Supporting Information for:

Synthesis of Trifluoromethylthioesters from Aldehydes via a Visible Light-Promoted Radical Process

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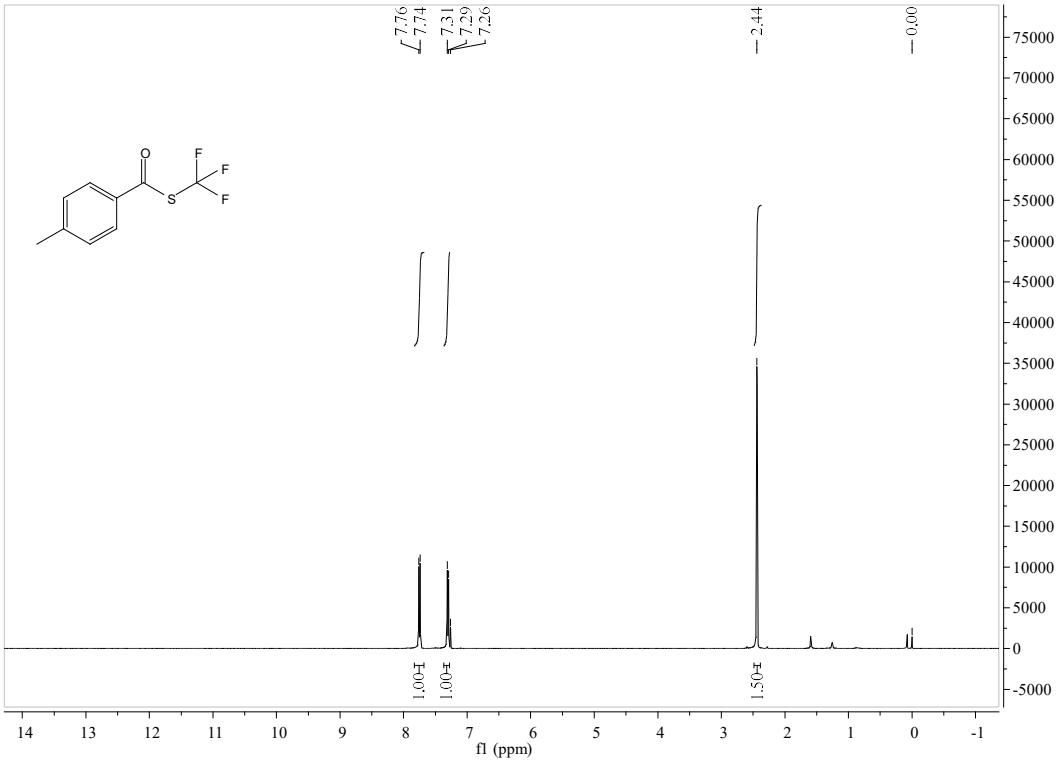
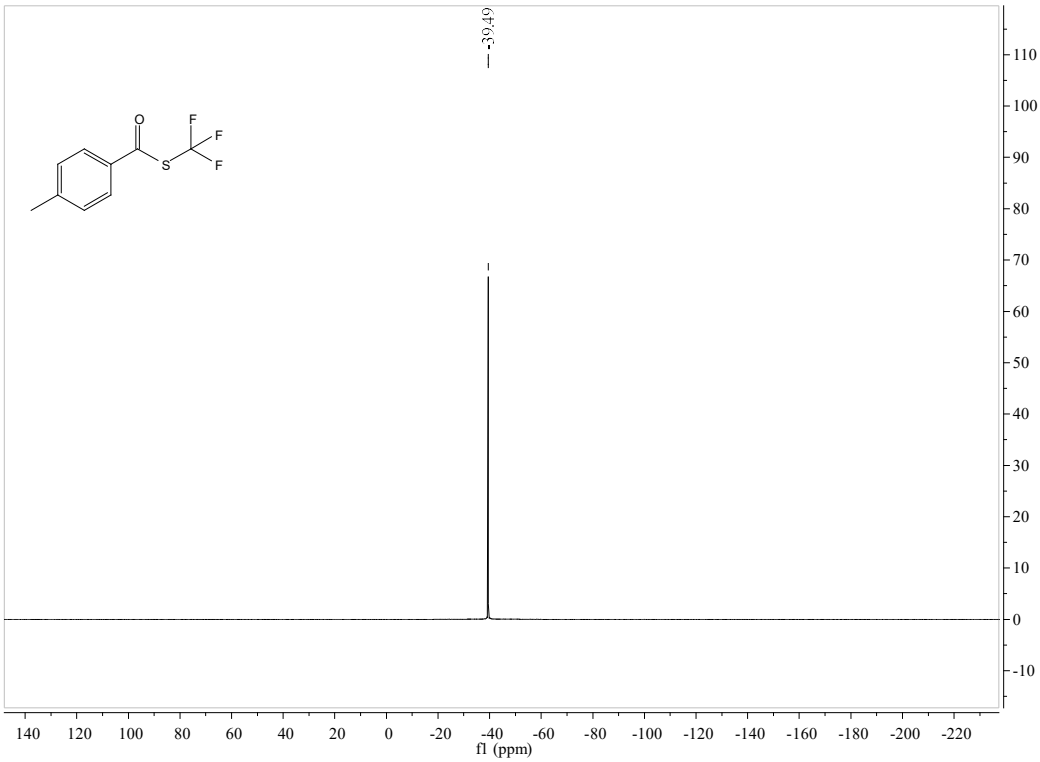
1. ^{1}H, ^{19}F, ^{13}C NMR spectra of compounds 3a – 3ad

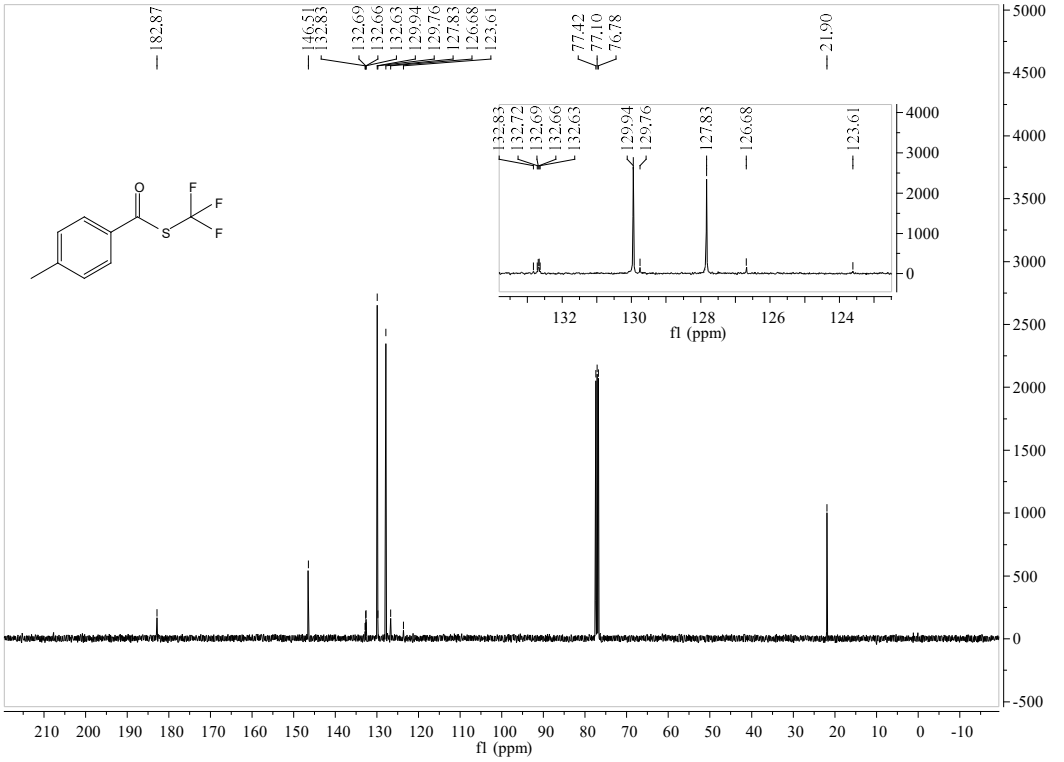
^{1}H NMR spectra of compound **3a**



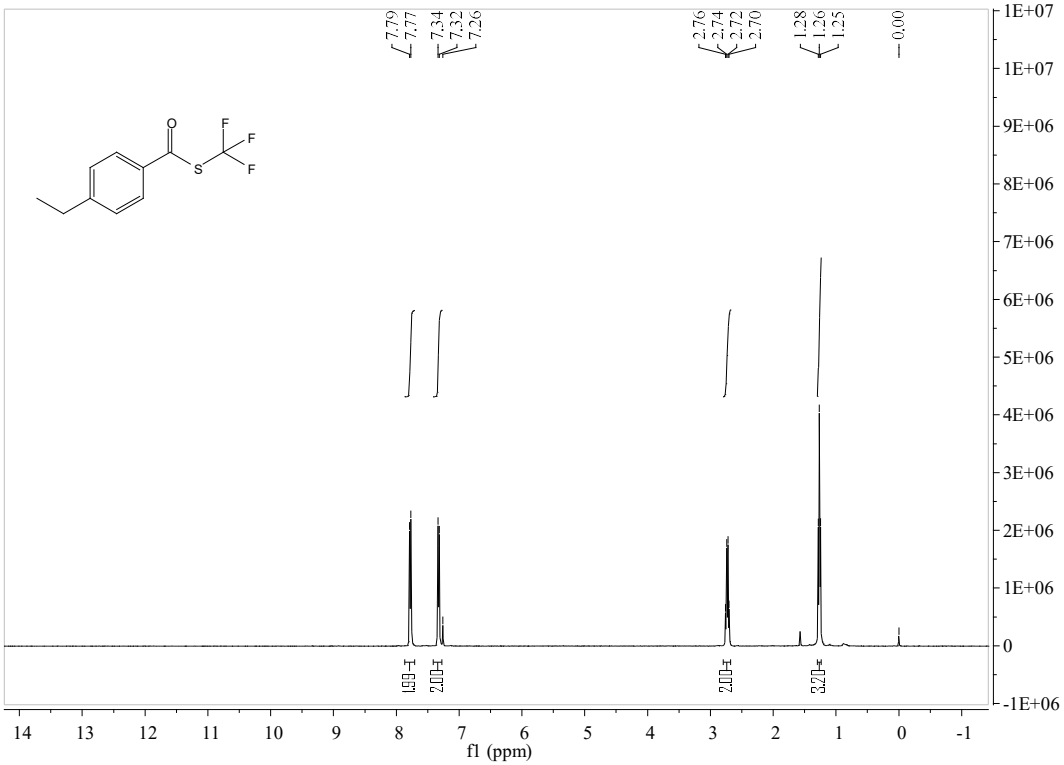
^{19}F NMR spectra of compound **3a**



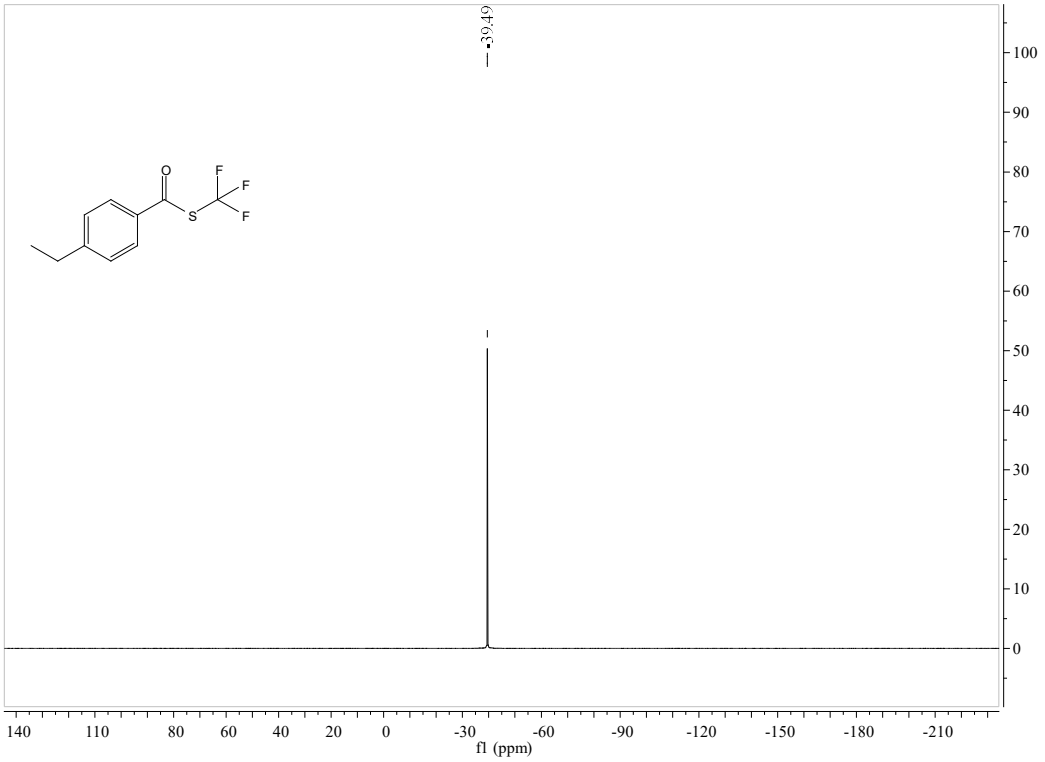
^{13}C NMR spectra of compound **3a**



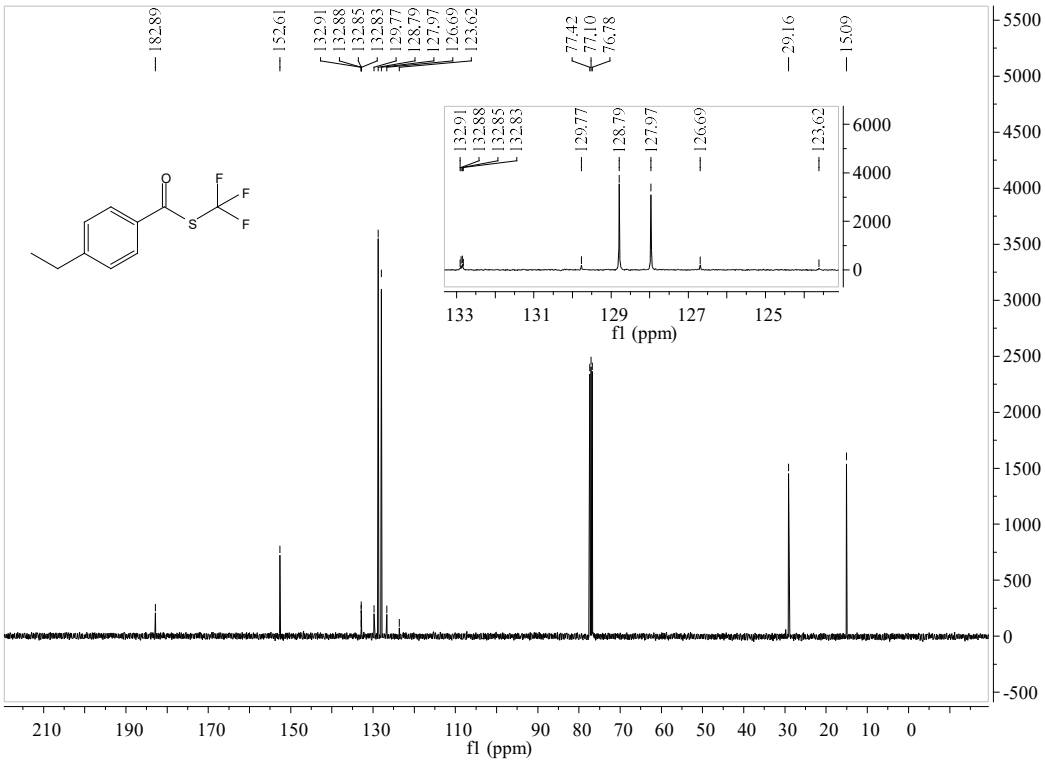
^{1}H NMR spectra of compound **3b**



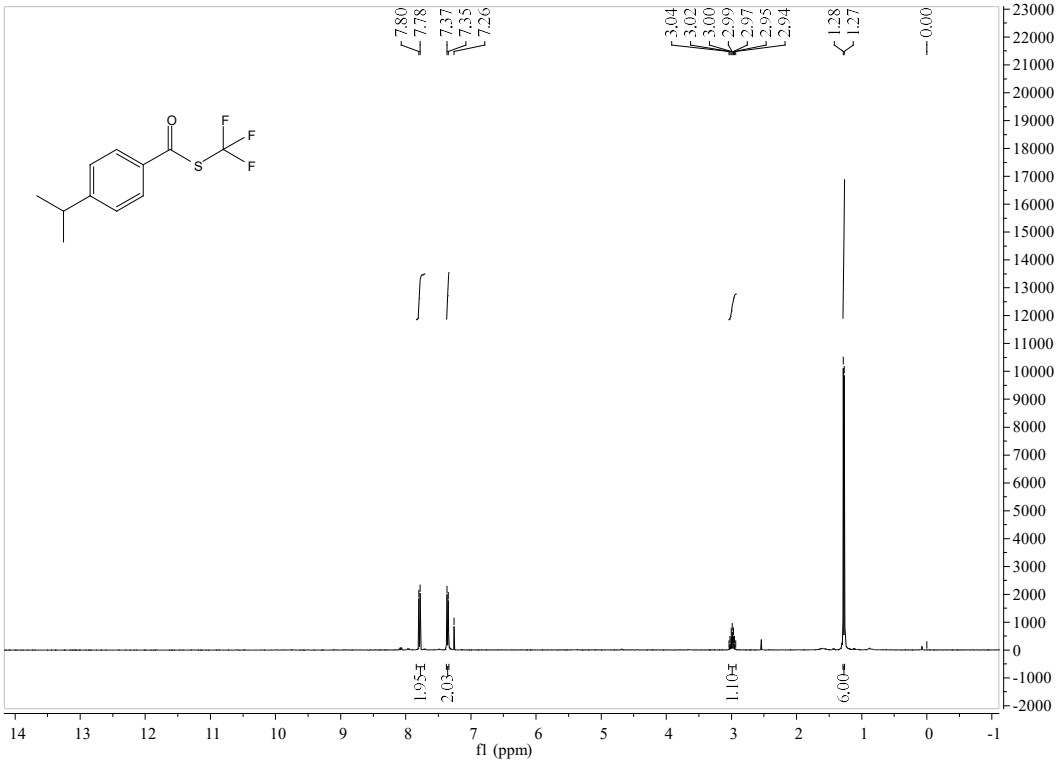
^{19}F NMR spectra of compound **3b**



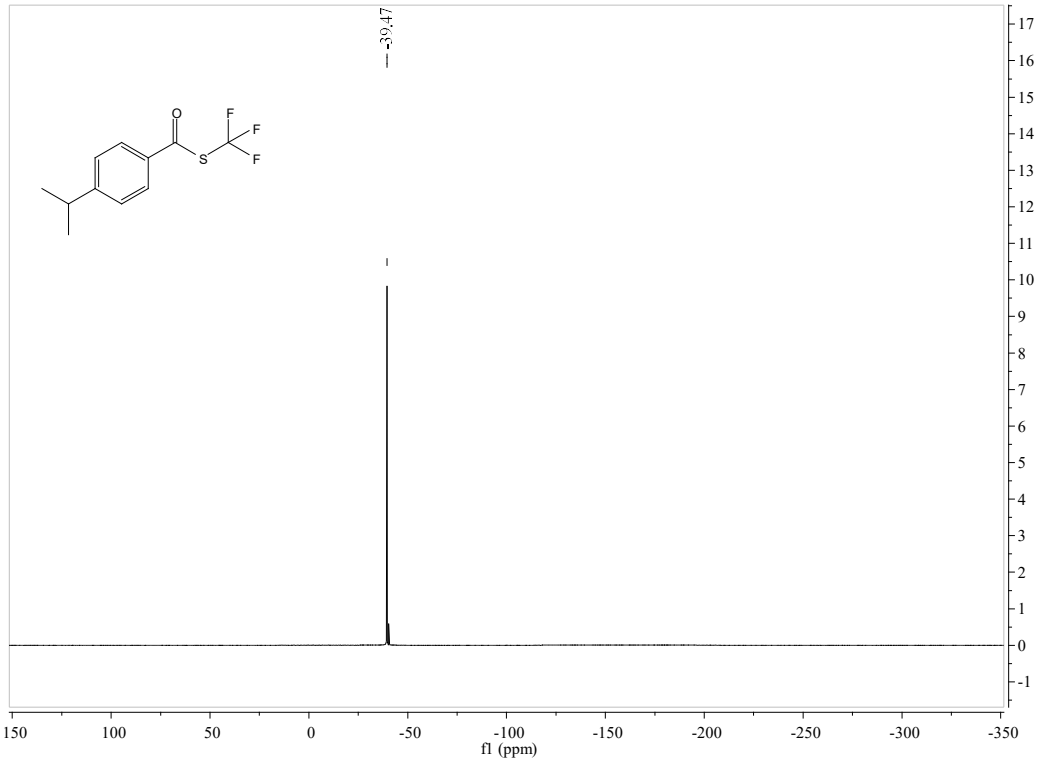
^{13}C NMR spectra of compound **3b**



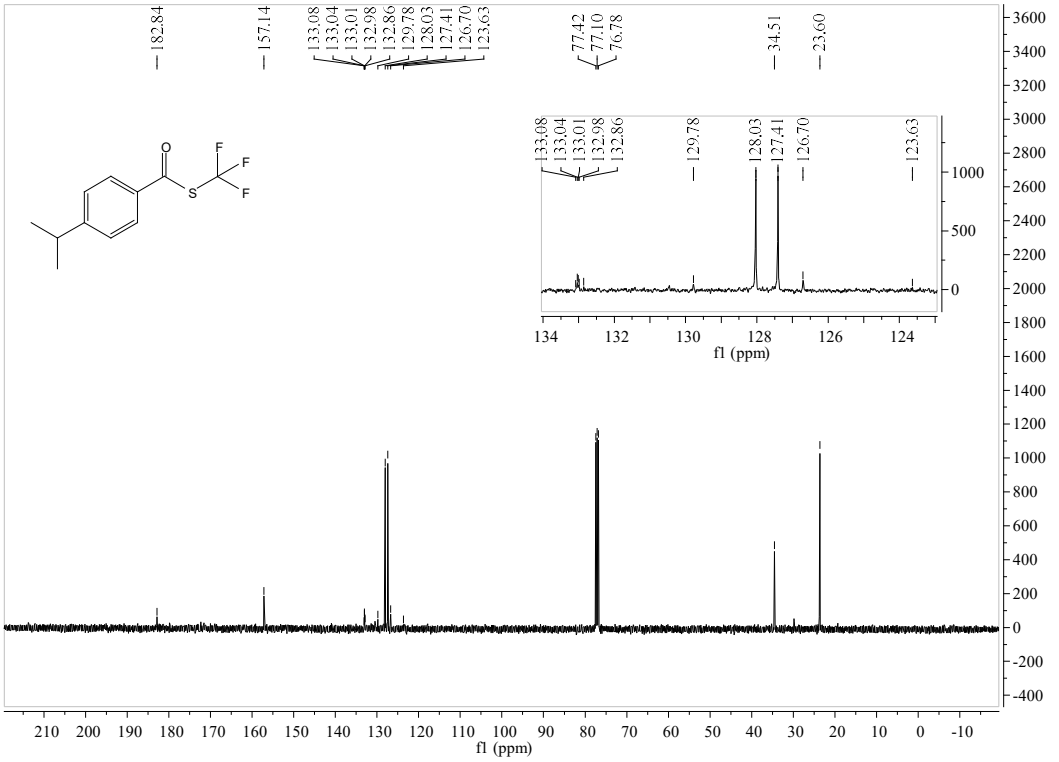
^{1}H NMR spectra of compound **3c**



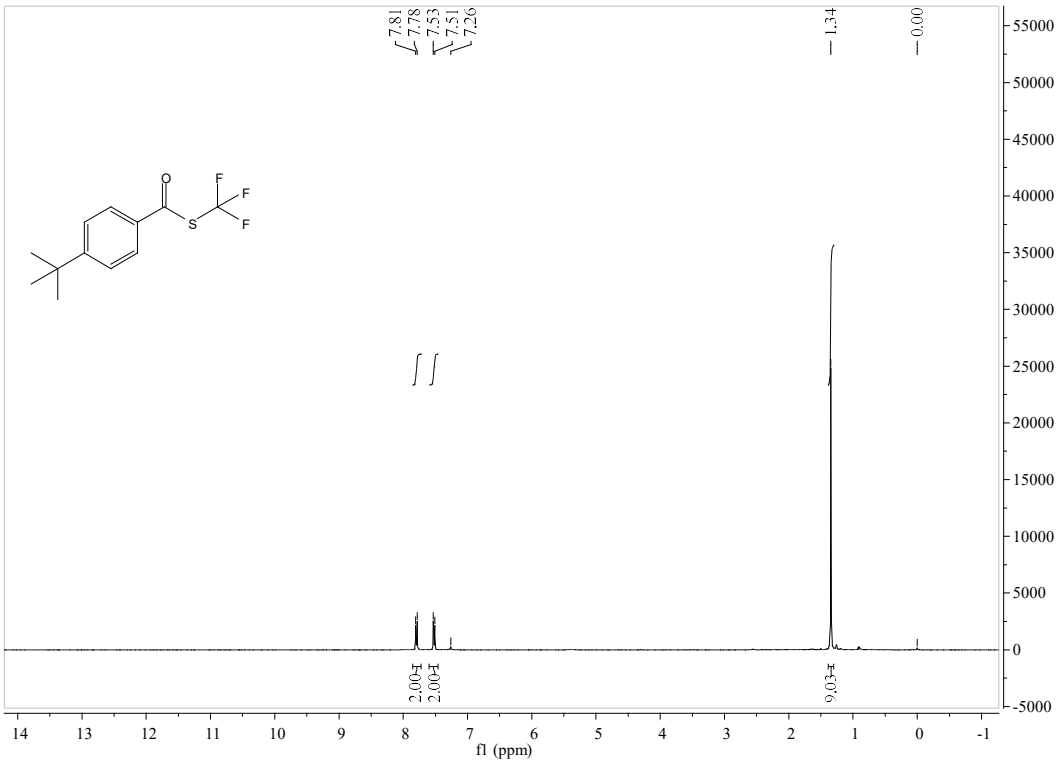
^{19}F NMR spectra of compound **3c**



^{13}C NMR spectra of compound **3c**

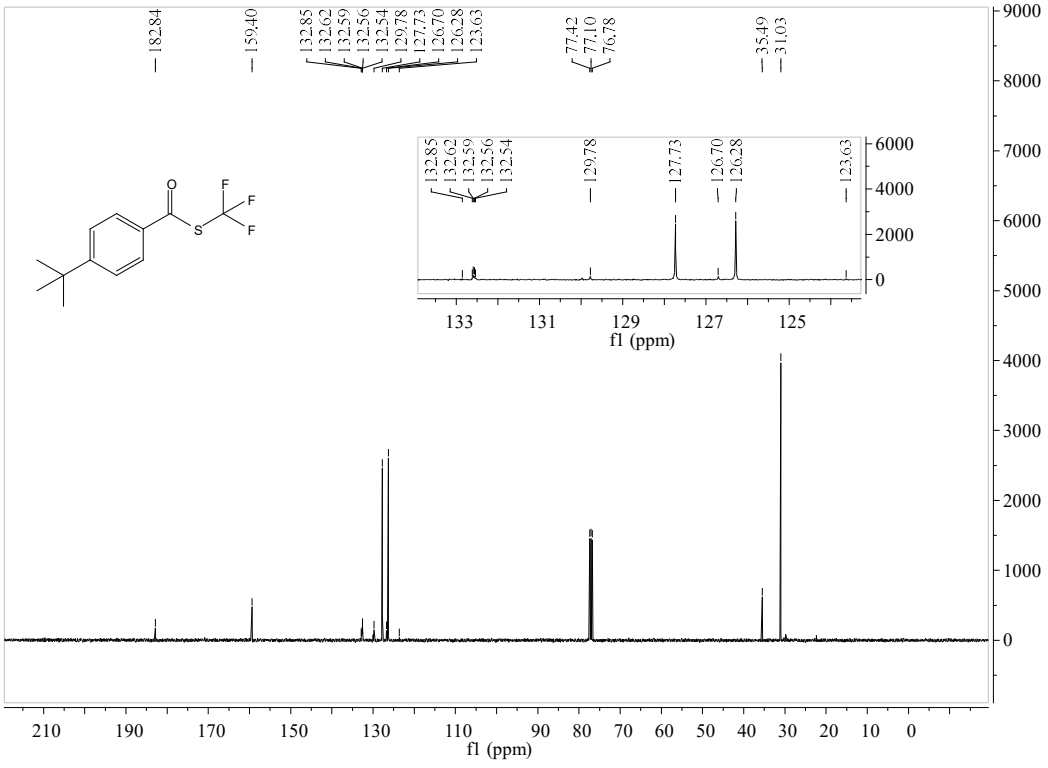


^{1}H NMR spectra of compound **3d**



^{19}F NMR spectra of compound **3d**

^{13}C NMR spectra of compound **3d**



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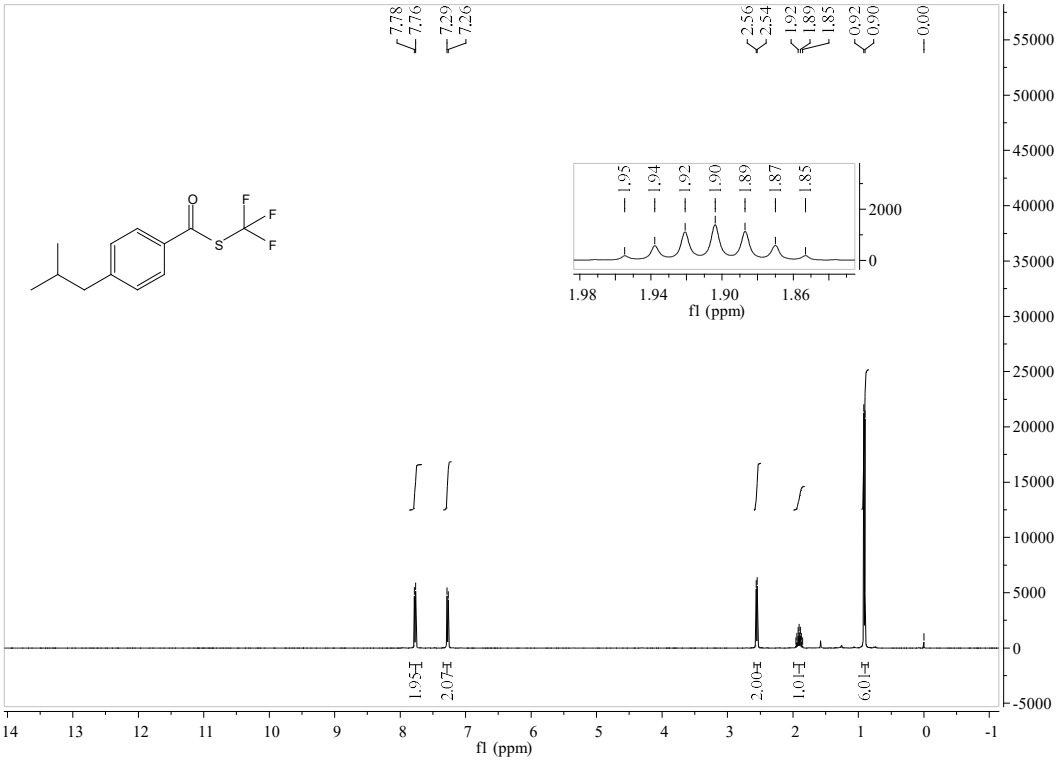
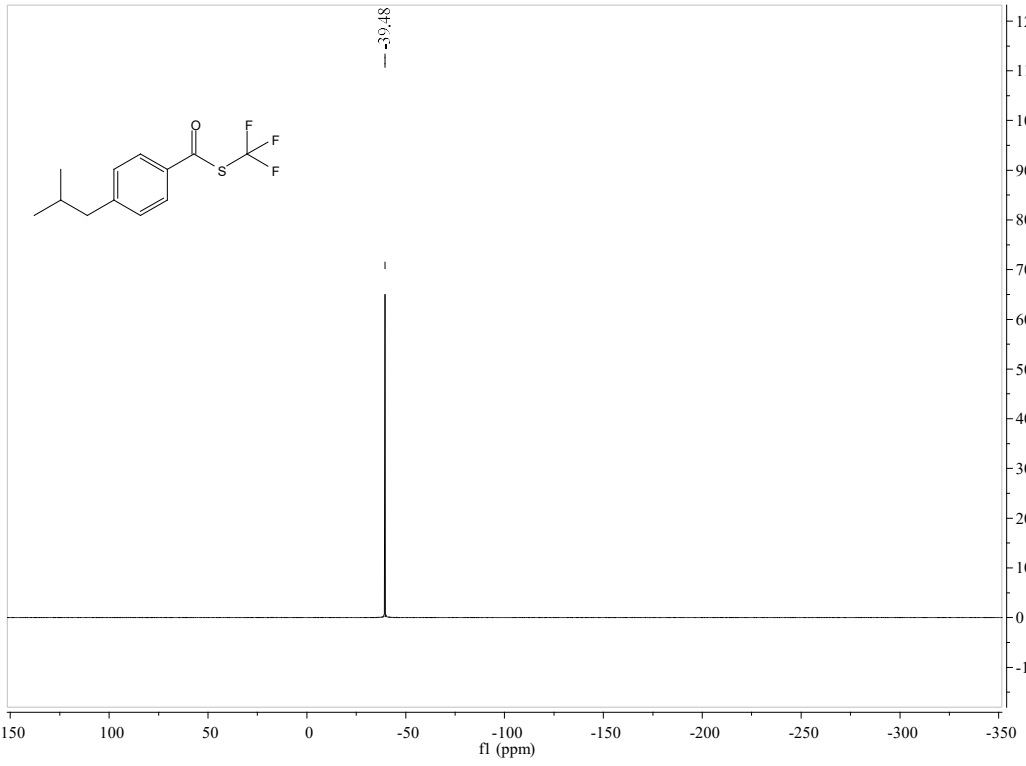
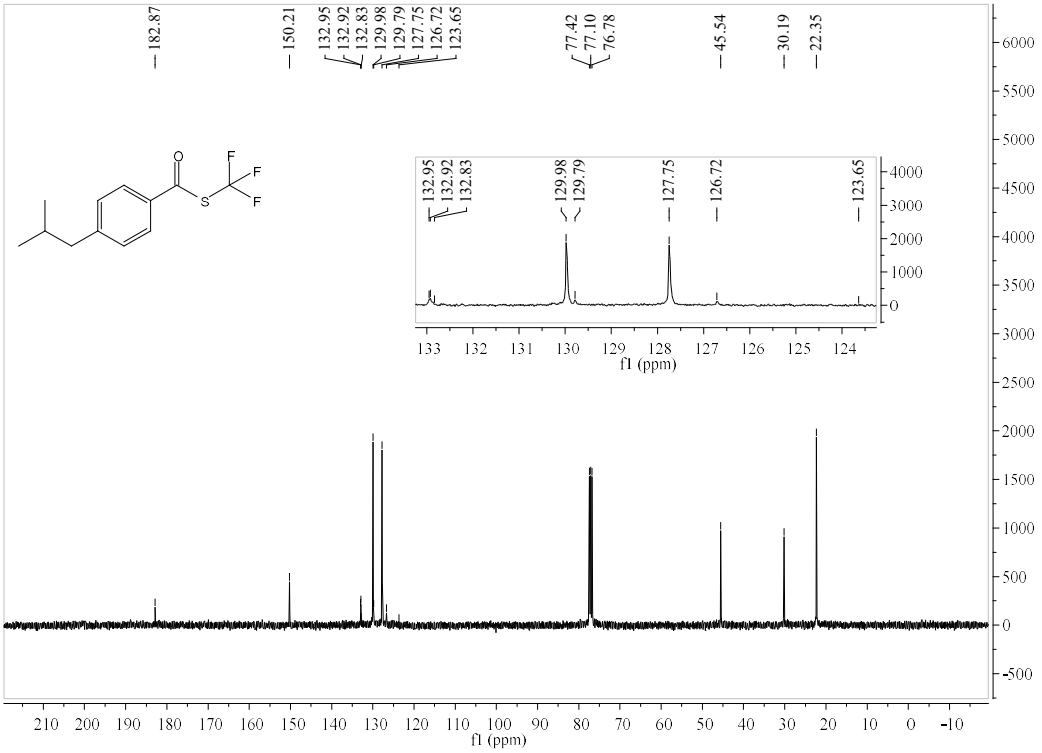


