Supporting Information

Half-Sandwich Iridium Complexes for One-Pot Synthesis of Amides: Preparation, Structure and Diverse Catalytic Activity

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General information

All reagents obtained from Admas-beta were used without further purification. ^{1}H NMR and ^{13}C spectra were recorded on Bruker AVANCE III 500 MHz (500 MHz for proton) spectrometer with tetramethylsilane as the internal reference using $CDCl_3$ as solvent in all cases, and chemical shifts were reported in parts per million (ppm, δ). FT-IR spectra were recorded on a Thermo fisher Nicolet 6700. GC analyses were performed on Shimadzu GC-2014 with a flame ionization detector equipped with an Rtx-1 capillary column (internal diameter = 0.25 mm, length = 30 m) or a Stabilwax capillary column (internal diameter = 0.25 mm, length = 30 m). GC mass spectra were recorded on Shimadzu GCMS-QP2010 with a capillary column (0.25 mm× 30 m). Column chromatography was performed using 200-300 mesh base-washed silica gel.

Characterizations of typical products

5a: ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.78–7.74 (m, 2H), 7.50 (t, J = 7.5 Hz, 1H), 7.48 (t, J = 7.5 Hz, 2H), 5.83 (brs, 2H) ppm. Data are in accordance with that previously published.[1-5]

5b: ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.45 (d, J = 7.5 Hz, 1H), 7.35 (d, J = 7.5 Hz 1H), 7.25–7.20 (m, 2H), 6.45 (brs, 1H), 6,10 (brs, 1H), 2.45 (s, 3H) ppm. Data are in accordance with that previously published.[1-5]

5c: ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.13 (s, 1H), 7.61 (s, 1H), 7.43 (s, 1H), 7.38 (d, J = 8.0 Hz, 1H), 7.31 (d, J = 7.5 Hz, 1H), 7.20 (d, J = 7.5 Hz, 1H), 2.36 (s, 3H) ppm. Data are in accordance with that previously published.[1-5]

5d: ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.10 (s, 2H), 7.52 (d, J = 7.5 Hz, 2H), 6.93 (d, J = 7.5 Hz, 2H), 3.84 (s, 3H) ppm. Data are in accordance with that previously published.[1-5]

5e: ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.95 (s, 1H), 7.62 (s, 1H), 7.48–7.45 (m, 4H). ppm. Data are in accordance with that previously published.[1-5]

5f: ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.15 (s, 1H), 8.02 (d, J = 6.5 Hz, 1H), 7.85 (d, J = 7.0 Hz, 1H), 7.73–7.69 (m, 1H), 7.55 (s, 1H), 7.40 (t, J = 7.5 Hz, 1H) ppm. Data are in accordance with that previously published.[1-5]

5g: ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.05 (s, 1H), 7.82 (d, J = 8.0 Hz, 2H), 7.62 (d, J = 8.0 Hz, 2H,), 7.47 (s, 1H) ppm. Data are in accordance with that previously published.[1-5]

5h: ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.00 (s, 1H), 7.89 (d, J = 7.5 Hz, 2H), 7.60 (d, J = 7.5 Hz, 2H,), 7.41 (s, 1H) ppm. Data are in accordance with that previously published.[1-5]

5i: ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.81 (d, J = 7.5 Hz, 2H), 7.53 (s, 1H), 7.03 (s, 1H), 6.99 (d, J = 7.5 Hz, 2H) 5.46 (s, 1H) ppm. Data are in accordance with that previously published.[1-5]

5j: ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.71 (d, J = 8.0 Hz, 2H), 7.61 (s, 1H), 6.98 (s, 1H), 6.64 (d, J = 7.5 Hz, 2H), 2.90 (s, 6H) ppm. Data are in accordance with that previously published.[1-5]

5k: ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.25 (d, J = 7.5 Hz, 2H), 8.23 (s, 1H), 7.98 (s, 1H), 7.79 (d, J = 7.0 Hz, 2H) ppm. Data are in accordance with that previously published.[1-5]

5l: ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.65–8.61 (m, 1H), 8.12 (brs, 1H), 8.02–7.97 (m, 2H), 7.63 (brs, 1H), 7.62–7.58 (m, 1H) ppm. Data are in accordance with that previously published.[1-5]

5m: ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.82 (s, 1H), 7.78 (d, J = 5.0 Hz, 1H), 7.36 (s, 1H), 7.12 (d, J = 7.0 Hz, 1H), 6.56 (dd, J = 7.0, 3.0 Hz, 1H) ppm. Data are in accordance with that previously published.[1-5]

5n: ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.95 (s, 1H), 7.79–7.73 (m, 2H), 7.39 (s, 1H), 7.12 (t, J = 7.0 Hz, 1H) ppm. Data are in accordance with that previously published.[1-5]

5o: ^{1}H NMR (500 MHz, $CDCl_3$): δ 6.16 (s, 1H), 5.90 (s, 1H), 2.09 (s, 3H) ppm. Data are in accordance with that previously published.[1-5]

5p: ^{1}H NMR (500 MHz, $CDCl_3$): δ 5.67 (brs, 1H), 5.48 (brs, 1H), 2.17 (t, J = 10.5 Hz, 1H), 1.87 (d, J = 12.0 Hz, 2H), 1.75 (d, J = 10.0 Hz, 2H), 1.65 (d, J = 10.5 Hz, 1H), 1.43 (q, J = 12.0 Hz, 2H), 1.23 (m, 3H) ppm. Data are in accordance with that previously published.[1-5]

