Supporting information

Electrochemical trifluoromethylation of 2-isocyanobiaryls using CF_3SO_2Na: Synthesis of 6-(trifluoromethyl)phenanthridines

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1. Cyclic voltammetry

Cyclic voltammetry experiments were conducted in a 4-neck flask that contained the analytes dissolved in a 0.1 M solution of tetrabutylammonium hexafluorophosphate in acetonitrile. A glassy carbon disc (Ø 3 mm), a Pt wire (Ø 0.5 mm), and Ag/AgCl electrode were used as a working electrode, a counter electrode, and a pseudo-reference electrode, respectively. The voltage was measured by PalmSens4 potentiostat in the presence of ferrocene as an external standard, at a scan rate of 0.1V/s (Fig. S1 and S2).

Fig. S1 Cyclic voltammetry experiment set up.

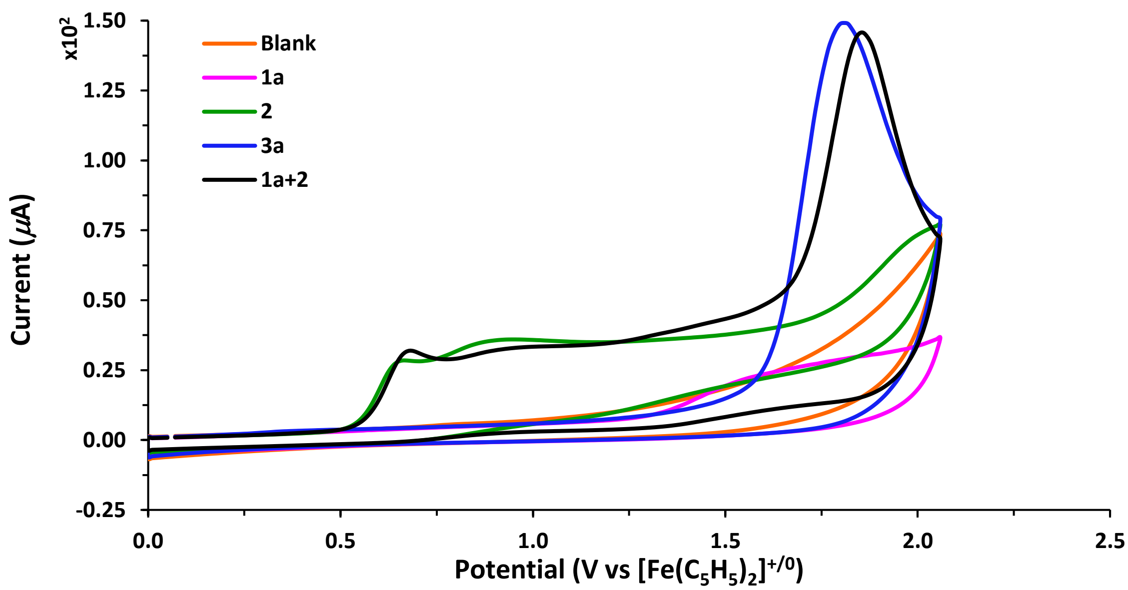


Fig. S2 Cyclic voltammograms of **Blank**, **1a**, **2**, and **3a**.

2. Faradaic calculation

$$Faradaic\ efficiency = \frac{\mathrm{Q\ experimental}}{\mathrm{Q\ theoretical}} \times 100$$

$$Faradaic\ efficiency = \frac{\mathrm{z \times n \times F}}{\mathrm{Q\ theoretical}} \times 100$$

With z = number of electron required for the reaction used = 2

n = mol of product obtained = (maybe use the number in moles here and list the mass in parentheses) 0.0447 g (88%, MW. of product = 247.2202 g/mol)

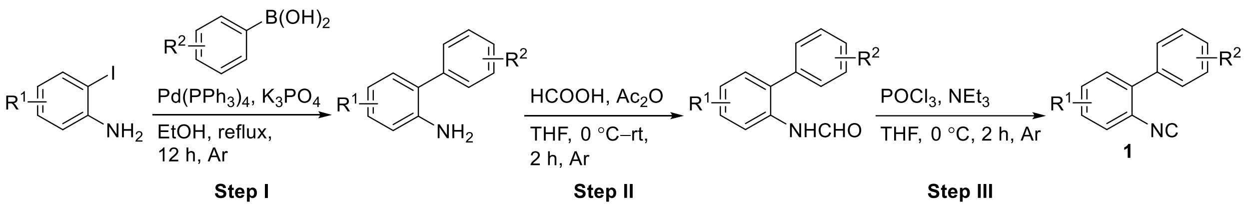
F = Faradaic constant (96485 C/mol)

$Q_{\text{theoretical}}$ = I (current, Ampere) × t (reaction time, second)

$$Faradaic\ efficiency = \frac{2 \times (\frac{0.0447\ g}{247.2202 g.mol}) \times 96485}{0.005\ \text{A} \times 7200\ \text{second}} \times 100$$

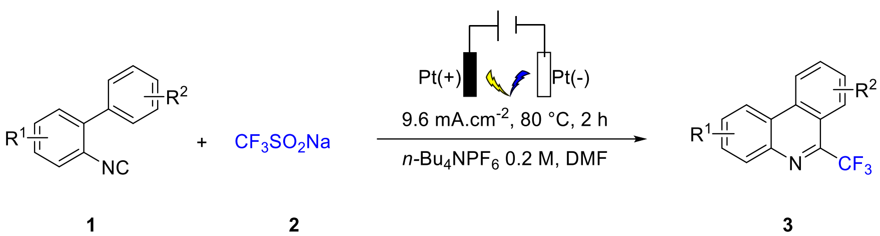
$$Faradaic\ efficiency = 94\%$$

3. General procedure A (Synthesis of 2-isocyanobiphenyls 1)



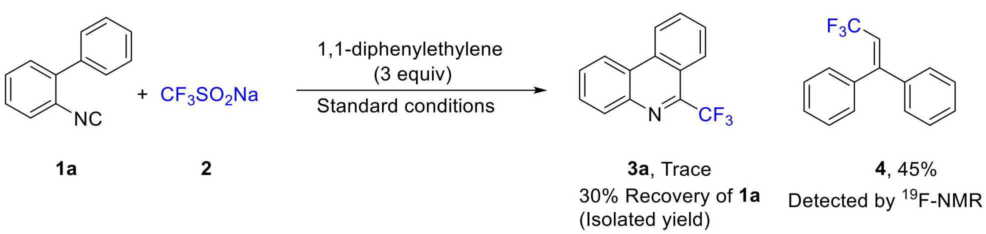
Scheme S1 Synthesis of 2-isocyanobiphenyls **1**

4. General procedure B (Synthesis of phenanthridines 3)



Scheme S2 Synthesis of phenanthridines **3**.

5. Radical trapping experiment



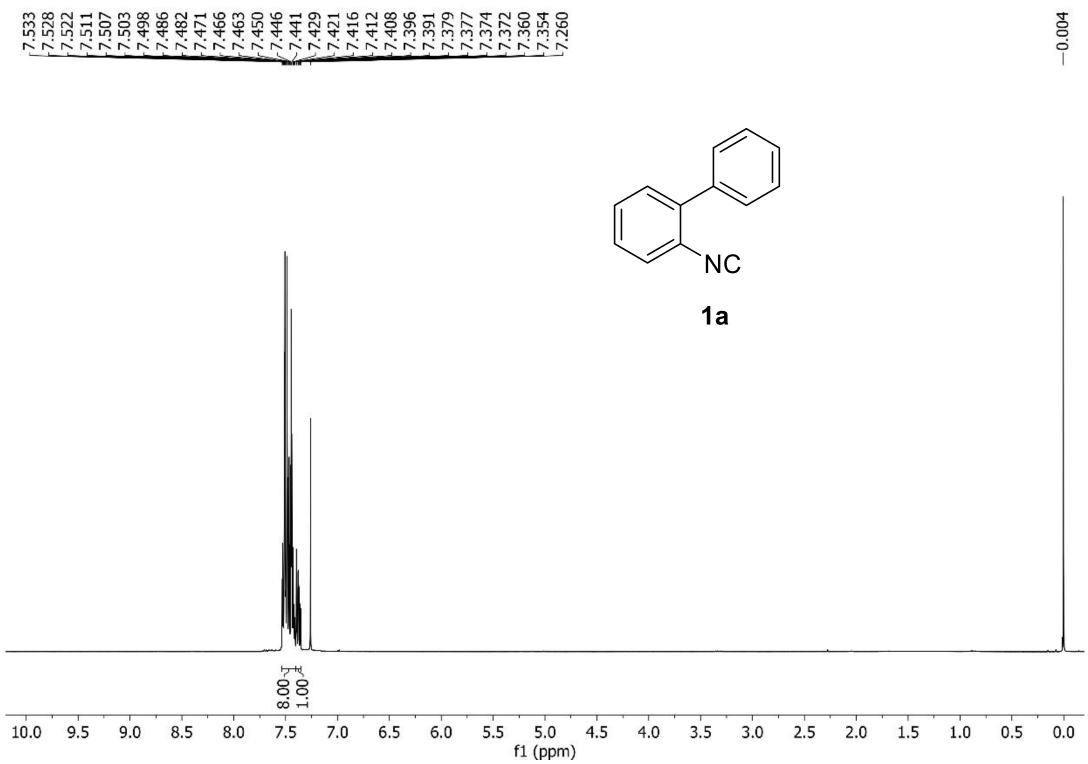
Scheme S3 Radical trapping experiment.

6. Picture of experiment set up

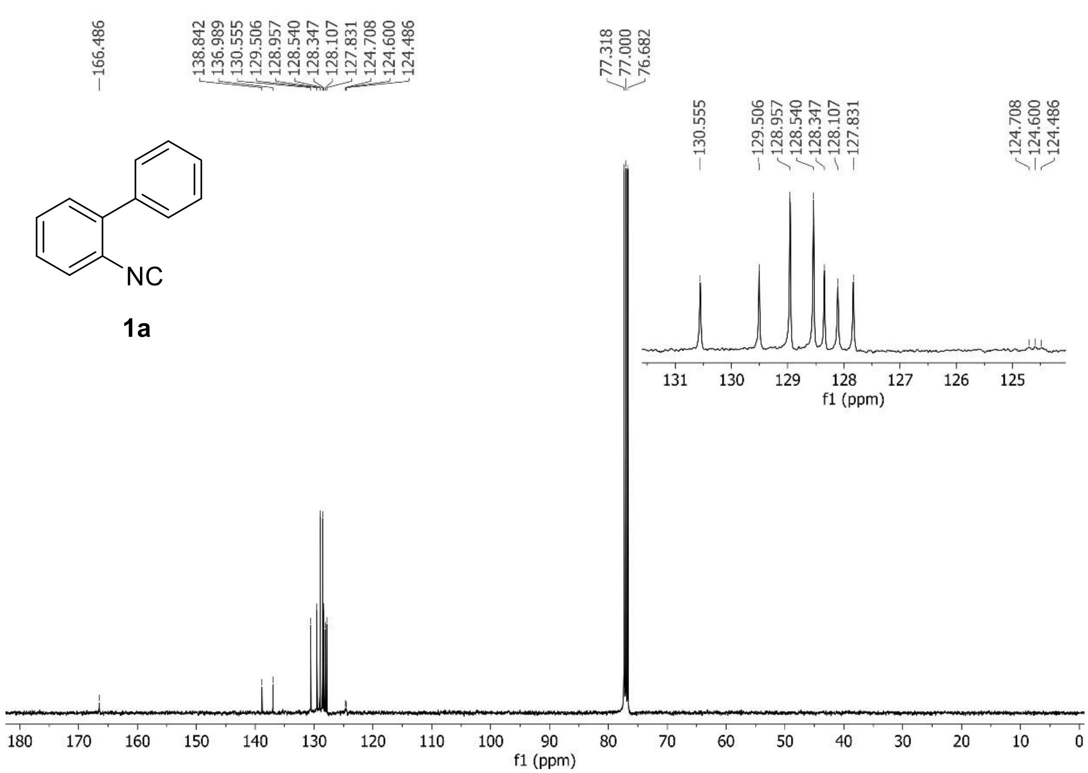
Fig. S3 Reactors set up and electrode.

7. NMR spectra of 2-isocyanobiphenyls 1a-1s

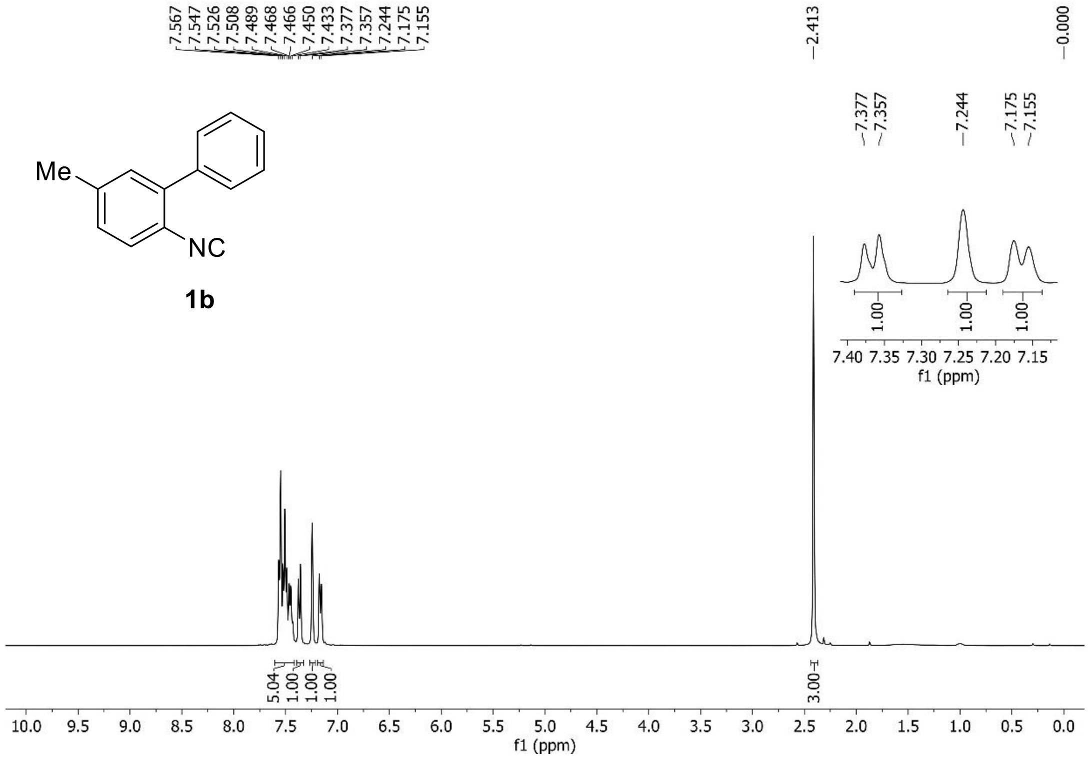
^{1}H NMR spectrum of **1a** (400 MHz, $CDCl_3$)



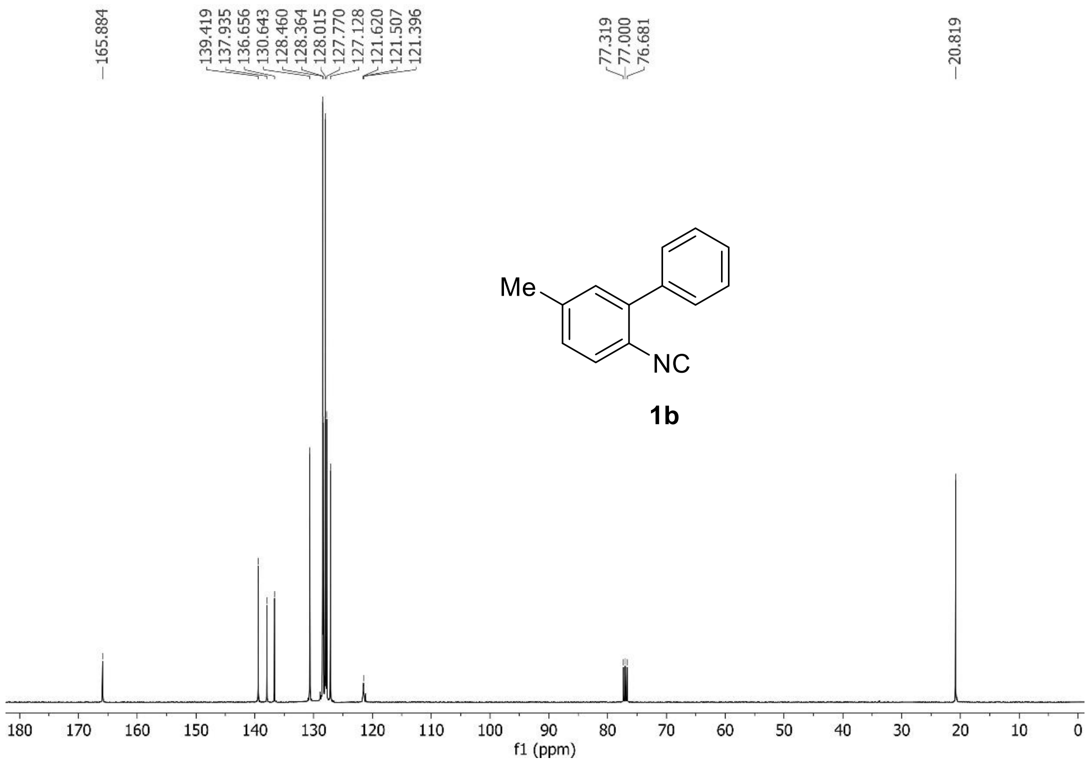
^{13}C NMR spectrum of **1a** (100 MHz, $CDCl_3$)



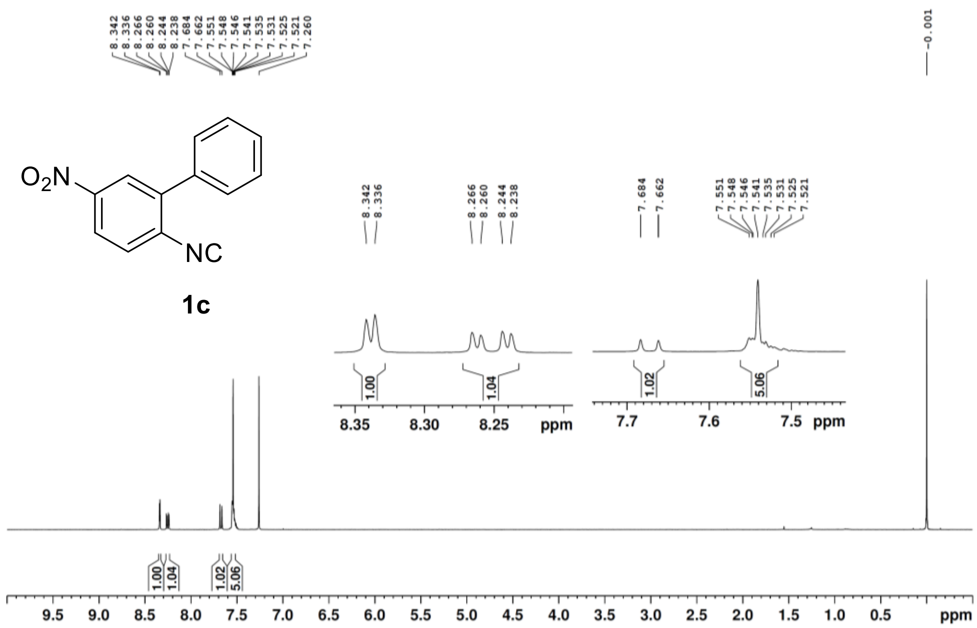
^{1}H NMR spectrum of **1b** (400 MHz, $CDCl_3$)



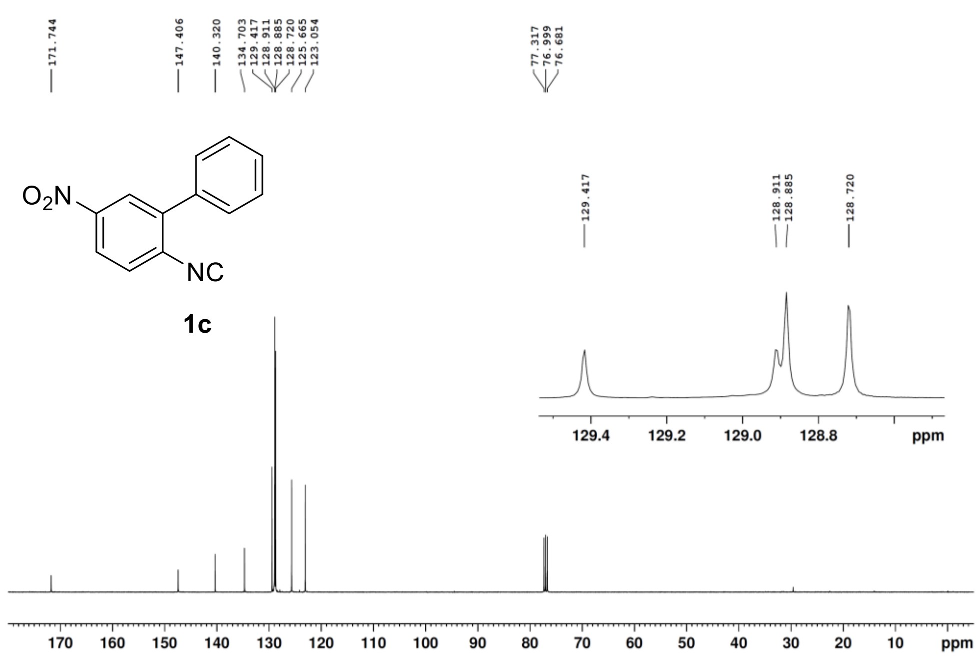
^{13}C NMR spectrum of **1b** (100 MHz, $CDCl_3$)



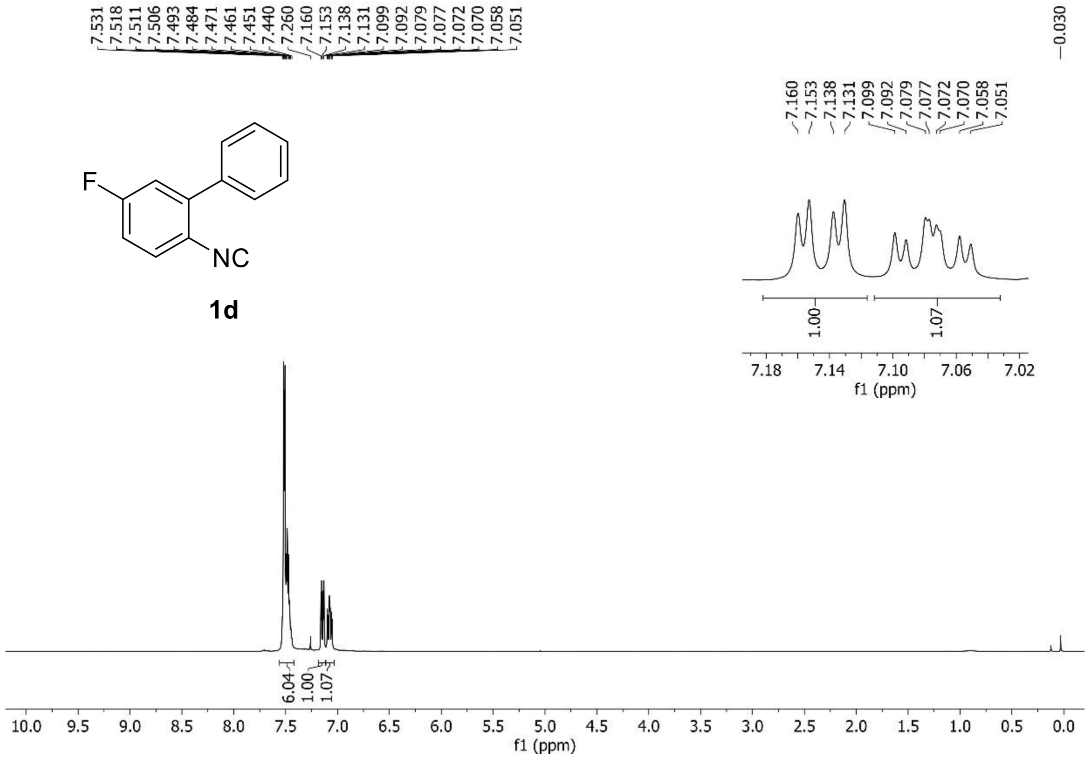
[1]H NMR spectrum of **1c** (400 MHz, $CDCl_3$)



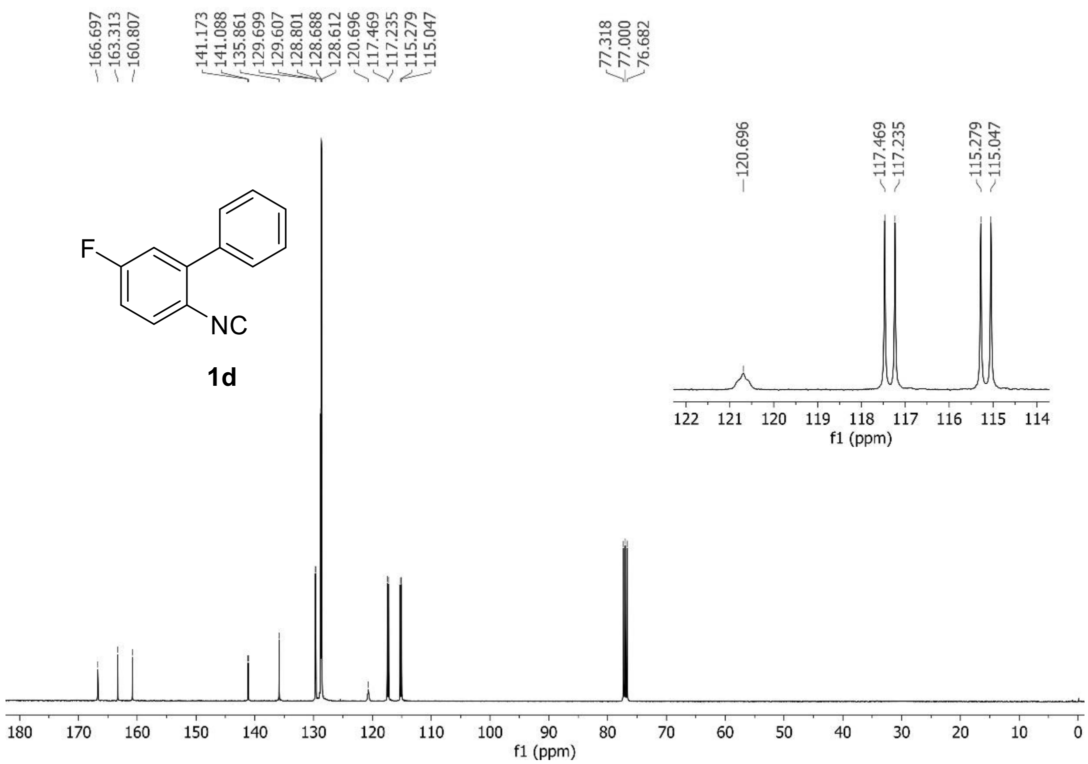
[13]C NMR spectrum of **1c** (100 MHz, $CDCl_3$)



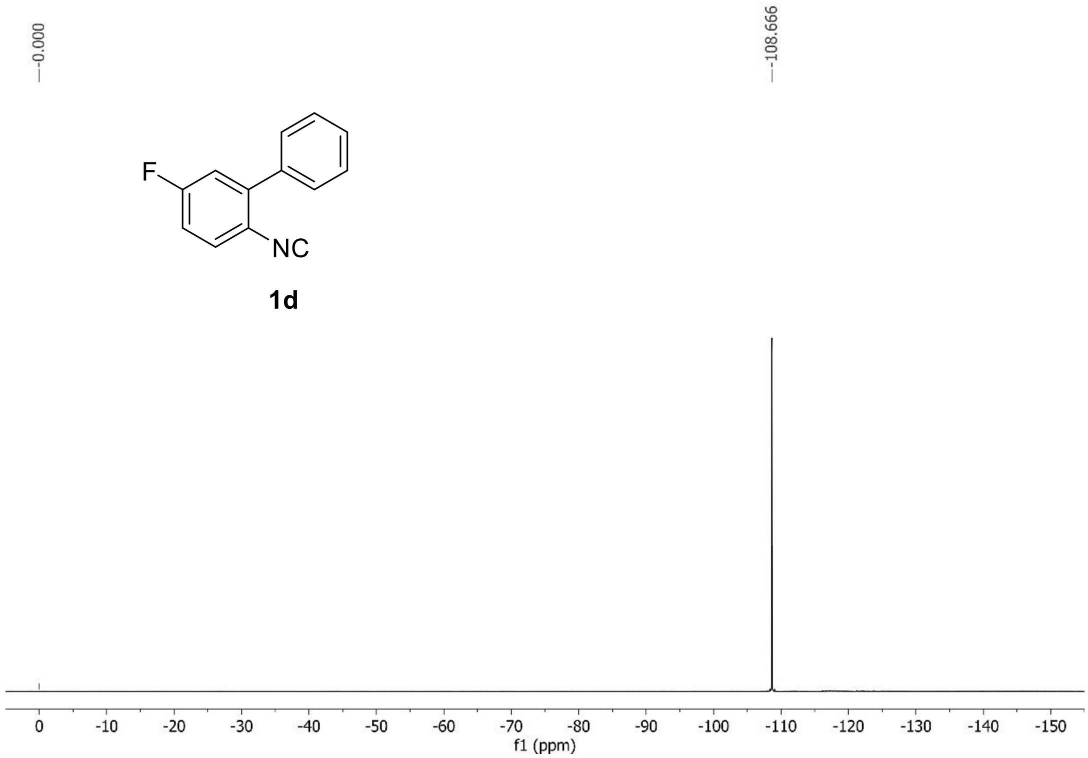
^{1}H NMR spectrum of **1d** (400 MHz, $CDCl_3$)



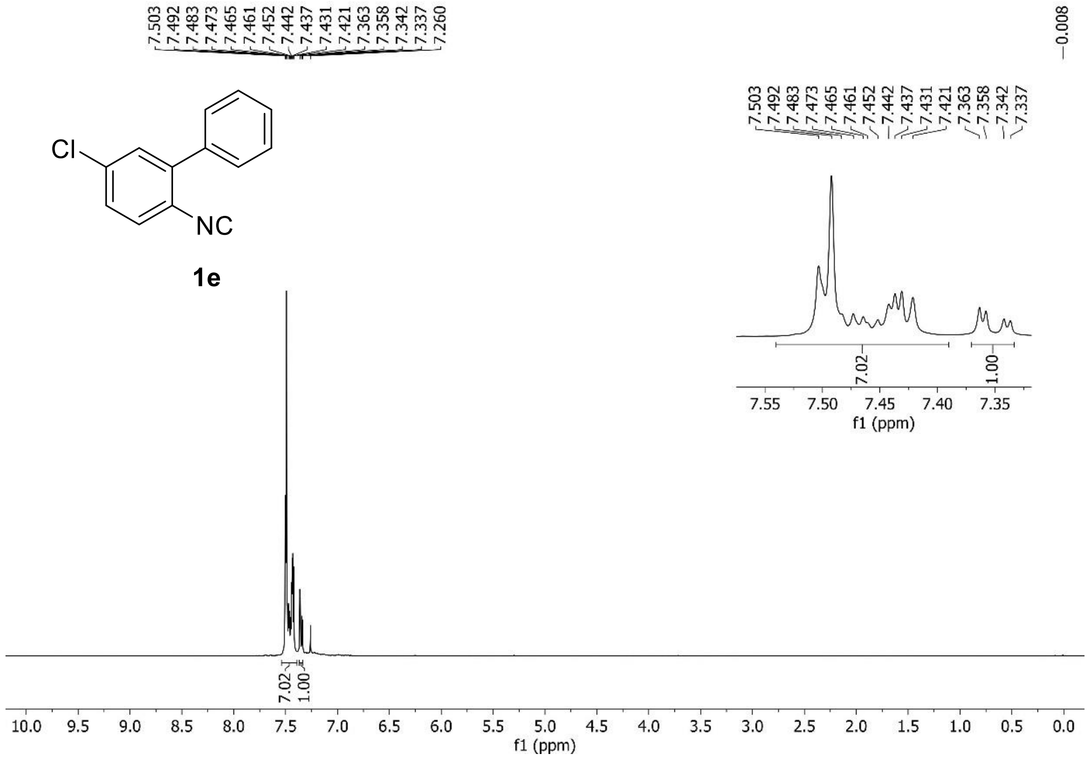
^{13}C NMR spectrum of **1d** (100 MHz, $CDCl_3$)



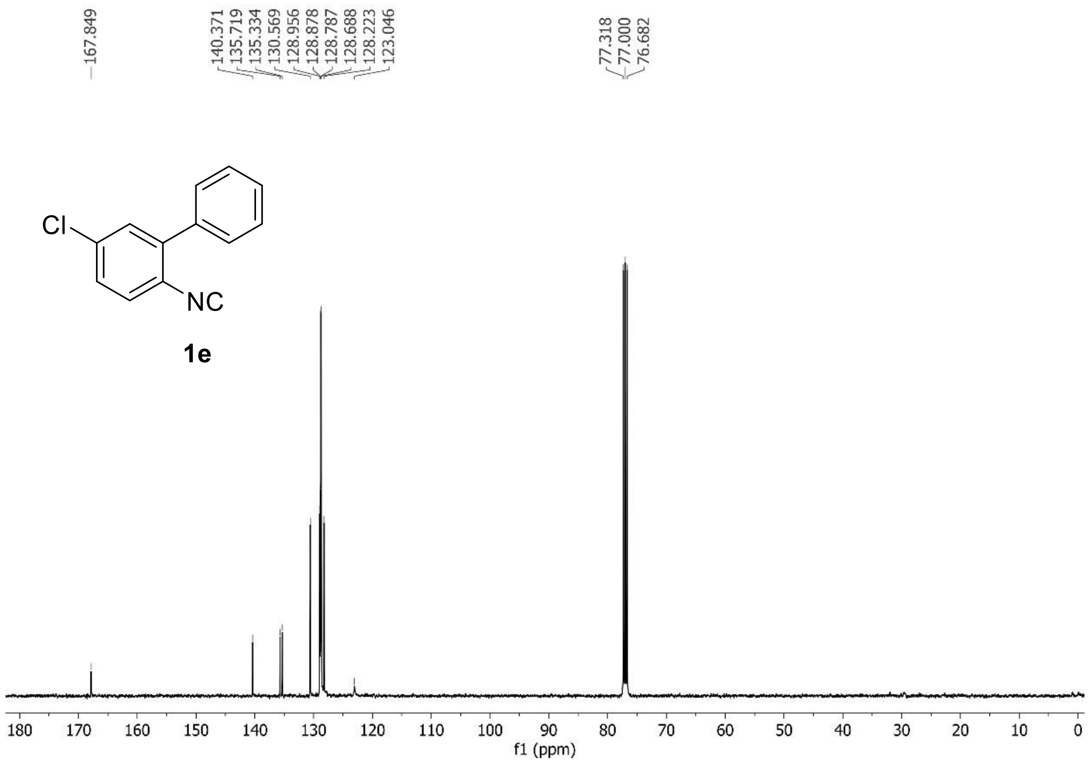
^{19}F NMR spectrum of **1d** (376 MHz, $CDCl_3$)



