

Supporting Information

The Role of Redox Active Non-innocent Ligand in Additive free C-C Glaser-Hay and Suzuki Coupling Reactions by *o*-aminophenol palladium(II) complex

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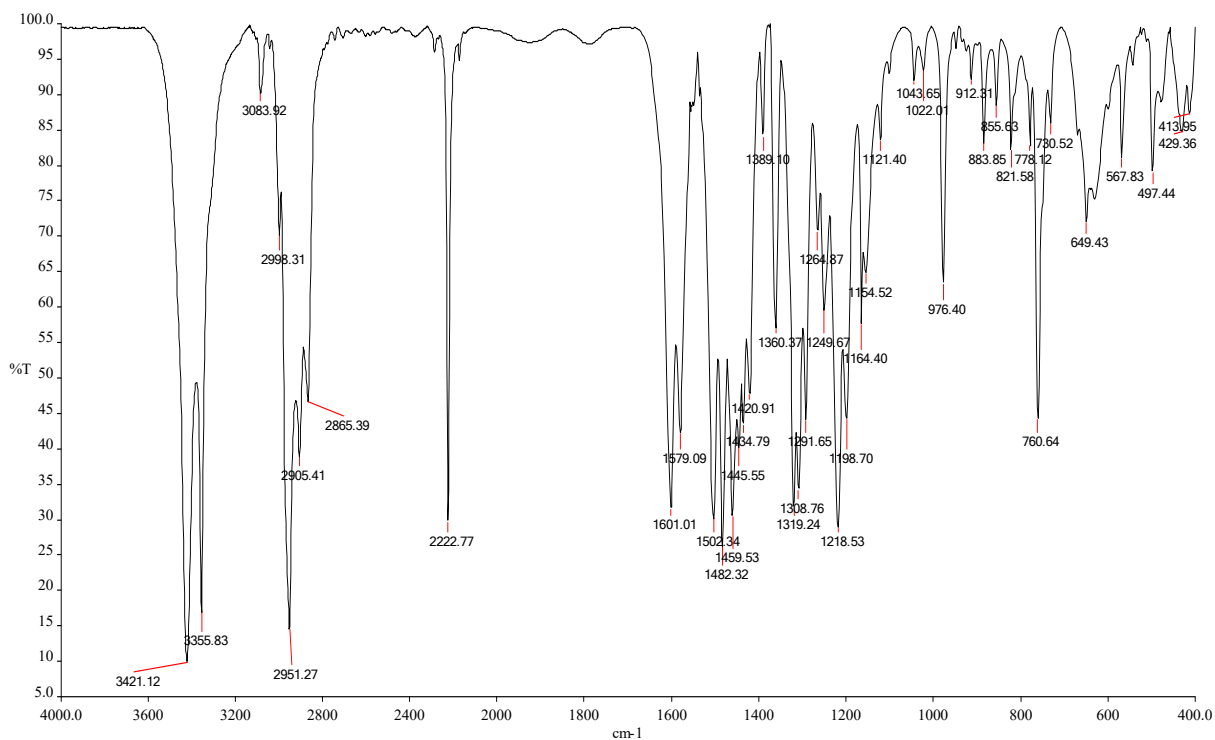


