

Supplementary Information

**New Blue Phosphorescent Heteroleptic Ir(III) Complexes with Imidazole- and
N-Methylimidazole Carboxylates as Ancillary Ligands**

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Section S6. ¹H-, ¹³C-, and ¹⁹F-NMR spectra of *Ir1-Ir4*.

Section S1. Absorption and Emission spectra of *Ir1-Ir4*.

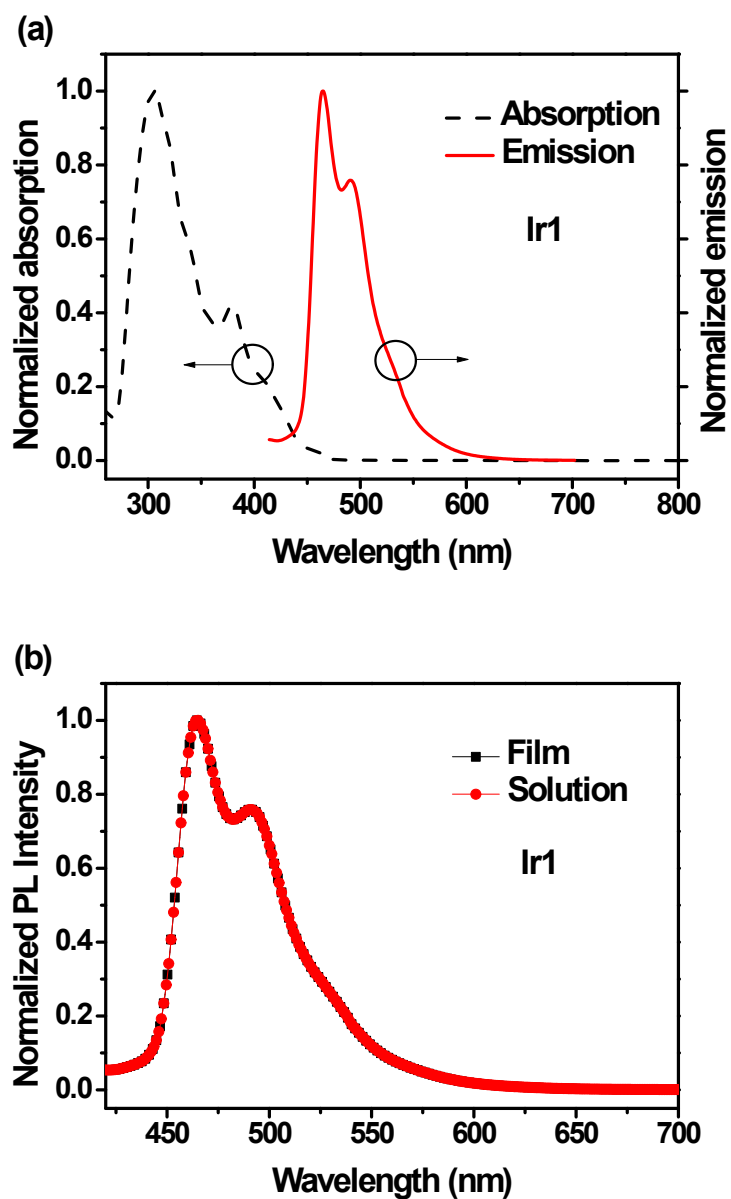


Figure S1. (a) UV-vis absorption (dotted) and emission spectra (line) in solution state and (b) comparison of emission spectra in film (square) vs. solution (circle) state of **Ir1**.

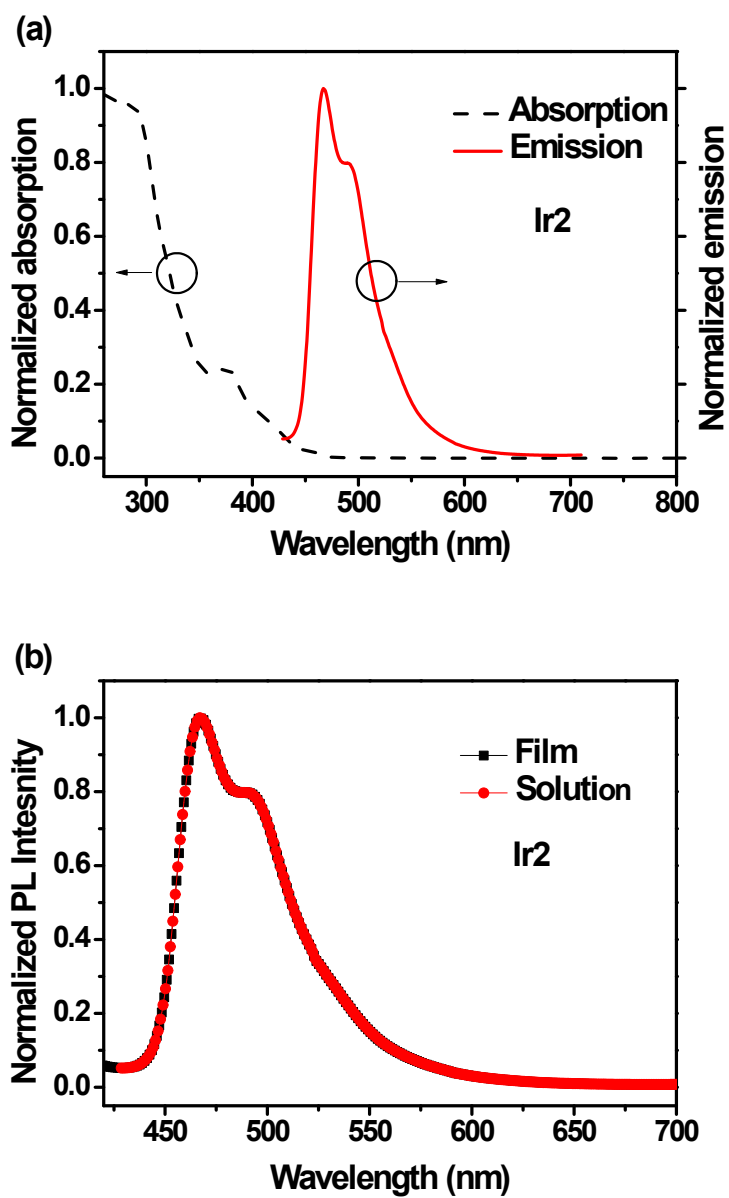


Figure S2. (a) UV-vis absorption (dotted) and emission spectra (line) in solution state and (b) comparison of emission spectra in film (square) vs. solution (circle) state of **Ir2**.

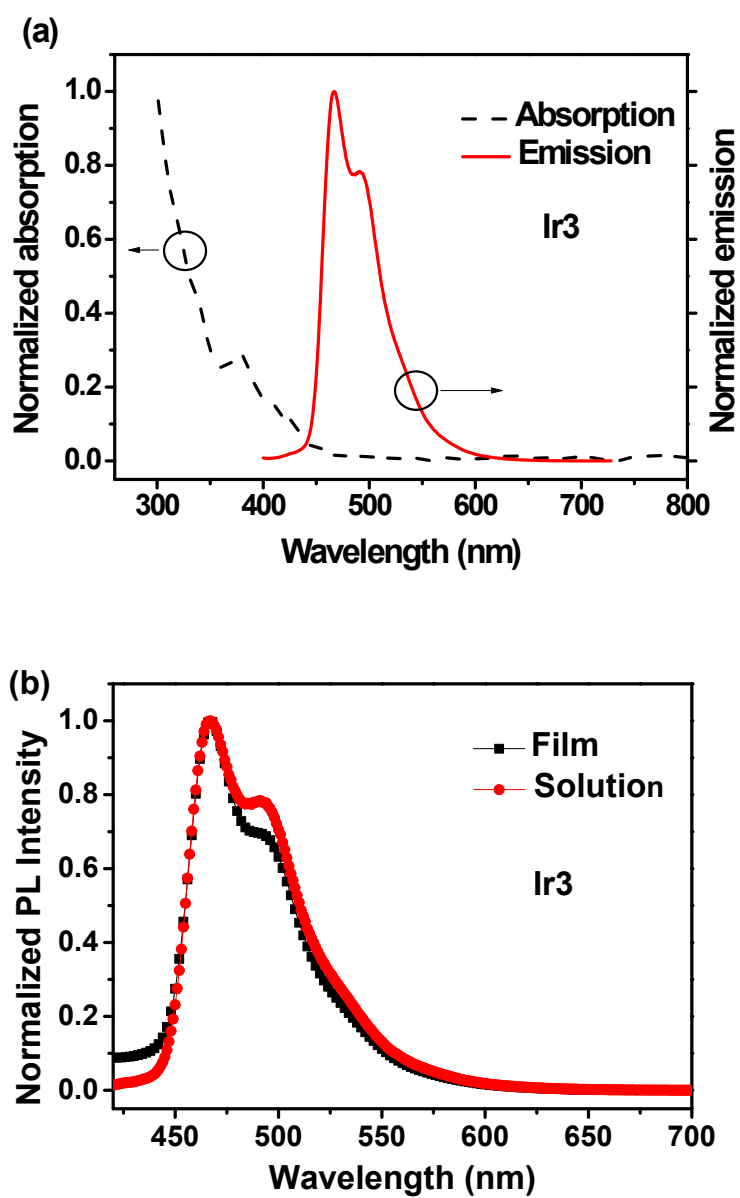


Figure S3. (a) UV-vis absorption (dotted) and emission spectra (line) in solution state and (b) comparison of emission spectra in film (square) vs. solution (circle) state of **Ir3**.

