-4.340860	-1.382861	-0.316912
C	-5.402884	0.388429	-0.161555
N	-6.336541	0.963594	0.187379
C	4.960471	0.890625	-0.152224
N	5.173663	1.971931	-0.484070
F	-0.467350	-0.139286	1.543256
H	-1.810477	-1.609361	-0.174121

Zero-point correction	=	0.238098
Thermal correction to Energy	=	0.252872
Thermal correction to Enthalpy	=	0.253816
Thermal correction to Gibbs Free Energy	=	0.193401
Sum of electronic and zero-point Energies	=	-599.191502
Sum of electronic and thermal Energies	=	-599.176728
Sum of electronic and thermal Enthalpies	=	-599.175784
Sum of electronic and thermal Free Energies	=	-599.236199
Number of imaginary frequencies/frequency	=	0

OPT-wB97xD-6-311+Gdp_18diCNoctane4FC_4.out

0 1

C	4.483337	-0.042248	-0.652230
C	3.053960	0.250558	-1.130081
H	4.634866	-1.118046	-0.522877
H	5.215331	0.305343	-1.385628
C	1.978410	-0.278589	-0.186062
H	2.934195	1.329501	-1.270920
H	2.942756	-0.214383	-2.114251
C	0.571597	-0.019715	-0.718823
H	2.123541	-1.353671	-0.037567
H	2.084074	0.194429	0.797658
H	0.424327	1.056553	-0.863893
H	0.442014	-0.494686	-1.698553
C	-0.525772	-0.505215	0.205349
C	-1.924441	-0.217731	-0.300541
H	-0.390100	-0.094947	1.211783
C	-3.018045	-0.696733	0.649700
H	-2.003163	0.865645	-0.444965
C	-4.432921	-0.407316	0.129274
H	-2.940112	-1.776530	0.793382
H	-2.890747	-0.229954	1.631276
H	-4.590868	-0.879122	-0.845281
H	-5.184276	-0.809744	0.813204
C	-4.693315	1.021186	-0.021046
N	-4.881475	2.151297	-0.131458
C	4.794681	0.602505	0.619638
N	5.029699	1.116431	1.622356
F	-0.390621	-1.912378	0.357166
H	-2.048762	-0.683289	-1.285217

Zero-point correction	=	0.238811
Thermal correction to Energy	=	0.253336
Thermal correction to Enthalpy	=	0.25428
Thermal correction to Gibbs Free Energy	=	0.194748
Sum of electronic and zero-point Energies	=	-599.191731
Sum of electronic and thermal Energies	=	-599.177206
Sum of electronic and thermal Enthalpies	=	-599.176262
Sum of electronic and thermal Free Energies	=	-599.235794
Number of imaginary frequencies/frequency	=	0

OPT-wB97xD-6-311+Gdp_18diCNoctane4FC_5.out

0 1

C	-4.336716	-0.378602	0.253427
C	-3.044286	0.343908	-0.150946
H	-4.431759	-1.328941	-0.280042
H	-4.333619	-0.604592	1.323747
C	-1.817892	-0.524437	0.113071
H	-3.094455	0.604713	-1.212750
H	-2.966593	1.282491	0.406658
C	-0.518351	0.202546	-0.223625
H	-1.804079	-0.830903	1.163785
H	-1.888170	-1.442909	-0.482580
H	-0.569753	0.594156	-1.246299
H	-0.382927	1.063090	0.441310
C	0.709893	-0.680569	-0.145305
C	2.005884	0.047541	-0.438909
H	0.597333	-1.549207	-0.803608
C	3.226545	-0.868347	-0.428587
H	1.905447	0.518763	-1.423242
C	4.528583	-0.140700	-0.792082
H	3.337610	-1.338960	0.551250
H	3.091618	-1.671313	-1.159527
H	5.362652	-0.845964	-0.829242
H	4.449976	0.326085	-1.778377
C	4.878881	0.904865	0.164251
N	5.146363	1.726982	0.923894
C	-5.527634	0.412323	-0.031911
N	-6.457402	1.050134	-0.262827
F	0.794567	-1.220177	1.165725
H	2.123443	0.854097	0.293618

Zero-point correction = 0.238208
Thermal correction to Energy = 0.252905
Thermal correction to Enthalpy = 0.253849
Thermal correction to Gibbs Free Energy = 0.1939
Sum of electronic and zero-point Energies = -599.191175
Sum of electronic and thermal Energies = -599.176477
Sum of electronic and thermal Enthalpies = -599.175533
Sum of electronic and thermal Free Energies = -599.235482
Number of imaginary frequencies/frequency = 0

OPT-wB97xD-6-311+Gdp_18diCNoctane4FC_6.out

0 1

C	-4.368402	1.075544	-0.284677
C	-2.977301	1.245075	0.343069
H	-5.071196	1.803637	0.128491
H	-4.324704	1.241305	-1.365273
C	-1.926468	0.317491	-0.259155
H	-2.683093	2.288482	0.193796
H	-3.046857	1.083927	1.423492
C	-0.544835	0.540515	0.350175
H	-2.224918	-0.725082	-0.110344
H	-1.875802	0.481206	-1.342660
H	-0.237304	1.581309	0.196949
H	-0.575554	0.371515	1.432837
C	0.529946	-0.342117	-0.250117
C	1.914107	-0.089164	0.311102
H	0.536799	-0.249652	-1.341657
C	2.989350	-0.969075	-0.319591
H	2.145372	0.967874	0.137768
C	4.389553	-0.706366	0.252553
H	2.761246	-2.022240	-0.142082
H	3.007224	-0.820182	-1.403766
H	4.398775	-0.855930	1.336208
H	5.117265	-1.398991	-0.177636
C	4.858834	0.649947	-0.013814
N	5.212712	1.722386	-0.236210
C	-4.932356	-0.252584	-0.062950
N	-5.370869	-1.300512	0.122019
F	0.188333	-1.697297	0.004116
H	1.890281	-0.240206	1.396600

Zero-point correction = 0.238209
Thermal correction to Energy = 0.252885
Thermal correction to Enthalpy = 0.253829
Thermal correction to Gibbs Free Energy = 0.193408
Sum of electronic and zero-point Energies = -599.191807
Sum of electronic and thermal Energies = -599.177131
Sum of electronic and thermal Enthalpies = -599.176187
Sum of electronic and thermal Free Energies = -599.236607
Number of imaginary frequencies/frequency = 0

