

Electronic supplementary information

for

Catalytic Sonogashira Couplings Mediated by an Amido Pincer Complex of Palladium

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Table S1. Data derived from competition reactions to construct Figure 3

	σ_p	yield	$\log(k/k_H)$
4-OMe	-0.27	3.9	-0.28
4-Me	-0.17	5.3	-0.15
H	0	7.5	0
4-C(O)Me	0.50	17.5	0.37

Table S2. Data derived from competition reactions to construct Figure 4

	σ_p	yield	$\log(k/k_H)$
4-OMe	-0.27	6.7	-0.38
4-Me	-0.17	8.9	-0.26
H	0	16.1	0
4-CF ₃	0.54	40.9	0.40
4-CN	0.66	60.3	0.57

Table S3. Crystal data and structure refinement for **1b**.

Identification code	5574	
Empirical formula	C ₂₄ H ₃₆ Cl N P ₂ Pd	
Formula weight	542.33	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 12.2739(3) Å	α = 90°.
	b = 10.0375(2) Å	β = 96.5990(10)°.
	c = 20.7695(6) Å	γ = 90°.
Volume	2541.83(11) Å ³	
Z	4	
Density (calculated)	1.417 Mg/m ³	
Absorption coefficient	0.972 mm ⁻¹	
F(000)	1120	
Crystal size	0.18 x 0.13 x 0.05 mm ³	
Theta range for data collection	2.26 to 25.35°.	
Index ranges	-14 ≤ h ≤ 14, -12 ≤ k ≤ 10, -19 ≤ l ≤ 25	
Reflections collected	16419	
Independent reflections	4643 [R(int) = 0.0729]	
Completeness to theta = 25.35°	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9674 and 0.7601	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	4643 / 0 / 262	
Goodness-of-fit on F ²	1.004	
Final R indices [I > 2σ(I)]	R1 = 0.0442, wR2 = 0.1039	
R indices (all data)	R1 = 0.0723, wR2 = 0.1209	
Largest diff. peak and hole	0.688 and -1.126 e.Å ⁻³	

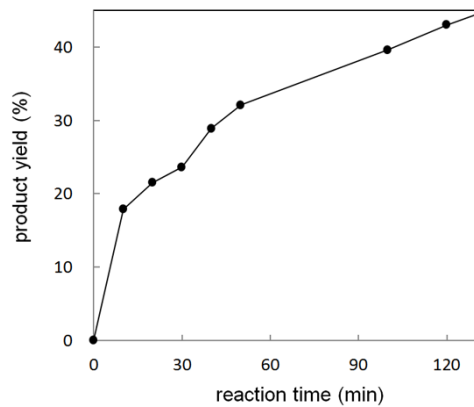


Figure S1. Reaction profile (product yields versus time) of the model reaction (Table 1, entry 1) conducted with 5-fold diluted initial substrate concentrations.

