

Supporting Information

Synthesis of strained 1,2-diazetidines via [3+1] cycloaddition of C,N-cyclic azomethine imines with isocyanides and synthetic derivation

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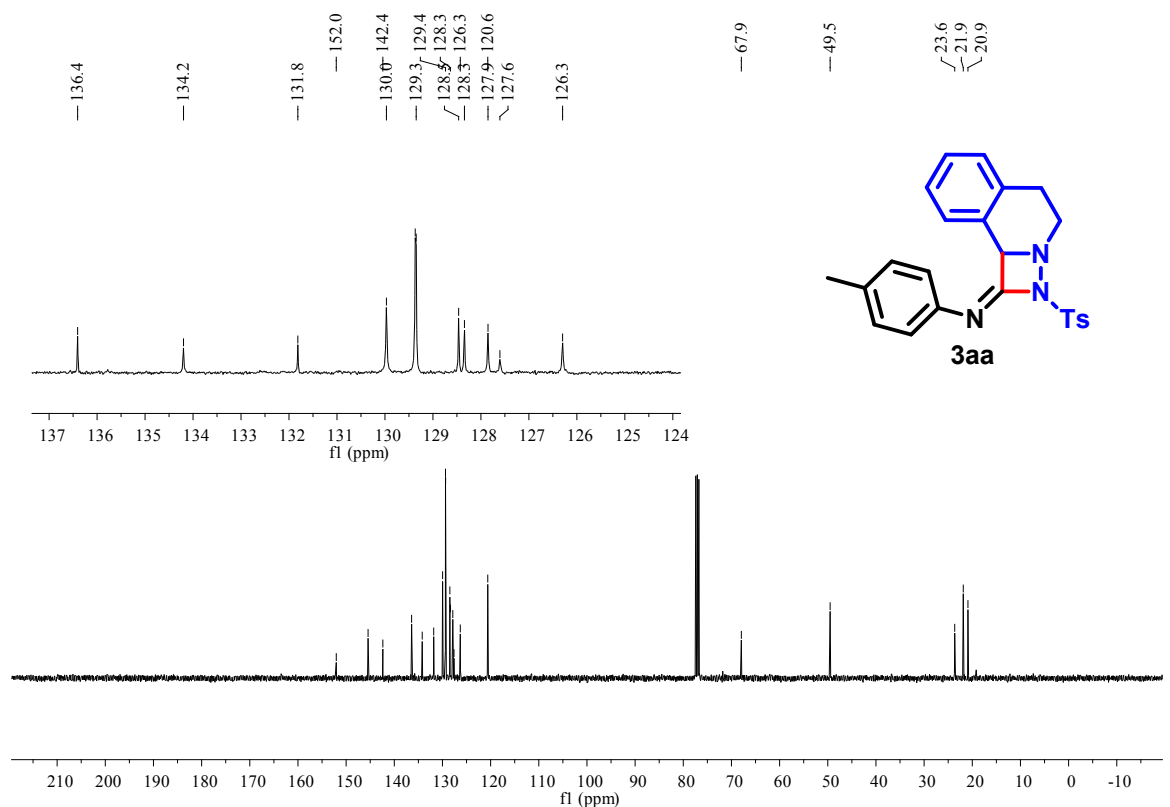
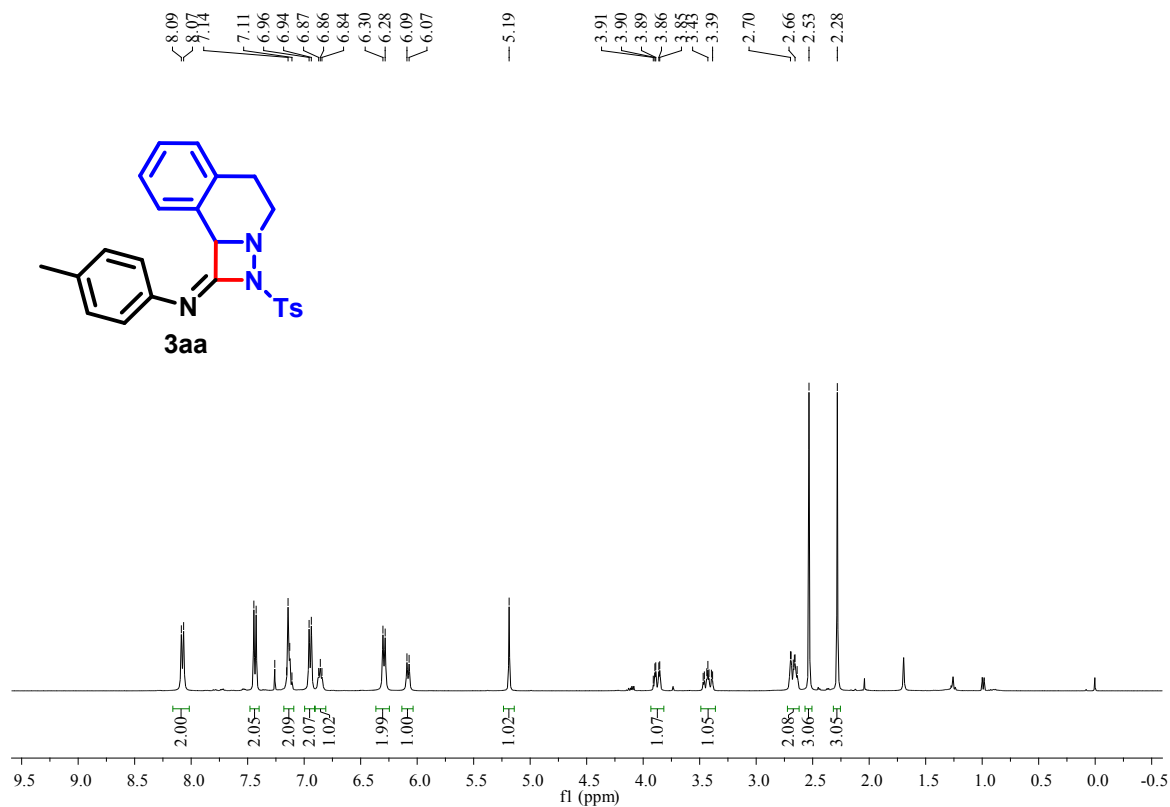
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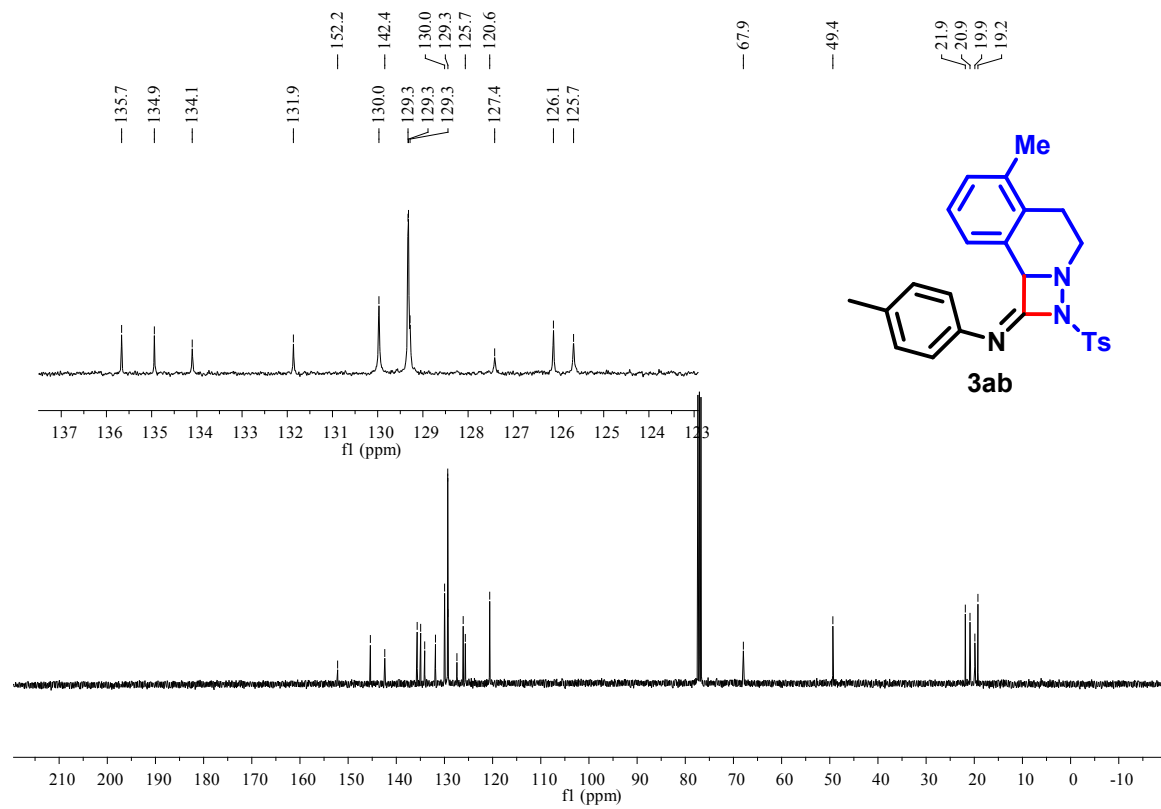
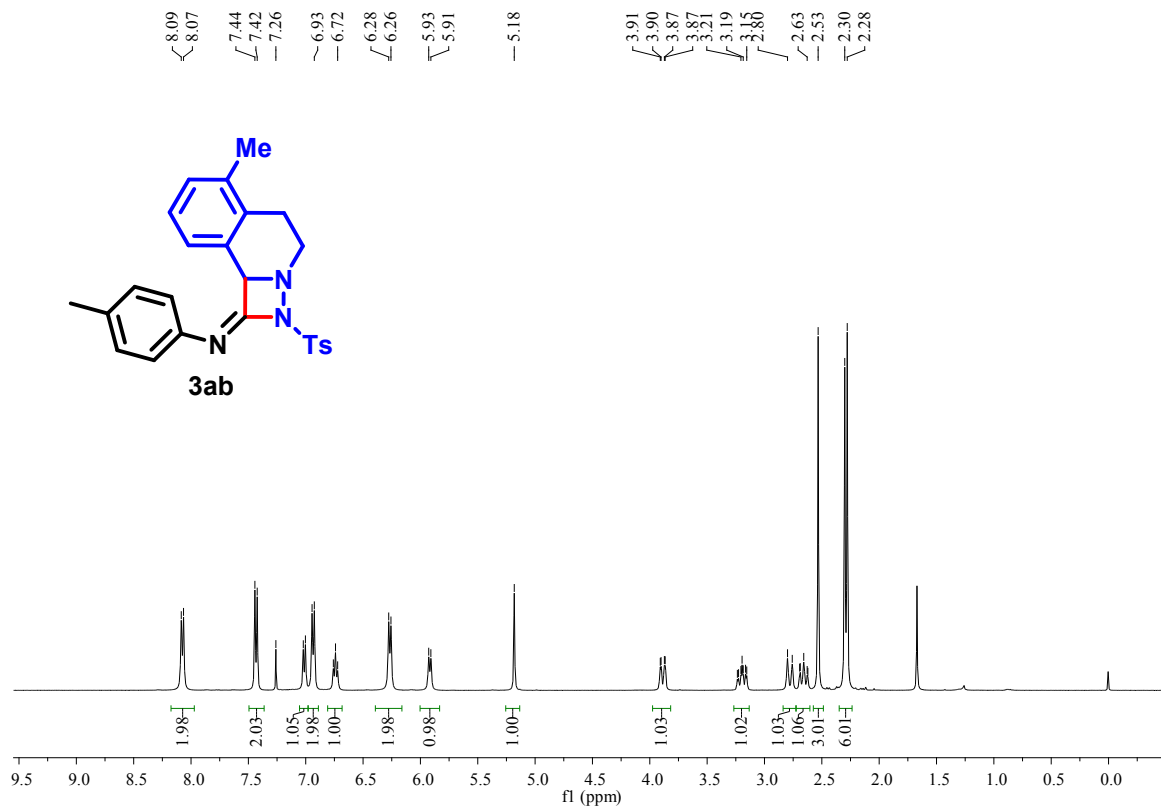
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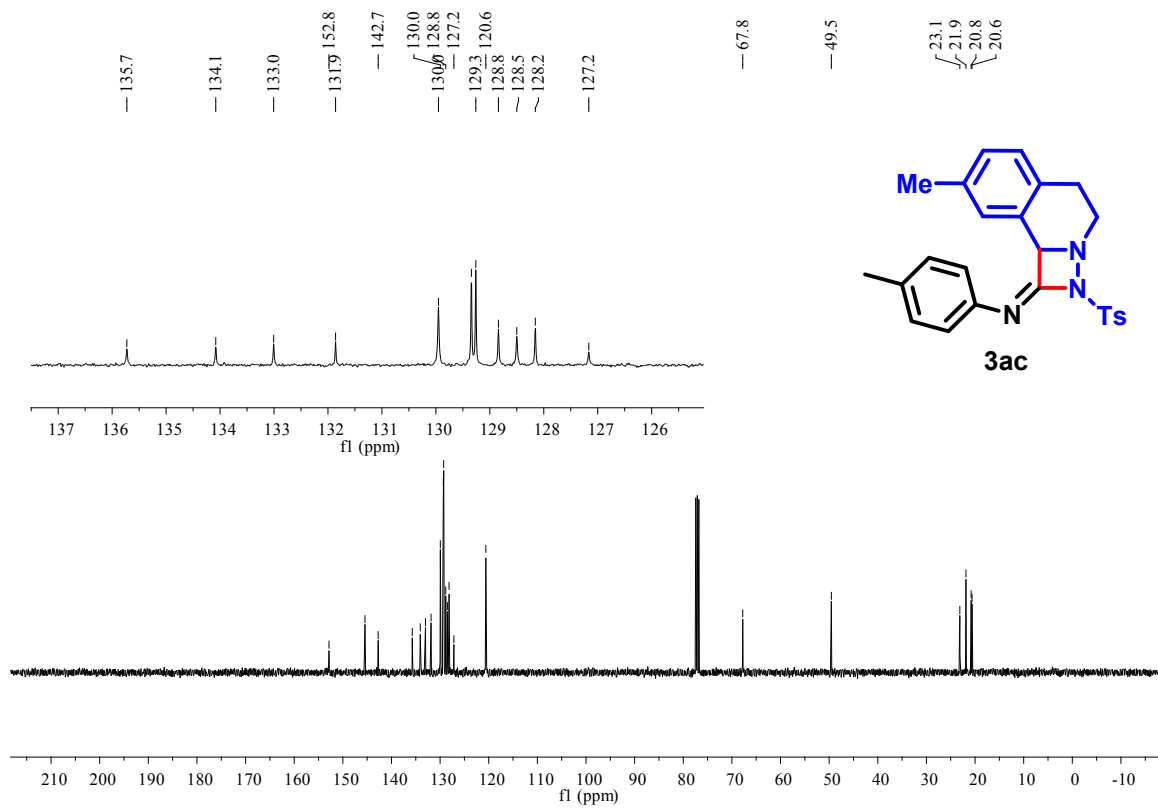
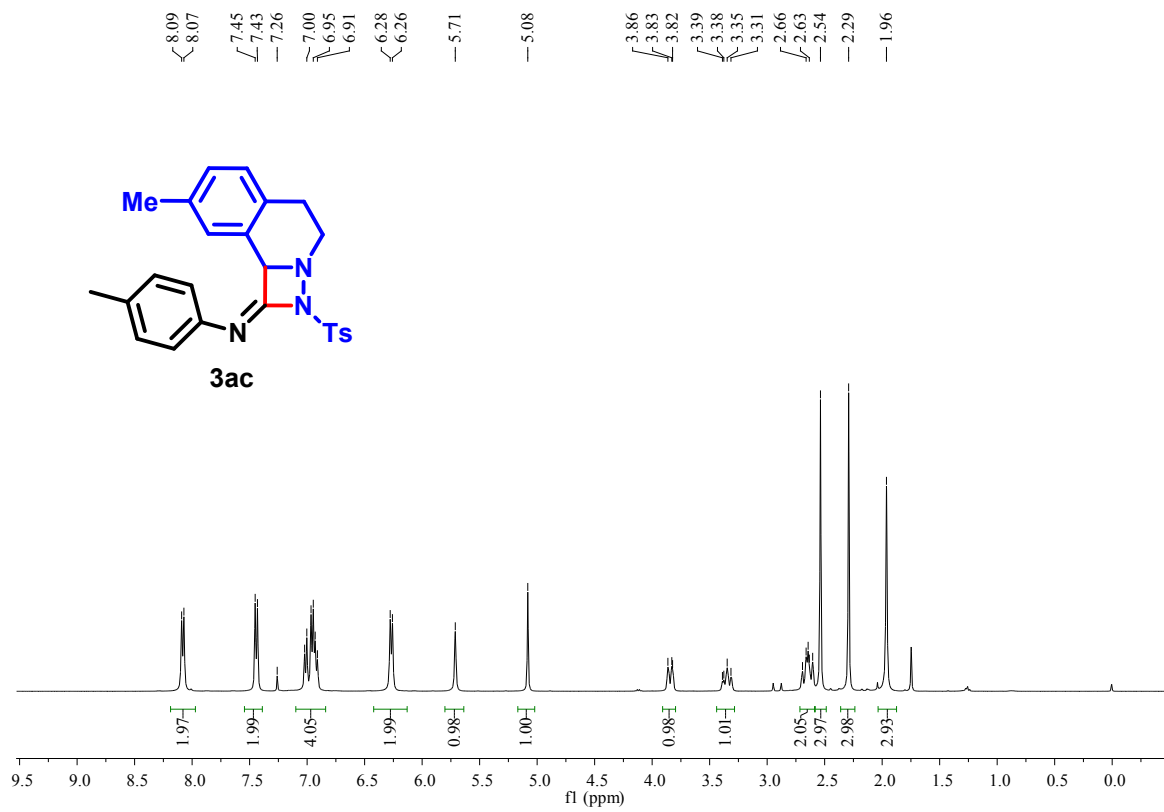
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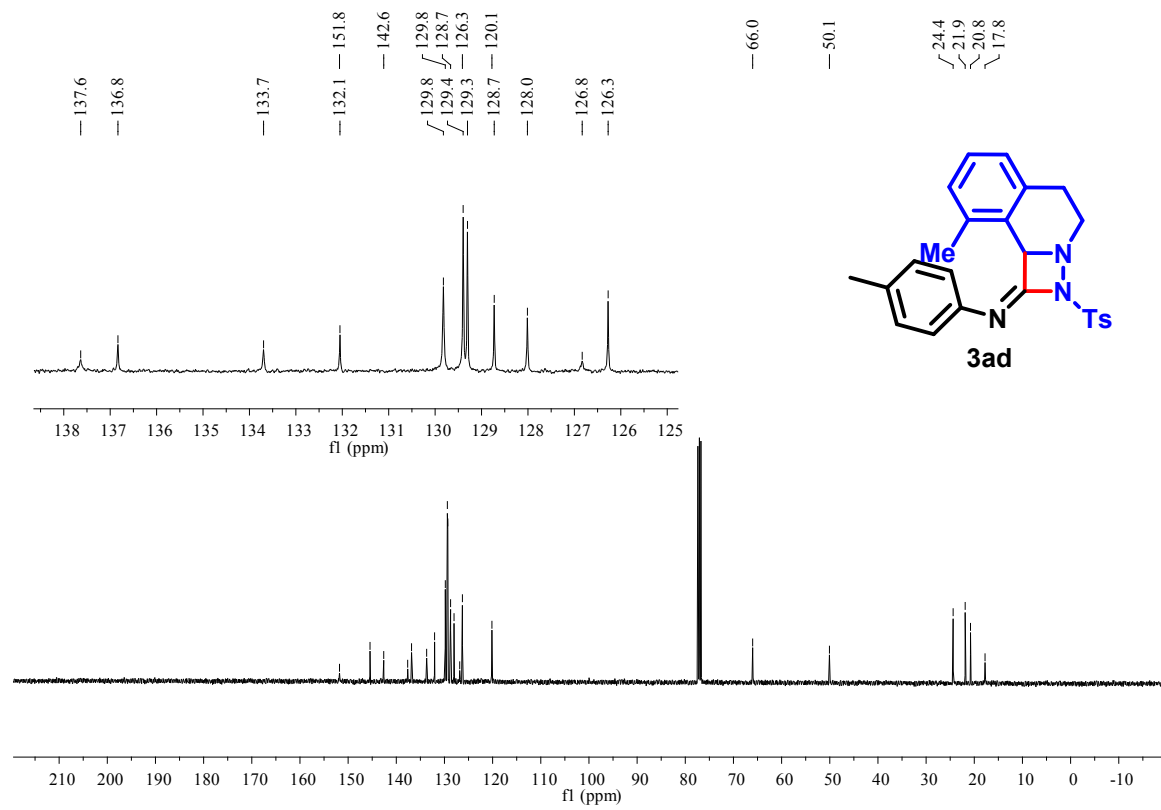
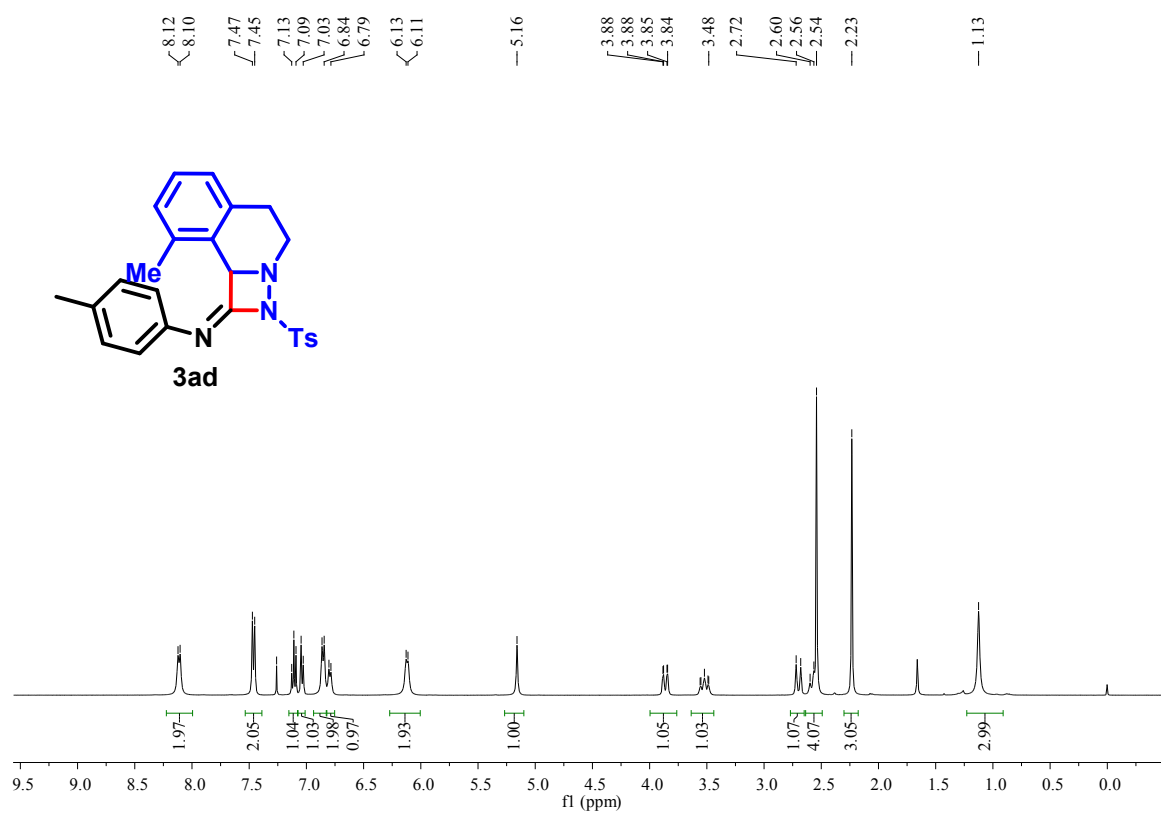
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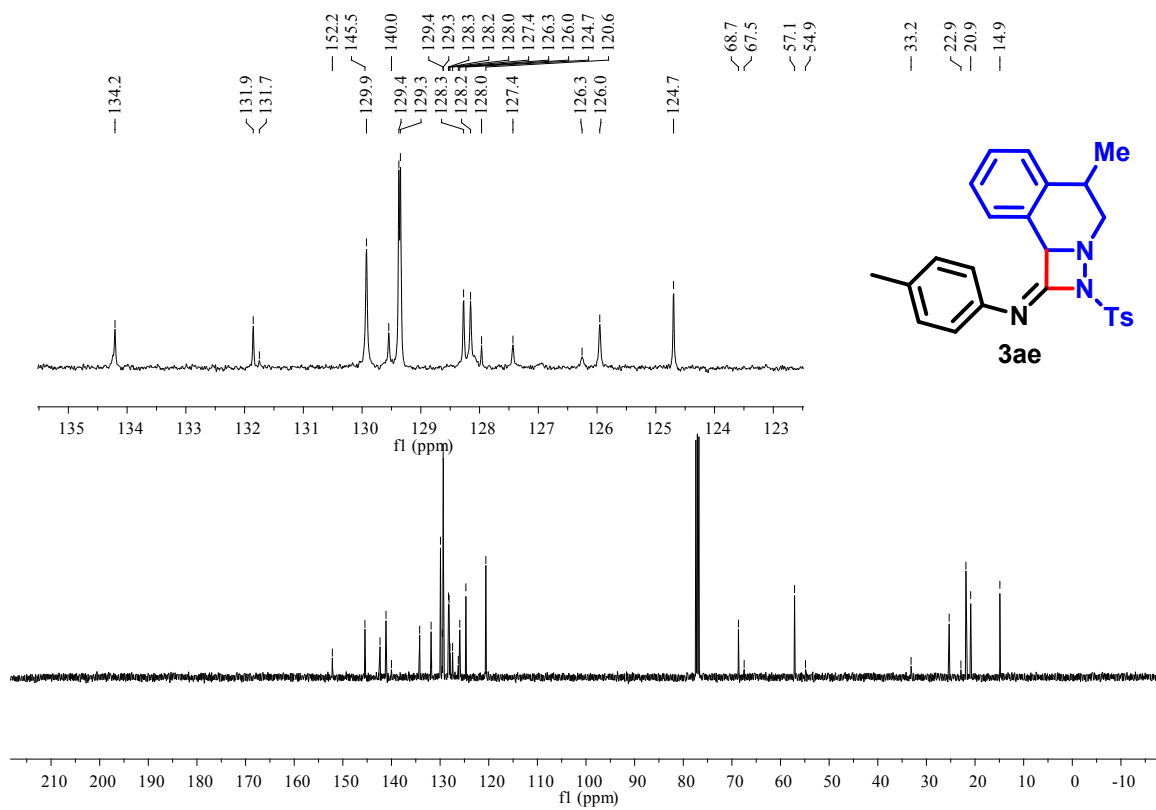
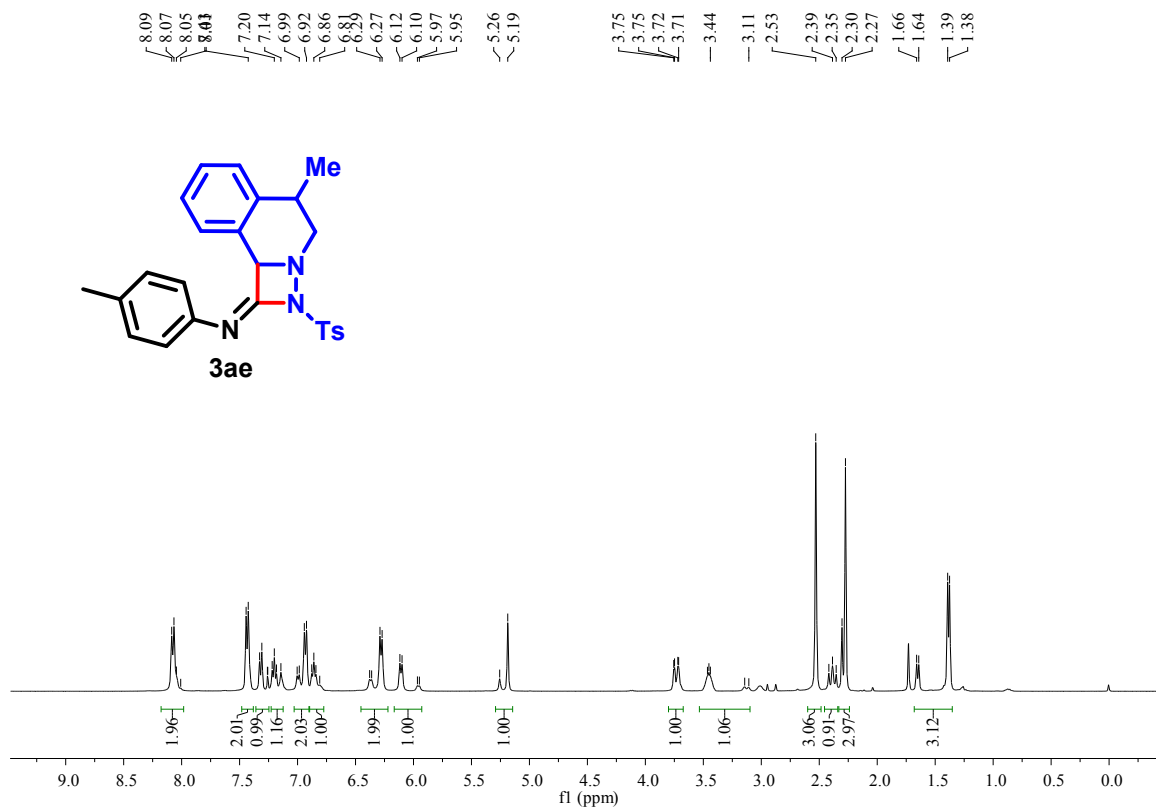
1. ^1H , ^{13}C and ^{19}F NMR spectra of all products

