Supporting Information

Access to α,α-Difluoro(arylthio)methyl Oxetanes from α,α-Difluoro(arylthio)methyl Ketones and Trimethylsulfoxonium Halides: Scope, Mechanism and Applications

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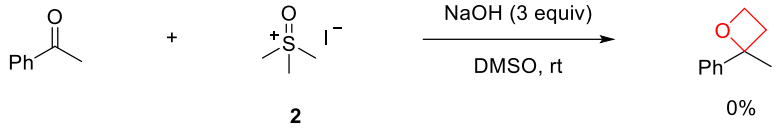
A. Other Tested Ketone

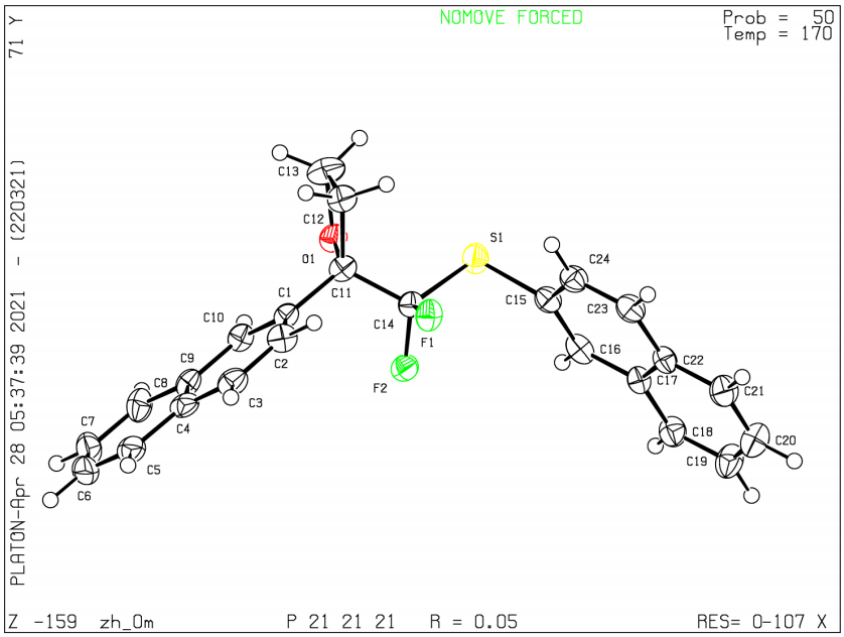
Acetophenone was not applicable to the standard reaction conditions, because no corresponding oxetane product was obtained.



2 0%

B. X-Ray Crystallographic Data

The obtained compound **3a** (30 mg) was dissolved in CH_2Cl_2 (0.2 mL) in a test tube at room temperature. Then petroleum ether (15 mL) was added to the solution slowly along the tube wall, resulting in a two-phase mixture. Finally, sealed the test tube with a rubber plug penetrated by a needle. Then the colorless crystal of **3a** was formed after the two-phase mixture has diffused. The X-ray crystallographic structures for **3a**. ORTEP representation with 50% probability thermal ellipsoids. Solvent and hydrogen are omitted for clarity. Crystal data have been deposited to CCDC, number 2118496.

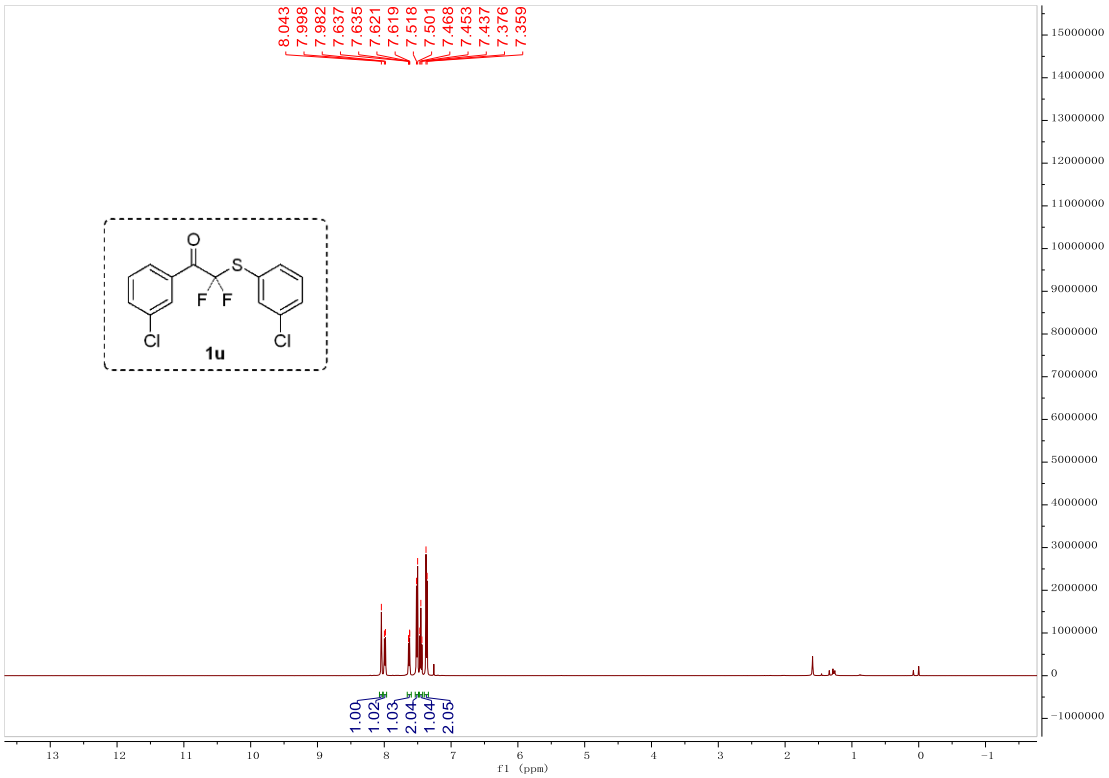


Empirical formula	$C_{24}H_{18}F_2OS$
Formula weight	392.44
Temperature	170.0 K
Wavelength	0.71073 Å

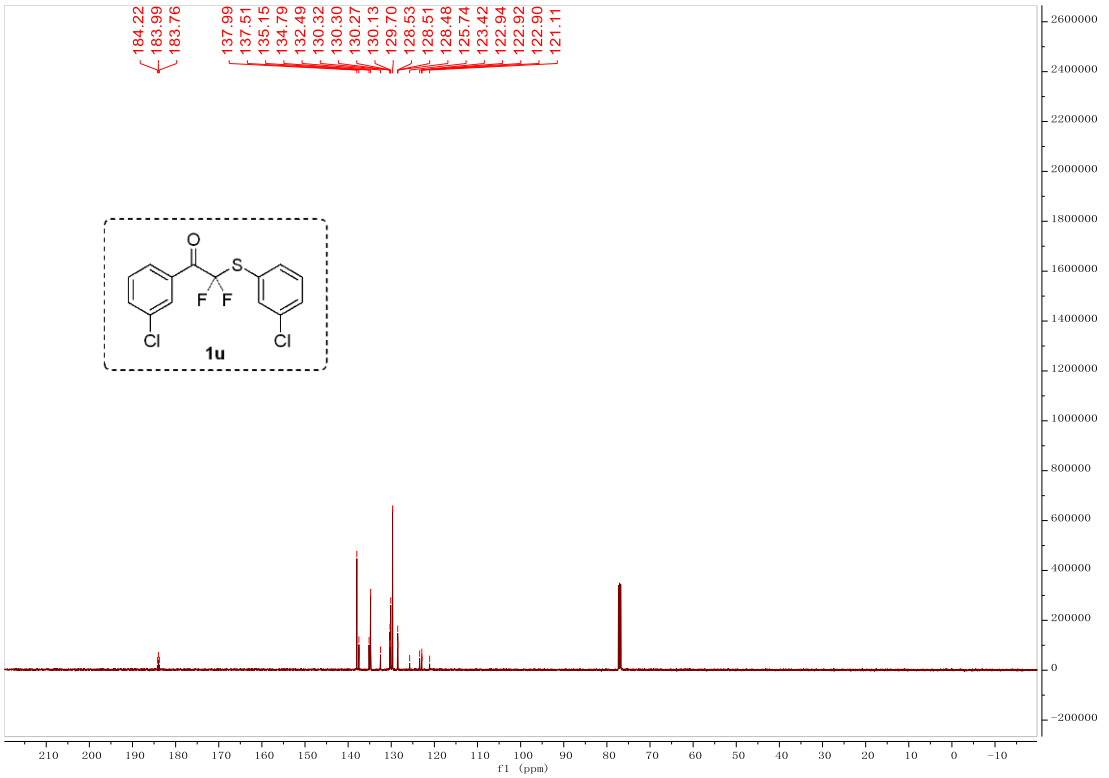
Crystal system, space group	orthorhombic, $P2_12_12_1$
Unit cell dimensions	a = 5.7949(4) Å alpha = 90 deg. b = 15.4144(12) Å beta = 90 deg. c = 21.1109(17) Å gamma = 90 deg.
Volume	1885.7(2) $Å^3$
Z, Calculated density	4
ρ_{calc}	1.382 g/cm^3
μ	0.203 mm^{-1}
F(000)	816.0
Crystal size	0.15 × 0.08 × 0.05 mm^3
Radiation	MoKα (λ = 0.71073)
Theta range for data collection	1.929 to 26.433 deg.
Index ranges	$-6 \leq h \leq 7$, $-19 \leq k \leq 16$, $-26 \leq l \leq 26$
Reflections collected	14420
Independent reflections	3865 [R_{int} = 0.0699, R_{sigma} = 0.0727]
Data / restraints / parameters	3865/0/253
Goodness-of-fit on F^2	1.095
Final R indexes [I>=2σ (I)]	R_1 = 0.0532, wR_2 = 0.1108
Final R indexes [all data]	R_1 = 0.0777, wR_2 = 0.1295

C. NMR Spectra of Compounds

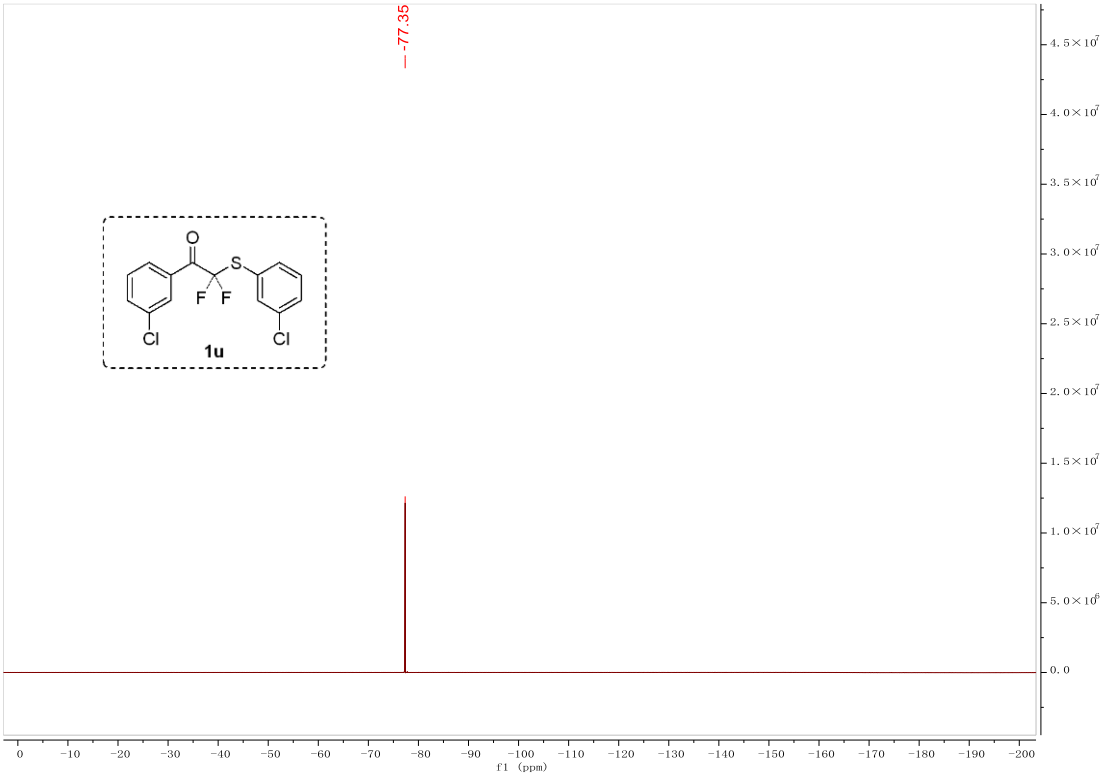
^{1}H NMR (500 MHz, $CDCl_3$) spectrum for 1u



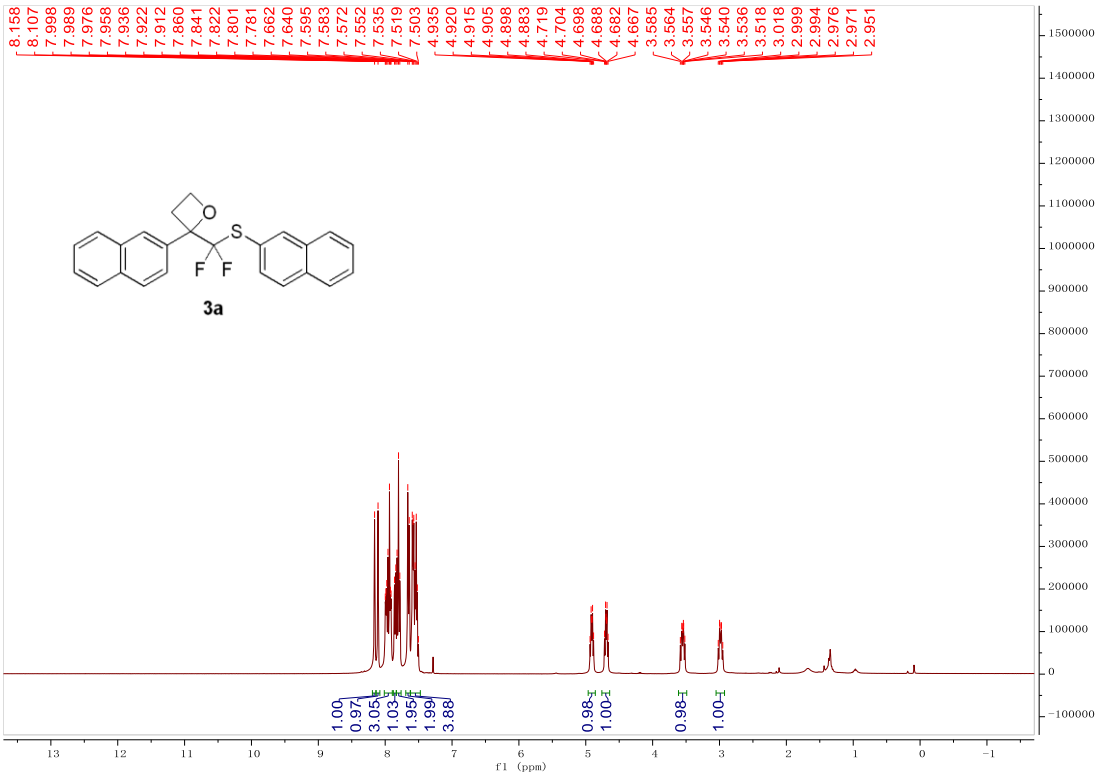
^{13}C NMR (126 MHz, $CDCl_3$) spectrum for 1u



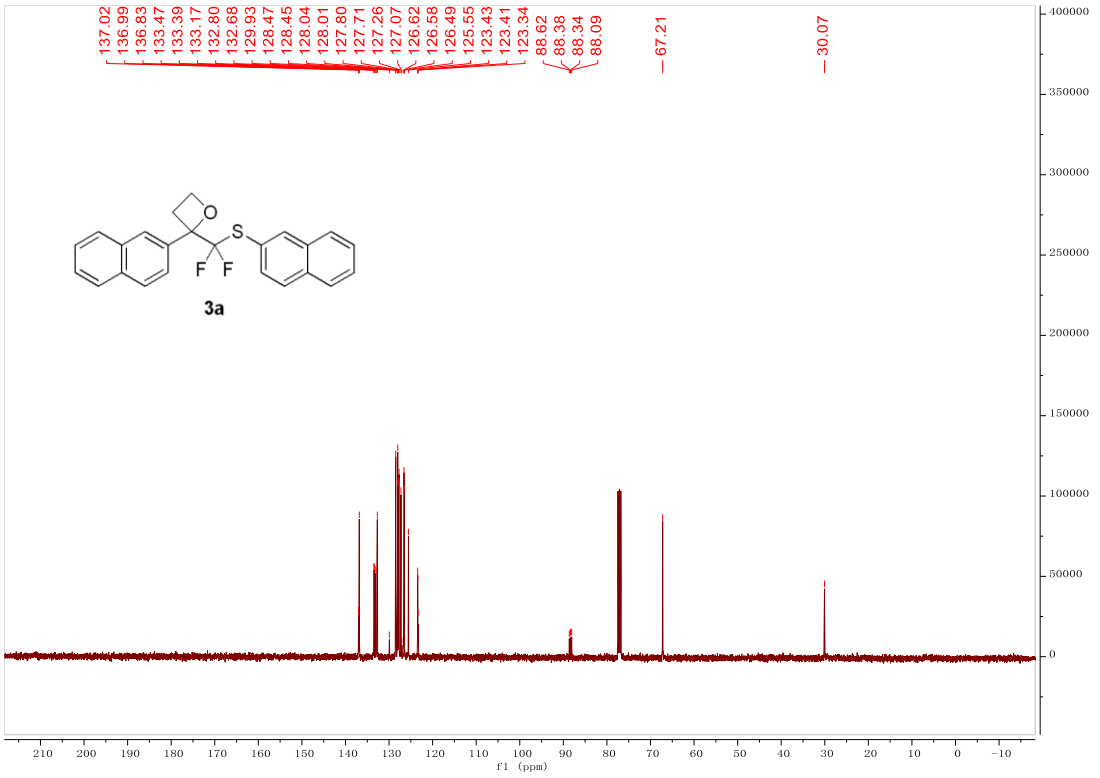
^{19}F NMR (471 MHz, $CDCl_3$) spectrum for 1u



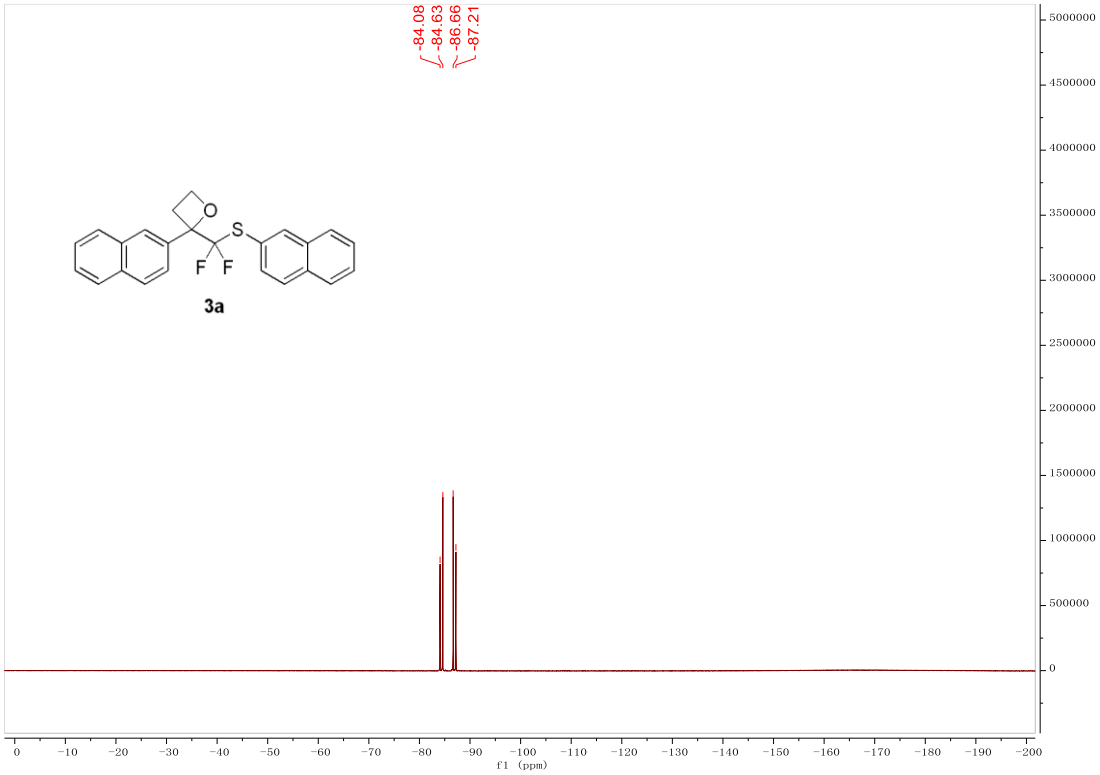
^{1}H NMR (400 MHz, $CDCl_3$) spectrum for 3a



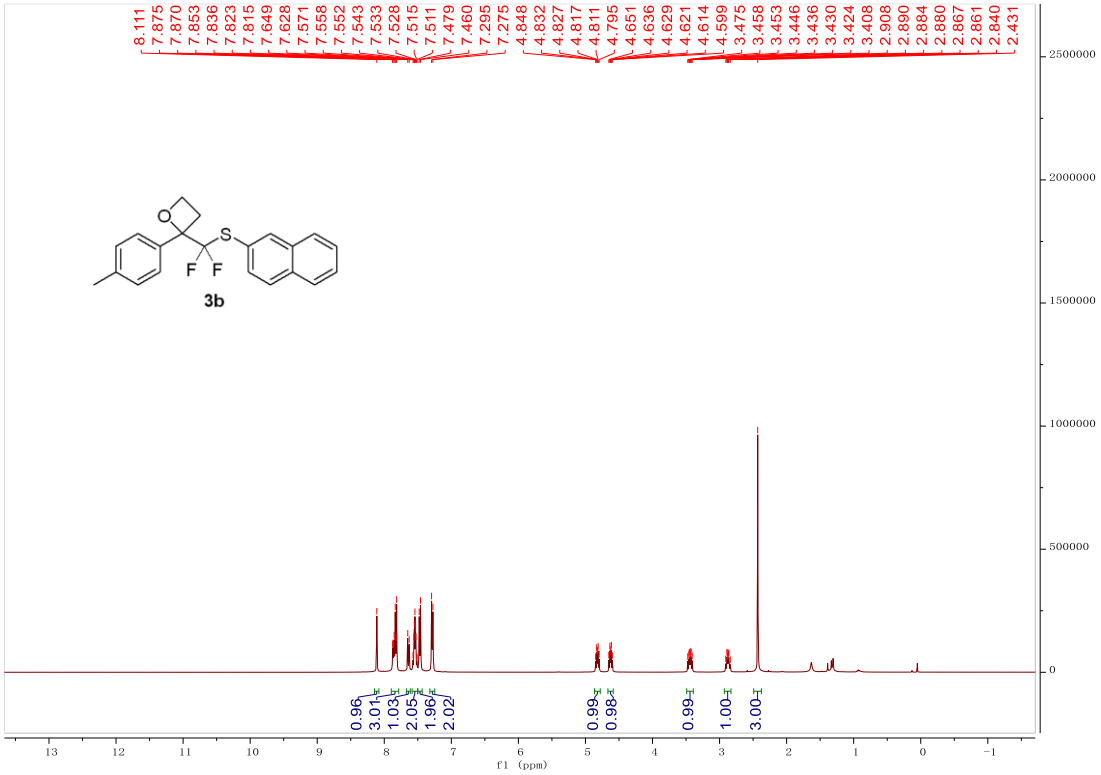
^{13}C NMR (101 MHz, $CDCl_3$) spectrum for 3a