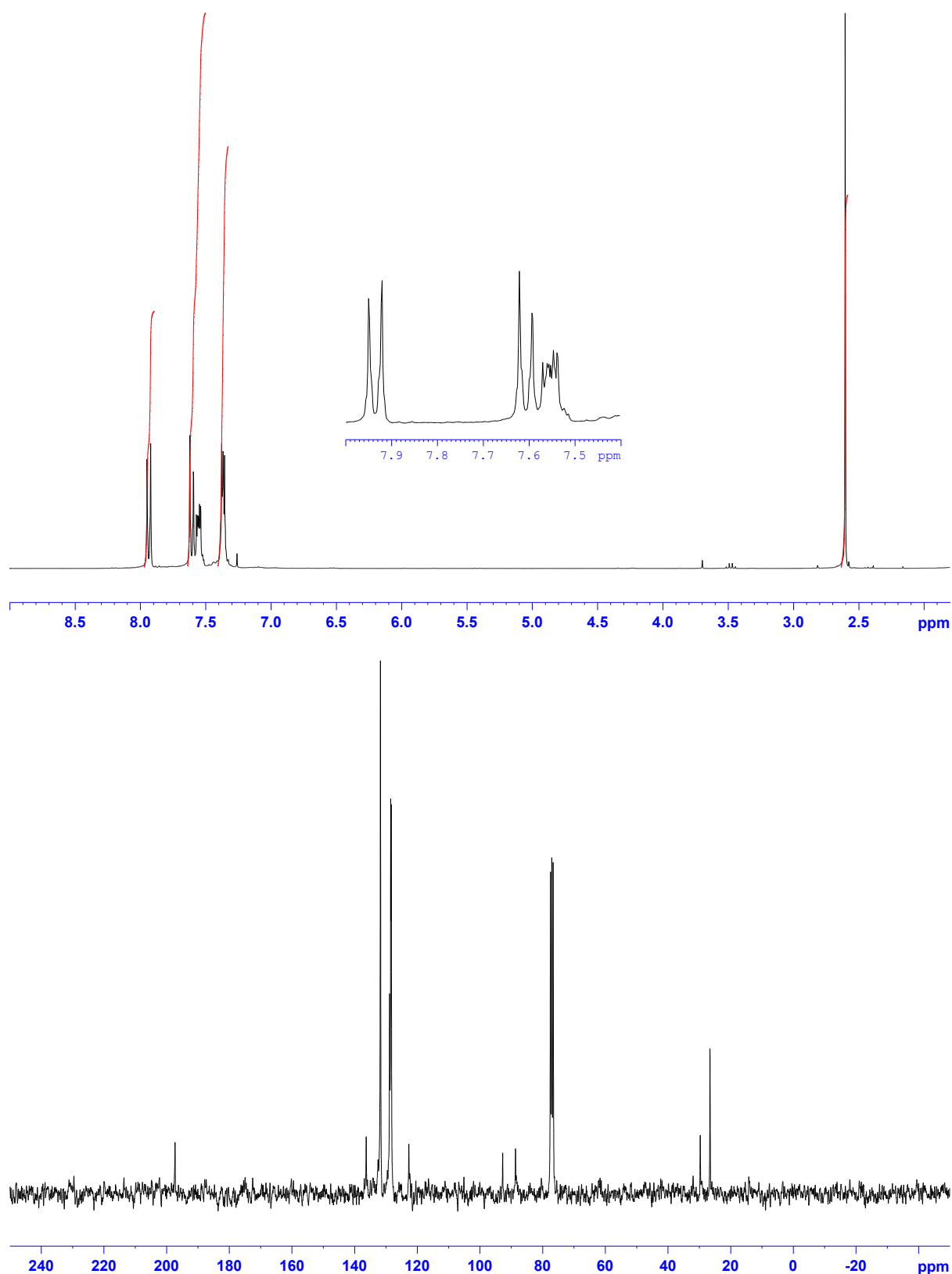


Figure S2. The ¹H (top, 300 MHz) and ¹³C{¹H} (bottom, 75 MHz) NMR spectra of 4-(phenylethynyl)acetophenone (**6e**) in CDCl₃ at room temperature

