Supplementary Materials

Regioselective Transfer Hydrogenative Defluorination of Polyfluoroarenes Catalyzed by Bifunctional Azairidacycle

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X-ray Crystallographic Data

Table S1. Crystallographic data for **7a** and **10**

	7a	**10**
Empirical Formula	$C_8H_2F_2N_2$	$C_6H_4F_2N_2O$
Formula Weight	164.11	158.11
Crystal Color, Habit	colorless, prism	colorless, prism
Crystal System	monoclinic	monoclinic
Space Group	$P2_1/c$ (#14)	$P2_1/c$ (#14)
Lattice Parameters	a = 5.657(7) Å	a = 3.691(2) Å
	b = 9.448(12) Å	b = 13.118 (8) Å
	c = 6.888(9) Å	c = 12.719(8) Å
	β = 101.70(2) °	β = 92.960(7) °
	V = 360.4(8) Å^3	V = 615.0(7) Å^3
Z value	2	4
D_{calc}	1.512 g/cm^3	1.707 g/cm^3
F_{000}	164.00	320.00
μ(Mo$K\alpha$)	1.306 cm^{-1}	1.600 cm^{-1}
Exposure Rate	16.0 sec./º	16.0 sec./°
No. of Reflections Measured	2738	4923
No. of Unique Reflections	809	1396
No. Variables	56	116
$R1$ (I>2.00σ(I))	0.0660	0.0500
w$R2$ (All Reflections)	0.1592	0.1131
GOF on F^2	1.000	1.000

$R1 = \Sigma\ ||F_o| - |F_c|| / \Sigma\ |F_o|$, $wR2 = [\ \Sigma\ (\ w\ (F_o^2 - F_c^2)^2\ )/\ \Sigma\ w(F_o^2)^2\ ]^{1/2}$.

