

Supporting Information

Synthesis of New Cyclazines and 4,5-Diaryl-1*H*-pyrrol-3(2*H*)-one unit in Discoipyrroles from Indolizinone-DMAD Cycloadducts

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General Experimental Information:

Various starting materials used such as 2-acetyl pyridine, phenylacetylenes and iodobenzenes were accessed through Spectrochem or Sigma Aldrich, and were used as received unless otherwise indicated. The solvents benzene (PhH), tetrahydrofuran (THF) and toluene (PhMe) were dried over sodium/benzophenone and distilled before use whereas dichloromethane (DCM) and acetonitrile (MeCN) were dried over CaH₂. Methanol was dried by refluxing over magnesium/iodine. Column chromatographic purification was carried out on 100-200 mesh silica gel using EtOAc-hexane solvent system in a gradient mode. Thin layer chromatography was done using 0.25 mm thick silica gel plates from Merck and was analysed using either 254 nm UV light or ninhydrin staining.

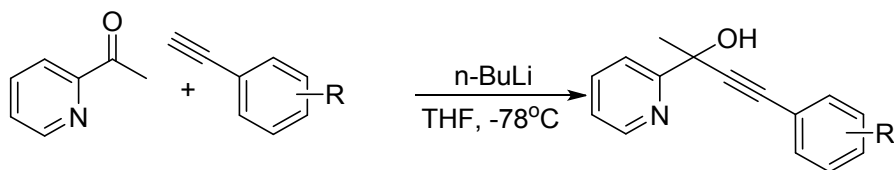
¹H NMR and ¹³C NMR spectra were recorded on Bruker Avance 400 MHz NMR spectrometer and the chemical shifts are reported in parts per million (ppm) relative to tetramethylsilane, with *J* values in Hertz. The splitting patterns in ¹H NMR are reported as follows: s = singlet, d = doublet, t = triplet, dd = doublet of doublets, bs = broad singlet, appt = apparent triplet. ¹³C NMR data are reported with solvent peak (CDCl₃ = 77.16, CD₃OD = 49.00) as the internal standard.

High-resolution mass spectra (HRMS) were recorded on a Waters Q-TOF *micro*™ spectrometer with lock spray source. Infrared spectra were recorded using Nicolet 6700 FT-IR spectrometer.

Single crystal X-ray crystallography: The intensity data collection during X-ray crystallographic analysis was carried out on a Bruker AXS (kappa apex II) diffractometer equipped with graphite monochromated Mo (K_α) radiation. The data were collected for θ up to 25° for Mo (K_α) radiation. ω and ϕ scans were employed to collect the data. The frame width for ω was set to 0.5 deg for data collection. The frames were integrated and data were reduced for Lorentz and polarization correction using SAINT-Plus. The multi-scan absorption correction was applied to the data. All structures were solved using SIR-92 and refined using SHELXL-97. The molecular and packing diagrams were solved using ORTEP -3 and Mercury 1.4.2. The non-hydrogen atoms were refined with anisotropic displacement parameter. All hydrogen atoms could be located in the difference Fourier map. However, the atoms bonded carbons were fixed at chemically meaningful positions and were allowed to ride with parent atom during the refinement.

Experimental procedure

General method for the synthesis of 4-aryl-2-(pyridin-2-yl)but-3-yn-2-ols



n-BuLi (1.1 equiv., 1.6 M solution in hexane) was added to a stirred solution of the alkyne (1.2 equiv.) in THF at -78°C under nitrogen atmosphere. After stirring for 15 min., a solution of 2-acetylpyridine (1.0 equiv.) in THF was slowly added and the mixture was stirred for an additional 1 h maintaining the temperature at -78°C. The reaction mixture was then quenched with saturated NH₄Cl at 0°C, diluted with ethyl acetate and washed with aqueous NH₄Cl (2 x 50 mL). The organic layer was dried over MgSO₄, concentrated under reduced pressure and the residue was purified by silica gel chromatography using ethyl acetate/hexane system to get the products in 88 – 95 % yields.