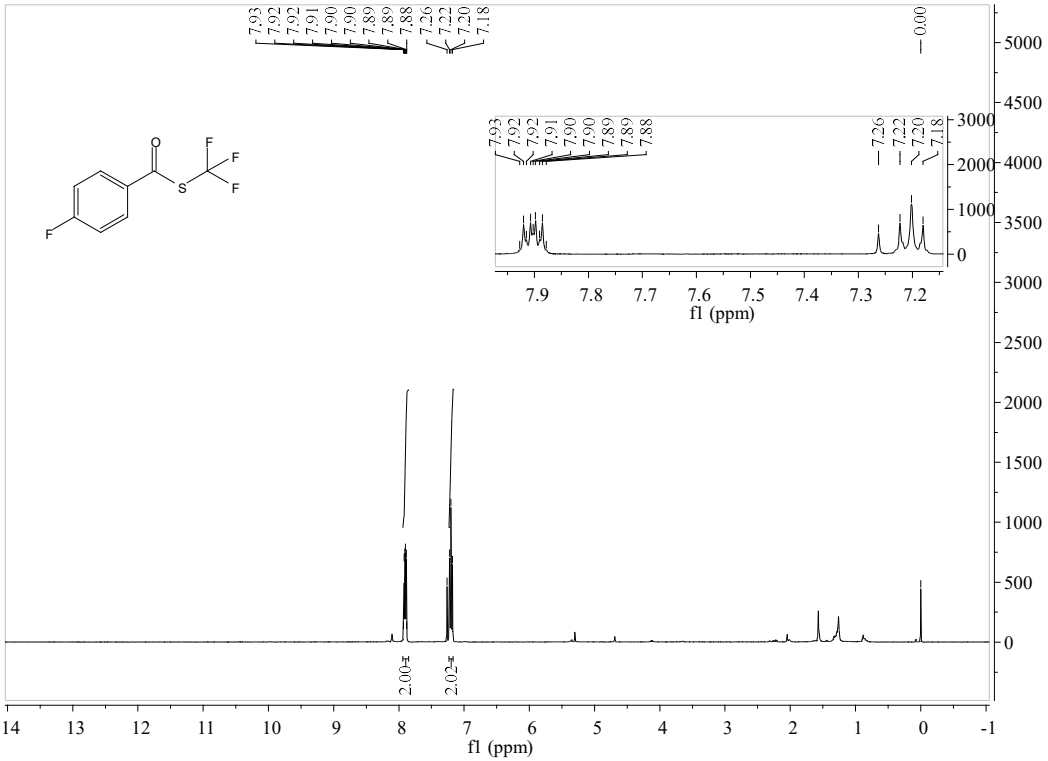
^{19}F NMR spectra of compound **3e**



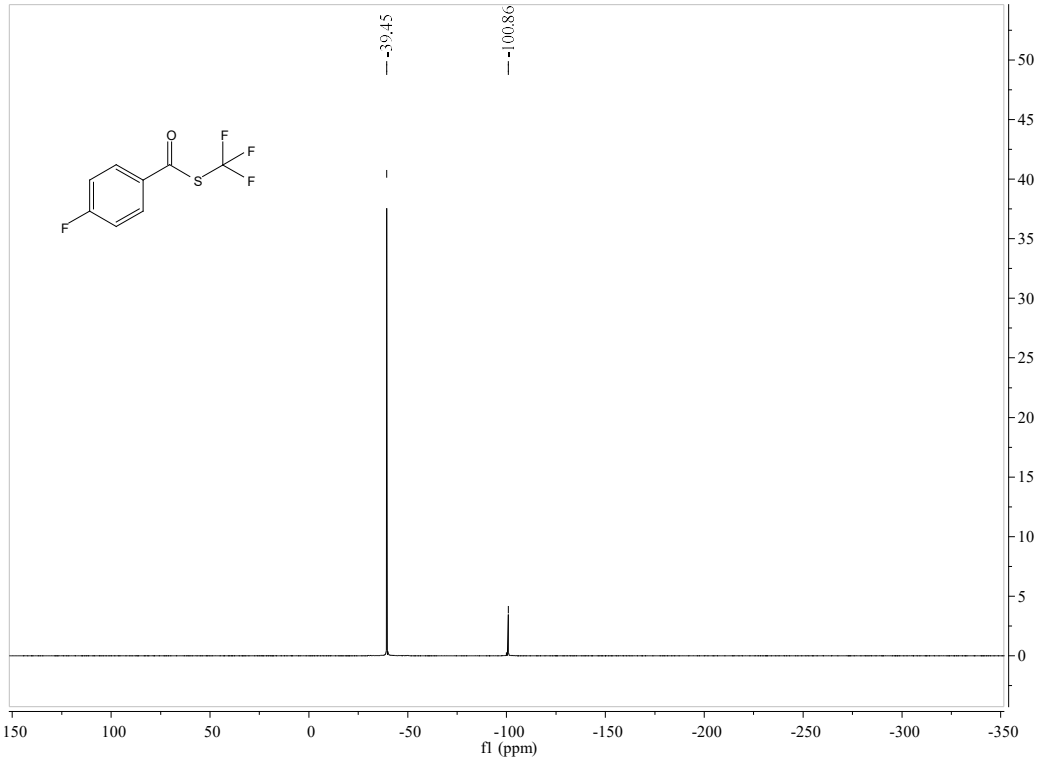
^{13}C NMR spectra of compound **3e**



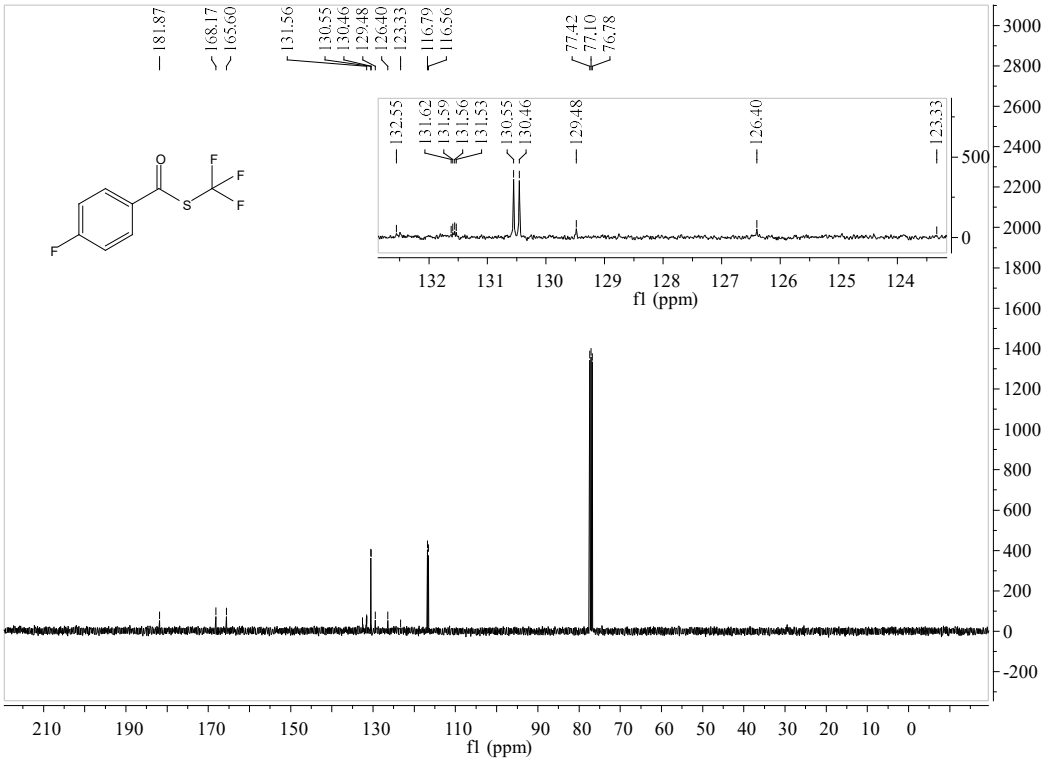
^{1}H NMR spectra of compound **3f**



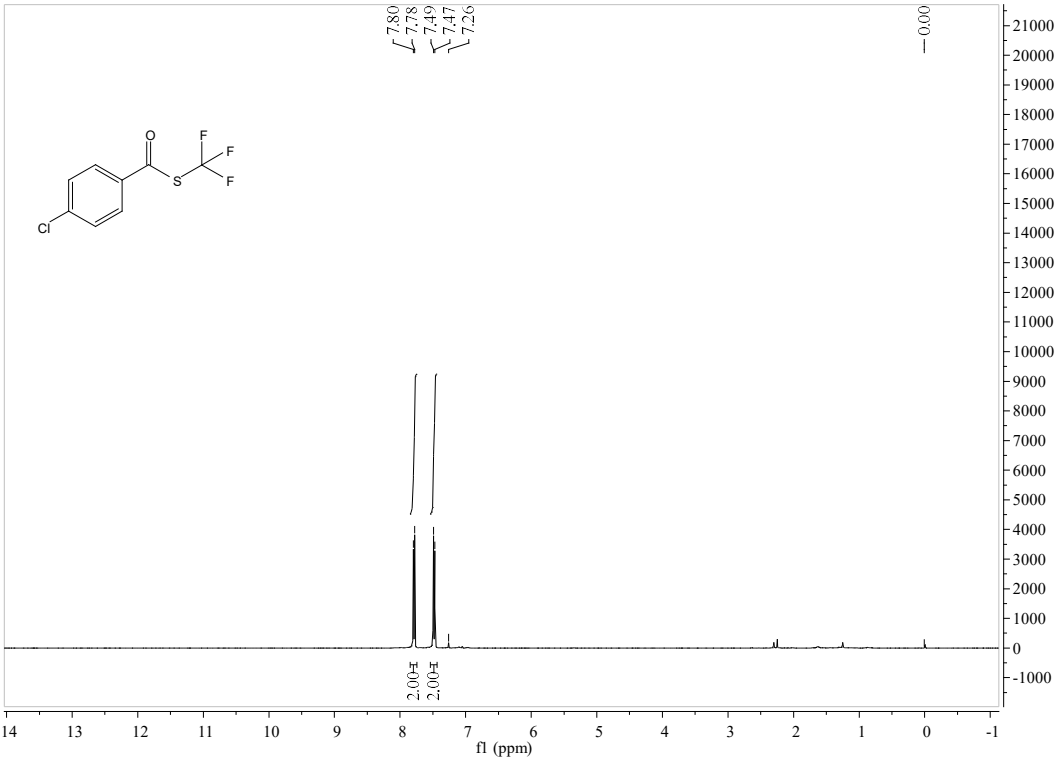
^{19}F NMR spectra of compound **3f**



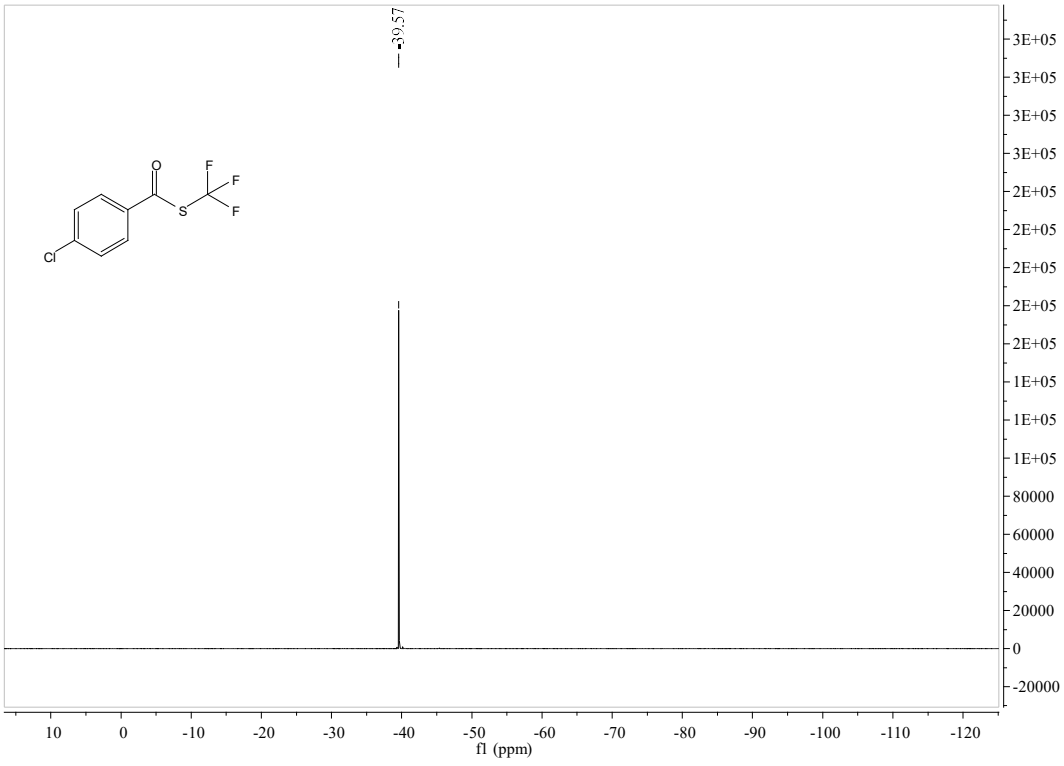
^{13}C NMR spectra of compound **3f**



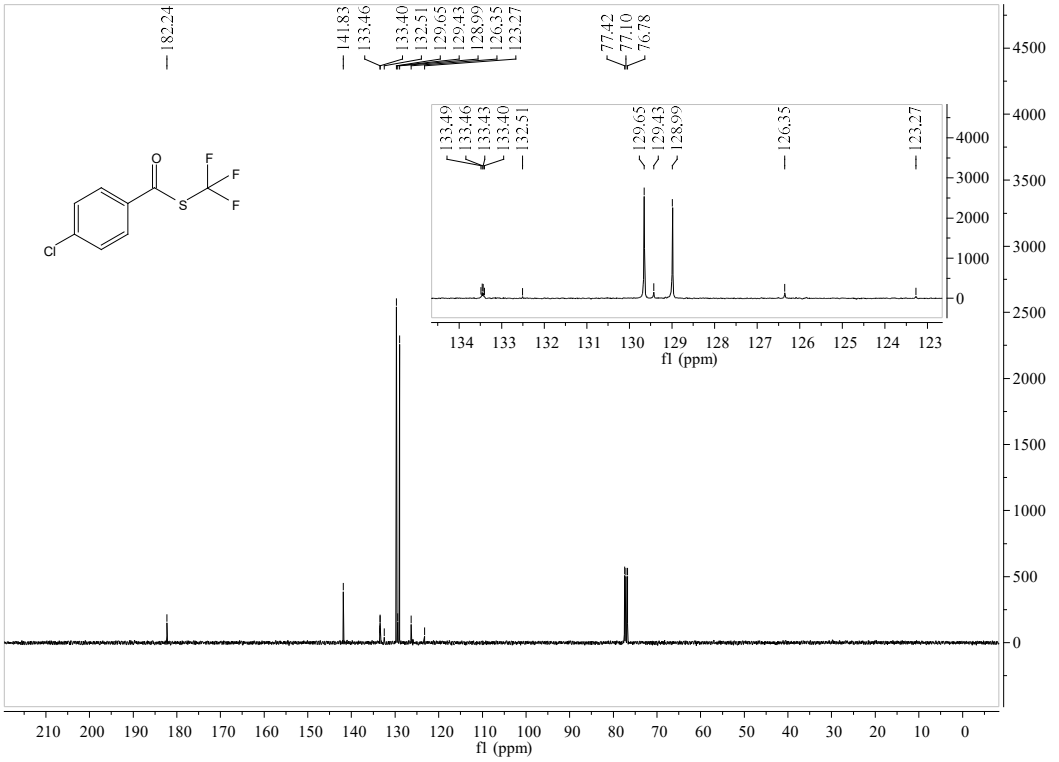
^{1}H NMR spectra of compound **3g**



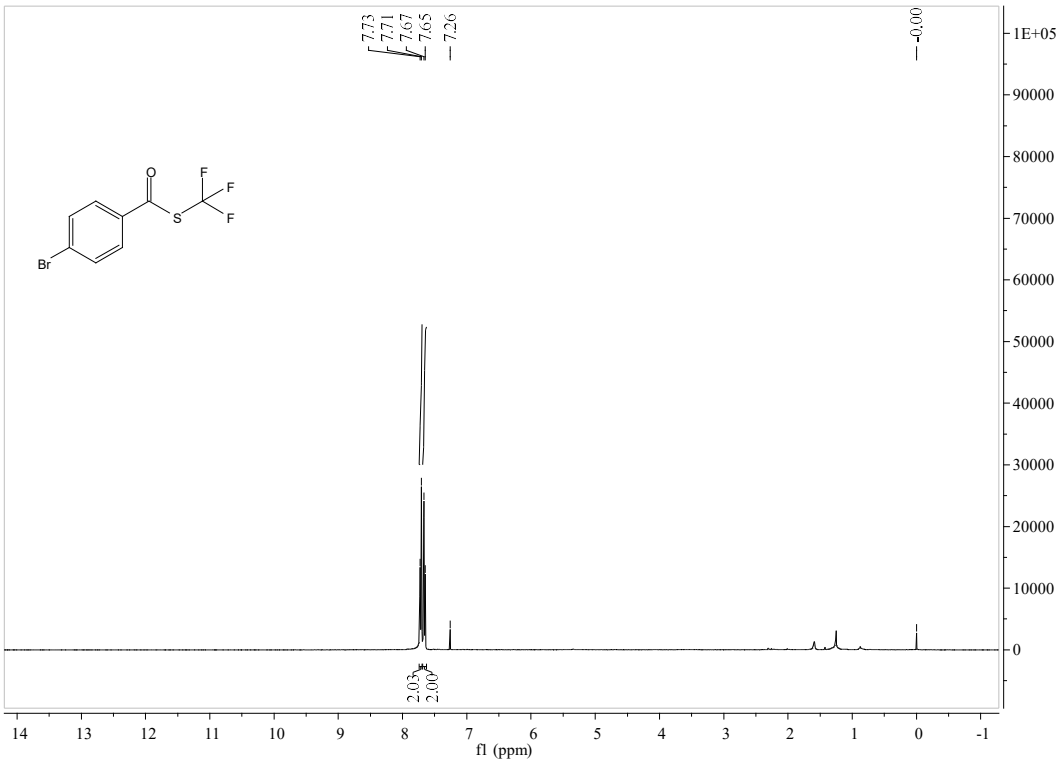
^{19}F NMR spectra of compound **3g**



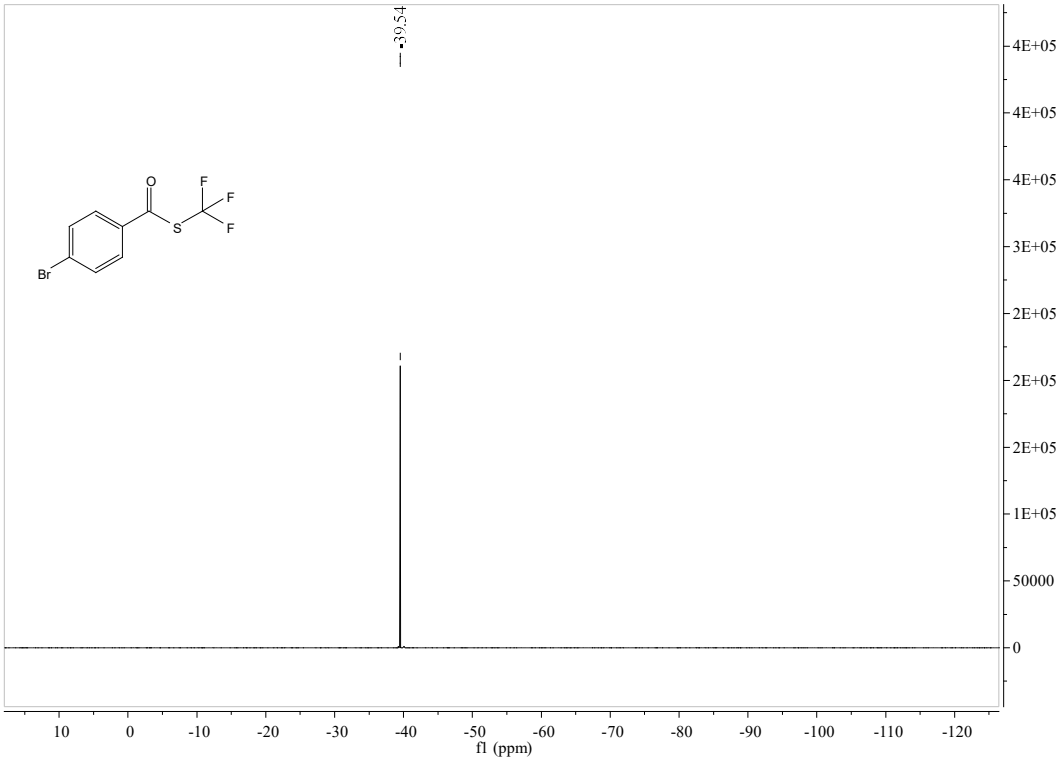
^{13}C NMR spectra of compound **3g**



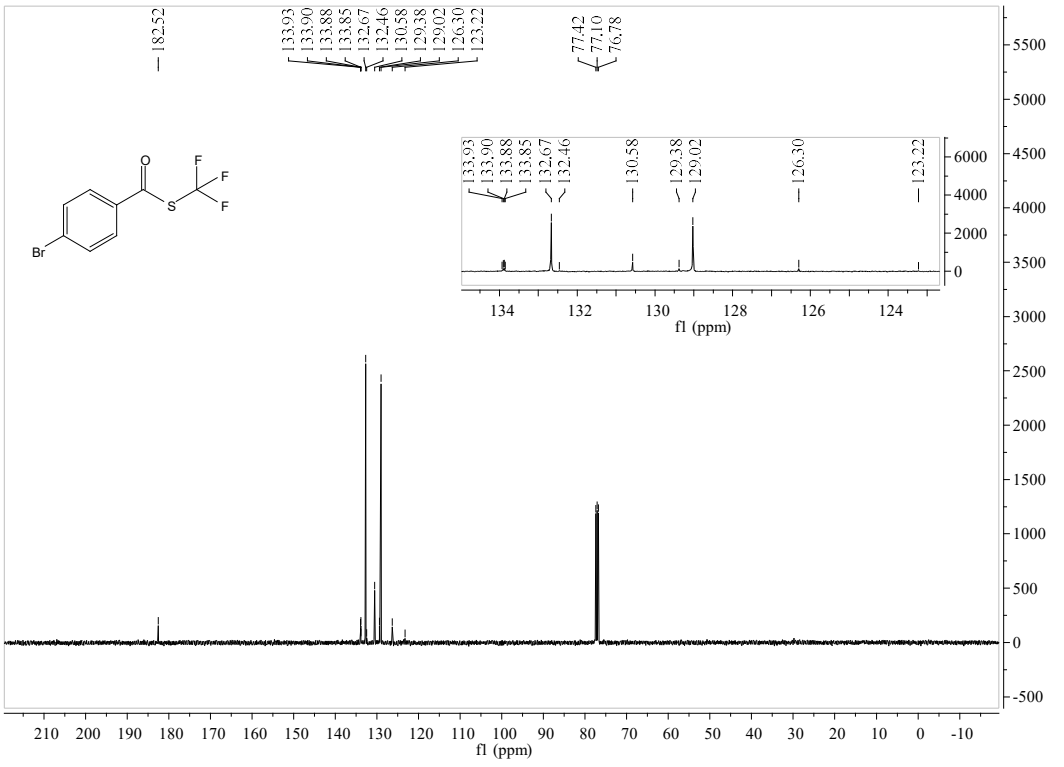
^{1}H NMR spectra of compound **3h**



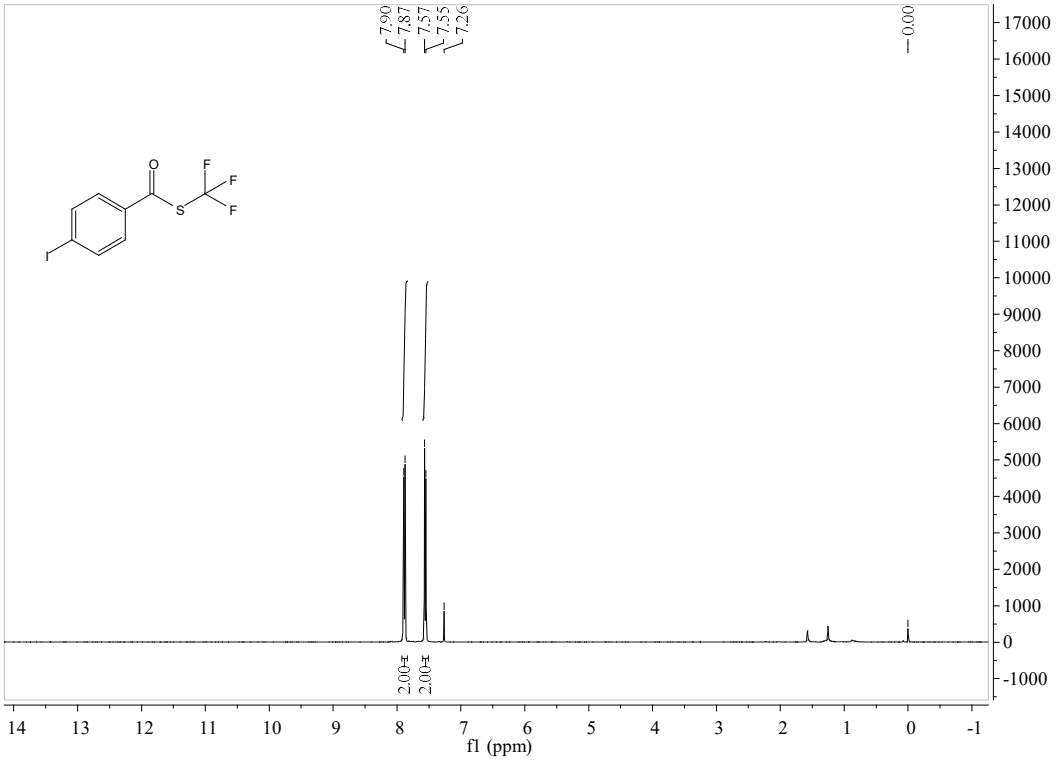
^{19}F NMR spectra of compound **3h**



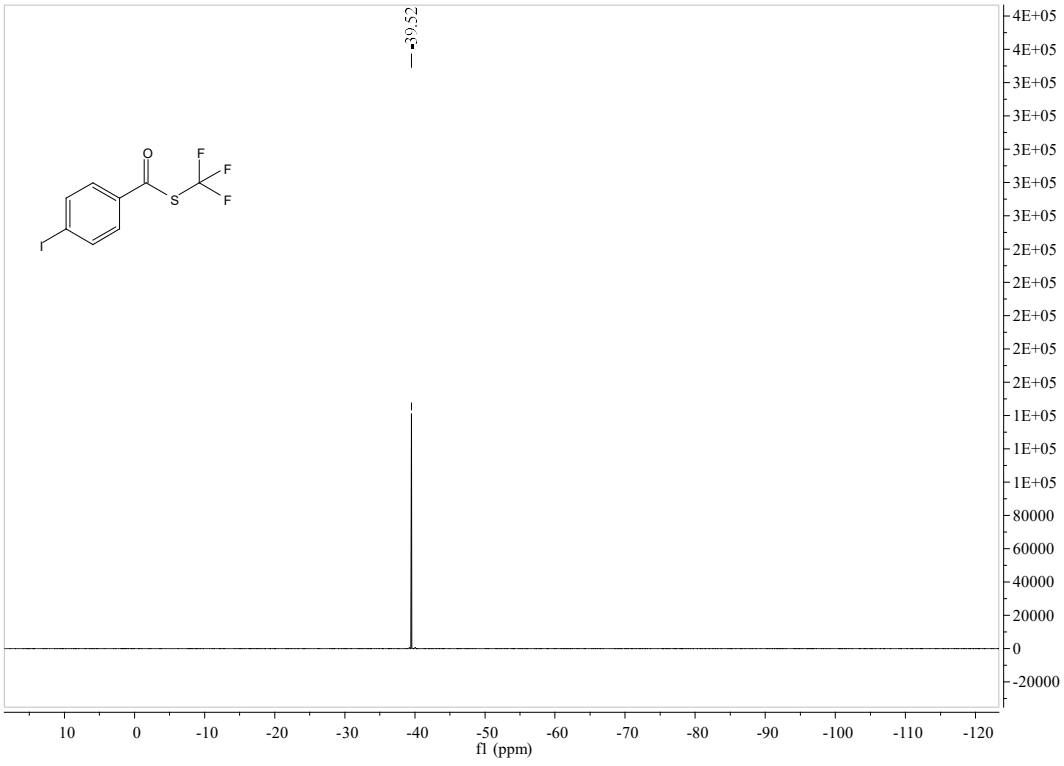
^{13}C NMR spectra of compound **3h**



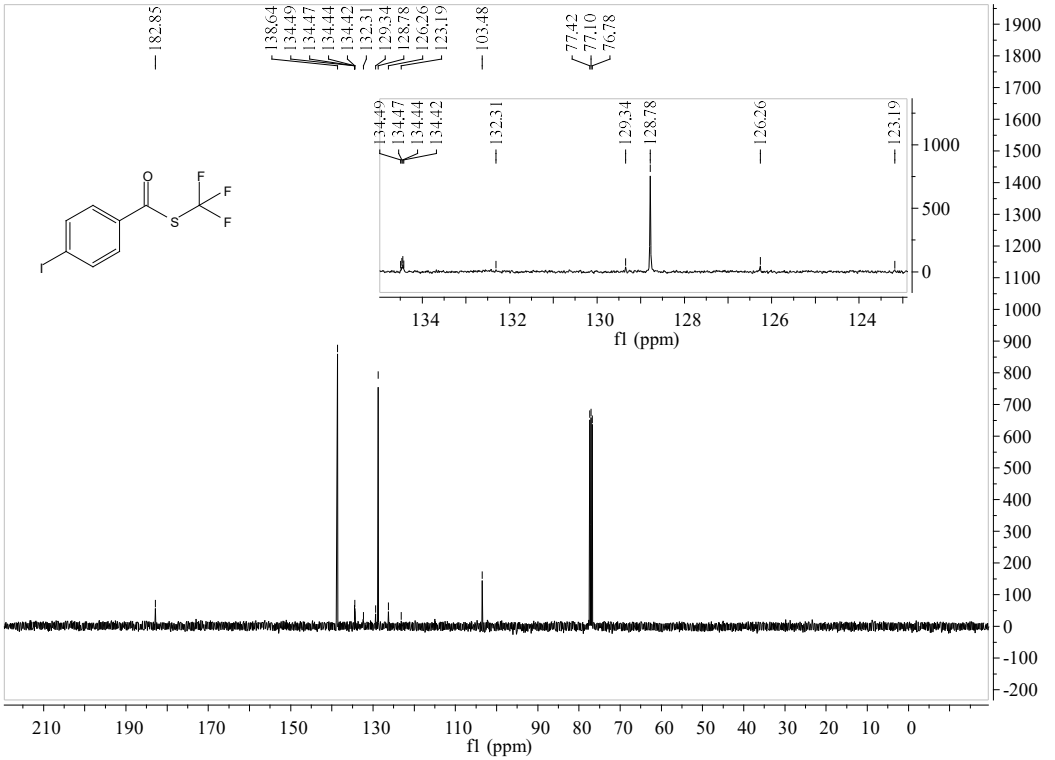
^{1}H NMR spectra of compound **3i**



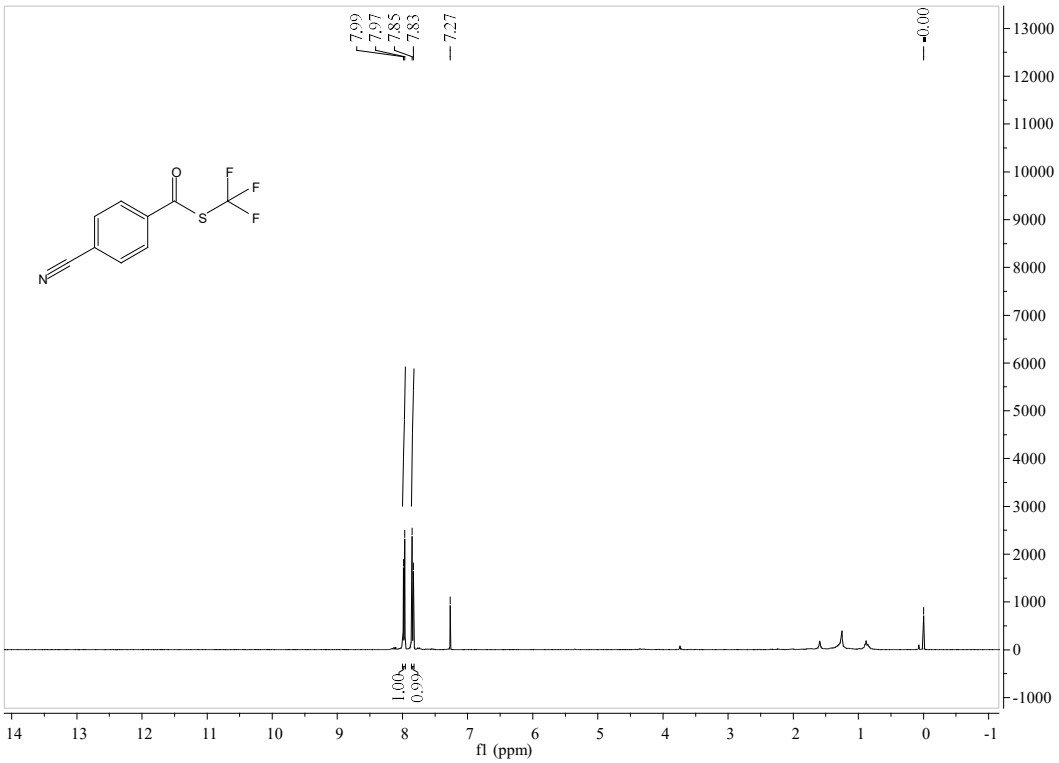
^{19}F NMR spectra of compound **3i**



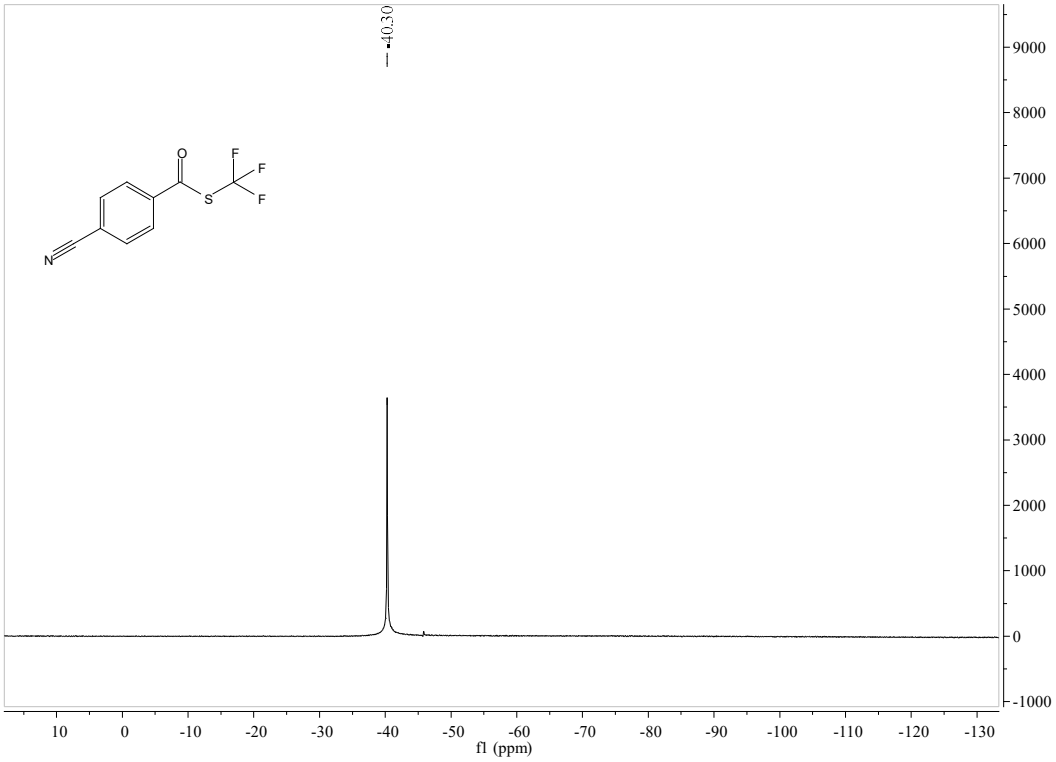
^{13}C NMR spectra of compound **3i**



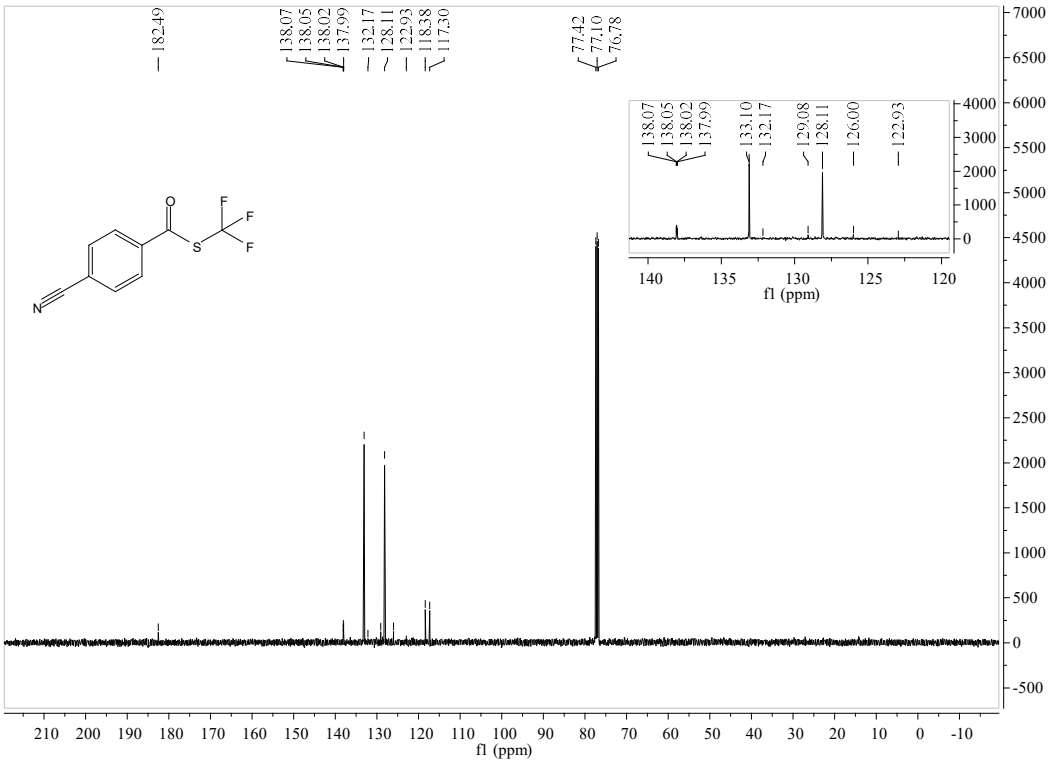
^{1}H NMR spectra of compound **3j**