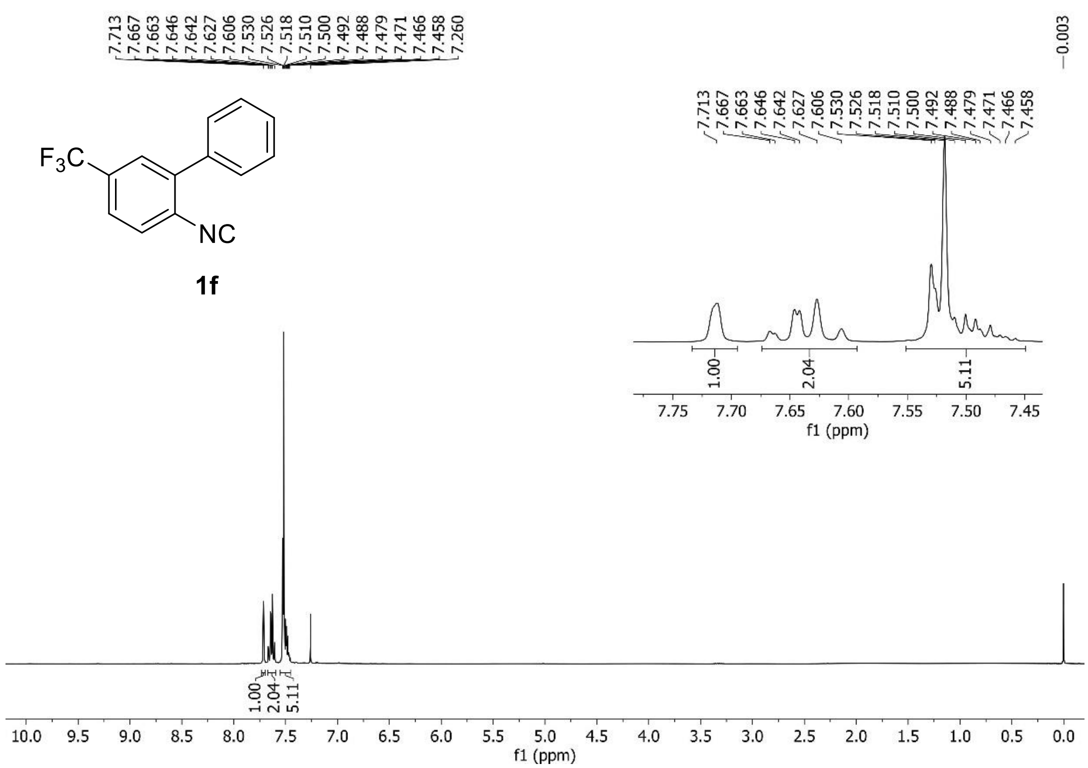
^{1}H NMR spectrum of **1e** (400 MHz, $CDCl_3$)



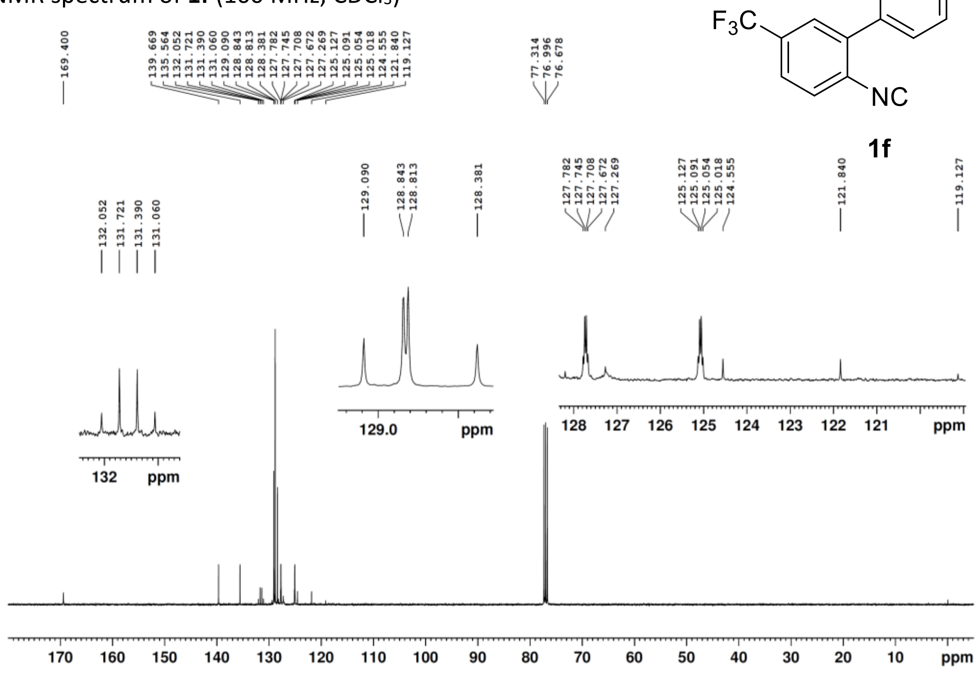
^{13}C NMR spectrum of **1e** (100 MHz, $CDCl_3$)



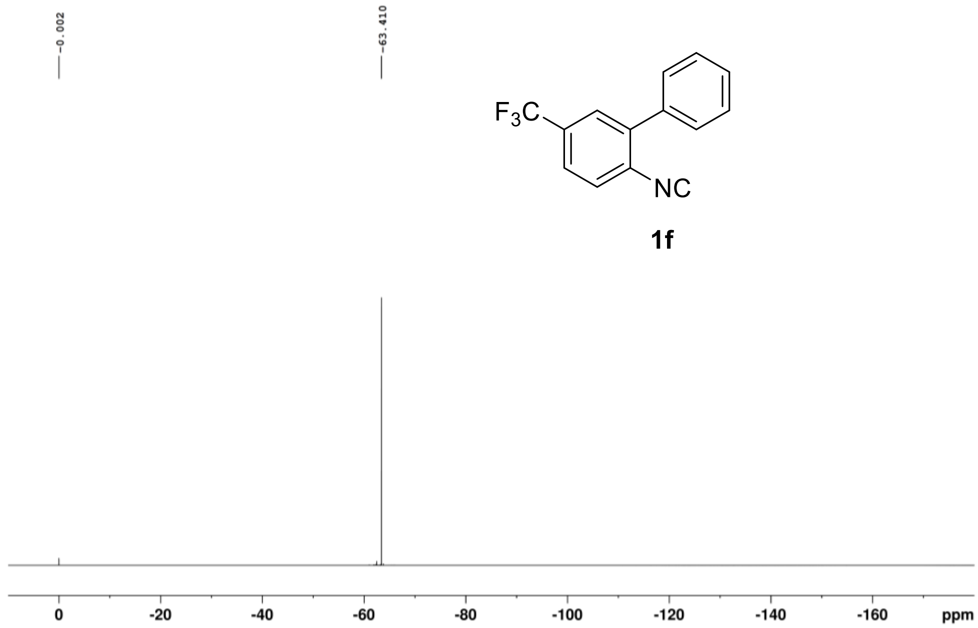
[1]H NMR spectrum of **1f** (400 MHz, $CDCl_3$)



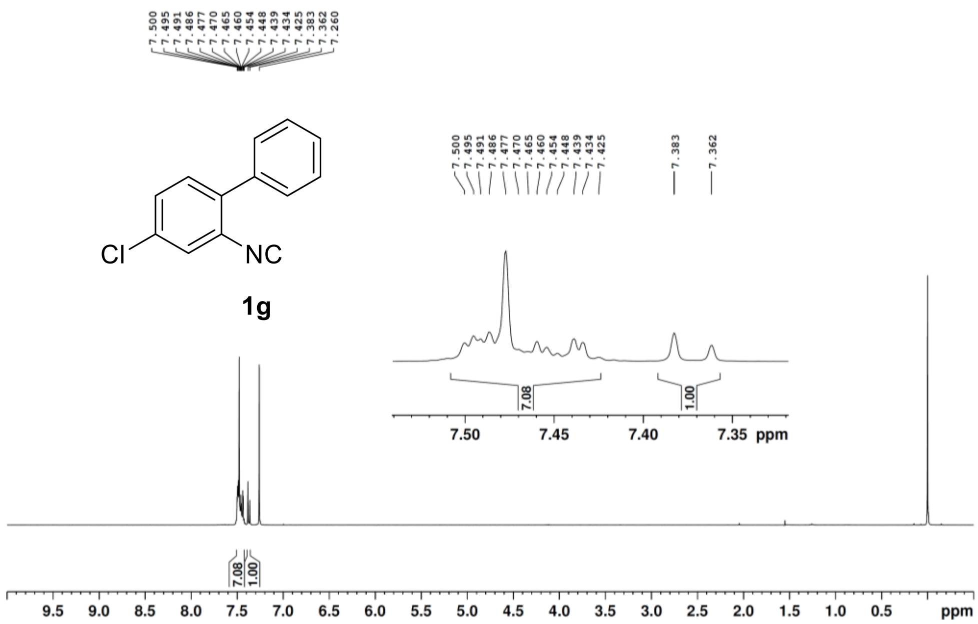
[13]C NMR spectrum of **1f** (100 MHz, $CDCl_3$)



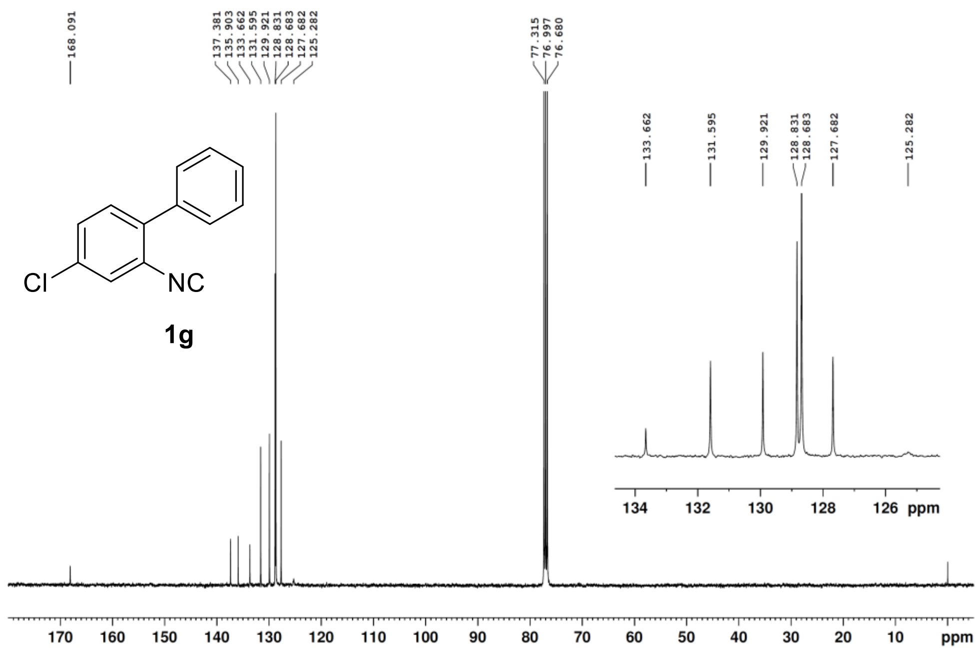
^{19}F NMR spectrum of **1f** (376 MHz, $CDCl_3$)



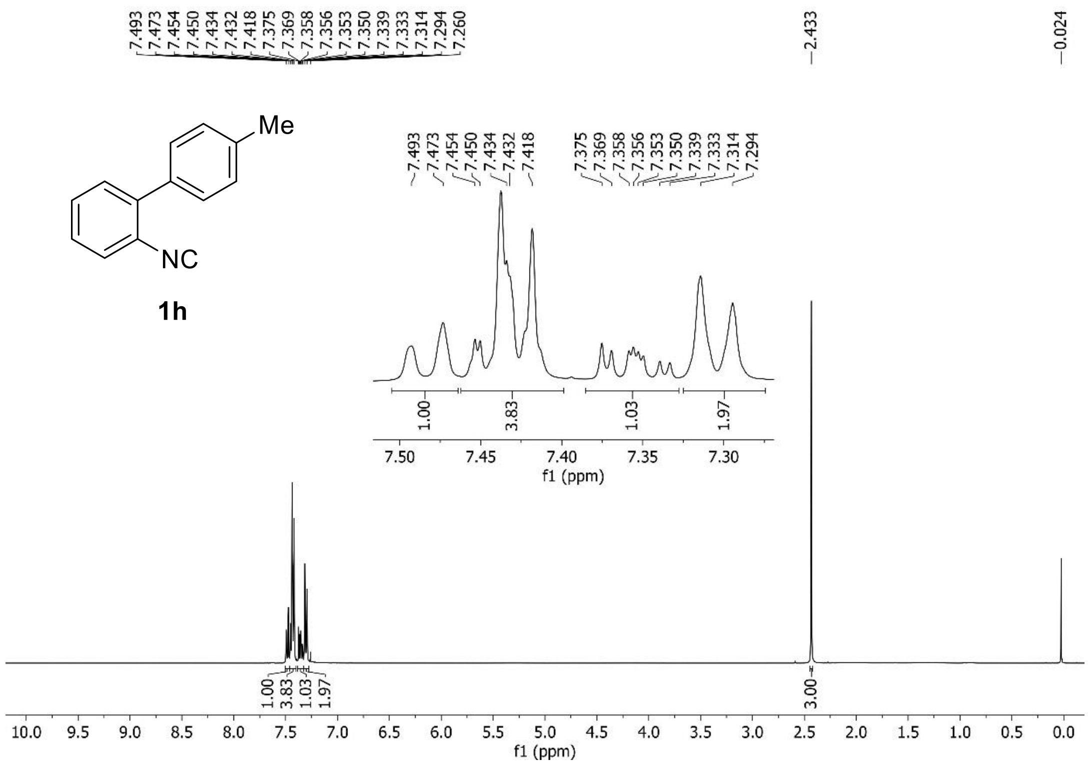
[1]H NMR spectrum of **1g** (400 MHz, $CDCl_3$)



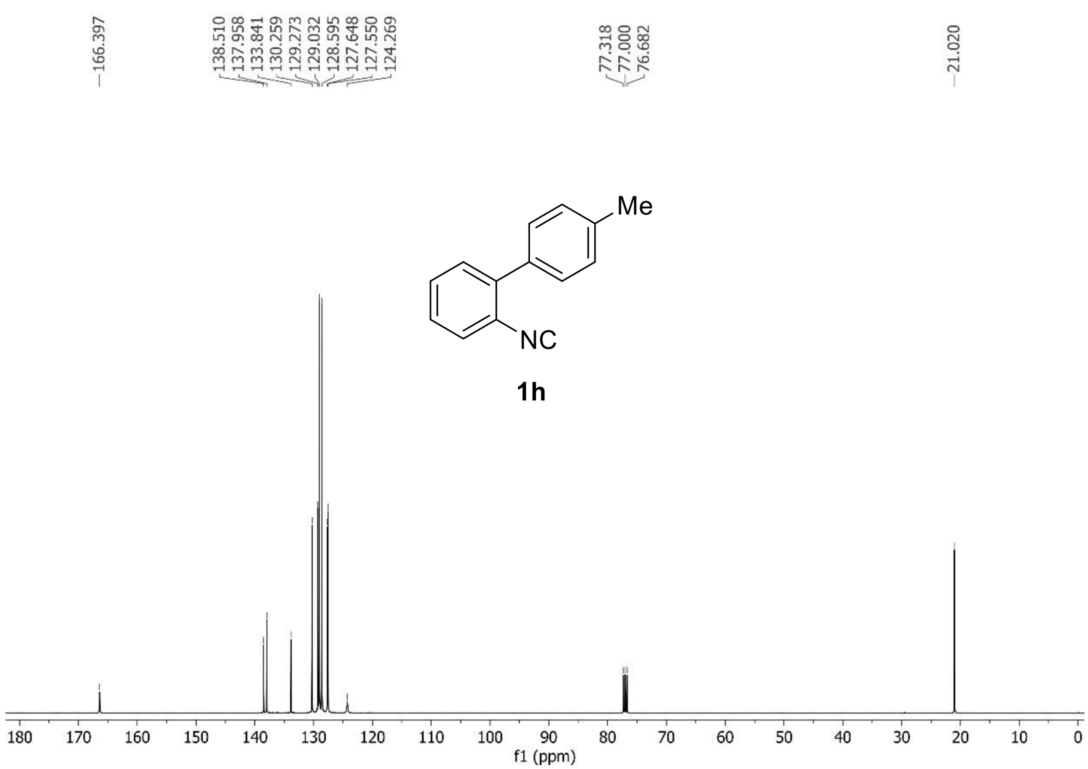
[13]C NMR spectrum of **1g** (100 MHz, $CDCl_3$)



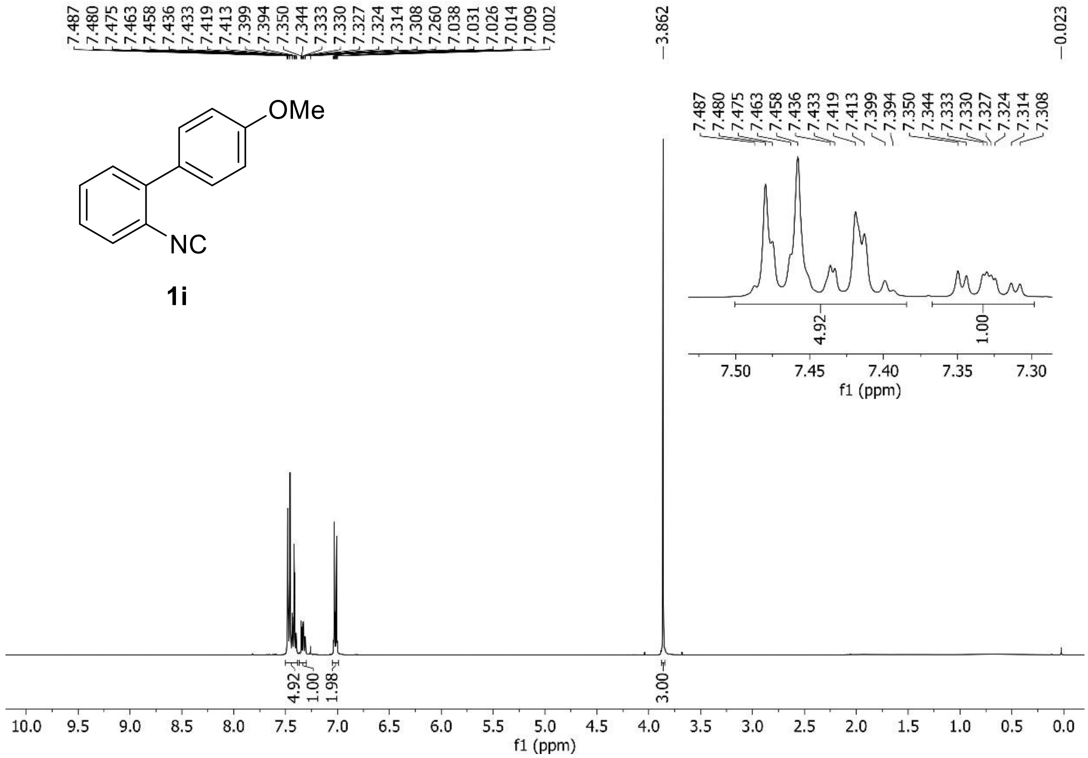
^{1}H NMR spectrum of **1h** (400 MHz, $CDCl_3$)



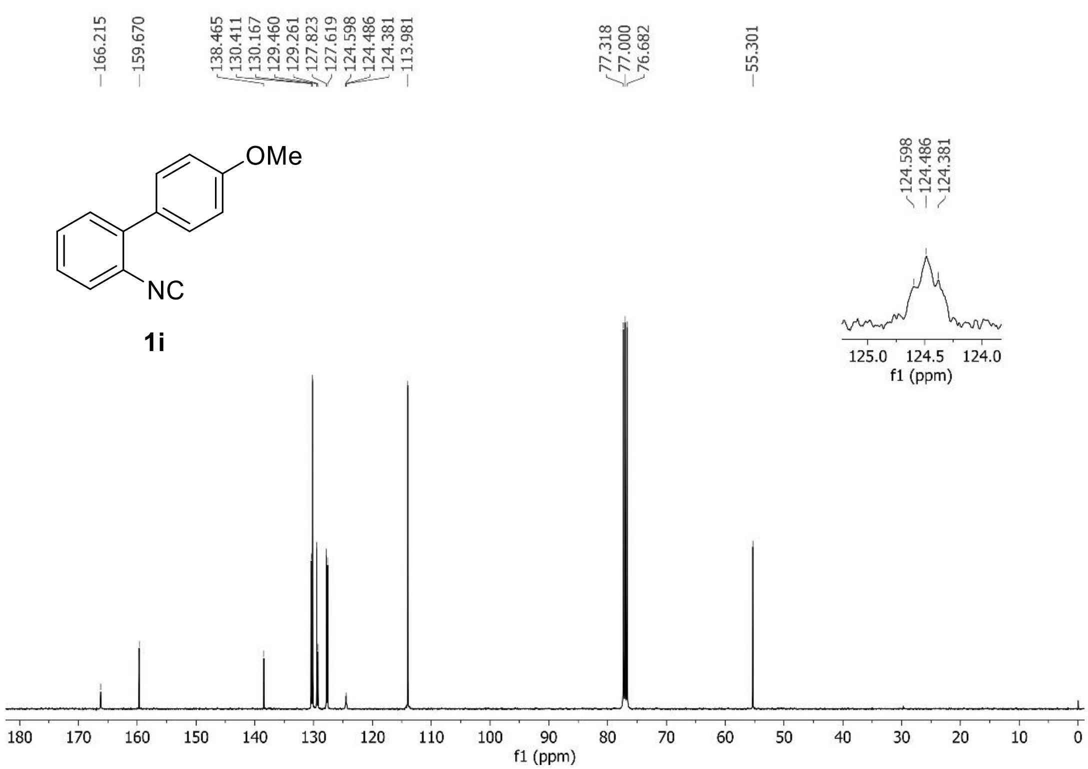
^{13}C NMR spectrum of **1h** (100 MHz, $CDCl_3$)



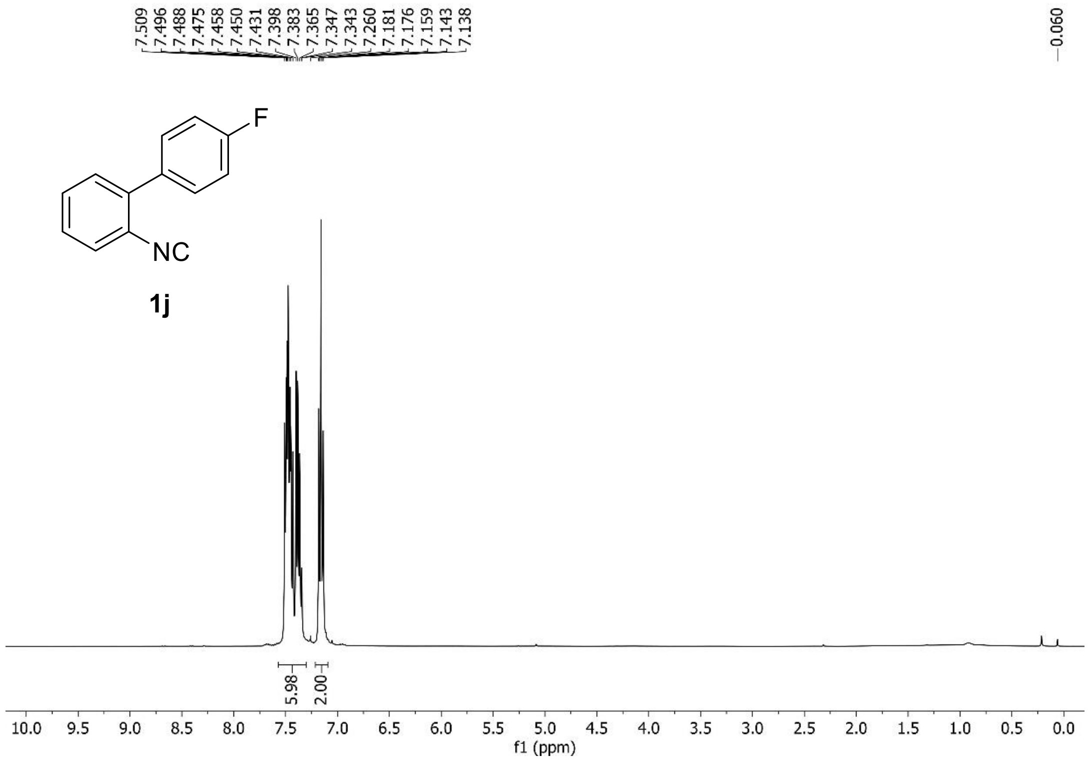
^{1}H NMR spectrum of **1i** (400 MHz, $CDCl_3$)



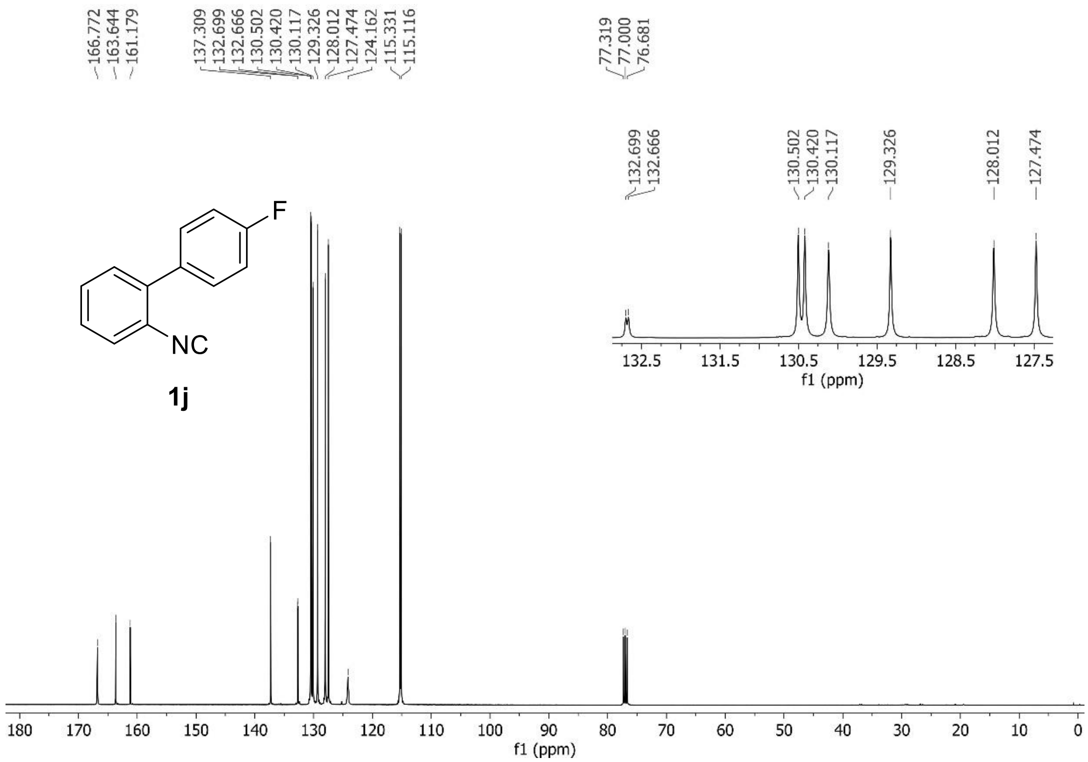
^{13}C NMR spectrum of **1i** (100 MHz, $CDCl_3$)



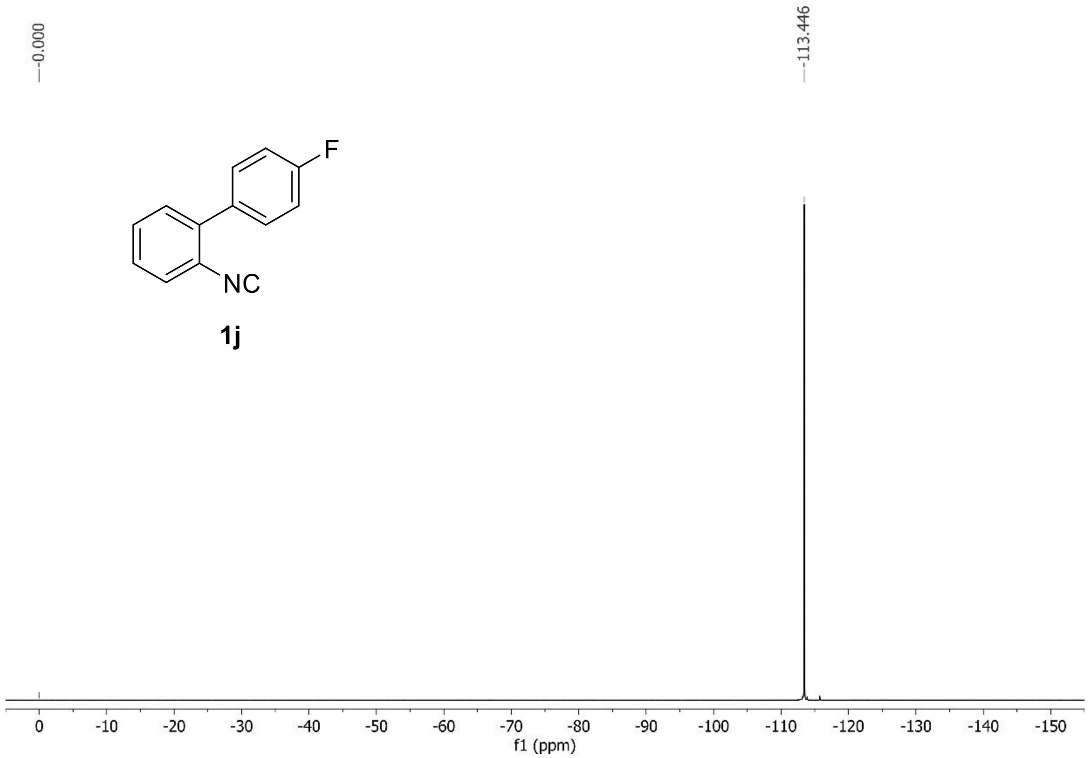
[1]H NMR spectrum of **1j** (400 MHz, $CDCl_3$)



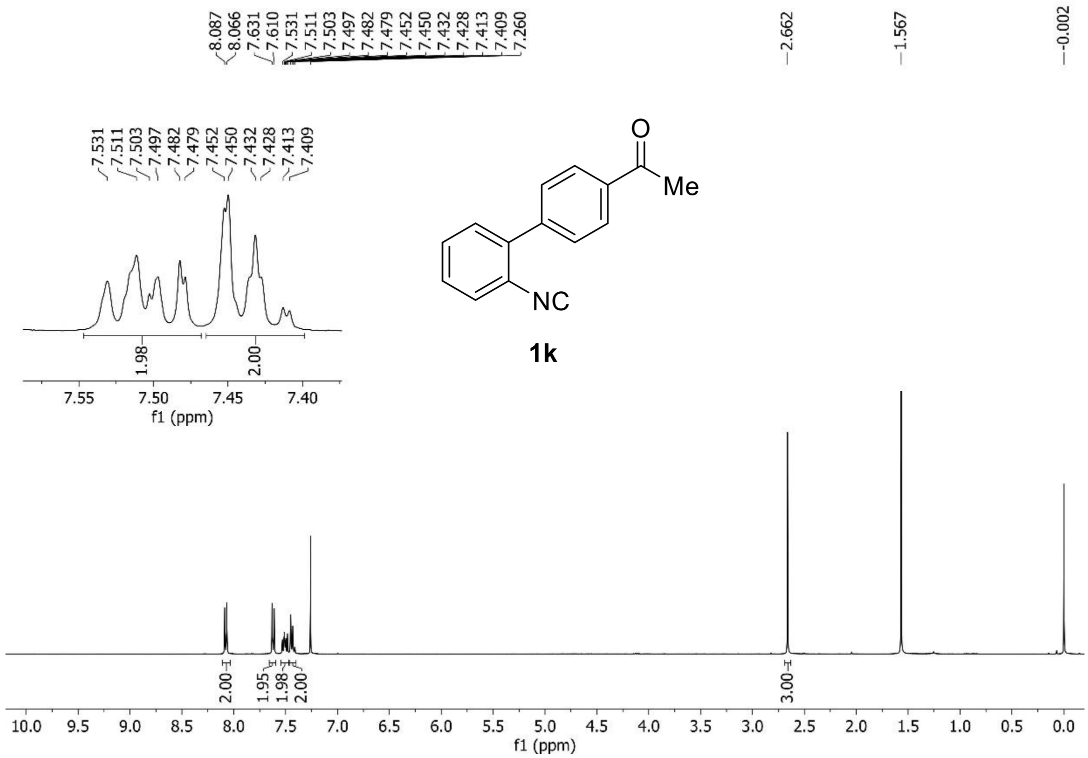
[13]C NMR spectrum of **1j** (100 MHz, $CDCl_3$)