^1H NMR, ^{13}C NMR spectra of compounds

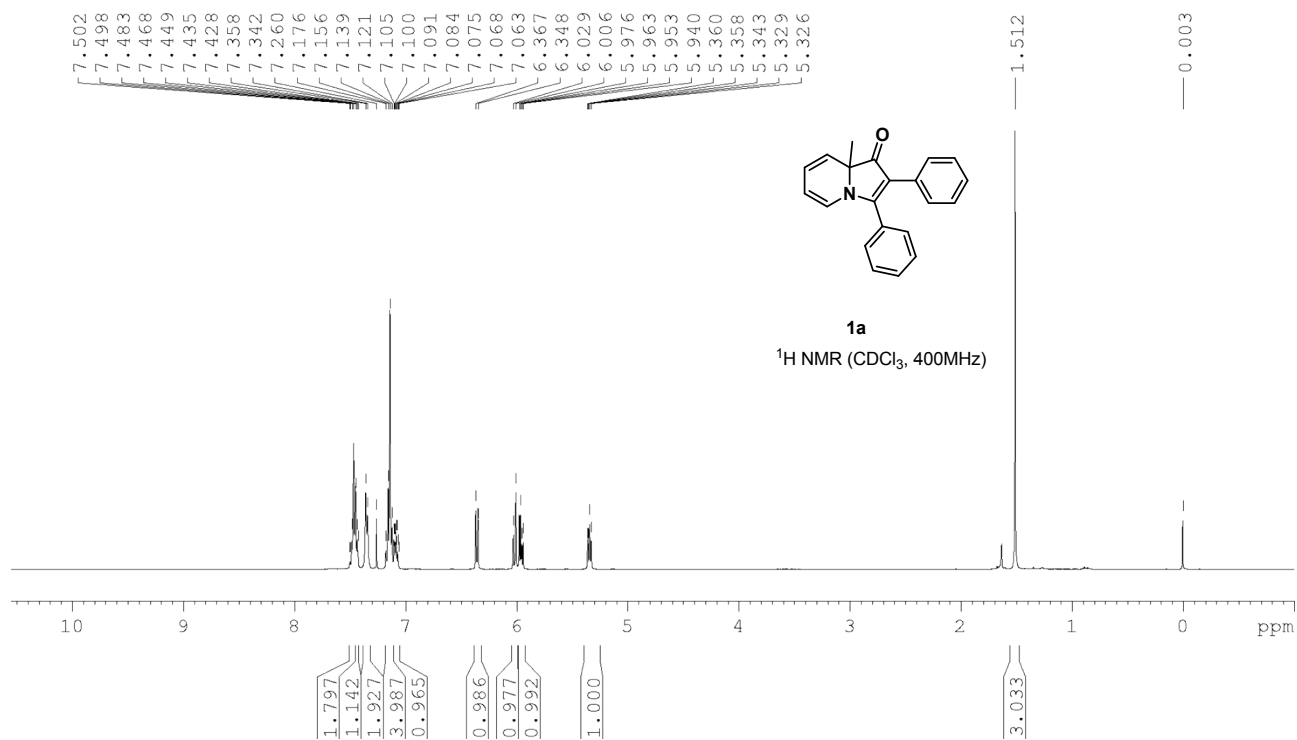


Figure 1: ^1H NMR (400 MHz) spectrum of **1a**

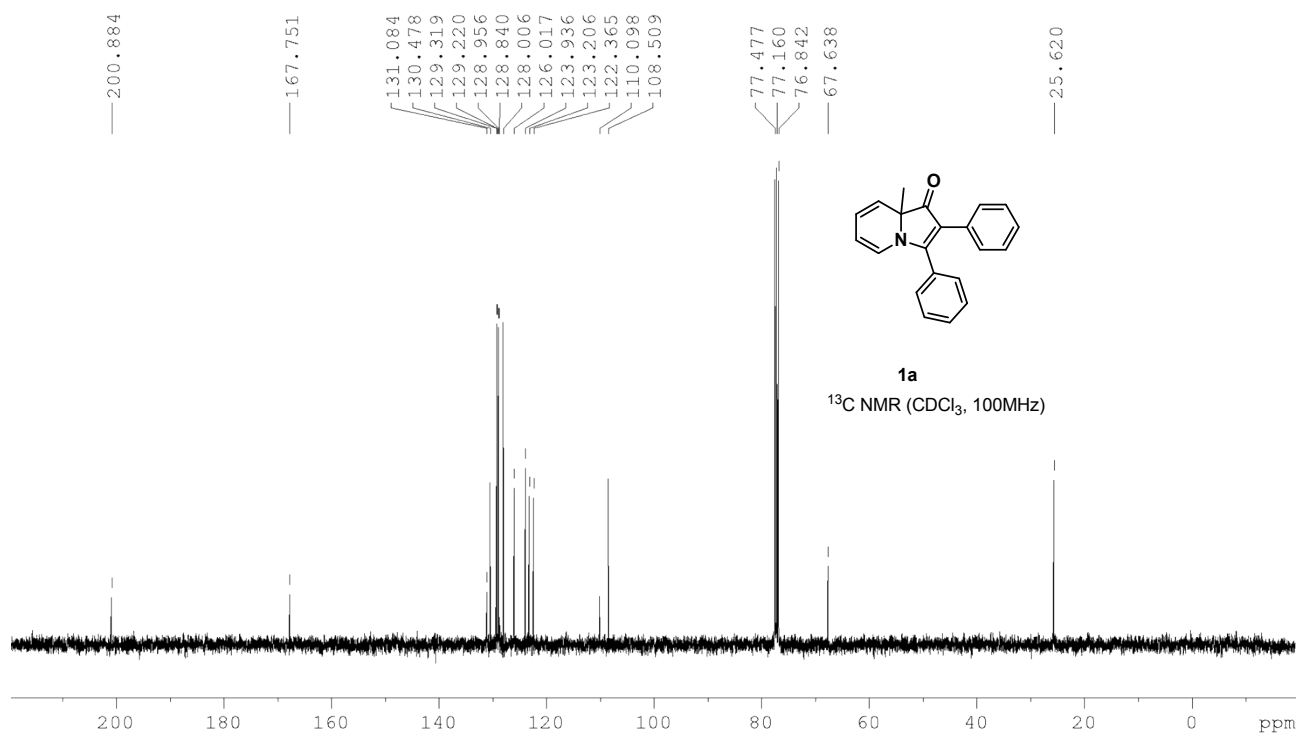


Figure 2: ^{13}C NMR (100 MHz) spectrum of **1a**

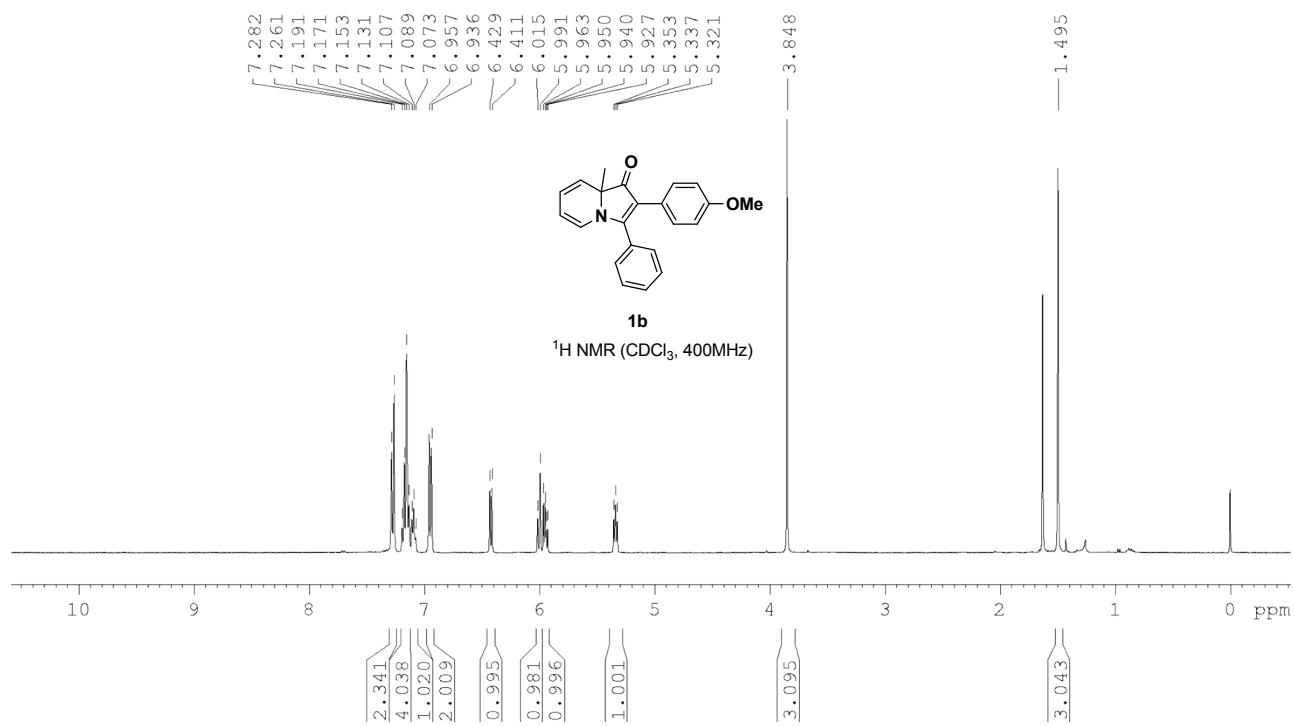


Figure 3: ¹H NMR (400 MHz) spectrum of **1b**

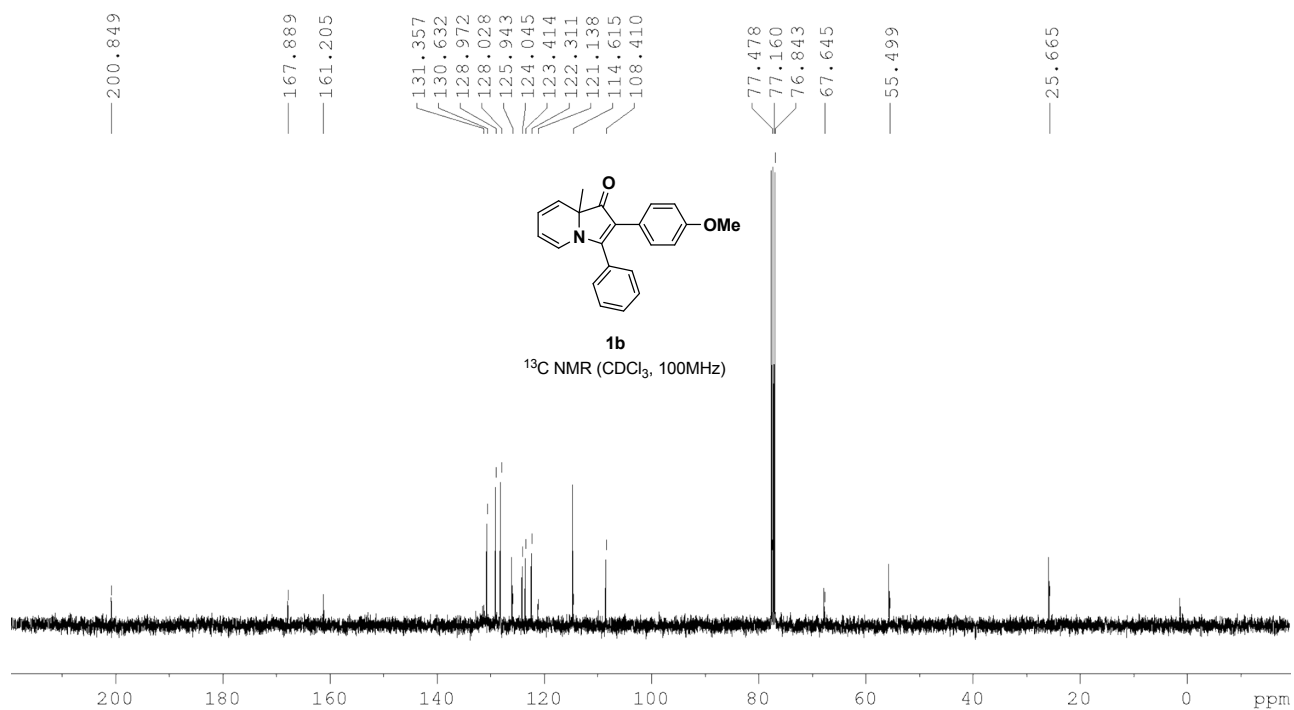


Figure 4: ¹³C NMR (100 MHz) spectrum of **1b**

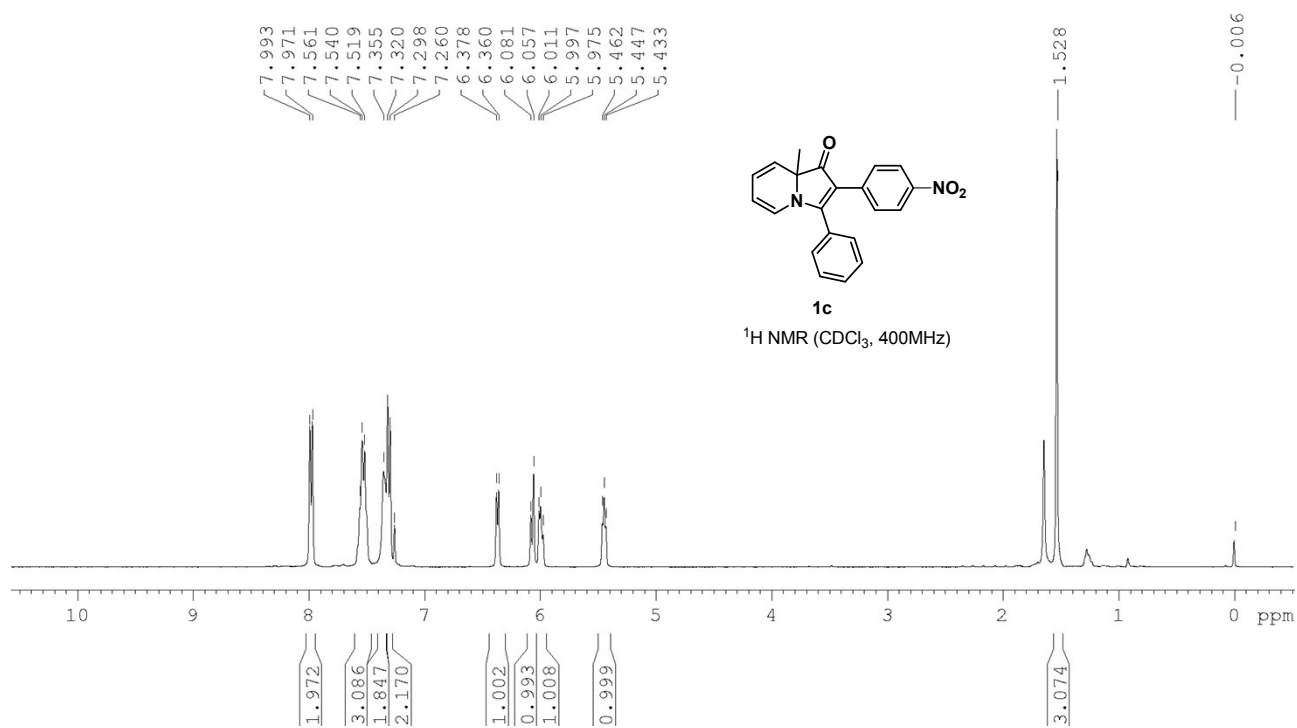


Figure 5: ¹H NMR (400 MHz) spectrum of **1c**

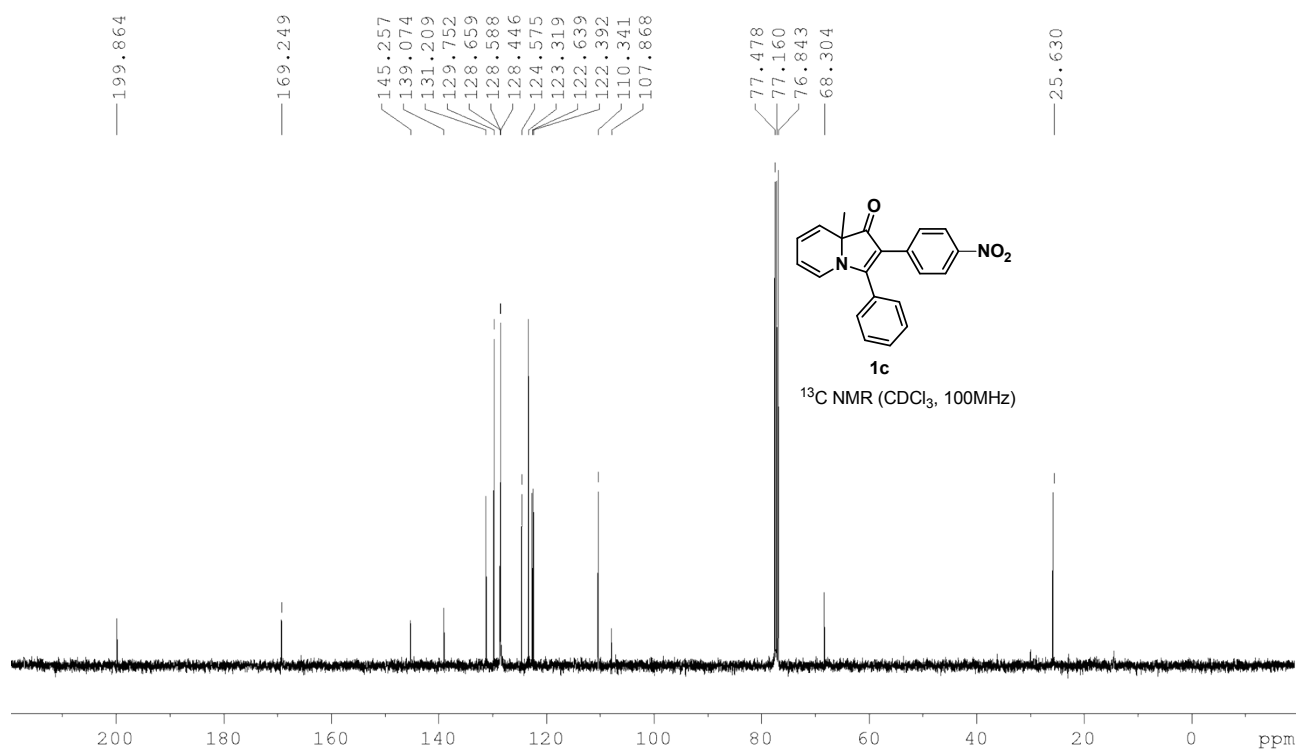


Figure 6: ¹³C NMR (100 MHz) spectrum of **1c**

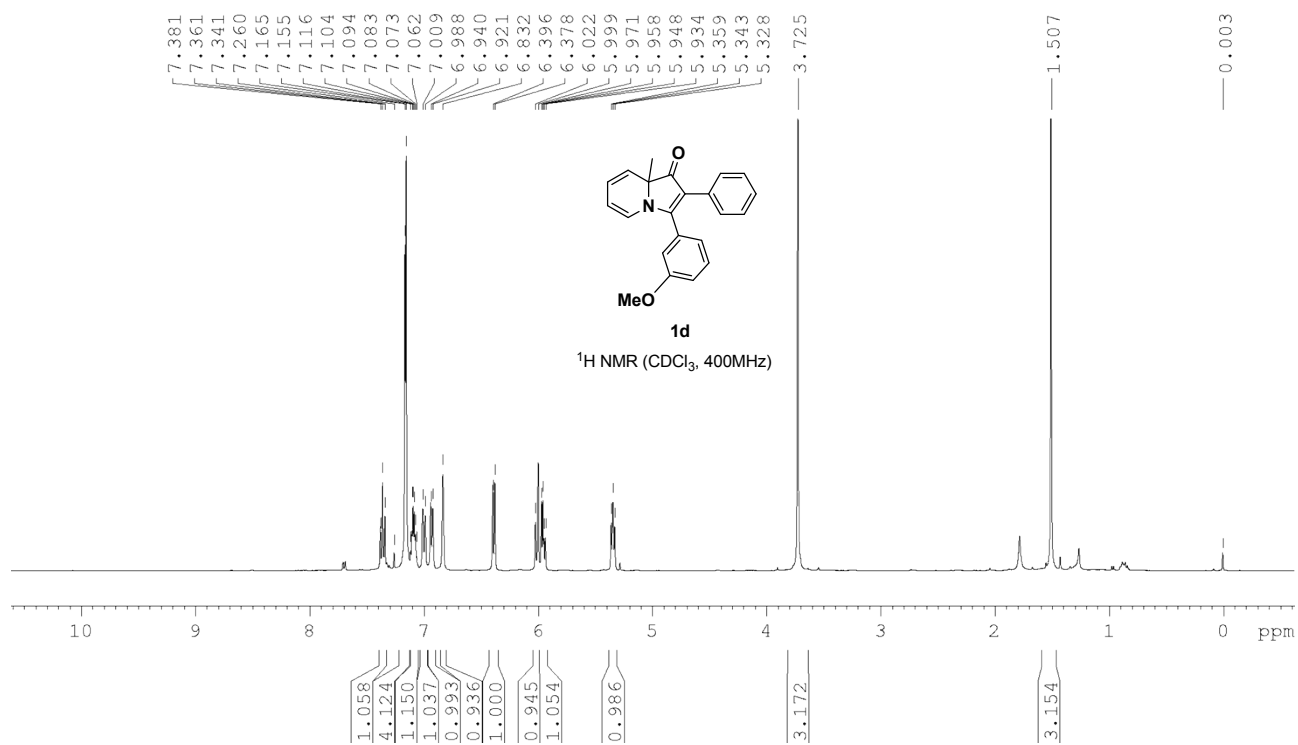


Figure 7: $^1\text{H NMR (400 MHz)}$ spectrum of **1d**

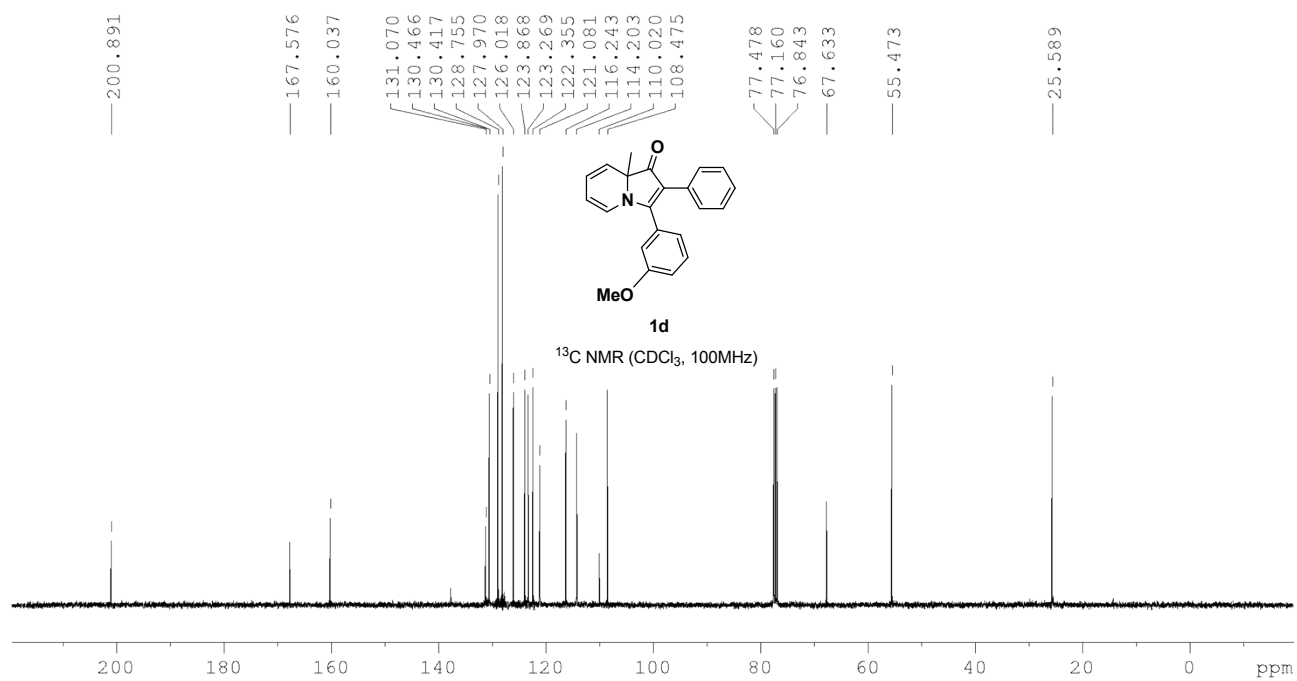


Figure 8: $^{13}\text{C NMR (100 MHz)}$ spectrum of **1d**

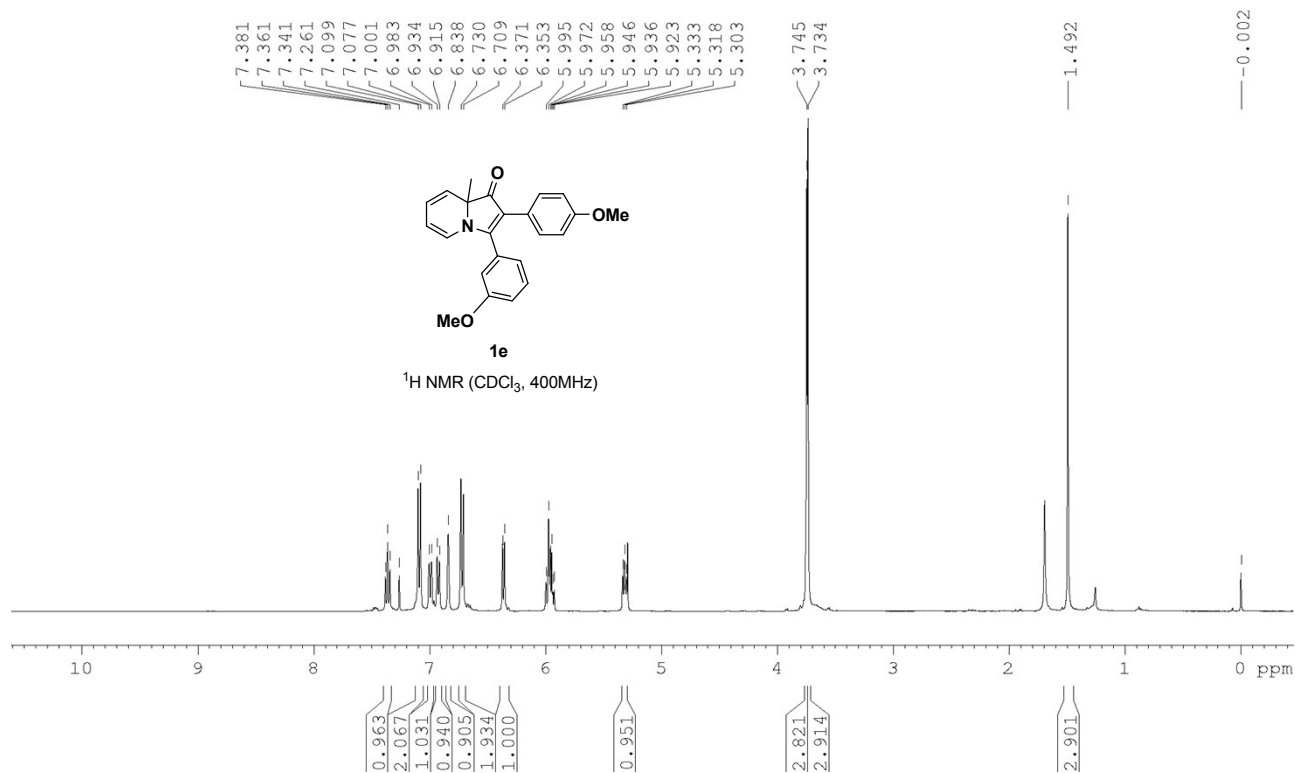


Figure 9: ¹H NMR (400 MHz) spectrum of **1e**

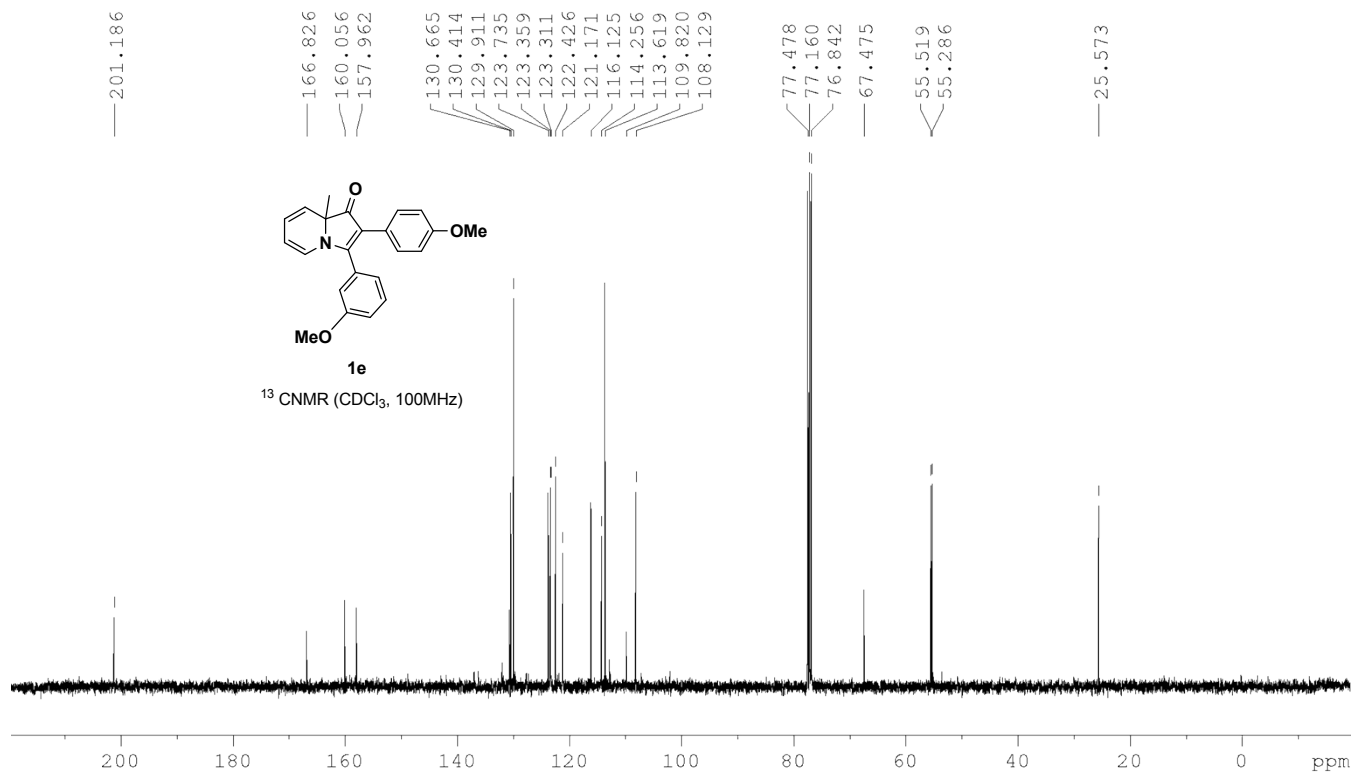


Figure 10: ¹³C NMR (100 MHz) spectrum of **1e**

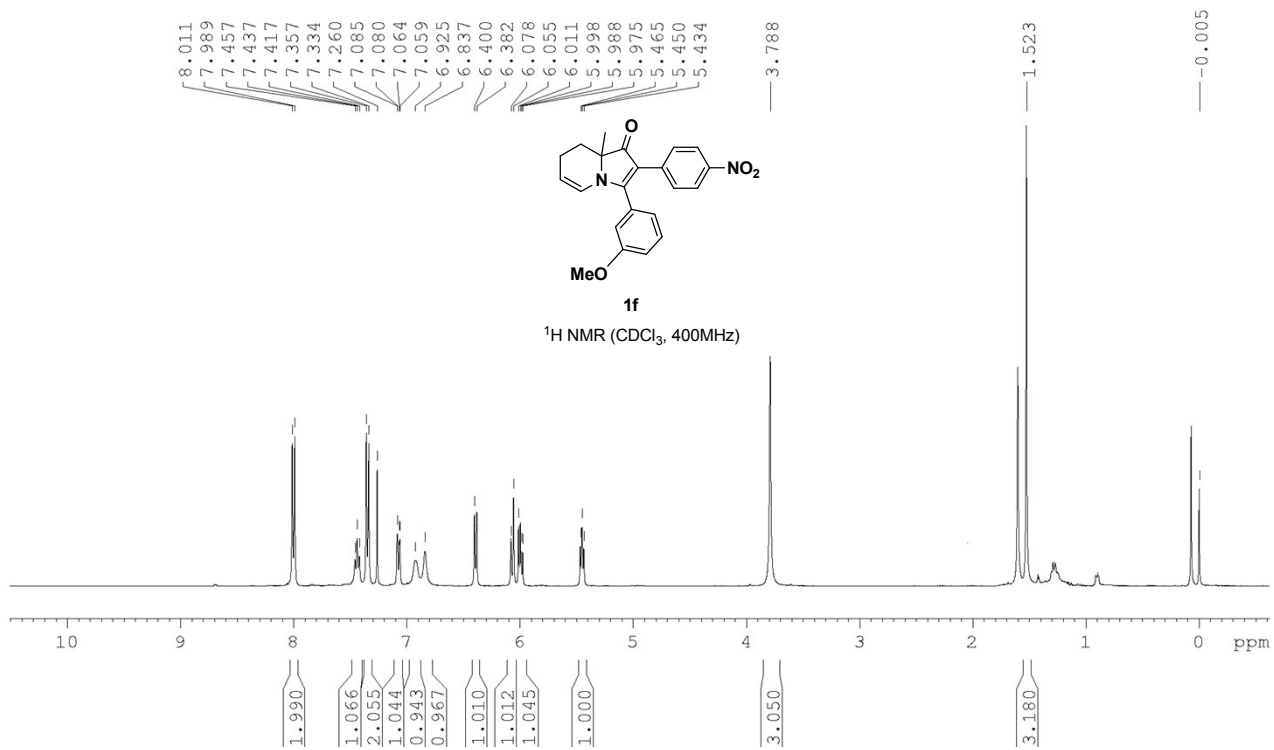


Figure 11: ¹H NMR (400 MHz) spectrum of **1f**

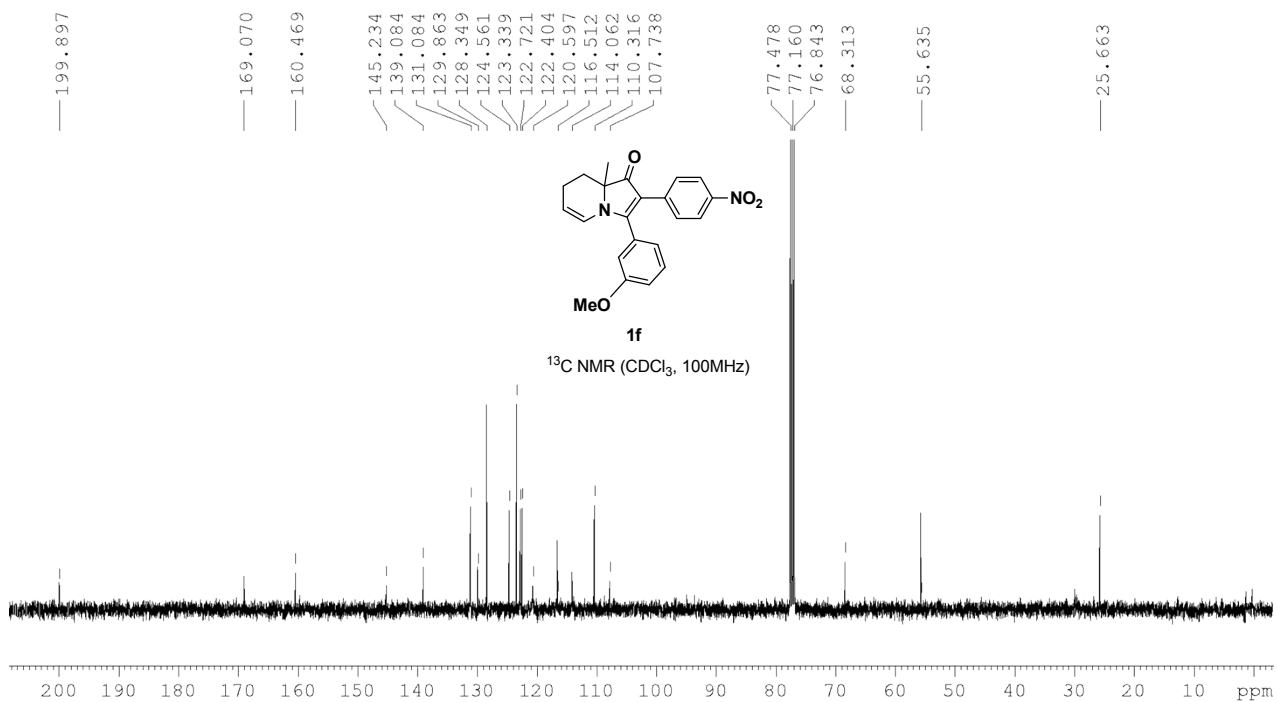


Figure 12: ¹³C NMR (100 MHz) spectrum of **1f**

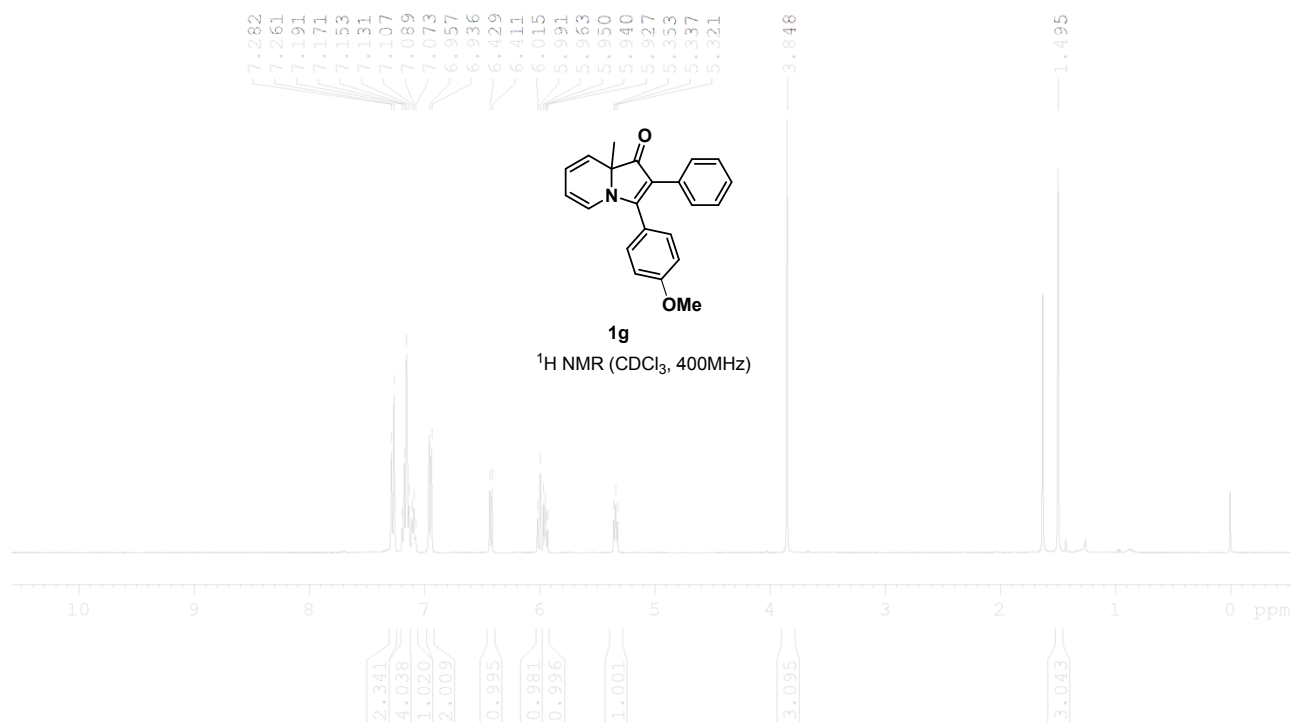


Figure 13: ¹H NMR (400 MHz) spectrum of **1g**

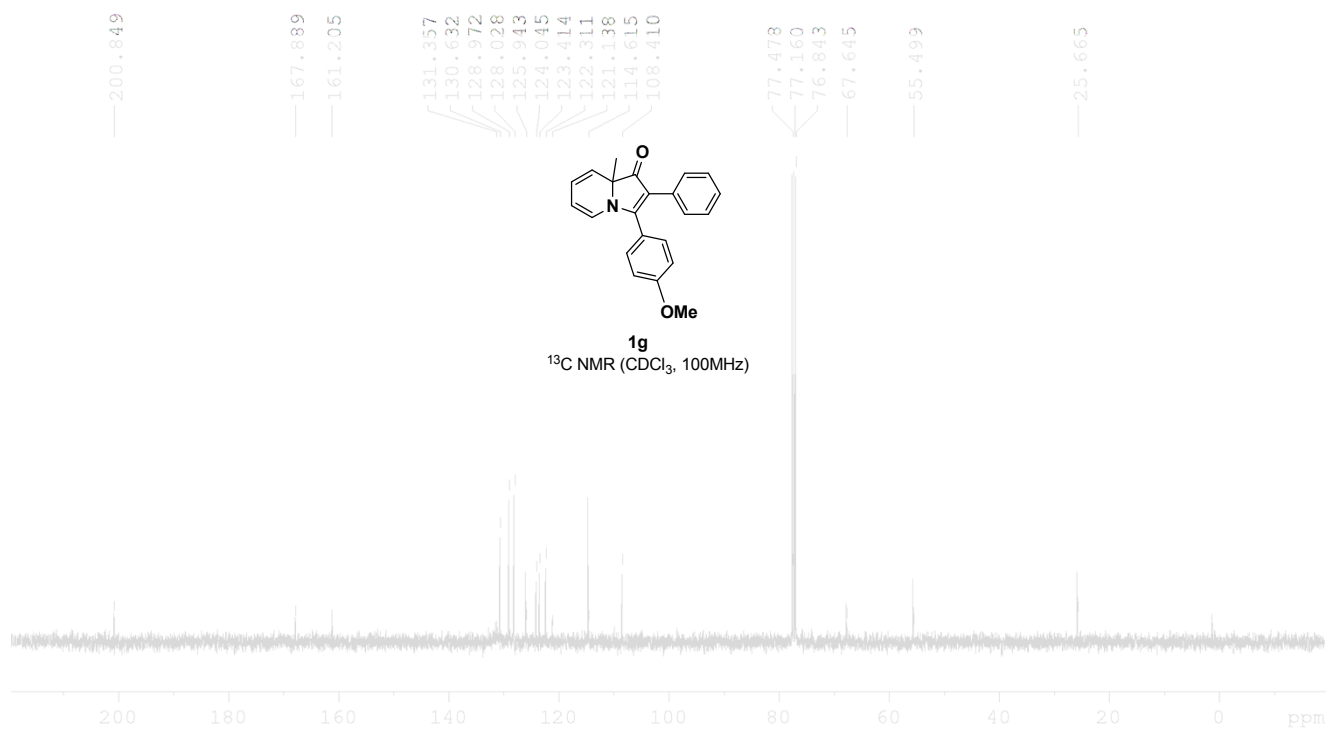


Figure 14: ¹³C NMR (100 MHz) spectrum of **1g**

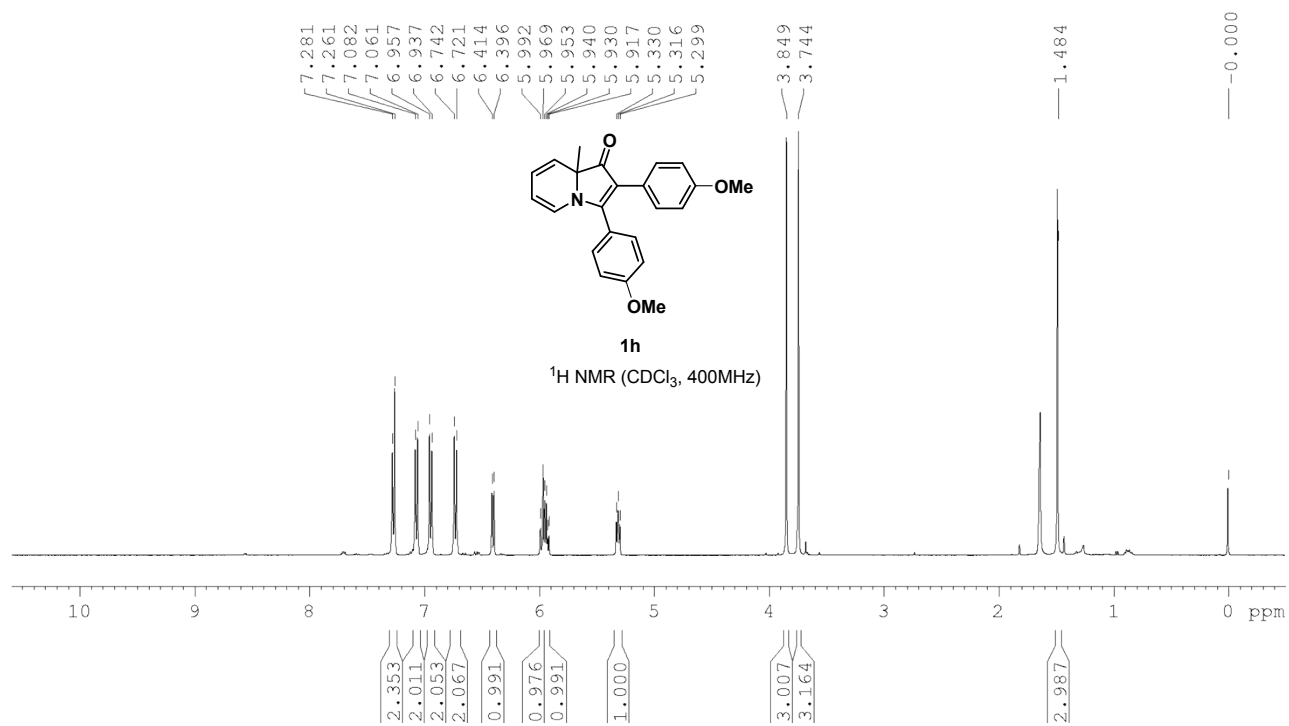


Figure 15: $^1\text{H NMR}$ (400 MHz) spectrum of **1h**

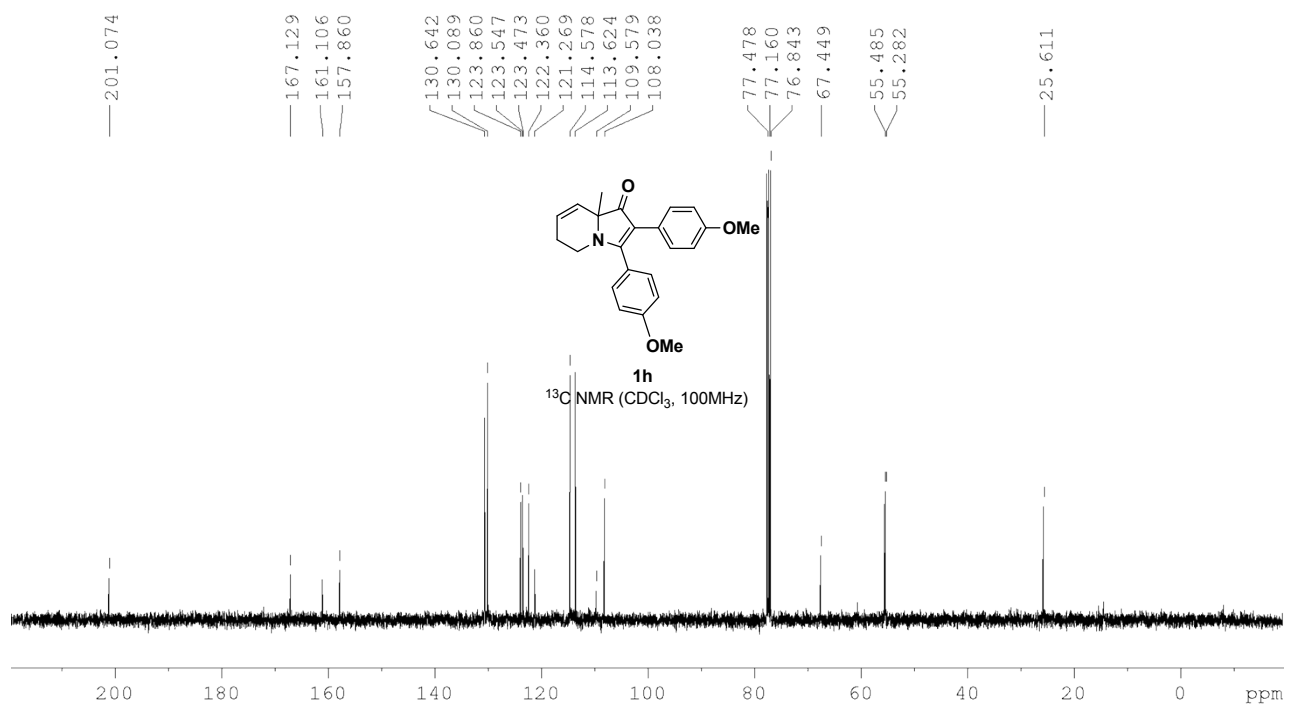


Figure 16: $^{13}\text{C NMR}$ (100 MHz) spectrum of **1h**

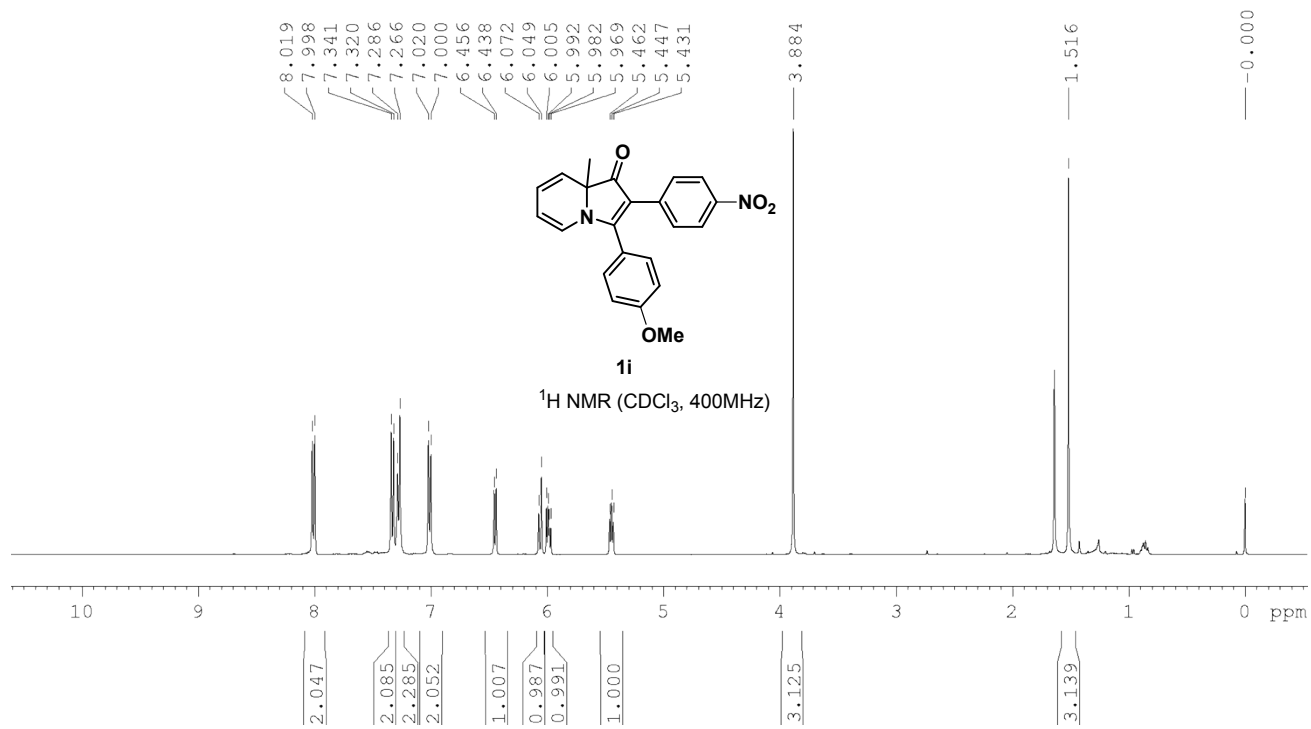


Figure 17: $^1\text{H NMR}$ (400 MHz) spectrum of **1i**

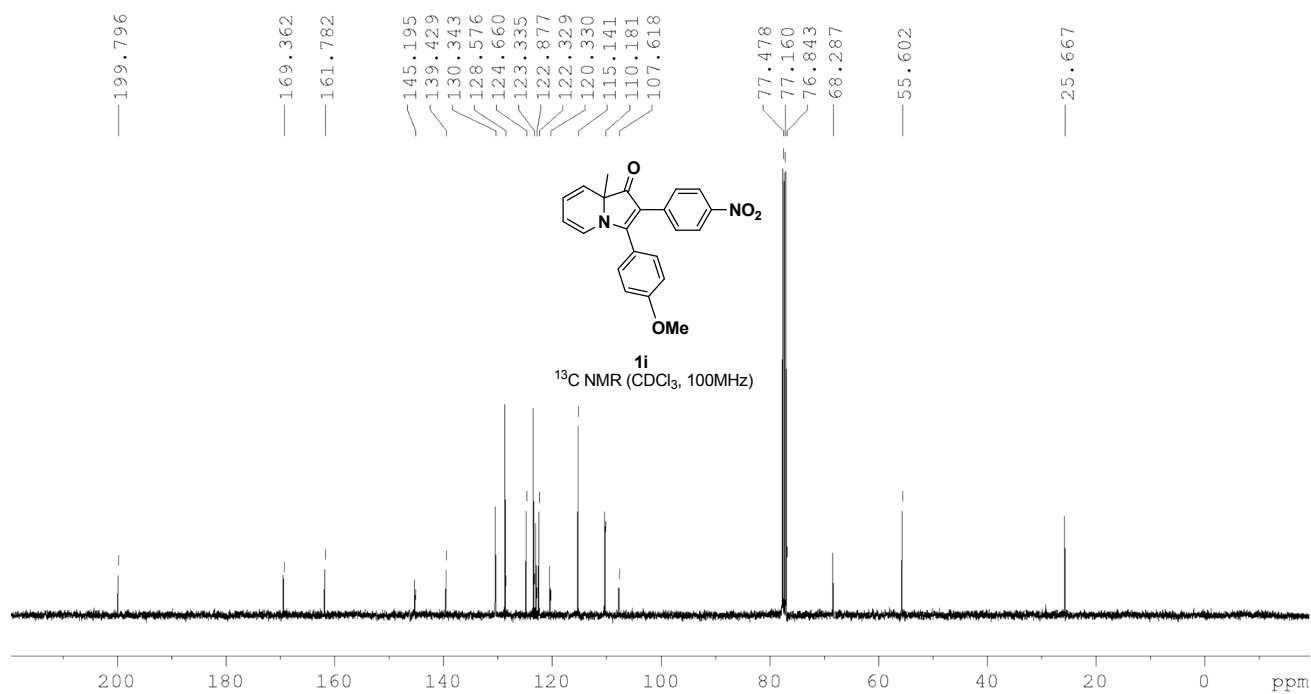


Figure 18: $^{13}\text{C NMR}$ (100 MHz) spectrum of **1i**

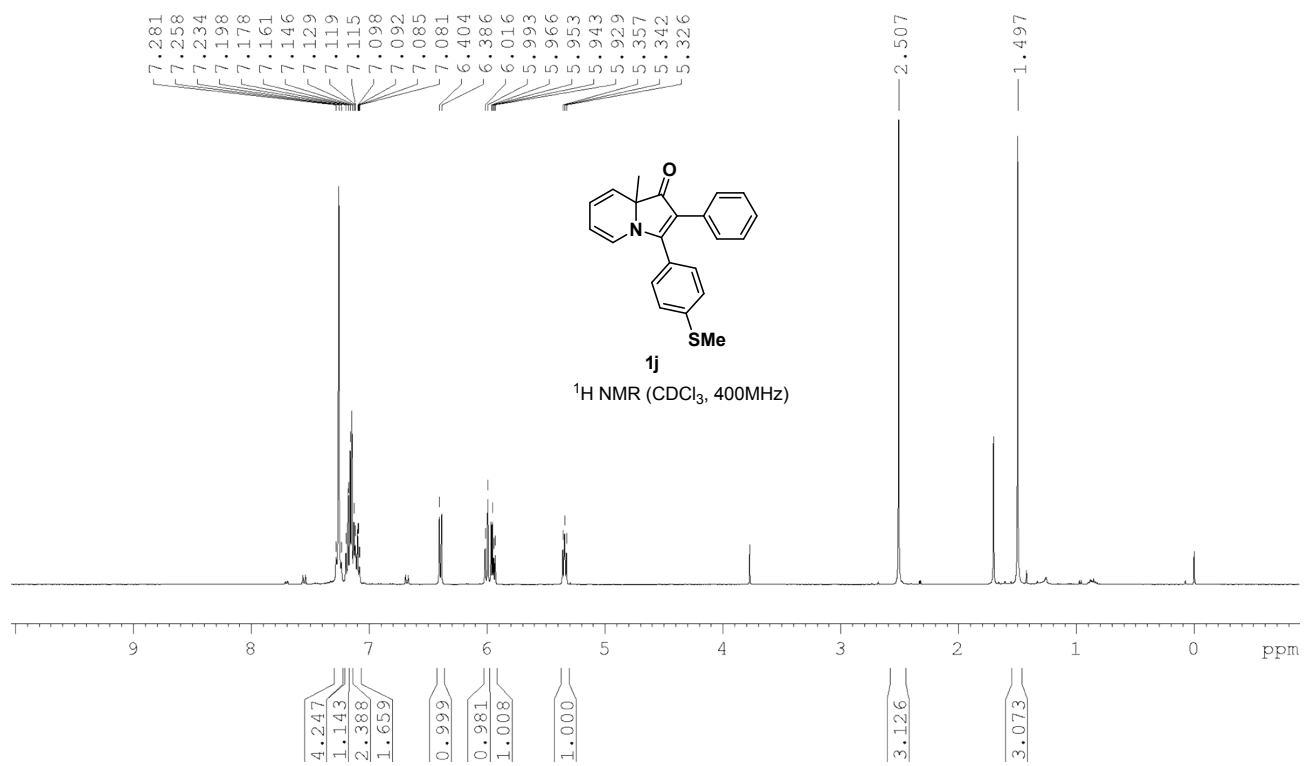


Figure 19: $^1\text{H NMR}$ (400 MHz) spectrum of **1j**

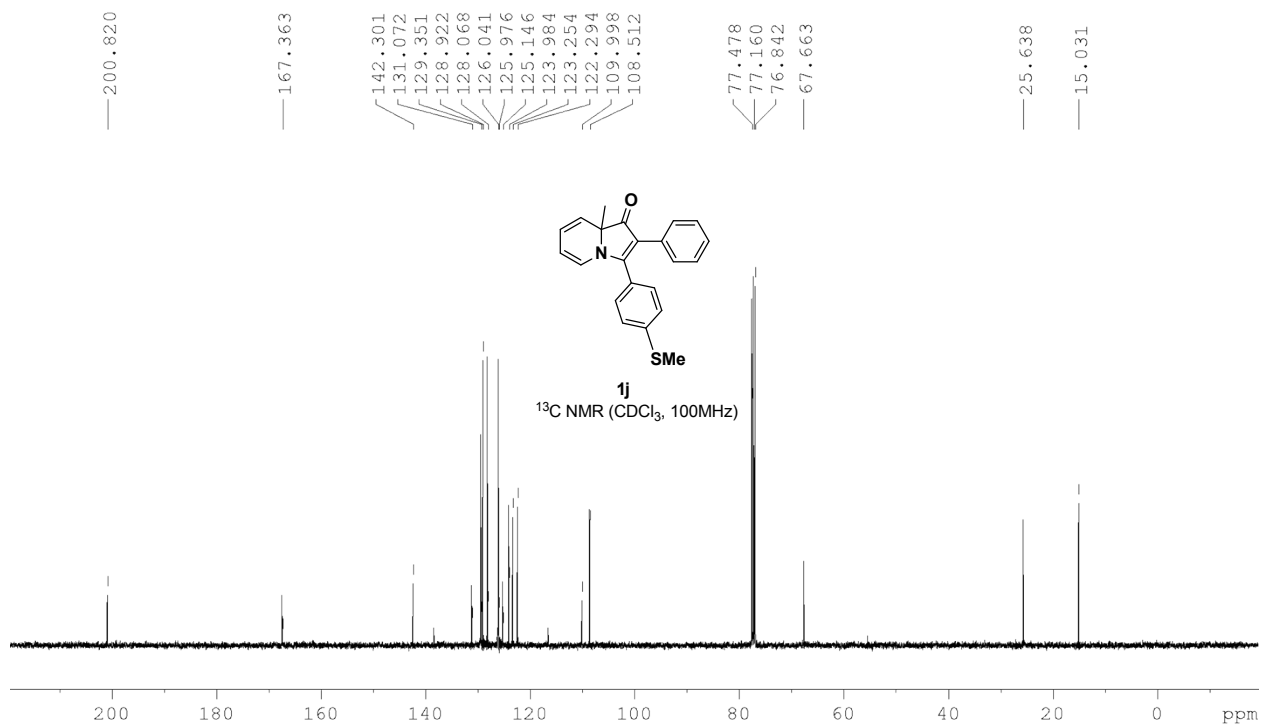


Figure 20: $^{13}\text{C NMR}$ (100 MHz) spectrum of **1j**

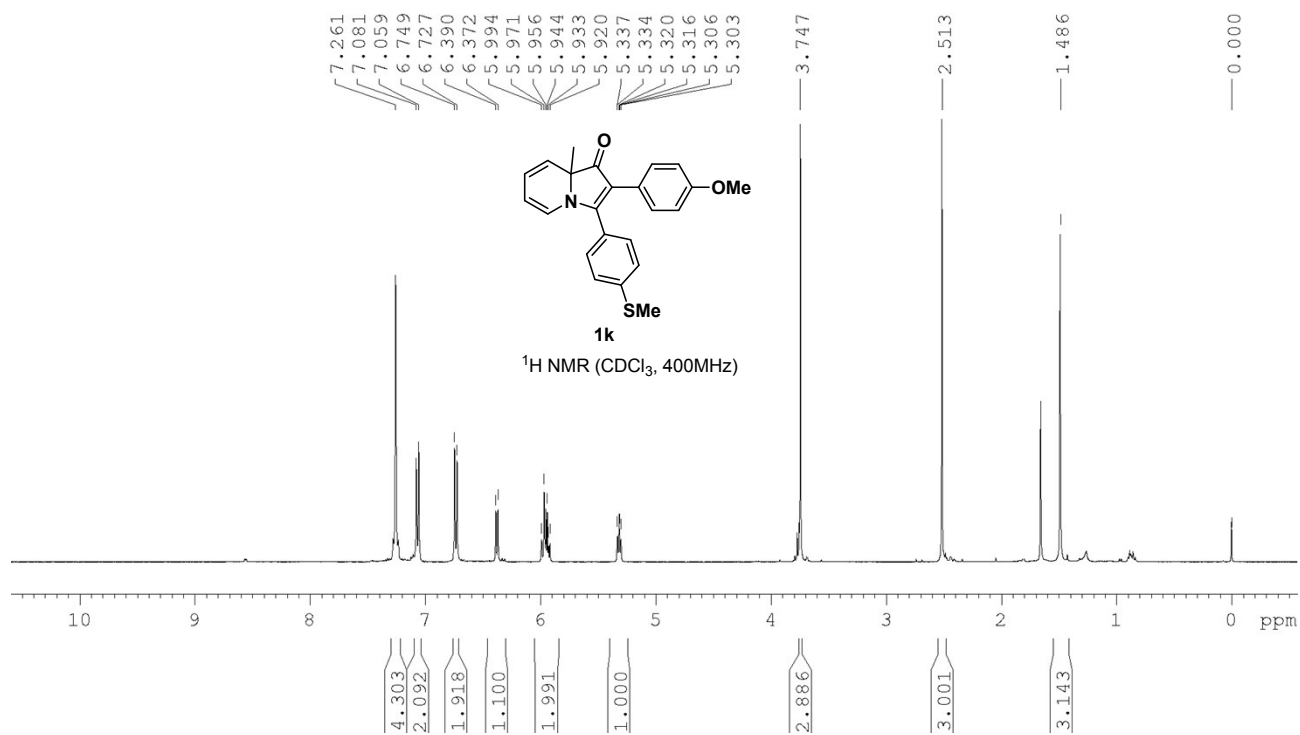


Figure 21: $^1\text{H NMR}$ (400 MHz) spectrum of **1k**

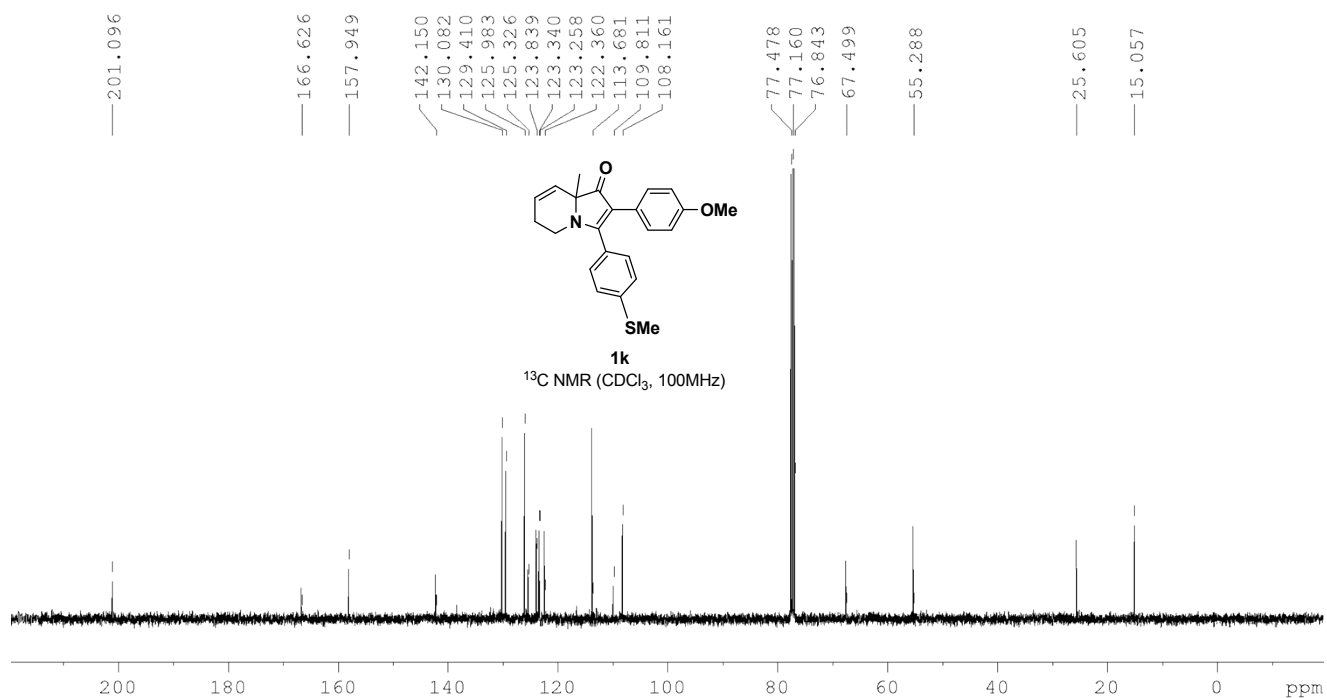


Figure 22: $^{13}\text{C NMR}$ (100 MHz) spectrum of **1k**

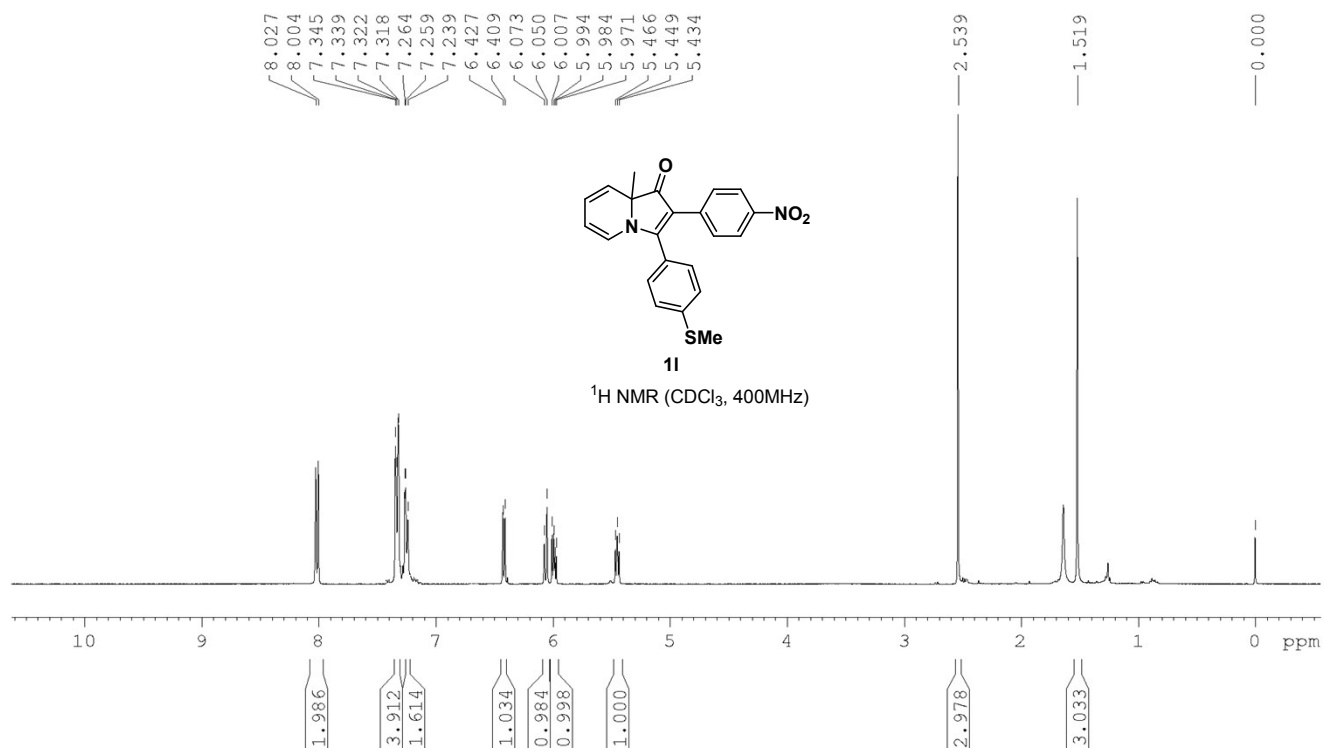


Figure 23: ¹H NMR (400 MHz) spectrum of **11**

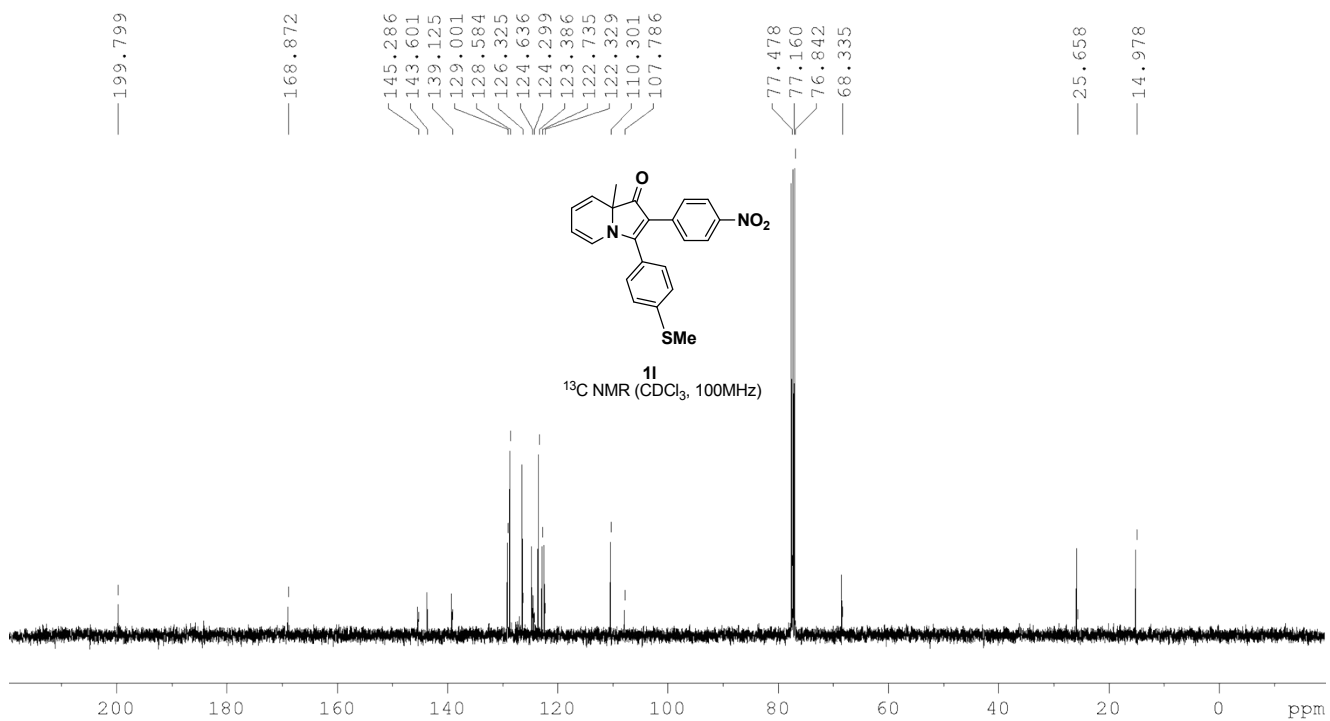


Figure 24: ¹³C NMR (100 MHz) spectrum of **11**

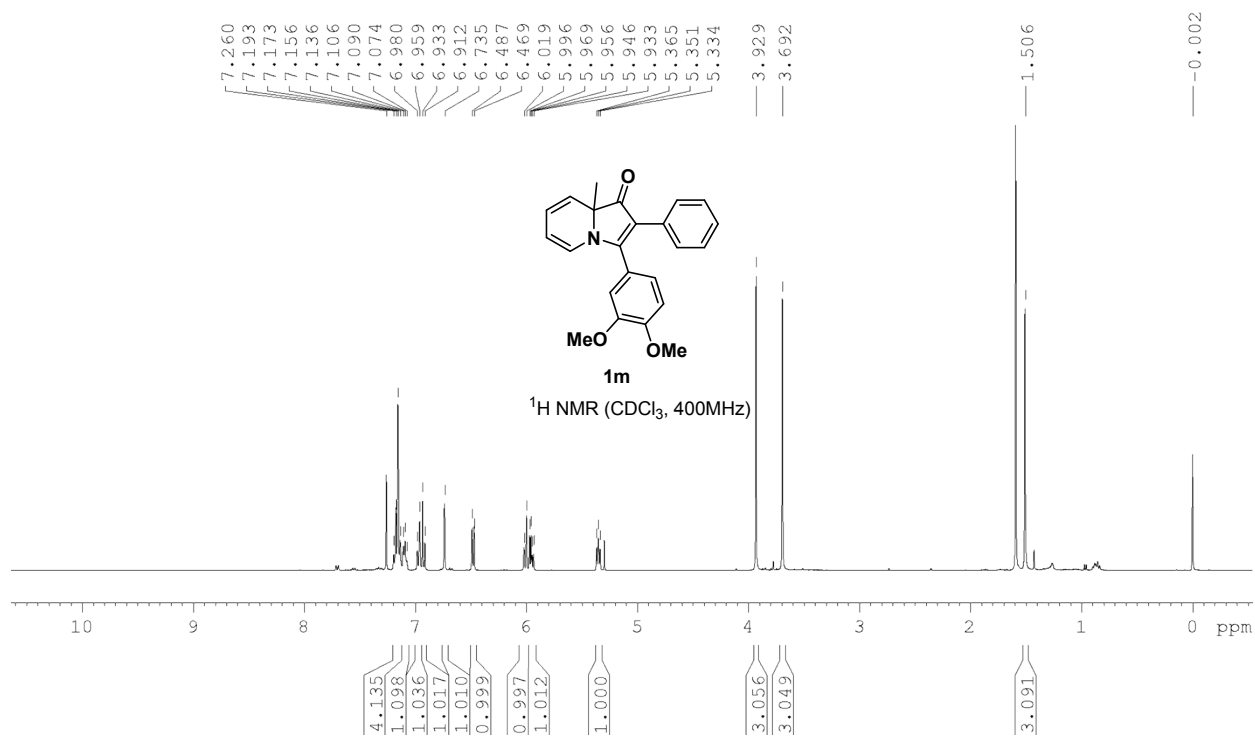


Figure 25: ¹H NMR (400 MHz) spectrum of **1m**

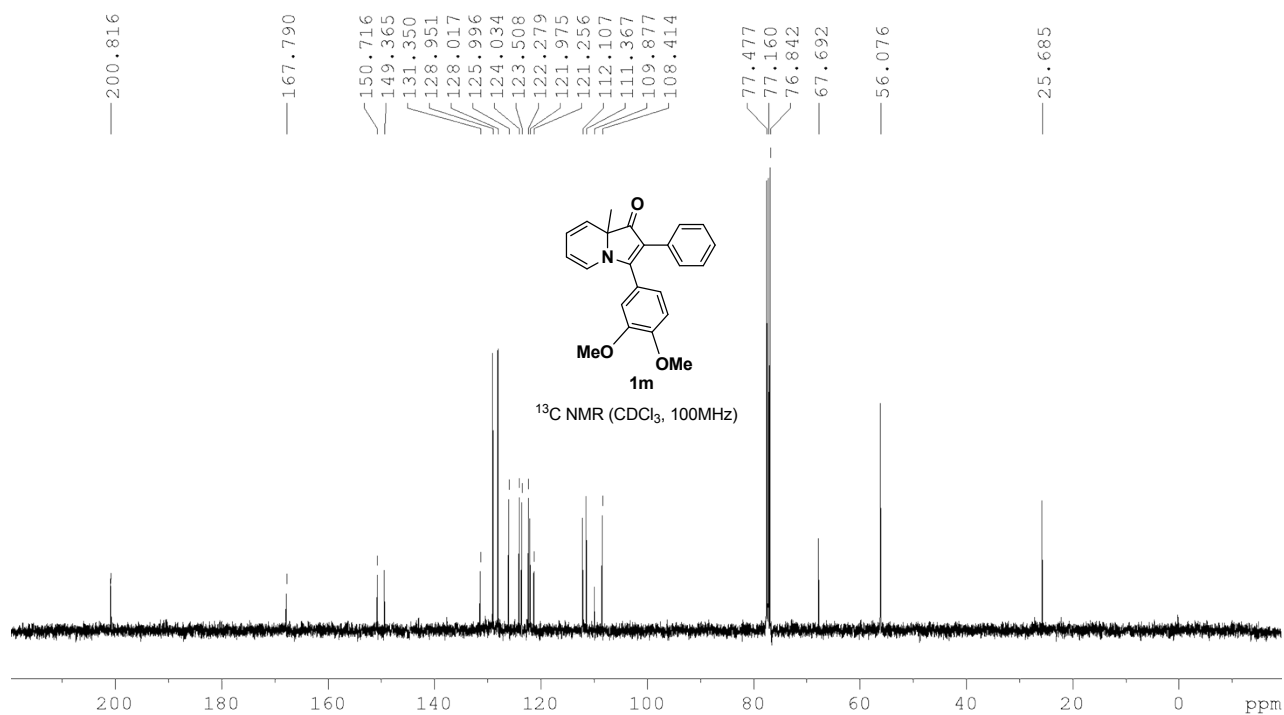


