

Supporting Information

Brønsted Acid-Catalyzed Synthesis of Benzo[*f*]indole and Naphtho[2,3-*b*]furan Derivatives via an Intramolecular Cascade Isomerization/Cyclisation/Aromatization

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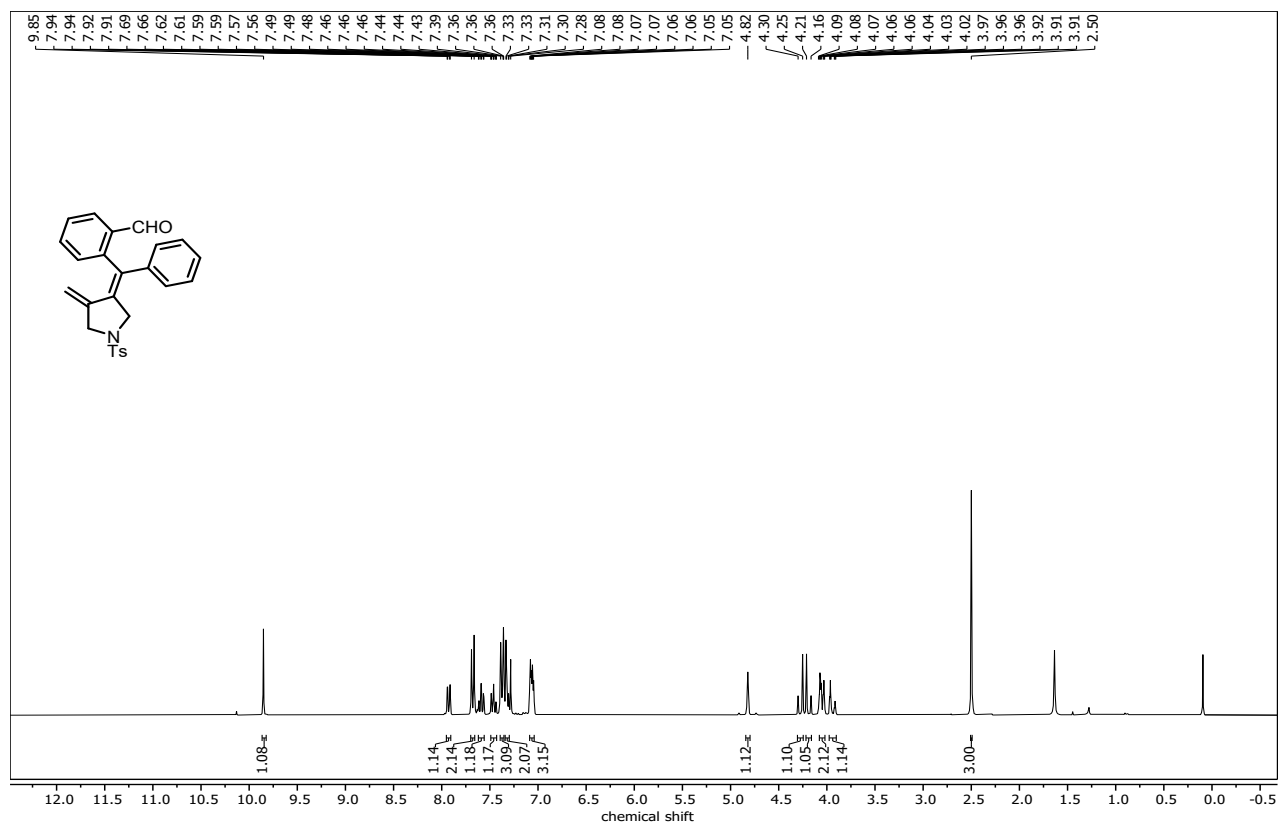
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Crystal structure determination for 4c and 7c	50- 53

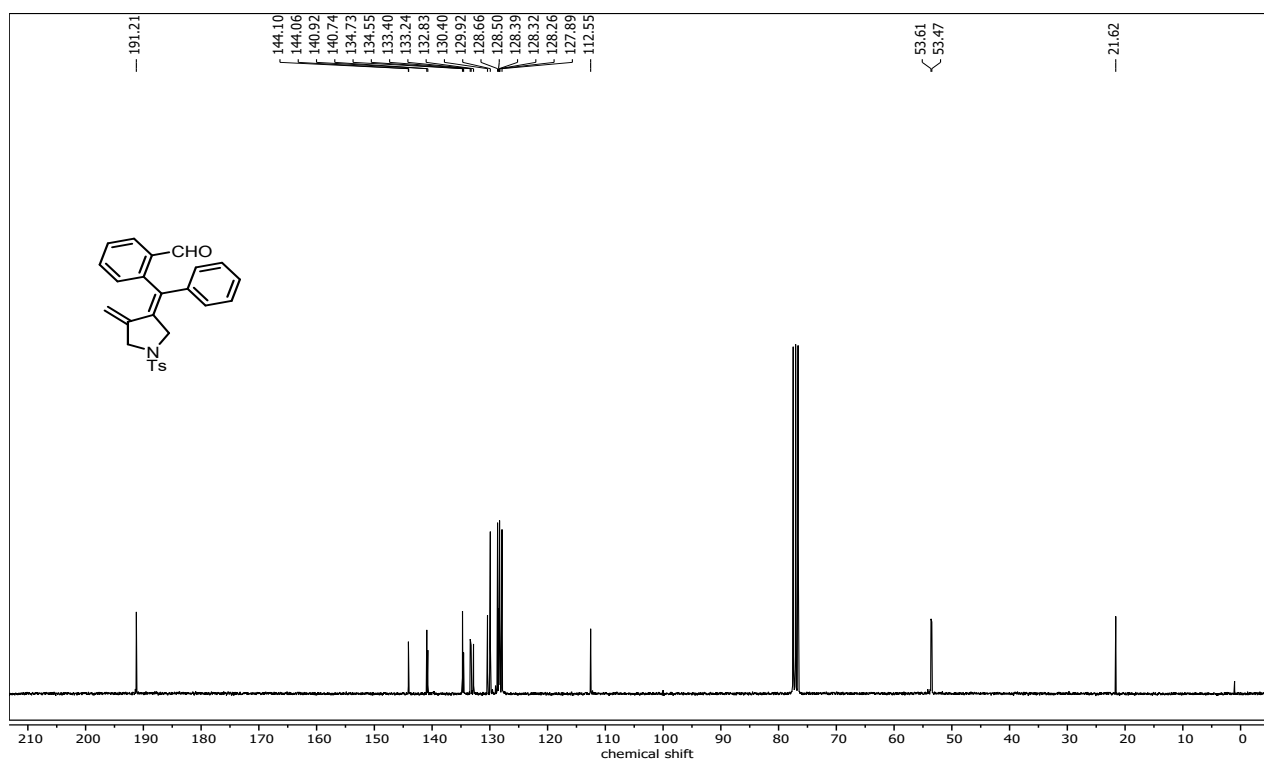
General Procedures. All ^1H NMR spectra were recorded with Bruker Avance III (300, 400) spectrometers in deuterated solvents (CDCl_3). Chemical shifts are reported in parts per million (ppm, δ) relative to tetramethylsilane (TMS), and the solvent resonances were referenced to internal standard CDCl_3 (δ 7.28 ppm). All coupling constants are absolute values and are expressed in Hz. The descriptions of the signals are reported as follows: s = singlet, d = doublet, dd = double of doublet, t = triplet, m = multiplet, and dt = doublet of triplets. ^{13}C NMR spectra were recorded with Bruker Avance III 300 (75 MHz) and 400 (100 MHz) spectrometers as solutions in CDCl_3 with complete proton decoupling. Chemical shifts are reported in parts per million (ppm, δ) and are referenced to internal standard CDCl_3 (δ = 77.16 ppm). High-resolution mass spectra were taken using a Q-ToF micro MS system by an electrospray ionization (ESI) technique. Crystallographic data were collected at room temperature on a Bruker D8 quest microfocus single crystal XRD machine. The routine monitoring of the reaction was performed with silica gel coated glass slides (Merck, silica gel G for TLC) and precoated Al plates which were analyzed with iodine and UV light, respectively. Solvents, reagents, and chemicals were purchased from Aldrich, Alfa Aesar, Merck, SRL, Spectrochem, and Process Chemicals. The final products were purified by column chromatography on Merck silica gel (60–120 mesh). All reactions involving moisture-sensitive reactants were executed with oven-dried glass ware.

NMR [^1H , $^{13}\text{C}\{^1\text{H}\}$, ^{19}F] spectra of synthesized products:

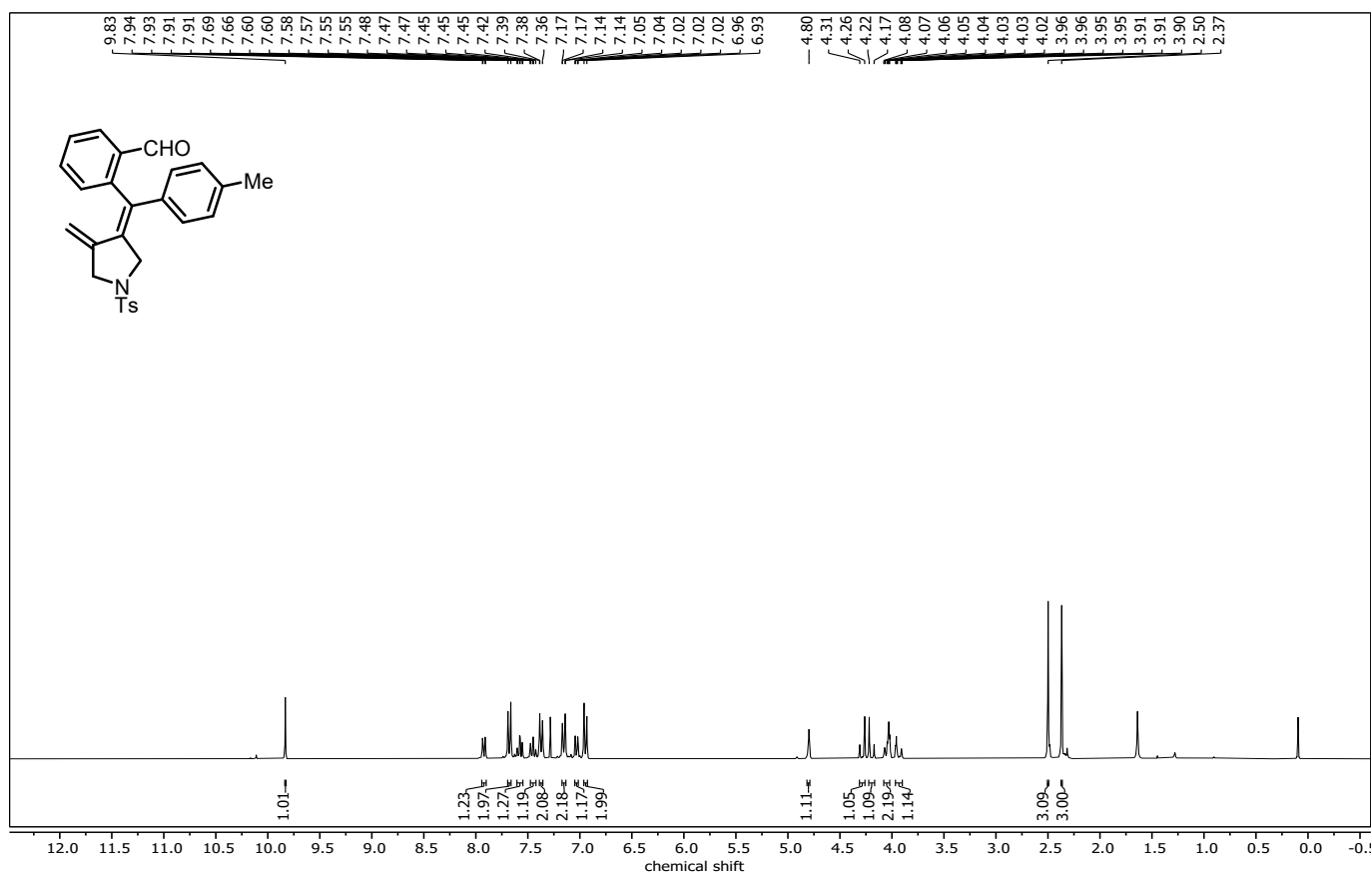
^1H NMR (400 MHz, CDCl_3) Spectrum of 3a



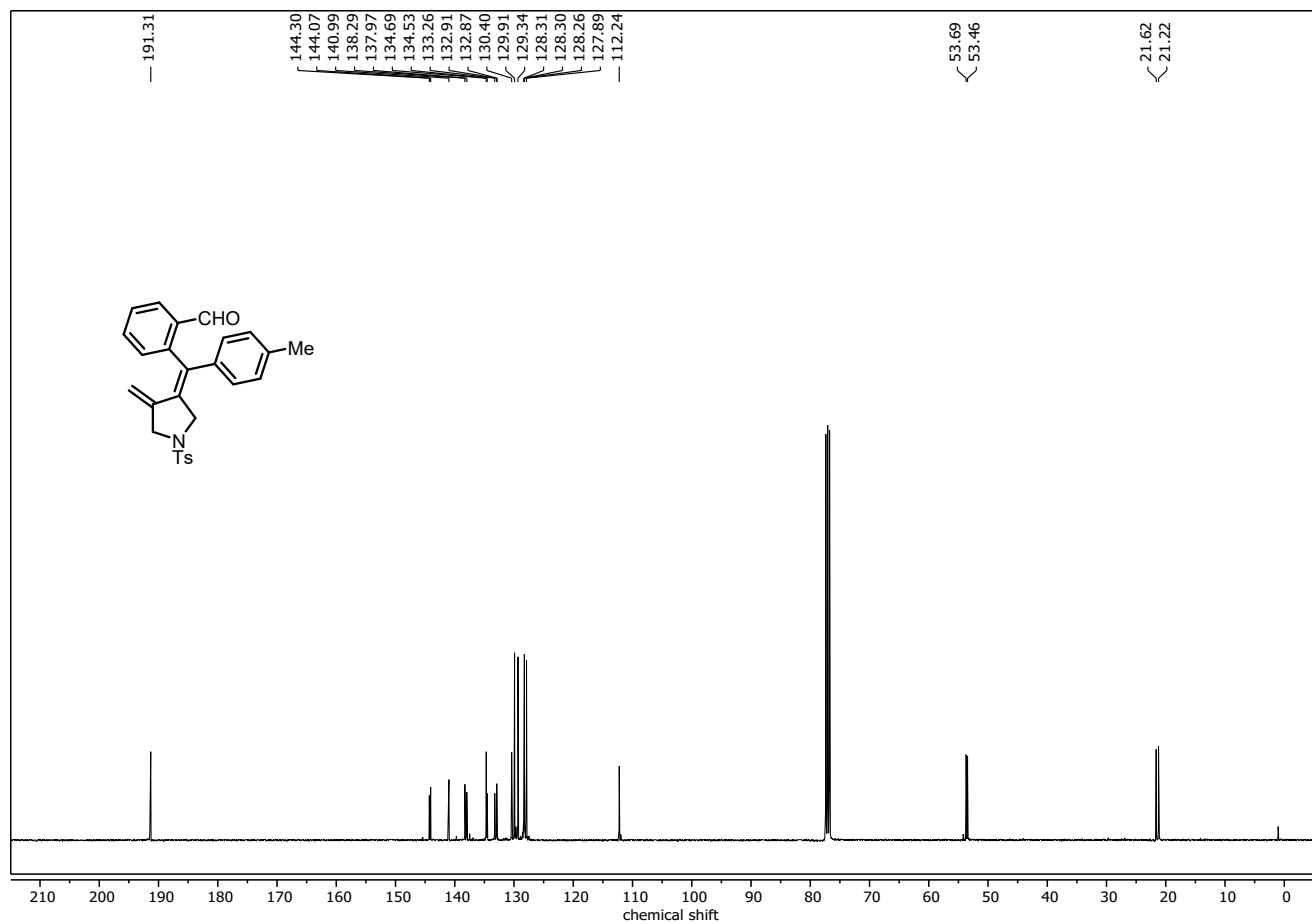
$^{13}\text{C}\{^1\text{H}\}$ (75 MHz, CDCl_3) NMR Spectrum of 3a.



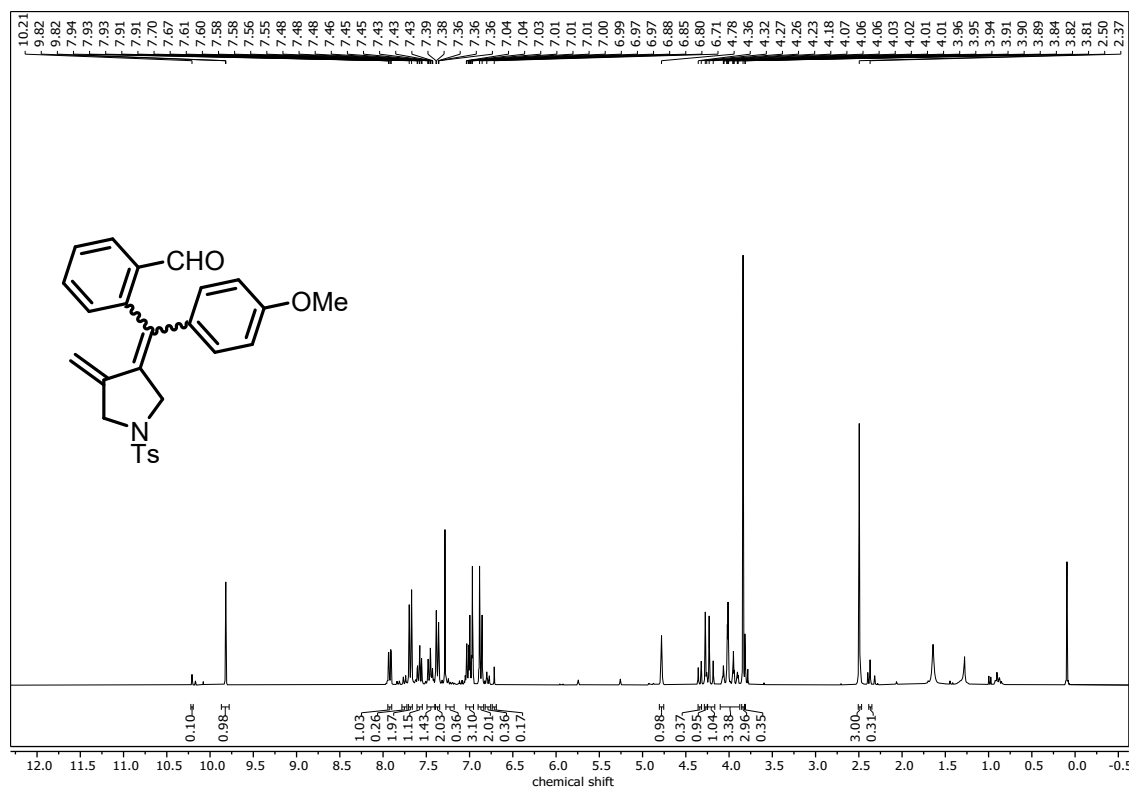
^1H NMR (400 MHz, CDCl_3) Spectrum of 3b.



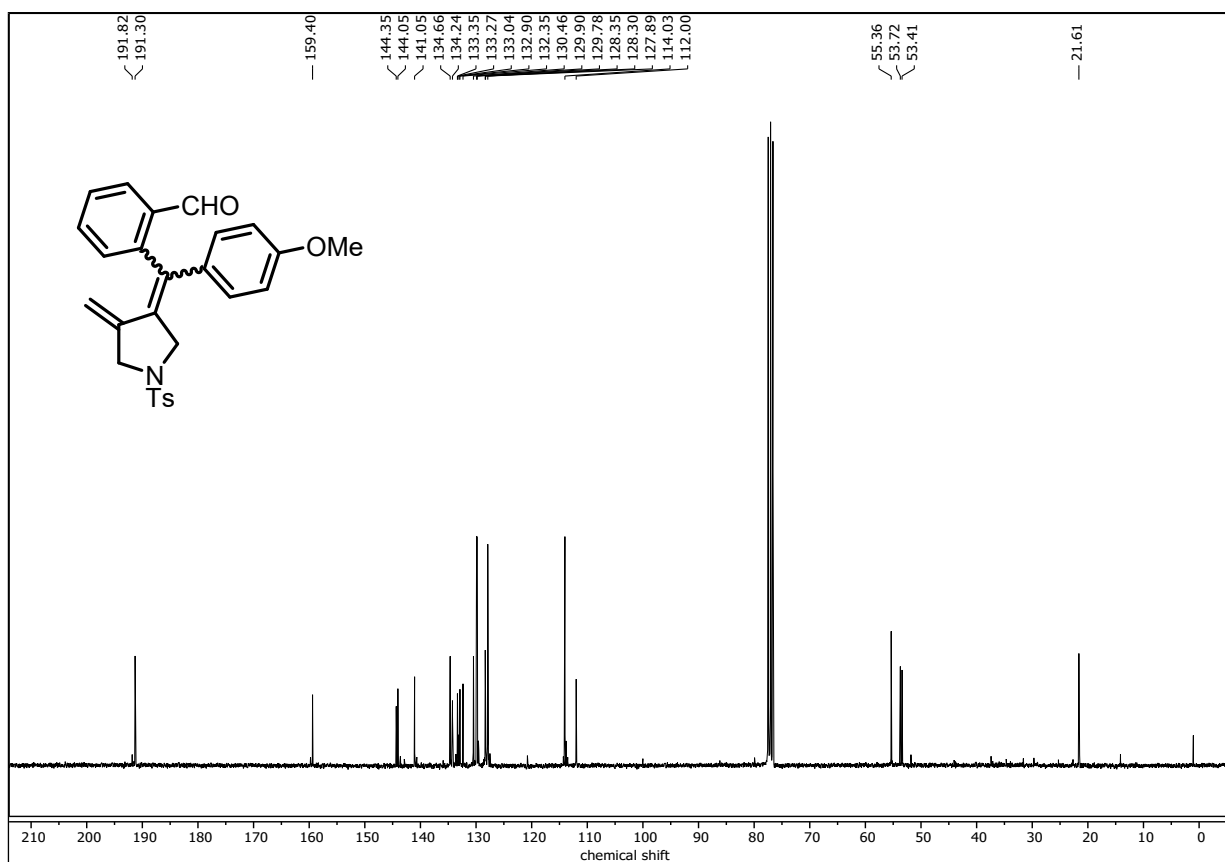
$^{13}\text{C}\{^1\text{H}\}$ (101 MHz, CDCl_3) NMR Spectrum of 3b.



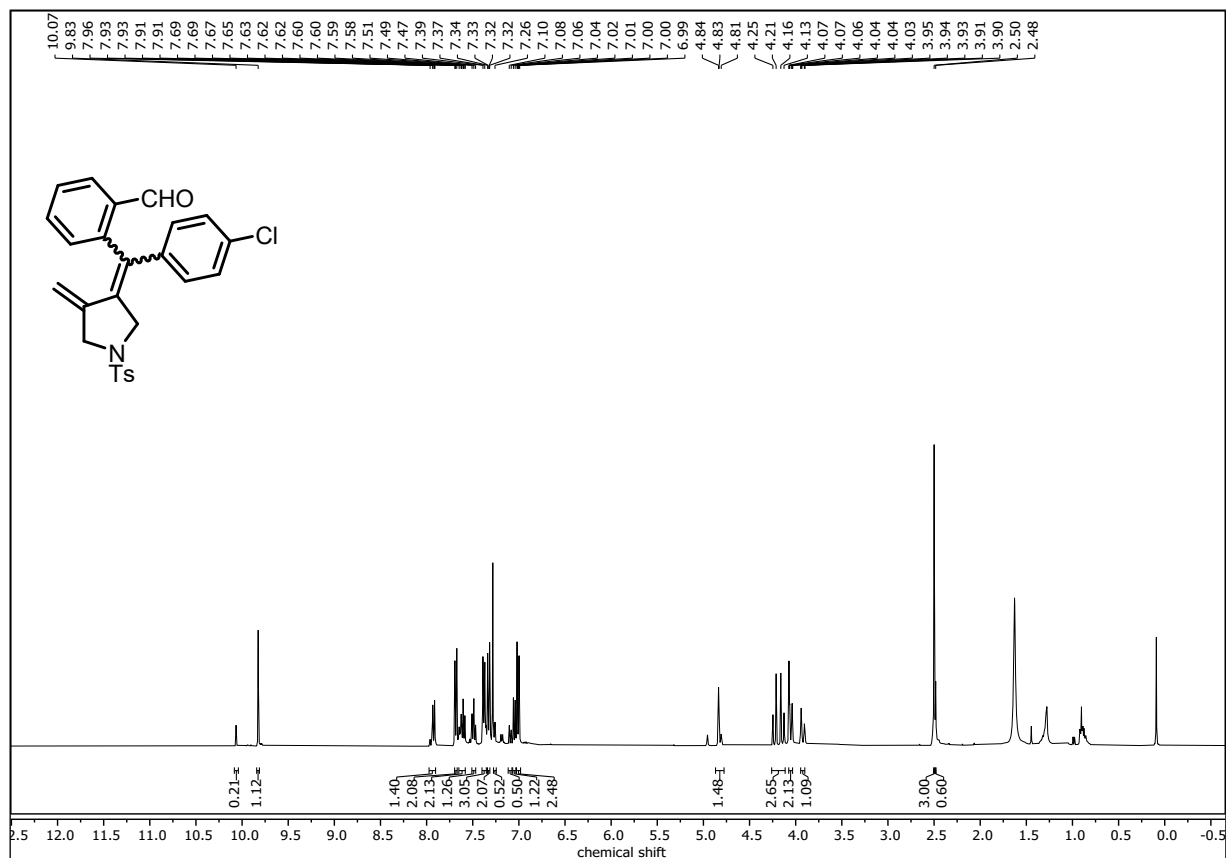
¹H NMR (400 MHz, CDCl₃) Spectrum of 3c.



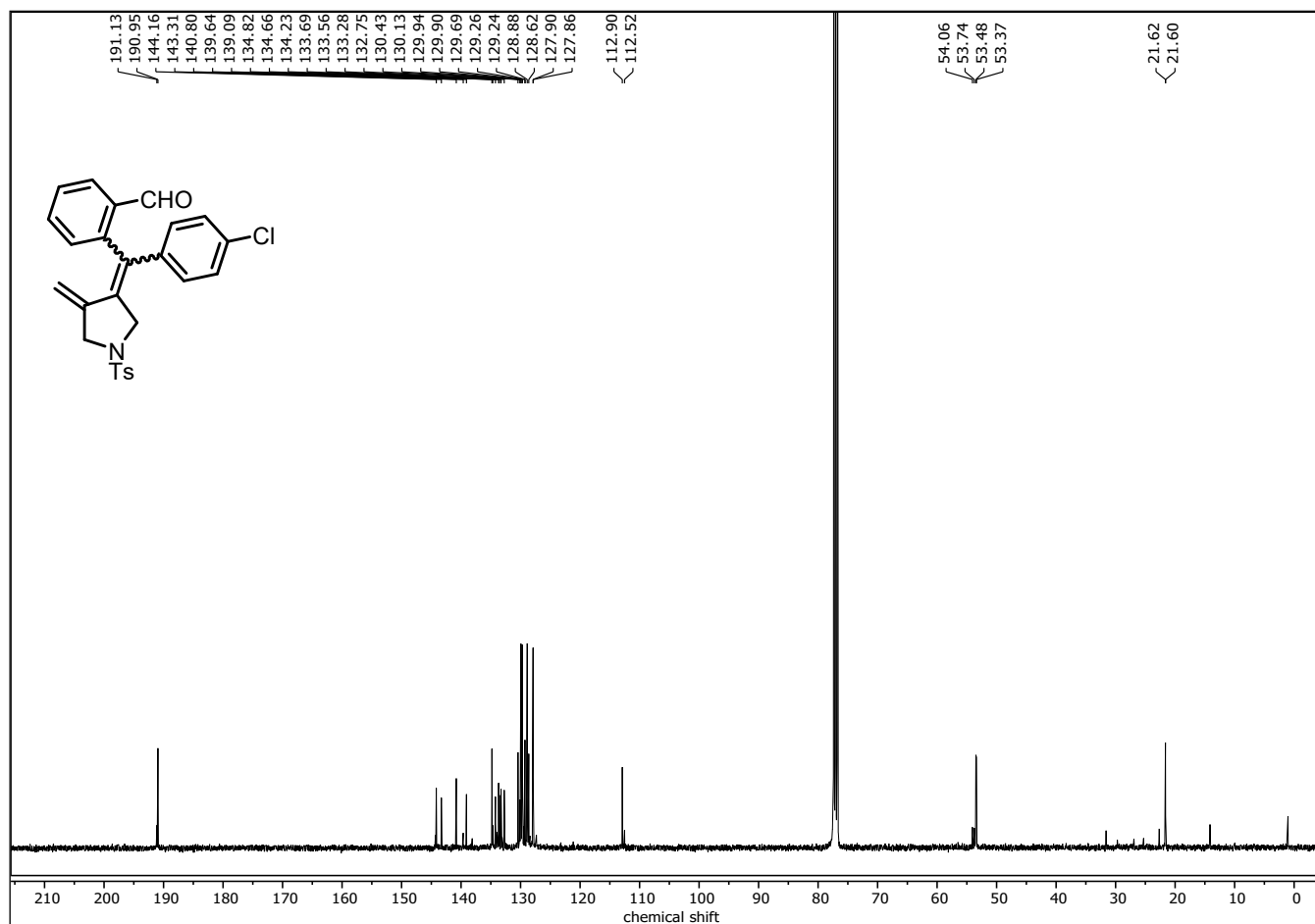
¹³C{¹H} (101 MHz, CDCl₃) NMR Spectrum of 3c.



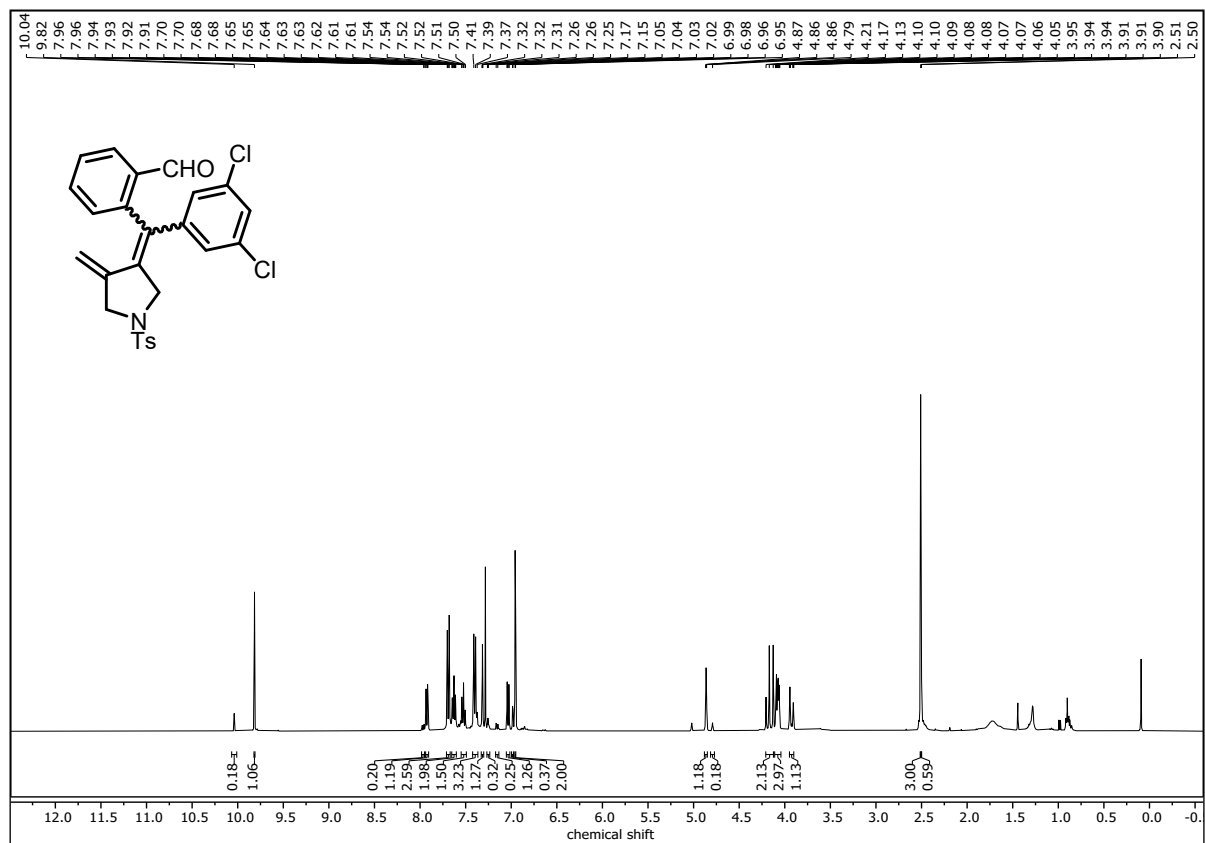
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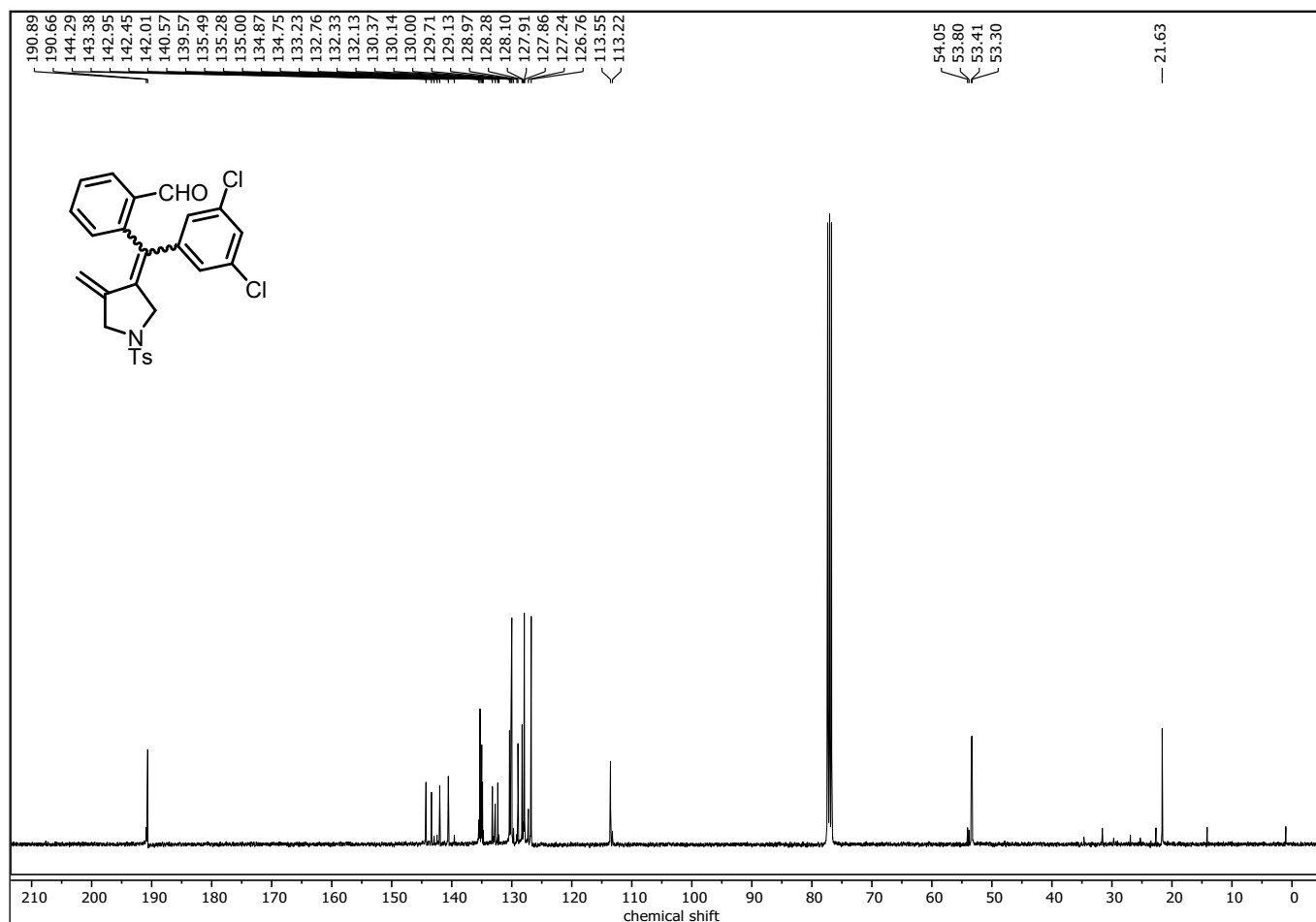
¹³C{¹H} (101 MHz, CDCl₃) NMR Spectrum of 3d.



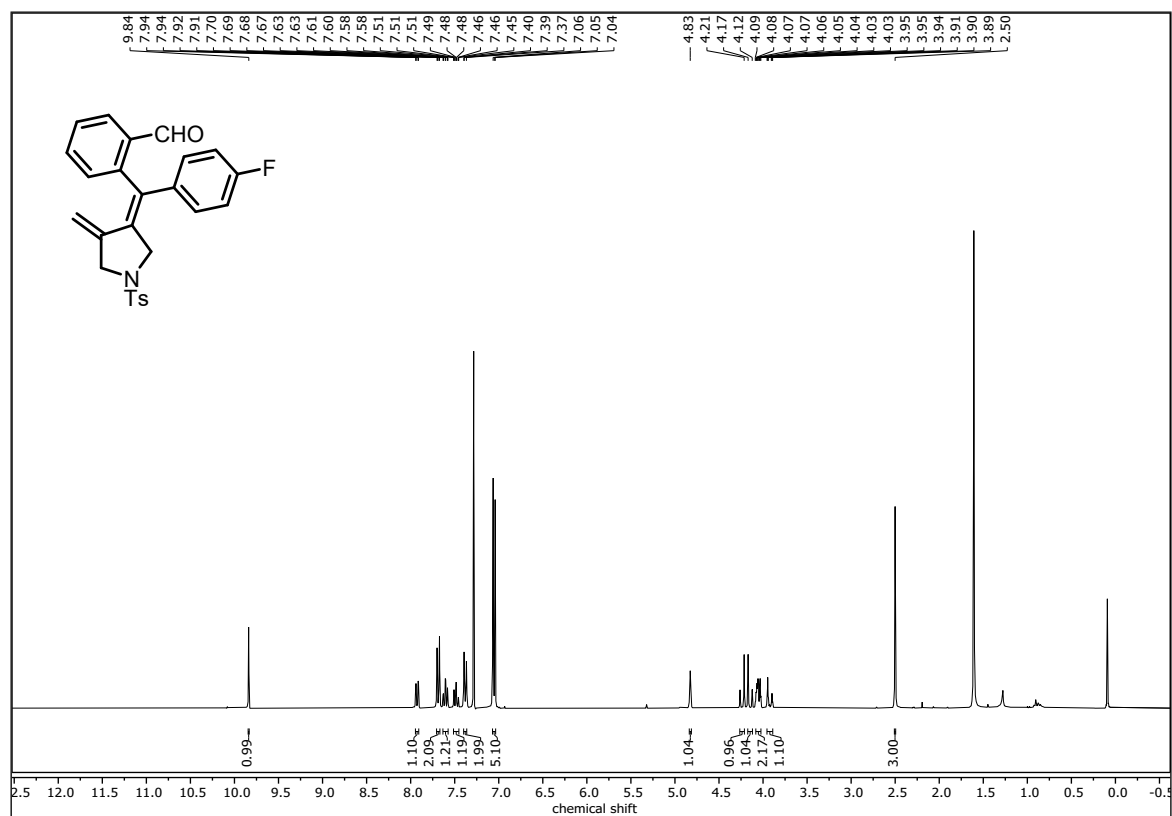
^1H NMR (400 MHz, CDCl_3) Spectrum of 3e.