Figure S1. IR spectrum of H_2L^{NAP}

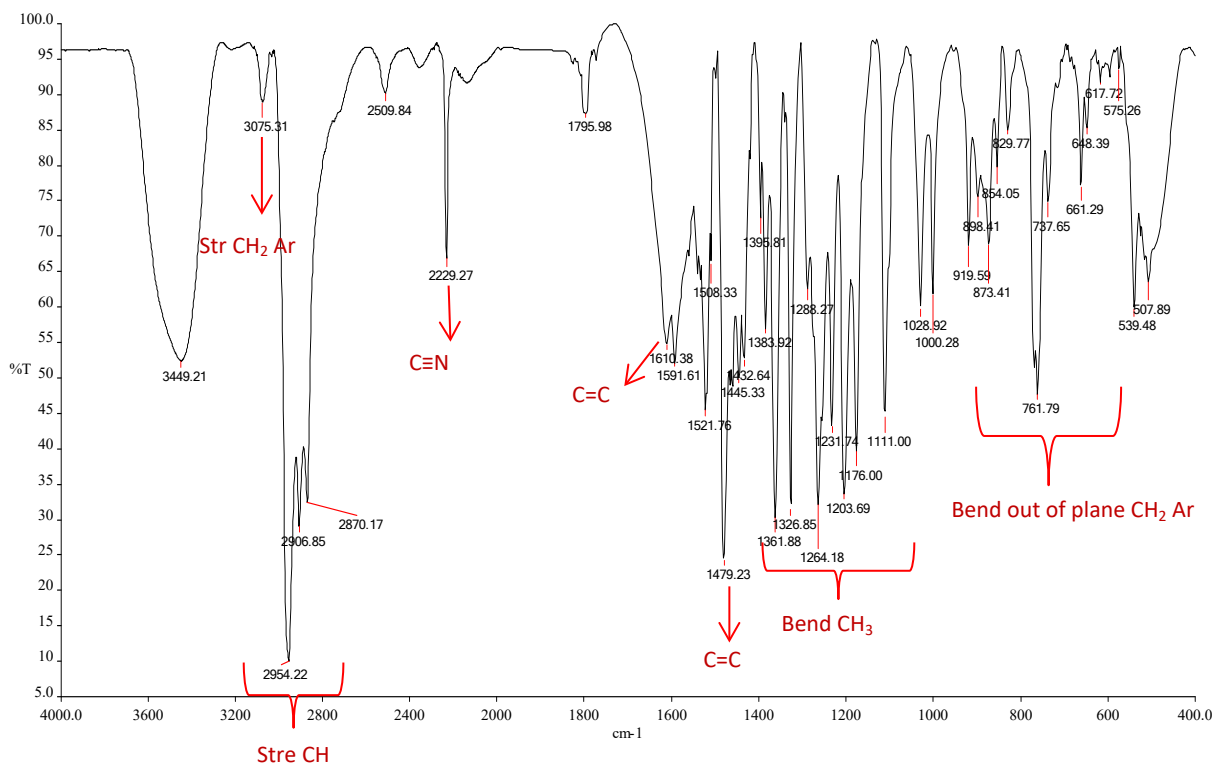


Figure S2. IR spectrum of PdL_2^{NIS}

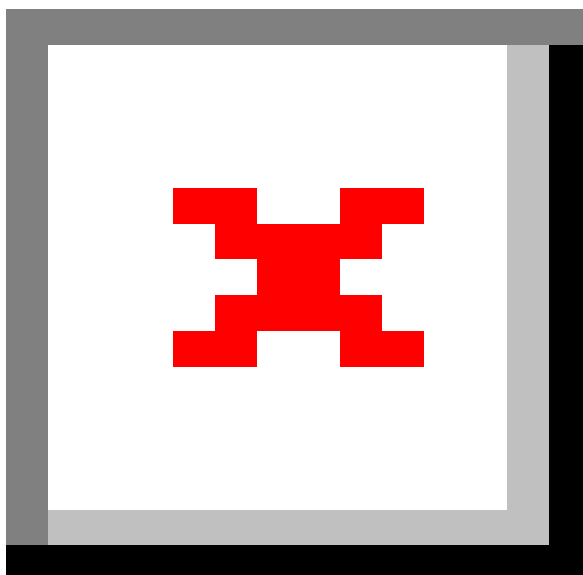


Figure S3. ^1H NMR spectrum of $\text{PdL}_2^{\text{NIS}}$ (CDCl_3 , 700 MHz)

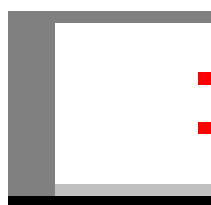


Figure S4. Regions between 7.3- 7.8 ppm were assigned as aromatic regions

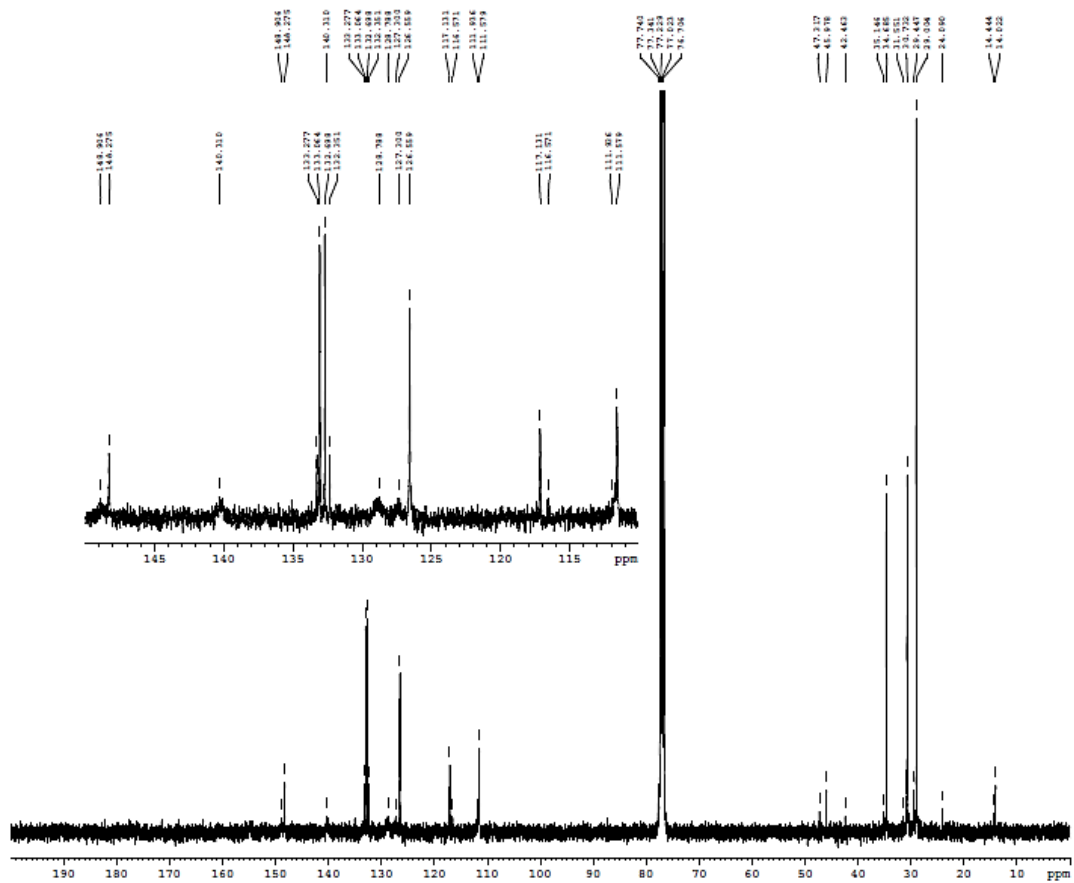


Figure S5. ^{13}C NMR spectrum of Pd_2NIS (CDCl_3 , 100 MHz)