5q: ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.95 (s, 1H), 7.76 (d, J = 7.5 Hz, 2H), 7.29 (s, 1H), 7.22 (d, J = 7.0 Hz, 2H), 2.33 (s, 3H) ppm. Data are in accordance with that previously published.[1-5]

5r: ^{1}H NMR (500 MHz, $CDCl_3$): δ 9.12 (d, J = 7.0 Hz, 1H), 8.73 (s, 1H), 7.95 (d, J = 7.0 Hz, 1H), 7.83 (dd, J = 7.0 Hz, J = 4.0 Hz, 1H), 7.82 (d, J = 7.5 Hz, 1H), 7.59–7.55 (m, 1H) 7.51–7.45 (m, 2H,), 7.12 (s, 1H) ppm. Data are in accordance with that previously published.[1-5]

5s: ^{1}H NMR (500 MHz, $CDCl_3$): δ 10.05 (s, 1H), 8.17 (s, 1H), 8.03 (d, J = 7.0 Hz, 2H), 7.96 (d, J = 7.0 Hz, 2H), 7.62 (s, 1H) ppm. Data are in accordance with that previously published.[1-5]

5u: ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.11 (s, 1H), 7.95 (s, 2H), 7.51 (s, 1H) ppm. Data are in accordance with that previously published.[1-5]

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(2) Zhang, S.; Xu, H.; Lou, C.; Senan, A. M.; Chen, Z.; Yin, G. Efficient Bimetallic Catalysis of Nitrile Hydration to Amides with a Simple $Pd(OAc)_2$/Lewis Acid Catalyst at Ambient Temperature. *Eur. J. Org. Chem*. **2017**, *2017*, 1870–1875.

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Aldoximes as the Water Source. *Org. Lett.* **2009**, *11*, 5598–5601.

