

Supporting Information for

Selective Hydration of Electron-Rich Aryl-Alkynes by a Schrock-type

Molybdenum Alkylidene Catalyst

by

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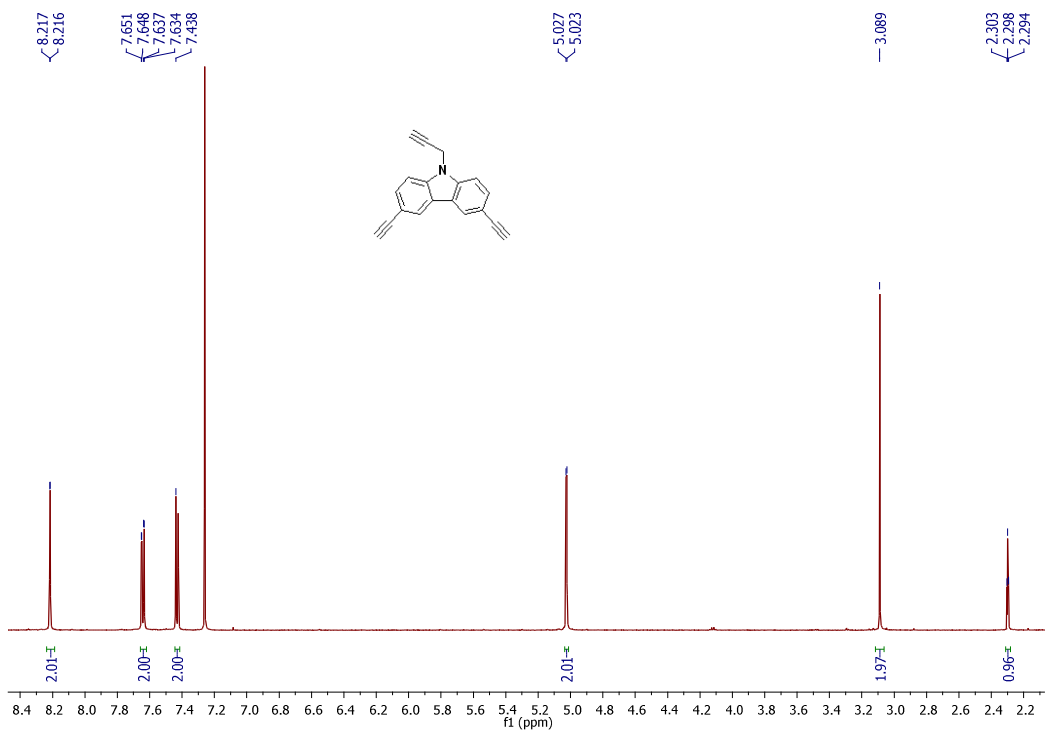