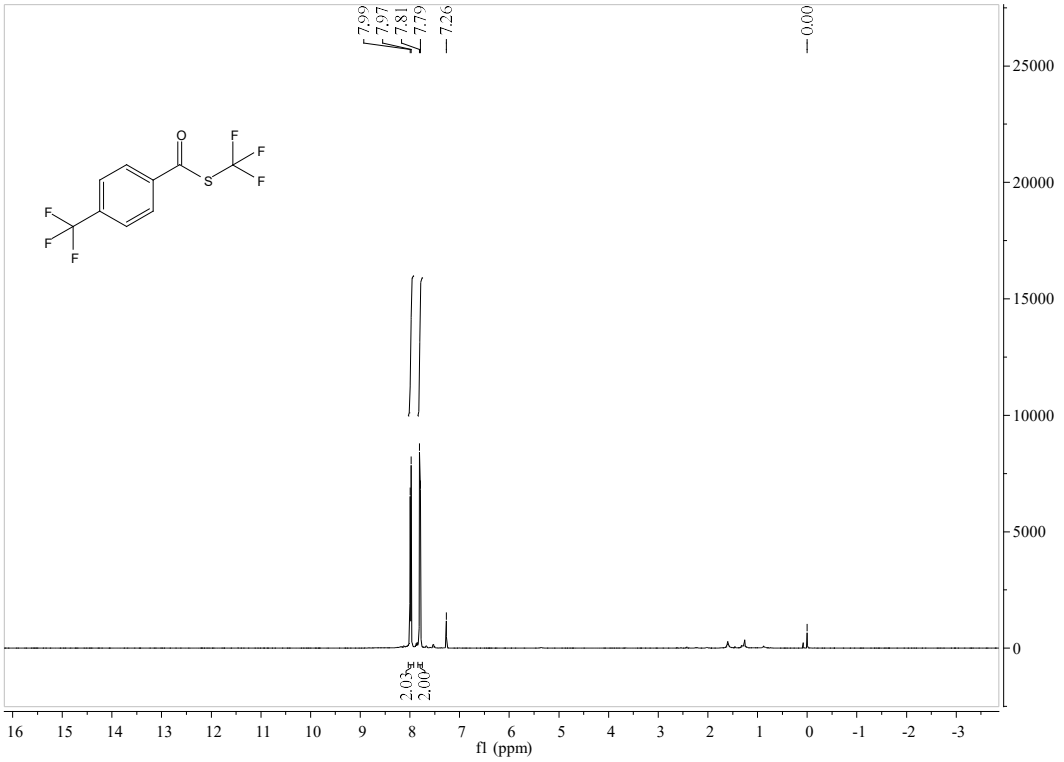
^{19}F NMR spectra of compound **3j**



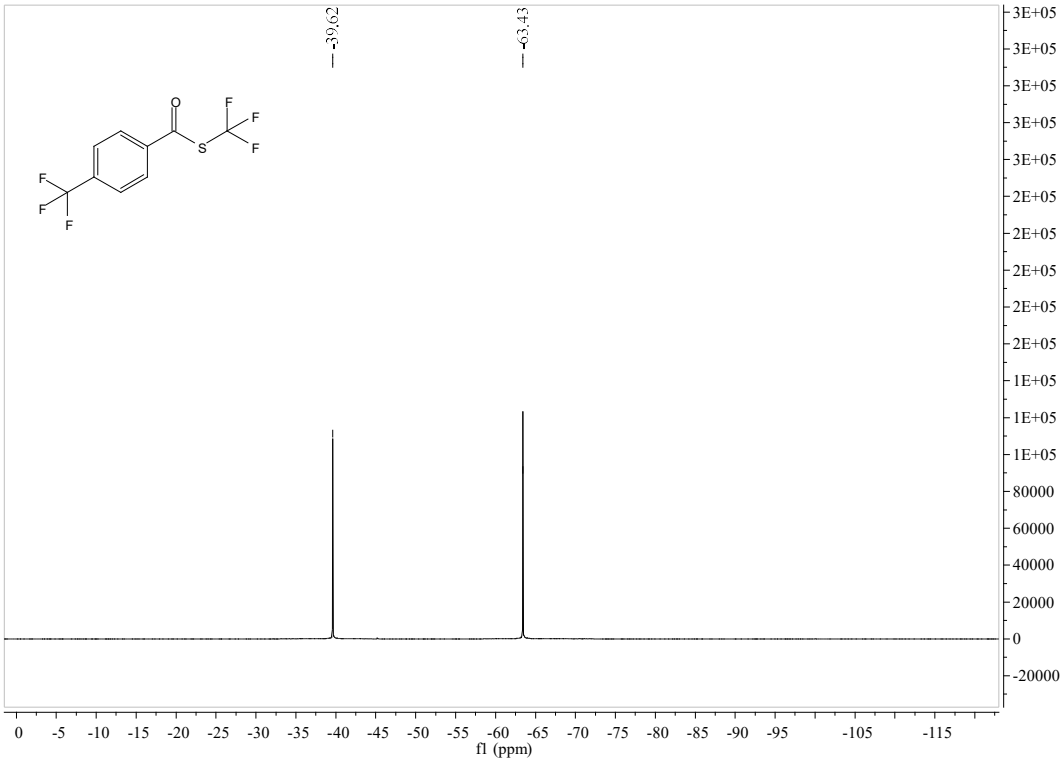
^{13}C NMR spectra of compound **3j**



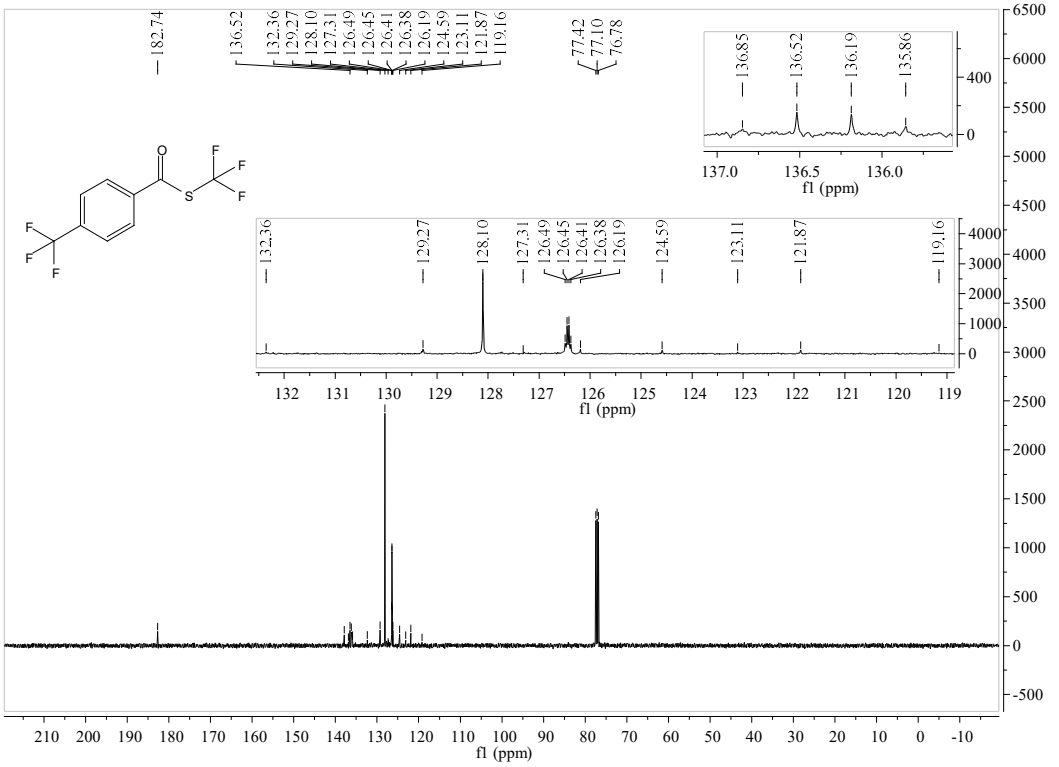
^{1}H NMR spectra of compound **3k**



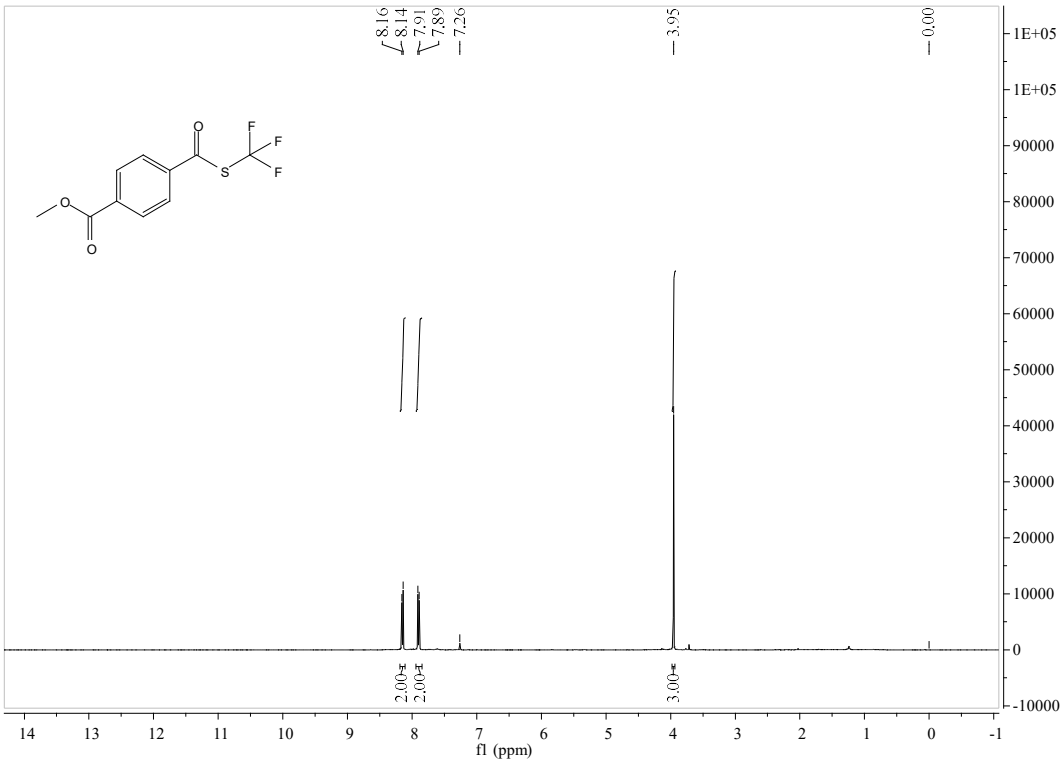
^{19}F NMR spectra of compound **3k**



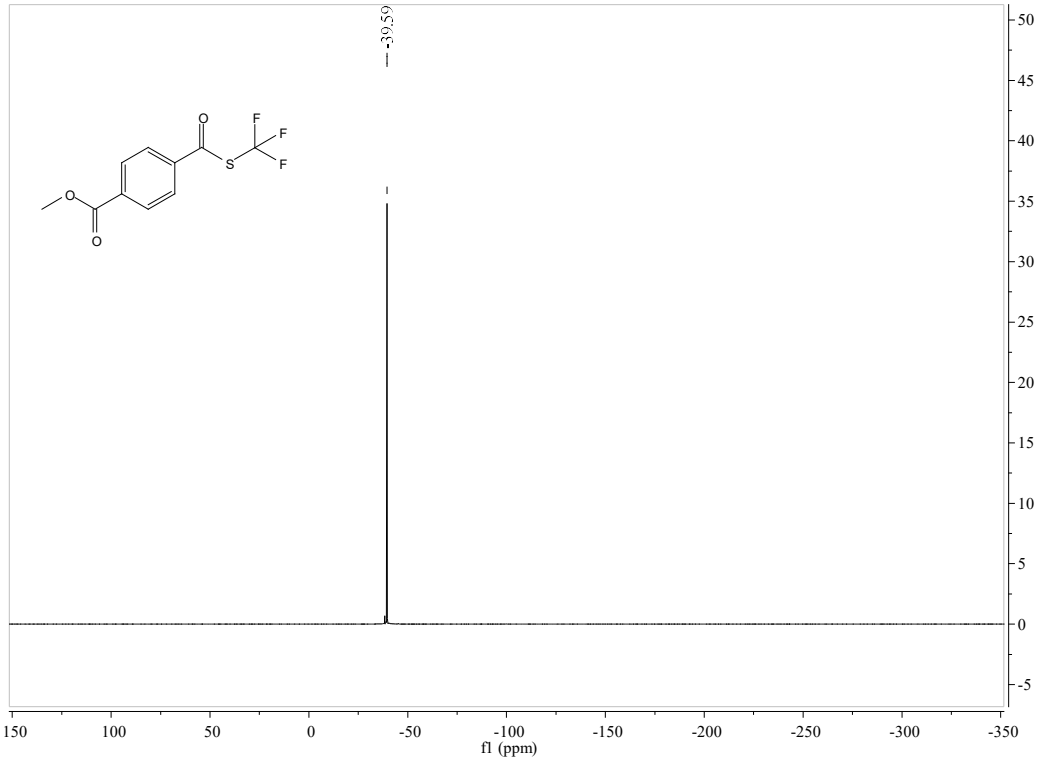
^{13}C NMR spectra of compound **3k**



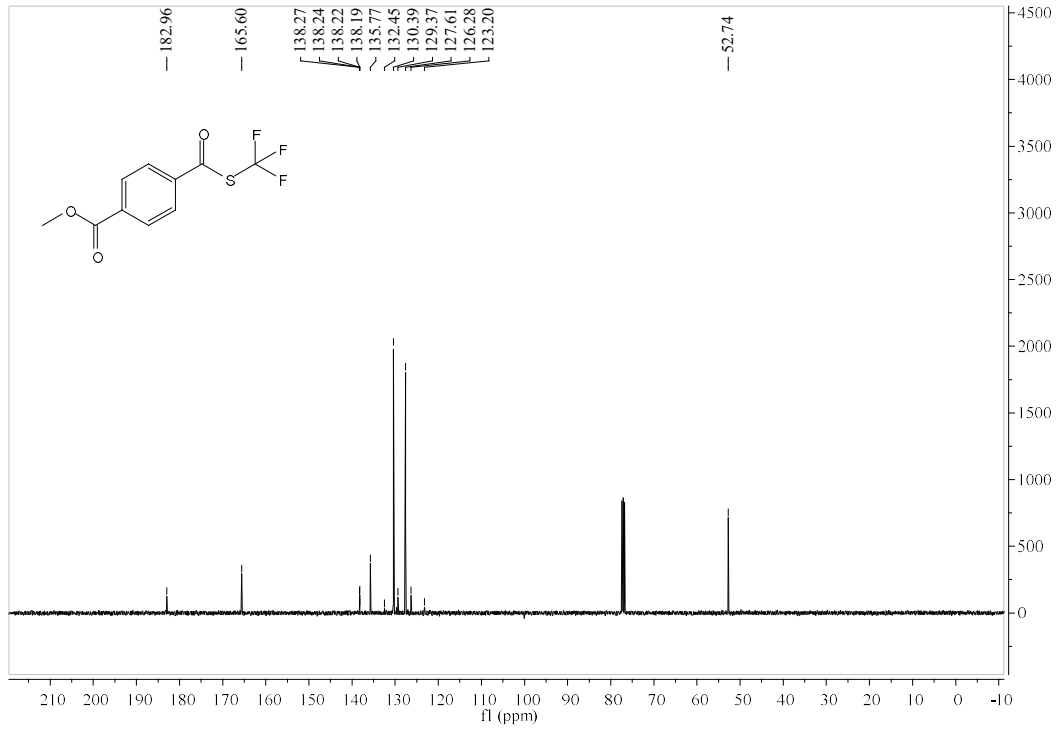
^{1}H NMR spectra of compound **3l**



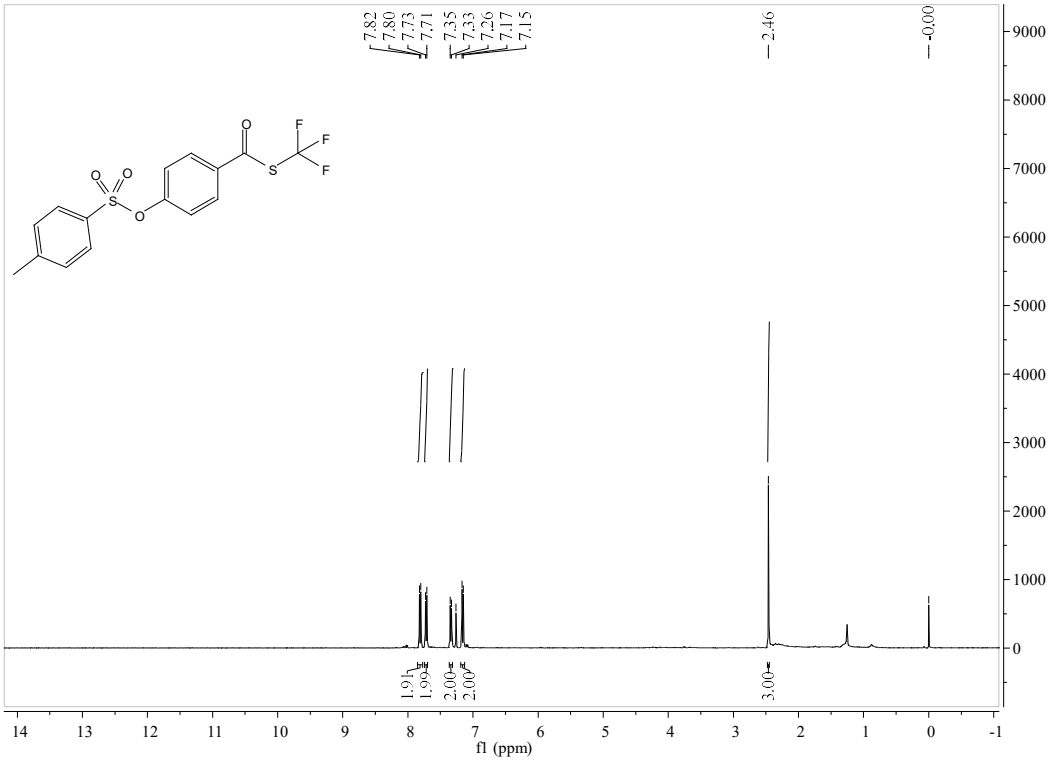
^{19}F NMR spectra of compound **3l**



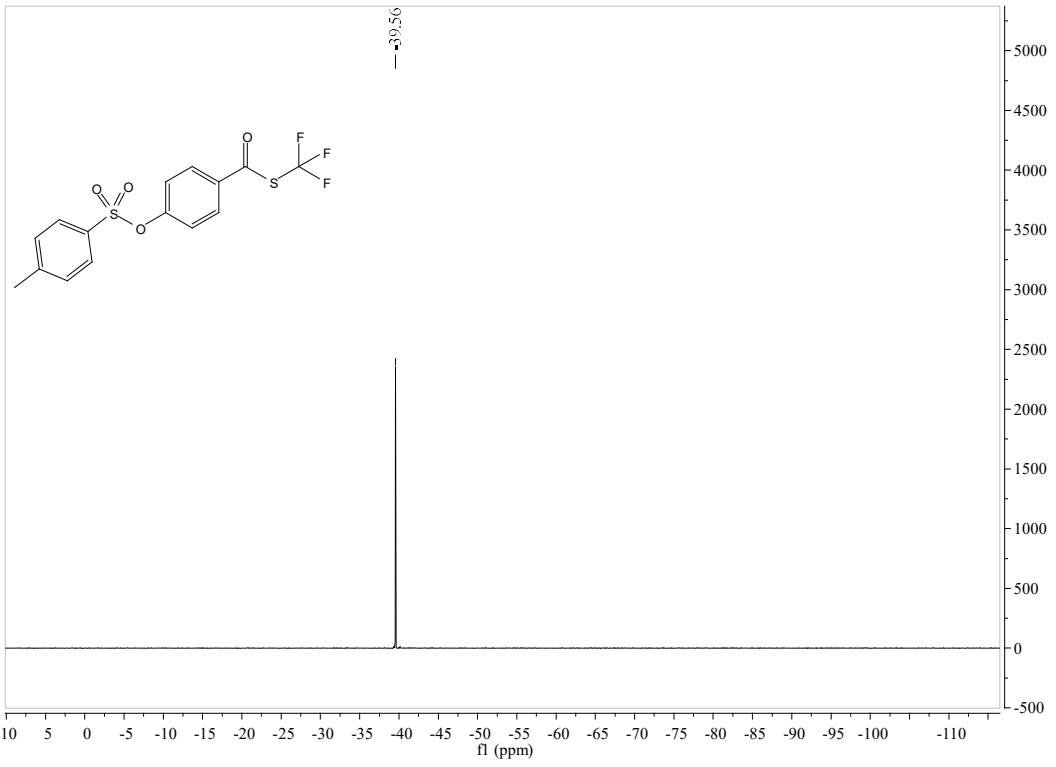
^{13}C NMR spectra of compound **3l**



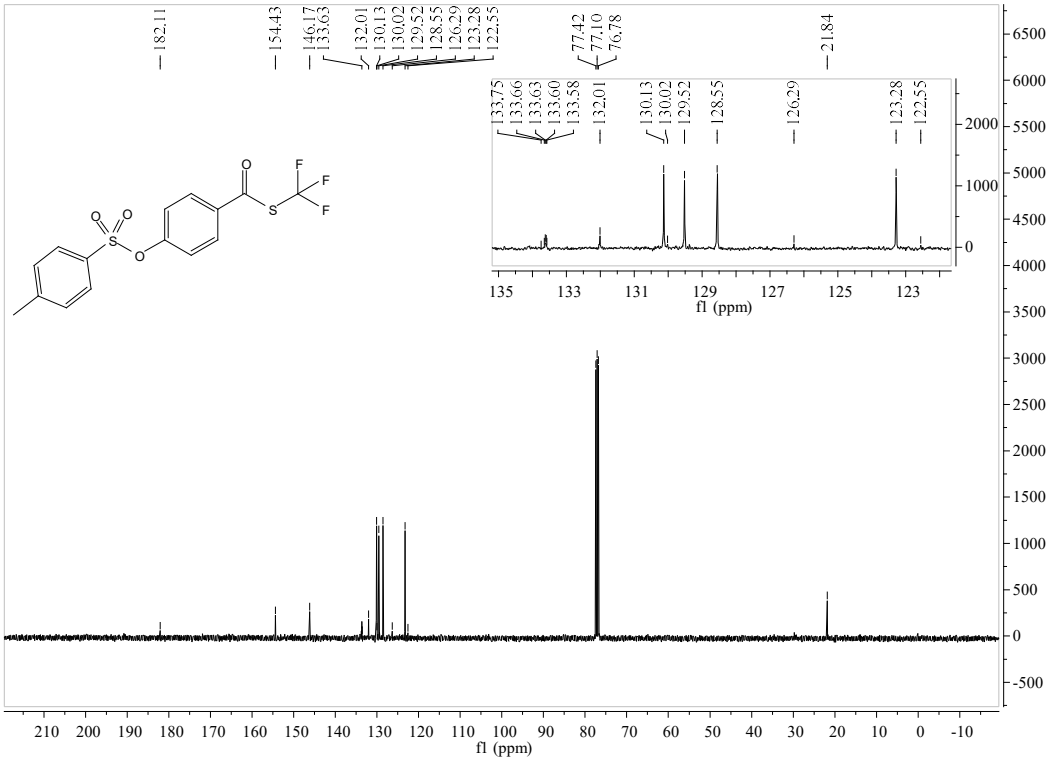
^{1}H NMR spectra of compound **3m**



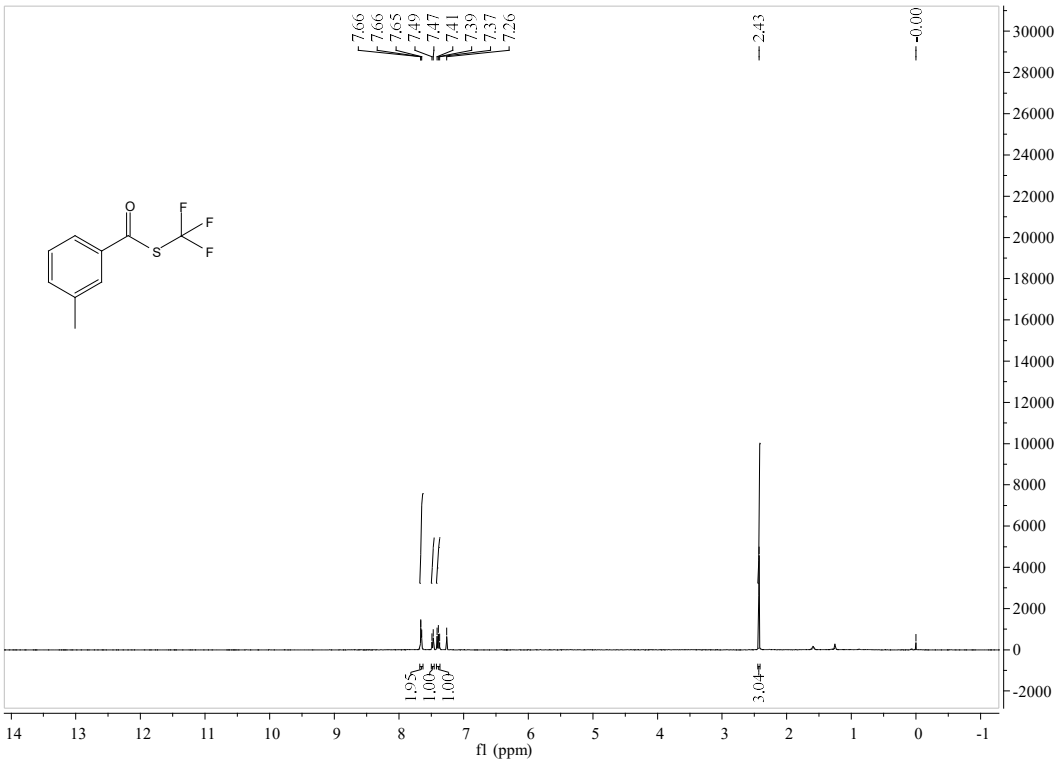
^{19}F NMR spectra of compound **3m**



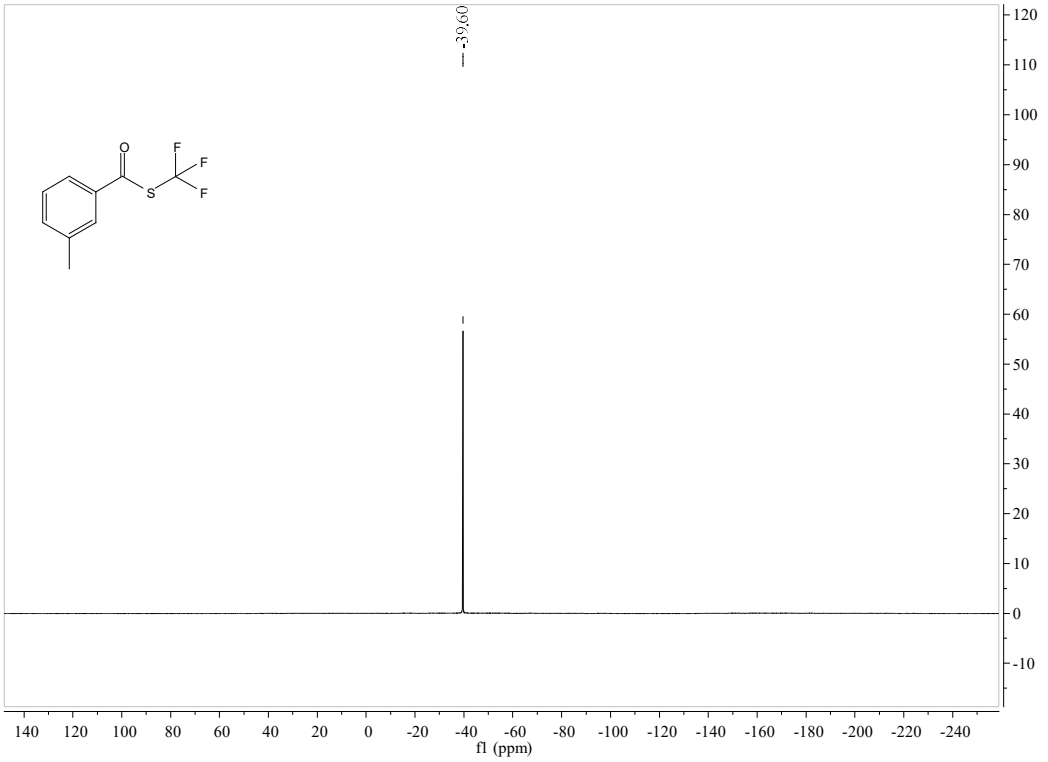
^{13}C NMR spectra of compound **3m**



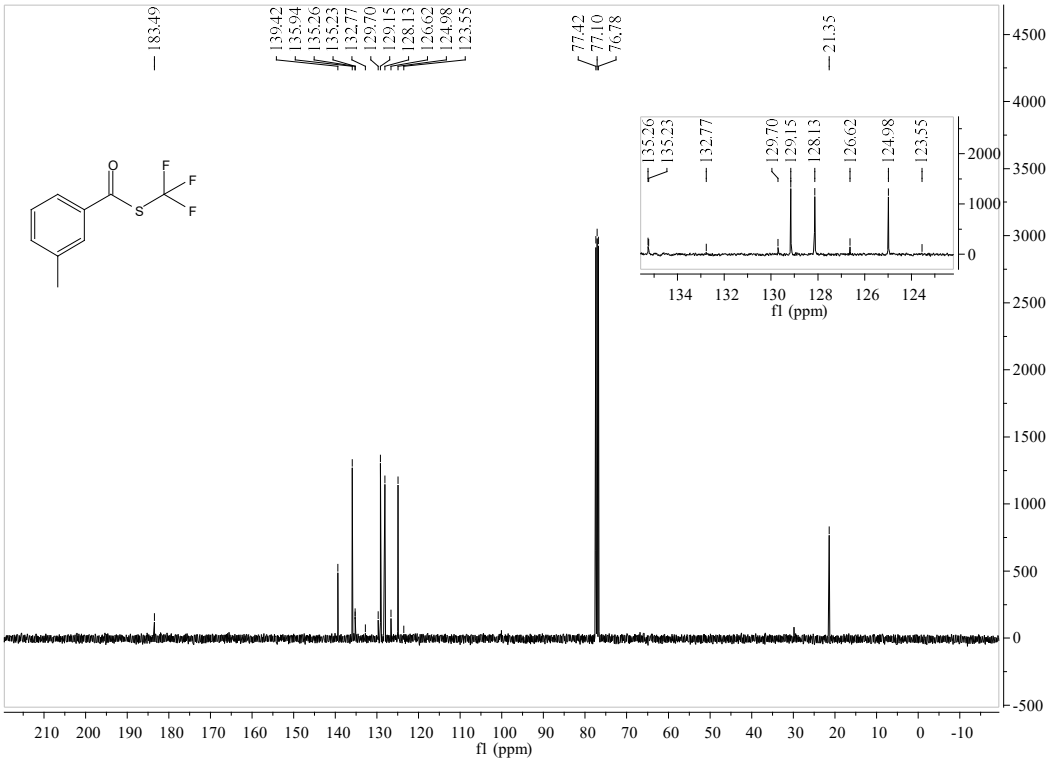
^{1}H NMR spectra of compound **3n**



^{19}F NMR spectra of compound **3n**



^{13}C NMR spectra of compound **3n**



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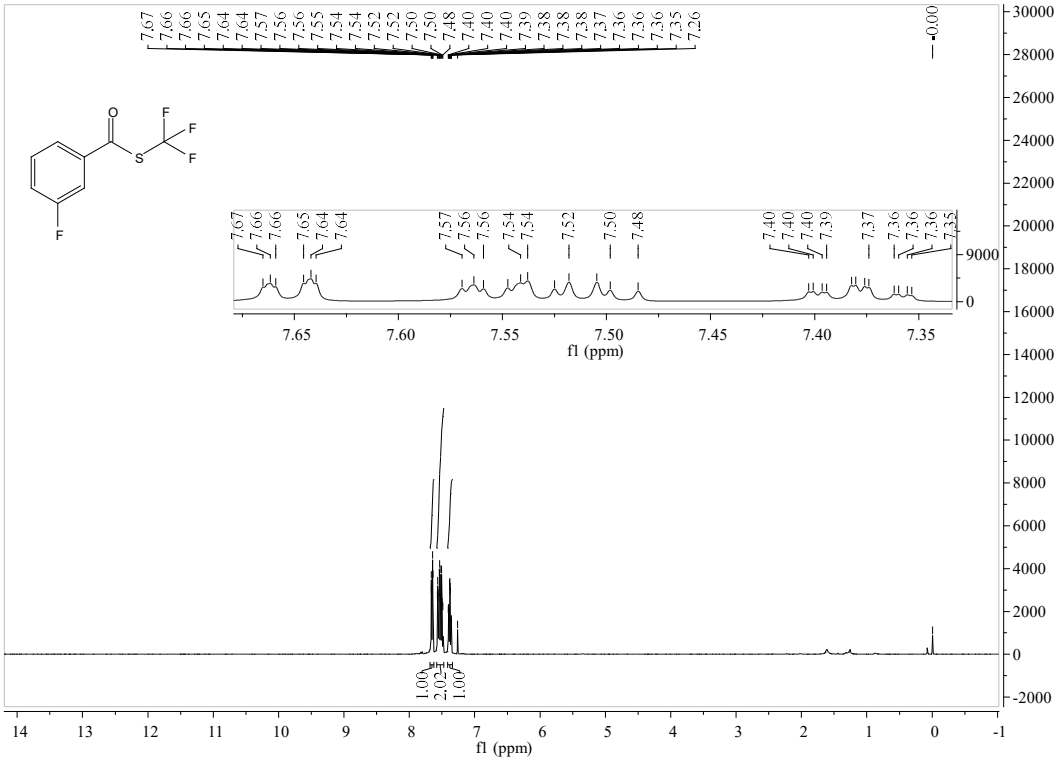
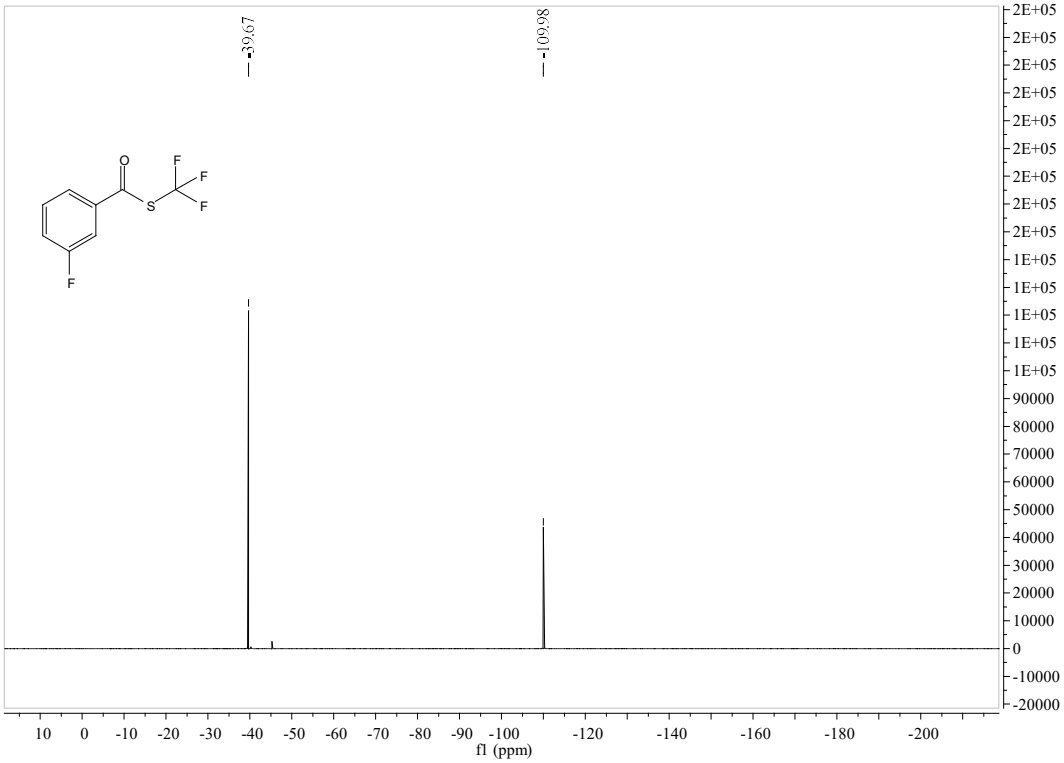
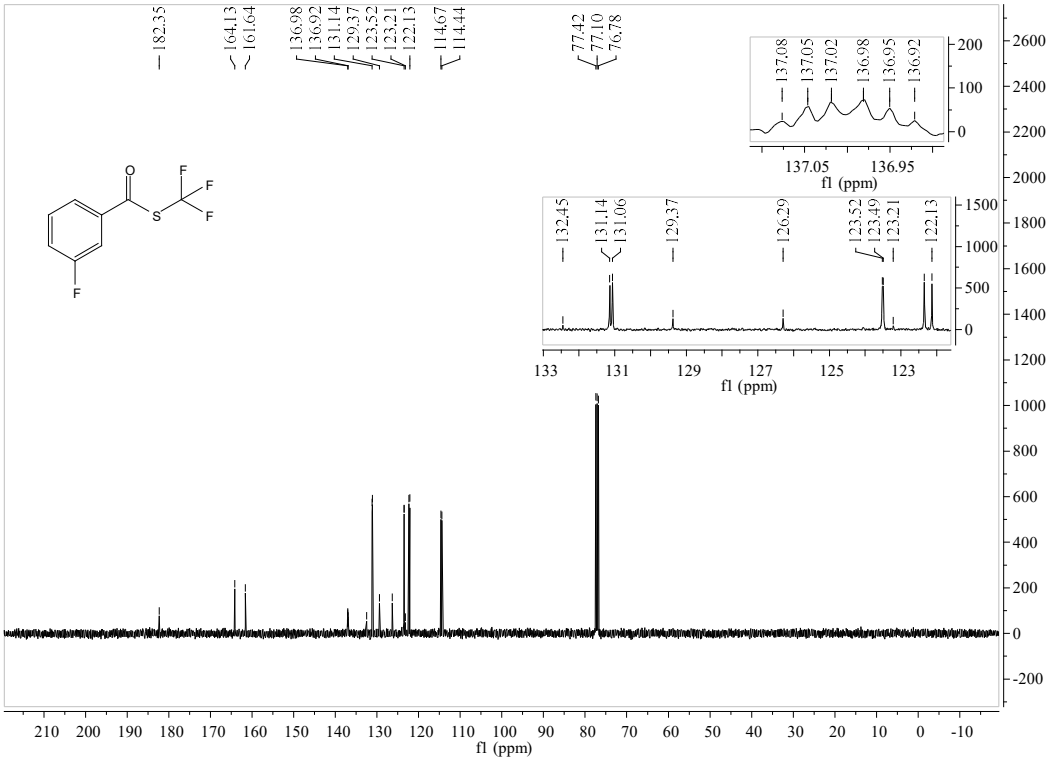