Figure 26: ¹³C NMR (100 MHz) spectrum of **1m**

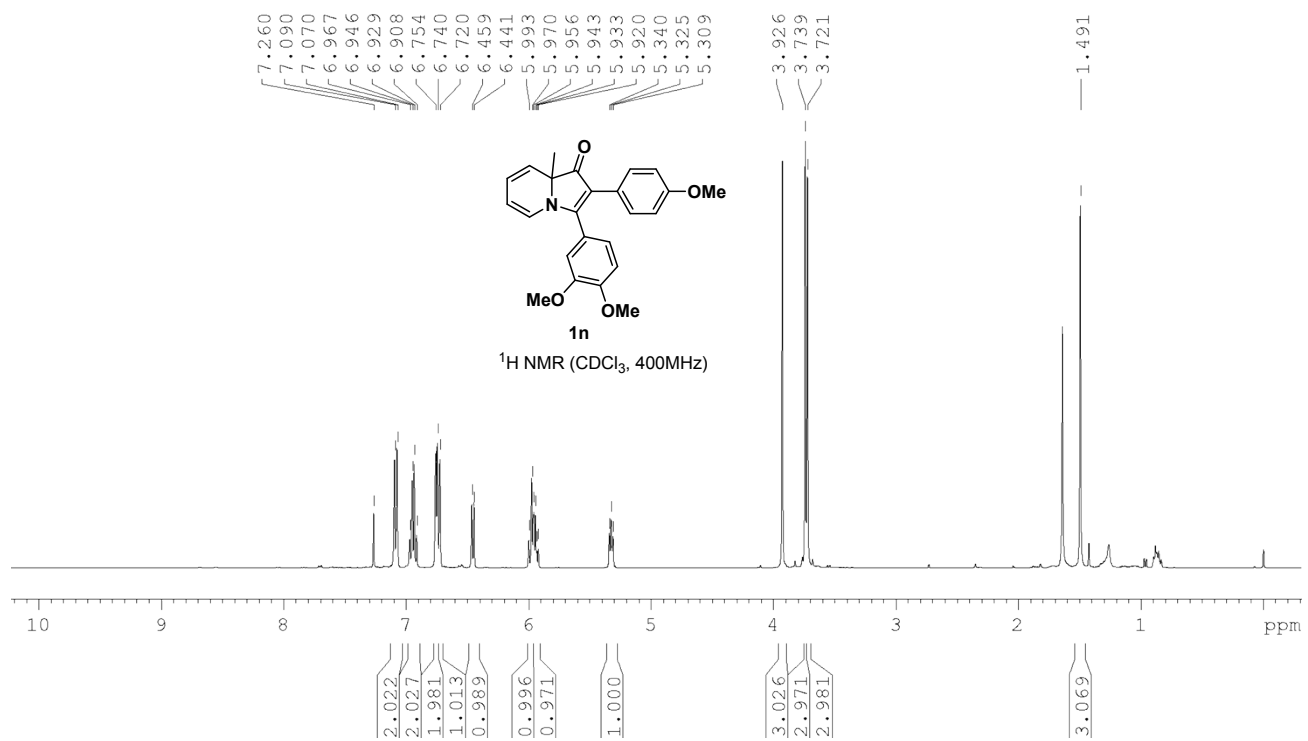


Figure 27: ¹H NMR (400 MHz) spectrum of **1n**

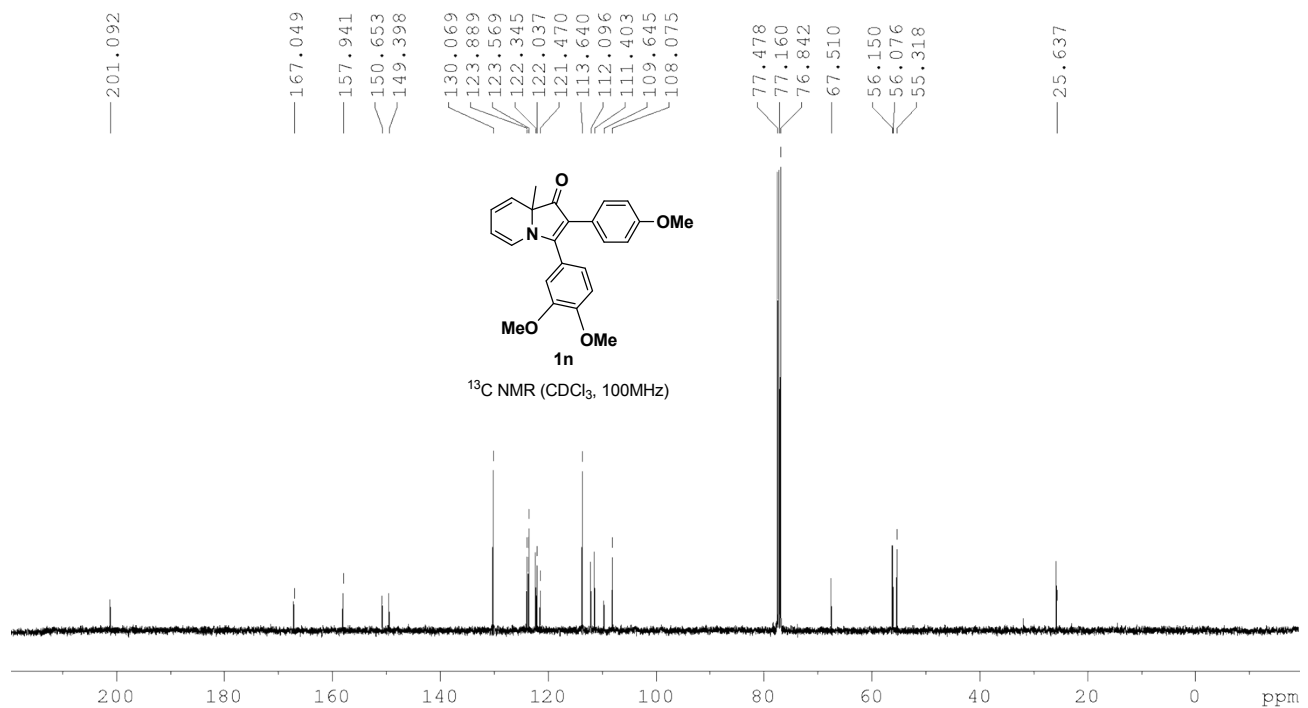


Figure 28: ¹³C NMR (100 MHz) spectrum of **1n**

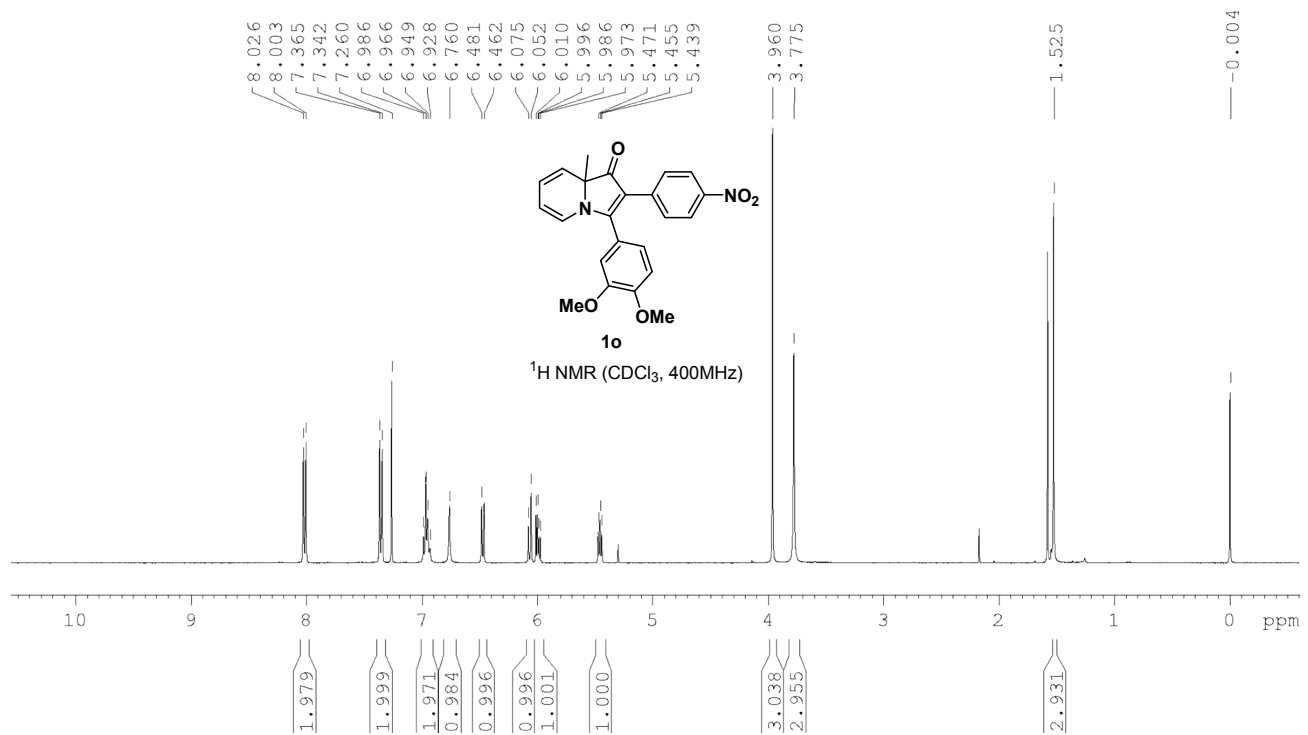


Figure 29: ¹H NMR (400 MHz) spectrum of **1o**

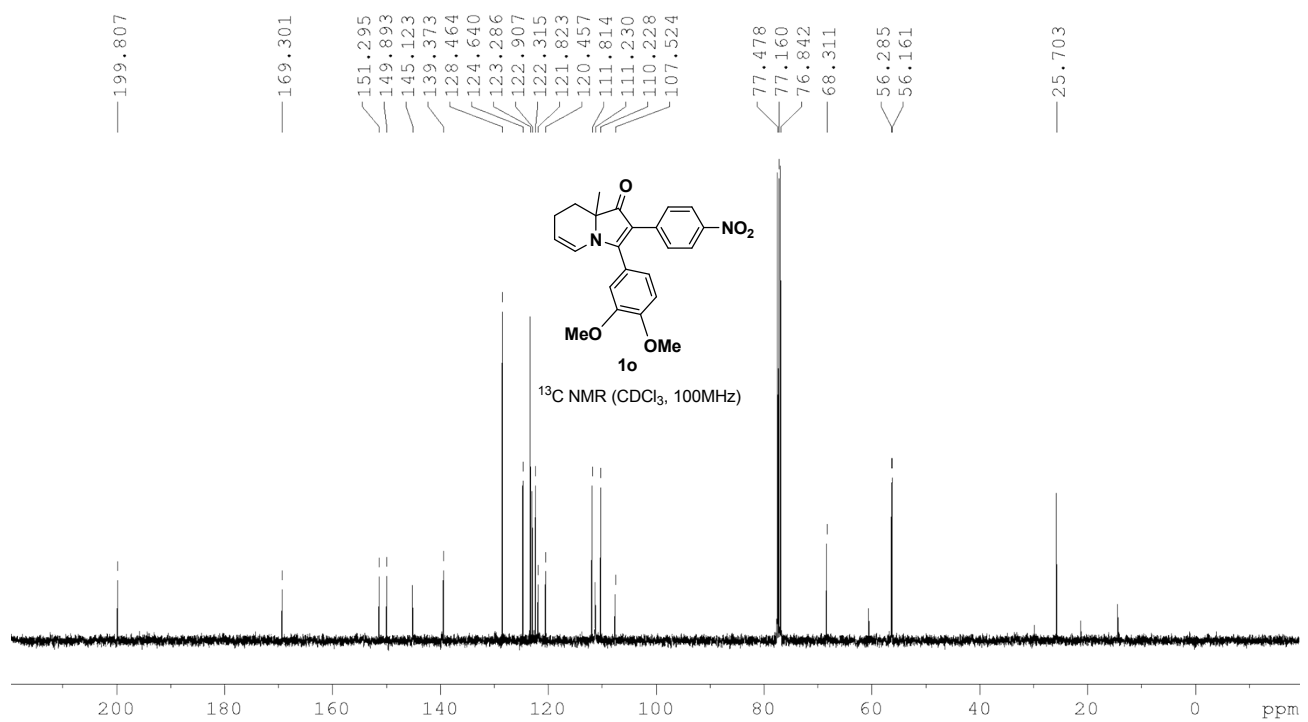


Figure 30: ¹³C NMR (100 MHz) spectrum of **1o**

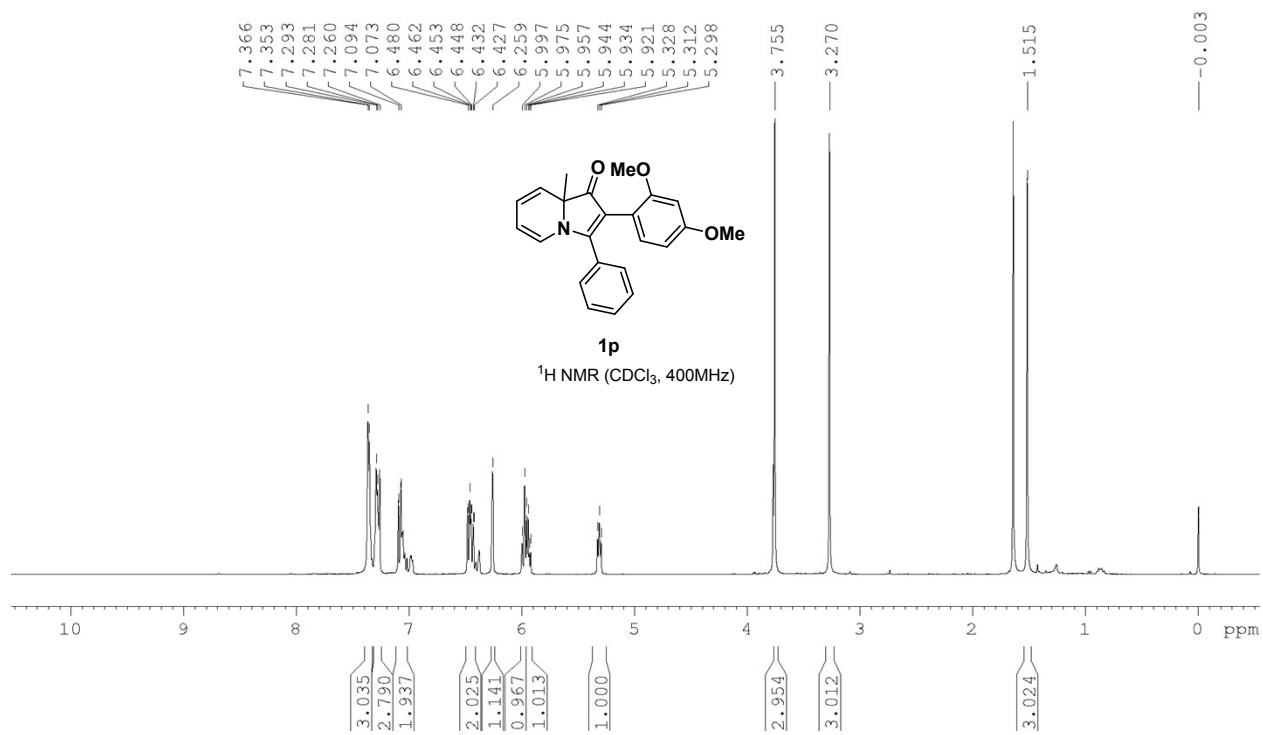


Figure 31: $^1\text{H NMR}$ (400 MHz) spectrum of **1p**

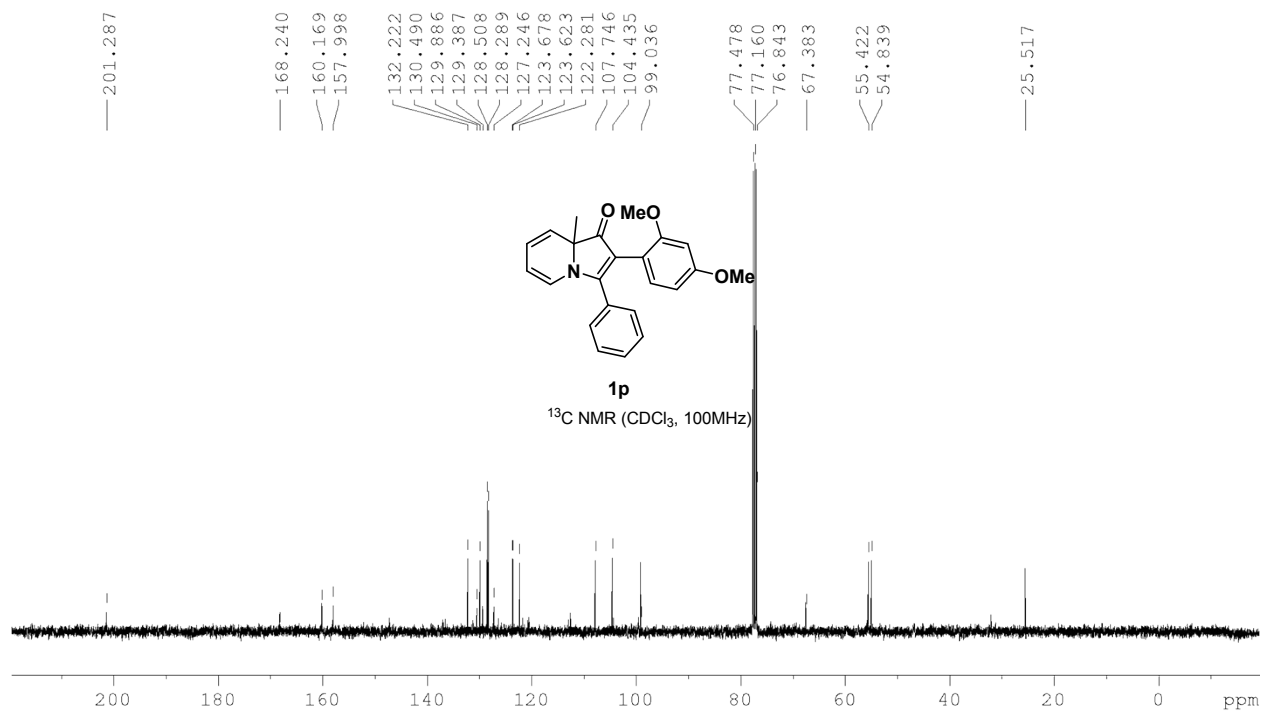


Figure 32: $^{13}\text{C NMR}$ (100 MHz) spectrum of **1p**

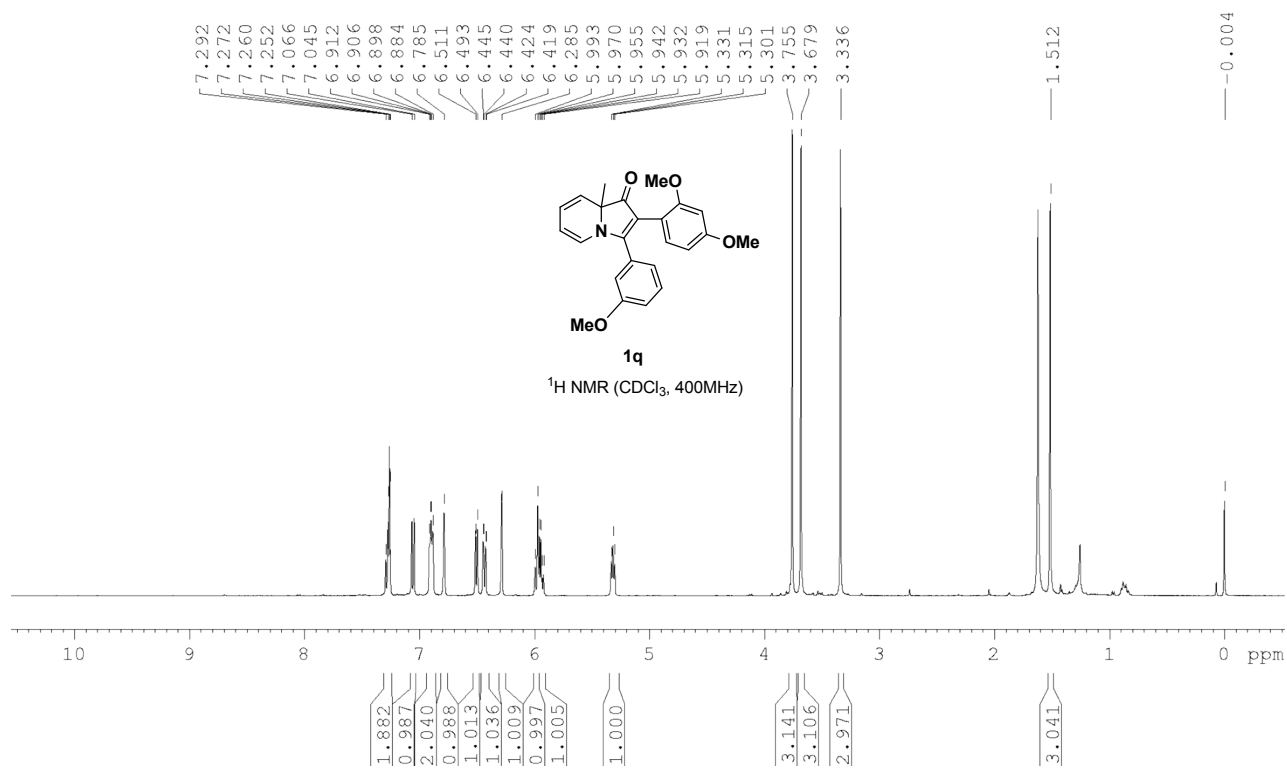


Figure 33: $^1\text{H NMR}$ (400 MHz) spectrum of **1q**

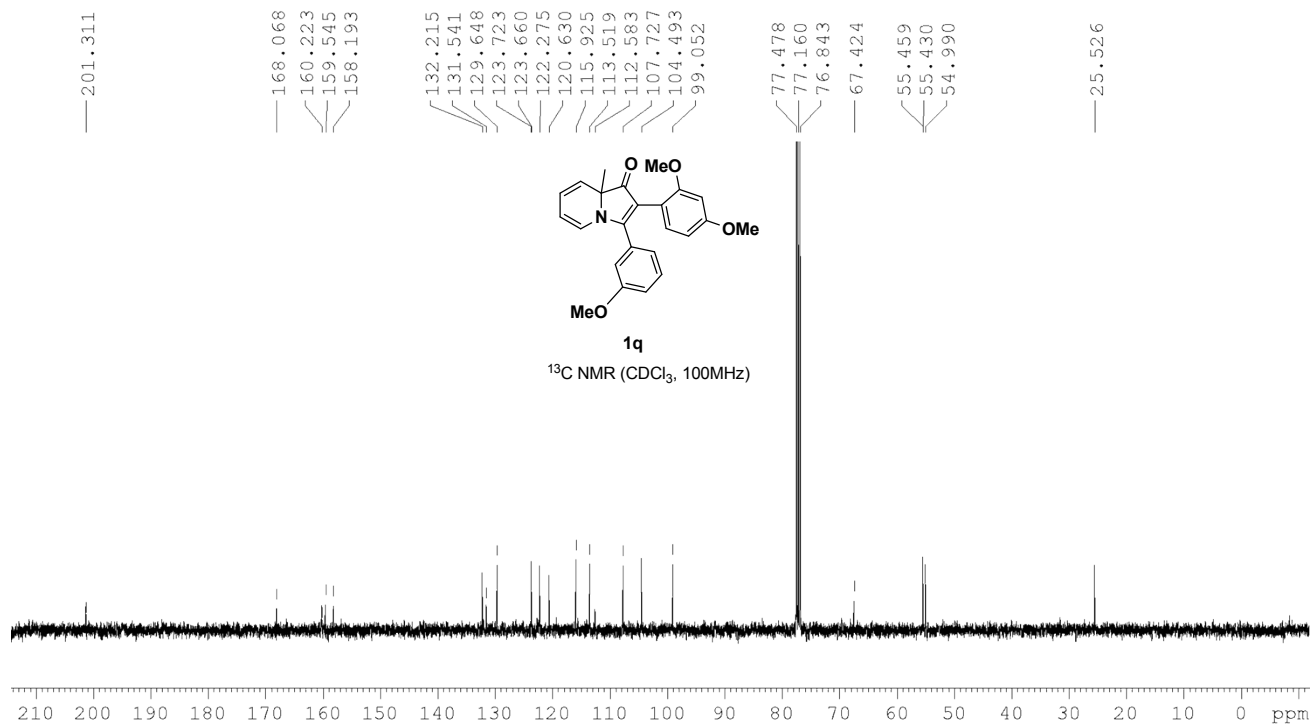


Figure 34: $^{13}\text{C NMR}$ (100 MHz) spectrum of **1q**

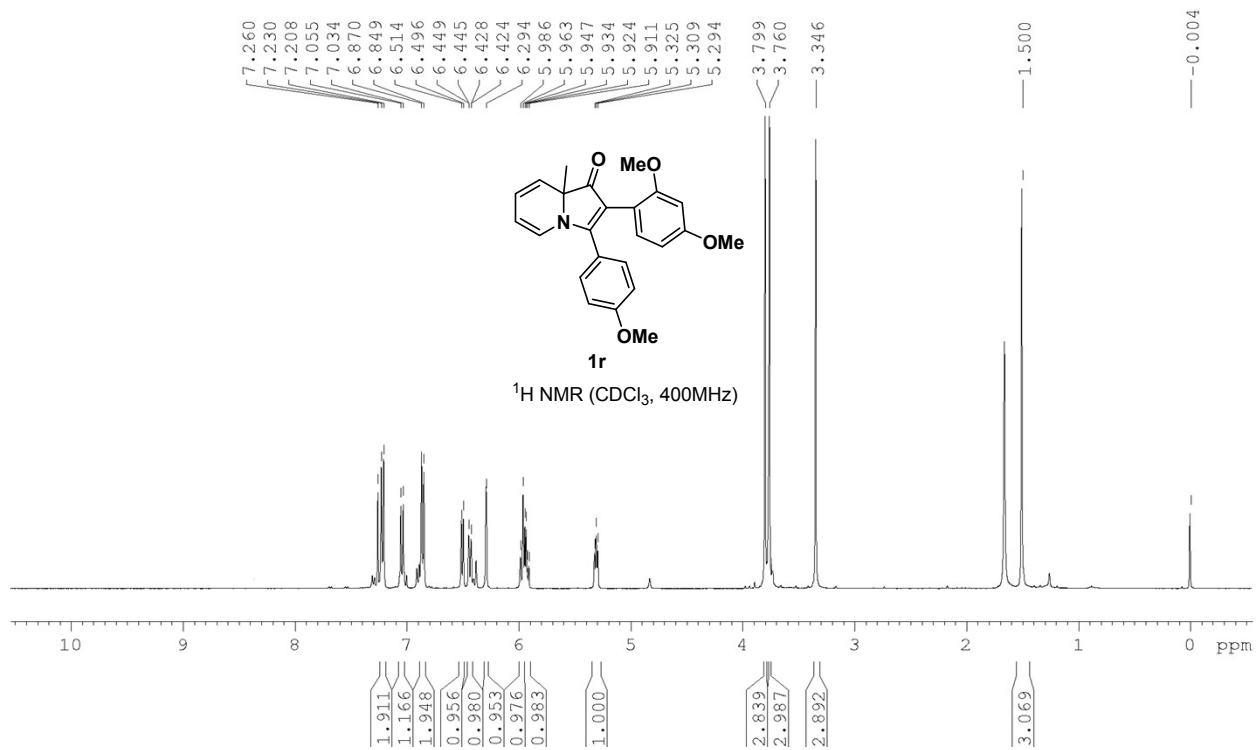


Figure 35: ¹H NMR (400 MHz) spectrum of **1r**

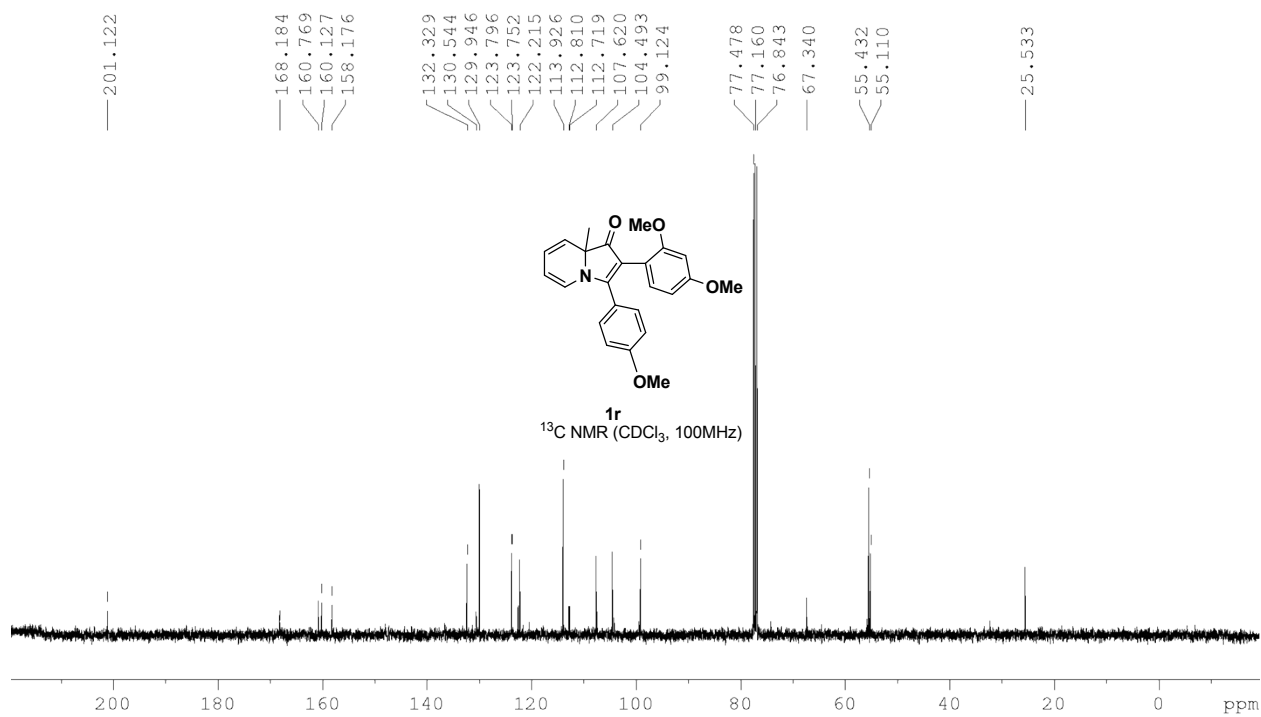


Figure 36: ¹³C NMR (100 MHz) spectrum of **1r**

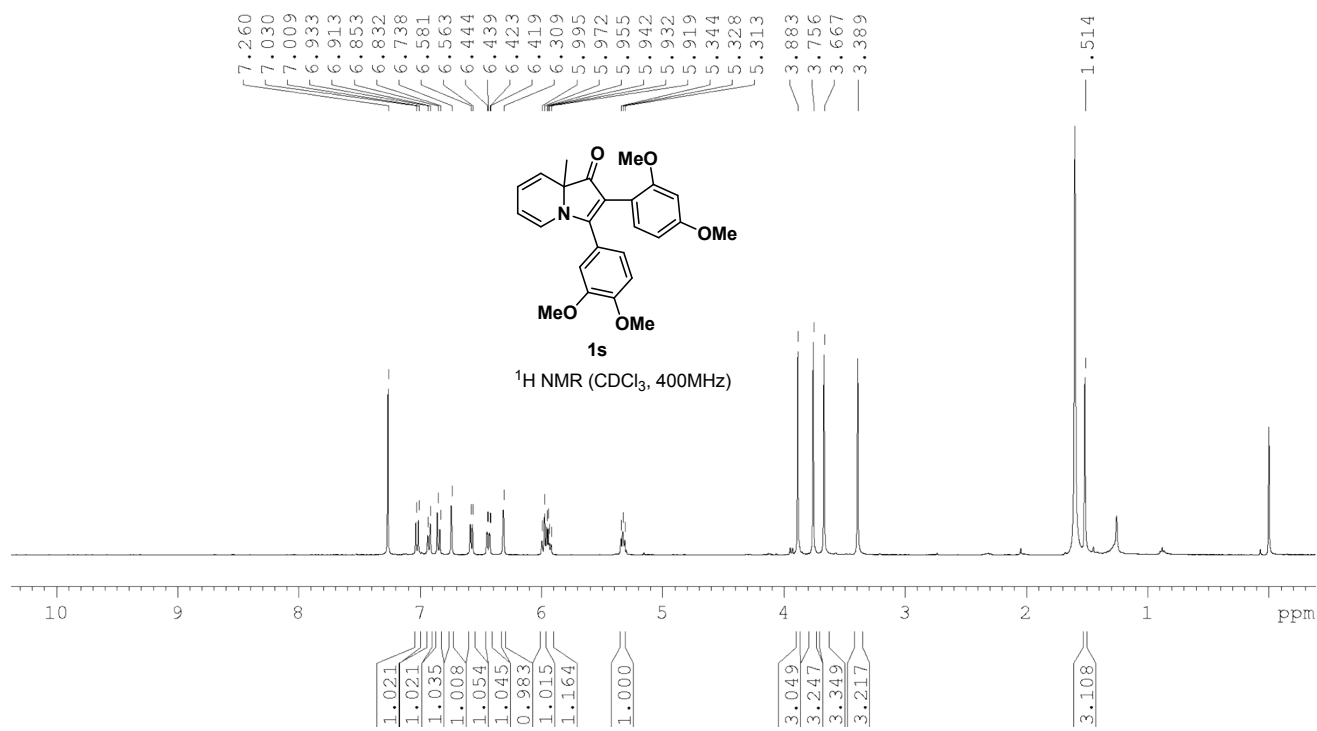


Figure 37: ¹H NMR (400 MHz) spectrum of **1s**

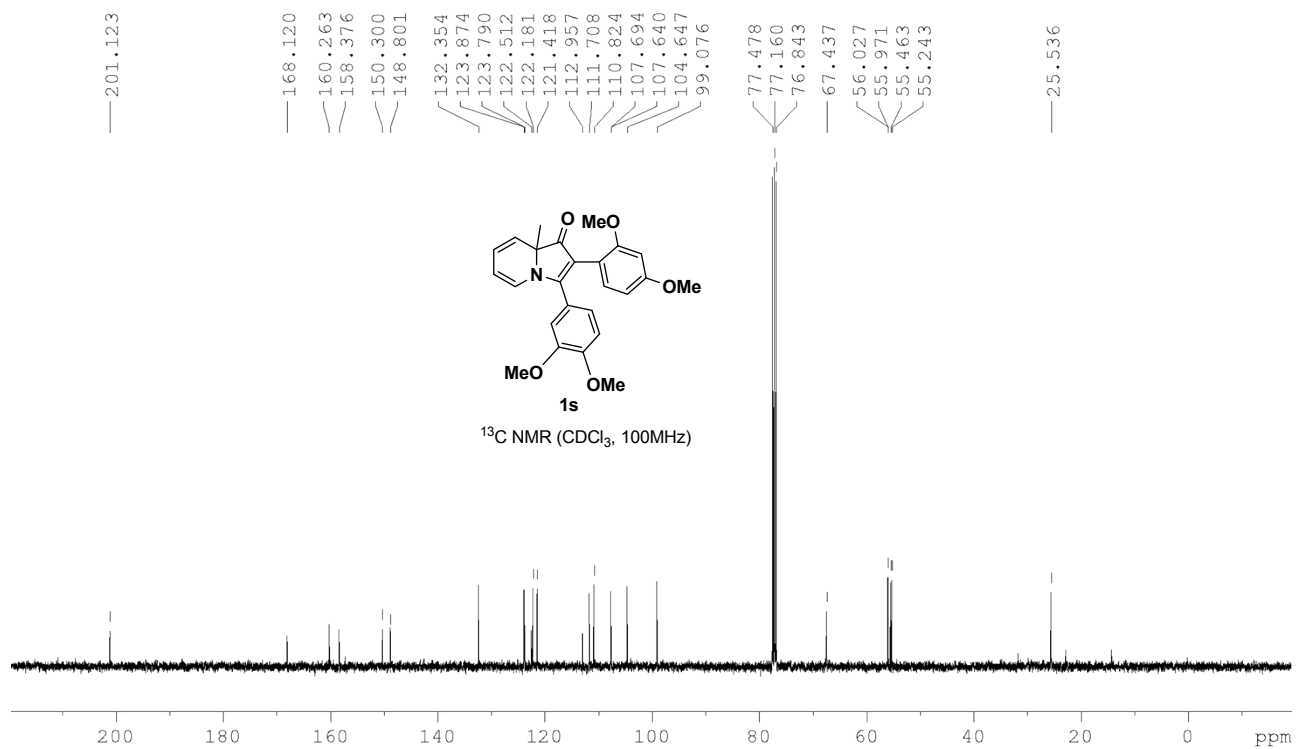


Figure 38: ¹³C NMR (100 MHz) spectrum of **1s**

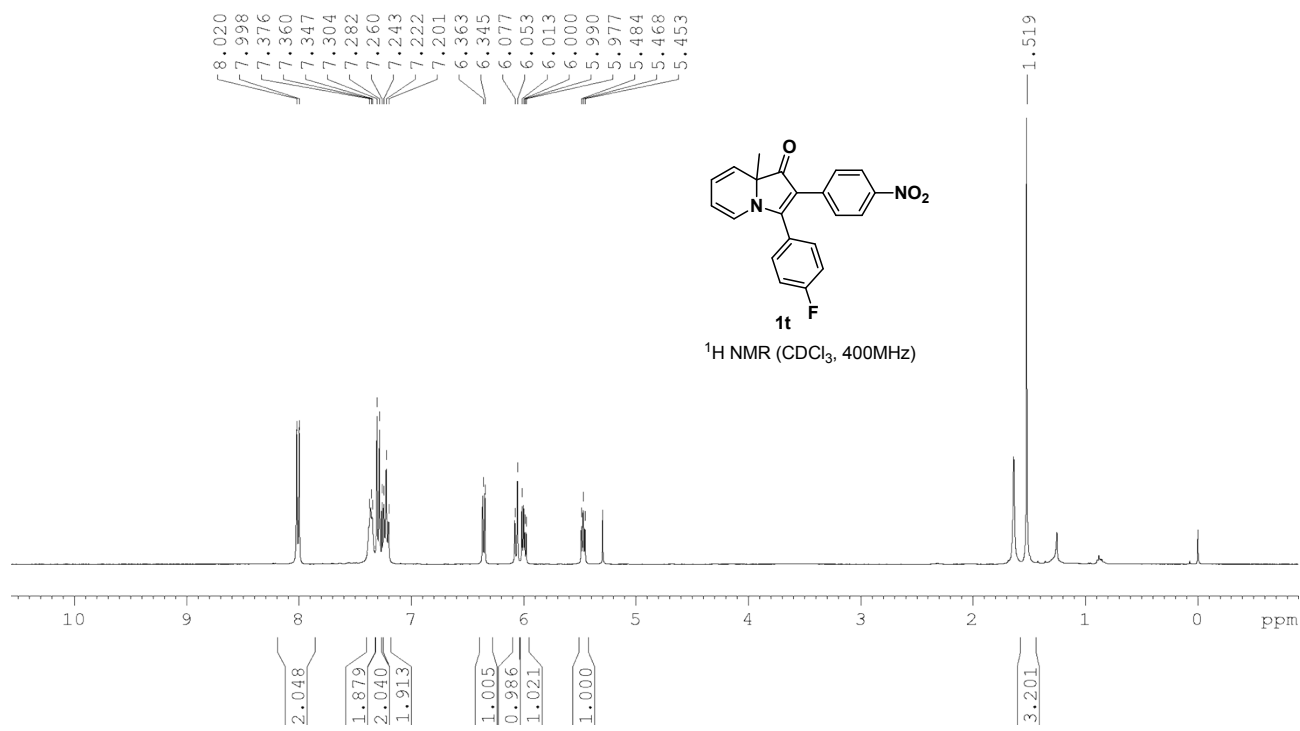


Figure 39: ¹H NMR (400 MHz) spectrum of **1t**

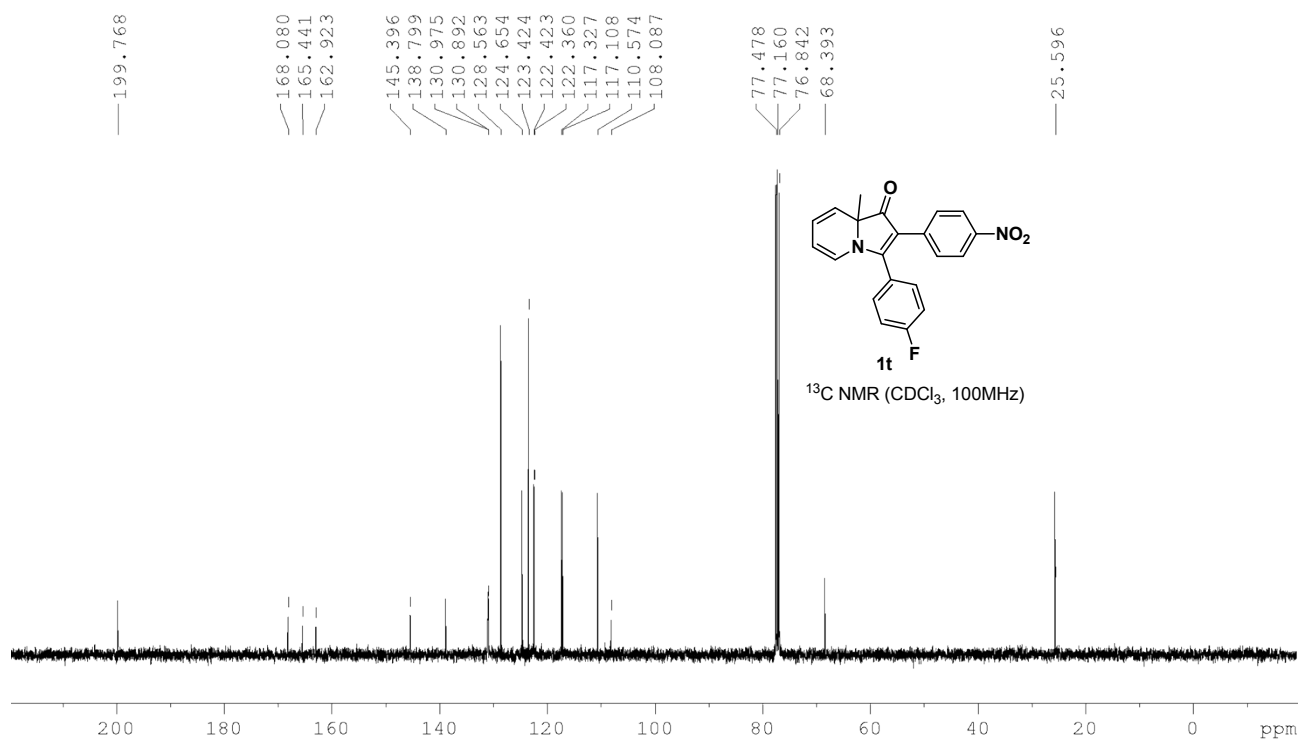


Figure 40: ¹³C NMR (100 MHz) spectrum of **1t**

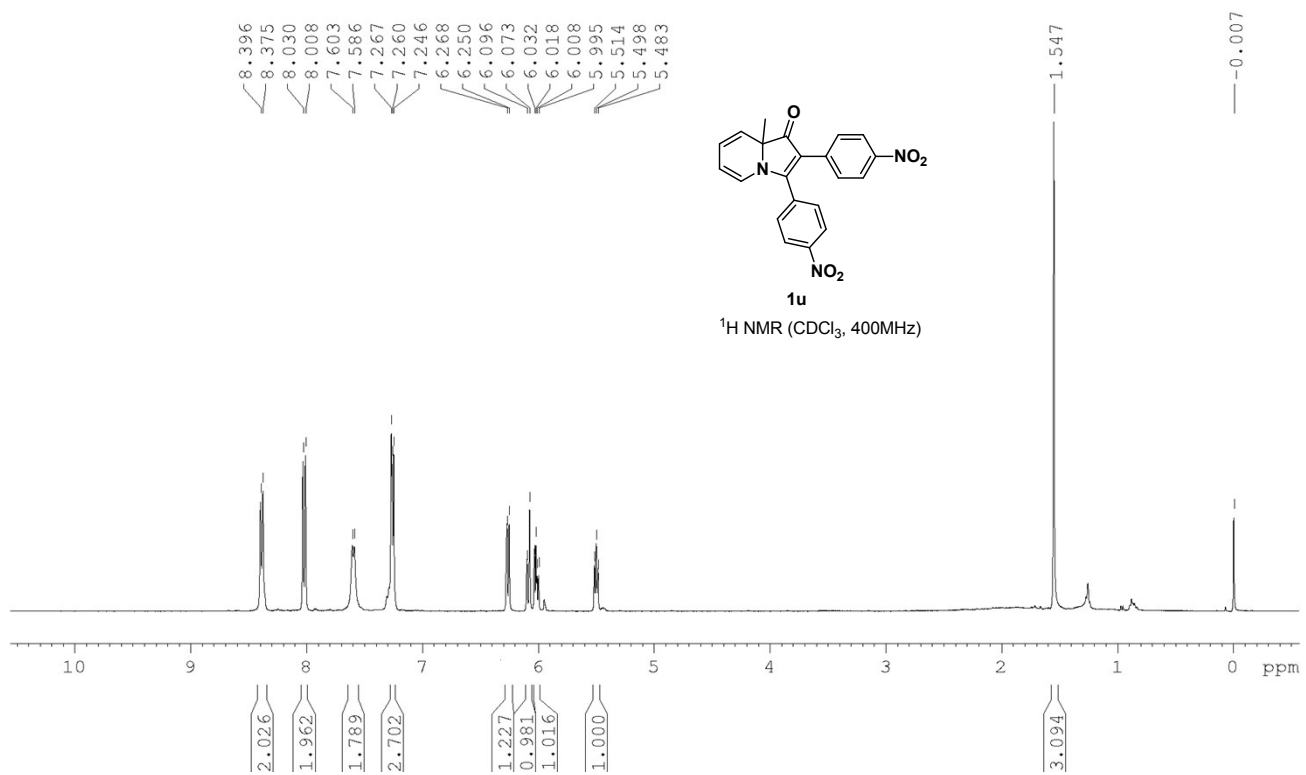


Figure 41: ¹H NMR (400 MHz) spectrum of **1u**

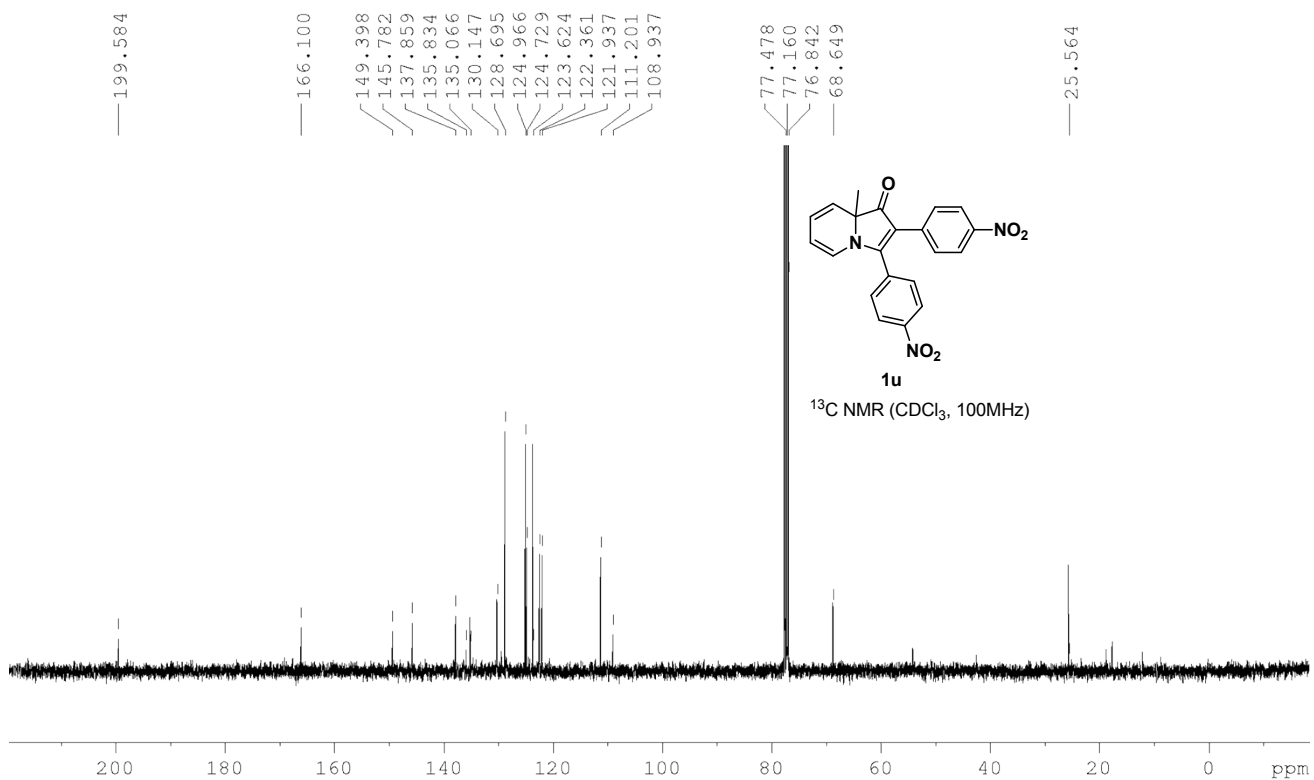


Figure 42: ¹³C NMR (100 MHz) spectrum of **1u**

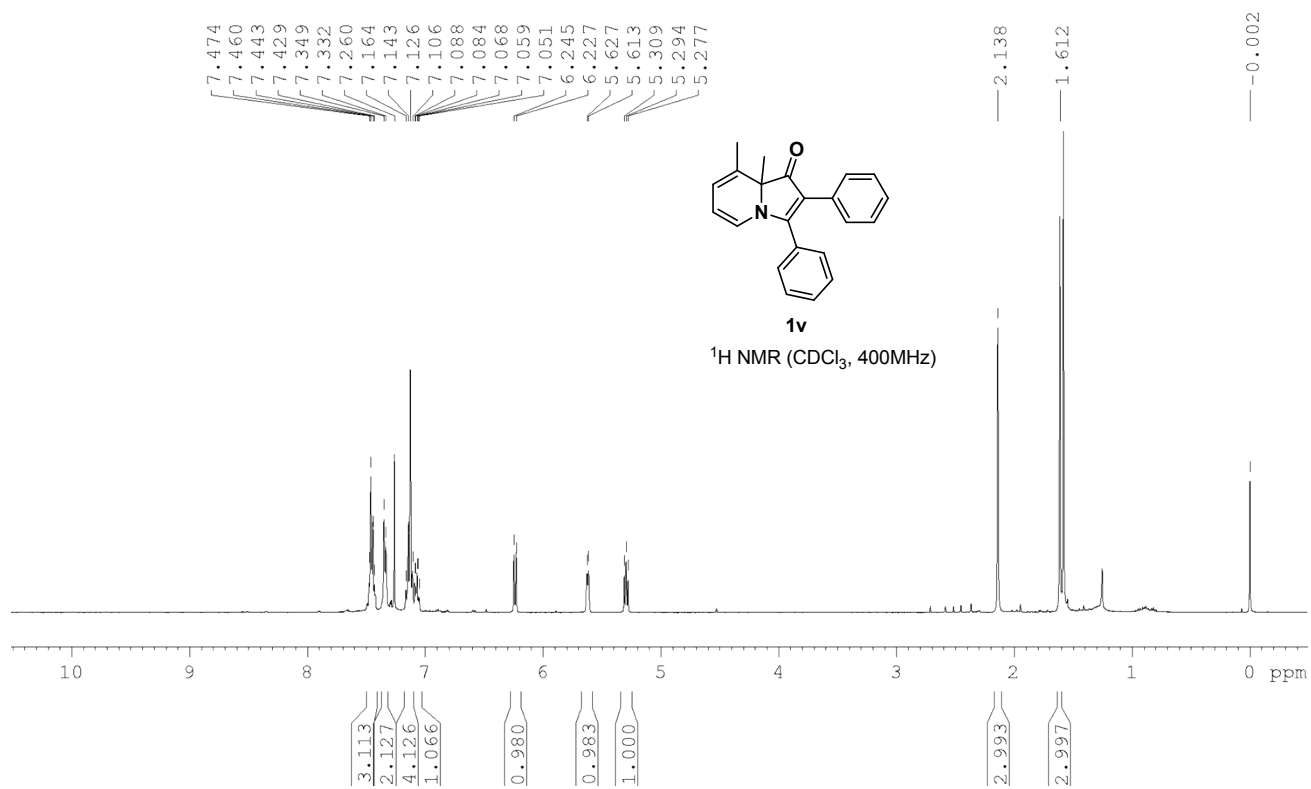


Figure 43: ¹H NMR (400 MHz) spectrum of **1v**

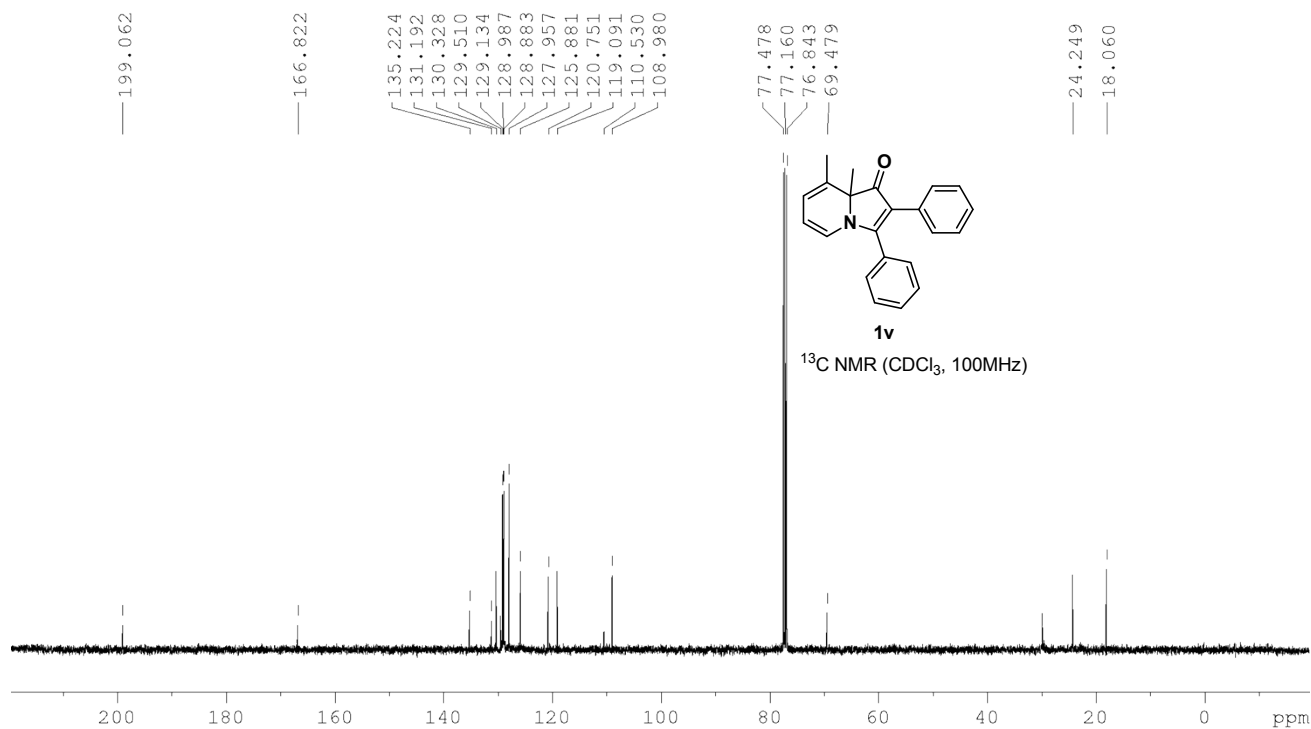


Figure 44: ¹³C NMR (100 MHz) spectrum of **1v**

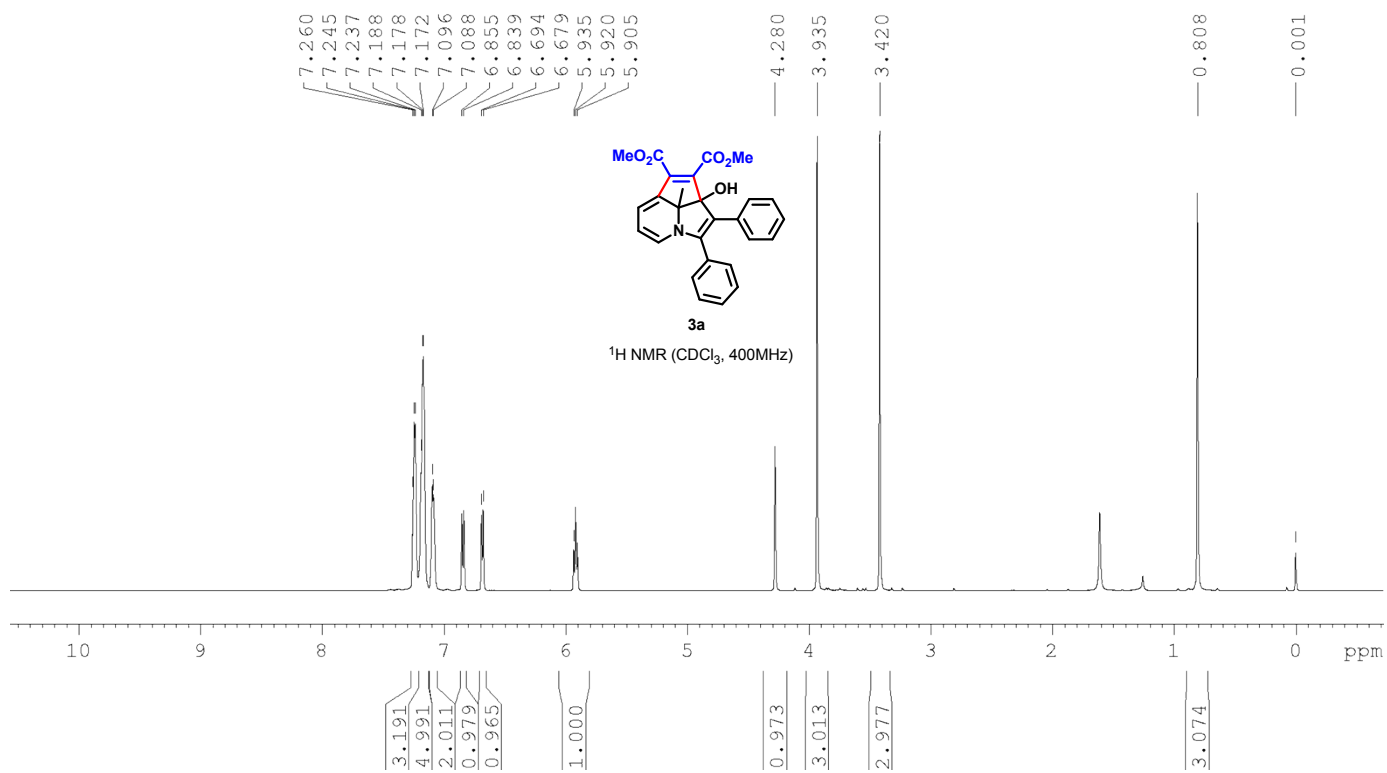


Figure 45: ¹H NMR (400 MHz) spectrum of **3a**

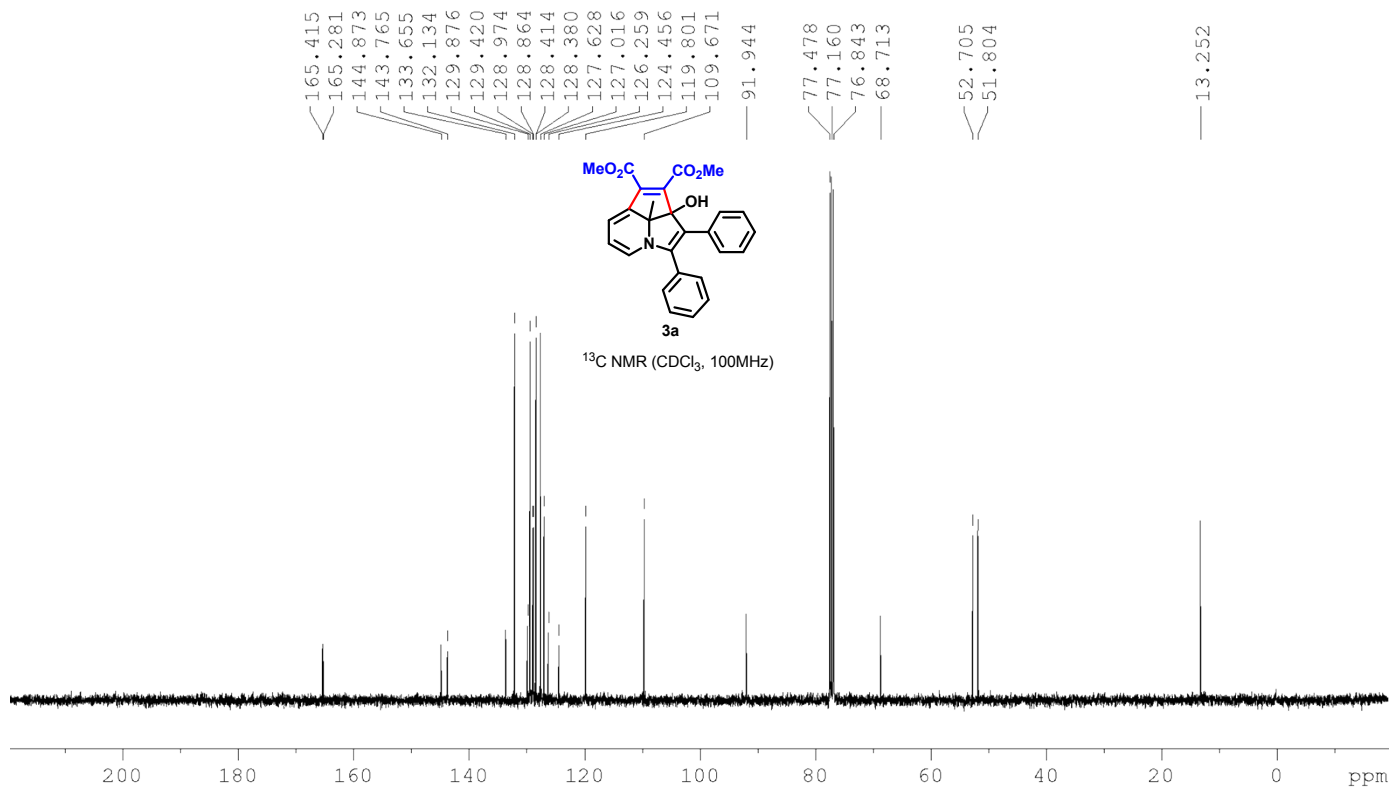


Figure 46: ¹³C NMR (100 MHz) spectrum of **3a**

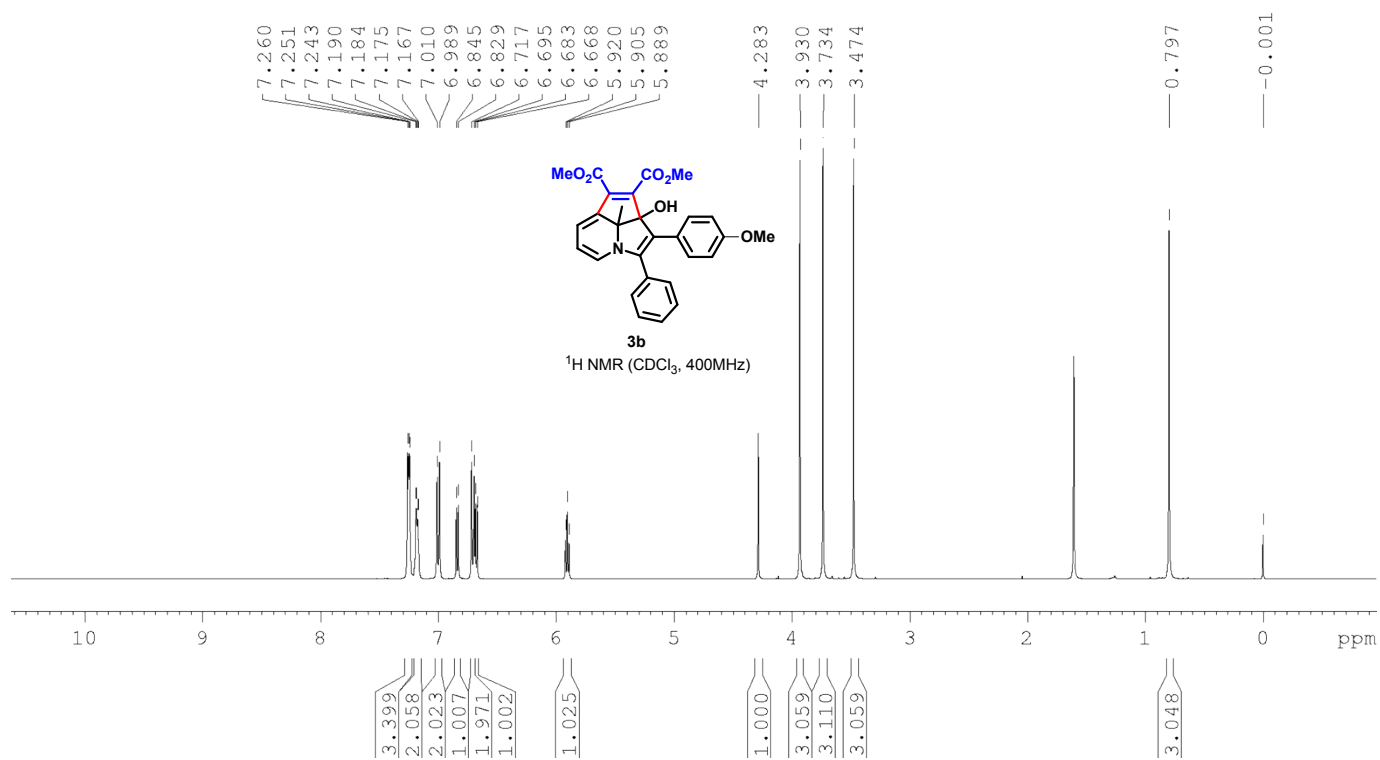


Figure 47: ¹H NMR (400 MHz) spectrum of **3b**

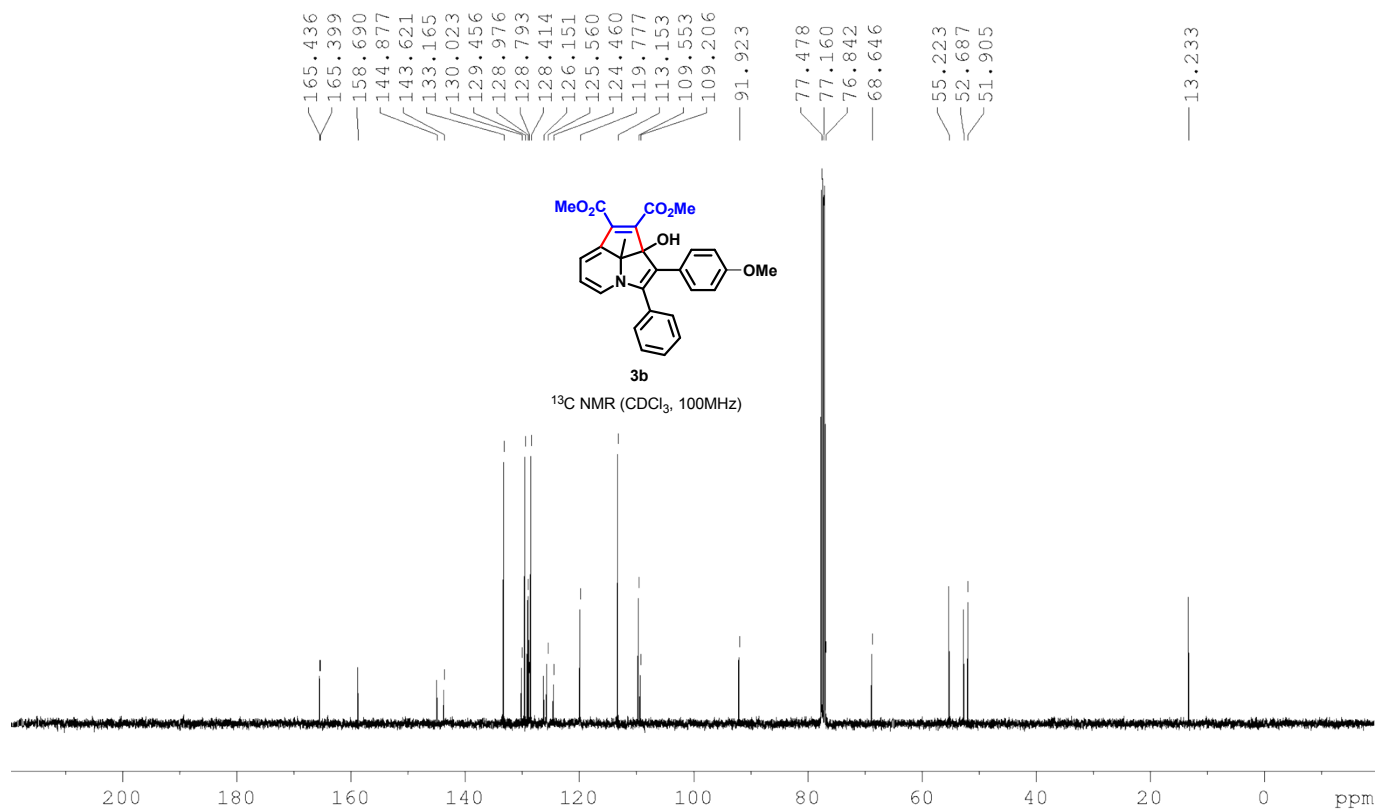


Figure 48: ¹³C NMR (100 MHz) spectrum of **3b**

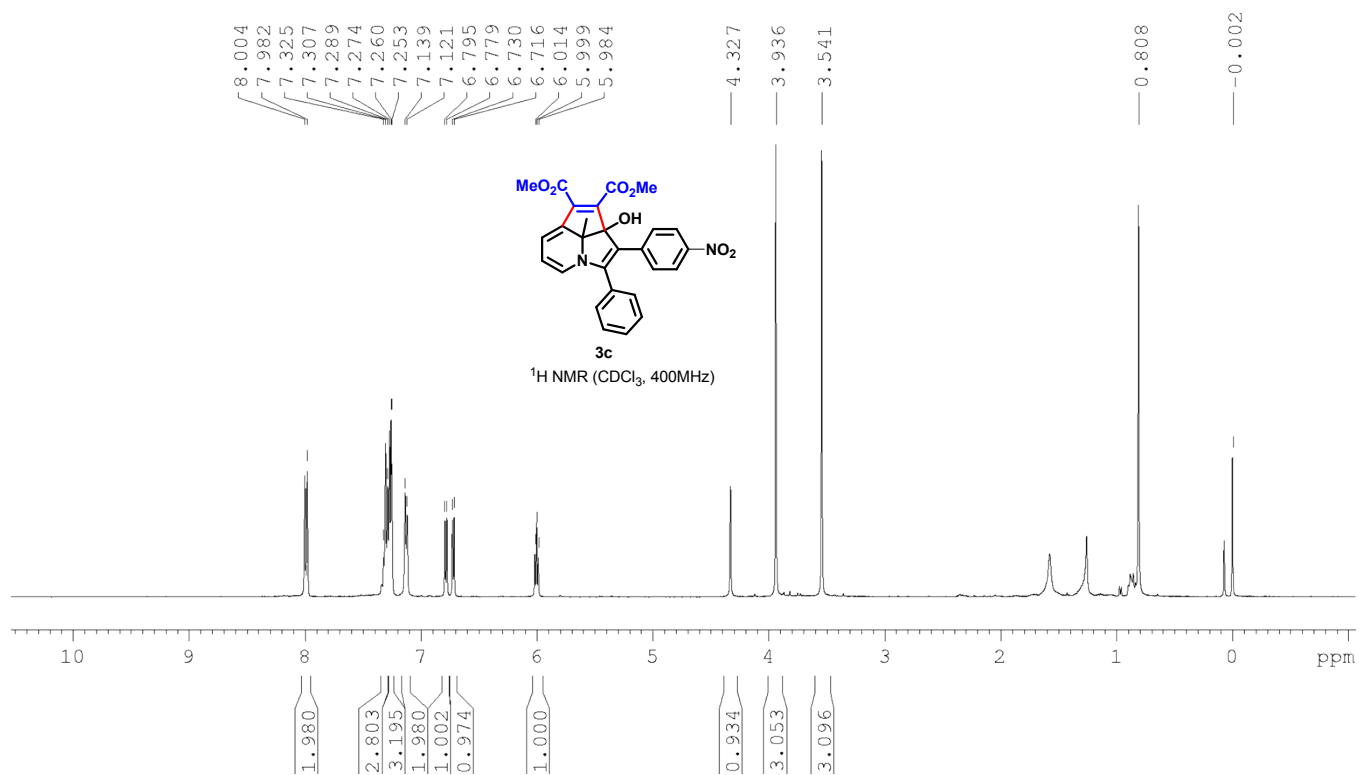


Figure 49: ¹H NMR (400 MHz) spectrum of **3c**

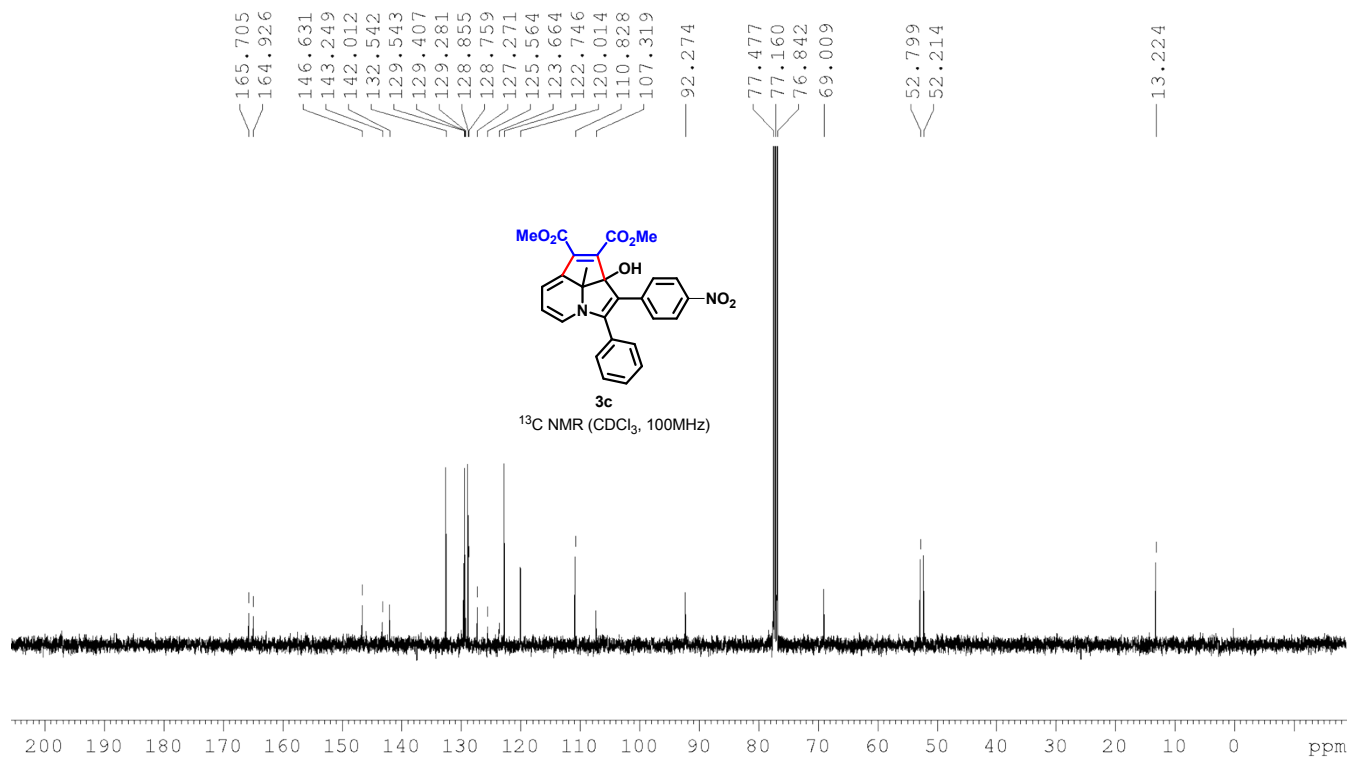


Figure 50: ¹³C NMR (100 MHz) spectrum of **3c**

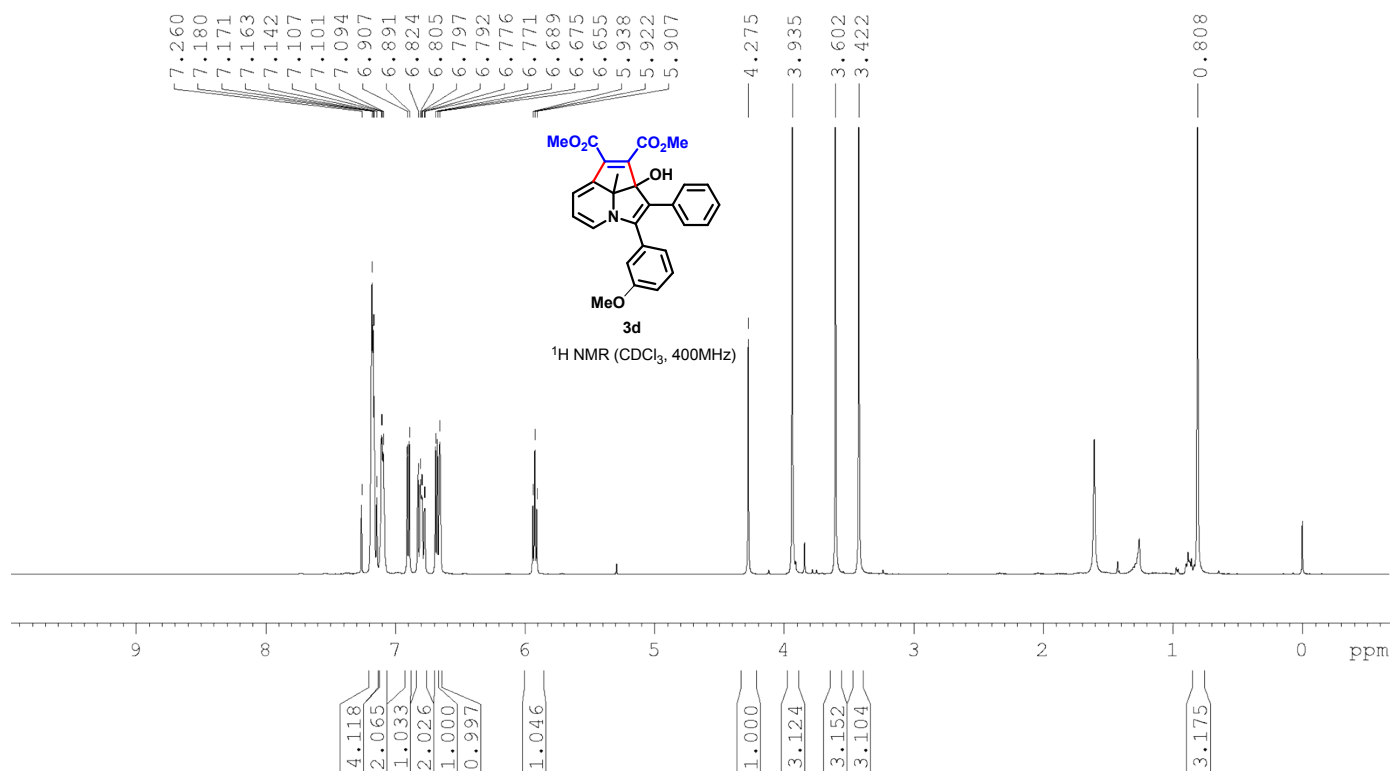


Figure 51: ¹H NMR (400 MHz) spectrum of **3d**

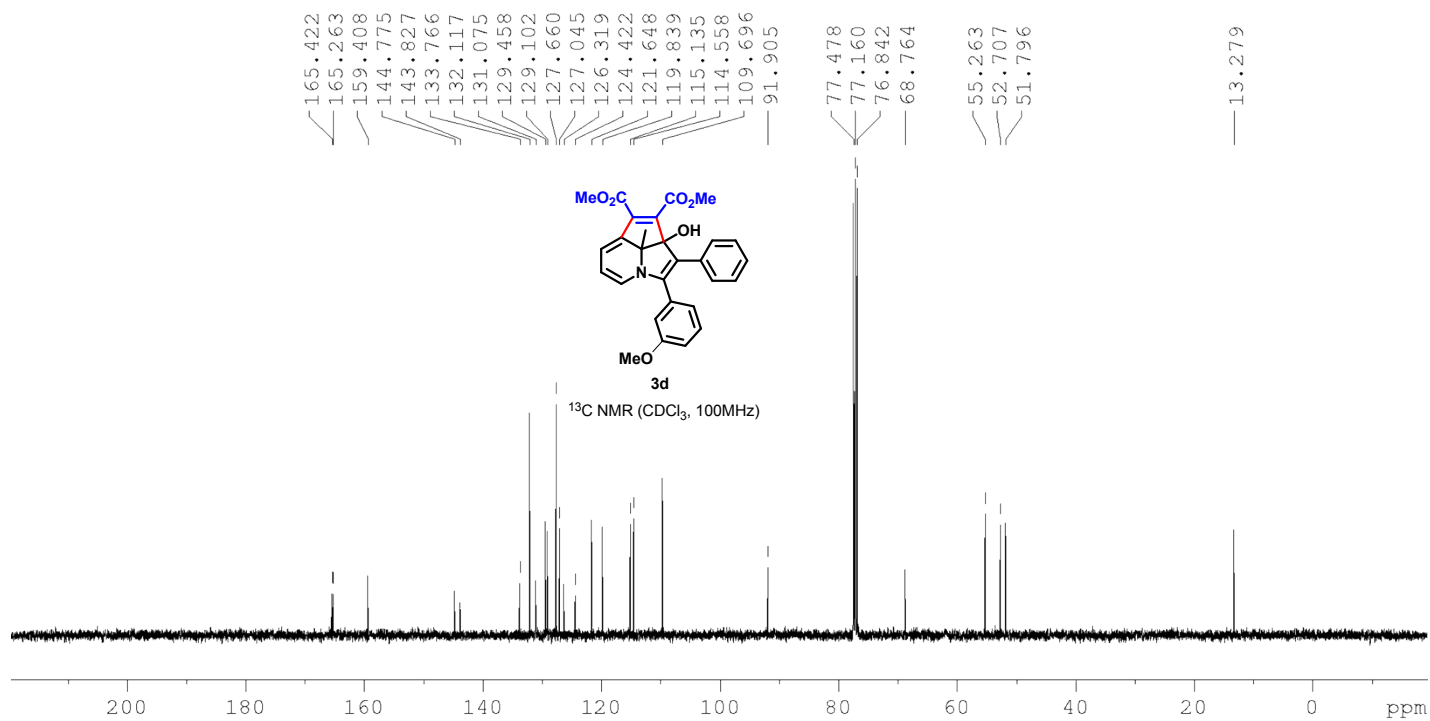


Figure 52: ¹³C NMR (100 MHz) spectrum of **3d**

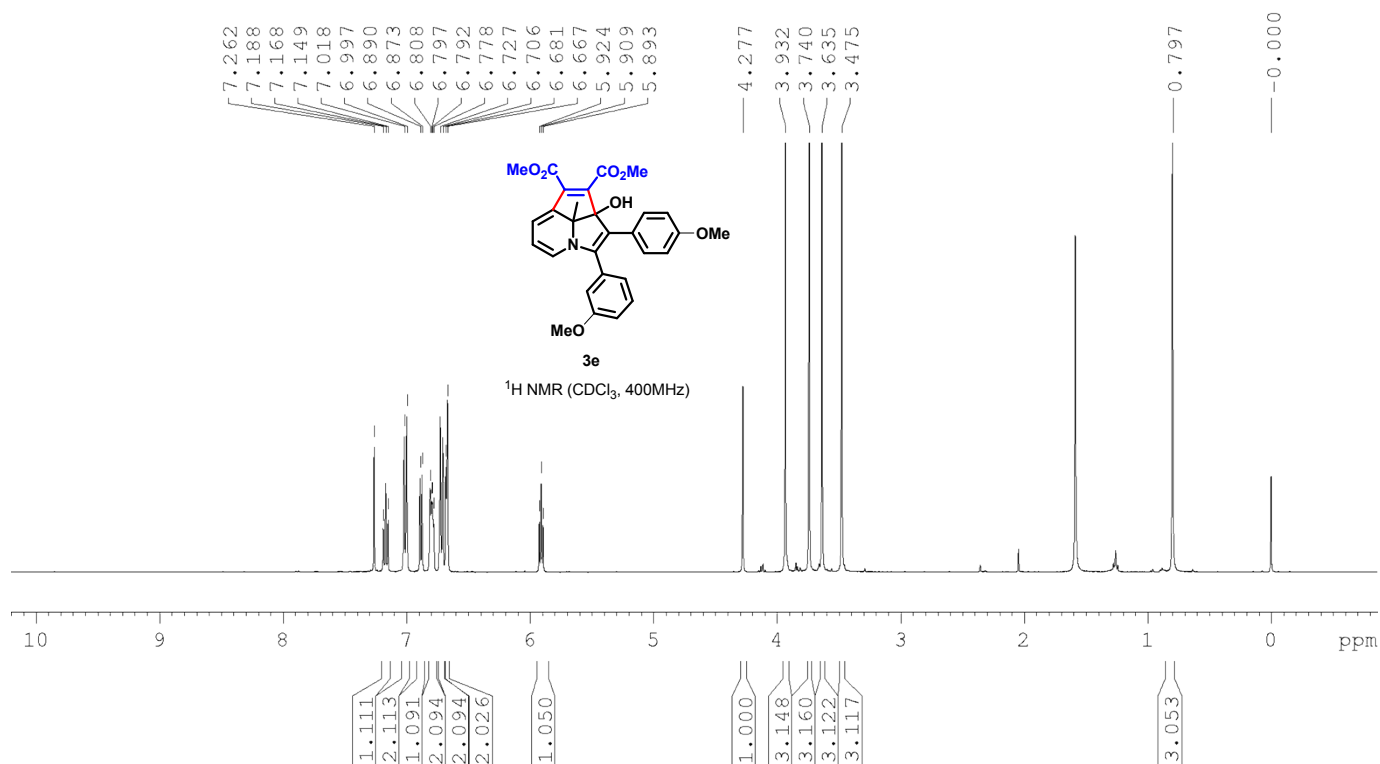