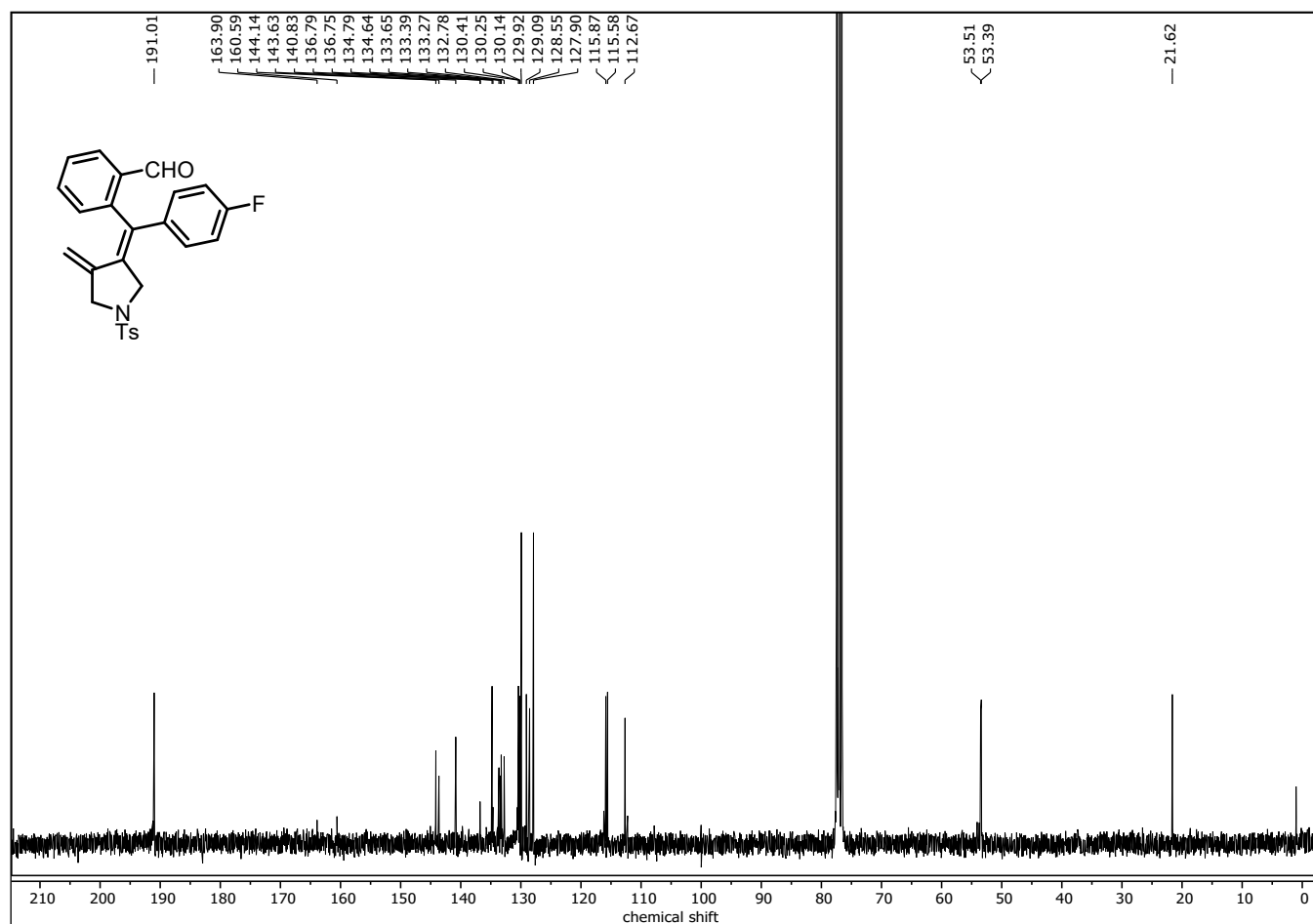
$^{13}\text{C}\{^1\text{H}\}$ (101 MHz, CDCl_3) NMR Spectrum of 3e.



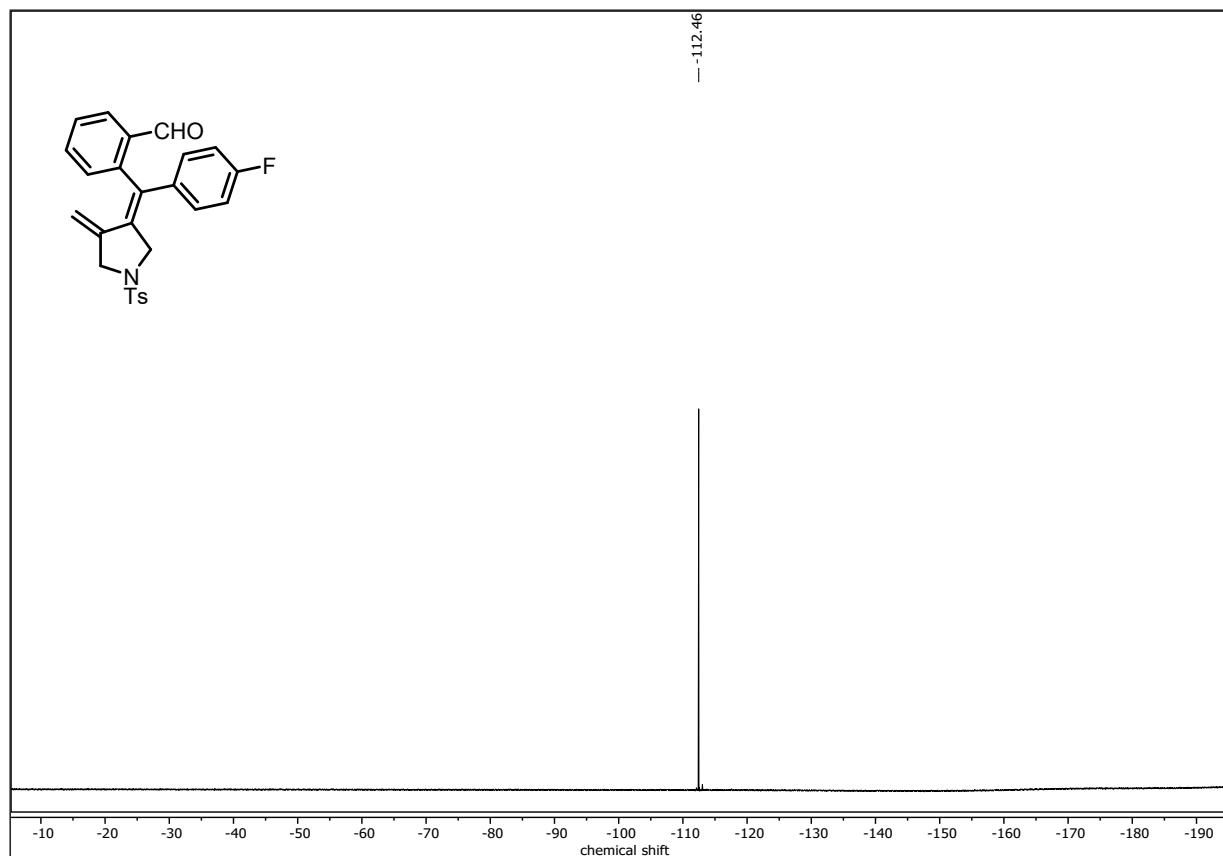
^1H NMR (300 MHz, CDCl_3) Spectrum of 3f.



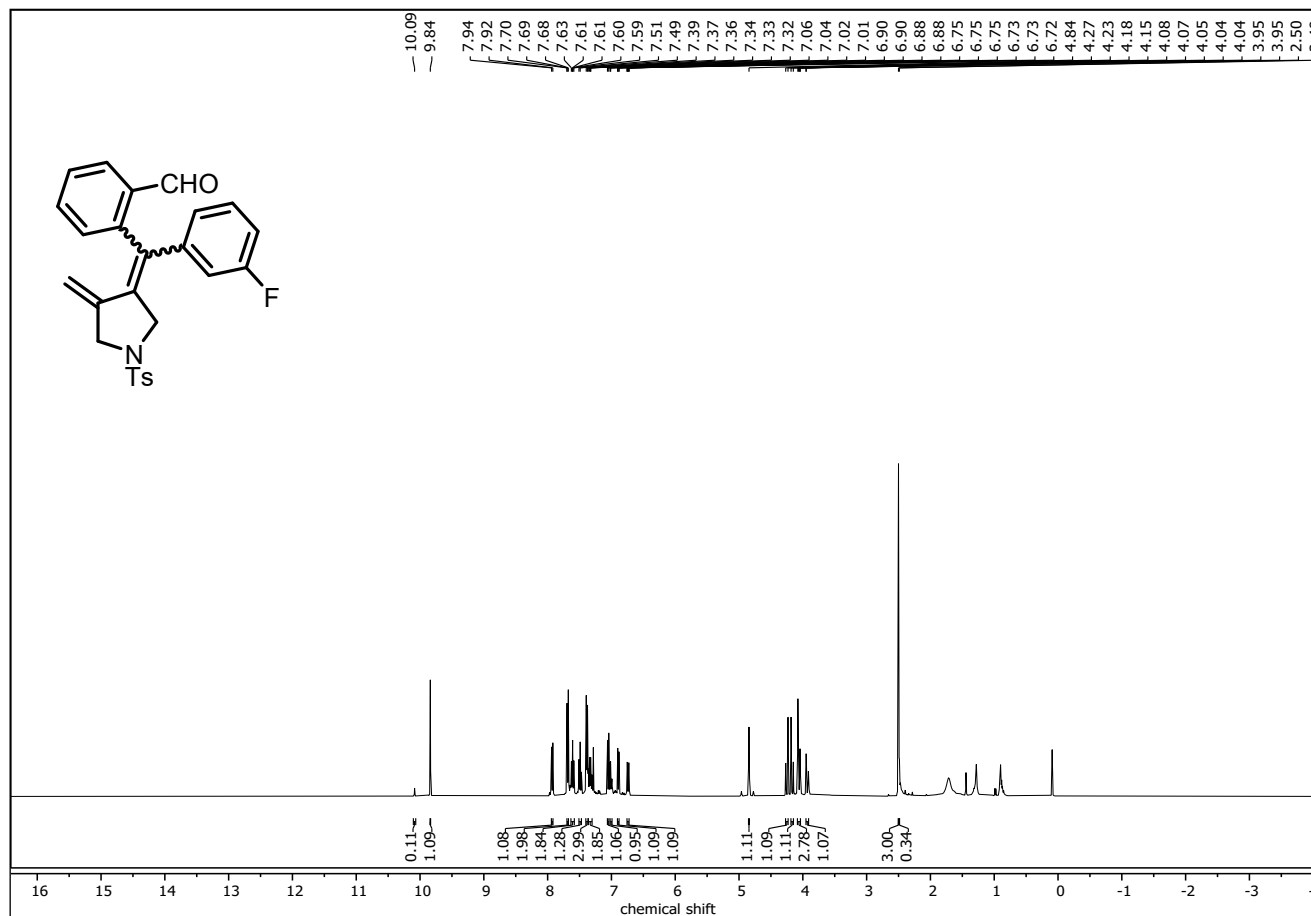
$^{13}\text{C}\{^1\text{H}\}$ (75 MHz, CDCl_3) NMR Spectrum of 3f.



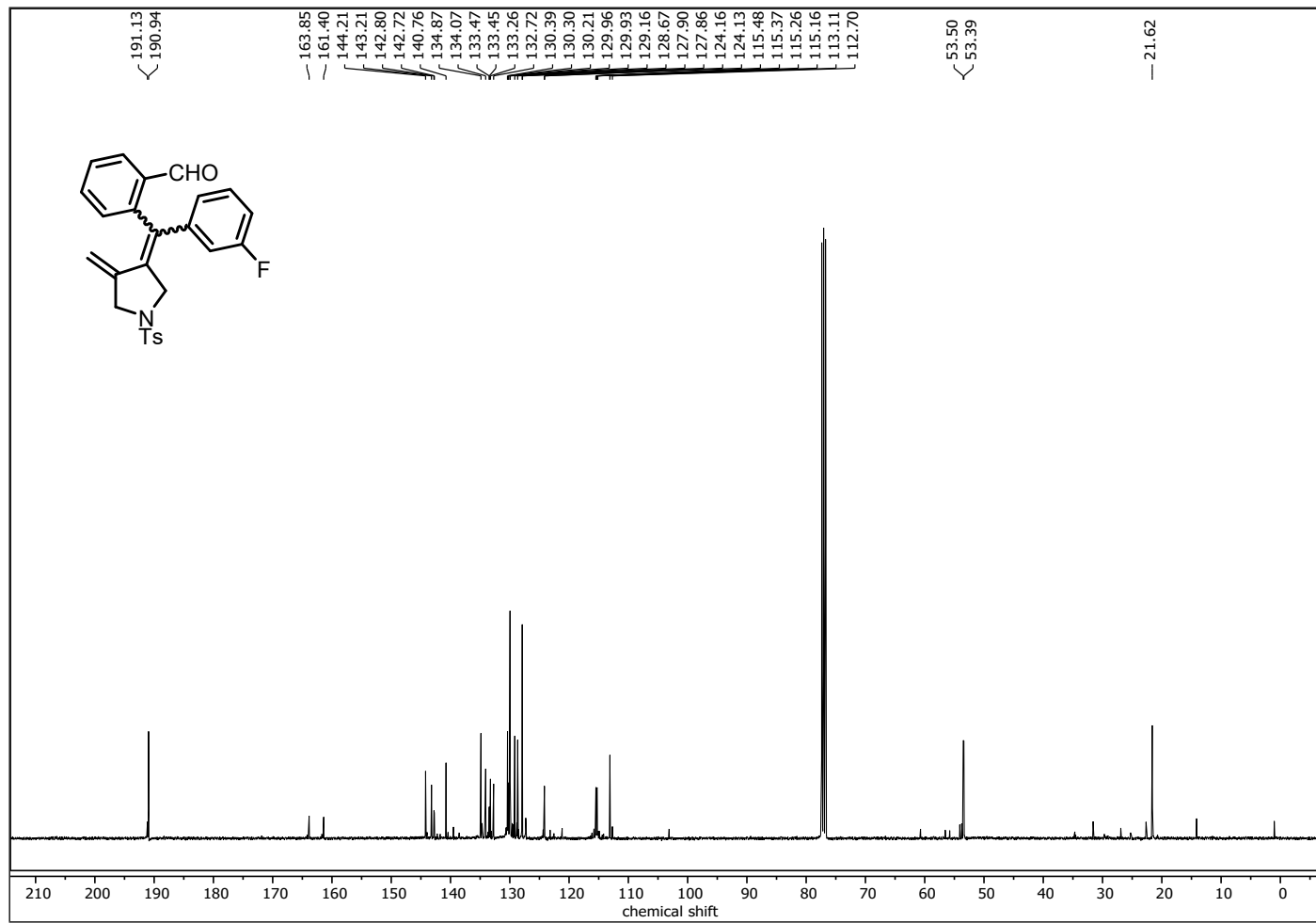
¹⁹F NMR (282 MHz, CDCl₃) Spectrum of 3f.



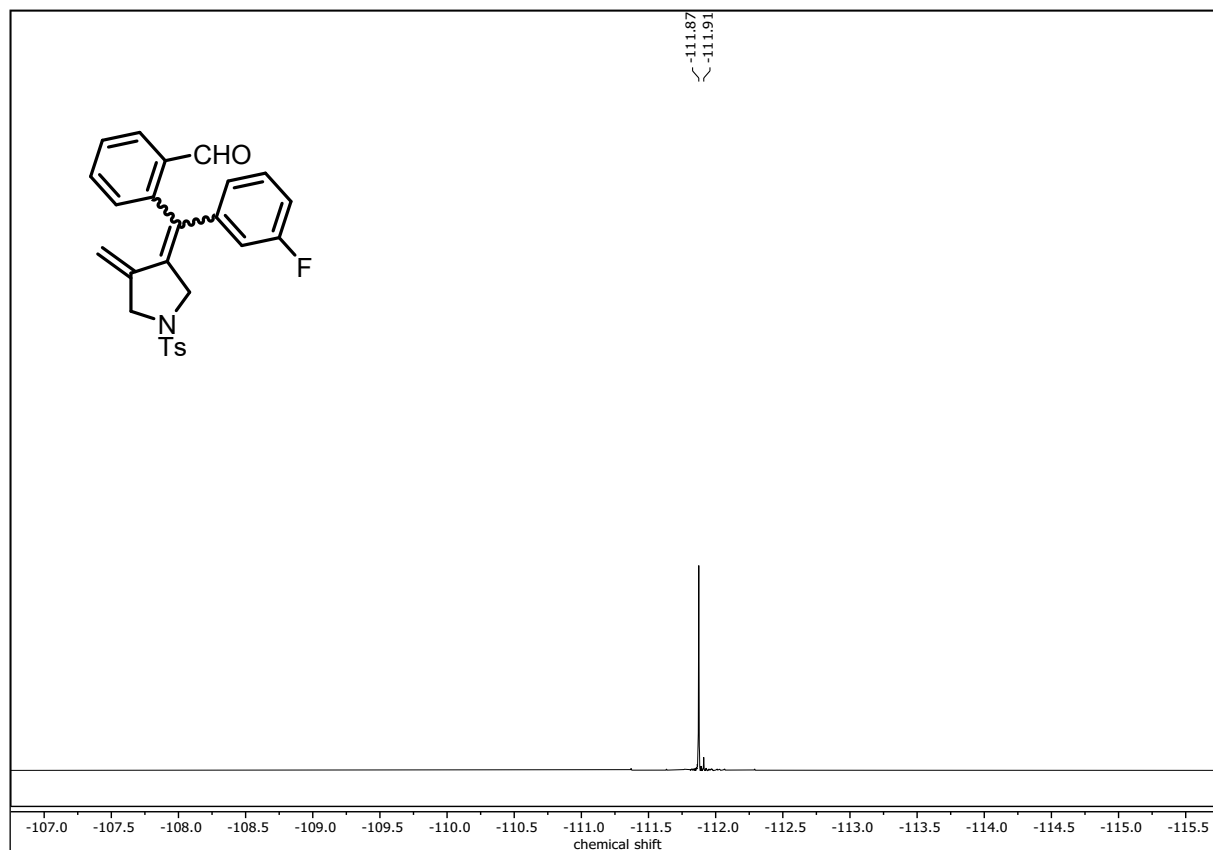
¹H NMR (400 MHz, CDCl₃) Spectrum of 3g.



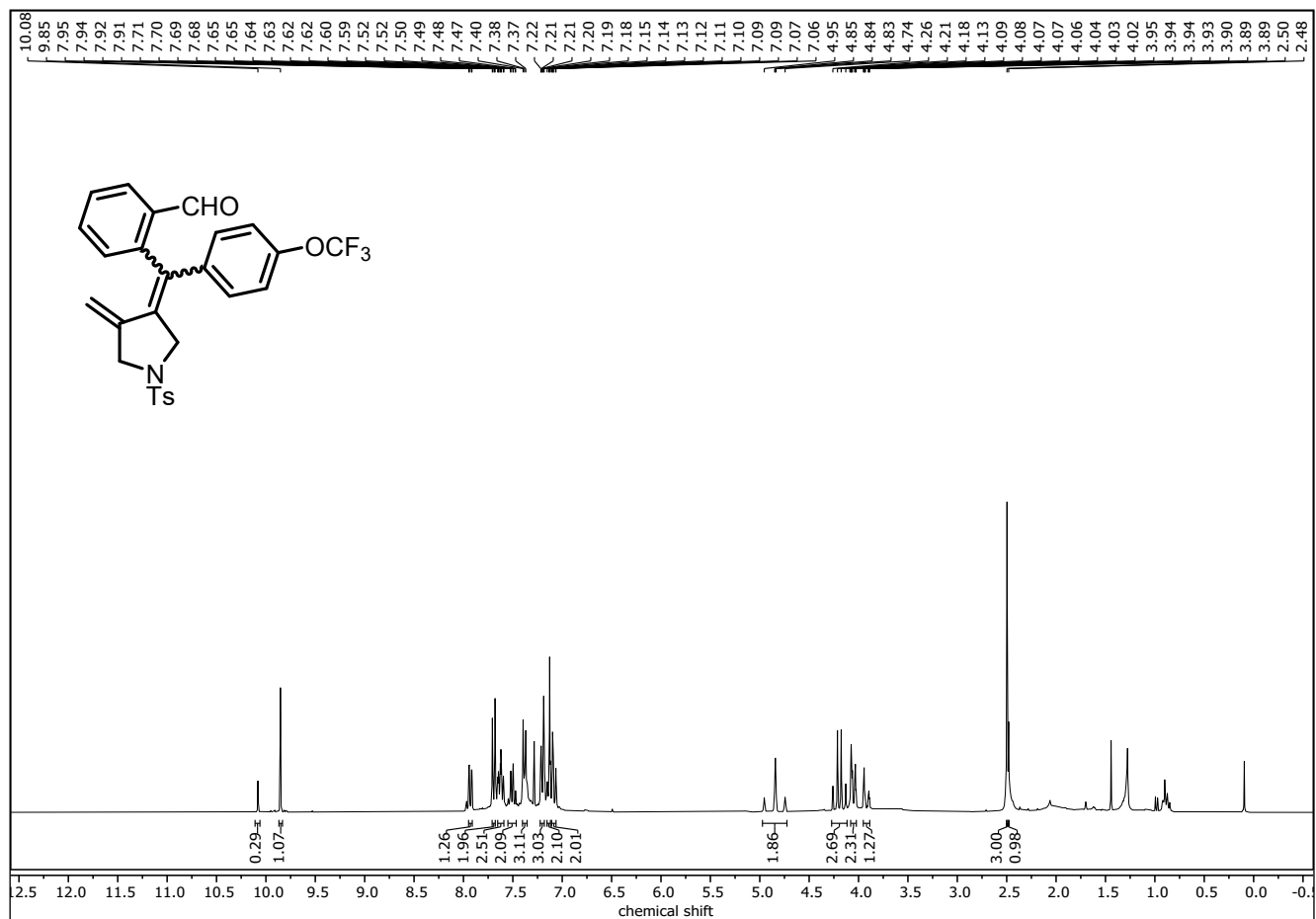
$^{13}\text{C}\{^1\text{H}\}$ (101 MHz, CDCl_3) NMR Spectrum of 3g.



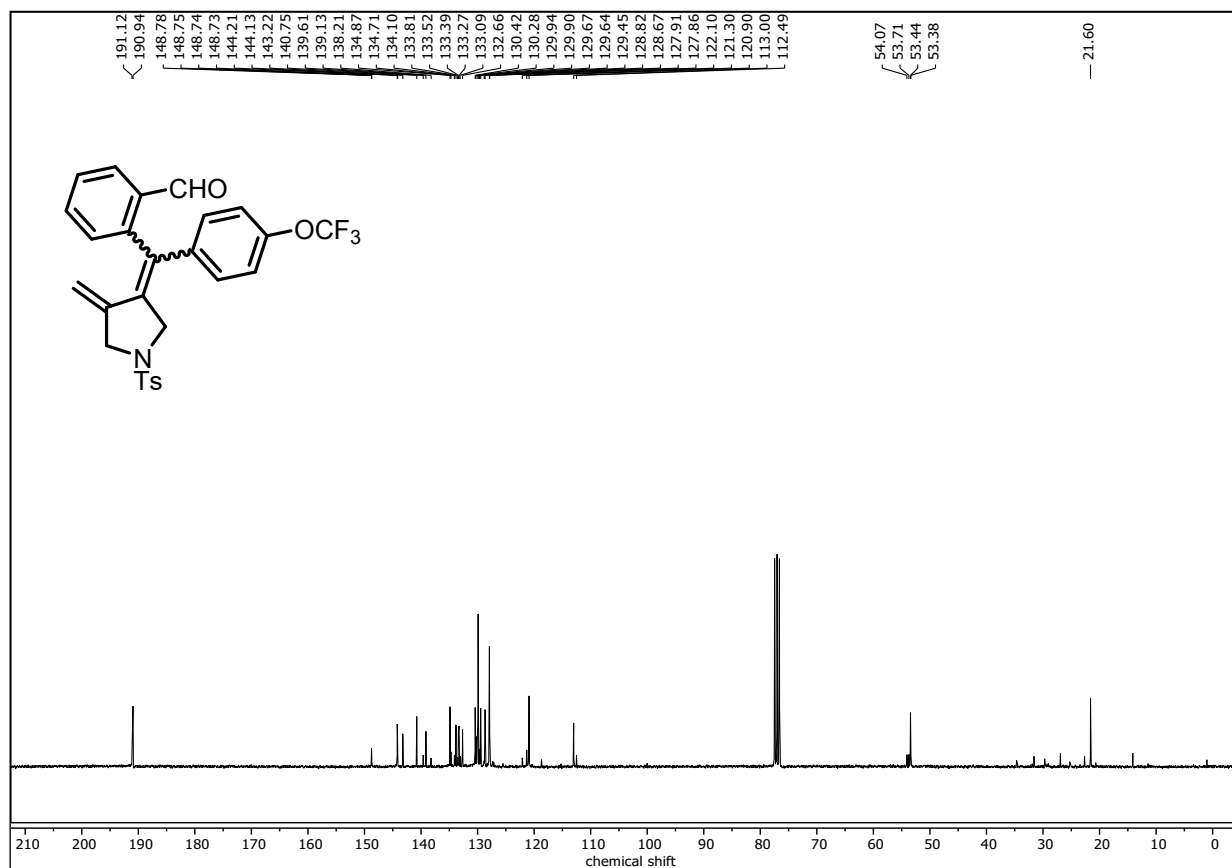
^{19}F NMR (377 MHz, CDCl_3) Spectrum of 3g.



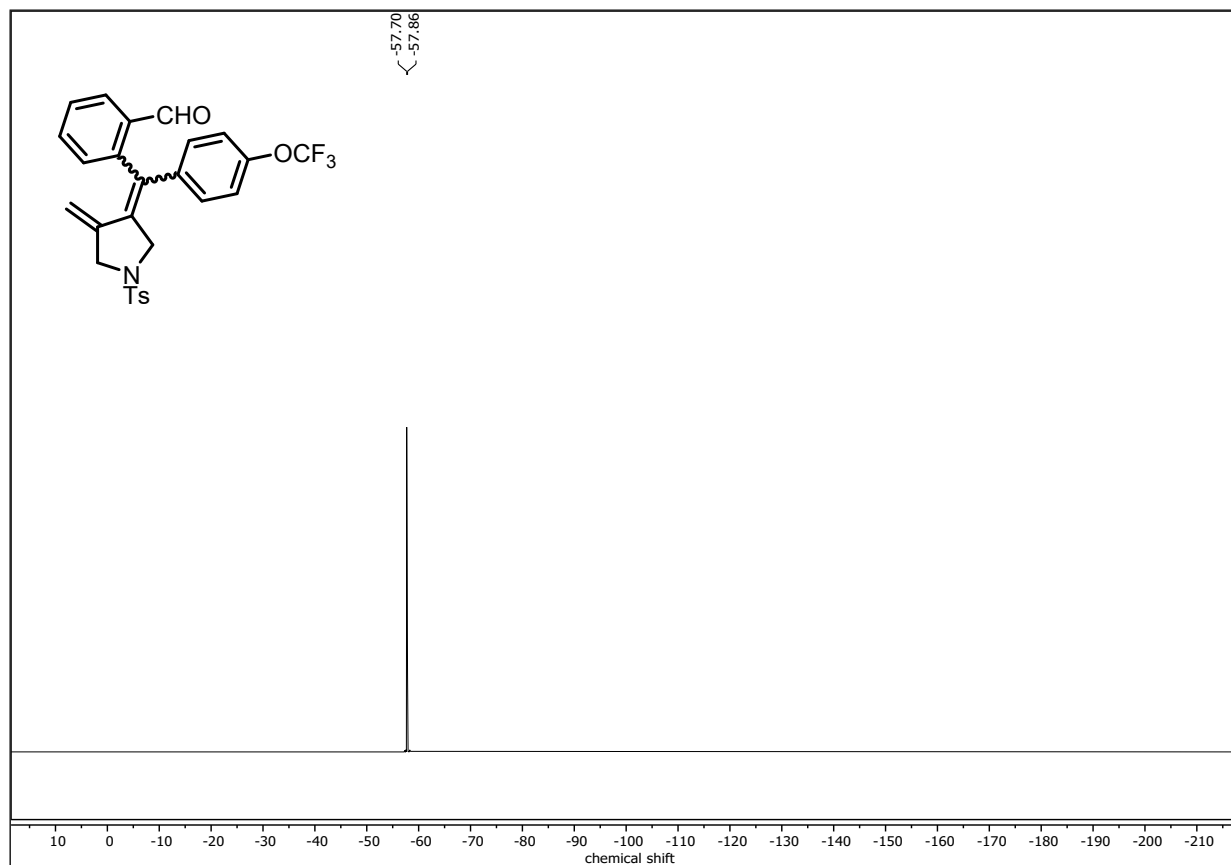
¹H NMR (300 MHz, CDCl₃) Spectrum of 3h.



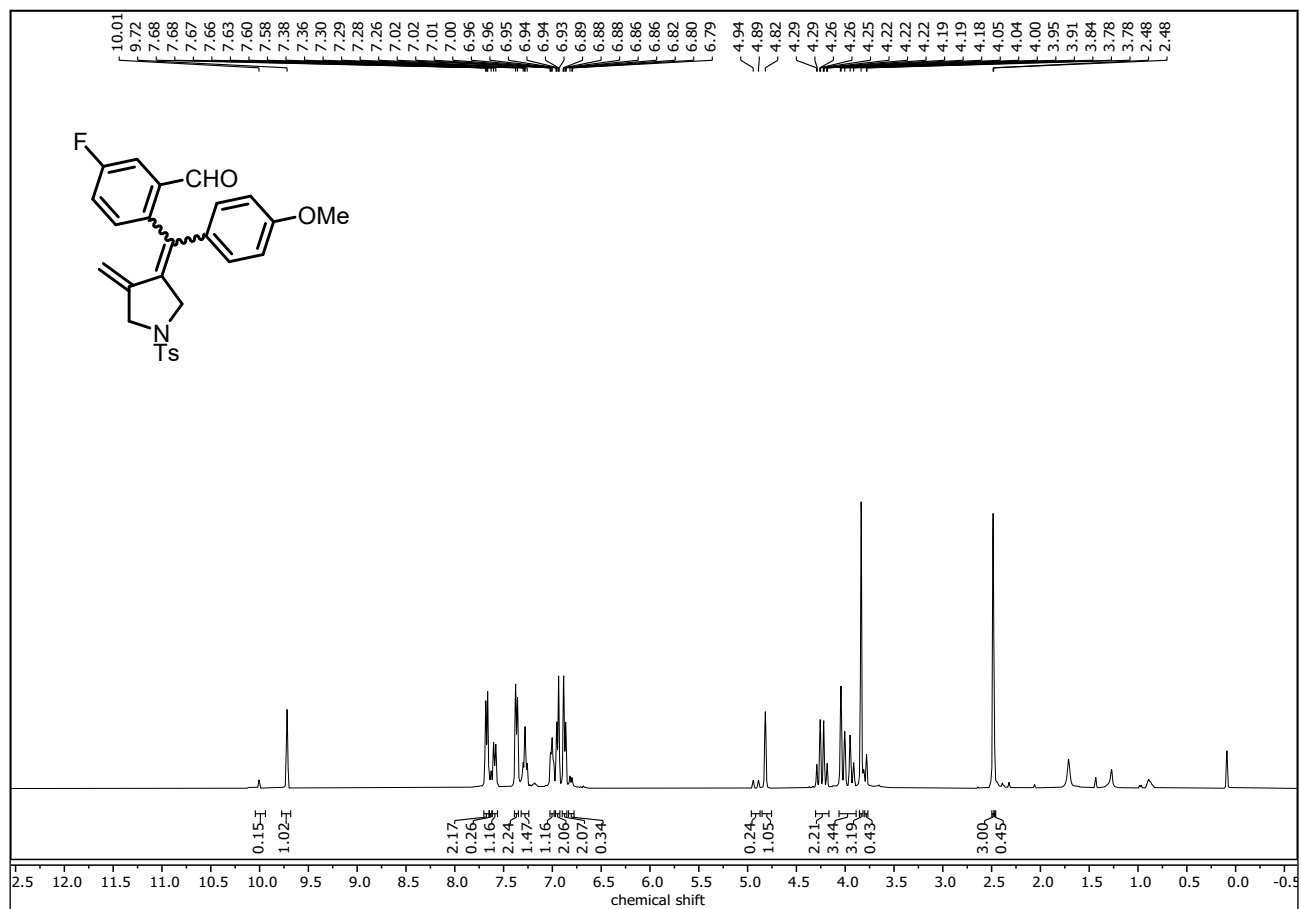
¹³C{¹H} (75 MHz, CDCl₃) NMR Spectrum of 3h.



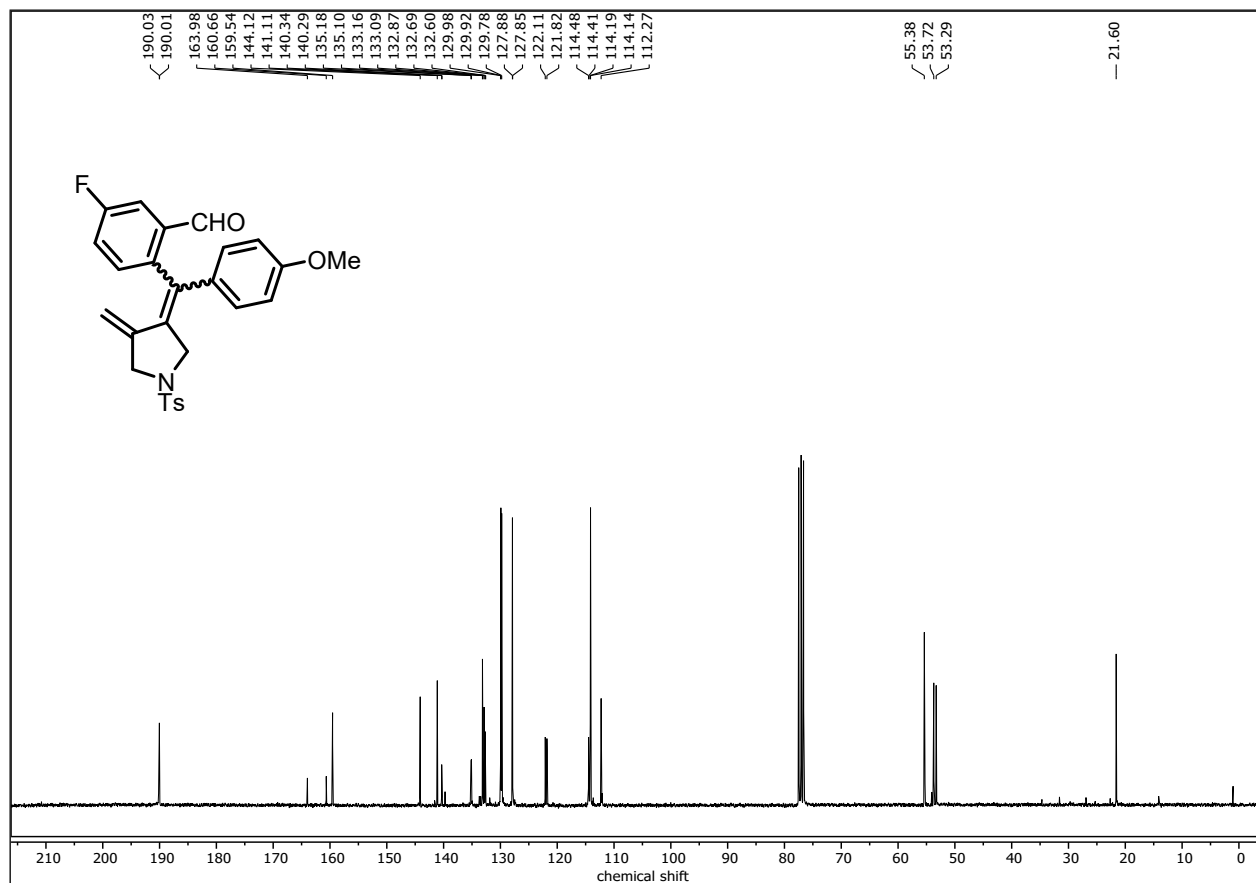
¹⁹F NMR (282 MHz, CDCl₃) Spectrum of 3h.



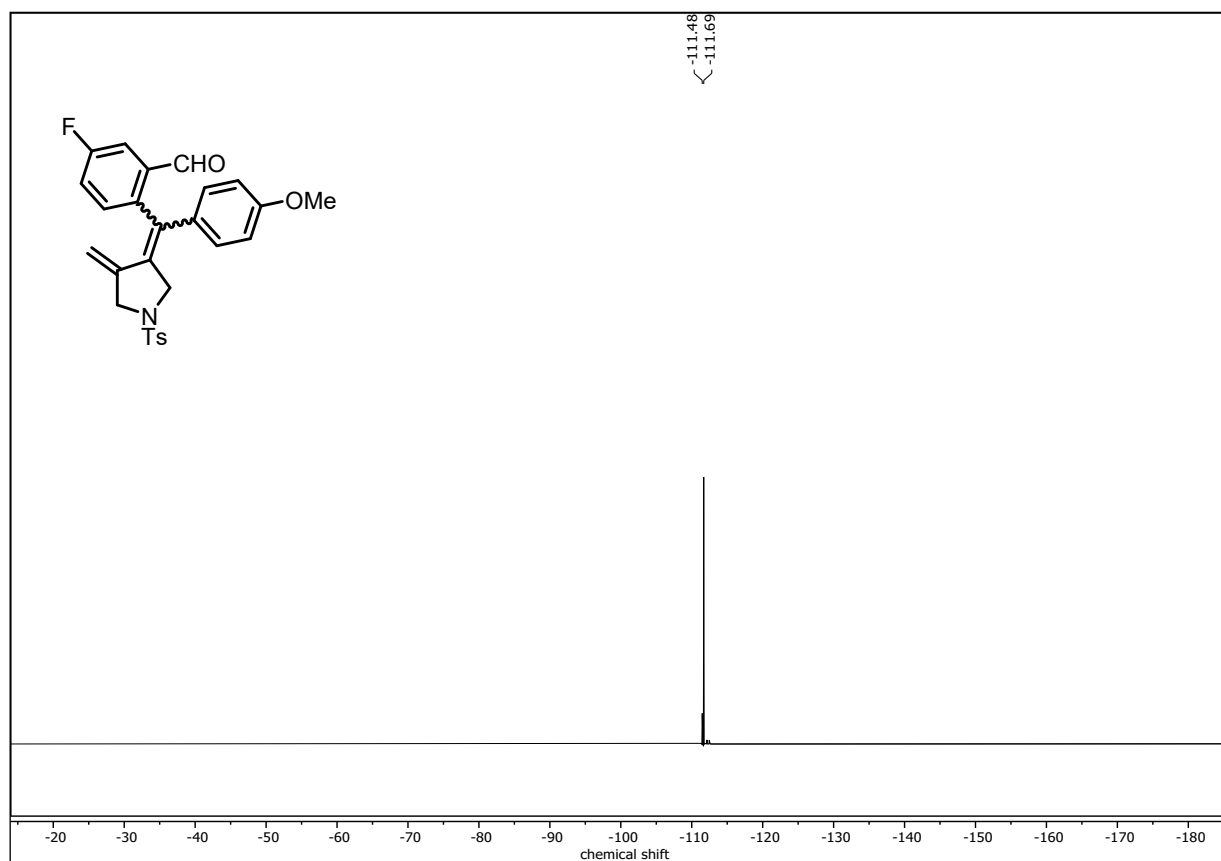
¹H NMR (400 MHz, CDCl₃) Spectrum of 3i.



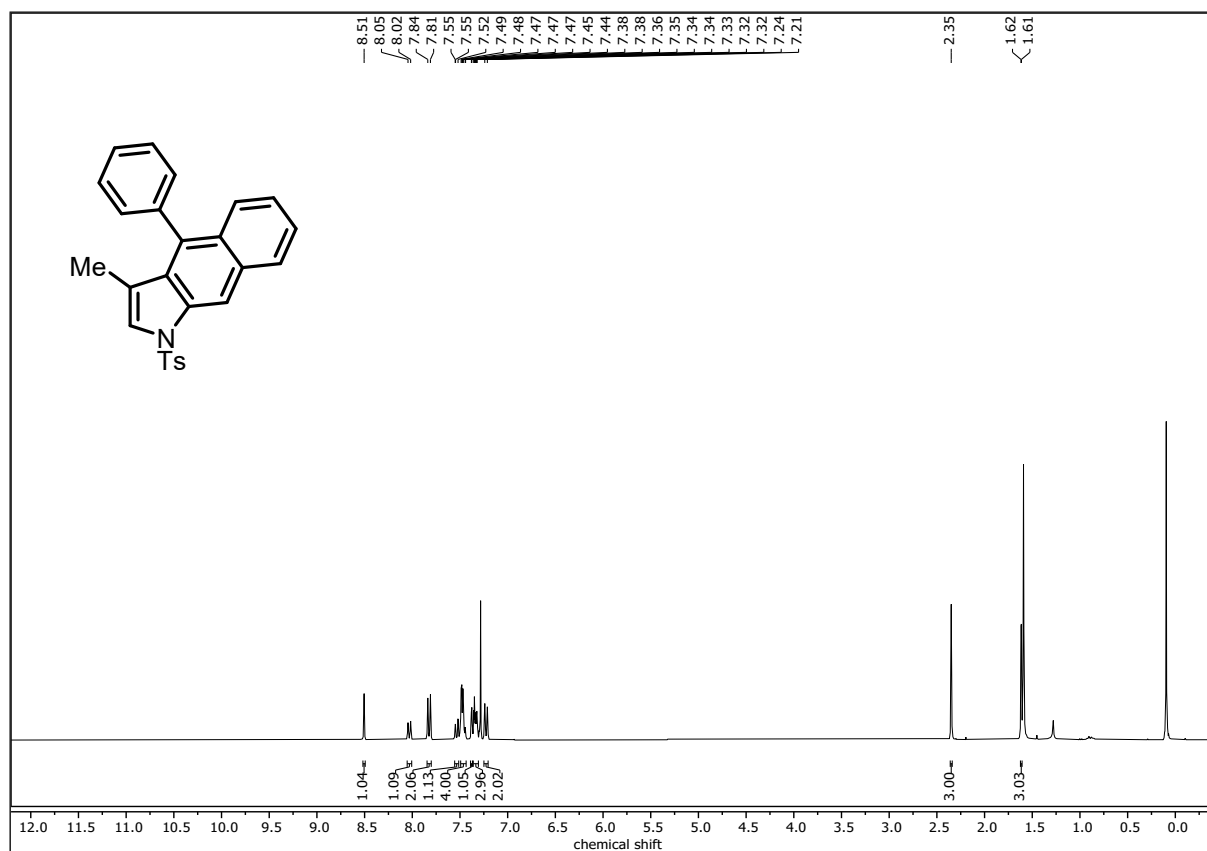
$^{13}\text{C}\{^1\text{H}\}$ (75 MHz, CDCl_3) NMR Spectrum of 3i.