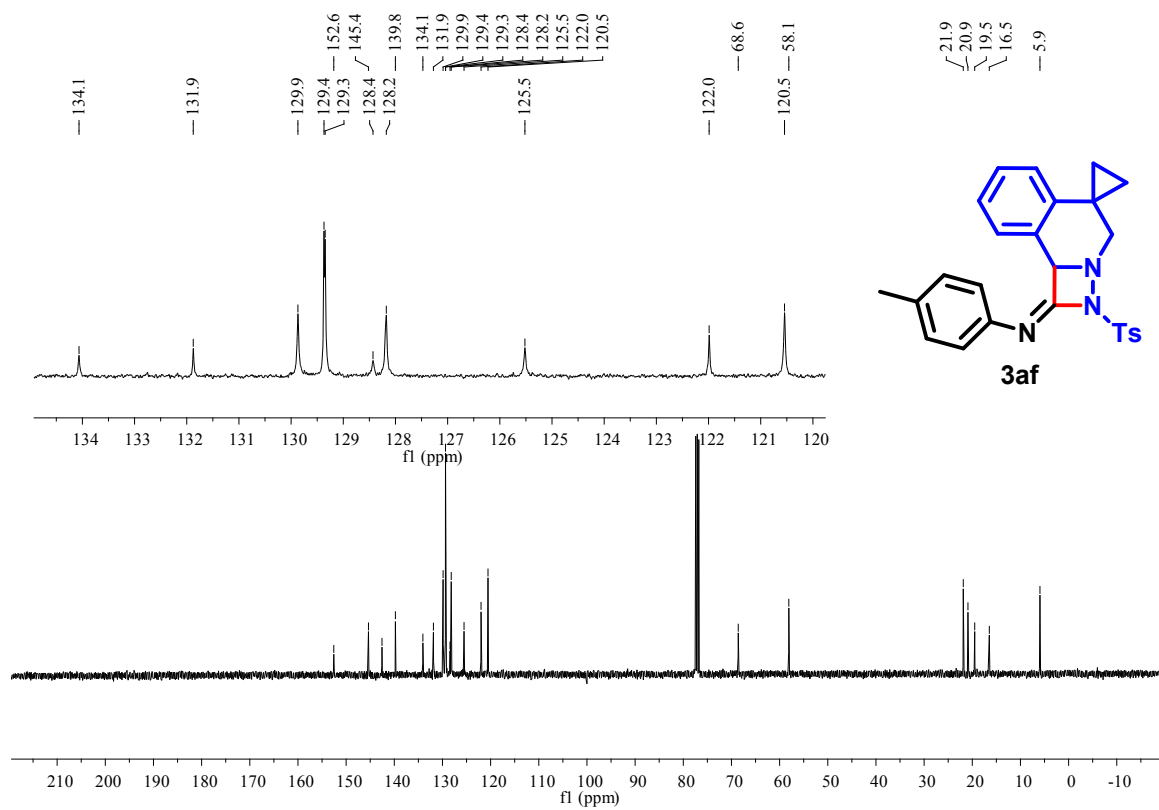
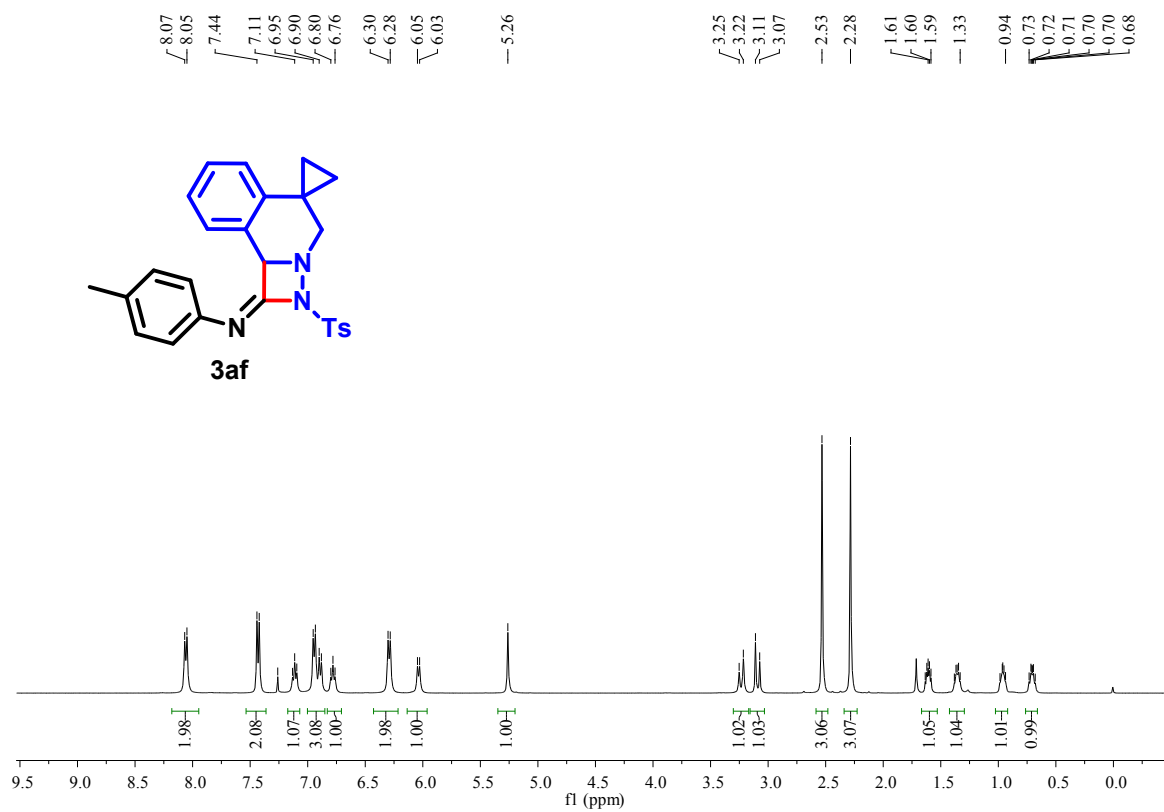


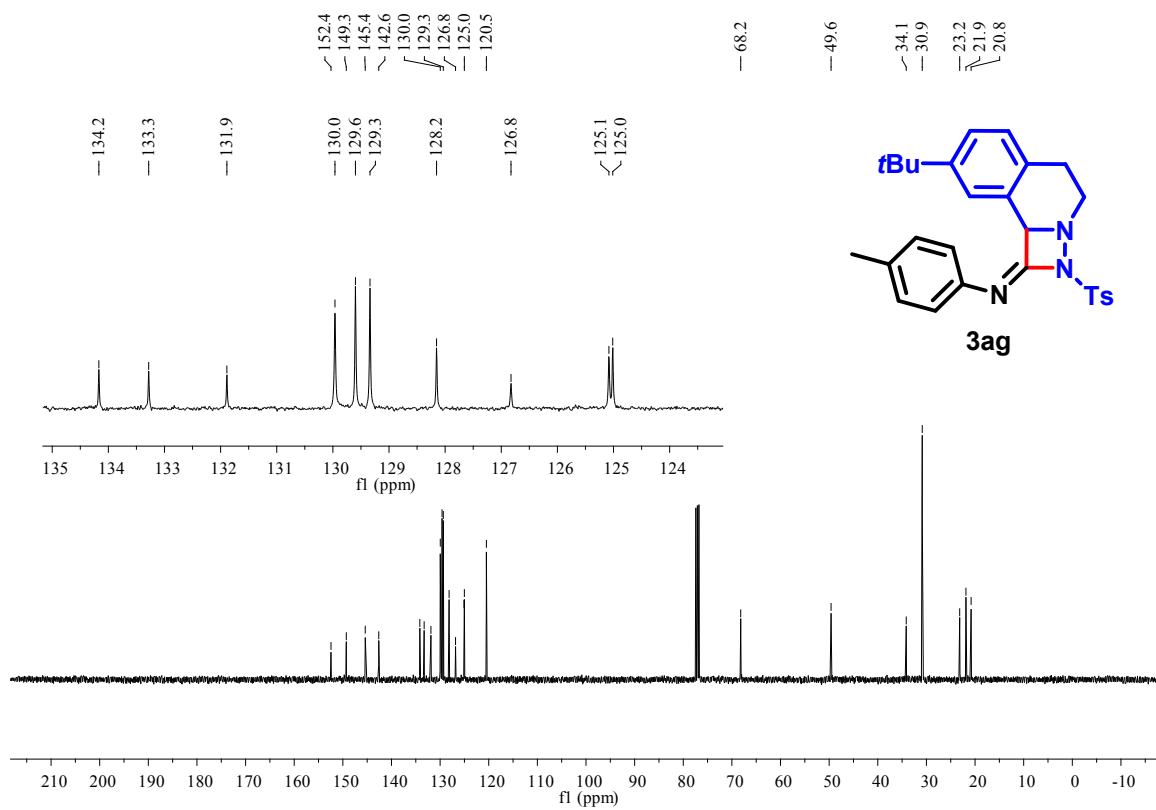
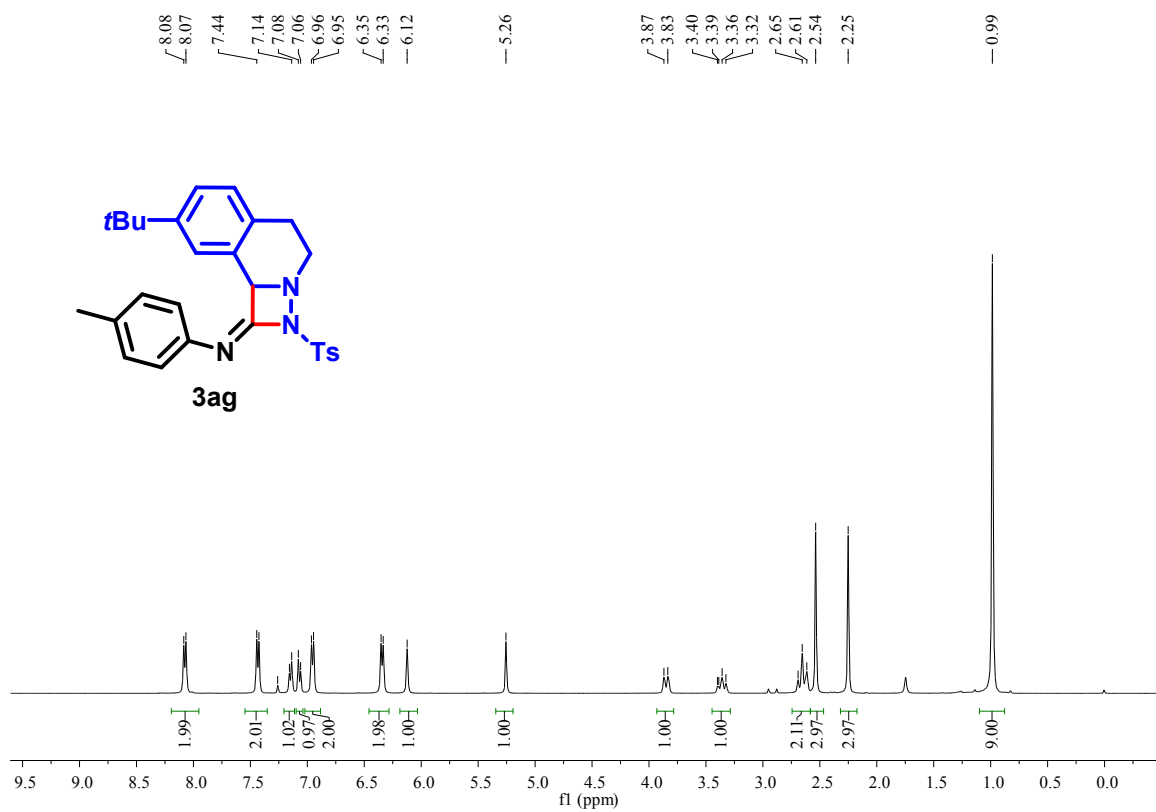


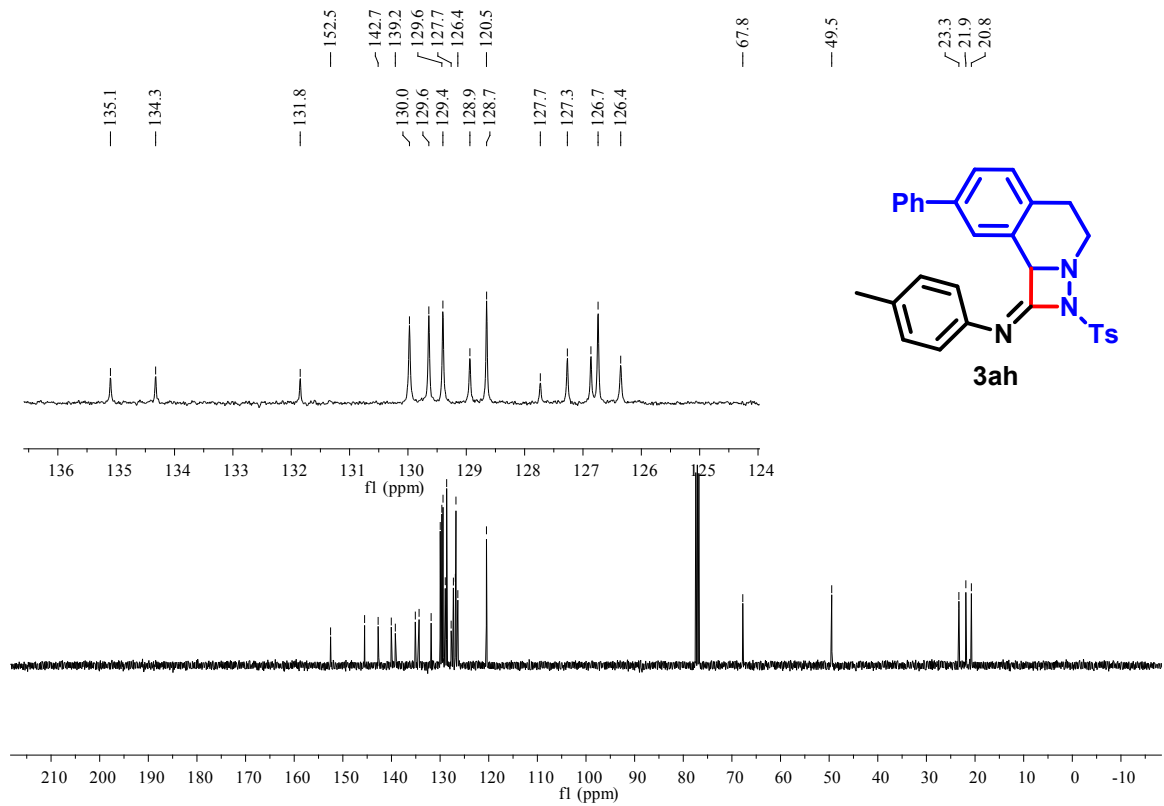
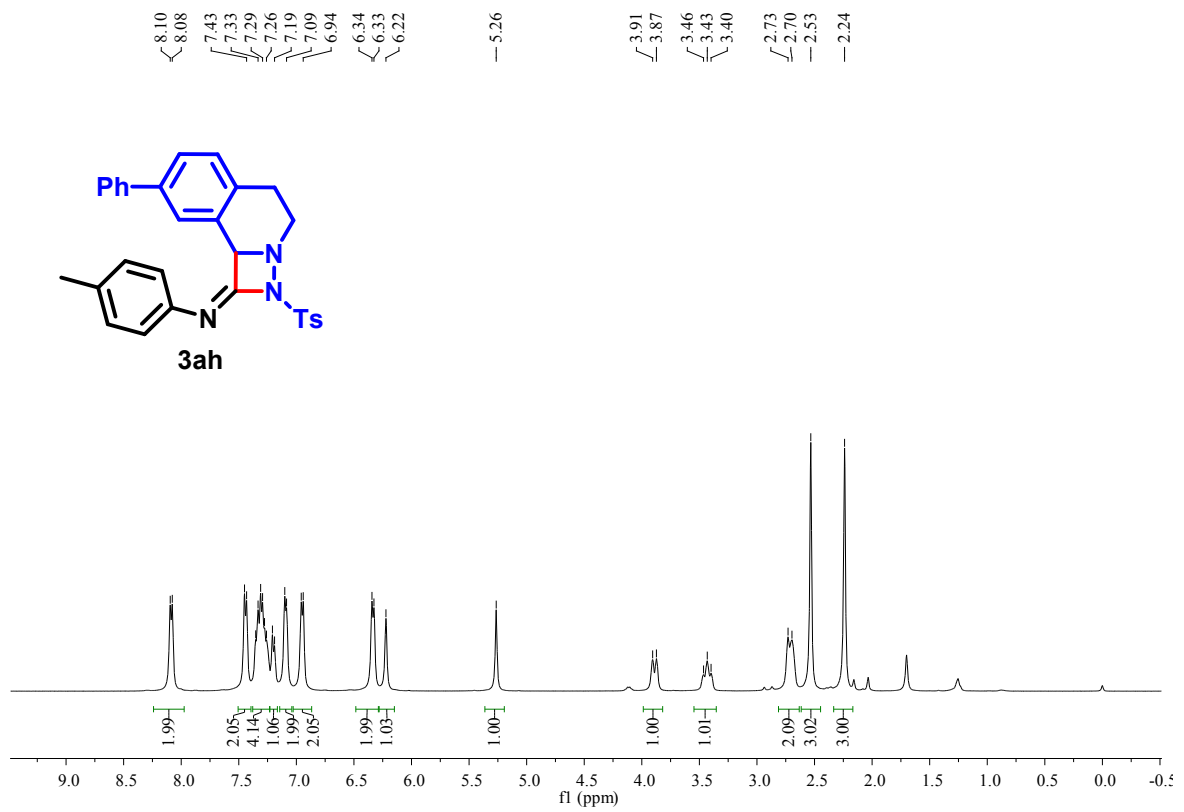


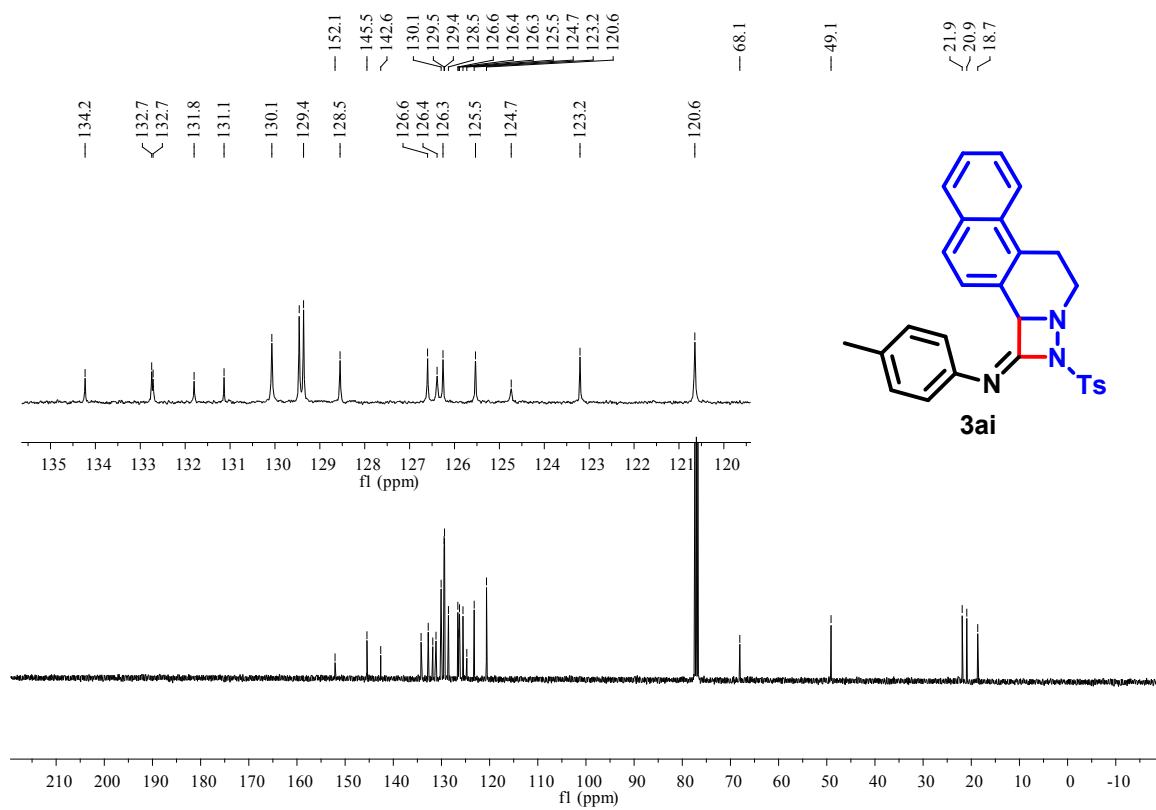
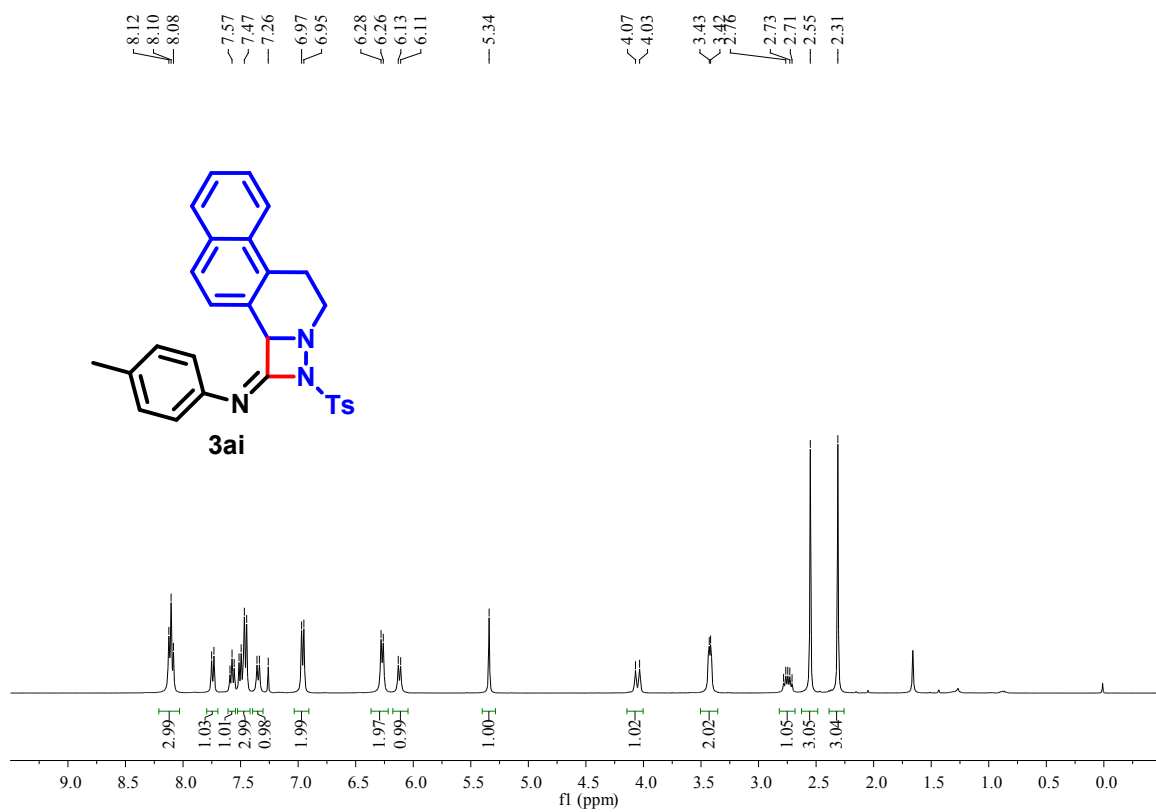