Identification code	e1470a_a
Empirical formula	C ₄₂ H ₄₈ N ₄ O ₂ Pd
Formula weight	747.24
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P2 ₁ /c
Unit cell dimensions	a = 16.674(2) Å
	b = 8.0975(7) Å
	c = 16.837(2) Å
	α = 90°
	β = 119.020(16)°
	γ = 90°
Volume	1987.8(5) Å ³
Z	2
Density (calculated)	1.248 Mg/m ³
Absorption coefficient	0.505 mm ⁻¹
F(000)	780
Crystal size	0.605 x 0.456 x 0.177 mm ³
Theta range for data collection	2.420 to 28.541°
Index ranges	-17<=h<=20, -6<=k<=10, -22<=l<=22
Reflections collected	8982
Independent reflections	4146 [R(int) = 0.0945]
Completeness to theta = 25.000°	93.0 %
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	4146 / 0 / 226
Goodness-of-fit on F ²	1.161
Final R indices [I>2sigma(I)]	R1 = 0.0813, wR2 = 0.2229
R indices (all data)	R1 = 0.1242, wR2 = 0.2610
Extinction coefficient	n/a
Largest diff. peak and hole	0.917 and -0.687 e.Å ⁻³

Table S2. Selected bond lengths [Å] and angles [°] for PdL ₂ ^{NIS}			
Bonds		Angles	
Pd(1)-N(1)	1.963(6)	N(1)#1-Pd(1)-N(1)	180.0(3)
Pd(1)-N(1)#1	1.963(6)	N(1)#1-Pd(1)-O(1)#1	81.4(2)
Pd(1)-O(1)	1.965(5)	N(1)-Pd(1)-O(1)#1	98.6(2)
Pd(1)-O(1)#1	1.965(5)	N(1)#1-Pd(1)-O(1)	98.6(2)
O(1)-C(1)	1.309(9)	N(1)-Pd(1)-O(1)	81.4(2)
C(1)-C(6)	1.424(10)	O(1)#1-Pd(1)-O(1)	180.0
C(1)-C(2)	1.425(10)	C(1)-O(1)-Pd(1)	113.7(4)
C(2)-C(3)	1.371(11)	O(1)-C(1)-C(6)	117.9(6)
C(2)-C(13)	1.530(11)	O(1)-C(1)-C(2)	122.3(7)
C(3)-C(4)	1.434(11)	C(6)-C(1)-C(2)	119.7(7)
C(4)-C(5)	1.368(11)	C(3)-C(2)-C(1)	116.3(7)
C(4)-C(17)	1.521(12)	C(3)-C(2)-C(13)	121.4(7)
C(5)-C(6)	1.409(11)	C(1)-C(2)-C(13)	122.2(7)
C(6)-N(1)	1.369(10)	C(2)-C(3)-C(4)	125.1(7)
N(1)-C(7)	1.396(9)	C(5)-C(4)-C(3)	117.7(7)
C(7)-C(8)	1.383(11)	C(5)-C(4)-C(17)	122.7(7)
C(8)-C(9)	1.392(13)	C(3)-C(4)-C(17)	119.5(7)
C(9)-C(10)	1.354(14)	C(4)-C(5)-C(6)	119.9(7)
C(10)-C(11)	1.361(14)	N(1)-C(6)-C(5)	126.3(7)
C(11)-C(12)	1.395(11)	N(1)-C(6)-C(1)	112.5(7)
C(12)-C(21)	1.438(12)	C(5)-C(6)-C(1)	121.2(7)
C(21)-N(2)	1.139(11)	C(6)-N(1)-C(7)	121.2(6)
C(13)-C(14)	1.520(13)	C(6)-N(1)-Pd(1)	114.4(5)
C(13)-C(15)	1.531(12)	C(7)-N(1)-Pd(1)	124.2(5)
C(13)-C(16)	1.541(12)	C(8)-C(7)-N(1)	122.4(7)
C(17)-C(18)	1.499(14)	C(8)-C(7)-C(12)	118.0(7)
C(17)-C(20)	1.518(16)	N(1)-C(7)-C(12)	119.3(6)
C(17)-C(19)	1.548(13)	C(7)-C(8)-C(9)	120.5(8)
		C(10)-C(9)-C(8)	120.1(8)
		C(9)-C(10)-C(11)	121.5(9)
		C(10)-C(11)-C(12)	119.1(8)
		C(11)-C(12)-C(7)	120.7(7)
		C(11)-C(12)-C(21)	120.1(7)
		C(7)-C(12)-C(21)	119.2(7)
		C(14)-C(13)-C(2)	108.9(7)
		C(14)-C(13)-C(15)	108.8(8)
		C(2)-C(13)-C(15)	112.2(7)
		C(14)-C(13)-C(16)	108.9(9)
		C(2)-C(13)-C(16)	109.7(7)

Table S2. Selected bond lengths [Å] and angles [°] for PdL ₂ ^{NIS} (continued)	
Angles	
C(18)-C(17)-C(20)	110.0(10)
C(18)-C(17)-C(4)	113.6(8)
C(20)-C(17)-C(4)	107.5(9)
C(18)-C(17)-C(19)	105.8(9)
C(20)-C(17)-C(19)	110.4(10)
C(4)-C(17)-C(19)	109.6(8)
C(15)-C(13)-C(16)	108.3(8)
N(2)-C(21)-C(12)	178.7(10)