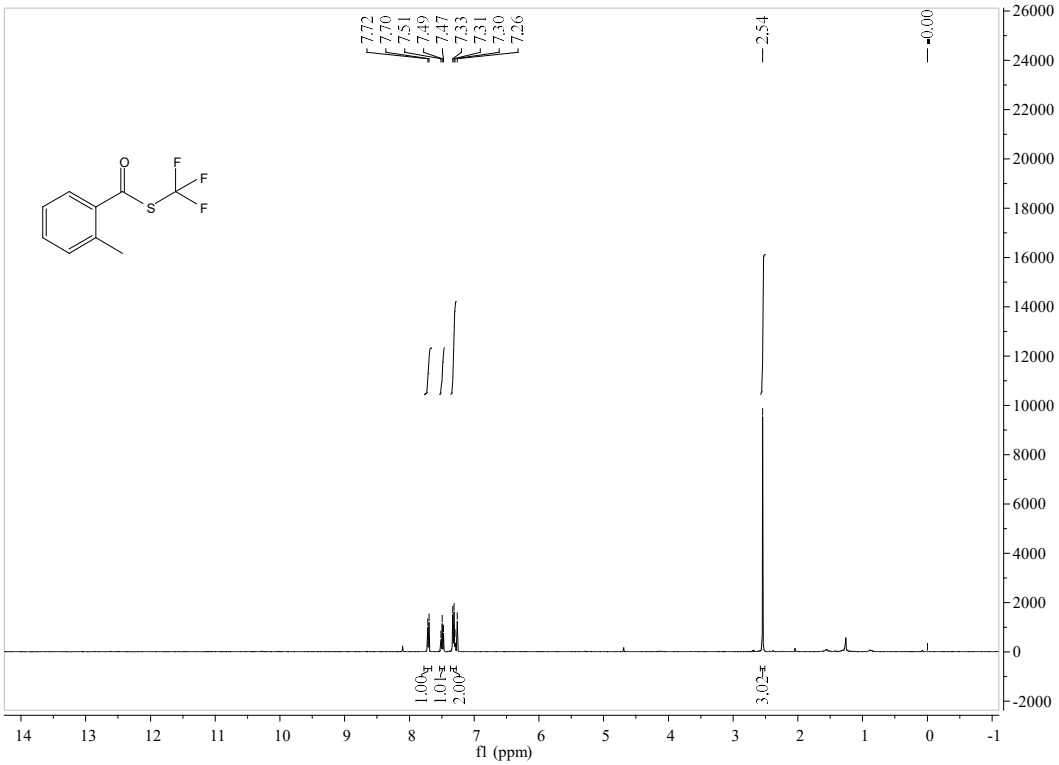
^{19}F NMR spectra of compound **3o**



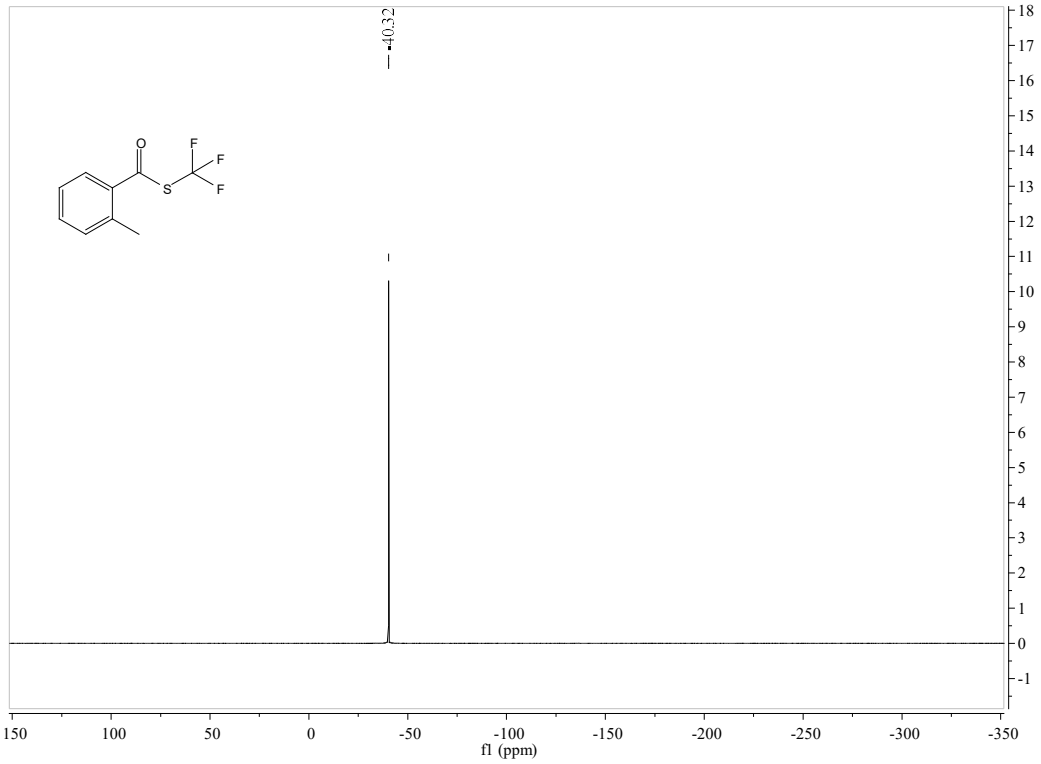
^{13}C NMR spectra of compound **3o**



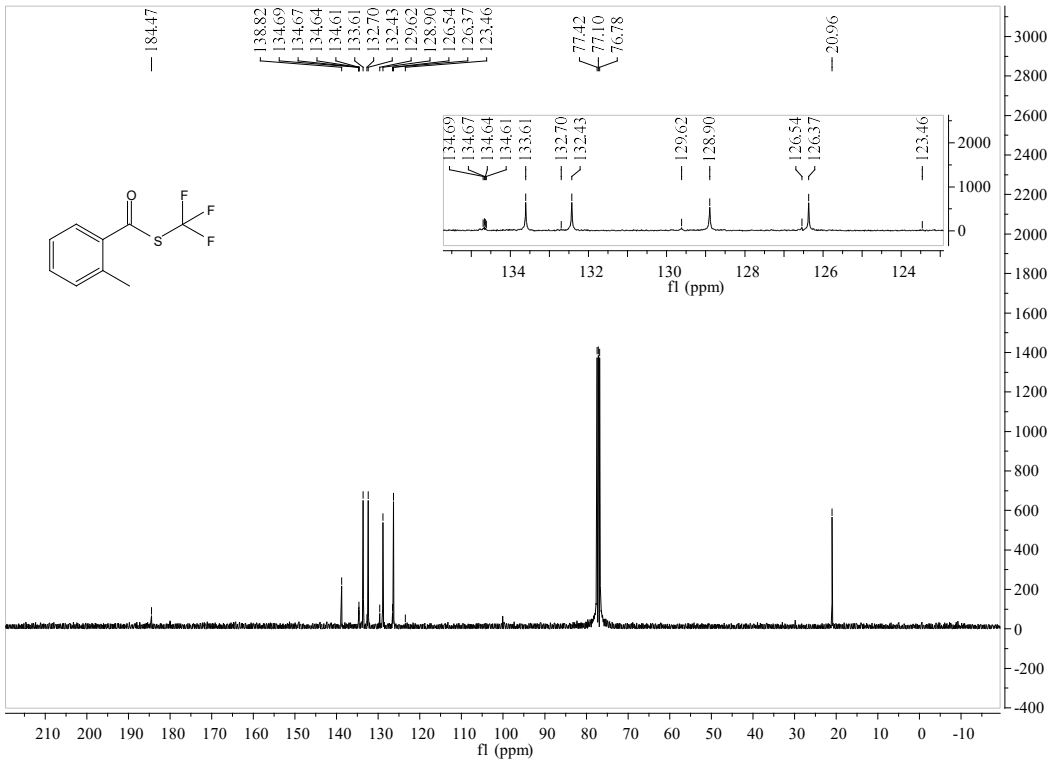
^{1}H NMR spectra of compound **3p**



^{19}F NMR spectra of compound **3p**

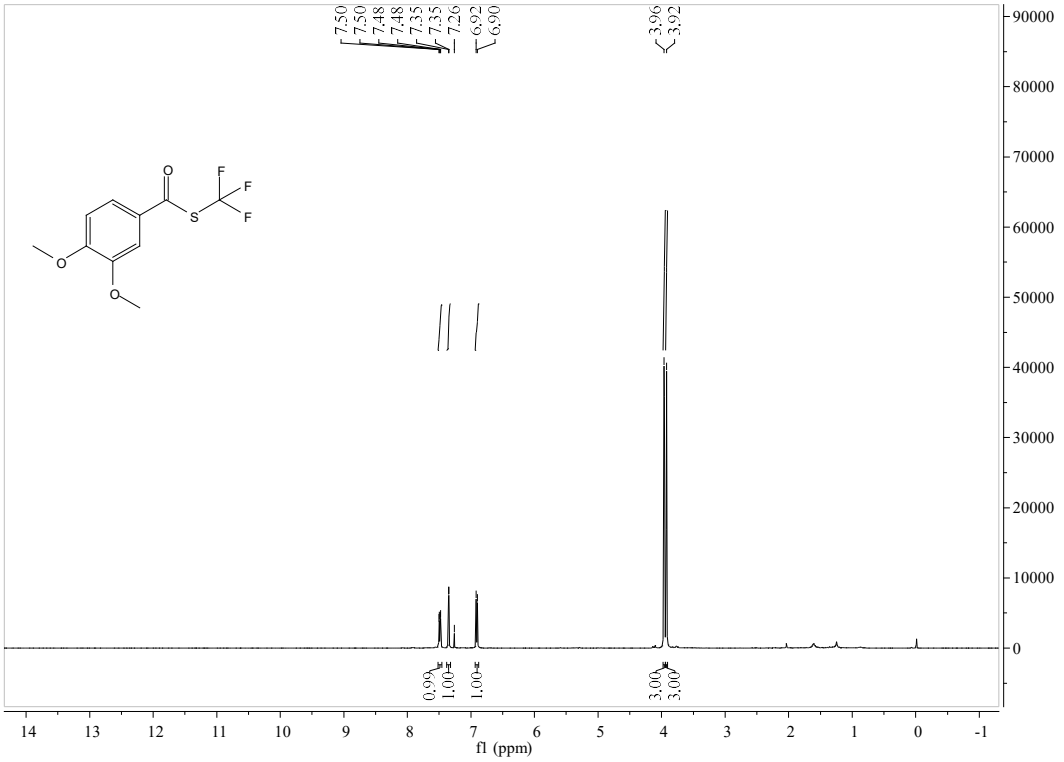


^{13}C NMR spectra of compound **3p**

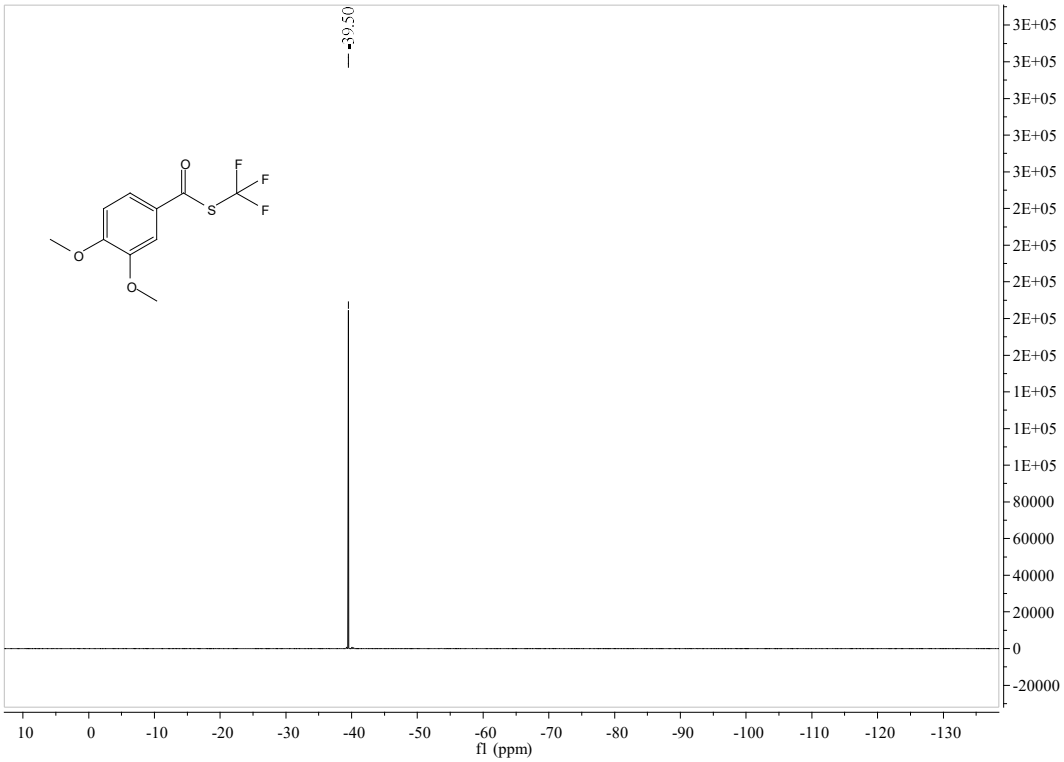


^{1}H

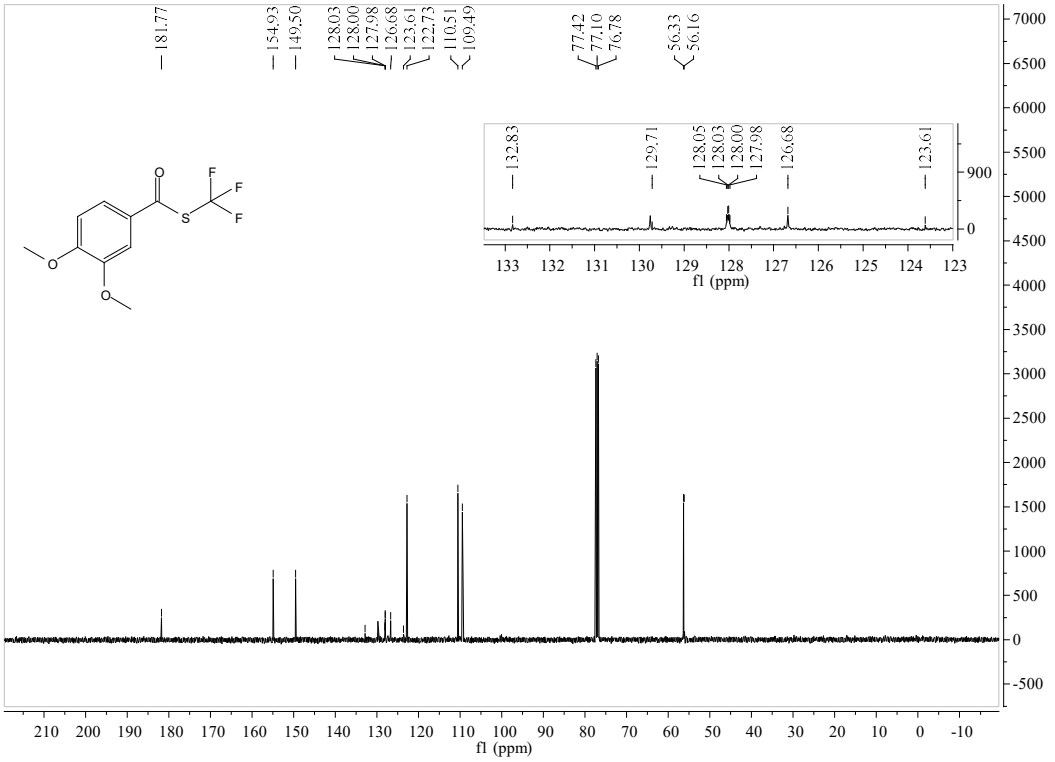
^{1}H NMR spectra of compound **3q**



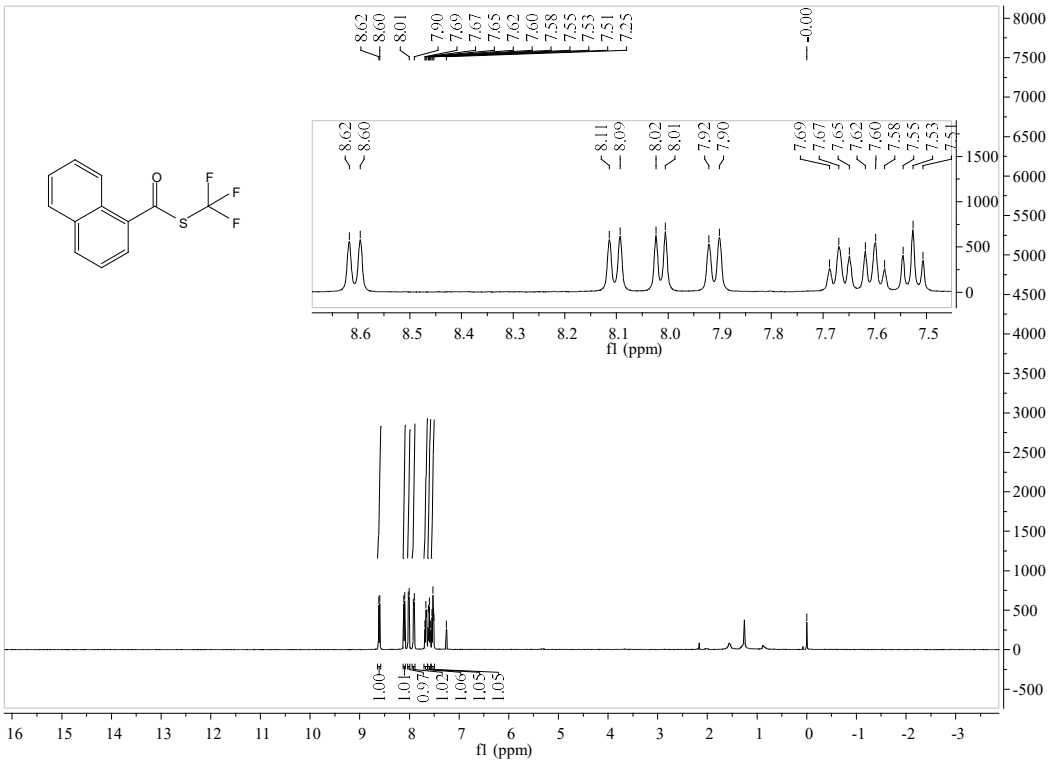
^{19}F NMR spectra of compound **3q**



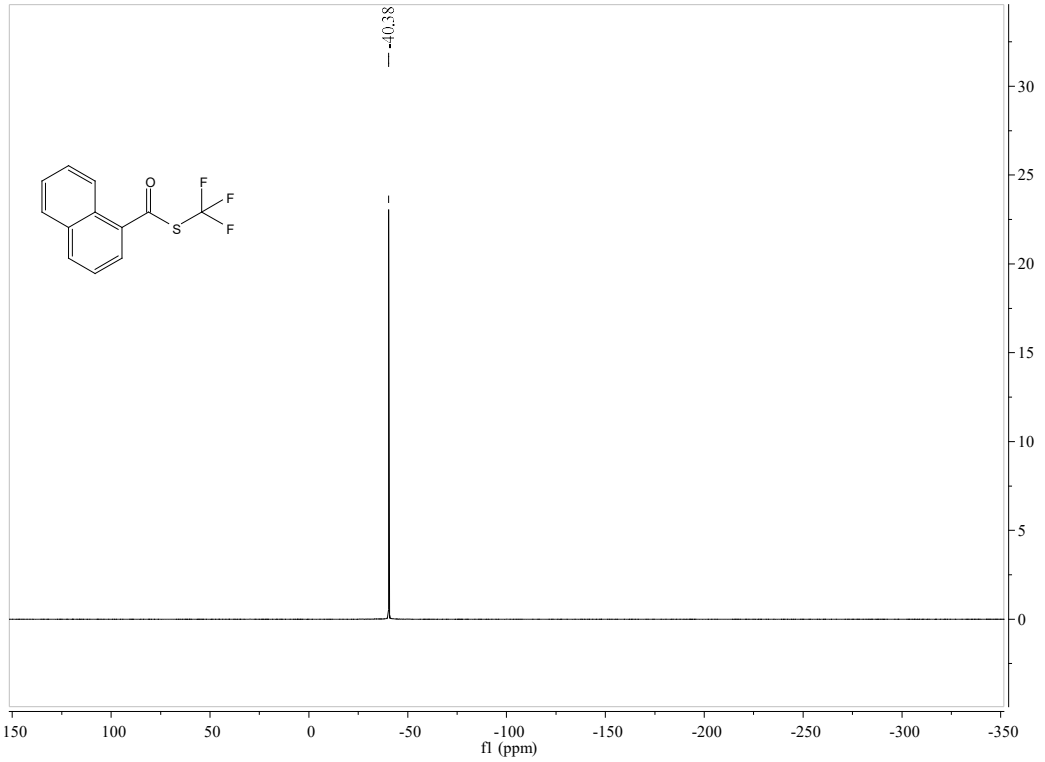
^{13}C NMR spectra of compound **3q**



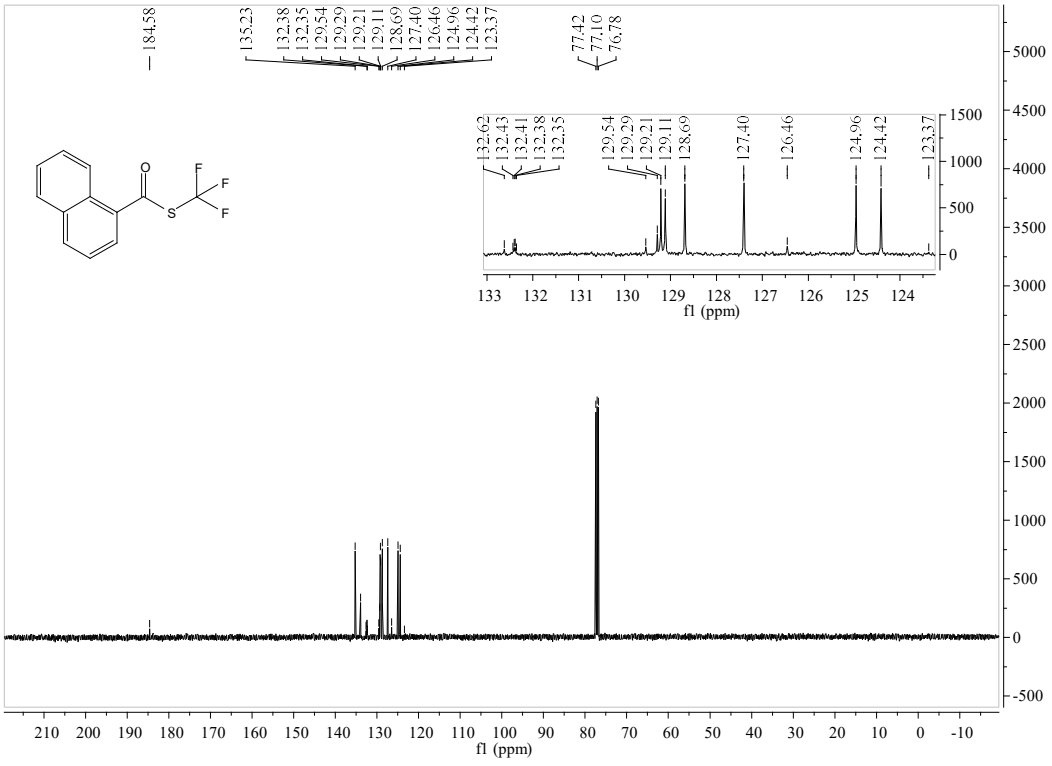
^{1}H NMR spectra of compound **3r**



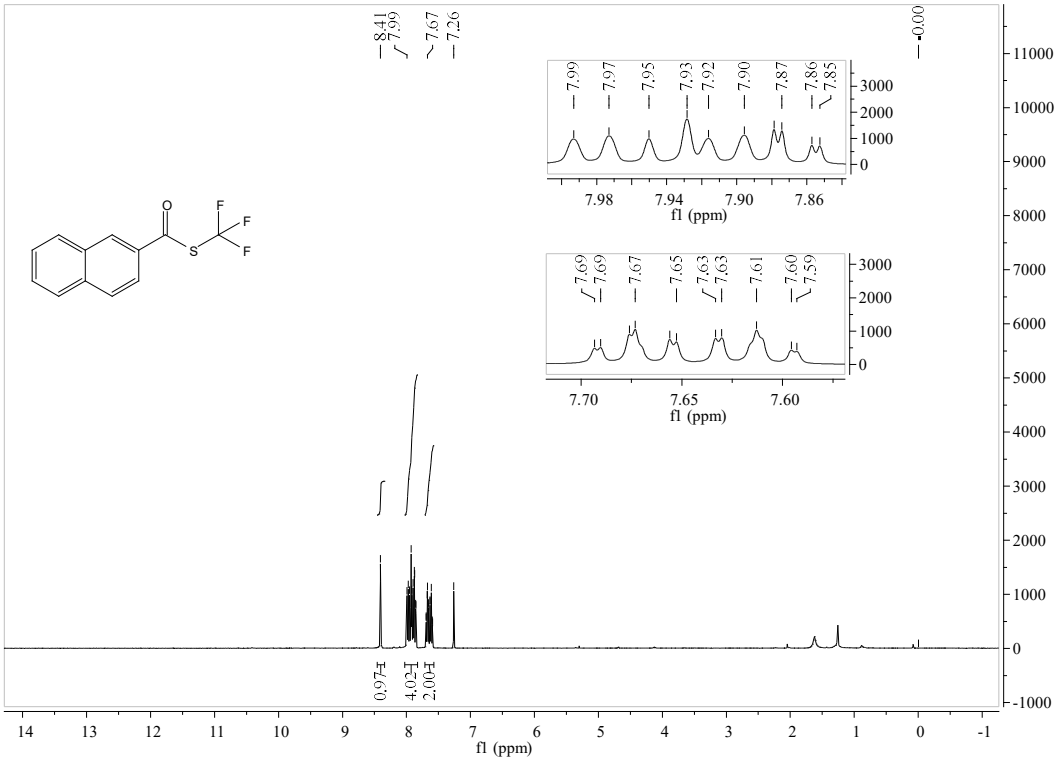
^{19}F NMR spectra of compound **3r**



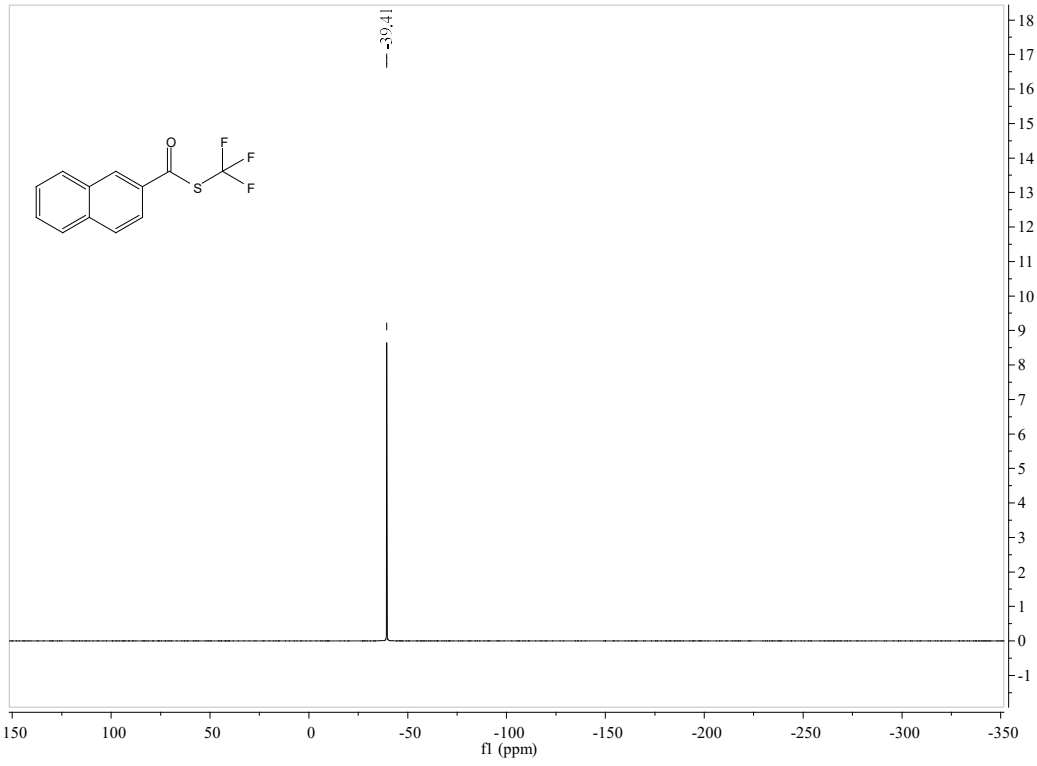
^{13}C NMR spectra of compound **3r**



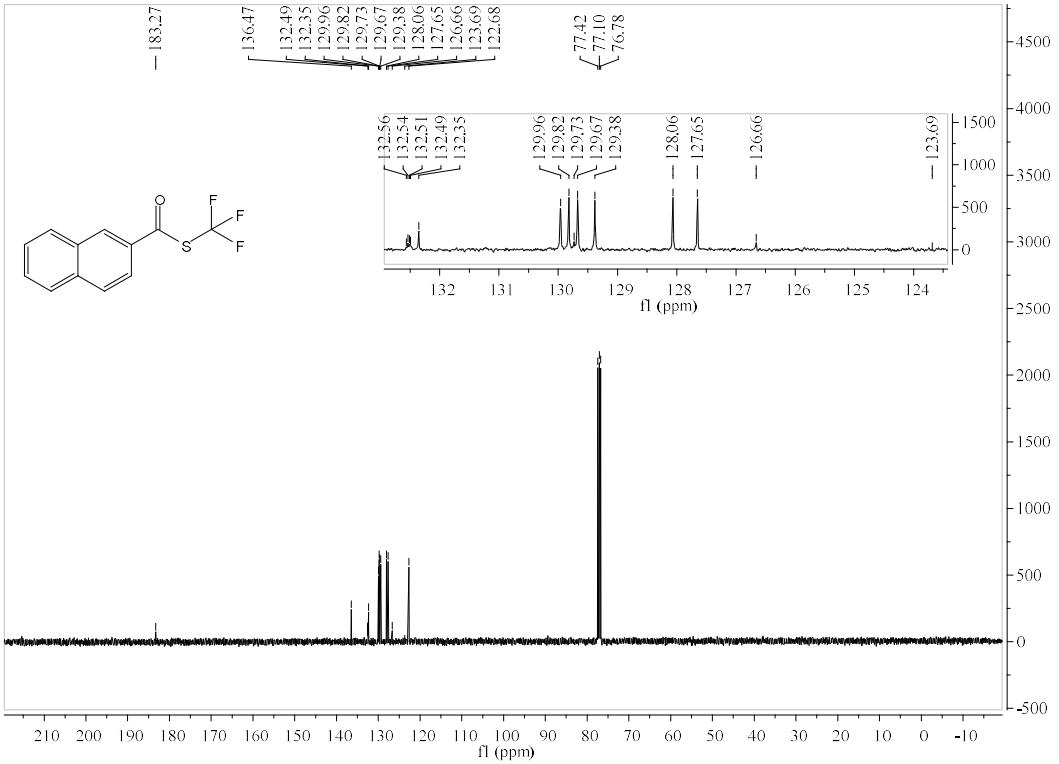
^{1}H NMR spectra of compound **3s**



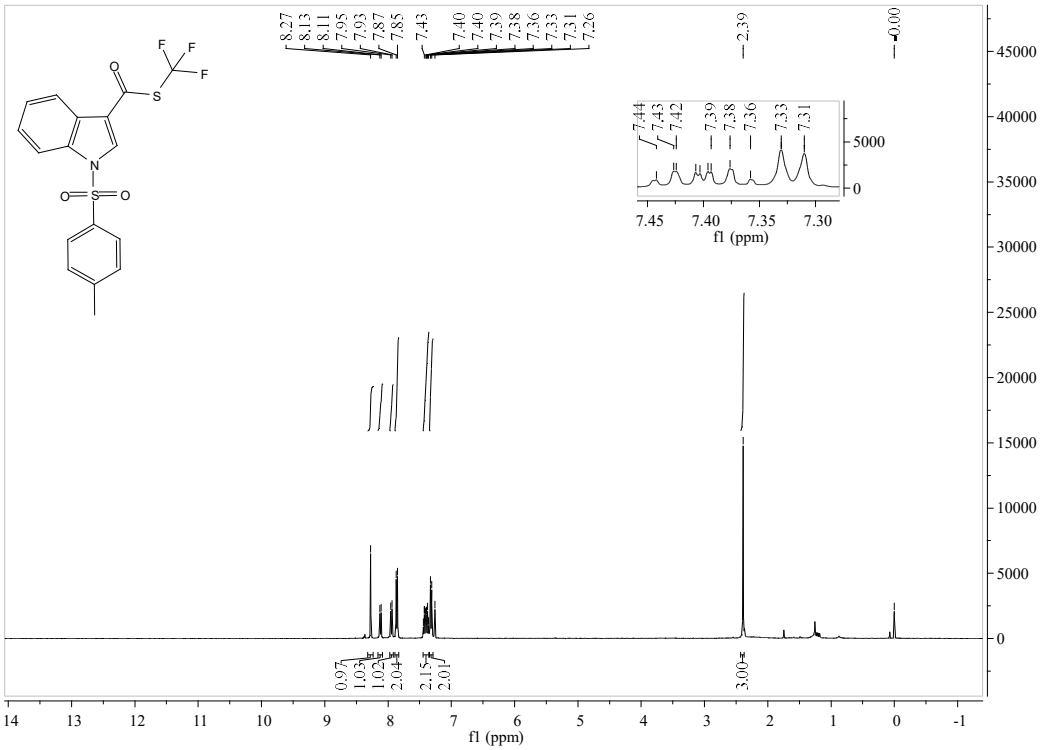
^{19}F NMR spectra of compound **3s**



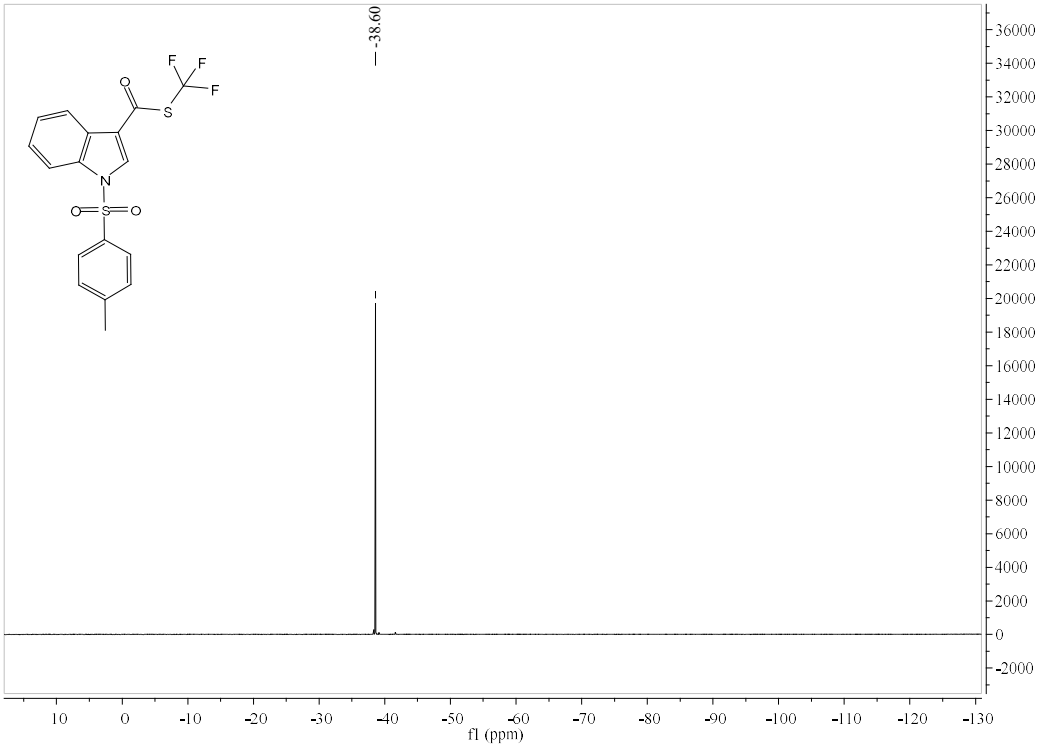
^{13}C NMR spectra of compound **3s**



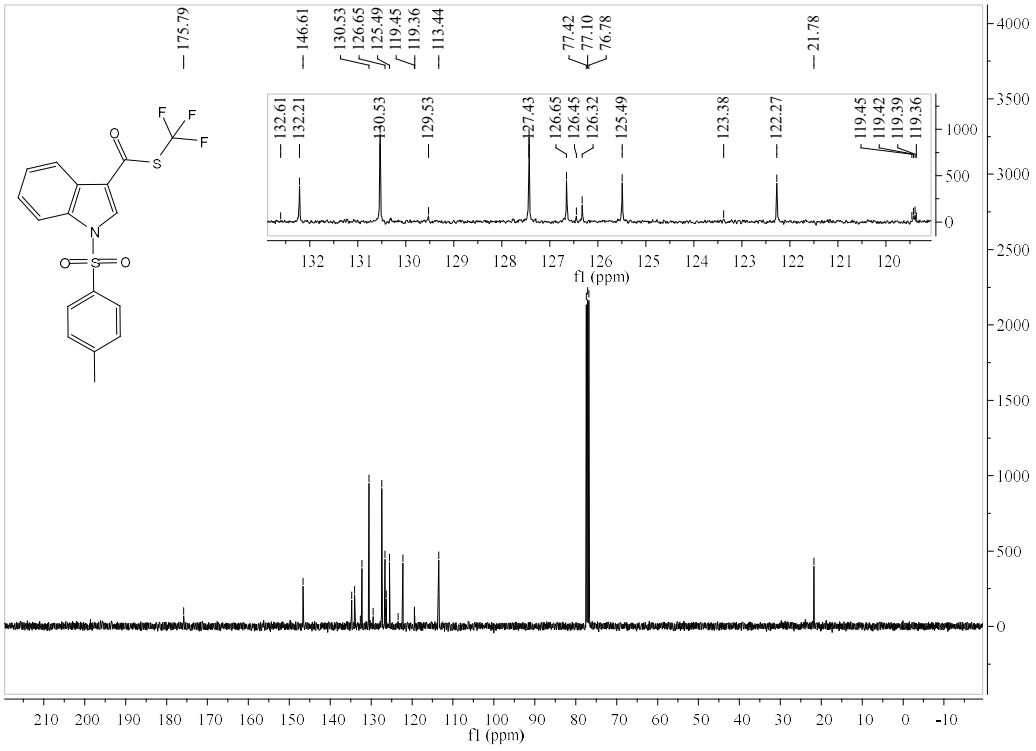
^{1}H NMR spectra of compound **3t**



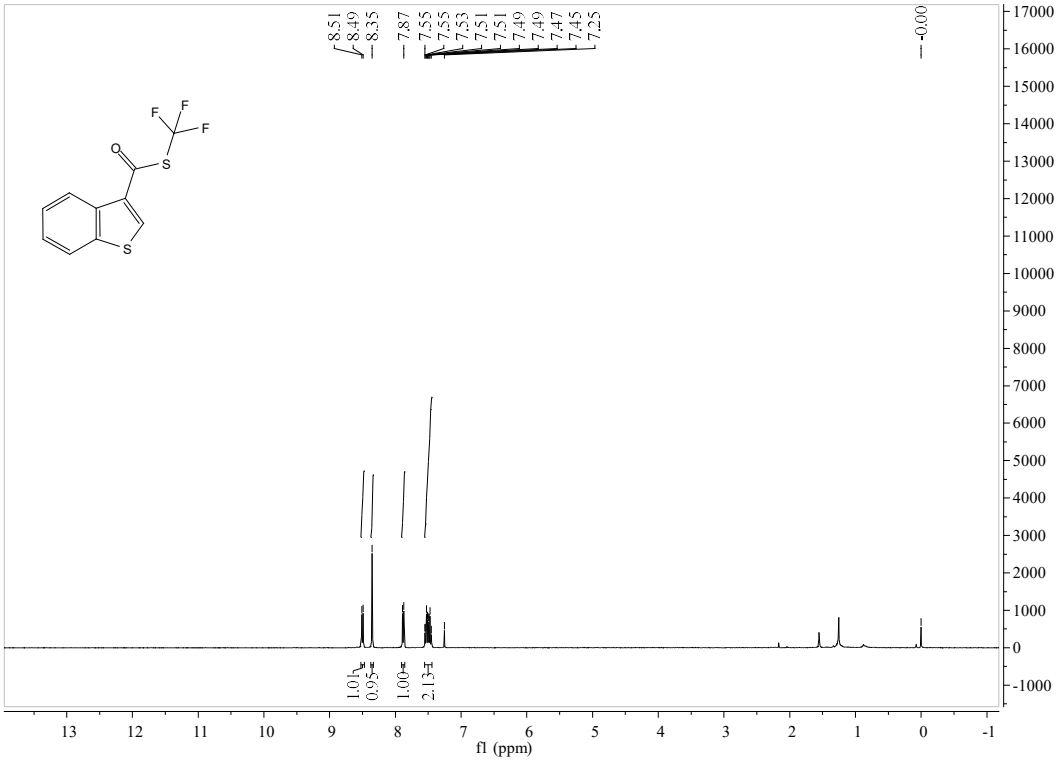
