

Supplementary information

Convenient One-Step Construction of Fused- or Zwitterionic Indanes from Tetraynes

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1. Crystallographic data of **2k** and **3e**

Table 1 Crystal data and structure refinement of **2k** and **3e**

Crystal data	2k	3e
Empirical formula	C ₉₀ H ₇₈ N ₂ O ₈	C ₂₉ H ₂₄ O ₆ Cl ₂ S
Formula weight	1315.54	571.44
Temperature/K	273.15	273.15
Crystal system	monoclinic	monoclinic
Space group	P2 ₁ /n	P2 ₁ /c
a (Å)	22.9592(9)	20.9343(11)
b (Å)	9.5176(4)	15.0713(8)
c (Å)	33.7688(13)	9.1726(5)
α (deg)	90	90
β (deg)	100.575(2)	93.192(2)
γ (deg)	90	90
Volume/Å ³	7253.7(5)	2889.5(3)
Z	4	4
ρ_{calc} (mg/m ³)	1.205	1.314
μ (mm ⁻¹)	0.602	3.031
F(000)	2784.0	1184.0
θ range (°)	4.312 - 136.83	11.306 - 136.988
Reflections collected	95633	42479
Independent reflections	13154	5279
R_{int}	0.0781	0.0537
Data/restraints/parameters	13154/0/910	5279/0/350
Goodness of fit on F^2	1.013	1.043
$R_1, wR_2 [I > 2\sigma(I)]$	0.0656, 0.1279	0.0567, 0.1717
R_1, wR_2 (all data)	0.1322, 0.1518	0.0663, 0.1786
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ (e.Å ⁻³)	0.21 and -0.16	0.50 and -0.45

2. ^1H NMR and ^{13}C NMR of **2a-2o** and **3a-3o**

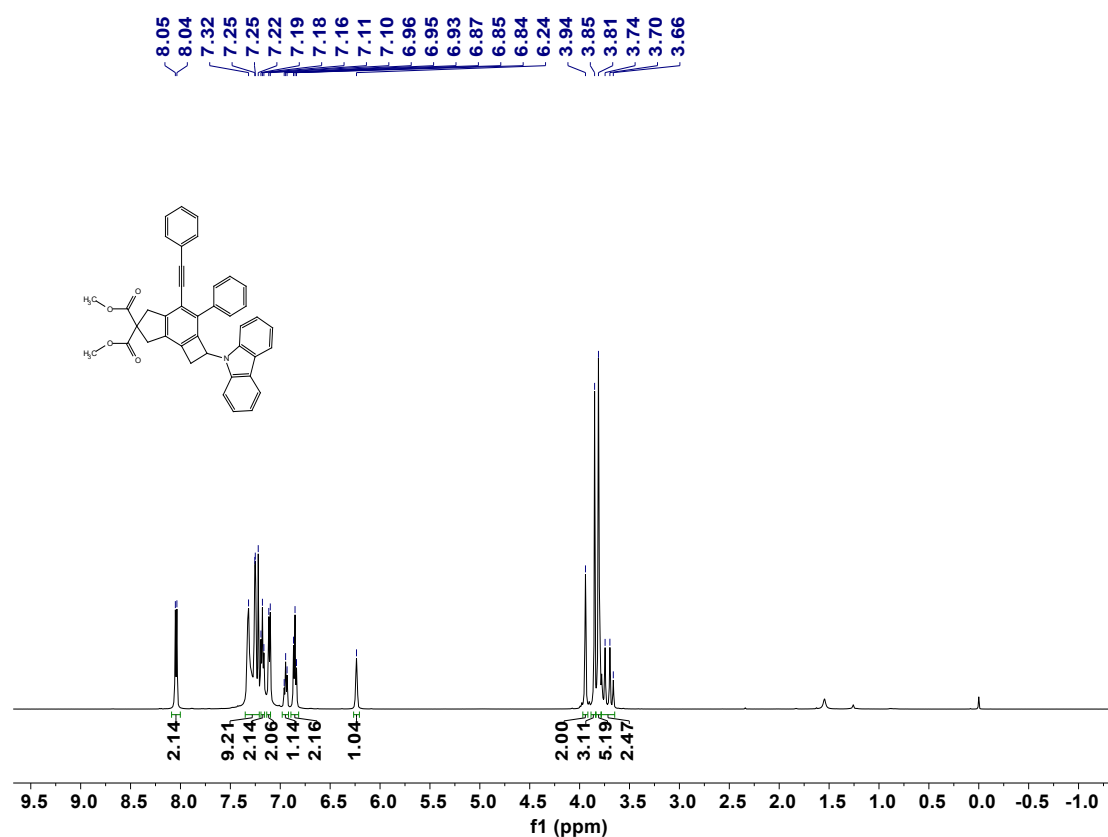


Figure 1 ^1H NMR spectrum of **2a** (500 MHz, CDCl_3).

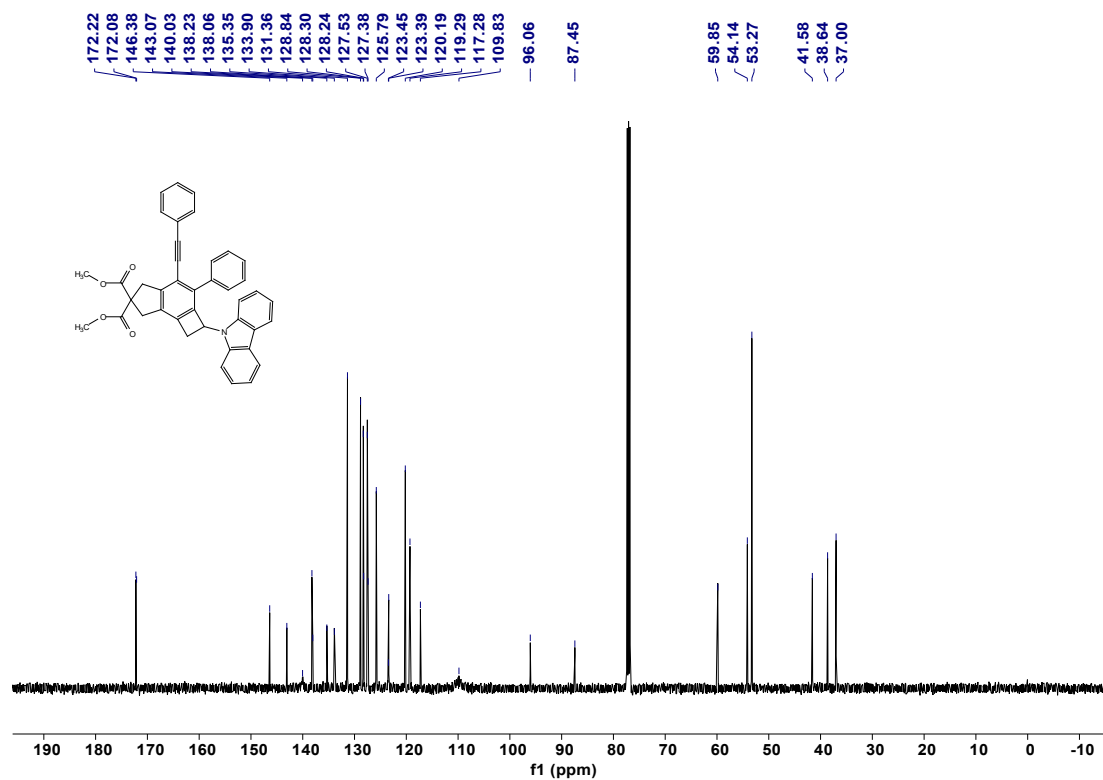


Figure 2 ^{13}C NMR spectrum of **2a** (125 MHz, CDCl_3).

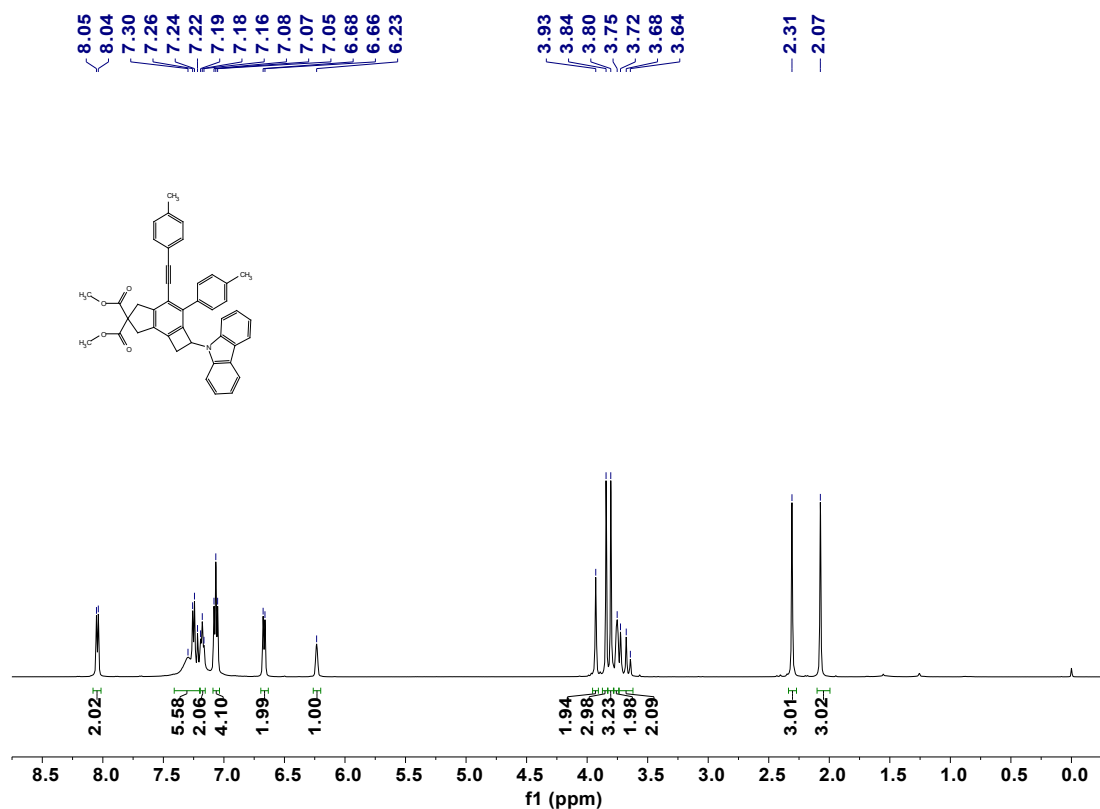


Figure 3 ¹H NMR spectrum of **2b** (500 MHz, CDCl₃).

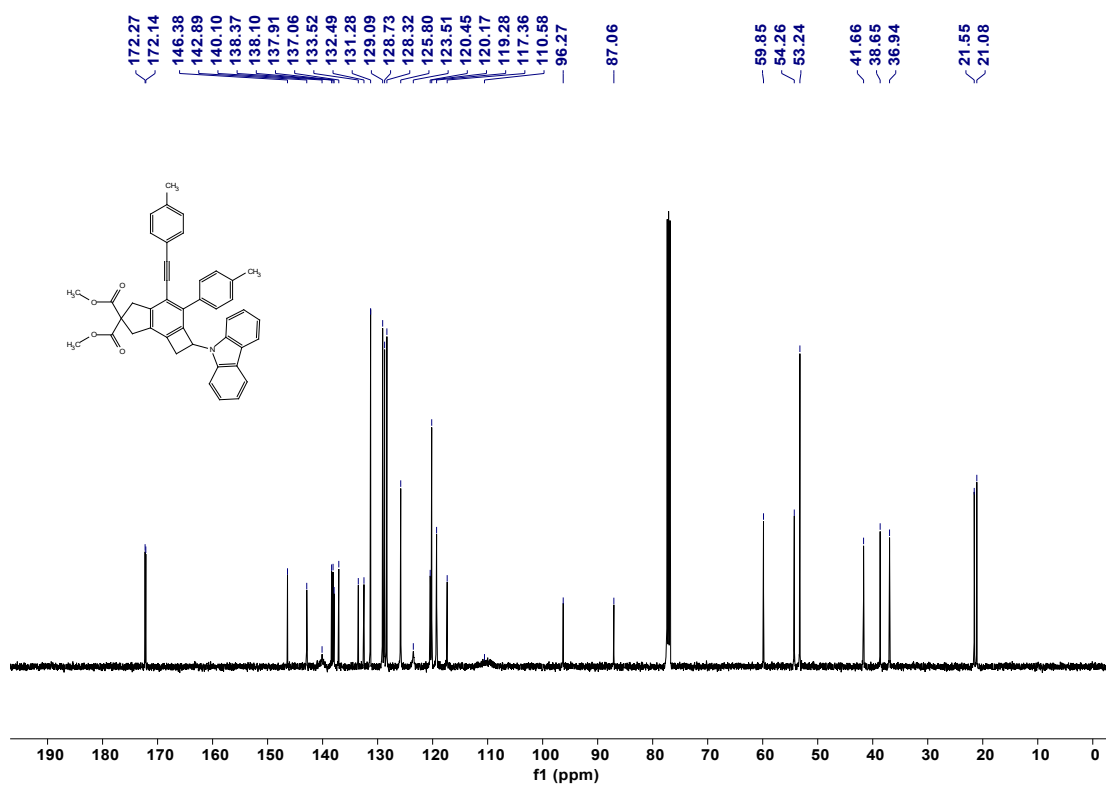


Figure 4 ¹³C NMR spectrum of **2b** (125 MHz, CDCl₃).

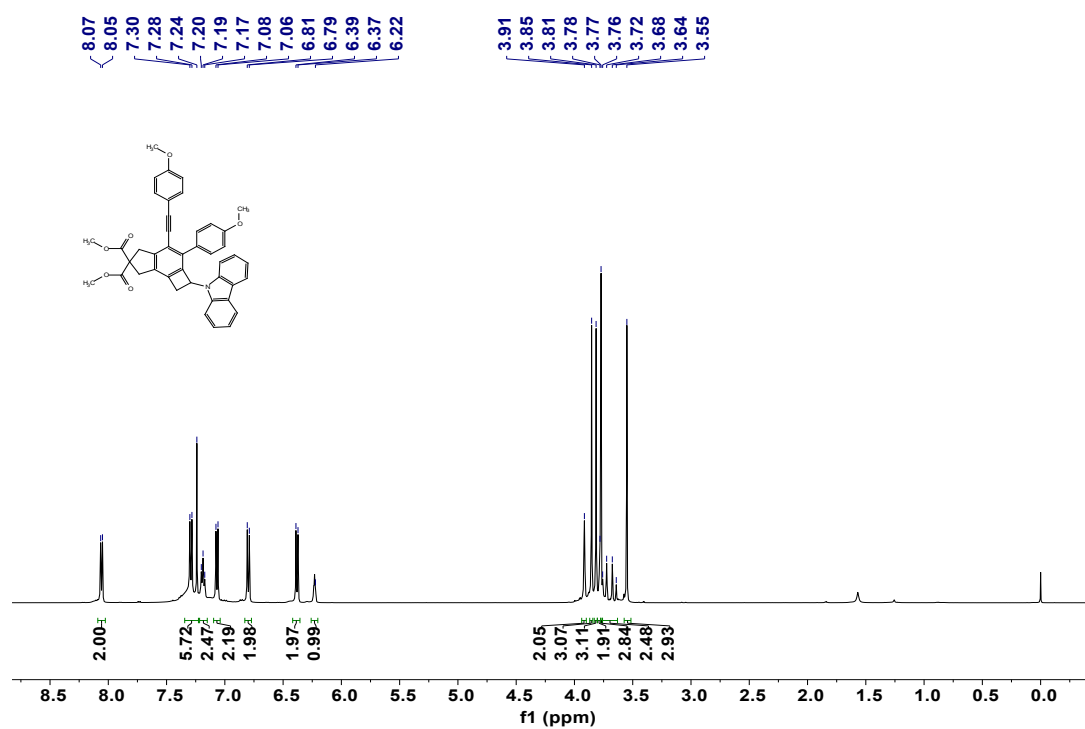


Figure 5 ¹H NMR spectrum of **2c** (500 MHz, CDCl₃).

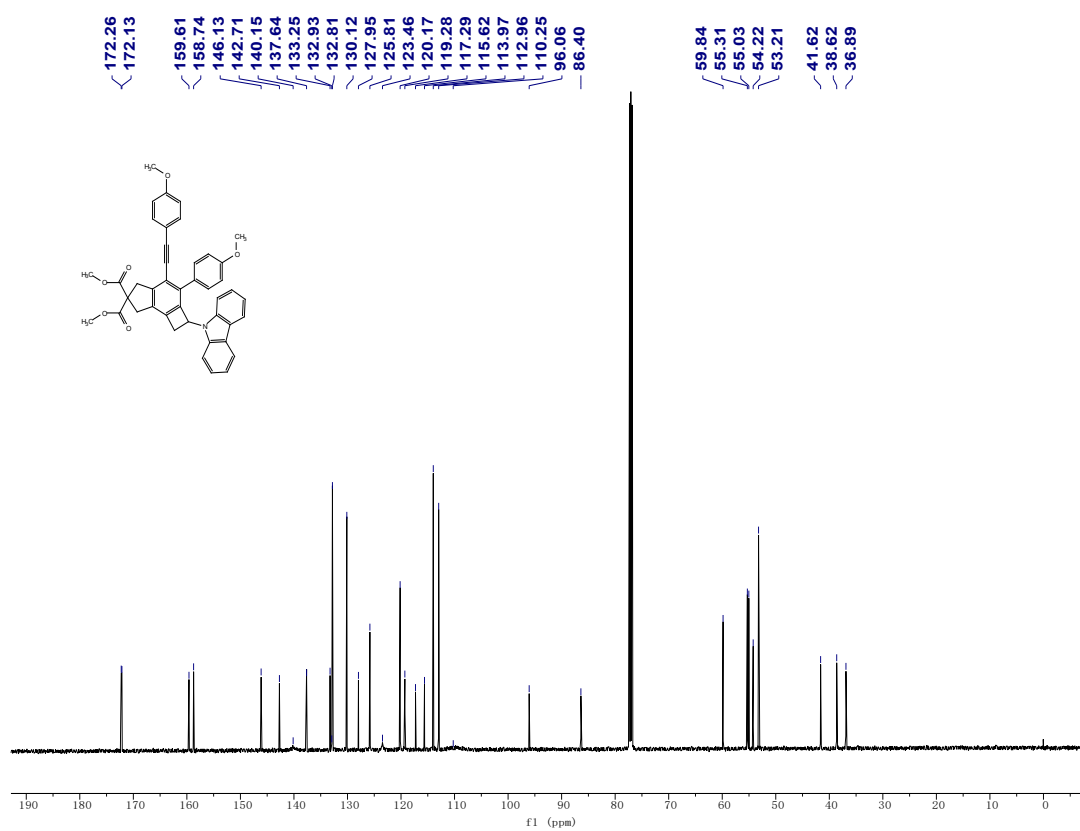


Figure 6 ¹³C NMR spectrum of **2c** (125 MHz, CDCl₃).

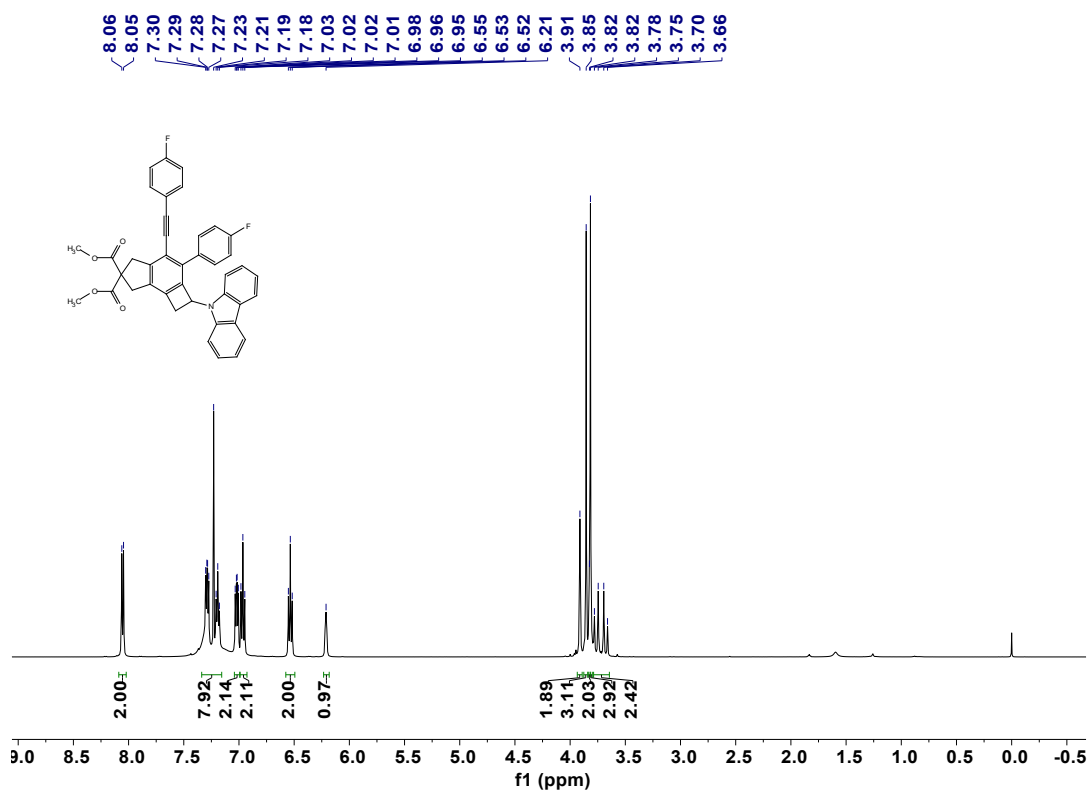


Figure 7 ¹H NMR spectrum of **2d** (500 MHz, CDCl₃).