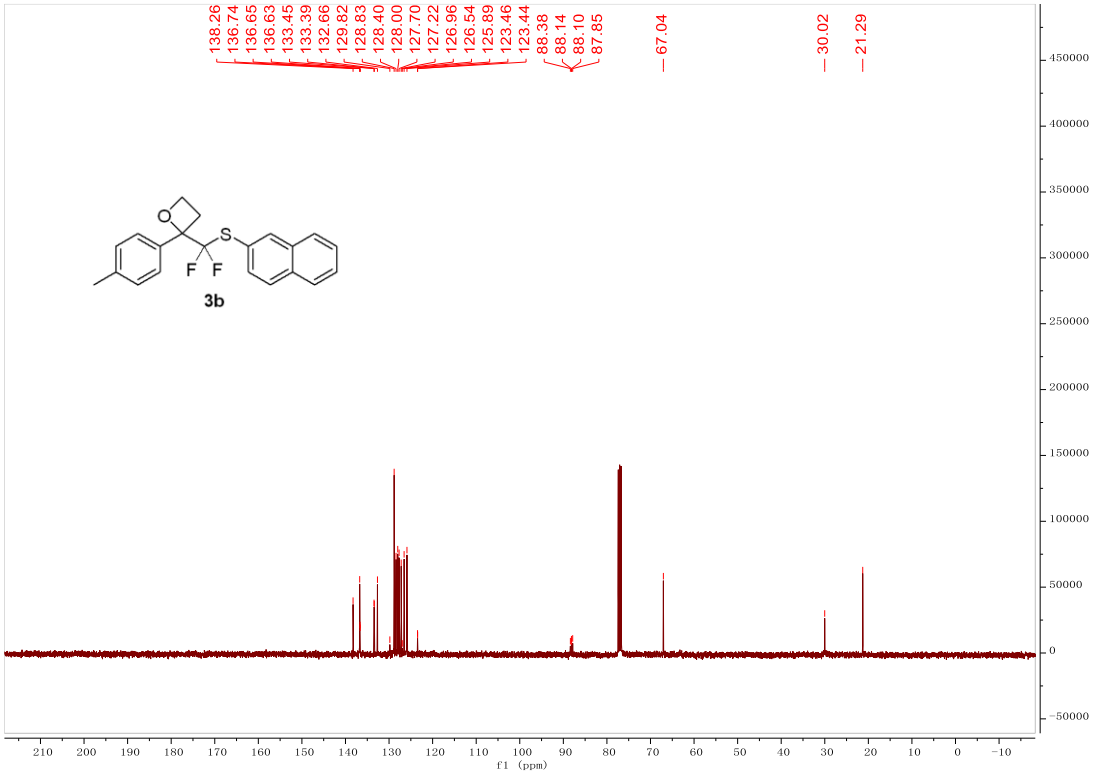
^{19}F NMR (376 MHz, $CDCl_3$) spectrum for 3a



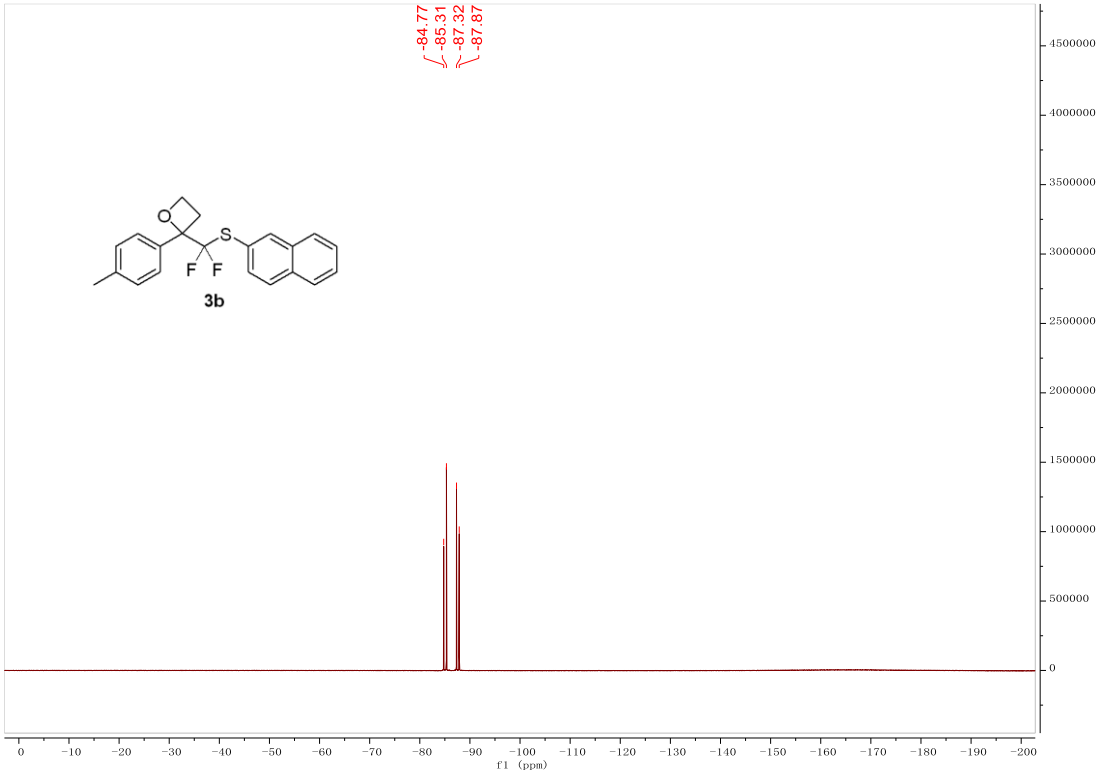
^{1}H NMR (400 MHz, $CDCl_3$) spectrum for 3b



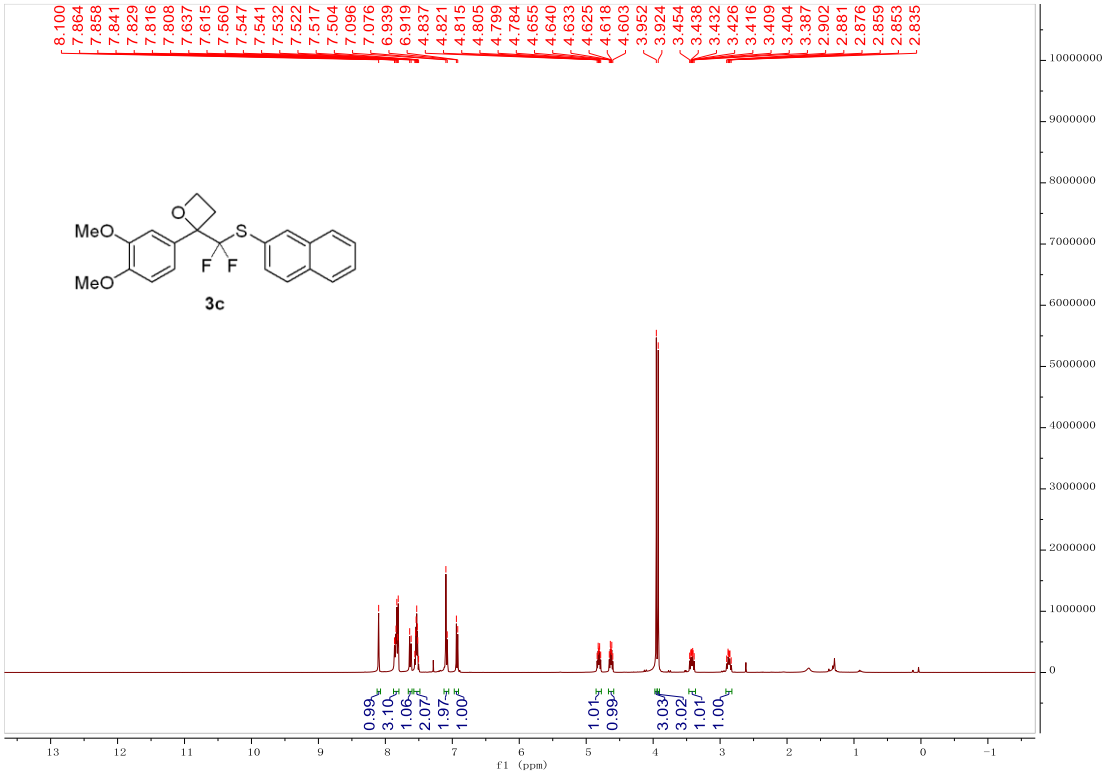
^{13}C NMR (101 MHz, $CDCl_3$) spectrum for 3b



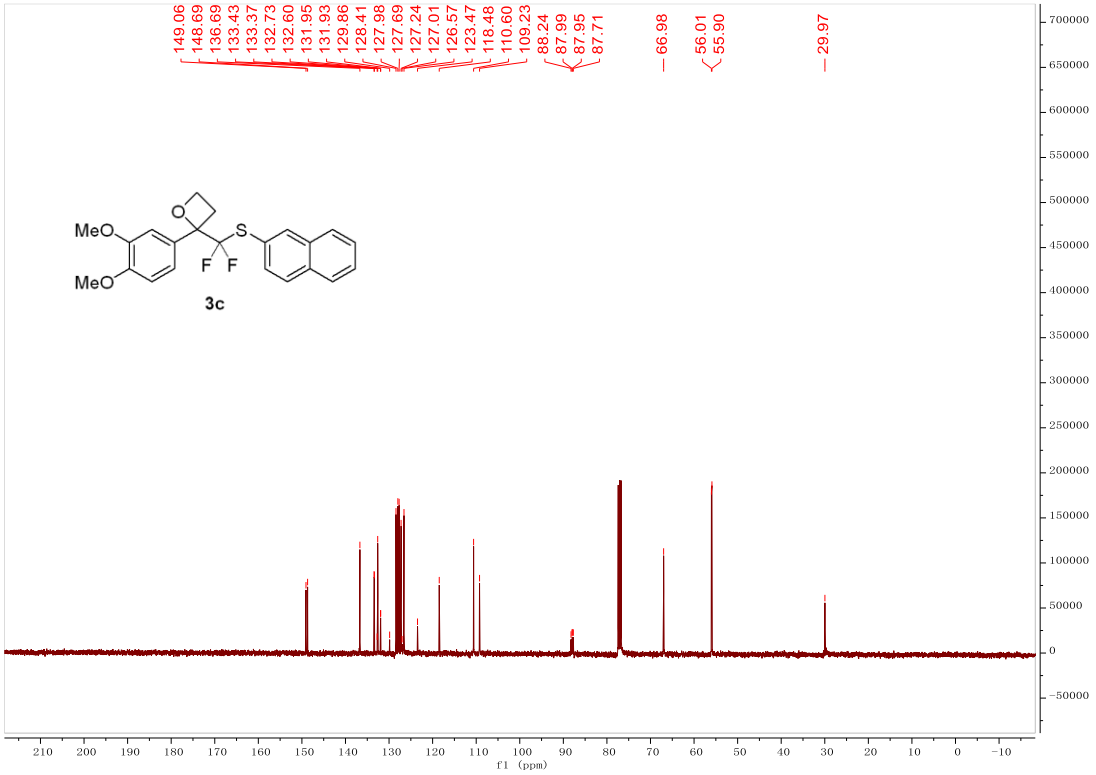
^{19}F NMR (376 MHz, $CDCl_3$) spectrum for 3b



^{1}H NMR (400 MHz, $CDCl_3$) spectrum for 3c

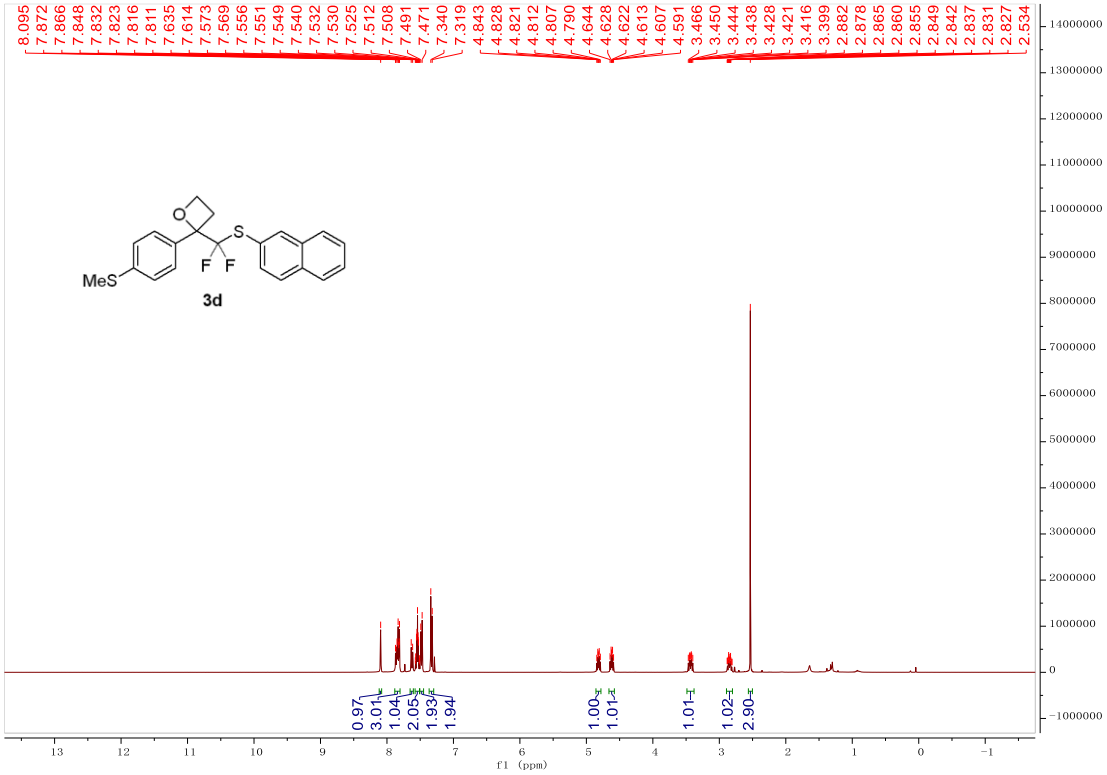


^{13}C NMR (101 MHz, $CDCl_3$) spectrum for 3c

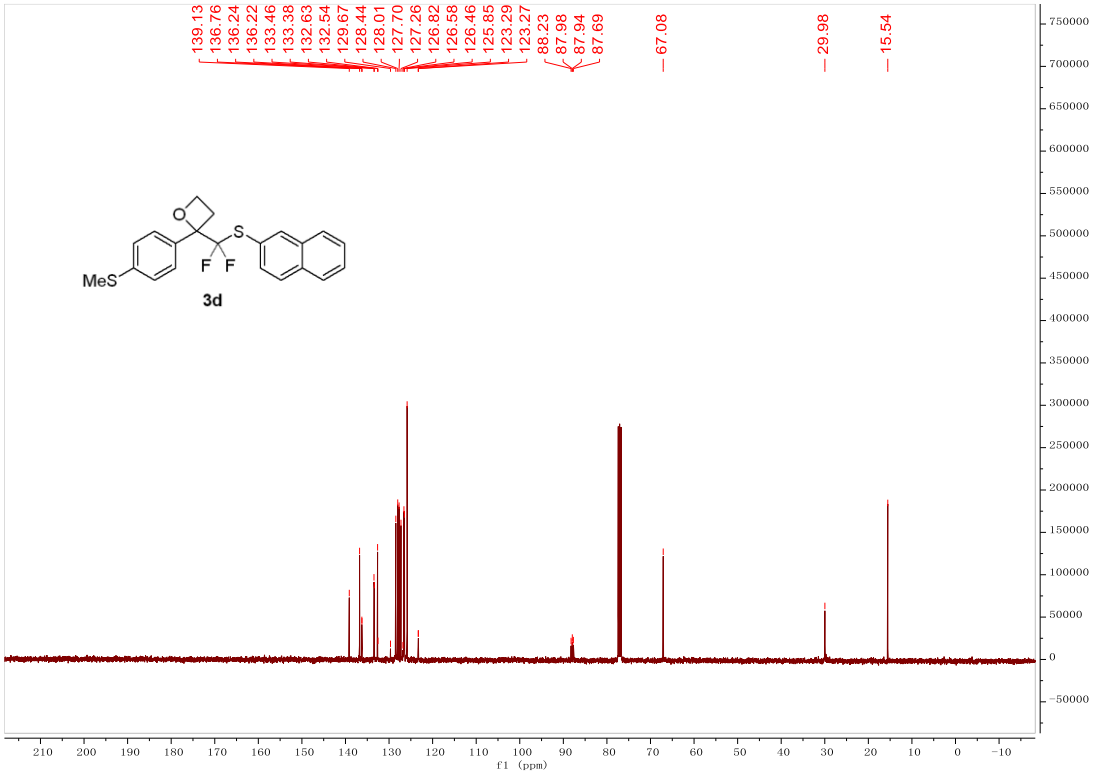


^{19}F NMR (376 MHz, $CDCl_3$) spectrum for 3c

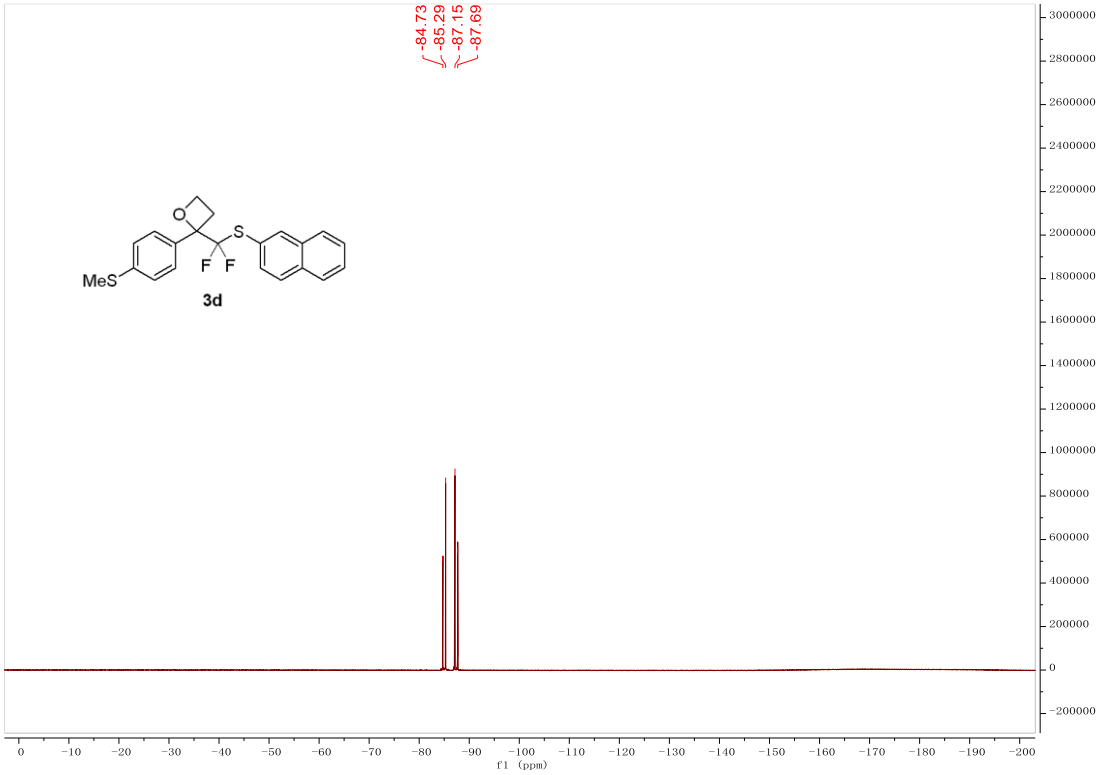
^{1}H NMR (400 MHz, $CDCl_3$) spectrum for 3d



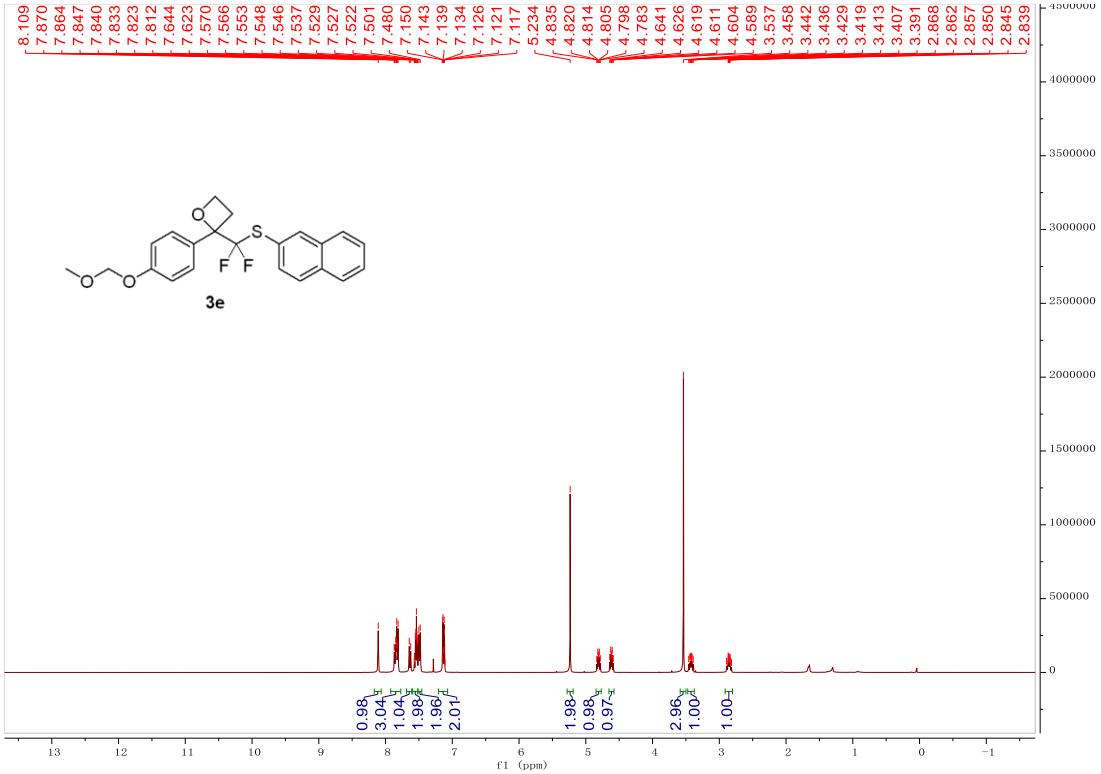
^{13}C NMR (101 MHz, $CDCl_3$) spectrum for 3d



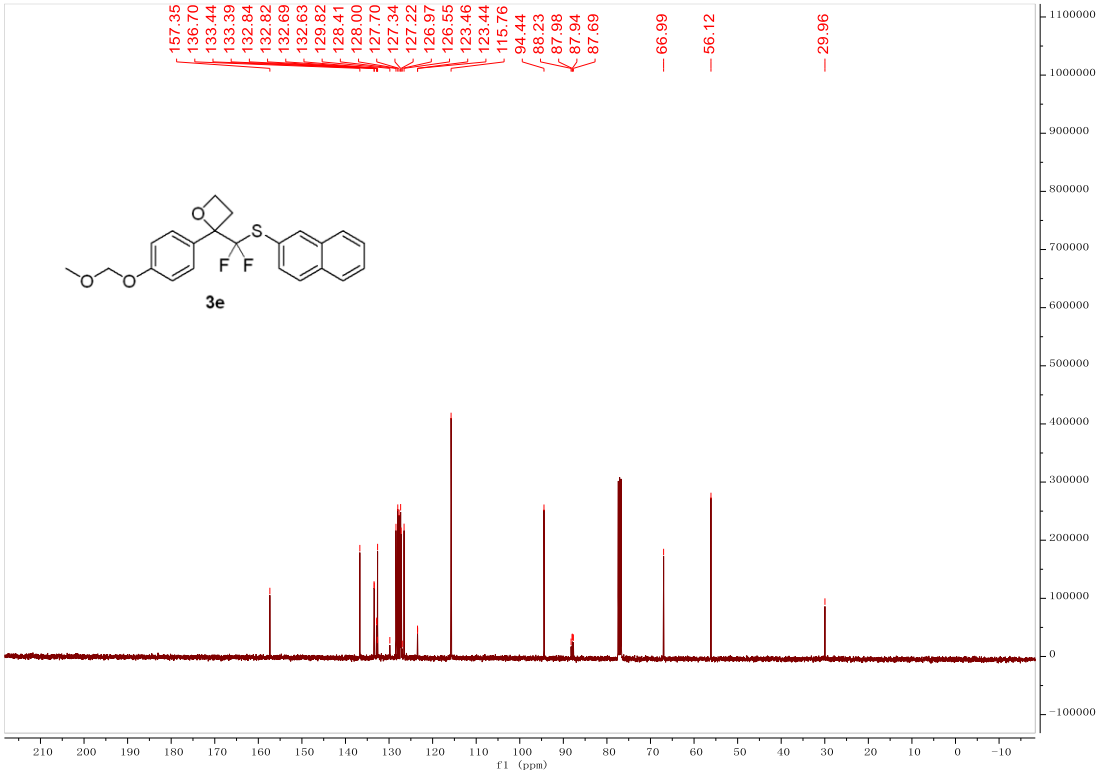
^{19}F NMR (376 MHz, $CDCl_3$) spectrum for 3d