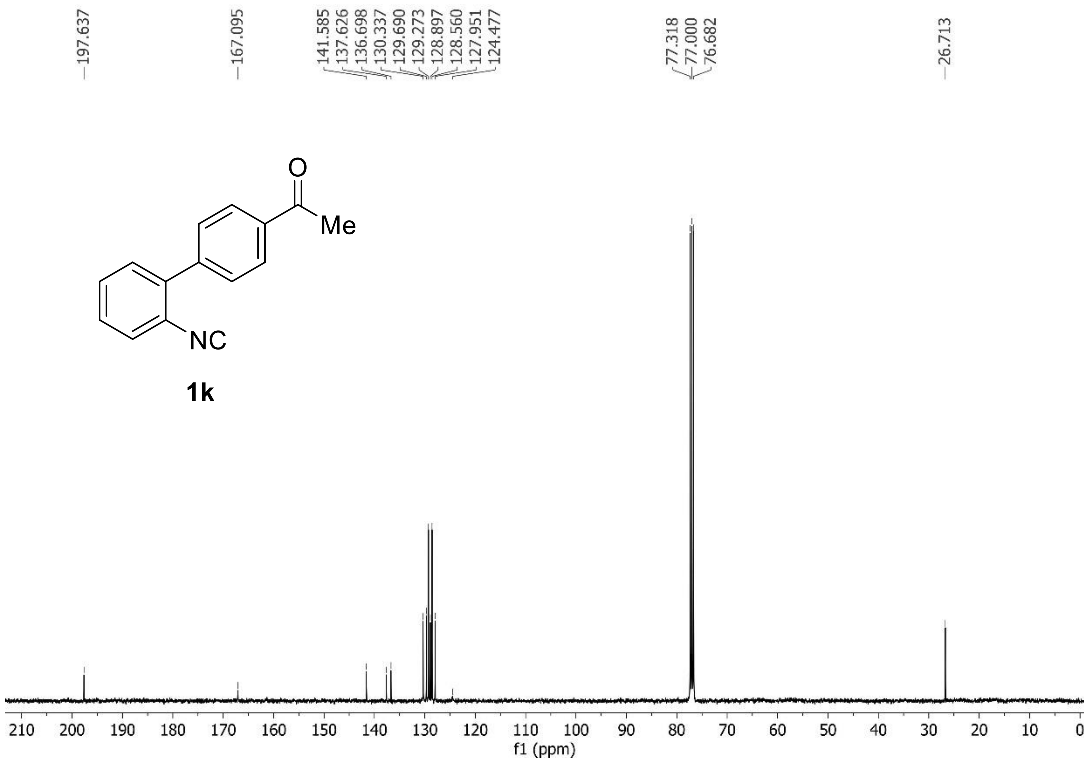
[19]F NMR spectrum of **1j** (376 MHz, $CDCl_3$)



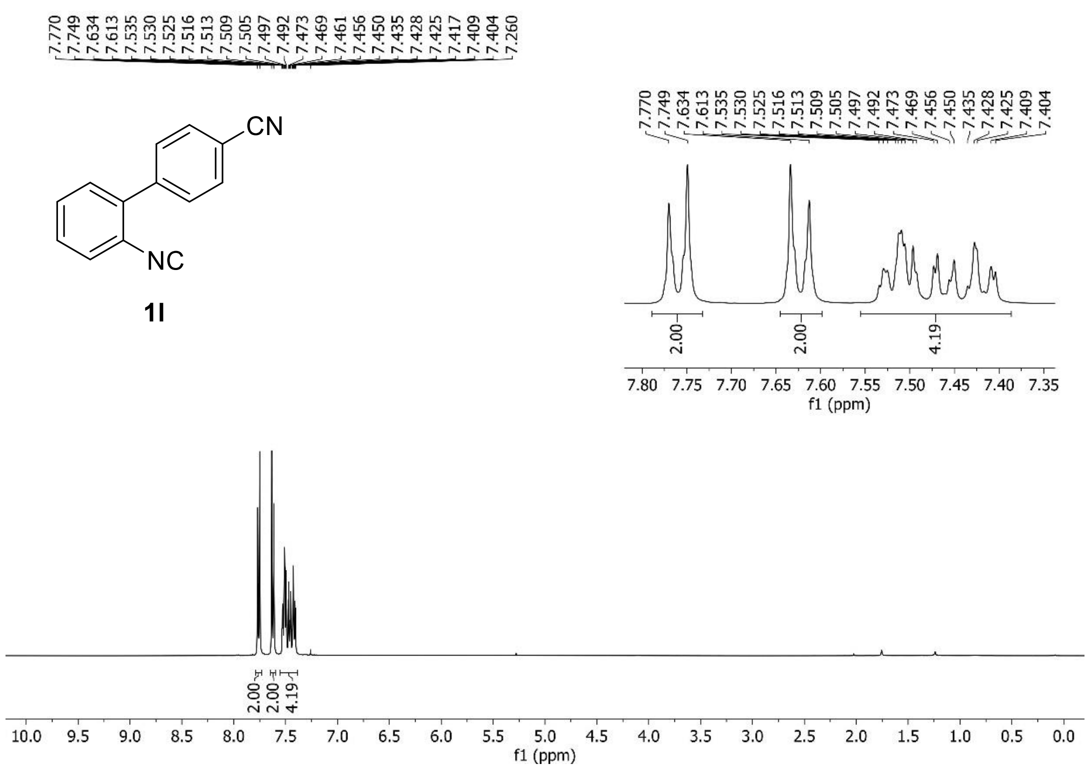
^{1}H NMR spectrum of **1k** (400 MHz, $CDCl_3$)



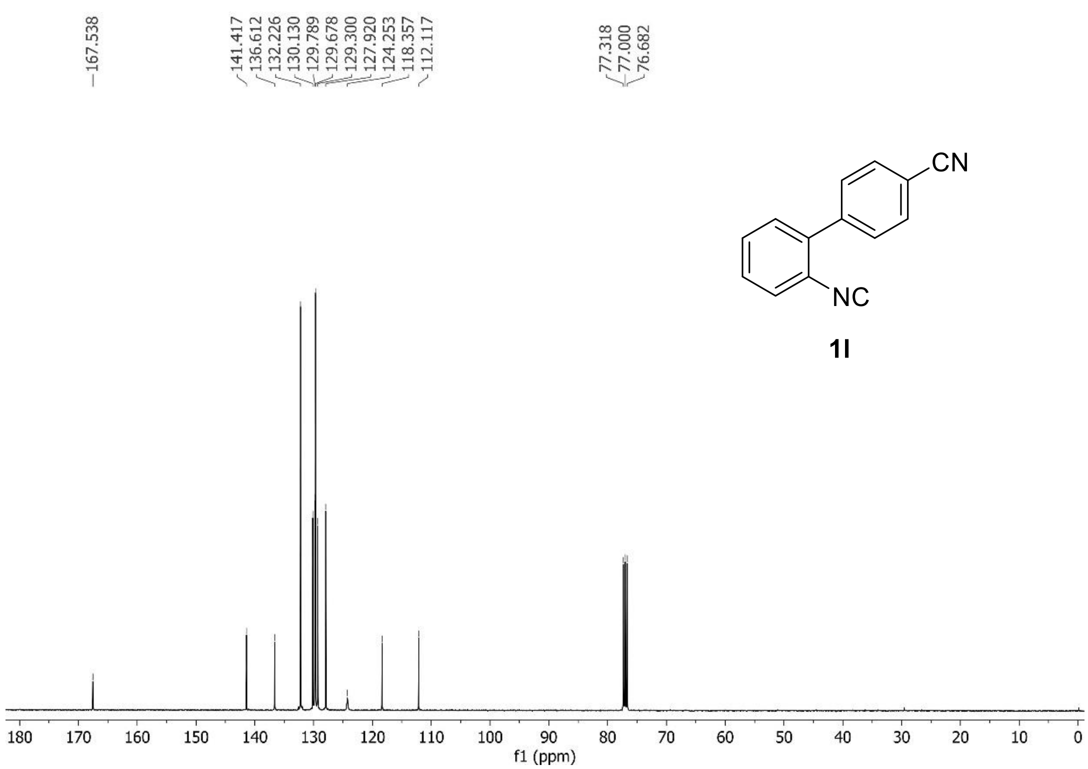
^{13}C NMR spectrum of **1k** (100 MHz, $CDCl_3$)



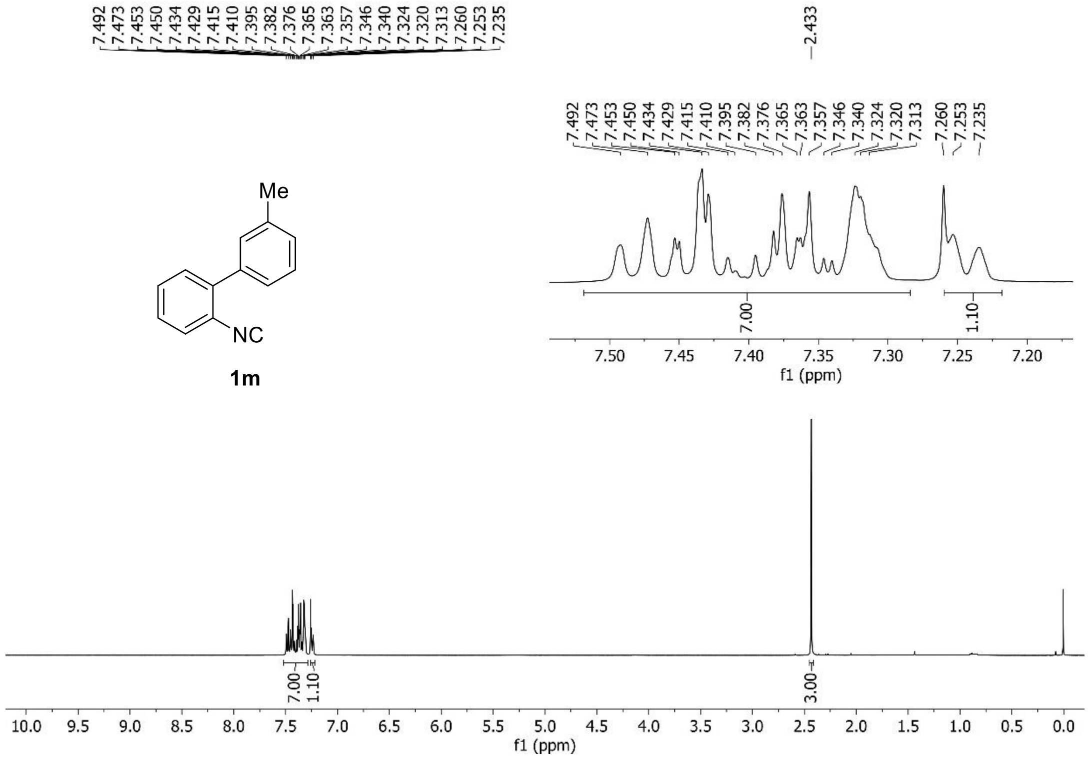
^{1}H NMR spectrum of **1l** (400 MHz, $CDCl_3$)



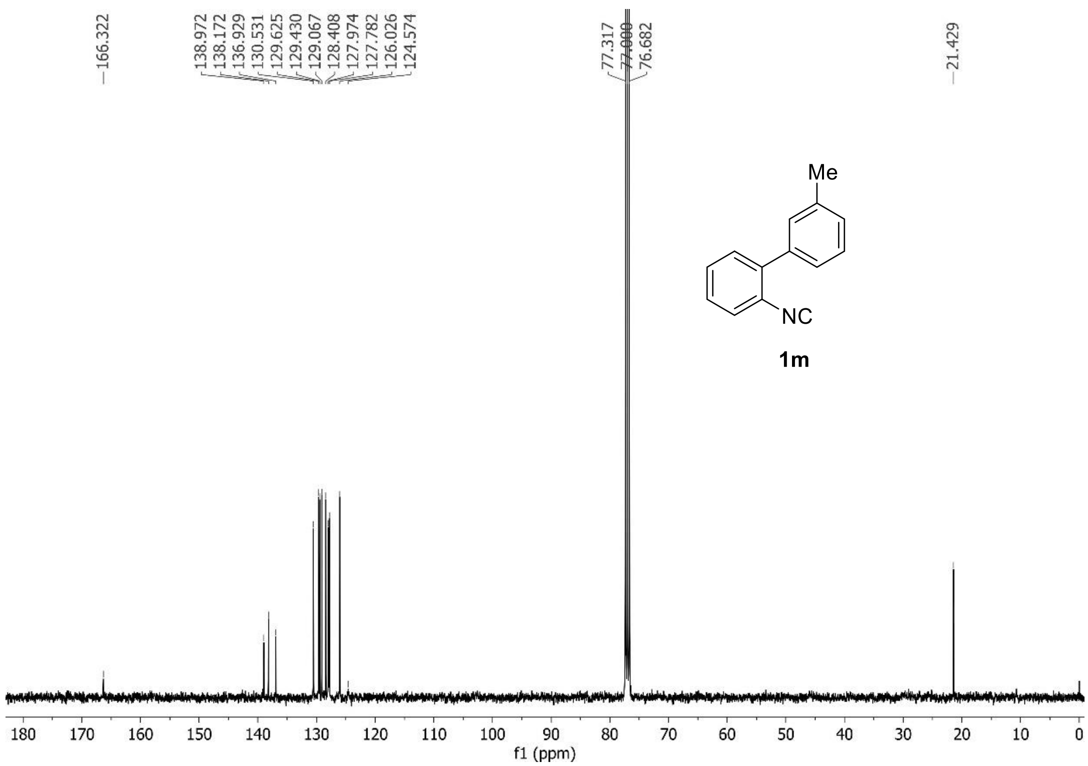
^{13}C NMR spectrum of **1l** (100 MHz, $CDCl_3$)



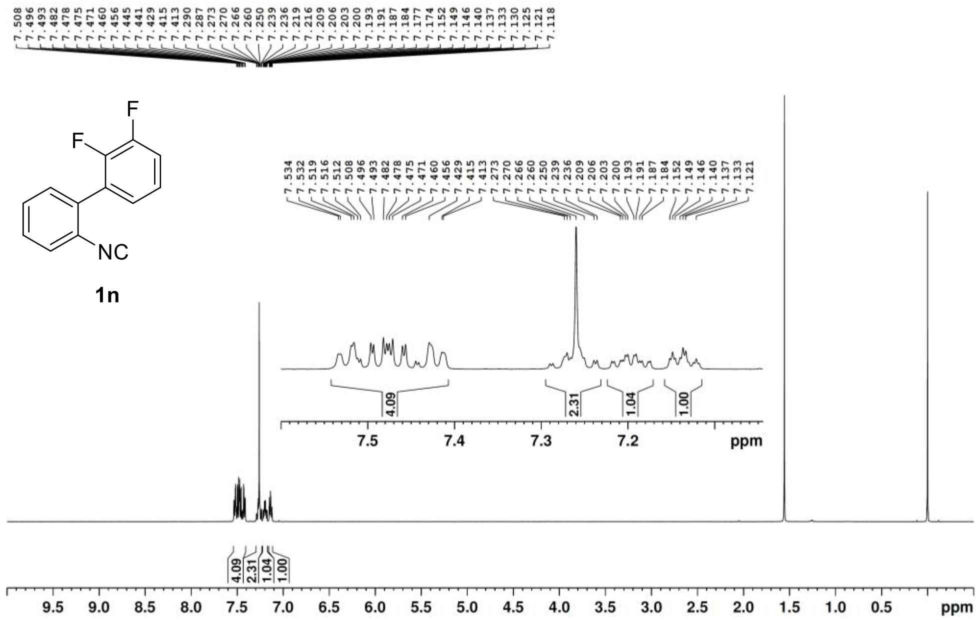
^{1}H NMR spectrum of **1m** (400 MHz, $CDCl_3$)



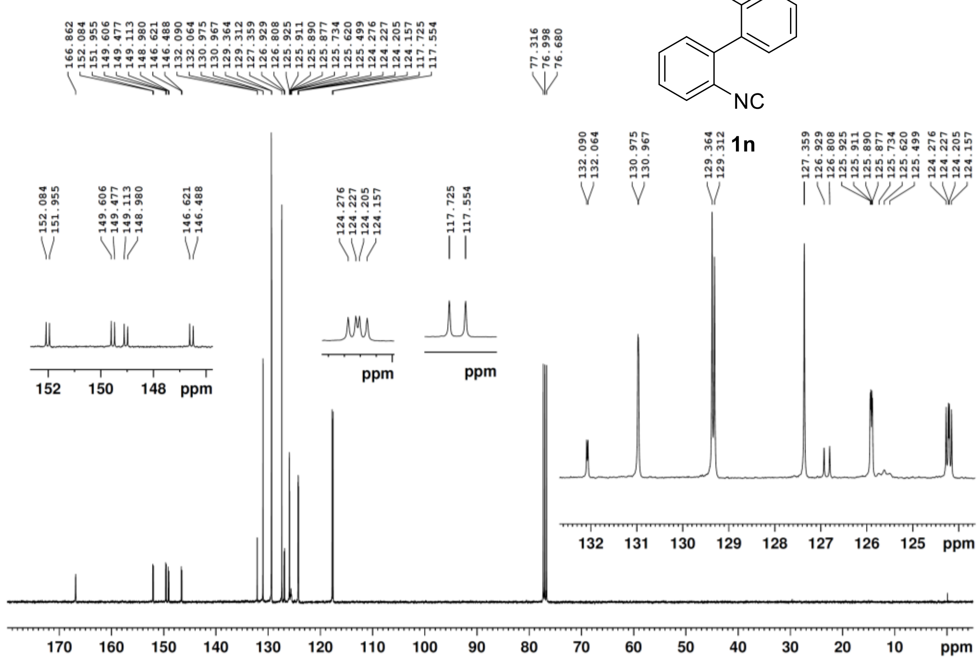
^{13}C NMR spectrum of **1m** (100 MHz, $CDCl_3$)



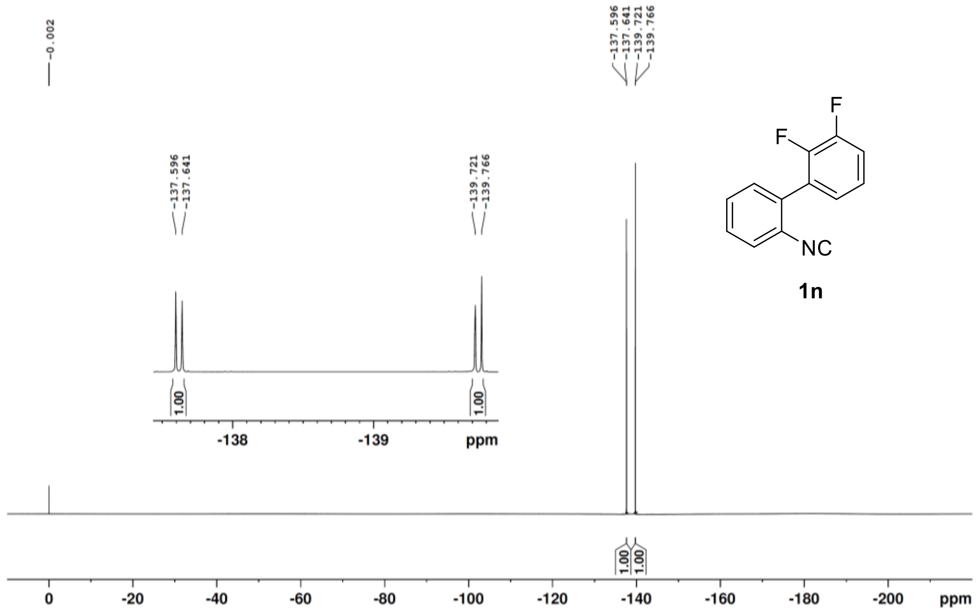
^{1}H NMR spectrum of **1n** (400 MHz, $CDCl_3$)



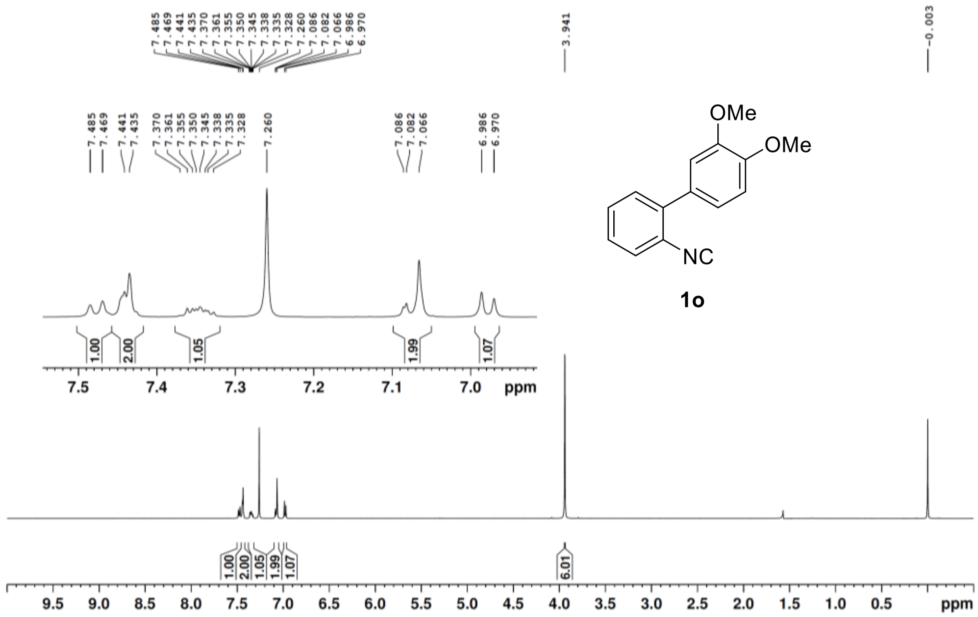
^{13}C NMR spectrum of **1n** (100 MHz, $CDCl_3$)



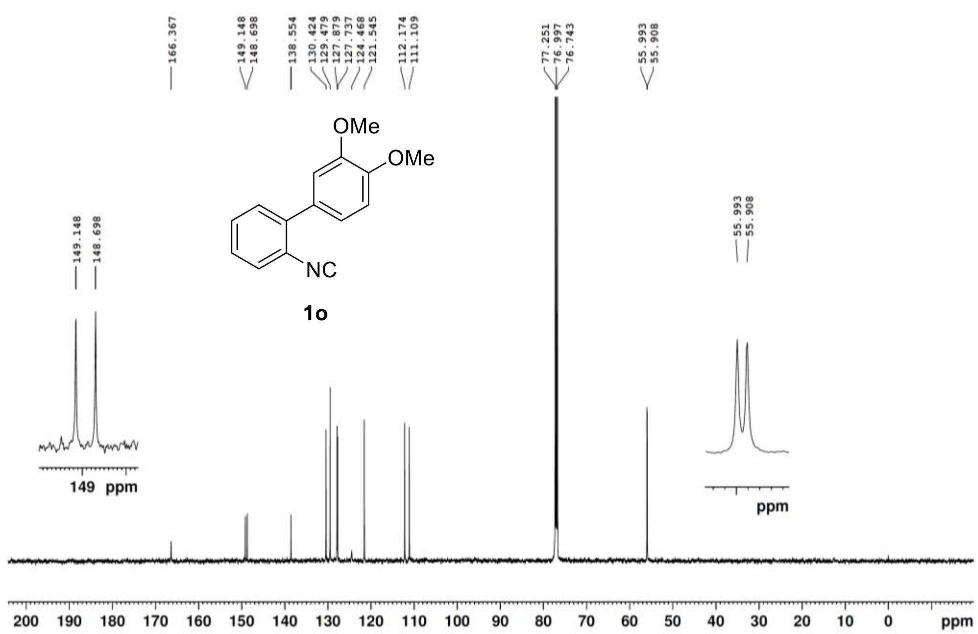
[19]F NMR spectrum of **1n** (470 MHz, $CDCl_3$)



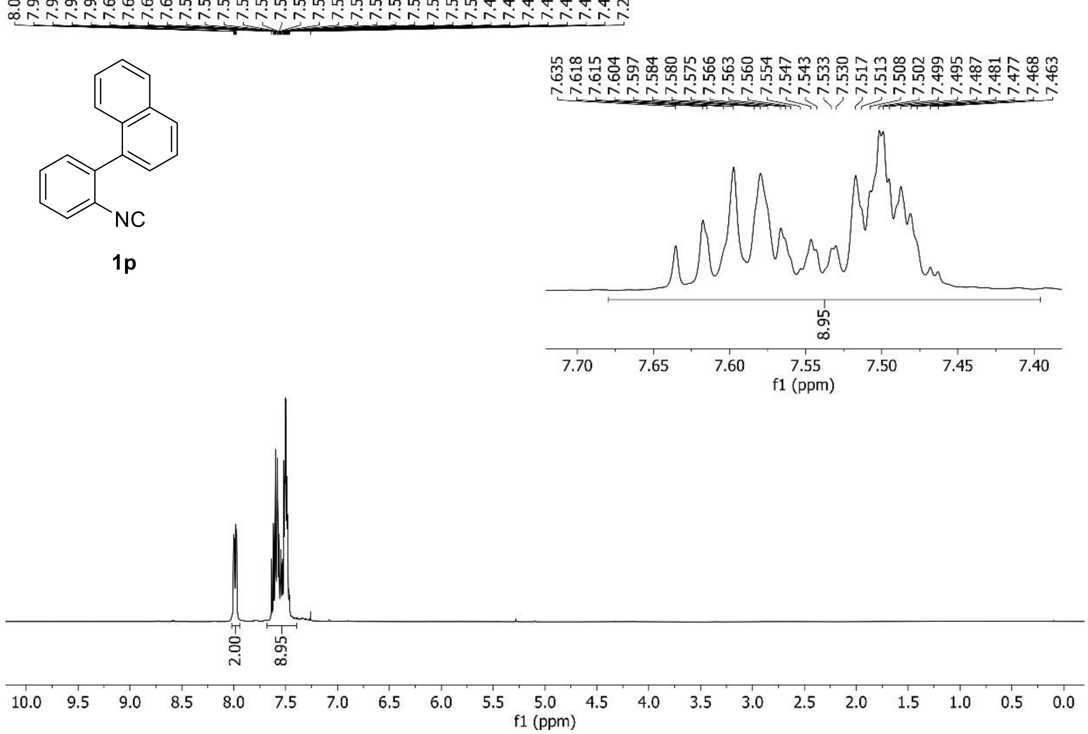
^{1}H NMR spectrum of **1o** (500 MHz, $CDCl_3$)



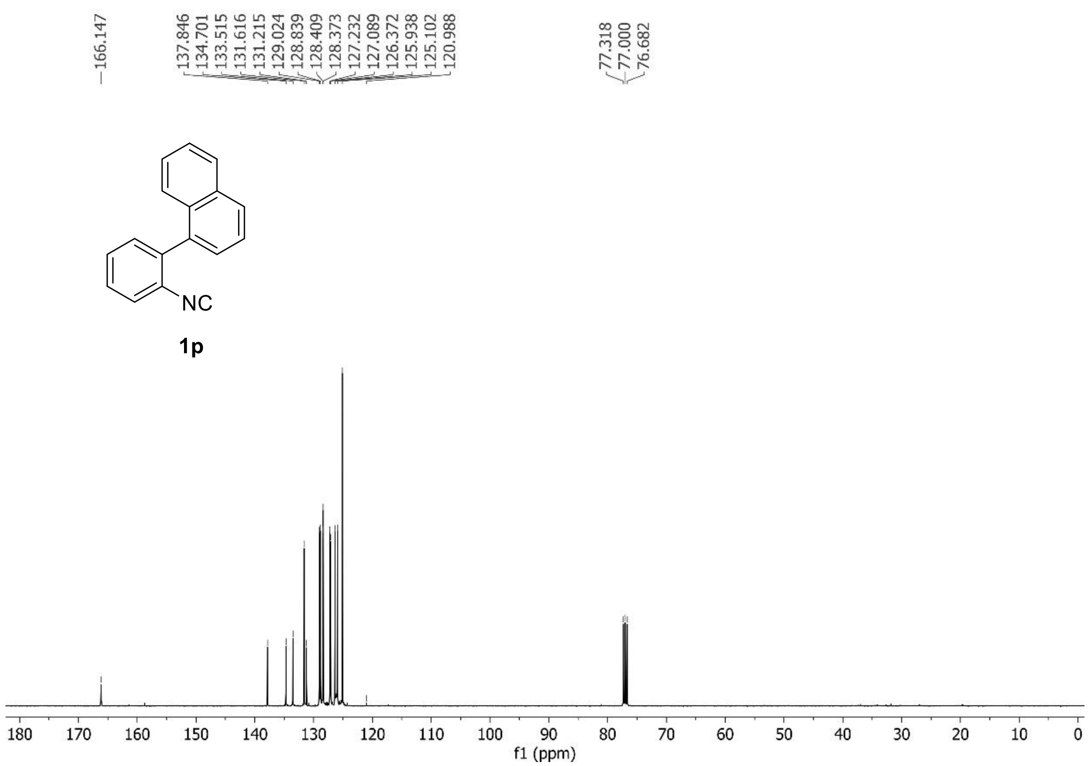
^{13}C NMR spectrum of **1o** (125 MHz, $CDCl_3$)



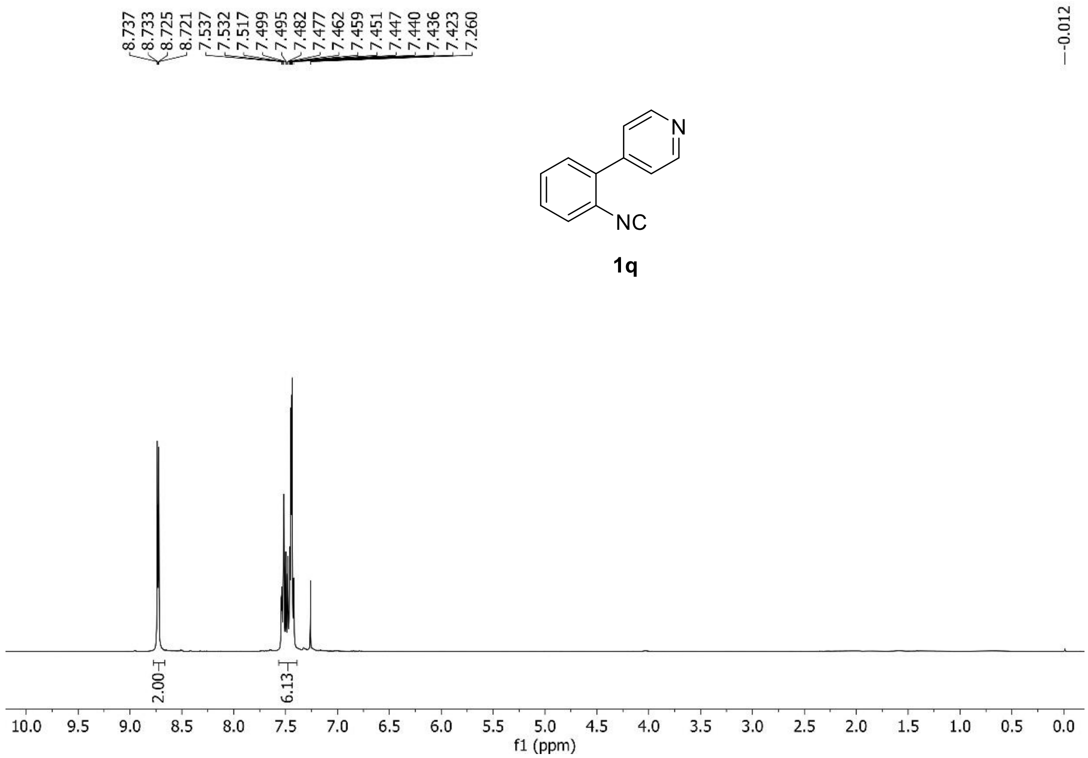
^{1}H NMR spectrum of **1p** (400 MHz, $CDCl_3$)



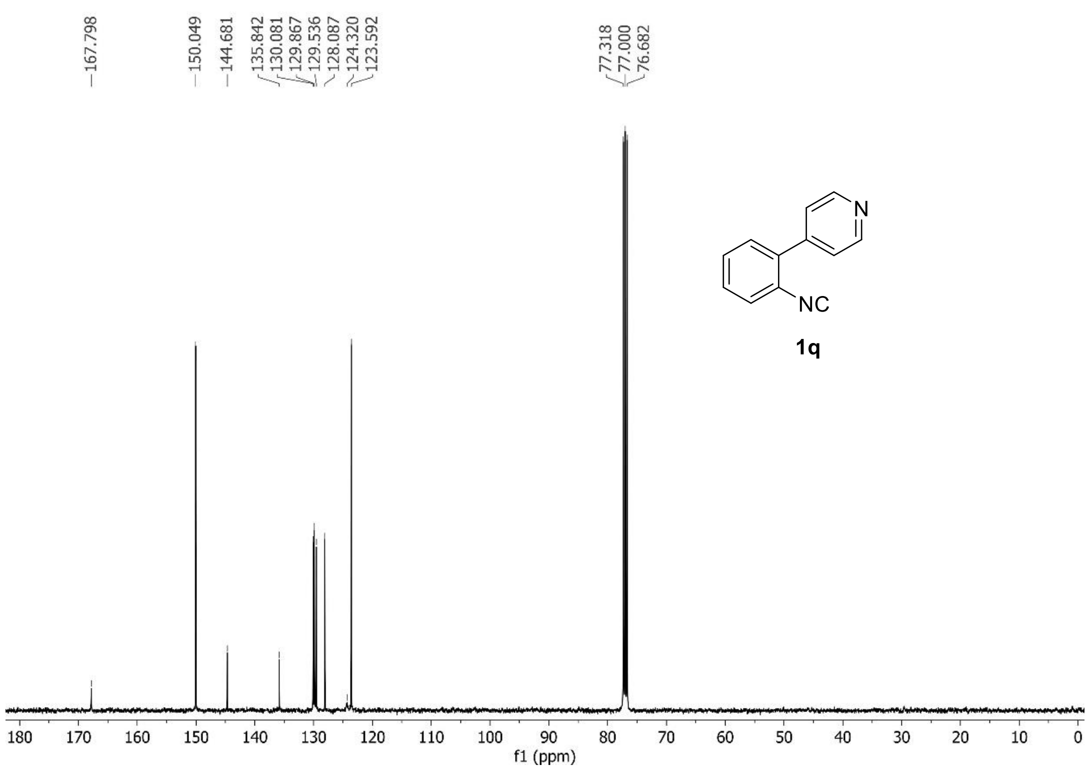
^{13}C NMR spectrum of **1p** (100 MHz, $CDCl_3$)