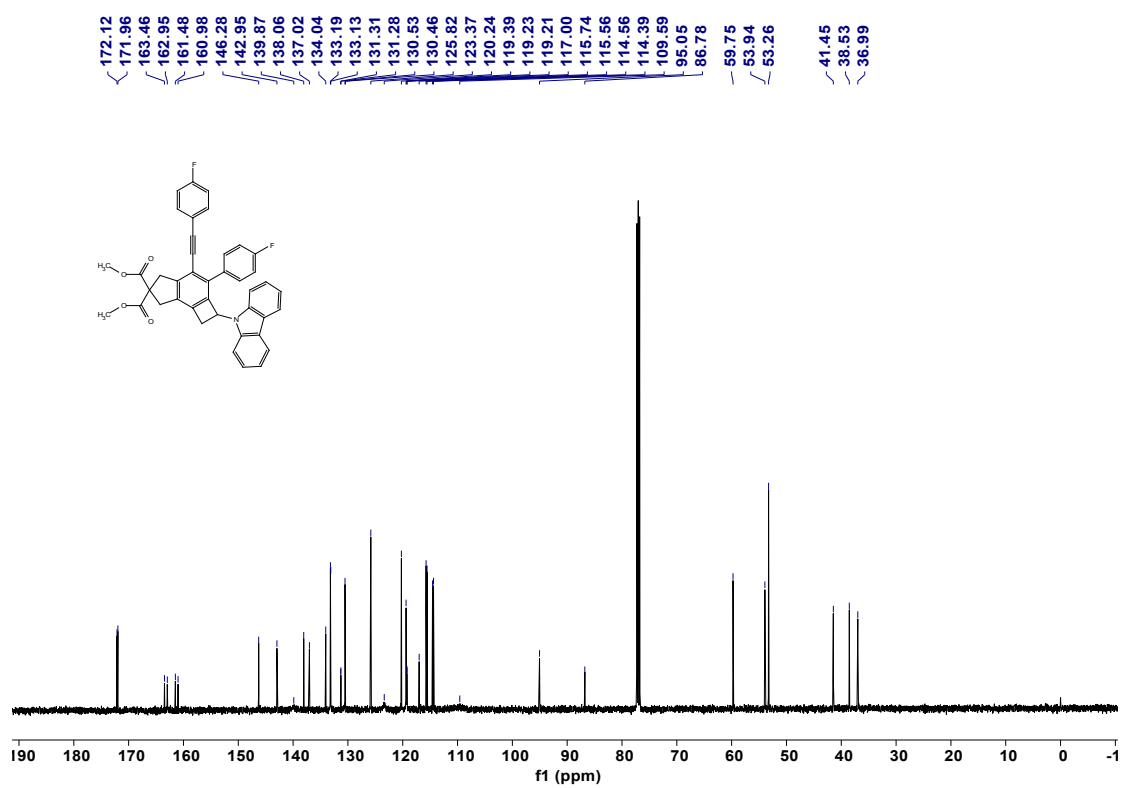


Figure 8 ¹³C NMR spectrum of **2d** (125 MHz, CDCl₃).

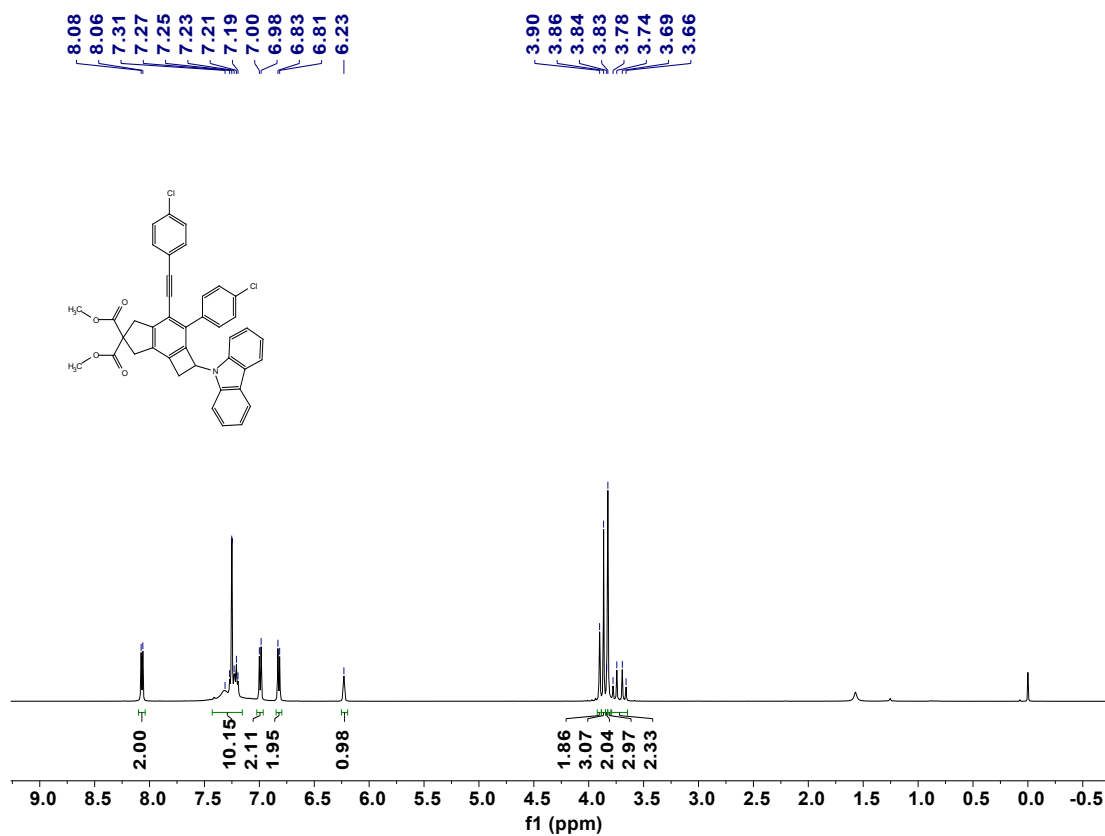


Figure 9 ¹H NMR spectrum of **2e** (500 MHz, CDCl₃).

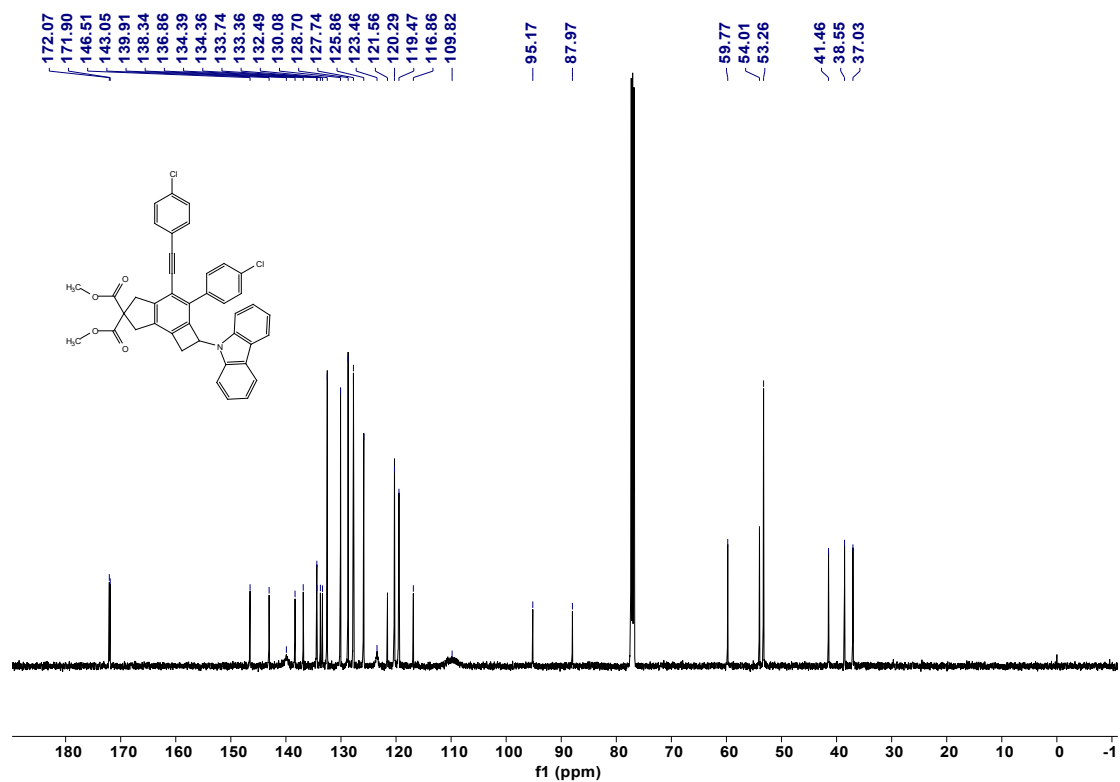


Figure 10 ¹³C NMR spectrum of **2e** (125 MHz, CDCl₃).

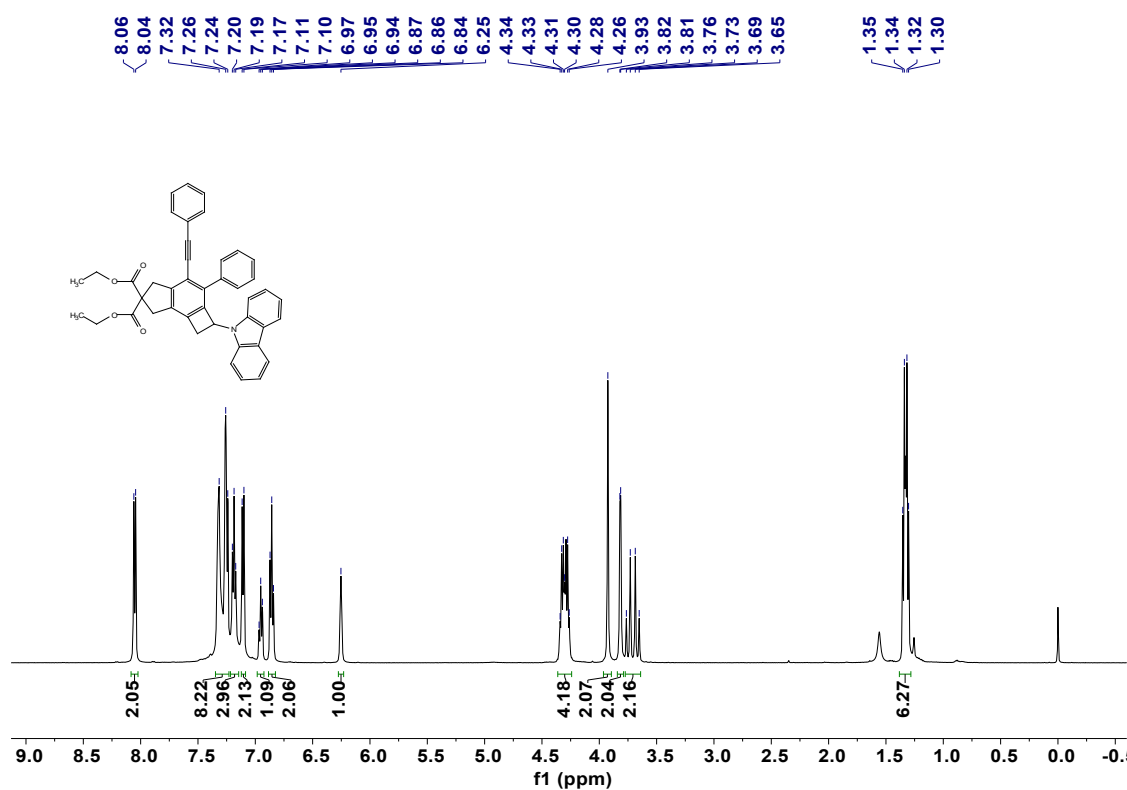


Figure 11 ^1H NMR spectrum of **2f** (500 MHz, CDCl_3).

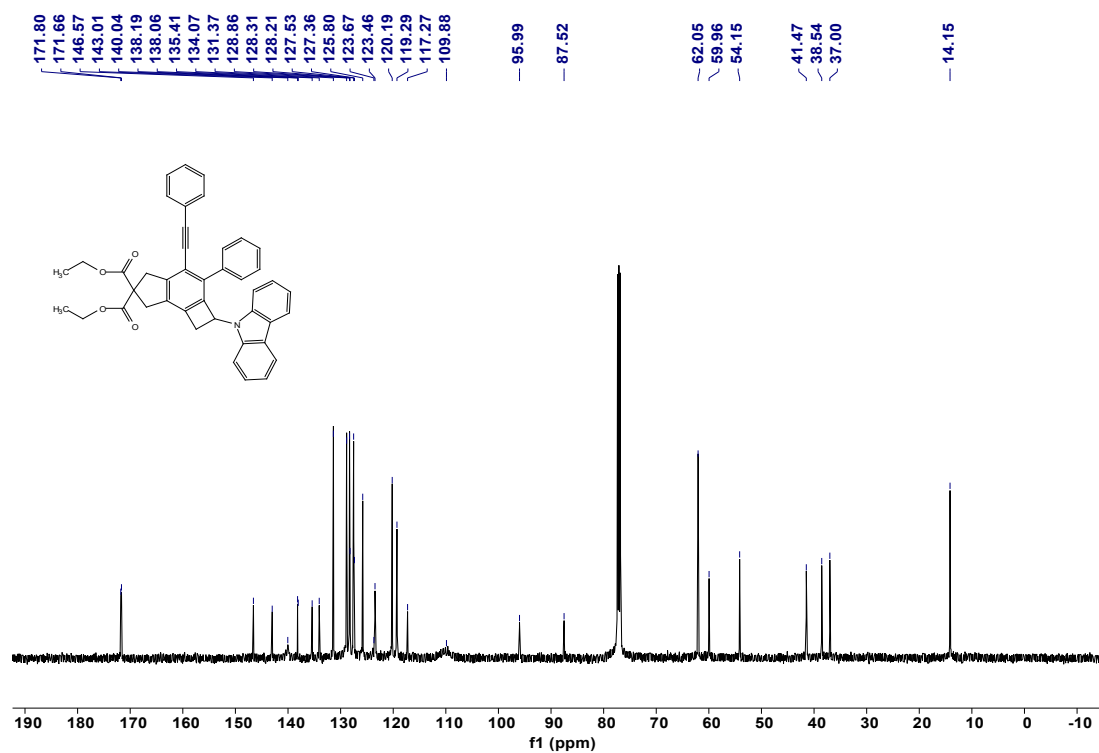


Figure 12 ^{13}C NMR spectrum of **2f** (125 MHz, CDCl_3).

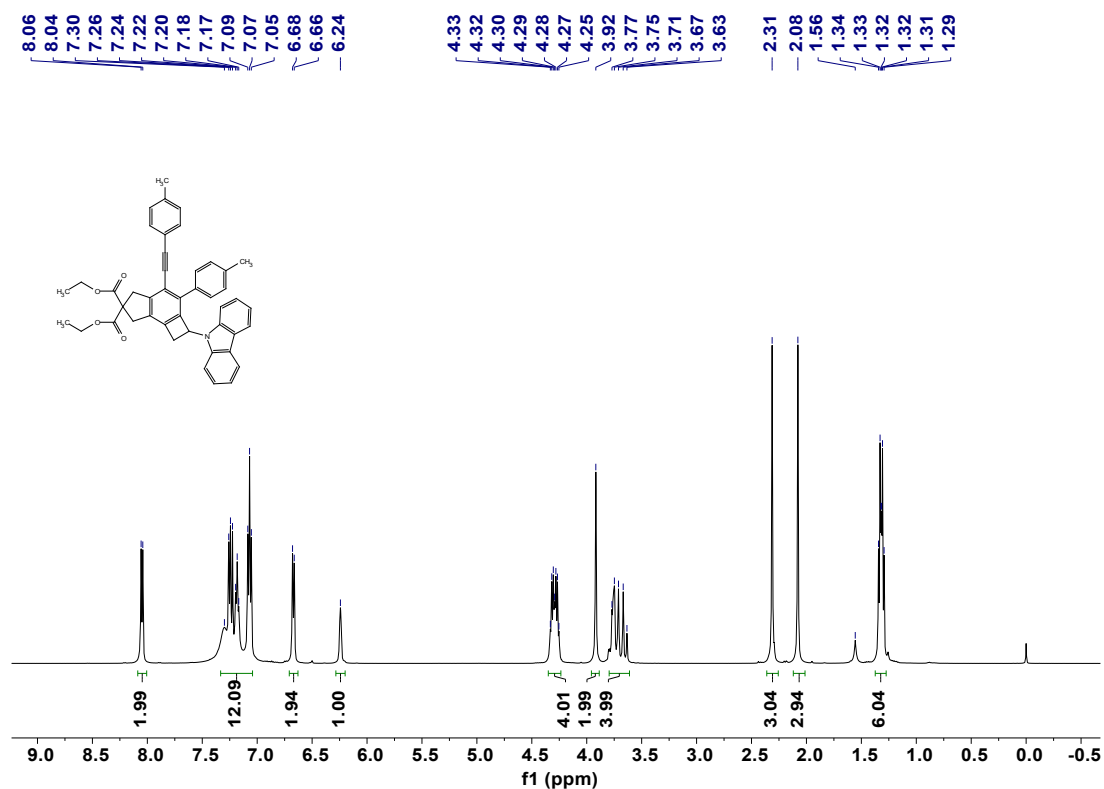


Figure 13 ¹H NMR spectrum of **2g** (500 MHz, CDCl₃).

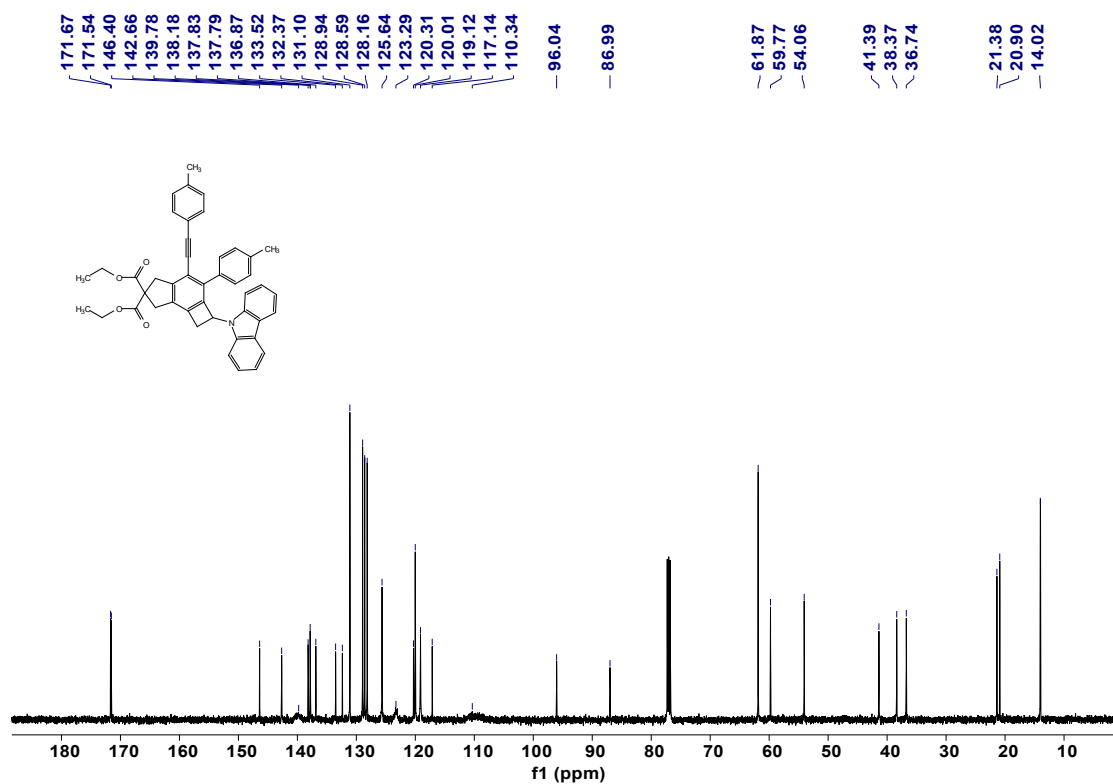


Figure 14 ¹³C NMR spectrum of **2g** (125 MHz, CDCl₃).

