Supplementary Information

Structure-Reactivity Relationship of Trifluoromethanesulfenates: Discovery of An Electrophilic Trifluoromethylthiolating Reagent

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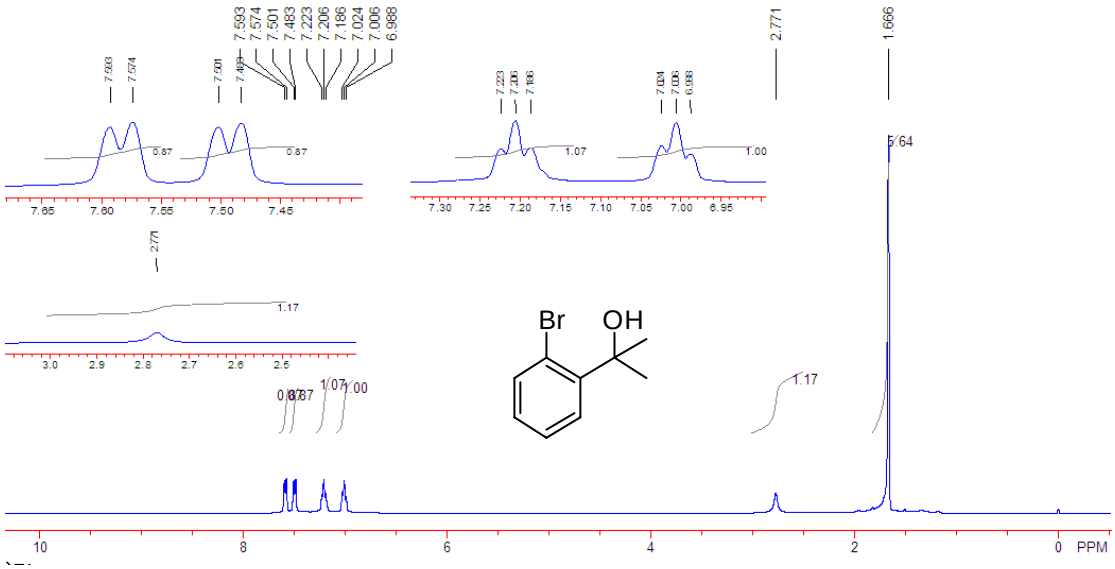
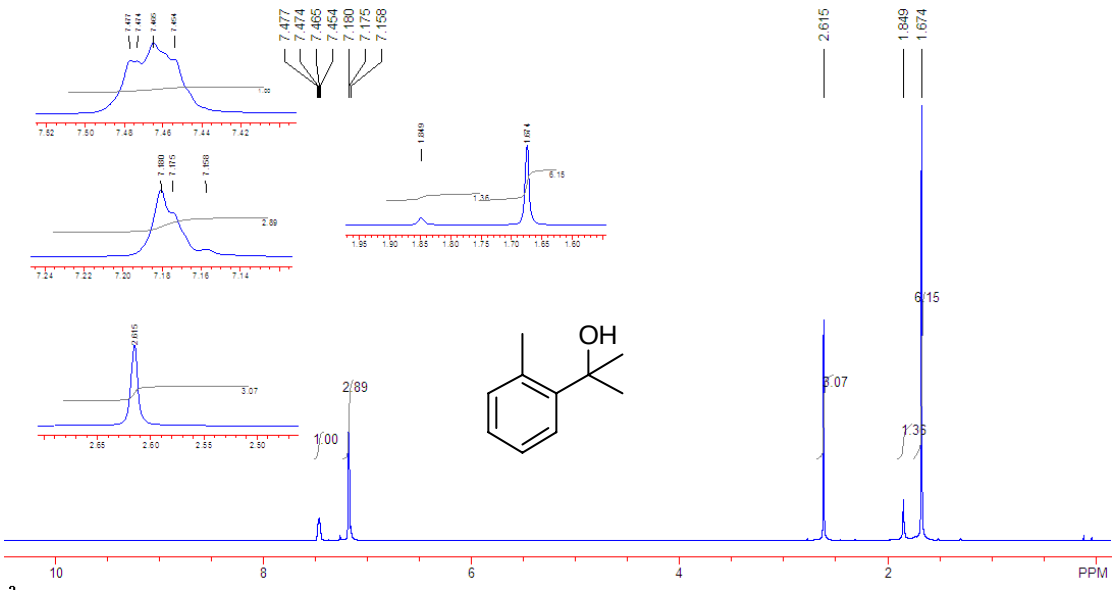


^{1}H NMR spectrum of 2-(O-tolyl)propan-2-ol



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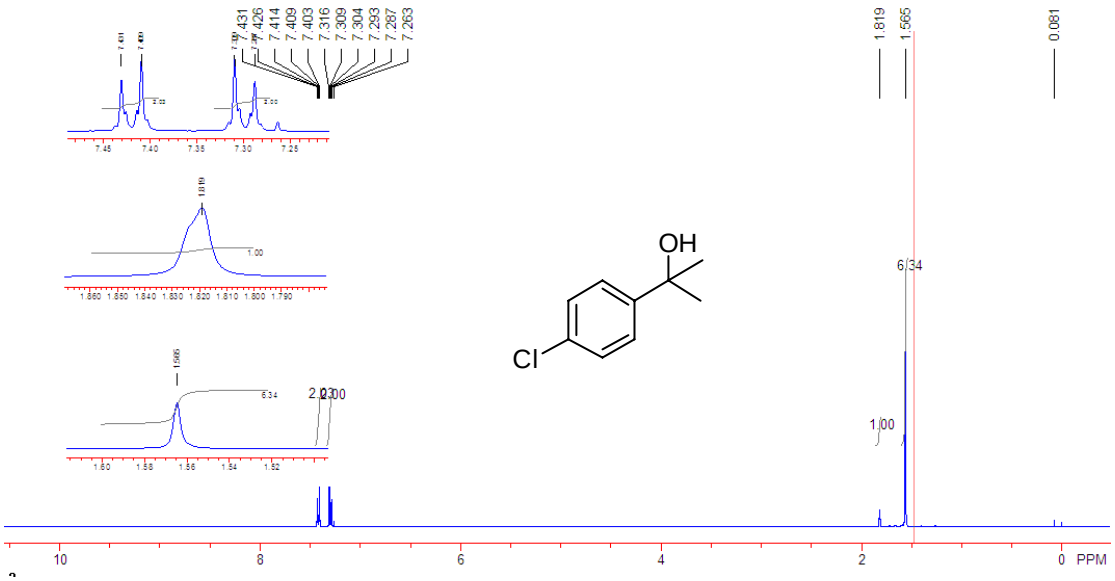

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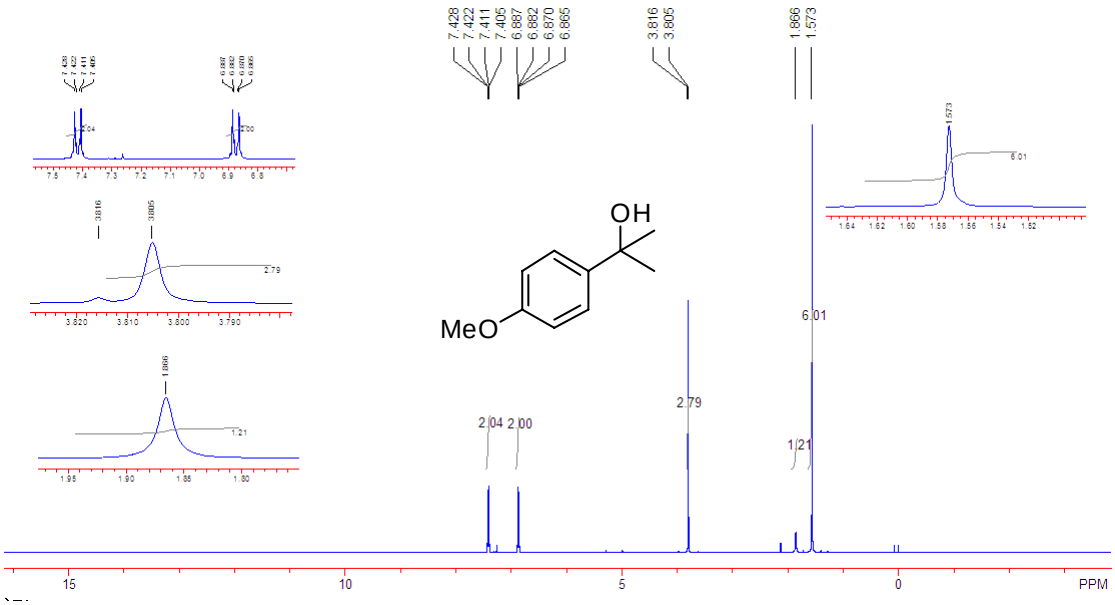

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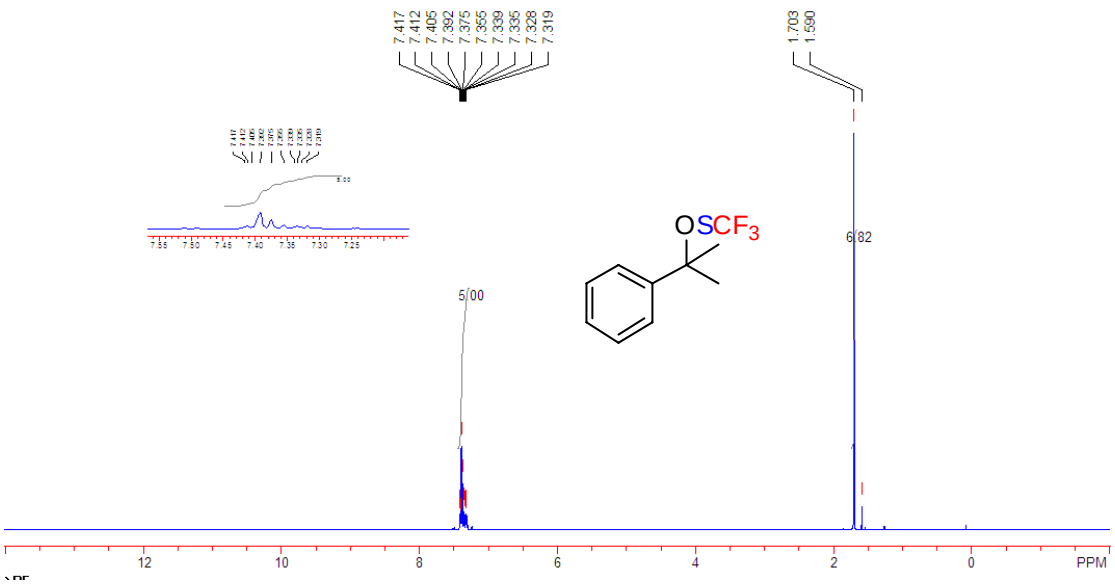

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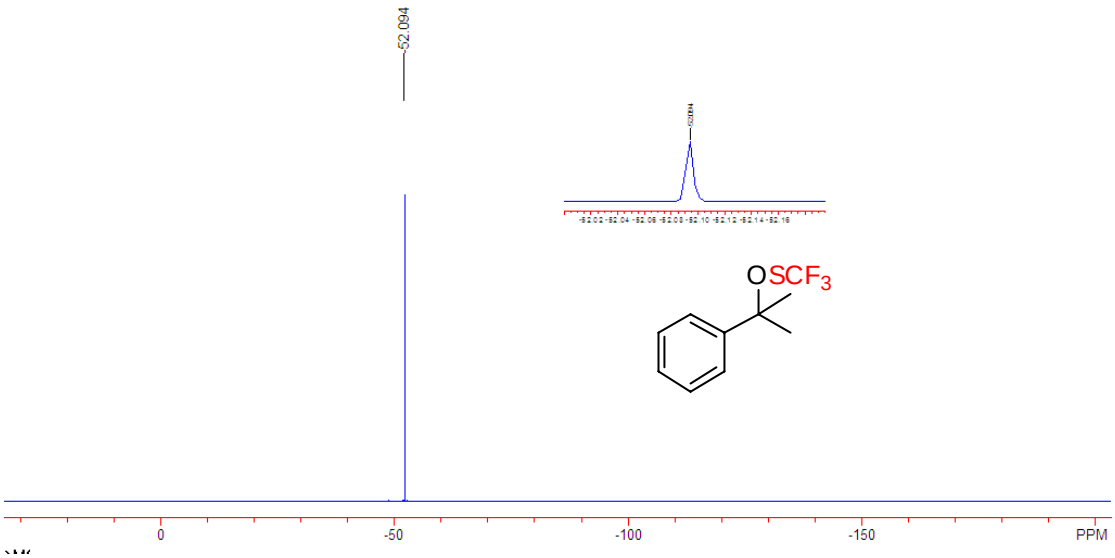

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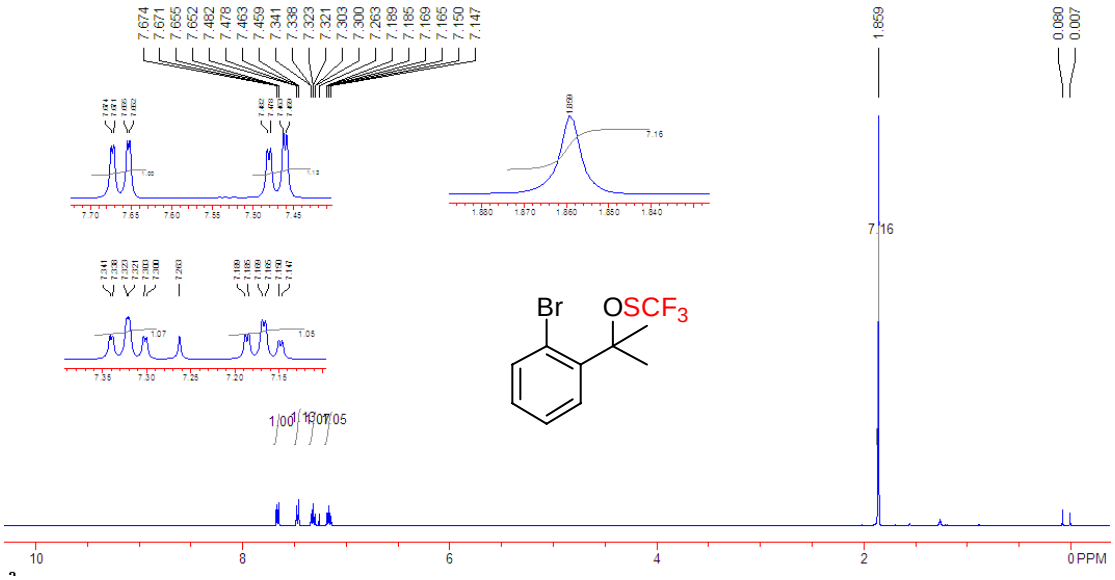

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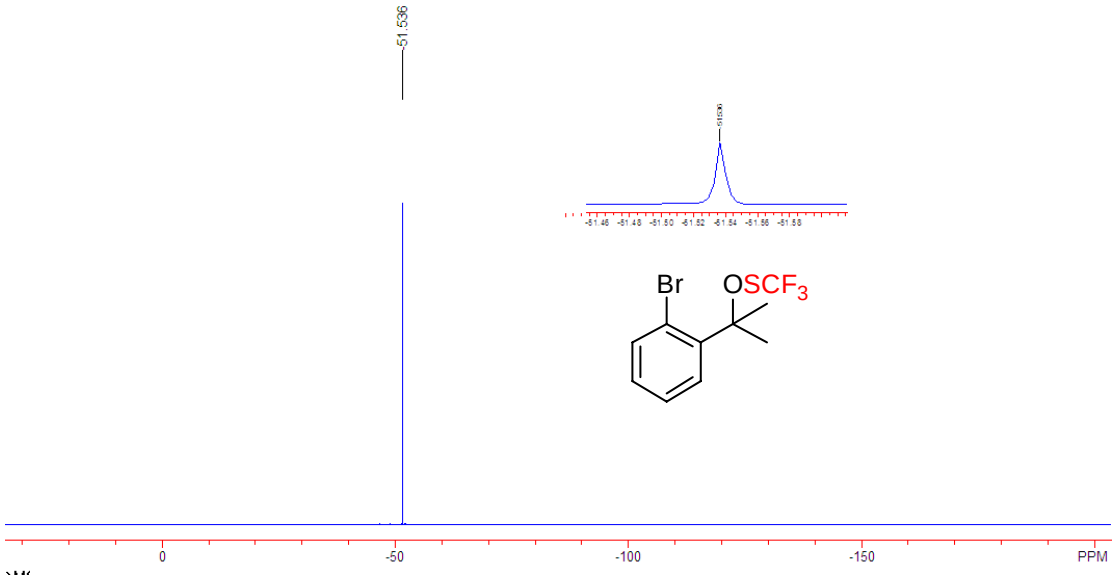

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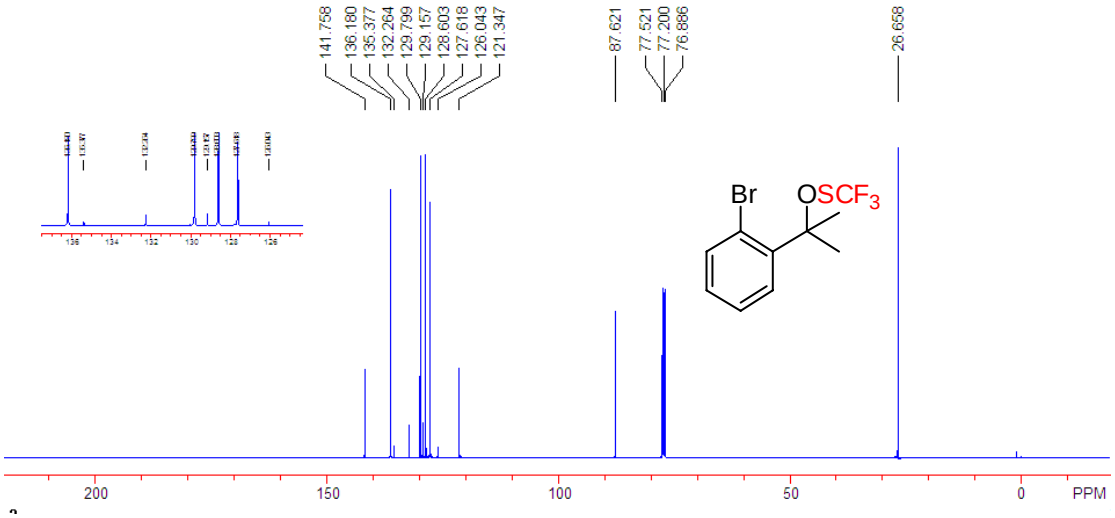

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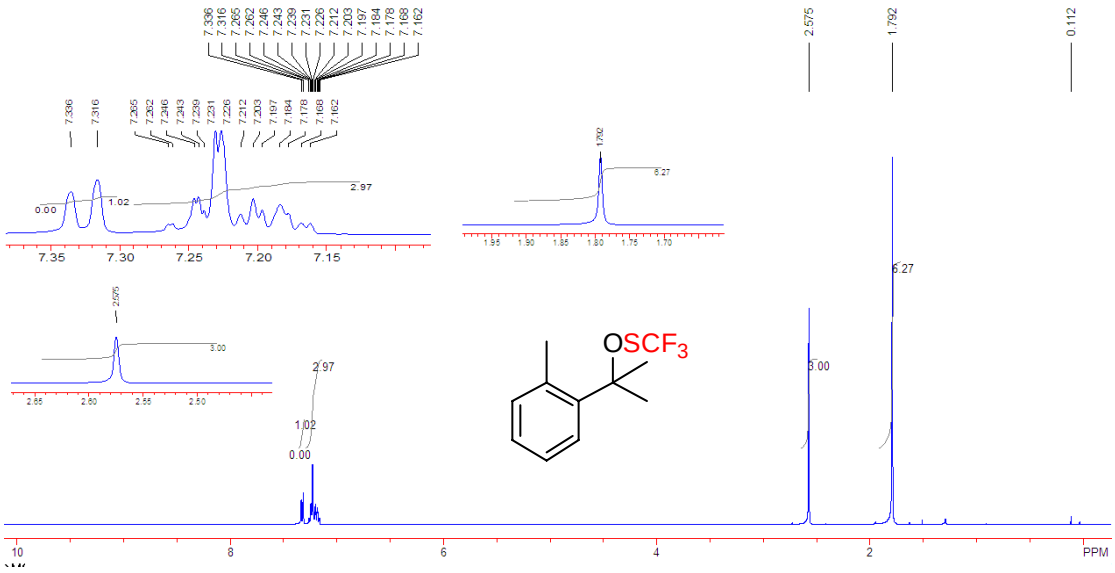

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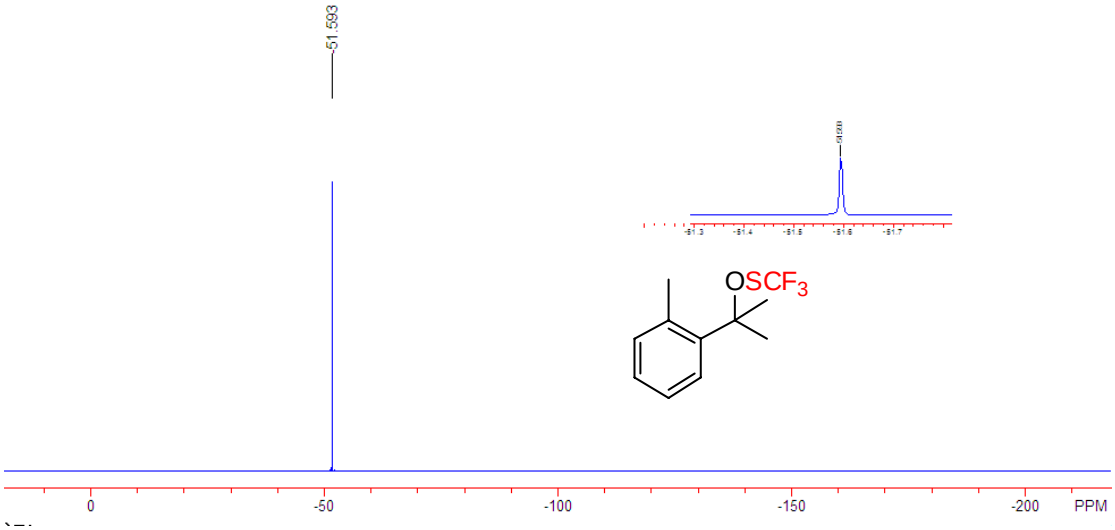

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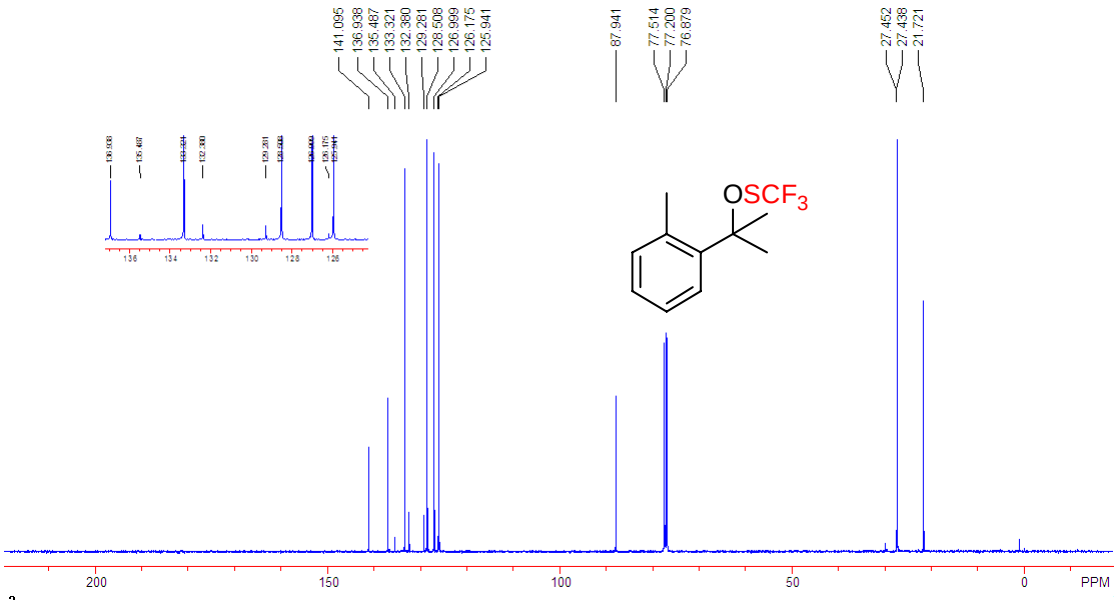

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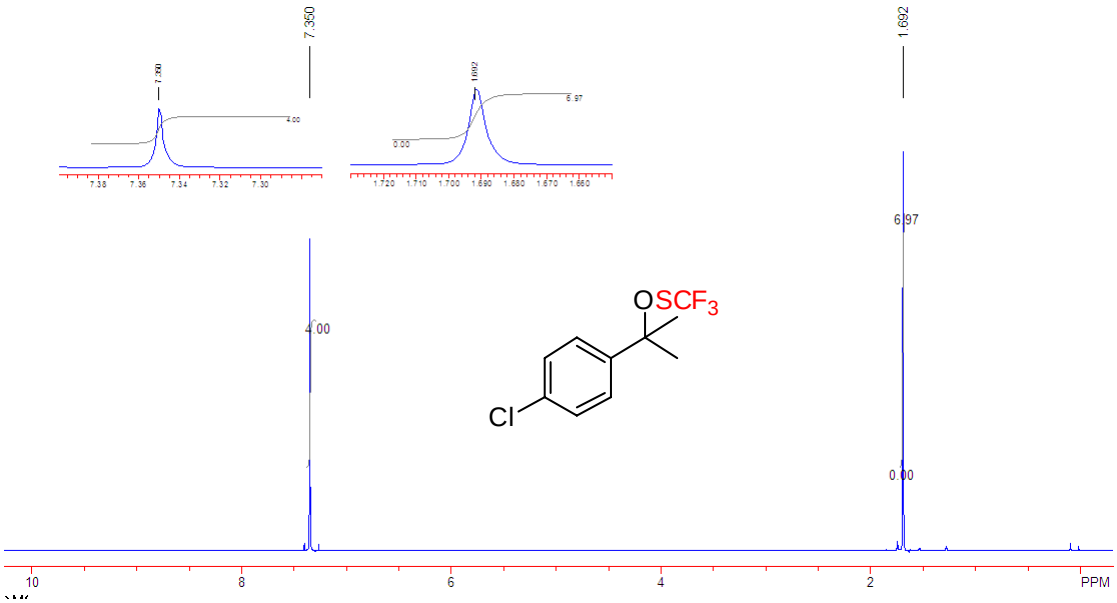

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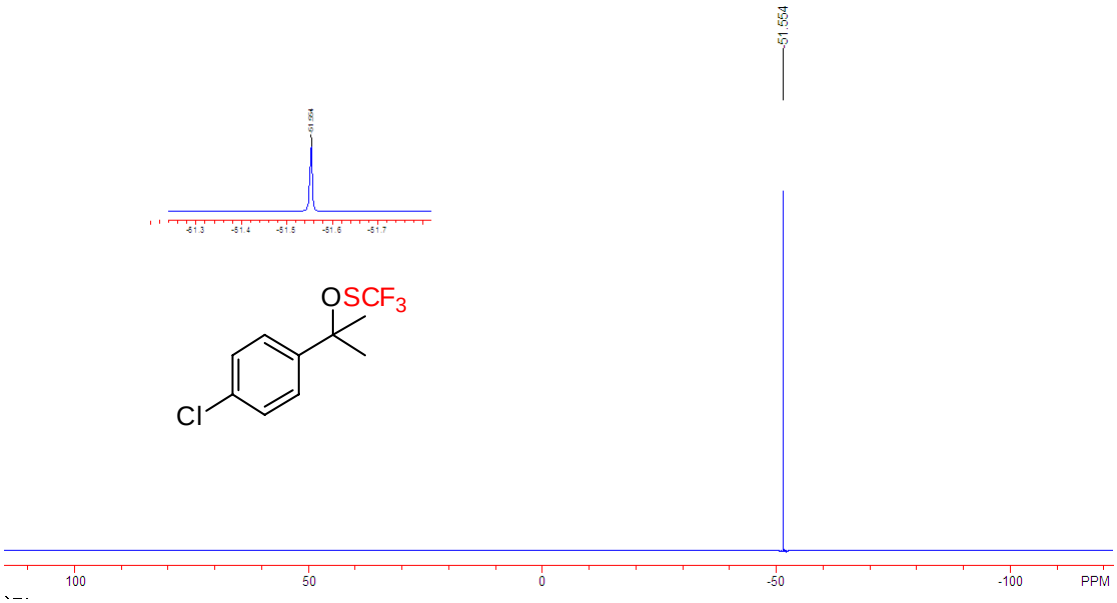

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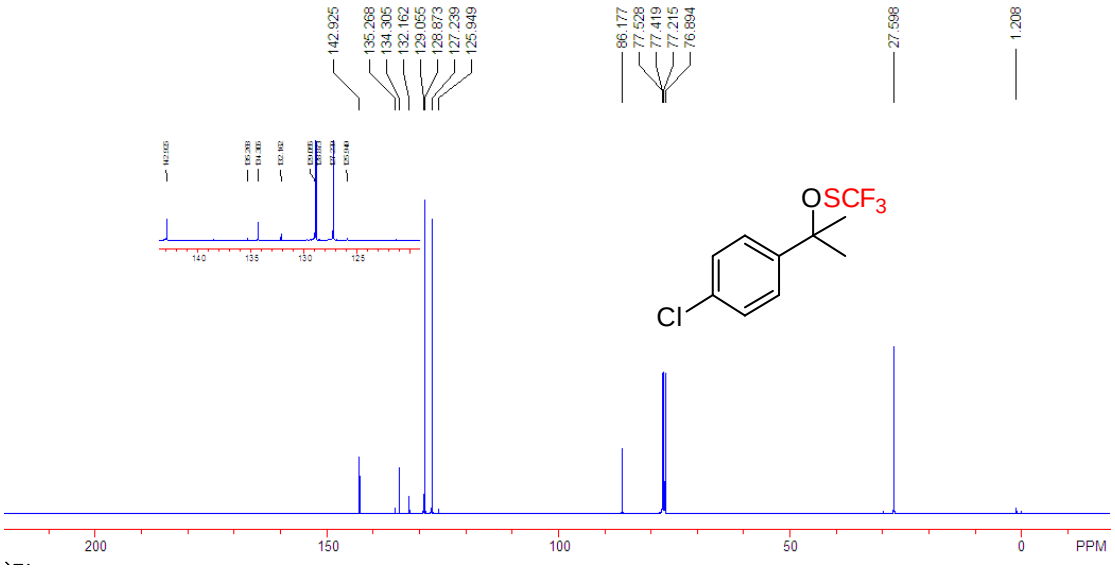

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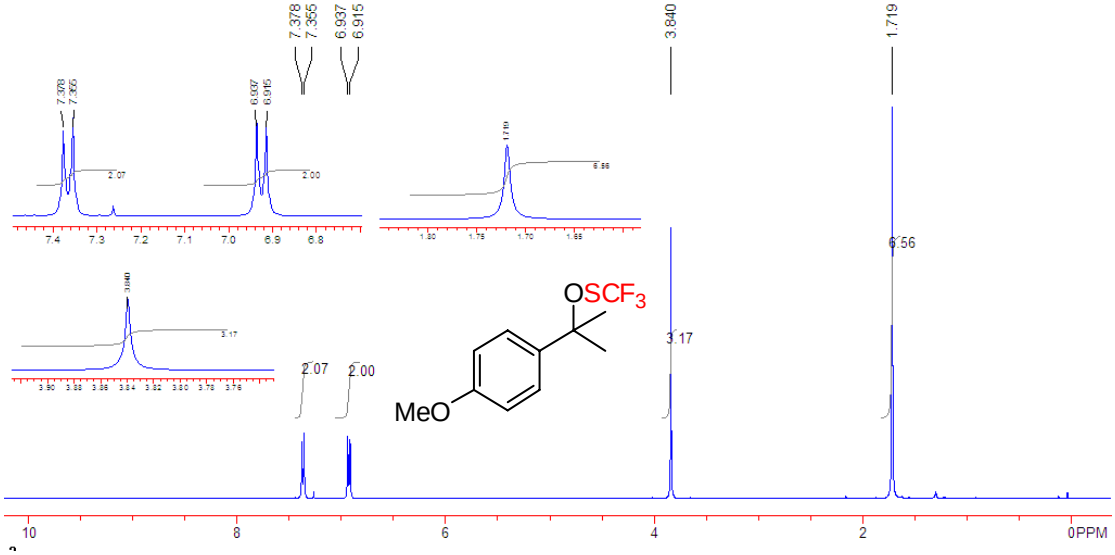

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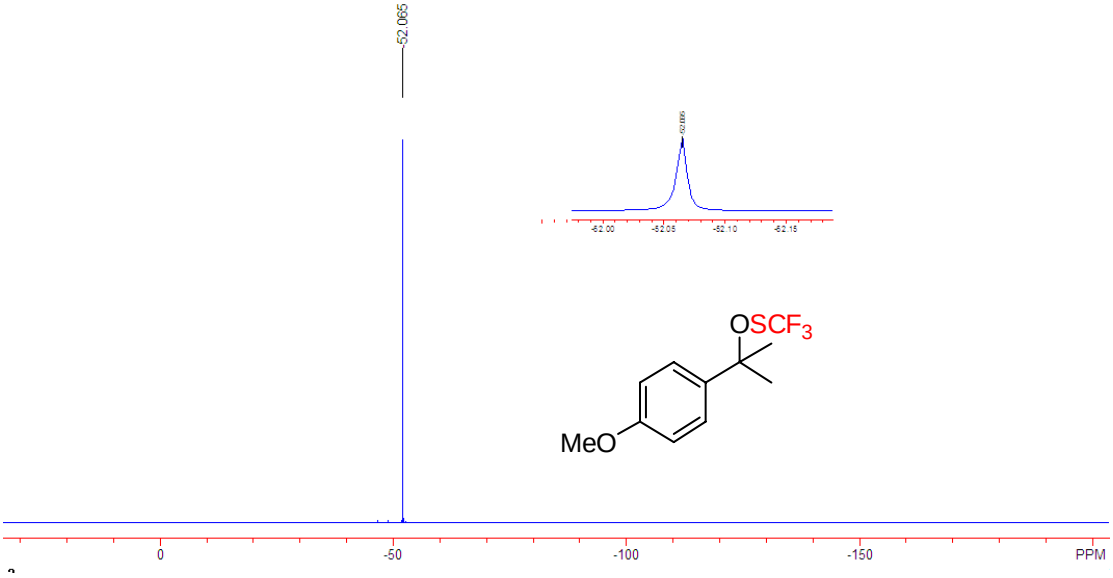

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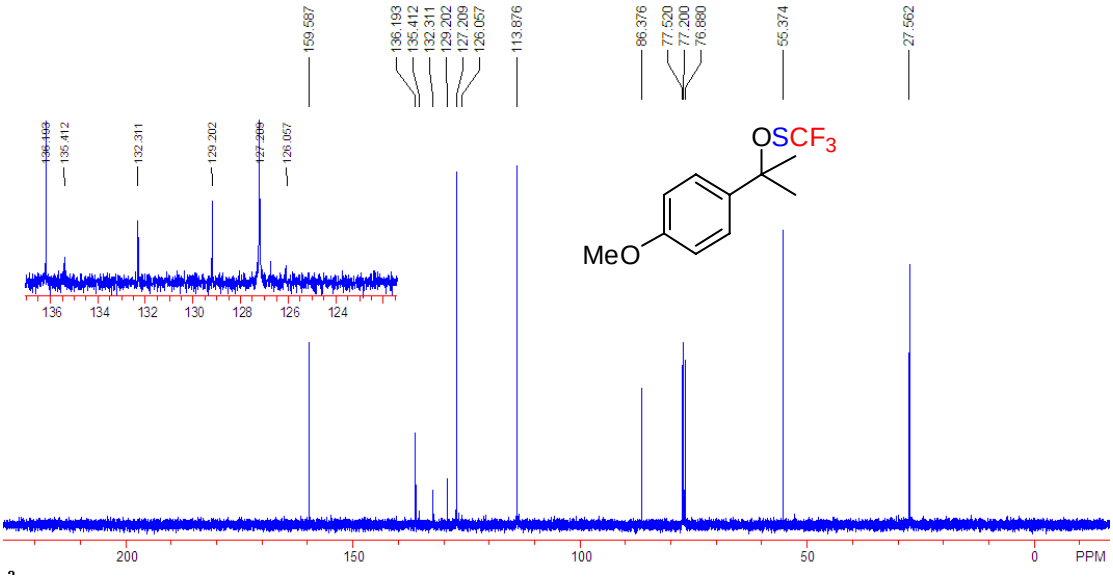
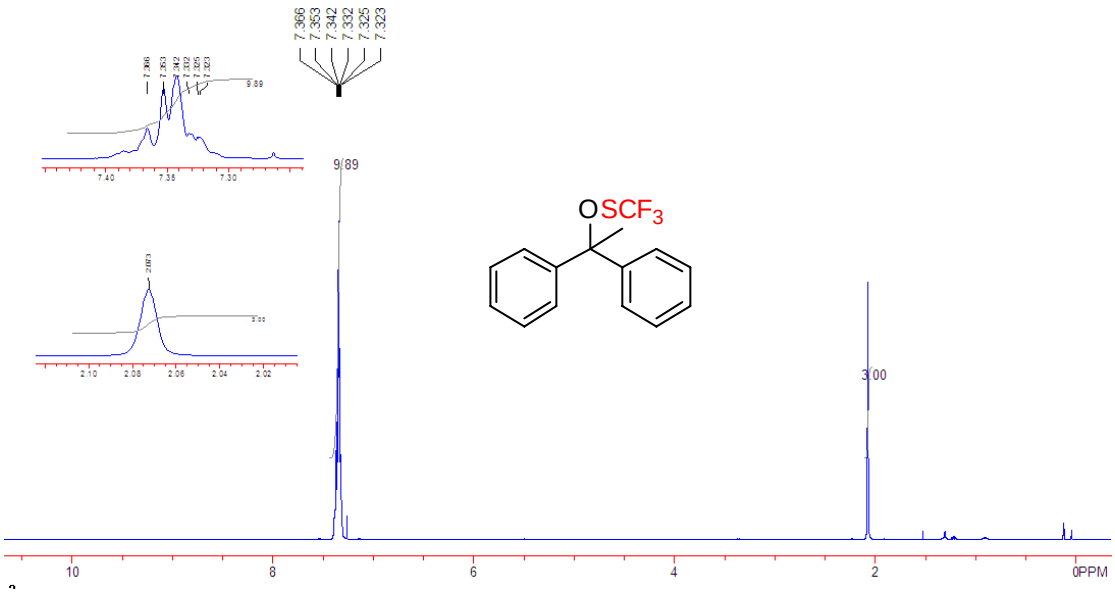


