Supporting Information for

Rhodium-Catalyzed Regioselective C8-H Amination of Quninoline *N*-oxides with Trifluoroacetamide at Room Temperature

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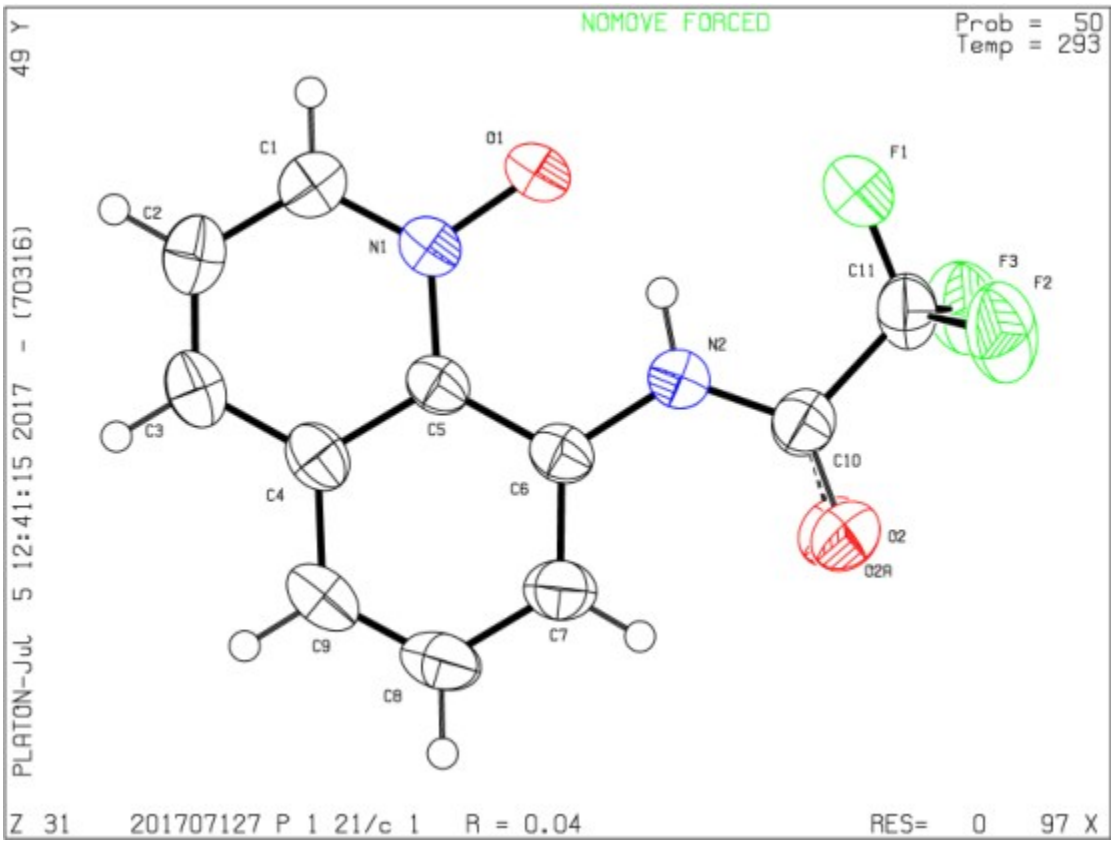
1. X-Ray Crystallographic Data of 3a



Single-crystal X-ray Structure of **3a**

Table 1 Crystal data and structure refinement for 3a.

Identification code	**3a**
Empirical formula	$C_{11}H_7F_3N_2O_2$
Formula weight	256.19
Temperature/K	293(2)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	4.5680(3)
b/Å	16.1861(8)
c/Å	15.8035(10)
α/°	90
β/°	115.336(7)
γ/°	90
Volume/Å^3	1056.09(12)
Z	4
ρ_{calc}g/cm^3	1.611

μ/mm^{-1}	1.303
F(000)	520.0
Crystal size/mm^3	0.21 × 0.15 × 0.12
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	8.256 to 134.138
Index ranges	-3 ≤ h ≤ 5, -19 ≤ k ≤ 12, -18 ≤ l ≤ 17
Reflections collected	3784
Independent reflections	1881 [R_{int} = 0.0231, R_{sigma} = 0.0314]
Data/restraints/parameters	1881/0/172
Goodness-of-fit on F^2	1.040
Final R indexes [I>=2σ (I)]	R_1 = 0.0438, wR_2 = 0.1310
Final R indexes [all data]	R_1 = 0.0513, wR_2 = 0.1427
Largest diff. peak/hole / e Å^{-3}	0.24/-0.25

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 3a. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

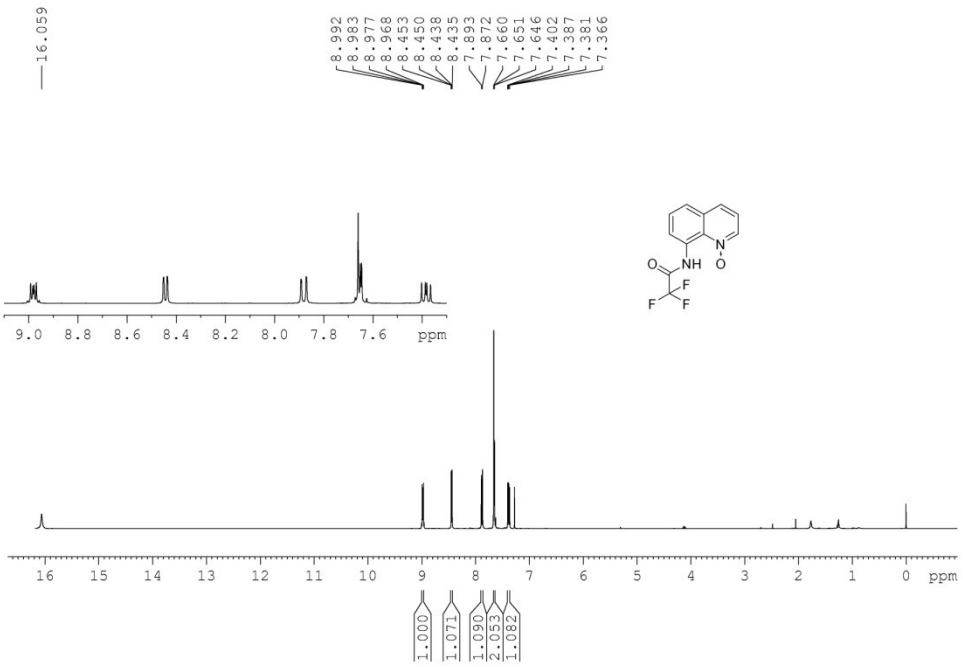
Atom	*x*	*y*	*z*	U(eq)
C1	-1295(6)	2042.7(14)	6840.6(16)	55.5(6)
C2	-3588(6)	1836.9(14)	5950.2(17)	57.0(6)
C3	-3687(5)	2253.2(13)	5196.1(15)	50.2(5)
C4	-1451(5)	2892.7(12)	5323.1(13)	43.1(5)
C5	872(4)	3103.5(11)	6233.1(12)	38.0(4)
C6	3149(5)	3748.5(12)	6360.8(13)	39.9(4)
C7	3020(5)	4155.7(14)	5580.6(14)	50.6(5)
C8	708(6)	3948.6(15)	4682.3(15)	58.3(6)
C9	-1467(5)	3338.2(14)	4550.3(14)	54.4(6)
C10	7679(5)	4525.1(13)	7547.1(15)	49.8(5)
C11	9627(5)	4578.7(14)	8611.6(15)	50.8(5)
F1	9187(3)	3944.5(9)	9075.8(9)	69.3(5)
F2	12755(3)	4631.3(12)	8840.4(12)	81.9(5)
F3	8813(4)	5257.8(10)	8934.3(11)	74.5(5)
N1	835(4)	2651.9(10)	6981.0(11)	45.5(4)
N2	5434(4)	3935(1)	7271.4(11)	43.0(4)
O1	2897(4)	2817.8(11)	7853(1)	71.0(6)
O2	8548(19)	4976(4)	7074(3)	71.5(14)
O2A	7380(50)	5155(11)	7077(10)	71.5(14)

Table 3 Anisotropic Displacement Parameters (Å^2×10^3) for 3a. The Anisotropic displacement factor exponent takes the form: -2π^2[h^{2}a*^{2}U_{11}+2hka*b*U_{12}+…].

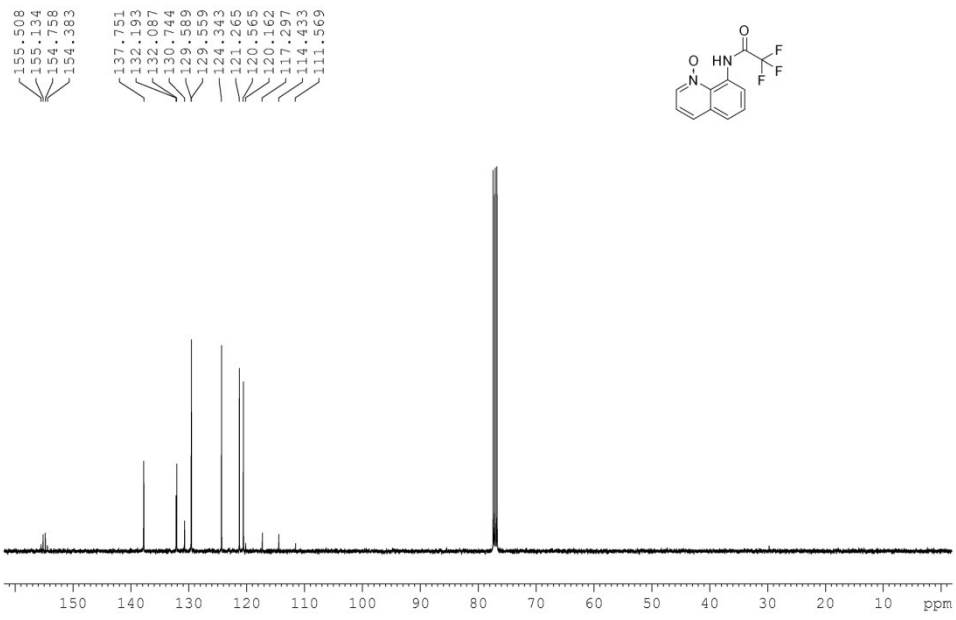
Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}

C1	60.7(13)	52.6(12)	51.7(12)	3.2(9)	22.5(10)	-10.4(10)
C2	55.1(12)	50.4(12)	62.3(13)	-9.8(10)	22(1)	-10.9(9)
C3	45.8(10)	53.9(12)	44.3(11)	-12.7(9)	13.0(8)	-0.4(8)
C4	42.8(10)	45.6(10)	37.8(9)	-5.3(8)	14.1(8)	6.2(8)
C5	40.8(9)	39.0(9)	33.3(9)	0.3(7)	15.0(7)	6.0(7)
C6	43.6(10)	41(1)	35.3(9)	0.0(7)	17.1(8)	4.0(7)
C7	60.4(12)	51.4(12)	42.4(11)	5.2(9)	24.3(9)	0.2(9)
C8	71.6(14)	65.6(14)	37.4(10)	9.8(10)	23(1)	4.3(11)
C9	57.8(12)	66.8(14)	31.5(10)	-2.0(9)	12.4(8)	5.1(10)
C10	52.4(12)	51.2(12)	48.3(11)	-4.6(9)	24.0(9)	-10.0(9)
C11	43.3(10)	59.5(12)	50.5(12)	-13.9(9)	21.0(9)	-10.4(9)
F1	70.0(9)	79.9(10)	44.7(7)	2.5(6)	11.8(6)	-16.7(7)
F2	42.6(8)	118.8(14)	80.7(10)	-23.4(9)	22.9(7)	-15.9(8)
F3	81.2(10)	74.9(10)	70.6(10)	-26.2(7)	35.4(8)	-4.5(7)
N1	45.9(9)	50.0(9)	34.7(8)	3.1(7)	11.7(6)	-4.5(7)
N2	46.2(9)	45.1(9)	36.6(8)	0.7(7)	16.6(7)	-4.5(7)
O1	76.0(11)	86.3(12)	32.4(8)	10.4(7)	5.7(7)	-32.3(9)
O2	74(3)	84(2)	59.5(11)	-1.7(13)	31.7(17)	-34(2)
O2A	74(3)	84(2)	59.5(11)	-1.7(13)	31.7(17)	-34(2)

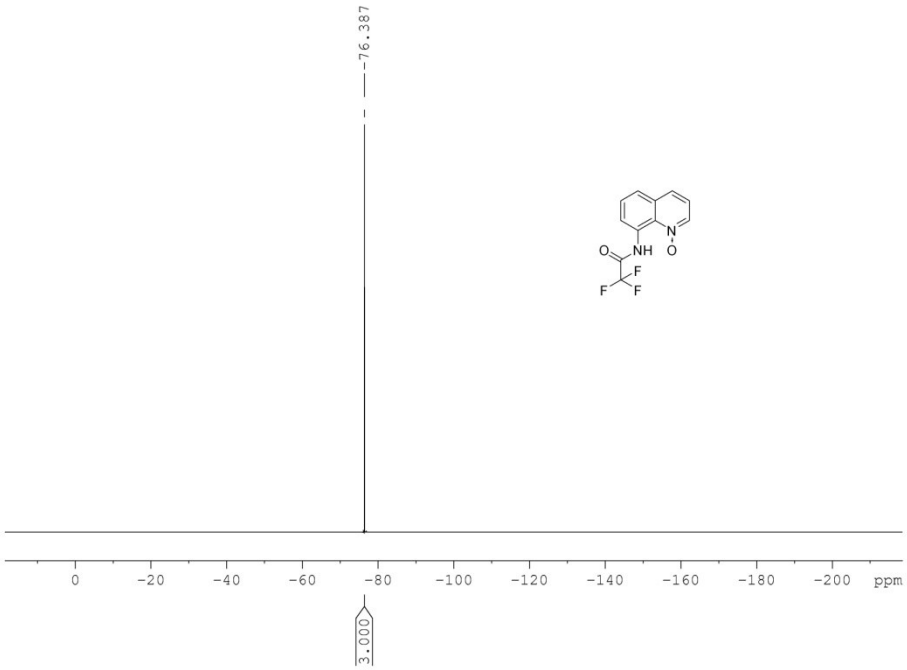
2. Copies of ^{1}H NMR, ^{13}C NMR and ^{19}F NMR Spectra