Figure S1. ¹H-NMR (600 MHz, CDCl₃) spectrum of compound **3**

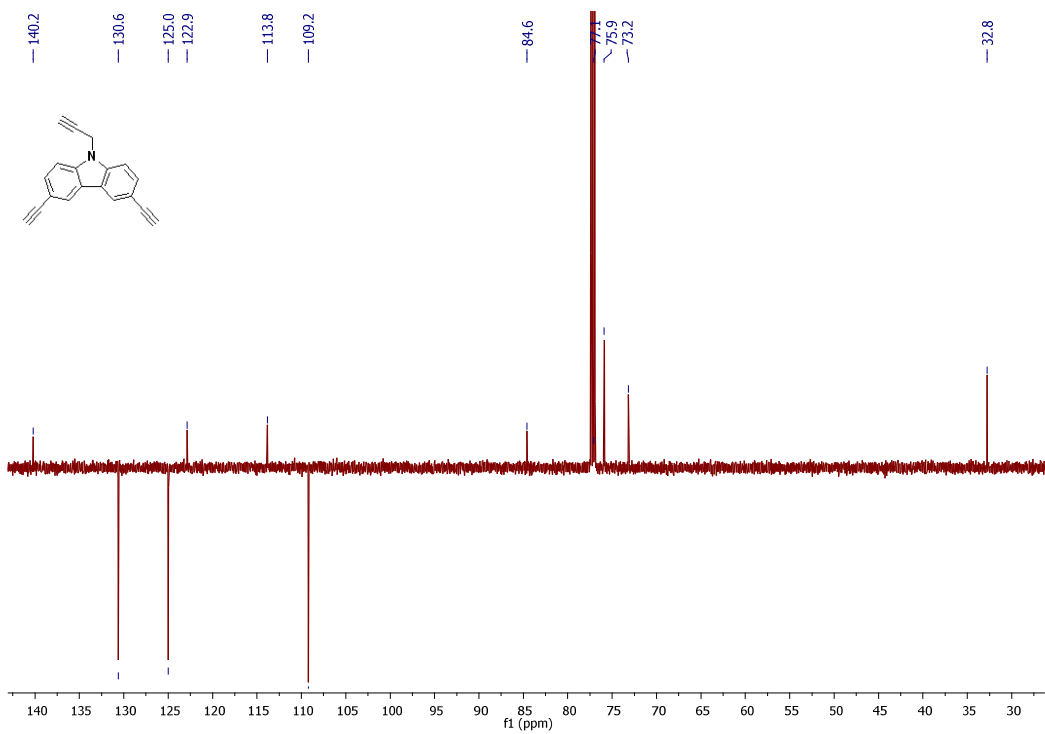


Figure S2. ^{13}C -NMR (100 MHz, CDCl_3) spectrum of compound **3**

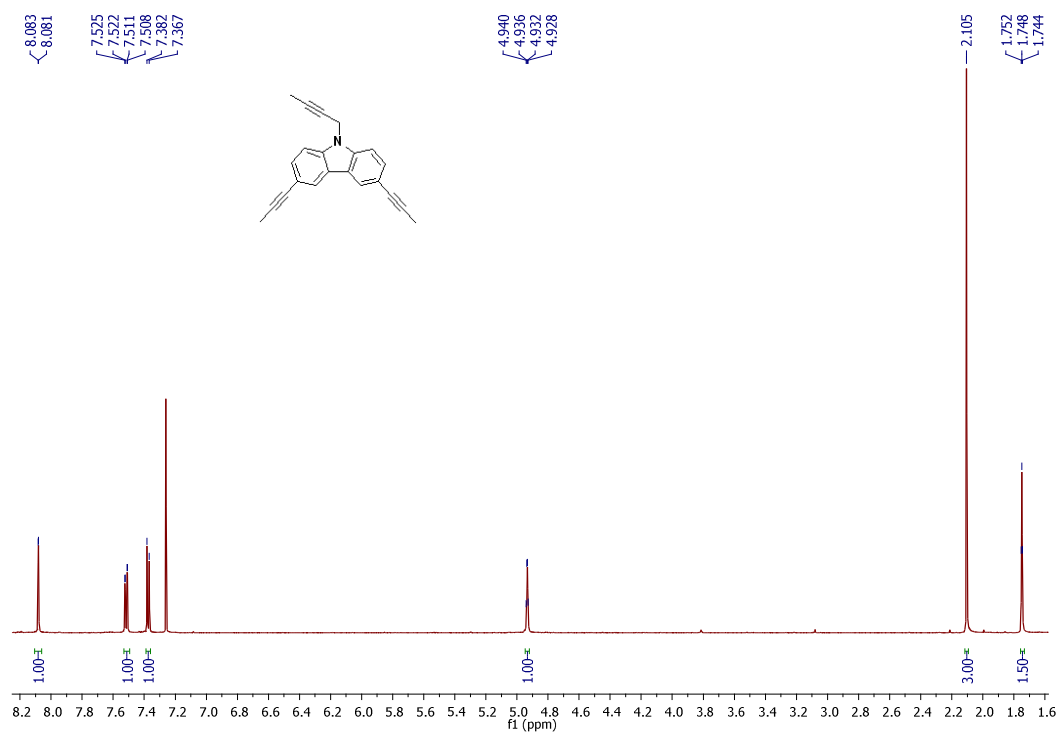


Figure S3. ^1H -NMR (600 MHz, CDCl_3) spectrum of compound **4**

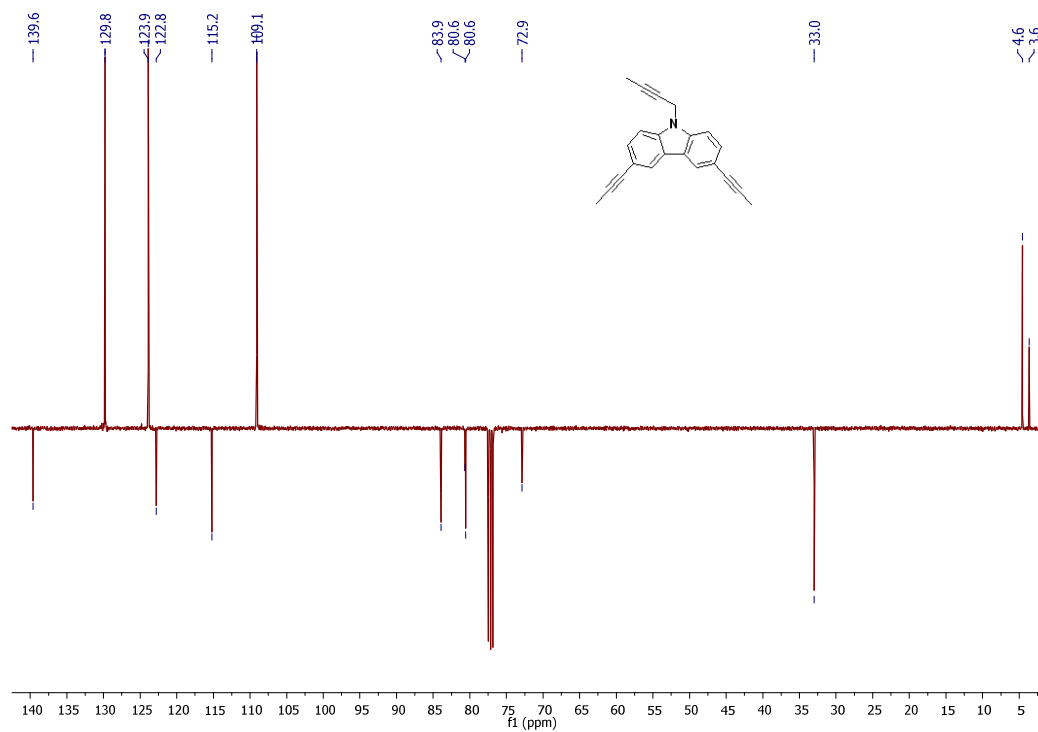


Figure S4. ^{13}C NMR (150 MHz, CDCl_3) spectrum of compound **4**

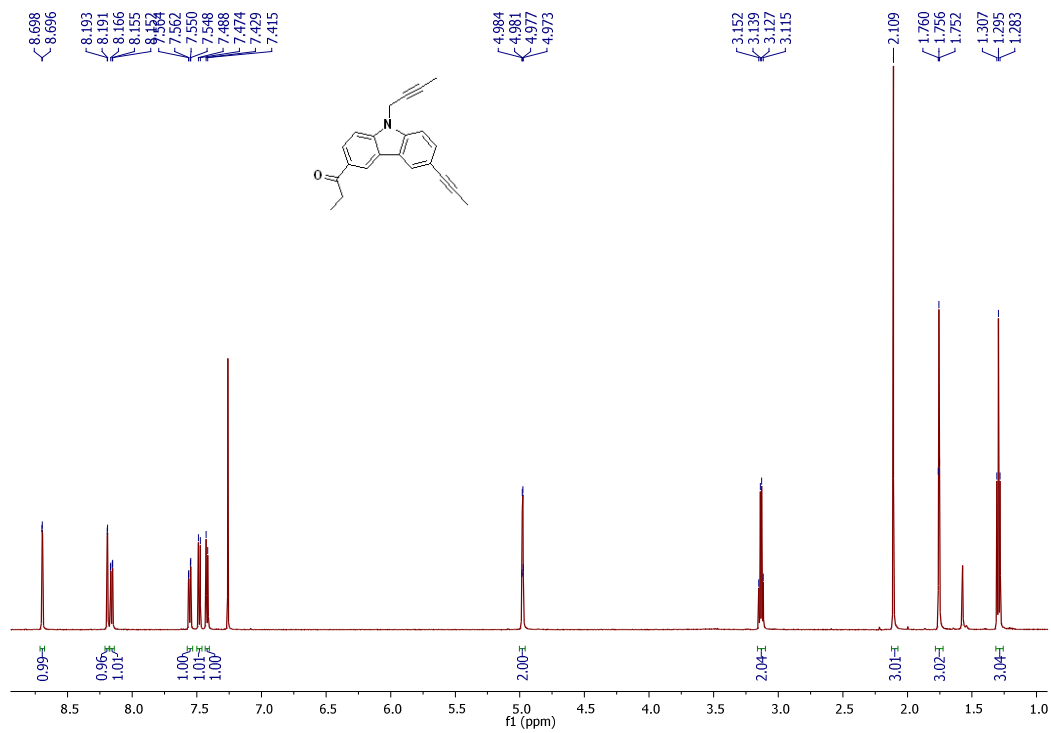


Figure S5. $^1\text{H-NMR}$ (600 MHz, CDCl_3) spectrum of compound **5**