^{1}H NMR spectrum of (1,1-Diphenylethoxy)(trifluoromethyl)sulfane 1h



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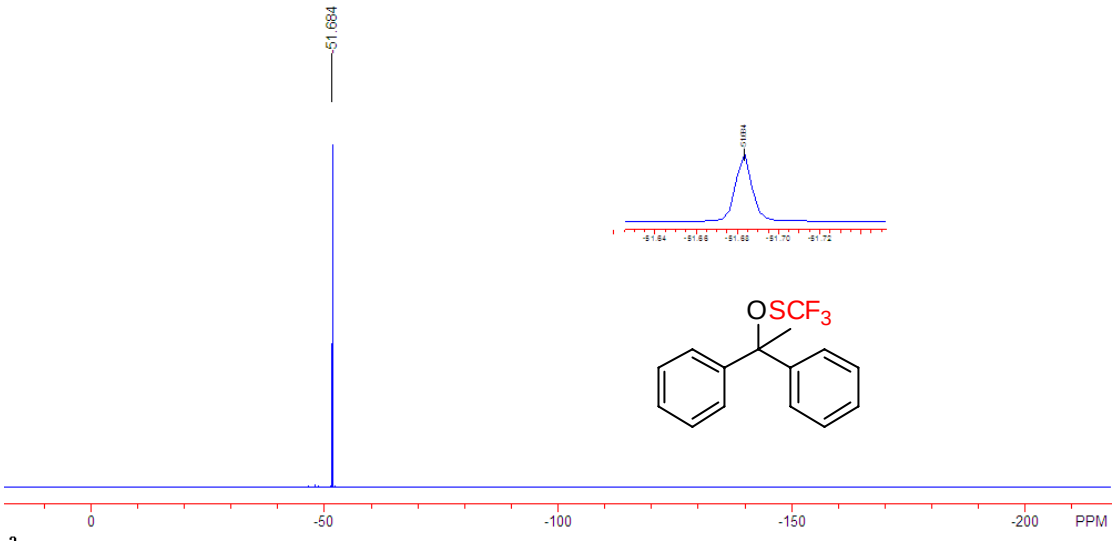

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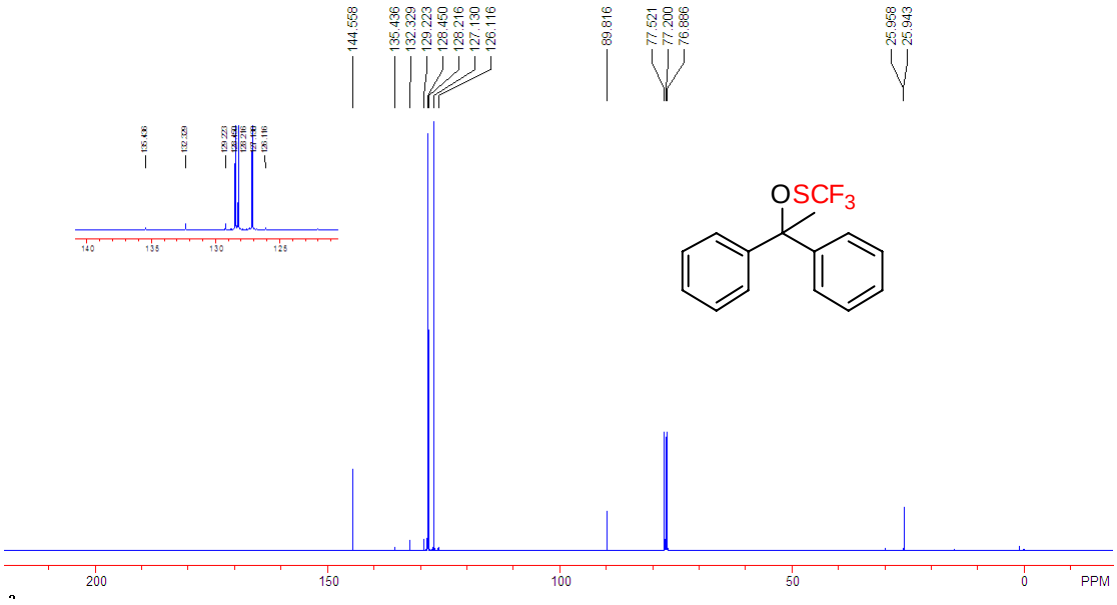

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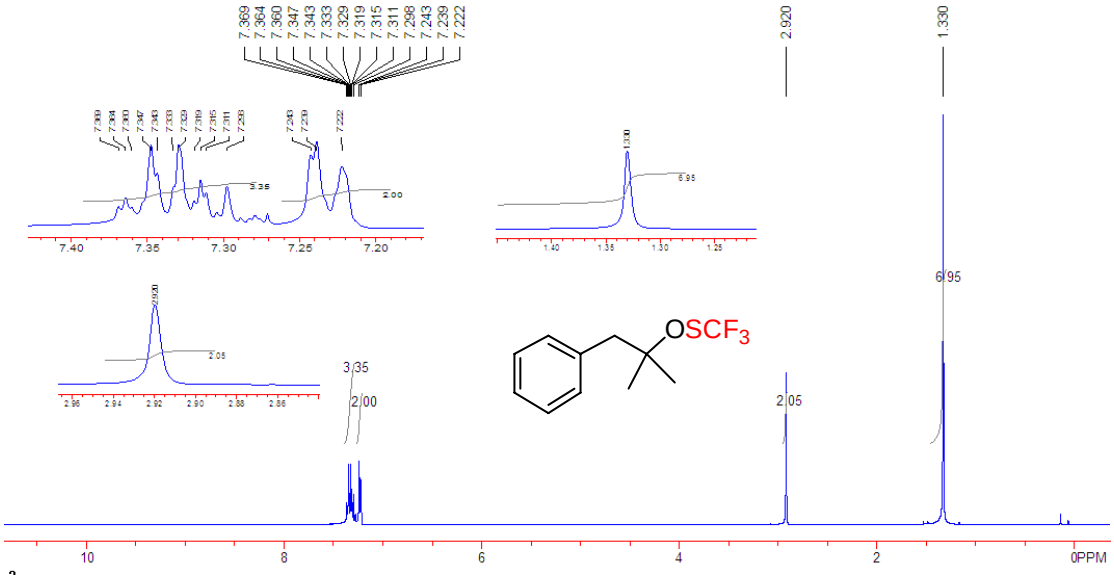

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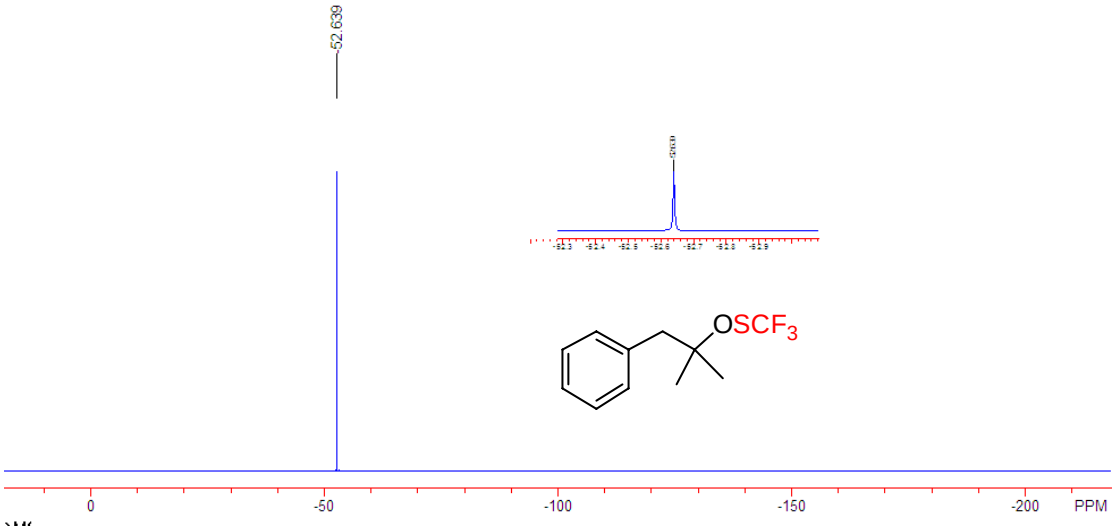

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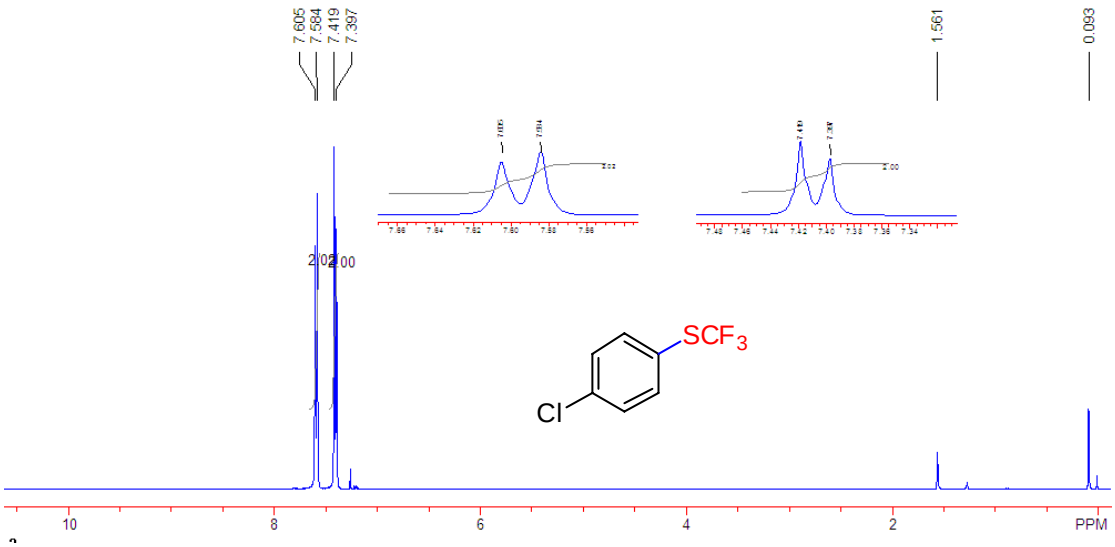

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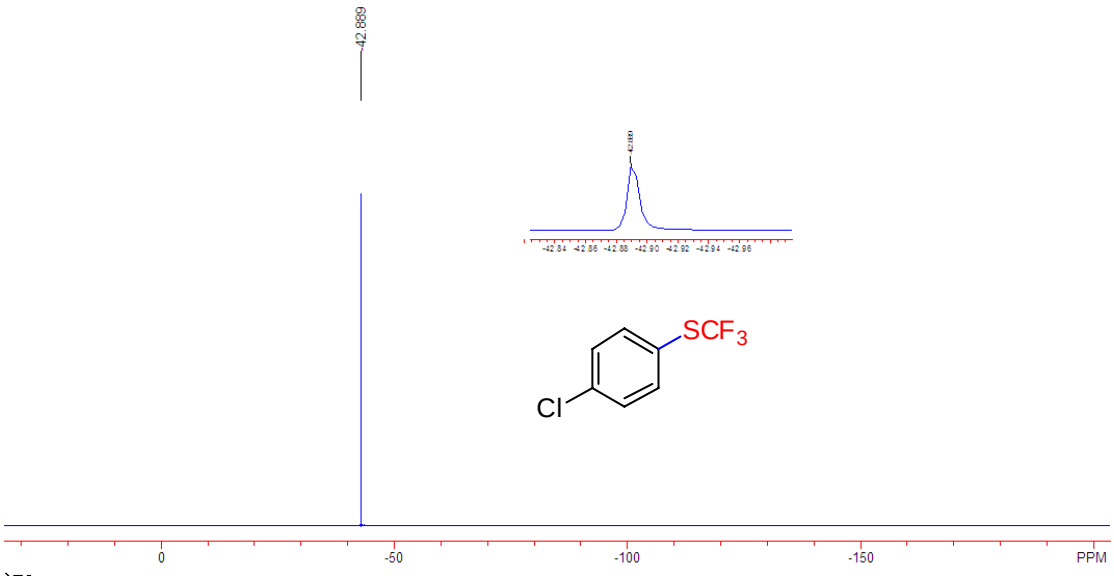

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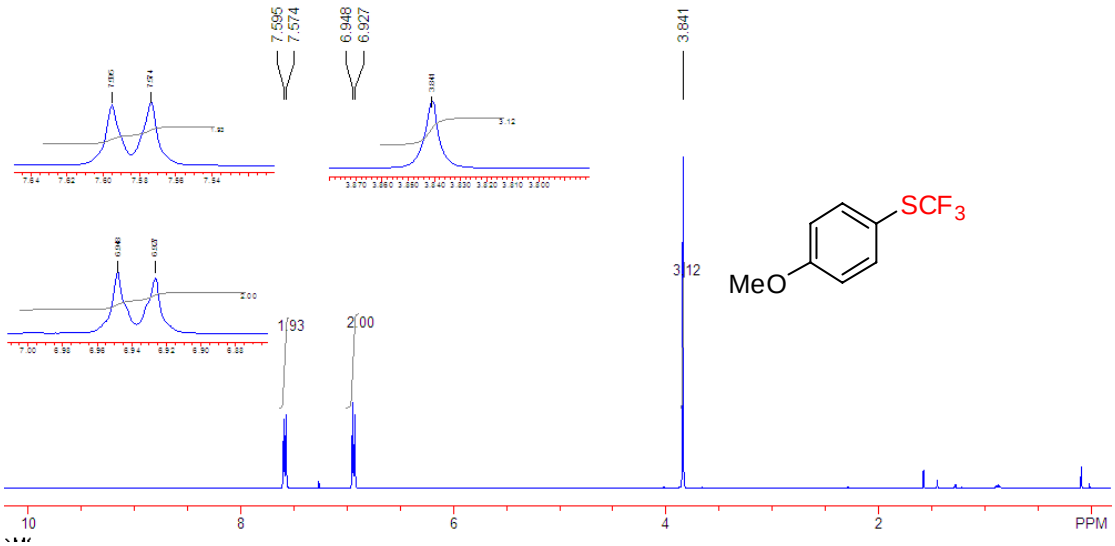

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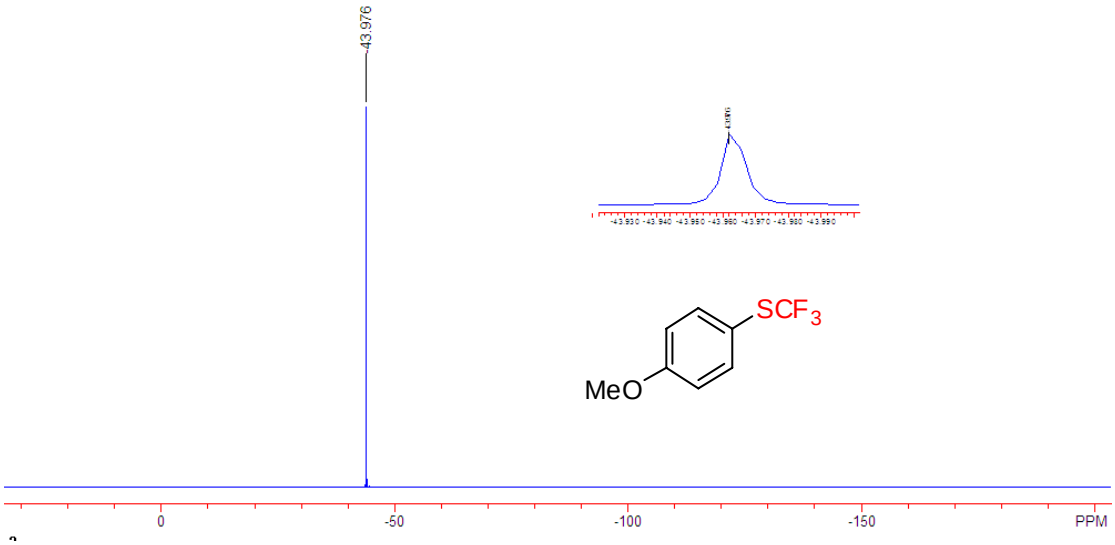

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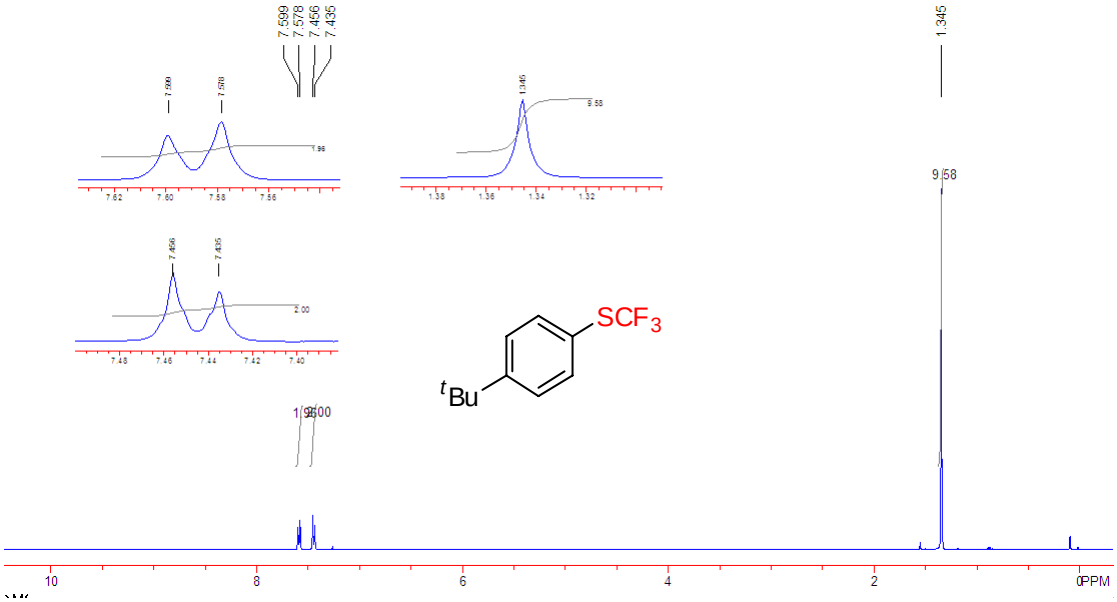

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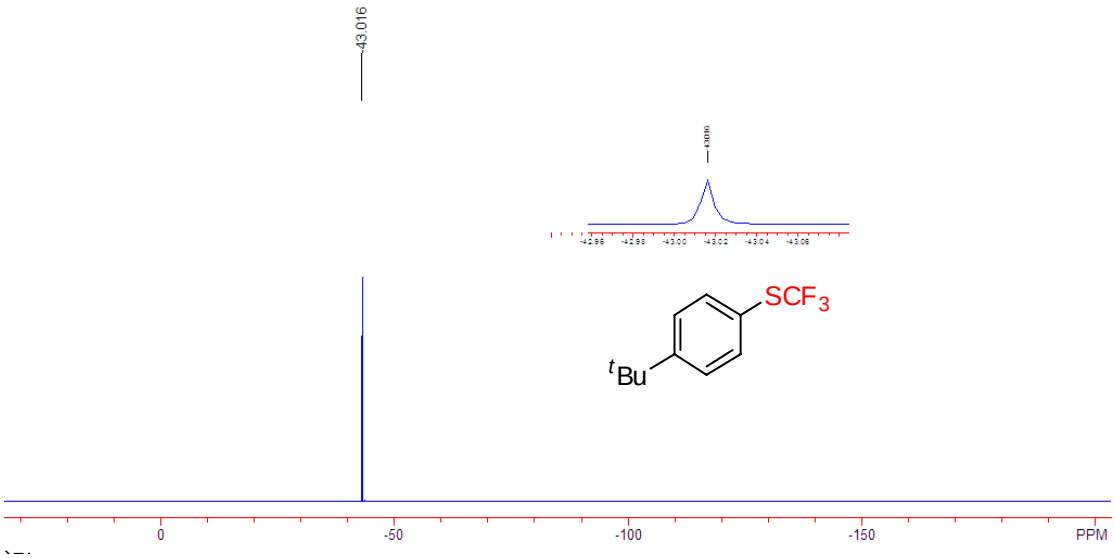

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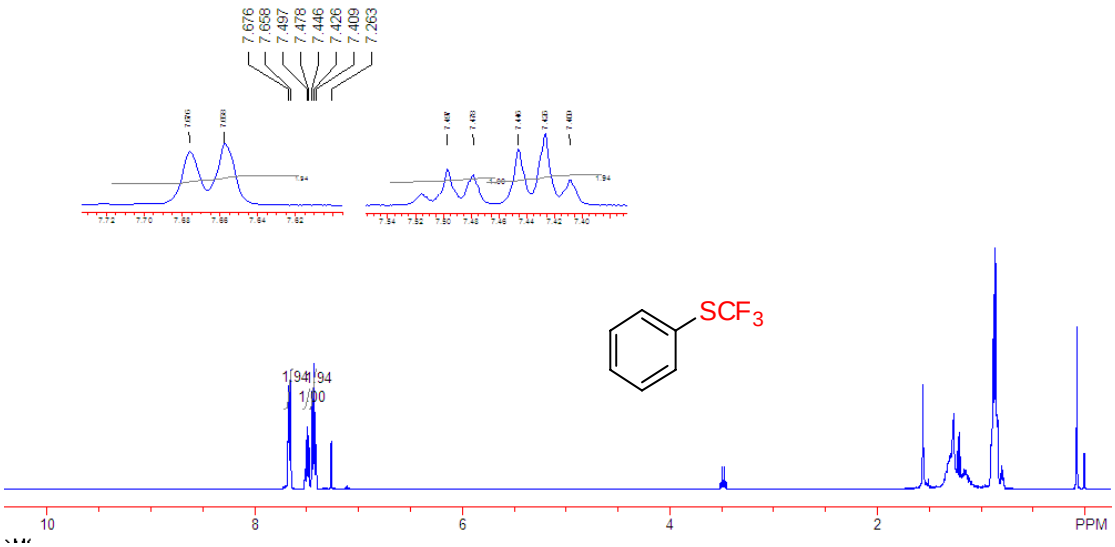

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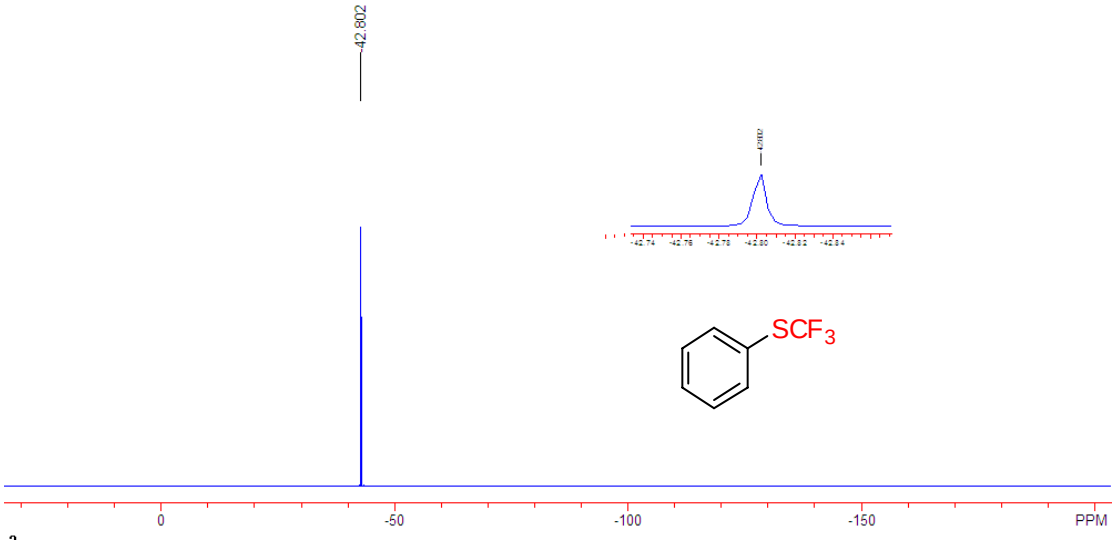

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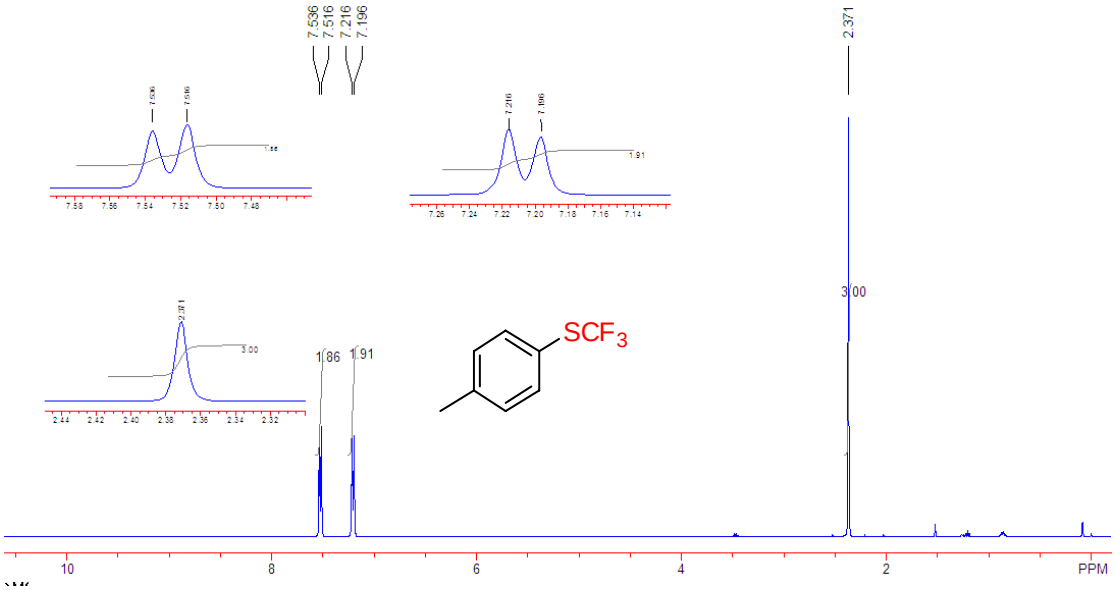

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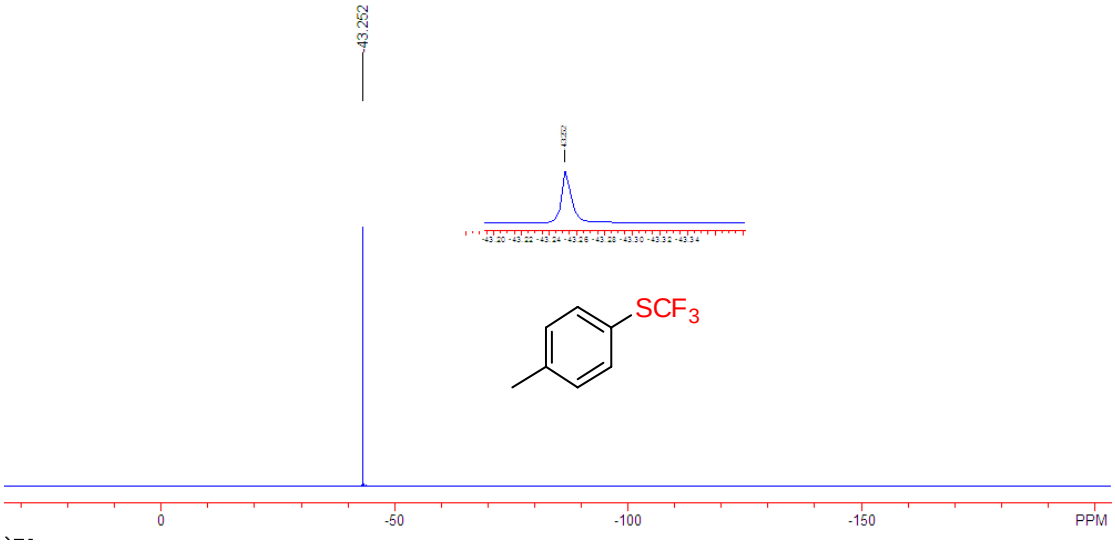

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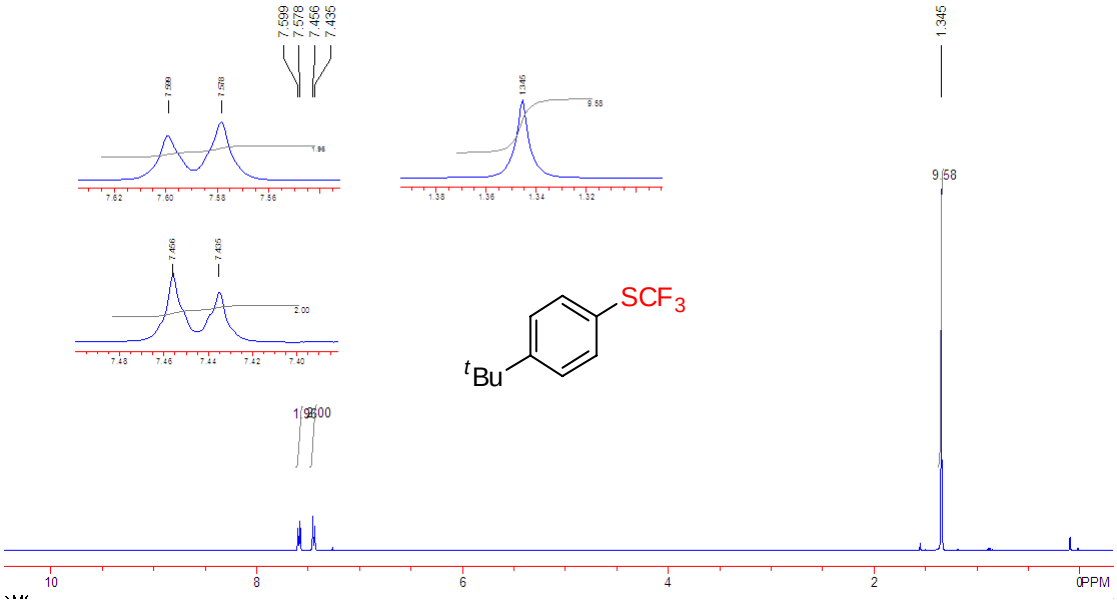

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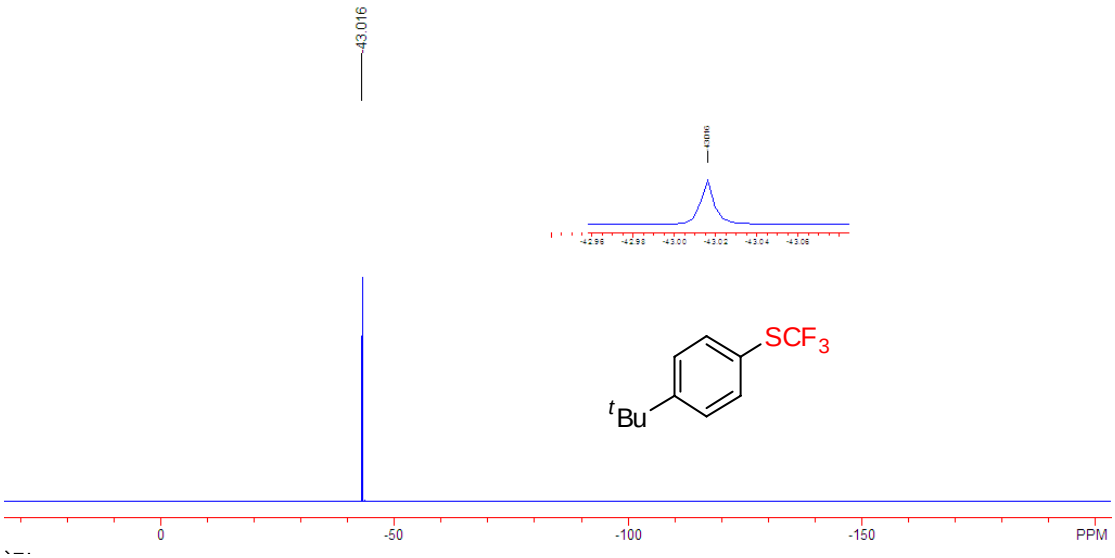

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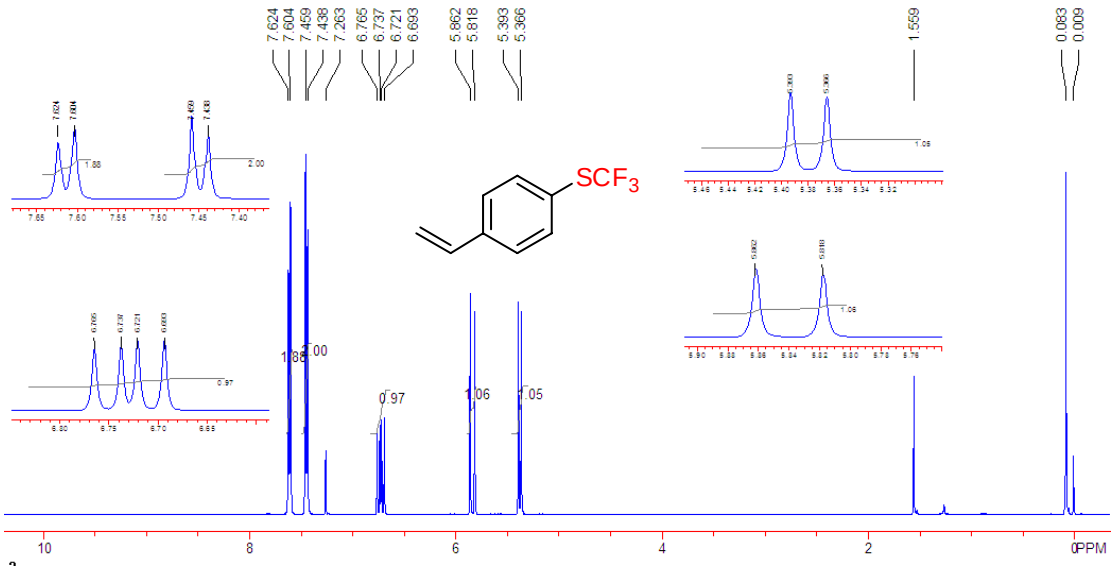

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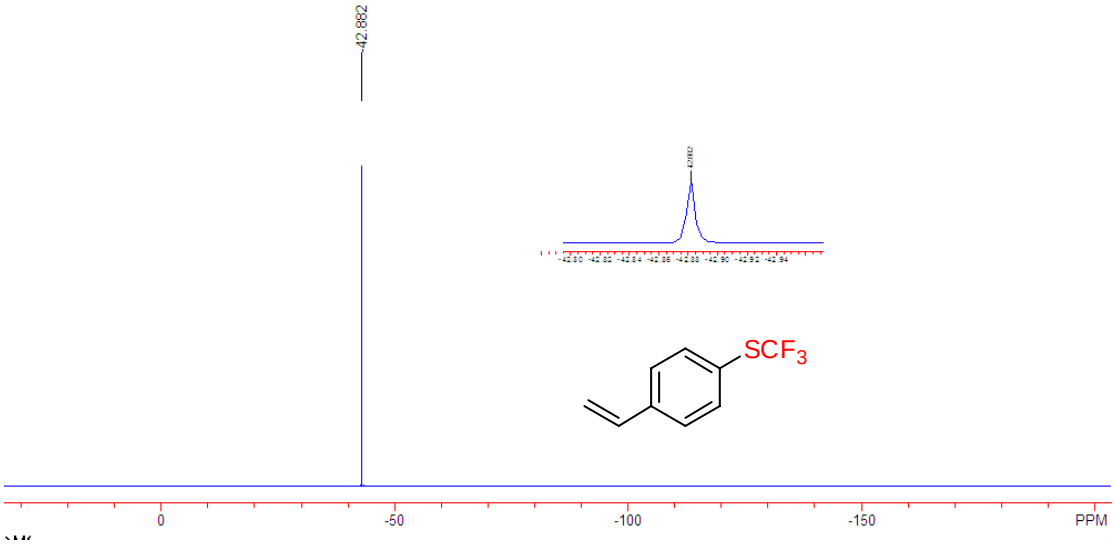

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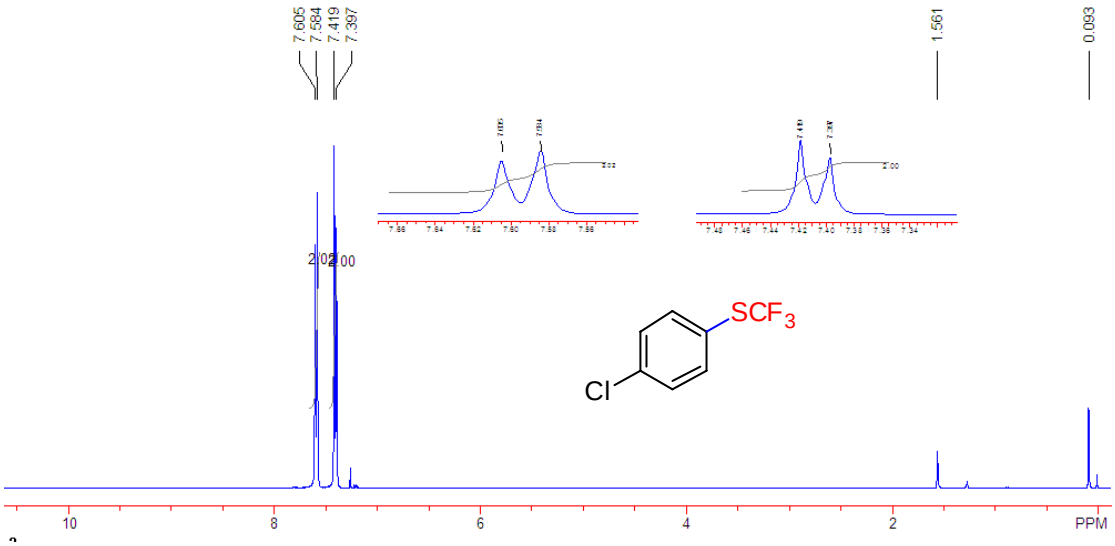