^{19}F NMR spectra of compound **3t**



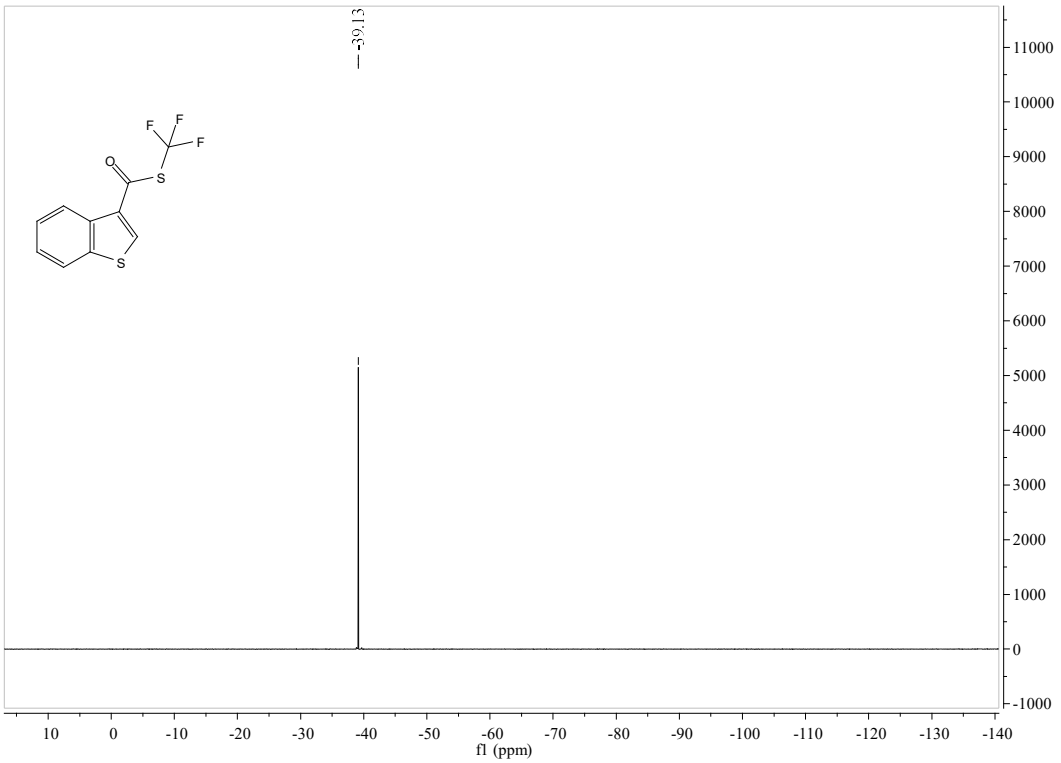
^{13}C NMR spectra of compound **3t**



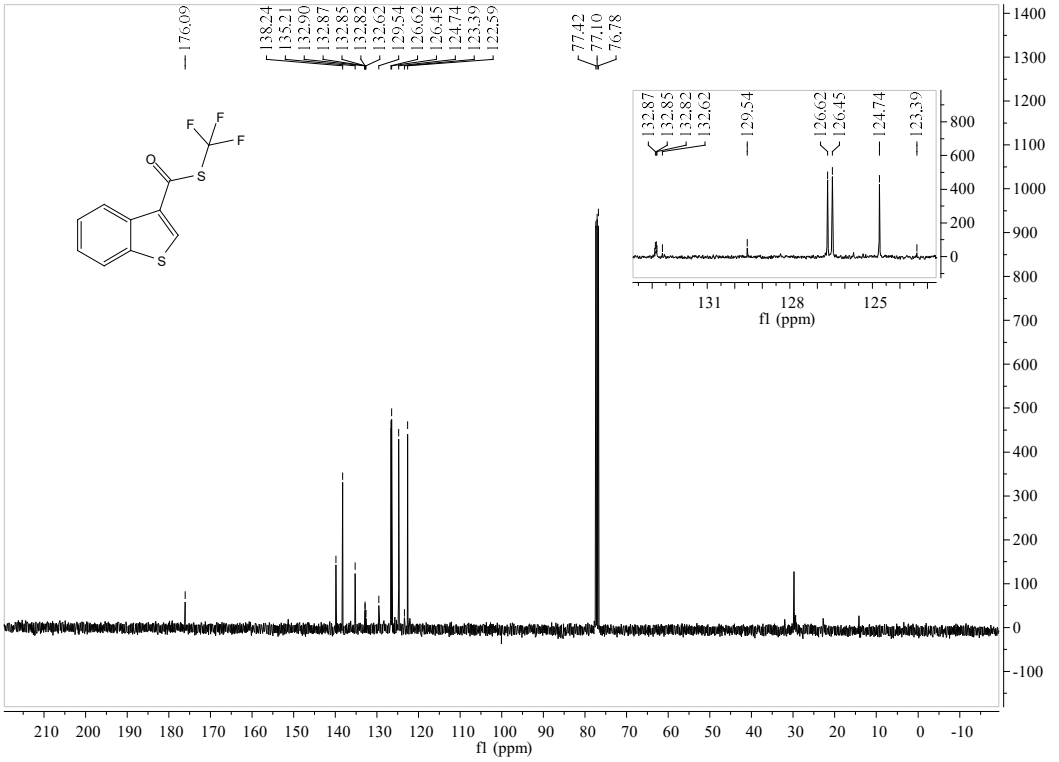
^{1}H NMR spectra of compound **3u**



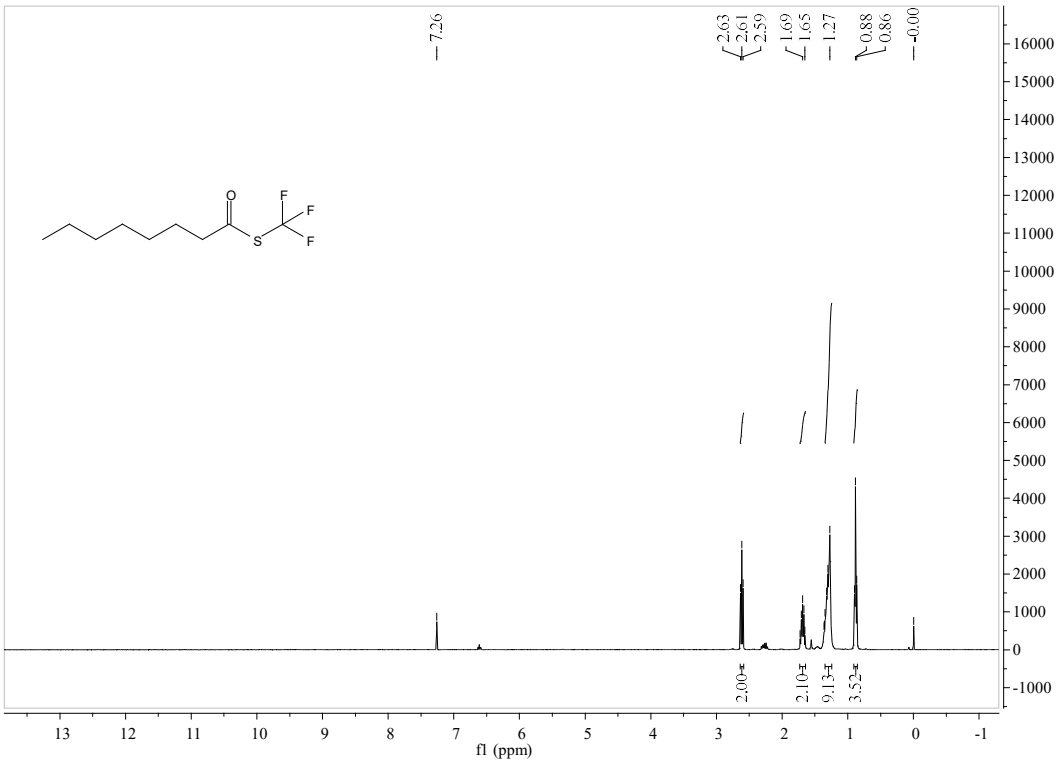
^{19}F NMR spectra of compound **3u**



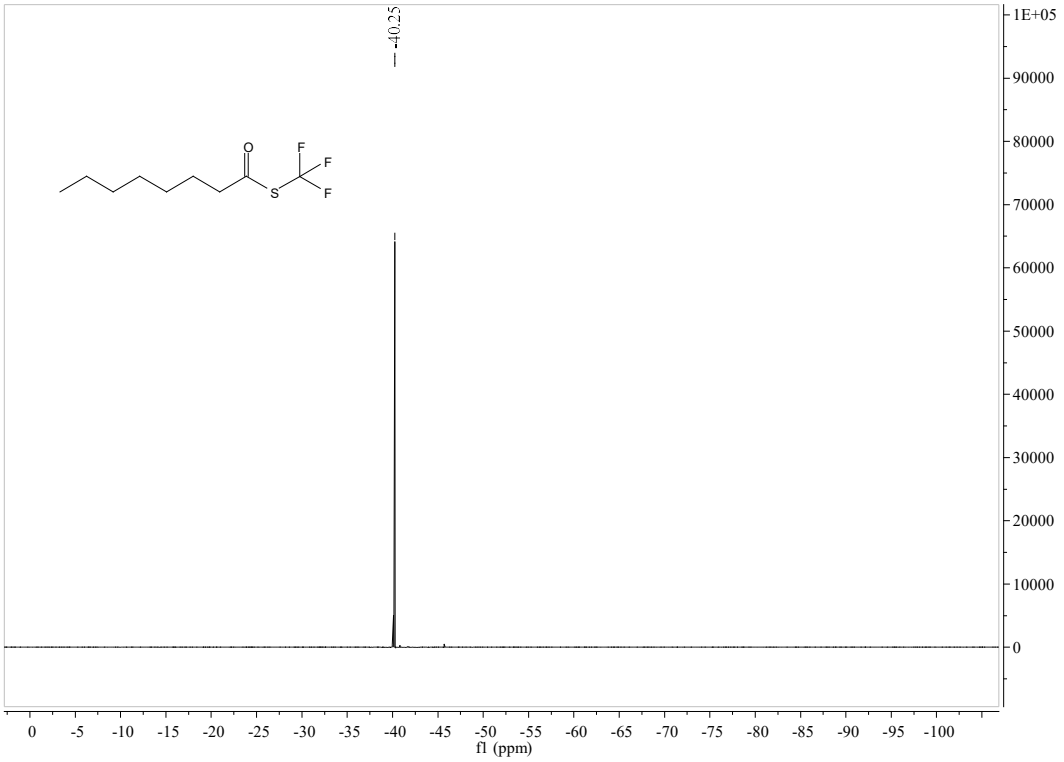
^{13}C NMR spectra of compound **3u**



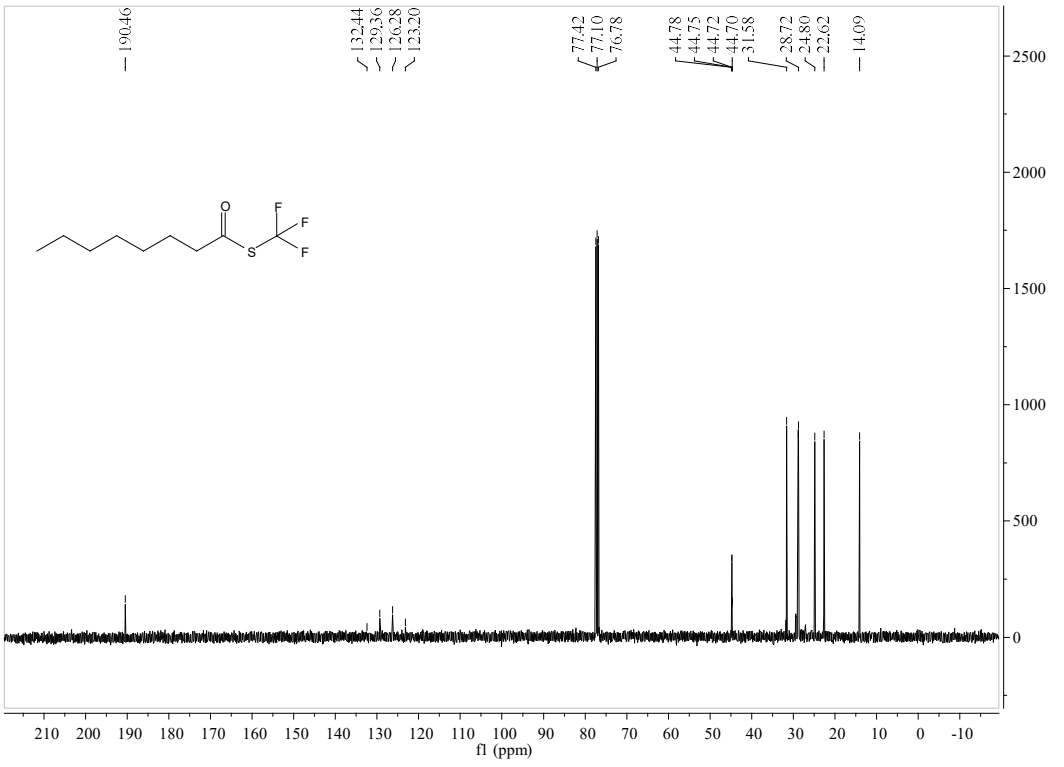
^{1}H NMR spectra of compound **3aa**



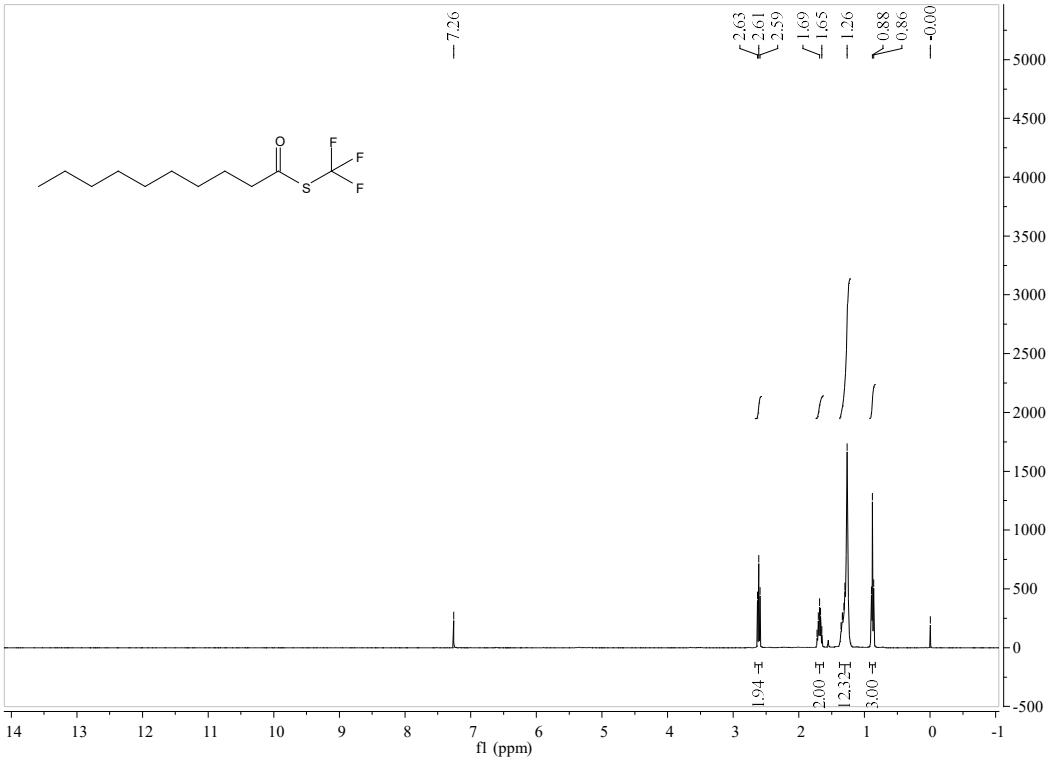
^{19}F NMR spectra of compound **3aa**



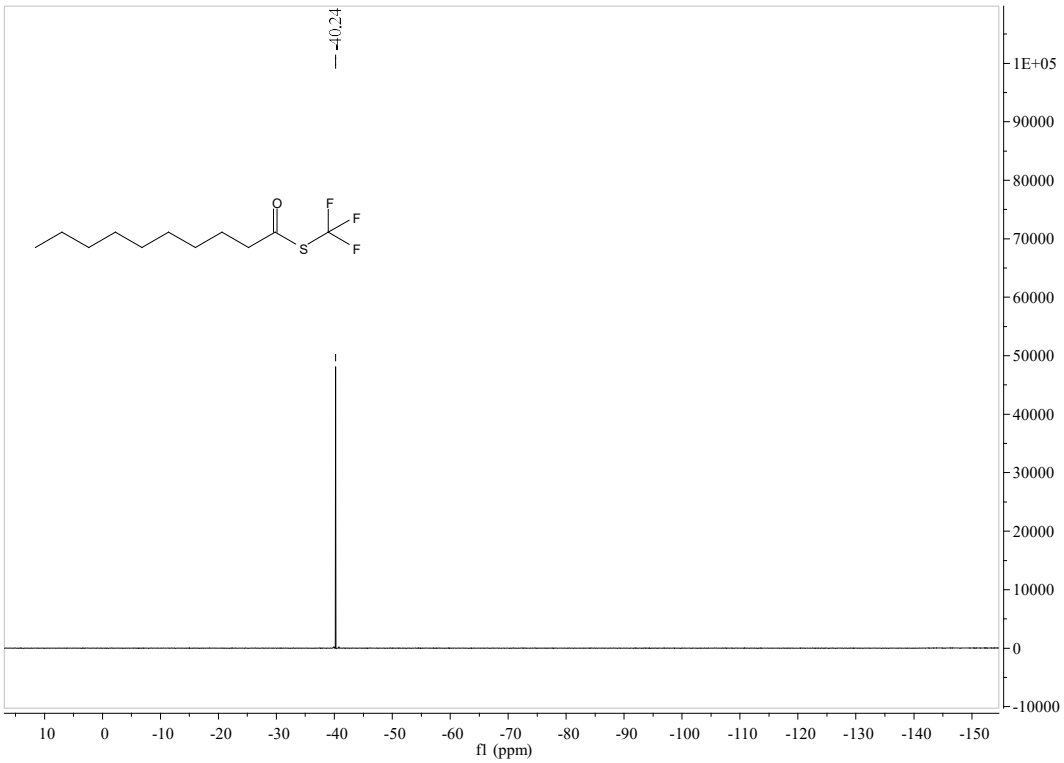
^{13}C NMR spectra of compound **3aa**



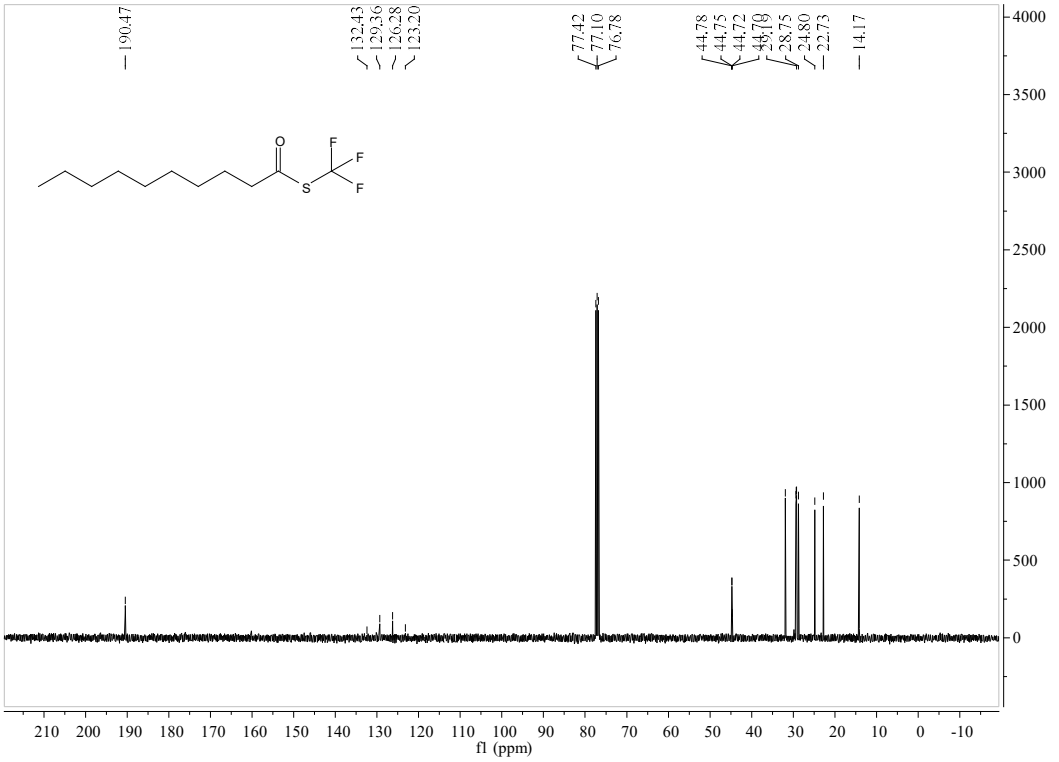
^{1}H NMR spectra of compound **3ab**



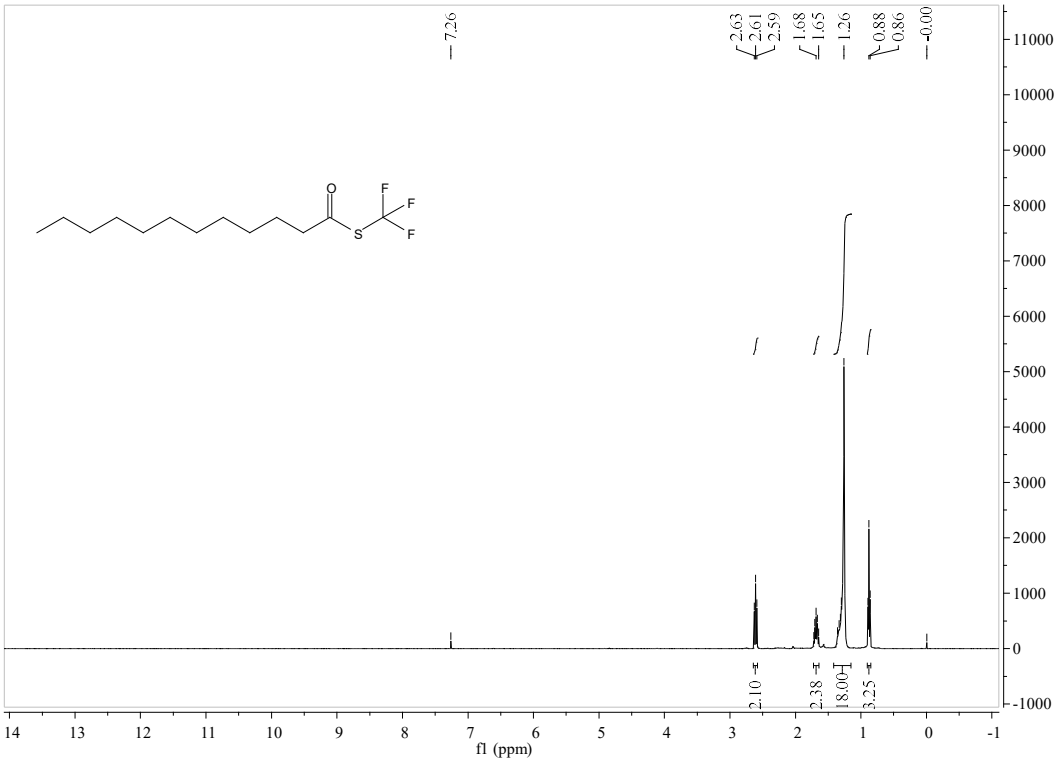
^{19}F NMR spectra of compound **3ab**



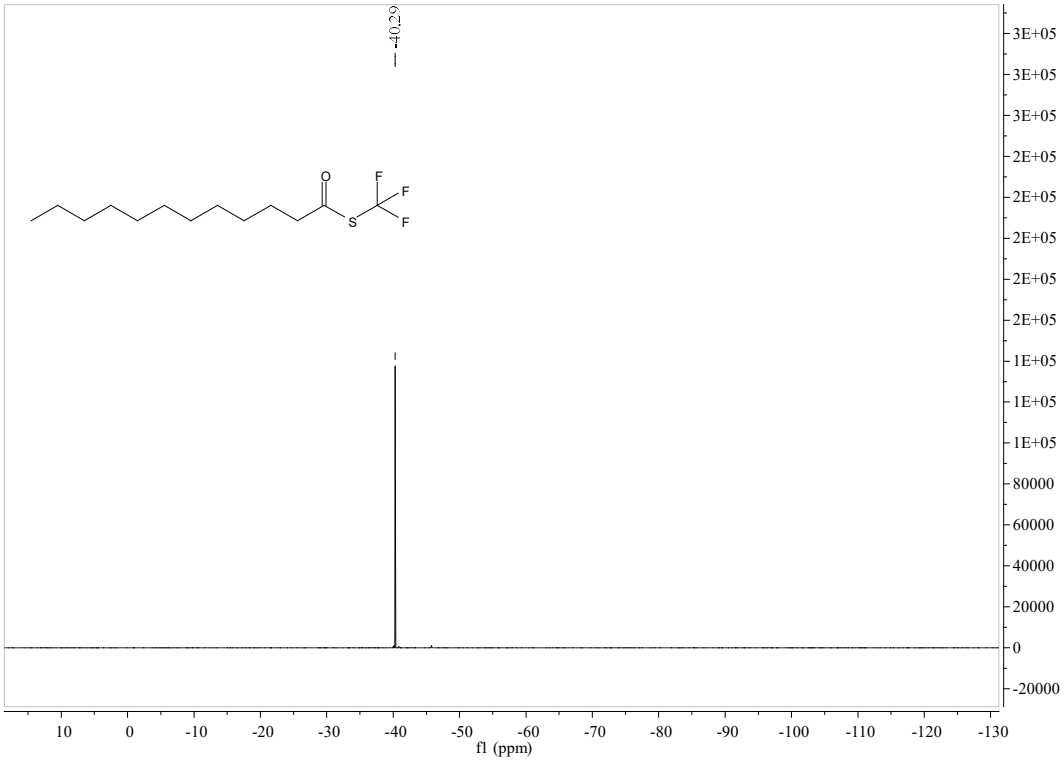
^{13}C NMR spectra of compound **3ab**



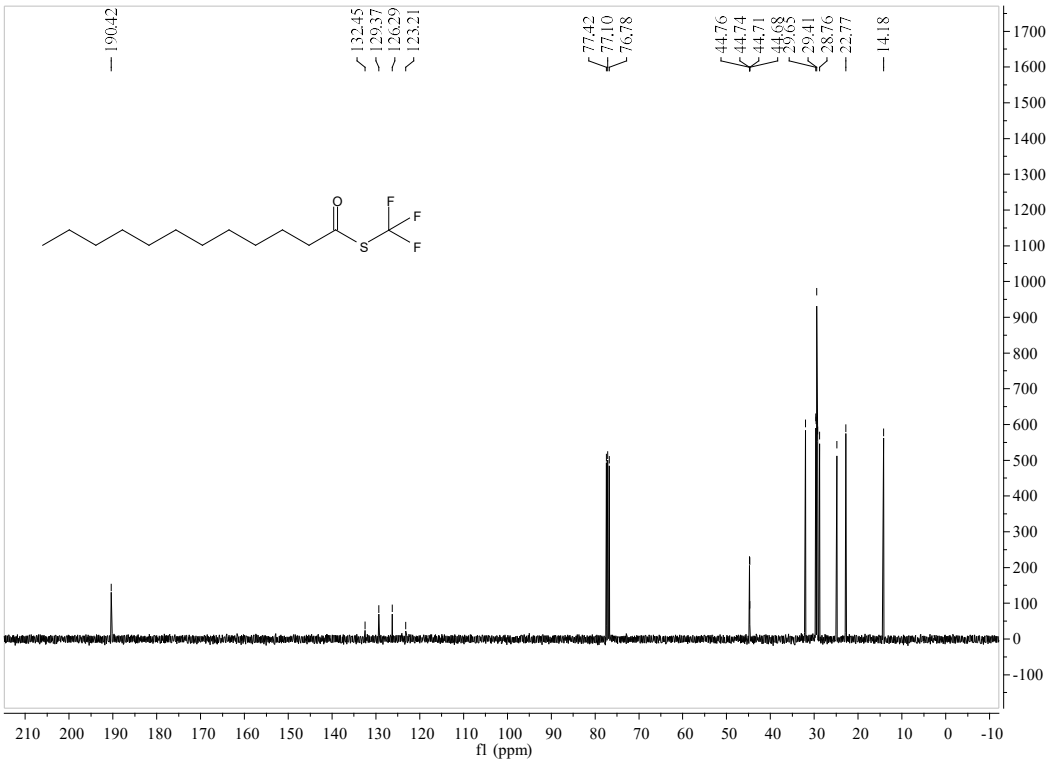
^{1}H NMR spectra of compound **3ac**



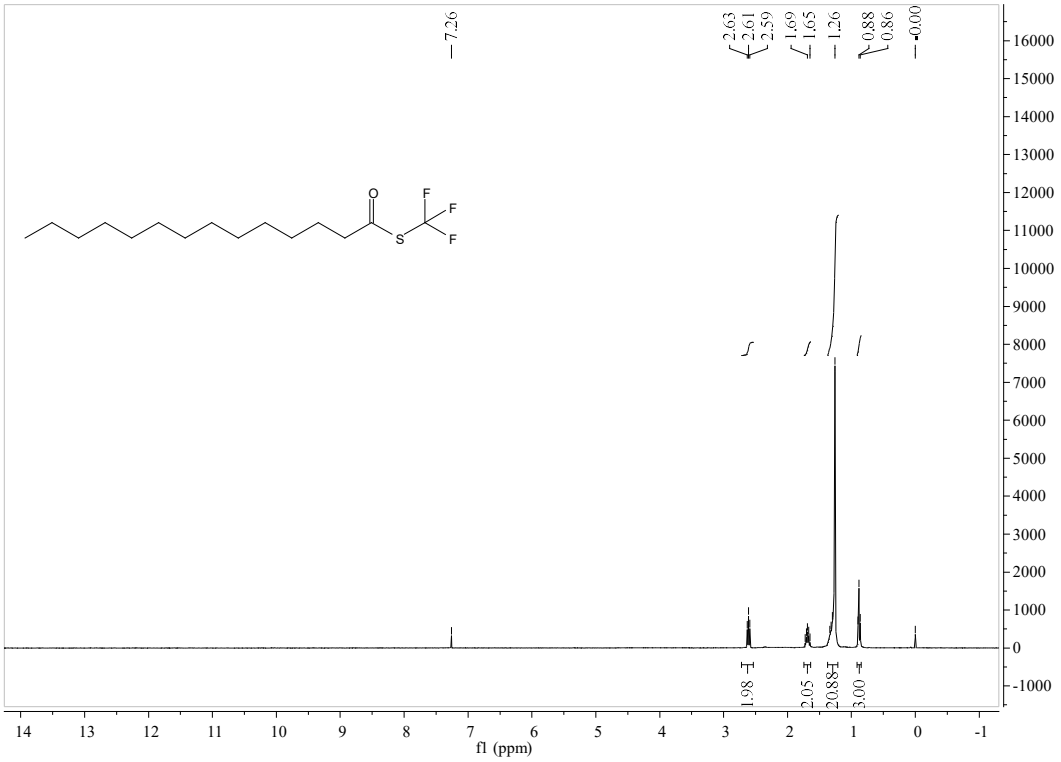
^{19}F NMR spectra of compound **3ac**



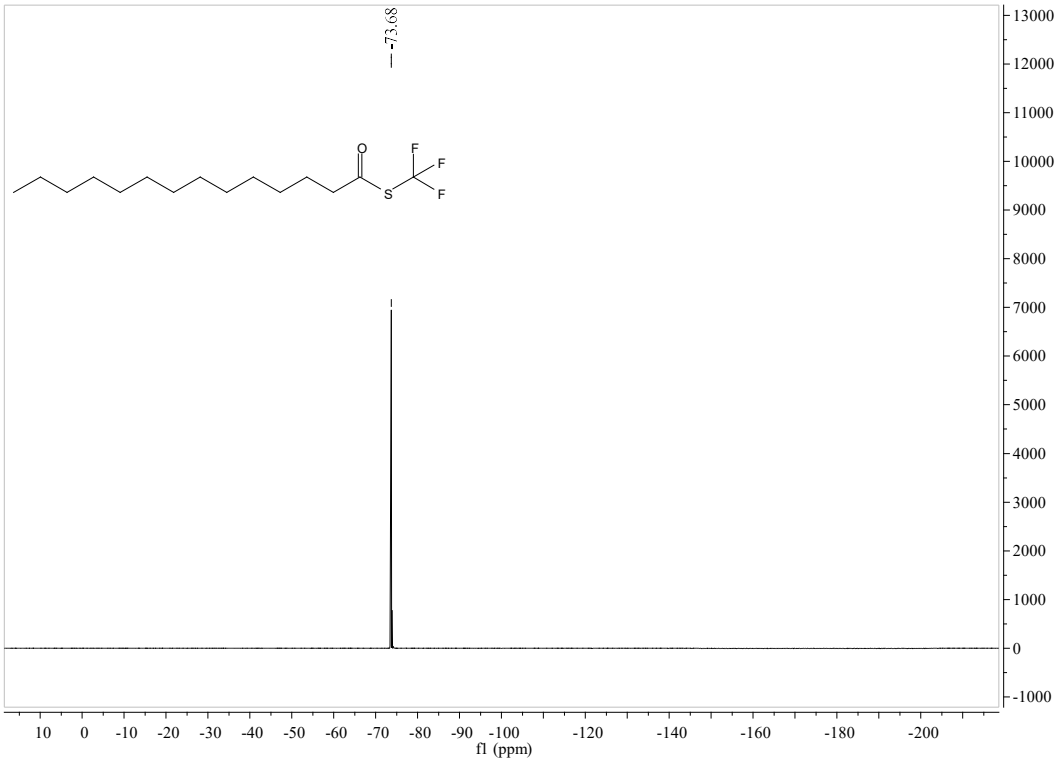
^{13}C NMR spectra of compound **3ac**



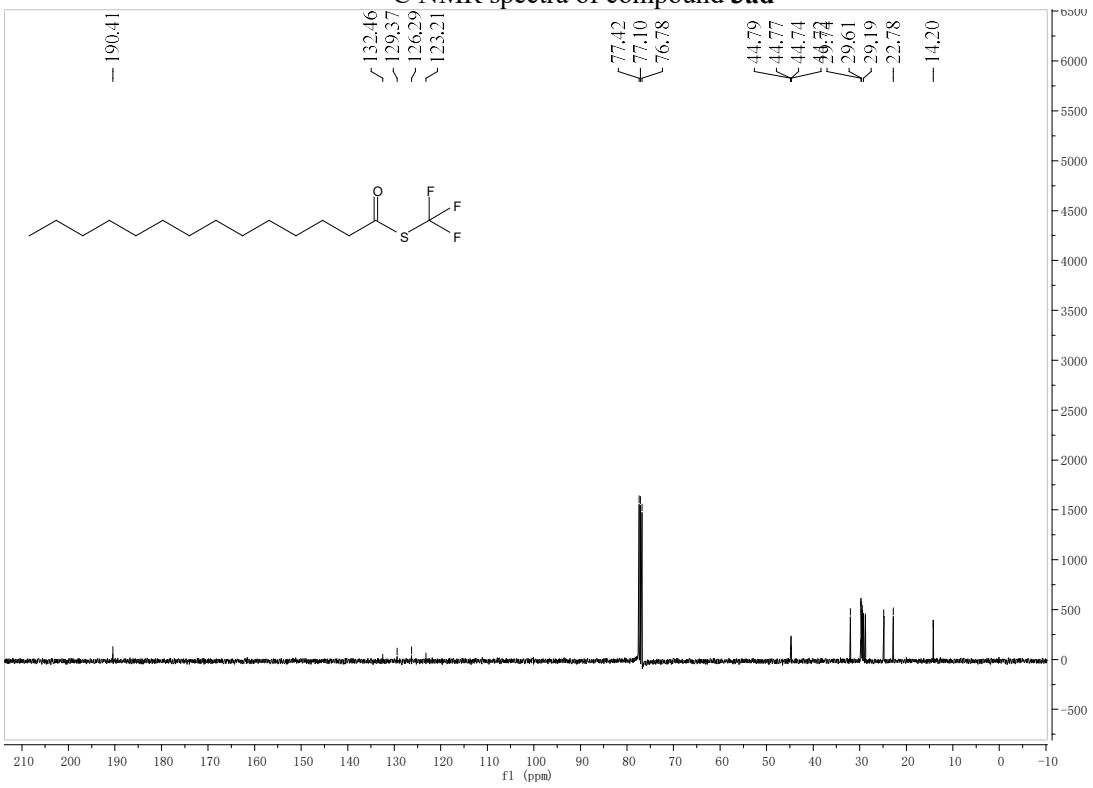
^{1}H NMR spectra of compound **3ad**



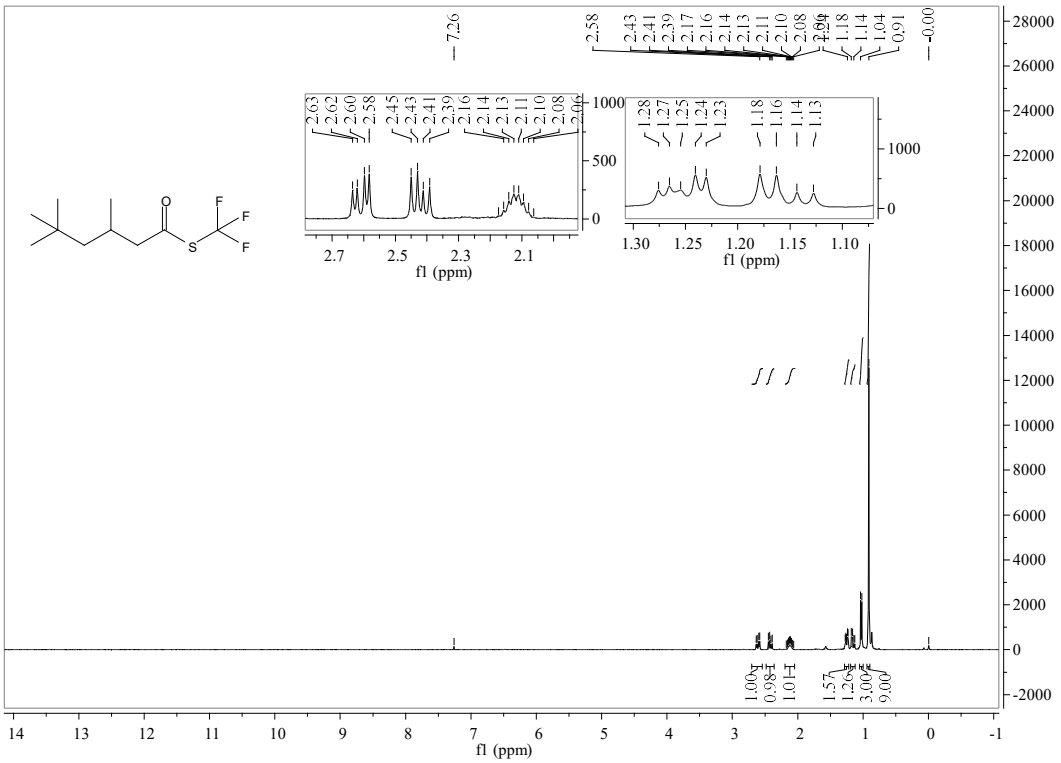
^{19}F NMR spectra of compound **3ad**