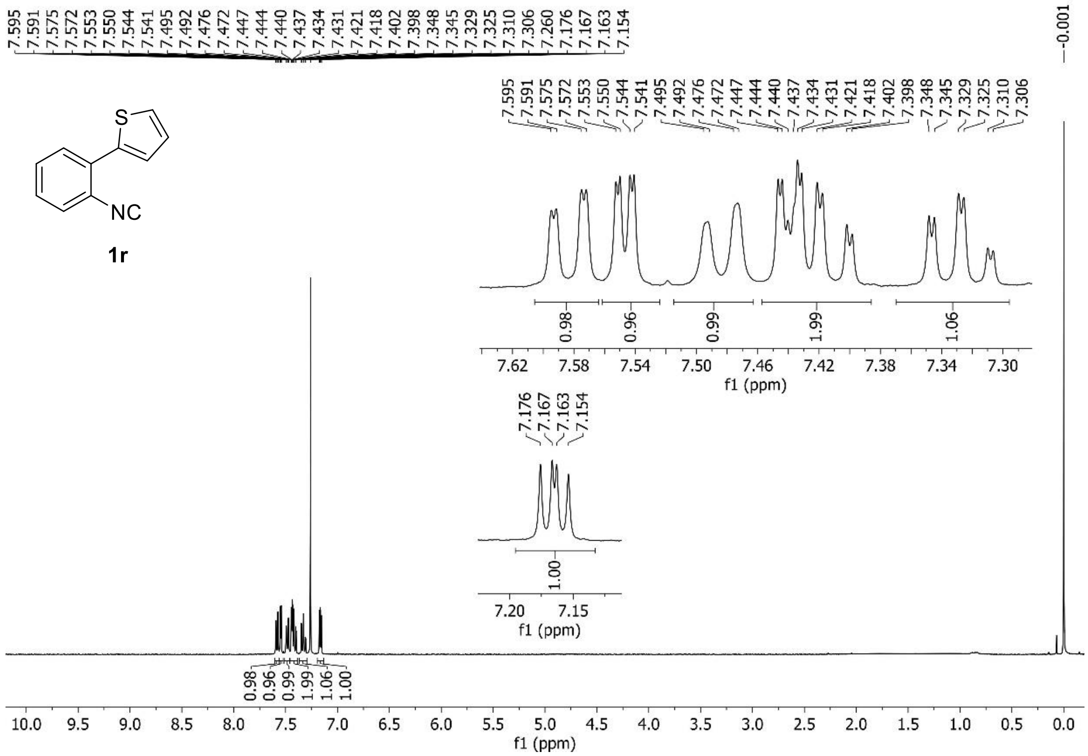
[1]H NMR spectrum of **1q** (400 MHz, $CDCl_3$)



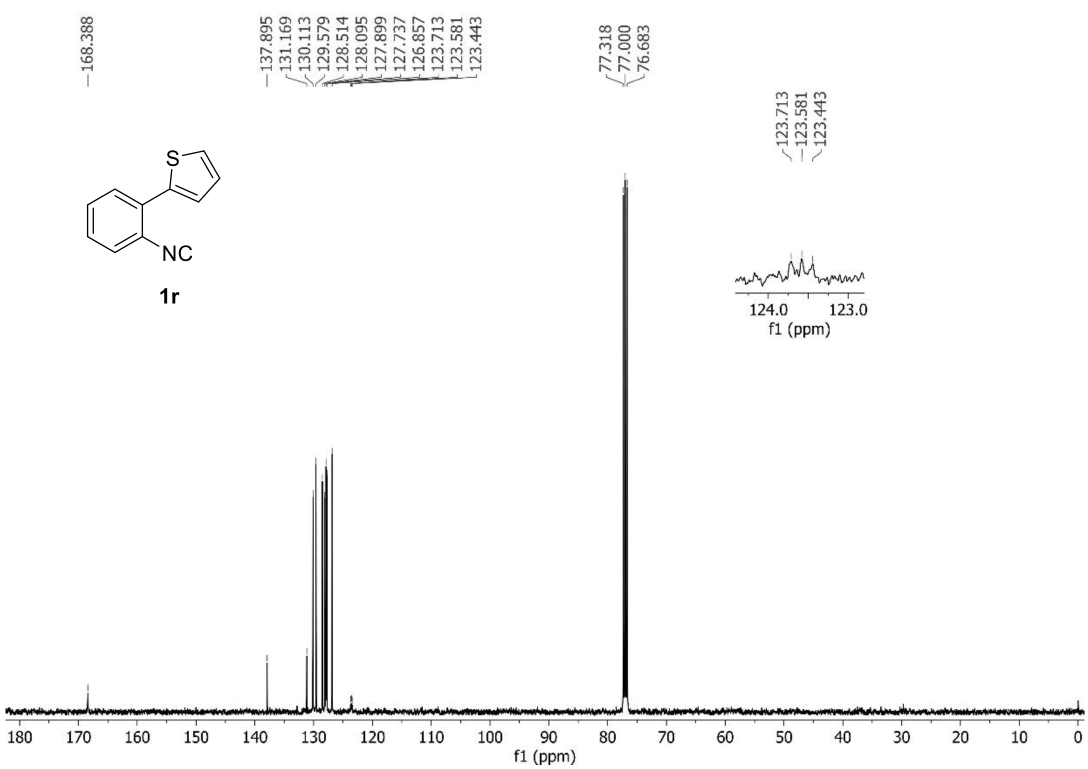
[13]C NMR spectrum of **1q** (100 MHz, $CDCl_3$)



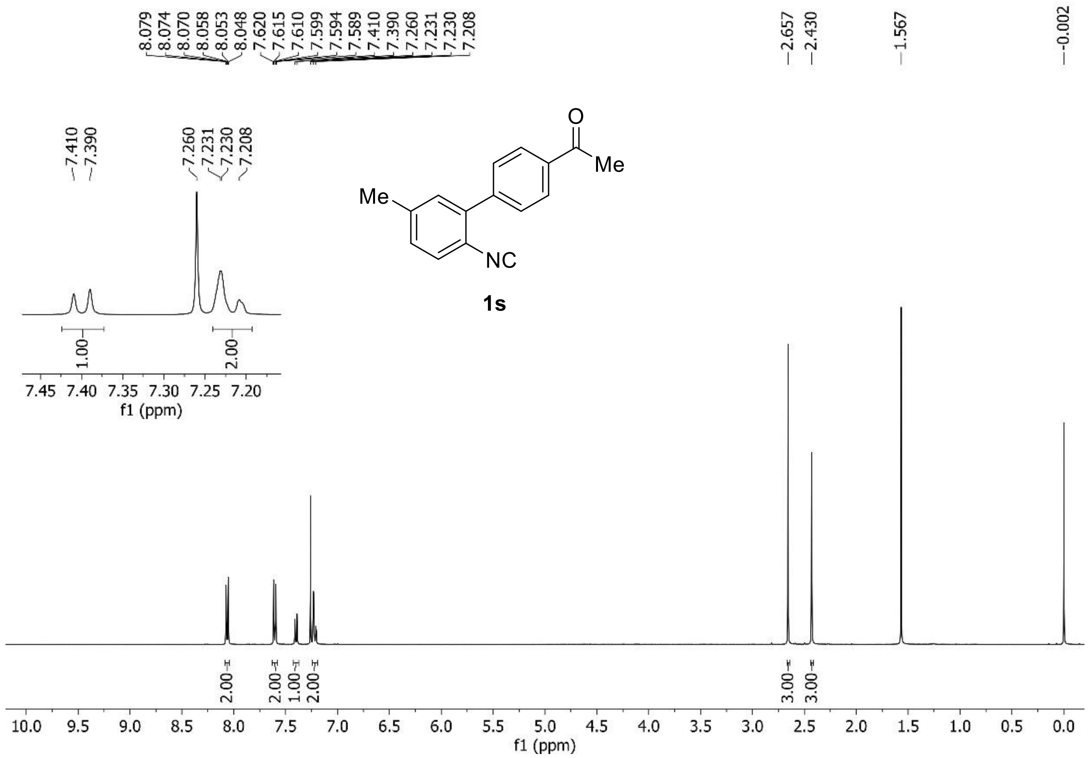
^{1}H NMR spectrum of **1r** (400 MHz, $CDCl_3$)



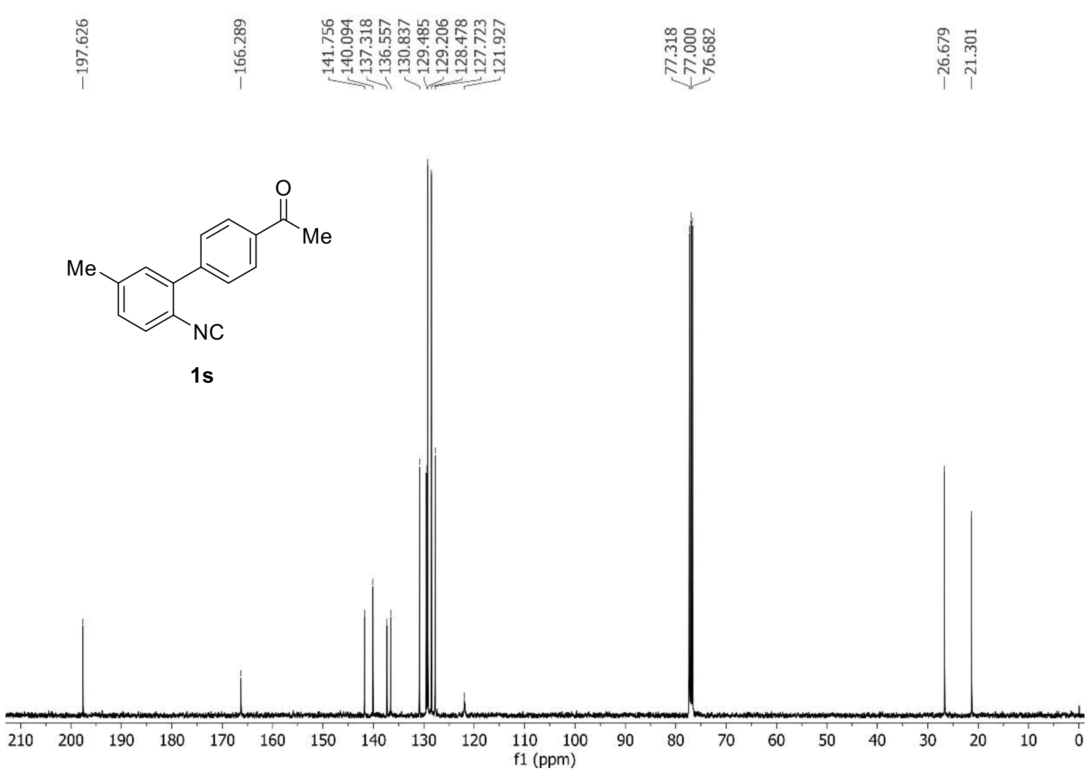
^{13}C NMR spectrum of **1r** (100 MHz, $CDCl_3$)



^{1}H NMR spectrum of **1s** (400 MHz, $CDCl_3$)

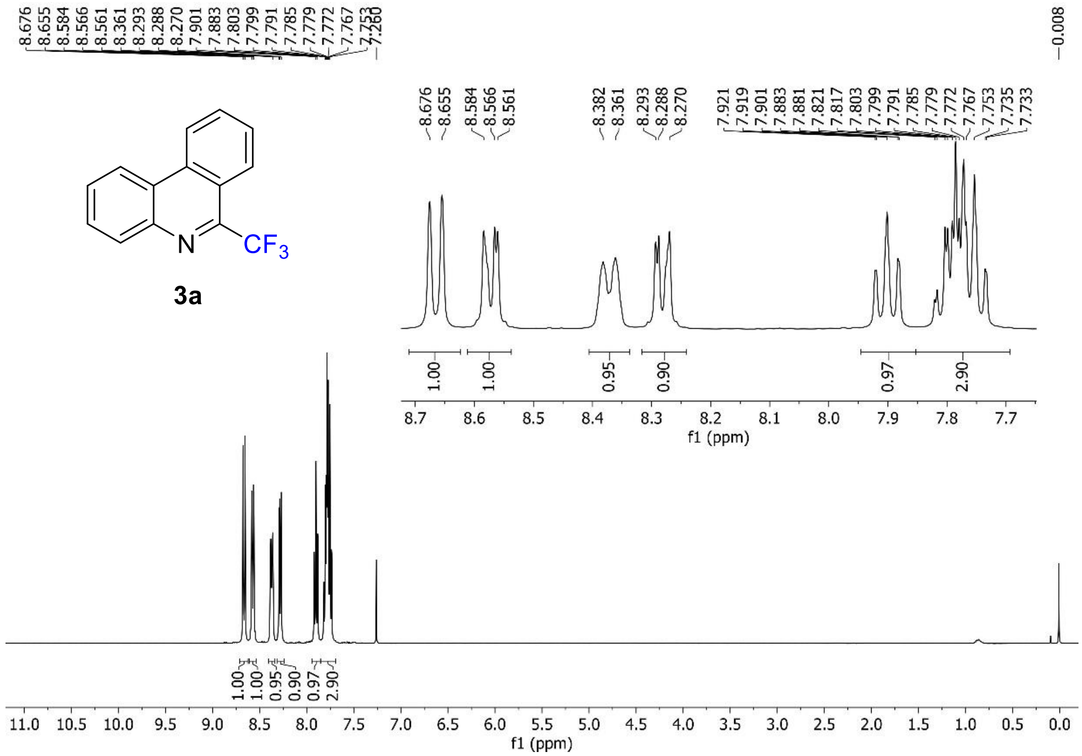


^{13}C NMR spectrum of **1s** (100 MHz, $CDCl_3$)

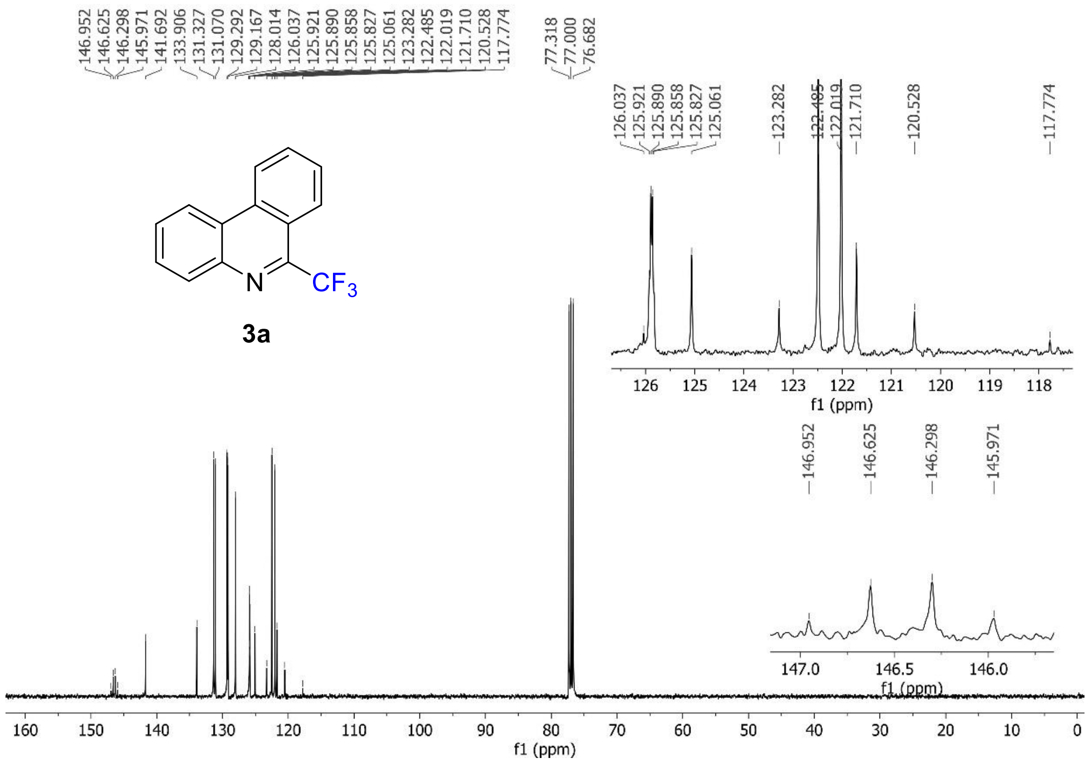


8. NMR spectra of 6-(trifluoromethyl)phenanthridines 3a-3s

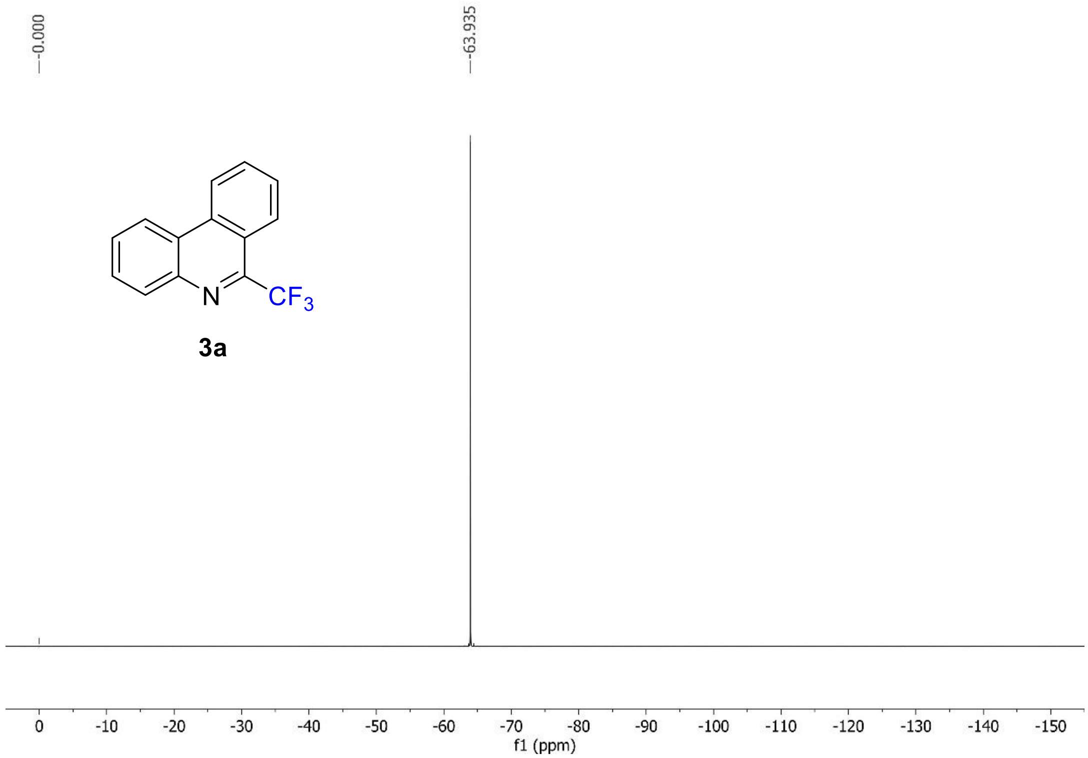
^{1}H NMR spectrum of **3a** (400 MHz, $CDCl_3$)



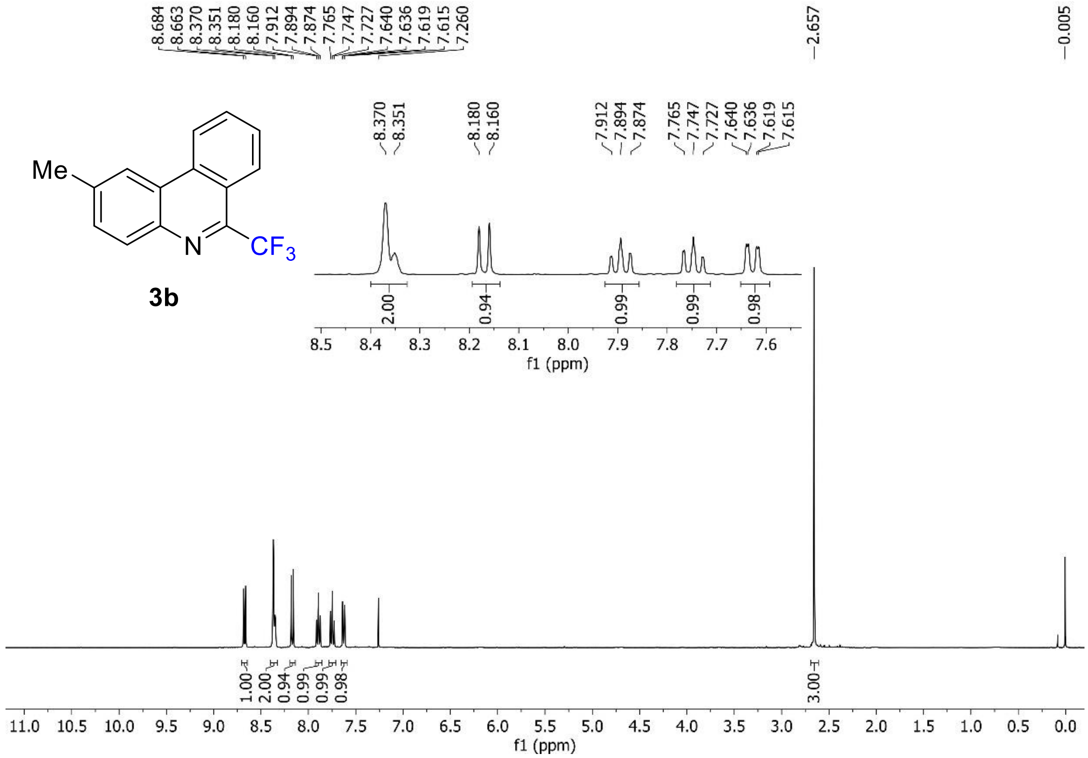
^{13}C NMR spectrum of **3a** (100 MHz, $CDCl_3$)



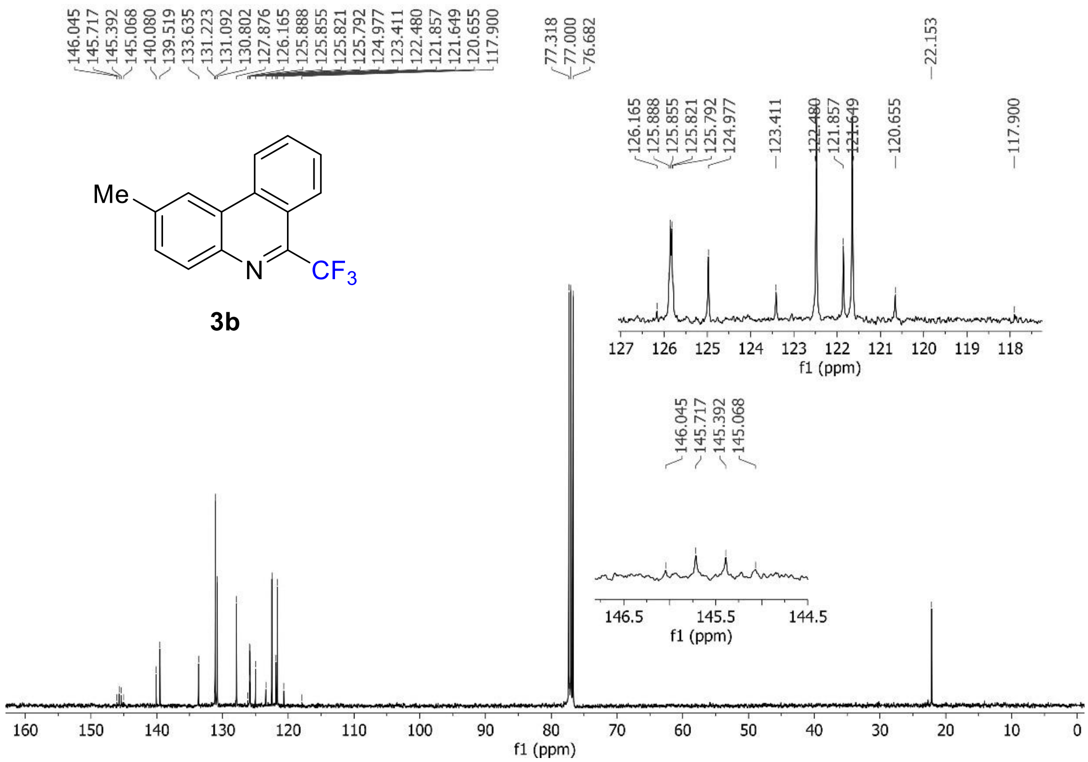
^{19}F NMR spectrum of **3a** (376 MHz, $CDCl_3$)



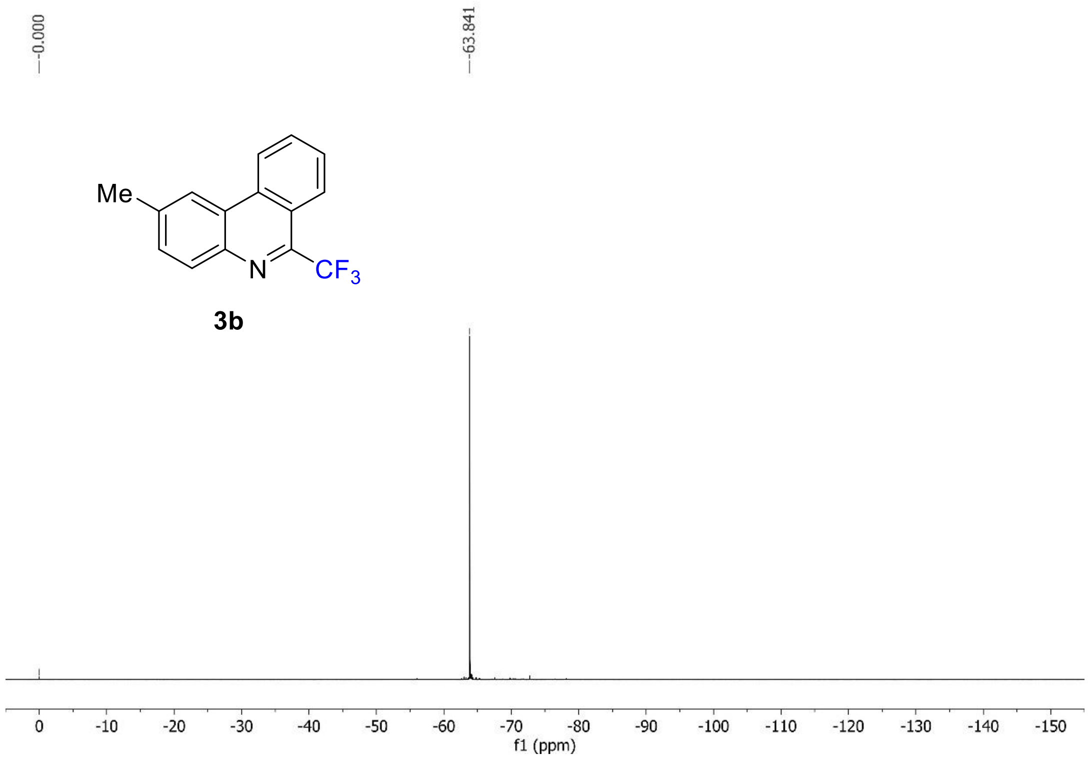
^{1}H NMR spectrum of **3b** (400 MHz, $CDCl_3$)



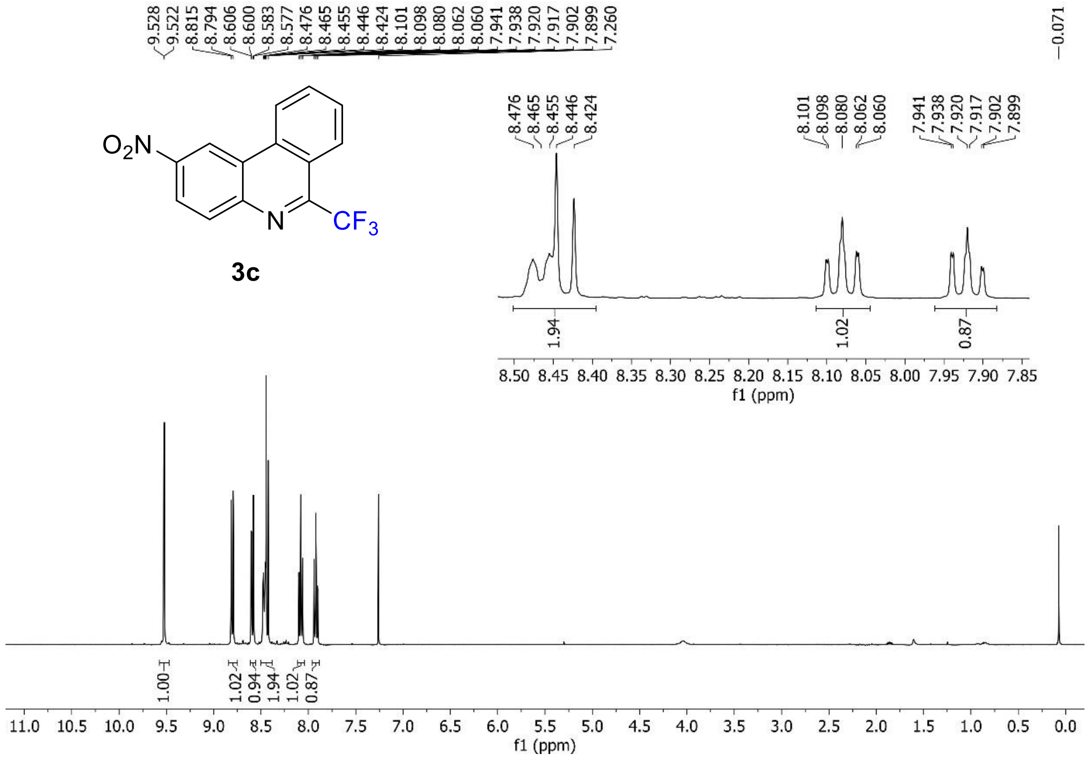
^{13}C NMR spectrum of **3b** (100 MHz, $CDCl_3$)



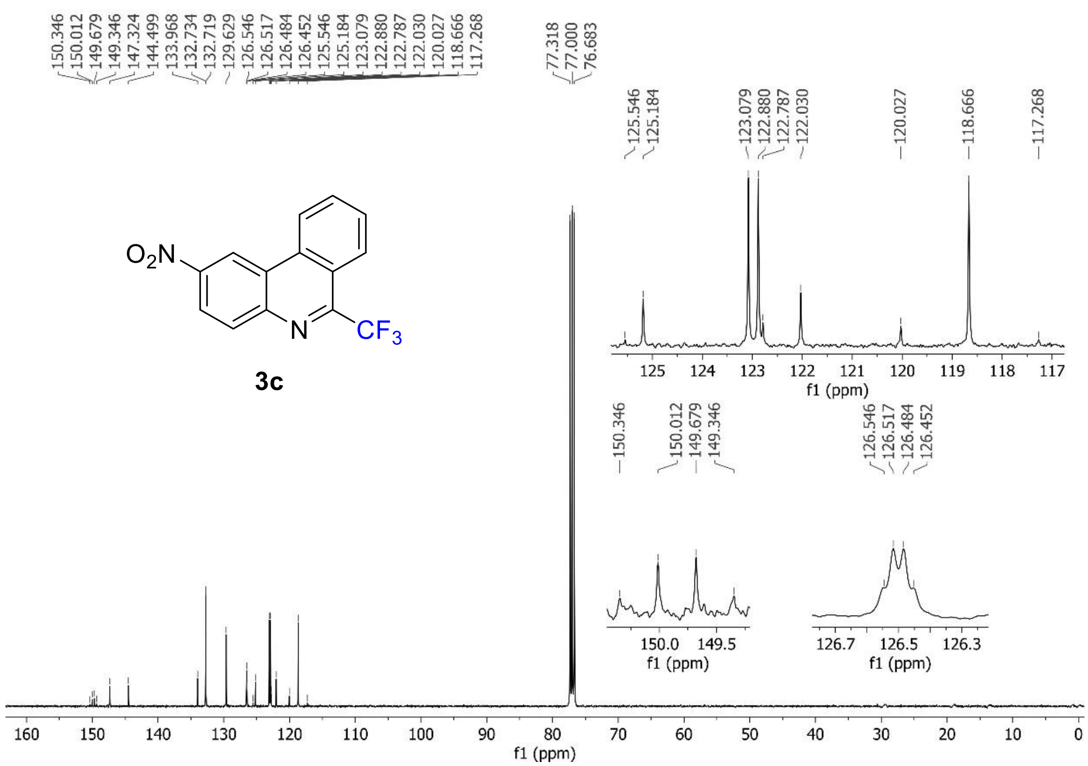
^{19}F NMR spectrum of **3b** (376 MHz, $CDCl_3$)