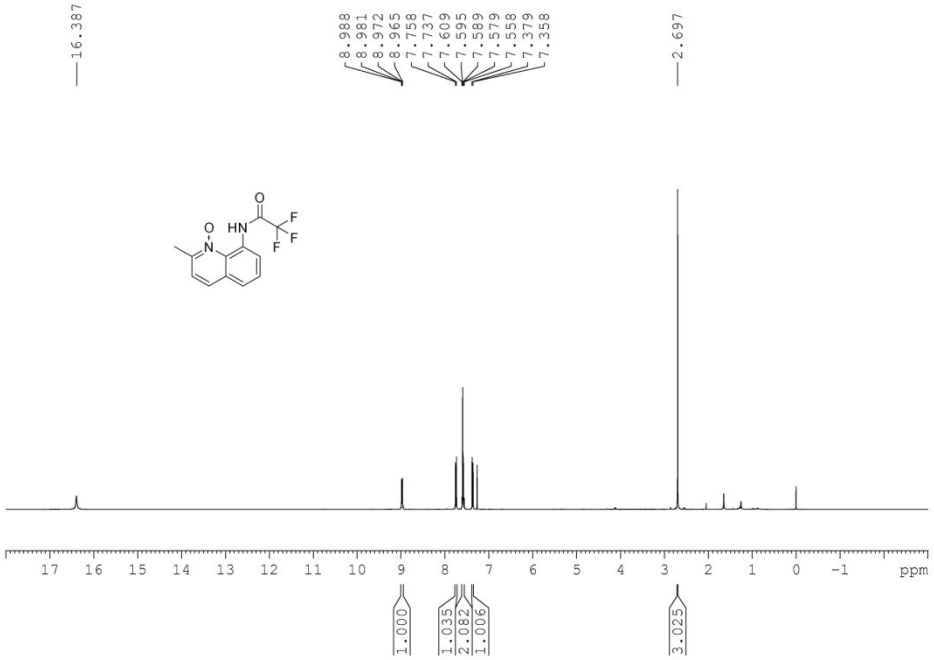
^{1}H NMR spectrum of compound **3a**



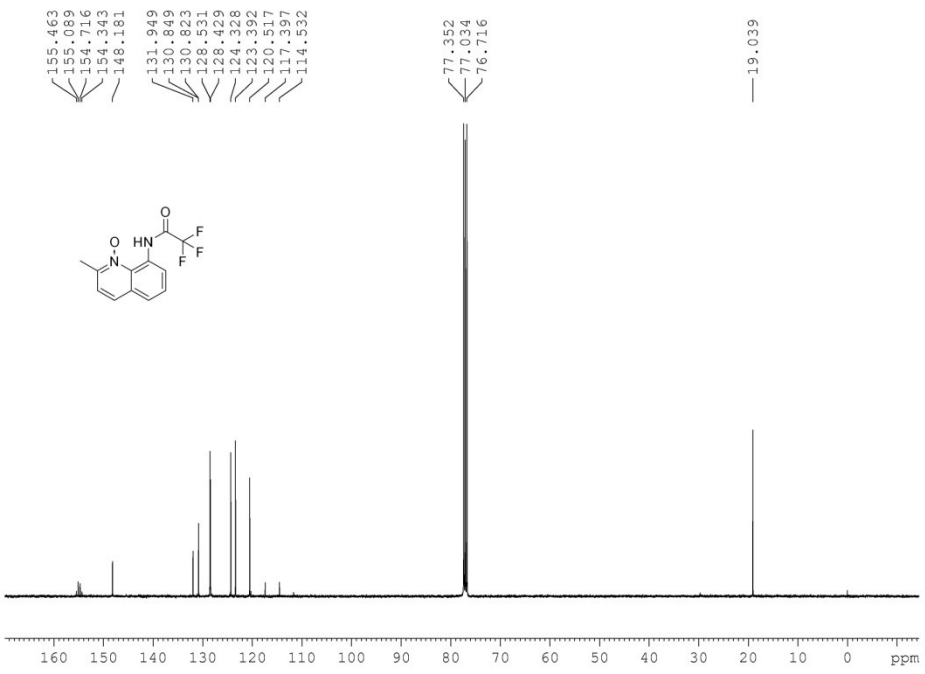
^{13}C NMR spectrum of compound **3a**



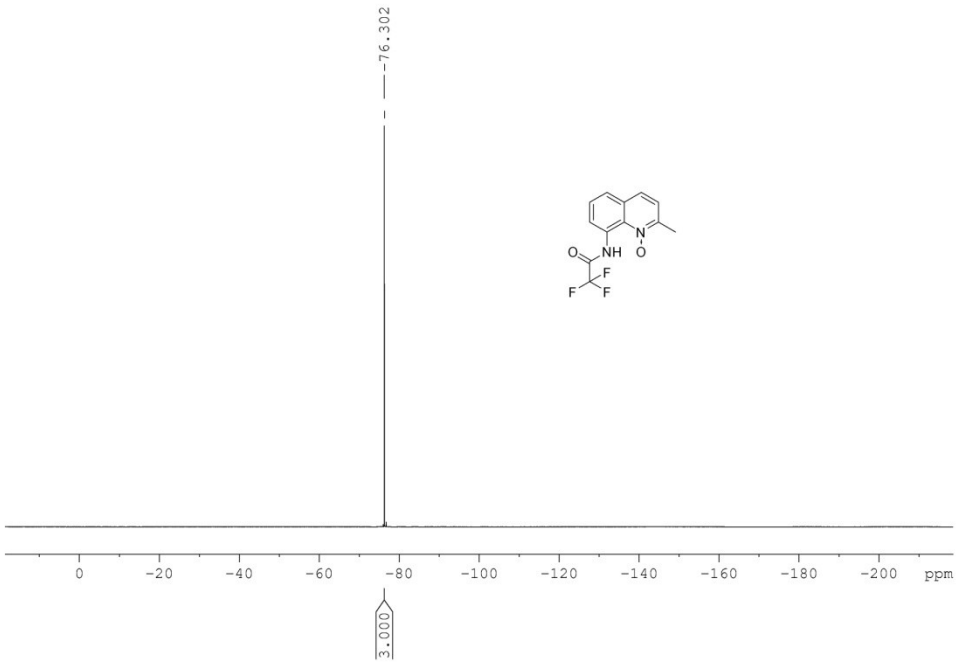
^{19}F NMR spectrum of compound **3a**



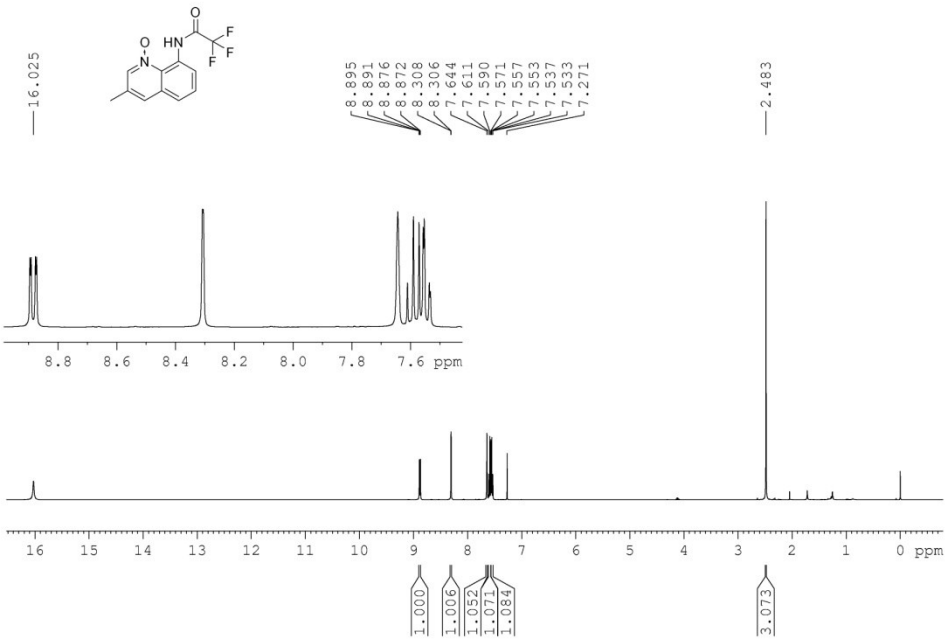
^{1}H NMR spectrum of compound **3b**



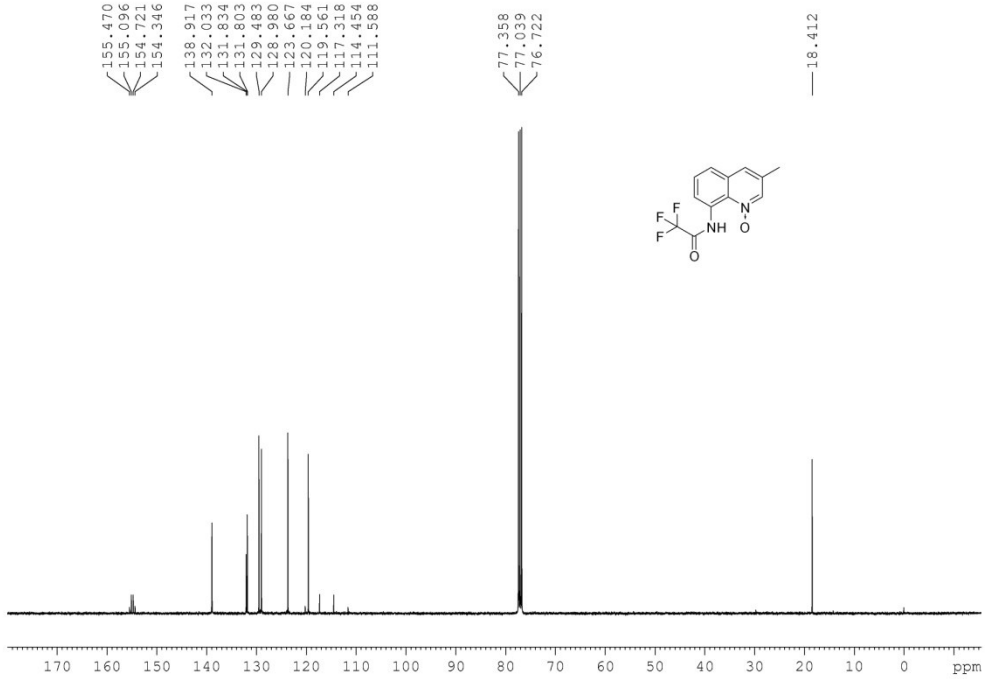
^{13}C NMR spectrum of compound **3b**



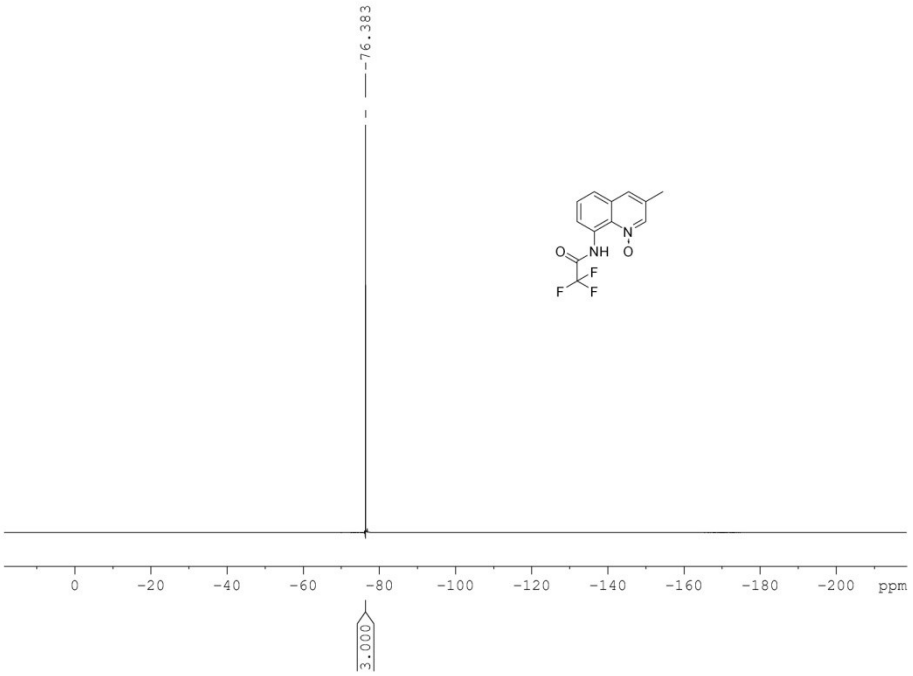
^{19}F NMR spectrum of compound **3b**



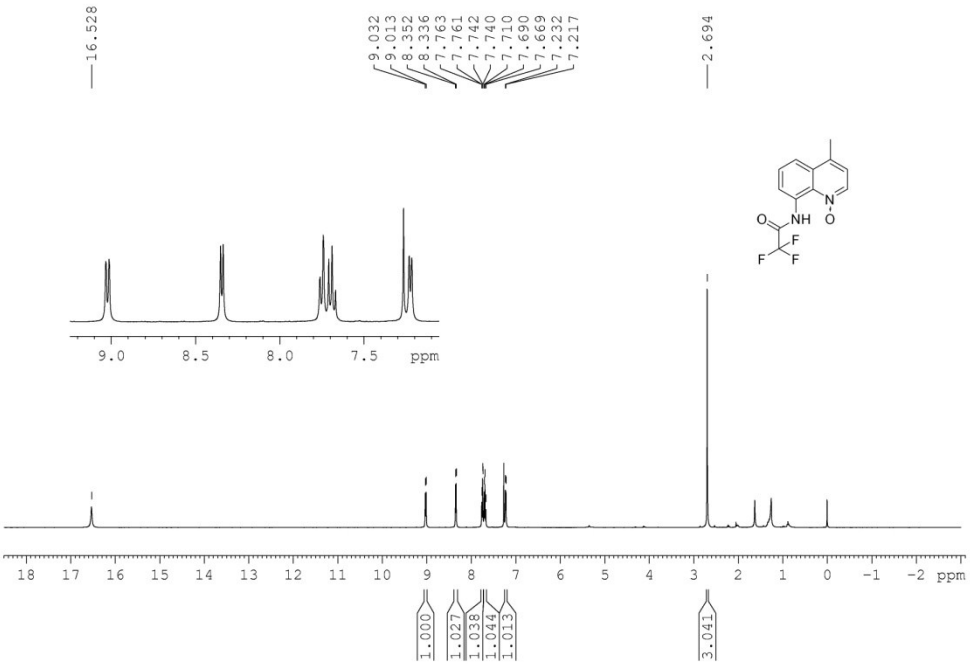
^{1}H NMR spectrum of compound **3c**



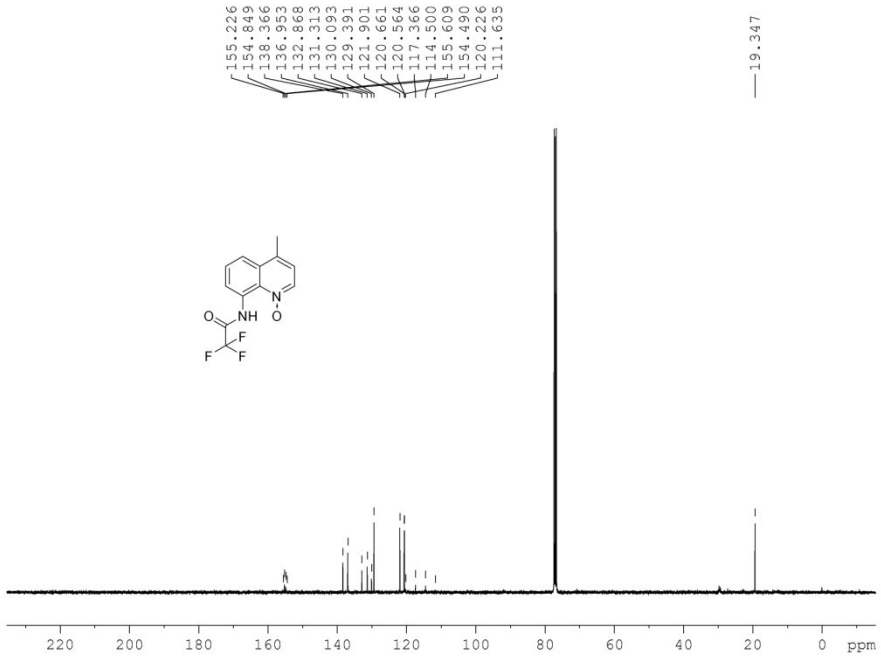
^{13}C NMR spectrum of compound **3c**



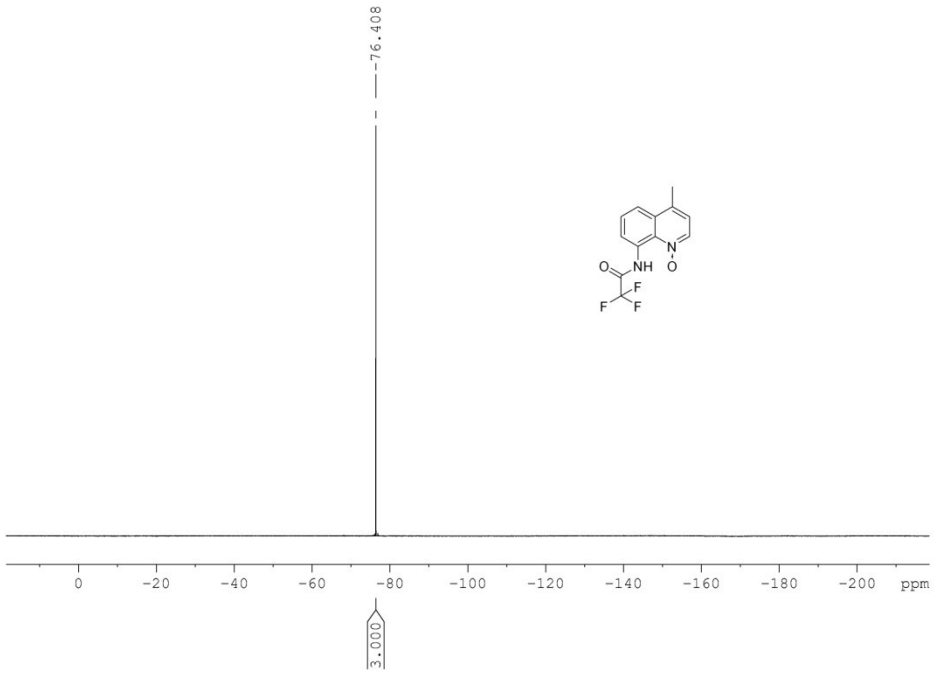
^{19}F NMR spectrum of compound **3c**