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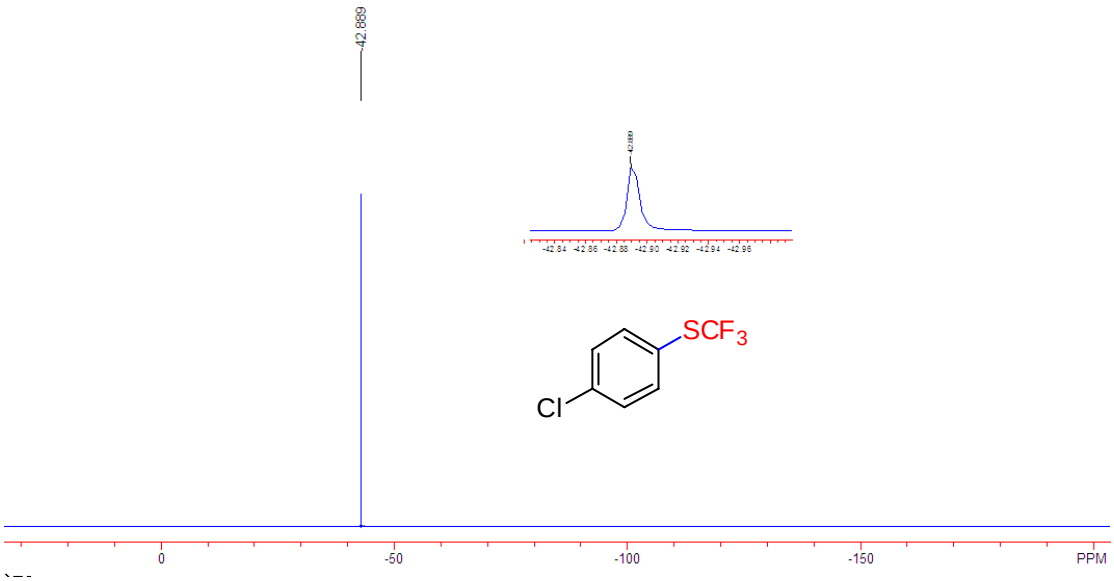

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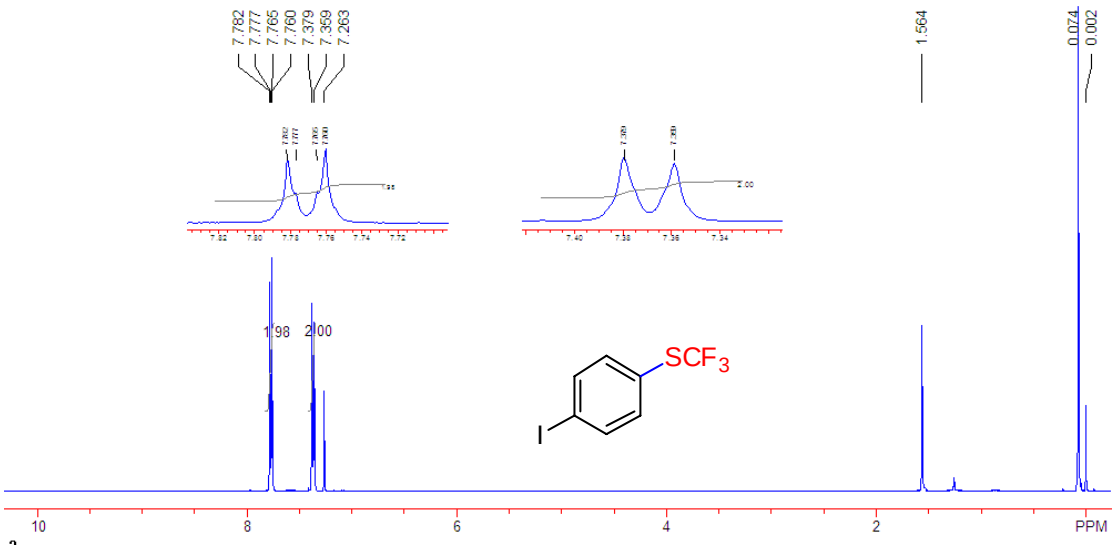

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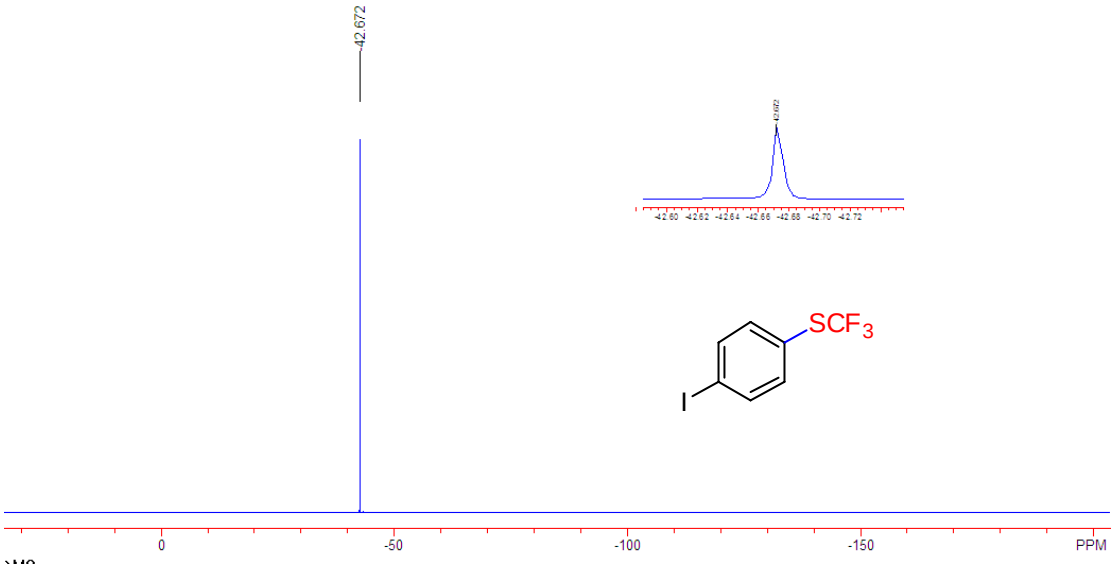

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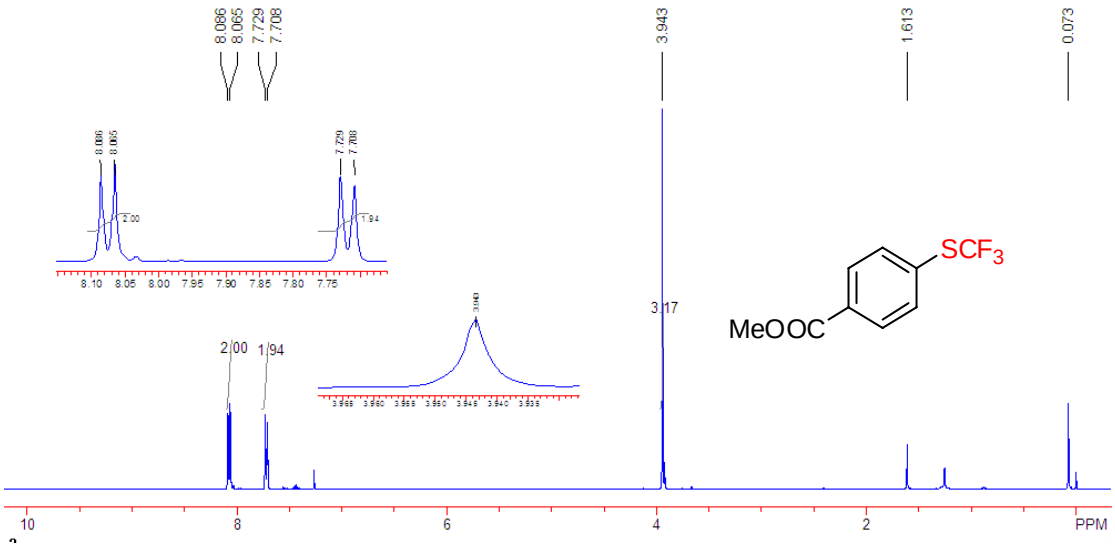
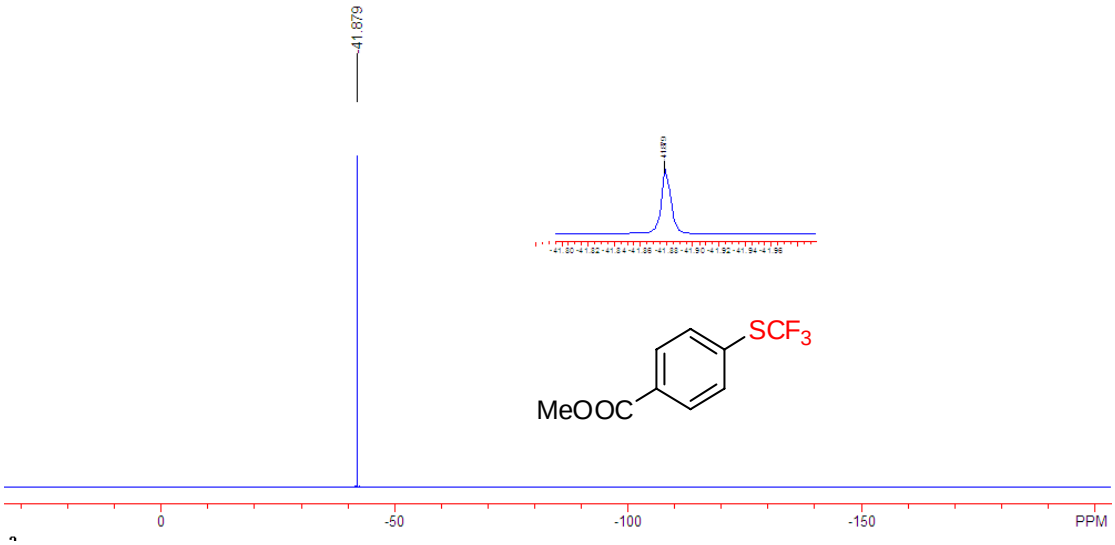


^{19}F NMR spectrum of Methyl 4-[(trifluoromethyl)thio]benzoate 6e



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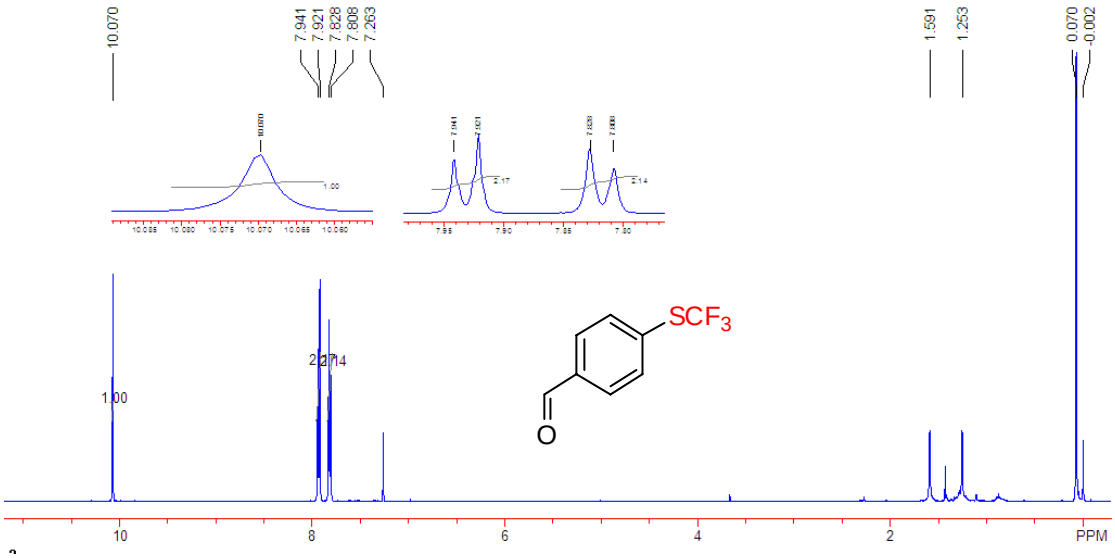

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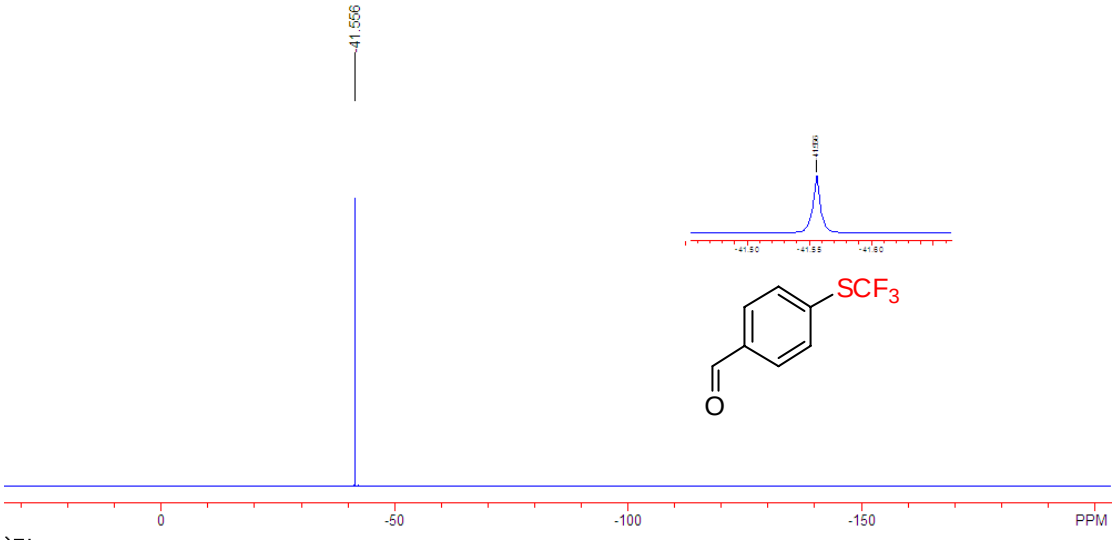
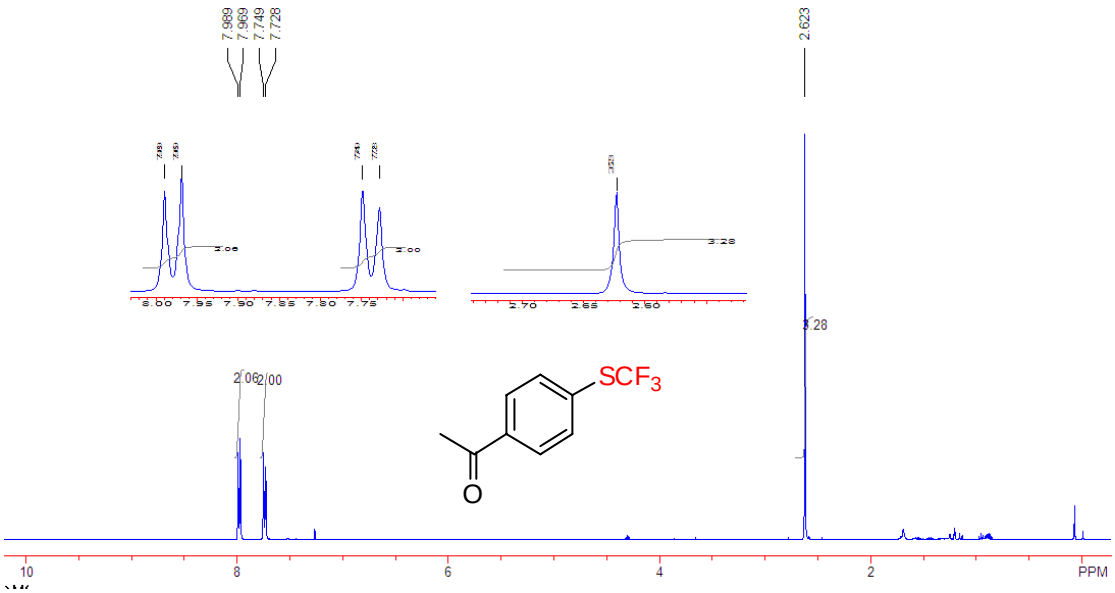


^{1}H NMR spectrum of 1-(4-Trifluoromethylsulfanyl-phenyl)-ethanone 6g



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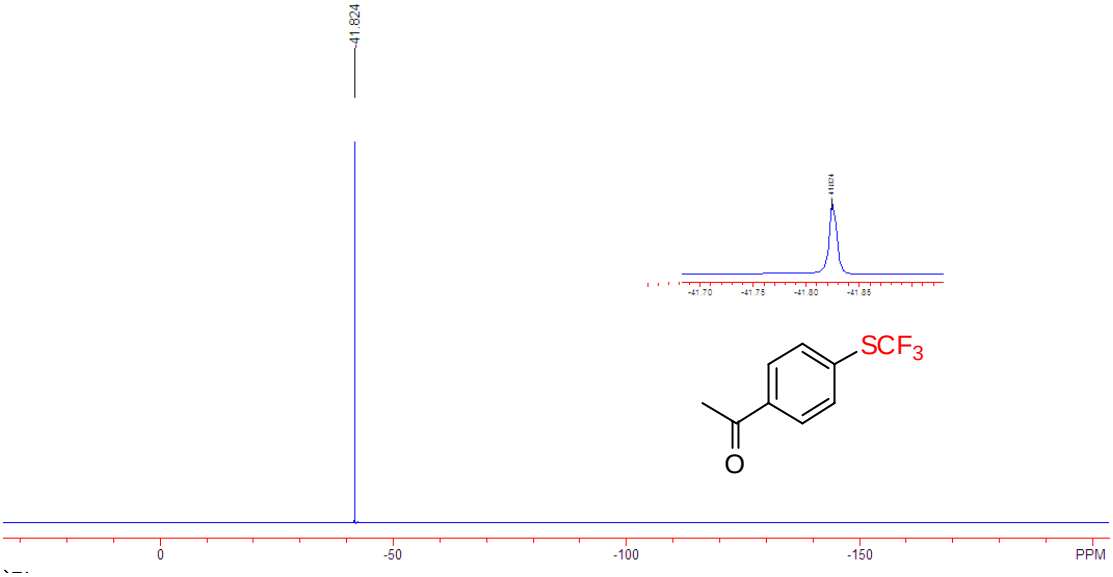

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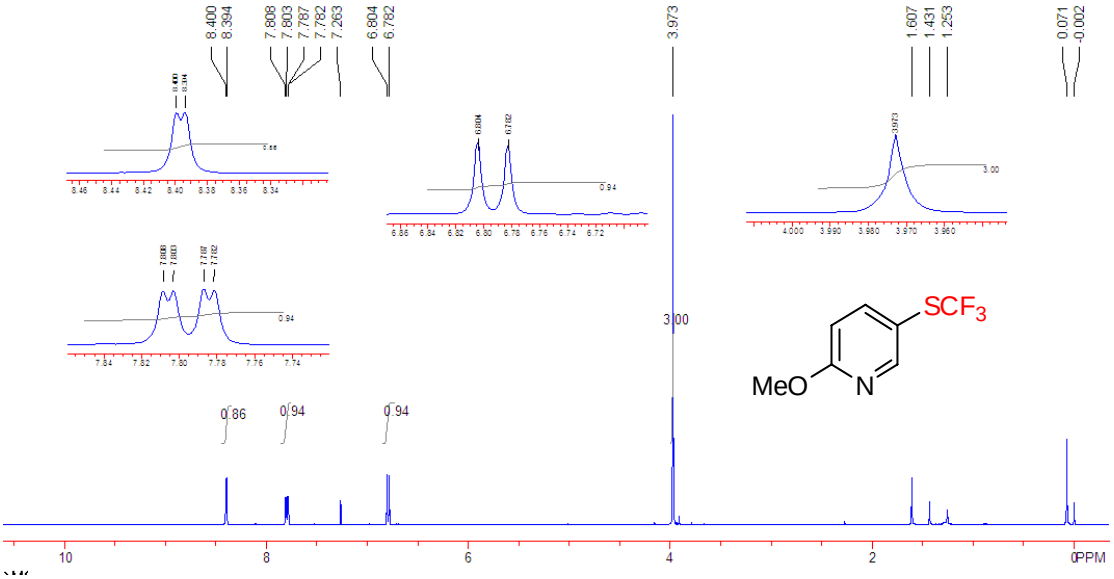

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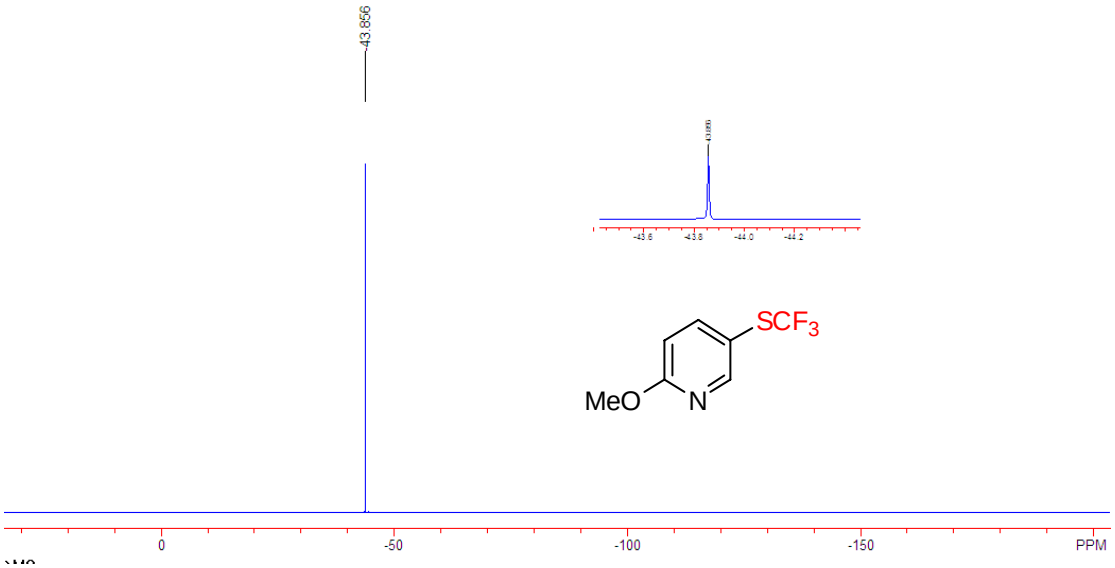
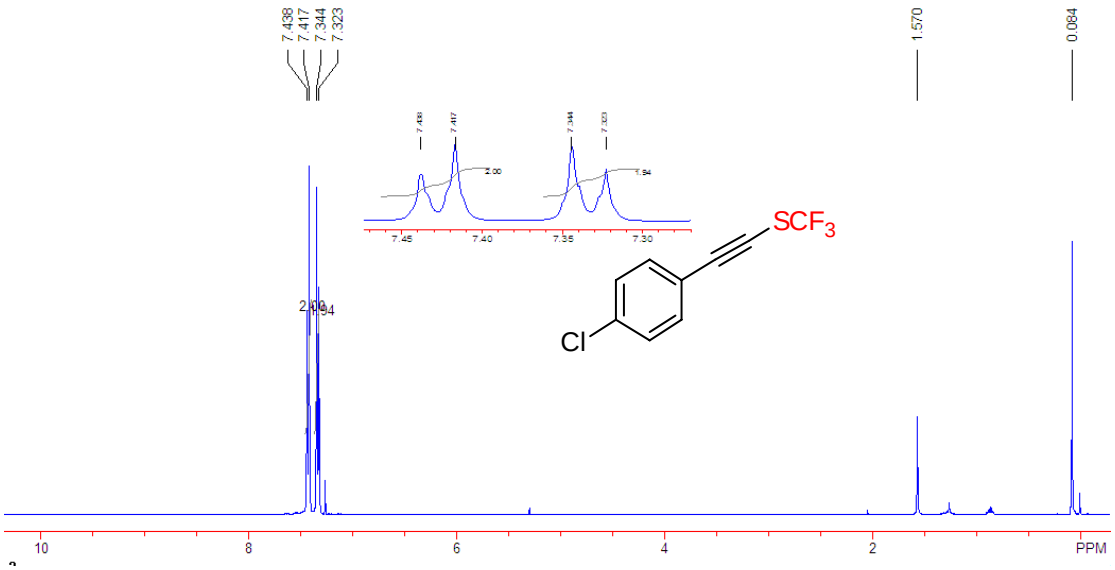
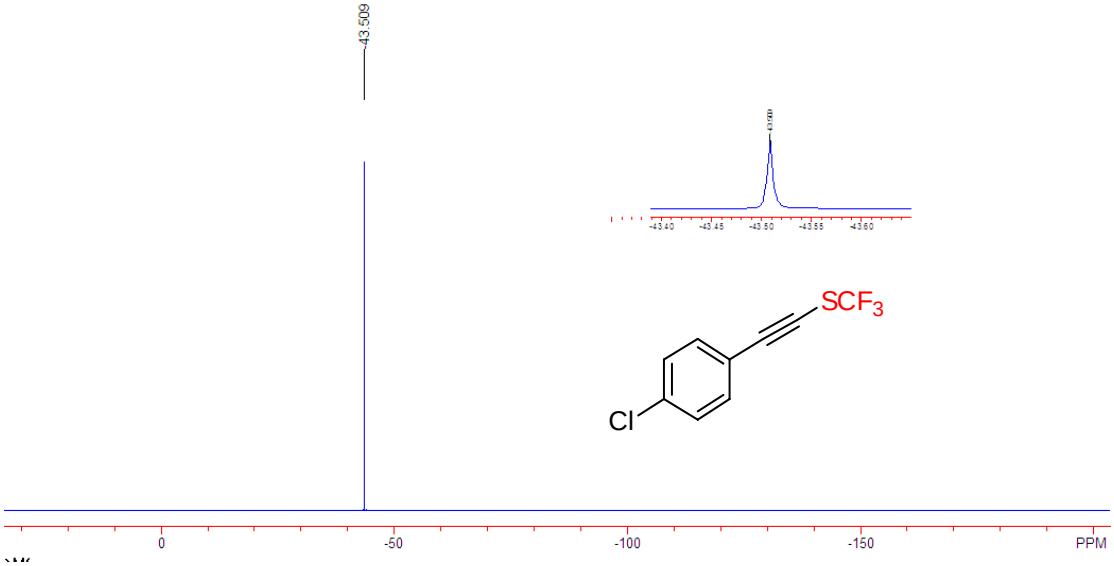


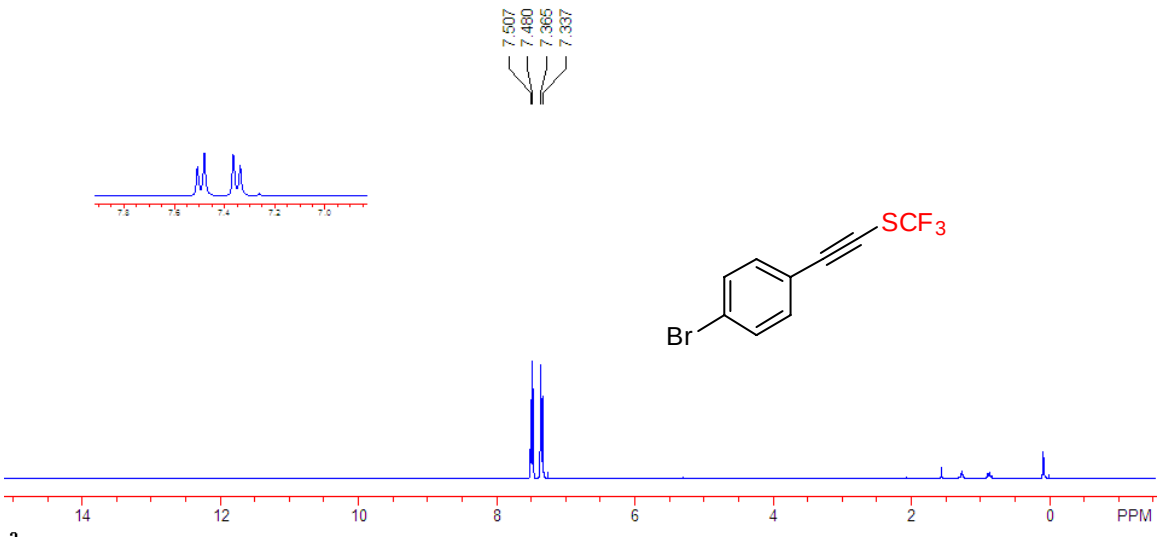
^{1}H NMR spectrum of ((4-Chlorophenyl)ethynyl)(trifluoromethyl)sulfane 7a



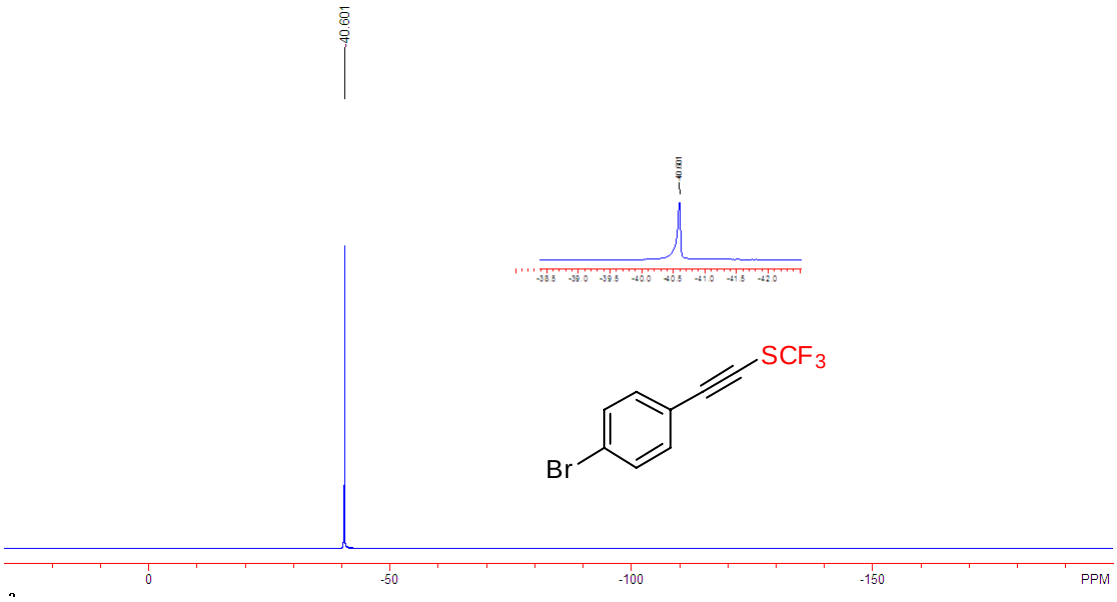
^{19}F NMR spectrum of ((4-Chlorophenyl)ethynyl)(trifluoromethyl)sulfane 7a



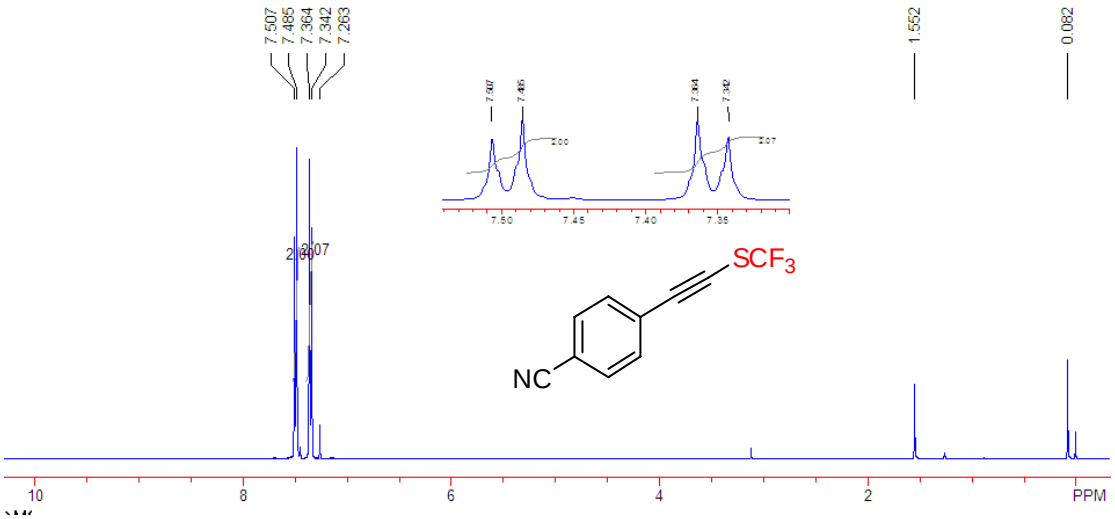
^{1}H NMR spectrum of ((4-Bromophenyl)ethynyl)(trifluoromethyl)sulfane 7b



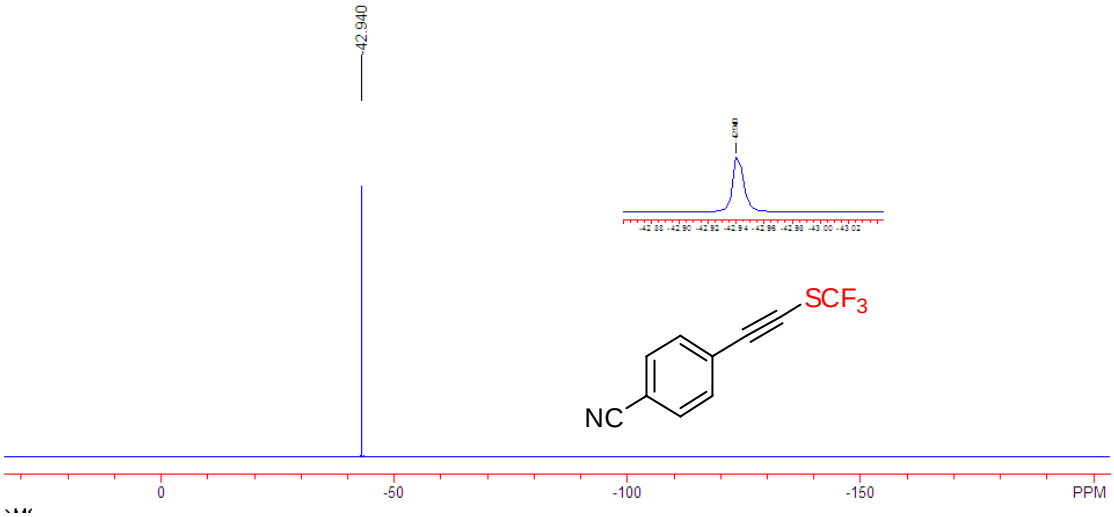
^{19}F NMR spectrum of ((4-Bromophenyl)ethynyl)(trifluoromethyl)sulfane 7b



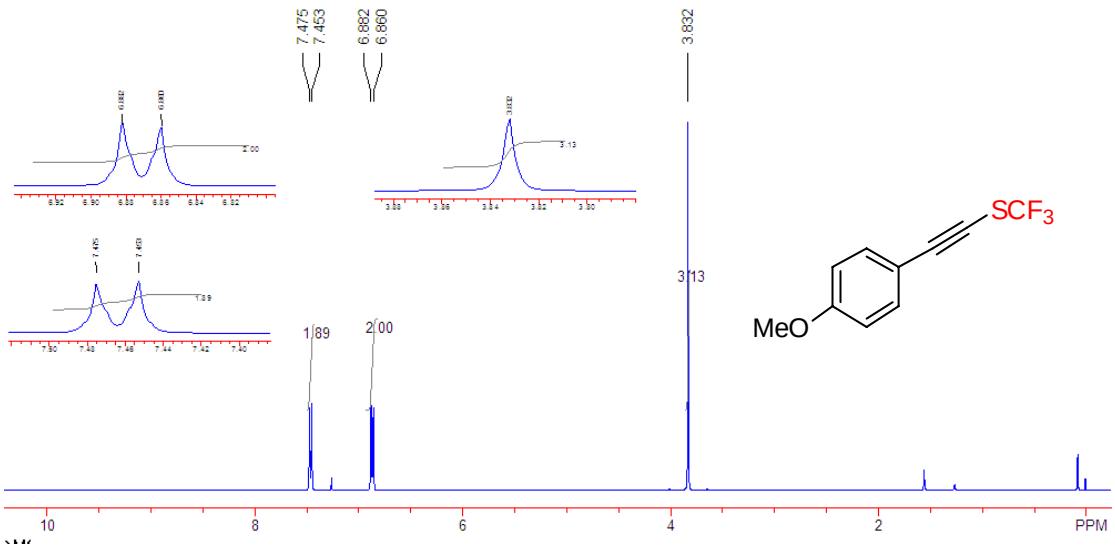
^{1}H NMR spectrum of 4-(((Trifluoromethyl)thio)ethynyl)benzonitrile 7c



