

Supporting Information

Radical Addition/Spirocyclization Cascade of Tryptamine-Derived Isocyanides with Aryl Boronic Acids: Efficient Access to Spiroindoline Derivatives

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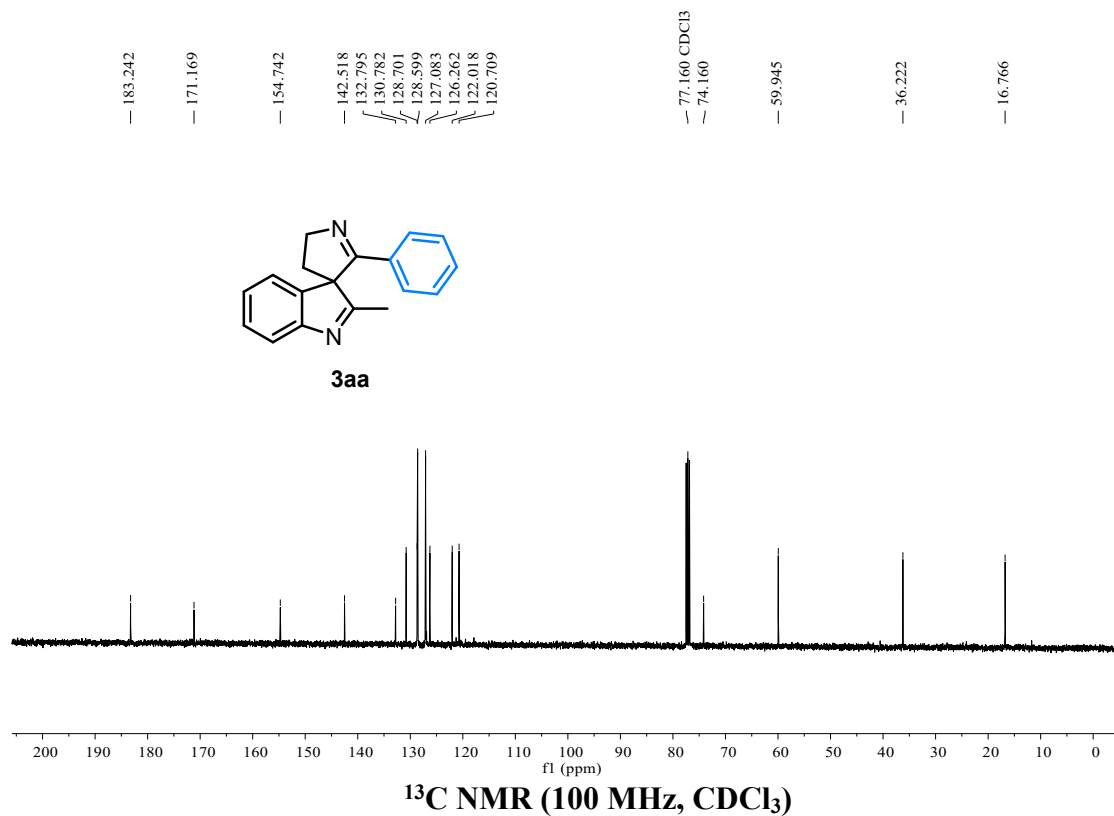
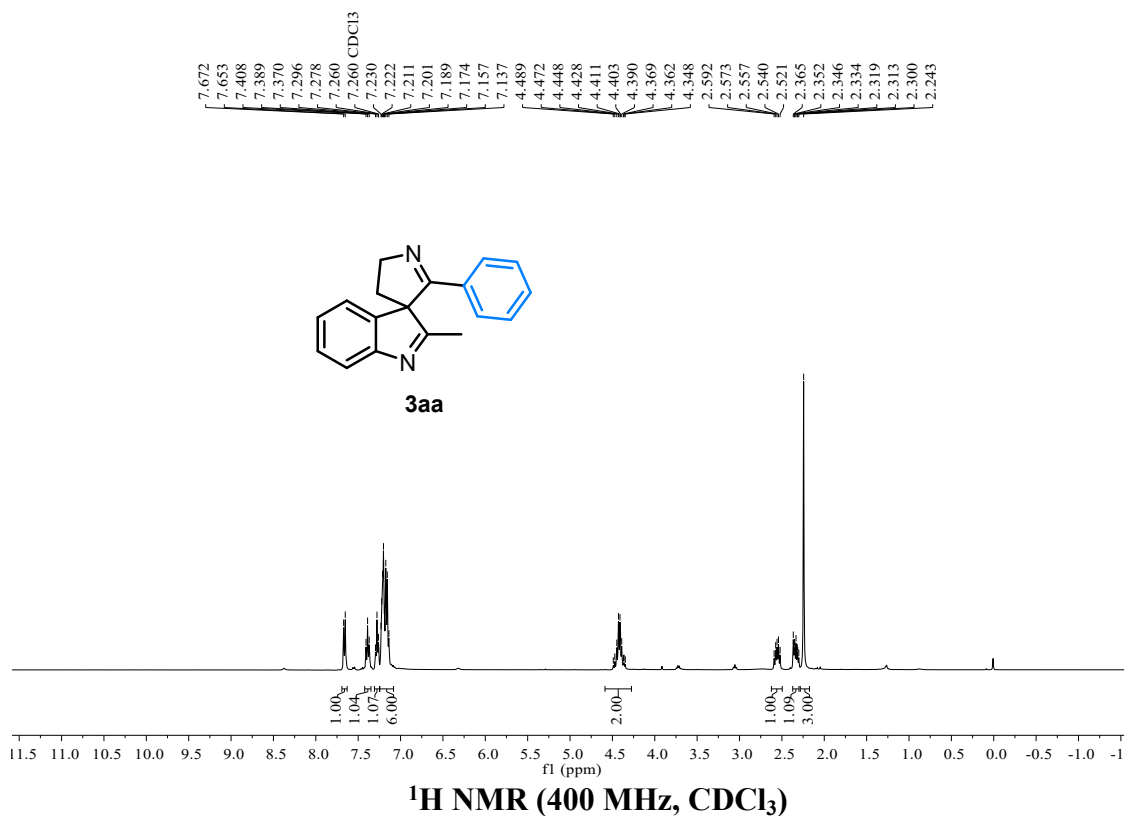
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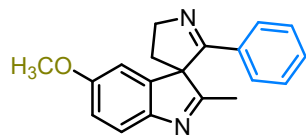
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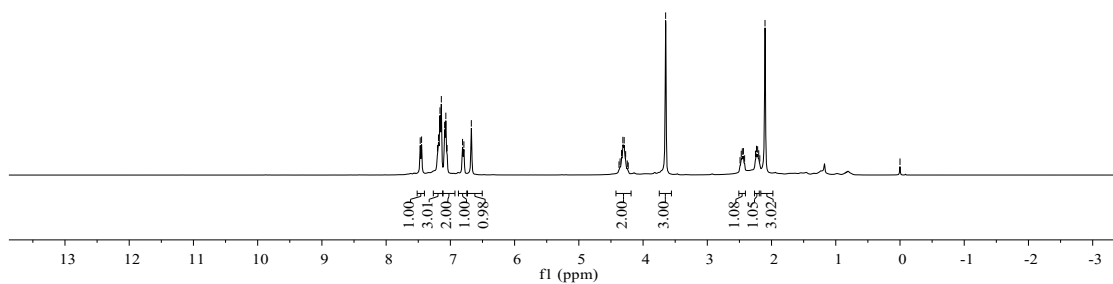
1. ^1H , ^{13}C and ^{19}F NMR spectra of all products



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7.051
6.810
6.674
6.674
4.375
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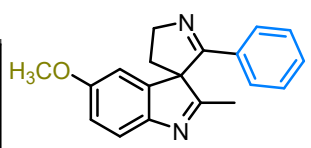


3ba

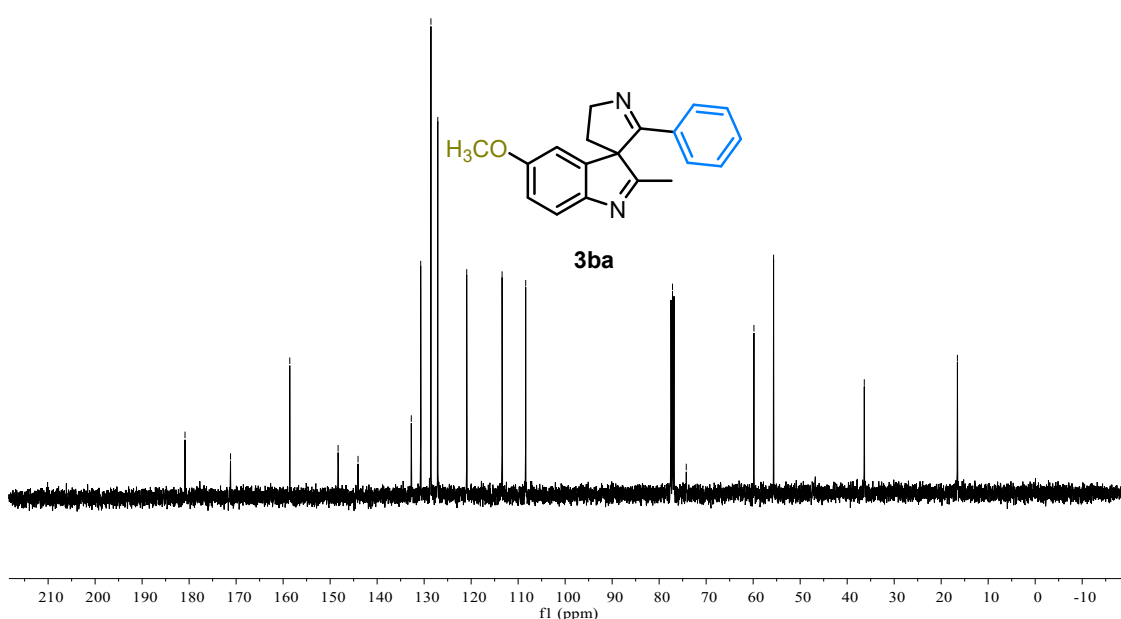


¹H NMR (400 MHz, CDCl₃)

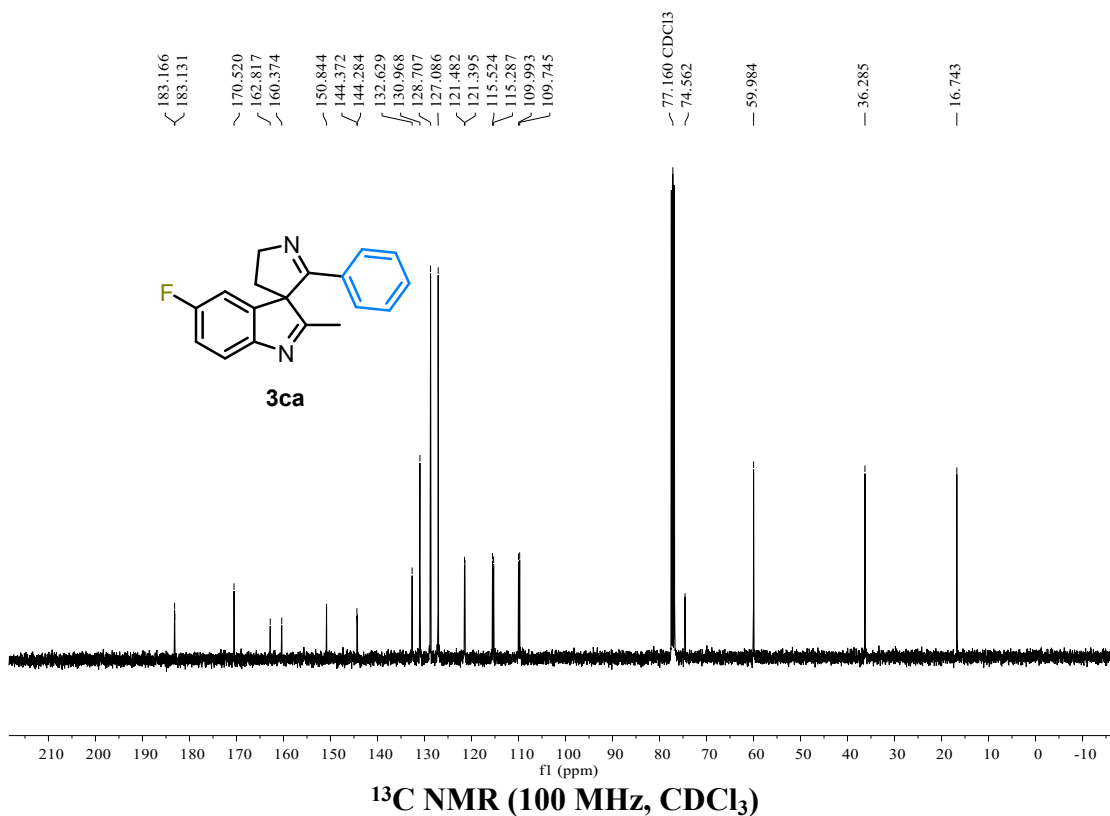
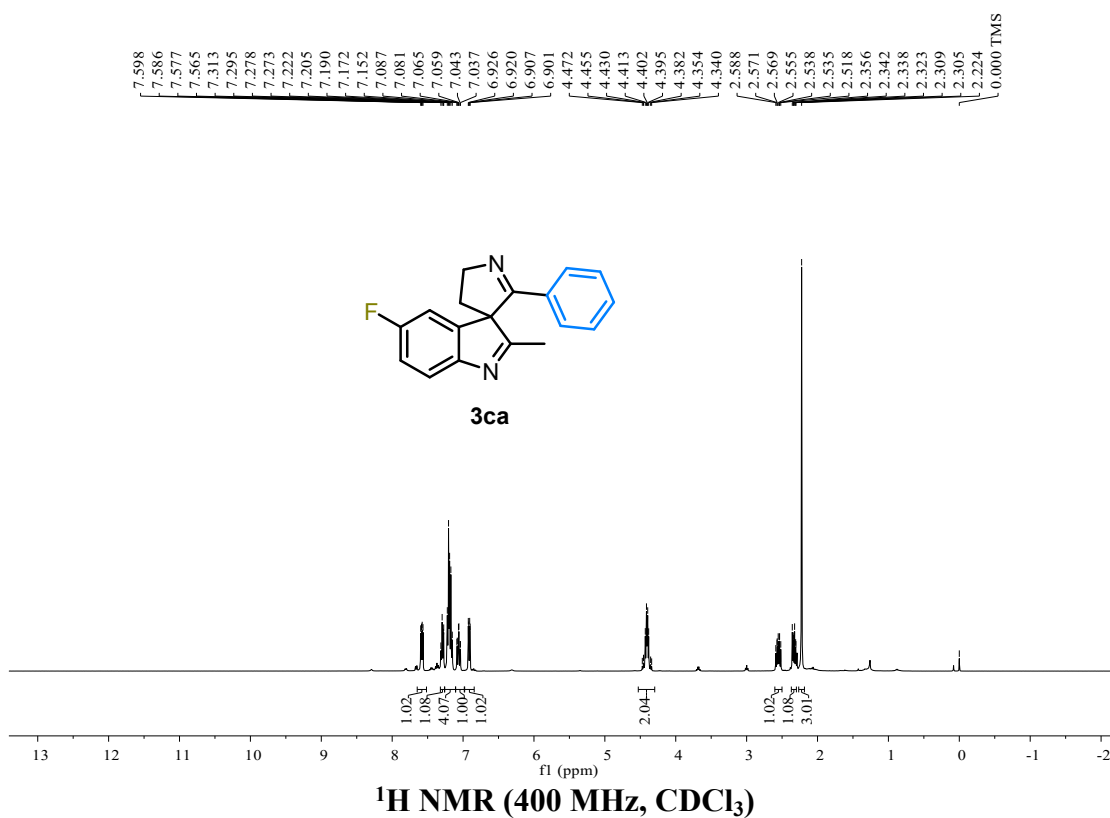
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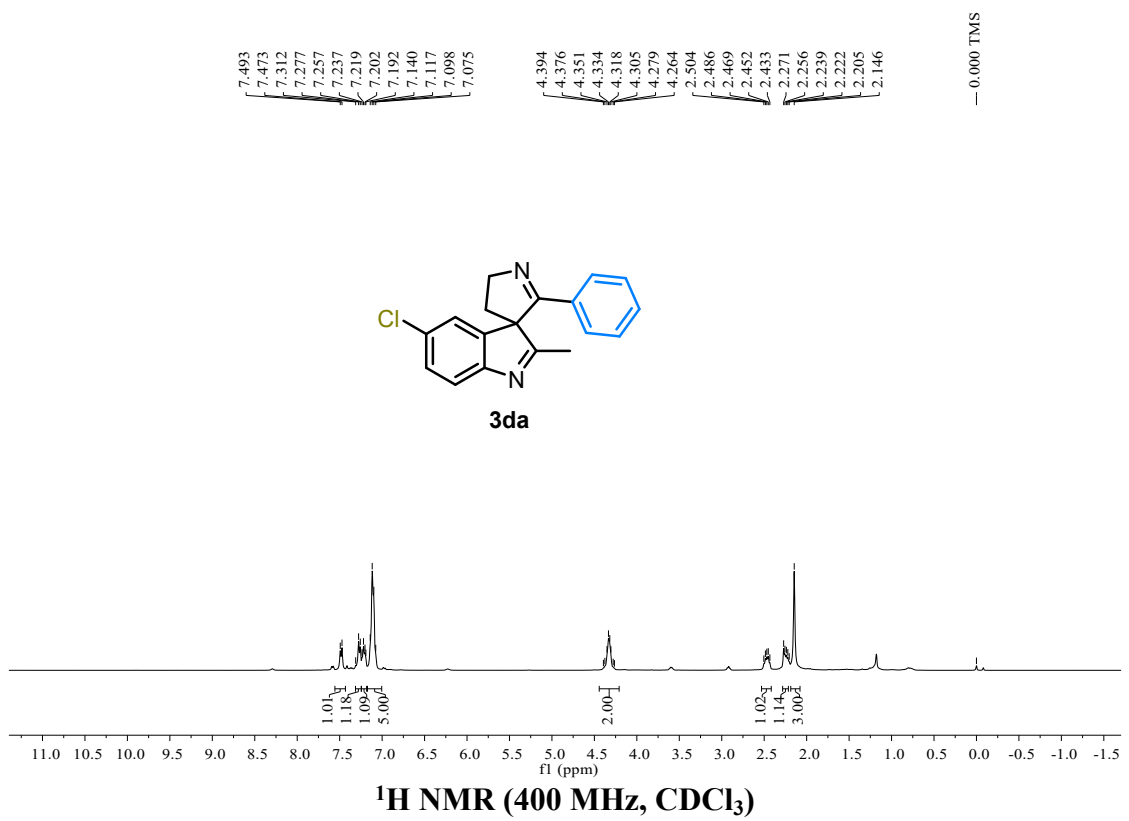
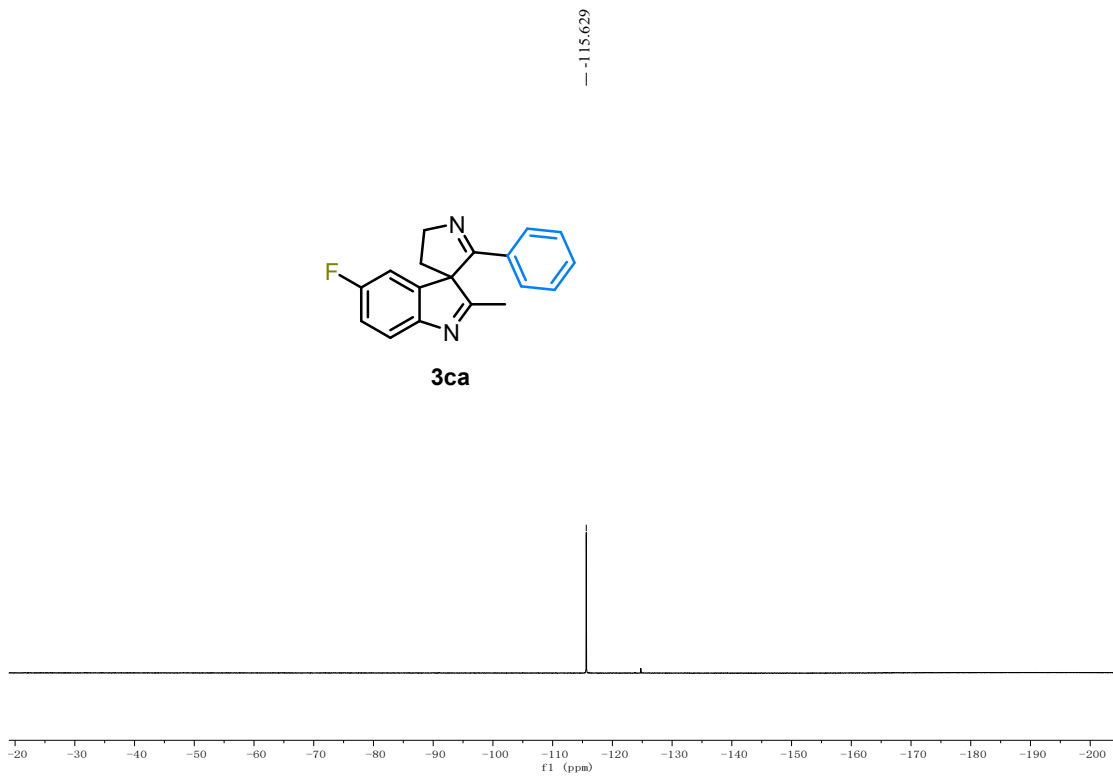


