Supporting Information

Tuning of the redox potential and catalytic activity of a new Cu(II) complex by *o*-iminobenzosemiquinone as an Electron-reservoir ligand

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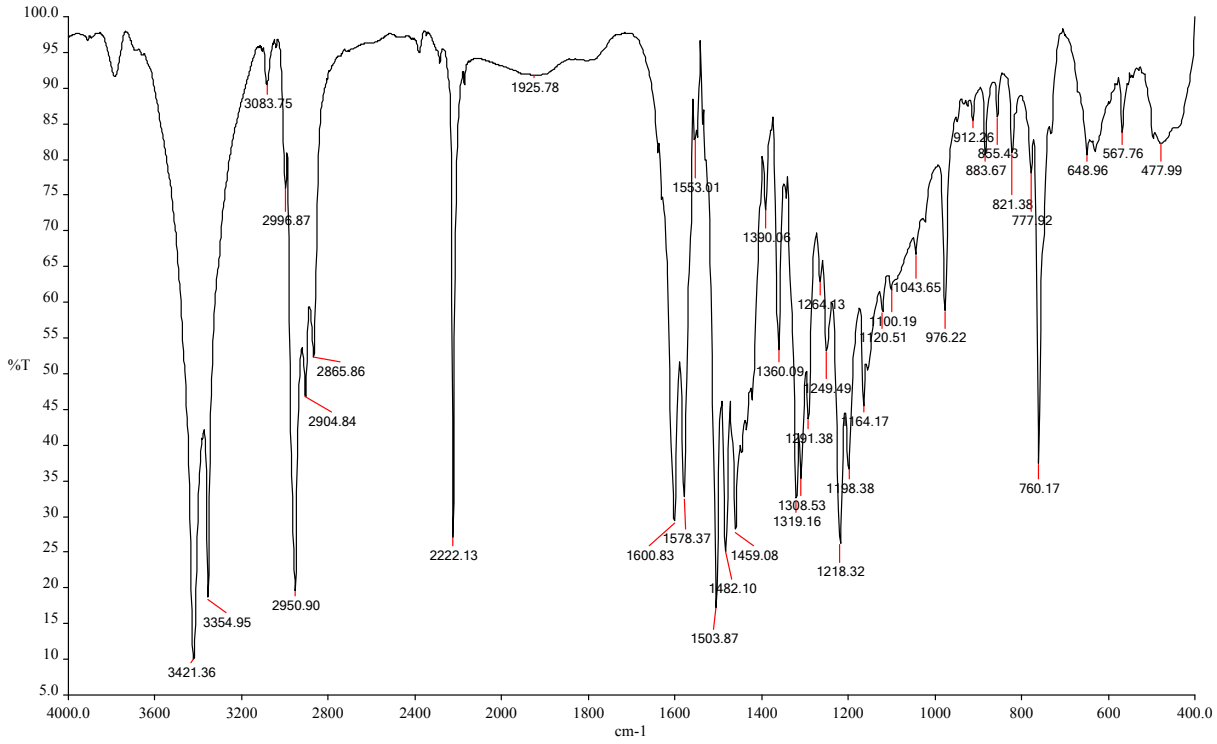


Figure S1 IR spectrum of H_2L^{NAP}.

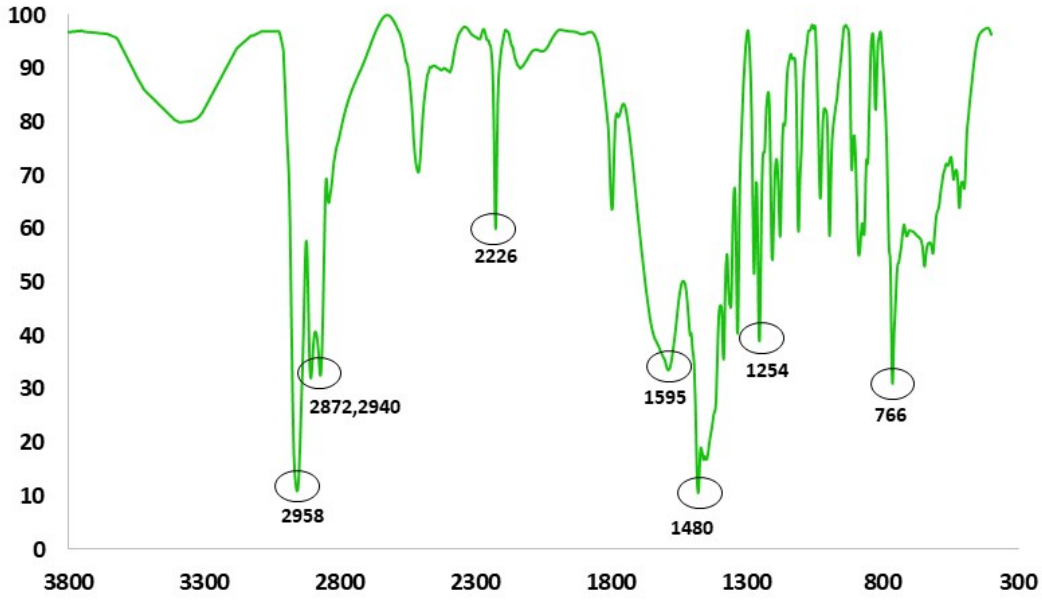


Figure S2 IR spectrum of CuL^{NIS}.

