

## Supplementary Materials

# Synthesis of Novel Benzo[*b*][1,6]naphthyridine Derivatives and Investigation of Their Potential as Scaffolds of MAO Inhibitors

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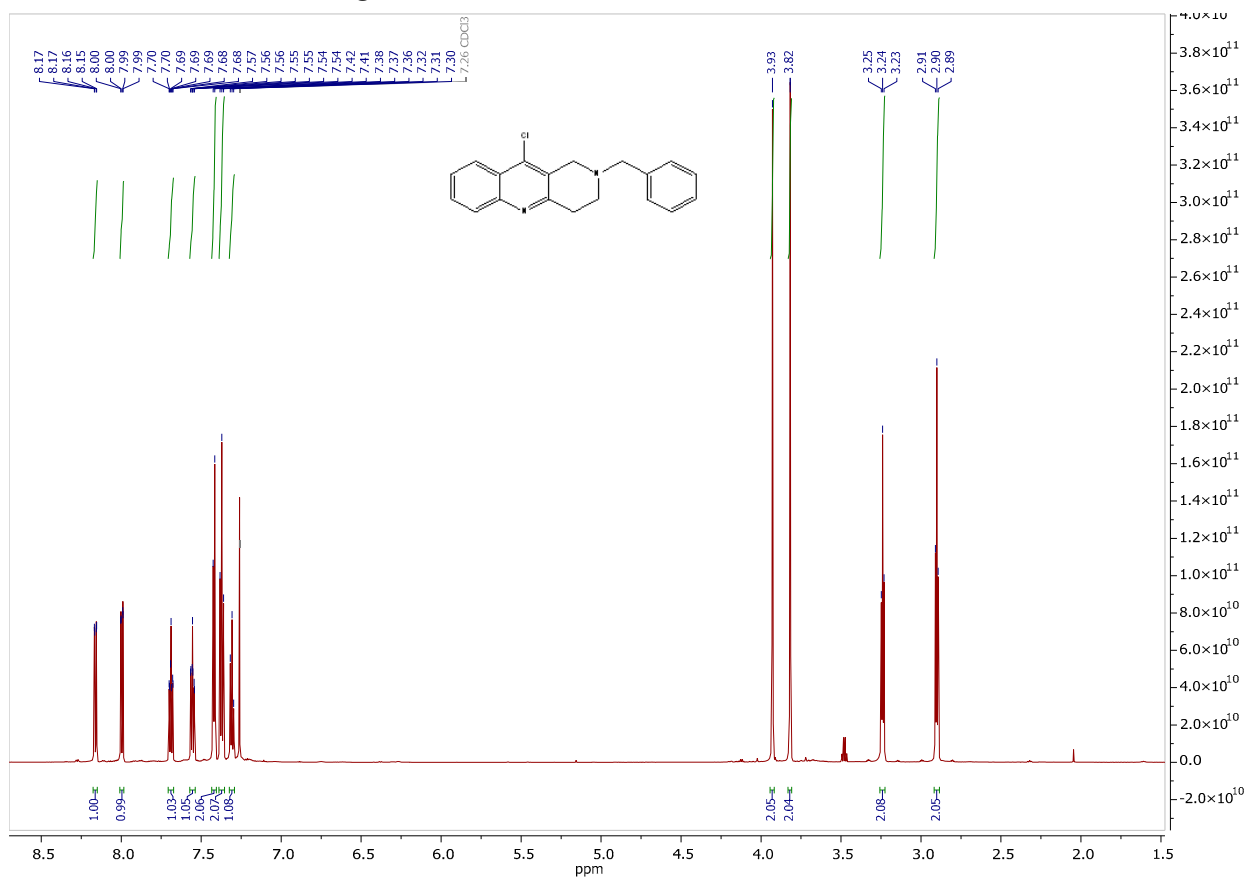
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### Table of Content

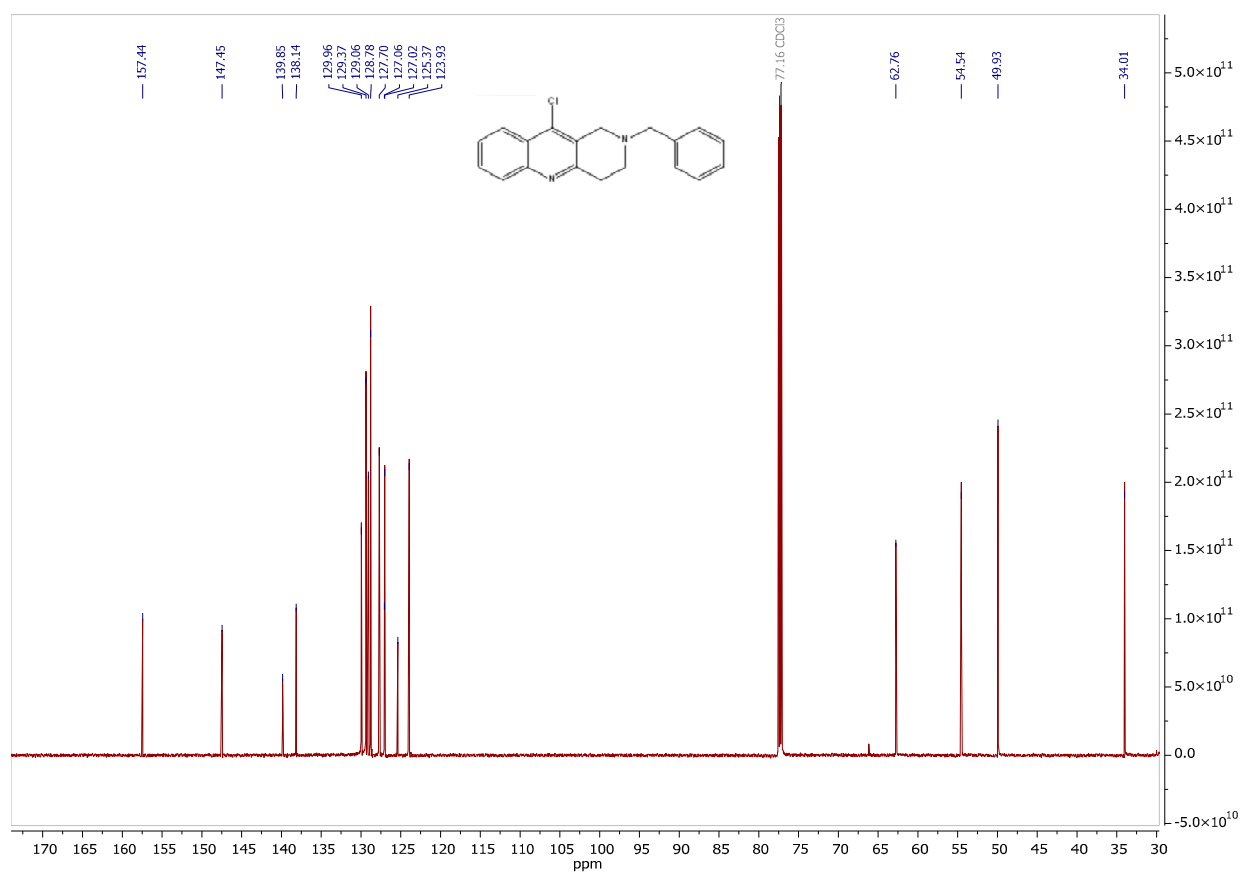
1. NMR Data of Derivatives (3-10)

2. A single crystal X-ray analysis of compound 5a

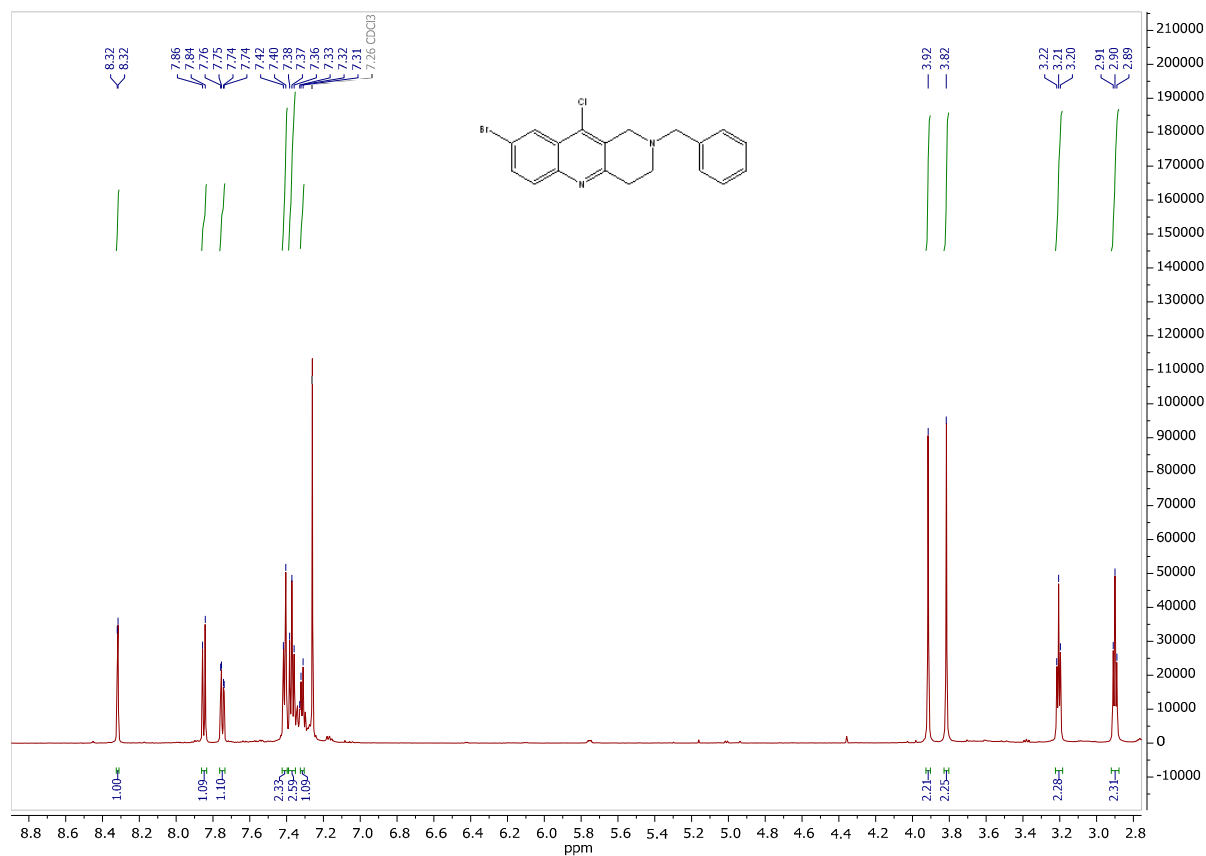
**Figure S1.** The <sup>1</sup>H NMR data of 3a



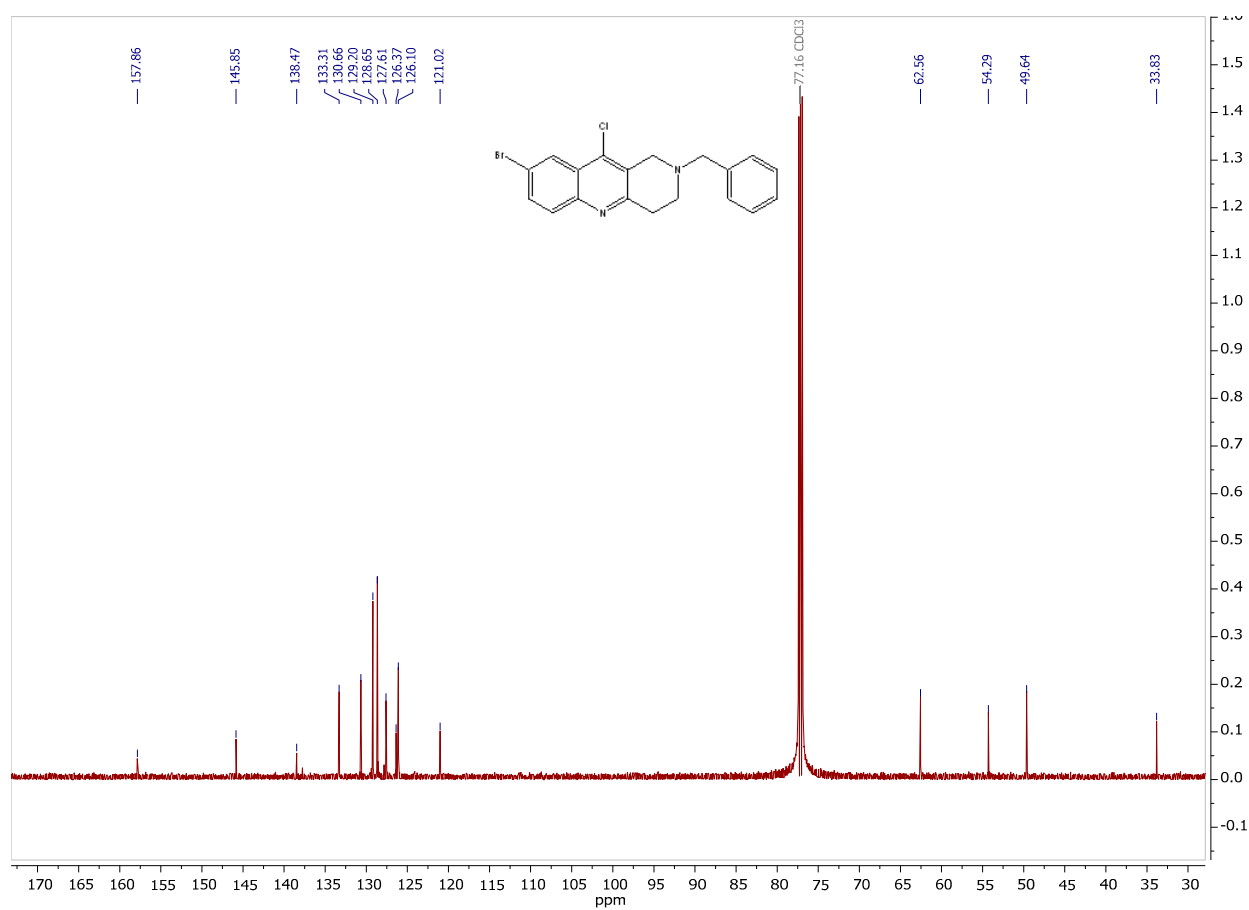
**Figure S2.** The  $^{13}\text{C}$  NMR data of **3a**



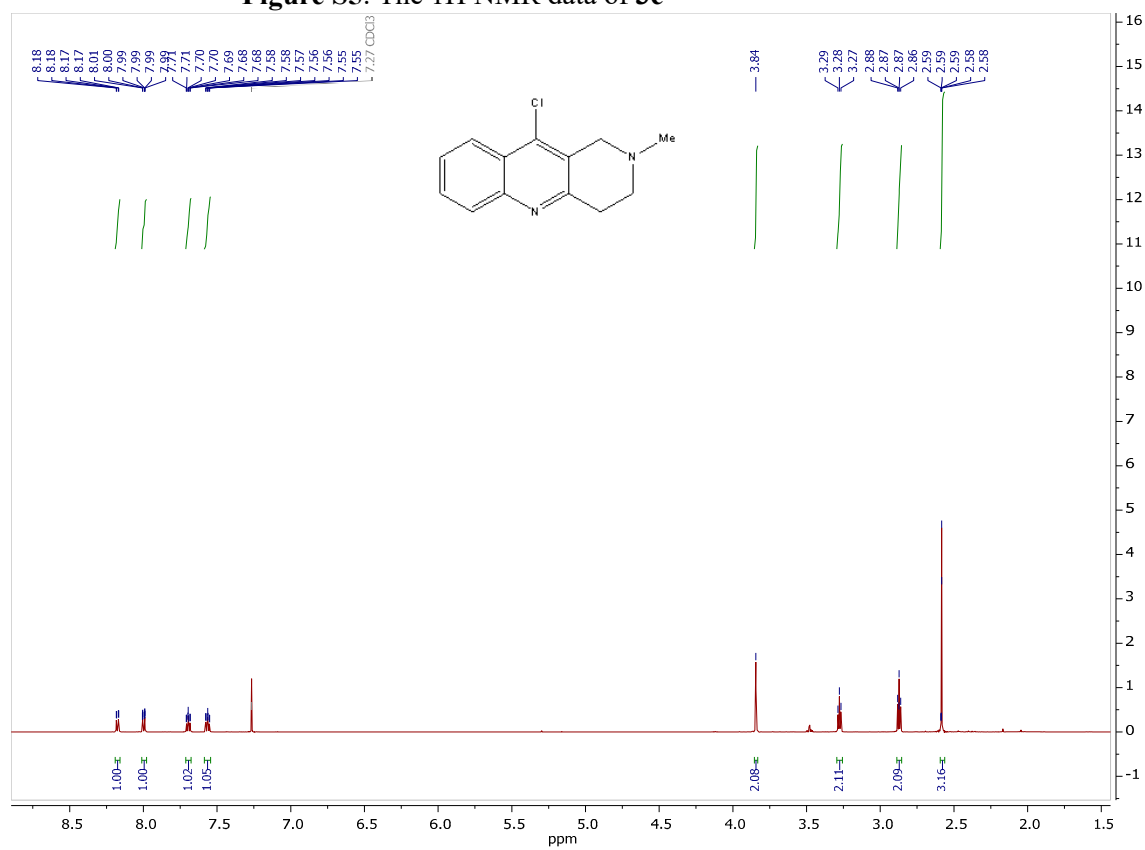
**Figure S3.** The  $^1\text{H}$  NMR data of **3b**



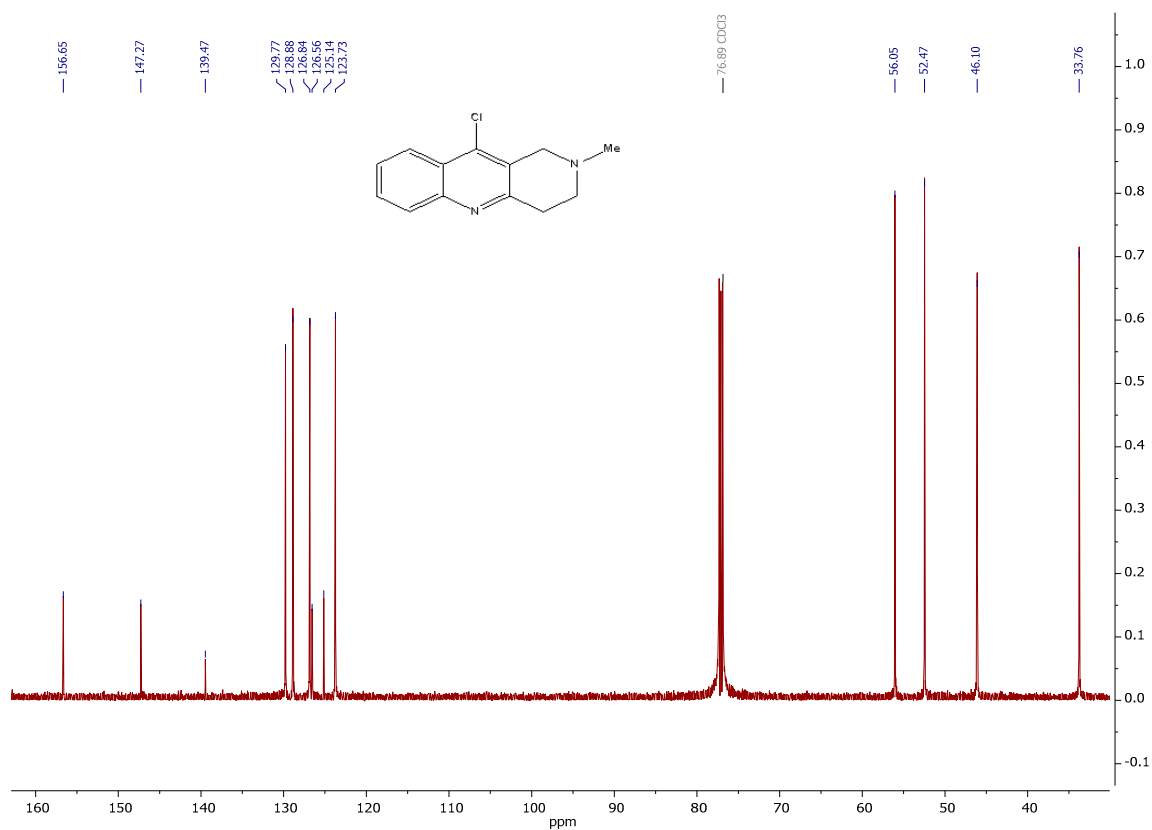
**Figure S4.** The  $^{13}\text{C}$  NMR data of **3b**