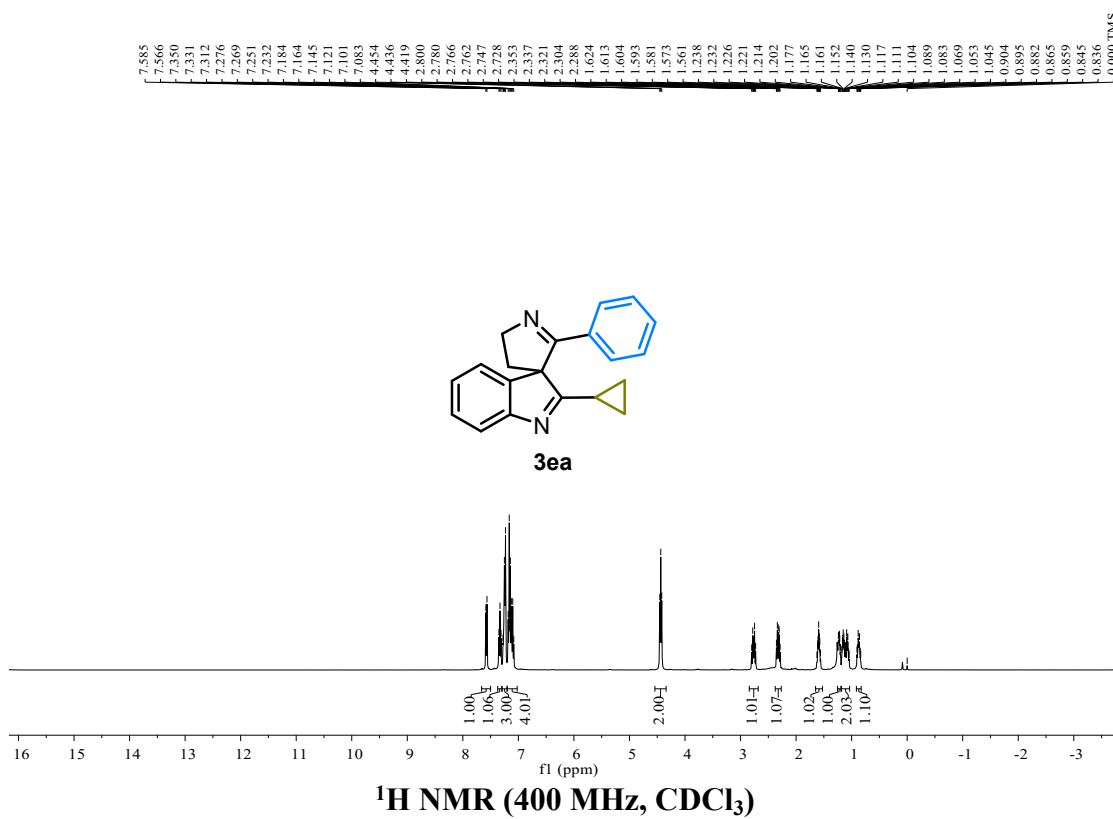
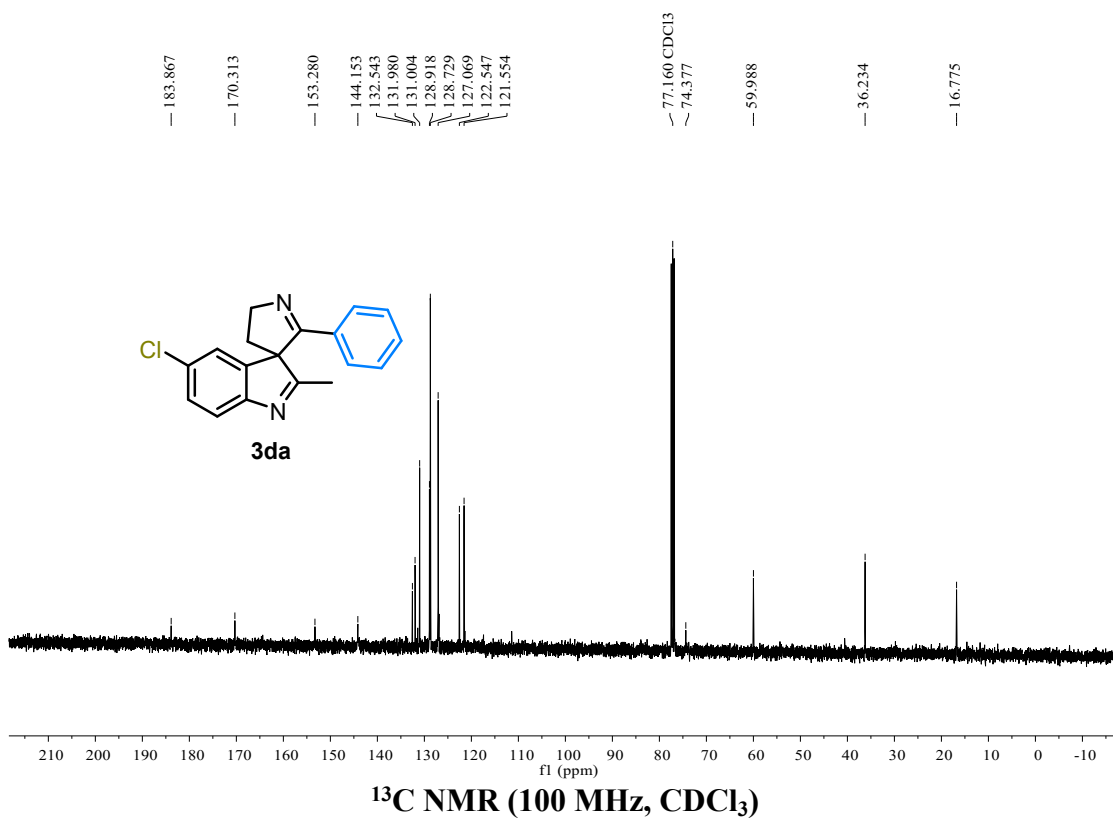
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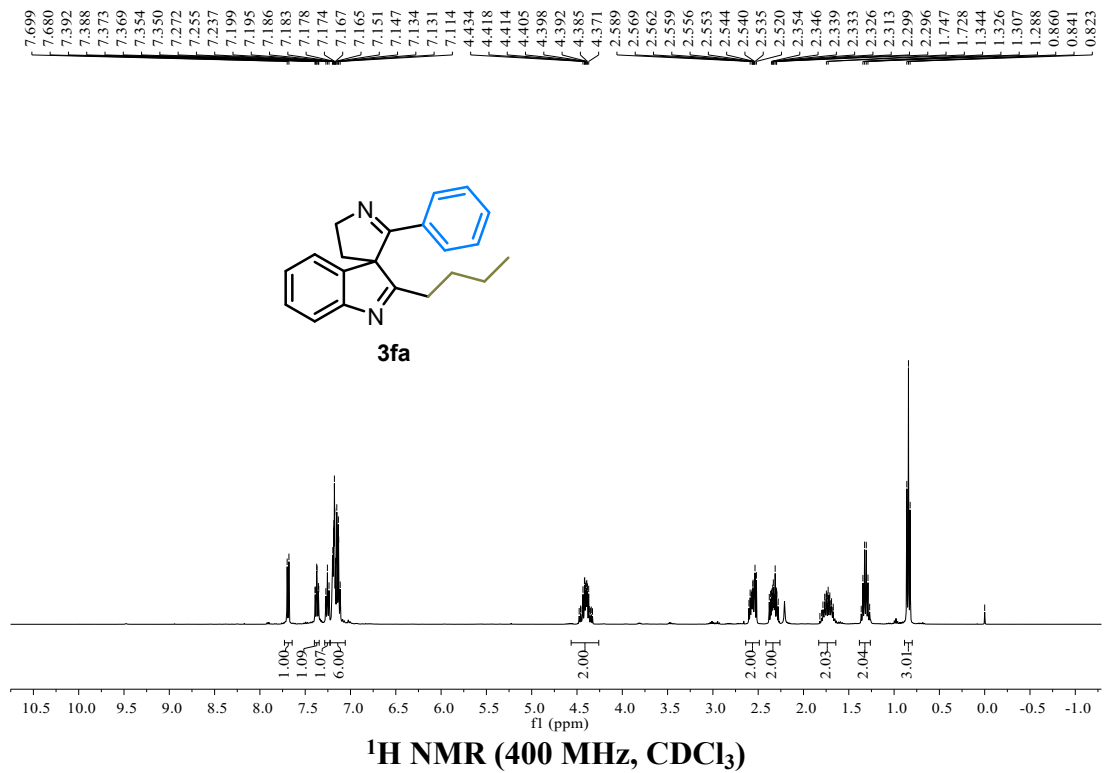
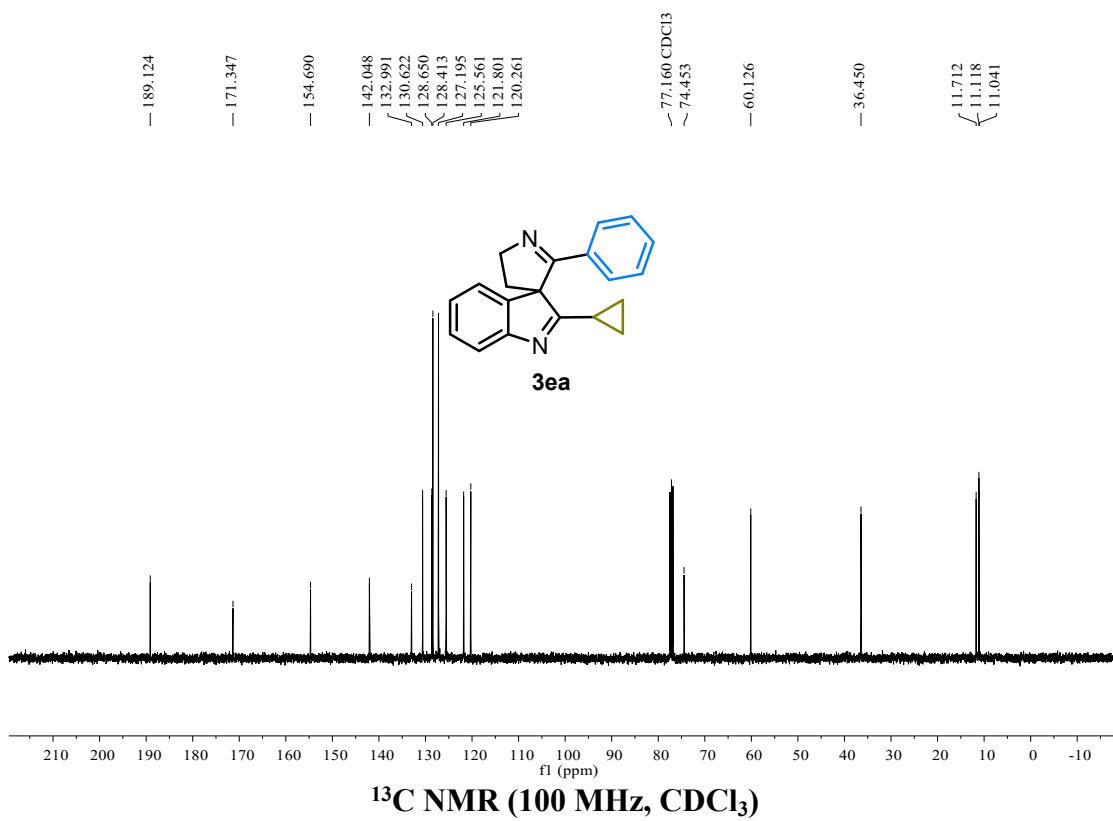


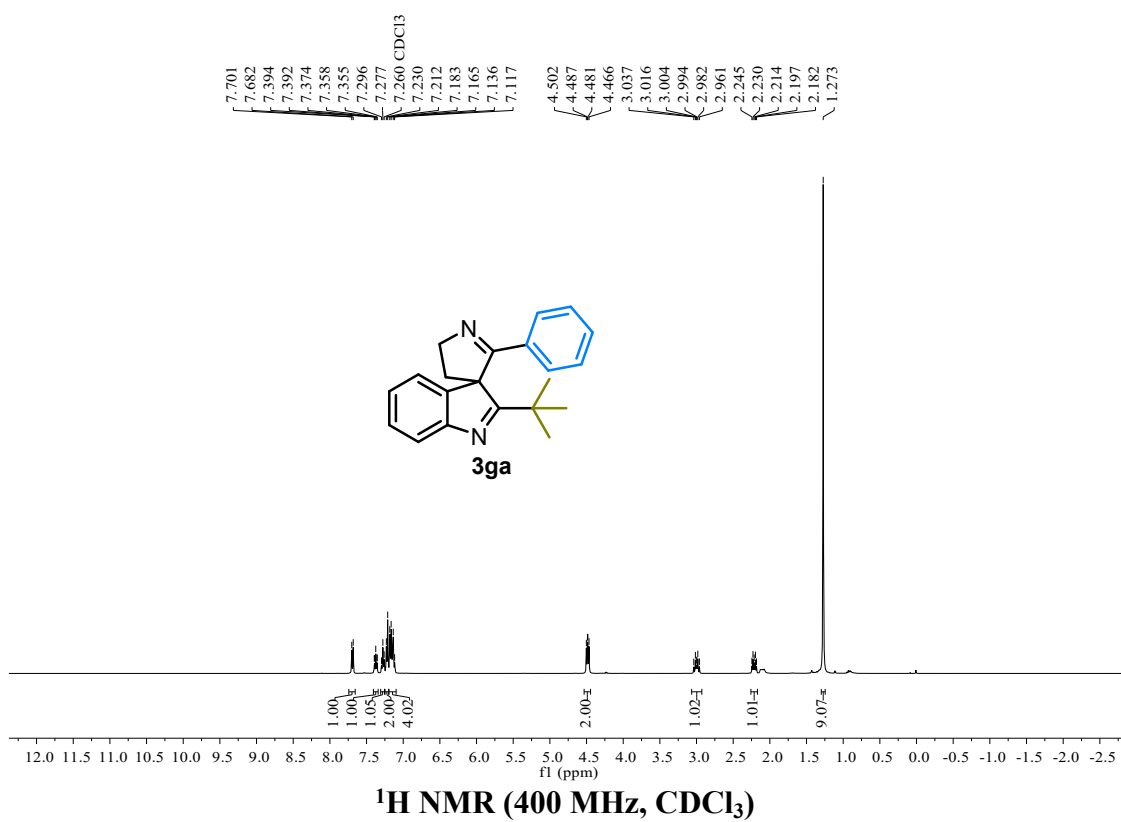
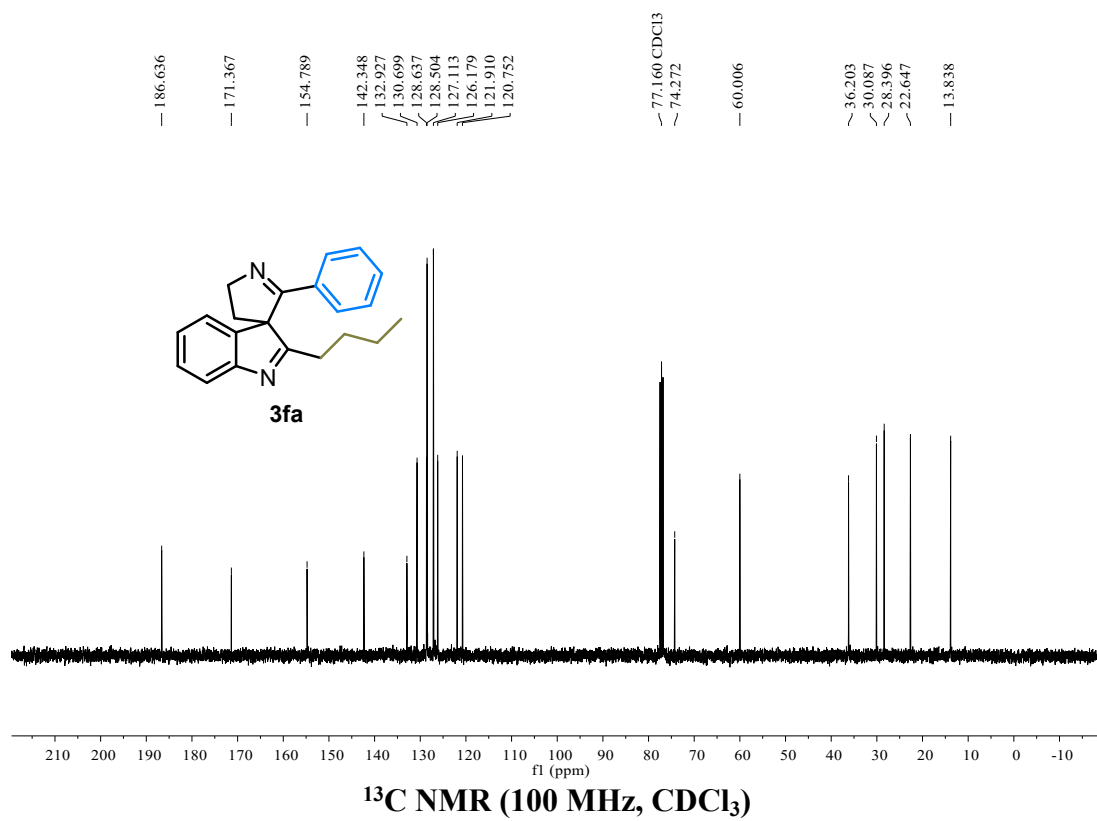
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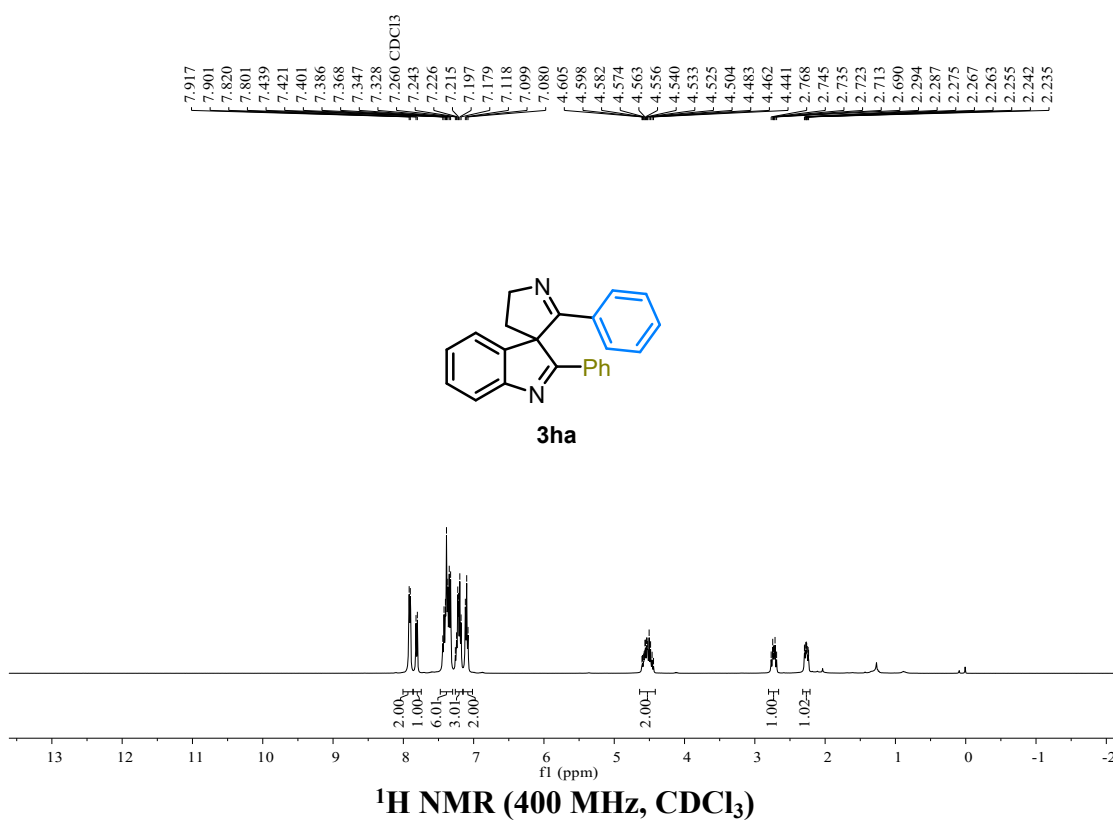
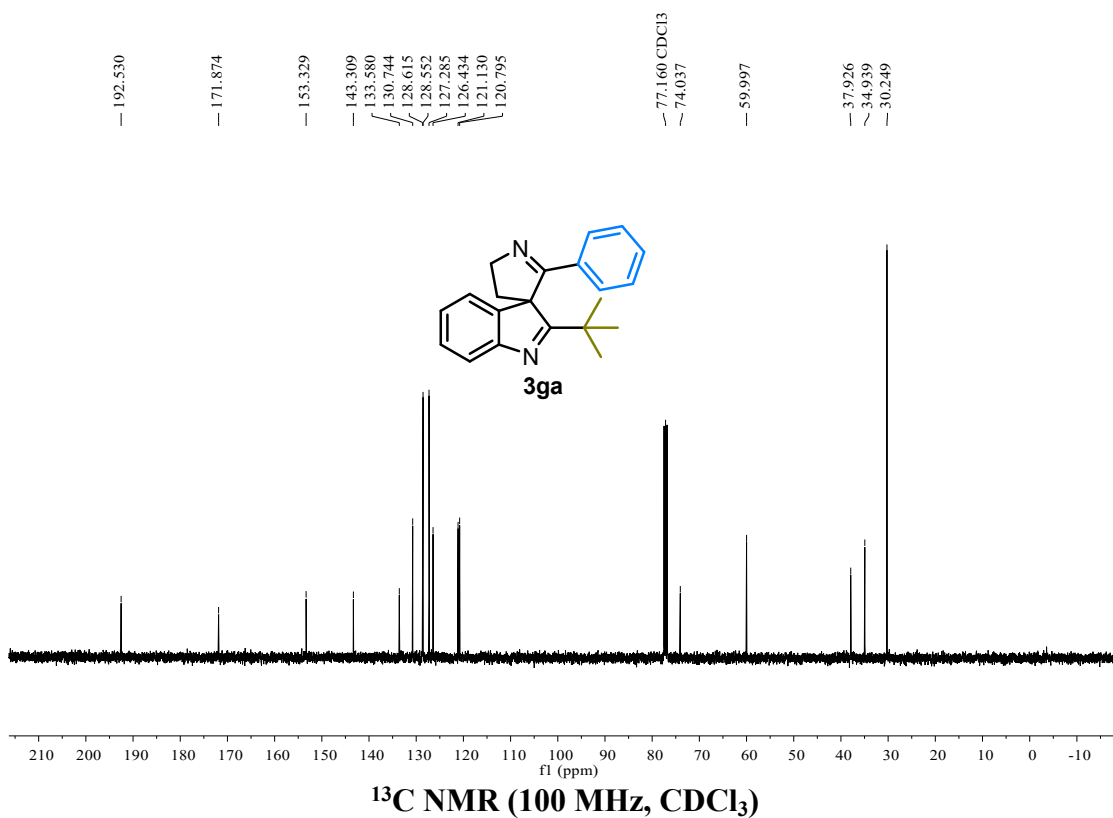