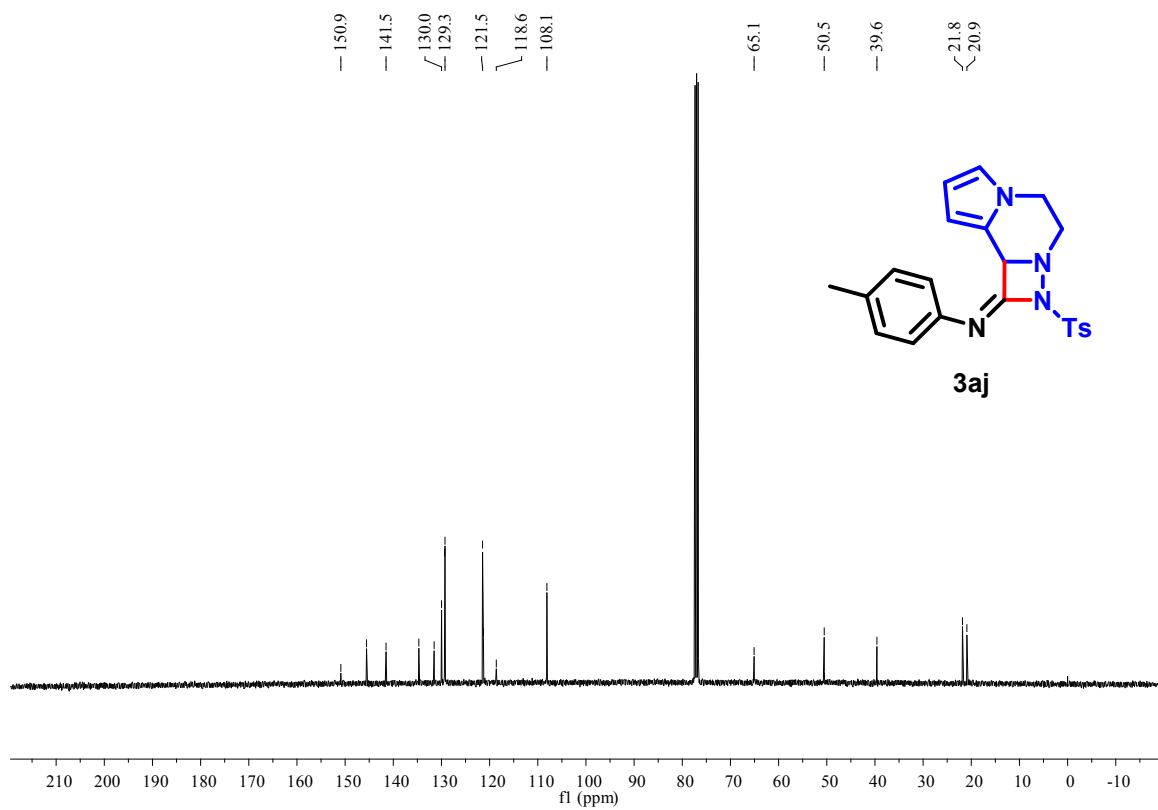
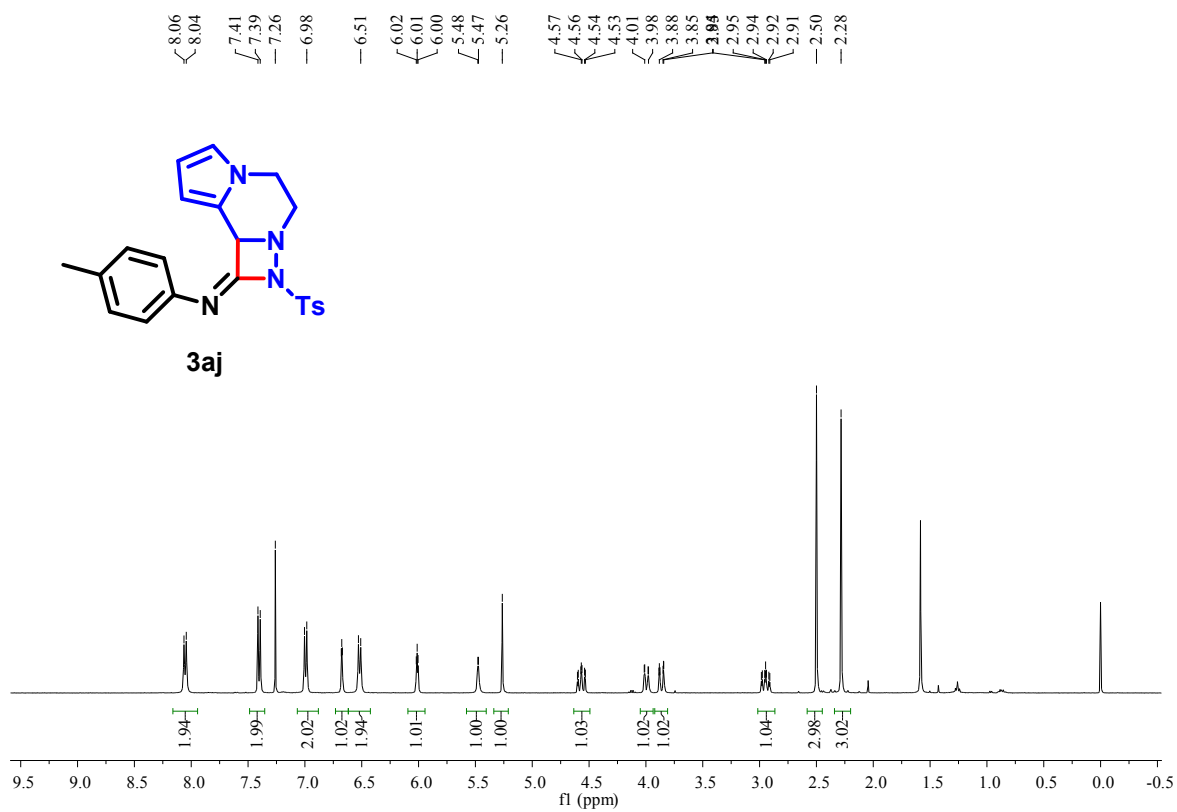


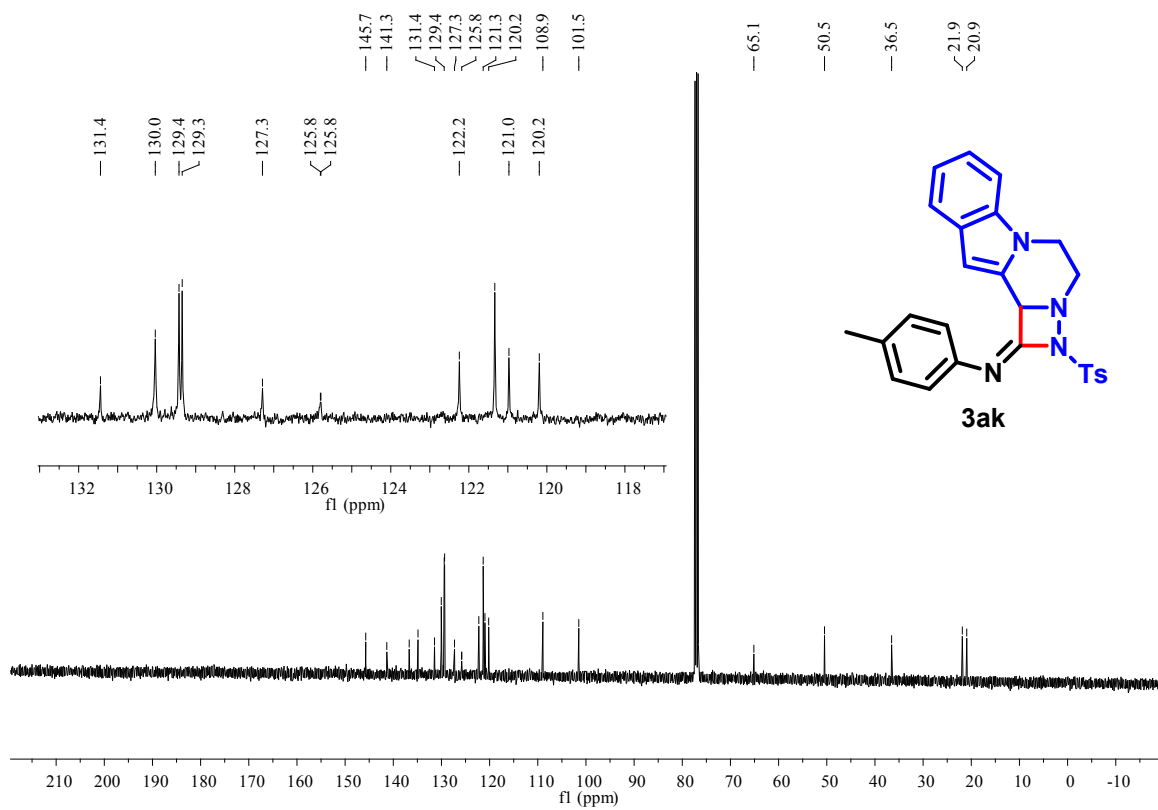
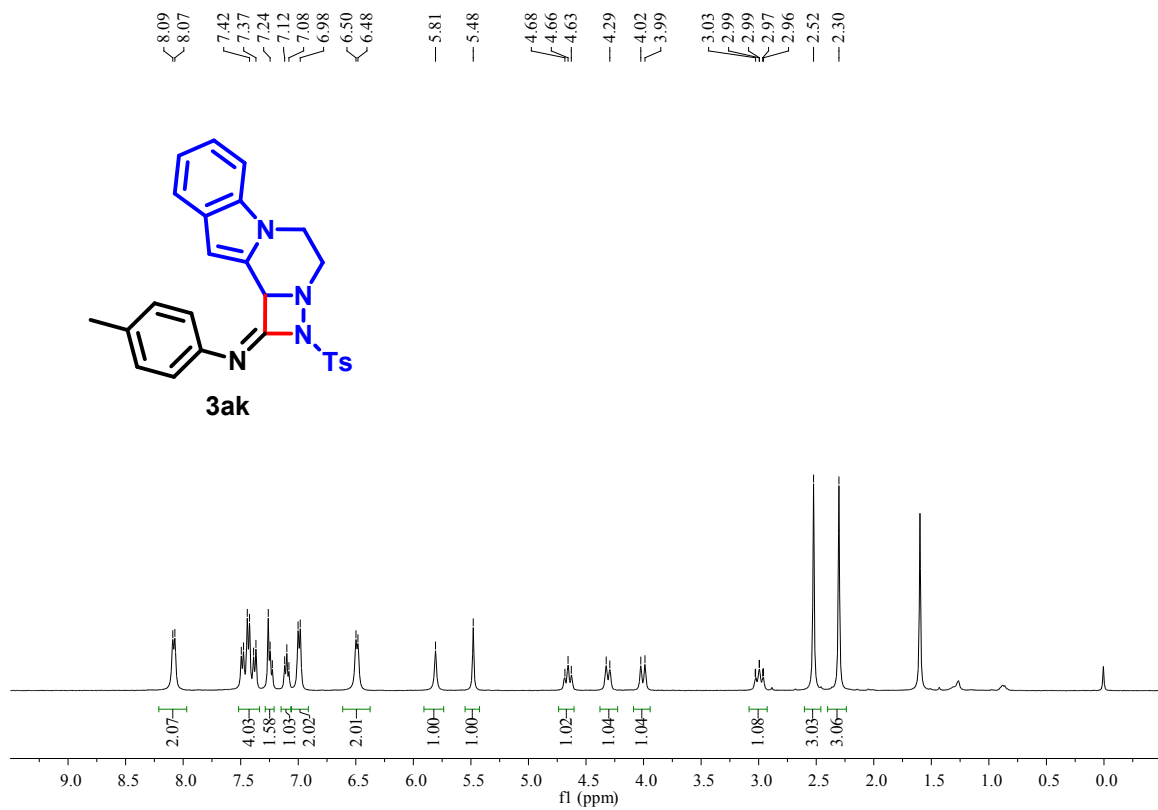


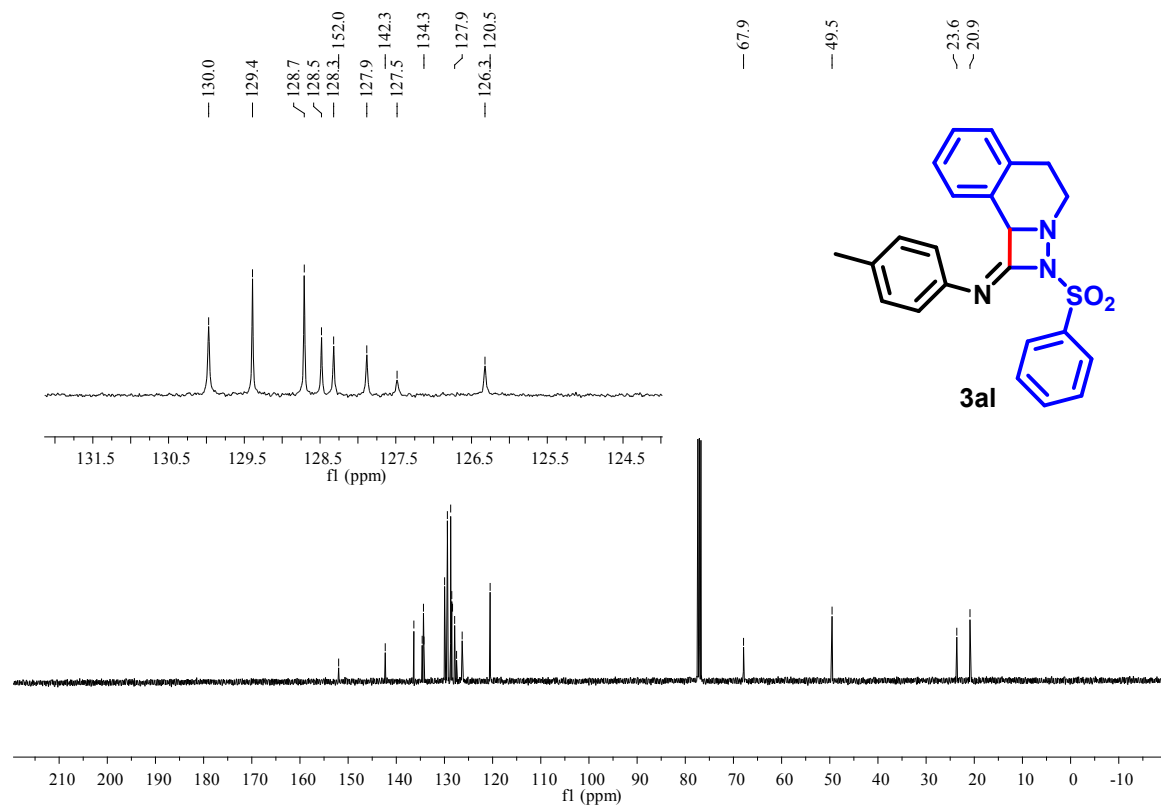
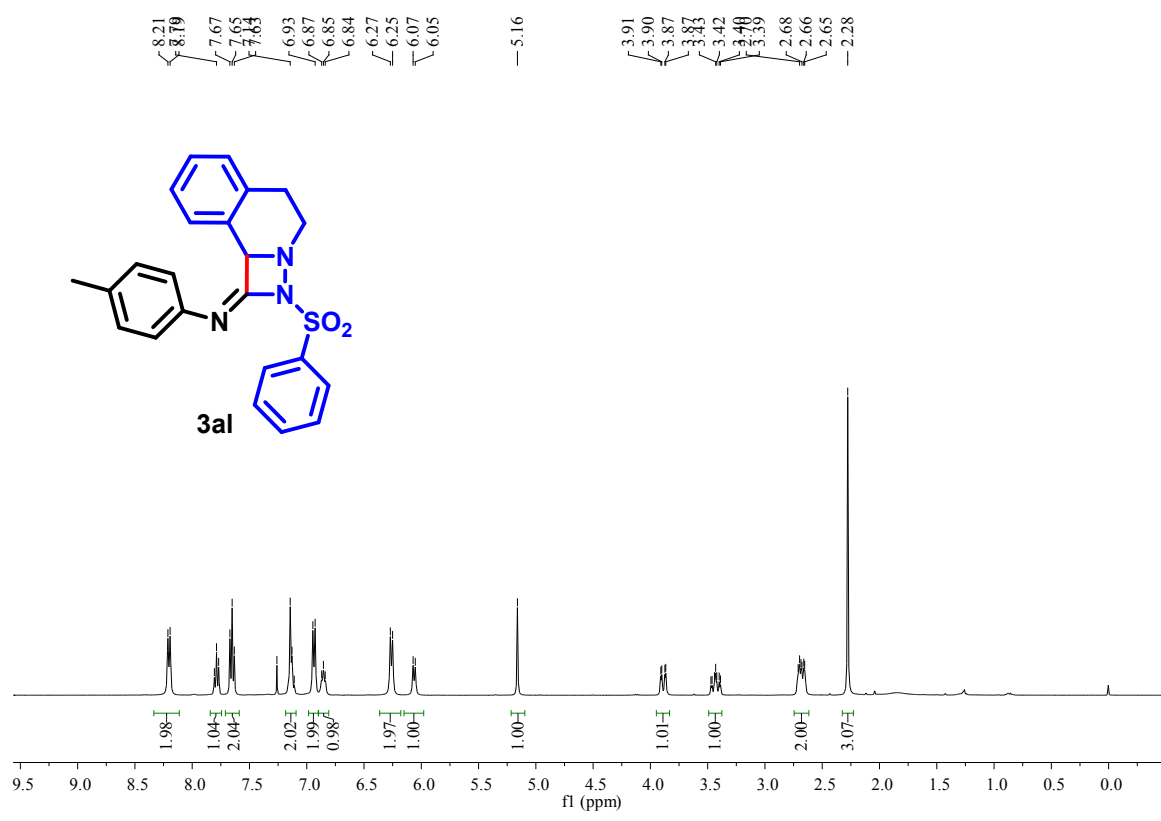


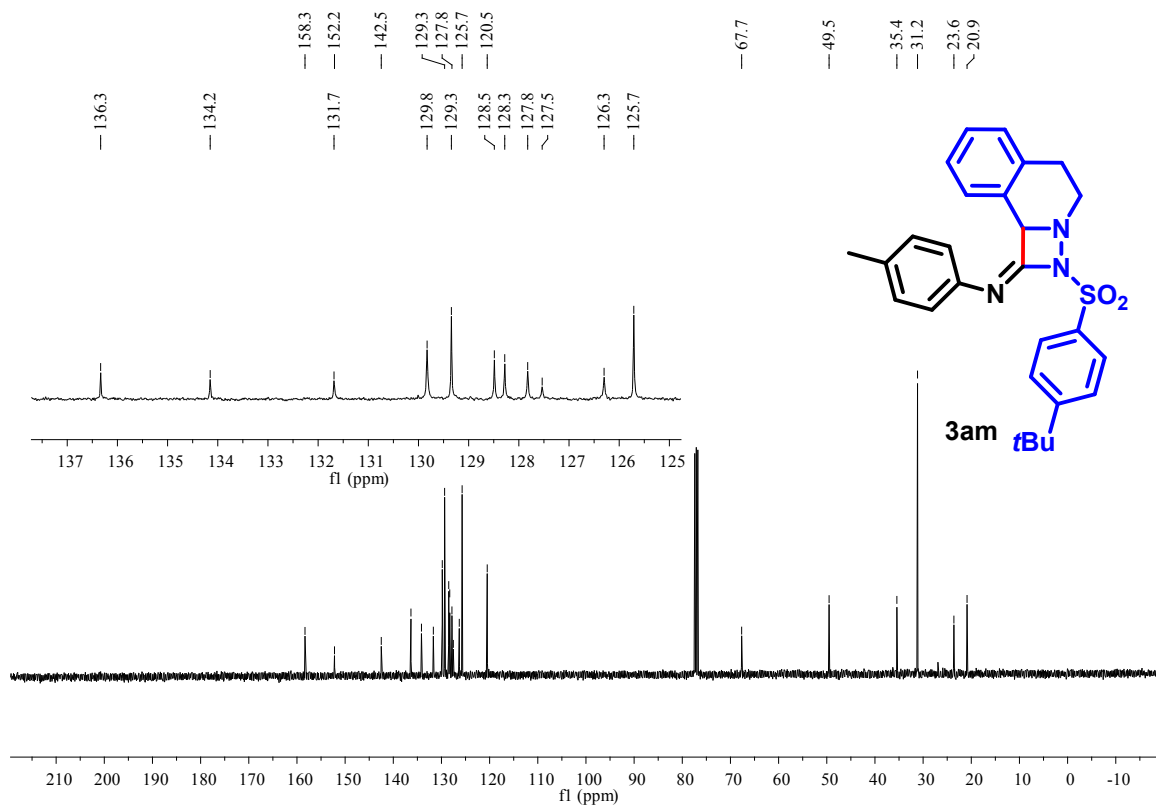
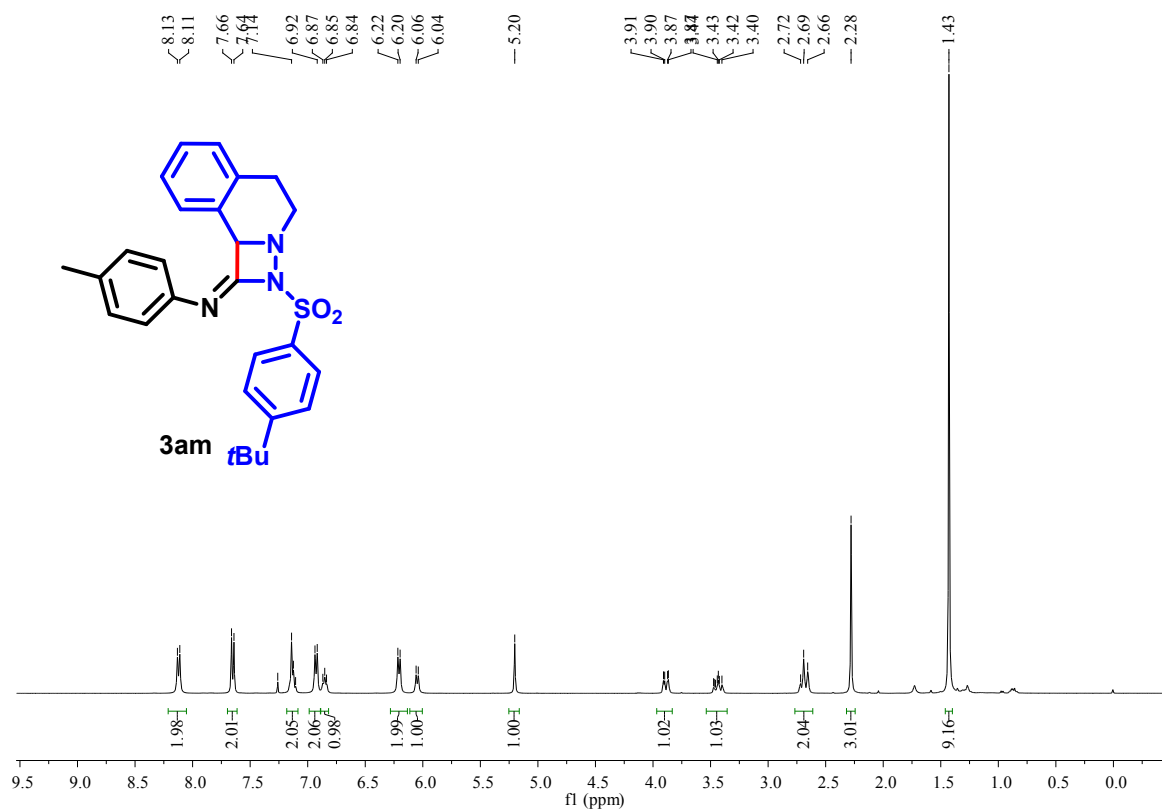