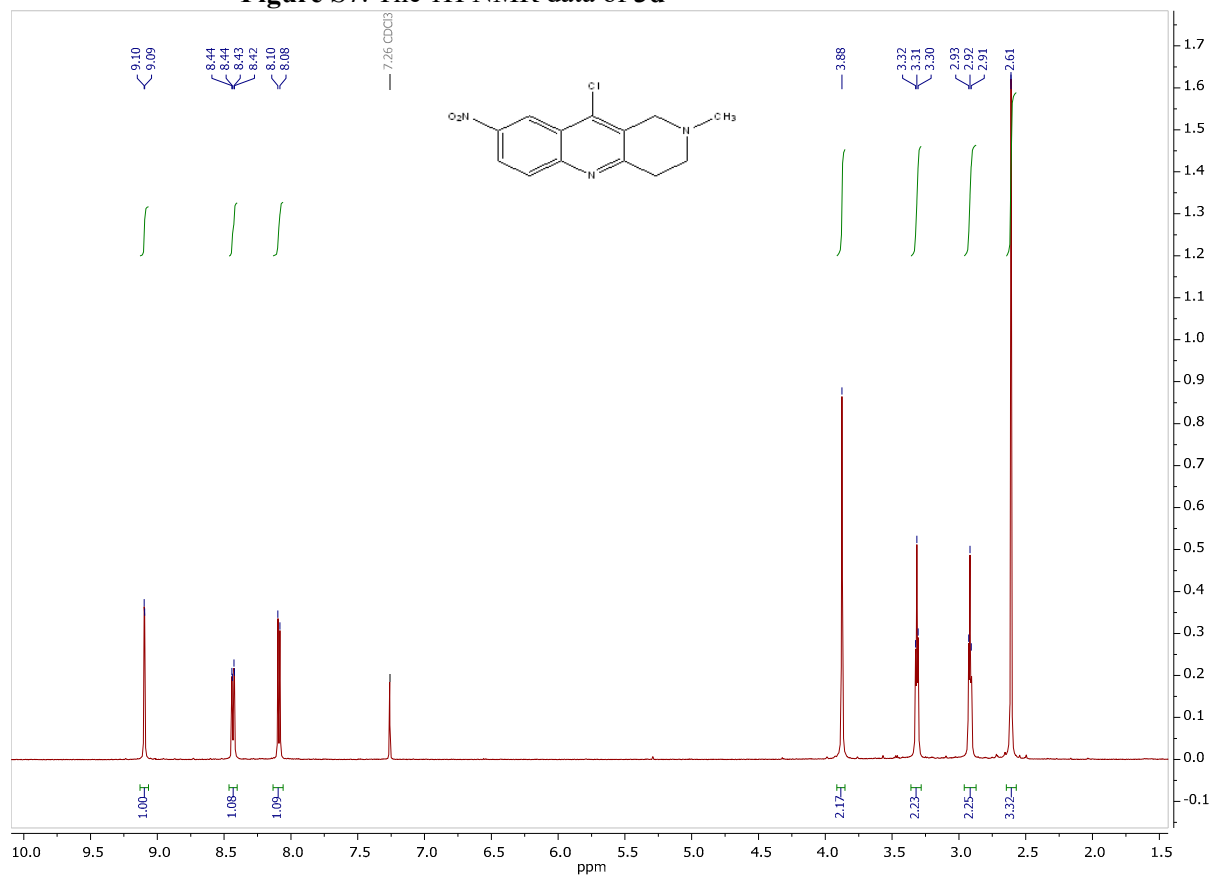
**Figure S5.** The  $^1\text{H}$  NMR data of **3c**



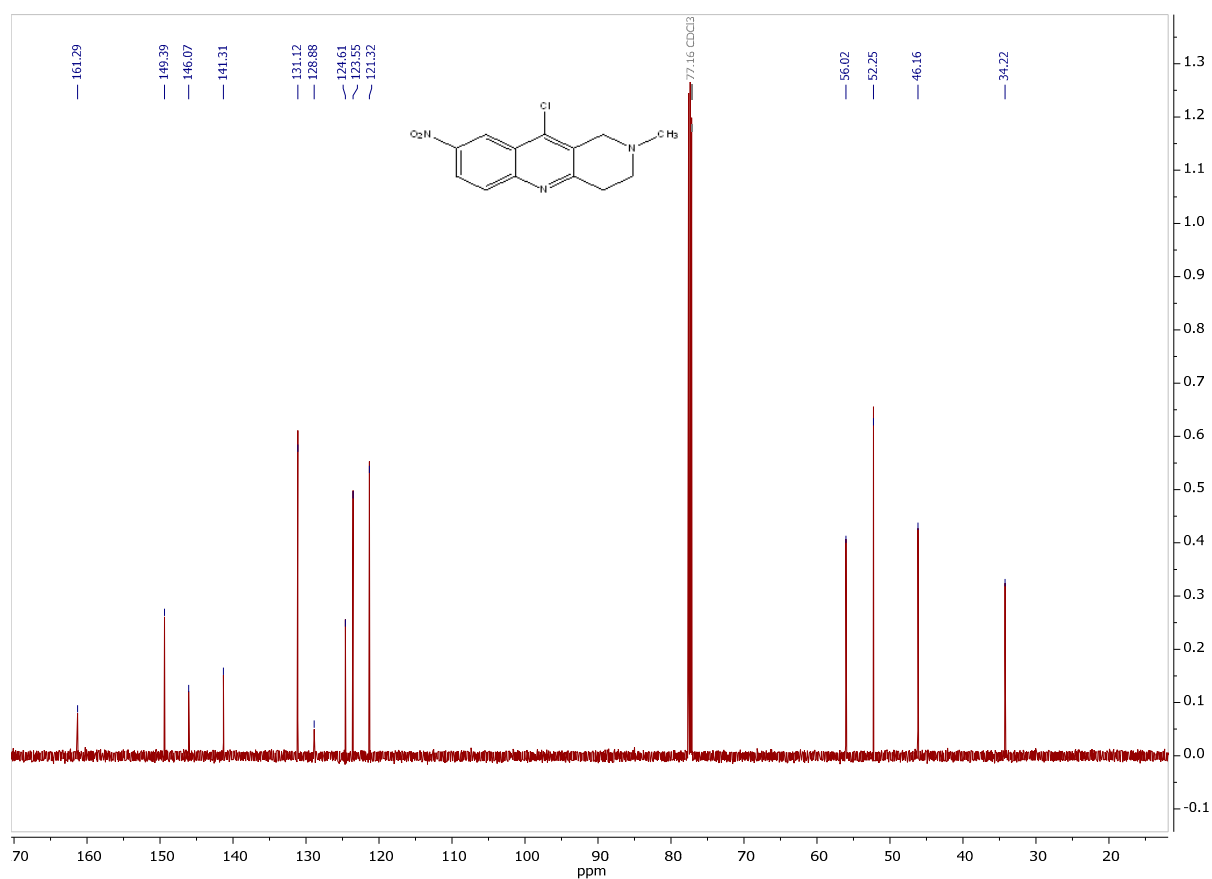
**Figure S6.** The  $^{13}\text{C}$  NMR data of **3c**



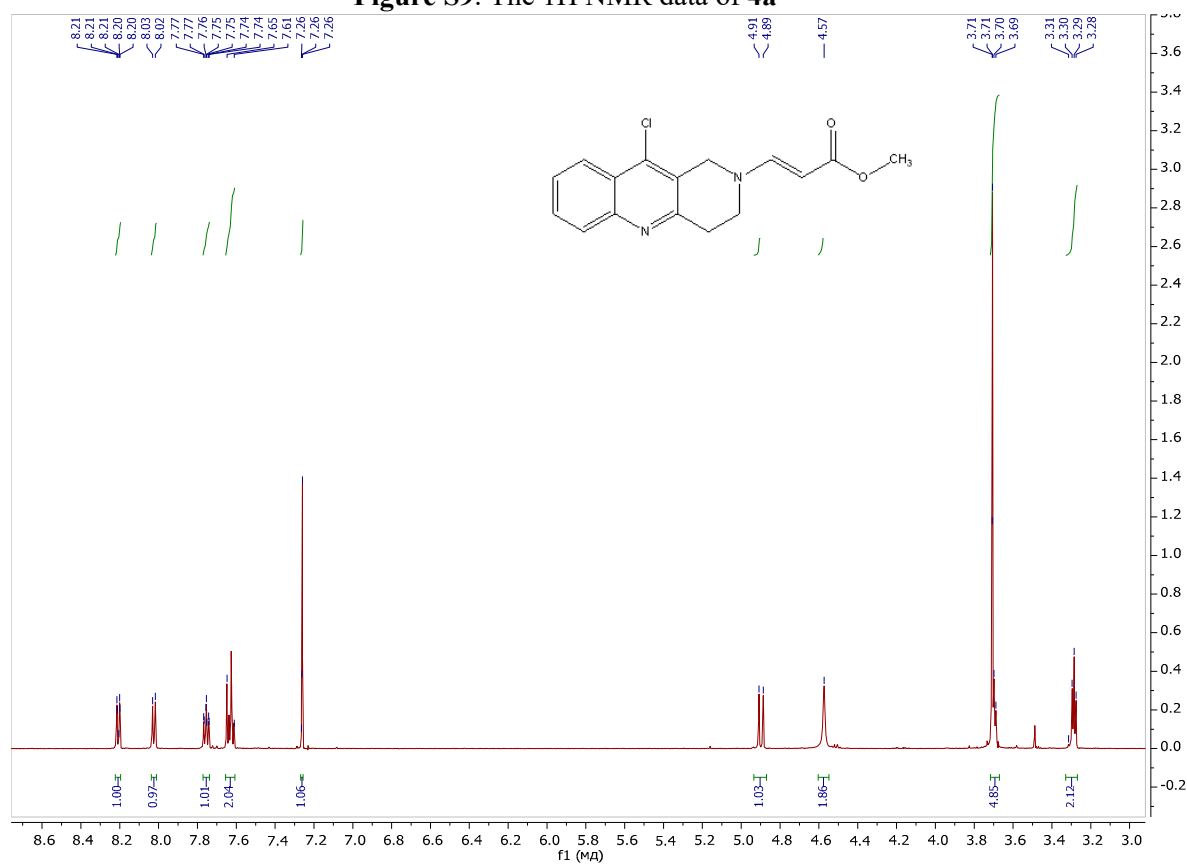
**Figure S7.** The  $^1\text{H}$  NMR data of **3d**



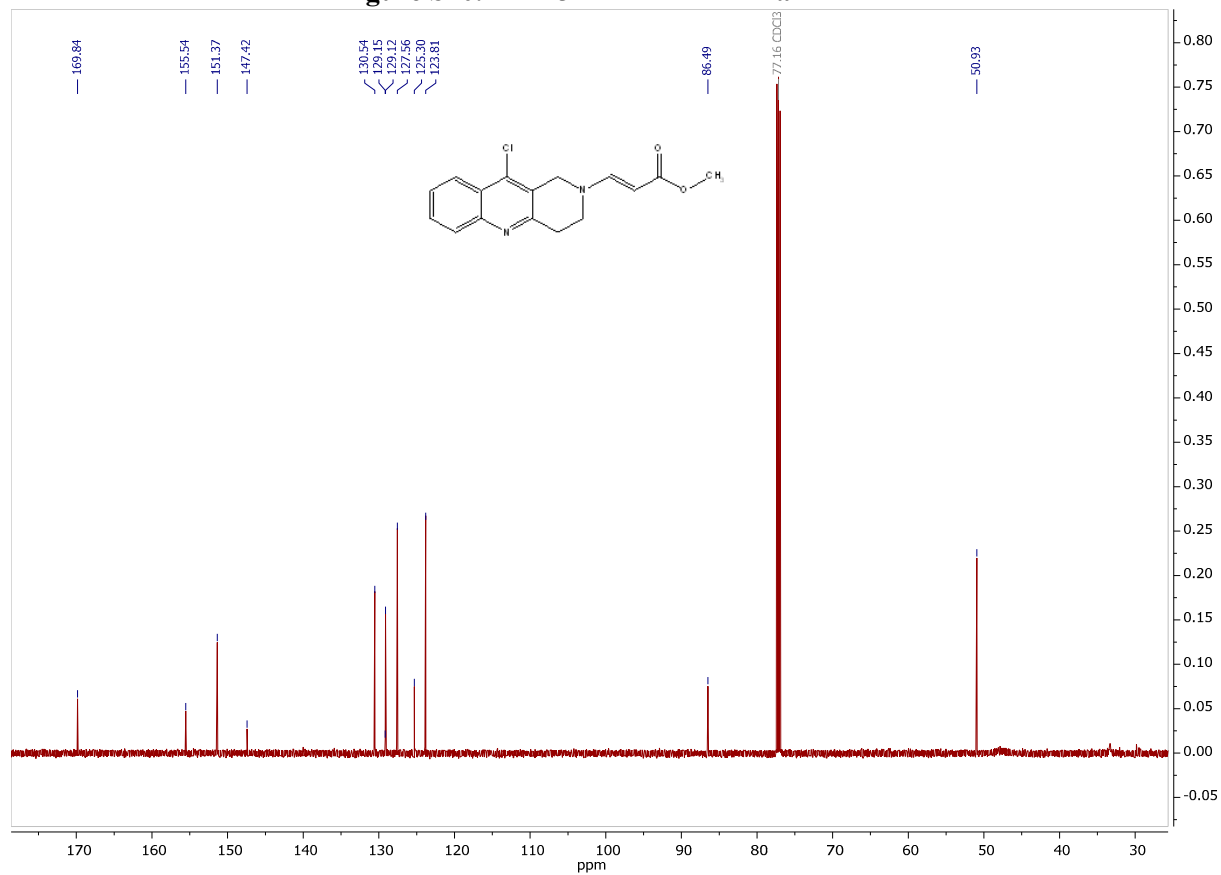
**Figure S8.** The  $^{13}\text{C}$  NMR data of **3d**



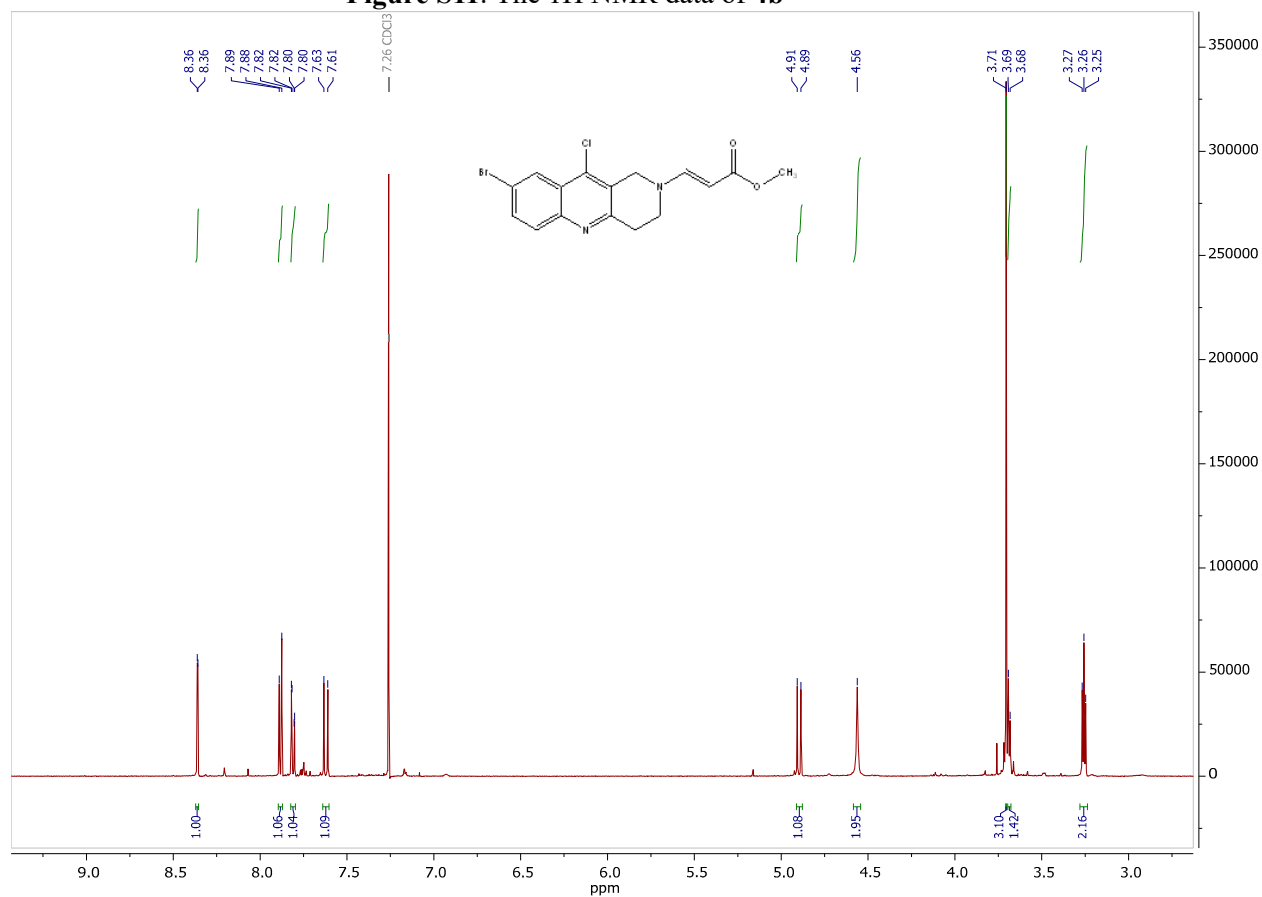
**Figure S9.** The  $^1\text{H}$  NMR data of **4a**



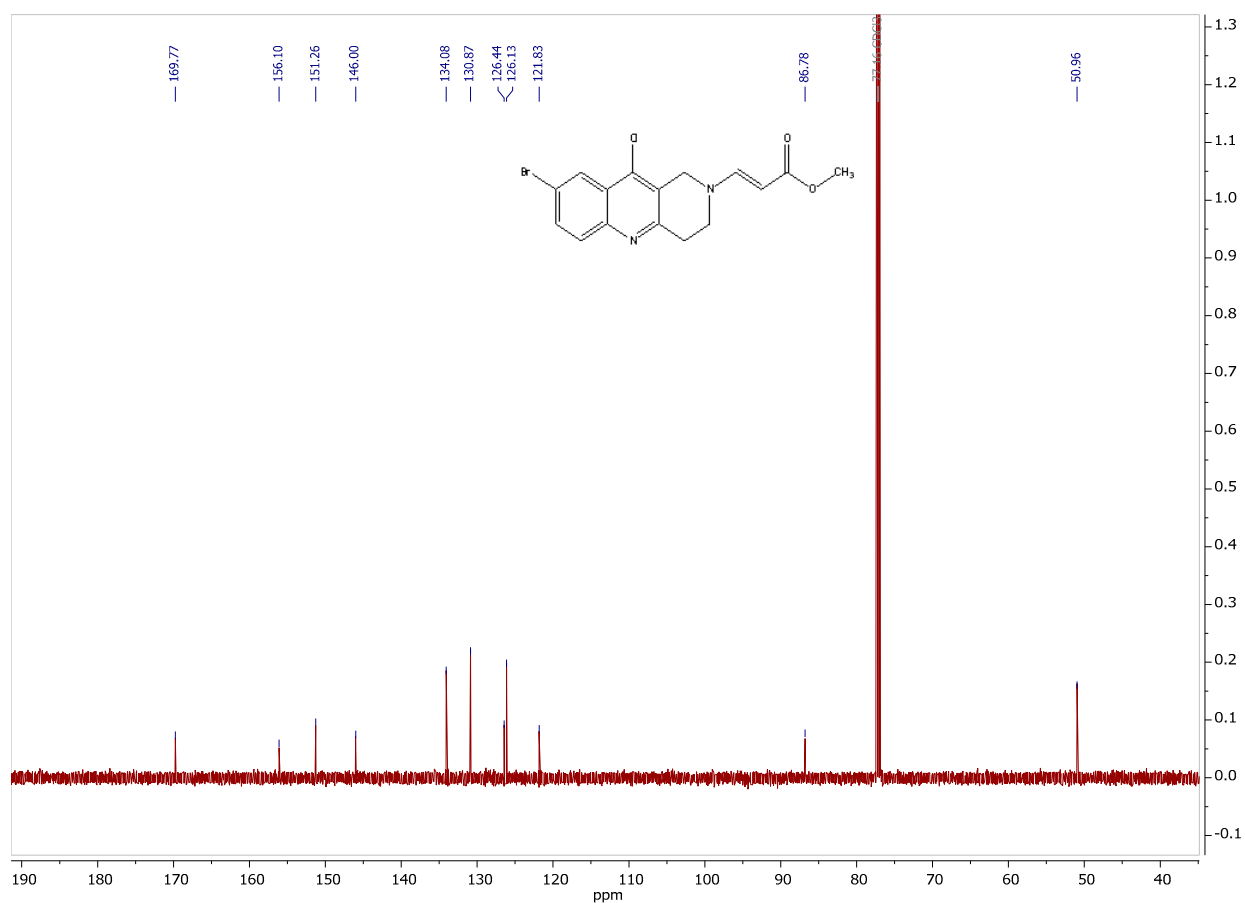
**Figure S10.** The <sup>13</sup>C NMR data of **4a**