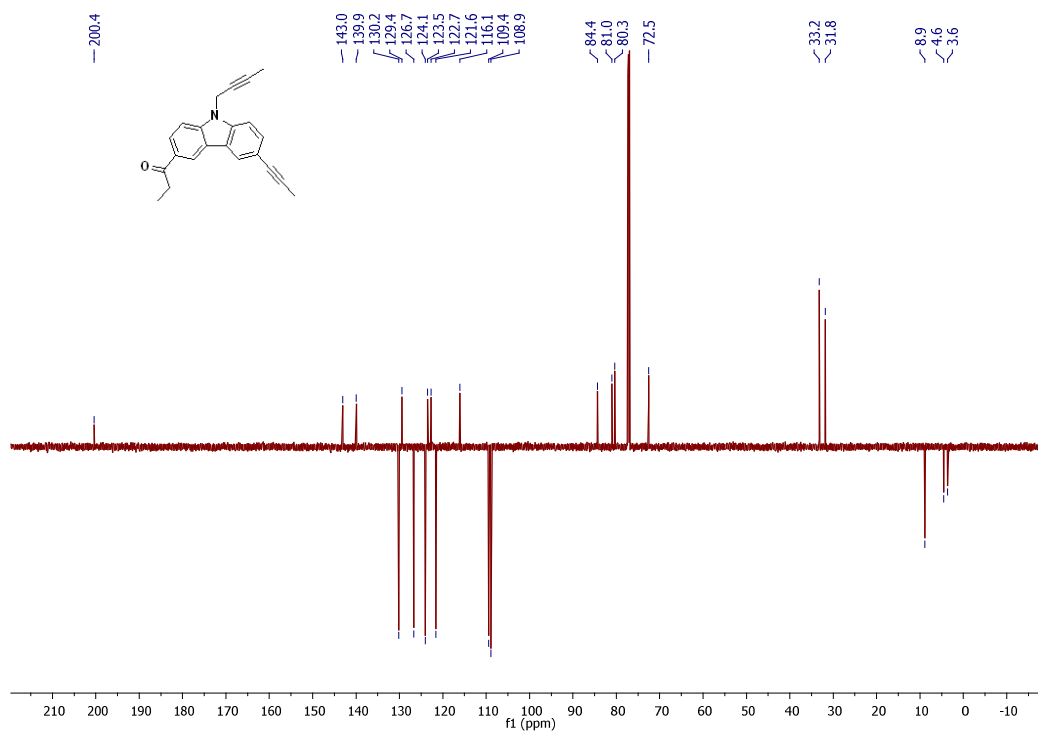


Figure S6. $^{13}\text{C NMR}$ (150 MHz, CDCl_3) spectrum of compound **5**

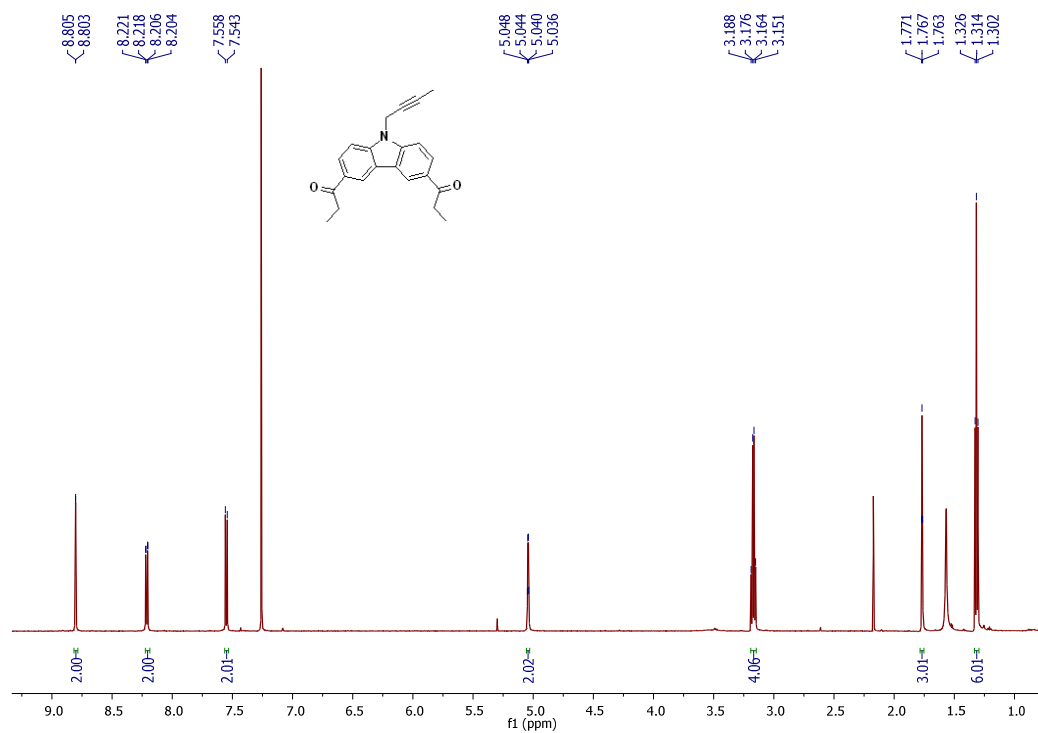


Figure S7. ^1H NMR (600 MHz, CDCl_3) spectrum of compound **6**

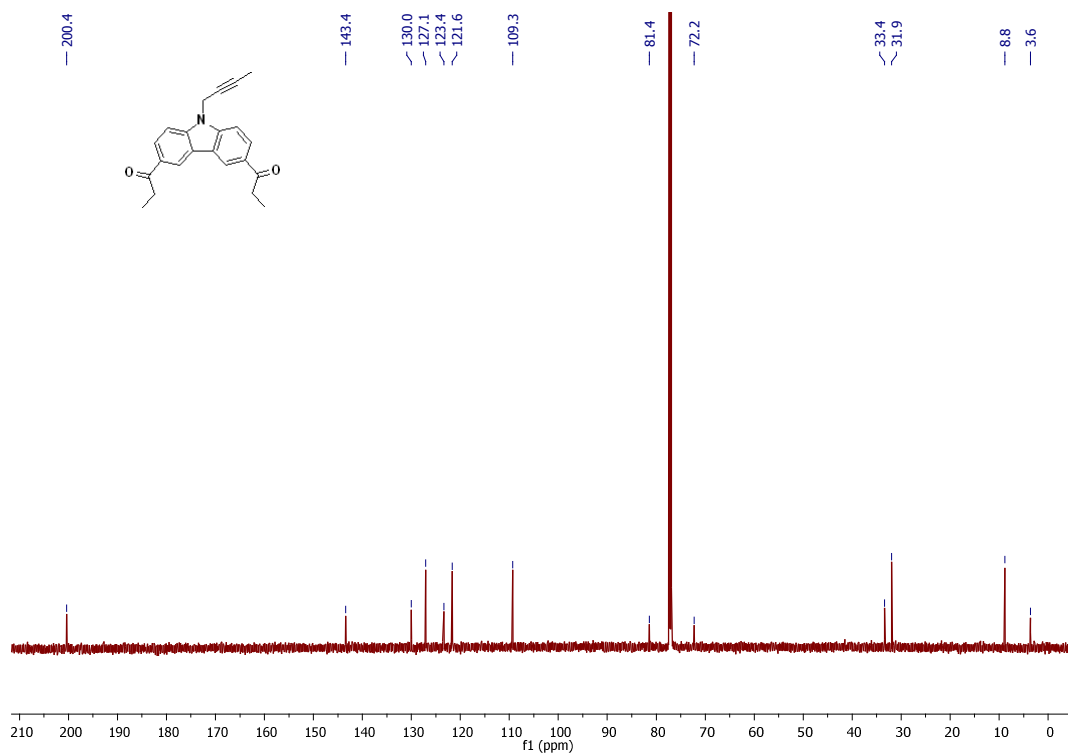


Figure S8. ^{13}C NMR (150 MHz, CDCl_3) spectrum of compound **6**

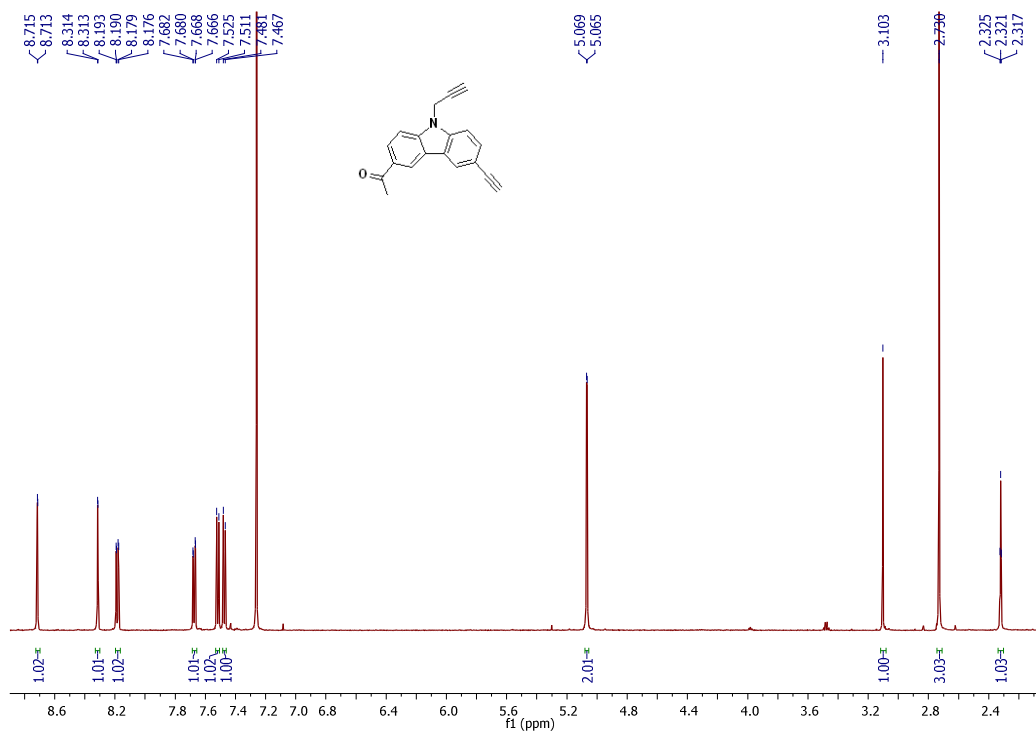


Figure S9. ^1H NMR (600 MHz, CDCl_3) spectrum of compound 7

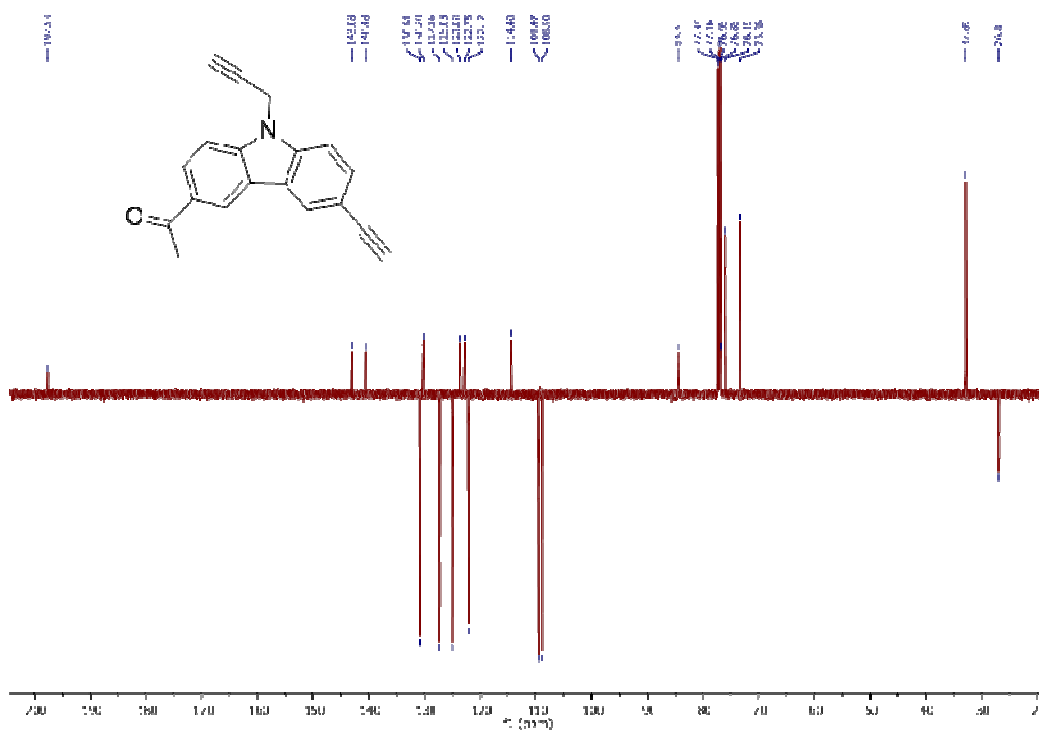