Figure 53: $^1\text{H NMR}$ (400 MHz) spectrum of **3e**

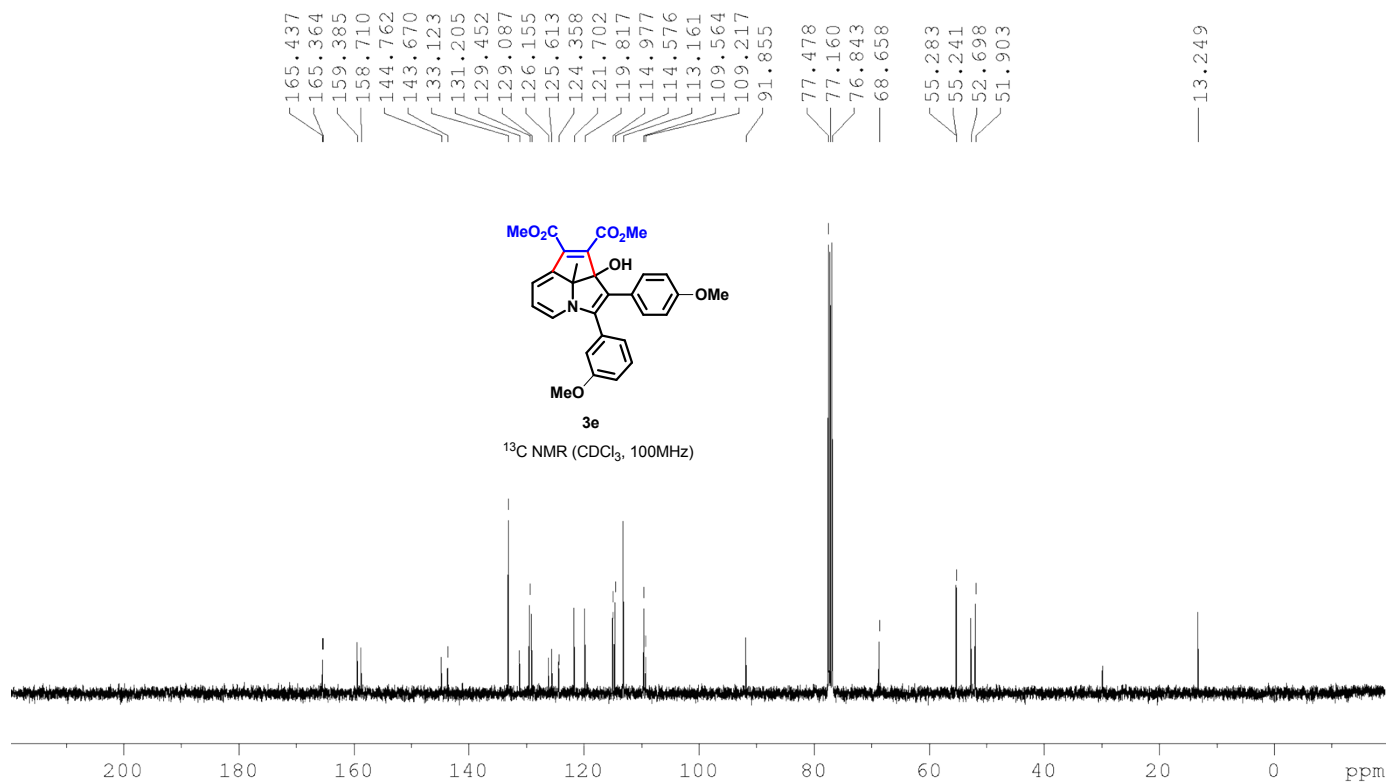


Figure 54: $^{13}\text{C NMR}$ (100 MHz) spectrum of **3e**

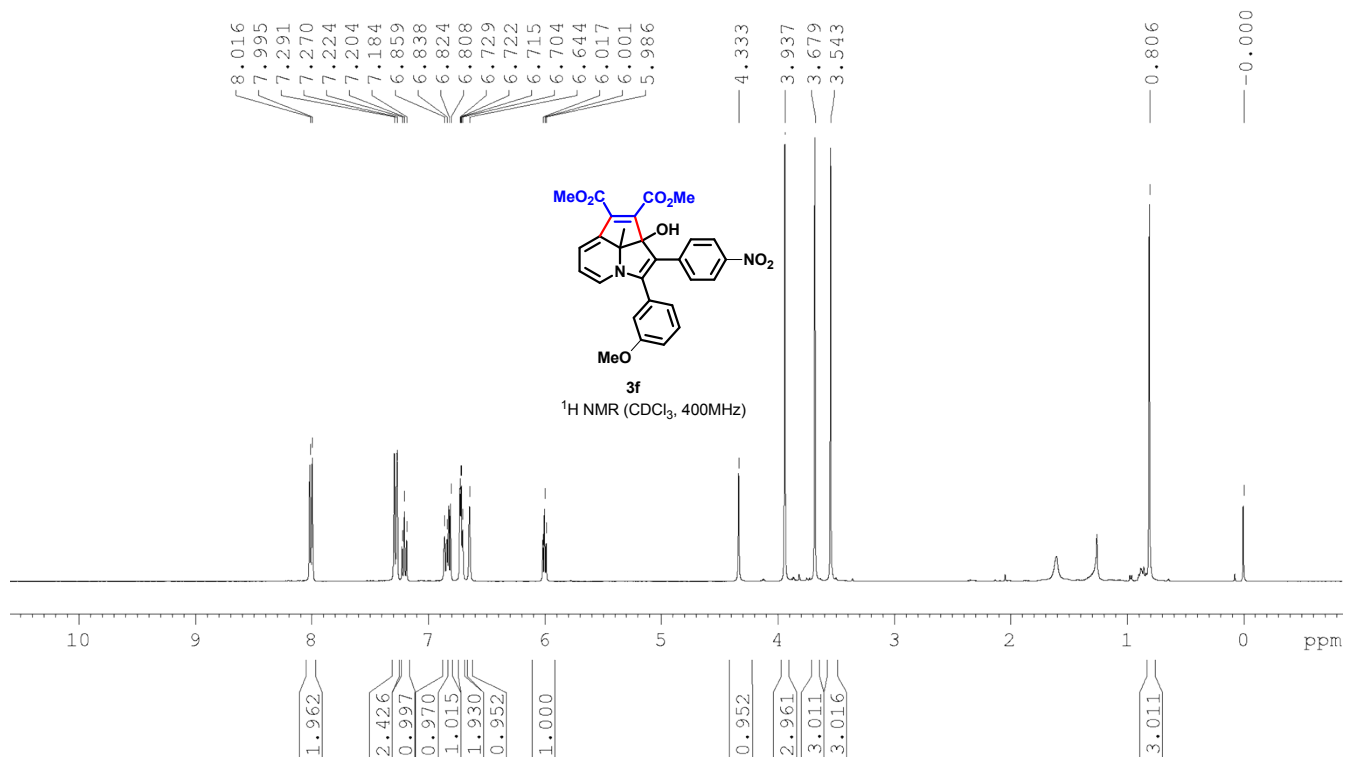


Figure 55: ¹H NMR (400 MHz) spectrum of **3f**

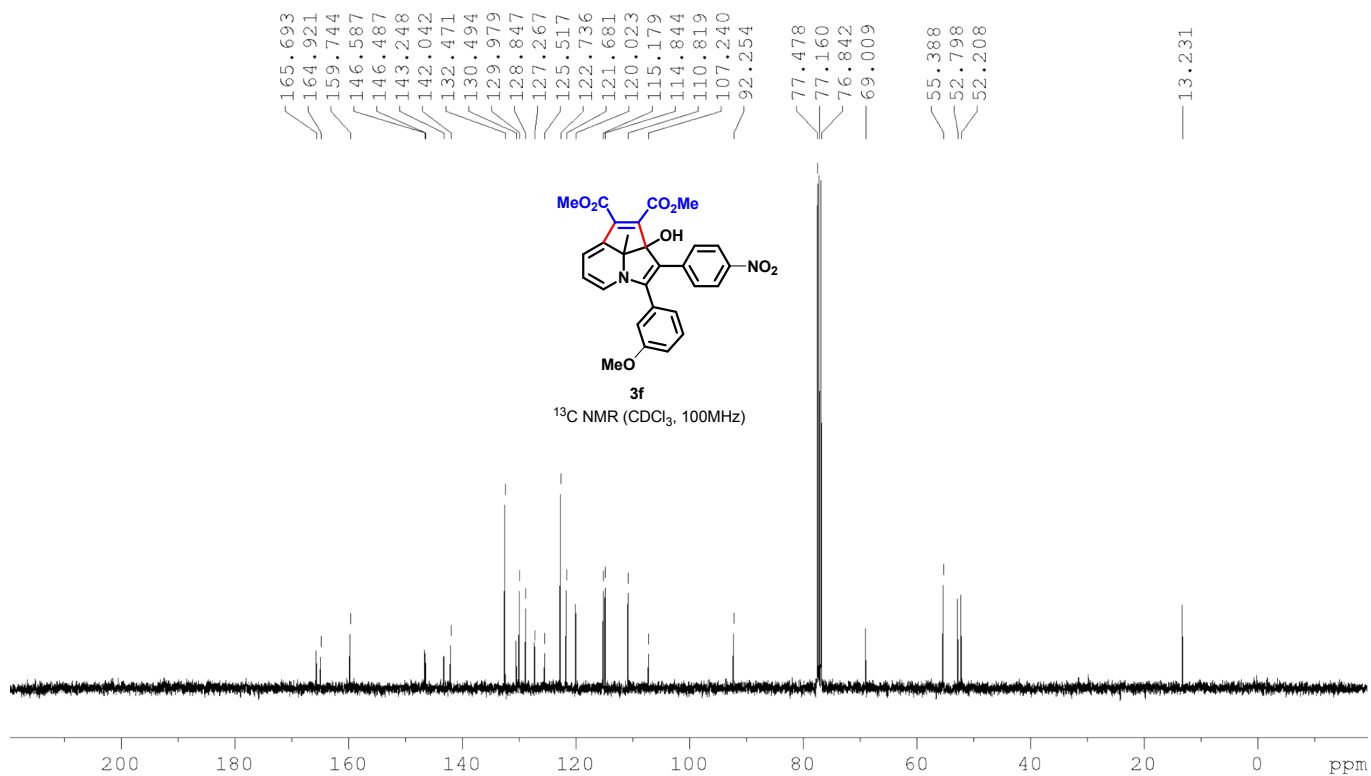


Figure 56: ¹³C NMR (100 MHz) spectrum of **3f**

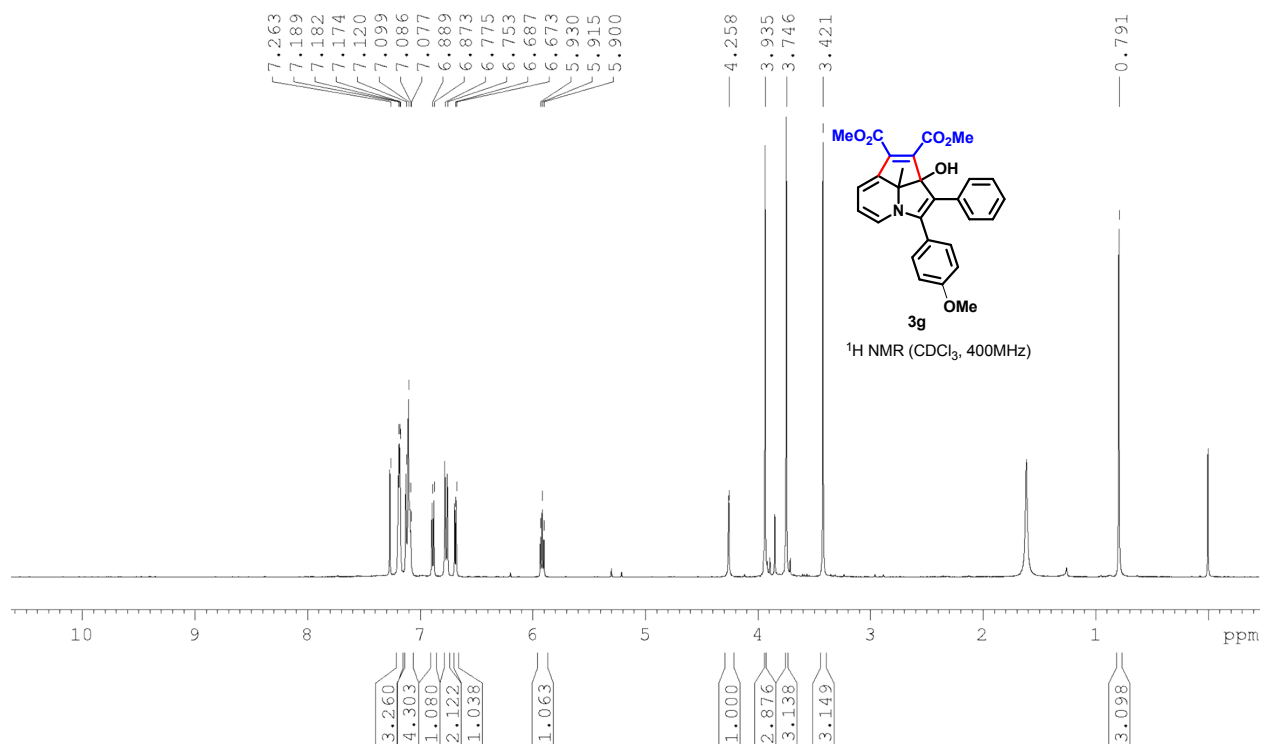


Figure 57: ¹H NMR (400 MHz) spectrum of 3g

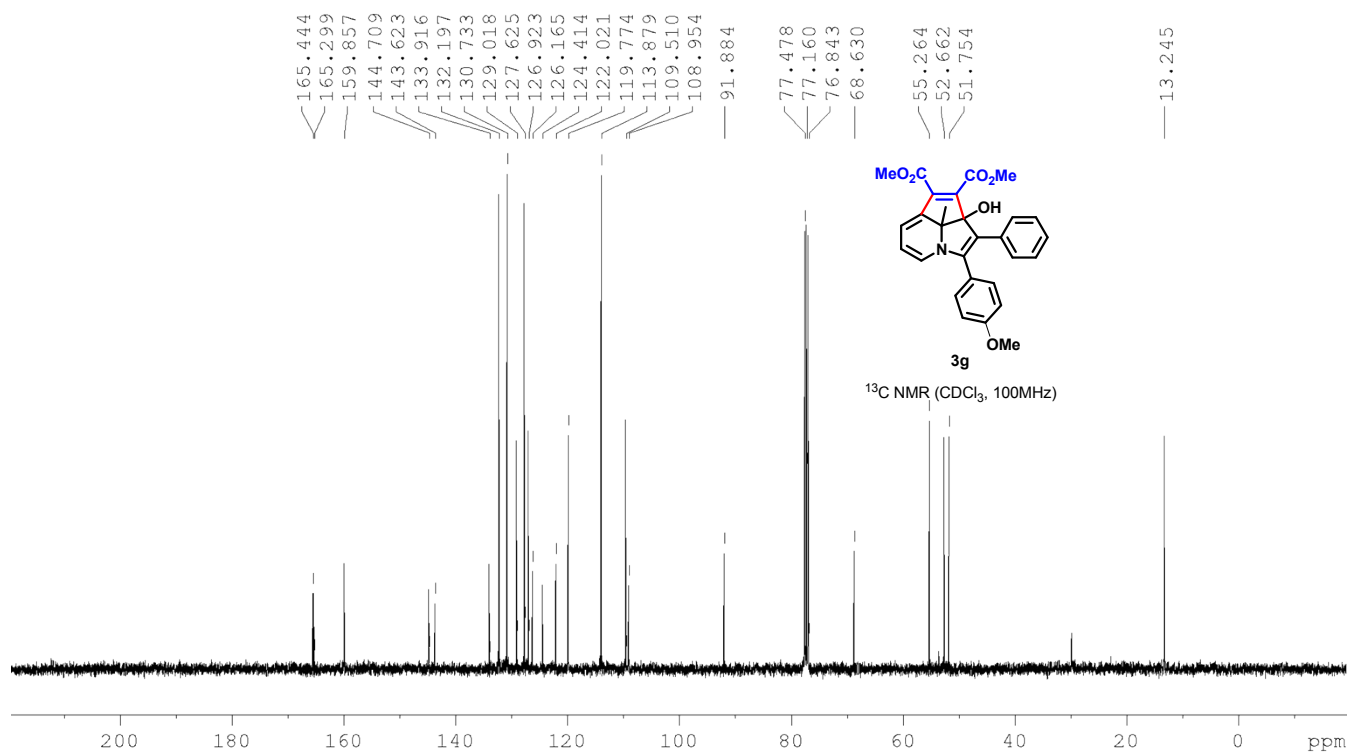


Figure 58: ¹³C NMR (100 MHz) spectrum of 3g

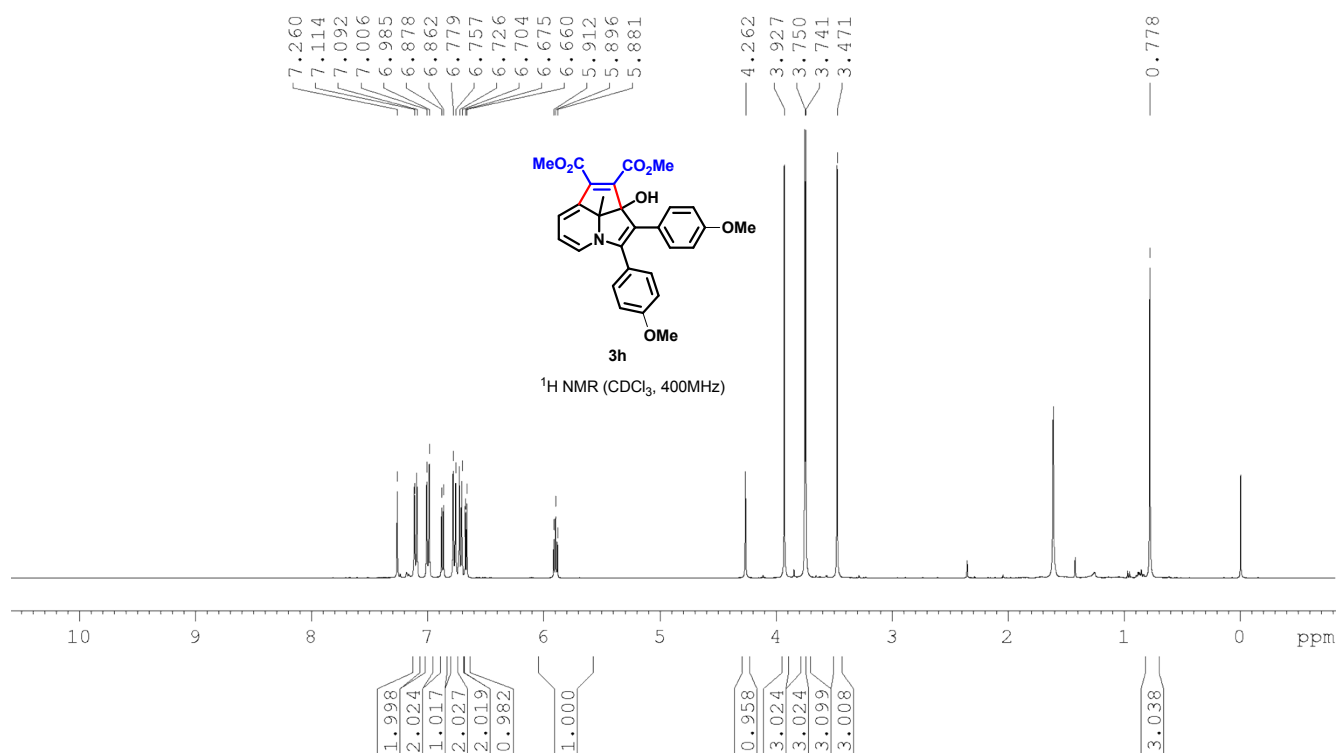


Figure 59: ¹H NMR (400 MHz) spectrum of **3h**

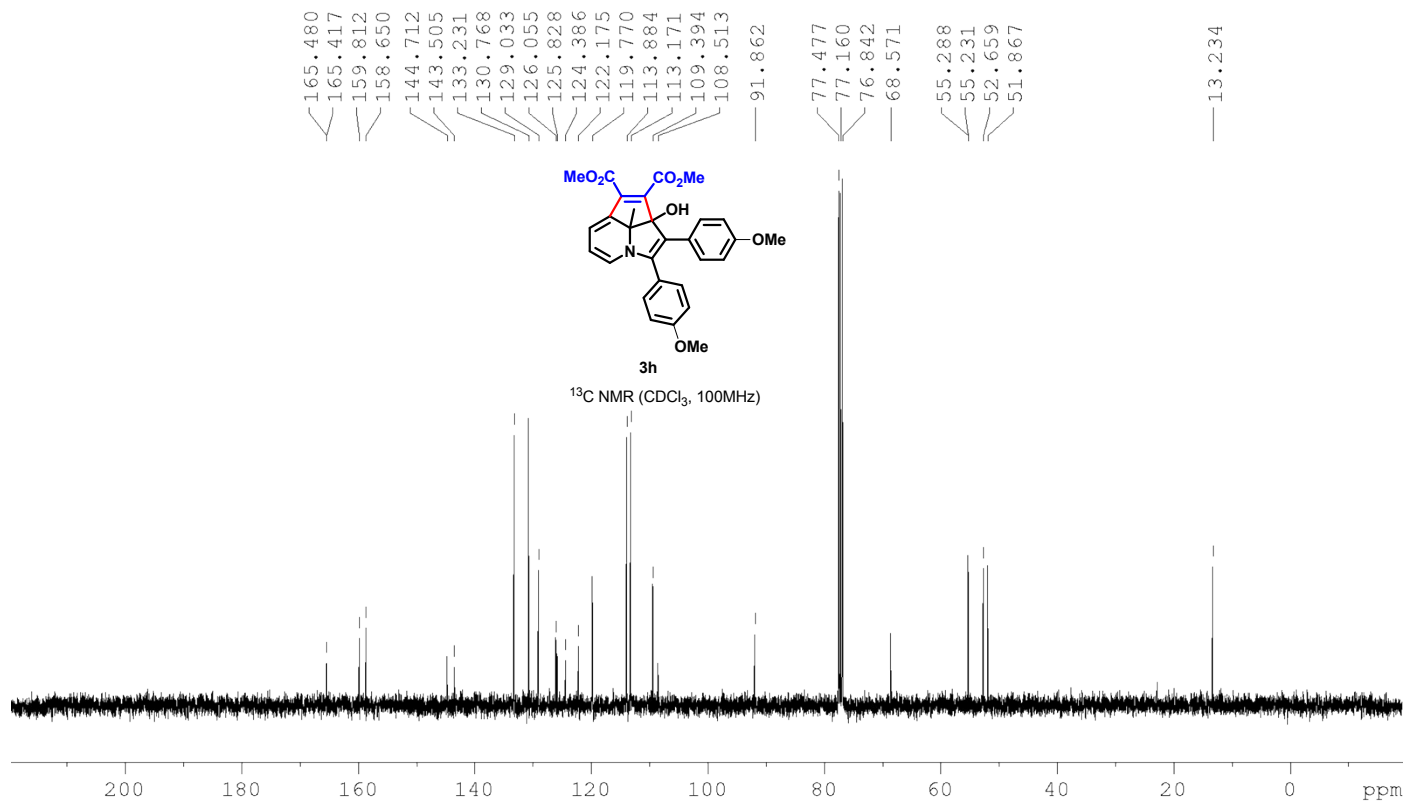


Figure 60: ¹³C NMR (100 MHz) spectrum of **3h**

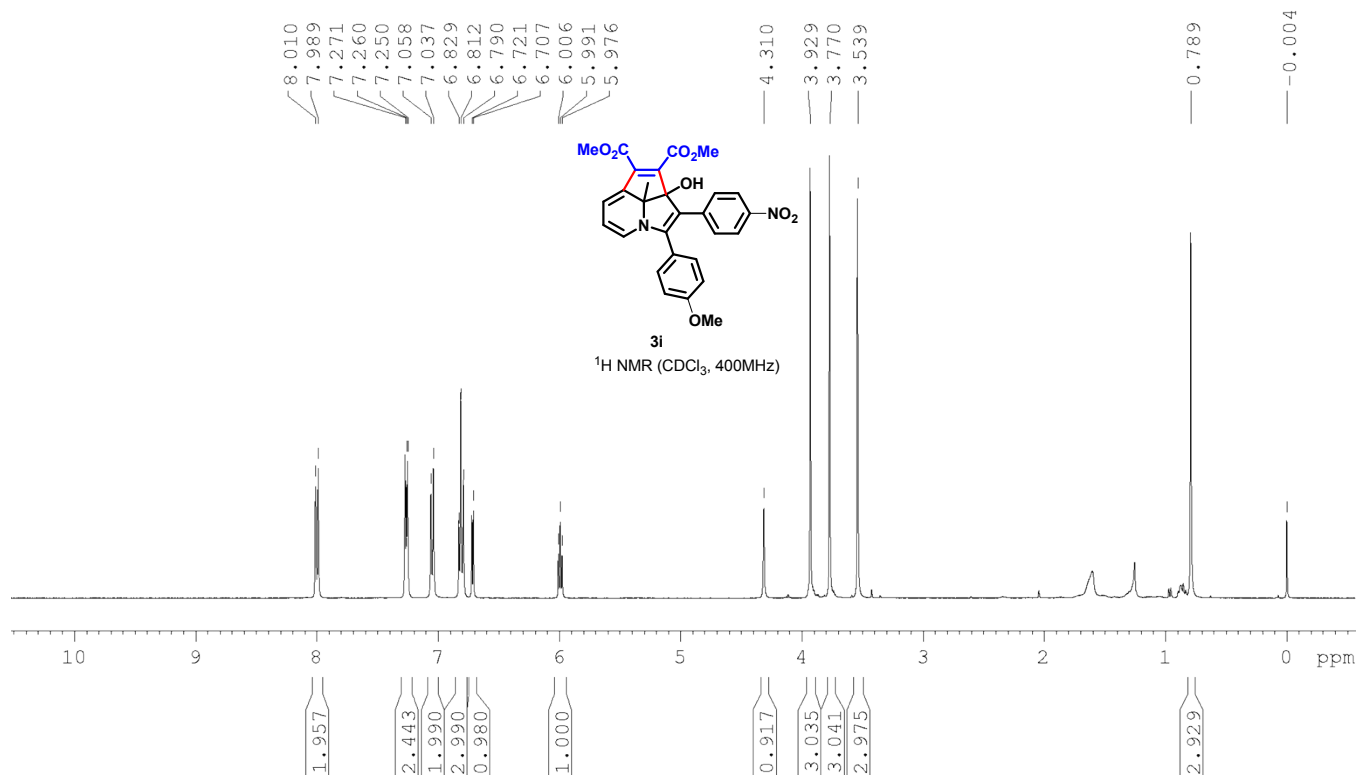


Figure 61: ¹H NMR (400 MHz) spectrum of **3i**

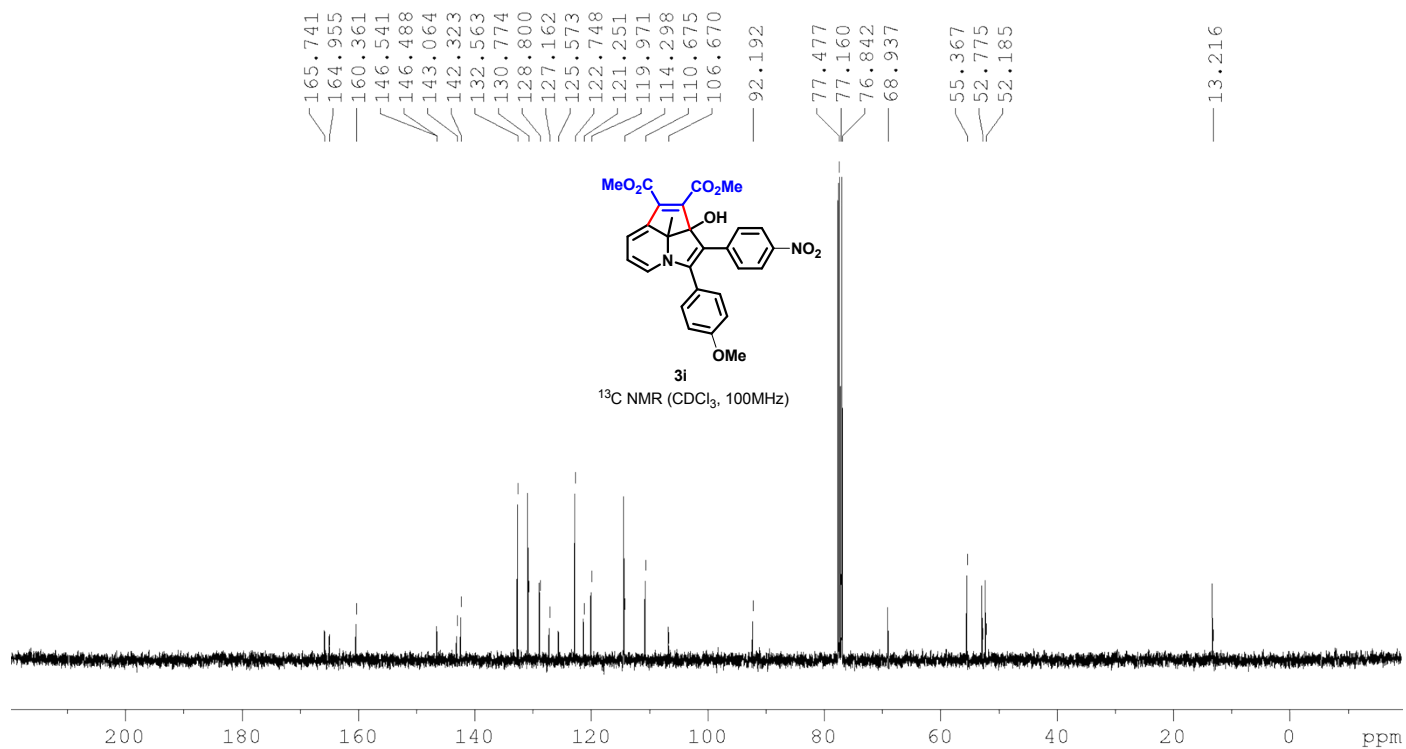


Figure 62: ¹³C NMR (100 MHz) spectrum of **3i**

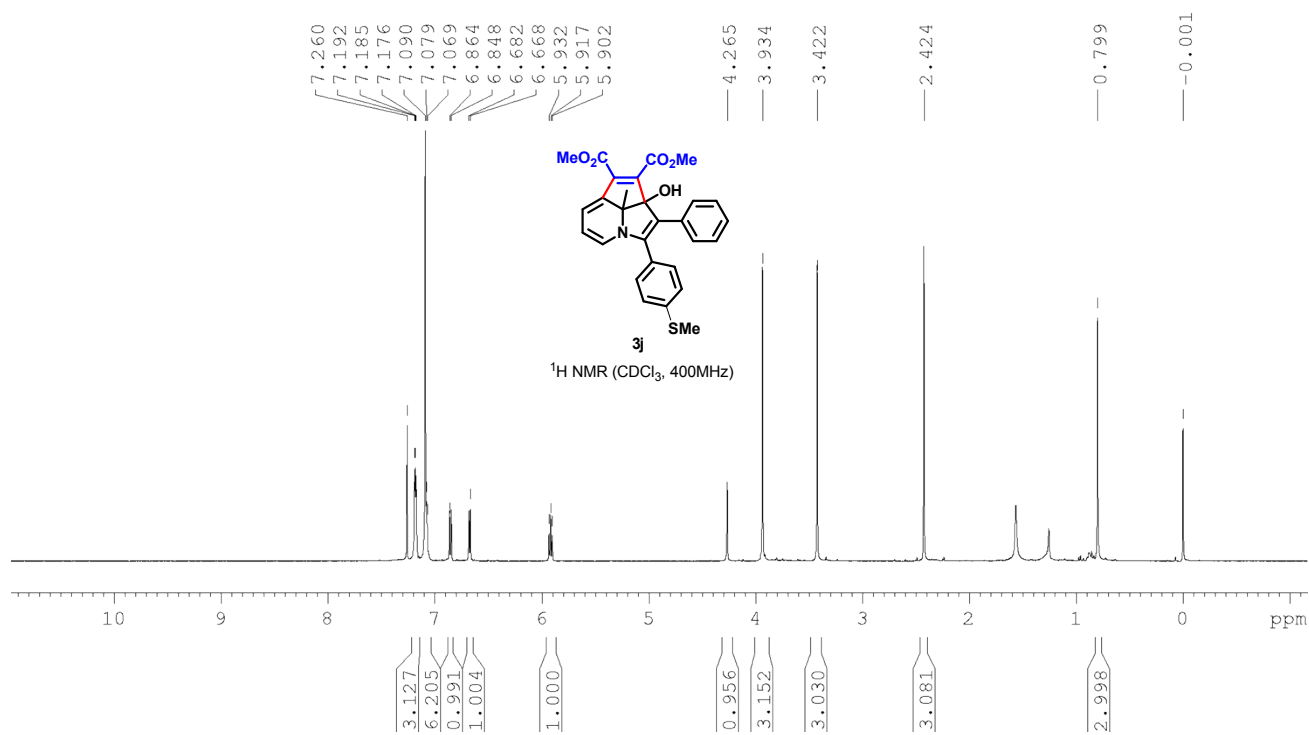


Figure 63: ^1H NMR (400 MHz) spectrum of **3j**

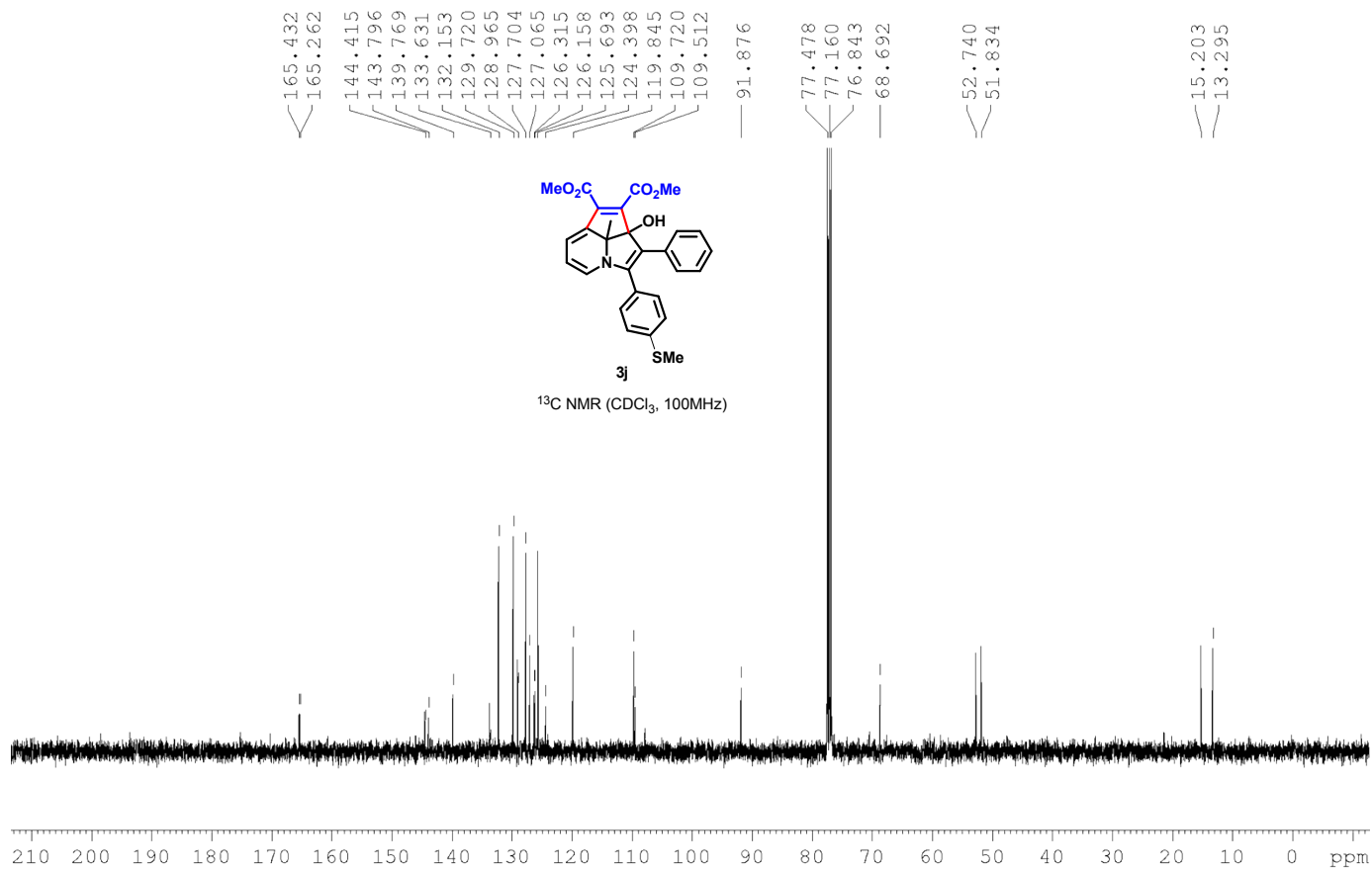


Figure 64: ^{13}C NMR (100 MHz) spectrum of **3j**

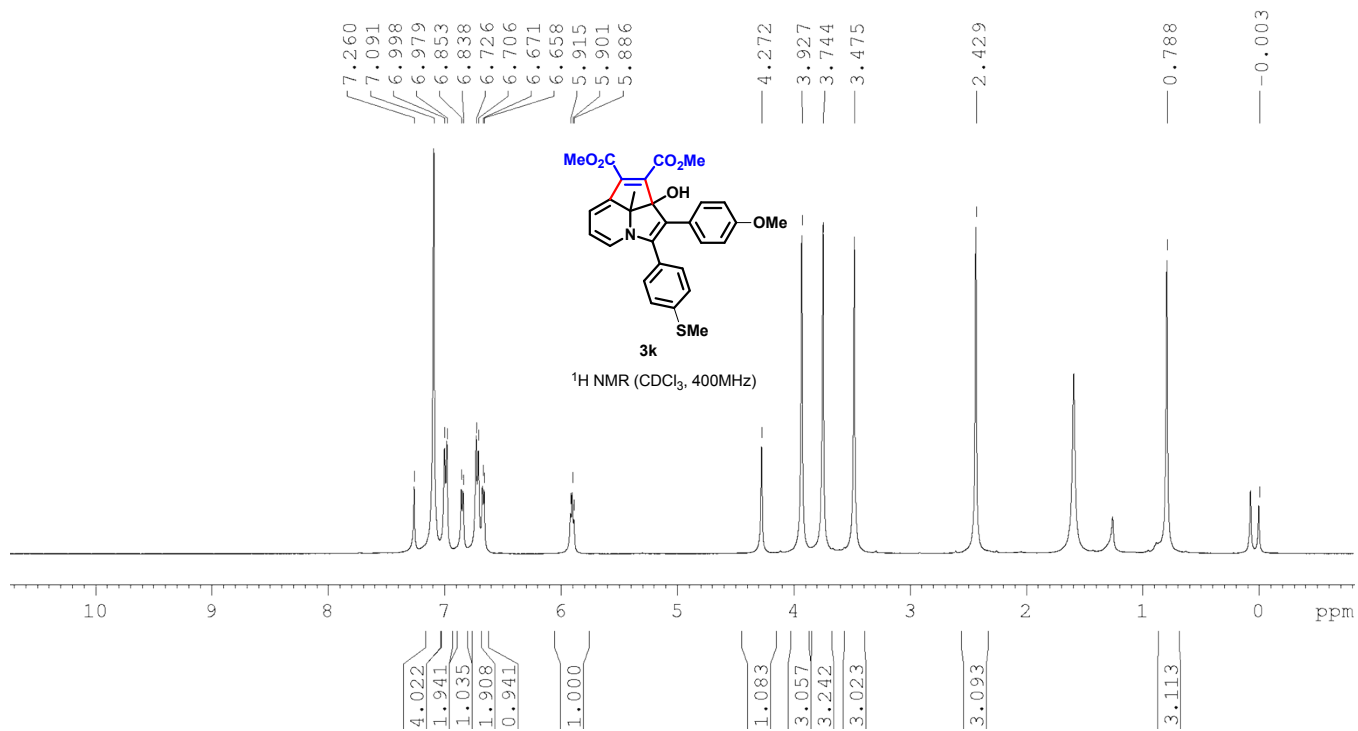


Figure 65: ¹H NMR (400 MHz) spectrum of **3k**

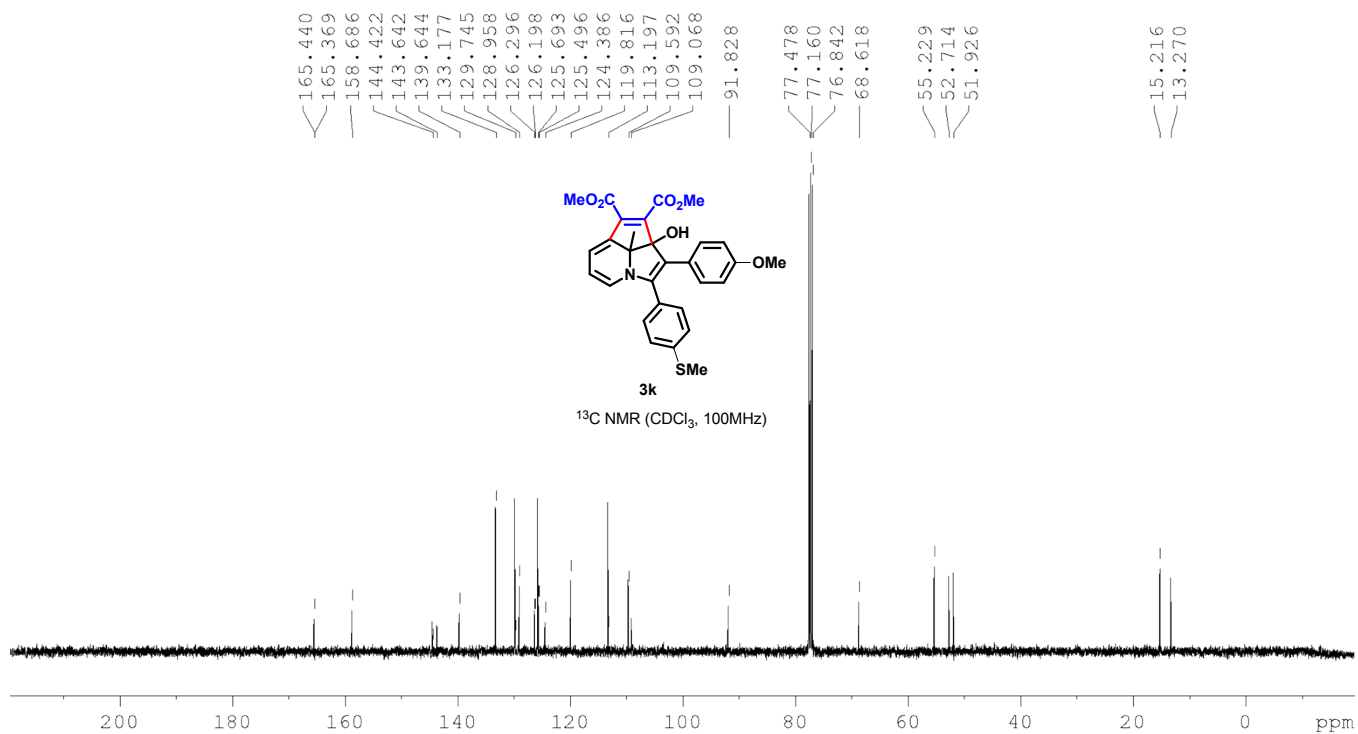


Figure 66: ¹³C NMR (100 MHz) spectrum of **3k**

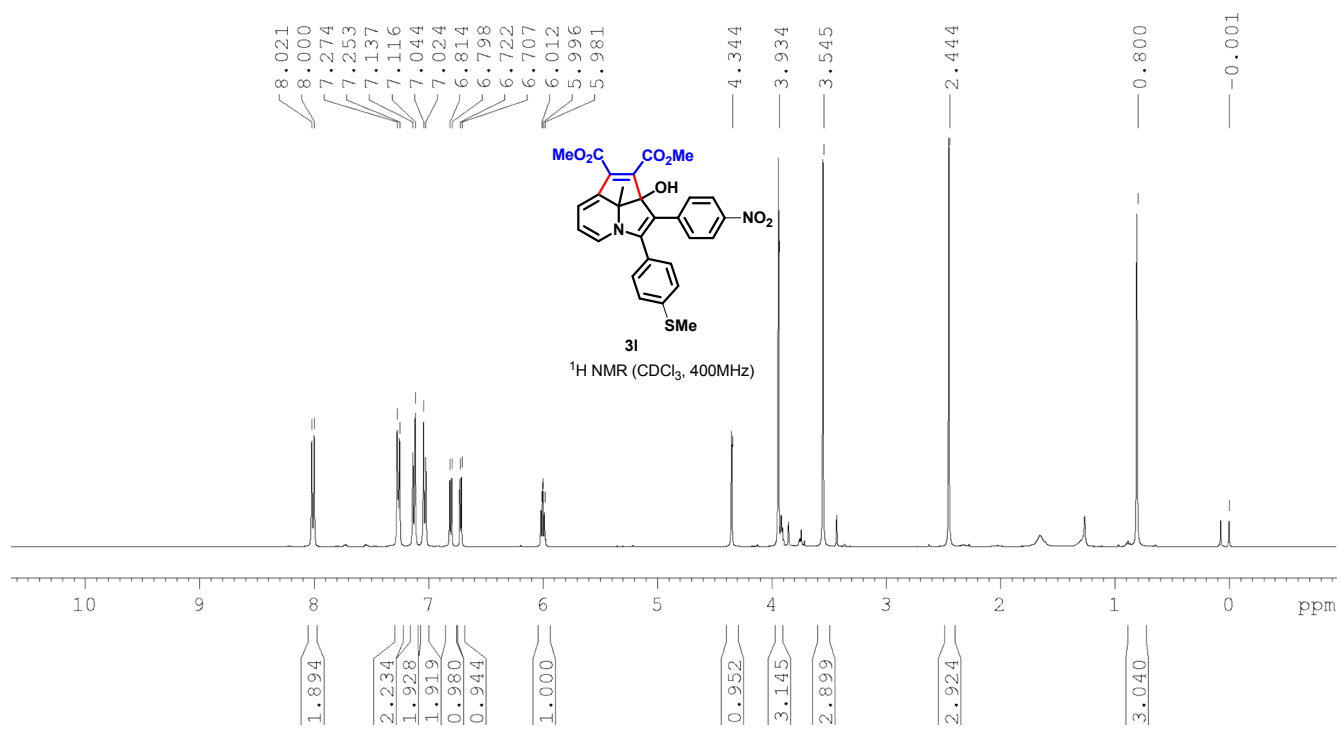


Figure 67: $^1\text{H NMR}$ (400 MHz) spectrum of **3I**

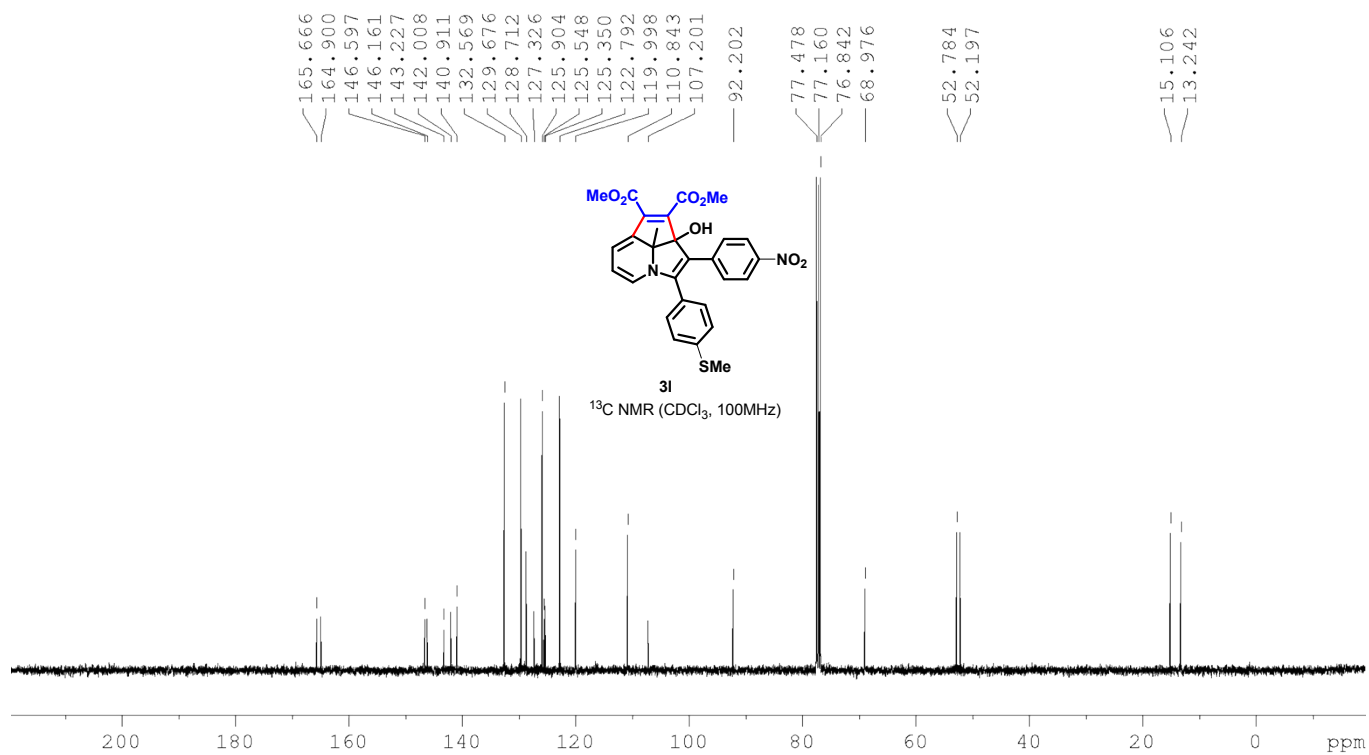


Figure 68: $^{13}\text{C NMR}$ (100 MHz) spectrum of **3I**

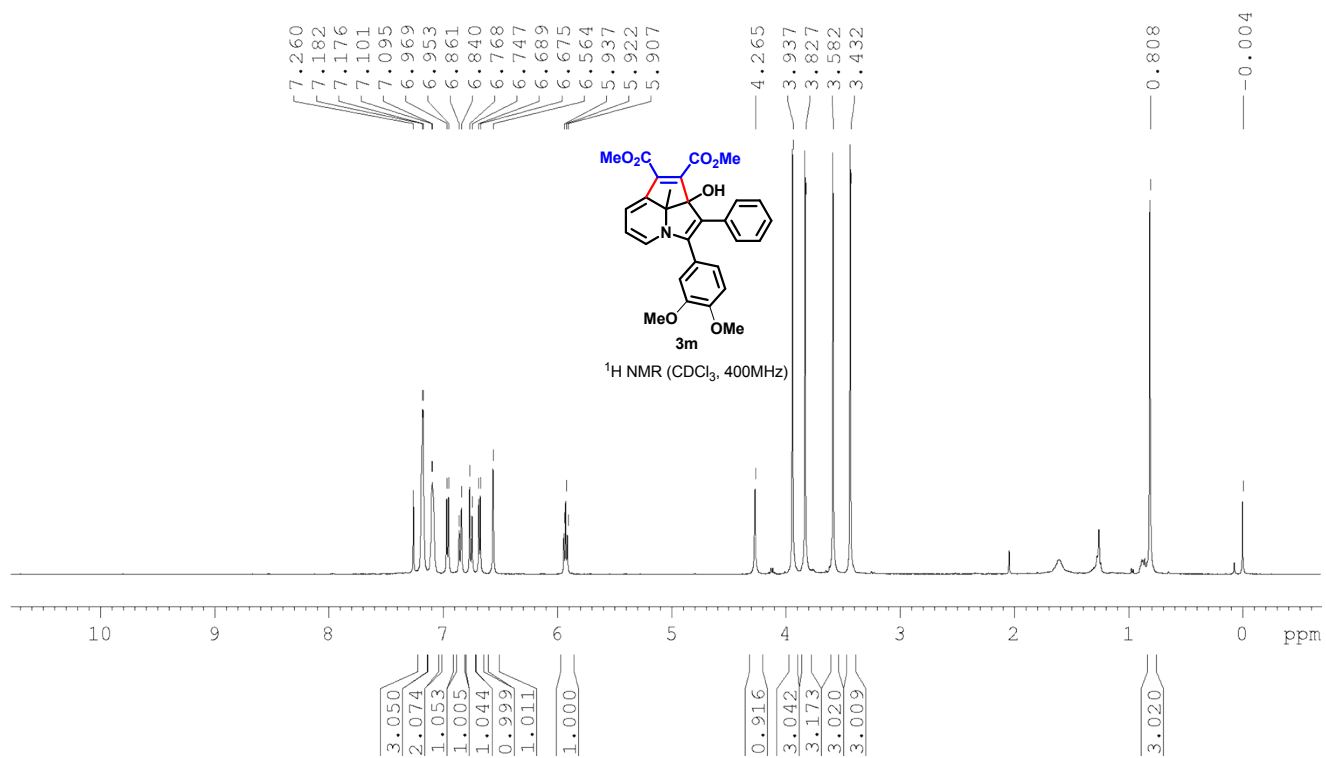


Figure 69: ¹H NMR (400 MHz) spectrum of **3m**

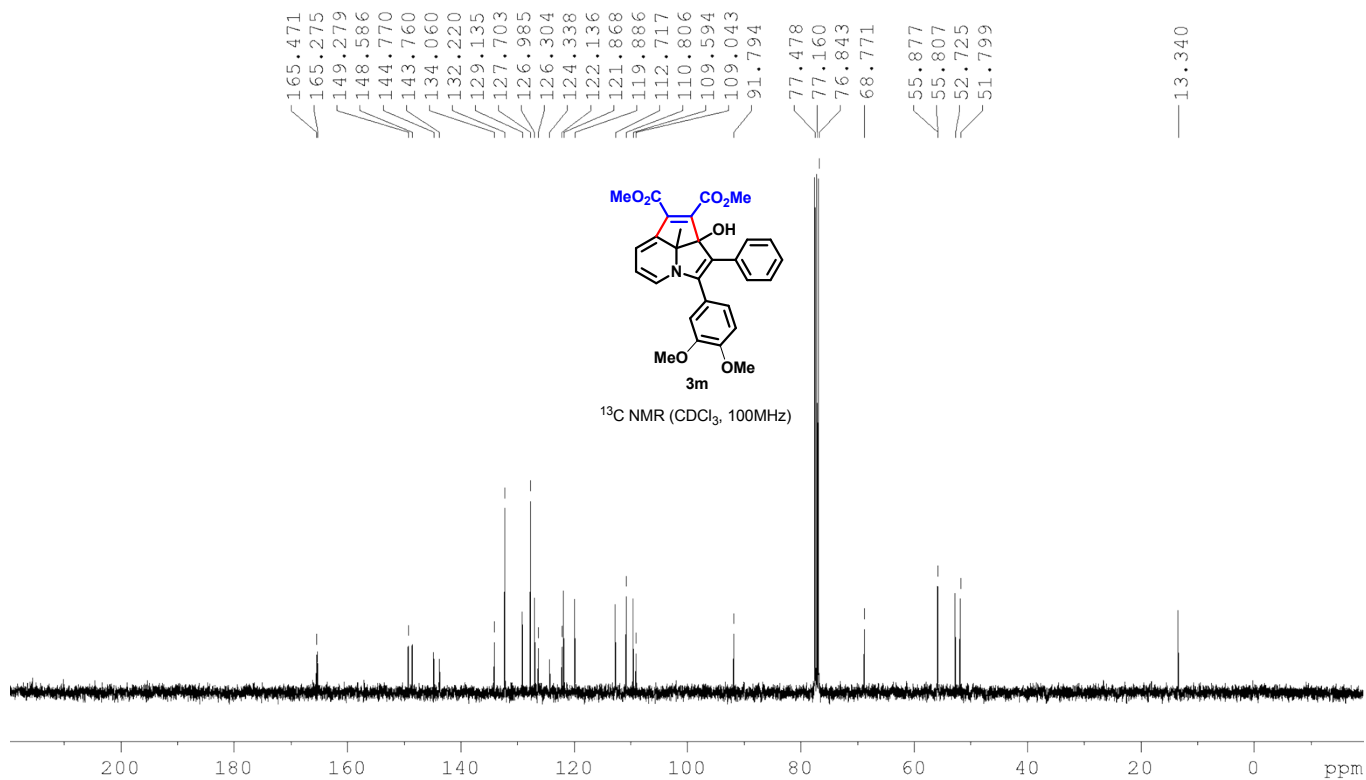


Figure 70: ¹³C NMR (100 MHz) spectrum of **3m**

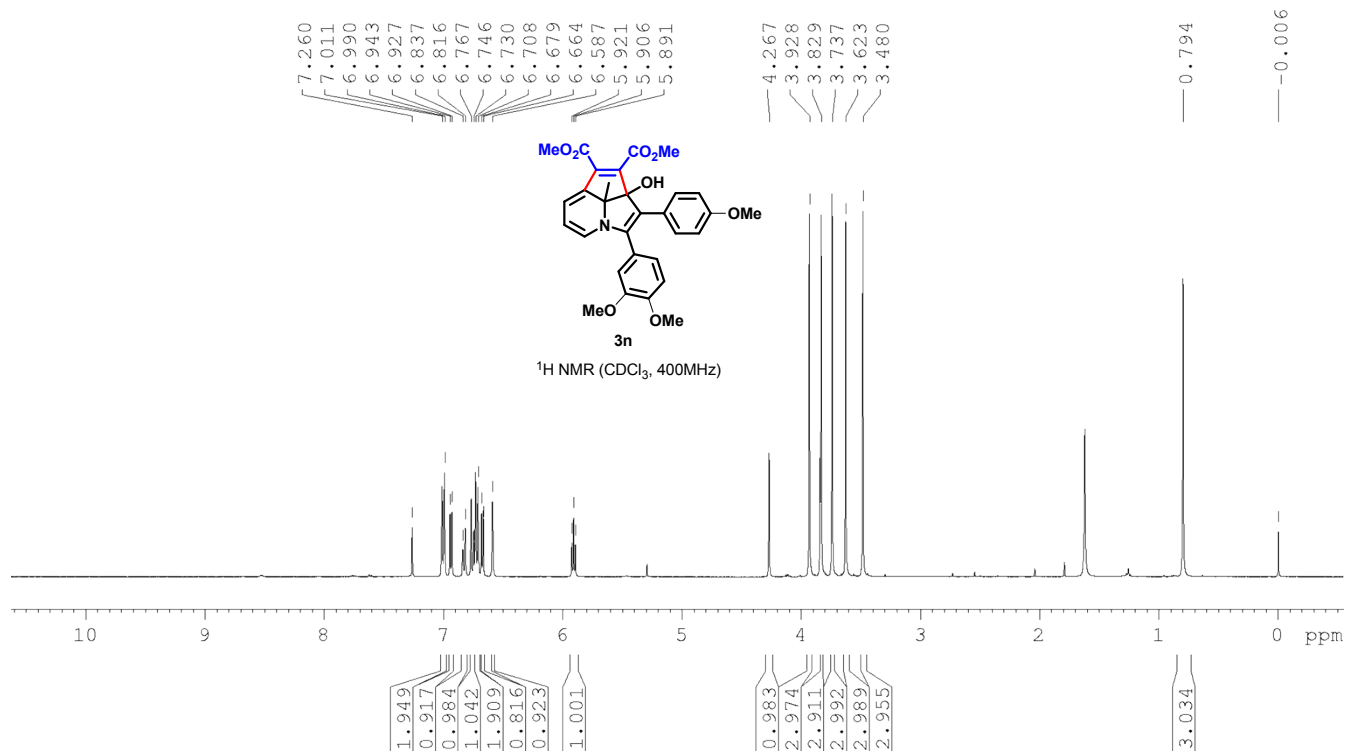


Figure 71: ¹H NMR (400 MHz) spectrum of **3n**

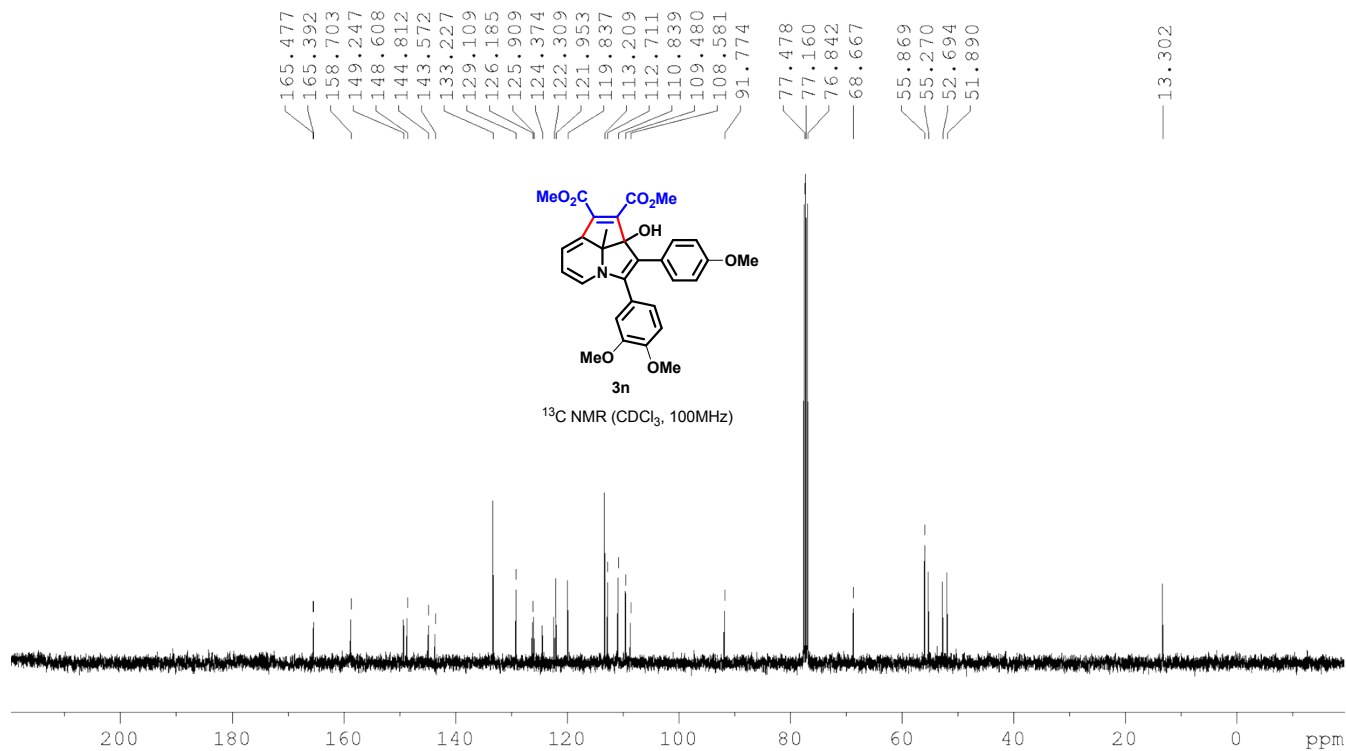


Figure 72: ¹³C NMR (100 MHz) spectrum of **3n**

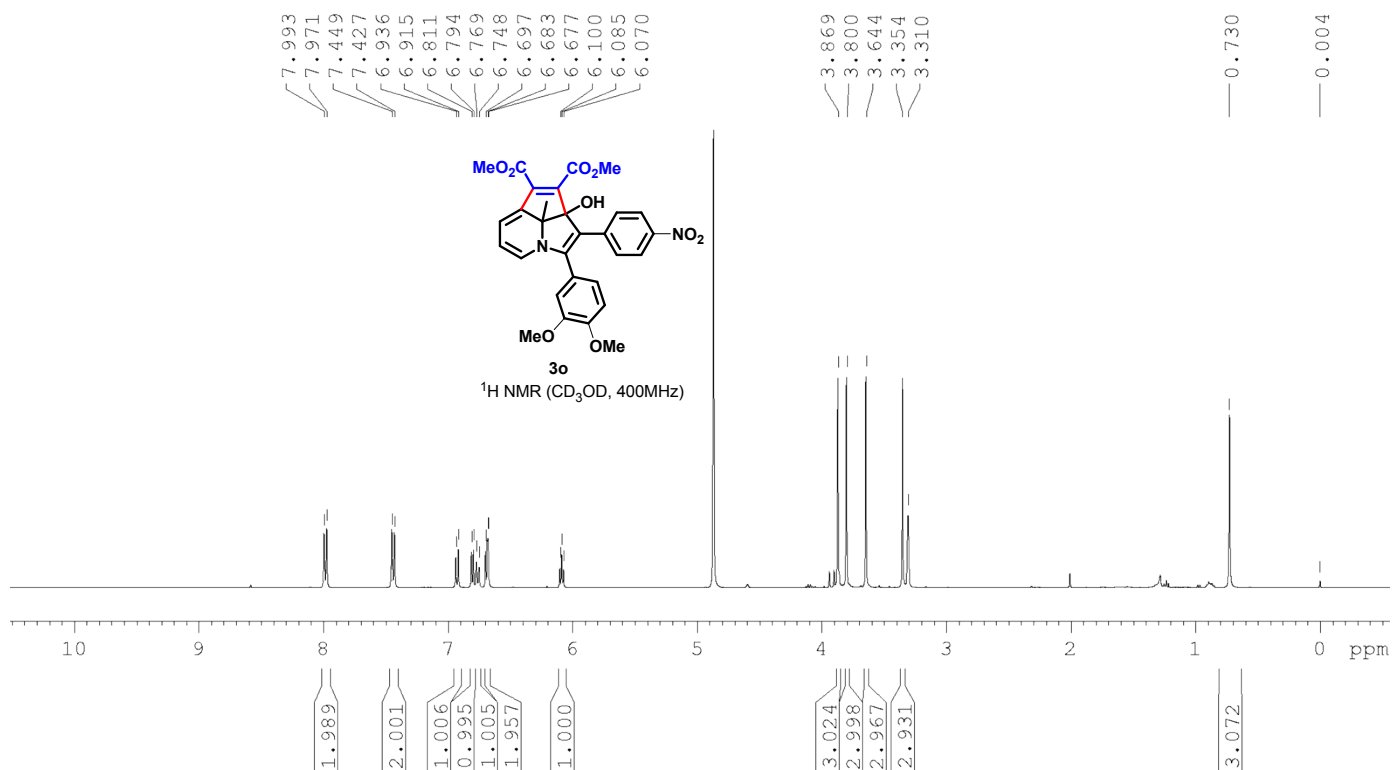


Figure 73: $^1\text{H NMR}$ (400 MHz) spectrum of **3o**

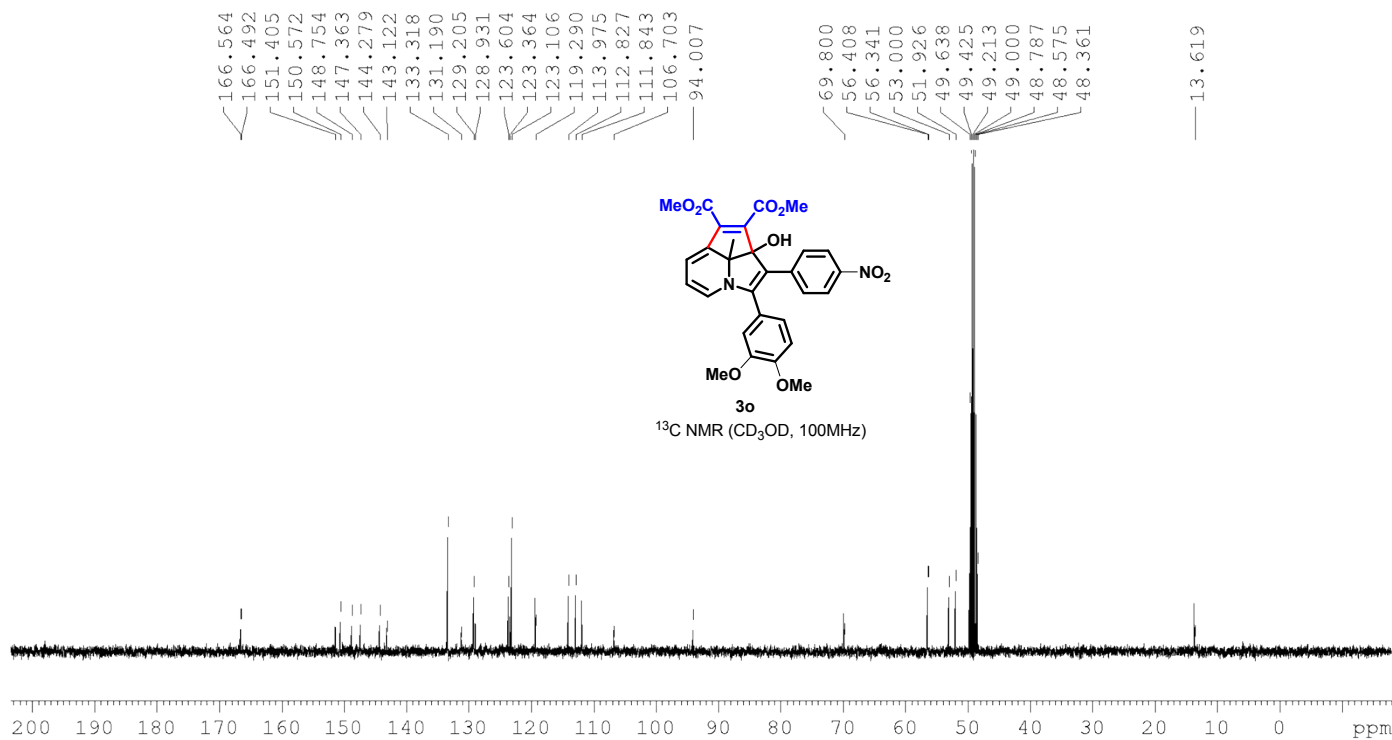


Figure 74: $^{13}\text{C NMR}$ (100 MHz) spectrum of **3o**

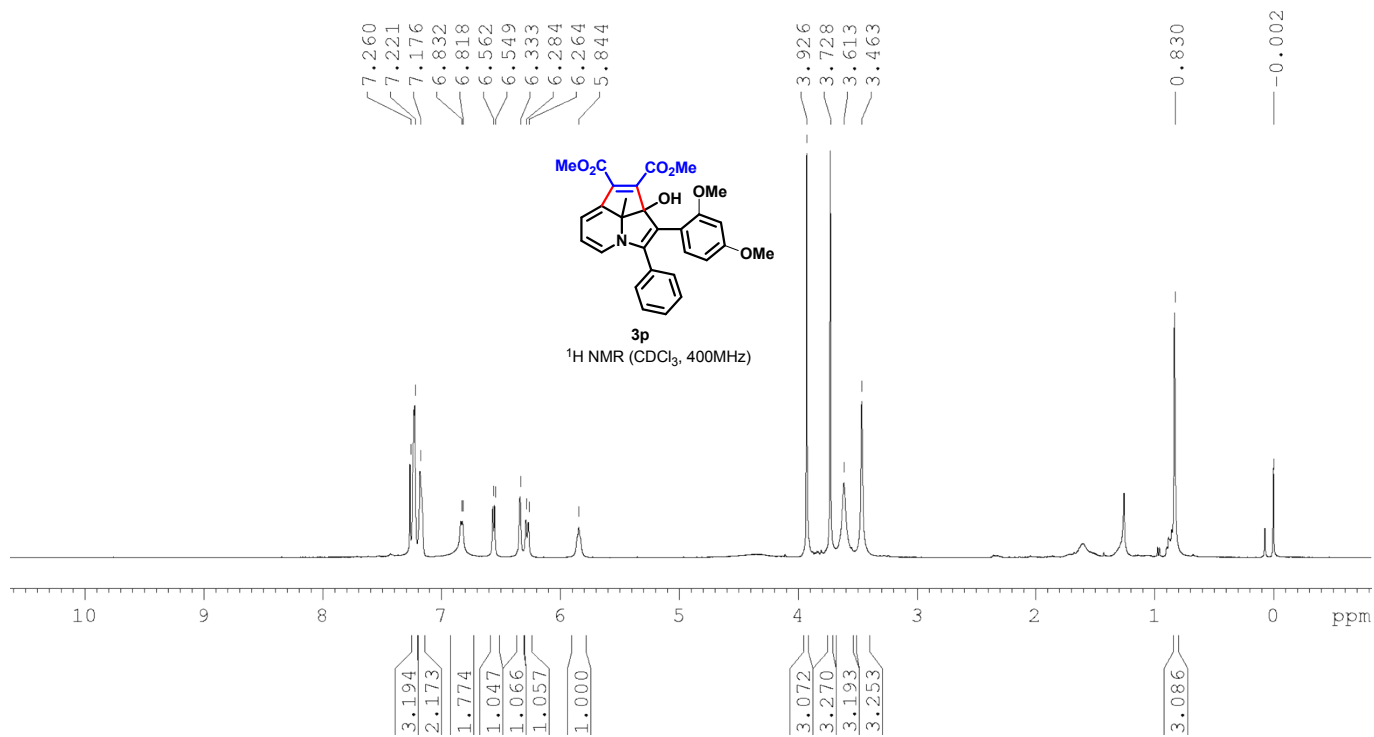


Figure 75: ¹H NMR (400 MHz) spectrum of **3p**

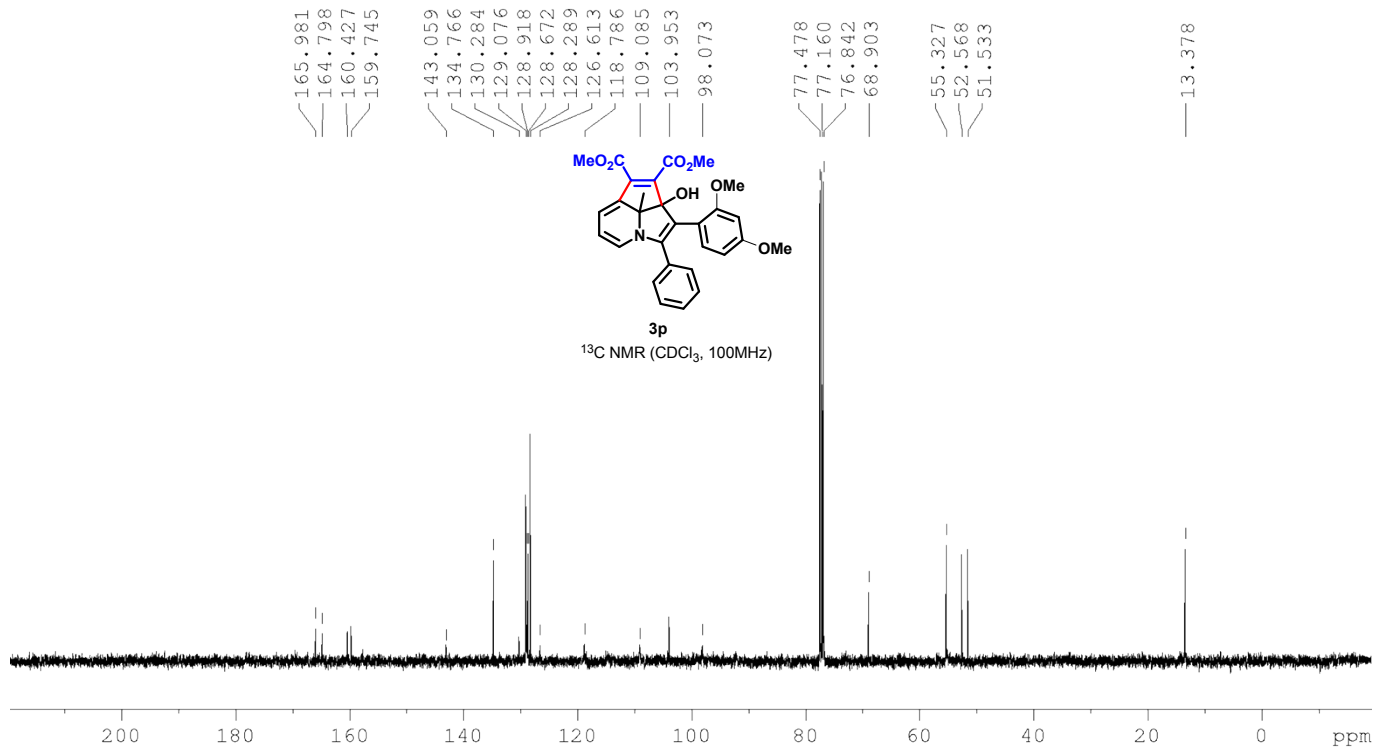


Figure 76: ¹³C NMR (100 MHz) spectrum of **3p**

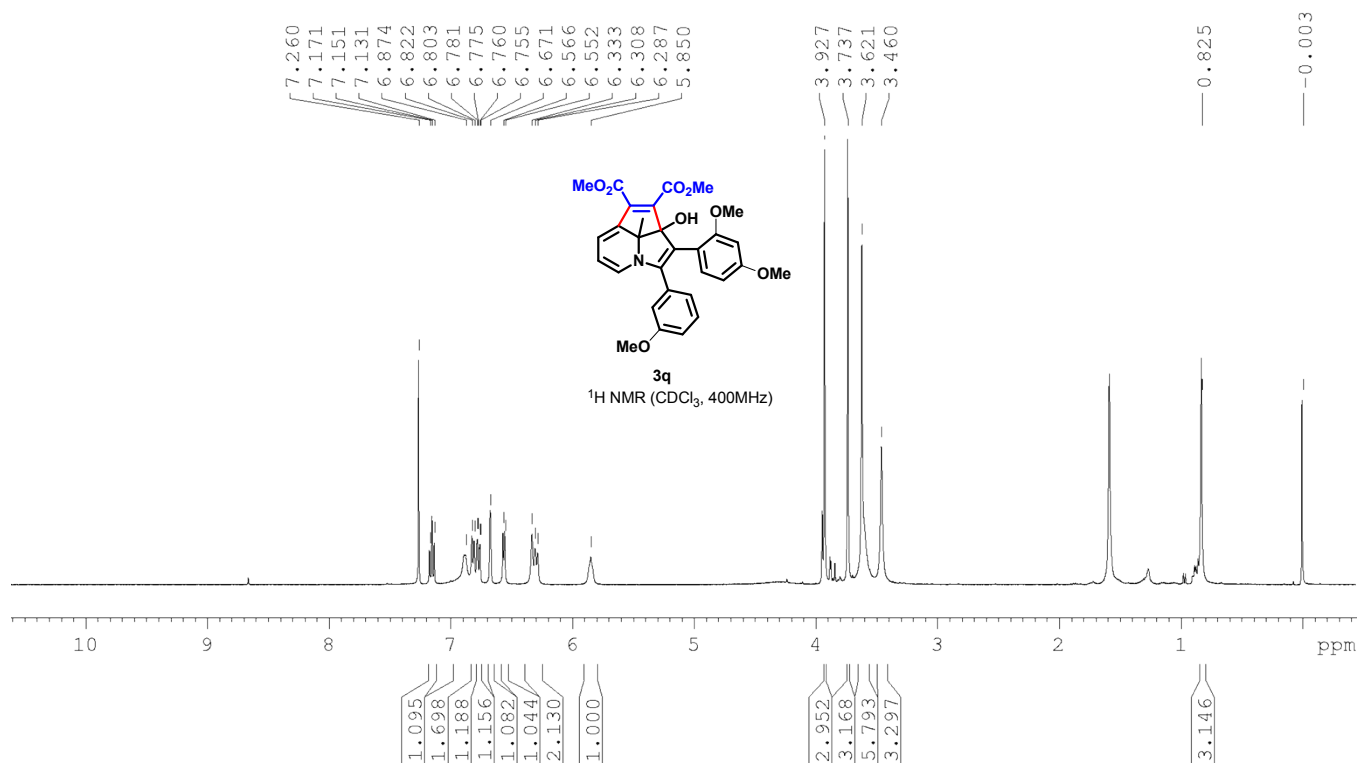


Figure 77: ^1H NMR (400 MHz) spectrum of **3q**

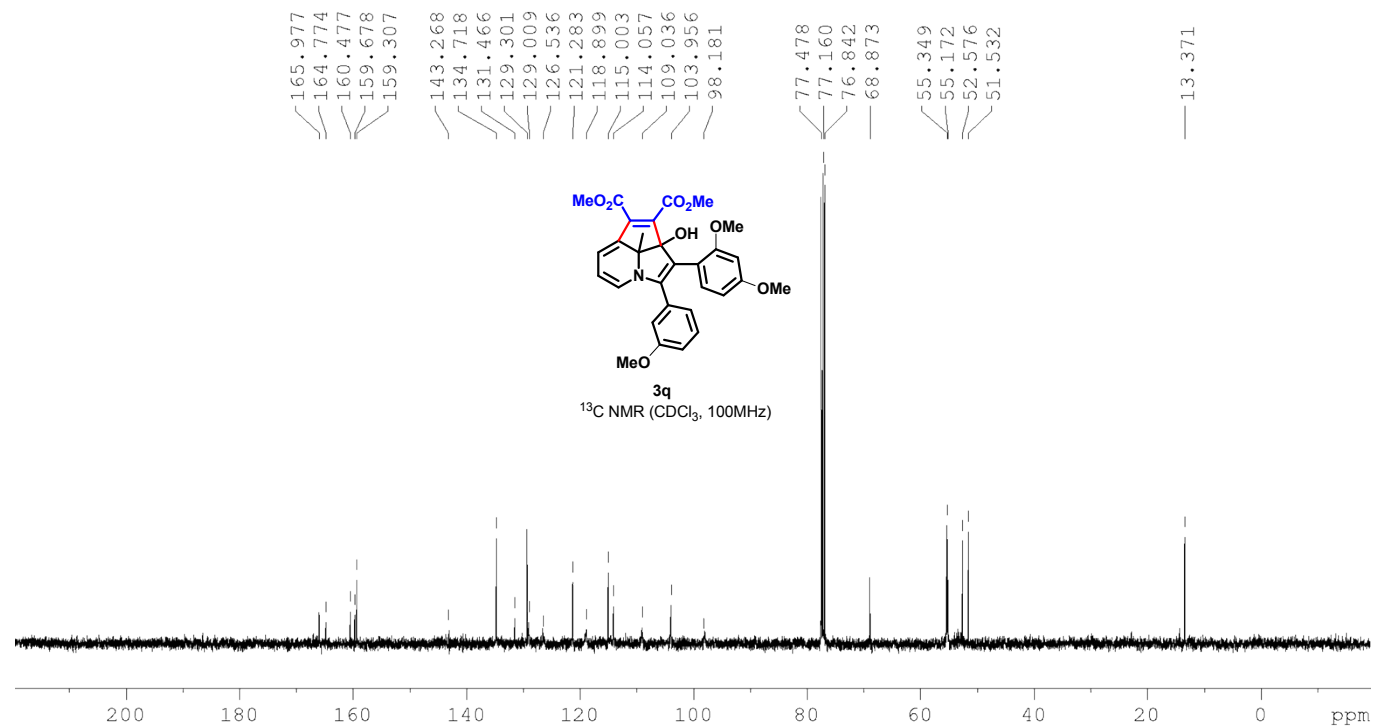


Figure 78: ^{13}C NMR (100 MHz) spectrum of **3q**

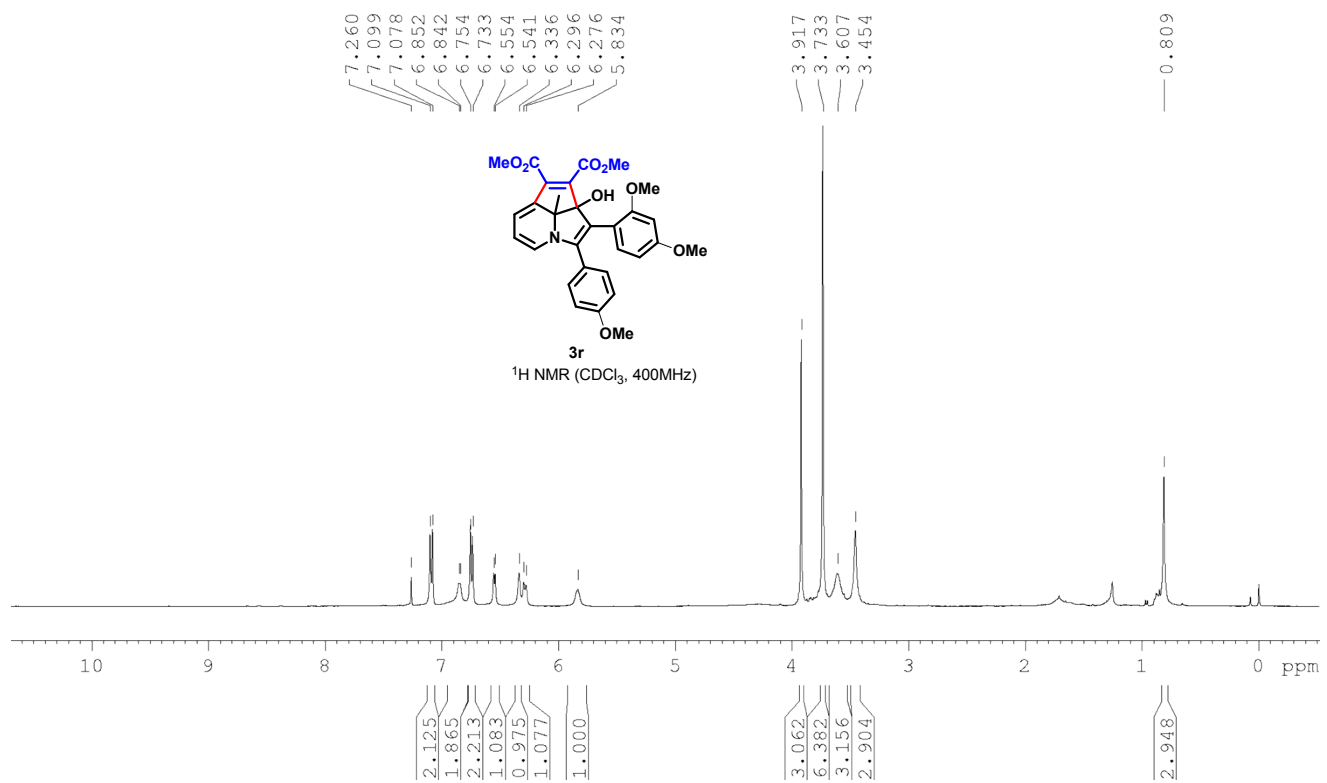


Figure 79: ¹H NMR (400 MHz) spectrum of **3r**