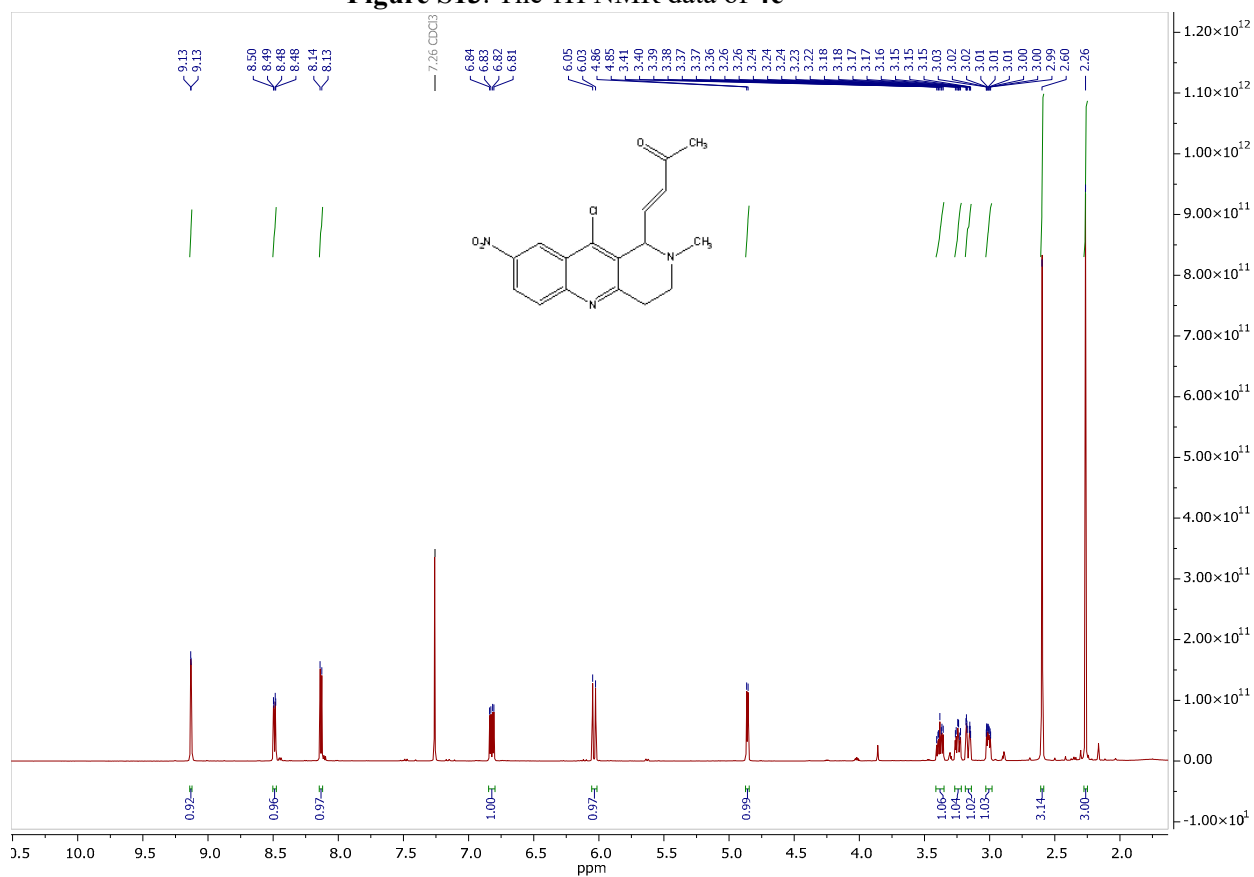
**Figure S11.** The <sup>1</sup>H NMR data of **4b**



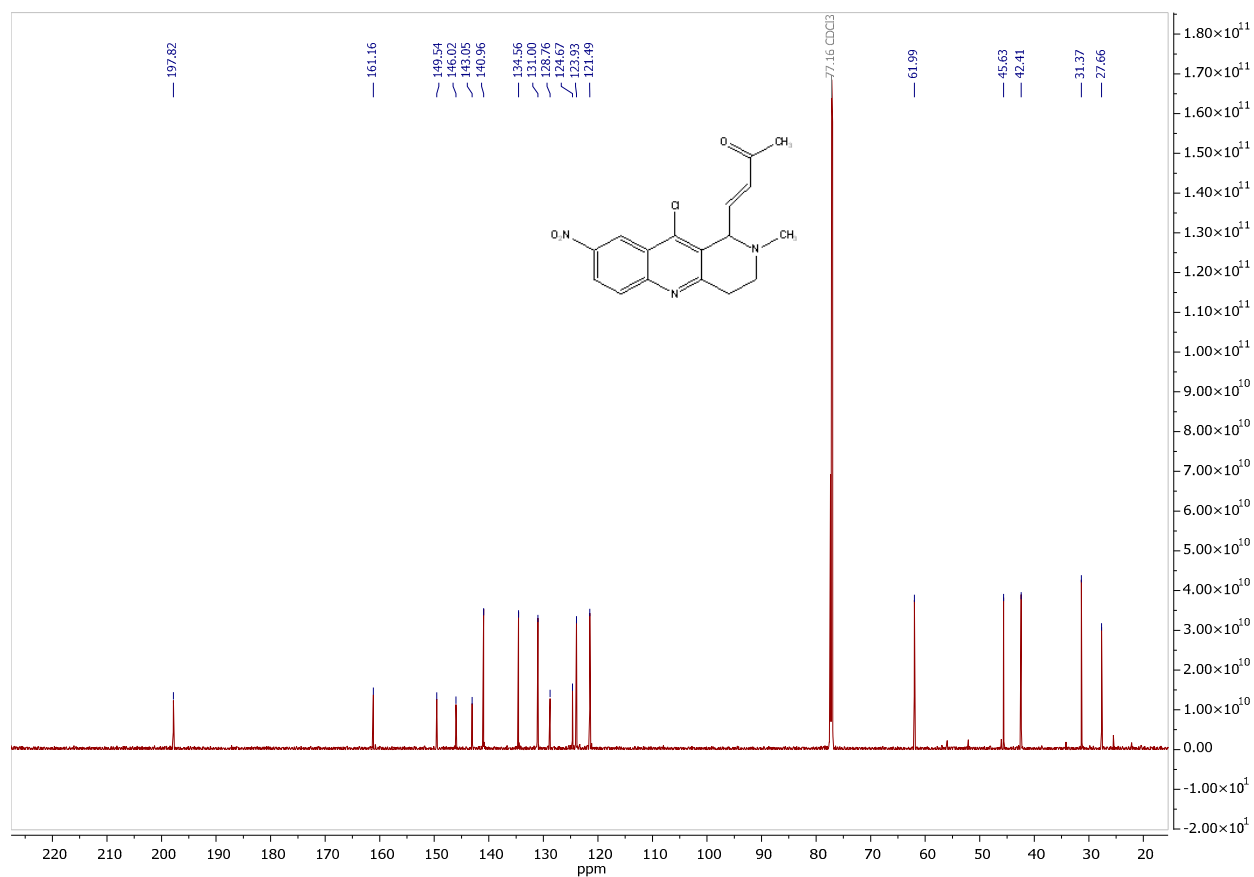
**Figure S12.** The  $^{13}\text{C}$  NMR data of **4b**



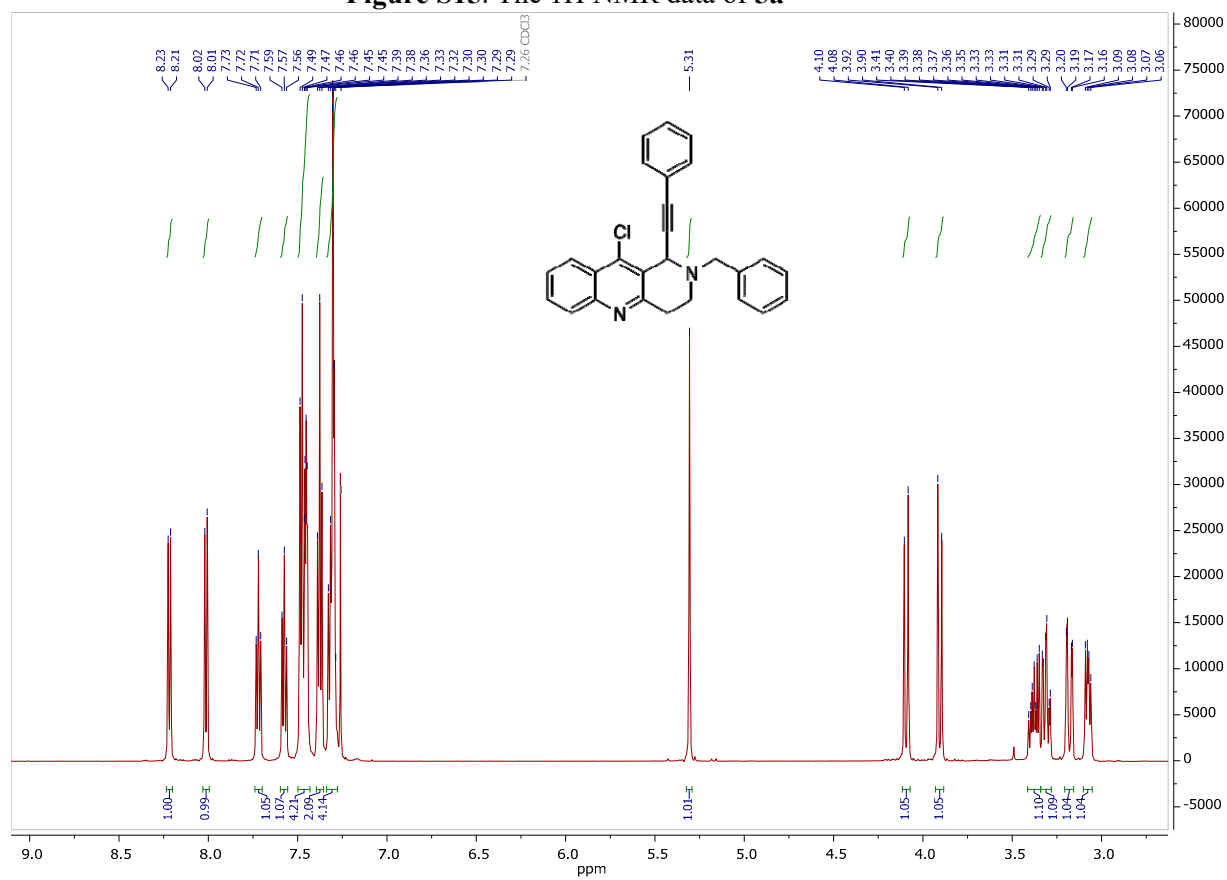
**Figure S13.** The  $^1\text{H}$  NMR data of **4c**



**Figure S14.** The  $^{13}\text{C}$  NMR data of **4c**

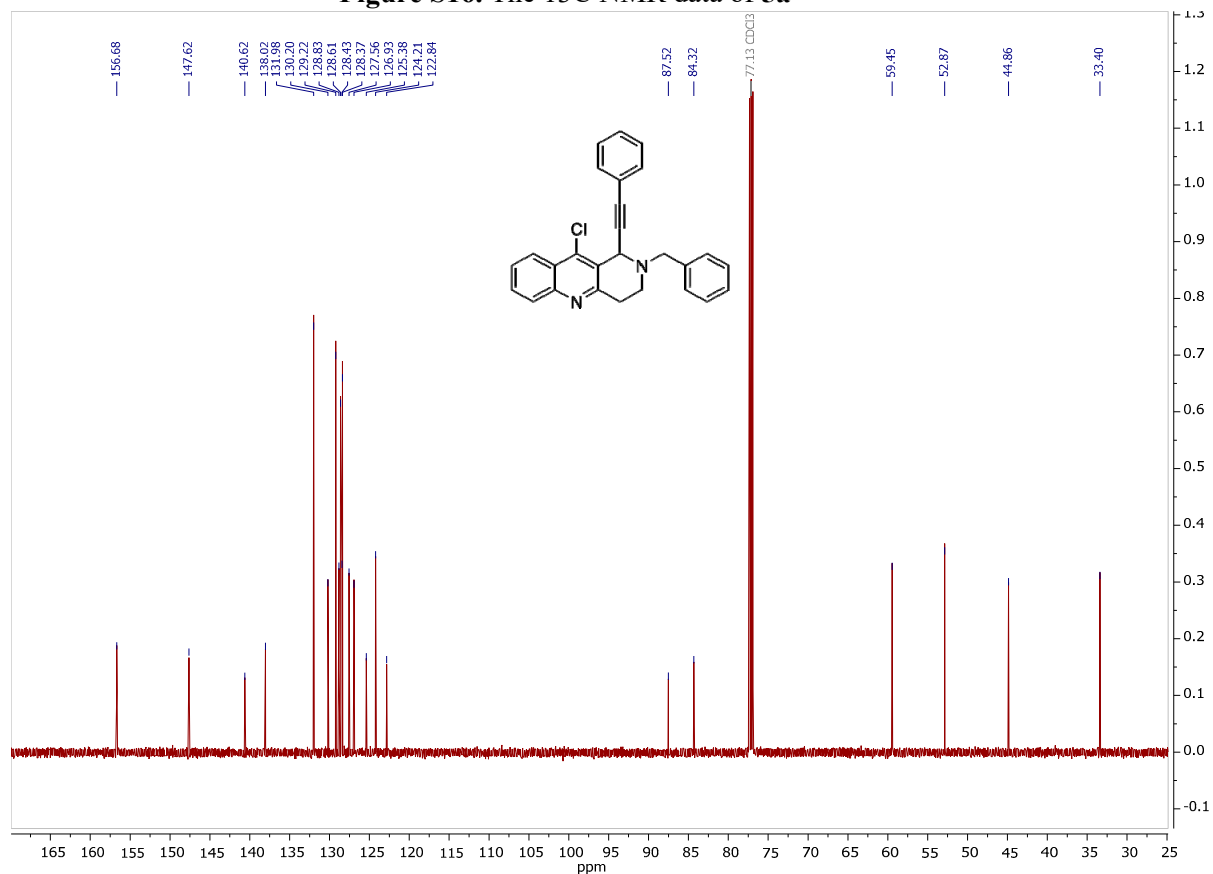


**Figure S15.** The  $^1\text{H}$  NMR data of **5a**

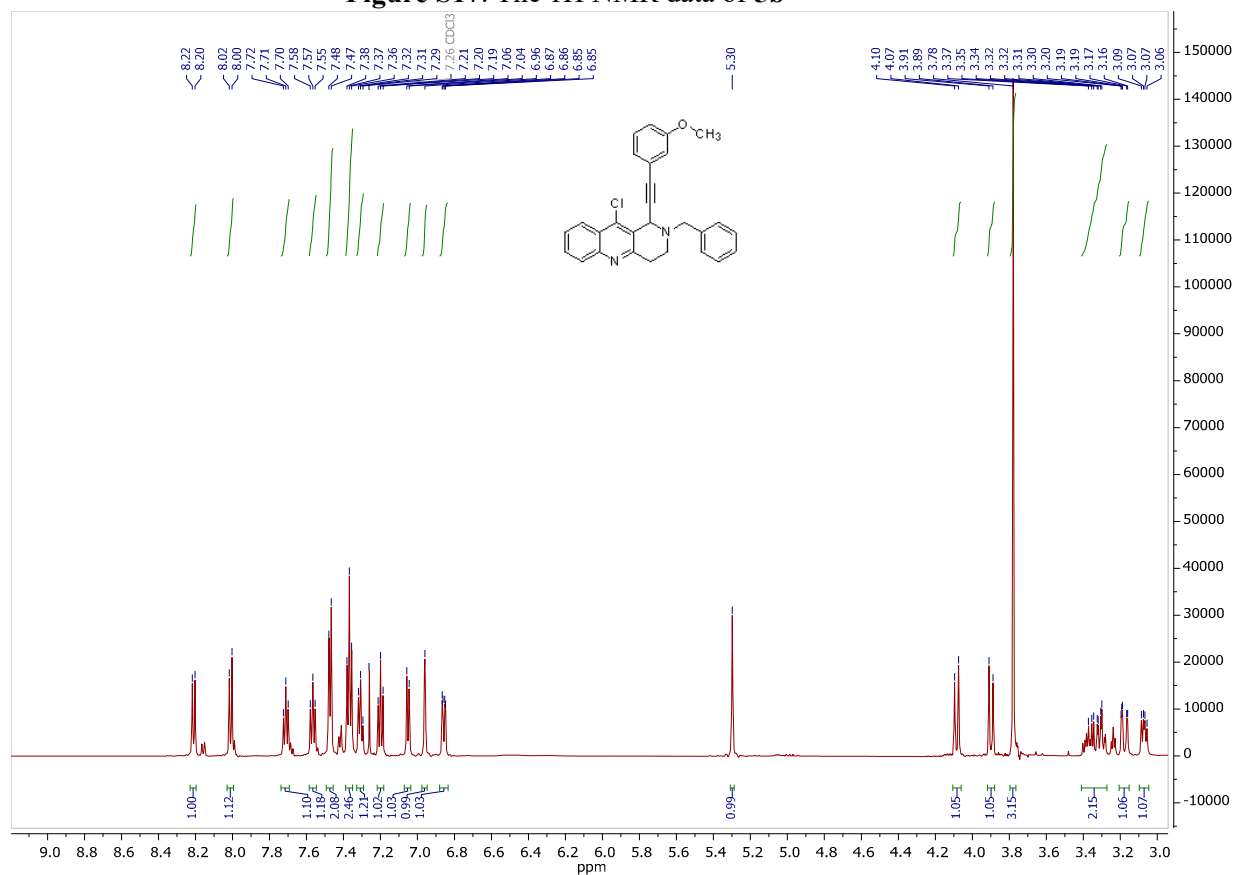




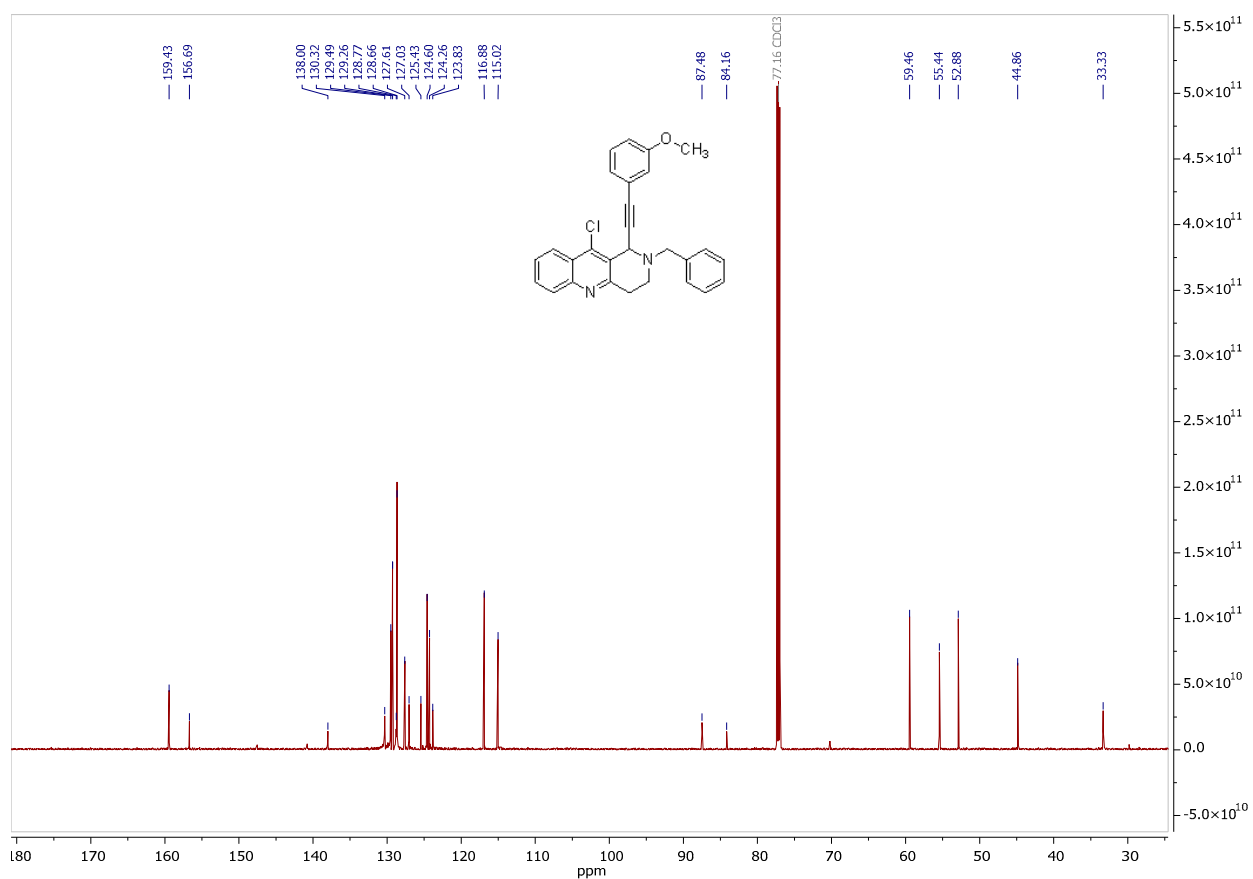
**Figure S16.** The  $^{13}\text{C}$  NMR data of **5a**