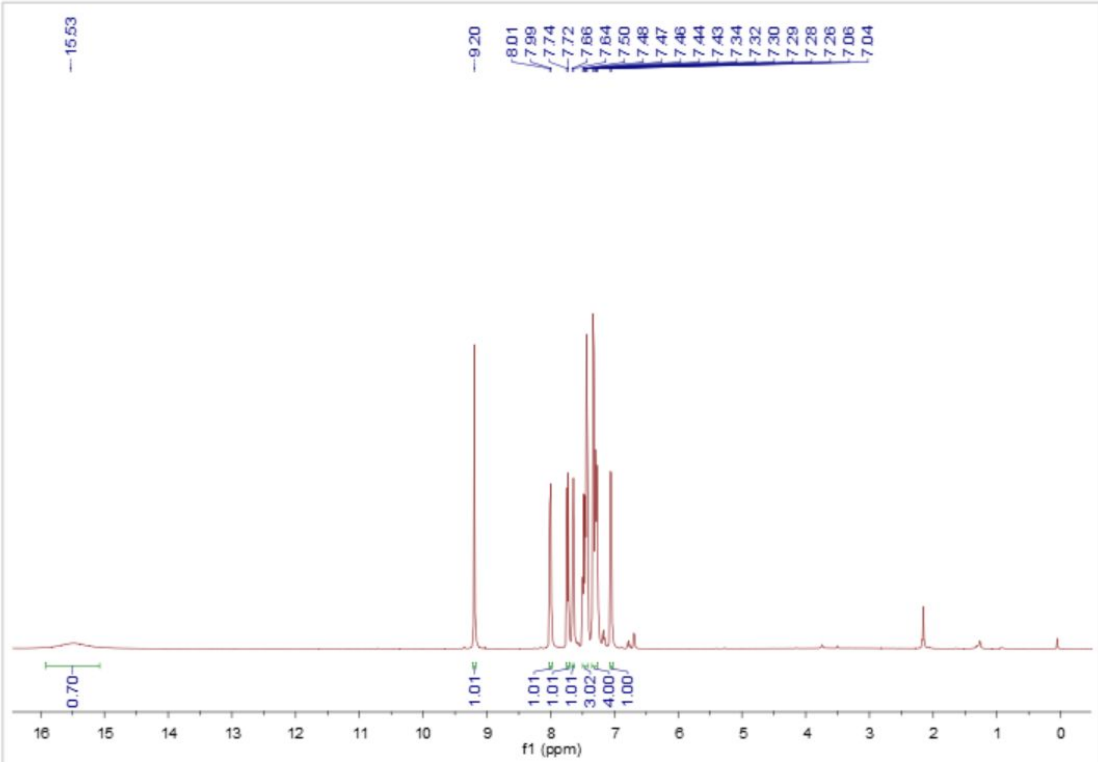

Figure S1. ^{1}H NMR spectra of **L1**

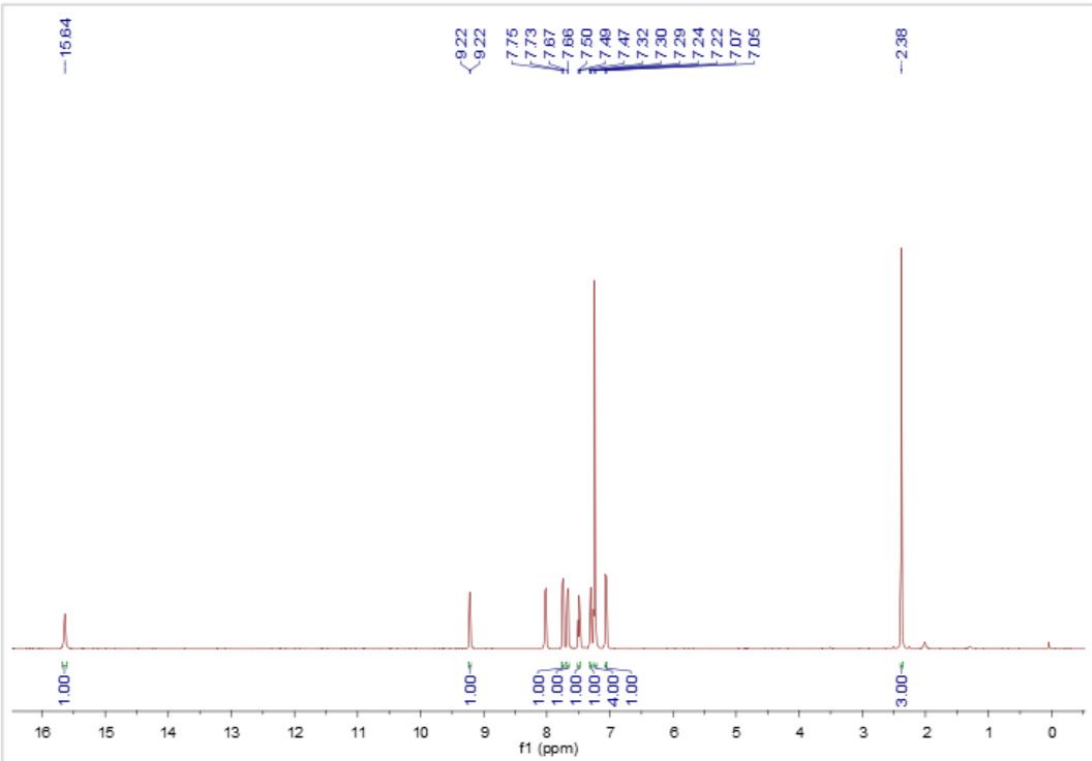

Figure S2. ^{1}H NMR spectra of **L2**