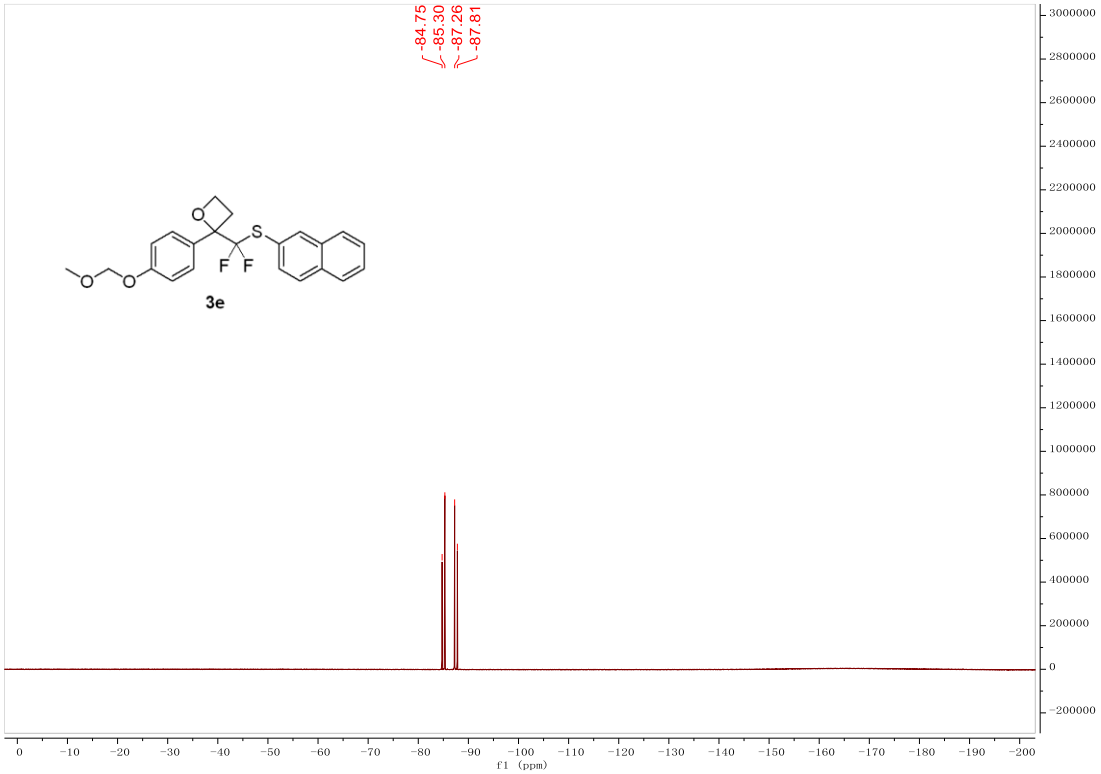
^{1}H NMR (400 MHz, $CDCl_3$) spectrum for 3e



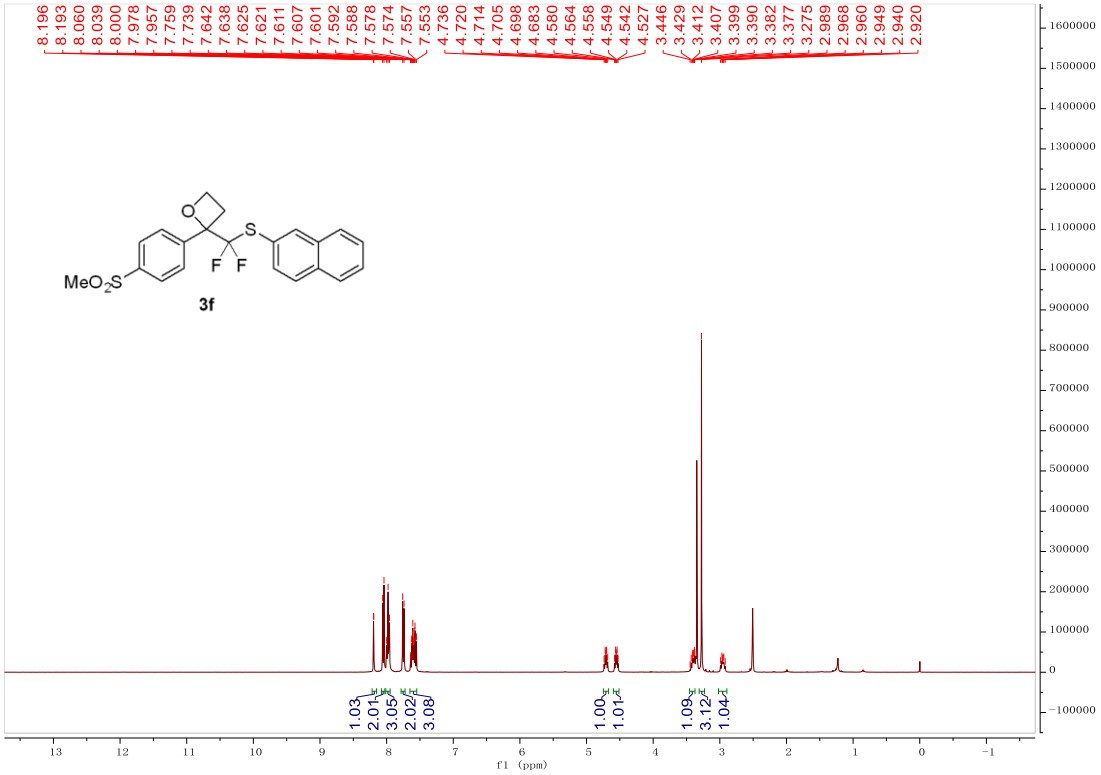
^{13}C NMR (101 MHz, $CDCl_3$) spectrum for 3e



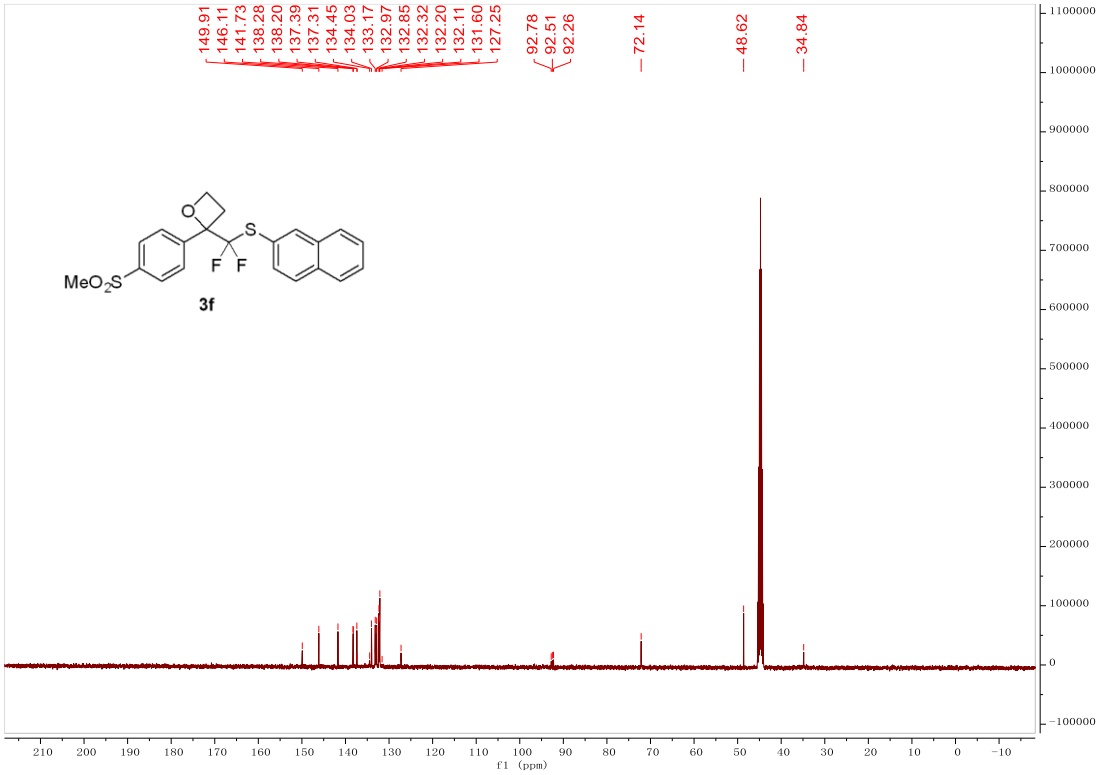
^{19}F NMR (376 MHz, $CDCl_3$) spectrum for 3e



^{1}H NMR (400 MHz, DMSO-d_6) spectrum for 3f

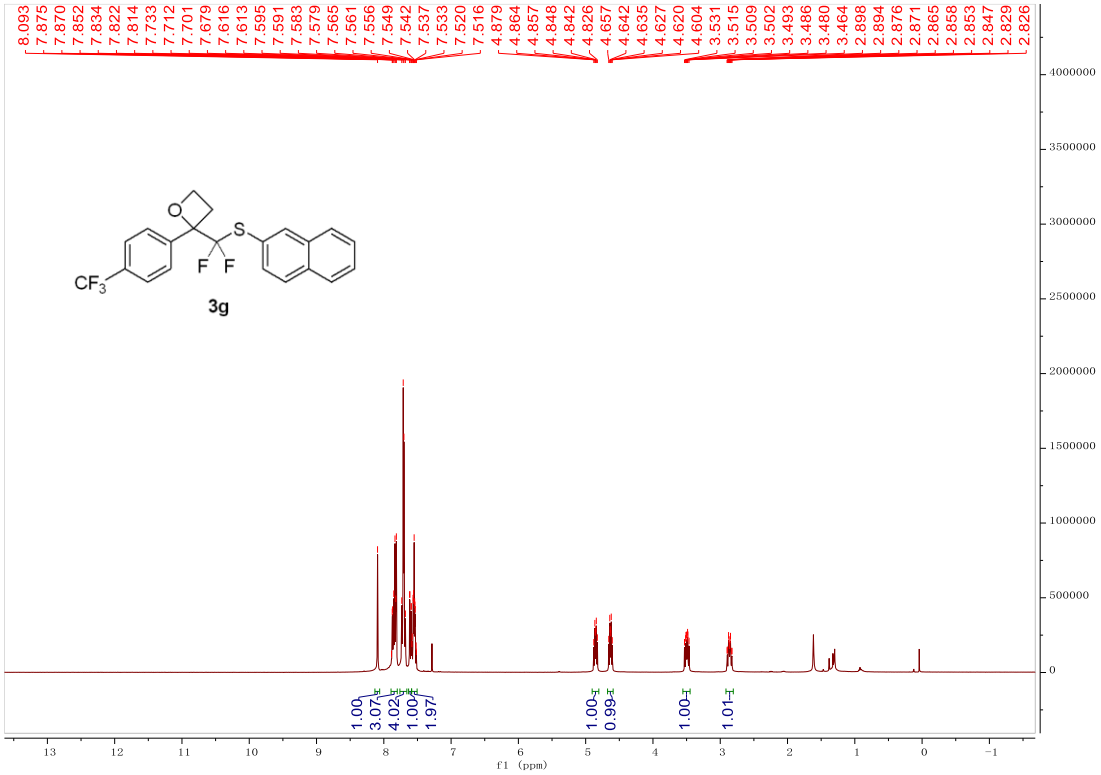


^{13}C NMR (101 MHz, DMSO-d_6) spectrum for 3f

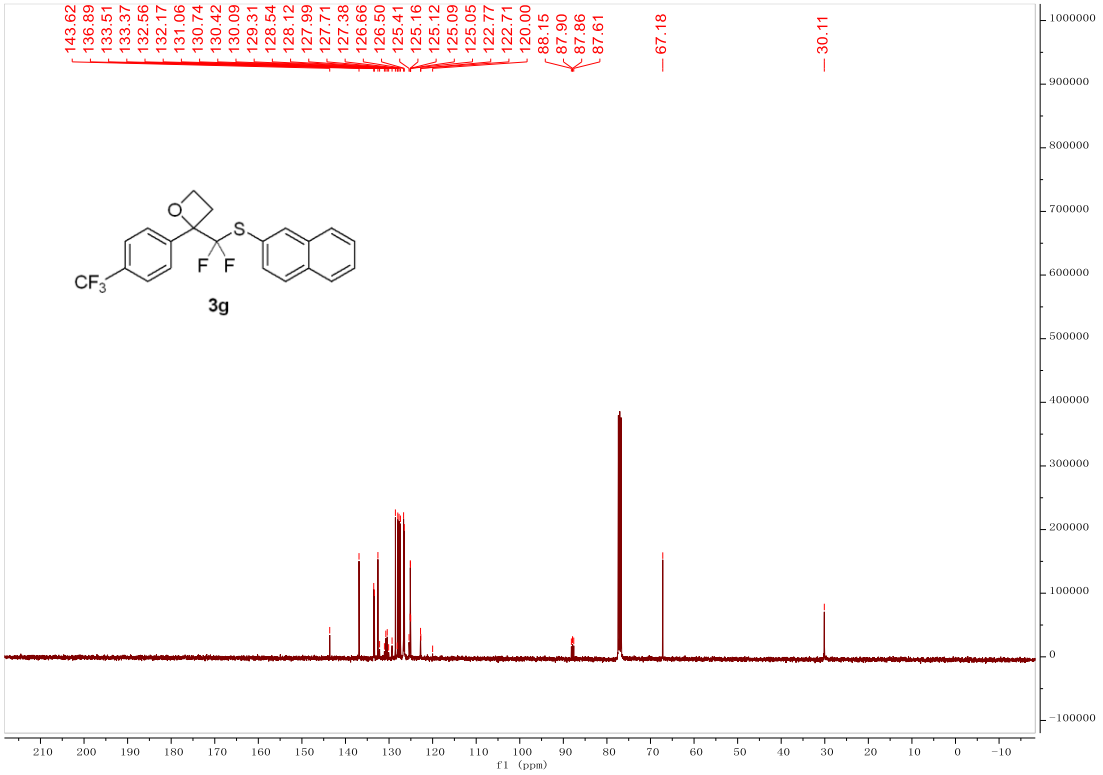


^{19}F NMR (376 MHz, DMSO-d_6) spectrum for 3f

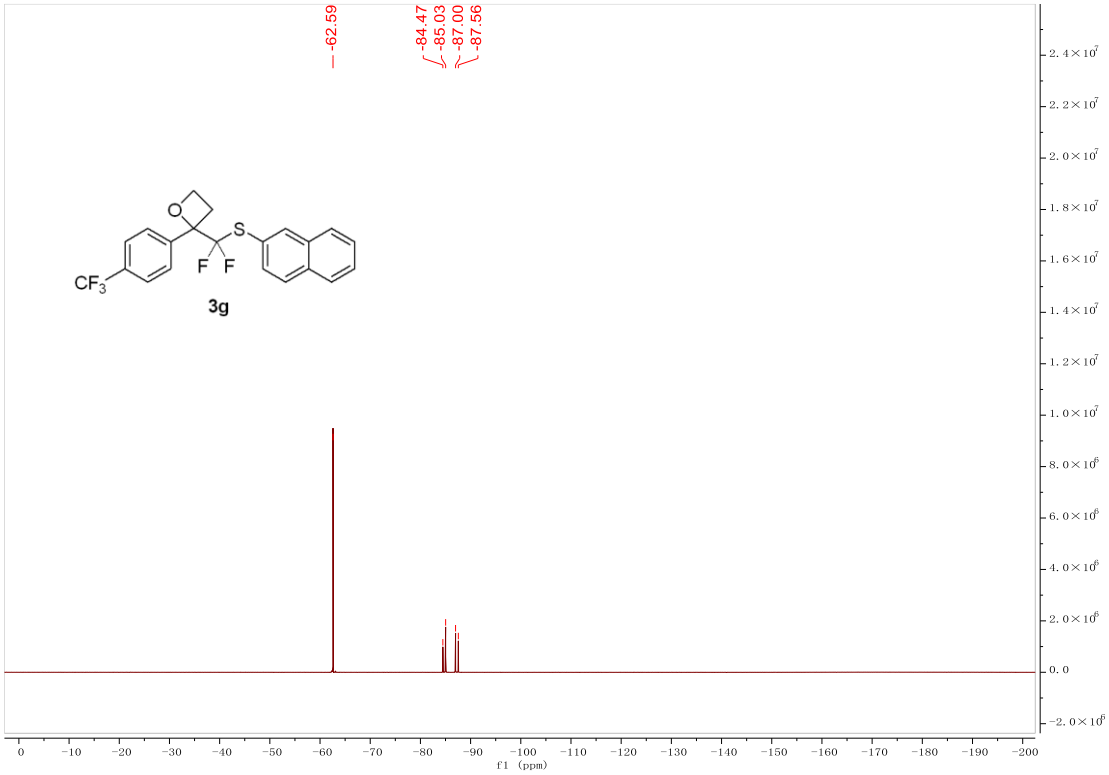
^{1}H NMR (400 MHz, $CDCl_3$) spectrum for 3g



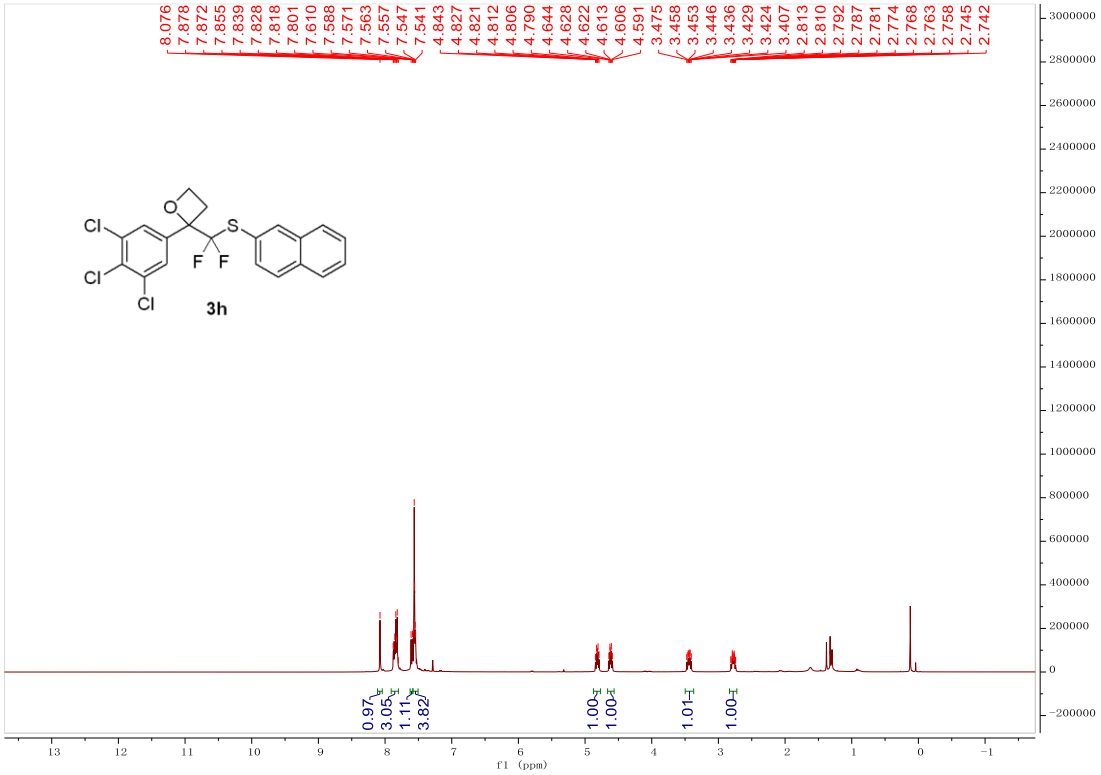
^{13}C NMR (101 MHz, $CDCl_3$) spectrum for 3g



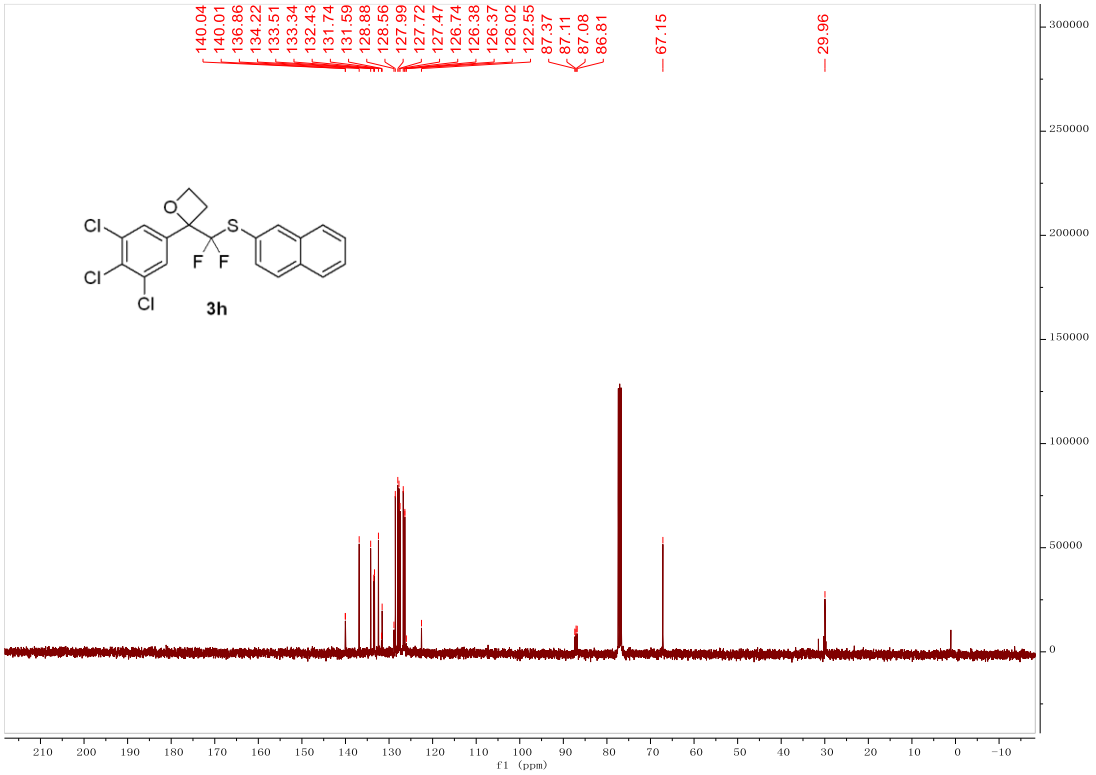
^{19}F NMR (376 MHz, $CDCl_3$) spectrum for 3g



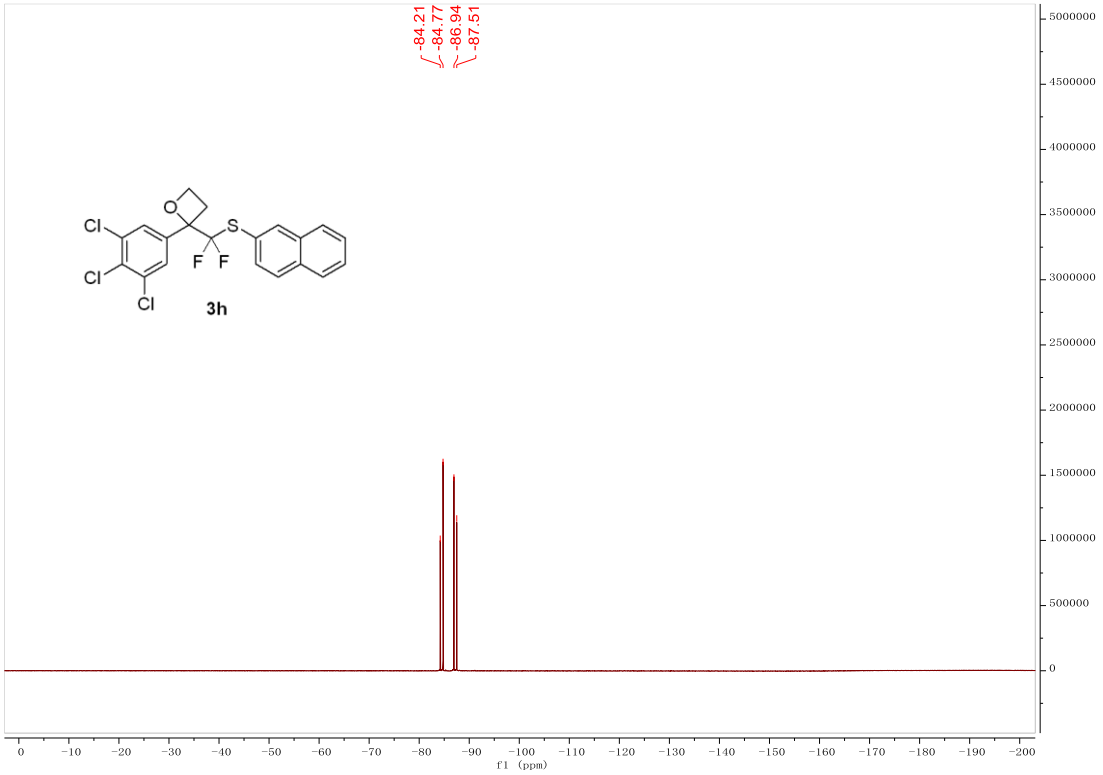
^{1}H NMR (400 MHz, $CDCl_3$) spectrum for 3h