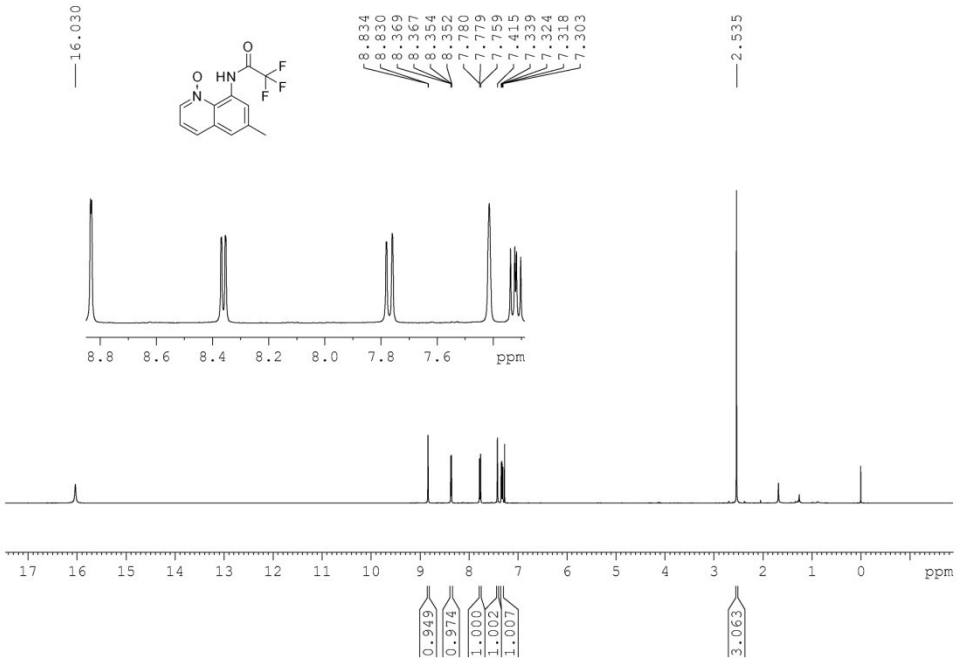
^{1}H NMR spectrum of compound **3d**



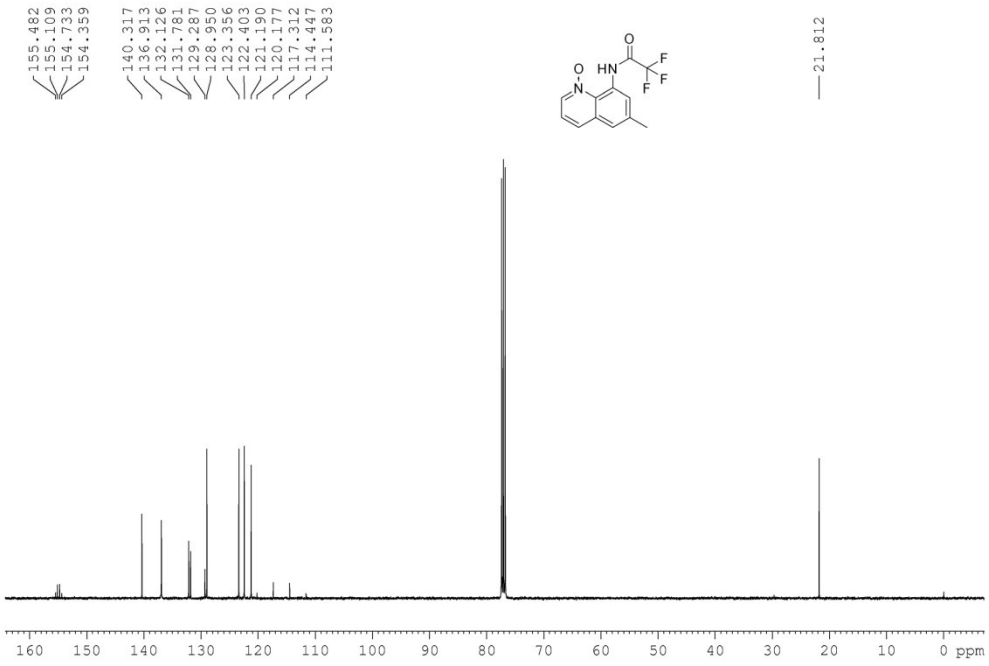
^{13}C NMR spectrum of compound **3d**



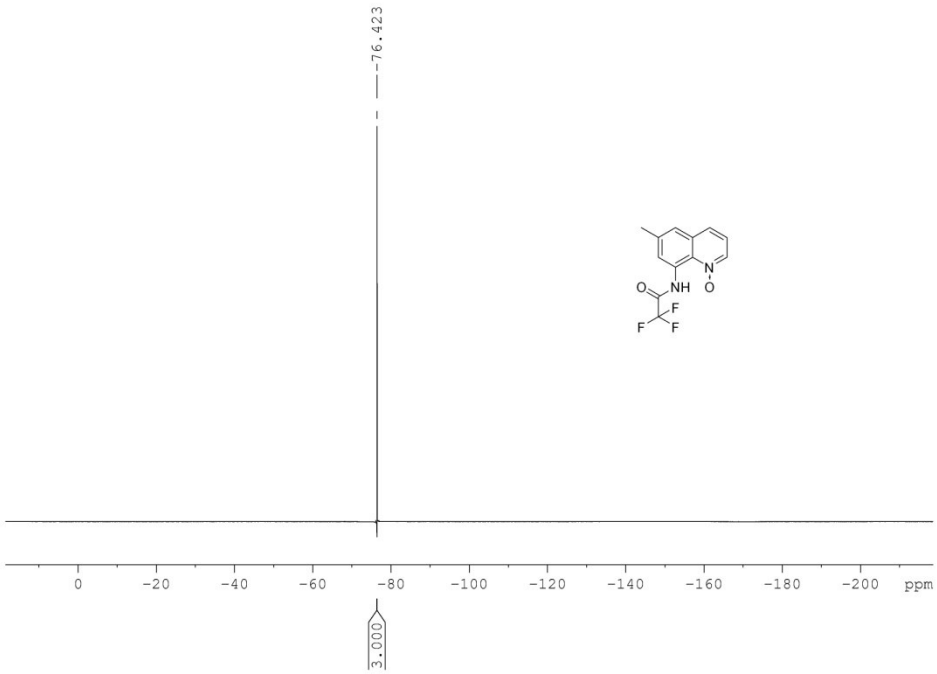
^{19}F NMR spectrum of compound **3d**



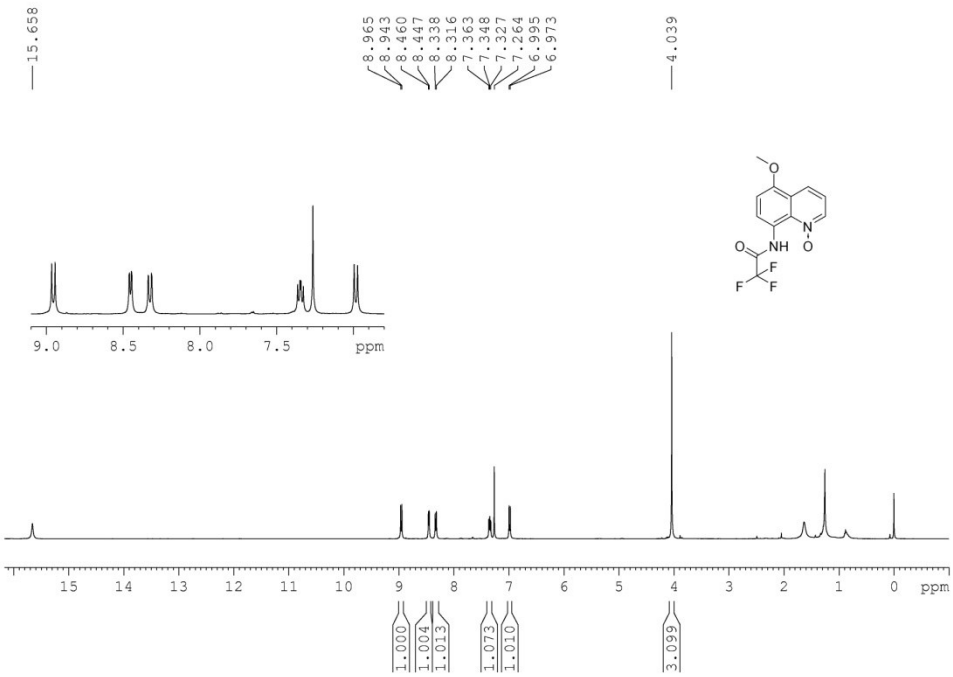
^{1}H NMR spectrum of compound **3e**



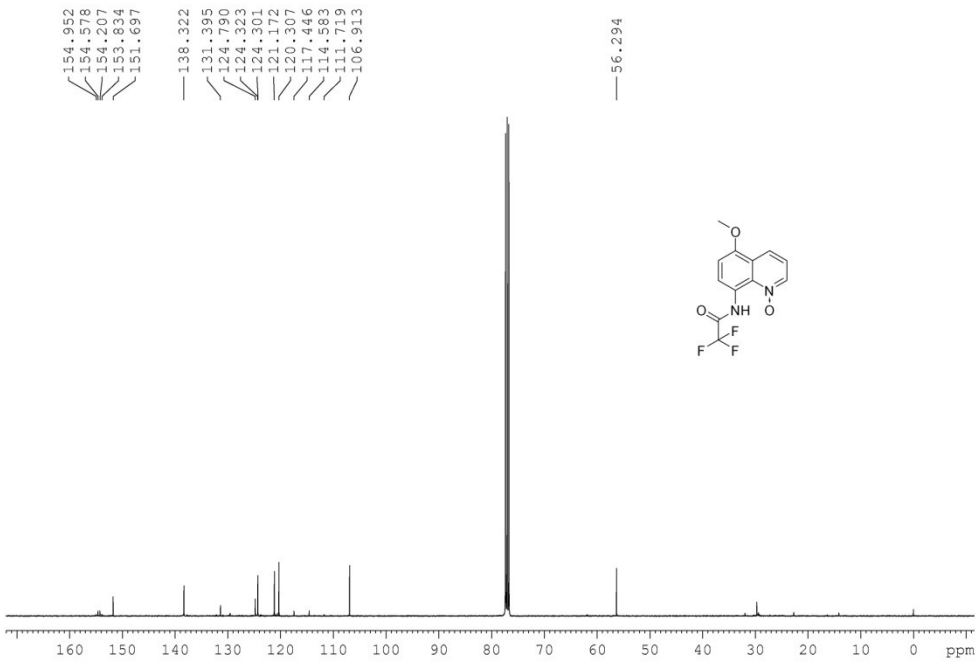
^{13}C NMR spectrum of compound **3e**



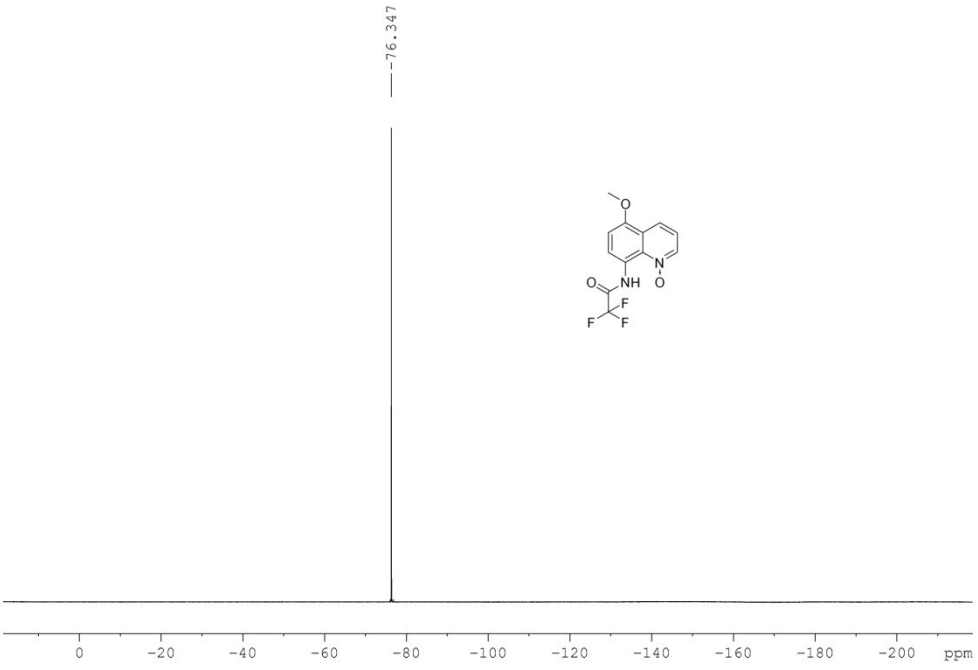
^{19}F NMR spectrum of compound **3e**



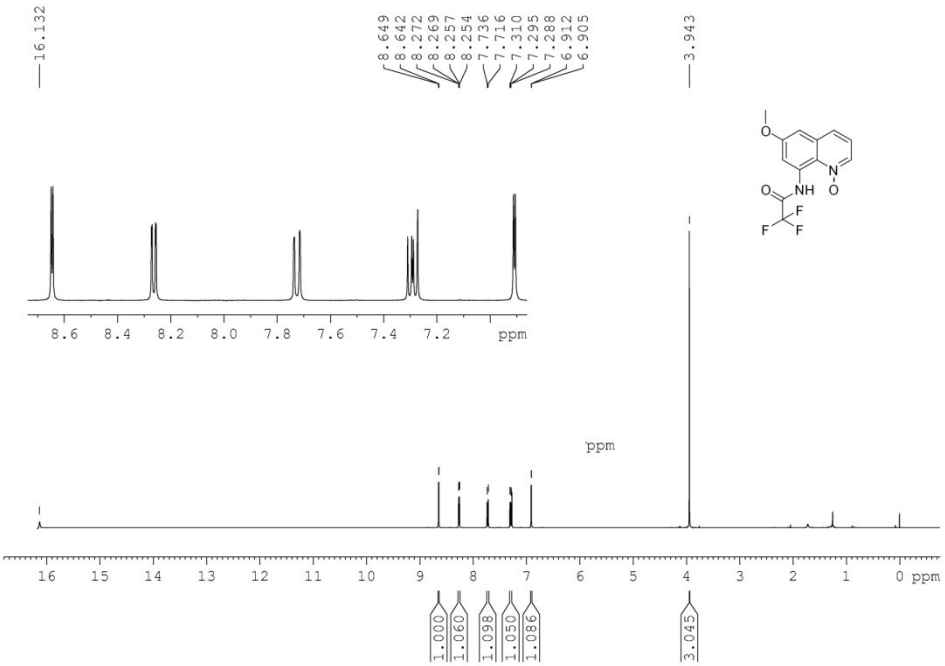
^{1}H NMR spectrum of compound **3g**



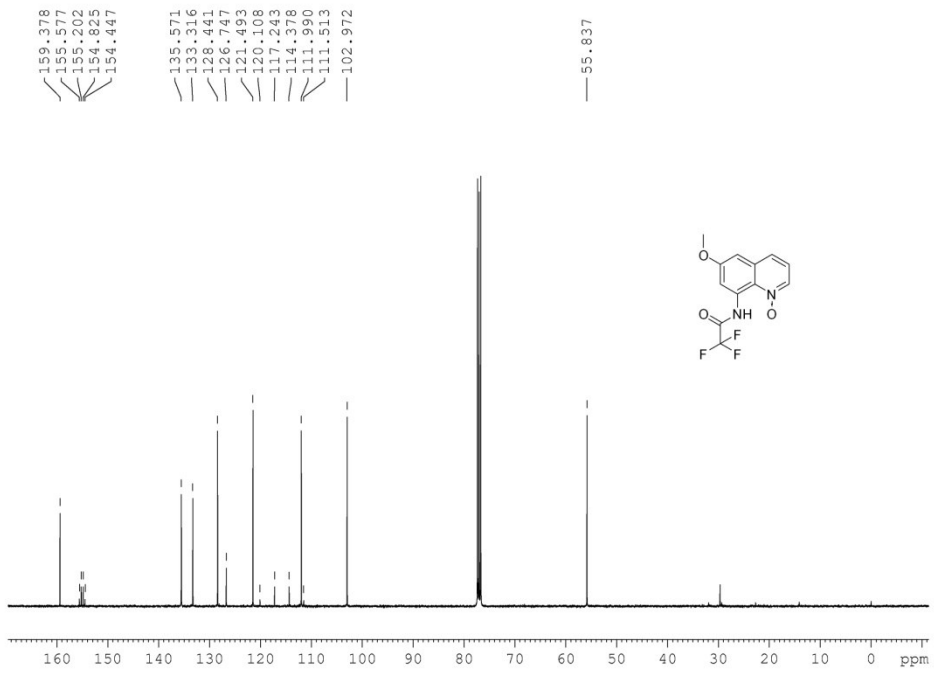
^{13}C NMR spectrum of compound **3g**



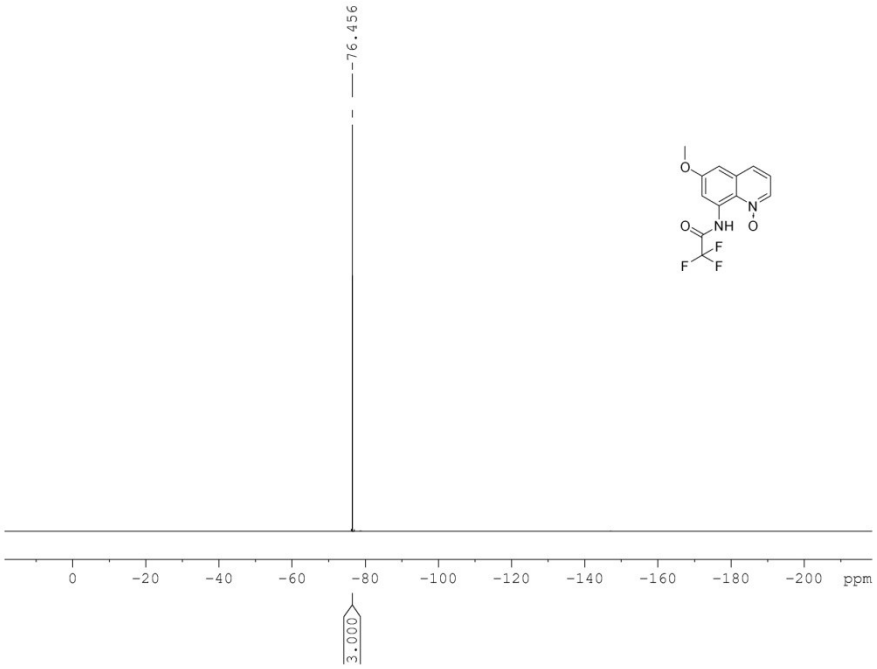