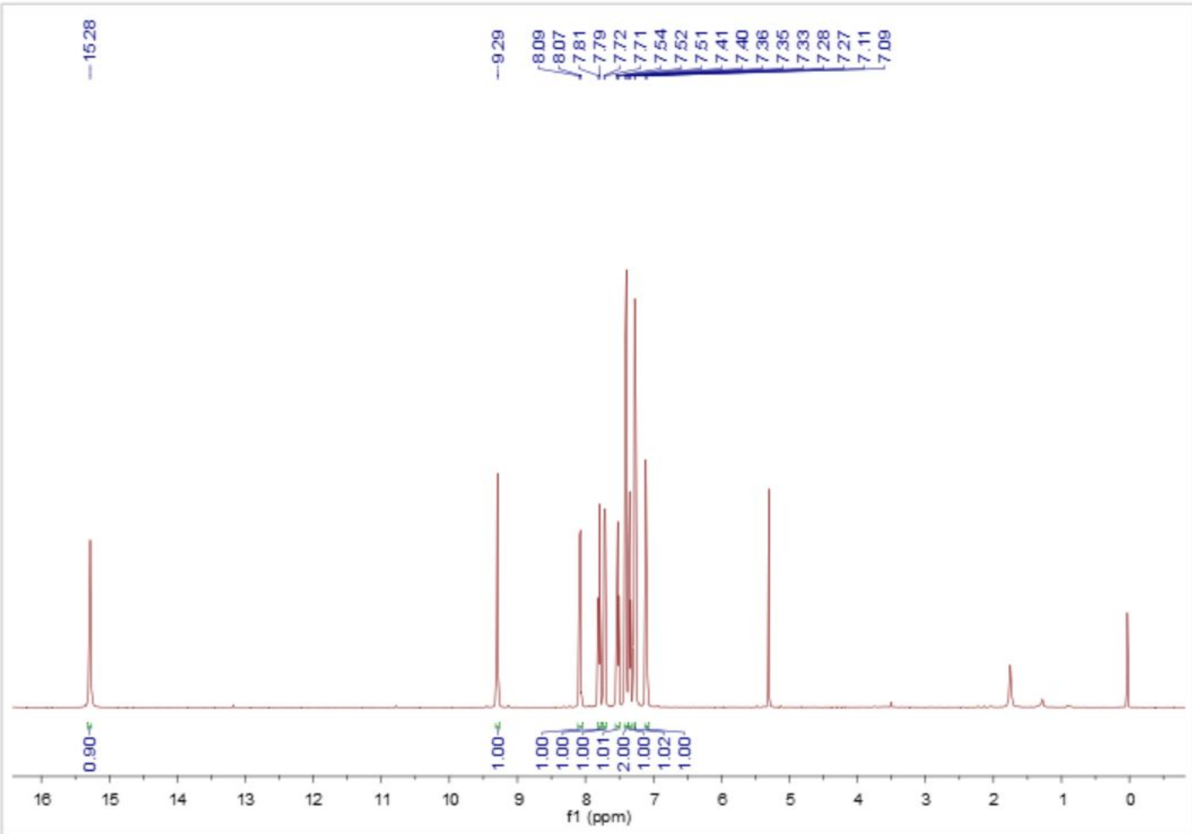

Figure S3. ^{1}H NMR spectra of **L3**

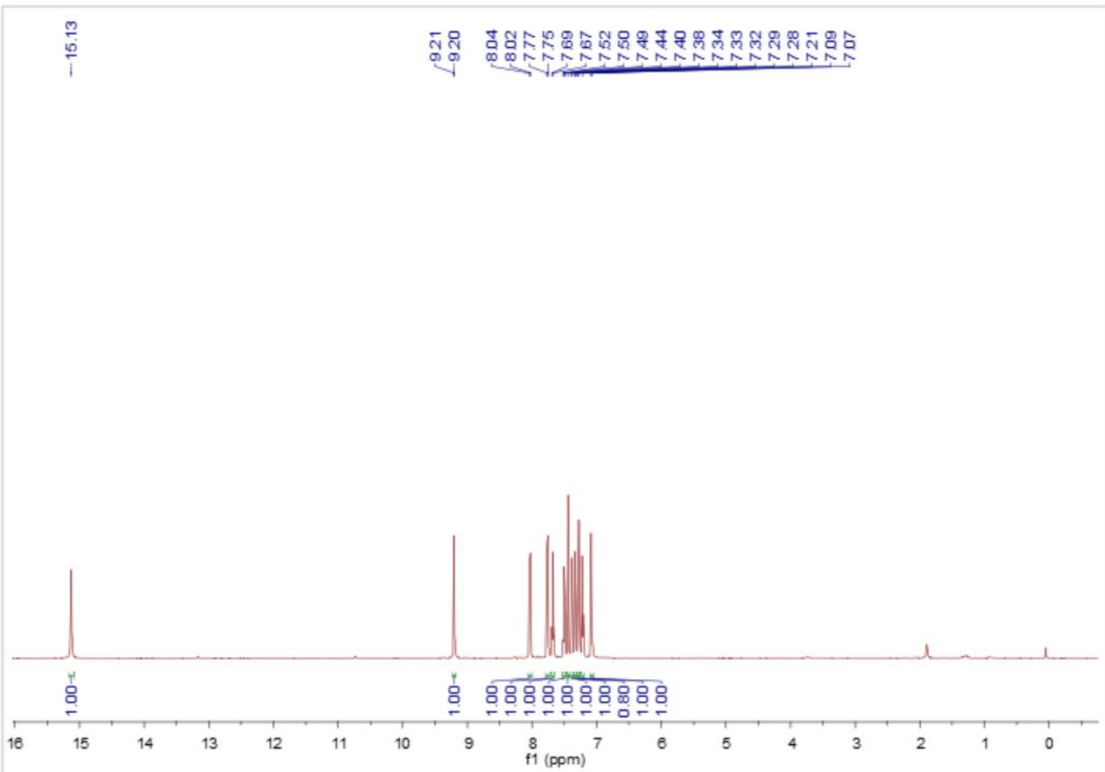

Figure S4. ^{1}H NMR spectra of **L4**

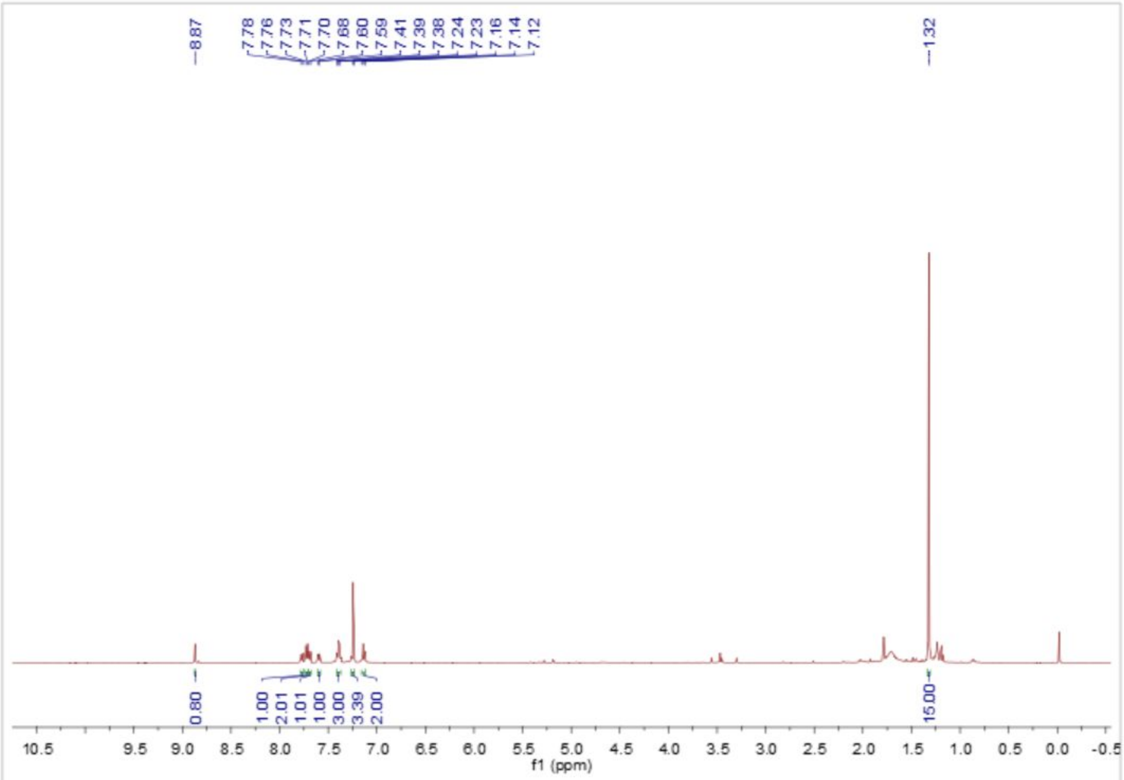