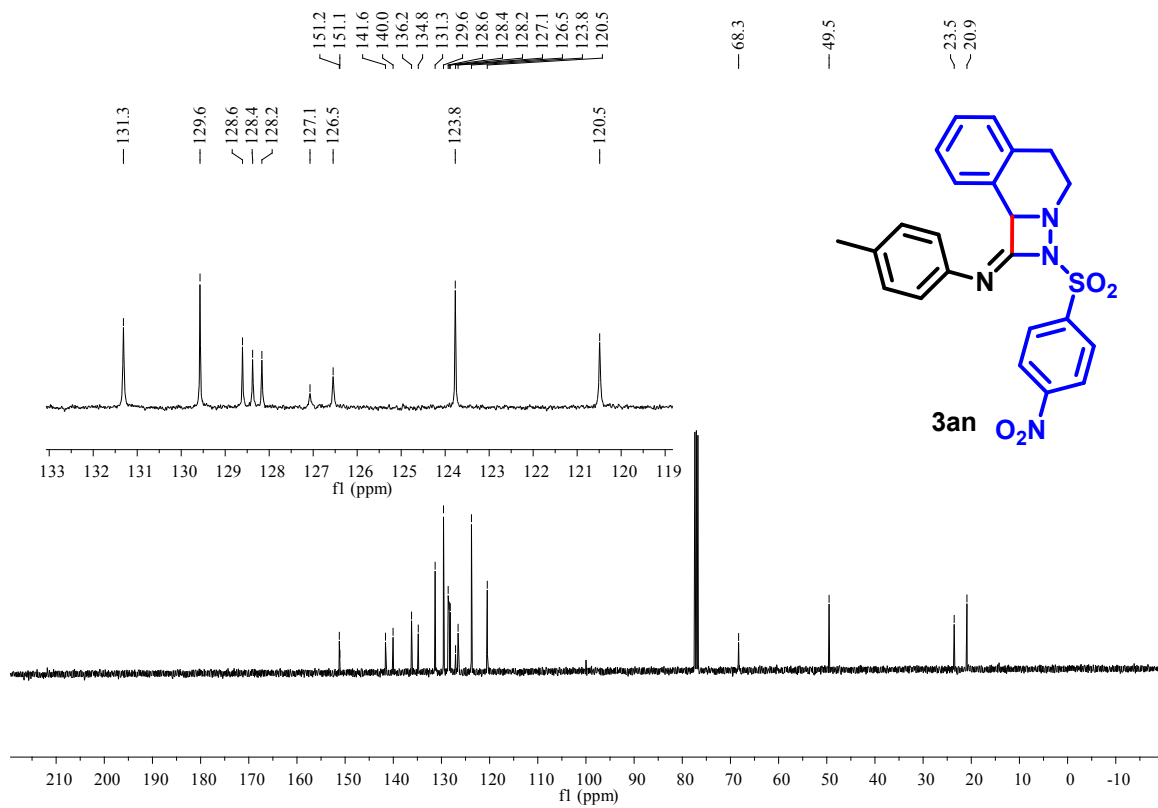
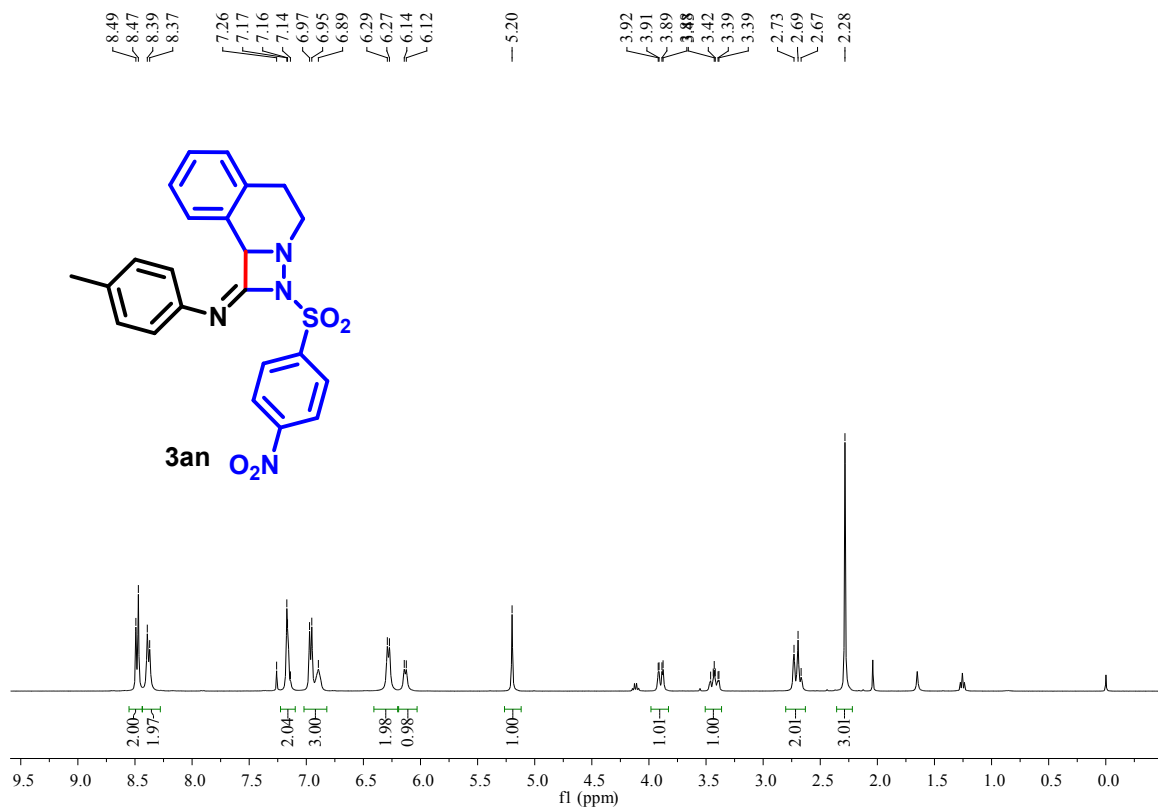


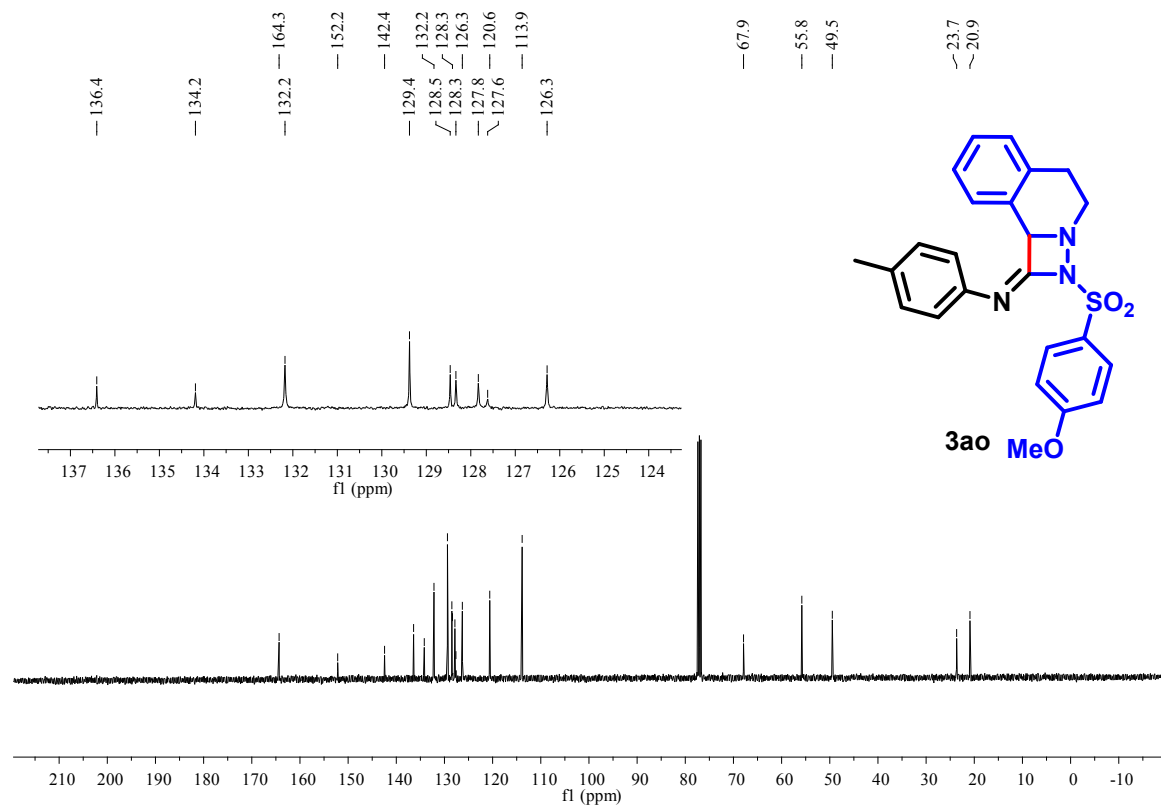
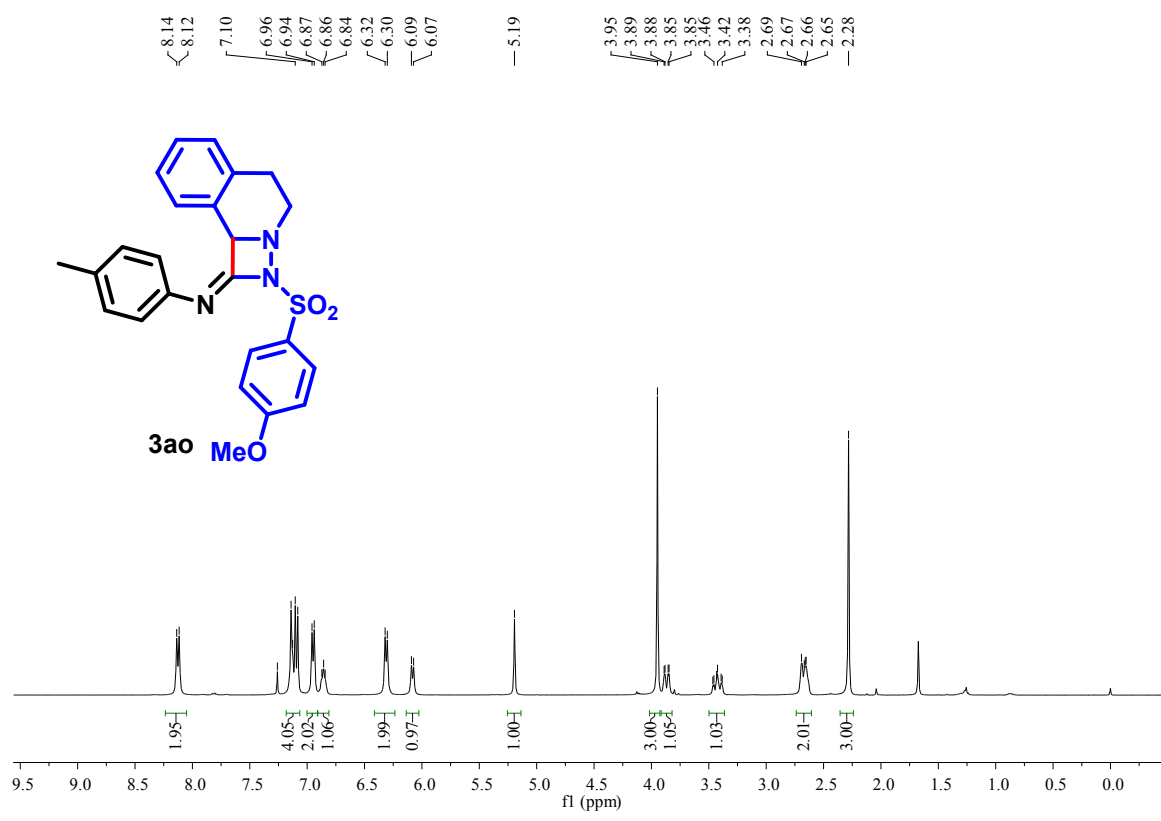


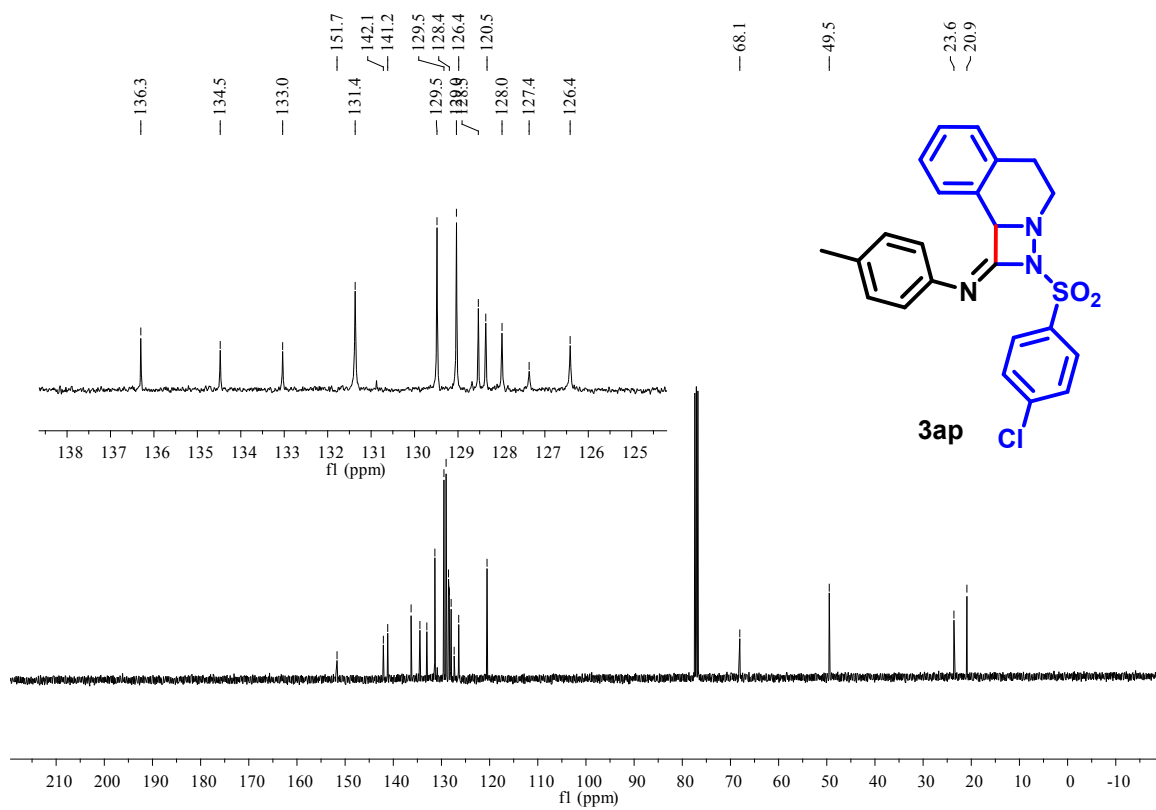
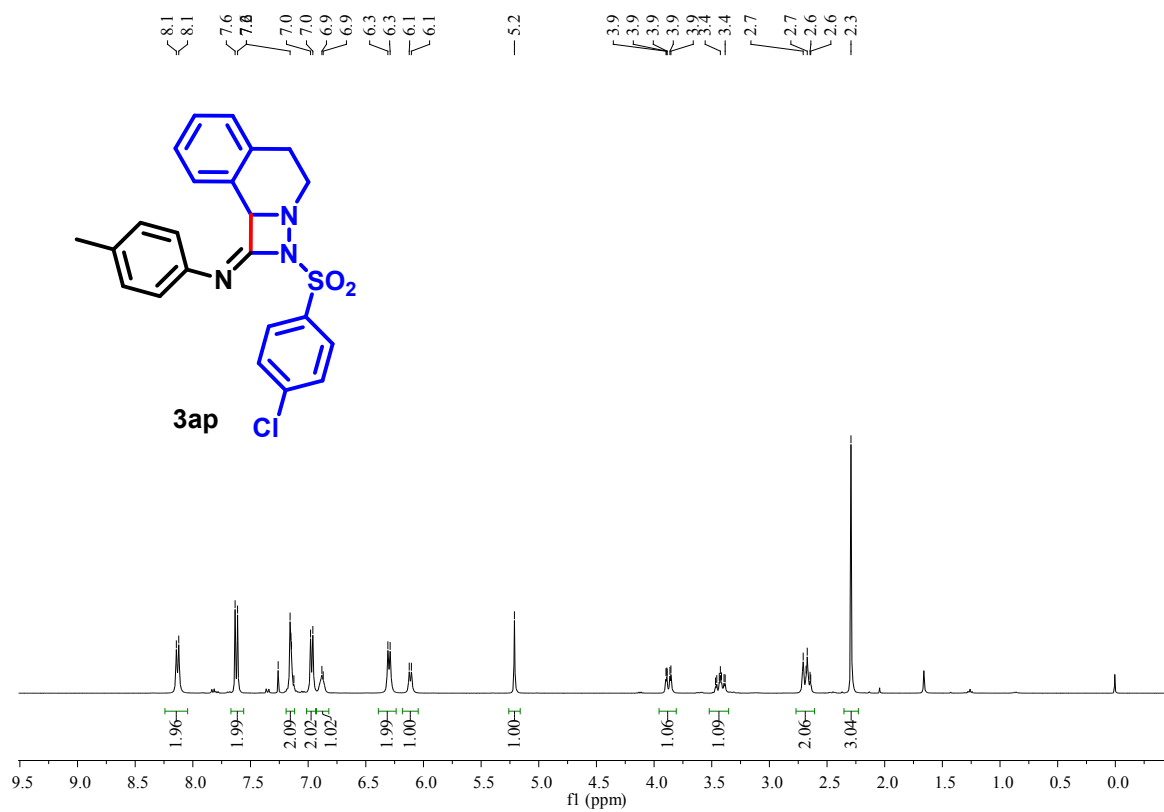


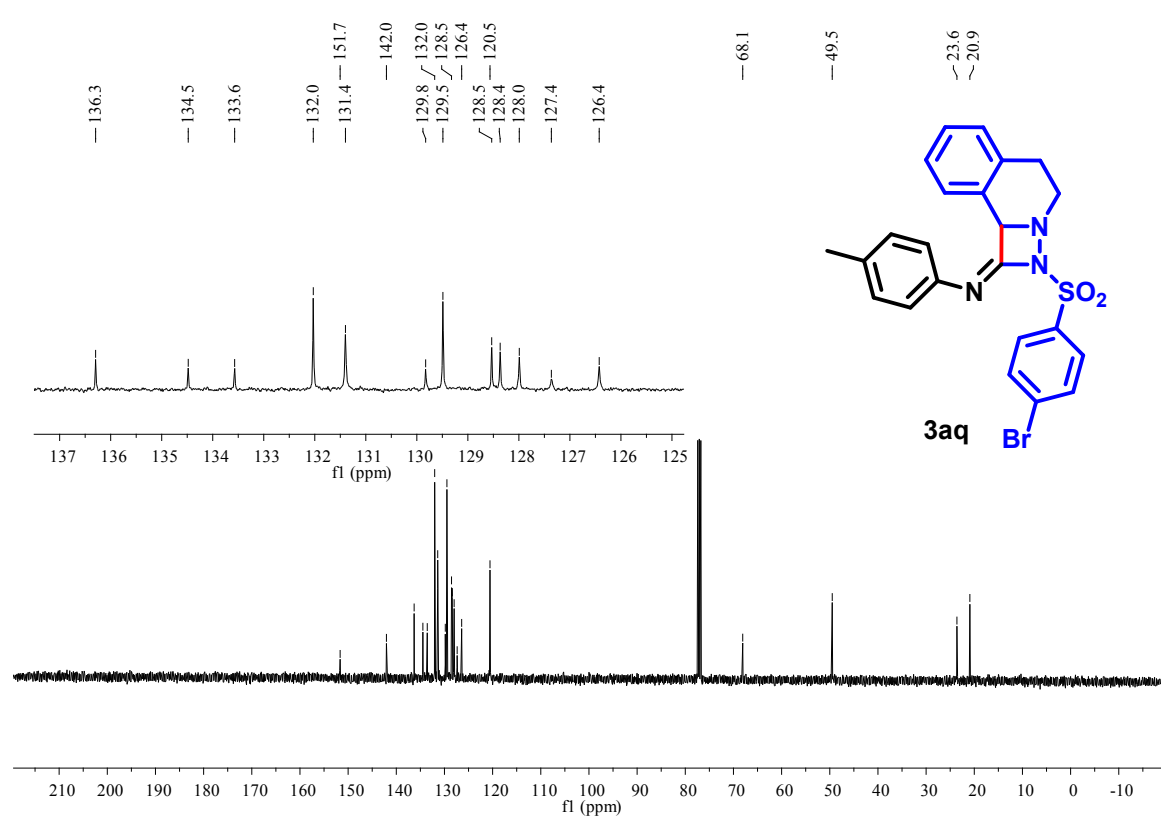
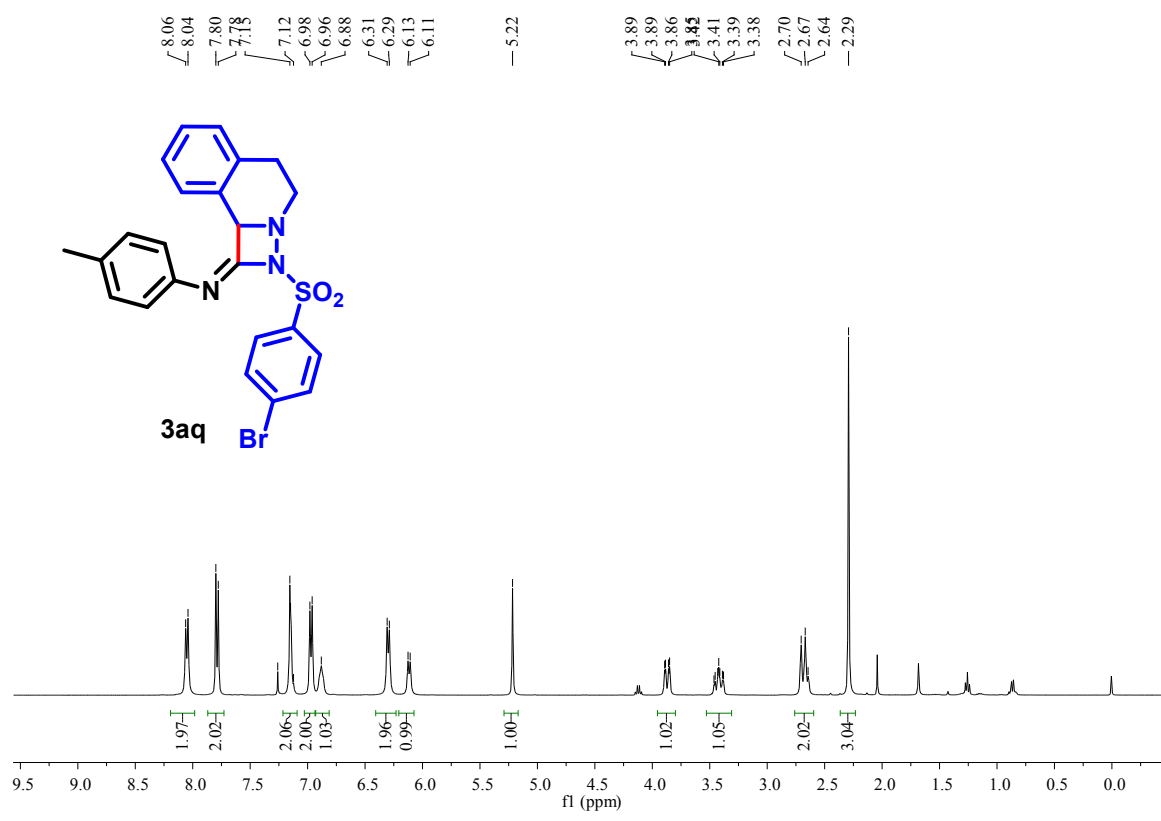


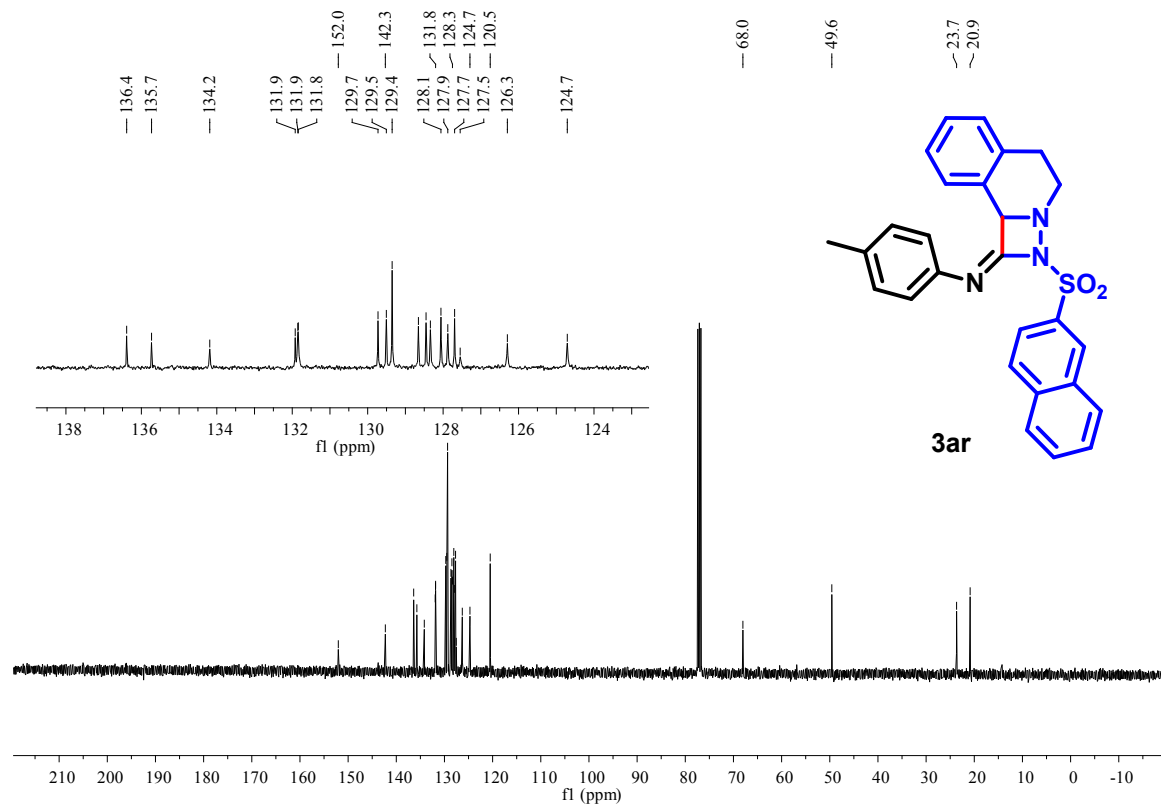
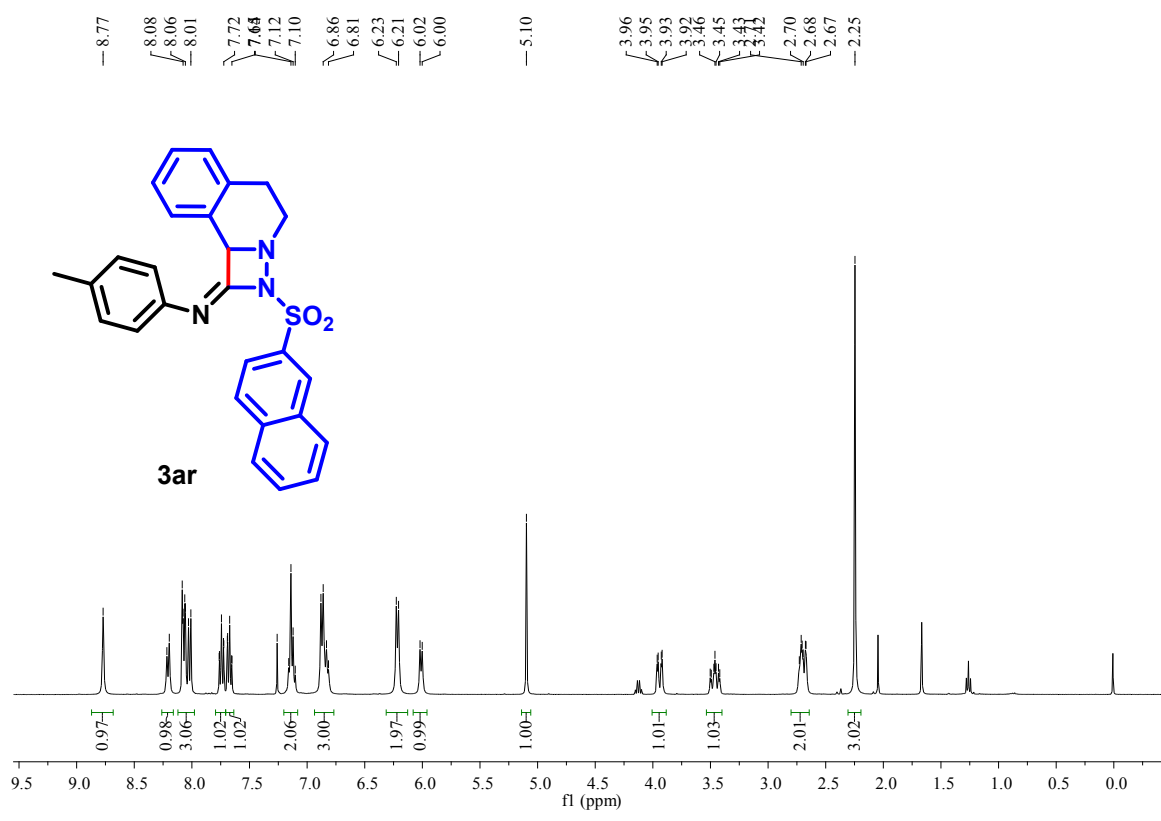