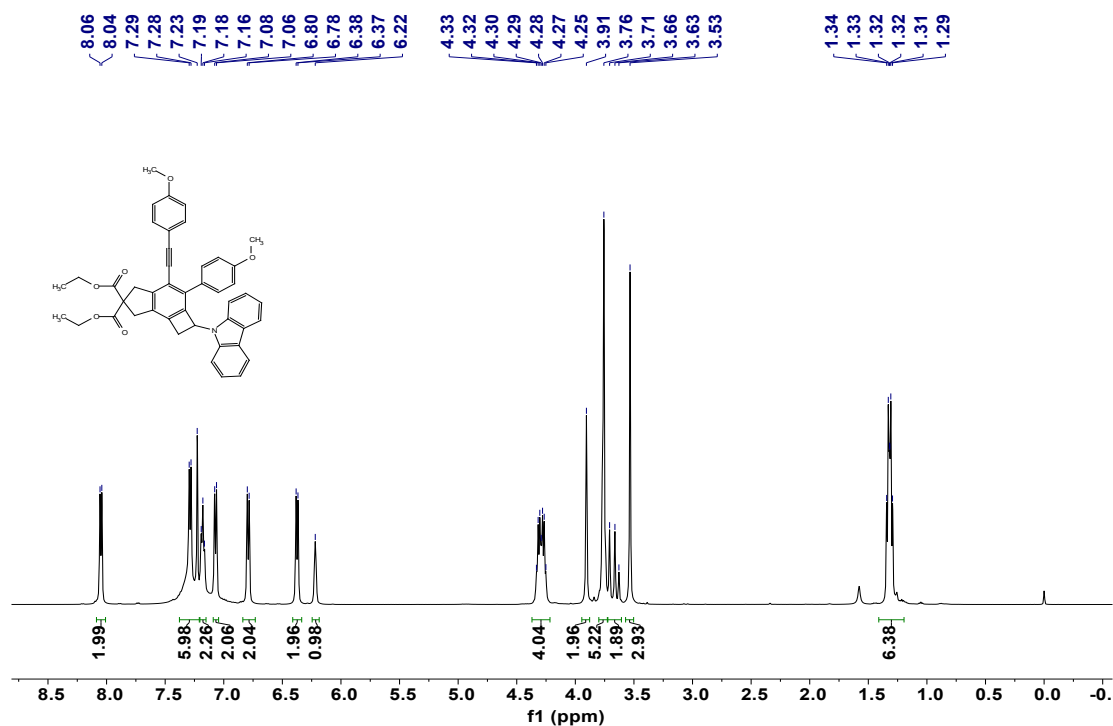


Figure 15 ¹H NMR spectrum of **2h** (500 MHz, CDCl₃).

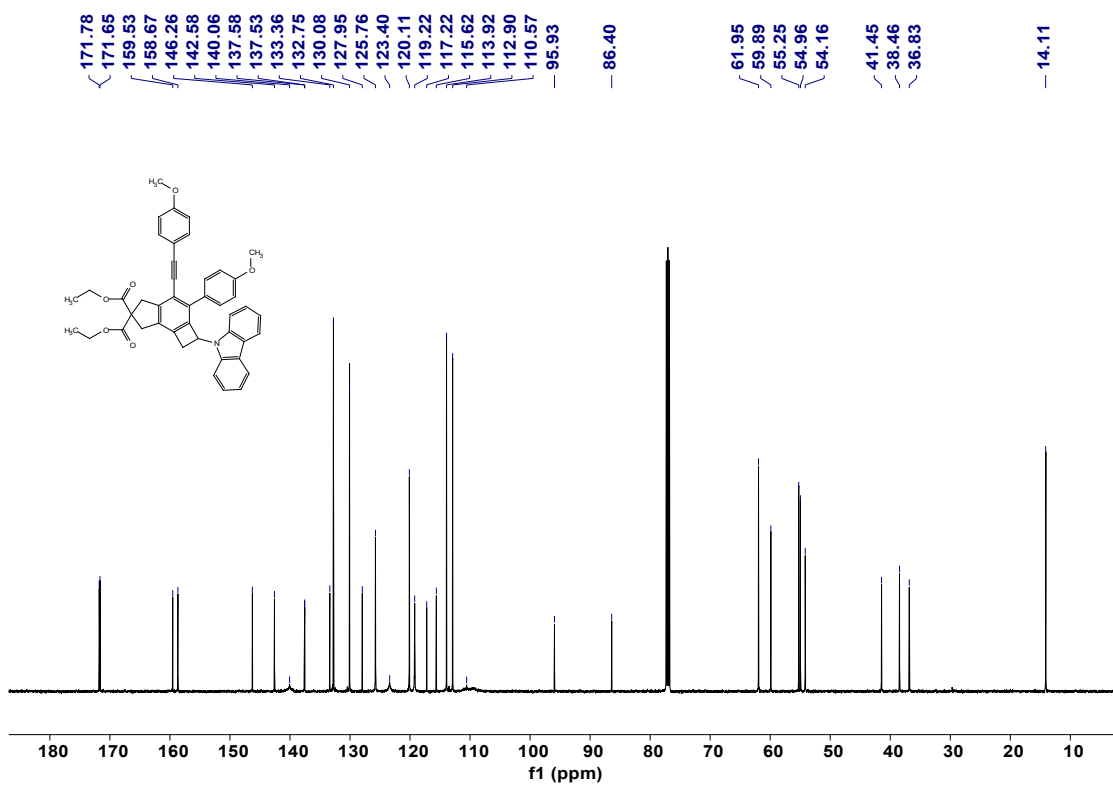


Figure 16 ¹³C NMR spectrum of **2h** (125 MHz, CDCl₃).

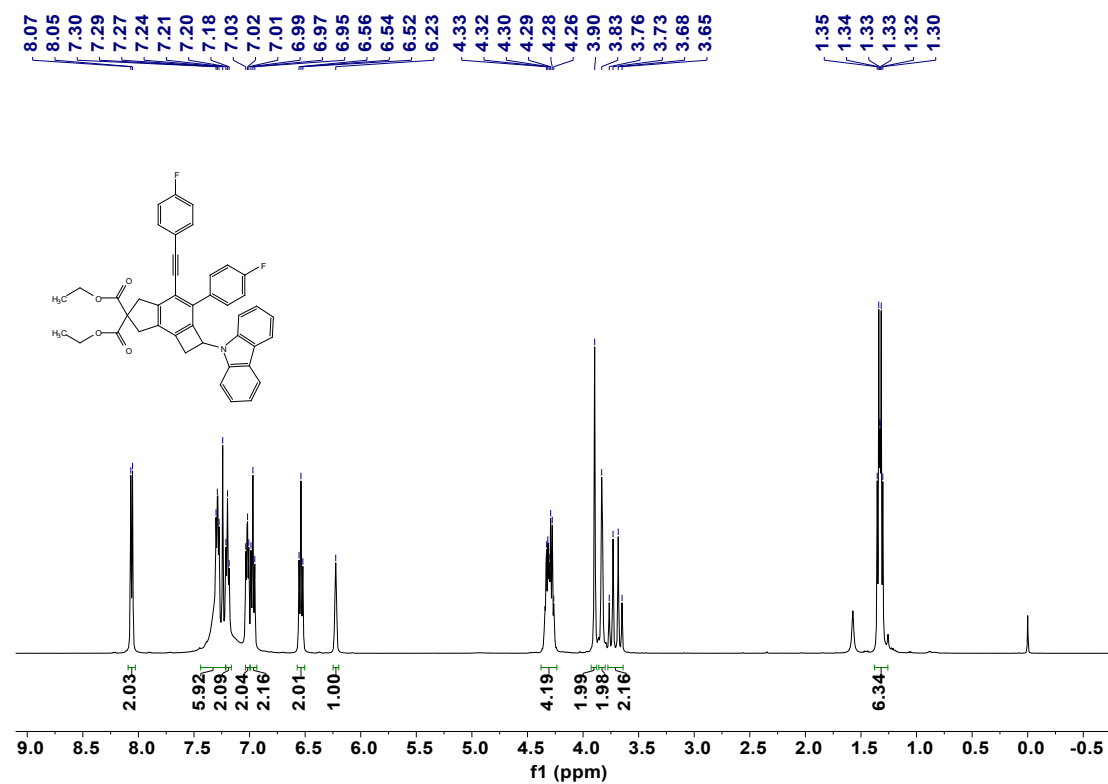


Figure 17 ¹H NMR spectrum of **2i** (500 MHz, CDCl₃).

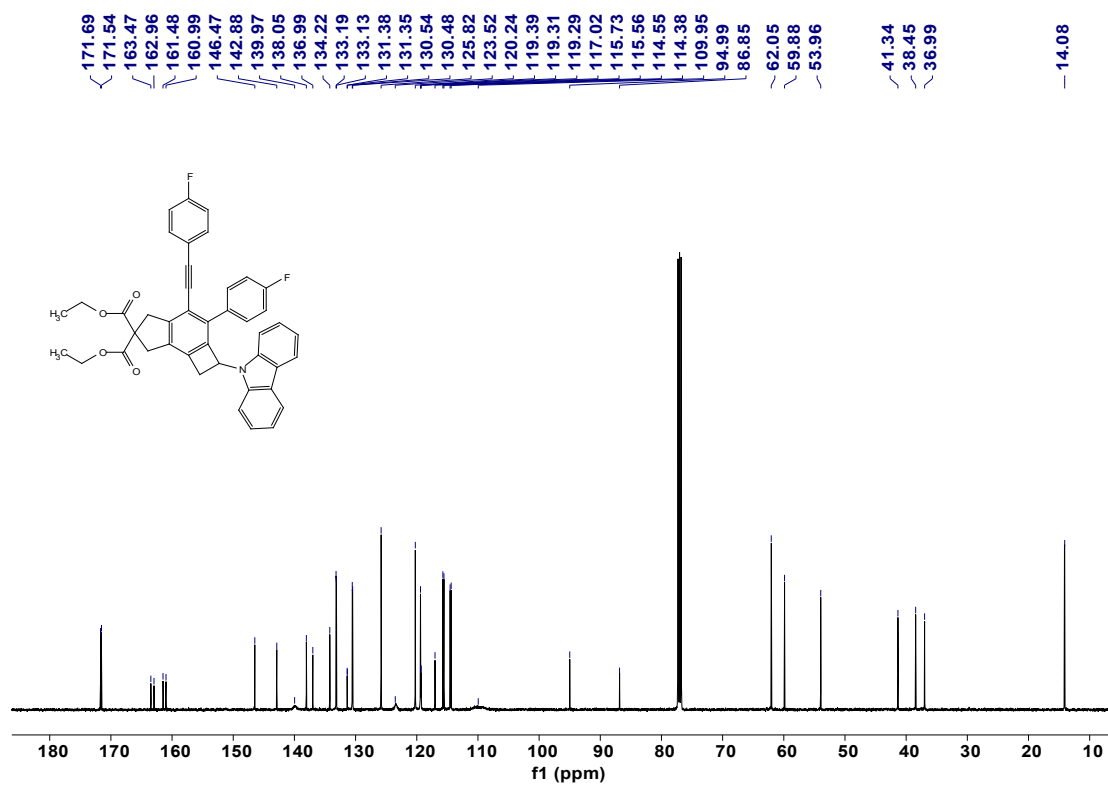


Figure 18 ¹³C NMR spectrum of **2i** (125 MHz, CDCl₃).

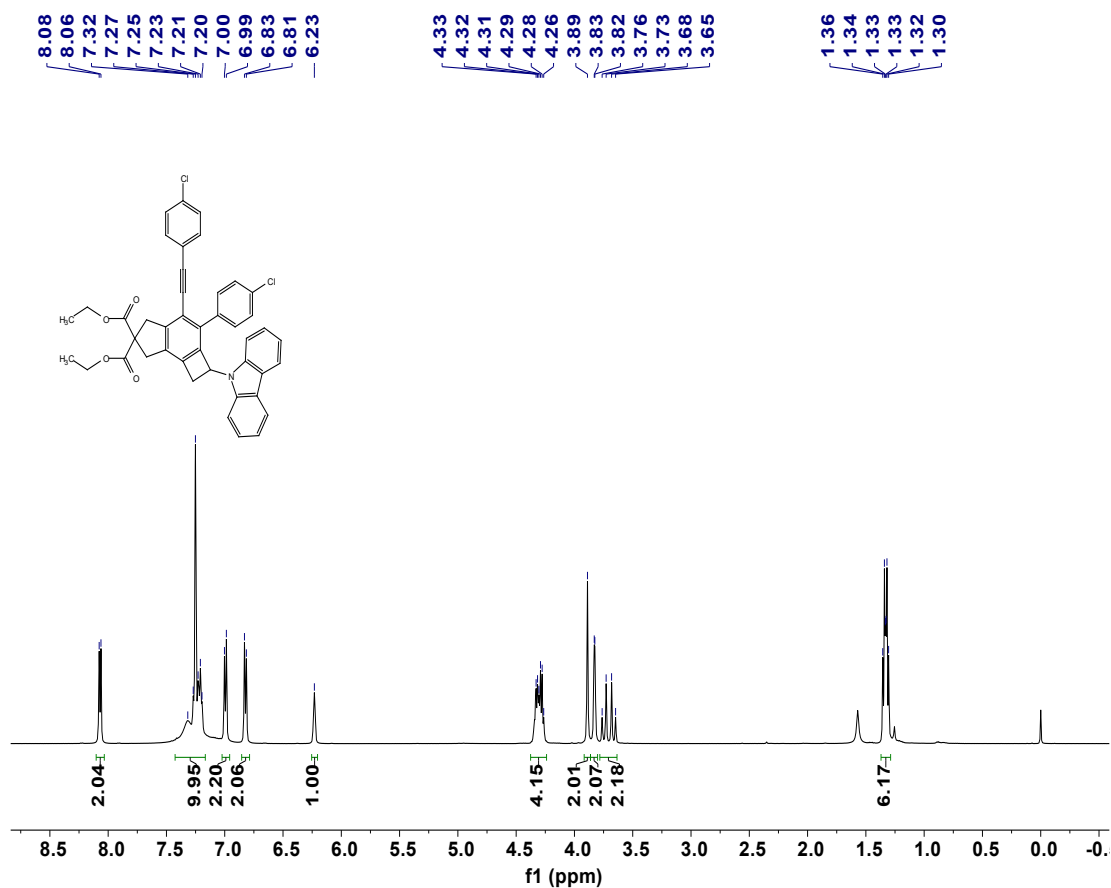


Figure 19 ^1H NMR spectrum of **2j** (500 MHz, CDCl_3).

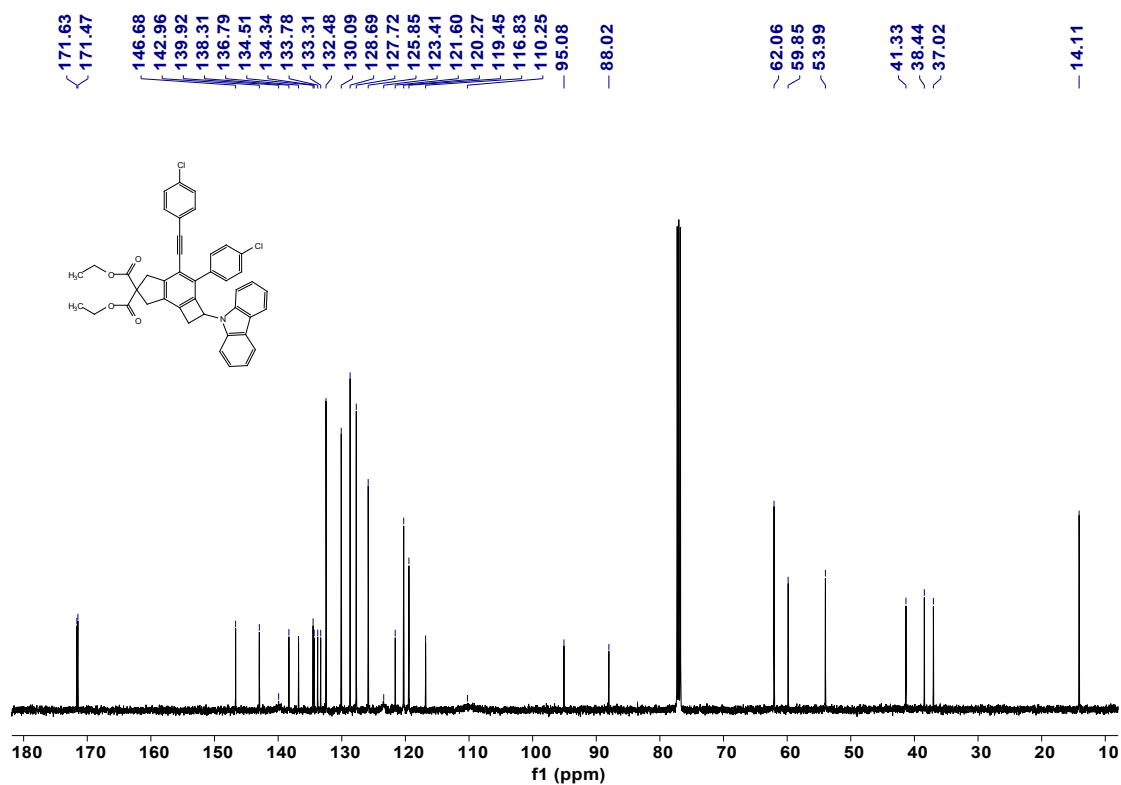


Figure 20 ^{13}C NMR spectrum of **2j** (125 MHz, CDCl_3).

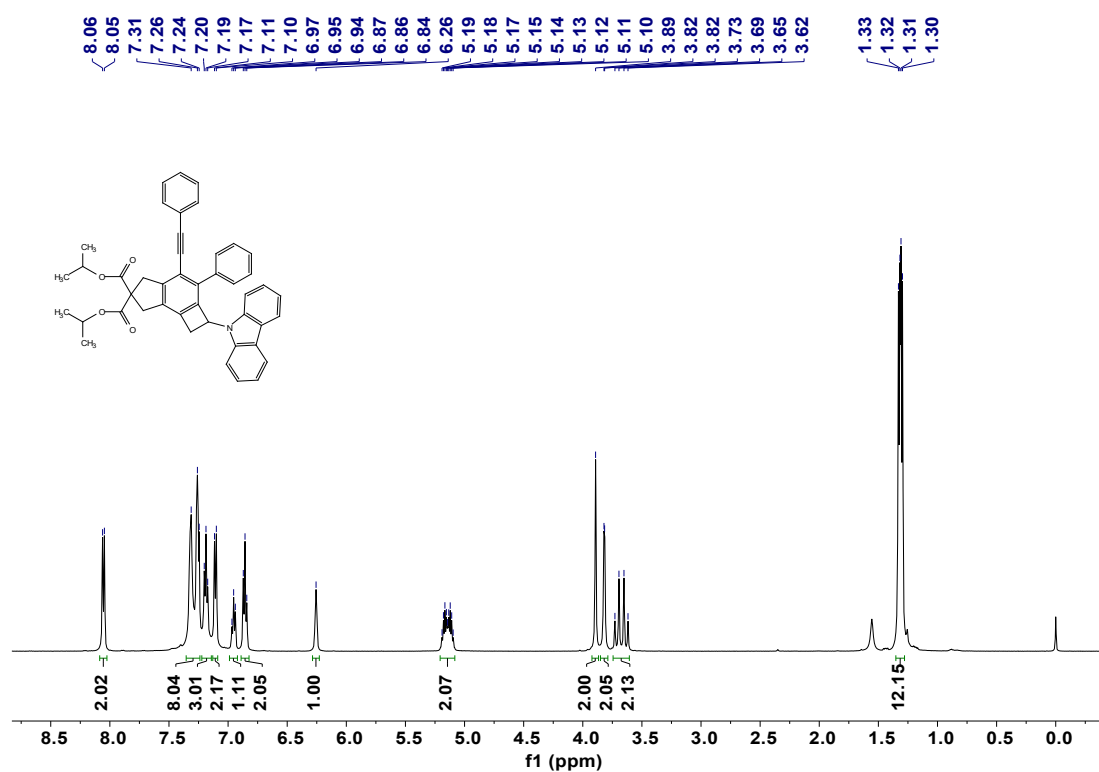


Figure 21 ^1H NMR spectrum of **2k** (500 MHz, CDCl_3).

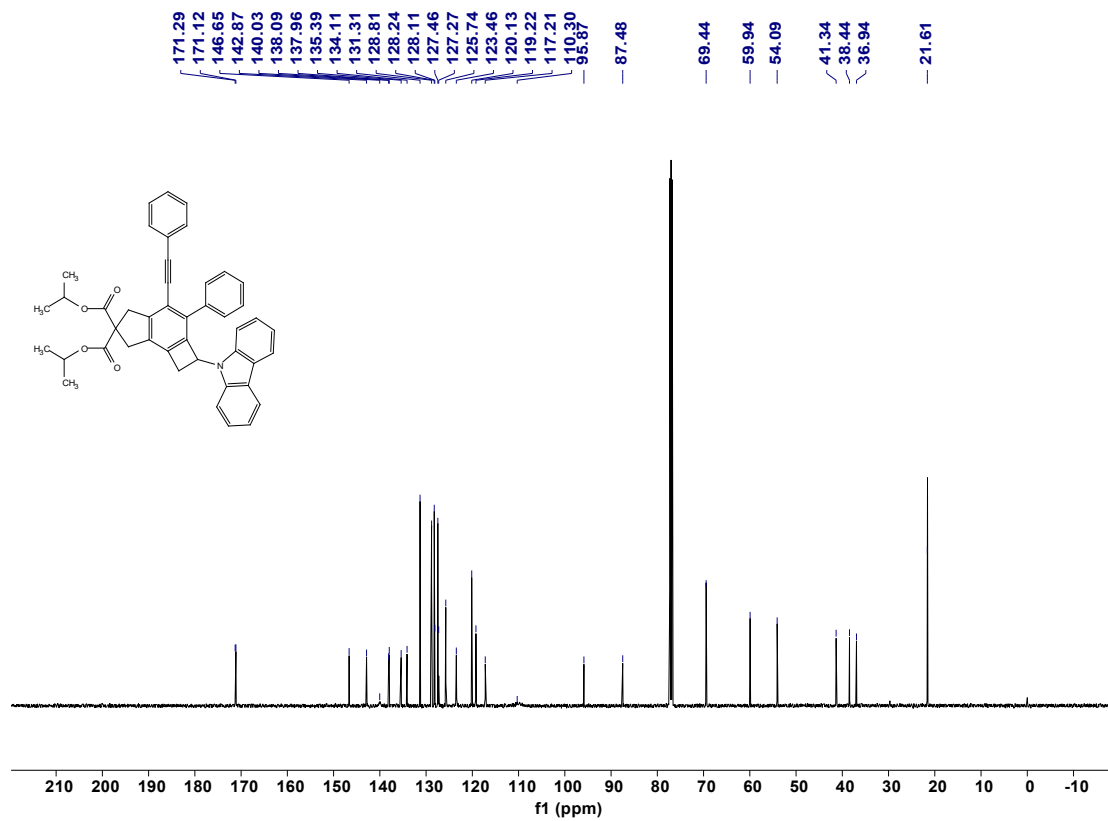


Figure 22 ^{13}C NMR spectrum of **2k** (125 MHz, CDCl_3).