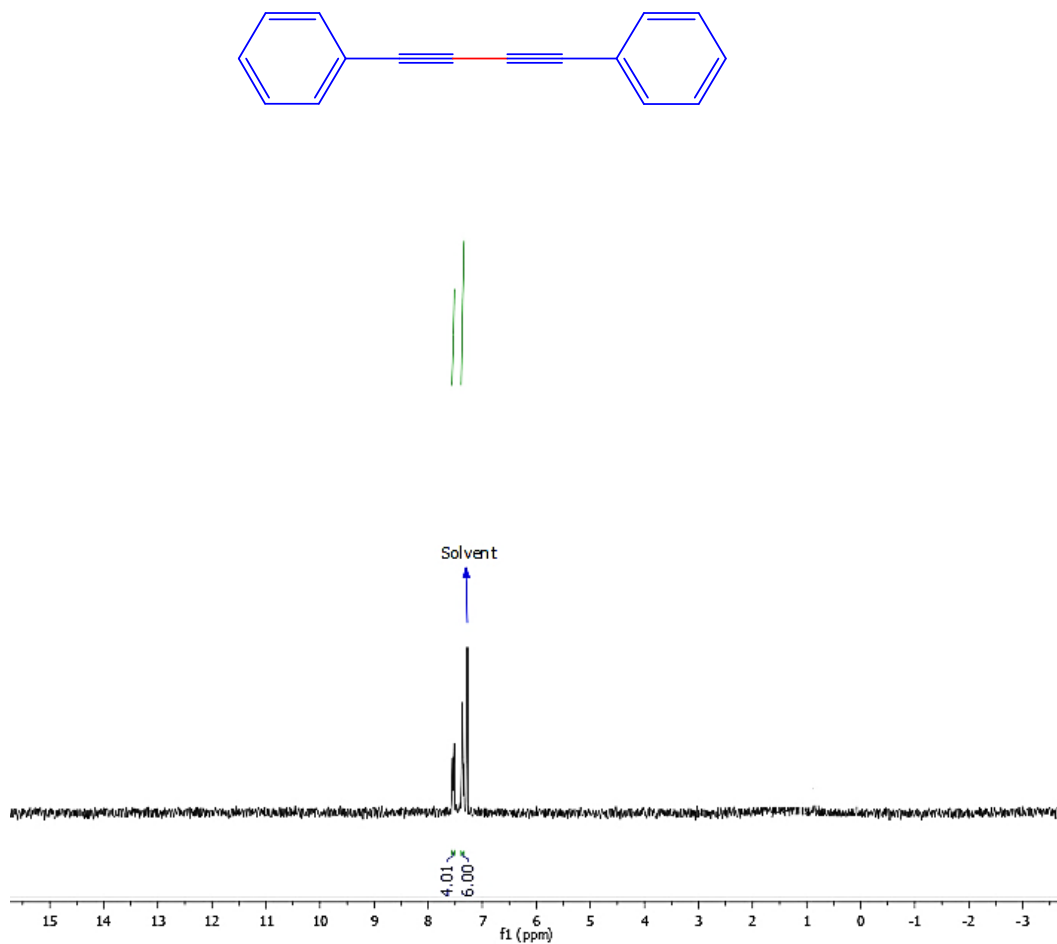


Figure S6. ¹H NMR spectrum of (4-phenyl-1,3-butadiynyl)benzene(CDCl₃, 250 MHz)

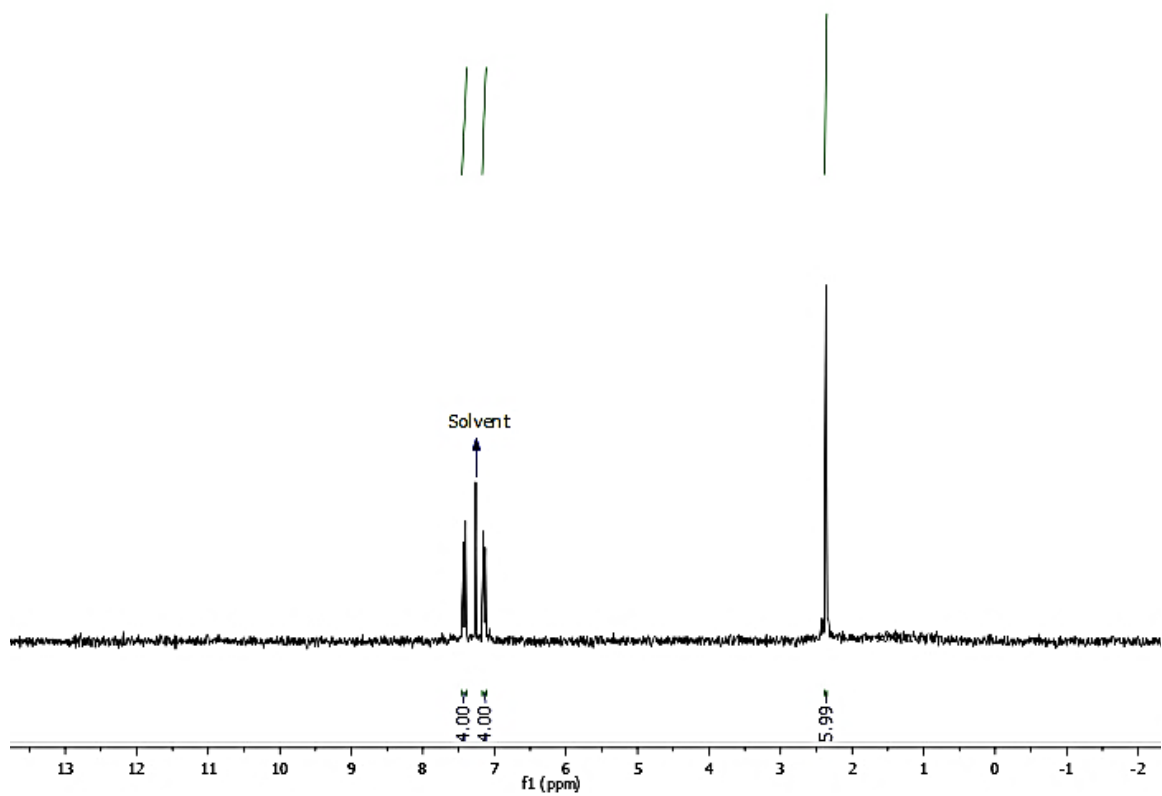
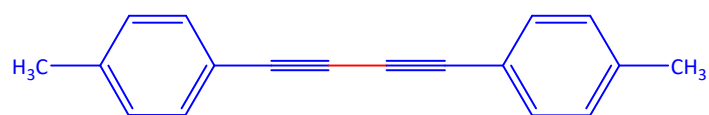