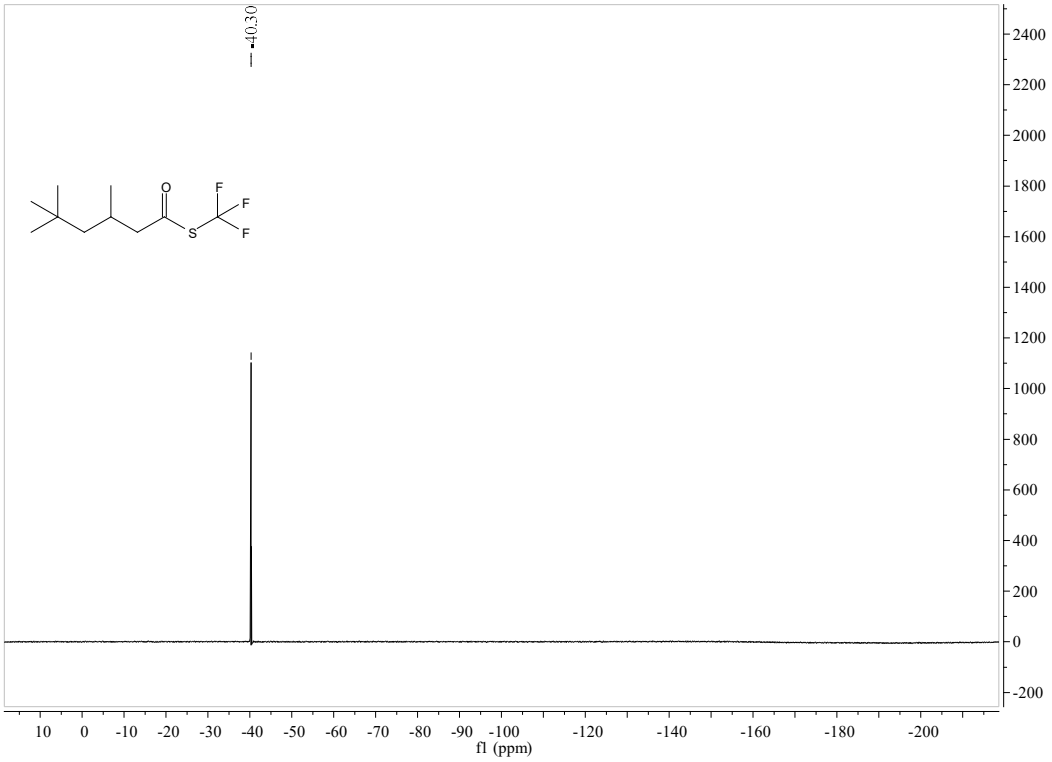
^{13}C NMR spectra of compound **3ad**



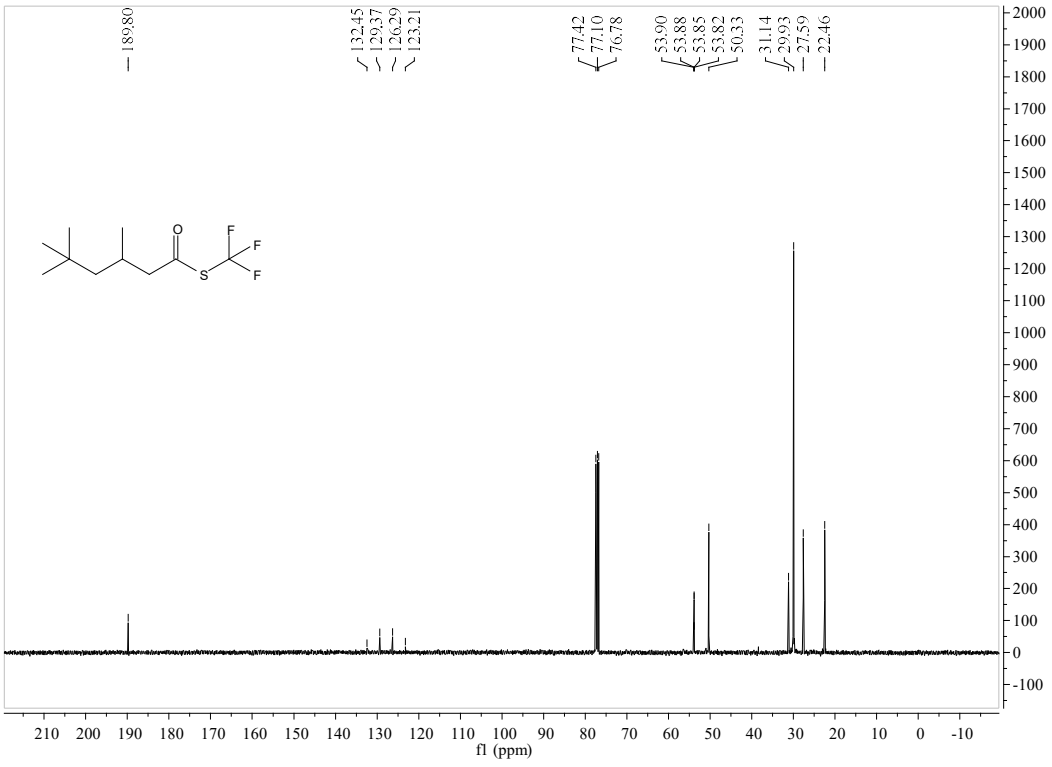
^{1}H NMR spectra of compound **3ae**



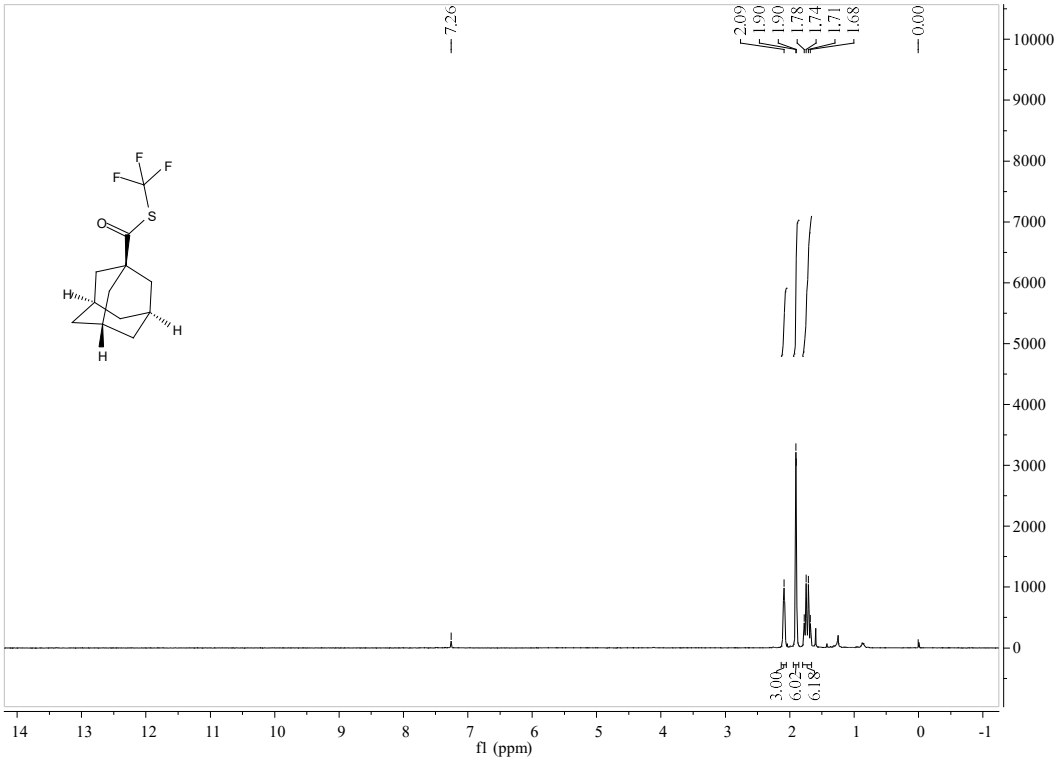
^{19}F NMR spectra of compound **3ae**



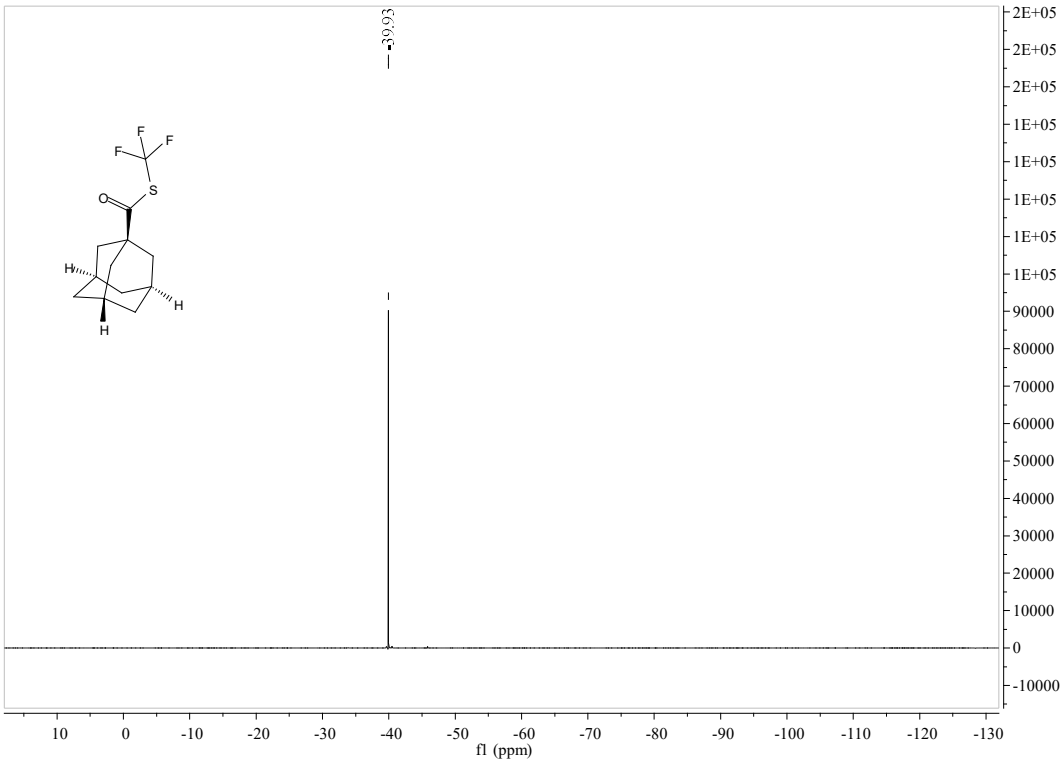
^{13}C NMR spectra of compound **3ae**



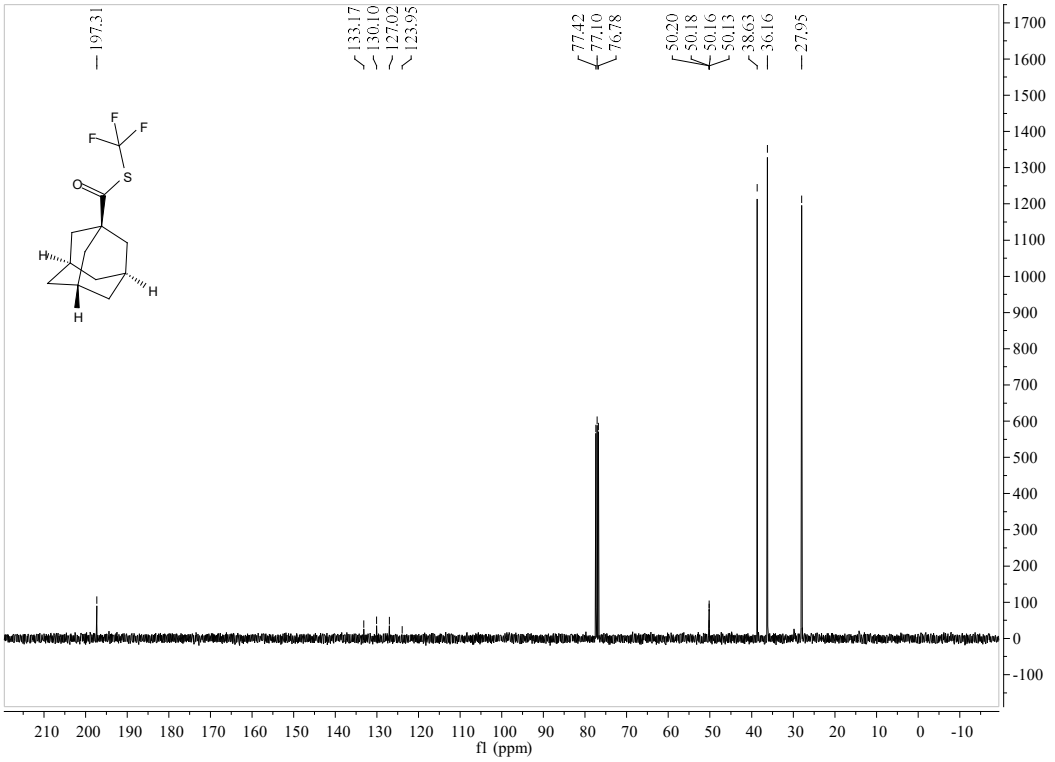
^{1}H NMR spectra of compound **3af**



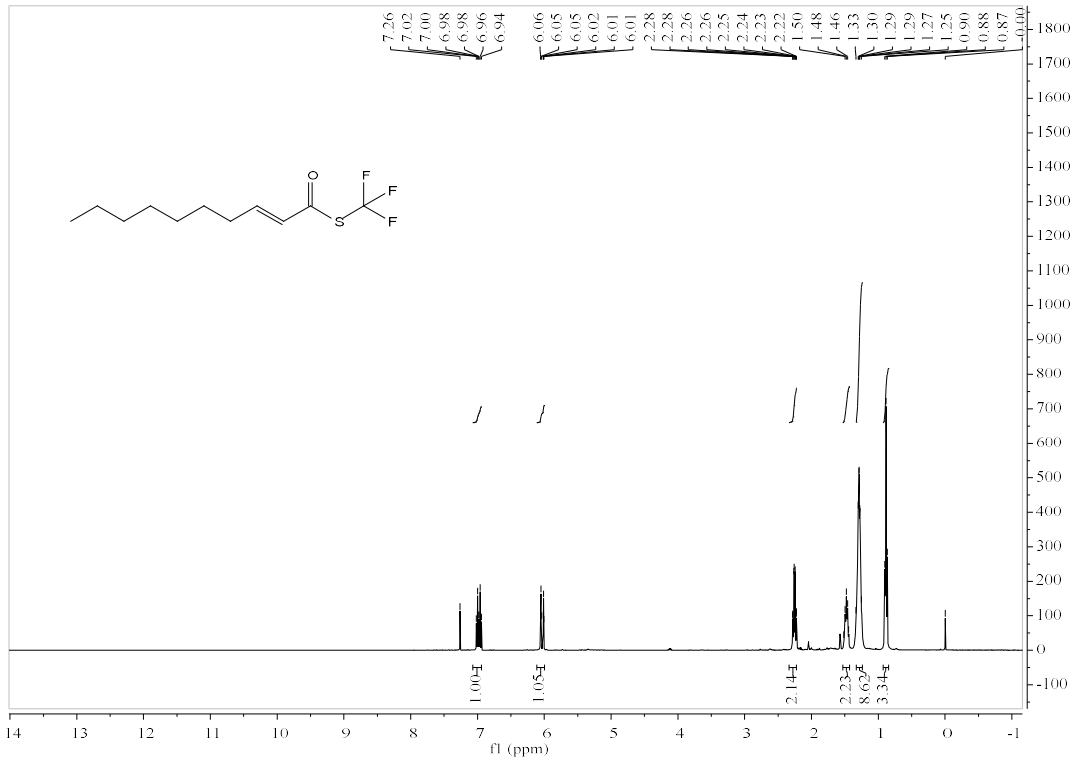
^{19}F NMR spectra of compound **3af**



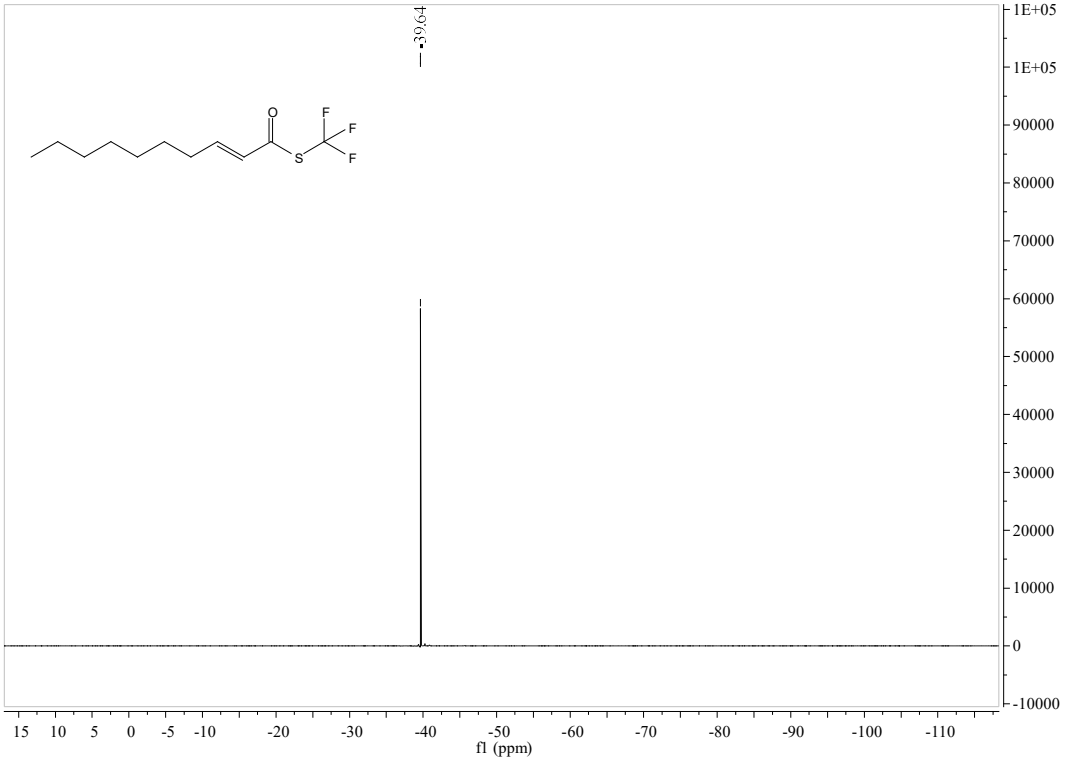
^{13}C NMR spectra of compound **3af**



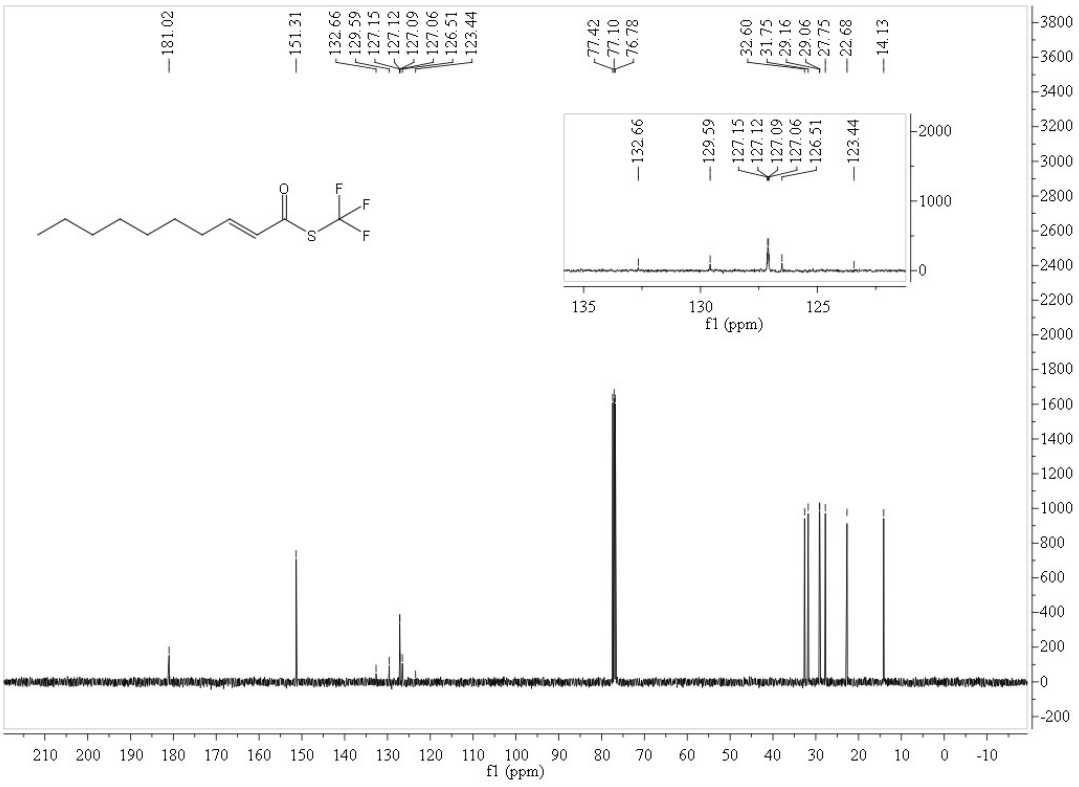
^{1}H NMR spectra of compound **3ag**



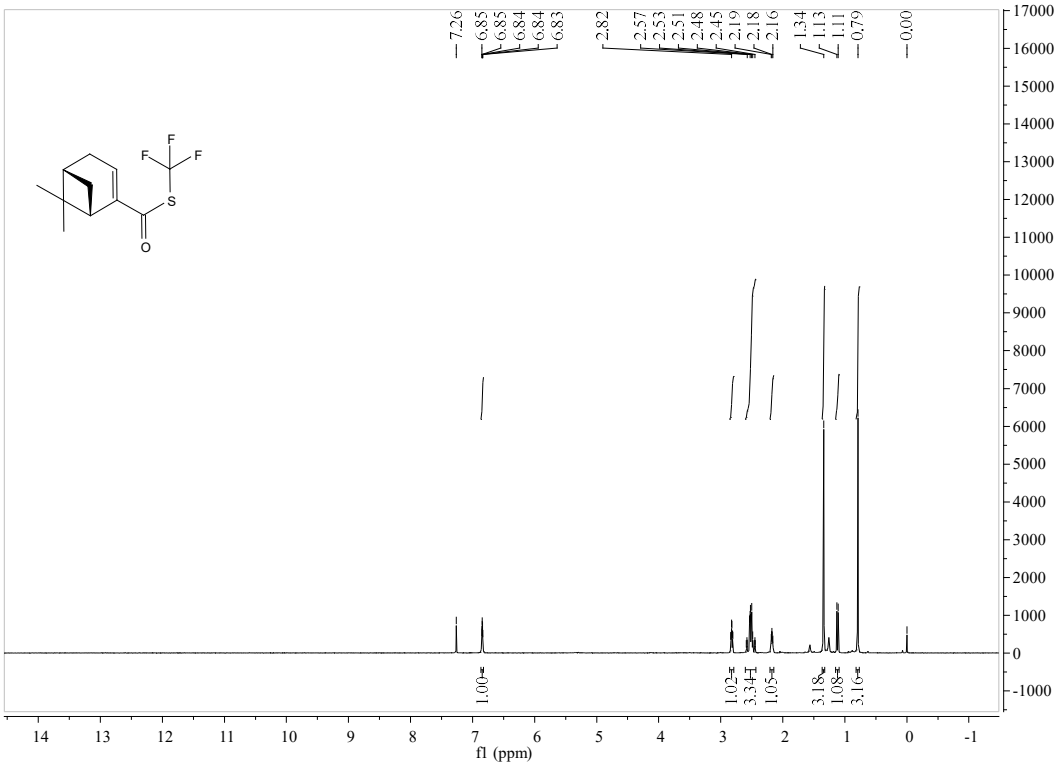
^{19}F NMR spectra of compound **3ag**



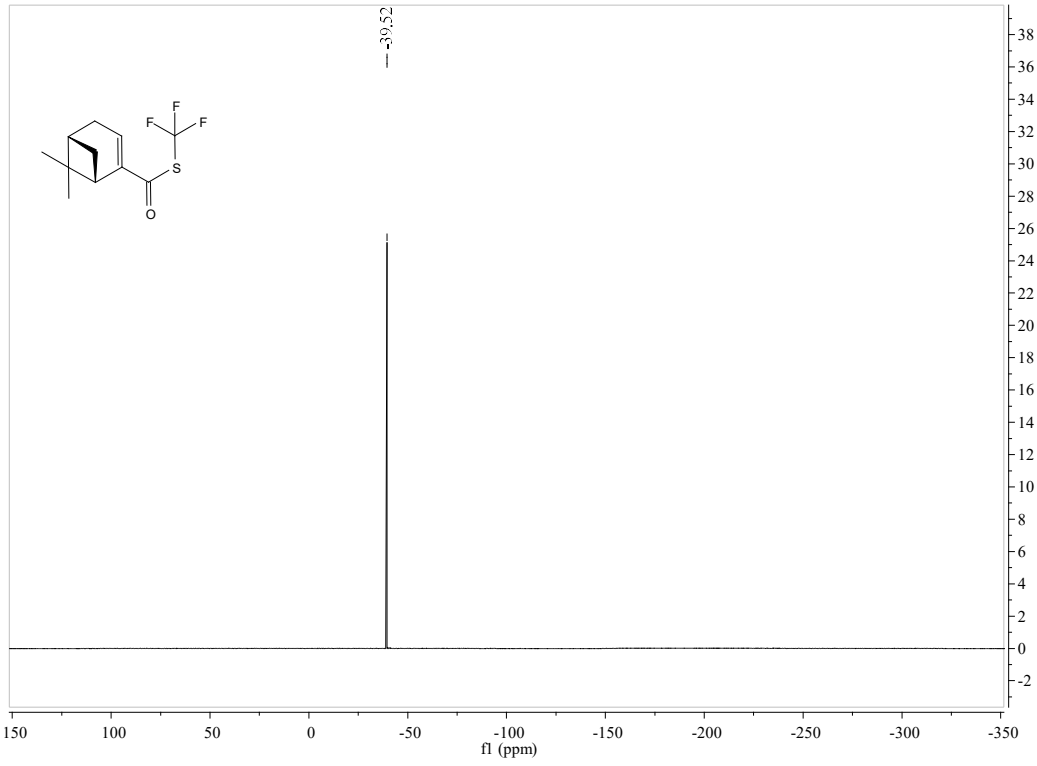
^{13}C NMR spectra of compound **3ag**



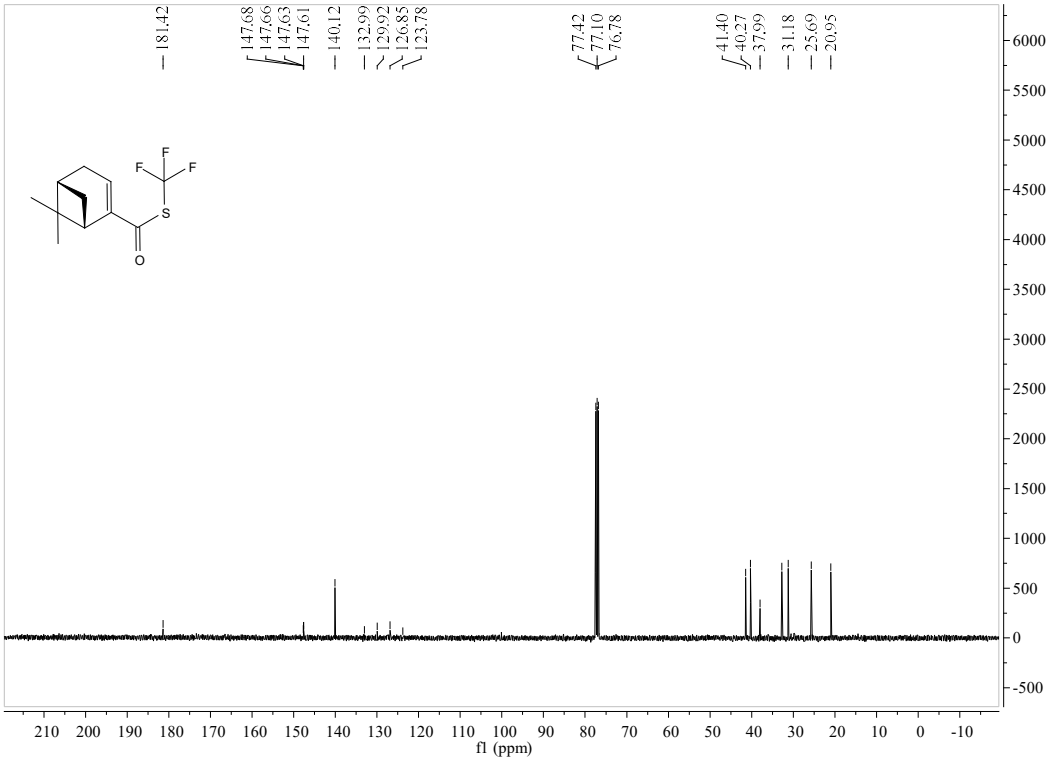
^{1}H NMR spectra of compound **3ah**



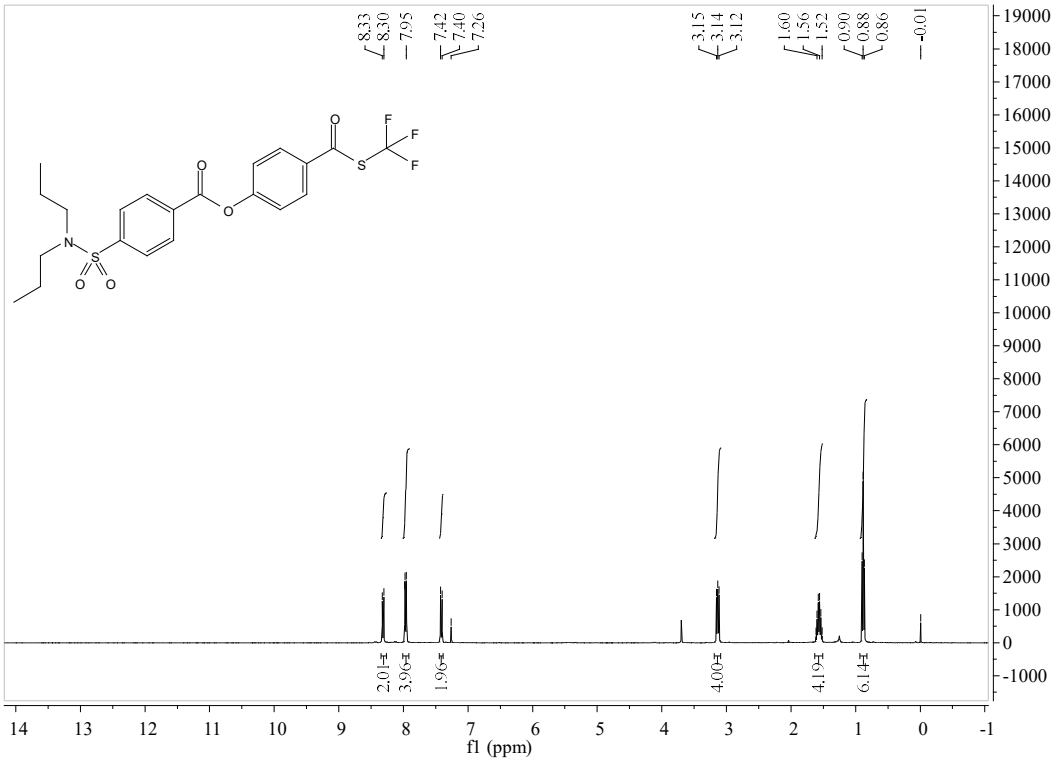
^{19}F NMR spectra of compound **3ah**



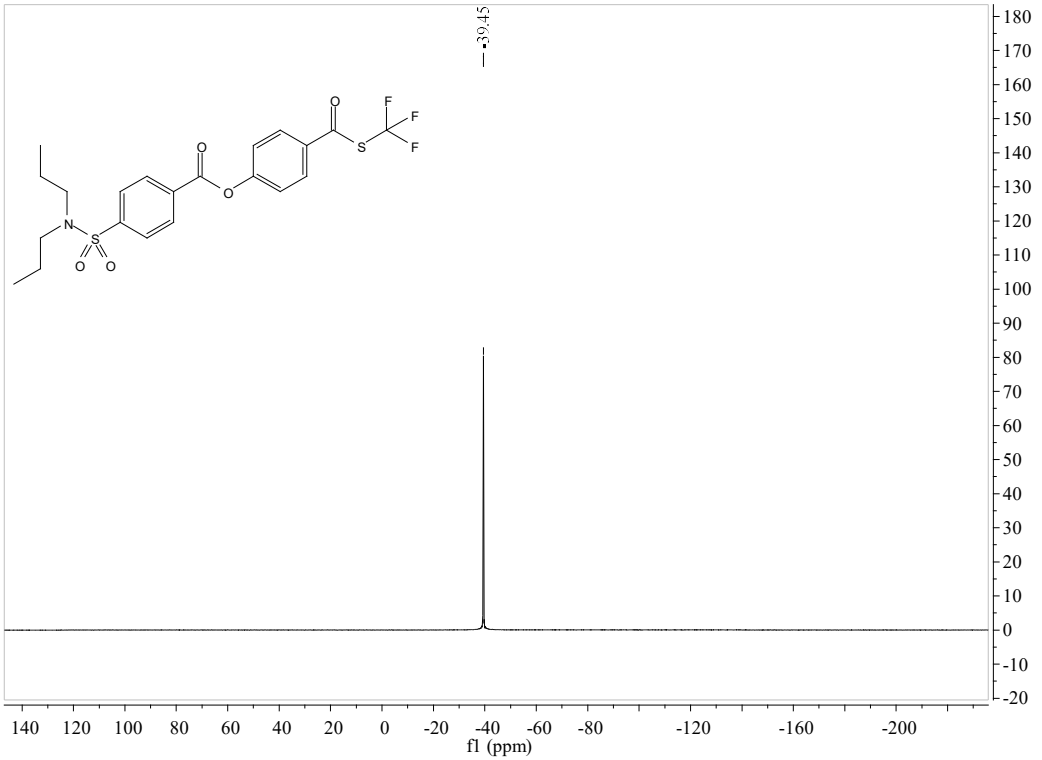
^{13}C NMR spectra of compound **3ah**



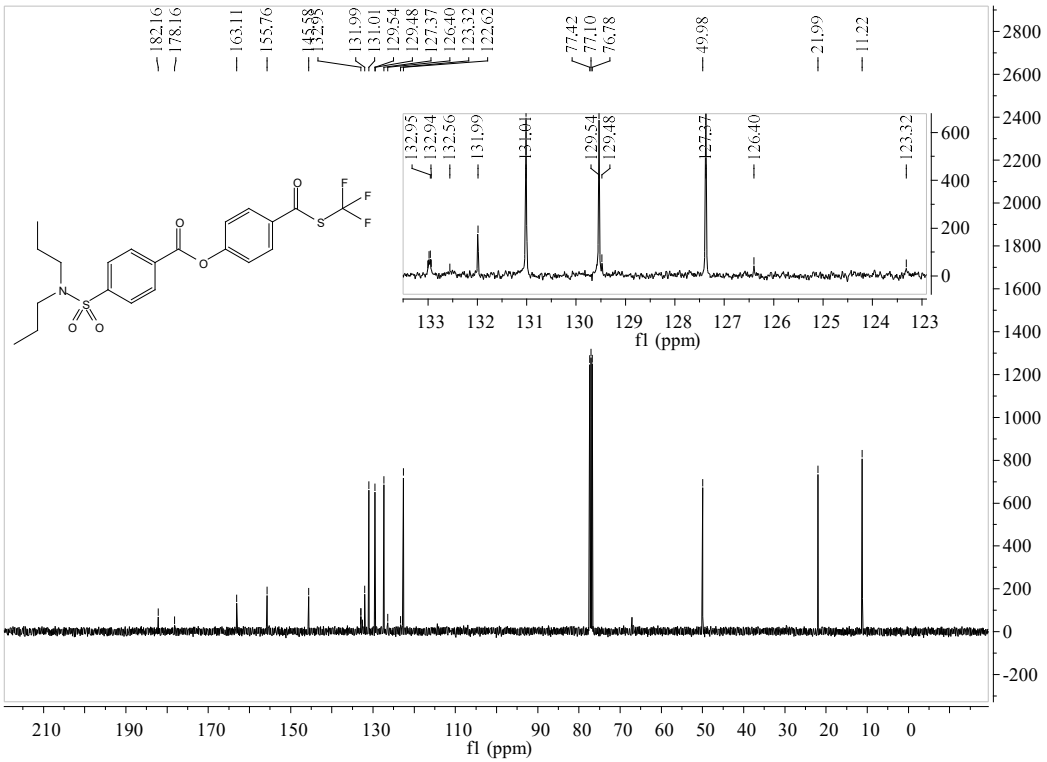
^{1}H NMR spectra of compound **3ba**



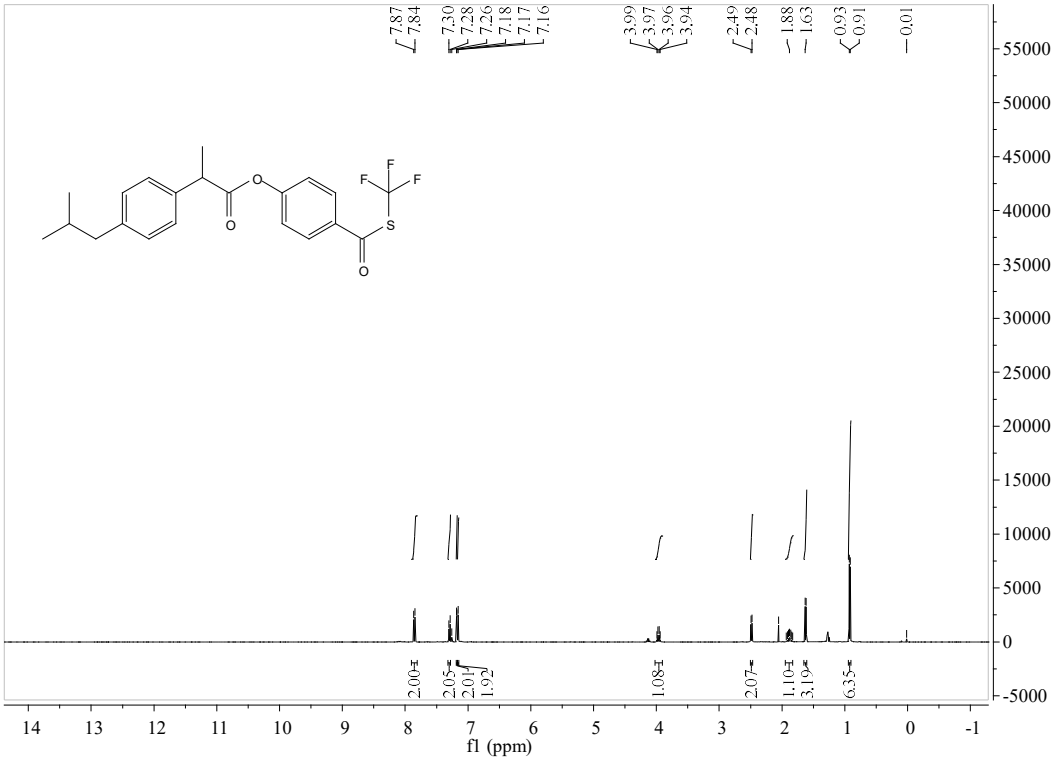
^{19}F NMR spectra of compound **3ba**



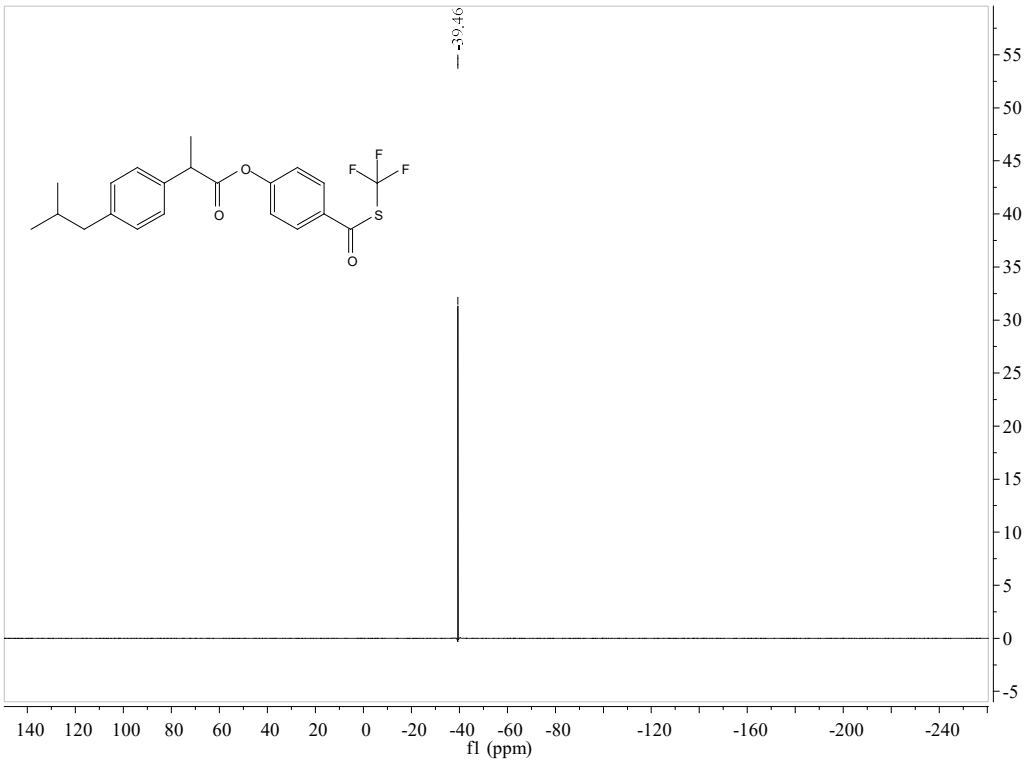