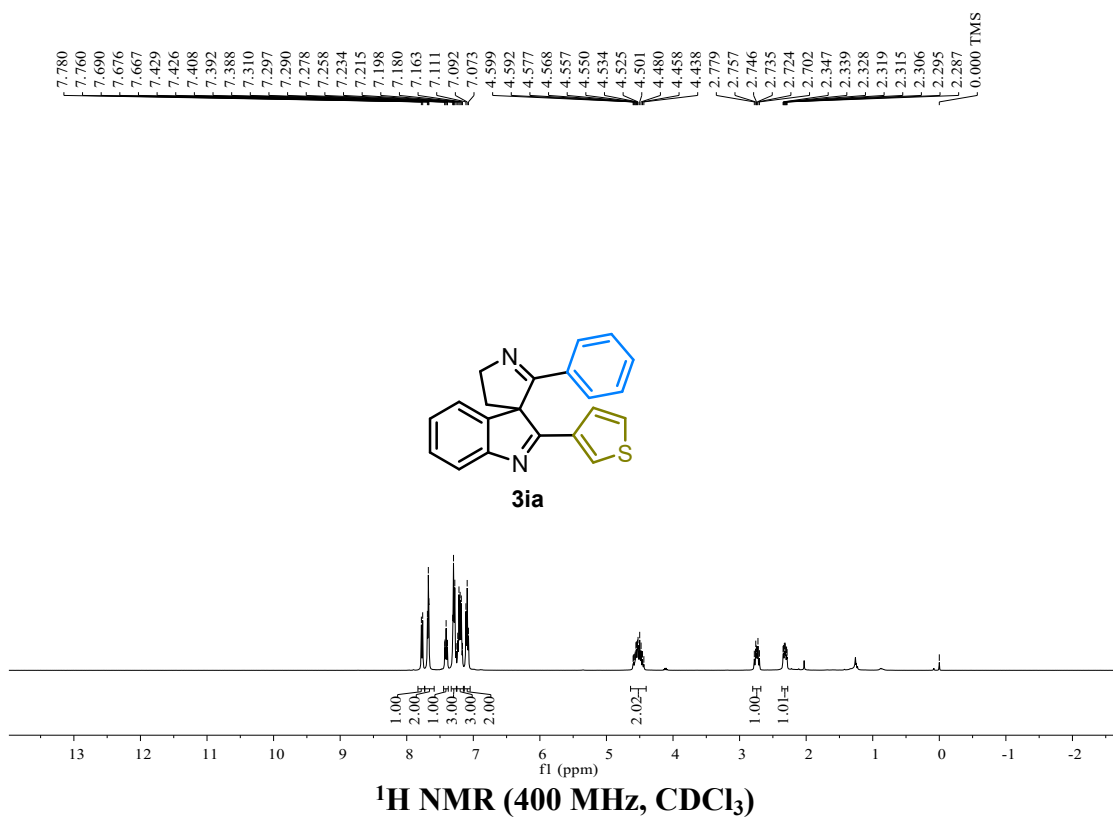
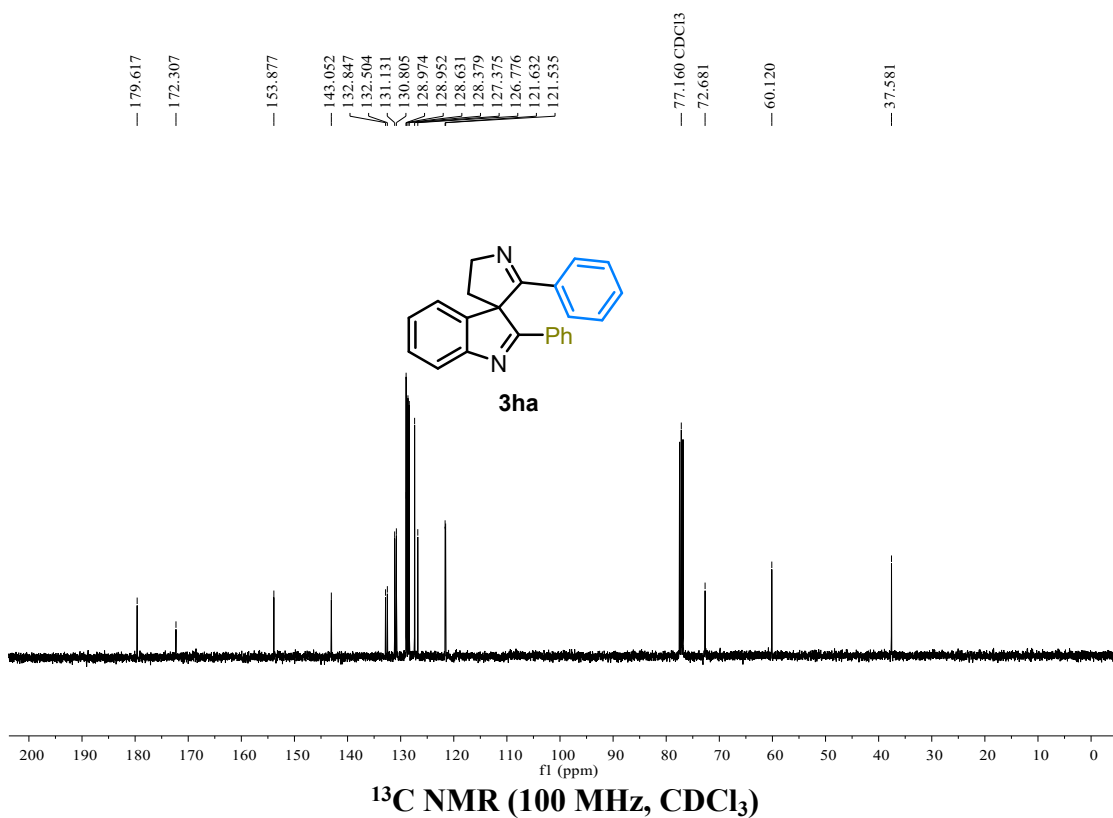


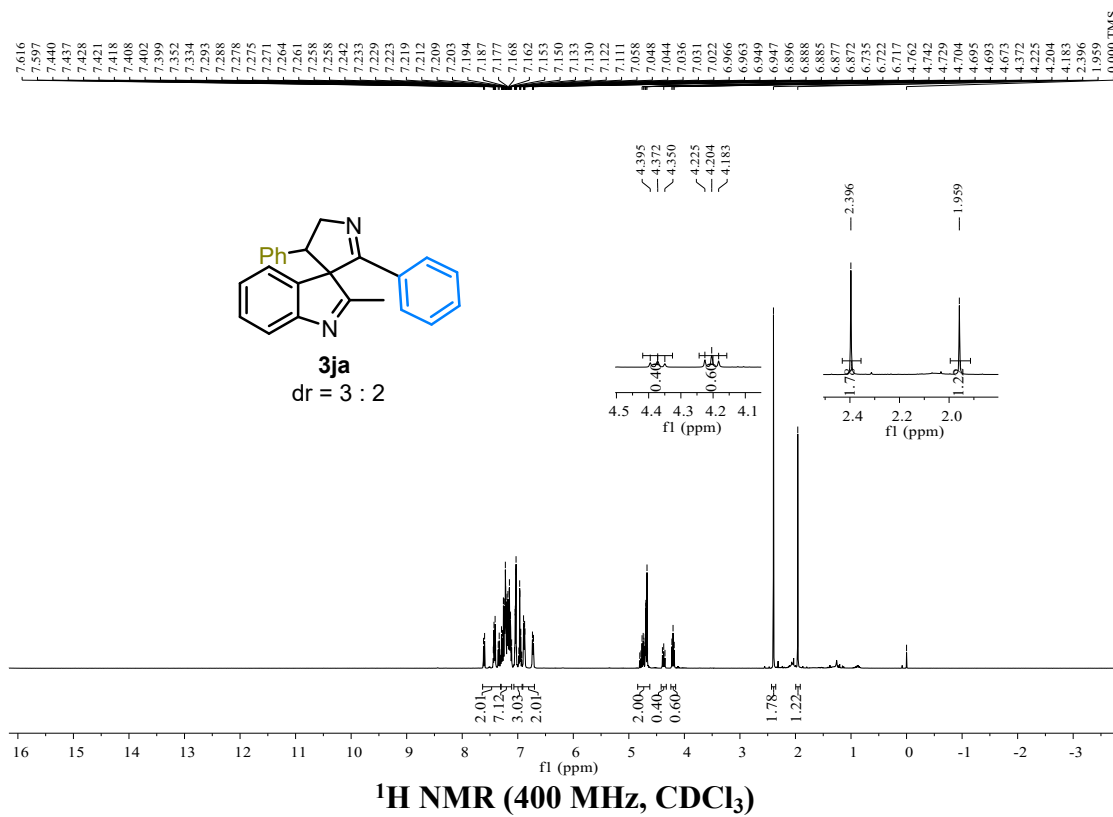
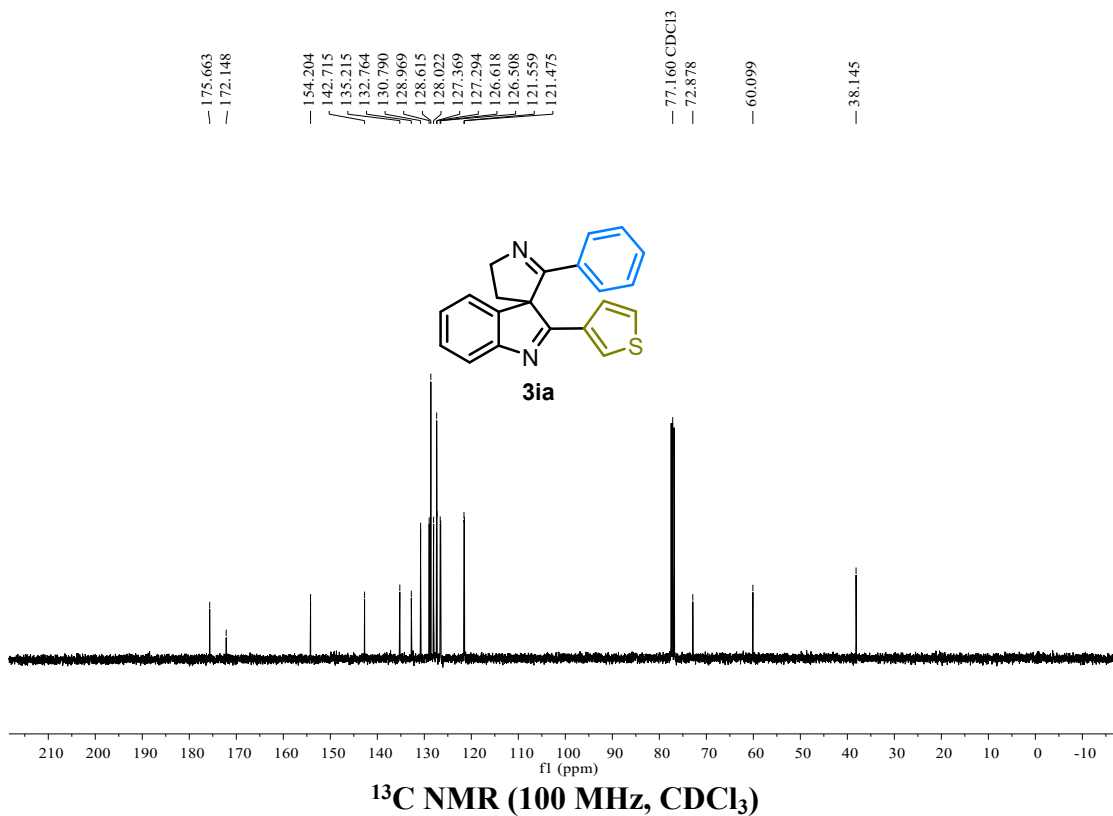


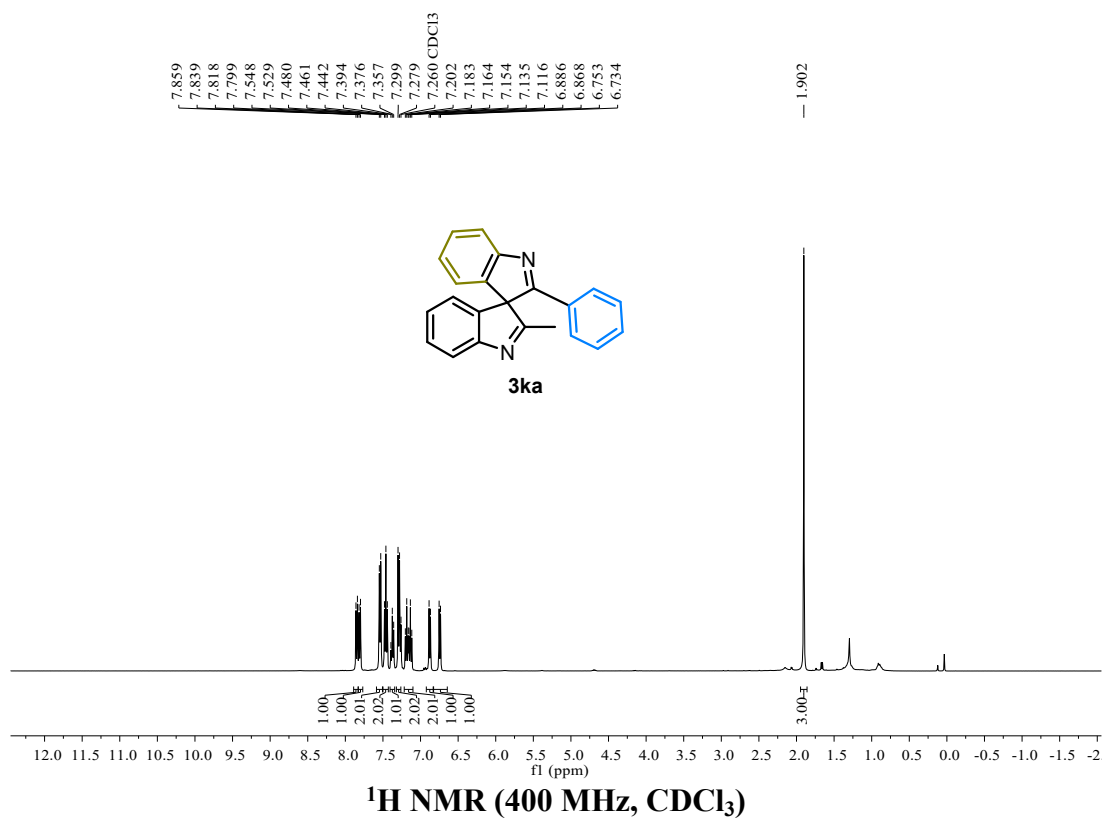
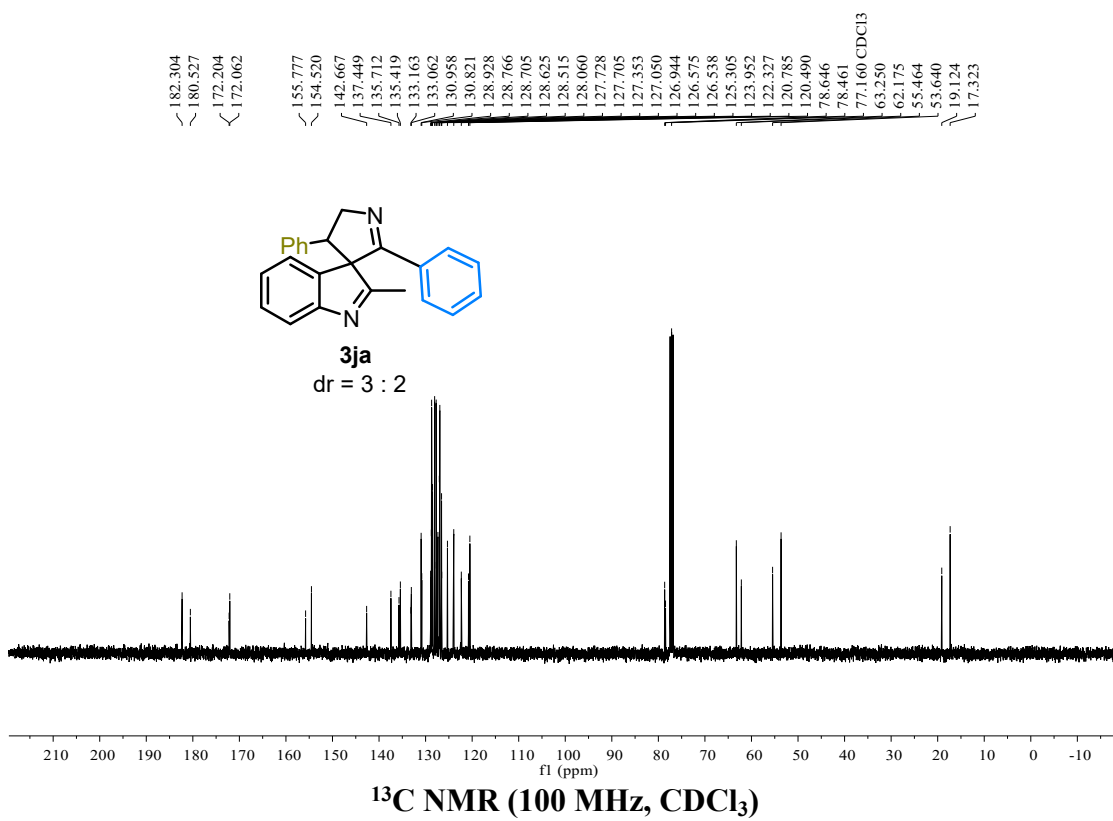


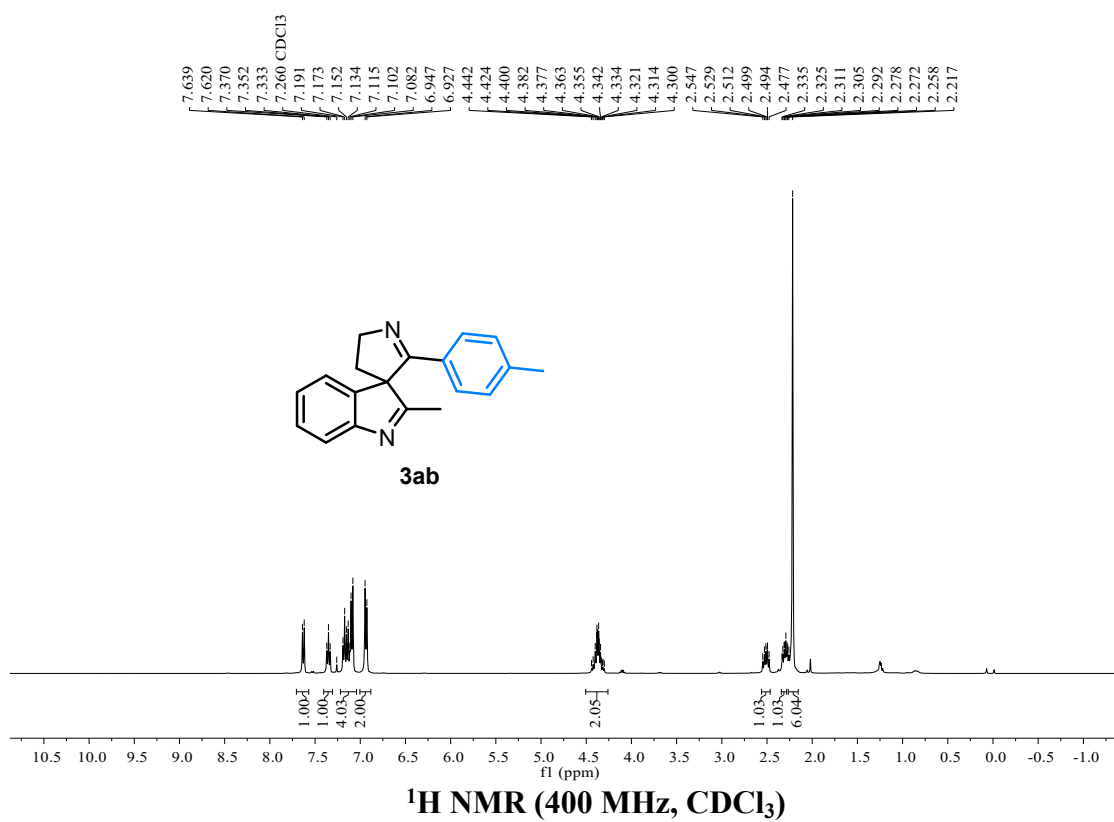
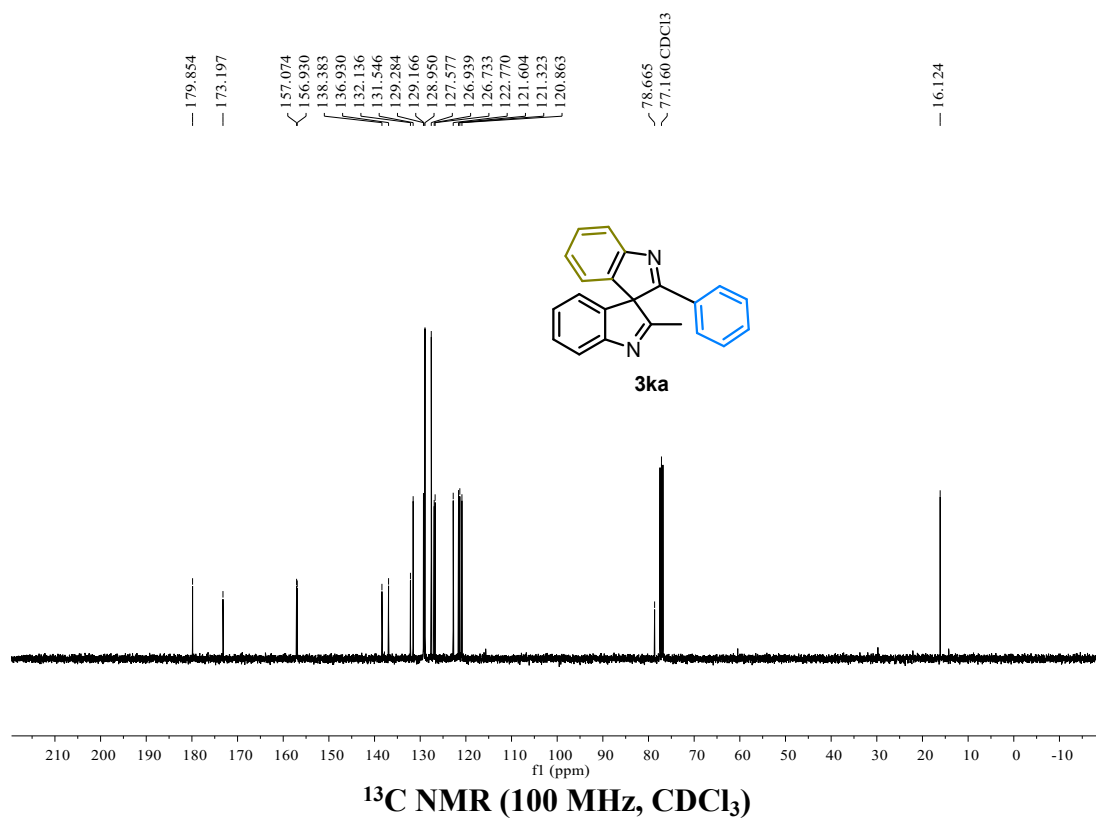