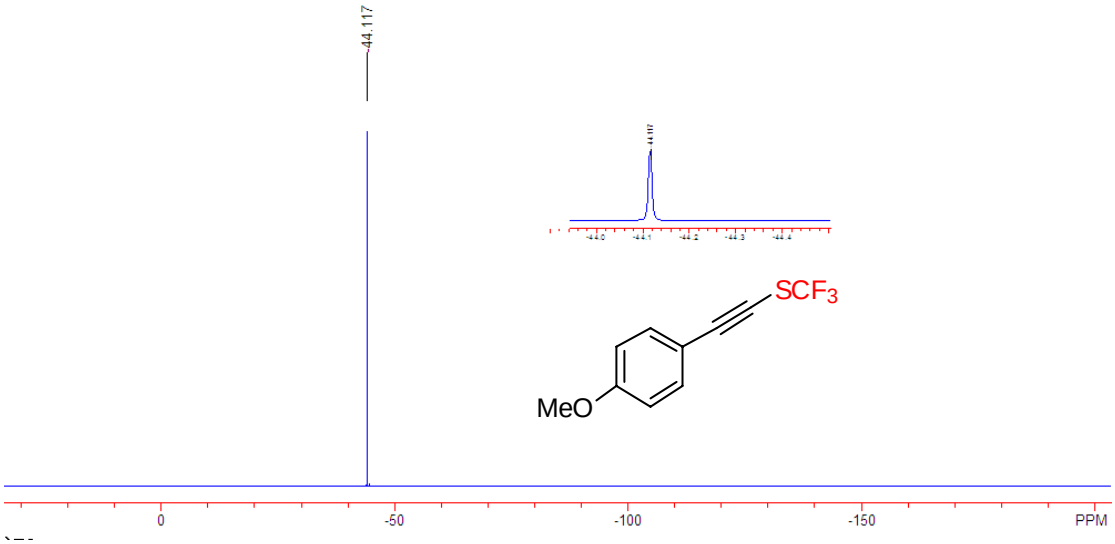
^{19}F NMR spectrum of 4-(((Trifluoromethyl)thio)ethynyl)benzonitrile 7c



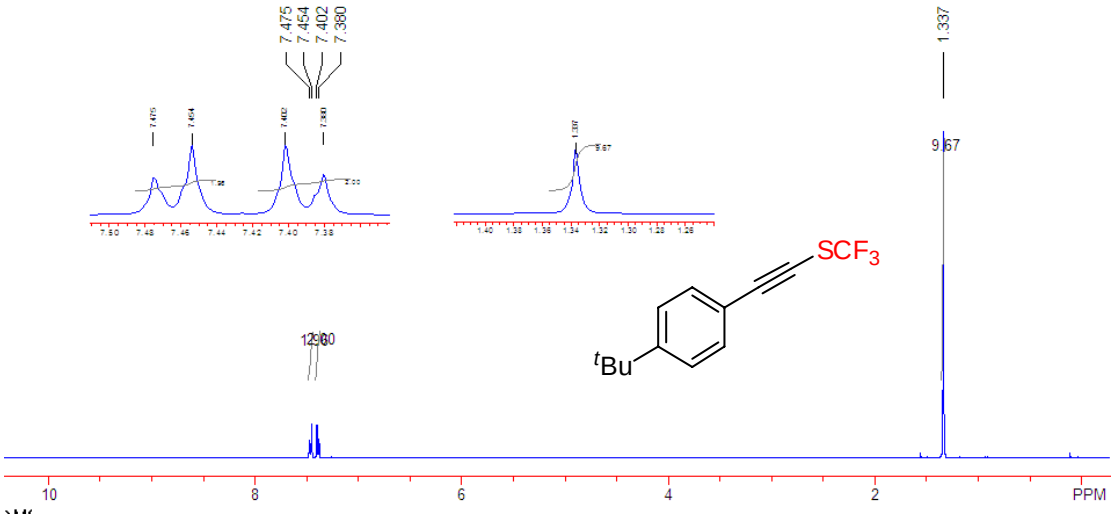
^{1}H NMR spectrum of ((4-Methoxyphenyl)ethynyl)(trifluoromethyl)sulfane 7d



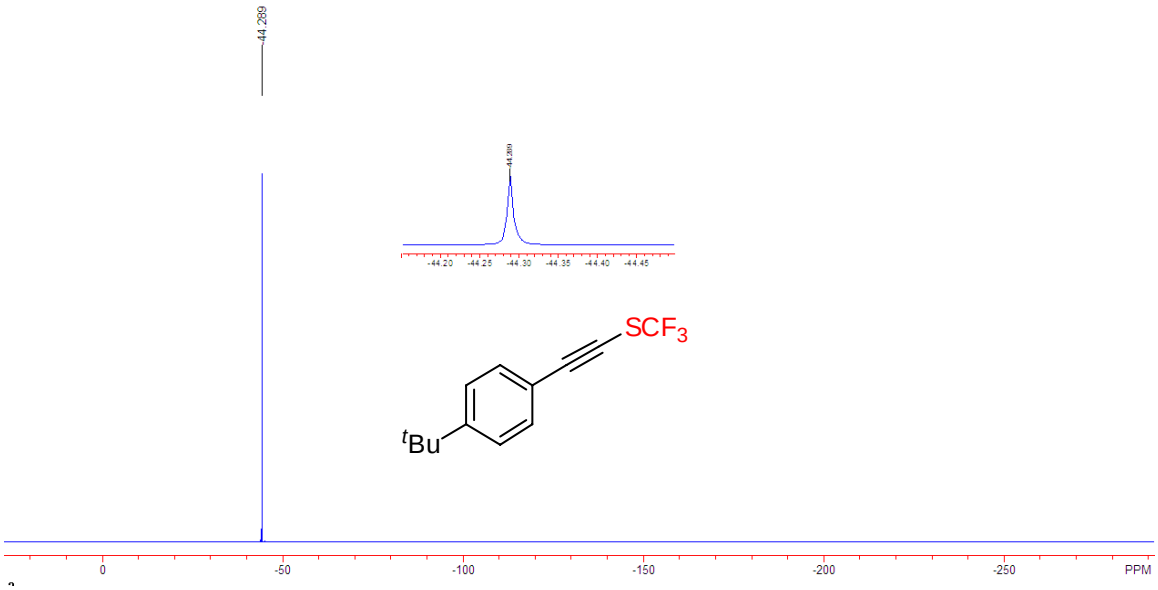
^{19}F NMR spectrum of ((4-Methoxyphenyl)ethynyl)(trifluoromethyl)sulfane 7d



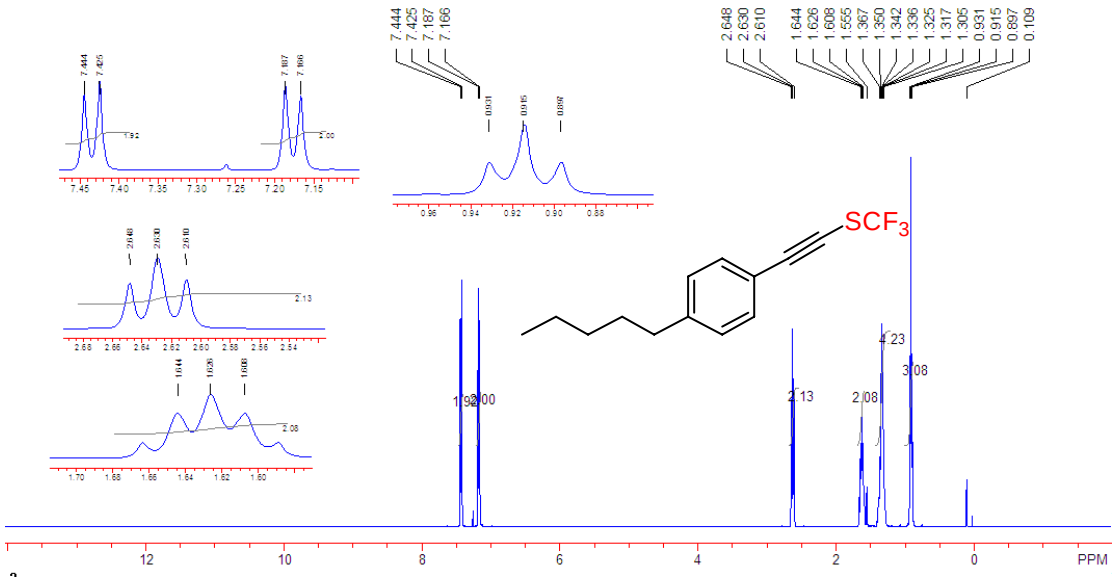
^{1}H NMR spectrum of ((4-*tert*-Butylphenyl)ethynyl)(trifluoromethyl)sulfane 7e



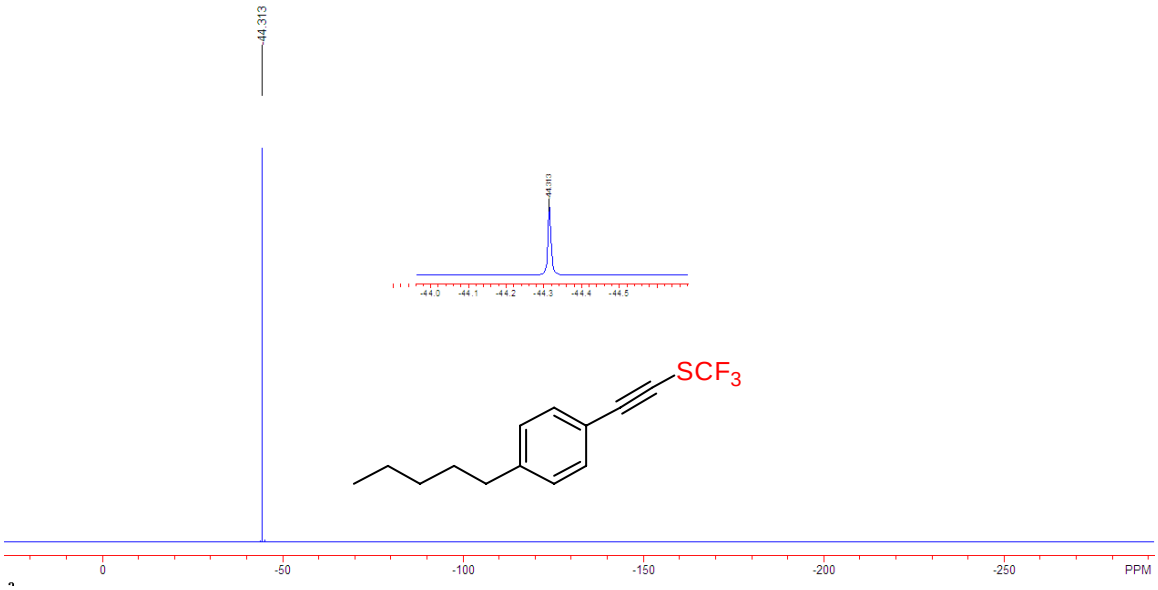
^{19}F NMR spectrum of ((4-*tert*-Butylphenyl)ethynyl)(trifluoromethyl)sulfane 7e



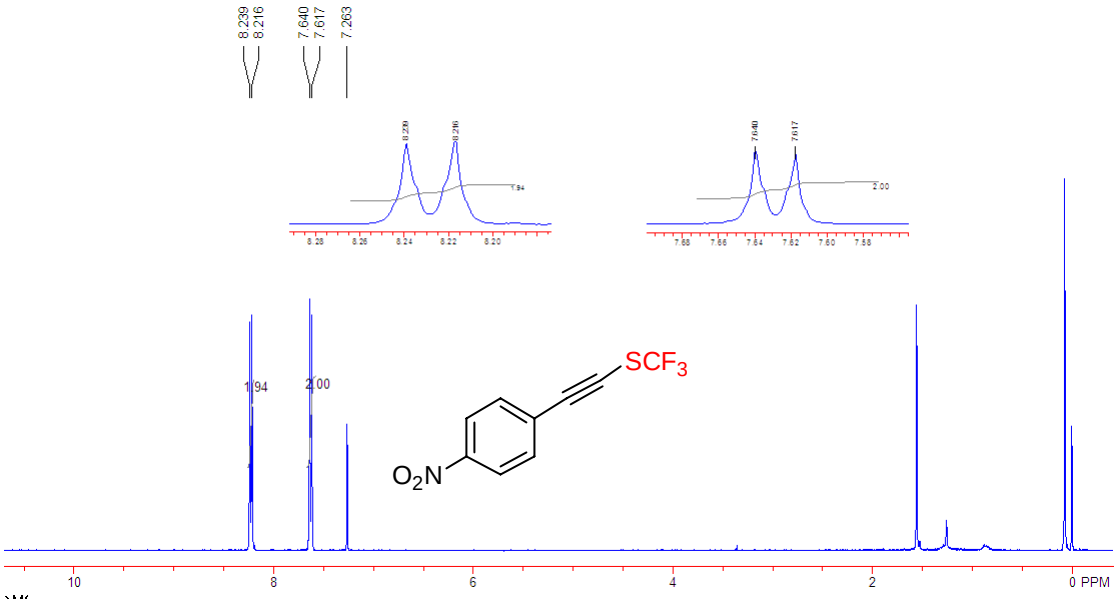
^{1}H NMR spectrum of ((4-pentylphenyl)ethynyl)(trifluoromethyl)sulfane 7f



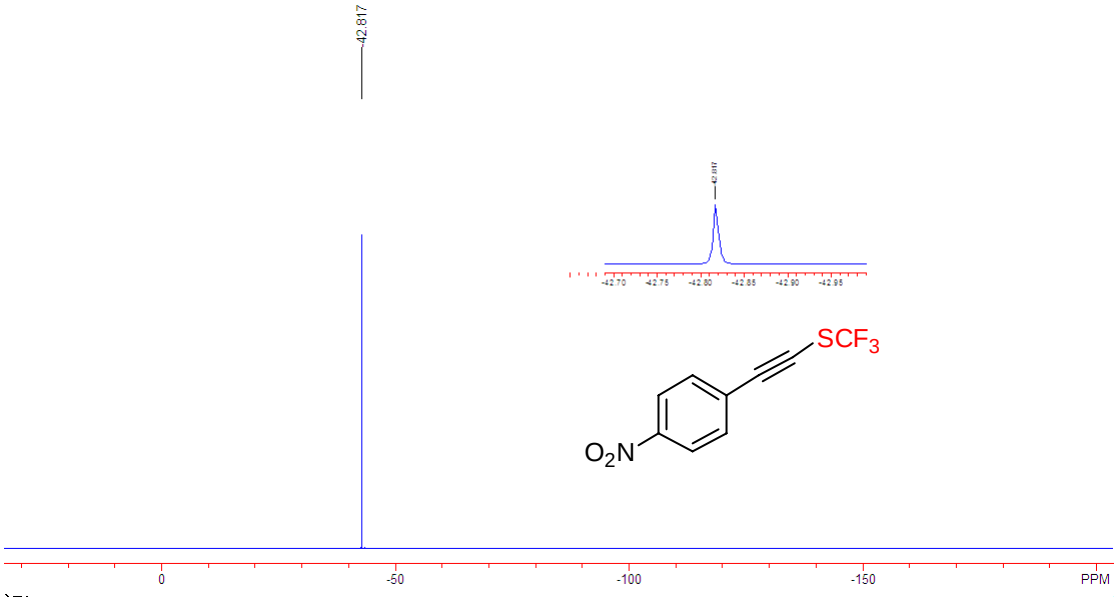
^{19}F NMR spectrum of ((4-pentylphenyl)ethynyl)(trifluoromethyl)sulfane 7f



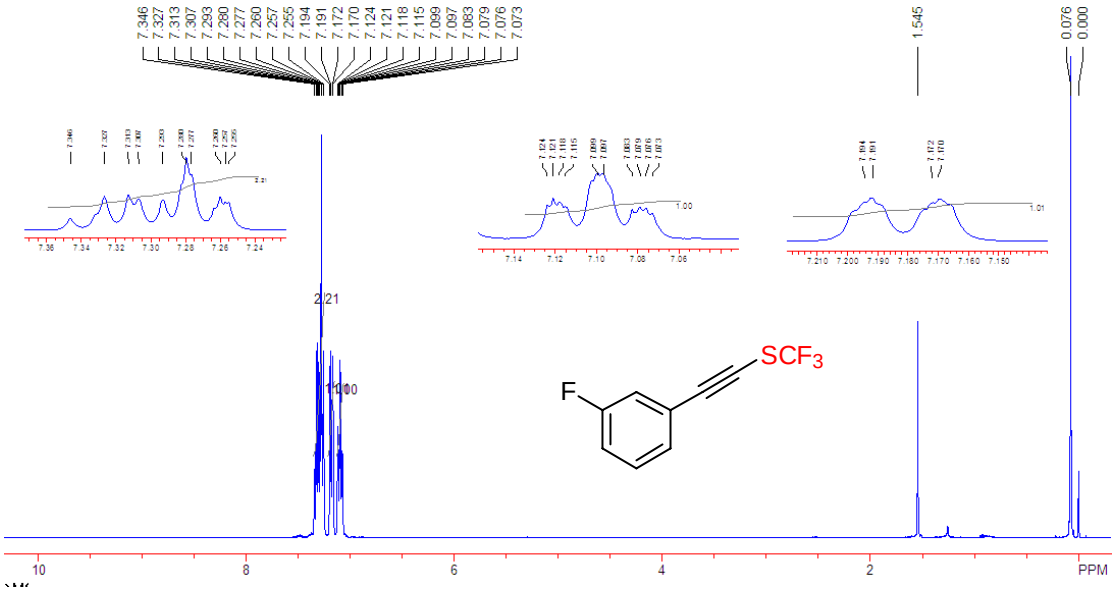
^{1}H NMR spectrum of ((4-Nitrophenyl)ethynyl)(trifluoromethyl)sulfane 7g



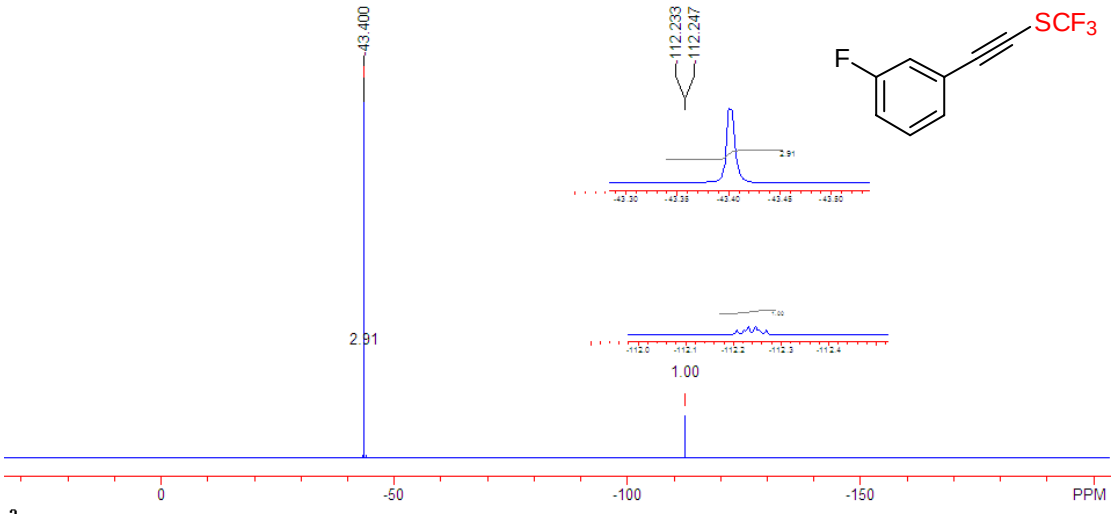
^{19}F NMR spectrum of ((4-Nitrophenyl)ethynyl)(trifluoromethyl)sulfane 7g



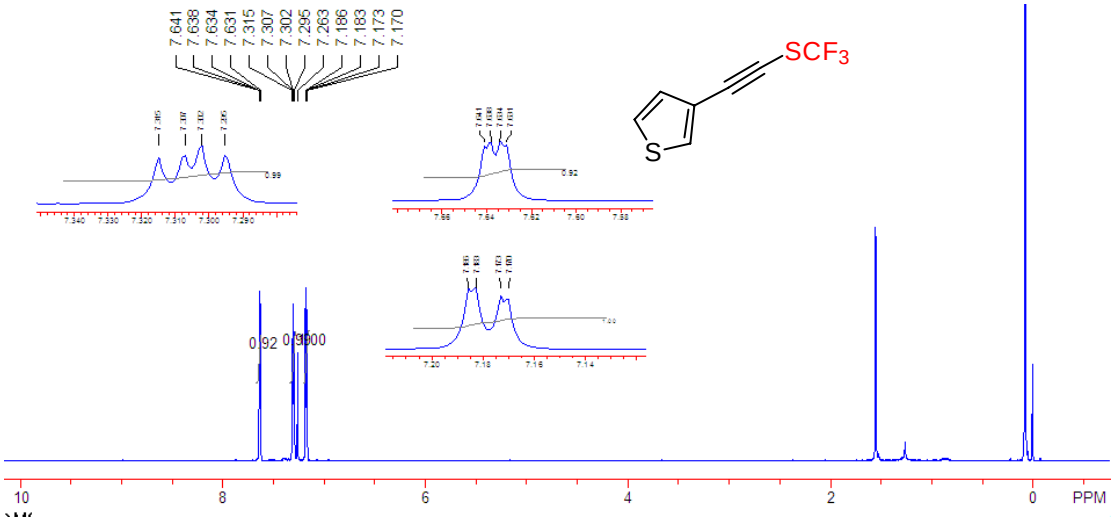
^{1}H NMR spectrum of ((3-Fluorophenyl)ethynyl)(trifluoromethyl)sulfane 7h



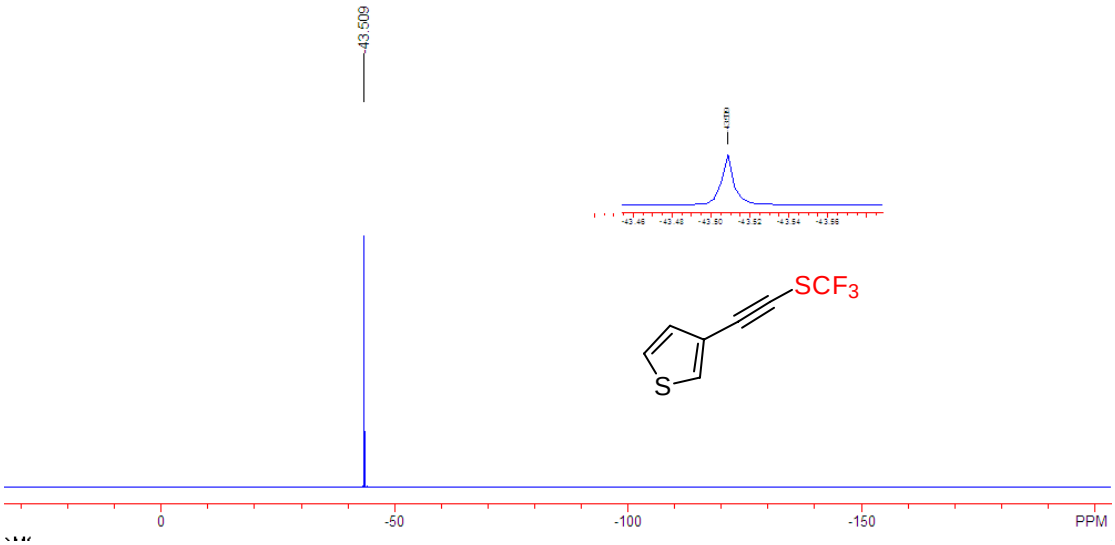
^{19}F NMR spectrum of ((3-Fluorophenyl)ethynyl)(trifluoromethyl)sulfane 7h



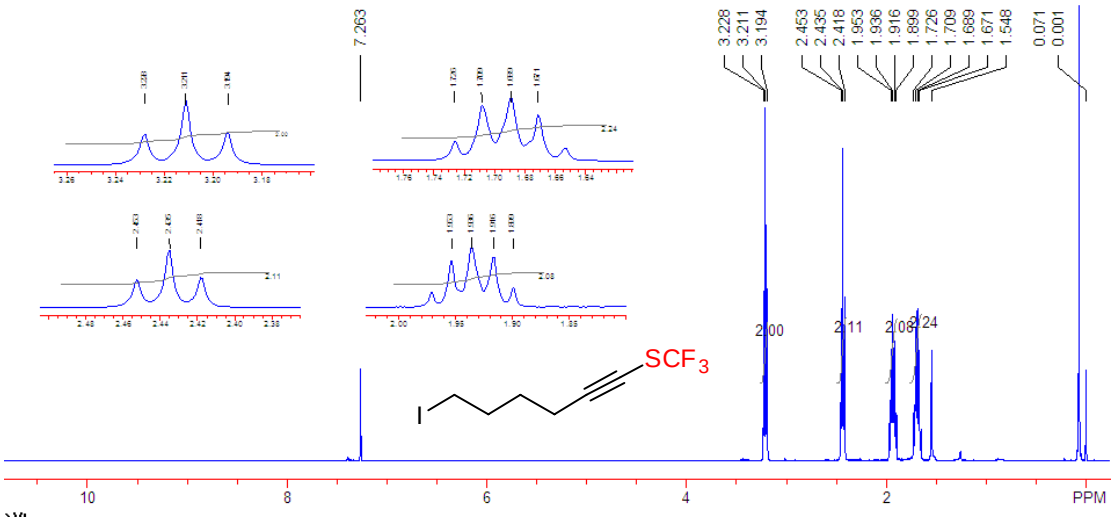
^{1}H NMR spectrum of 3-((Trifluoromethylthio)ethynyl)thiophene 7i



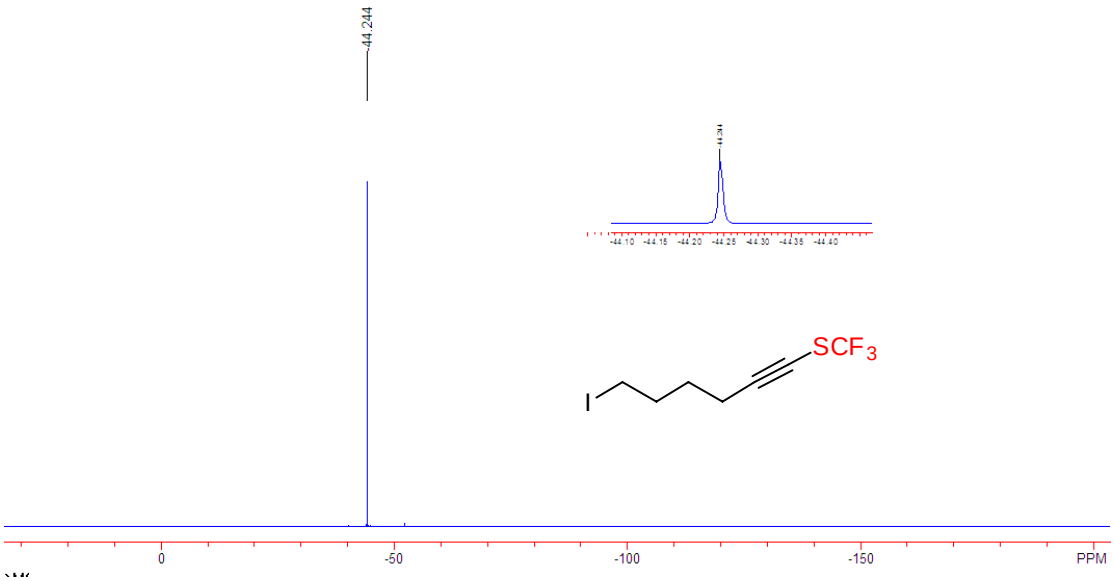
^{19}F NMR spectrum of 3-((Trifluoromethylthio)ethynyl)thiophene 7i



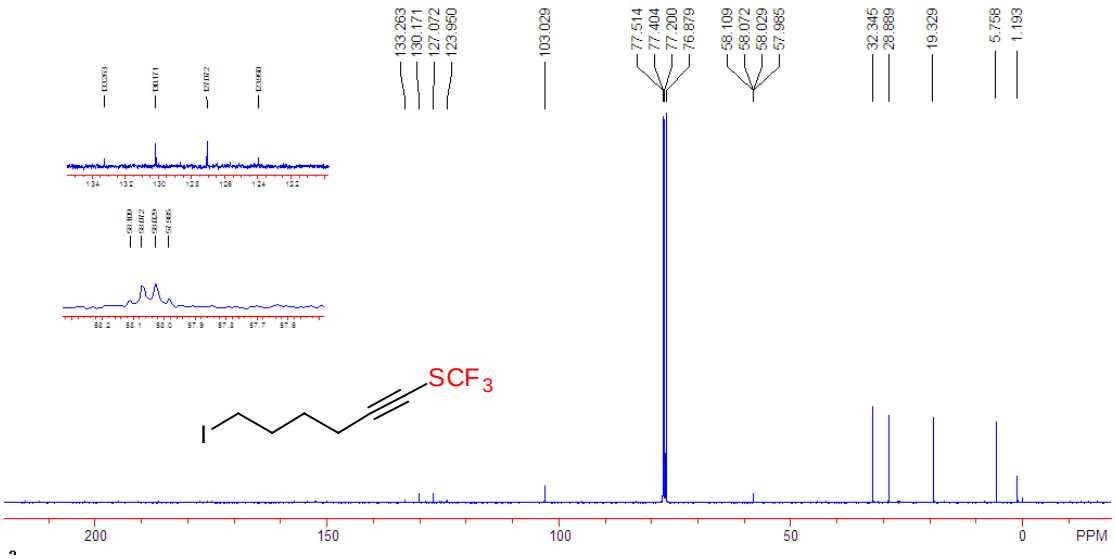
^{1}H NMR spectrum of (6-Iodohex-1-yn-1-yl)(trifluoromethyl)sulfane 7j



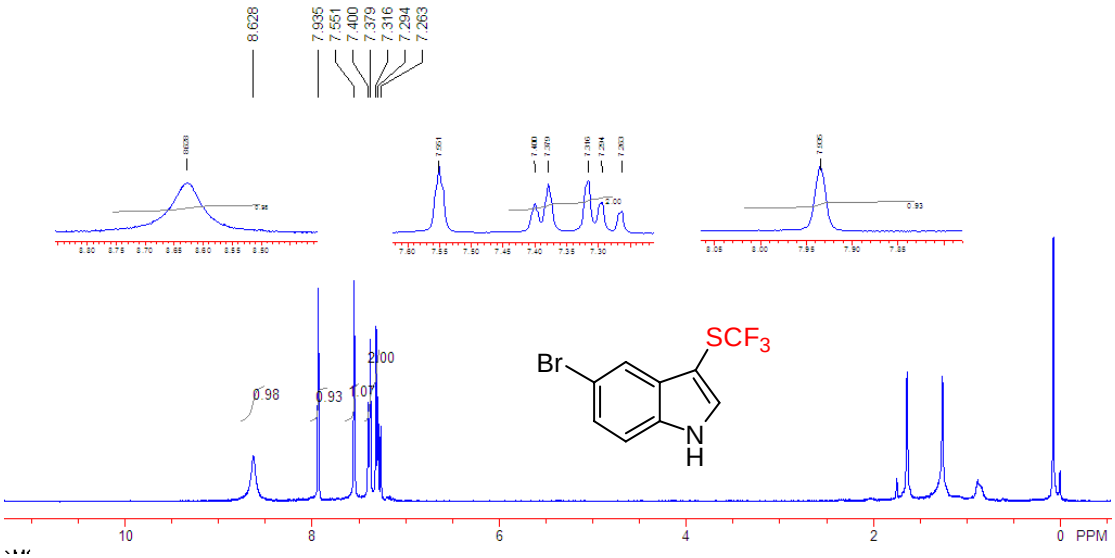
^{19}F NMR spectrum of (6-Iodohex-1-yn-1-yl)(trifluoromethyl)sulfane 7j



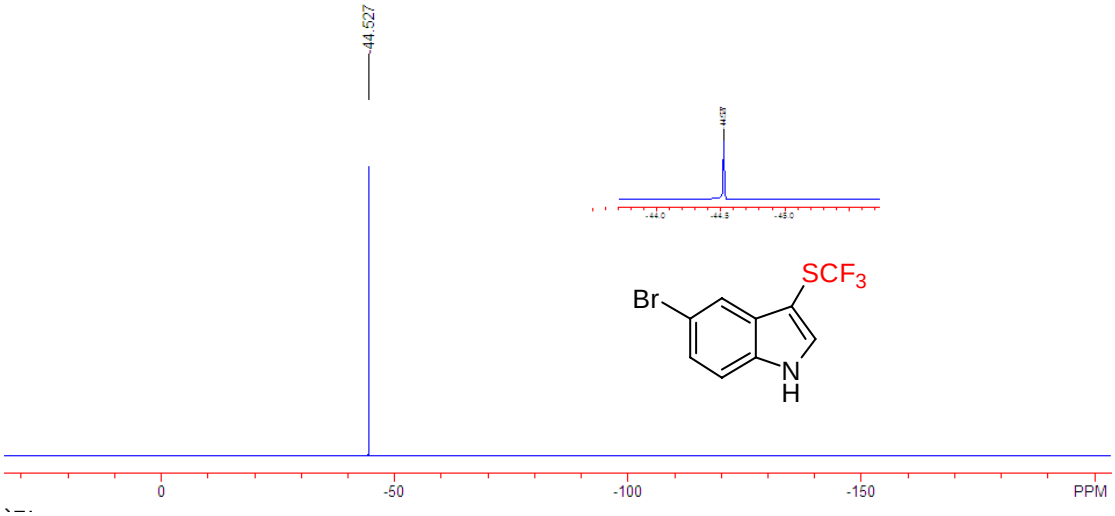
^{13}C NMR spectrum of (6-Iodohex-1-yn-1-yl)(trifluoromethyl)sulfane 7j



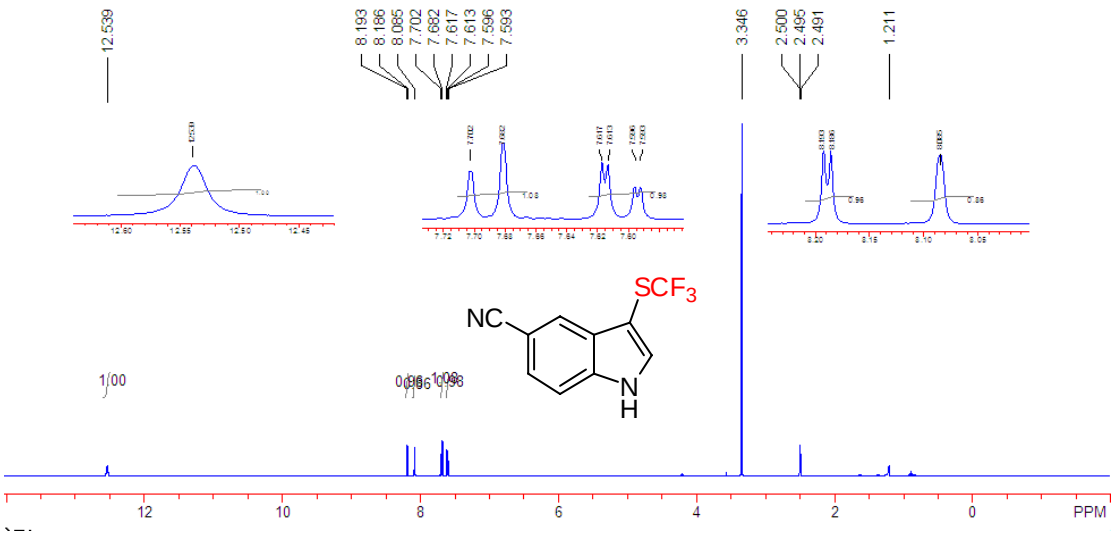
^{1}H NMR spectrum of 5-bromo-3-((trifluoromethyl)thio)-1H-indole 8a



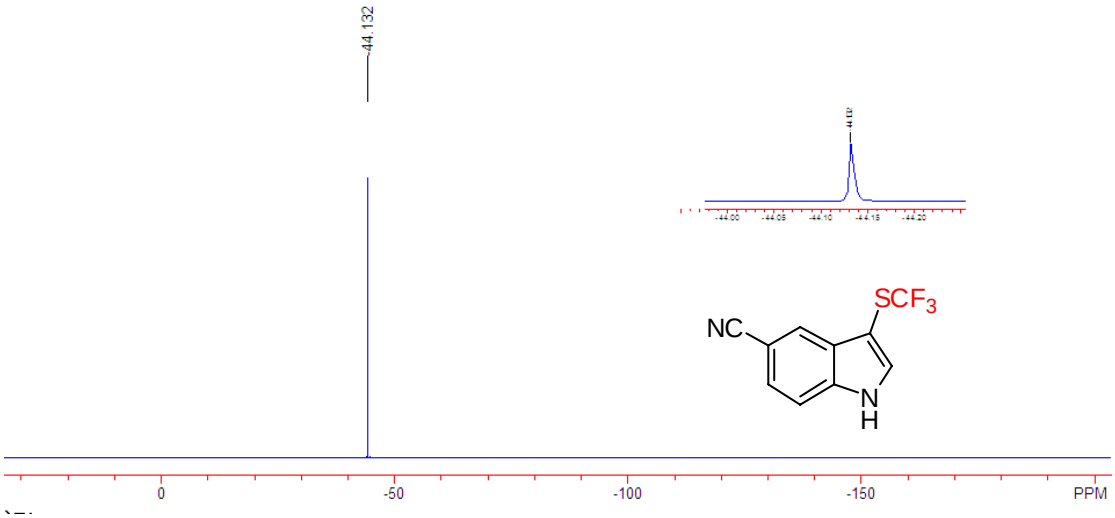
^{19}F NMR spectrum of5-bromo-3-((trifluoromethyl)thio)-1H-indole 8a