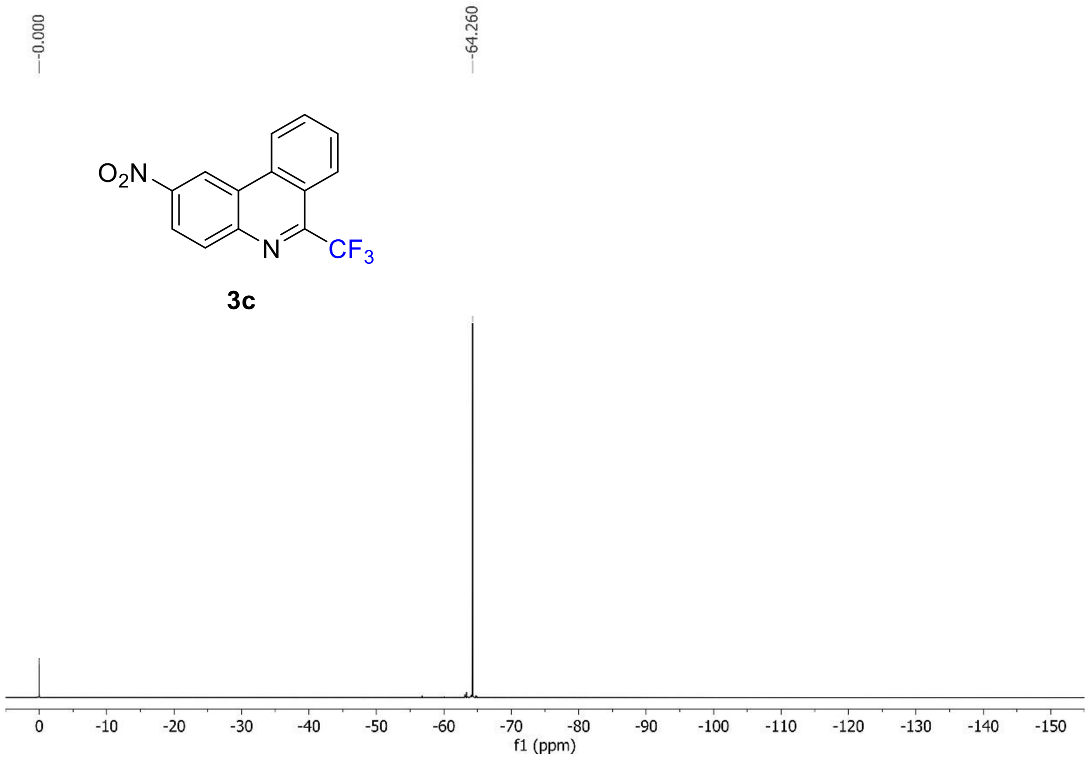
^{1}H NMR spectrum of **3c** (400 MHz, $CDCl_3$)



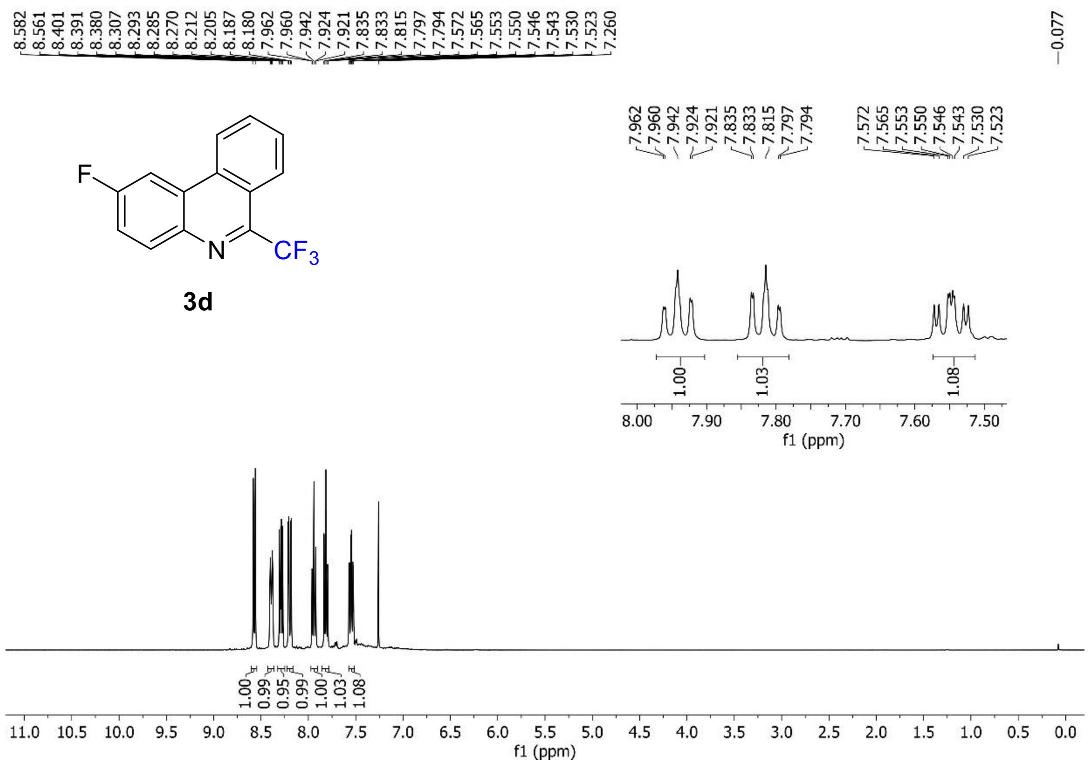
^{13}C NMR spectrum of **3c** (100 MHz, $CDCl_3$)



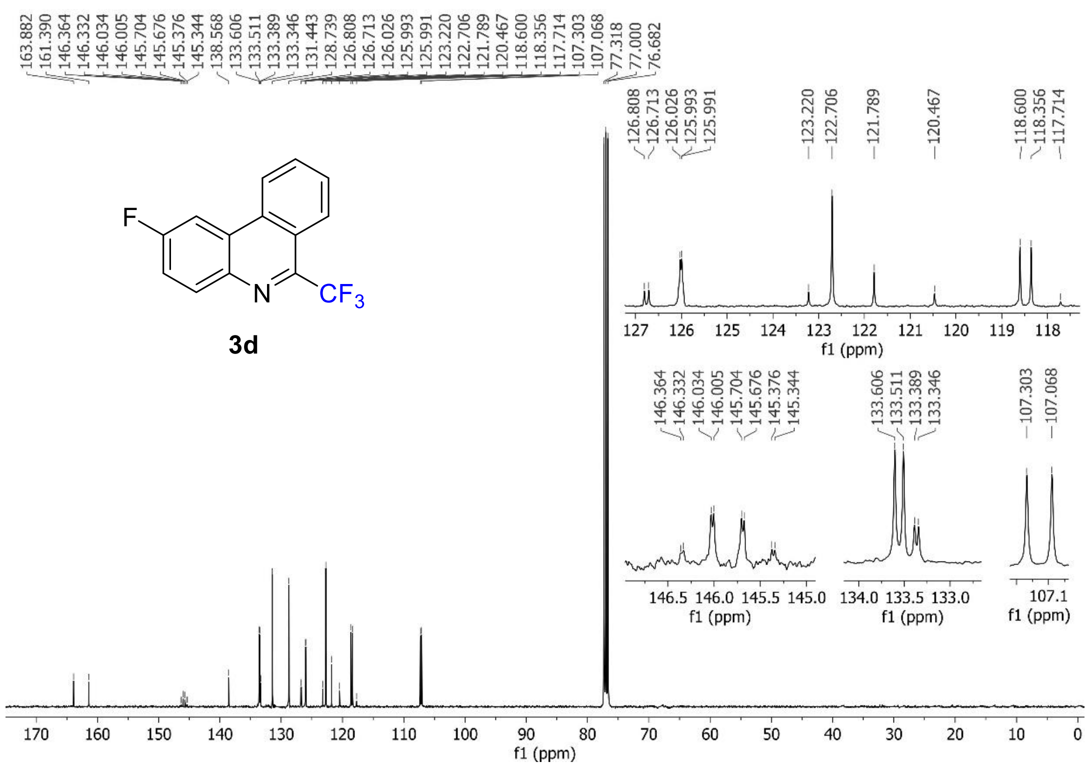
^{19}F NMR spectrum of **3c** (376 MHz, $CDCl_3$)



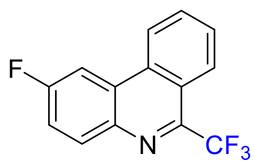
[1]H NMR spectrum of **3d** (400 MHz, $CDCl_3$)



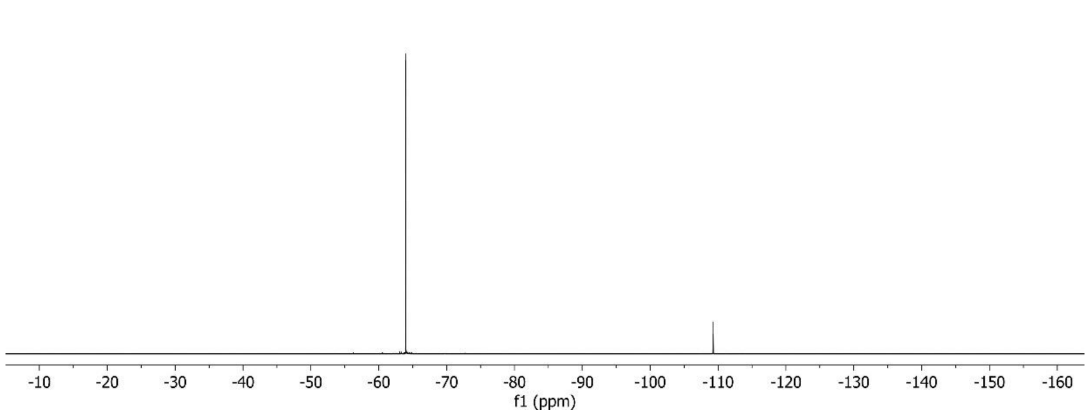
[13]C NMR spectrum of **3d** (100 MHz, $CDCl_3$)



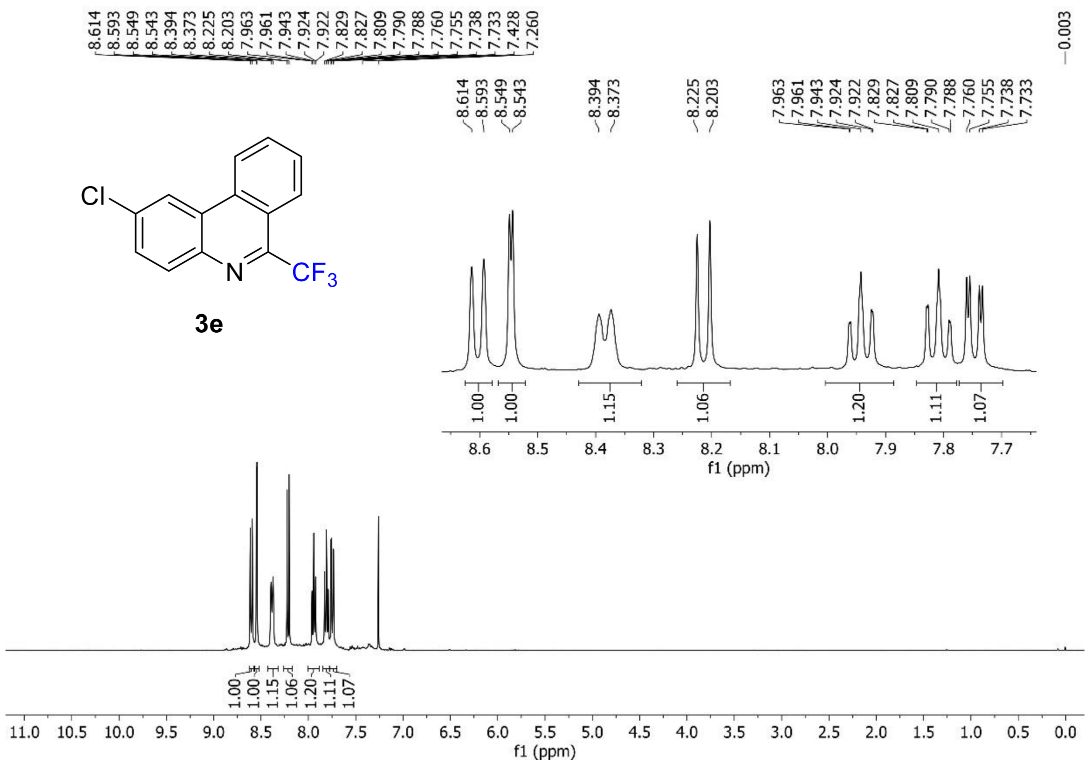
^{19}F NMR spectrum of **3d** (376 MHz, $CDCl_3$)



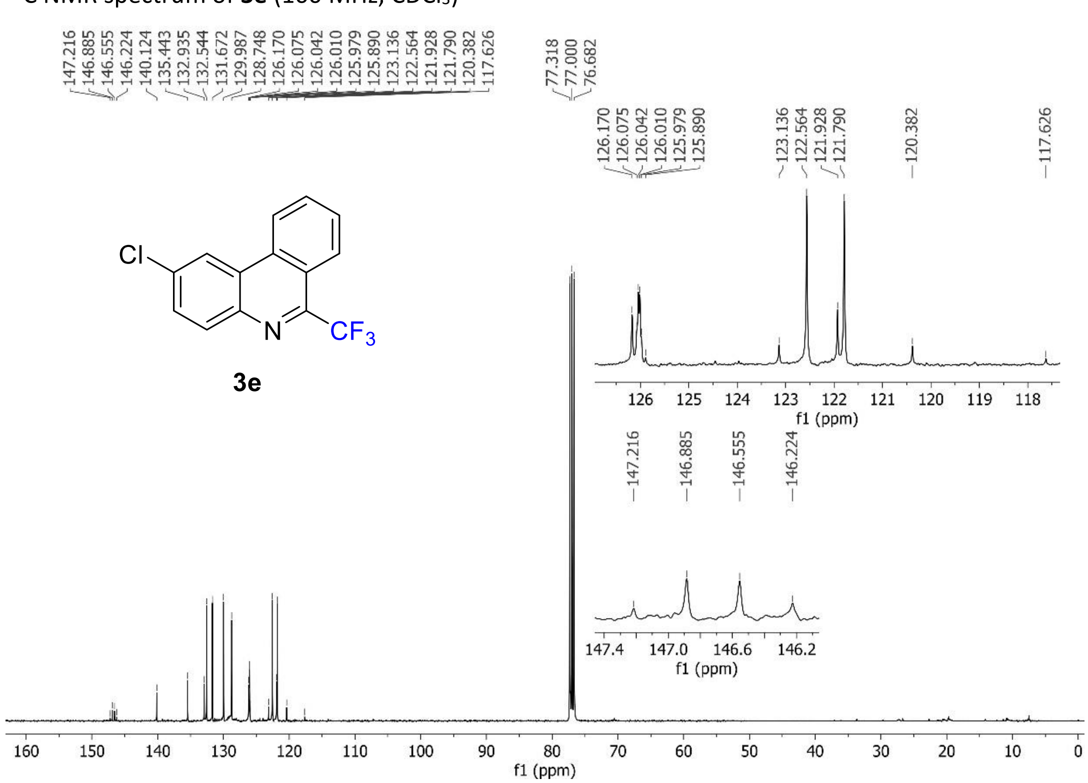
3d



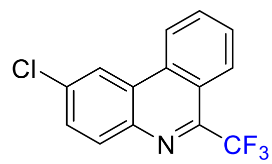
[1]H NMR spectrum of **3e** (400 MHz, $CDCl_3$)



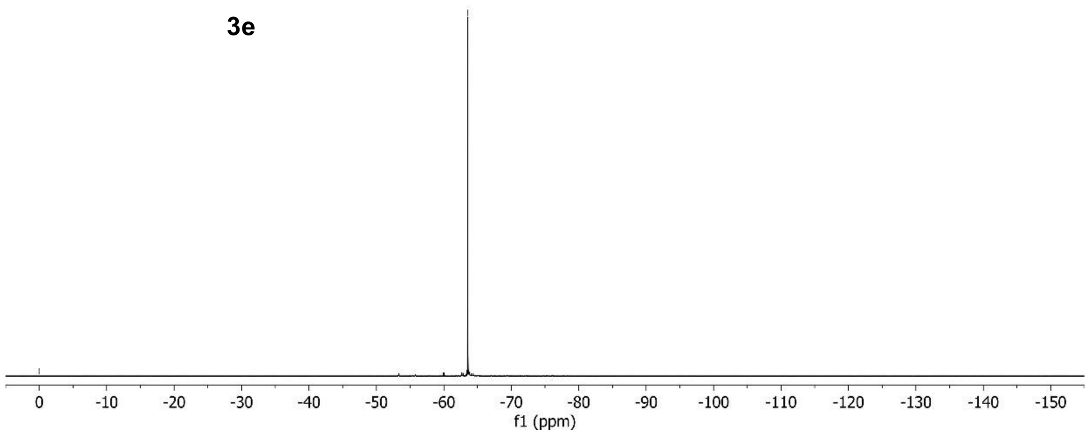
[13]C NMR spectrum of **3e** (100 MHz, $CDCl_3$)



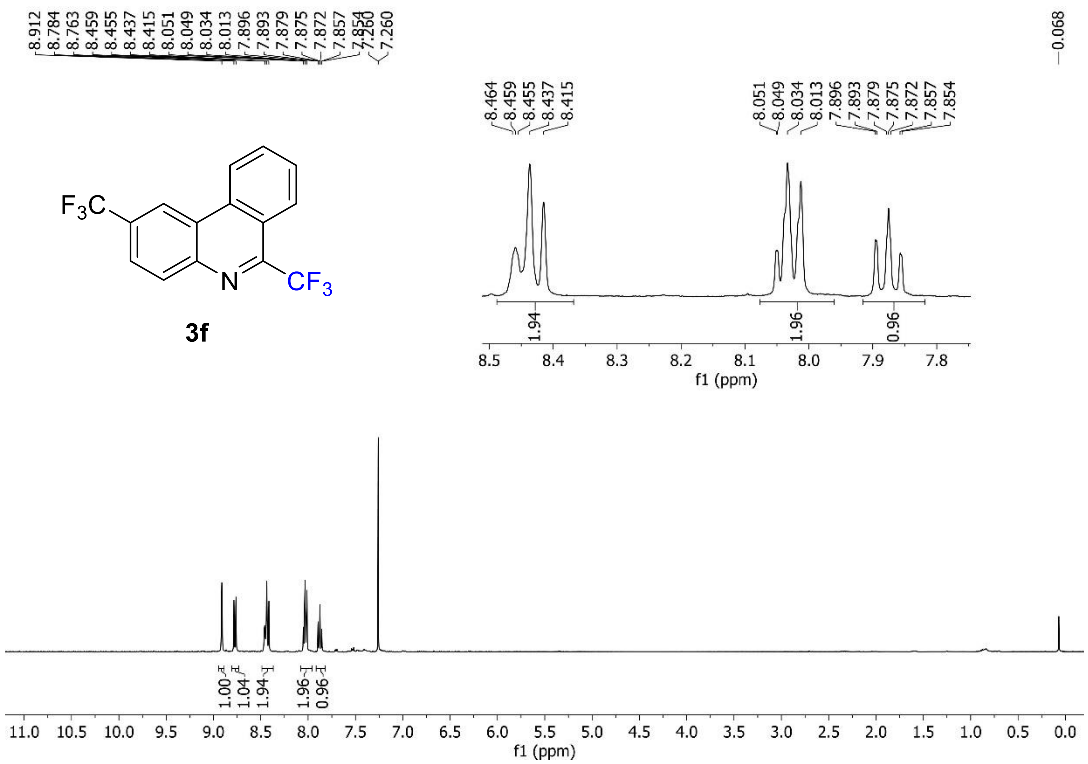
^{19}F NMR spectrum of **3e** (376 MHz, $CDCl_3$)



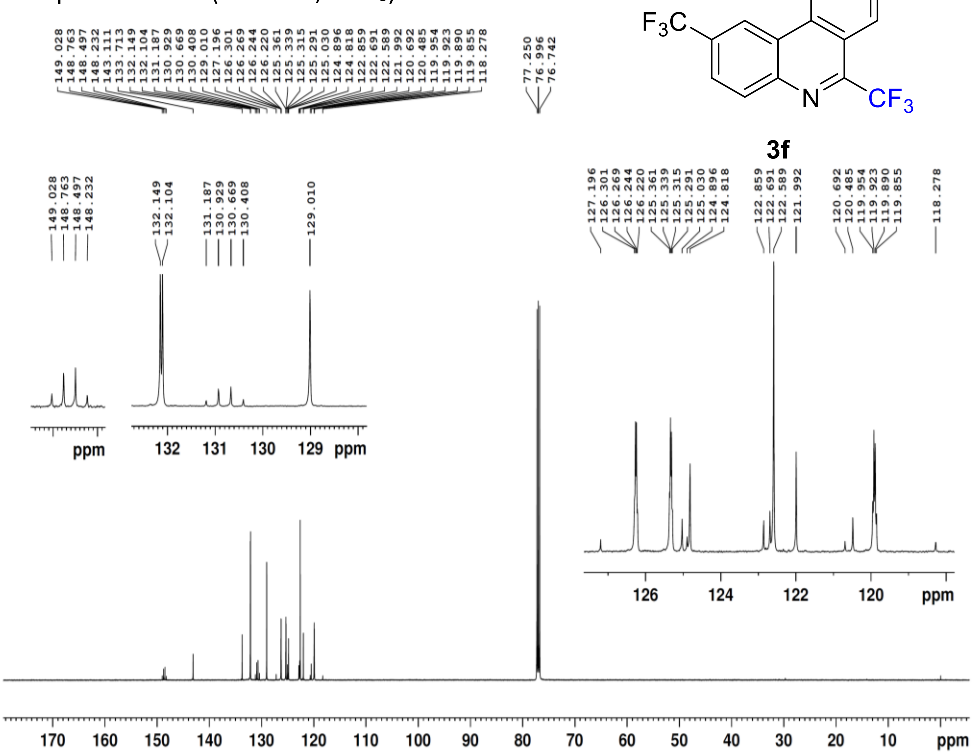
3e



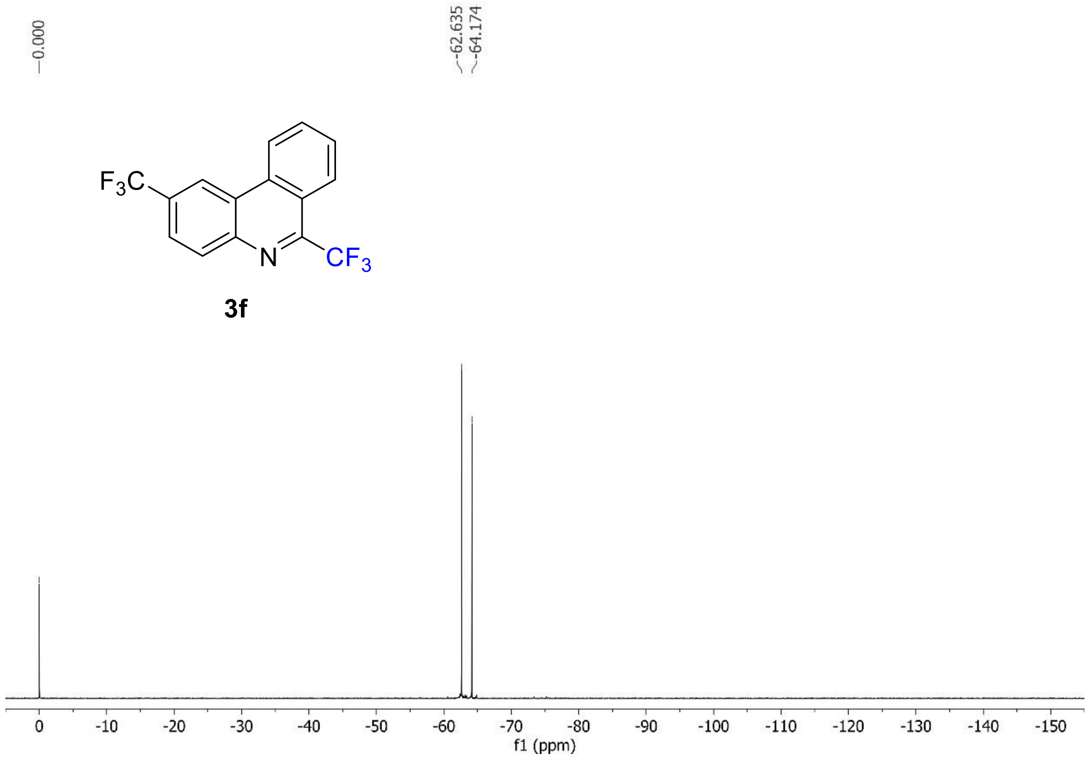
^{1}H NMR spectrum of **3f** (400 MHz, $CDCl_3$)



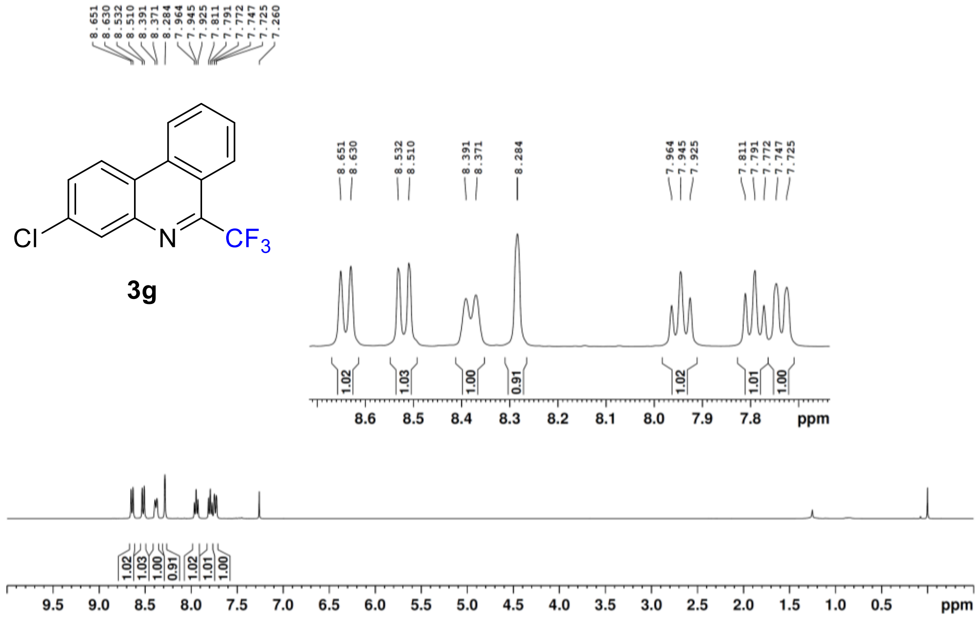
^{13}C NMR spectrum of **3f** (125 MHz, $CDCl_3$)



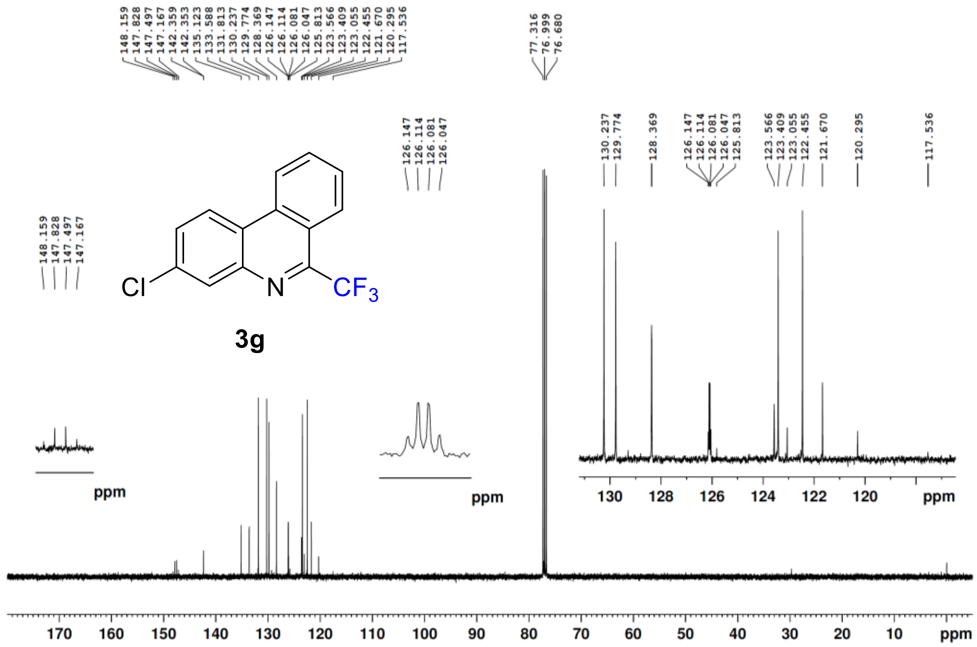
^{19}F NMR spectrum of **3f** (376 MHz, $CDCl_3$)



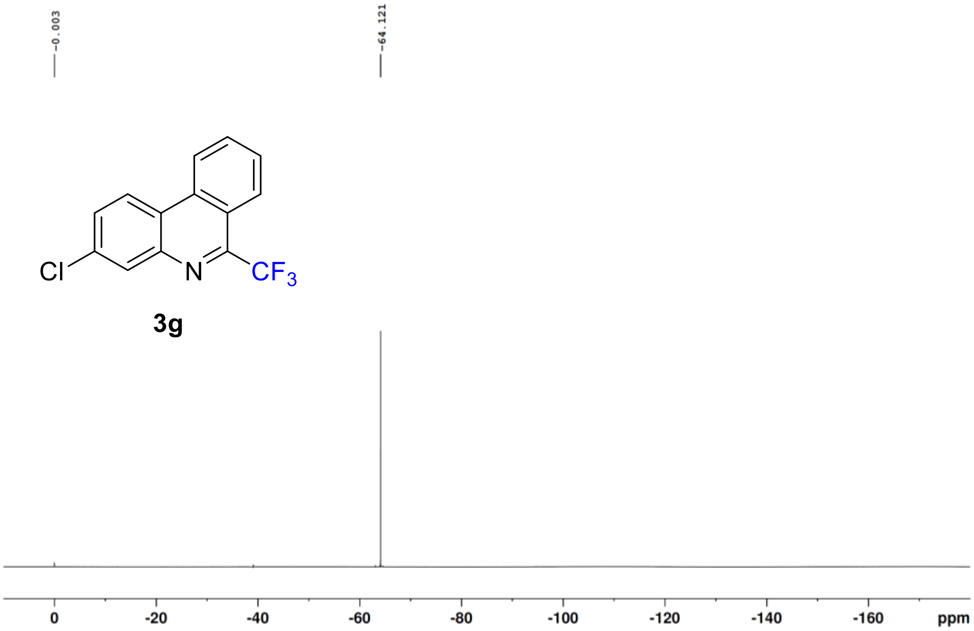
^{1}H NMR spectrum of **3g** (400 MHz, $CDCl_3$)



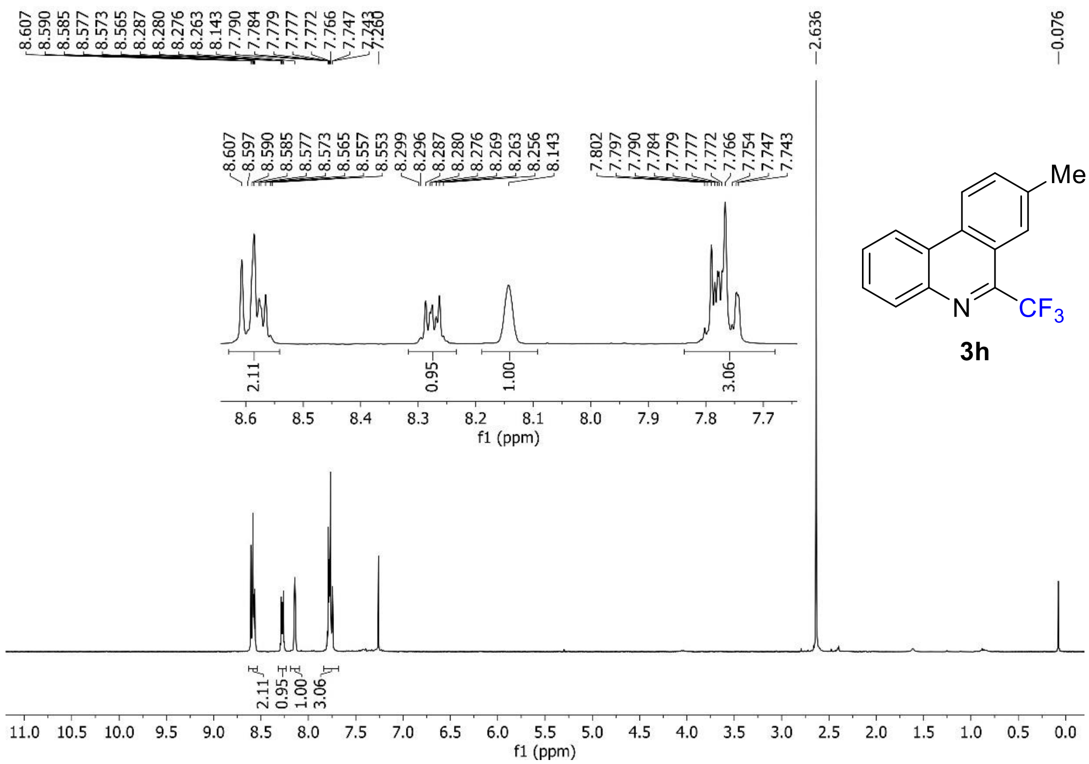
^{13}C NMR spectrum of **3g** (100 MHz, $CDCl_3$)