Figure S10. ^{13}C NMR (150 MHz, CDCl_3) spectrum of compound 7

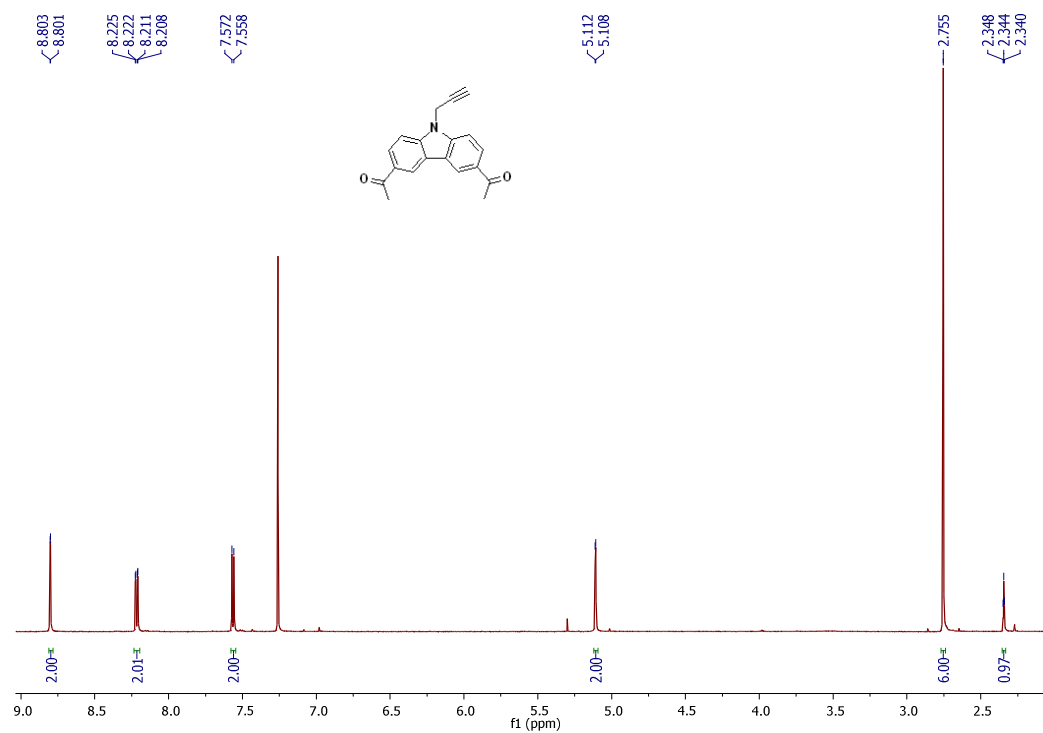


Figure S11. ^1H NMR (600 MHz, CDCl_3) spectrum of compound **8**

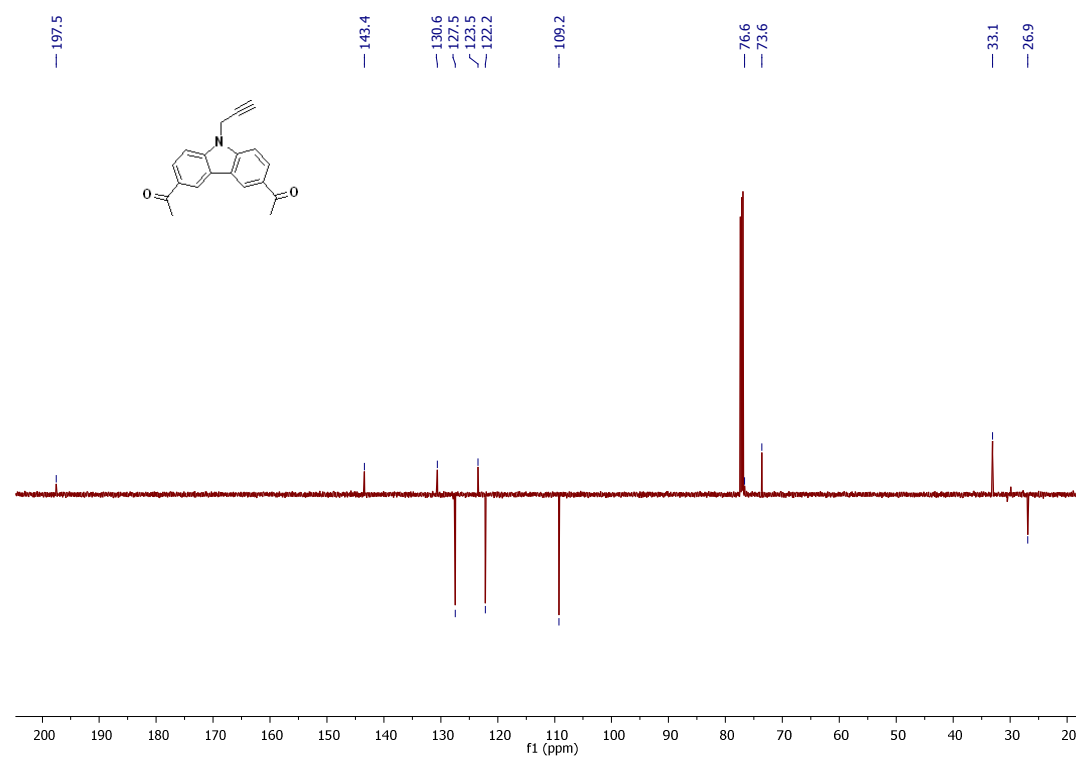


Figure S12. ^{13}C NMR (150 MHz, CDCl_3) spectrum of compound **8**

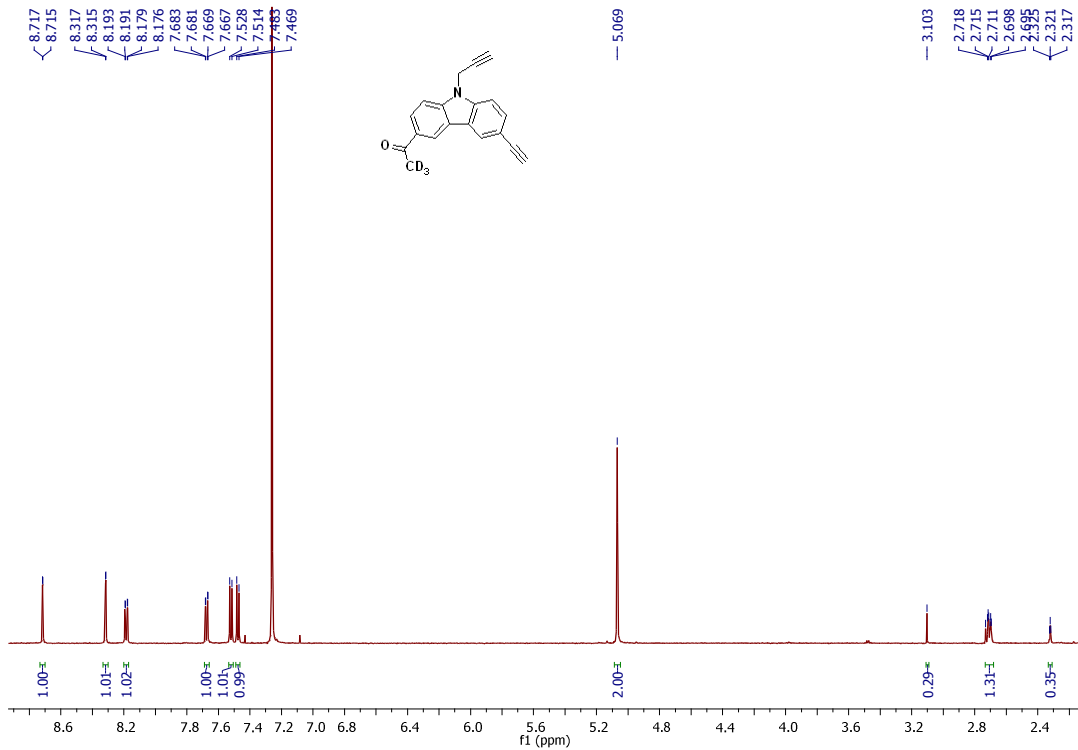


Figure S13. ^1H NMR (600 MHz, CDCl_3) spectrum of compound **9**

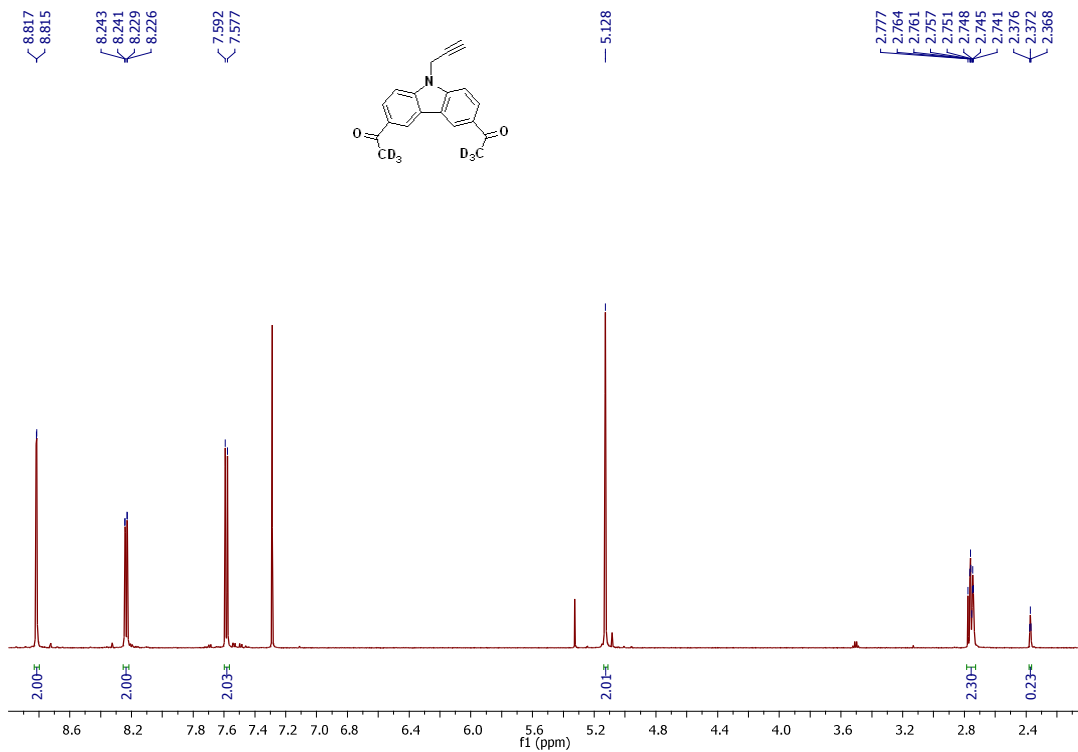