OPT-wB97xD-6-311+Gdp_18diCNoctane4FC_7.out

0 1

C	-4.638864	-0.630429	0.482520
C	-3.310575	-1.131497	-0.102607
H	-5.455589	-1.307199	0.219091
H	-4.587744	-0.588523	1.574718
C	-2.106286	-0.296632	0.322479
H	-3.181926	-2.165559	0.231554
H	-3.385339	-1.156512	-1.194327
C	-0.801477	-0.832512	-0.260822
H	-2.245421	0.742655	0.008514
H	-2.039201	-0.289129	1.417404
H	-0.670615	-1.882120	0.026894
H	-0.836661	-0.803296	-1.356249
C	0.426930	-0.081117	0.209644
C	1.726583	-0.611402	-0.362077
H	0.467607	-0.061718	1.304398
C	2.958646	0.103695	0.184384
H	1.784253	-1.679858	-0.125754
C	4.242783	-0.457543	-0.440702
H	2.893631	1.174116	-0.024206
H	3.004262	-0.014054	1.271277
H	4.334371	-1.530239	-0.245889
H	4.233739	-0.322061	-1.526179
C	5.441711	0.189998	0.077813
N	6.380608	0.708343	0.495082
C	-5.001994	0.700433	0.005166
N	-5.282676	1.747459	-0.381590
F	0.298429	1.277695	-0.179602
H	1.688506	-0.524325	-1.454055

Zero-point correction = 0.238113
Thermal correction to Energy = 0.252831
Thermal correction to Enthalpy = 0.253775
Thermal correction to Gibbs Free Energy = 0.193887
Sum of electronic and zero-point Energies = -599.190938
Sum of electronic and thermal Energies = -599.17622
Sum of electronic and thermal Enthalpies = -599.175276
Sum of electronic and thermal Free Energies = -599.235164
Number of imaginary frequencies/frequency = 0

OPT-wB97xD-6-311+Gdp_18diCNoctane4FC_8.out

0 1

C	-3.862432	-0.303156	-0.499164
C	-3.365991	0.540581	0.686458
H	-3.801580	0.270731	-1.428920
H	-3.257108	-1.203316	-0.633078
C	-1.958059	1.090962	0.461229
H	-4.057954	1.373736	0.835931
H	-3.393690	-0.065733	1.597846
C	-0.873231	0.016558	0.404163
H	-1.943254	1.678814	-0.462564
H	-1.725932	1.784687	1.276314
H	-0.879202	-0.559357	1.336934
H	-1.059397	-0.692074	-0.410346
C	0.521011	0.581657	0.223360
C	1.613109	-0.468559	0.229570
H	0.726031	1.352434	0.974299
C	3.011308	0.114989	0.048222
H	1.554394	-0.996449	1.188127
C	4.077048	-0.987401	0.112332
H	3.082152	0.630032	-0.912465
H	3.208800	0.855500	0.829287
H	4.037086	-1.510916	1.072040
H	3.910684	-1.731603	-0.672113
C	5.427625	-0.463340	-0.051679
N	6.488605	-0.036596	-0.180086
C	-5.245635	-0.729970	-0.329304
N	-6.338505	-1.059114	-0.181063
F	0.564037	1.259222	-1.024231
H	1.403425	-1.203441	-0.556285

Zero-point correction = 0.238432
Thermal correction to Energy = 0.253078

Thermal correction to Enthalpy	=	0.254022	
Thermal correction to Gibbs Free Energy	=	0.194395	
Sum of electronic and zero-point Energies	=	-599.190194	
Sum of electronic and thermal Energies	=	-599.175549	
Sum of electronic and thermal Enthalpies	=	-599.174605	
Sum of electronic and thermal Free Energies	=	-599.234231	
Number of imaginary frequencies/frequency	=	0	

OPT-wB97xD-6-311+Gdp_18diCNoctane4FC_9.out

0 1

C	3.689582	0.186747	-0.532819
C	3.127570	-0.116295	0.865295
H	3.843493	-0.740590	-1.092838
H	3.003074	0.808667	-1.113130
C	1.820504	-0.906392	0.815096
H	3.872851	-0.686633	1.426152
H	2.973284	0.825327	1.401966
C	0.660590	-0.138324	0.182777
H	1.980732	-1.847604	0.279095
H	1.548818	-1.174717	1.841789
H	0.558474	0.835979	0.675048
H	0.846331	0.058098	-0.879089
C	-0.672058	-0.847439	0.308965
C	-1.838748	-0.061630	-0.252662
H	-0.862396	-1.121980	1.352252
C	-3.179604	-0.771086	-0.088547
H	-1.859357	0.901712	0.269295
C	-4.356564	0.035616	-0.654806
H	-3.161813	-1.728929	-0.613129
H	-3.363094	-0.984498	0.969001
H	-4.202201	0.251476	-1.716107
H	-5.288085	-0.529198	-0.568926
C	-4.546862	1.308257	0.034296
N	-4.680339	2.306324	0.591789
C	4.965499	0.888858	-0.469363
N	5.970957	1.444770	-0.400867
F	-0.588263	-2.082720	-0.389523
H	-1.649517	0.149836	-1.311516

Zero-point correction	=	0.238906	
Thermal correction to Energy	=	0.253454	
Thermal correction to Enthalpy	=	0.254398	
Thermal correction to Gibbs Free Energy	=	0.194733	
Sum of electronic and zero-point Energies	=	-599.190636	
Sum of electronic and thermal Energies	=	-599.176088	
Sum of electronic and thermal Enthalpies	=	-599.175144	
Sum of electronic and thermal Free Energies	=	-599.234809	
Number of imaginary frequencies/frequency	=	0	

OPT-wB97xD-6-311+Gdp_18diCNoctane4FC_10.out

0 1

C	4.267979	0.262279	-0.475975
C	3.345057	-0.689613	0.298585
H	5.316899	0.062576	-0.241868
H	4.141924	0.127251	-1.554354
C	1.869841	-0.516979	-0.051309
H	3.663563	-1.709833	0.064639
H	3.497831	-0.545607	1.373050
C	0.985476	-1.495302	0.719395
H	1.563618	0.512119	0.165363
H	1.733636	-0.669060	-1.127580
H	1.368150	-2.514447	0.597336
H	1.026281	-1.273119	1.792022
C	-0.476317	-1.500552	0.310543
C	-1.172553	-0.154910	0.358573
H	-1.021701	-2.227987	0.919586
C	-2.673041	-0.253530	0.099523
H	-0.993828	0.277727	1.349752
C	-3.331149	1.131280	0.156320
H	-2.854486	-0.700253	-0.881100
H	-3.137019	-0.906645	0.844928
H	-3.171916	1.597619	1.133179
H	-2.897213	1.796635	-0.595826
C	-4.768818	1.073081	-0.078578
N	-5.902951	1.012748	-0.264242
C	4.008187	1.666222	-0.171488
N	3.792816	2.768254	0.081567
F	-0.564657	-1.993629	-1.020175
H	-0.710846	0.516814	-0.372376

Zero-point correction	=	0.238572	
Thermal correction to Energy	=	0.253153	
Thermal correction to Enthalpy	=	0.254097	
Thermal correction to Gibbs Free Energy	=	0.194659	
Sum of electronic and zero-point Energies	=	-599.190806	
Sum of electronic and thermal Energies	=	-599.176225	
Sum of electronic and thermal Enthalpies	=	-599.175281	
Sum of electronic and thermal Free Energies	=	-599.23472	
Number of imaginary frequencies/frequency	=	0	