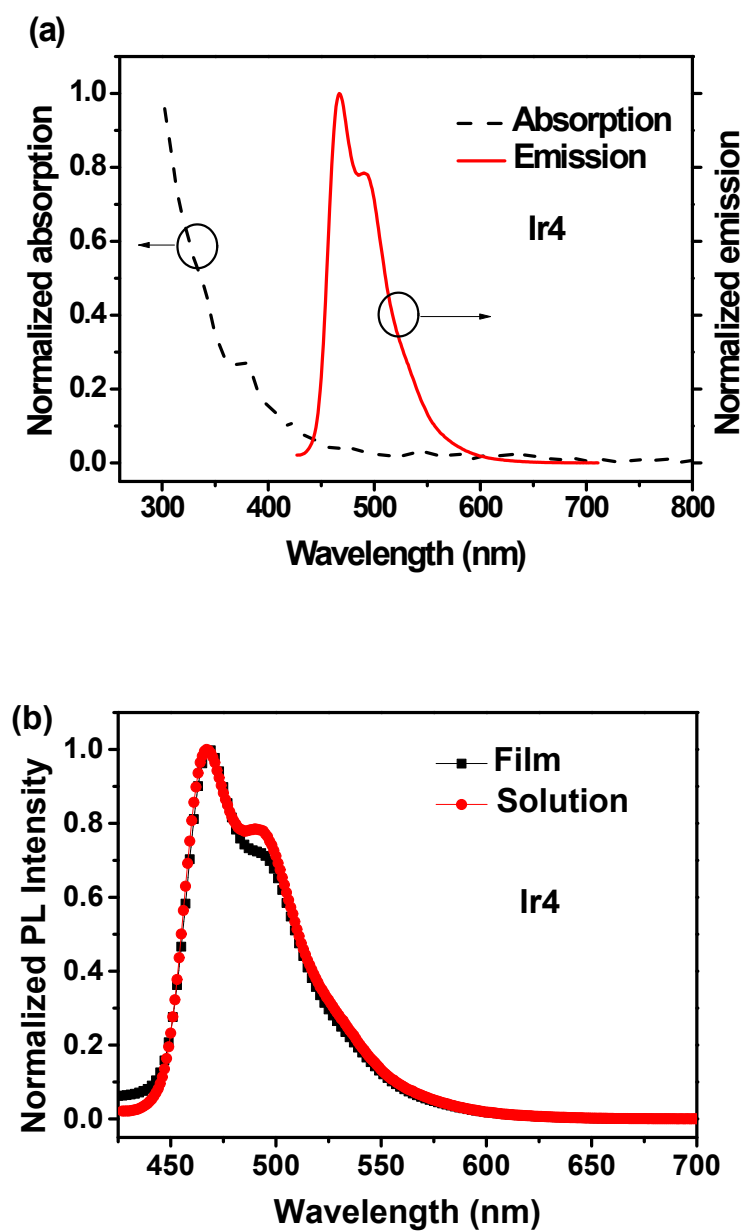


Figure S4. (a) UV-vis absorption (dotted) and emission spectra (line) in solution state and (b) comparison of emission spectra in film (square) vs. solution (circle) state of **Ir4**.

Section S2. Electrochemical properties of *Ir1-Ir4*.

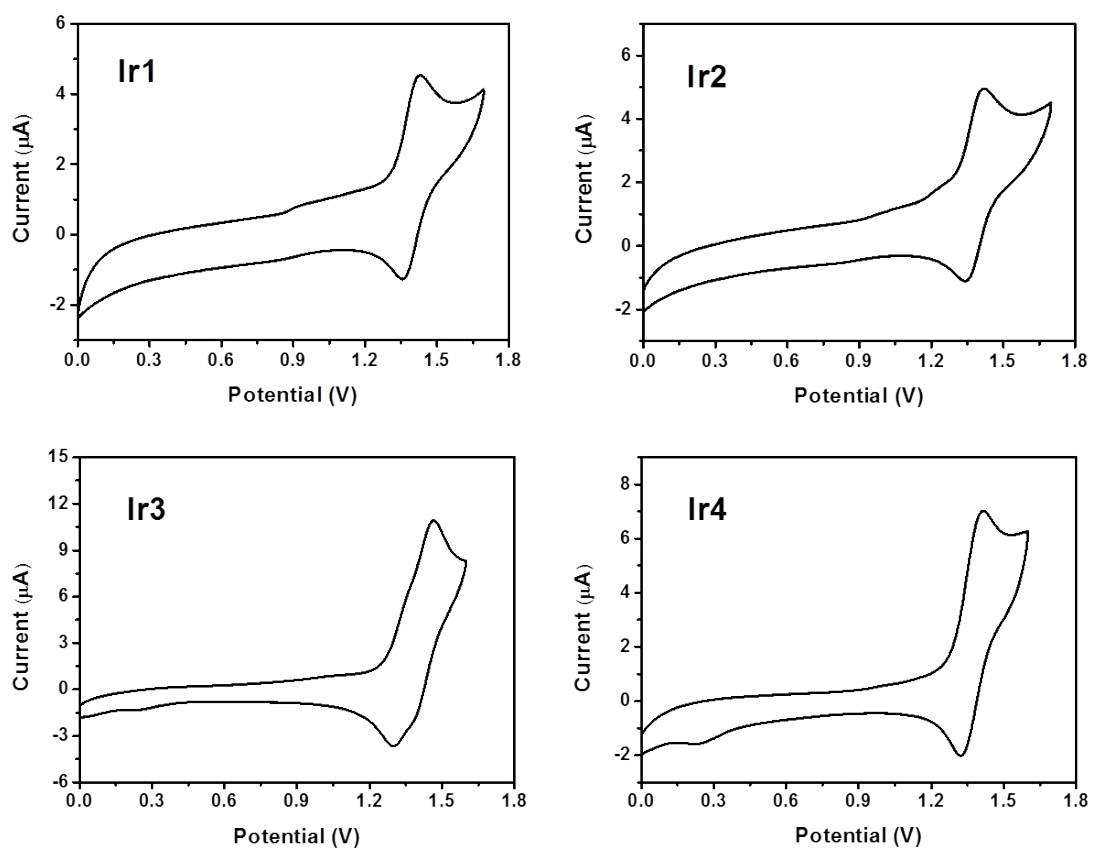


Figure S5. Cyclic voltammograms (CV) of iridium (III) complexes, **Ir1~Ir4**.

Section S3. Thermal properties of *Ir3* and *Ir4*.

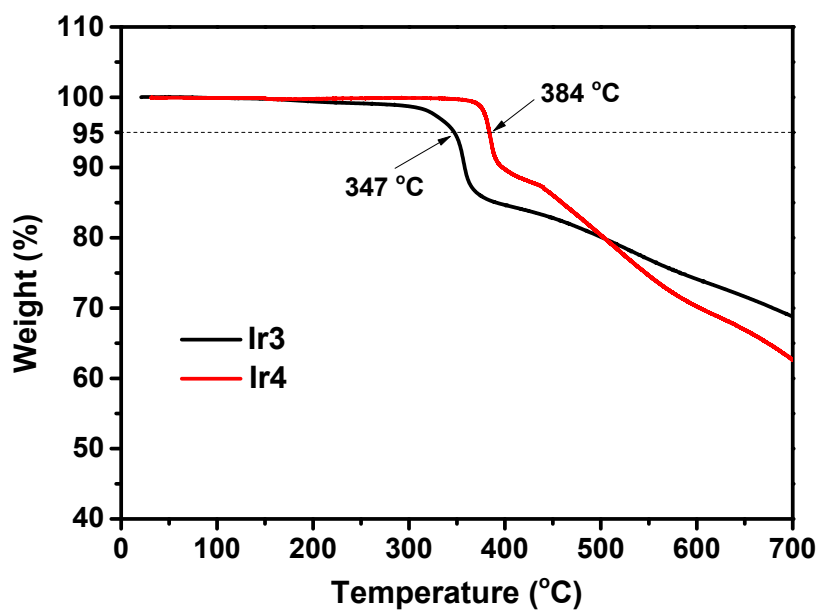


Figure S6. TGA curves of Ir(III) complexes, **Ir3** and **Ir4**.

Section S4. Device performances of *Ir3*, *Ir4*, and *Flrpic* (reference).