Figure S14. ^1H NMR (600 MHz, CDCl_3) spectrum of compound **10**

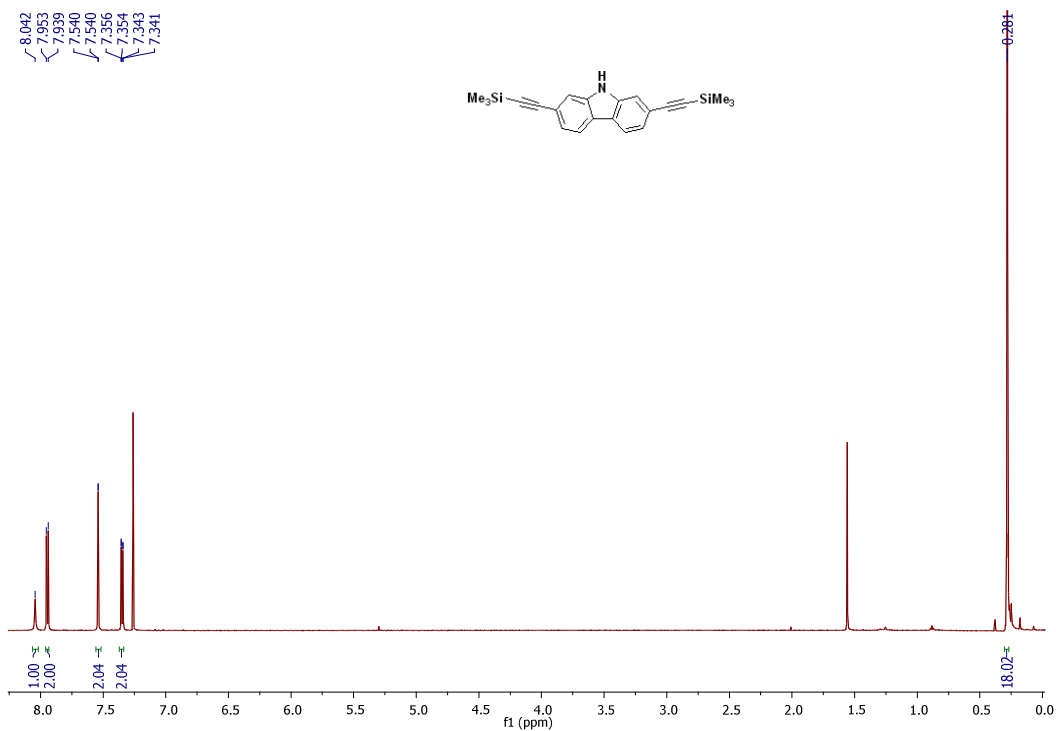


Figure S15. ^1H NMR (600 MHz, CDCl_3) spectrum of compound **11**

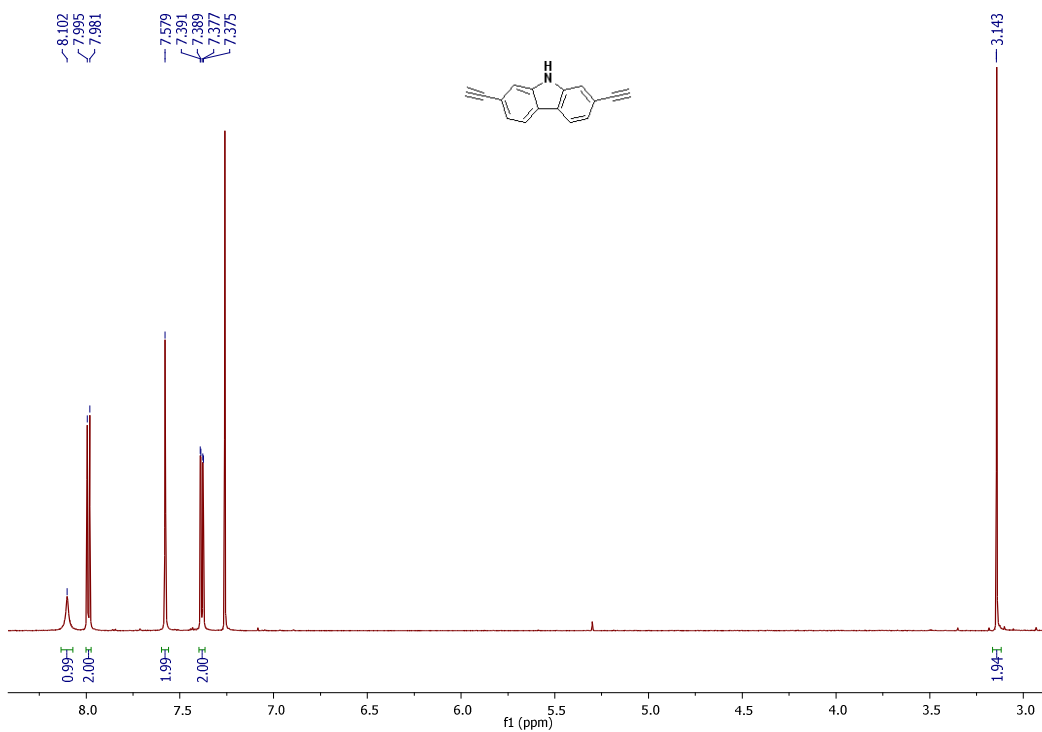


Figure S16. ^1H NMR (600 MHz, CDCl_3) spectrum of compound **12**

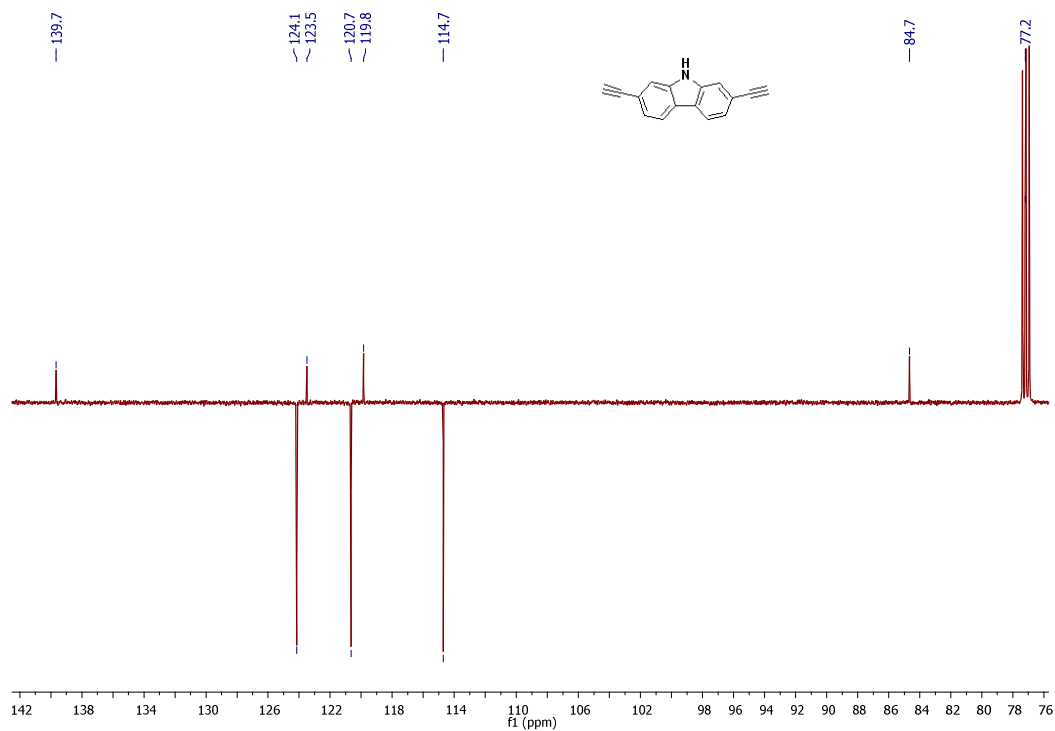


Figure S17. ^{13}C NMR (150 MHz, CDCl_3) spectrum of compound **12**

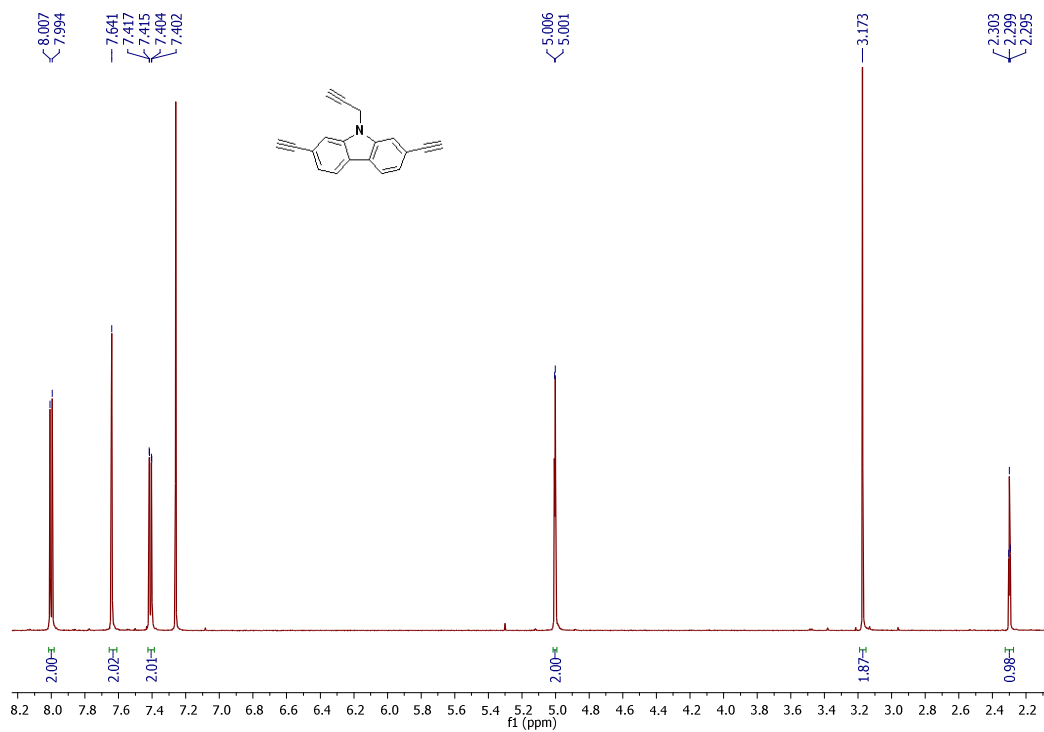


Figure S18. ^1H NMR (600 MHz, CDCl_3) spectrum of compound **13**