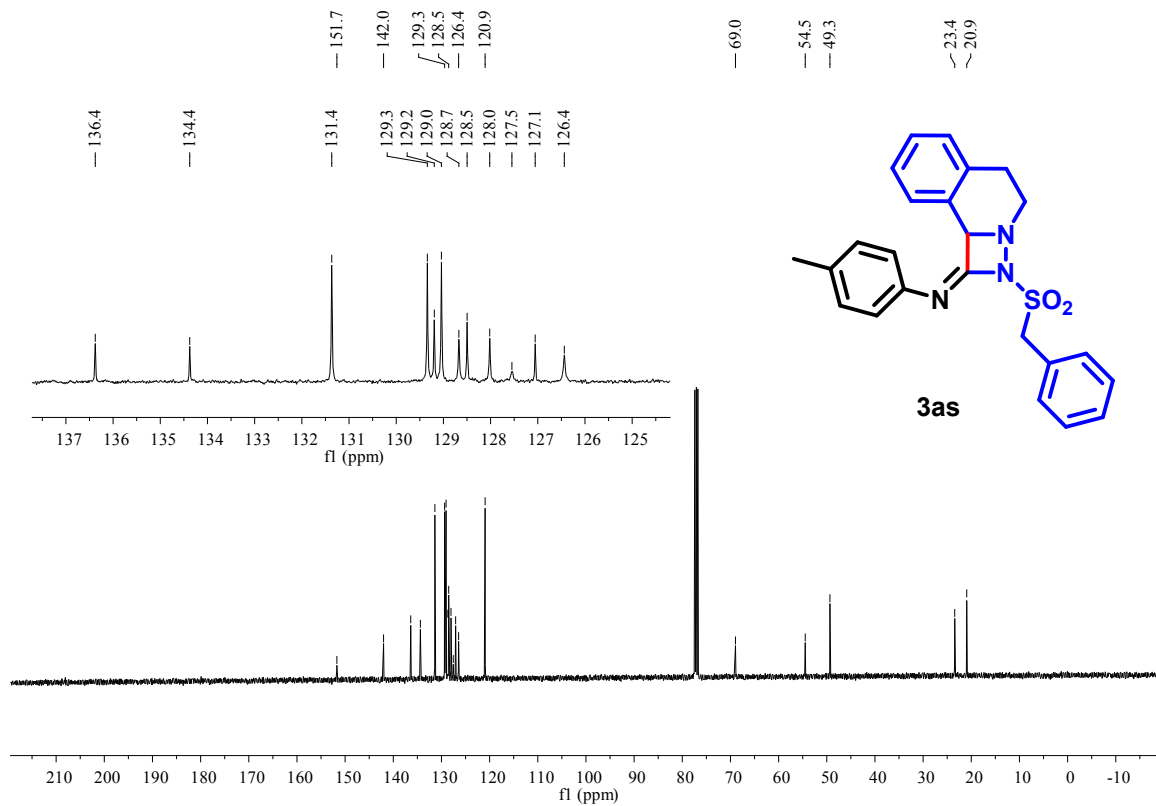
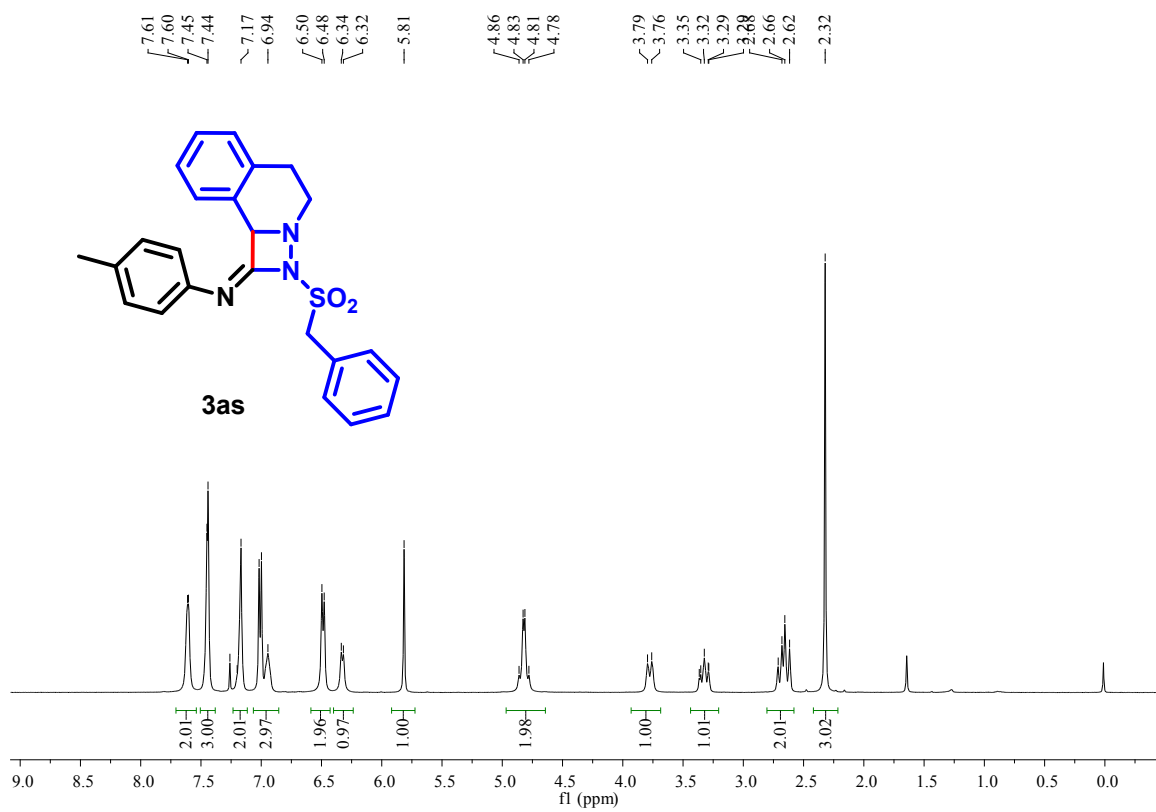


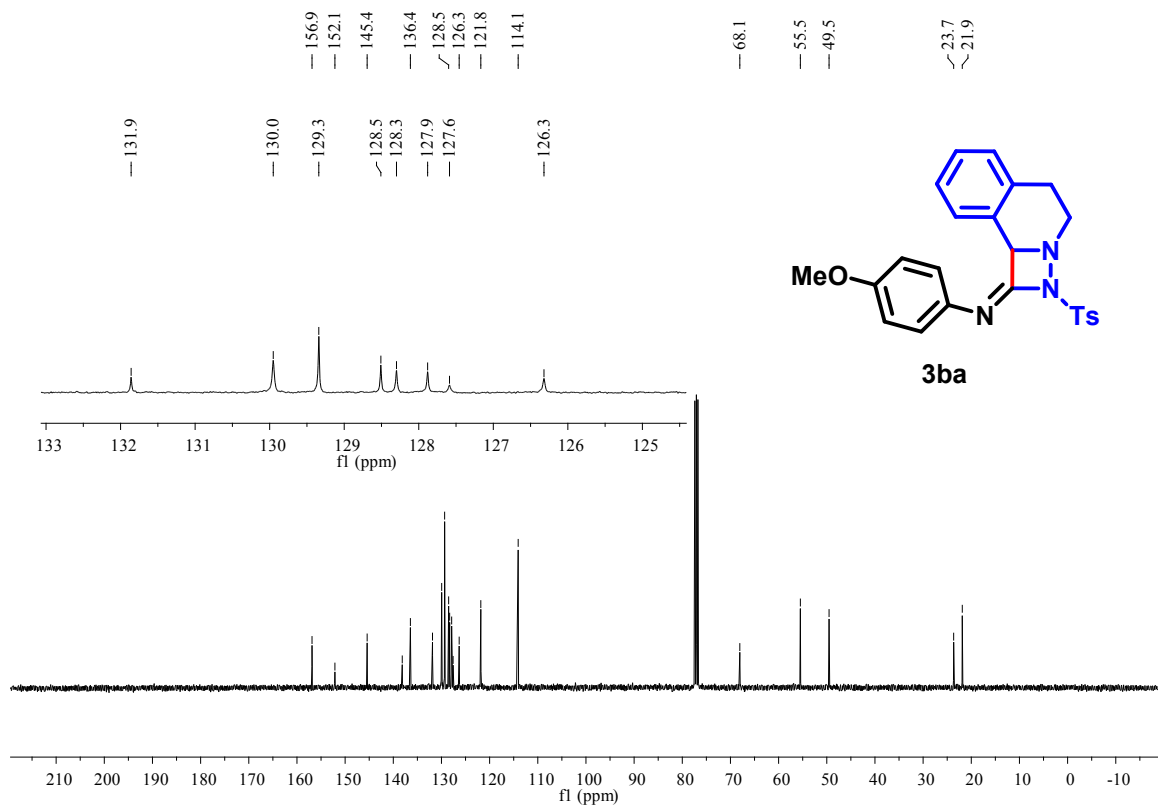
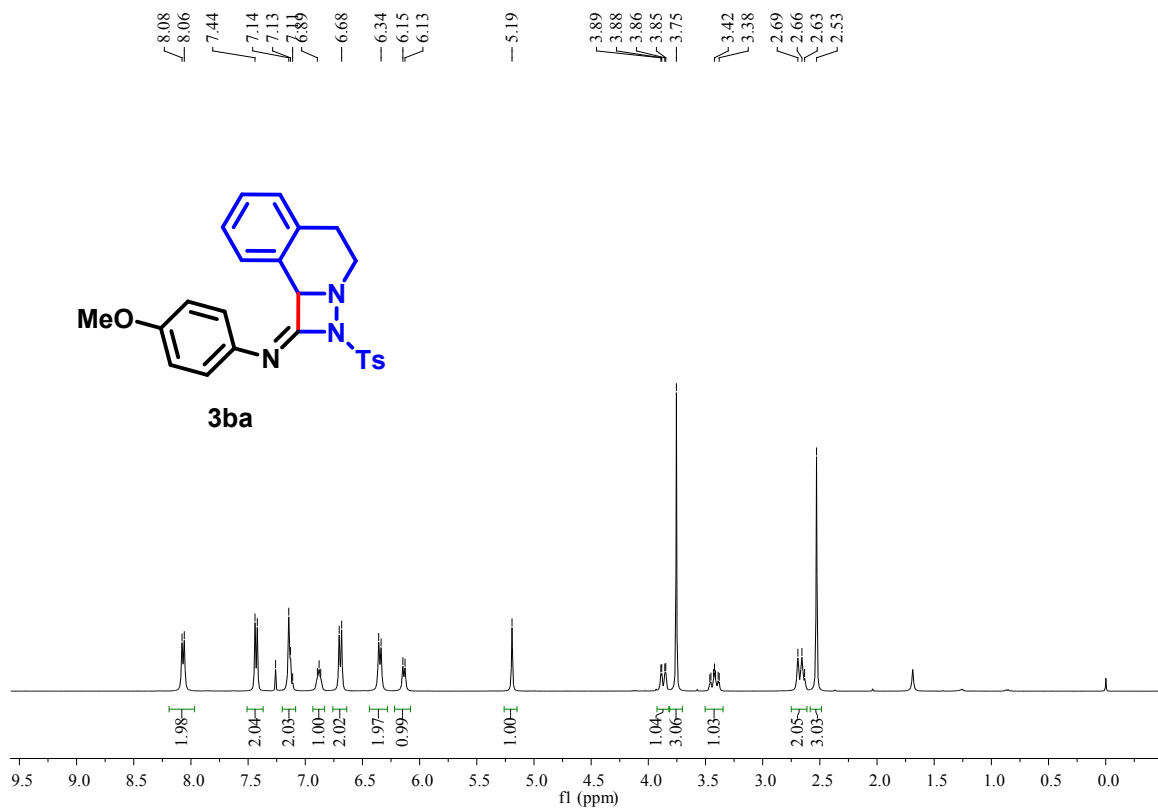


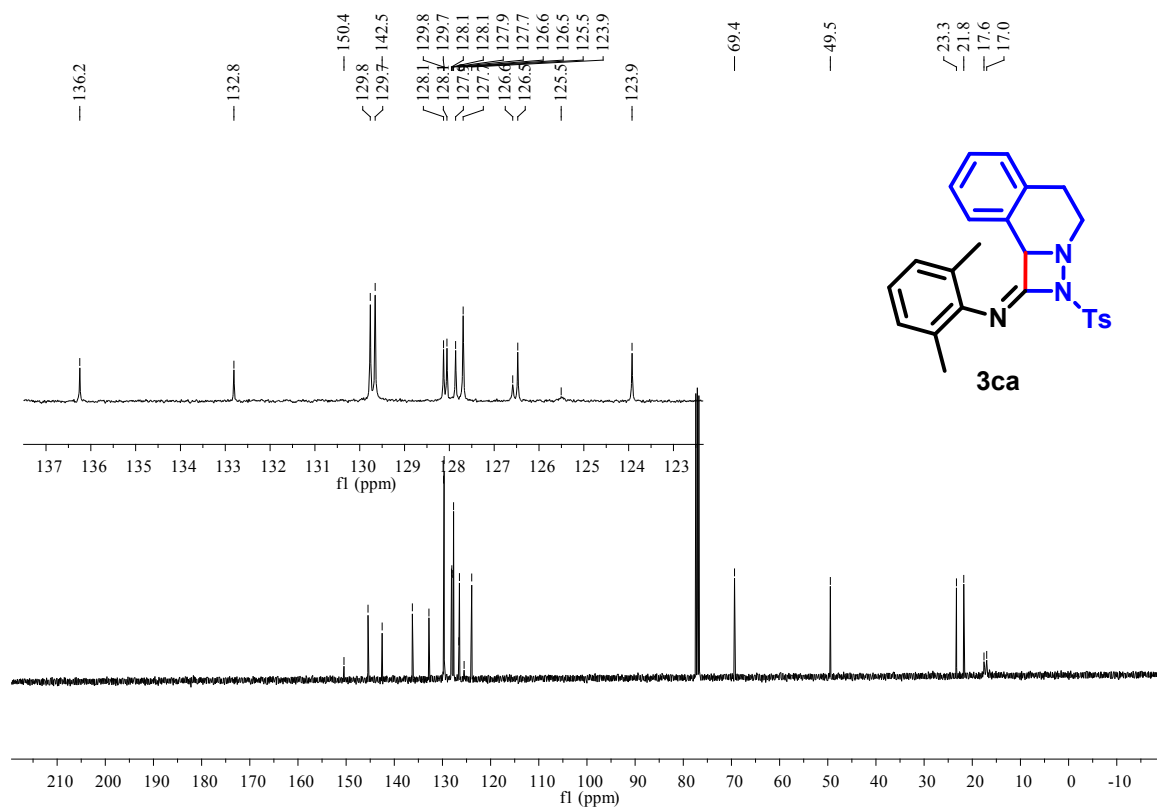
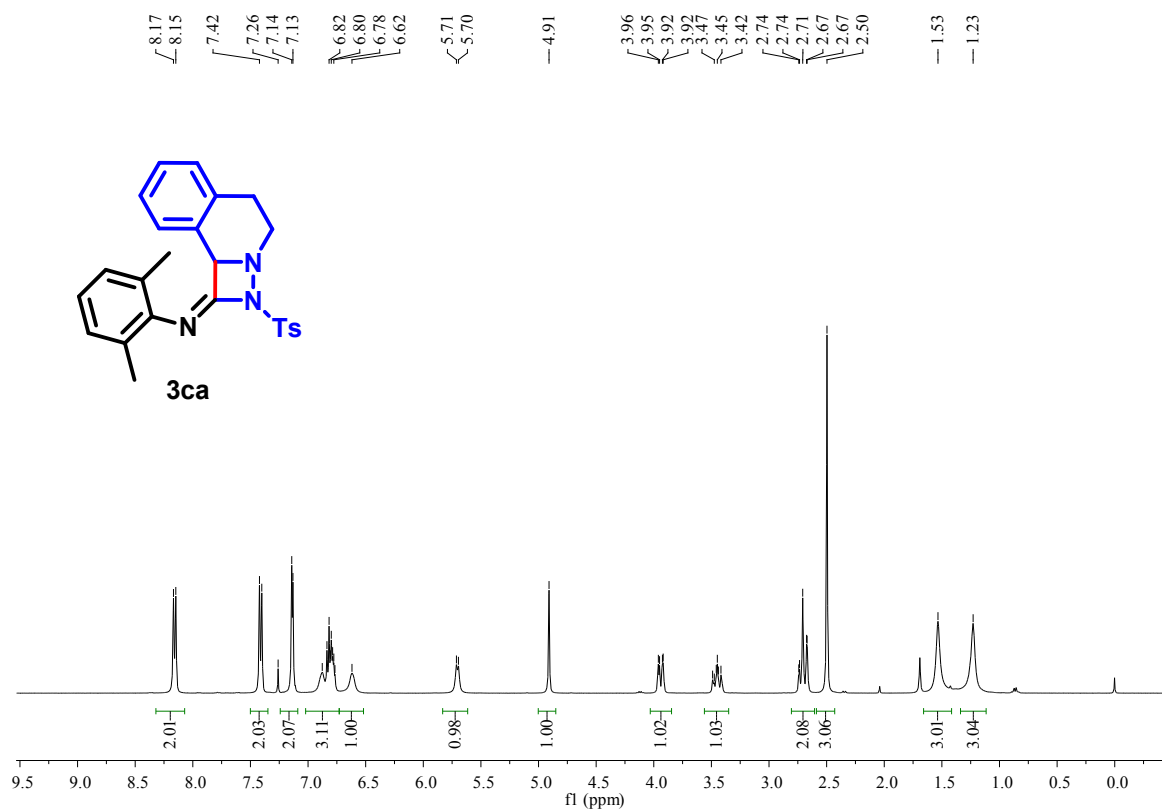


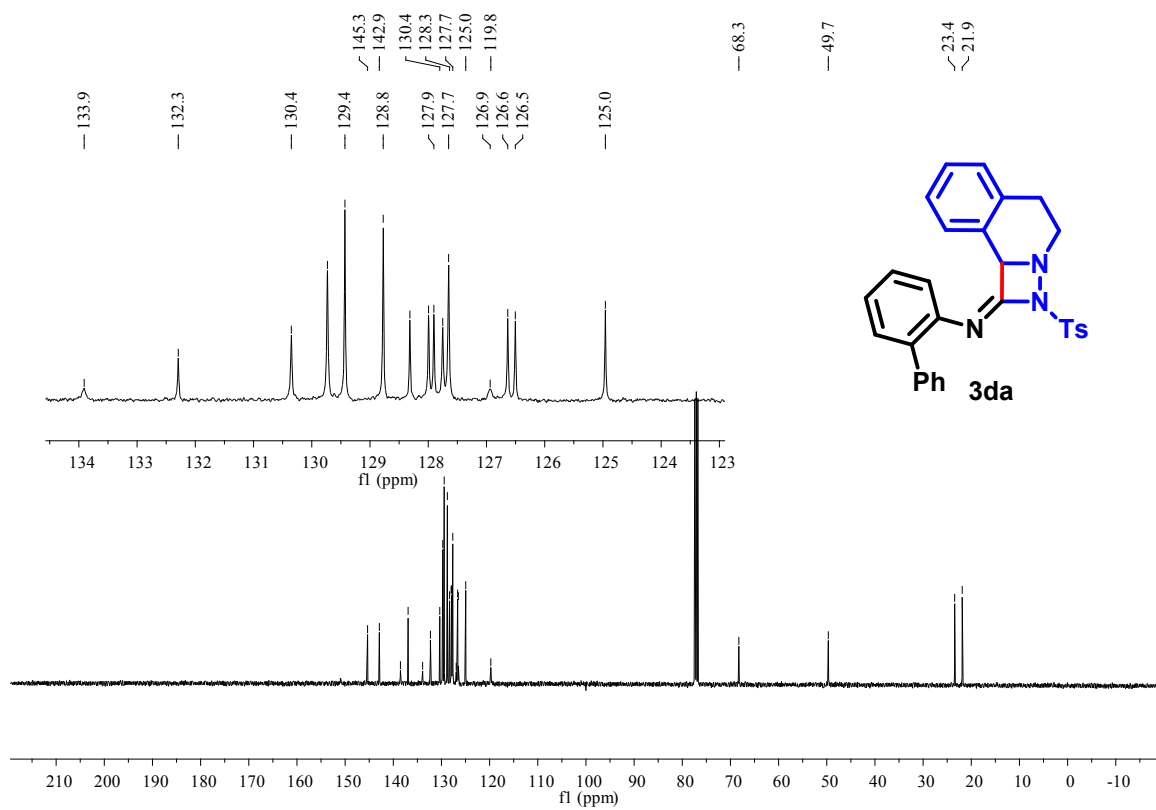
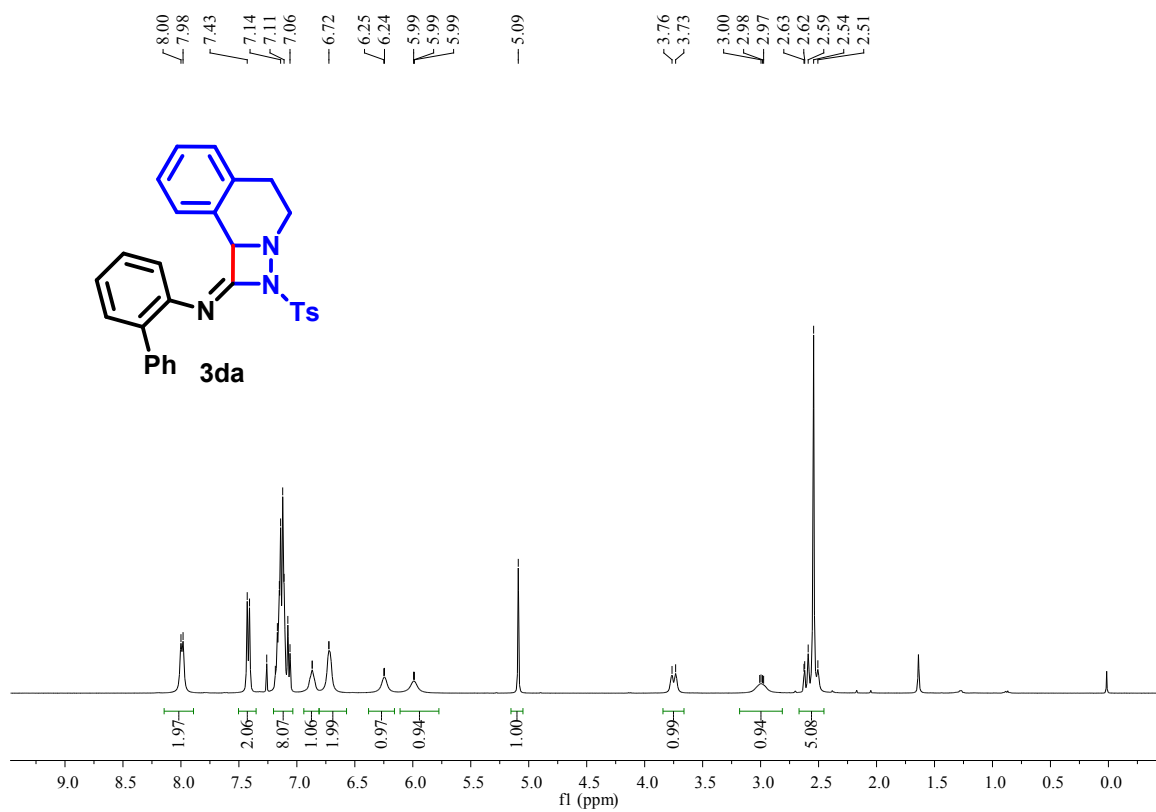


