

Electronic Supplementary Information

Catalyst-Free Assembly of Poly-Functionalized 1,2,4-Triazole-Fused *N*-Heterocycle, 6-Acylated Pyrrolo[1,2-*a*][1,2,4]triazolo[5,1-*c*]pyrazine

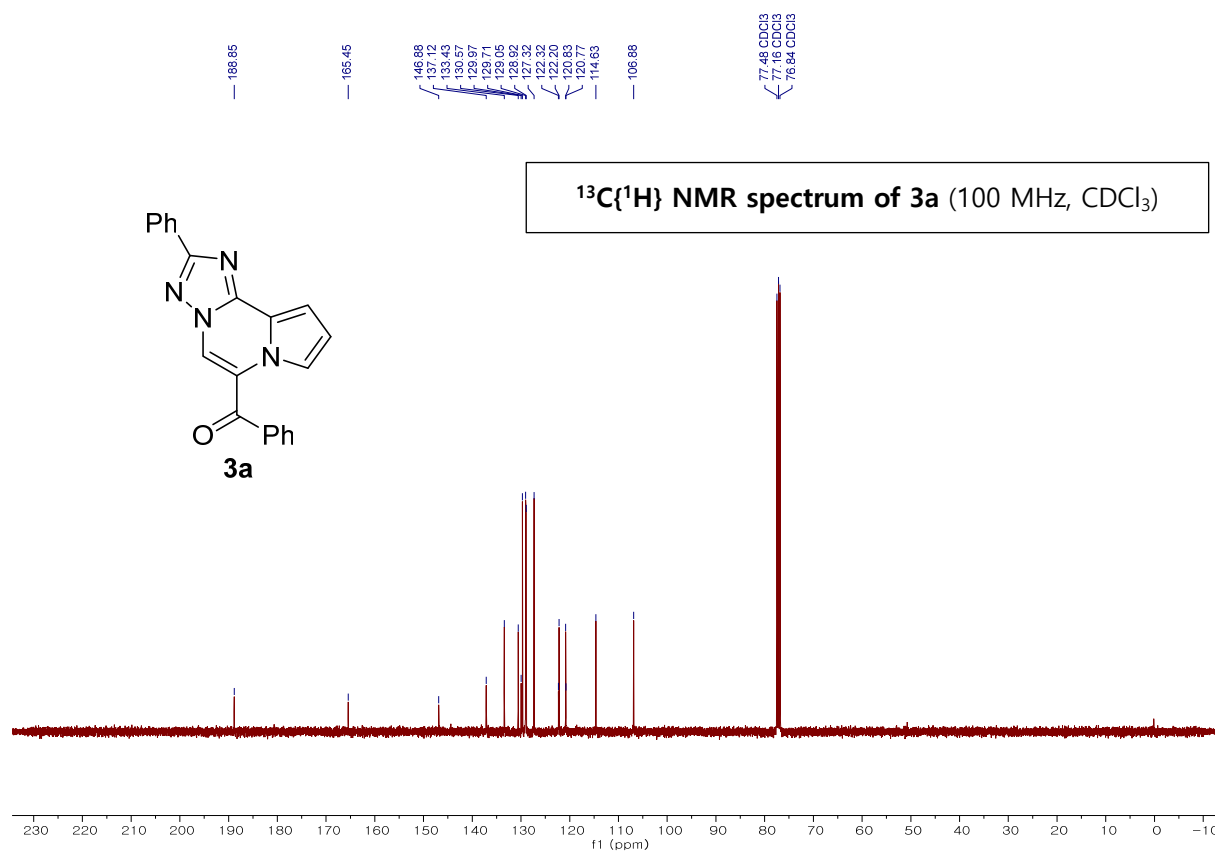
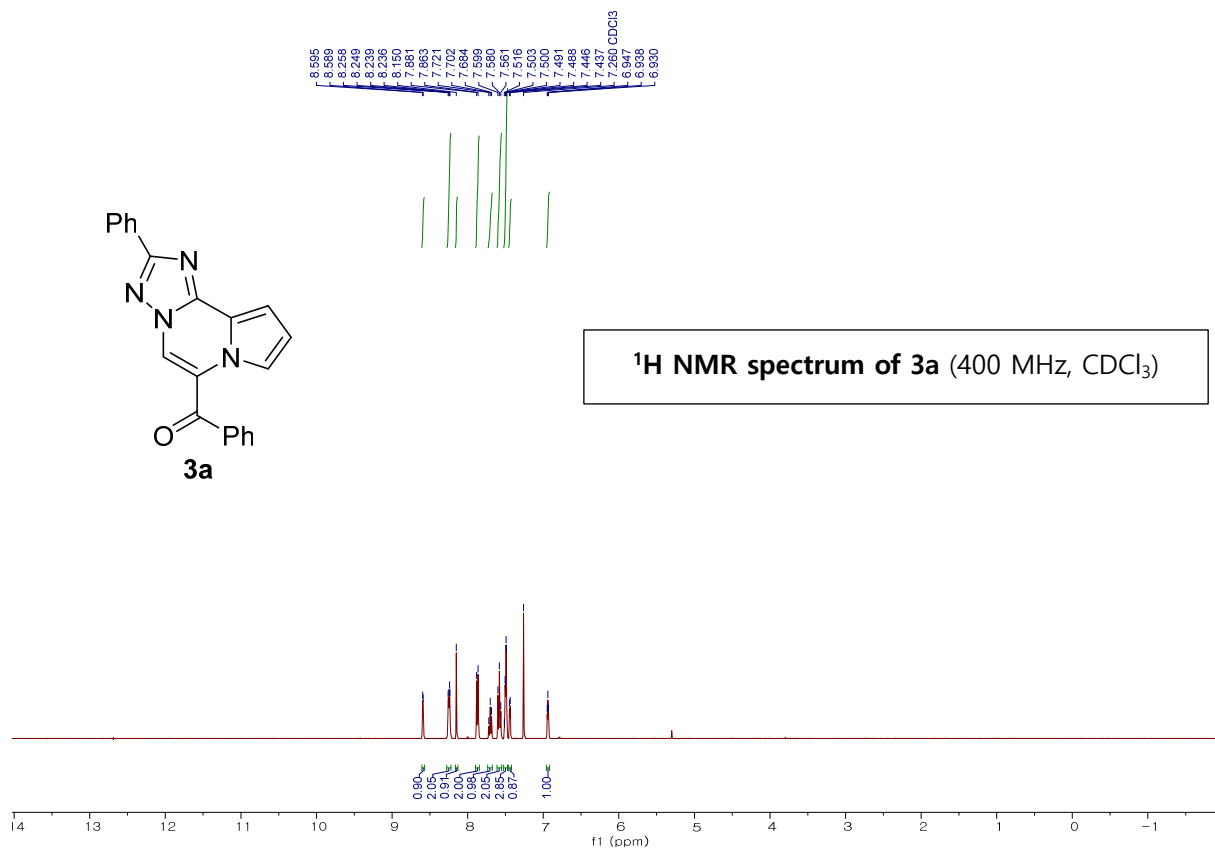
Hyunjin Oh and Ikyon Kim*

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85 Songdogwahak-ro, Yeonsu-gu, Incheon, 21983, Republic of Korea

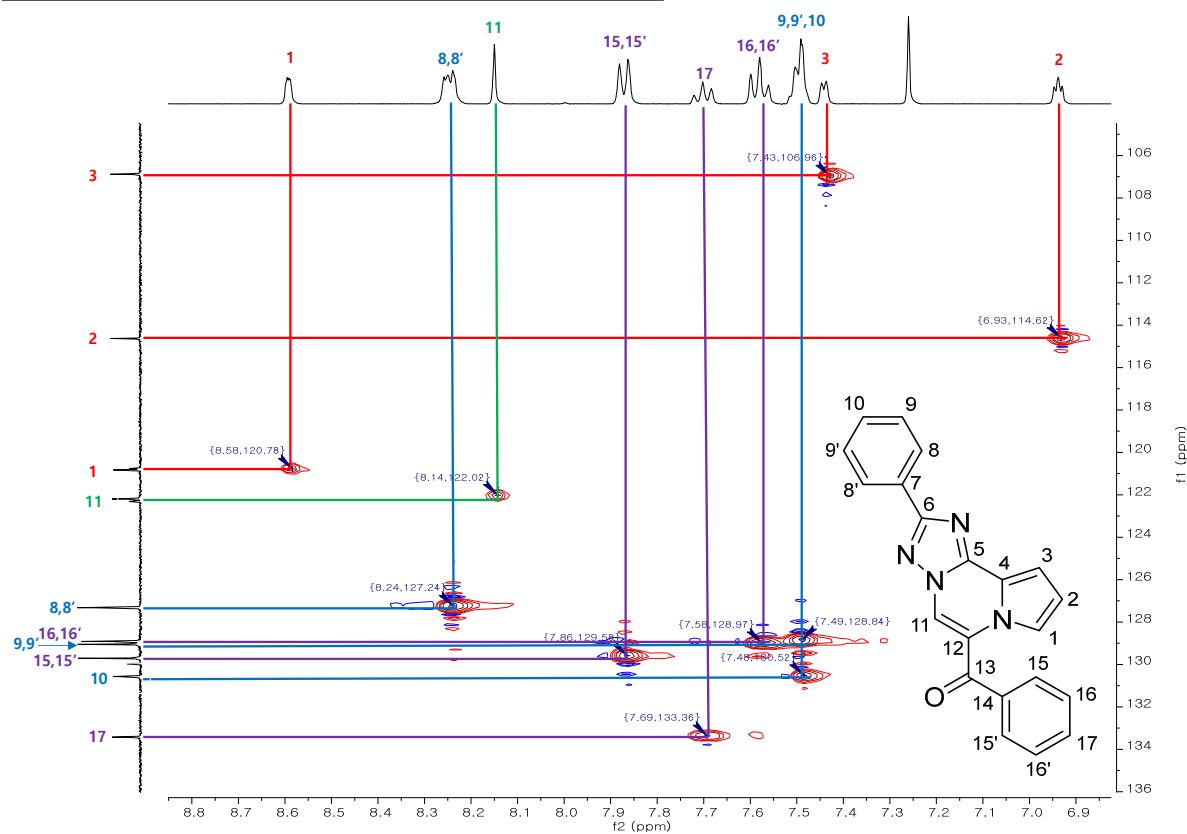
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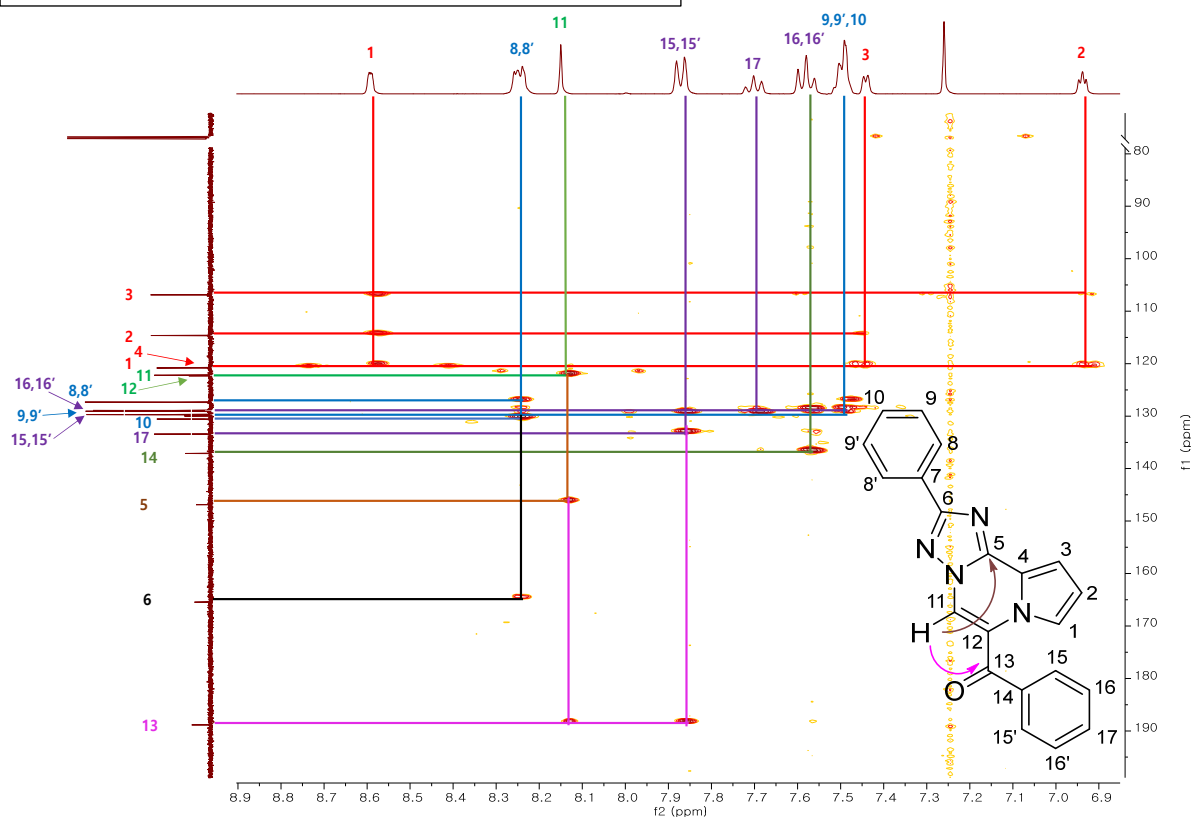
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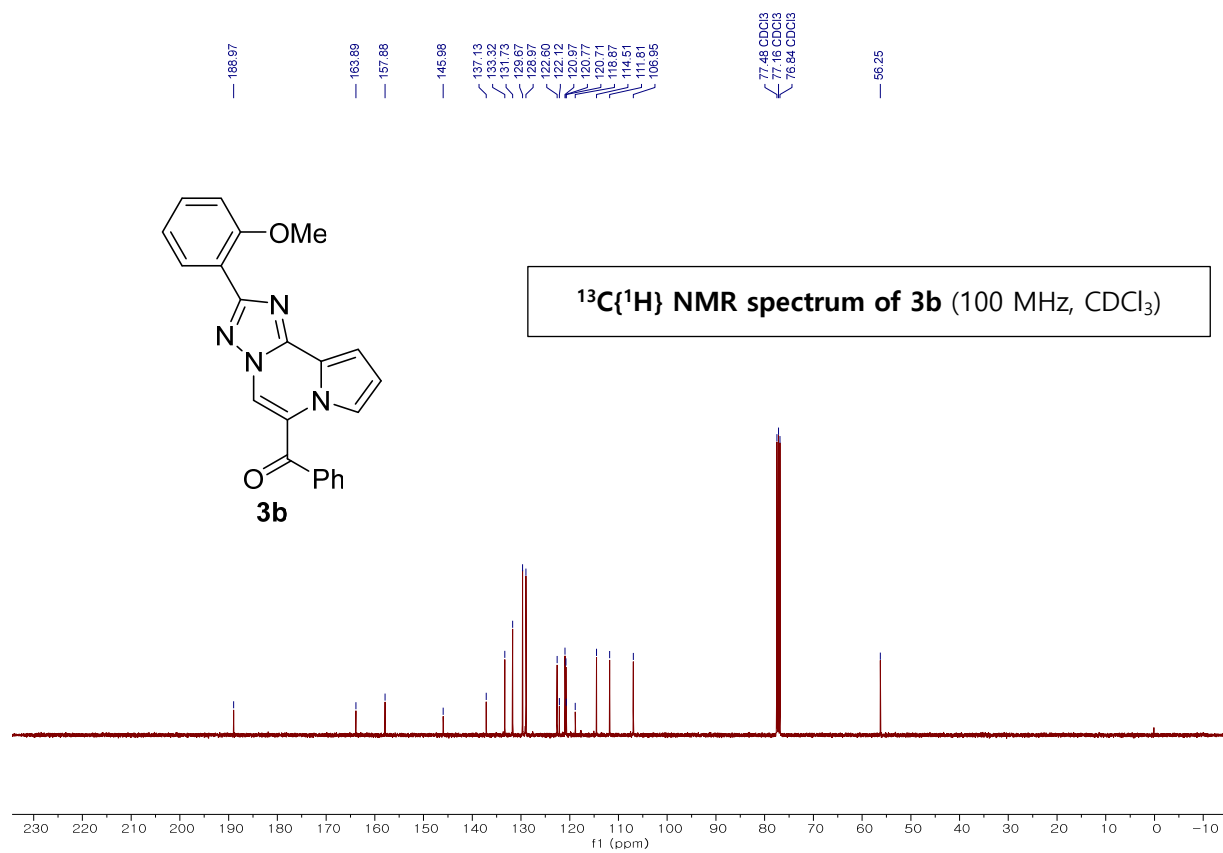
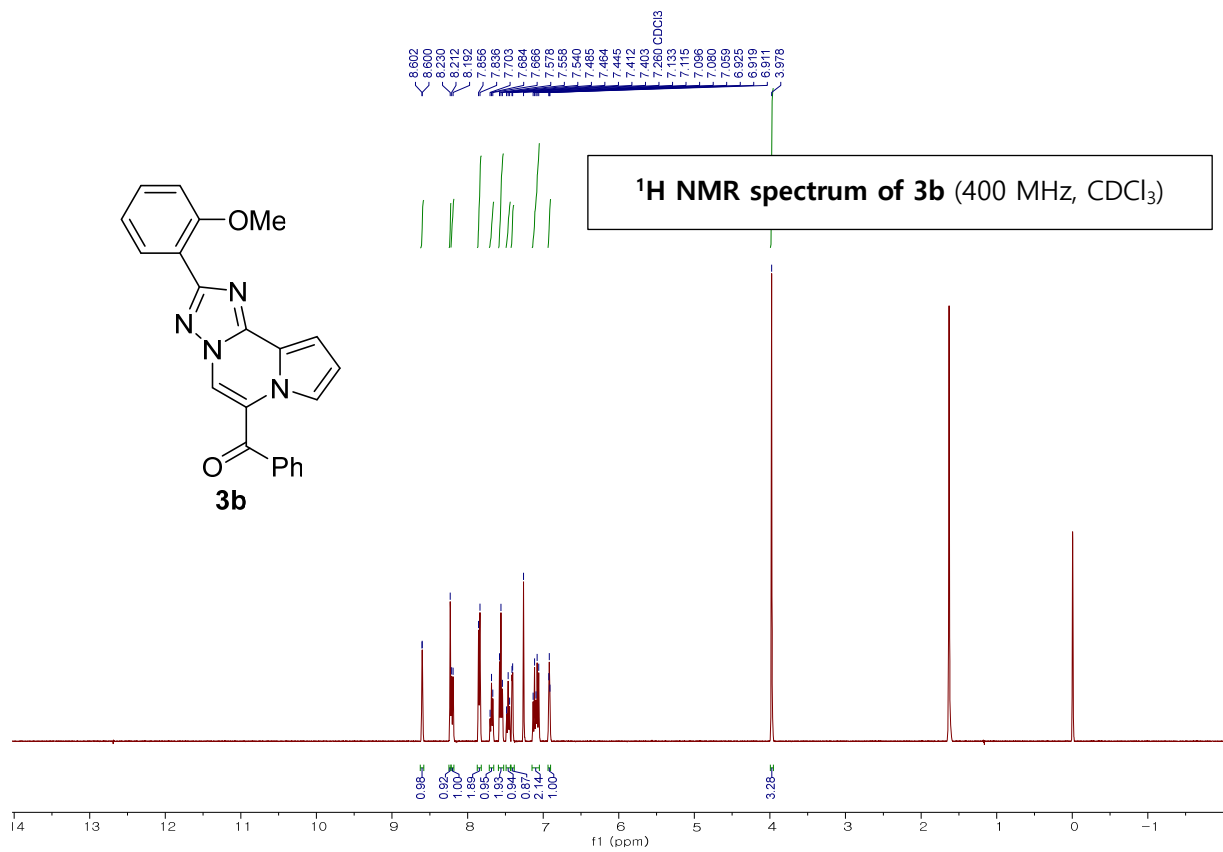


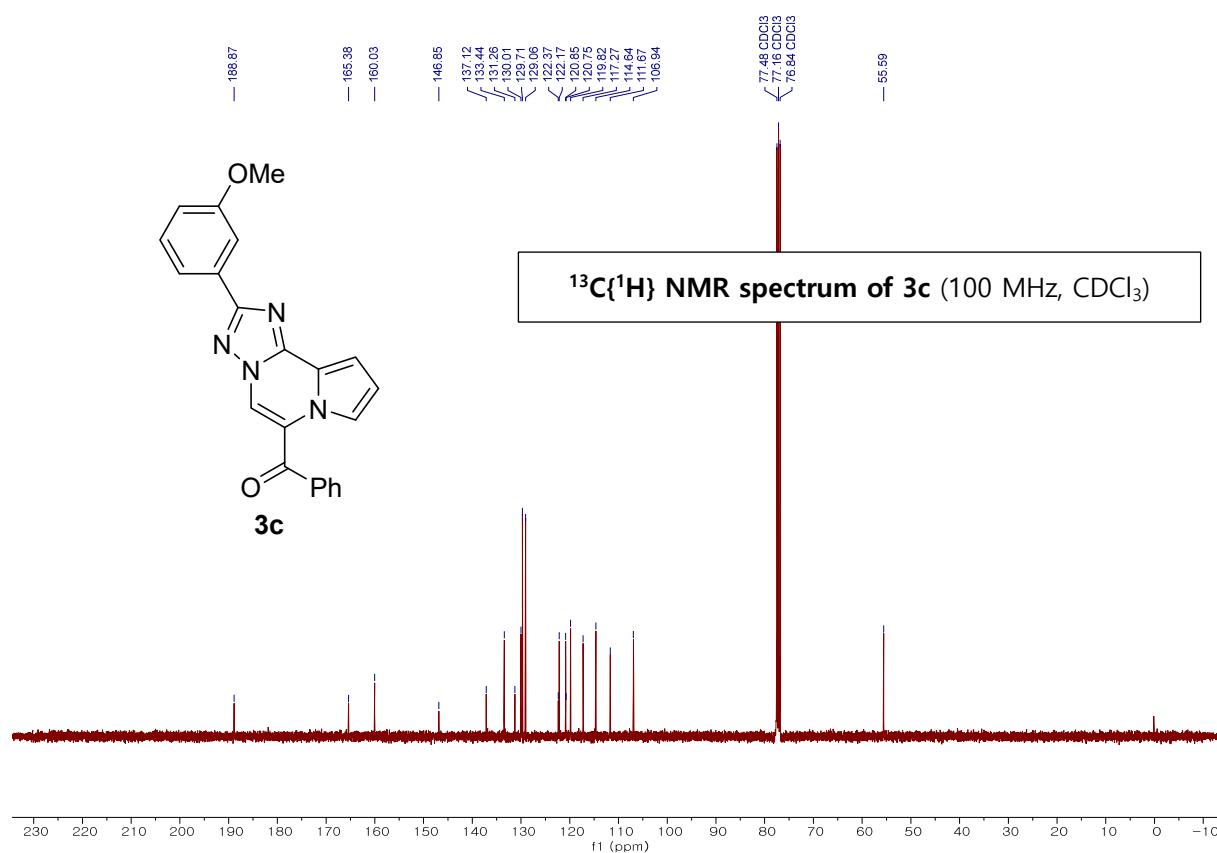
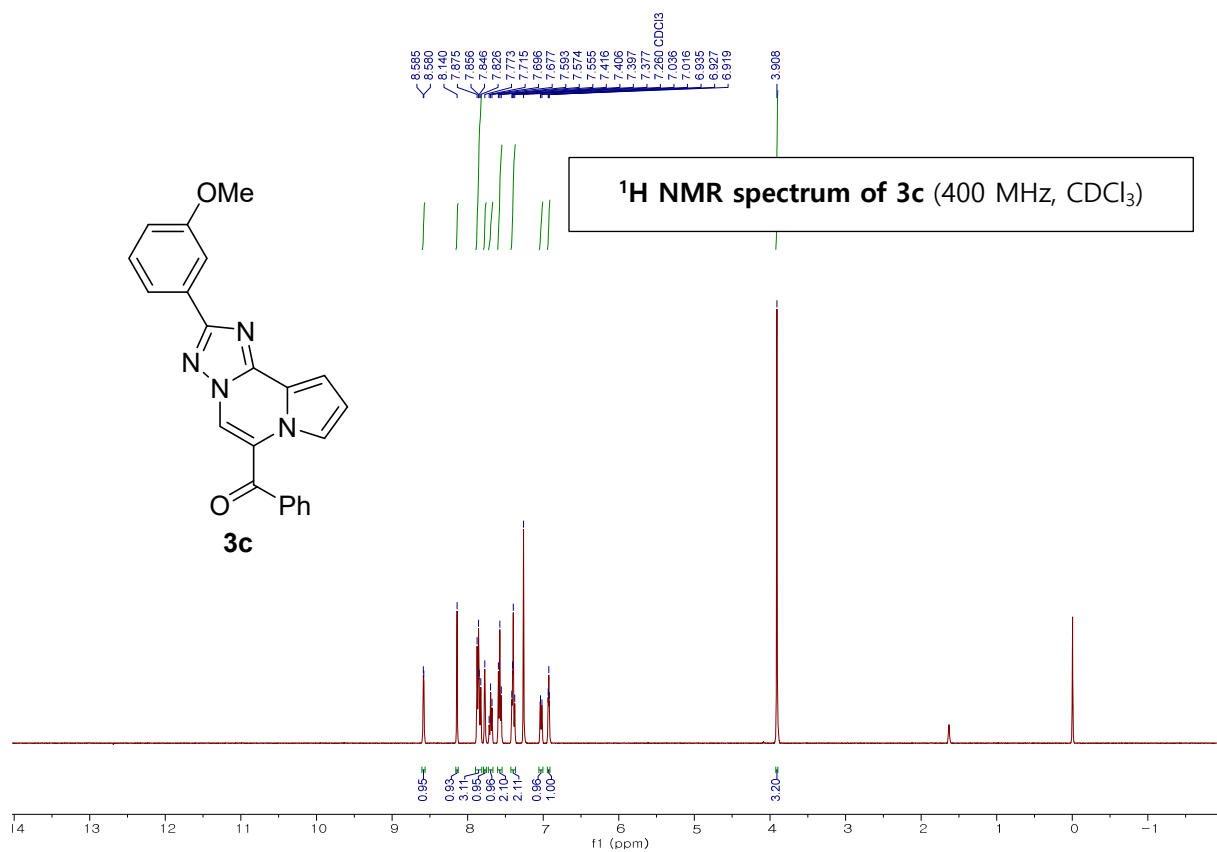
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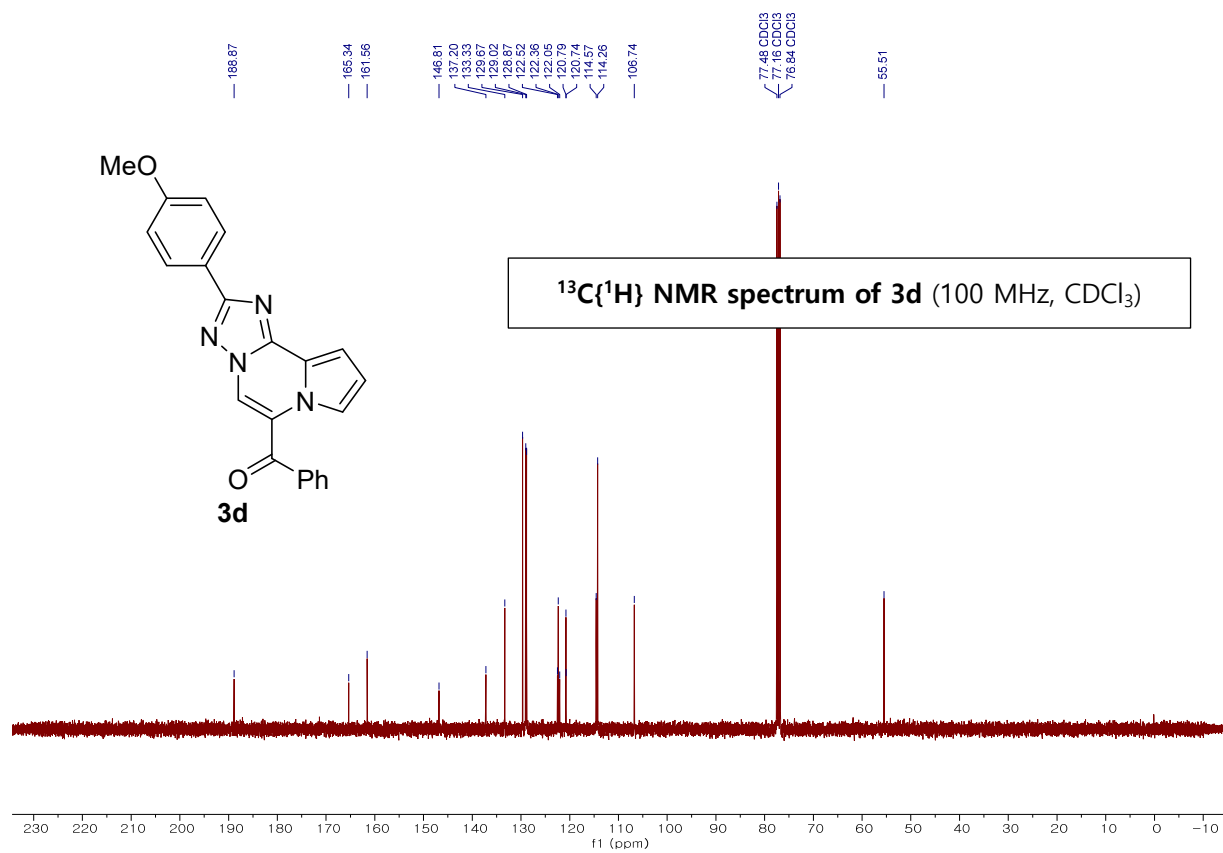
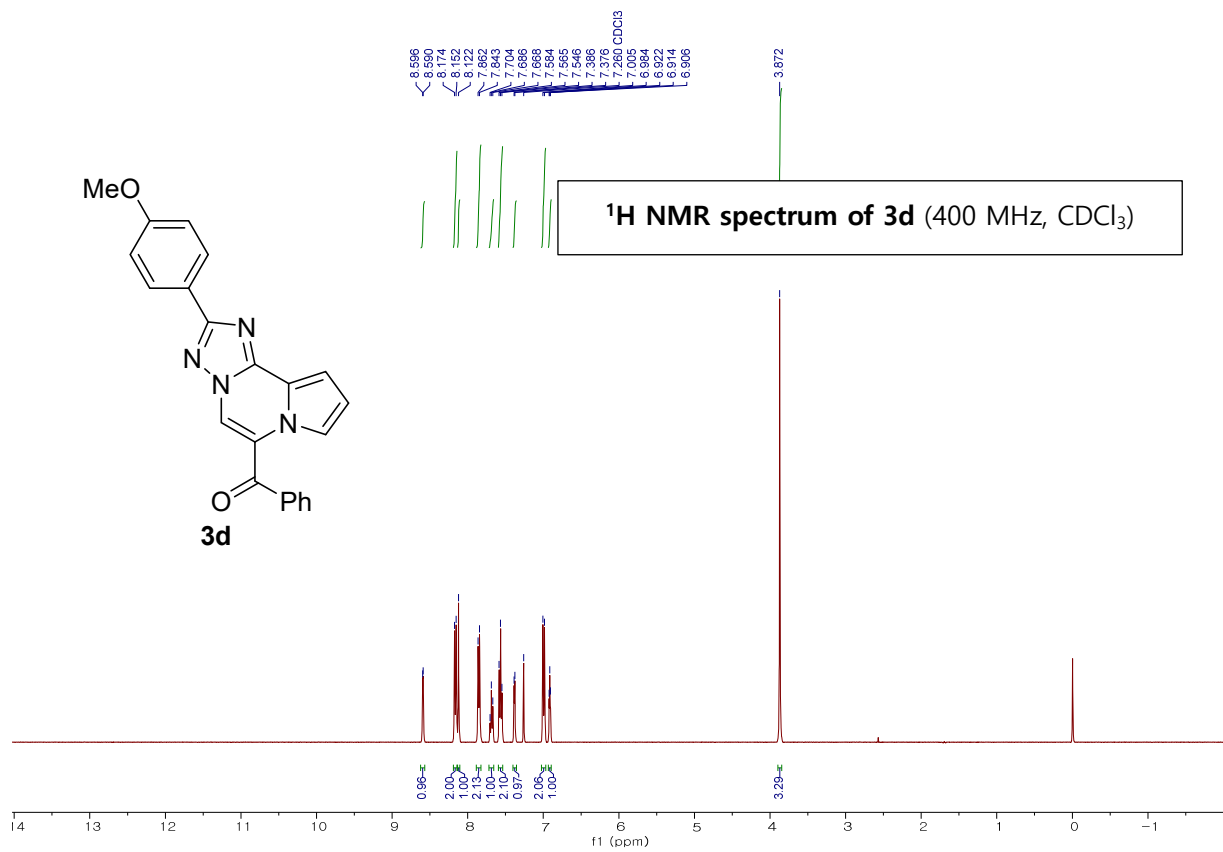


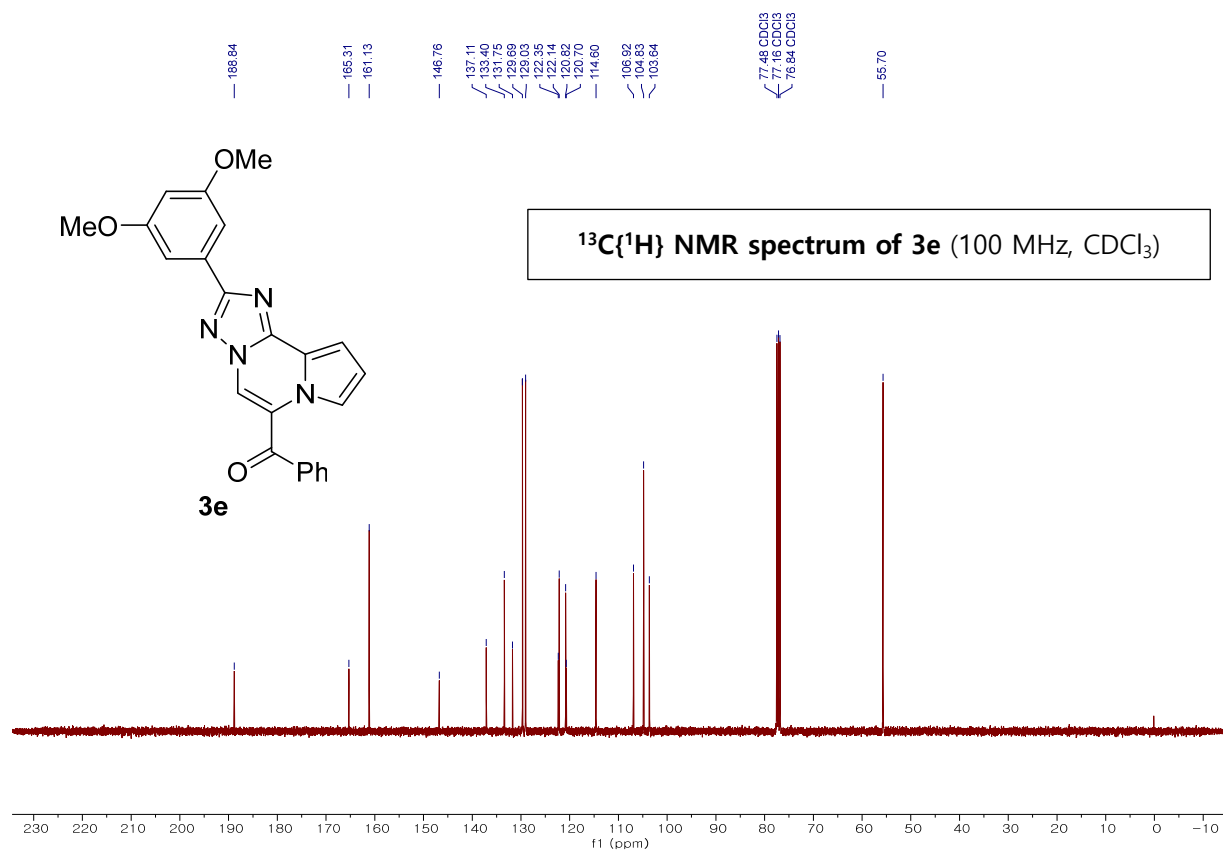
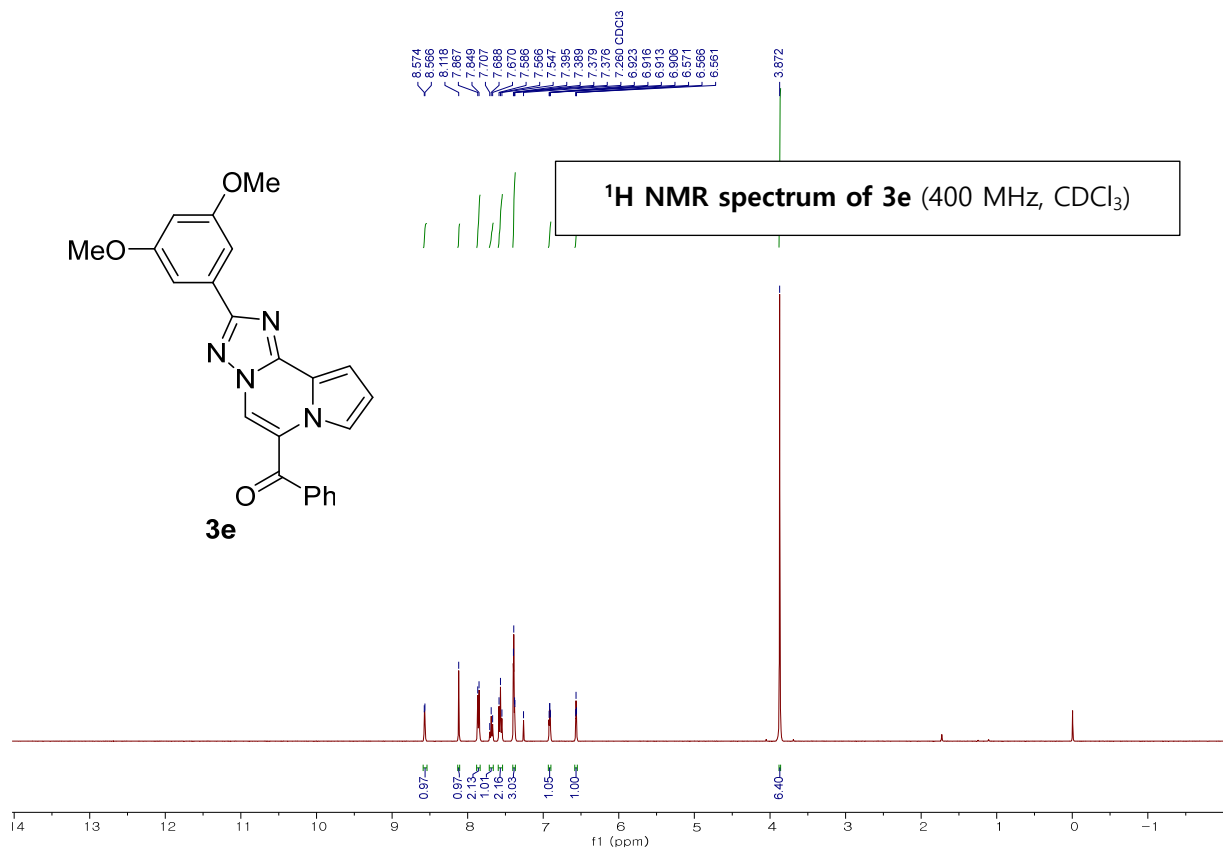
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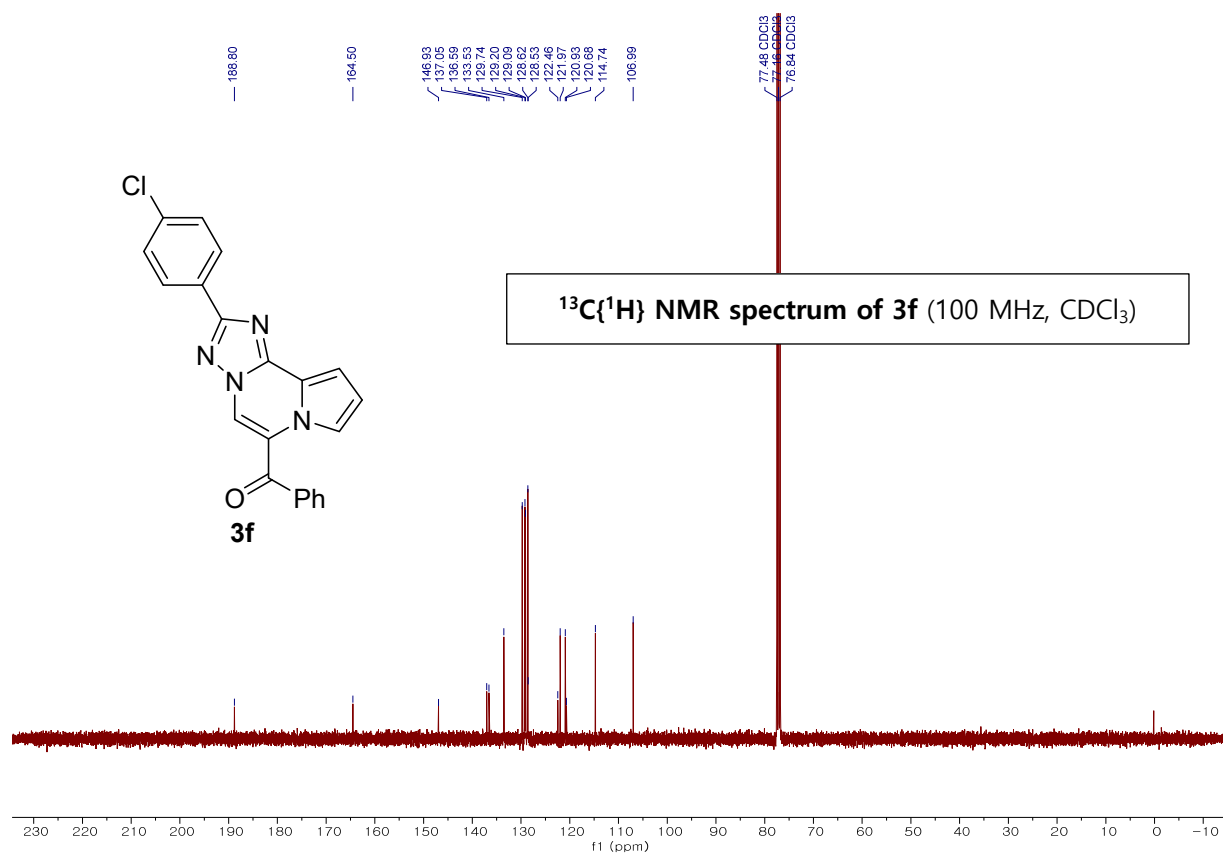
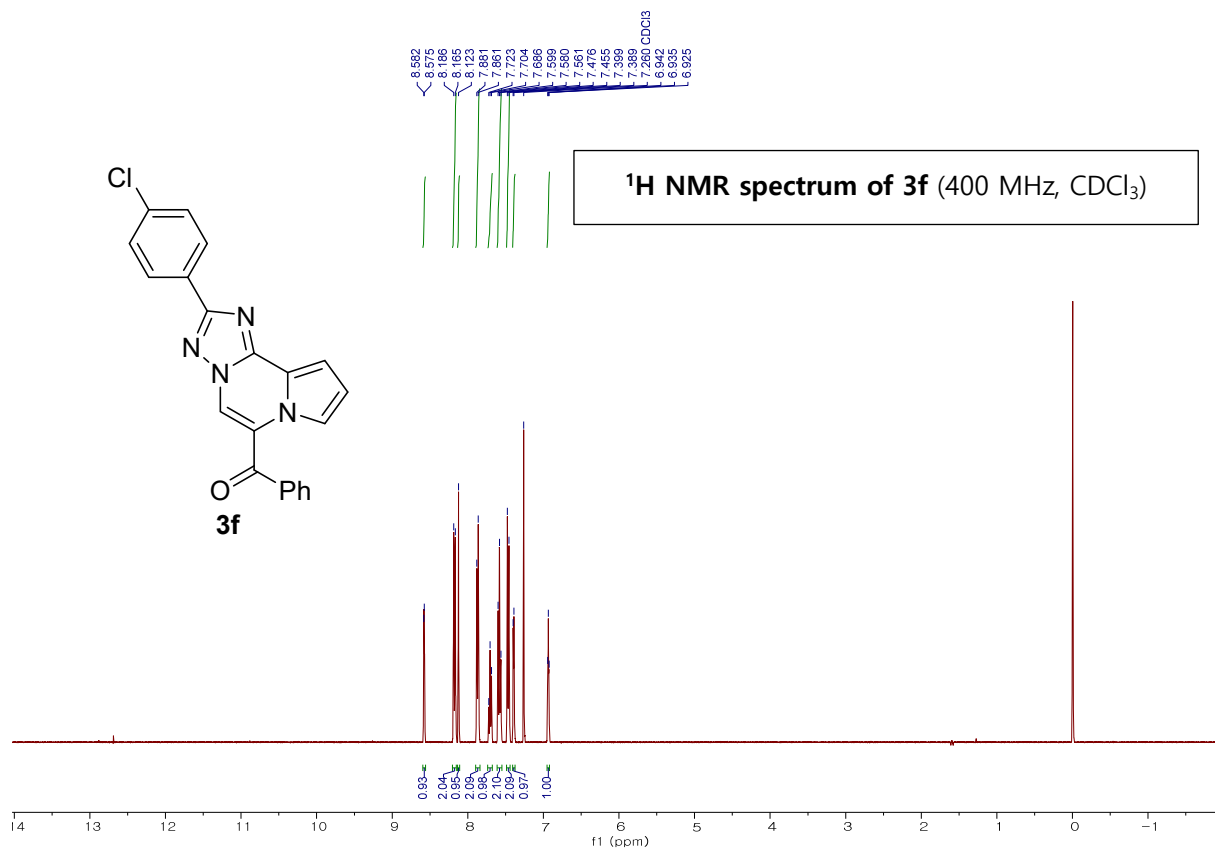