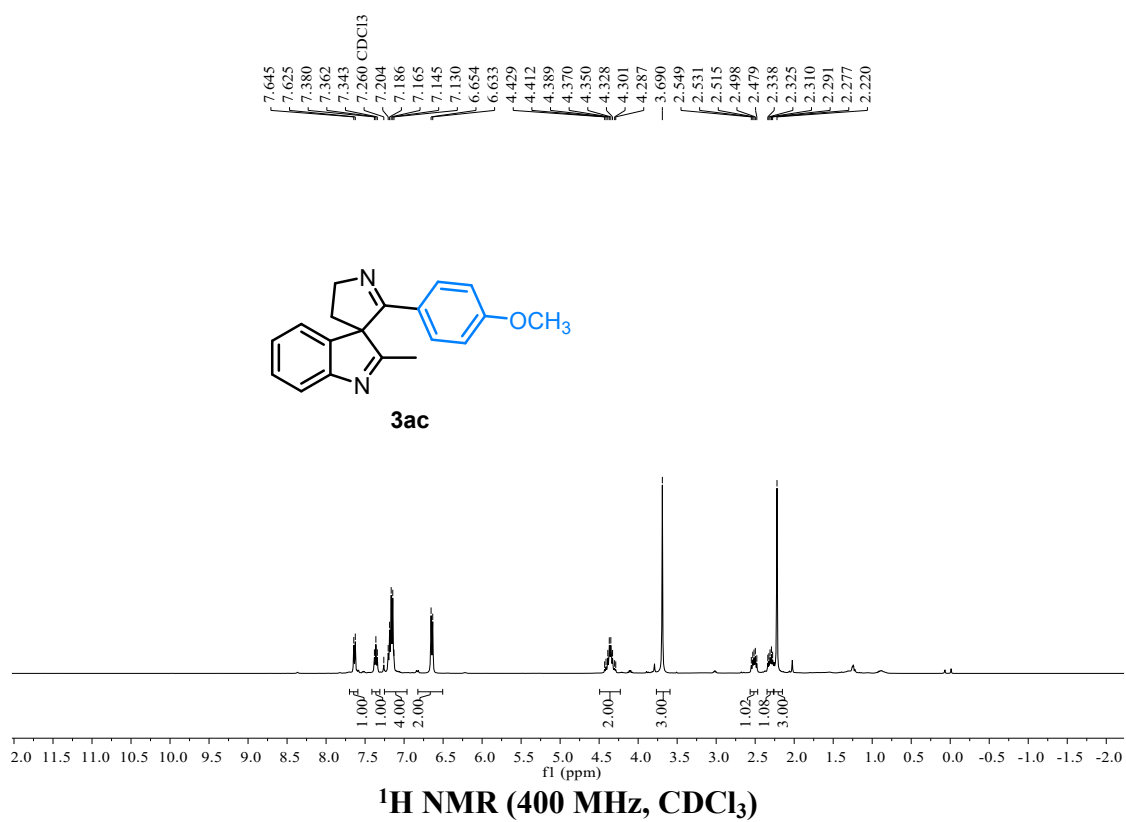
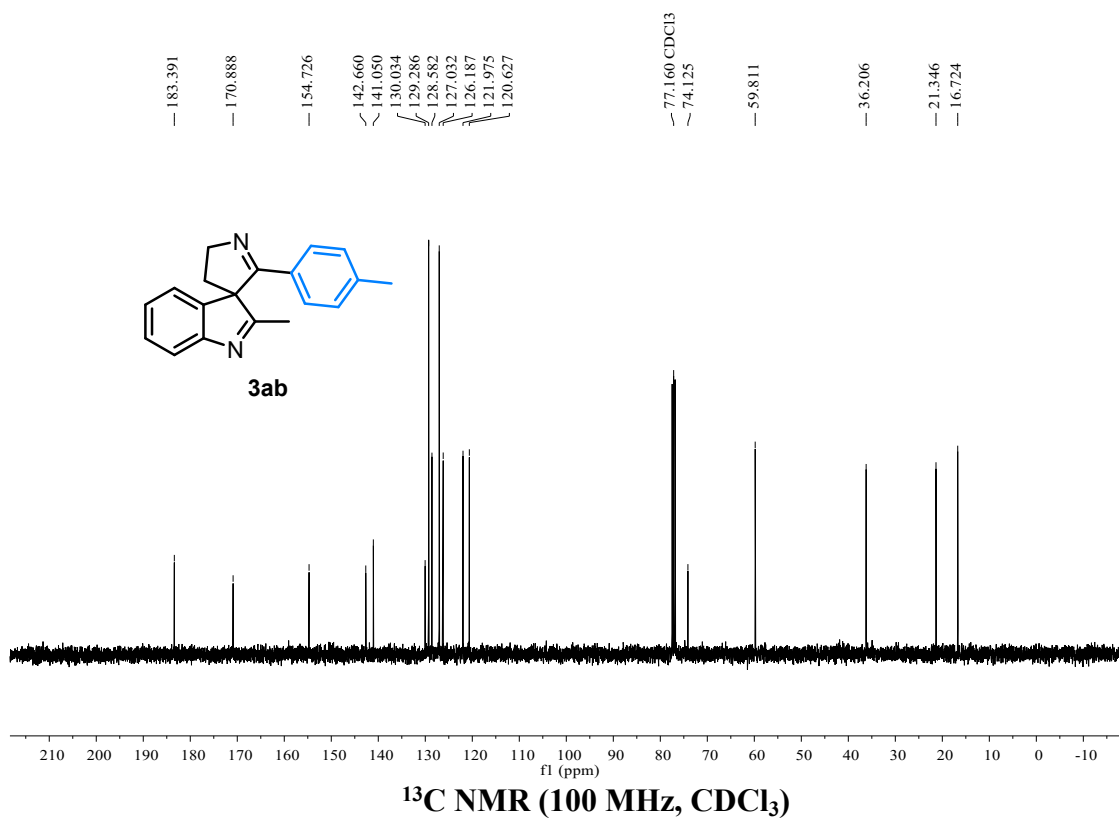


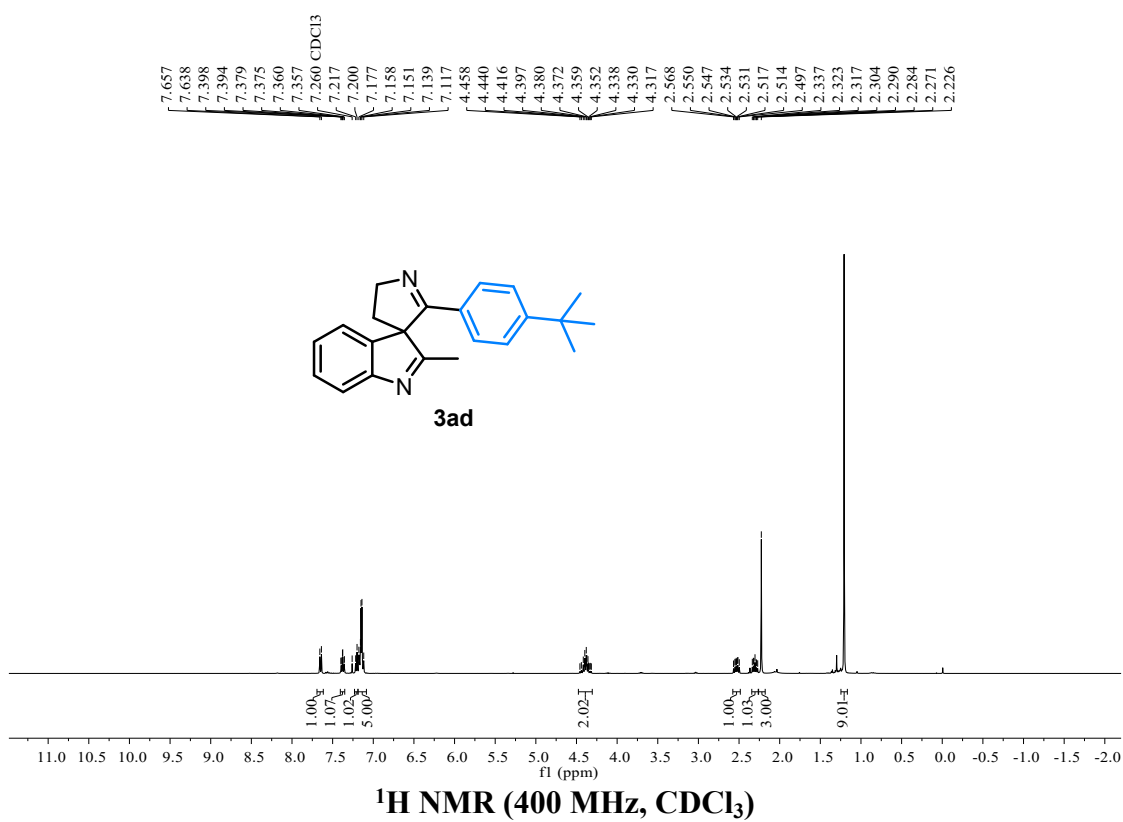
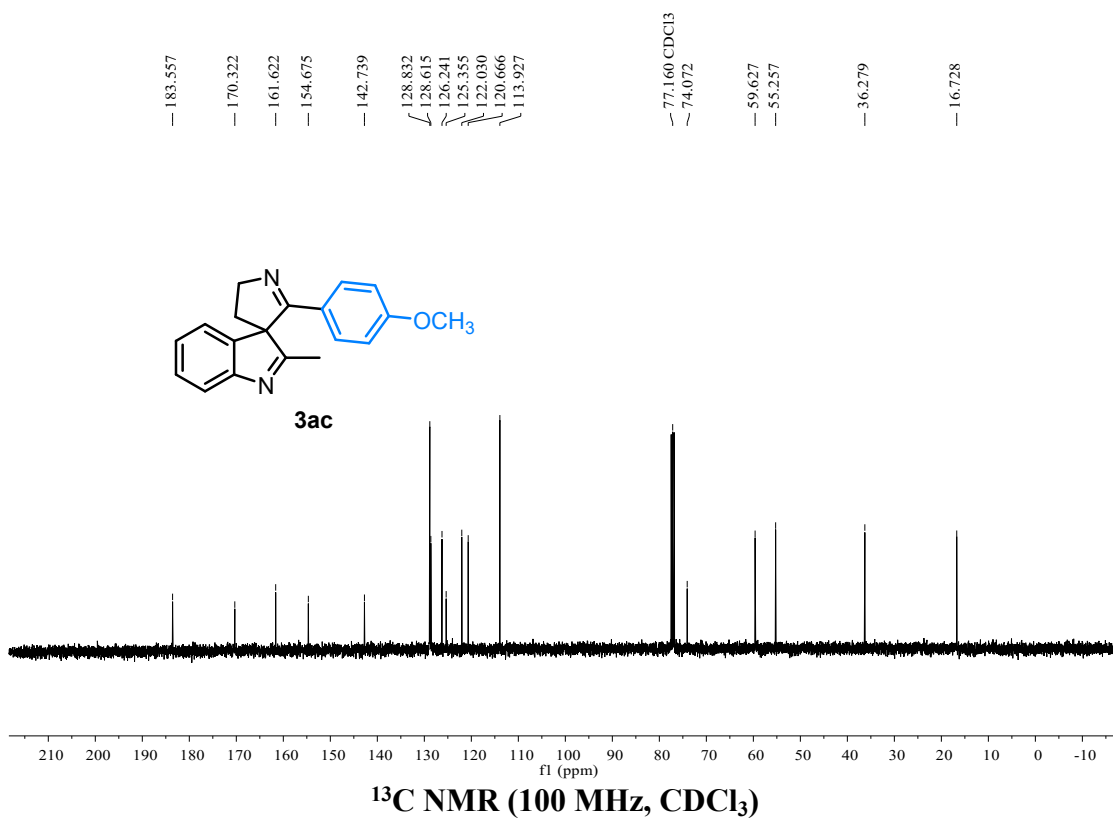


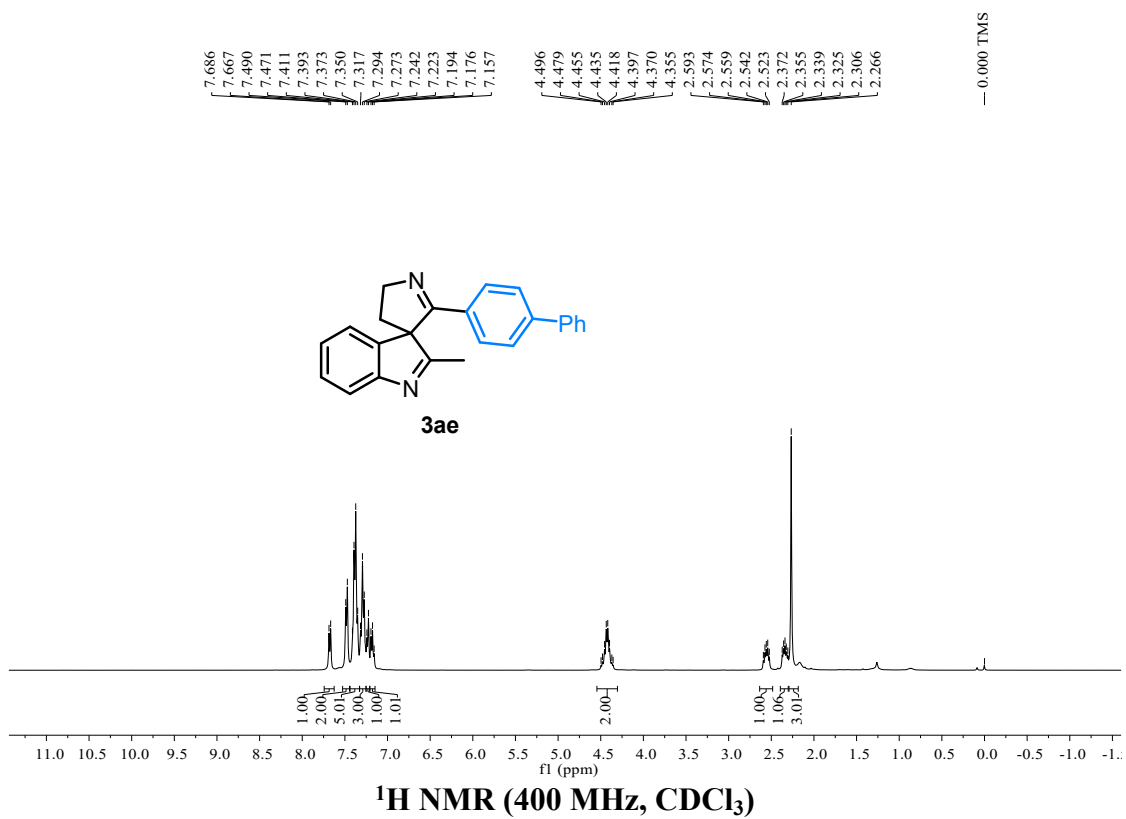
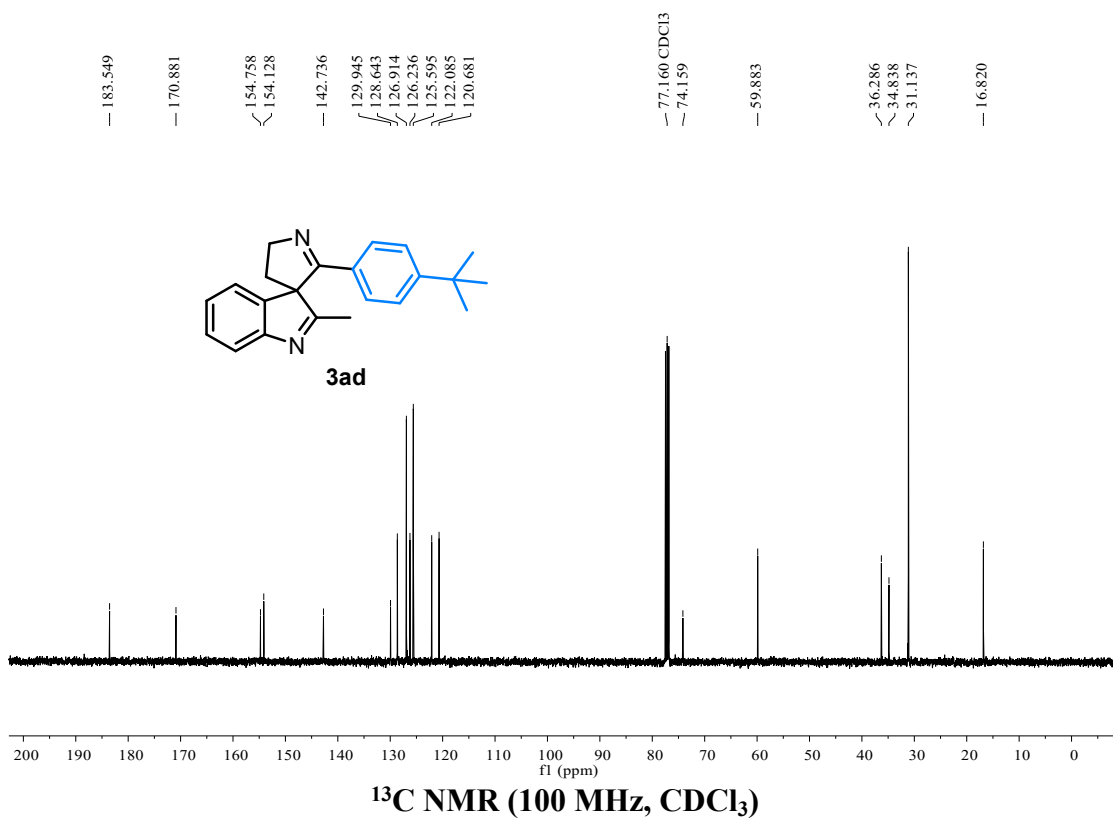


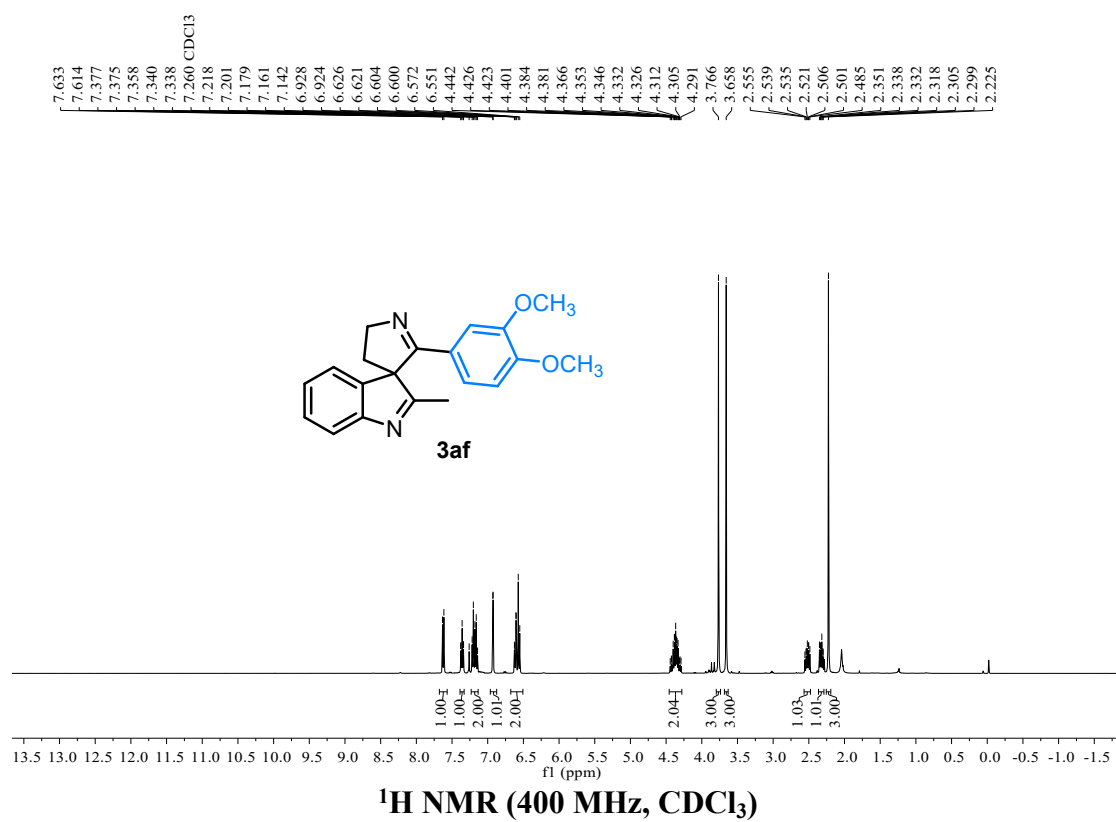
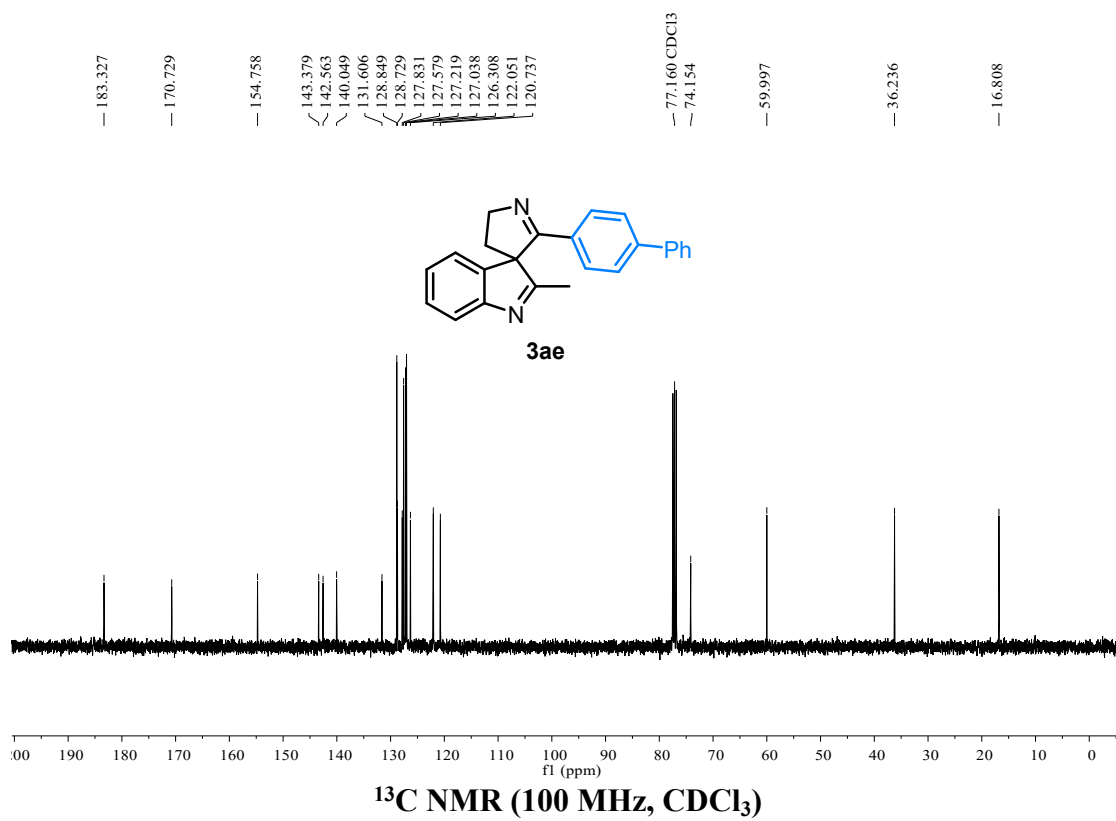