Figure S7. ^1H NMR spectrum of 4-methyl-1-[4-(4-methylphenyl)buta-1,3-dienyl]benzene(CDCl_3 , 250 MHz)

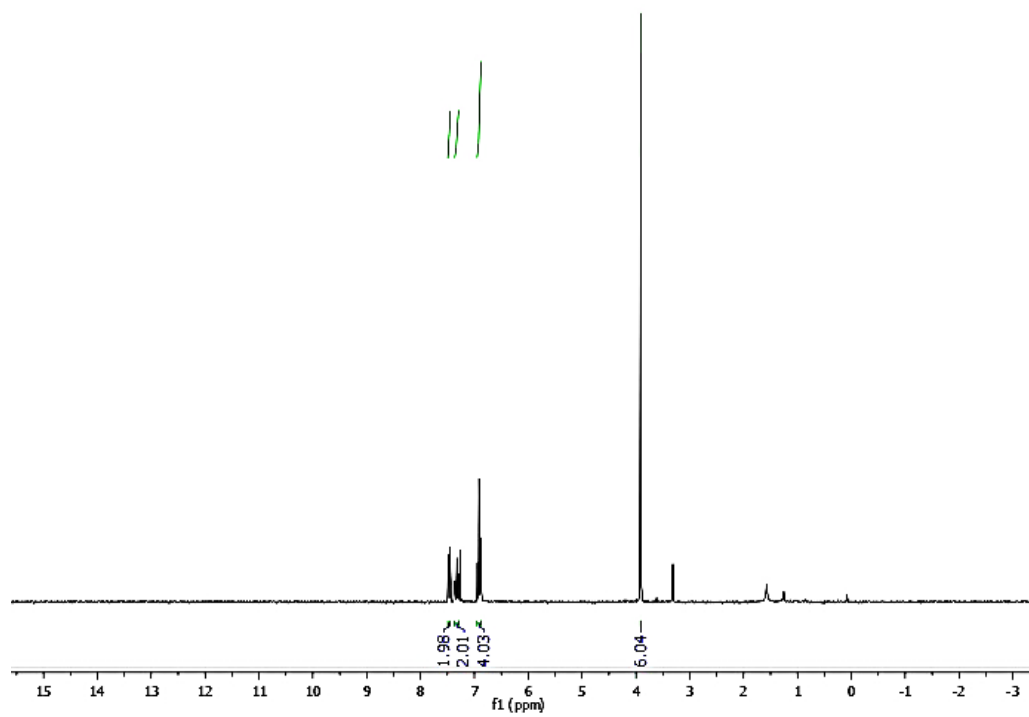
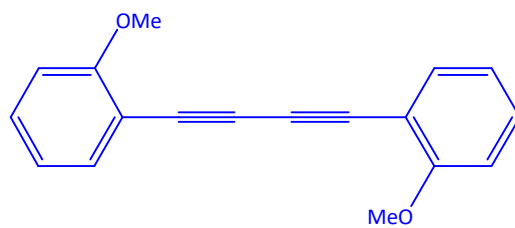


Figure S8. ¹H NMR spectrum of 1,1'-(1,3-Butadiyne-1,4-diyl)bis(2-methoxybenzene) (CDCl₃, 250 MHz)