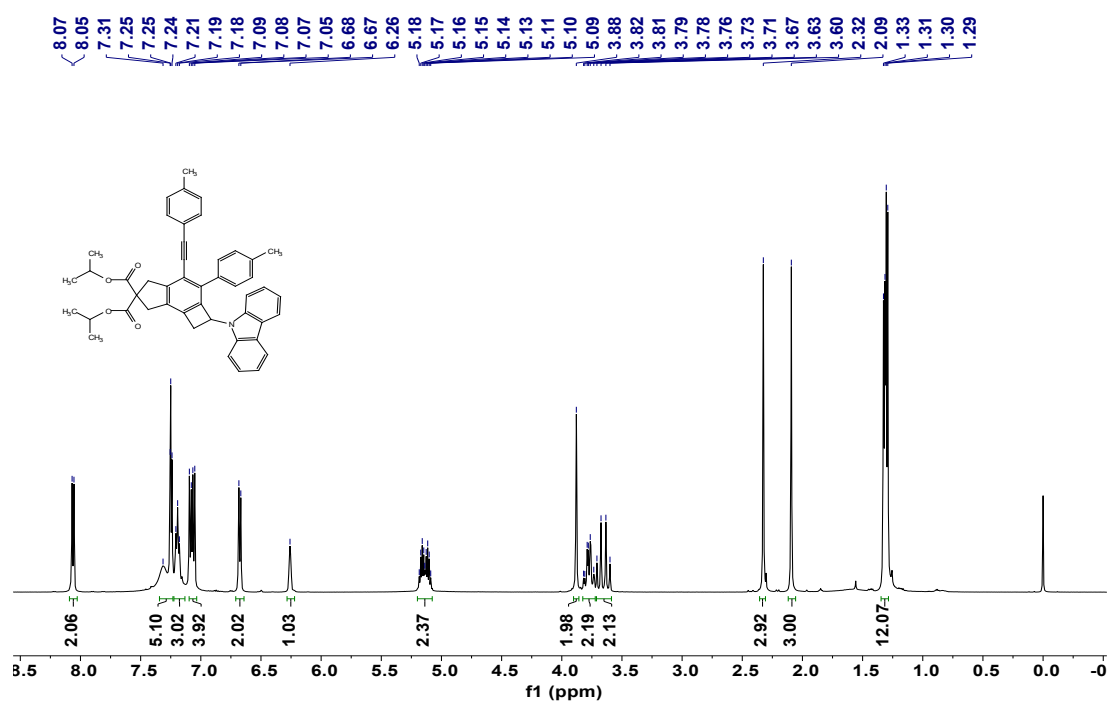


Figure 23 ¹H NMR spectrum of **2I** (500 MHz, CDCl₃).

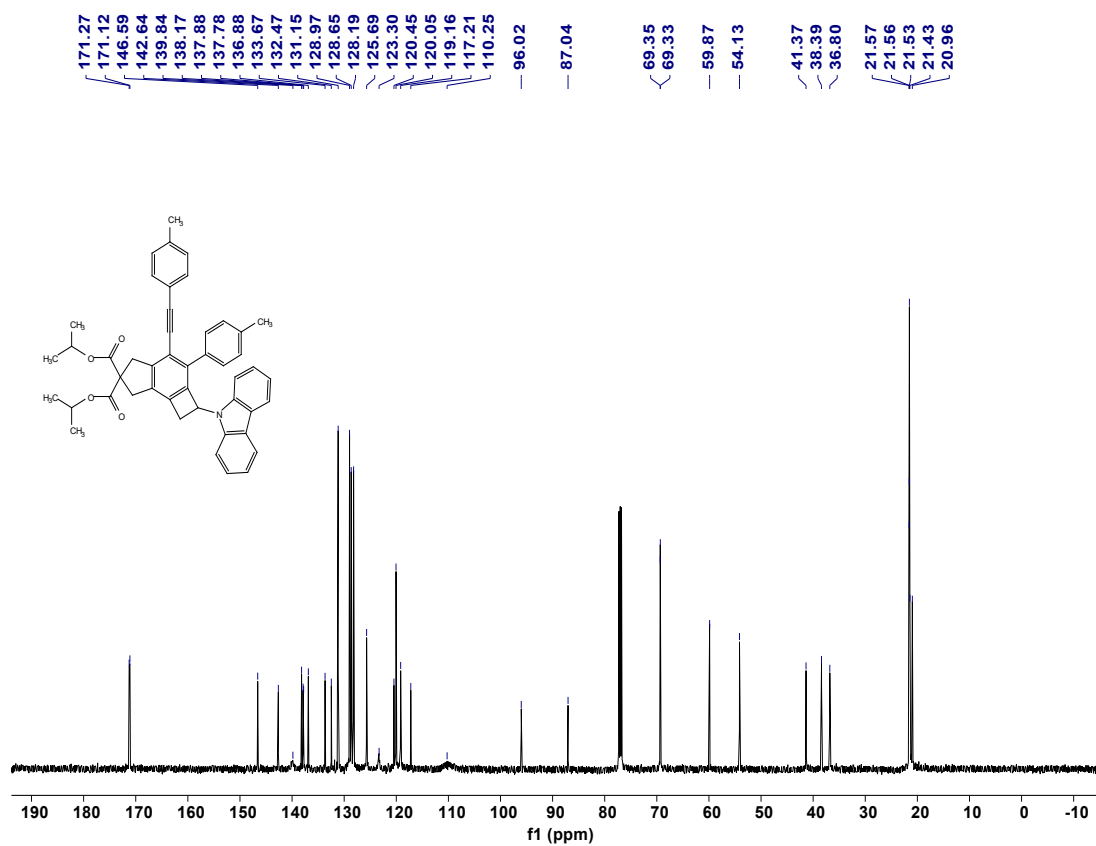


Figure 24 ¹³C NMR spectrum of **2I** (125 MHz, CDCl₃).

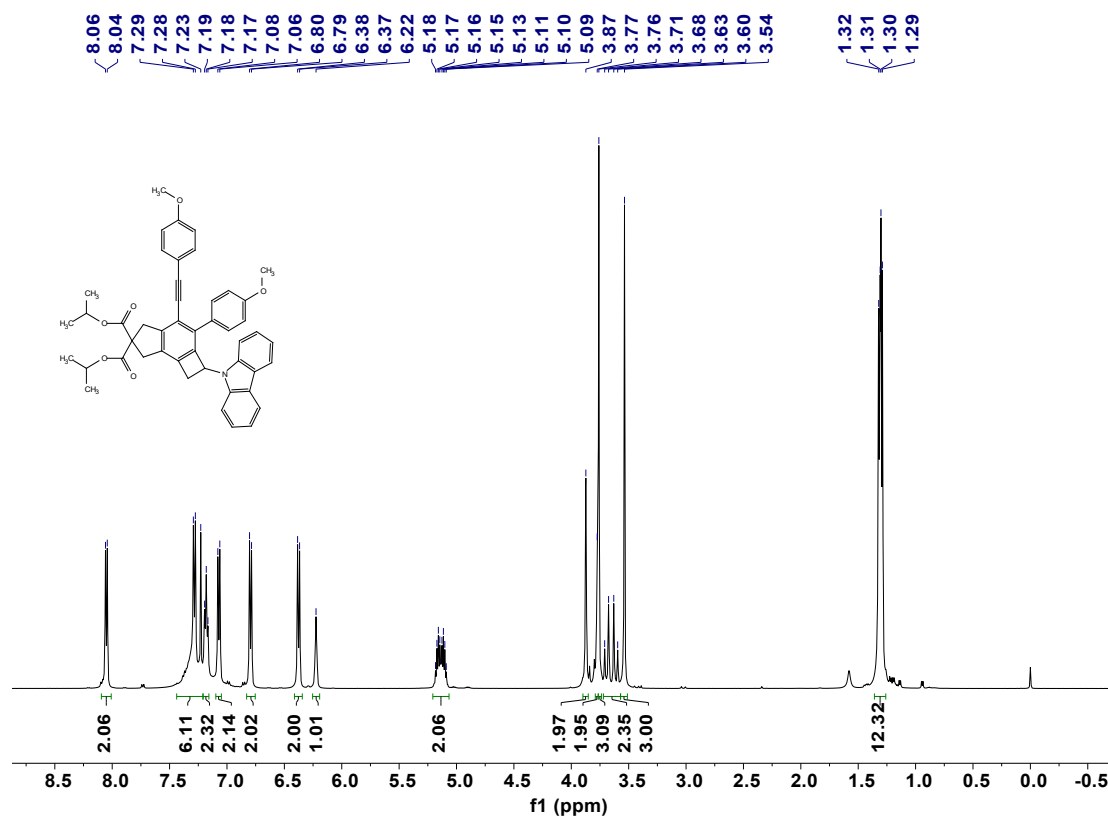


Figure 25 ¹H NMR spectrum of **2m** (500 MHz, CDCl₃).

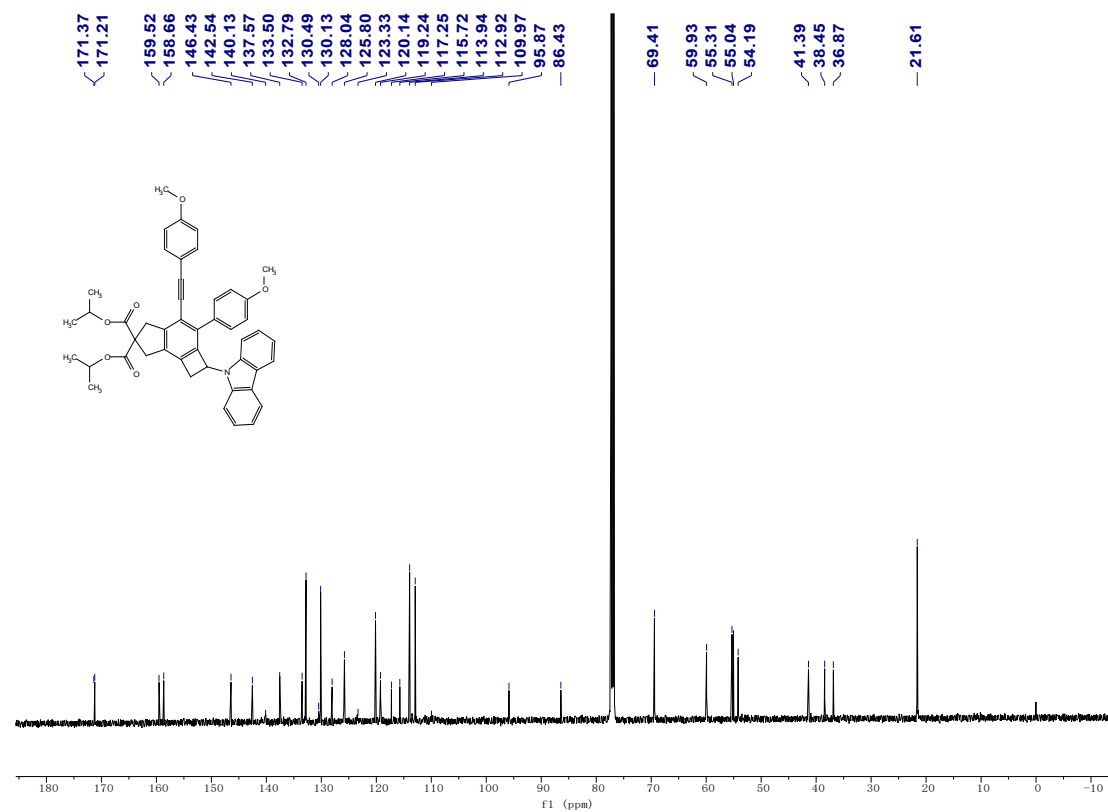


Figure 26 ¹³C NMR spectrum of **2m** (125 MHz, CDCl₃).

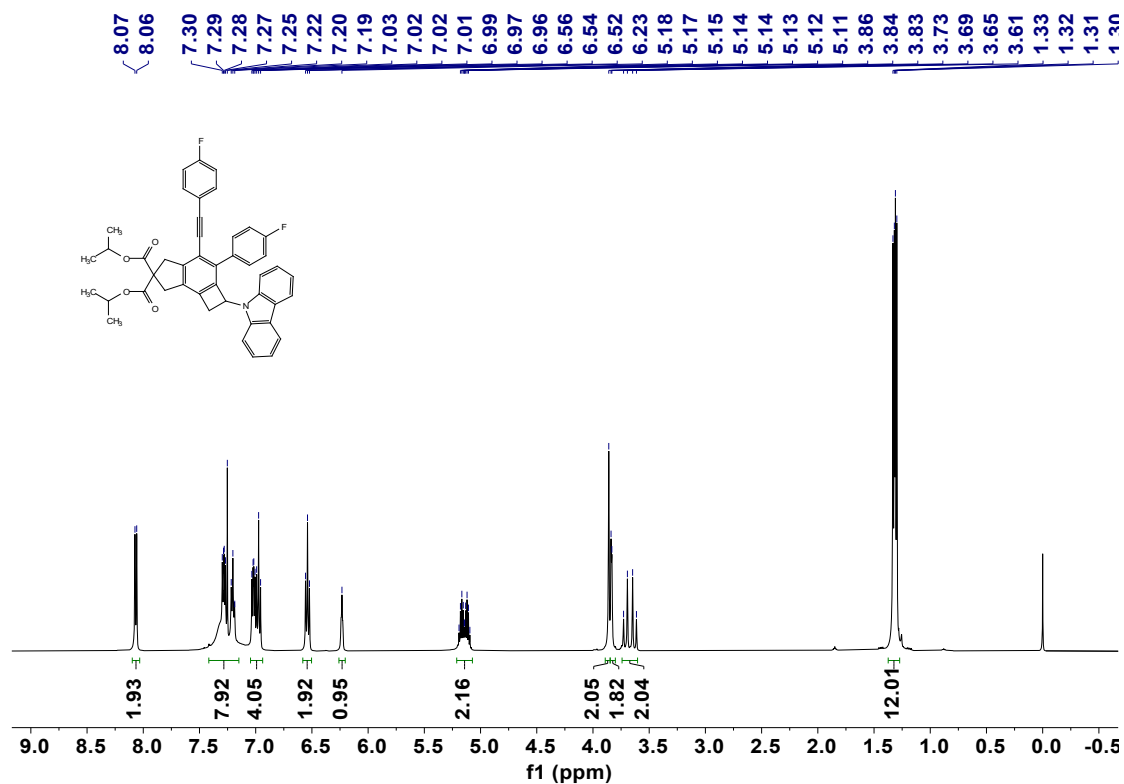


Figure 27 ^1H NMR spectrum of **2n** (500 MHz, CDCl_3).

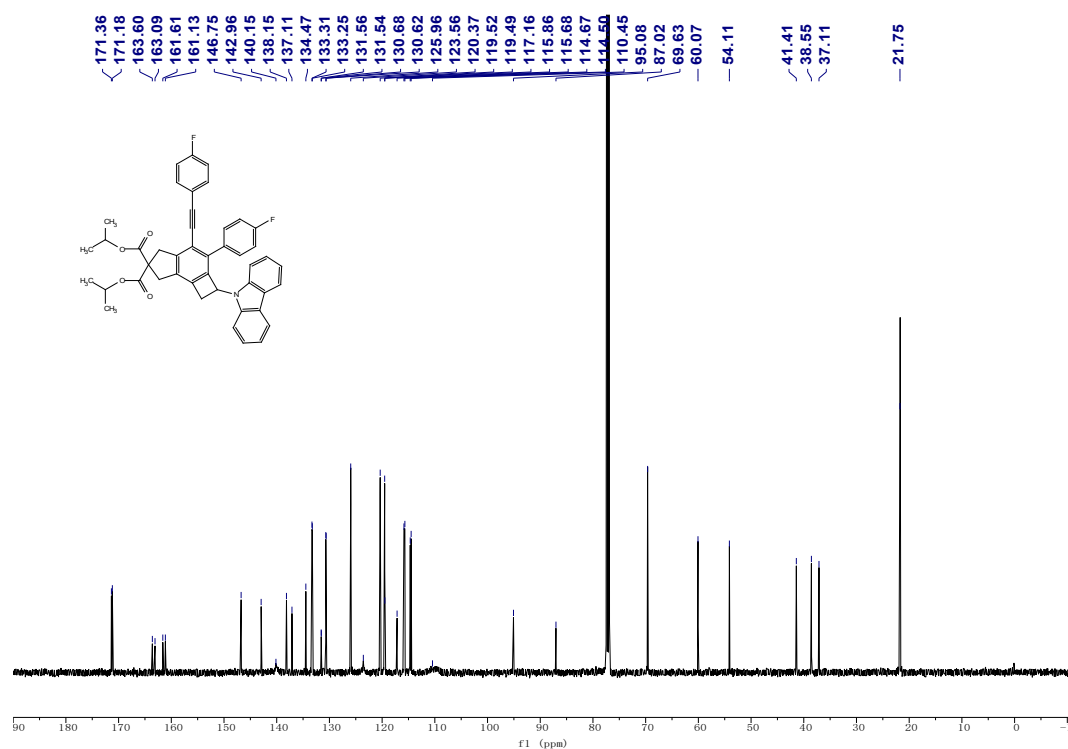


Figure 28 ^{13}C NMR spectrum of **2n** (125 MHz, CDCl_3).

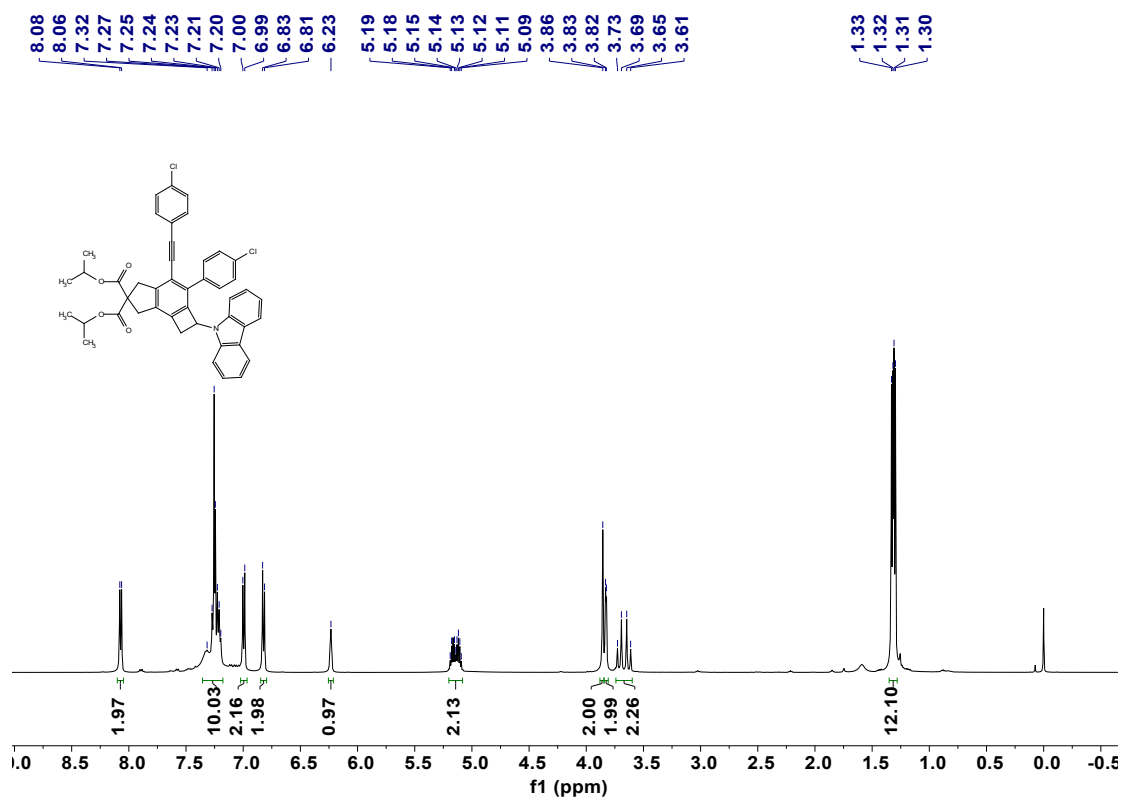


Figure 29 ^1H NMR spectrum of **2o** (500 MHz, CDCl_3).