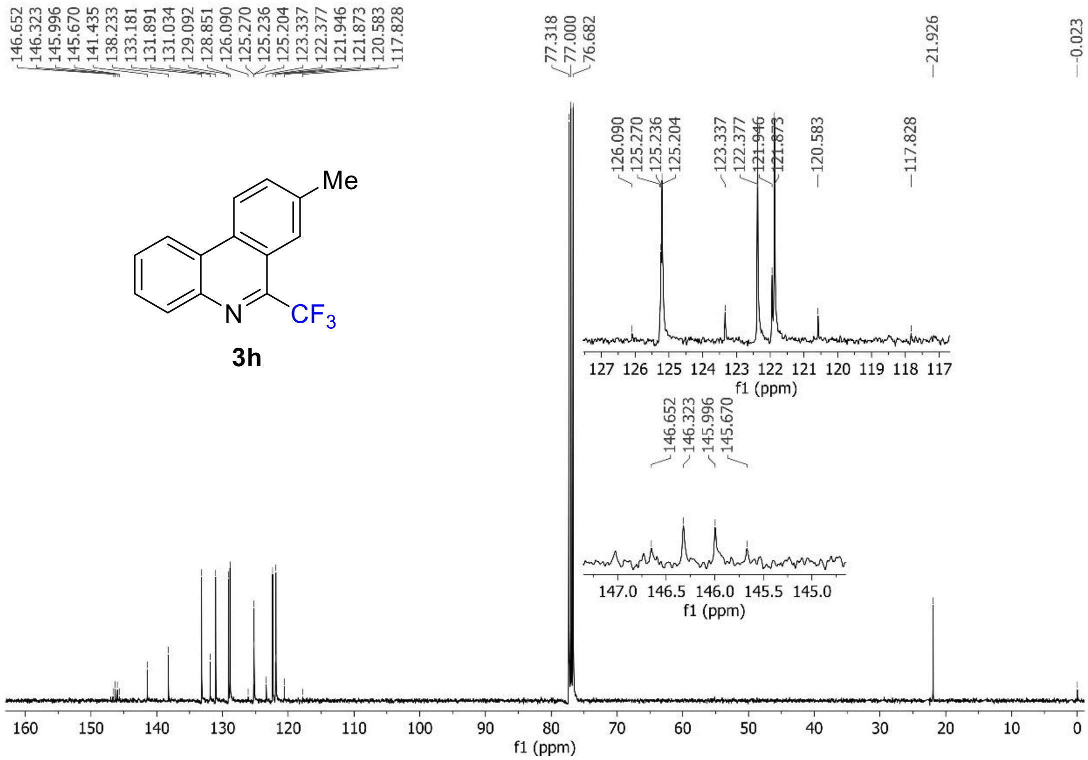
^{19}F NMR spectrum of **3g** (376 MHz, $CDCl_3$)



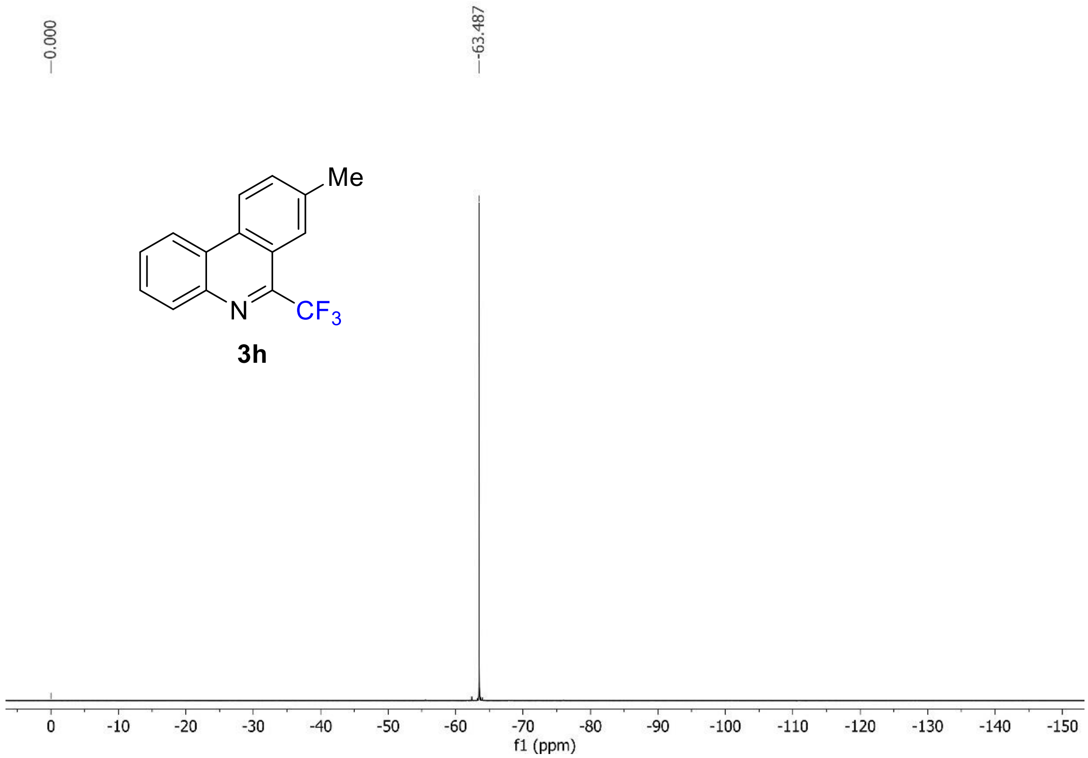
^{1}H NMR spectrum of **3h** (400 MHz, $CDCl_3$)



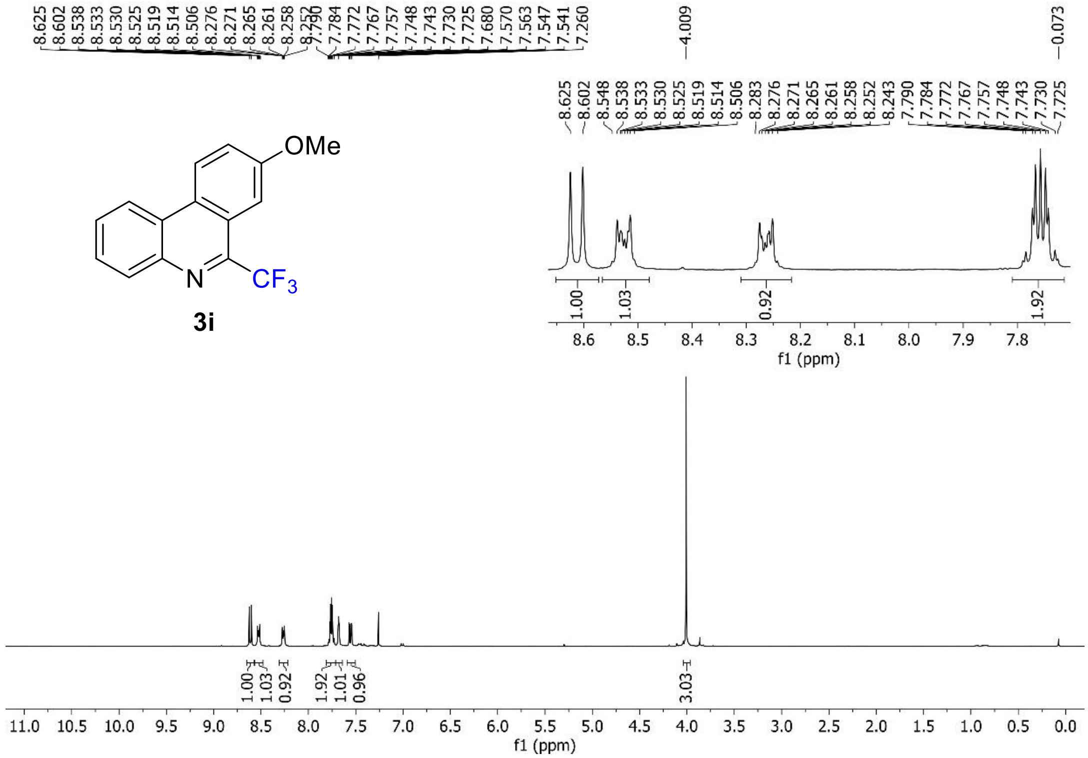
^{13}C NMR spectrum of **3h** (100 MHz, $CDCl_3$)



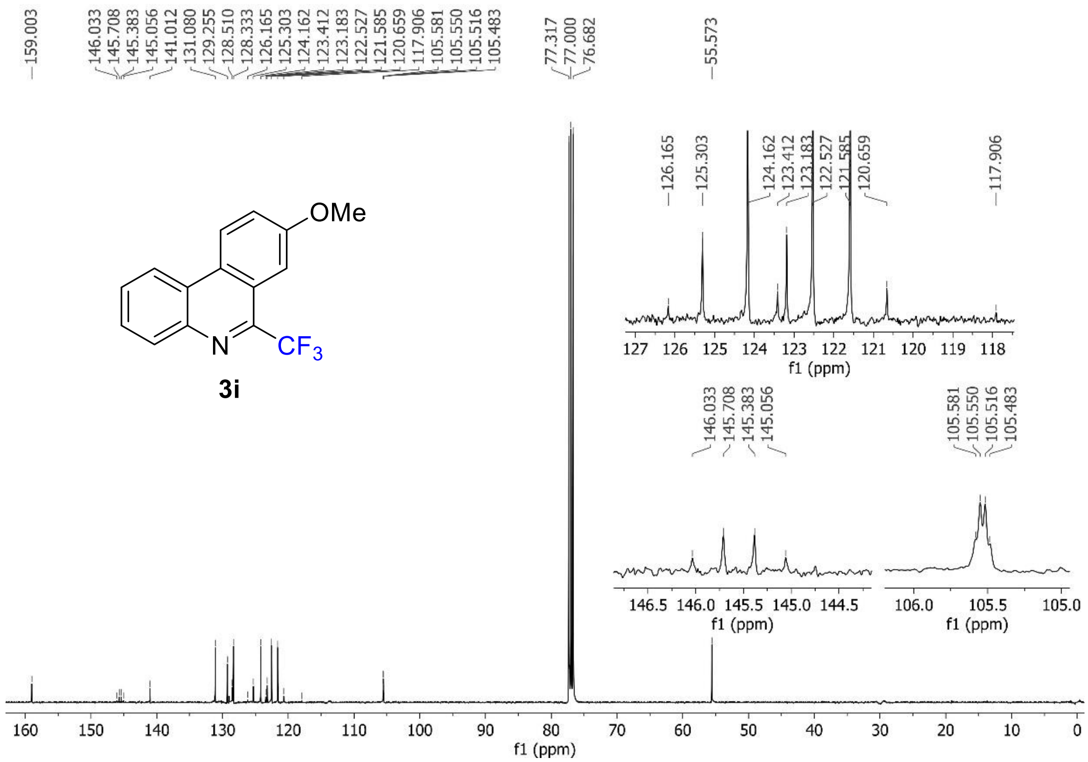
^{19}F NMR spectrum of **3h** (376 MHz, $CDCl_3$)



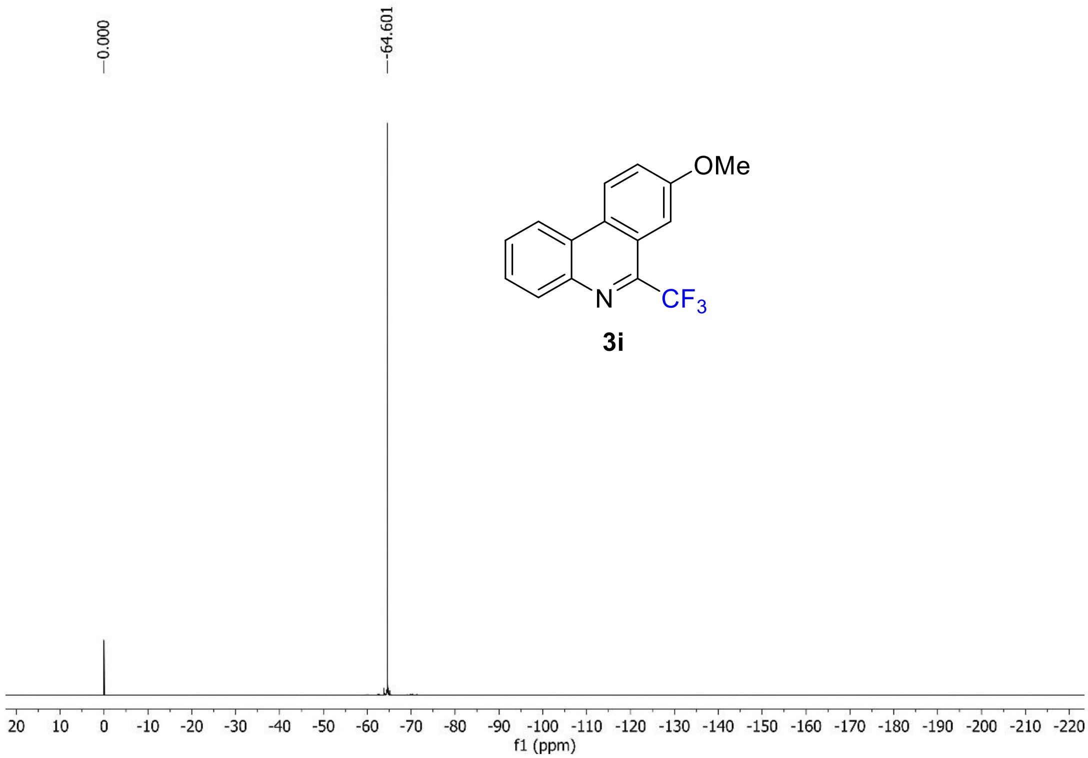
^{1}H NMR spectrum of **3i** (400 MHz, $CDCl_3$)



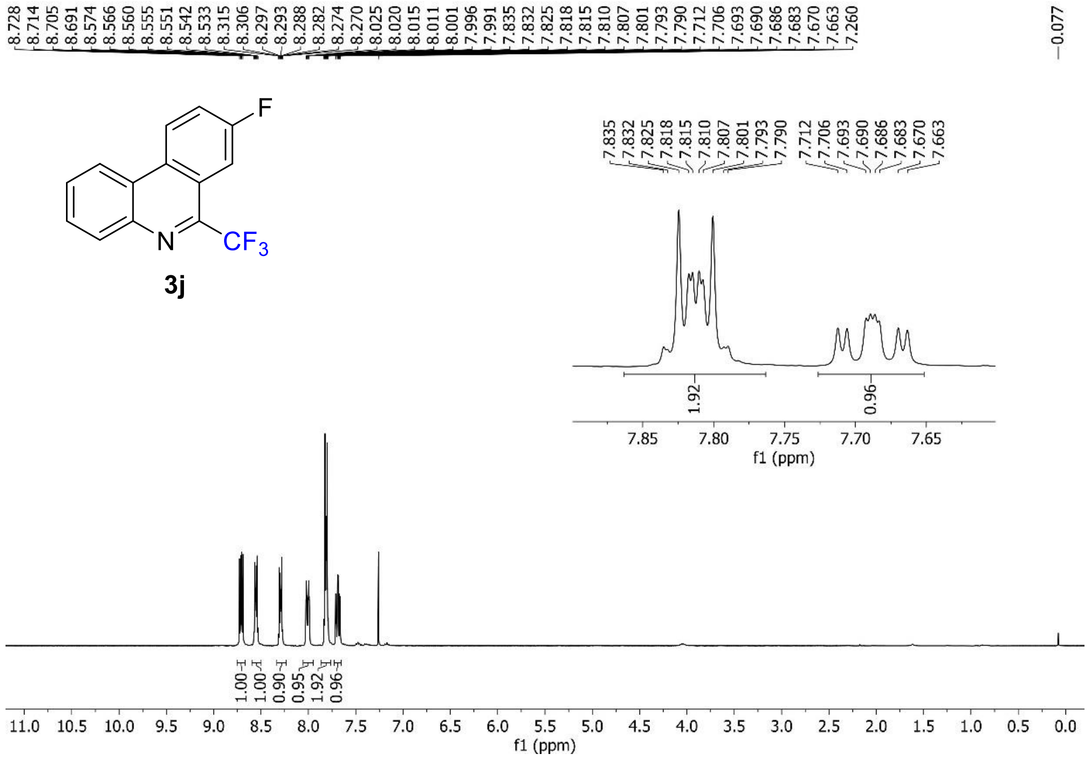
^{13}C NMR spectrum of **3i** (100 MHz, $CDCl_3$)



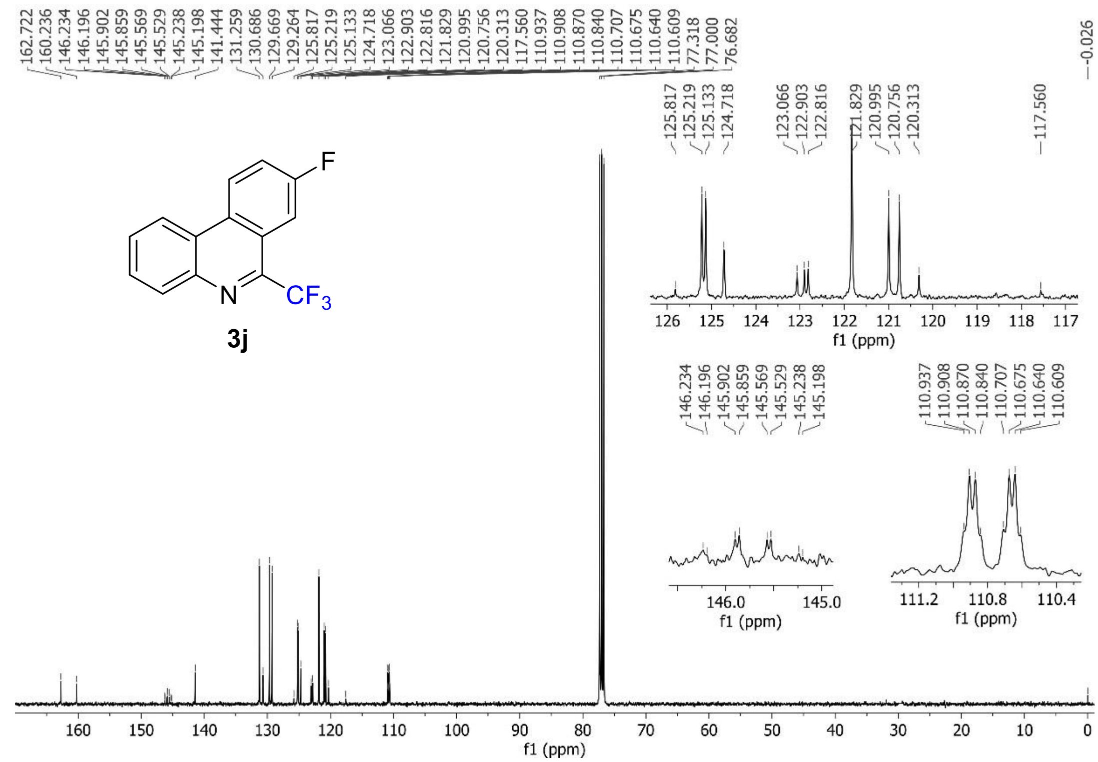
^{19}F NMR spectrum of **3i** (376 MHz, $CDCl_3$)



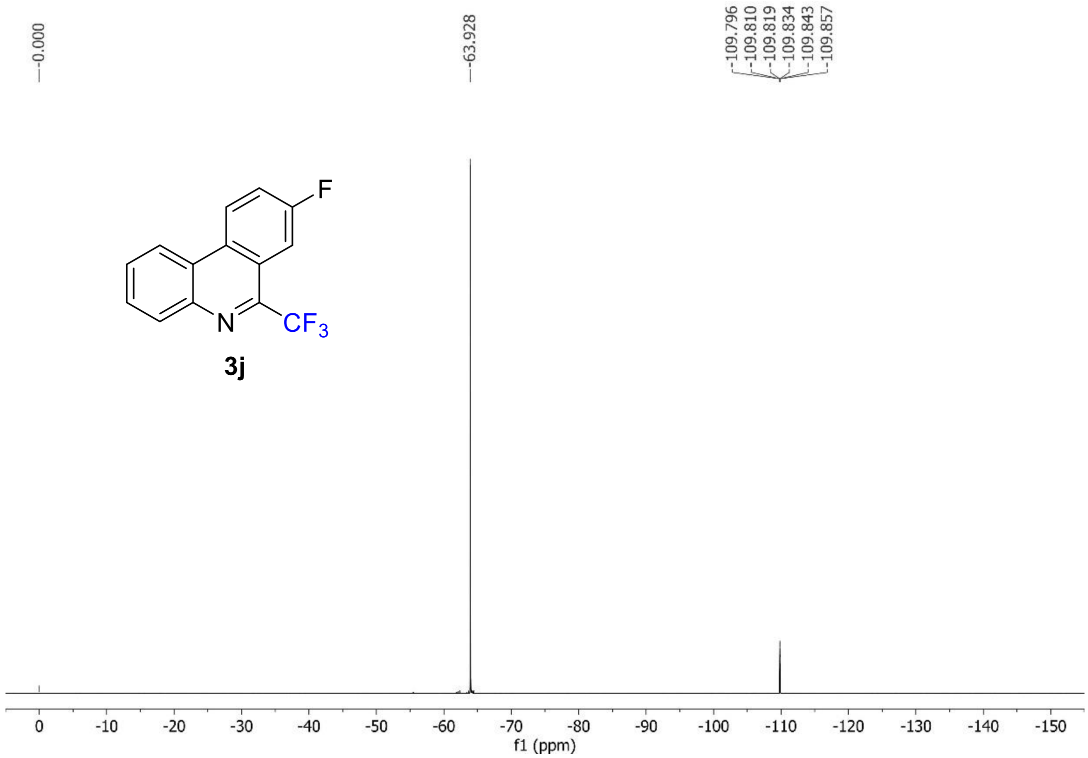
^{1}H NMR spectrum of **3j** (400 MHz, $CDCl_3$)



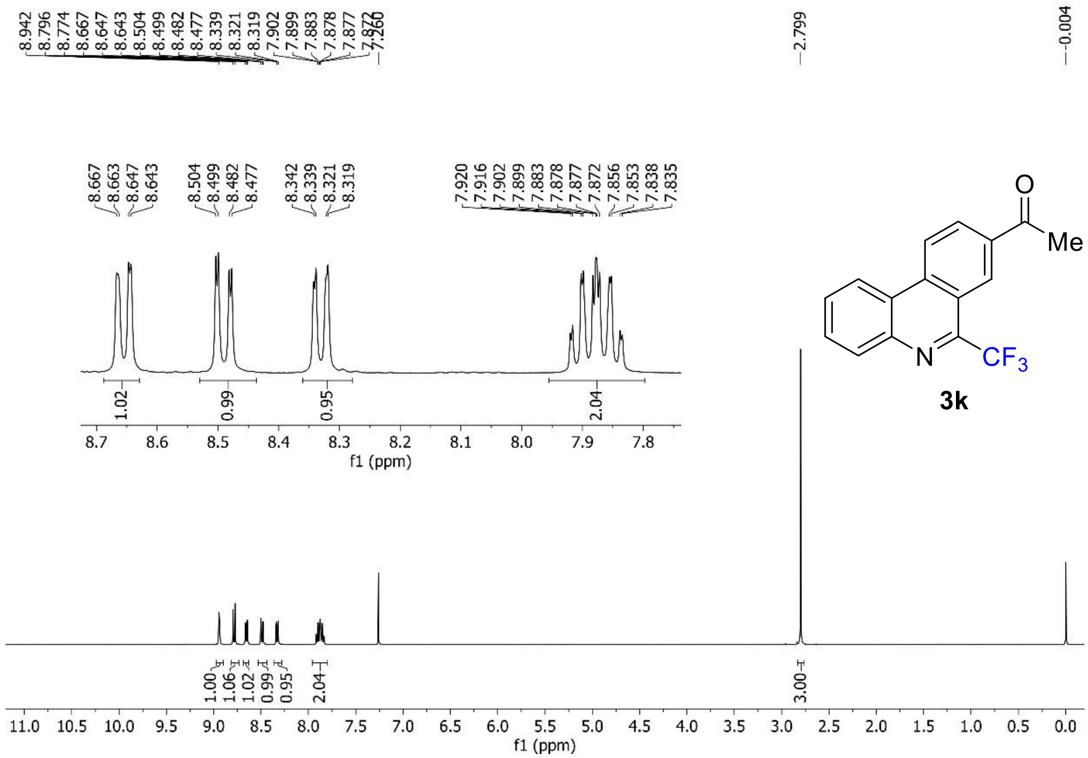
^{13}C NMR spectrum of **3j** (100 MHz, $CDCl_3$)



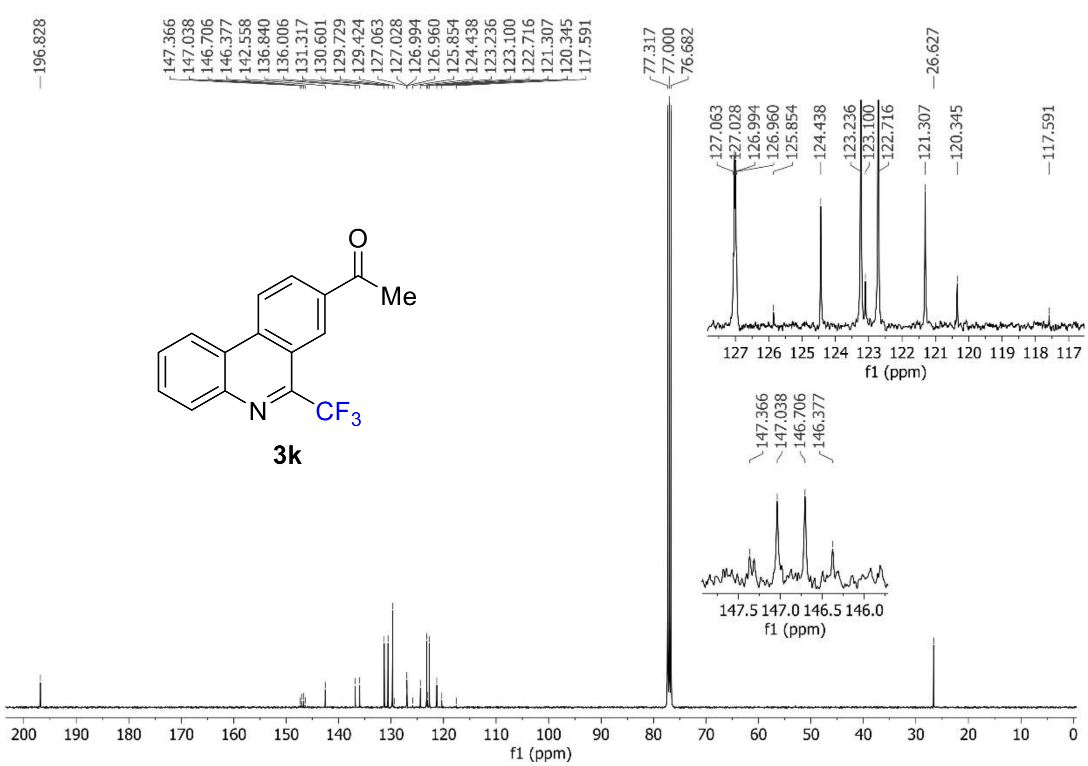
^{19}F NMR spectrum of **3j** (376 MHz, $CDCl_3$)



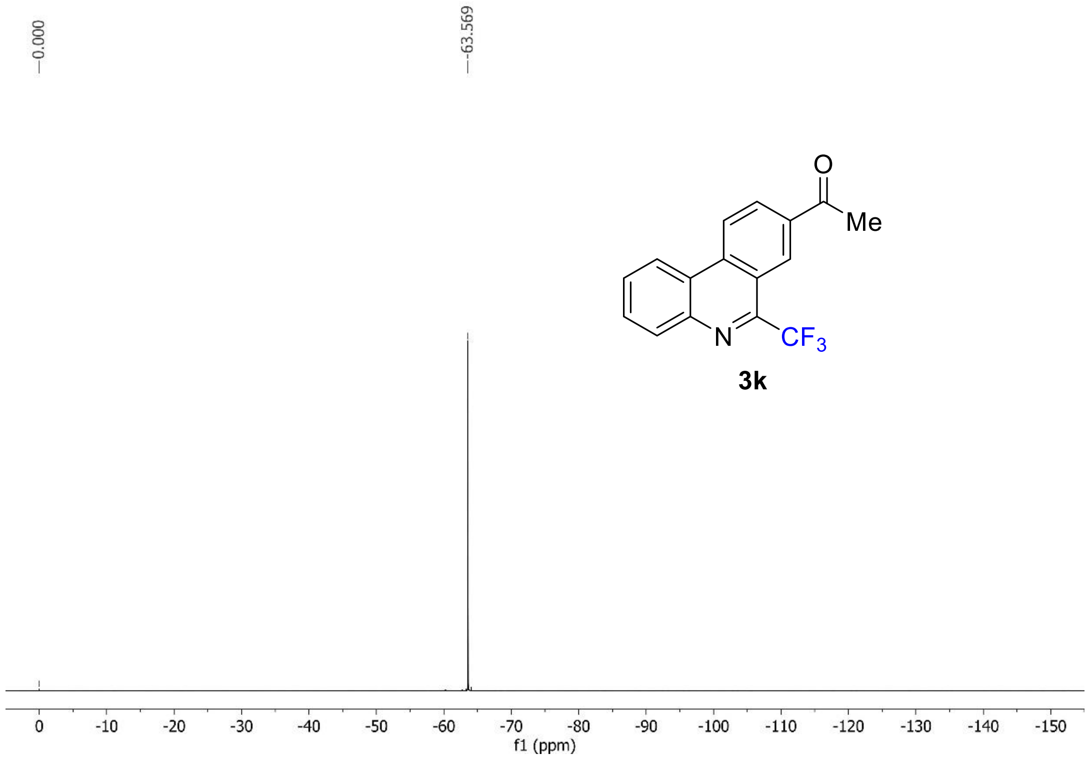
^{1}H NMR spectrum of **3k** (400 MHz, $CDCl_3$)



^{13}C NMR spectrum of **3k** (100 MHz, $CDCl_3$)

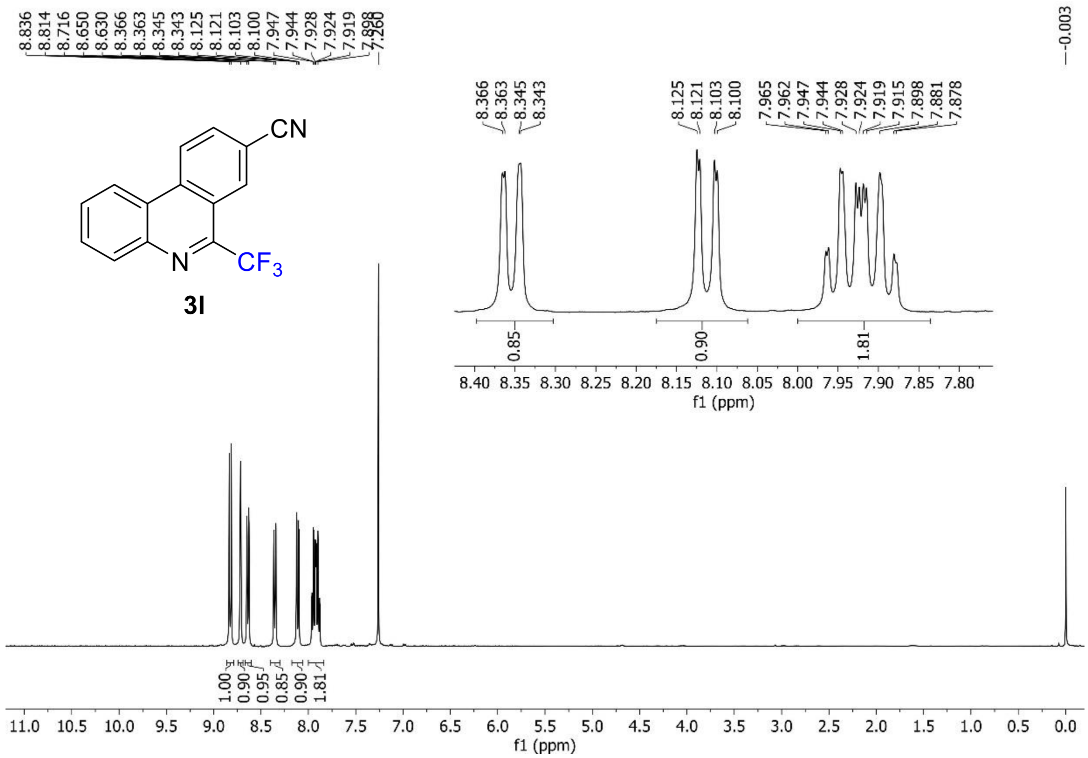


^{19}F NMR spectrum of **3k** (376 MHz, $CDCl_3$)