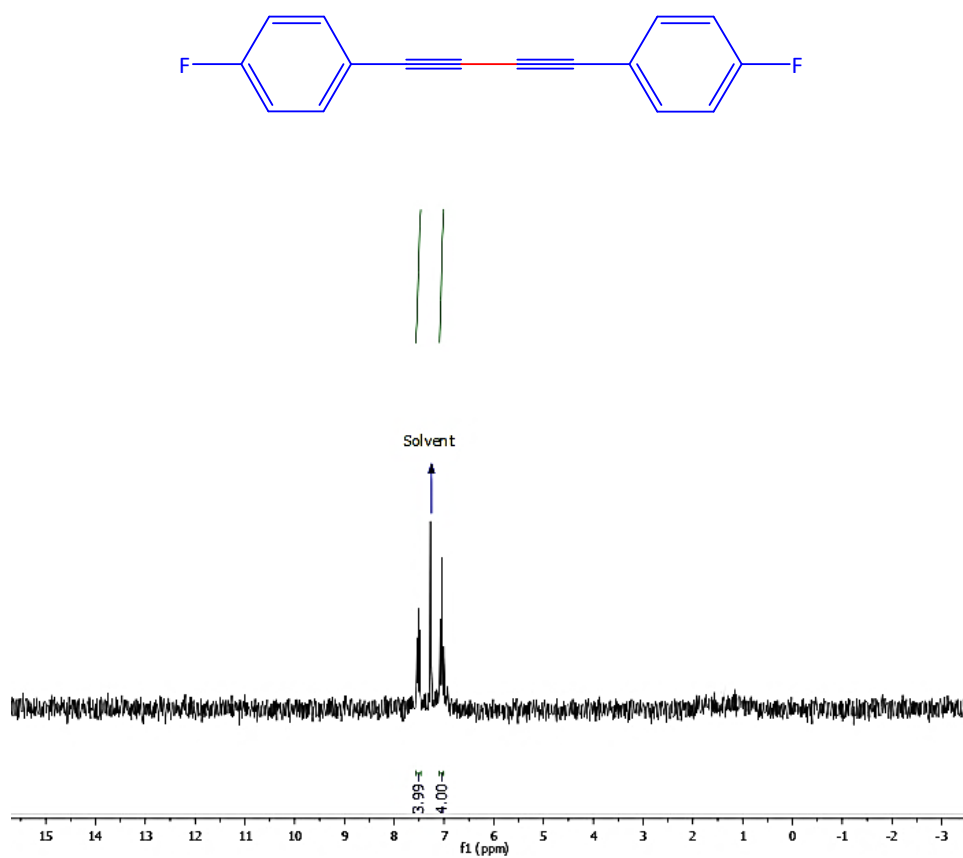


Figure S9. ¹H NMR spectrum of 1,1'-(1,3-Butadiyne-1,4-diyl)bis(4-fluorobenzene) (CDCl₃, 250 MHz)

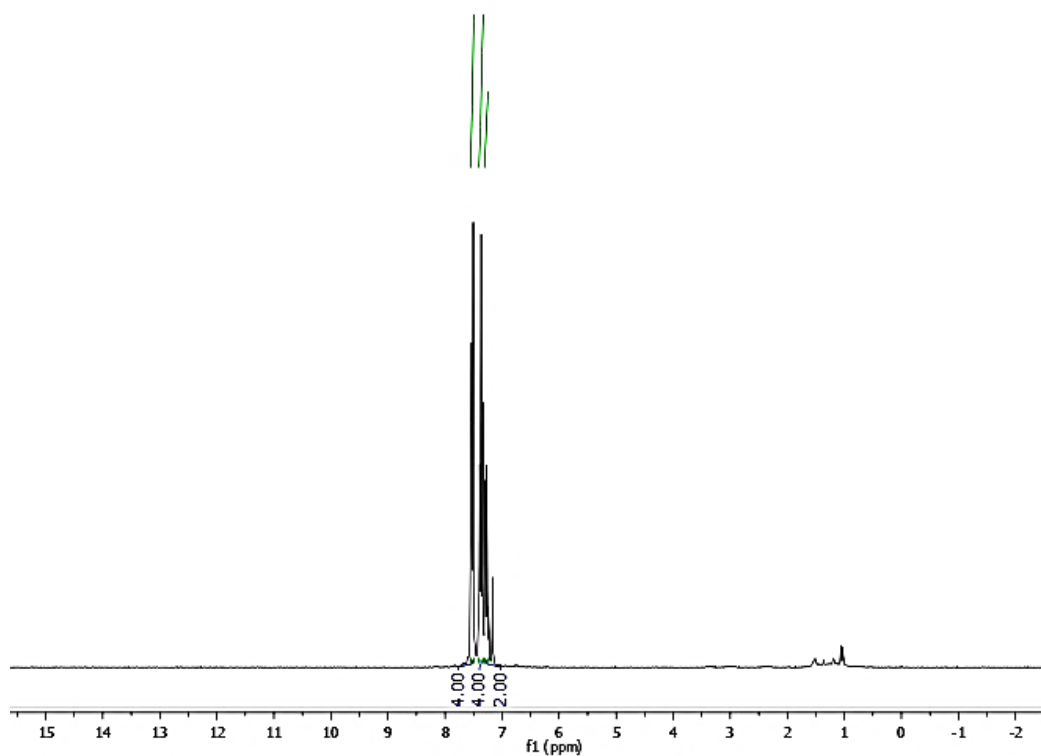
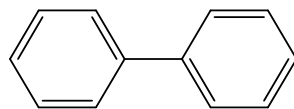


Figure S10. ¹H NMR spectrum of Biphenyl (CDCl₃, 250 MHz)