Figure S5. ^{1}H NMR spectra of **1**

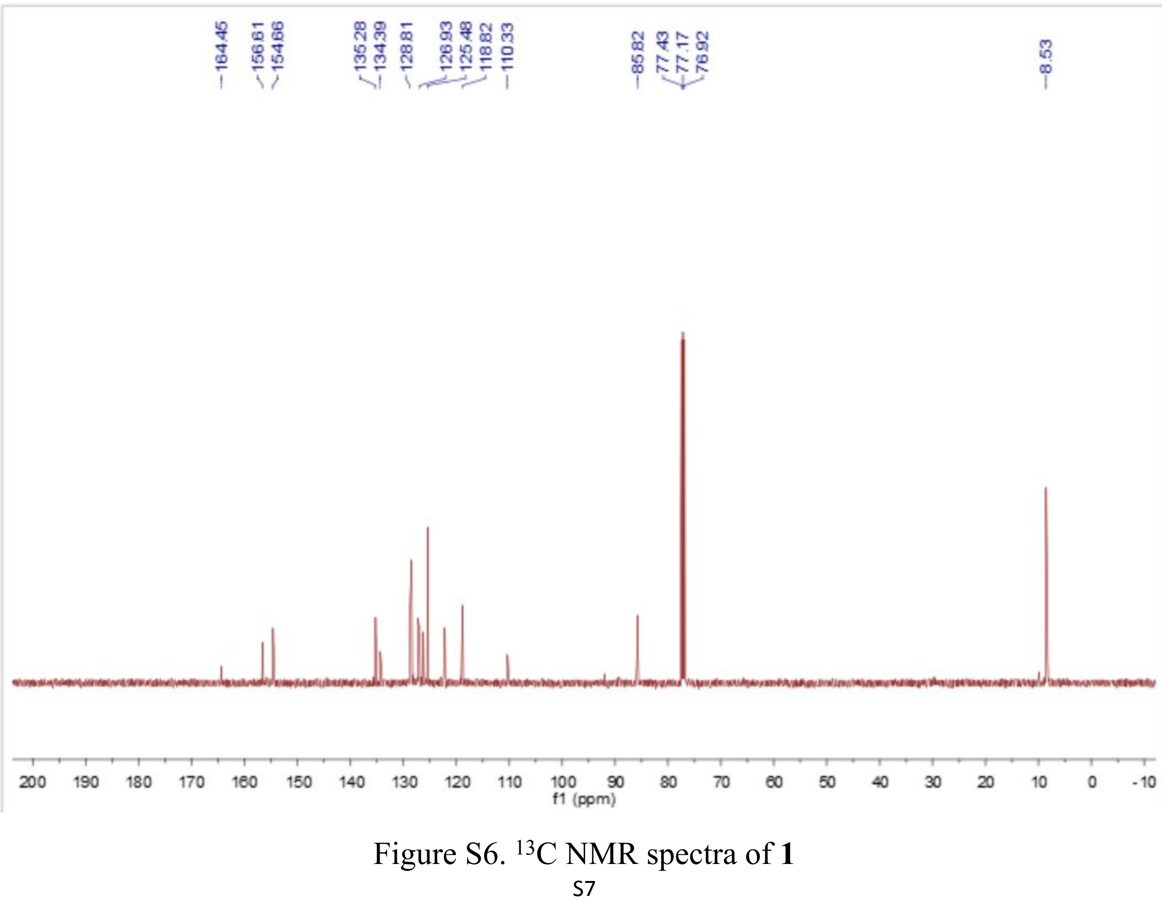

Figure S6. ^{13}C NMR spectra of **1**

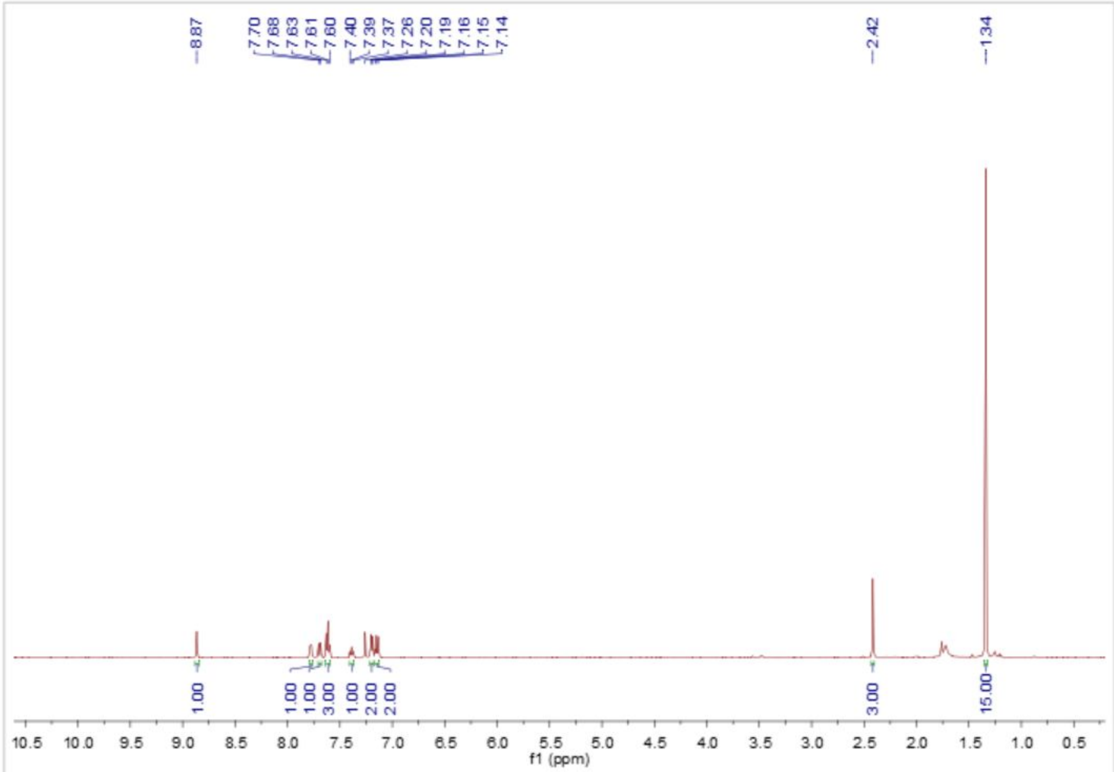