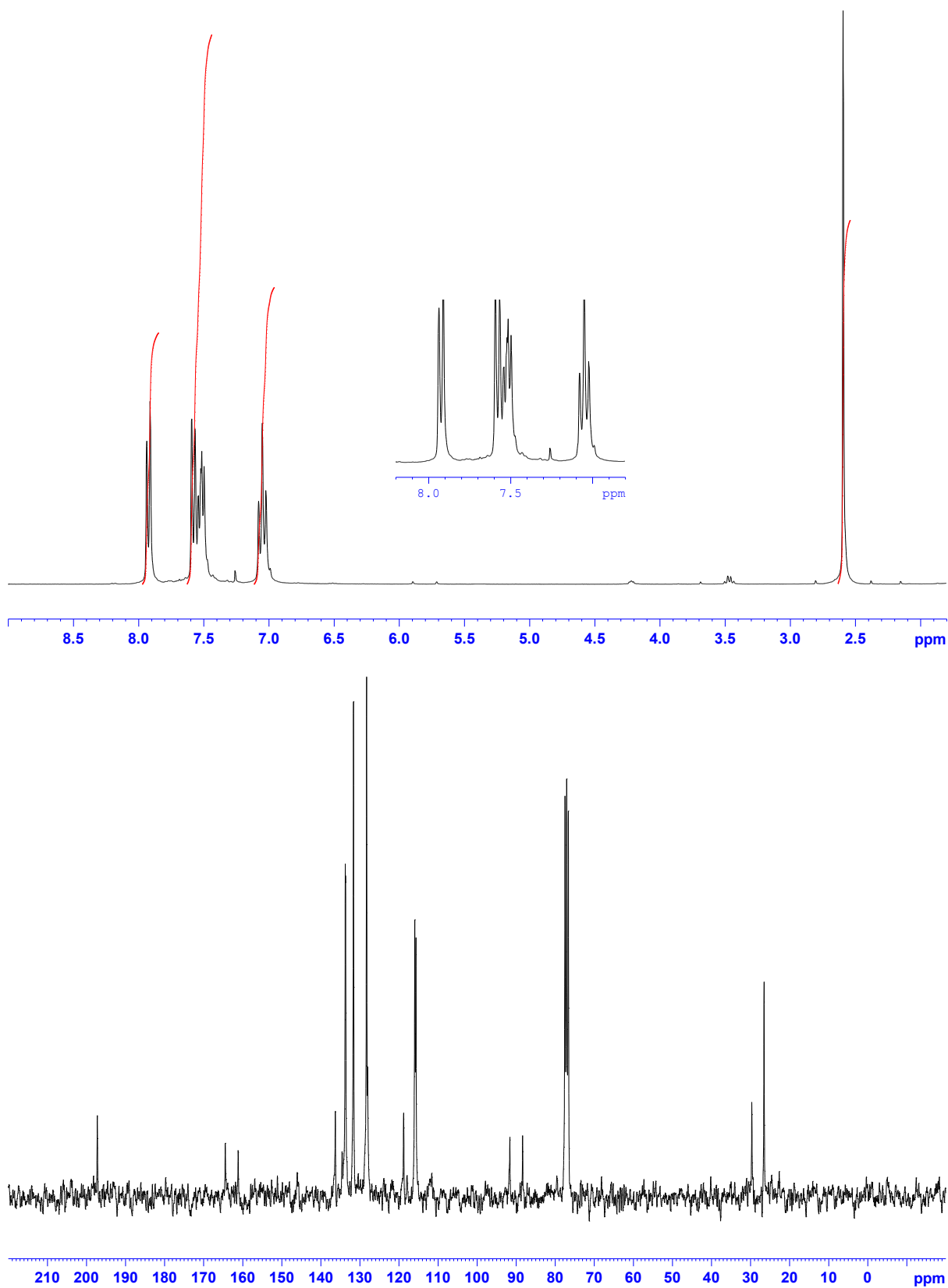


Figure S3. The ¹H (top, 300 MHz) and ¹³C{¹H} (bottom, 75 MHz) NMR spectra of 4-(4-fluorophenylethynyl)acetophenone (**7e**) in CDCl₃ at room temperature