**Figure S17.** The  $^1\text{H}$  NMR data of **5b**



**Figure S18.** The  $^{13}\text{C}$  NMR data of **5b**



**Figure S19.** The  $^1\text{H}$  NMR data of **5c**

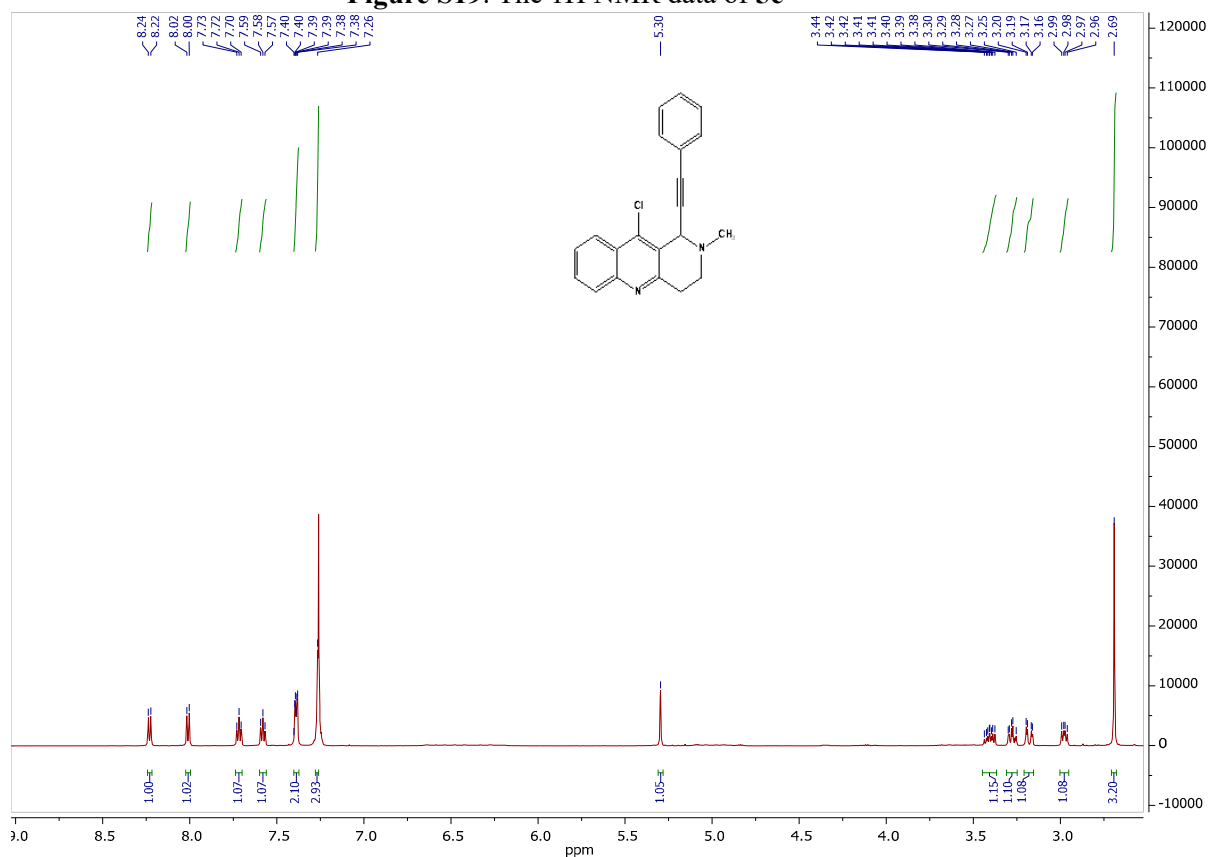


Figure S20. The  $^1\text{H}$  NMR data of **5d**

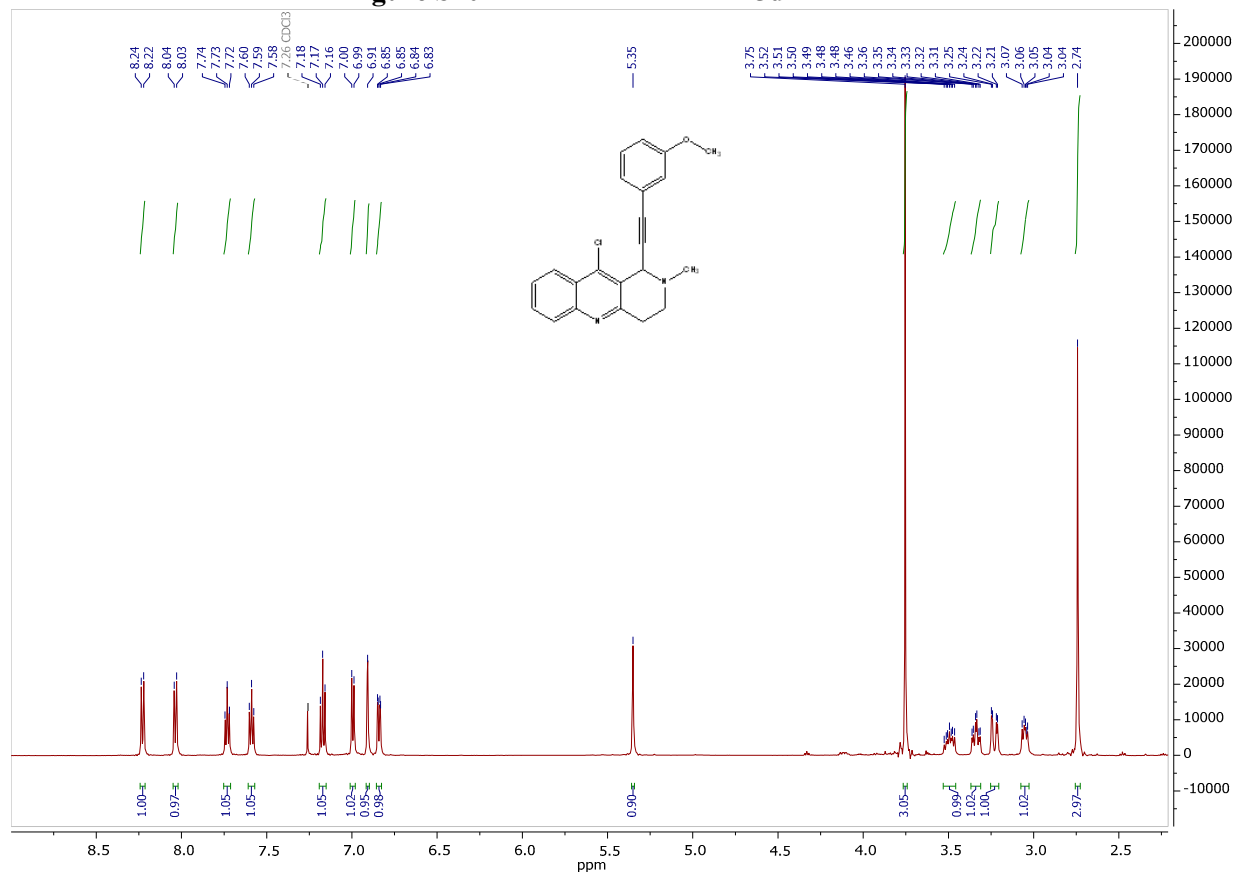
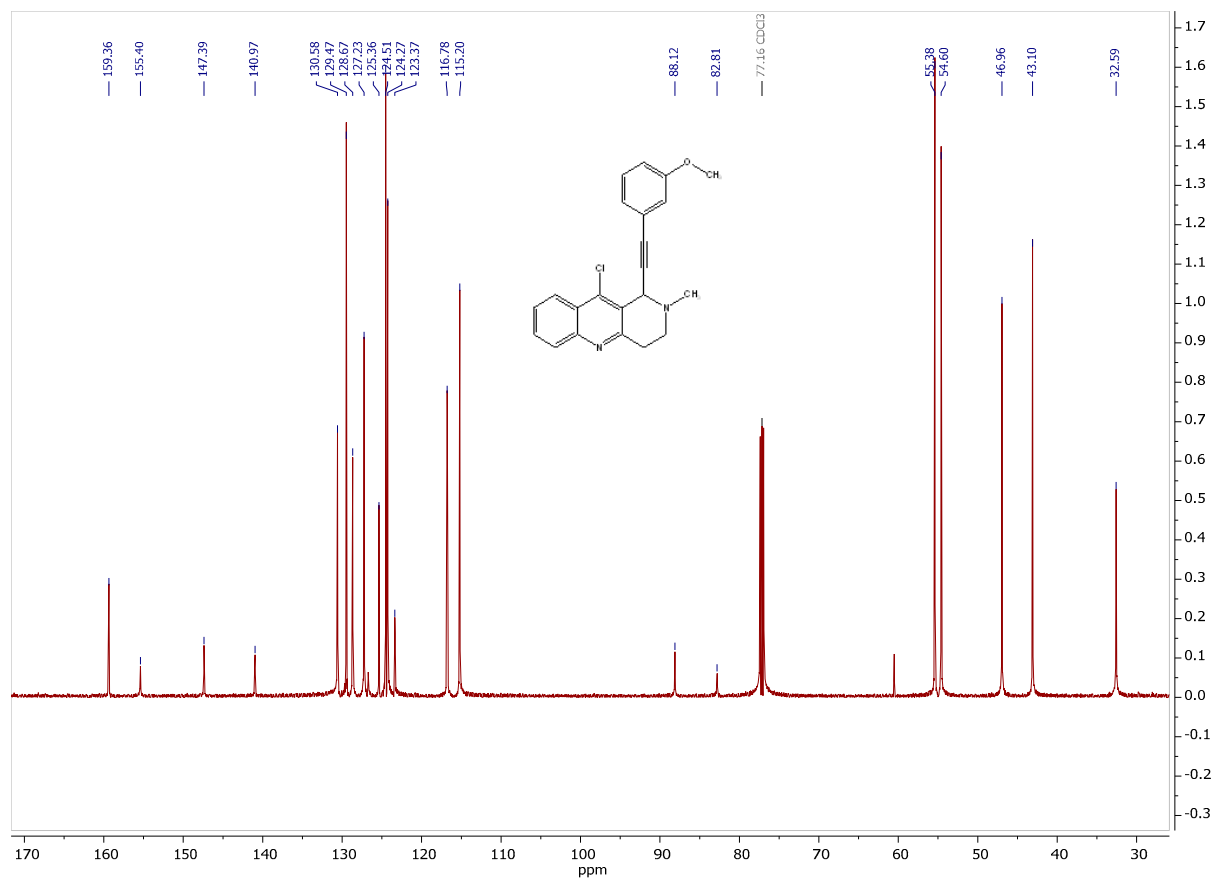
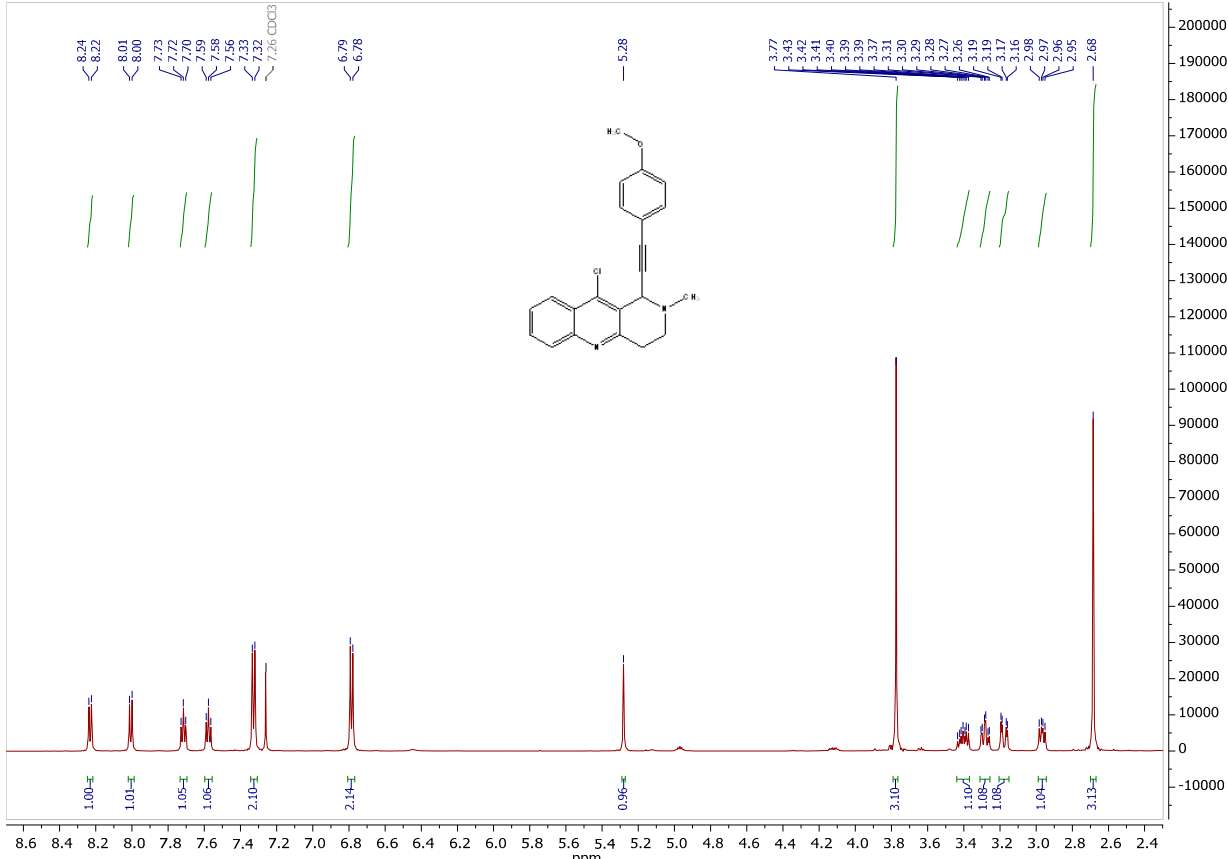


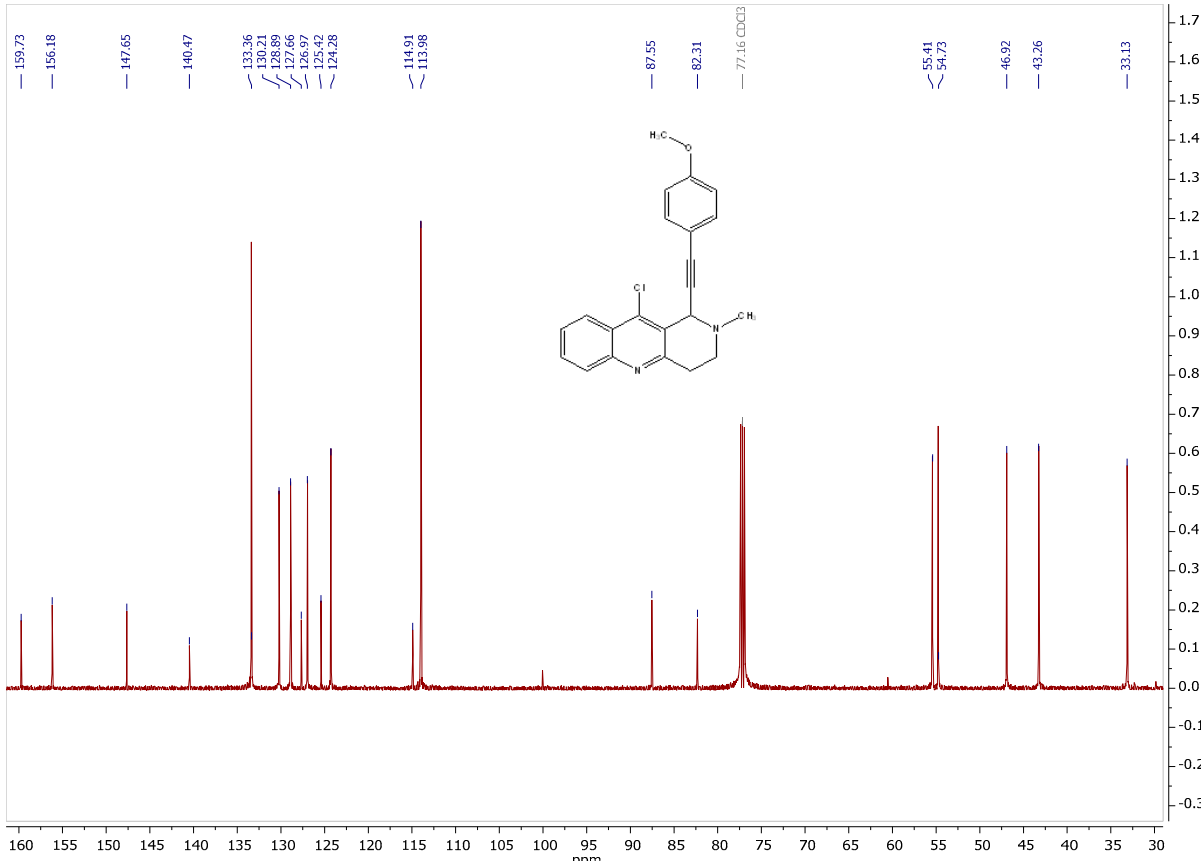
Figure S21. The  $^{13}\text{C}$  NMR data of **5d**



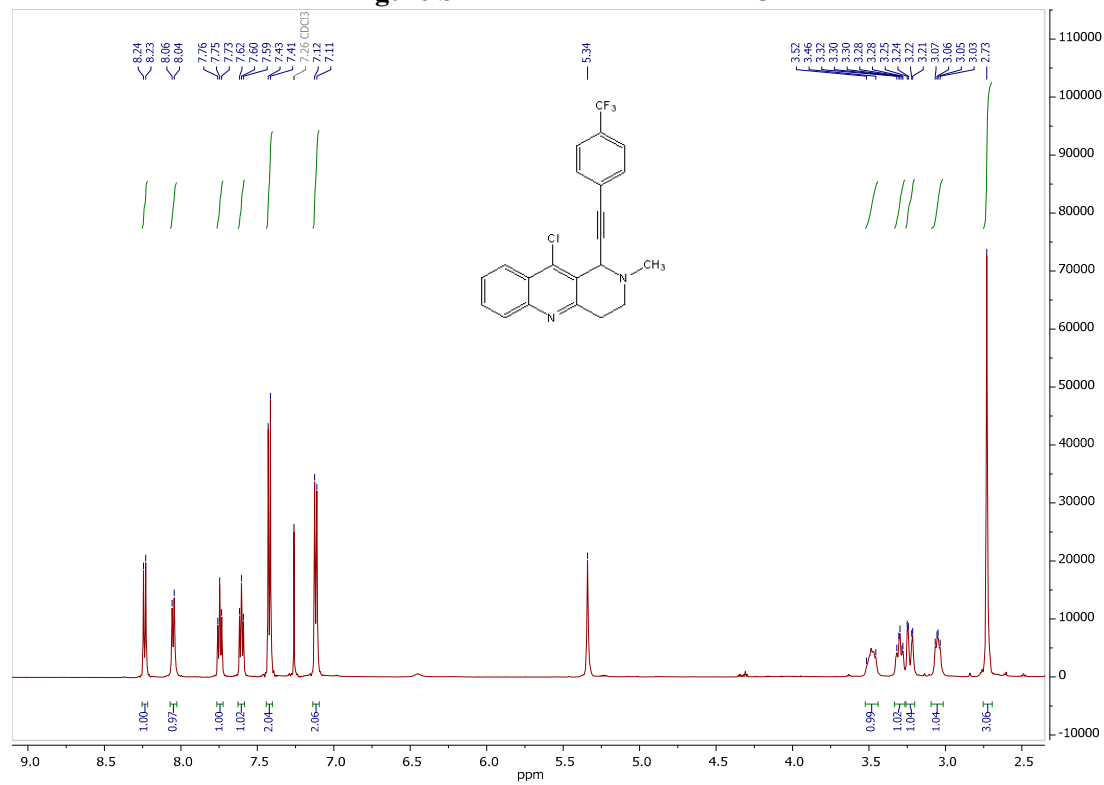
**Figure S22.** The  $^1\text{H}$  NMR data of **5e**