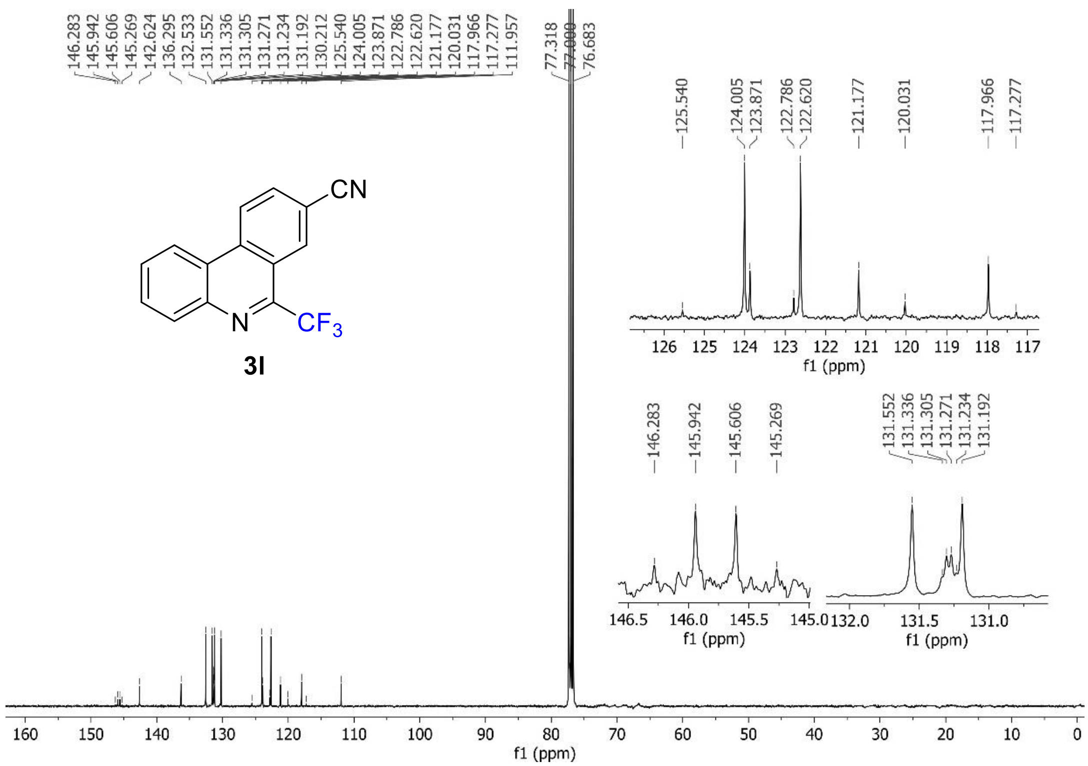


3k

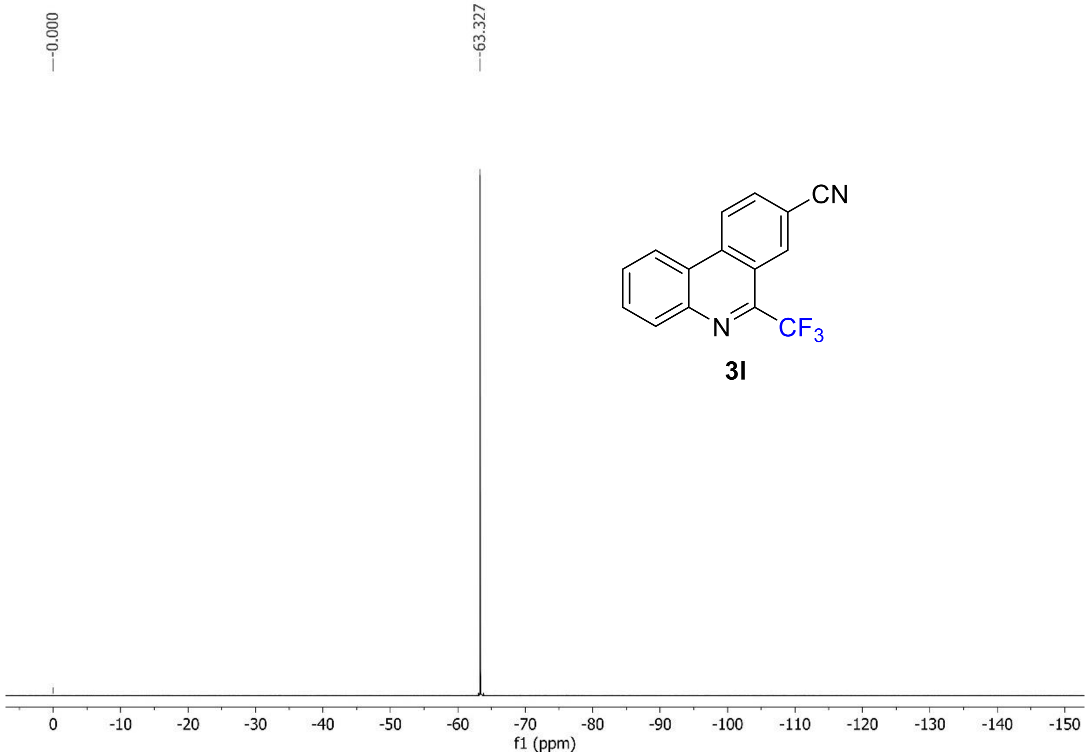
^{1}H NMR spectrum of **3l** (400 MHz, $CDCl_3$)



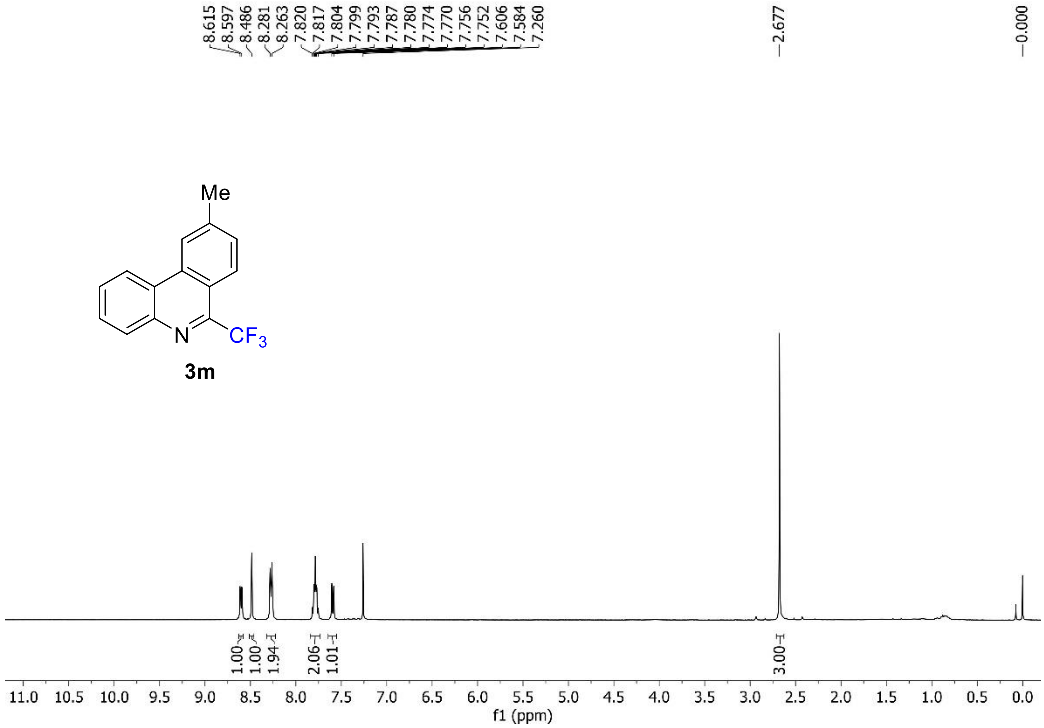
^{13}C NMR spectrum of **3l** (100 MHz, $CDCl_3$)



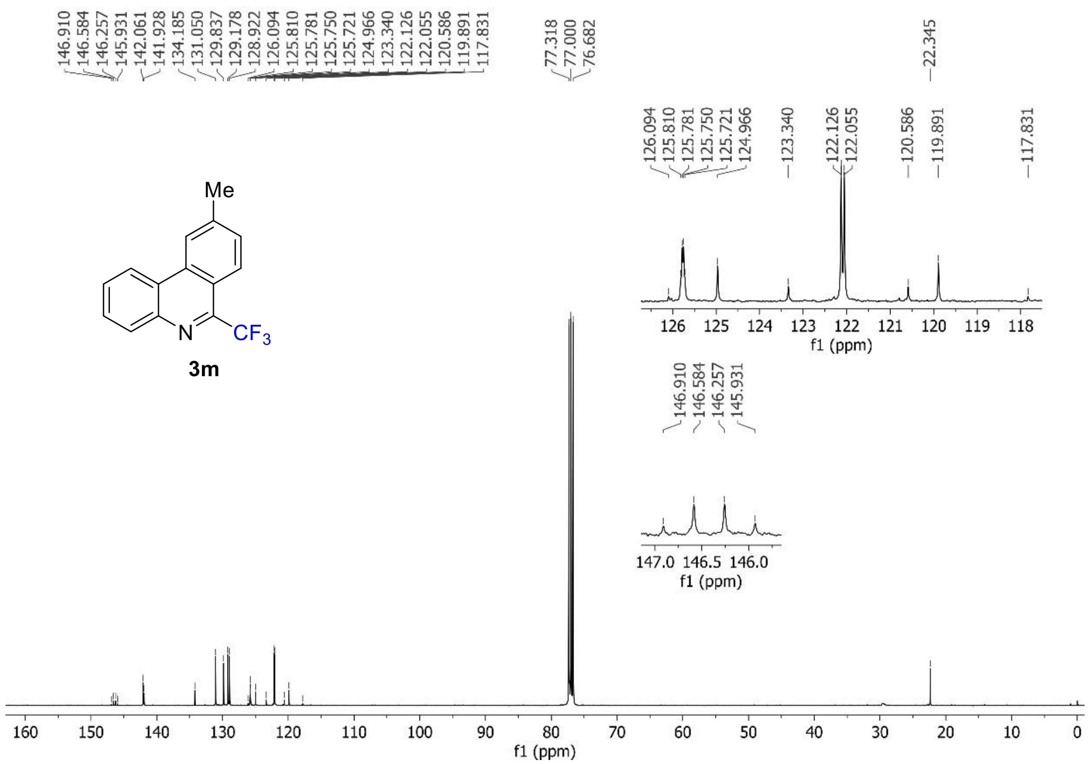
^{19}F NMR spectrum of **3l** (376 MHz, $CDCl_3$)



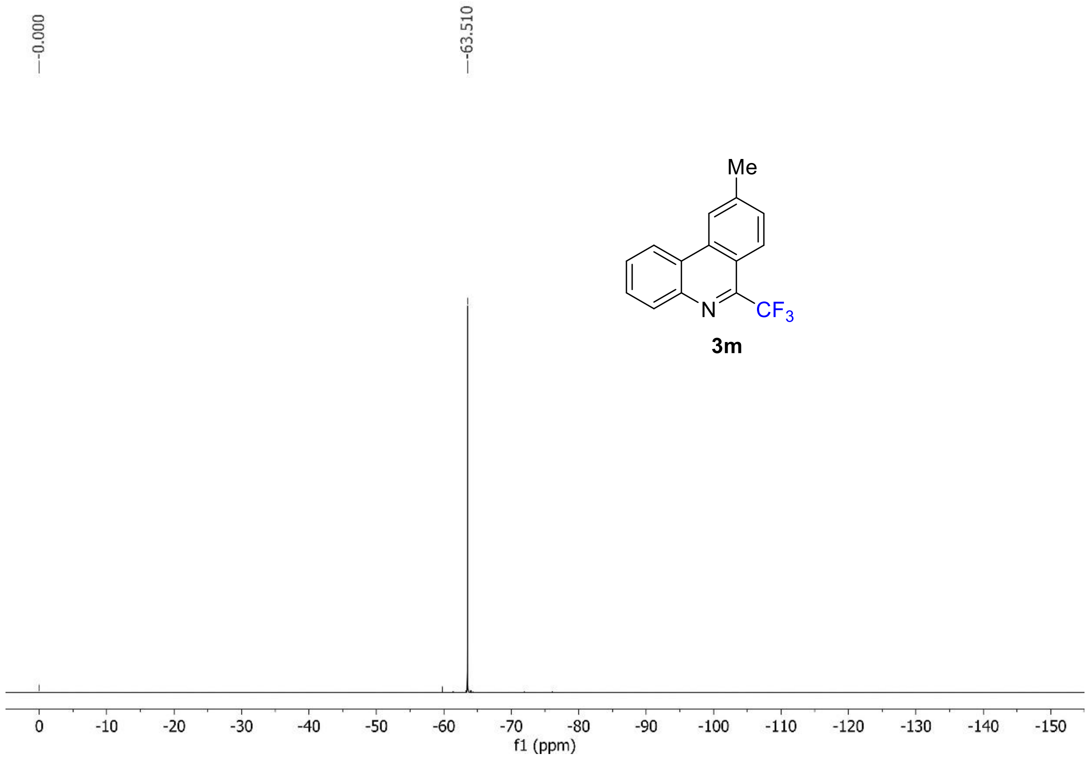
^{1}H NMR spectrum of **3m** (400 MHz, $CDCl_3$)



^{13}C NMR spectrum of **3m** (100 MHz, $CDCl_3$)

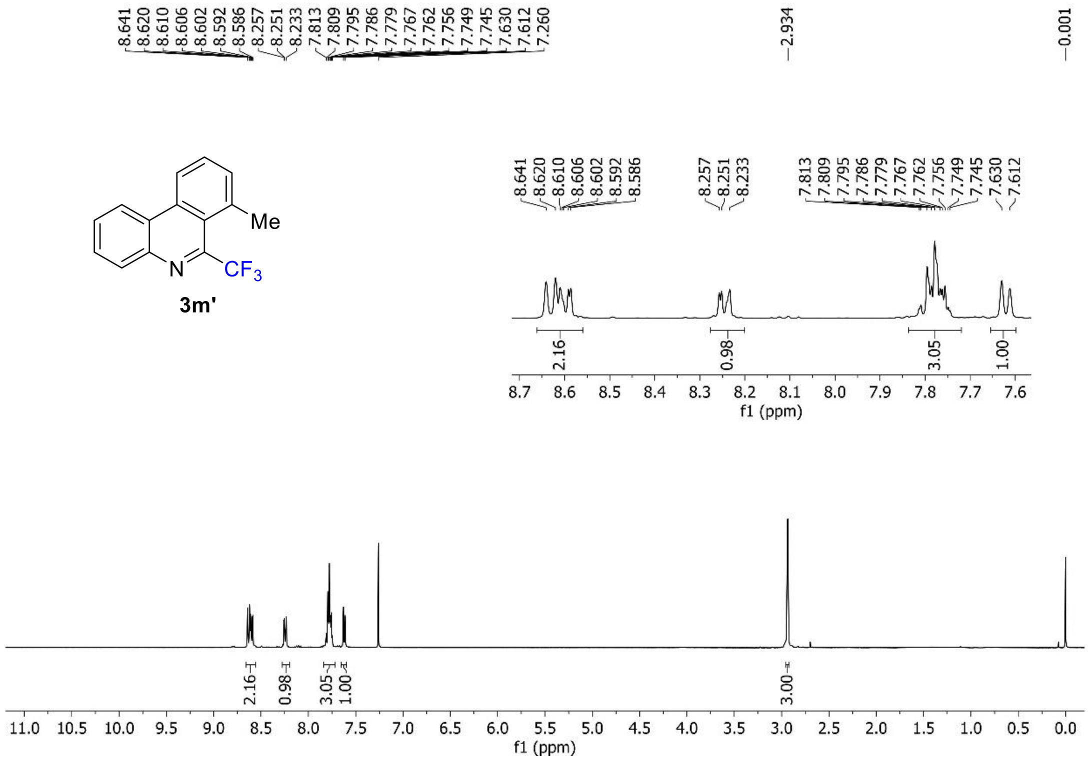


^{19}F NMR spectrum of **3m** (376 MHz, $CDCl_3$)

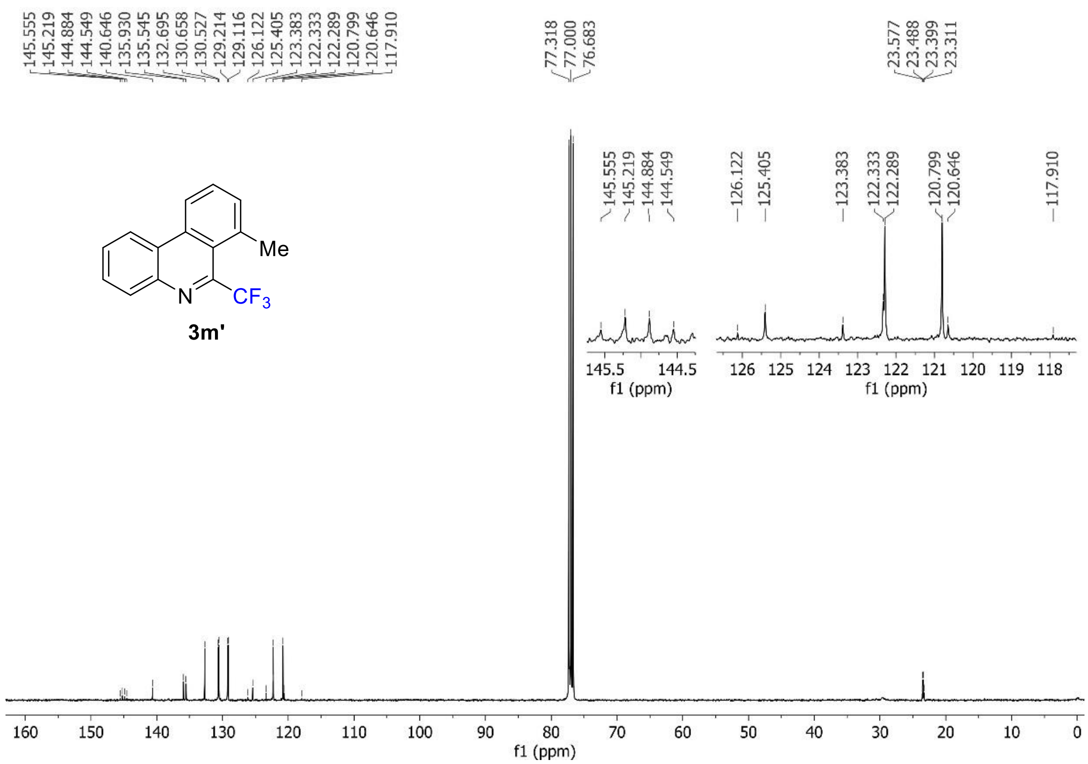


3m

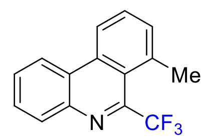
^{1}H NMR spectrum of **3m’** (400 MHz, $CDCl_3$)



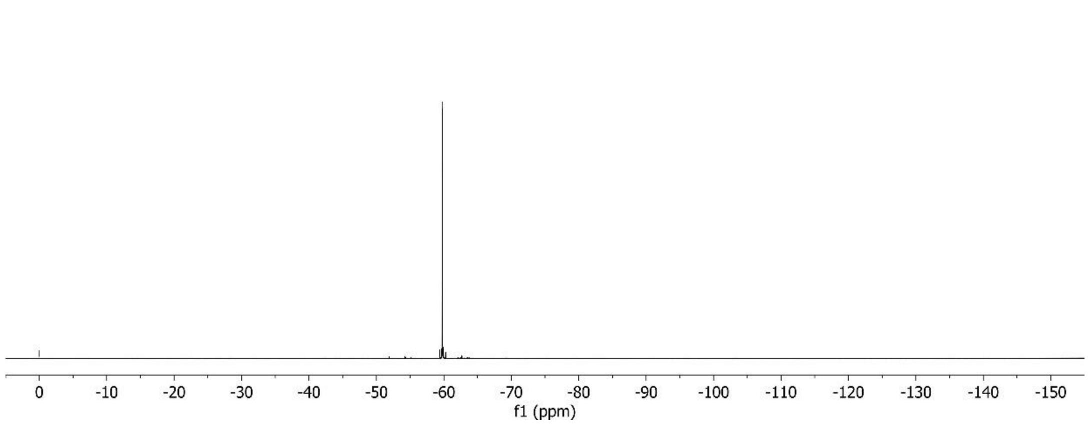
^{13}C NMR spectrum of **3m’** (100 MHz, $CDCl_3$)



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

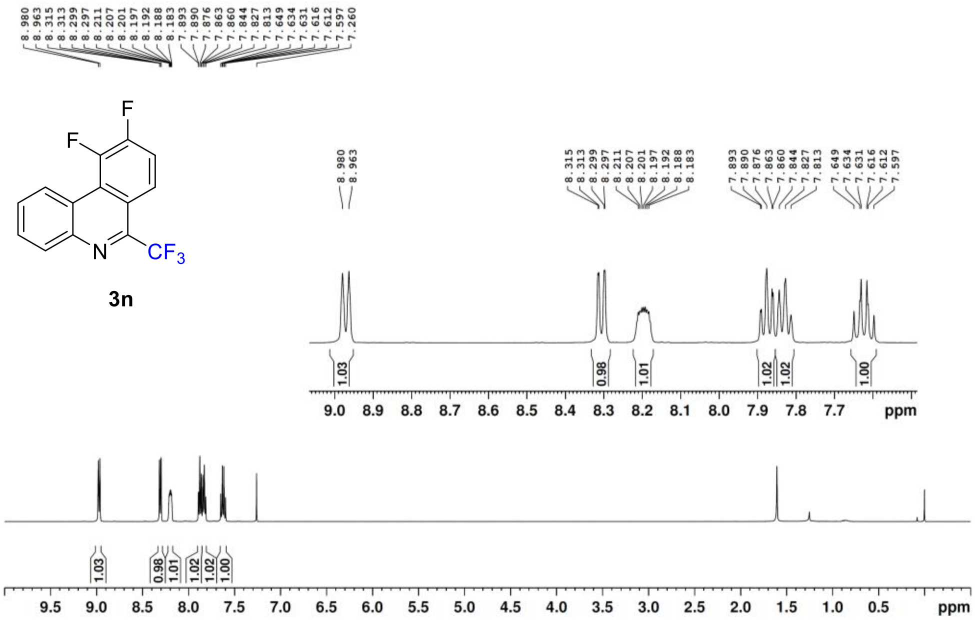


3m'



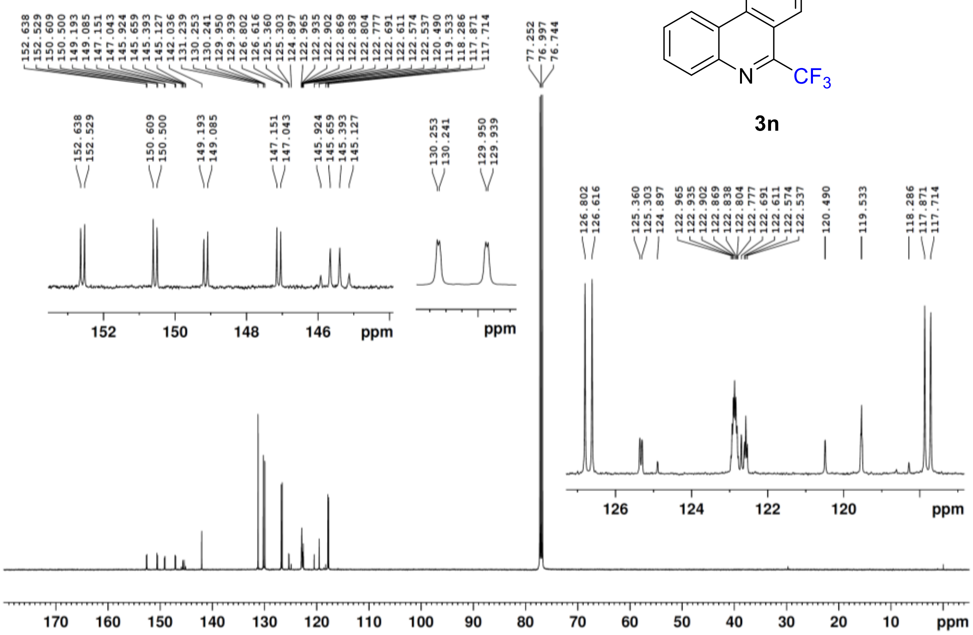
[1]H NMR spectrum of **3n** (500 MHz, $CDCl_3$)

3n

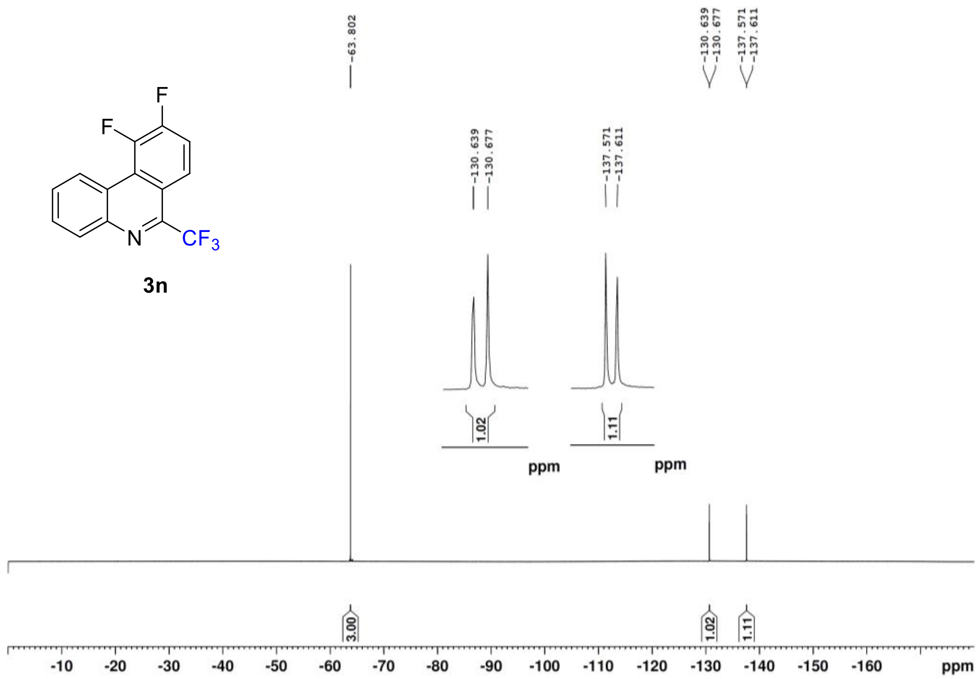


[13]C NMR spectrum of **3n** (125 MHz, $CDCl_3$)

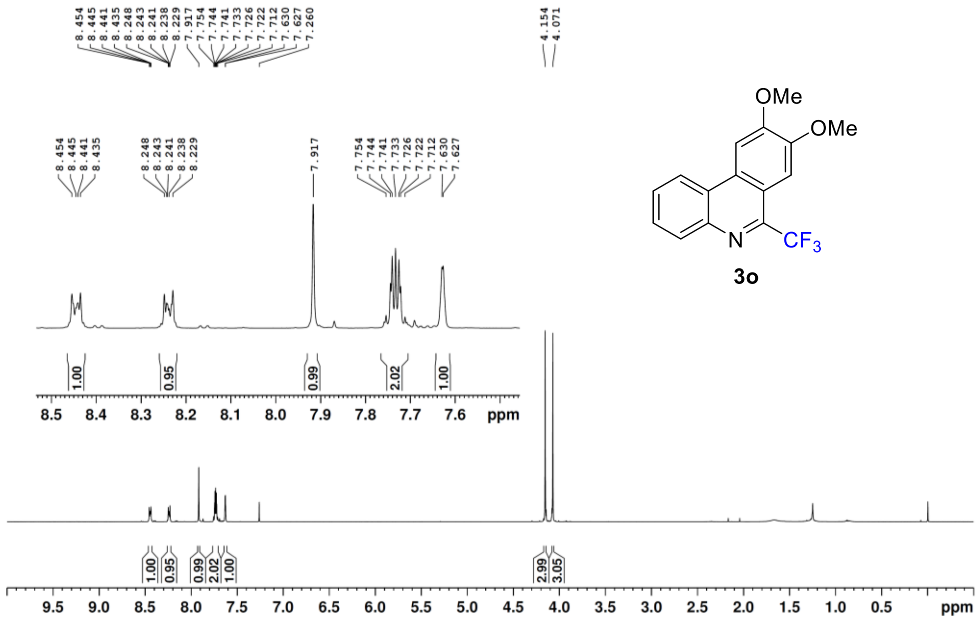
3n



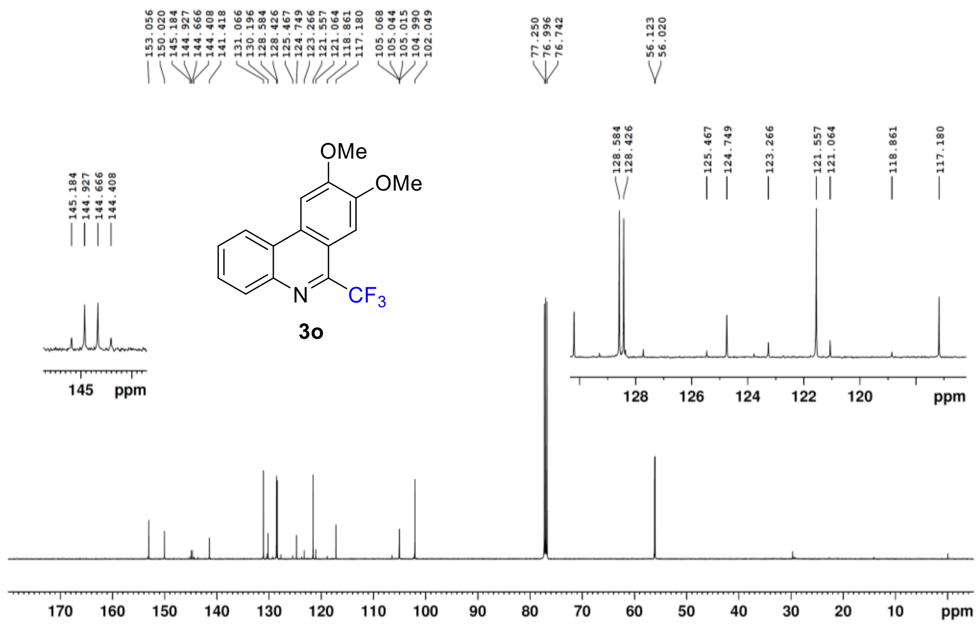
^{19}F NMR spectrum of **3n** (470 MHz, $CDCl_3$)



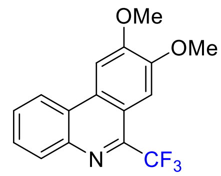
^{1}H NMR spectrum of **3o** (500 MHz, $CDCl_3$)



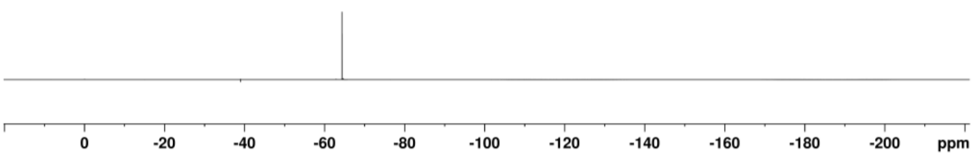
^{13}C NMR spectrum of **3o** (125 MHz, $CDCl_3$)



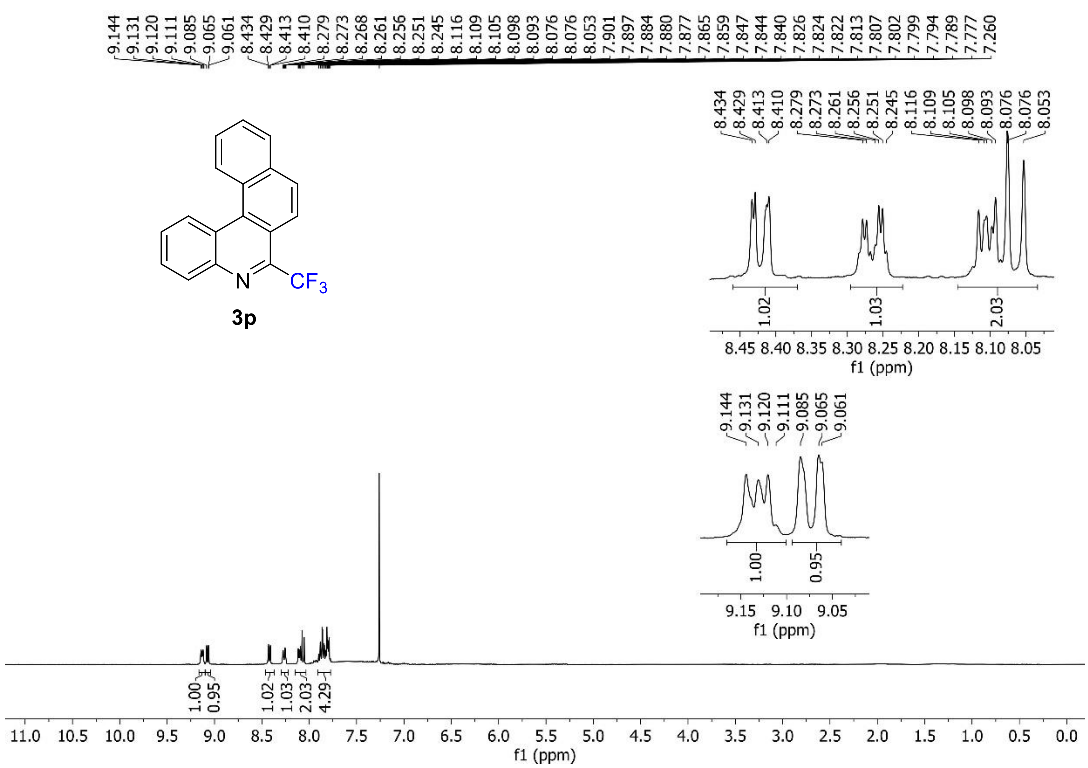
^{19}F NMR spectrum of **3o** (470 MHz, $CDCl_3$)