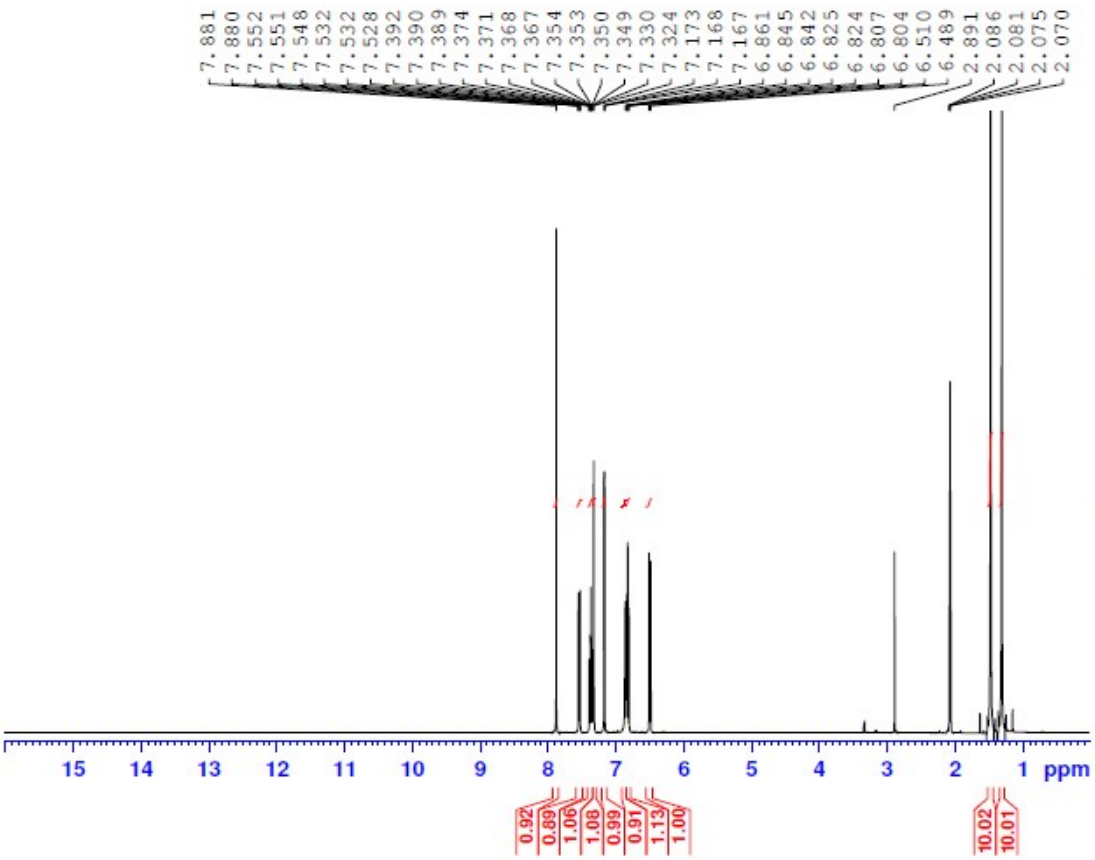


Figure S3 ^{1}H NMR spectrum of H_2L^{NAP}.

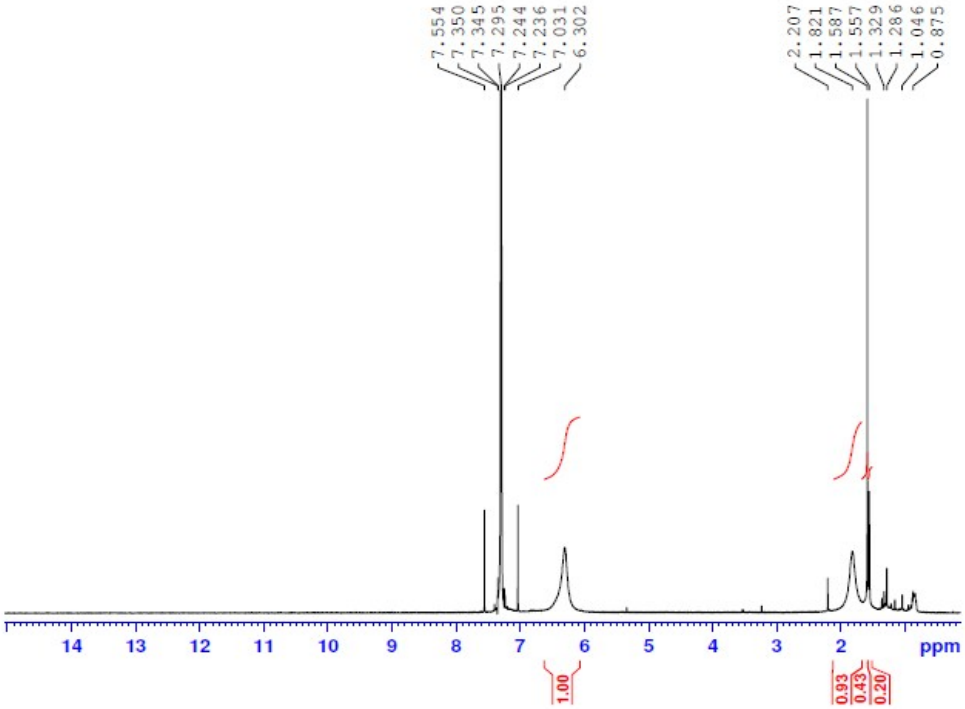


Figure S4 ^{1}H NMR spectrum of CuL^{NIS}.