^{13}C NMR spectra of compound **3ba**



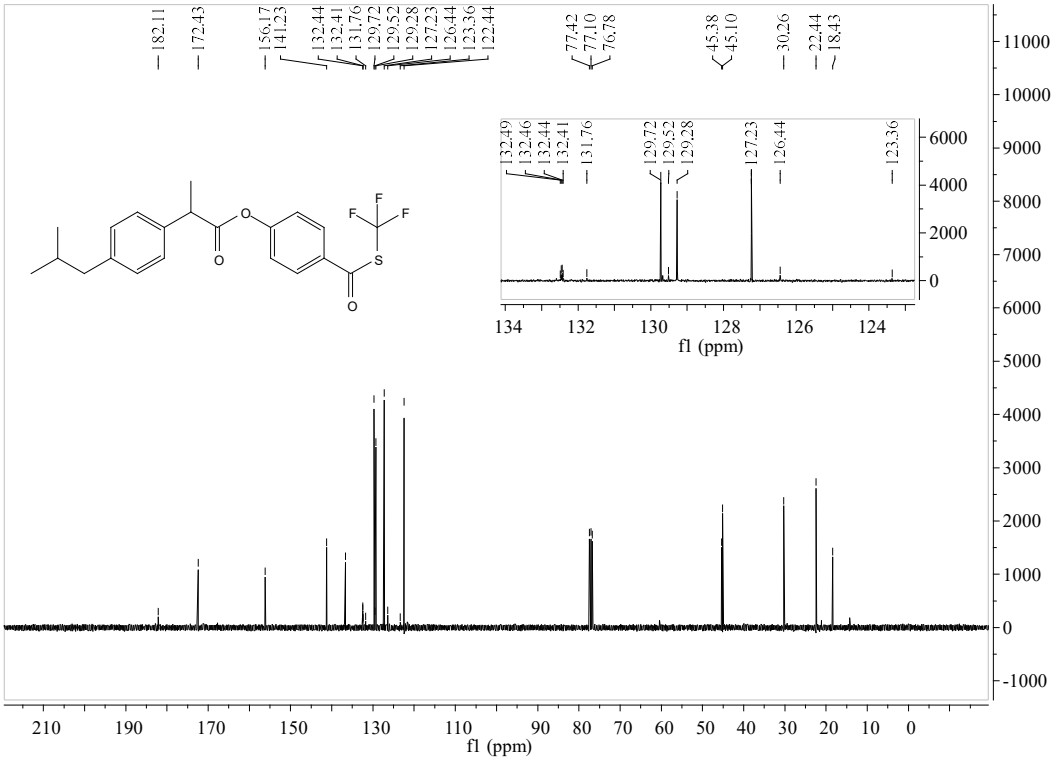
[1]H NMR spectra of compound **3bb**



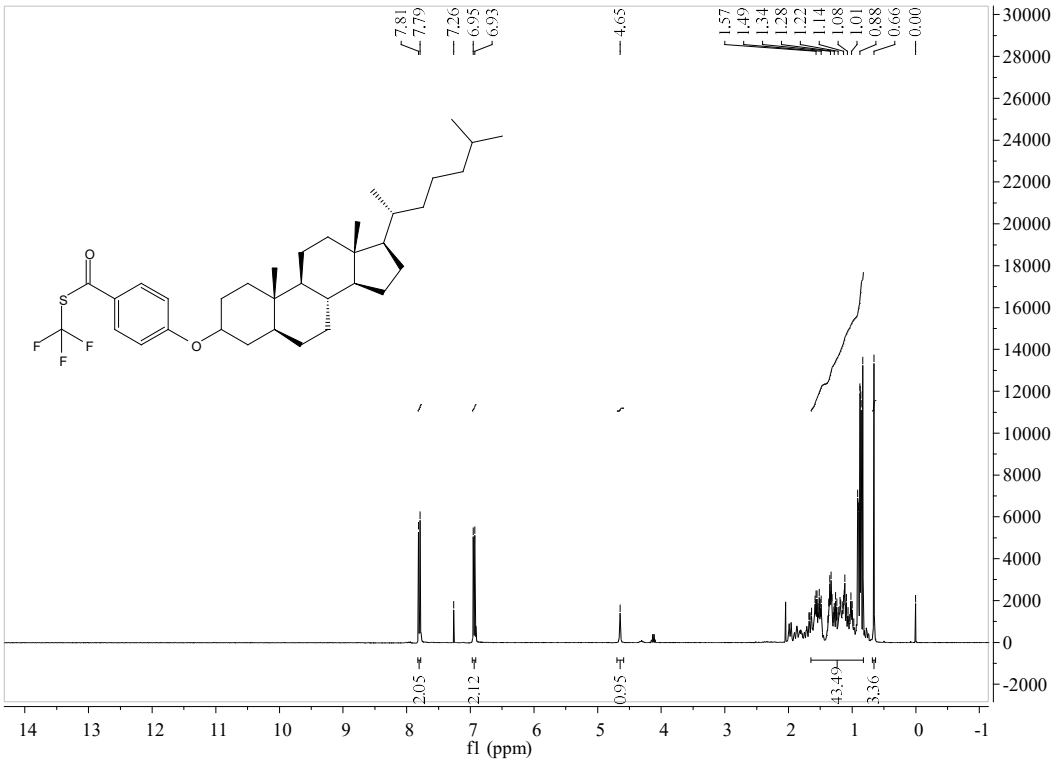
[19]F NMR spectra of compound **3bb**



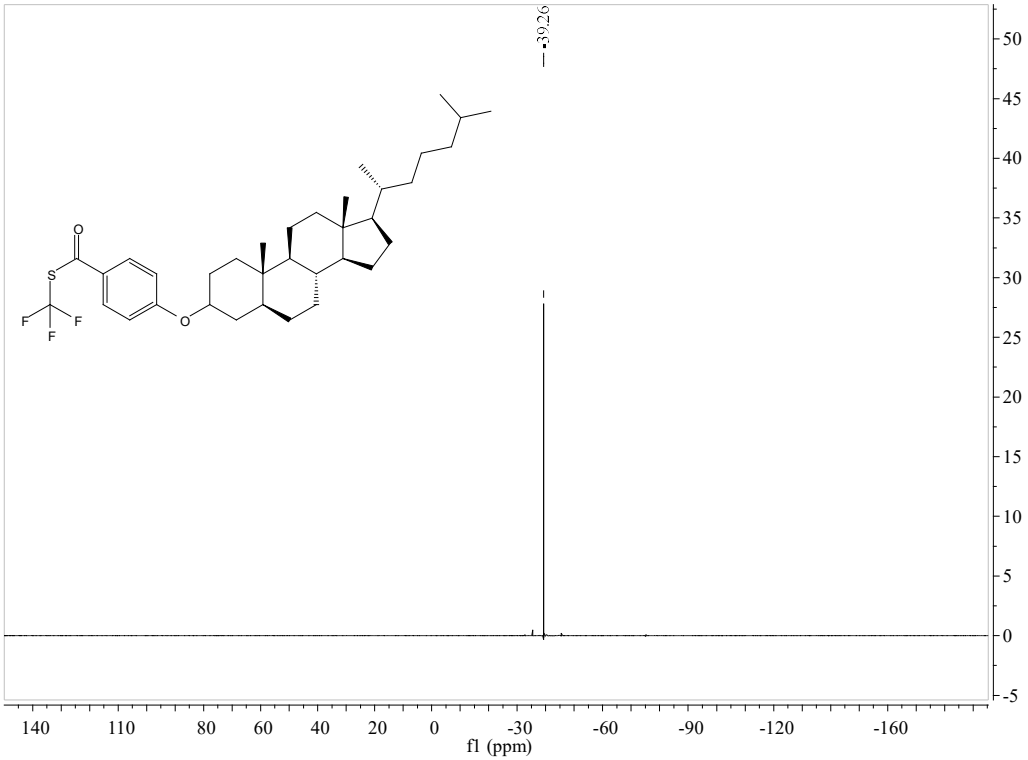
^{13}C NMR spectra of compound **3bb**



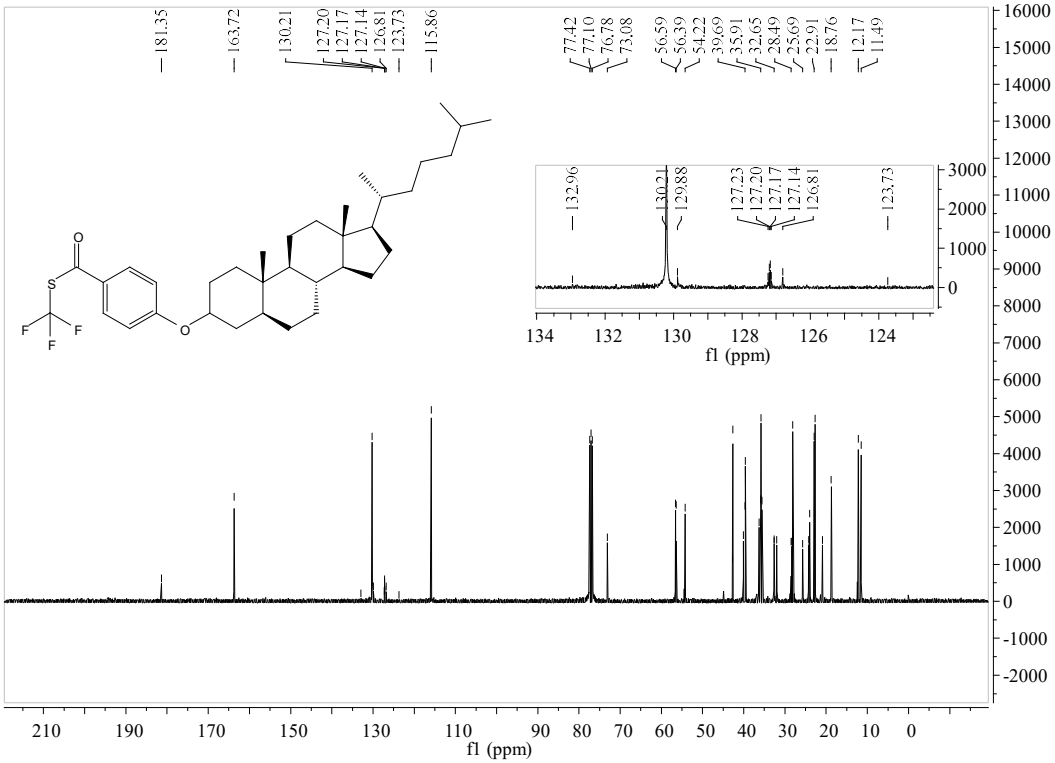
^{1}H NMR spectra of compound **3bc**



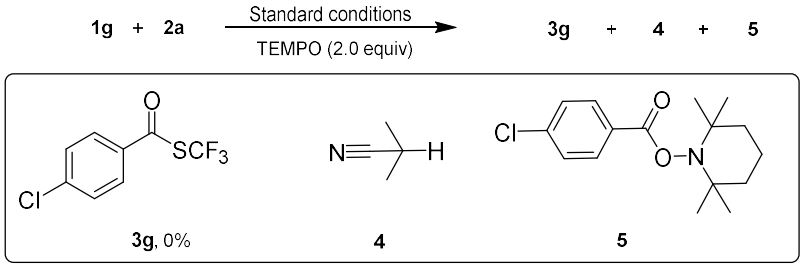
^{19}F NMR spectra of compound **3bc**

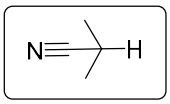


^{13}C NMR spectra of compound **3bc**



2. HRMS(ESI) Data of Procedures for free radical mechanism experiments





:HRMS (ESI) for $C_4H_7NNa(M+Na^+)$: Calcd: 92.0471, Found: 92.0474

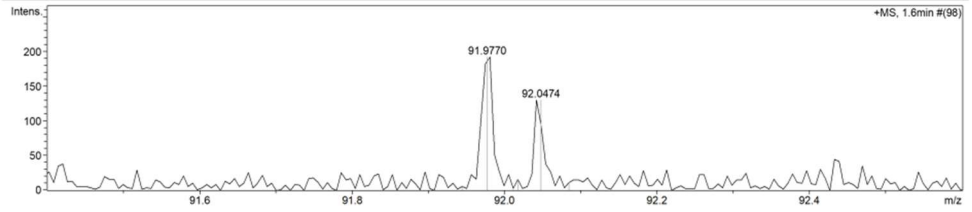
Mass Spectrum SmartFormula Report

Analysis Info

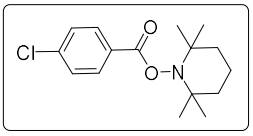
Analysis Name	F:\WYQ-20200628-WMY-1AAA.d	Acquisition Date	2020/6/28 9:53:23
Method	tune_low 50-500.m	Operator	service
Sample Name		Instrument / Ser#	micrOTOF-Q II 10280
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	110.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Formula	m/z	err [ppm]	Mean err [ppm]	rdb	N-Rule	e¡¥Conf	mSigma	Std I	Std Mean m/z	Std I VarNorm	Std m/z Diff	Std Comb Dev
92.0474														