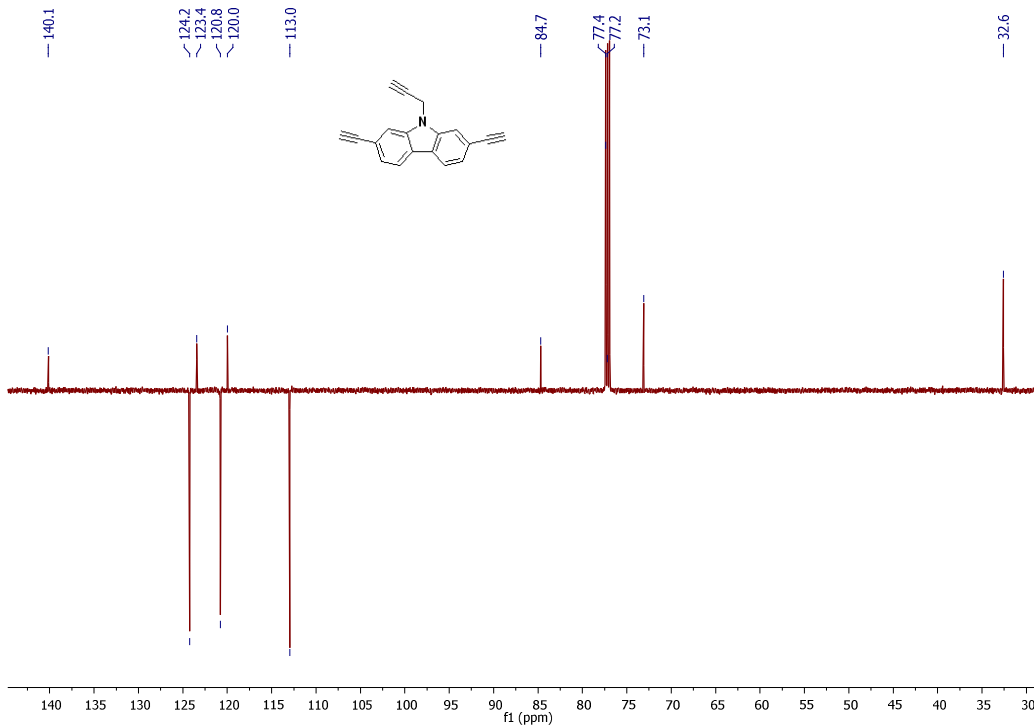


Figure S19. ¹³C NMR (150 MHz, CDCl₃) spectrum of compound **13**

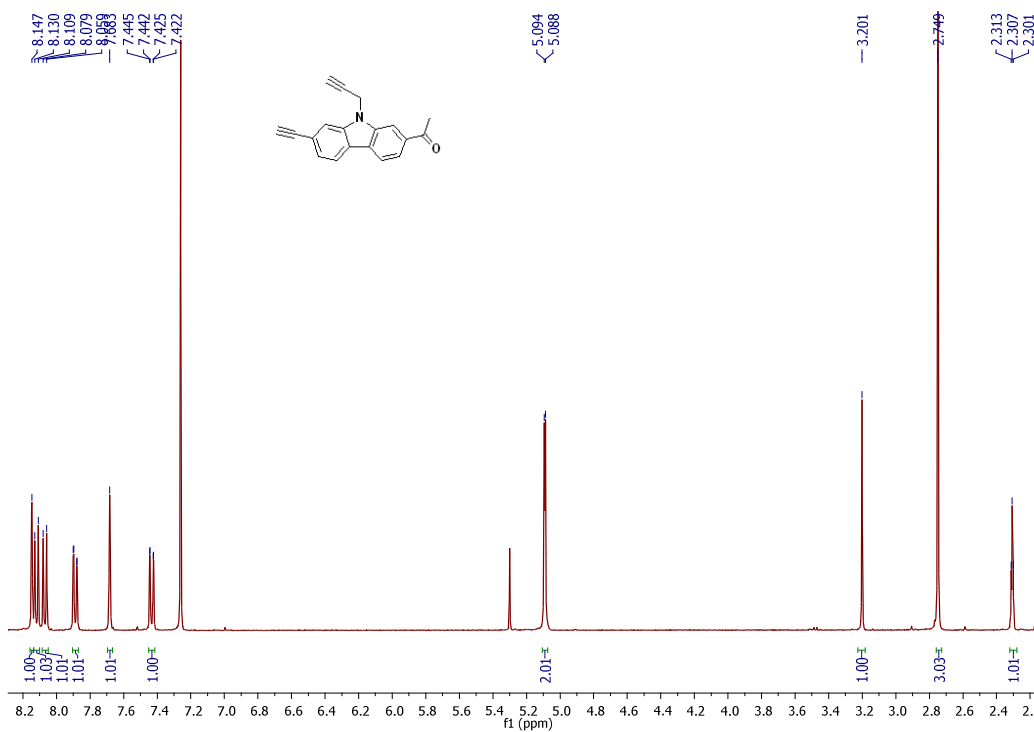


Figure S20. ¹H NMR (600 MHz, CDCl₃) spectrum of compound **14**

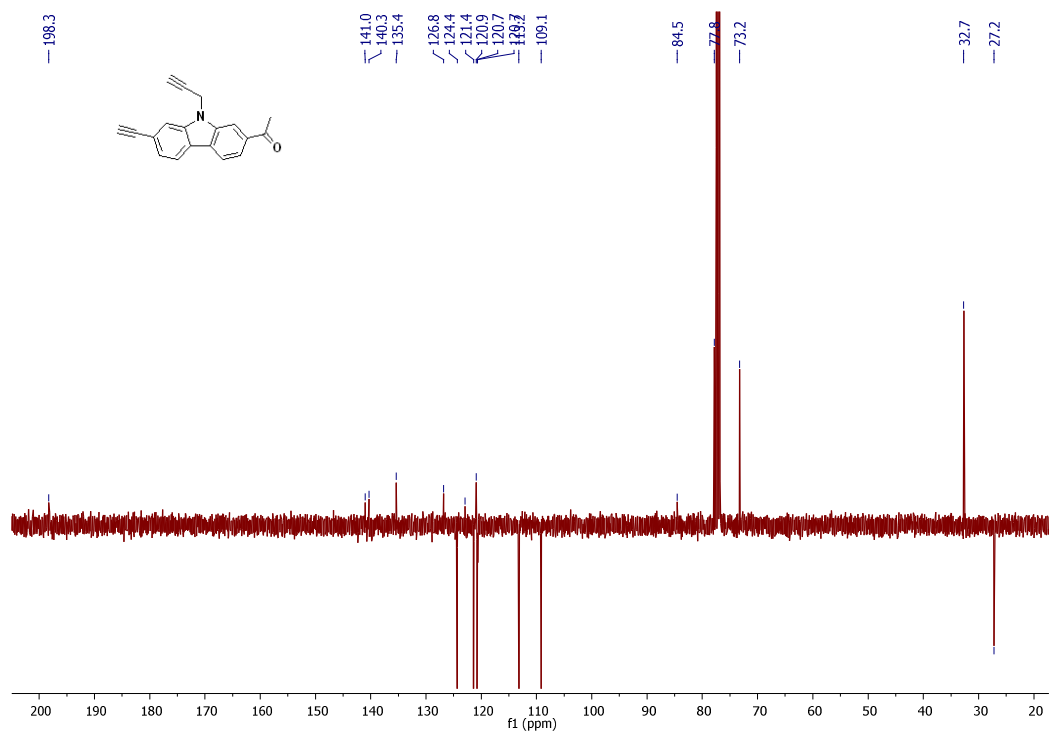


Figure S21. ^{13}C NMR (150 MHz, CDCl_3) spectrum of compound 14

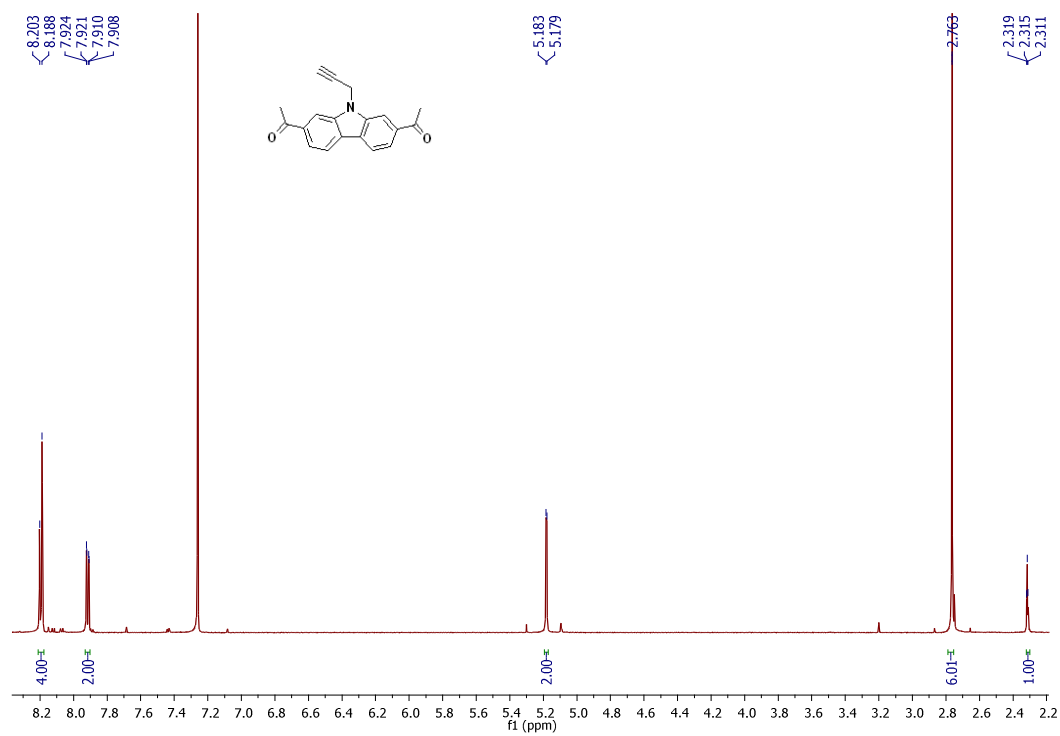


Figure S22. ^1H NMR (600 MHz, CDCl_3) spectrum of compound 15

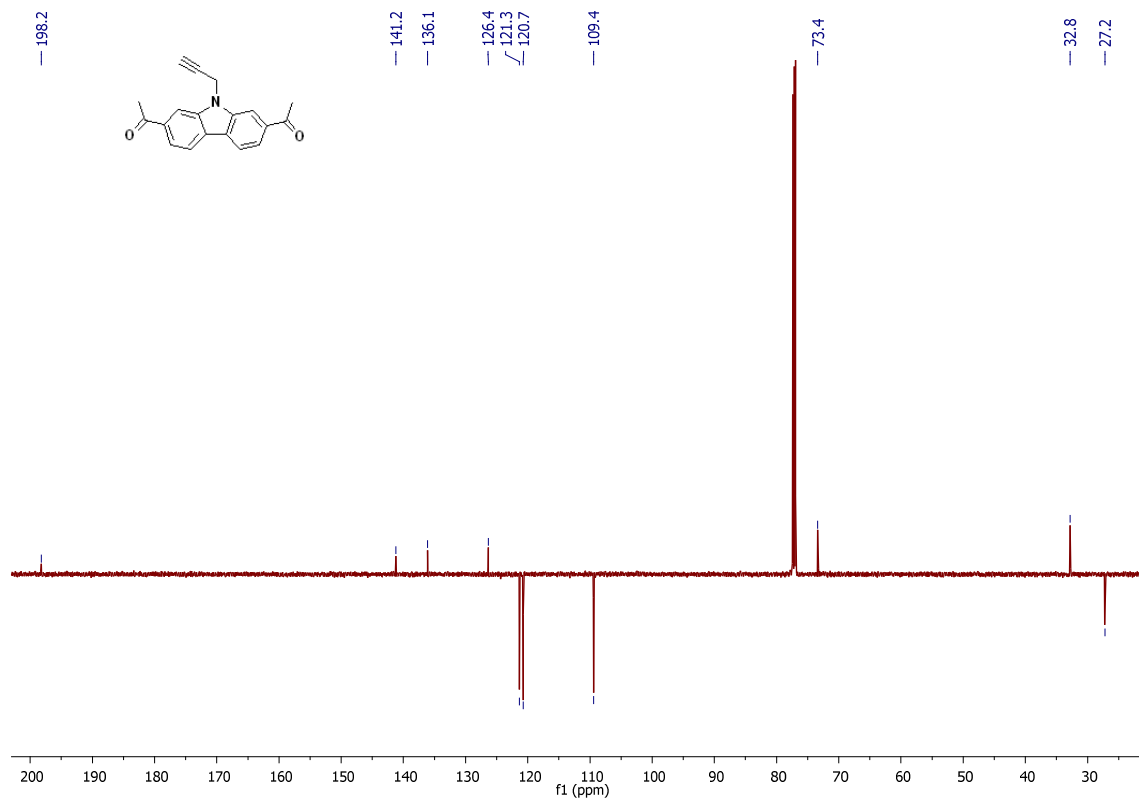