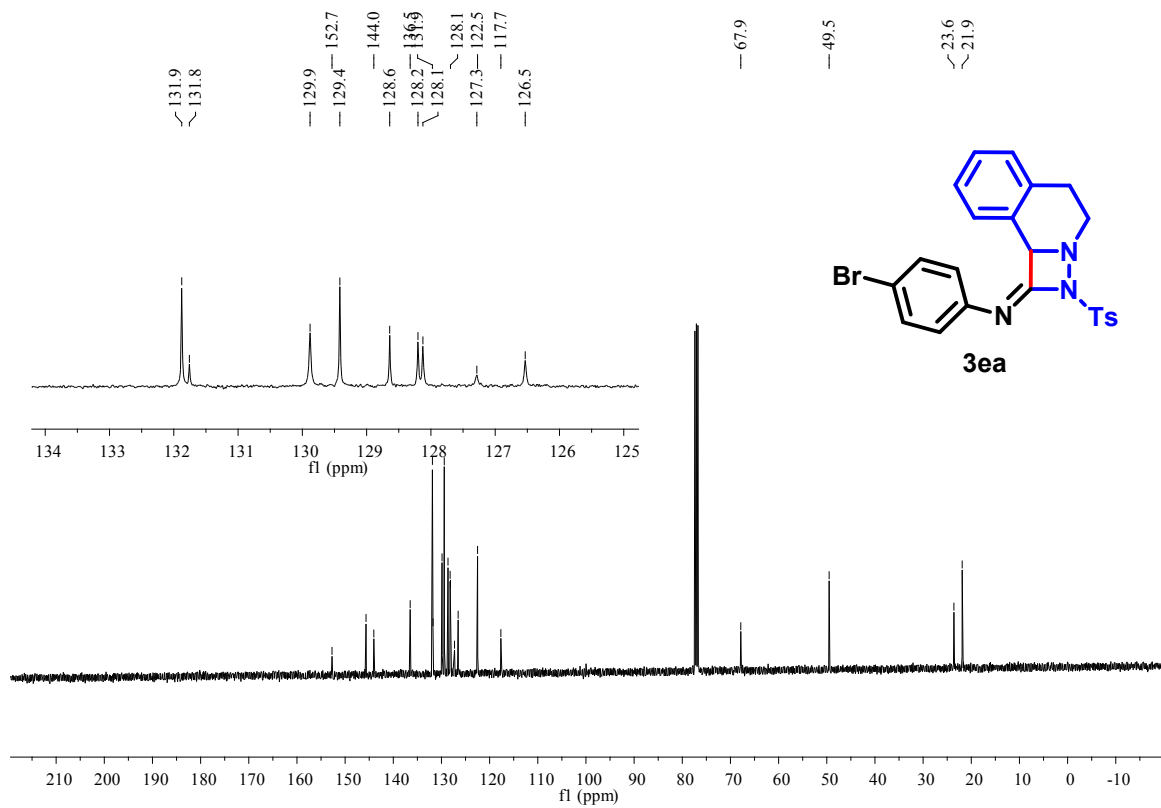
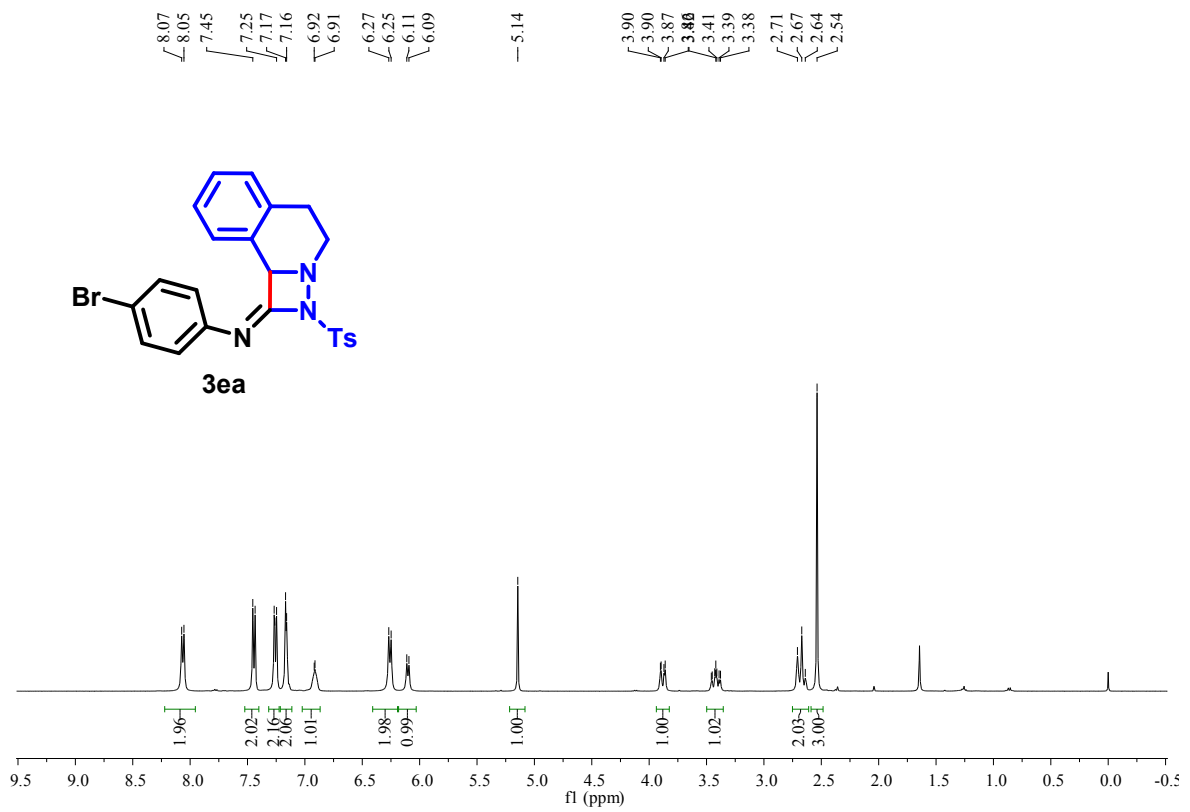


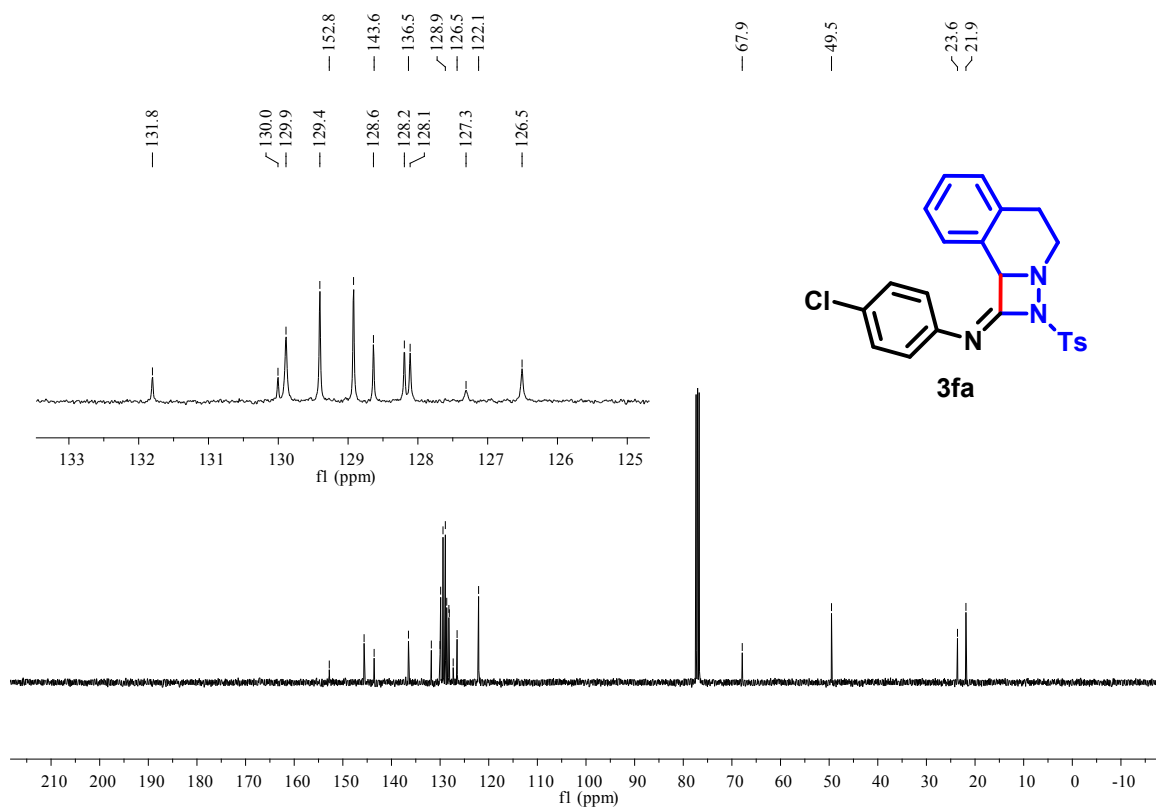
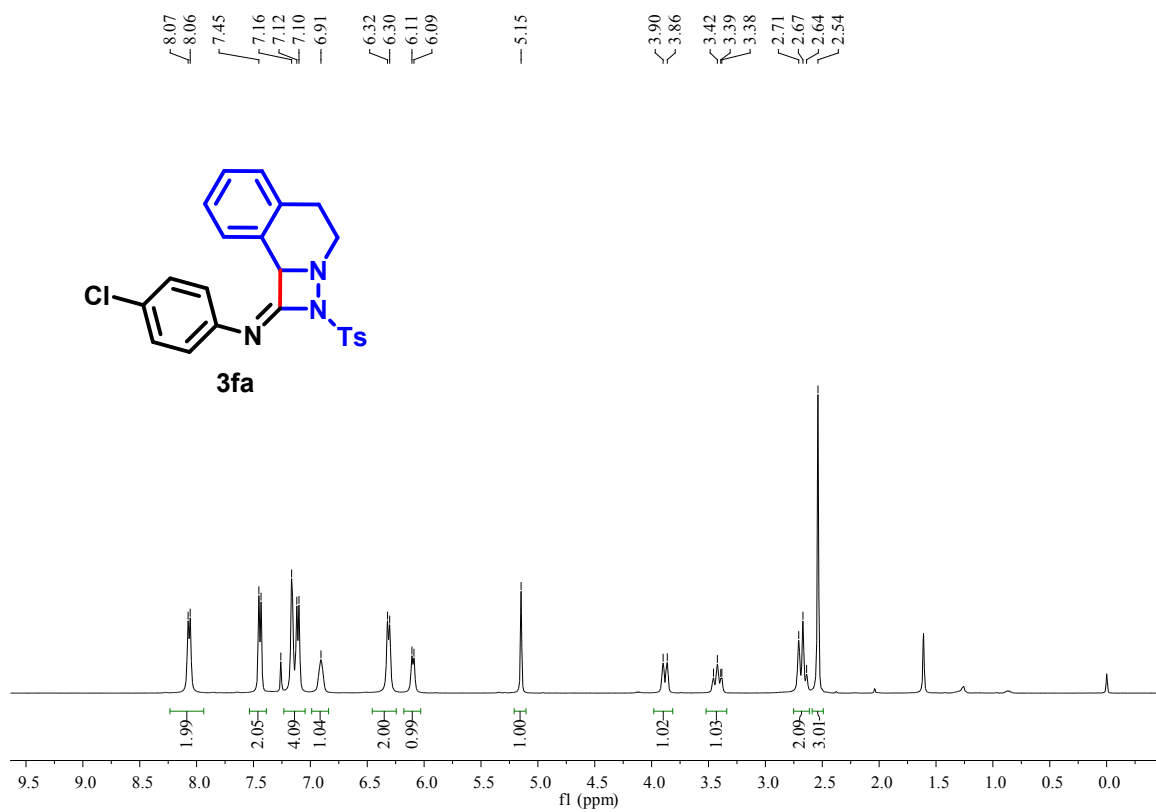


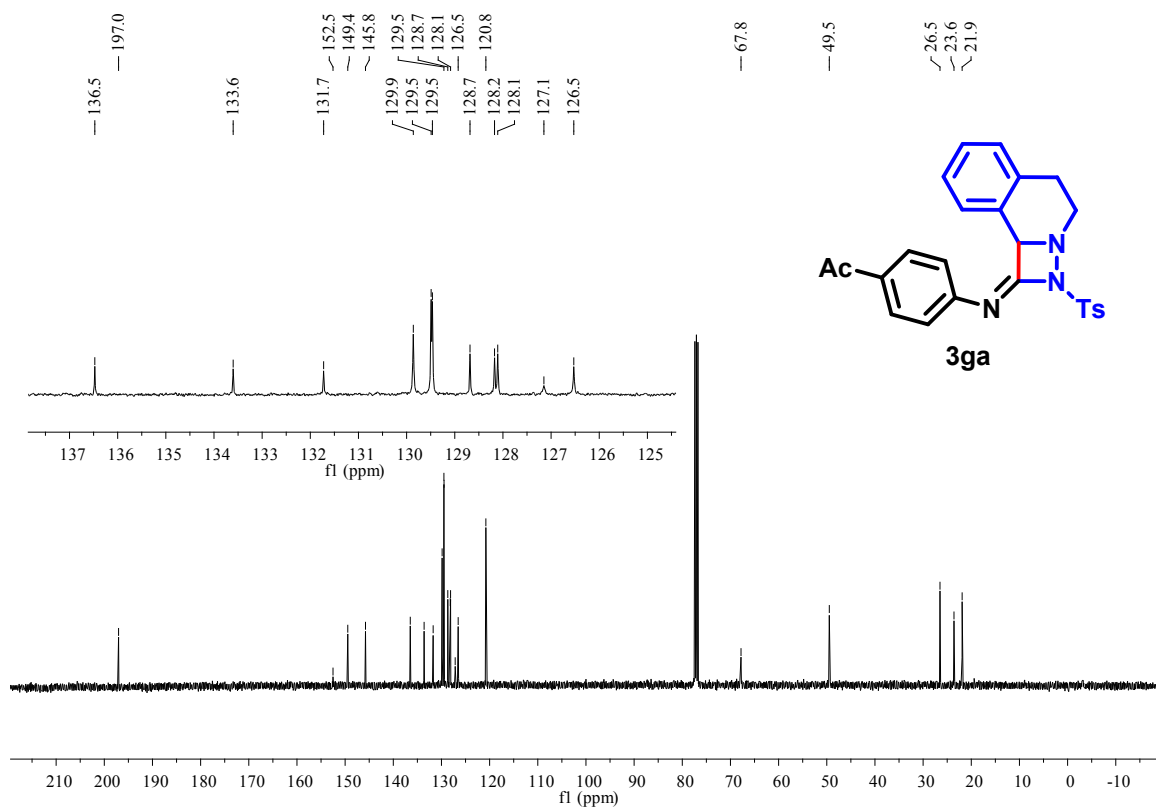
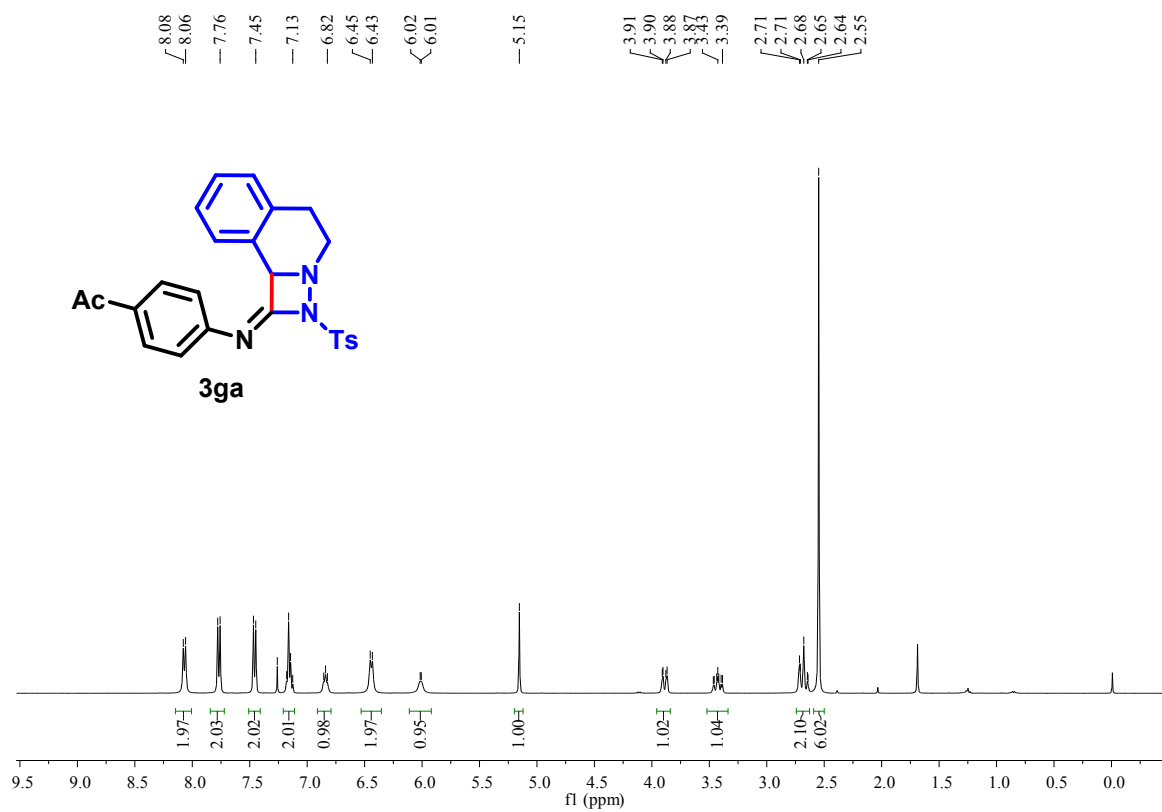


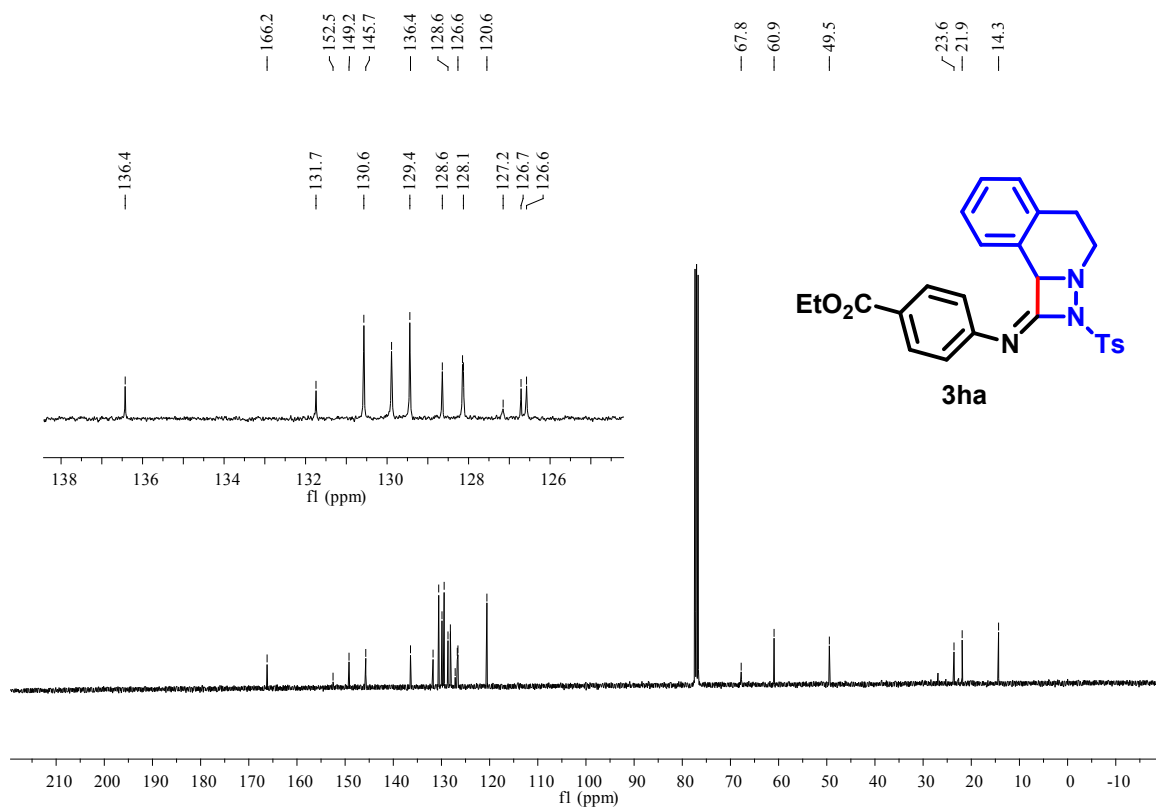
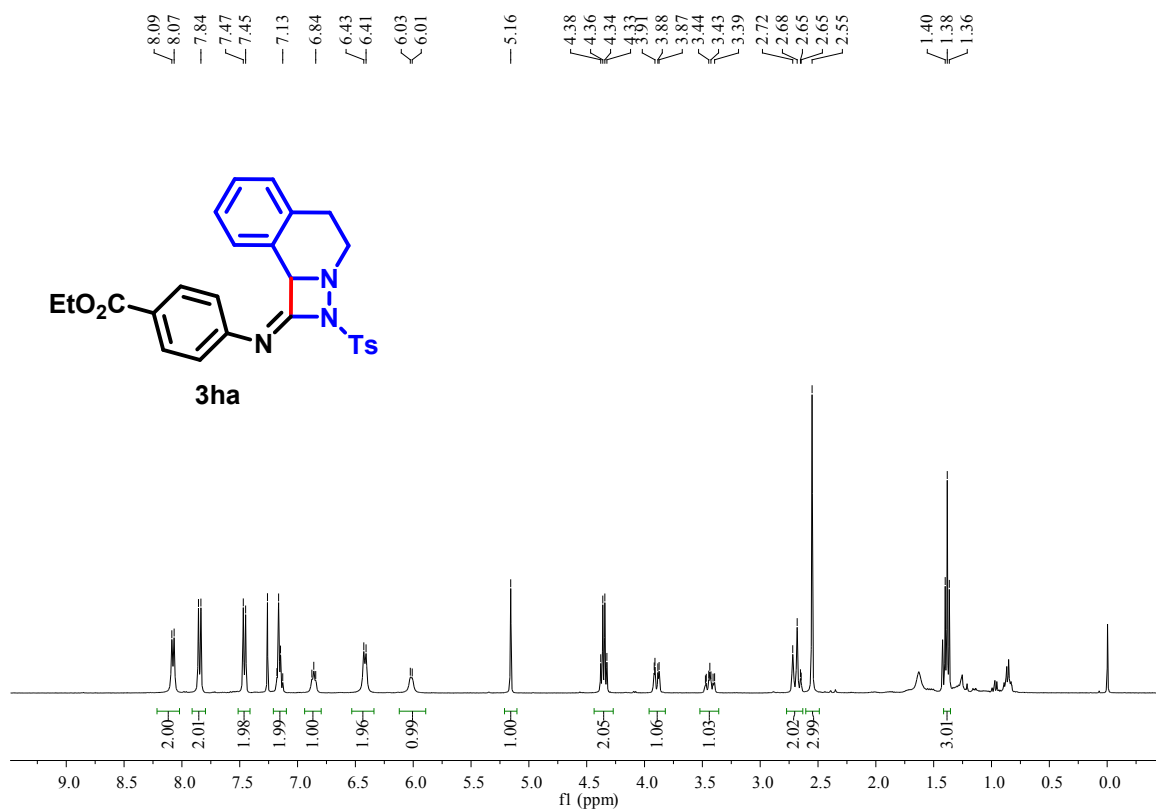


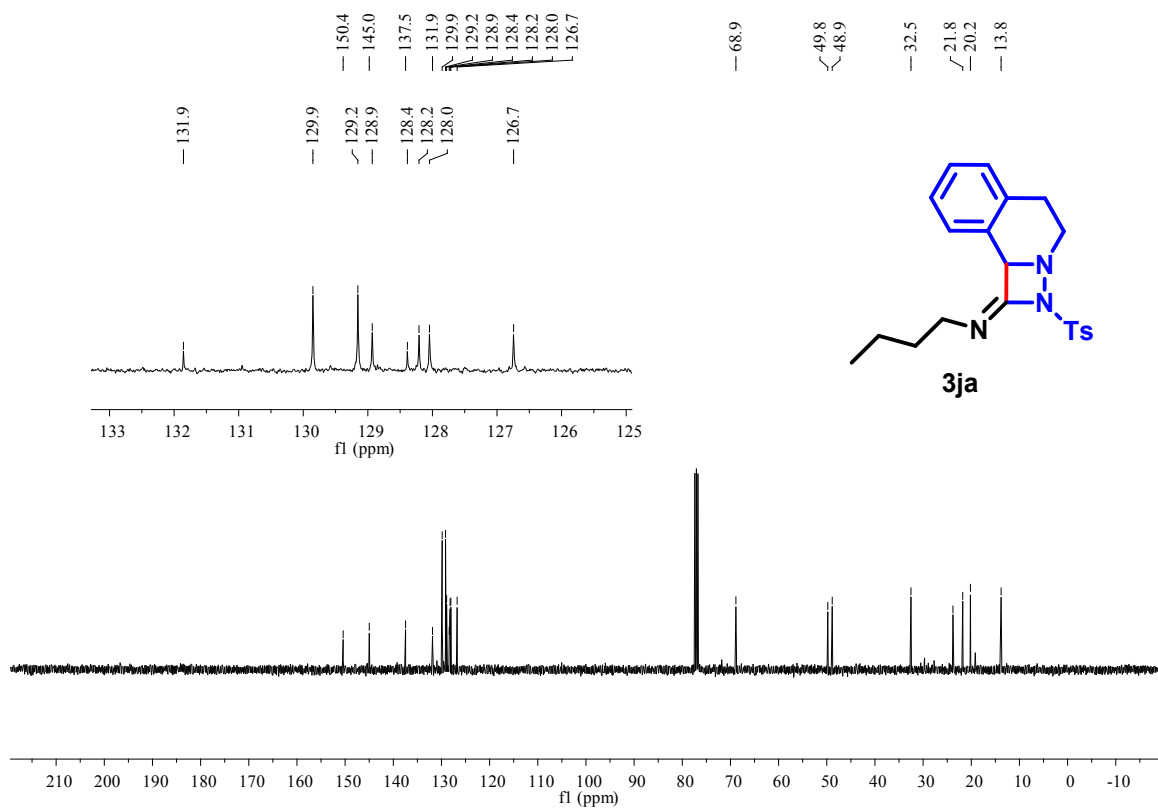
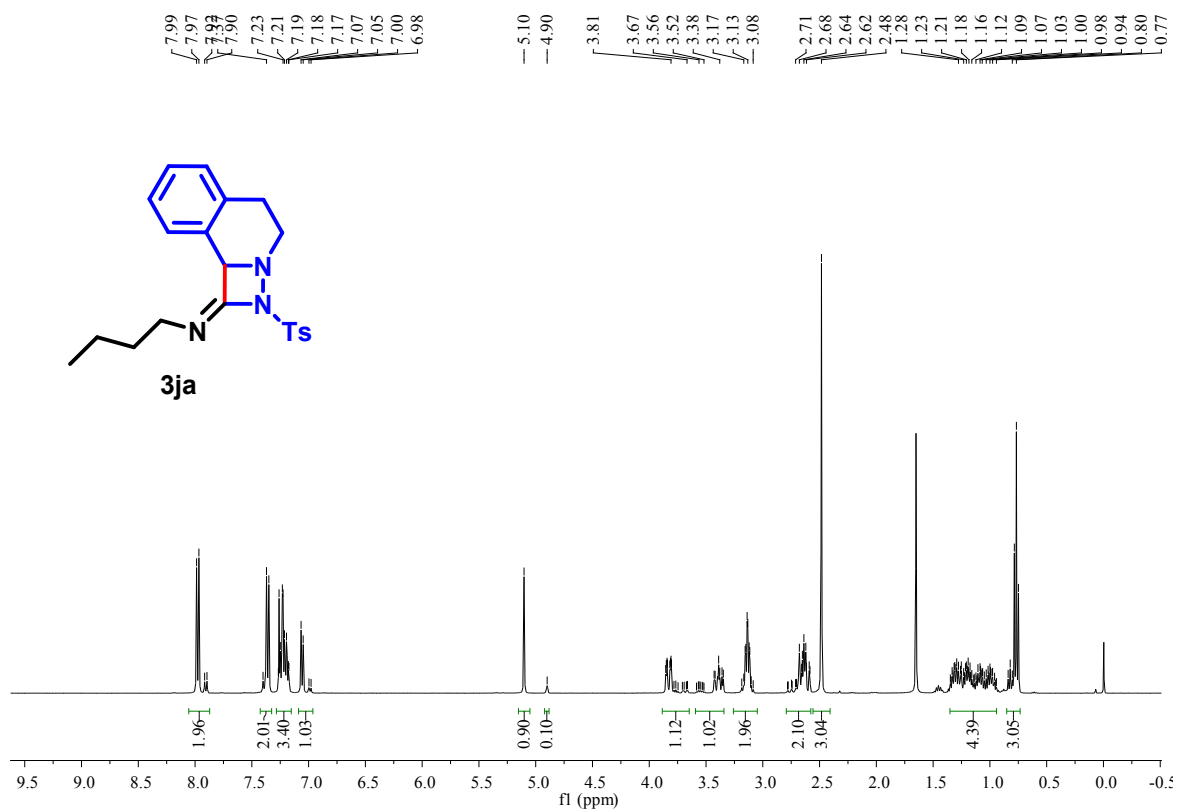