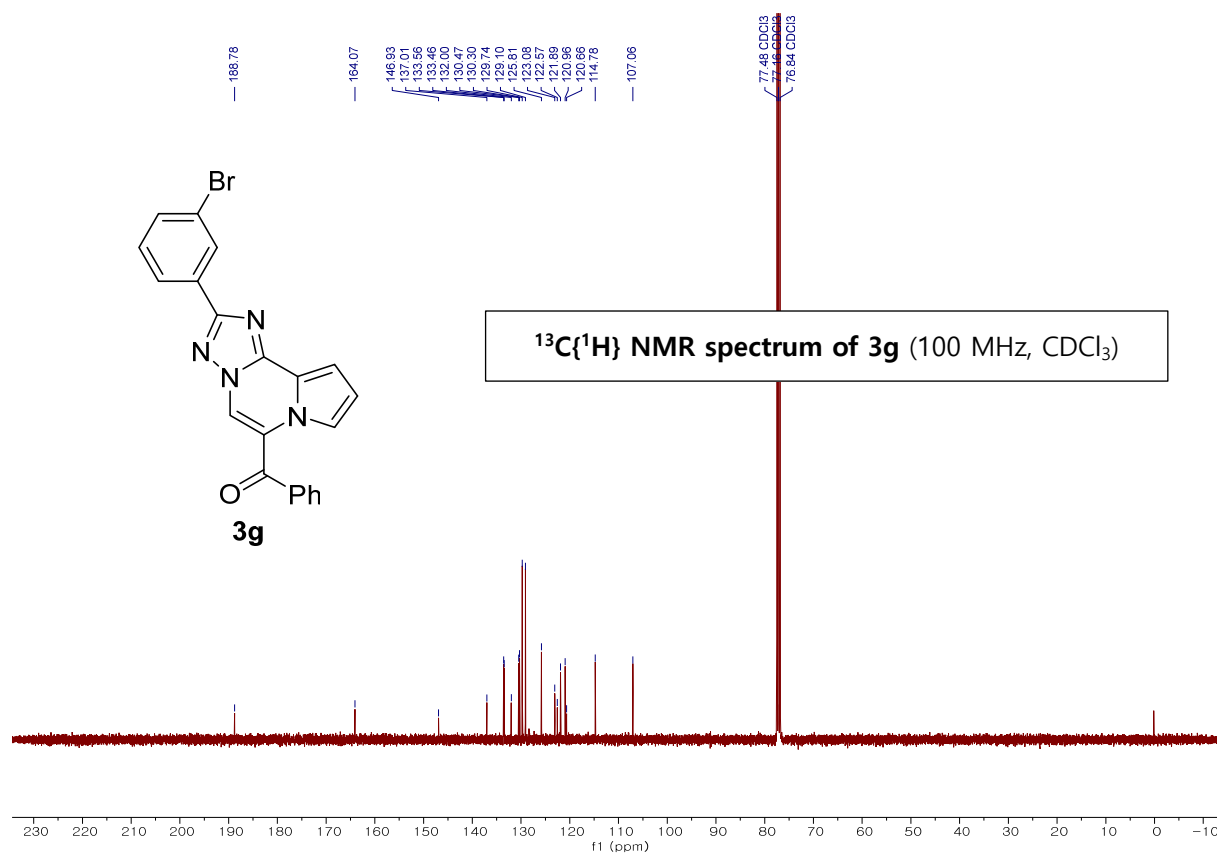
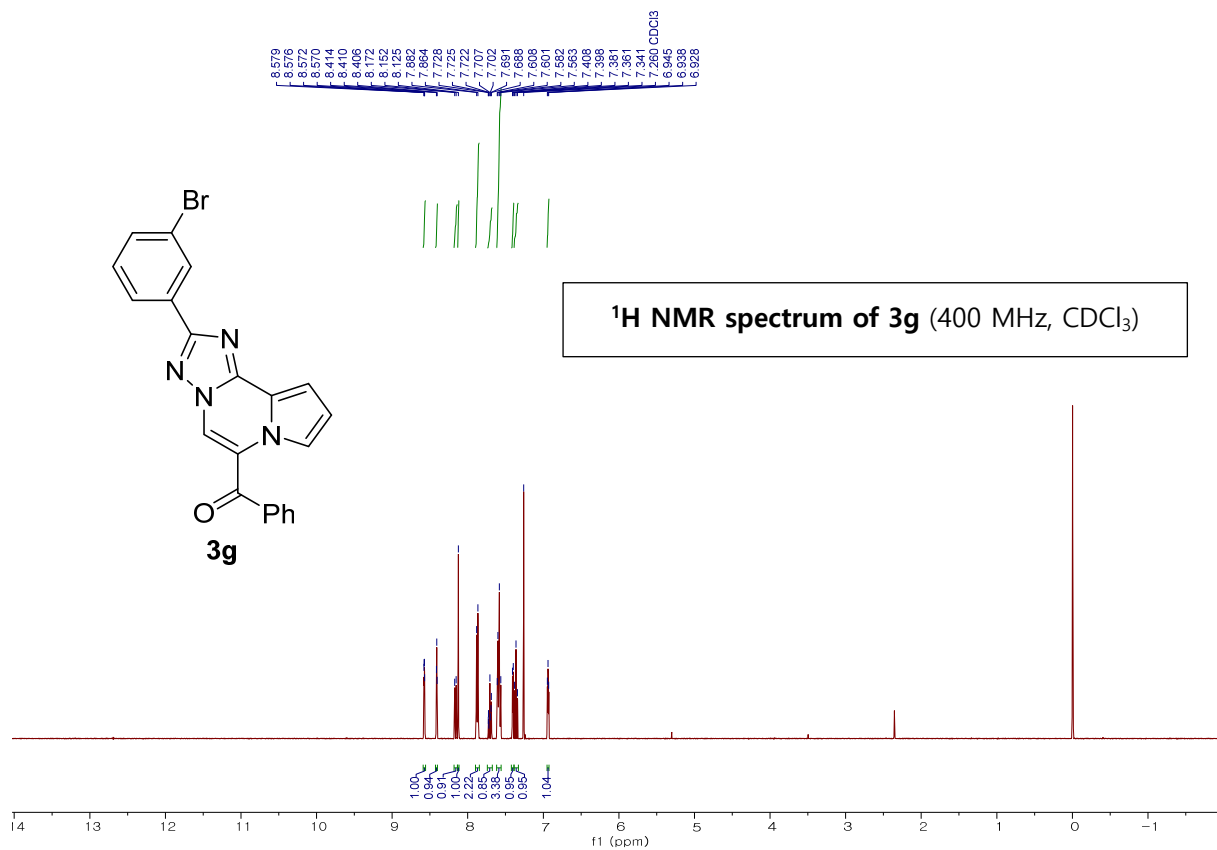


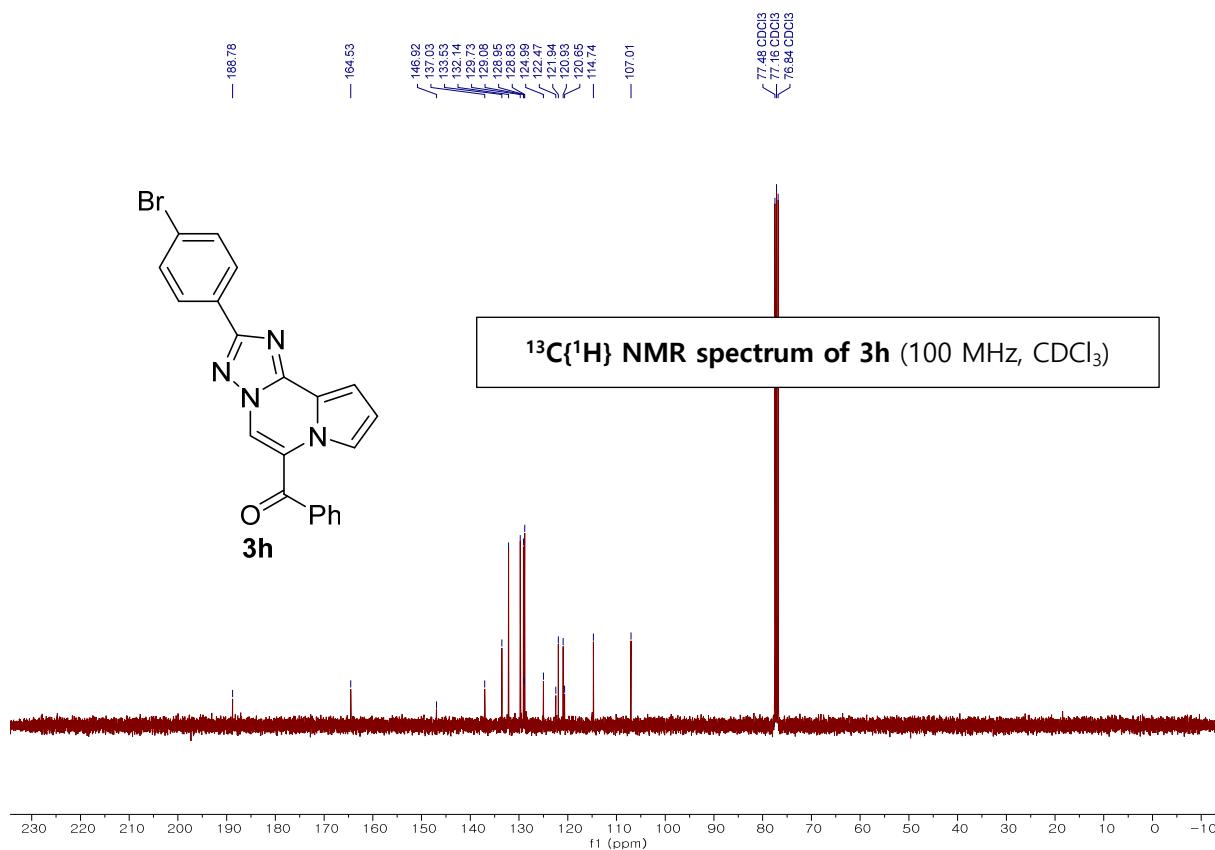
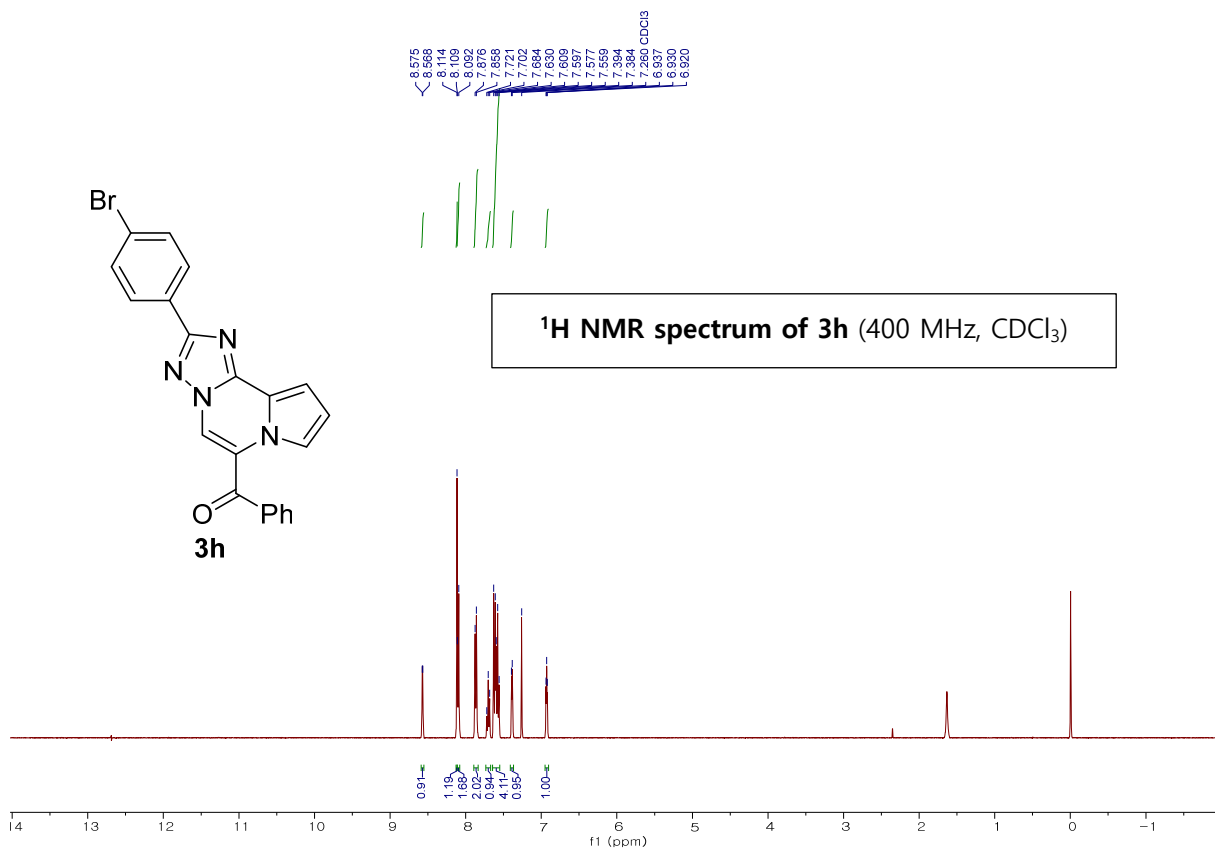


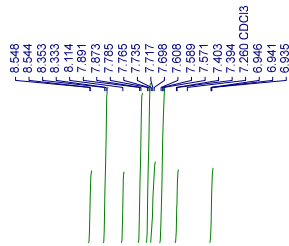
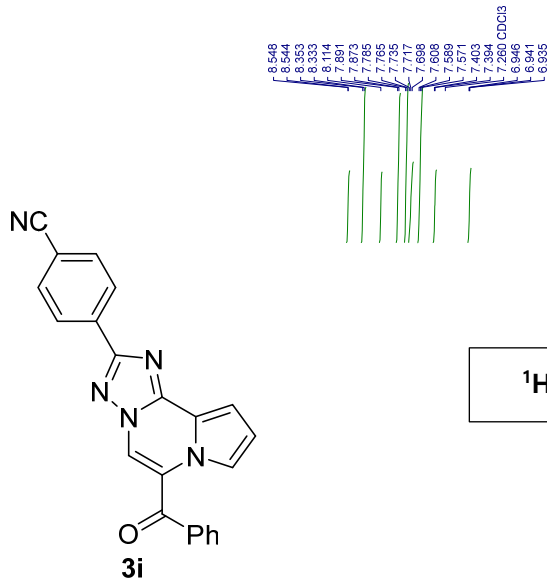




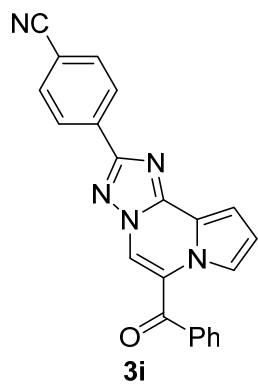
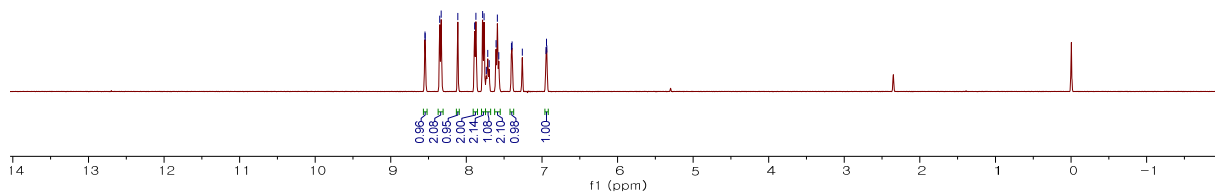




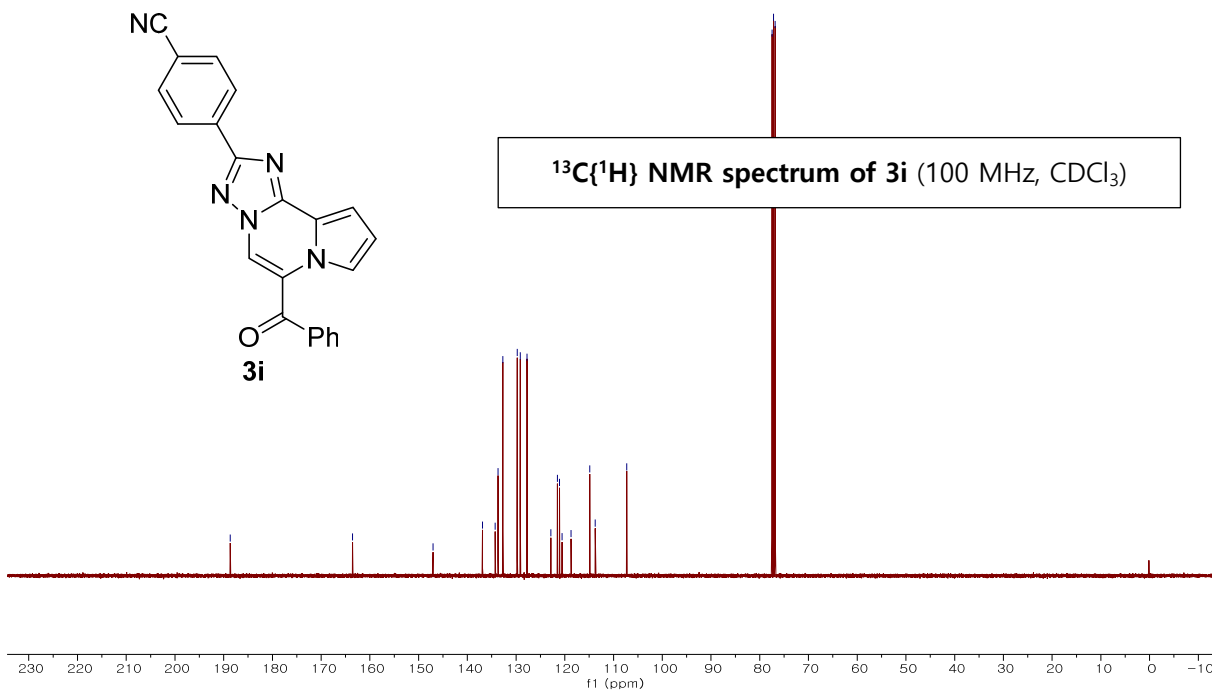


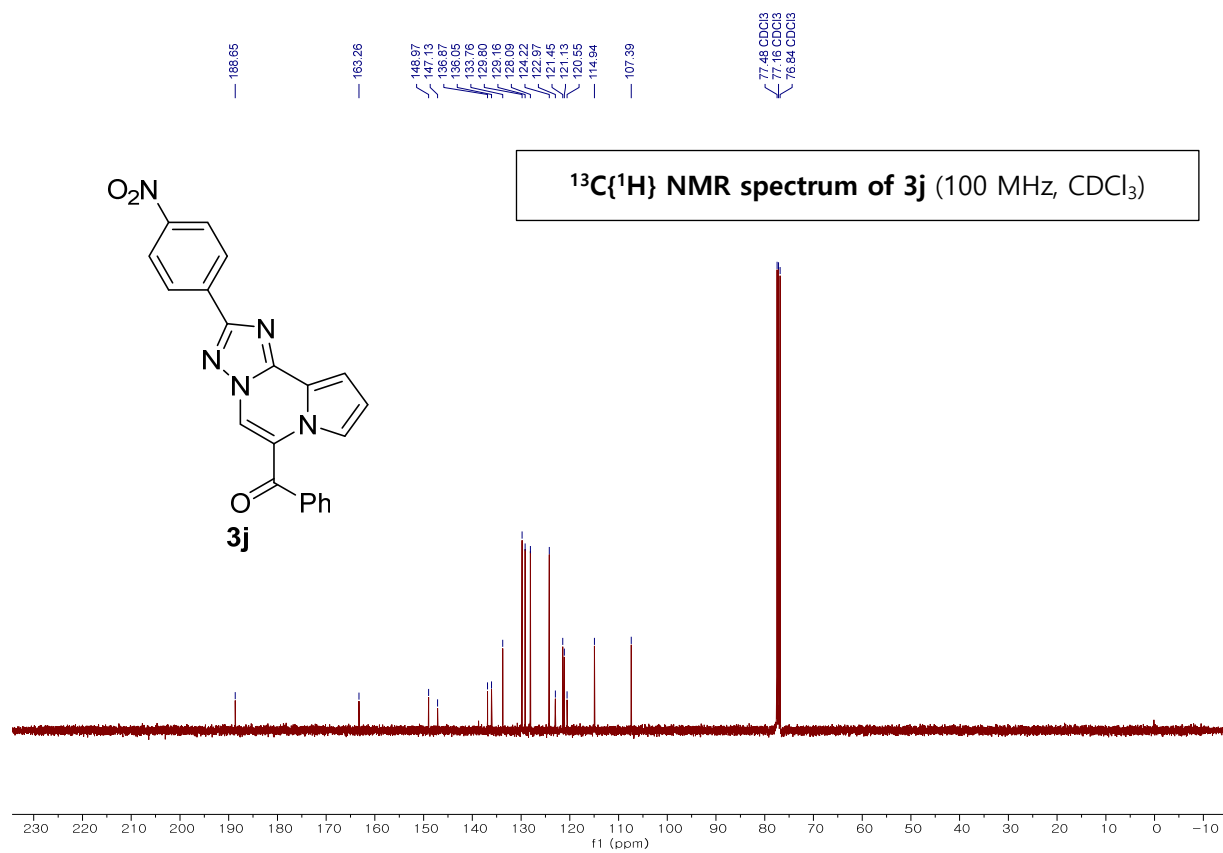
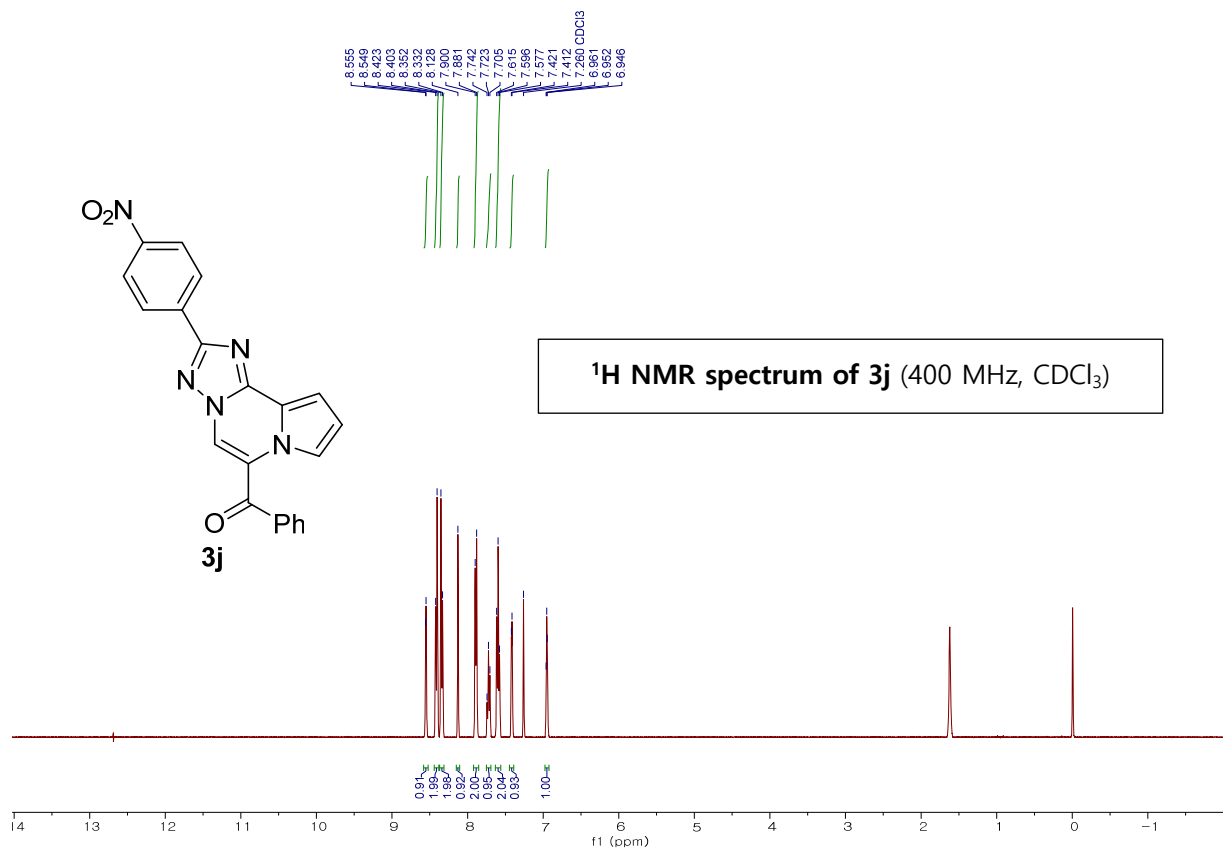


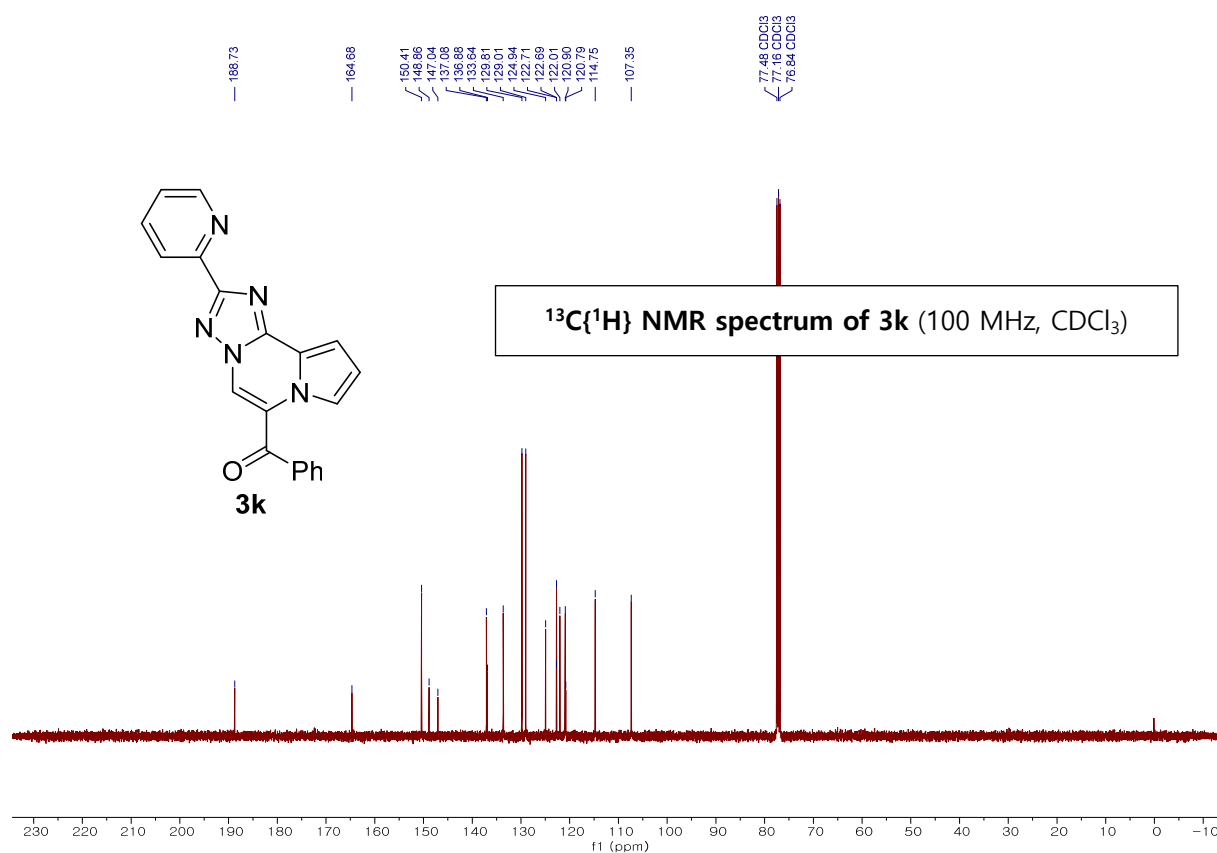
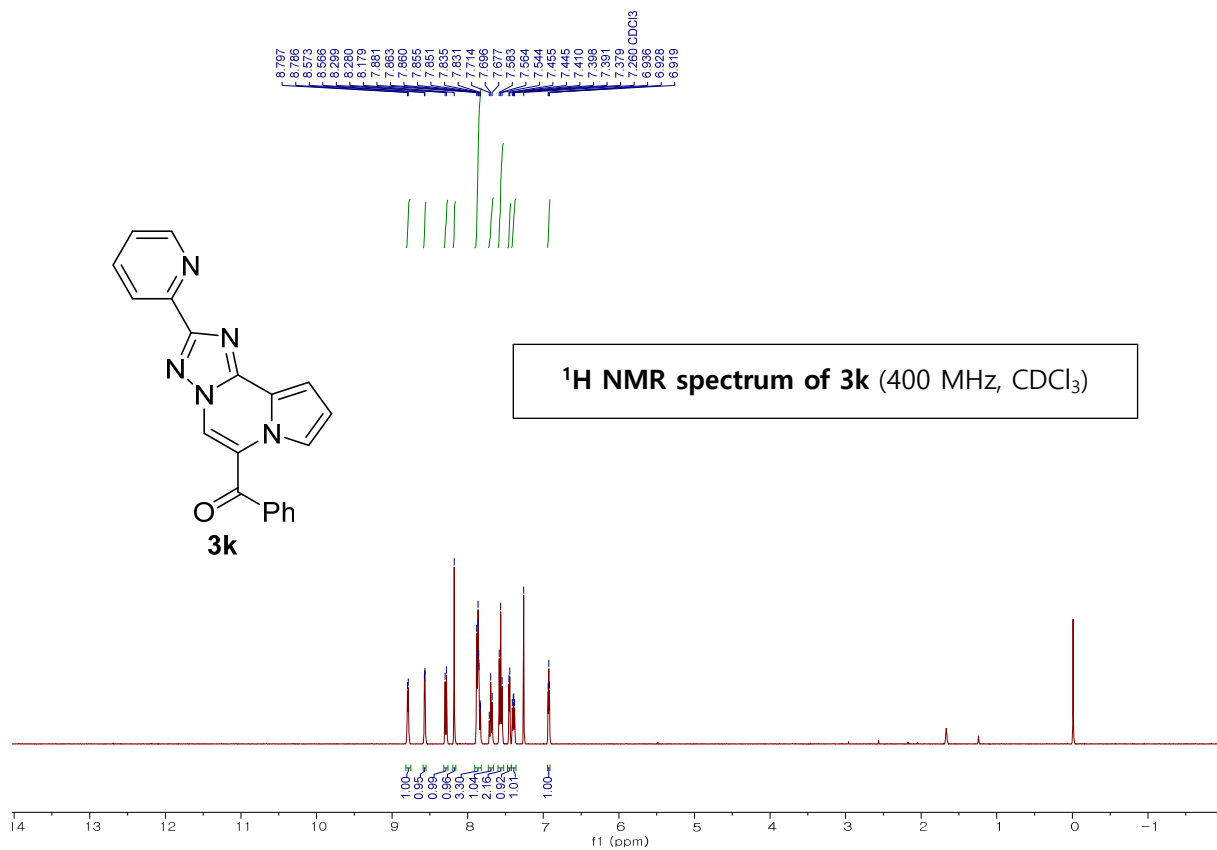
¹H NMR spectrum of **3i** (400 MHz, CDCl₃)

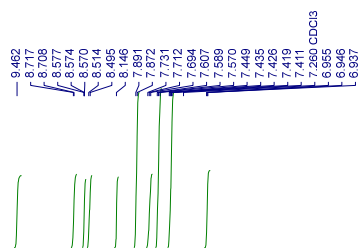
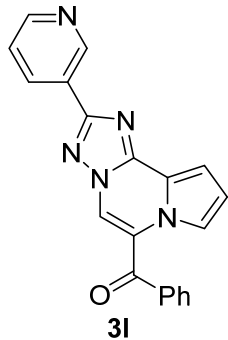


¹³C{¹H} NMR spectrum of **3i** (100 MHz, CDCl₃)

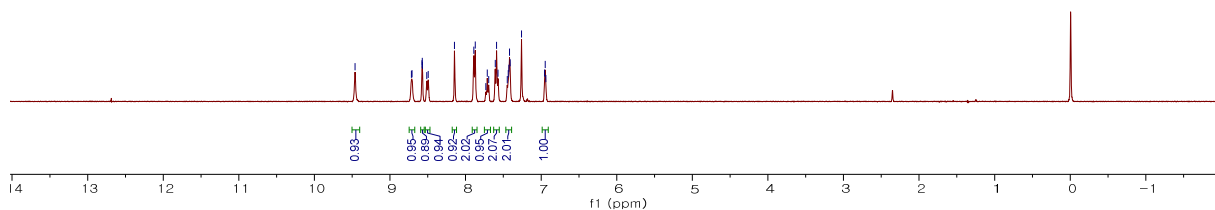




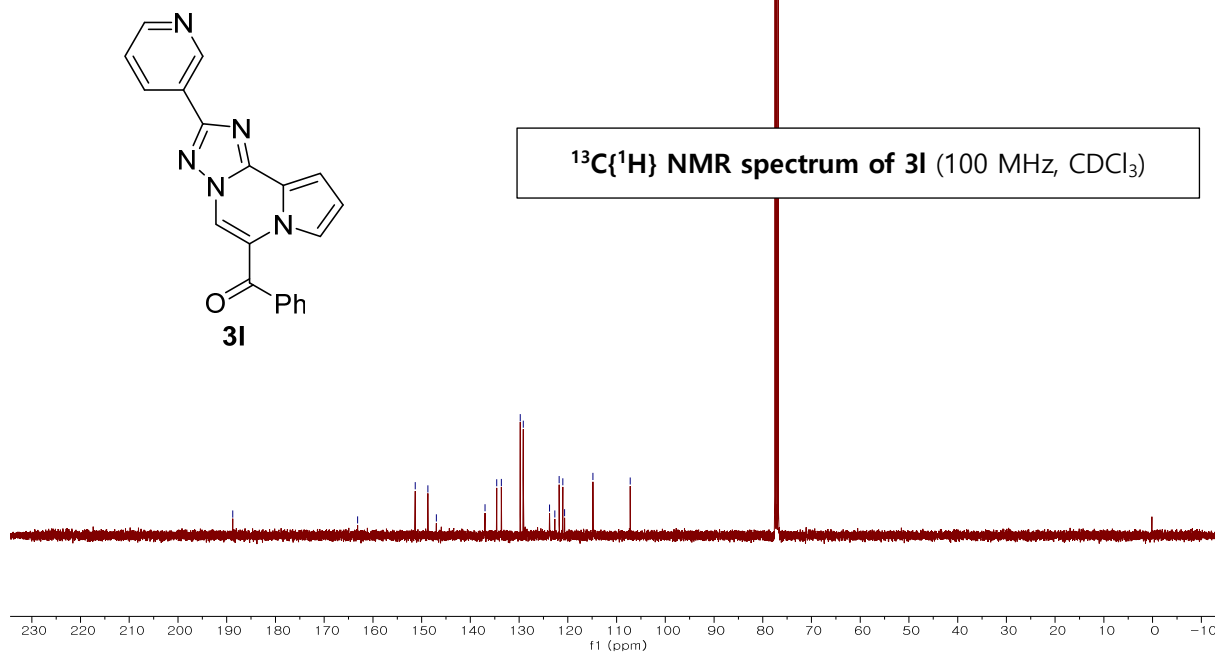


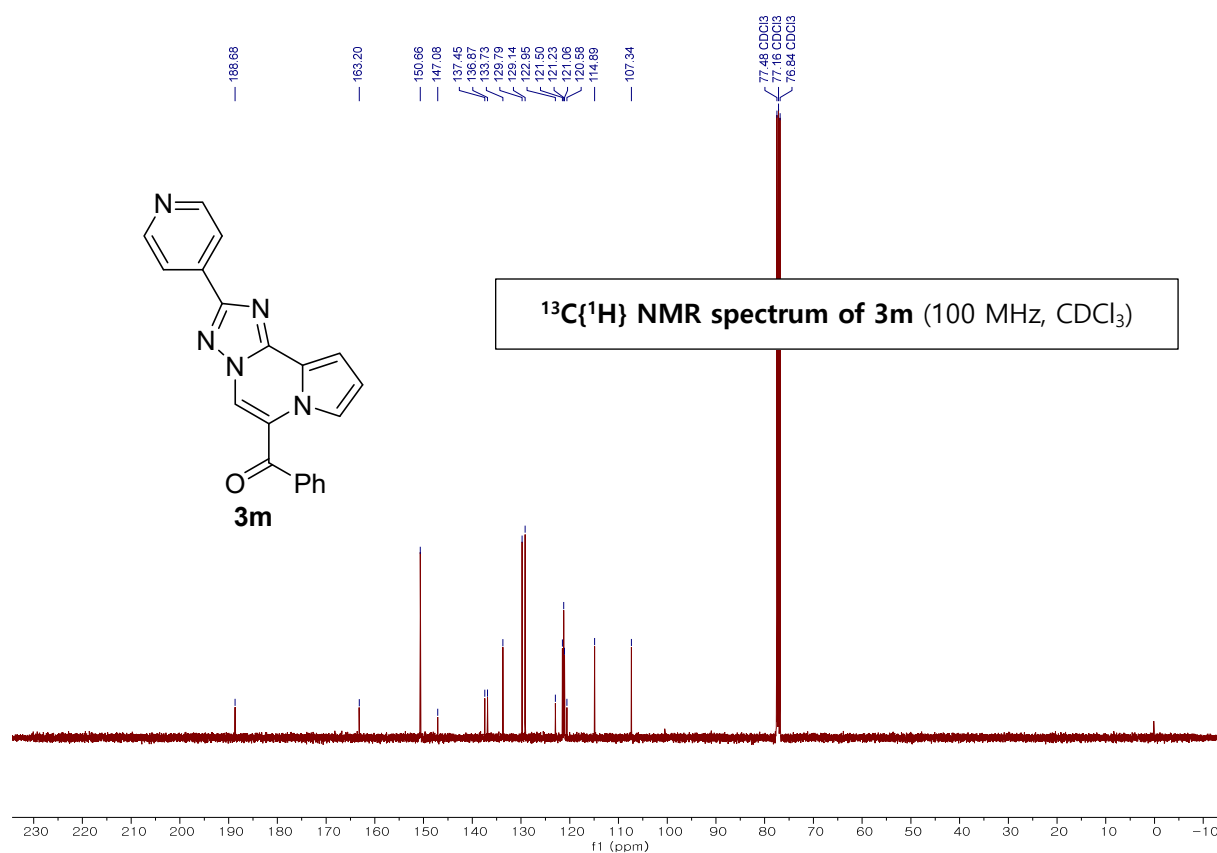
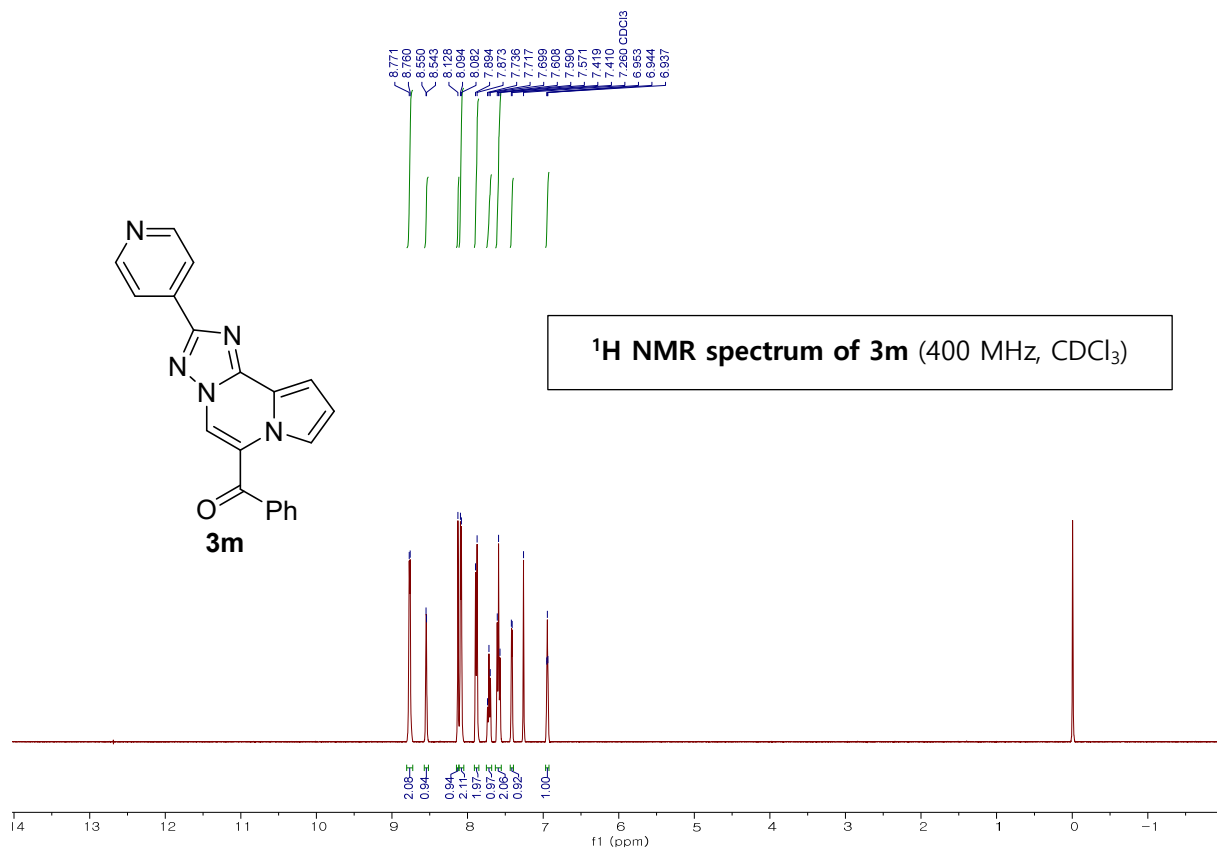