OPT-wB97xD-6-311+Gdp_18diCNoctane4FC_11.out

0 1

C	3.563104	0.949173	0.303059
C	2.795553	-0.305794	-0.134301
H	3.158558	1.839719	-0.186587
H	3.469023	1.101660	1.382261
C	1.315613	-0.198575	0.220686
H	2.912140	-0.443626	-1.213544
H	3.232057	-1.184336	0.350373
C	0.531984	-1.436328	-0.215310
H	1.212542	-0.062903	1.304348
H	0.898198	0.698555	-0.248907
H	0.518013	-1.511440	-1.308472
H	1.031703	-2.332958	0.165373
C	-0.893958	-1.454225	0.302992
C	-1.807129	-0.401628	-0.289850
H	-0.899713	-1.391931	1.396688
C	-3.212548	-0.425166	0.303857
H	-1.348649	0.576736	-0.109886
C	-4.138771	0.639300	-0.300756
H	-3.679184	-1.396692	0.127264
H	-3.159541	-0.284054	1.387910
H	-4.237495	0.497967	-1.380985
H	-5.139953	0.566428	0.130905
C	-3.654783	1.997515	-0.072587
N	-3.254293	3.059722	0.117469
C	4.984152	0.873233	-0.012547
N	6.104209	0.798989	-0.266353
F	-1.440897	-2.729640	-0.001062
H	-1.848358	-0.542380	-1.376457

Zero-point correction	=	0.238649	
Thermal correction to Energy	=	0.253249	
Thermal correction to Enthalpy	=	0.254193	
Thermal correction to Gibbs Free Energy	=	0.194488	
Sum of electronic and zero-point Energies	=	-599.190991	
Sum of electronic and thermal Energies	=	-599.176392	
Sum of electronic and thermal Enthalpies	=	-599.175448	
Sum of electronic and thermal Free Energies	=	-599.235152	
Number of imaginary frequencies/frequency	=	0	

OPT-wB97xD-6-311+Gdp_18diCNoctane4FC_12.out

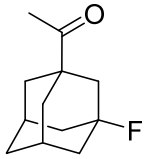
0 1

C	-4.173716	1.105367	0.556361
C	-2.686858	1.230983	0.194624
H	-4.293107	0.685201	1.559377
H	-4.657070	2.085563	0.552787
C	-1.929886	-0.090736	0.274565
H	-2.594961	1.658529	-0.809166
H	-2.246250	1.952095	0.889521
C	-0.459173	0.063912	-0.103333
H	-2.008911	-0.493184	1.290208
H	-2.394808	-0.825206	-0.393986
H	-0.378668	0.405795	-1.141870
H	0.011216	0.830083	0.522246
C	0.327942	-1.225614	0.020922
C	1.729240	-1.196323	-0.561247
H	-0.228533	-2.053906	-0.427830
C	2.619002	-0.070144	-0.040650
H	2.198541	-2.164886	-0.358201
C	4.042228	-0.212834	-0.597173
H	2.216725	0.902228	-0.335903
H	2.654203	-0.091302	1.051680
H	4.492847	-1.153871	-0.269256
H	4.030308	-0.221036	-1.691286
C	4.917221	0.872763	-0.171379

N	5.596355	1.736807	0.169991
C	-4.907196	0.250222	-0.371743
N	-5.473261	-0.423252	-1.113924
F	0.426199	-1.550963	1.401482
H	1.628193	-1.117909	-1.649805

Zero-point correction	=	0.238113
Thermal correction to Energy	=	0.25296
Thermal correction to Enthalpy	=	0.253904
Thermal correction to Gibbs Free Energy	=	0.191424
Sum of electronic and zero-point Energies	=	-599.190943
Sum of electronic and thermal Energies	=	-599.176097
Sum of electronic and thermal Enthalpies	=	-599.175153
Sum of electronic and thermal Free Energies	=	-599.237633
Number of imaginary frequencies/frequency	=	0

	Calculated 19F NMR Shielding Tensor
OPT-wB97xD-6-311+Gdp_18diCNoctane3FC_1.out	380.6212
OPT-wB97xD-6-311+Gdp_18diCNoctane3FC_2.out	383.5863
OPT-wB97xD-6-311+Gdp_18diCNoctane3FC_3.out	380.7001
OPT-wB97xD-6-311+Gdp_18diCNoctane3FC_4.out	383.2081
OPT-wB97xD-6-311+Gdp_18diCNoctane3FC_5.out	389.6546
OPT-wB97xD-6-311+Gdp_18diCNoctane3FC_6.out	382.0414
OPT-wB97xD-6-311+Gdp_18diCNoctane3FC_7.out	380.6922
OPT-wB97xD-6-311+Gdp_18diCNoctane3FC_8.out	379.6953
OPT-wB97xD-6-311+Gdp_18diCNoctane3FC_9.out	384.5465
OPT-wB97xD-6-311+Gdp_18diCNoctane3FC_10.out	368.5254
OPT-wB97xD-6-311+Gdp_18diCNoctane3FC_11.out	382.3124
OPT-wB97xD-6-311+Gdp_18diCNoctane3FC_12.out	385.1057



1-((1r,3s,5R,7S)-3-fluoroadamantan-1-yl)ethan-1-one

OPT-wB97xD-6-311+Gdp_MethylKetoneAdamantaneTerF-C_1.out

0 1

C	0.561954	-0.664201	1.320280
H	0.779789	-0.006962	2.168968
H	1.194104	-1.551819	1.419408
C	0.881958	0.077049	-0.003343
C	-0.916247	-1.080412	1.337812
H	-1.130856	-1.594507	2.278633
C	-1.803795	0.171272	1.229762
H	-1.614033	0.853063	2.064566
H	-2.862917	-0.104055	1.247886
C	-0.025837	1.316329	-0.105288
H	0.176920	1.858034	-1.034063
H	0.166664	1.998073	0.726322
C	-1.480370	0.871639	-0.080798
C	-1.788312	-0.031203	-1.265819
H	-2.846968	-0.308532	-1.251373
H	-1.590353	0.507361	-2.197917
C	0.579310	-0.867491	-1.188242
H	1.206200	-1.762100	-1.132054
H	0.811196	-0.361228	-2.131843
C	-1.203025	-2.014007	0.153266
H	-0.587573	-2.917044	0.229123
H	-2.250857	-2.331905	0.171846
C	-0.899434	-1.281365	-1.161228
H	-1.102992	-1.940402	-2.009266
F	-2.293835	2.032795	-0.180527
C	2.349205	0.498137	0.014211
O	2.670118	1.656388	0.182150
C	3.400835	-0.564470	-0.185432
H	4.357432	-0.207794	0.196625
H	3.135395	-1.510797	0.288944
H	3.504964	-0.753311	-1.259354