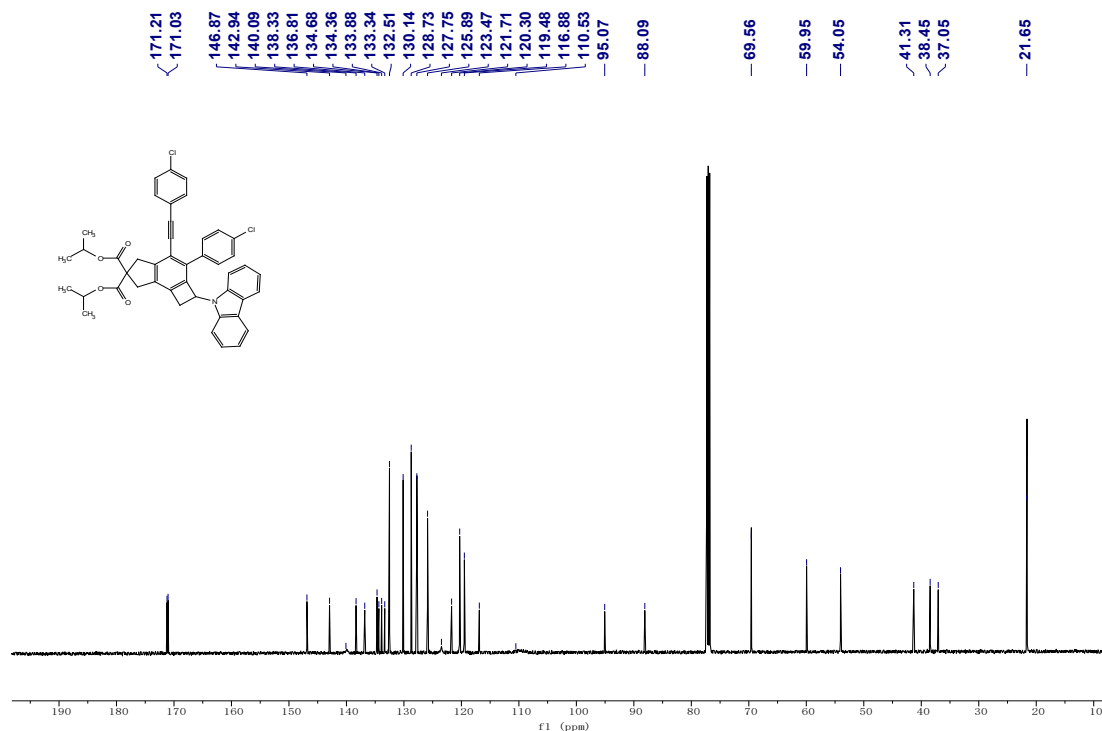


Figure 30 ^{13}C NMR spectrum of **2o** (125 MHz, CDCl_3).

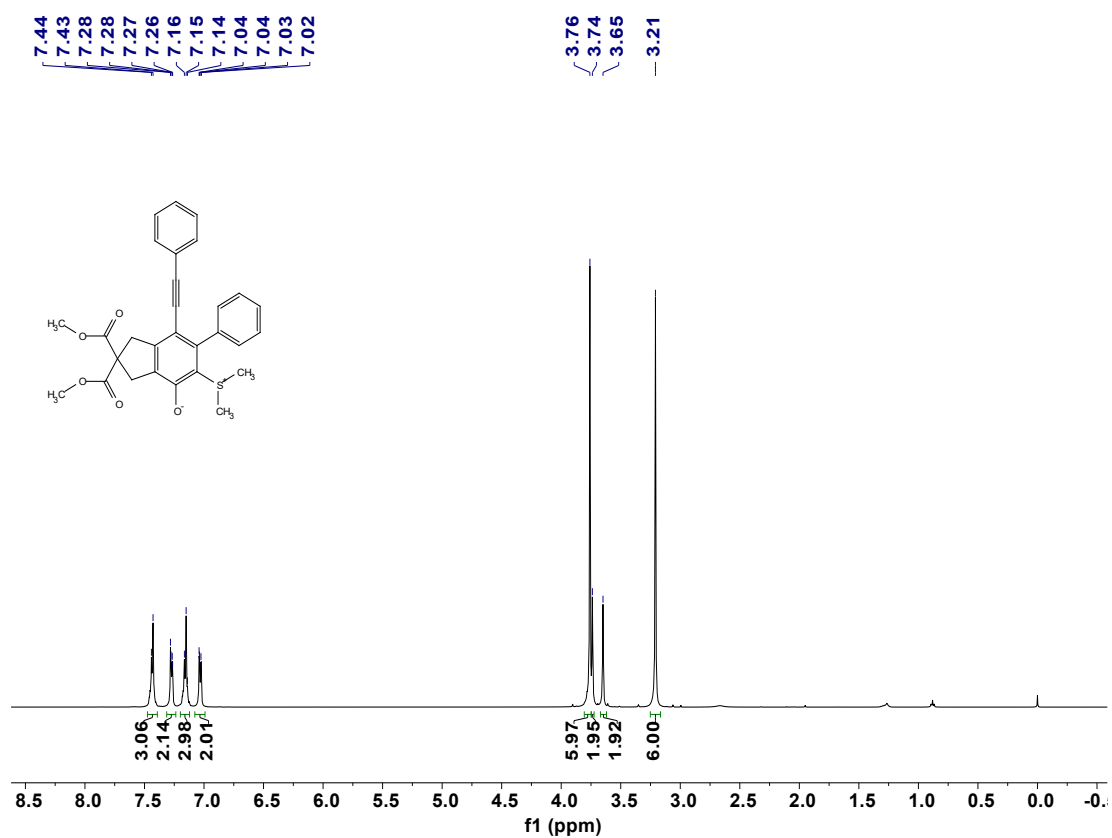


Figure 31 ¹H NMR spectrum of **3a** (500 MHz, CDCl₃).

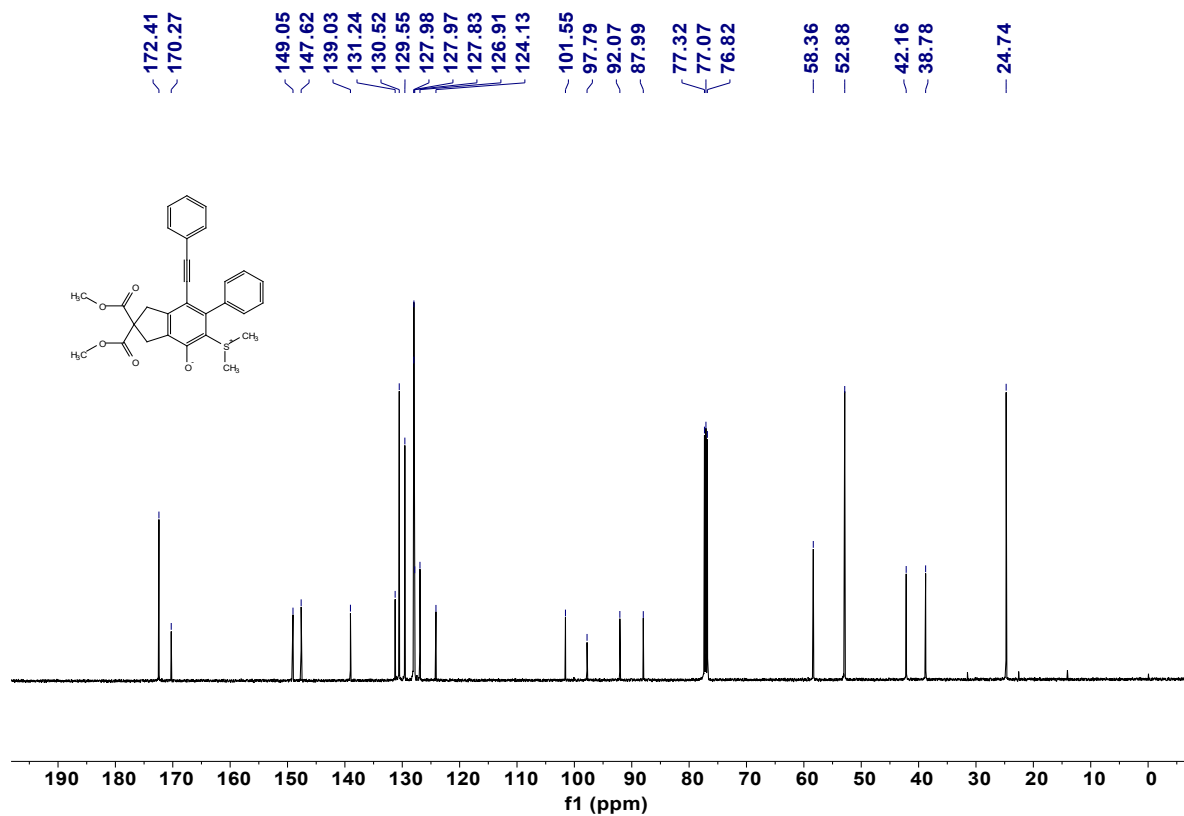


Figure 32 ¹³C NMR spectrum of **3a** (125 MHz, CDCl₃).

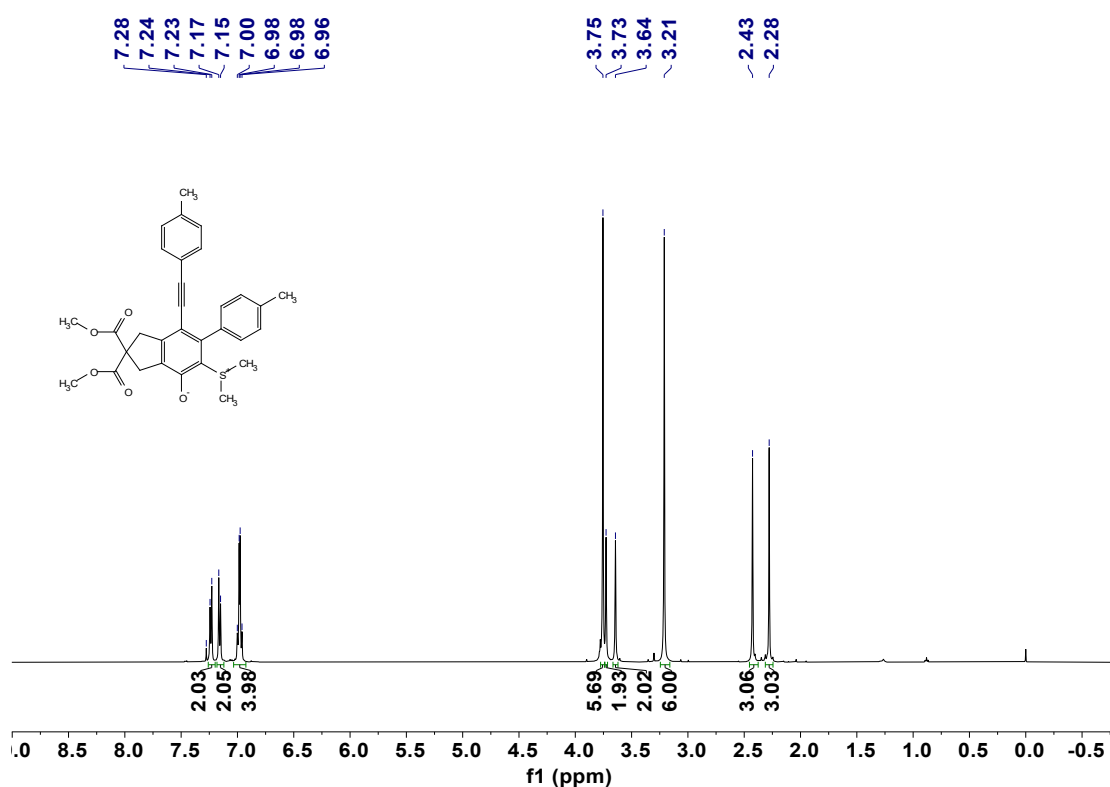


Figure 33 ^1H NMR spectrum of **3b** (500 MHz, CDCl_3).

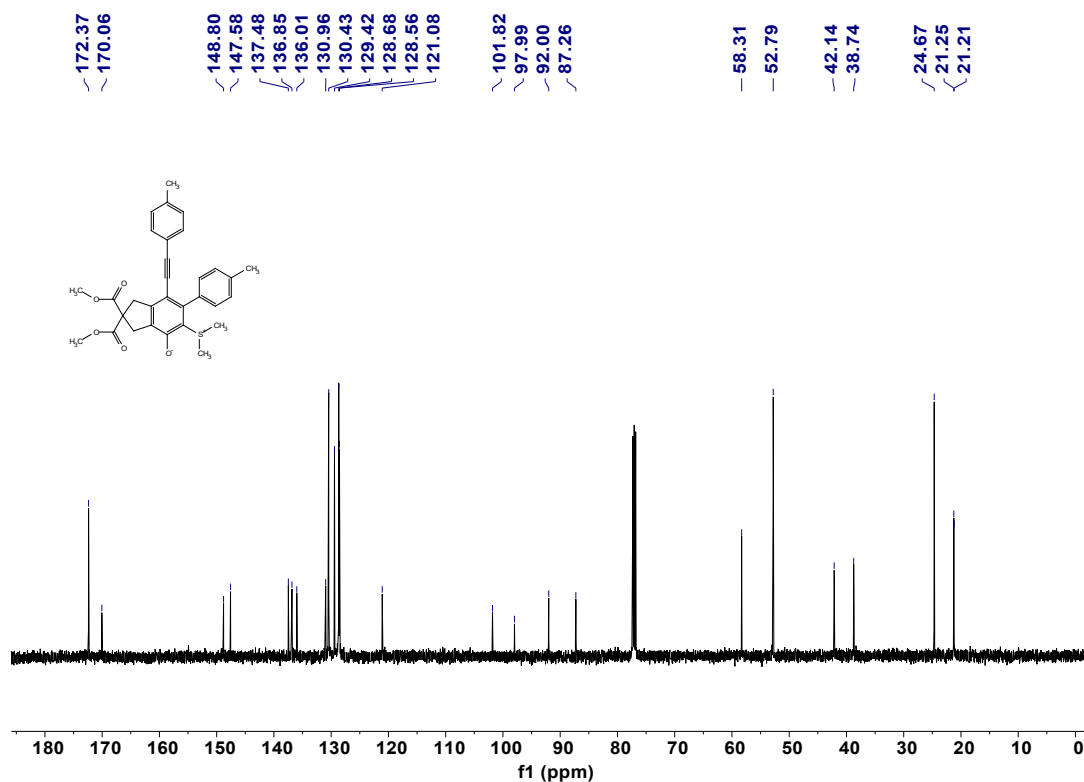


Figure 34 ^{13}C NMR spectrum of **3b** (125 MHz, CDCl_3).

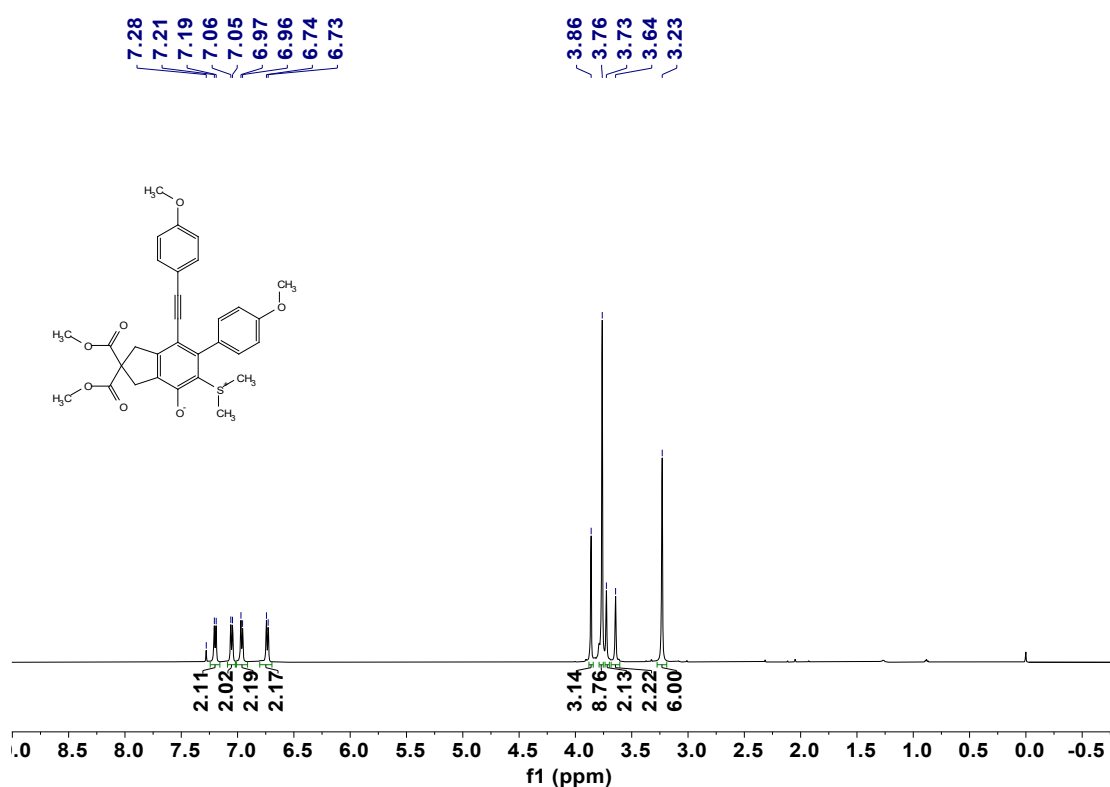


Figure 35 ^1H NMR spectrum of **3c** (500 MHz, CDCl_3).

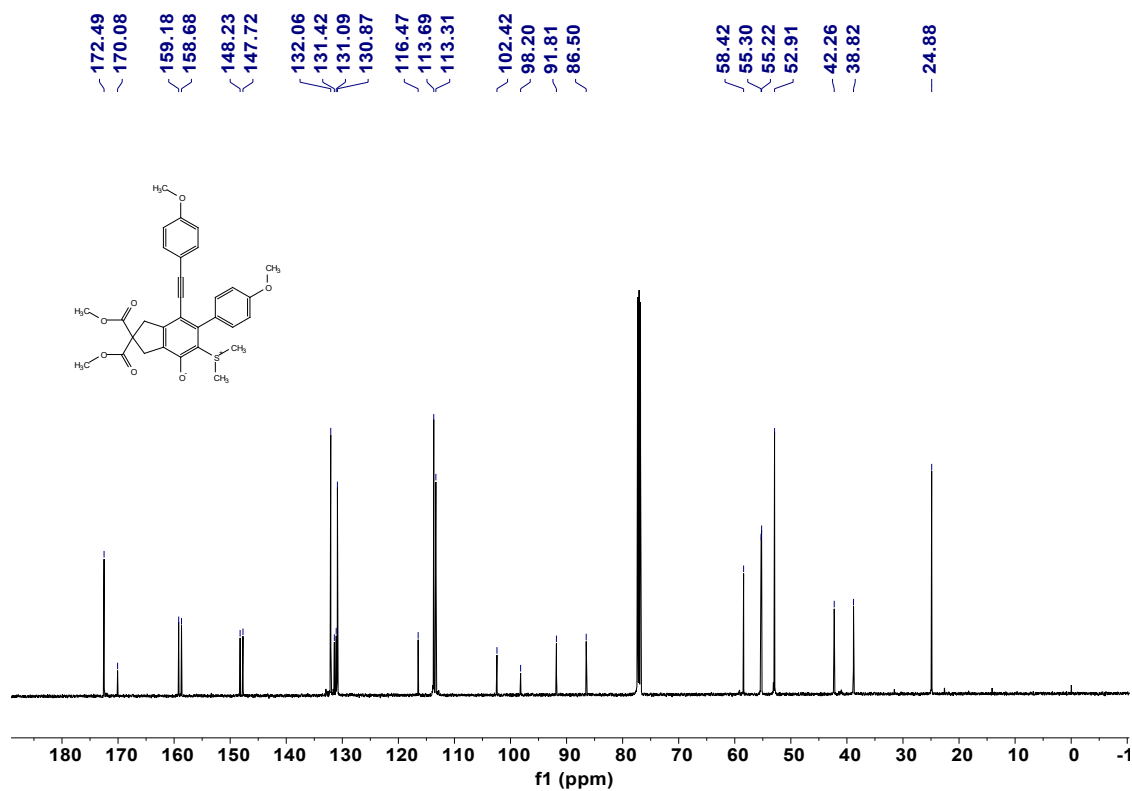


Figure 36 ^{13}C NMR spectrum of **3c** (125 MHz, CDCl_3).