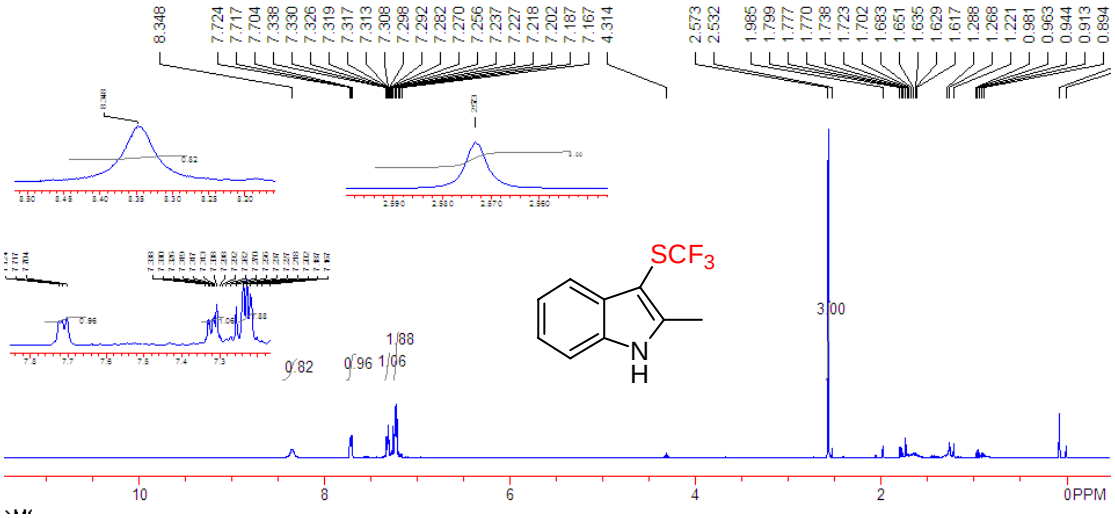
^{1}H NMR spectrum of 3-((Trifluoromethyl)thio)-1H-indole-5-carbonitrile 8b



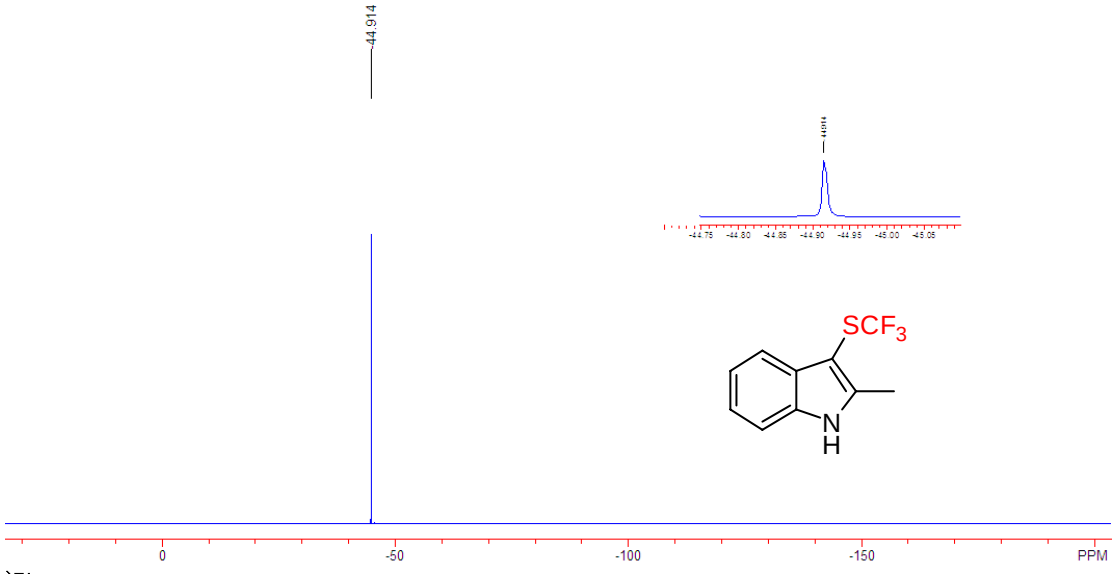
^{19}F NMR spectrum of 3-((Trifluoromethyl)thio)-1H-indole-5-carbonitrile 8b



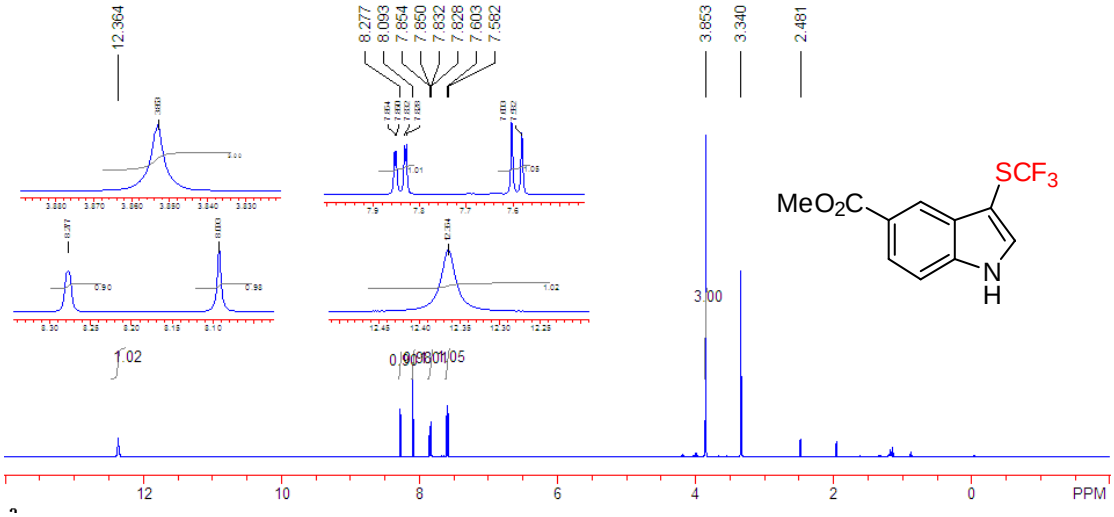
^{1}H NMR spectrum of 2-Methyl-3-((trifluoromethyl)thio)-1H-indole 8c



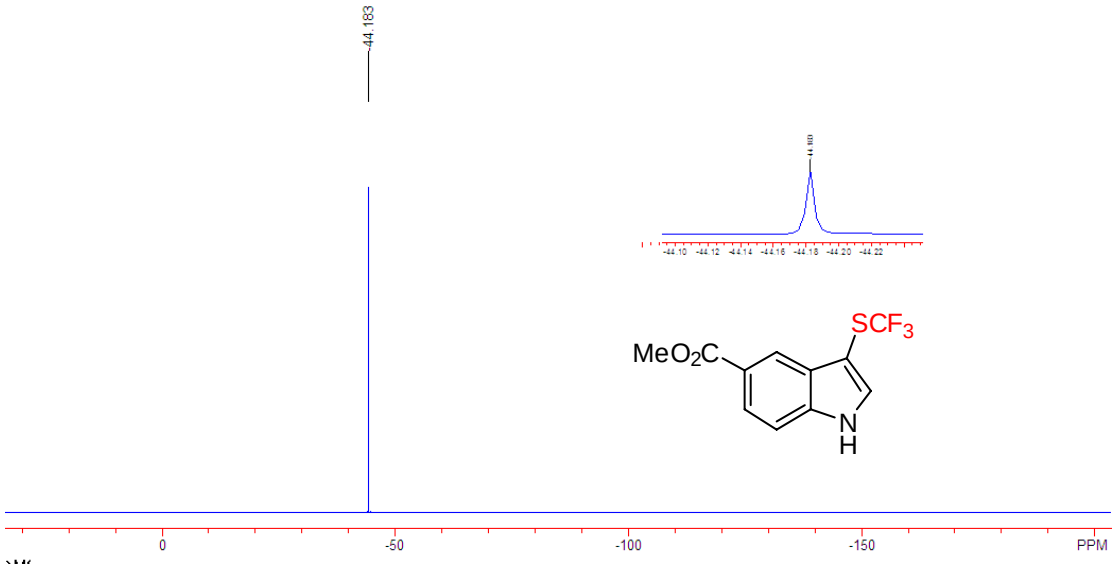
^{19}F NMR spectrum of 2-Methyl-3-((trifluoromethyl)thio)-1H-indole 8c



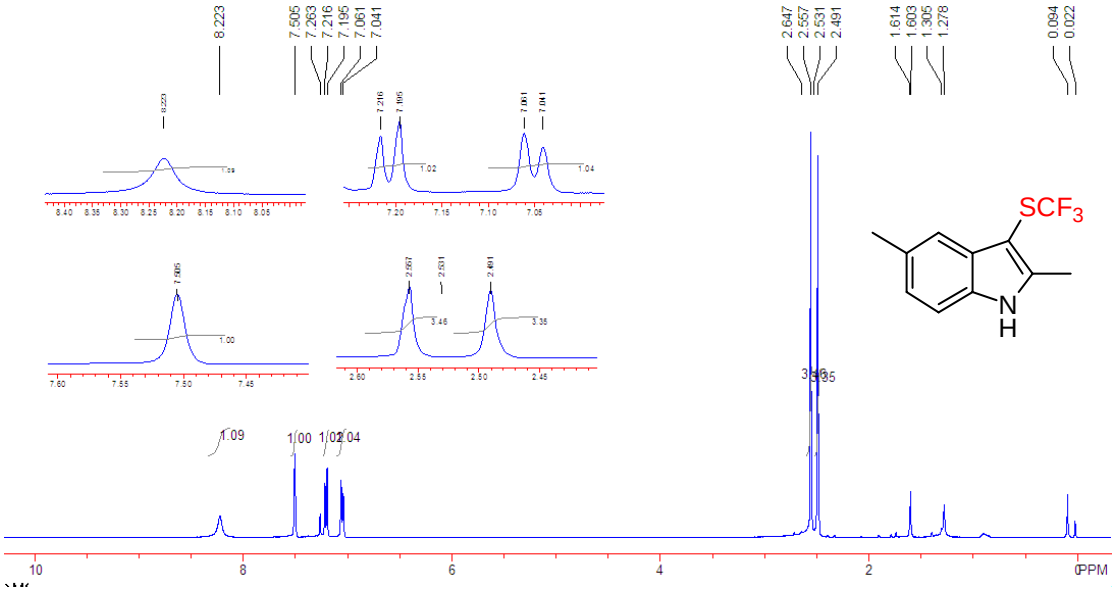
^{1}H NMR spectrum of 2-Methyl-3-((trifluoromethyl)thio)-1H-indole 8d



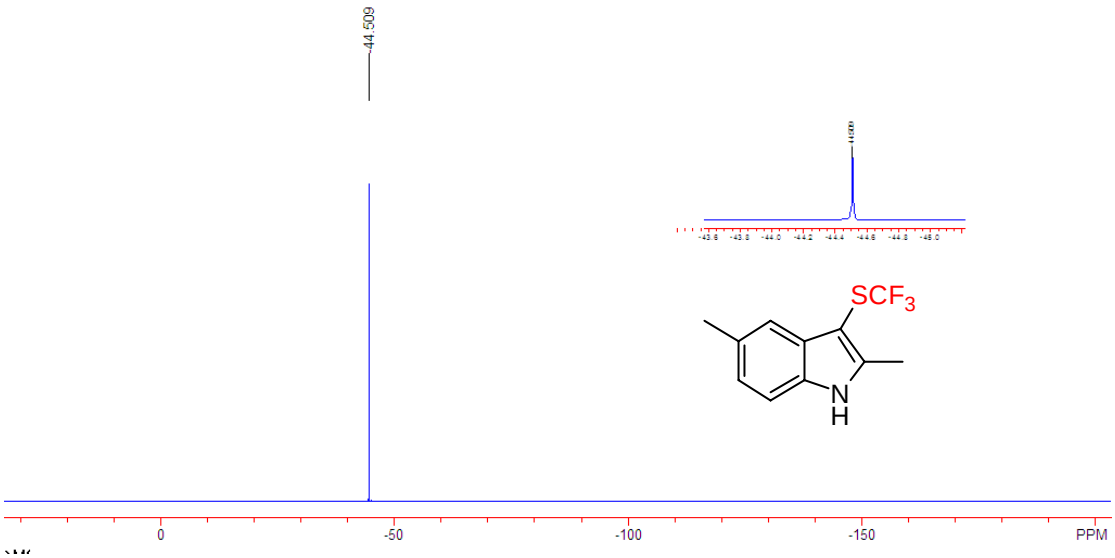
^{19}F NMR spectrum of 2-Methyl-3-((trifluoromethyl)thio)-1H-indole 8d



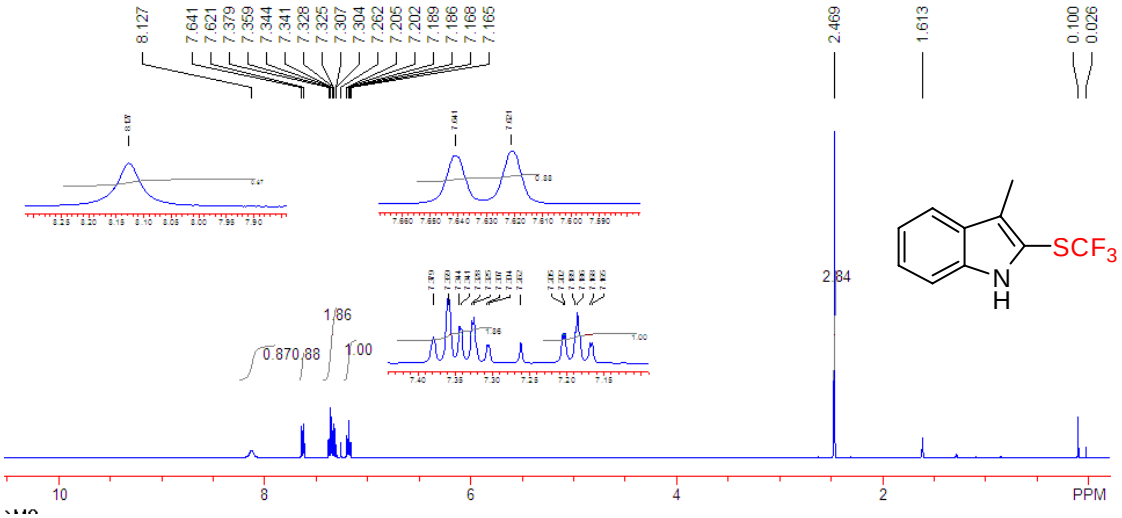
^{1}H NMR spectrum of 2,5-Dimethyl-3-((trifluoromethyl)thio)-1H-indole 8e



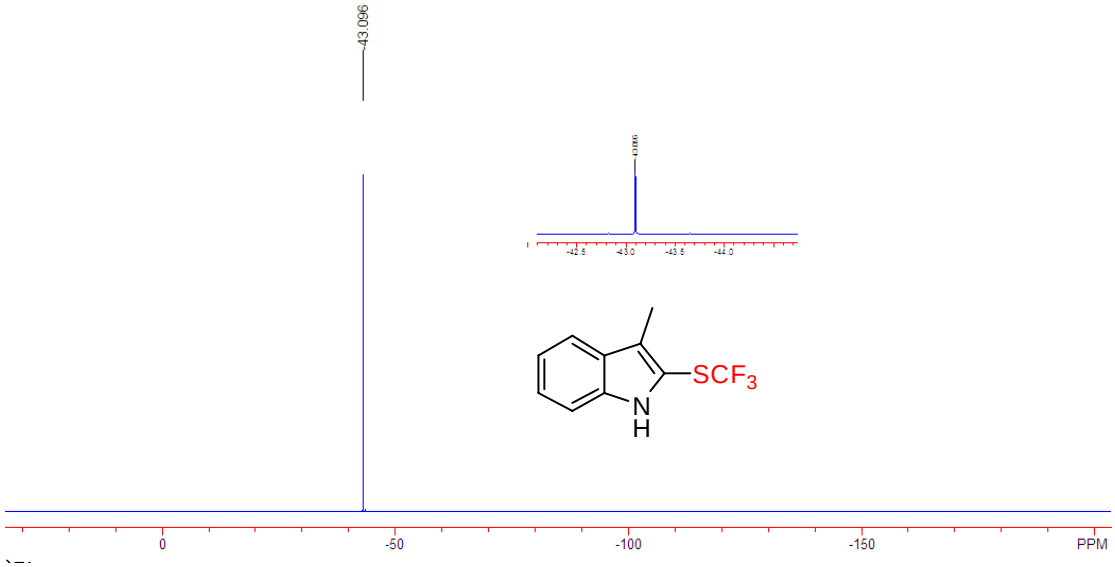
^{19}F NMR spectrum of 2,5-Dimethyl-3-((trifluoromethyl)thio)-1H-indole 8e



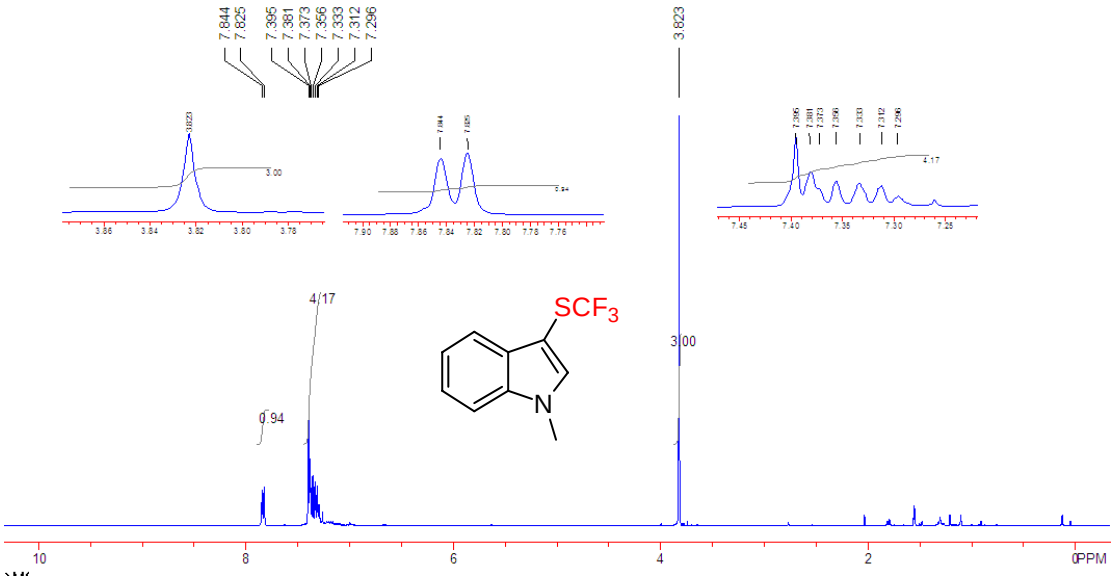
^{1}H NMR spectrum of 3-Methyl-2-((trifluoromethyl)thio)-1H-indole 8f



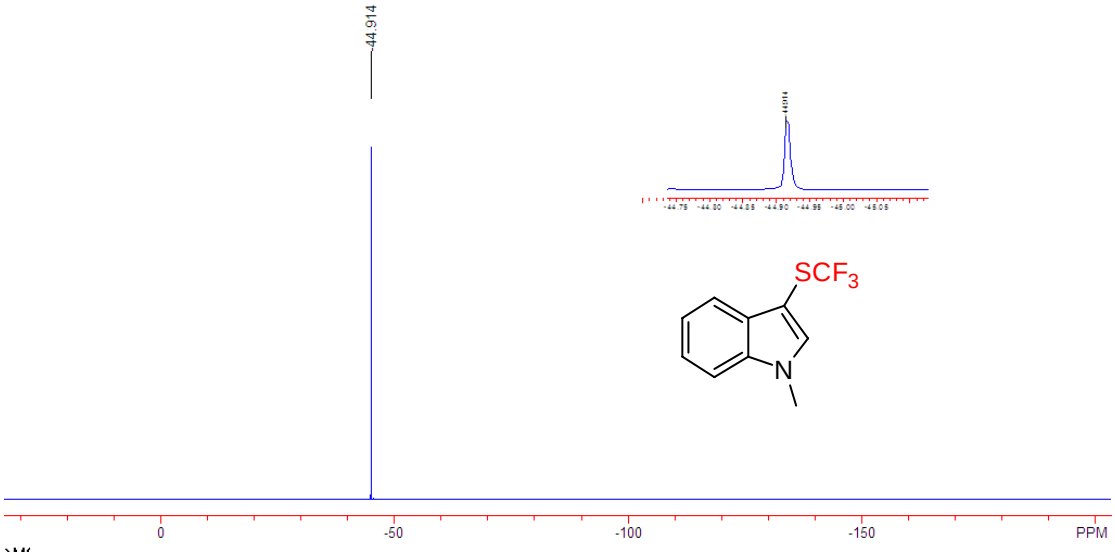
^{19}F NMR spectrum of 3-Methyl-2-((trifluoromethyl)thio)-1H-indole 8f



^{1}H NMR spectrum of 1-Methyl-3-((trifluoromethyl)thio)-1H-indole 8g

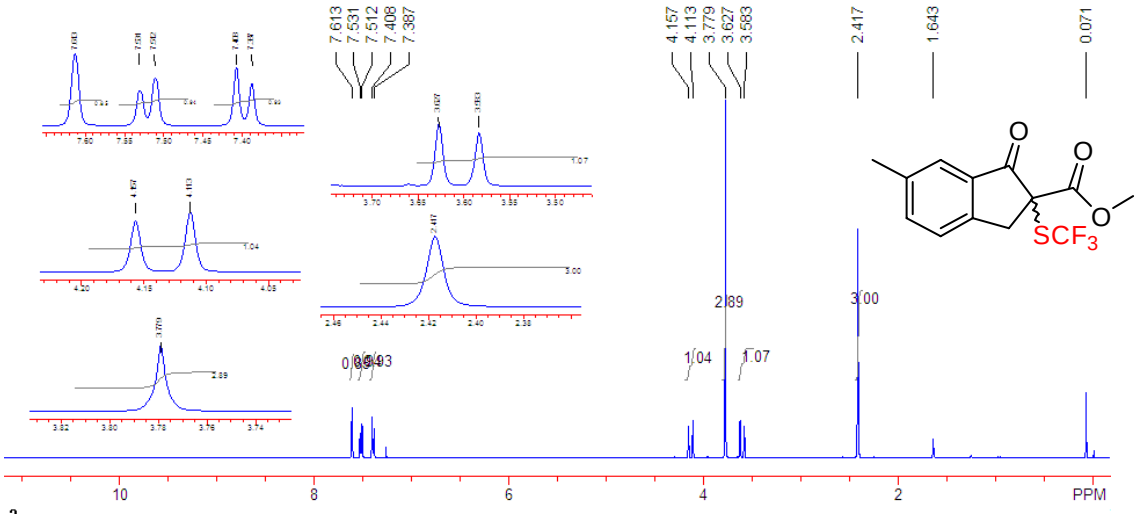


^{19}F NMR spectrum of 1-Methyl-3-((trifluoromethyl)thio)-1H-indole 8g



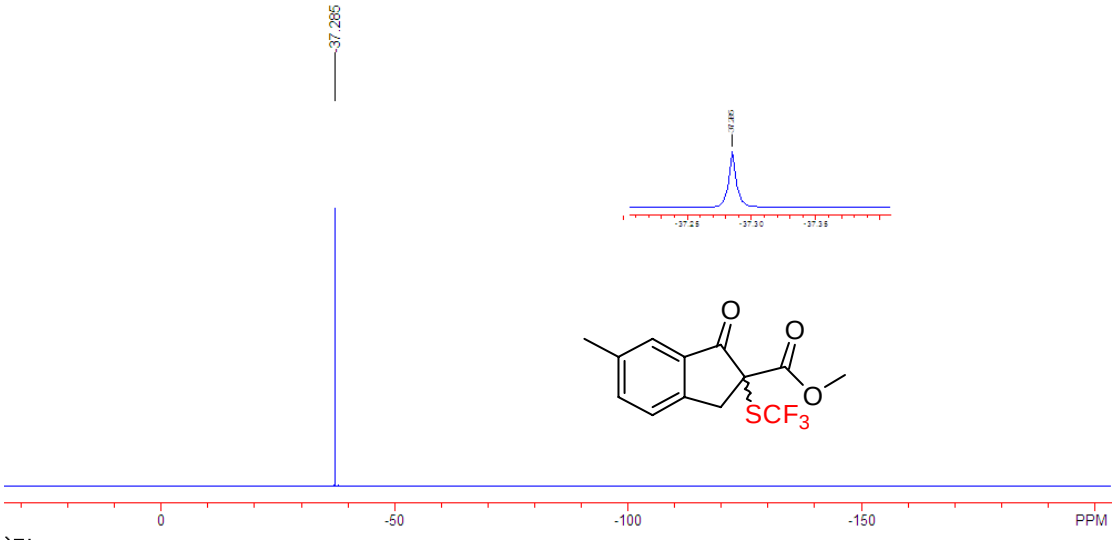
^{1}H NMR spectrum of Methyl

6-methyl-1-oxo-2-((trifluoromethyl)thio)-2,3-dihydro-1H-indene-2-carboxylate 9a



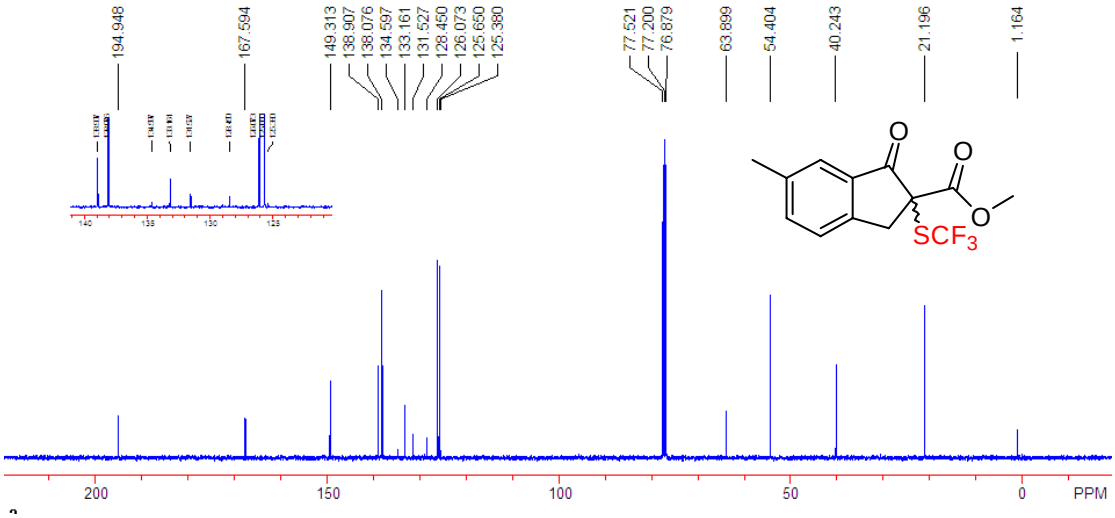
^{19}F NMR spectrum of Methyl

6-methyl-1-oxo-2-((trifluoromethyl)thio)-2,3-dihydro-1H-indene-2-carboxylate ate 9a

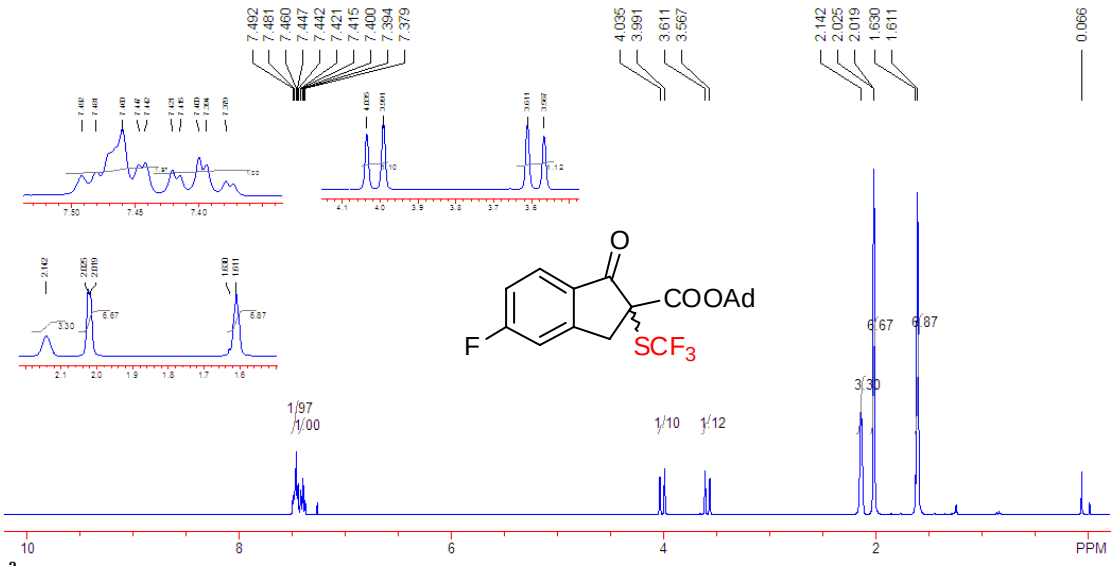


^{13}C NMR spectrum of Methyl

6-methyl-1-oxo-2-((trifluoromethyl)thio)-2,3-dihydro-1H-indene-2-carboxylate 9a

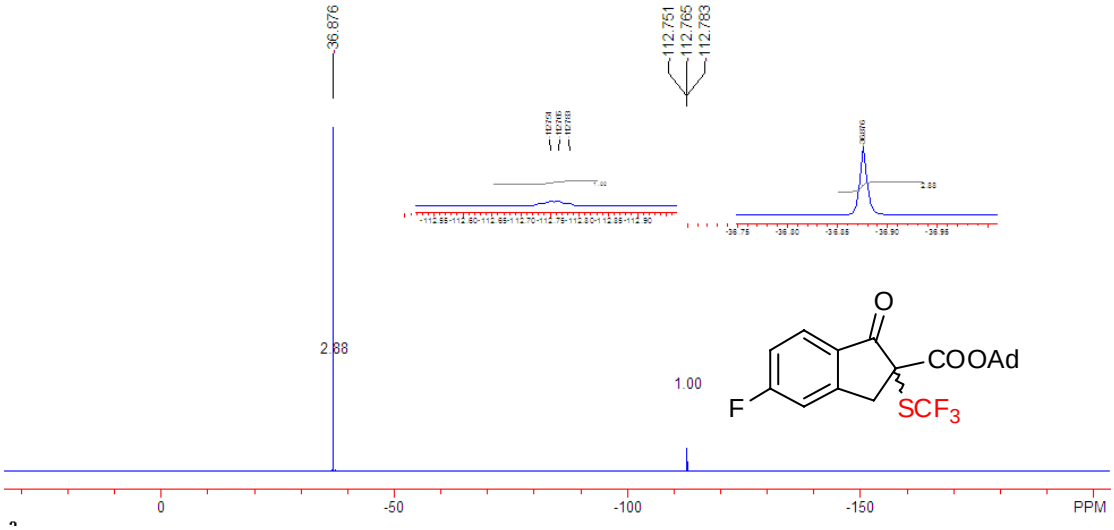


^{1}H NMR spectrum of Adamantan-1-yl 5-fluoro-1-oxo-2-((trifluoromethyl)thio)-2,3-dihydr o-1H-indene-2-carboxylate 9b



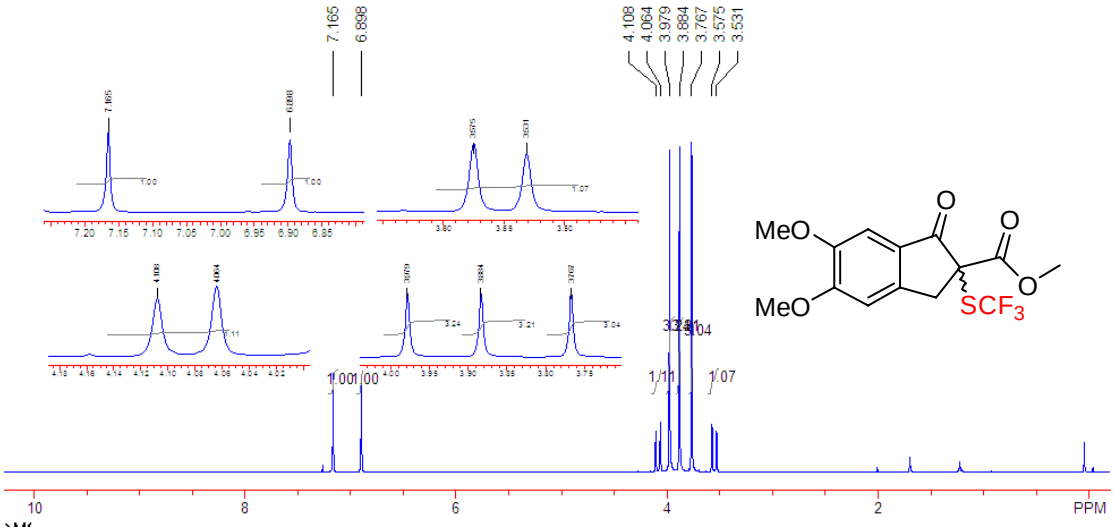
^{19}F NMR spectrum of Adamantan-1-yl

5-fluoro-1-oxo-2-((trifluoromethyl)thio)-2,3-dihydro-1H-indene-2-carboxylate 9b



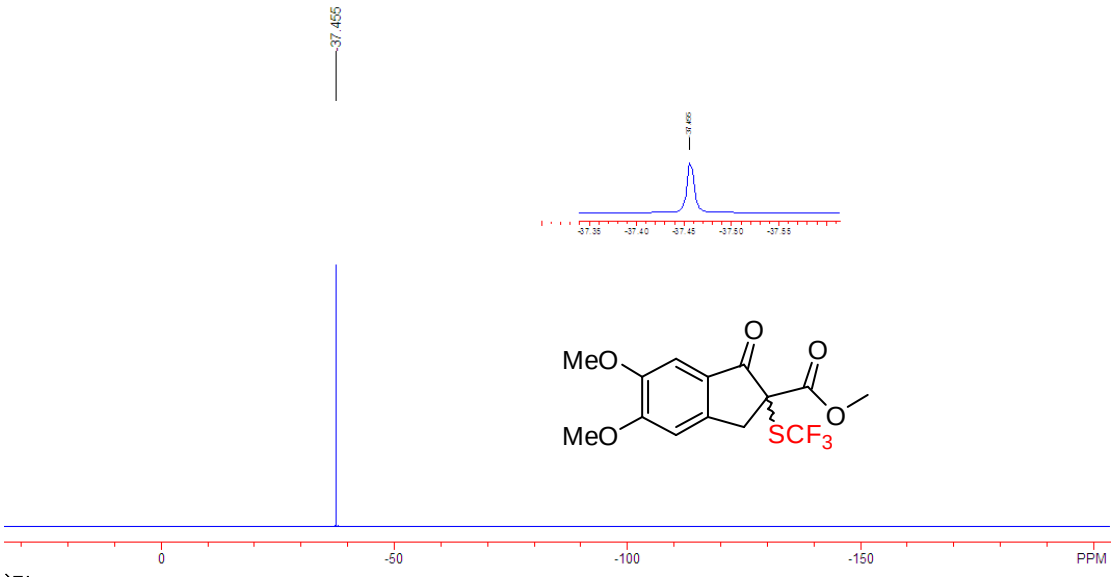
^{1}H NMR spectrum of Methyl

5,6-dimethoxy-1-oxo-2-((trifluoromethyl)thio)-2,3-dihydro-1*H*-indene-2-carboxylate 9c



^{19}F NMR spectrum of Methyl

5,6-dimethoxy-1-oxo-2-((trifluoromethyl)thio)-2,3-dihydro-1*H*-indene-2-carboxylate 9c



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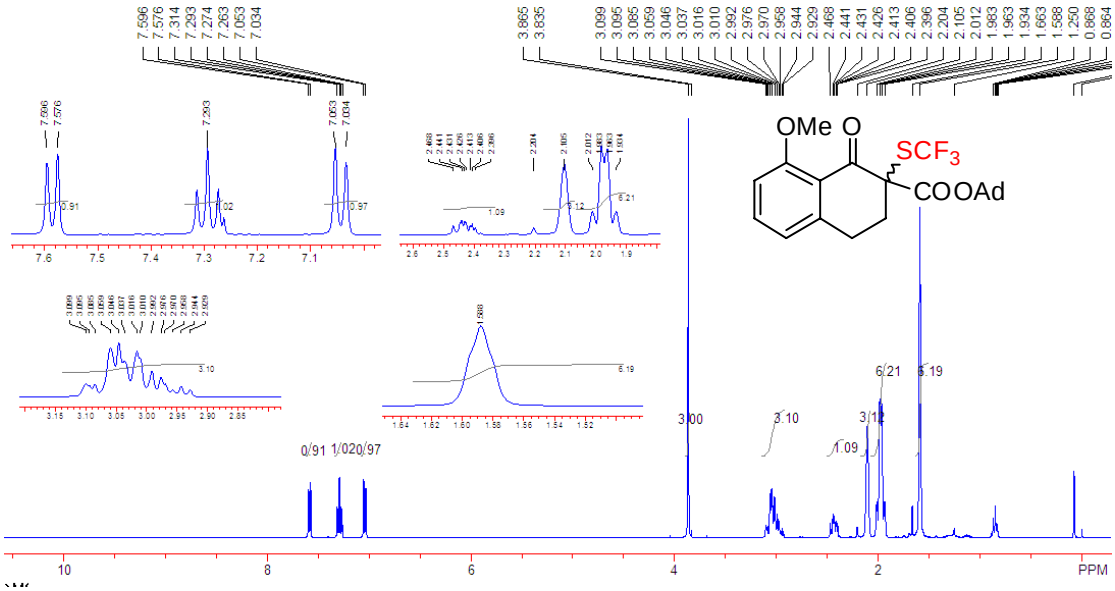
^{1}H NMR spectrum of Adamantanyl

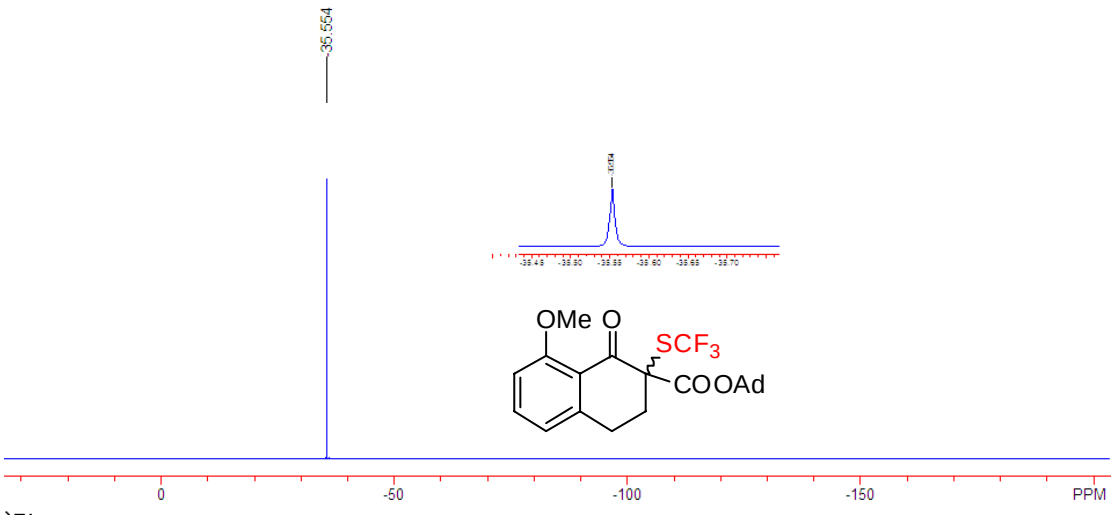
5-methoxy-1-oxo-2-((trifluoromethyl)thio)-1,2,3,4-tetrahydronaphthalene-2-carboxylate ate