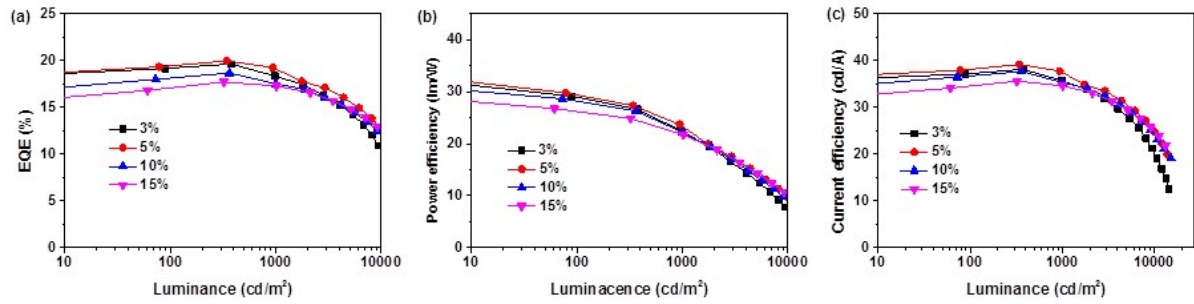


Figure S7. (a) *EQE-L*, (b) *PE-L*, and (c) *CE-L* curves of **Ir3** at different doping ratio.

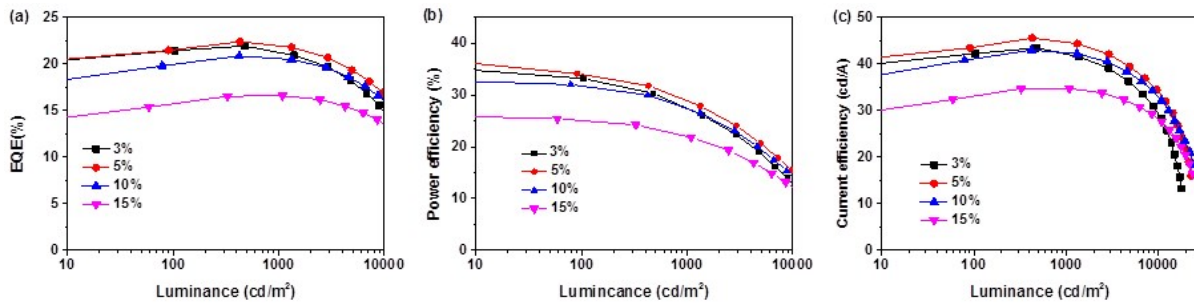


Figure S8. (a) *EQE-L*, (b) *PE-L*, and (c) *CE-L* curves of **Ir4** at different doping ratio.

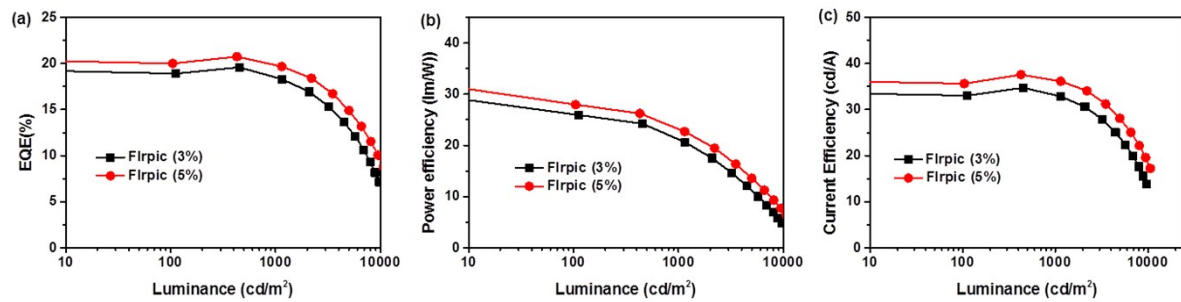


Figure S9. (a) *EQE-L*, (b) *PE-L*, and (c) *CE-L* curves of **Flrpic** as a reference device at different doping ratio.

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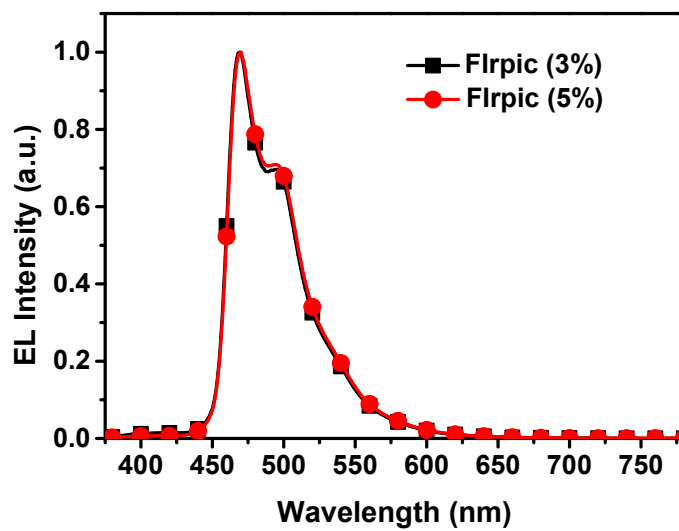


Figure S10. Electroluminescence (EL) spectra of **Flrpic** at different doping ratio.

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Section S5. Crystal data of *Ir1*.

The CCDC deposit numbers of Ir(III) crystals are as follows. **Ir1** (1504882) and **Ir3** (2032373).

Table S1. Crystal data and structure refinement of **Ir1**.

Identification code	Ir1	
Empirical formula	C _{34.86} H _{25.71} Cl _{8.57} F _{4.57} Ir _{1.14} N _{4.57} O _{2.86}	
Formula weight	1164.69	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 17.8294(6) Å	$\alpha = 90^\circ$.
	b = 18.6005(6) Å	$\beta = 97.526(2)^\circ$.
	c = 22.9797(7) Å	$\gamma = 90^\circ$.
Volume	7555.2(4) Å ³	
Z	7	
Density (calculated)	1.792 Mg/m ³	
Absorption coefficient	4.121 mm ⁻¹	
F(000)	3952	
Crystal size	0.31 x 0.28 x 0.06 mm ³	
Theta range for data collection	1.15 to 27.54°.	
Index ranges	-23 ≤ h ≤ 23, -24 ≤ k ≤ 20, -28 ≤ l ≤ 29	
Reflections collected	70108	
Independent reflections	17349 [R(int) = 0.1221]	
Completeness to theta = 27.54°	99.6 %	
Absorption correction	SADABS	
Max. and min. transmission	0.7901 and 0.3568	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	17349 / 6 / 894	
Goodness-of-fit on F ²	1.047	
Final R indices [I > 2σ(I)]	R1 = 0.0618, wR2 = 0.1863	
R indices (all data)	R1 = 0.0814, wR2 = 0.1970	
Largest diff. peak and hole	3.797 and -4.279 e.Å ⁻³	

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Table S2. Crystal data and structure refinement of **Ir3**.

Identification code	Ir3	
Empirical formula	C ₂₉ H ₂₁ F ₄ Ir N ₄ O ₂	
Formula weight	725.70	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2 ₁ /c	
Unit cell dimensions	a = 10.365(2) Å	α = 90°.
	b = 10.696(2) Å	β = 98.90(3)°.
	c = 23.837(5) Å	γ = 90°.
Volume	2610.6(9) Å ³	
Z	4	
Density (calculated)	1.846 Mg/m ³	
Absorption coefficient	5.178 mm ⁻¹	
F(000)	1408	
Crystal size	0.300 x 0.300 x 0.300 mm ³	
Theta range for data collection	3.084 to 27.483°.	
Index ranges	-13 ≤ h ≤ 13, -13 ≤ k ≤ 13, -30 ≤ l ≤ 30	
Reflections collected	22582	
Independent reflections	5944 [R(int) = 0.1389]	
Completeness to theta = 25.242°	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.211 and 0.048	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	5944 / 0 / 364	
Goodness-of-fit on F ²	1.155	
Final R indices [I > 2σ(I)]	R1 = 0.1046, wR2 = 0.2200	
R indices (all data)	R1 = 0.1281, wR2 = 0.2305	
Extinction coefficient	n/a	
Largest diff. peak and hole	4.262 and -5.326 e.Å ⁻³	

Section S6. ^1H -, ^{13}C -, and ^{19}F -NMR spectra of *Ir1-Ir4*.