Zero-point correction	=	0.273464
Thermal correction to Energy	=	0.28476
Thermal correction to Enthalpy	=	0.285704
Thermal correction to Gibbs Free Energy	=	0.237179
Sum of electronic and zero-point Energies	=	-642.352283
Sum of electronic and thermal Energies	=	-642.340987
Sum of electronic and thermal Enthalpies	=	-642.340043
Sum of electronic and thermal Free Energies	=	-642.388569
Number of imaginary frequencies/frequency	=	0

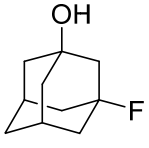
OPT-wB97xD-6-311+Gdp_MethylKetoneAdamantaneTerF-C_2.out

0 1

C	-0.410966	-1.191286	-1.059871
H	-0.668451	-0.884618	-2.079049
H	-0.930423	-2.133613	-0.868406
C	-0.892122	-0.124322	-0.063022
C	1.105888	-1.389427	-0.932325
H	1.433170	-2.141961	-1.654441
C	1.826126	-0.061852	-1.225797
H	1.602458	0.283210	-2.240193
H	2.910237	-0.182480	-1.138141
C	-0.152691	1.203107	-0.349761
H	-0.452526	1.980812	0.357527
H	-0.381297	1.554459	-1.361217
C	1.346423	0.969979	-0.217512
C	1.695689	0.543071	1.200344
H	2.779798	0.424283	1.291194
H	1.378350	1.317946	1.905340
C	-0.537501	-0.587859	1.373404
H	-1.056728	-1.527287	1.589853
H	-0.873565	0.152402	2.106181
C	1.446079	-1.850035	0.491884
H	0.952665	-2.804625	0.702926
H	2.524831	-2.011558	0.590664
C	0.980083	-0.786572	1.495227
H	1.217537	-1.104505	2.513994
F	1.998980	2.203288	-0.487555
C	-2.405279	0.062919	-0.144175
O	-3.109353	-0.748196	-0.708852
C	-3.011736	1.284203	0.501583
H	-4.070369	1.109447	0.693766
H	-2.502455	1.568265	1.424299
H	-2.919187	2.124238	-0.195364

Zero-point correction	=	0.273912
Thermal correction to Energy	=	0.28517
Thermal correction to Enthalpy	=	0.286114
Thermal correction to Gibbs Free Energy	=	0.237565
Sum of electronic and zero-point Energies	=	-642.35194
Sum of electronic and thermal Energies	=	-642.340682
Sum of electronic and thermal Enthalpies	=	-642.339737
Sum of electronic and thermal Free Energies	=	-642.388287
Number of imaginary frequencies/frequency	=	0

	Calculated 19F NMR Shielding Tensor
OPT-wB97xD-6-311+Gdp_MethylKetoneAdamantaneTerF-C_1.out	328.179
OPT-wB97xD-6-311+Gdp_MethylKetoneAdamantaneTerF-C_2.out	326.384



(1r,3s,5R,7S)-3-fluoroadamantan-1-ol

OPT-wB97xD-6-311+Gdp_OHadamantaneTerFC1.out

0 1

C	1.235638	0.328876	-1.251916
H	1.274709	-0.306243	-2.142993
H	2.124455	0.971215	-1.260690
C	1.261752	-0.557920	0.000000
C	-0.038412	1.189021	-1.254349
H	-0.057347	1.811649	-2.152550
C	-1.271279	0.267170	-1.252053
H	-1.275858	-0.374019	-2.139040
H	-2.193490	0.856281	-1.252829
C	0.028837	-1.467650	0.000000
H	0.041083	-2.107650	0.887462
H	0.041083	-2.107650	-0.887463
C	-1.221518	-0.597157	0.000000
C	-1.271279	0.267170	1.252052
H	-2.193490	0.856280	1.252829
H	-1.275858	-0.374020	2.139039
C	1.235637	0.328876	1.251917
H	2.124454	0.971215	1.260691
H	1.274708	-0.306244	2.142994
C	-0.062794	2.075098	0.000000
H	0.800209	2.749720	0.000001
H	-0.962837	2.699449	0.000000
C	-0.038412	1.189020	1.254349
H	-0.057348	1.811648	2.152550
O	2.397350	-1.416304	0.000000
H	3.188024	-0.868896	0.000001
F	-2.353369	-1.454147	-0.000001

Zero-point correction	=	0.240155
Thermal correction to Energy	=	0.249143
Thermal correction to Enthalpy	=	0.250087
Thermal correction to Gibbs Free Energy	=	0.207153
Sum of electronic and zero-point Energies	=	-564.970706
Sum of electronic and thermal Energies	=	-564.961719
Sum of electronic and thermal Enthalpies	=	-564.960774
Sum of electronic and thermal Free Energies	=	-565.003709
Number of imaginary frequencies/frequency	=	0

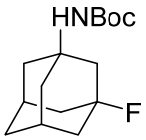
OPT-wB97xD-6-311+Gdp_OHadamantaneTerFC2.out

0 1

C	1.230995	0.365841	-1.254599
H	1.273465	-0.254996	-2.155468
H	2.111908	1.015621	-1.255298
C	1.274695	-0.534897	-0.019987
C	-0.055470	1.206426	-1.237278
H	-0.084864	1.842224	-2.125725
C	-1.279665	0.272918	-1.243602
H	-1.282206	-0.355186	-2.139941
H	-2.207446	0.853083	-1.231516
C	0.046253	-1.461955	-0.027359
H	0.065566	-2.118167	0.850189
H	0.062262	-2.086625	-0.925565
C	-1.215506	-0.608633	-0.004723
C	-1.266577	0.235174	1.260889
H	-2.194934	0.814217	1.276660
H	-1.259654	-0.420302	2.137541
C	1.243132	0.331300	1.245969
H	2.124435	0.980566	1.256966
H	1.292331	-0.313961	2.131779
C	-0.085837	2.074693	0.029399
H	0.768299	2.760074	0.035428
H	-0.994443	2.686387	0.042799
C	-0.044136	1.170751	1.270451
H	-0.065475	1.779683	2.177882
O	2.476218	-1.293116	-0.097658
H	2.540810	-1.840206	0.690802
F	-2.338567	-1.478577	-0.011137

Zero-point correction	=	0.240246
Thermal correction to Energy	=	0.249195
Thermal correction to Enthalpy	=	0.25014
Thermal correction to Gibbs Free Energy	=	0.207292
Sum of electronic and zero-point Energies	=	-564.970751
Sum of electronic and thermal Energies	=	-564.961801
Sum of electronic and thermal Enthalpies	=	-564.960857
Sum of electronic and thermal Free Energies	=	-565.003704
Number of imaginary frequencies/frequency	=	0