Table S1. Crystallographic data for CuL^{NIS}	
Identification code	e1317a
Empirical formula	C42 H48 Cu N4 O2
Formula weight	704.38
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	a = 8.5030(5) Å
	b = 10.8824(8) Å
	c = 11.7661(10) Å
	α = 114.768(8)°.
	β = 90.404(6)°.
	γ = 92.966(5)°.
Volume	986.78(14) $Å^3$
Z	1
Density (calculated)	1.185 Mg/m^3
Absorption coefficient	0.591 mm^{-1}
F(000)	373
Crystal size	0.518 x 0.298 x 0.130 mm^3
Theta range for data collection	2.143 to 28.412°.
Index ranges	-7<=h<=11, -13<=k<=13, -10<=l<=15
Reflections collected	6811
Independent reflections	4344 [R(int) = 0.0512]
Completeness to theta = 25.000°	99.5 %
Absorption correction	Analytical
Max. and min. transmission	0.944680 and 0.838343
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4344 / 0 / 257
Goodness-of-fit on F^2	1.003
Final R indices [I>2sigma(I)]	R1 = 0.0554, wR2 = 0.1439
R indices (all data)	R1 = 0.0799, wR2 = 0.1741
Extinction coefficient	n/a
Largest diff. peak and hole	0.612 and -0.519 $e.Å^{-3}$

Table S2. Selected bond lengths [Å] and angles [°] for CuL^{NIS}			
Bonds		Angles	
Cu1-O1	1.9210(19)	O1-Cu1-O1#1	180.0
Cu1-O1#1	1.9210(19)	O1-Cu1-N1#1	96.82(8)
Cu1-N1#1	1.928(2)	O1#1-Cu1-N1#1	83.18(8)
Cu1-N1	1.928(2)	O1-Cu1-N1	83.18(8)
O1-C1	1.298(3)	O1#1-Cu1-N1	96.82(8)
C1-C2	1.424(4)	N1#1-Cu1-N1	180.0
C1-C6	1.448(4)	C1-O1-Cu1	113.53(17)
C2-C3	1.371(4)	O1-C1-C2	123.9(2)
C2-C14	1.529(4)	O1-C1-C6	116.6(2)
C3-C4	1.428(4)	C2-C1-C6	119.5(2)
C4-C5	1.361(4)	C3-C2-C1	116.7(2)
C4-C18	1.539(4)	C3-C2-C14	122.5(2)
C5-C6	1.416(4)	C1-C2-C14	120.8(2)
C6-N1	1.340(3)	C2-C3-C4	124.7(3)
N1-C7	1.412(3)	C5-C4-C3	118.9(2)
C7-C8	1.380(4)	C5-C4-C18	122.0(3)
C7-C12	1.395(4)	C3-C4-C18	119.1(2)
C8-C9	1.381(5)	C4-C5-C6	119.7(3)
C9-C10	1.373(6)	N1-C6-C5	126.4(2)
C10-C11	1.374(5)	N1-C6-C1	113.1(2)
C11-C12	1.383(4)	C5-C6-C1	120.4(2)
C12-C13	1.446(5)	C6-N1-C7	120.4(2)
C13-N2	1.133(5)	C6-N1-Cu1	113.56(18)
C14-C17	1.530(5)	C7-N1-Cu1	125.82(17)
C14-C15	1.534(4)	C8-C7-C12	118.6(3)
C14-C16	1.538(4)	C8-C7-N1	121.5(3)
C18-C21	1.485(7)	C12-C7-N1	119.8(3)
C18-C20	1.511(8)	C7-C8-C9	121.1(3)
C18-C20B	1.512(11)	C10-C9-C8	120.0(3)
C18-C21B	1.528(11)	C9-C10-C11	119.6(3)
C18-C19	1.532(8)	C10-C11-C12	120.9(3)
C18-C19B	1.536(11)	C11-C12-C7	119.8(3)
		C11-C12-C13	121.2(3)
		C7-C12-C13	119.0(3)
		N2-C13-C12	178.4(4)
		C2-C14-C17	109.7(2)
		C2-C14-C15	111.3(3)
		C17-C14-C15	109.2(3)
		C2-C14-C16	109.6(3)
		C17-C14-C16	109.2(3)
		C15-C14-C16	107.8(3)
		C21-C18-C20	111.4(6)
		C20B-C18-C21B	108.0(9)
		C21-C18-C19	106.6(6)
		C20-C18-C19	108.8(6)
		C20B-C18-C19B	111.1(9)
		C21B-C18-C19B	107.2(7)
		C21-C18-C4	109.9(4)
		C20-C18-C4	108.6(4)
		C20B-C18-C4	113.4(5)
		C21B-C18-C4	107.7(5)
		C19-C18-C4	111.5(3)
		C19B-C18-C4	109.2(4)