^{19}F NMR Monitoring Experiments

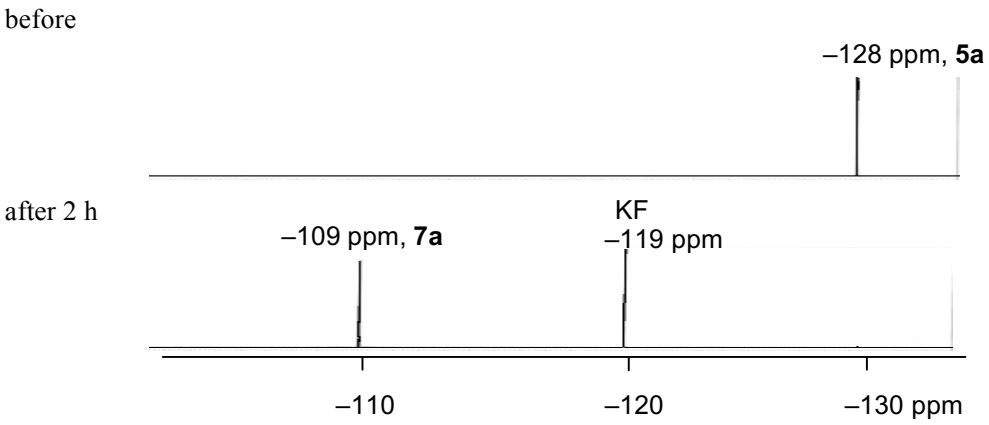
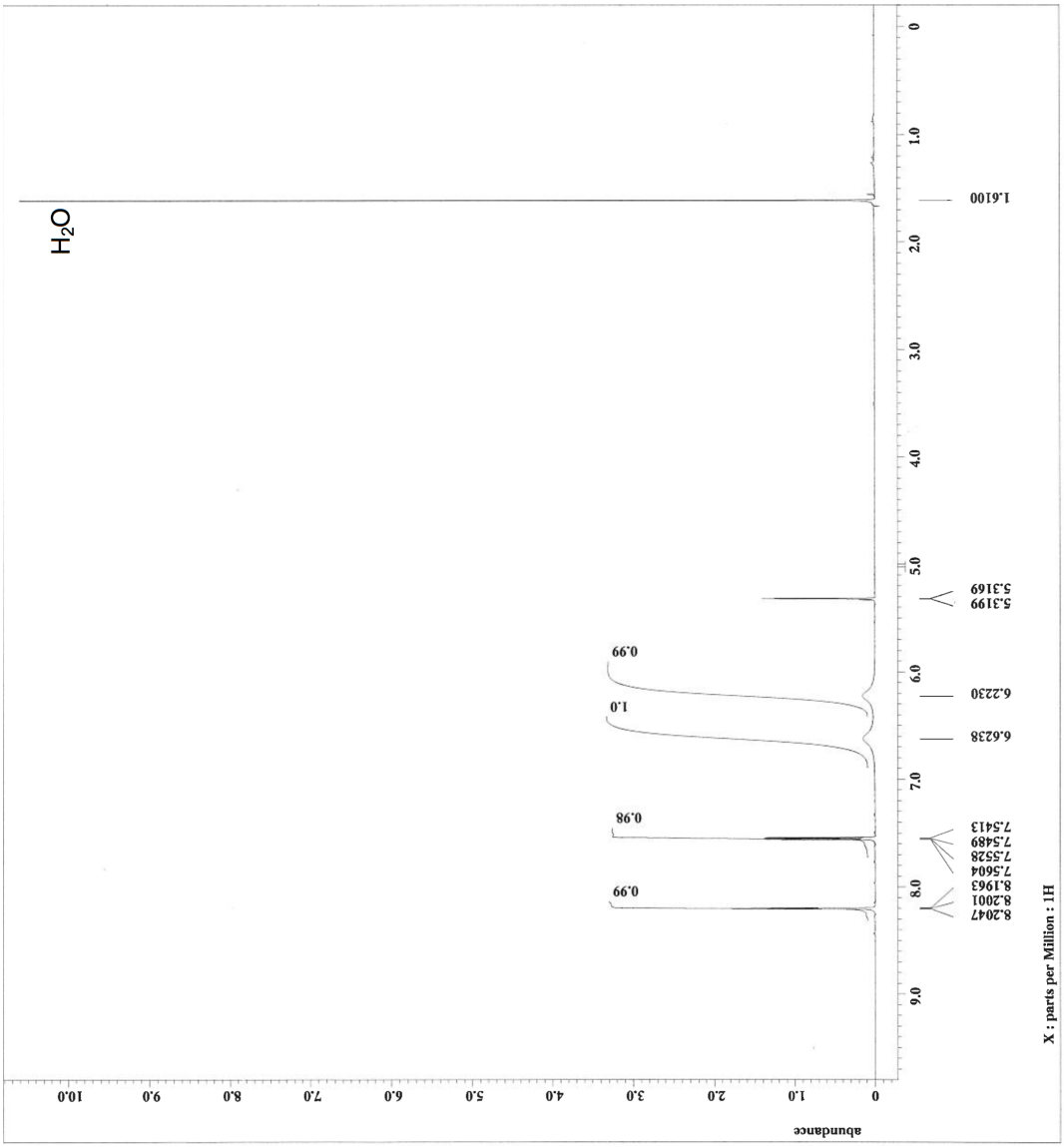
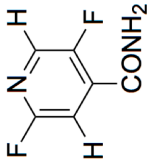


Figure S1. HDF of **5a** Monitored by ^{19}F NMR Spectroscopy.

Copies of NMR Spectra of 10, 12a, and 12b





10

Figure S2. ^{1}H NMR Spectrum of **10**.