^{19}F NMR spectrum of compound **3g**



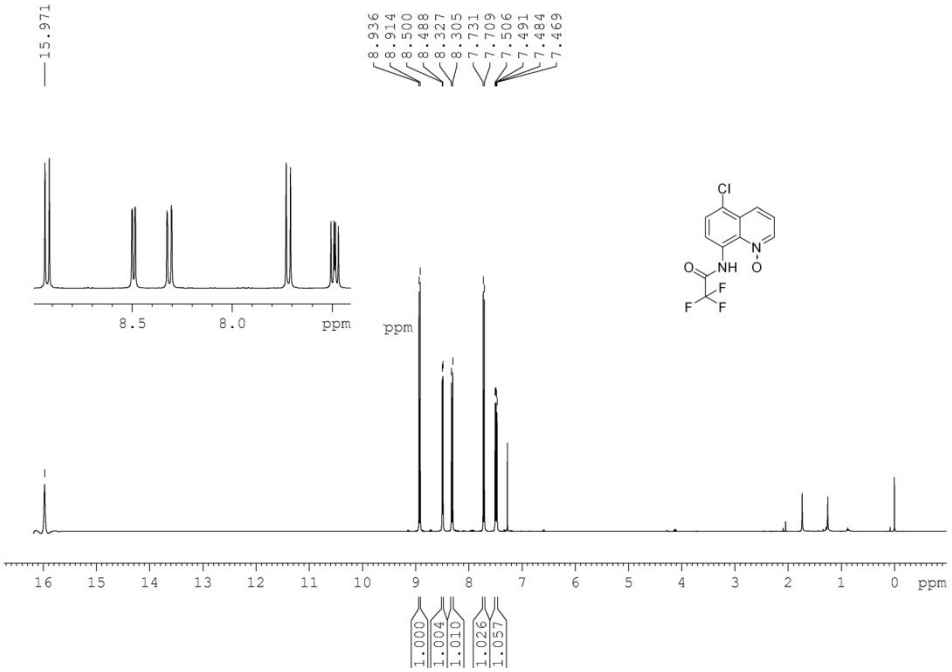
^{1}H NMR spectrum of compound **3h**



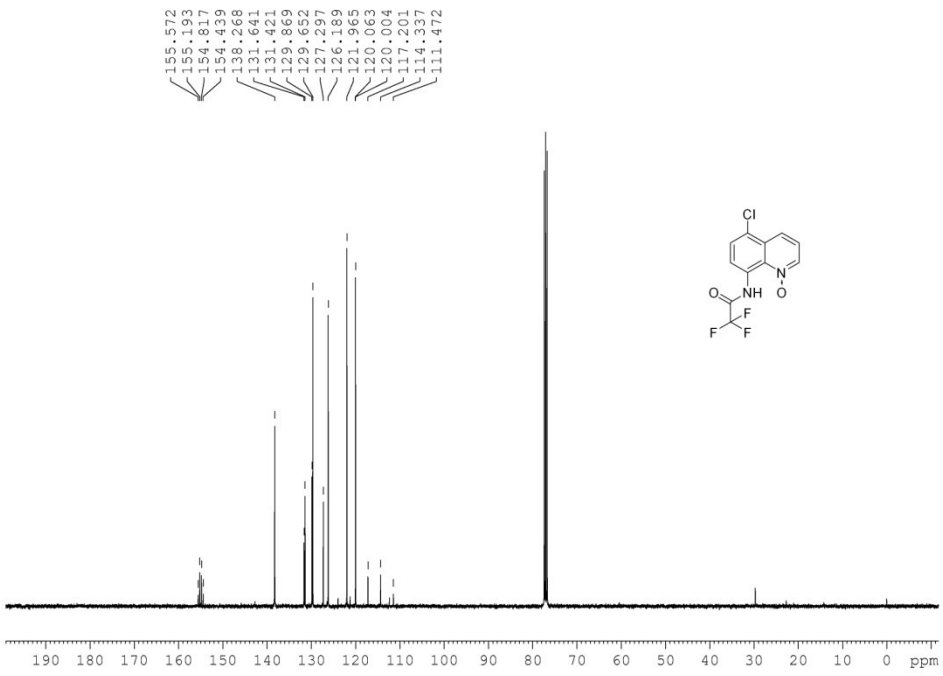
^{13}C NMR spectrum of compound **3h**



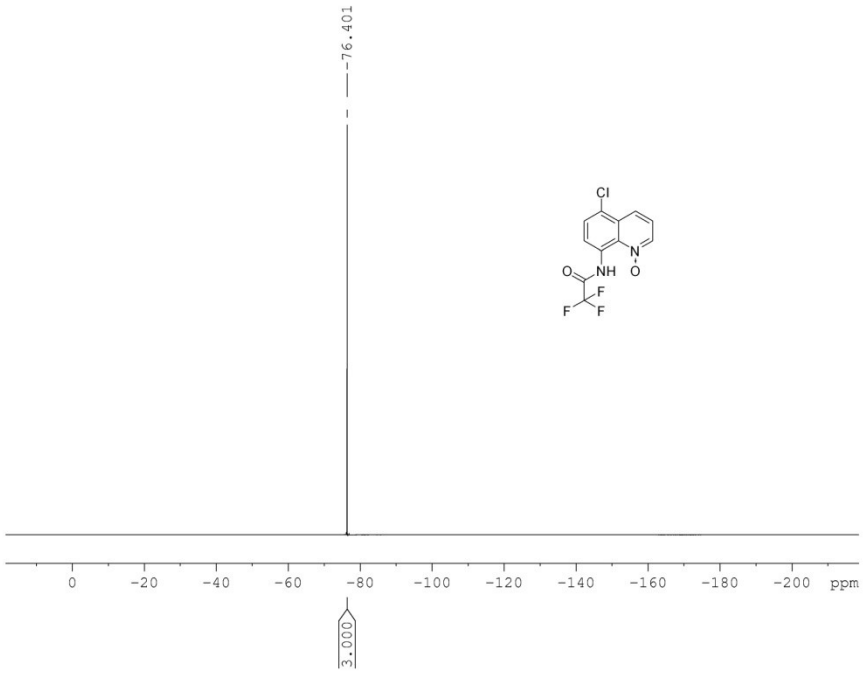
^{19}F NMR spectrum of compound **3h**



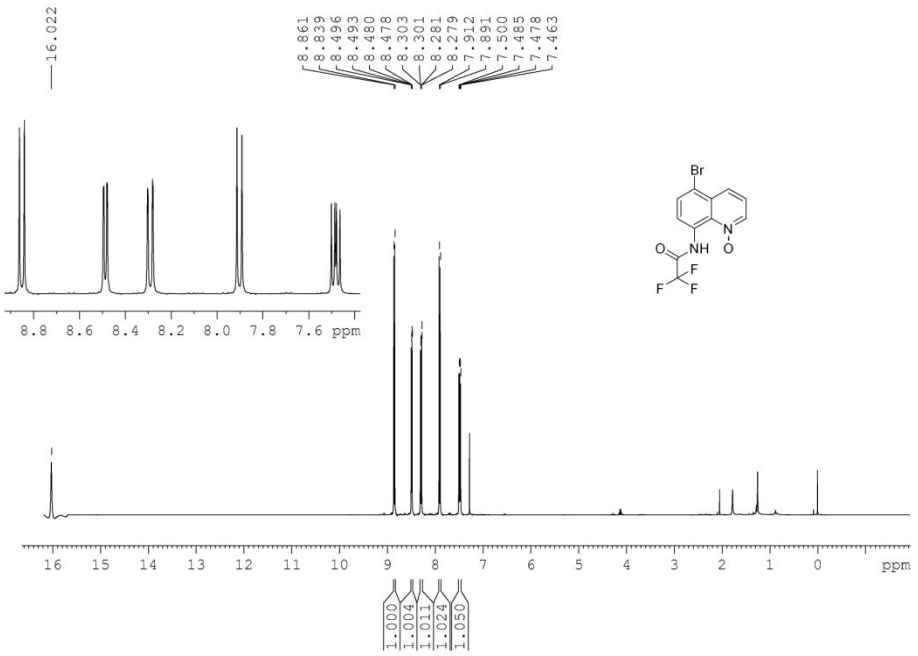
^{1}H NMR spectrum of compound **3i**



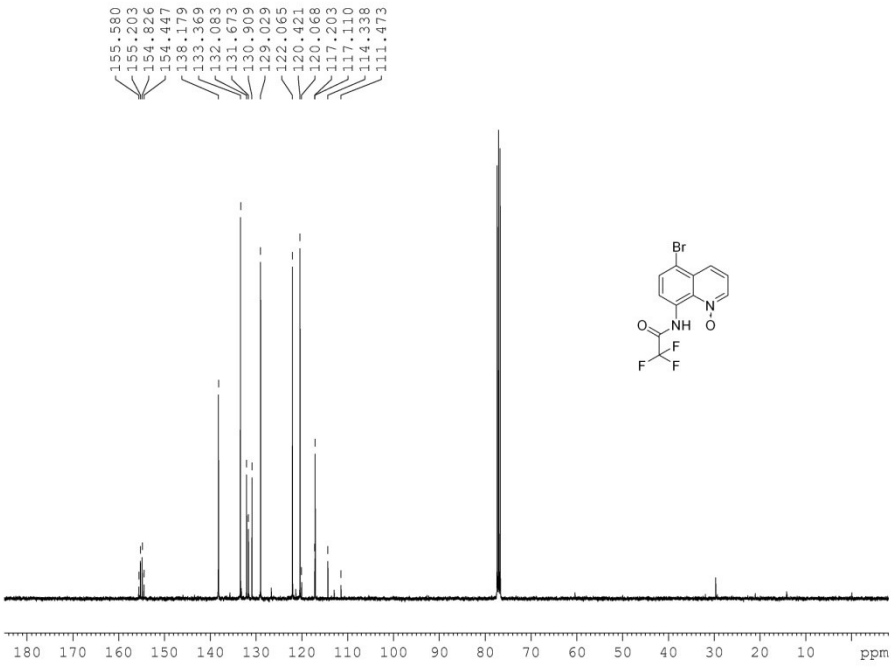
^{13}C NMR spectrum of compound **3i**



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



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



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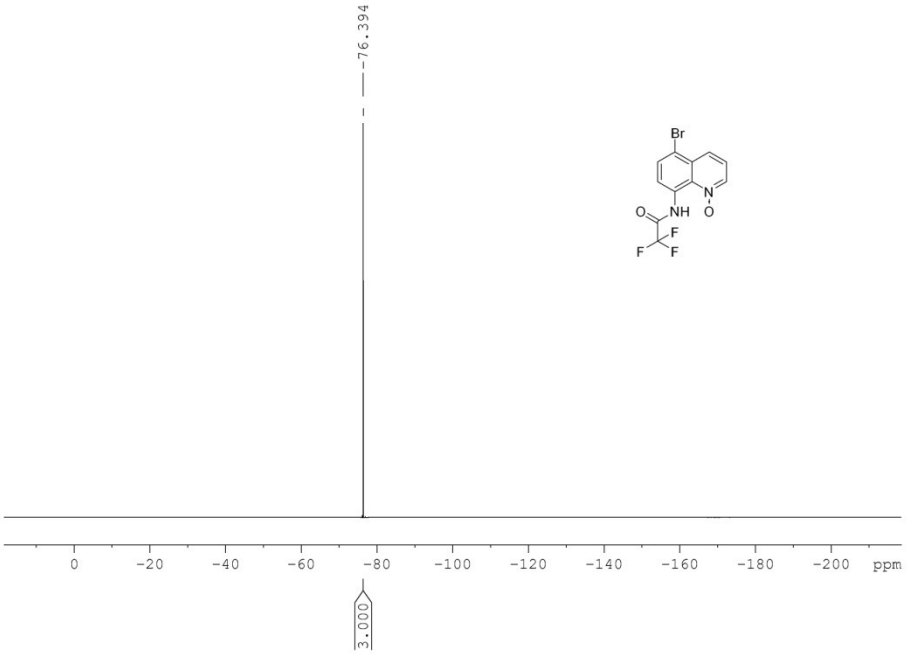
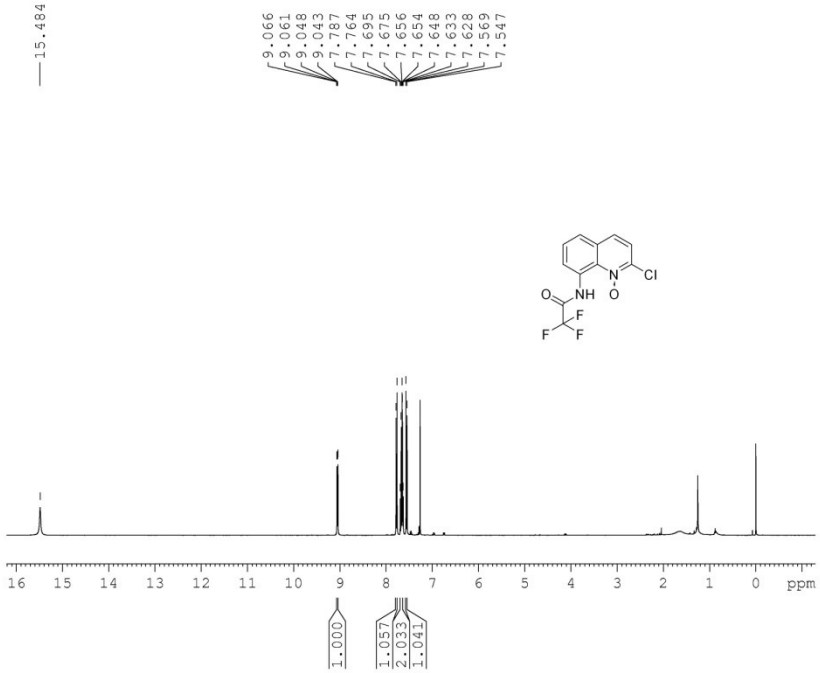
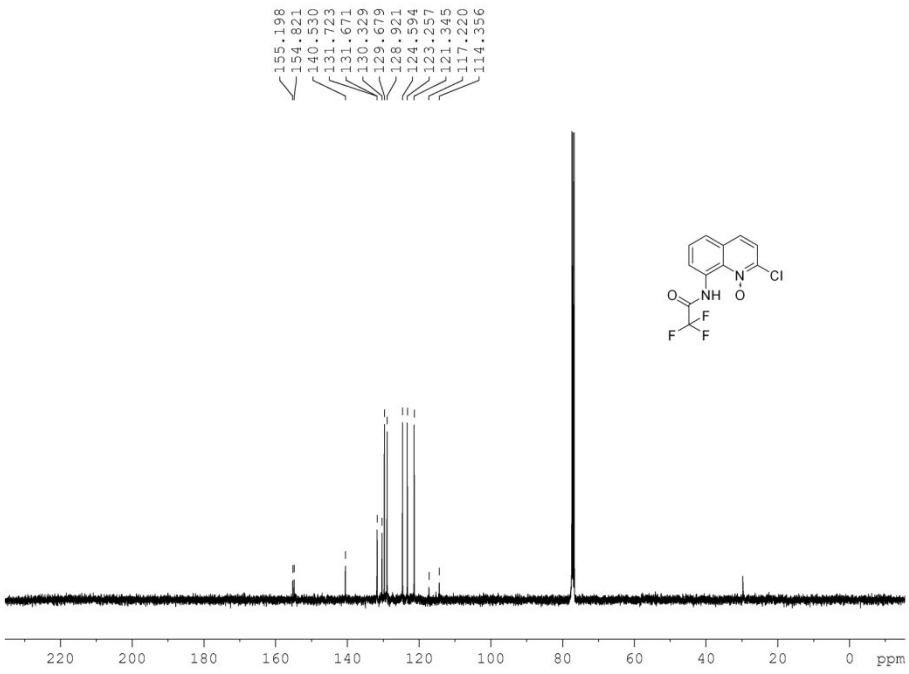