Figure S7. ^{1}H NMR spectra of **2**

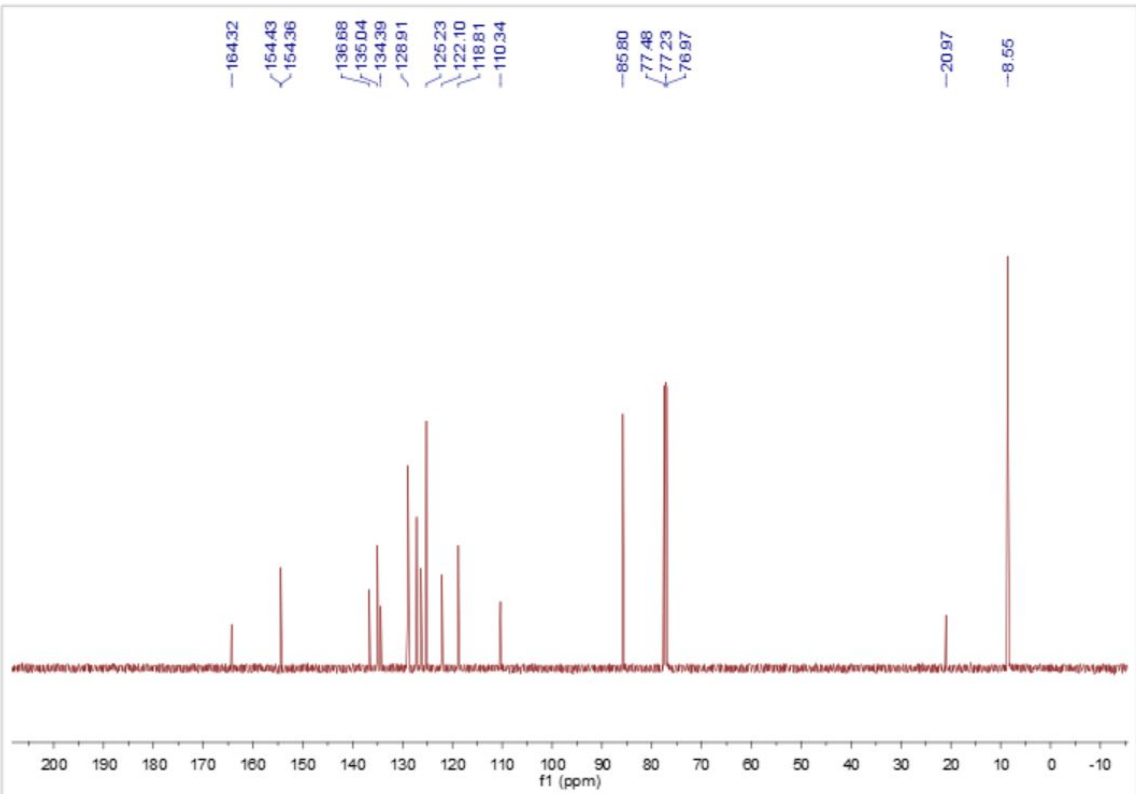

Figure S8. ^{13}C NMR spectra of **2**

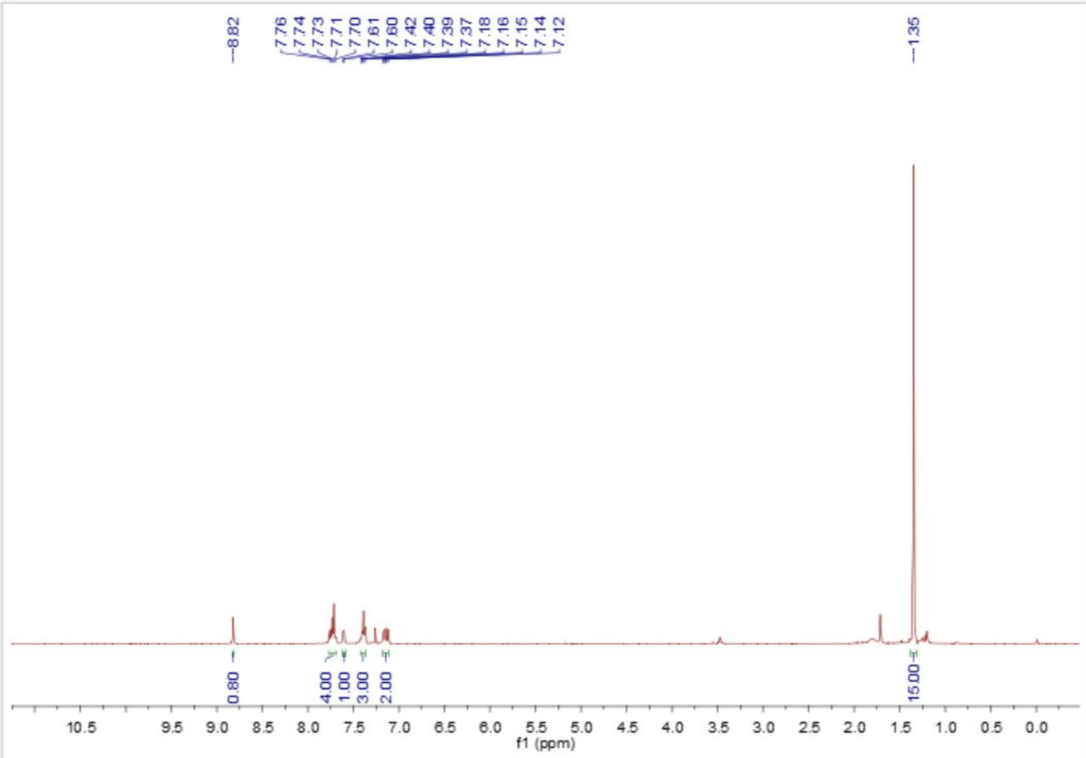