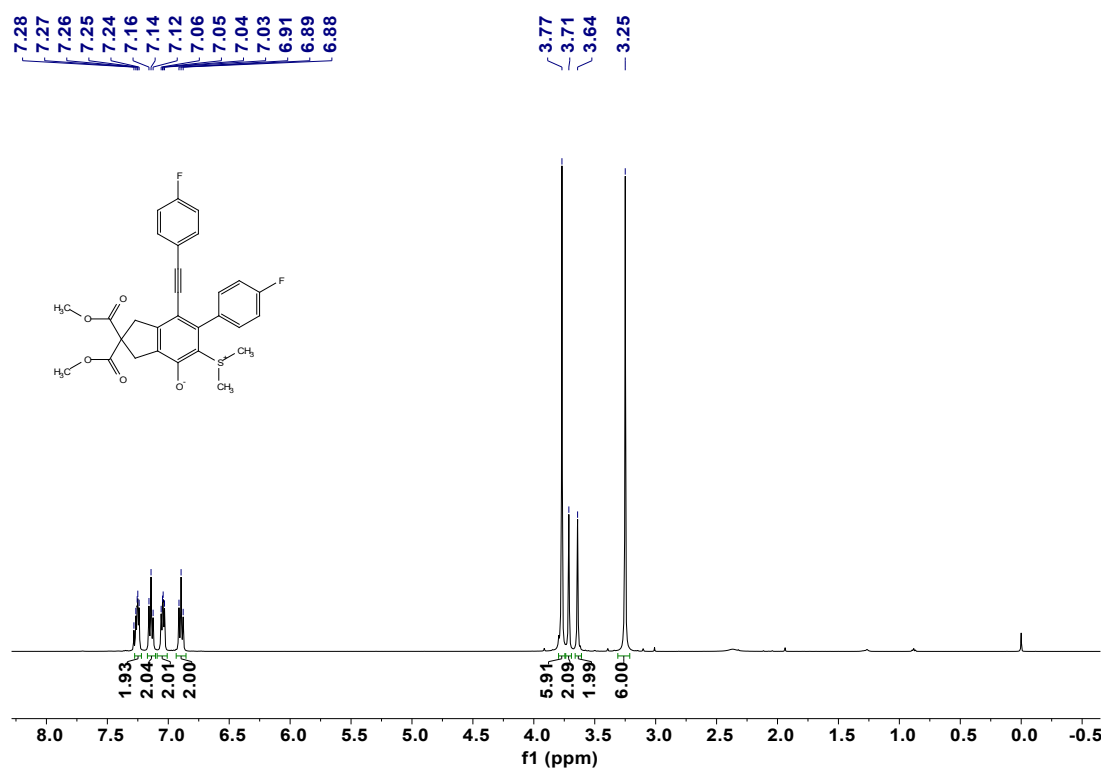


Figure 37 ¹H NMR spectrum of **3d** (500 MHz, CDCl₃).

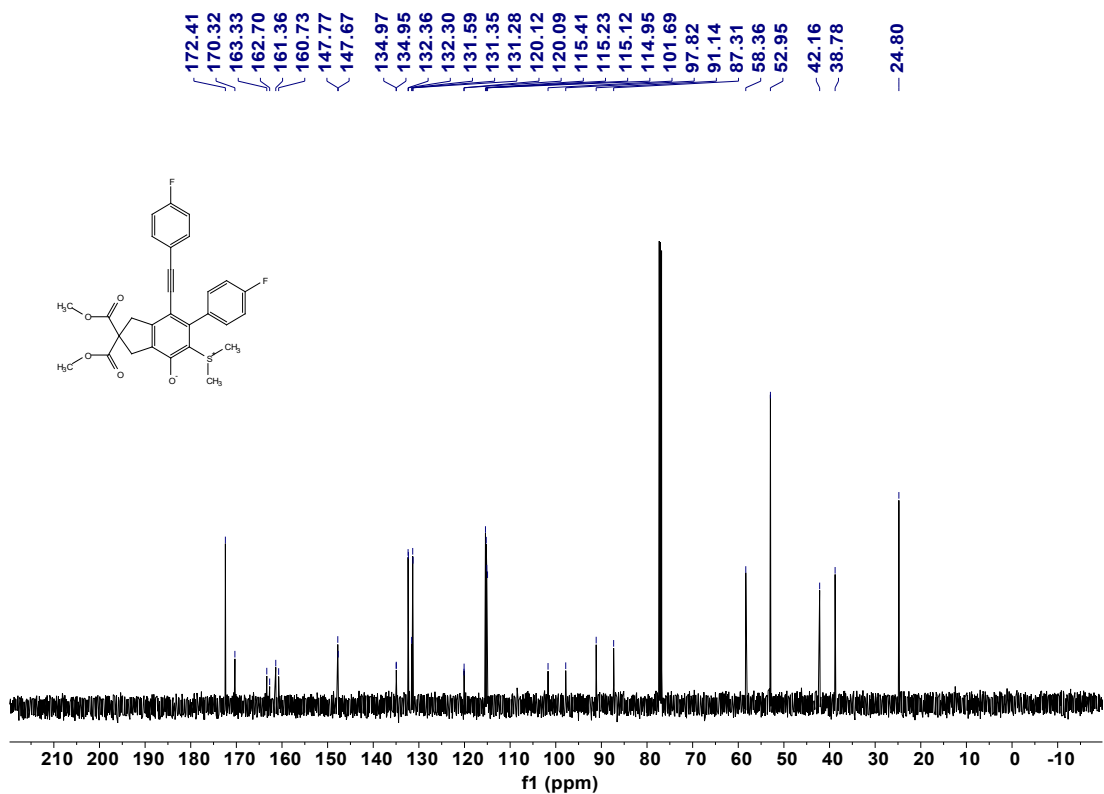


Figure 38 ¹³C NMR spectrum of **3d** (125 MHz, CDCl₃).

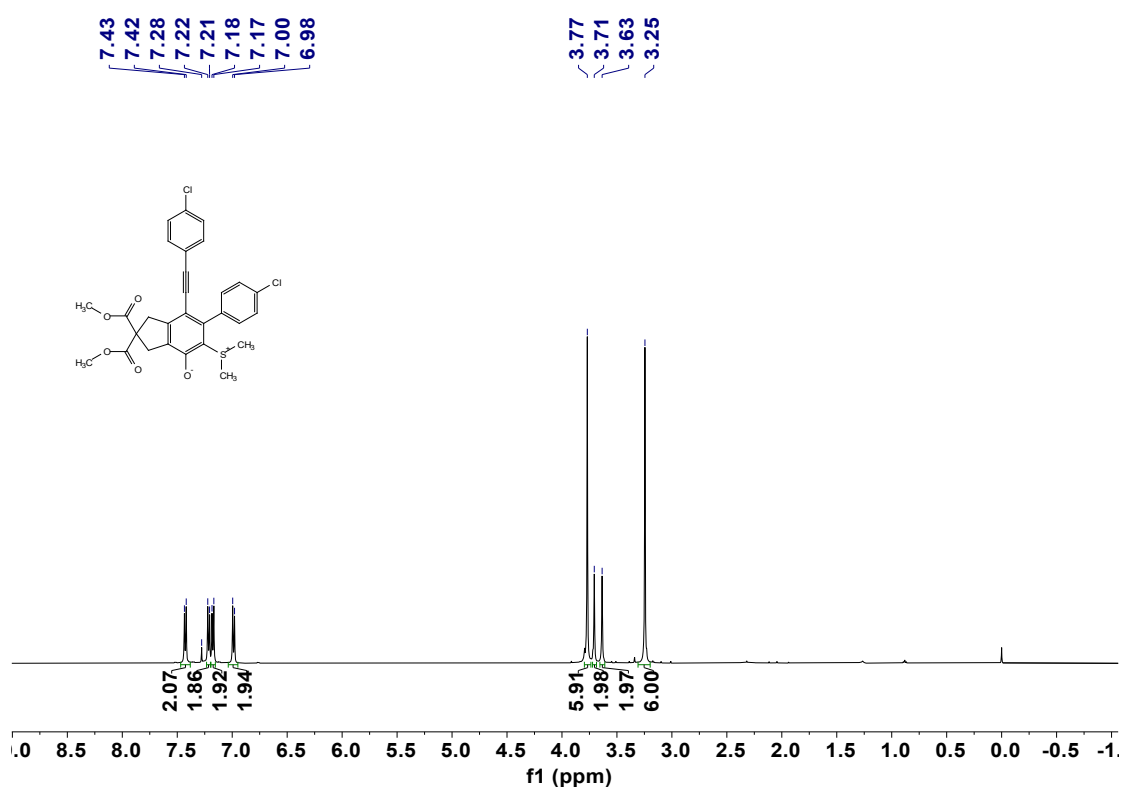


Figure 39 ¹H NMR spectrum of **3e** (500 MHz, CDCl₃).

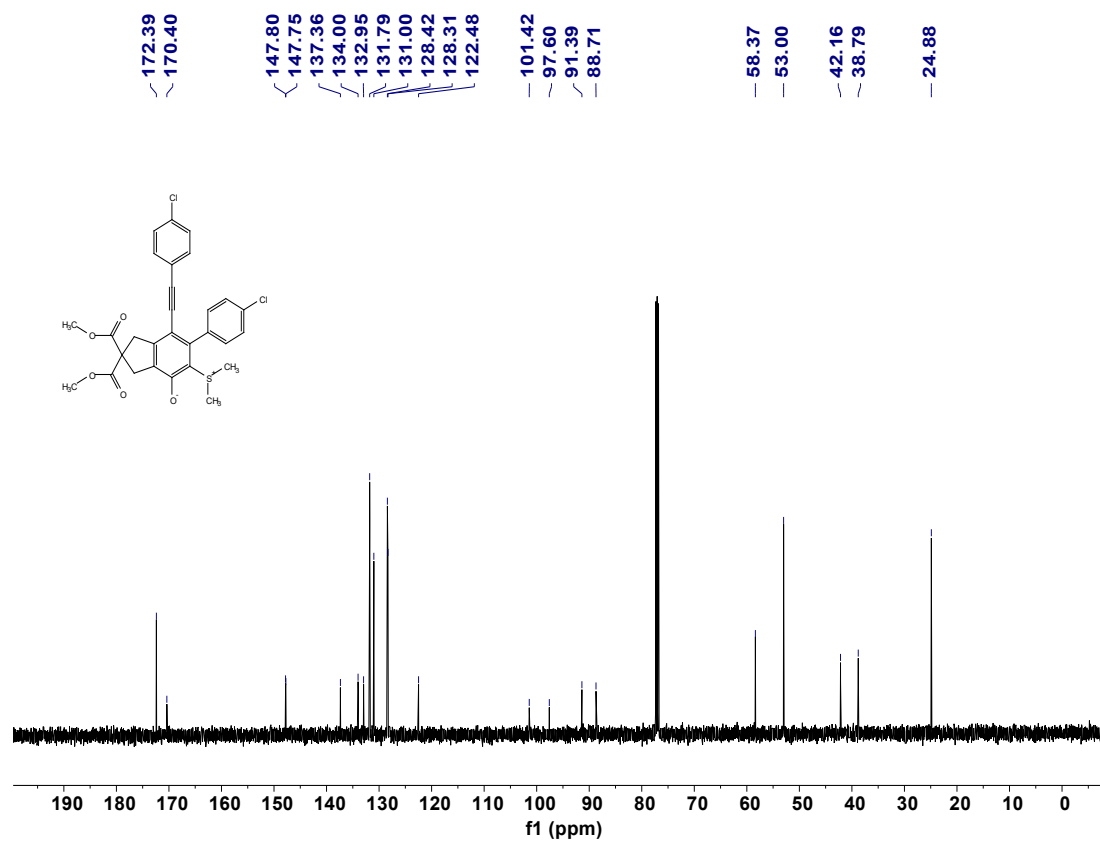


Figure 40 ¹³C NMR spectrum of **3e** (125 MHz, CDCl₃).

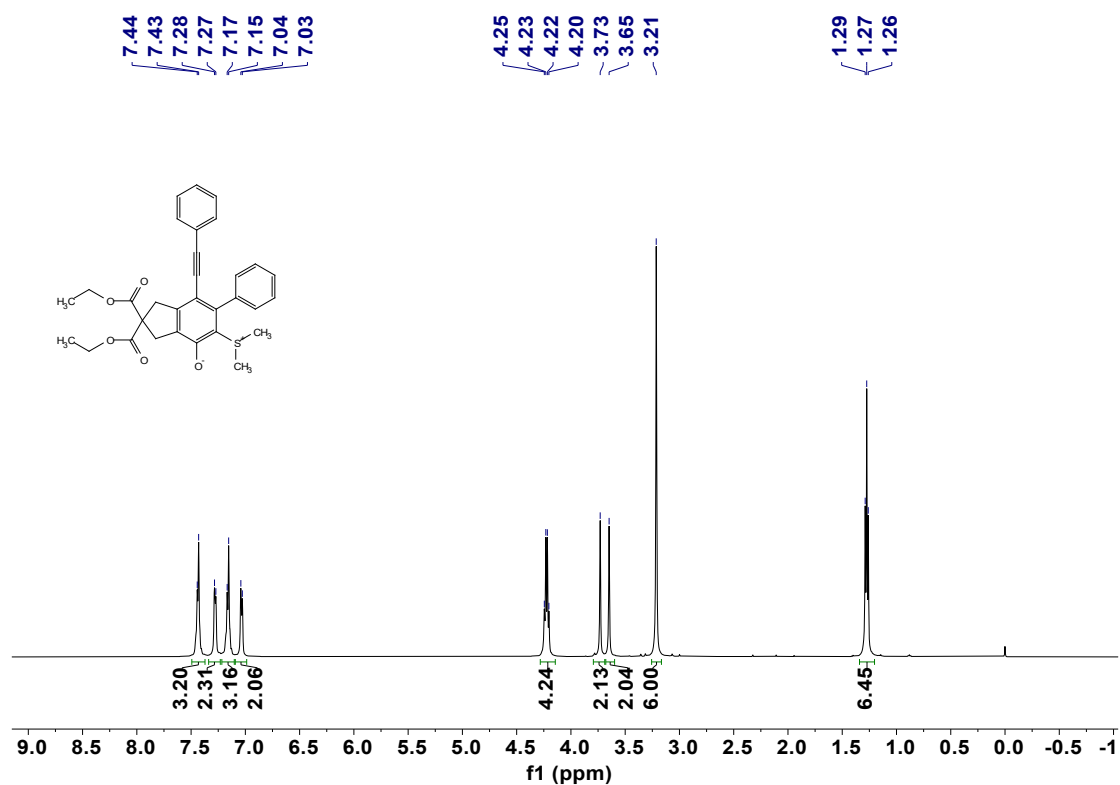


Figure 41 ¹H NMR spectrum of **3f** (500 MHz, CDCl₃).

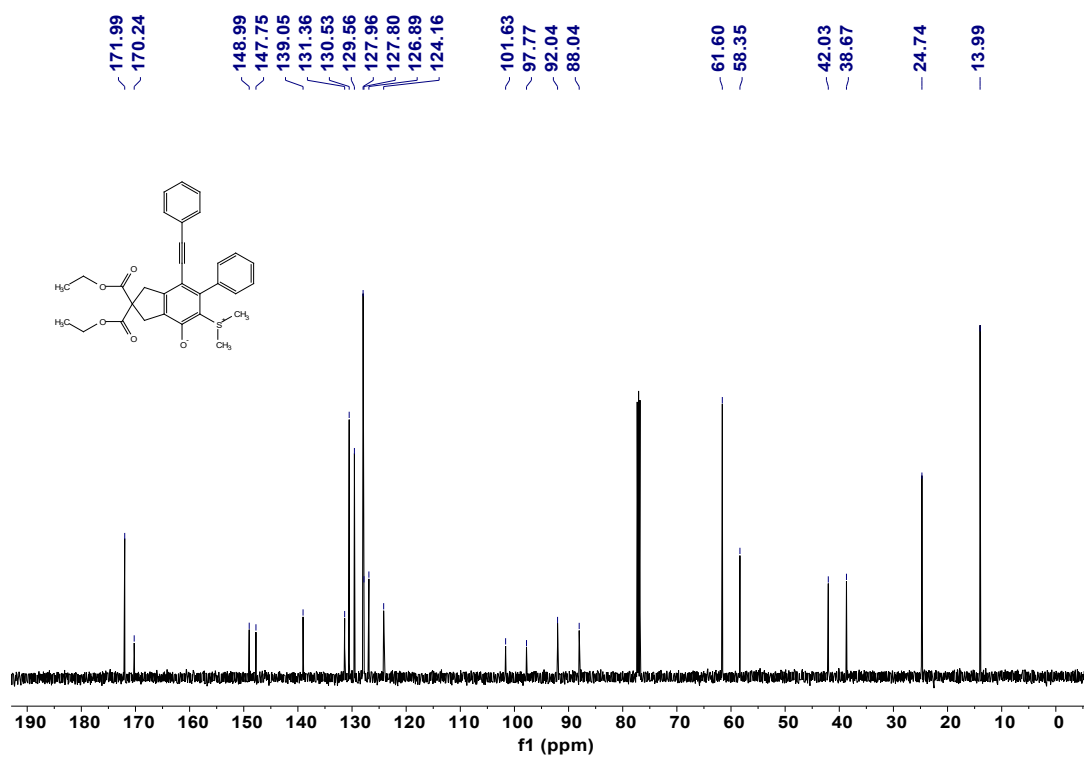


Figure 42 ¹³C NMR spectrum of **3f** (125 MHz, CDCl₃).

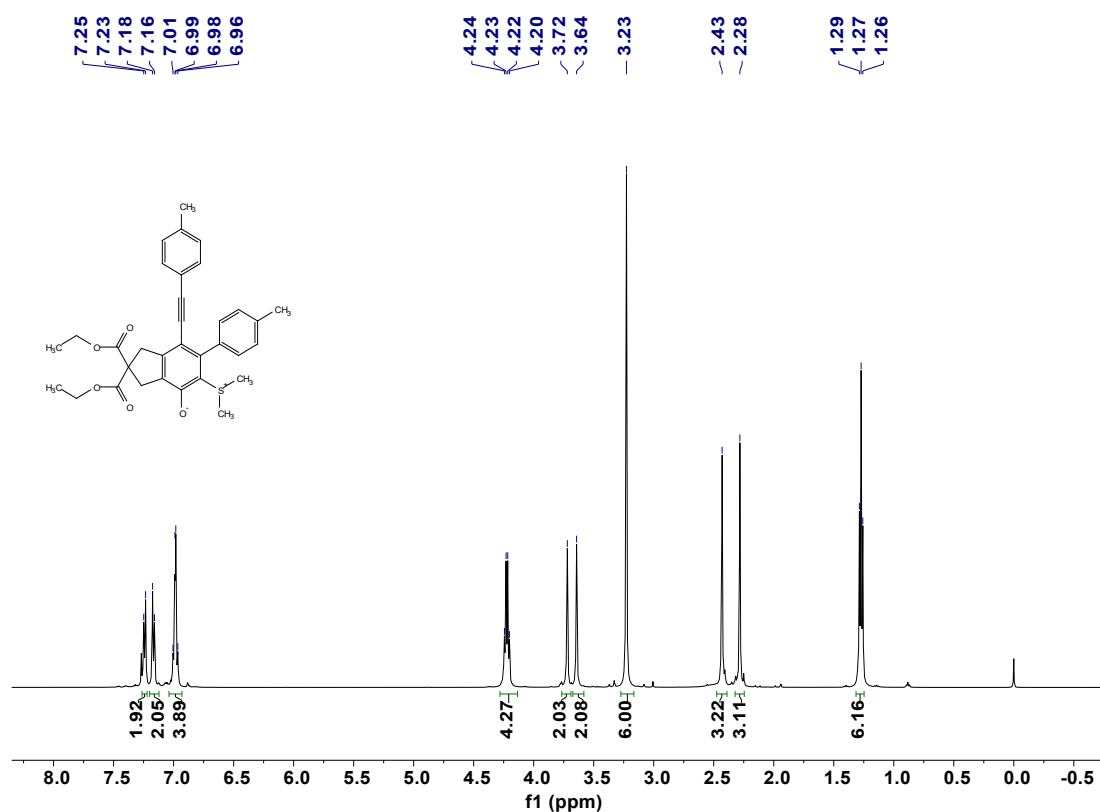


Figure 43 ^1H NMR spectrum of **3g** (500 MHz, CDCl_3).