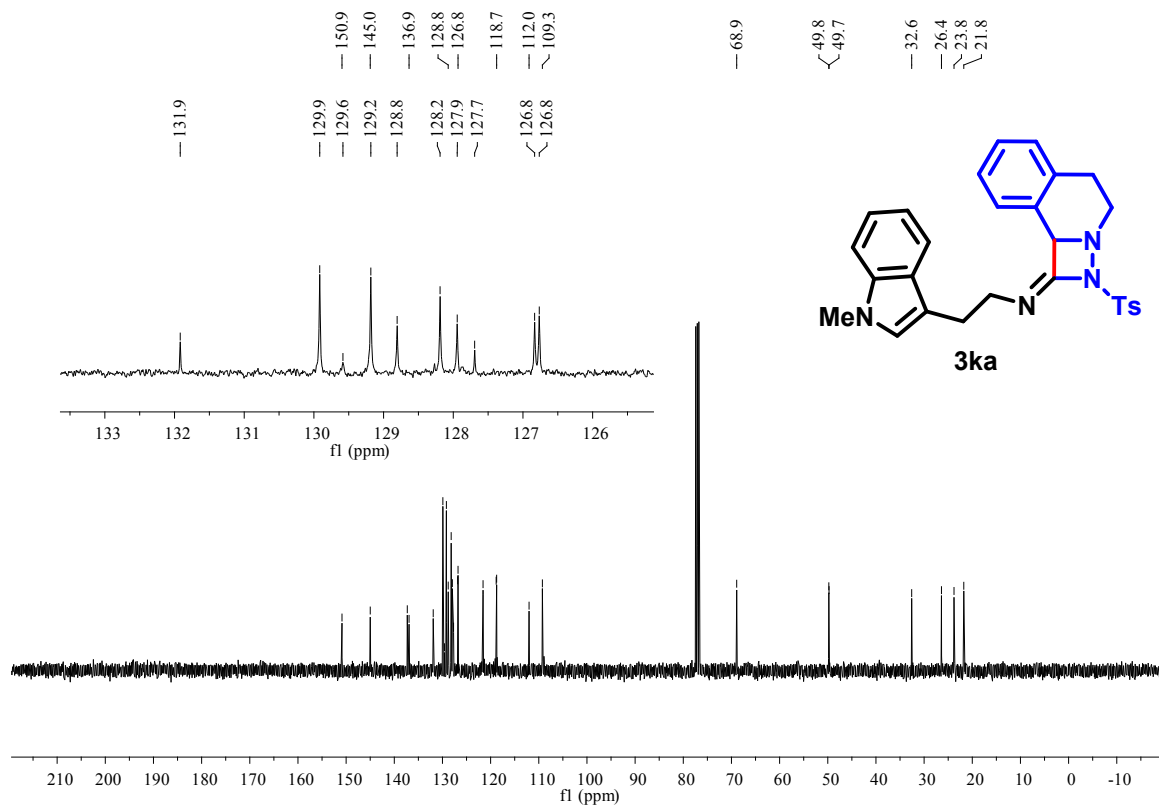
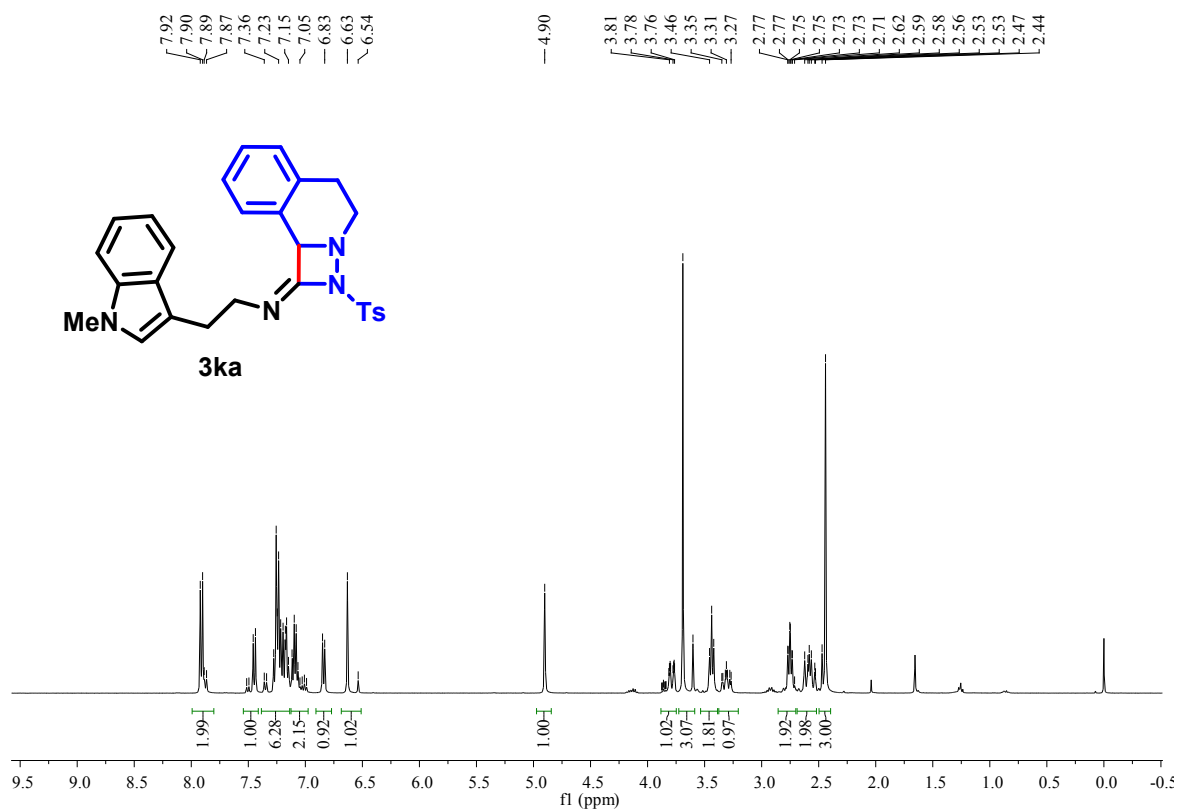


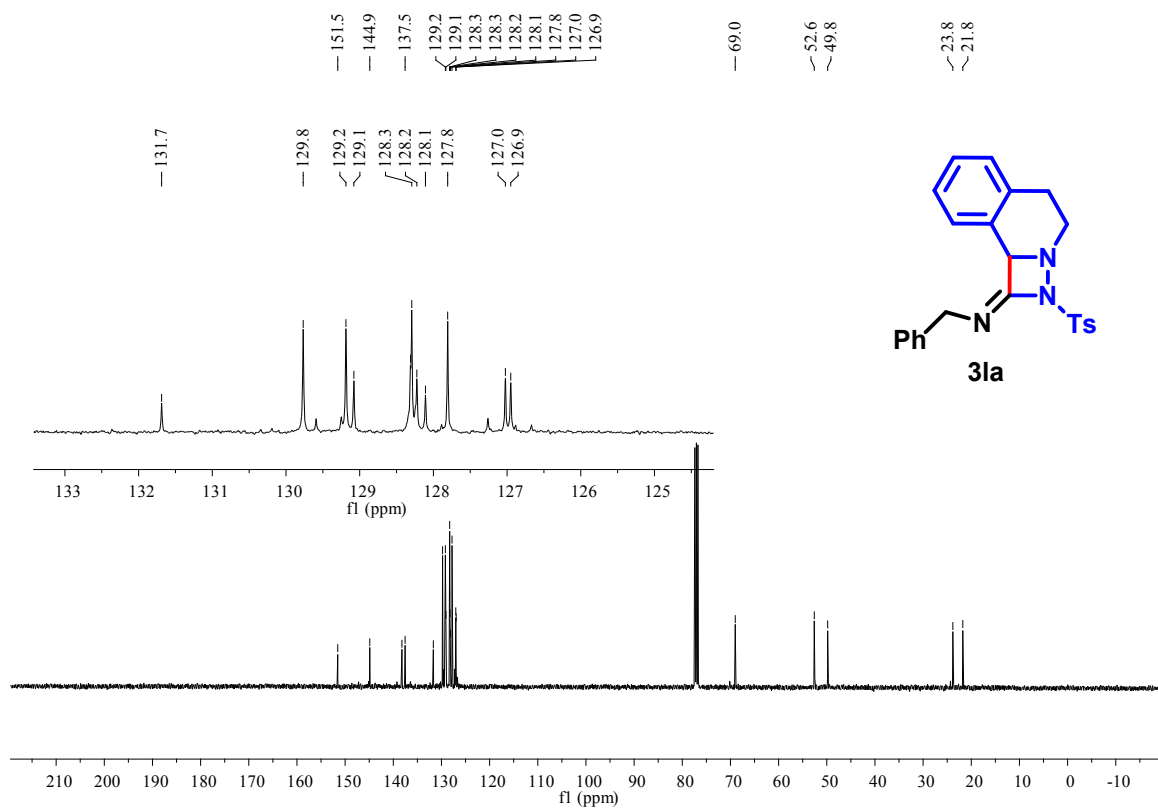
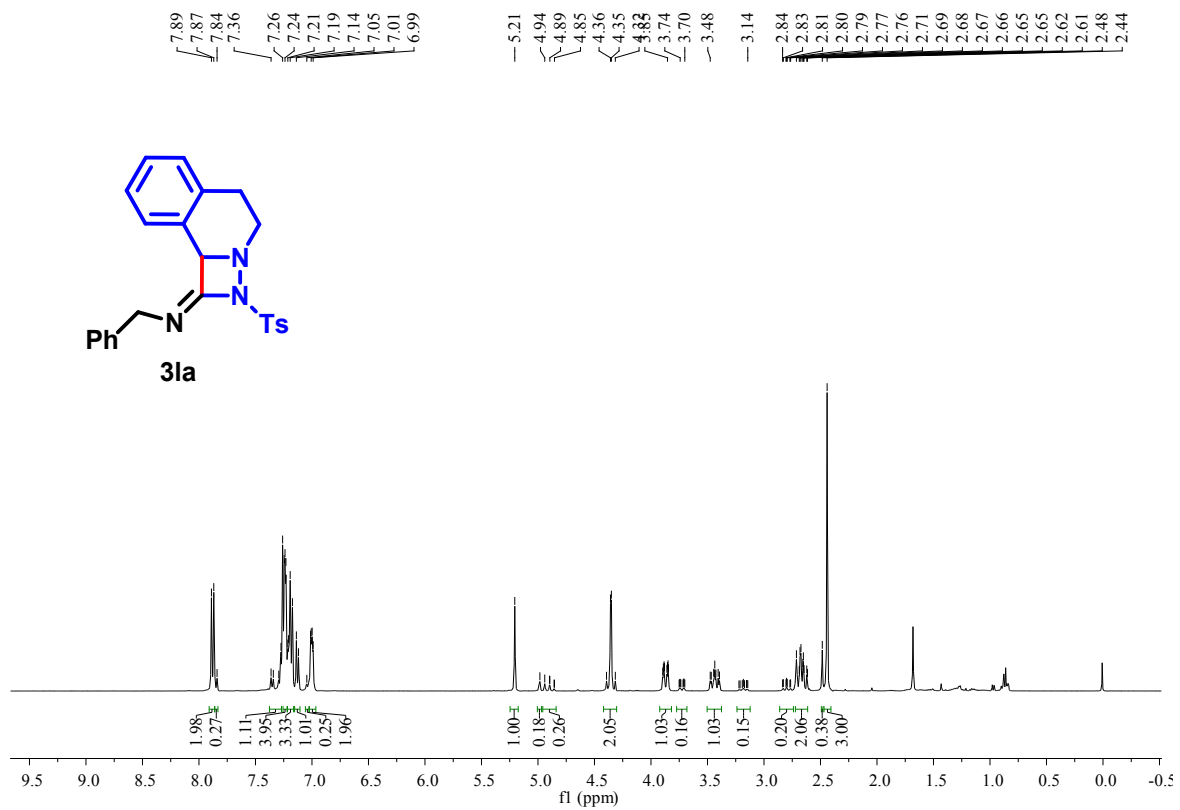


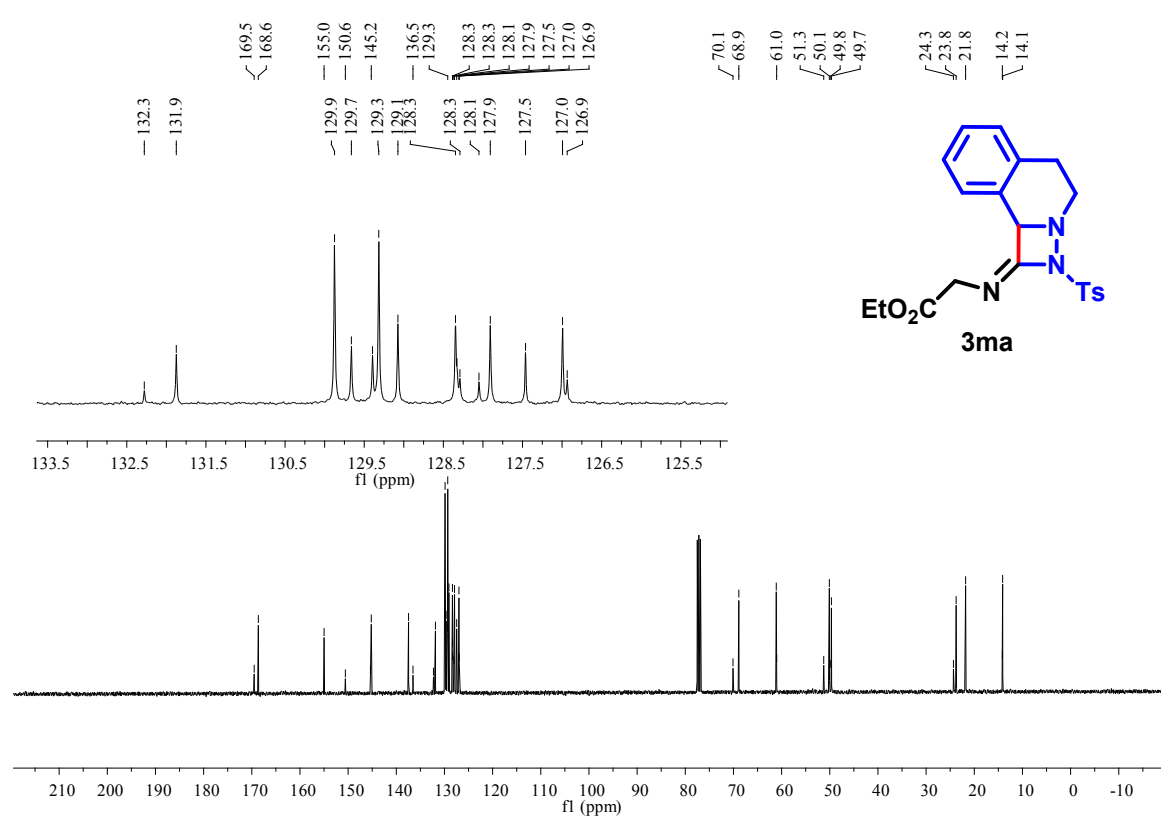
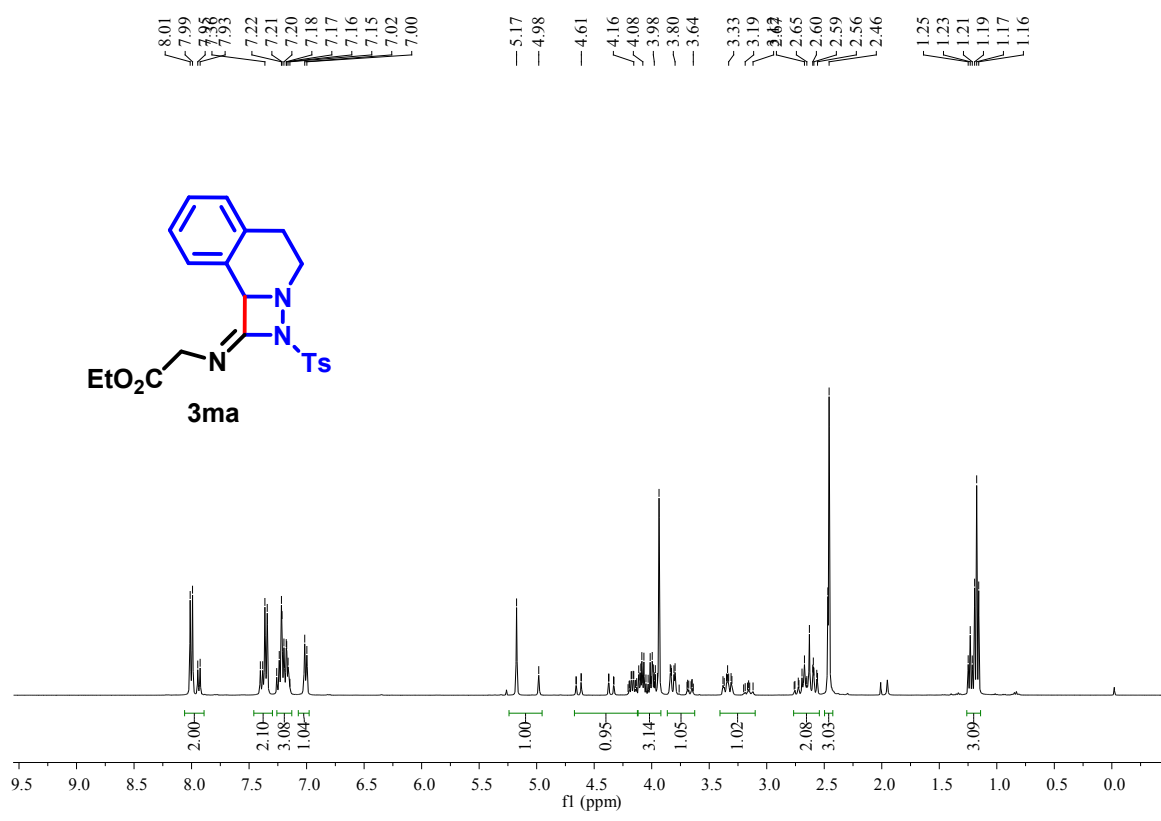


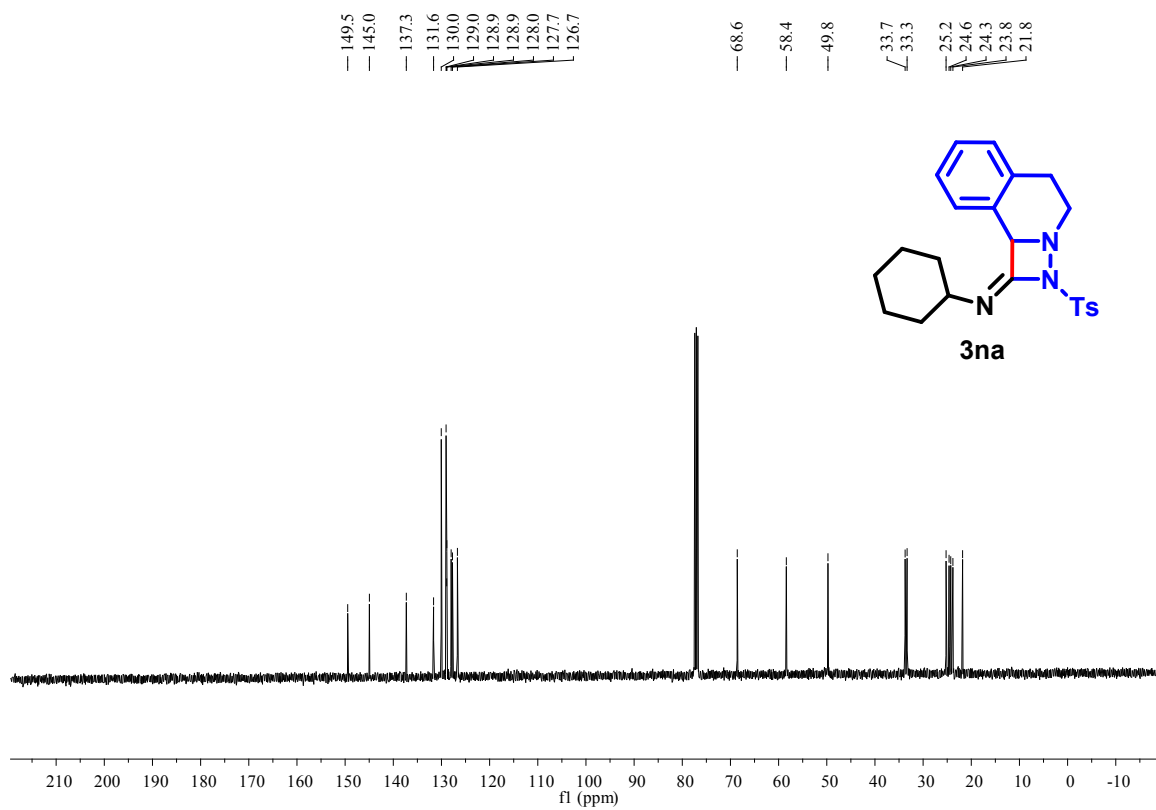
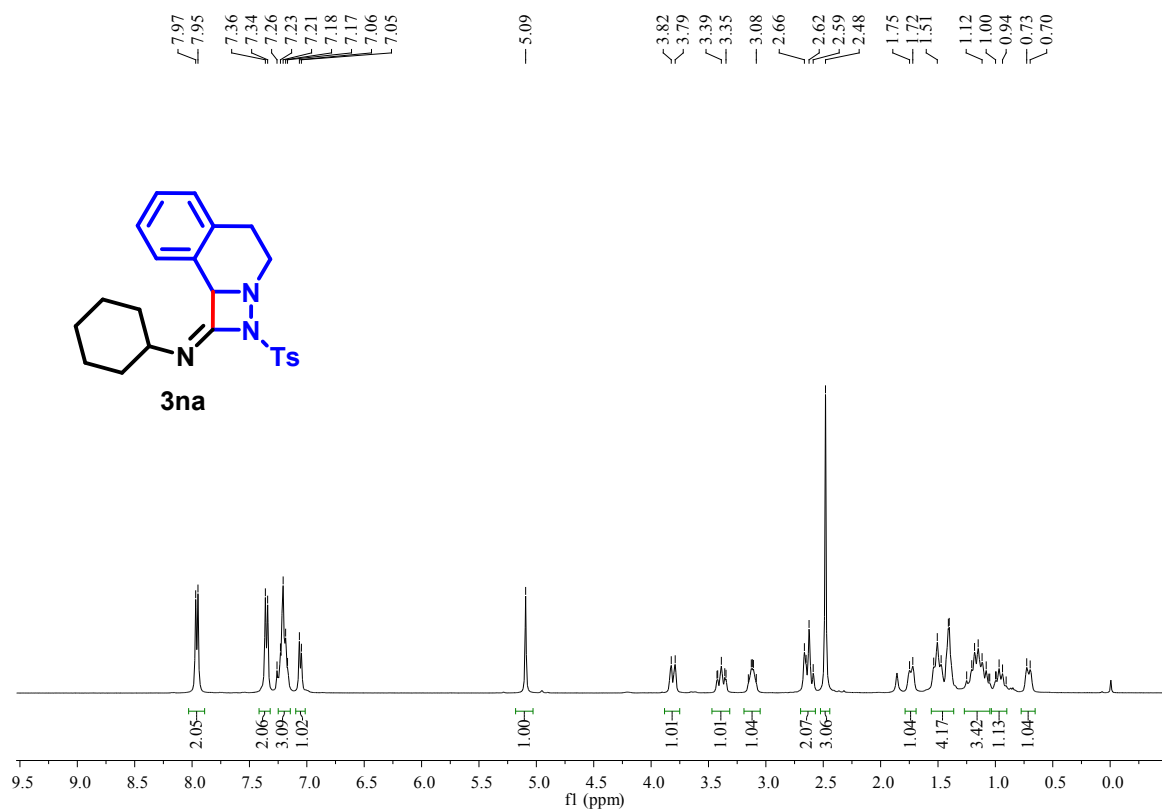