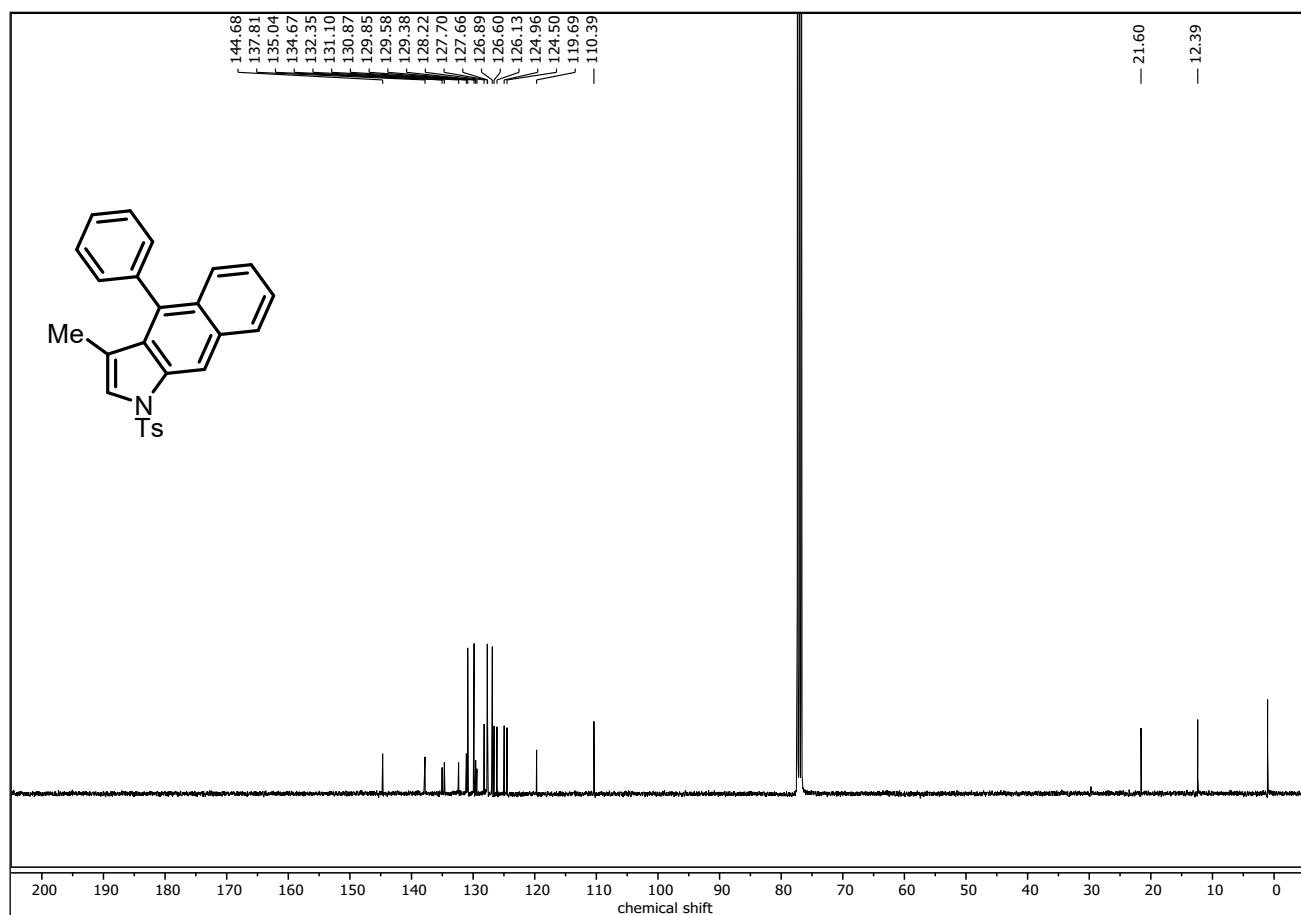
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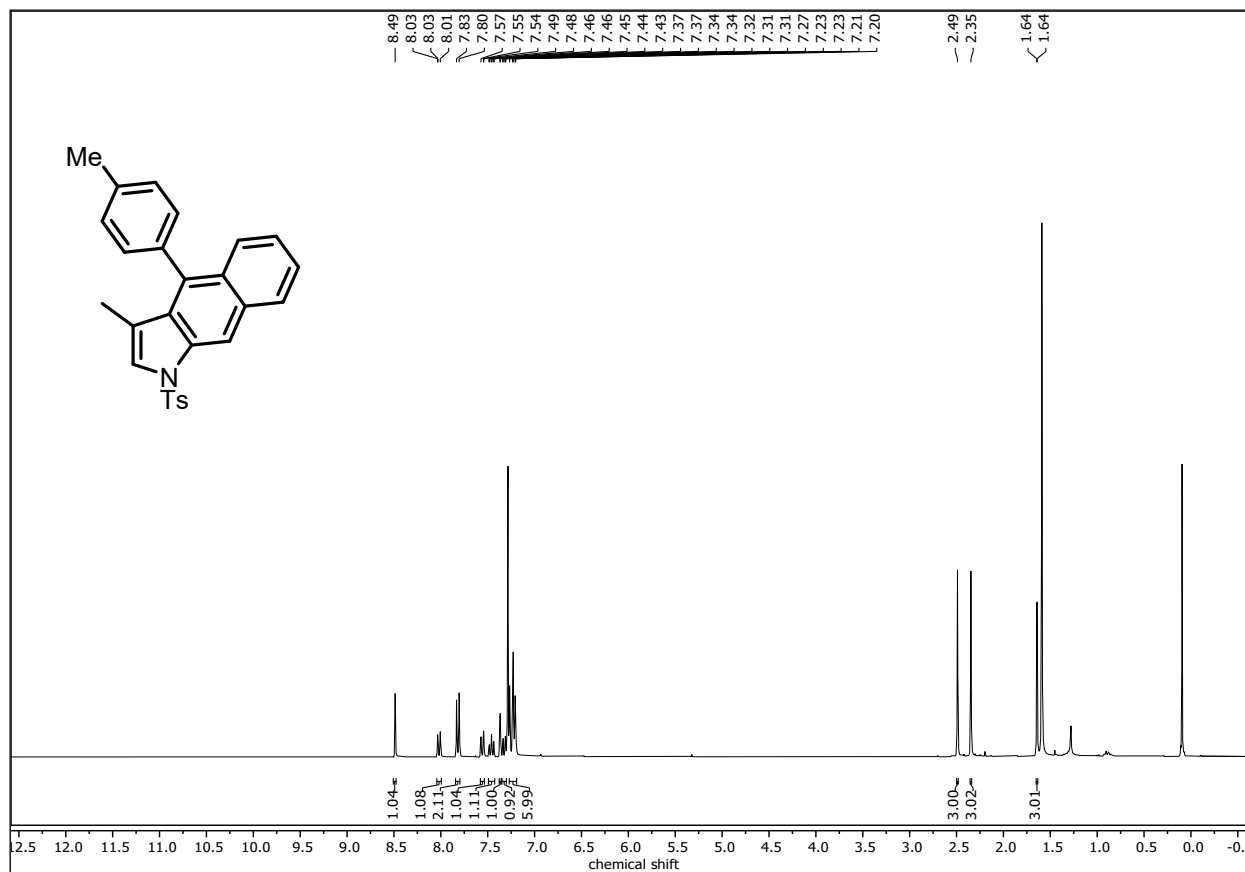
¹H NMR (300 MHz, CDCl₃) Spectrum of 4a.



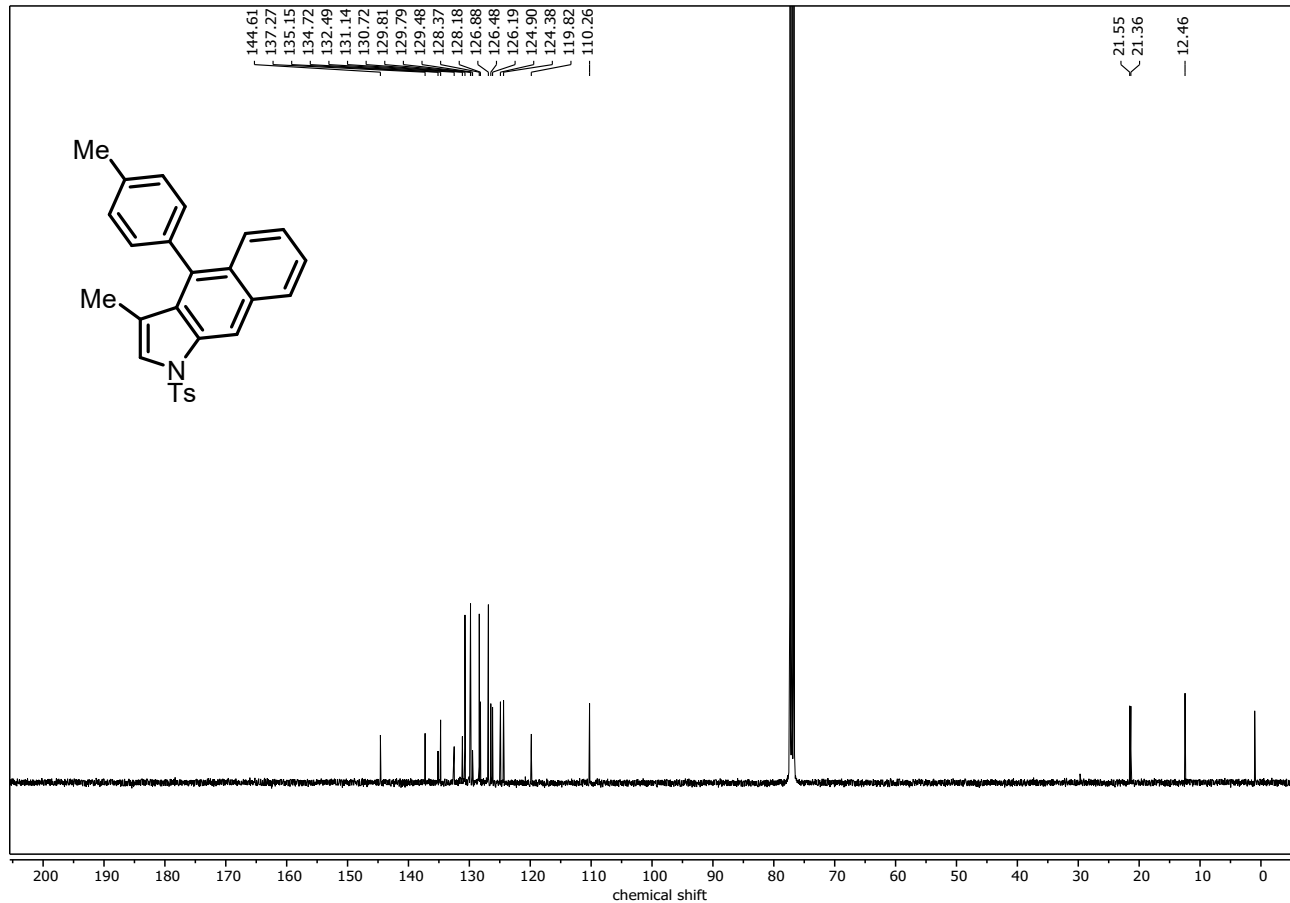
¹³C{¹H} (101 MHz, CDCl₃) NMR Spectrum of 4a.



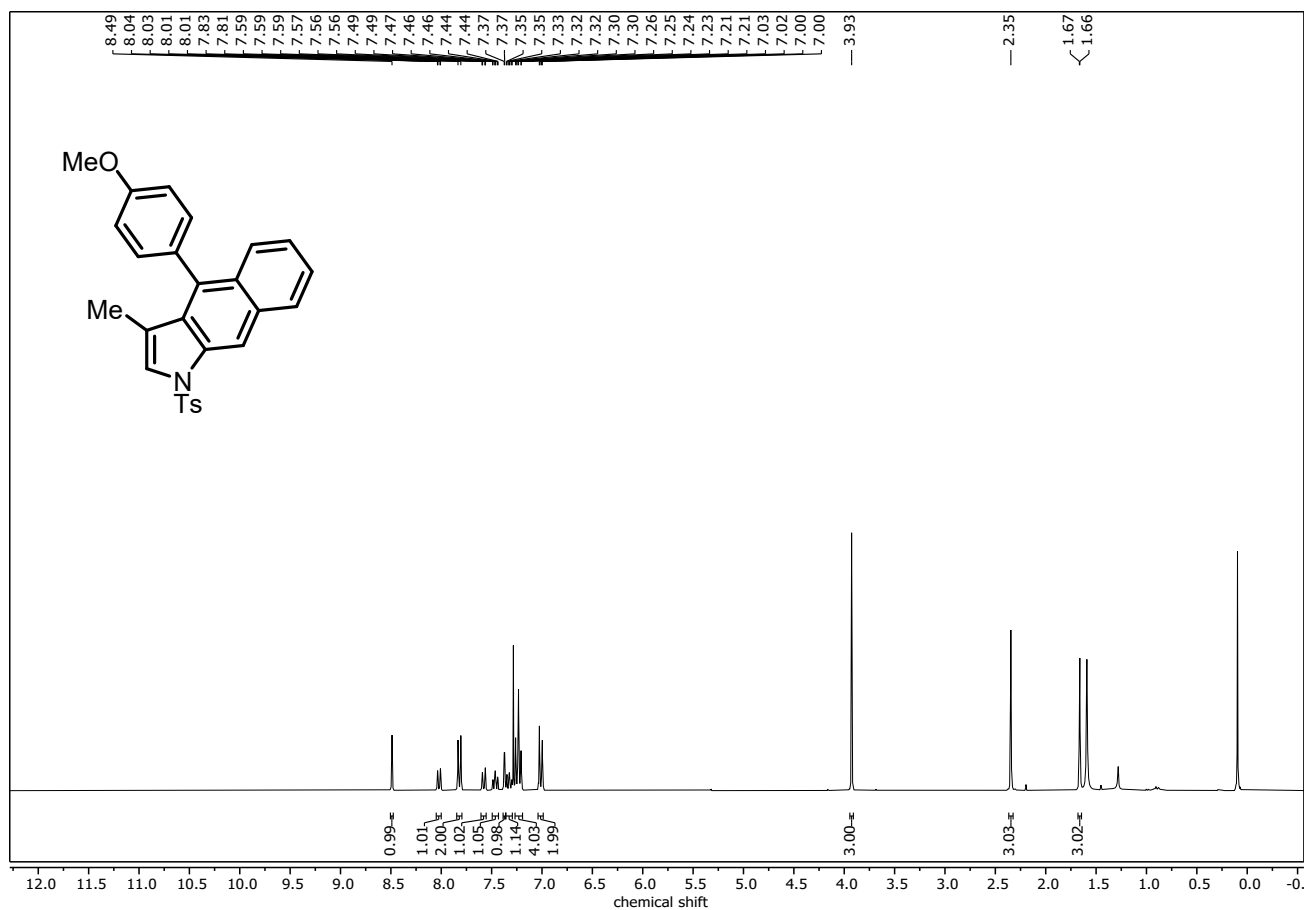
^1H NMR (300 MHz, CDCl_3) Spectrum of 4b.



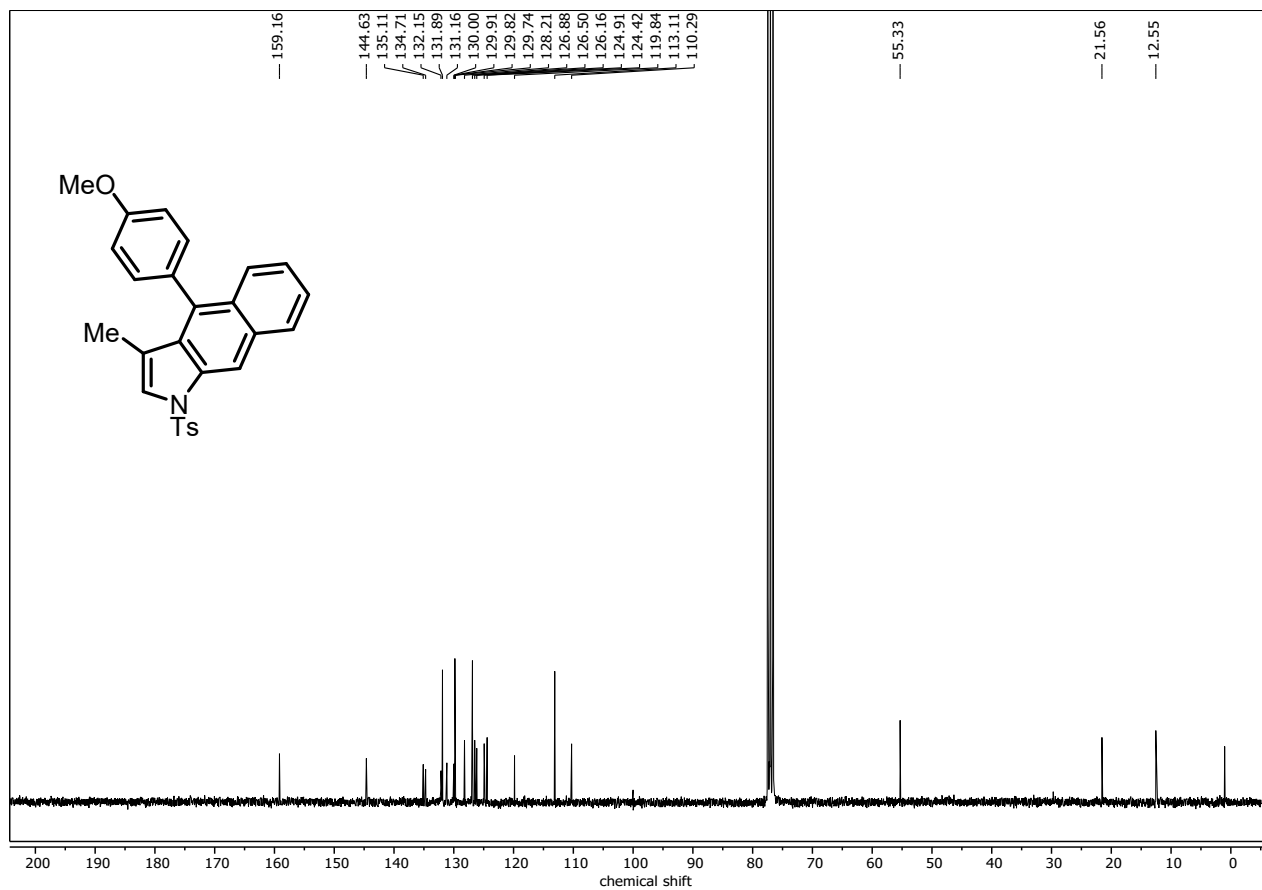
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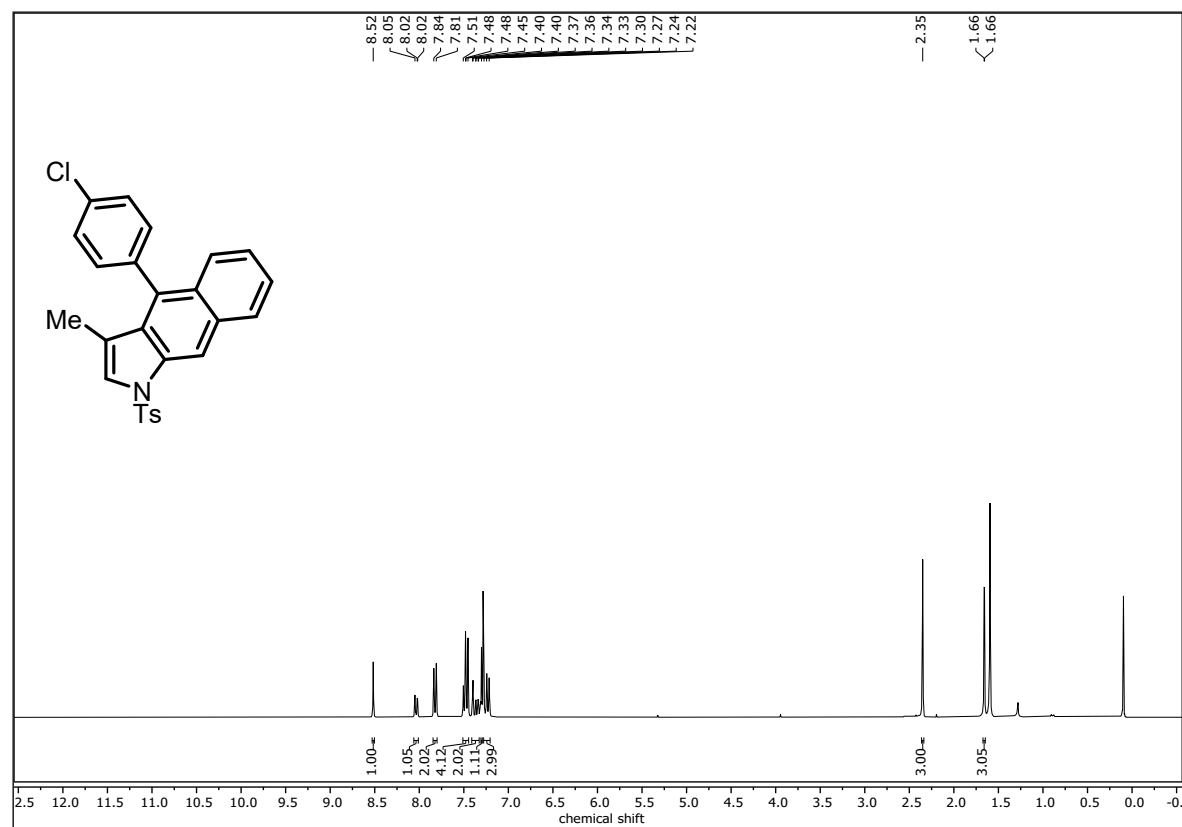
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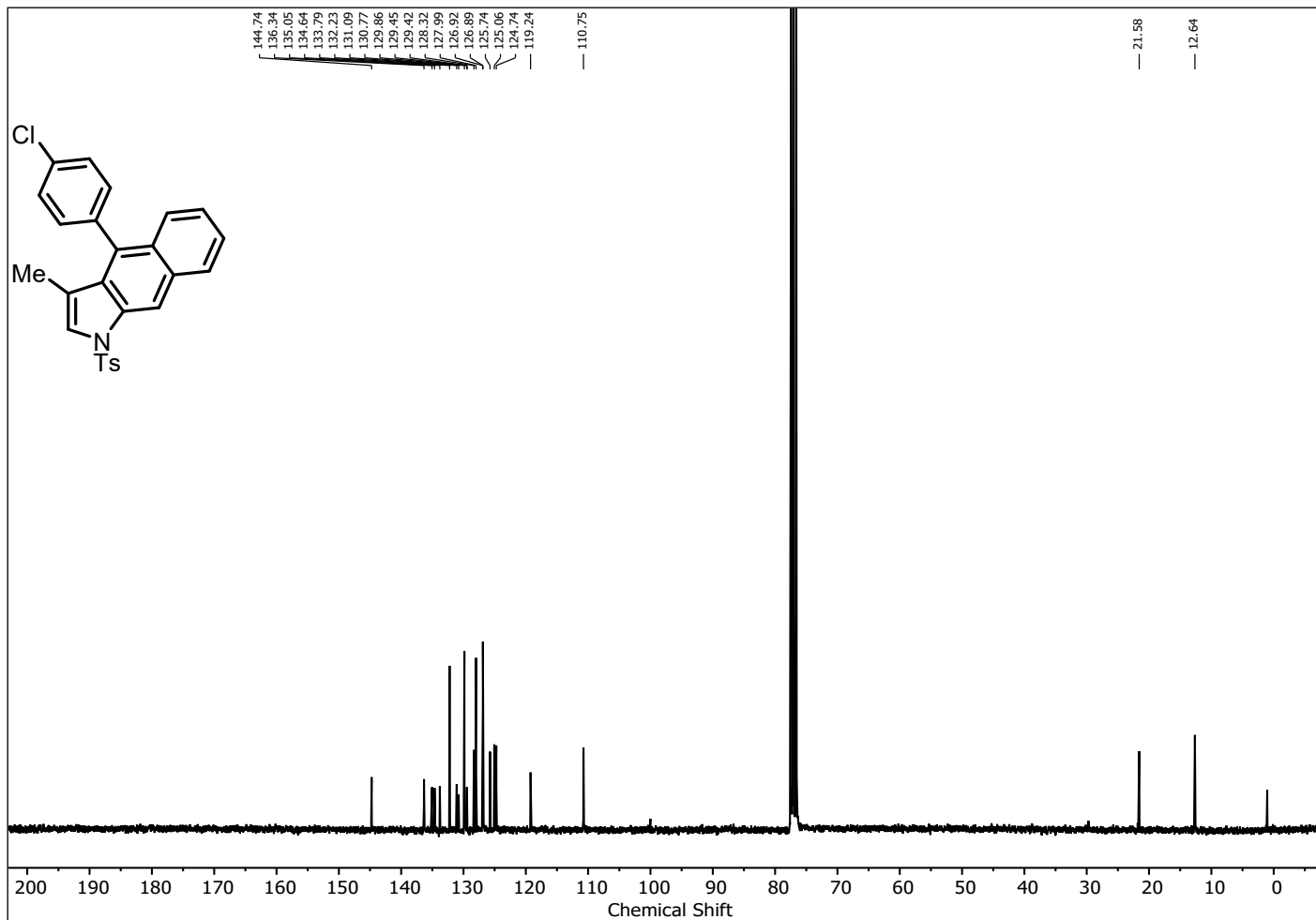
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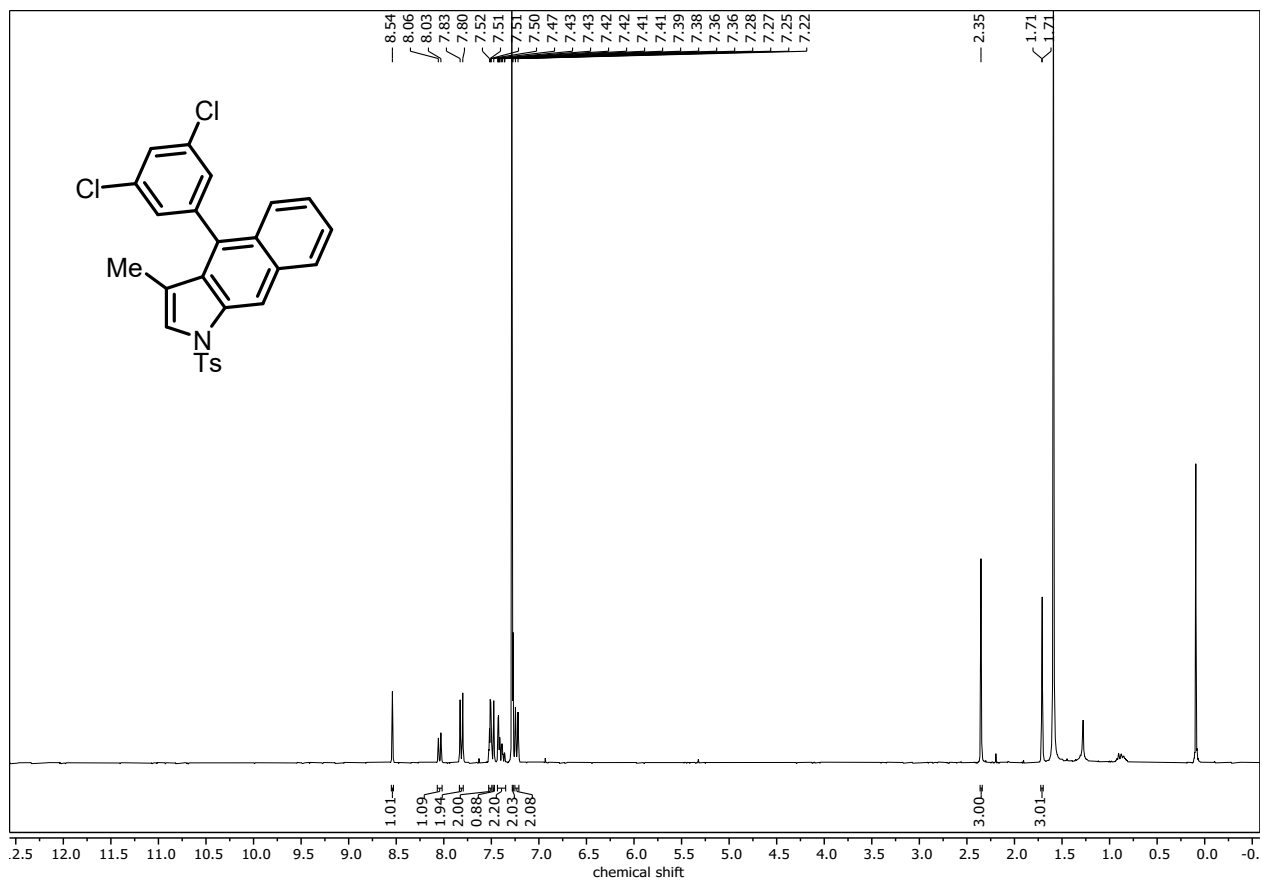
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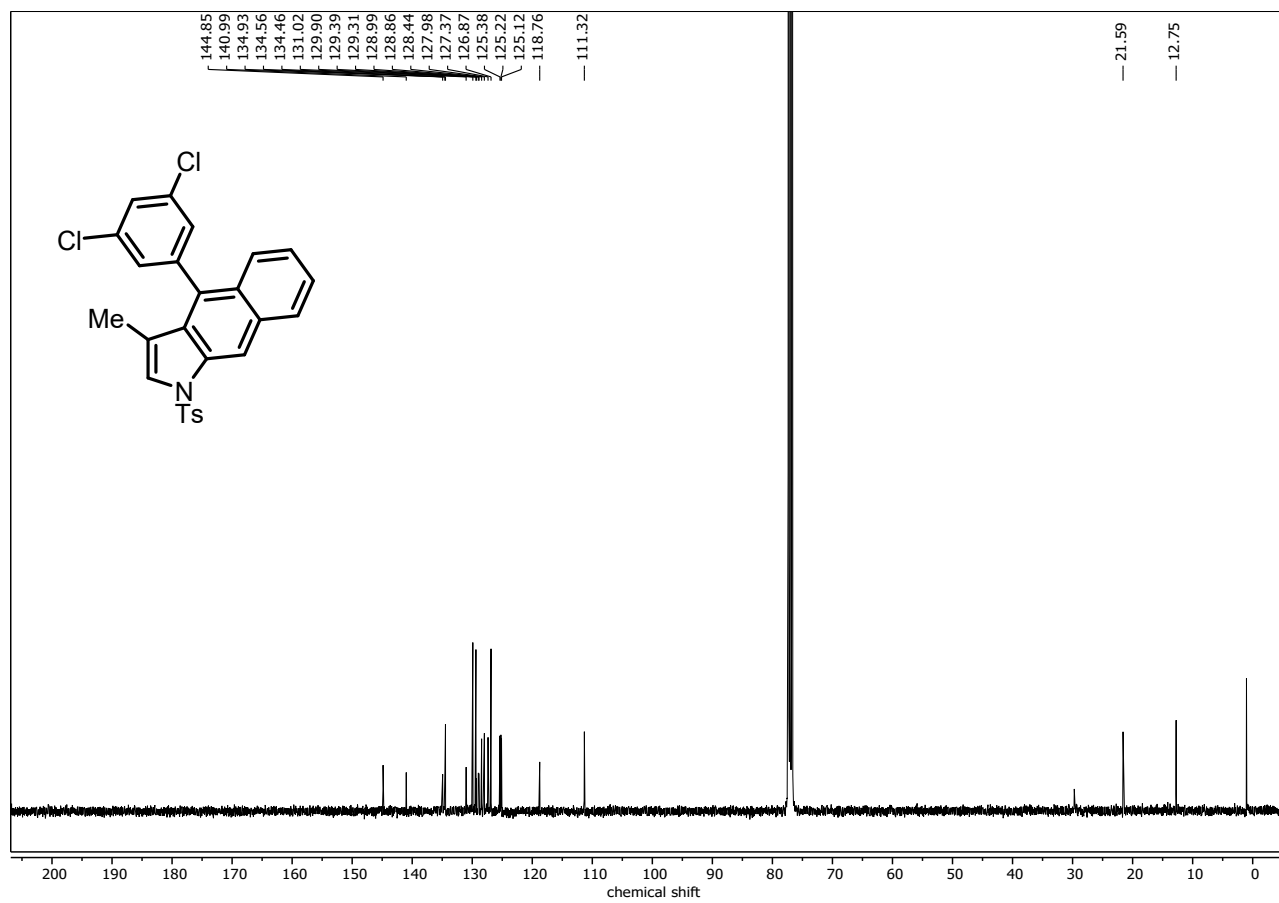
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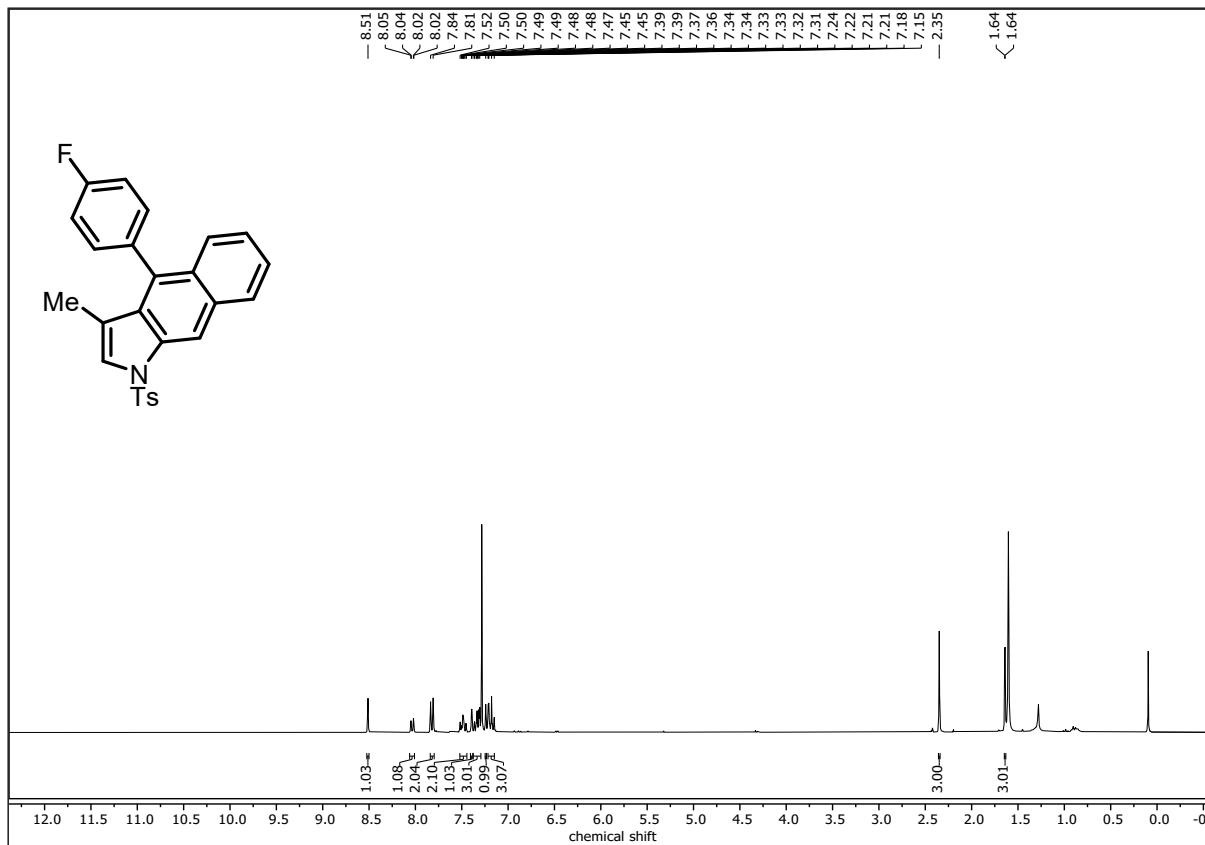
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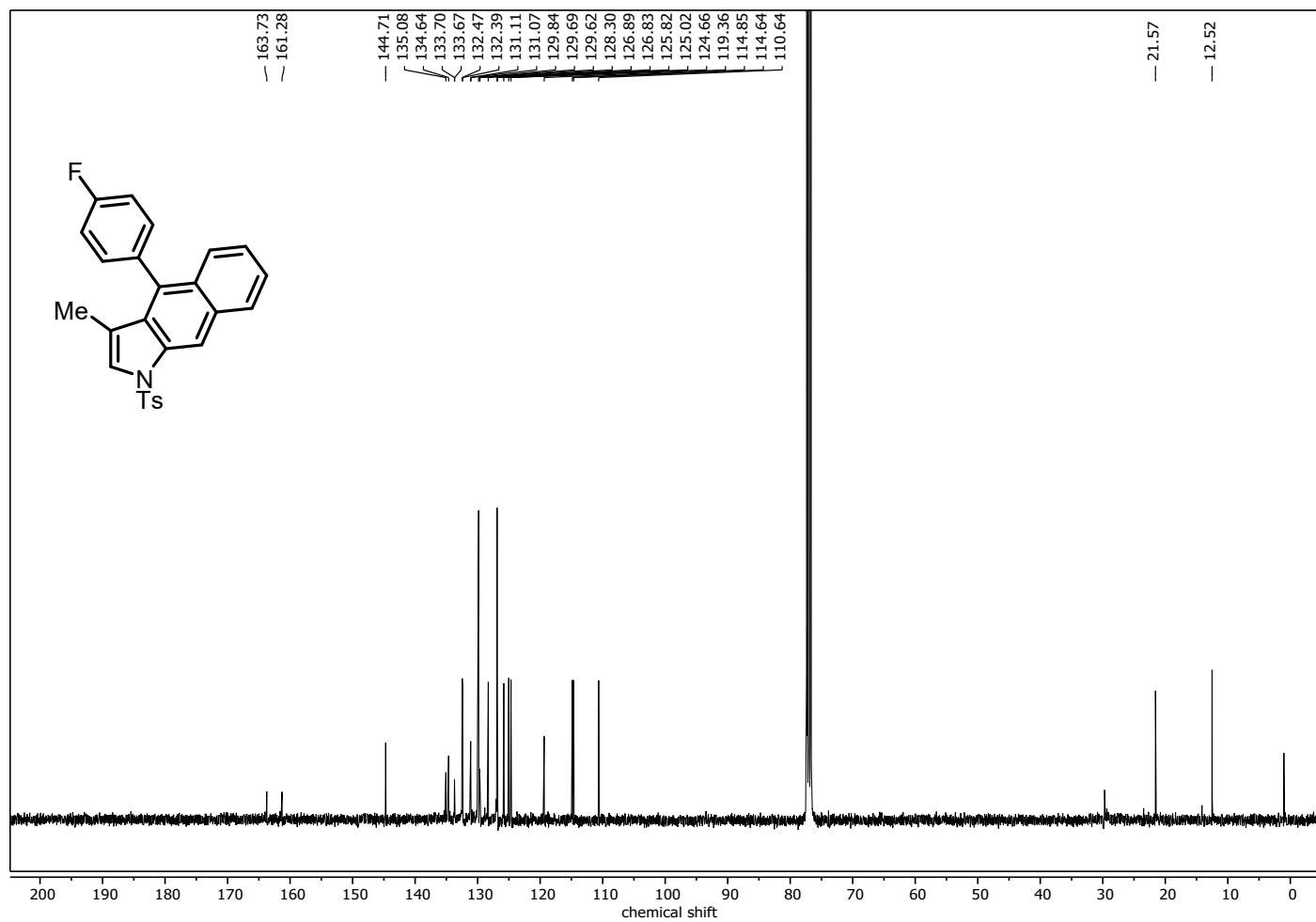
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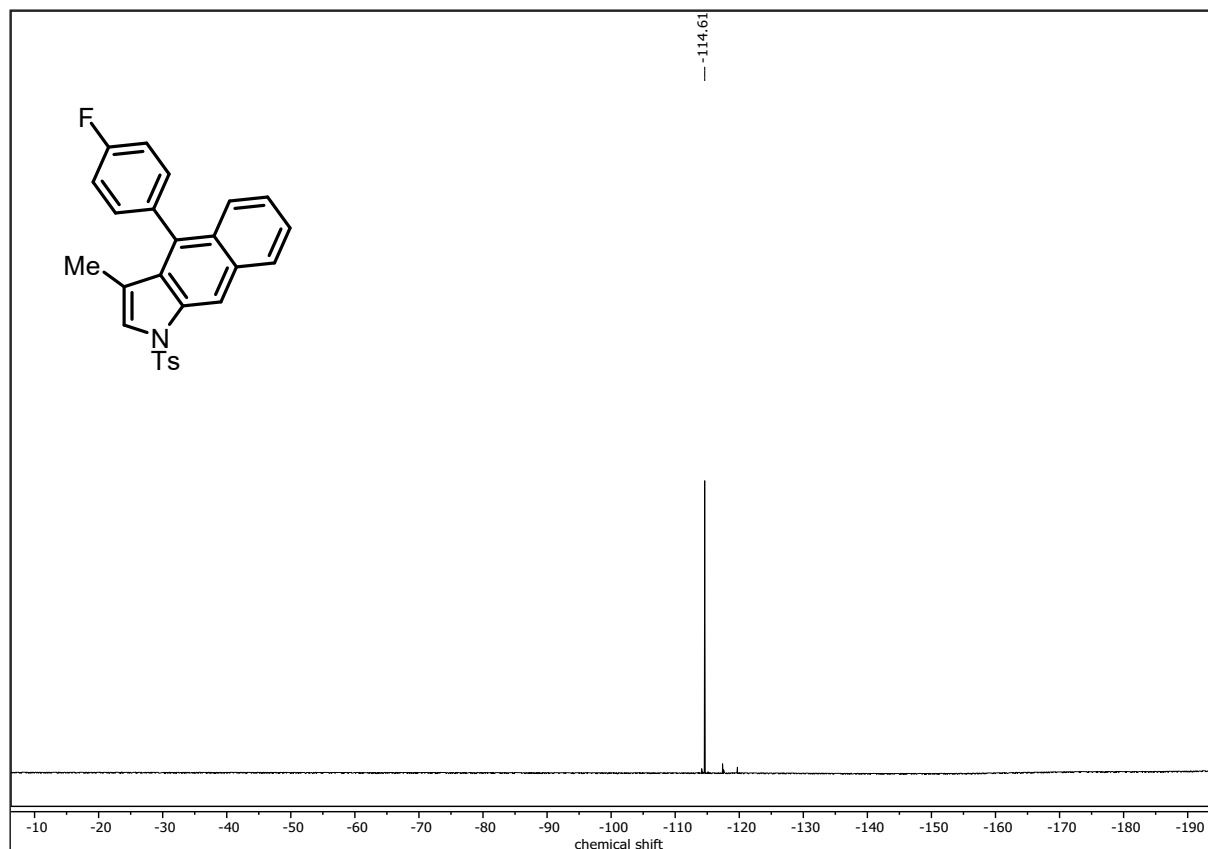
^1H NMR (300 MHz, CDCl_3) Spectrum of 4f.