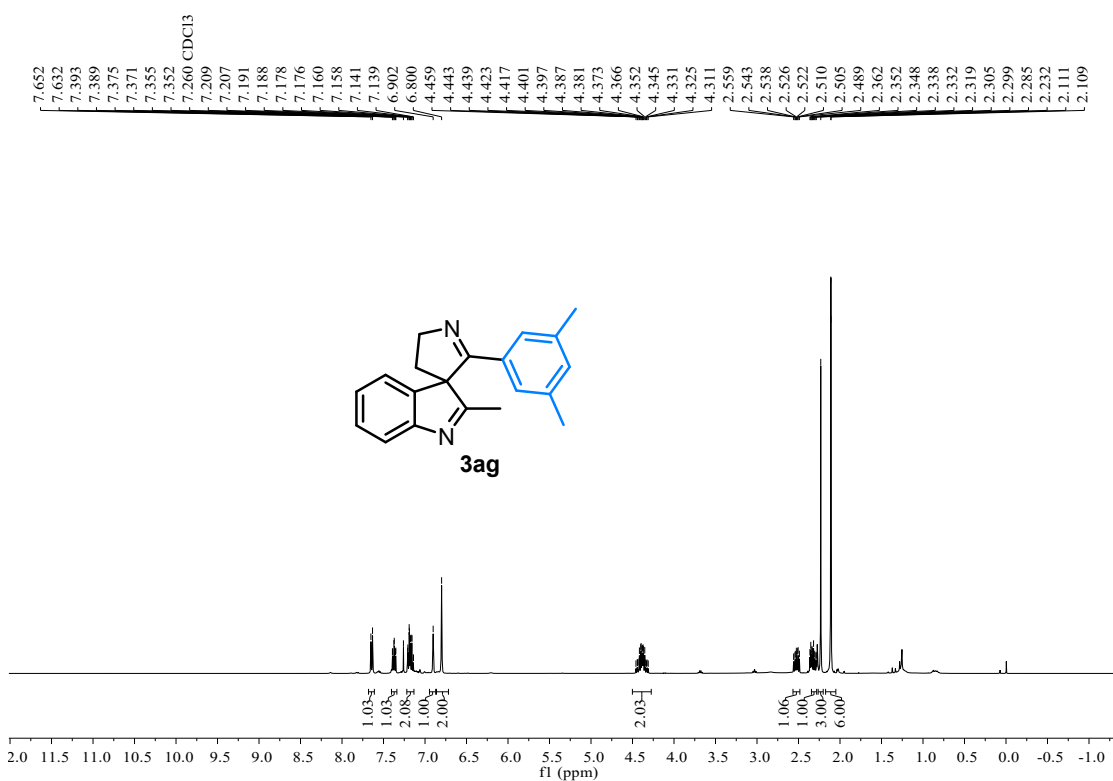
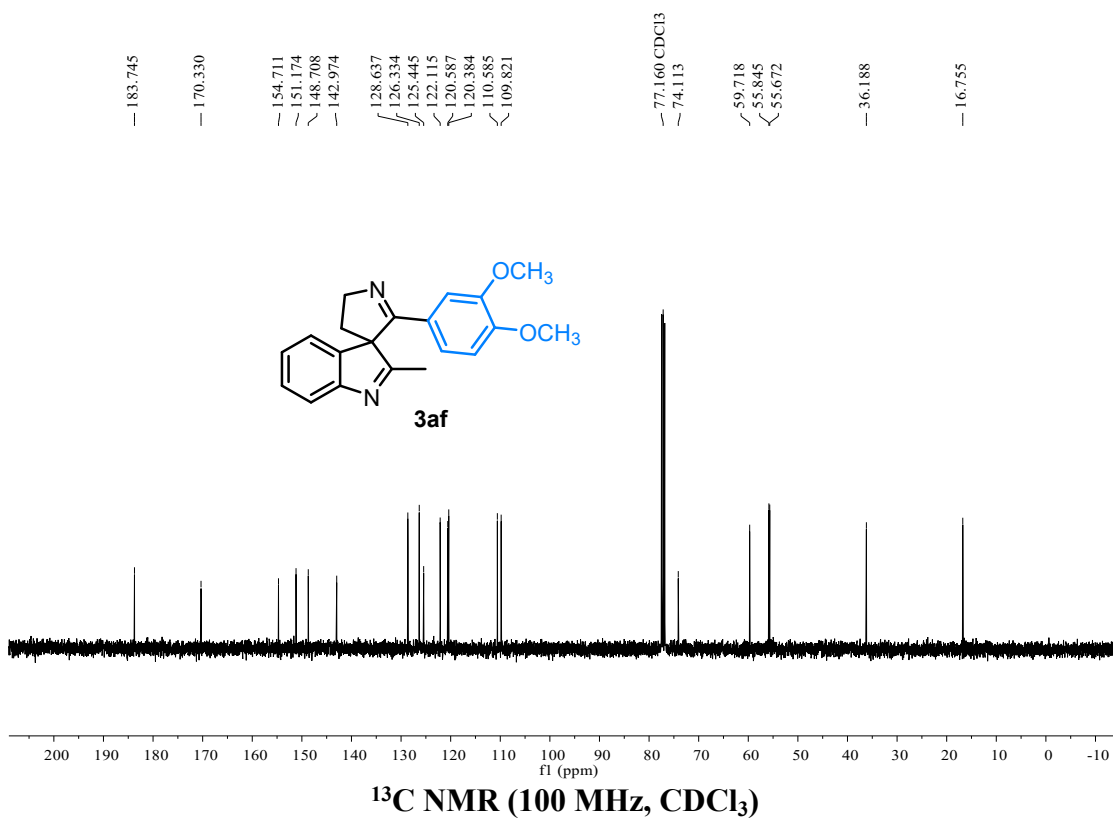


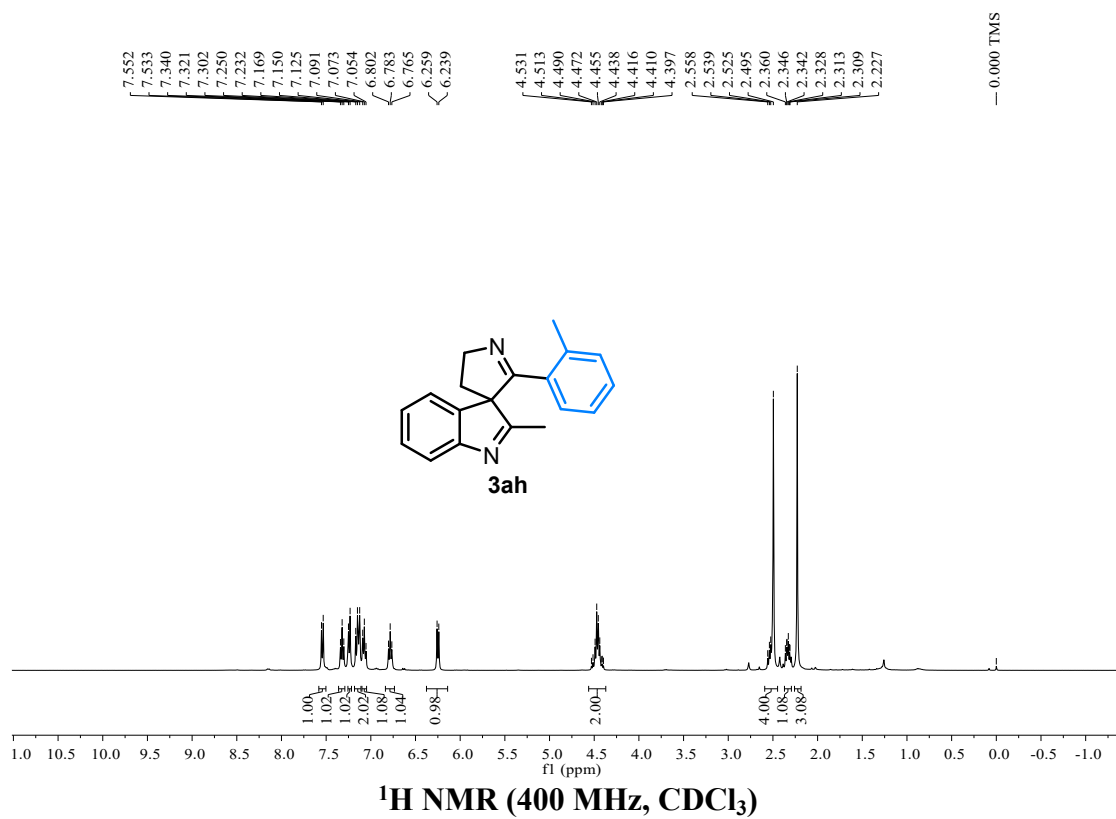
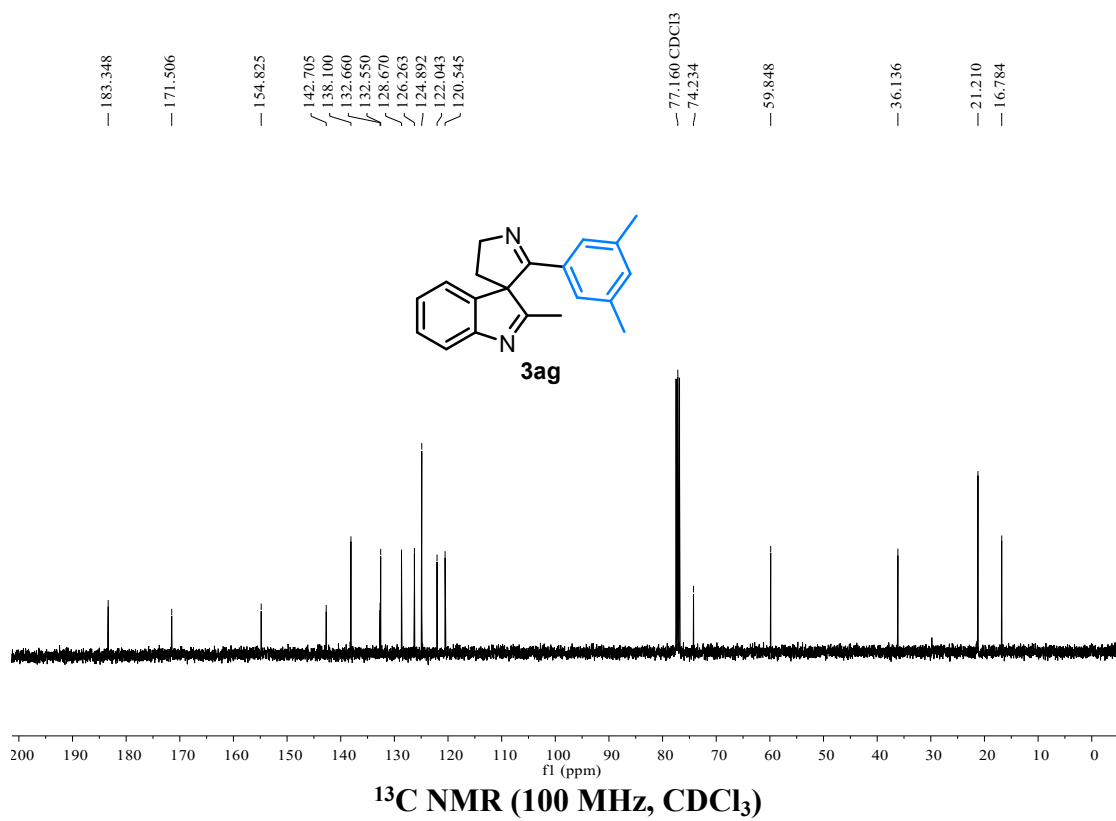


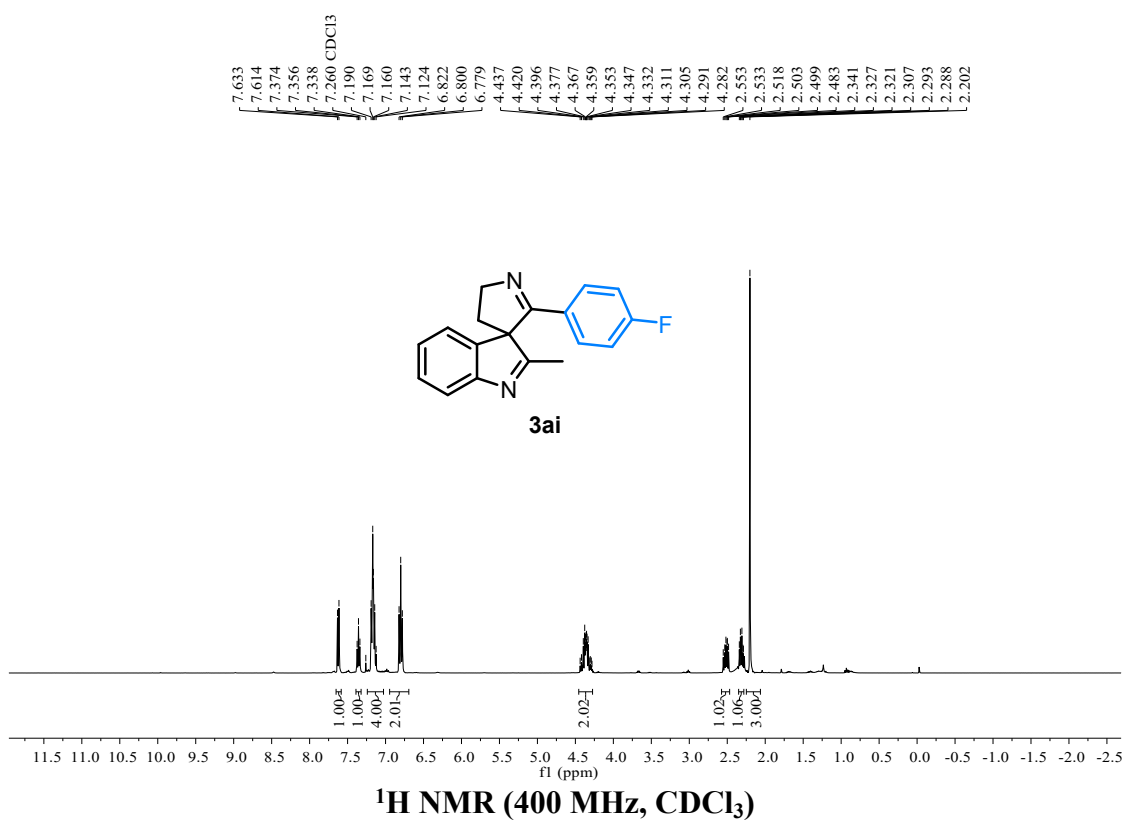
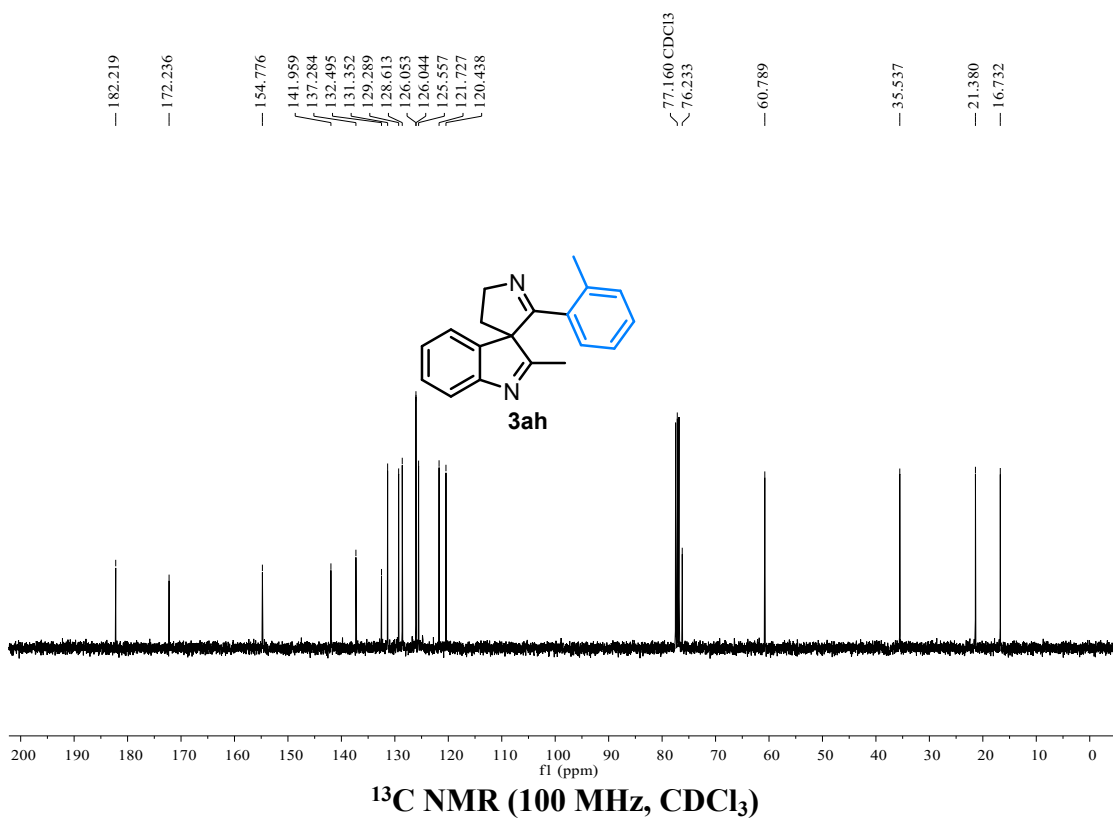


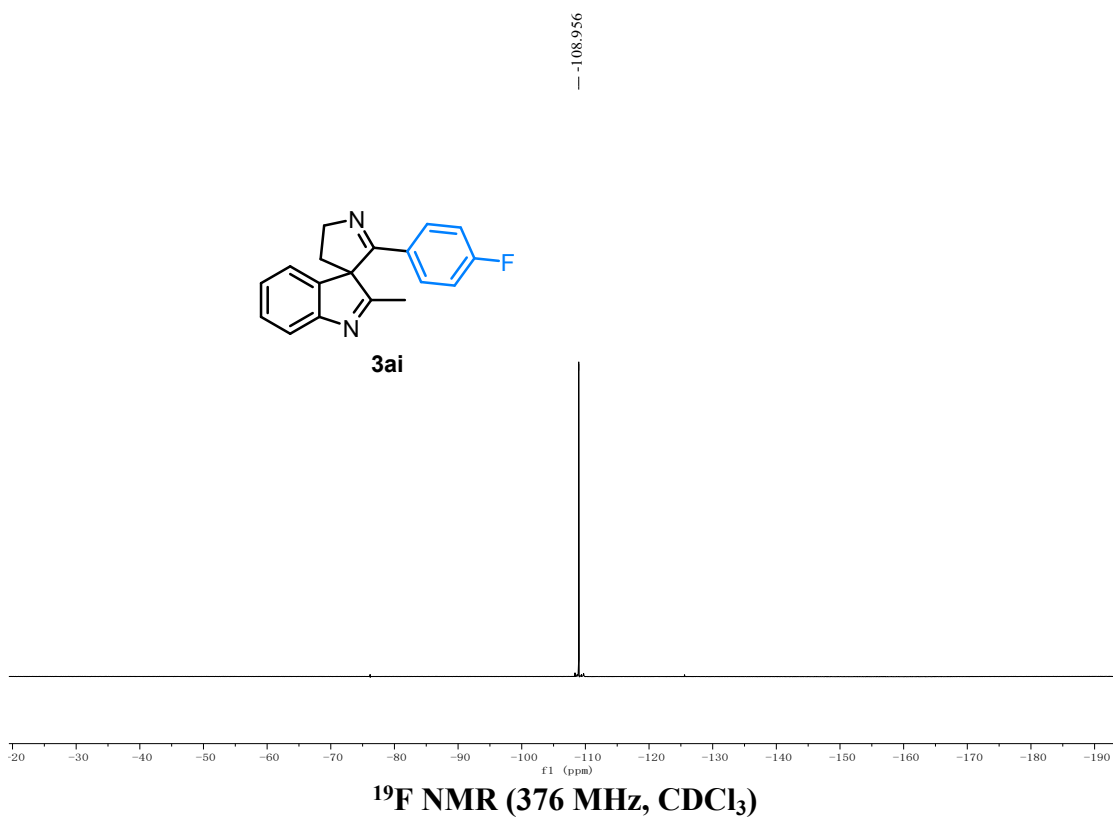
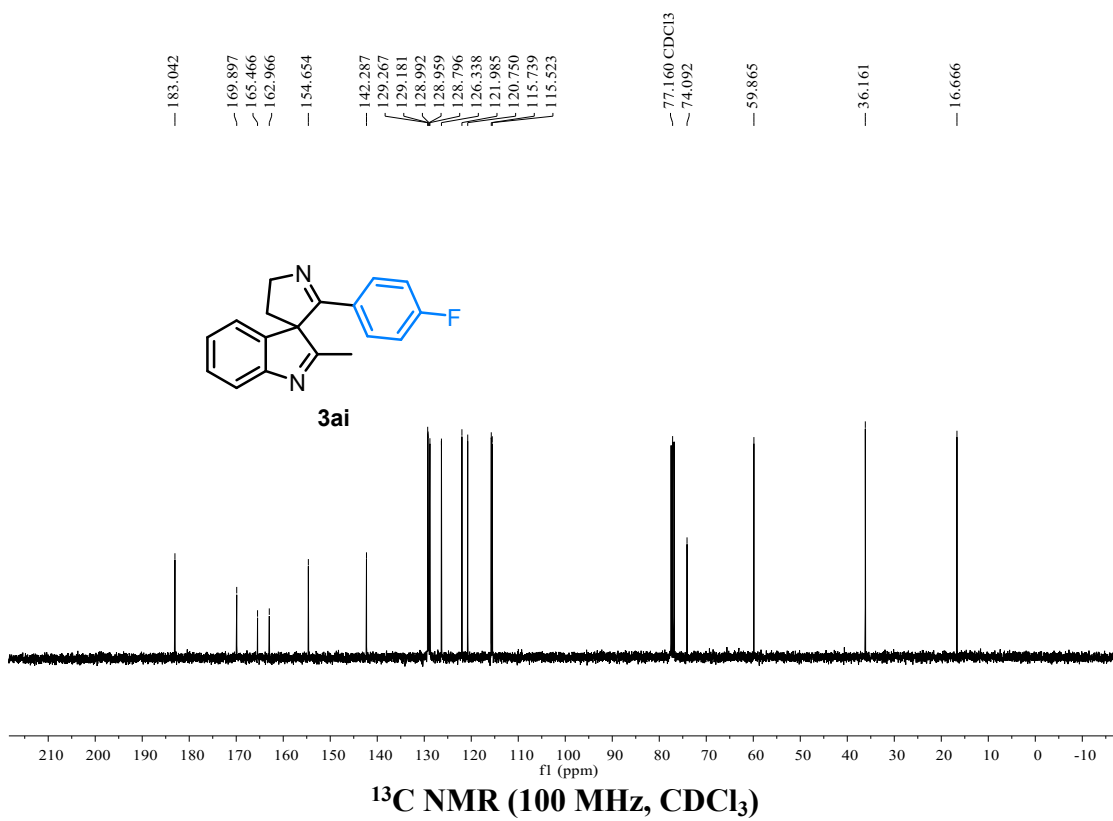