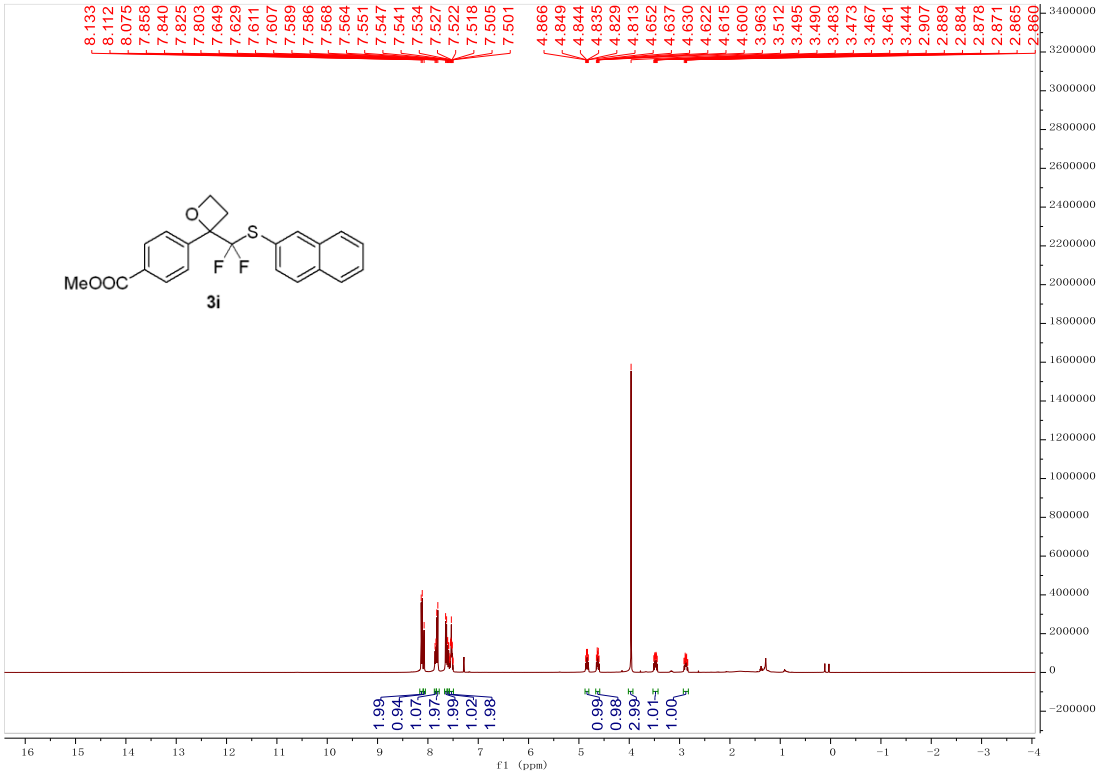
^{13}C NMR (101 MHz, $CDCl_3$) spectrum for 3h



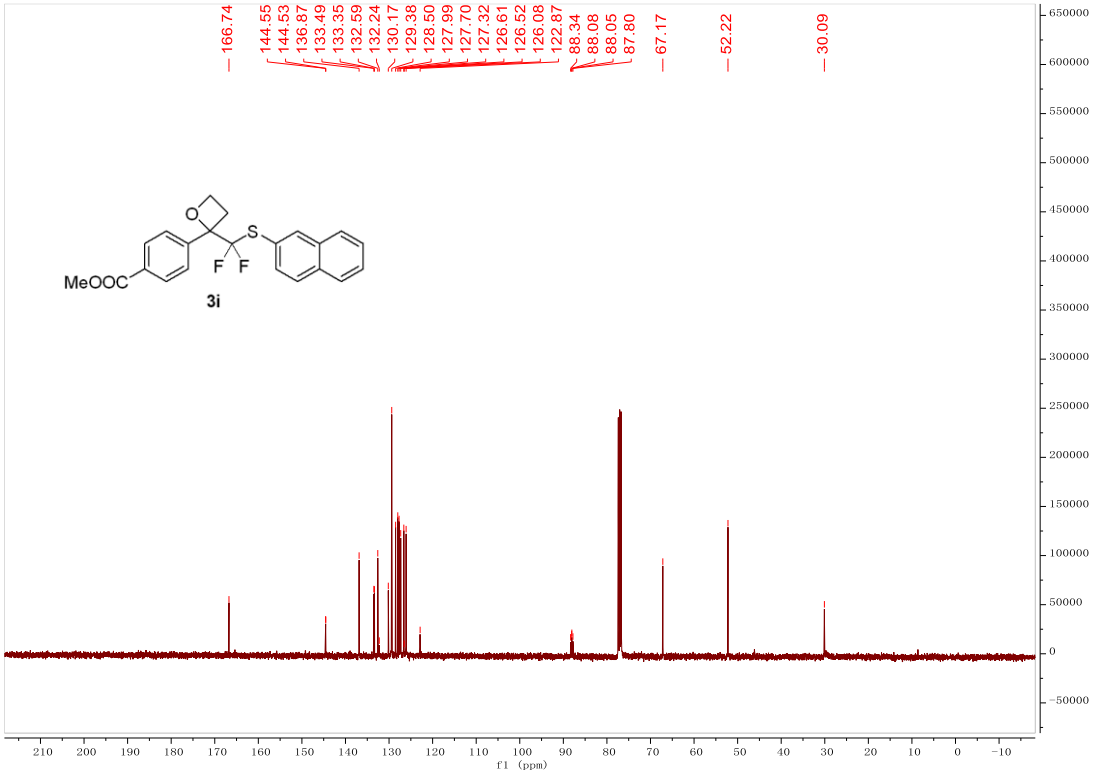
^{19}F NMR (376 MHz, $CDCl_3$) spectrum for 3h



^{1}H NMR (400 MHz, $CDCl_3$) spectrum for 3i

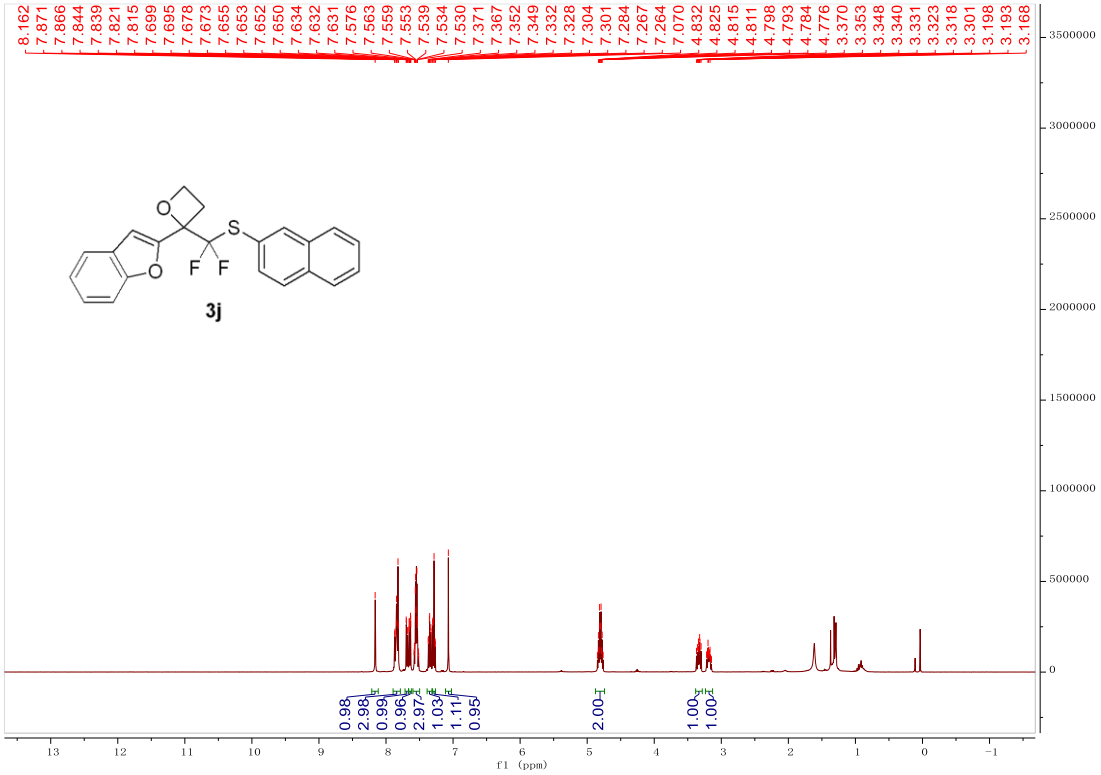


^{13}C NMR (101 MHz, $CDCl_3$) spectrum for 3i

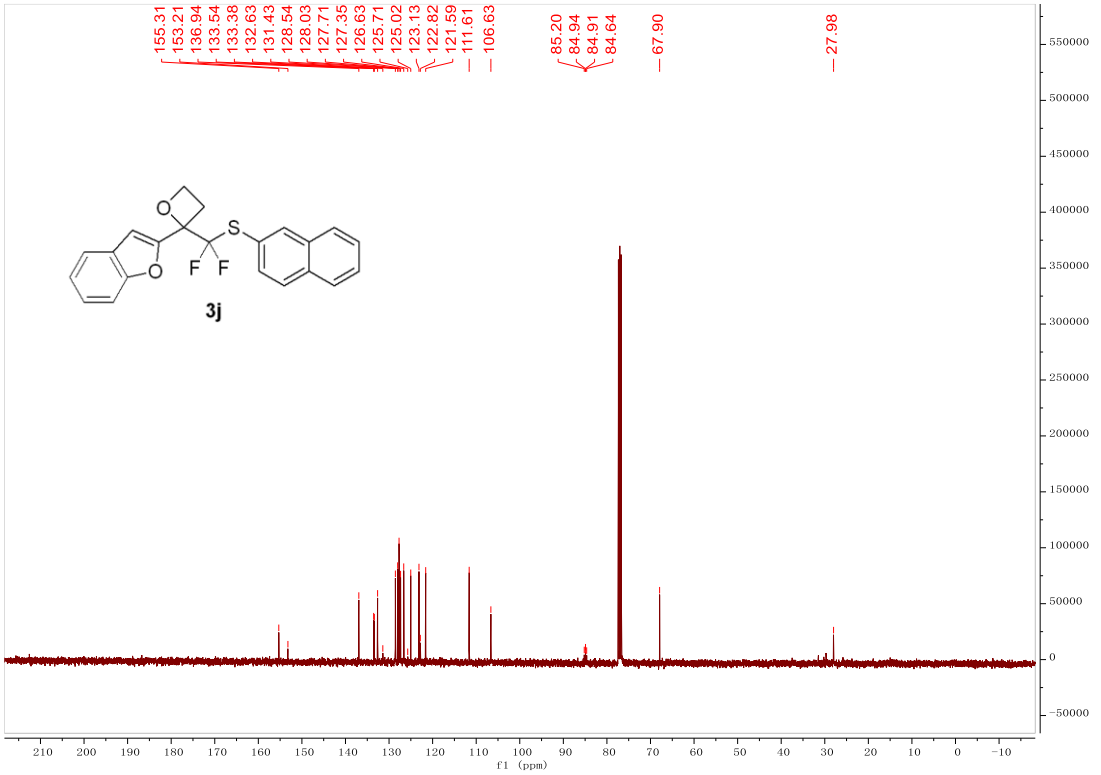


^{19}F NMR (376 MHz, $CDCl_3$) spectrum for 3i

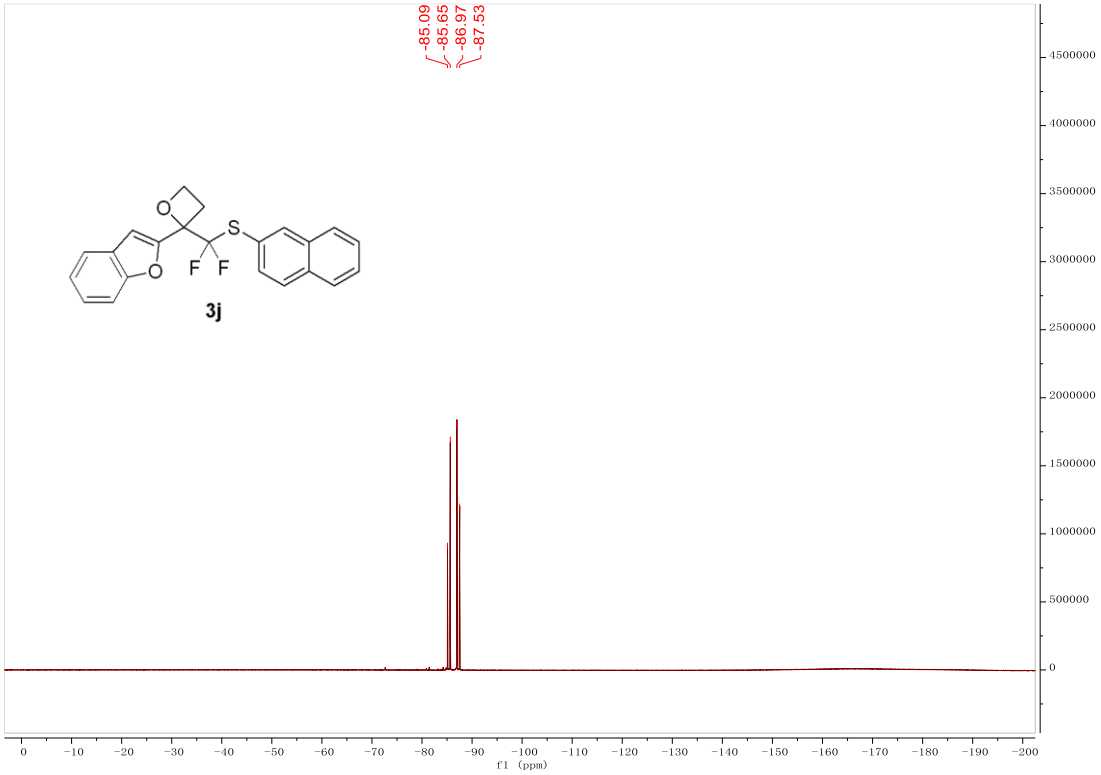
^{1}H NMR (400 MHz, $CDCl_3$) spectrum for 3j



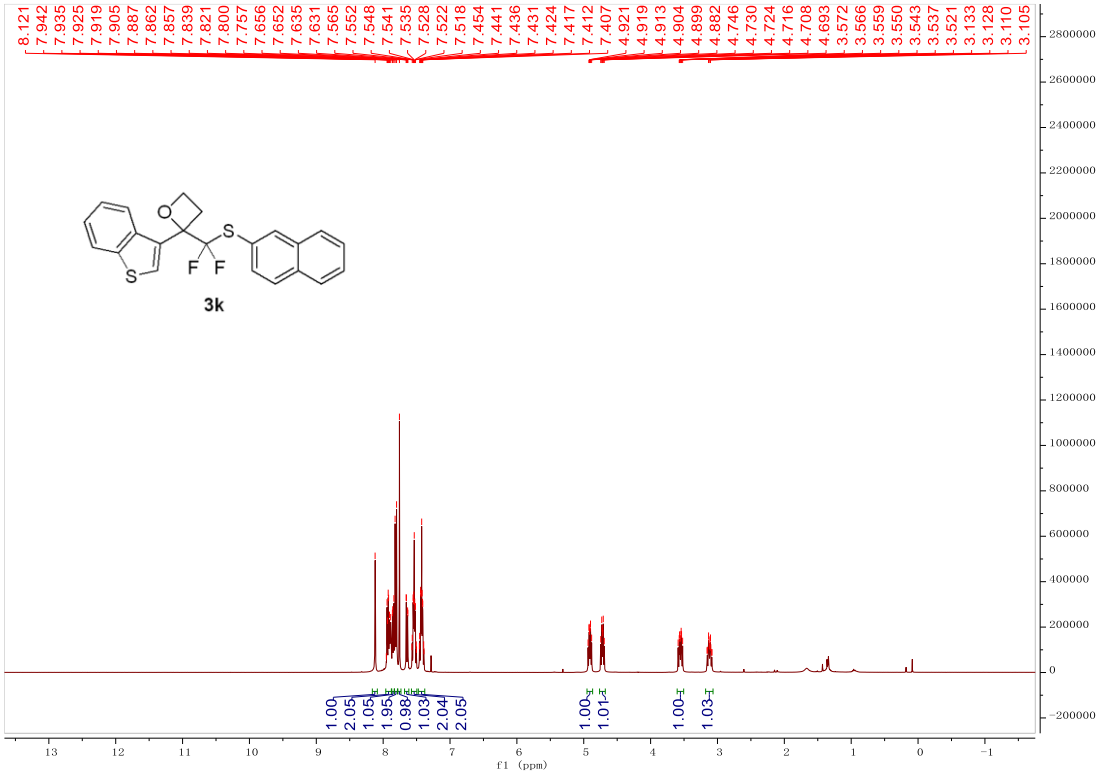
^{13}C NMR (101 MHz, $CDCl_3$) spectrum for 3j



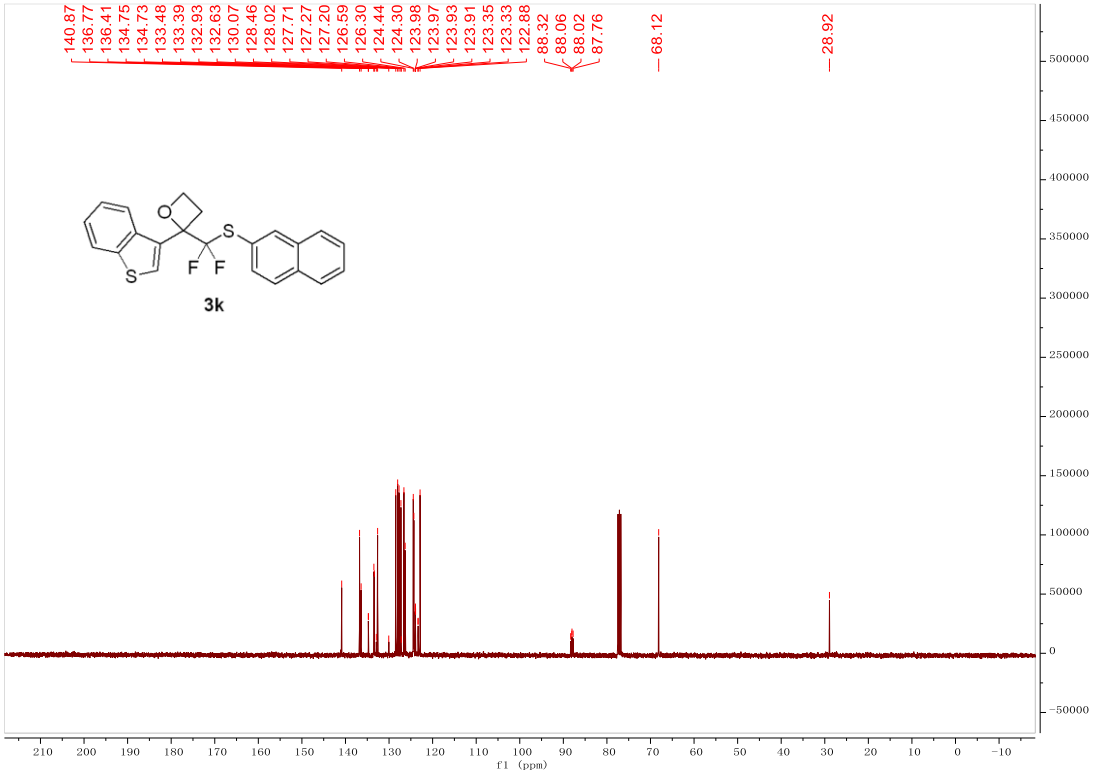
^{19}F NMR (376 MHz, $CDCl_3$) spectrum for 3j



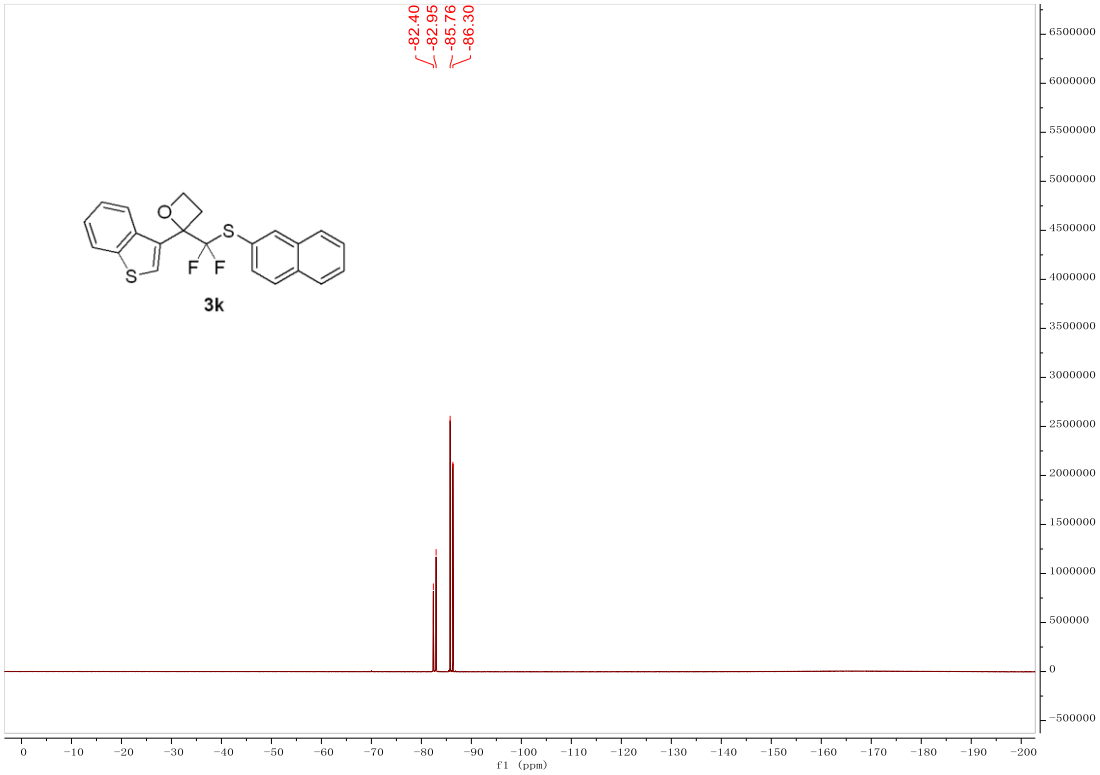
^{1}H NMR (400 MHz, $CDCl_3$) spectrum for 3k



