Conjugated, Rigidified Bibenzimidazole Ancillary Ligands for Enhanced Photoluminescence Quantum Yields of Orange/Red-Emitting Iridium(III) Complexes

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Supporting Information

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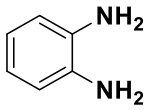
Experimental Section

General Synthetic Procedures. All reactions were performed using standard Schlenk techniques under inert (N_2) atmosphere with reagent grade solvents. The compounds 4-mesityl-2-chloropyridine and 4-mesityl-2-phenylpyridine were synthesized according to previously published procedures, and their characterization matches that previously reported.[1] Flash column chromatography was performed using silica gel (60 Å, 40-63 μm). Analytical thin layer chromatography (TLC) was performed using silica plates with aluminum backings (250 μm with indicator F-254). Compounds were visualized under UV light. ^{1}H and ^{13}C spectra were recorded on a Bruker Avance spectrometer at 400 MHz and 126 MHz, respectively. The following abbreviations have been used for multiplicity assignments: "s" for singlet, "d" for doublet, "t" for triplet, and "m" for multiplet. Deuterated chloroform ($CDCl_3$), deuterated dichloromethane (CD_2Cl_2) and deuterated dimethyl sulfoxide (DMSO-d_6) were used as the solvents of record. ^{1}H NMR spectra were referenced to the solvent peak. High-resolution mass spectra were recorded at the EPSRC UK National Mass Spectrometry Facility at Swansea University on a quadrupole time-of-flight (ESI-Q-TOF), model ABSciex 5600 Triple TOF in positive electrospray ionization mode and spectra were recorded using sodium formate solution as the calibrant. Elemental analyses were performed by Mr. Stephen Boyer, London Metropolitan University.

***o*-Phenylendiamine.**



The synthesis of this compound follows a previously reported method.[2] To a solution of 2-nitroaniline (2.70 g, 20 mmol, 1.0 equiv.) in ethanol (25 mL) were added concentrated HCl (6 mL) and anhydrous $SnCl_2$ (18.34 g, 72 mmol, 3.6 equiv.). The reaction was stirred under nitrogen at 60 °C for 16 h. Water was added to the reaction mixture and the resulting mixture was poured into an agitated aqueous solution of NaOH (3 M) resulting in the formation of a white precipitate. Saturated, aqueous $NaHCO_3$ solution was added for an additional 5 min. The fine white precipitate was removed by filtration through celite. The precipitate was repeatedly washed with DCM, then the organic phases were combined, washed with brine, dried over Na_2SO_4 and concentrated to give the compound as a white solid (2.10 g). **Yield**: 95%. **Mp:** 99 – 101 °C. **Litt.:**[2] 101 – 102 °C. **^{1}H NMR (500 MHz, $CDCl_3$) δ (ppm):** 6.74 – 6.70 (m, 4H), 3.19 (br s, 4H). The data matches that previously reported.[3]