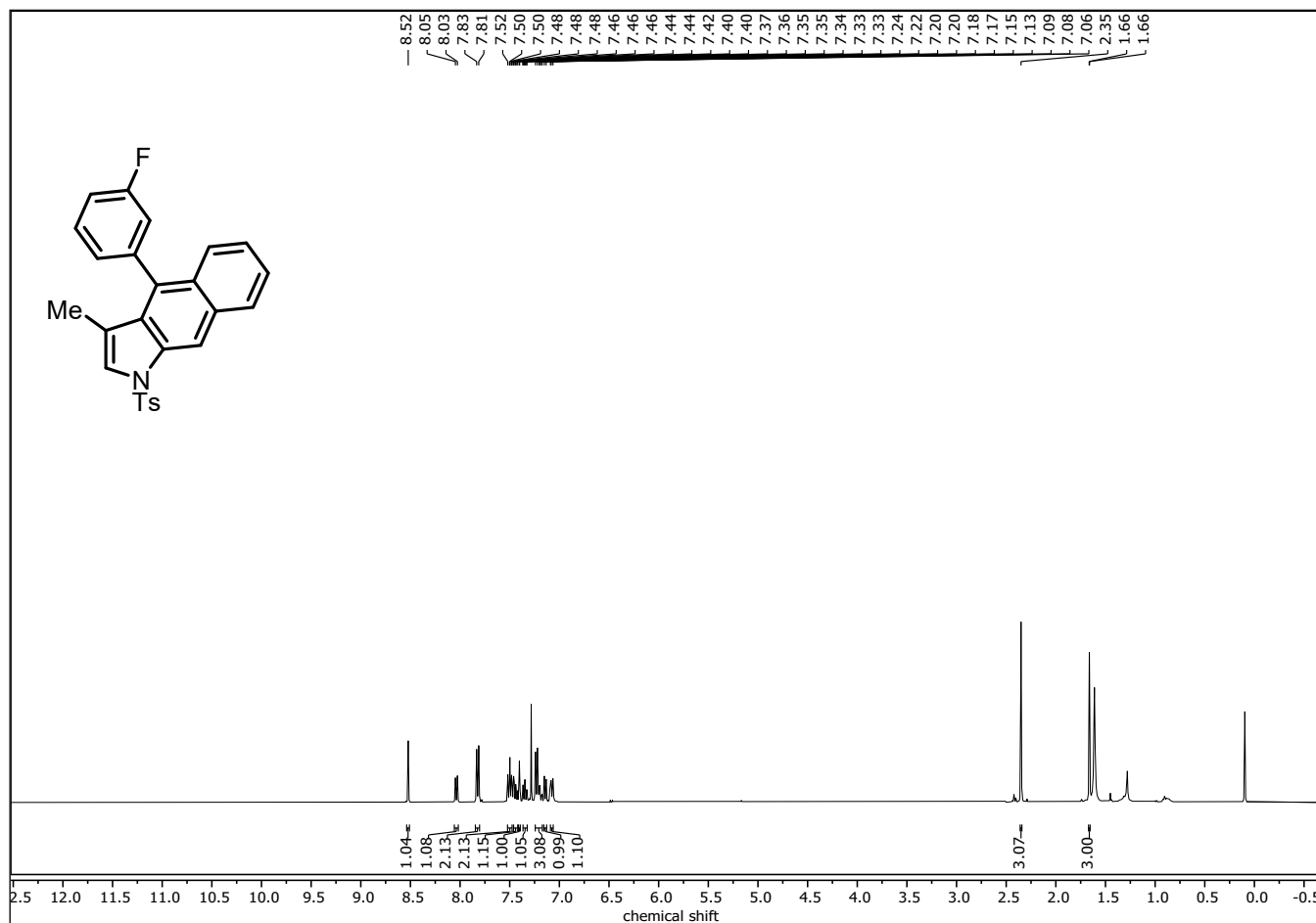
¹³C{¹H} (101 MHz, CDCl₃) NMR Spectrum of 4f.



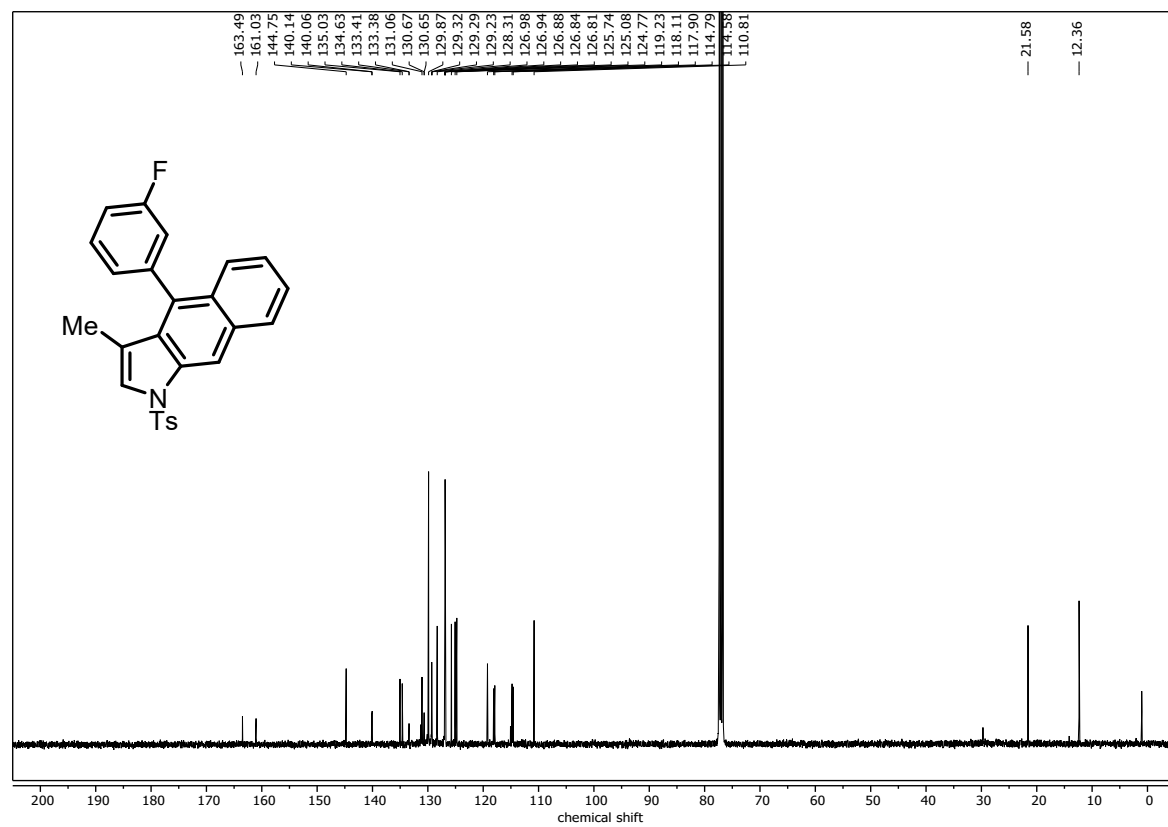
¹⁹F NMR (282 MHz, CDCl₃) Spectrum of 4f.



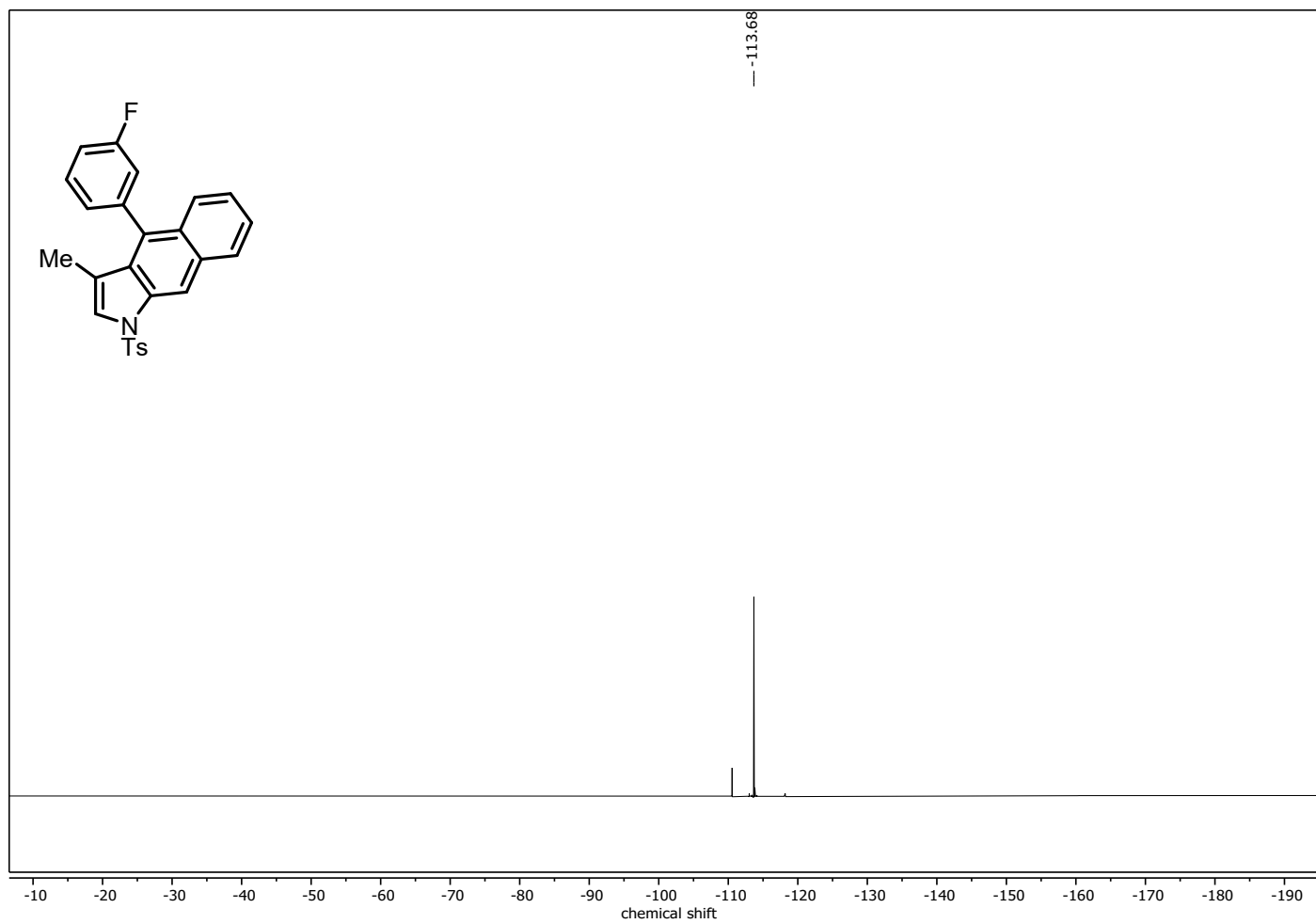
¹H NMR (400 MHz, CDCl₃) Spectrum of 4g.



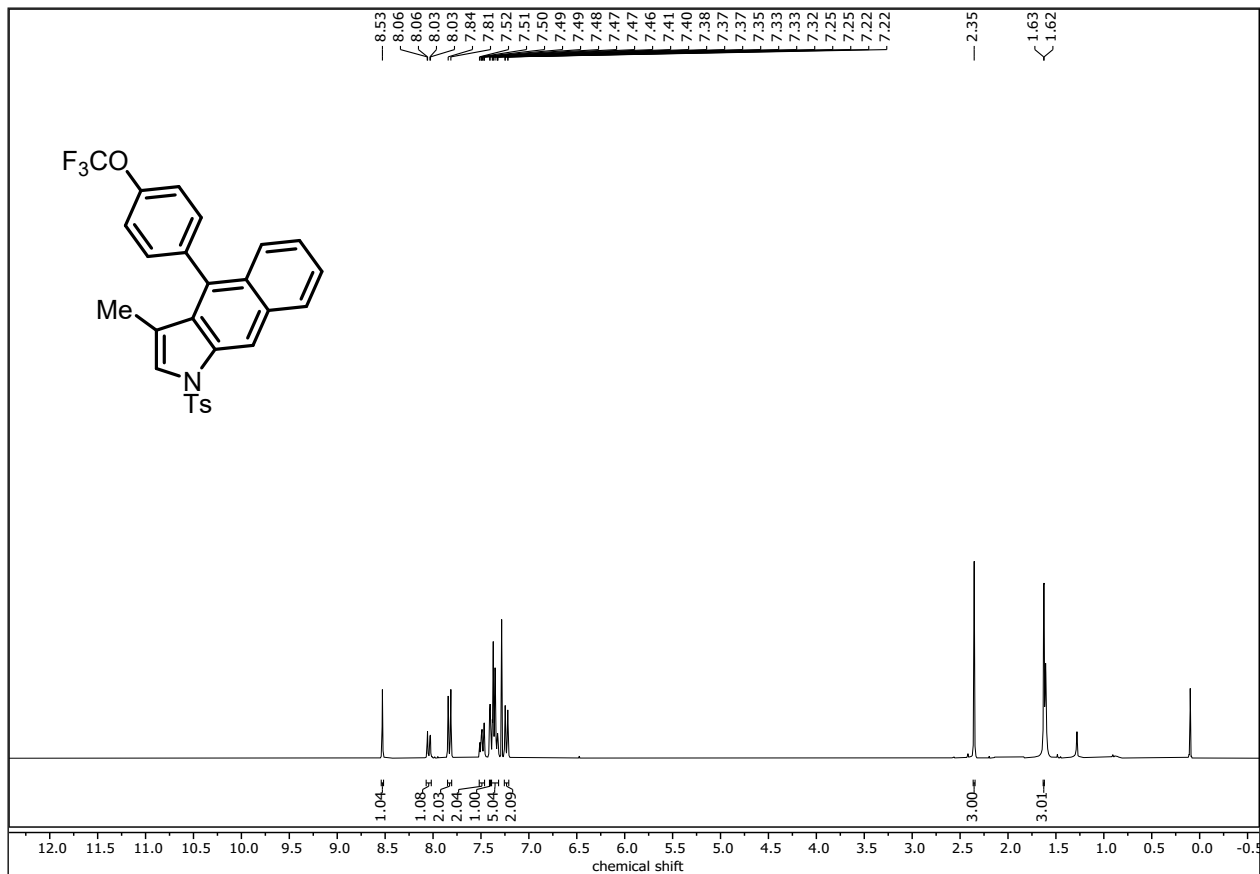
$^{13}\text{C}\{^1\text{H}\}$ (101 MHz, CDCl_3) NMR Spectrum of 4g.



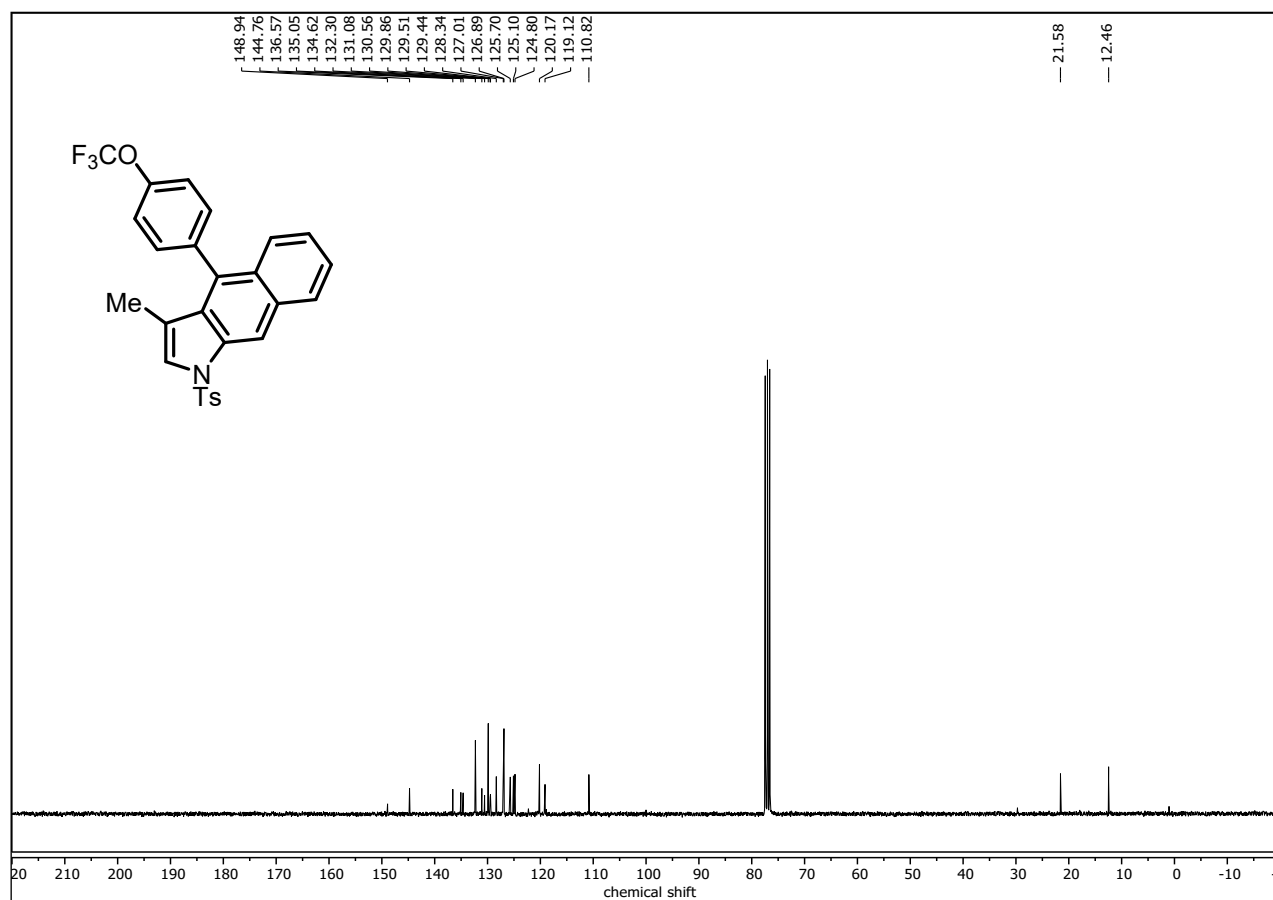
^{19}F NMR (377 MHz, CDCl_3) Spectrum of 4g.



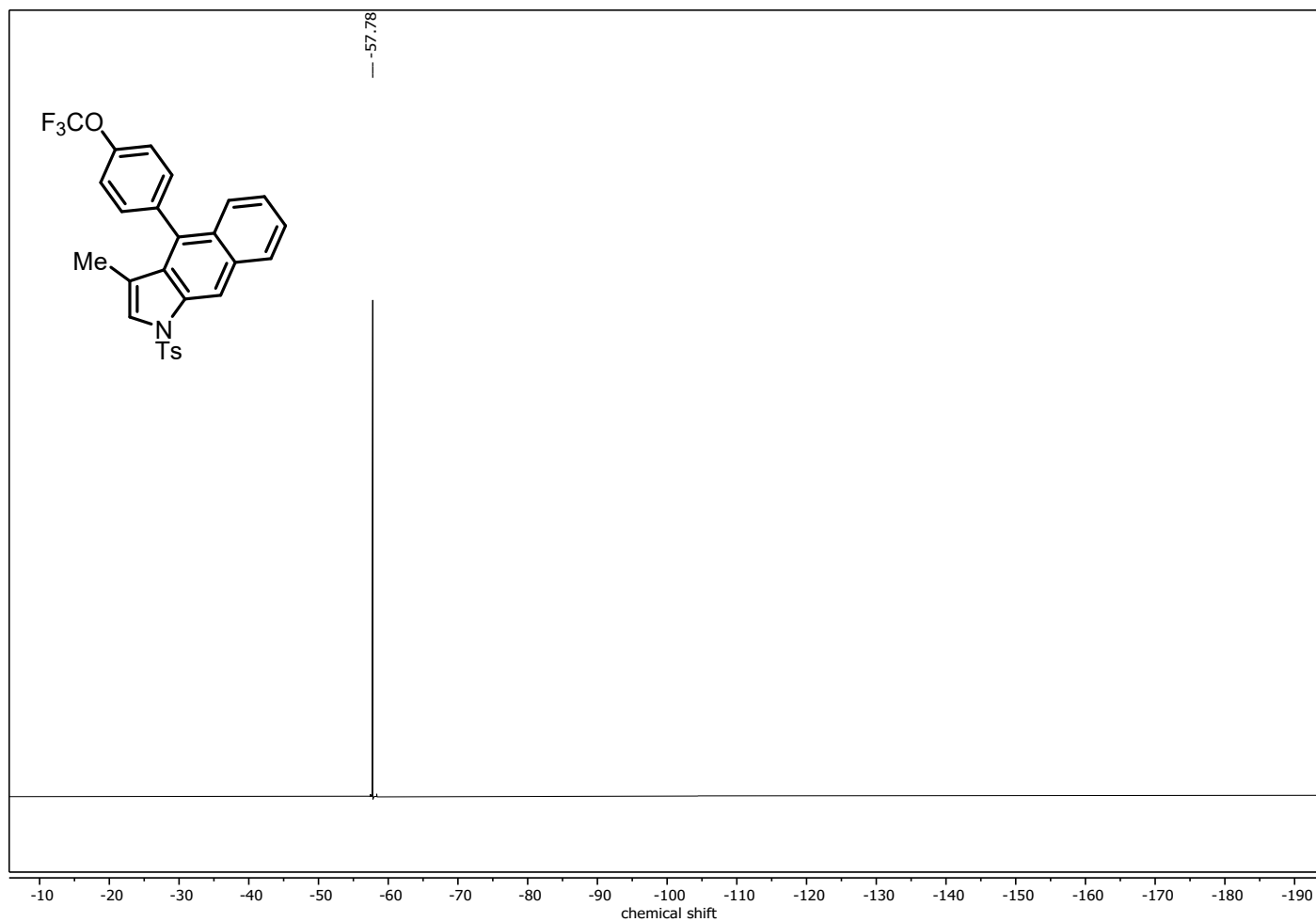
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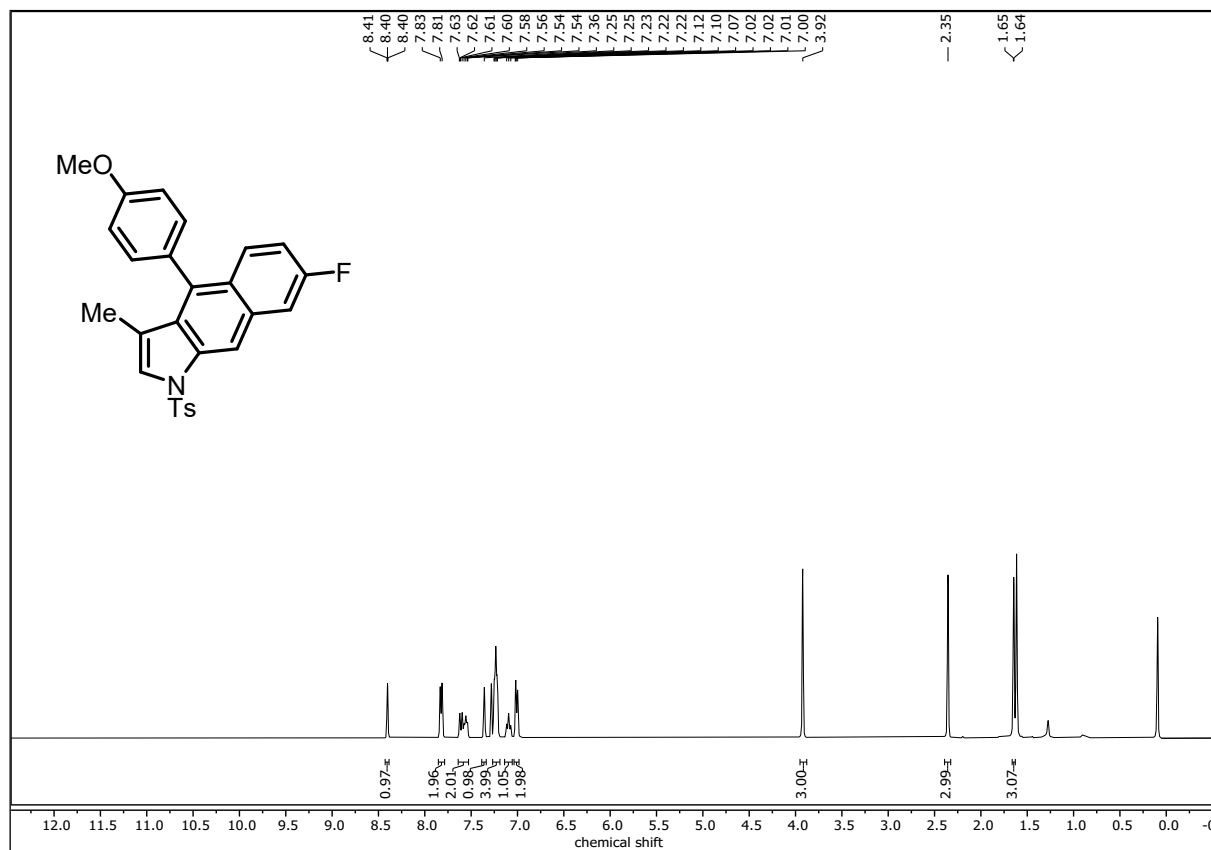
$^{13}\text{C}\{^1\text{H}\}$ (75 MHz, CDCl_3) NMR Spectrum of 4h.



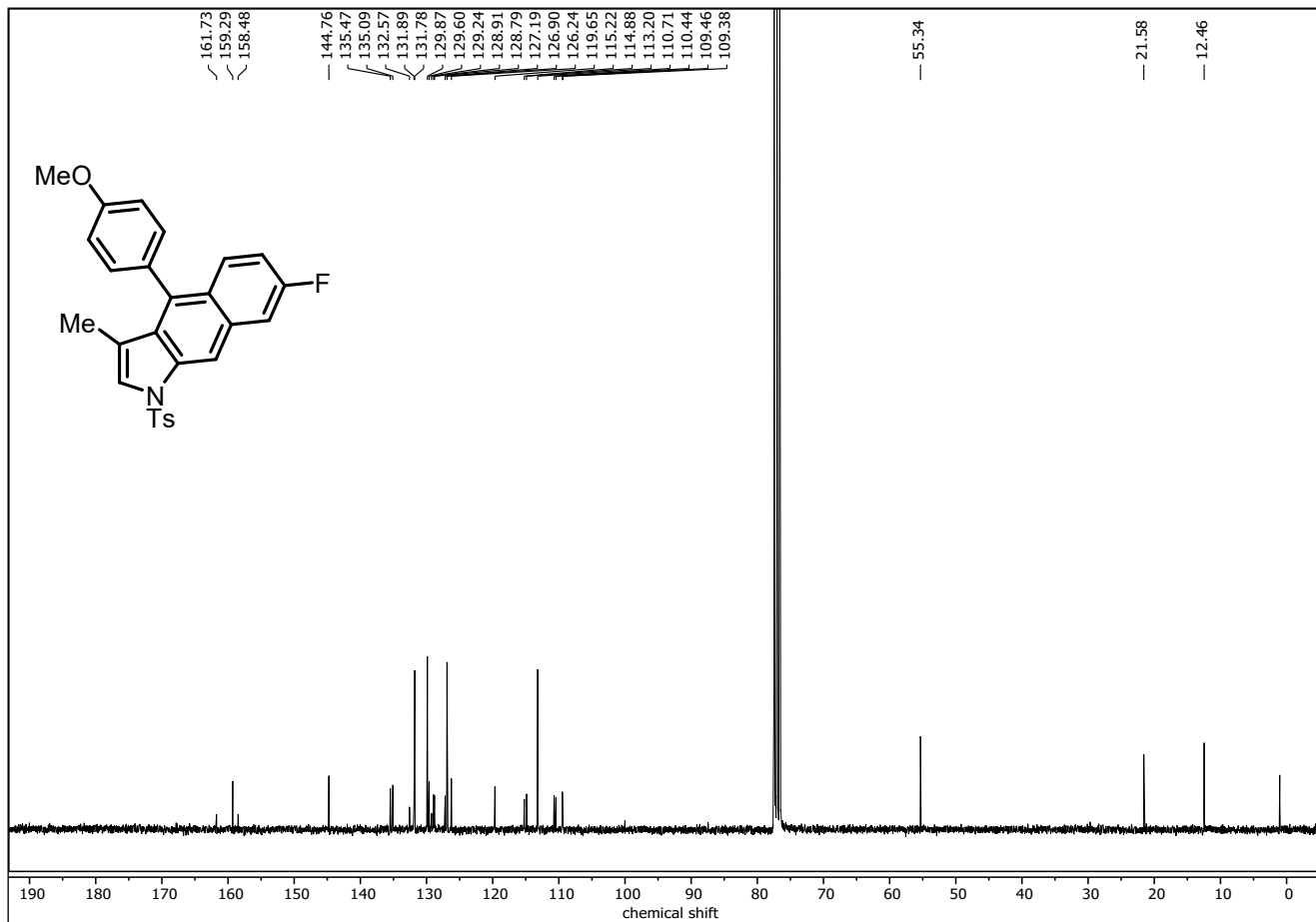
^{19}F NMR (282 MHz, CDCl_3) Spectrum of 4h.



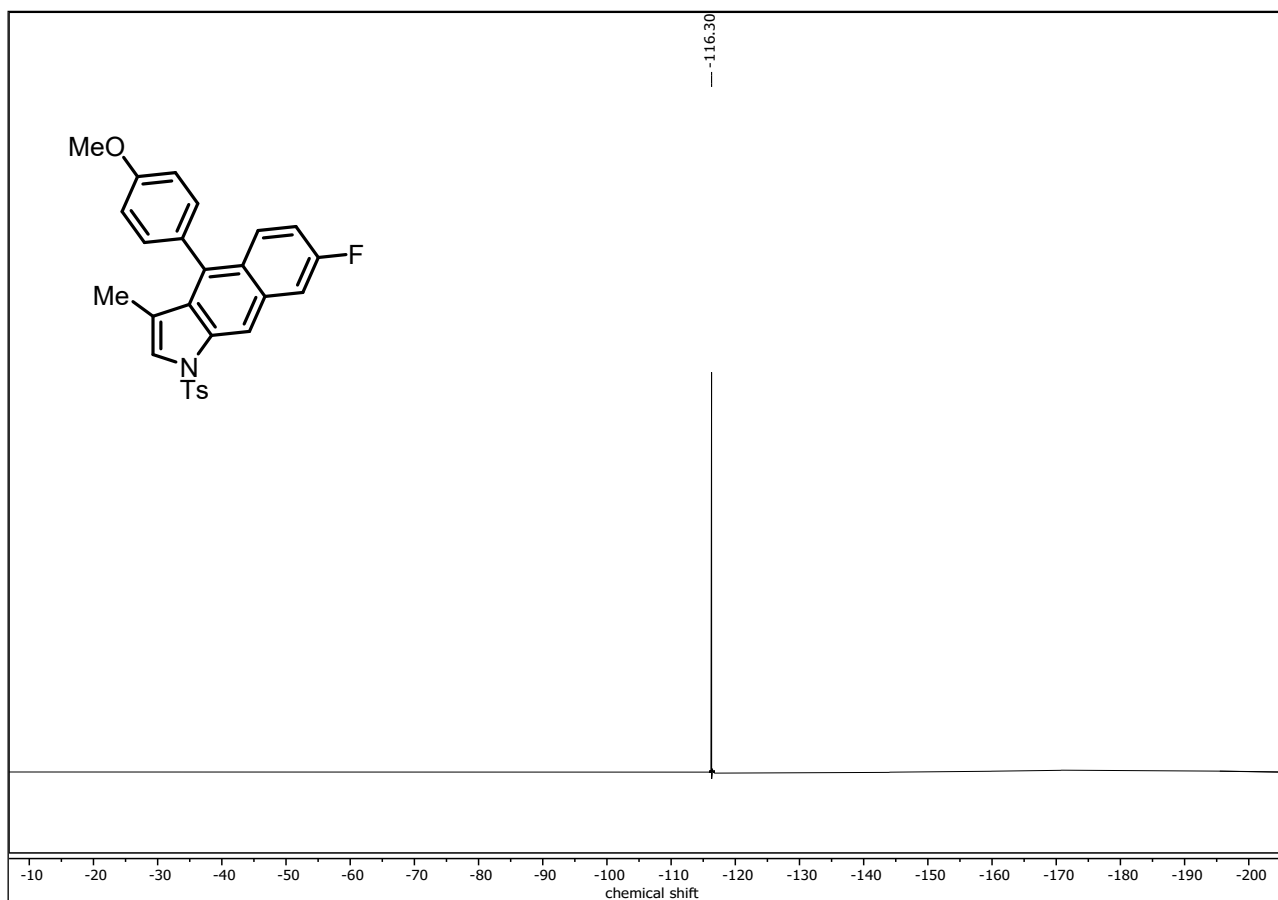
¹H NMR (400 MHz, CDCl₃) Spectrum of 4i.



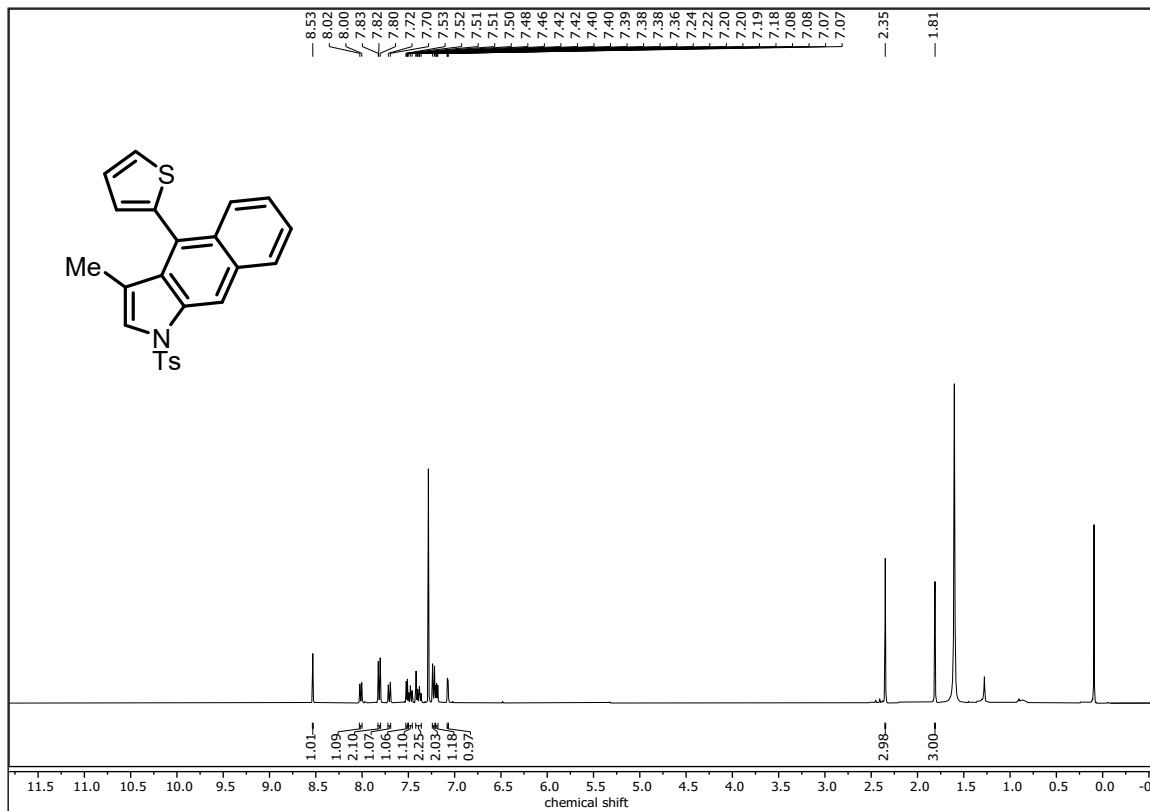
¹³C{¹H} (75 MHz, CDCl₃) NMR Spectrum of 4i.



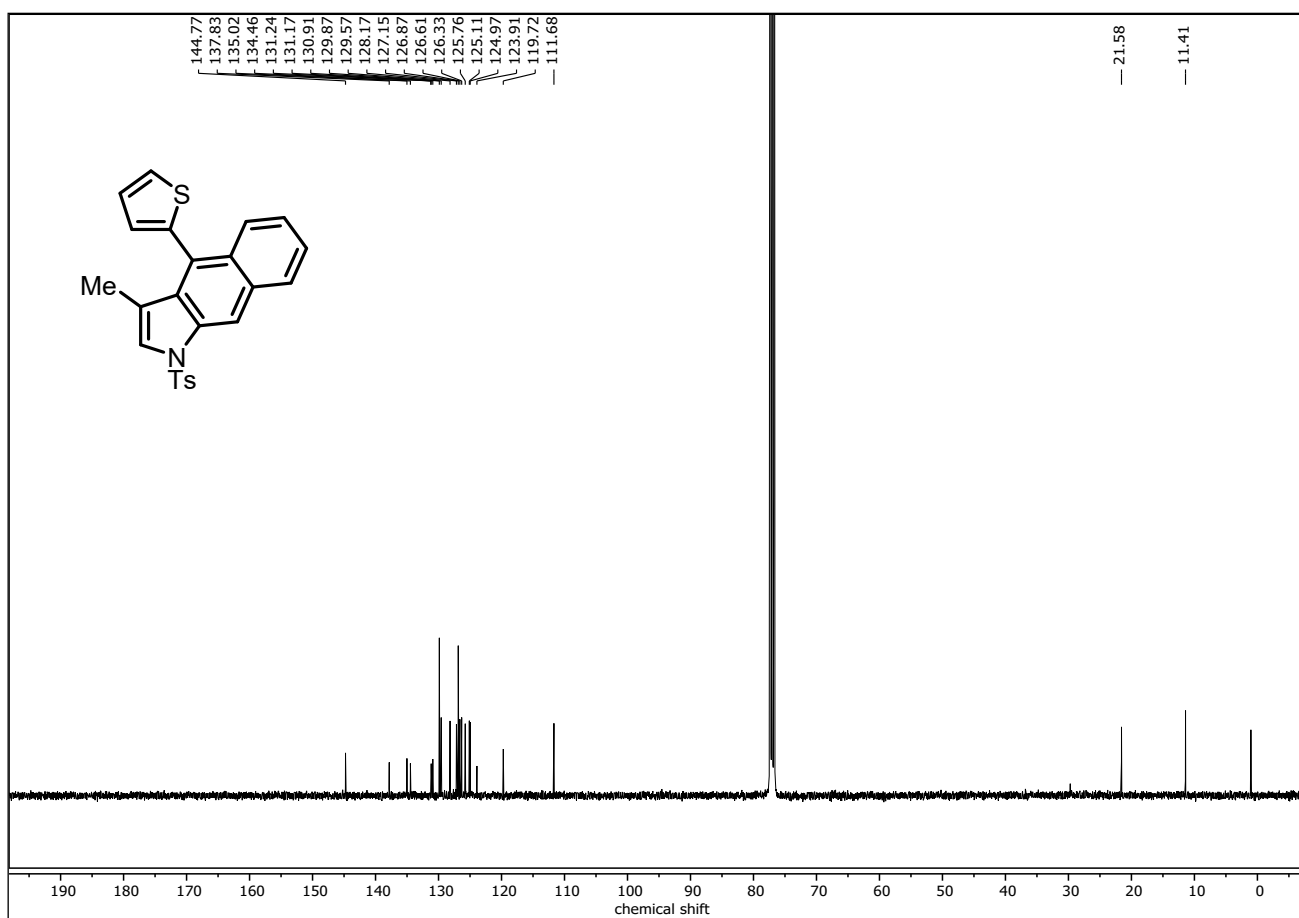
¹⁹F NMR (377 MHz, CDCl₃) Spectrum of 4i.