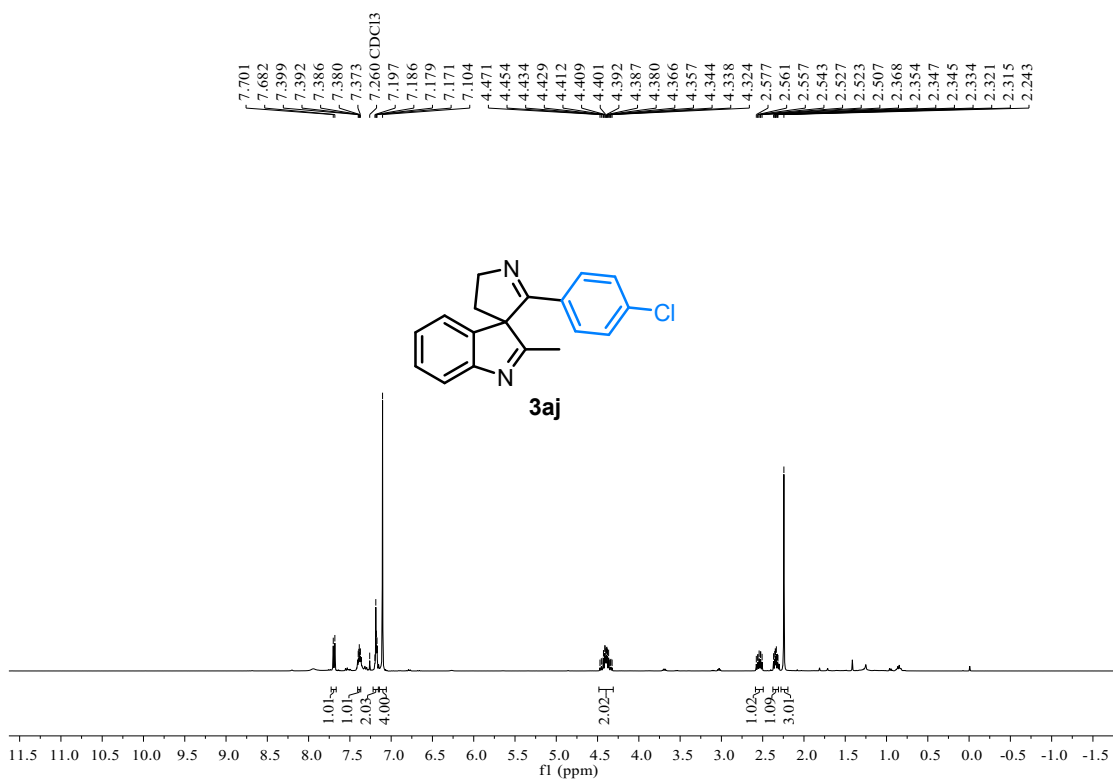




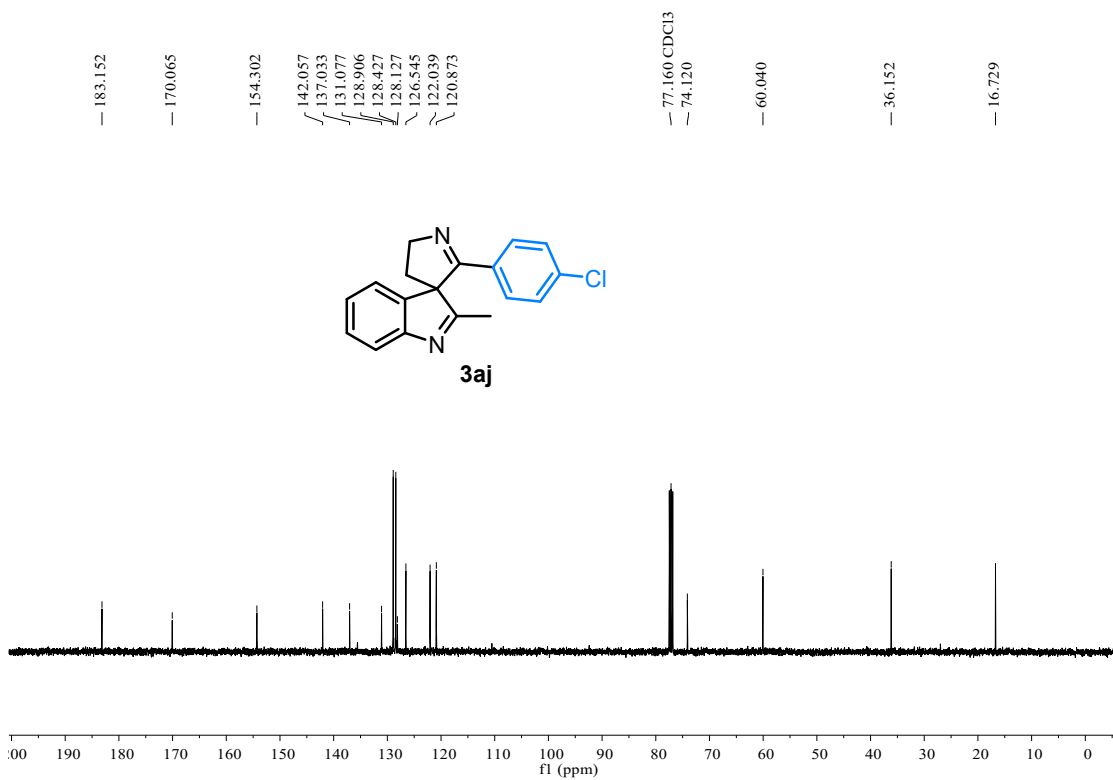




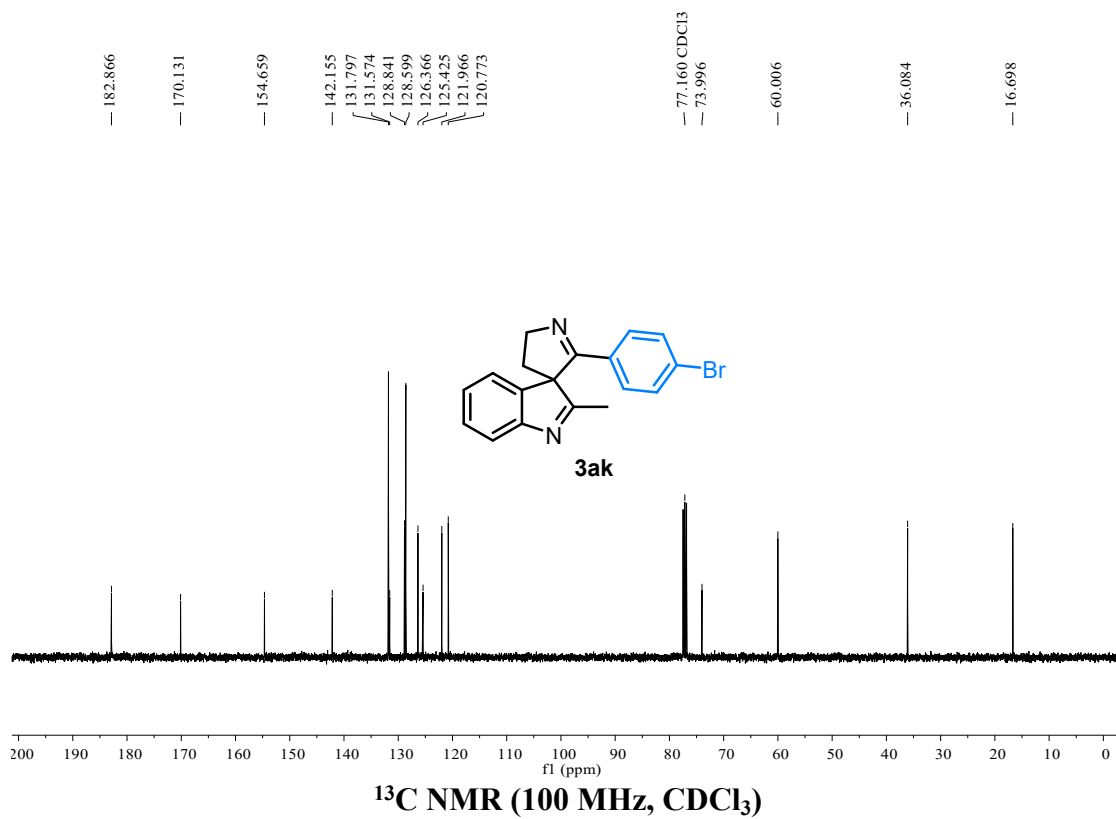
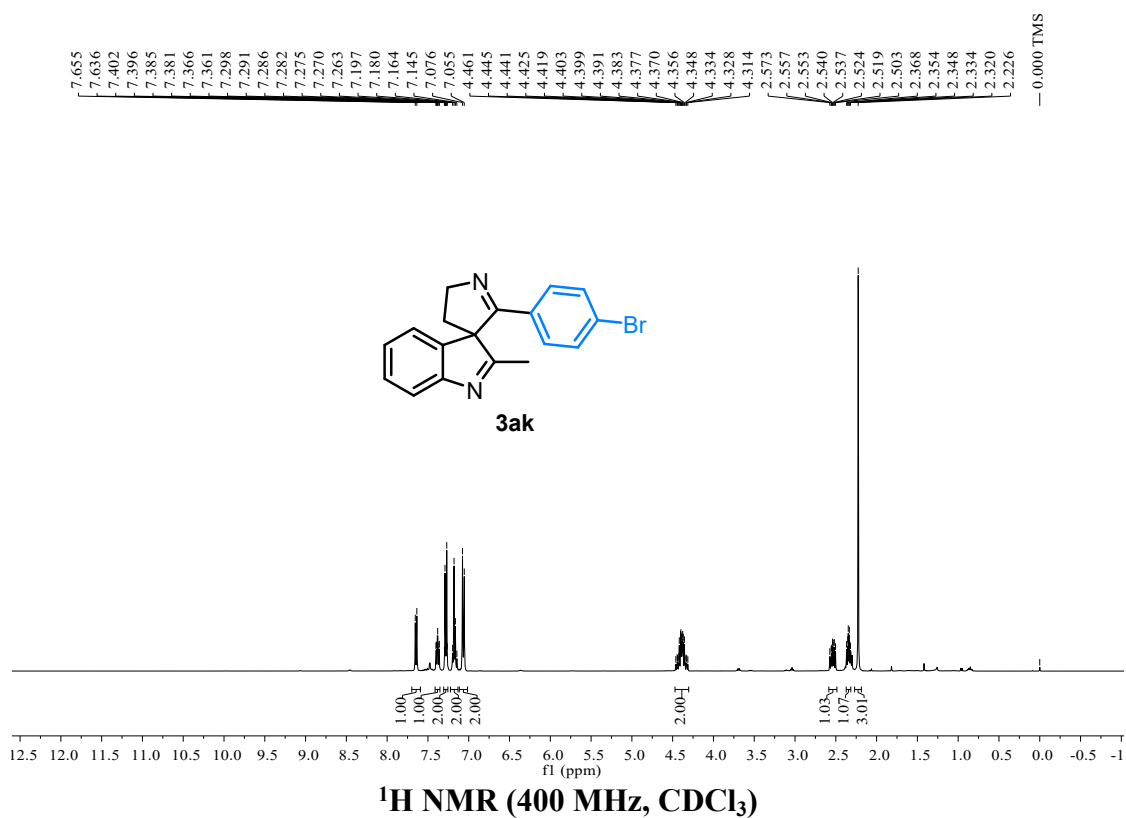


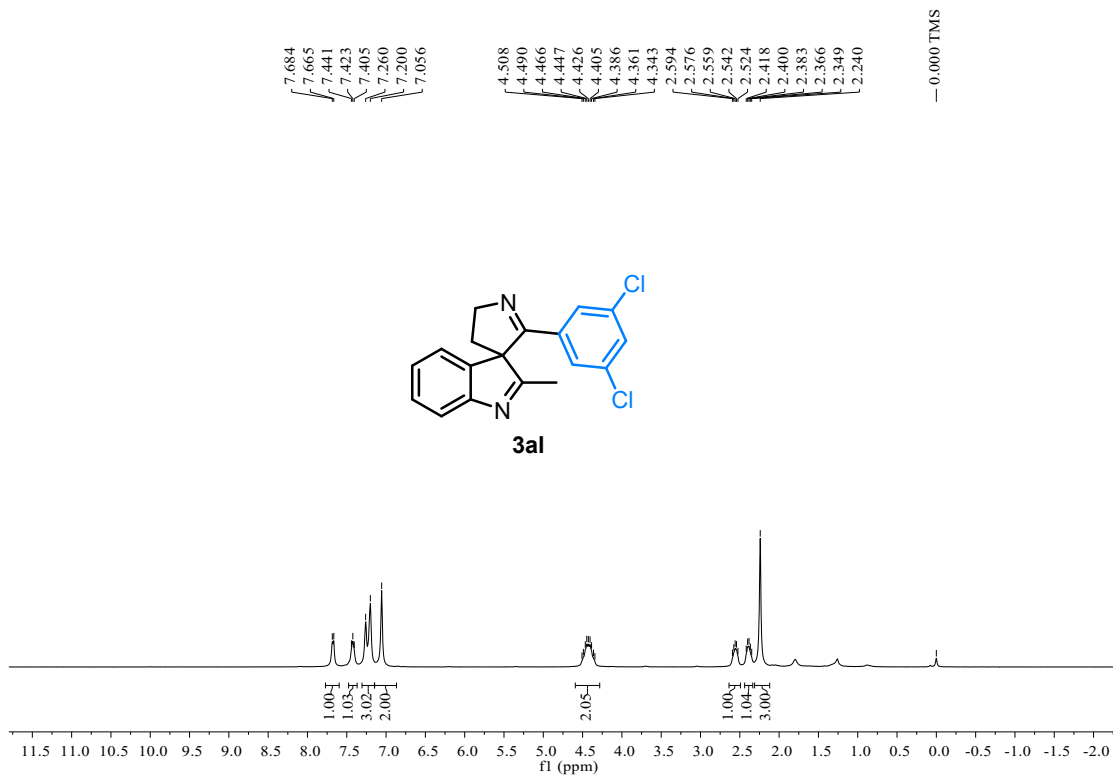


¹H NMR (400 MHz, CDCl₃)

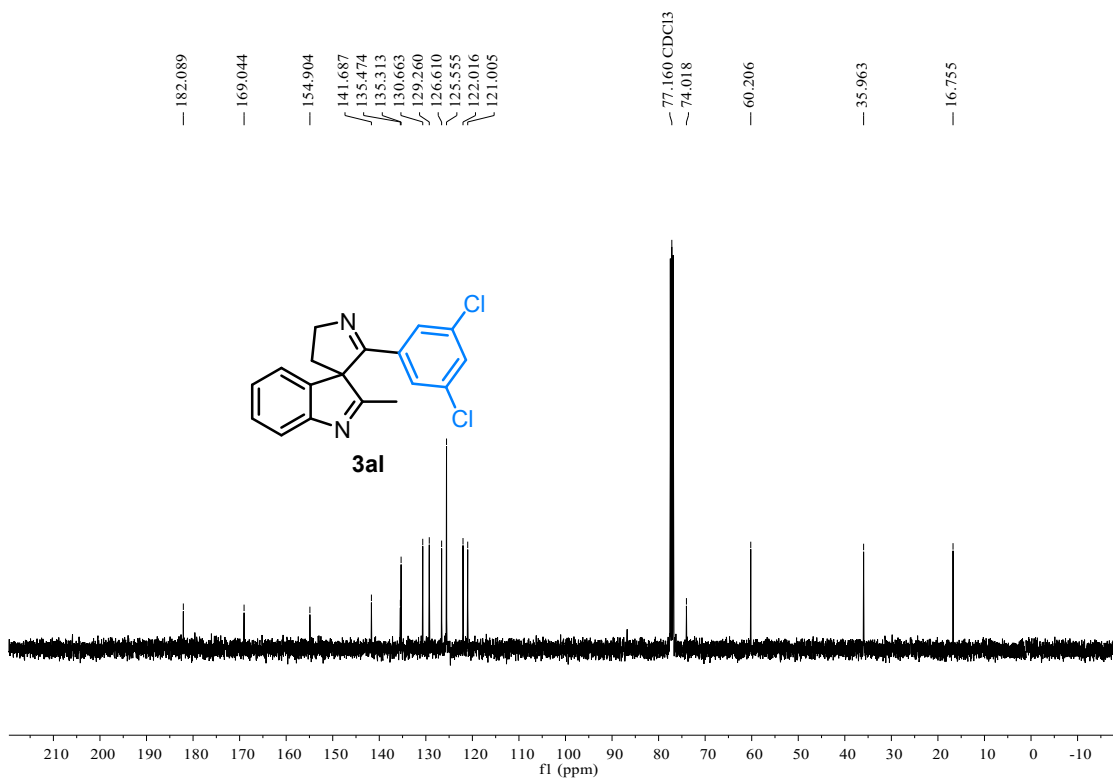


¹³C NMR (100 MHz, CDCl₃)

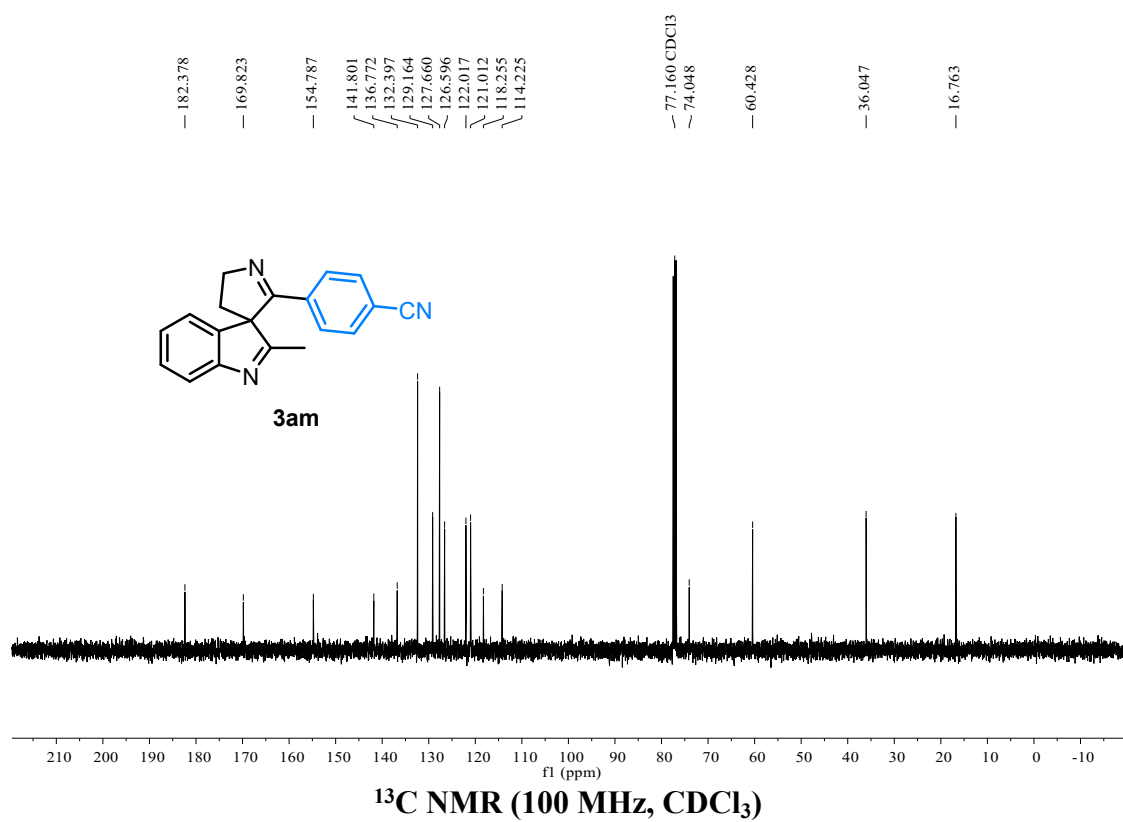
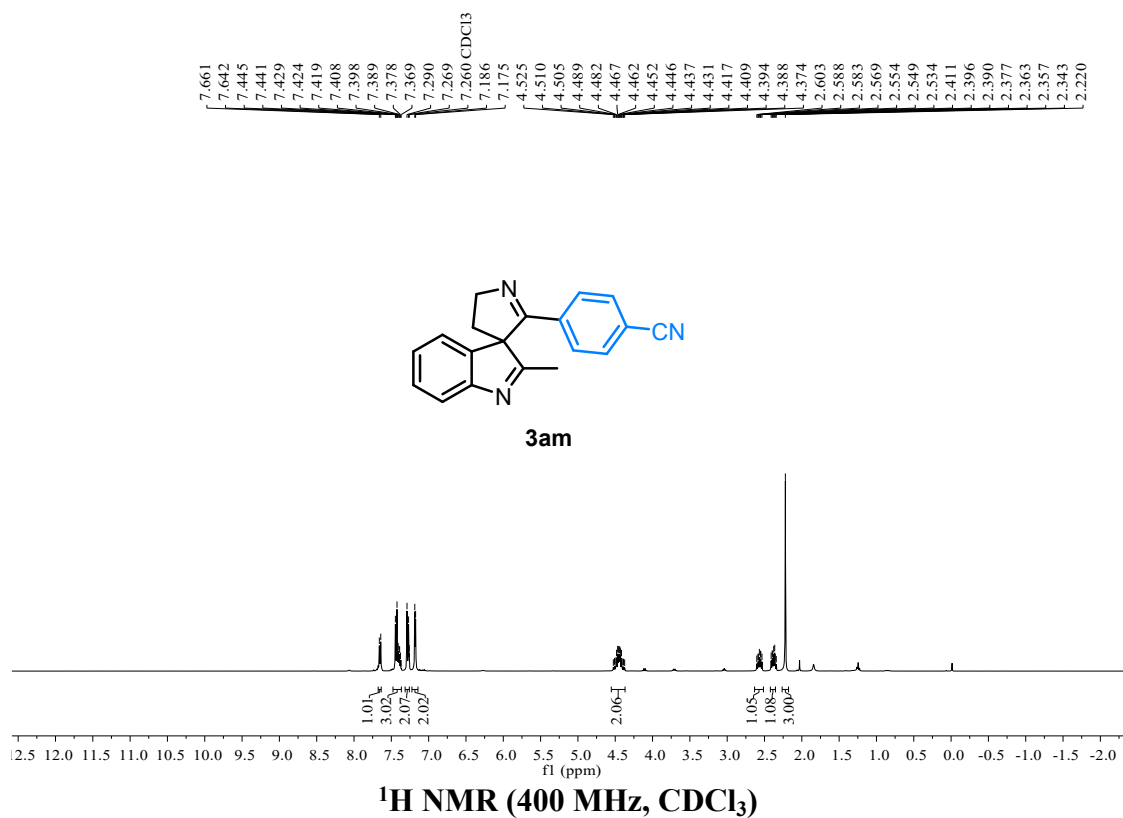