	Calculated 19F NMR Shielding Tensor
OPT-wB97xD-6-311+Gdp_OHadamantaneTerFC1.out	329.0816
OPT-wB97xD-6-311+Gdp_OHadamantaneTerFC2.out	327.429



tert-butyl ((1r,3s,5R,7S)-3-fluoroadamantan-1-yl)carbamate

C6 omitted due to presence of 1 imaginary frequency

OPT-wB97xD-6-311+Gdp_NBocadamantaneTerF-C_1.out

0 1

C	1.613411	-1.335928	-1.219600
H	1.356948	-1.047599	-2.246161
H	1.361951	-2.395038	-1.097465
C	0.785777	-0.500139	-0.229308
C	3.113147	-1.117515	-0.971521
H	3.684918	-1.711048	-1.689336
C	3.454150	0.370915	-1.160006
H	3.219851	0.696218	-2.178539
H	4.519904	0.545060	-0.983425
C	1.144513	0.988490	-0.423417
H	0.567438	1.606393	0.268249
H	0.904118	1.293340	-1.447117
C	2.632290	1.176860	-0.165482
C	2.978298	0.785314	1.262897
H	4.041785	0.967923	1.445208
H	2.400135	1.399726	1.959664
C	1.146969	-0.933023	1.202654
H	0.897980	-1.992268	1.326779
H	0.550358	-0.362989	1.916522
C	3.465762	-1.542423	0.460849
H	3.249070	-2.606730	0.600547
H	4.536827	-1.399895	0.639813
C	2.645416	-0.705759	1.451560
H	2.886244	-0.998097	2.476988
F	2.937676	2.553507	-0.341720
N	-0.625429	-0.739141	-0.529943
H	-0.840049	-1.142903	-1.429351
C	-1.664037	-0.137321	0.106204
O	-1.582867	0.497857	1.139387
O	-2.799955	-0.363820	-0.578126
C	-4.102991	0.076827	-0.076814
C	-4.420382	-0.636927	1.232824
C	-4.143199	1.595708	0.065005
C	-5.052805	-0.375955	-1.178713
H	-4.334890	-1.719772	1.105985
H	-3.749830	-0.319564	2.031720
H	-5.447624	-0.408657	1.529767
H	-3.515308	1.941064	0.885272
H	-3.810337	2.073572	-0.860688
H	-5.173348	1.908561	0.257020
H	-6.082098	-0.126159	-0.909468
H	-4.813733	0.121001	-2.122687
H	-4.986718	-1.456758	-1.327095

Zero-point correction	=	0.380721
Thermal correction to Energy	=	0.398072
Thermal correction to Enthalpy	=	0.399016
Thermal correction to Gibbs Free Energy	=	0.336146
Sum of electronic and zero-point Energies	=	-890.796938
Sum of electronic and thermal Energies	=	-890.779587

Sum of electronic and thermal Enthalpies = -890.778643
Sum of electronic and thermal Free Energies = -890.841513
Number of imaginary frequencies/frequency = 0

OPT-wB97xD-6-311+Gdp_NBocadamantaneTerF-C_2.out

0 1

C	1.070441	-0.675528	-1.261277
H	0.857446	-0.076641	-2.153501
H	0.415375	-1.549324	-1.281374
C	0.762457	0.164041	-0.007540
C	2.542723	-1.111793	-1.248397
H	2.750969	-1.703266	-2.143885
C	3.446764	0.133345	-1.246454
H	3.264140	0.742893	-2.137150
H	4.502907	-0.153440	-1.240196
C	1.680668	1.400295	-0.007356
H	1.481933	2.013052	0.878317
H	1.490672	2.006899	-0.899162
C	3.133426	0.945205	0.001046
C	3.435051	0.141587	1.256706
H	4.491209	-0.145121	1.262523
H	3.243758	0.756971	2.141569
C	1.058806	-0.667076	1.254688
H	0.403573	-1.540611	1.274856
H	0.837739	-0.062026	2.140802
C	2.822459	-1.947807	0.008952
H	2.193320	-2.844029	0.008978
H	3.866187	-2.280008	0.014958
C	2.531061	-1.103473	1.258147
H	2.730730	-1.689046	2.159449
F	3.948812	2.108112	0.001028
N	-0.609169	0.666550	-0.015744
H	-0.748773	1.664695	-0.024926
C	-1.730713	-0.093117	-0.014304
O	-1.761589	-1.308839	-0.001603
O	-2.808960	0.713686	-0.029876
C	-4.173207	0.188742	0.002721
C	-4.448195	-0.656121	-1.237111
C	-4.410036	-0.583796	1.296268
C	-5.016719	1.458018	-0.020650
H	-5.514892	-0.892993	-1.281679
H	-4.185961	-0.100406	-2.141879
H	-3.885139	-1.589036	-1.219894
H	-4.133285	0.027174	2.160230
H	-5.472447	-0.828527	1.380793
H	-3.837192	-1.510701	1.320731
H	-6.078479	1.201082	0.008598
H	-4.789333	2.088011	0.843198
H	-4.825108	2.031640	-0.931206

Zero-point correction = 0.379706
Thermal correction to Energy = 0.3973
Thermal correction to Enthalpy = 0.398244
Thermal correction to Gibbs Free Energy = 0.334594
Sum of electronic and zero-point Energies = -890.797902
Sum of electronic and thermal Energies = -890.780308
Sum of electronic and thermal Enthalpies = -890.779364
Sum of electronic and thermal Free Energies = -890.843014
Number of imaginary frequencies/frequency = 0

OPT-wB97xD-6-311+Gdp_NBocadamantaneTerF-C_3.out

0 1

C	1.899097	-1.750020	-0.498044
H	1.867975	-1.995918	-1.565603
H	1.824521	-2.688000	0.063551
C	0.697536	-0.852946	-0.149699
C	3.214661	-1.038155	-0.157548
H	4.051788	-1.689573	-0.420640
C	3.315176	0.267238	-0.965239
H	3.297885	0.060341	-2.039850
H	4.247092	0.792073	-0.734001
C	0.819072	0.454014	-0.961764
H	-0.018181	1.116604	-0.737698
H	0.804435	0.224222	-2.031791
C	2.127106	1.142481	-0.597614
C	2.153066	1.494088	0.882648
H	3.080441	2.026843	1.114950
H	1.311974	2.154326	1.116410
C	0.746719	-0.530591	1.355528
H	0.669606	-1.466310	1.919020
H	-0.106990	0.094132	1.625400
C	3.250372	-0.714670	1.342511
H	3.201673	-1.640819	1.924901
H	4.192155	-0.216737	1.596254
C	2.060330	0.188763	1.693366
H	2.075632	0.427668	2.759849
F	2.207519	2.346889	-1.347617
N	-0.504071	-1.605690	-0.514150
H	-0.368808	-2.531171	-0.891037
C	-1.812492	-1.251756	-0.433765
O	-2.716415	-1.989847	-0.786459
O	-1.967739	-0.022529	0.069650
C	-3.282853	0.604471	0.207367
C	-4.144126	-0.188505	1.183330
C	-2.939335	1.971250	0.786764
C	-3.939007	0.756297	-1.160417
H	-5.064614	0.366363	1.384791
H	-4.408217	-1.165064	0.778609
H	-3.616310	-0.327073	2.131095
H	-2.432618	1.867373	1.749695
H	-2.290122	2.529557	0.107271
H	-3.855196	2.547592	0.939737
H	-4.849904	1.352081	-1.057107
H	-3.267415	1.276924	-1.848753
H	-4.204673	-0.210355	-1.587523