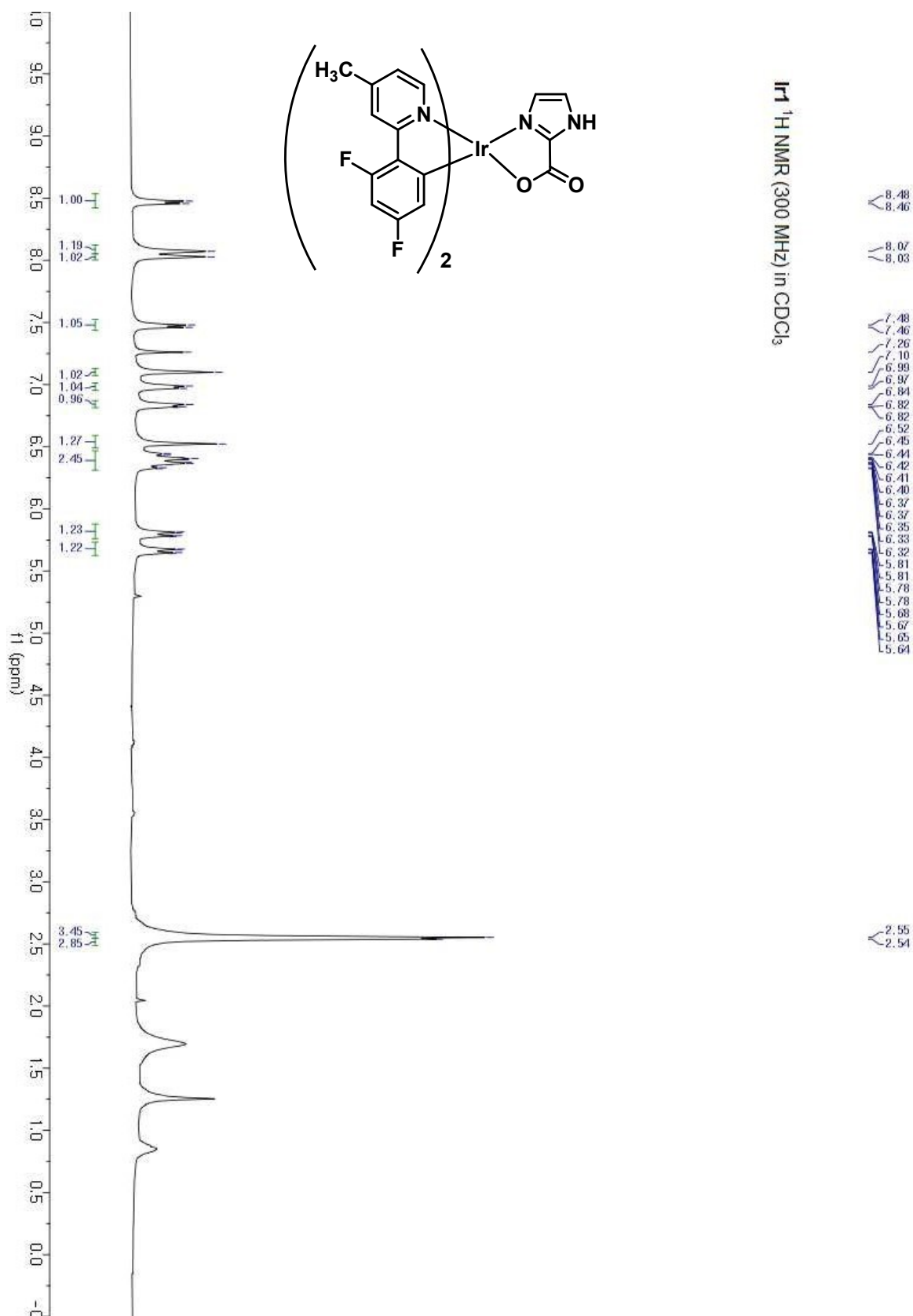


Figure S11. ^1H -NMR spectra of **Ir1**.

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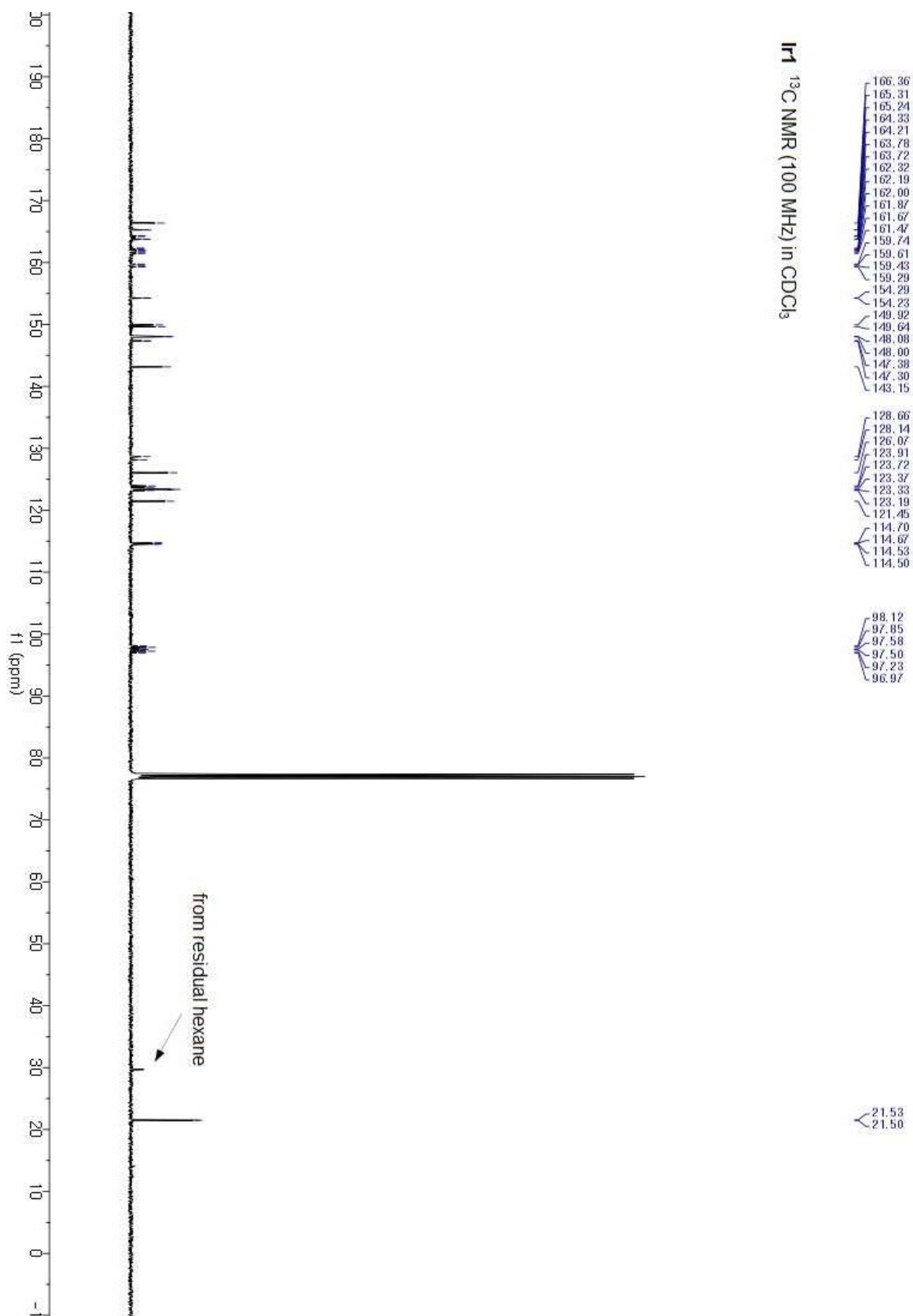
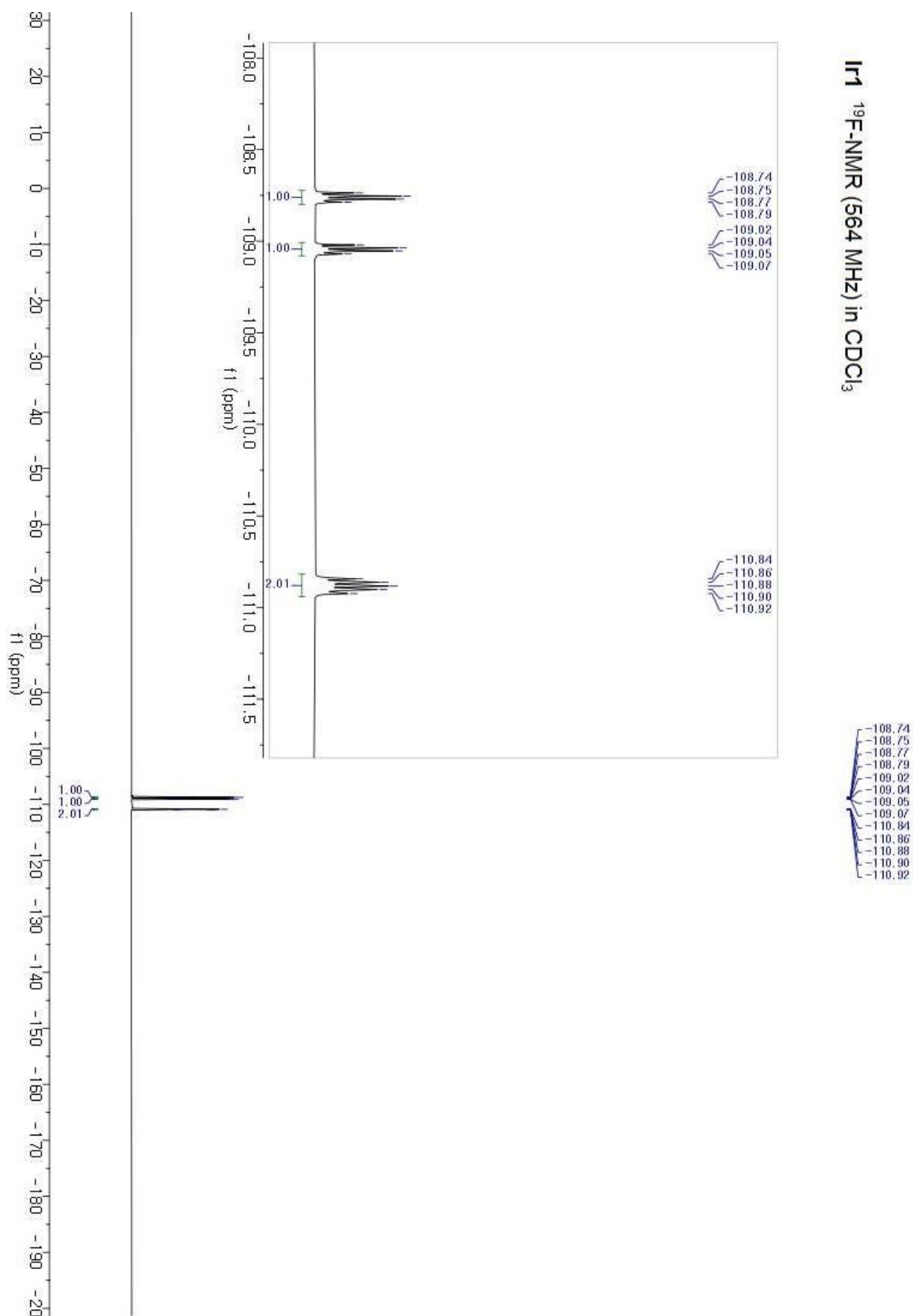


Figure S12. ^{13}C -NMR spectra of **Ir1**.