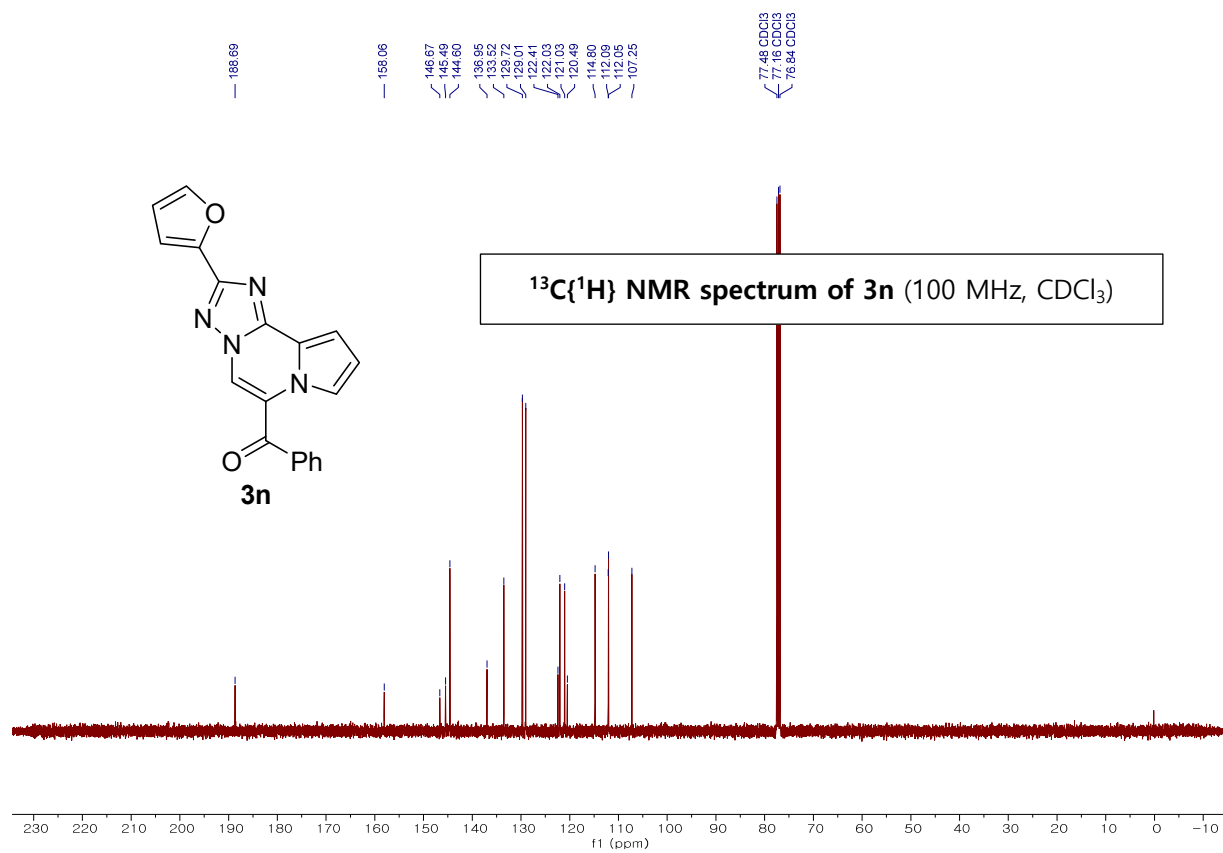
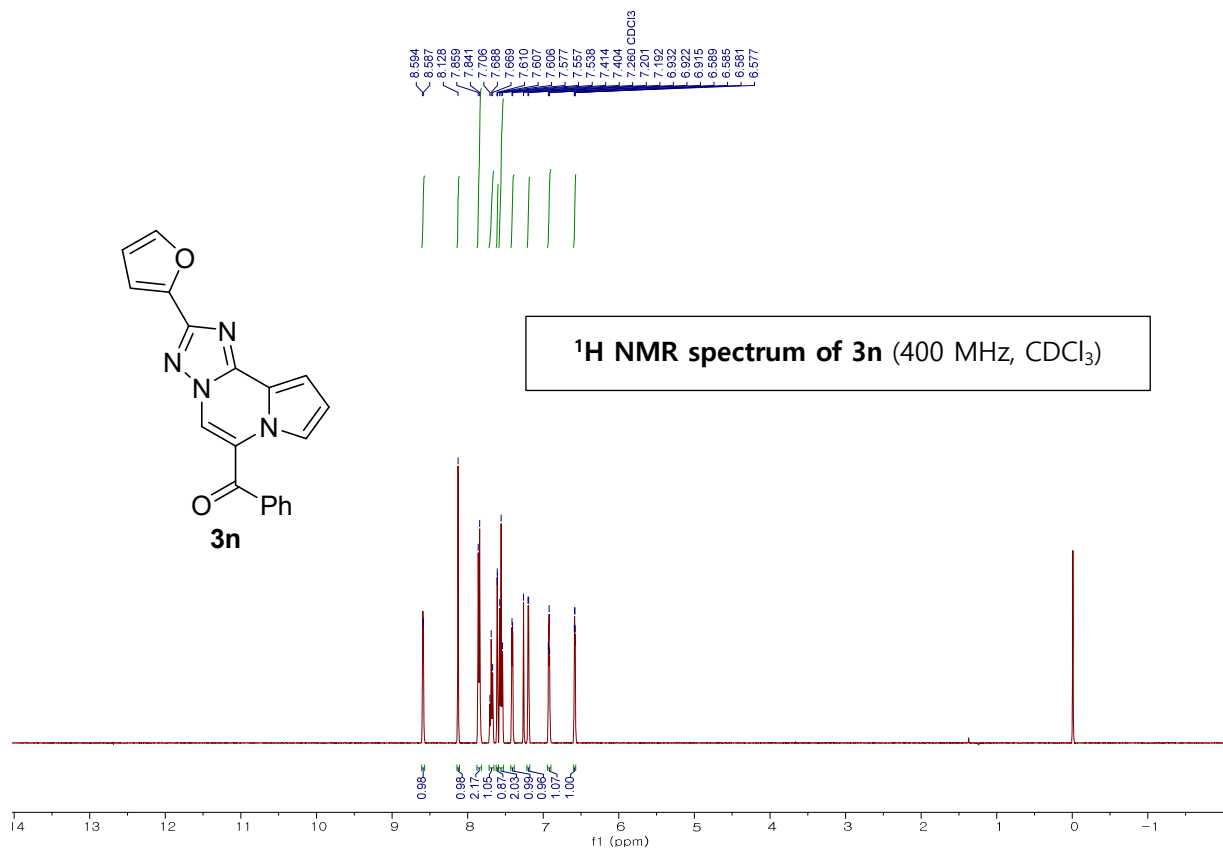
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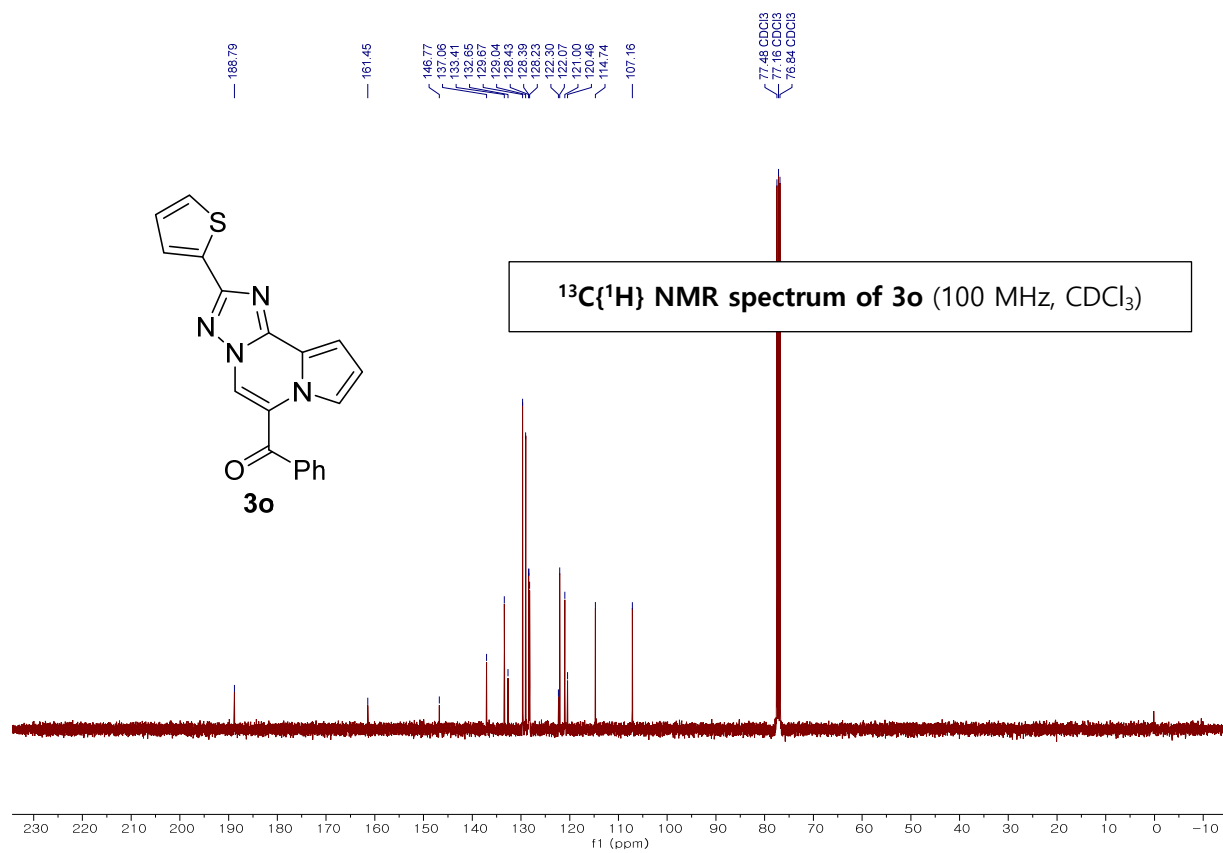
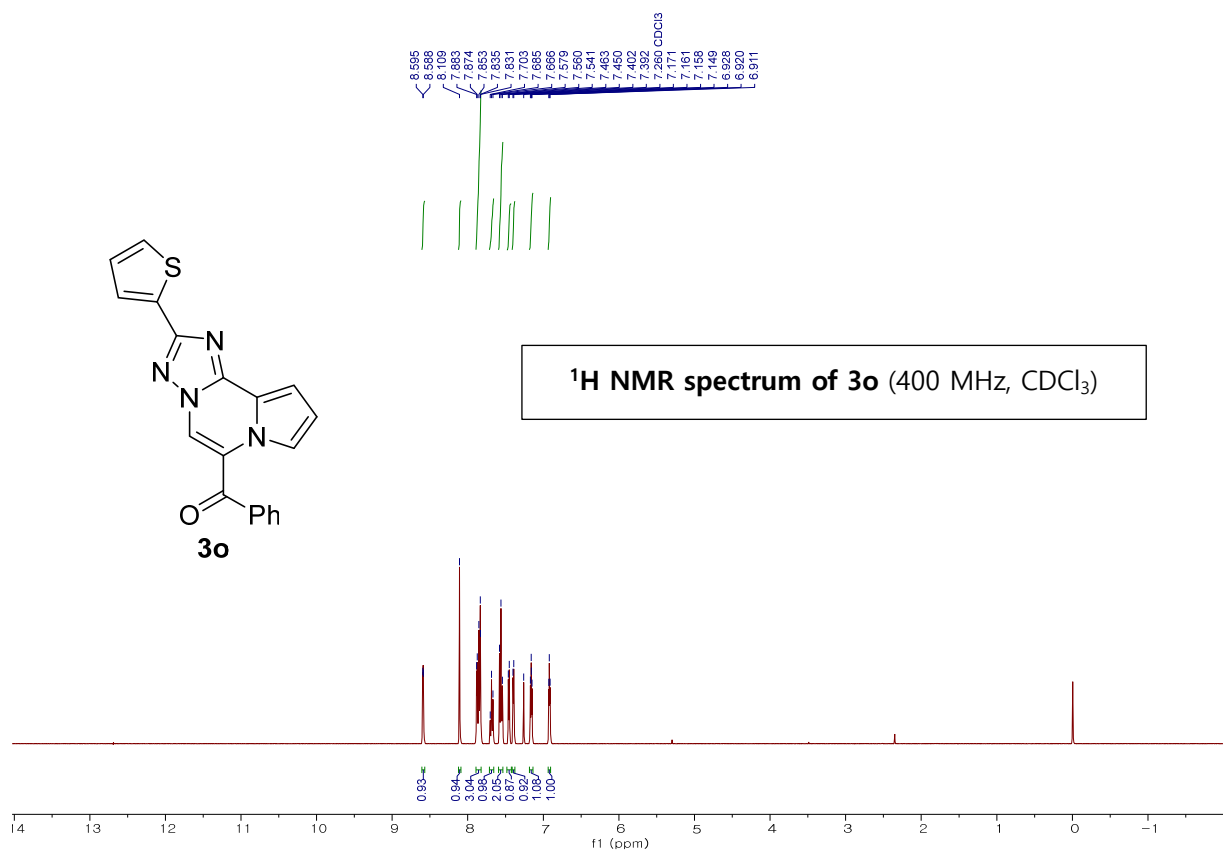


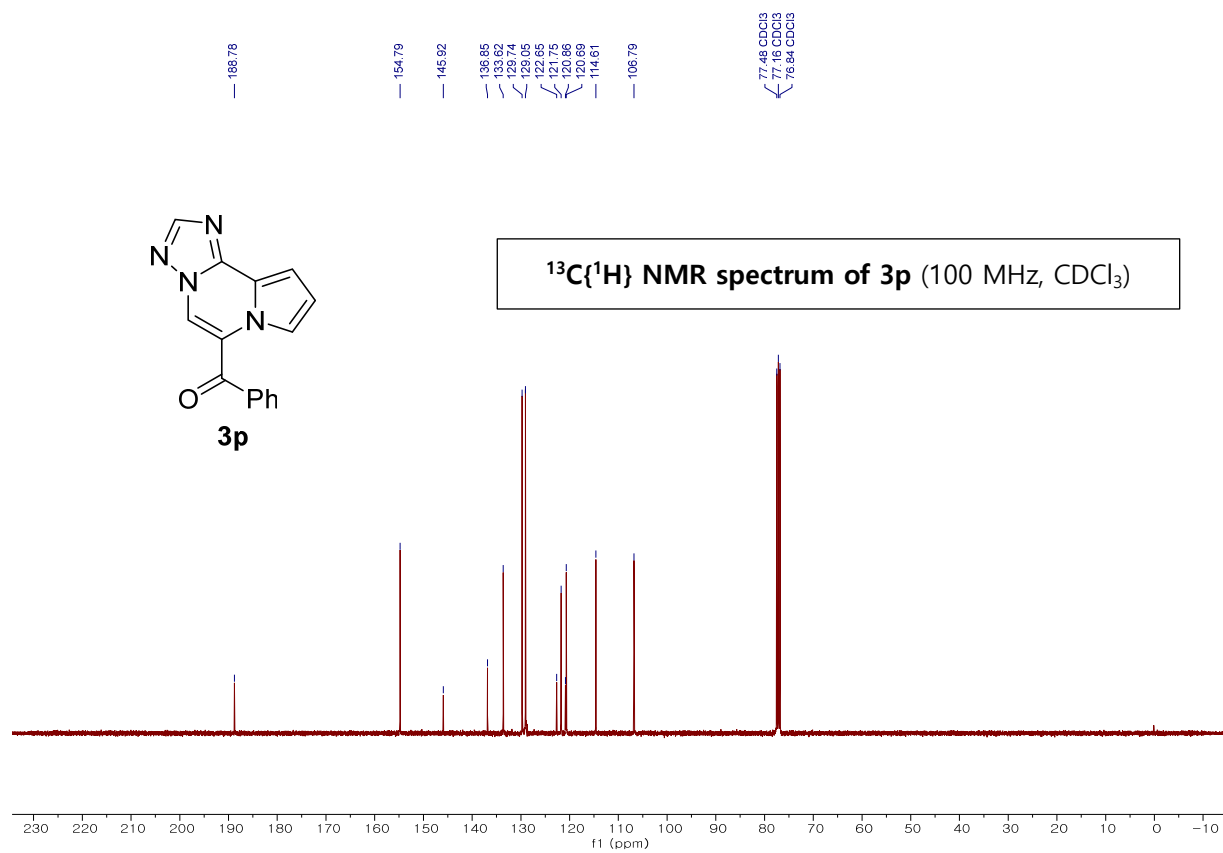
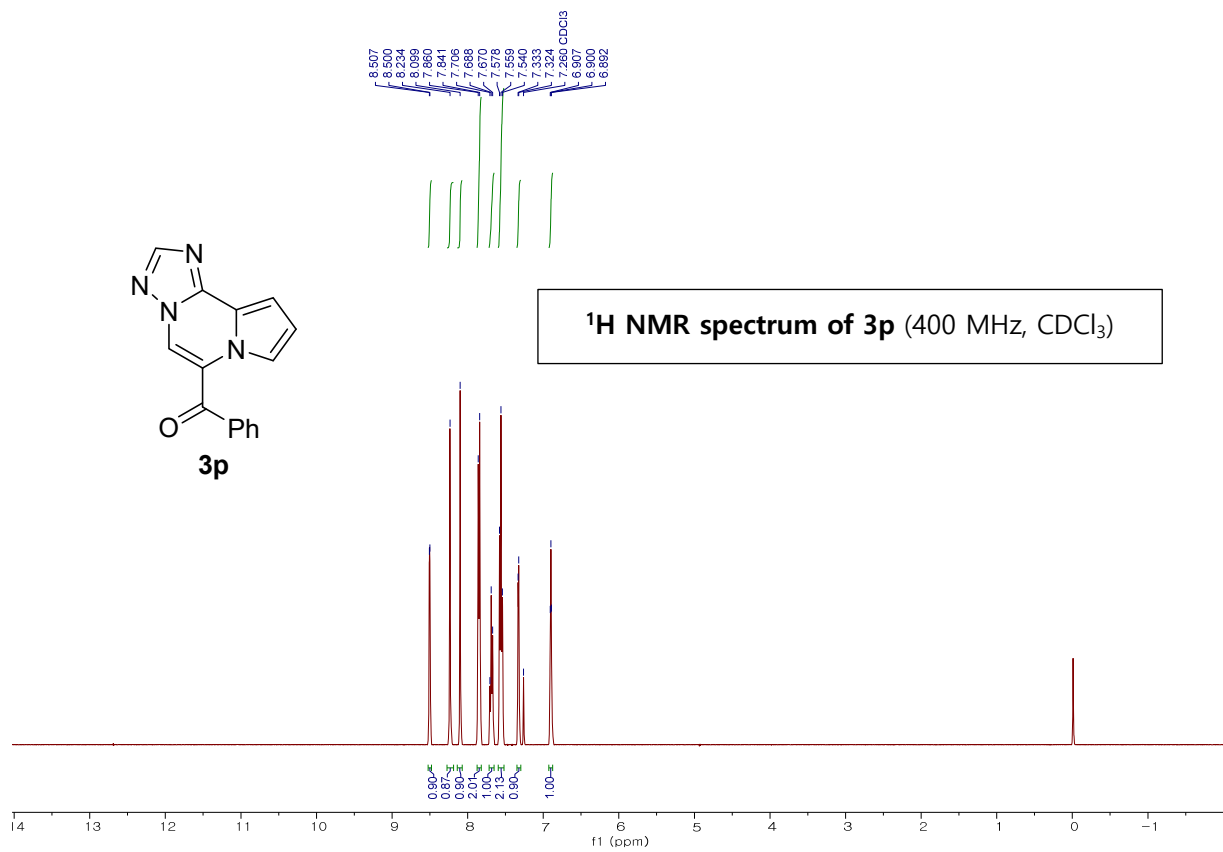
¹³C{¹H} NMR spectrum of 3I (100 MHz, CDCl₃)

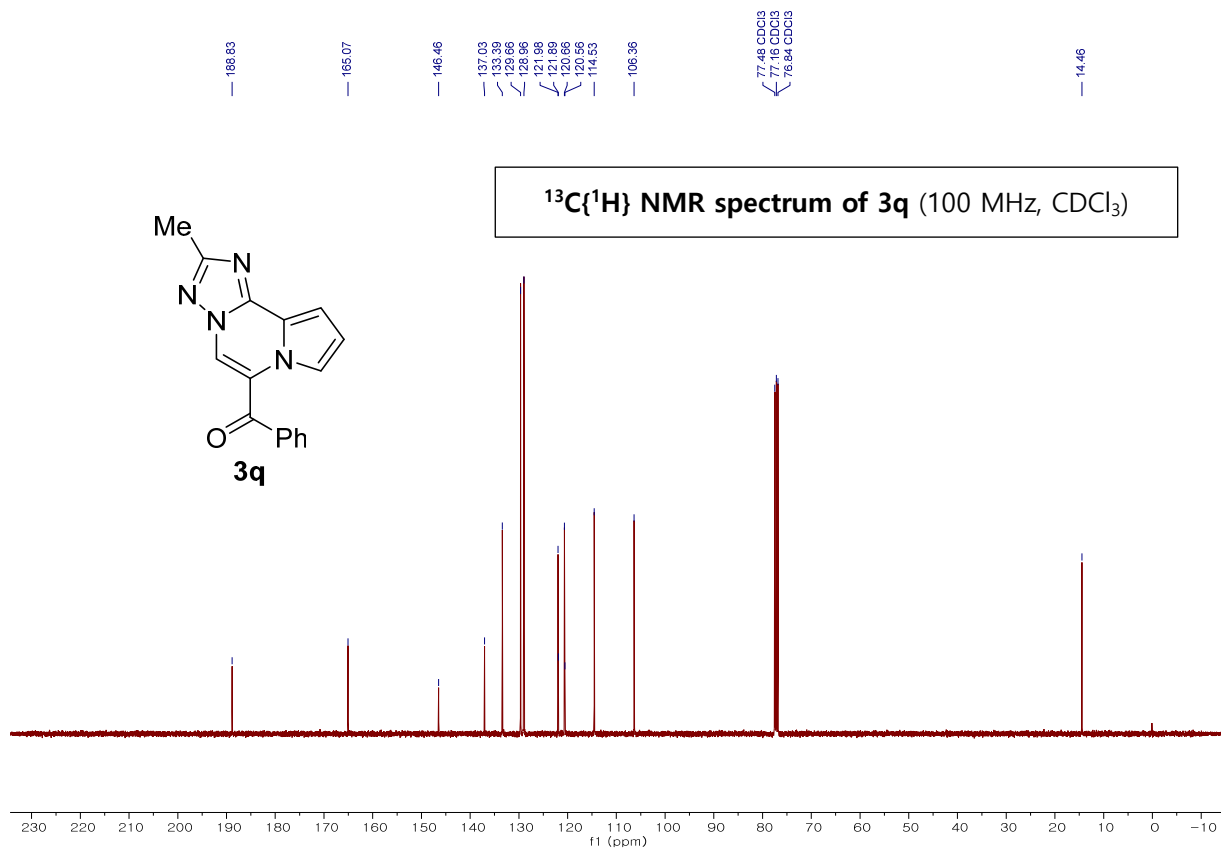
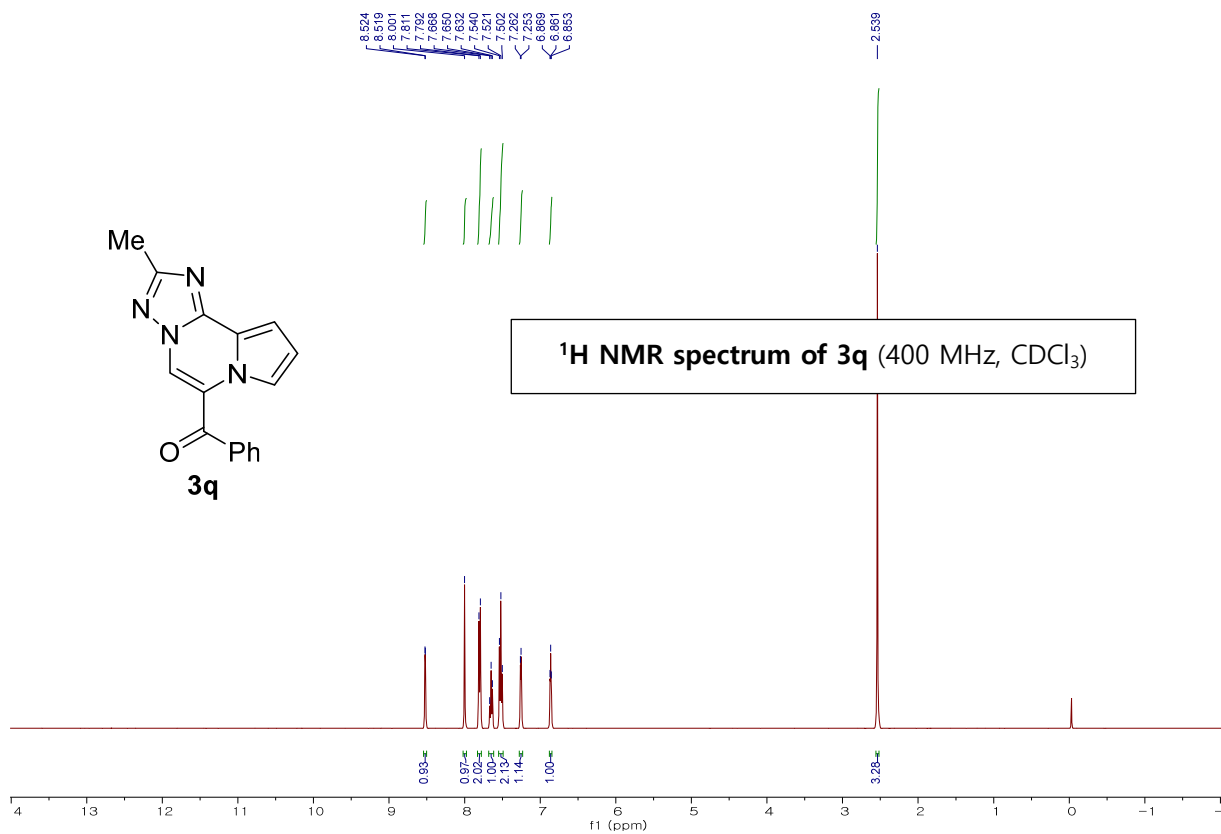


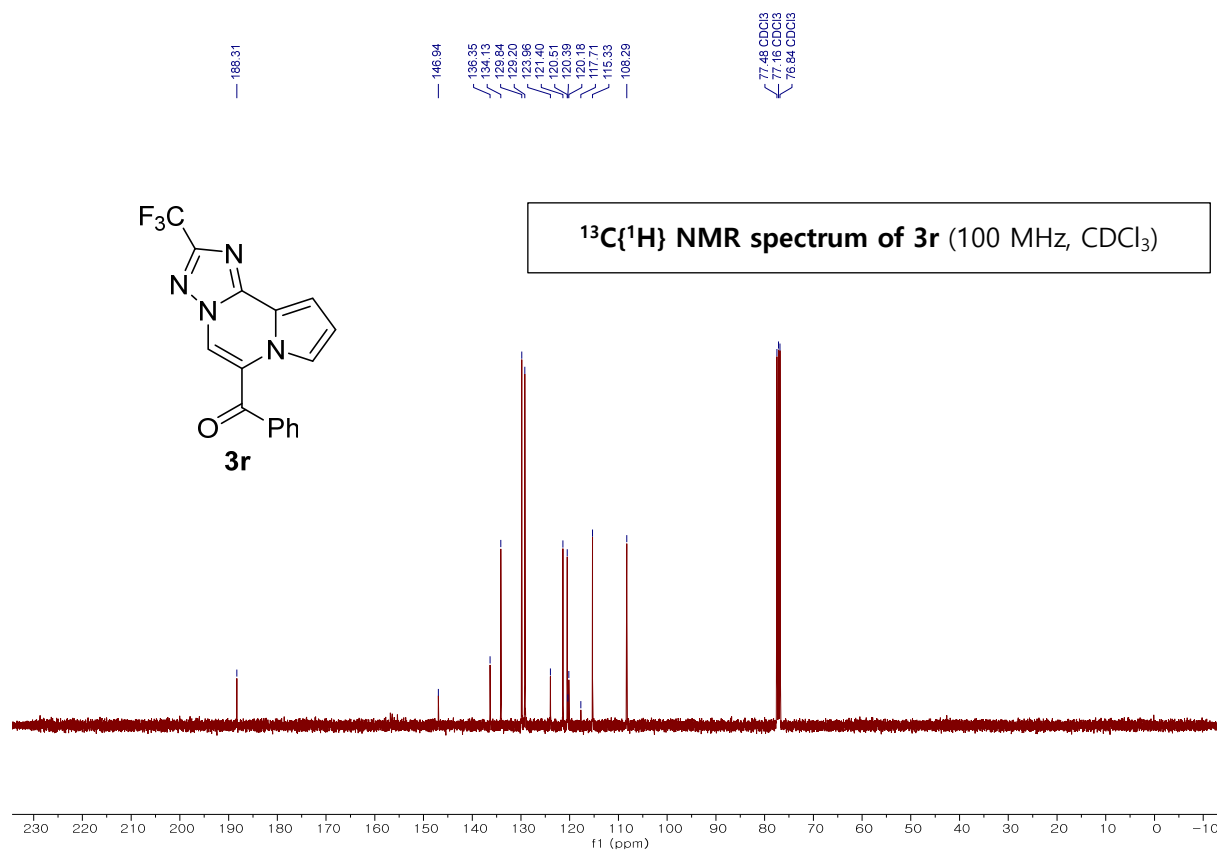
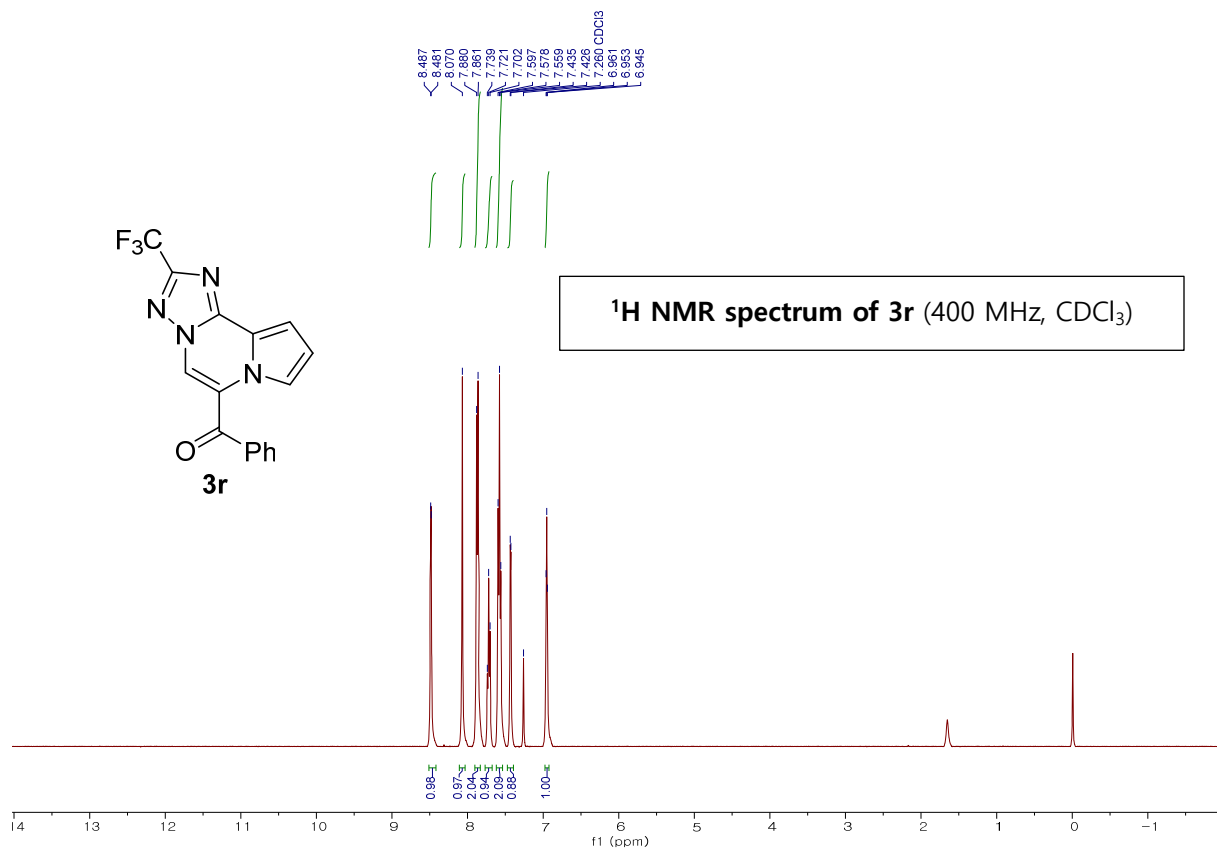