**Figure S23.** The  $^{13}\text{C}$  NMR data of **5e**



**Figure S24. The  $^1\text{H}$  NMR data of **5f****



**Figure S25. The  $^{13}\text{C}$  NMR data of **5f****

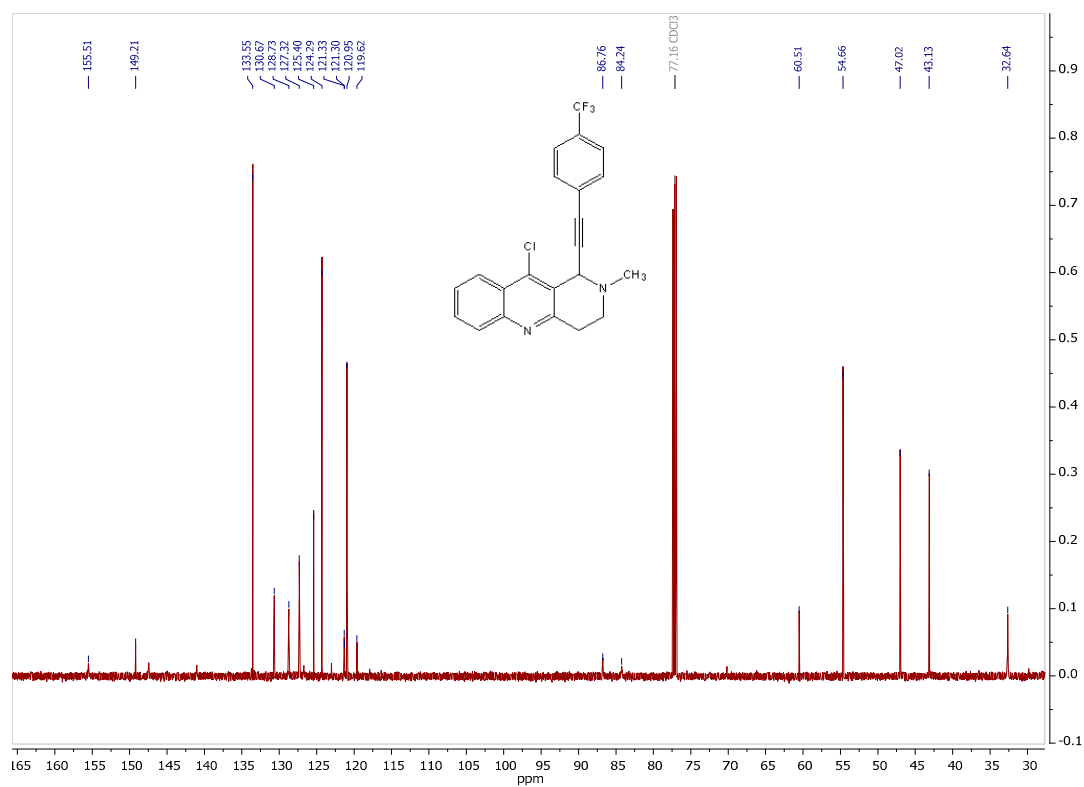


Figure S26. The  $^1\text{H}$  NMR data of **5g**

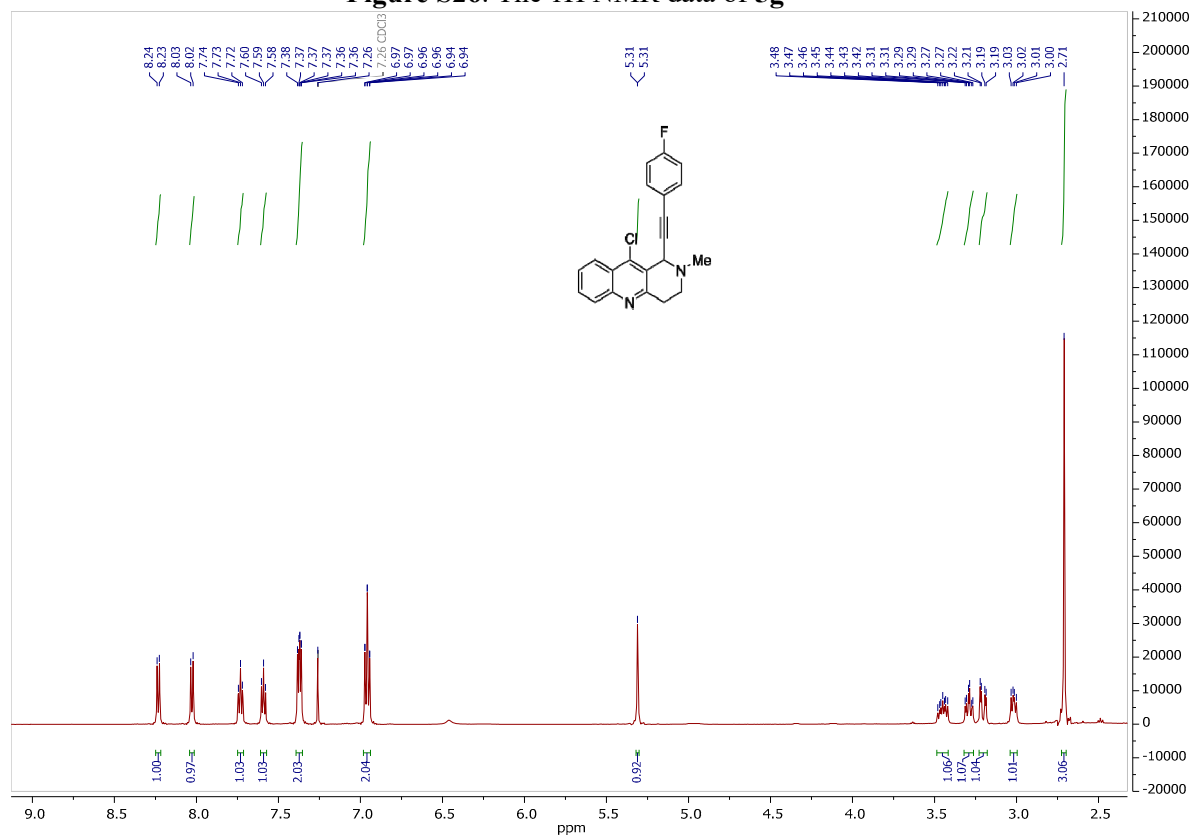
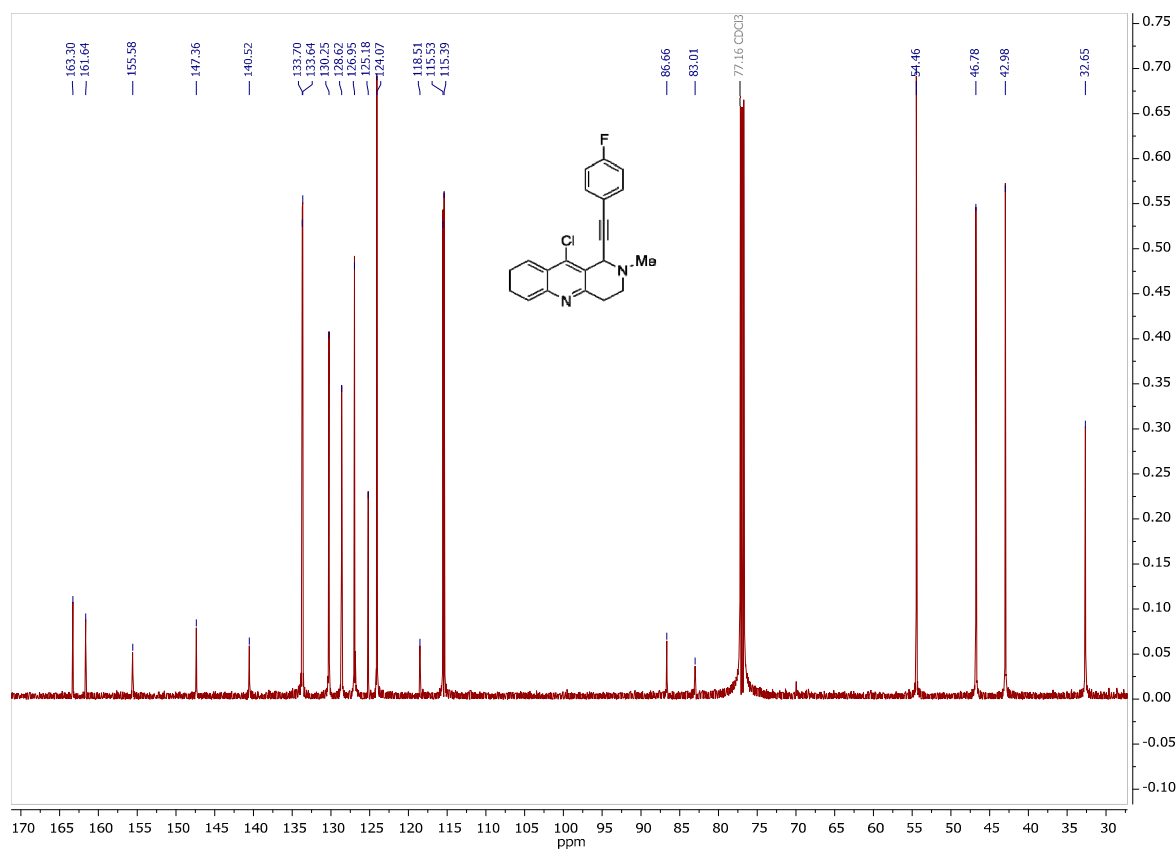
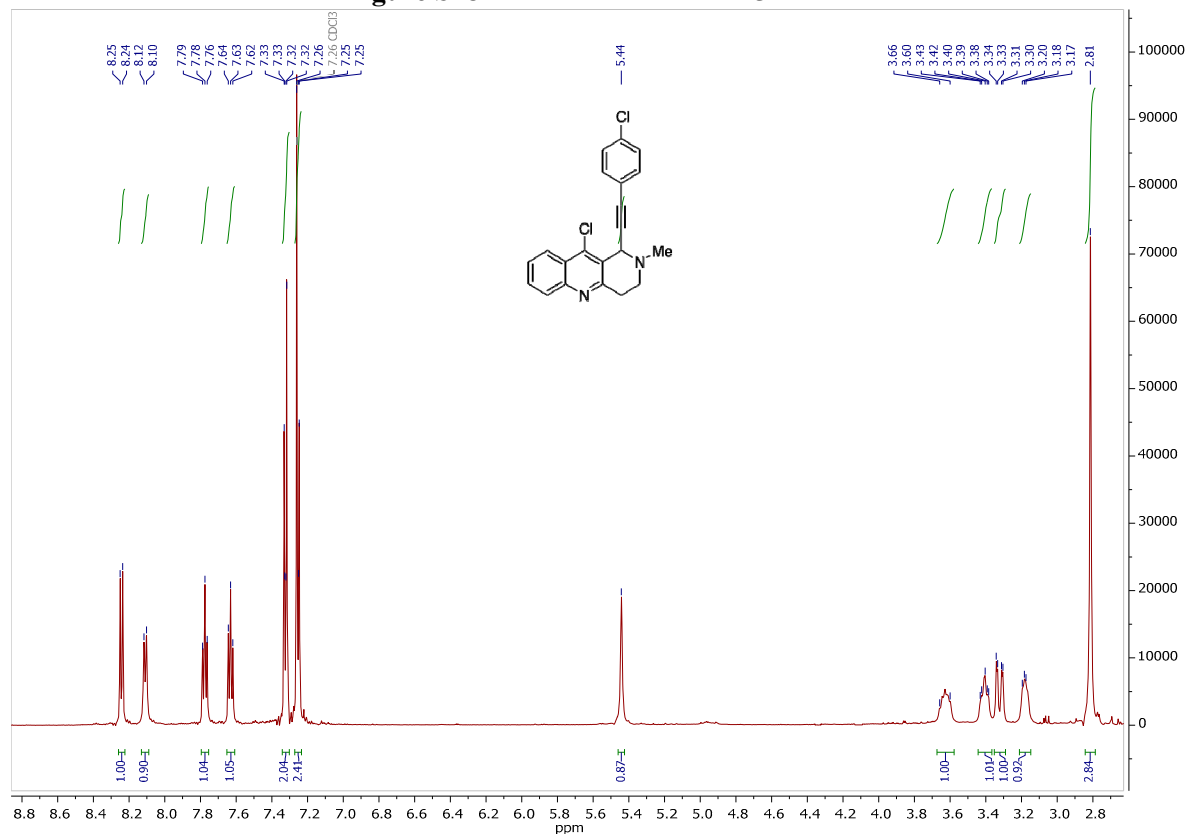


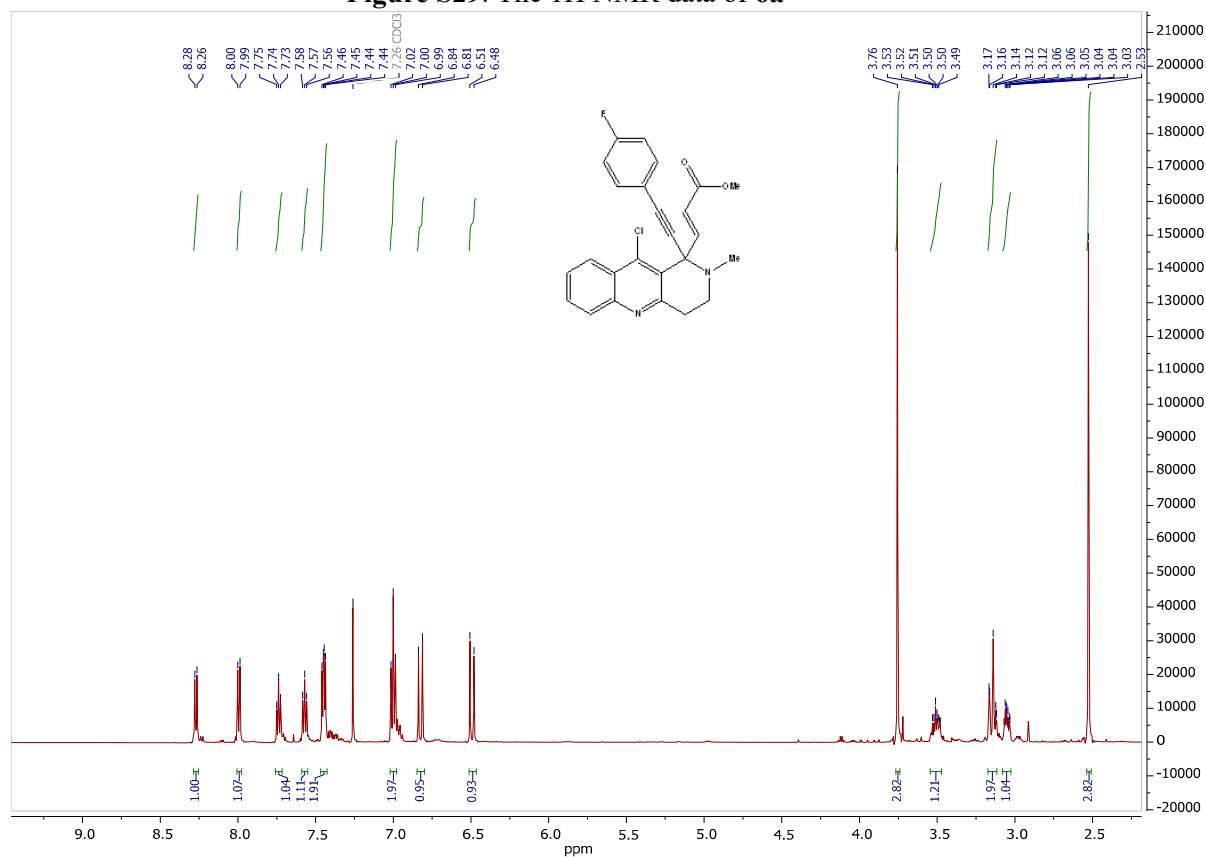
Figure S27. The  $^{13}\text{C}$  NMR data of **5g**



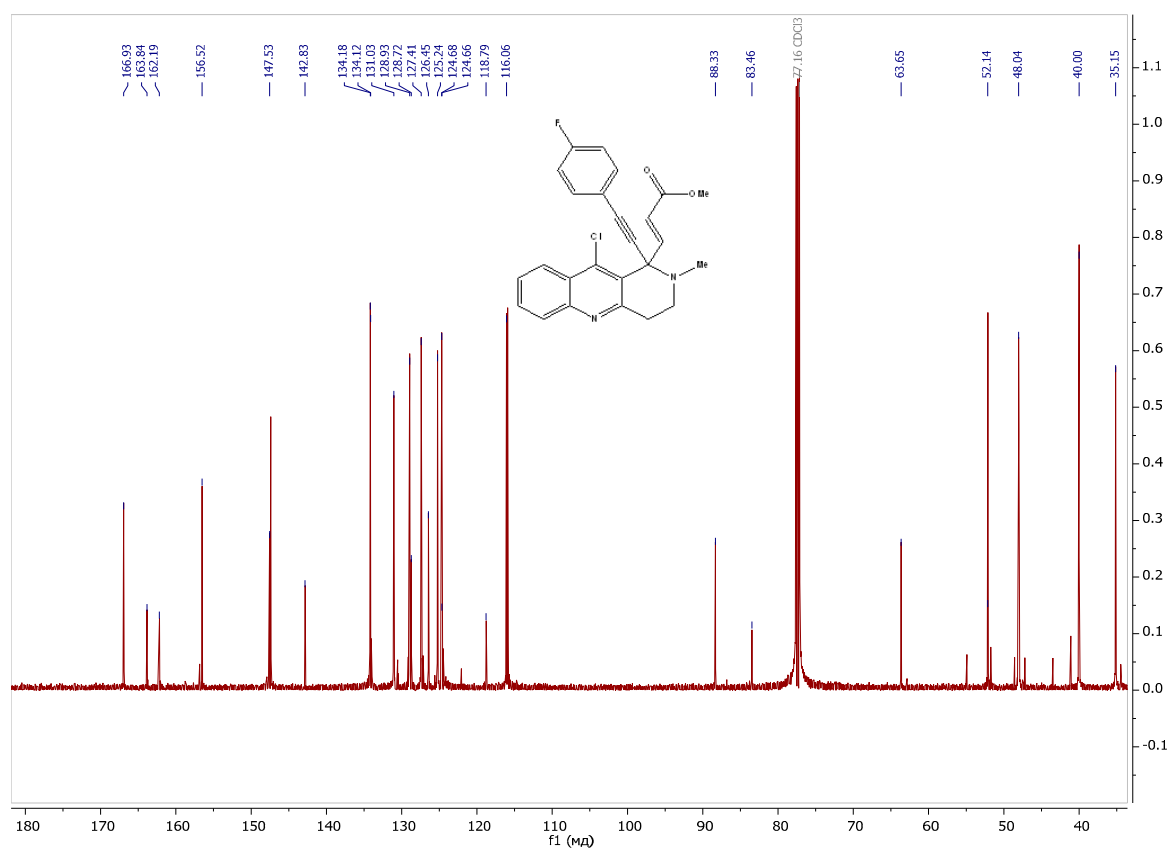
**Figure S28.** The  $^1\text{H}$  NMR data of **5h**