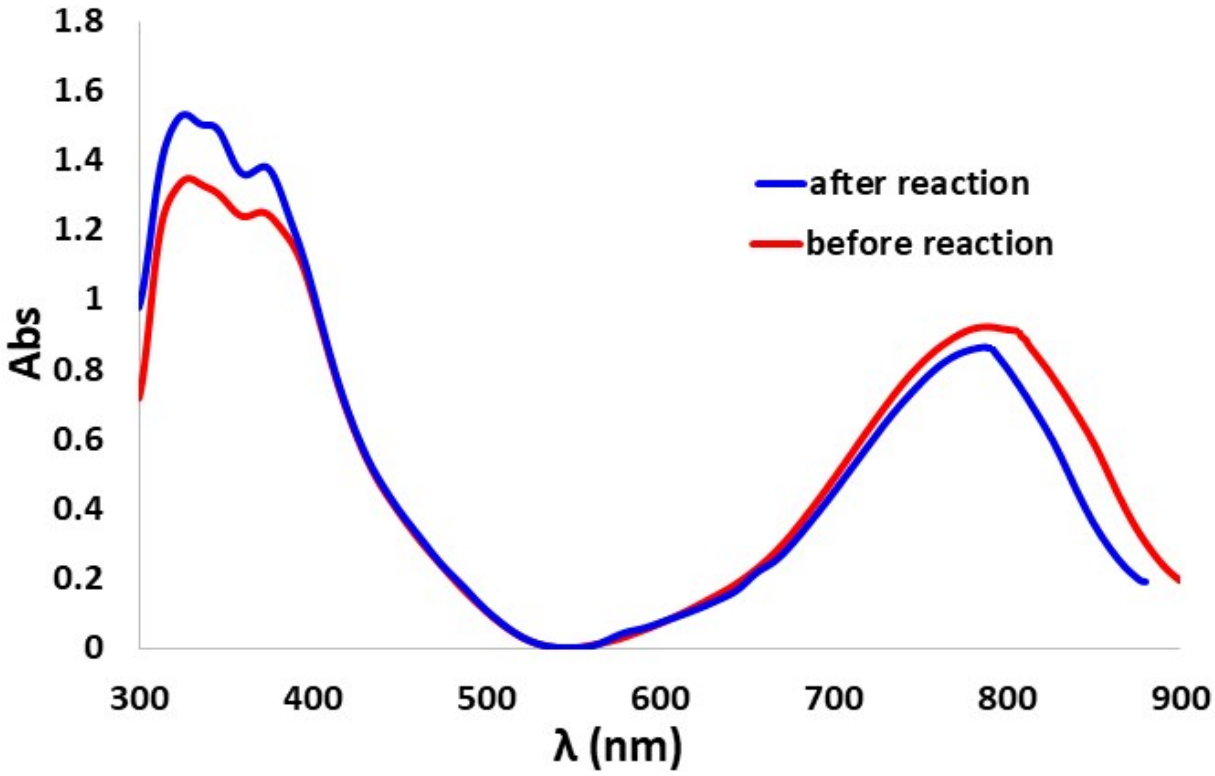


Figure S5 Electronic spectrum of $L_2^{NIS}Cu^{II}$ solution in THF before coupling reaction

(without KOH and phenyl acetylene addition) (_) after reaction (with KOH and phenyl acetylene addition) (_).