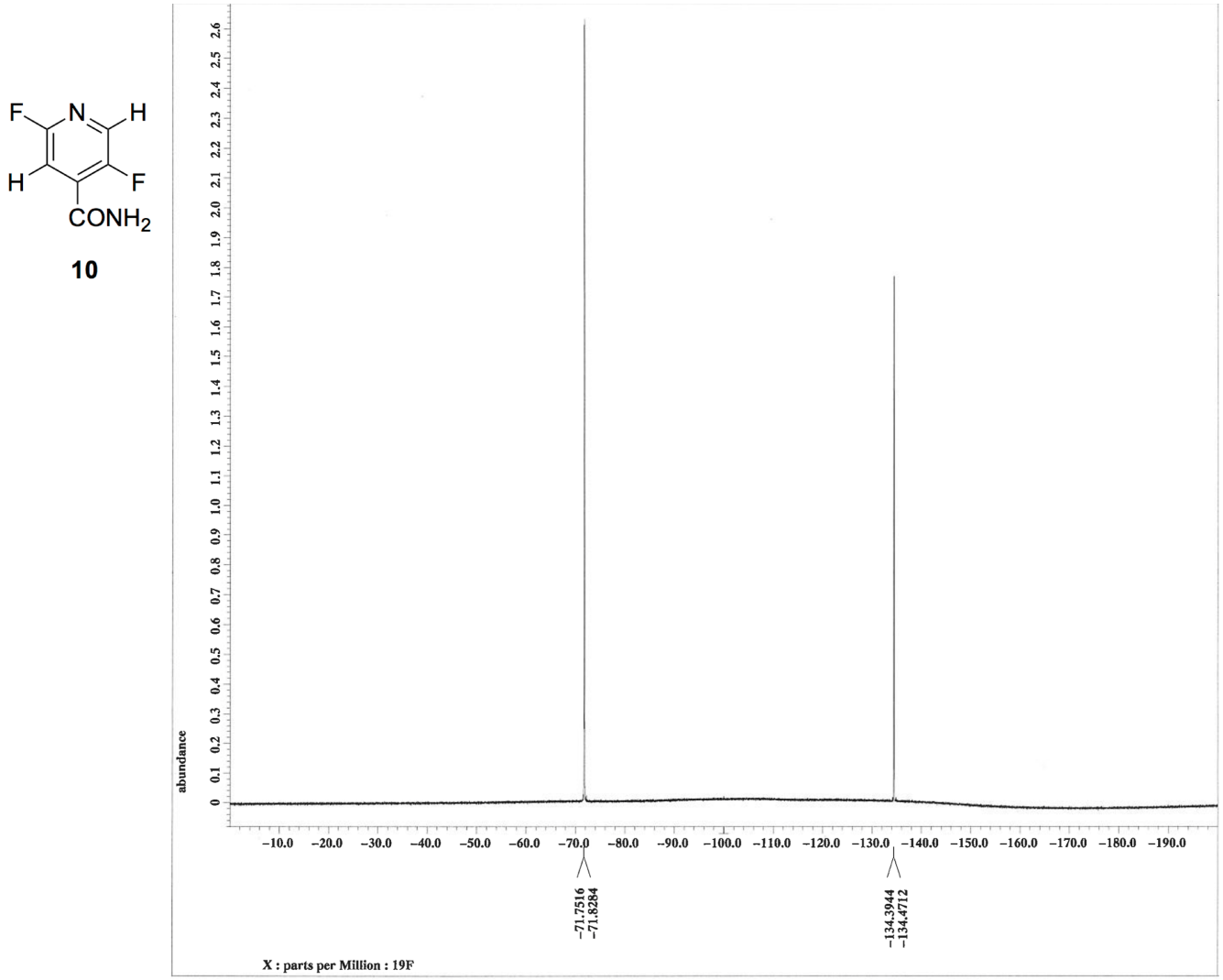


Figure S3. ^{19}F NMR Spectrum of **10**.