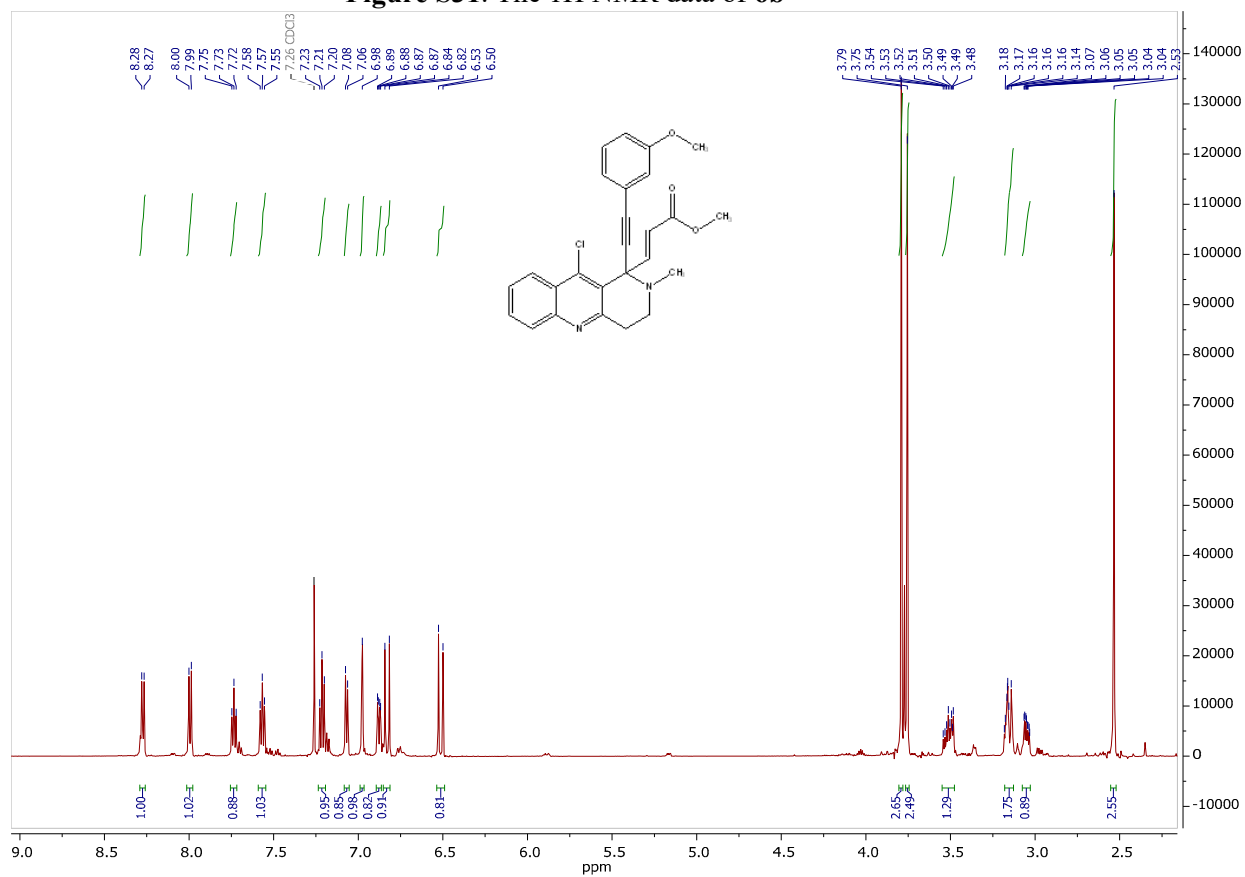
**Figure S29.** The  $^1\text{H}$  NMR data of **6a**



**Figure S30.** The  $^{13}\text{C}$  NMR data of **6a**

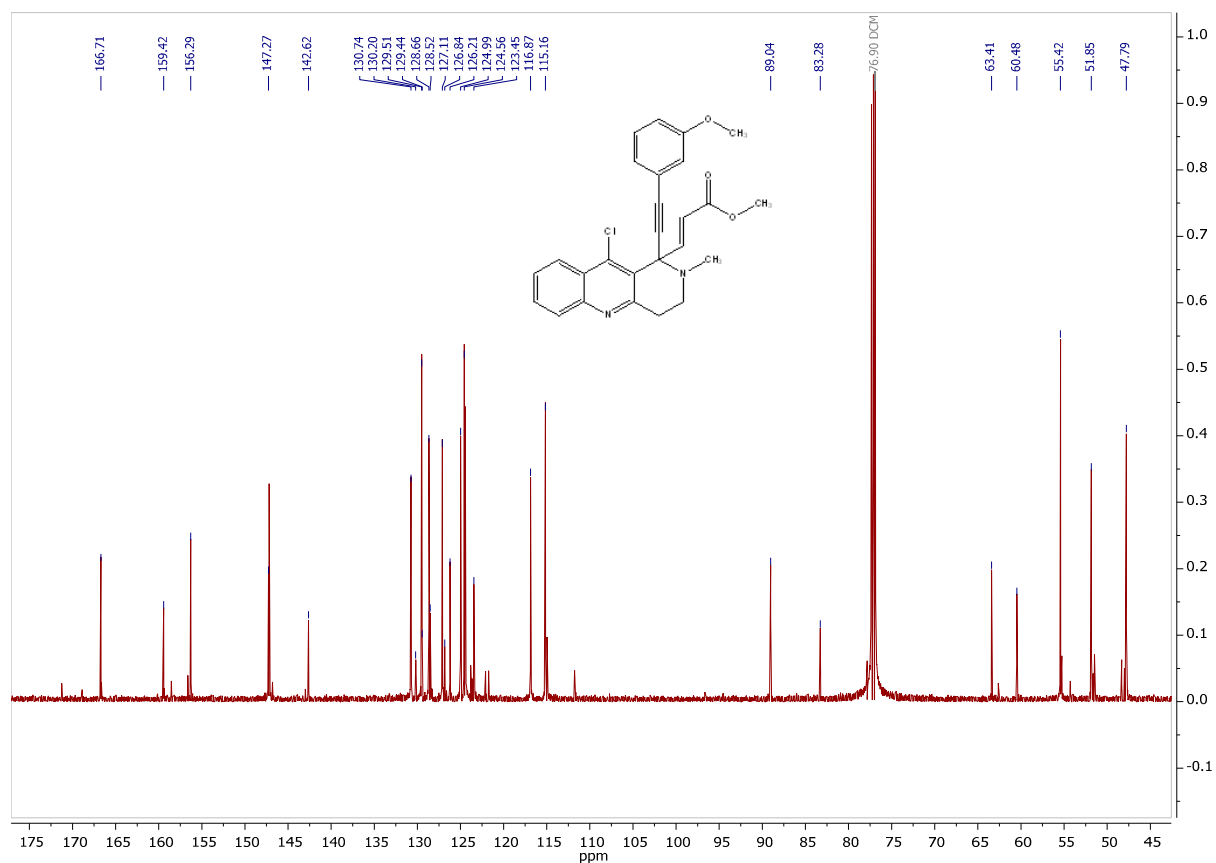


**Figure S31.** The  $^1\text{H}$  NMR data of **6b**

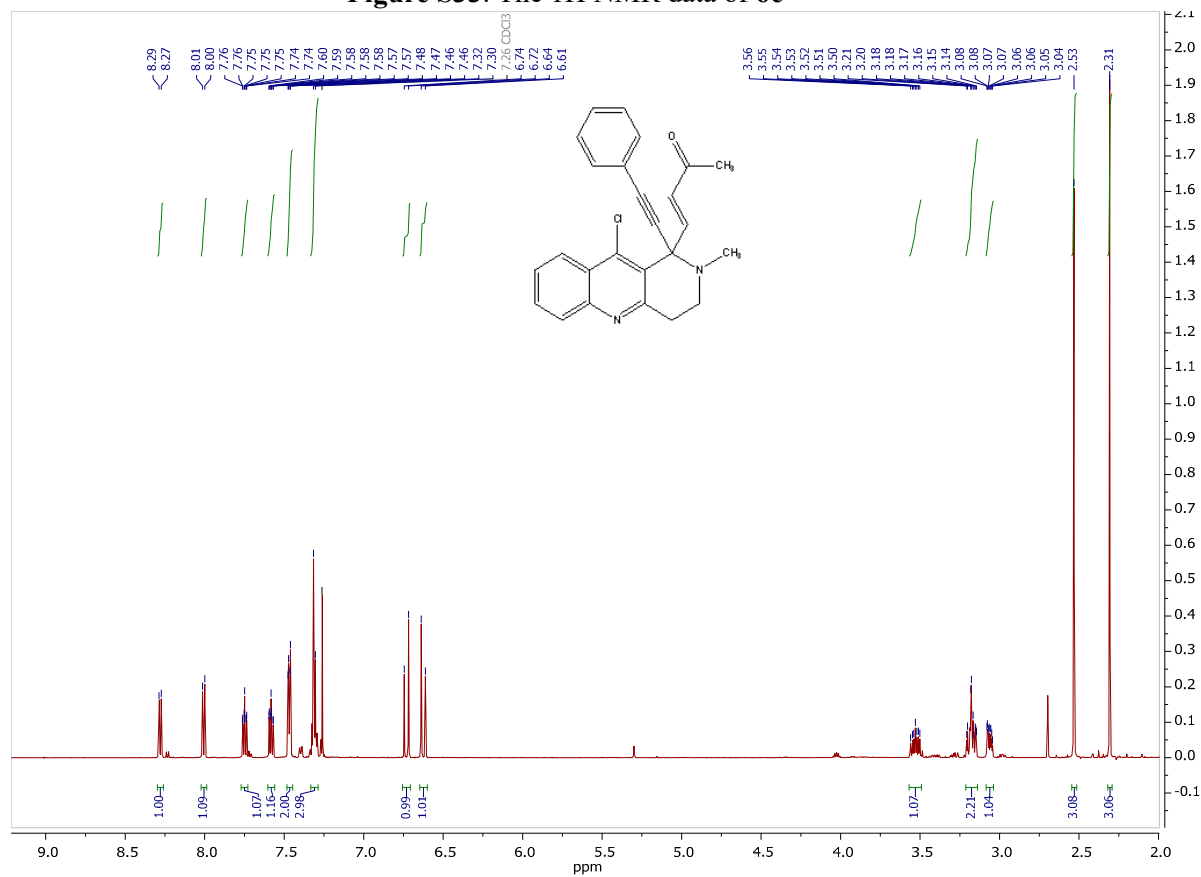




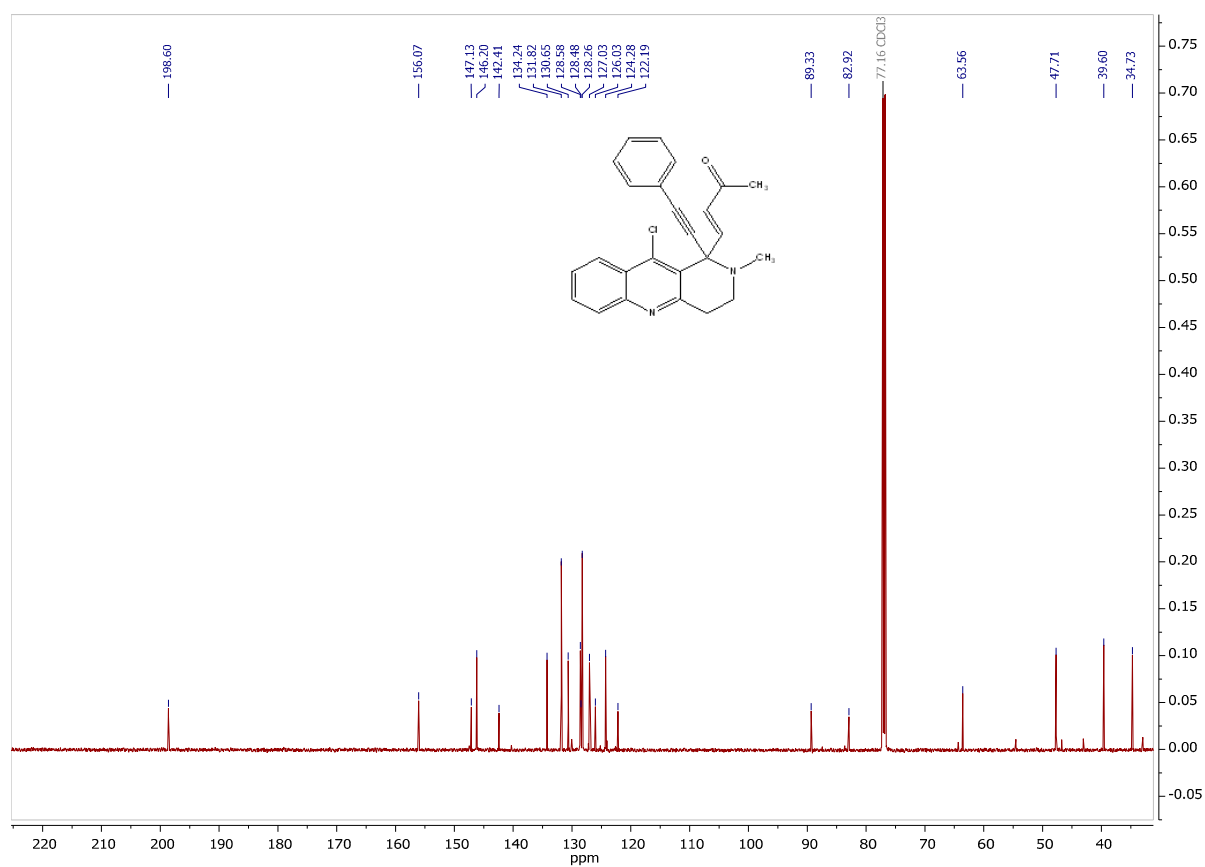
**Figure S32.** The  $^{13}\text{C}$  NMR data of **6b**