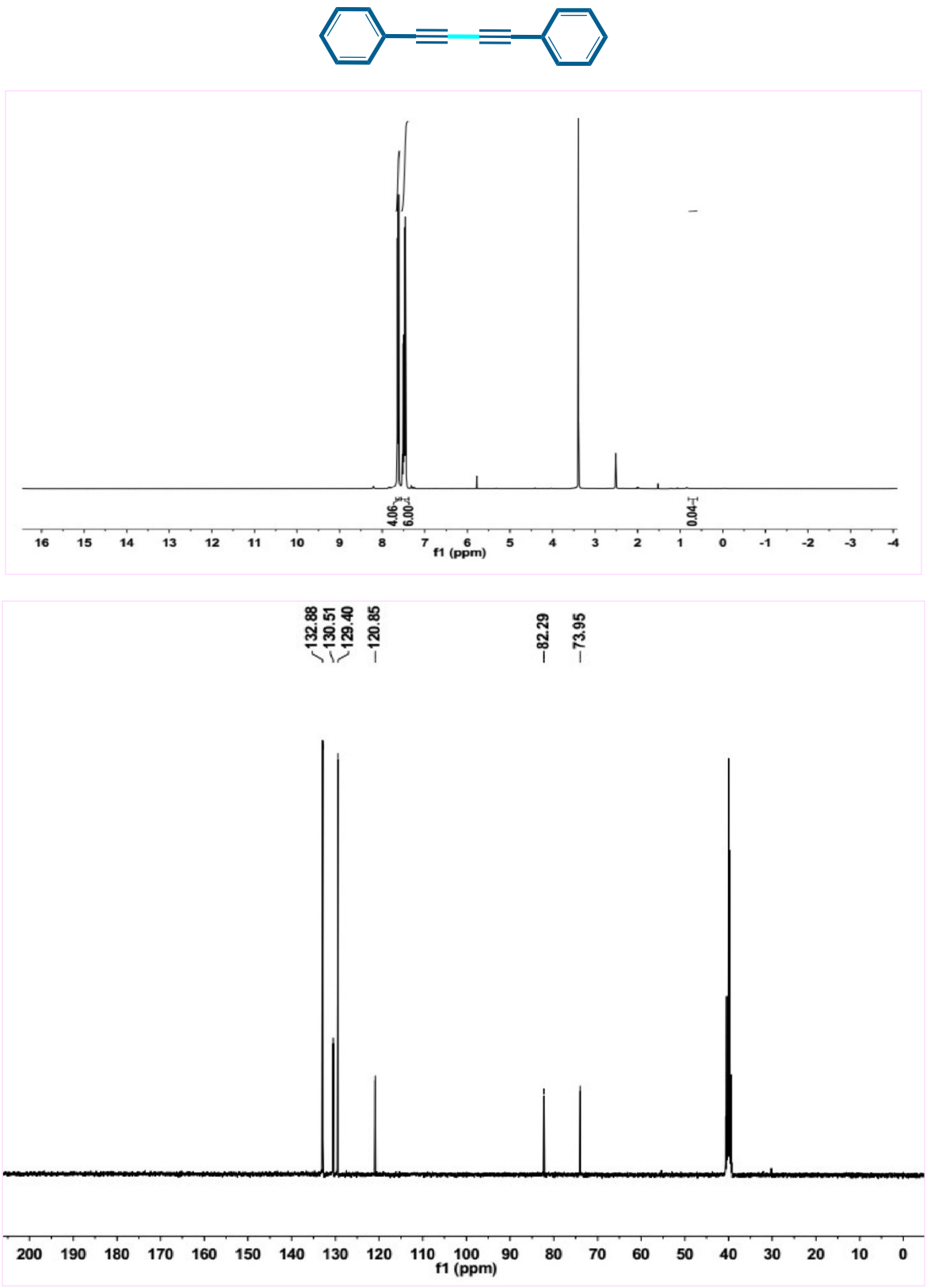
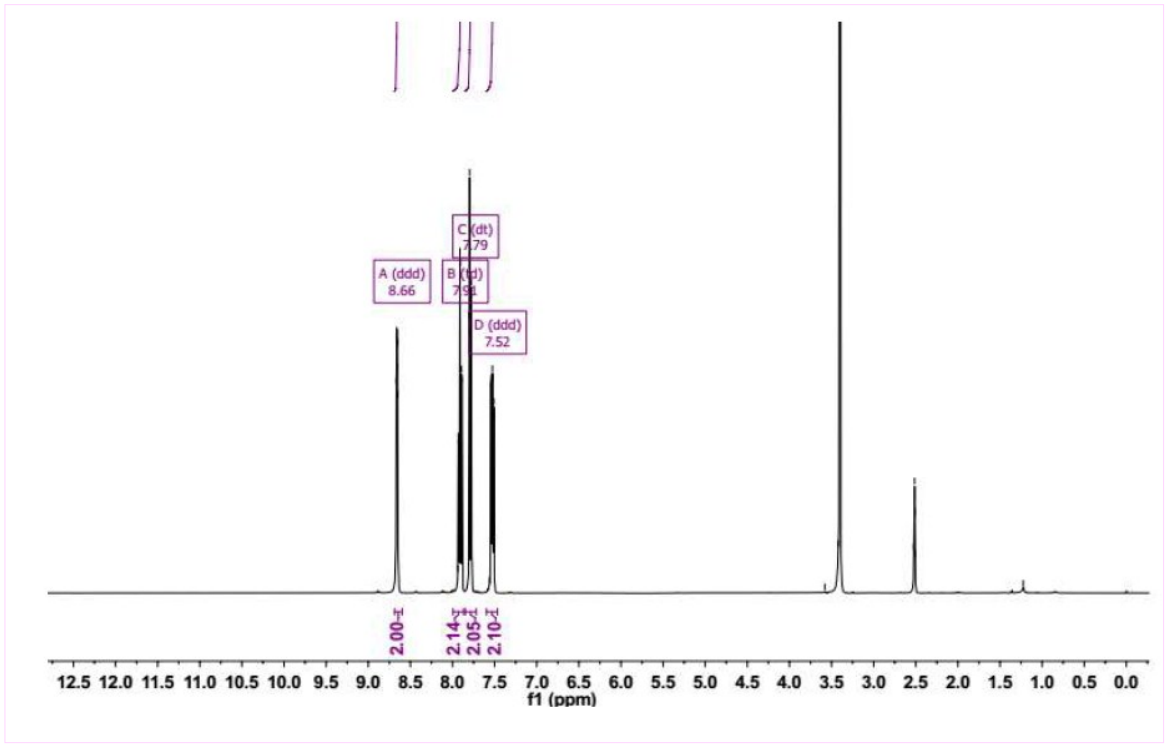


Figure S6 ^{1}H NMR and ^{13}C NMR spectrum of 1,4-diphenyl buta-1,3-diyne.