Zero-point correction = 0.380368
Thermal correction to Energy = 0.397853
Thermal correction to Enthalpy = 0.398797
Thermal correction to Gibbs Free Energy = 0.335629
Sum of electronic and zero-point Energies = -890.797073
Sum of electronic and thermal Energies = -890.779588
Sum of electronic and thermal Enthalpies = -890.778644
Sum of electronic and thermal Free Energies = -890.841812
Number of imaginary frequencies/frequency = 0

OPT-wB97xD-6-311+Gdp_NBocadamantaneTerF-C_4.out

0 1

C	0.634286	0.302909	1.254093
H	0.637238	-0.347004	2.135956
H	-0.281803	0.895862	1.279879
C	0.644401	-0.573237	-0.013206
C	1.862020	1.225827	1.261552
H	1.842805	1.842949	2.163735
C	3.144536	0.376160	1.258793
H	3.180860	-0.270335	2.141178
H	4.033237	1.014729	1.266600
C	1.939239	-1.409354	-0.013488
H	1.974772	-2.041845	-0.906891
H	1.966009	-2.057008	0.869441
C	3.143755	-0.478116	0.000778
C	3.157778	0.395668	-1.243631
H	4.046209	1.034574	-1.232013
H	3.203737	-0.236790	-2.135687
C	0.646971	0.322597	-1.266348
H	-0.268327	0.916431	-1.291828
H	0.658534	-0.313078	-2.158409
C	1.838220	2.121242	0.013968
H	0.931170	2.735392	0.014003
H	2.694547	2.804313	0.023453
C	1.874908	1.244835	-1.246694
H	1.864984	1.875994	-2.139245
F	4.312087	-1.284876	0.000875
N	-0.458618	-1.538218	-0.026345
H	-0.216632	-2.516642	0.002836
C	-1.799055	-1.322641	-0.013343
O	-2.612506	-2.230205	0.016429
O	-2.094674	-0.018847	-0.042421
C	-3.471197	0.474043	0.000938
C	-3.278808	1.985239	-0.046422
C	-4.244393	-0.004547	-1.222614
C	-4.135571	0.060078	1.308984
H	-2.685938	2.326695	0.806217
H	-2.769617	2.281665	-0.967131
H	-4.249883	2.485076	-0.012621
H	-5.214640	0.498712	-1.254557
H	-3.701072	0.245911	-2.138223

H	-4.409907	-1.081211	-1.192884
H	-5.102282	0.563201	1.397966
H	-4.299873	-1.016384	1.351696
H	-3.517674	0.358392	2.160849

Zero-point correction = 0.380663
Thermal correction to Energy = 0.397971
Thermal correction to Enthalpy = 0.398915
Thermal correction to Gibbs Free Energy = 0.336261
Sum of electronic and zero-point Energies = -890.796349
Sum of electronic and thermal Energies = -890.779041
Sum of electronic and thermal Enthalpies = -890.778097
Sum of electronic and thermal Free Energies = -890.840751
Number of imaginary frequencies/frequency = 0

OPT-wB97xD-6-311+Gdp_NBocadamantaneTerF-C_5.out

0 1

C	-1.001218	1.469497	-0.729850
H	-0.535299	1.351517	-1.715137
H	-0.646158	2.414829	-0.303097
C	-0.568673	0.306975	0.179834
C	-2.529689	1.495622	-0.863732
H	-2.819546	2.322137	-1.517321
C	-3.009150	0.169936	-1.480244
H	-2.571184	0.023469	-2.472609
H	-4.098413	0.165926	-1.584695
C	-1.060218	-1.014217	-0.444152
H	-0.764523	-1.857776	0.182192
H	-0.614456	-1.142799	-1.435514
C	-2.577838	-0.964435	-0.562731
C	-3.216580	-0.819277	0.810124
H	-4.306273	-0.829425	0.709255
H	-2.922956	-1.664275	1.440193
C	-1.213238	0.492165	1.565333
H	-0.860636	1.434657	1.997826
H	-0.895821	-0.317716	2.225621
C	-3.165507	1.673420	0.522396
H	-2.845053	2.623587	0.962626
H	-4.256342	1.706267	0.430830
C	-2.742525	0.508540	1.427728
H	-3.192383	0.622926	2.417157
F	-3.009424	-2.190964	-1.134027
N	0.892884	0.343003	0.244872
H	1.332200	1.172761	-0.116172
C	1.671771	-0.534147	0.919615
O	1.252292	-1.460707	1.583999
O	3.005906	-0.314160	0.873865
C	3.771189	0.101859	-0.305400
C	3.343672	-0.708911	-1.523421
C	3.662330	1.608577	-0.546912
C	5.199979	-0.246305	0.095796
H	2.314833	-0.492946	-1.818295
H	3.993998	-0.461773	-2.366603
H	3.433246	-1.779372	-1.322377
H	4.484447	1.927646	-1.192648
H	2.741165	1.901940	-1.058053
H	3.741176	2.154453	0.396494
H	5.497401	0.318247	0.983313
H	5.285884	-1.312347	0.317081
H	5.887905	-0.001135	-0.717138

Zero-point correction = 0.380459
Thermal correction to Energy = 0.397847
Thermal correction to Enthalpy = 0.398792
Thermal correction to Gibbs Free Energy = 0.336141
Sum of electronic and zero-point Energies = -890.787603
Sum of electronic and thermal Energies = -890.770214
Sum of electronic and thermal Enthalpies = -890.76927
Sum of electronic and thermal Free Energies = -890.831921
Number of imaginary frequencies/frequency = 0

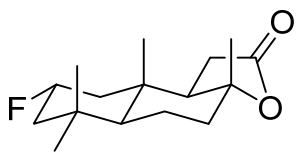
OPT-wB97xD-6-311+Gdp_NBocadamantaneTerF-C_7.out