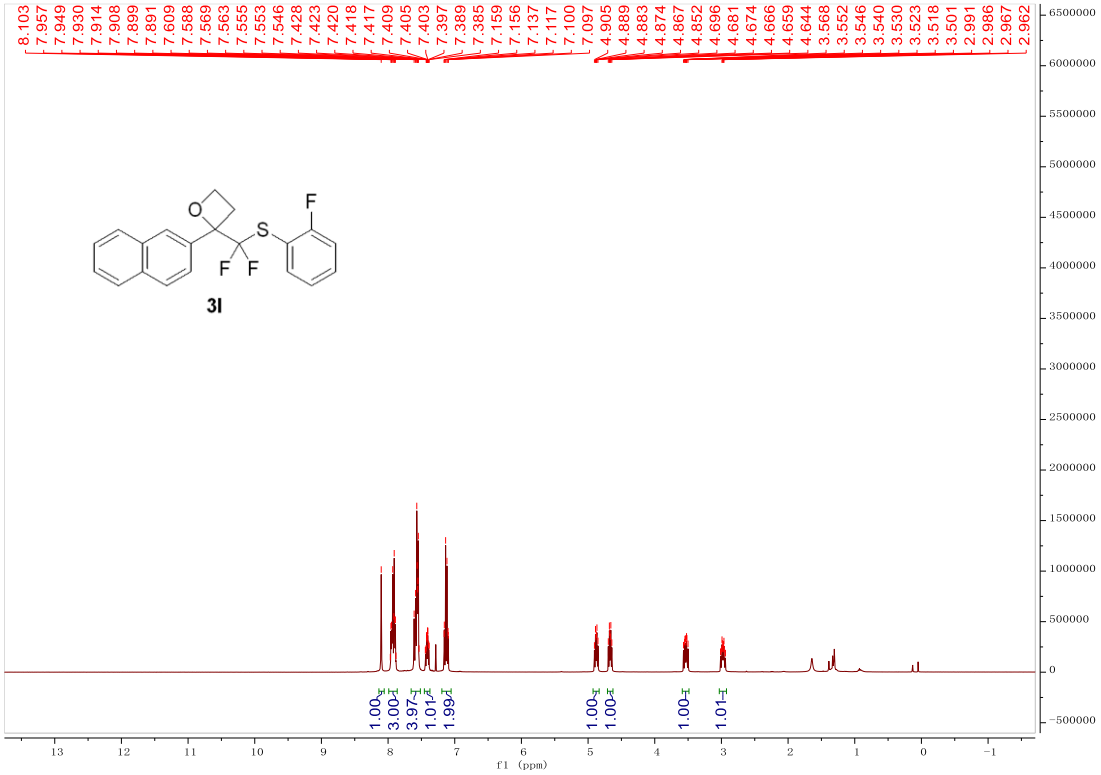
^{13}C NMR (101 MHz, $CDCl_3$) spectrum for 3k



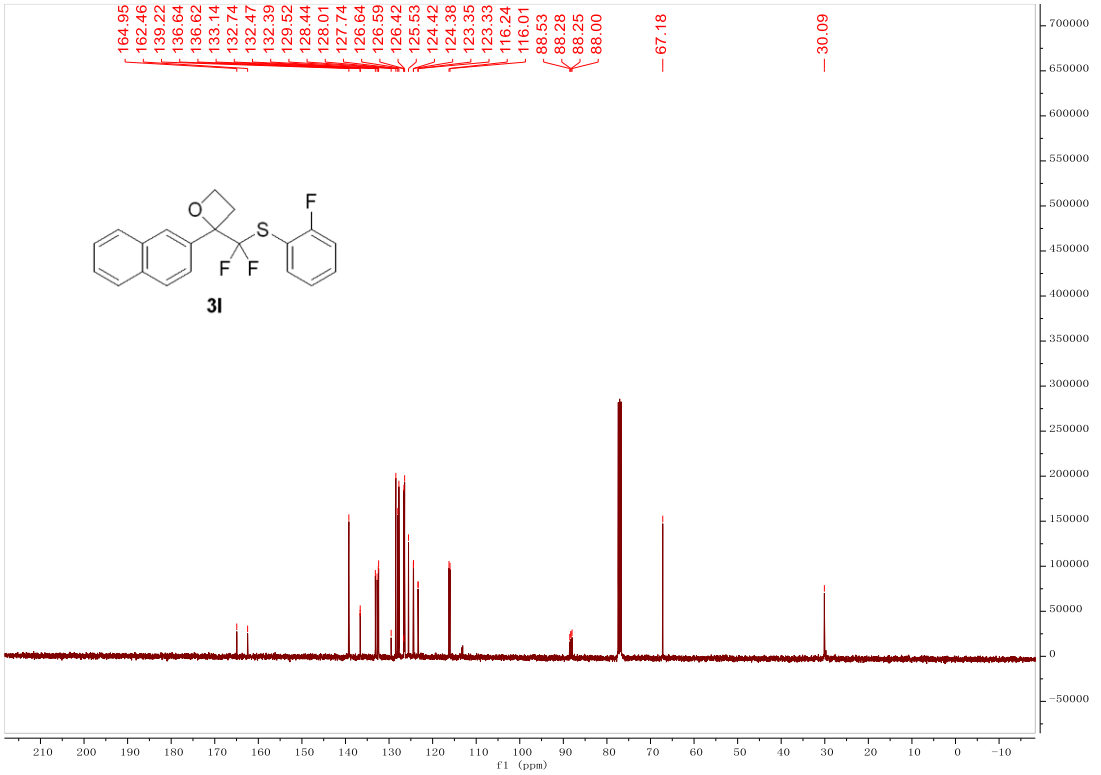
^{19}F NMR (376 MHz, $CDCl_3$) spectrum for 3k



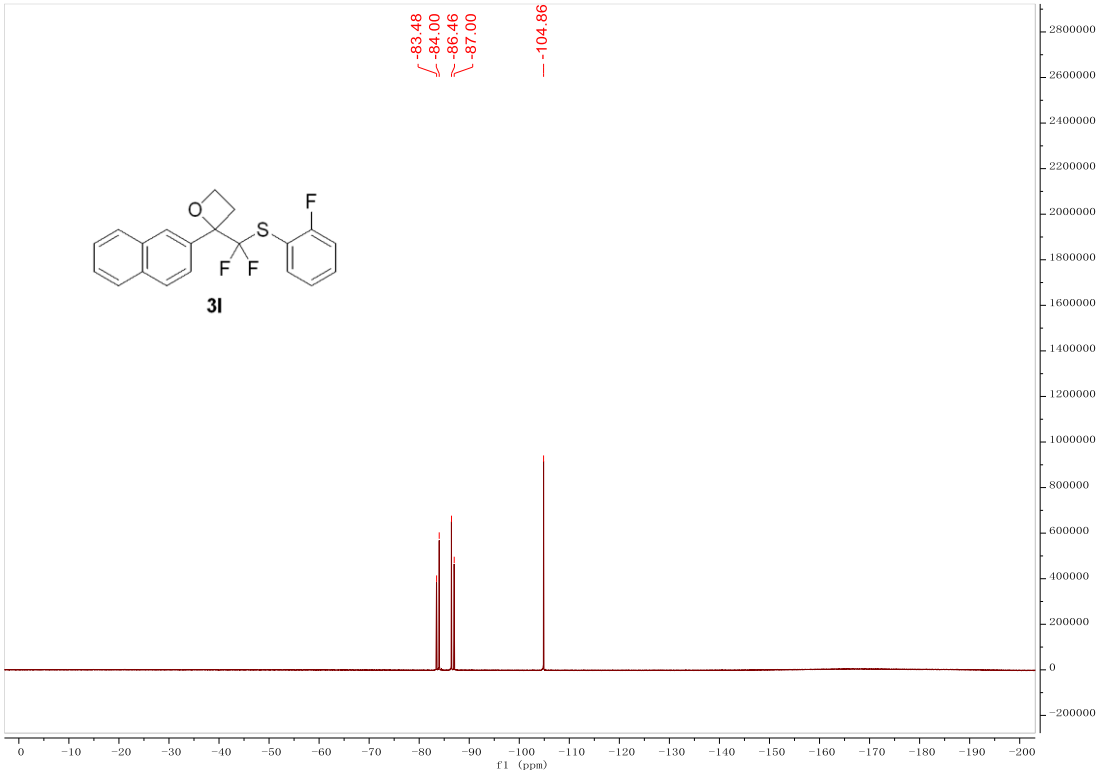
^{1}H NMR (400 MHz, $CDCl_3$) spectrum for 3l



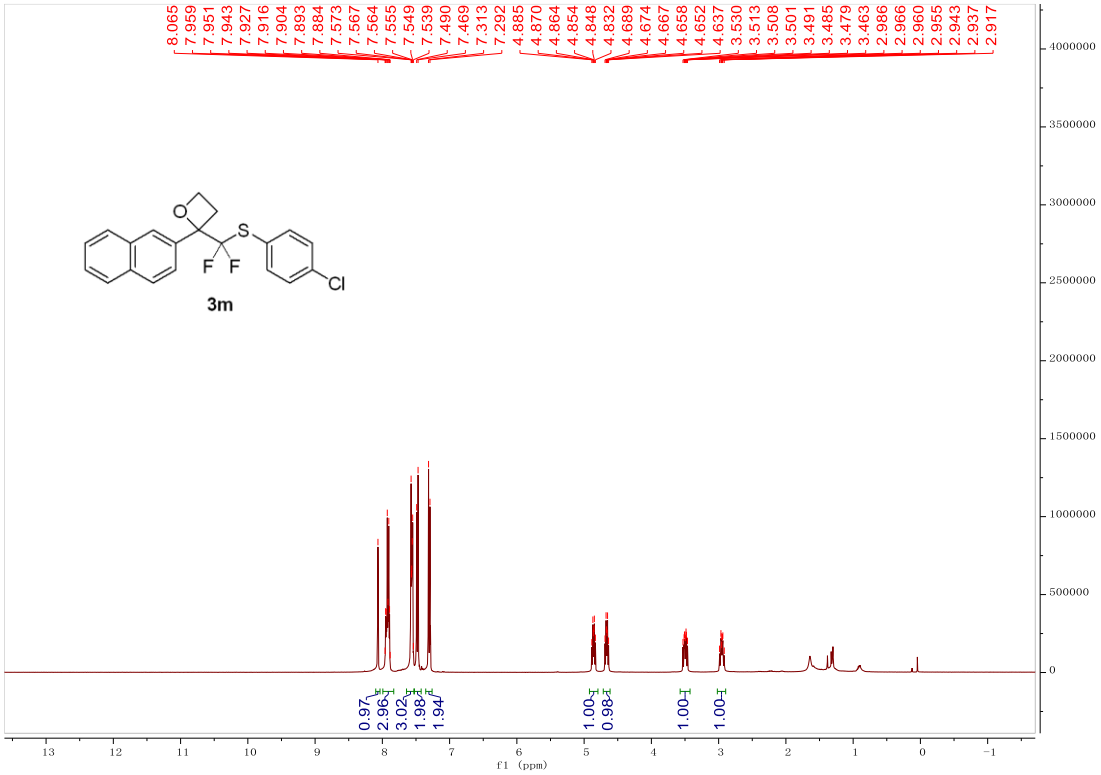
^{13}C NMR (101 MHz, $CDCl_3$) spectrum for 3l



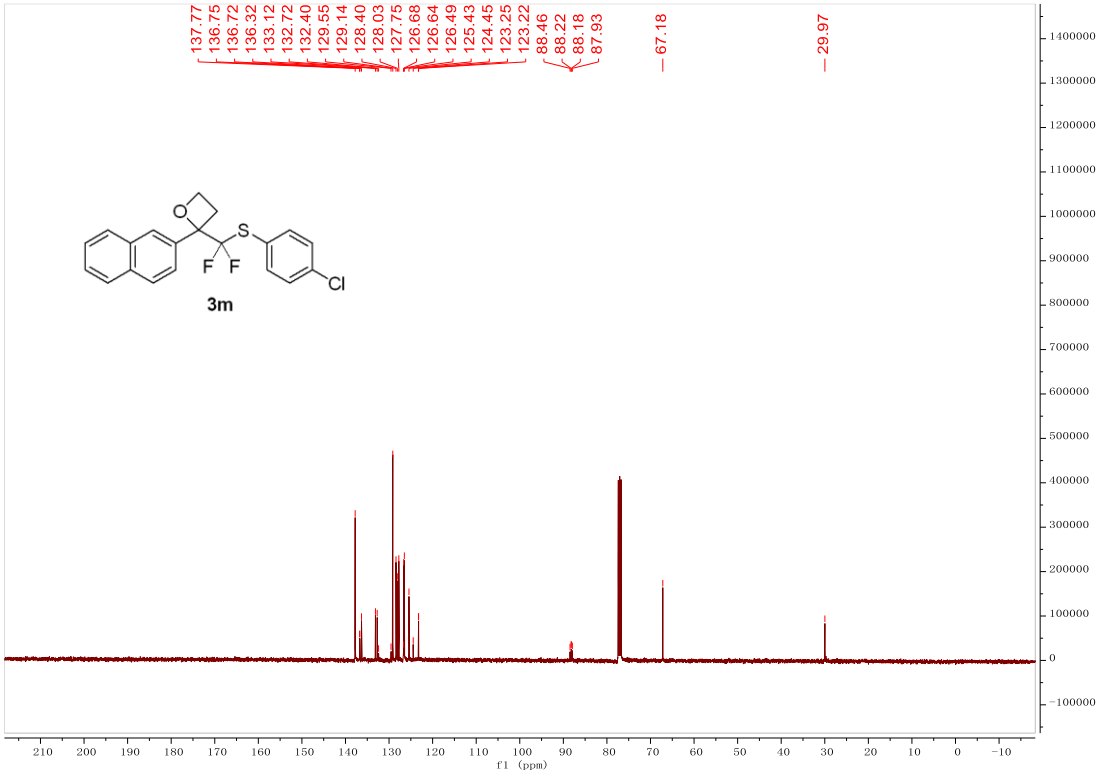
^{19}F NMR (376 MHz, $CDCl_3$) spectrum for 3l



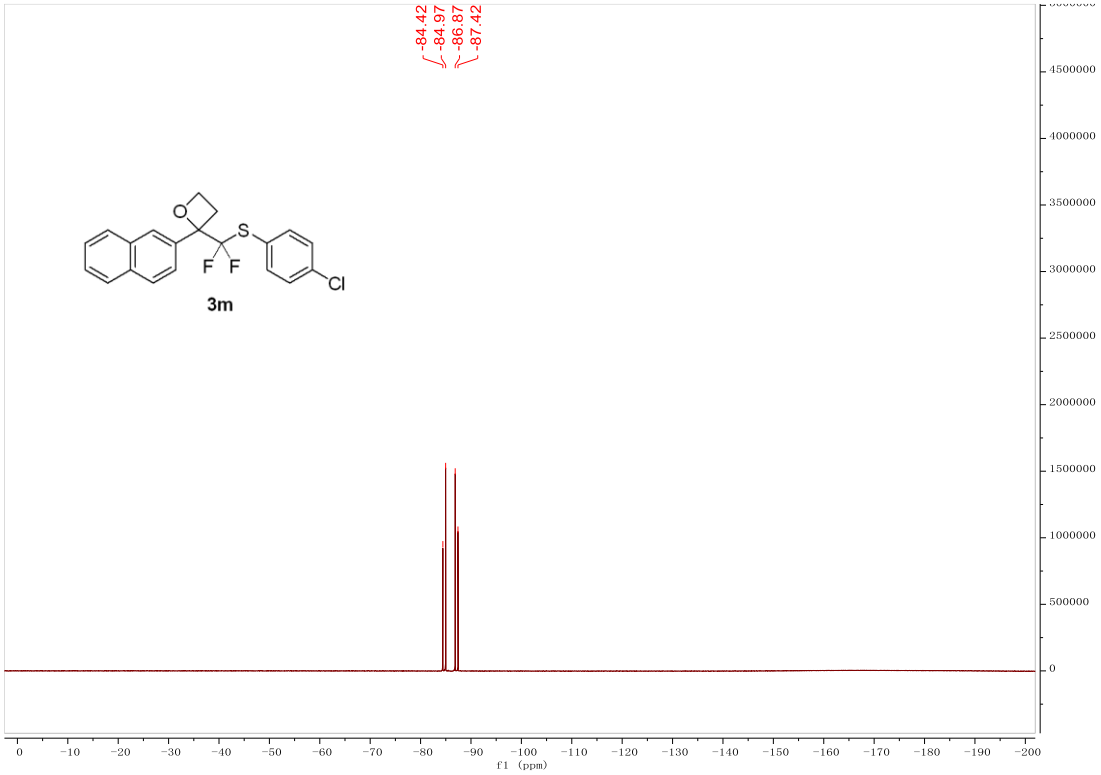
^{1}H NMR (400 MHz, $CDCl_3$) spectrum for 3m



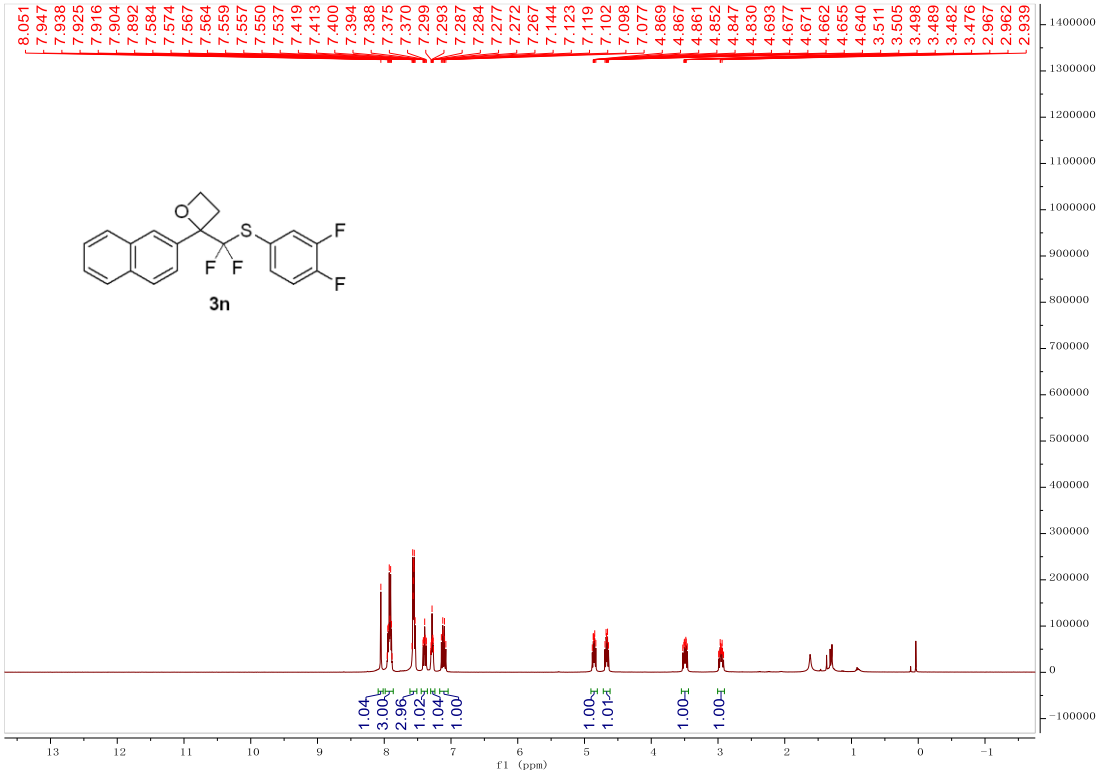
^{13}C NMR (101 MHz, $CDCl_3$) spectrum for 3m



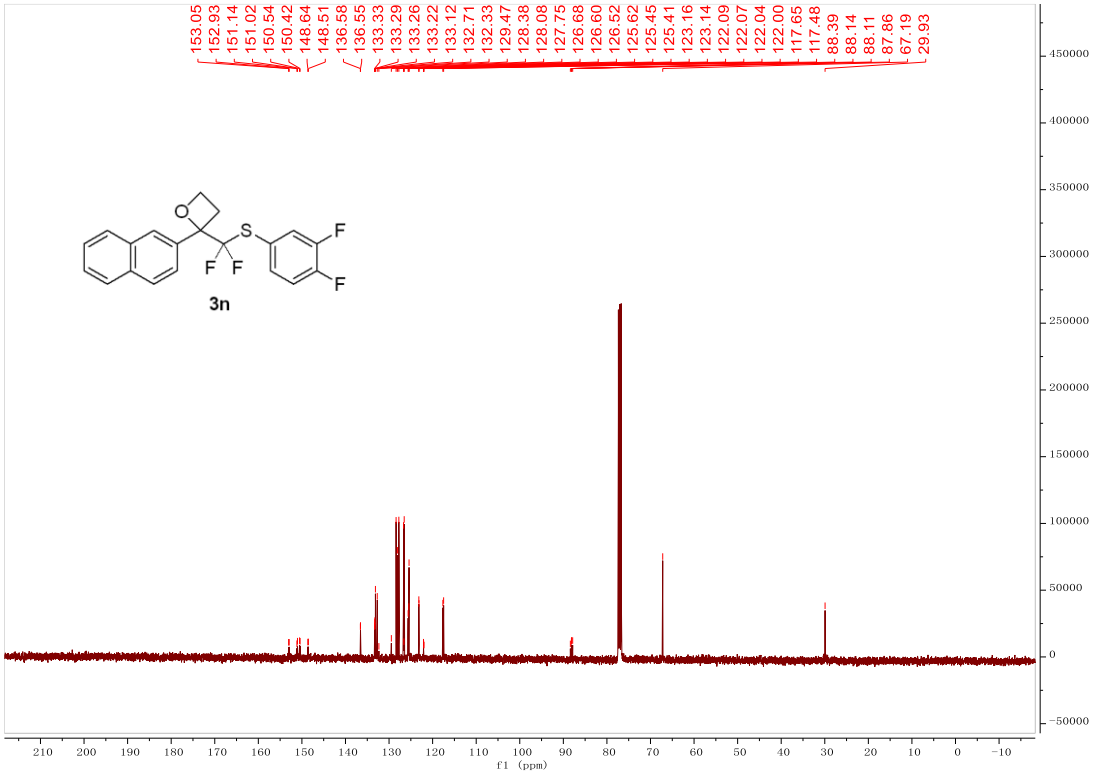
^{19}F NMR (376 MHz, $CDCl_3$) spectrum for 3m



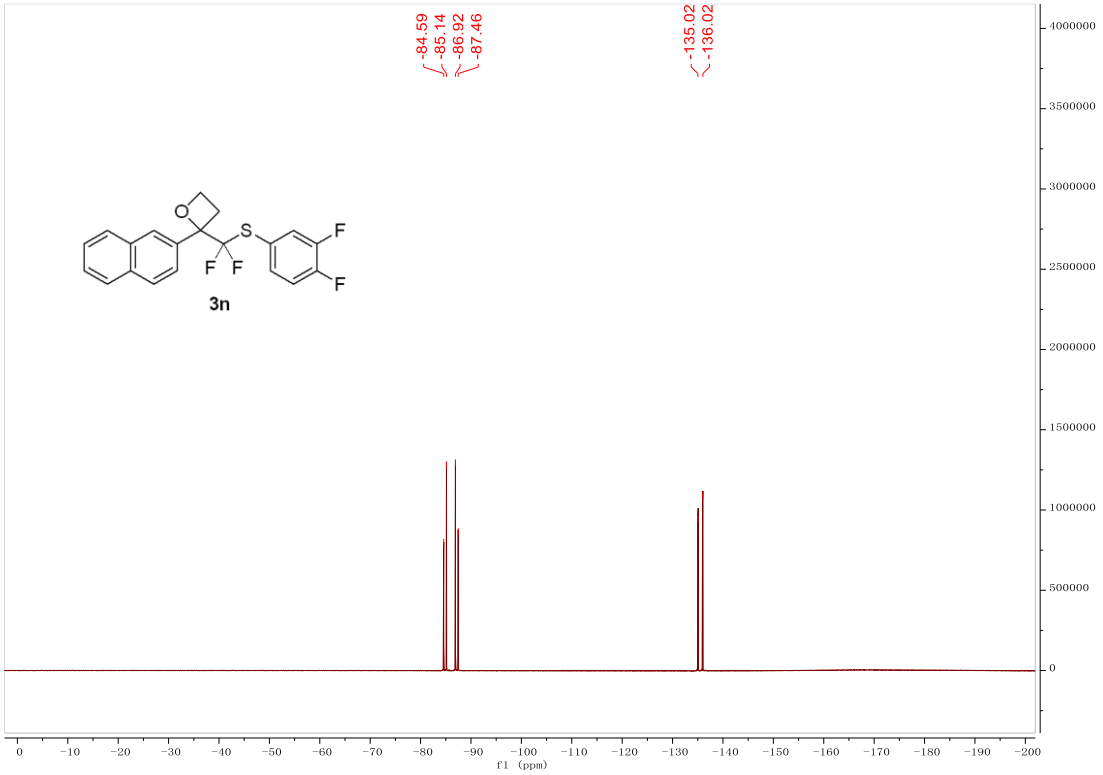
^{1}H NMR (400 MHz, $CDCl_3$) spectrum for 3n