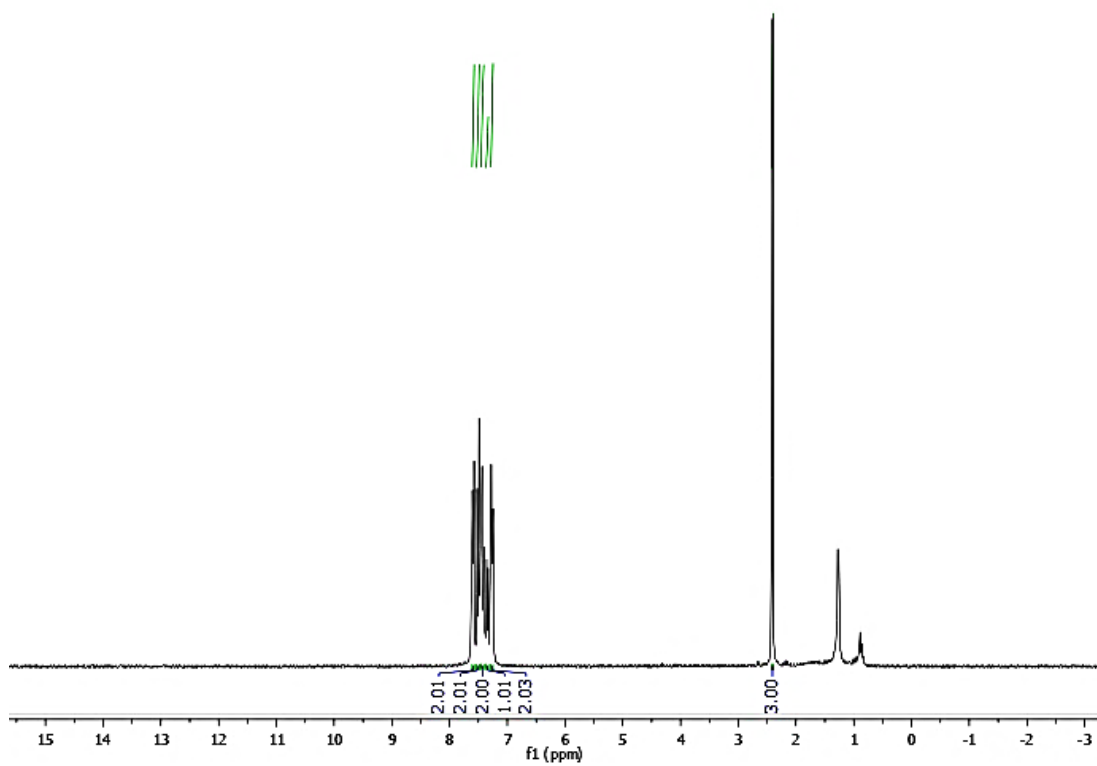
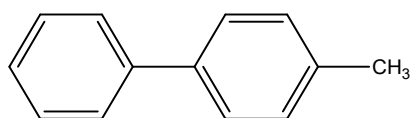


Figure S11. ¹H NMR spectrum of 4-Methylbiphenyl (CDCl₃, 250 MHz)

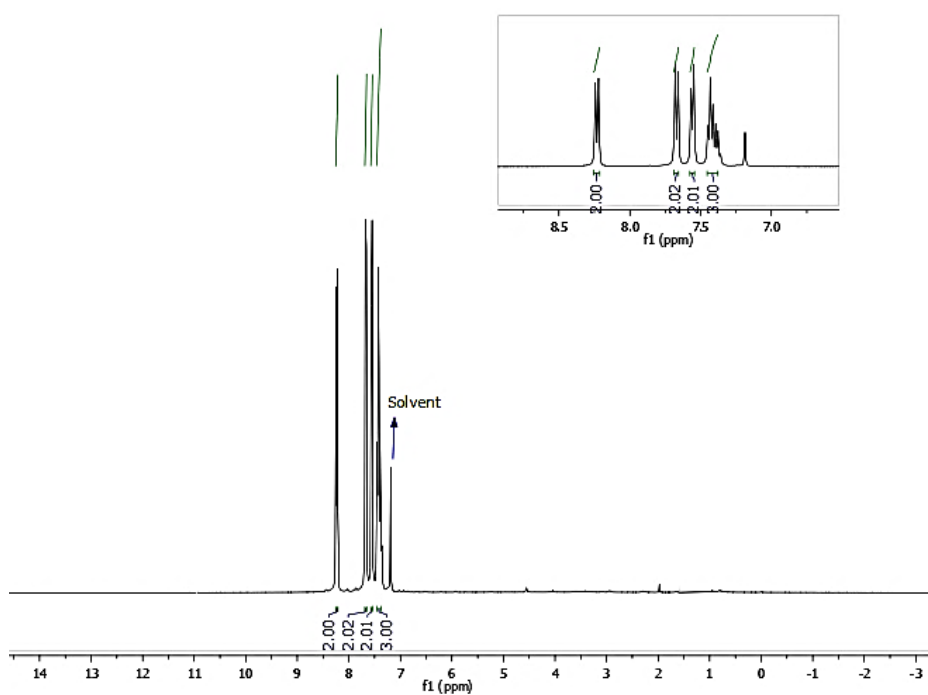
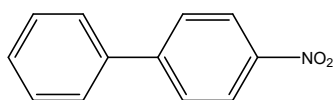


Figure S12. ^1H NMR spectrum of 4-Nitrobiphenyl(CDCl_3 , 400 MHz)