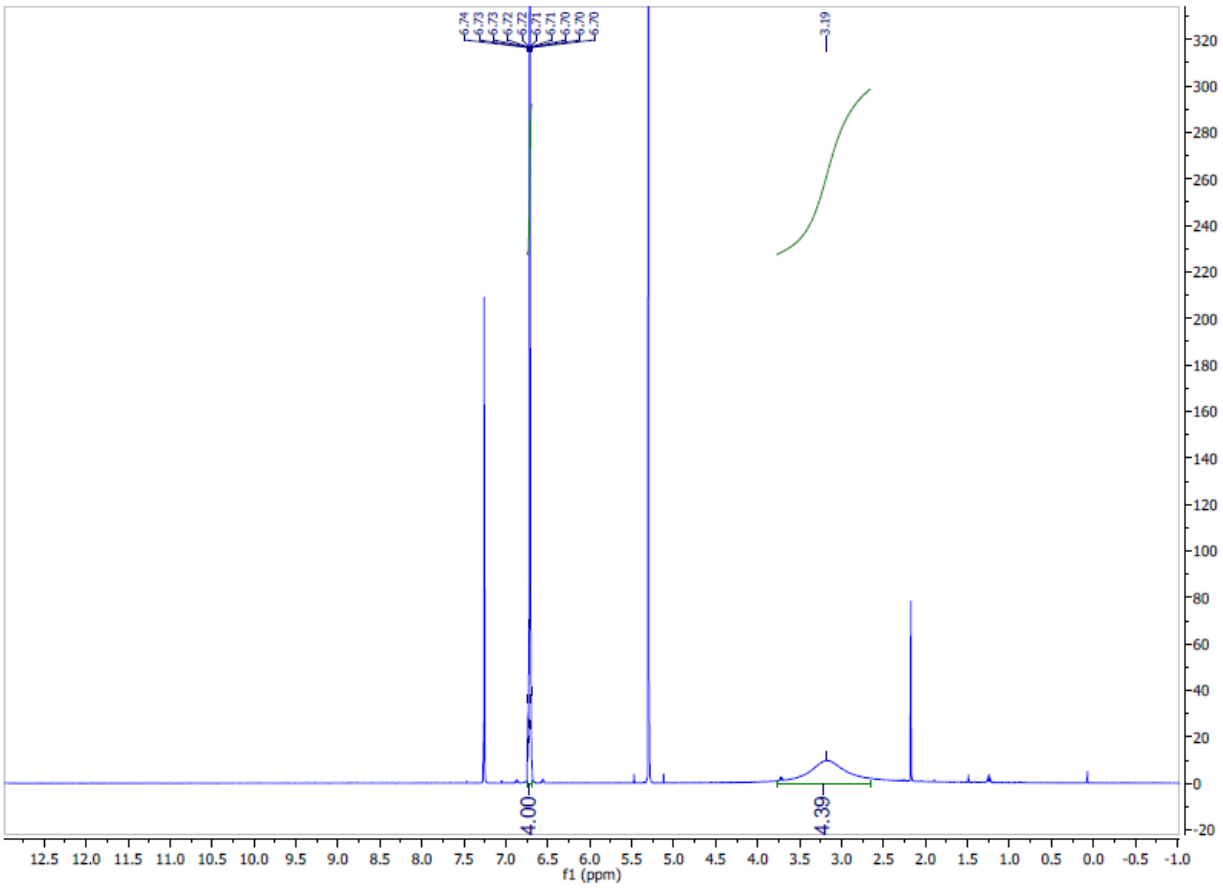
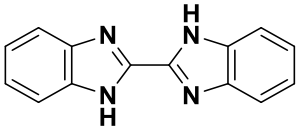


Figure **S1**. ^{1}H NMR spectrum of ***o*-phenylenediamine** in $CDCl_3$.

1*H*,1'*H*-2,2'-Bibenzimidazole (H_2biben).



The synthesis of this compound follows a previously reported method.[2] To a solution of *o*-phenylenediamine (1.24 g, 11.47 mmol, 2.0 equiv.) in methanol (50 mL) was added methyl-2,2,2-trichloroacetimidate (1.01 g, 5.74 mmol, 1.0 equiv.), followed by concentrated HCl (0.05 mL) at 0 °C under N_2, and the obtained mixture was stirred at room temperature. To this mixture three portions of K_2CO_3 (393 mg, 2.80 mmol, 0.5 equiv.; 786 mg, 5.60 mmol, 1.0 equiv.; 786 mg, 5.60 mmol, 1.0 equiv.) were added at intervals of 3 h, 3h and 15 h. The reaction mixture was stirred another 24 h after the final addition, and then water and Et_2O were added. The resulting precipitate was filtered, washed with water and Et_2O, and dried in vacuum. Orange solid (1.24 g). **Yield**: 92%. **Mp:** > 300 °C. **^{1}H NMR (500 MHz, DMSO-d_6) δ (ppm):** 7.75 (d, J = 7.8 Hz, 2H), 7.55 (d, J = 7.8 Hz, 2H), 7.34 – 7.23 (m, 4H). The data matches that previously reported.[4]