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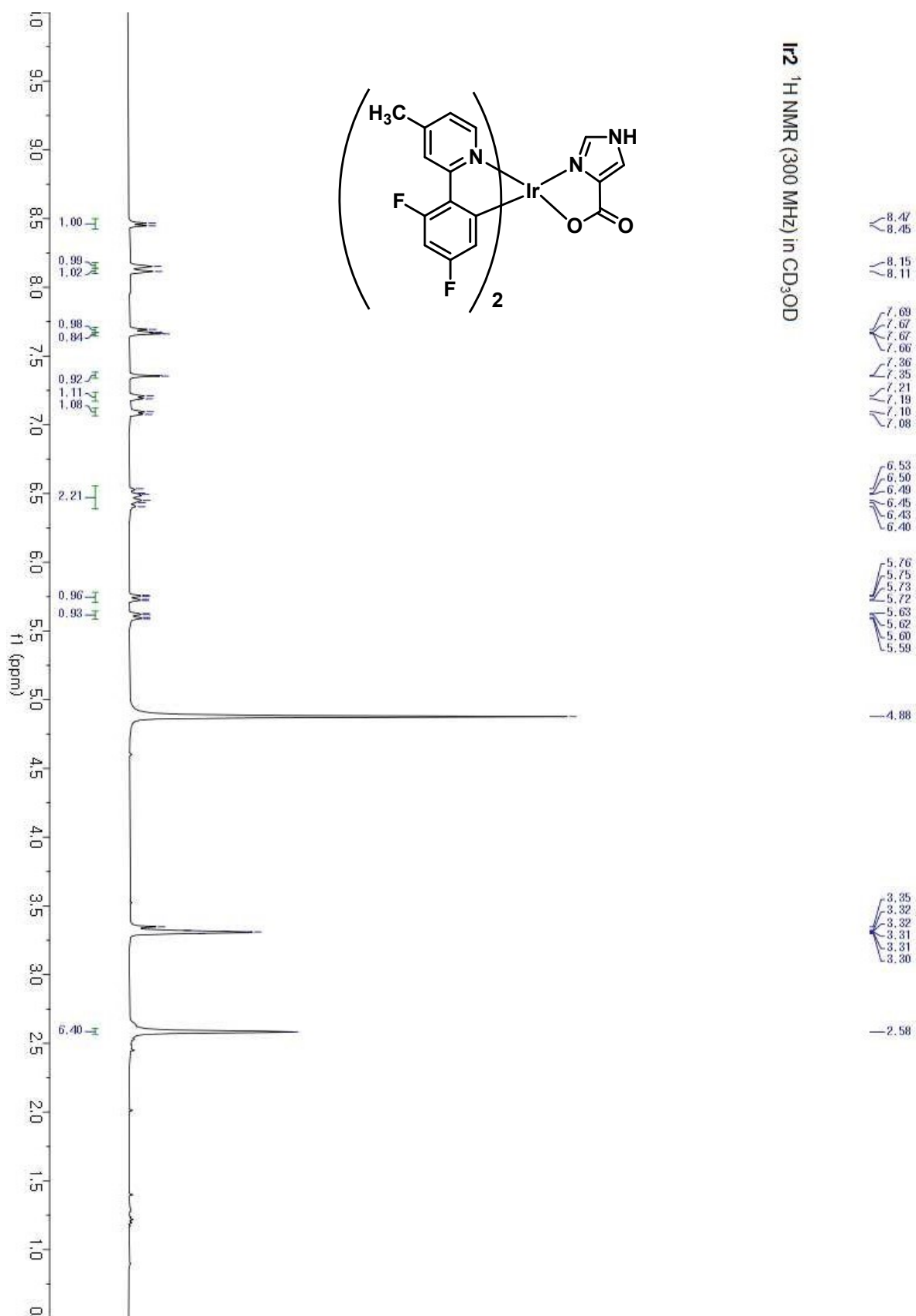


Figure S14. ¹H-NMR spectra of **Ir2**.

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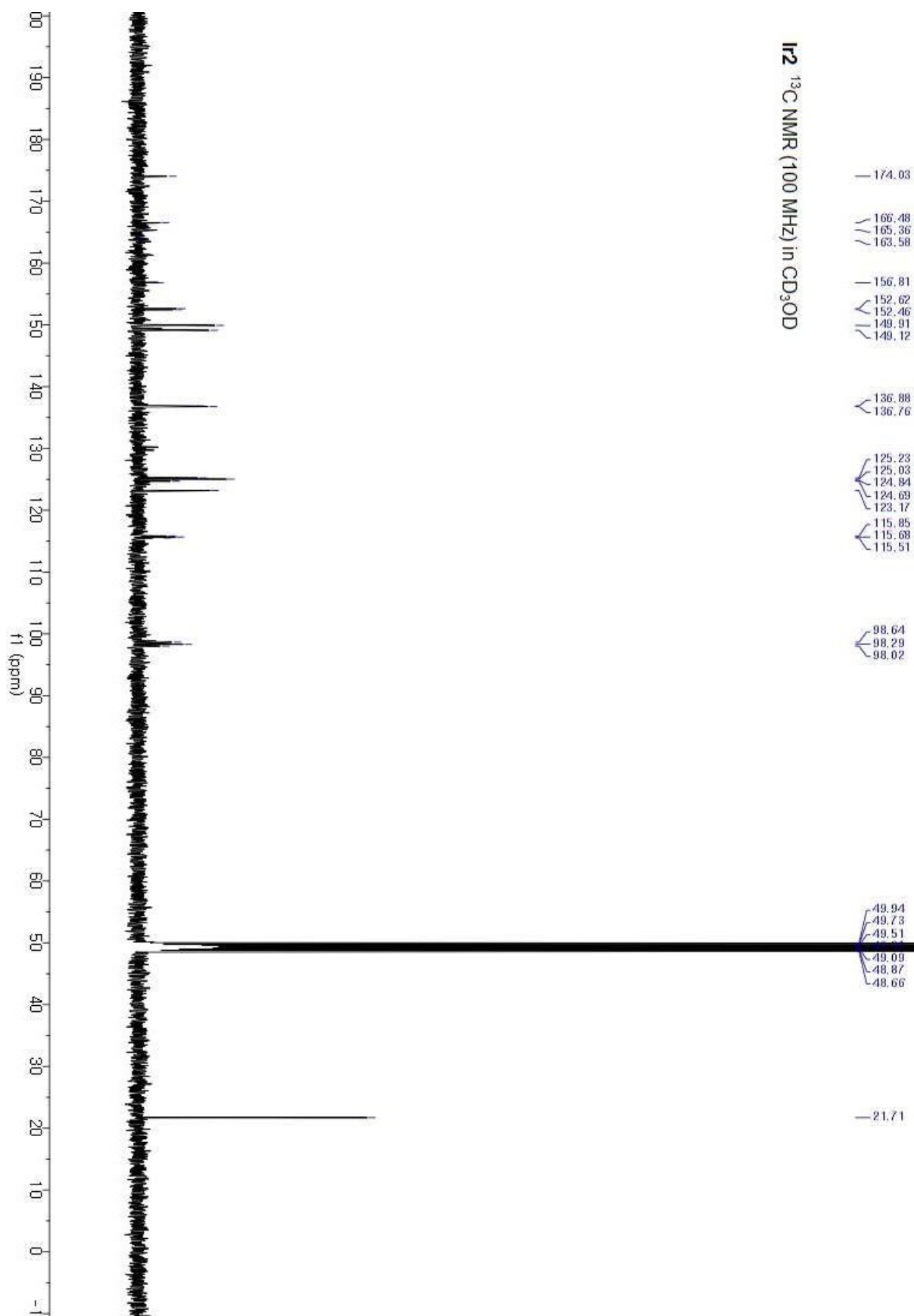


Figure S15. ^{13}C -NMR spectra of **Ir2**.