**Figure S33.** The  $^1\text{H}$  NMR data of **6c**



**Figure S34.** The  $^{13}\text{C}$  NMR data of **6c**



**Figure S35.** The  $^1\text{H}$  NMR data of **6d**

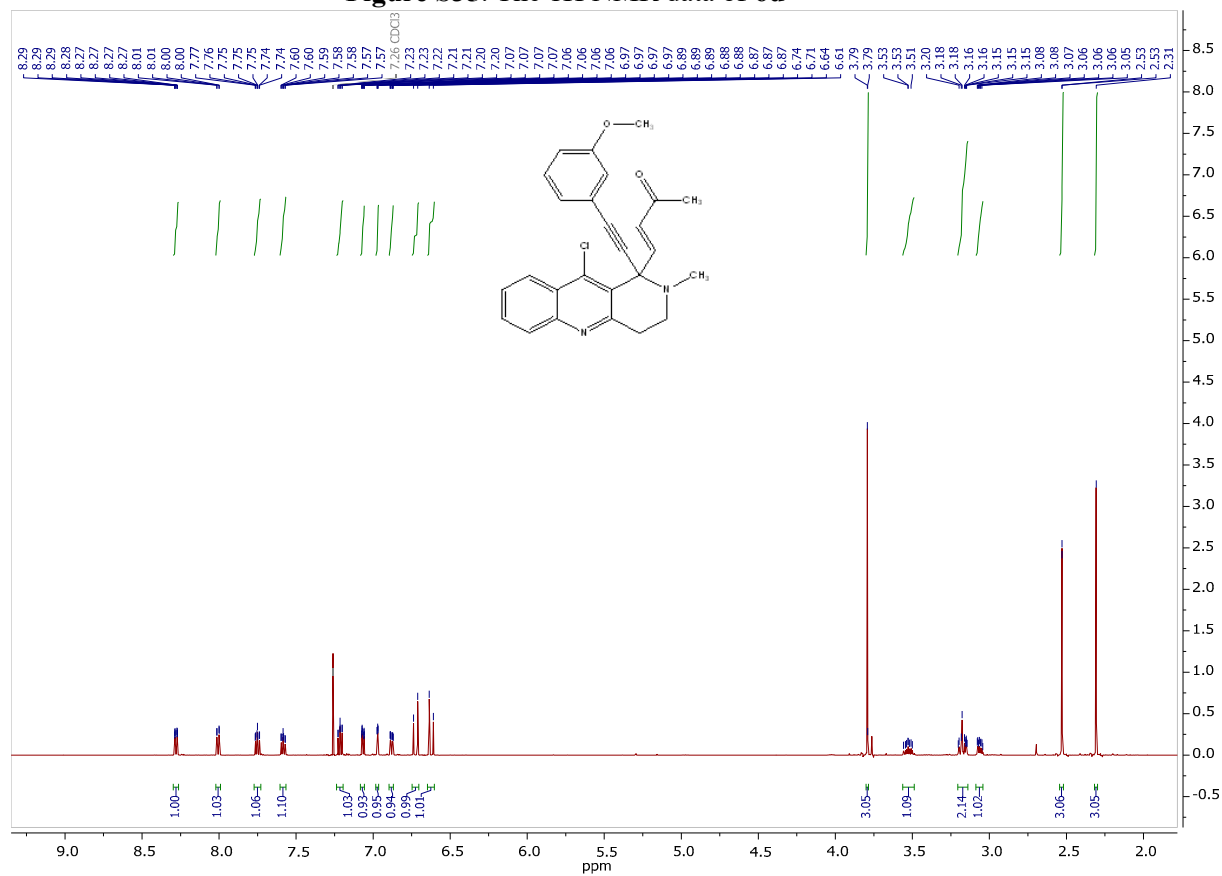


Figure S36. The  $^{13}\text{C}$  NMR data of **6d**

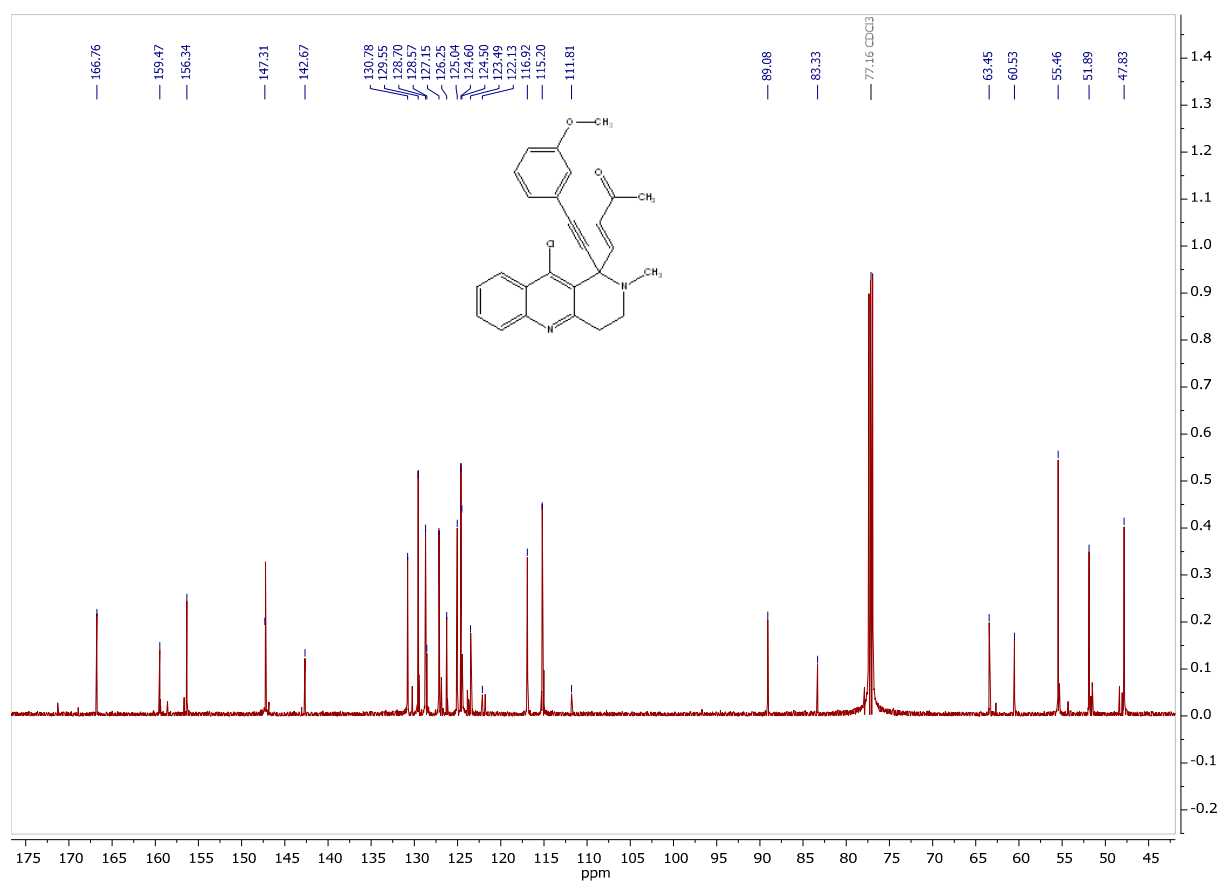
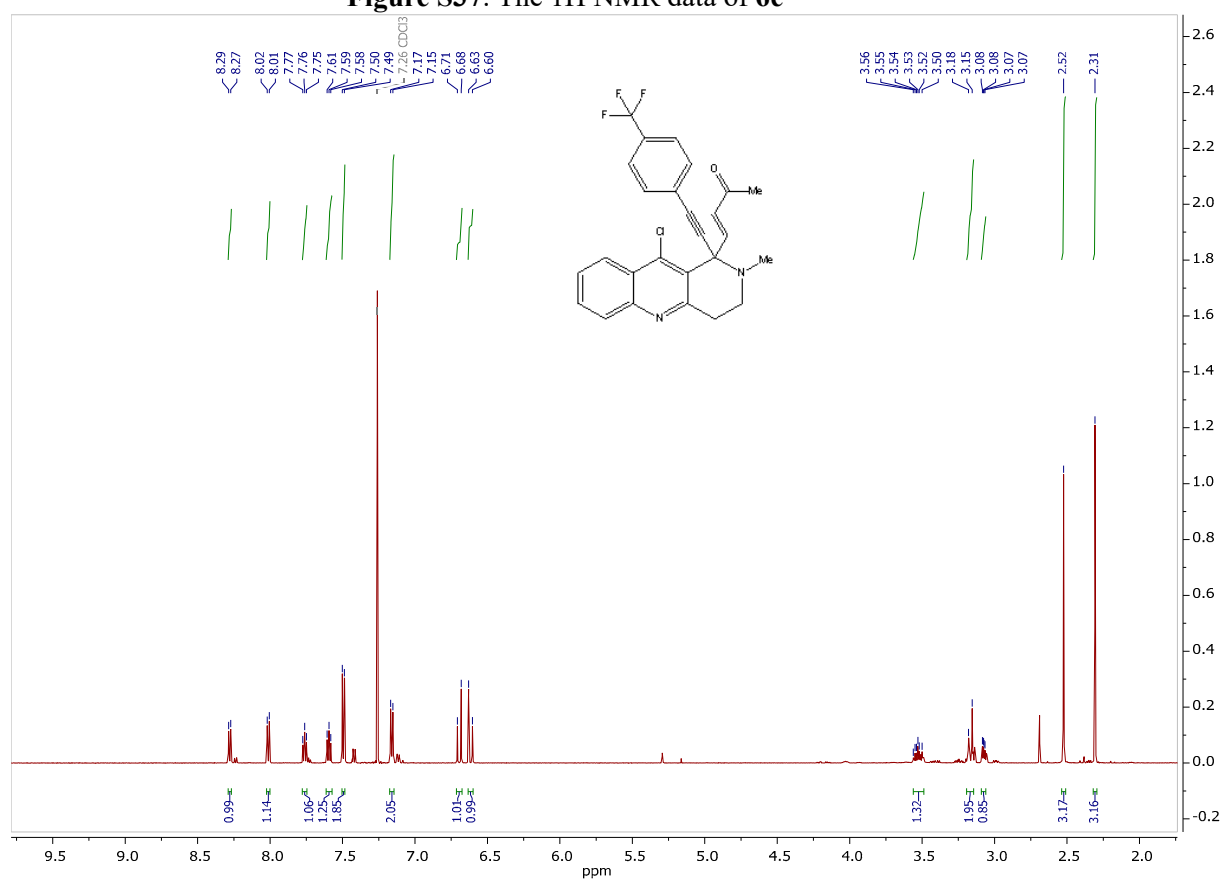
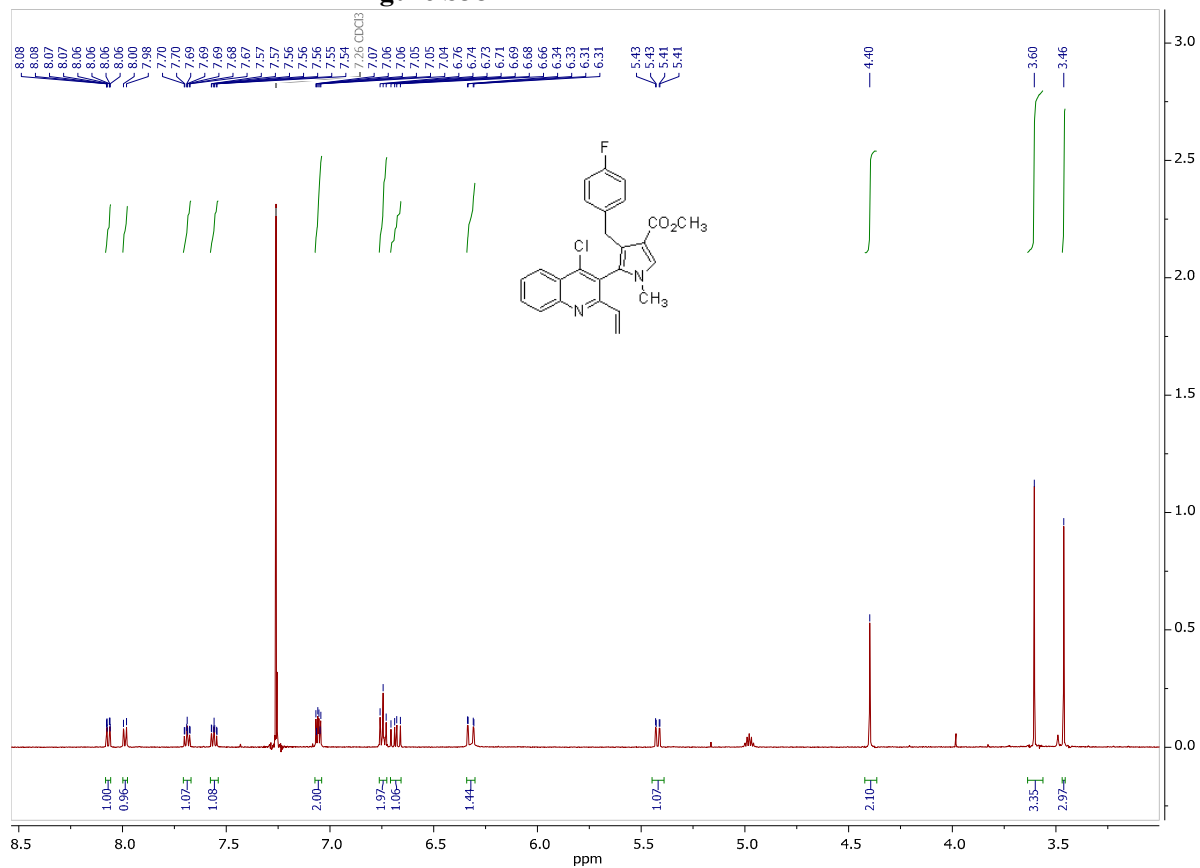