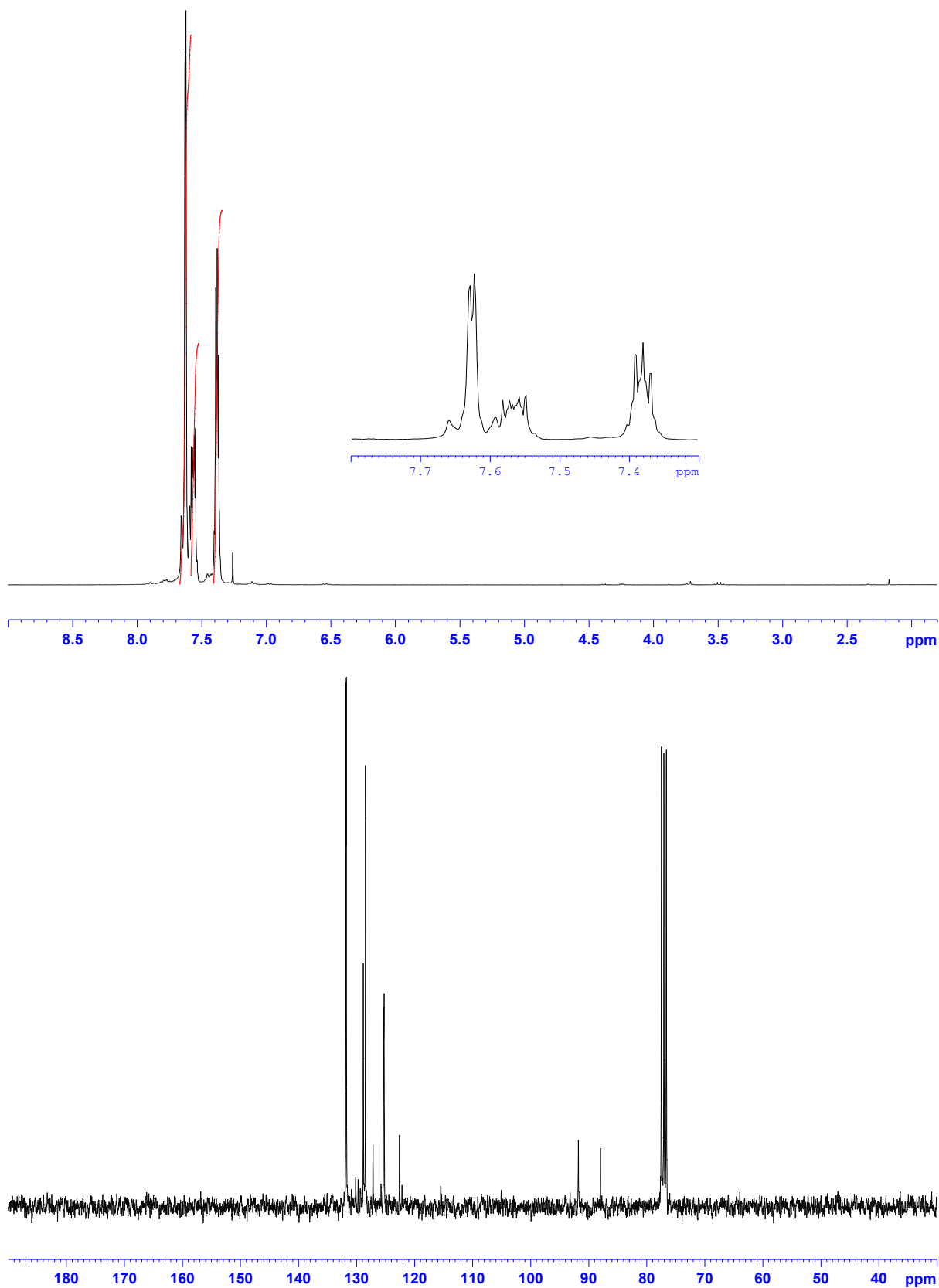


Figure S4. The ^1H (top, 300 MHz) and $^{13}\text{C}\{^1\text{H}\}$ (bottom, 75 MHz) NMR spectra of 1-(phenylethynyl)-4-(trifluoromethyl)benzene (**8a**) in CDCl_3 at room temperature