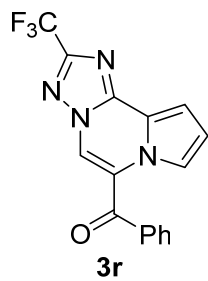




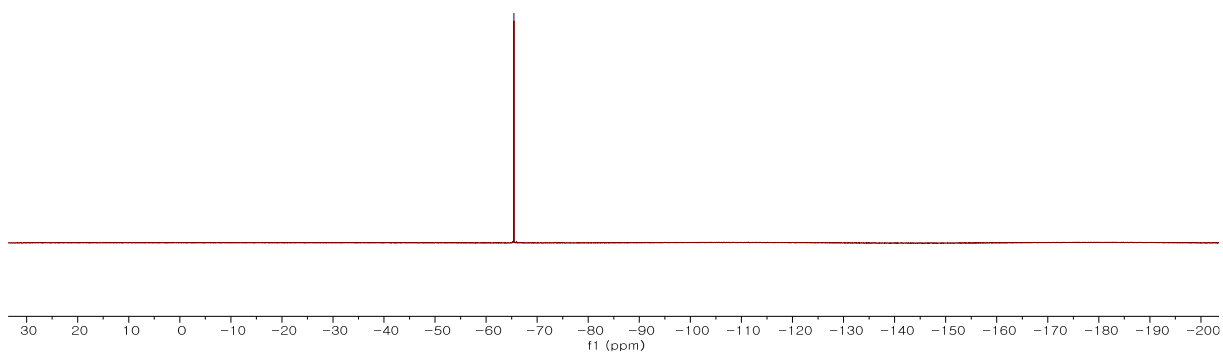


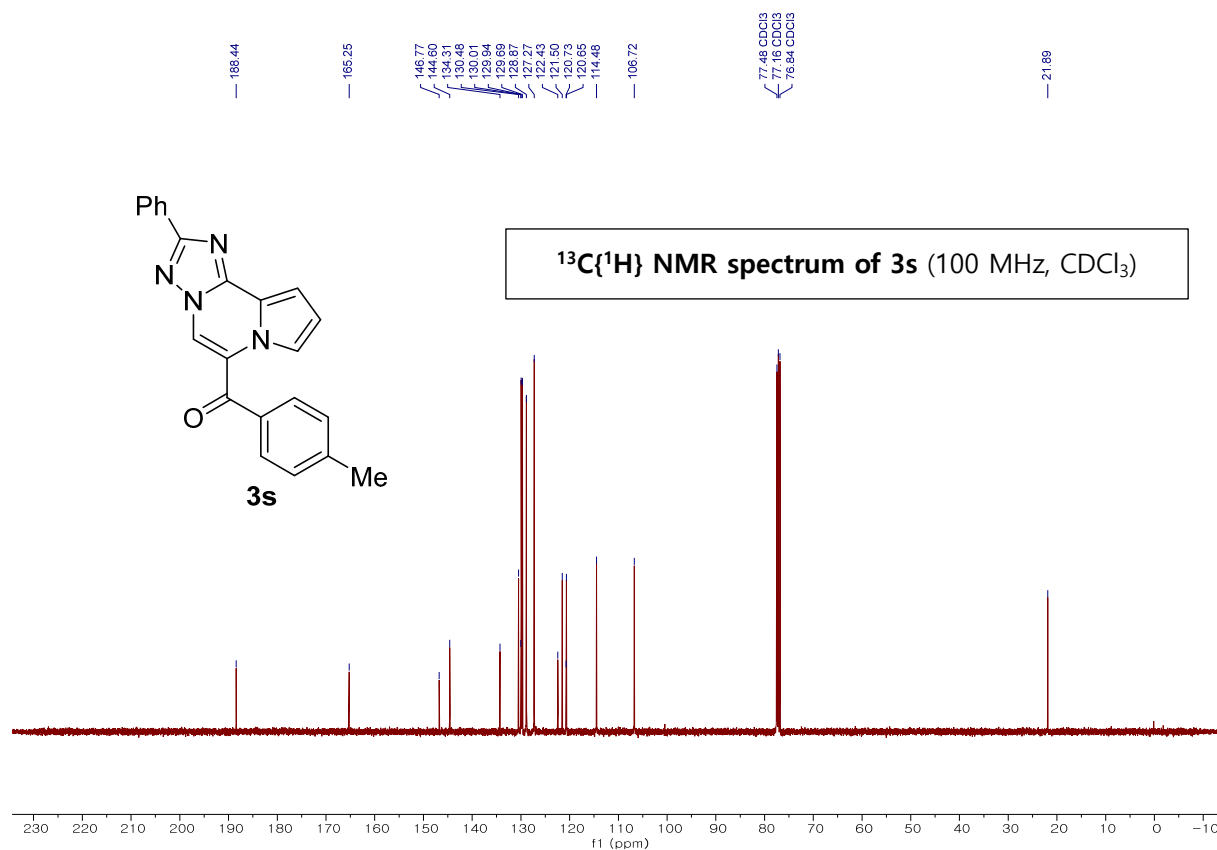
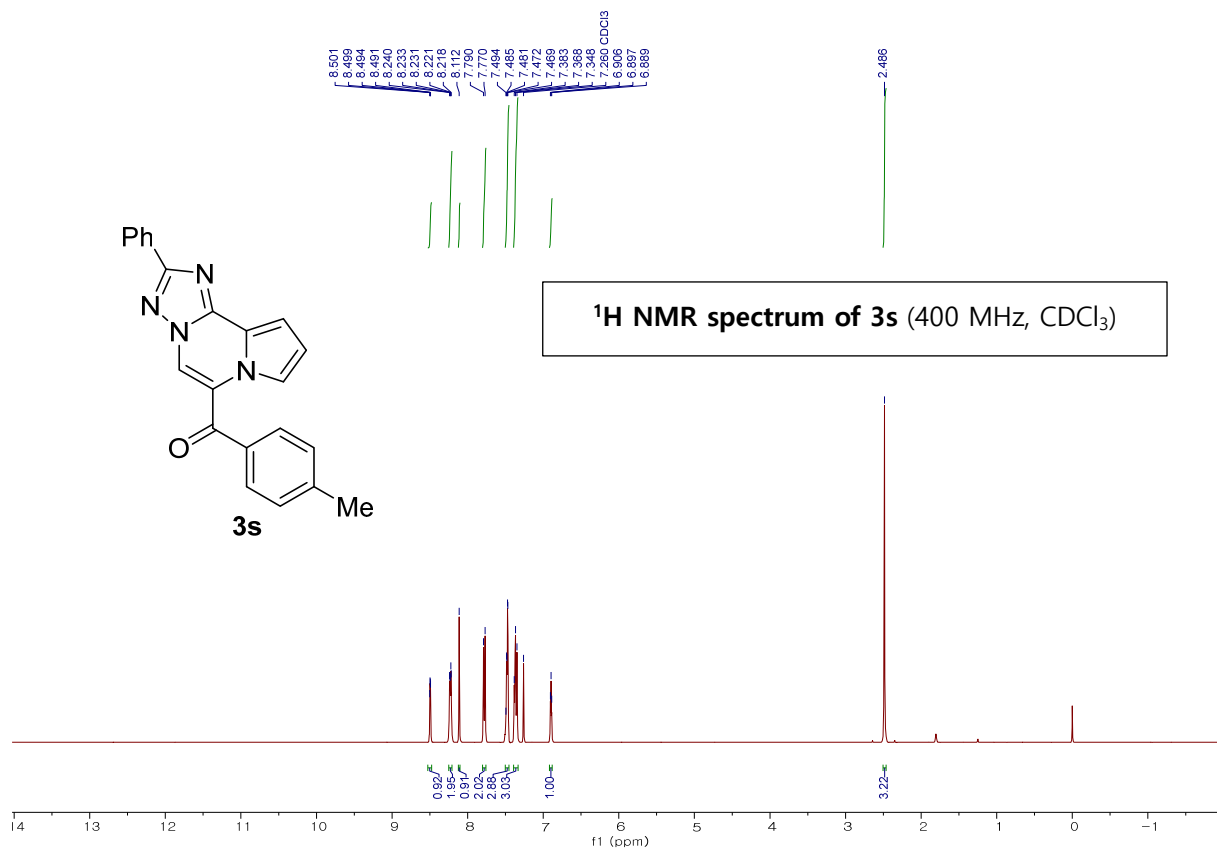


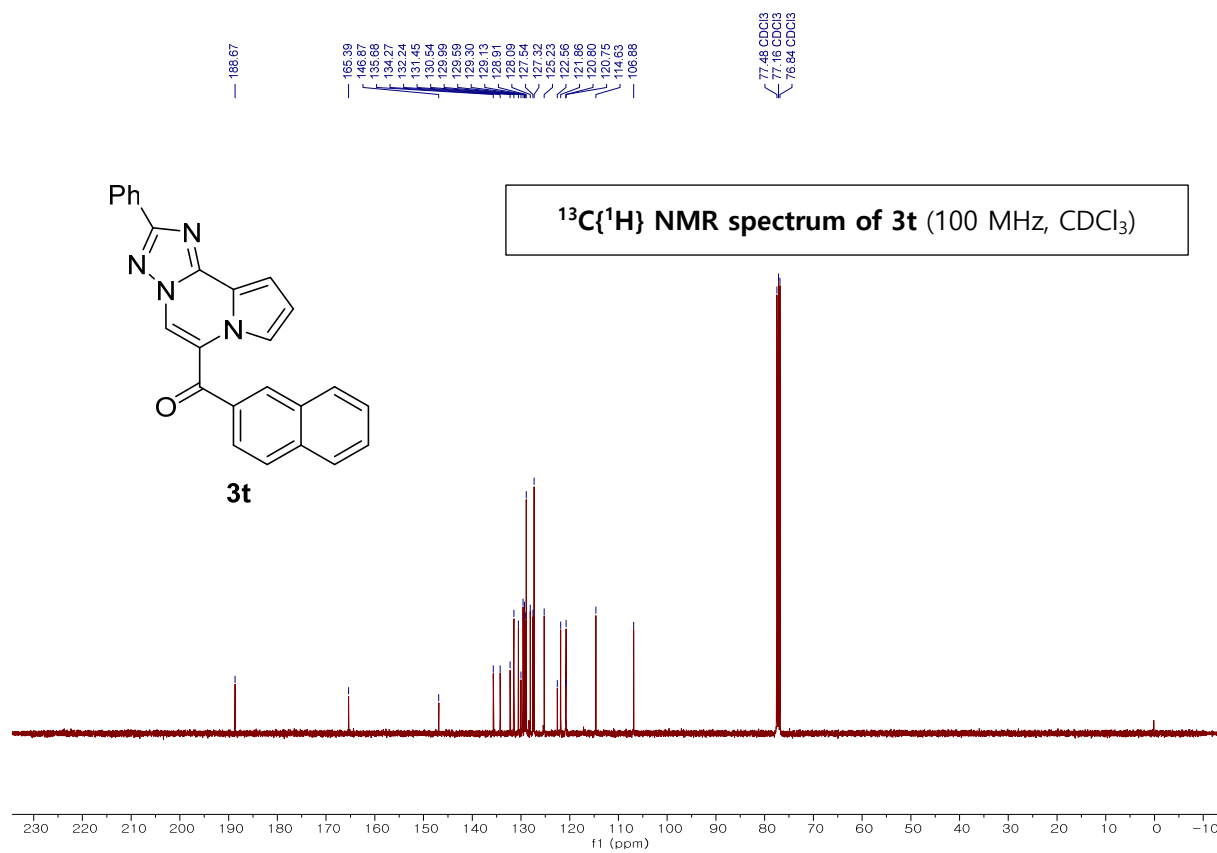
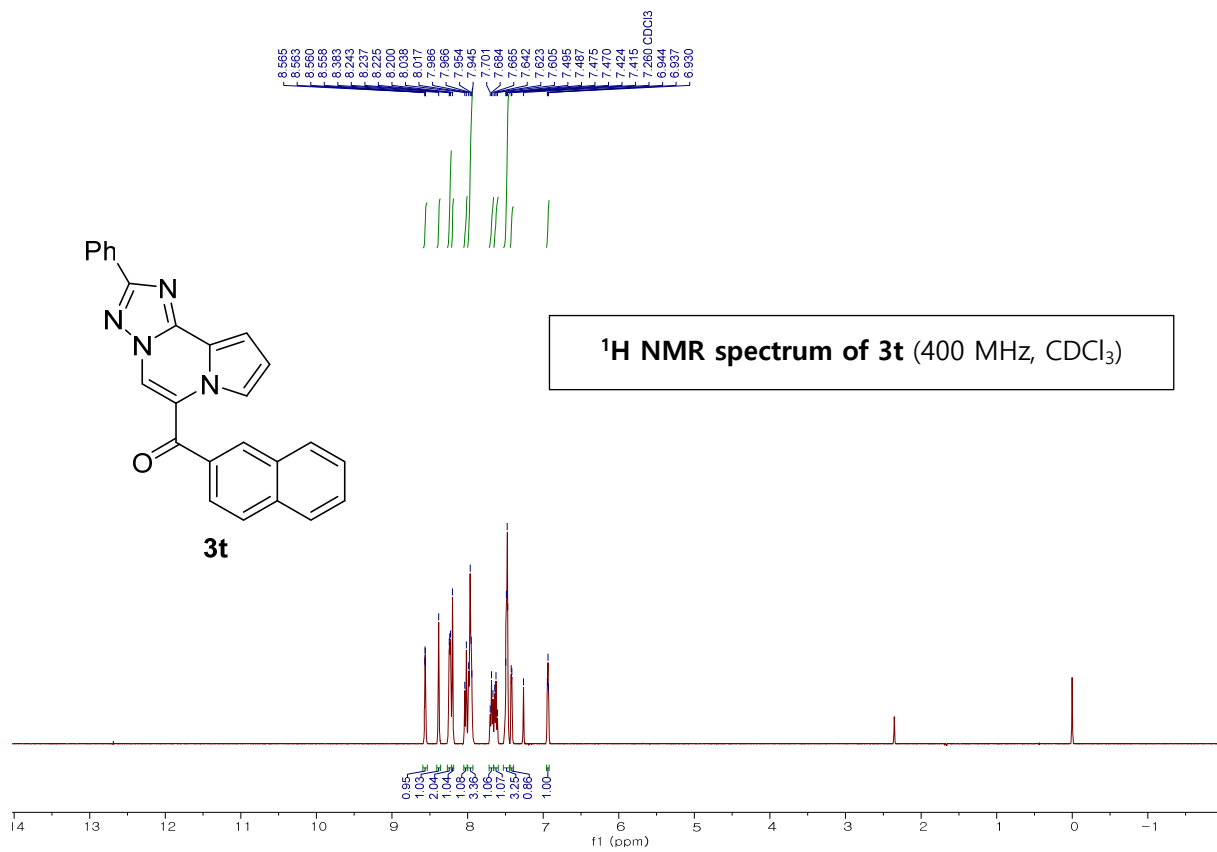
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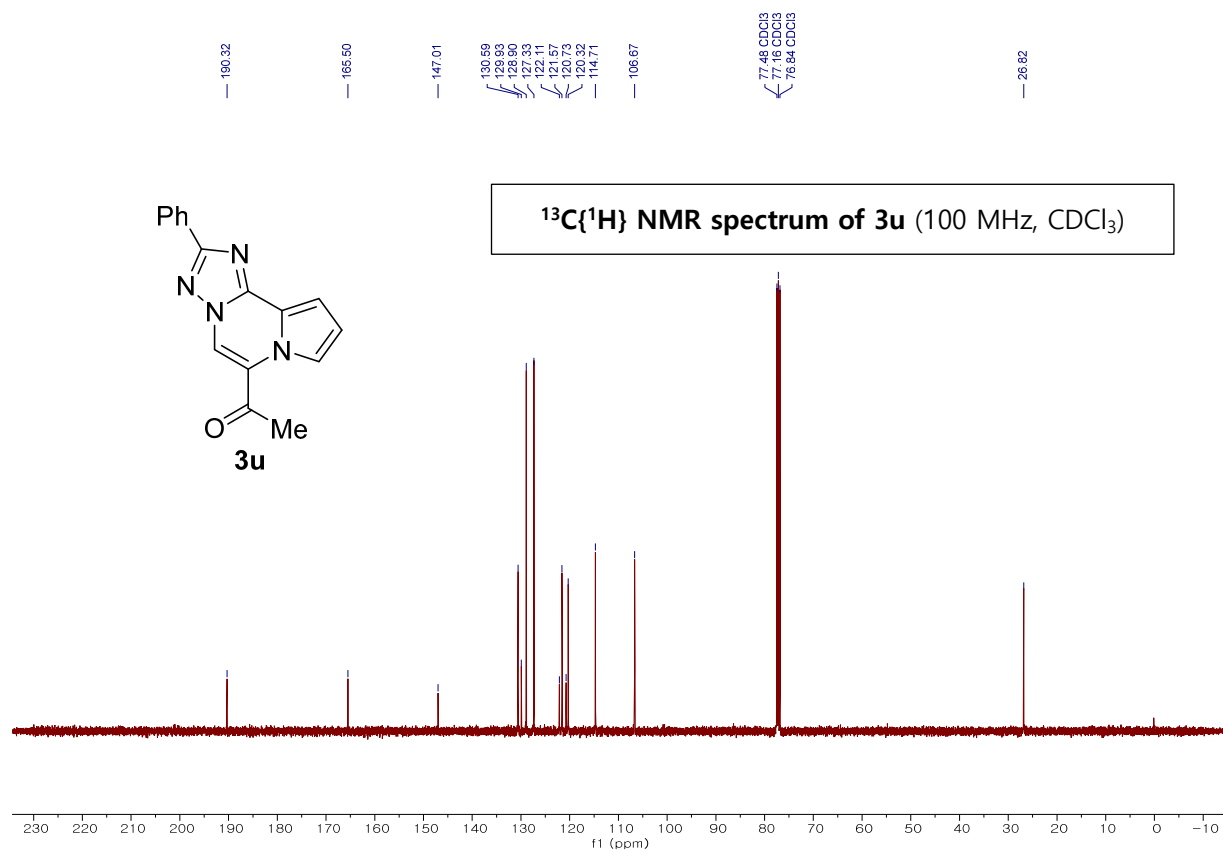
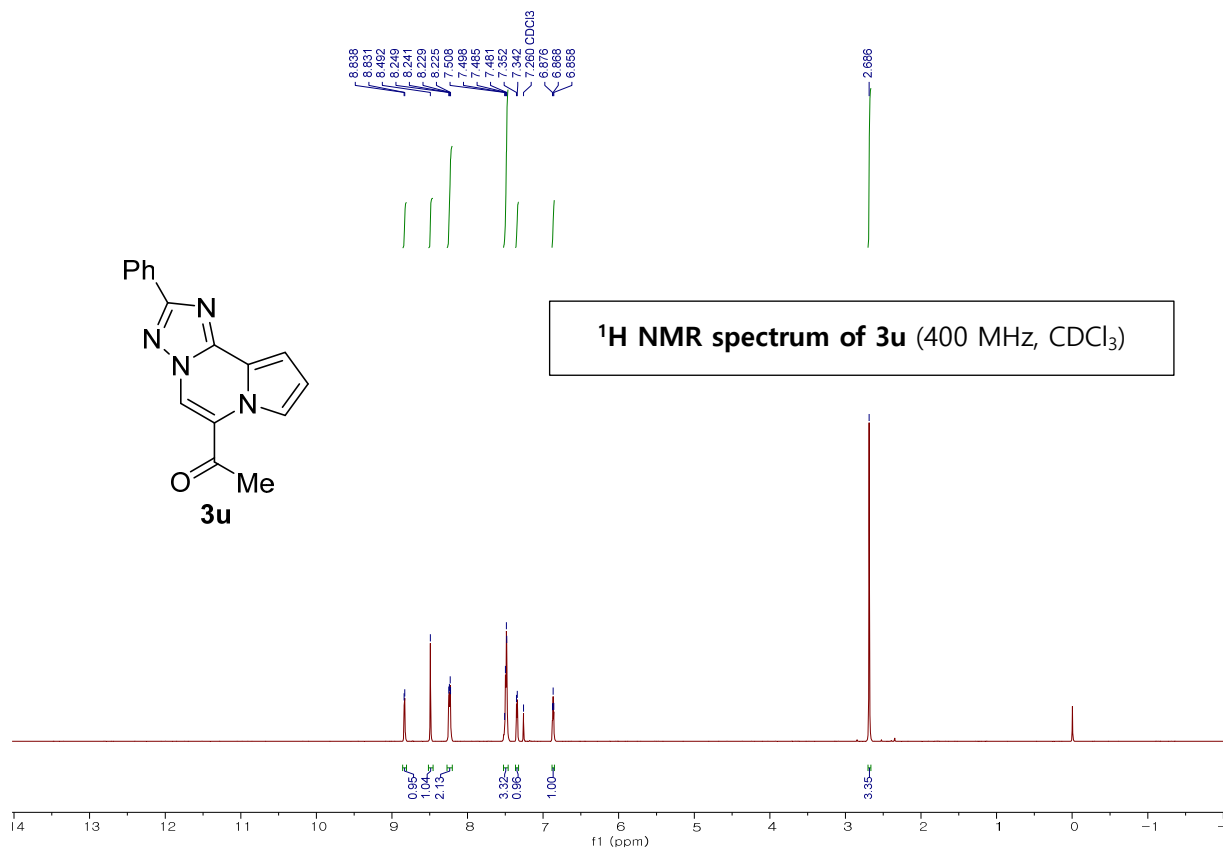


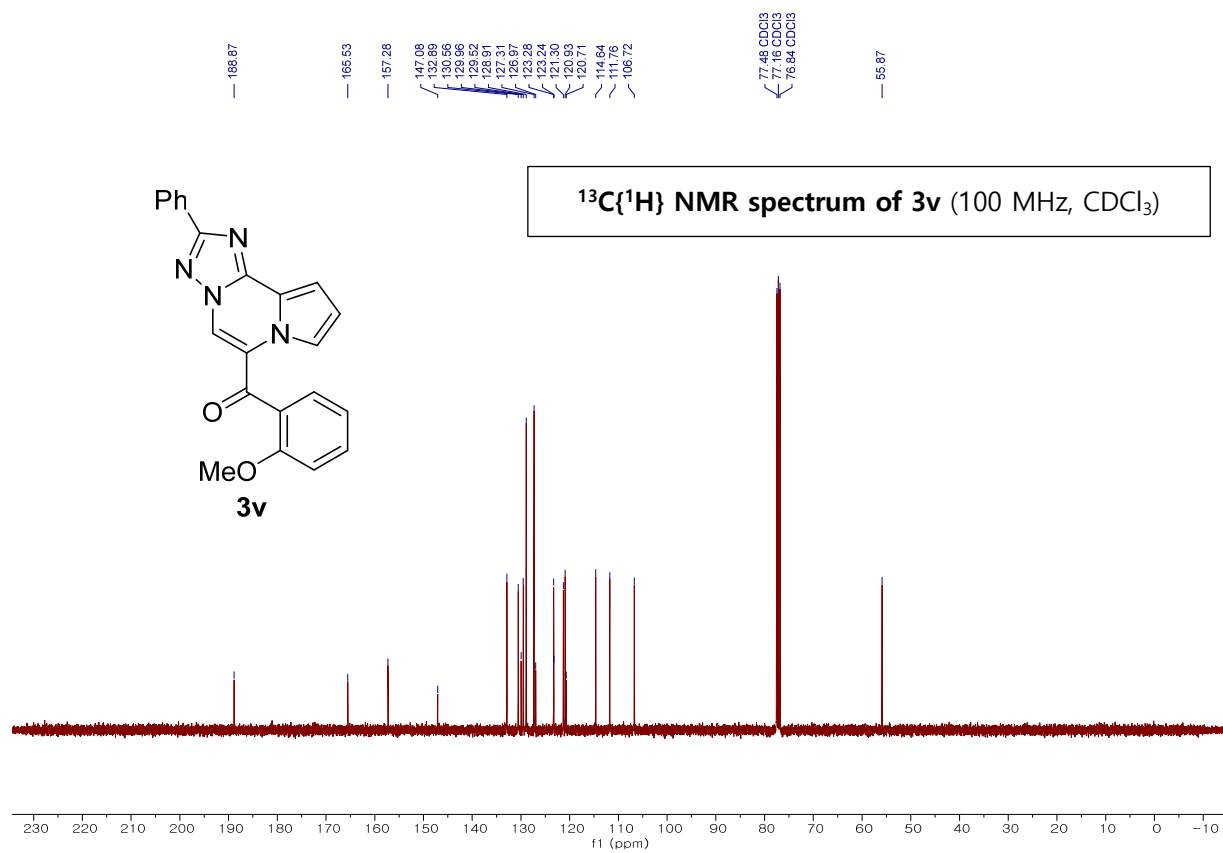
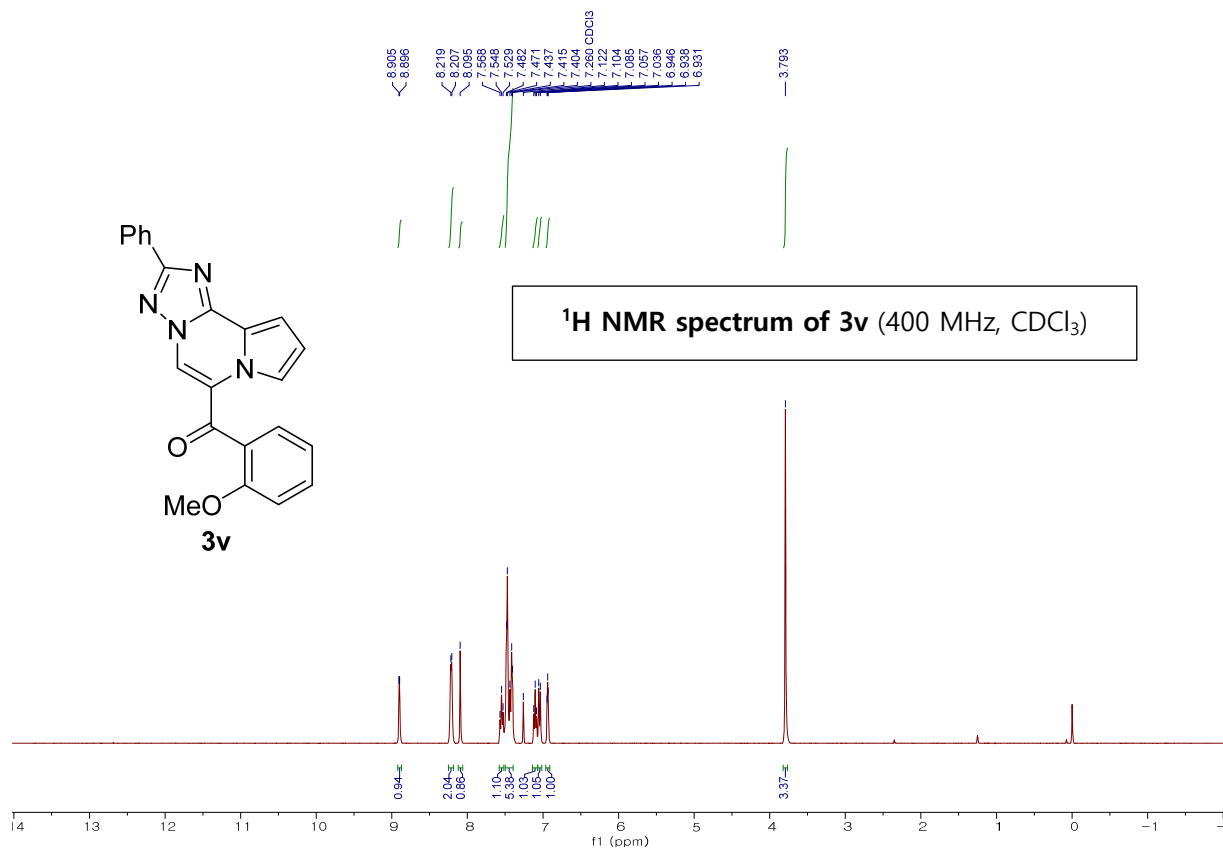
¹⁹F NMR spectrum of 3r (376 MHz, CDCl₃)

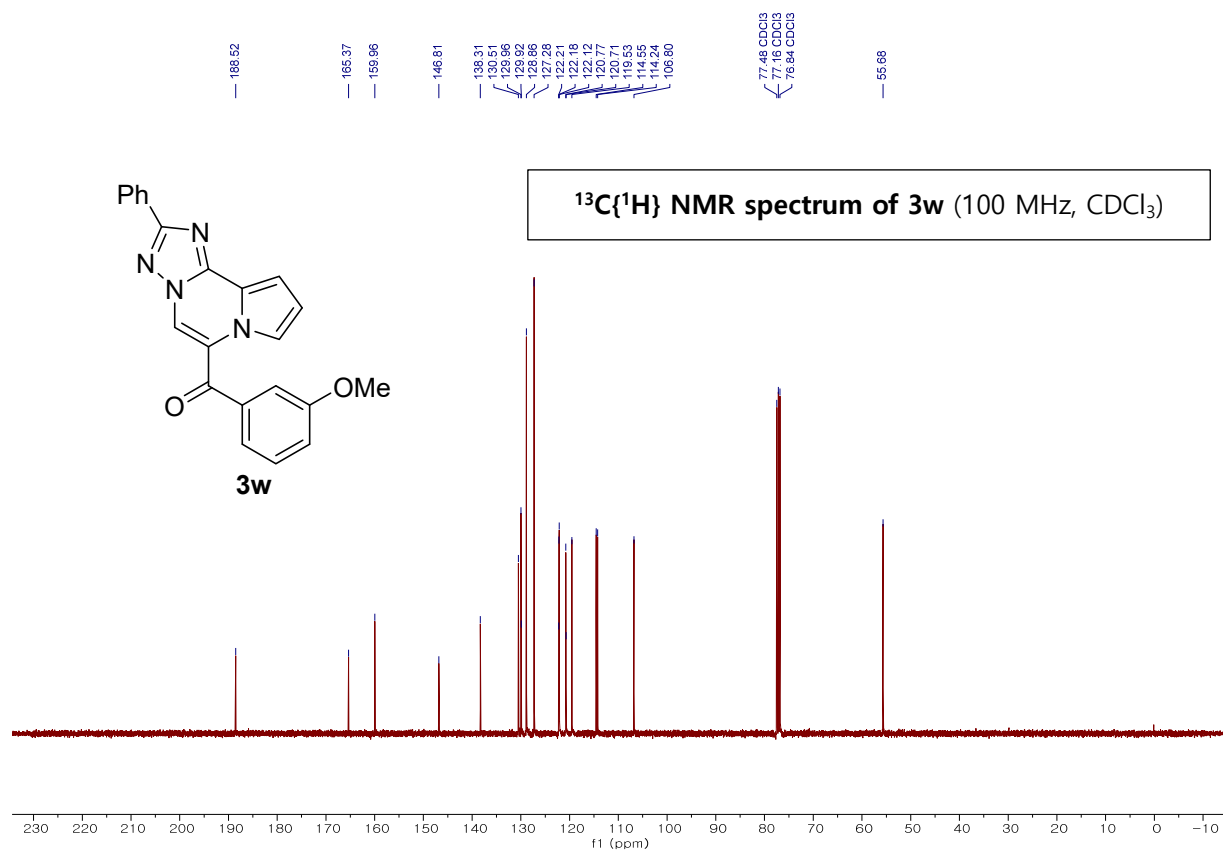
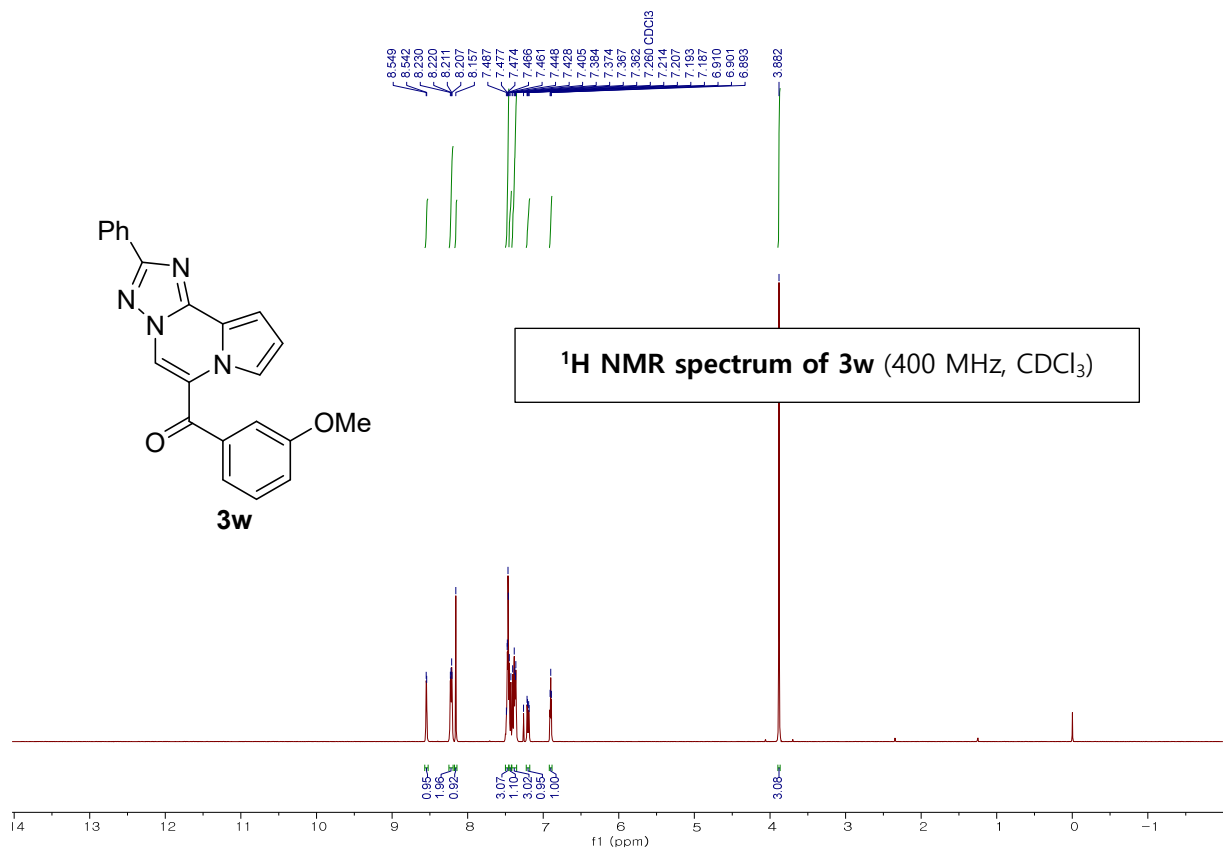


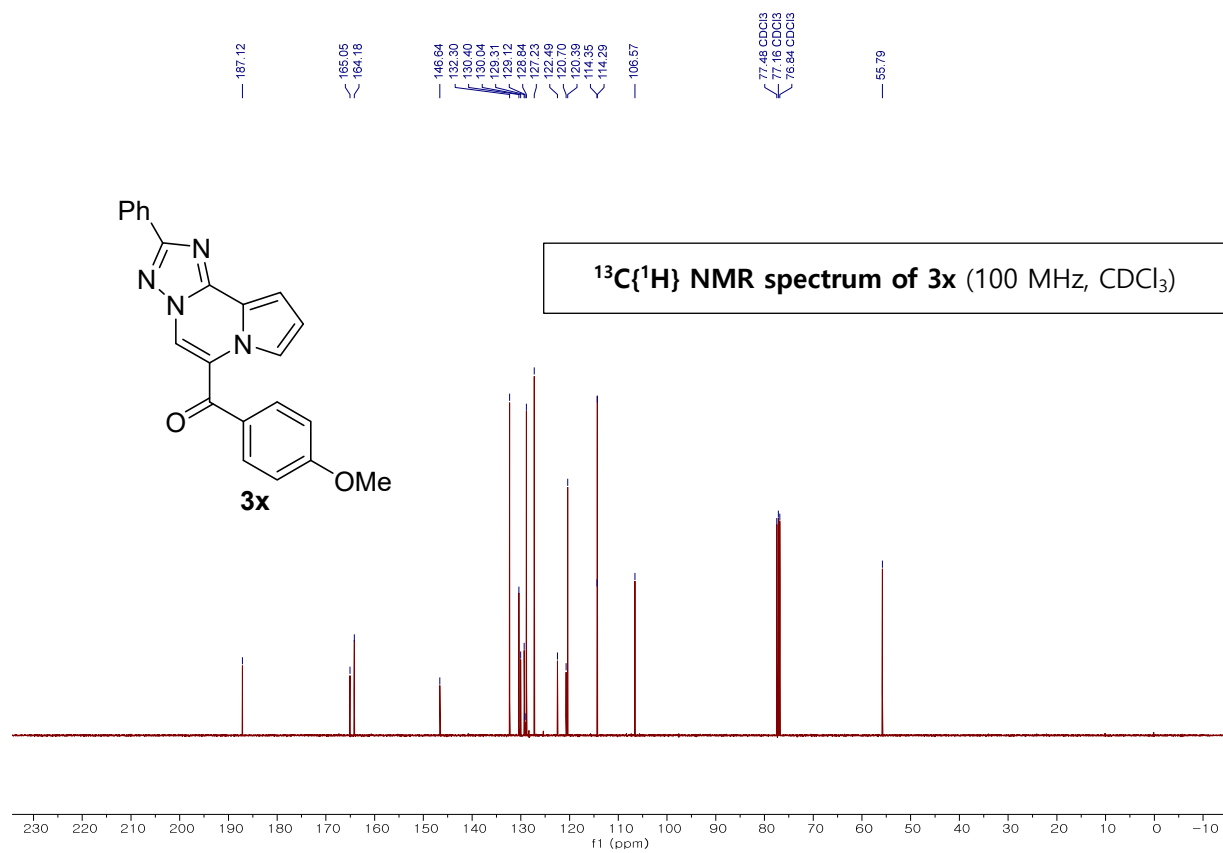
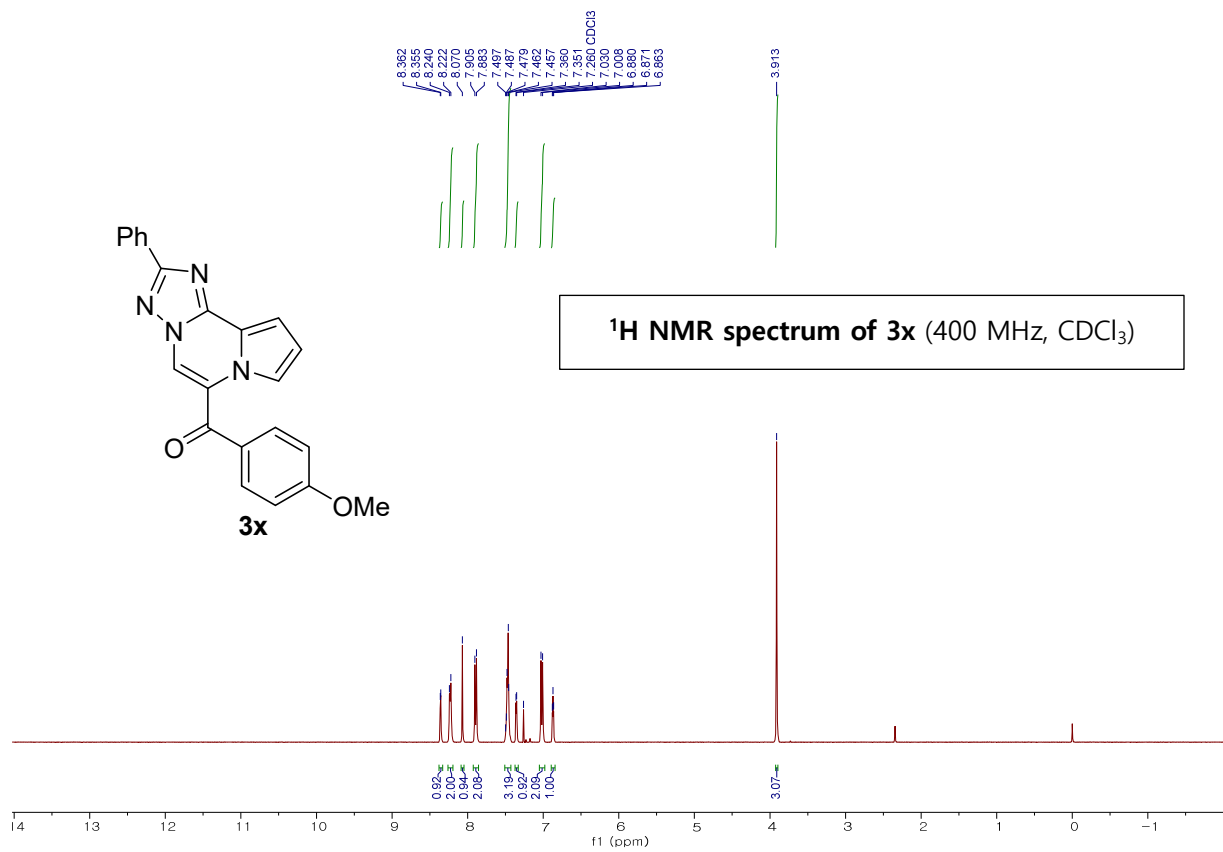


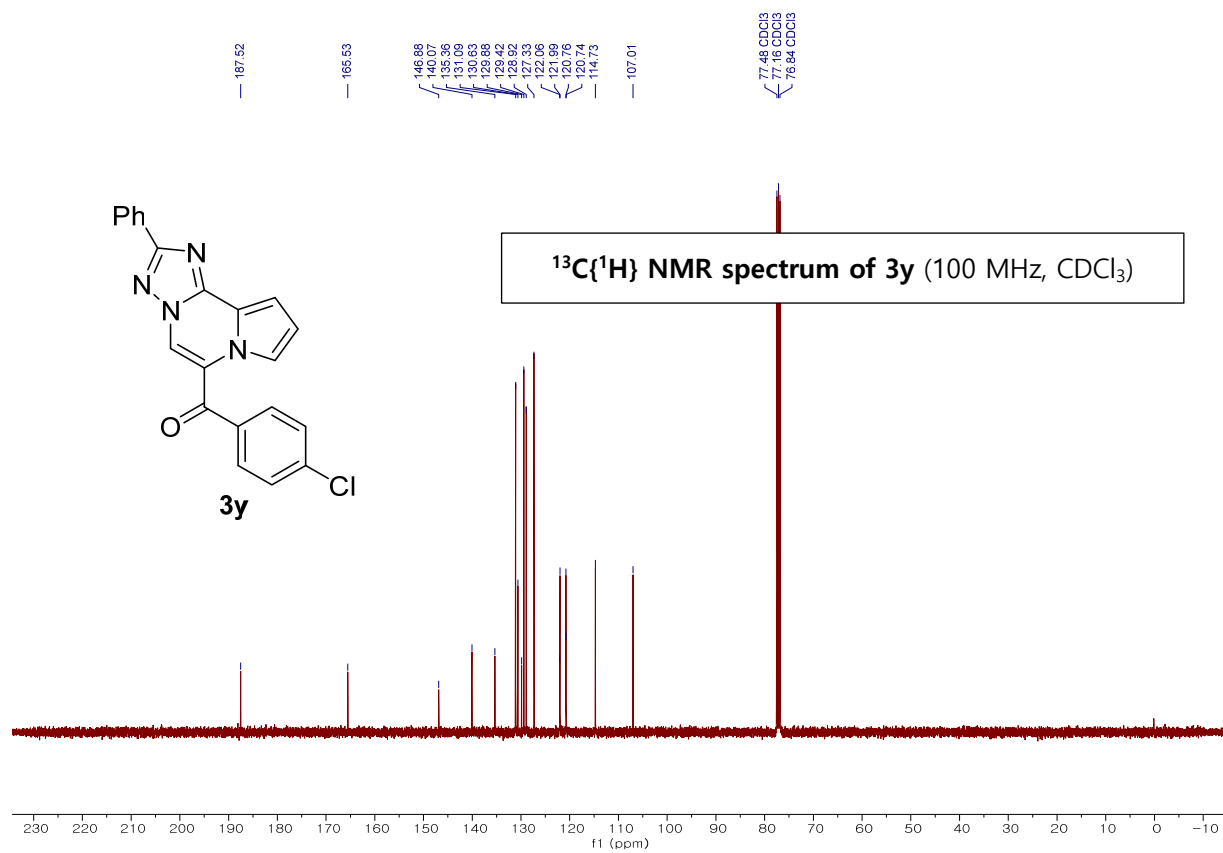
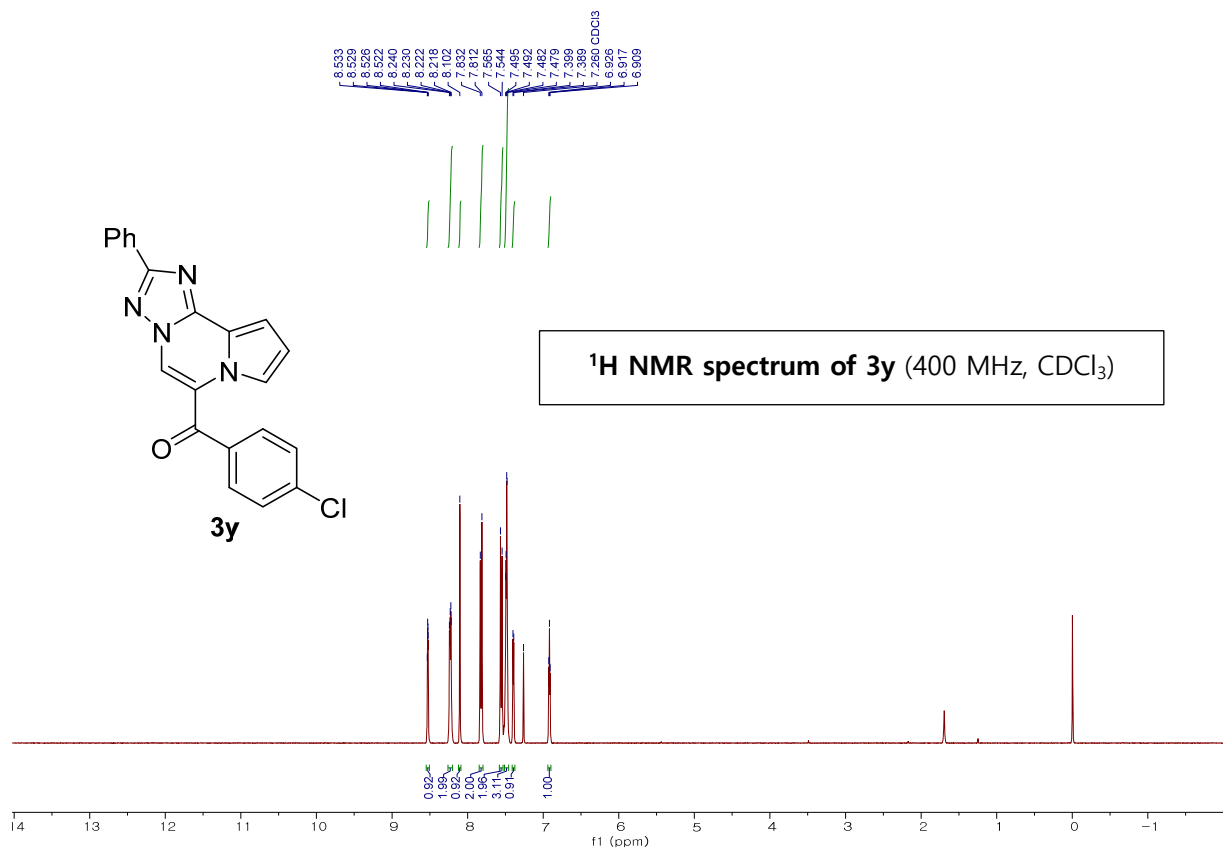