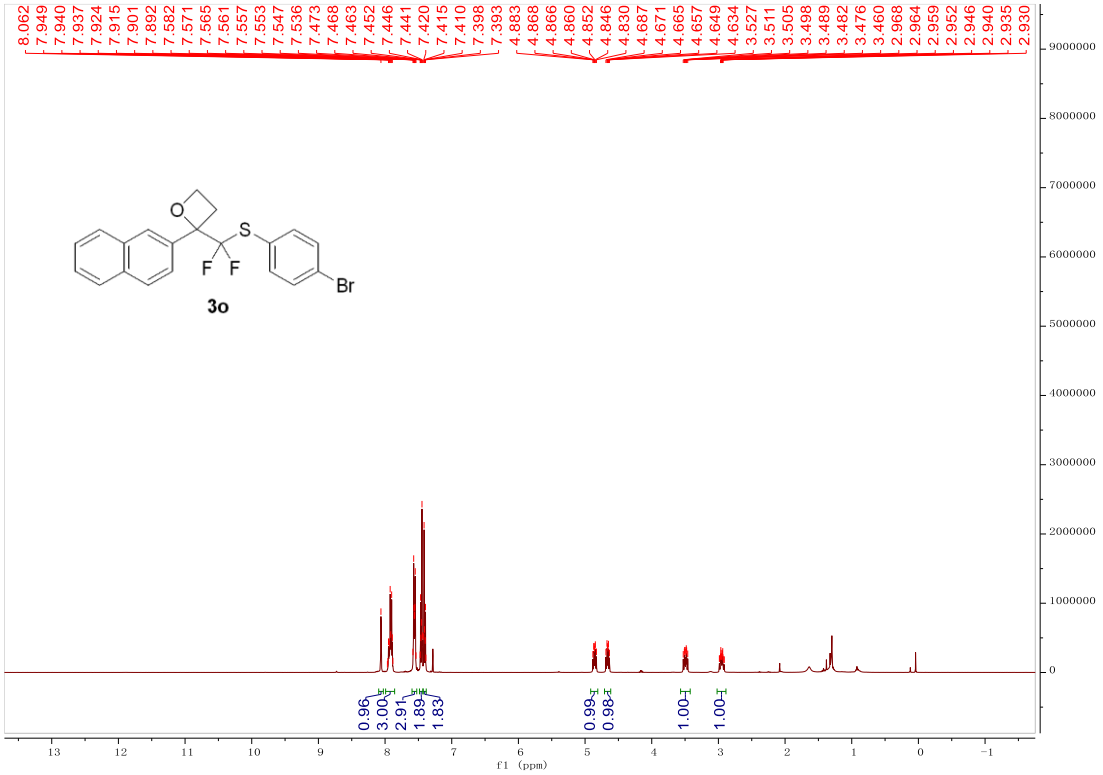
^{13}C NMR (101 MHz, $CDCl_3$) spectrum for 3n



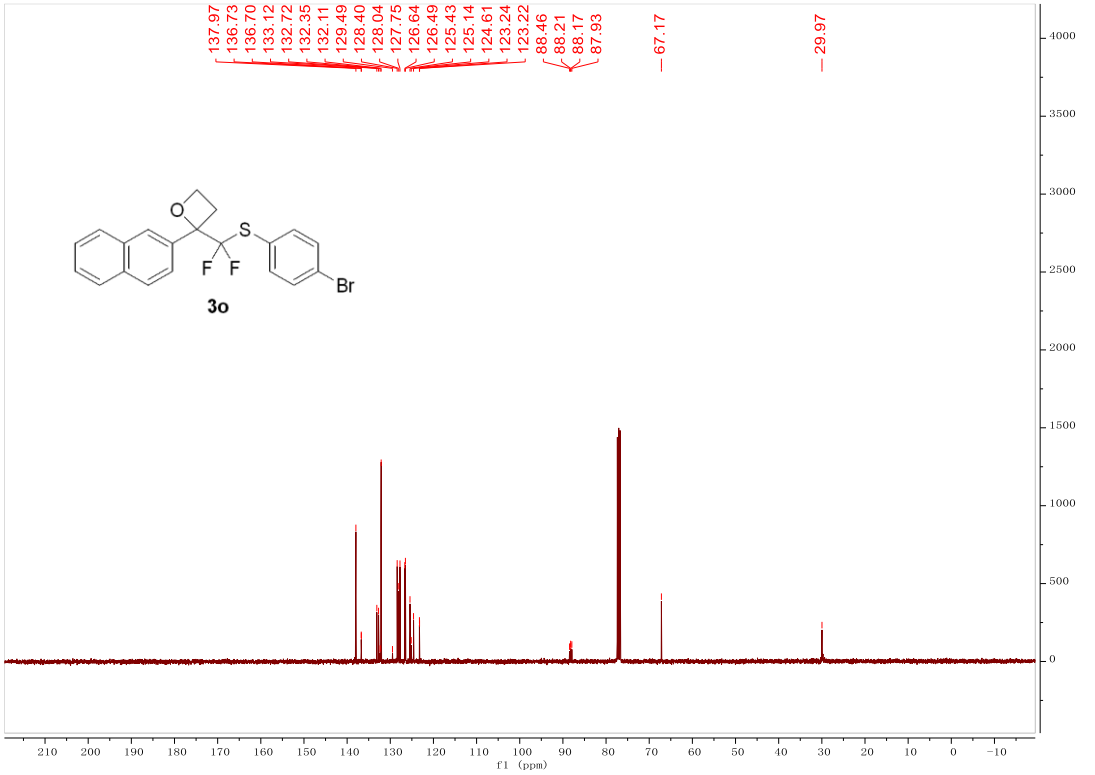
^{19}F NMR (376 MHz, $CDCl_3$) spectrum for 3n



^{1}H NMR (400 MHz, $CDCl_3$) spectrum for 3o

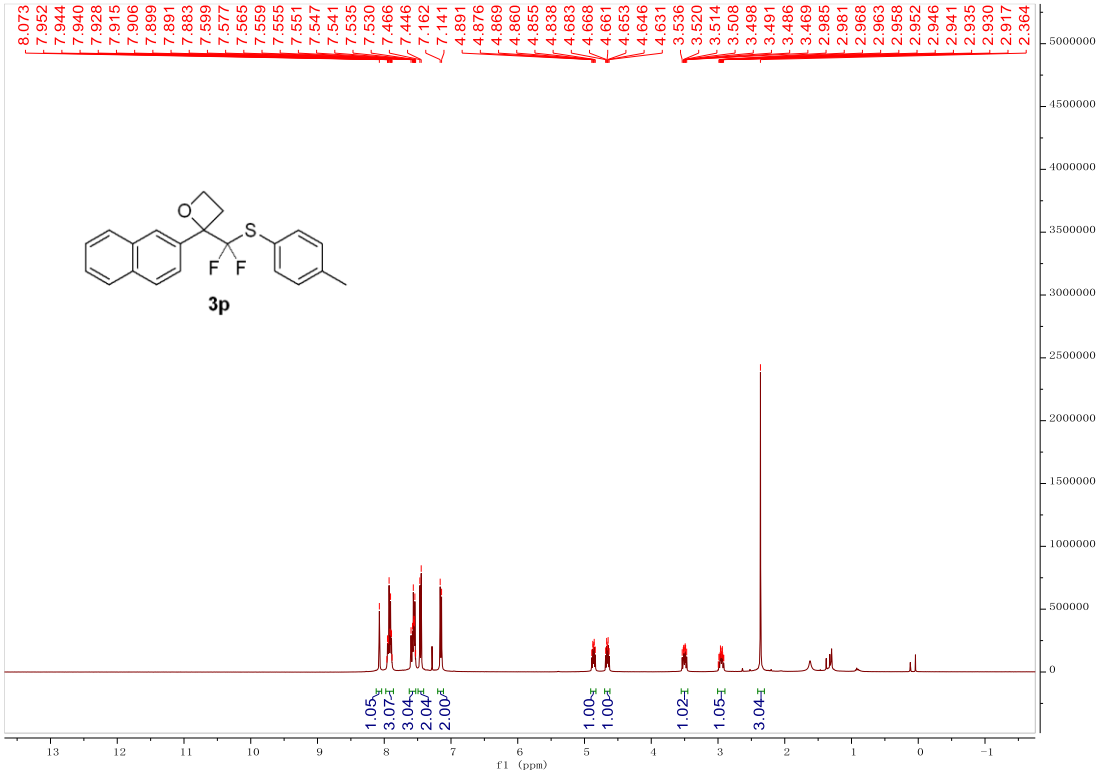


^{13}C NMR (101 MHz, $CDCl_3$) spectrum for 3o

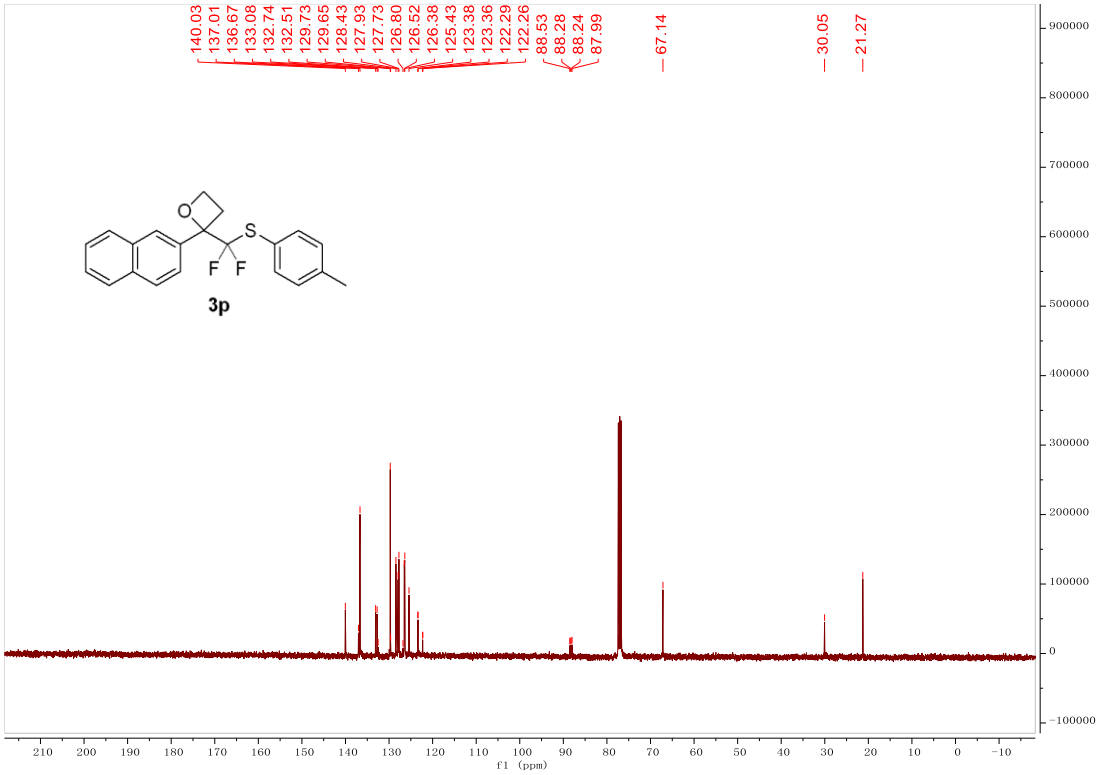


^{19}F NMR (376MHz, $CDCl_3$) spectrum for 3o

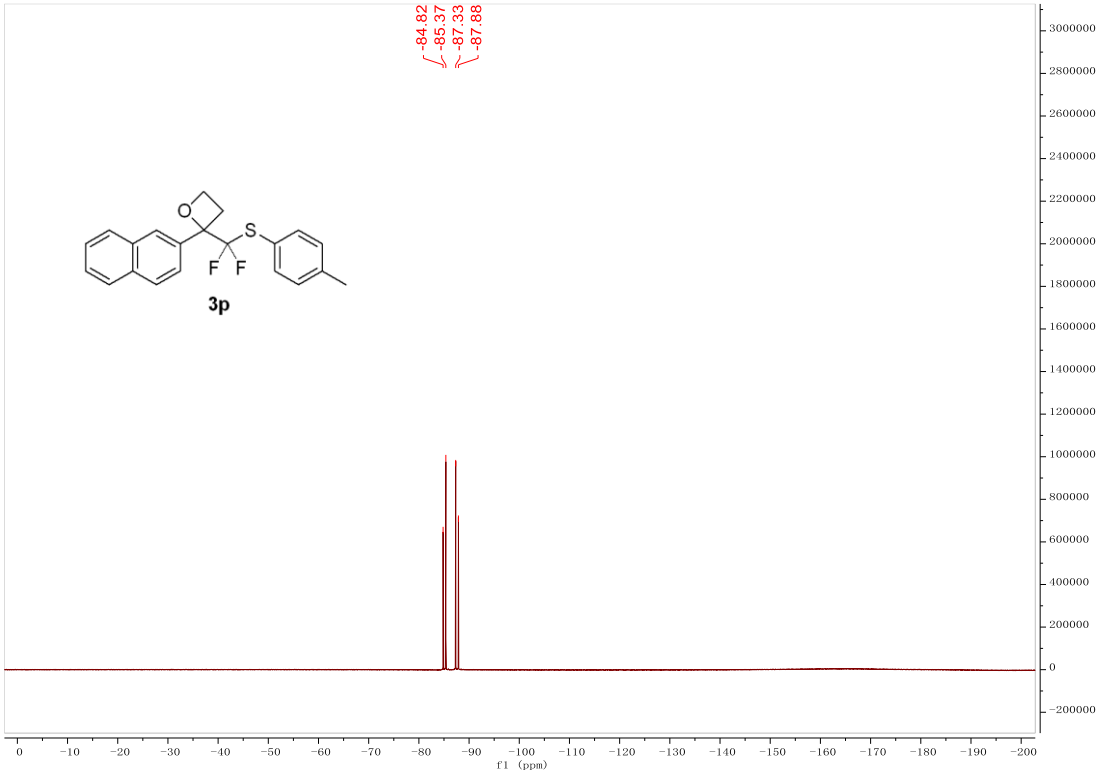
^{1}H NMR (400 MHz, $CDCl_3$) spectrum for 3p



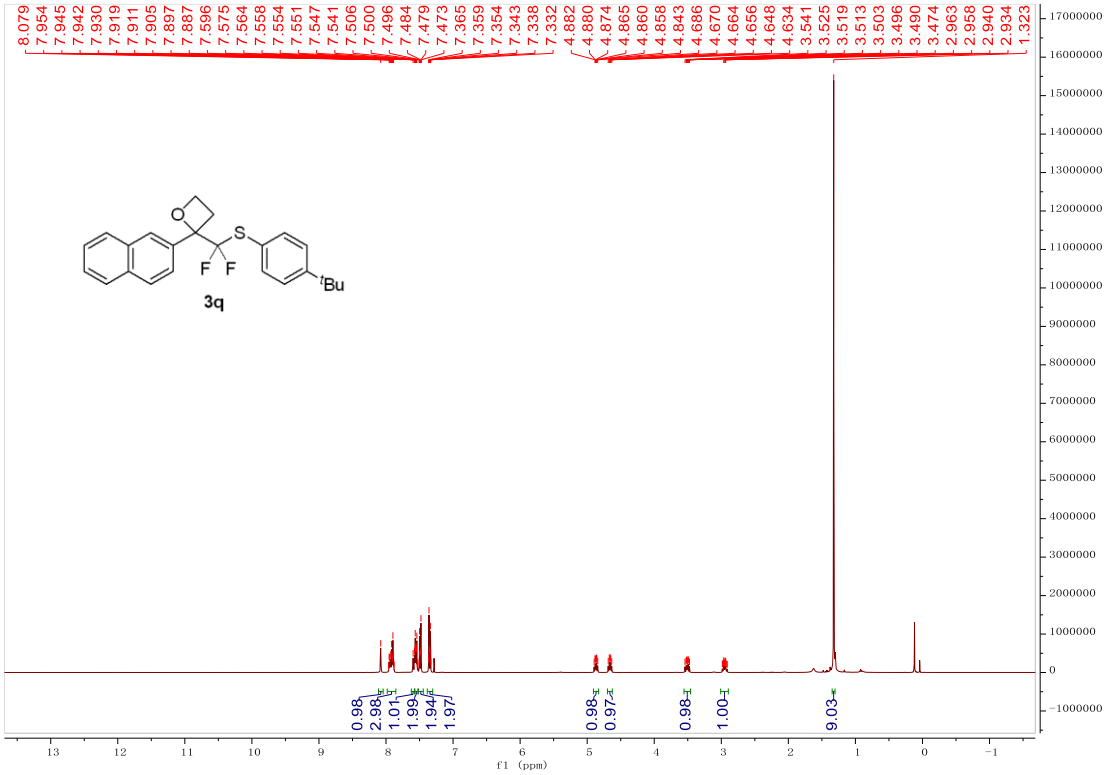
^{13}C NMR (101 MHz, $CDCl_3$) spectrum for 3p



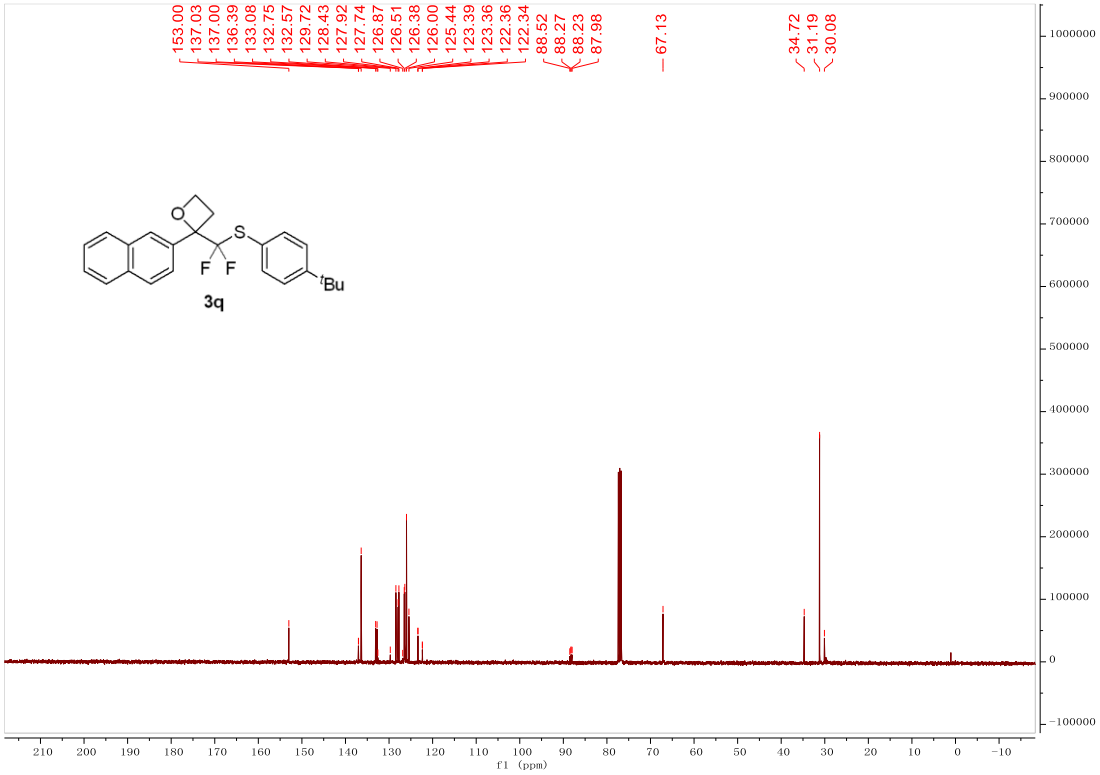
^{19}F NMR (376 MHz, $CDCl_3$) spectrum for 3p