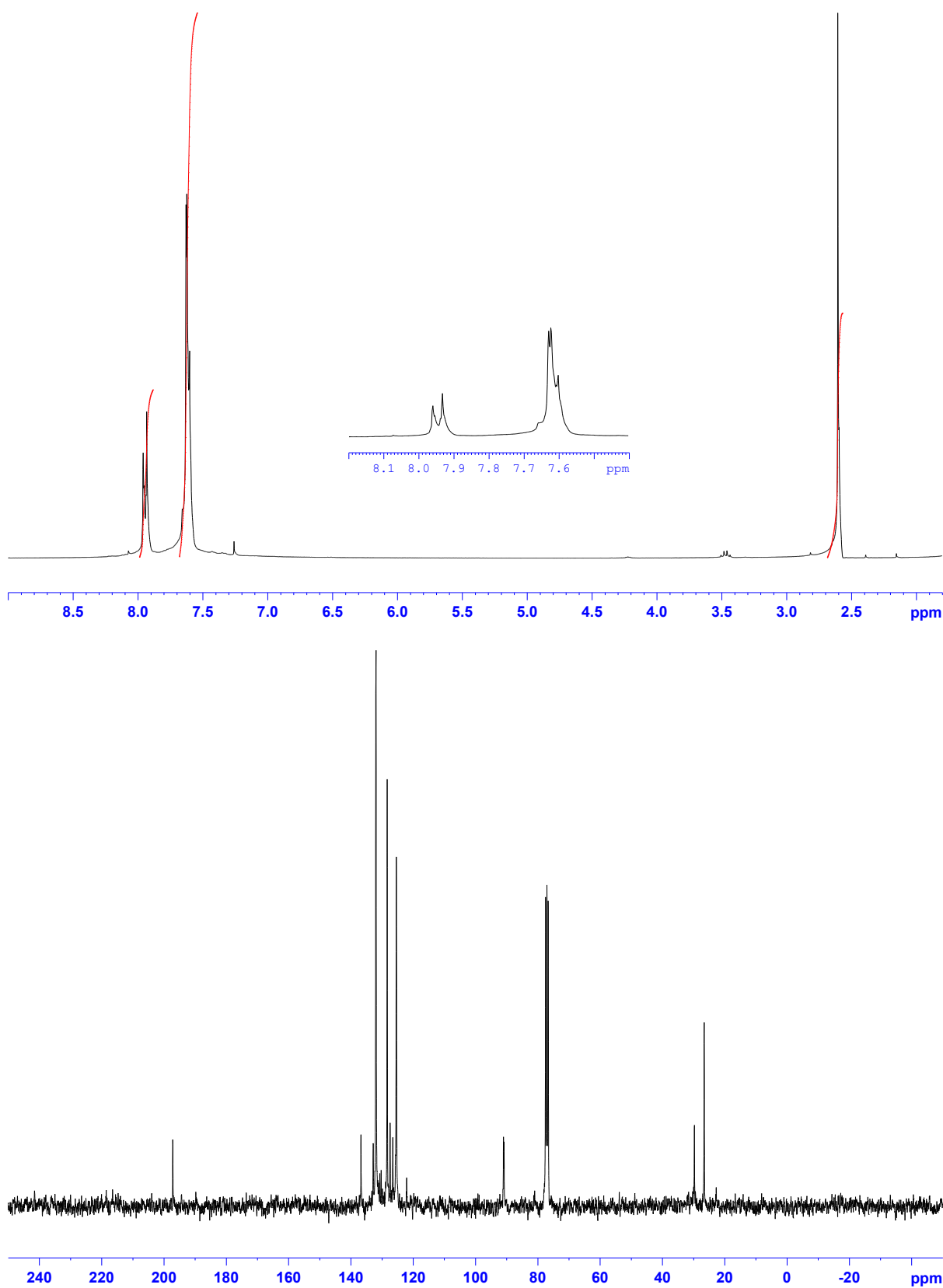


Figure S5. The ^1H (top, 300 MHz) and $^{13}\text{C}\{^1\text{H}\}$ (bottom, 75 MHz) NMR spectra of 4-(4-trifluoromethylphenylethynyl)acetophenone (**8e**) in CDCl_3 at room temperature