0 1

C	0.955990	1.456098	0.688945
H	0.539246	1.364539	1.698794
H	0.525487	2.353286	0.229092
C	0.558921	0.221595	-0.137913
C	2.483675	1.581980	0.754084
H	2.746803	2.459887	1.349755
C	3.071110	0.323618	1.416365
H	2.685202	0.205265	2.433794
H	4.161798	0.392368	1.471867
C	1.158615	-1.030540	0.531990
H	0.890852	-1.924222	-0.034131
H	0.762381	-1.130338	1.547428
C	2.673879	-0.882844	0.578574
C	3.244770	-0.773470	-0.827699
H	4.336151	-0.710500	-0.775249
H	2.980150	-1.668253	-1.399242
C	1.131860	0.368615	-1.558753
H	0.702244	1.261838	-2.024817
H	0.840081	-0.495763	-2.159104
C	3.048251	1.722604	-0.666438
H	2.650348	2.626965	-1.138920
H	4.137663	1.827469	-0.627085
C	2.661645	0.486820	-1.491036
H	3.061315	0.575301	-2.504317
F	3.204794	-2.048378	1.192399
N	-0.904053	0.172494	-0.137058
H	-1.366565	0.979239	0.242585
C	-1.657713	-0.778174	-0.736432
O	-1.203710	-1.722370	-1.353832
O	-2.999359	-0.658162	-0.661338
C	-3.793067	0.155053	0.262250
C	-3.443963	-0.176548	1.710149
C	-3.672213	1.649269	-0.048604
C	-5.212039	-0.308842	-0.050768
H	-2.424426	0.107949	1.976633
H	-4.126038	0.361883	2.373427
H	-3.562176	-1.247486	1.891871
H	-4.522921	2.172002	0.395428
H	-2.775648	2.121374	0.362608
H	-3.694708	1.817756	-1.127820
H	-5.465996	-0.087937	-1.090420
H	-5.304612	-1.385224	0.109060
H	-5.925177	0.203406	0.599654

Zero-point correction = 0.381011
Thermal correction to Energy = 0.398315
Thermal correction to Enthalpy = 0.39926
Thermal correction to Gibbs Free Energy = 0.337061
Sum of electronic and zero-point Energies = -890.786975
Sum of electronic and thermal Energies = -890.76967
Sum of electronic and thermal Enthalpies = -890.768726
Sum of electronic and thermal Free Energies = -890.830924
Number of imaginary frequencies/frequency = 0

	Calculated 19F NMR Shielding Tensor
OPT-wB97xD-6-311+Gdp_NBocadamantaneTerF-C_1.out	328.1366
OPT-wB97xD-6-311+Gdp_NBocadamantaneTerF-C_2.out	326.6604
OPT-wB97xD-6-311+Gdp_NBocadamantaneTerF-C_3.out	327.4076
OPT-wB97xD-6-311+Gdp_NBocadamantaneTerF-C_4.out	327.0034
OPT-wB97xD-6-311+Gdp_NBocadamantaneTerF-C_5.out	328.2686
OPT-wB97xD-6-311+Gdp_NBocadamantaneTerF-C_7.out	328.2789



2F(eq)-Sclareolide

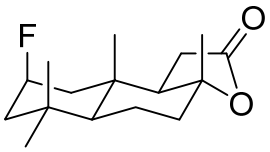
OPT-wB97xD-6-311+Gdp-2FeqSclareolide.out

0 1

C	-0.144125	-2.075232	-0.218518

C	-0.901309	-0.747026	-0.393420
C	-0.211592	0.430066	0.375828
C	1.219932	0.429686	-0.182825
C	2.021929	-0.863272	0.028649
C	1.319933	-1.997382	-0.696398
H	-0.774196	-0.478309	-1.452850
H	-0.176949	-2.403018	0.825740
H	-0.641912	-2.857405	-0.794843
H	1.091735	0.480123	-1.272066
H	1.343994	-1.799337	-1.772991
H	1.827220	-2.950444	-0.520407
C	-0.892074	1.747006	-0.044449
C	-2.444047	-0.842162	-0.230437
C	-3.038217	0.539837	-0.585436
C	-2.392006	1.687039	0.160631
H	-0.475300	2.586797	0.520847
H	-0.703761	1.935203	-1.108197
H	-2.649990	1.661735	1.221401
H	-2.896243	0.717959	-1.658532
H	-4.116002	0.539511	-0.393072
C	2.261527	1.494379	0.126491
H	2.099836	2.453873	-0.363534
H	2.414915	1.675963	1.194848
C	3.503041	0.828517	-0.446139
O	4.544888	1.343668	-0.754668
O	3.288764	-0.491760	-0.612339
C	-2.910619	-1.296157	1.161105
H	-3.990248	-1.477435	1.143676
H	-2.426817	-2.233072	1.451914
H	-2.716852	-0.562642	1.943711
C	-3.006563	-1.841933	-1.253910
H	-4.095246	-1.744908	-1.313696
H	-2.598288	-1.661685	-2.253826
H	-2.788059	-2.877097	-0.979020
C	-0.232546	0.318530	1.913564
H	-1.119787	0.781756	2.345434
H	-0.210365	-0.712828	2.263719
H	0.628297	0.834697	2.346726
C	2.402380	-1.260853	1.453316
H	1.573337	-1.721975	1.986059
H	3.210051	-1.994688	1.392068
H	2.761203	-0.413700	2.041808
F	-2.952628	2.899935	-0.318576

Zero-point correction	=	0.392915
Thermal correction to Energy	=	0.410135
Thermal correction to Enthalpy	=	0.411079
Thermal correction to Gibbs Free Energy	=	0.350888
Sum of electronic and zero-point Energies	=	-874.709462
Sum of electronic and thermal Energies	=	-874.692242
Sum of electronic and thermal Enthalpies	=	-874.691298
Sum of electronic and thermal Free Energies	=	-874.751489
Number of imaginary frequencies/frequency	=	0



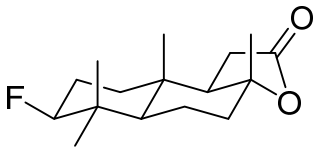
2F(axial)-Sclareolide

OPT-wB97xD-6-311+Gdp-2FaxSclareolide.out

0 1

C	0.216253	2.037999	0.033129
C	0.911973	0.736649	-0.404684
C	0.214173	-0.535993	0.183250
C	-1.243971	-0.389025	-0.281841
C	-1.981481	0.870236	0.197888
C	-1.273401	2.090658	-0.361385
H	0.730566	0.659631	-1.488163
H	0.319559	2.182295	1.113223
H	0.712365	2.891392	-0.432784
H	-1.176241	-0.245834	-1.368918
H	-1.366514	2.085730	-1.452375
H	-1.729850	3.013251	0.008773
C	0.808076	-1.776898	-0.508743
C	2.461839	0.755260	-0.298053
C	2.991299	-0.544578	-0.942422
C	2.325944	-1.840951	-0.523716
H	0.414955	-2.693953	-0.058208
H	0.496912	-1.783871	-1.560908
H	2.846957	-0.469423	-2.027657
H	4.070244	-0.633698	-0.778623
C	-2.312087	-1.458969	-0.105891
H	-2.213720	-2.322285	-0.763385
H	-2.419546	-1.820967	0.921226
C	-3.551951	-0.663730	-0.484306
O	-4.626248	-1.082701	-0.826418
O	-3.293957	0.656988	-0.423927
C	3.002721	0.928202	1.129342
H	4.087873	1.070820	1.092309
H	2.573630	1.813793	1.607925
H	2.811480	0.068488	1.767868
C	3.020349	1.915602	-1.140211
H	4.099840	1.792680	-1.275897
H	2.560052	1.949204	-2.133357
H	2.863375	2.884239	-0.658801
C	0.317598	-0.703750	1.711180
H	1.227058	-1.228942	1.992750
H	0.309408	0.246511	2.243361
H	-0.518961	-1.301525	2.084537
C	-2.272780	1.028539	1.688558
H	-1.406645	1.387740	2.240764
H	-3.068418	1.770292	1.795385
H	-2.614307	0.099744	2.150108
F	2.810730	-2.228779	0.757770
H	2.647676	-2.646096	-1.188892