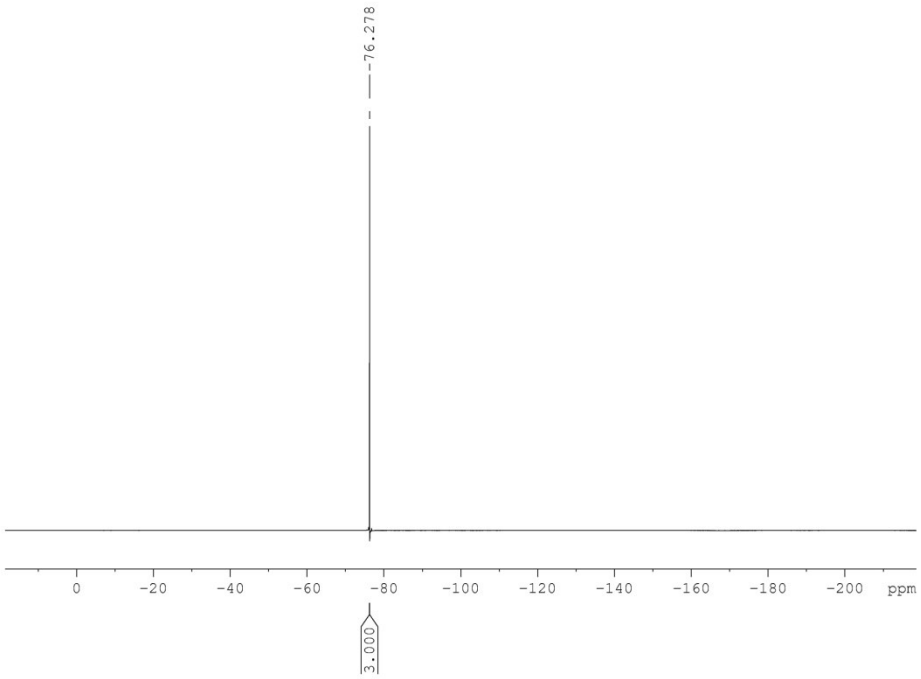
^{19}F NMR spectrum of compound **3j**



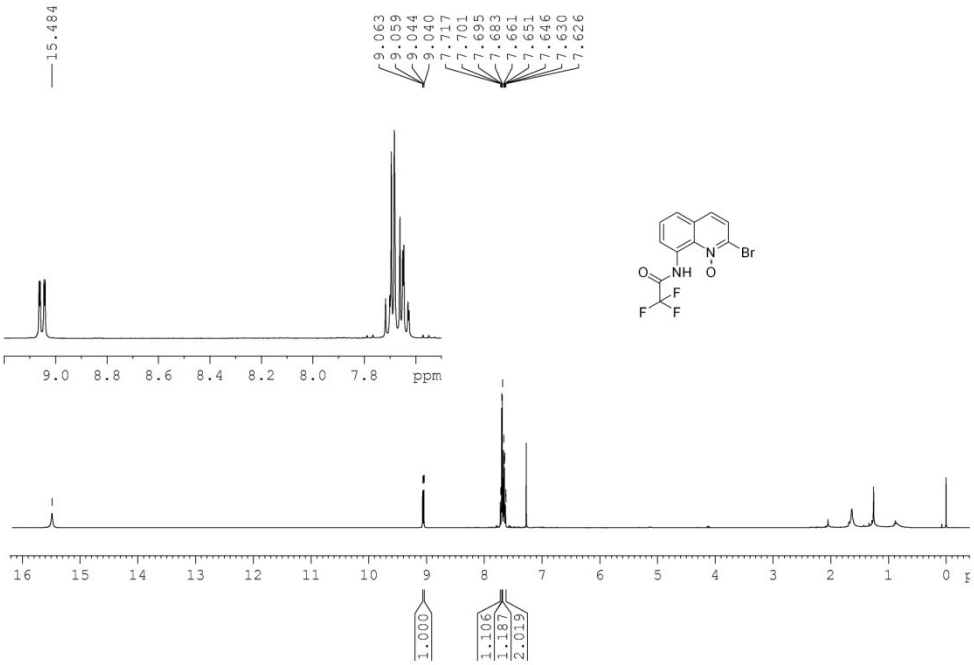
^{1}H NMR spectrum of compound **3k**



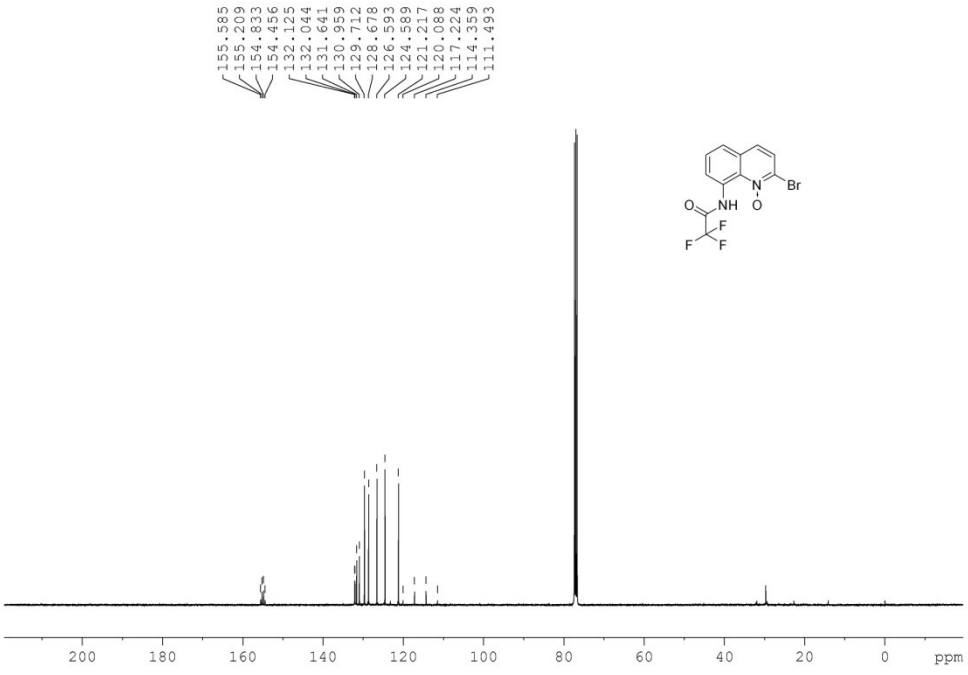
^{13}C NMR spectrum of compound **3k**



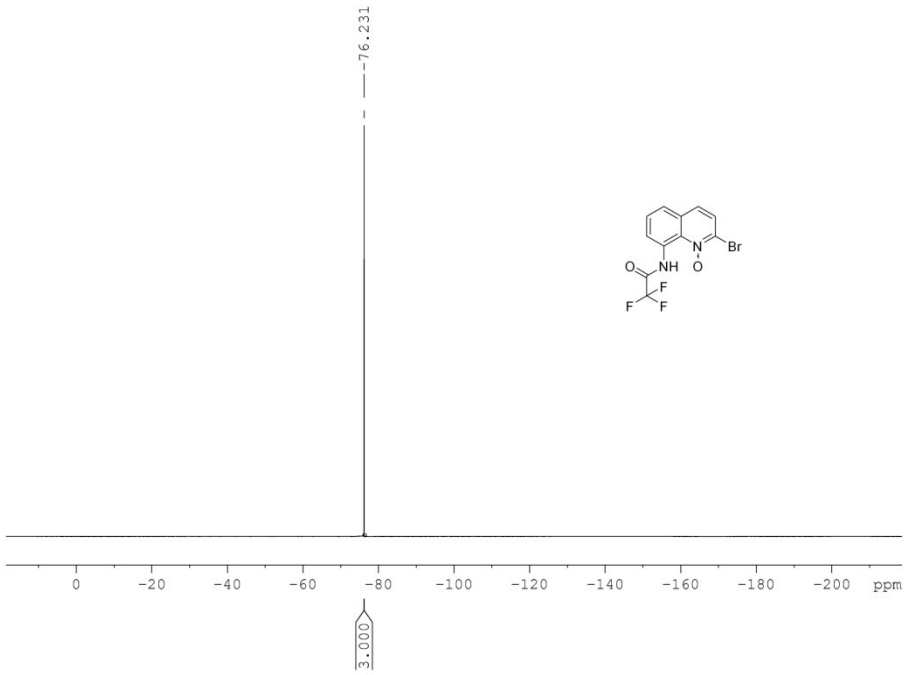
^{19}F NMR spectrum of compound **3k**



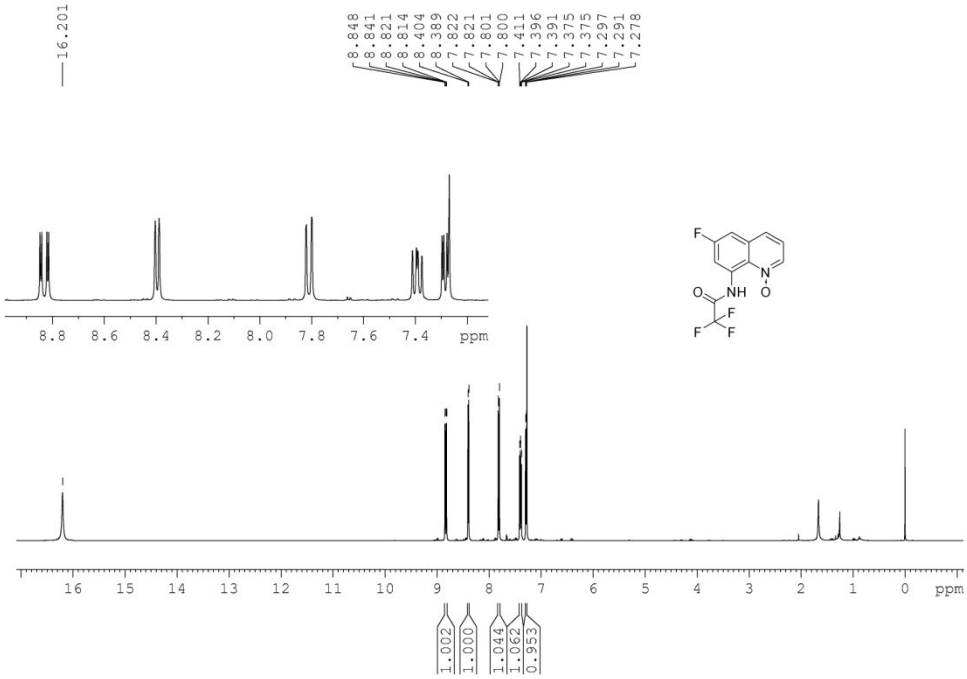
^{1}H NMR spectrum of compound **3l**



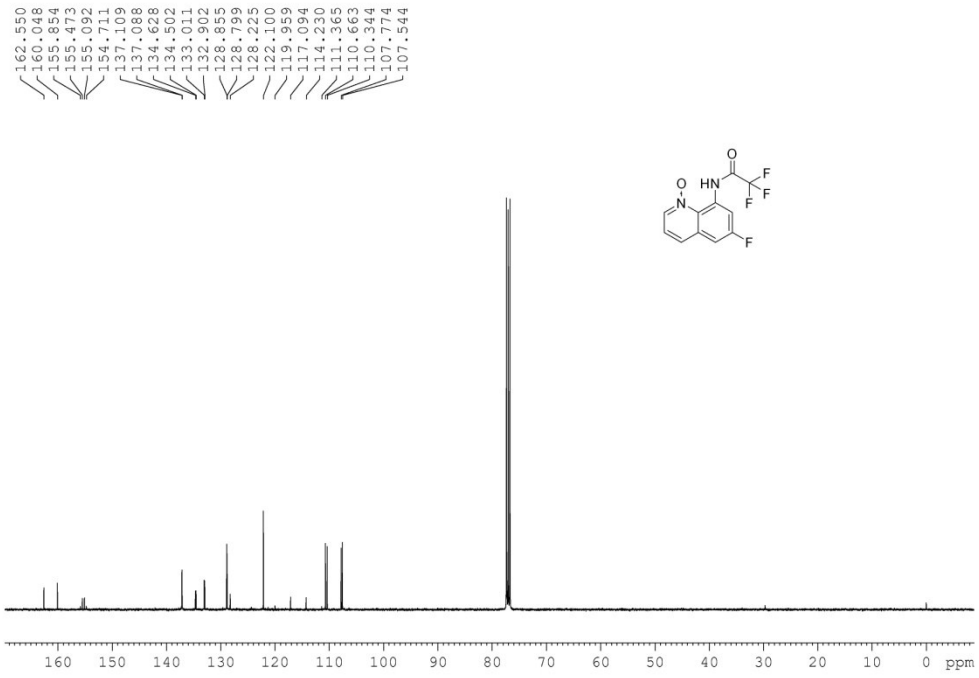
^{13}C NMR spectrum of compound **3l**



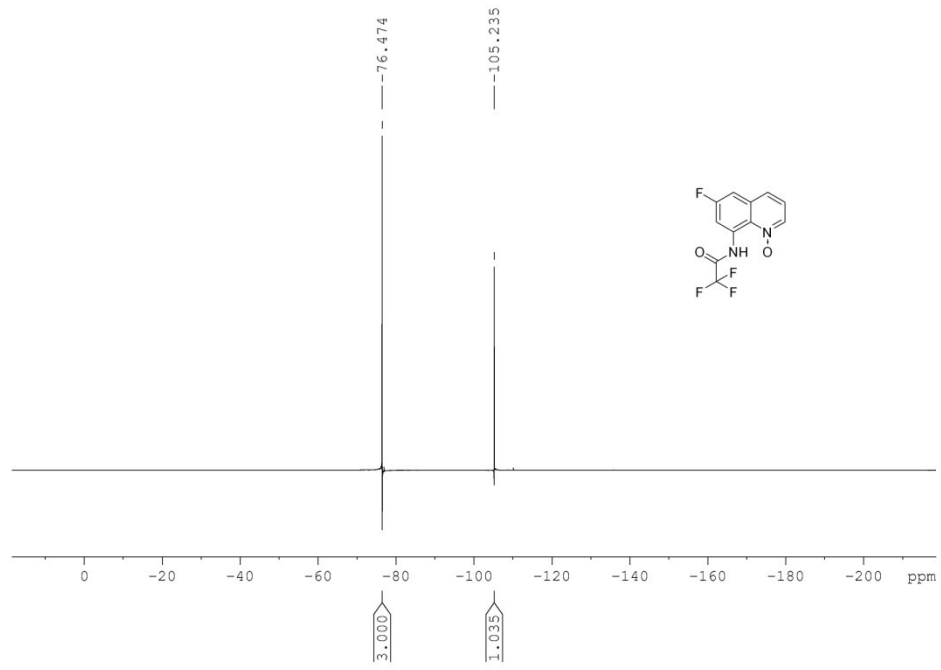
^{19}F NMR spectrum of compound **3l**



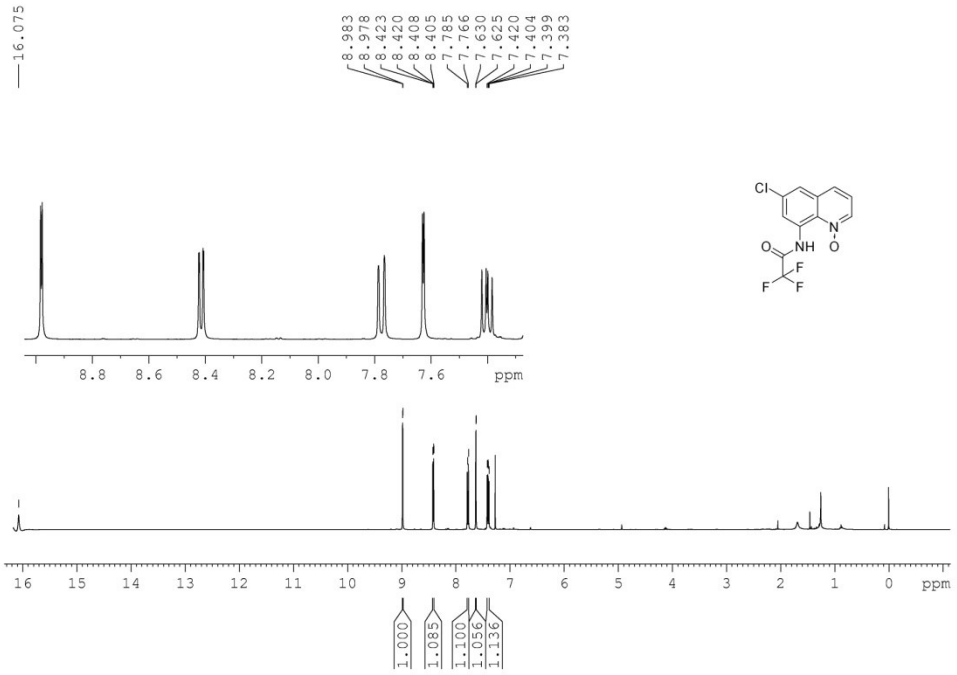
^{1}H NMR spectrum of compound **3m**



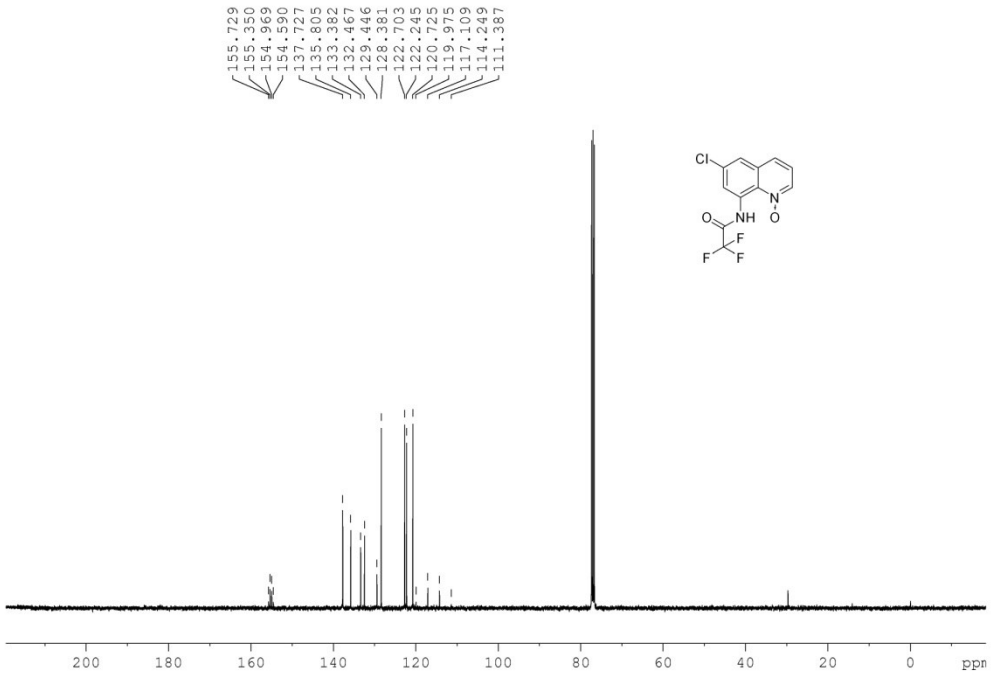
^{13}C NMR spectrum of compound **3m**



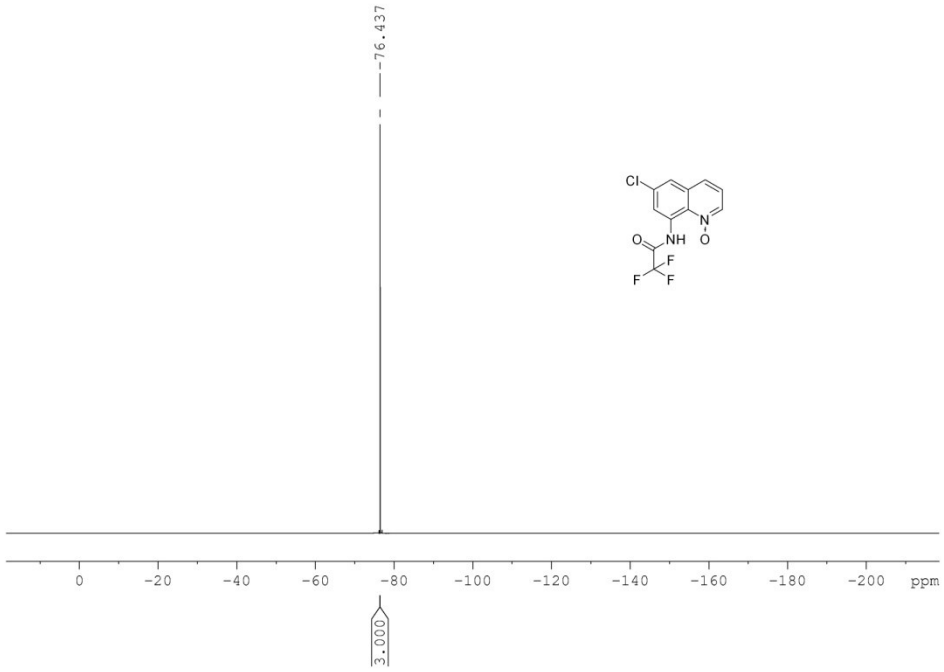