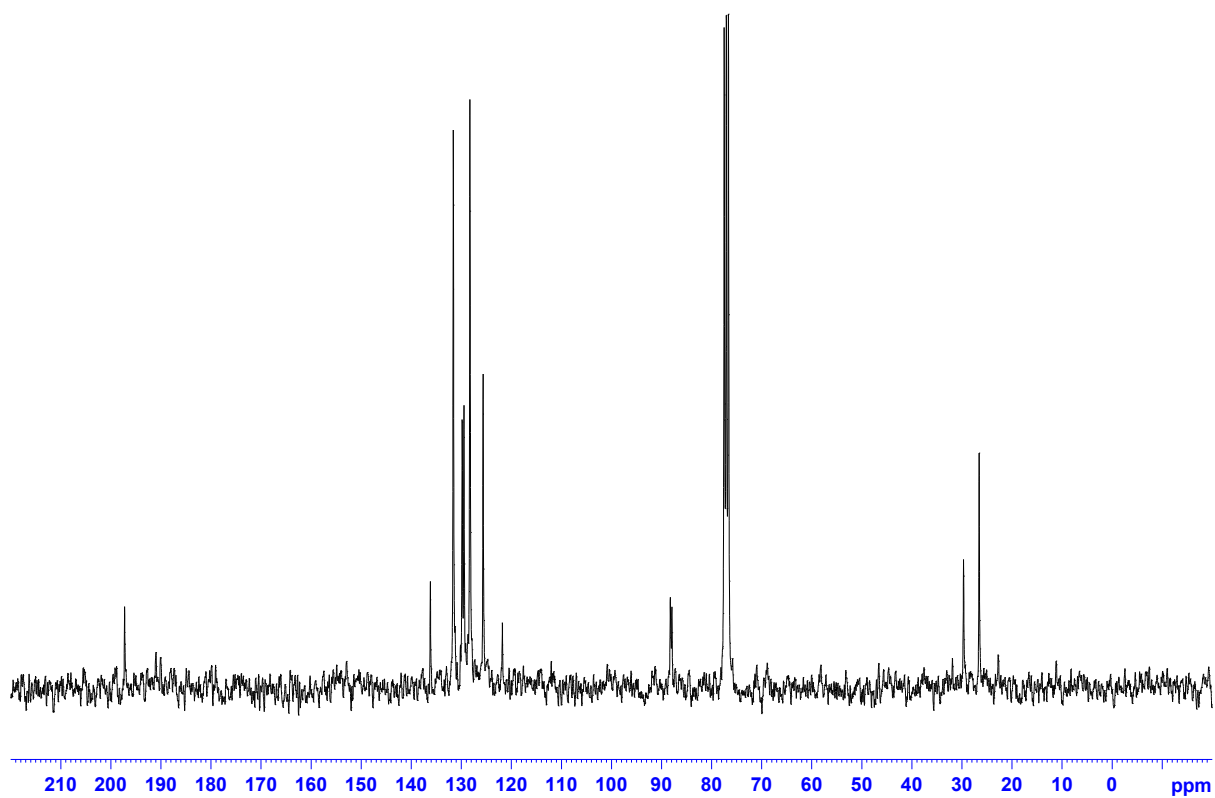
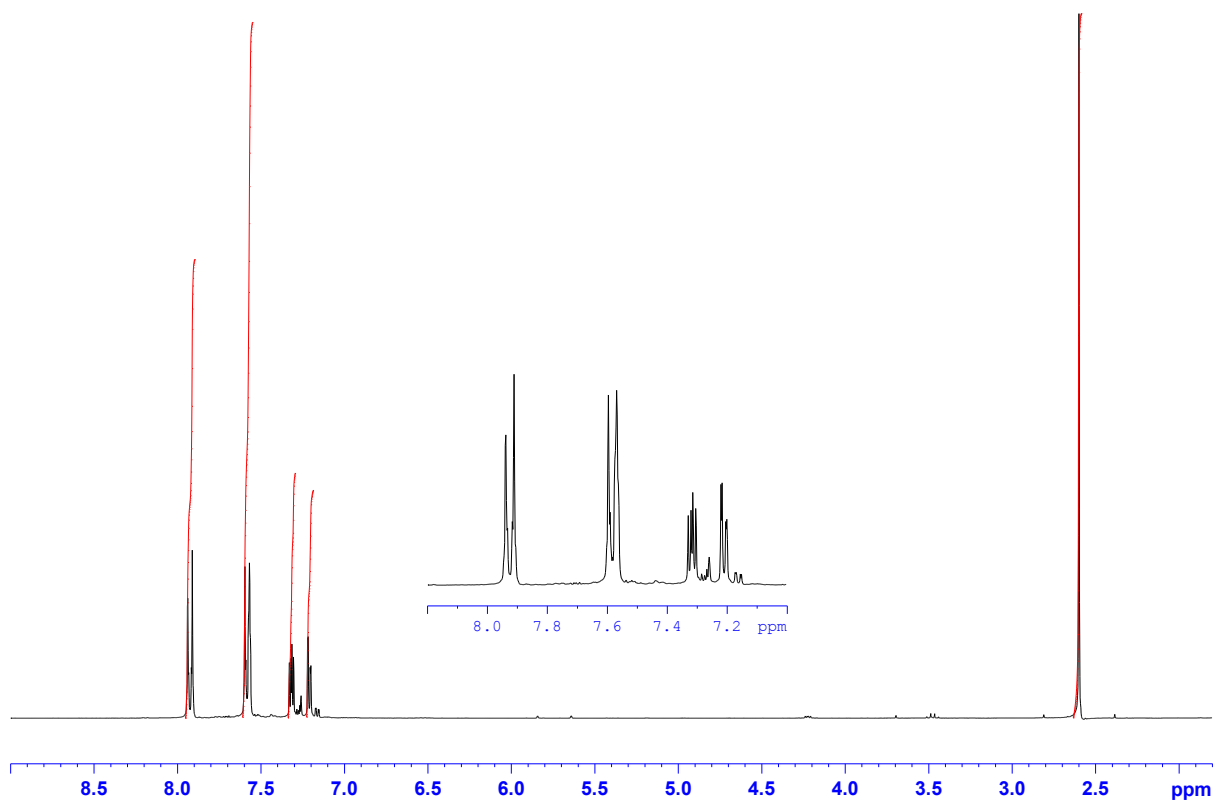