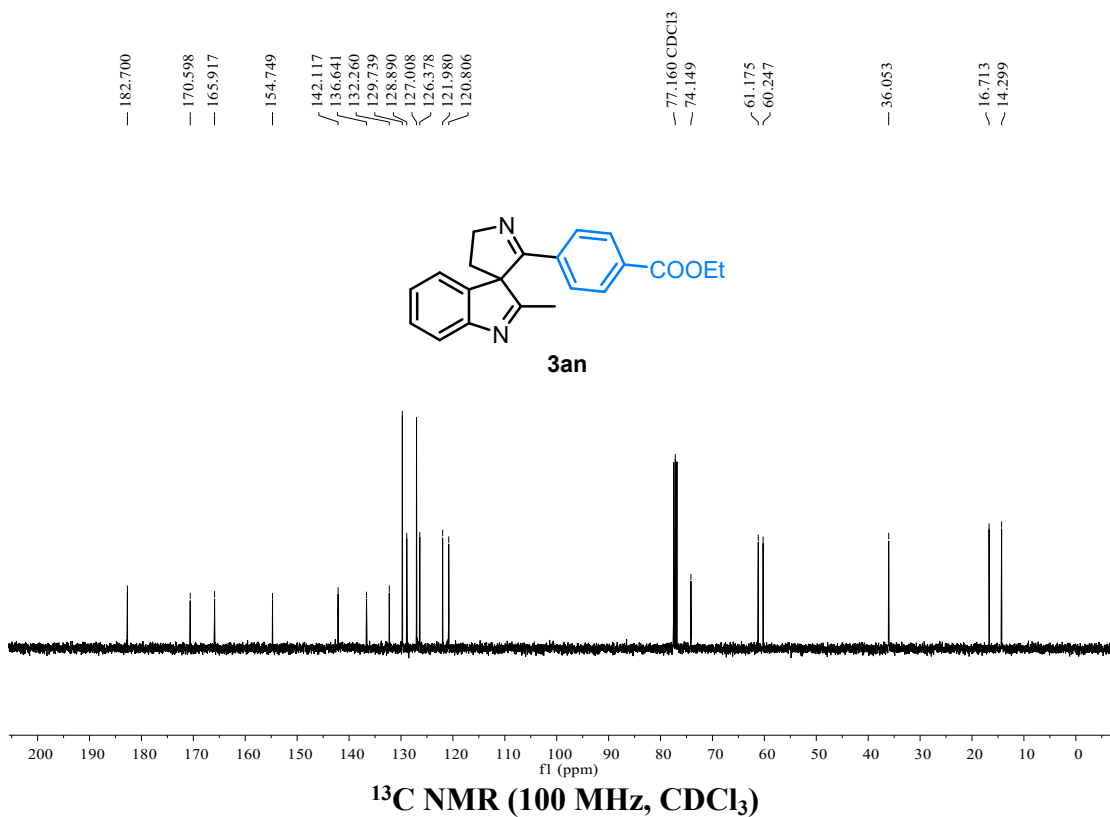
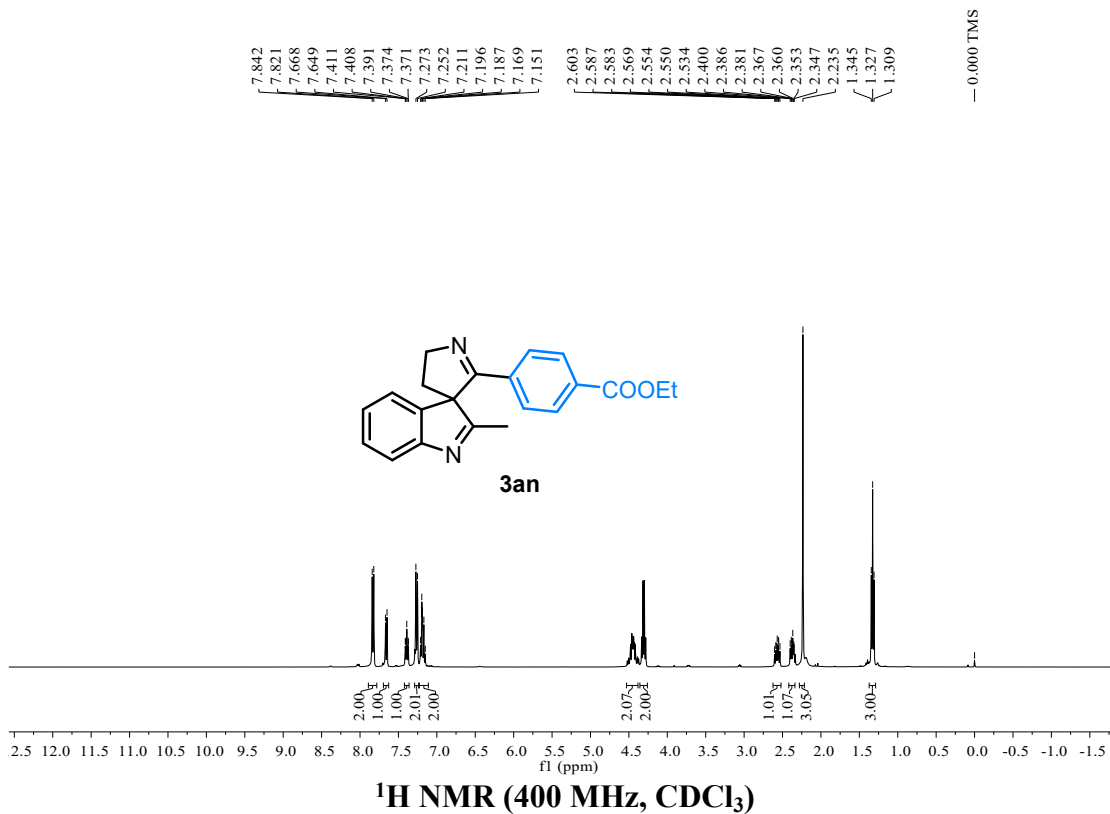


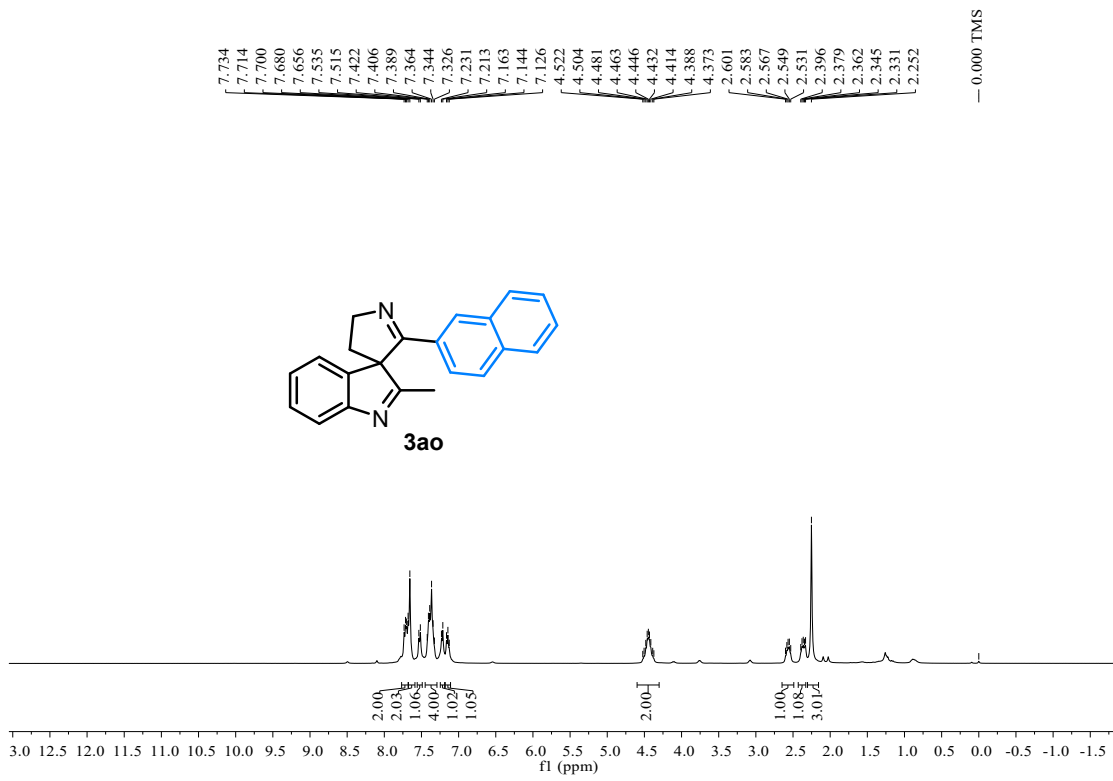
$^1\text{H NMR}$ (400 MHz, CDCl_3)



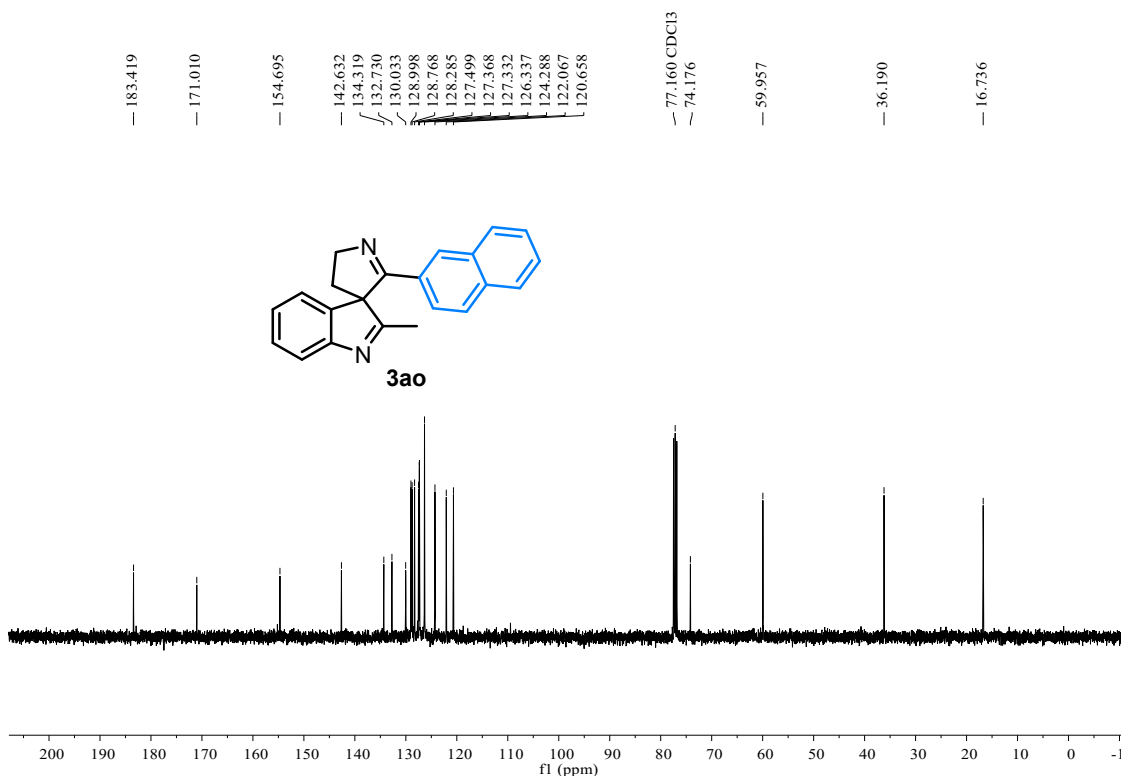
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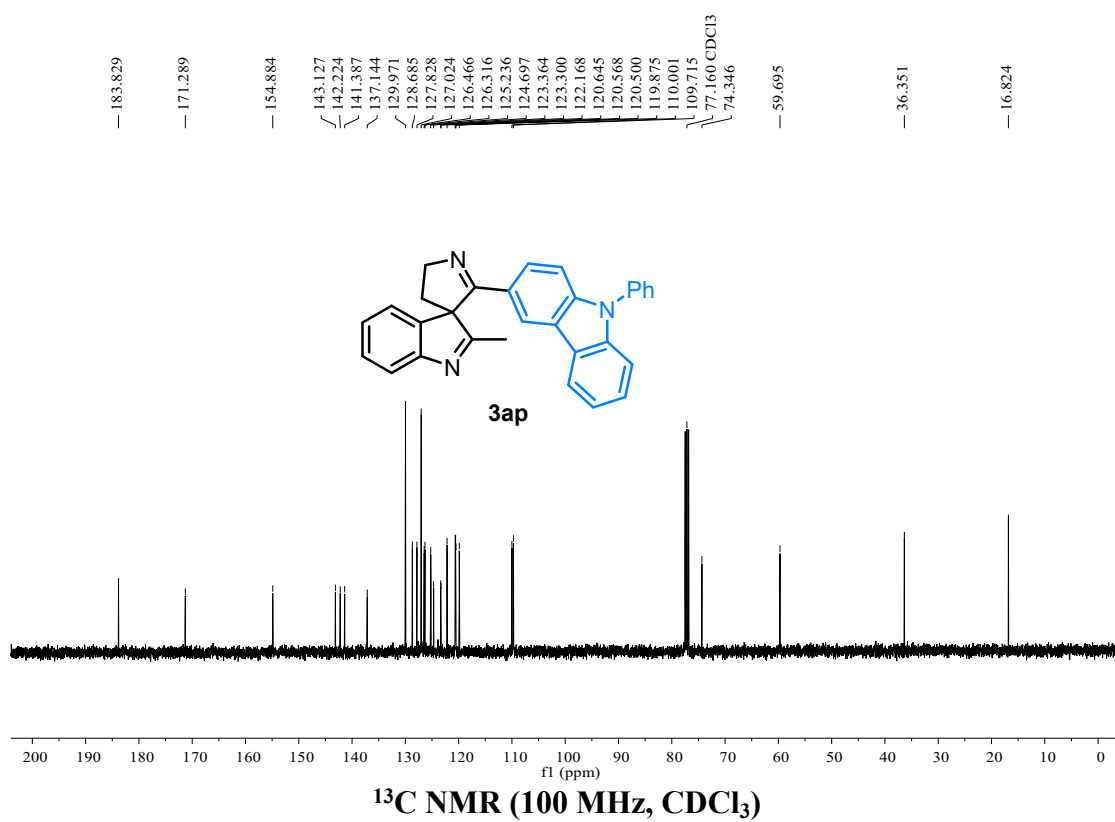
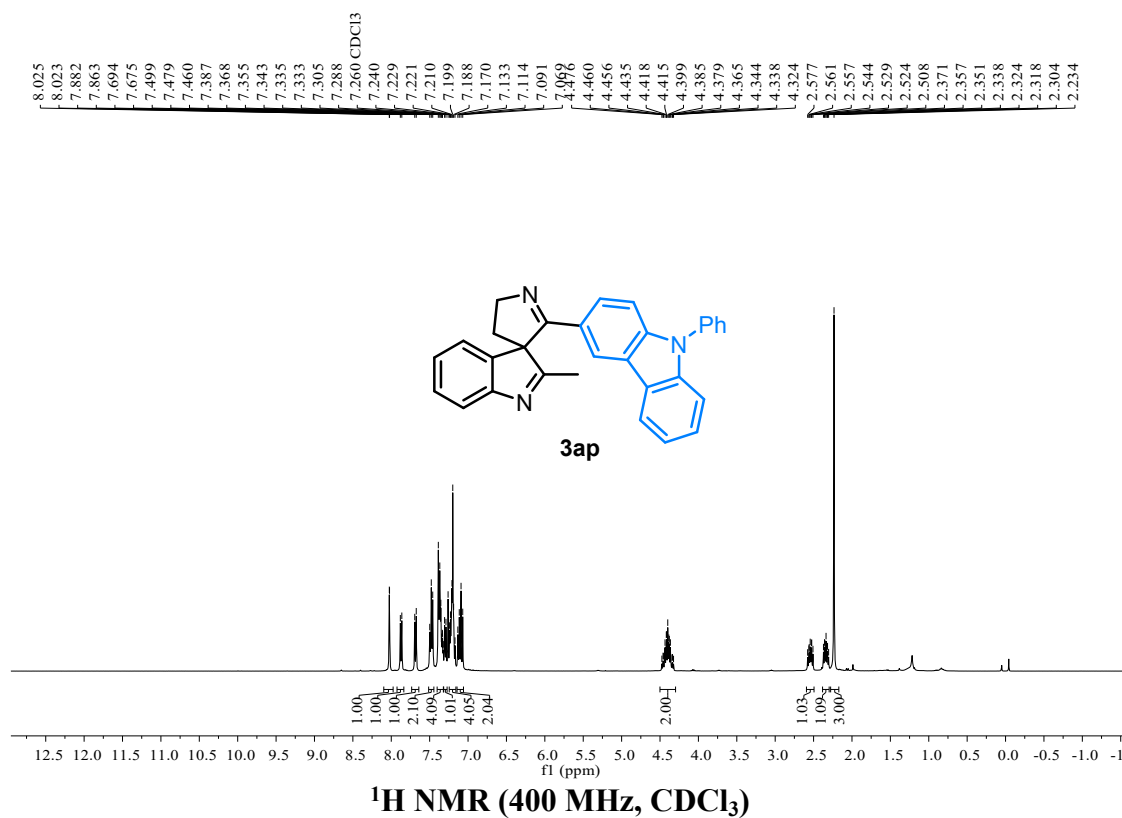


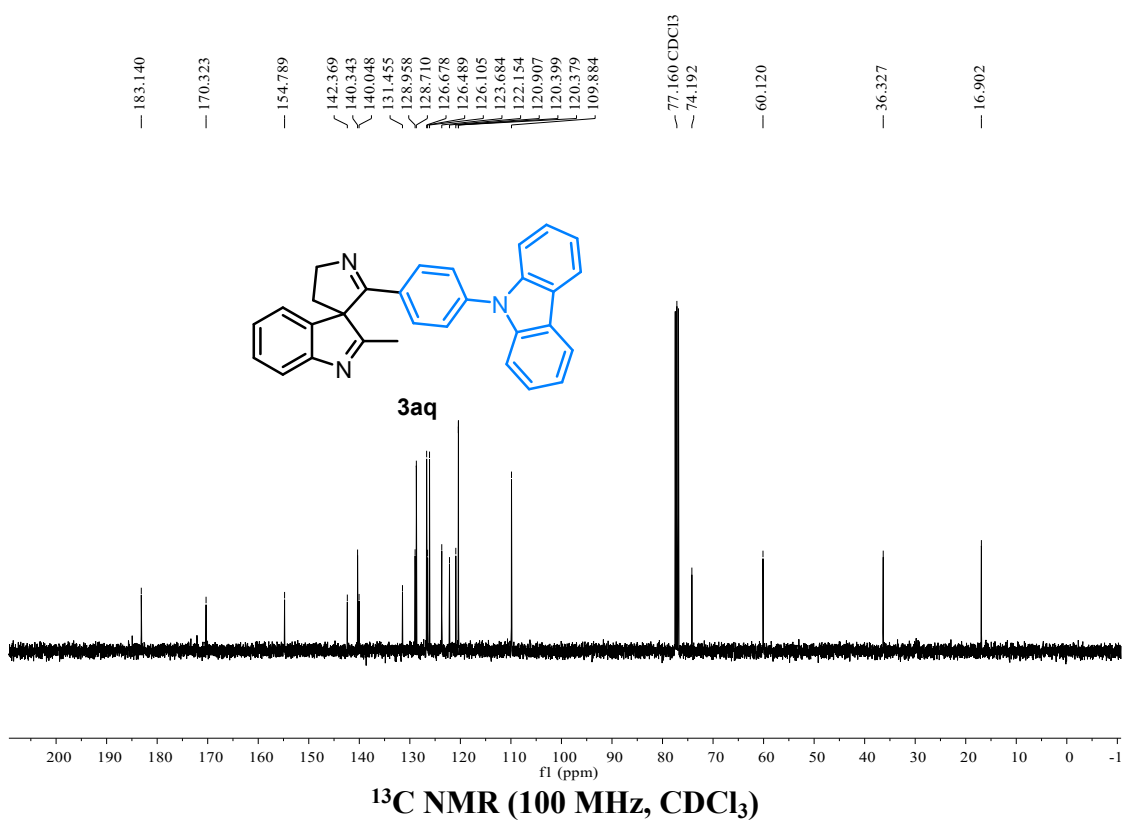
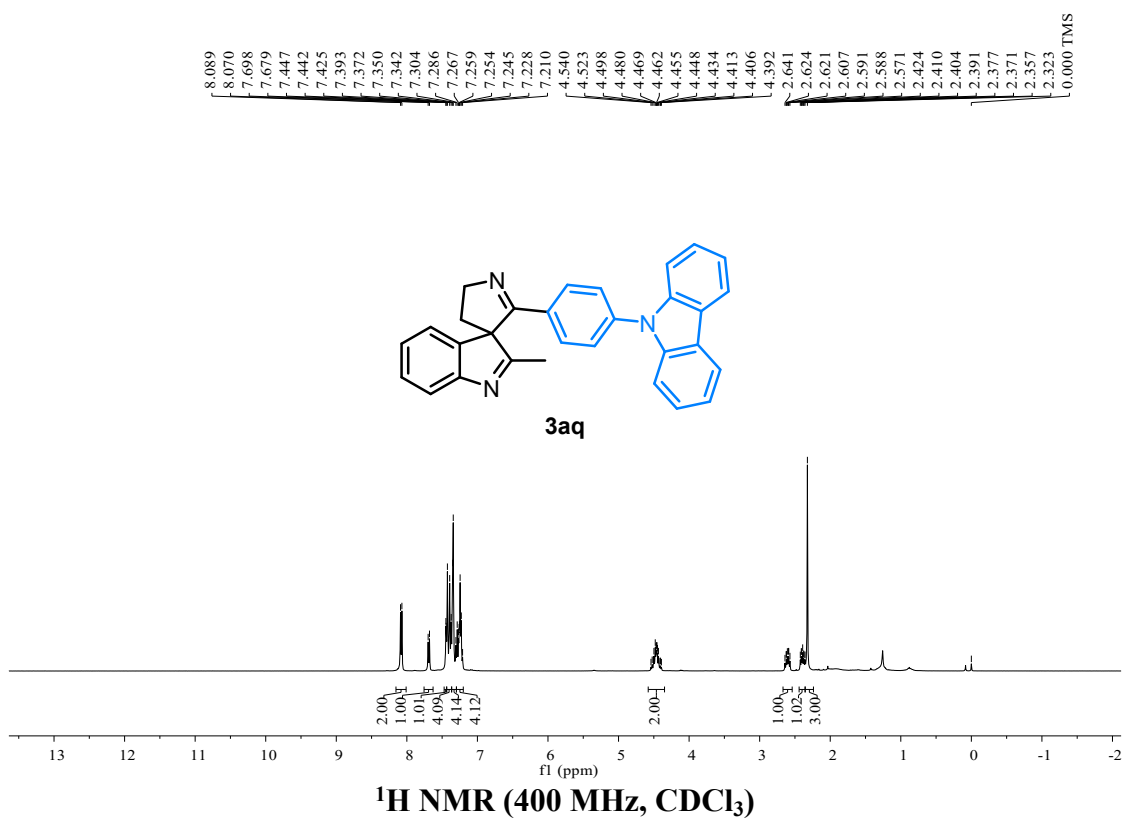