^{19}F NMR spectrum of compound **3m**



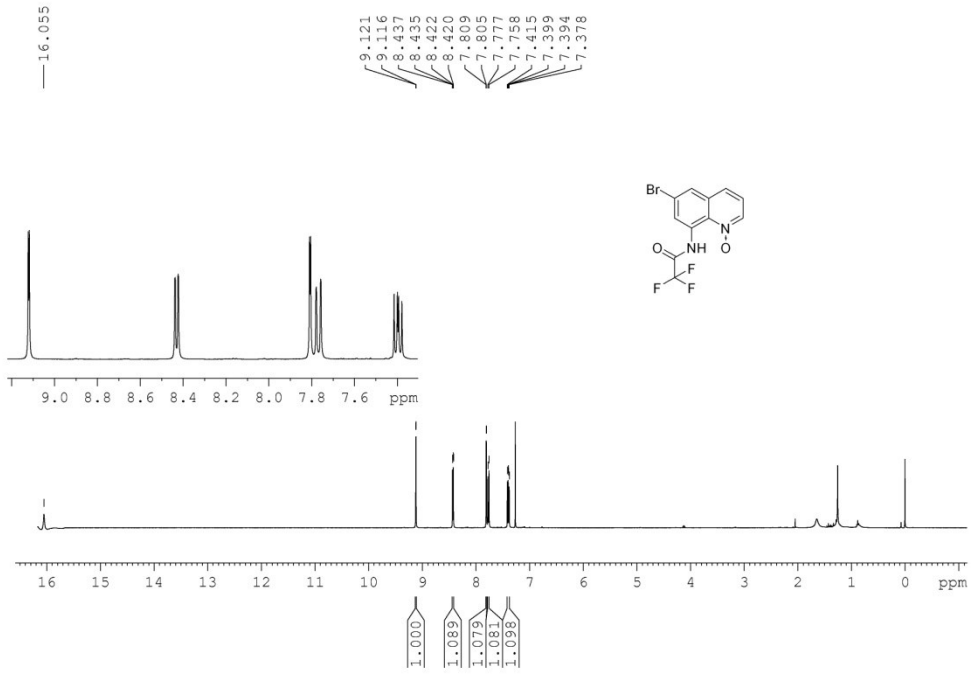
^{1}H NMR spectrum of compound **3n**



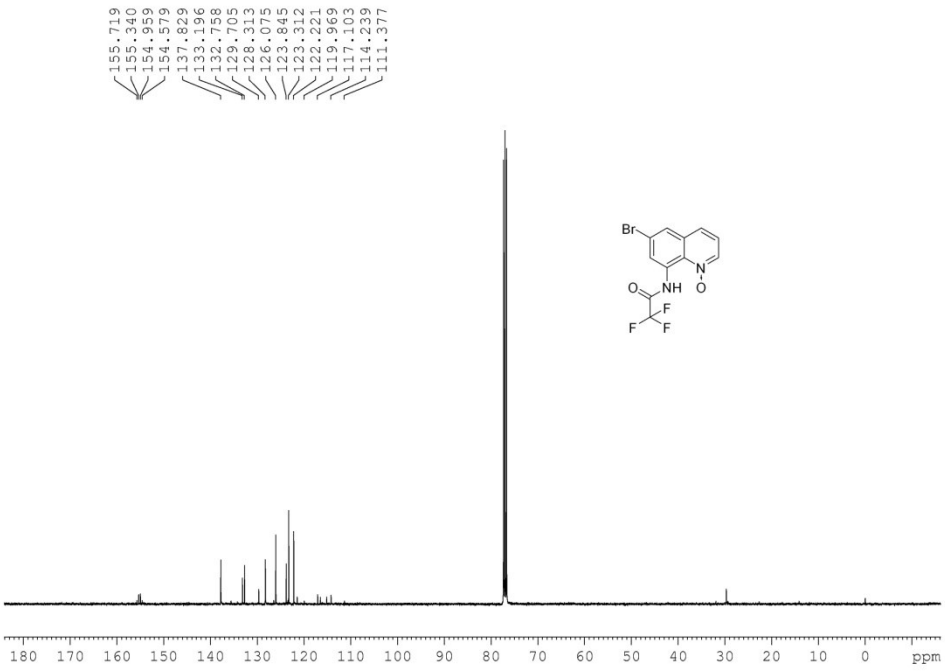
^{13}C NMR spectrum of compound **3n**



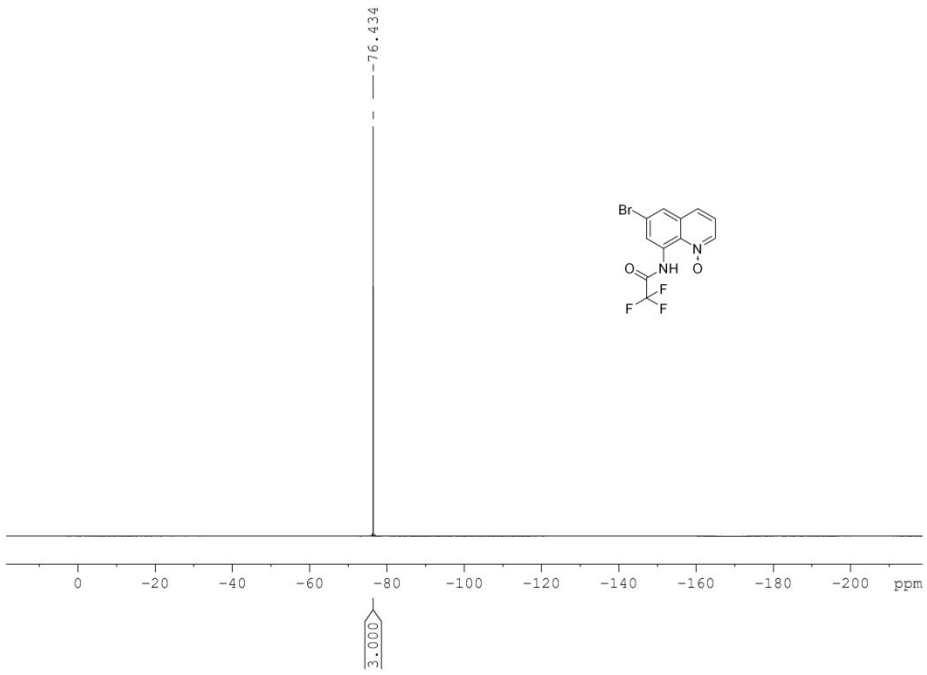
^{19}F NMR spectrum of compound **3n**



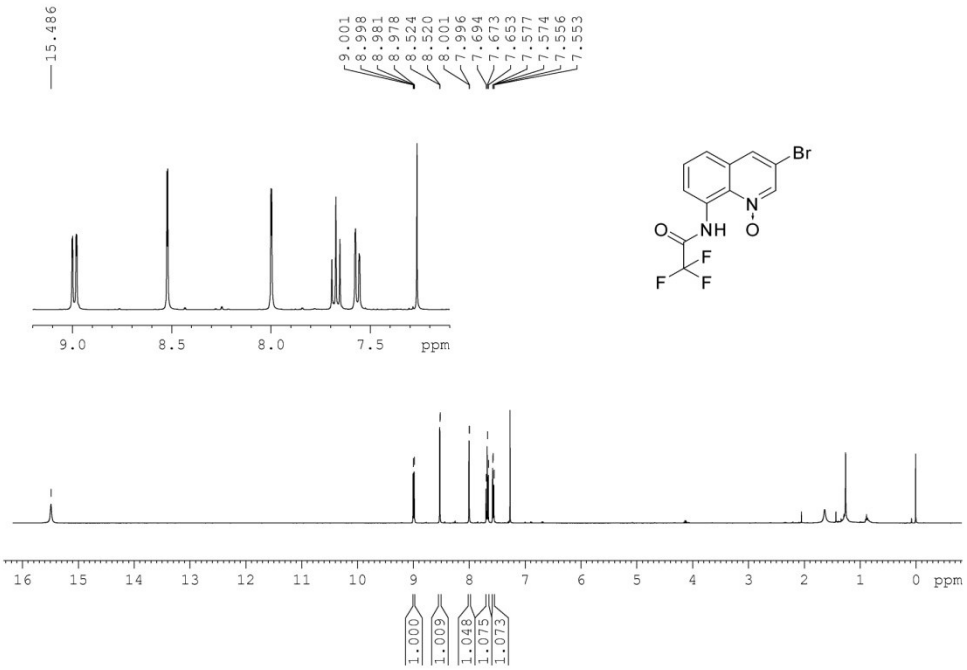
^{1}H NMR spectrum of compound **3o**



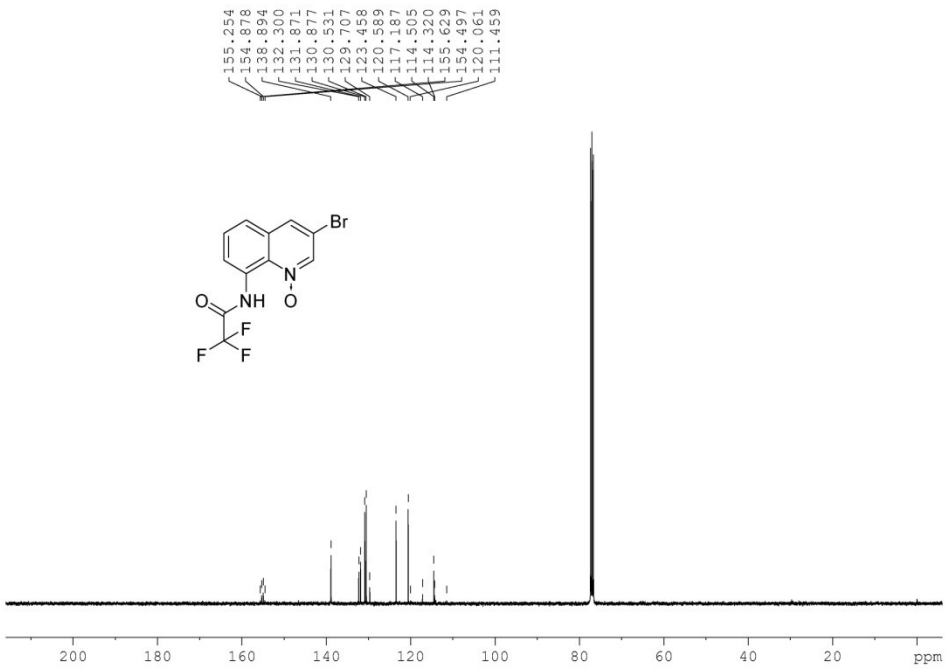
^{13}C NMR spectrum of compound **3o**



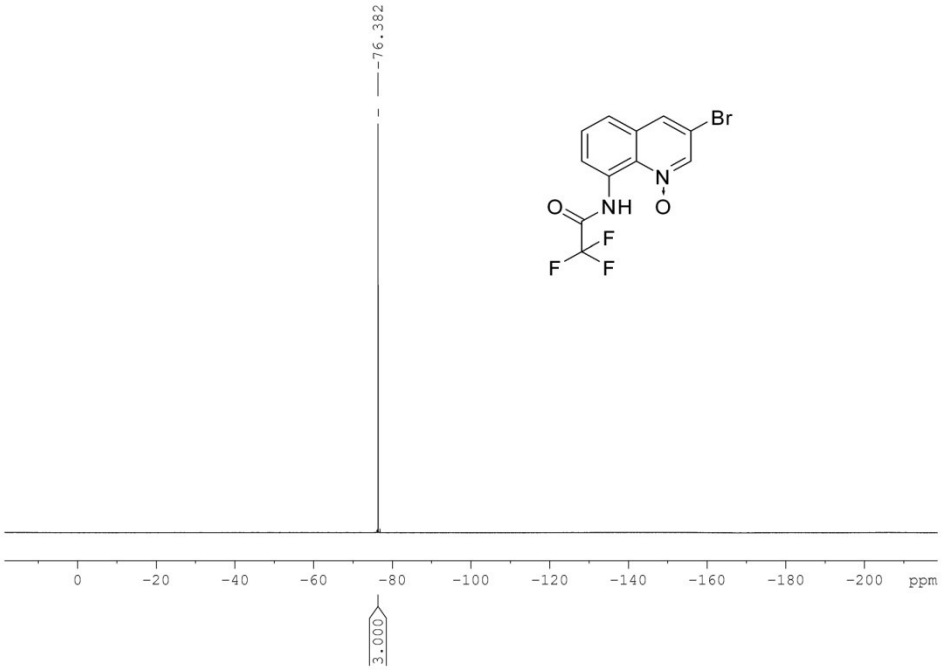
^{19}F NMR spectrum of compound **3o**



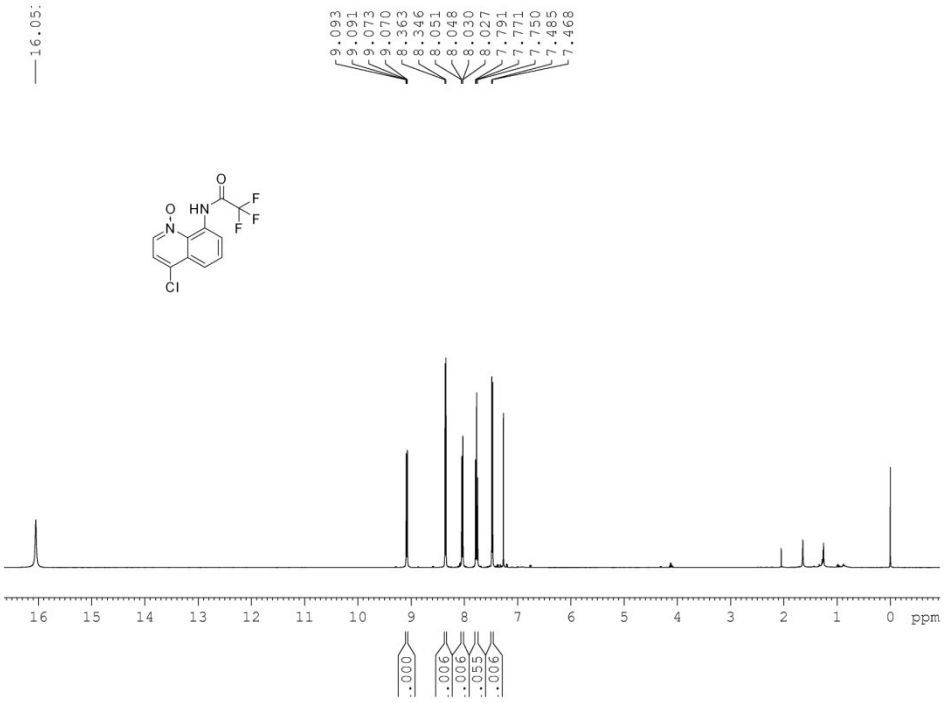
^{1}H NMR spectrum of compound **3p**



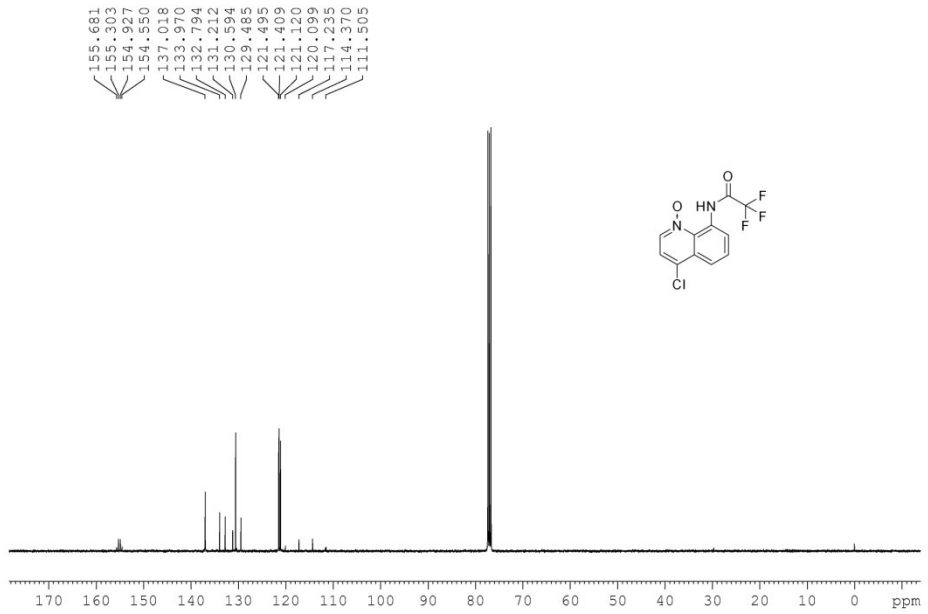
^{13}C NMR spectrum of compound **3p**



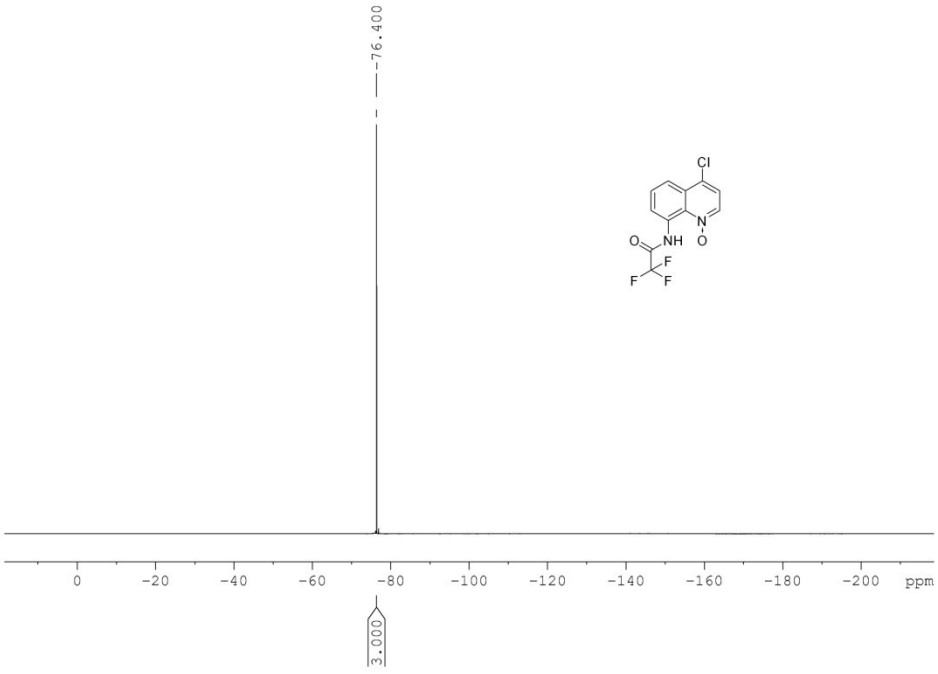
^{19}F NMR spectrum of compound **3p**