Figure S6. The ^1H (top, 300 MHz) and $^{13}\text{C}\{^1\text{H}\}$ (bottom, 75 MHz) NMR spectra of 3-(4-acetylphenylethynyl)thiophene (**9e**) in CDCl_3 at room temperature

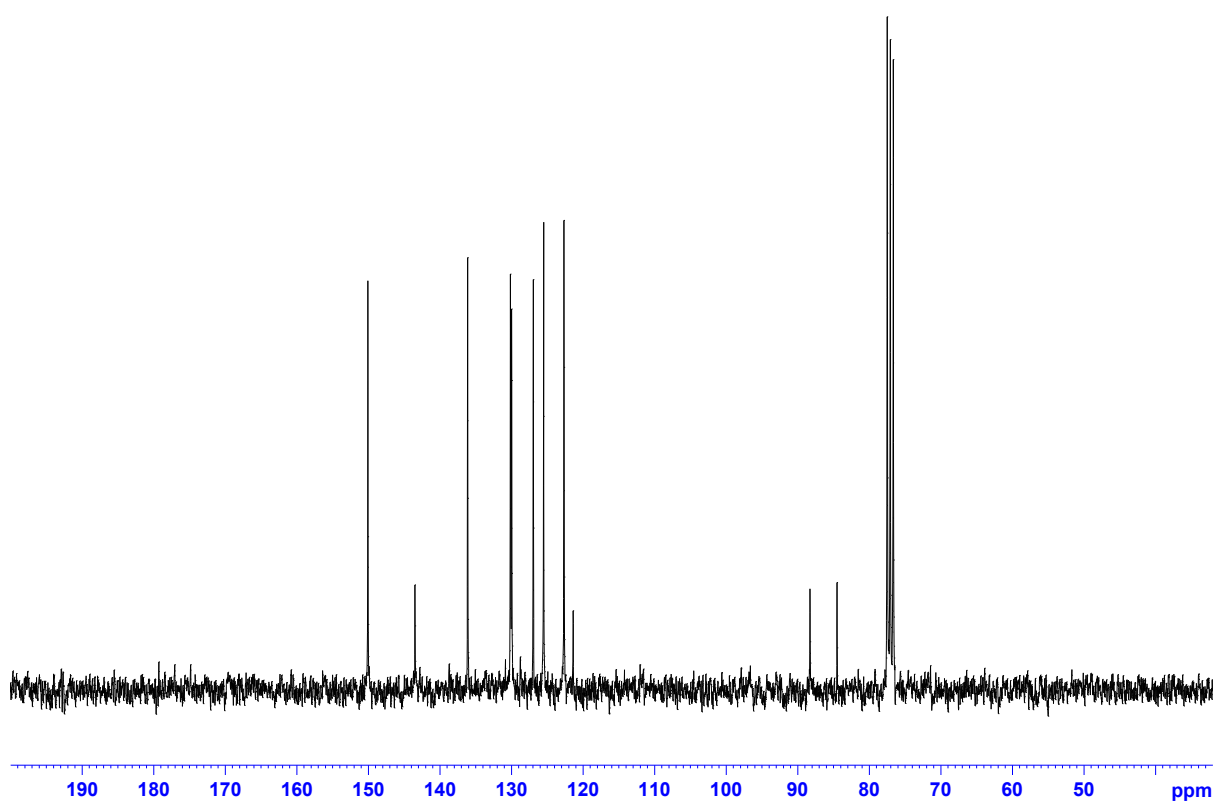