Figure S23. ¹H NMR (150 MHz, CDCl₃) spectrum of compound **15**

Table S1. Crystal data and structure refinement for mono-ketone **7**

Identification code	shelx	
Empirical formula	C ₁₉ H ₁₃ NO	
Formula weight	271.30	
Temperature	294(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 13.0200(18) Å	a = 90°.
	b = 8.4402(12) Å	b = 107.069(2)°.
	c = 13.3130(19) Å	g = 90°.
Volume	1398.5(3) Å ³	
Z	4	
Density (calculated)	1.289 Mg/m ³	
Absorption coefficient	0.080 mm ⁻¹	
F(000)	568	
Crystal size	0.390 x 0.321 x 0.220 mm ³	
Theta range for data collection	1.636 to 24.994°.	
Index ranges	-15 ≤ h ≤ 15, -10 ≤ k ≤ 10, -15 ≤ l ≤ 15	
Reflections collected	13048	
Independent reflections	2464 [R(int) = 0.0751]	
Completeness to theta = 24.994°	100.0 %	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	2464 / 0 / 191	
Goodness-of-fit on F ²	1.103	
Final R indices [I > 2σ(I)]	R1 = 0.0811, wR2 = 0.1837	
R indices (all data)	R1 = 0.1047, wR2 = 0.1957	
Largest diff. peak and hole	0.455 and -0.211 e.Å ⁻³	