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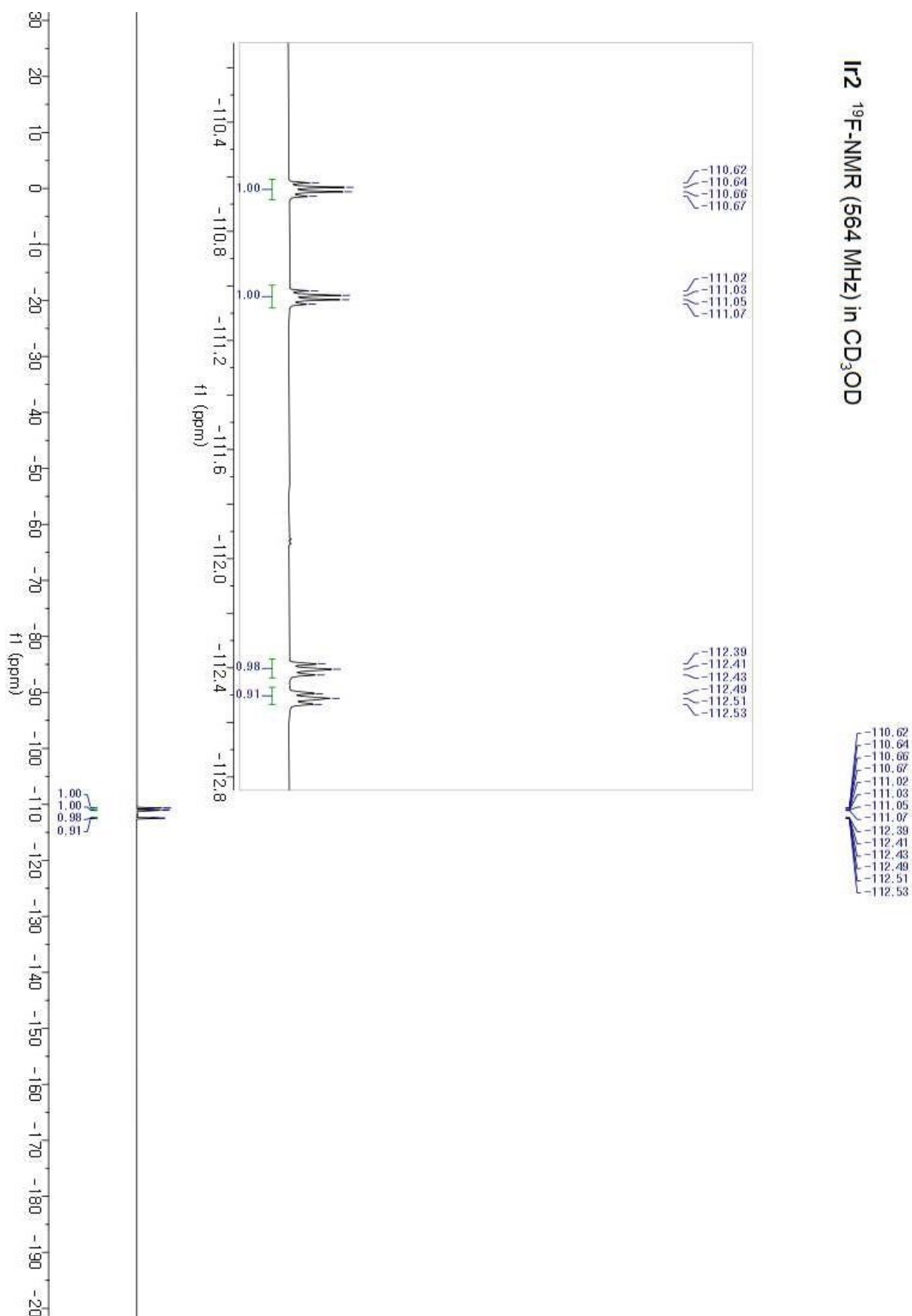


Figure S16. ^{19}F -NMR spectra of **Ir2**.

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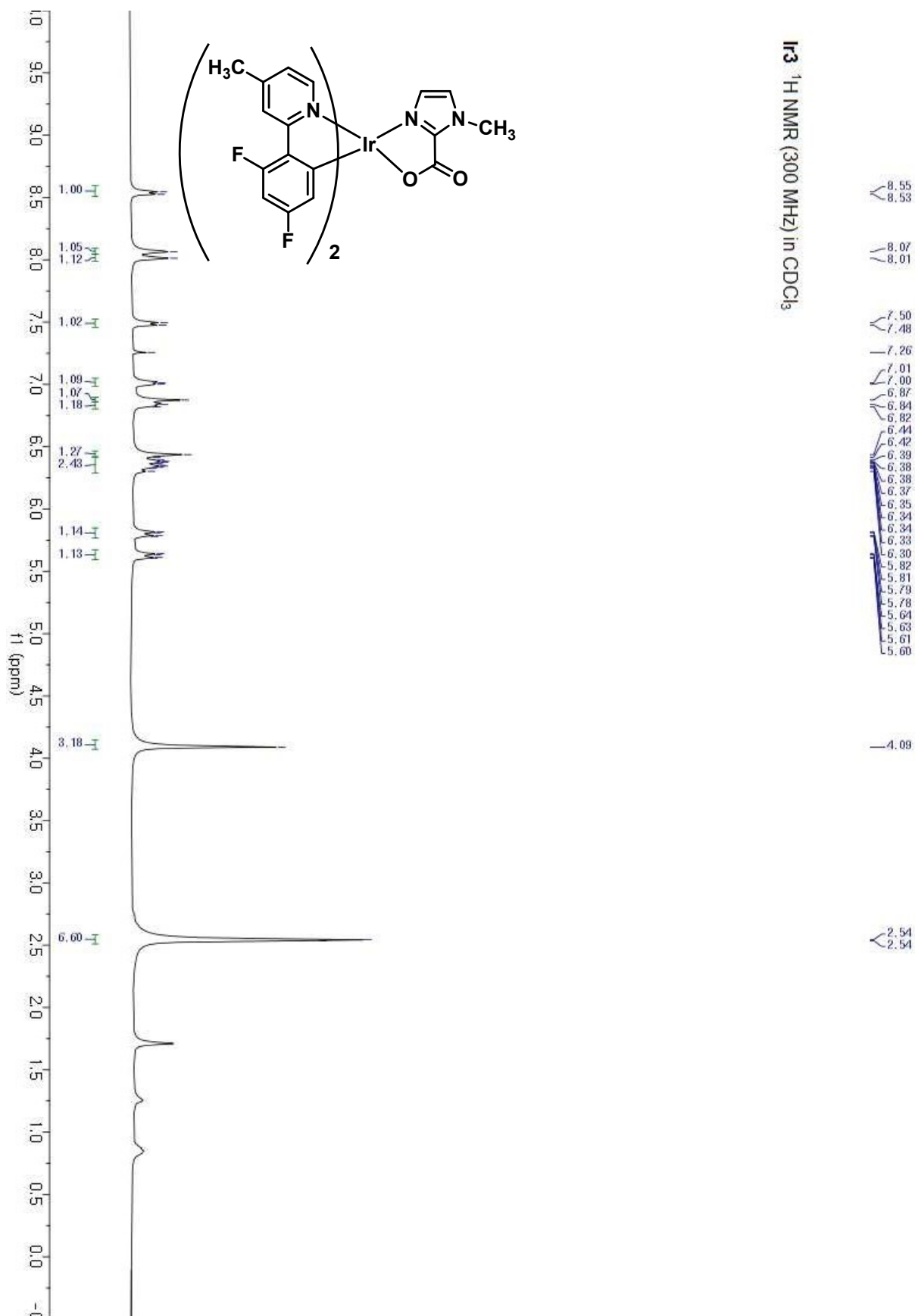


Figure S17. ¹H-NMR spectra of Ir3.