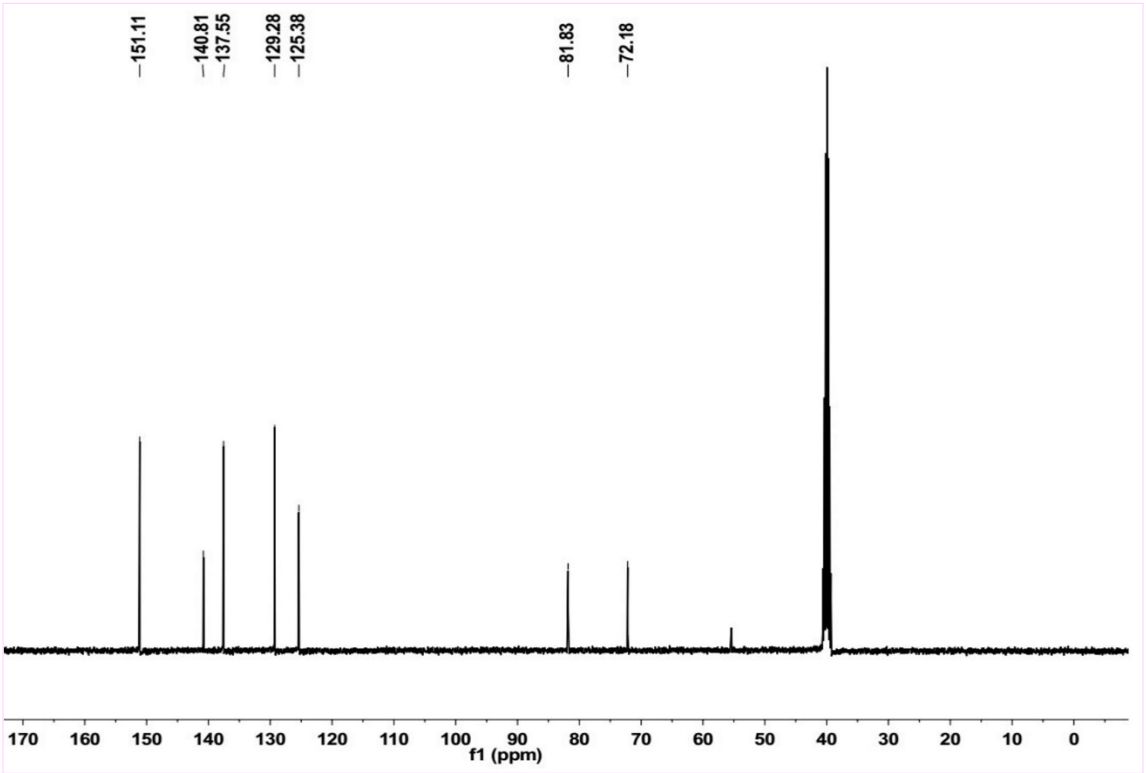


Figure S7 ^{1}H NMR and ^{13}C NMR spectrum of 1,4-di(pyridin-2-yl)buta-1,3-diyne.

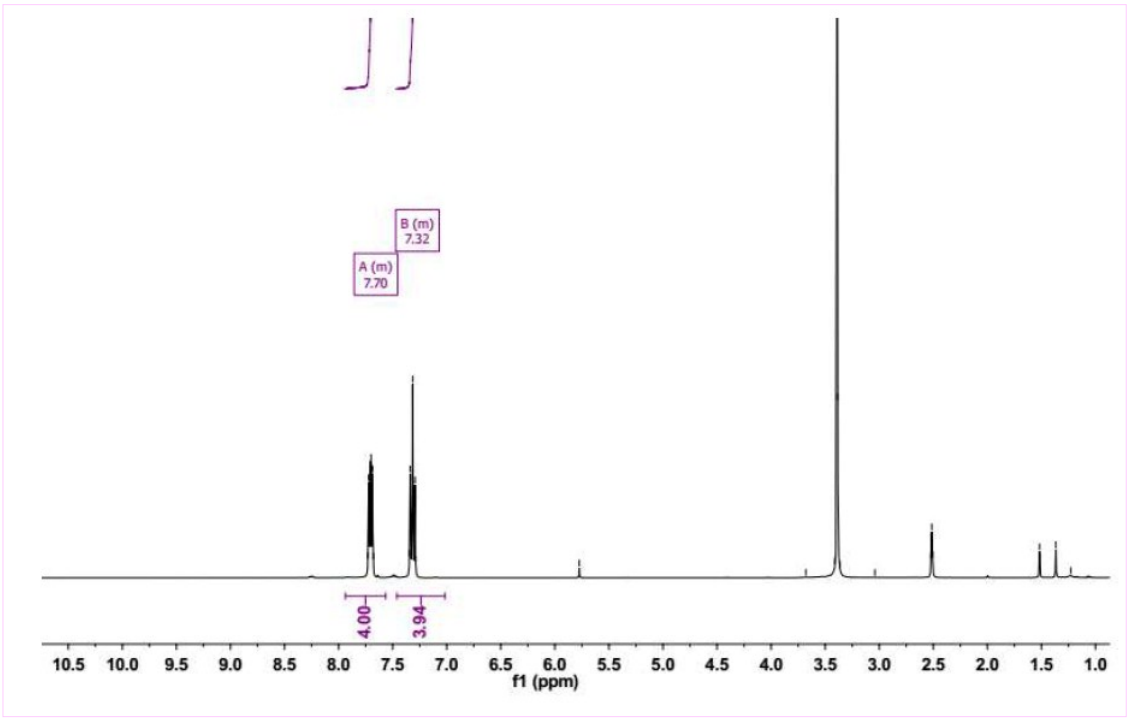


Figure S8 ^{1}H NMR and ^{13}C NMR spectrum of 1,4-*bis*(*p*-fluorophenyl)buta-1,3-diyne.