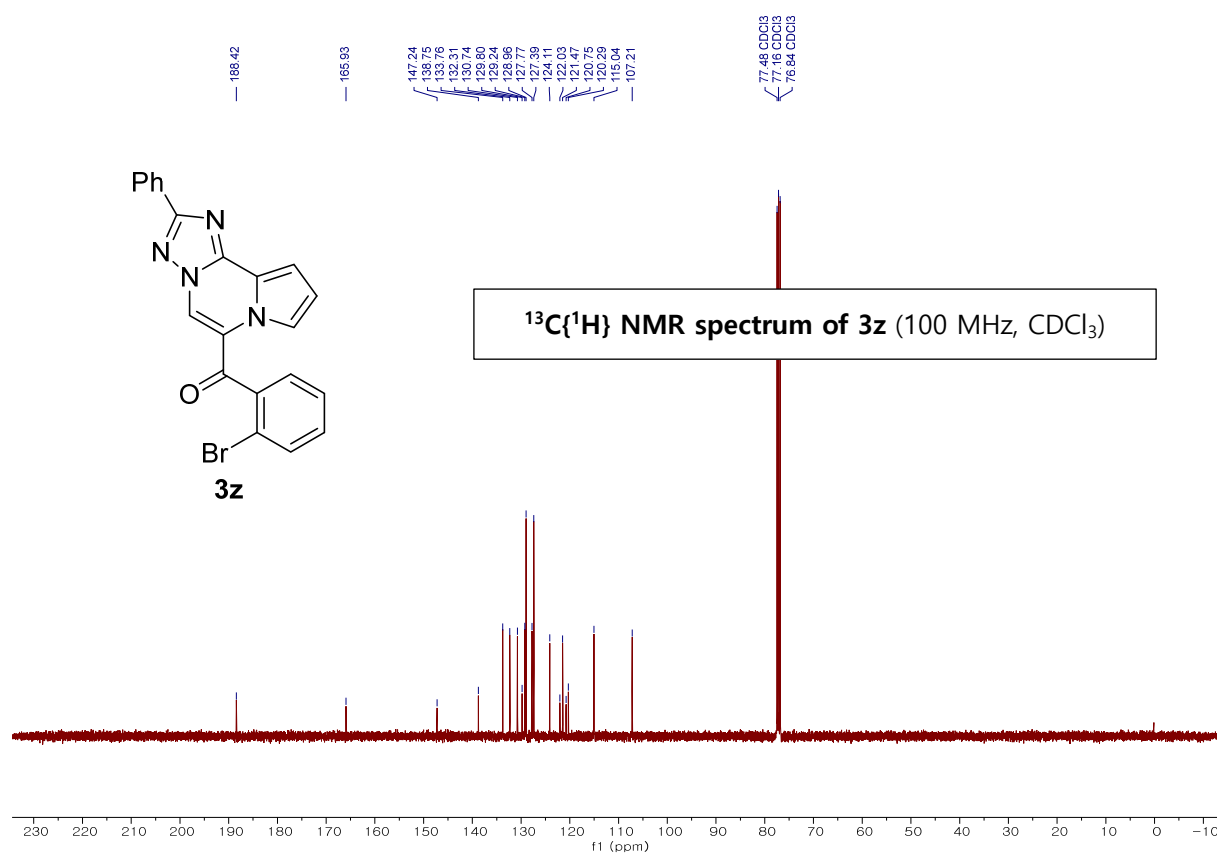
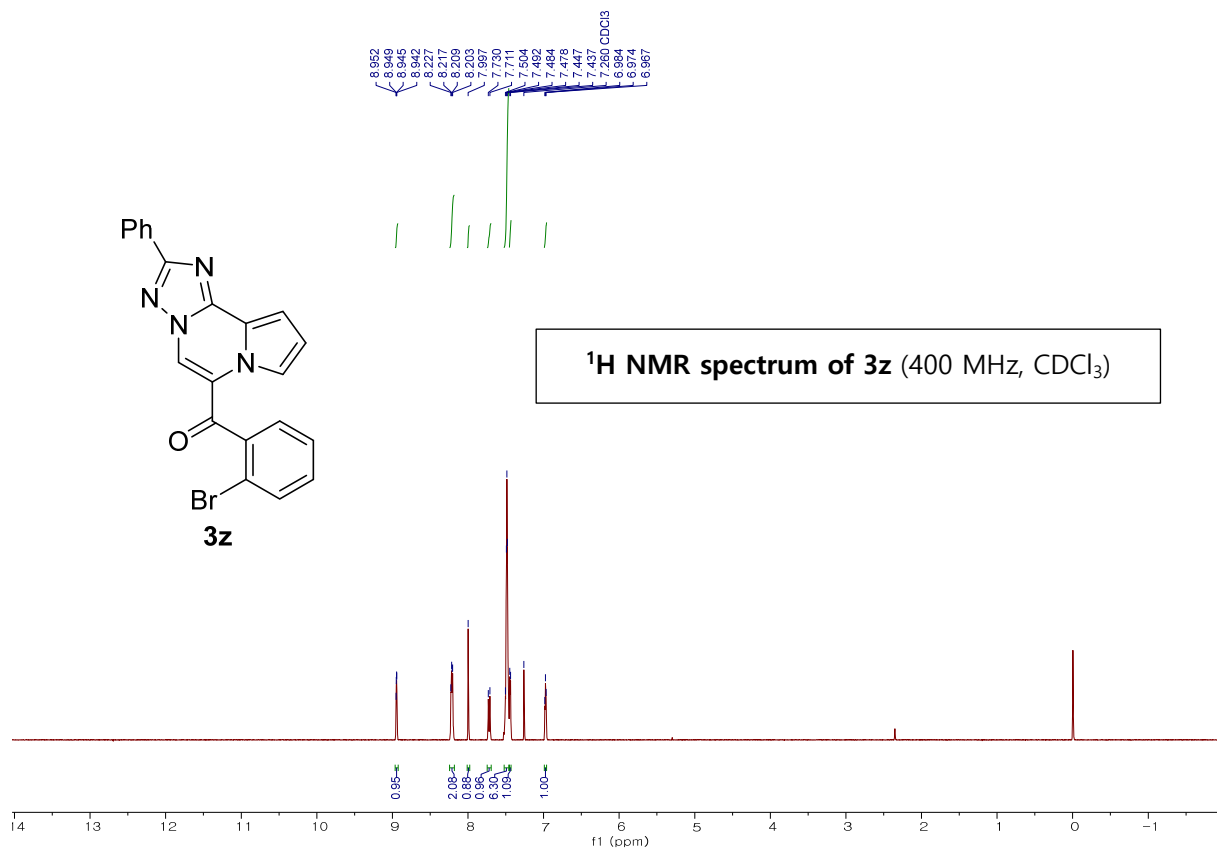


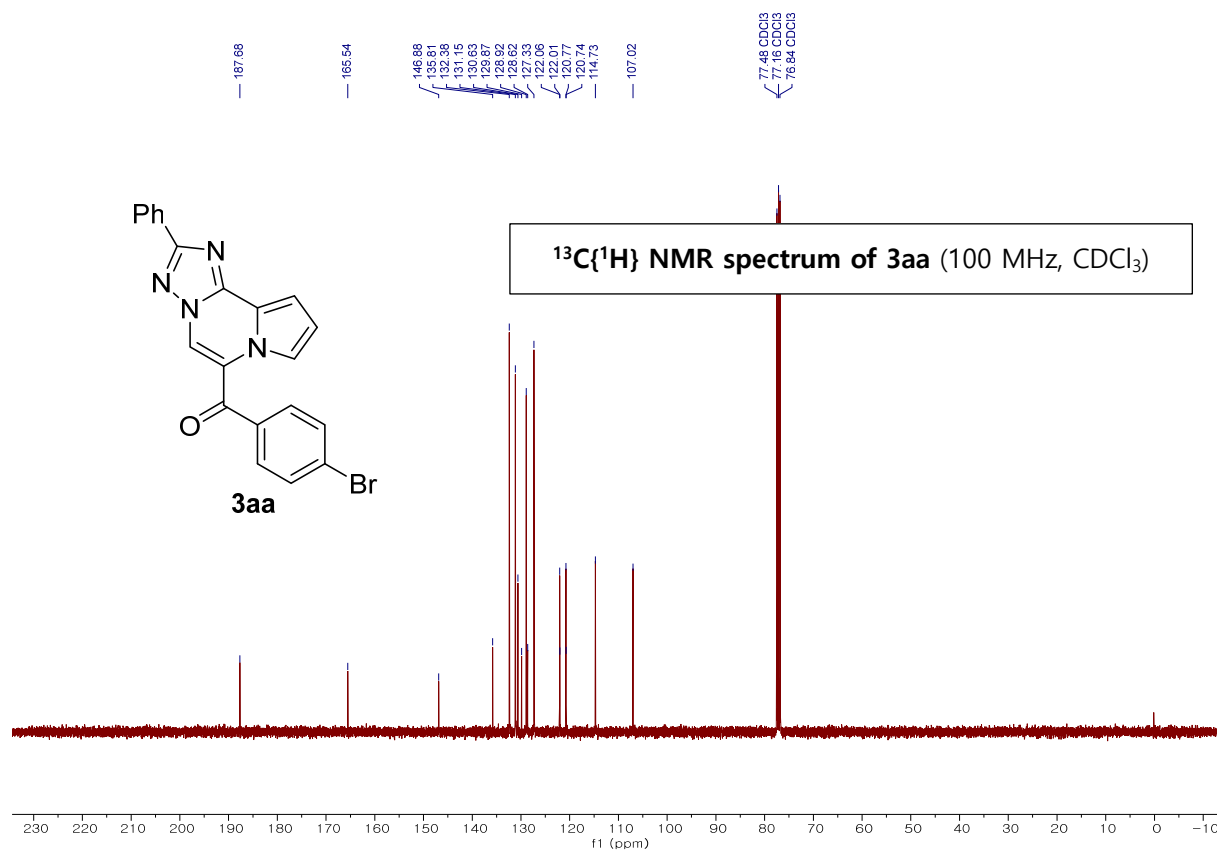
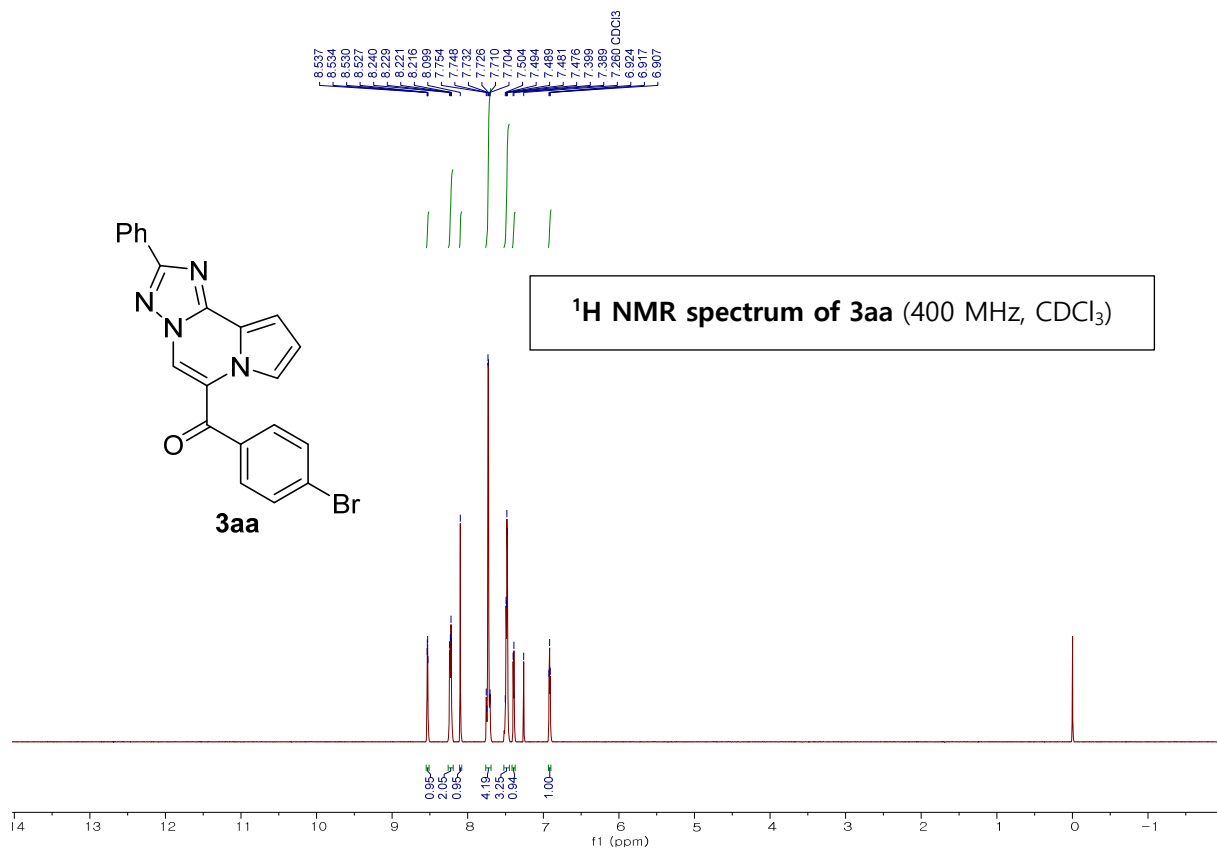


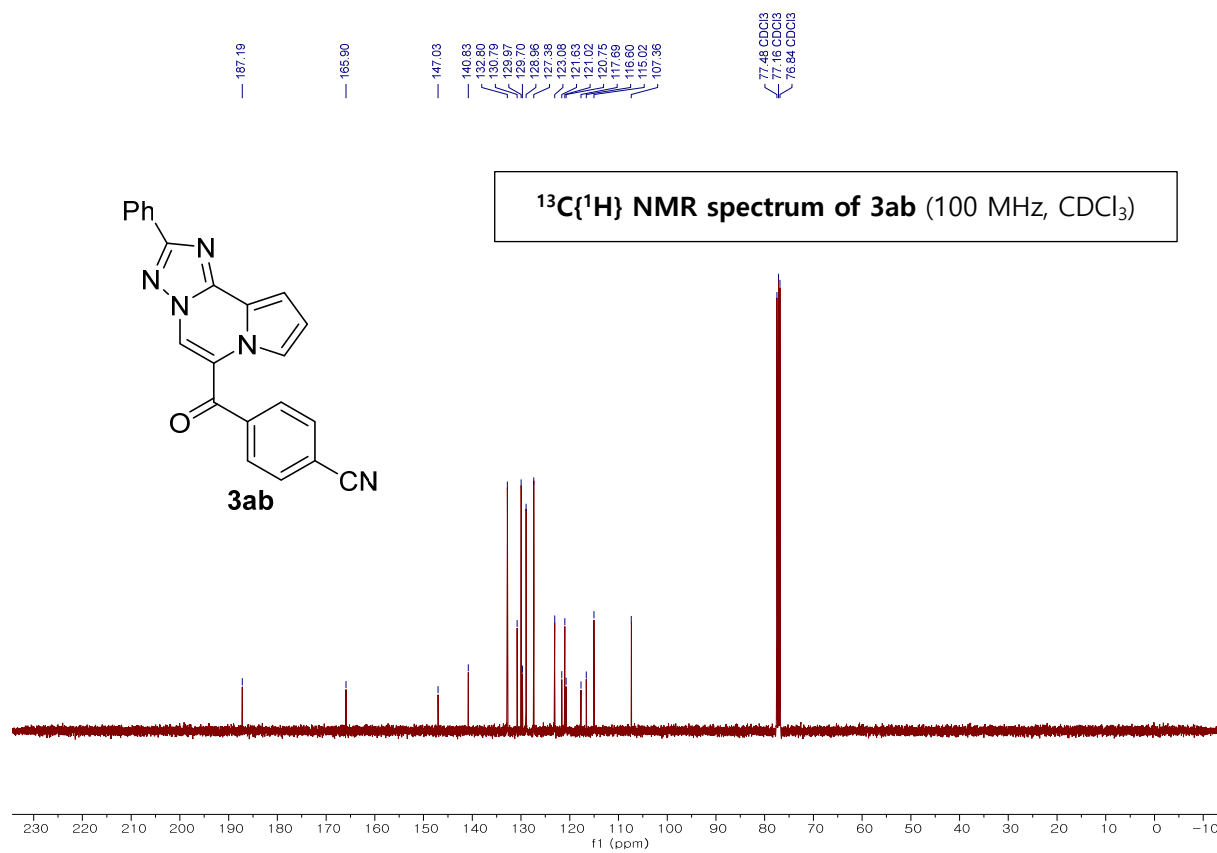
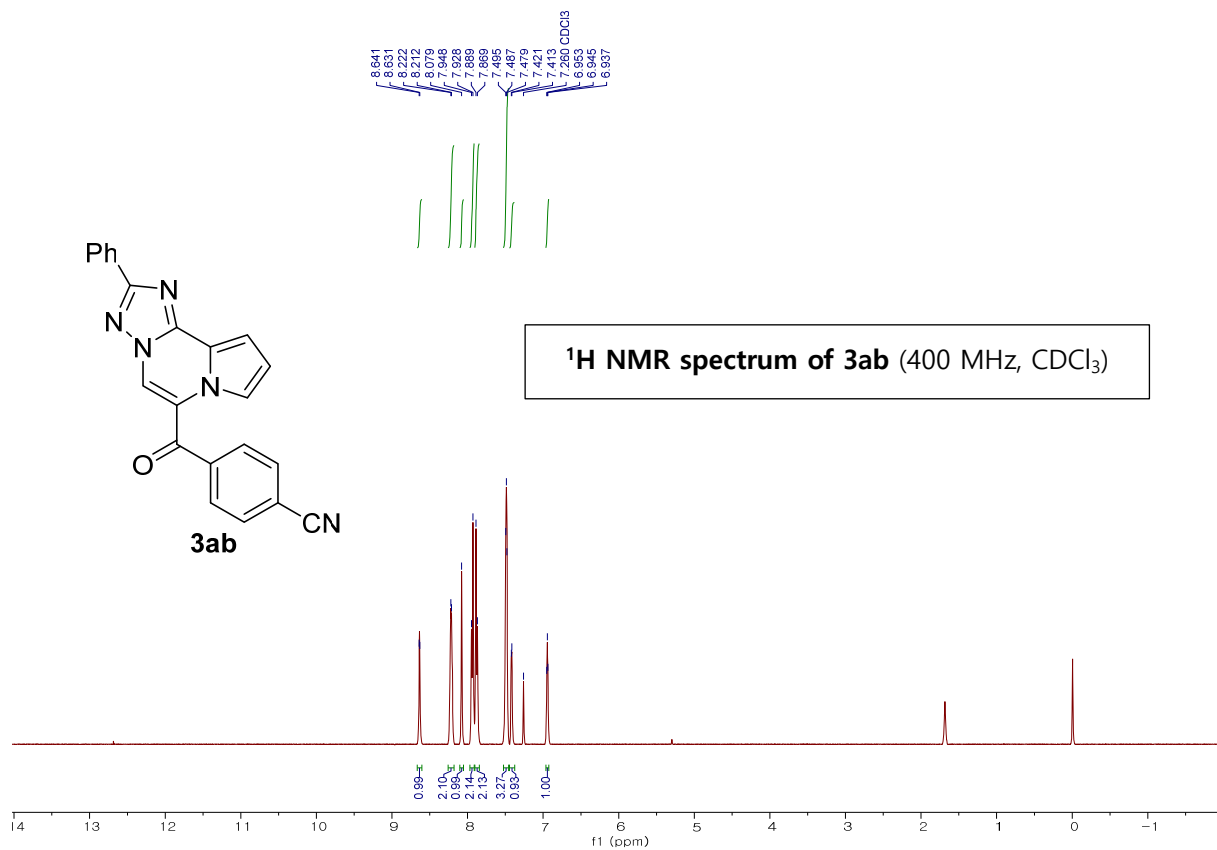


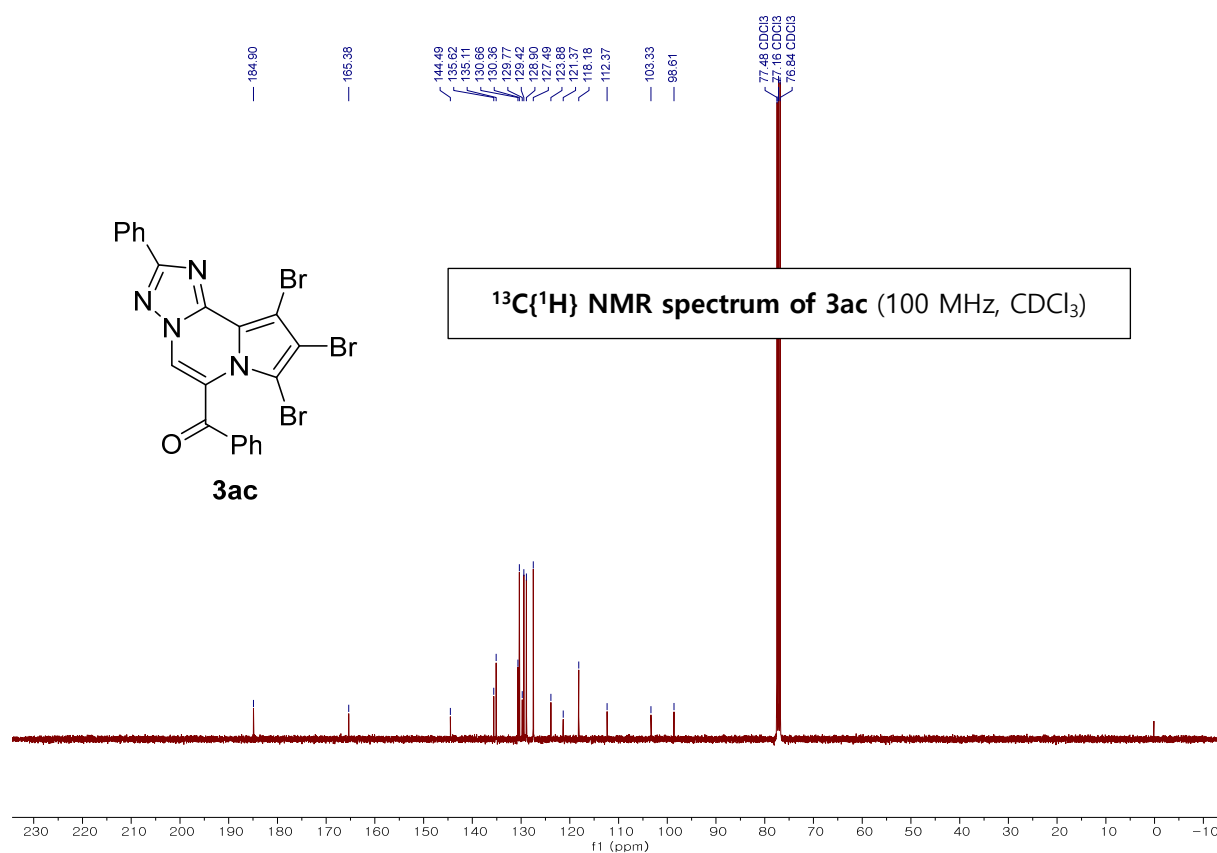
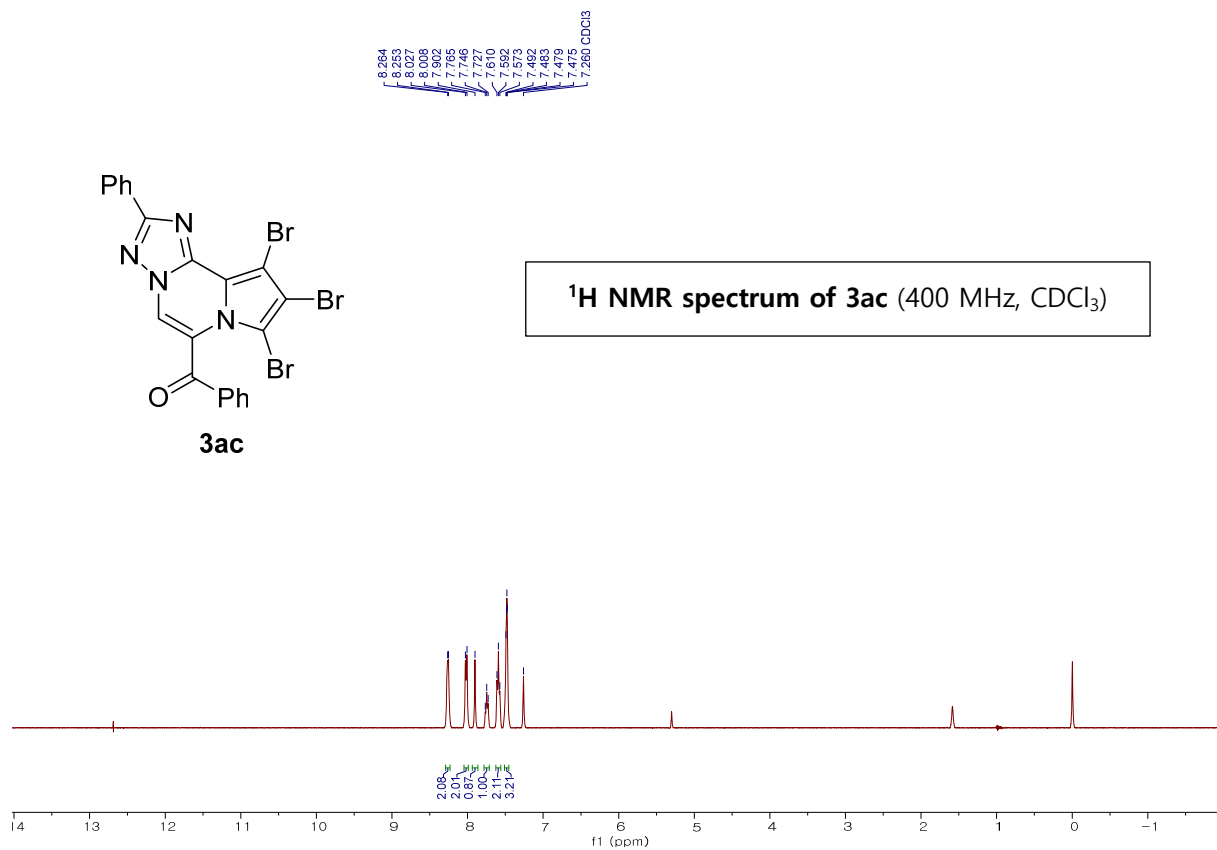


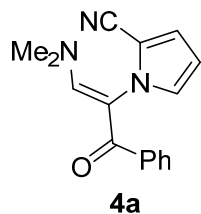




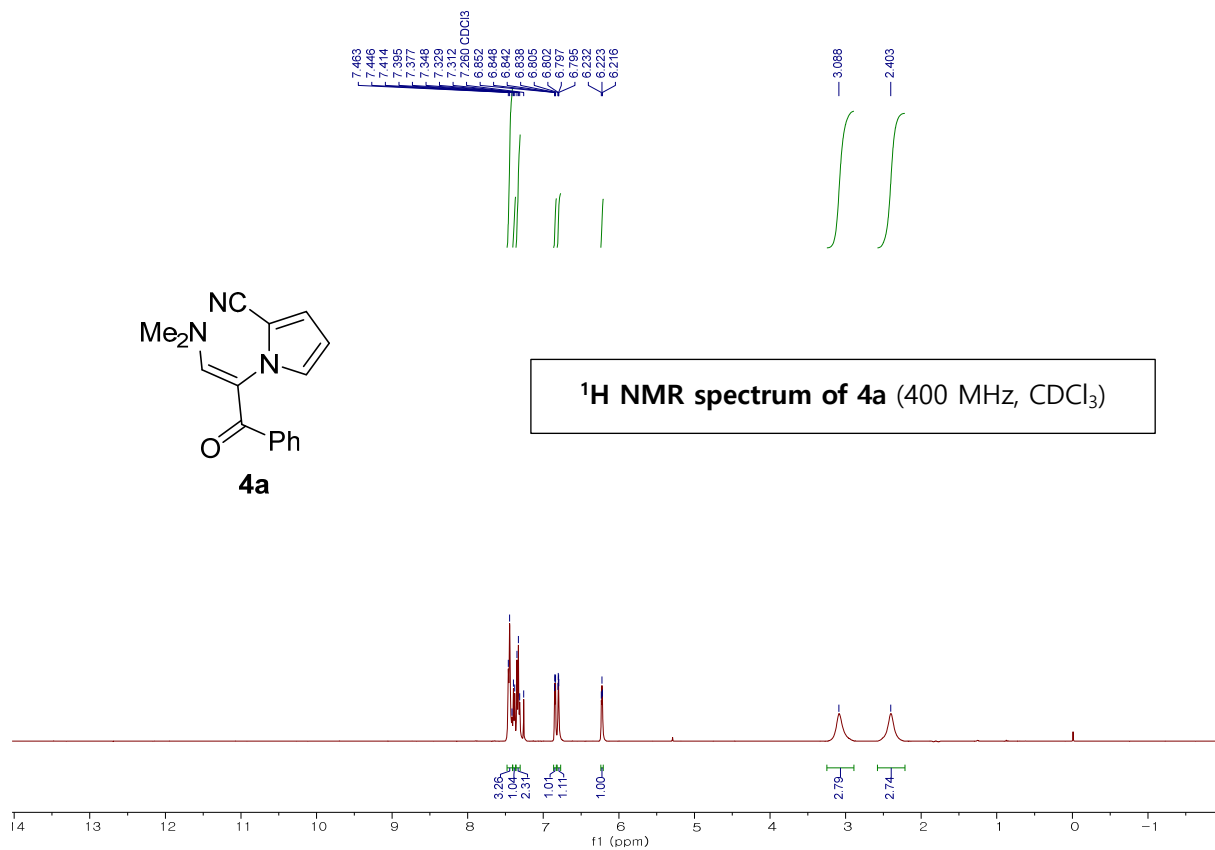




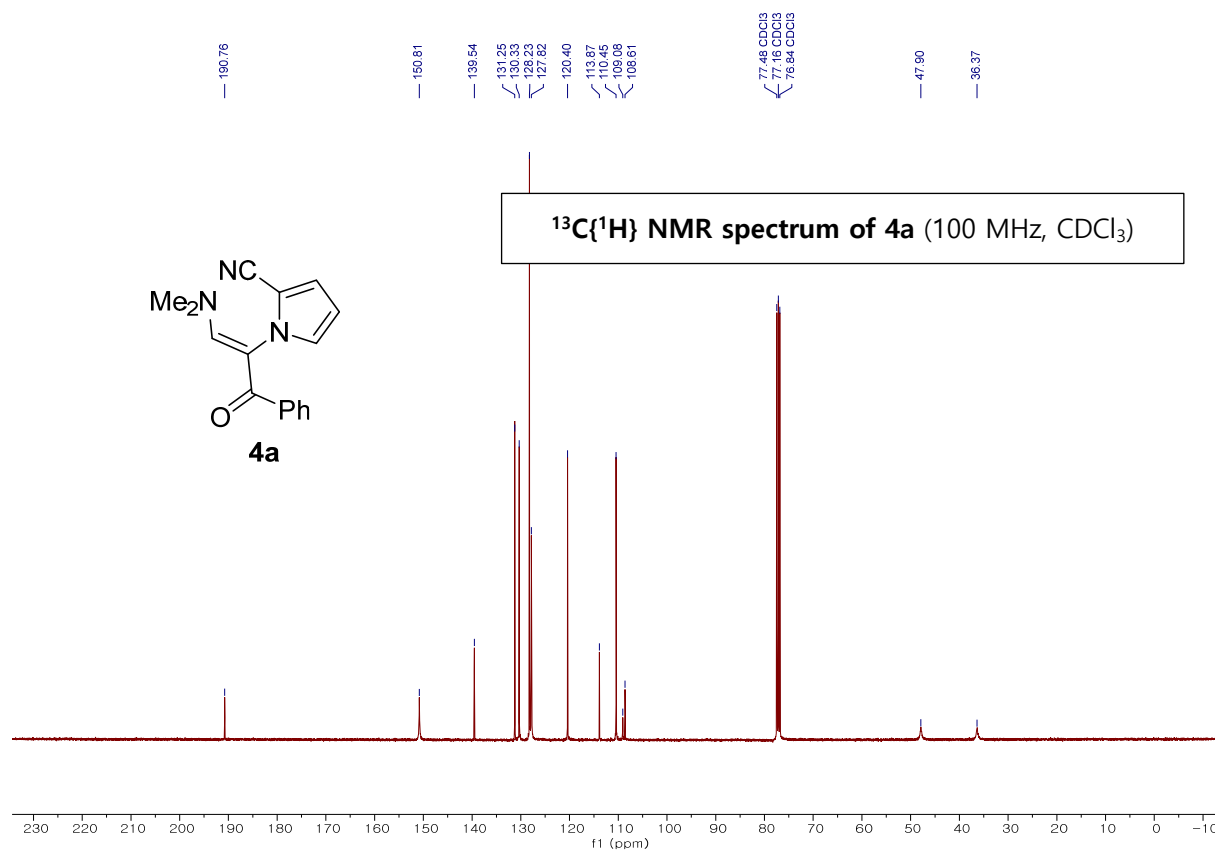


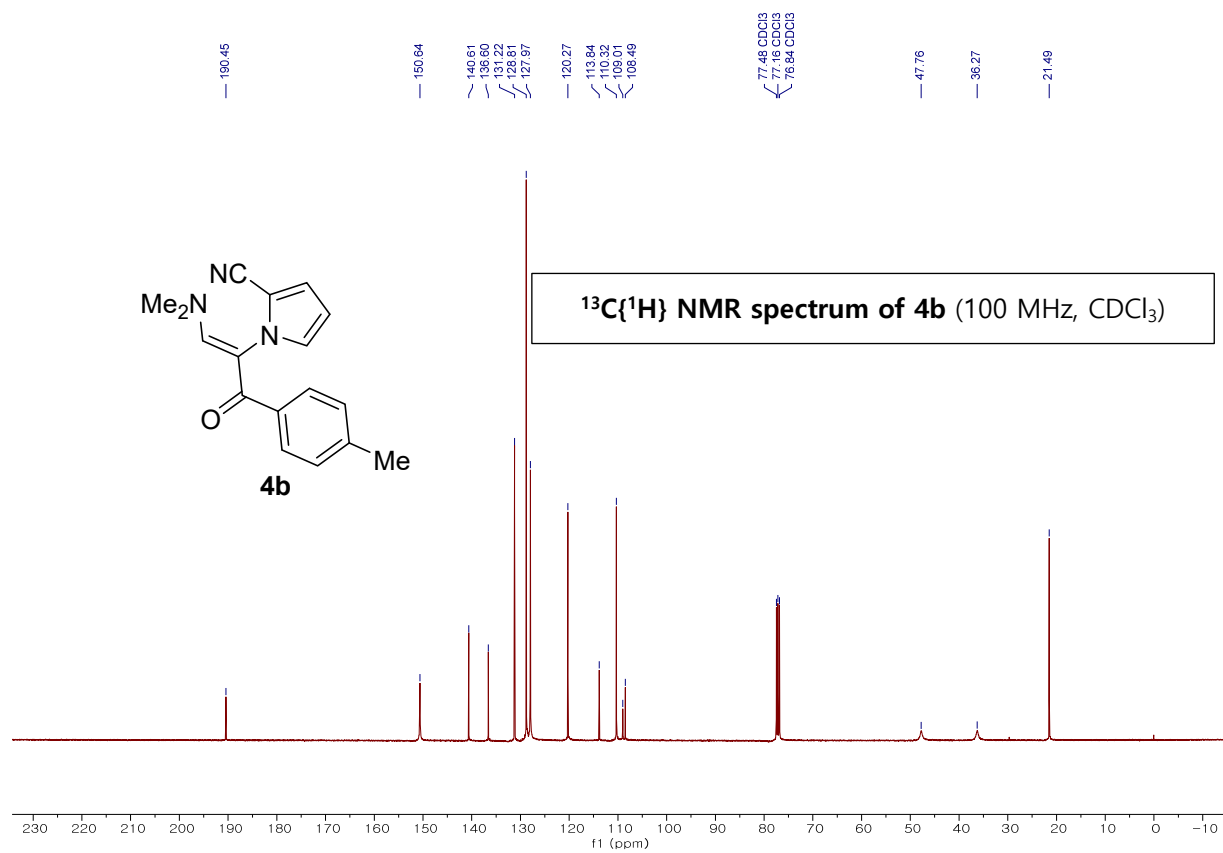
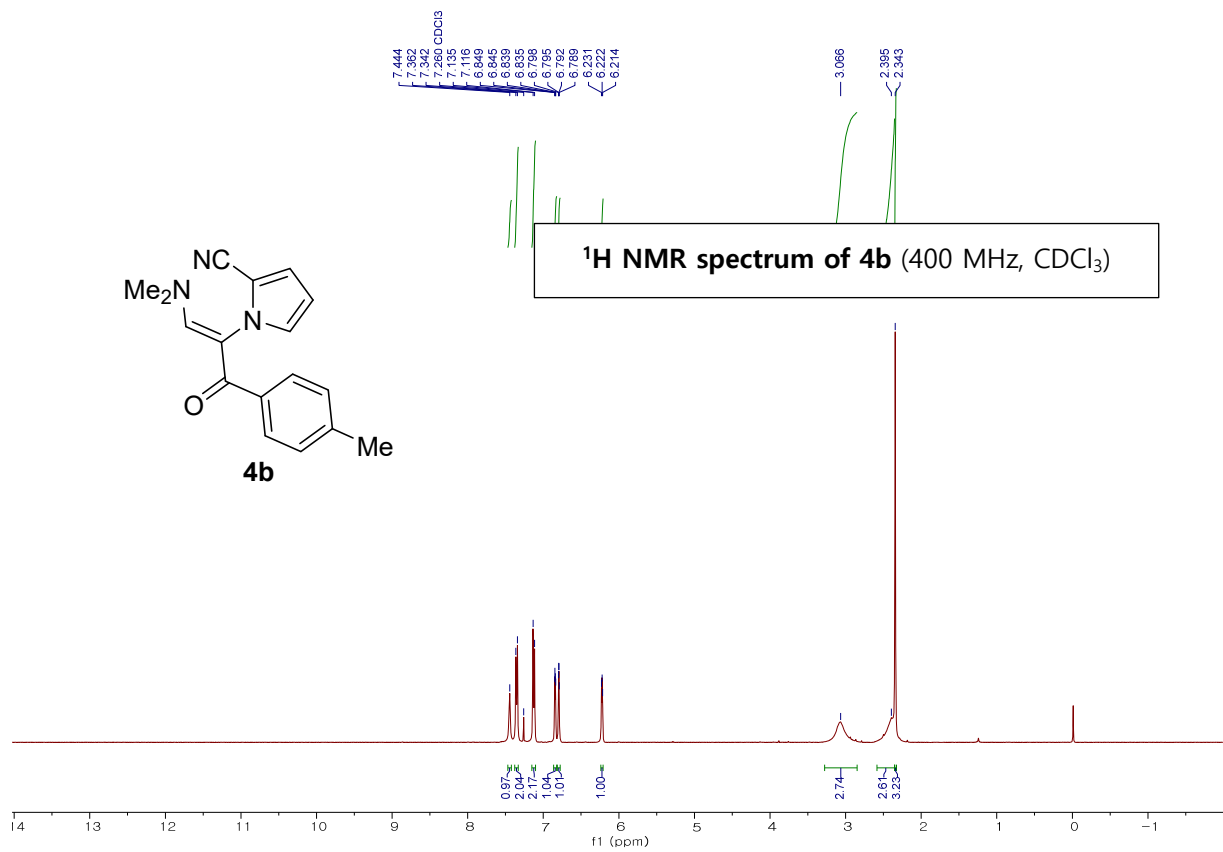