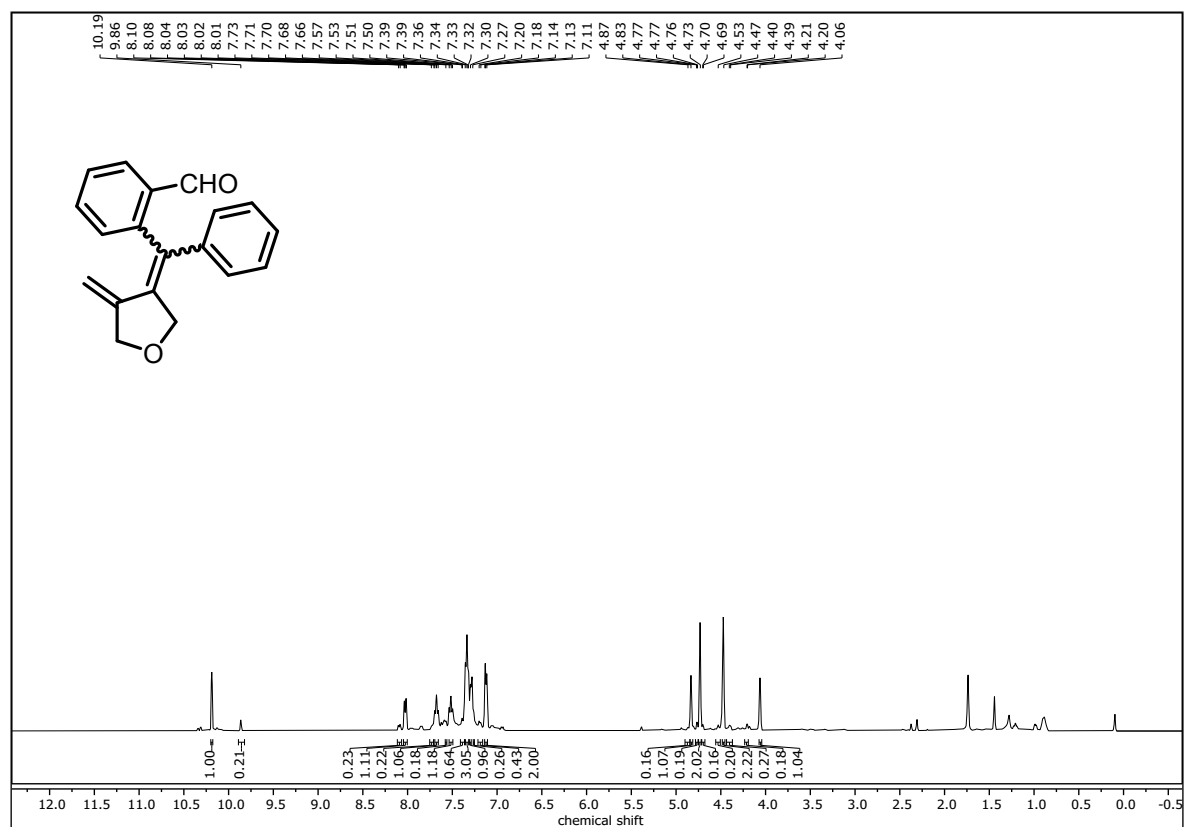
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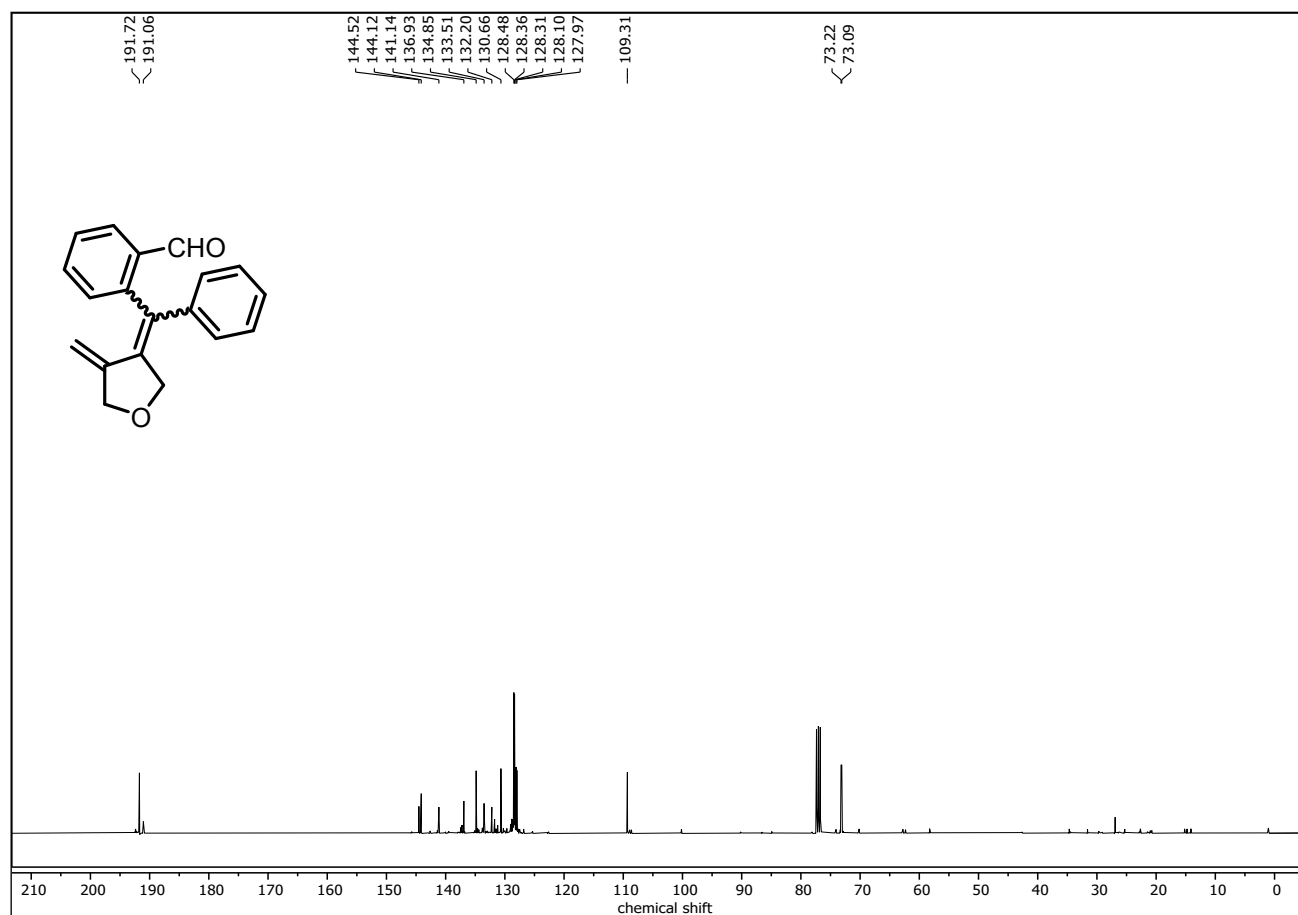
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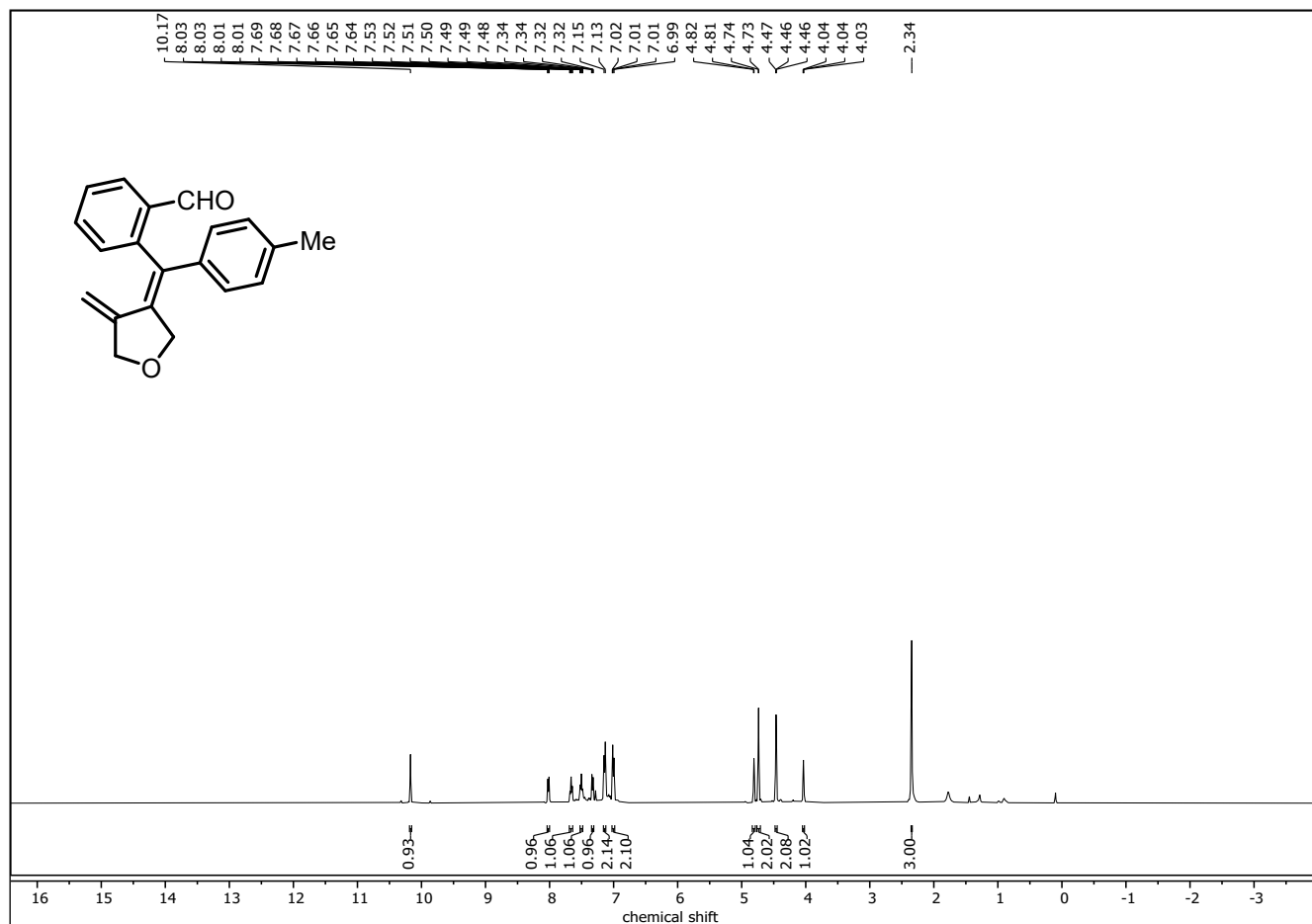
^1H NMR (400 MHz, CDCl_3) Spectrum of 6a.



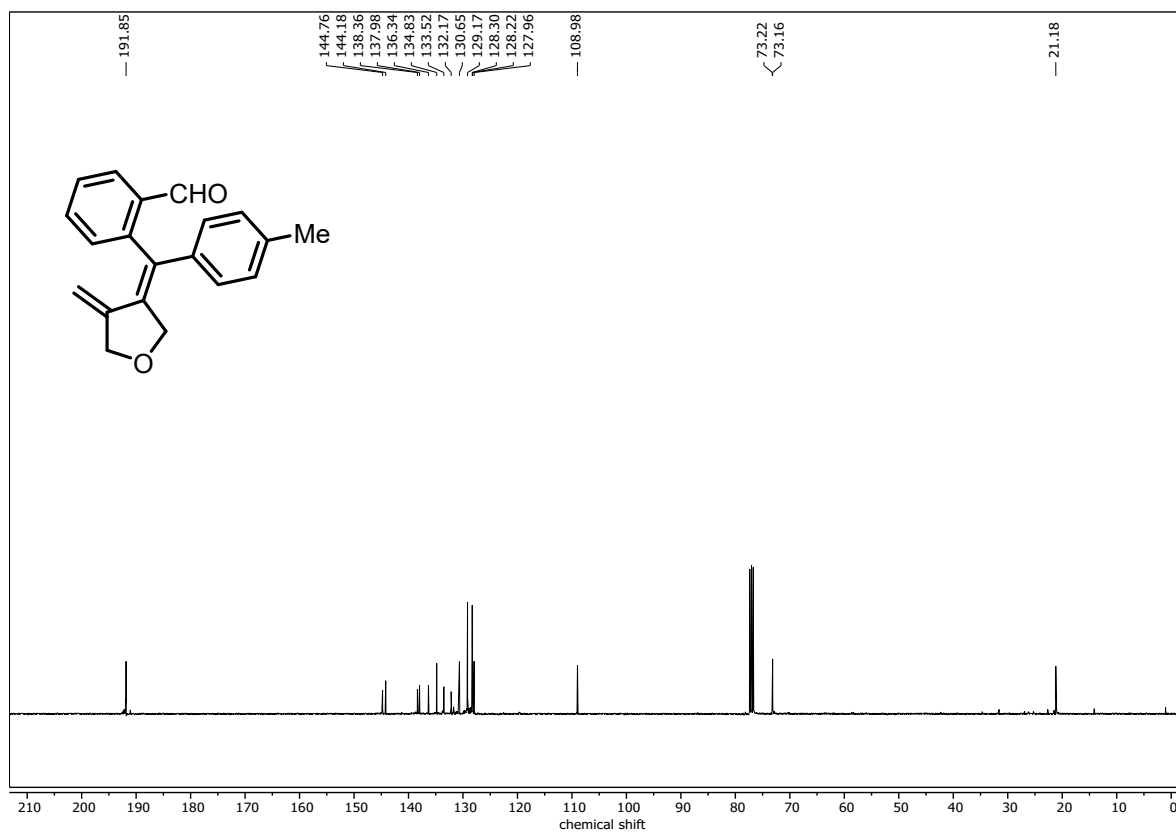
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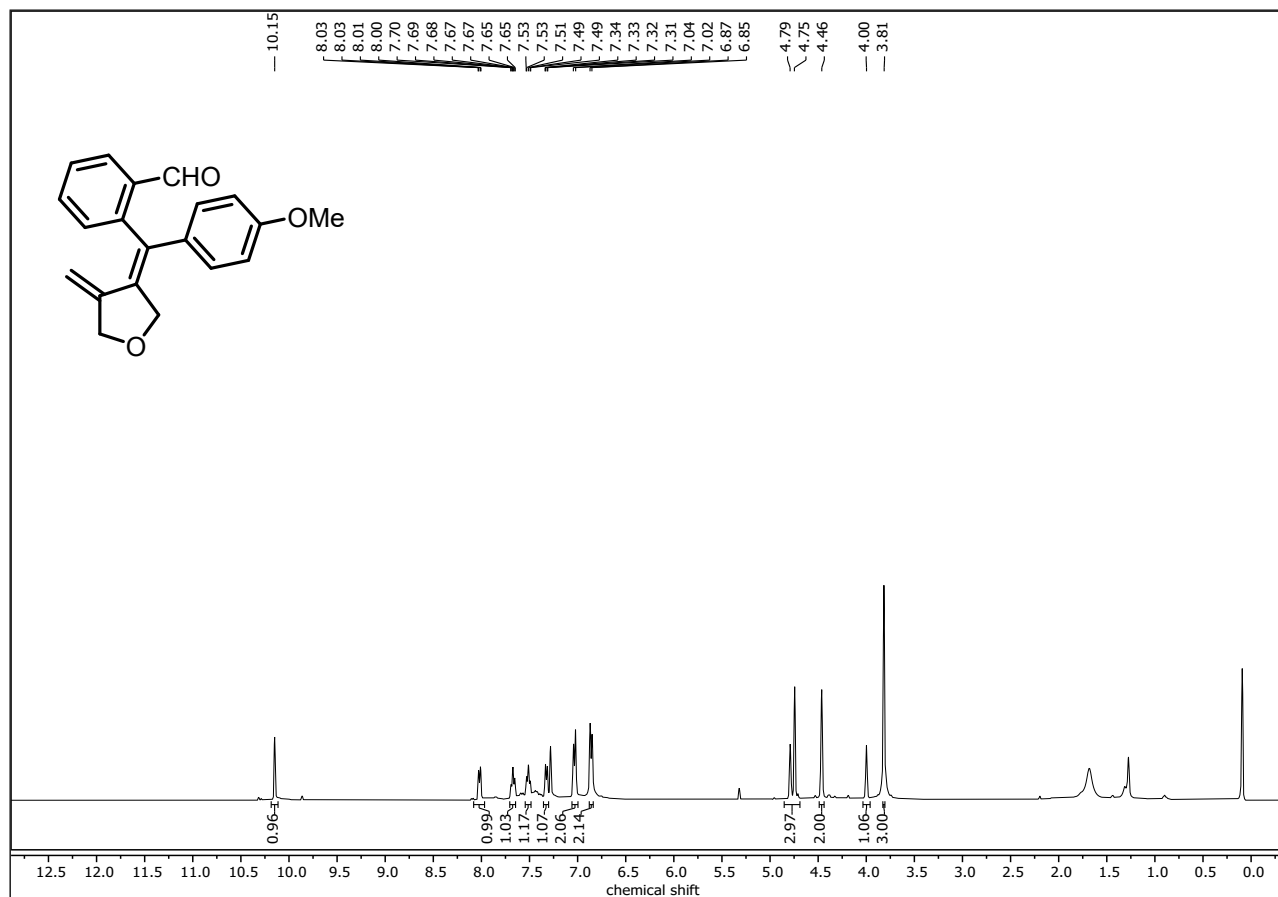
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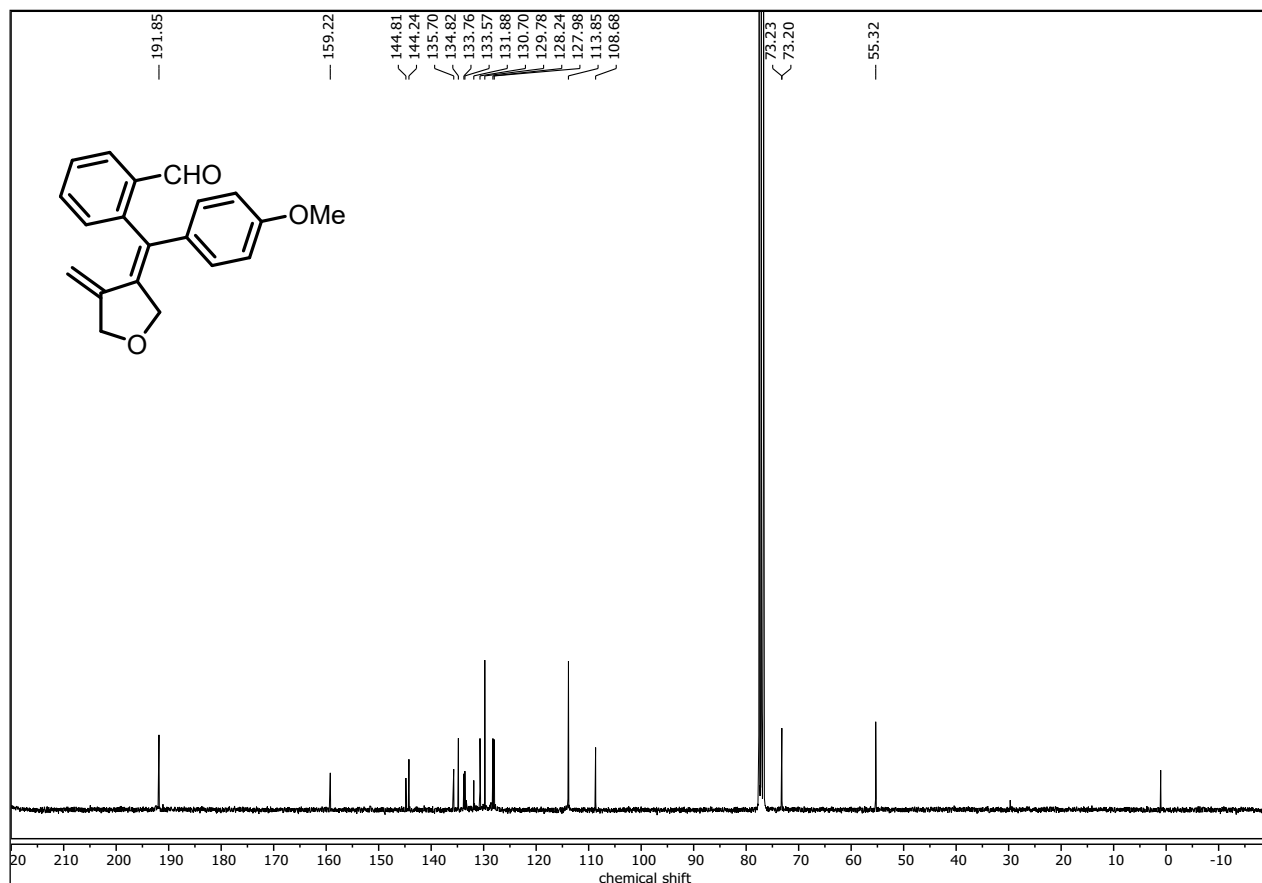
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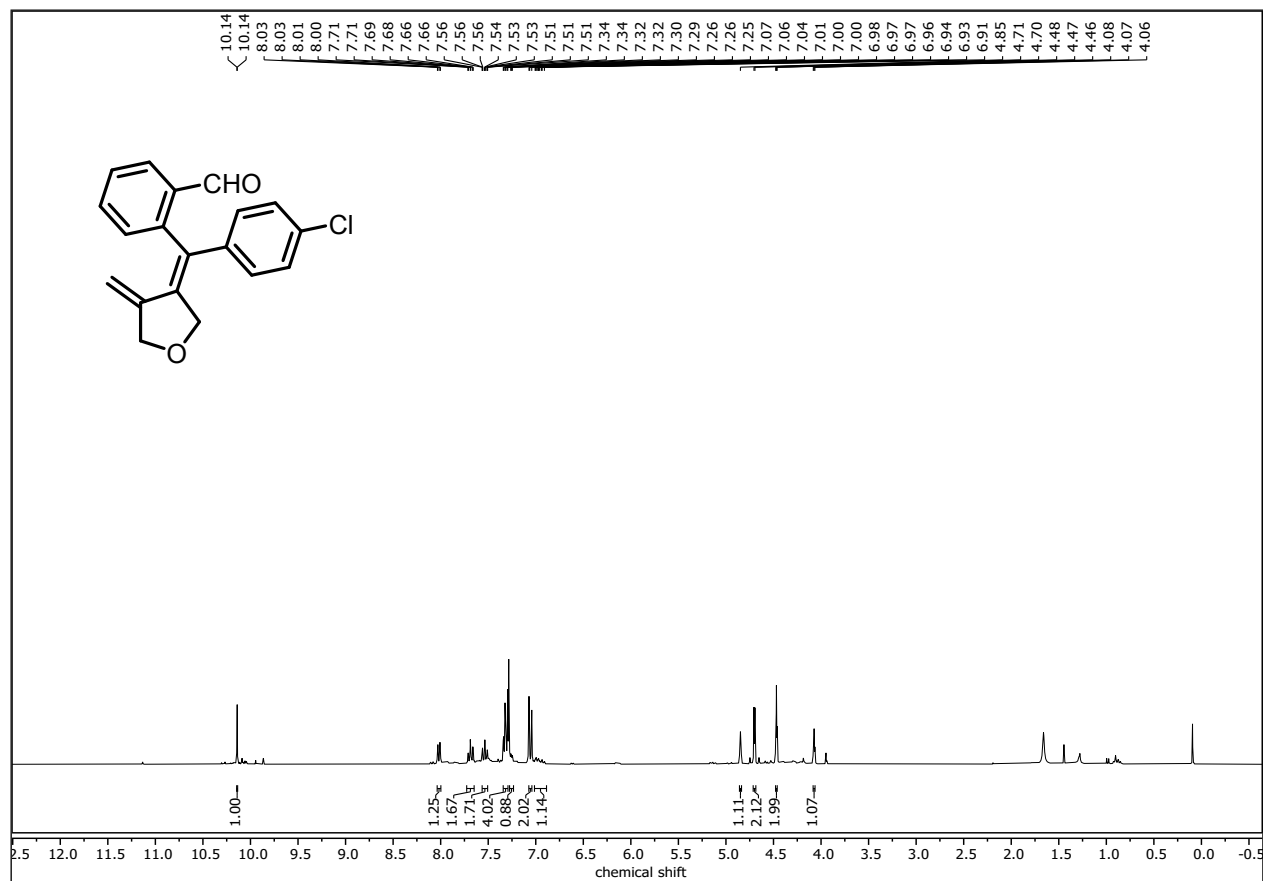
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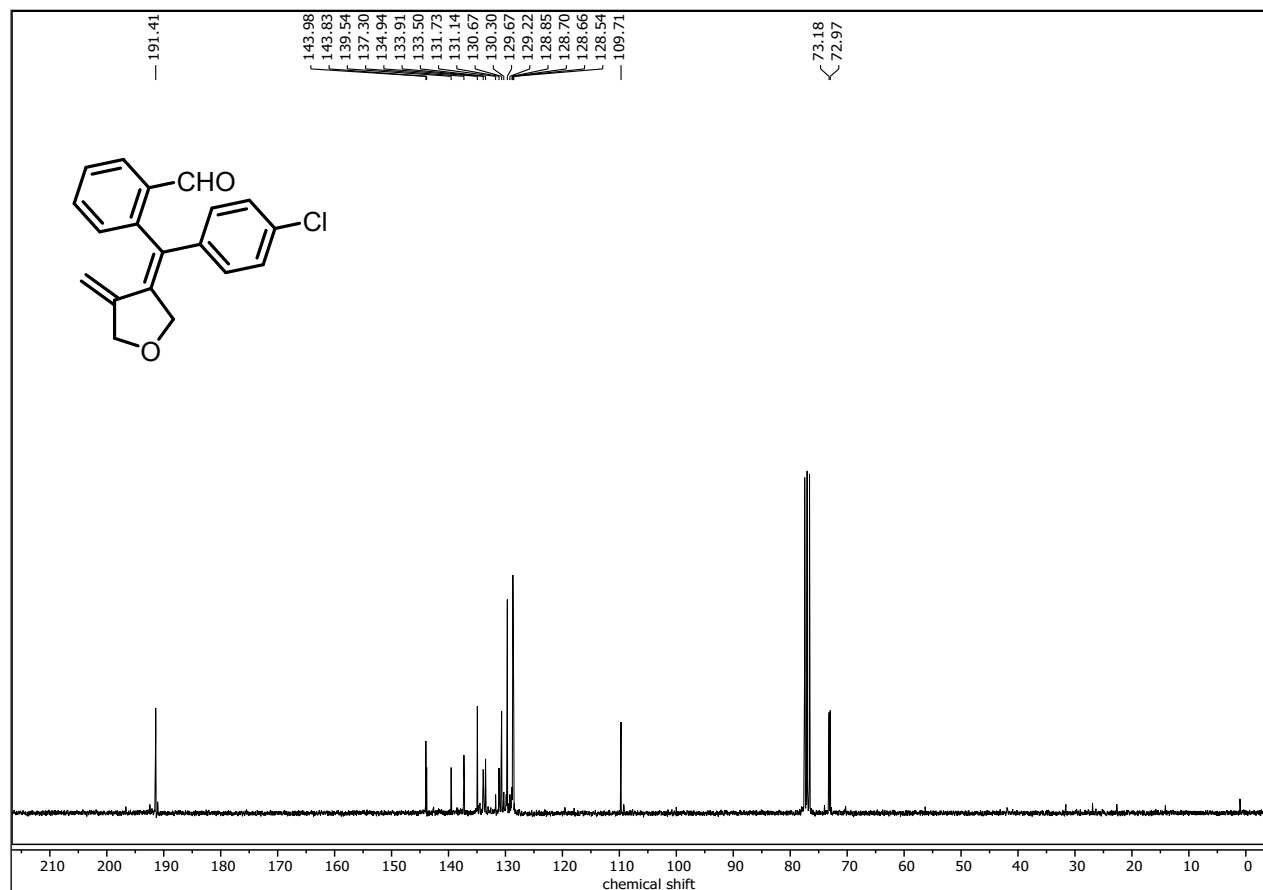
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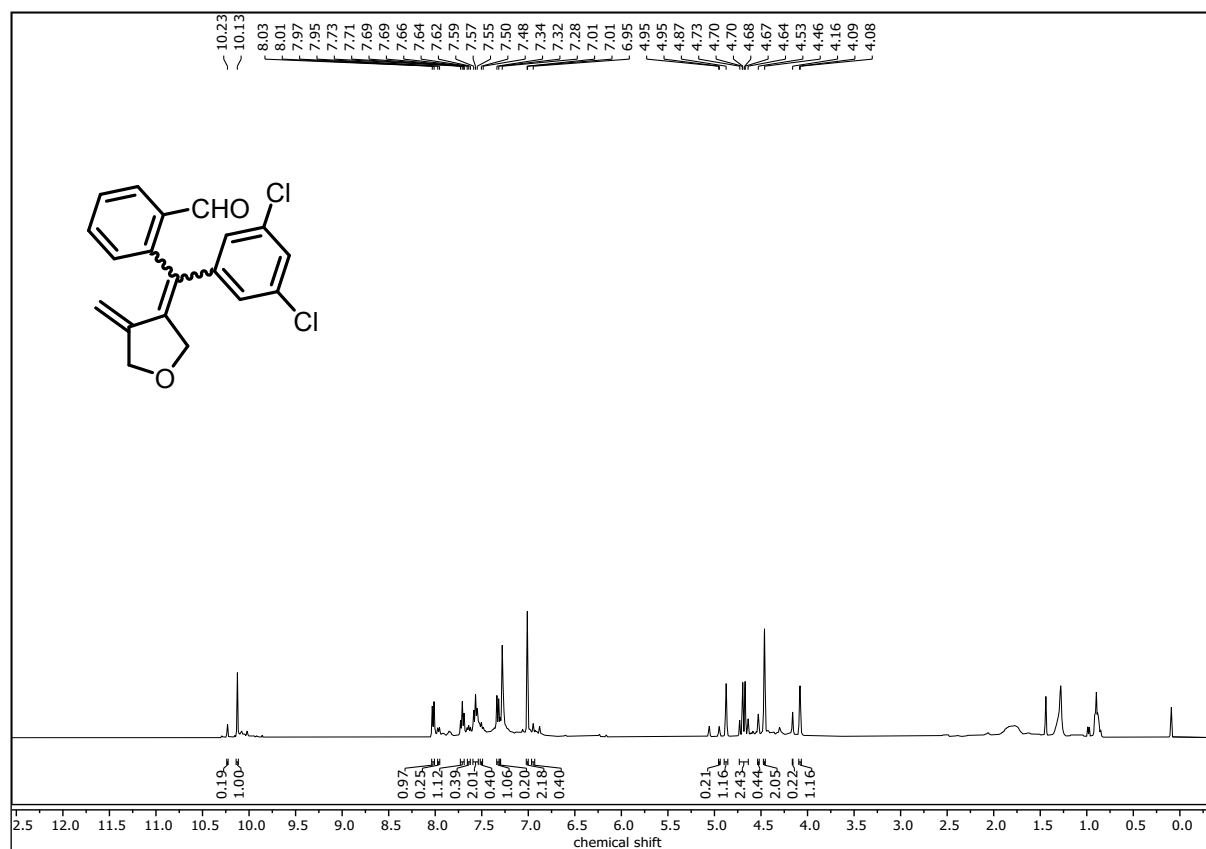
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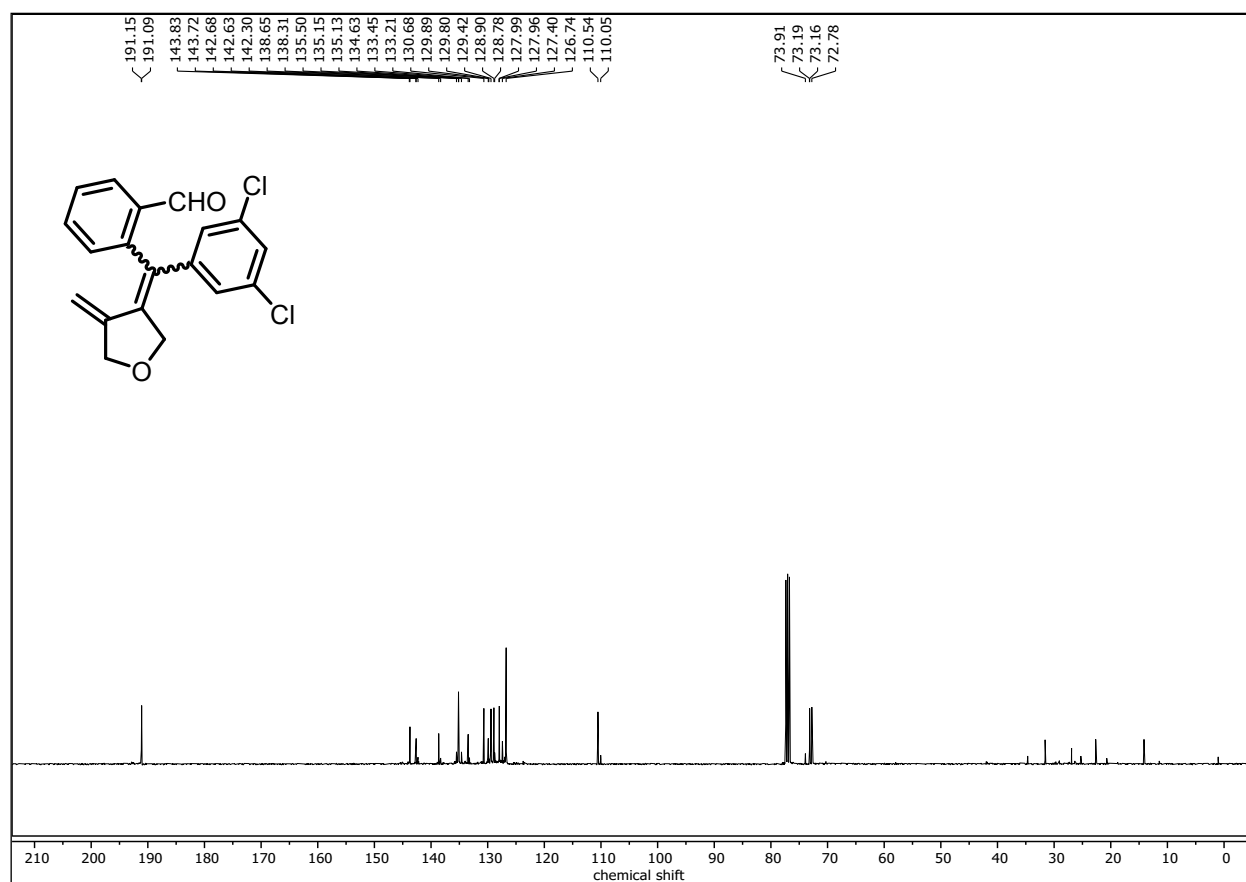
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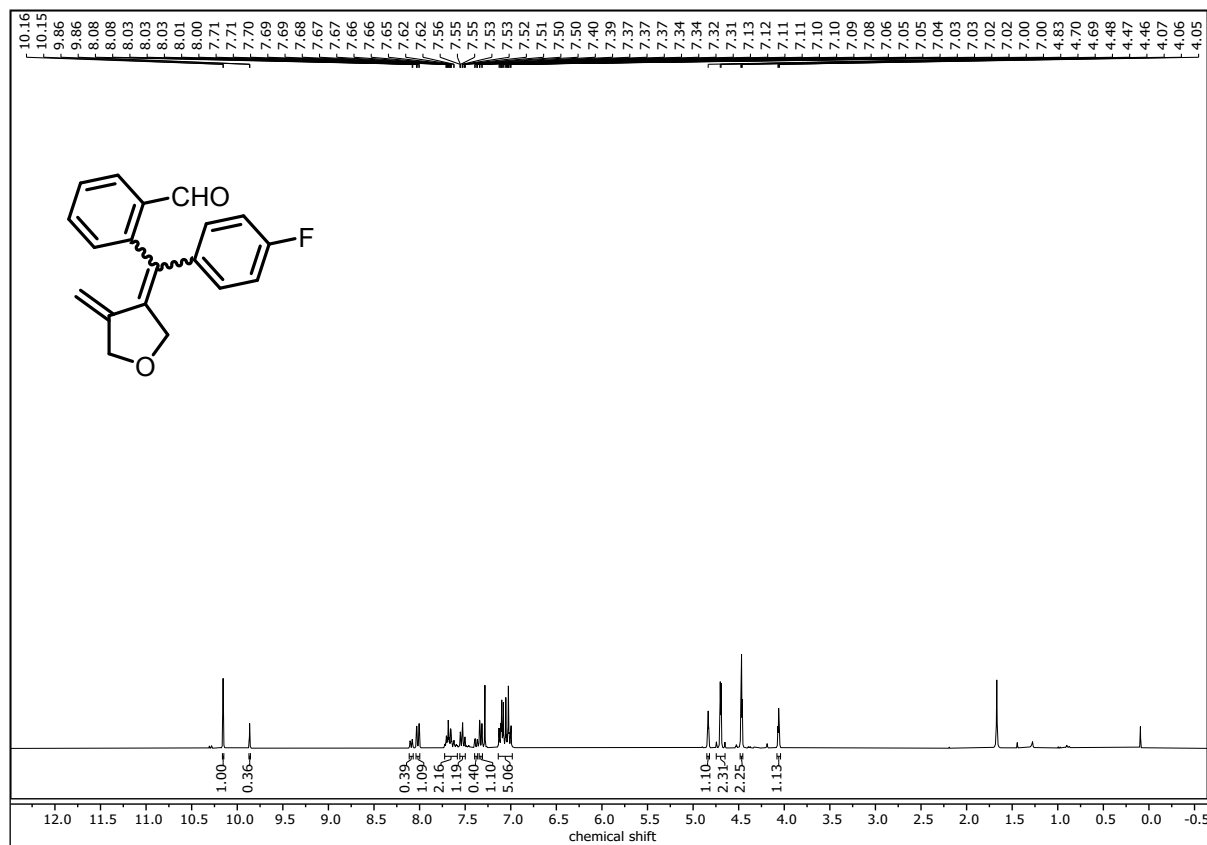
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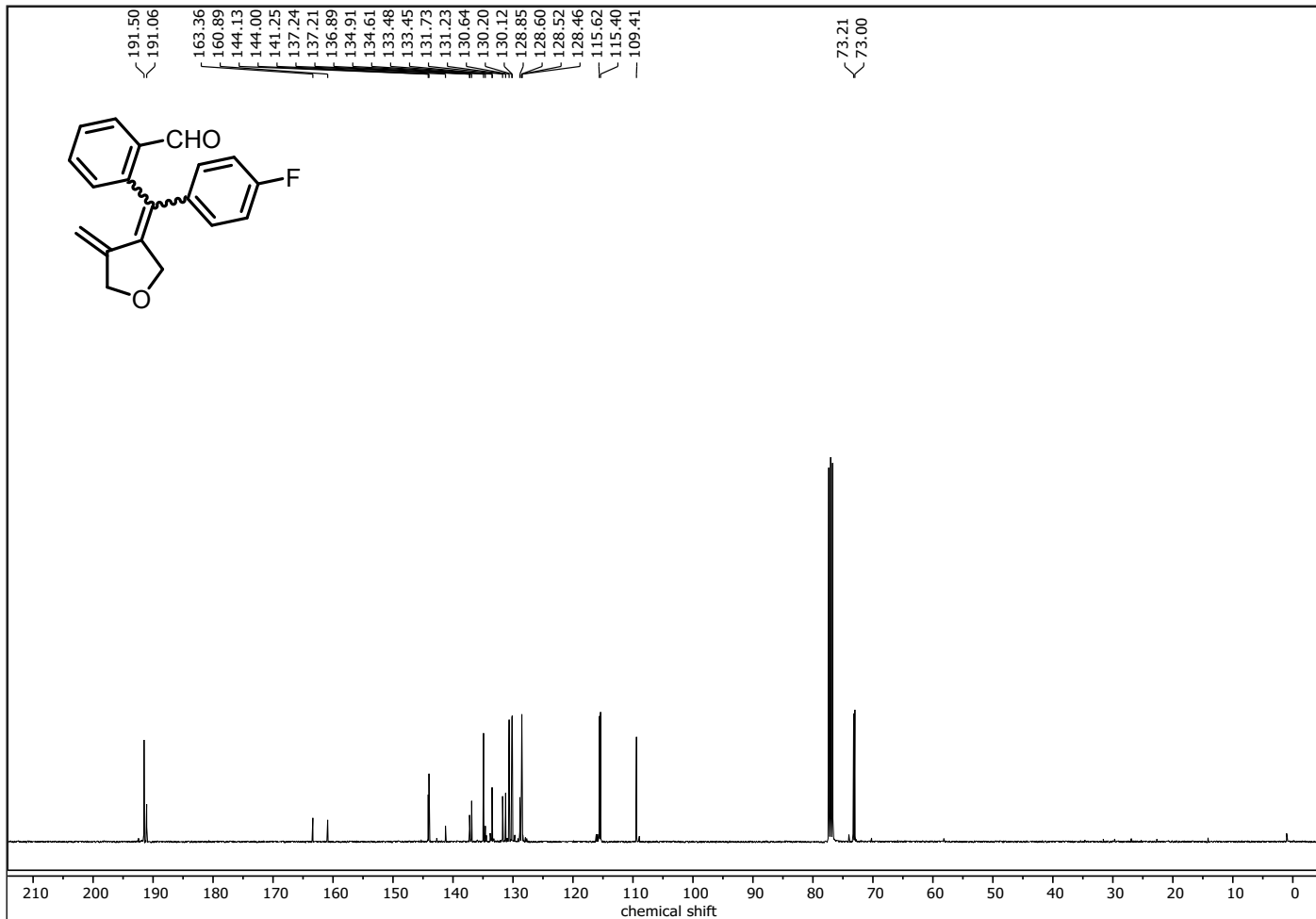
¹³C{¹H} (101 MHz, CDCl₃) NMR Spectrum of 6e.