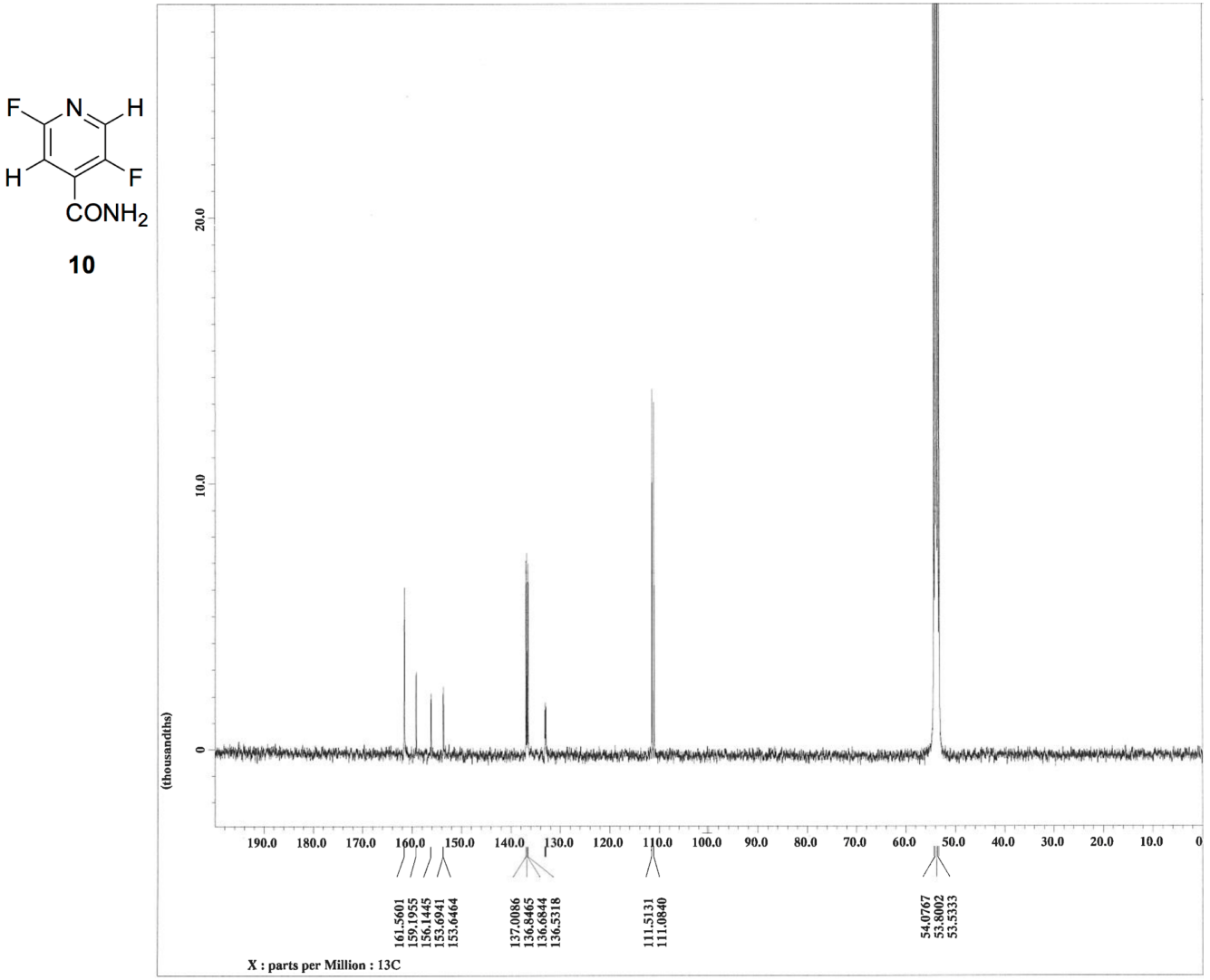


Figure S4. $^{13}C\{^{1}H\}$ NMR Spectrum of **10**.