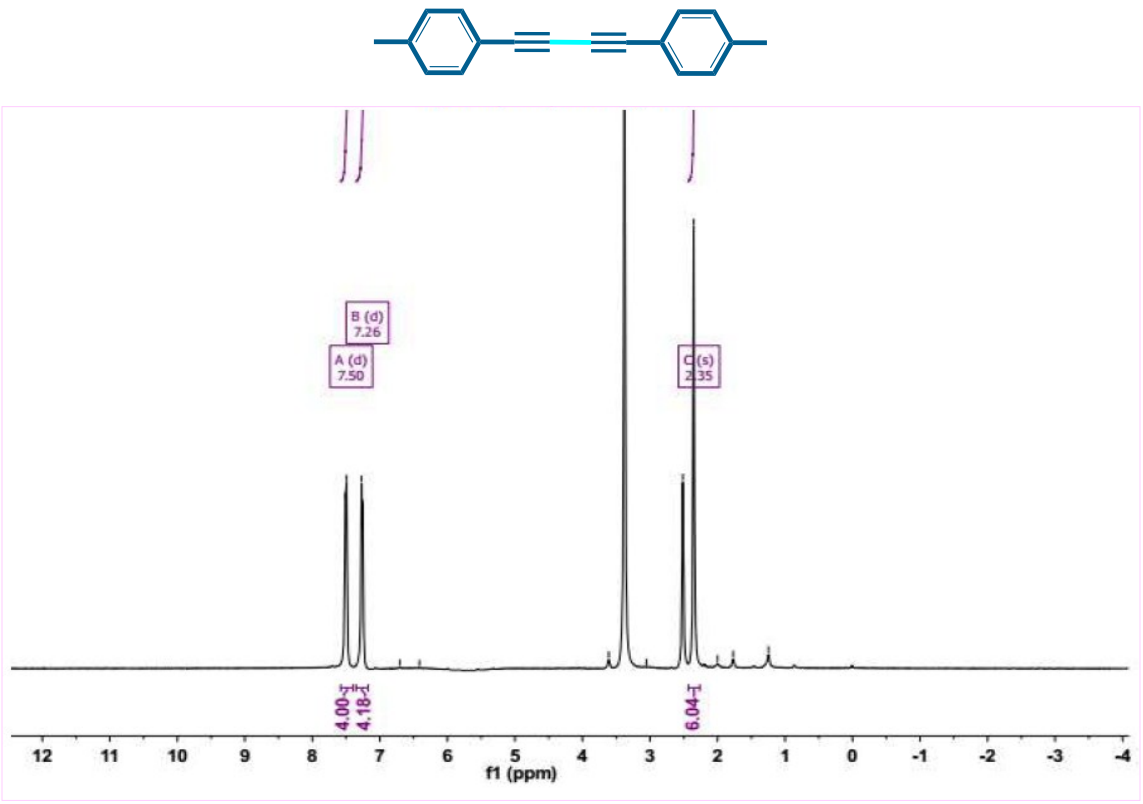


Figure S9 ^{1}H NMR and ^{13}C NMR spectrum of 1,4-*bis*(*p*-tolyl)buta-1,3-diyne.