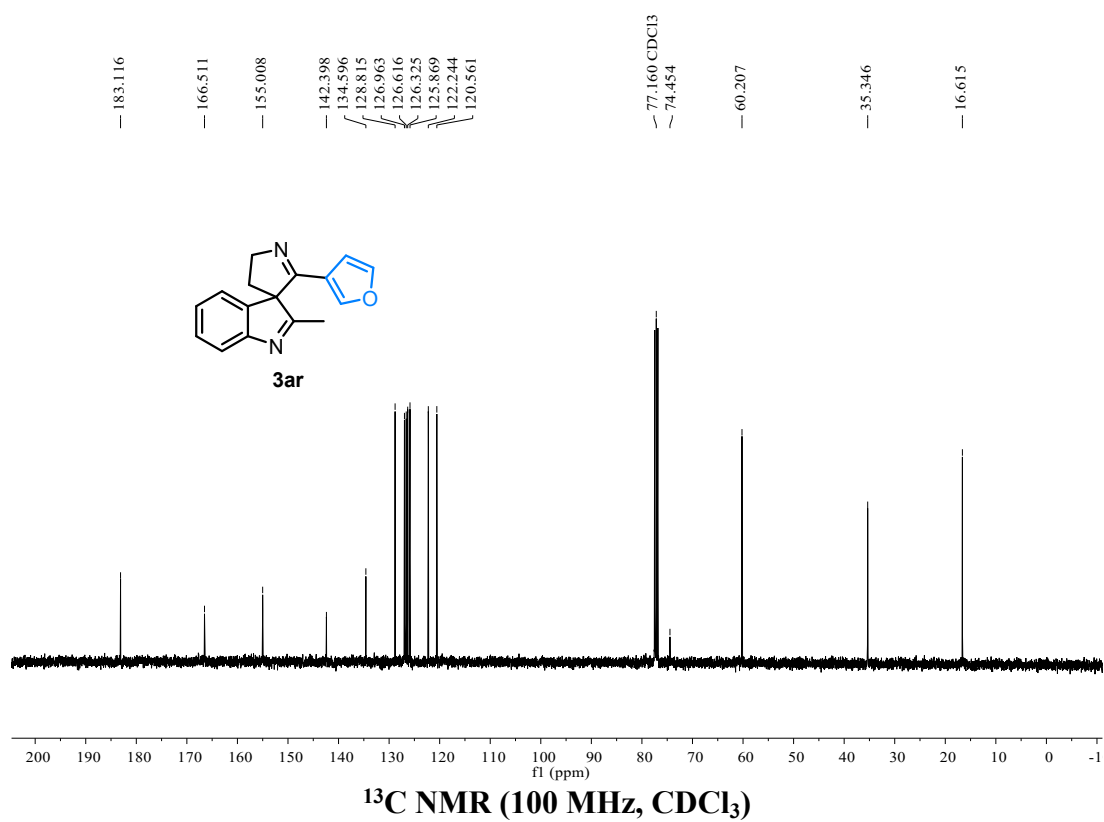
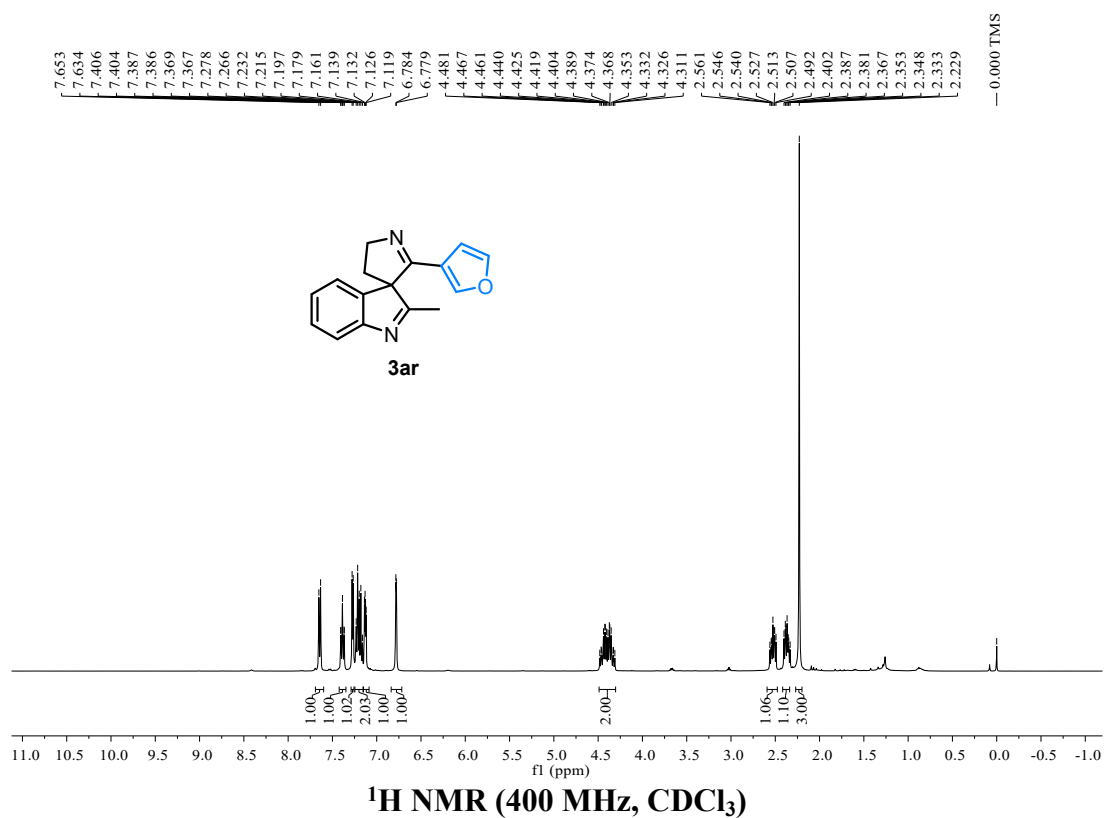
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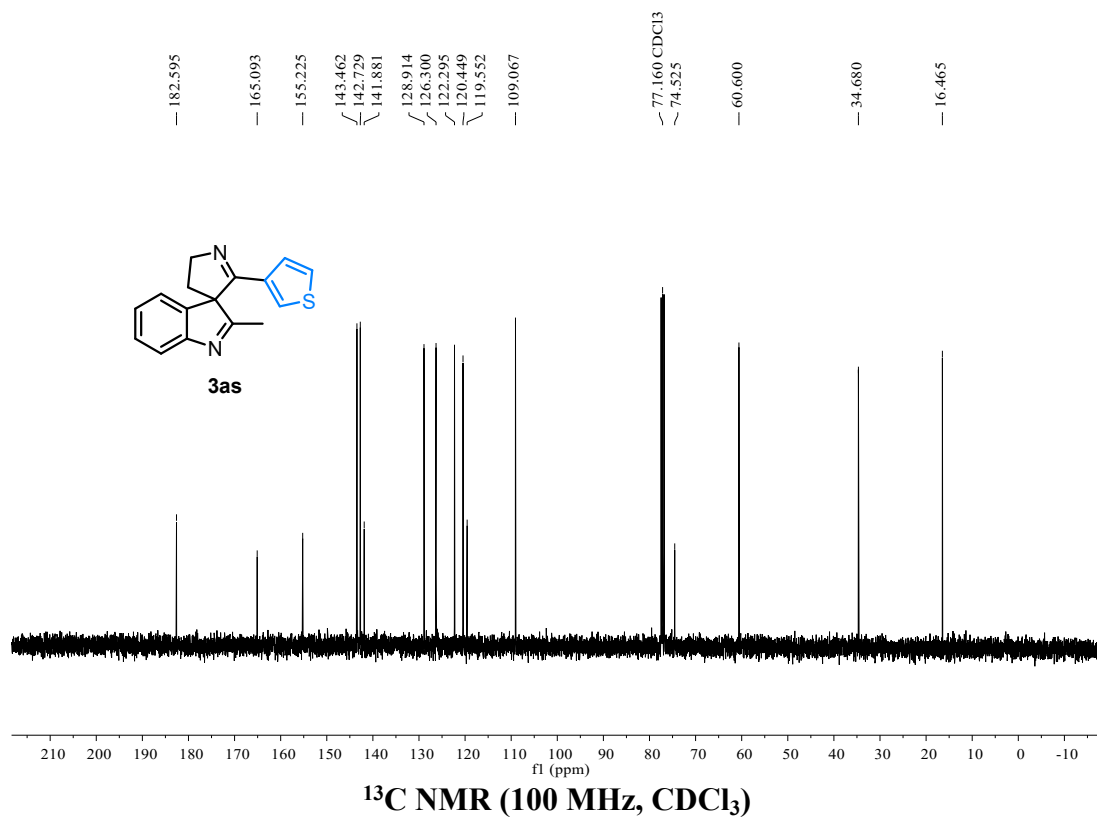
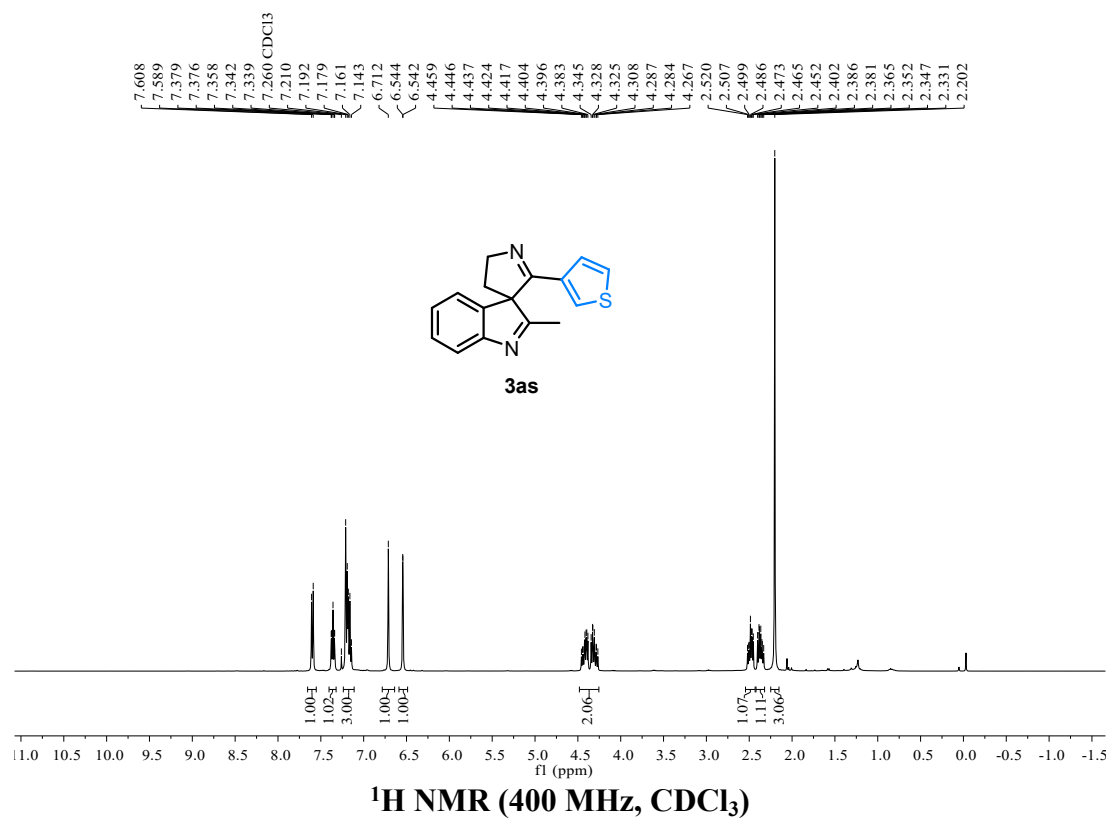


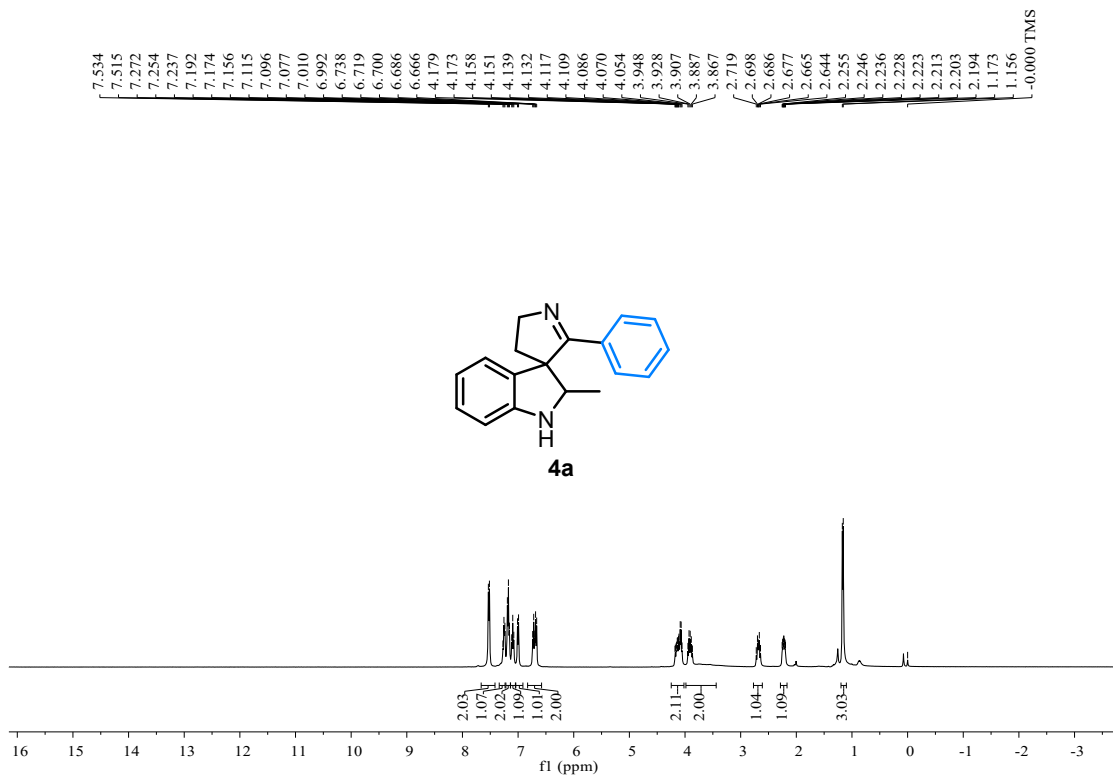
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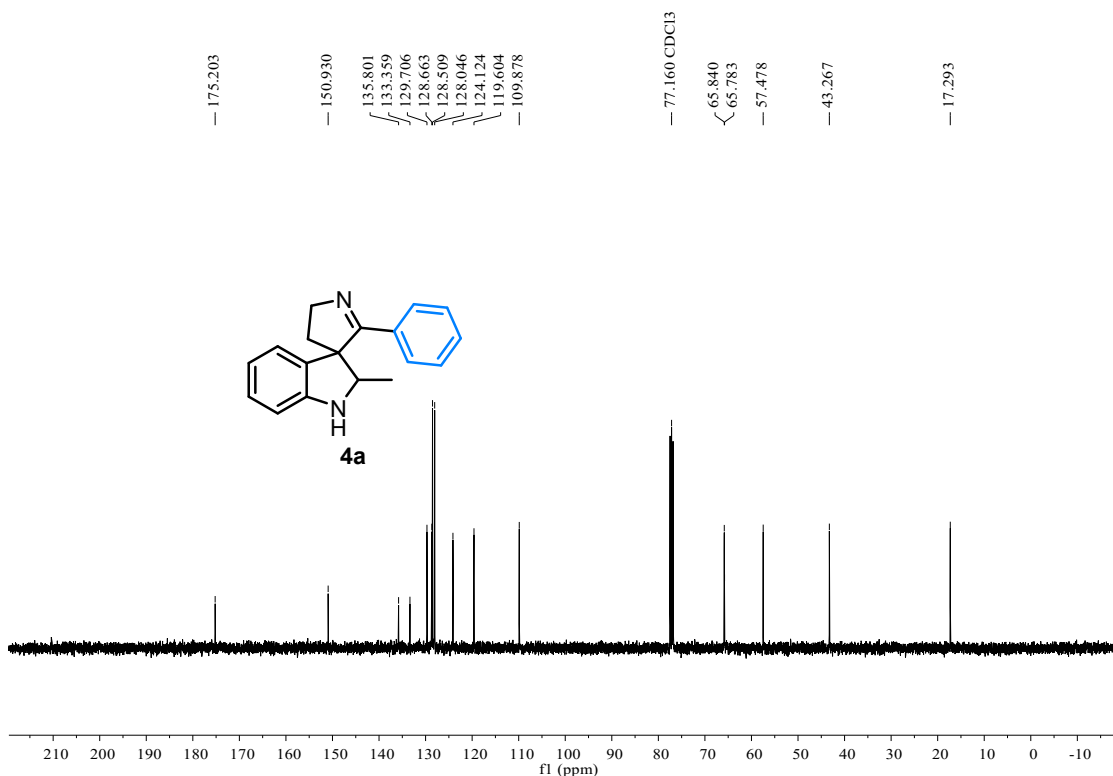




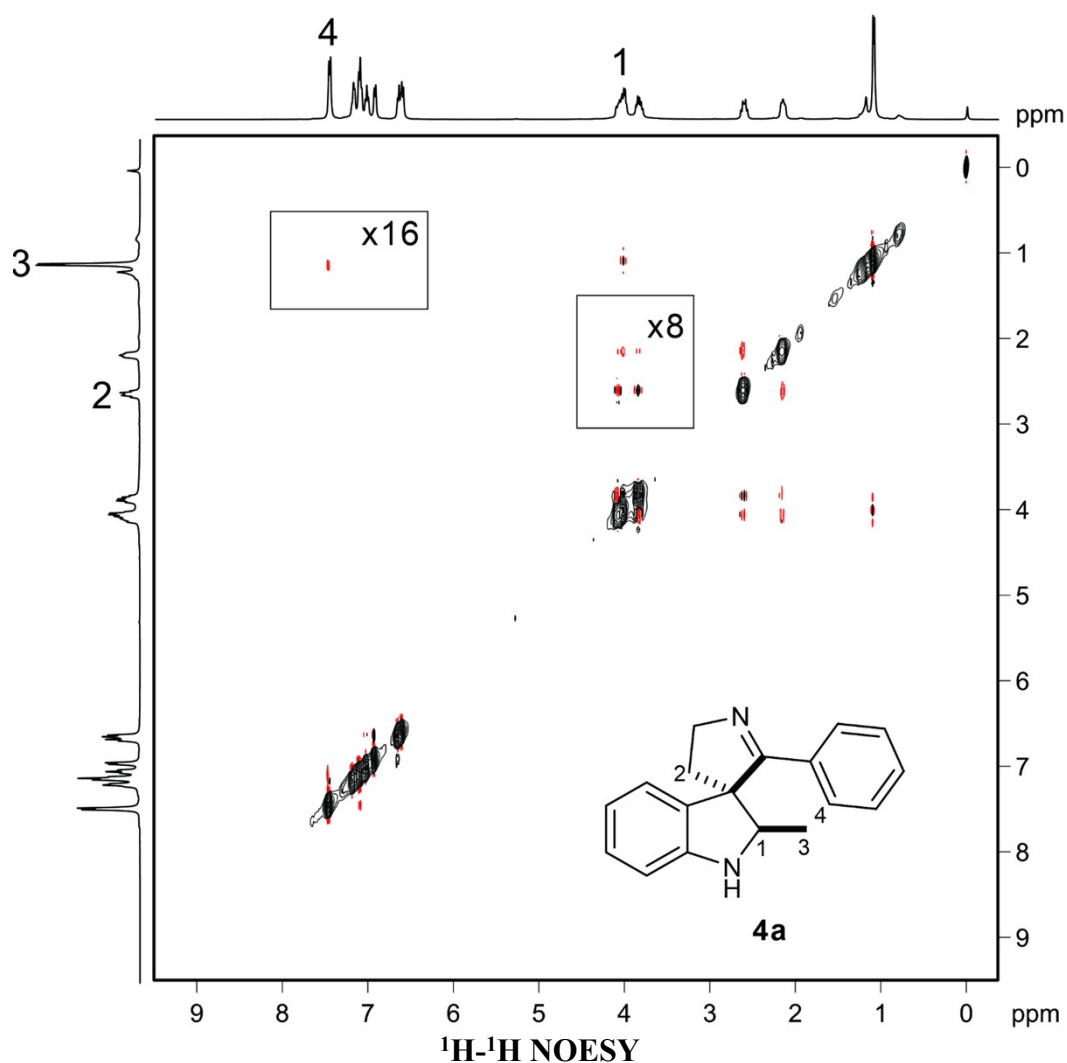




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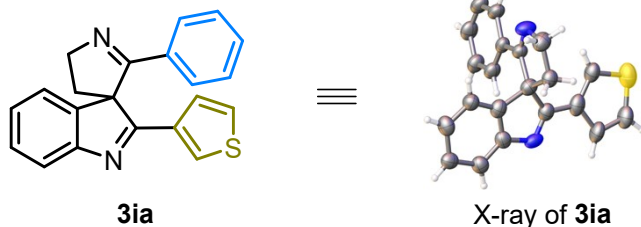


¹³C NMR (100 MHz, CDCl₃)



2. Crystal data and structure refinement for **3ia**.

Compound **3ia**: (The crystal structure of compound **3ia** has been deposited at the Cambridge Crystallographic Data Centre (CCDC 2102830). The data is available free of charge at www.ccdc.cam.ac.uk/conts/retrieving.html.)



Crystal data and structure refinement for **3ia**.

Empirical formula

$C_{21}H_{16}N_2S$

Formula weight	328.42	
Temperature/K	296	
Wavelength	1.54184 Å	
Crystal system	monoclinic	
Space group	P 1 21/c 1	
Unit cell dimensions	a = 9.3674(7) Å	$\alpha = 90.000^\circ$
	b = 23.7692(18) Å	$\beta = 114.905^\circ$
	c = 8.4101(6) Å	$\gamma = 90.000^\circ$
Volume/Å ³	1698.4(2)	
Z	4	
Density (calculated) g/cm ³	1.284	
Absorption coefficient/mm ⁻¹	1.699	
F(000)	688	
Crystal size/mm ³	0.4 × 0.35 × 0.3	
Theta range for data collection/°	3.7190 to 77.4550	
Index ranges	-11 ≤ h ≤ 11, -28 ≤ k ≤ 30, -10 ≤ l ≤ 6	
Reflections collected	3598	
Independent reflections	2474 [R(int) = 0.1459]	
Completeness to theta = 80.95 °	99.8%	
Absorption correction	Multi-scan	
Data / restranits / parameters	3598/529/217	
Goodness-of-fit on F ²	1.542	
Final R indices [I>2sigma(I)]	R ₁ = 0.1459, wR ₂ = 0.3972	
Final R indices [all data]	R ₁ = 0.1780, wR ₂ = 0.4383	