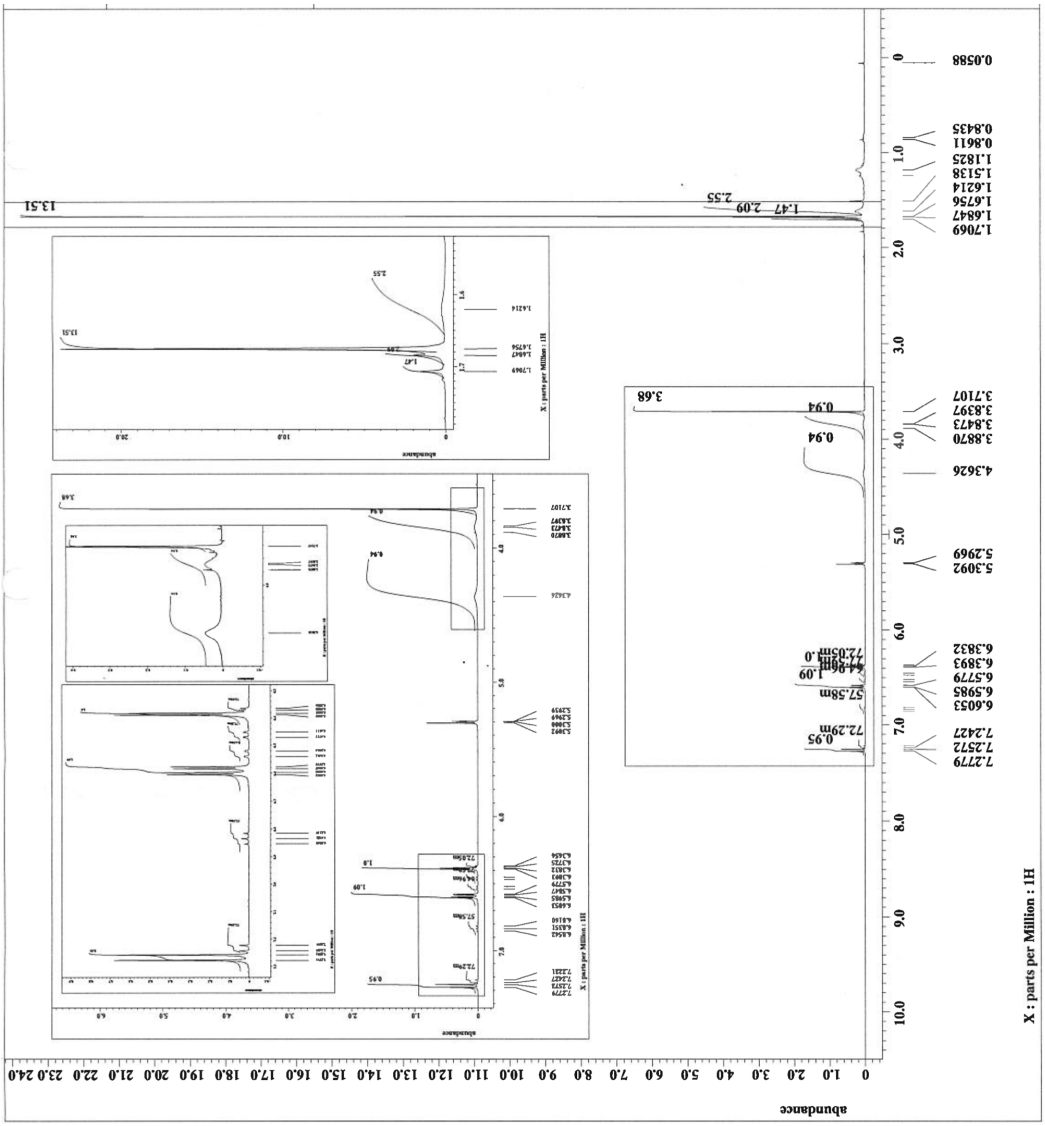


Figure S5. ^{1}H NMR Spectrum of **12a**.