^{1}H NMR (400 MHz, $CDCl_3$) spectrum for 3q

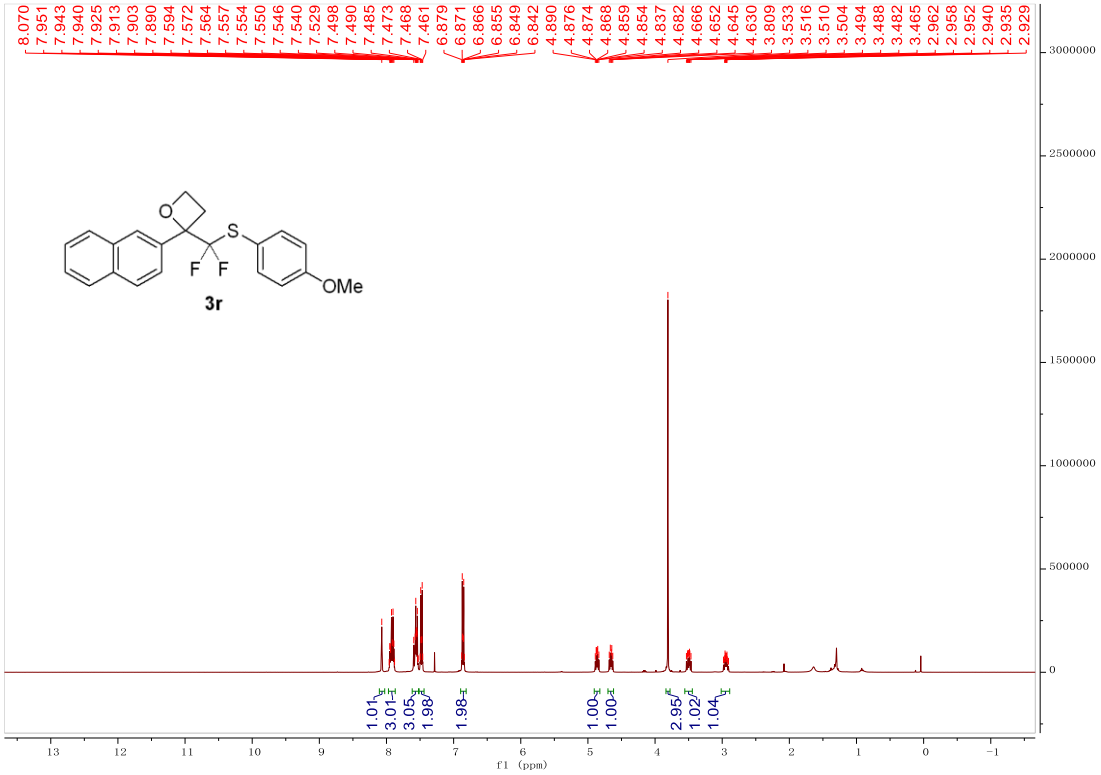


^{13}C NMR (101 MHz, $CDCl_3$) spectrum for 3q

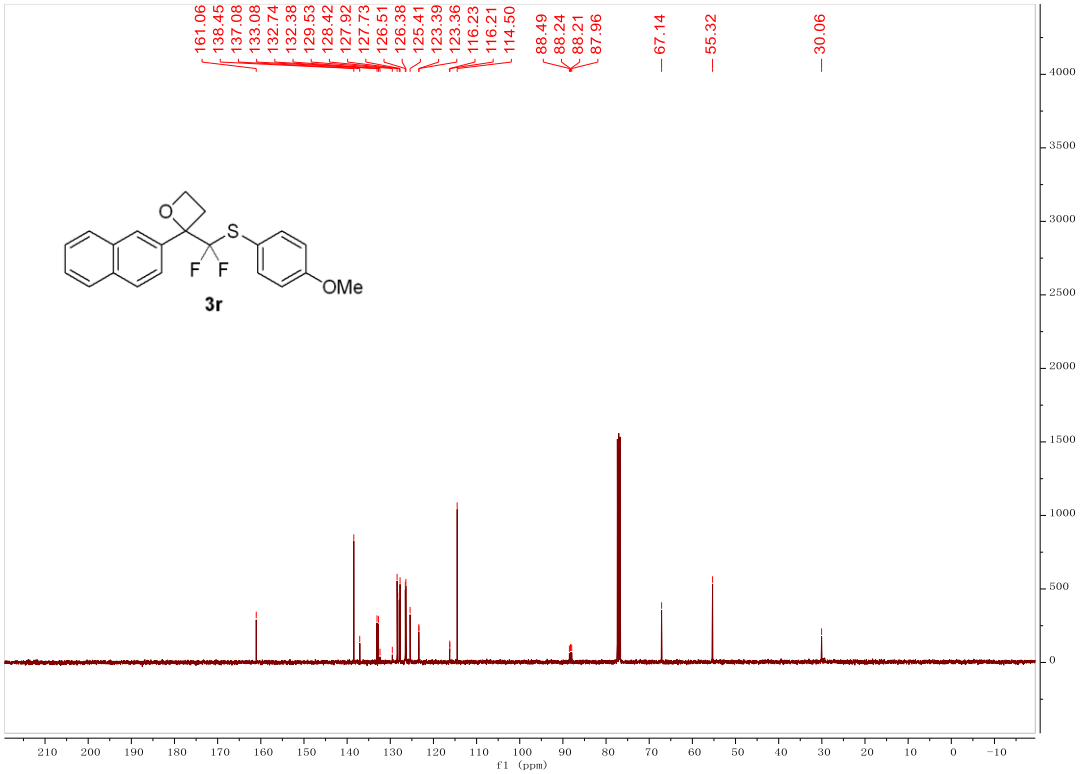


^{19}F NMR (376 MHz, $CDCl_3$) spectrum for 3q

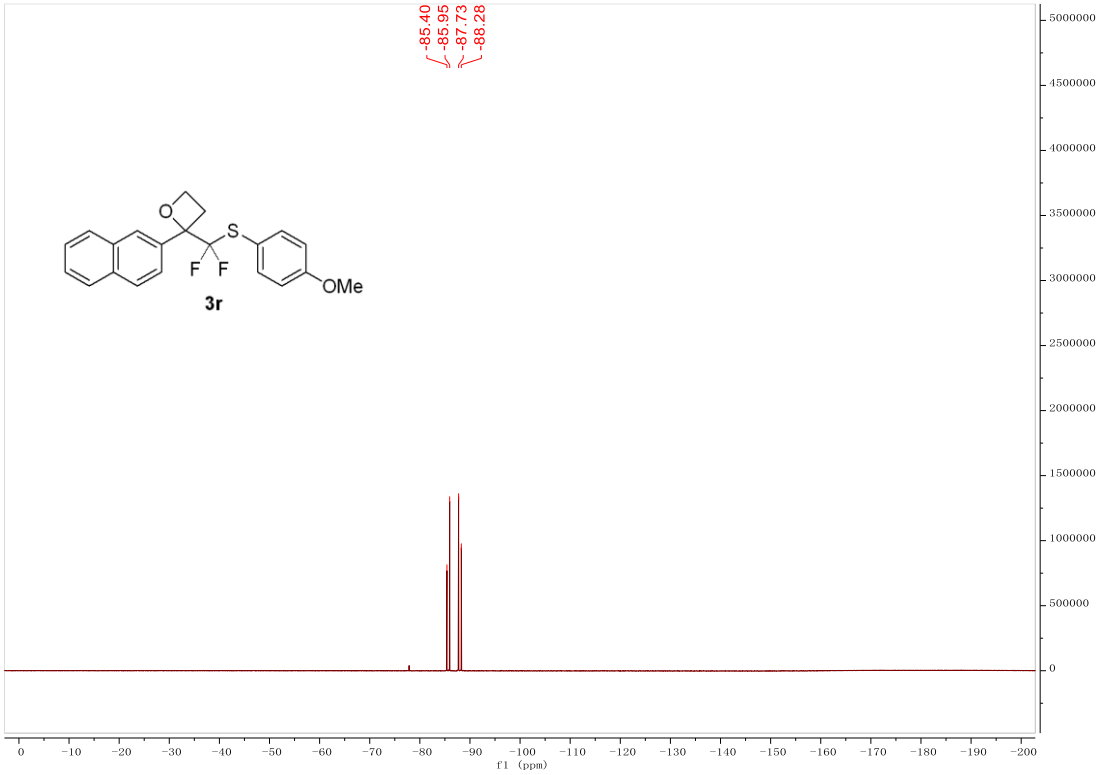
^{1}H NMR (400 MHz, $CDCl_3$) spectrum for 3r



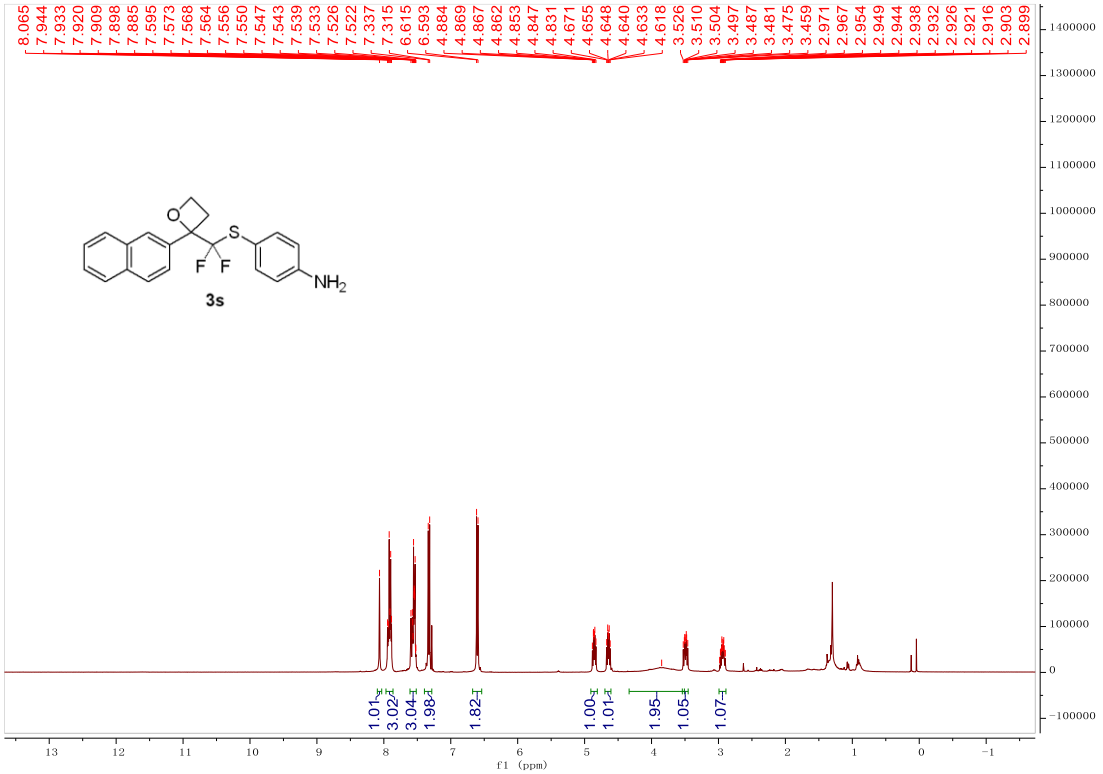
^{13}C NMR (101 MHz, $CDCl_3$) spectrum for 3r



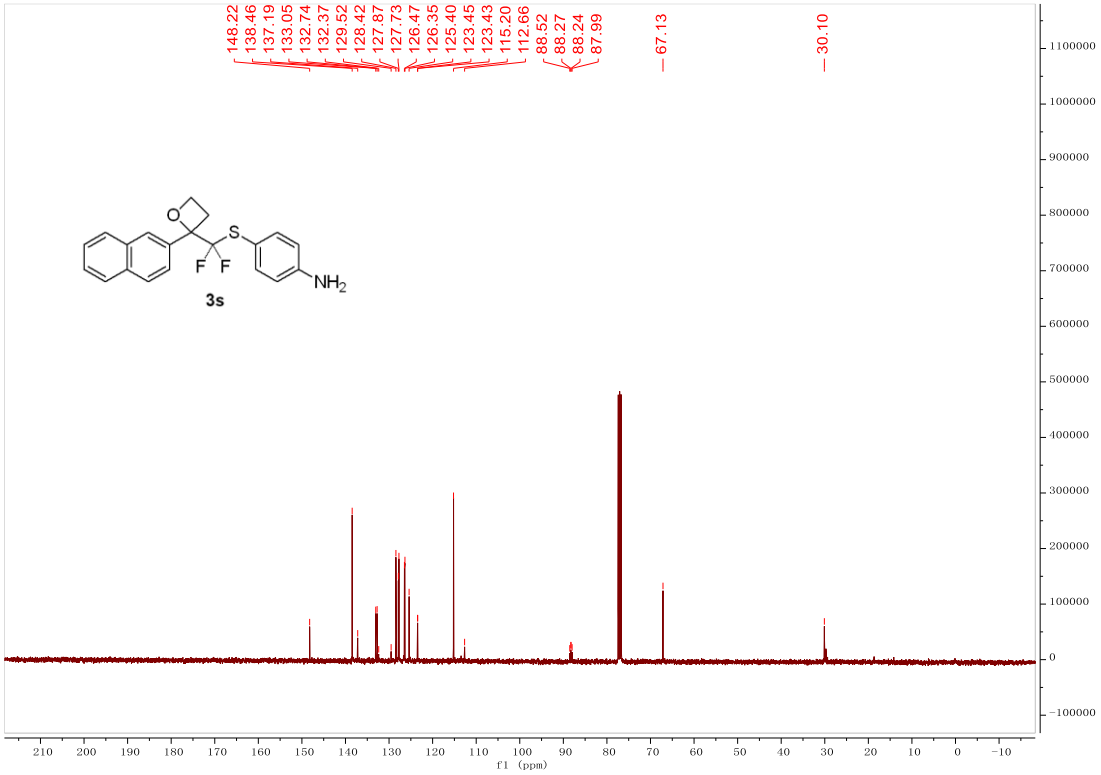
^{19}F NMR (376 MHz, $CDCl_3$) spectrum for 3r



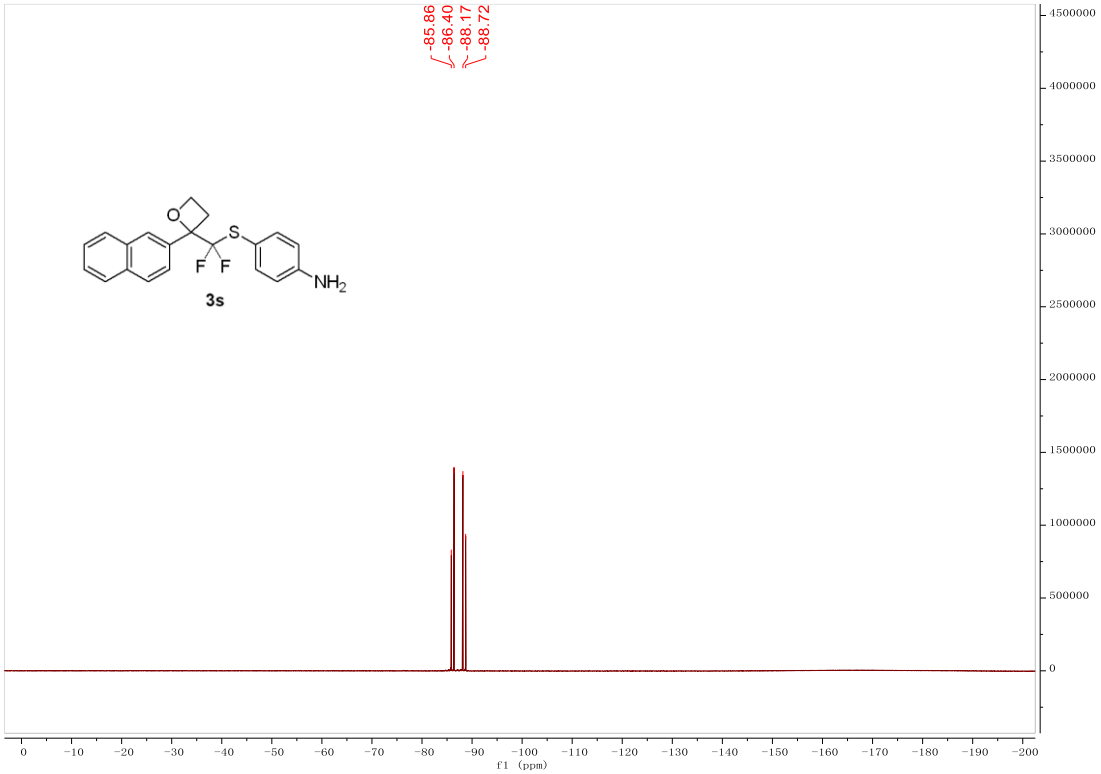
^{1}H NMR (400 MHz, $CDCl_3$) spectrum for 3s



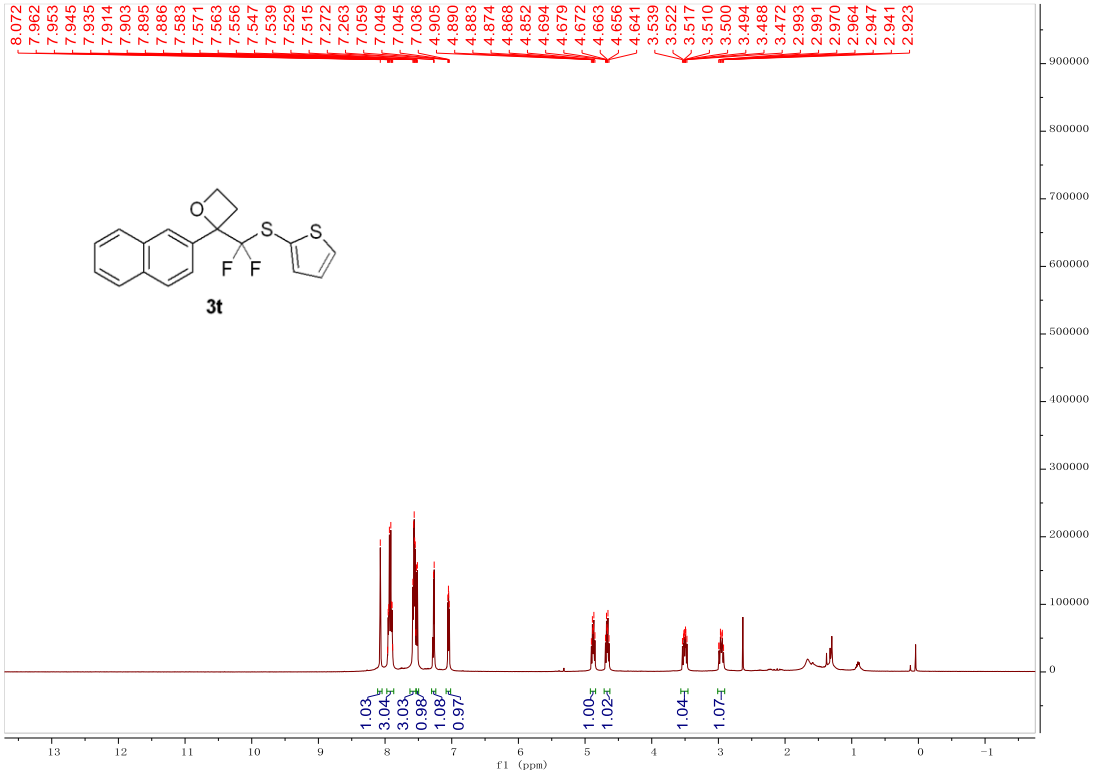
^{13}C NMR (101 MHz, $CDCl_3$) spectrum for 3s



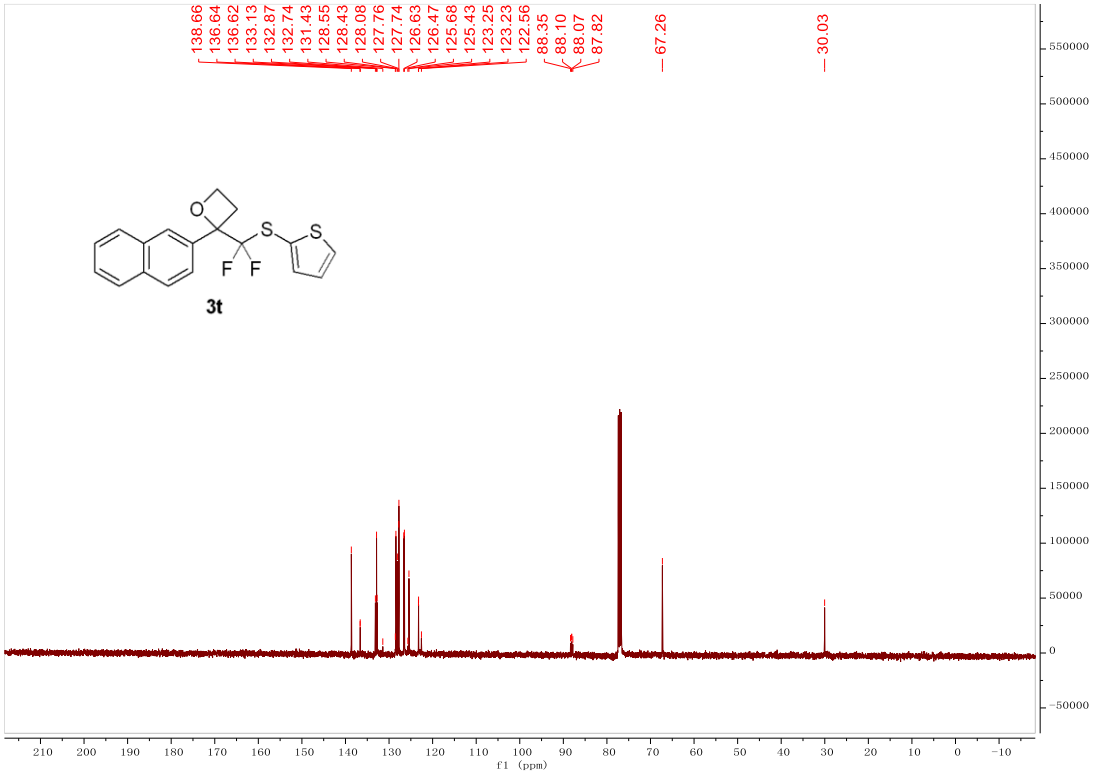
^{19}F NMR (376 MHz, $CDCl_3$) spectrum for 3s



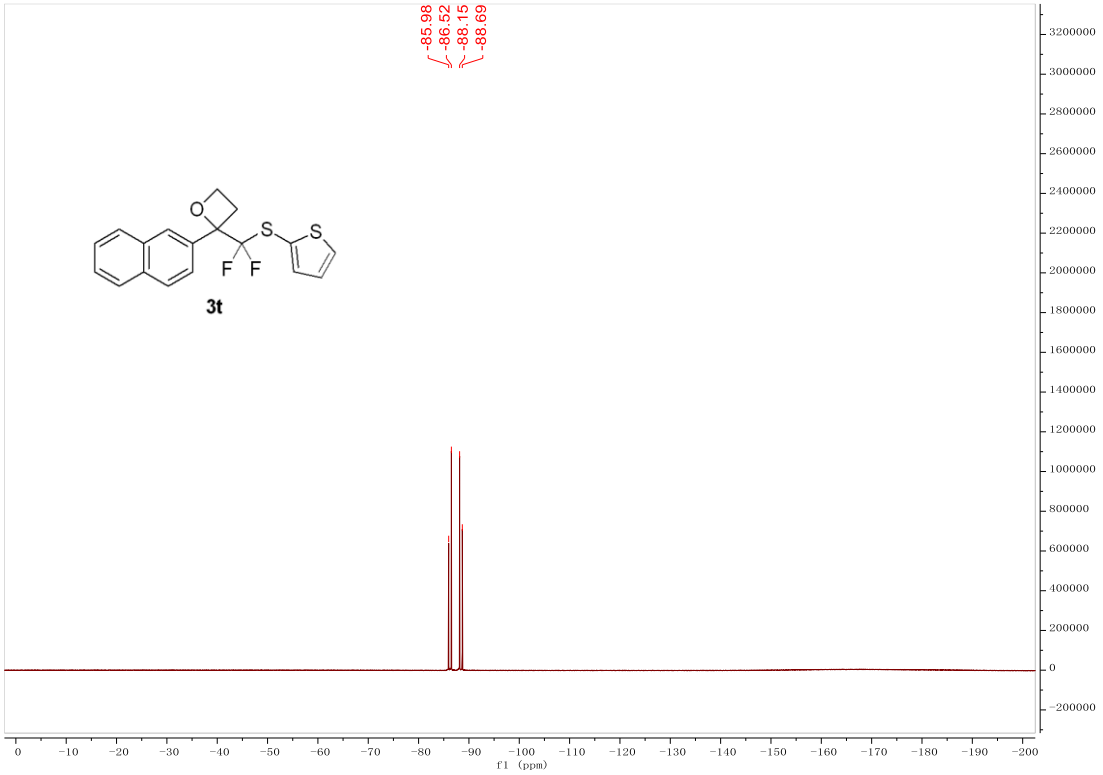
^{1}H NMR (400 MHz, $CDCl_3$) spectrum for 3t



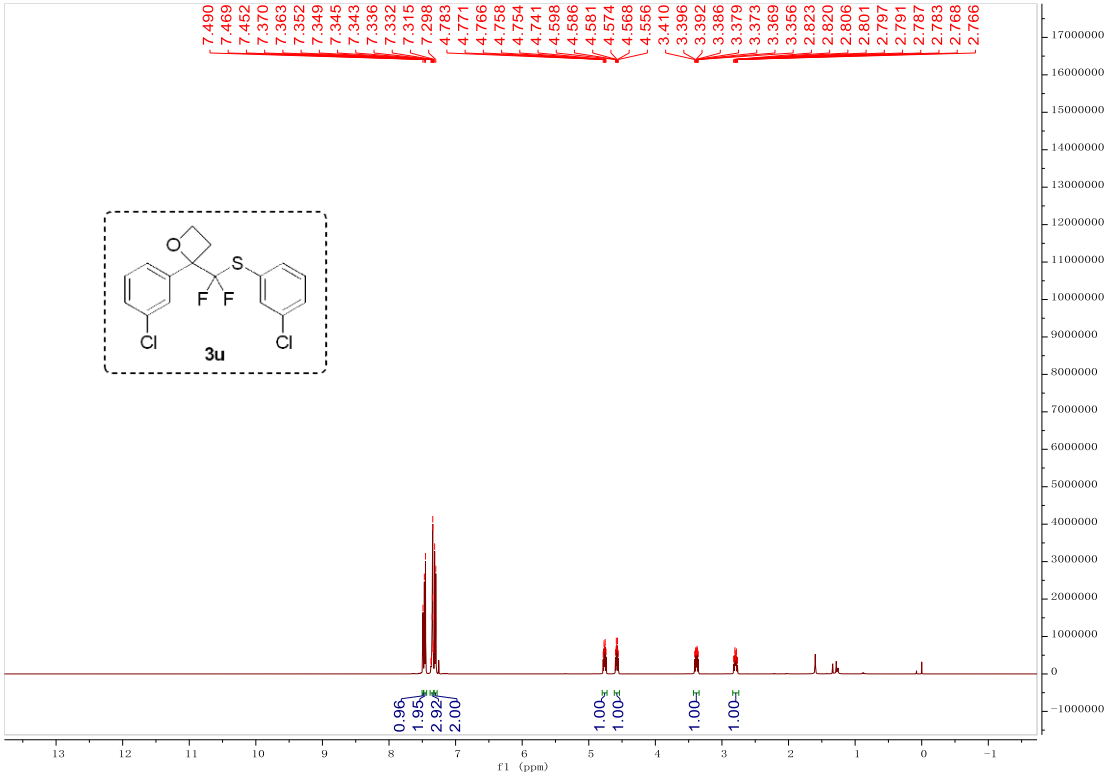
^{13}C NMR (101 MHz, $CDCl_3$) spectrum for 3t