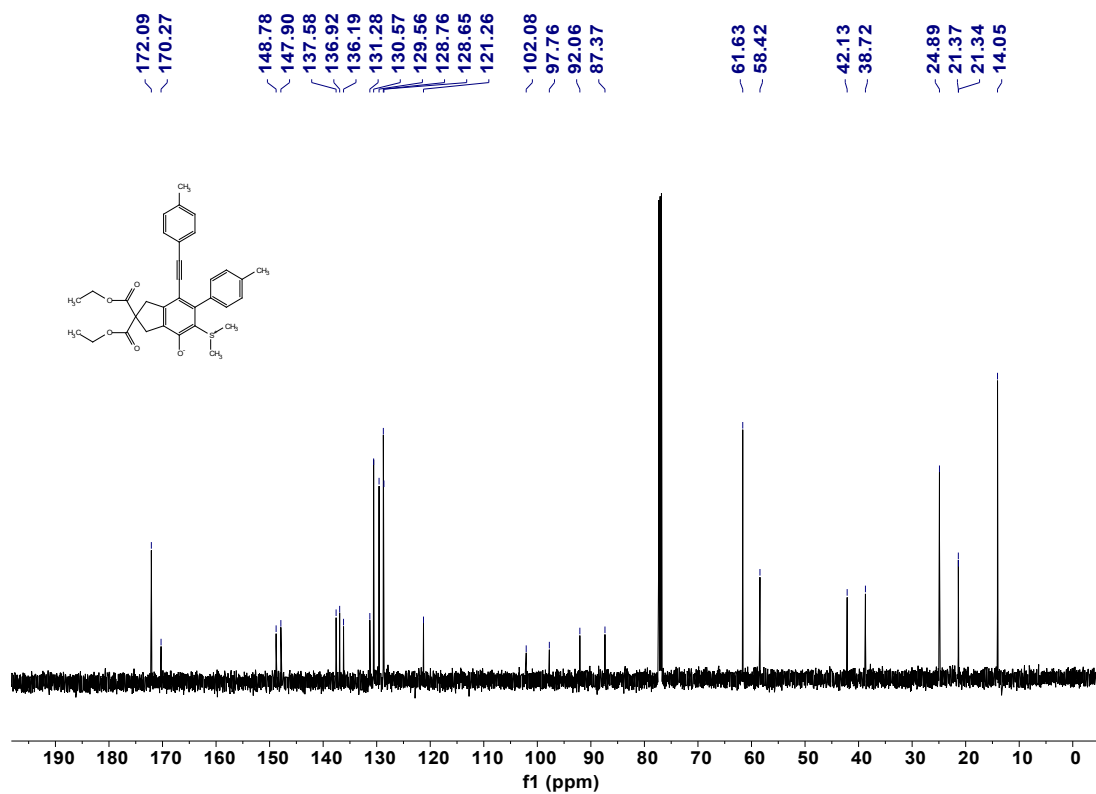


Figure 44 ^{13}C NMR spectrum of **3g** (125 MHz, CDCl_3).

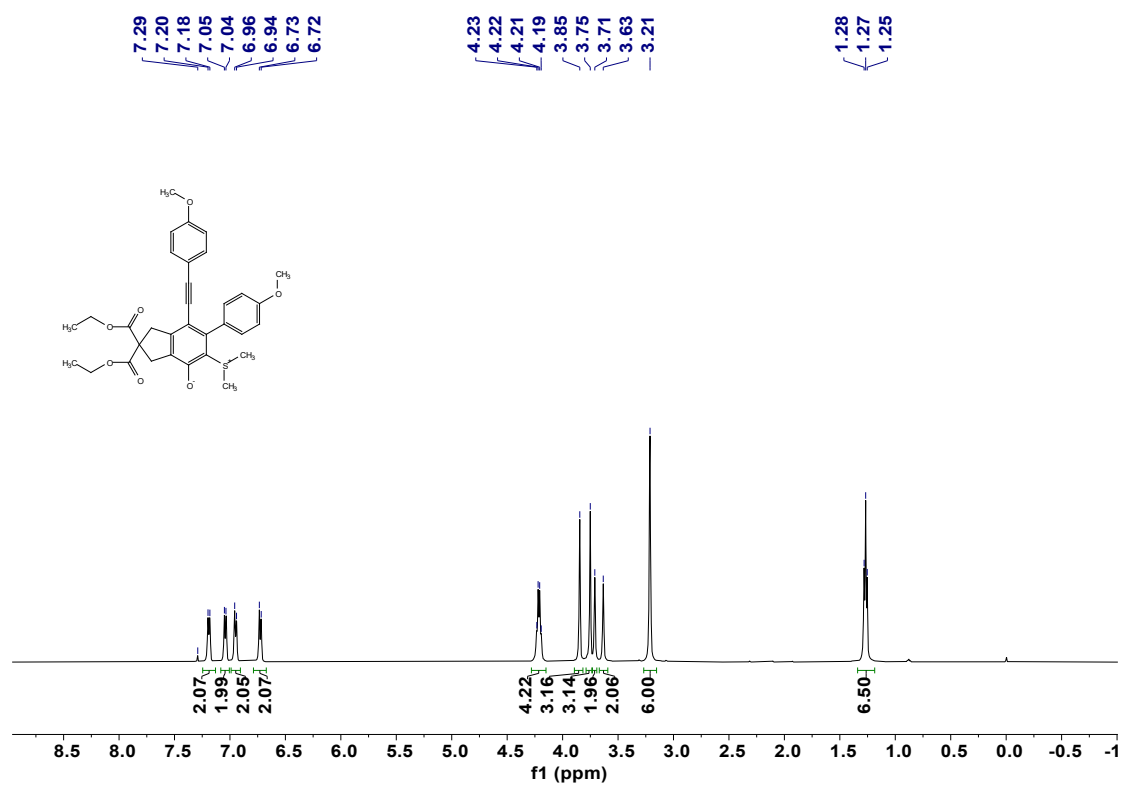


Figure 45 ^1H NMR spectrum of **3h** (500 MHz, CDCl_3).

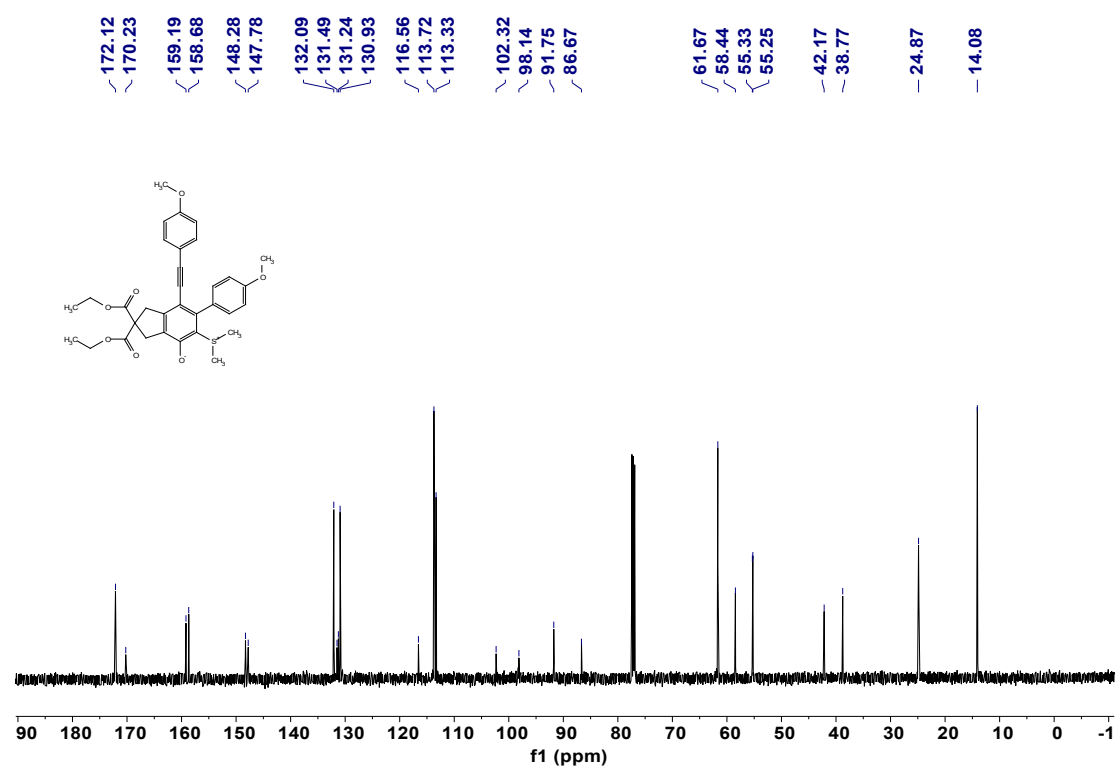


Figure 46 ^{13}C NMR spectrum of **3h** (125 MHz, CDCl_3).

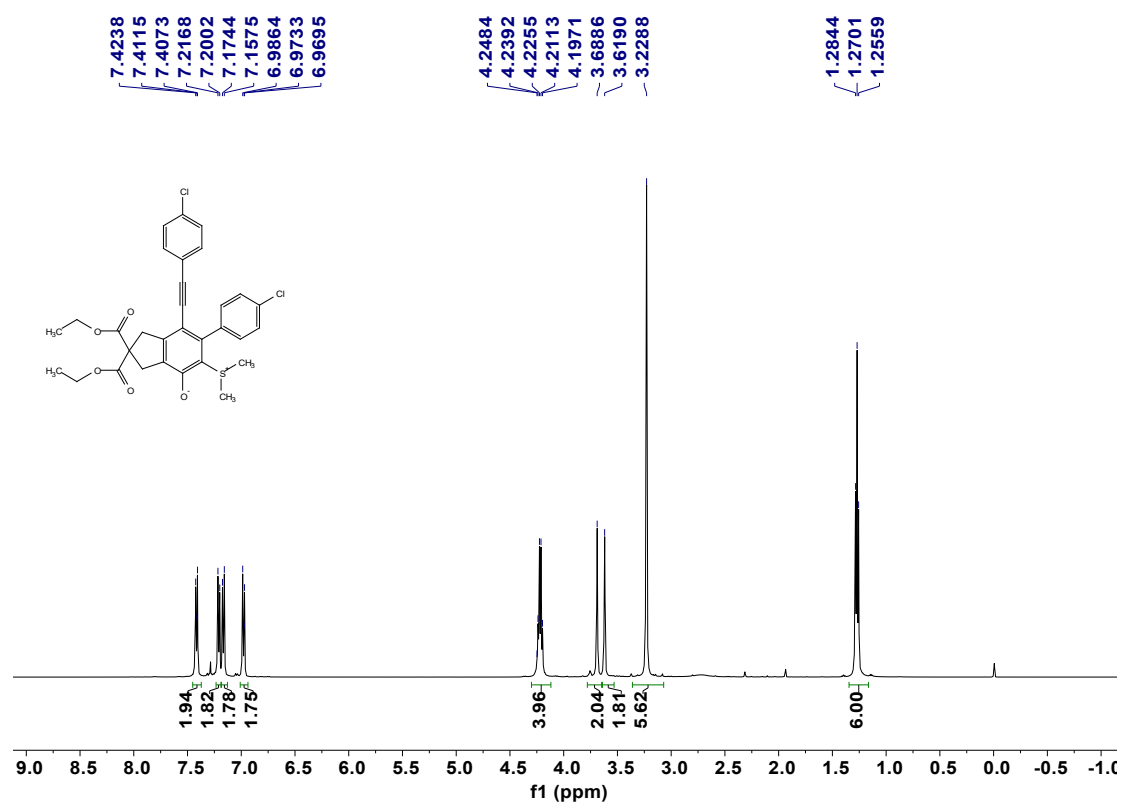


Figure 49 ¹H NMR spectrum of **3j** (500 MHz, CDCl₃).

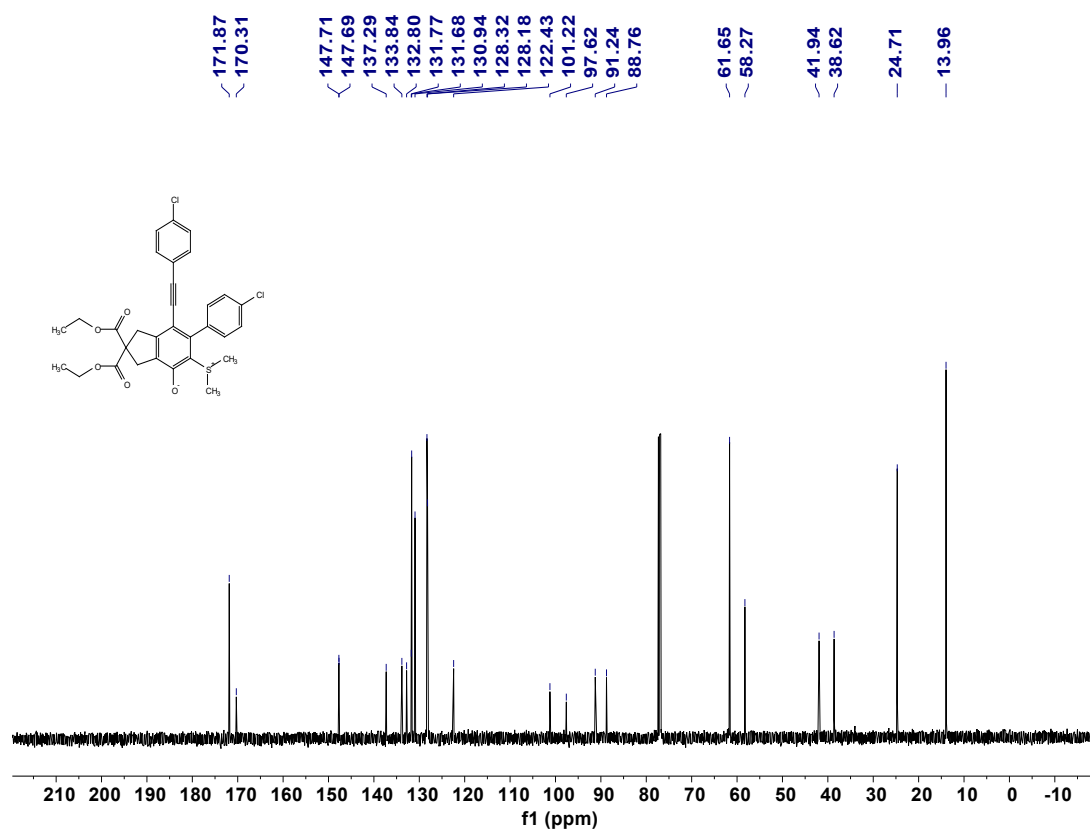


Figure 50 ¹³C NMR spectrum of **3j** (125 MHz, CDCl₃).

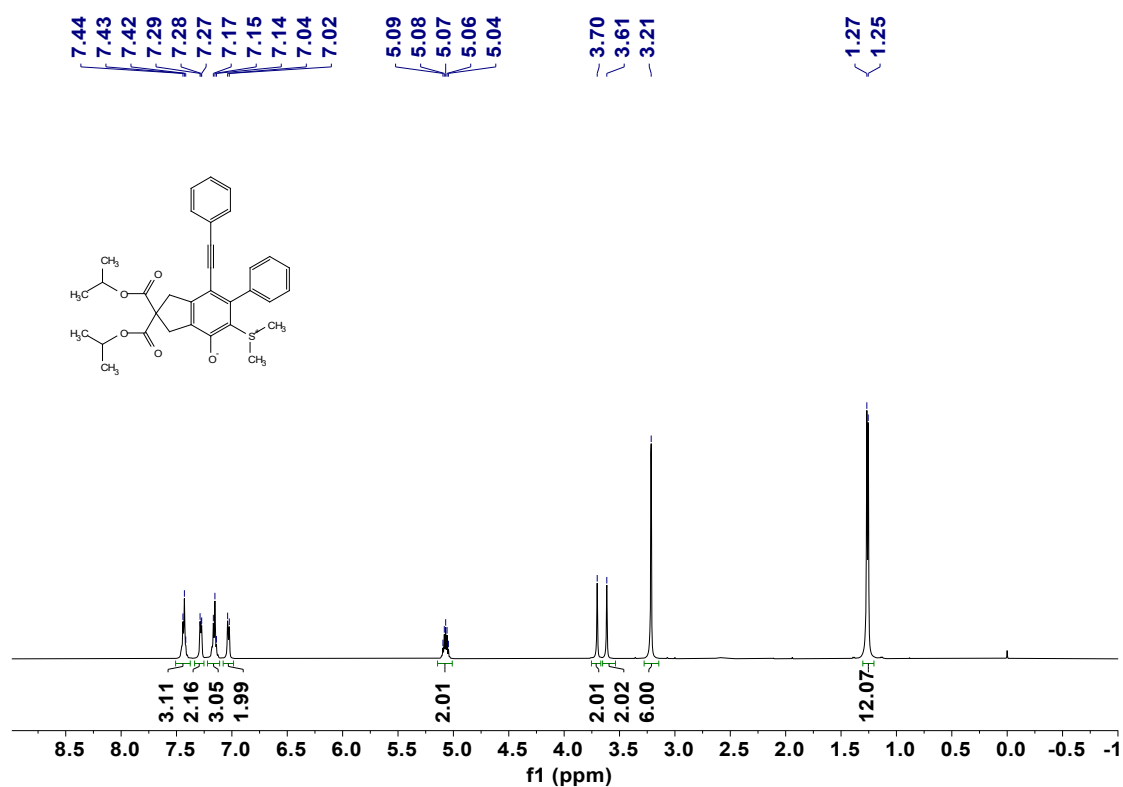


Figure 51 ¹H NMR spectrum of **3k** (500 MHz, CDCl₃).

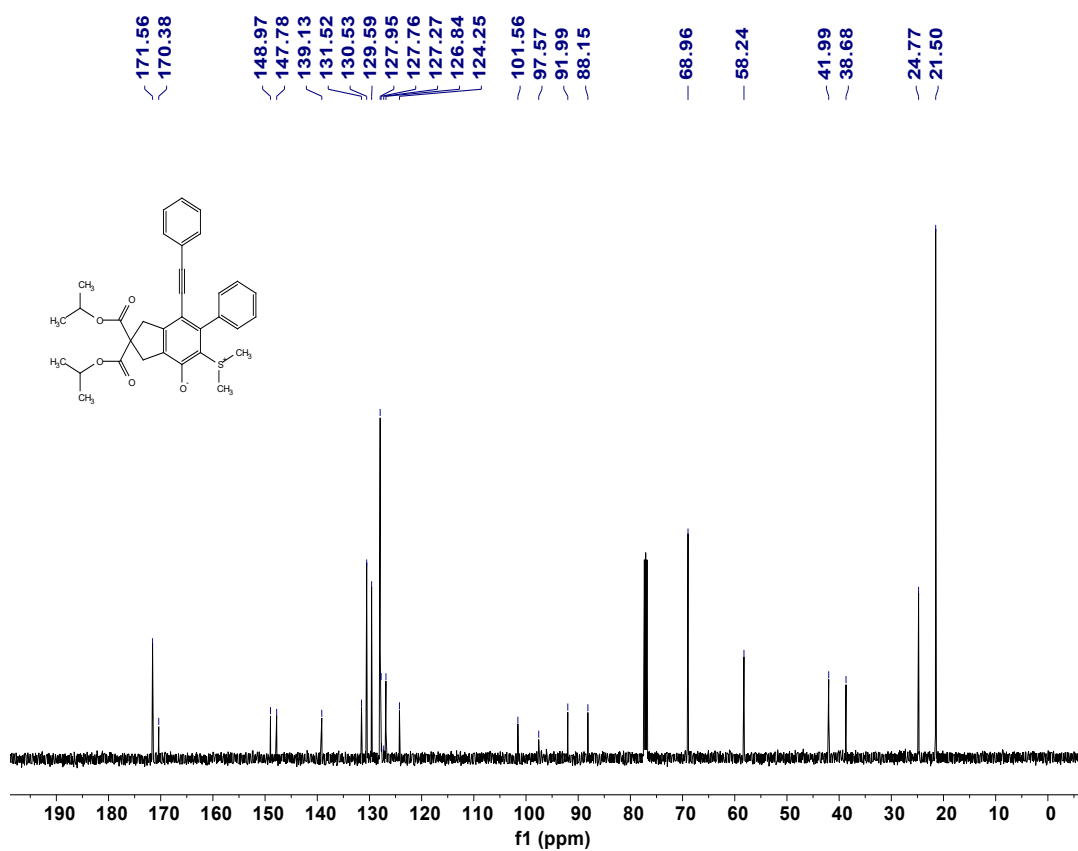


Figure 52 ¹³C NMR spectrum of **3k** (125 MHz, CDCl₃).

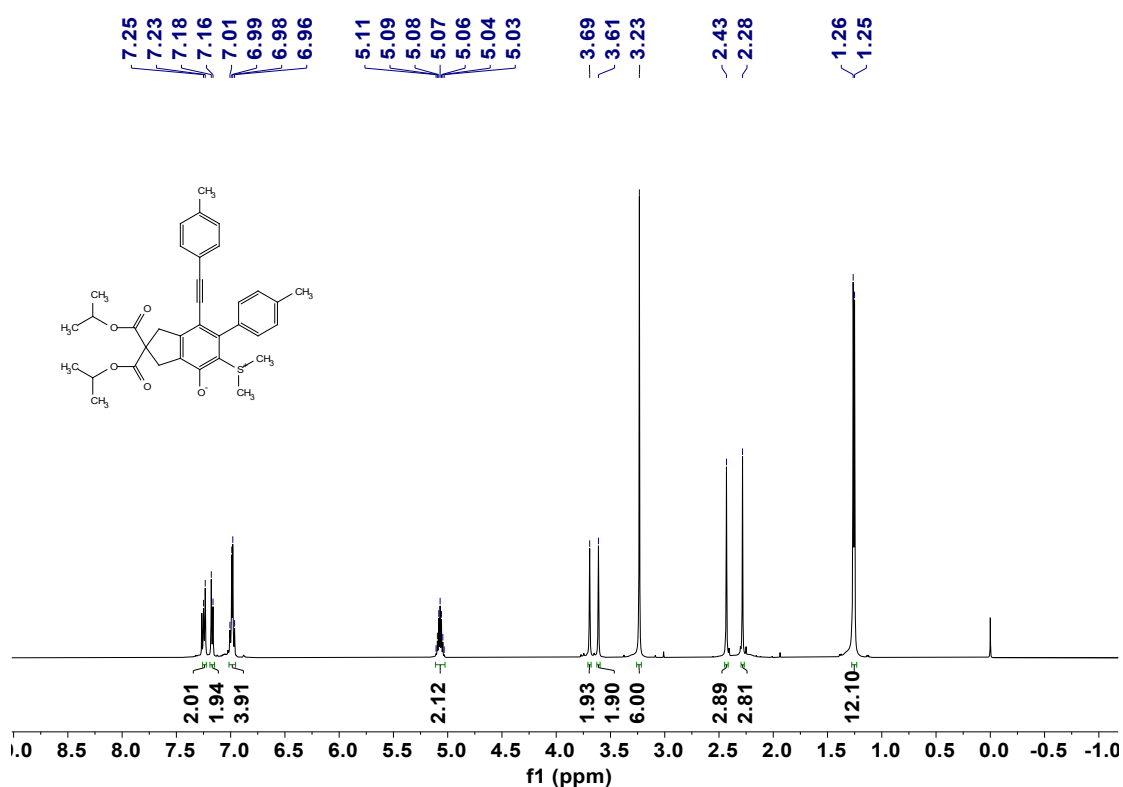


Figure 53 ^1H NMR spectrum of **3I** (500 MHz, CDCl_3).