Figure S9. ^{1}H NMR spectra of **3**

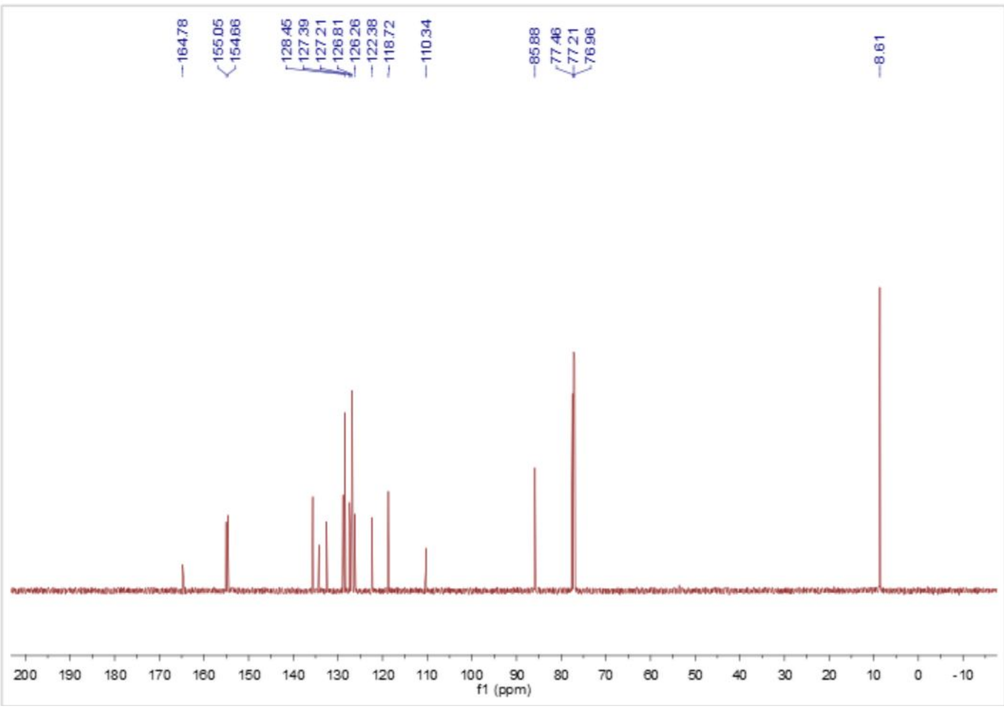

Figure S10. ^{13}C NMR spectra of **3**

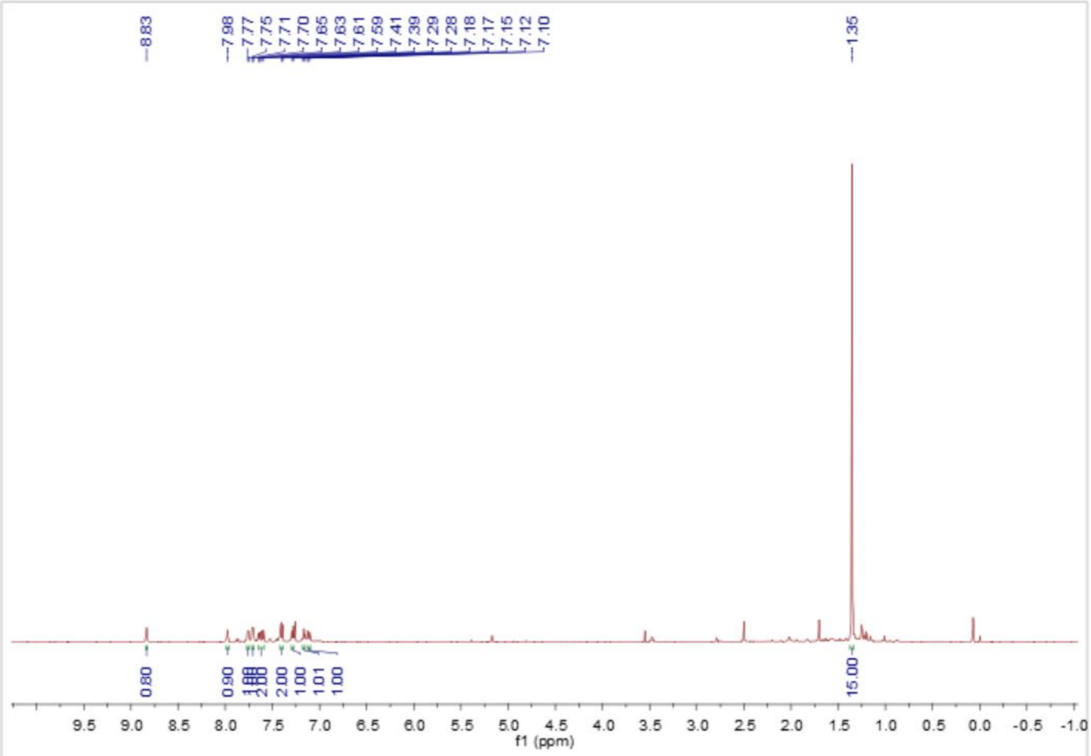