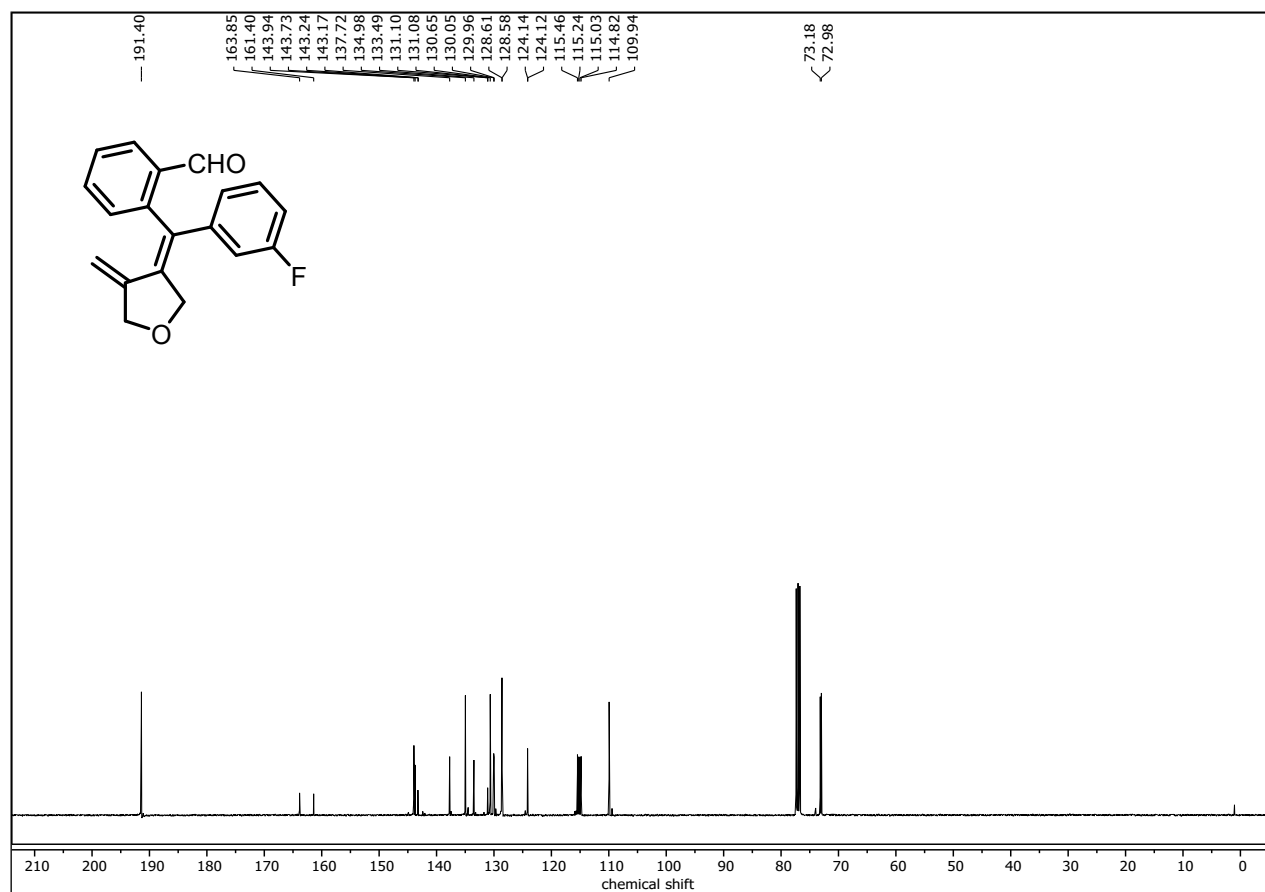
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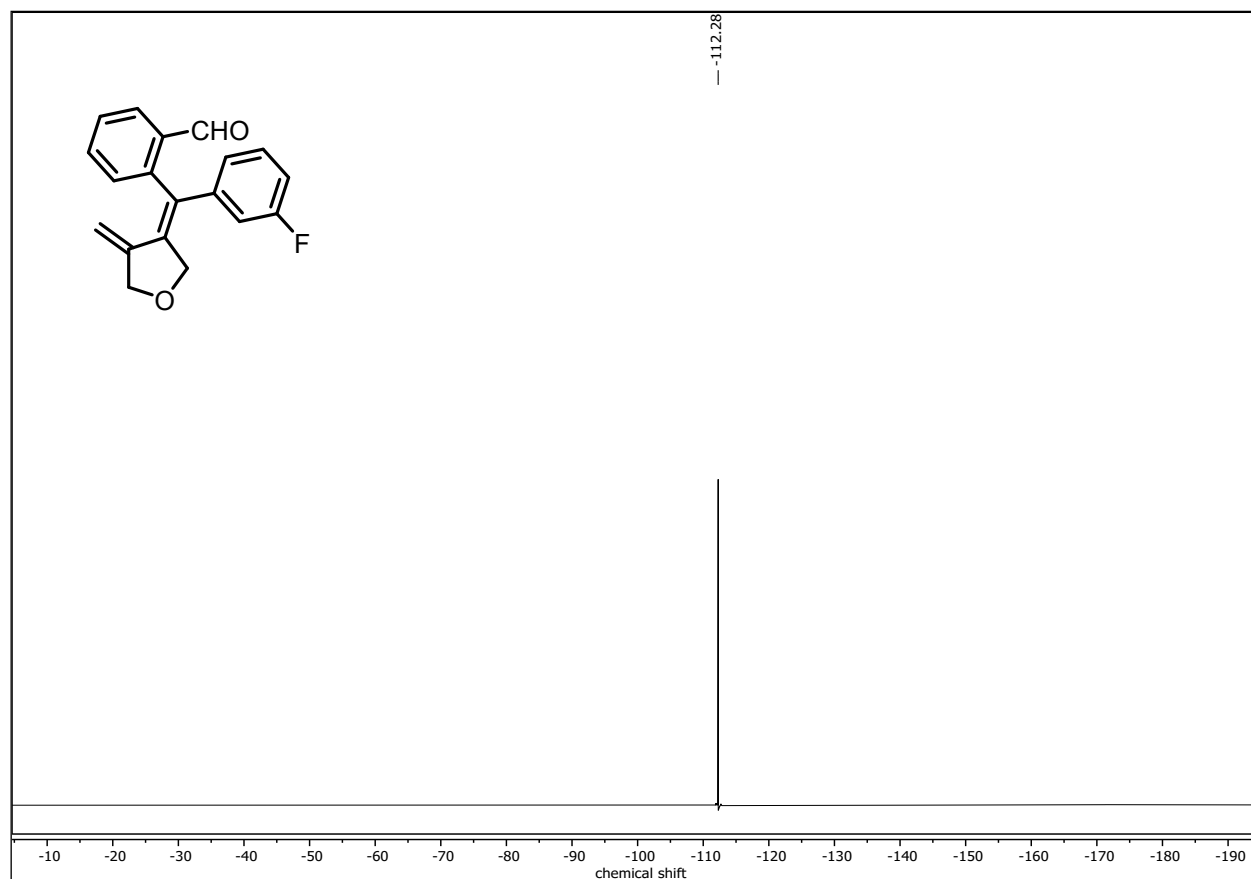
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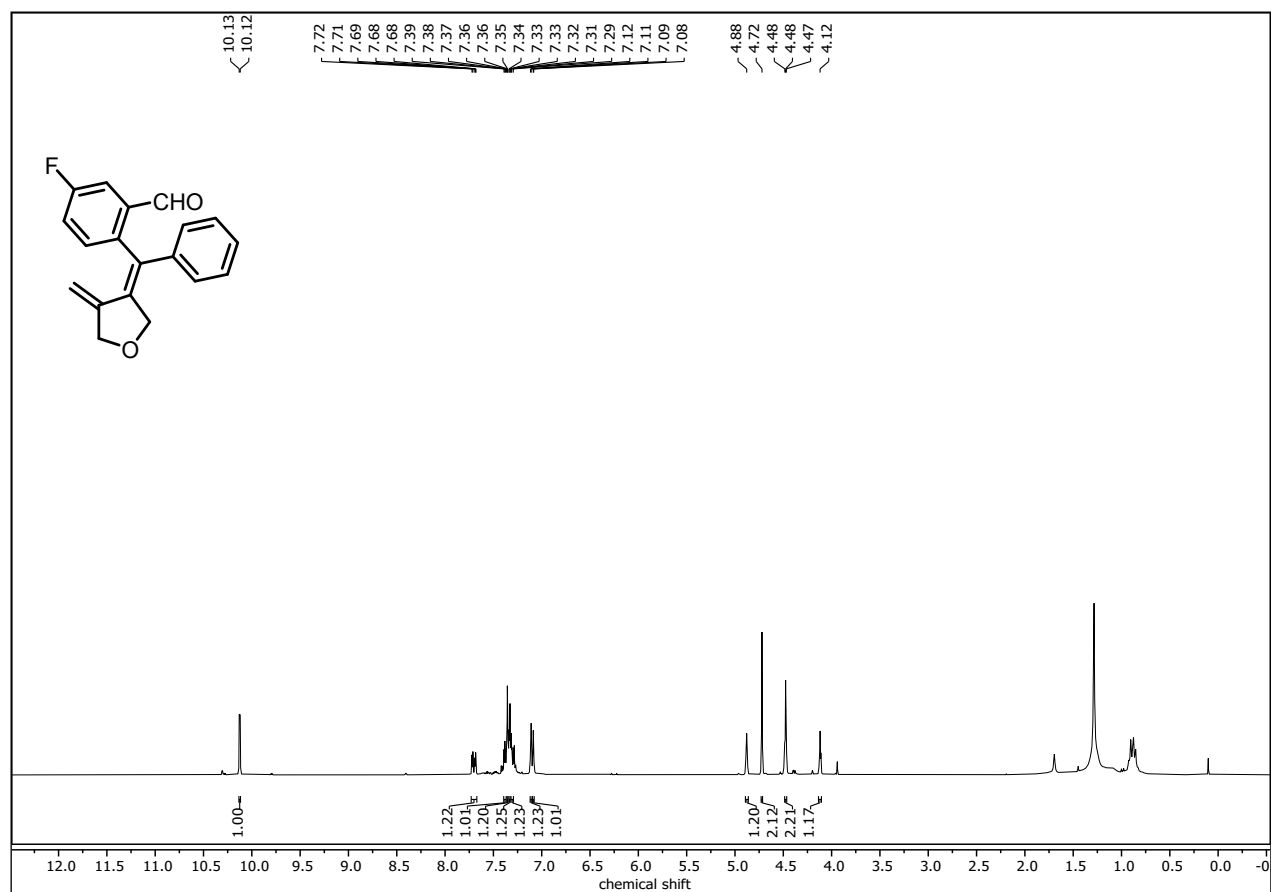
$^{13}\text{C}\{^1\text{H}\}$ (101 MHz, CDCl_3) NMR Spectrum of 6g.



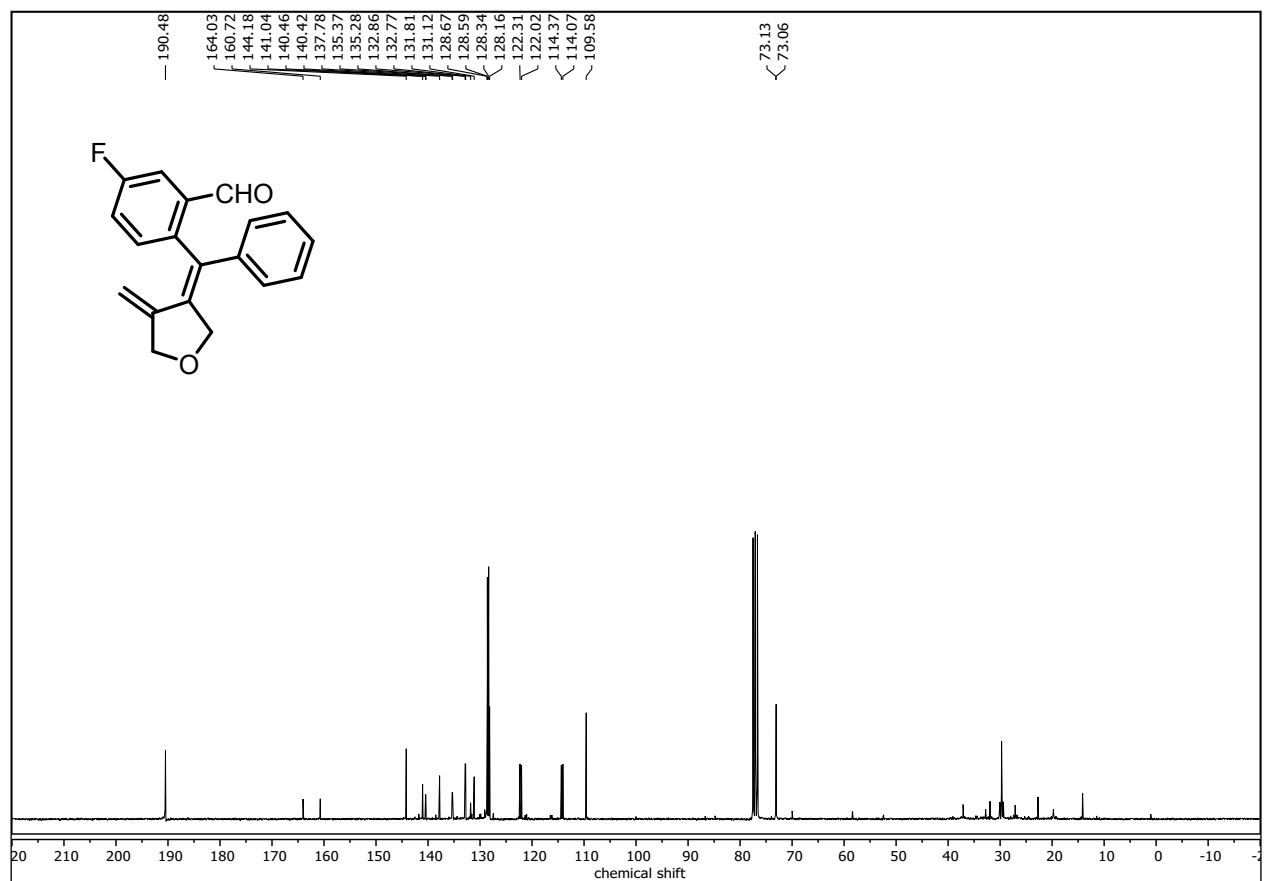
^{19}F NMR (377 MHz, CDCl_3) Spectrum of 6g.



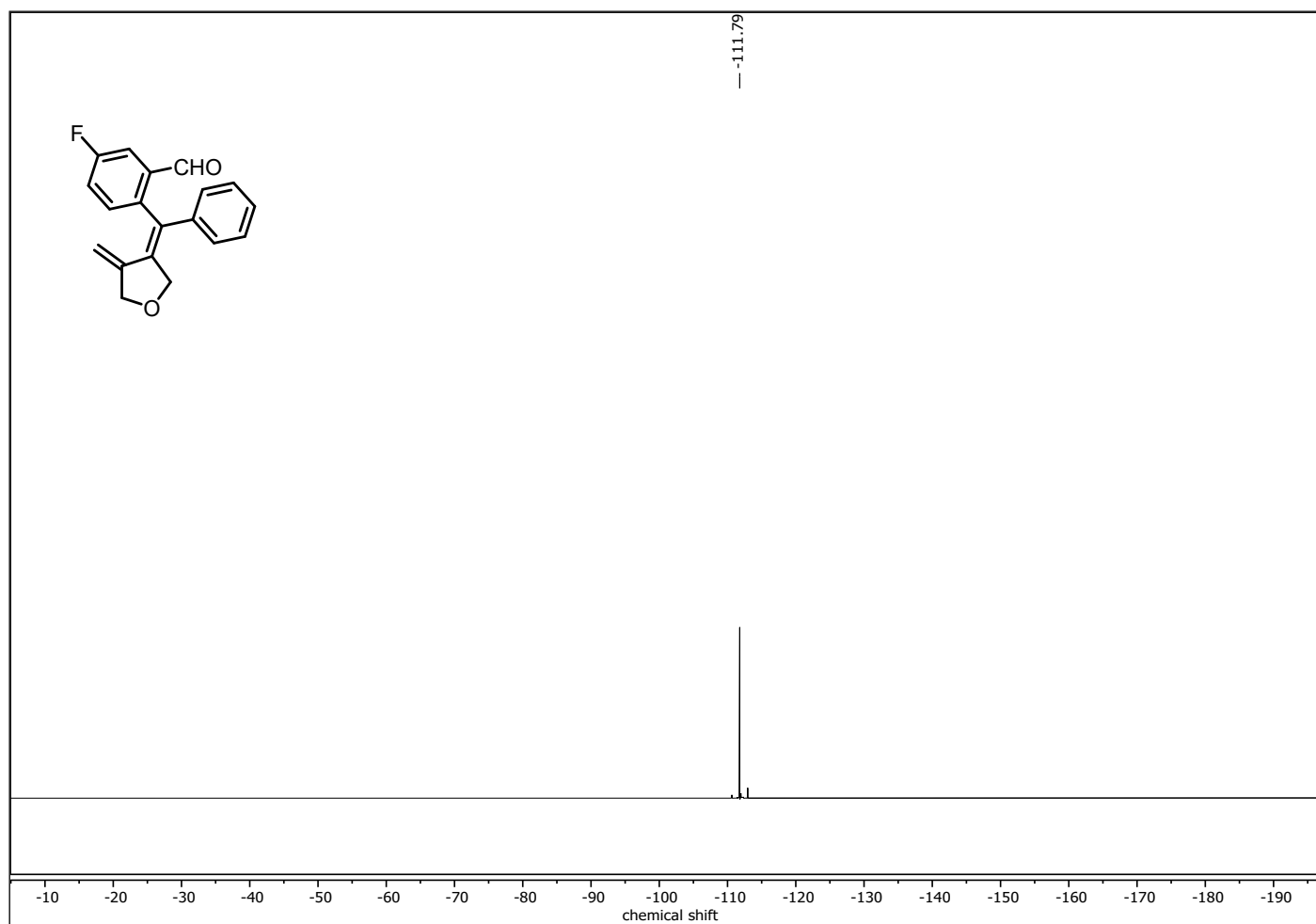
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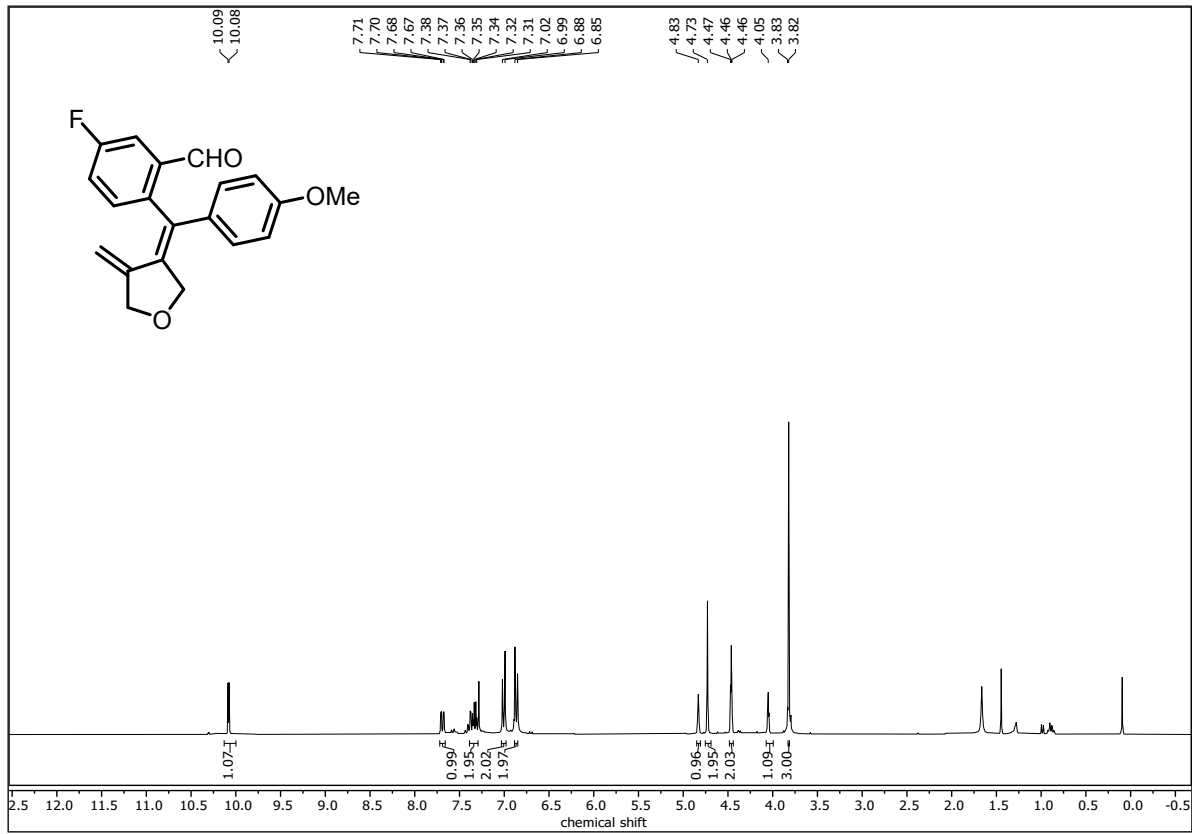
¹³C{¹H} (75 MHz, CDCl₃) NMR Spectrum of 6h.



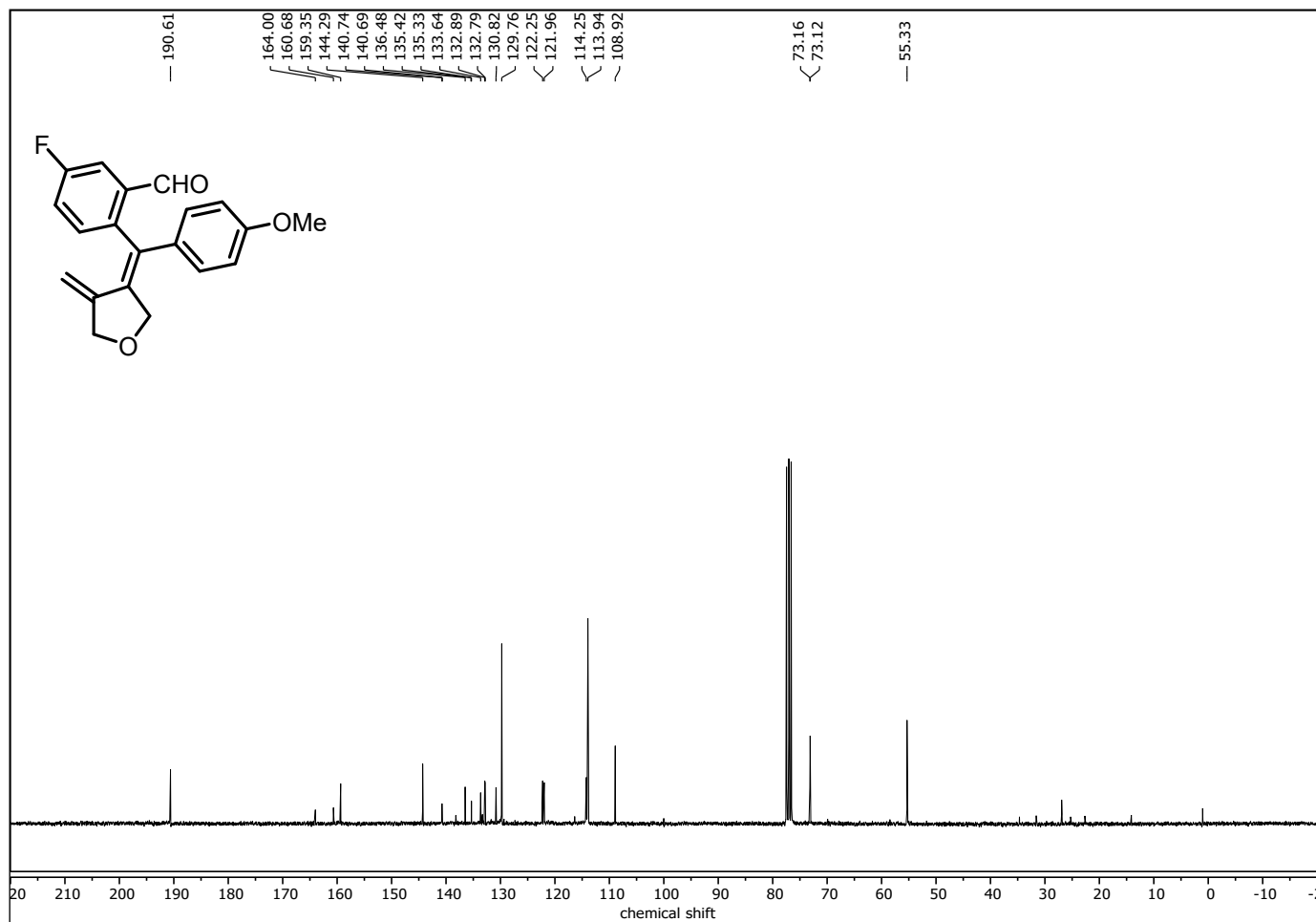
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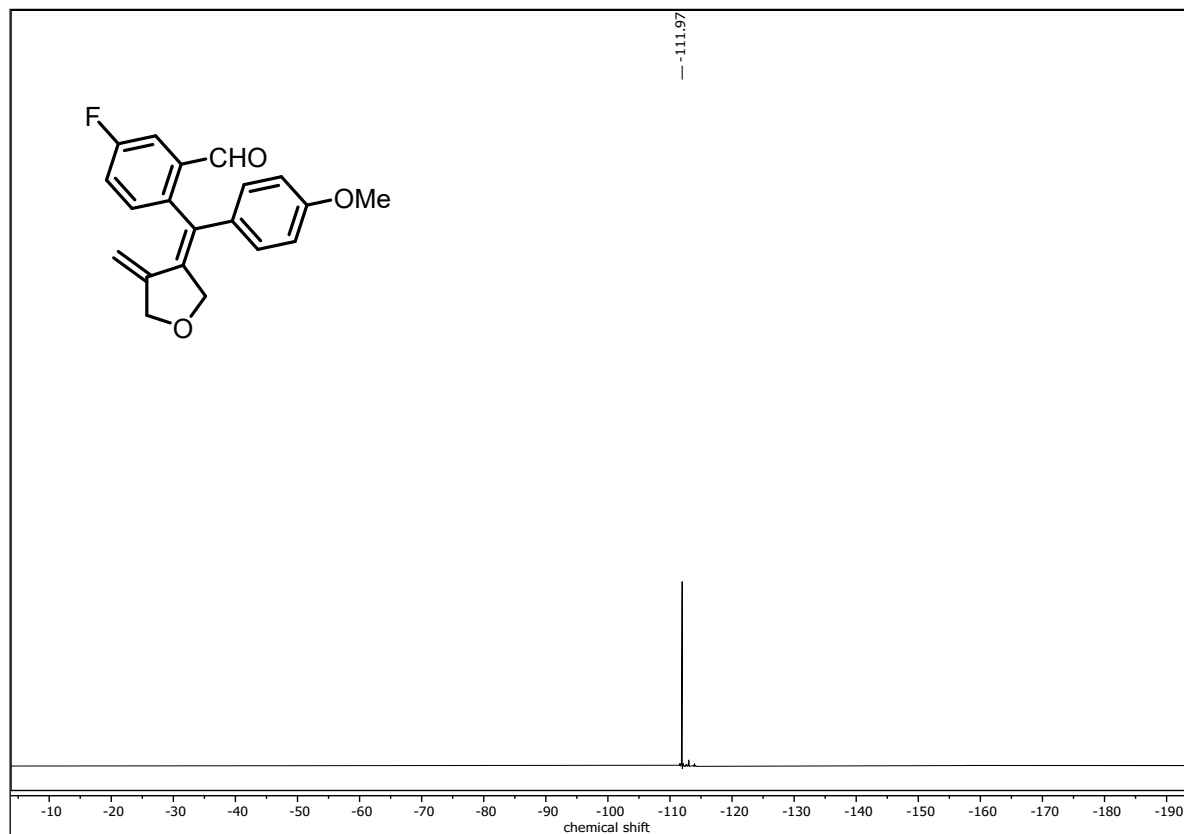
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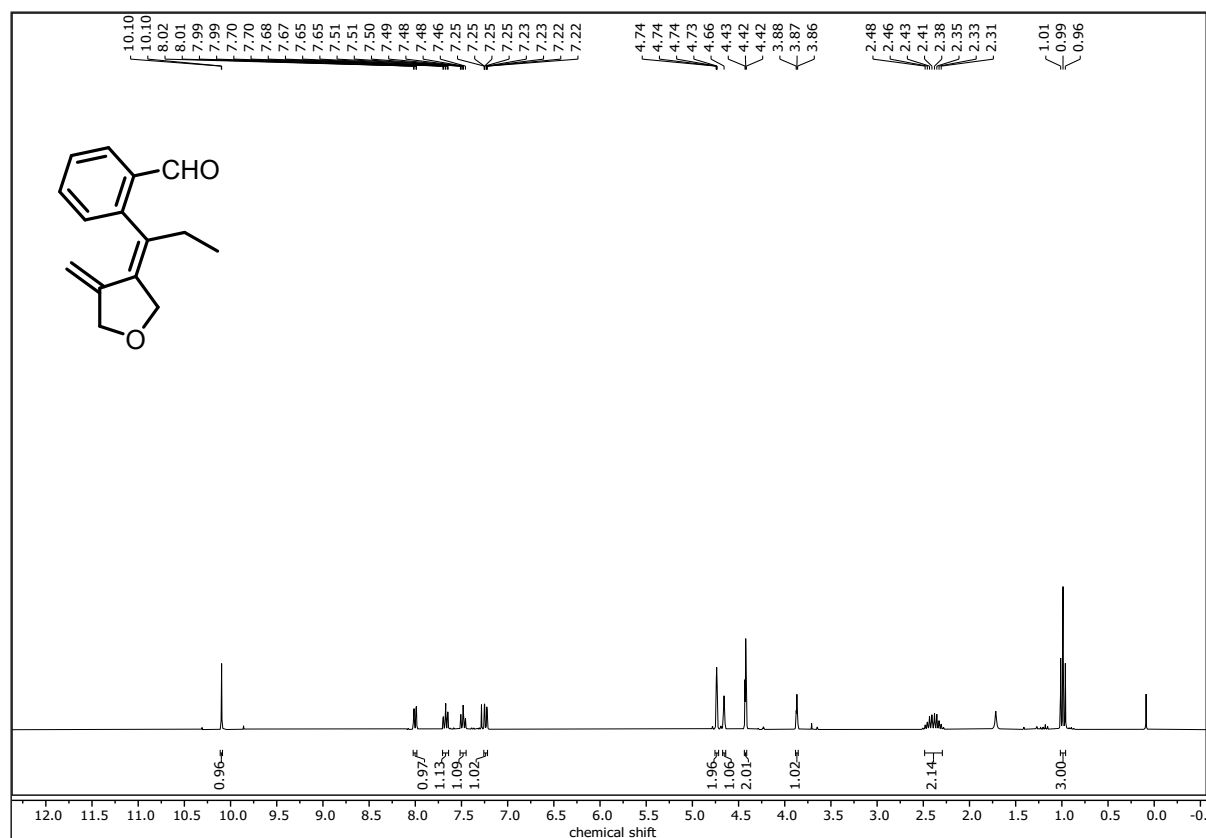
$^{13}\text{C}\{^1\text{H}\}$ (75 MHz, CDCl_3) NMR Spectrum of 6i.



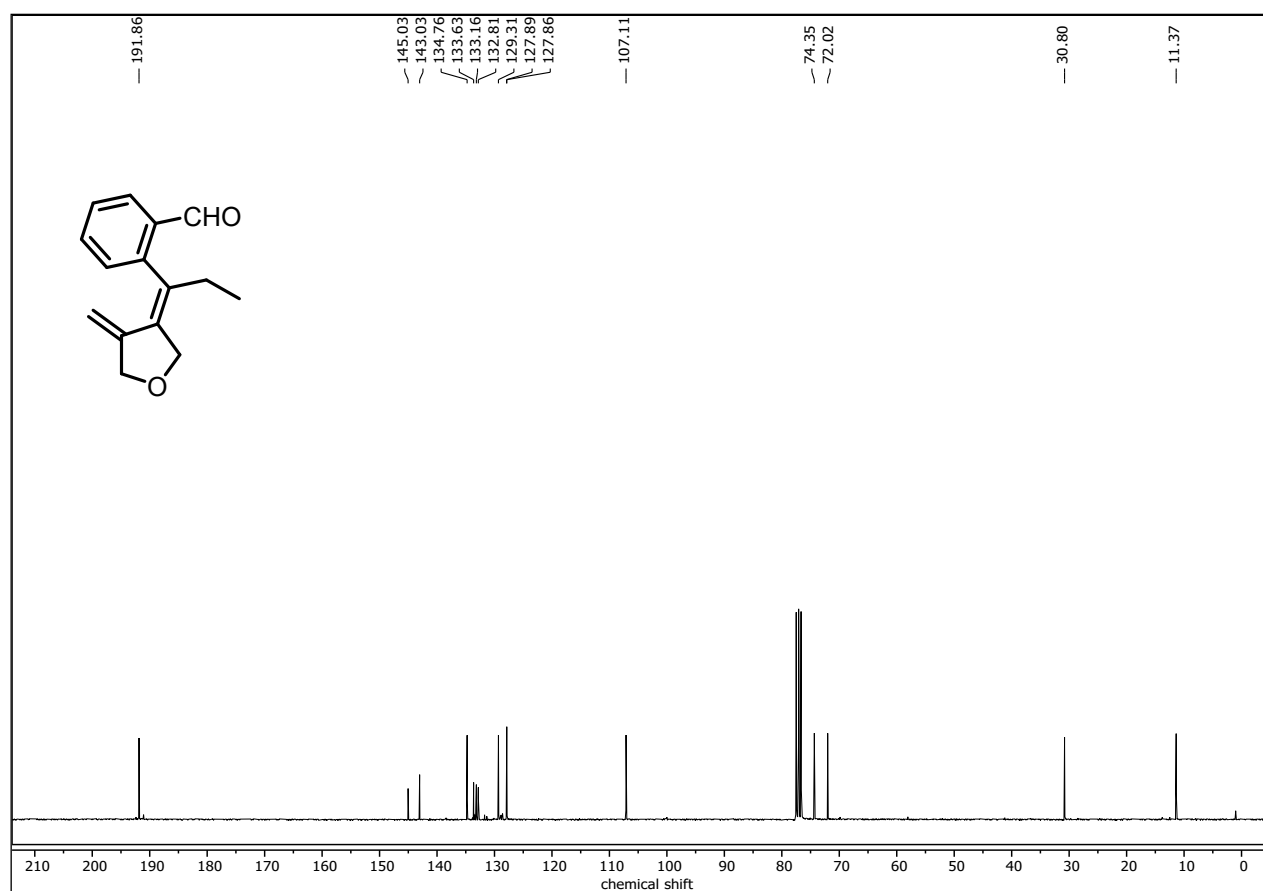
^{19}F NMR (282 MHz, CDCl_3) Spectrum of 6i.



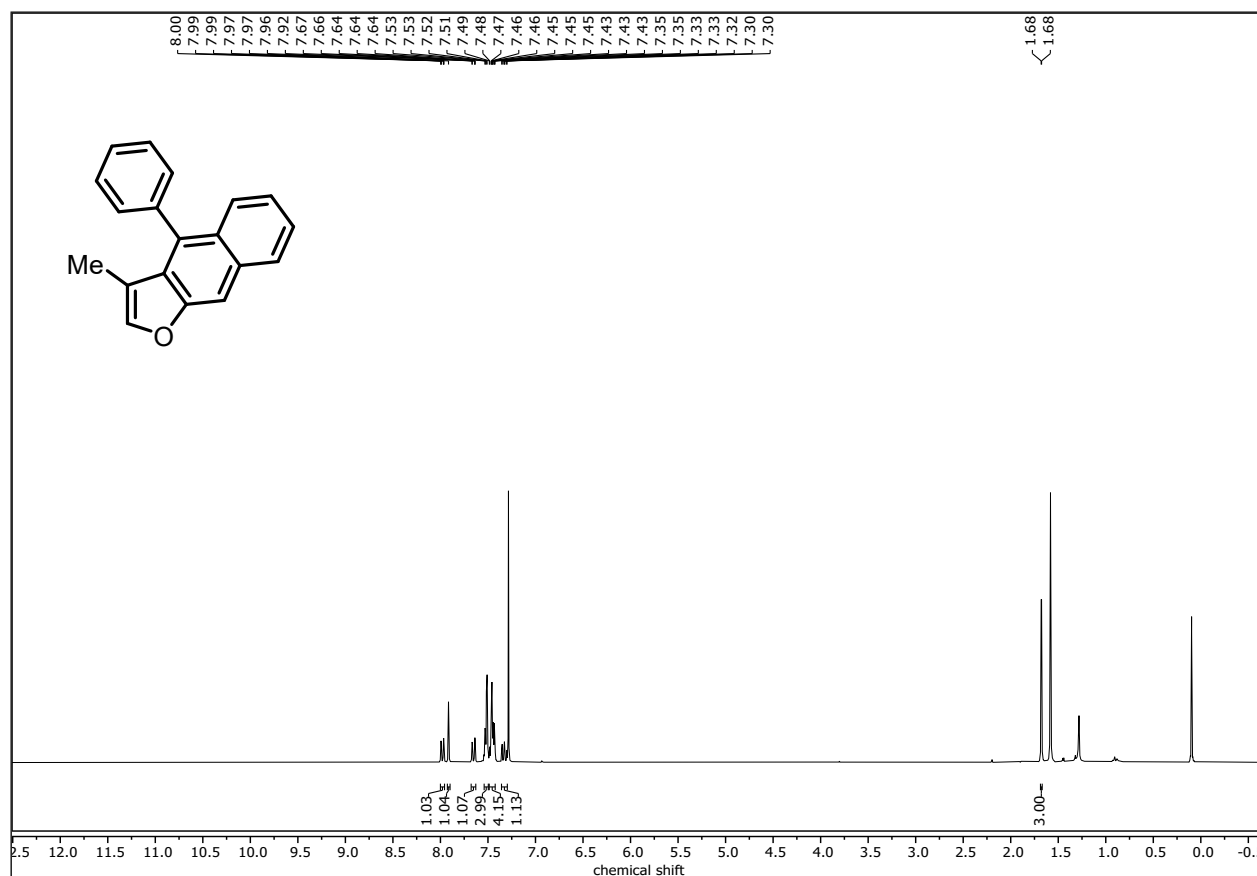
¹H NMR (300 MHz, CDCl₃) Spectrum of 6k.



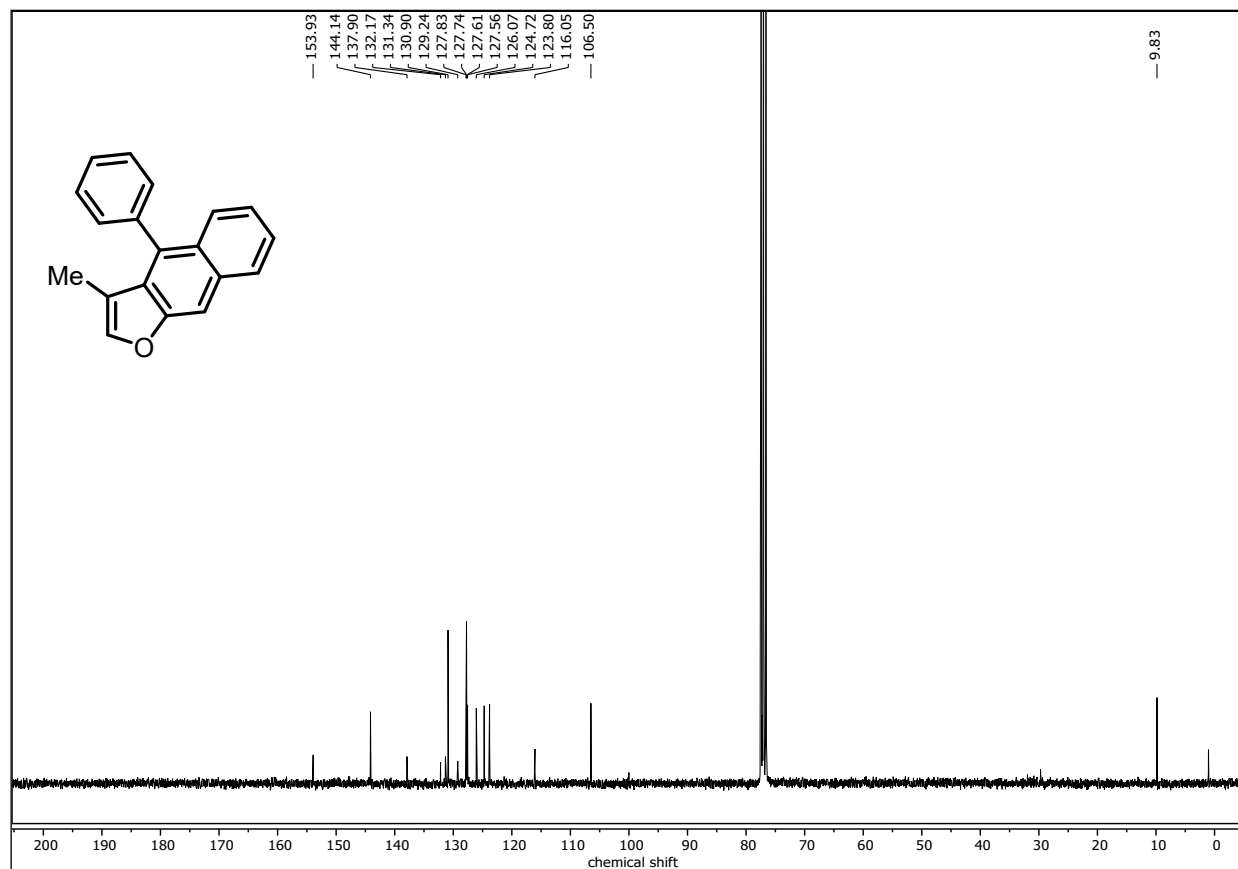
¹³C{¹H} (75 MHz, CDCl₃) NMR Spectrum of 6k.