9d



^{19}F NMR spectrum of Adamantanyl

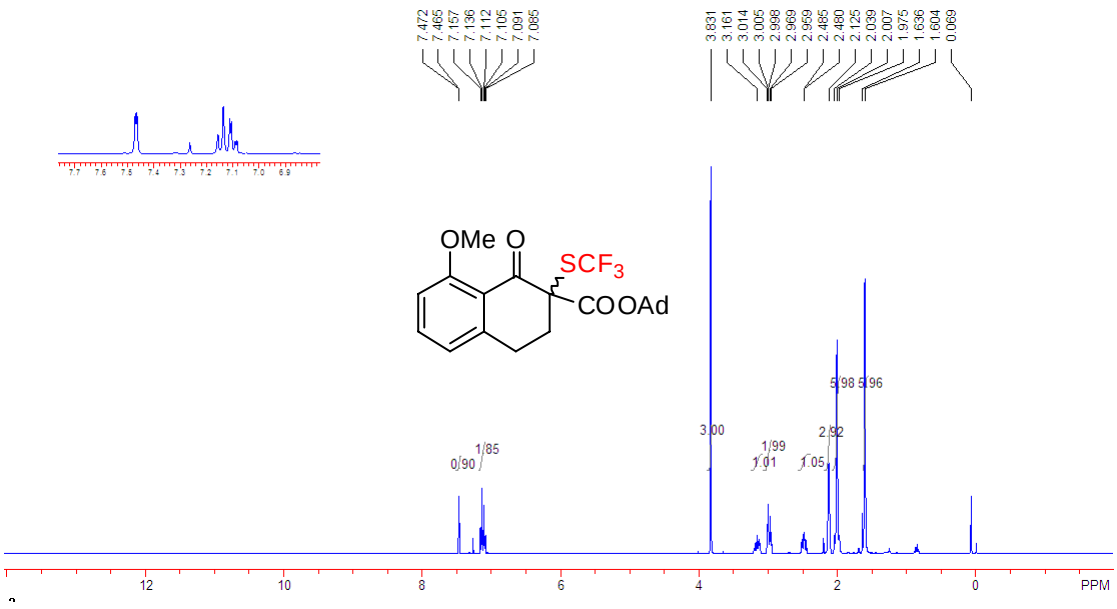
5-methoxy-1-oxo-2-((trifluoromethyl)thio)-1,2,3,4-tetrahydronaphthalene-2-carboxylate 9d



^{1}H NMR spectrum of Adamantanyl

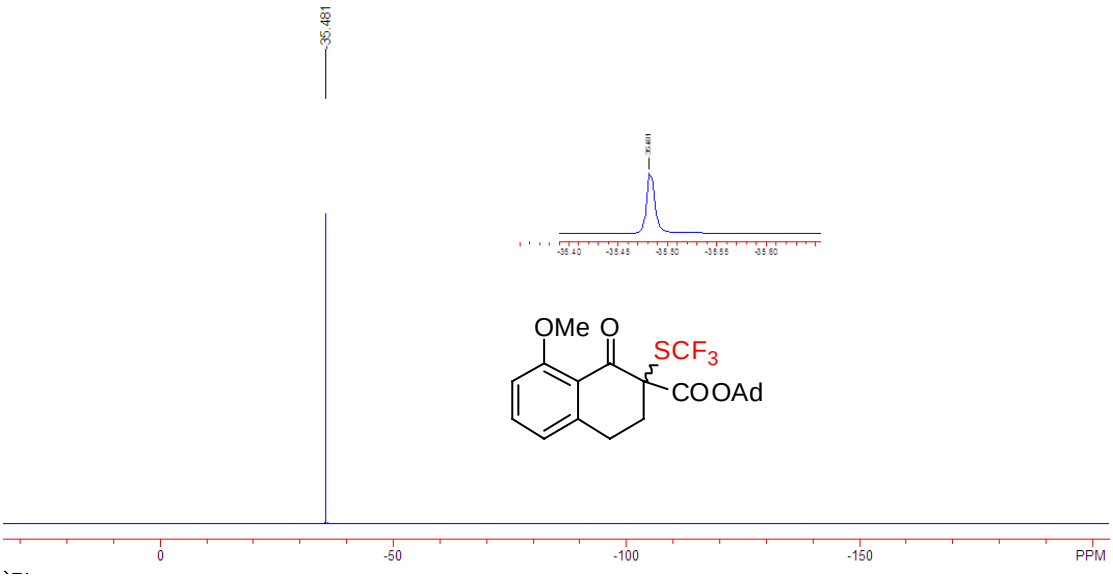
8-methoxy-1-oxo-2-((trifluoromethyl)thio)-1,2,3,4-tetrahydronaphthalene-2-carboxylate ate

9e



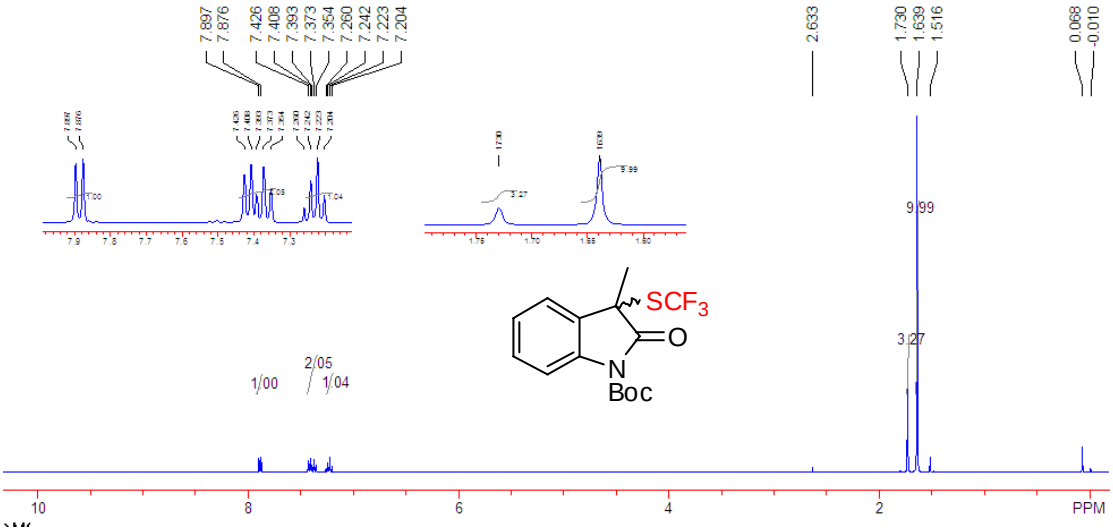
^{19}F NMR spectrum of Adamantanyl

8-methoxy-1-oxo-2-((trifluoromethyl)thio)-1,2,3,4-tetrahydronaphthalene-2-carboxylate 9e



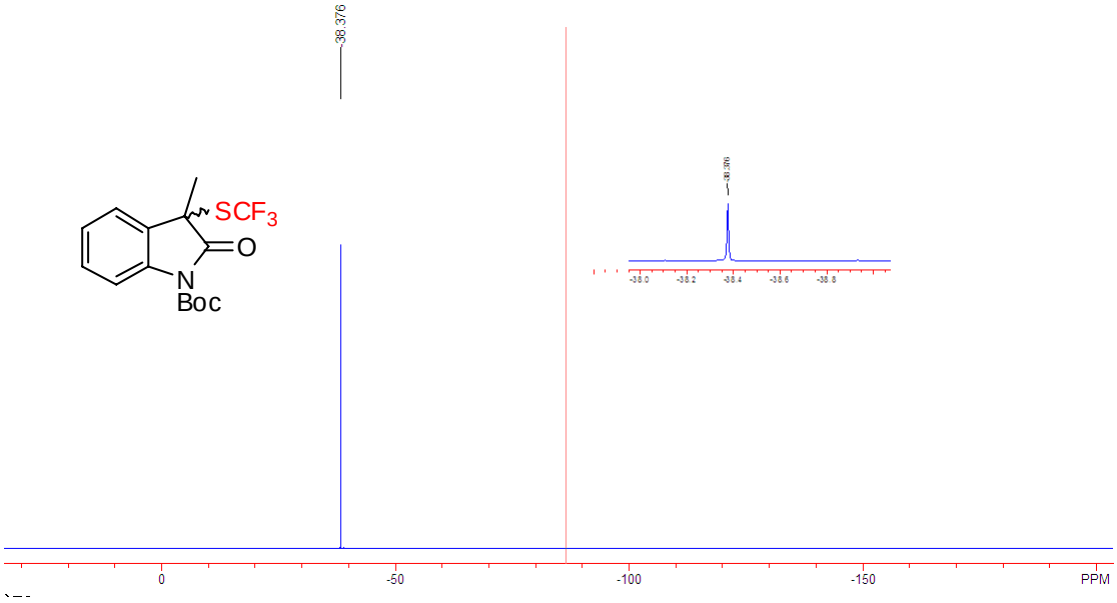
^{1}H NMR spectrum of *tert*-Butyl

3-methyl-2-oxo-3-((trifluoromethyl)thio)indoline-1-carboxylate 9f



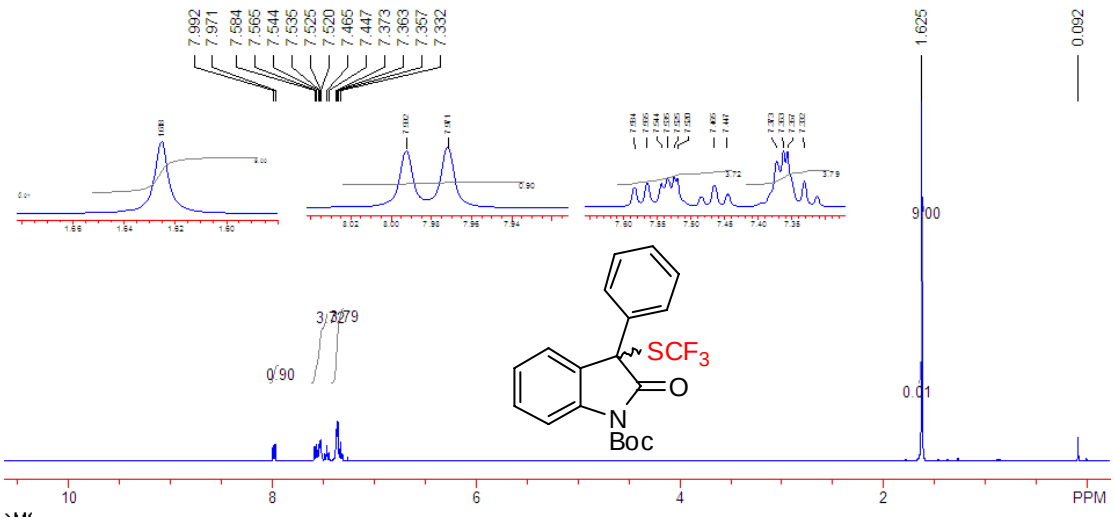
^{19}F NMR spectrum of tert-Butyl

3-methyl-2-oxo-3-((trifluoromethyl)thio)indoline-1-carboxylate 9f



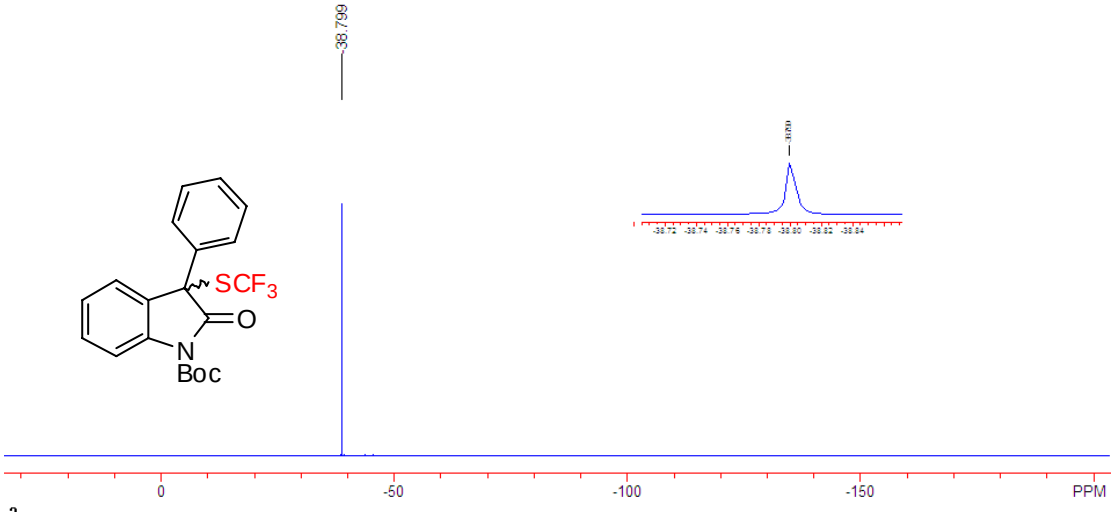
^{1}H NMR spectrum of *tert*-butyl

2-oxo-3-phenyl-3-((trifluoromethyl)thio)indoline-1-carboxylate 9g



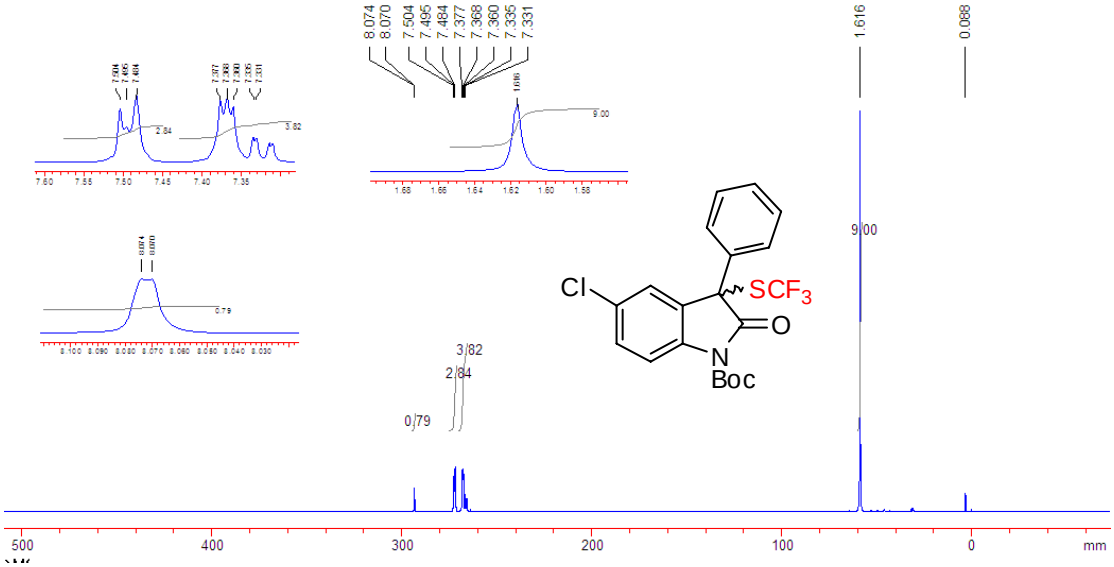
^{19}F NMR spectrum of tert-butyl

2-oxo-3-phenyl-3-((trifluoromethyl)thio)indoline-1-carboxylate 9g



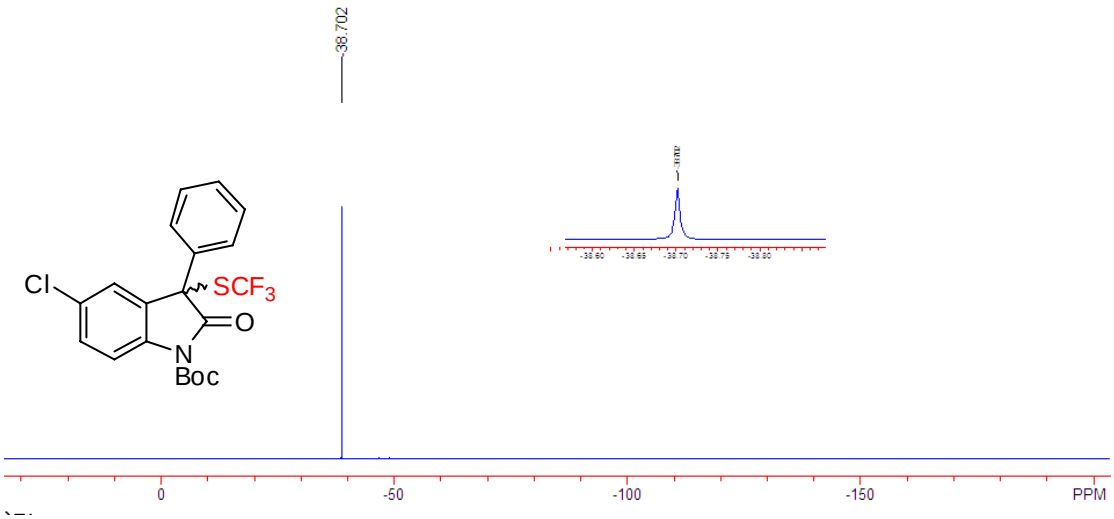
^{1}H NMR spectrum of *tert*-Butyl

5-chloro-2-oxo-3-phenyl-3-((trifluoromethyl)thio)indoline-1-carboxylate 9h



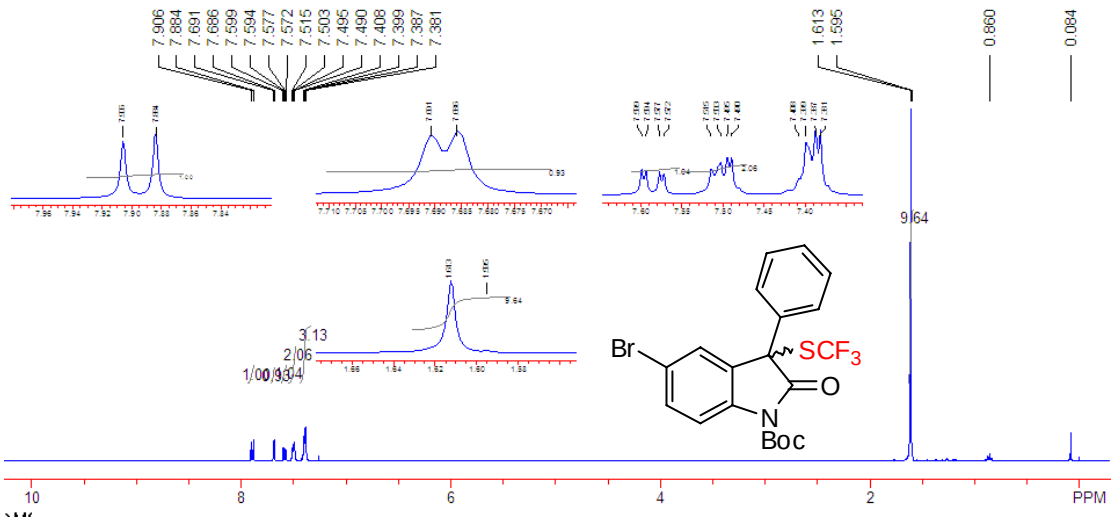
^{19}F NMR spectrum of *tert*-Butyl

5-chloro-2-oxo-3-phenyl-3-((trifluoromethyl)thio)indoline-1-carboxylate 9h



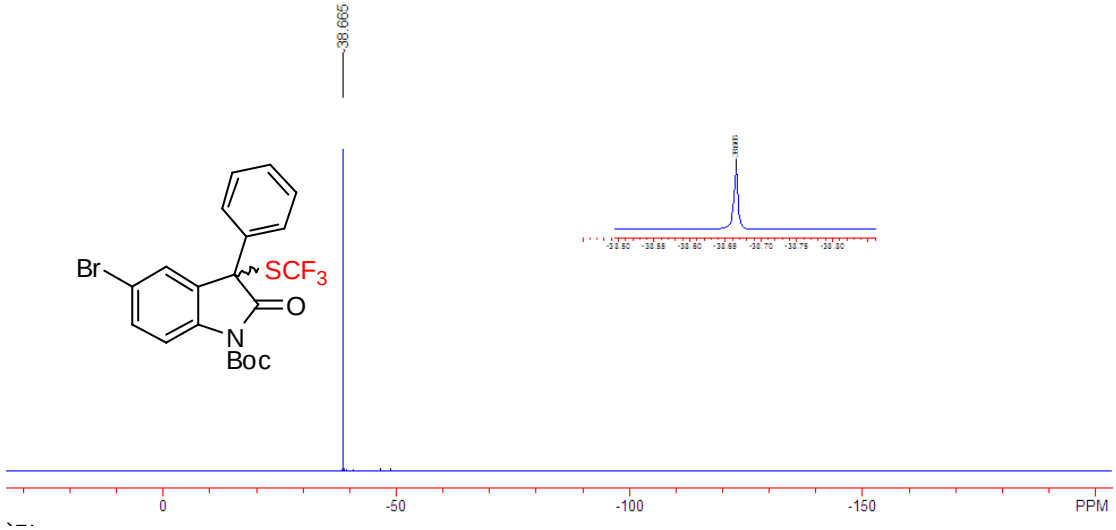
^{1}H NMR spectrum of *tert*-Butyl

5-bromo-2-oxo-3-phenyl-3-((trifluoromethyl)thio)indoline-1-carboxylate 9i



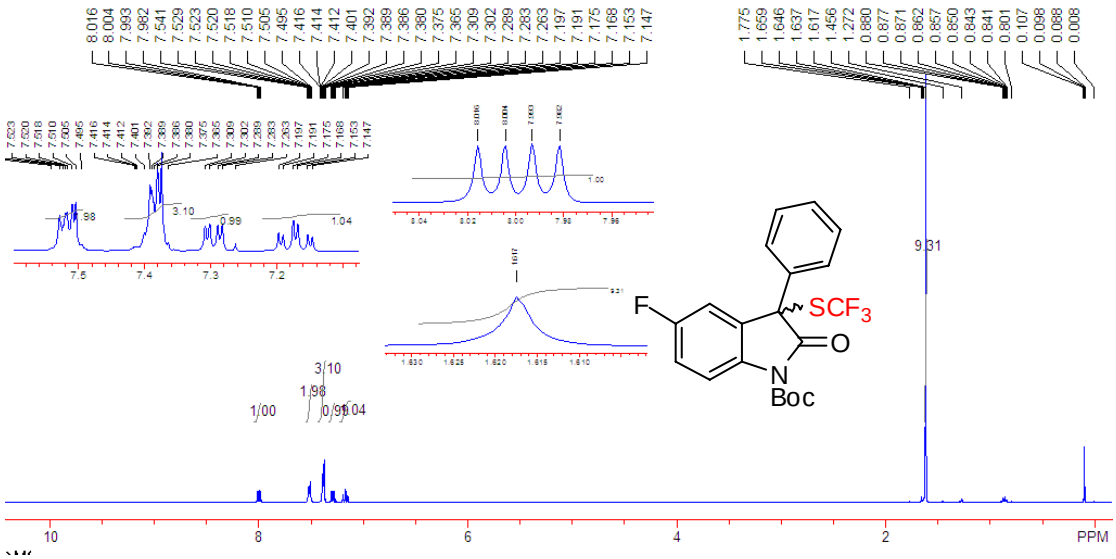
^{19}F NMR spectrum of *tert*-Butyl

5-bromo-2-oxo-3-phenyl-3-((trifluoromethyl)thio)indoline-1-carboxylate 9i



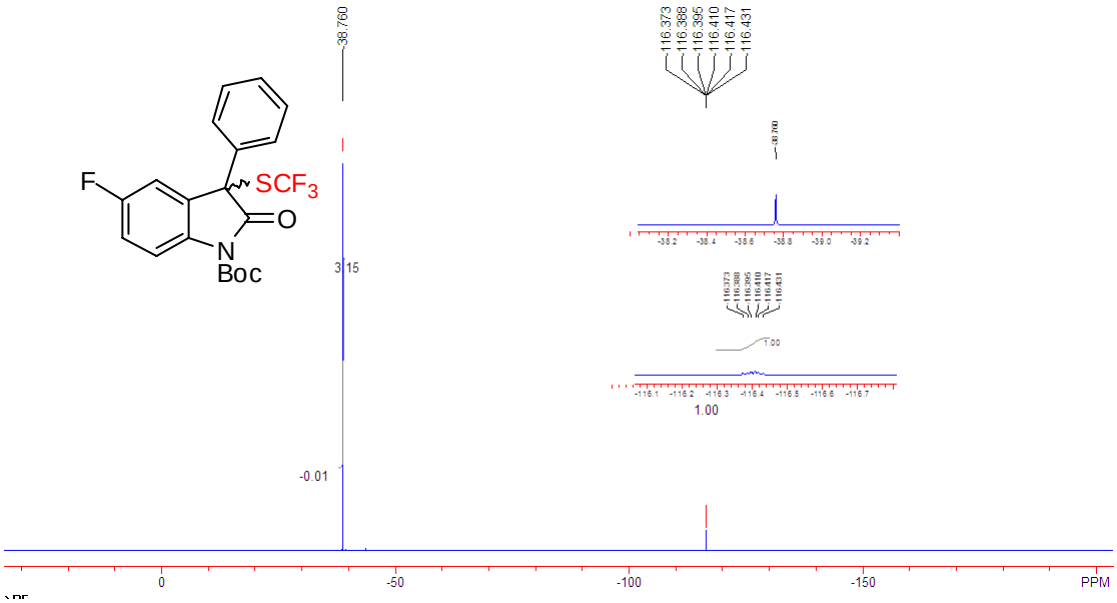
^{1}H NMR spectrum of *tert*-Butyl

5-bromo-2-oxo-3-phenyl-3-((trifluoromethyl)thio)indoline-1-carboxylate 9j



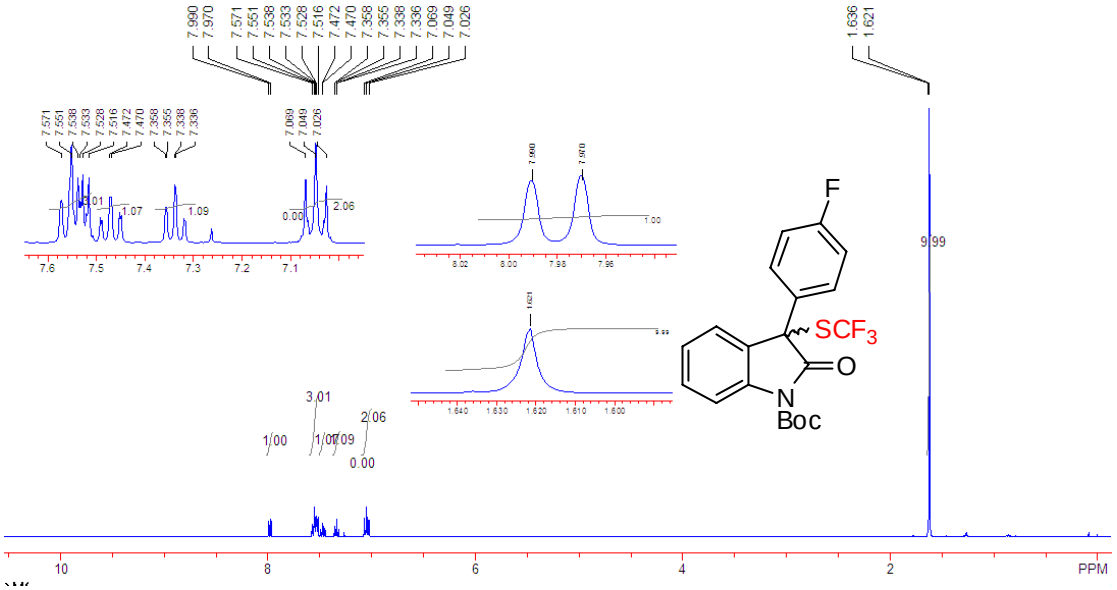
^{19}F NMR spectrum of *tert*-Butyl

5-bromo-2-oxo-3-phenyl-3-((trifluoromethyl)thio)indoline-1-carboxylate 9j



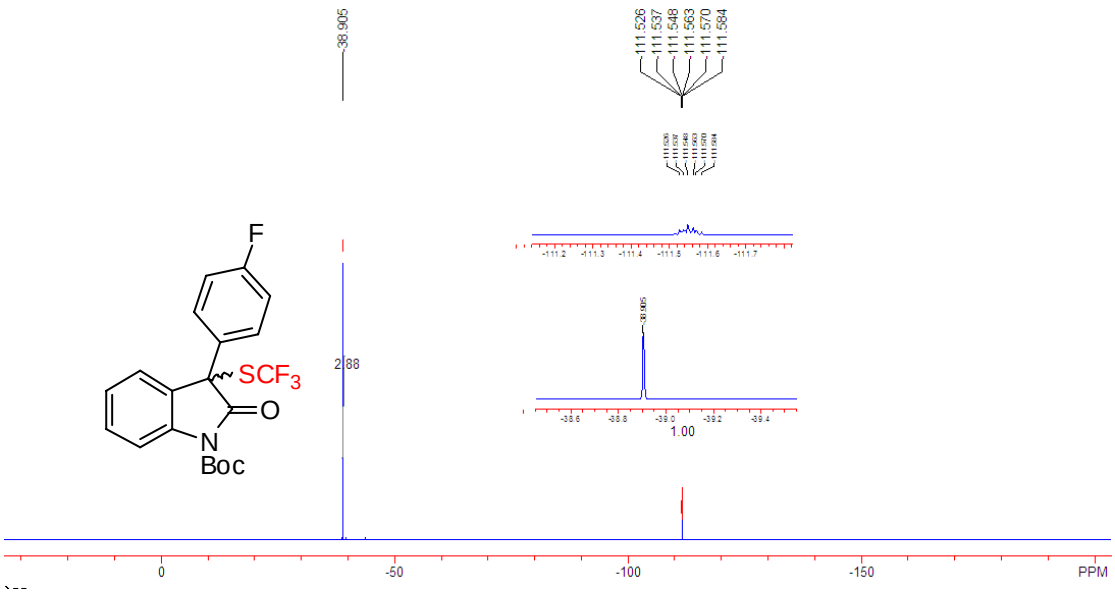
^{1}H NMR spectrum of *tert*-Butyl

3-(4-fluorophenyl)-2-oxo-3-((trifluoromethyl)thio)indoline-1-carboxylate 9k



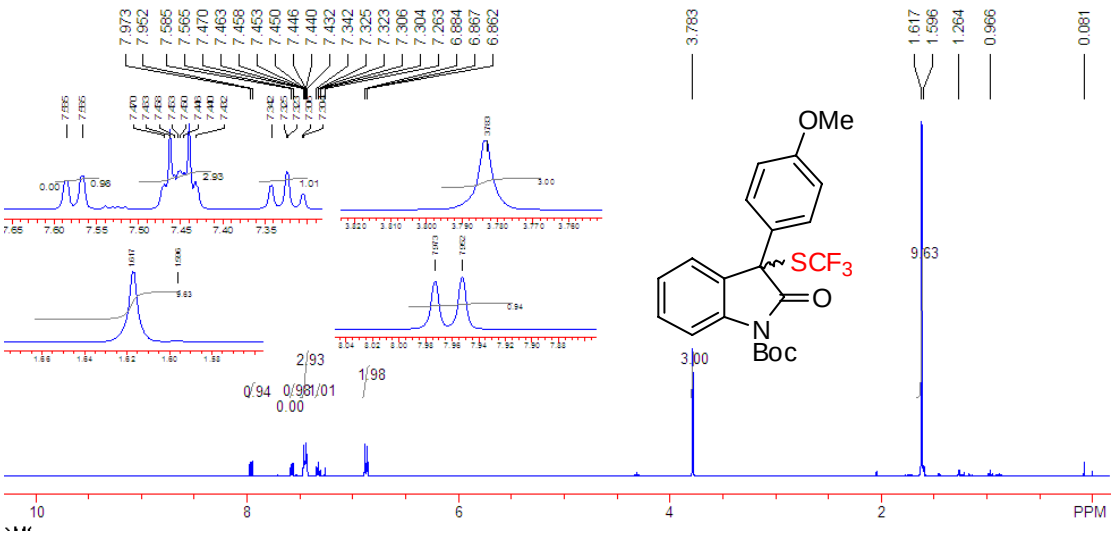
^{19}F NMR spectrum of *tert*-Butyl

3-(4-fluorophenyl)-2-oxo-3-((trifluoromethyl)thio)indoline-1-carboxylate 9k



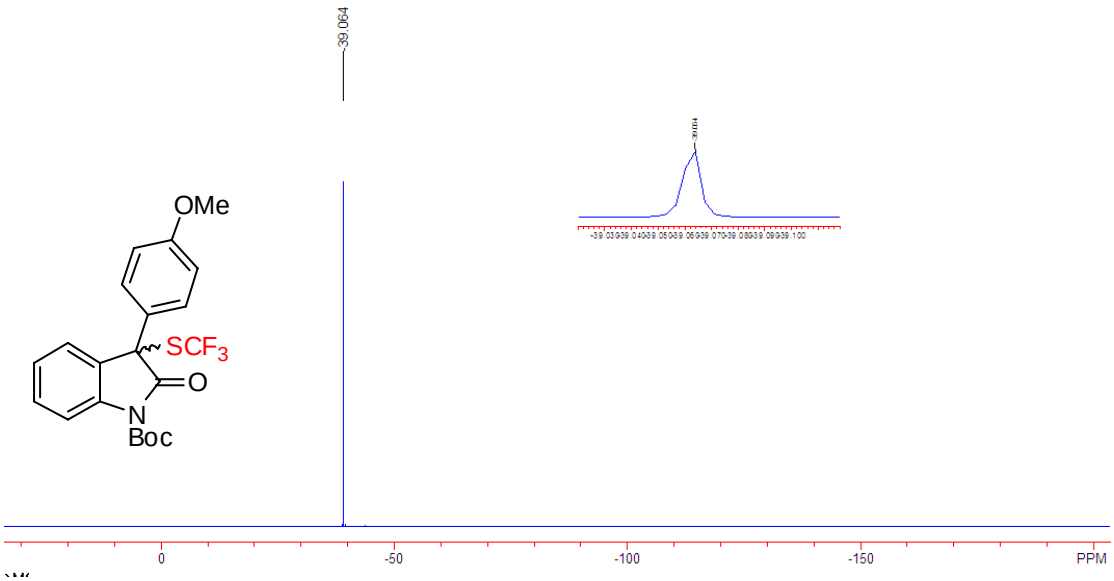
^{1}H NMR spectrum of tert-Butyl

3-(4-methoxyphenyl)-2-oxo-3-((trifluoromethyl)thio)indoline-1-carboxylate 9l

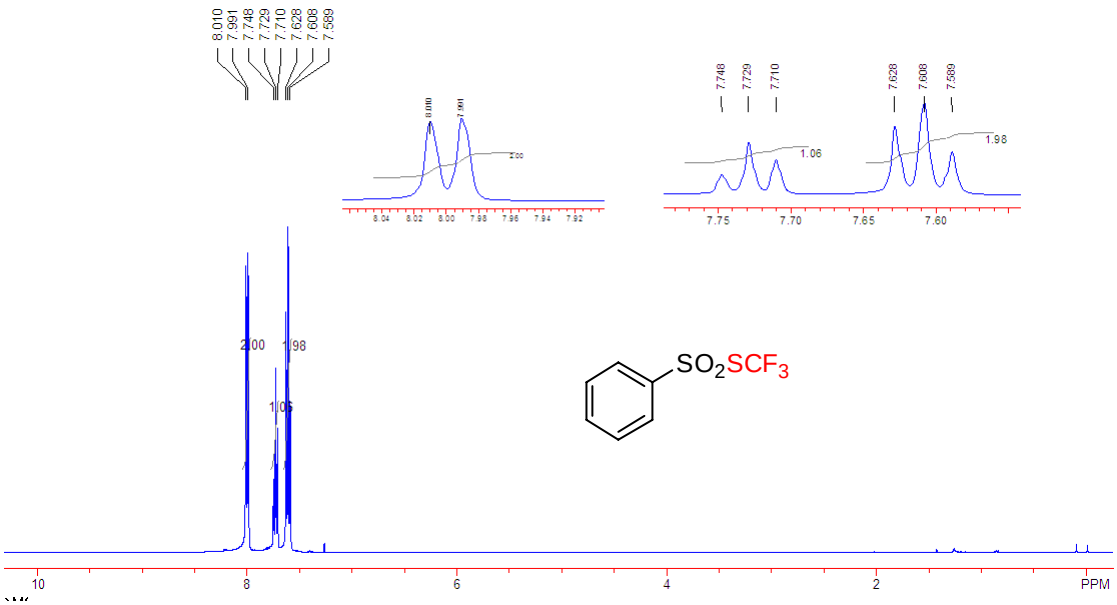


^{19}F NMR spectrum of tert-Butyl

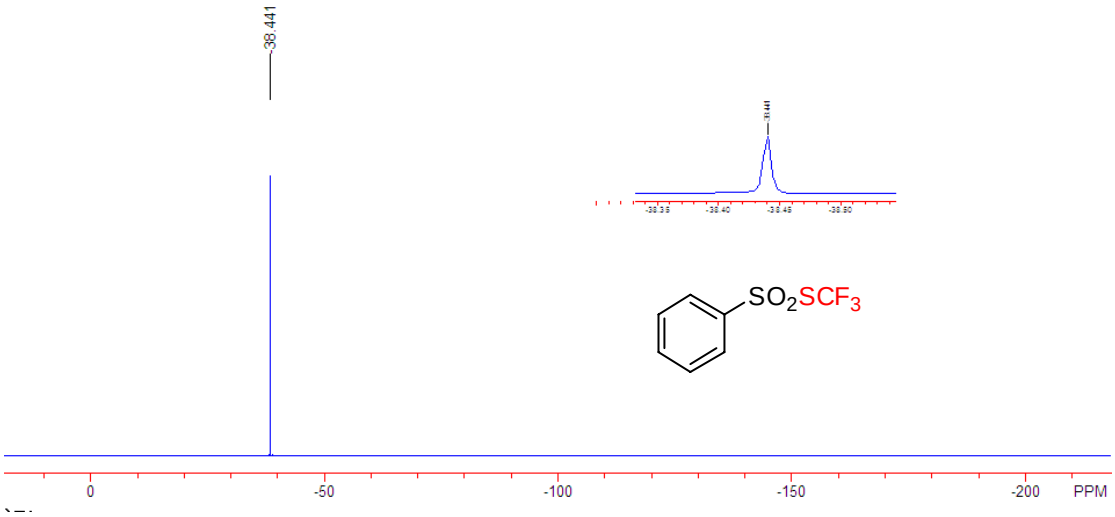
3-(4-methoxyphenyl)-2-oxo-3-((trifluoromethyl)thio)indoline-1-carboxylate 9l