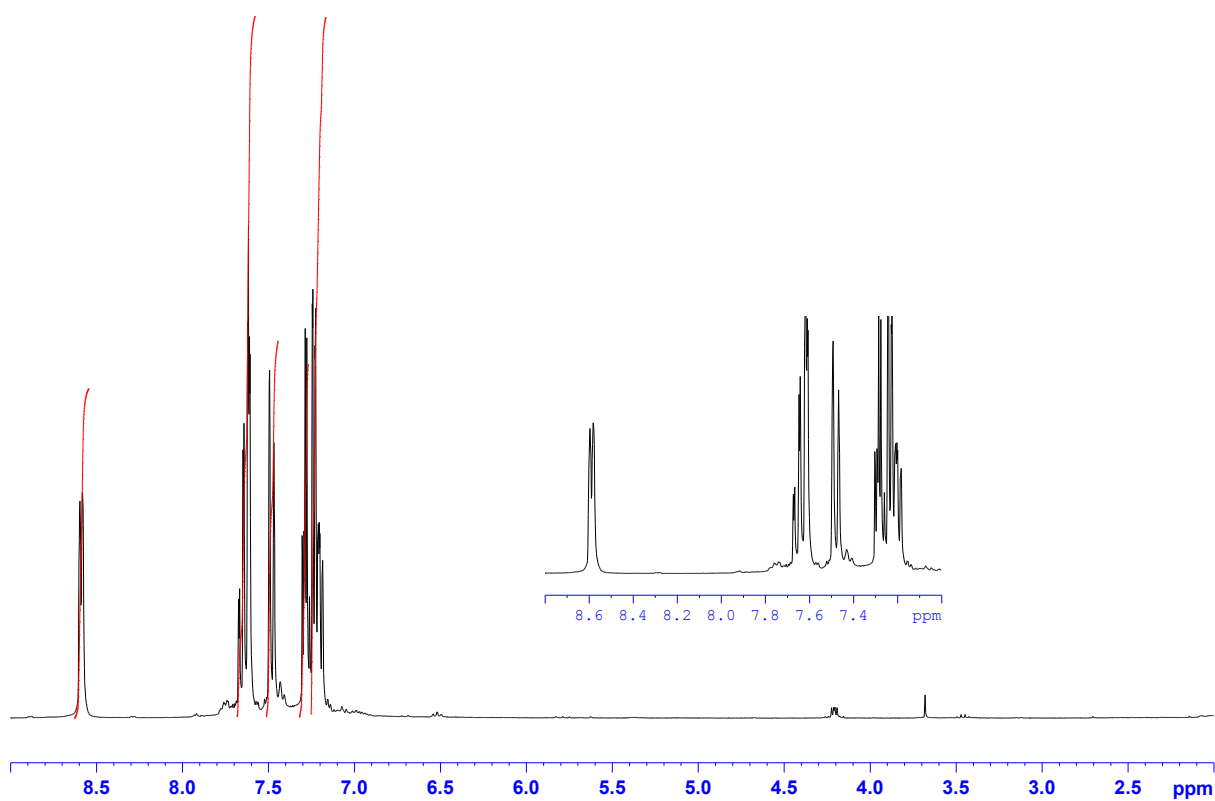


Figure S7. The ^1H (top, 300 MHz) and $^{13}\text{C}\{^1\text{H}\}$ (bottom, 75 MHz) NMR spectra of 3-(2-pyridylethynyl)thiophene (**9g**) in CDCl_3 at room temperature