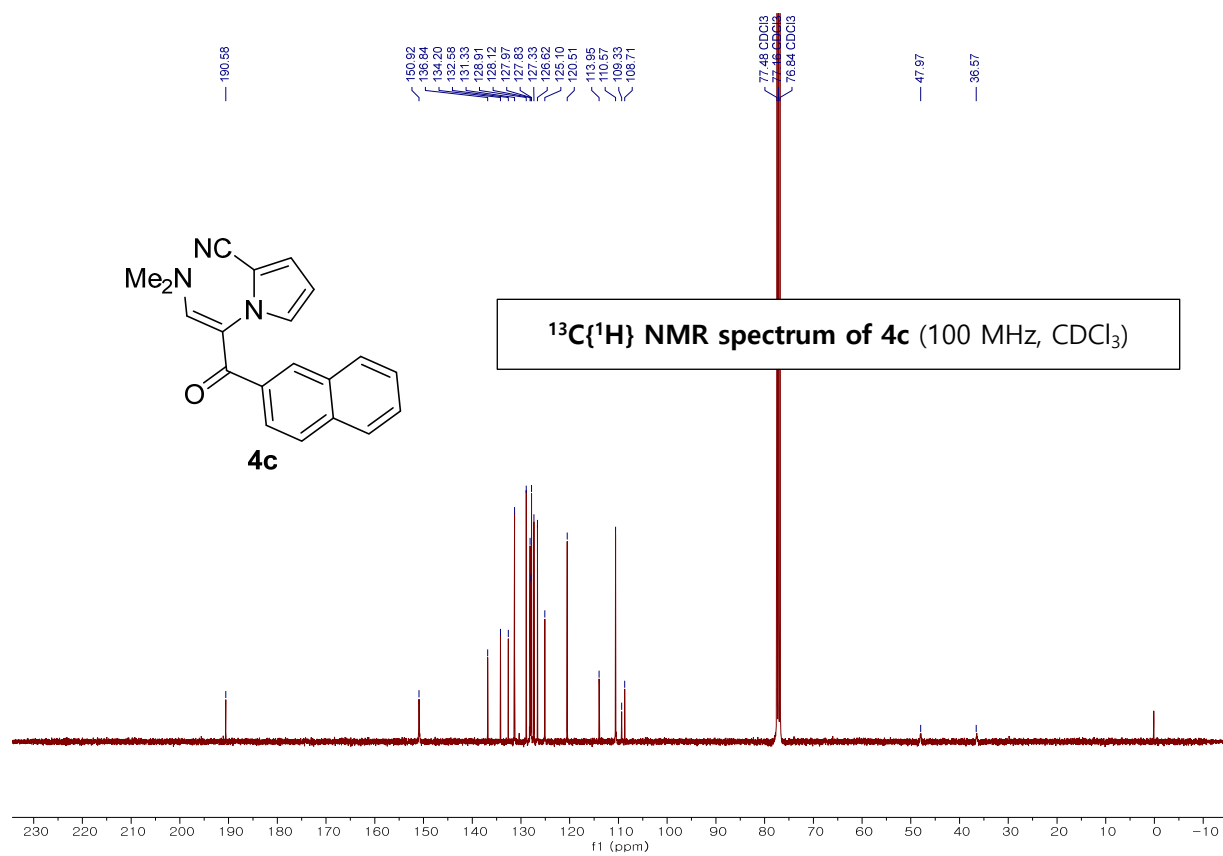
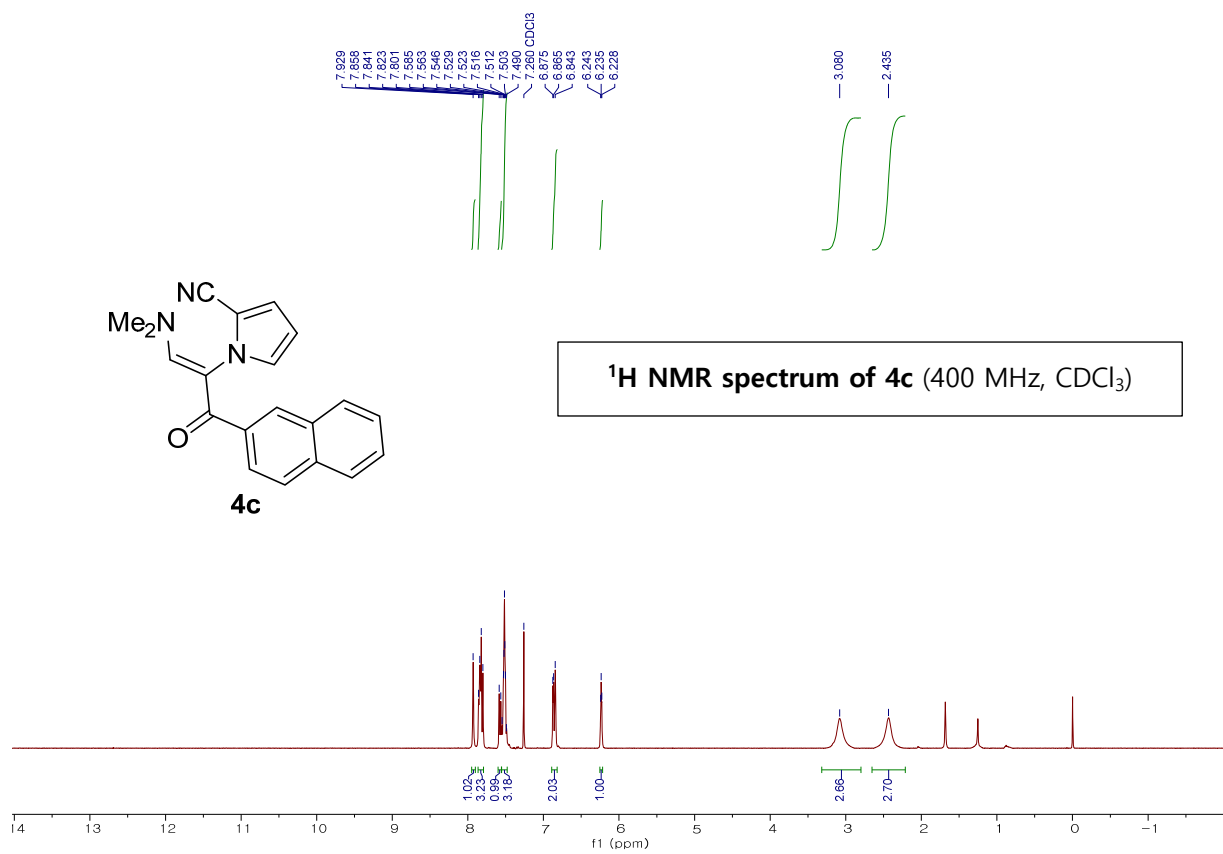
¹H NMR spectrum of 4a (400 MHz, CDCl₃)

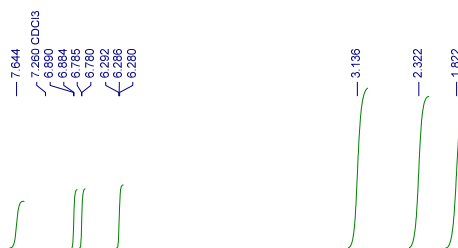
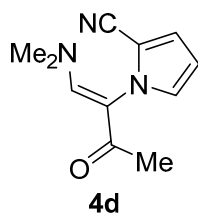


¹³C{¹H} NMR spectrum of 4a (100 MHz, CDCl₃)

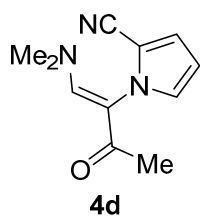
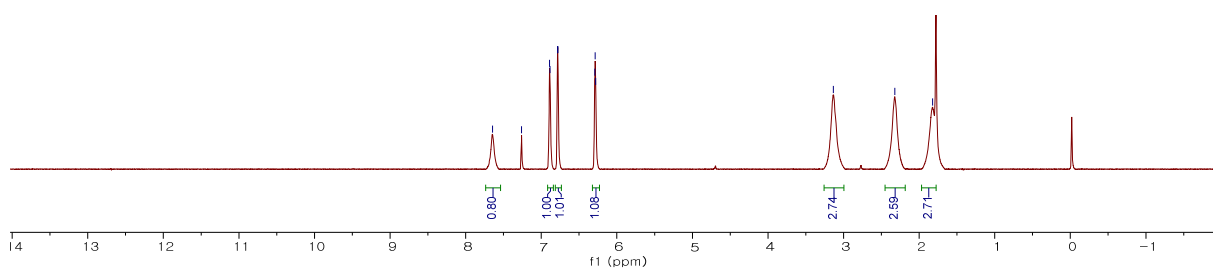




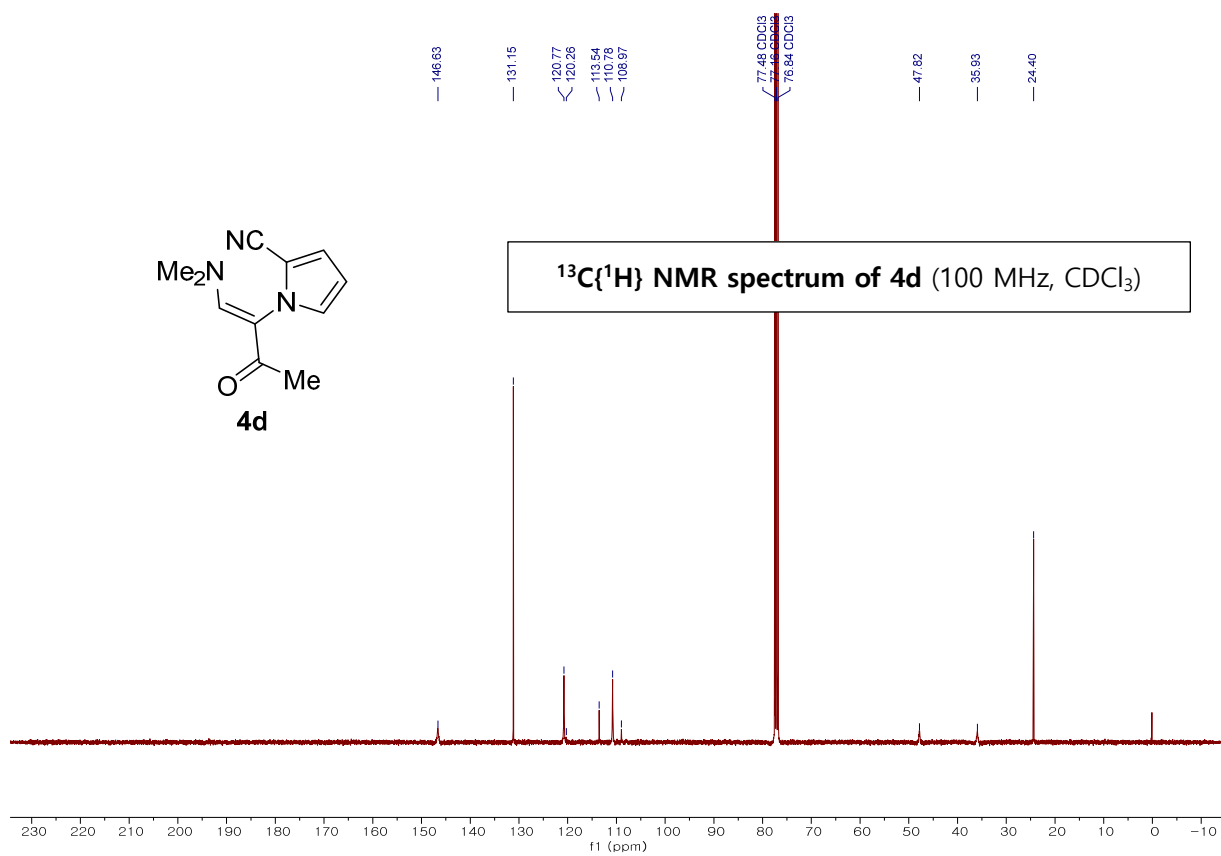


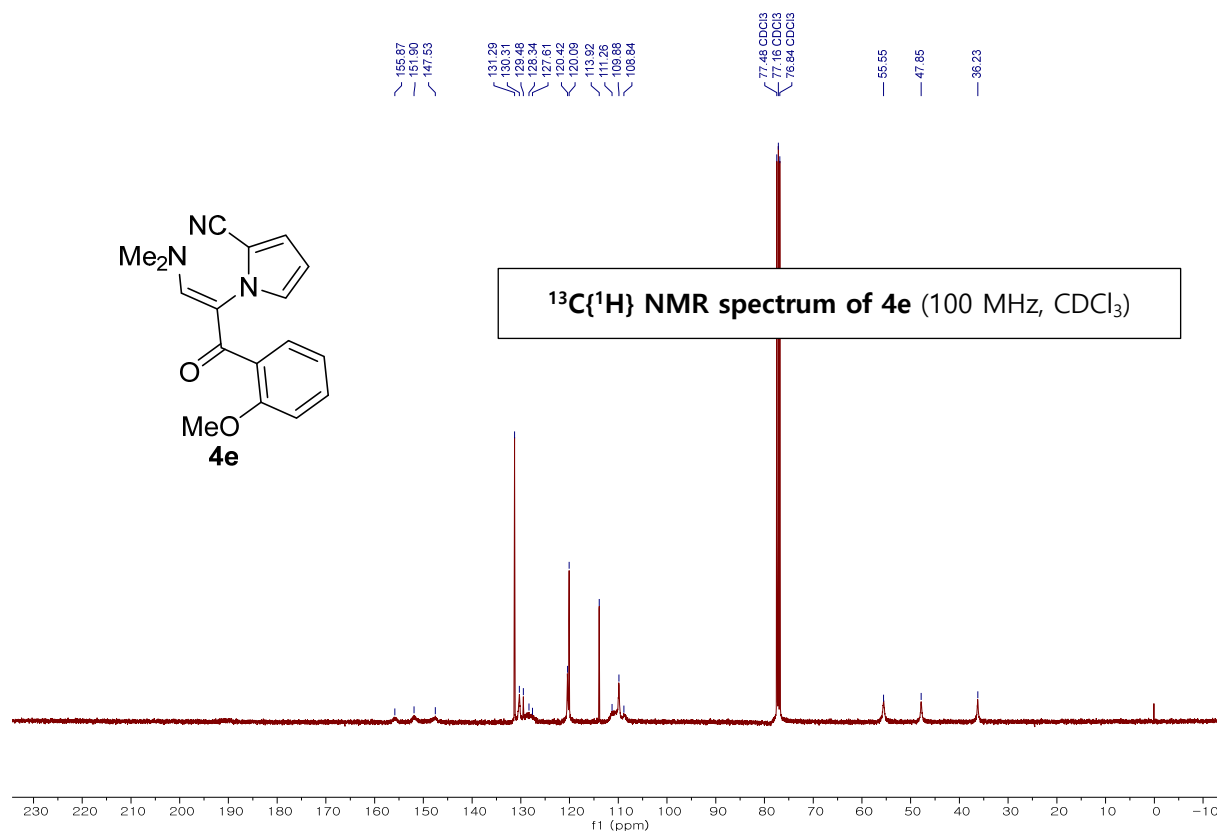
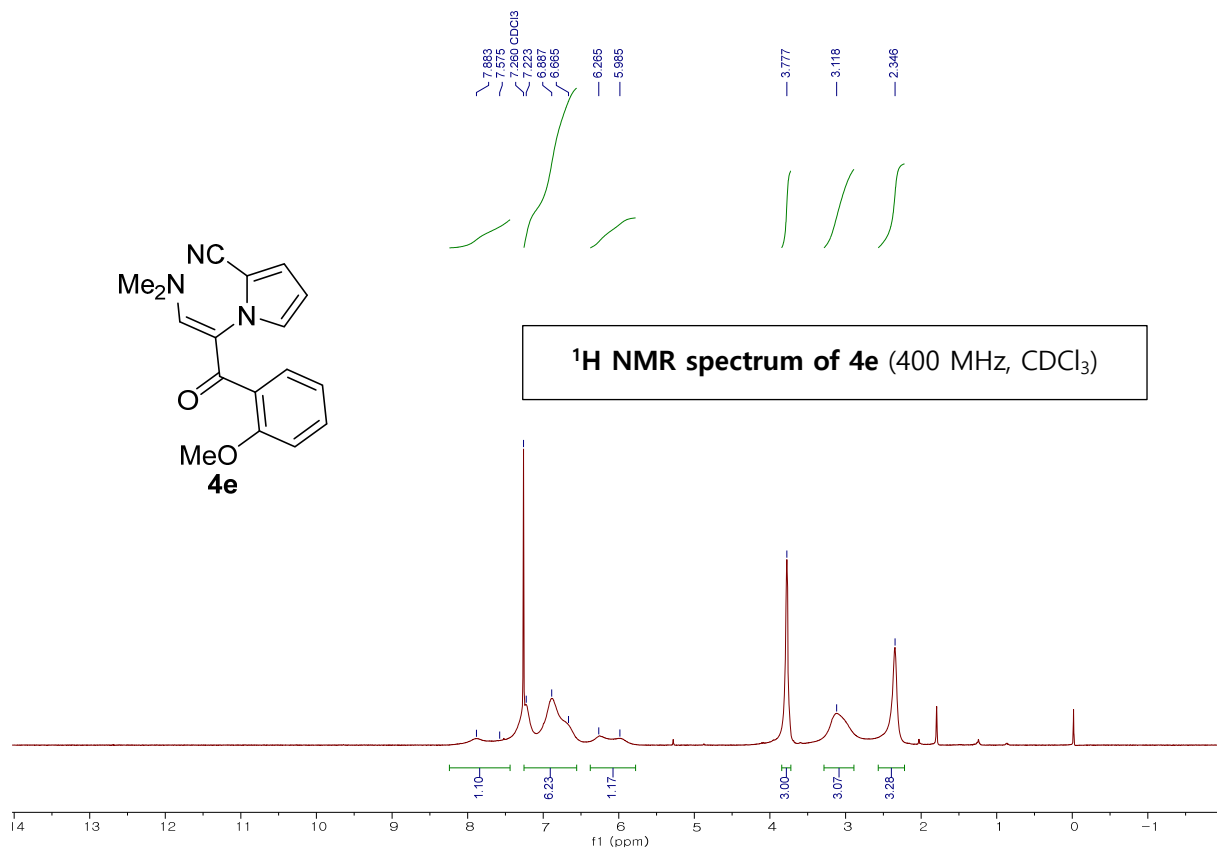
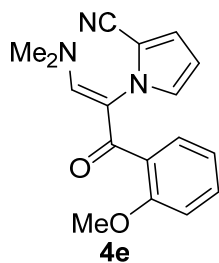


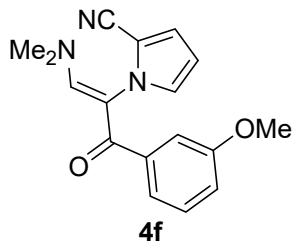
^1H NMR spectrum of 4d (400 MHz, CDCl_3)



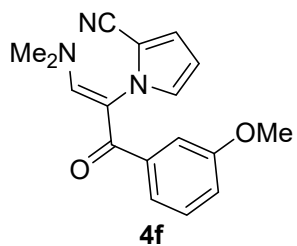
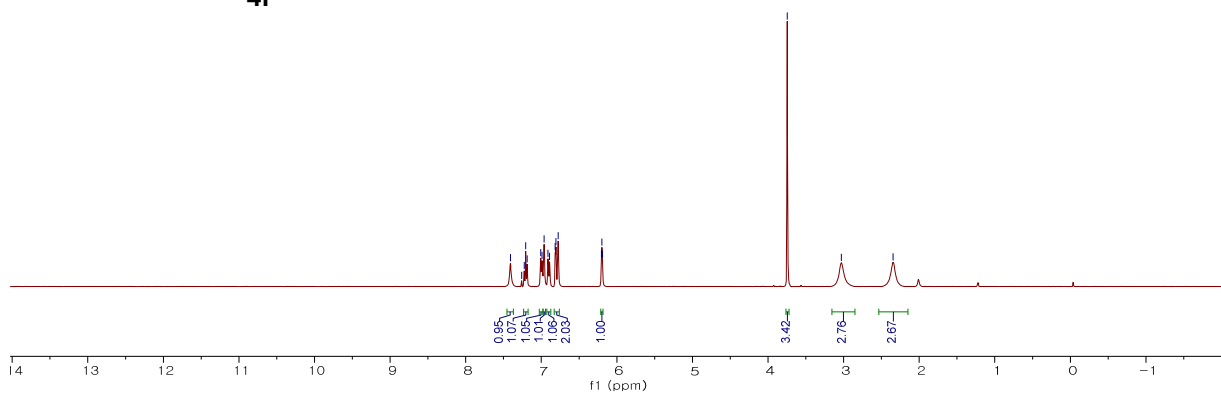
$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of 4d (100 MHz, CDCl_3)



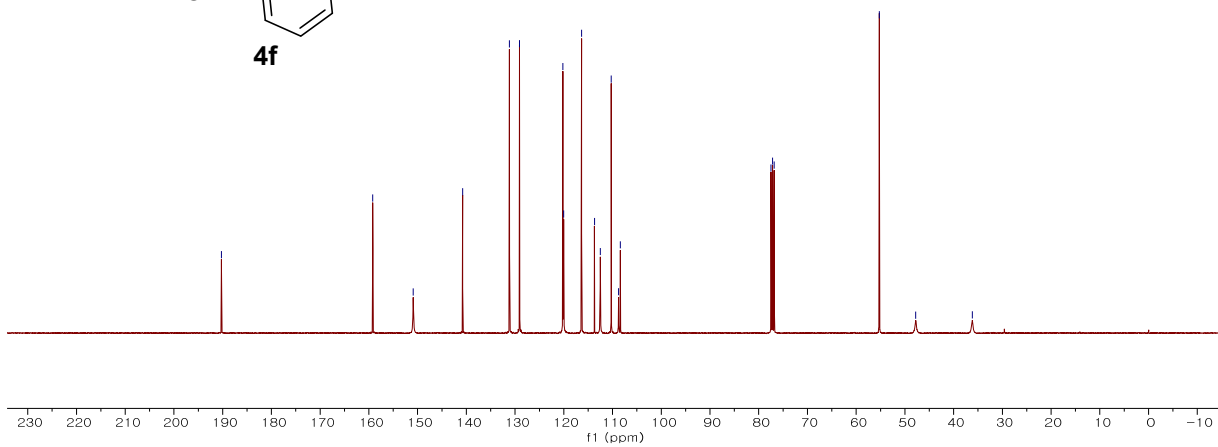


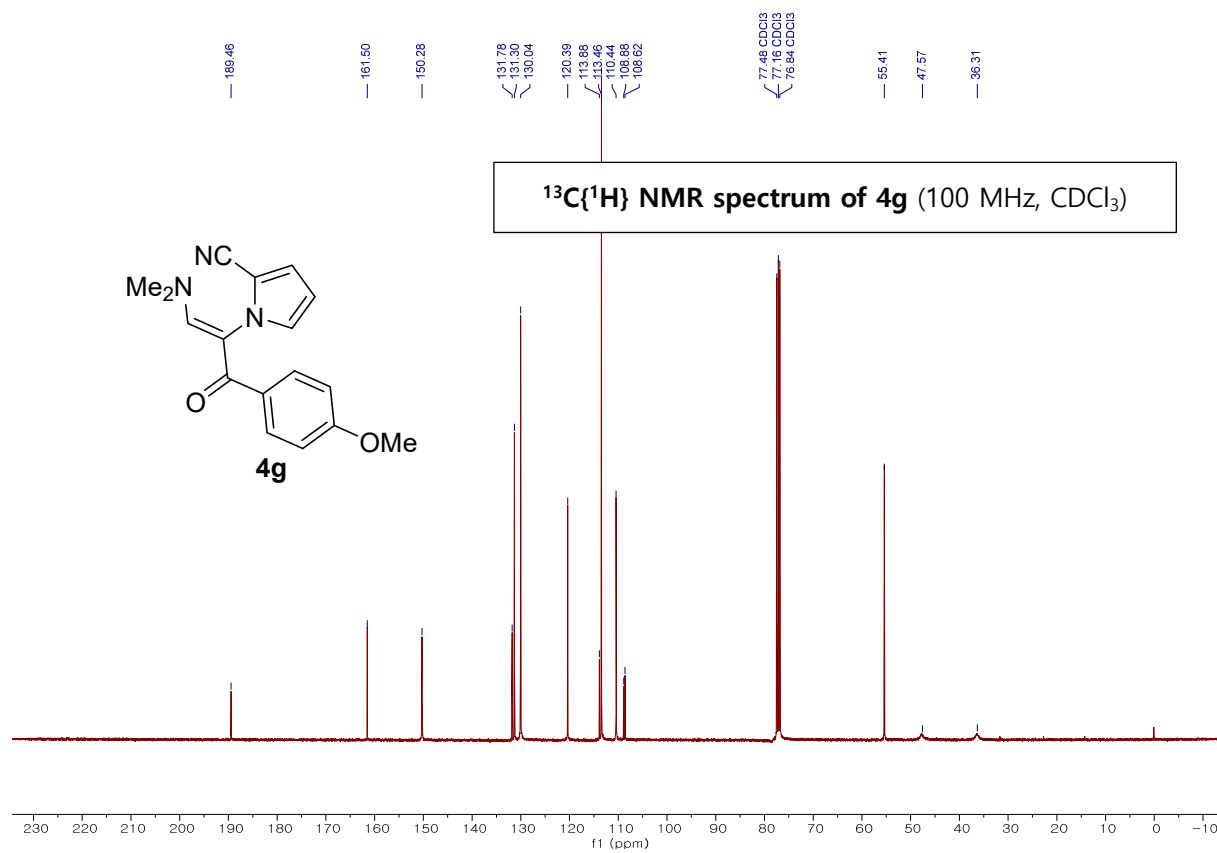
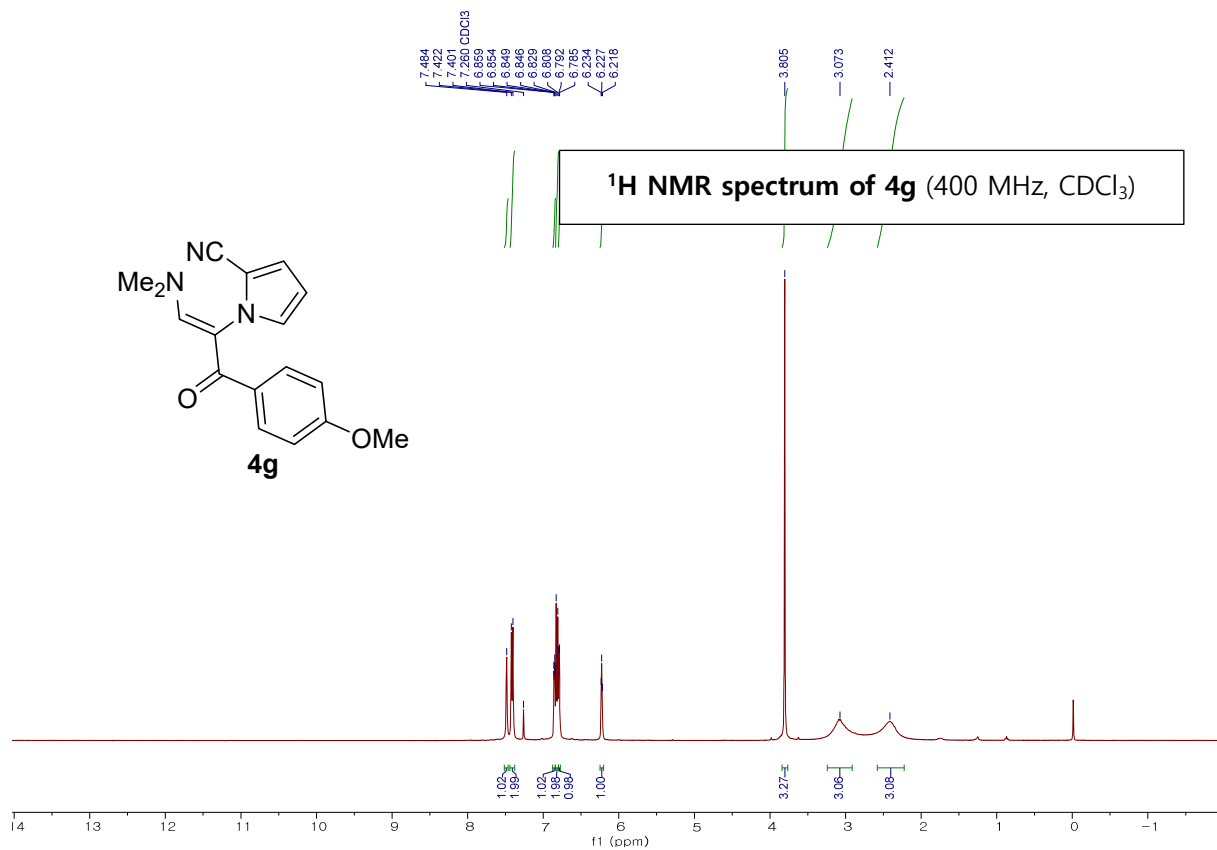


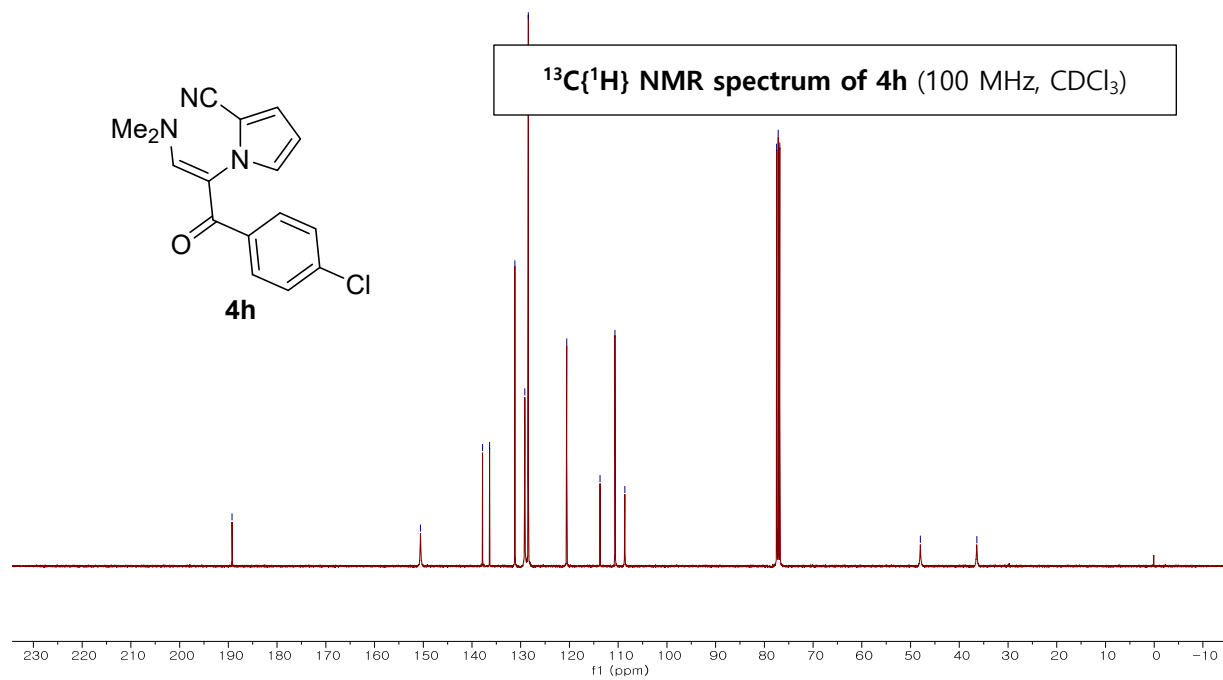
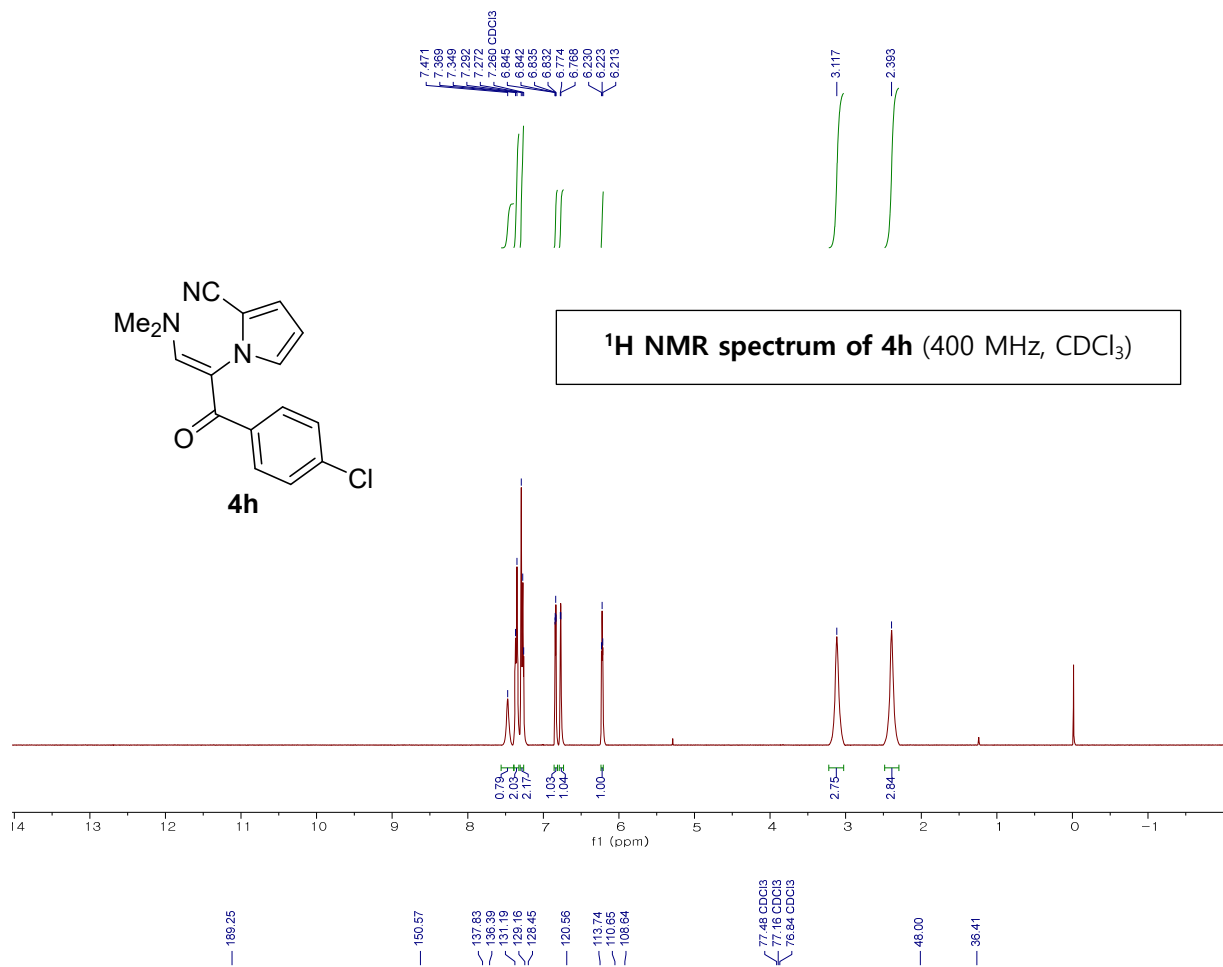
¹H NMR spectrum of 4f (400 MHz, CDCl₃)

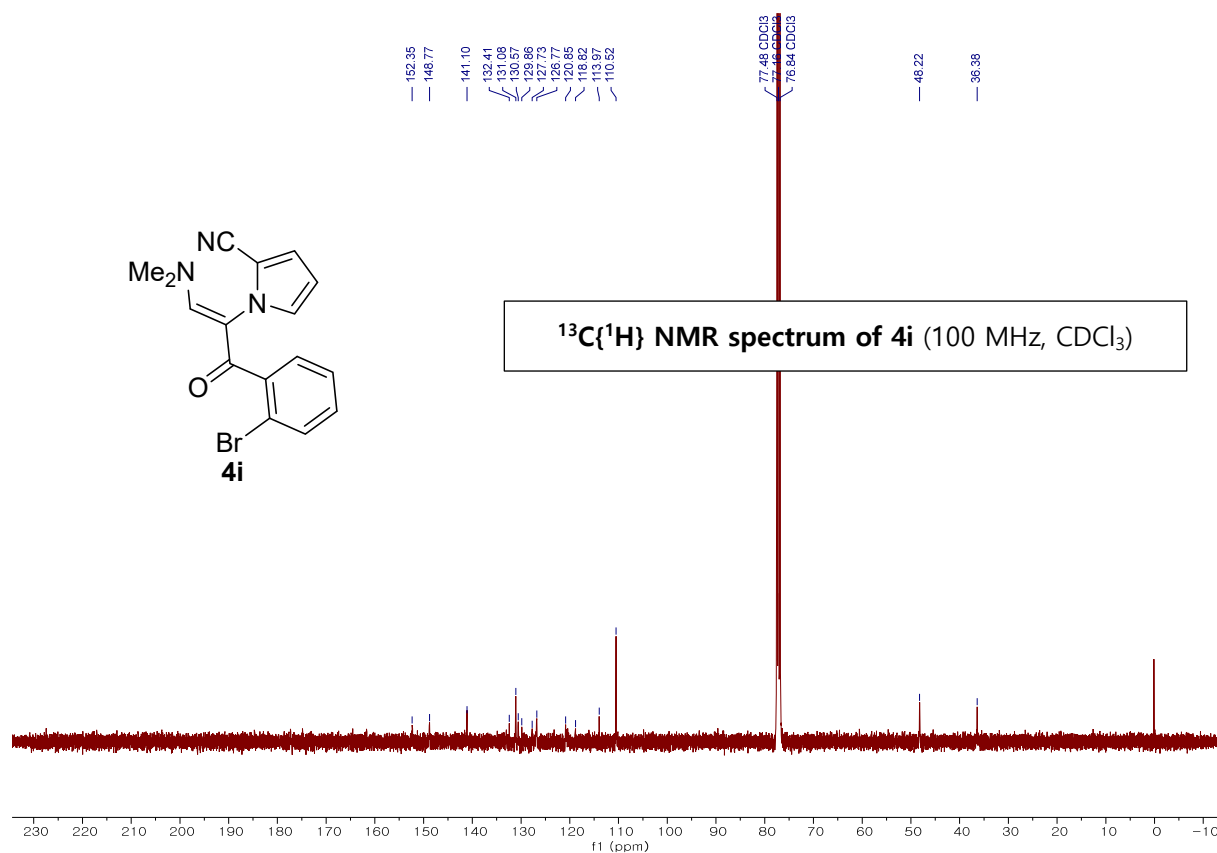
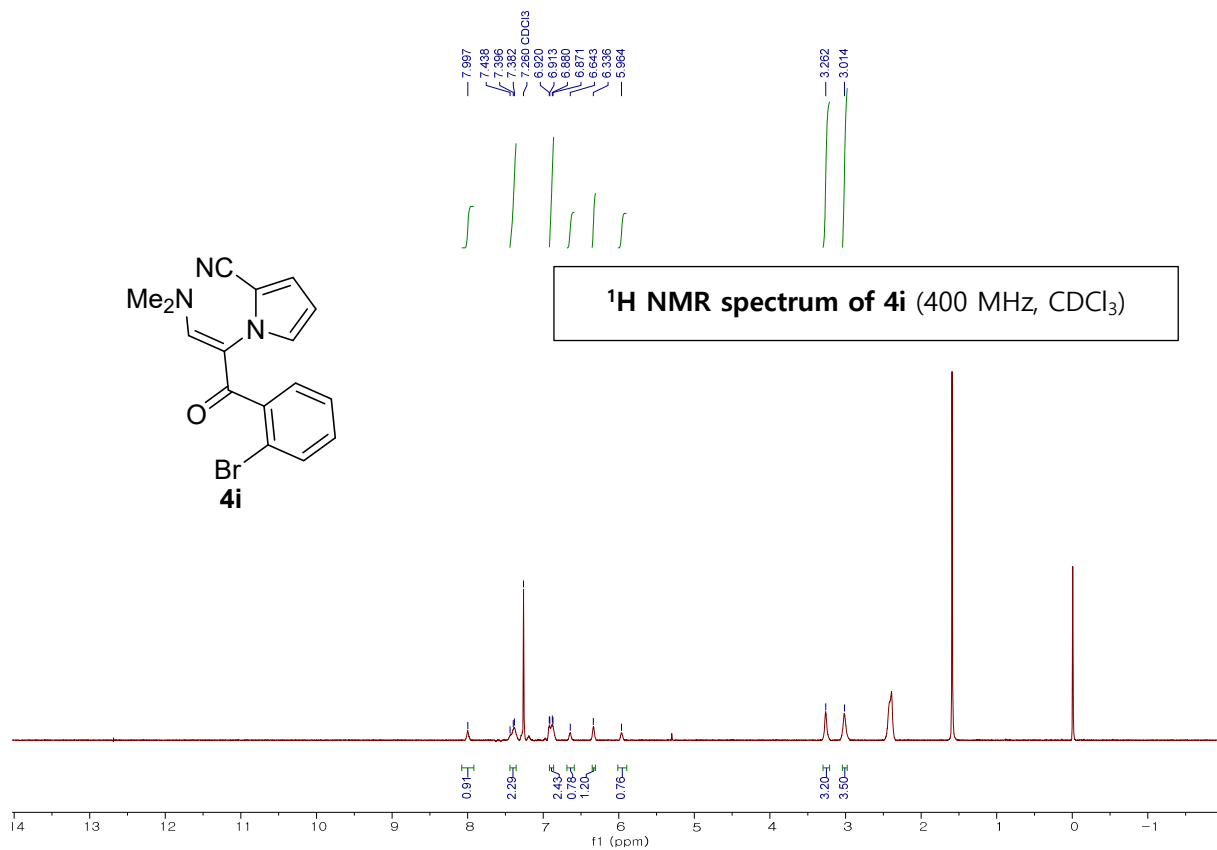