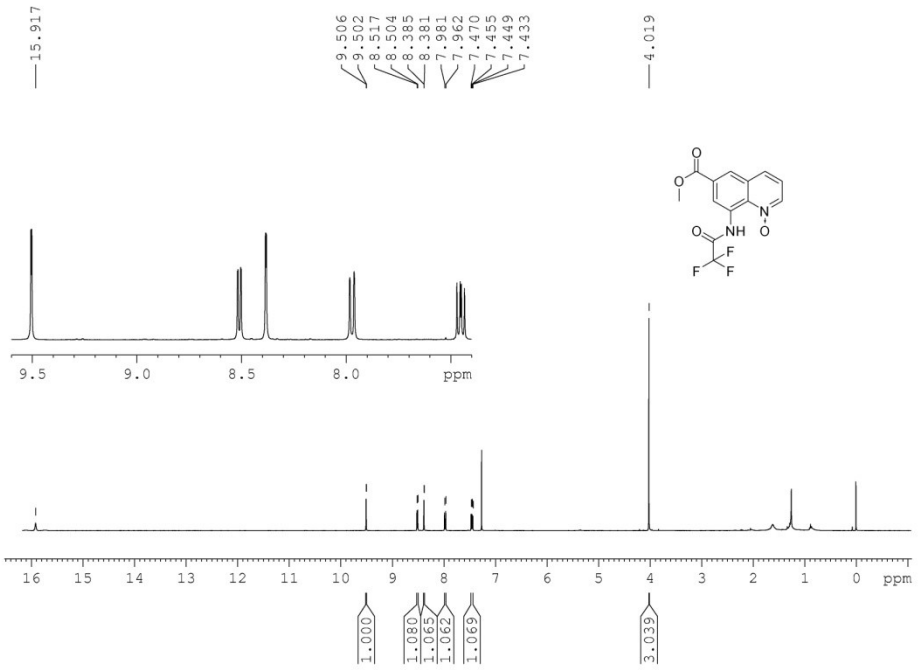
^{1}H NMR spectrum of compound **3q**



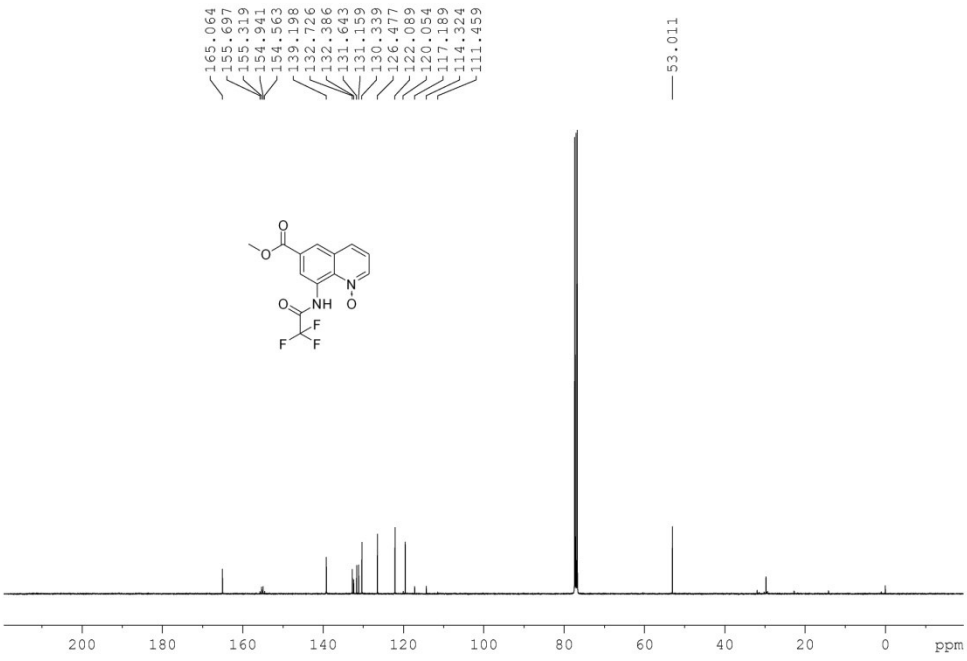
^{13}C NMR spectrum of compound **3q**



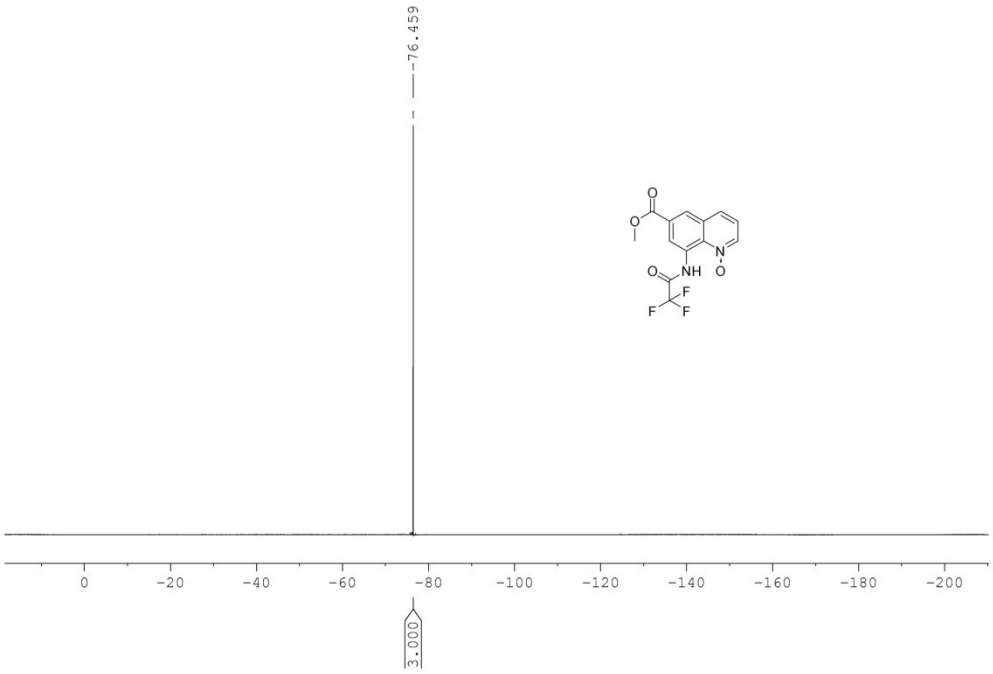
^{19}F NMR spectrum of compound **3q**



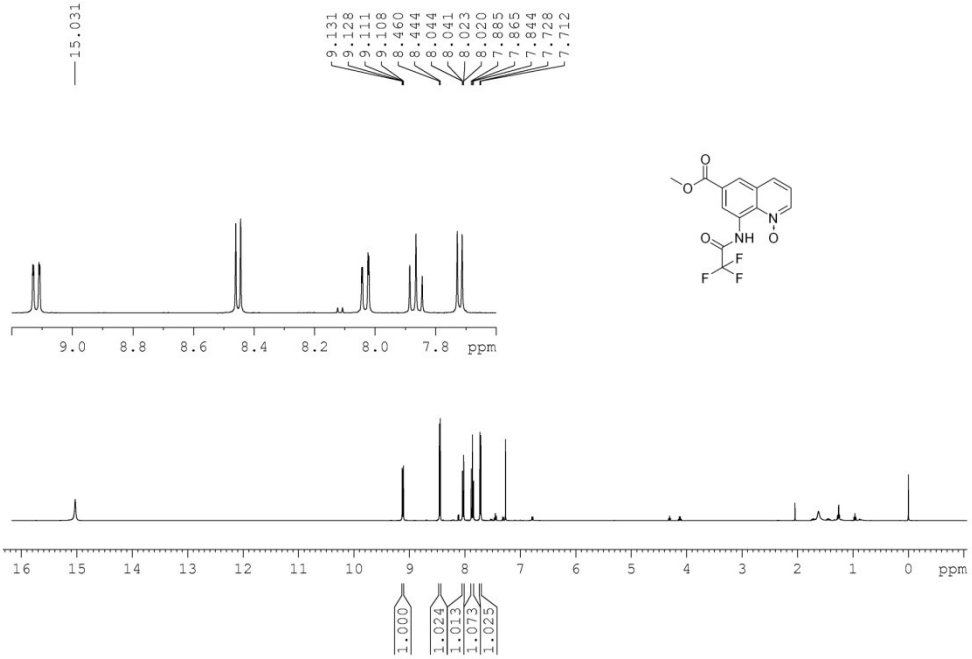
^{1}H NMR spectrum of compound **3r**



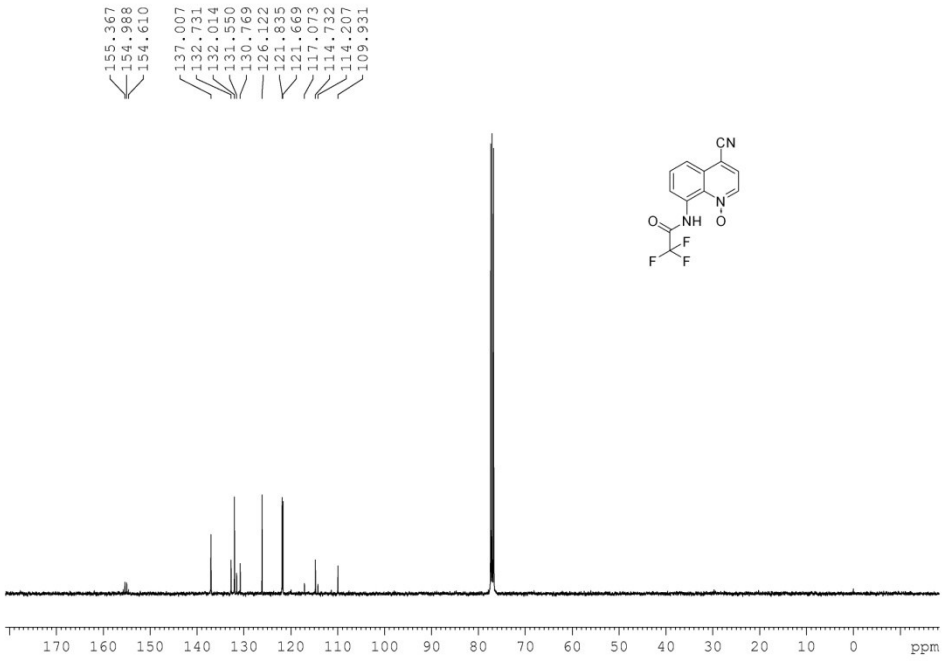
^{13}C NMR spectrum of compound **3r**



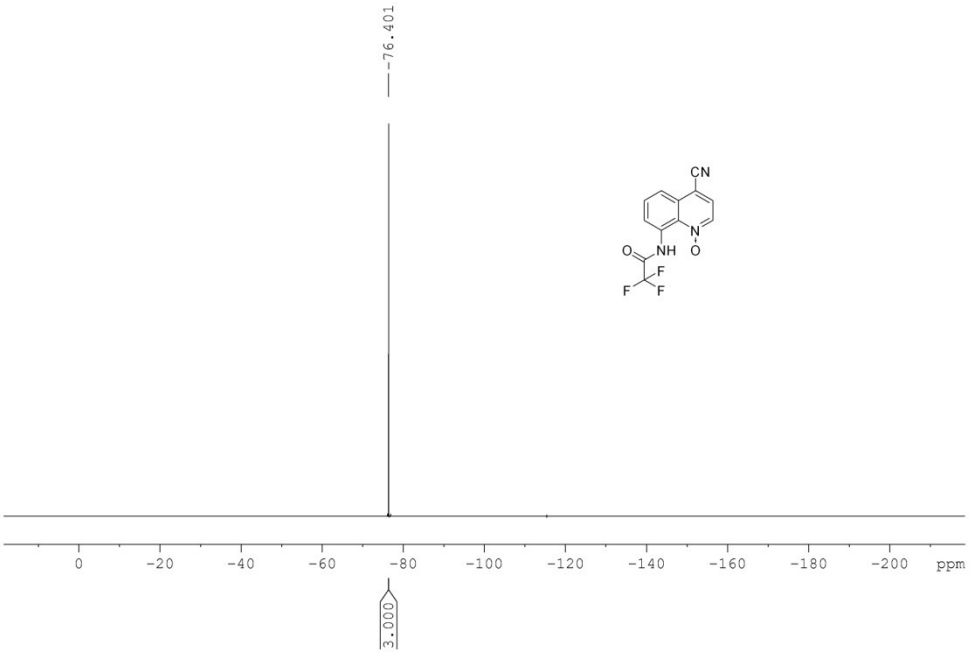
^{19}F NMR spectrum of compound **3r**



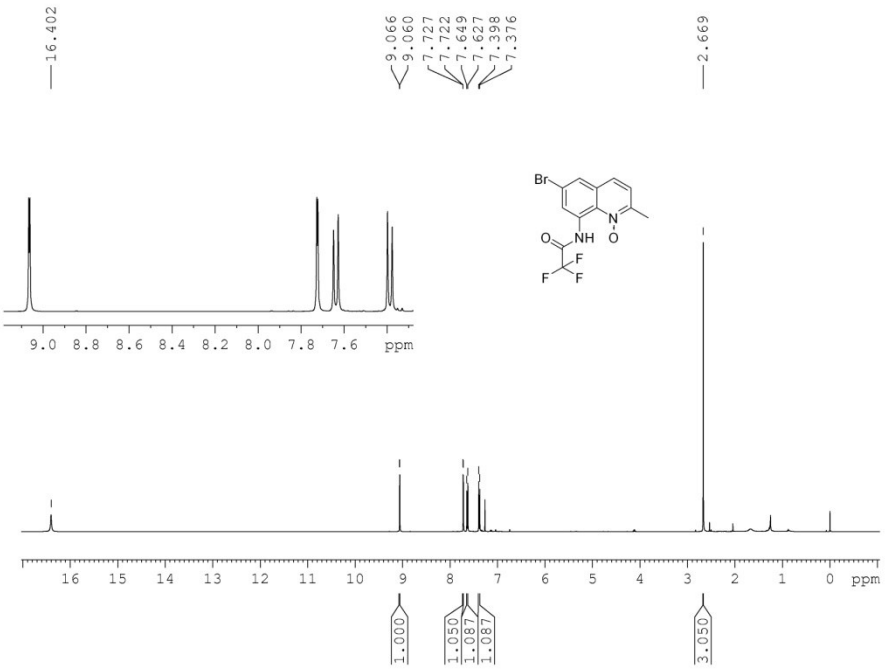
^{1}H NMR spectrum of compound **3s**



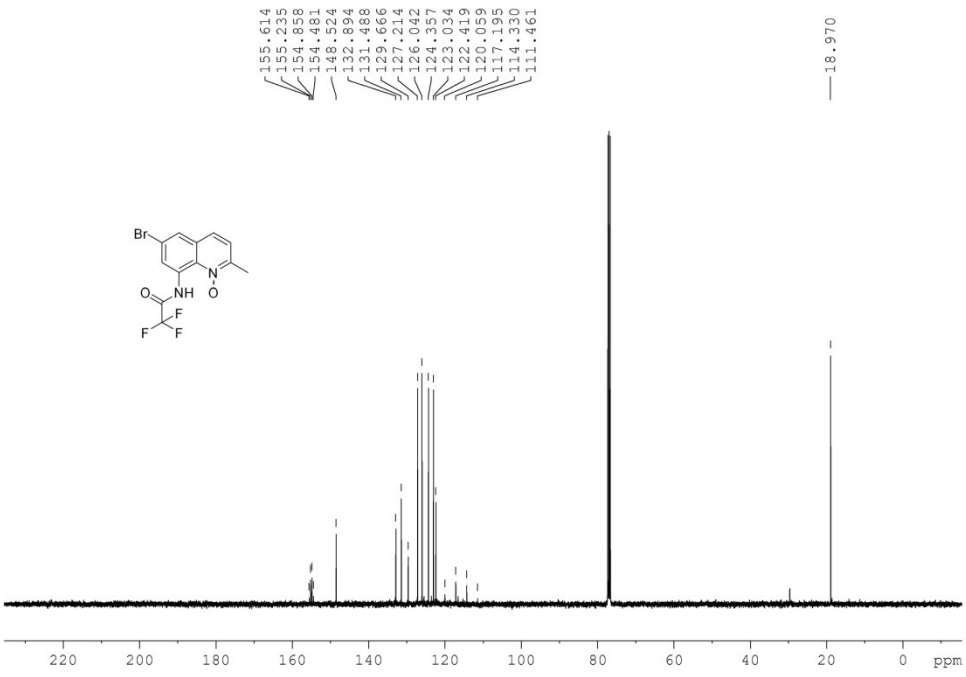
^{13}C NMR spectrum of compound **3s**



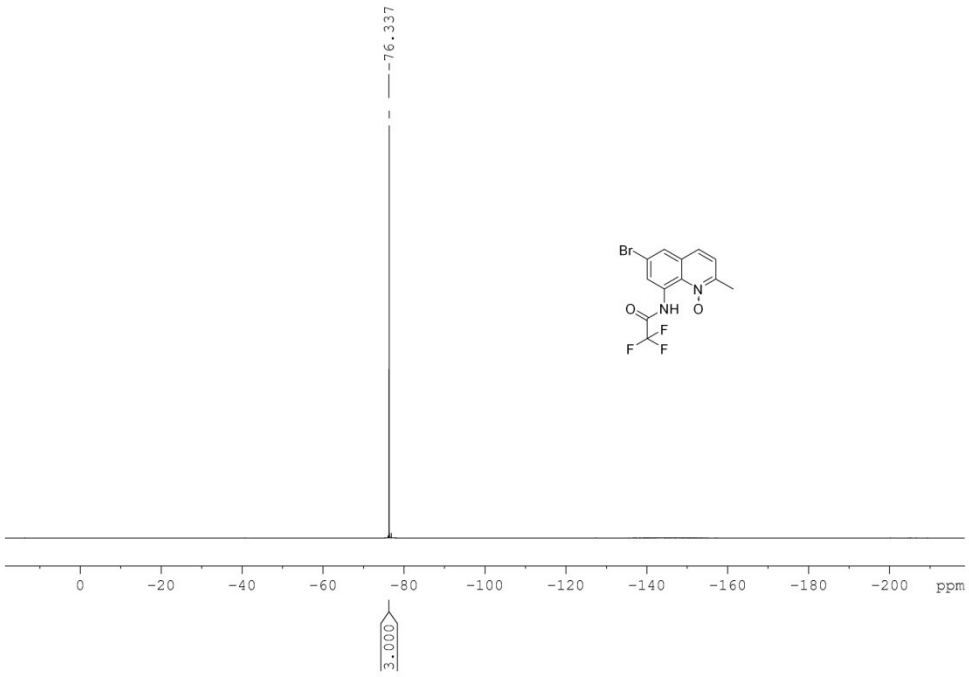
^{19}F NMR spectrum of compound **3s**



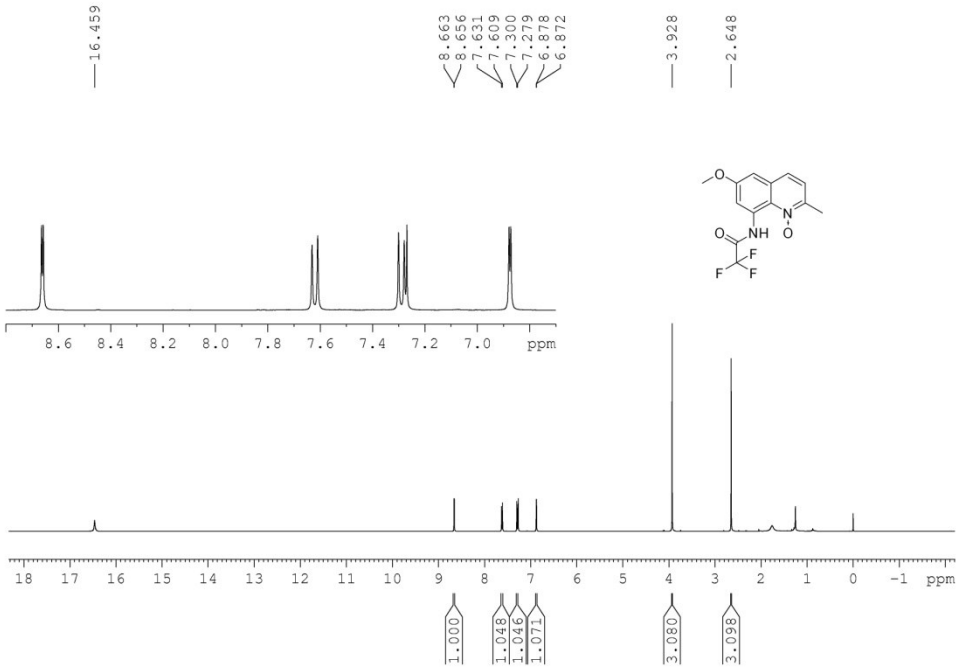
^{1}H NMR spectrum of compound **3t**