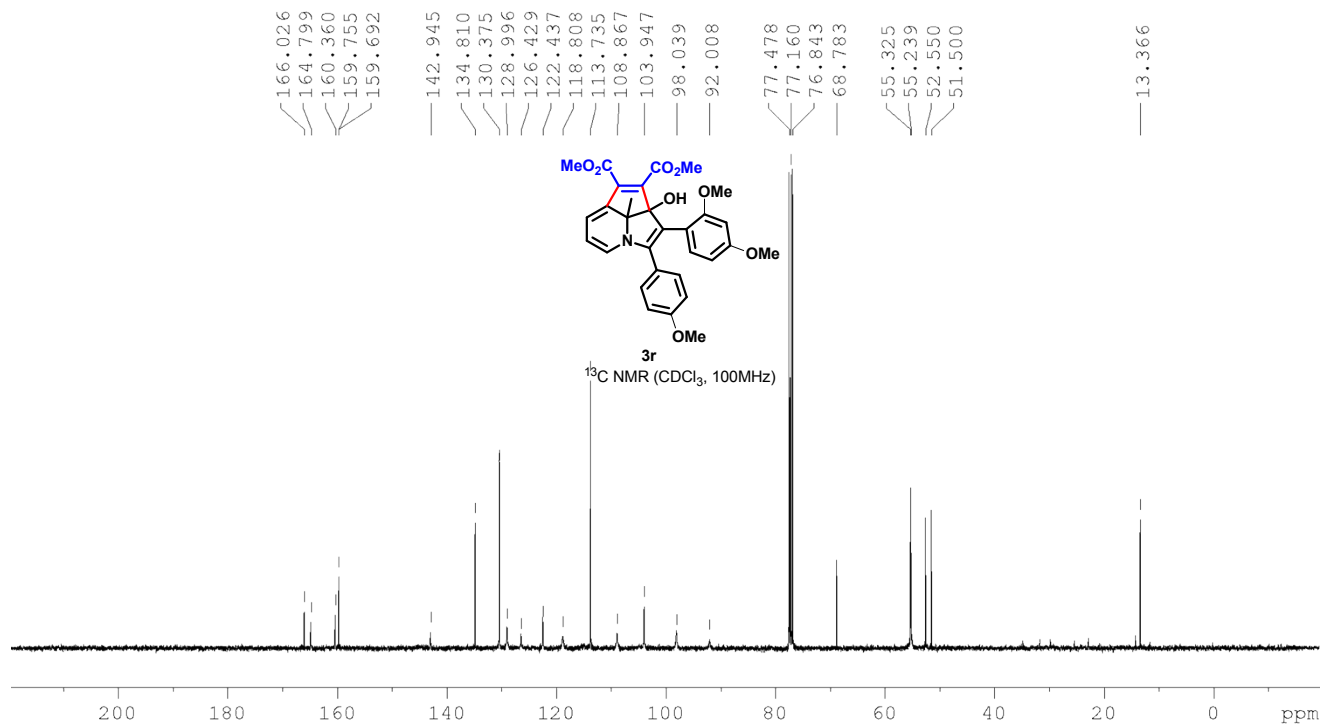


Figure 80: ¹³C NMR (100 MHz) spectrum of **3r**

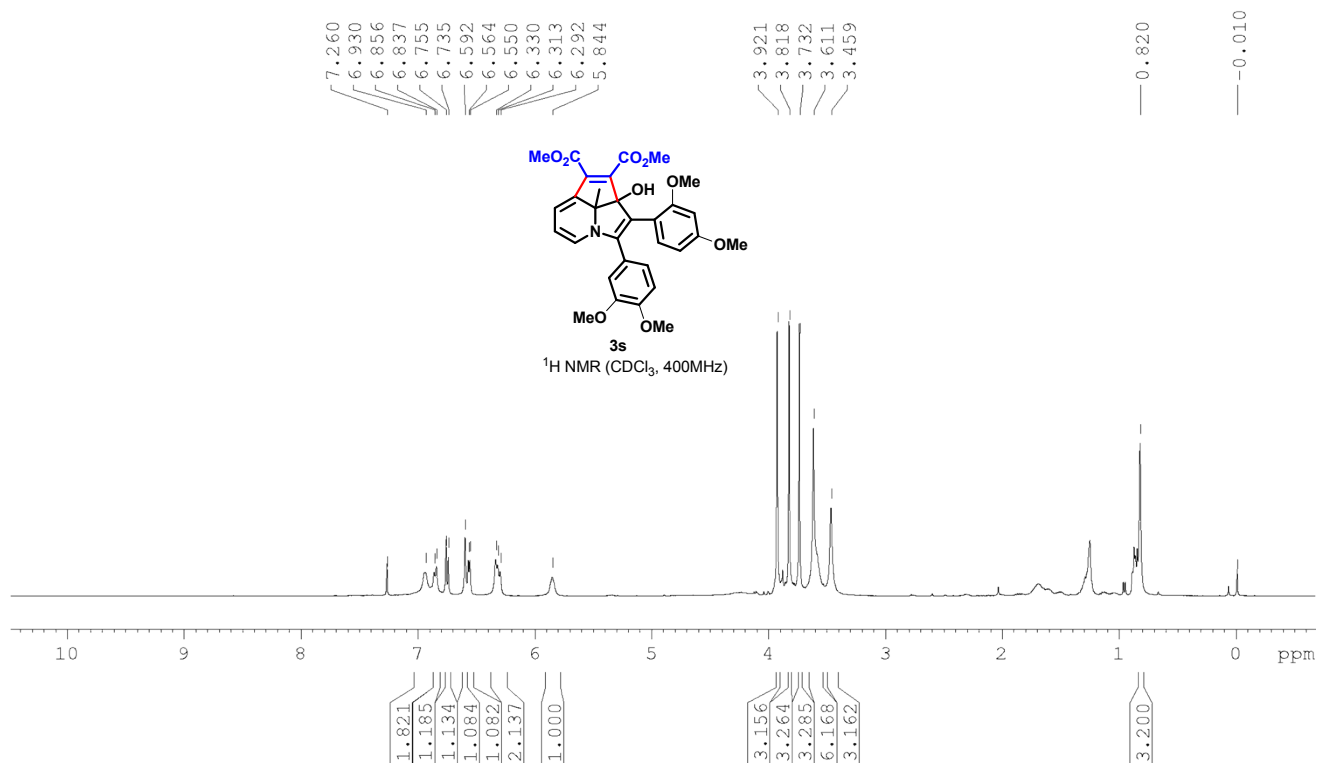


Figure 81: ¹H NMR (400 MHz) spectrum of **3s**

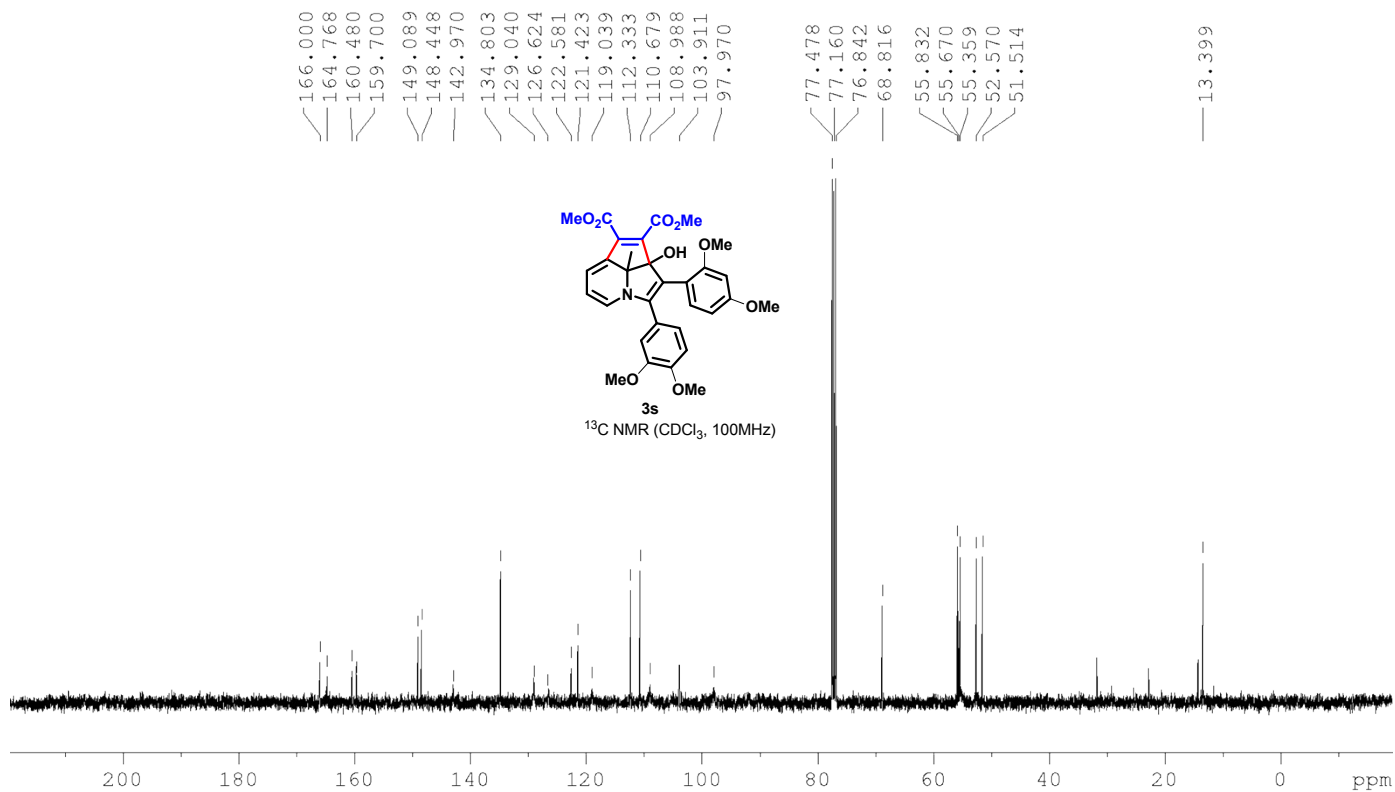


Figure 82: ¹³C NMR (100 MHz) spectrum of **3s**

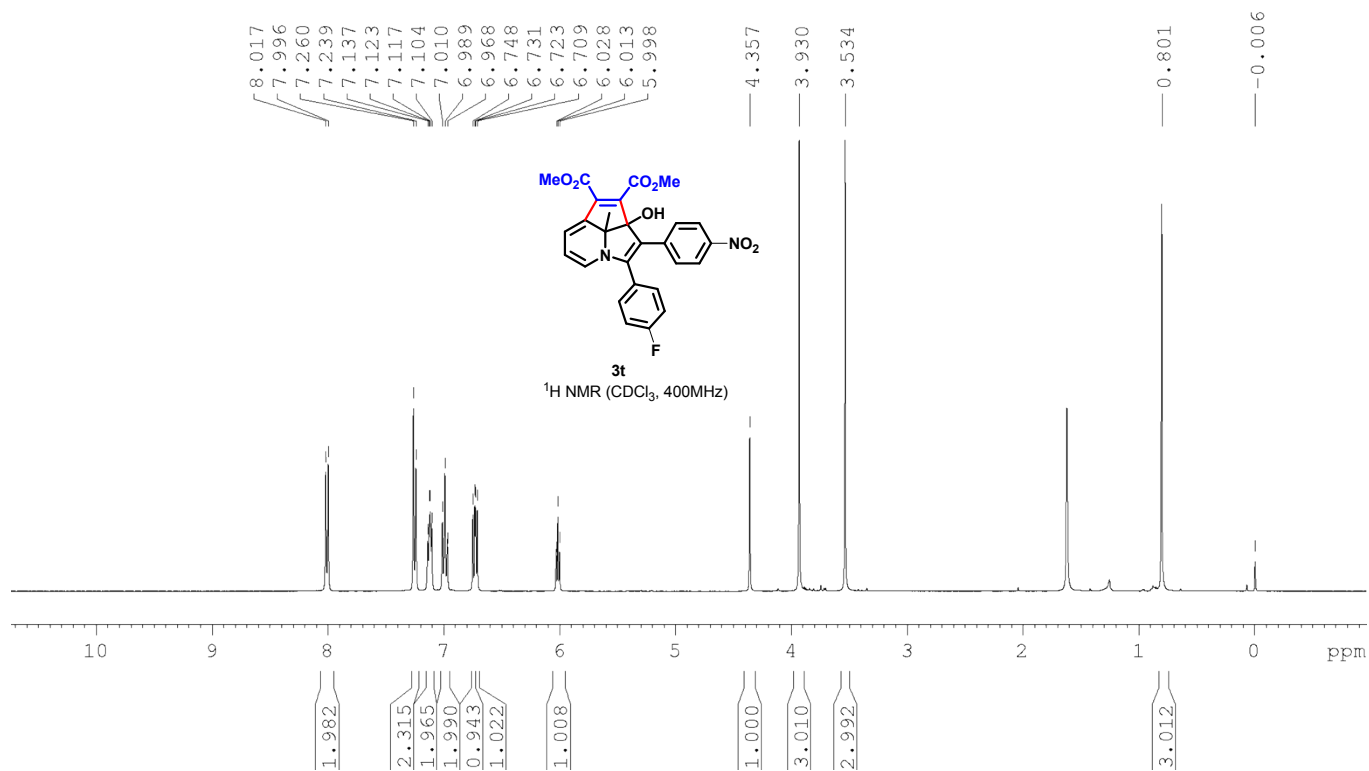


Figure 83: ¹H NMR (400 MHz) spectrum of **3t**

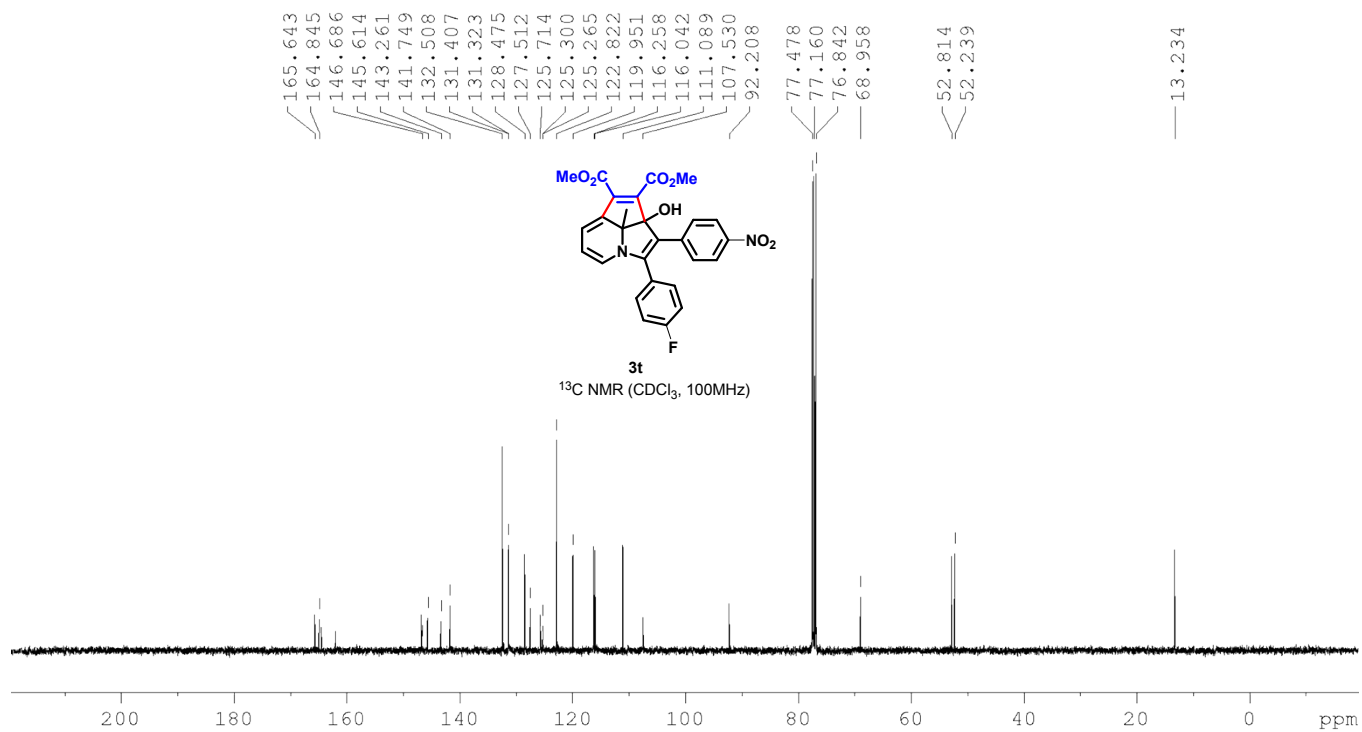


Figure 84: ¹³C NMR (100 MHz) spectrum of **3t**

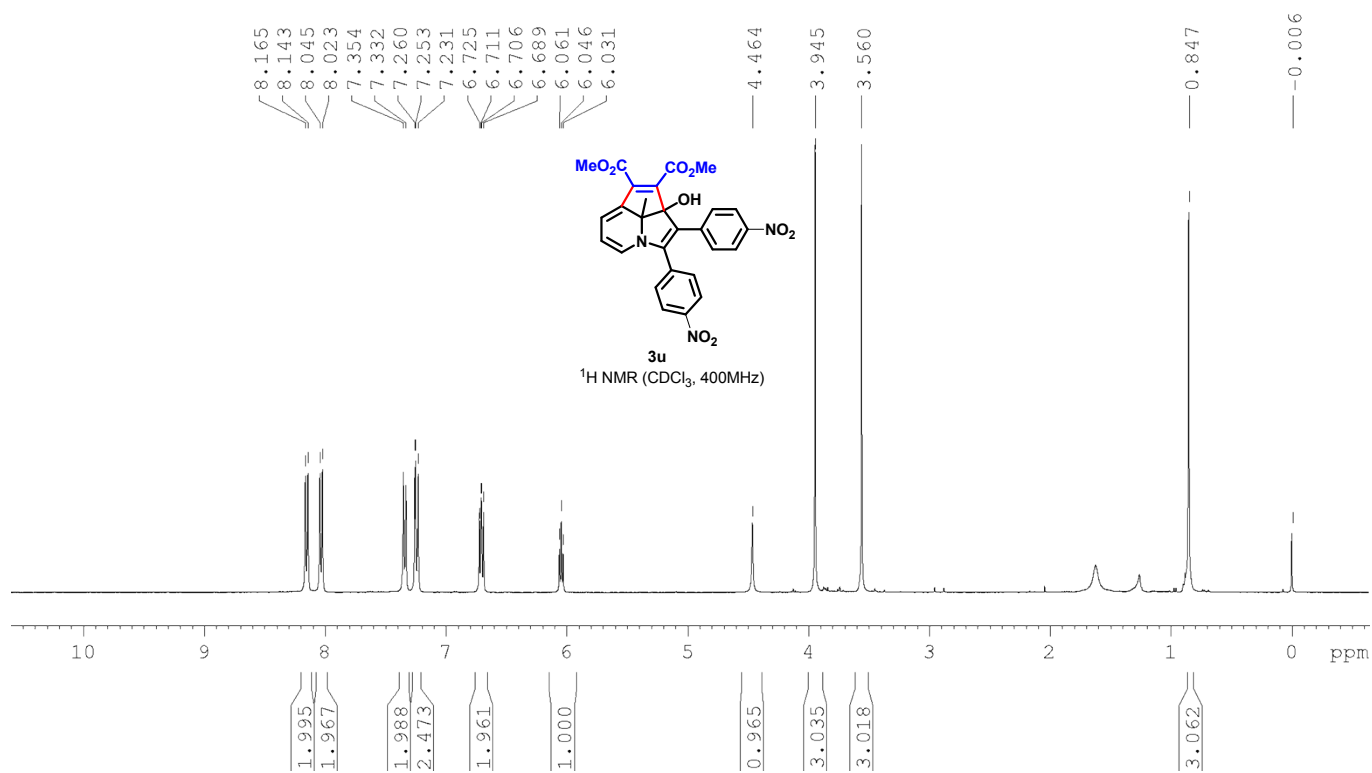


Figure 85: $^1\text{H NMR}$ (400 MHz) spectrum of **3u**

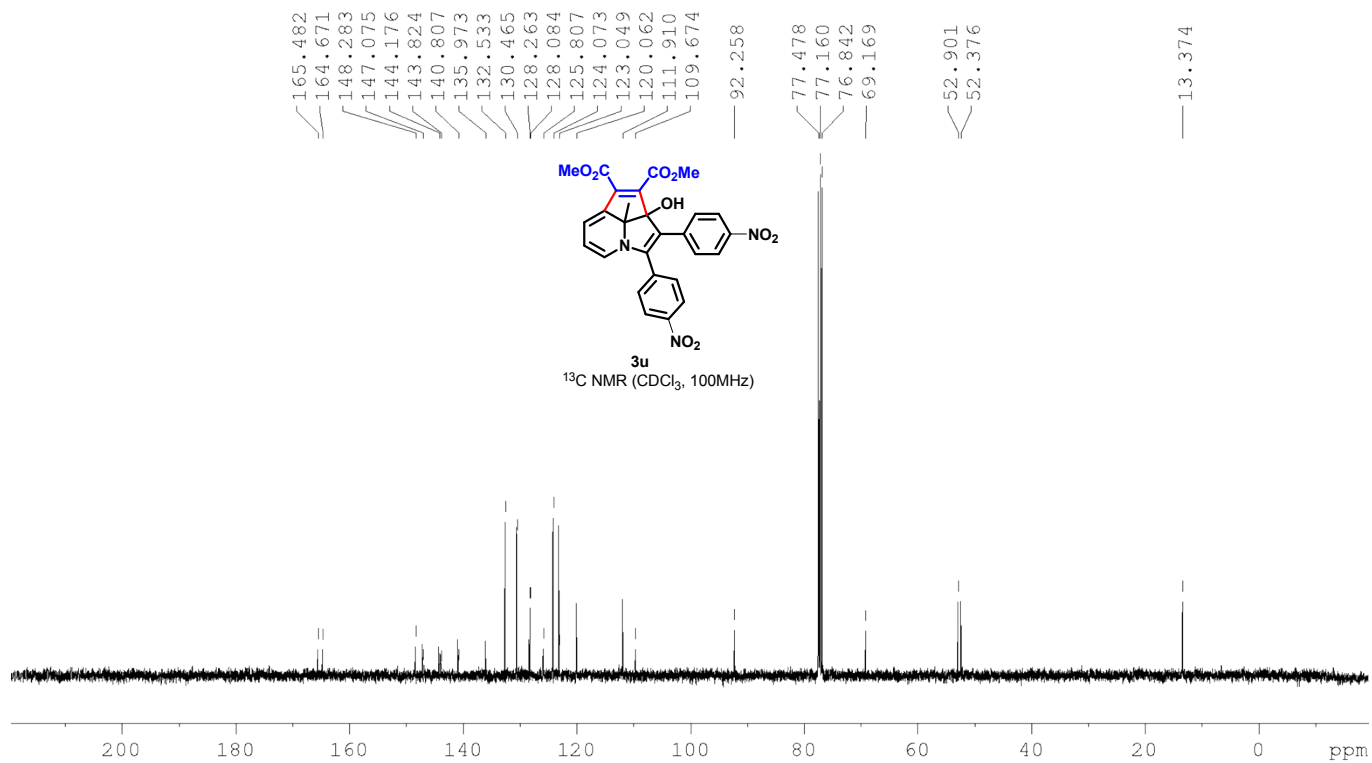


Figure 86: $^{13}\text{C NMR}$ (100 MHz) spectrum of **3u**

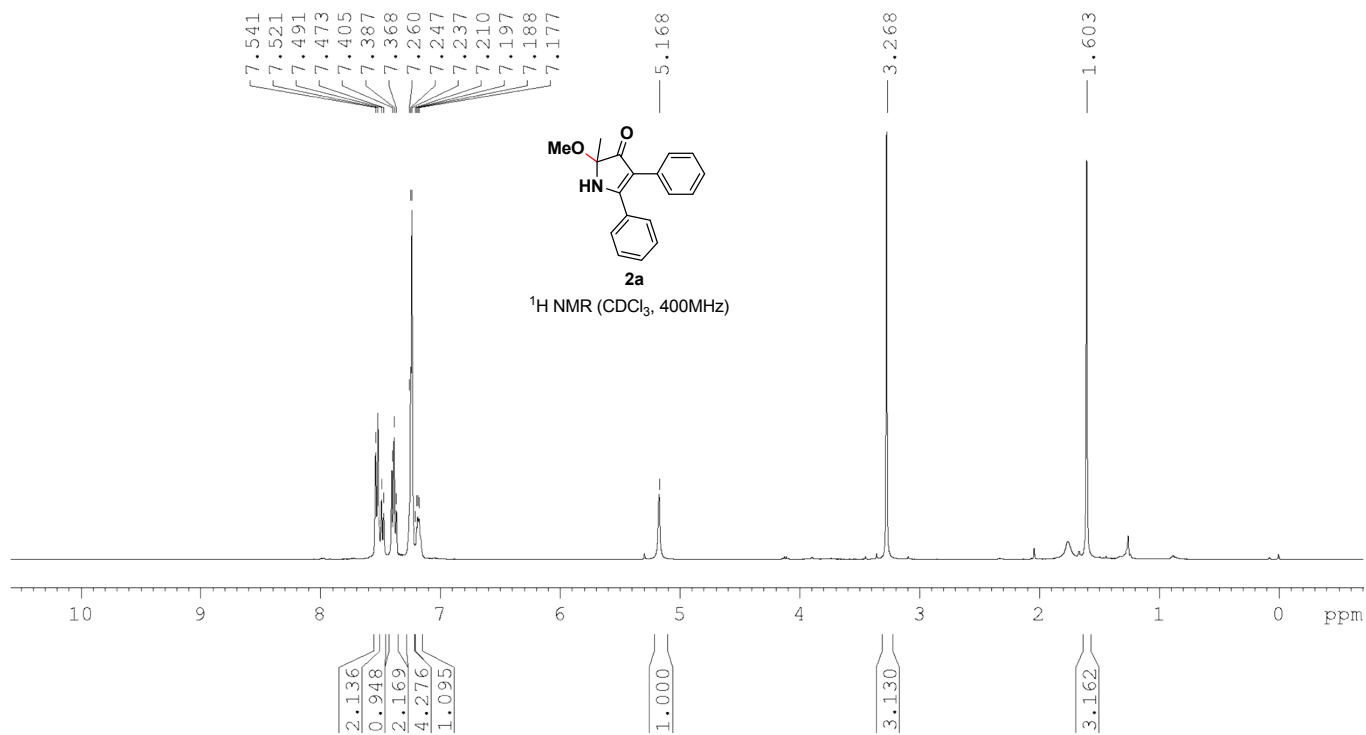


Figure 87: $^1\text{H NMR}$ (400 MHz) spectrum of **2a**

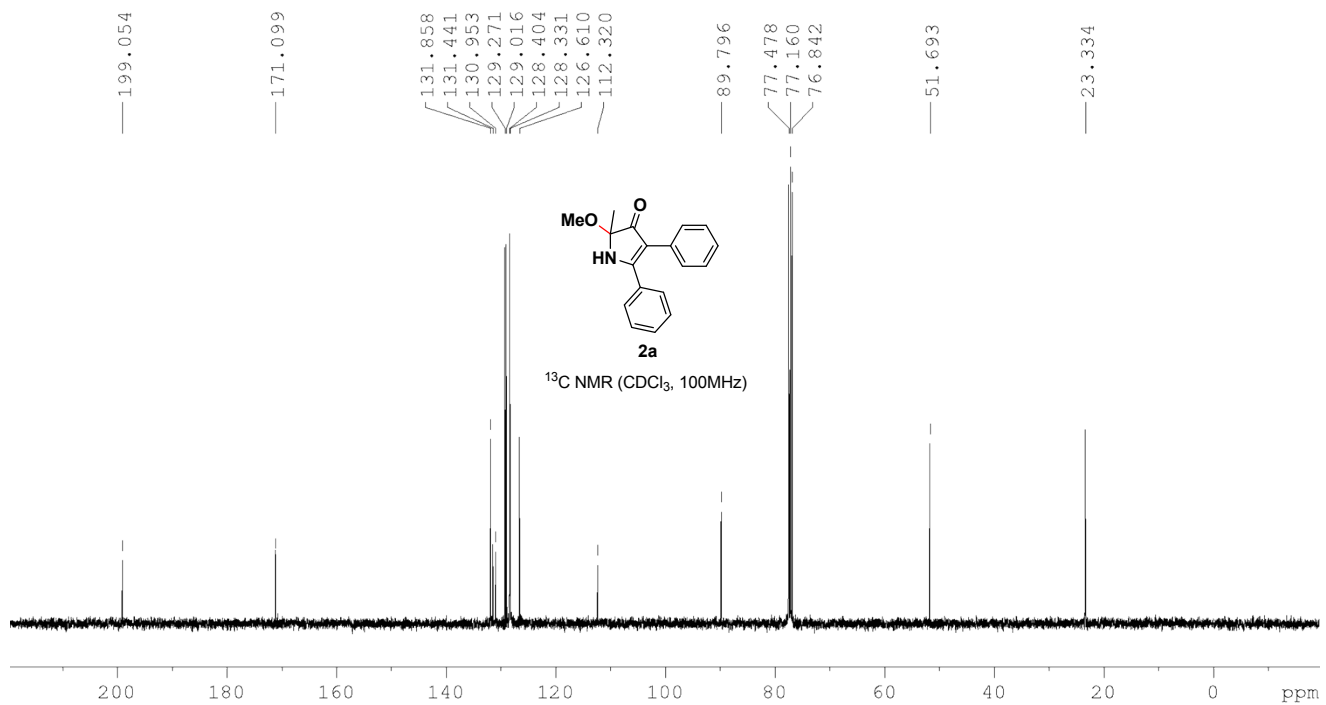


Figure 88: $^{13}\text{C NMR}$ (100 MHz) spectrum of **2a**

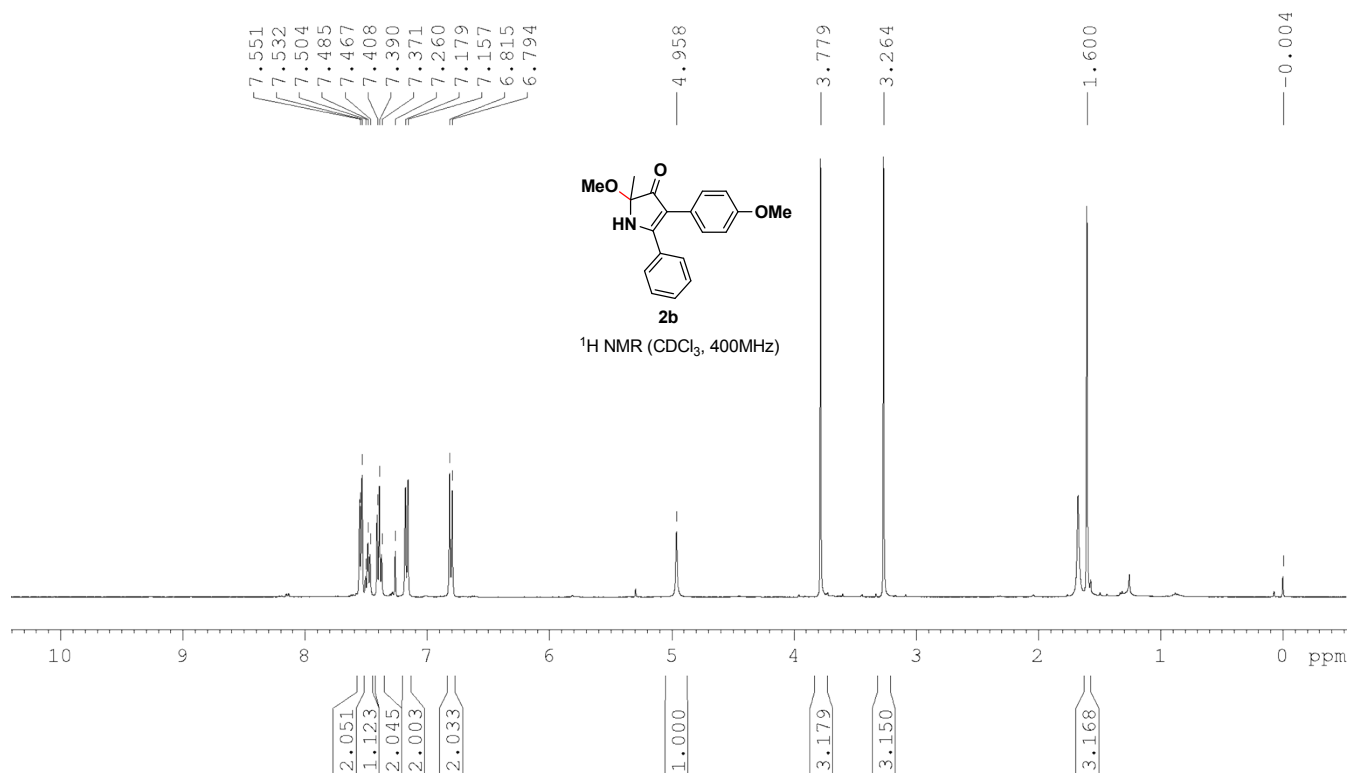


Figure 89: ¹H NMR (400 MHz) spectrum of **2b**

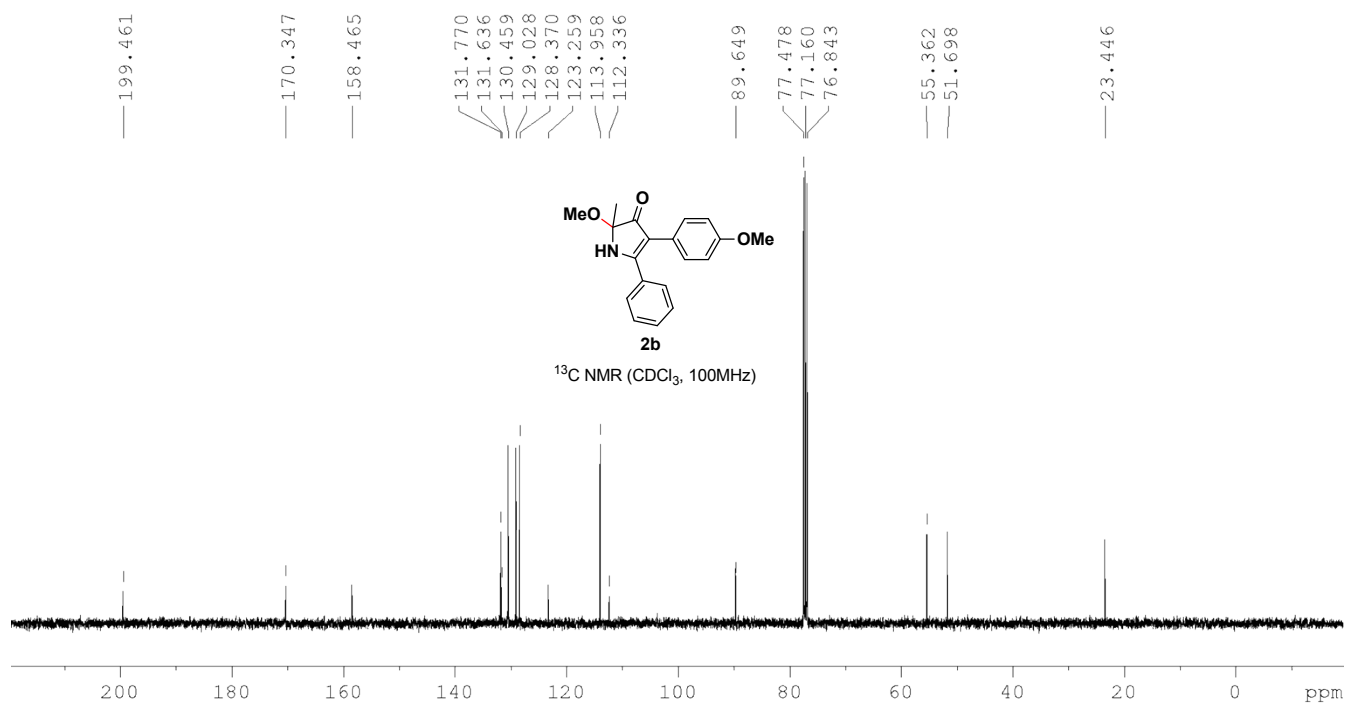


Figure 90: ¹³C NMR (100 MHz) spectrum of **2b**

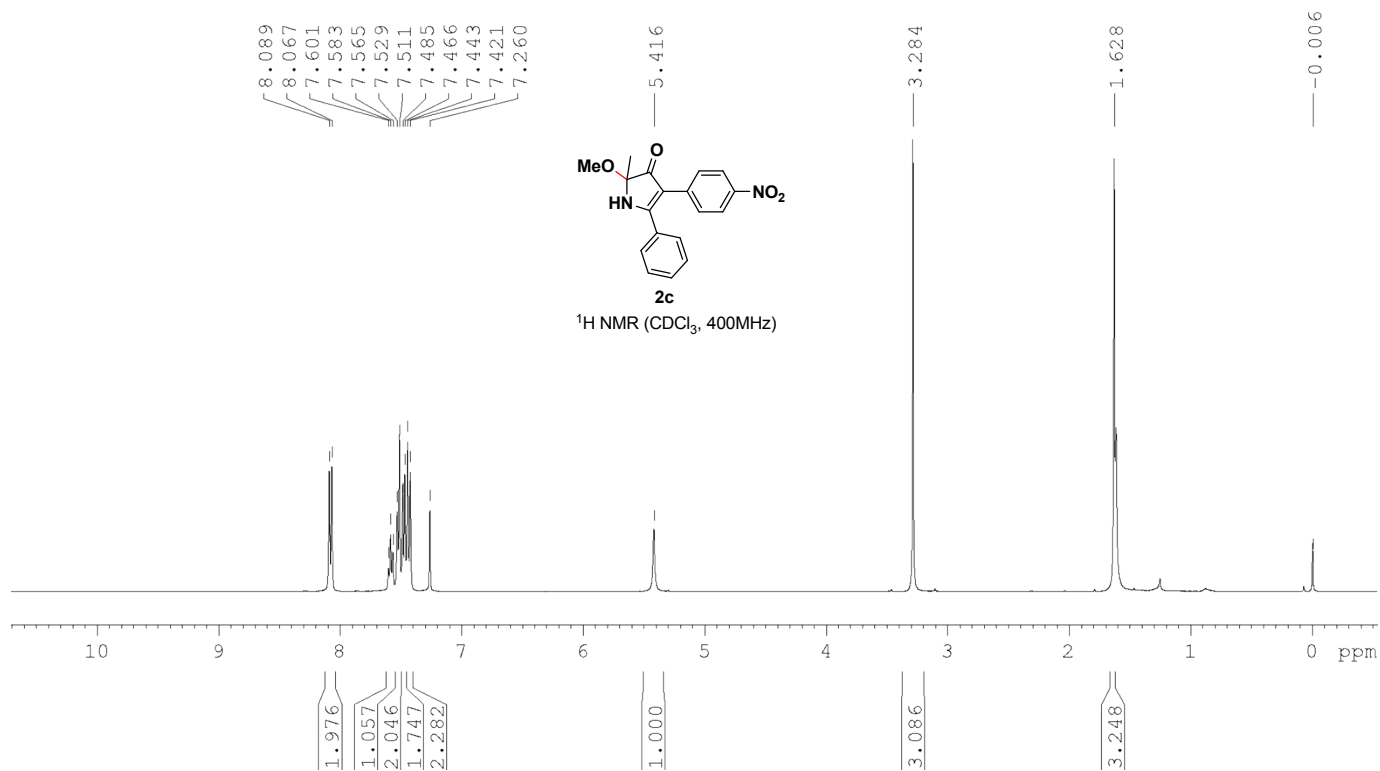


Figure 91: ¹H NMR (400 MHz) spectrum of **2c**

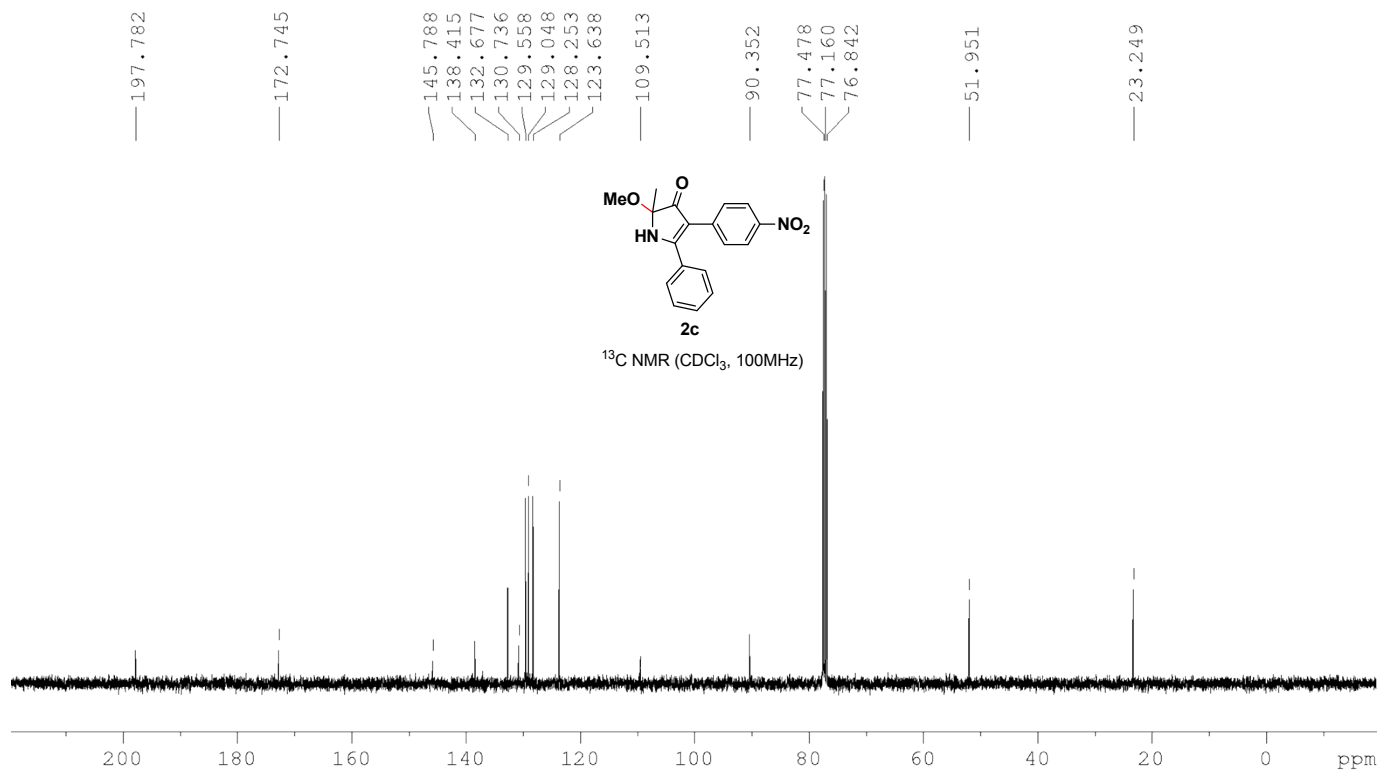


Figure 92: ¹³C NMR (100 MHz) spectrum of **2c**

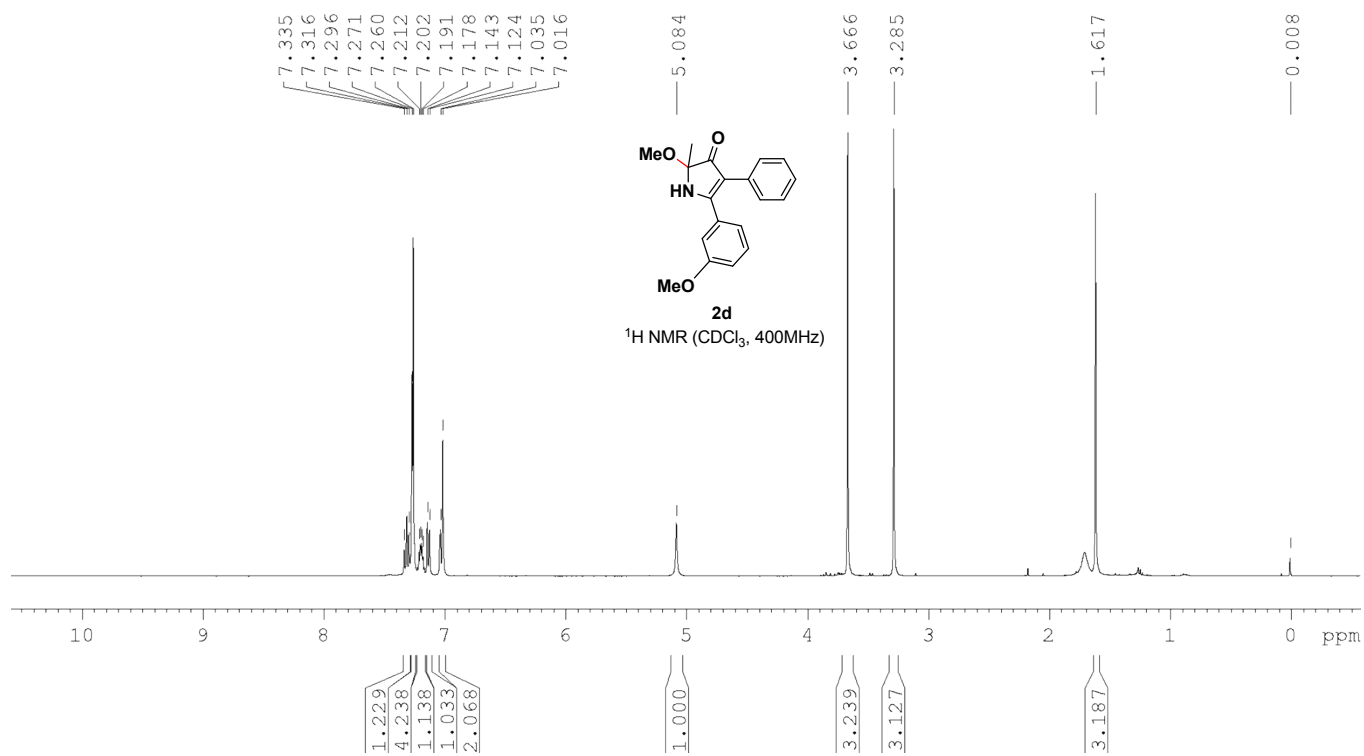


Figure 93: ¹H NMR (400 MHz) spectrum of **2d**

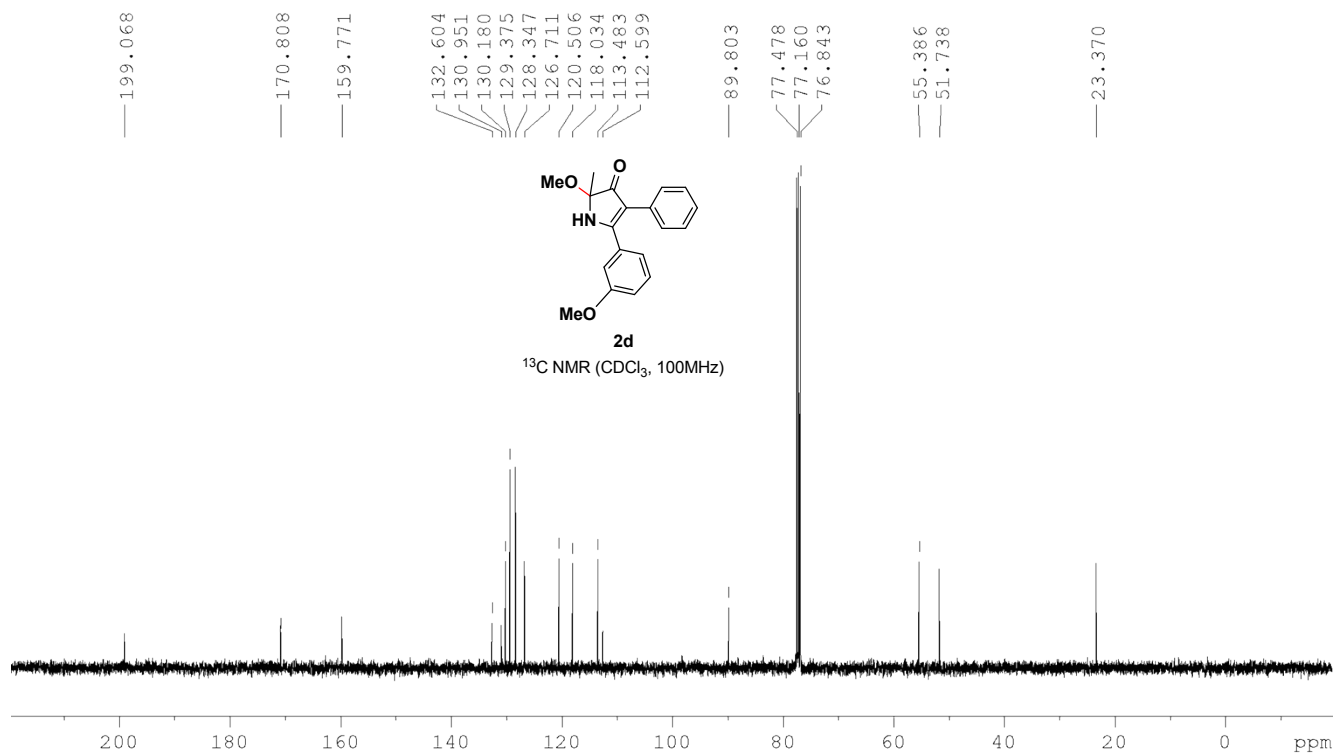


Figure 94: ¹³C NMR (100 MHz) spectrum of **2d**

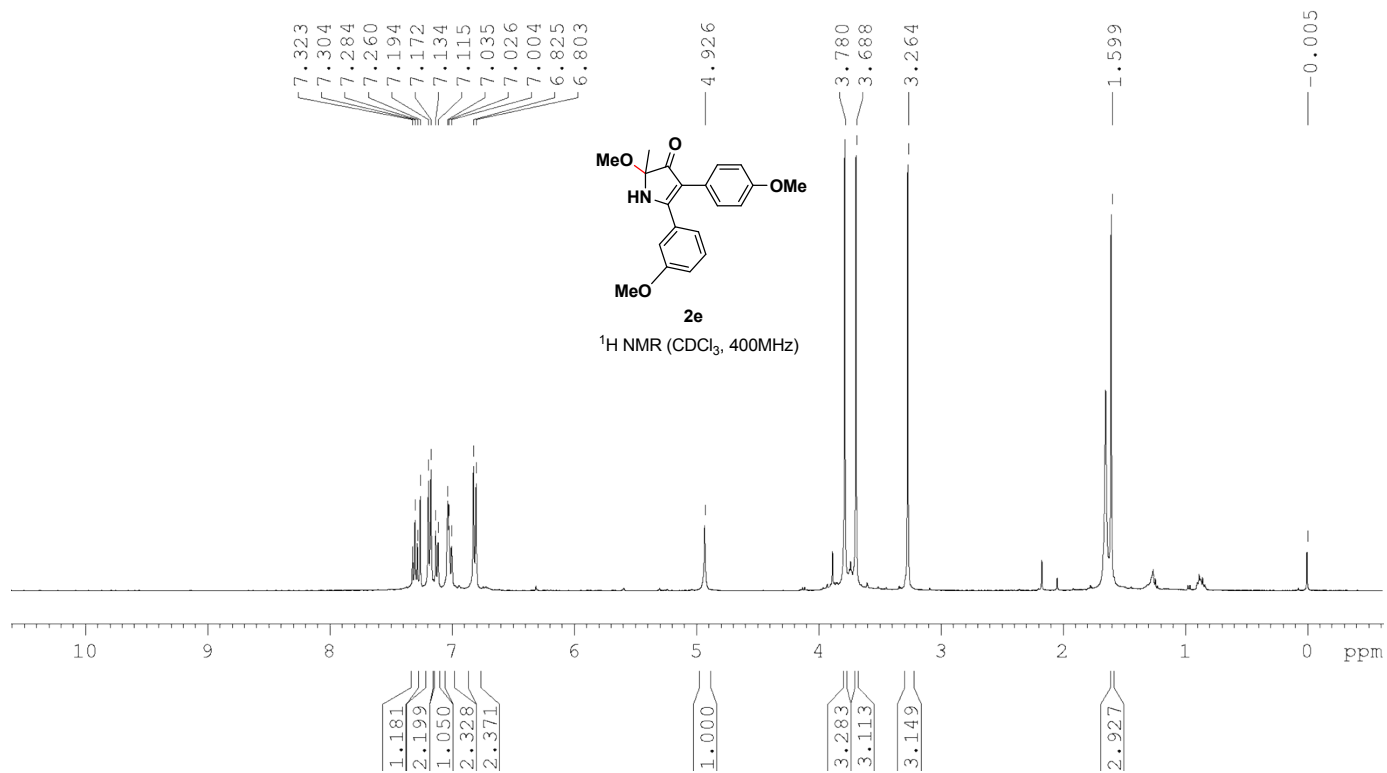


Figure 95: ¹H NMR (400 MHz) spectrum of **2e**

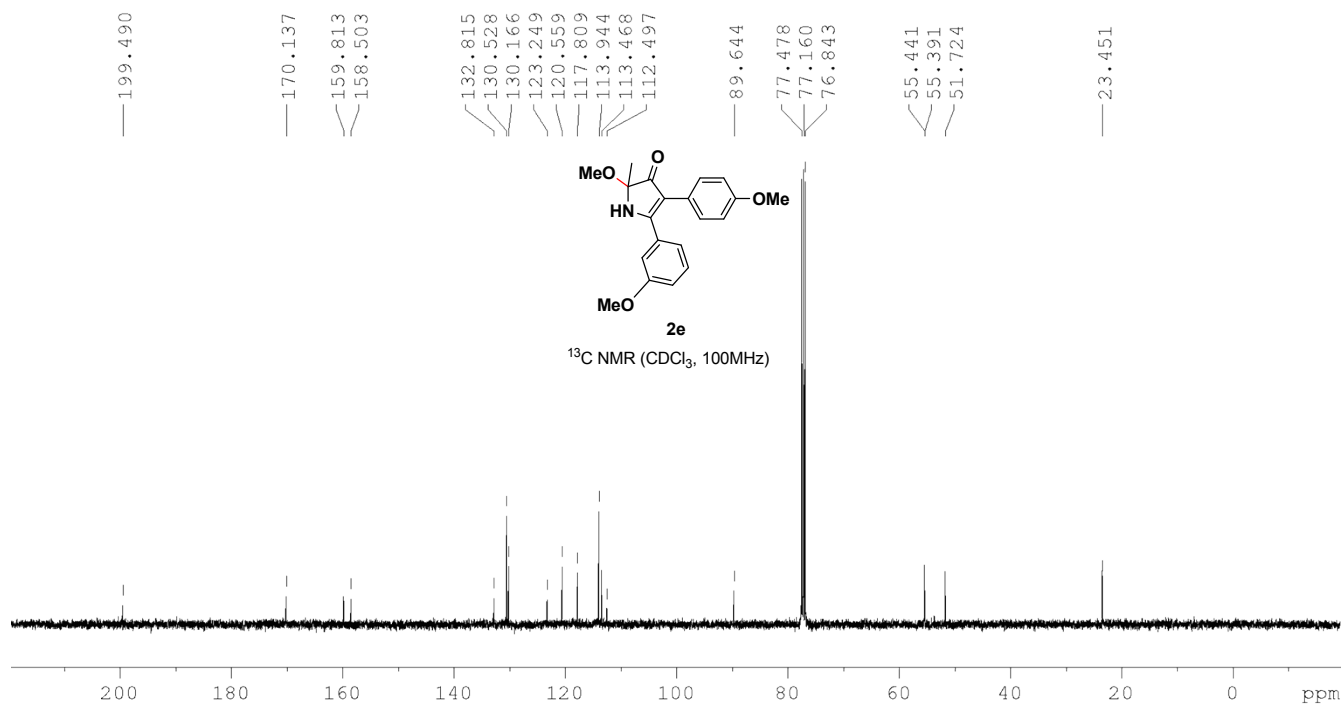


Figure 96: ¹³C NMR (100 MHz) spectrum of **2e**

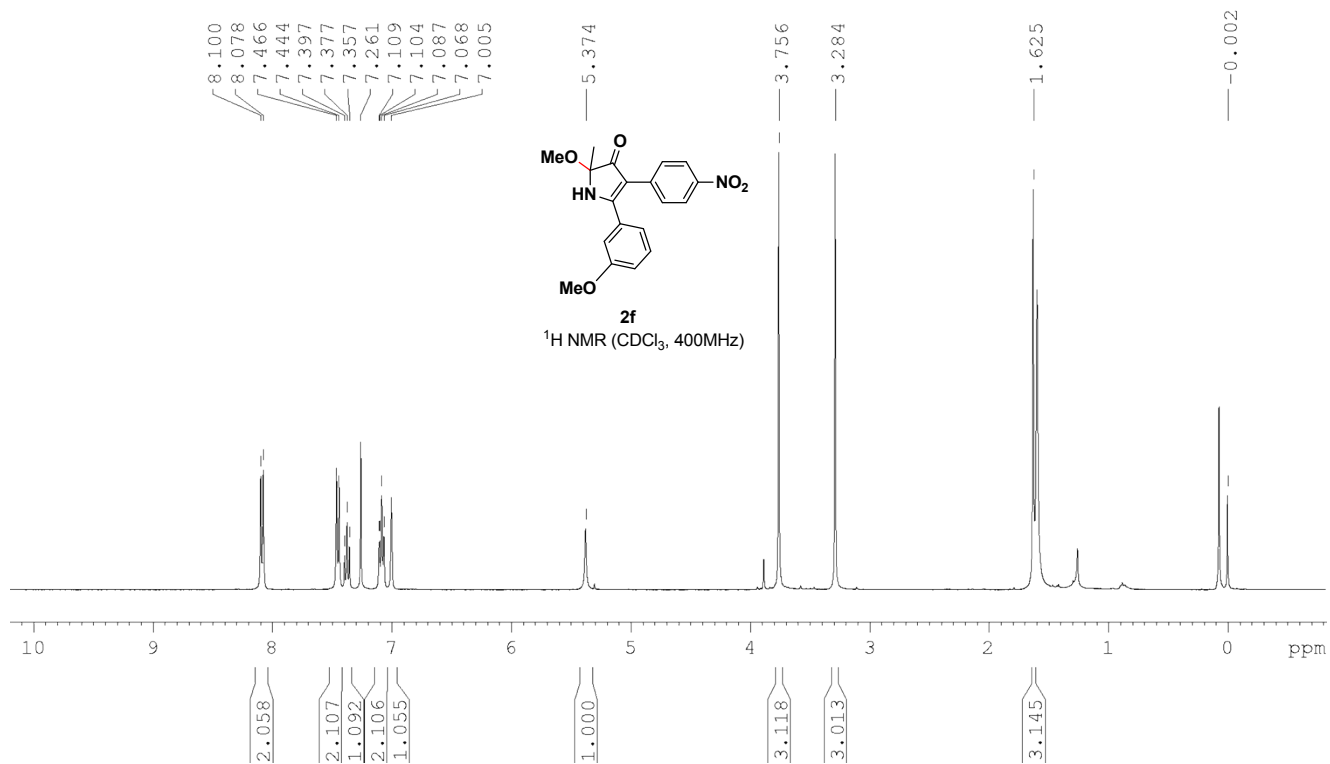


Figure 97: ¹H NMR (400 MHz) spectrum of **2f**

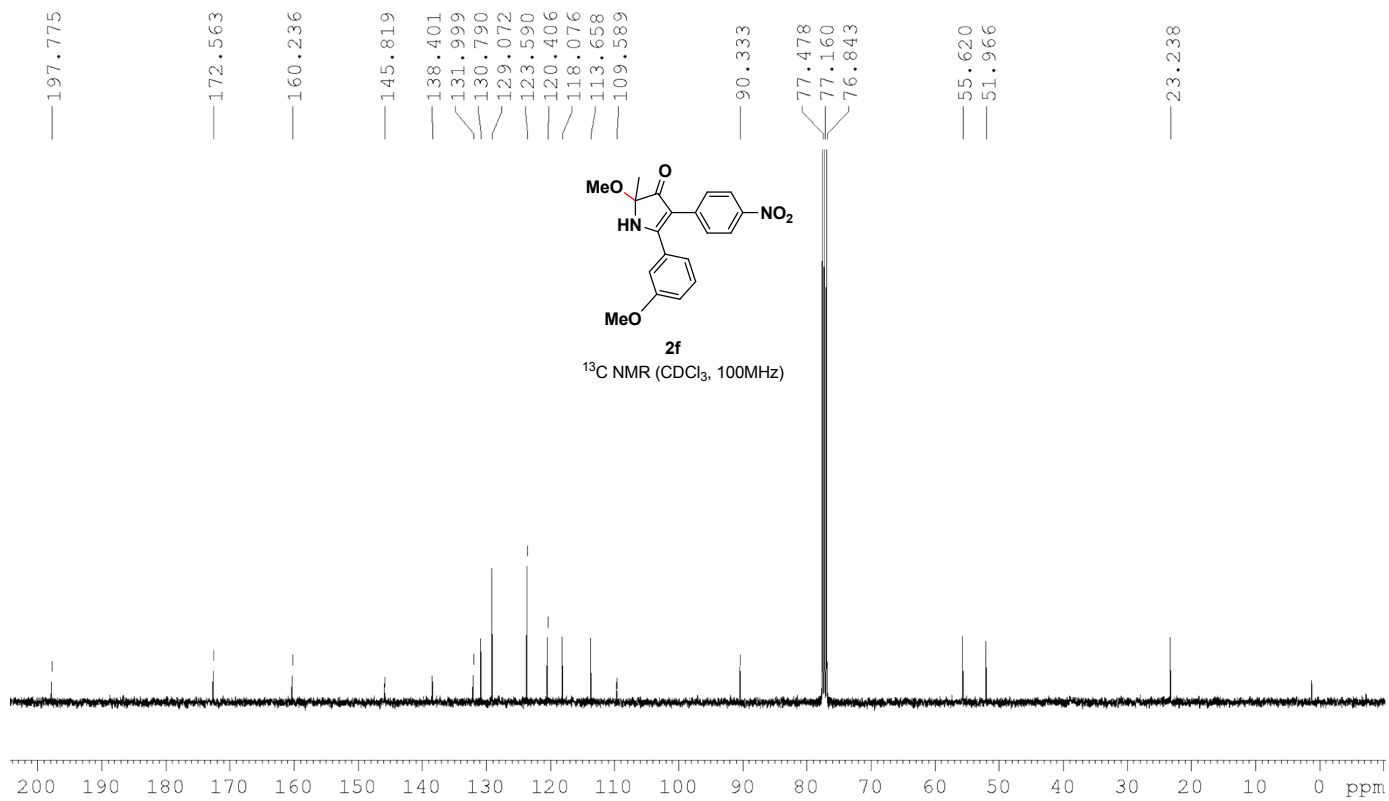


Figure 98: ¹³C NMR (100 MHz) spectrum of **2f**

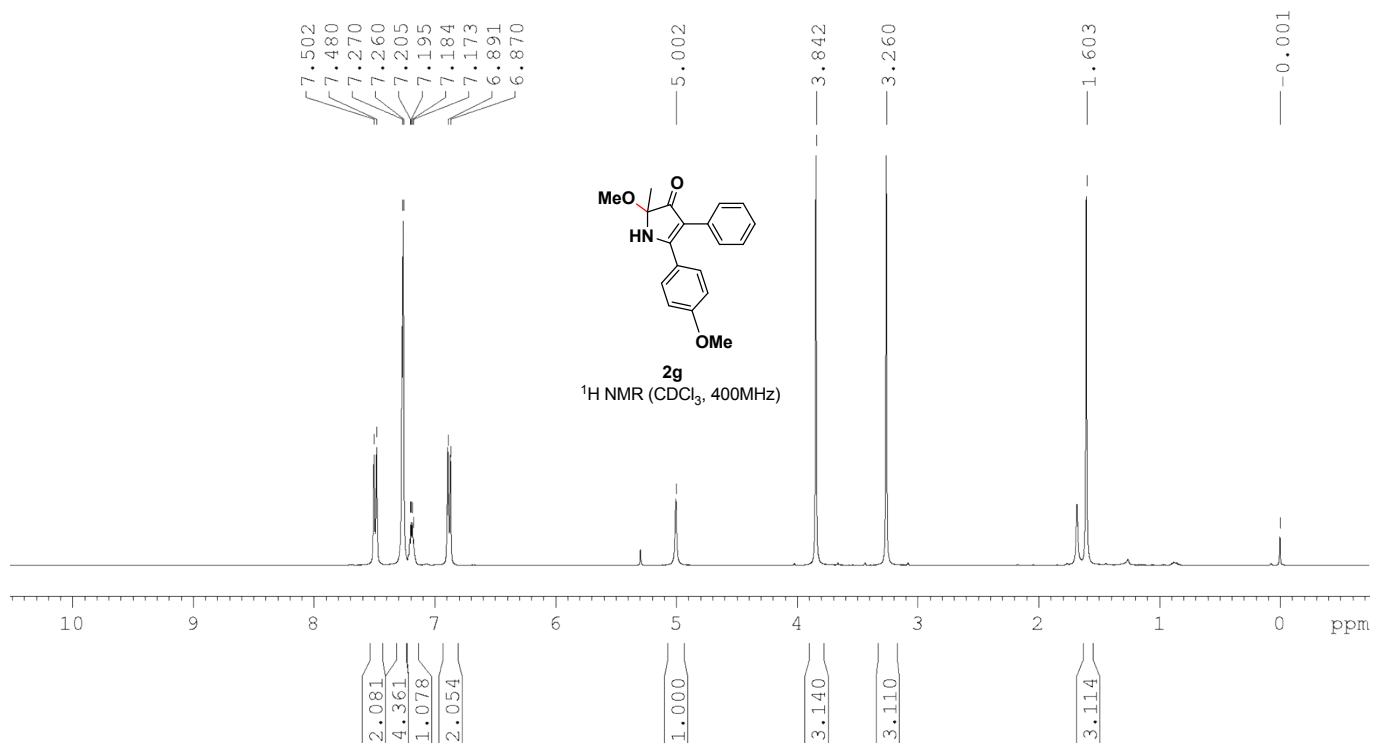


Figure 99: ¹H NMR (400 MHz) spectrum of **2g**

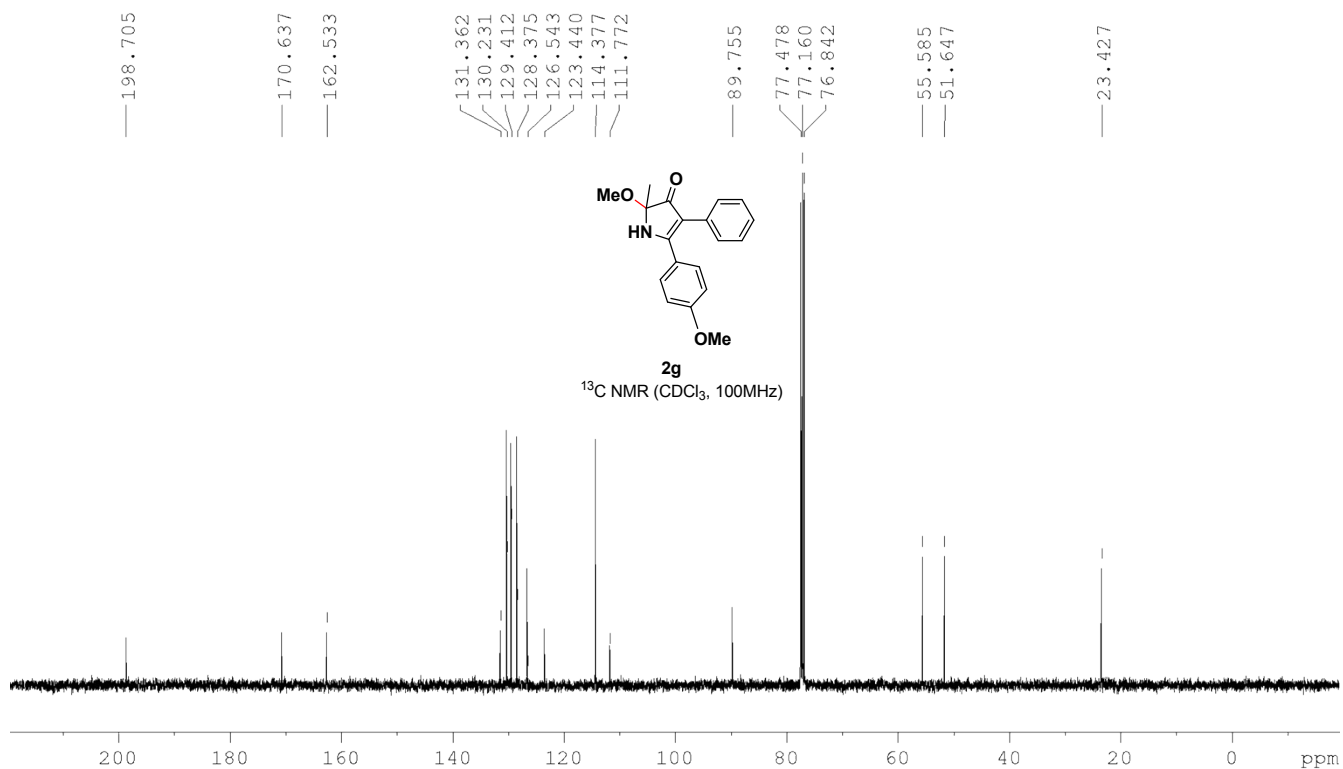


Figure 100: ¹³C NMR (100 MHz) spectrum of **2g**

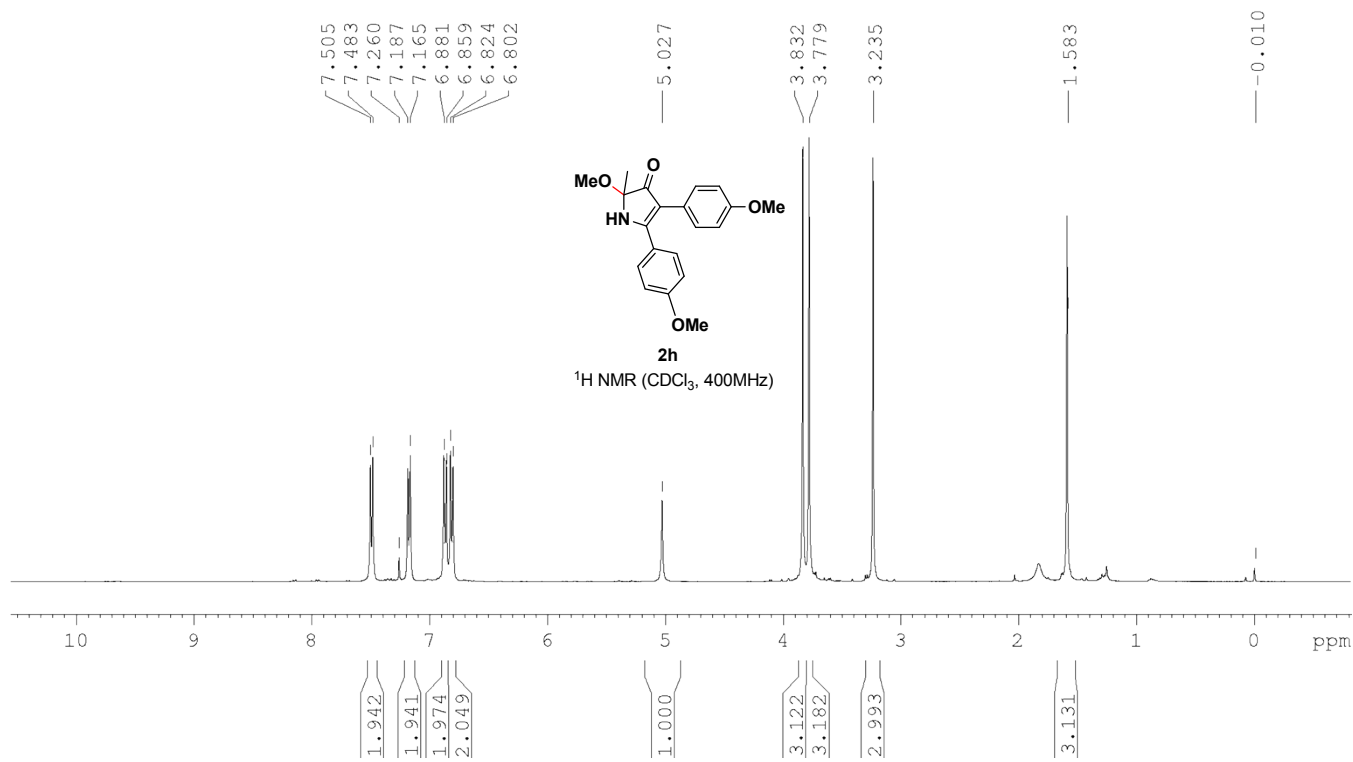


Figure 101: ¹H NMR (400 MHz) spectrum of **2h**

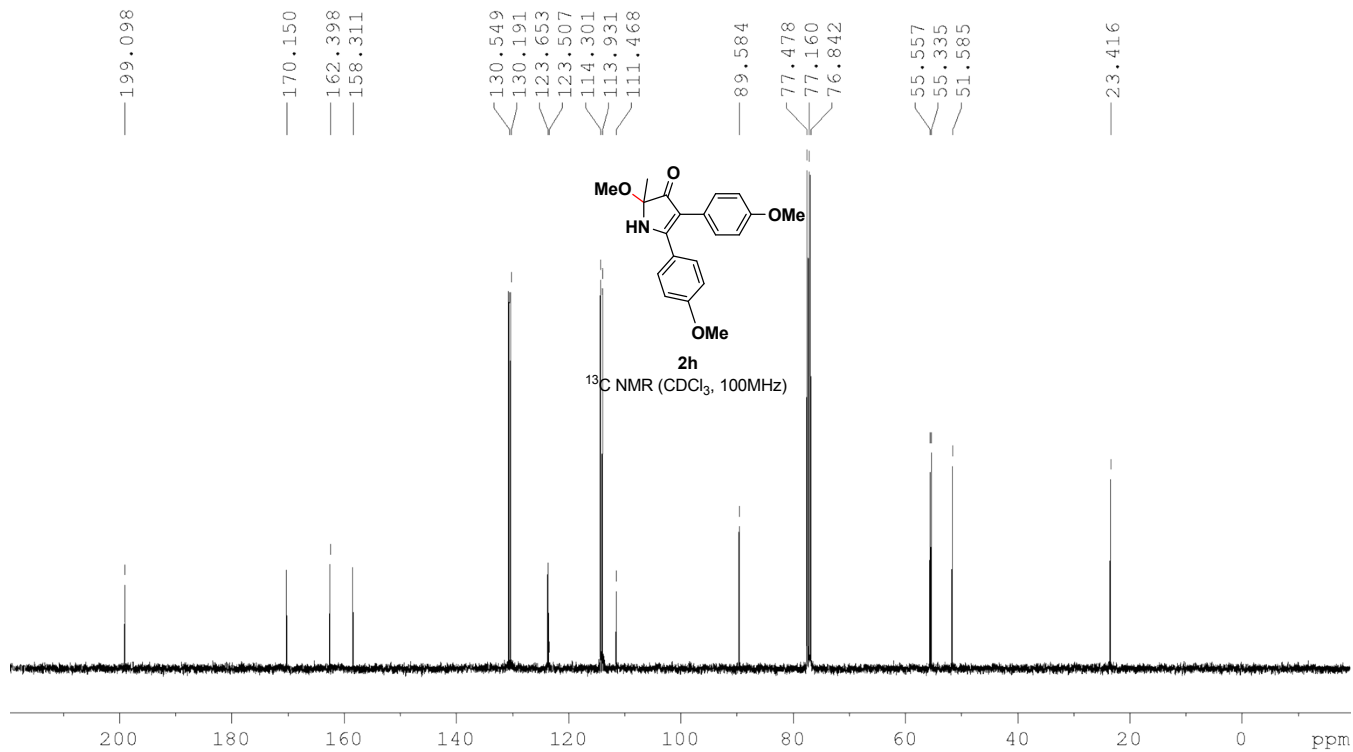


Figure 102: ¹³C NMR (100 MHz) spectrum of **2h**

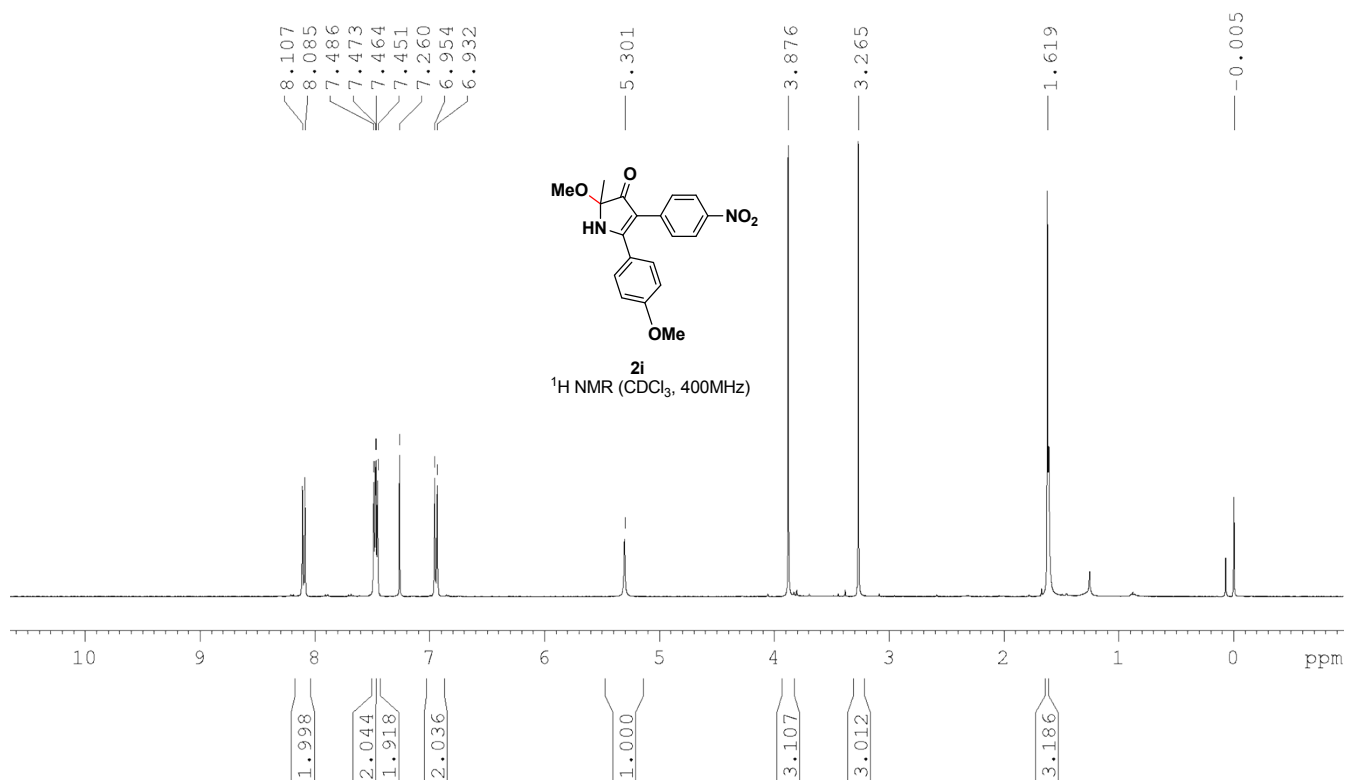


Figure 103: $^1\text{H NMR}$ (400 MHz) spectrum of **2i**

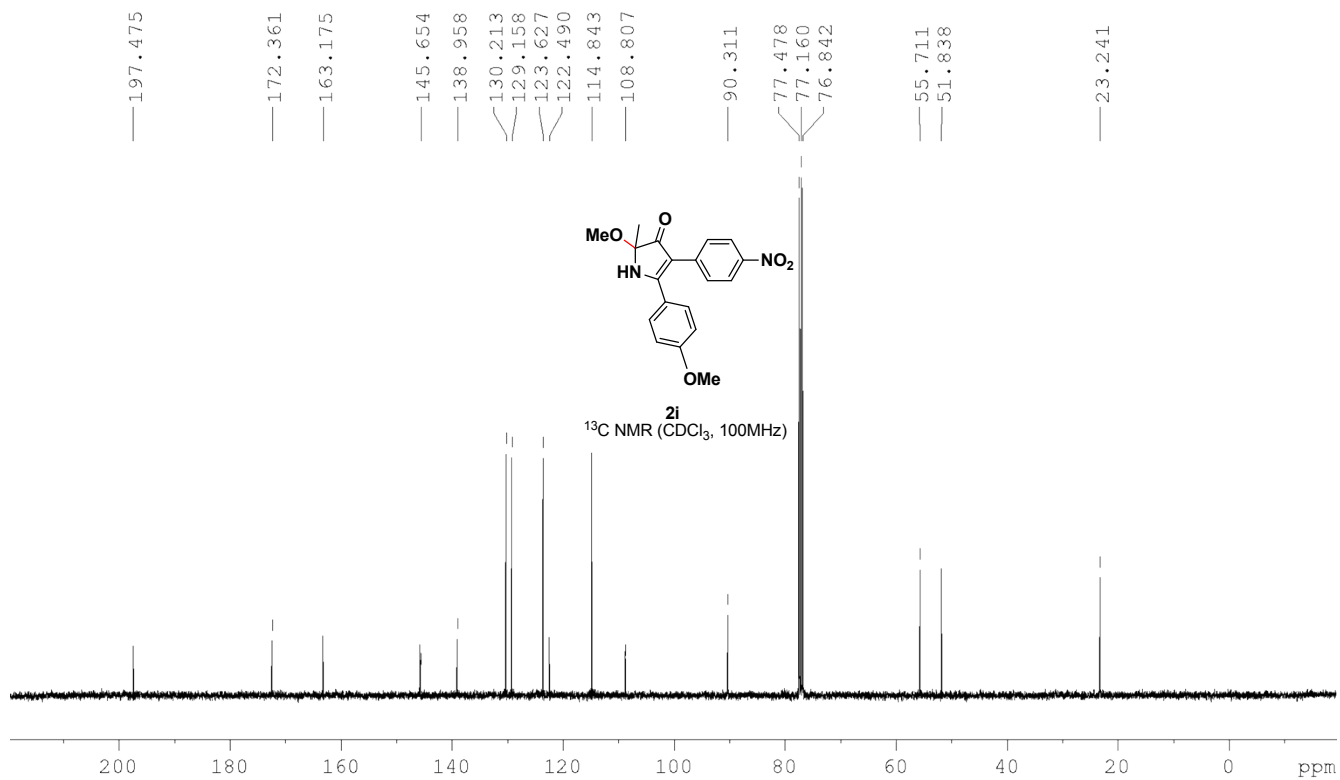


Figure 104: $^{13}\text{C NMR}$ (100 MHz) spectrum of **2i**

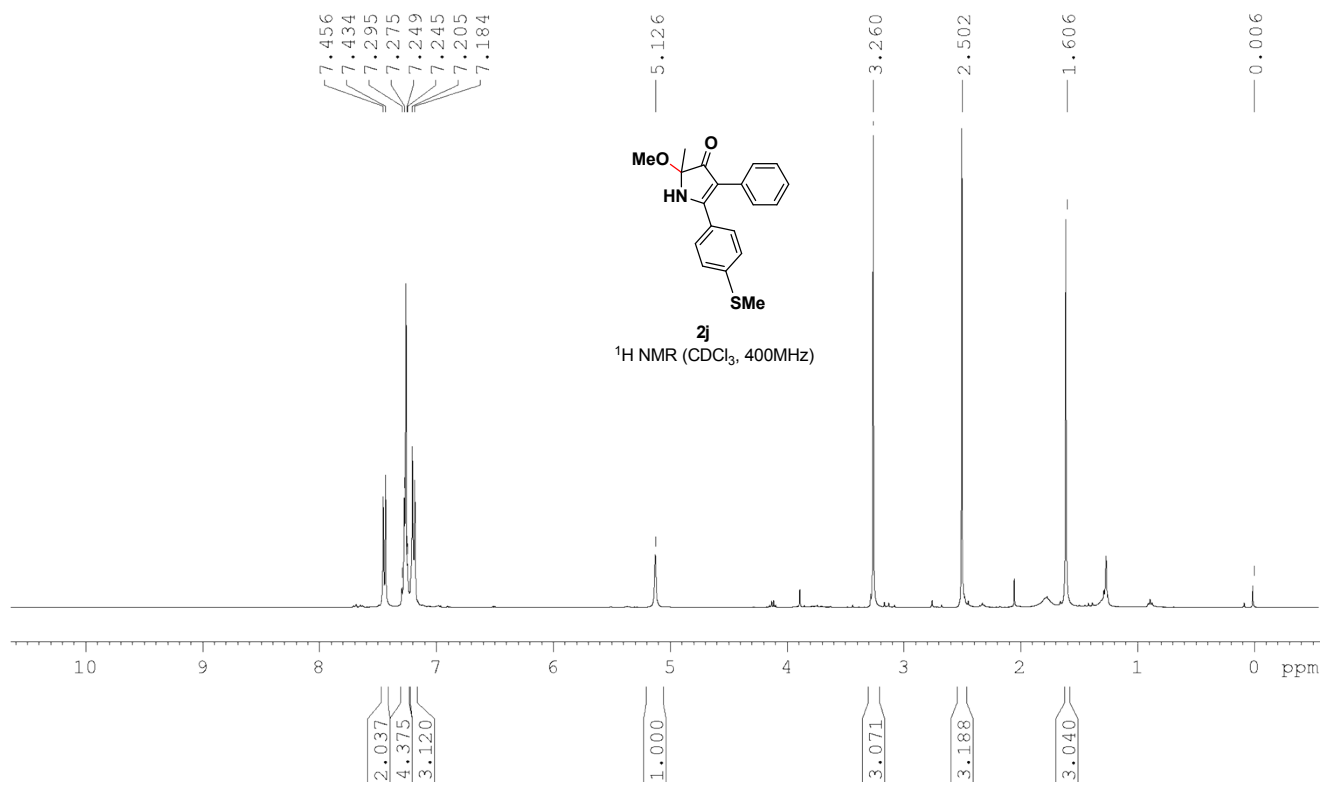


Figure 105: ¹H NMR (400 MHz) spectrum of **2j**

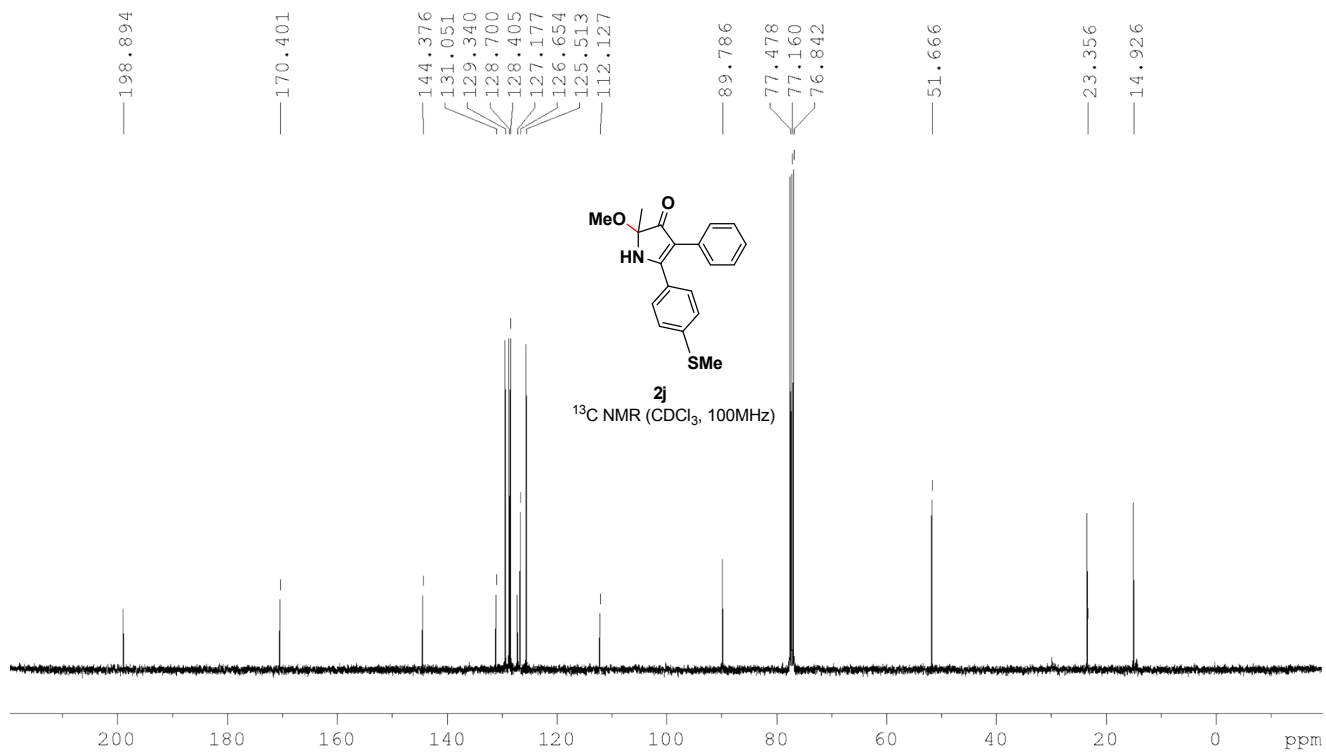