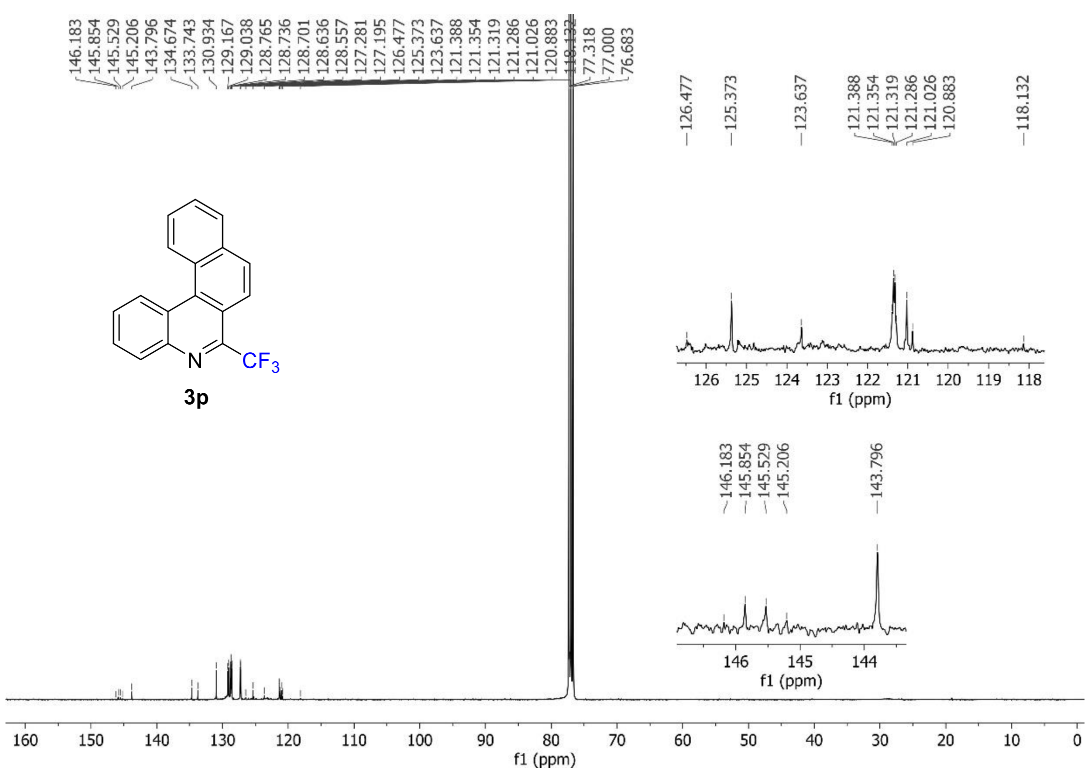
3o



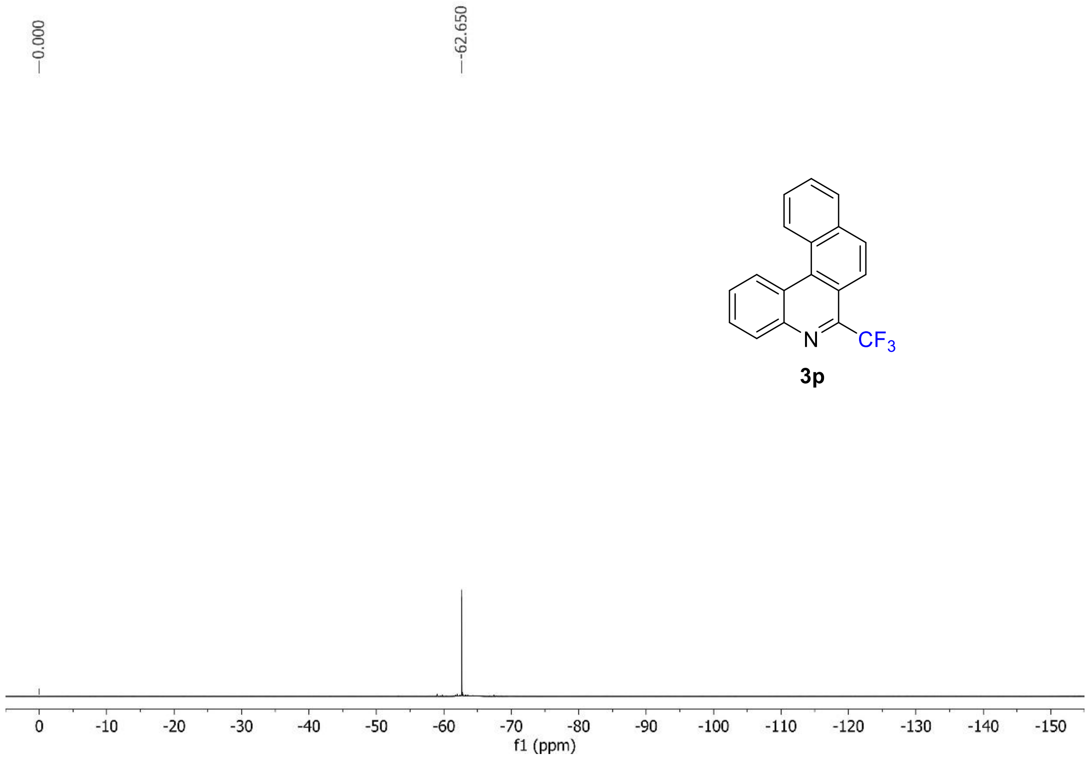
^{1}H NMR spectrum of **3p** (400 MHz, $CDCl_3$)



^{13}C NMR spectrum of **3p** (100 MHz, $CDCl_3$)

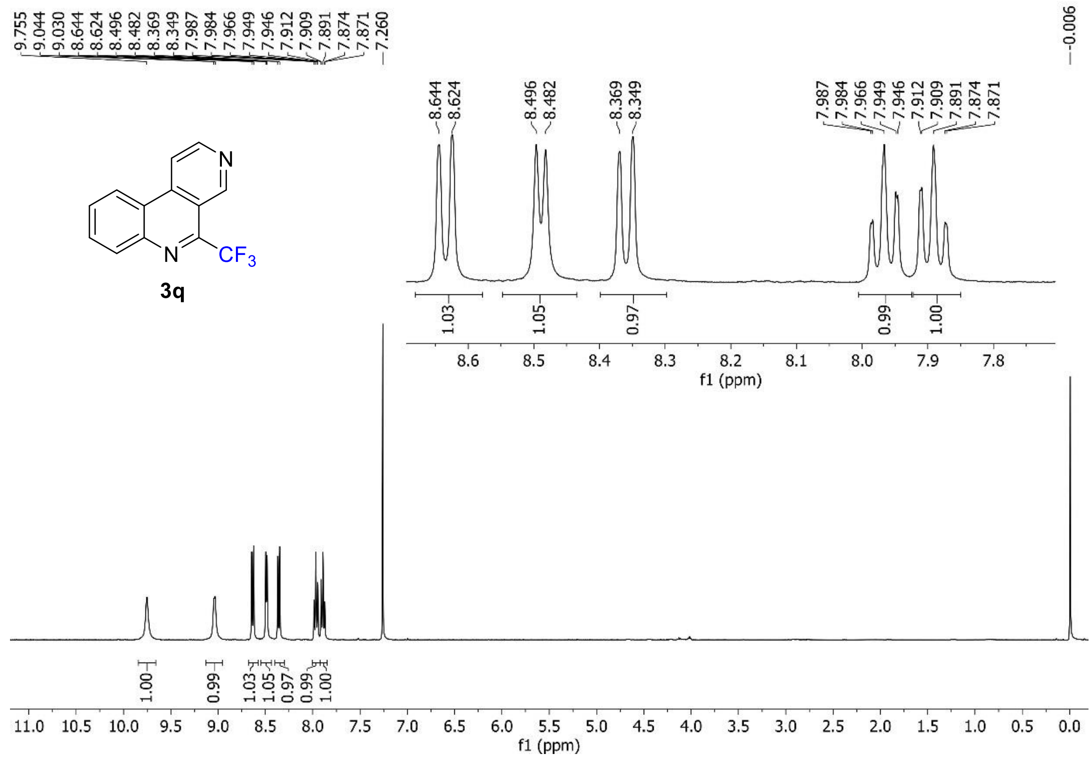


^{19}F NMR spectrum of **3p** (376 MHz, $CDCl_3$)

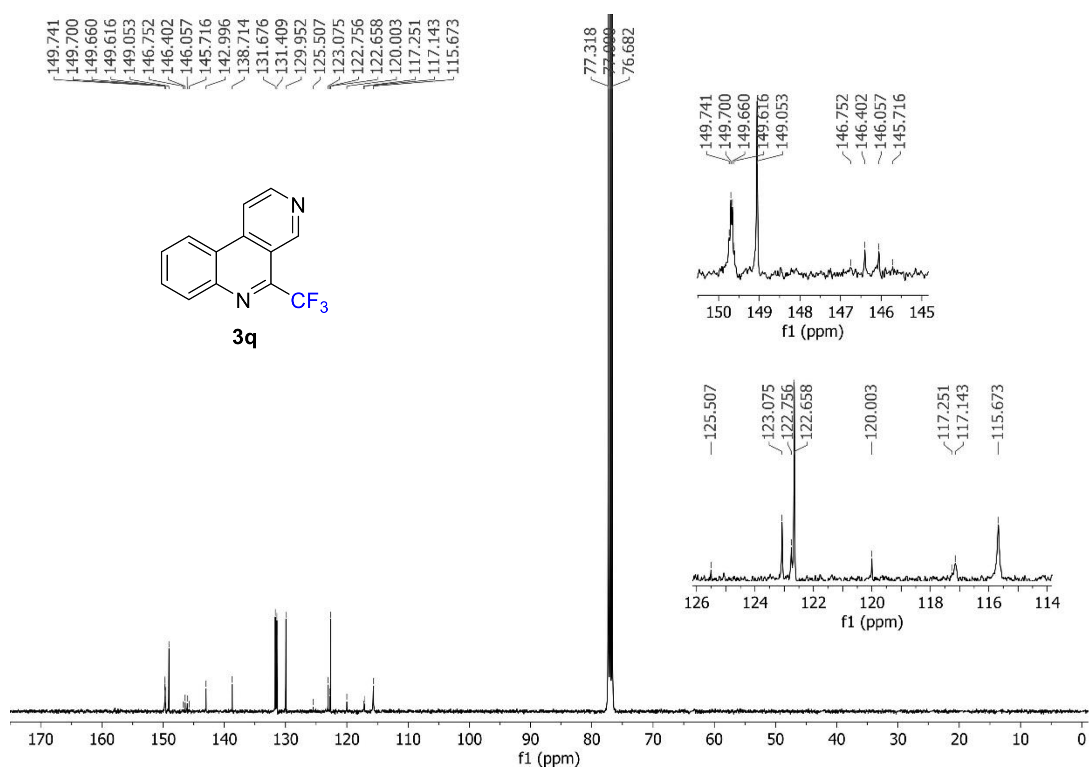


3p

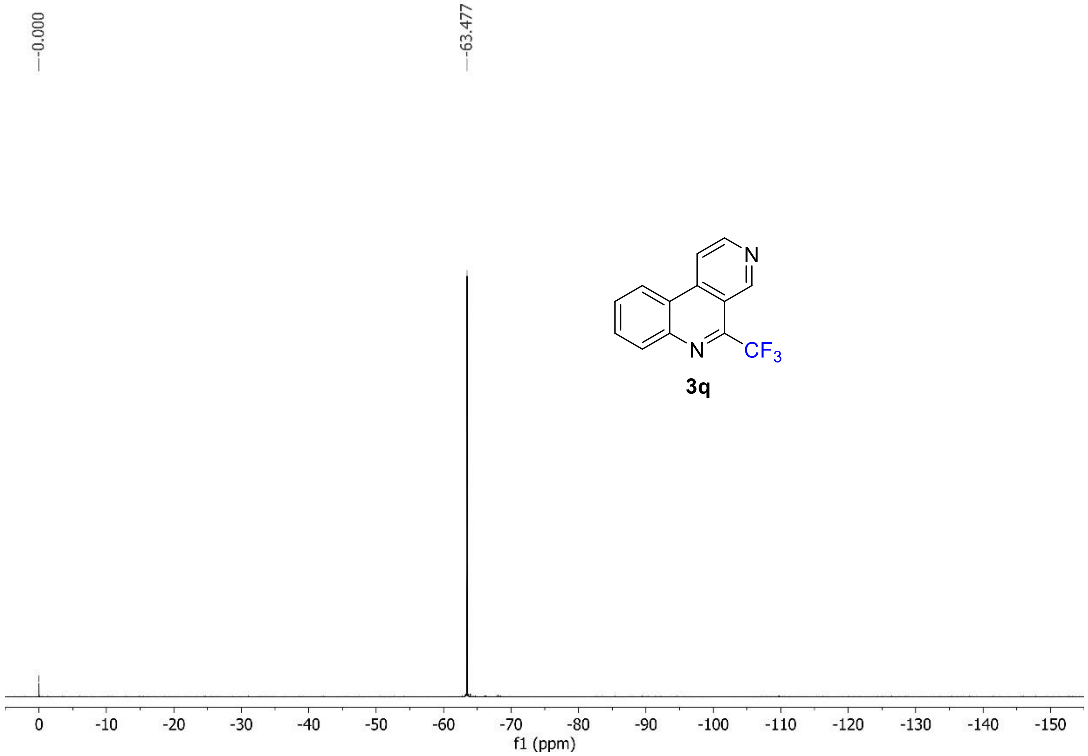
^{1}H NMR spectrum of **3q** (400 MHz, $CDCl_3$)



^{13}C NMR spectrum of **3q** (100 MHz, $CDCl_3$)

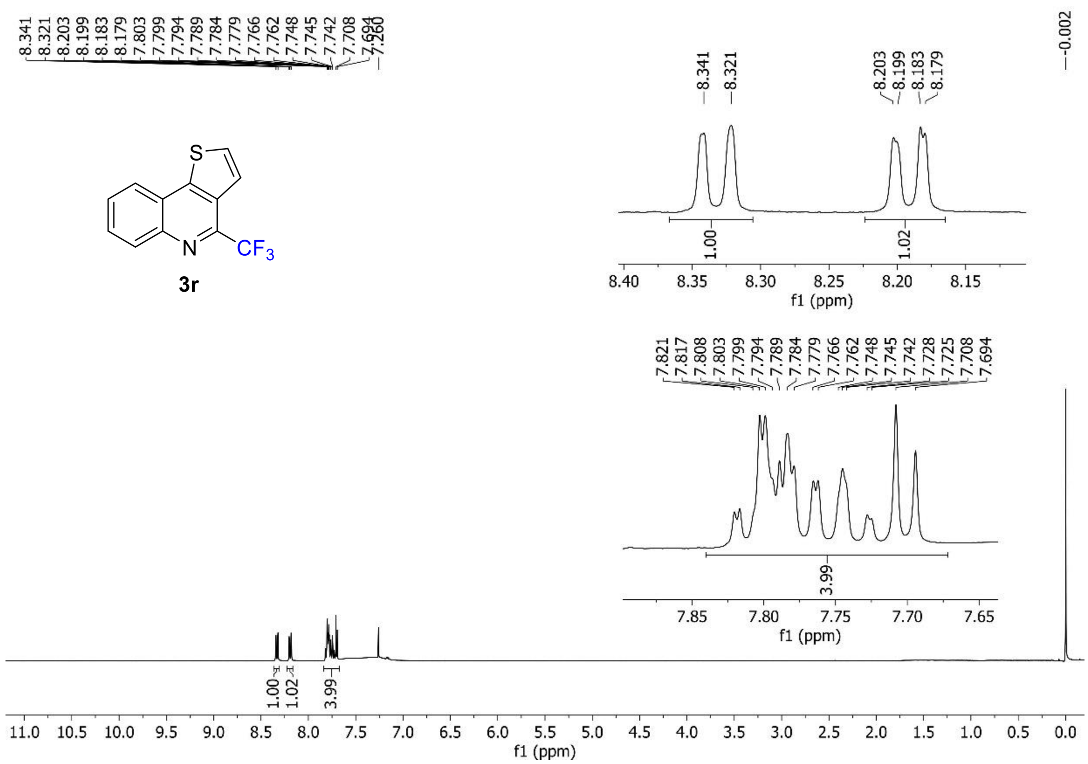


^{19}F NMR spectrum of **3q** (376 MHz, $CDCl_3$)

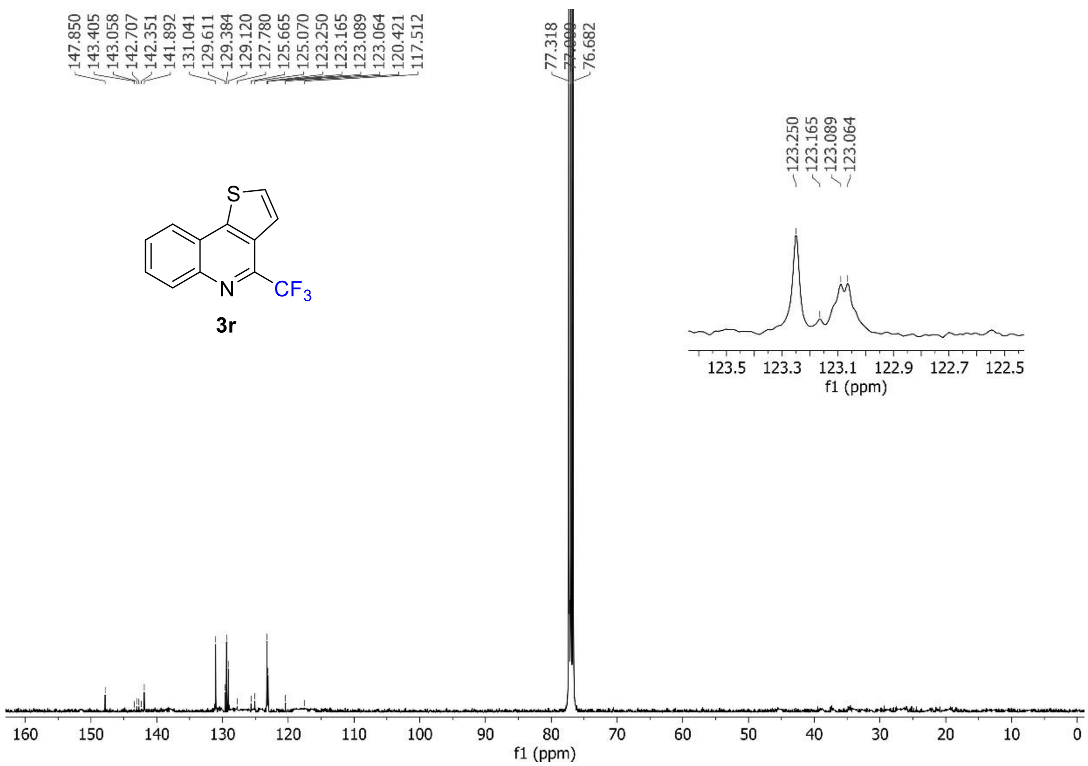


3q

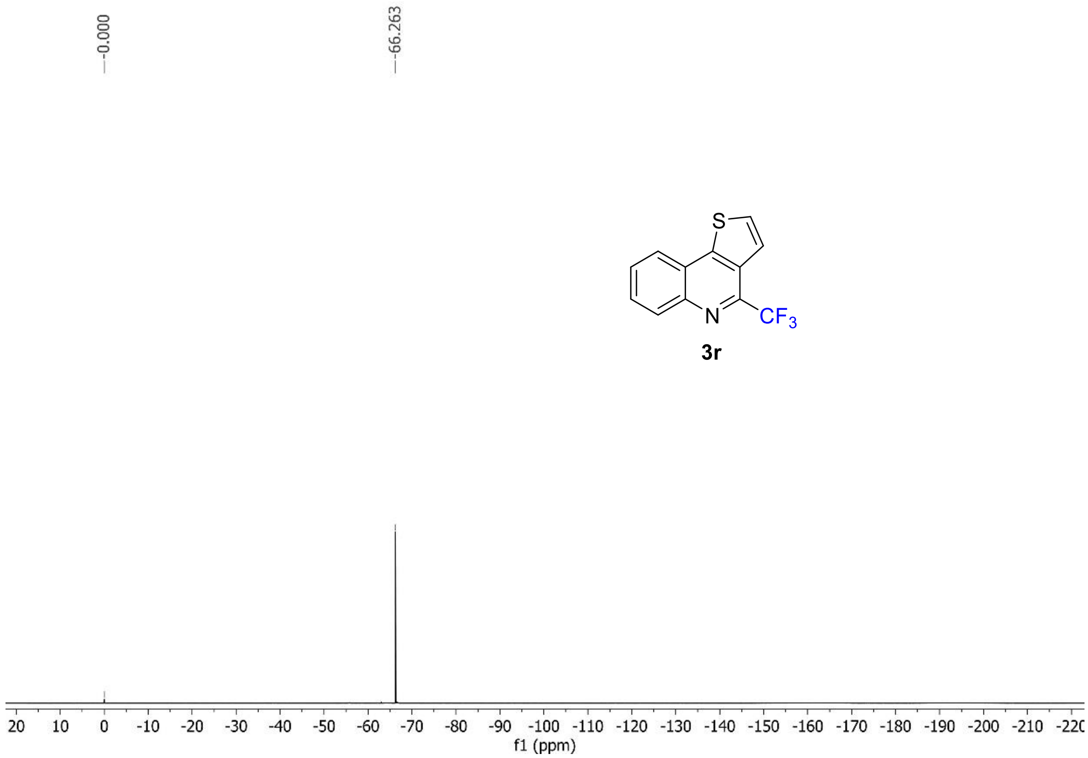
^{1}H NMR spectrum of **3r** (400 MHz, $CDCl_3$)



^{13}C NMR spectrum of **3r** (100 MHz, $CDCl_3$)

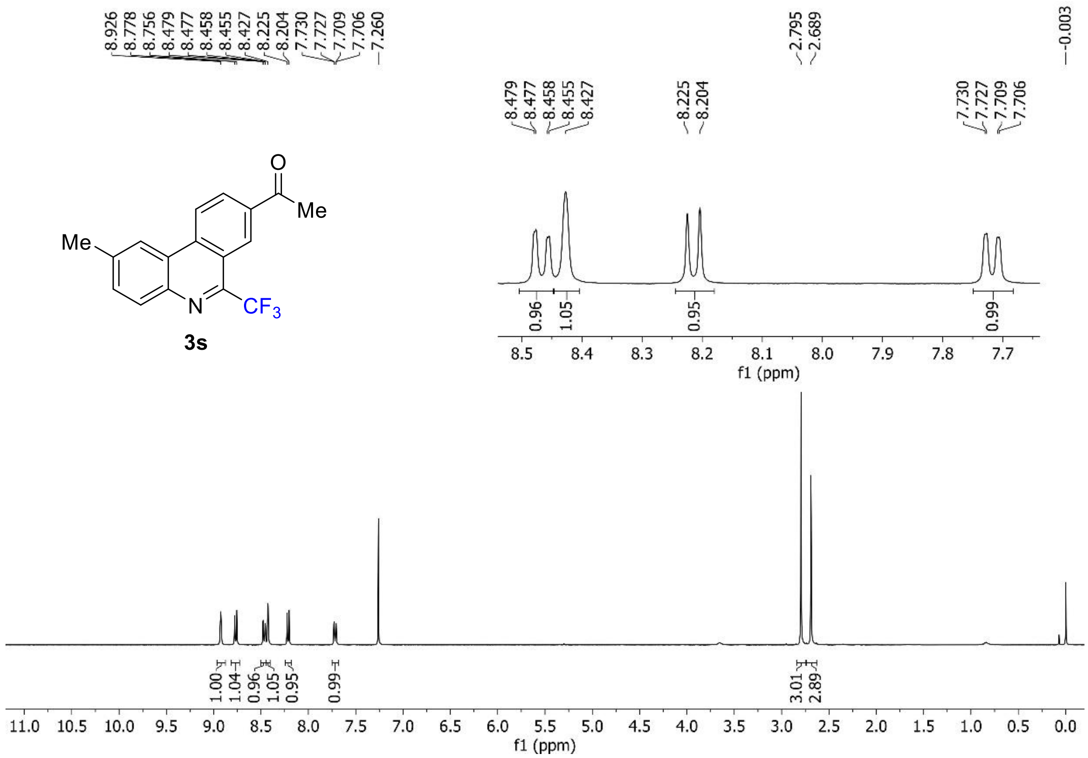


^{19}F NMR spectrum of **3r** (376 MHz, $CDCl_3$)

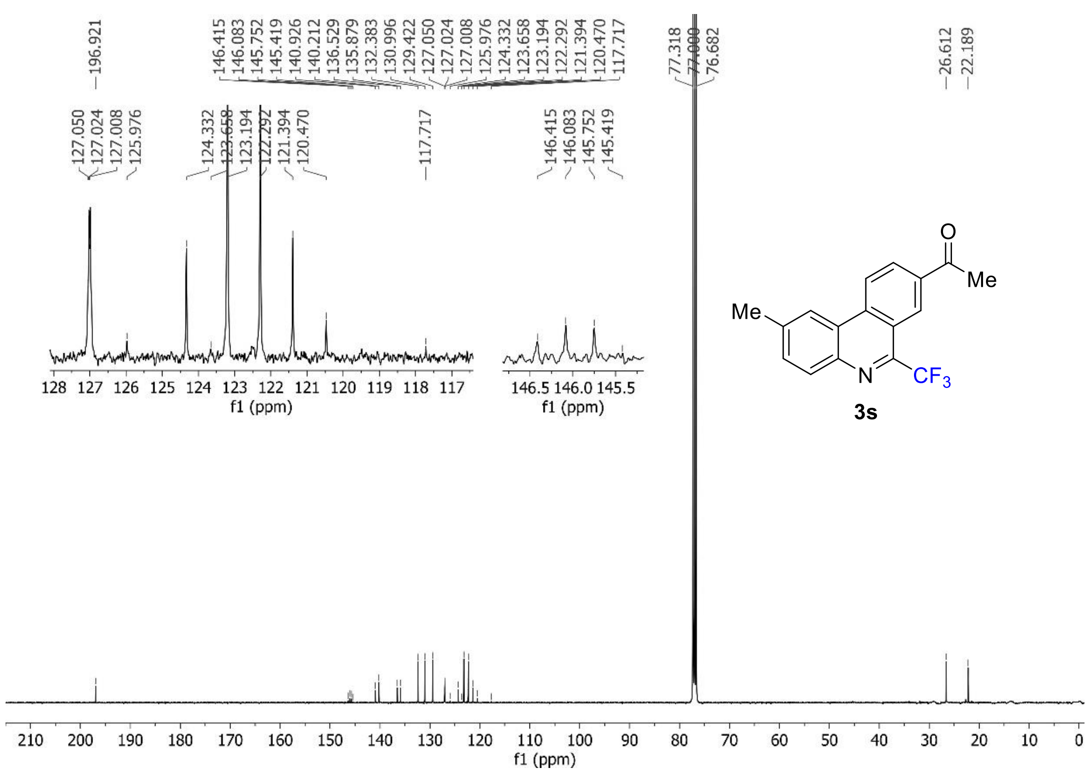


3r

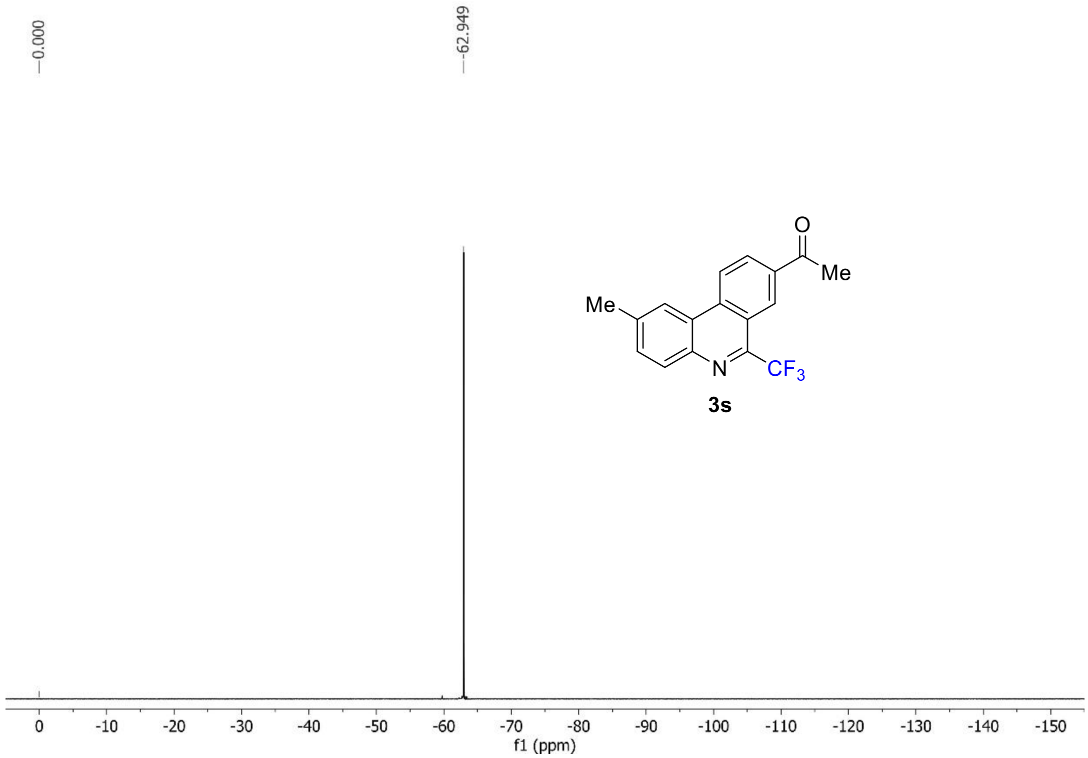
^{1}H NMR spectrum of **3s** (400 MHz, $CDCl_3$)



^{13}C NMR spectrum of **3s** (100 MHz, $CDCl_3$)



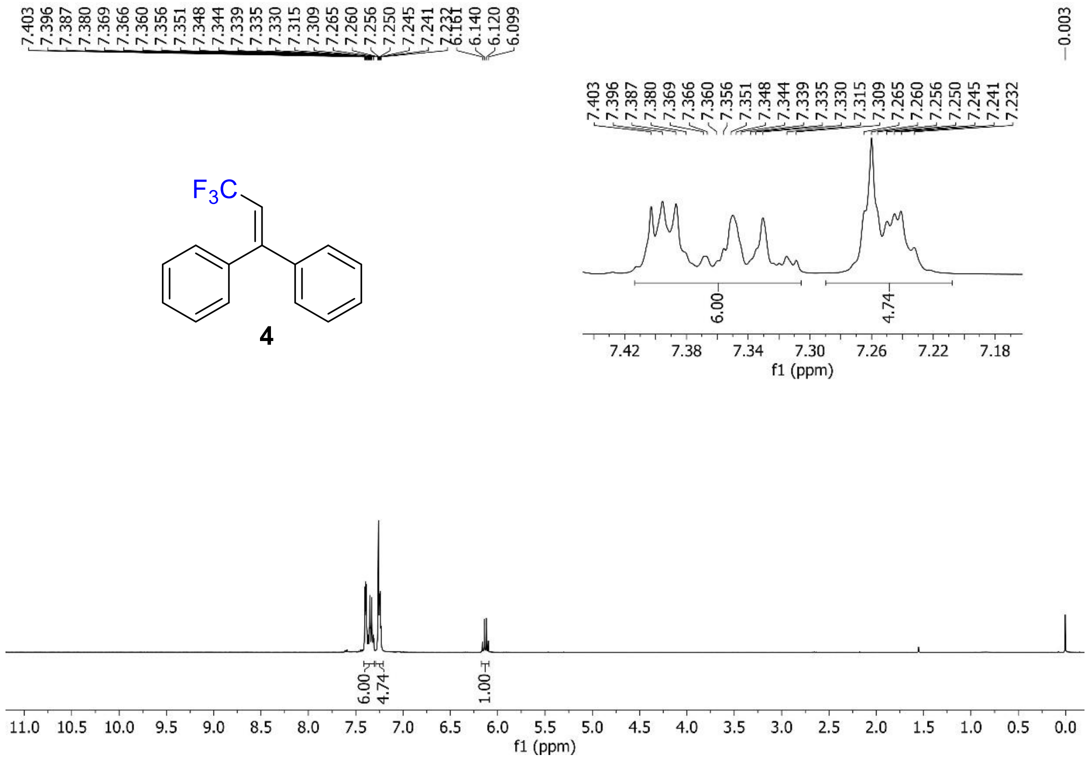
^{19}F NMR spectrum of **3s** (376 MHz, $CDCl_3$)



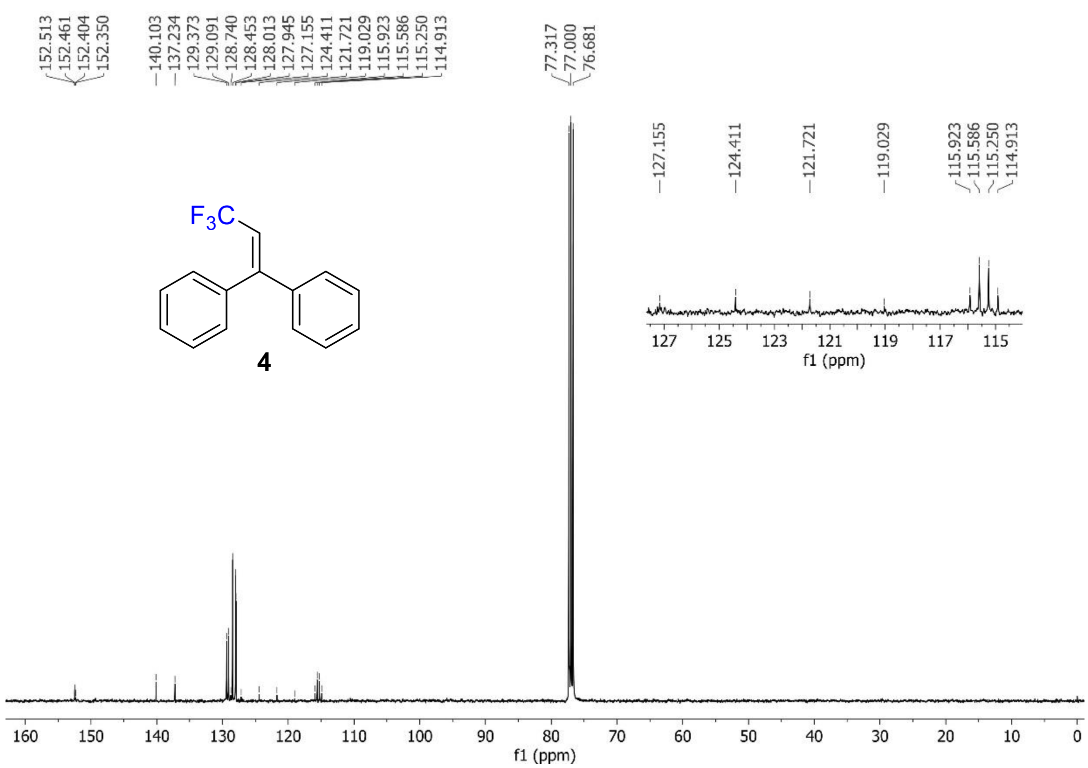
3s

9. NMR spectra of (3,3,3-trifluoroprop-1-ene-1,1-diyl)dibenzene 4

^{1}H NMR spectrum of **4** (400 MHz, $CDCl_3$)



^{13}C NMR spectrum of **4** (100 MHz, $CDCl_3$)



^{19}F NMR spectrum of **4** (376 MHz, $CDCl_3$)