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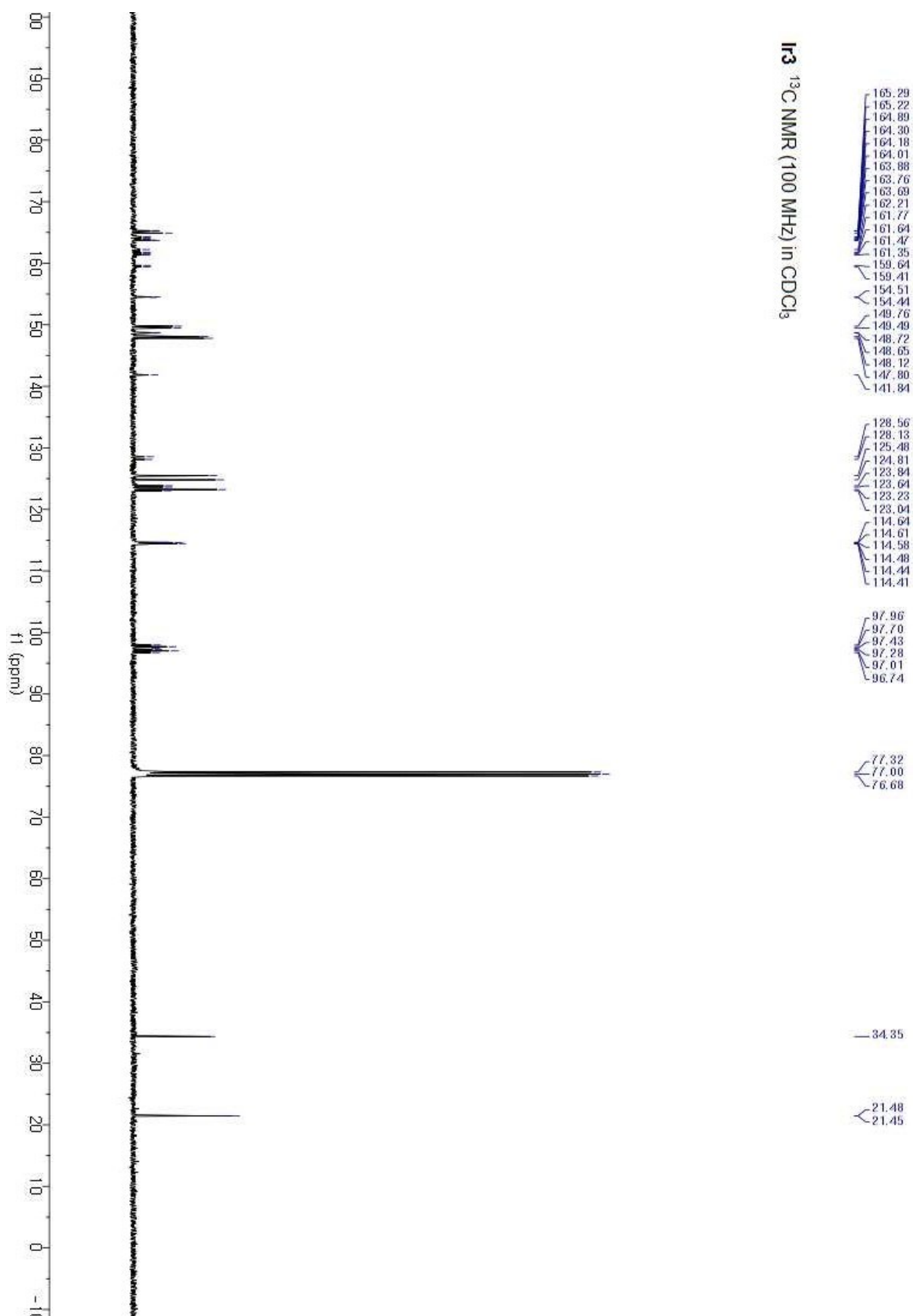


Figure S18. ^{13}C -NMR spectra of **Ir3**.

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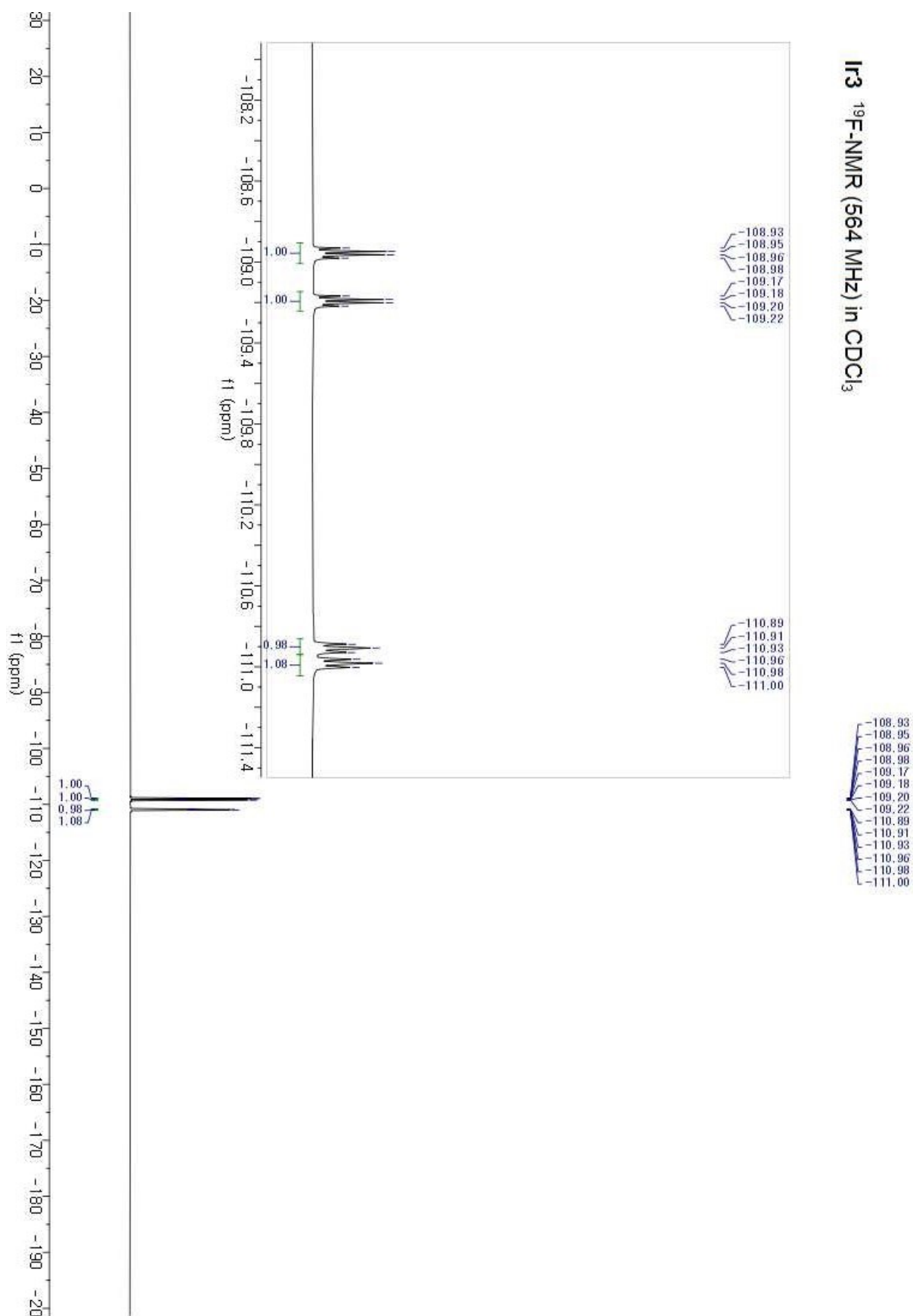


Figure S19. ^{19}F -NMR spectra of **Ir3**.

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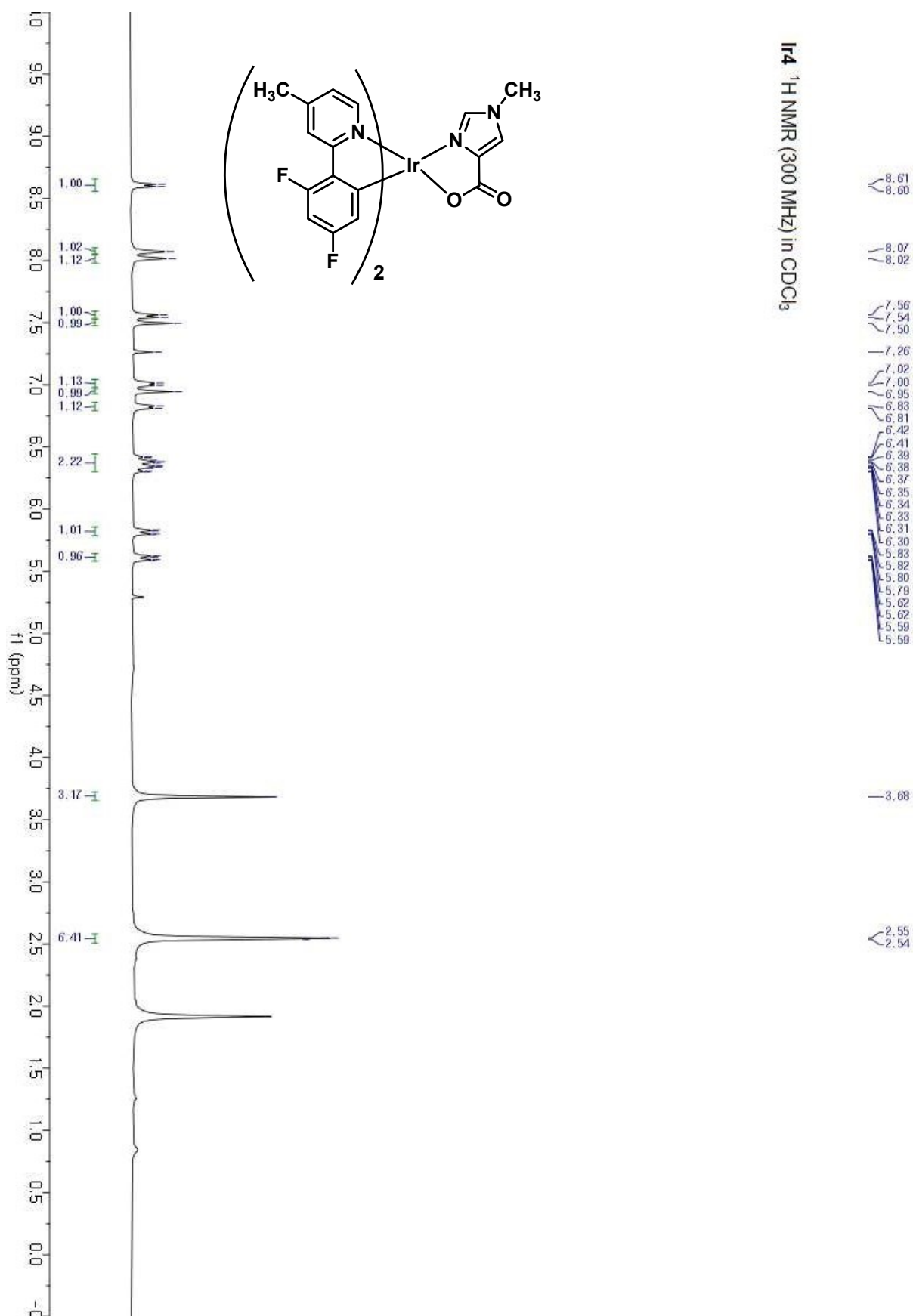


Figure S20. ^1H -NMR spectra of **Ir4**.