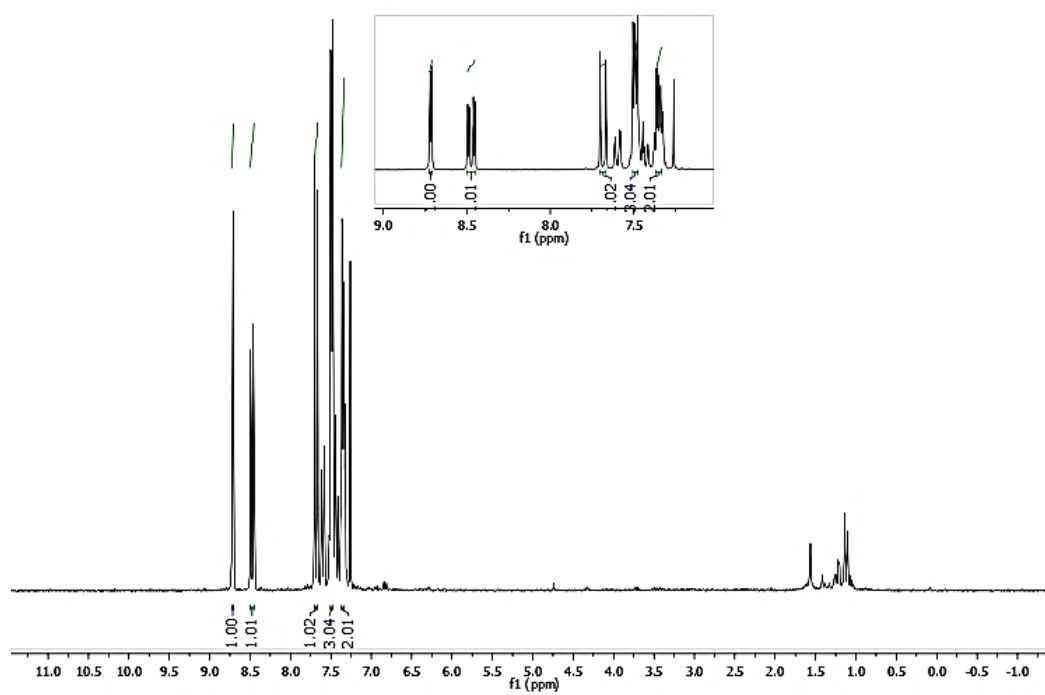
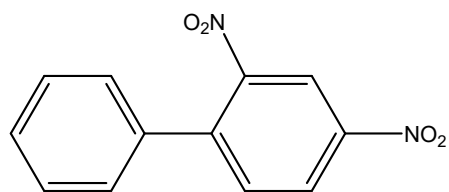


Figure S13. ^1H NMR spectrum of 2,4-Dinitrophenyl(CDCl_3 , 250 MHz)

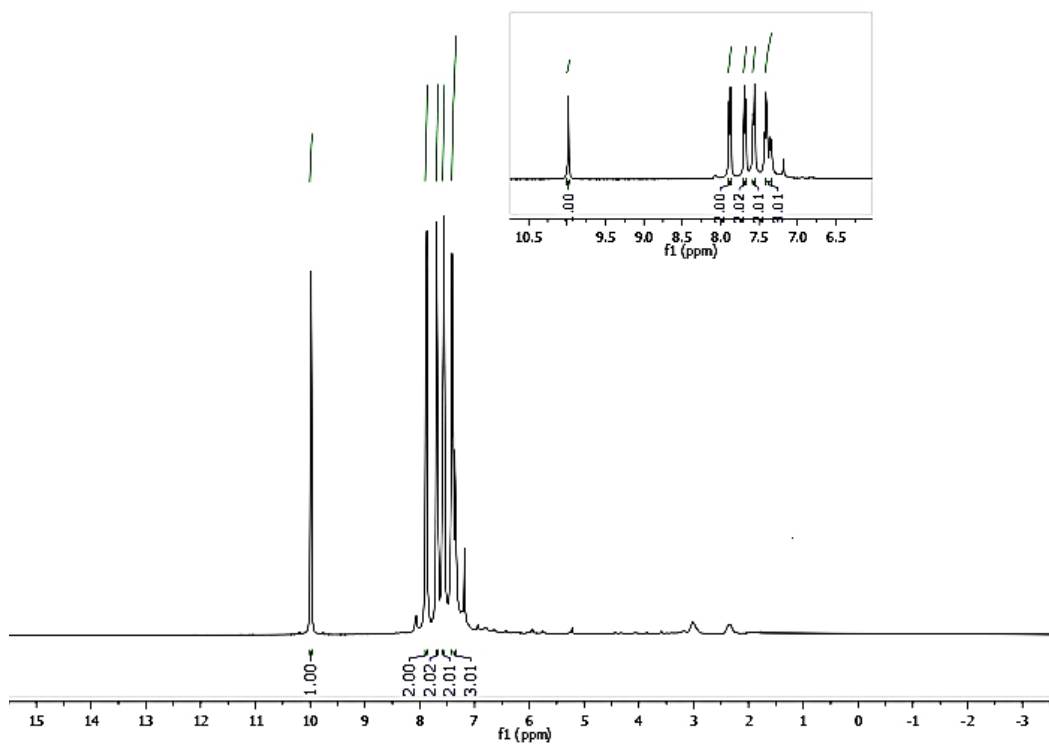
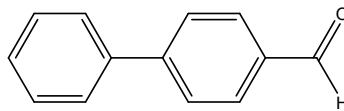


Figure S14. ¹H NMR spectrum of 4-Biphenylcarbaldehyd(CDCl₃, 400 MHz)