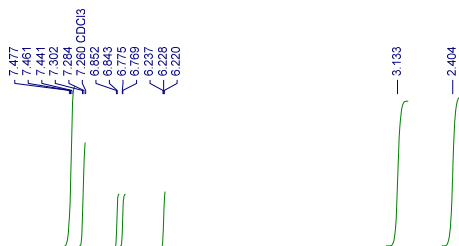
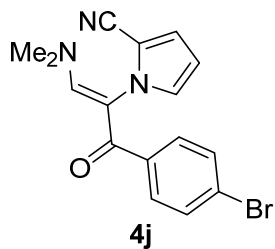
¹³C{¹H} NMR spectrum of 4f (100 MHz, CDCl₃)



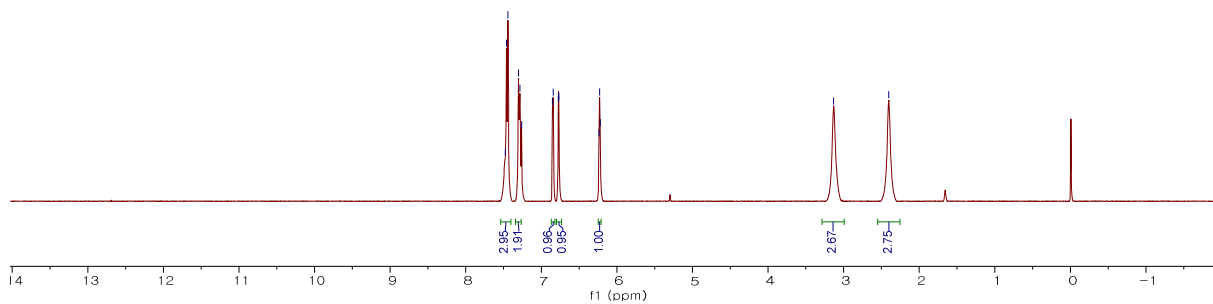




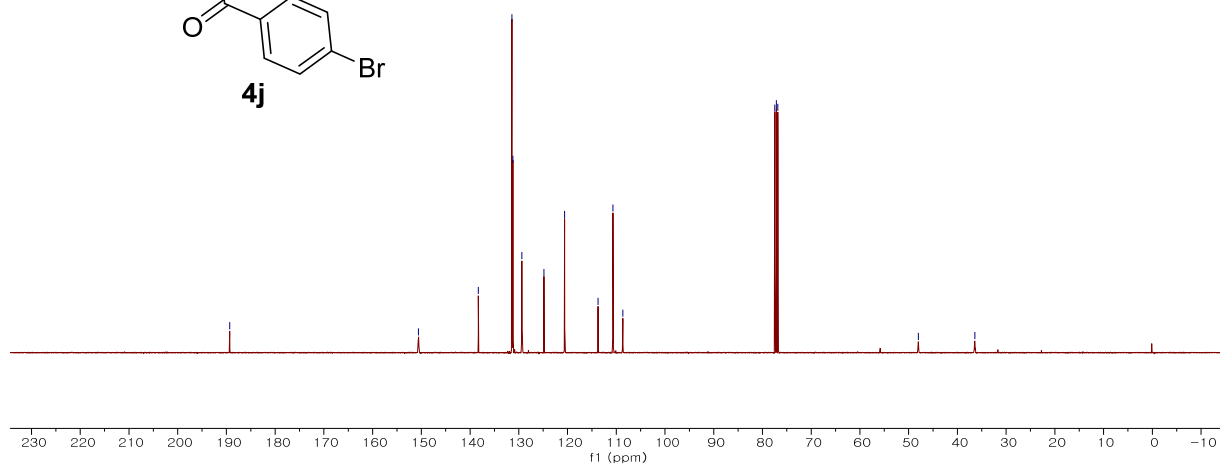


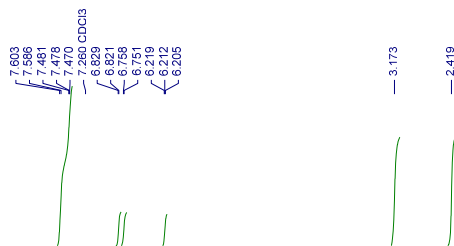
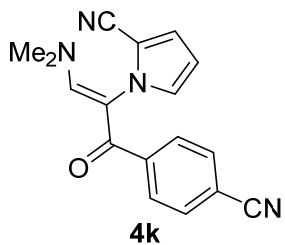


¹H NMR spectrum of 4j (400 MHz, CDCl₃)

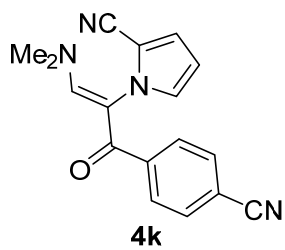
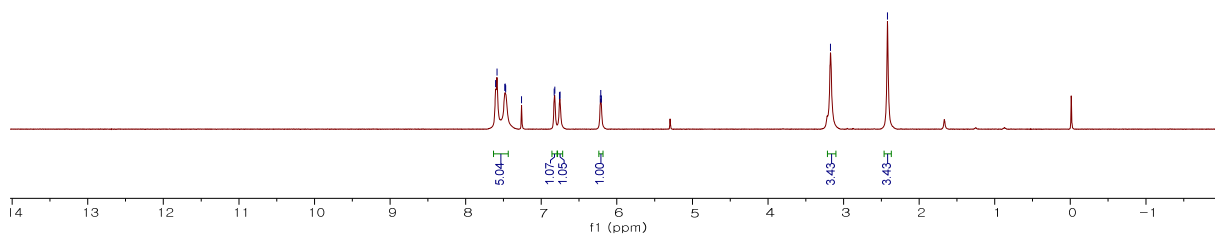


¹³C{¹H} NMR spectrum of 4j (100 MHz, CDCl₃)

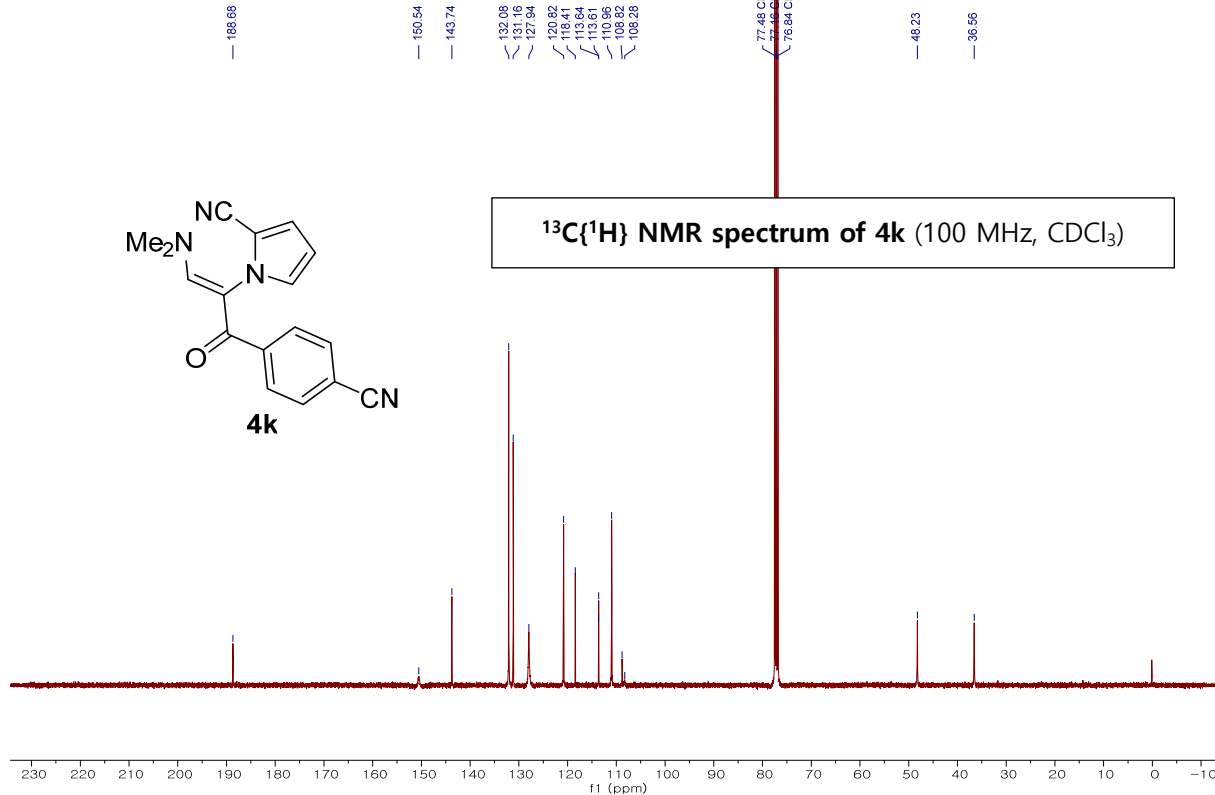


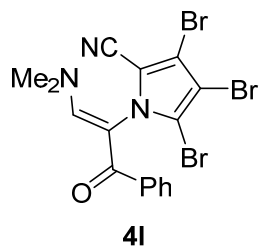


¹H NMR spectrum of 4k (400 MHz, CDCl₃)



¹³C{¹H} NMR spectrum of 4k (100 MHz, CDCl₃)

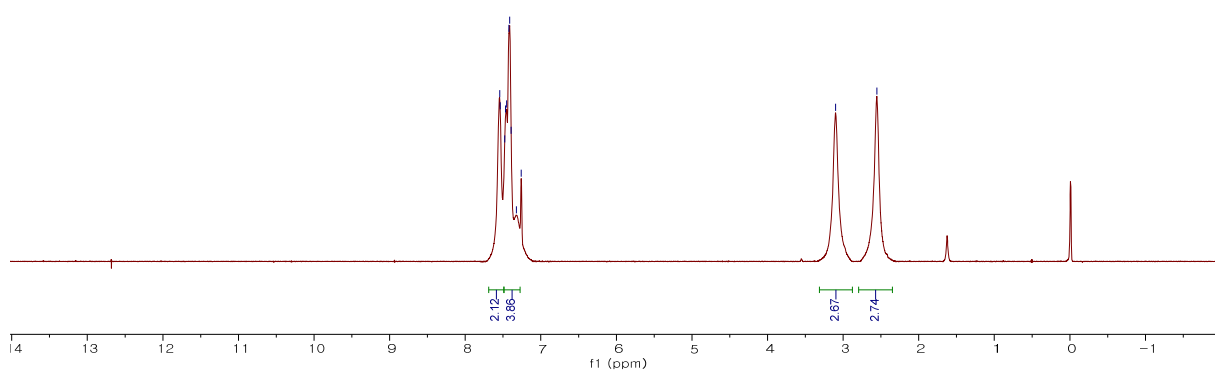




7.543
7.537
7.477
7.466
7.432
7.411
7.392
7.322
7.260 CDCl₃

3.099
2.553

¹H NMR spectrum of 4I (400 MHz, CDCl₃)



189.83

152.02

138.94

130.85

128.50

128.26

115.93

111.92

110.84

110.31

108.44

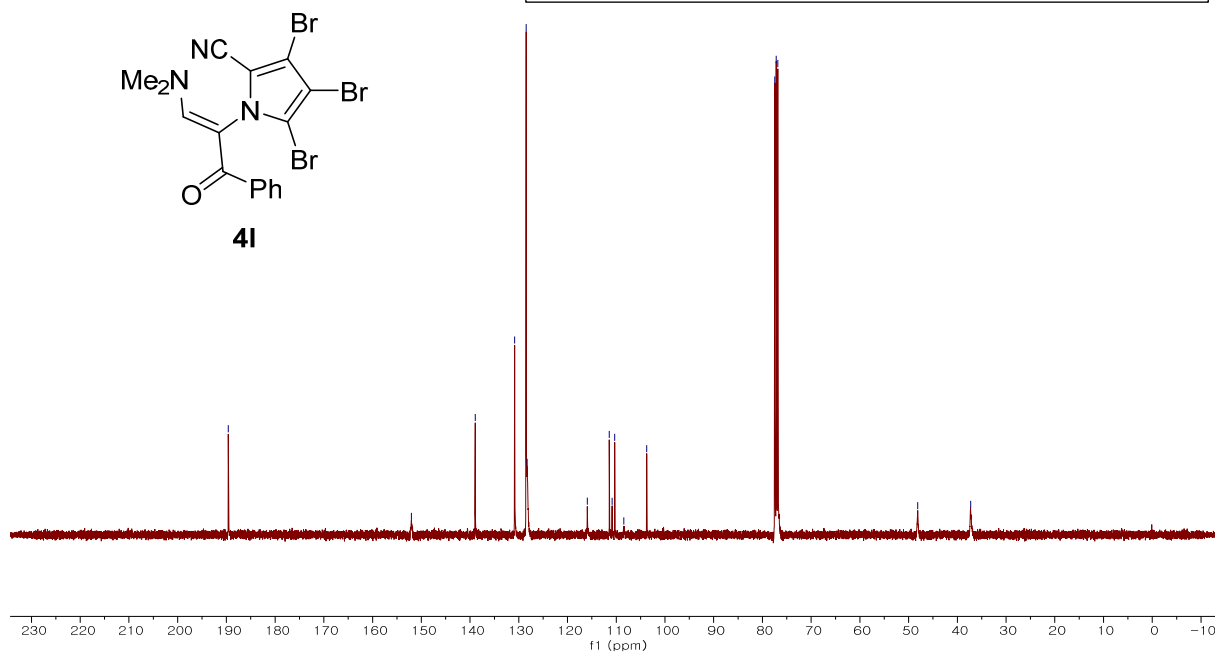
103.74

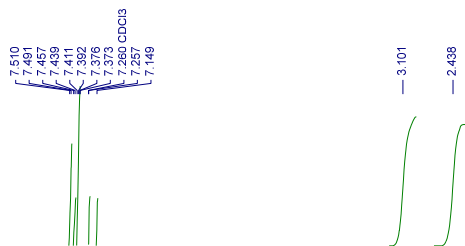
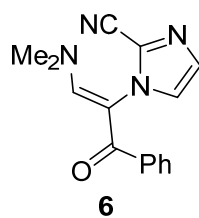
77.48 CDCl₃
77.16 CDCl₃
76.84 CDCl₃

46.15

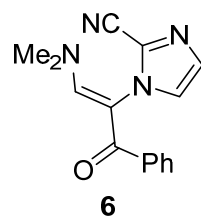
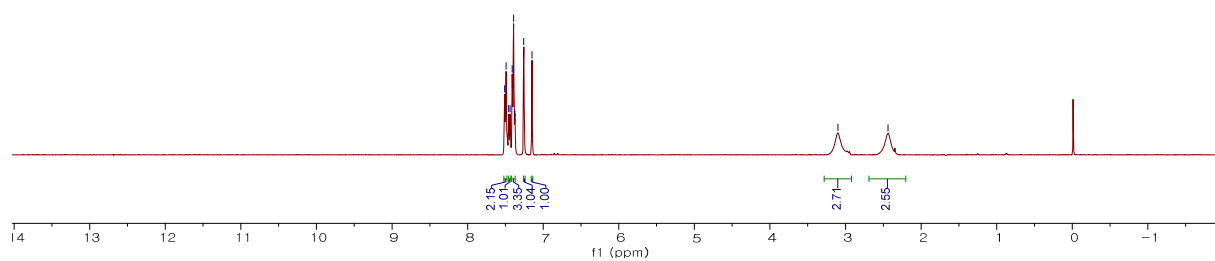
37.27

¹³C{¹H} NMR spectrum of 4I (100 MHz, CDCl₃)

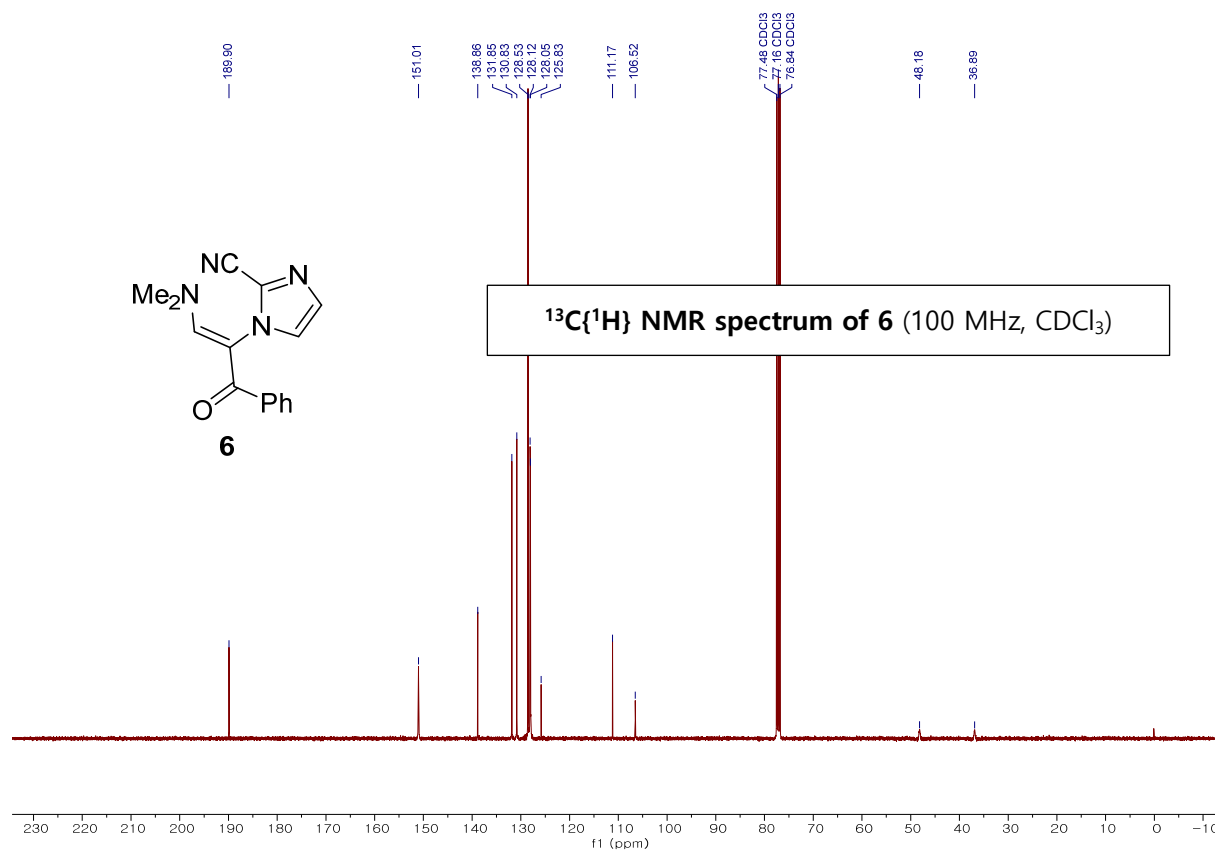


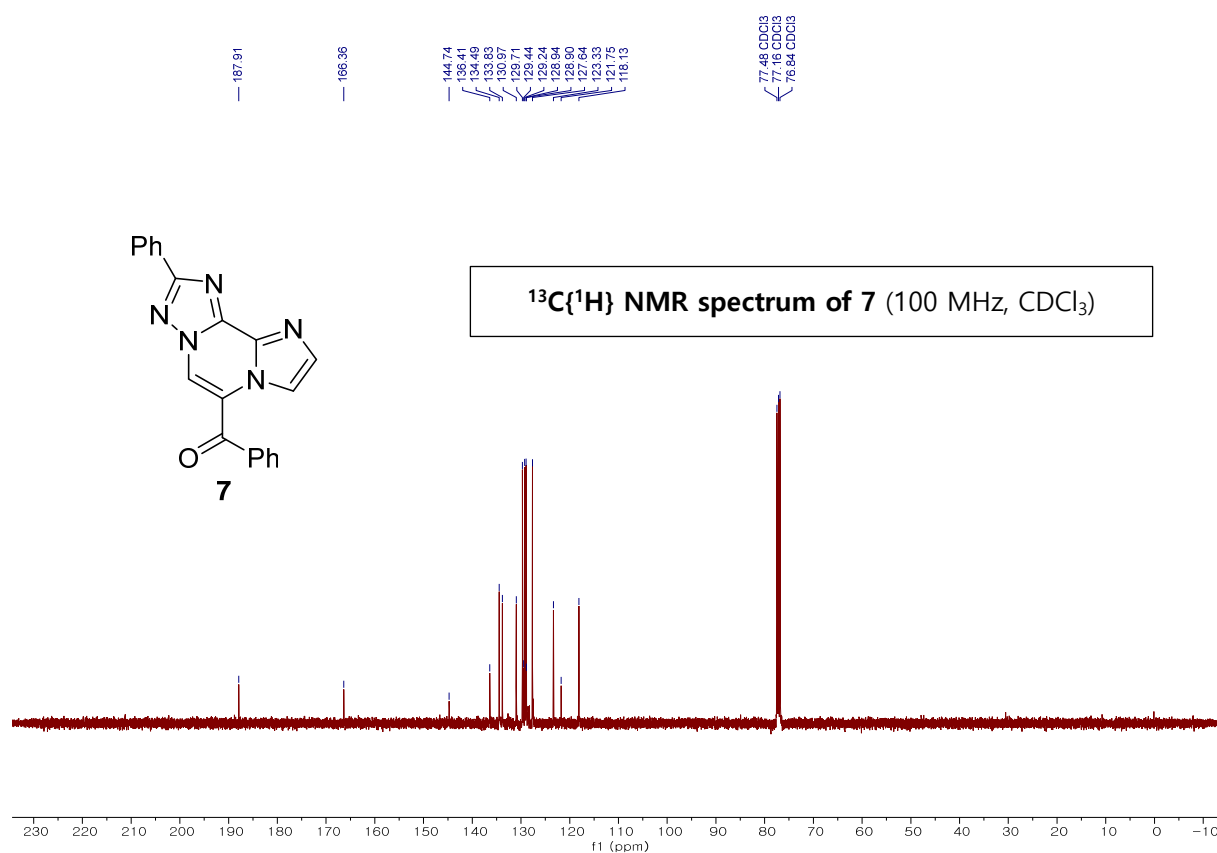
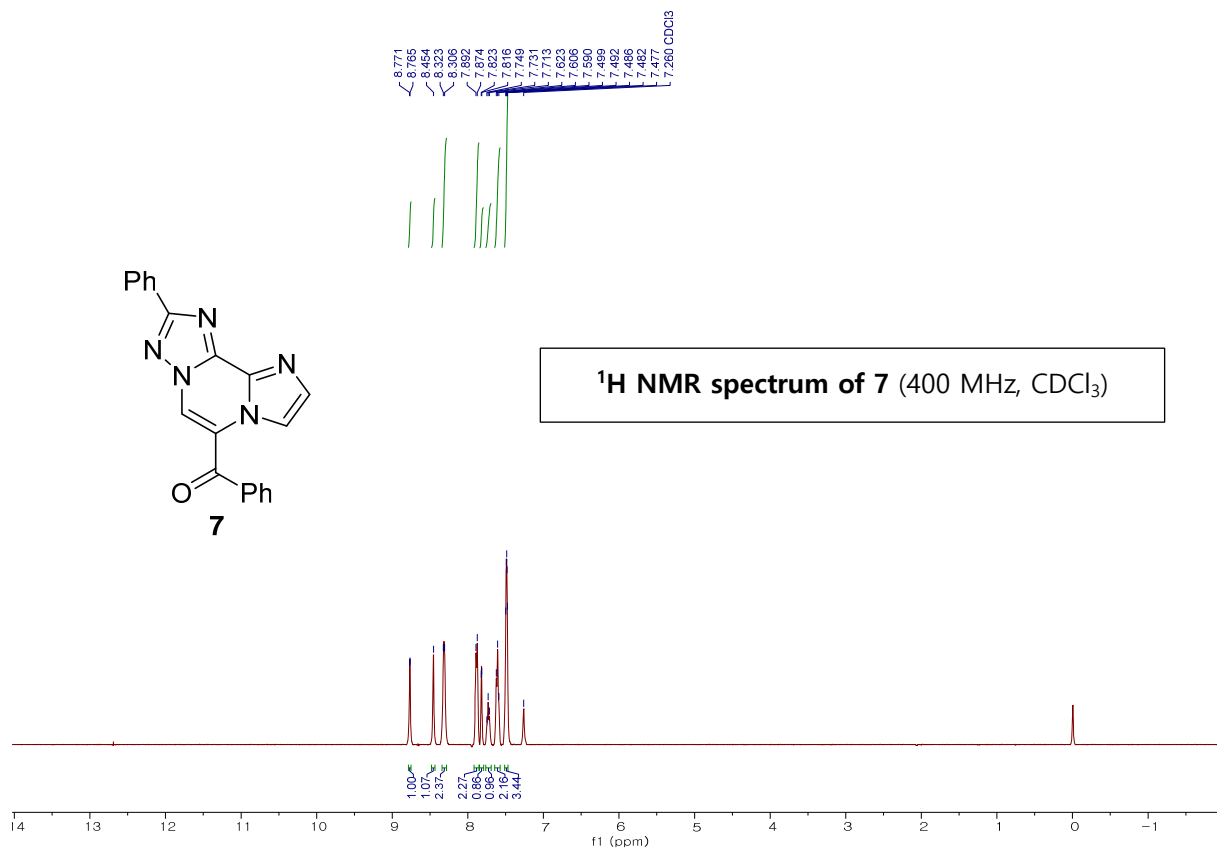


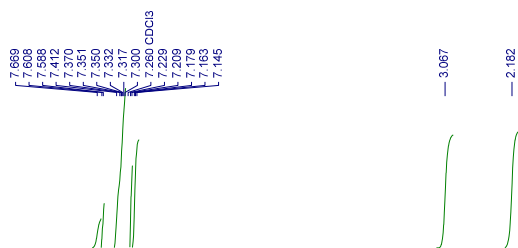
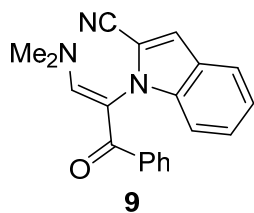
¹H NMR spectrum of 6 (400 MHz, CDCl₃)



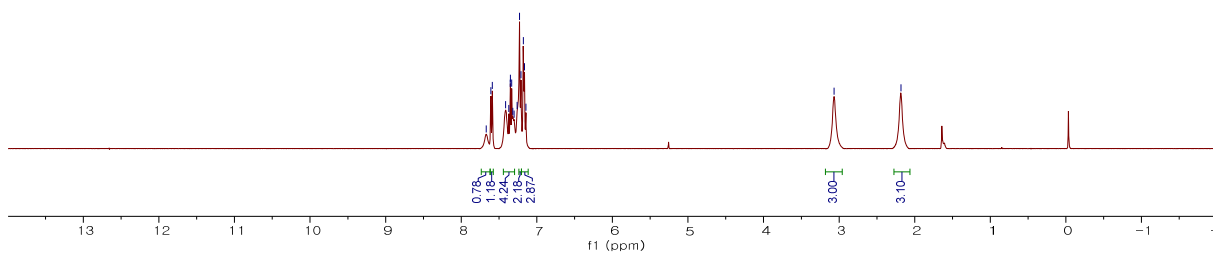
¹³C{¹H} NMR spectrum of 6 (100 MHz, CDCl₃)



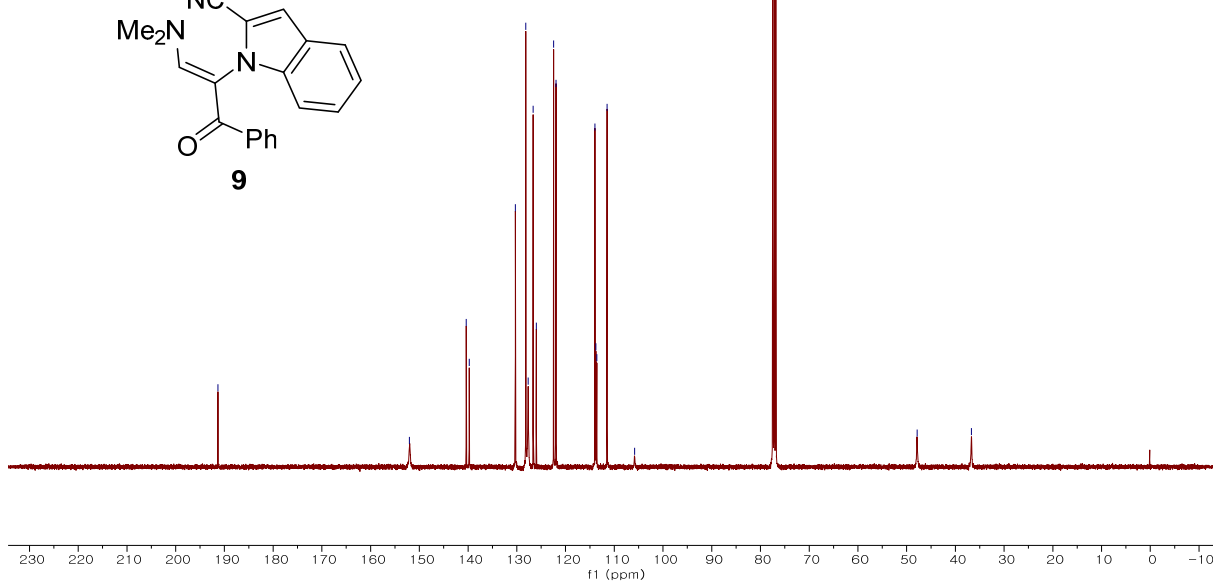
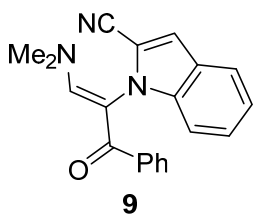


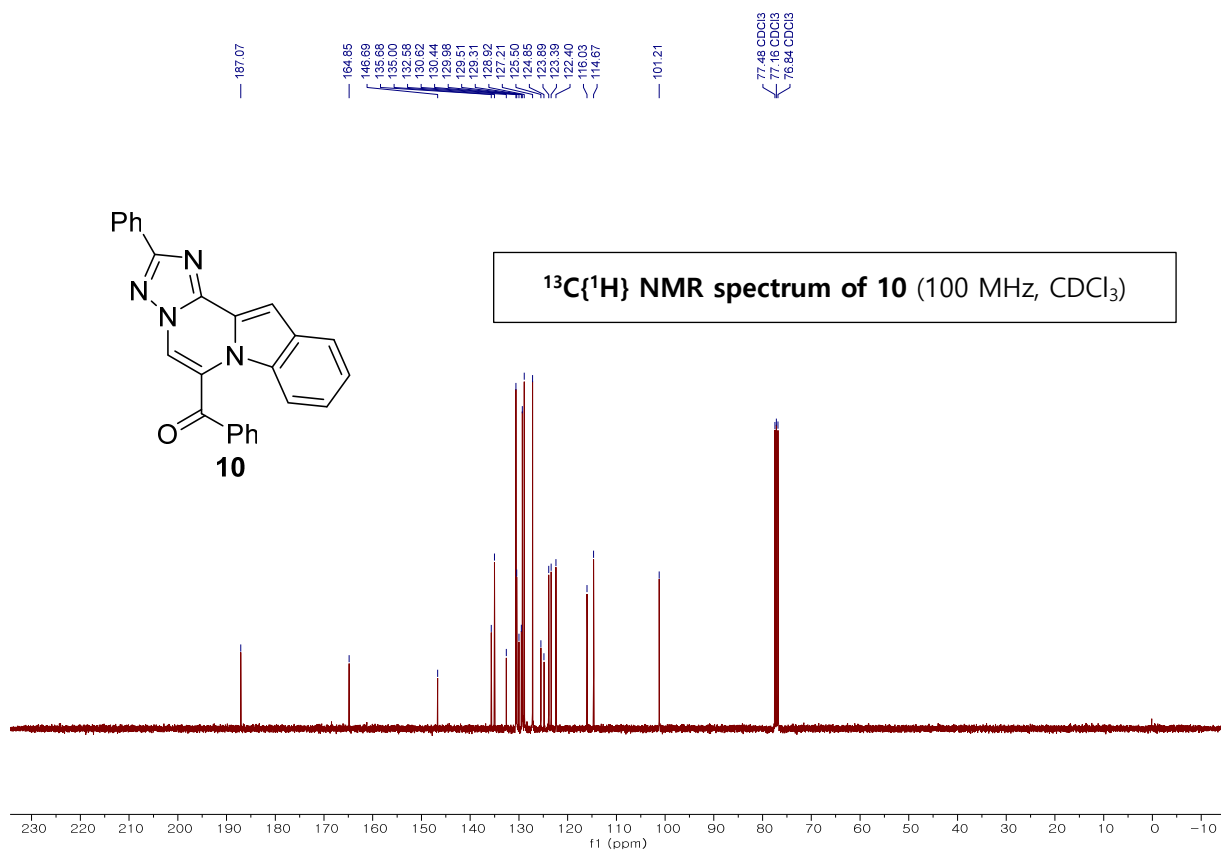
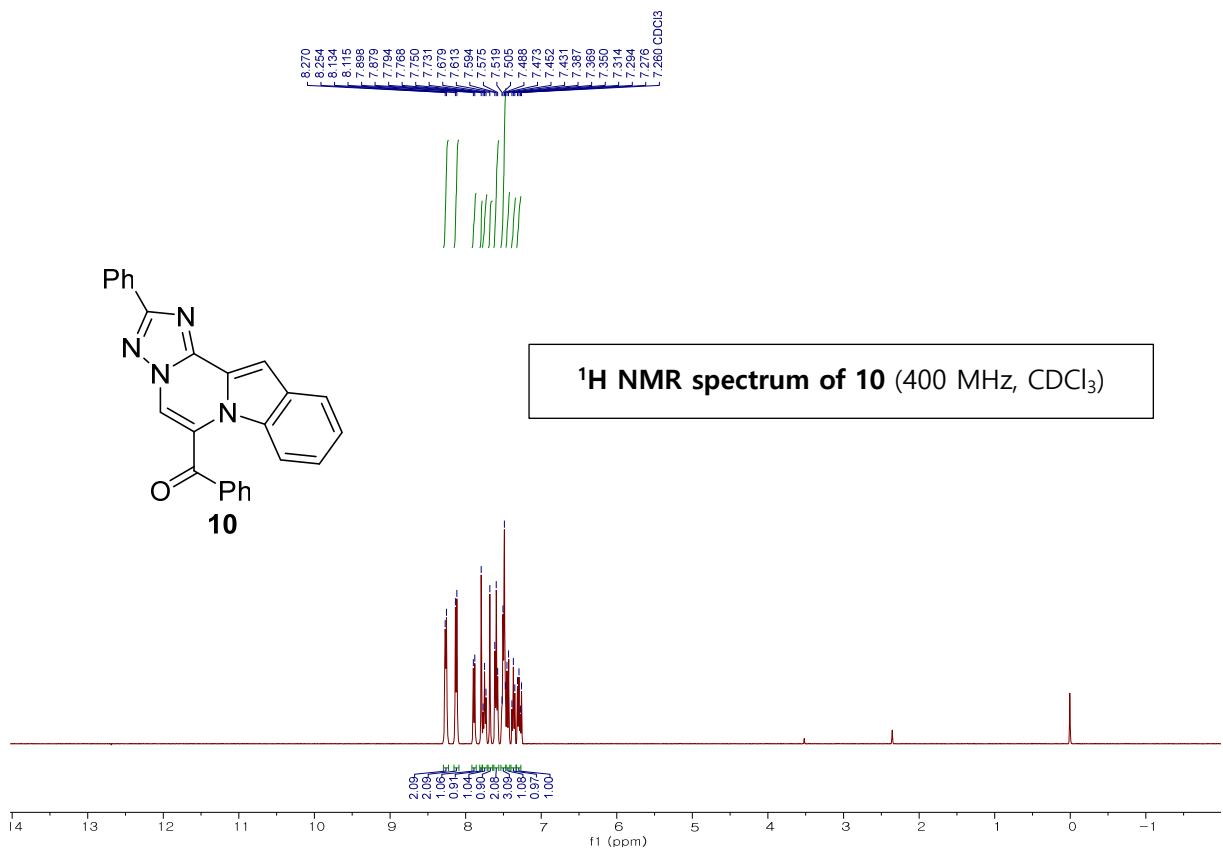


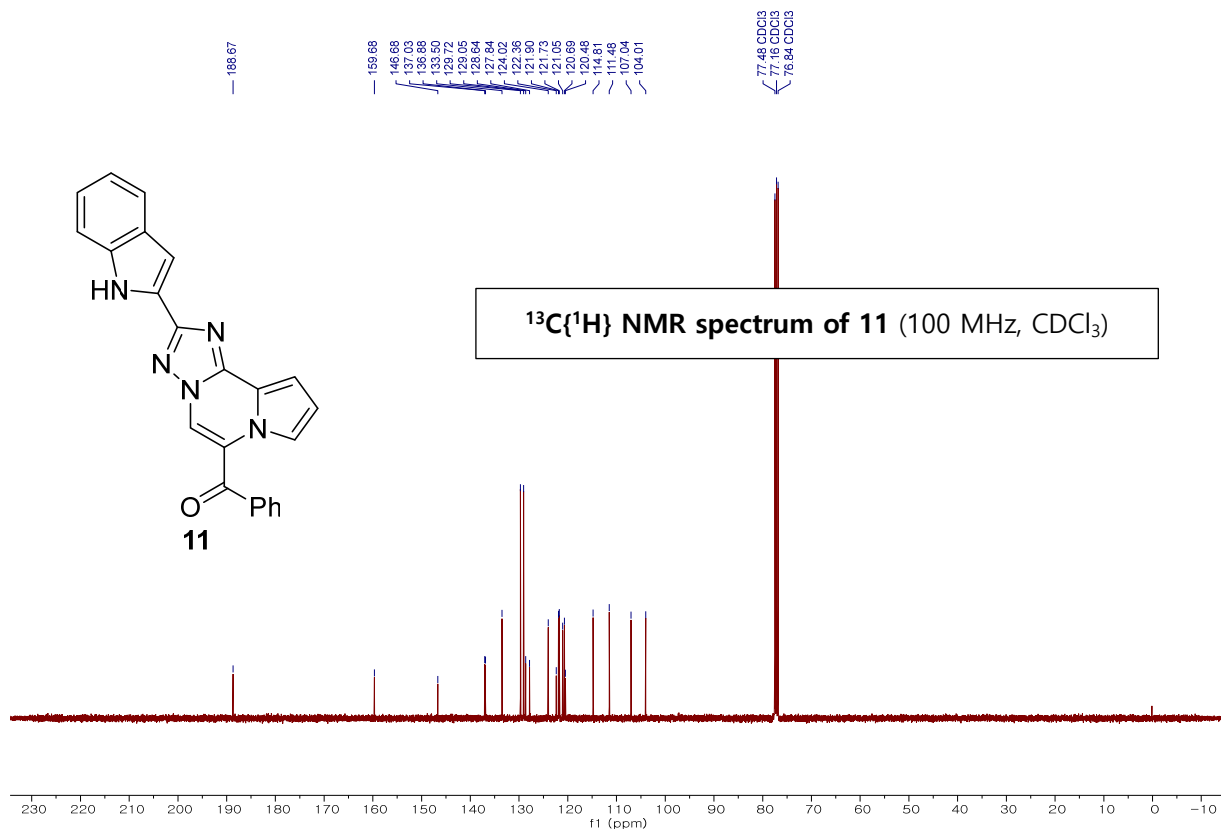
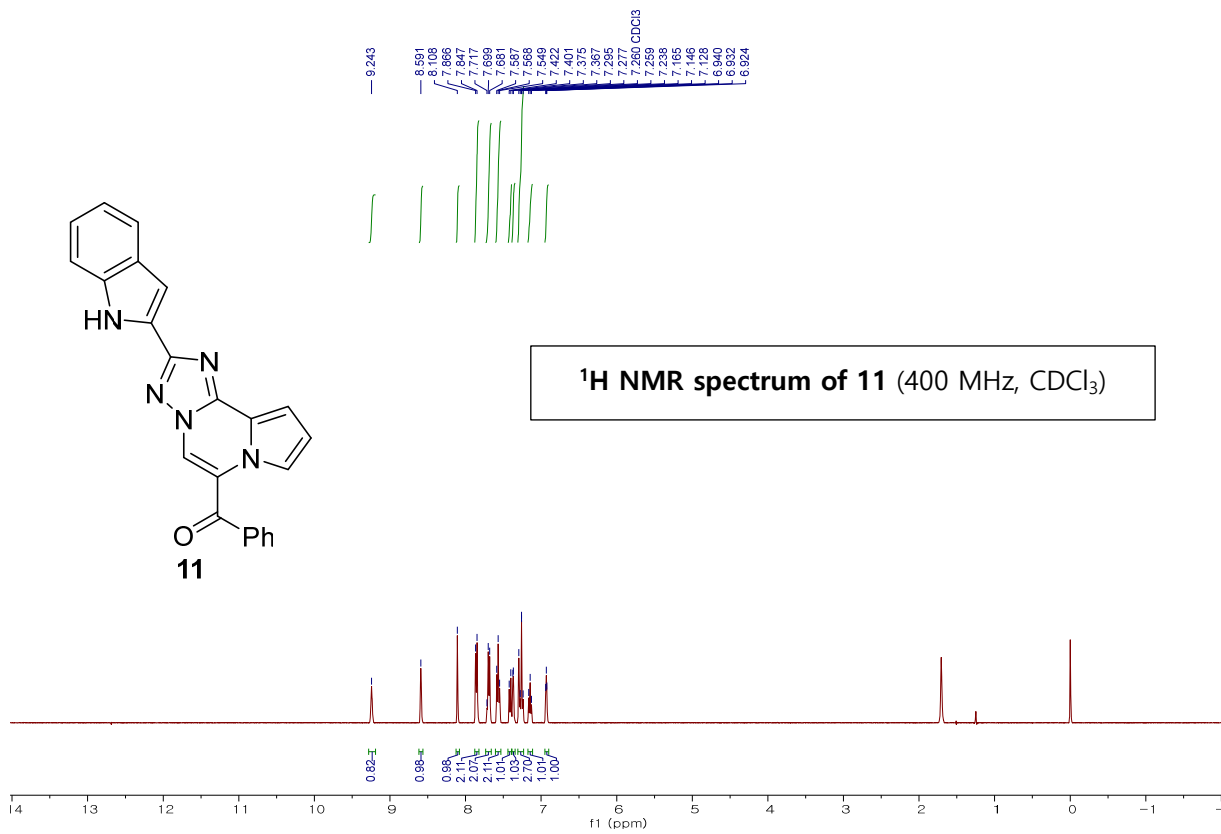
¹H NMR spectrum of 9 (400 MHz, CDCl₃)