Figure S37. The  $^1\text{H}$  NMR data of **6e**



**Figure S38.** The  $^1\text{H}$  NMR data of **7**



**Figure S39.** The  $^{13}\text{C}$  NMR data of **7**

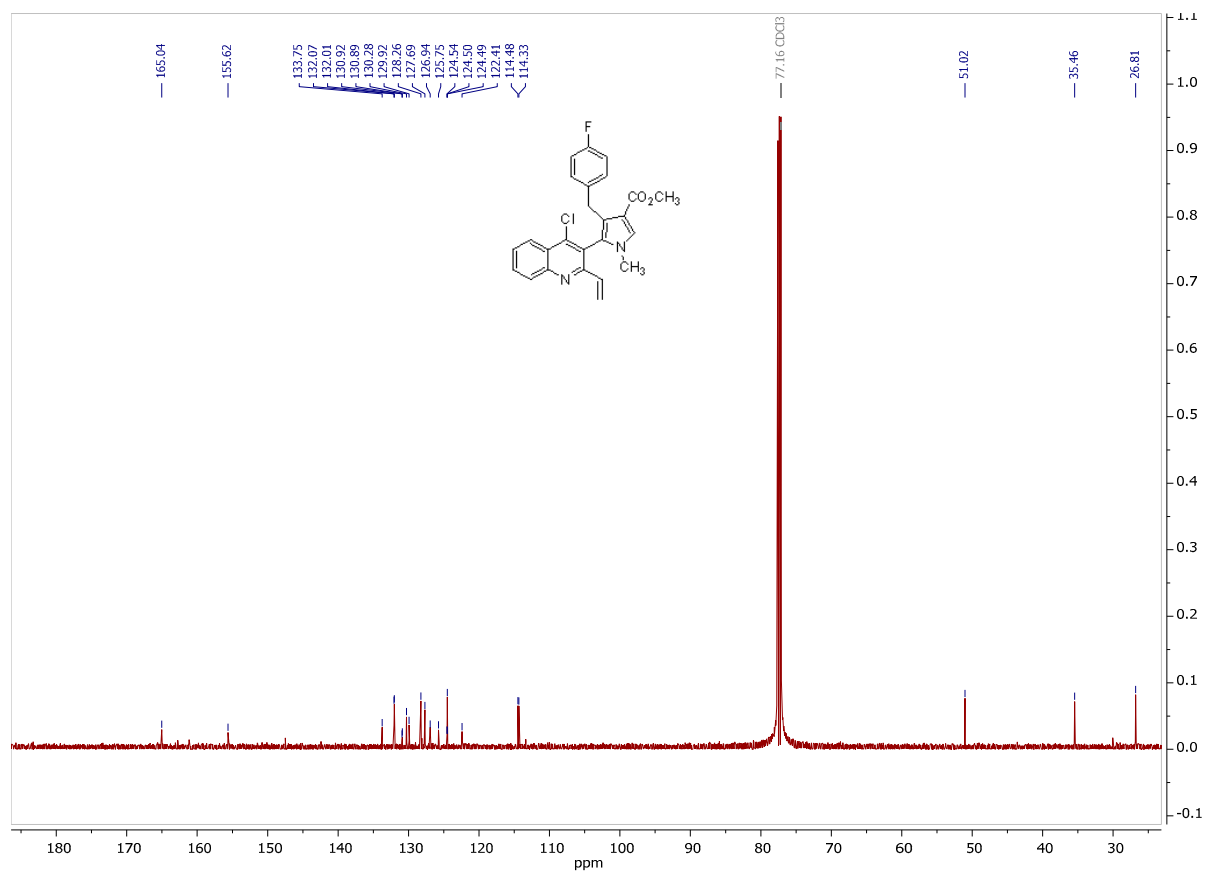


Figure S40. The  $^1\text{H}$  NMR data of **8a**

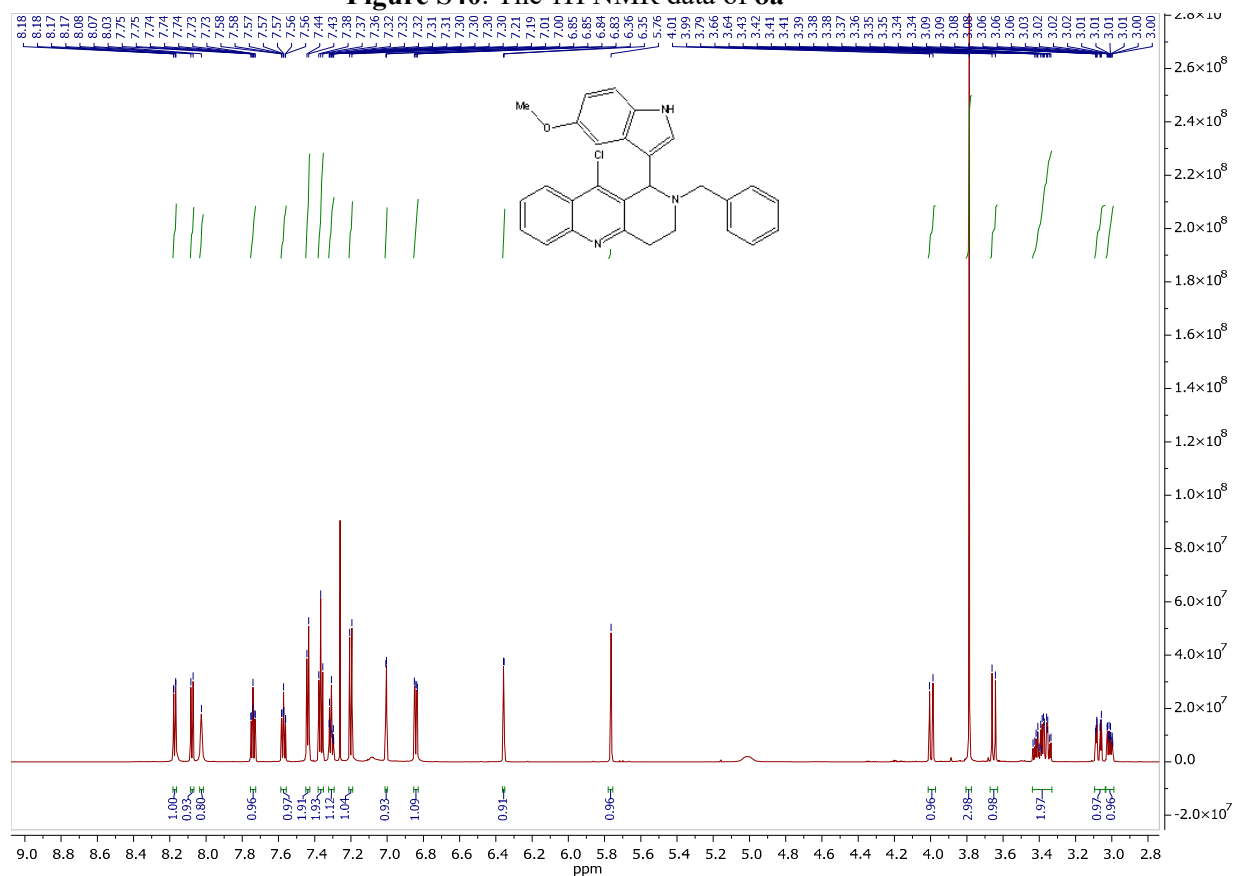


Figure S41. The  $^{13}\text{C}$  NMR data of **8a**

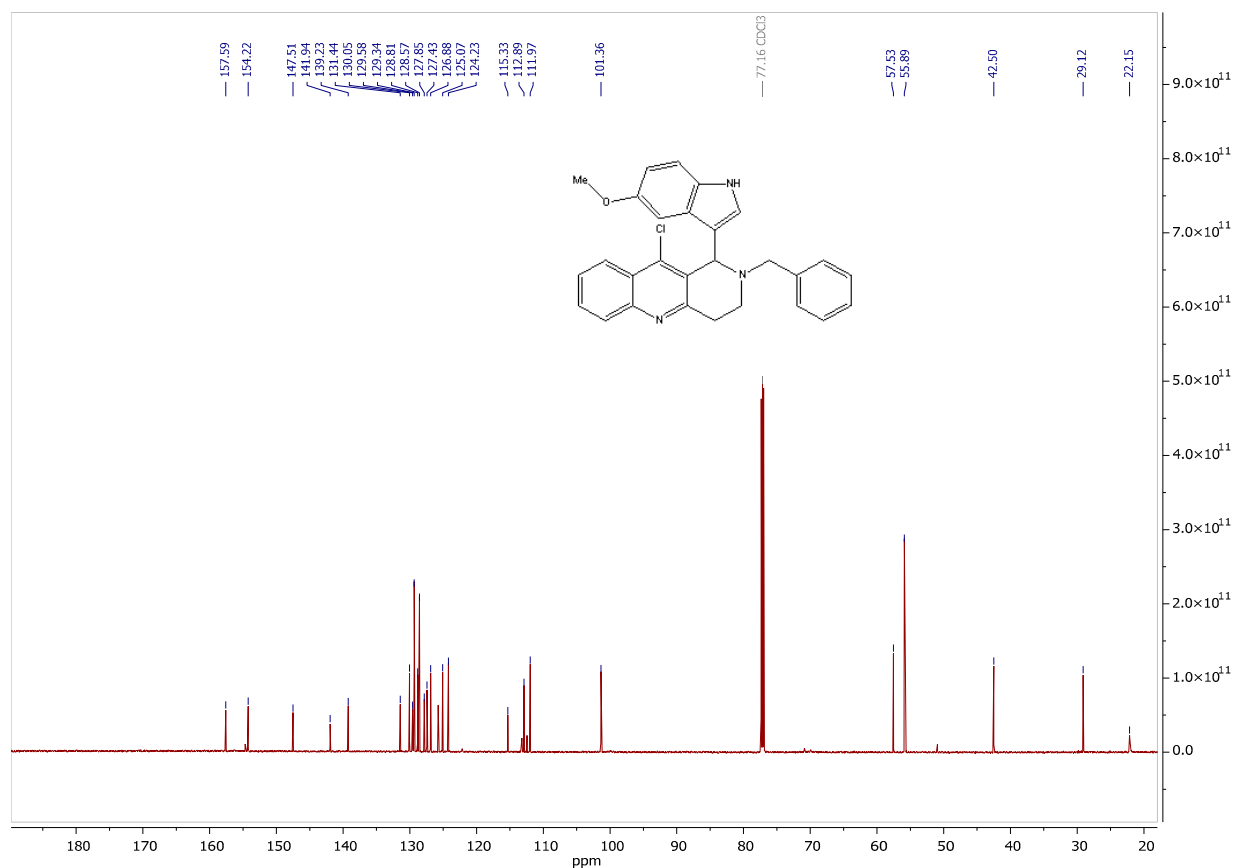


Figure S42. The  $^1\text{H}$  NMR data of **8b**

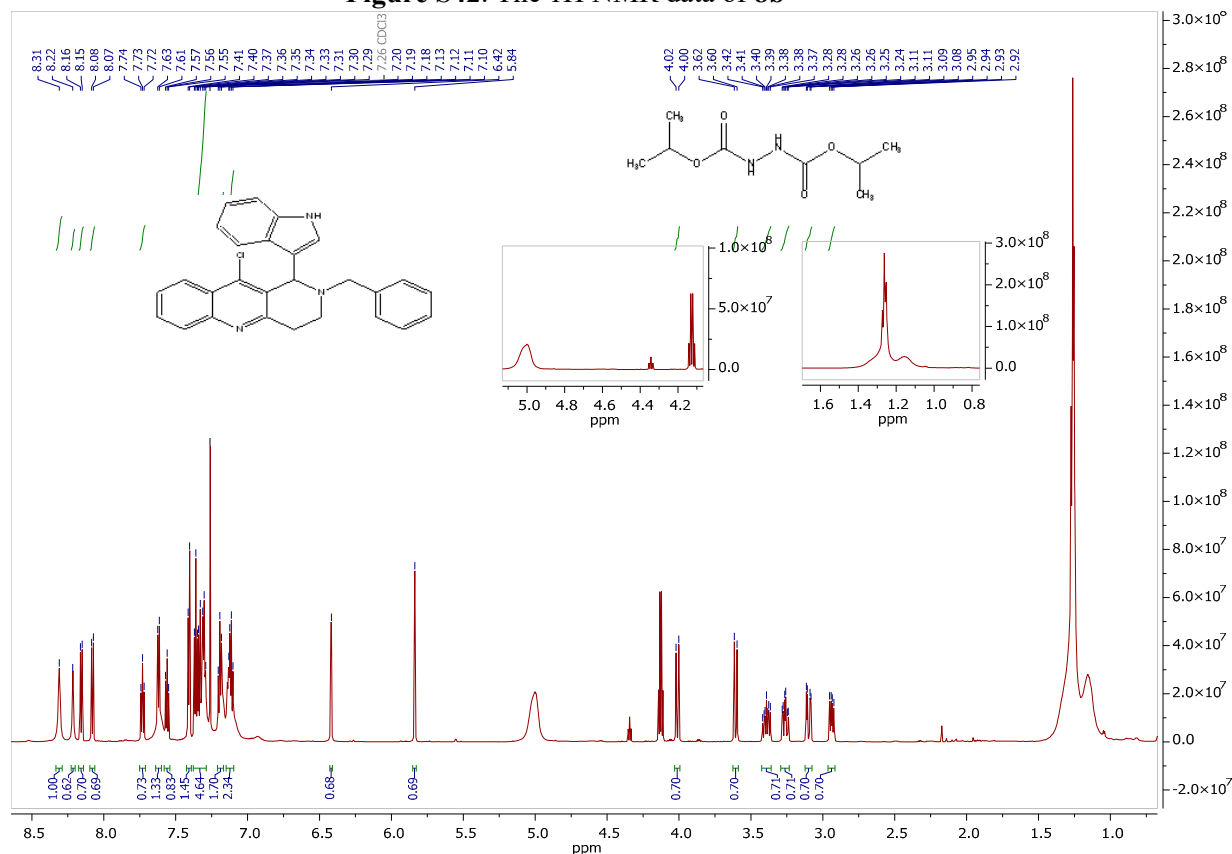
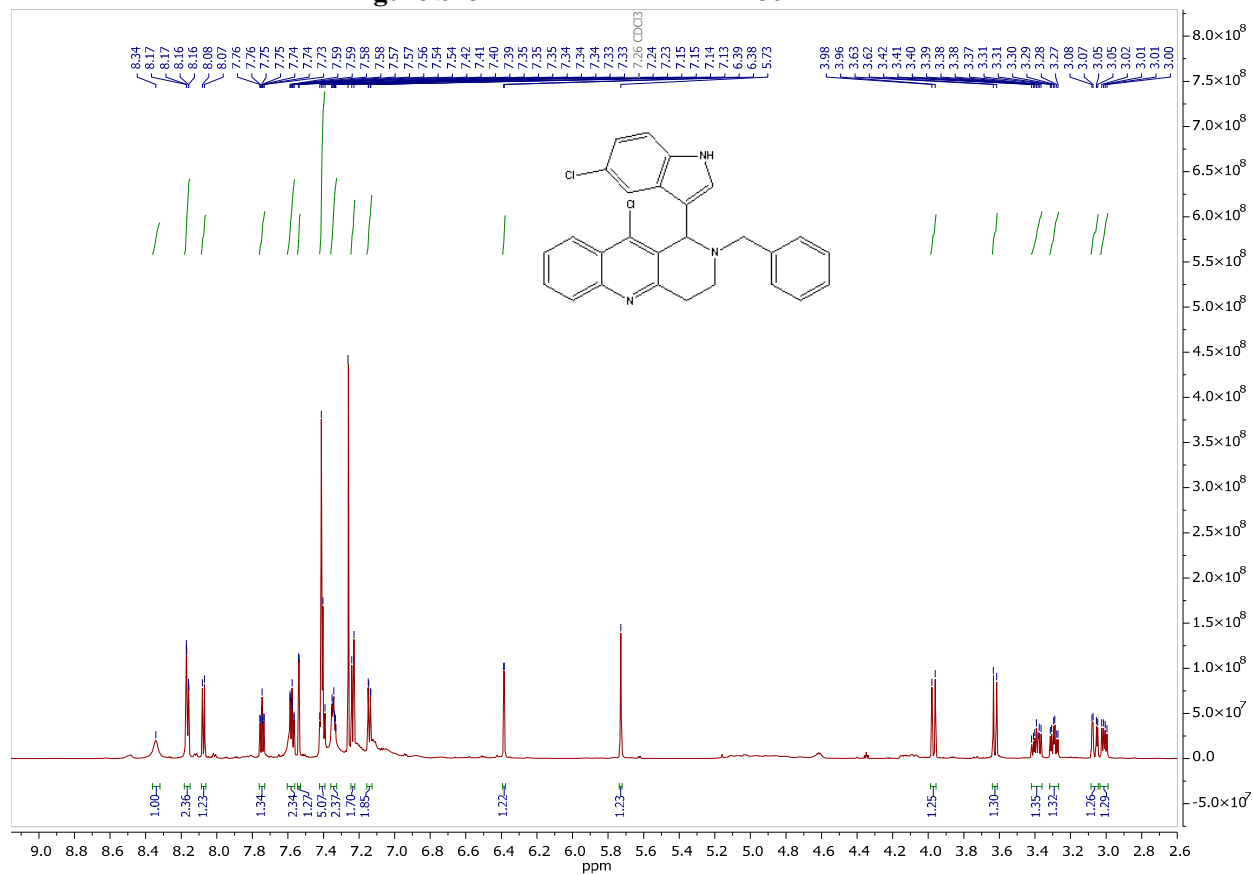
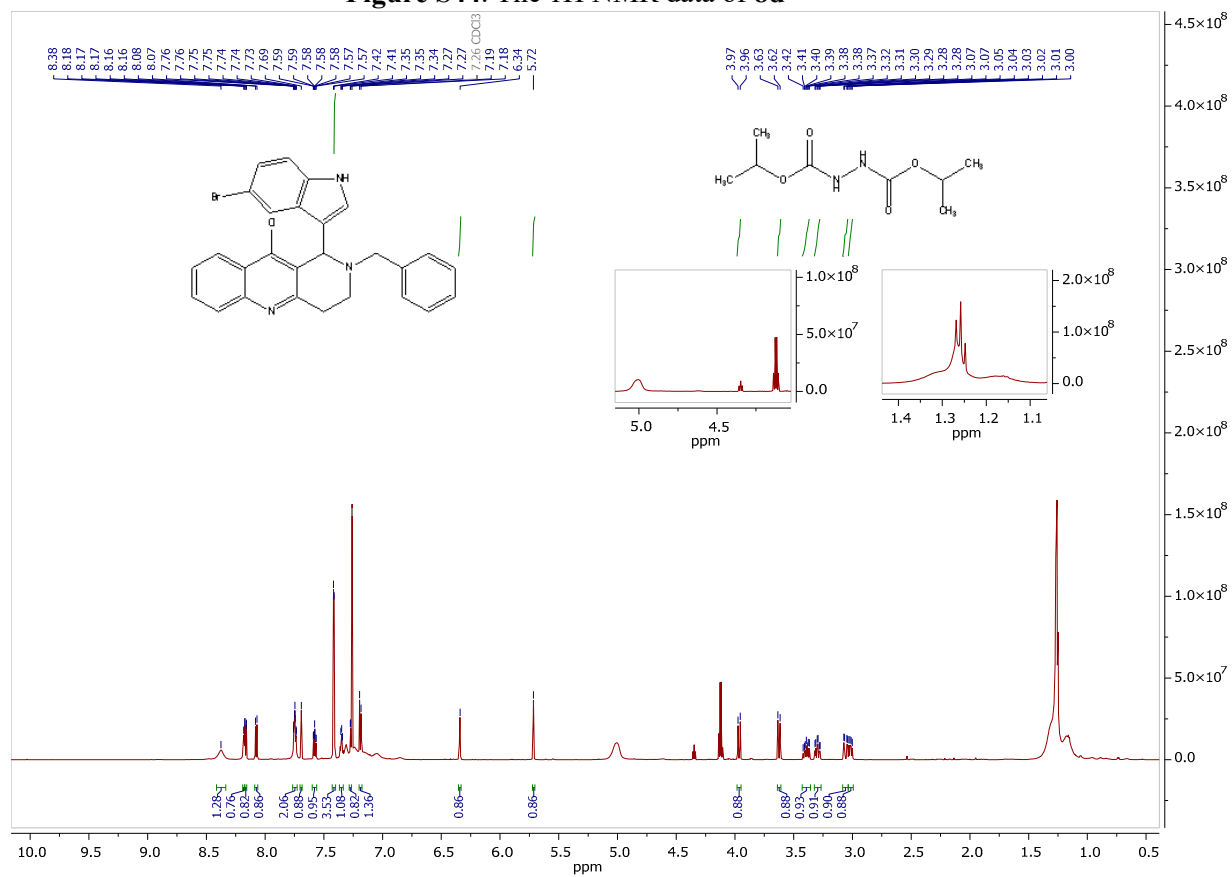


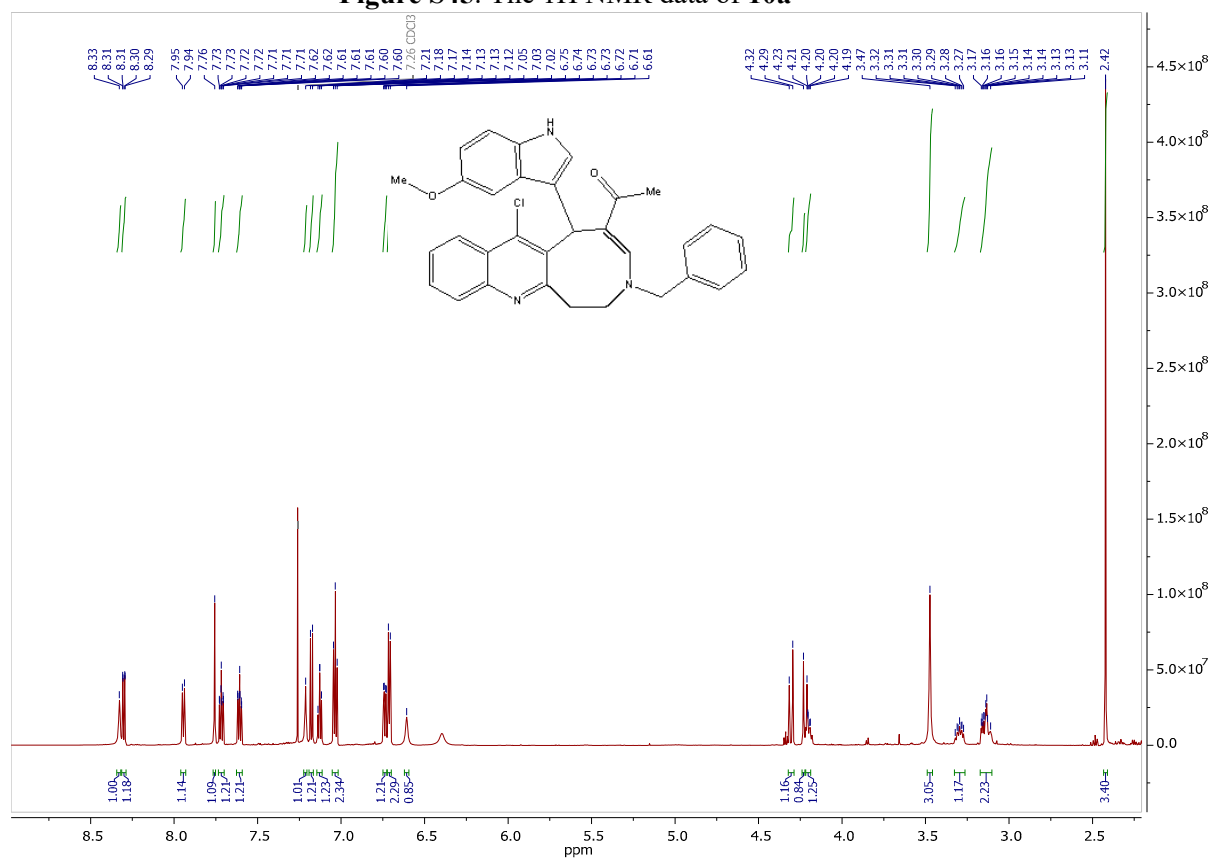
Figure S43. The  $^1\text{H}$  NMR data of **8c**



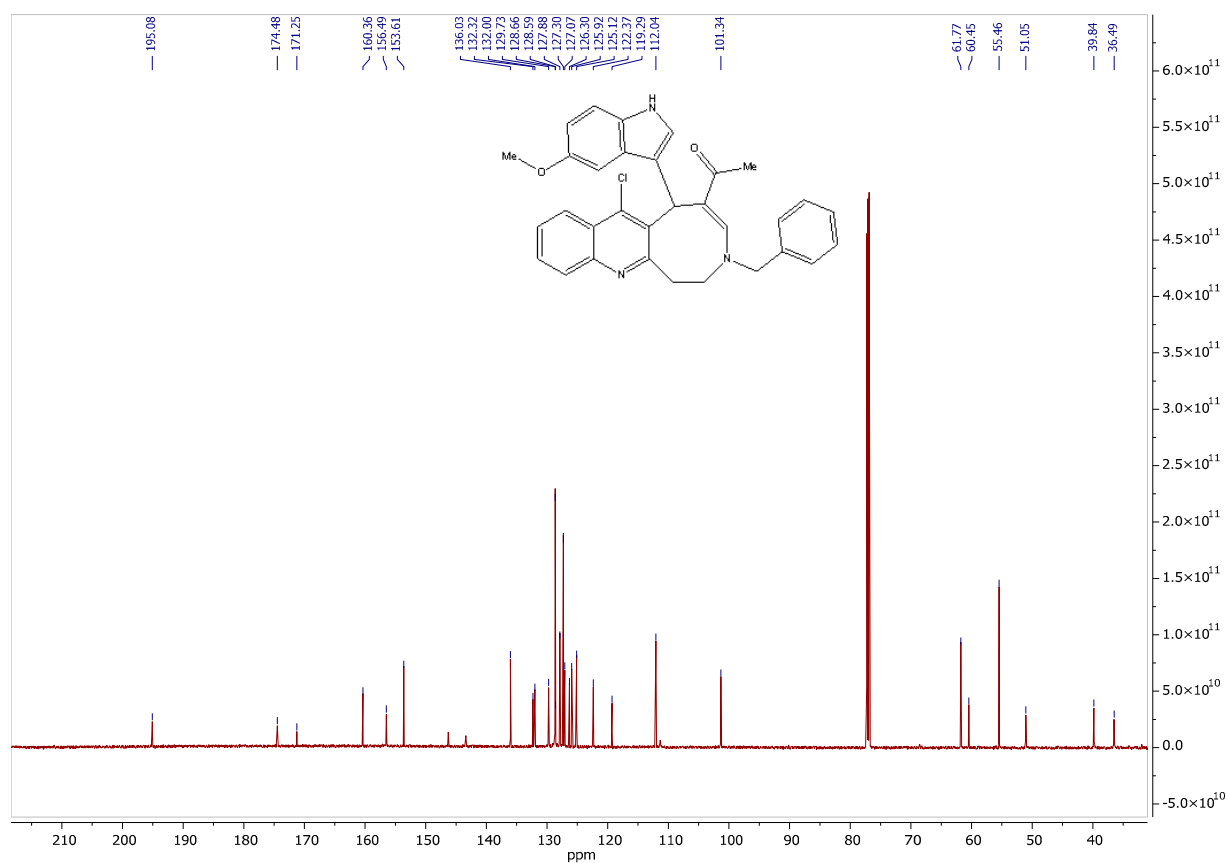
**Figure S44. The  $^1\text{H}$  NMR data of **8d****



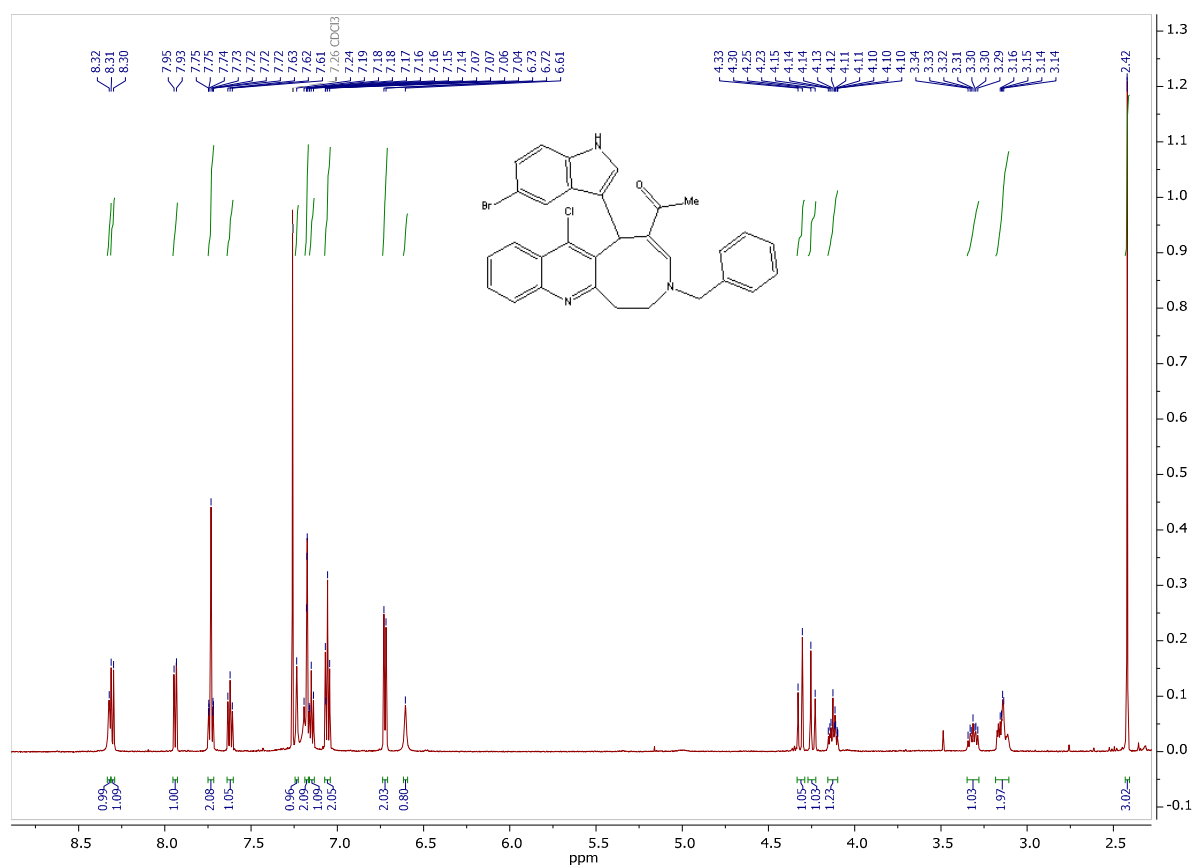
**Figure S45. The  $^1\text{H}$  NMR data of **10a****



**Figure S46.** The  $^{13}\text{C}$  NMR data of **10a**

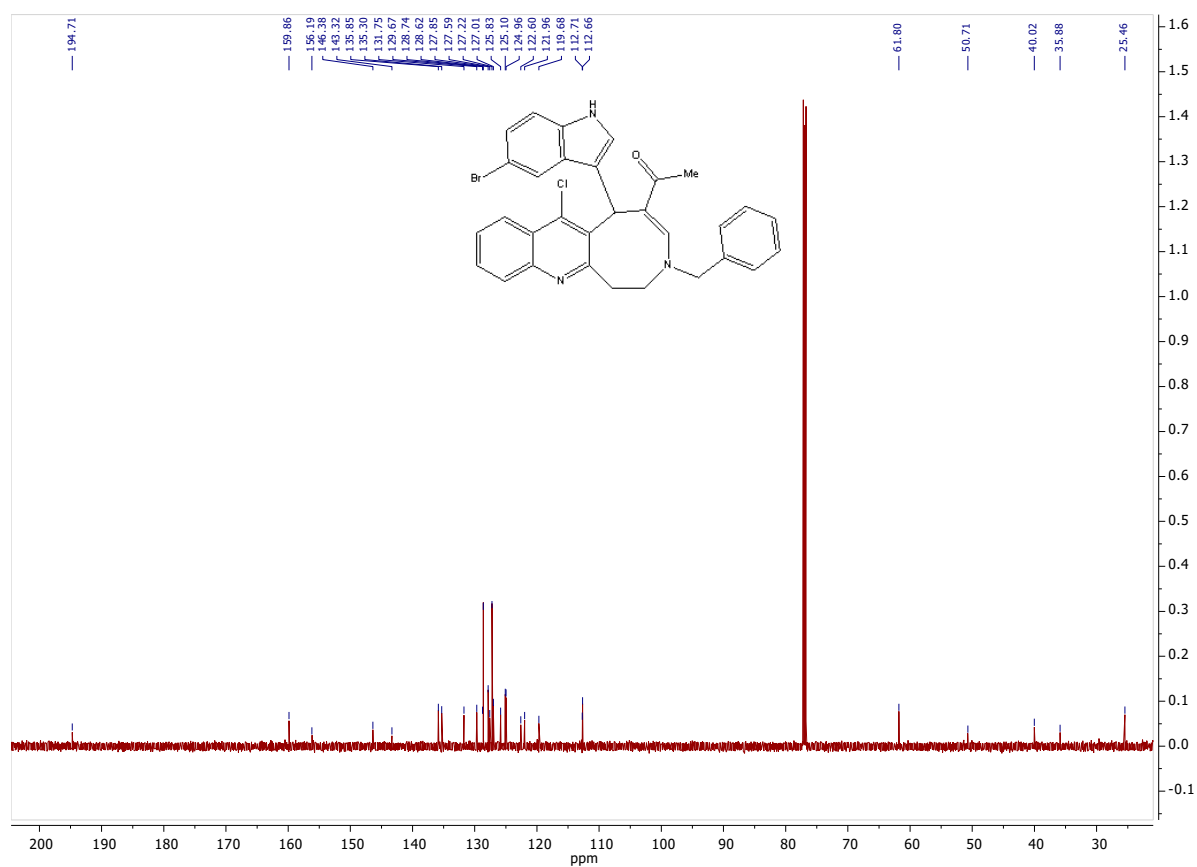


**Figure S47.** The  $^1\text{H}$  NMR data of **10b**

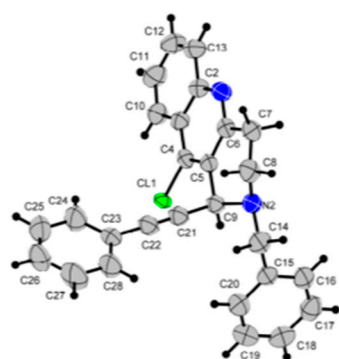




**Figure S48.** The  $^{13}\text{C}$  NMR data of **10b**



The crystallographic data compound **5a**.



A single crystal X-ray analysis of compound **5a**.

**Table S1.** Crystal data and structure refinement for **5a**.

Empirical formula	$\text{C}_{27}\text{H}_{21}\text{ClN}_2$
Formula weight	408.91
Temperature	295(2) K
Wavelength	1.54186 Å
Crystal system	Triclinic
Space group	P -1

Unit cell dimensions	a = 8.711(3) Å	$\alpha$ = 84.483(3)°.
	b = 9.2683(3) Å	$\beta$ = 77.132(3)°.
	c = 14.6665(5) Å	$\gamma$ = 67.091(3)°.
Volume	1063.2(4) Å <sup>3</sup>	
Z	2	
Density (calculated)	1.277 Mg/m <sup>3</sup>	
Absorption coefficient	1.698 mm <sup>-1</sup>	
F(000)	428	
Theta range for data collection	5.181 to 67.500°.	
Index ranges	-9<=h<=10, -7<=k<=11, -16<=l<=17	
Reflections collected	10522	
Independent reflections	3611 [R(int) = 0.0414]	
Completeness to theta = 67.500°	94.2 %	
Refinement method	Full-matrix least-squares on F <sup>2</sup>	
Data / restraints / parameters	3611 / 0 / 276	
Goodness-of-fit on F <sup>2</sup>	0.834	
Final R indices [I>2sigma(I)]	R1 = 0.0372, wR2 = 0.0798	
R indices (all data)	R1 = 0.0698, wR2 = 0.0871	
Extinction coefficient	0.0067(4)	
Largest diff. peak and hole	0.152 and -0.191 e. Å <sup>-3</sup>	