	1	C 4 H 7 N Na	92.0471	-3.5	-3.5	1.5	ok	even	27.11	0.0400	0.0003	0.0244	0.0003	0.8427



:HRMS (ESI) for $C_{16}H_{23}ClNO_2(M+H^+)$: Calcd: 296.1412, Found: 296.1414

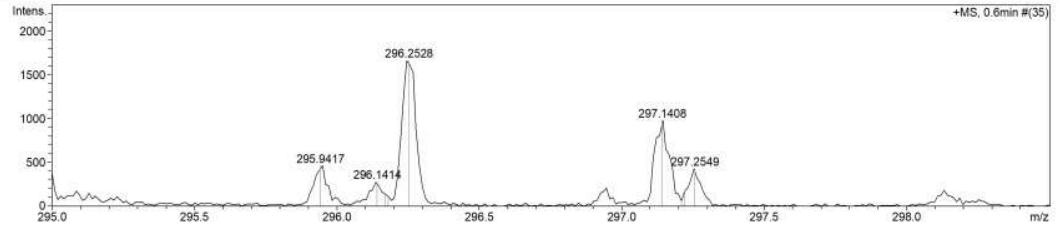
Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name	F:\wyq-20200628-WMY-1AAA.d	Acquisition Date	2020/6/30 14:55:46
Method	tune_low 50-500.m	Operator	service
Sample Name	tyf127-ag-2	Instrument / Ser#	micrOTOF-Q II 10280
Comment			

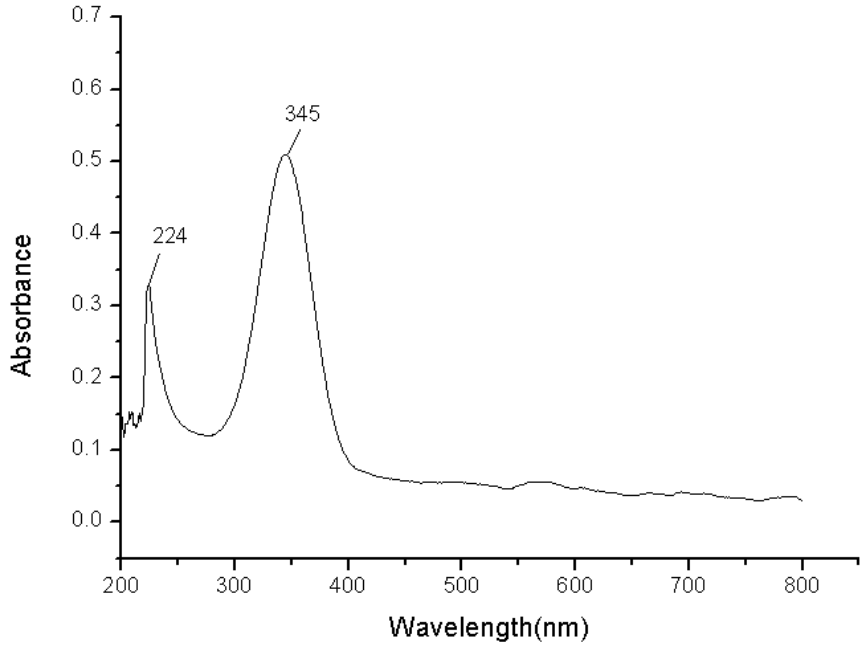
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	110.0 Vpp	Set Divert Valve	Source

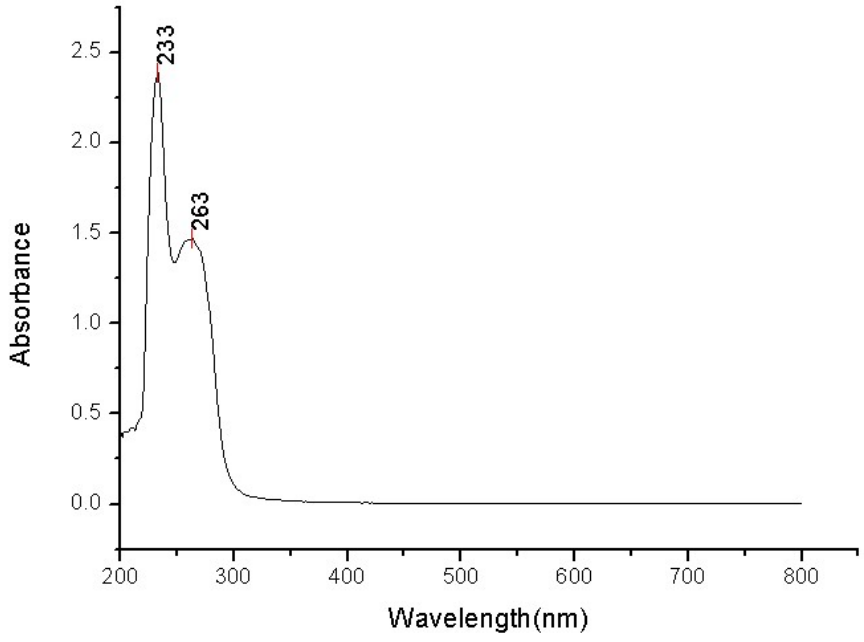


Meas. m/z	#	Formula	m/z	err [ppm]	Mean err [ppm]	rdb	N-Rule	e¡¥Conf	mSigma	Std I	Std Mean m/z	Std I VarNorm	Std m/z Diff	Std Comb Dev
296.1414														
	1	C 16 H 23 Cl N O 2	296.1412	-0.6	25.3	5.5	ok	even	530.53	0.8525	0.0116	0.2680	0.0147	0.8427

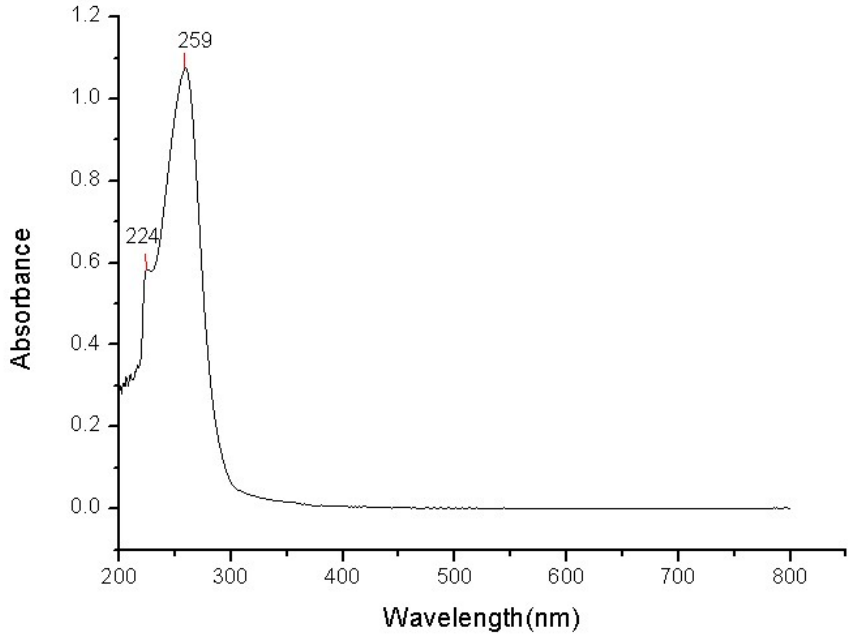
3. UV-vis absorption spectra of AIBN, $PhSO_2SCF_3$, and the standard reaction mixture



UV-vis absorption spectra of AIBN (Solvent:DCE)



UV-vis absorption spectra of $PhSO_2SCF_3$ (Solvent:DCE)



UV-vis absorption spectra of the standard reaction mixture (Solvent:DCE)

4. X-ray Crystal Structure of *S*-(trifluoromethyl)- 3,4-dimethoxybenzothioate (3q) (CCDC: 1976664)