Figure 106: ¹³C NMR (100 MHz) spectrum of **2j**

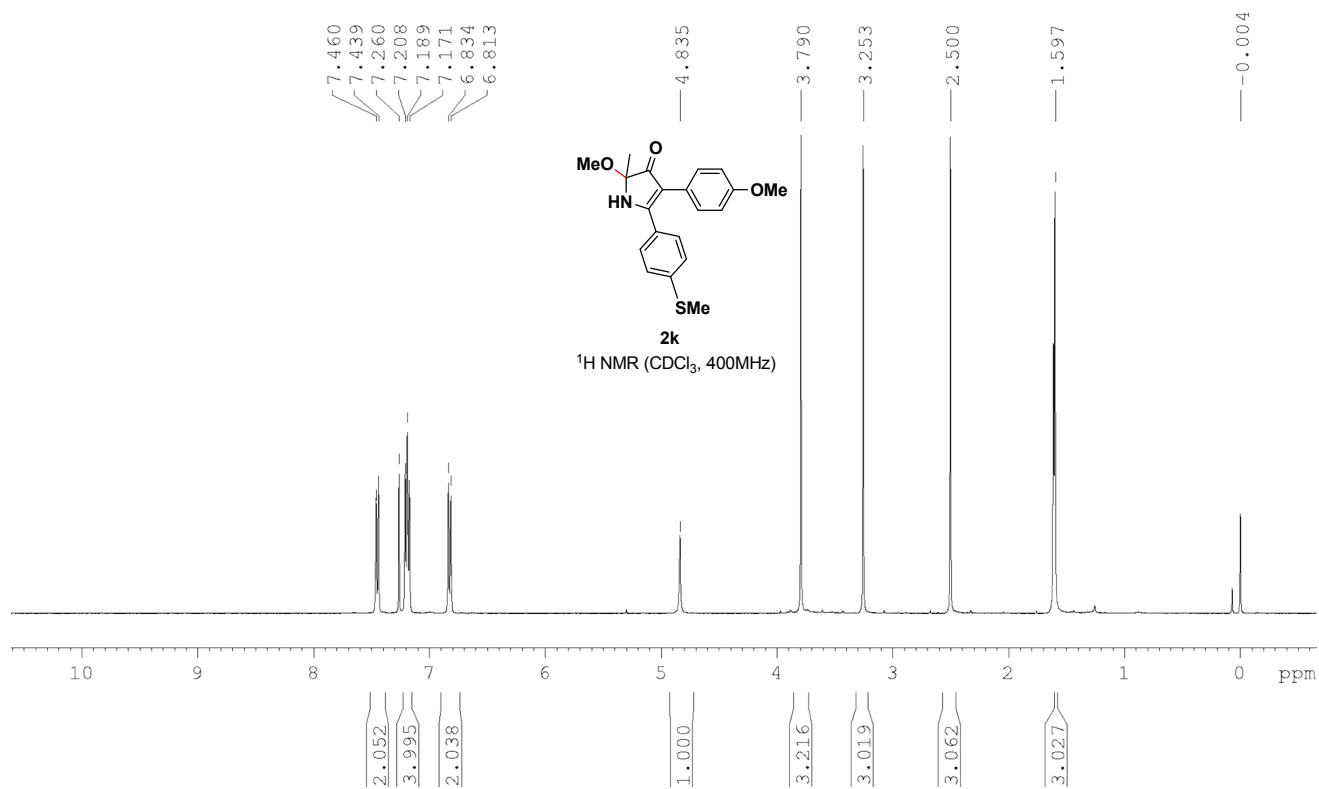


Figure 107: ¹H NMR (400 MHz) spectrum of **2k**

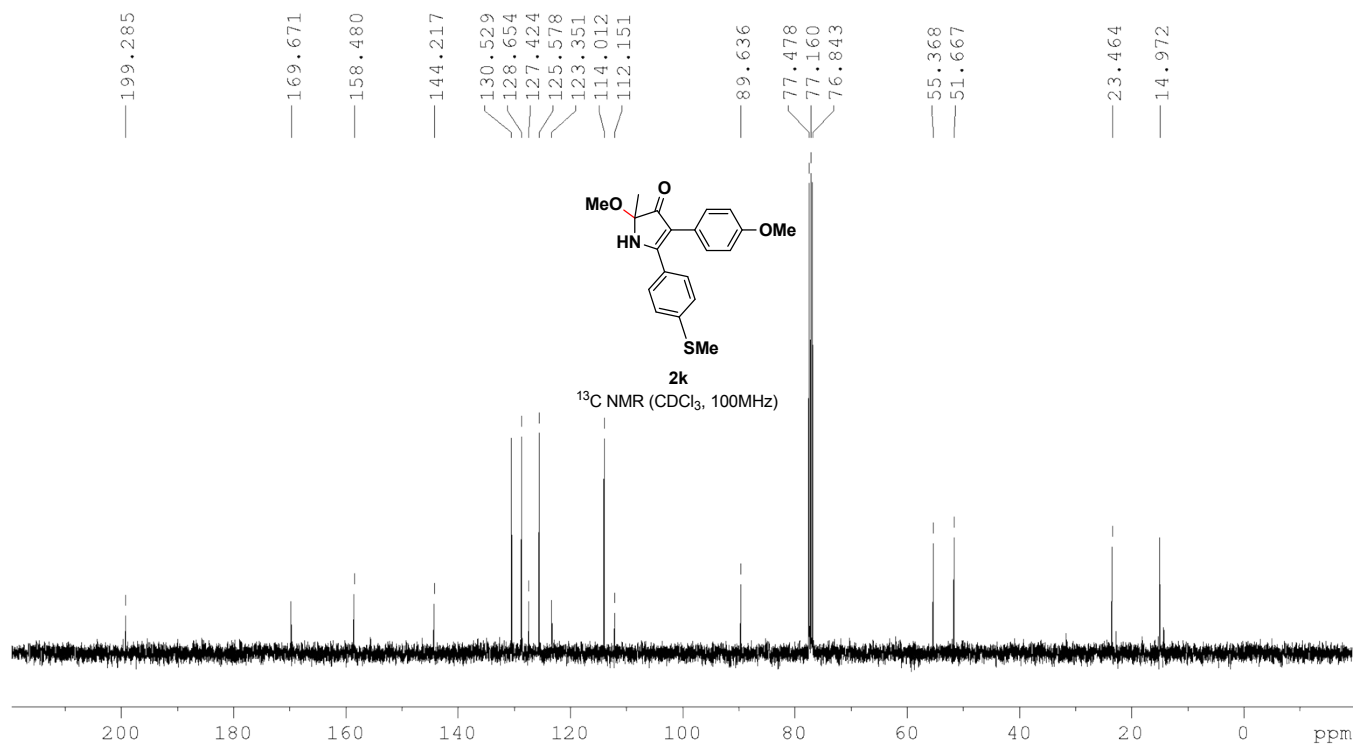


Figure 108: ¹³C NMR (100 MHz) spectrum of **2k**

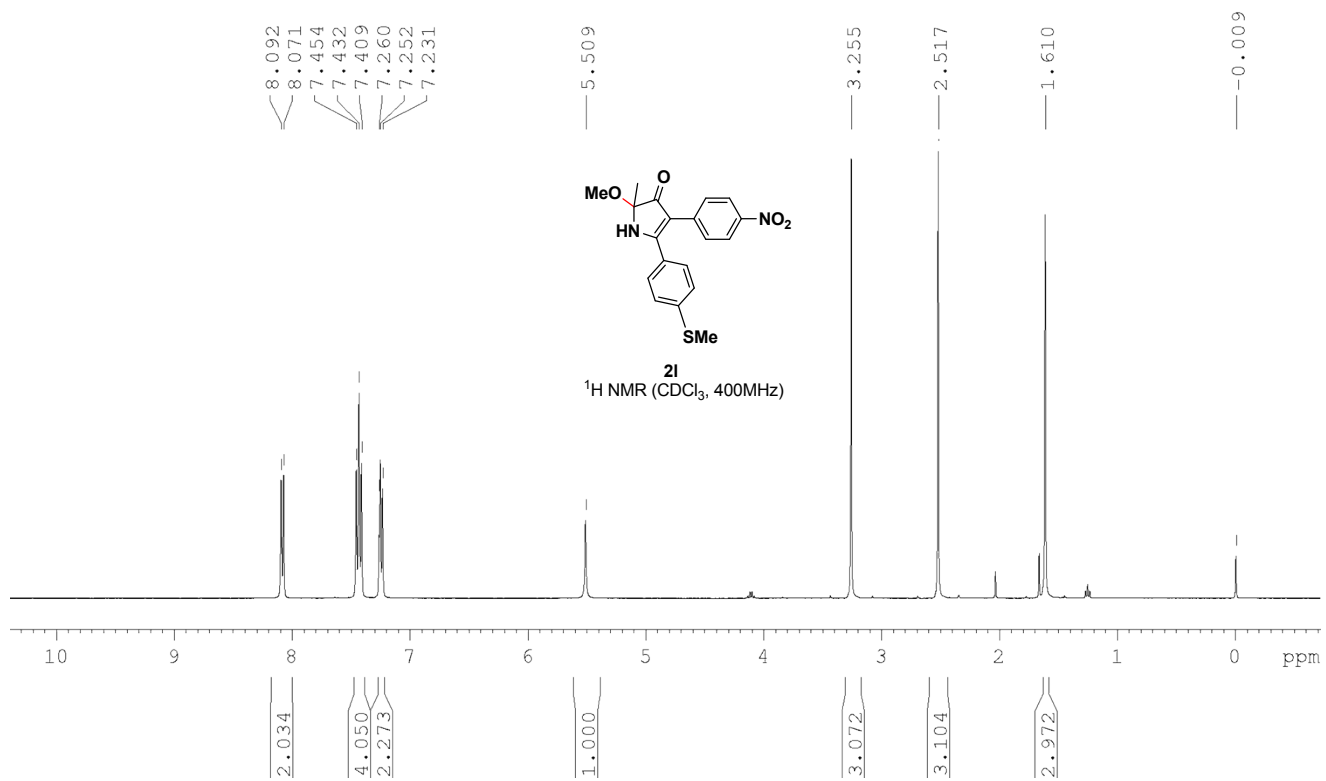


Figure 109: ¹H NMR (400 MHz) spectrum of **21**

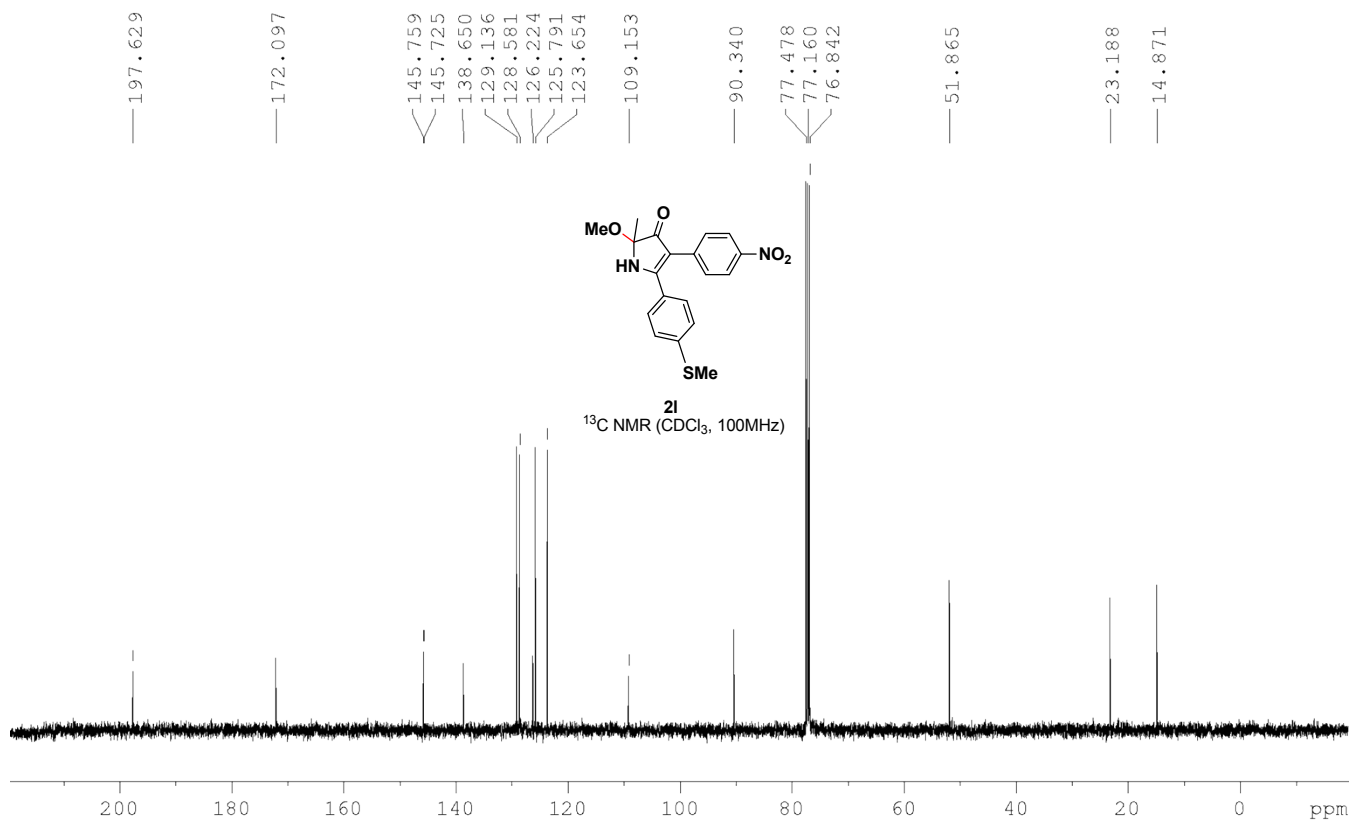


Figure 110: ¹³C NMR (100 MHz) spectrum of **21**

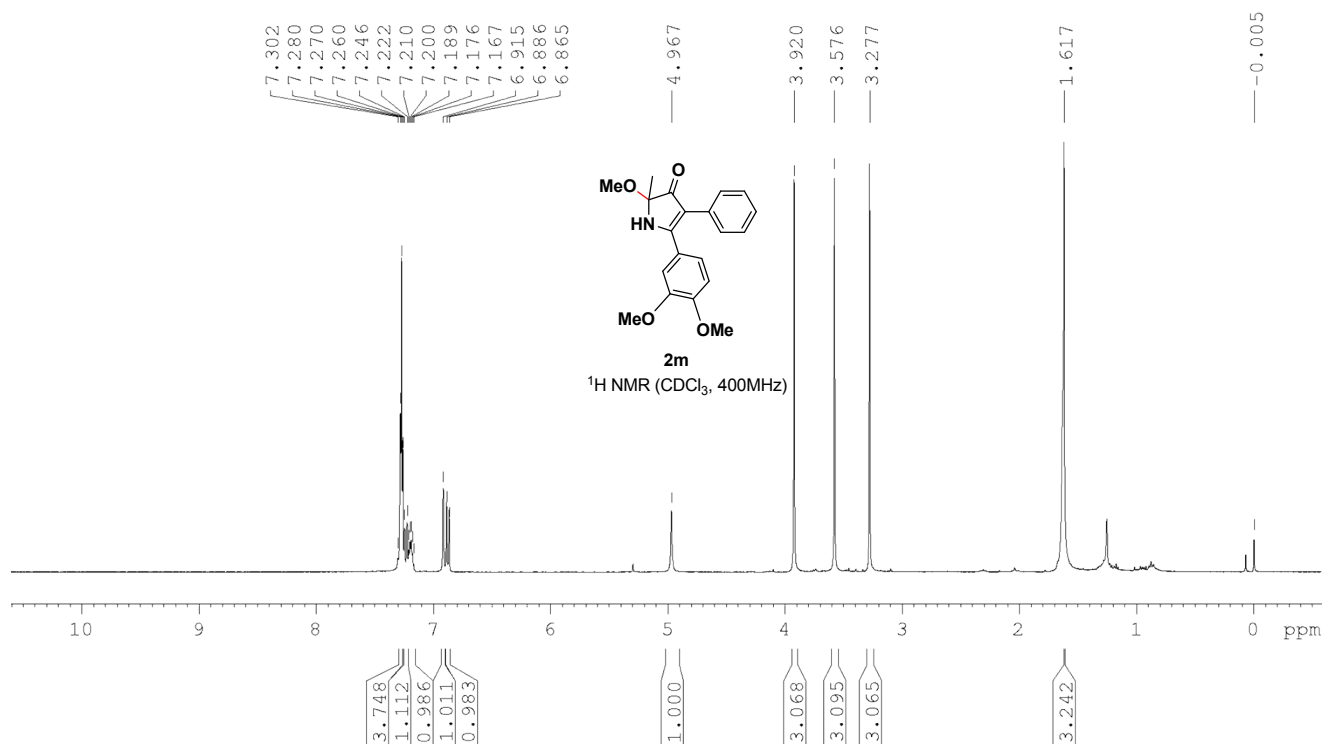


Figure 111: ¹H NMR (400 MHz) spectrum of **2m**

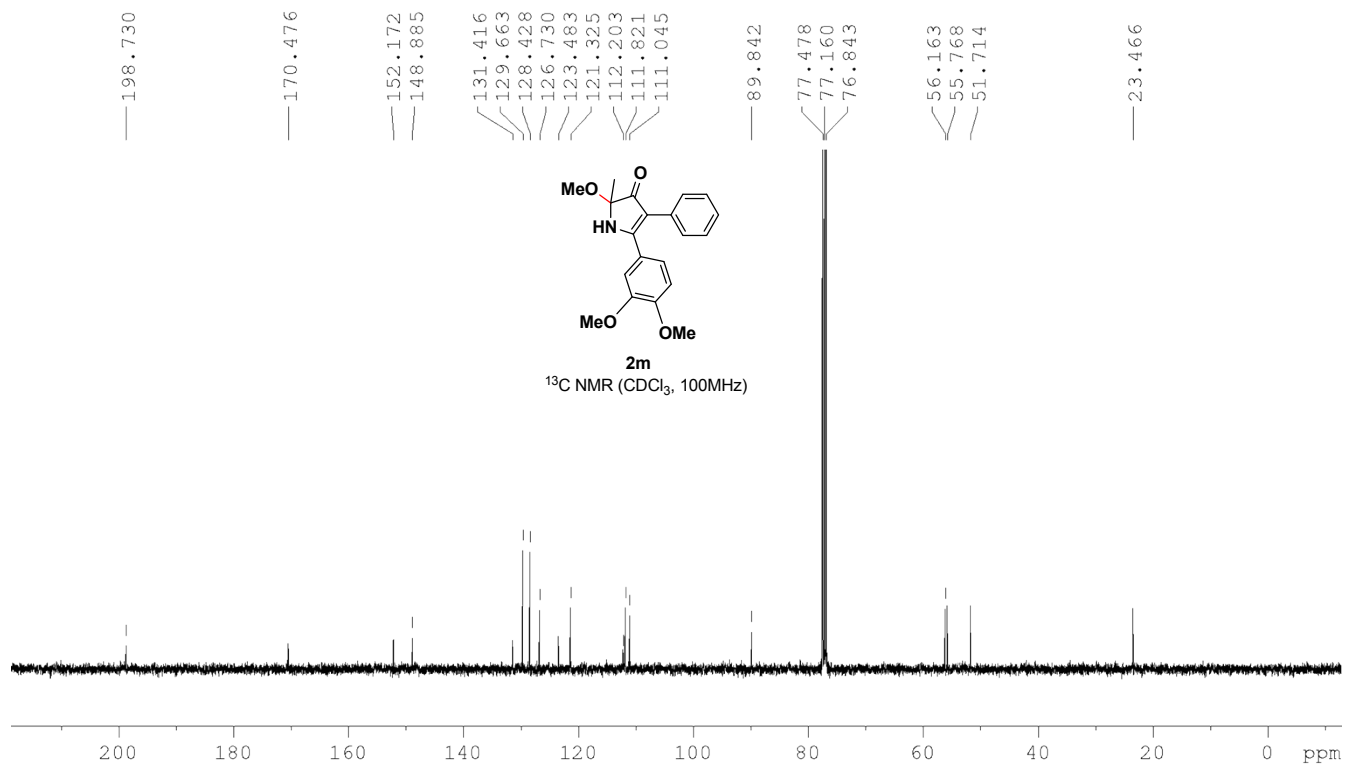


Figure 112: ¹³C NMR (100 MHz) spectrum of **2m**

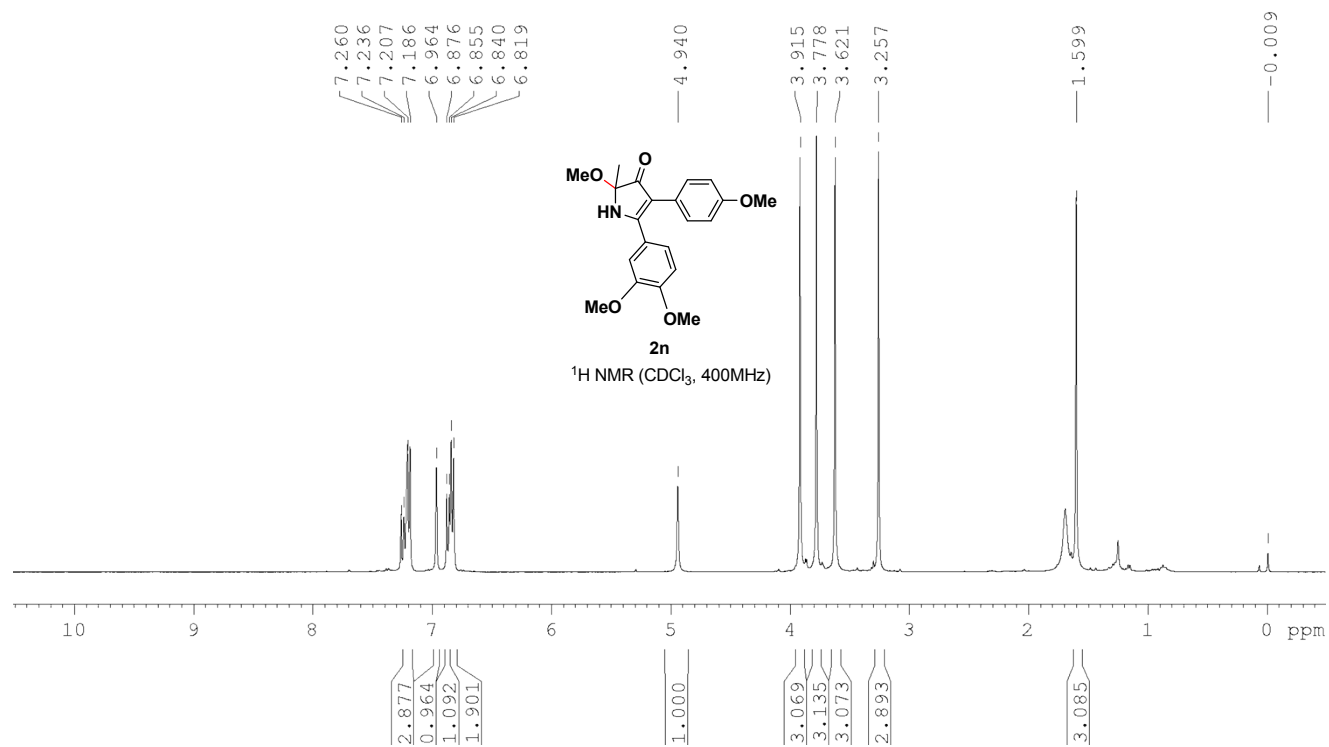


Figure 113: ¹H NMR (400 MHz) spectrum of **2n**

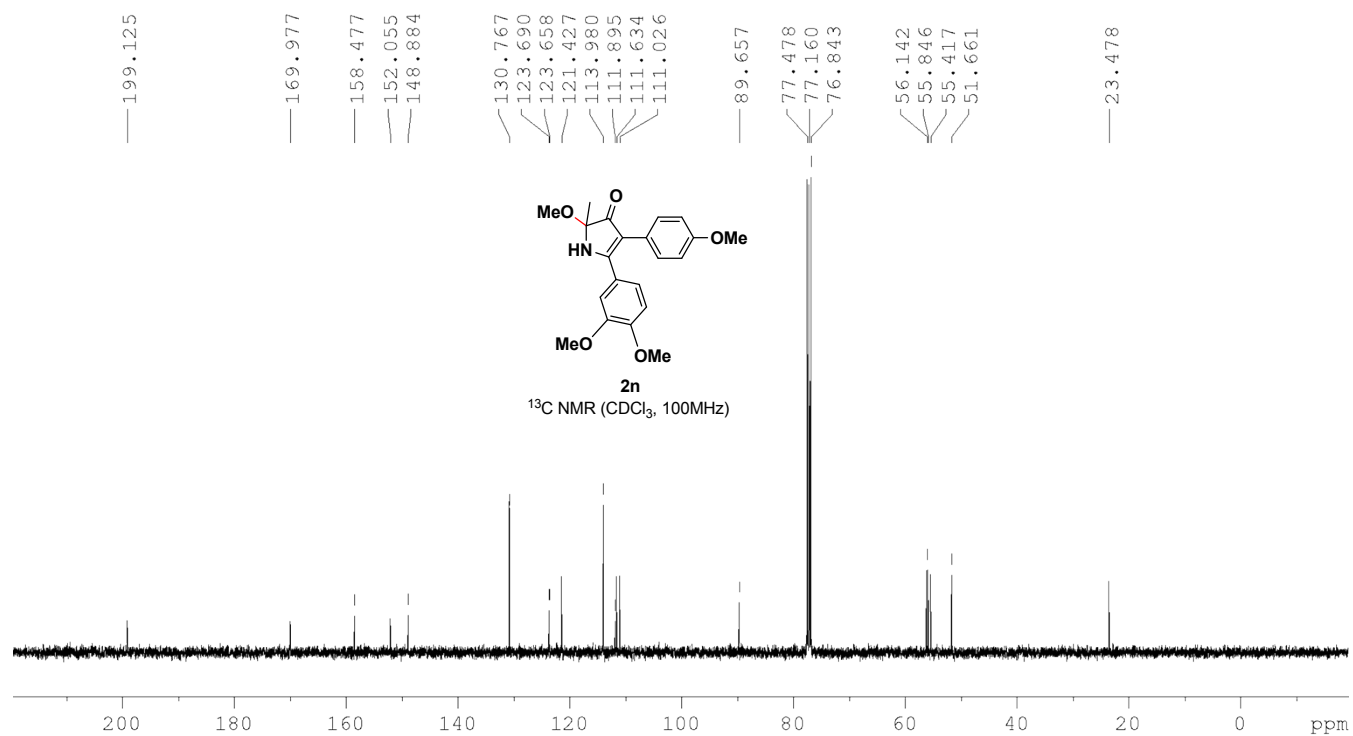


Figure 114: ¹³C NMR (100 MHz) spectrum of **2n**

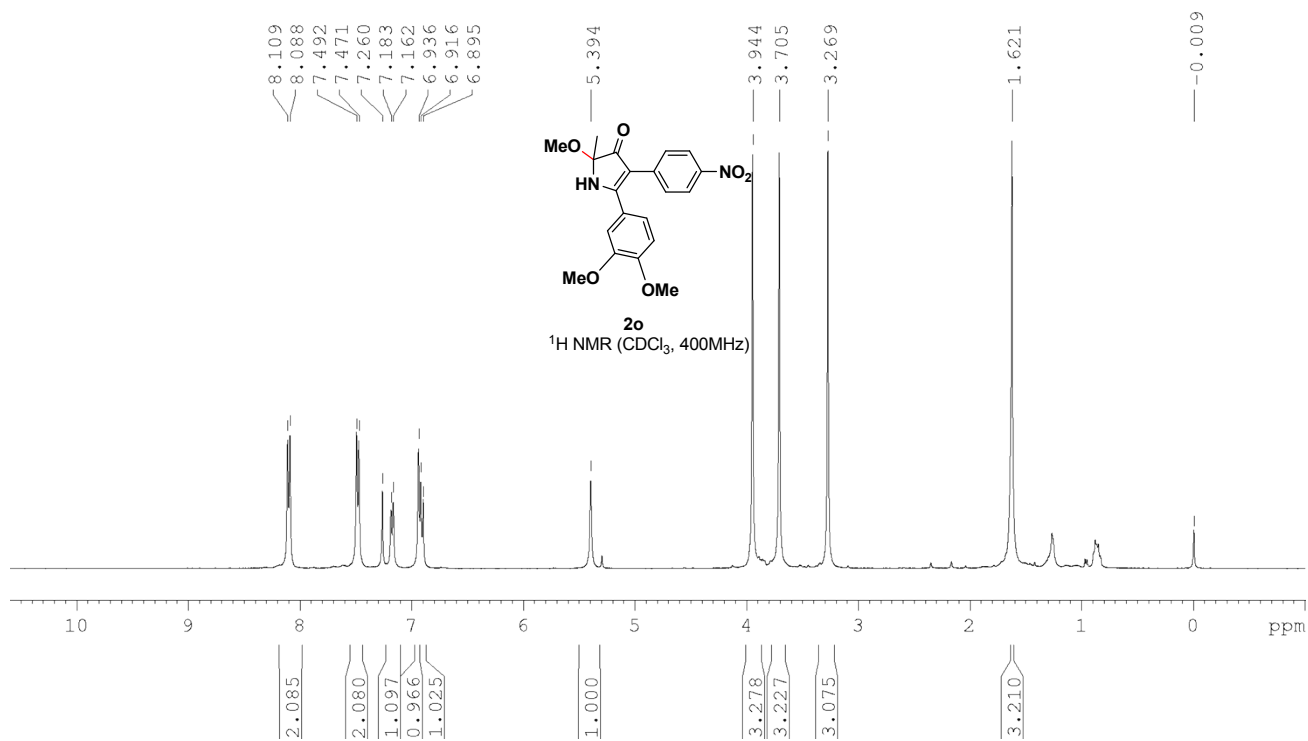


Figure 115: ¹H NMR (400 MHz) spectrum of **2o**

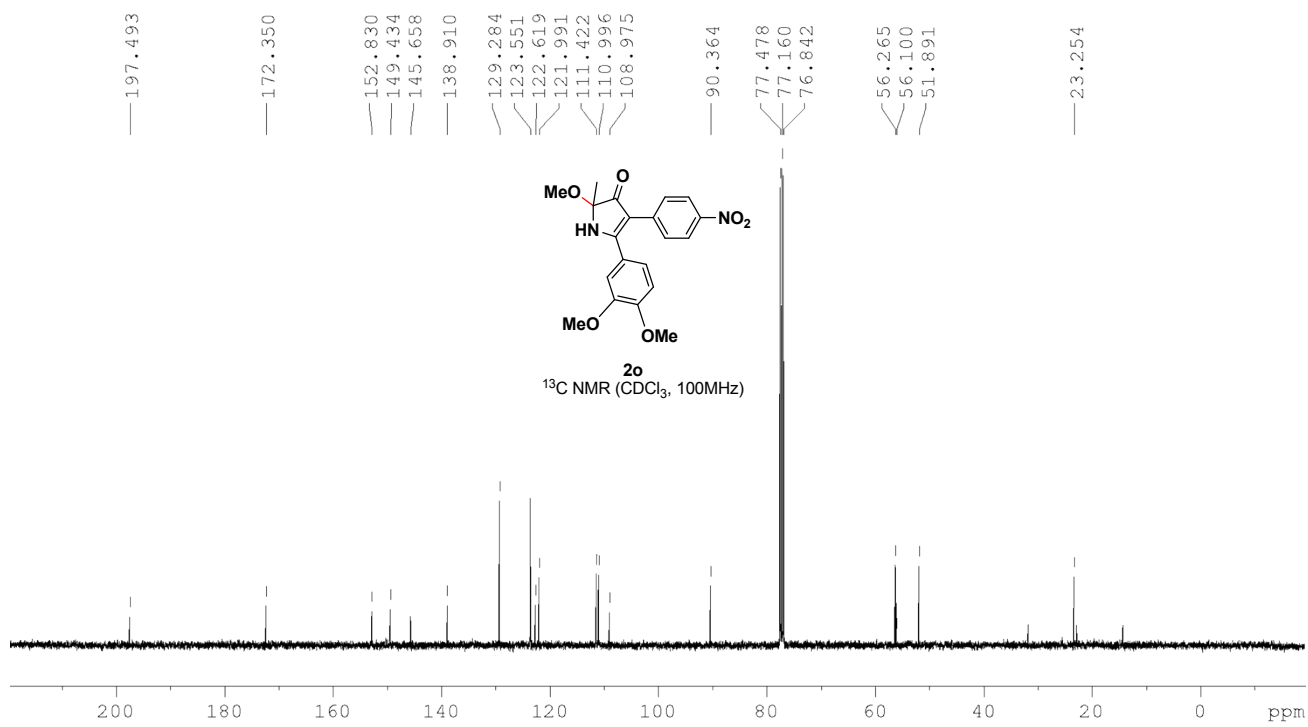


Figure 116: ¹³C NMR (100 MHz) spectrum of **2o**

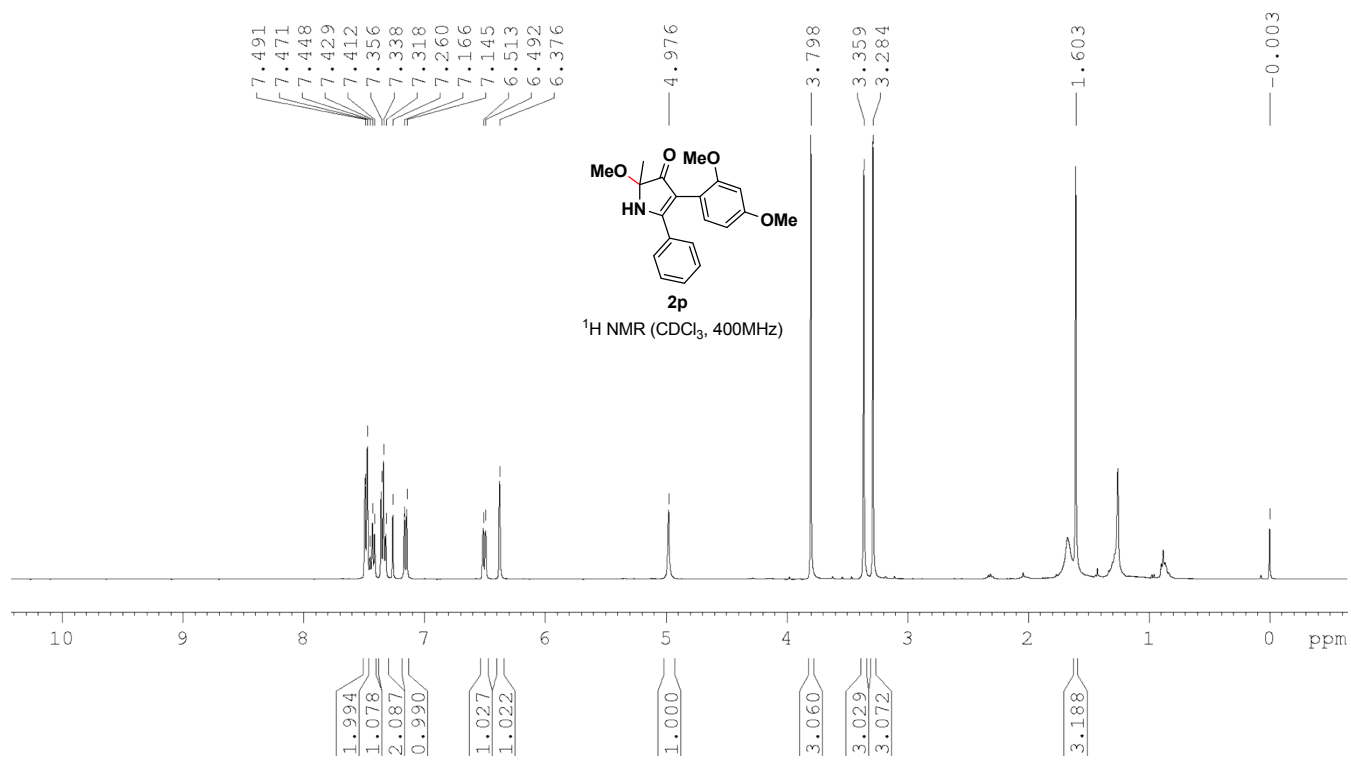


Figure 117: ¹H NMR (400 MHz) spectrum of **2p**

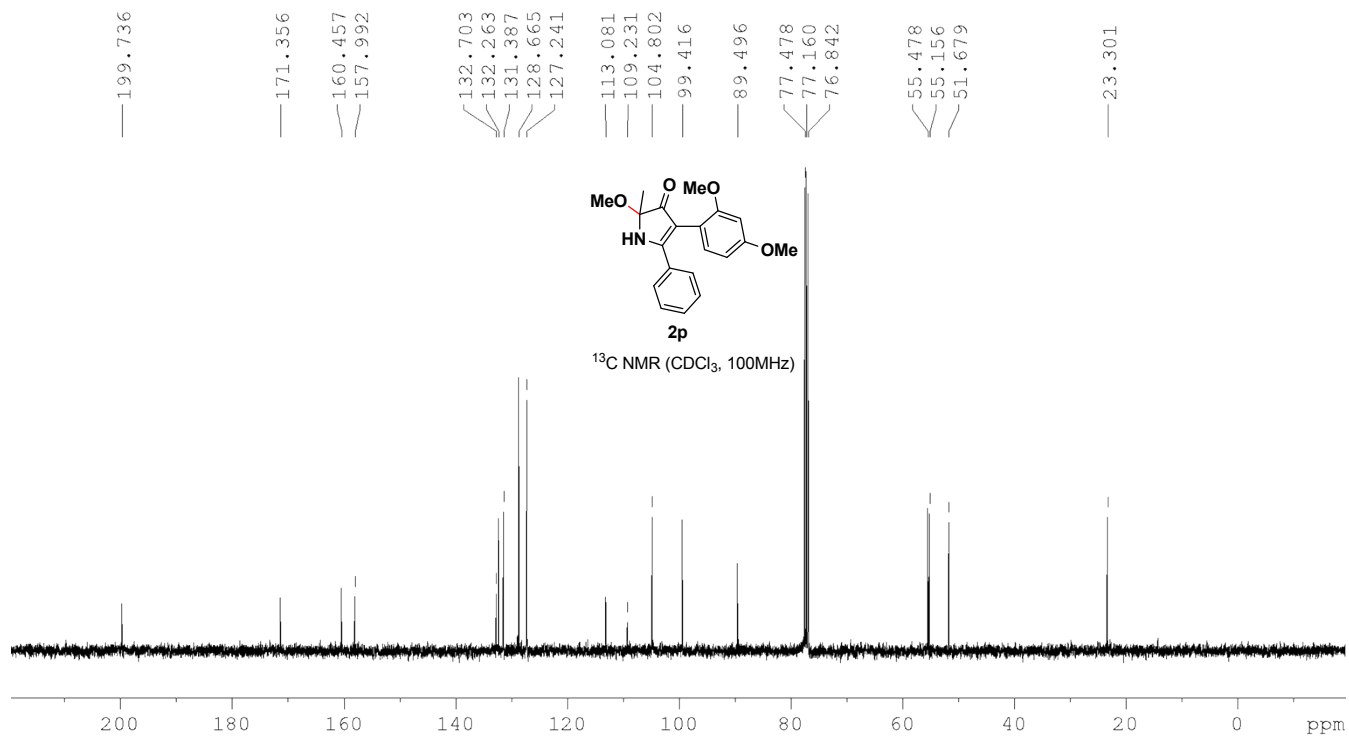


Figure 118: ¹³C NMR (100 MHz) spectrum of **2p**

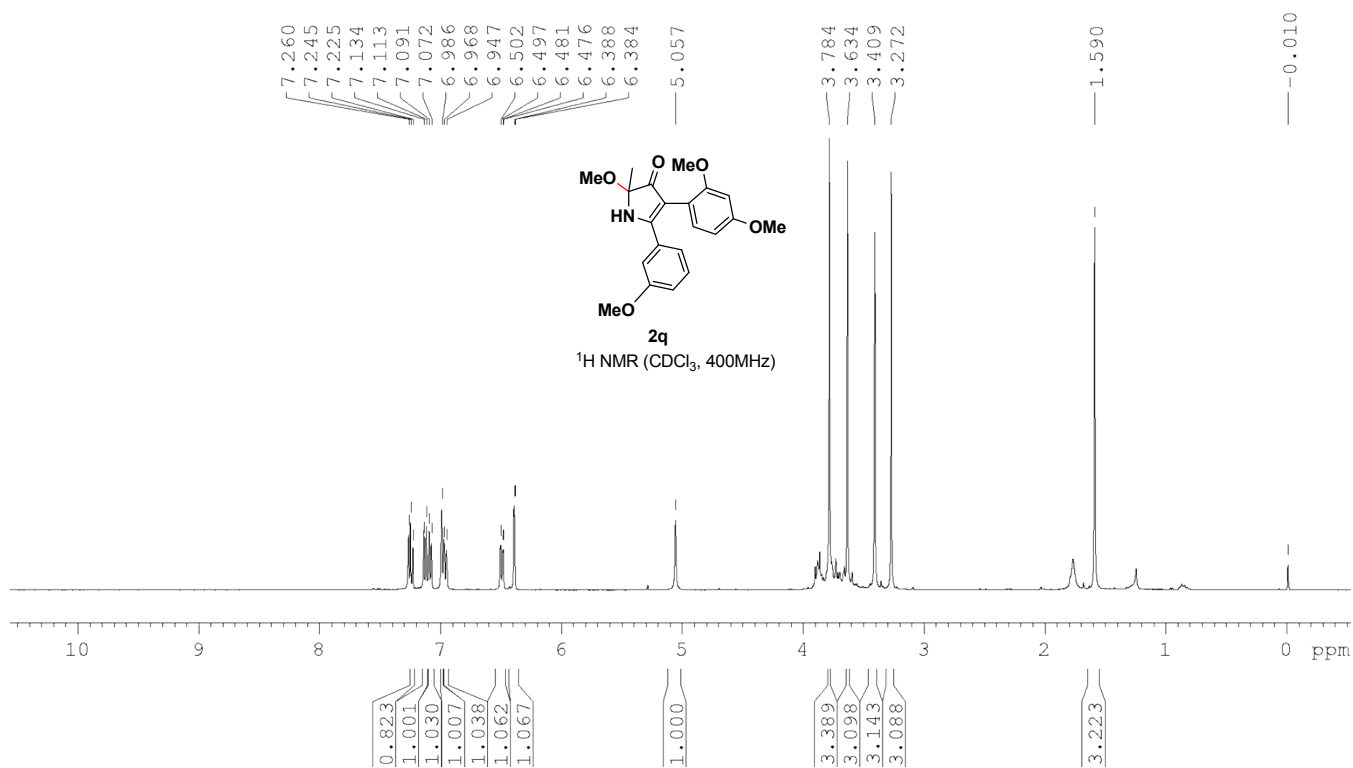


Figure 119: ¹H NMR (400 MHz) spectrum of **2q**

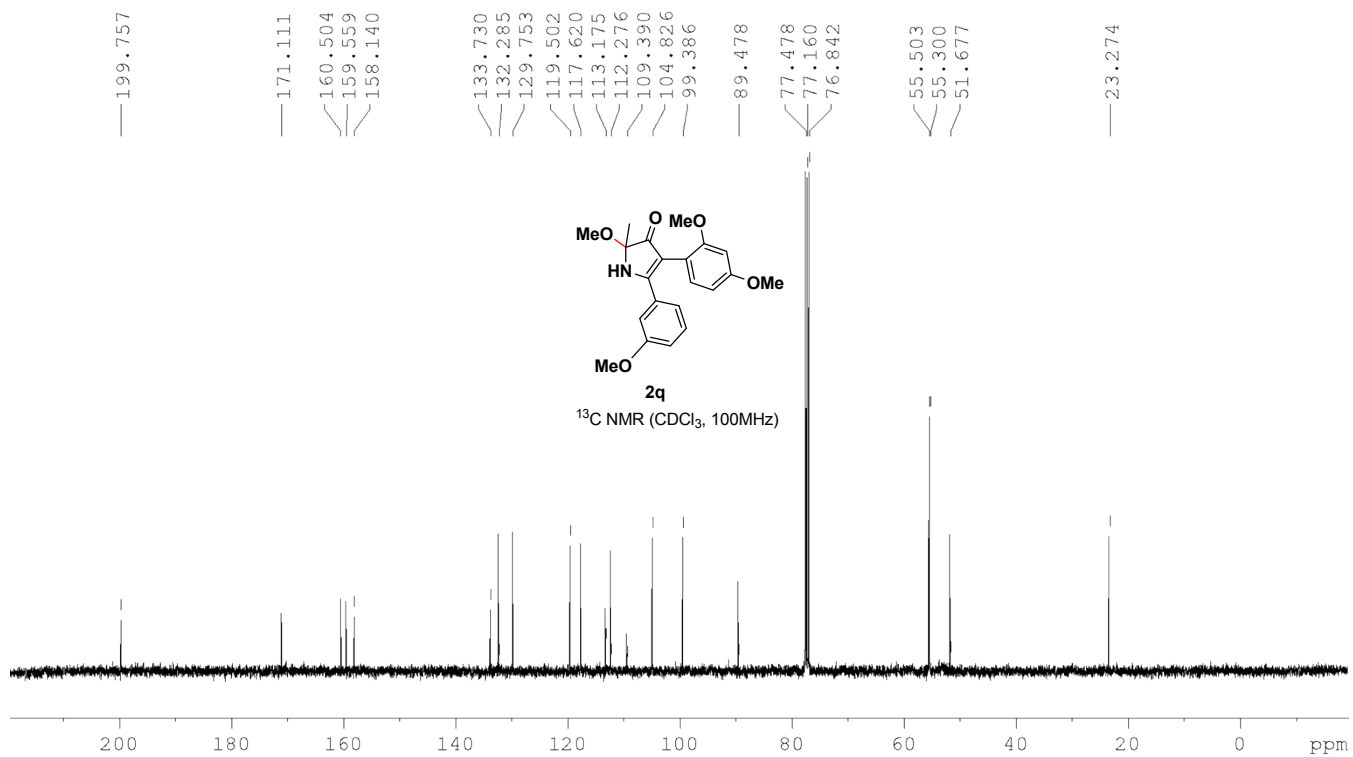


Figure 120: ¹³C NMR (100 MHz) spectrum of **2q**

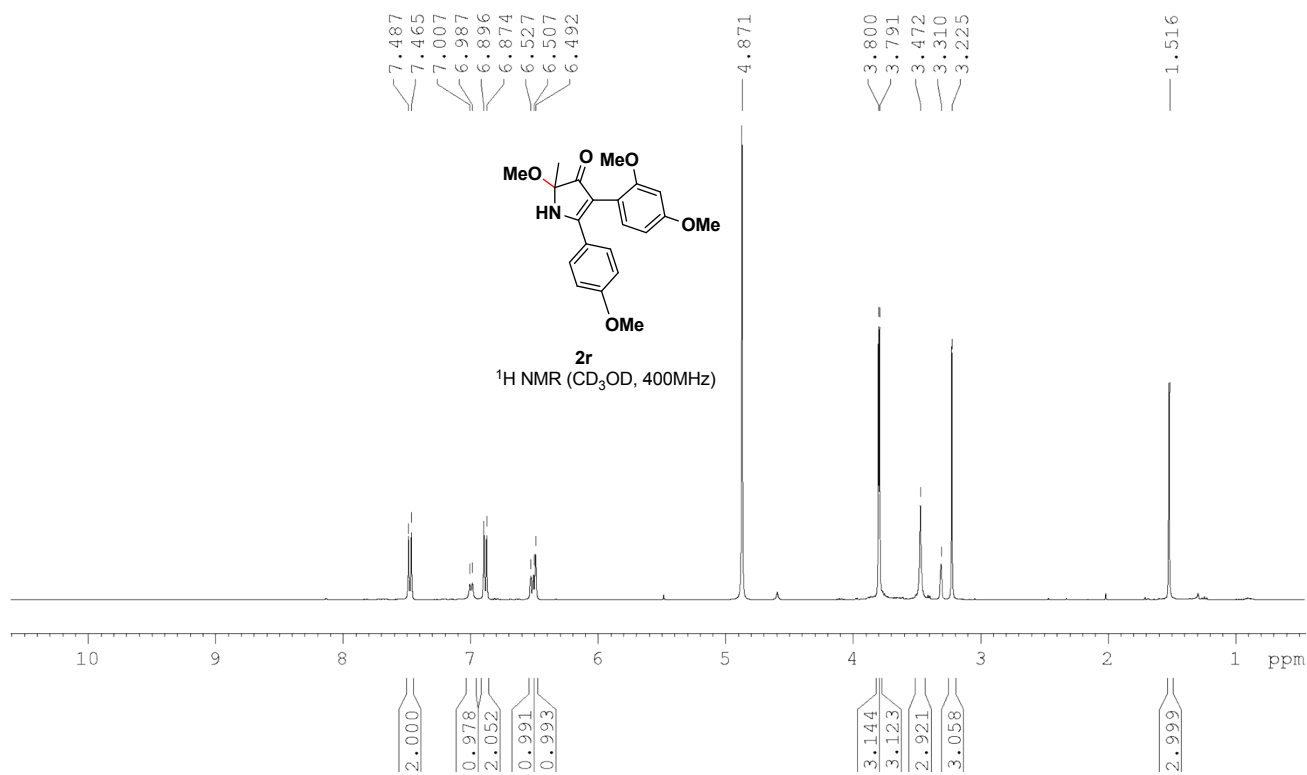


Figure 121: ¹H NMR (400 MHz) spectrum of **2r**

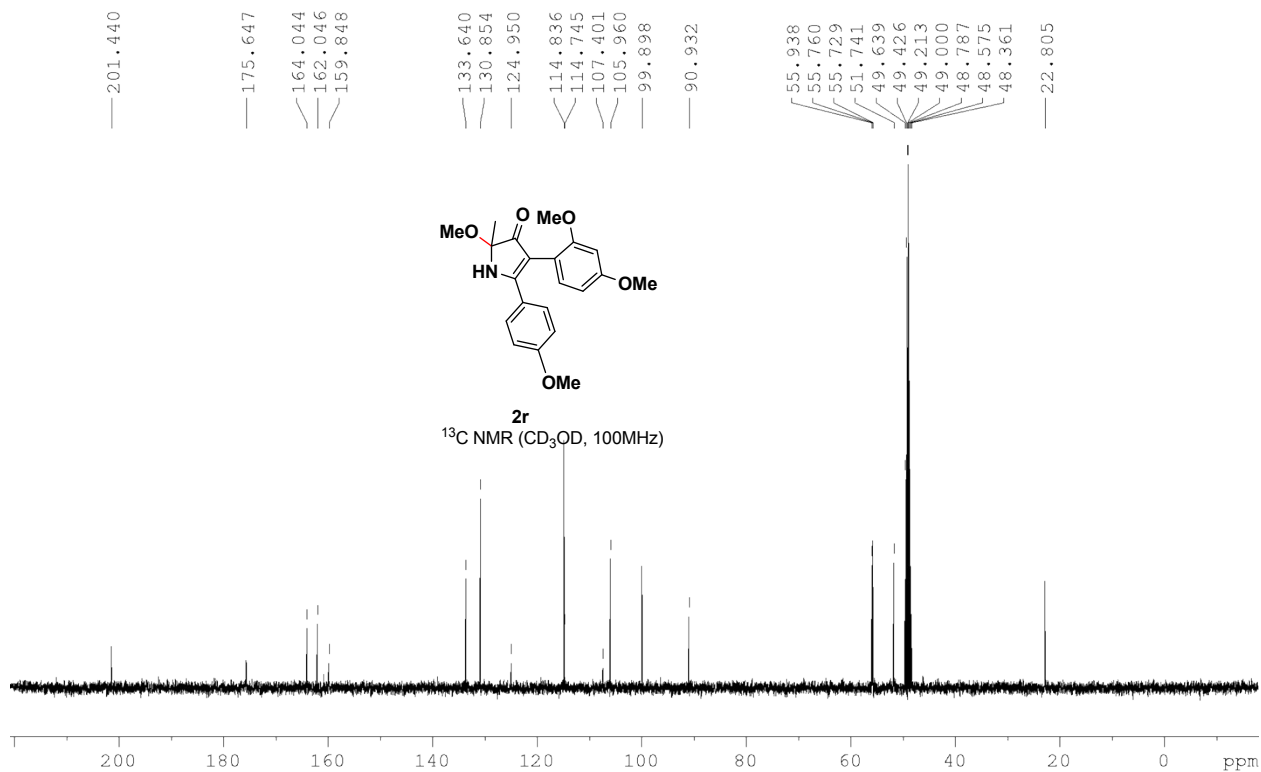


Figure 122: ¹³C NMR (100 MHz) spectrum of **2r**

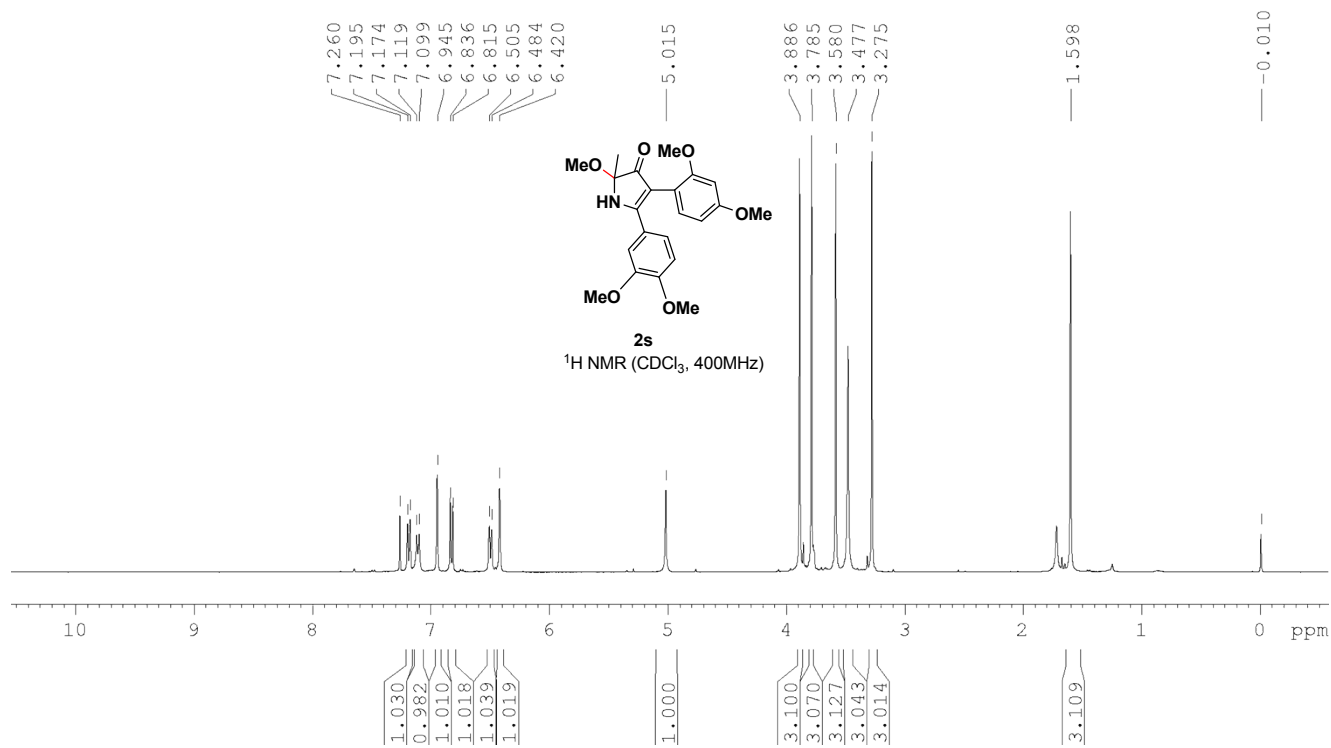


Figure 123: $^1\text{H NMR}$ (400 MHz) spectrum of **2s**

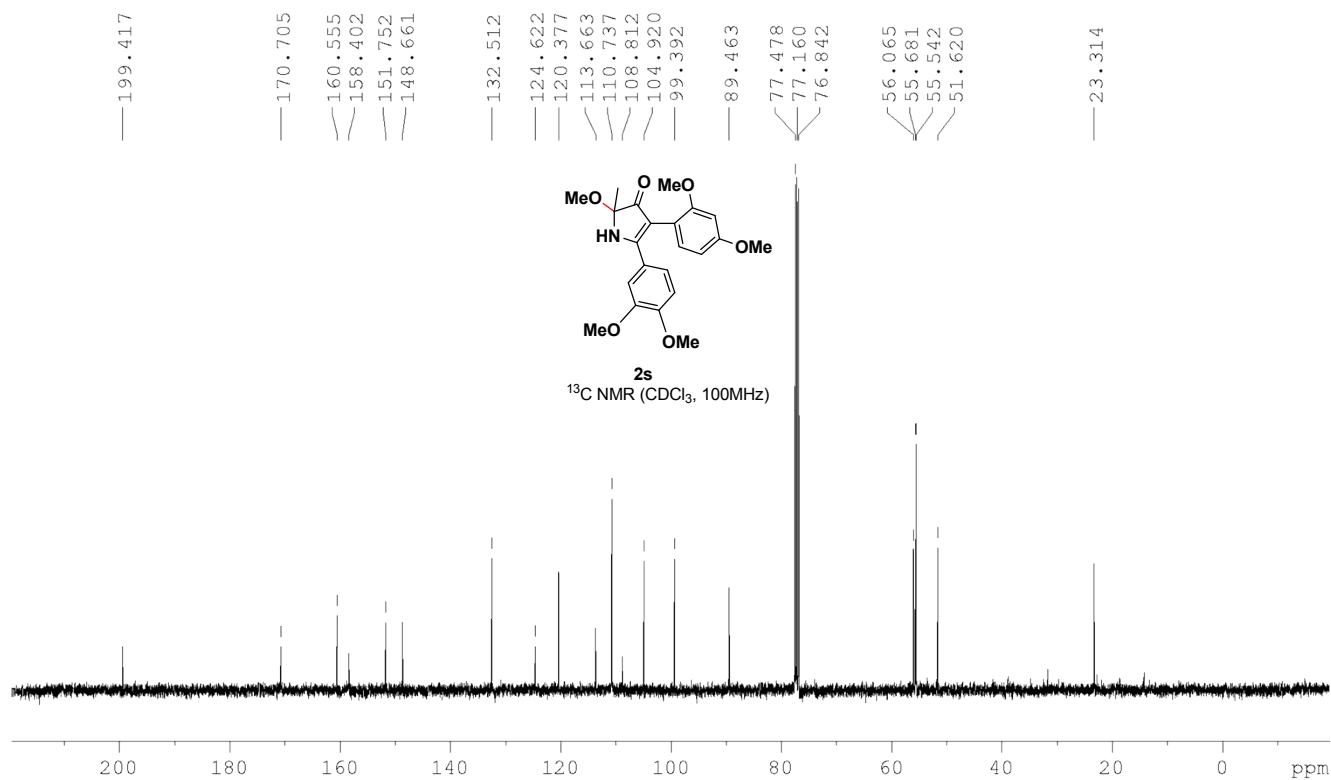


Figure 124: $^{13}\text{C NMR}$ (100 MHz) spectrum of **2s**

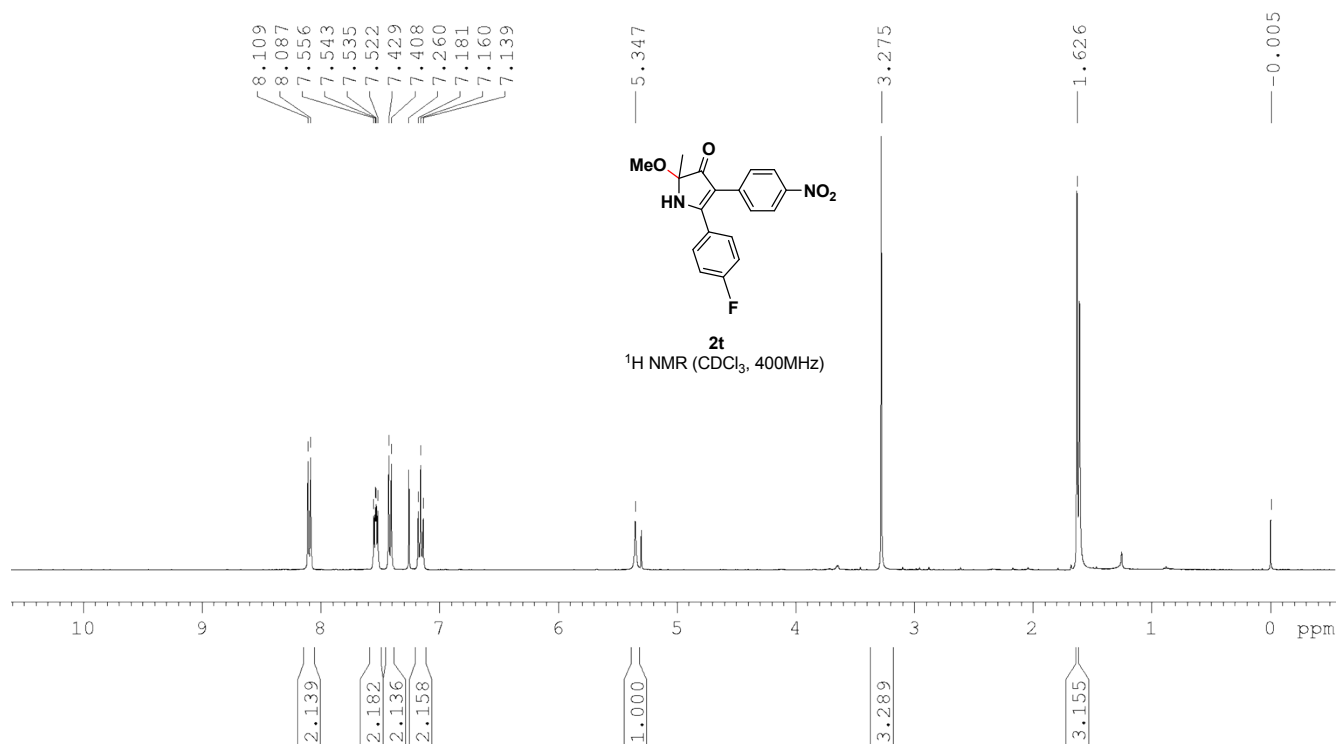


Figure 125: $^1\text{H NMR}$ (400 MHz) spectrum of **2t**

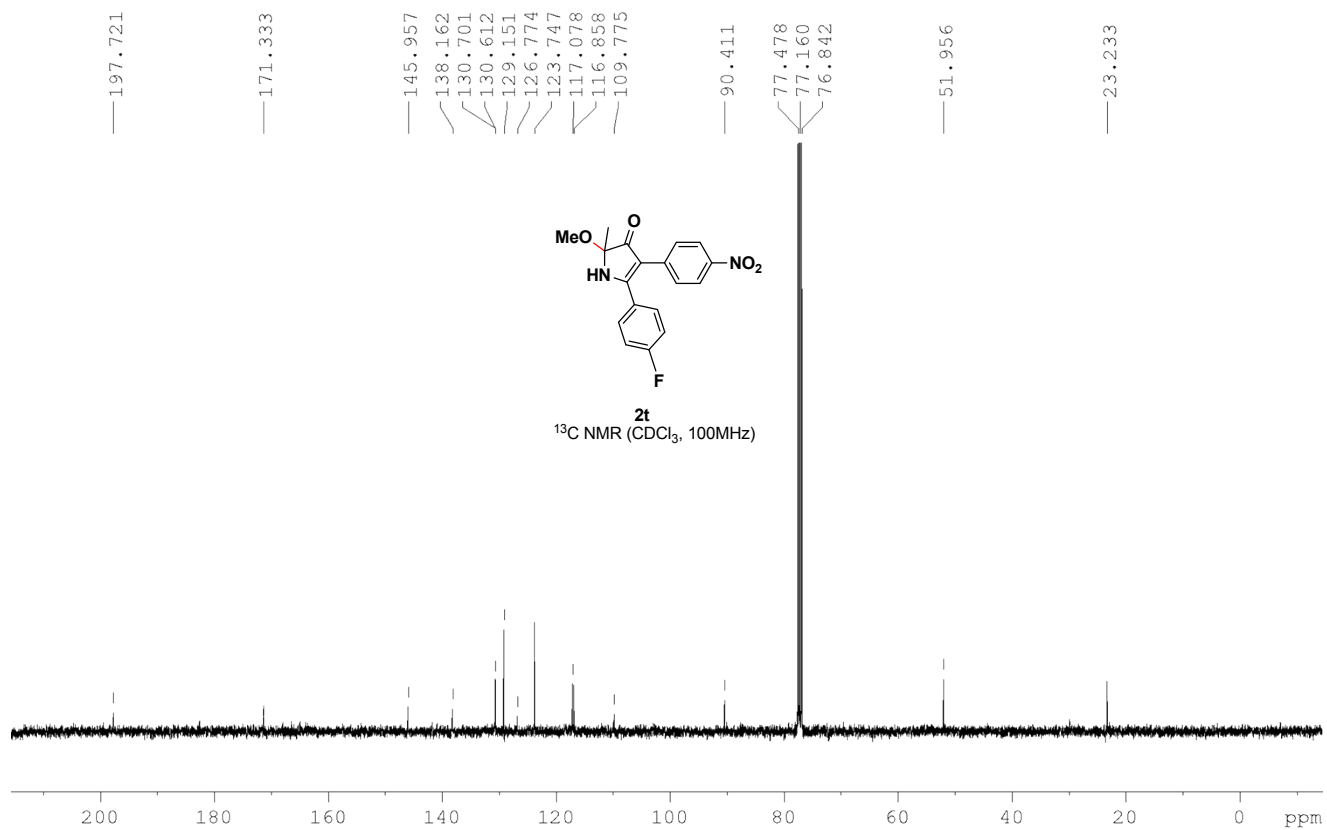


Figure 126: $^{13}\text{C NMR}$ (100 MHz) spectrum of **2t**

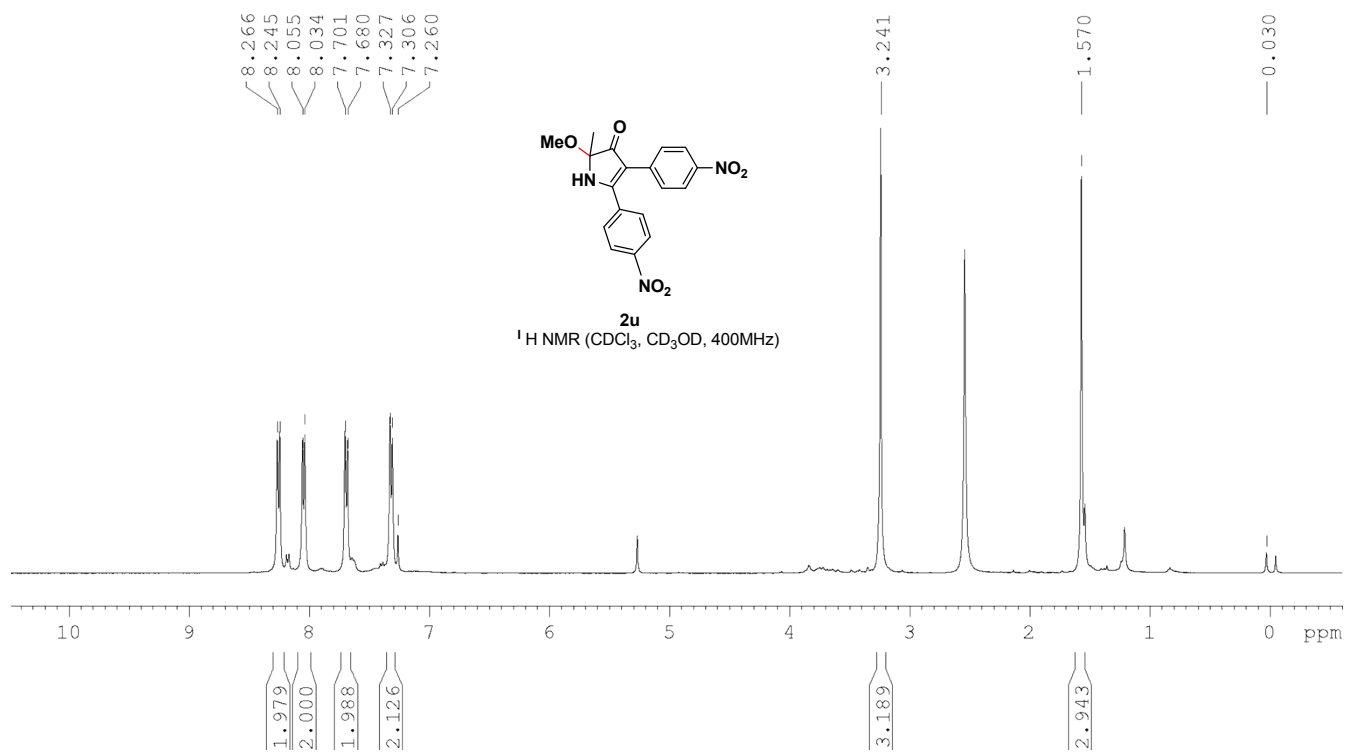


Figure 127: $^1\text{H NMR}$ (400 MHz) spectrum of **2u**

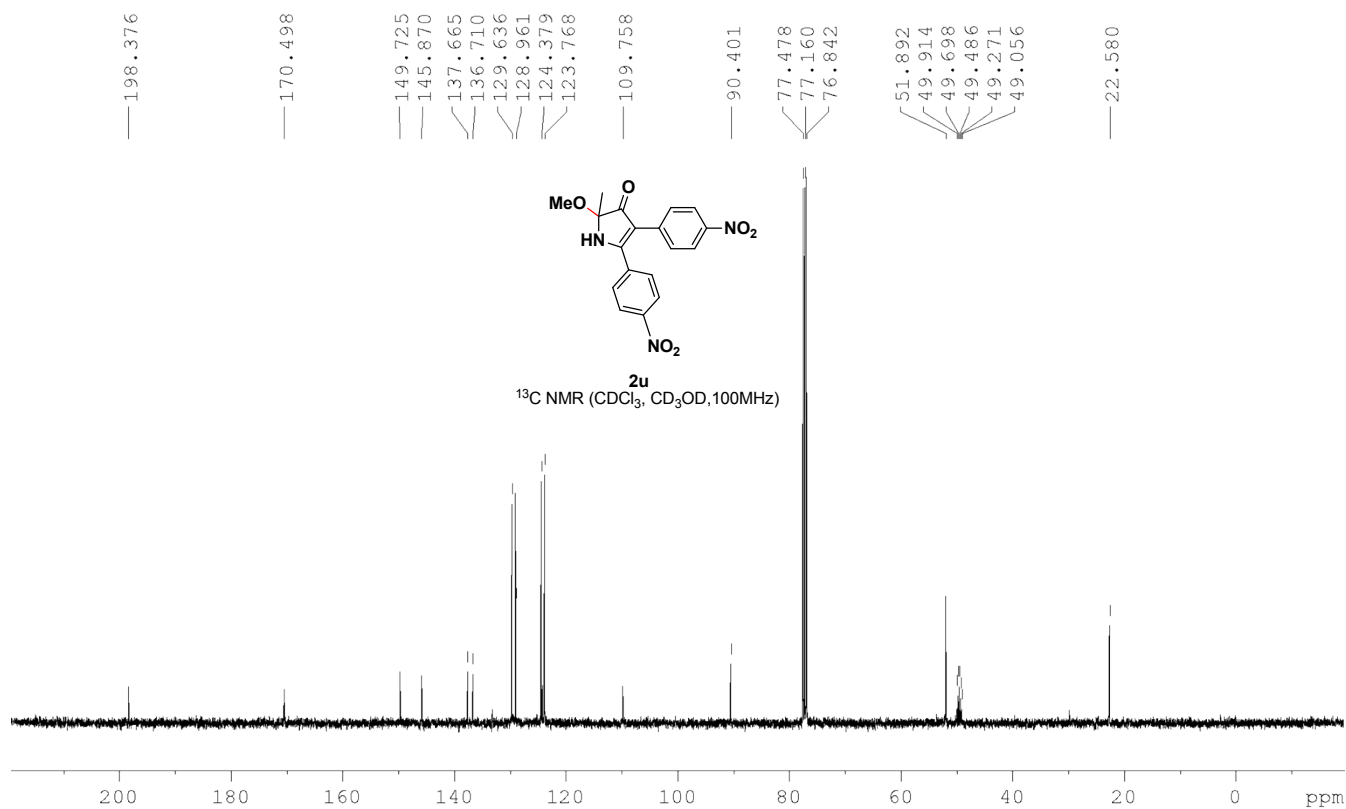


Figure 128: $^{13}\text{C NMR}$ (100 MHz) spectrum of **2u**

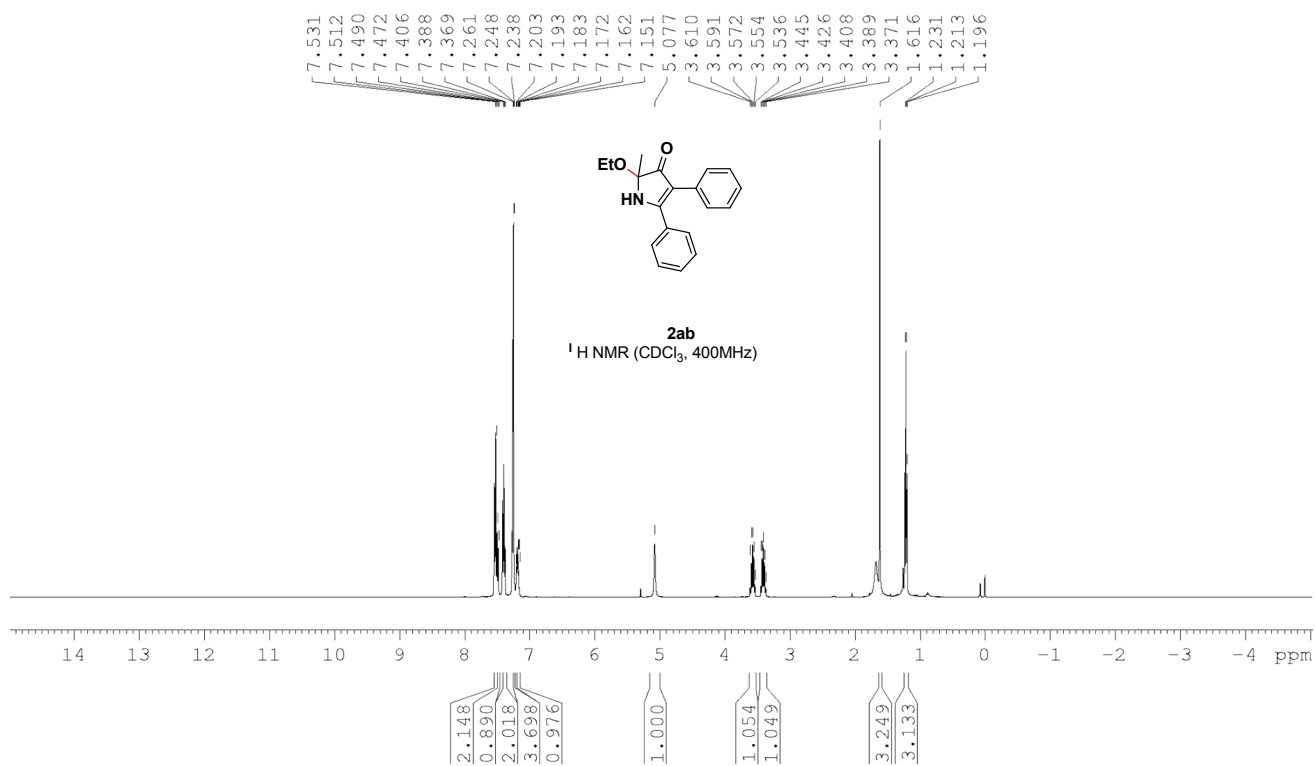


Figure 129: ¹H NMR (400 MHz) spectrum of **2ab**

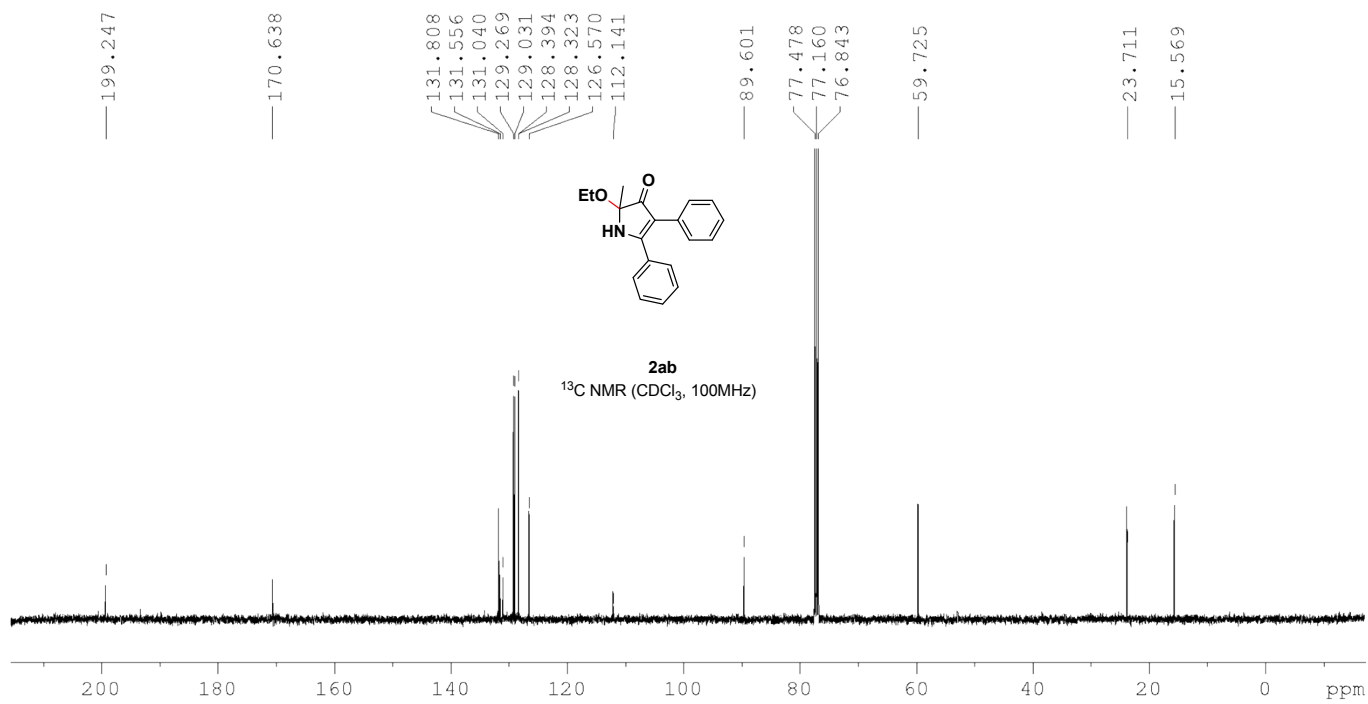


Figure 130: ¹³C NMR (100 MHz) spectrum of **2ab**

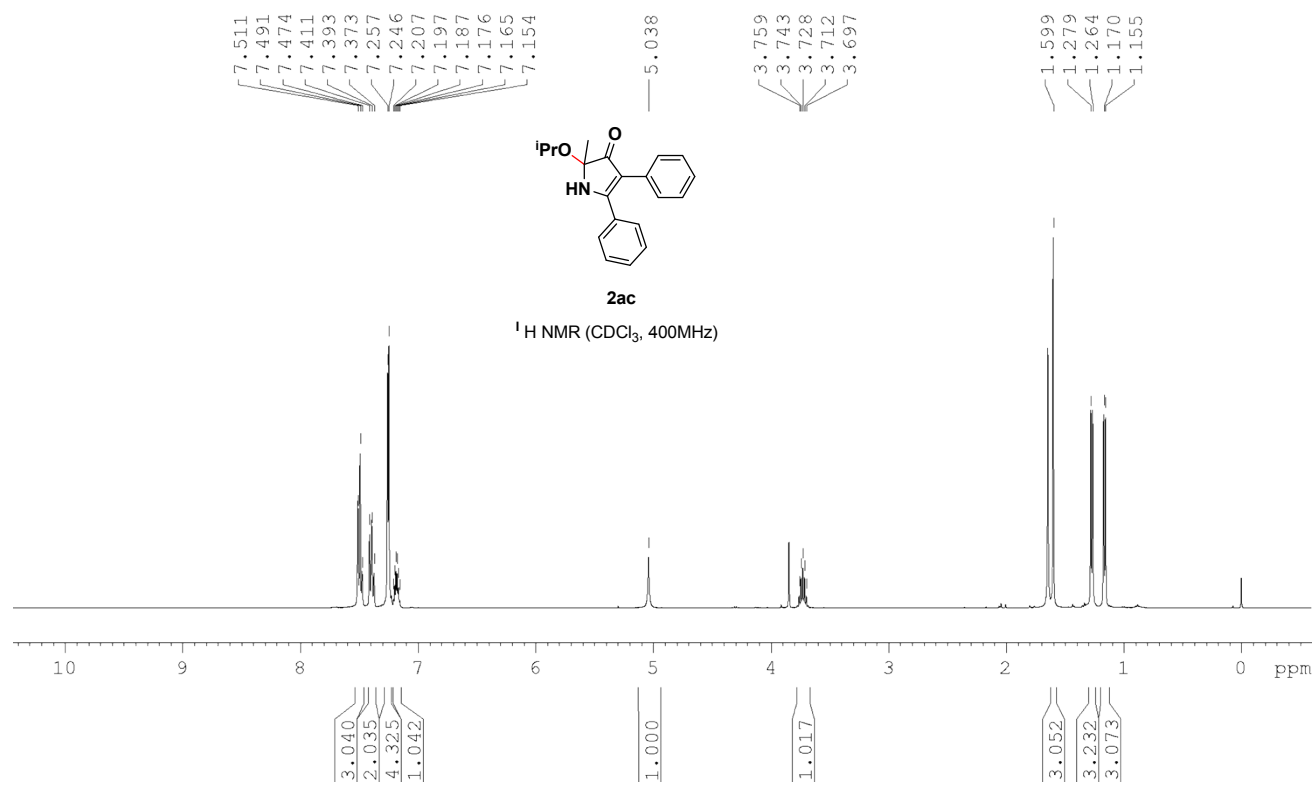


Figure 131: ¹H NMR (400 MHz) spectrum of **2ac**

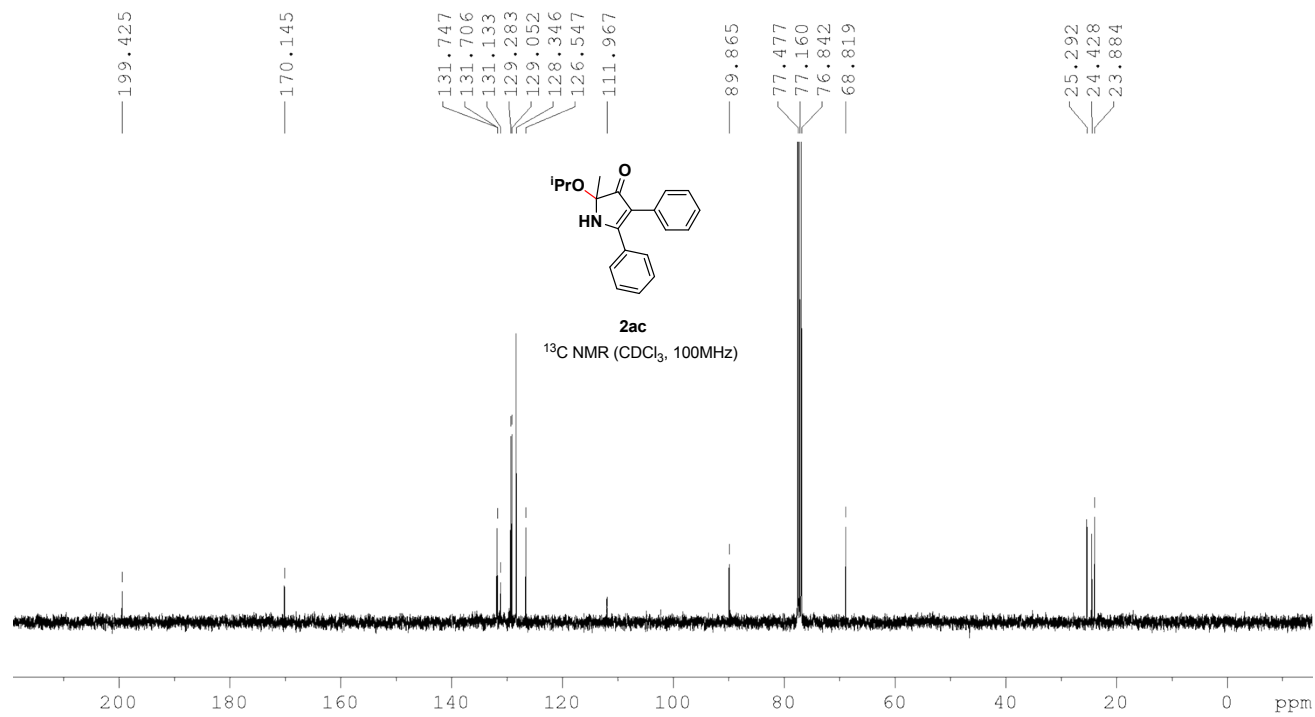