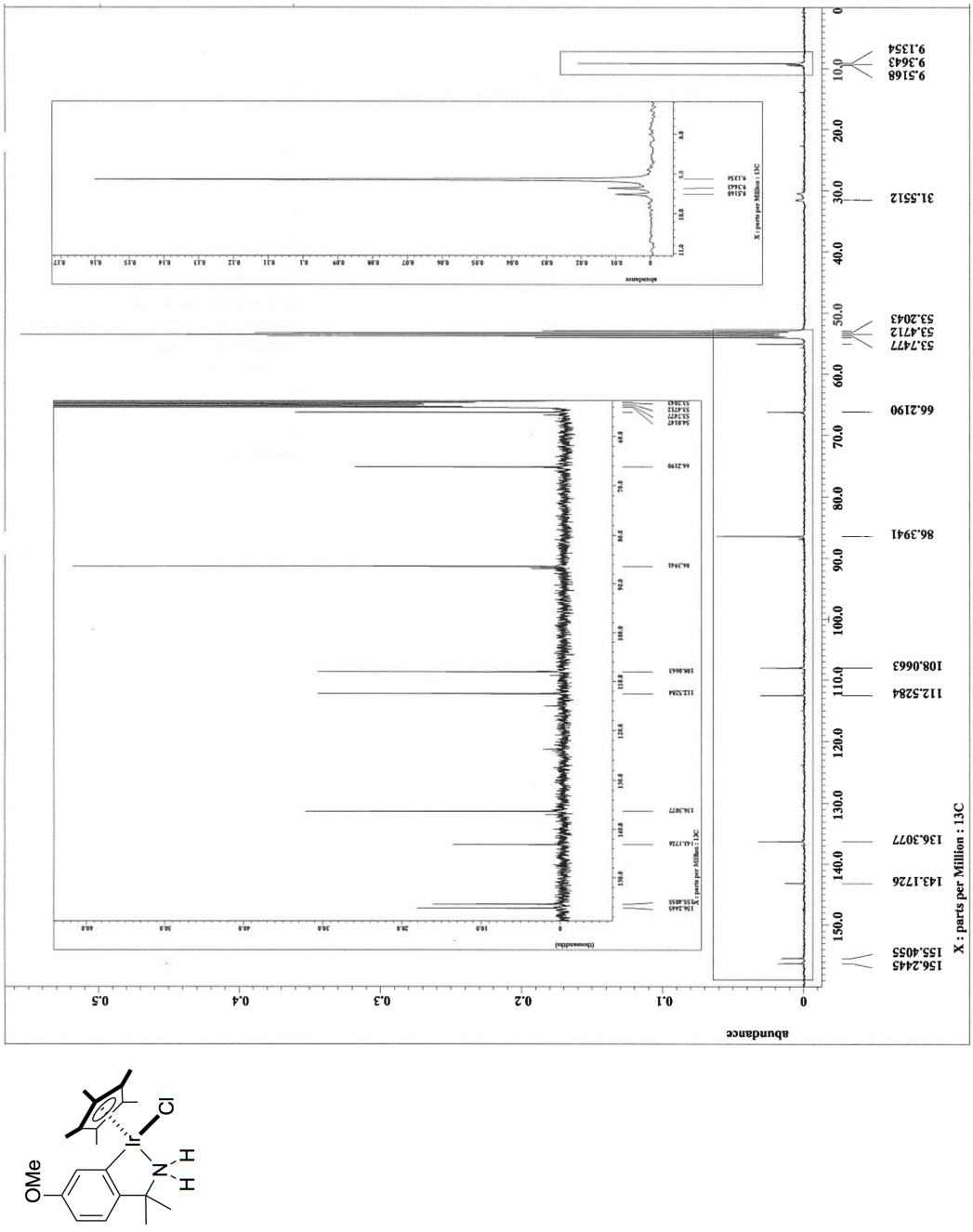


Figure S6. ^{13}C NMR Spectrum of **12a.**