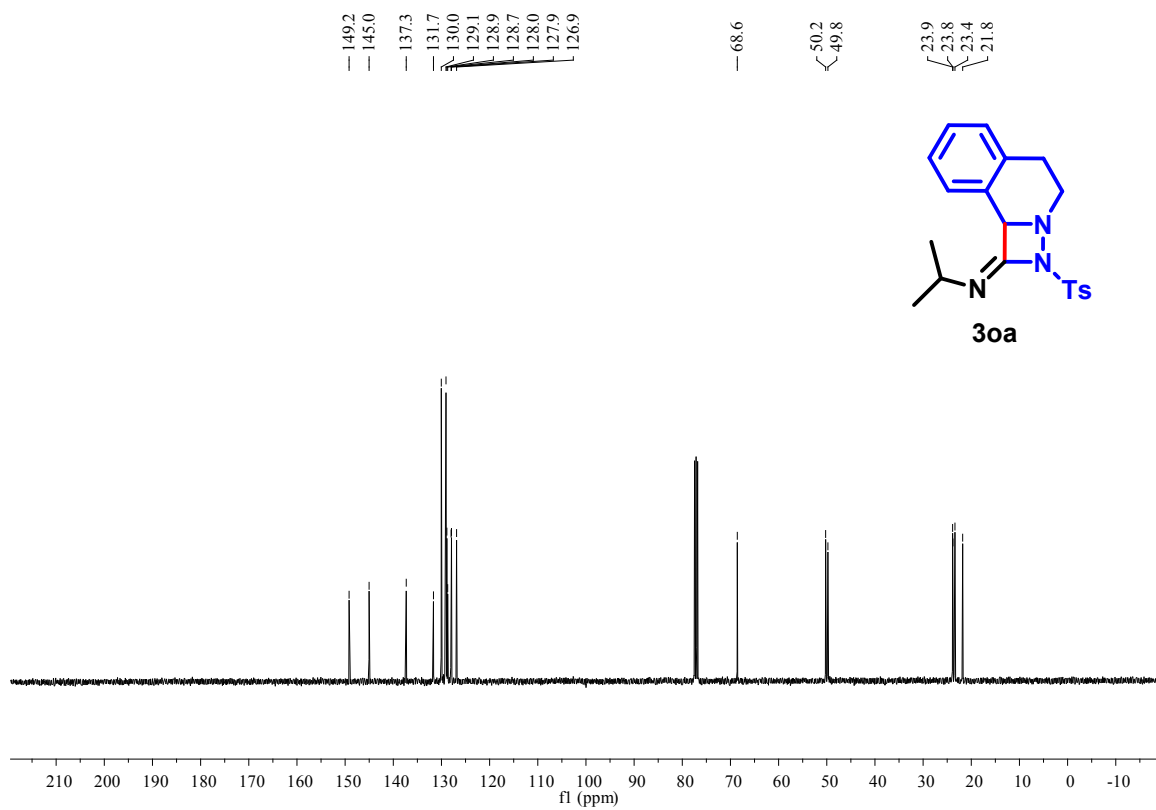
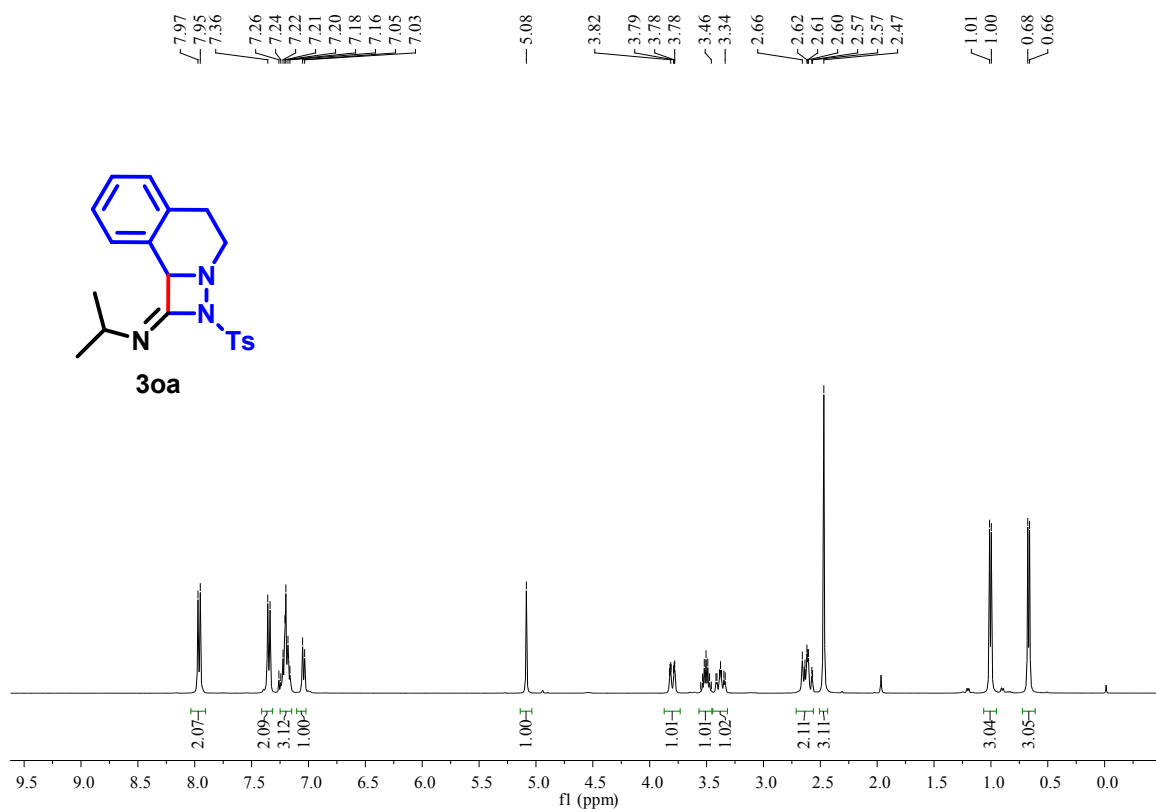


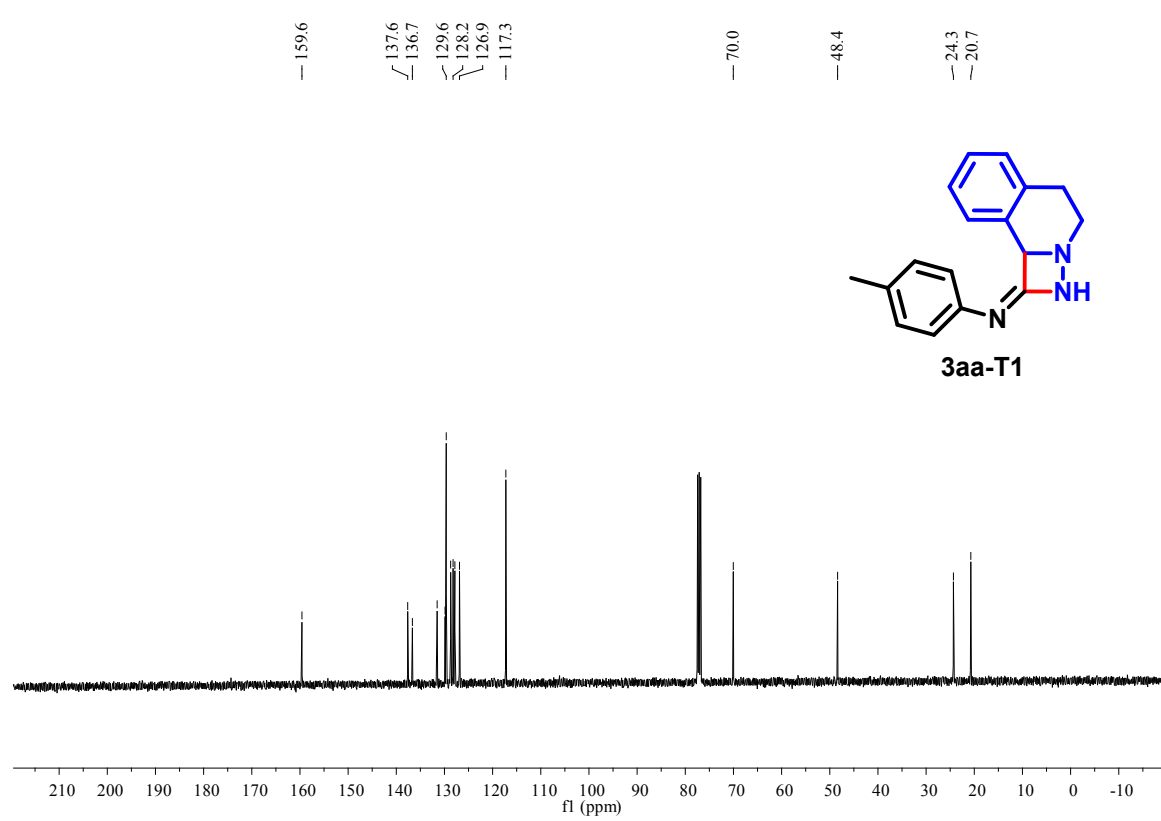
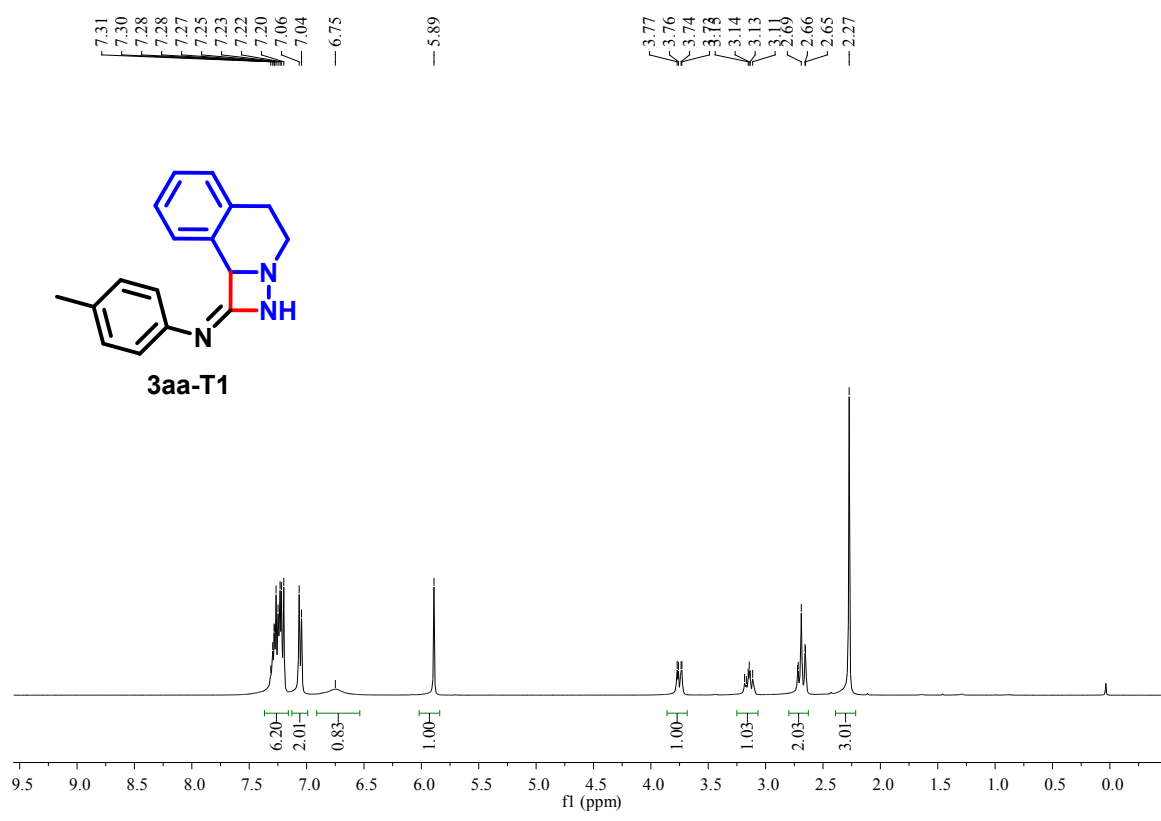


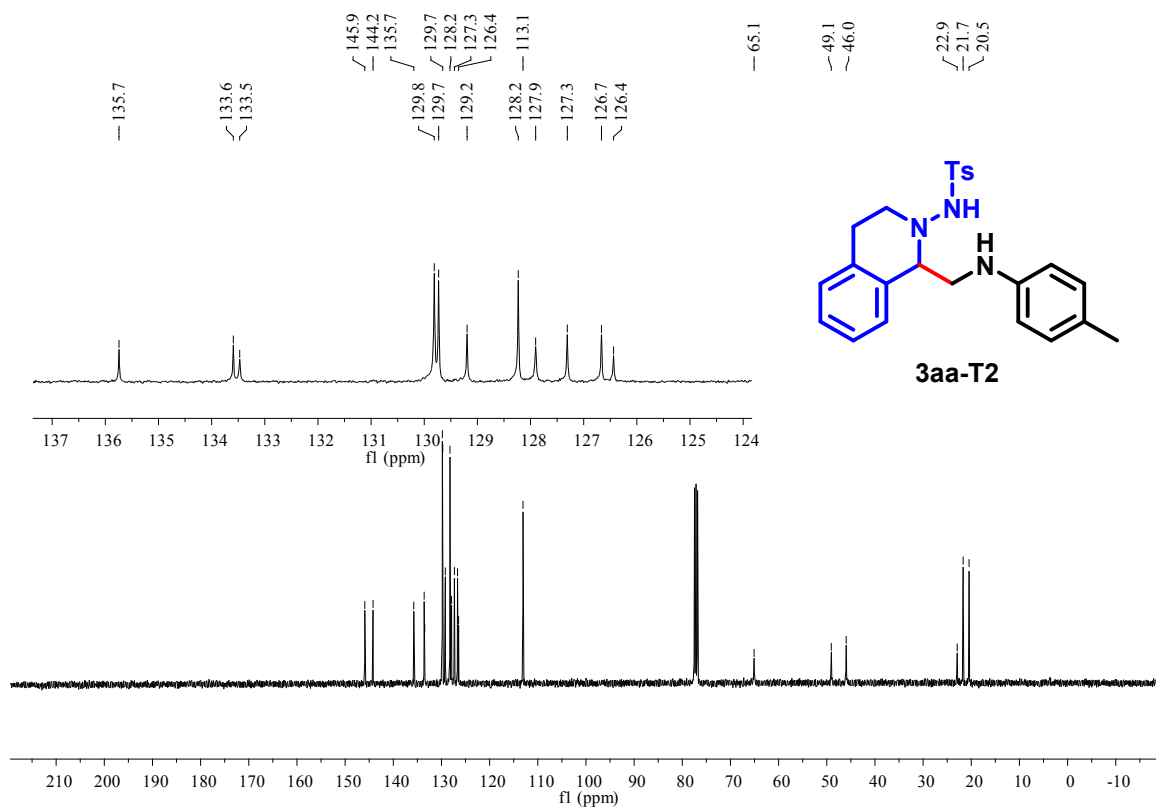
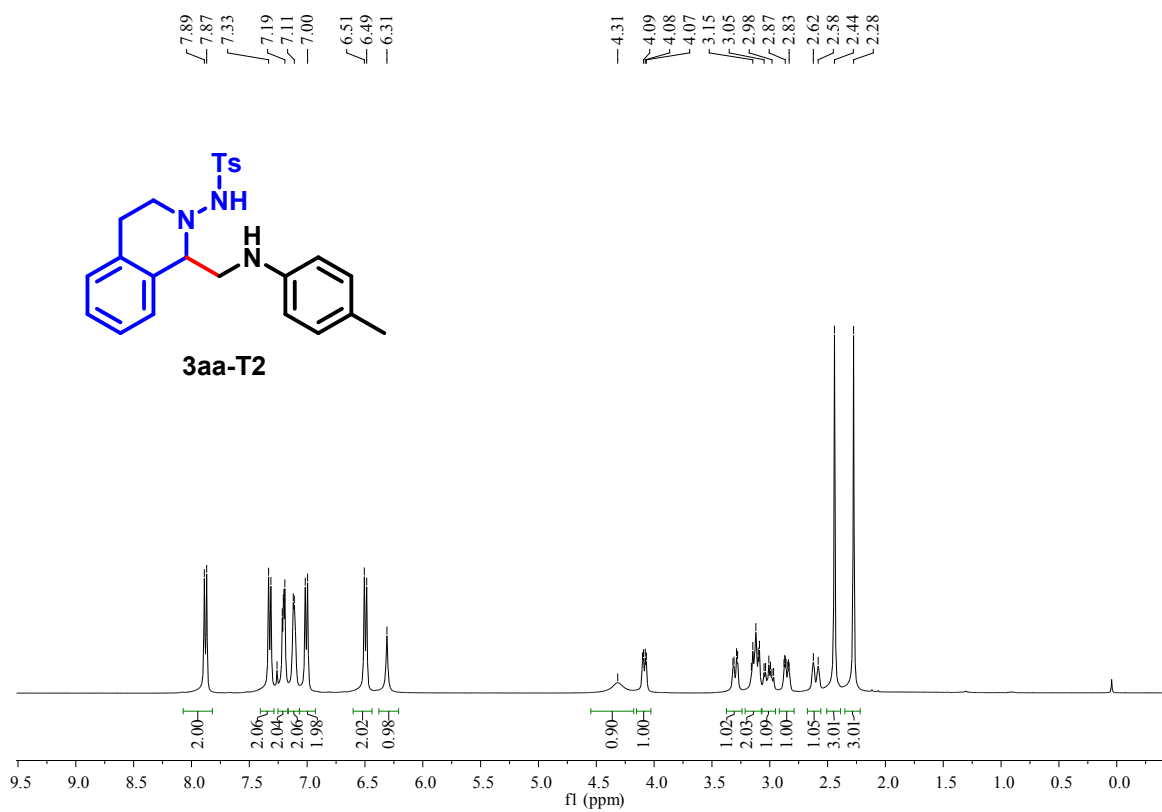


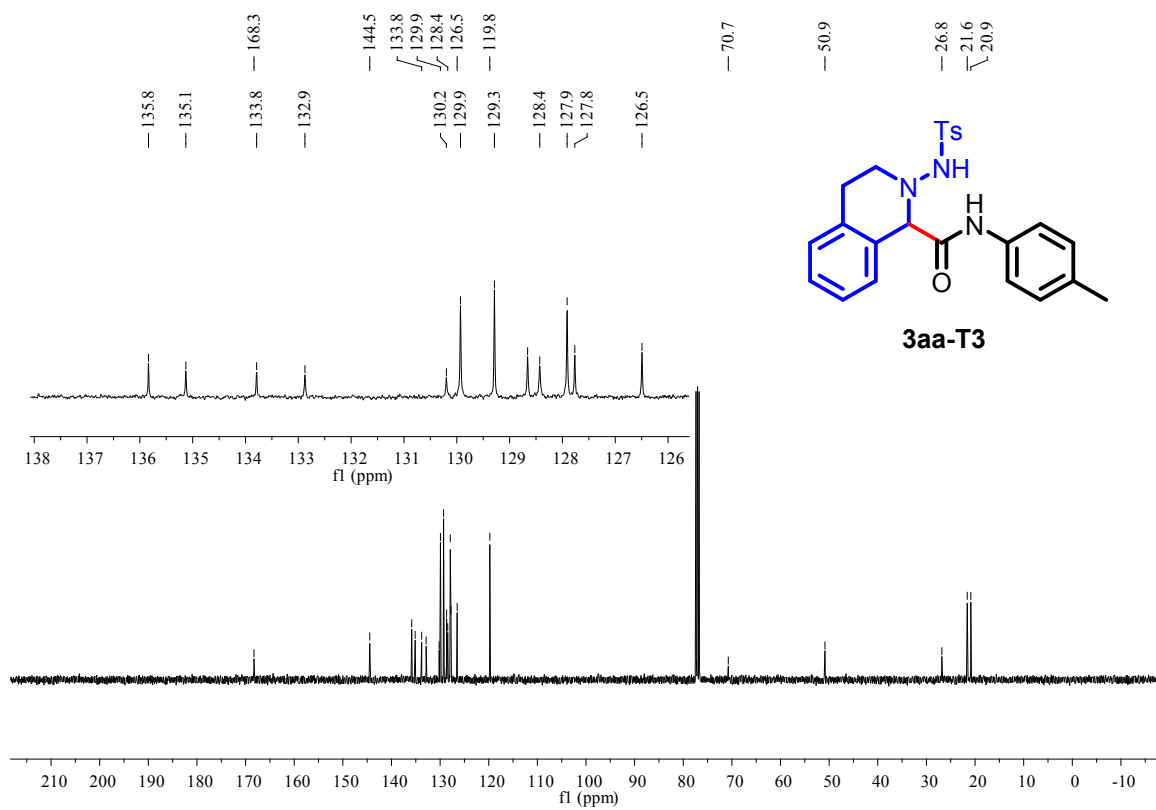
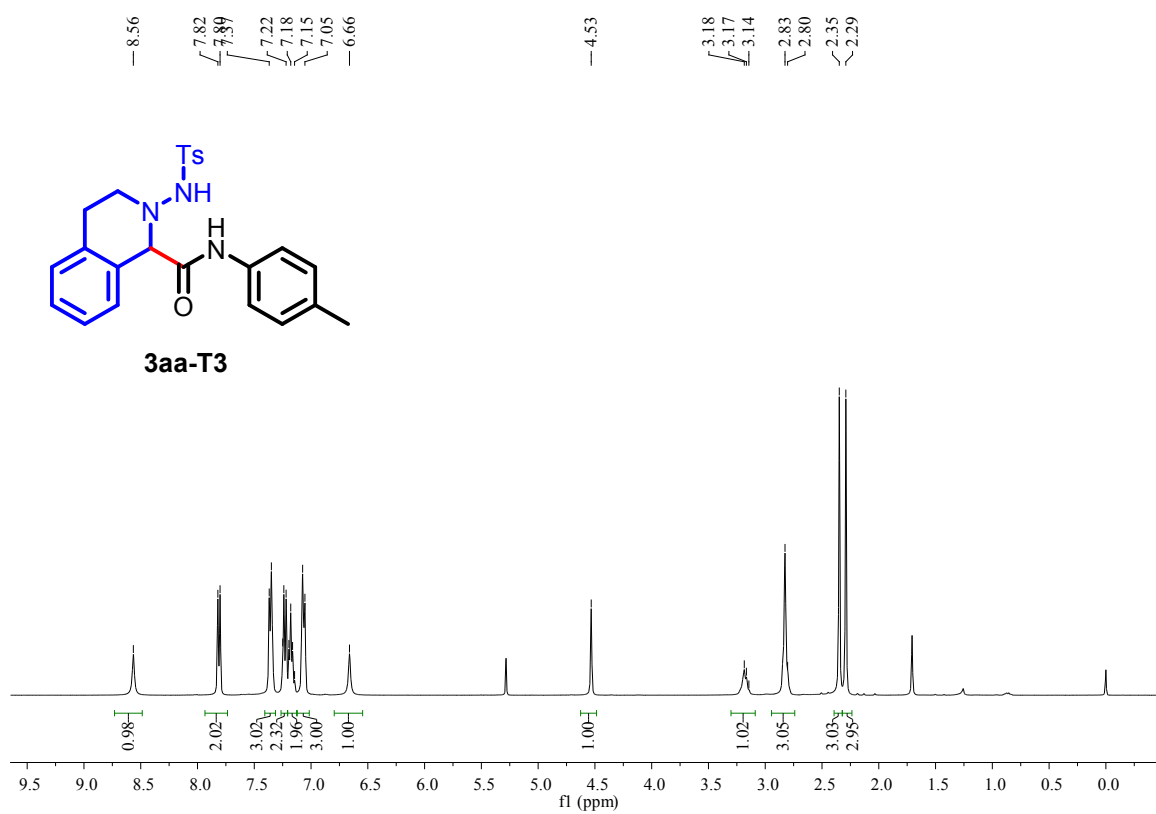






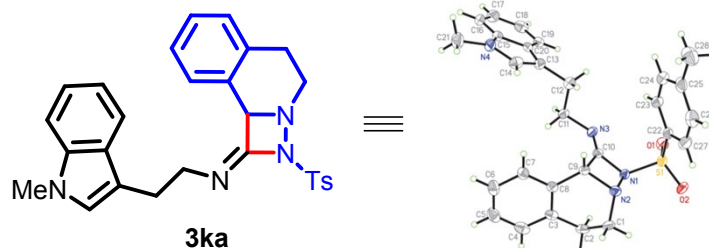






2. Crystal data and structure refinement

Compound **3ka**: (The crystal structure of compound **3ka** has been deposited at the Cambridge Crystallographic Data Centre (CCDC [2034479](https://www.ccdc.cam.ac.uk/conts/retrieving.html)). The data is available free of charge at www.ccdc.cam.ac.uk/conts/retrieving.html.)

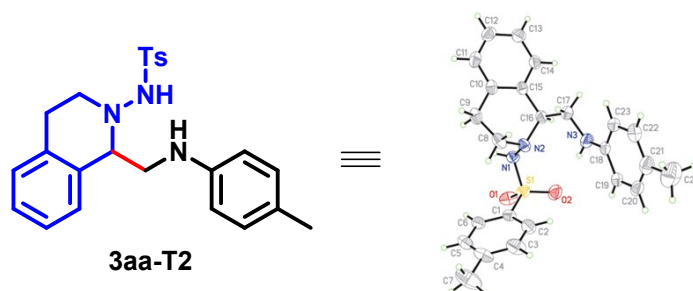


Crystal data and structure refinement for **3ka**.

Empirical formula	C ₂₈ H ₂₈ N ₄ O ₂ S	
Formula weight	484.60	
Temperature/K	296	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	P 21 P 21	
Unit cell dimensions	a = 10.6532(6) Å	α = 90 °
	b = 11.4210(7) Å	β = 99.632 °
	c = 20.3231(13) Å	γ = 90 °
Volume/Å ³	2437.9 (3)	
Z	4	
Density (calculated) g/cm ³	1.320	
Absorption coefficient/mm ⁻¹	0.167	
F(000)	1024	
Crystal size/mm ³	0.20 × 0.15 × 0.10	
Theta range for data collection/°	2.335 to 27.551	
Index ranges	-13 ≤ h ≤ 13, -14 ≤ k ≤ 14, -26 ≤ l ≤ 26	
Reflections collected	10854	
Independent reflections	6928 [R(int) = 0.0564]	
Completeness to theta = 25.242 °	99.2%	
Absorption correction	Multi-scan	
Data / restranits / parameters	10854/1/635	

Goodness-of-fit on F^2	1.016
Final R indices [$I > 2\sigma(I)$]	$R_1 = 0.0564$, $wR_2 = 0.0876$
Final R indices [all data]	$R_1 = 0.1224$, $wR_2 = 0.1018$

Compound **3aa-T2**: (The crystal structure of compound **3aa-T2** has been deposited at the Cambridge Crystallographic Data Centre (CCDC 2054283). The data is available free of charge at www.ccdc.cam.ac.uk/conts/retrieving.html.)



Crystal data and structure refinement for **3aa-T2**.

Empirical formula	$C_{24}H_{27}N_3O_2S$
Formula weight	421.55
Temperature/K	296
Wavelength	0.71073 Å
Crystal system	triclinic
Space group	$P -1 P -1$
Unit cell dimensions	$a = 10.6667(5)$ Å $\alpha = 87.4762^\circ$ $b = 13.4081(7)$ Å $\beta = 79.9020^\circ$ $c = 16.0716(8)$ Å $\gamma = 81.4307^\circ$
Volume/Å ³	2237.32(19)
Z	4
Density (calculated) g/cm ³	1.251
Absorption coefficient/mm ⁻¹	0.170
F(000)	896.0
Crystal size/mm ³	0.60 × 0.40 × 0.36
Theta range for data collection/°	2.46 to 27.30
Index ranges	$-13 \leq h \leq 13$, $-17 \leq k \leq 17$, $-20 \leq l \leq 20$
Reflections collected	10257

Independent reflections	50241 [R(int) = 0.0348]
Completeness to theta = 25.242 °	99.7%
Absorption correction	Multi-scan
Data / restranits / parameters	10257/0/557
Goodness-of-fit on F ²	1.080
Final R indices [I>2sigma(I)]	R ₁ = 0.0435, wR ₂ = 0.0930
Final R indices [all data]	R ₁ = 0.0700, wR ₂ = 0.1022