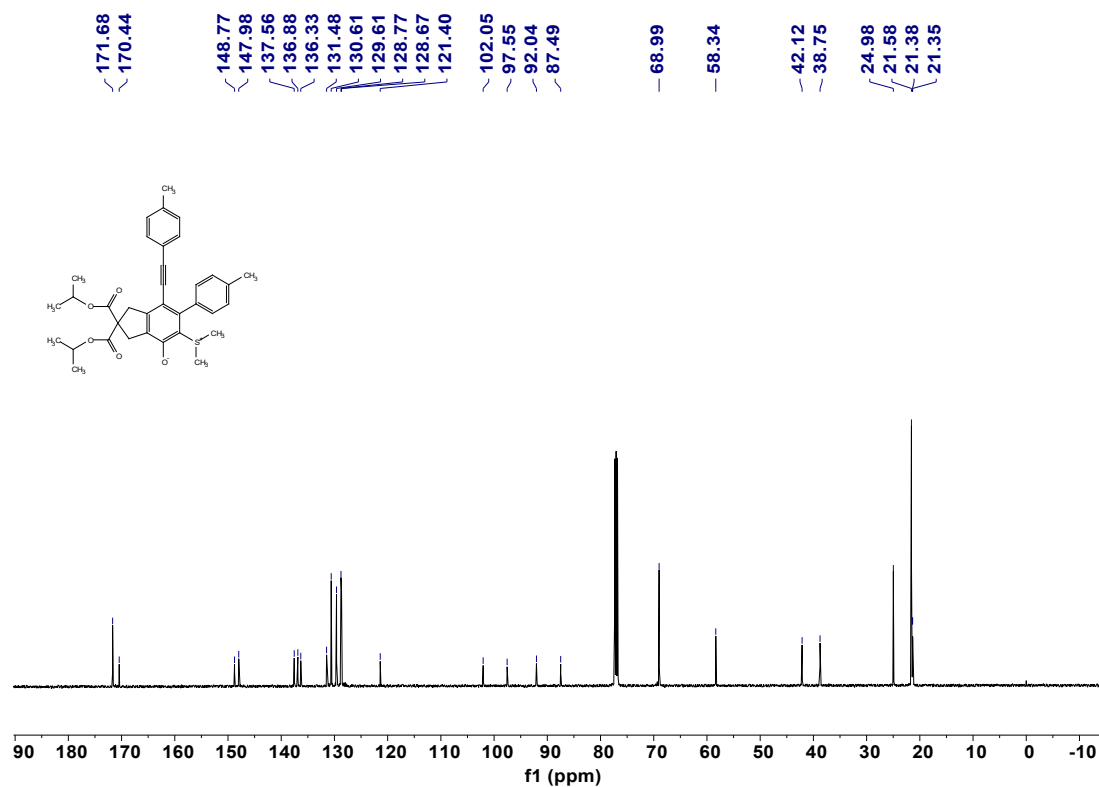


Figure 54 ^{13}C NMR spectrum of **3I** (125 MHz, CDCl_3).

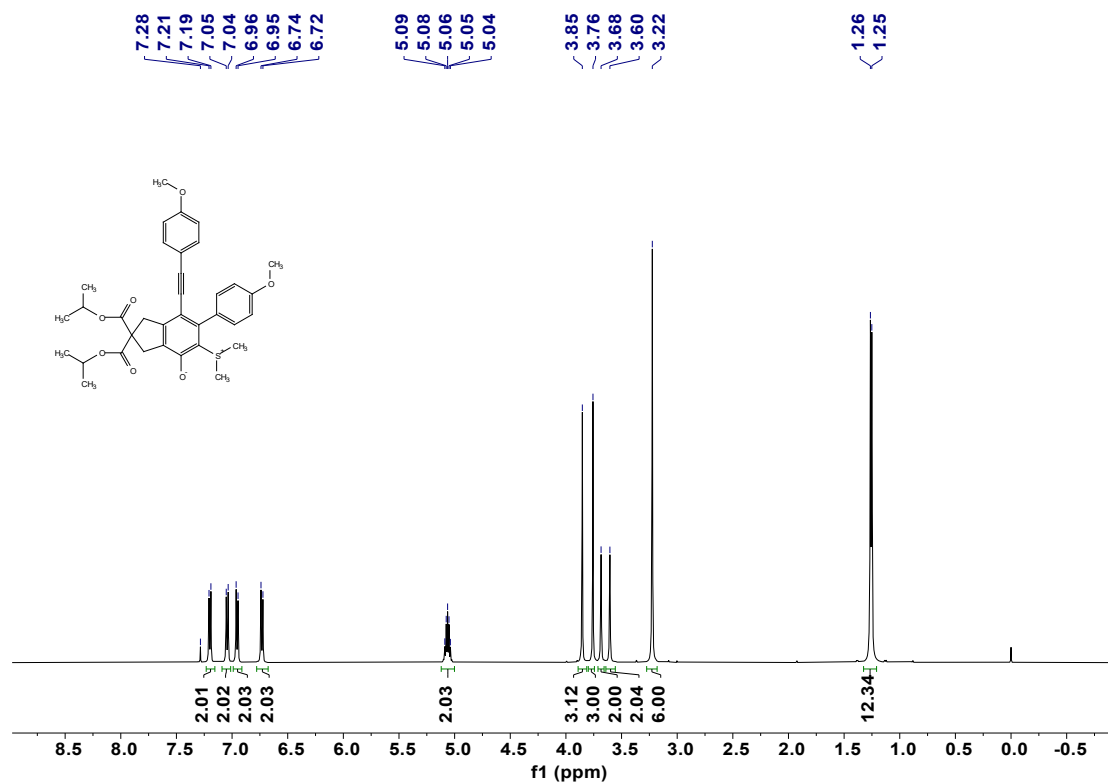


Figure 55 ¹H NMR spectrum of **3m** (500 MHz, CDCl₃).

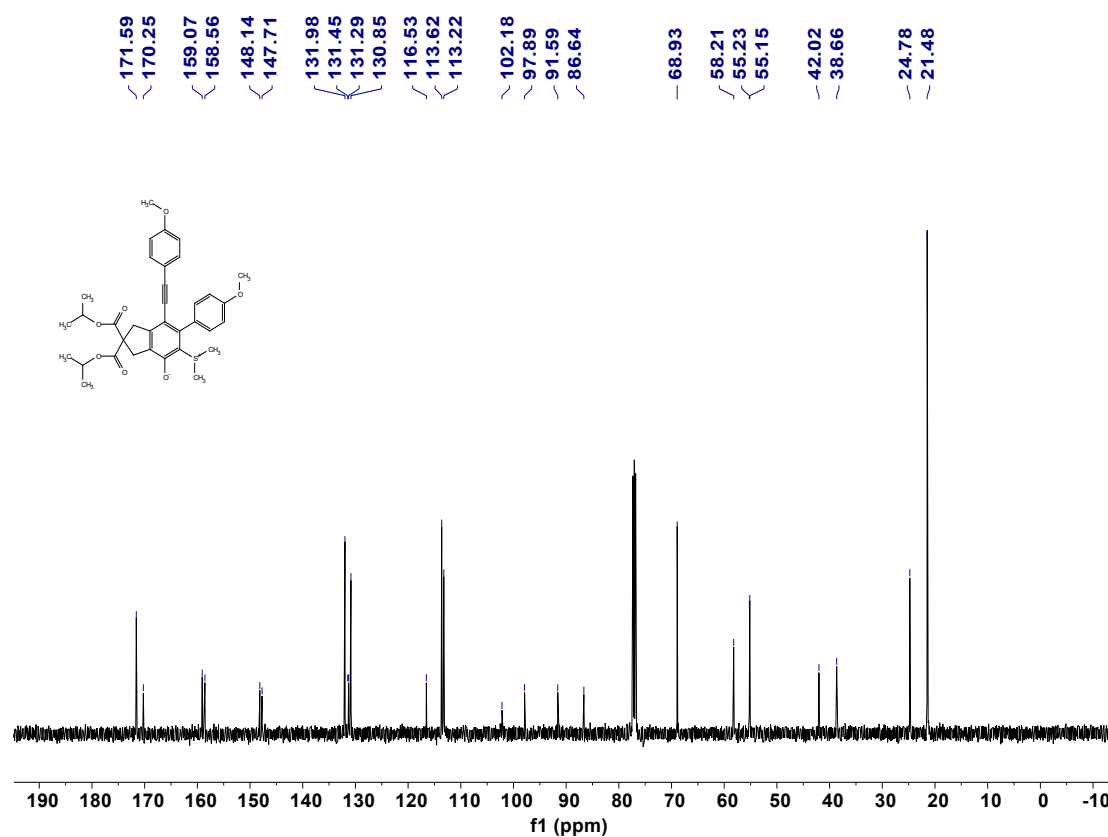


Figure 56 ¹³C NMR spectrum of **3m** (125 MHz, CDCl₃).

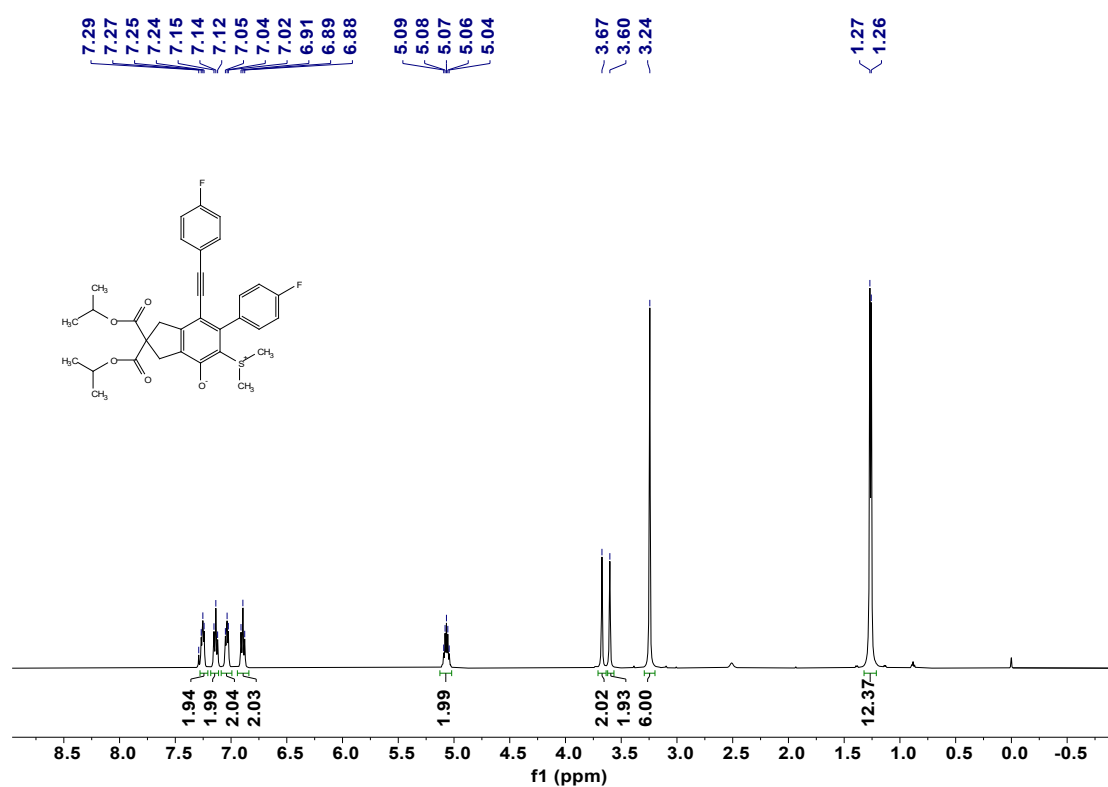


Figure 57 ¹H NMR spectrum of **3n** (500 MHz, CDCl₃).

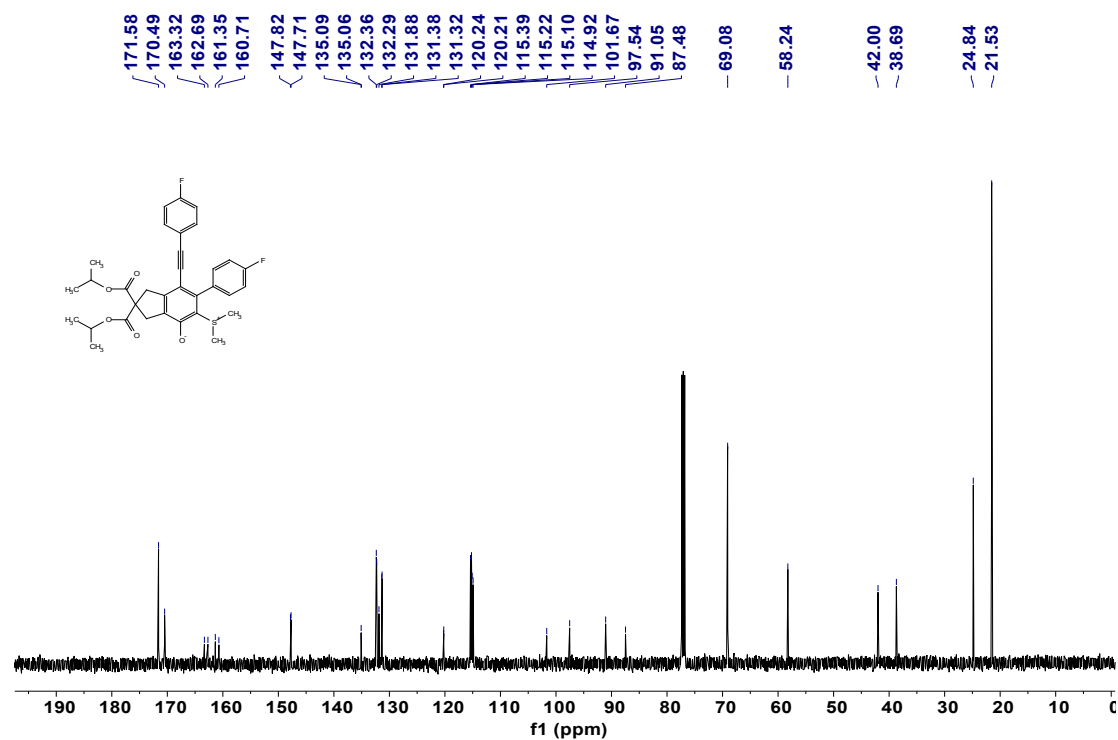


Figure 58 ¹³C NMR spectrum of **3n** (125 MHz, CDCl₃).

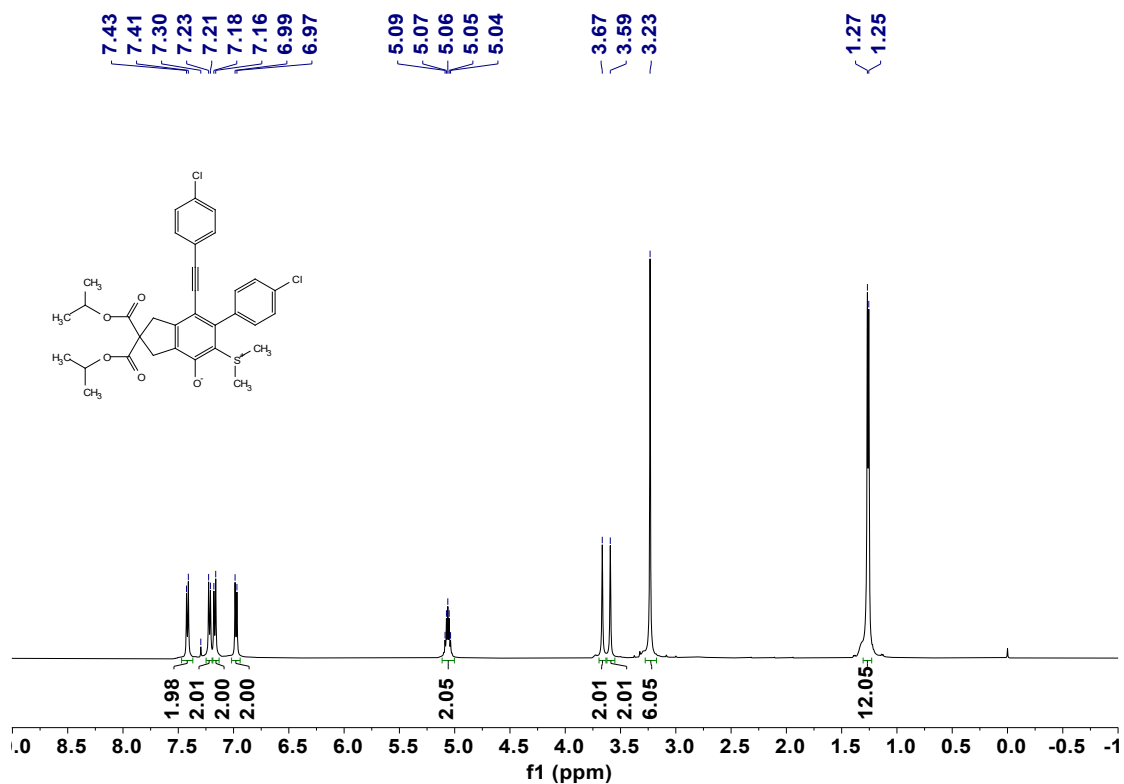


Figure 59 ¹H NMR spectrum of **3o** (500 MHz, CDCl₃).

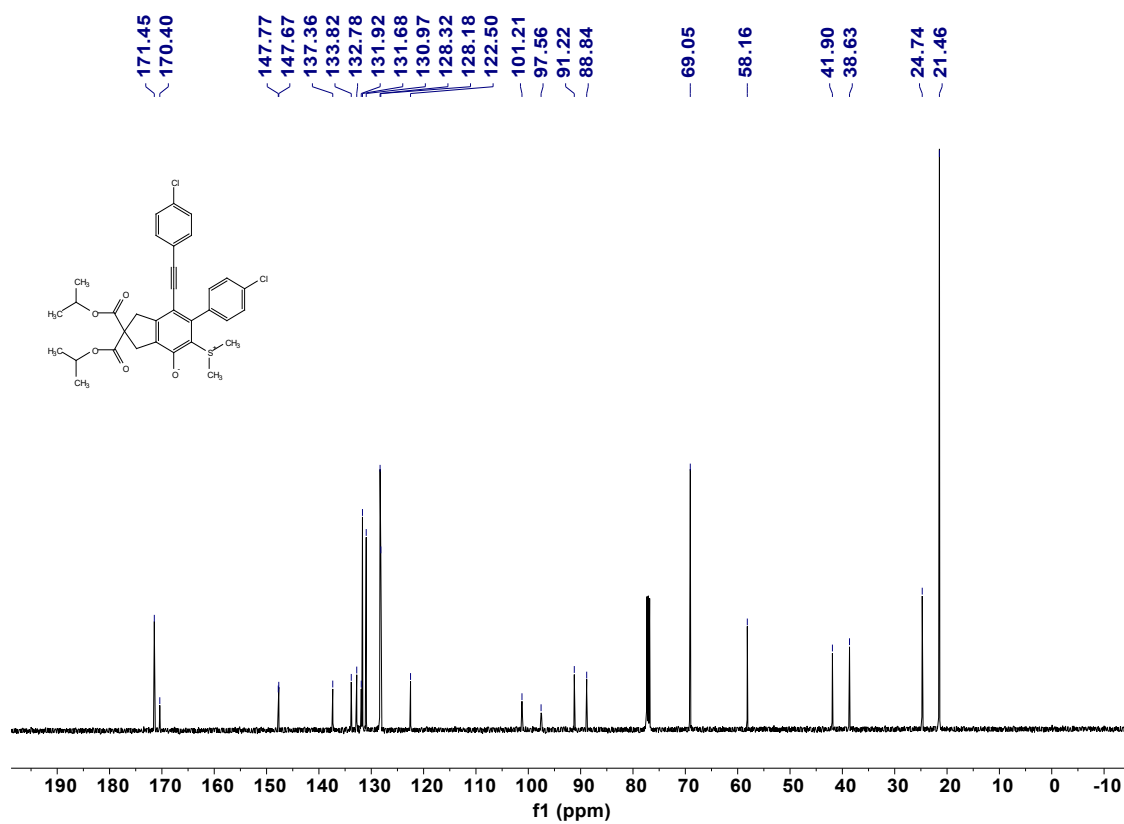


Figure 60 ¹³C NMR spectrum of **3o** (125 MHz, CDCl₃).