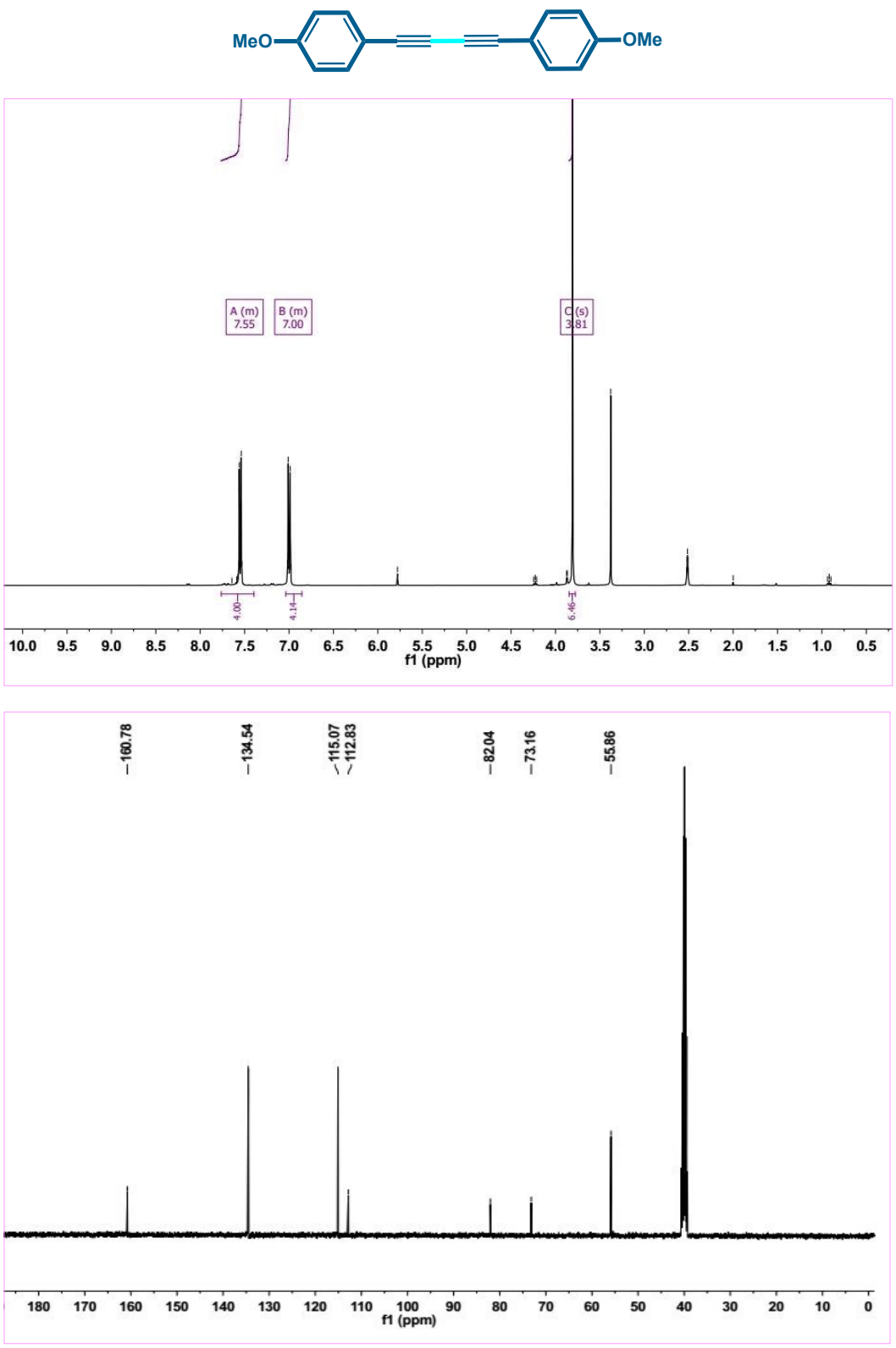


Figure S10 ^{1}H NMR and ^{13}C NMR spectrum of 1,4-bis(4-methoxyphenyl)buta-1,3-diyne.

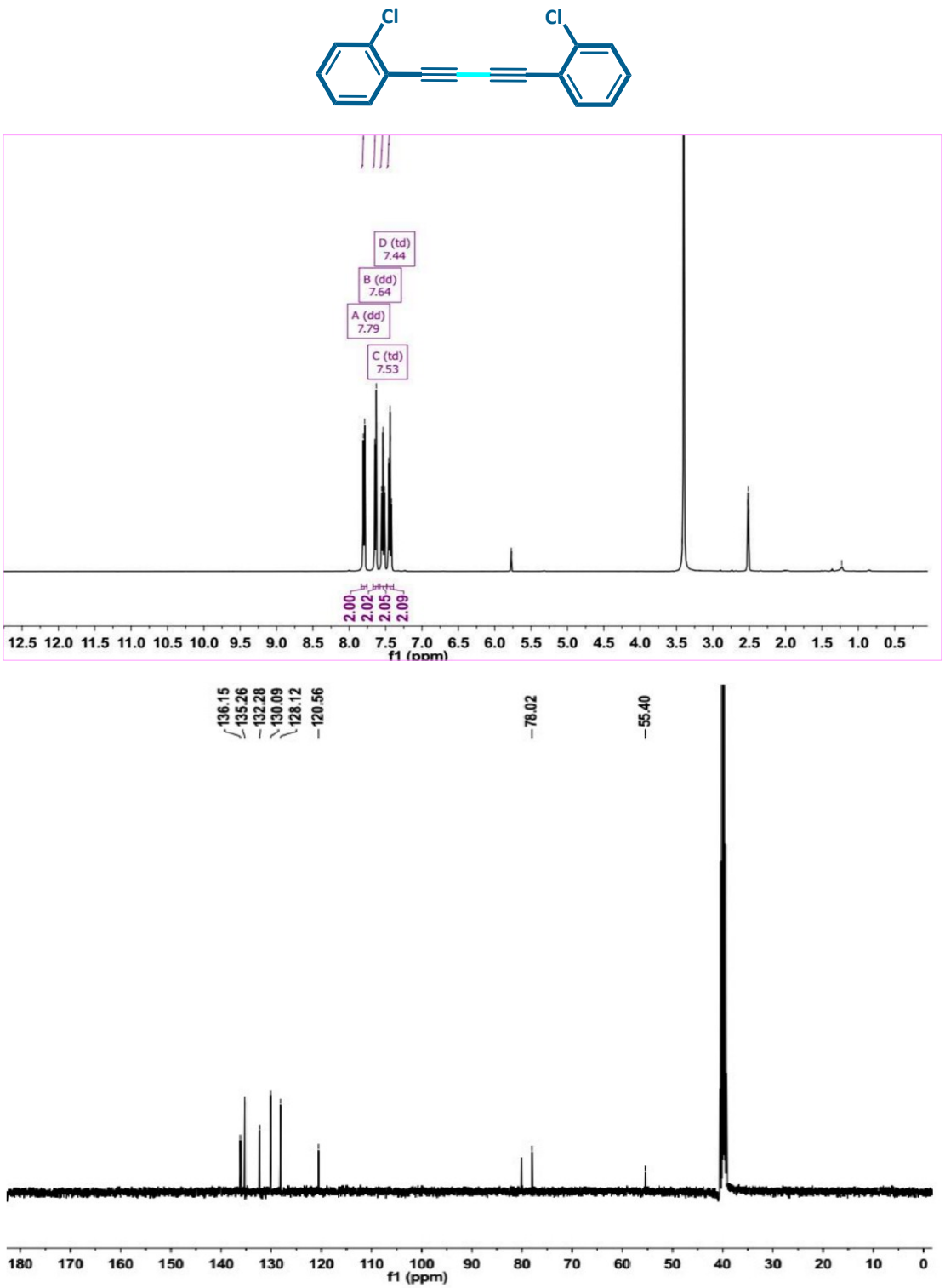


Figure S11 ^{1}H NMR and ^{13}C NMR spectrum of 1,4-bis(2-chlorophenyl)buta-1,3-diyne.