Figure 132: ¹³C NMR (100 MHz) spectrum of **2ac**

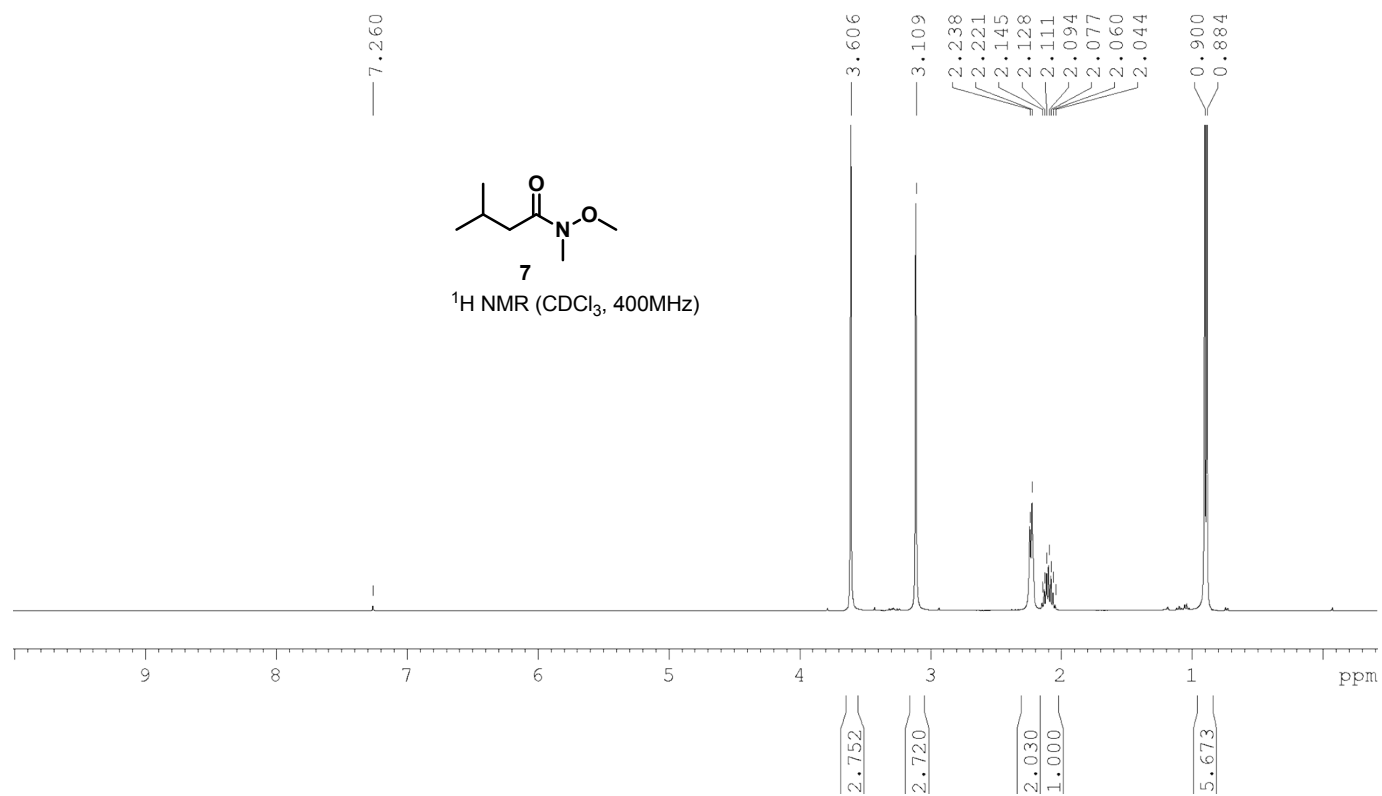


Figure 133: ¹H NMR (400 MHz) spectrum of **7**

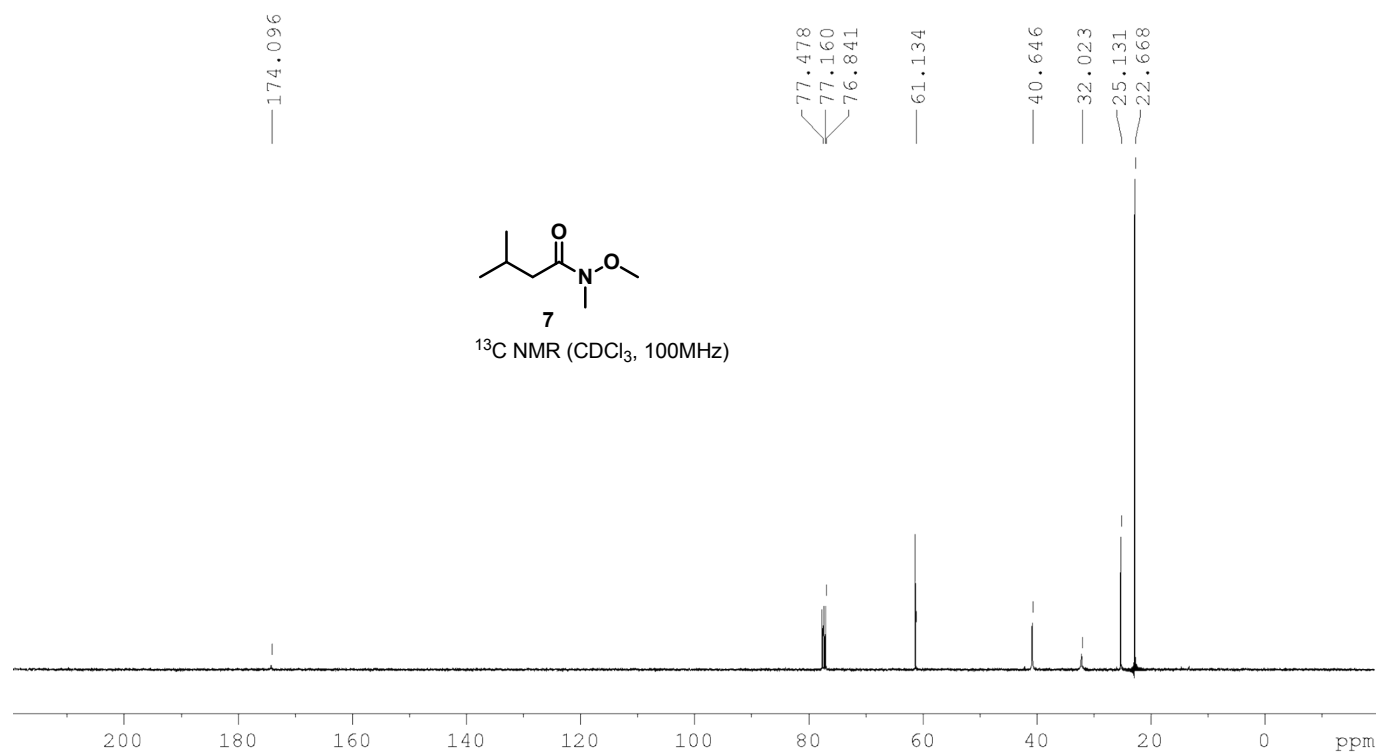


Figure 134: ¹³C NMR (100 MHz) spectrum of **7**

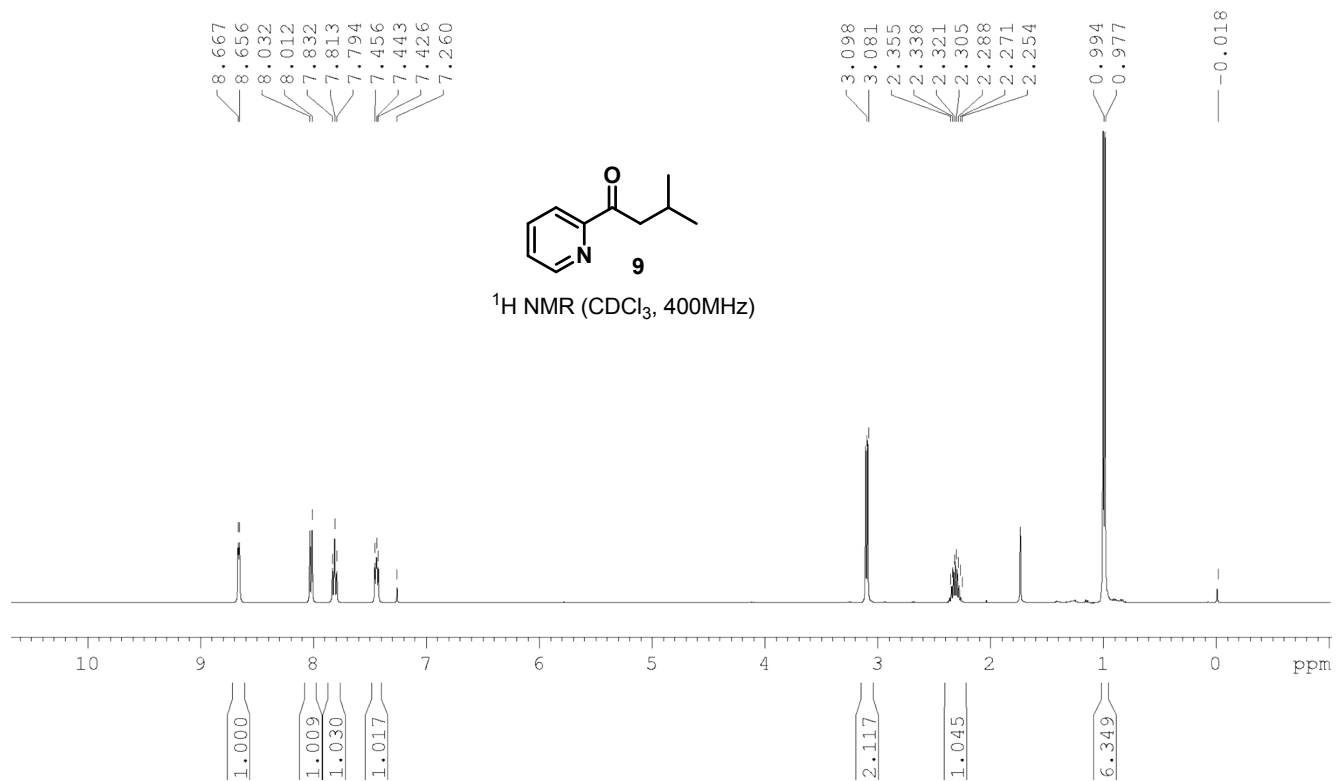


Figure 135: ¹H NMR (400 MHz) spectrum of 9

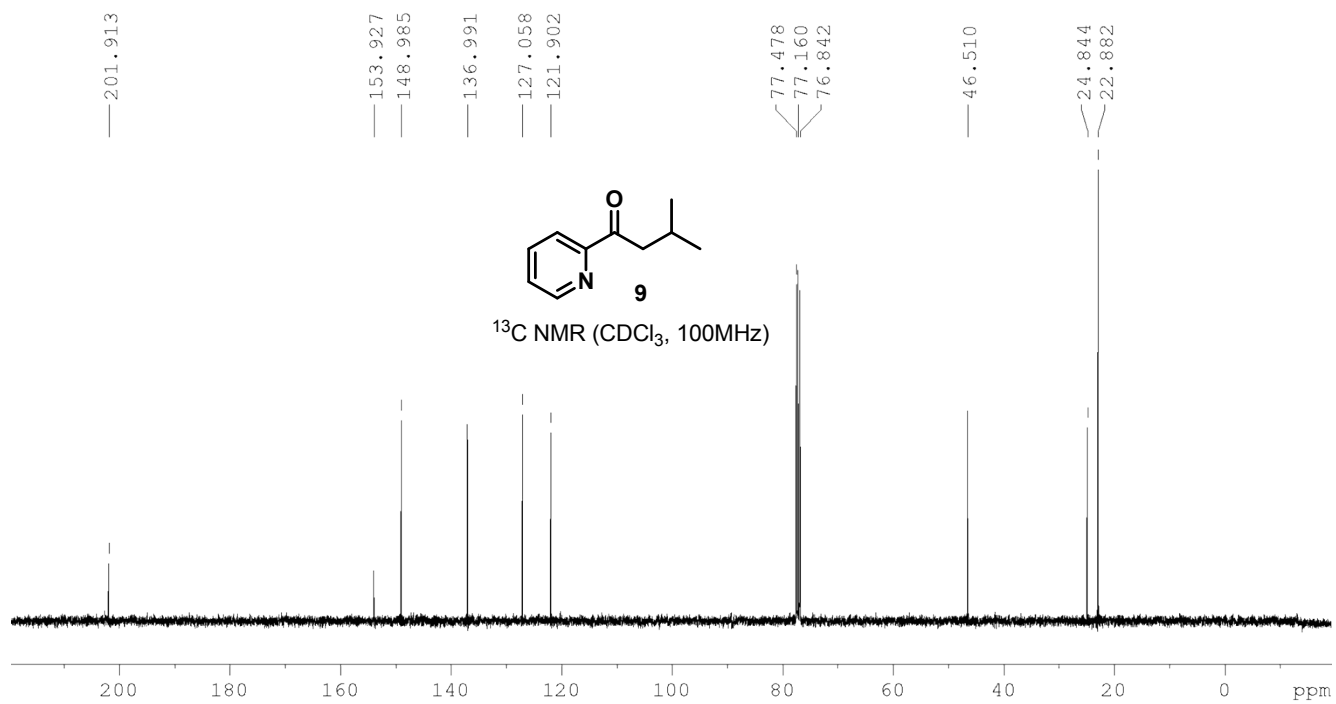


Figure 136: ¹³C NMR (100 MHz) spectrum of 9

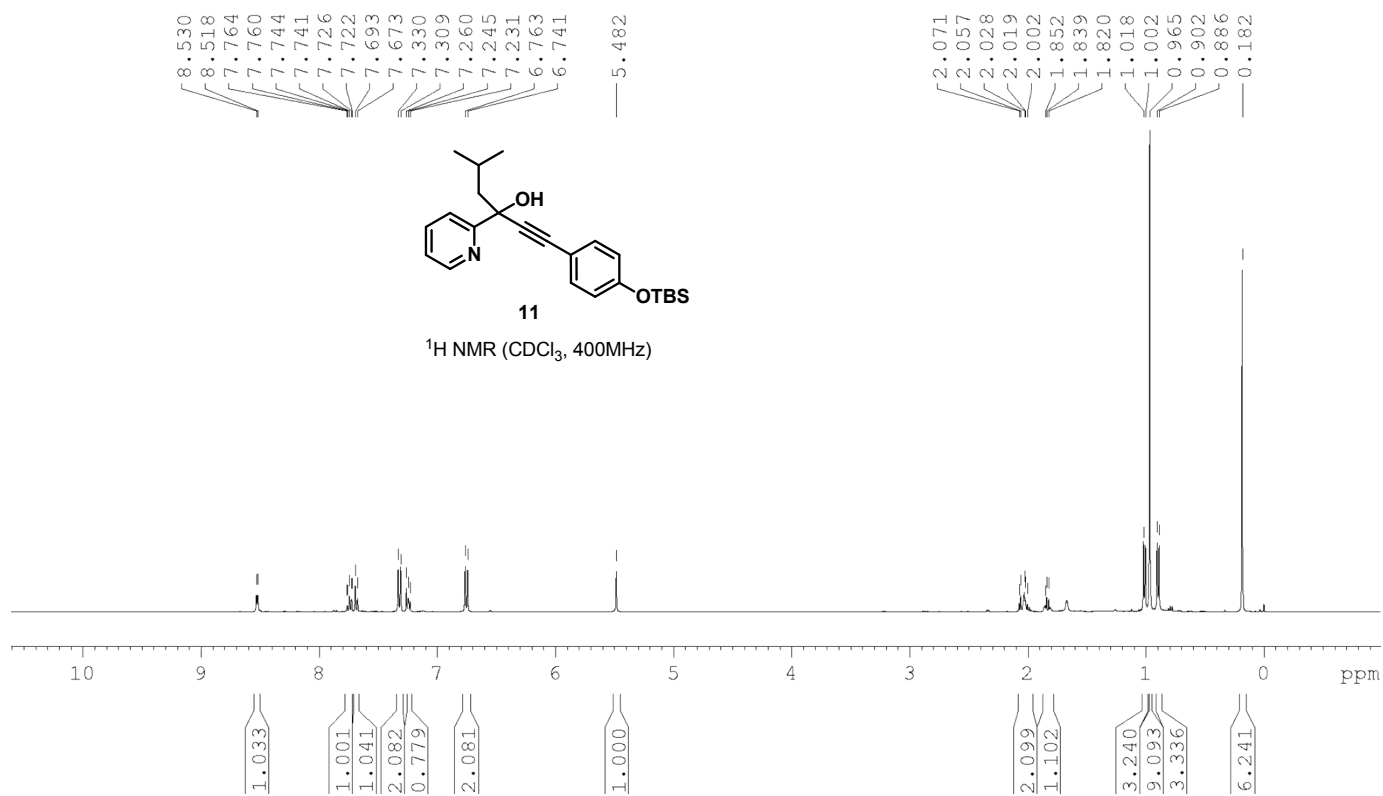


Figure 137: $^1\text{H NMR}$ (400 MHz) spectrum of **11**

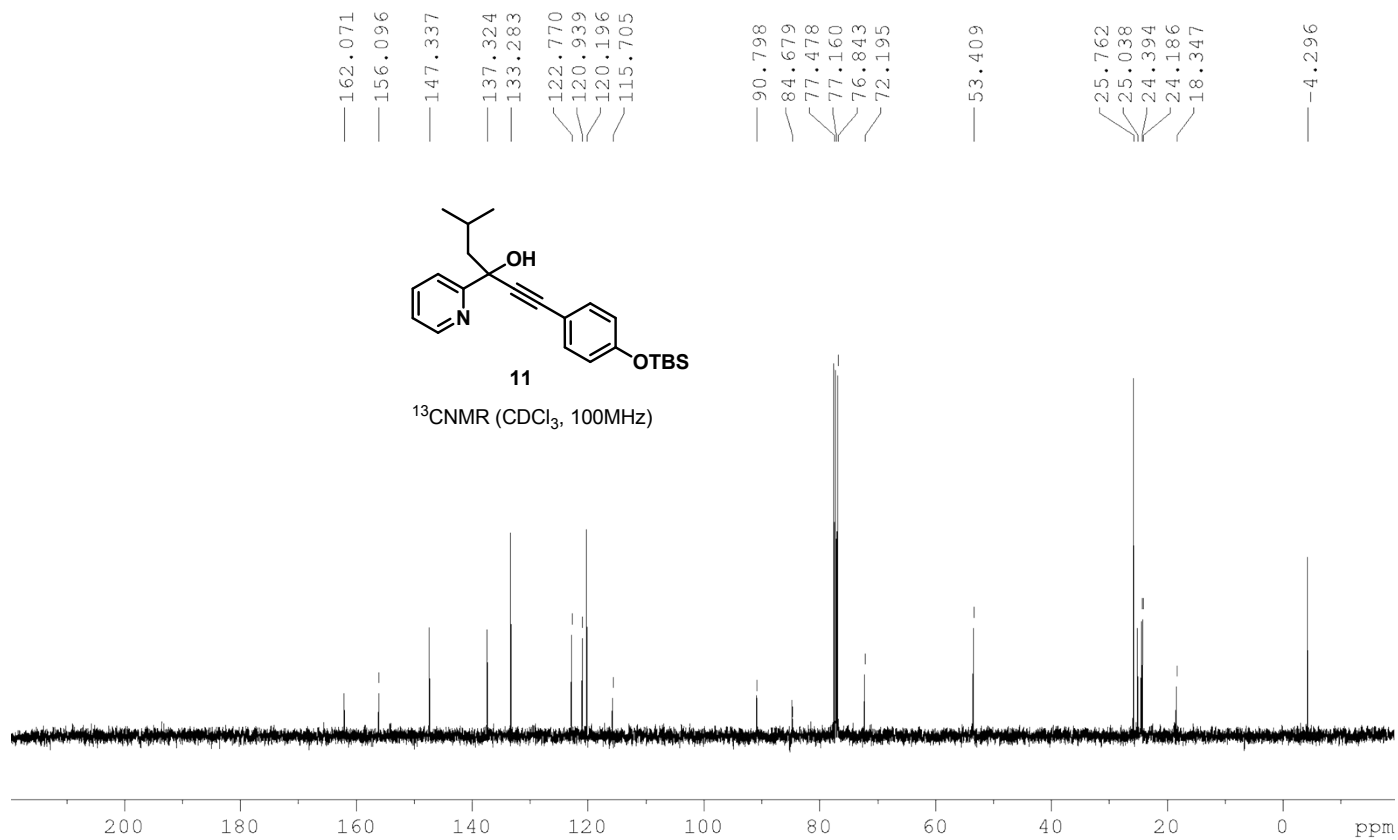


Figure 138: $^{13}\text{C NMR}$ (100 MHz) spectrum of **11**

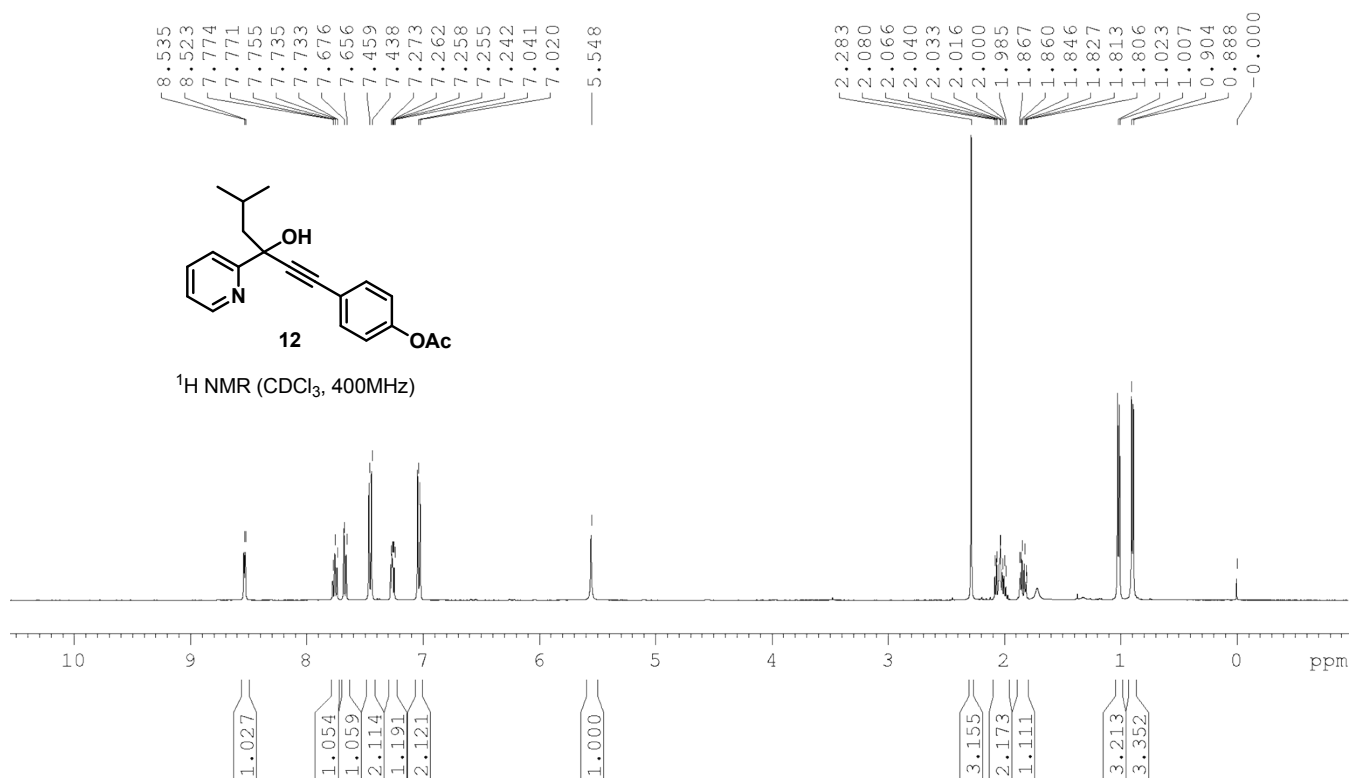


Figure 139: ^1H NMR (400 MHz) spectrum of **12**

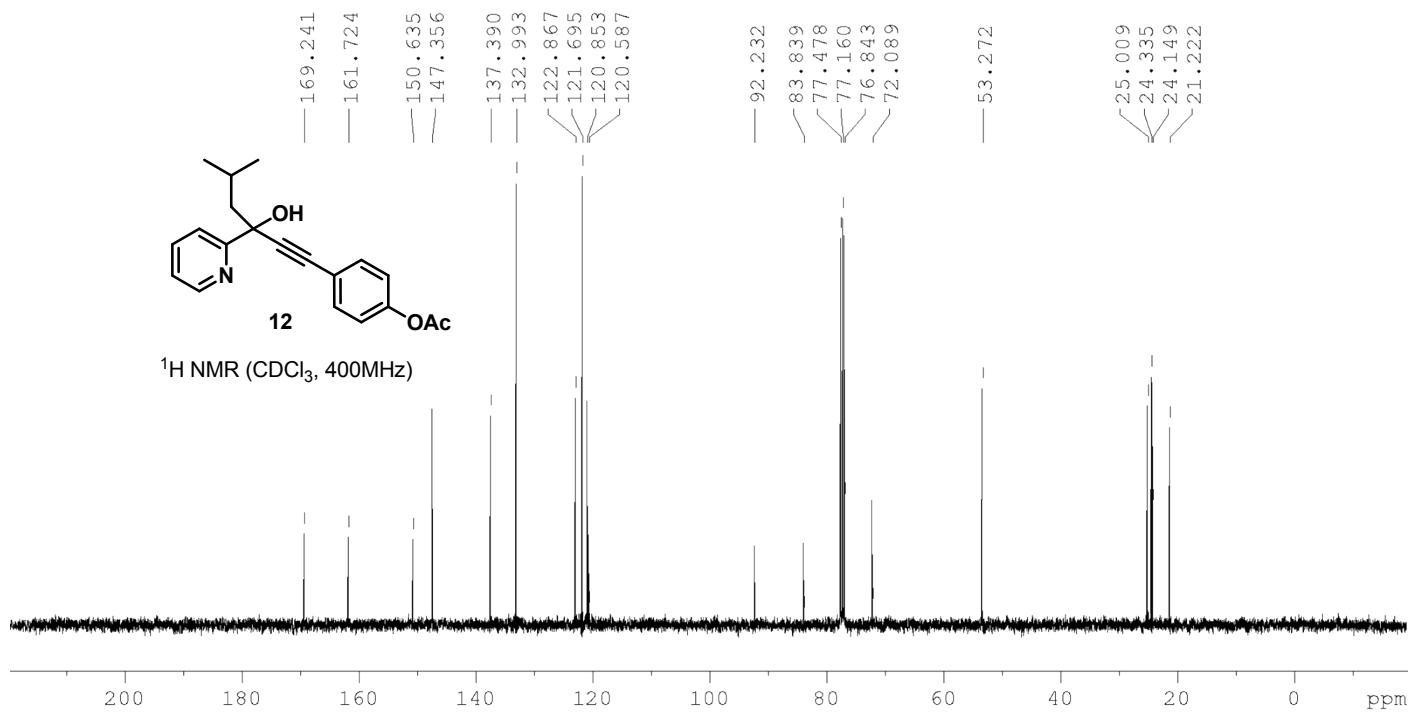


Figure 140: ^{13}C NMR (100 MHz) spectrum of **12**

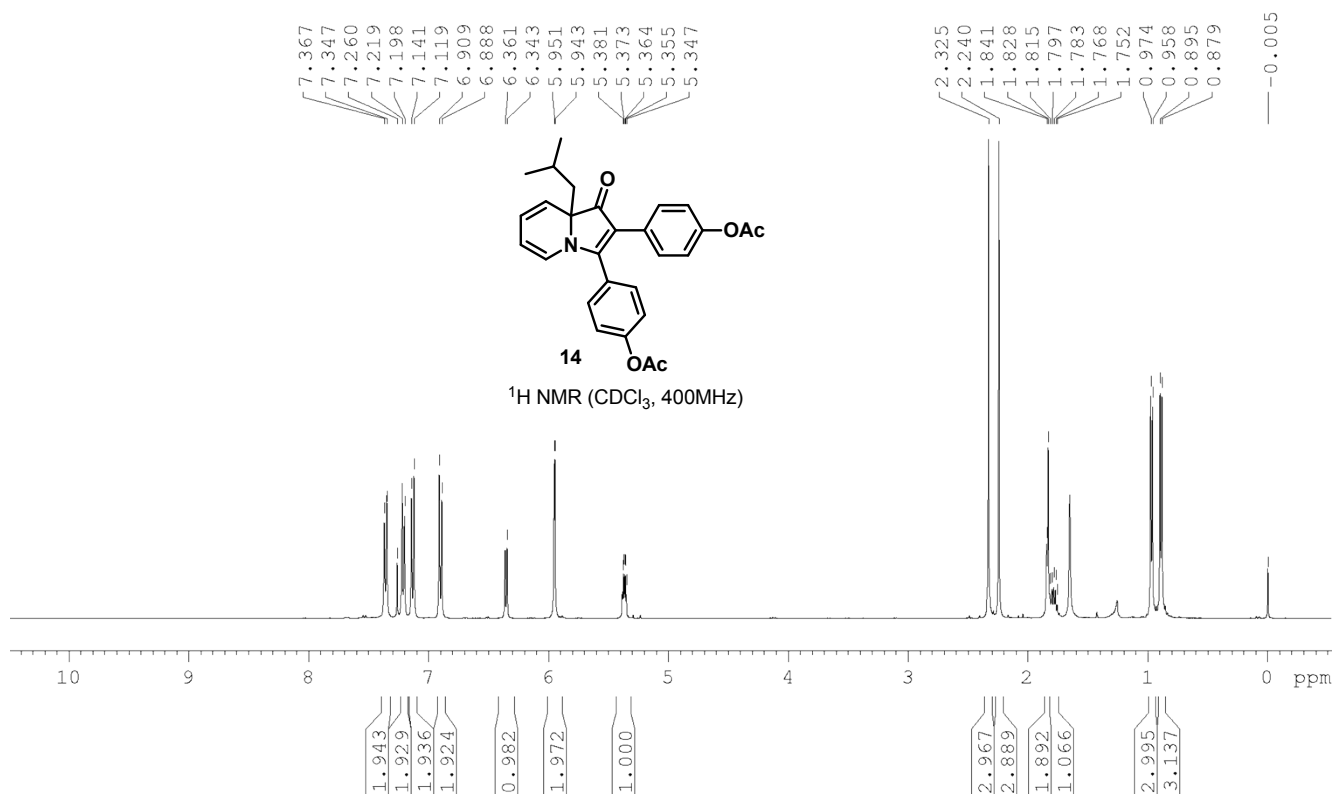


Figure 141: $^1\text{H NMR}$ (400 MHz) spectrum of **14**

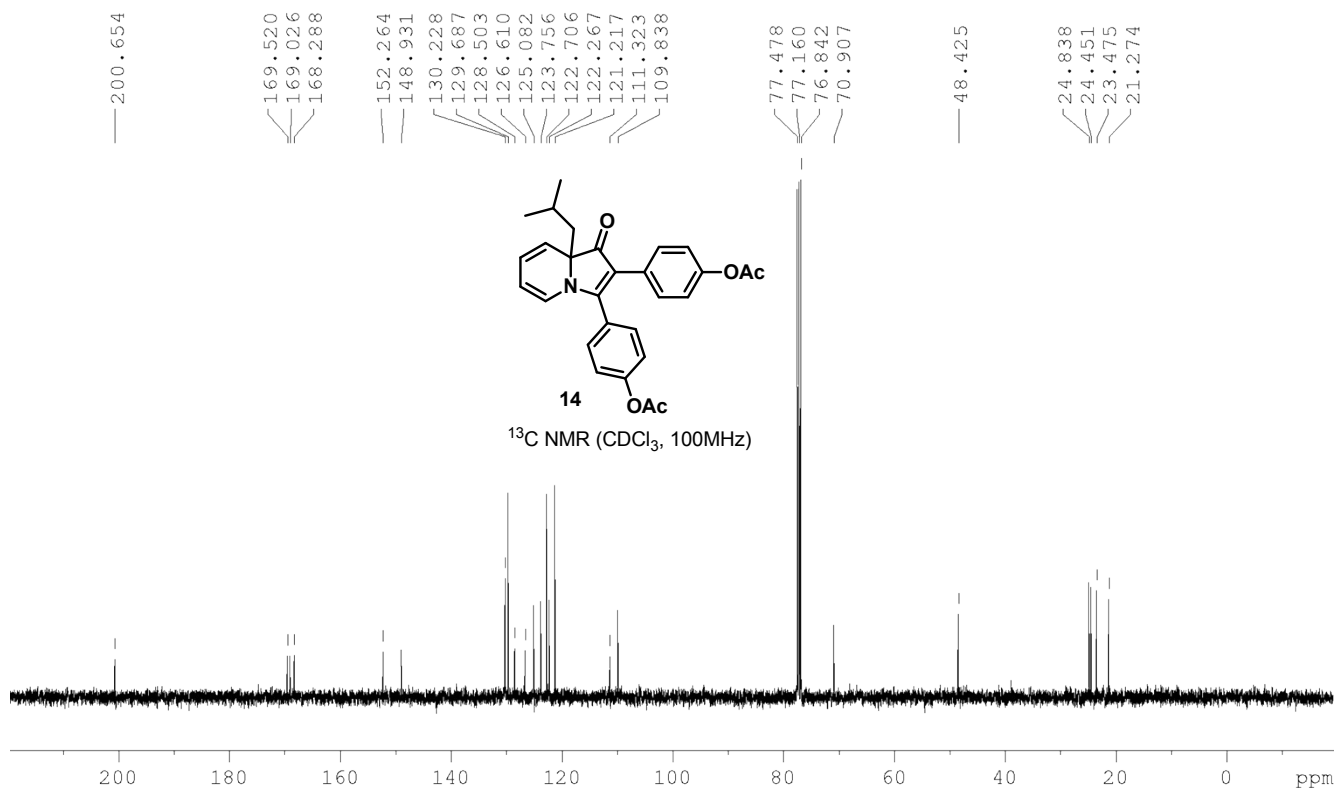


Figure 142: $^{13}\text{C NMR}$ (100 MHz) spectrum of **14**

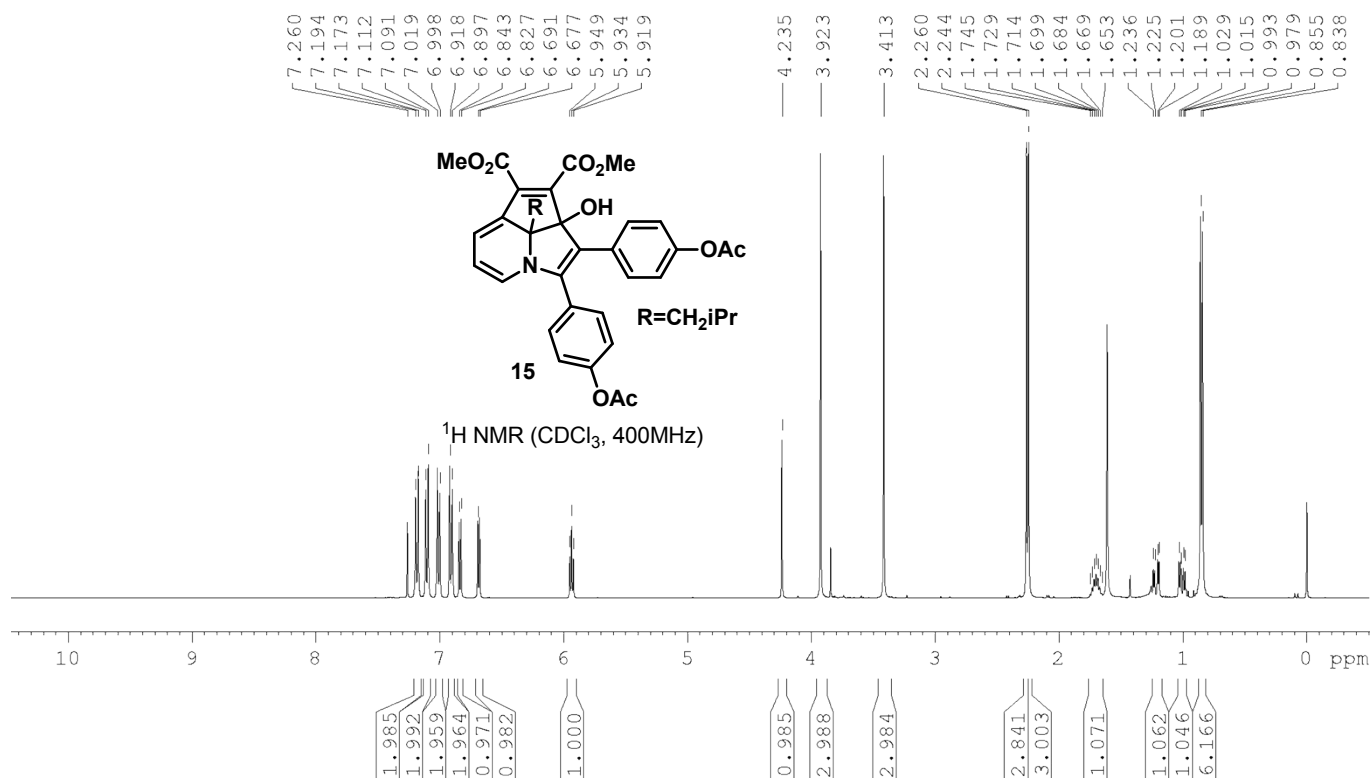


Figure 143: ¹H NMR (400 MHz) spectrum of **15**

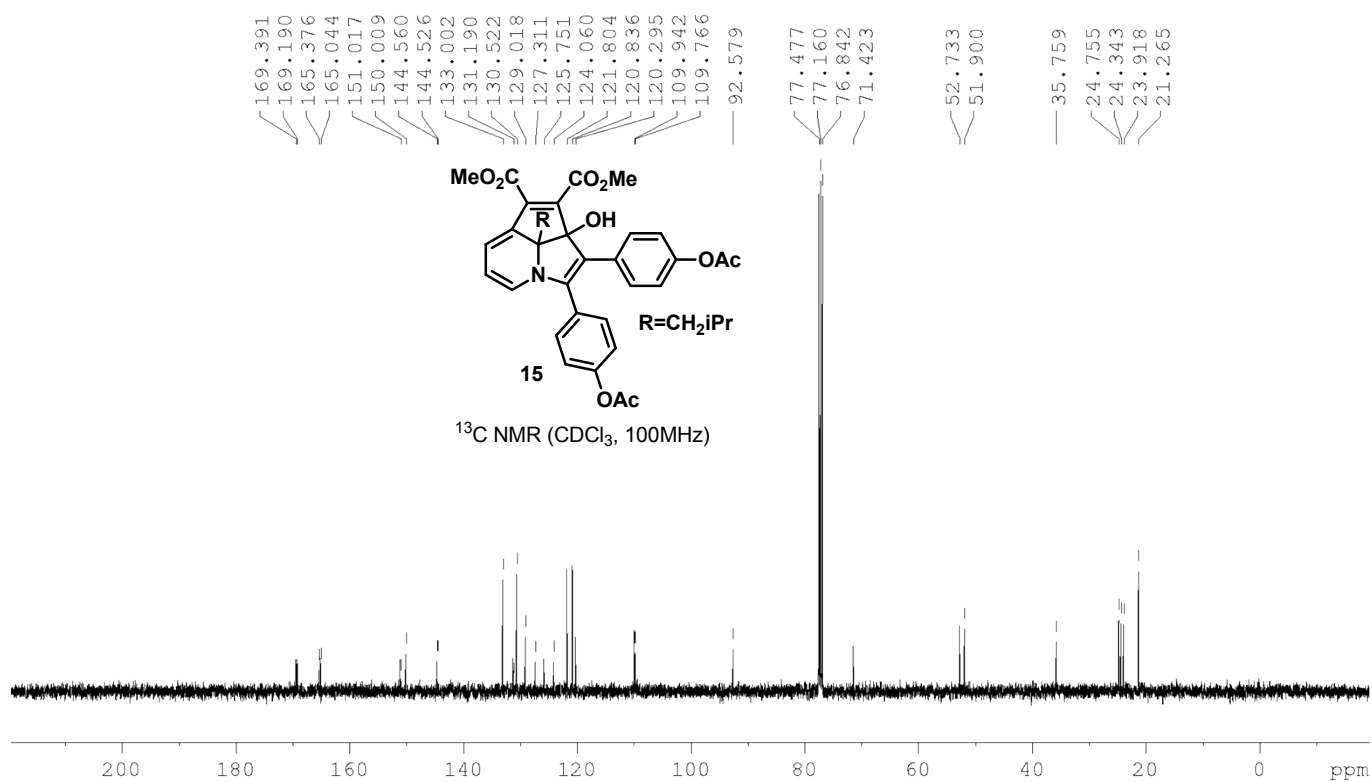


Figure 144: ¹³C NMR (100 MHz) spectrum of **15**

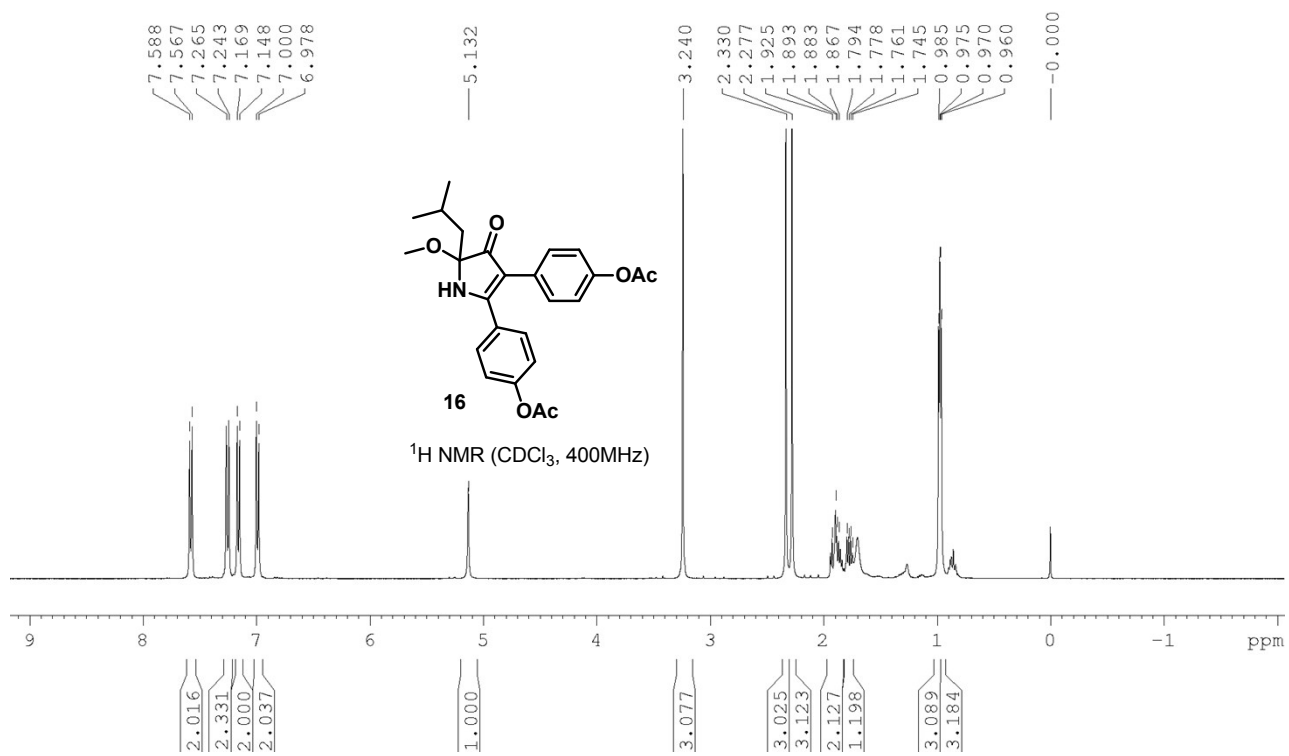


Figure 145: ¹H NMR (400 MHz) spectrum of **16**

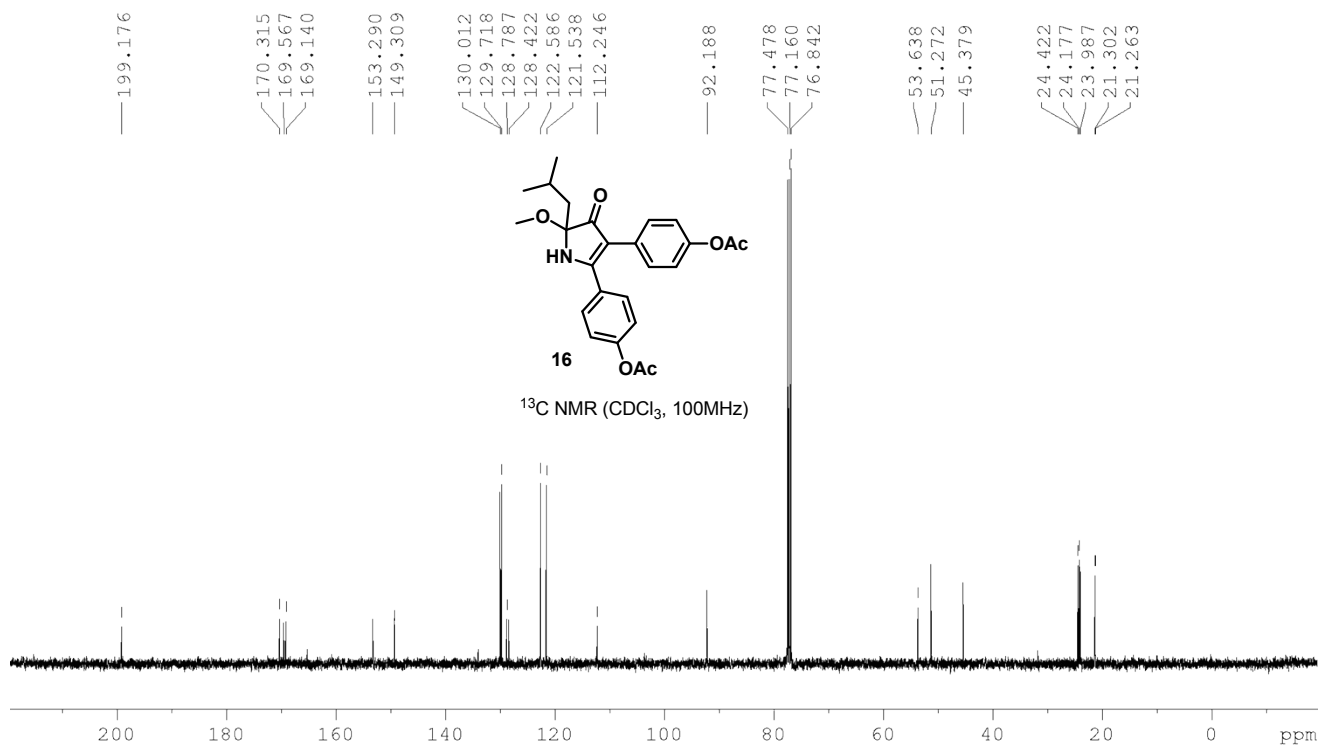


Figure 146: ¹³C NMR (100 MHz) spectrum of **16**

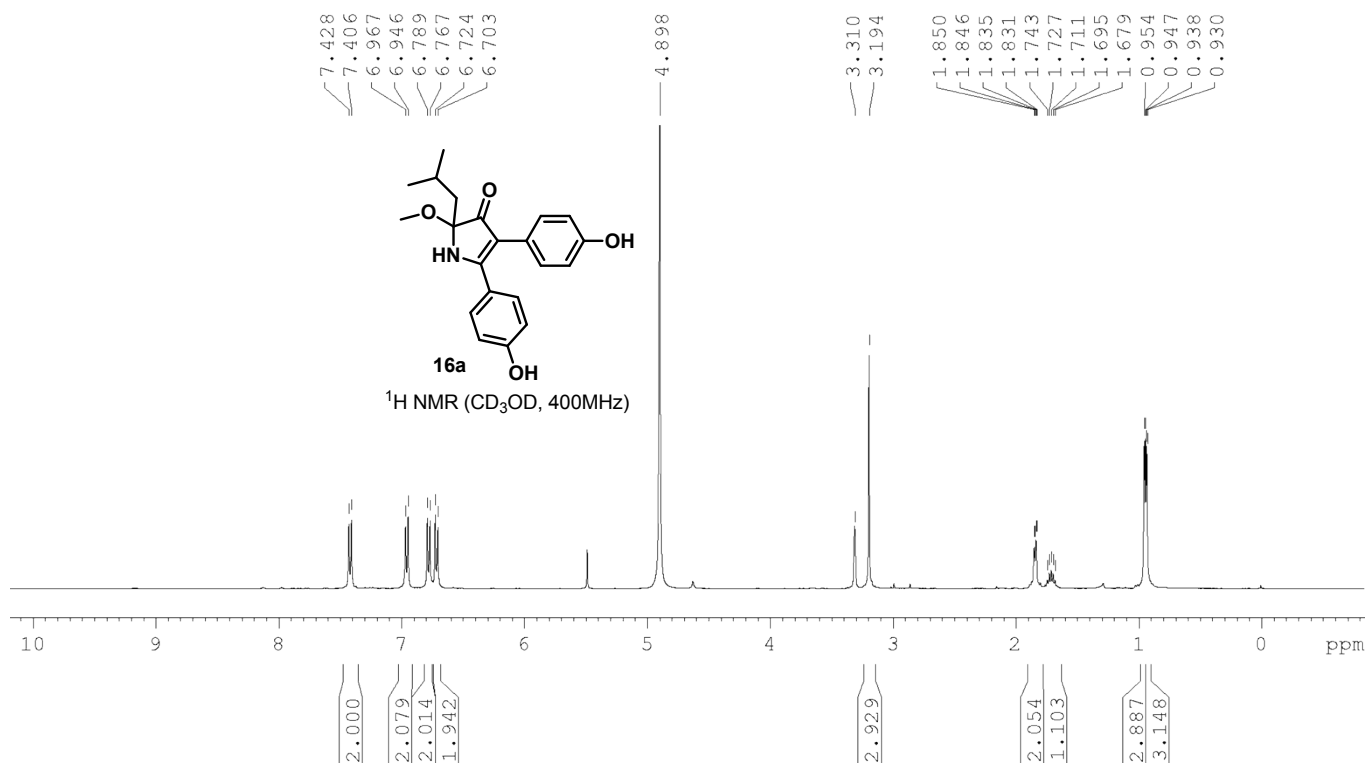


Figure 147: ¹H NMR (400 MHz) spectrum of **16a**

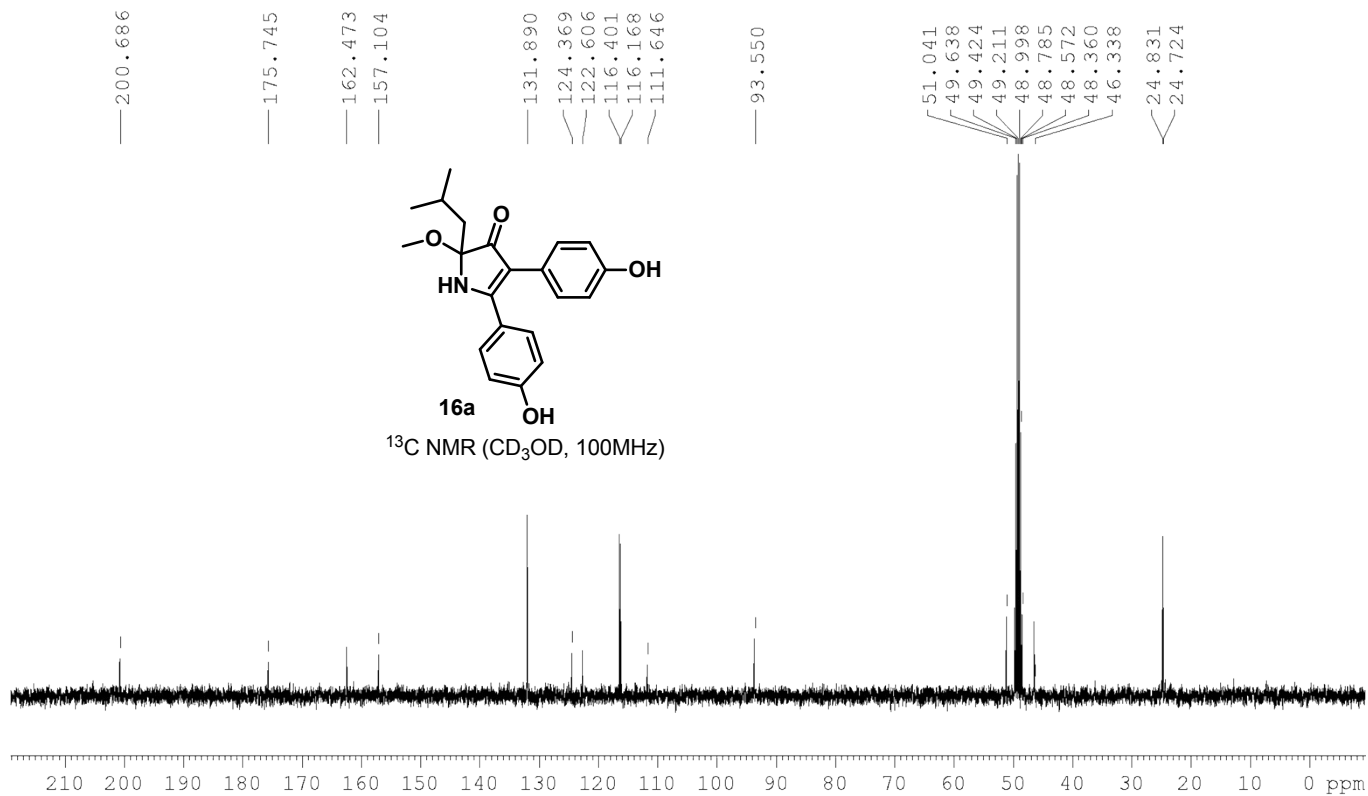


Figure 148: ¹³C NMR (100 MHz) spectrum of **16a**

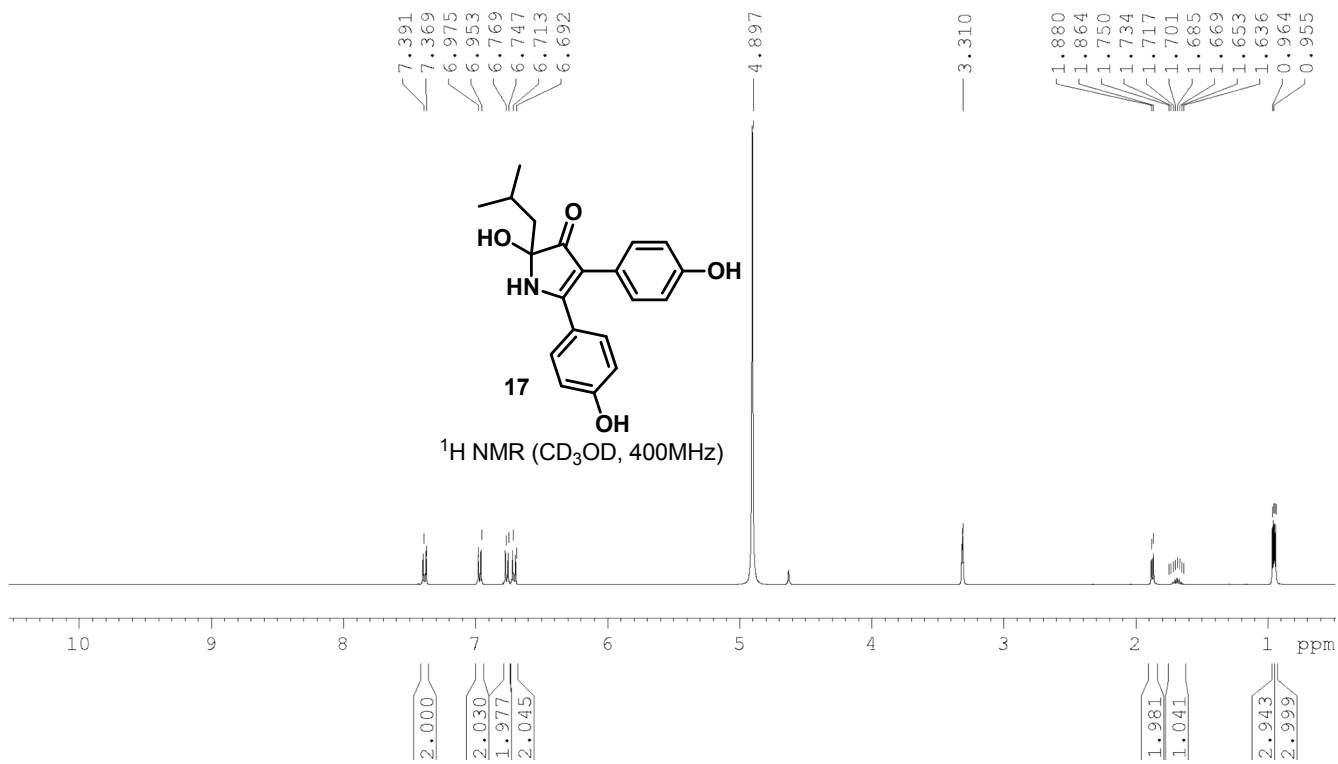


Figure 149: $^1\text{H NMR}$ (400 MHz) spectrum of **17**

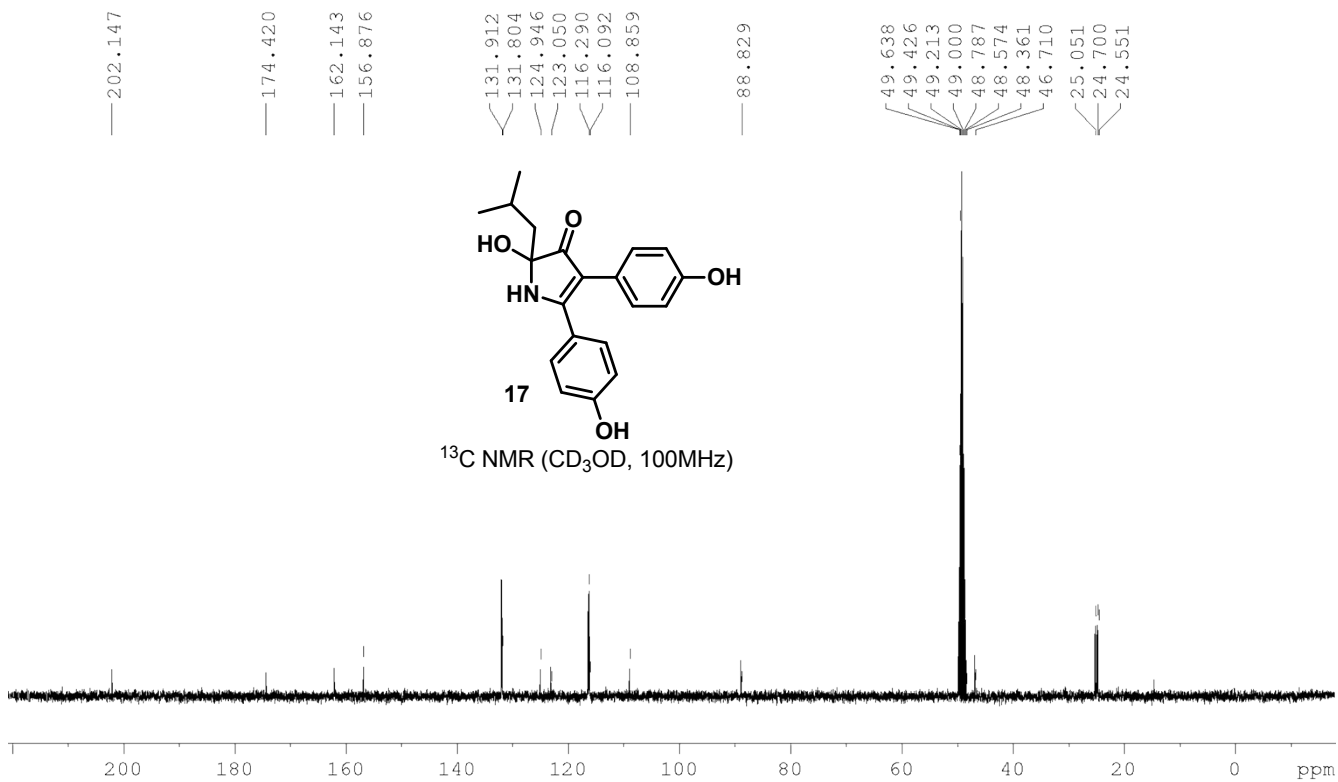


Figure 150: $^{13}\text{C NMR}$ (100 MHz) spectrum of **17**

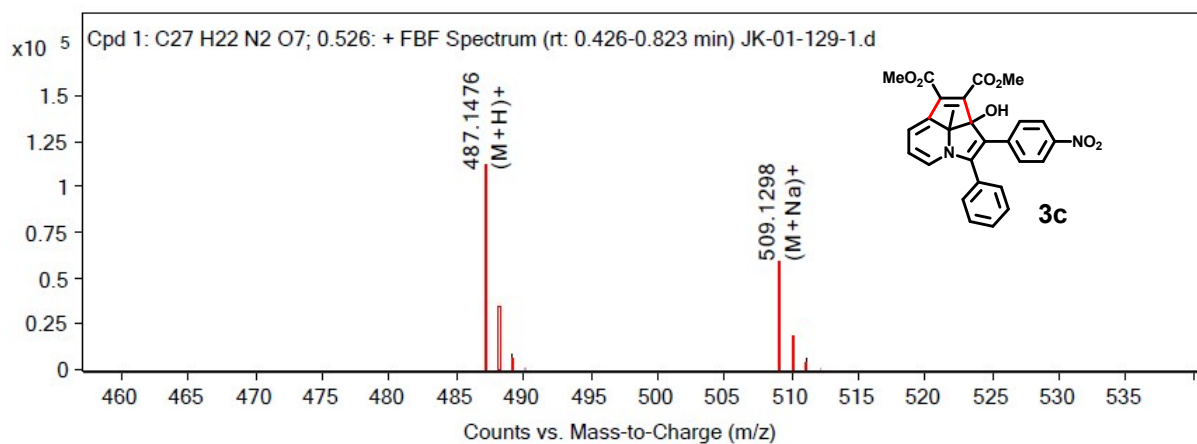
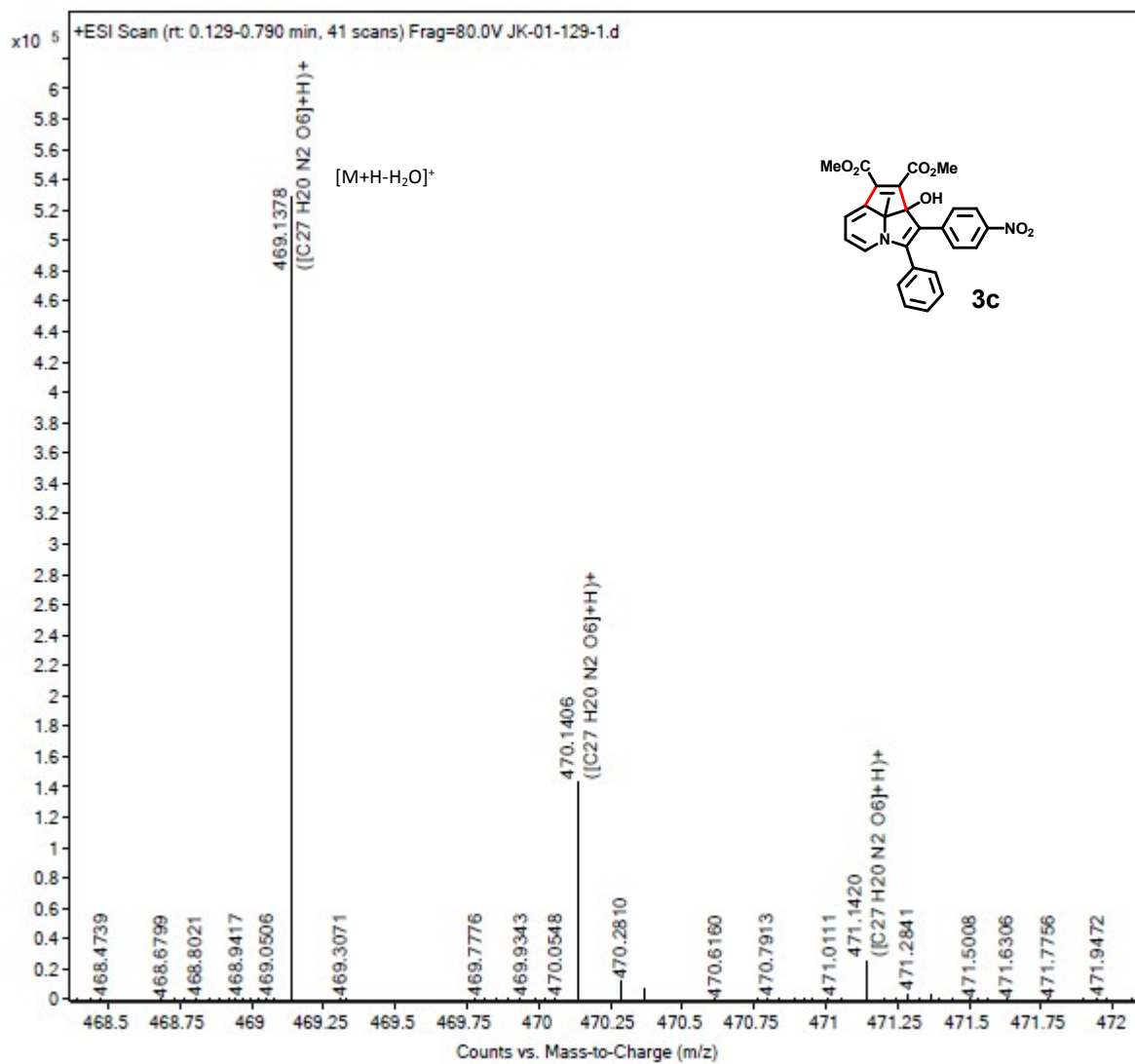


Figure 151: HRMS spectrum of **3c**

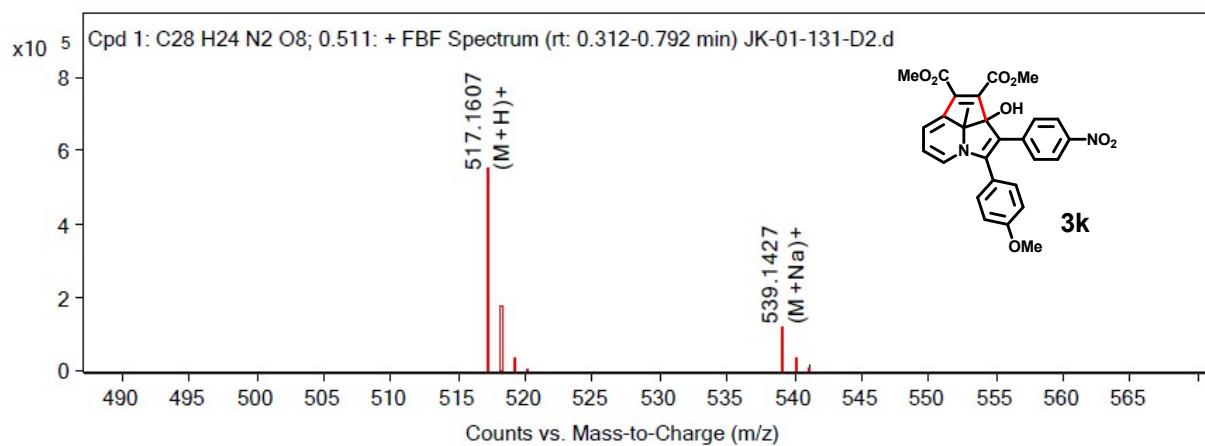
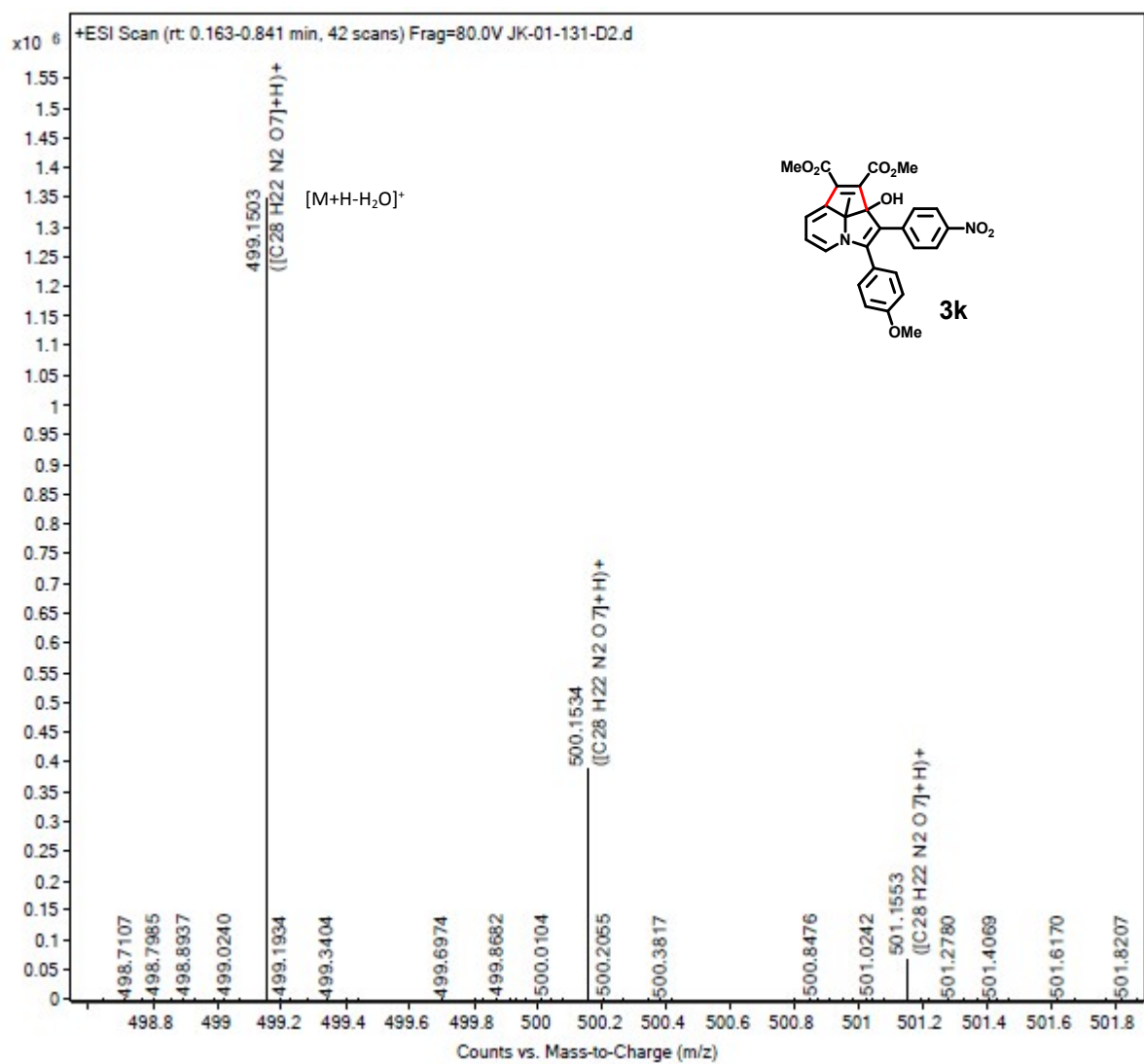


Figure 152: HRMS spectrum of **3k**

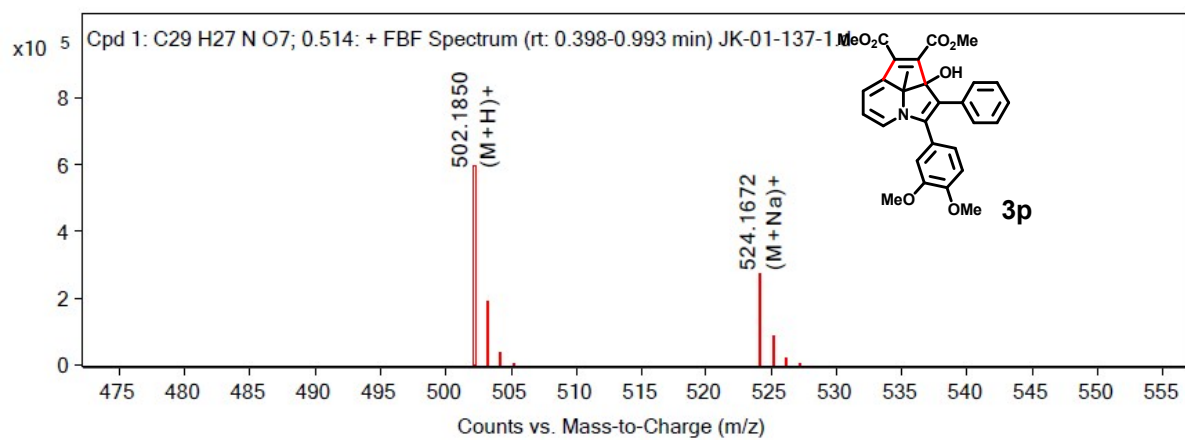
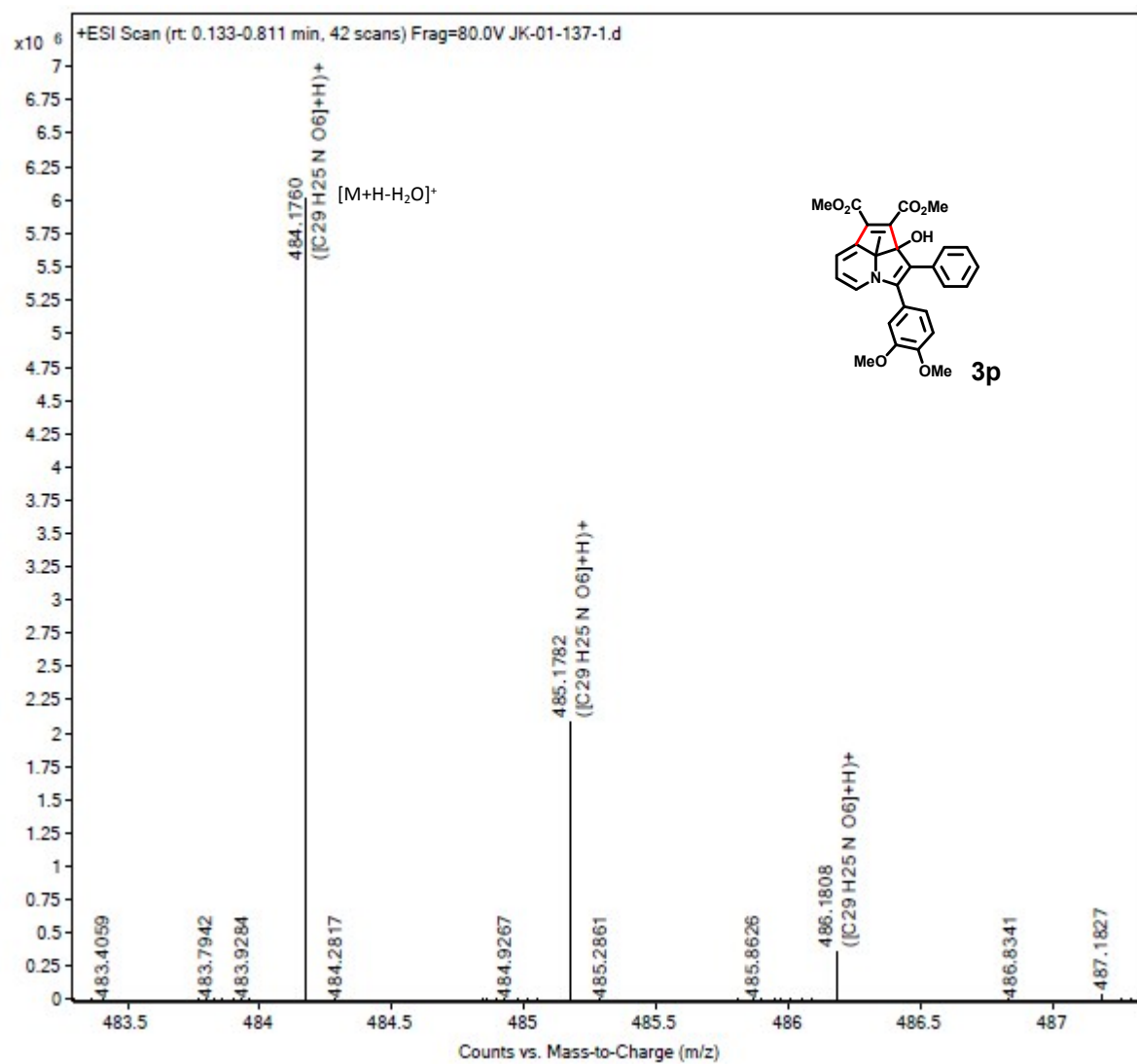


Figure 153: HRMS spectrum of 3p

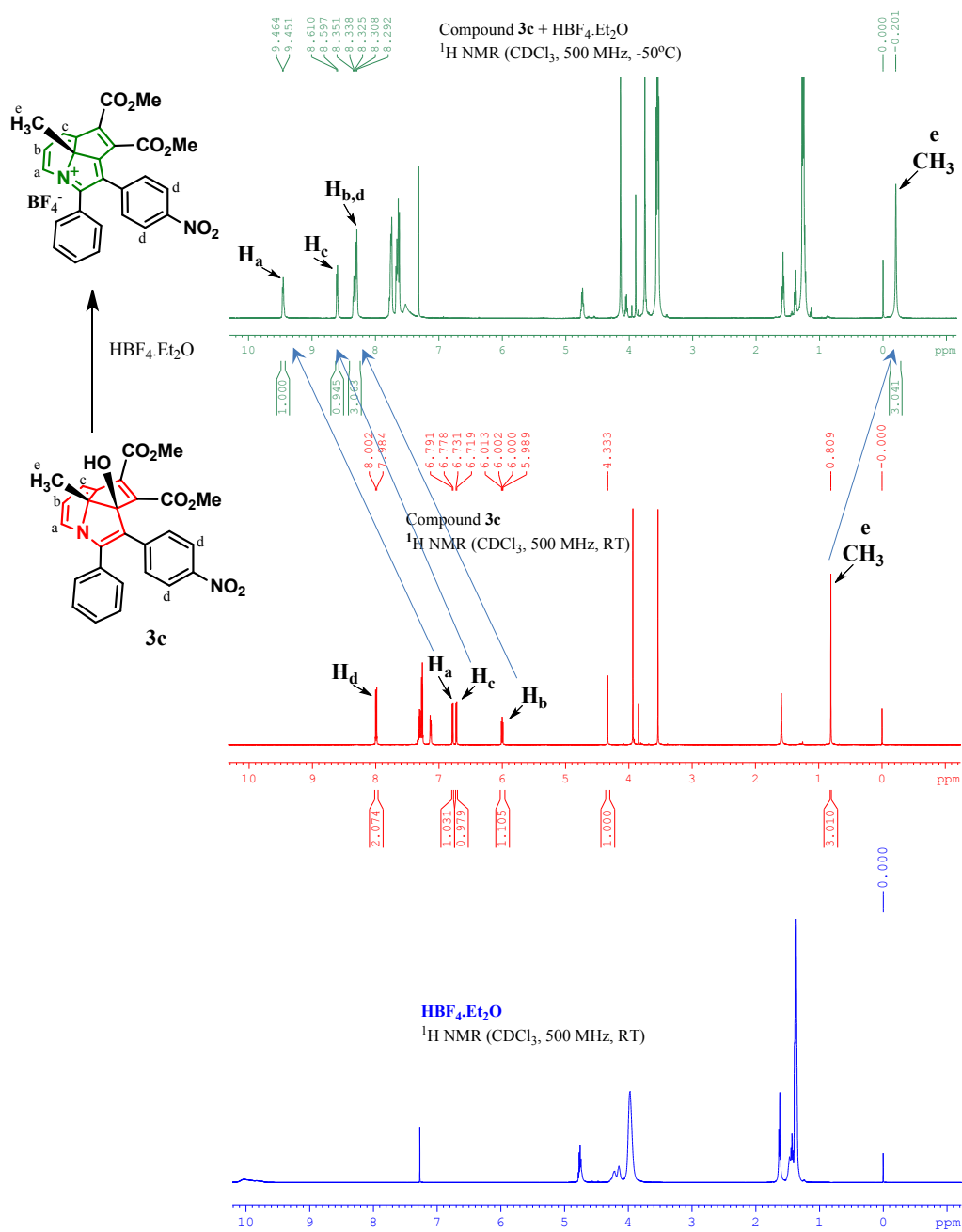
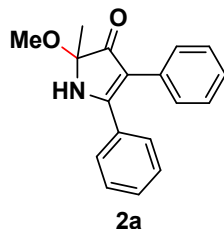


Figure 154: ¹H NMR spectra showing the formation of aromatic 10-electron species from **3c** on treatment with HBF₄.Et₂O

X-ray crystallography Data of **2a**, **3a** and **17**



CCDC deposition number of **2a** is 1908547.

Bond precision: C-C = 0.0072 Å

Wavelength=0.71073

Cell: a=11.6409 (14)