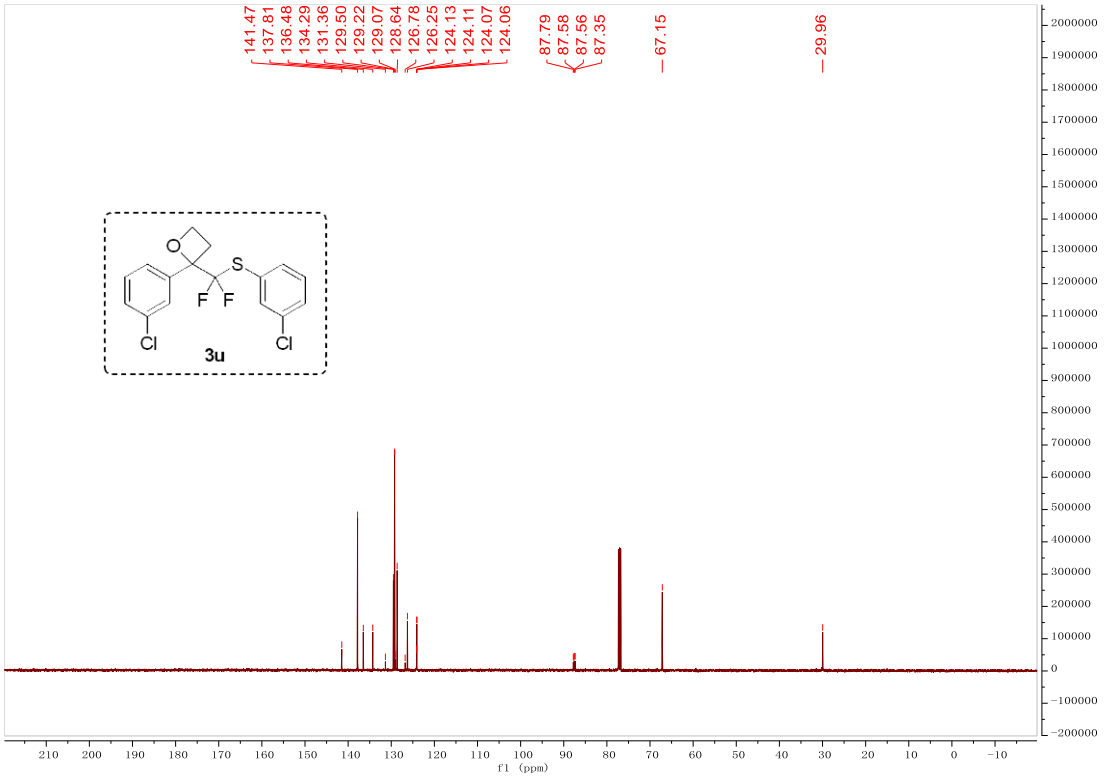
^{19}F NMR (376 MHz, $CDCl_3$) spectrum for 3t



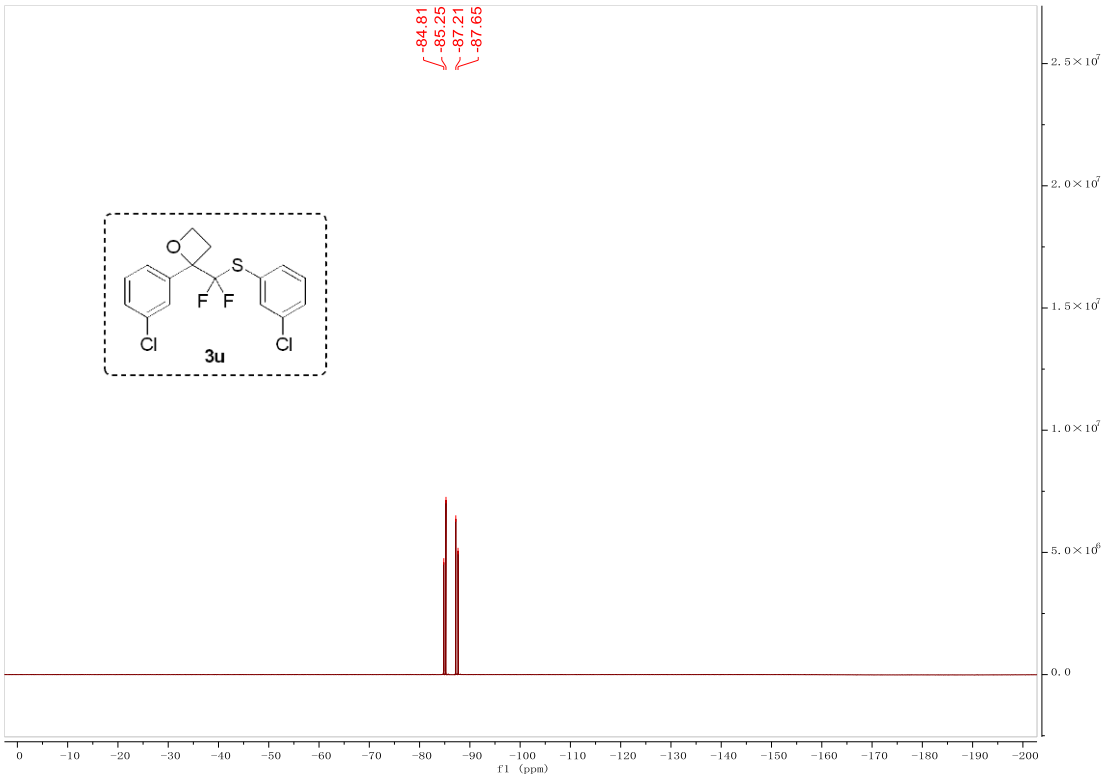
^{1}H NMR (500 MHz, $CDCl_3$) spectrum for 3u



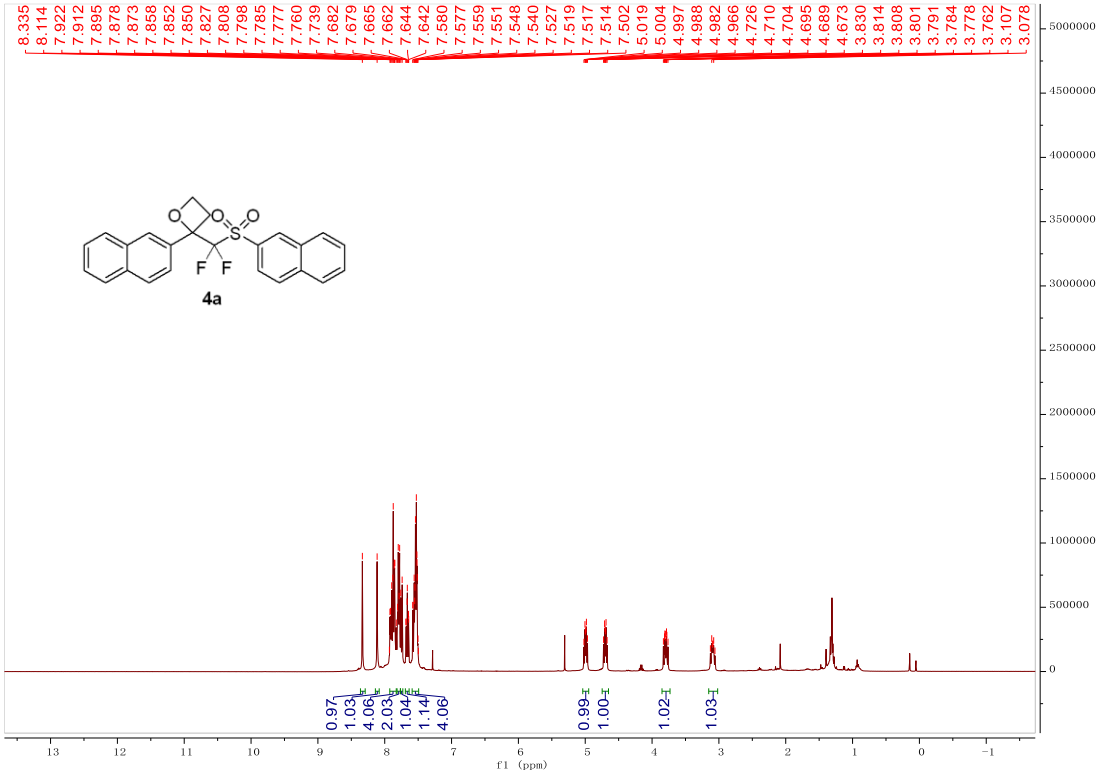
^{13}C NMR (126 MHz, $CDCl_3$) spectrum for 3u



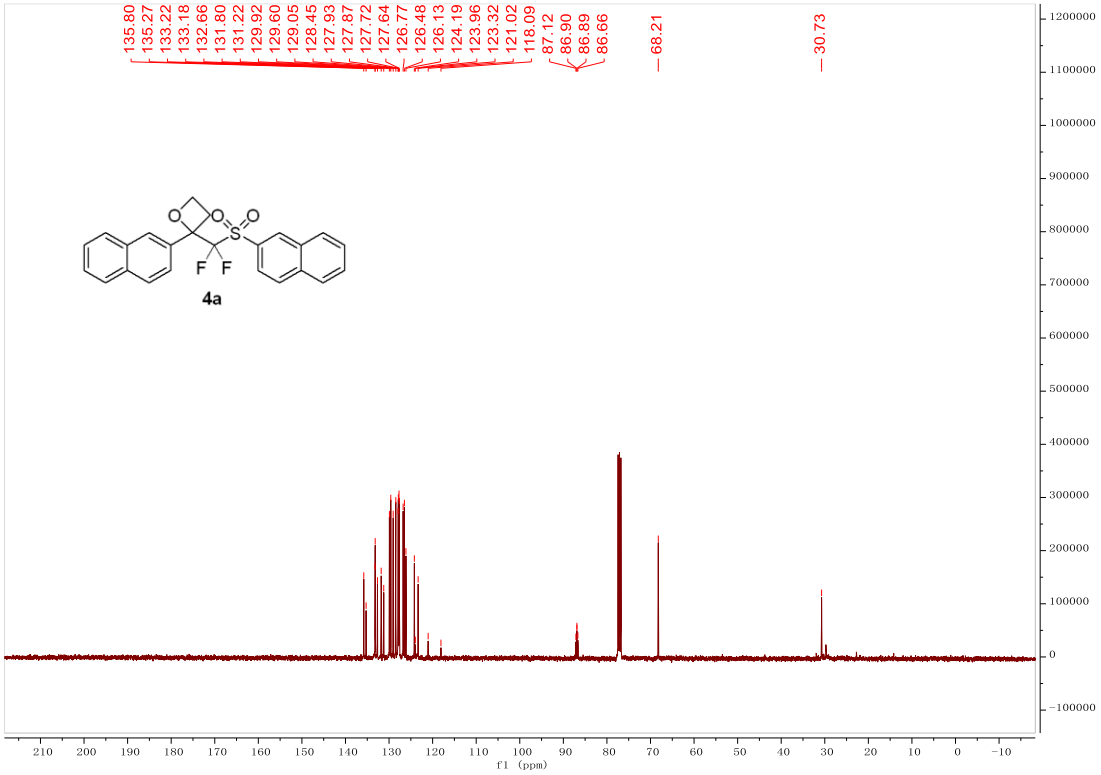
^{19}F NMR (471 MHz, $CDCl_3$) spectrum for 3u



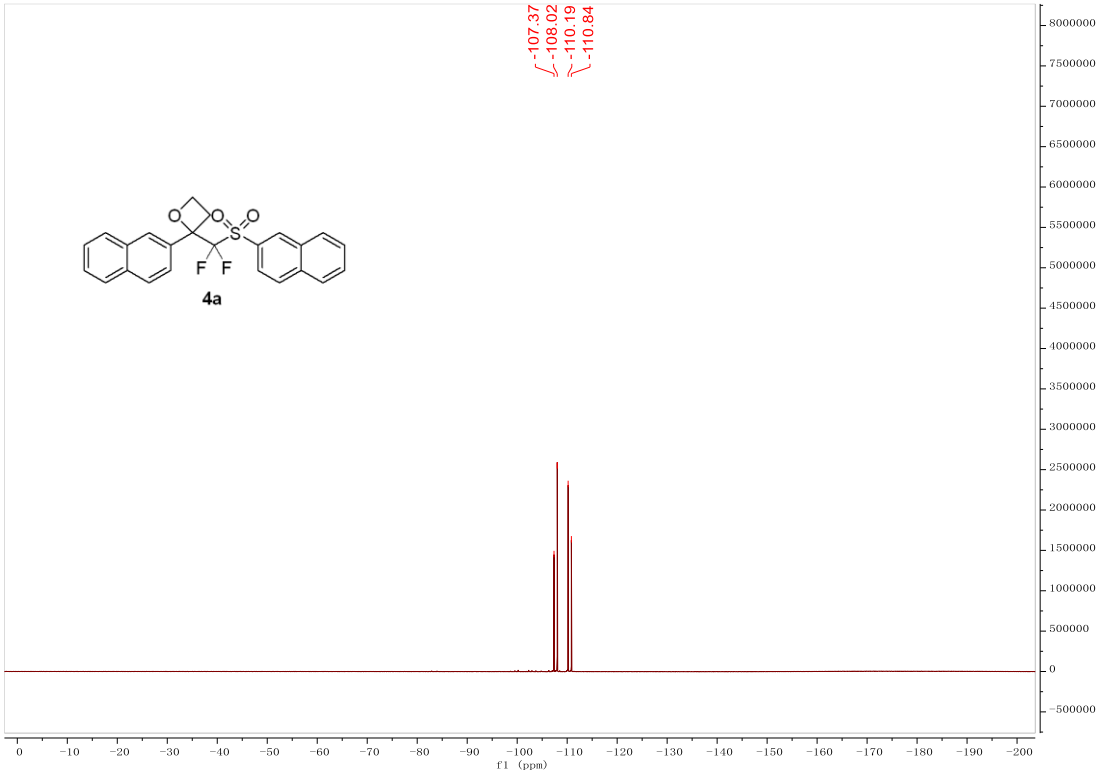
^{1}H NMR (400 MHz, $CDCl_3$) spectrum for 4a



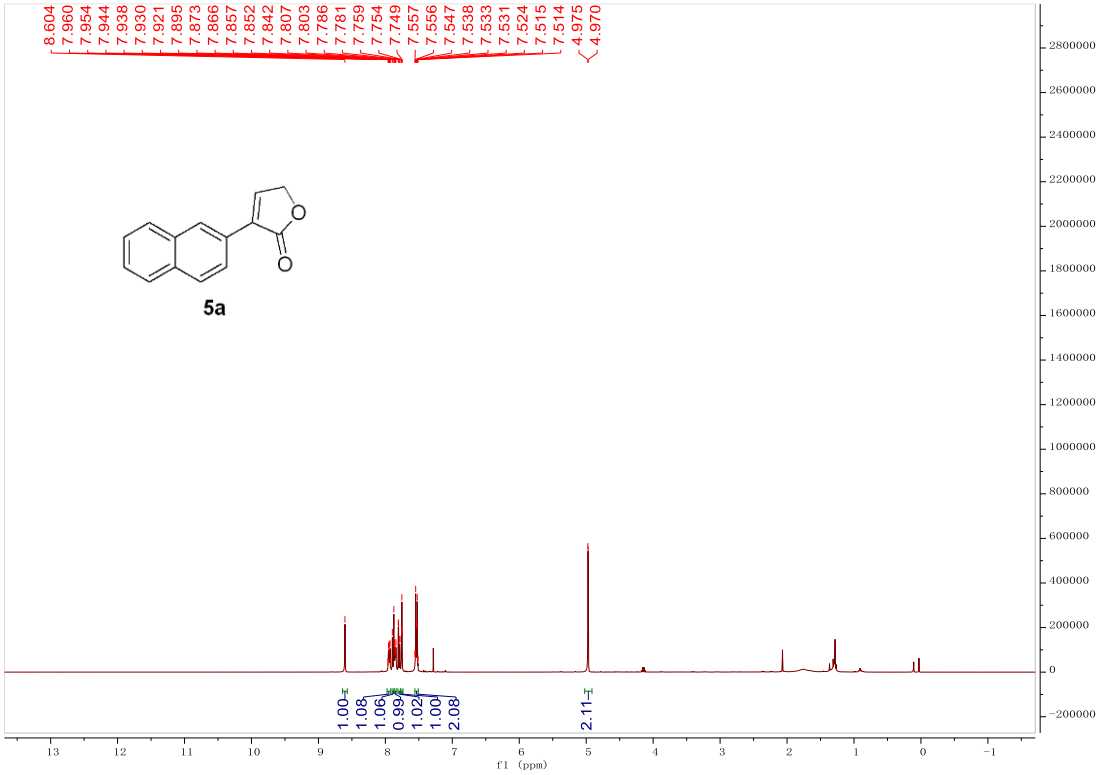
^{13}C NMR (101 MHz, $CDCl_3$) spectrum for 4a



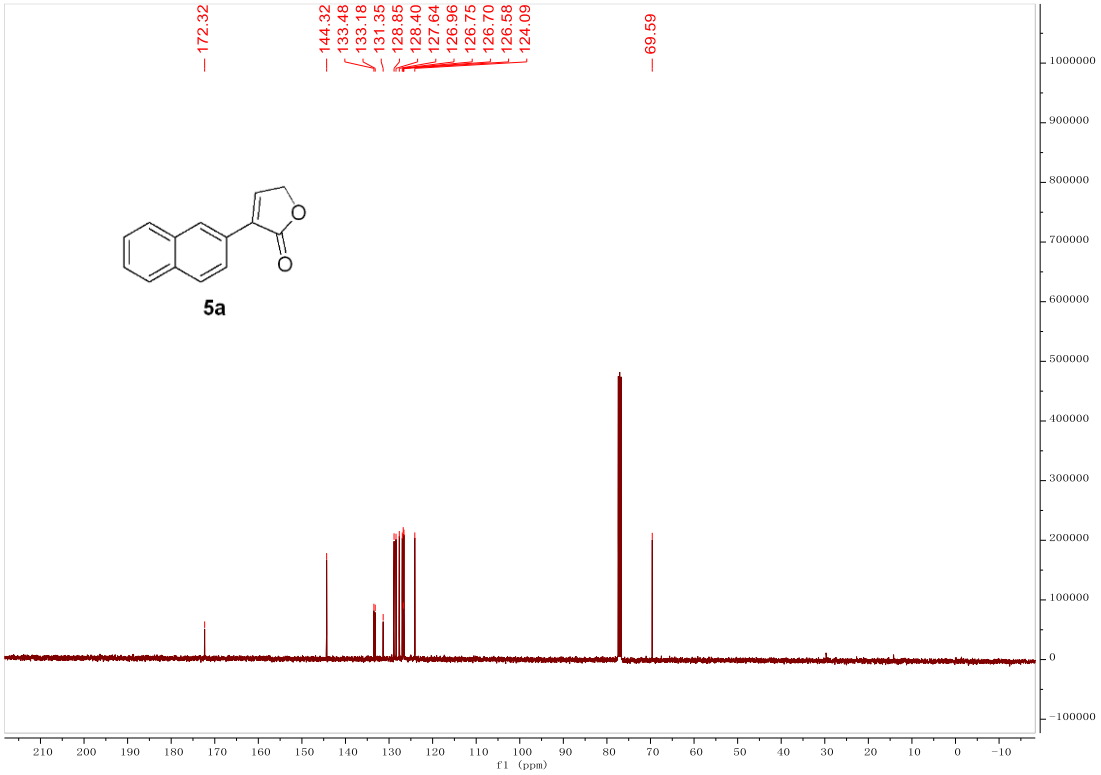
^{19}F NMR (376 MHz, $CDCl_3$) spectrum for 4a



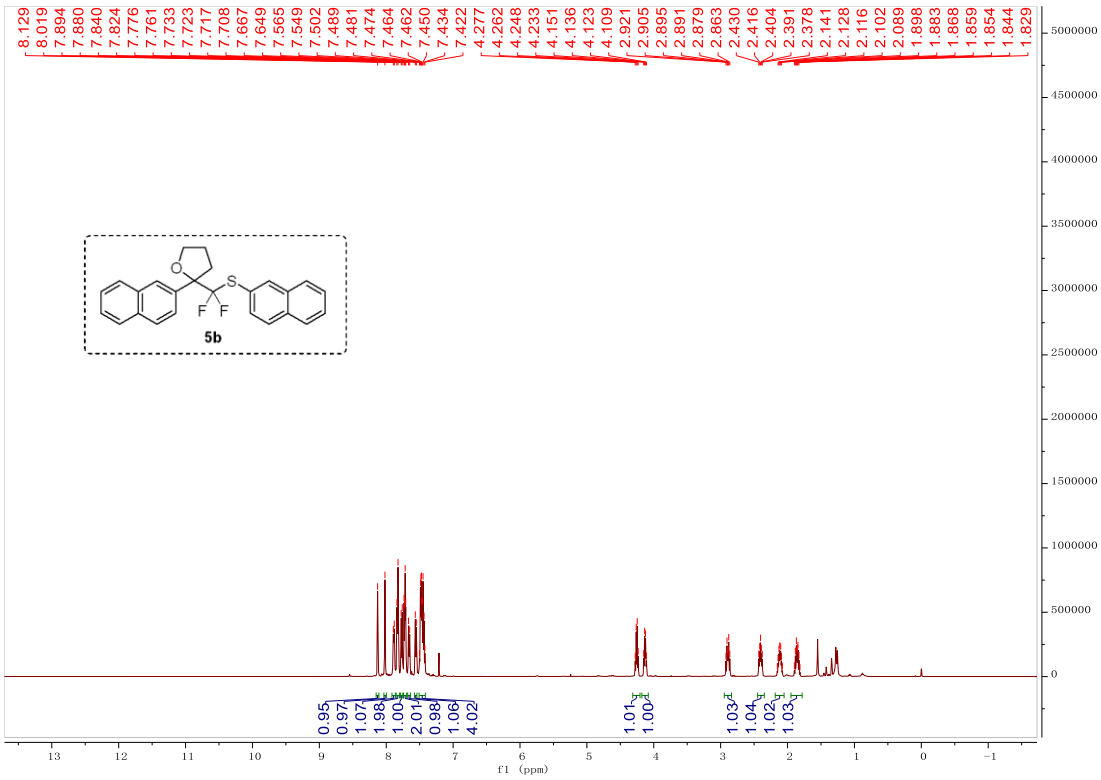
^{1}H NMR (400 MHz, $CDCl_3$) spectrum for 5a



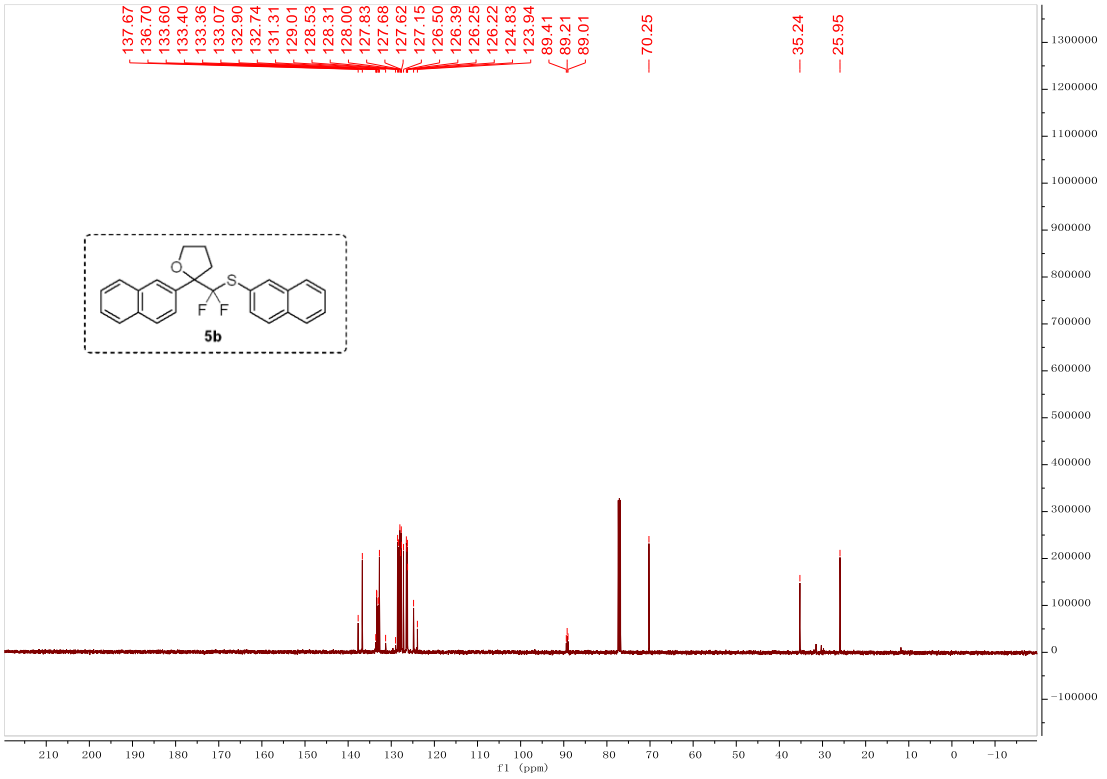
^{13}C NMR (101 MHz, $CDCl_3$) spectrum for 5a



^{1}H NMR (500 MHz, $CDCl_3$) spectrum for 5b



^{13}C NMR (126 MHz, $CDCl_3$) spectrum for 5b



^{19}F NMR (471 MHz, $CDCl_3$) spectrum for 5b