Zero-point correction	=	0.393311
Thermal correction to Energy	=	0.410328
Thermal correction to Enthalpy	=	0.411272
Thermal correction to Gibbs Free Energy	=	0.351556
Sum of electronic and zero-point Energies	=	-874.706654
Sum of electronic and thermal Energies	=	-874.689636
Sum of electronic and thermal Enthalpies	=	-874.688692
Sum of electronic and thermal Free Energies	=	-874.748408
Number of imaginary frequencies/frequency	=	0



3F(eq)-Sclareolide

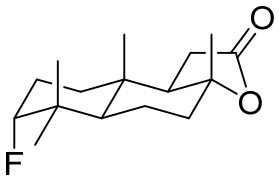
OPT-wB97xD-6-311+Gdp-3FeqSclareolide.out

0 1

C	0.198784	1.939557	-0.147082
C	0.862485	0.567545	-0.364956
C	0.089053	-0.589807	0.353377
C	-1.336126	-0.464417	-0.206772
C	-2.045921	0.871950	0.055364
C	-1.265406	1.980283	-0.627362
H	0.729005	0.348615	-1.435499
H	0.251669	2.223868	0.908716
H	0.749579	2.706422	-0.694467
H	-1.208500	-0.479523	-1.297633
H	-1.301177	1.822885	-1.710387
H	-1.706196	2.958945	-0.417345
C	0.684572	-1.927596	-0.122742
C	2.409724	0.565004	-0.178751
C	2.879618	-0.832297	-0.617814
C	2.199289	-1.994694	0.073580
H	0.207258	-2.758012	0.407596
H	0.458186	-2.061346	-1.188169
H	2.460124	-1.988149	1.135802
H	2.745891	-0.919893	-1.702120
C	-2.452532	-1.464310	0.057263
H	-2.354603	-2.414773	-0.466135
H	-2.626416	-1.672320	1.117479
C	-3.640177	-0.690368	-0.493683
O	-4.711743	-1.118011	-0.833143
O	-3.334288	0.617560	-0.599372
C	2.883804	0.894024	1.243800
H	3.964067	1.059417	1.247396

H	2.411111	1.812317	1.601846
H	2.671143	0.104601	1.963712
C	3.043273	1.588253	-1.137307
H	4.121006	1.421441	-1.208977
H	2.619869	1.508416	-2.144062
H	2.897017	2.612013	-0.785340
C	0.115919	-0.545902	1.892424
H	0.972781	-1.086913	2.294516
H	0.165019	0.467280	2.290101
H	-0.776840	-1.022970	2.305523
C	-2.398796	1.238805	1.495464
H	-1.542613	1.629913	2.041670
H	-3.163296	2.019233	1.464635
H	-2.804180	0.392113	2.053637
F	4.274841	-0.952076	-0.403179
H	2.589394	-2.927470	-0.342573

Zero-point correction	=	0.393401
Thermal correction to Energy	=	0.410486
Thermal correction to Enthalpy	=	0.41143
Thermal correction to Gibbs Free Energy	=	0.351578
Sum of electronic and zero-point Energies	=	-874.708657
Sum of electronic and thermal Energies	=	-874.691573
Sum of electronic and thermal Enthalpies	=	-874.690629
Sum of electronic and thermal Free Energies	=	-874.75048
Number of imaginary frequencies/frequency	=	0



3F(axial)-Sclareolide

OPT-wB97xD-6-311+Gdp-3FaxSclareolide.out

0 1

C	0.307630	1.919938	-0.283855
C	0.959834	0.526251	-0.308725
C	0.141292	-0.533567	0.504226
C	-1.256885	-0.461158	-0.127575
C	-1.957403	0.903393	-0.054229
C	-1.134701	1.917047	-0.828630
H	0.871987	0.184553	-1.349528
H	0.319150	2.333674	0.729662
H	0.892264	2.607592	-0.897604
H	-1.084802	-0.606715	-1.202365
H	-1.126650	1.635982	-1.886741
H	-1.570605	2.917344	-0.751220
C	0.740447	-1.922349	0.213559
C	2.493068	0.525450	-0.051603
C	3.014956	-0.909367	-0.242783
C	2.241565	-1.984071	0.495404
H	0.223917	-2.681926	0.810027
H	0.565543	-2.172585	-0.838840
H	4.077737	-0.949069	0.015680
C	-2.397159	-1.412319	0.206358
H	-2.294281	-2.415892	-0.205033
H	-2.610617	-1.499940	1.276241
C	-3.553229	-0.695718	-0.473456
O	-4.620222	-1.148614	-0.794759
O	-3.223552	0.585880	-0.725039
C	2.911286	1.009252	1.346523
H	3.996932	1.145212	1.382665
H	2.454916	1.977015	1.569310
H	2.639130	0.319930	2.144800
C	3.199748	1.430356	-1.076004
H	4.276666	1.233513	-1.075963
H	2.829148	1.267767	-2.090598
H	3.063134	2.485447	-0.826907
C	0.099291	-0.313062	2.028335
H	0.928818	-0.812907	2.529368
H	0.143420	0.738277	2.312359
H	-0.817627	-0.732343	2.451369
C	-2.362449	1.444640	1.315304
H	-1.523396	1.895149	1.842264
H	-3.115481	2.221412	1.159320
H	-2.799806	0.677242	1.957627
H	2.642680	-2.959012	0.205739
H	2.443834	-1.875774	1.564962
F	2.960048	-1.233374	-1.627255

Zero-point correction	=	0.393028
Thermal correction to Energy	=	0.410177
Thermal correction to Enthalpy	=	0.411122
Thermal correction to Gibbs Free Energy	=	0.351092
Sum of electronic and zero-point Energies	=	-874.708992
Sum of electronic and thermal Energies	=	-874.691842
Sum of electronic and thermal Enthalpies	=	-874.690898
Sum of electronic and thermal Free Energies	=	-874.750928
Number of imaginary frequencies/frequency	=	0