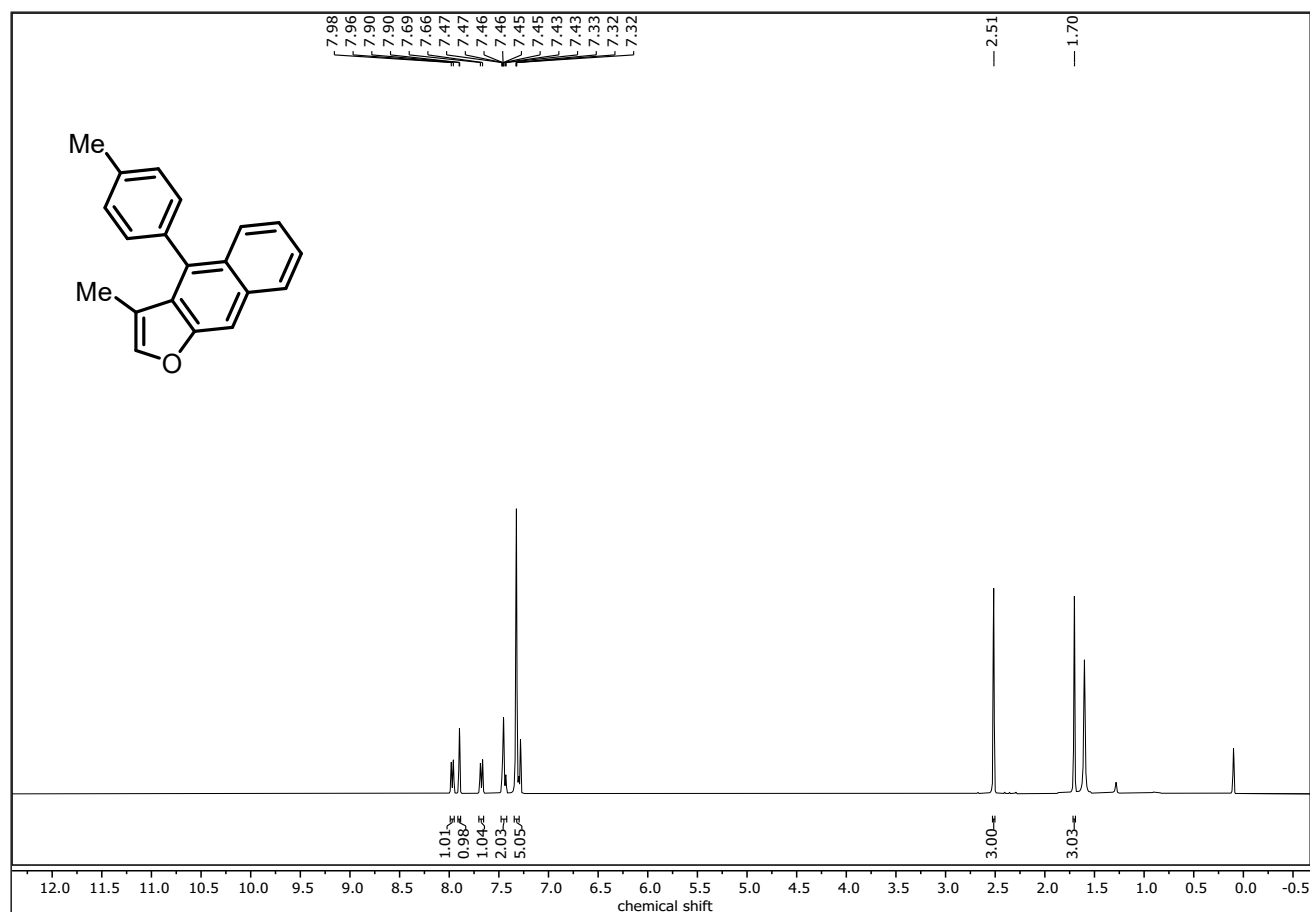
¹H NMR (300 MHz, CDCl₃) Spectrum of 7a.



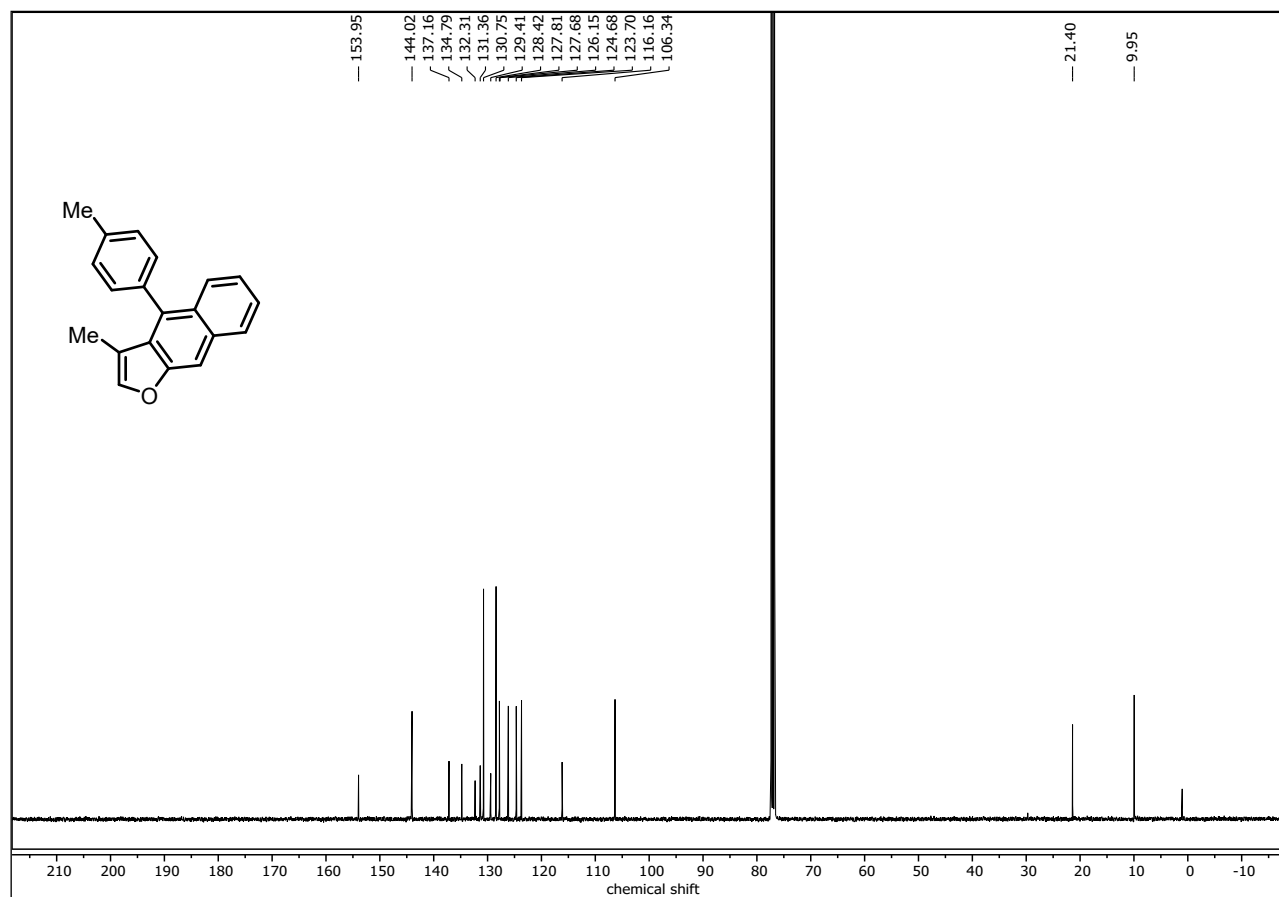
¹³C{¹H} (75 MHz, CDCl₃) NMR Spectrum of 7a.



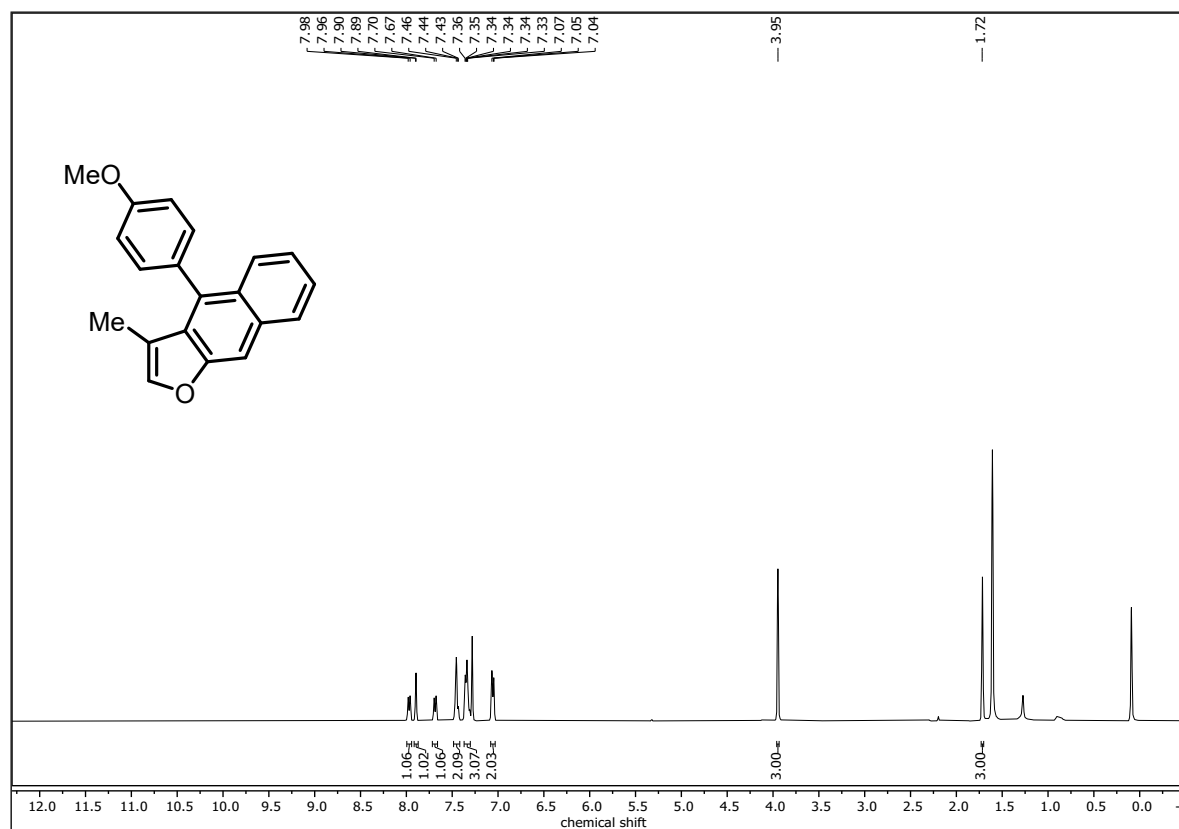
¹H NMR (400 MHz, CDCl₃) Spectrum of 7b.



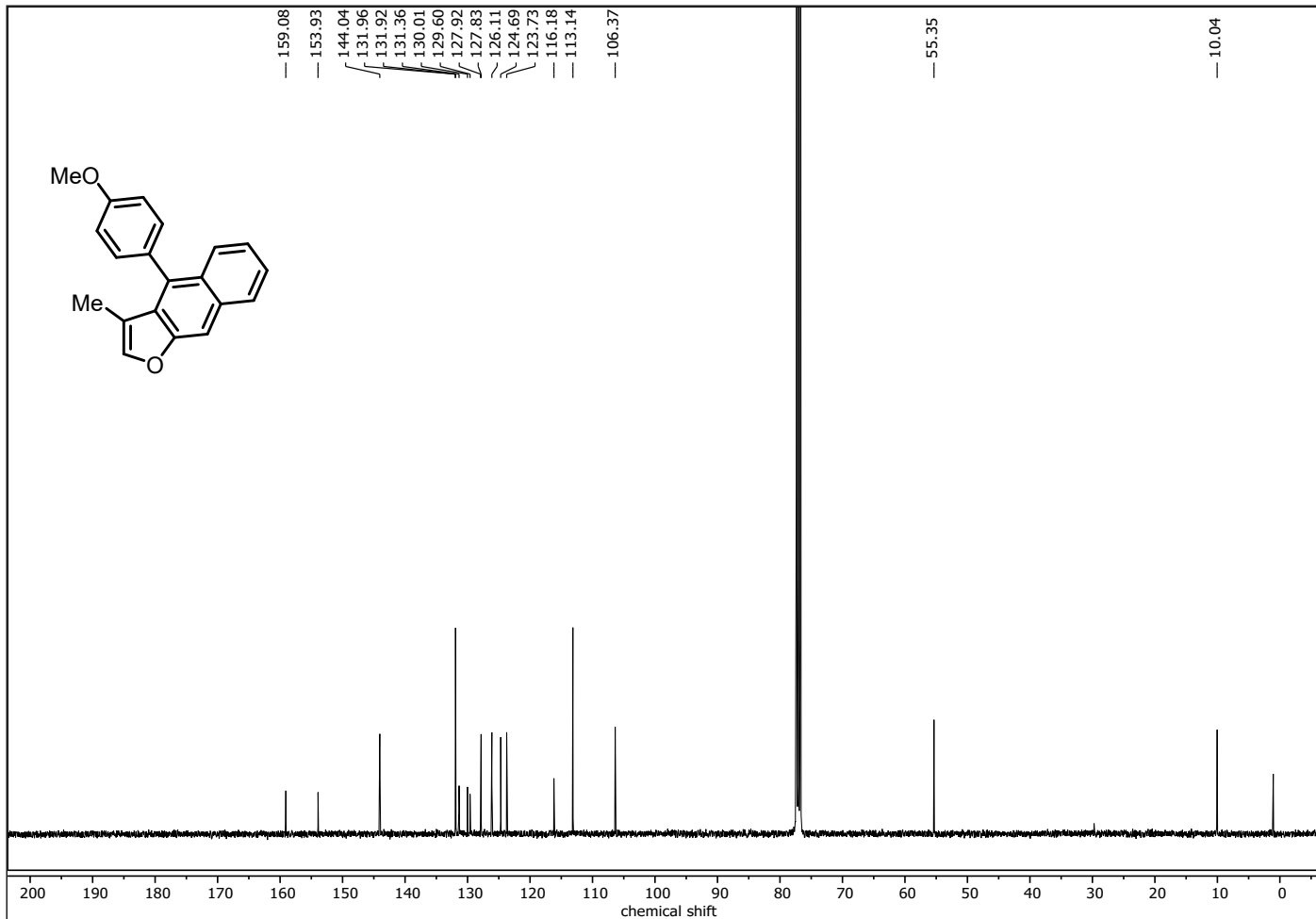
¹³C{¹H} (101 MHz, CDCl₃) NMR Spectrum of 7b.



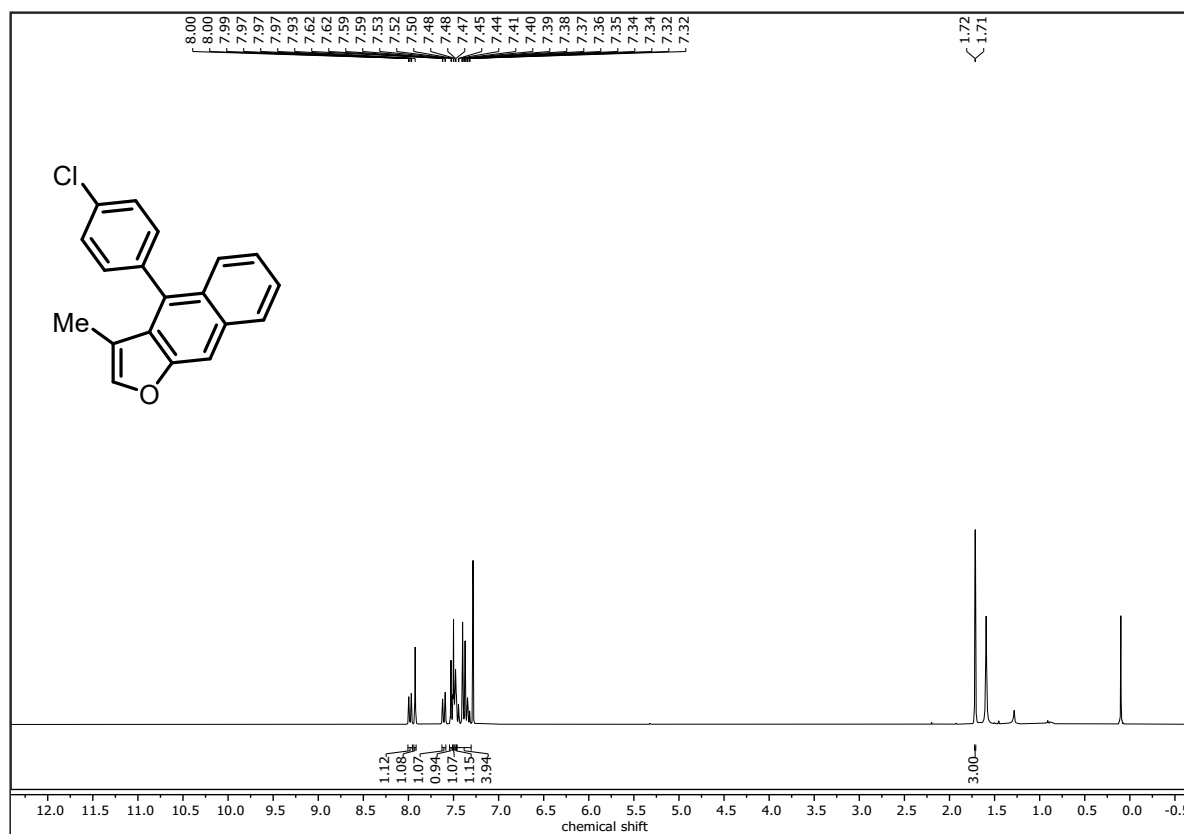
^1H NMR (400 MHz, CDCl_3) Spectrum of 7c.



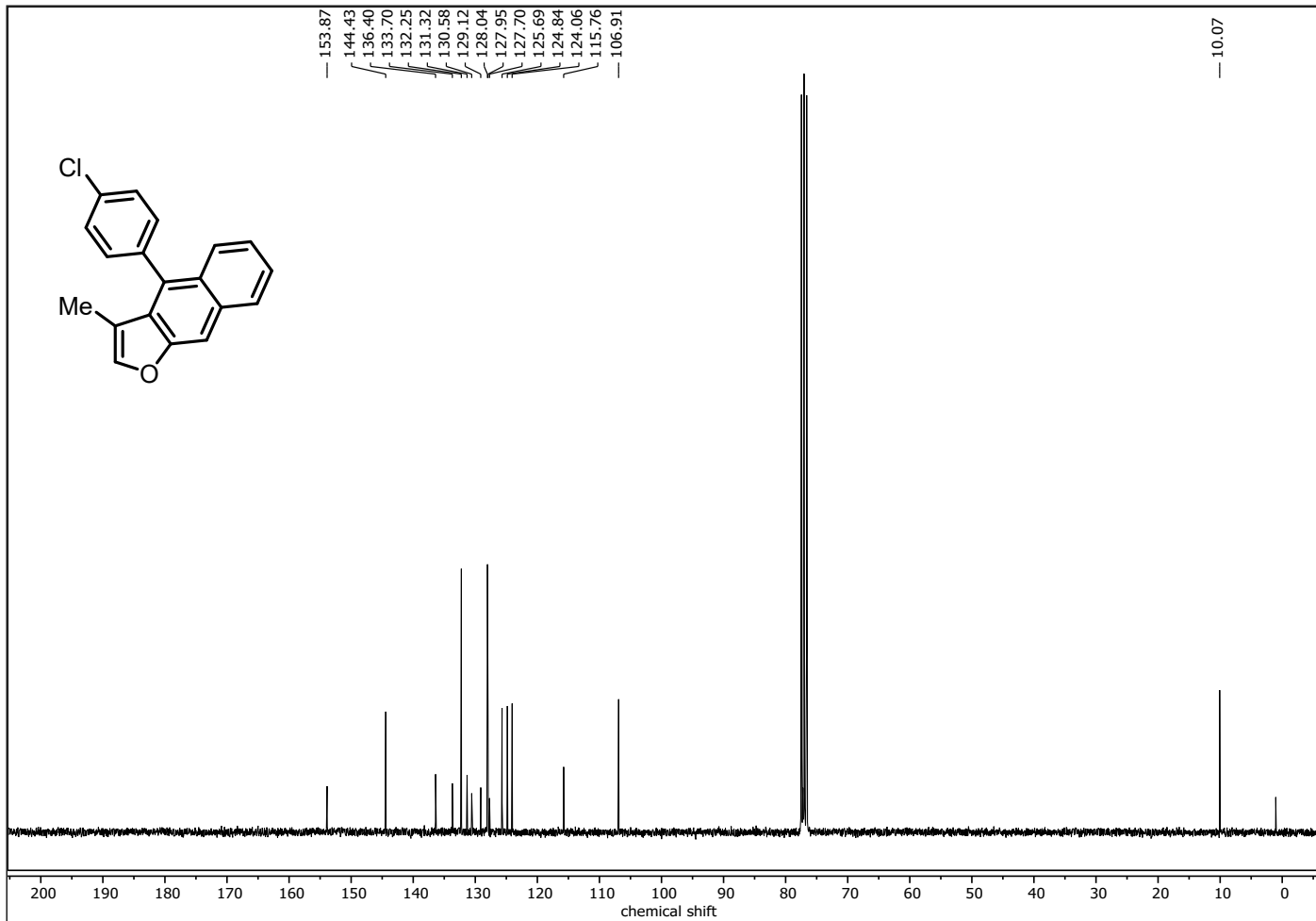
$^{13}\text{C}\{^1\text{H}\}$ (101 MHz, CDCl_3) NMR Spectrum of 7c.



^1H NMR (300 MHz, CDCl_3) Spectrum of 7d.



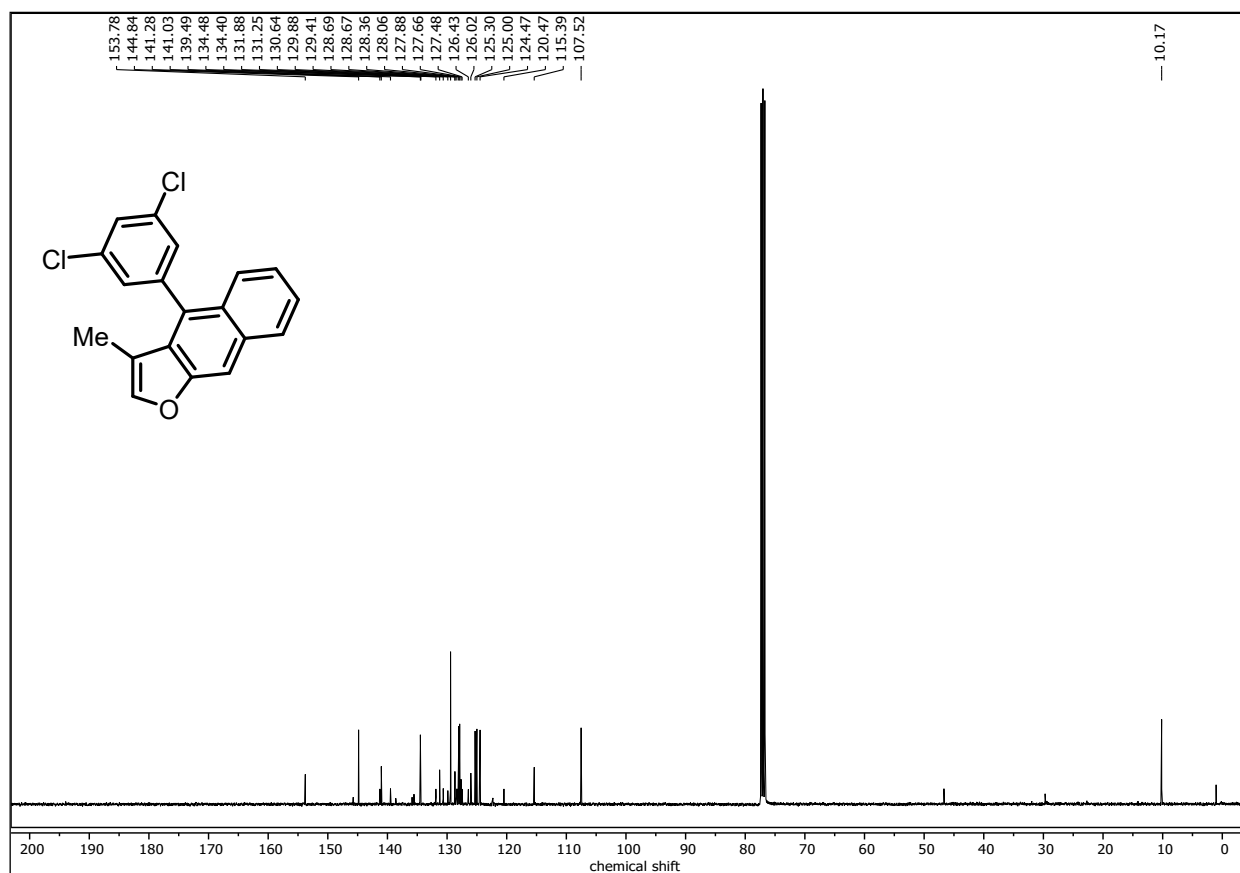
$^{13}\text{C}\{^1\text{H}\}$ (75 MHz, CDCl_3) NMR Spectrum of 7d.



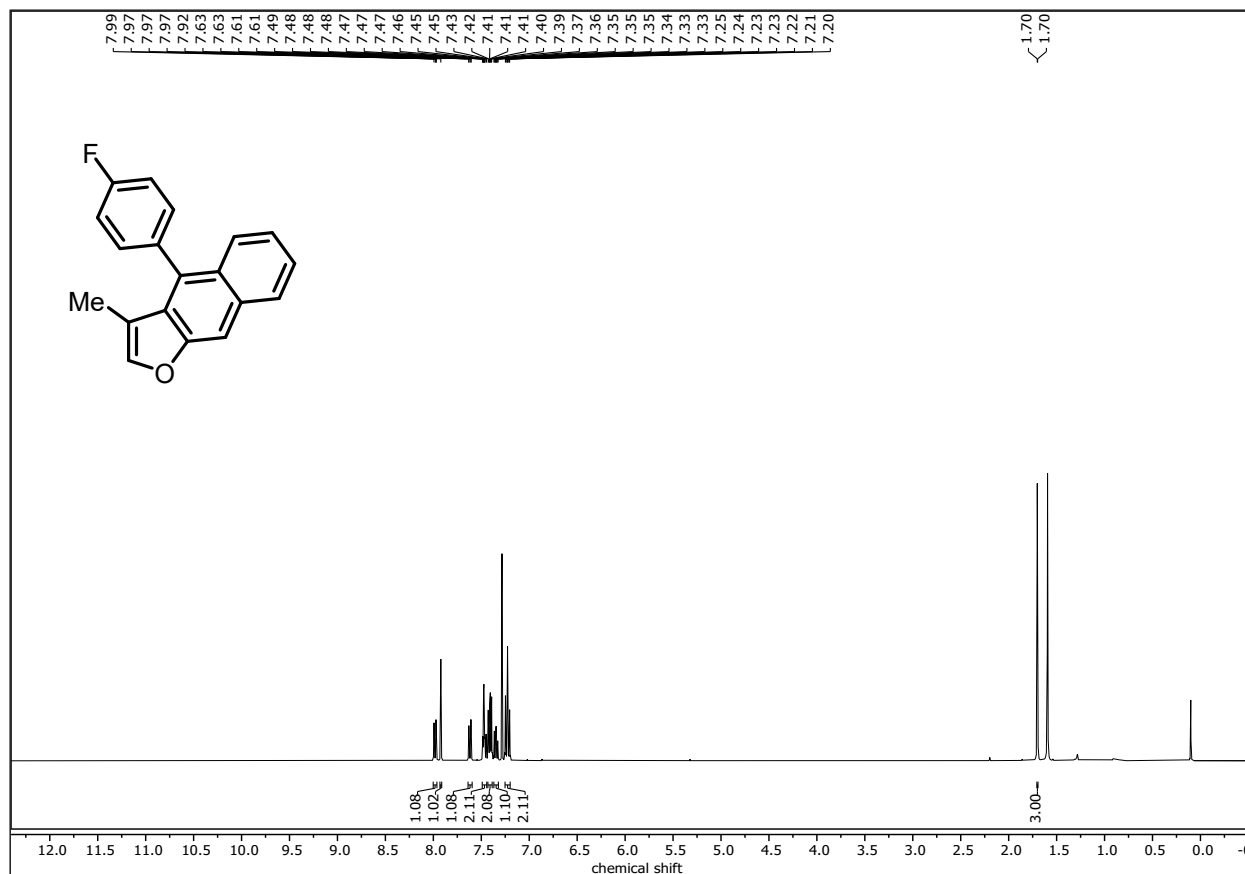
^1H NMR (400 MHz, CDCl_3) Spectrum of 7e.



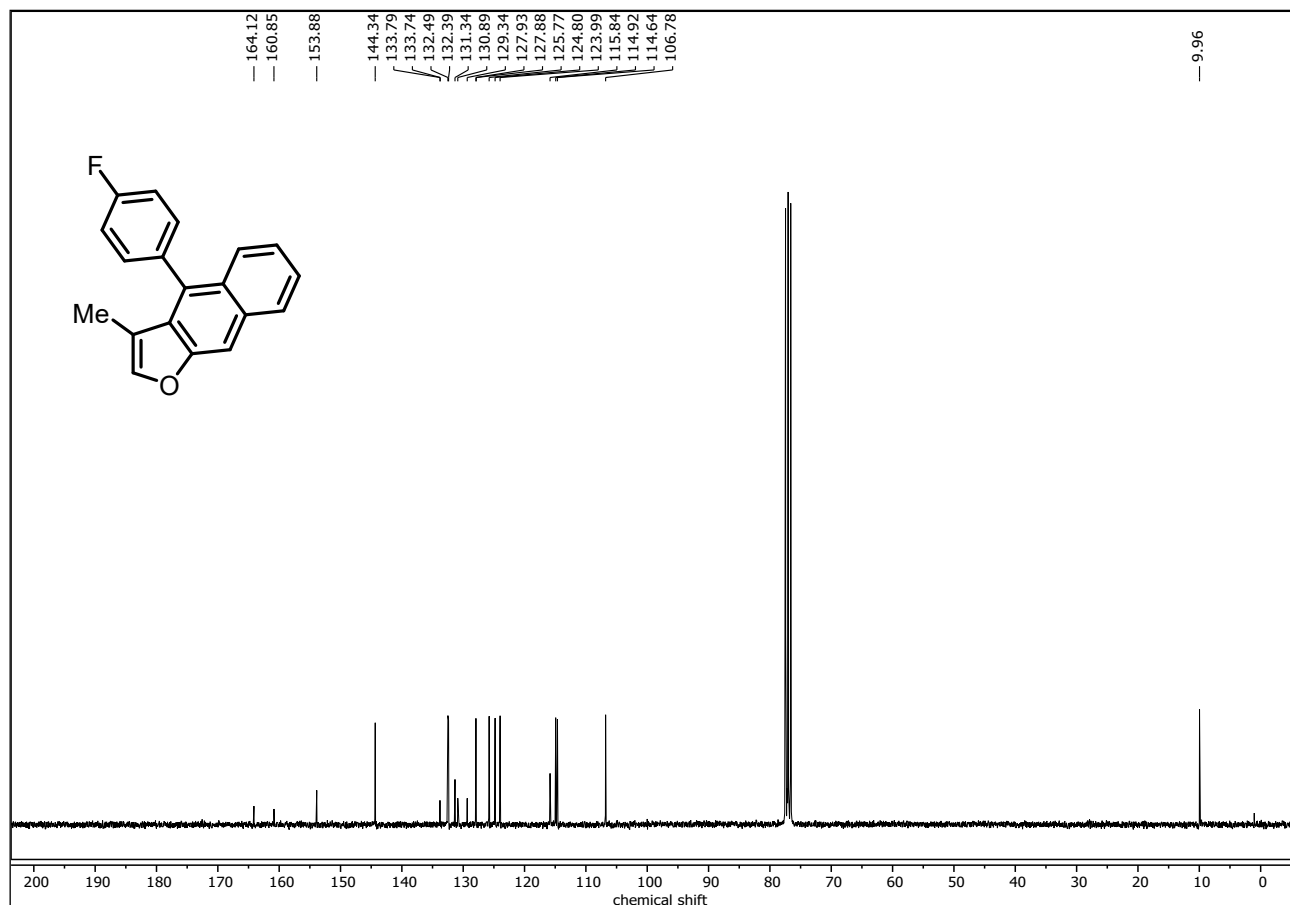
$^{13}\text{C}\{^1\text{H}\}$ (101 MHz, CDCl_3) NMR Spectrum of 7e.



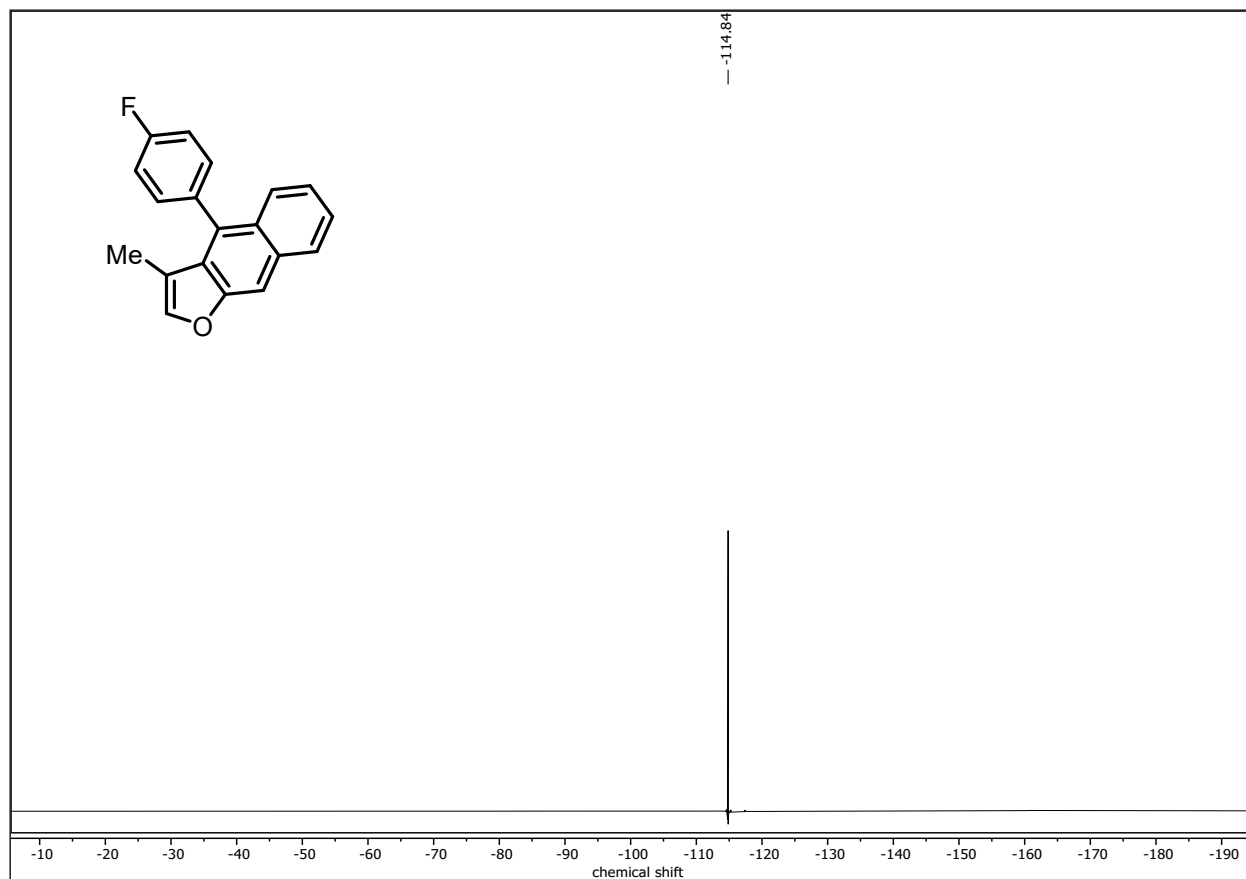
^1H NMR (400 MHz, CDCl_3) Spectrum of 7f.



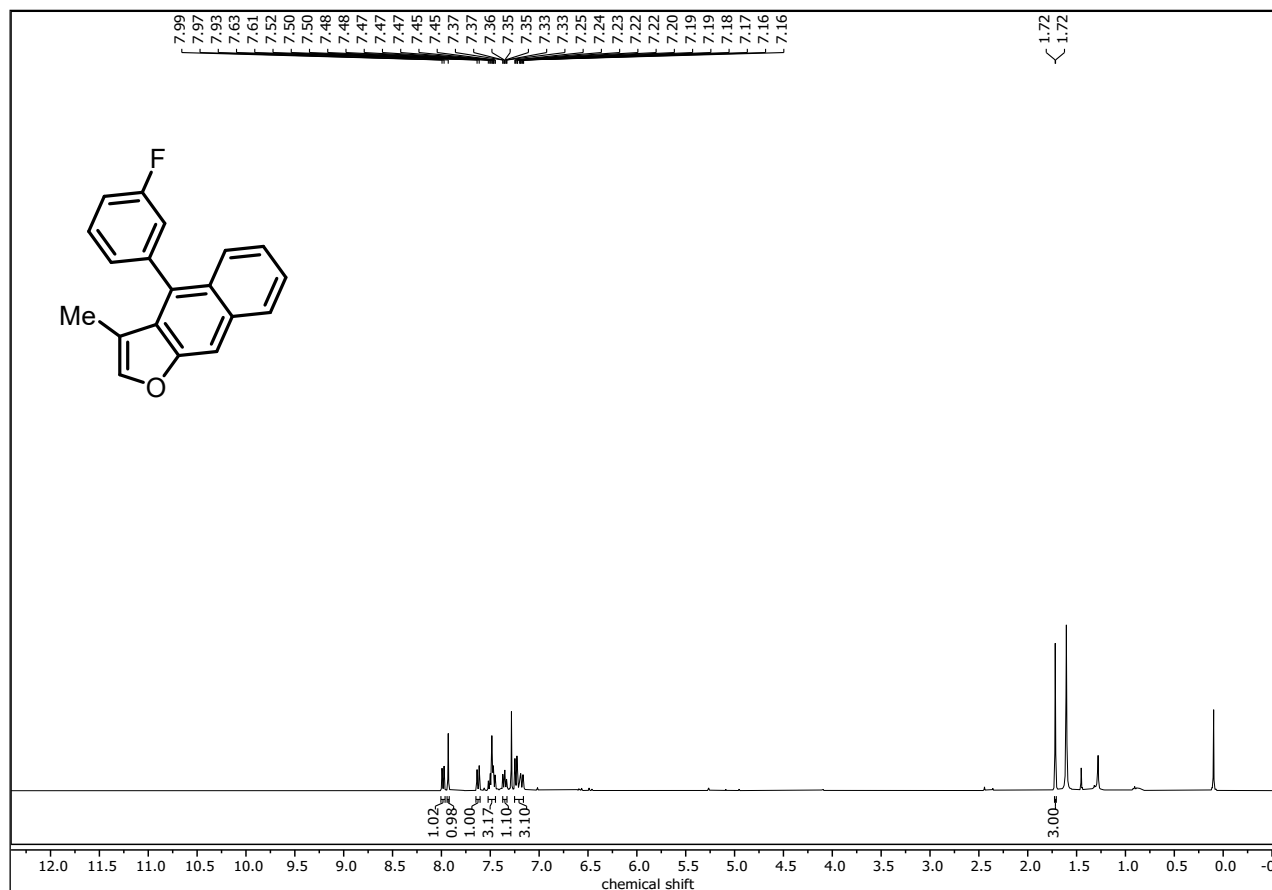
$^{13}\text{C}\{^1\text{H}\}$ (75 MHz, CDCl_3) NMR Spectrum of 7f.