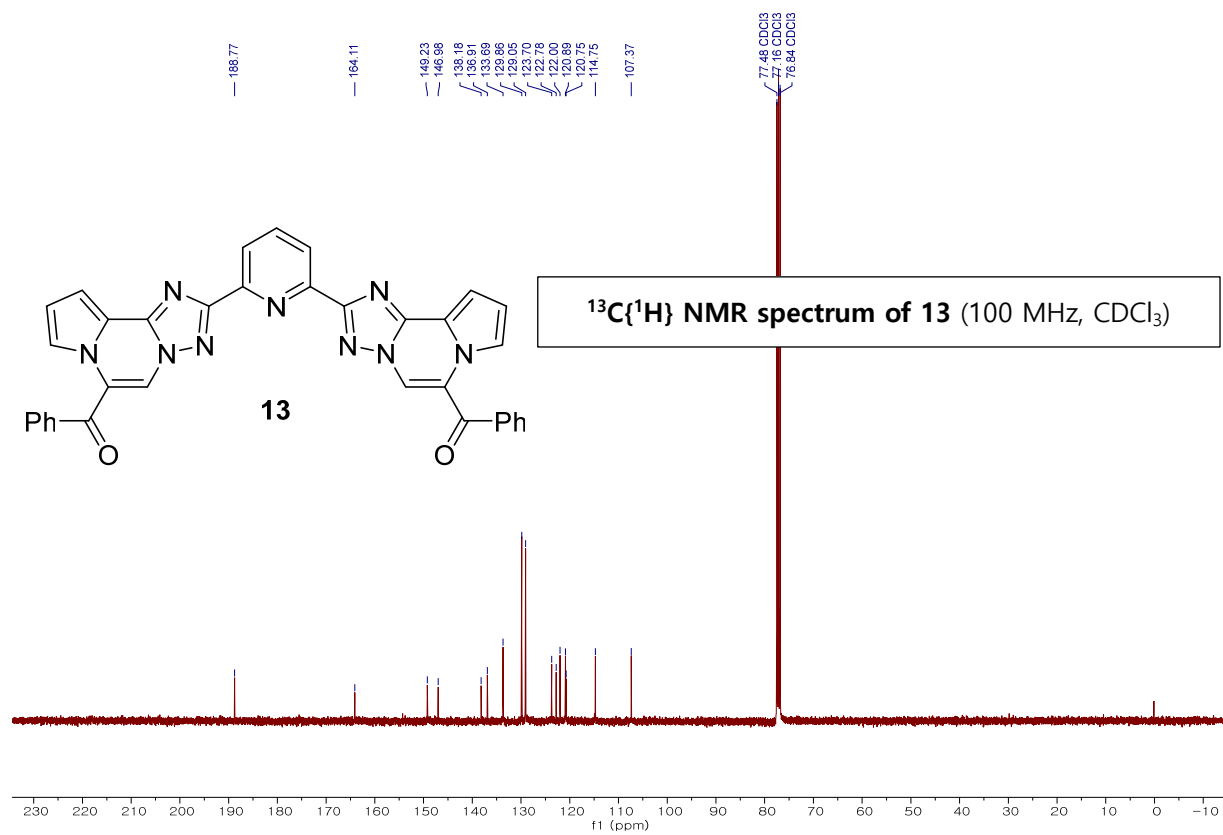
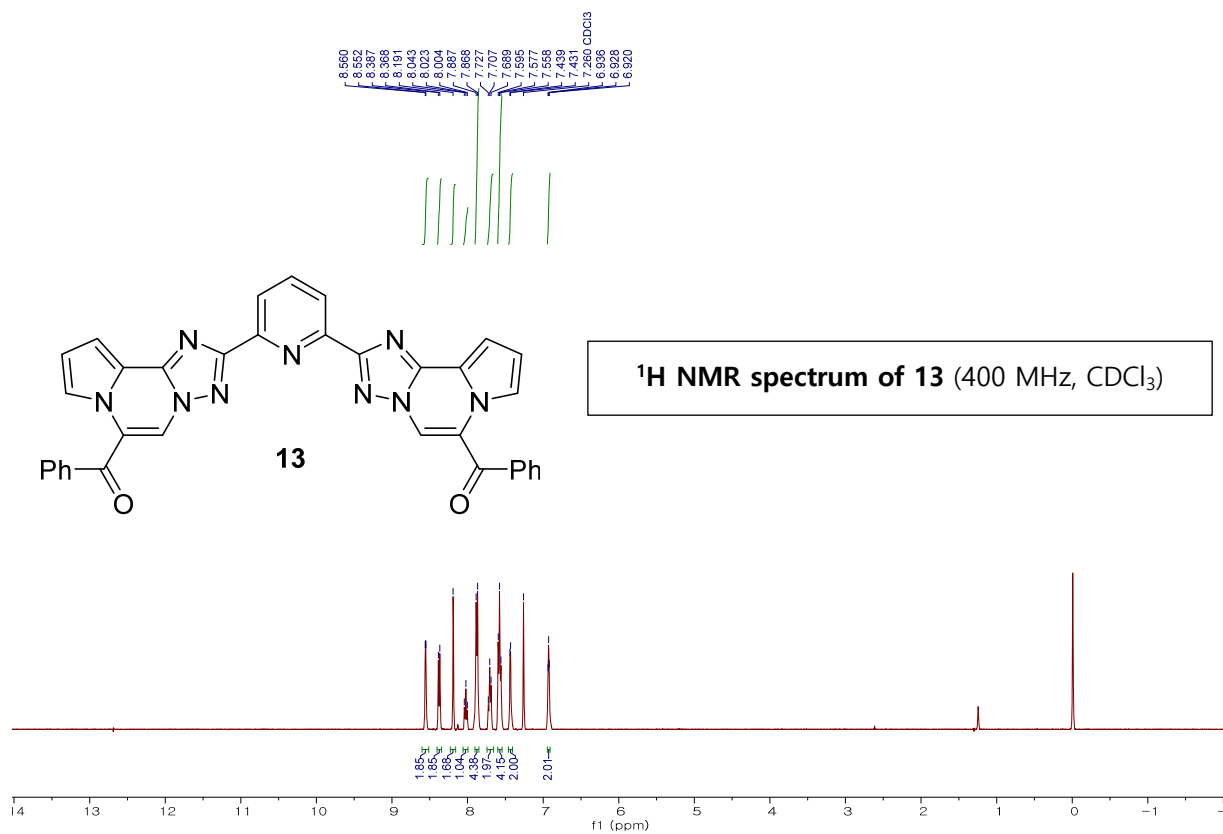


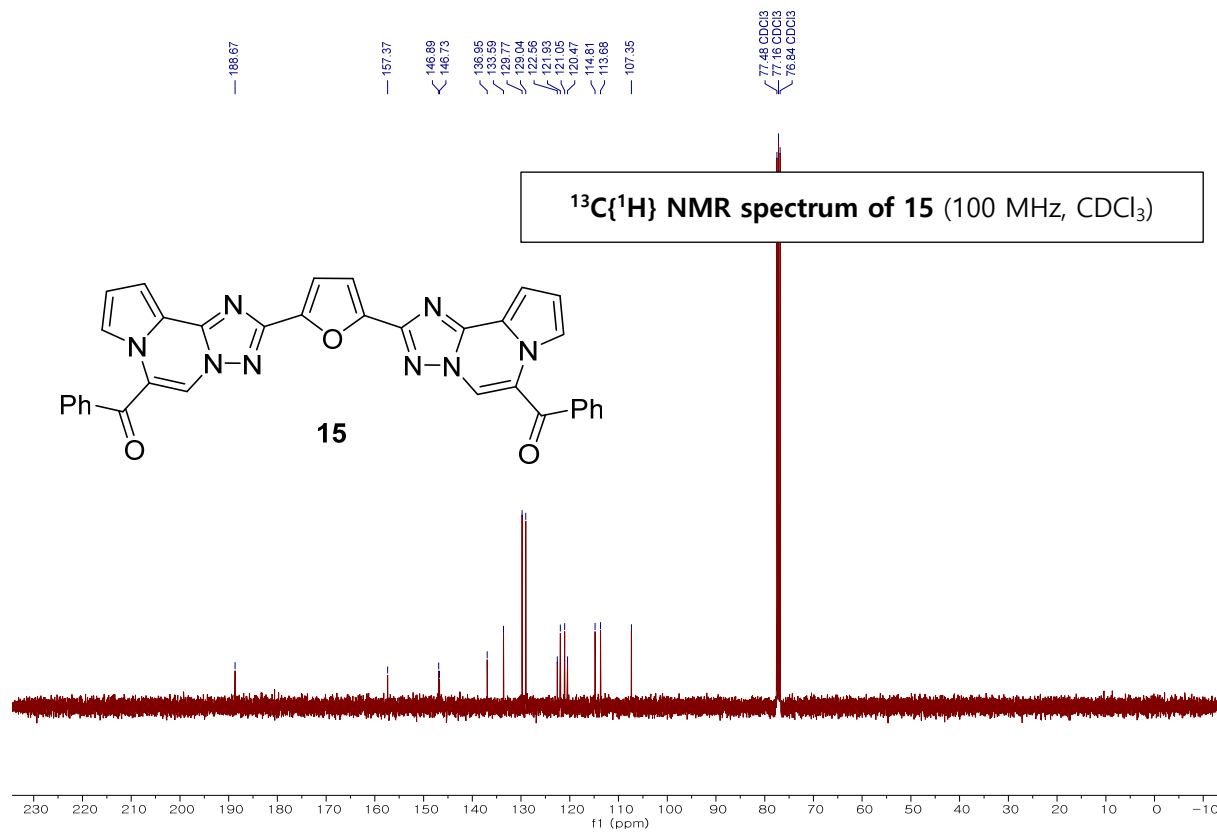
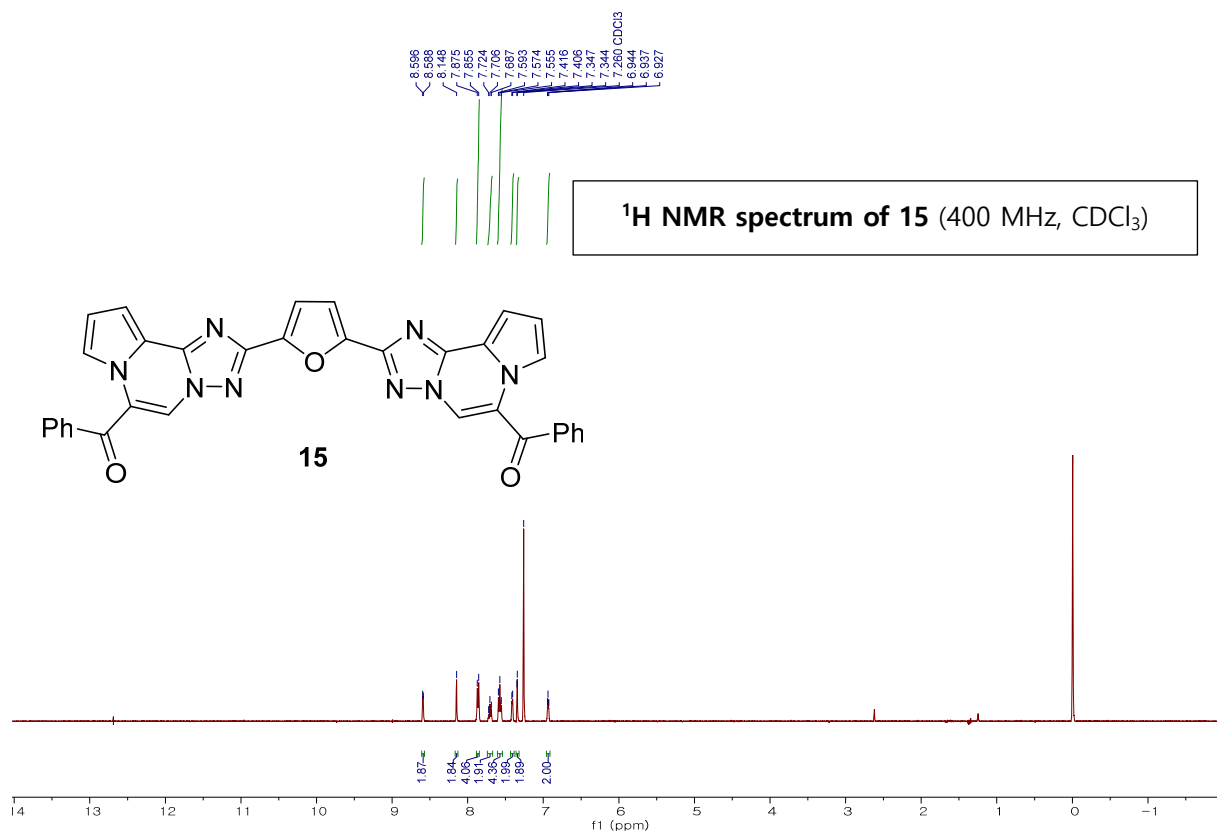
¹³C{¹H} NMR spectrum of 9 (100 MHz, CDCl₃)

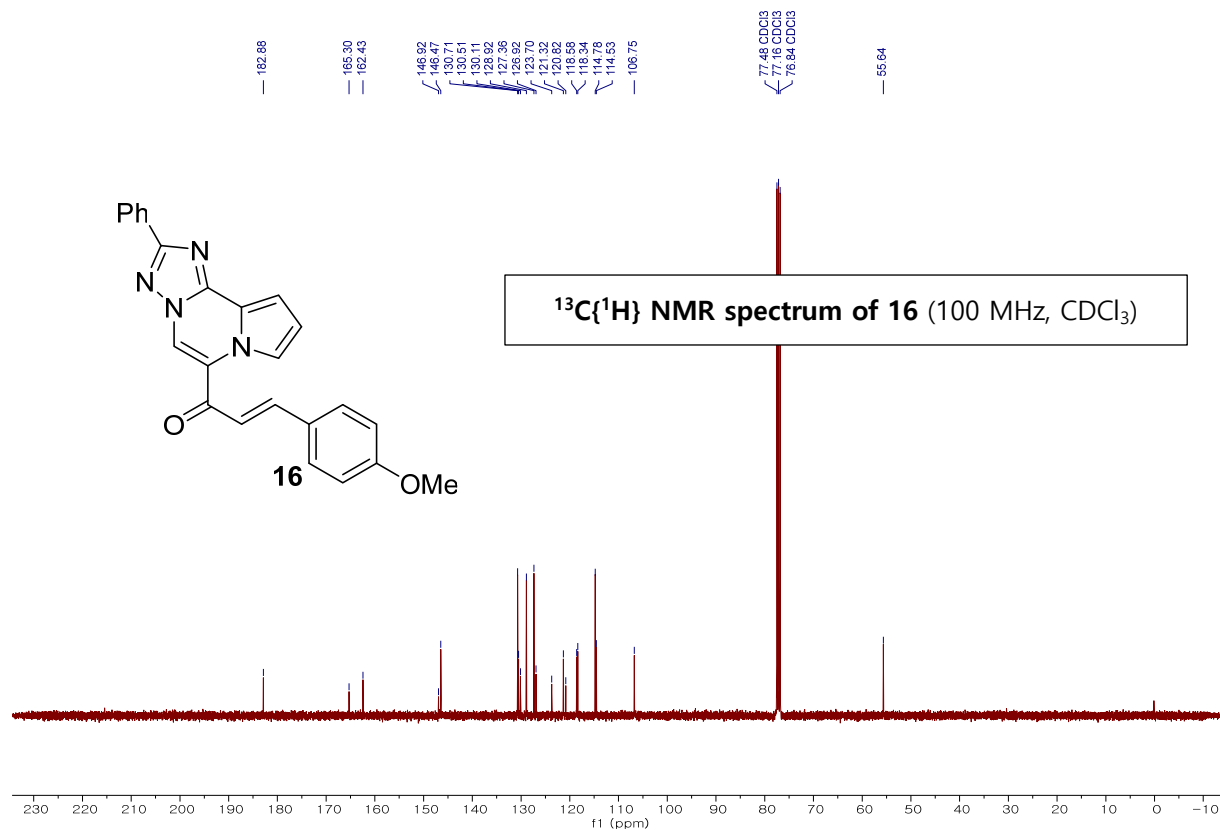
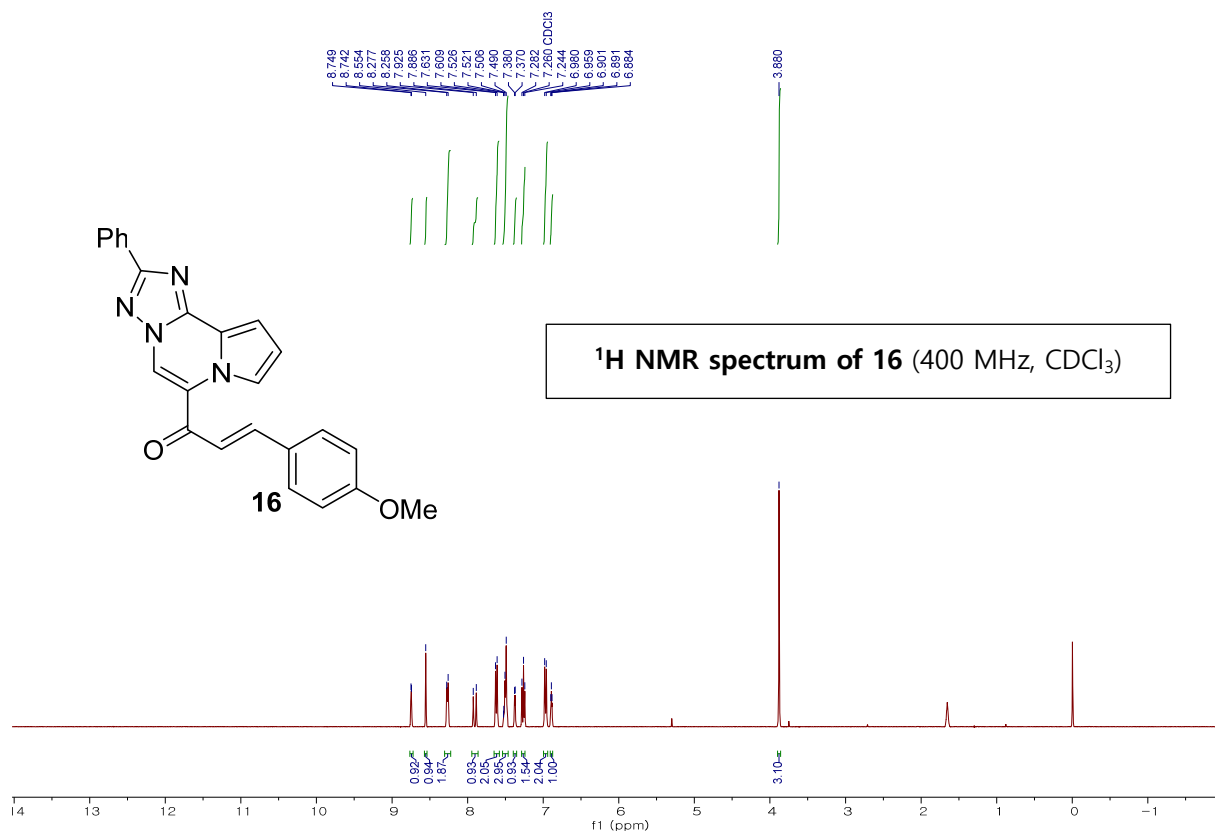


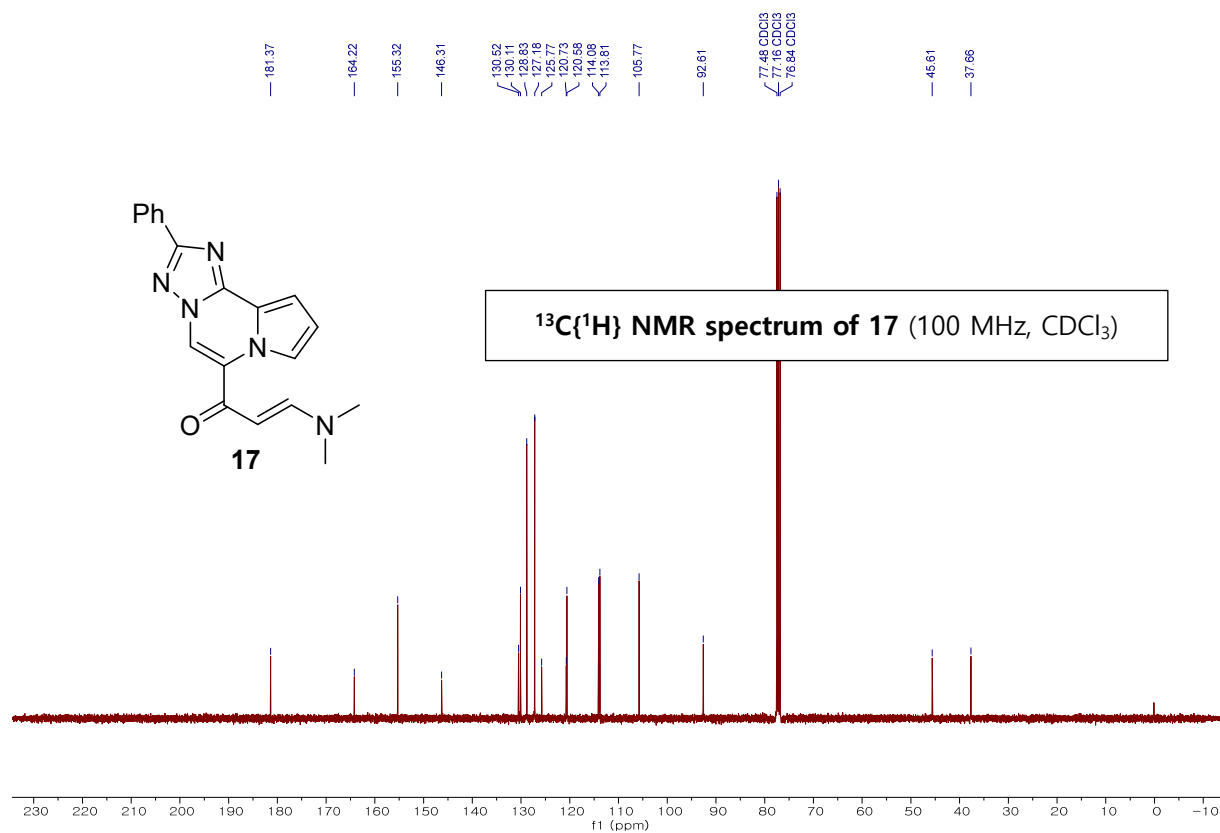
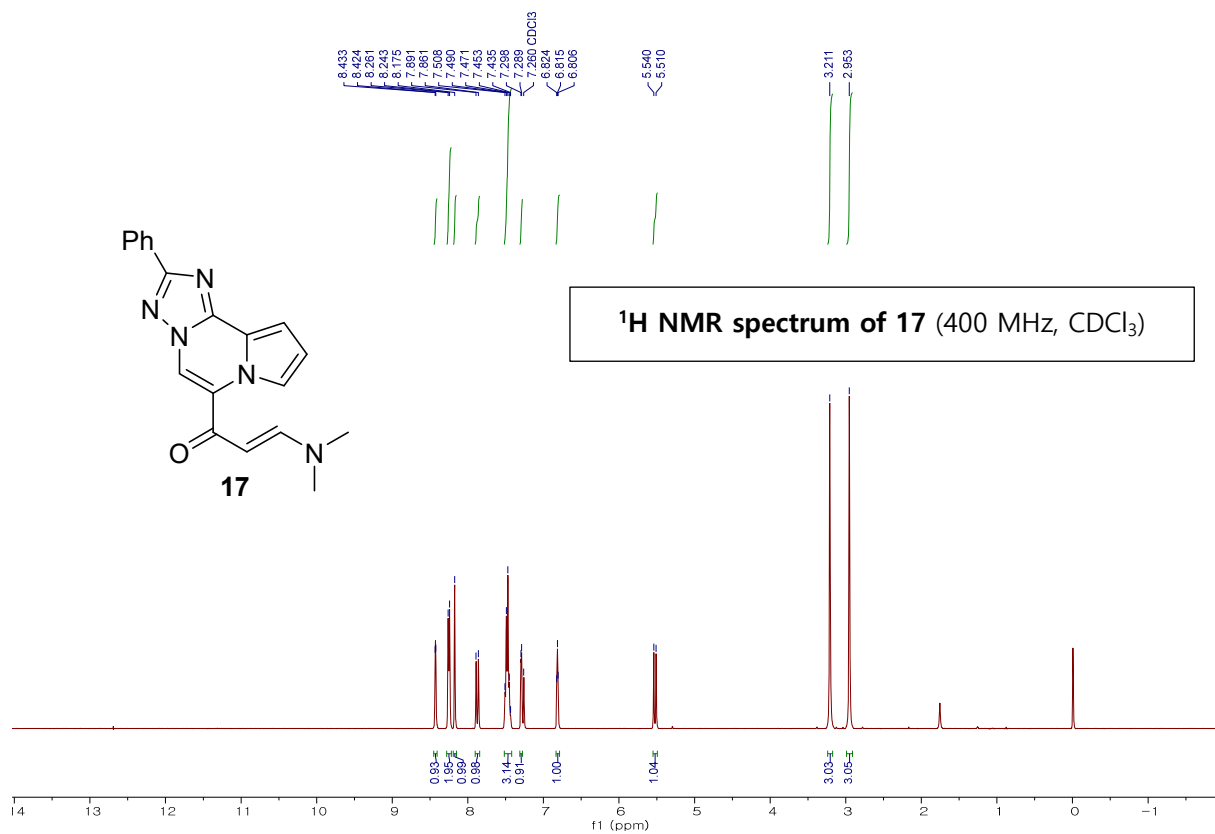


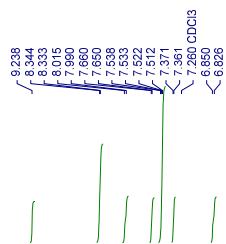
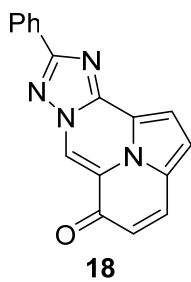




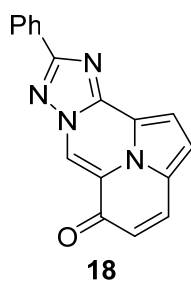
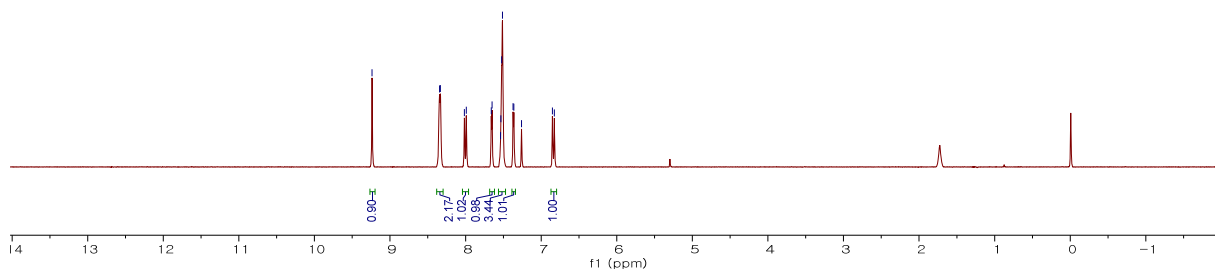




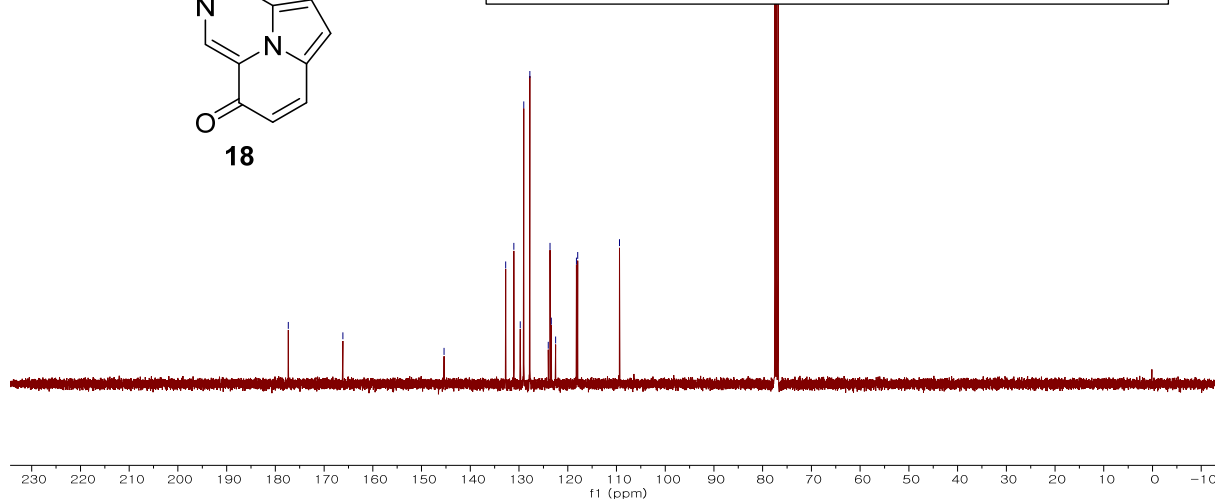


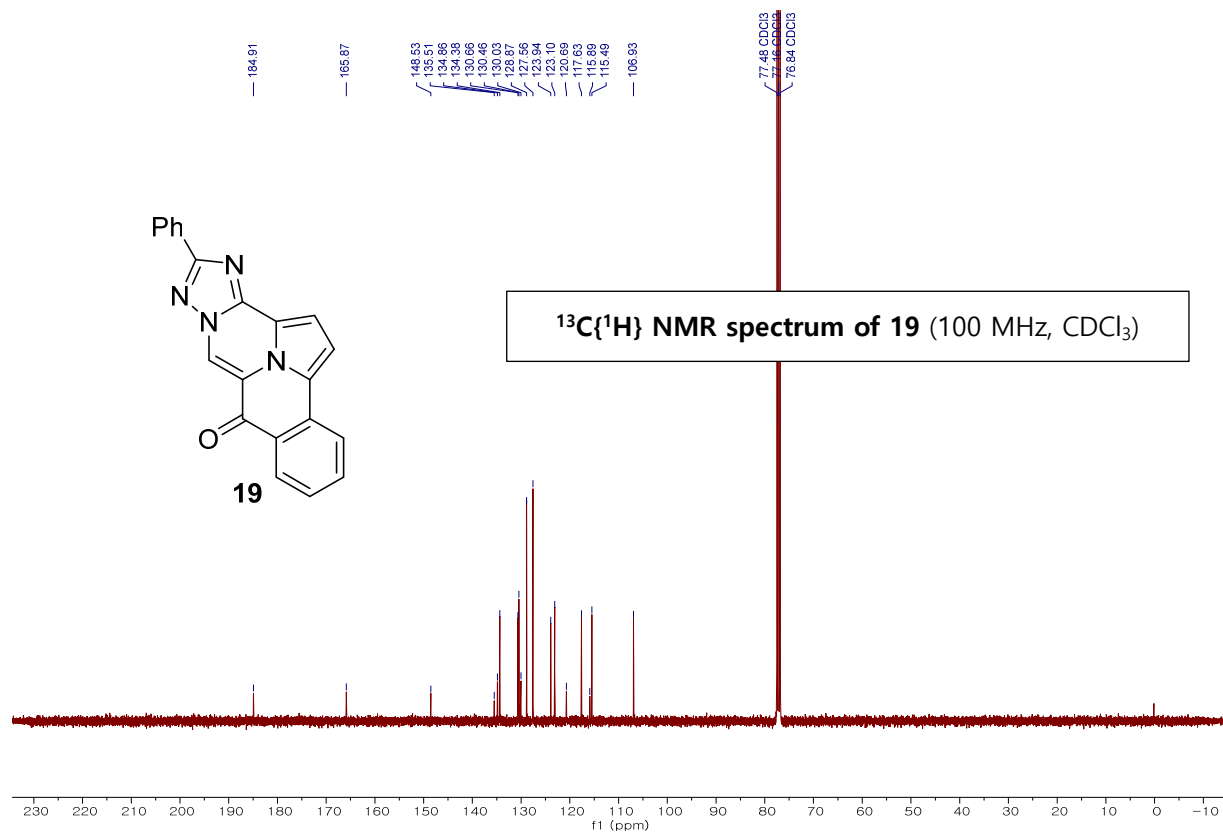
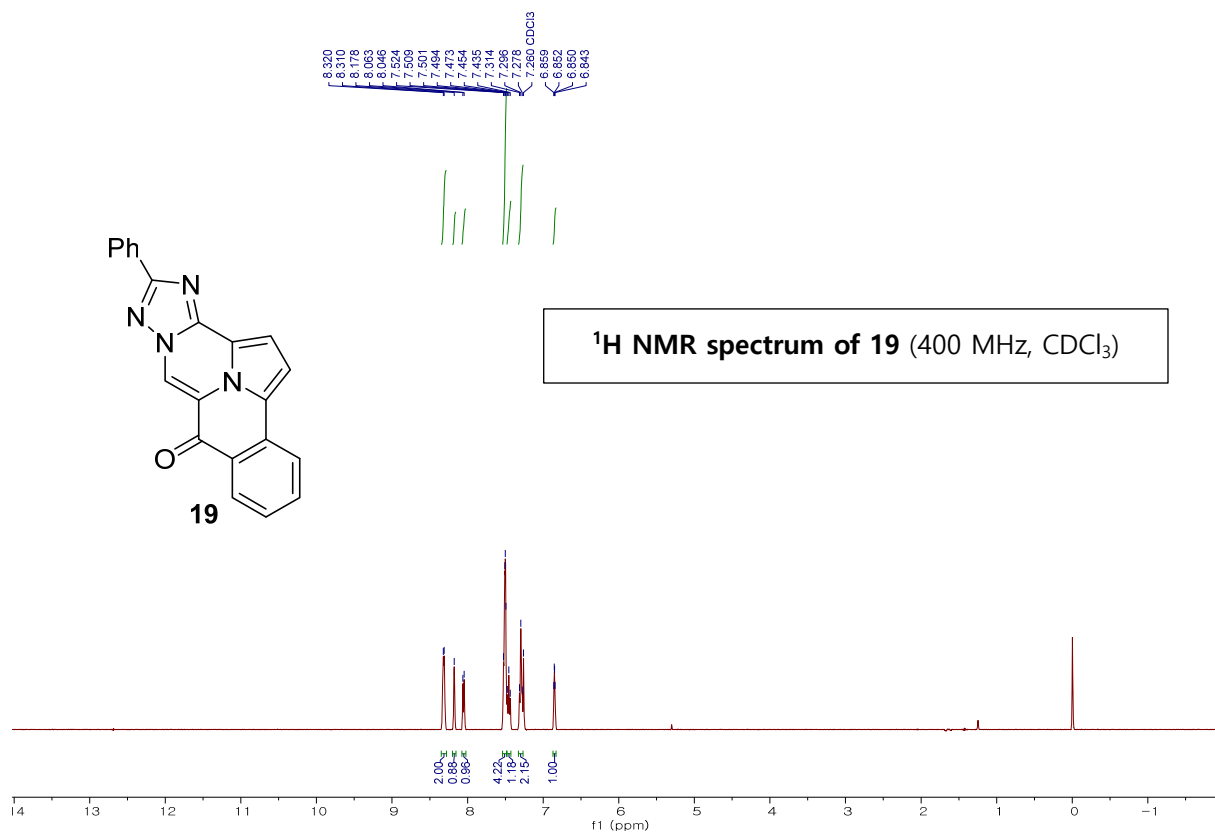


¹H NMR spectrum of 18 (400 MHz, CDCl₃)



¹³C{¹H} NMR spectrum of 18 (100 MHz, CDCl₃)





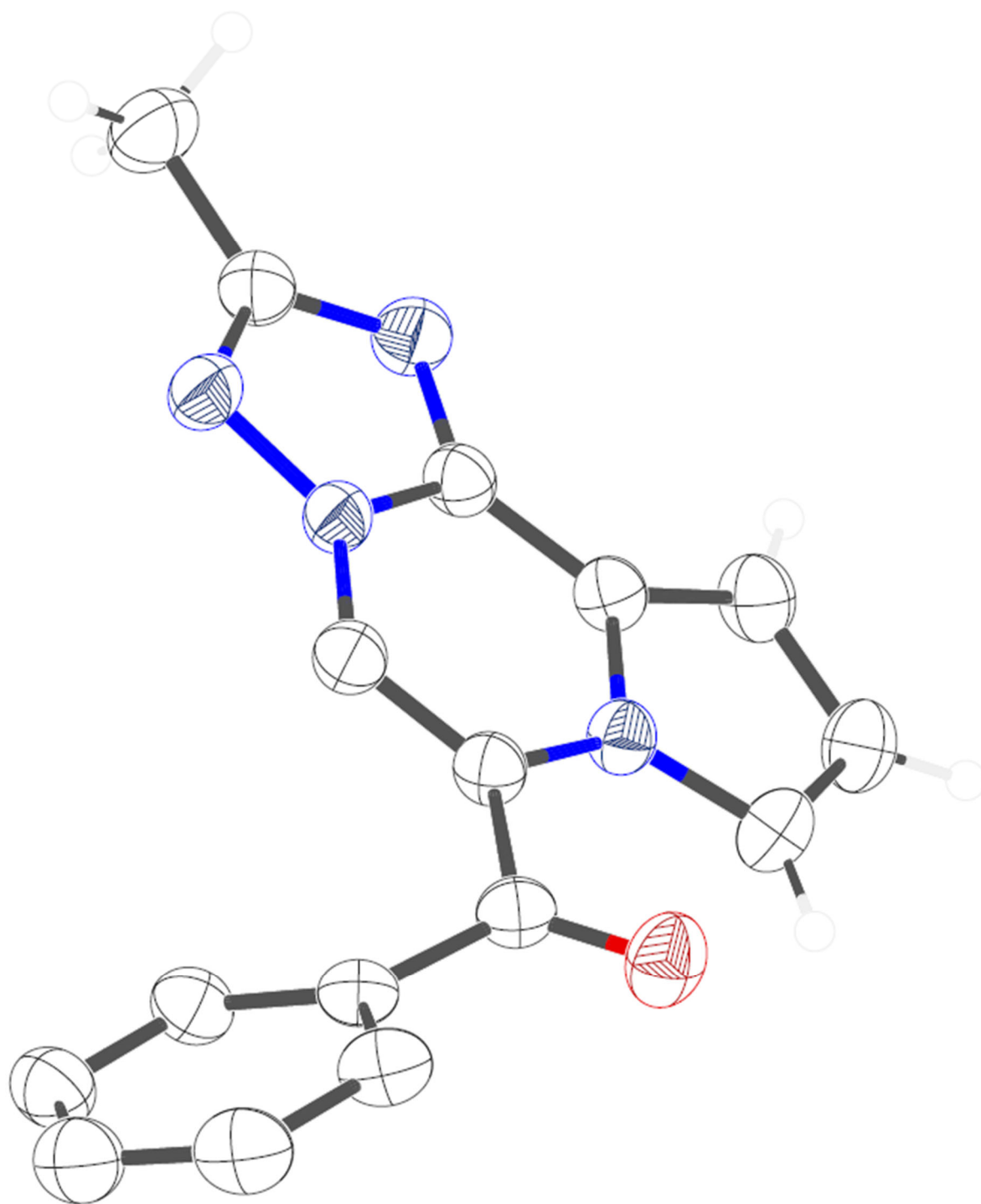


Figure S1. Thermal ellipsoid plot for **3q** with 50 % probability

The crystal **3q** for X-ray crystallographic analysis was obtained via dissolution of the compound in a mixed solvent (EtOAc:EtOH, 1:1) and slow evaporation of the solvent at room temperature.

Table S1. Crystal data for 1,2,4-triazole-acylpyrrolopyrazine 3q.

Identification code	1,2,4-triazole-acylpyrrolopyrazine 3q	
Chemical formula	C ₁₆ H ₁₂ N ₄ O	
Formula weight	276.30 g/mol	
Temperature/K	296(2) K	
Wavelength	0.71073 Å	
Crystal size	0.300 × 0.350 × 0.700 mm	
Crystal habit	Clear yellow block	
Crystal system	orthorhombic	
Space group	Pbca	
Unit cell dimensions	a = 17.3854(19) Å	α = 90°
	b = 7.5604(8) Å	β = 90°
	c = 20.364(2) Å	γ = 90°
Volume	2676.7(5) Å ³	
Z	8	
Density (calculated)	1.371 g/cm ³	
Absorption coefficient	0.090 mm ⁻¹	
F(000)	1152	