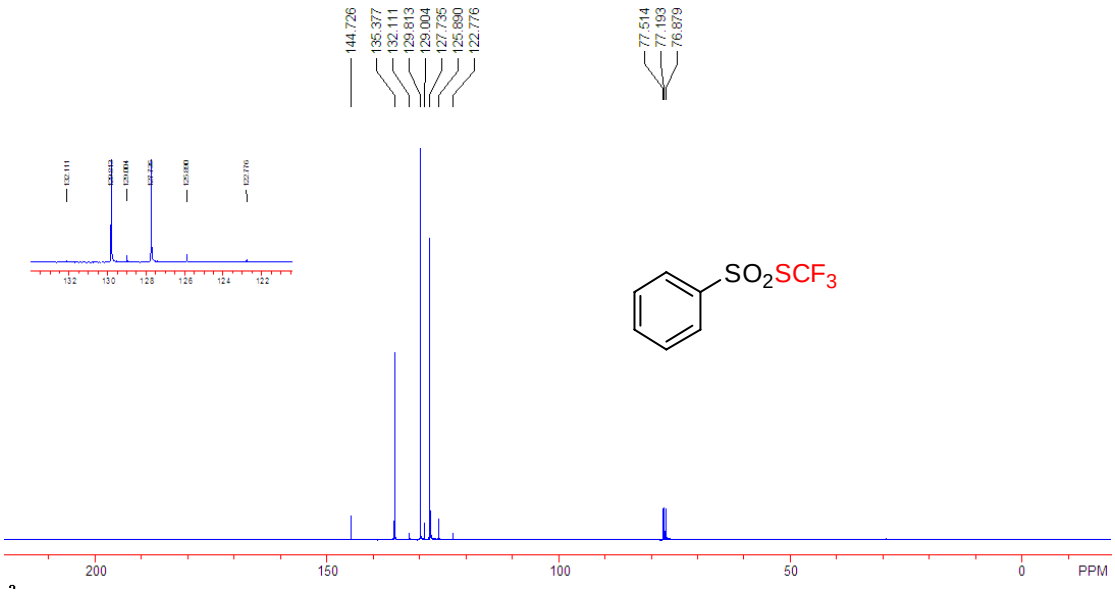
^{1}H NMR spectrum of *S*-(Trifluoromethyl) benzenesulfonothioate 10a



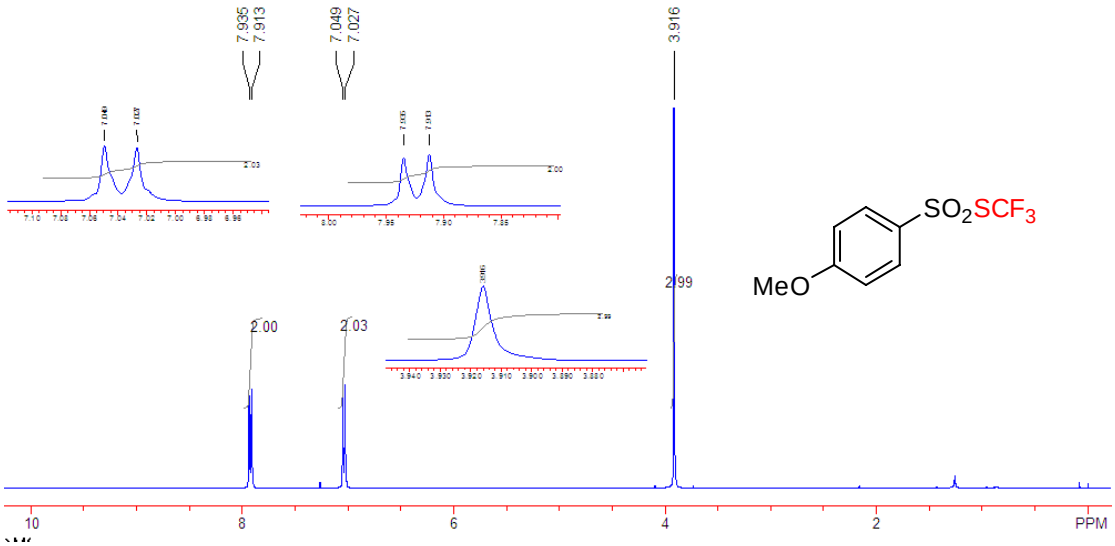
^{19}F NMR spectrum of *S*-(Trifluoromethyl) benzenesulfonothioate 10a



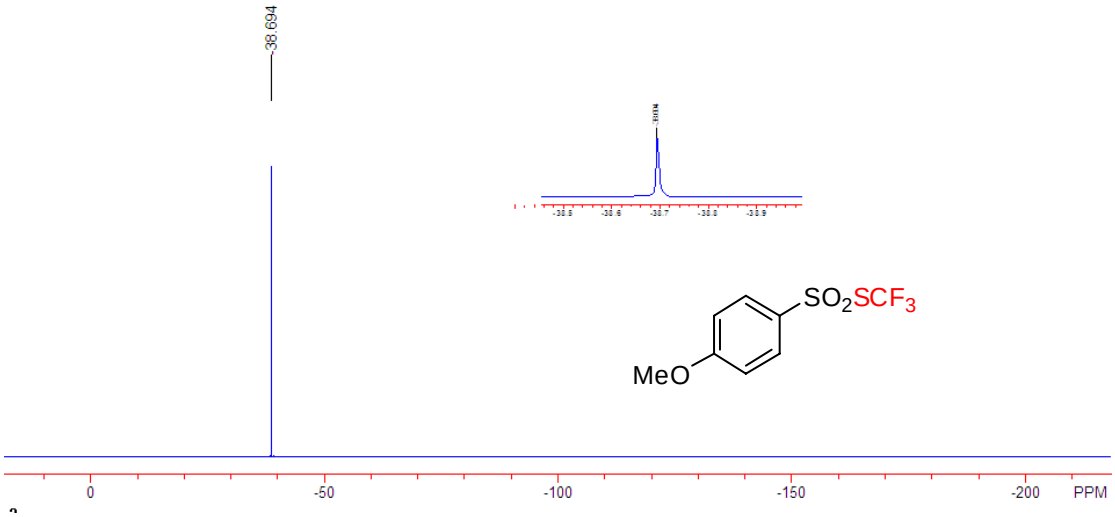
^{13}C NMR spectrum of *S*-(Trifluoromethyl) benzenesulfonothioate 10a



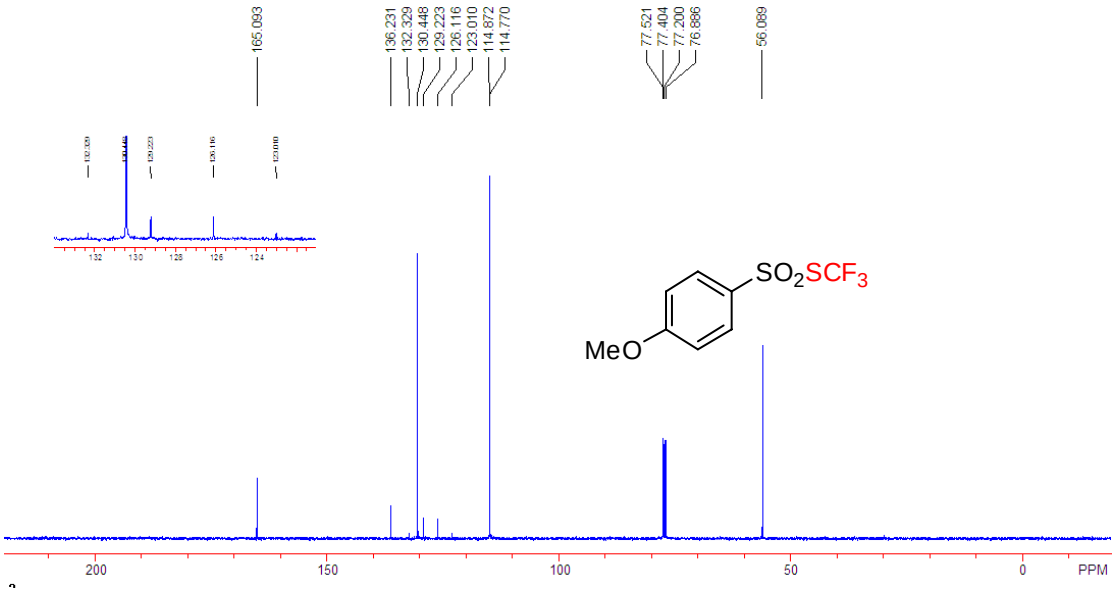
^{1}H NMR spectrum of S-(trifluoromethyl) 4-methoxybenzenesulfonothioate 10b



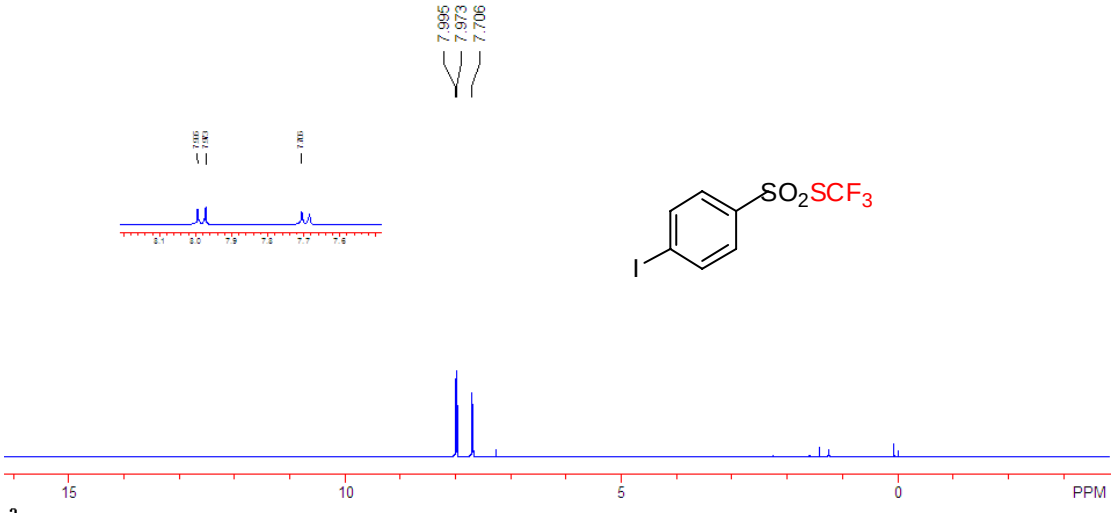
^{19}F NMR spectrum of S-(trifluoromethyl) 4-methoxybenzenesulfonothioate 10b



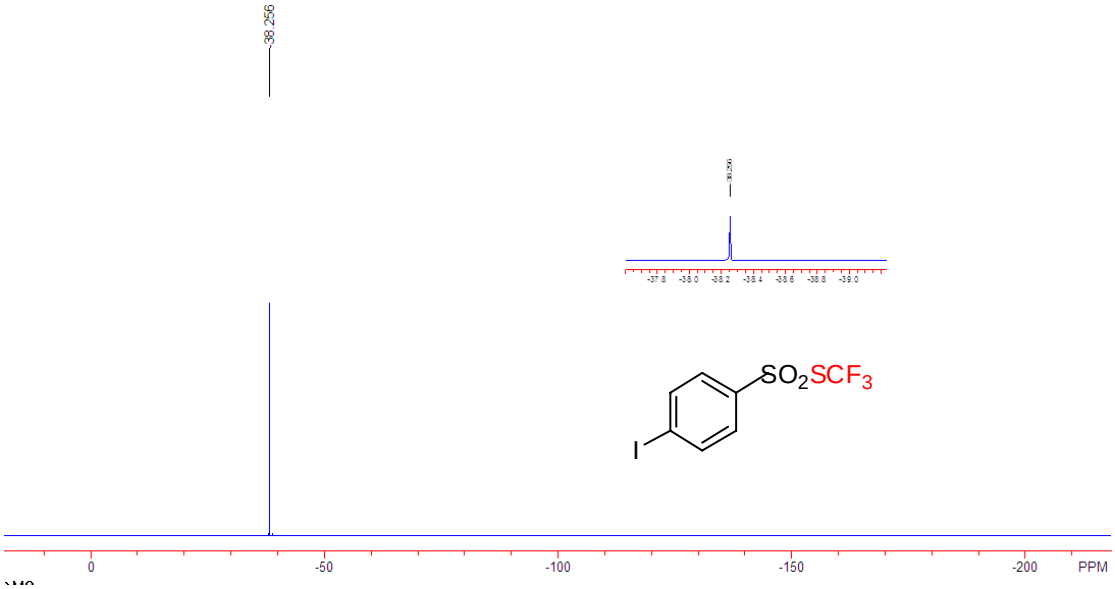
^{13}C NMR spectrum of S-(trifluoromethyl) 4-methoxybenzenesulfonothioate 10b



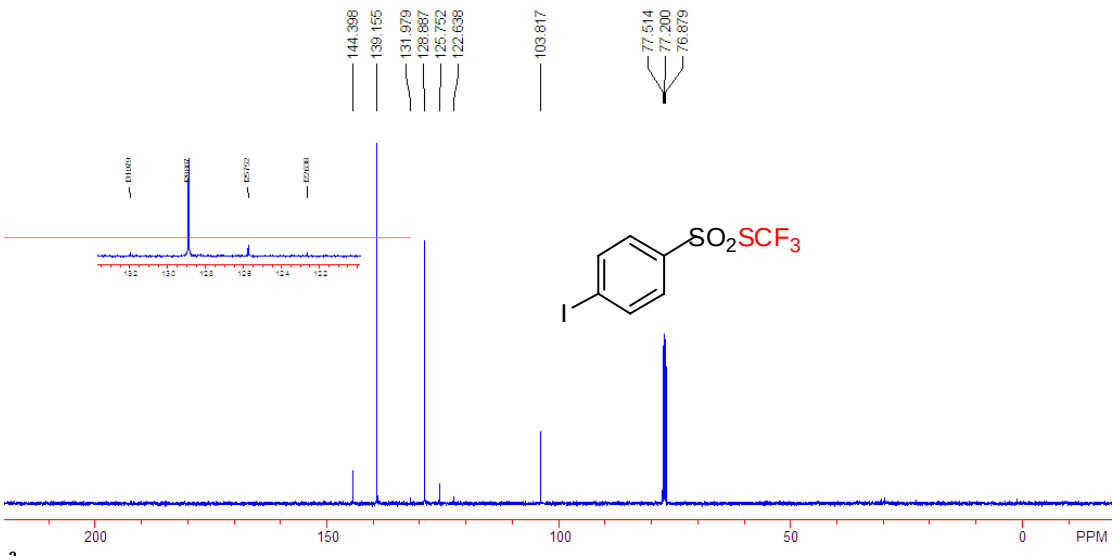
^{1}H NMR spectrum of S-(trifluoromethyl) 4-iodobenzenesulfonothioate 10c



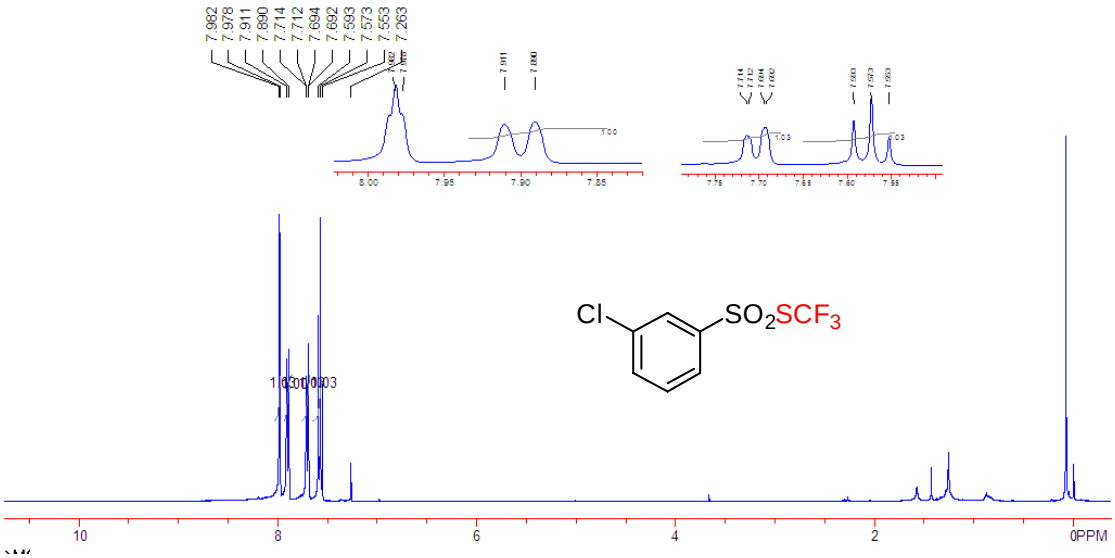
^{19}F NMR spectrum of S-(trifluoromethyl) 4-iodobenzenesulfonothioate 10c



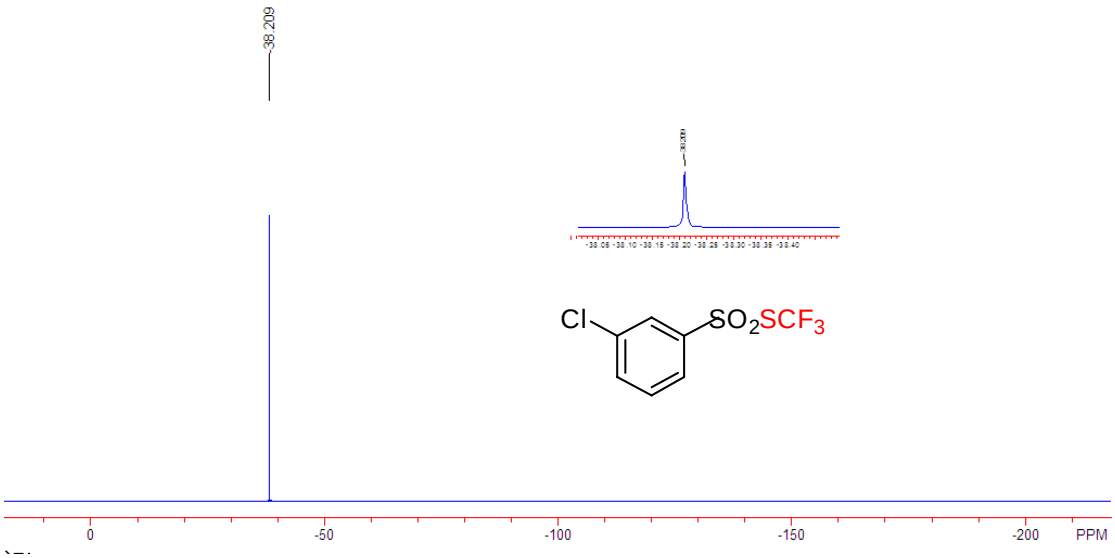
^{13}C NMR spectrum of S-(trifluoromethyl) 4-iodobenzenesulfonothioate 10c



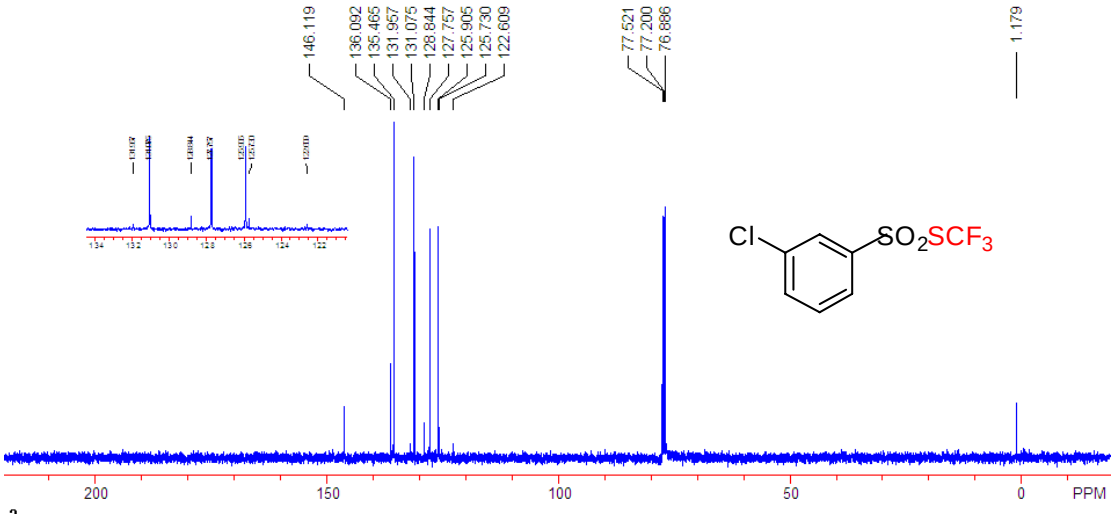
^{1}H NMR spectrum of S-(trifluoromethyl) 3-chlorobenzenesulfonothioate 10d



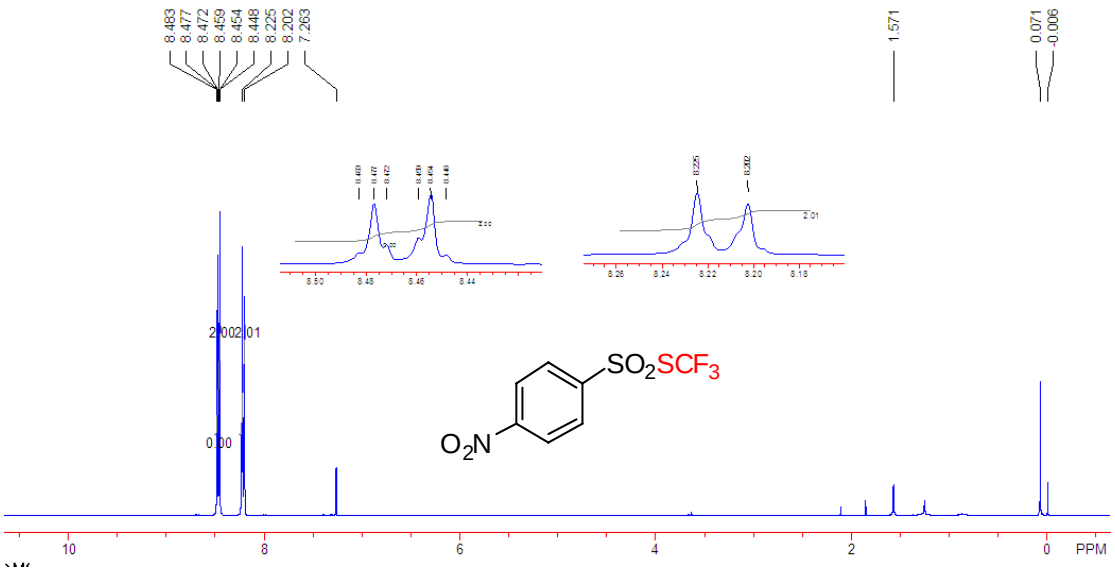
^{19}F NMR spectrum of S-(trifluoromethyl) 3-chlorobenzenesulfonothioate 10d



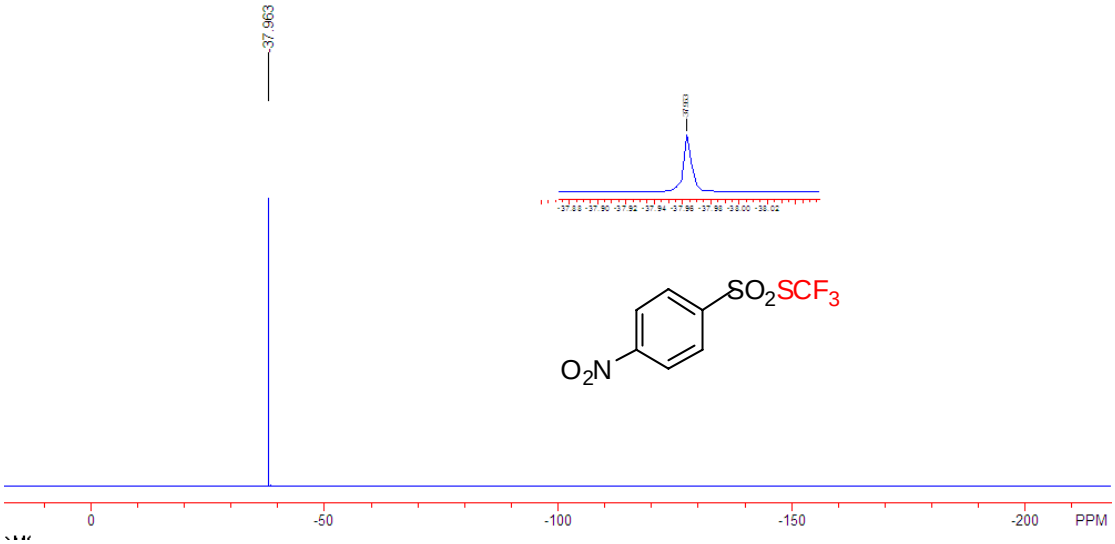
^{13}C NMR spectrum of S-(trifluoromethyl) 3-chlorobenzenesulfonothioate 10d



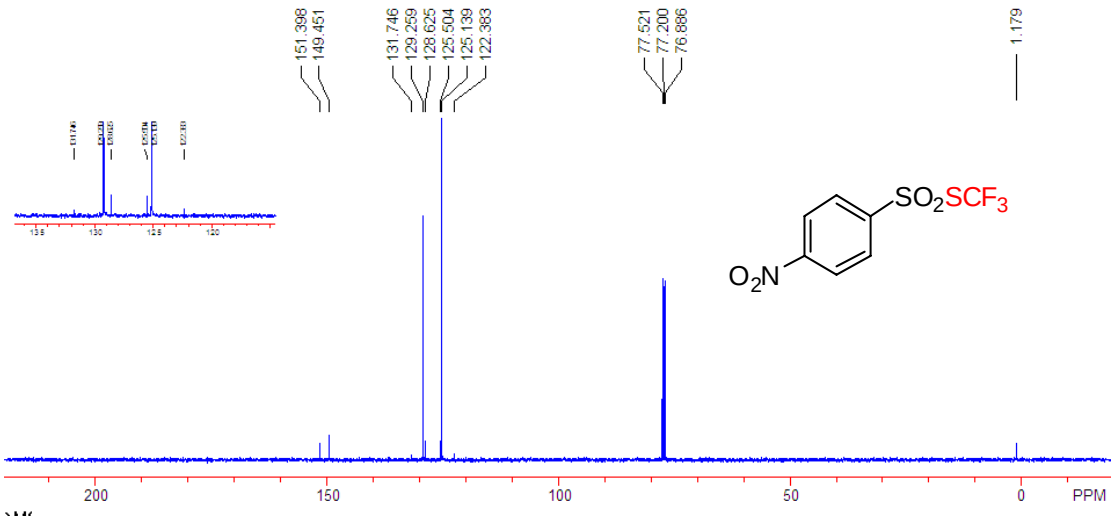
^{1}H NMR spectrum of S-(trifluoromethyl) 4-nitrobenzenesulfonothioate 10e



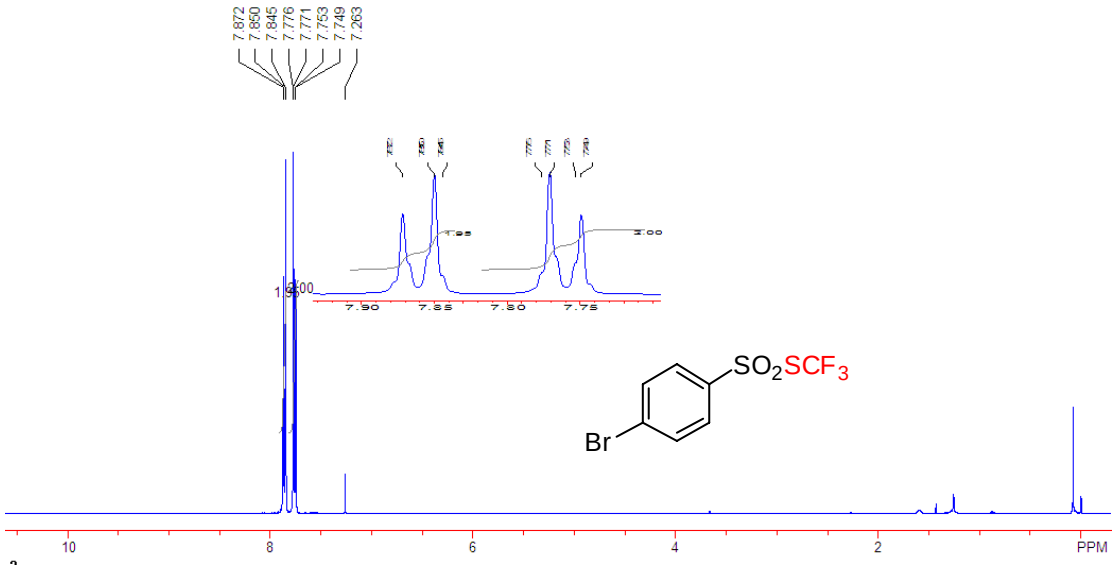
^{19}F NMR spectrum of S-(trifluoromethyl) 4-nitrobenzenesulfonothioate 10e



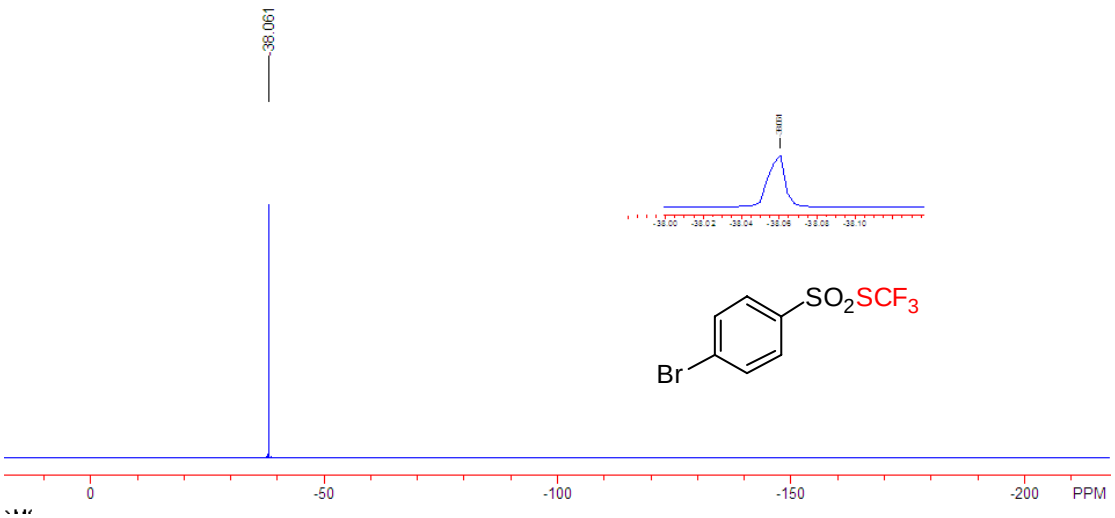
^{13}C NMR spectrum of S-(trifluoromethyl) 4-nitrobenzenesulfonothioate 10e



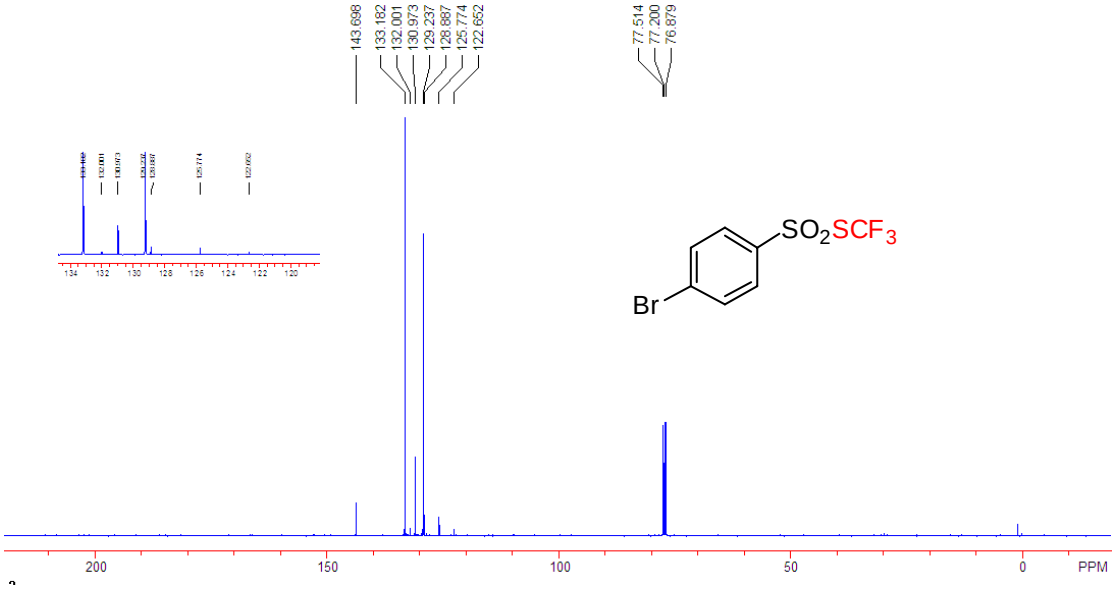
^{1}H NMR spectrum of S-(trifluoromethyl) 4-nitrobenzenesulfonothioate 10e