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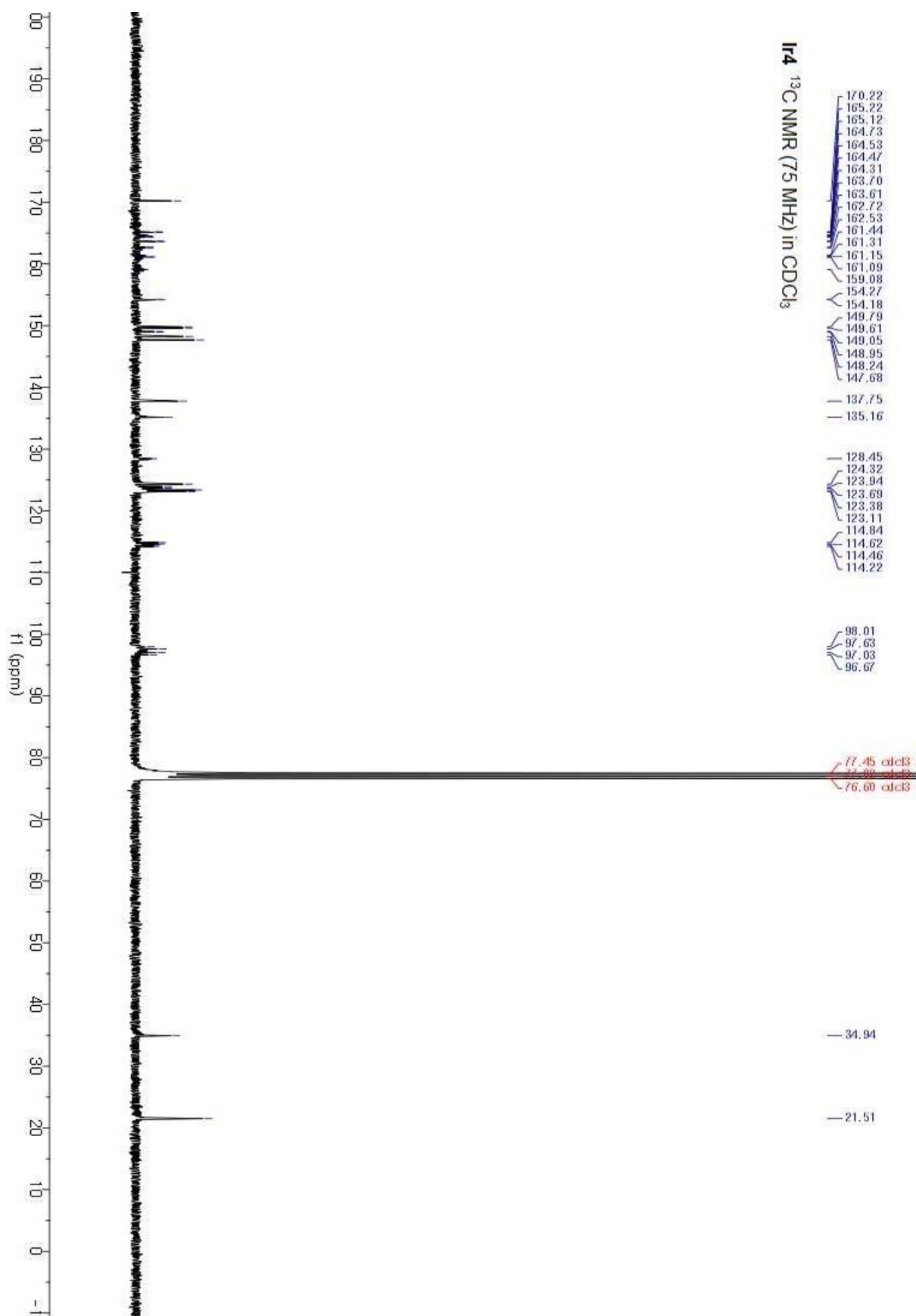


Figure S21. ^{13}C -NMR spectra of **Ir4**.

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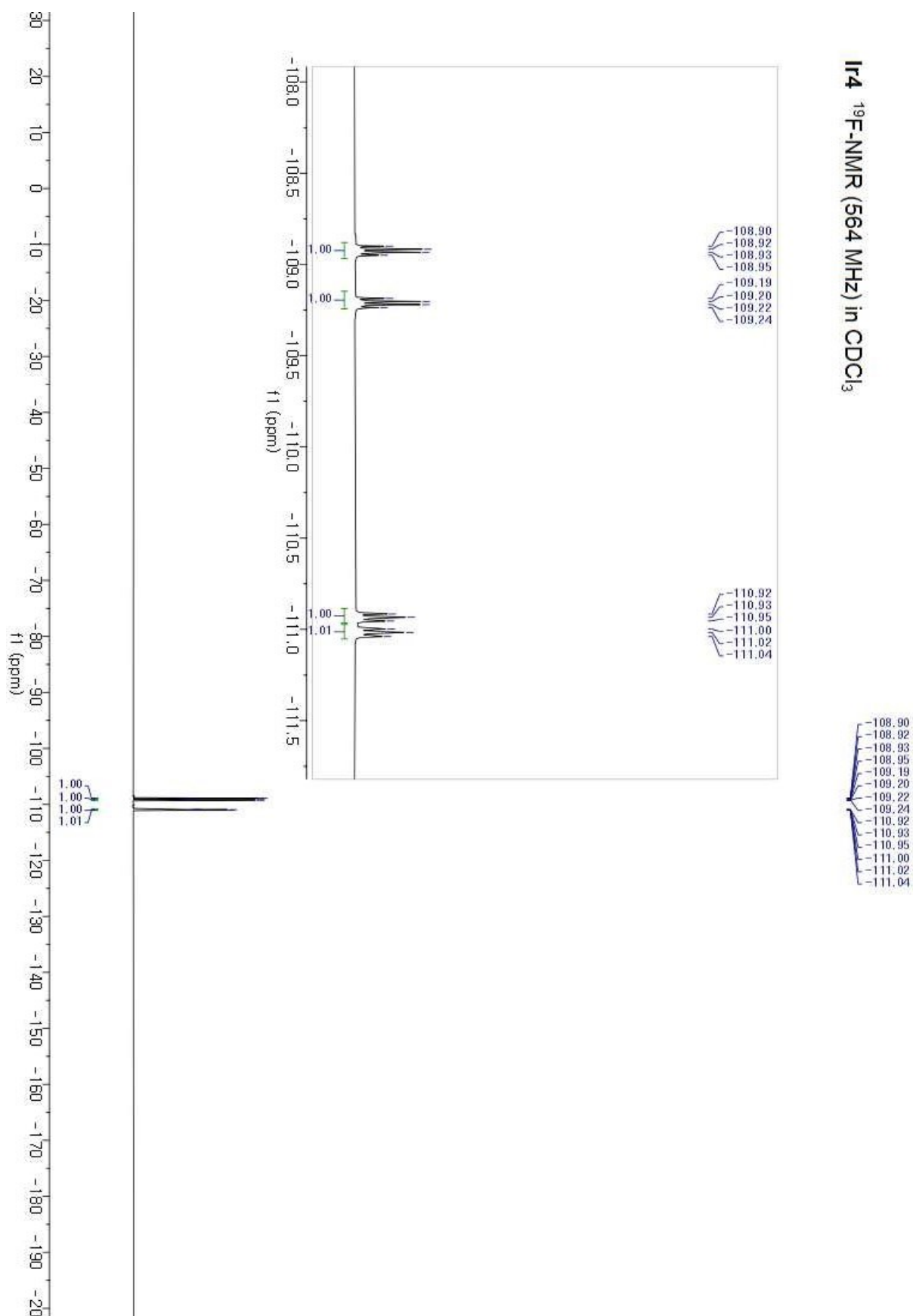


Figure S22. ^{19}F -NMR spectra of **Ir4**.