alpha=67.133 (5)

b=11.8981 (11)
beta=76.352 (5)

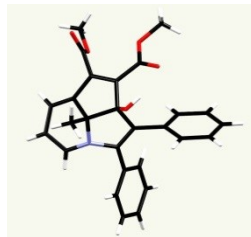
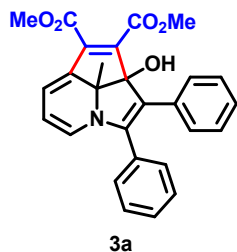
c=12.5461 (14)
gamma=89.759 (5)

Temperature: 296 K

	Calculated	Reported
Volume	1548.5 (3)	1548.5 (3)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C18 H17 N O2	C36 H34 N2 O4
Sum formula	C18 H17 N O2	C36 H34 N2 O4
Mr	279.33	558.65
Dx, g cm ⁻³	1.198	1.198
Z	4	2
Mu (mm ⁻¹)	0.078	0.078
F000	592.0	592.0
F000'	592.26	
h, k, lmax	12, 12, 13	12, 12, 13
Nref	4121	4085
Tmin, Tmax	0.989, 0.992	0.980, 0.992
Tmin'	0.980	
Correction method=	# Reported T Limits: Tmin=0.980 Tmax=0.992	
AbsCorr =	MULTI-SCAN	
Data completeness=	0.991	Theta(max)= 22.629
R(reflections)=	0.0563 (1991)	wR2(reflections)= 0.1580 (4085)

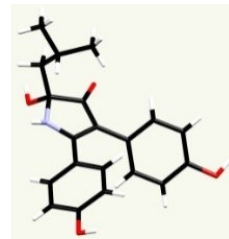
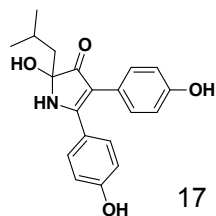
S = 0.949

Npar= 392



CCDC deposition number of **3a** is 1907329.

Bond precision:	C-C = 0.0030 Å	Wavelength=0.71073	
Cell:	a=6.0337 (2) alpha=83.2254 (14)	b=12.7989 (4) beta=79.7254 (12)	c=15.3967 (5) gamma=82.5173 (12)
Temperature:	296 K		
Calculated	Reported Volume	1154.49 (6)	
	1154.49 (6)		
Space group	P -1	P -1	
Hall group	-P 1	-P 1	
Moiety formula	C ₂₇ H ₂₃ N O ₅	C ₂₇ H ₂₃ N O ₅	
Sum formula	C ₂₇ H ₂₃ N O ₅	C ₂₇ H ₂₃ N O ₅	
Mr	441.46	441.46	
Dx, g cm ⁻³	1.270	1.270	
Z	2	2	
Mu (mm ⁻¹)	0.088	0.088	
F000	464.0	464.0	
F000'	464.23		
h, k, lmax	7, 15, 18	7, 15, 18	
Nref	4067	4053	
Tmin, Tmax	0.977, 0.991	0.976, 0.991	
Tmin'	0.976		
Correction method=	# Reported T Limits: Tmin=0.976 Tmax=0.991		
AbsCorr =	MULTI-SCAN		
Data completeness=	0.997	Theta (max)= 25.000	
R (reflections)=	0.0478 (3315)	wR2 (reflections)= 0.1318 (4053)	
S =	1.026	Npar= 306	



CCDC deposition number of **17** is 1908557.

Bond precision: C-C = 0.0035 Å Wavelength=0.71073

Cell: a=9.9320(3) b=12.9438(4) c=18.2127(4)
 alpha=90 beta=92.2716(14) gamma=90 Temperature: 296 K

Calculated	Reported Volume	2339.55(11)
	2339.55(11)	
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn Moiety
formula	C20 H21 N O4, C4 H8 O2	C24 H29 N O6
Sum formula	C24 H29 N O6	C24 H29 N O6
Mr	427.48	427.48
Dx, g cm ⁻³	1.214	1.214
Z	4	4
Mu (mm ⁻¹)	0.087	0.087
F000	912.0	912.0
F000'	912.48	
h, k, lmax	11, 15, 21	11, 15, 21
Nref	4118	4118
Tmin, Tmax	0.978, 0.991	0.979, 0.991
Tmin'	0.978	
Correction method=	# Reported T Limits: Tmin=0.979 Tmax=0.991	
AbsCorr =	MULTI-SCAN	
Data completeness=	1.000	Theta(max)= 24.992
R(reflections)=	0.0490(2871)	wR2(reflections)= 0.1384(4118)
S =	1.045	Npar= 301