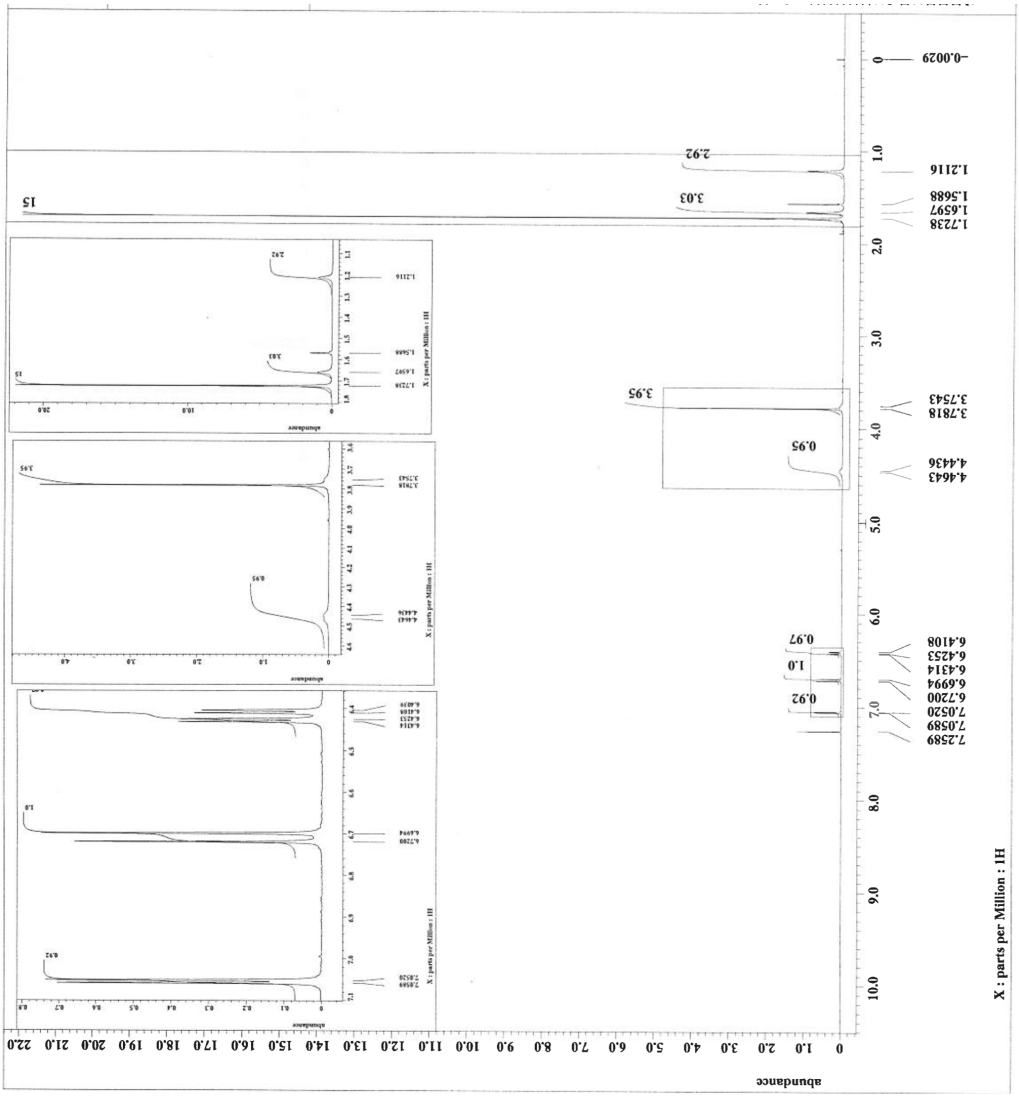


Figure S7. ^{1}H NMR Spectrum of **12b**.