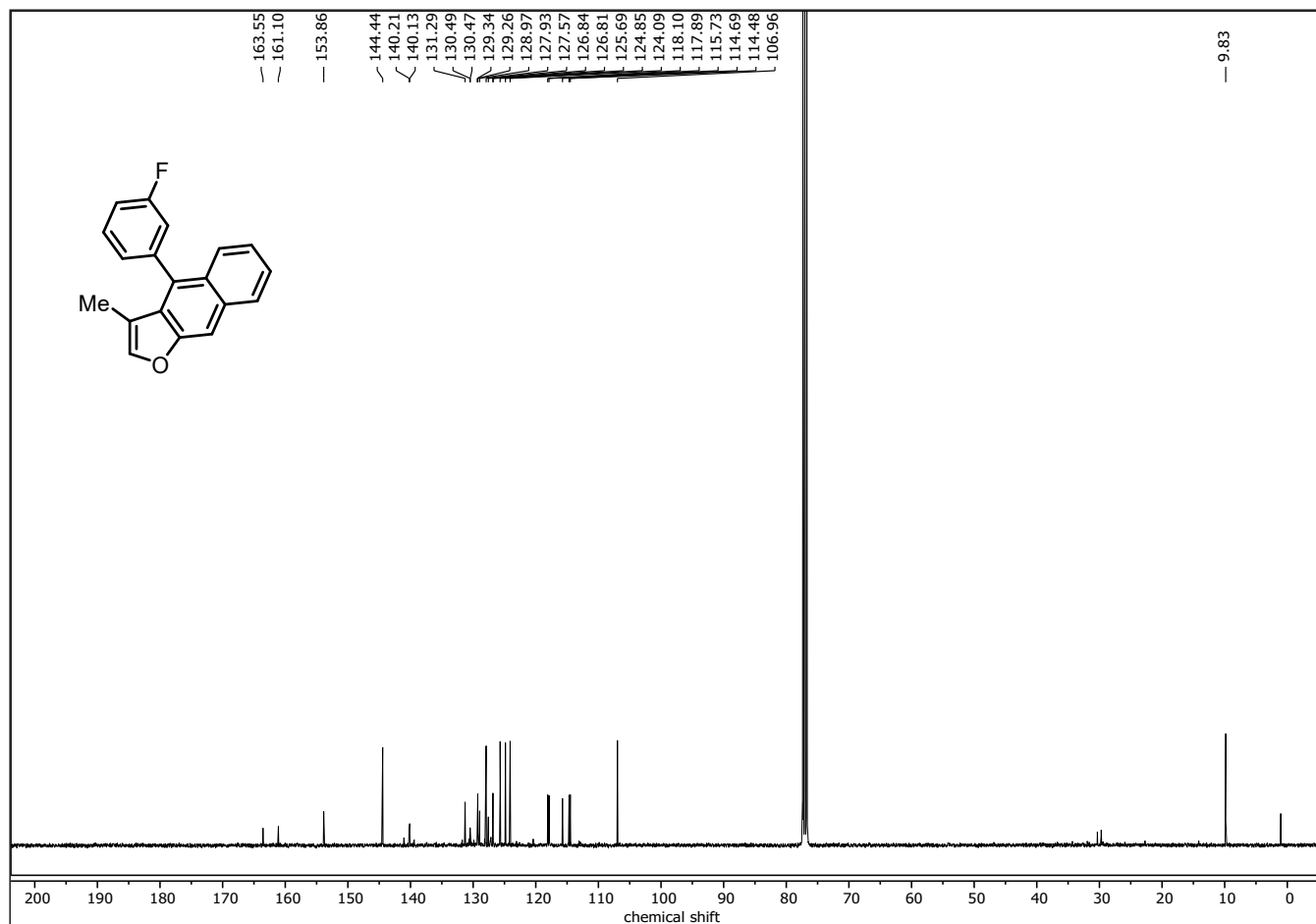
¹⁹F NMR (377 MHz, CDCl₃) Spectrum of 7f.



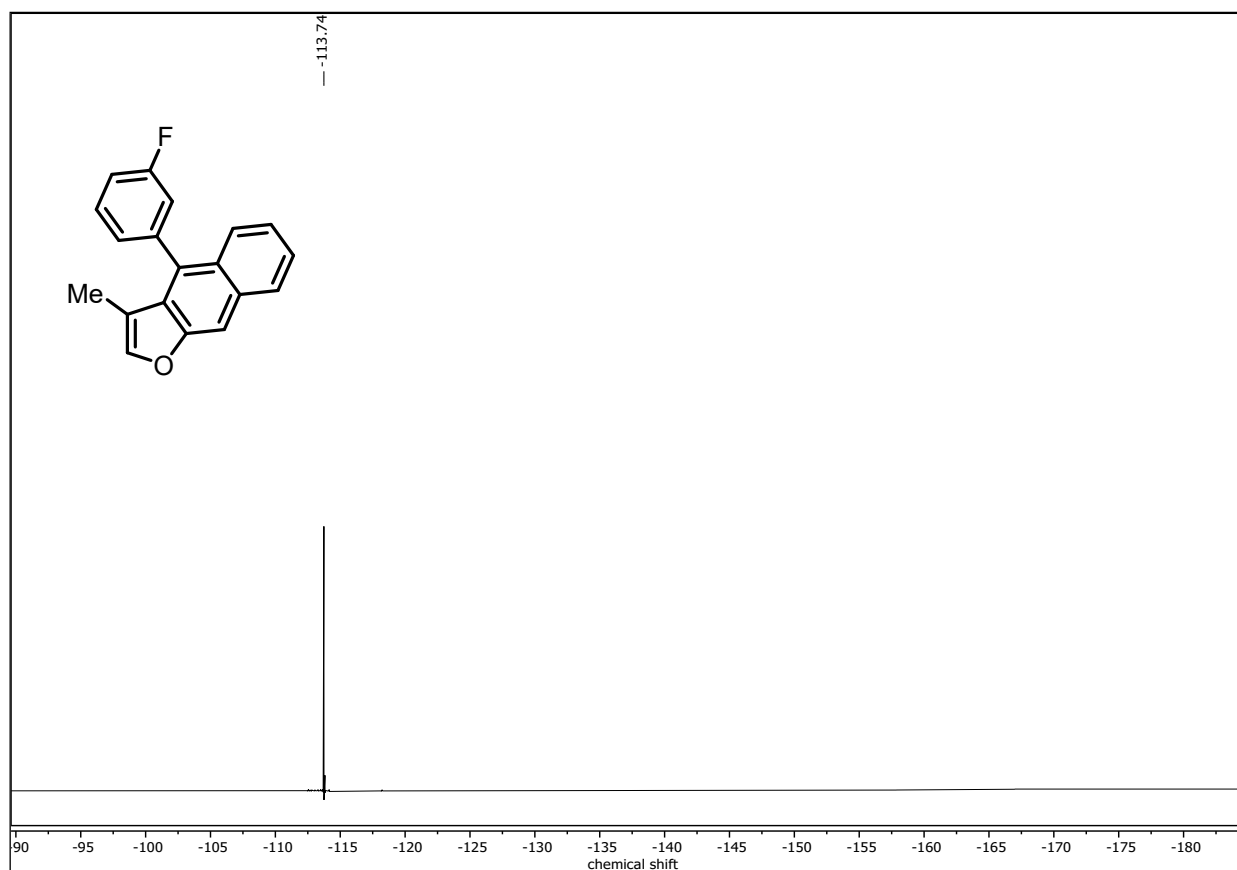
¹H NMR (400 MHz, CDCl₃) Spectrum of 7g.



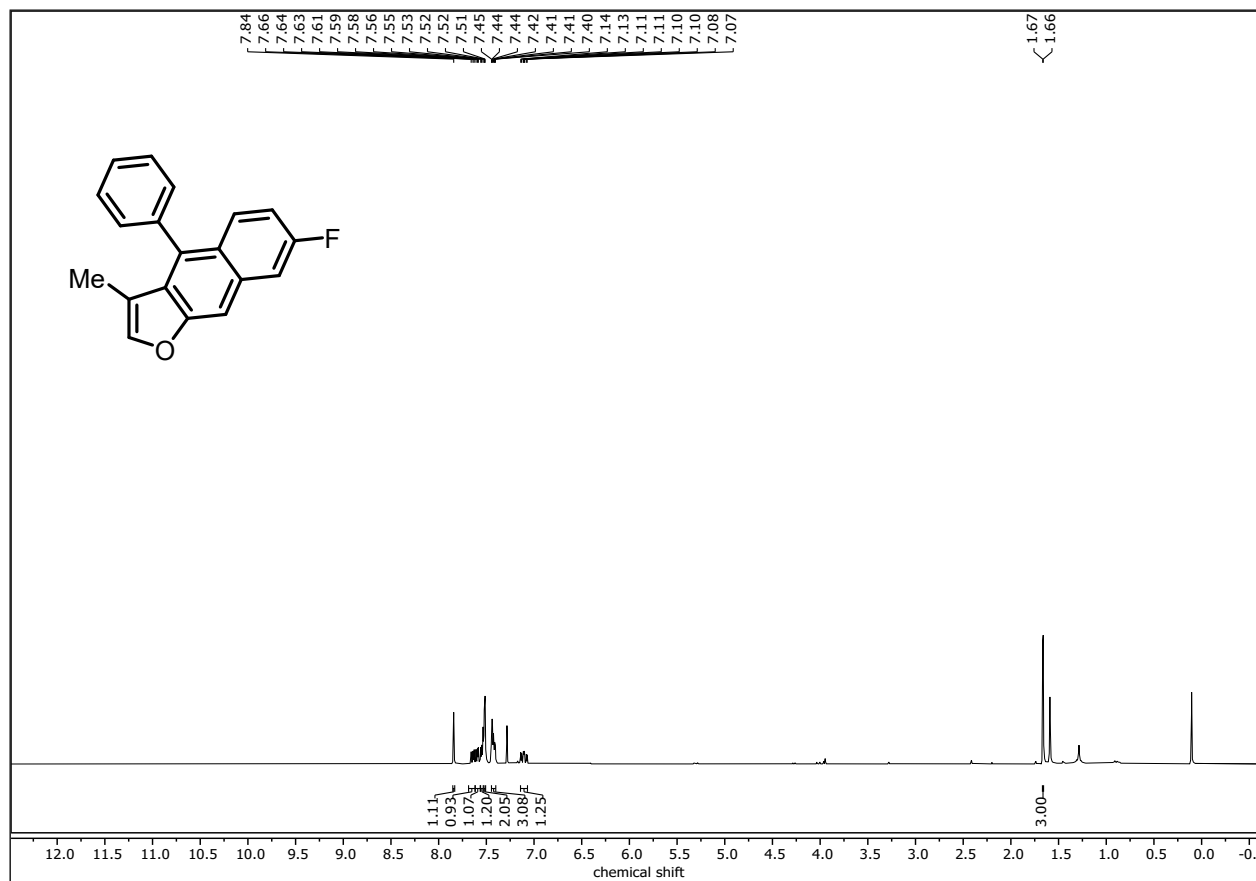
$^{13}\text{C}\{^1\text{H}\}$ (101 MHz, CDCl_3) NMR Spectrum of 7g.



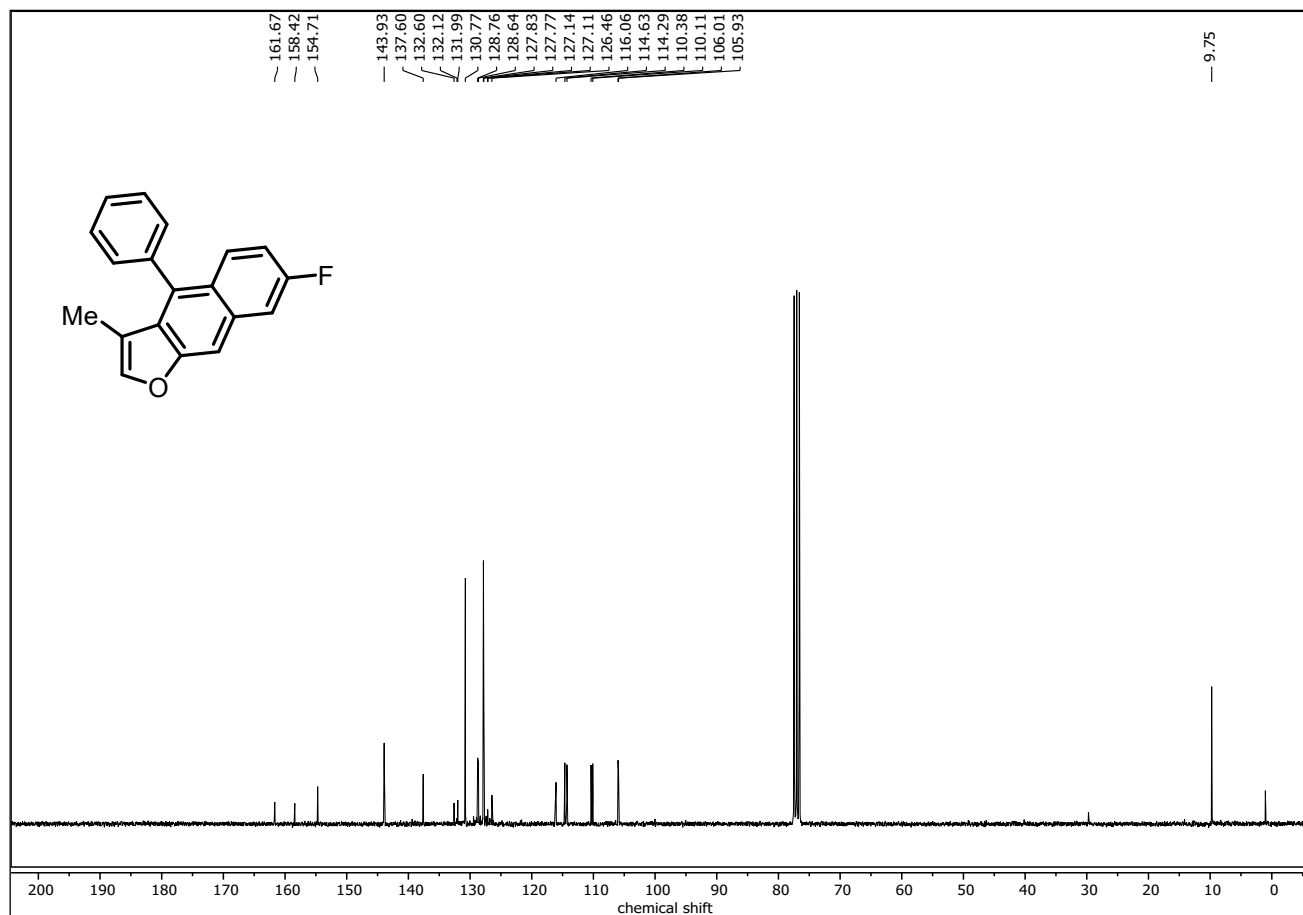
^{19}F NMR (377 MHz, CDCl_3) Spectrum of 7g.



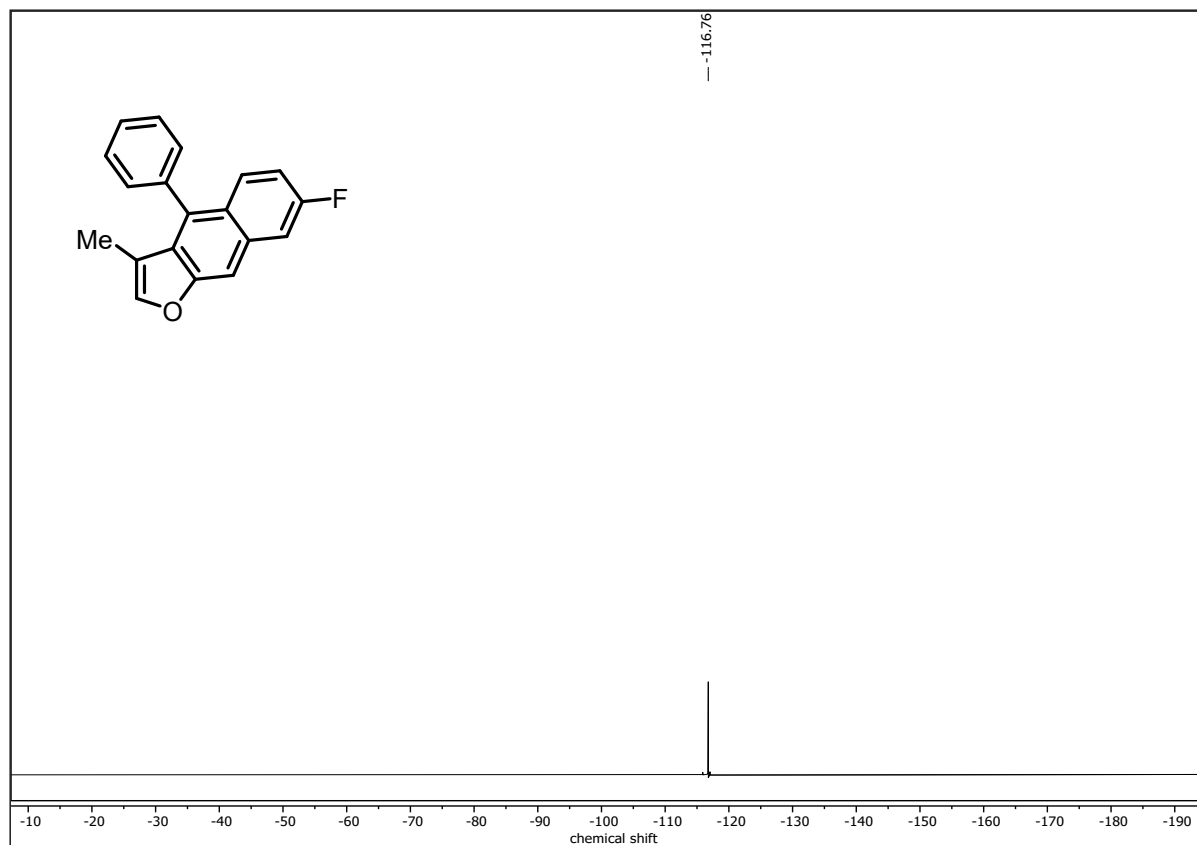
¹H NMR (300 MHz, CDCl₃) Spectrum of 7h.



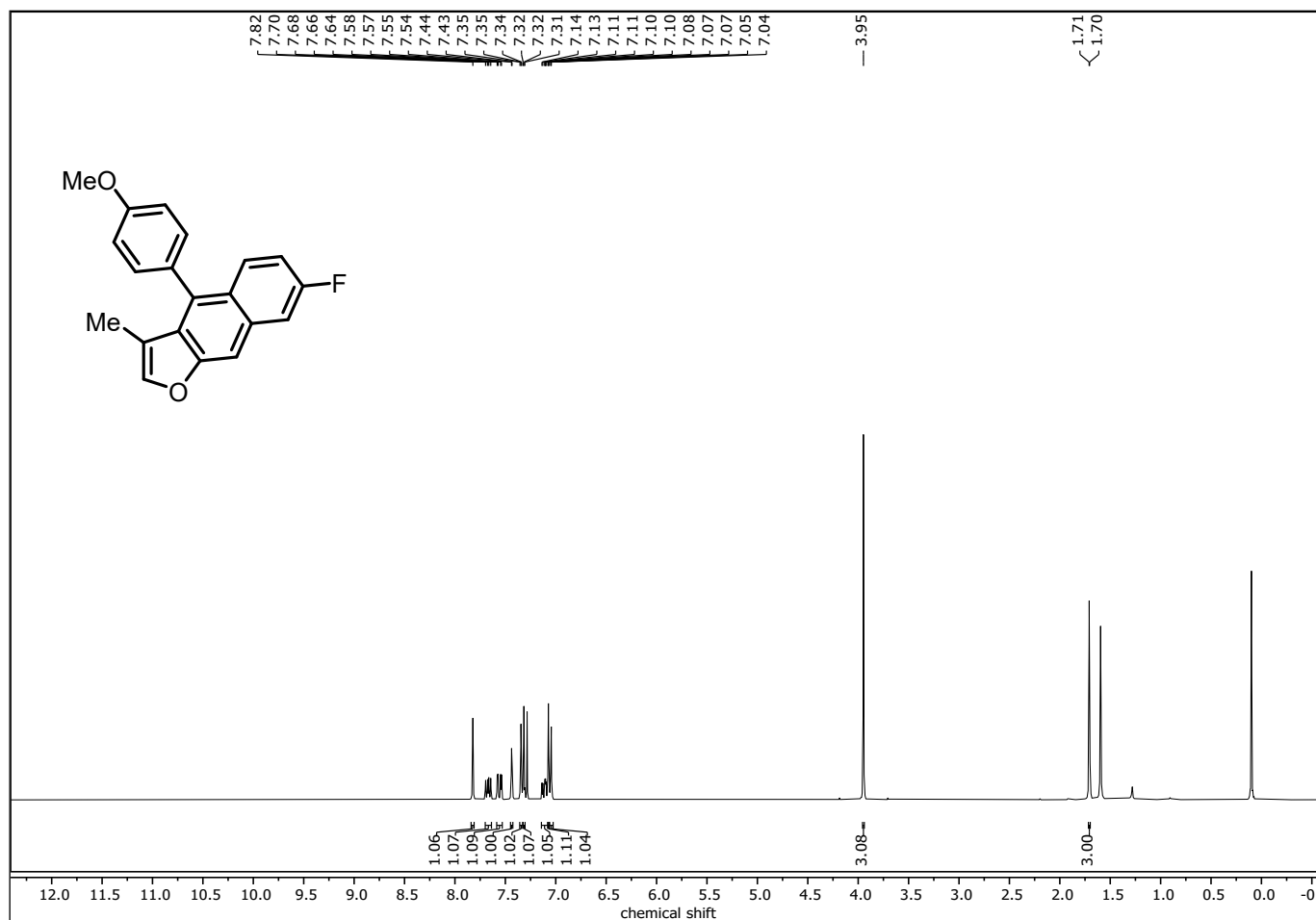
¹³C{¹H} (75 MHz, CDCl₃) NMR Spectrum of 7h.



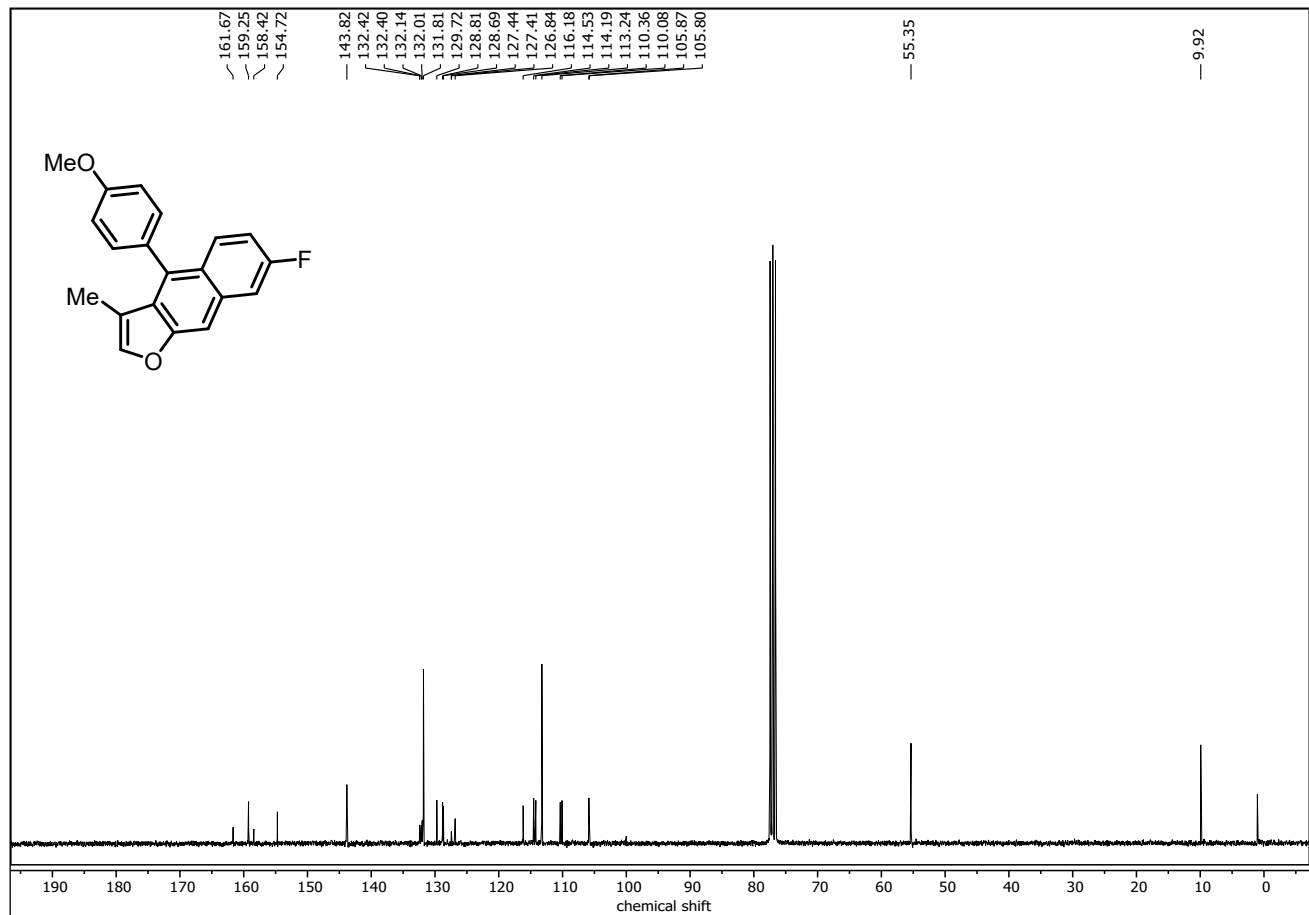
¹⁹F NMR (282 MHz, CDCl₃) Spectrum of 7h.



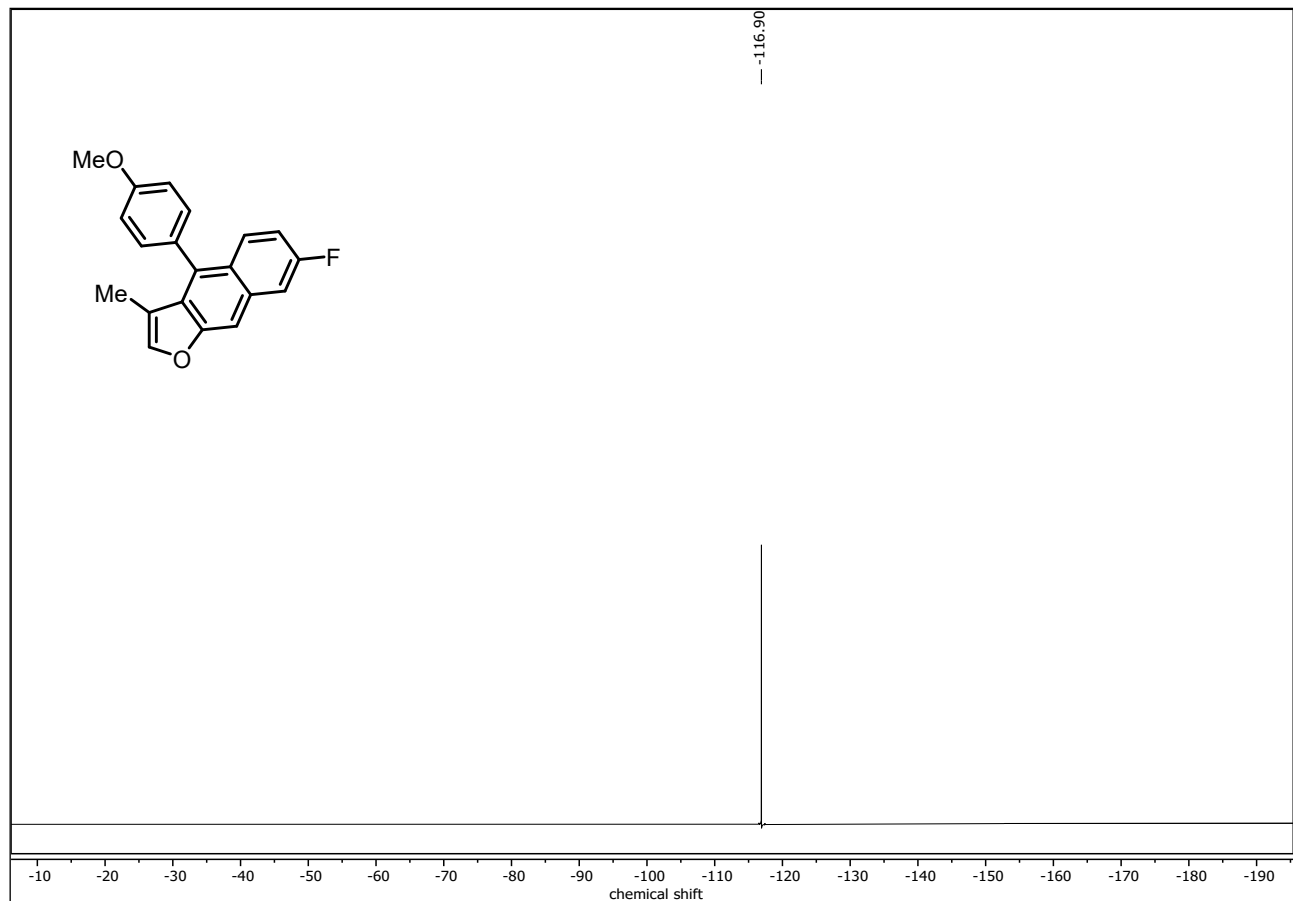
¹H NMR (300 MHz, CDCl₃) Spectrum of 7i.



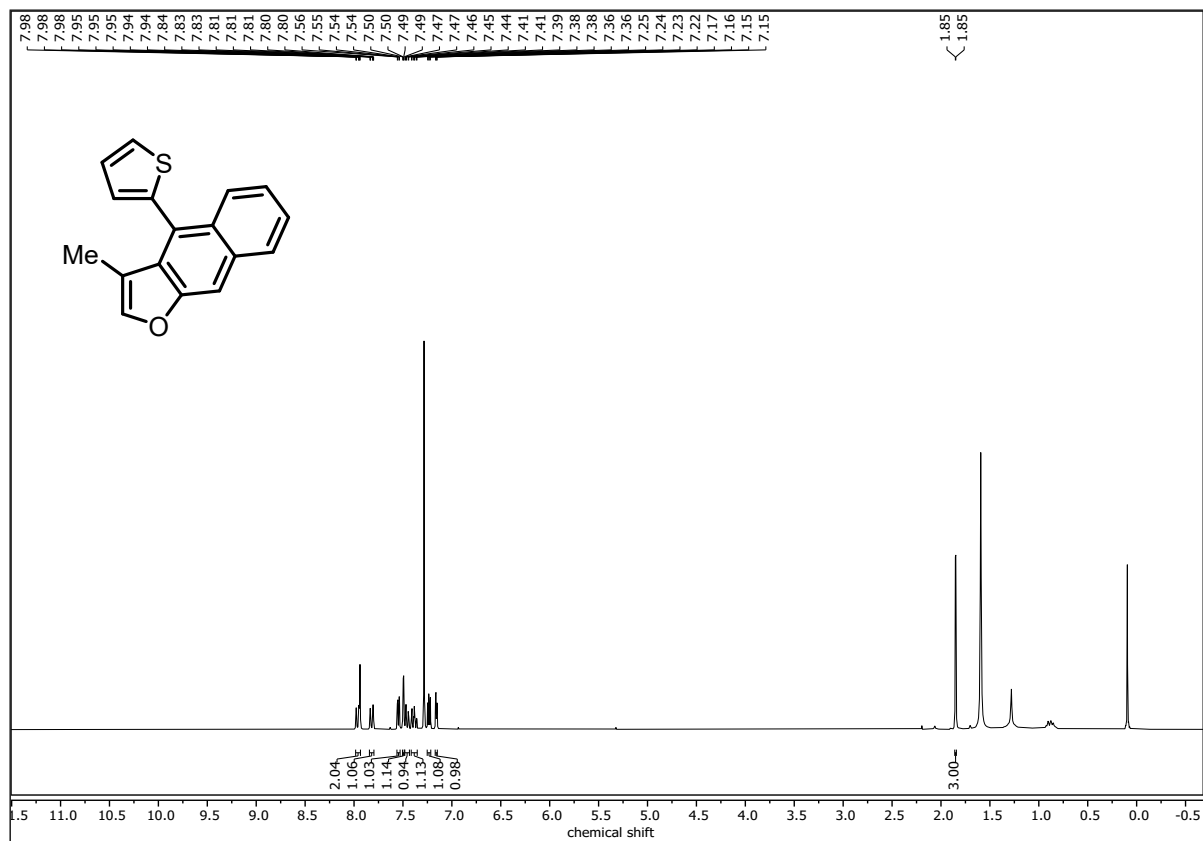
$^{13}\text{C}\{^1\text{H}\}$ (75 MHz, CDCl_3) NMR Spectrum of 7i.



^{19}F NMR (282 MHz, CDCl_3) Spectrum of 7i.



¹H NMR (300 MHz, CDCl₃) Spectrum of 7j.



¹³C{¹H} (75 MHz, CDCl₃) NMR Spectrum of 7j.

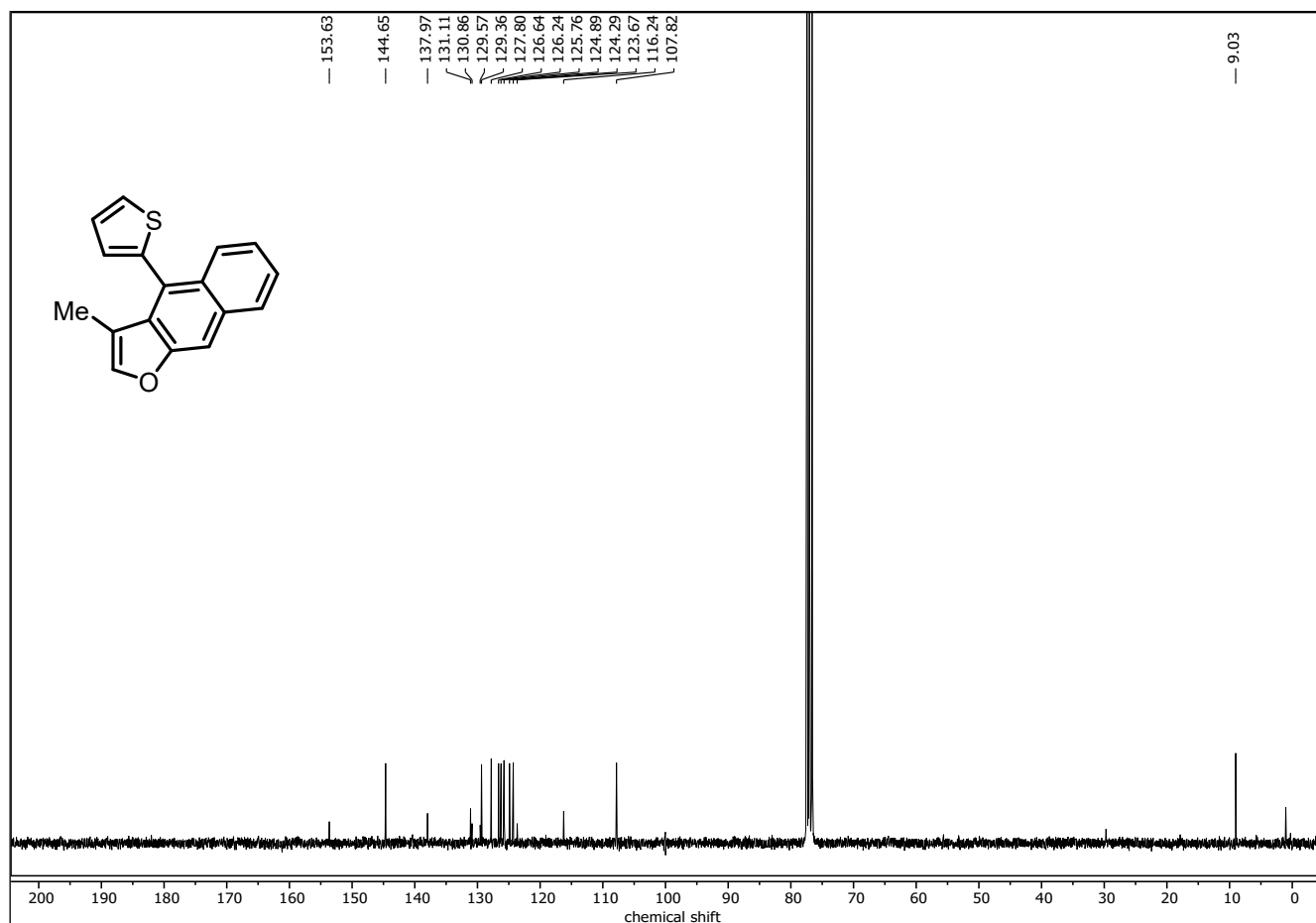


Table for crystallographic data and structural refinement parameters for 4c (CCDC No-2525614)

Empirical formula	C ₂₇ H ₂₃ NO ₃ S
Formula weight	441.52
Temperature/K	273
Crystal system	monoclinic
Space group	P 21/n
a/Å	10.1335(6)
b/Å	18.6755(10)
c/Å	12.0712(7)
α/°	90
β/°	92.907(2)
γ/°	90
Volume/Å ³	2281.5(2)
Z	4
μ/mm ⁻¹	0.171
F (000)	928.0
Index ranges	-12 ≤ h ≤ 12, -23 ≤ k ≤ 23, -15 ≤ l ≤ 15
Radiation	MoKα (λ = 0.71073)
ρ _{calc} g/cm ³	1.285

ORTEP diagram of the crystal structure of 4C.

Datablock uj_rks_2011 - ellipsoid plot

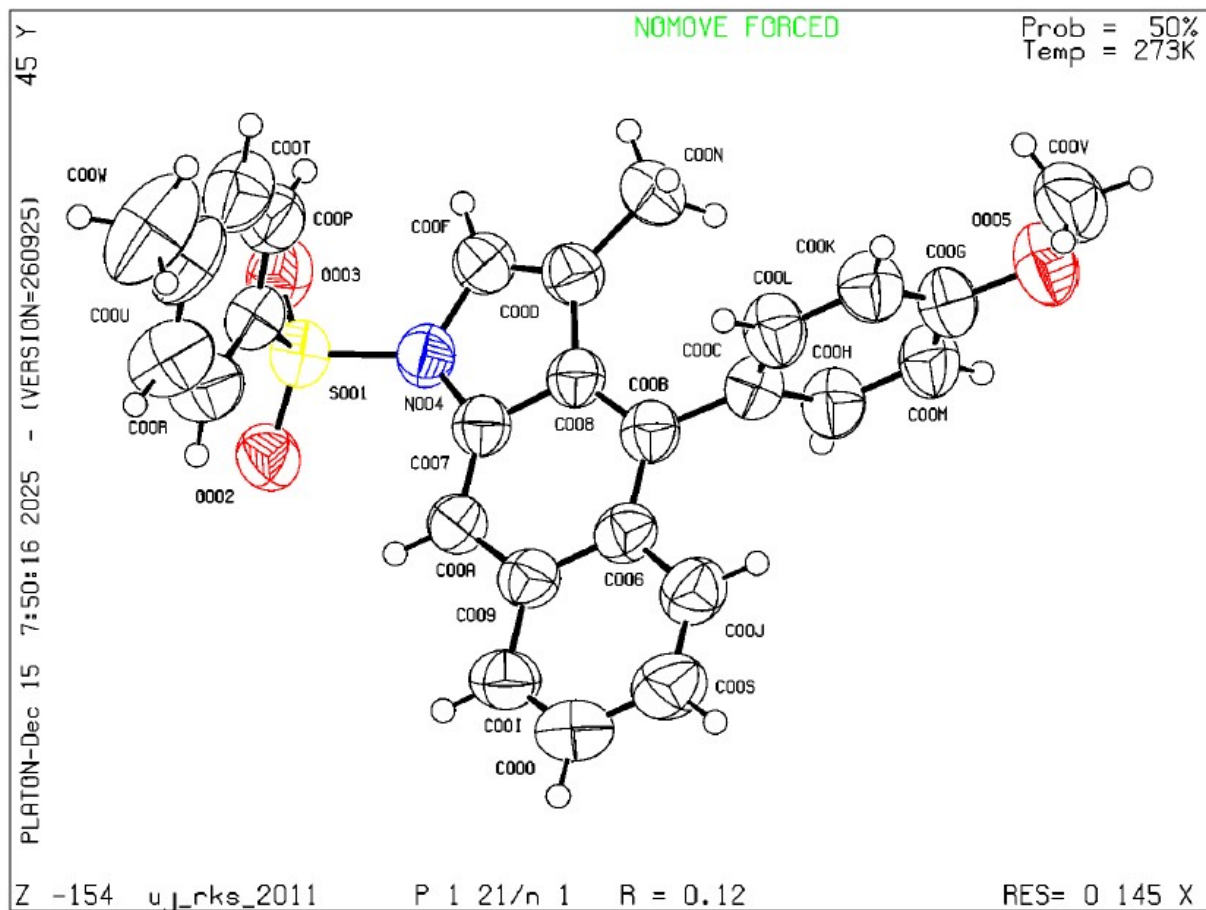


Table for crystallographic data and structural refinement parameters for 7c (CCDC No-2525616)

Empirical formula	C ₂₀ H ₁₆ O ₂
Formula weight	288.33
Temperature/K	273
Crystal system	monoclinic
Space group	P 21/n
a/Å	12.635(2)
b/Å	8.3274(14)
c/Å	14.396(3)
α/°	90
β/°	96.948(6)
γ/°	90
Volume/Å ³	1503.6(5)
Z	4
μ/mm ⁻¹	0.081
F (000)	608.0
Index ranges	-15 ≤ h ≤ 16, -10 ≤ k ≤ 10, -18 ≤ l ≤ 18
Radiation	MoKα (λ = 0.71073)
ρ _{calc} g/cm ³	1.274

ORTEP diagram of the crystal structure of 7C.

Datablock uj_rks_ea - ellipsoid plot