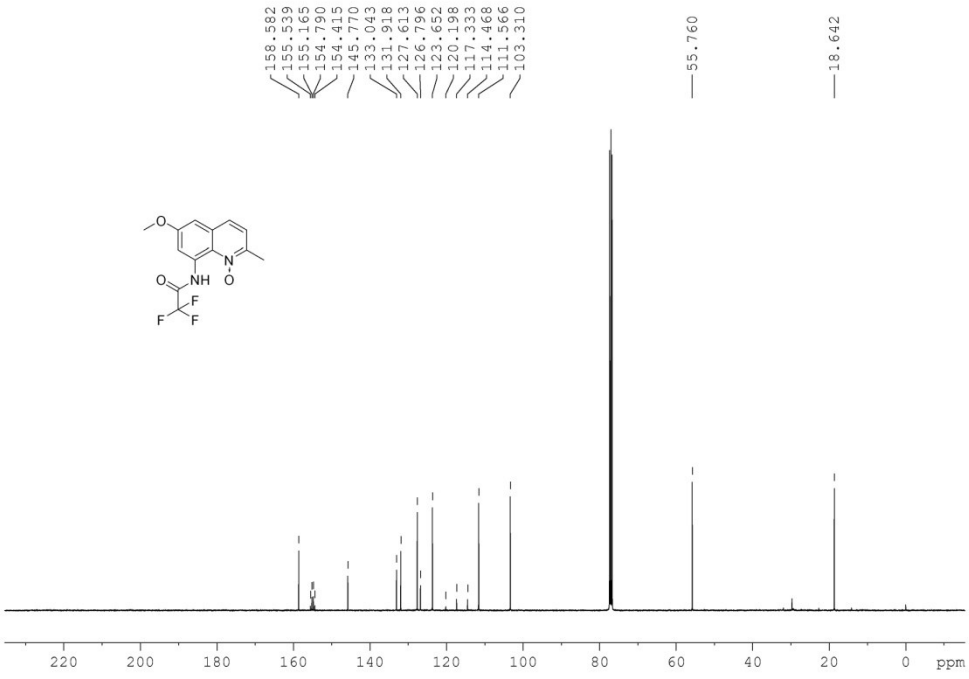
^{13}C NMR spectrum of compound **3t**



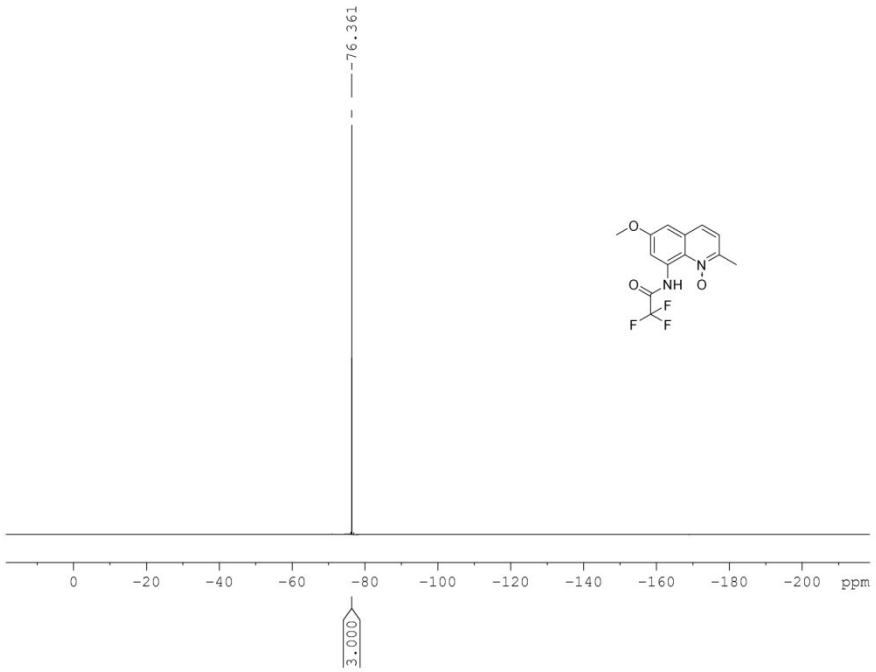
^{19}F NMR spectrum of compound **3t**



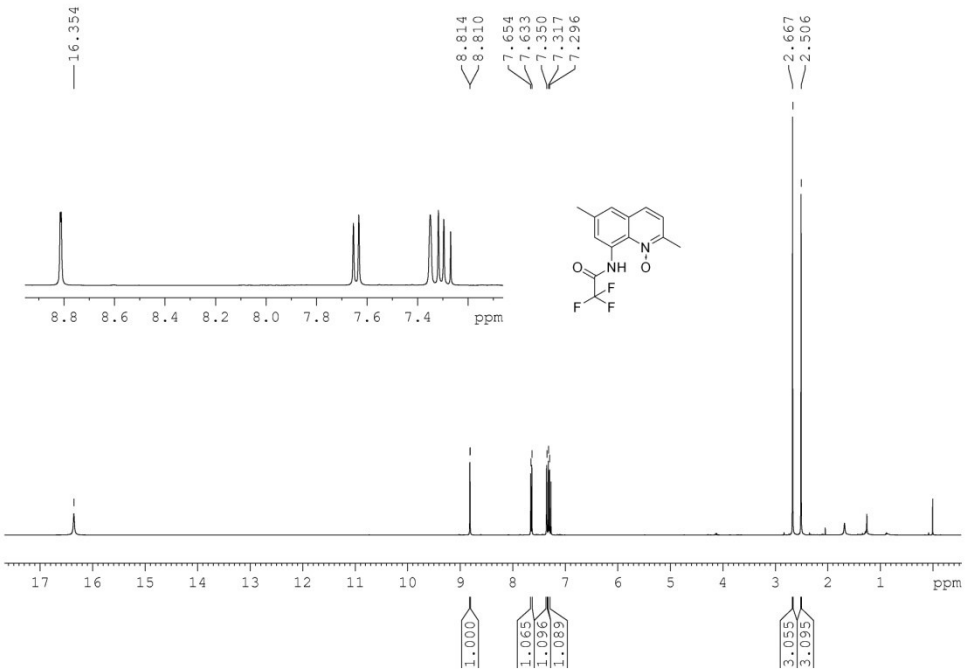
^{1}H NMR spectrum of compound **3u**



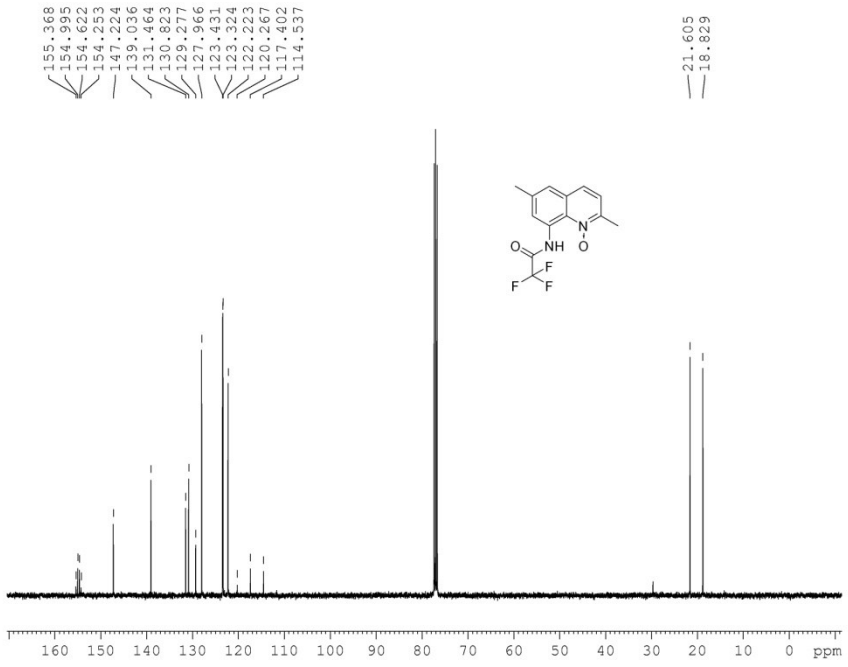
^{13}C NMR spectrum of compound **3u**



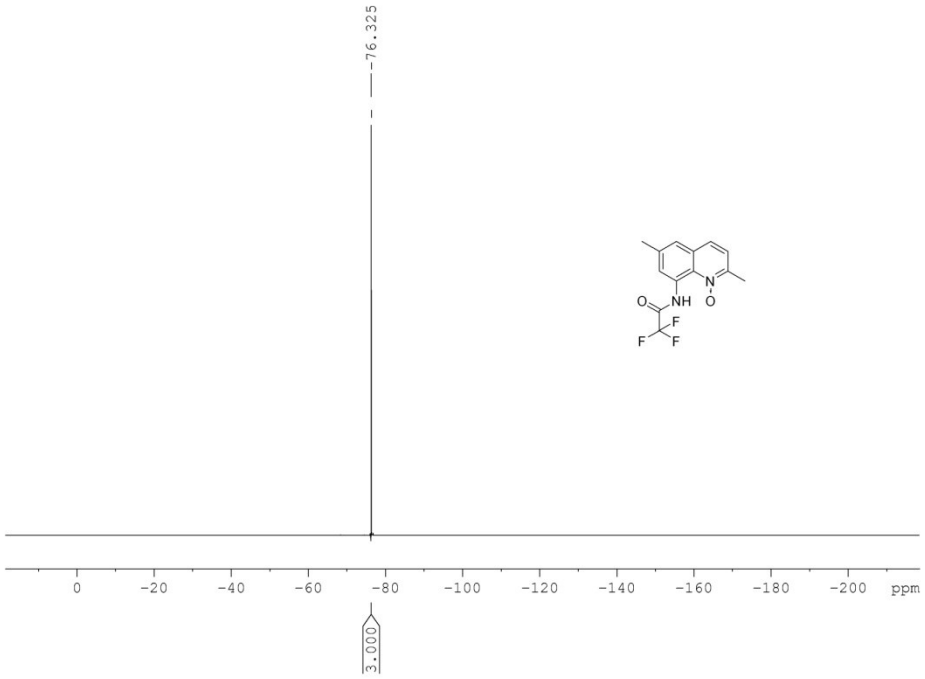
^{19}F NMR spectrum of compound **3u**



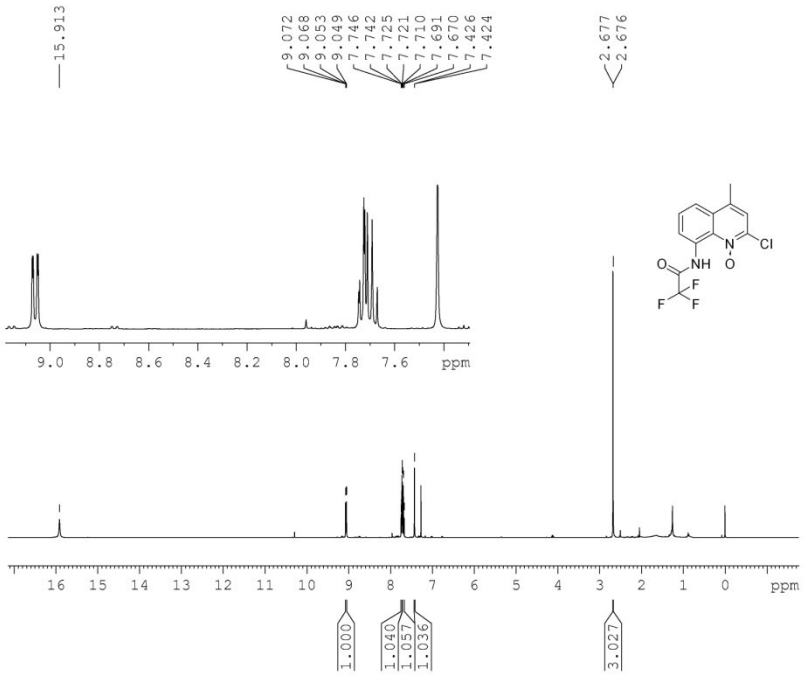
^{1}H NMR spectrum of compound **3v**



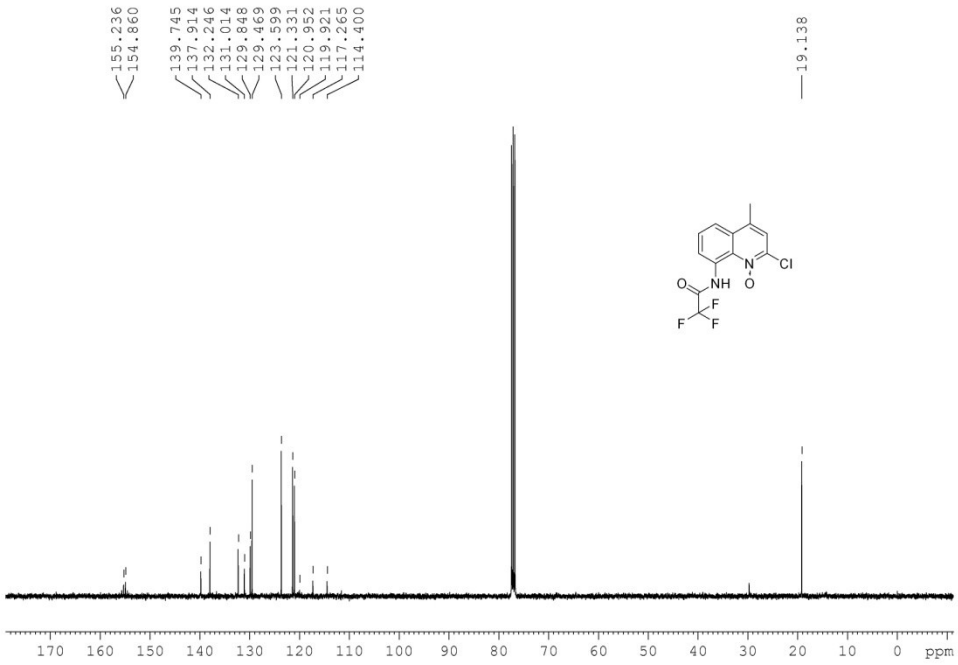
^{13}C NMR spectrum of compound **3v**



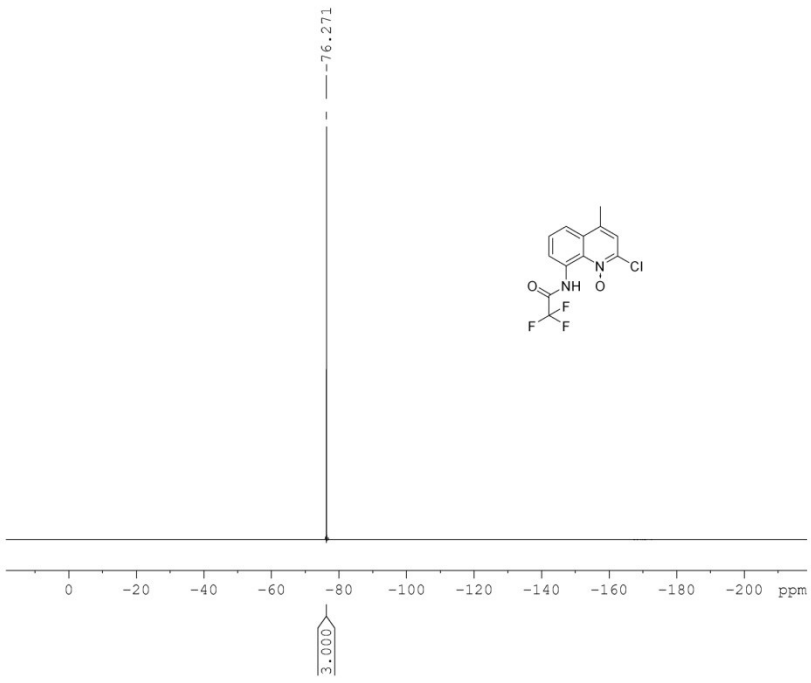
^{19}F NMR spectrum of compound **3v**



^{1}H NMR spectrum of compound **3w**



^{13}C NMR spectrum of compound **3w**



^{19}F NMR spectrum of compound **3w**