^{19}F NMR spectrum of S-(trifluoromethyl) 4-nitrobenzenesulfonothioate 10f

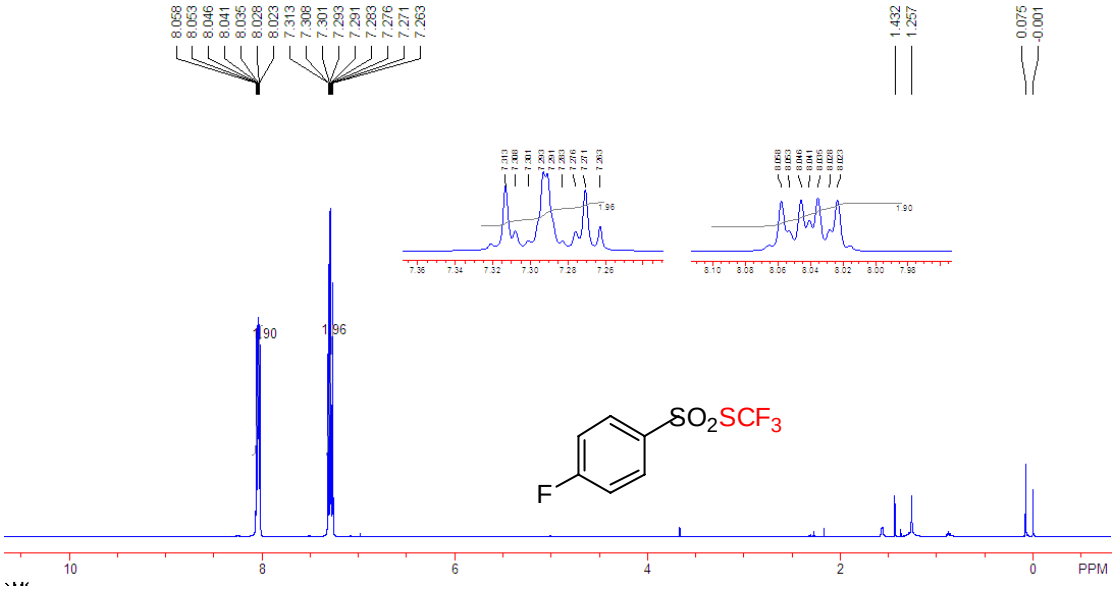


^{13}C NMR spectrum of S-(trifluoromethyl) 4-nitrobenzenesulfonothioate 10f

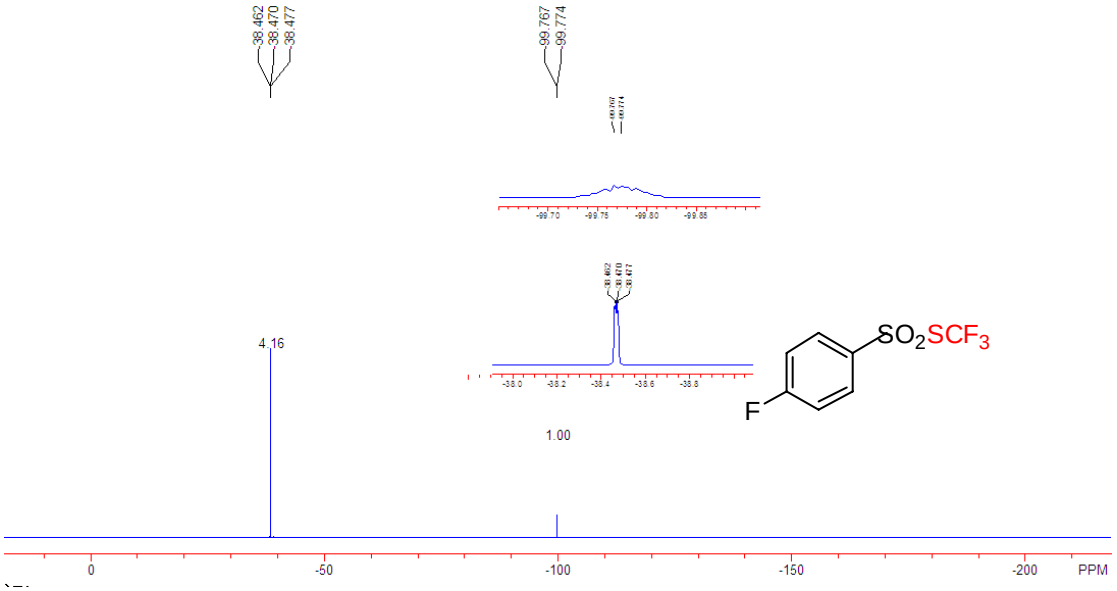


^{1}H NMR spectrum of *S*-(trifluoromethyl) 4-fluorobenzenesulfonothioate

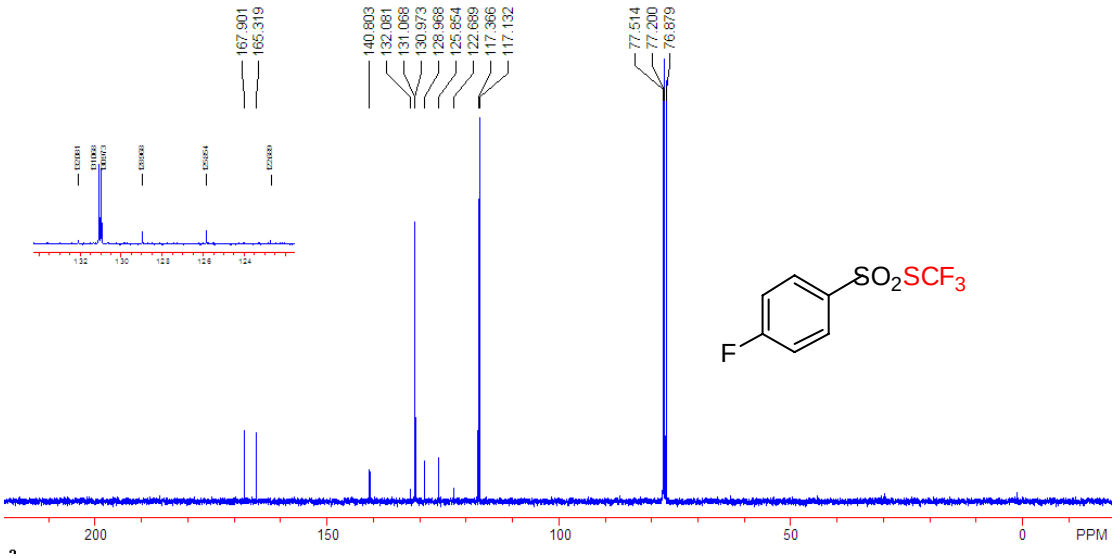
10g



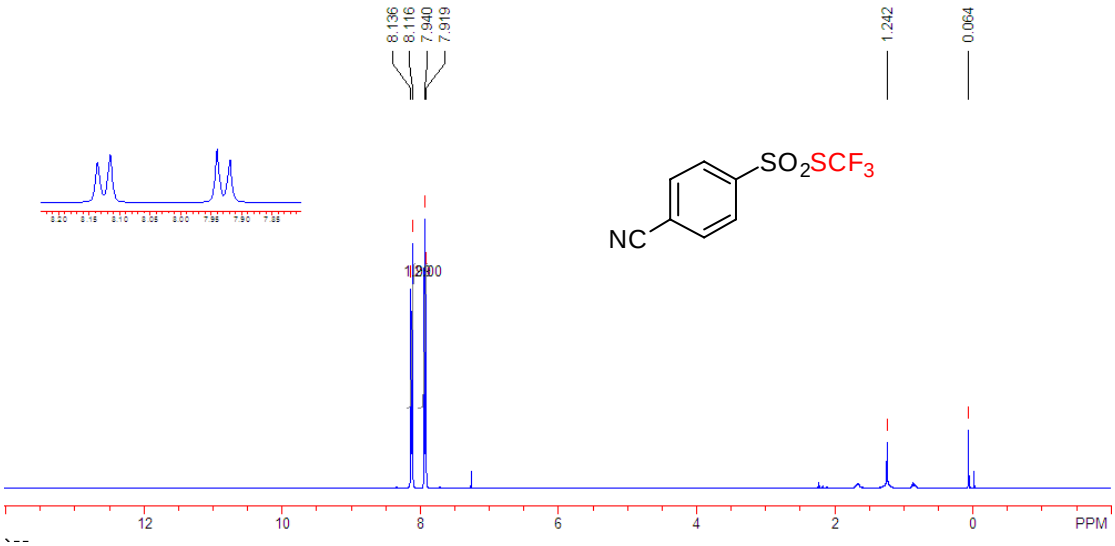
^{19}F NMR spectrum of *S*-(trifluoromethyl) 4-fluorobenzenesulfonothioate 10g



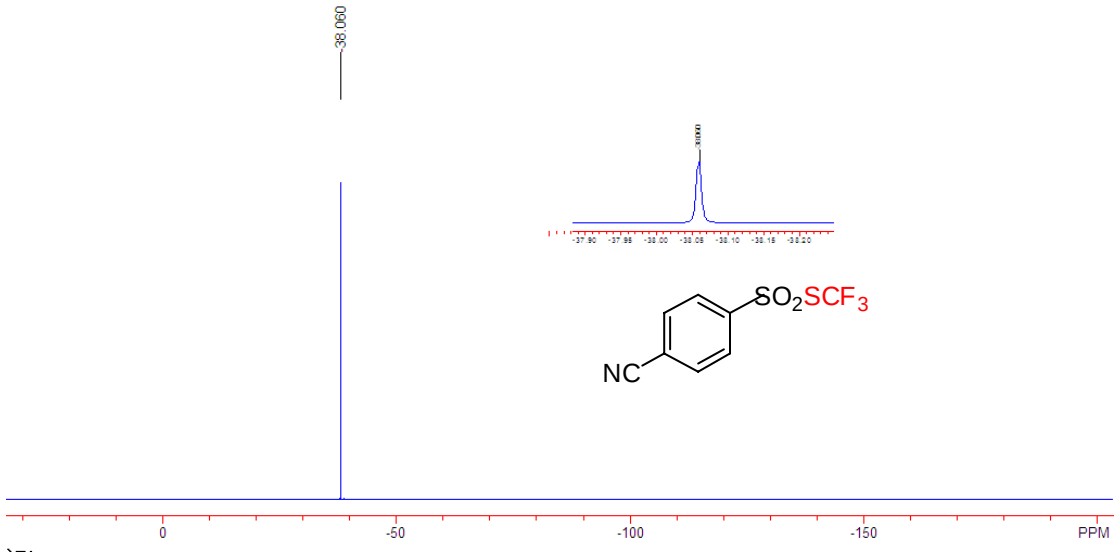
^{13}C NMR spectrum of *S*-(trifluoromethyl) 4-fluorobenzenesulfonothioate 10g



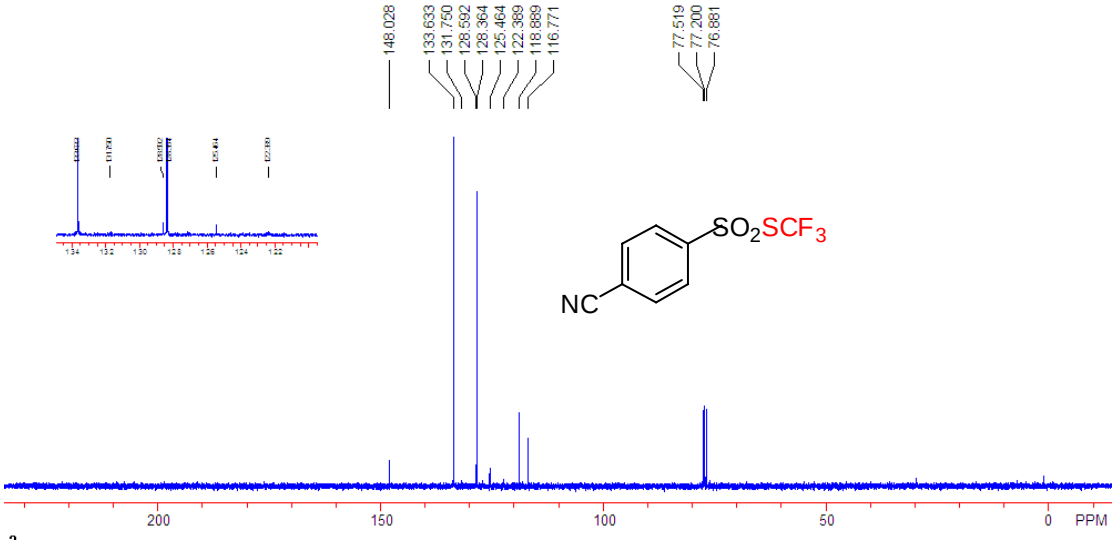
^{1}H NMR spectrum of *S*-(trifluoromethyl) 4-cyanobenzenesulfonothioate 10h



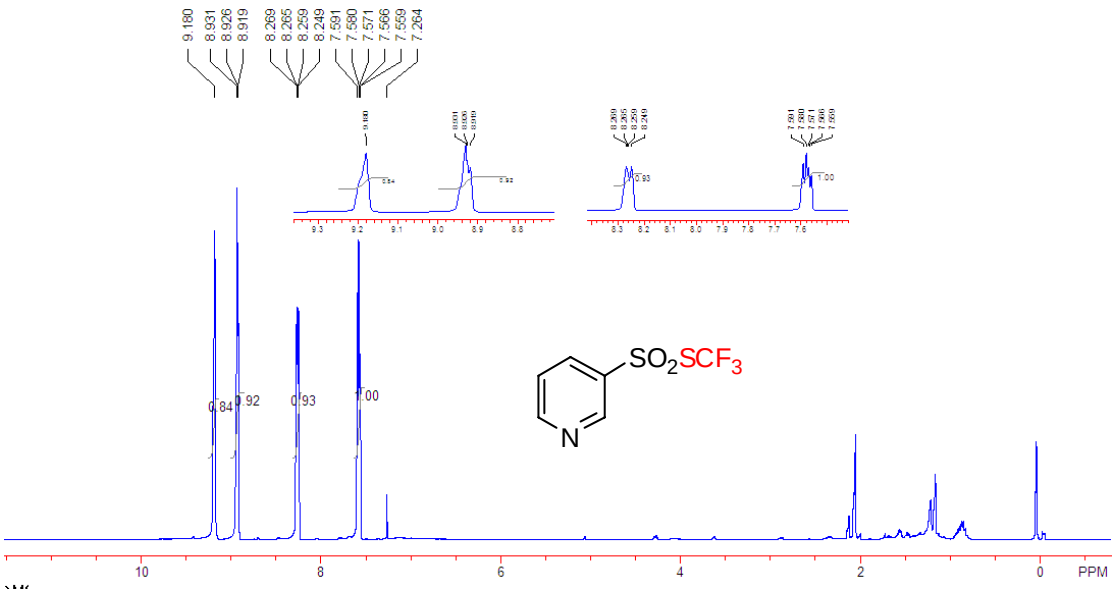
^{19}F NMR spectrum of *S*-(trifluoromethyl) 4-cyanobenzenesulfonothioate 10h



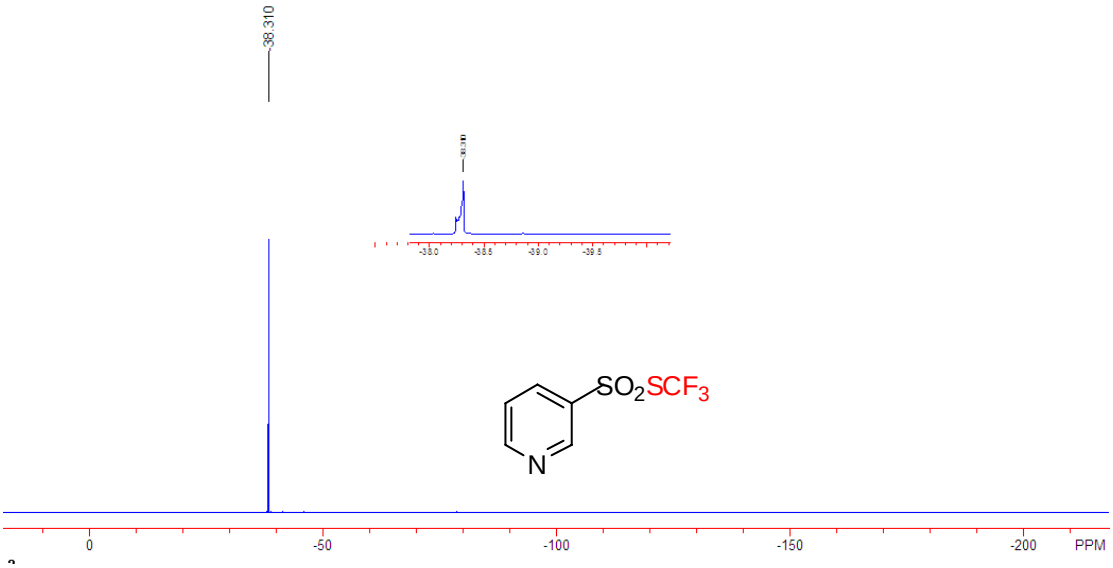
^{13}C NMR spectrum of *S*-(trifluoromethyl) 4-cyanobenzenesulfonothioate 10h



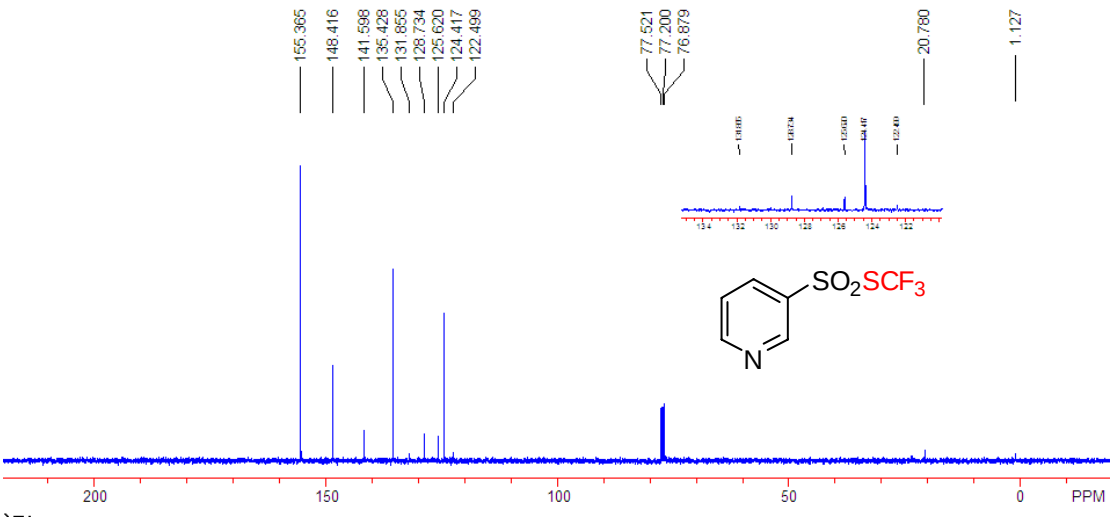
^{1}H NMR spectrum of S-(trifluoromethyl) pyridine-3-sulfonothioate 10i



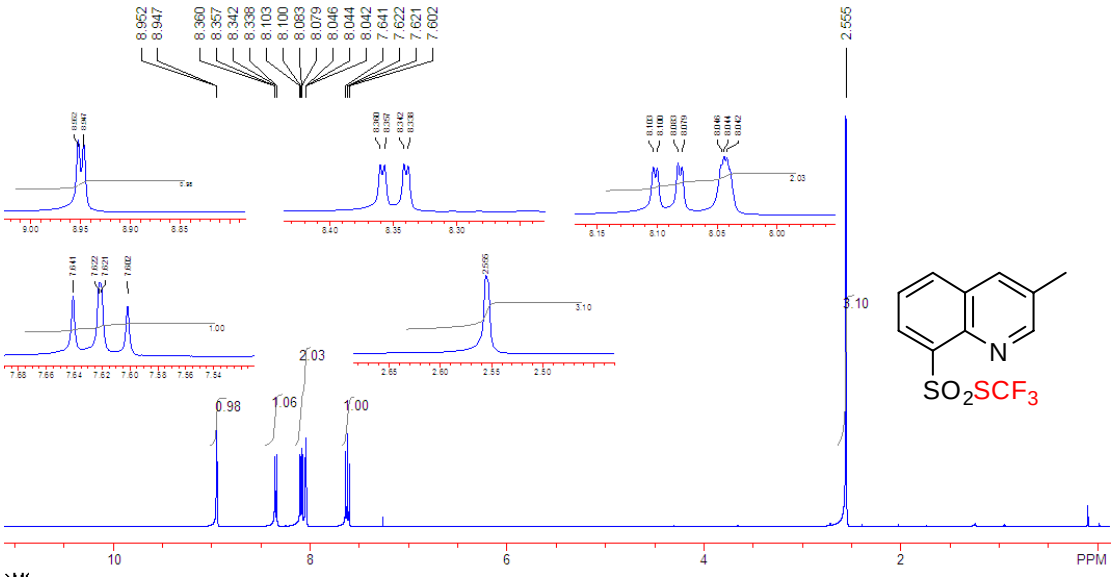
^{19}F NMR spectrum of *S*-(trifluoromethyl) S-(trifluoromethyl) pyridine-3-sulfonothioate 10i



^{13}C NMR spectrum of S-(trifluoromethyl) pyridine-3-sulfonothioate 10i

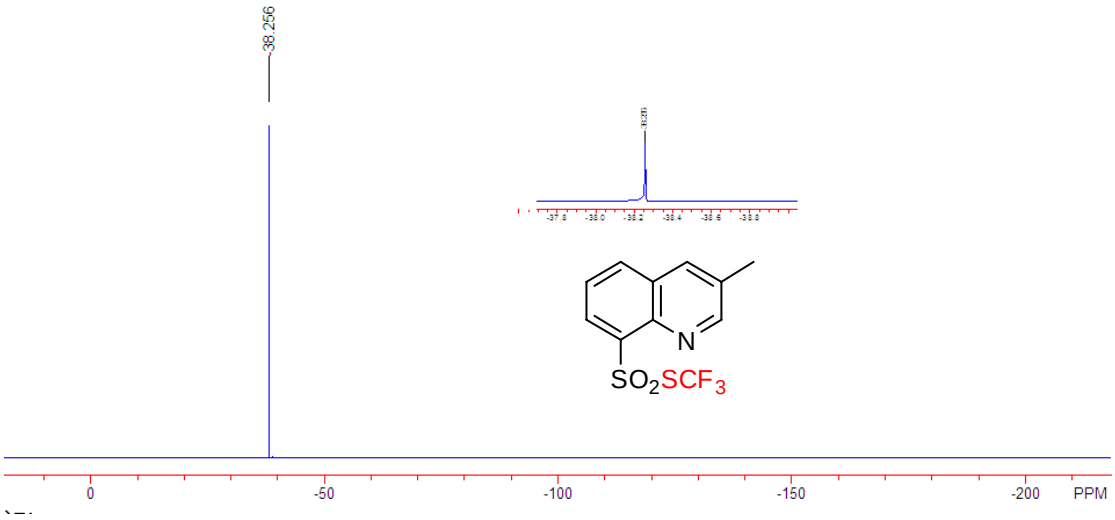


^{1}H NMR spectrum of S-(trifluoromethyl) 3-methylquinoline-8-sulfonothioate

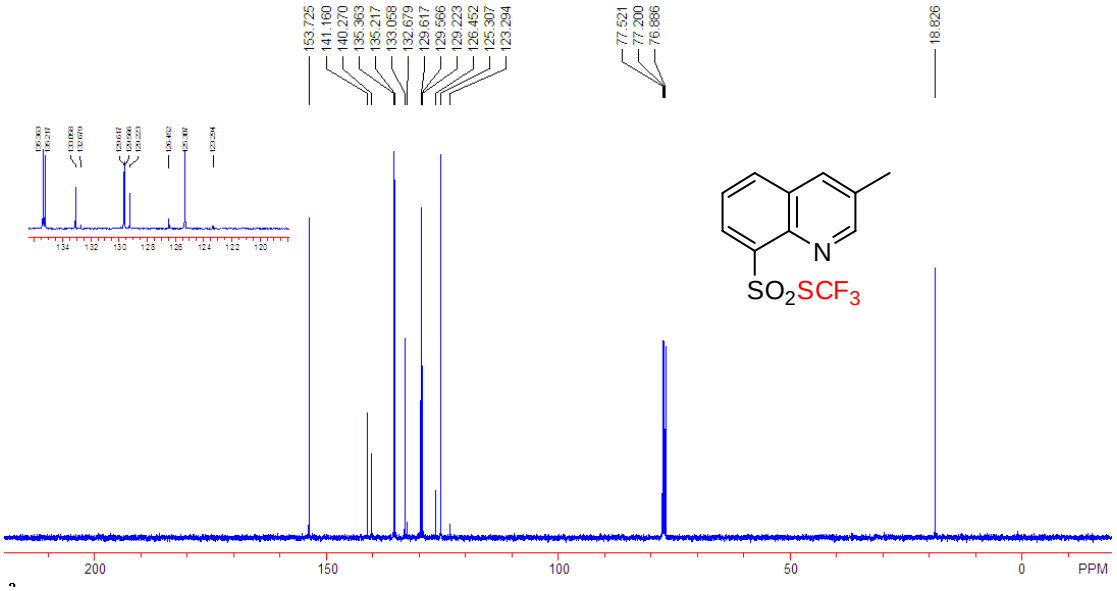


^{19}F NMR spectrum of S-(trifluoromethyl) 3-methylquinoline-8-sulfonothioate

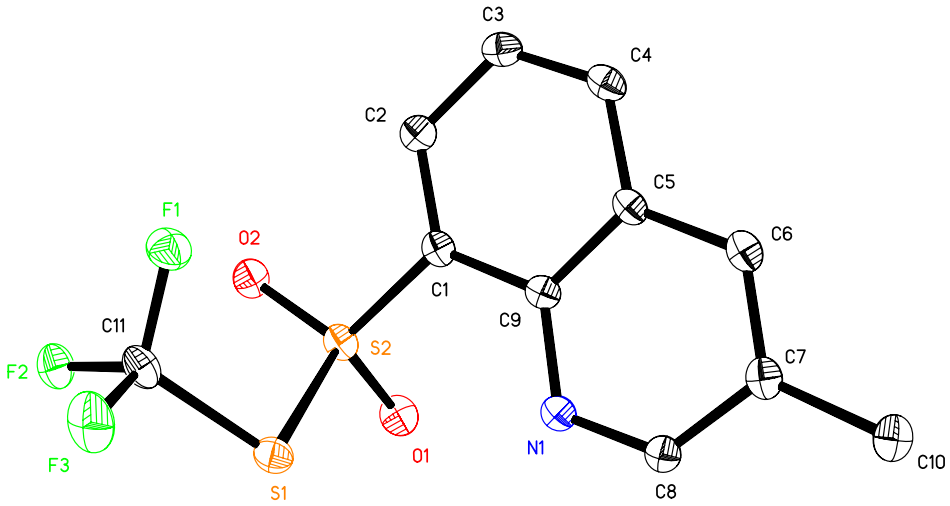
10j

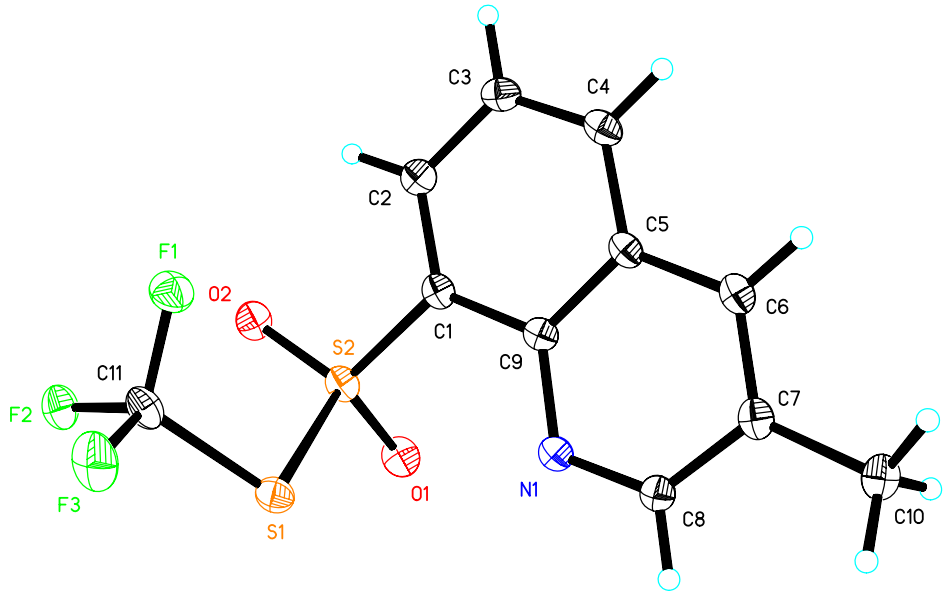


^{13}C NMR spectrum of S-(trifluoromethyl) 3-methylquinoline-8-sulfonothioate 10j



Crystallographic data of 10j





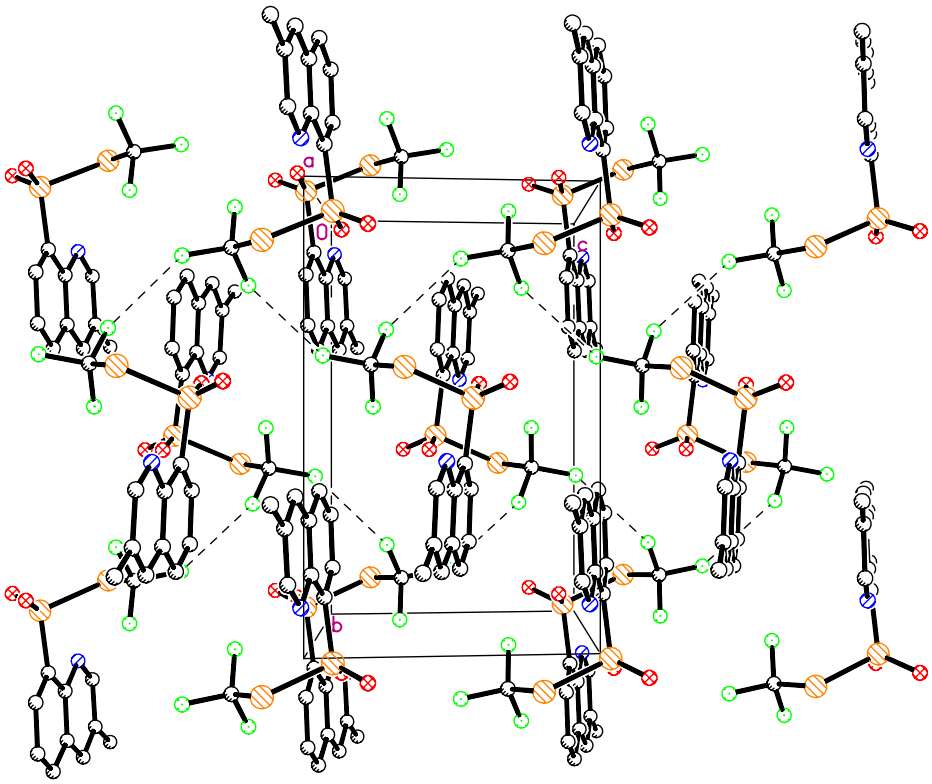


Table 1. Crystal data and structure refinement for dm14611.

Identification code	dm14611	
Empirical formula	C11 H8 F3 N O2 S2	
Formula weight	307.30	
Temperature	130 K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 1 21/c 1	
Unit cell dimensions	a = 13.839(6) Å	α= 90°.
	b = 11.892(5) Å	β= 99.943(7)°.
	c = 7.497(3) Å	γ = 90°.
Volume	1215.2(10) $Å^3$	
Z	4	
Density (calculated)	1.680 Mg/m^3	
Absorption coefficient	0.472 mm^{-1}	

F(000)	624
Crystal size	0.18 x 0.12 x 0.05 mm^3
Theta range for data collection	1.494 to 30.756°.
Index ranges	-19<=h<=19, -17<=k<=15, -10<=l<=10
Reflections collected	11227
Independent reflections	3717 [R(int) = 0.0740]
Completeness to theta = 25.242°	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7461 and 0.4578
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3717 / 0 / 174
Goodness-of-fit on F^2	0.926
Final R indices [I>2sigma(I)]	R1 = 0.0522, wR2 = 0.1197
R indices (all data)	R1 = 0.1069, wR2 = 0.1439
Extinction coefficient	0.017(2)
Largest diff. peak and hole	0.518 and -0.492 e.$Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3)
for dm14611. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
S(1)	7418(1)	11117(1)	8251(1)	32(1)
S(2)	7139(1)	10435(1)	10705(1)	27(1)
F(1)	5674(1)	10245(1)	7036(2)	39(1)
F(2)	5639(1)	12010(1)	7520(2)	36(1)
F(3)	6263(2)	11393(2)	5269(2)	49(1)
O(1)	7974(2)	10783(2)	11996(3)	36(1)
O(2)	6170(2)	10761(2)	10932(3)	33(1)
N(1)	8817(2)	9052(2)	9764(3)	25(1)
C(1)	7161(2)	8967(2)	10409(3)	24(1)
C(2)	6338(2)	8375(2)	10625(3)	28(1)
C(3)	6348(2)	7184(2)	10555(3)	29(1)
C(4)	7166(2)	6630(2)	10231(3)	28(1)
C(5)	8016(2)	7231(2)	9954(3)	23(1)
C(6)	8879(2)	6688(2)	9585(3)	27(1)
C(7)	9681(2)	7313(2)	9331(3)	27(1)
C(8)	9594(2)	8502(2)	9420(3)	26(1)
C(9)	8026(2)	8419(2)	10034(3)	23(1)
C(10)	10623(2)	6786(2)	8988(4)	32(1)
C(11)	6178(2)	11194(2)	6996(4)	31(1)

Table 3. Bond lengths [Å] and angles [°] for dm14611.

S(1)-S(2)	2.1065(12)
S(1)-C(11)	1.812(3)
S(2)-O(1)	1.435(2)
S(2)-O(2)	1.434(2)
S(2)-C(1)	1.761(3)
F(1)-C(11)	1.329(3)
F(2)-C(11)	1.324(3)
F(3)-C(11)	1.341(3)
N(1)-C(8)	1.322(4)
N(1)-C(9)	1.372(3)
C(1)-C(2)	1.372(4)
C(1)-C(9)	1.433(4)
C(2)-H(2)	0.9500
C(2)-C(3)	1.417(4)
C(3)-H(3)	0.9500
C(3)-C(4)	1.366(4)
C(4)-H(4)	0.9500
C(4)-C(5)	1.422(4)
C(5)-C(6)	1.425(4)
C(5)-C(9)	1.414(4)
C(6)-H(6)	0.9500
C(6)-C(7)	1.376(4)
C(7)-C(8)	1.421(4)
C(7)-C(10)	1.508(4)
C(8)-H(8)	0.9500
C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800
C(10)-H(10C)	0.9800
C(11)-S(1)-S(2)	99.94(10)
O(1)-S(2)-S(1)	103.32(10)
O(1)-S(2)-C(1)	109.97(12)
O(2)-S(2)-S(1)	108.40(9)
O(2)-S(2)-O(1)	120.23(13)
O(2)-S(2)-C(1)	108.66(13)
C(1)-S(2)-S(1)	105.16(9)

C(8)-N(1)-C(9)	116.9(2)
C(2)-C(1)-S(2)	117.5(2)
C(2)-C(1)-C(9)	121.9(3)
C(9)-C(1)-S(2)	120.6(2)
C(1)-C(2)-H(2)	120.2
C(1)-C(2)-C(3)	119.7(3)
C(3)-C(2)-H(2)	120.2
C(2)-C(3)-H(3)	120.0
C(4)-C(3)-C(2)	120.1(3)
C(4)-C(3)-H(3)	120.0
C(3)-C(4)-H(4)	119.5
C(3)-C(4)-C(5)	121.0(3)
C(5)-C(4)-H(4)	119.5
C(4)-C(5)-C(6)	122.9(3)
C(9)-C(5)-C(4)	119.9(3)
C(9)-C(5)-C(6)	117.2(3)
C(5)-C(6)-H(6)	119.8
C(7)-C(6)-C(5)	120.4(3)
C(7)-C(6)-H(6)	119.8
C(6)-C(7)-C(8)	117.0(3)
C(6)-C(7)-C(10)	122.7(3)
C(8)-C(7)-C(10)	120.3(3)
N(1)-C(8)-C(7)	125.4(3)
N(1)-C(8)-H(8)	117.3
C(7)-C(8)-H(8)	117.3
N(1)-C(9)-C(1)	119.6(2)
N(1)-C(9)-C(5)	123.0(3)
C(5)-C(9)-C(1)	117.4(2)
C(7)-C(10)-H(10A)	109.5
C(7)-C(10)-H(10B)	109.5
C(7)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
F(1)-C(11)-S(1)	113.54(19)
F(1)-C(11)-F(3)	107.8(2)
F(2)-C(11)-S(1)	114.48(19)
F(2)-C(11)-F(1)	106.9(3)

F(2)-C(11)-F(3)	107.7(2)
F(3)-C(11)-S(1)	106.0(2)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for dm14611. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
S(1)	34(1)	34(1)	28(1)	7(1)	10(1)	-1(1)
S(2)	36(1)	27(1)	19(1)	0(1)	7(1)	2(1)
F(1)	45(1)	32(1)	39(1)	-4(1)	1(1)	-5(1)
F(2)	42(1)	31(1)	36(1)	0(1)	8(1)	9(1)
F(3)	62(1)	64(1)	22(1)	12(1)	12(1)	15(1)
O(1)	45(1)	34(1)	25(1)	-6(1)	-2(1)	-1(1)
O(2)	37(1)	35(1)	31(1)	1(1)	17(1)	7(1)
N(1)	29(1)	26(1)	20(1)	1(1)	4(1)	0(1)
C(1)	32(2)	26(1)	14(1)	1(1)	4(1)	2(1)
C(2)	31(2)	35(2)	18(1)	3(1)	7(1)	0(1)
C(3)	32(2)	34(2)	20(1)	4(1)	4(1)	-6(1)
C(4)	40(2)	26(1)	17(1)	4(1)	2(1)	-4(1)
C(5)	33(2)	23(1)	14(1)	2(1)	2(1)	0(1)
C(6)	36(2)	26(1)	17(1)	1(1)	1(1)	3(1)
C(7)	33(2)	31(1)	15(1)	2(1)	2(1)	4(1)
C(8)	28(2)	29(1)	21(1)	1(1)	4(1)	1(1)
C(9)	29(1)	25(1)	14(1)	0(1)	4(1)	-2(1)
C(10)	35(2)	37(2)	24(1)	-2(1)	6(1)	6(1)
C(11)	44(2)	26(1)	24(1)	2(1)	8(1)	4(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for dm14611.

	x	y	z	U(eq)
H(2)	5765	8761	10820	33
H(3)	5786	6770	10734	35
H(4)	7166	5832	10191	33
H(6)	8900	5891	9514	32
H(8)	10140	8937	9214	31
H(10A)	11064	6669	10144	48
H(10B)	10938	7285	8220	48
H(10C)	10479	6061	8377	48

Table 6. Torsion angles [°] for dm14611.

S(1)-S(2)-C(1)-C(2)	-122.59(18)
S(1)-S(2)-C(1)-C(9)	60.1(2)
S(2)-S(1)-C(11)-F(1)	-49.1(2)
S(2)-S(1)-C(11)-F(2)	74.1(2)
S(2)-S(1)-C(11)-F(3)	-167.30(17)
S(2)-C(1)-C(2)-C(3)	-174.59(19)
S(2)-C(1)-C(9)-N(1)	-5.1(3)
S(2)-C(1)-C(9)-C(5)	175.13(18)
O(1)-S(2)-C(1)-C(2)	126.8(2)
O(1)-S(2)-C(1)-C(9)	-50.6(2)
O(2)-S(2)-C(1)-C(2)	-6.7(2)
O(2)-S(2)-C(1)-C(9)	175.96(18)
C(1)-C(2)-C(3)-C(4)	-1.6(4)
C(2)-C(1)-C(9)-N(1)	177.6(2)
C(2)-C(1)-C(9)-C(5)	-2.1(3)
C(2)-C(3)-C(4)-C(5)	-0.2(4)
C(3)-C(4)-C(5)-C(6)	-179.0(2)
C(3)-C(4)-C(5)-C(9)	0.8(4)
C(4)-C(5)-C(6)-C(7)	-179.9(2)
C(4)-C(5)-C(9)-N(1)	-179.4(2)
C(4)-C(5)-C(9)-C(1)	0.3(3)
C(5)-C(6)-C(7)-C(8)	-1.2(4)
C(5)-C(6)-C(7)-C(10)	178.3(2)
C(6)-C(5)-C(9)-N(1)	0.4(4)
C(6)-C(5)-C(9)-C(1)	-179.9(2)
C(6)-C(7)-C(8)-N(1)	1.6(4)
C(8)-N(1)-C(9)-C(1)	-179.8(2)
C(8)-N(1)-C(9)-C(5)	-0.1(3)
C(9)-N(1)-C(8)-C(7)	-0.9(4)
C(9)-C(1)-C(2)-C(3)	2.7(4)
C(9)-C(5)-C(6)-C(7)	0.3(3)
C(10)-C(7)-C(8)-N(1)	-177.9(2)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for dm14611 [Å and °].

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