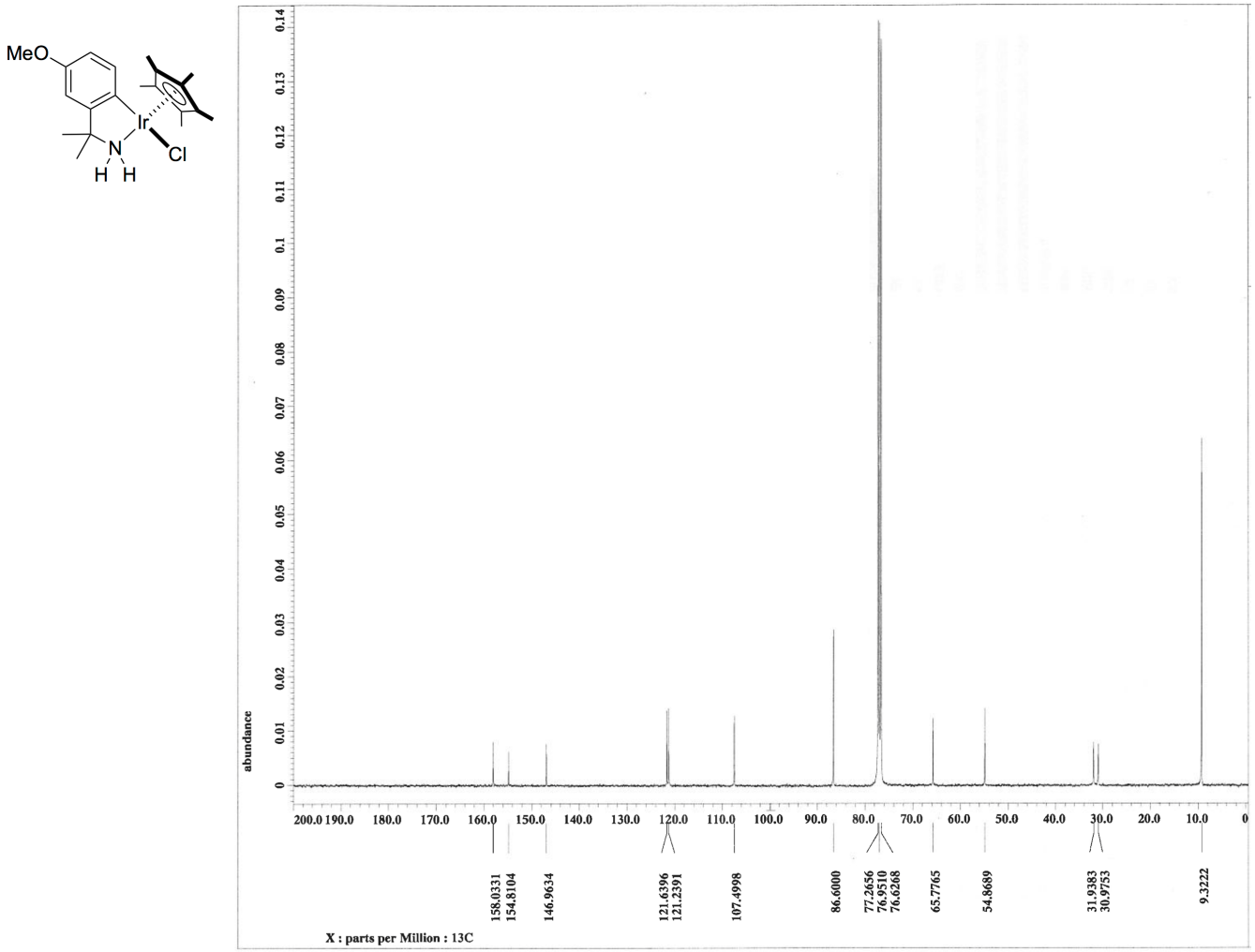


Figure S8. ^{13}C NMR Spectrum of **12b**.