Figure S11. [1]H NMR spectra of **4**

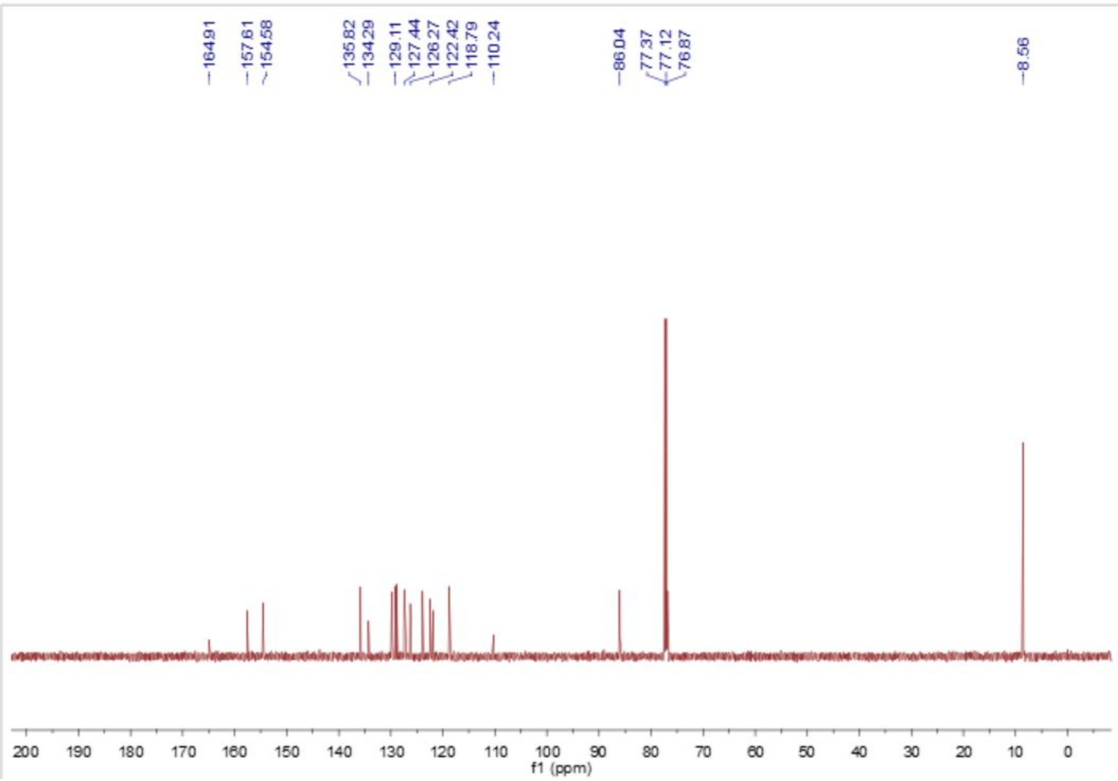

Figure S12. [13]C NMR spectra of **4**

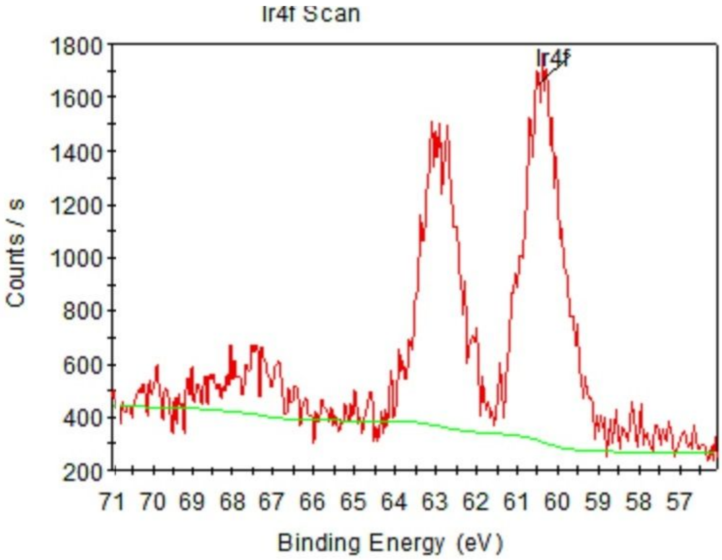

Figure S13. XPS of complex **1**