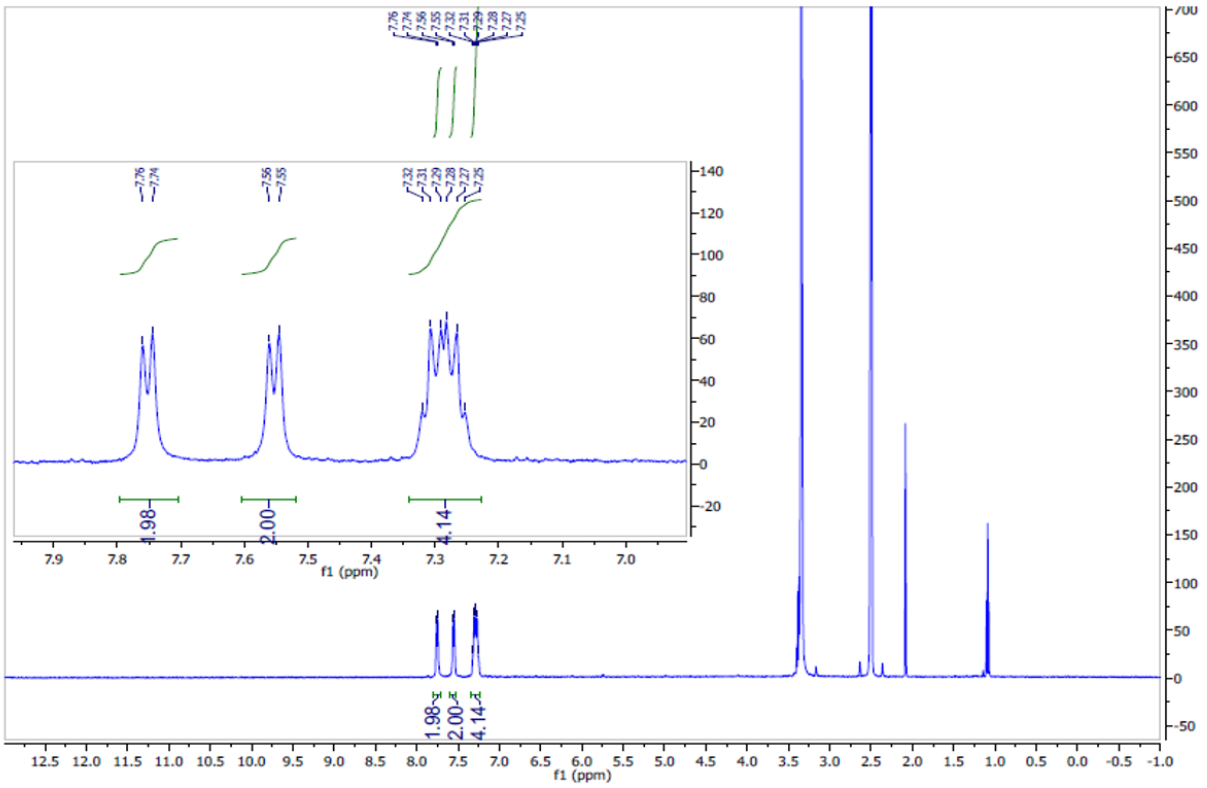
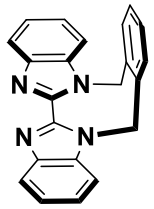


Figure **S2**. ^{1}H NMR spectrum of **1*H*,1'*H*-2,2'-Bibenzimidazole (H_2biben).** in DMSO-d_6.

1,1'-(α,α'-*o*-xylylene)-2,2'-Bibenzimidazole (*o*-Xylbiben).



The synthesis of this compound follows a previously reported method.[5] To a solution containing α,α'-dibromo-*o*-xylene (250 mg, 1.07 mmol, 1.0 equiv.) in acetonitrile (30 mL) was added with stirring 1*H*,1'*H*-2,2'-bibenzimidazole (375 mg, 1.61 mmol, 1.2 equiv.) followed by aqueous sodium hydroxide (30 mg, 0.75 mmol, 5.6 equiv., dissolved in 2 mL of water) under N_2. The temperature was increased to reflux, where after about 10 minutes a yellow solution formed. The reaction mixture was maintained at reflux for 19 h before being cooled to room temperature, then evaporating the crude mixture to dryness. Water was added, and the mixture was extracted multiple times with dichloromethane. The organic fractions were combined, dried over $MgSO_4$, filtered and evaporated to dryness. Et_2O was added to the solid to give a suspension, which was filtered, washed multiple times with Et_2O and dried to give the final compound as a yellow solid. **Yield**: 60%. **Mp:** > 300 °C. **Litt.:**[5] > 300 °C. **^{1}H NMR (500 MHz, DMSO-d_6) δ (ppm):** 7.86 (d, J = 8.0 Hz, 2H), 7.79 – 7.72 (m, 4H), 7.47 – 7.33 (m, 6H), 5.30 (s, 4H). The data matches that previously reported.[5]

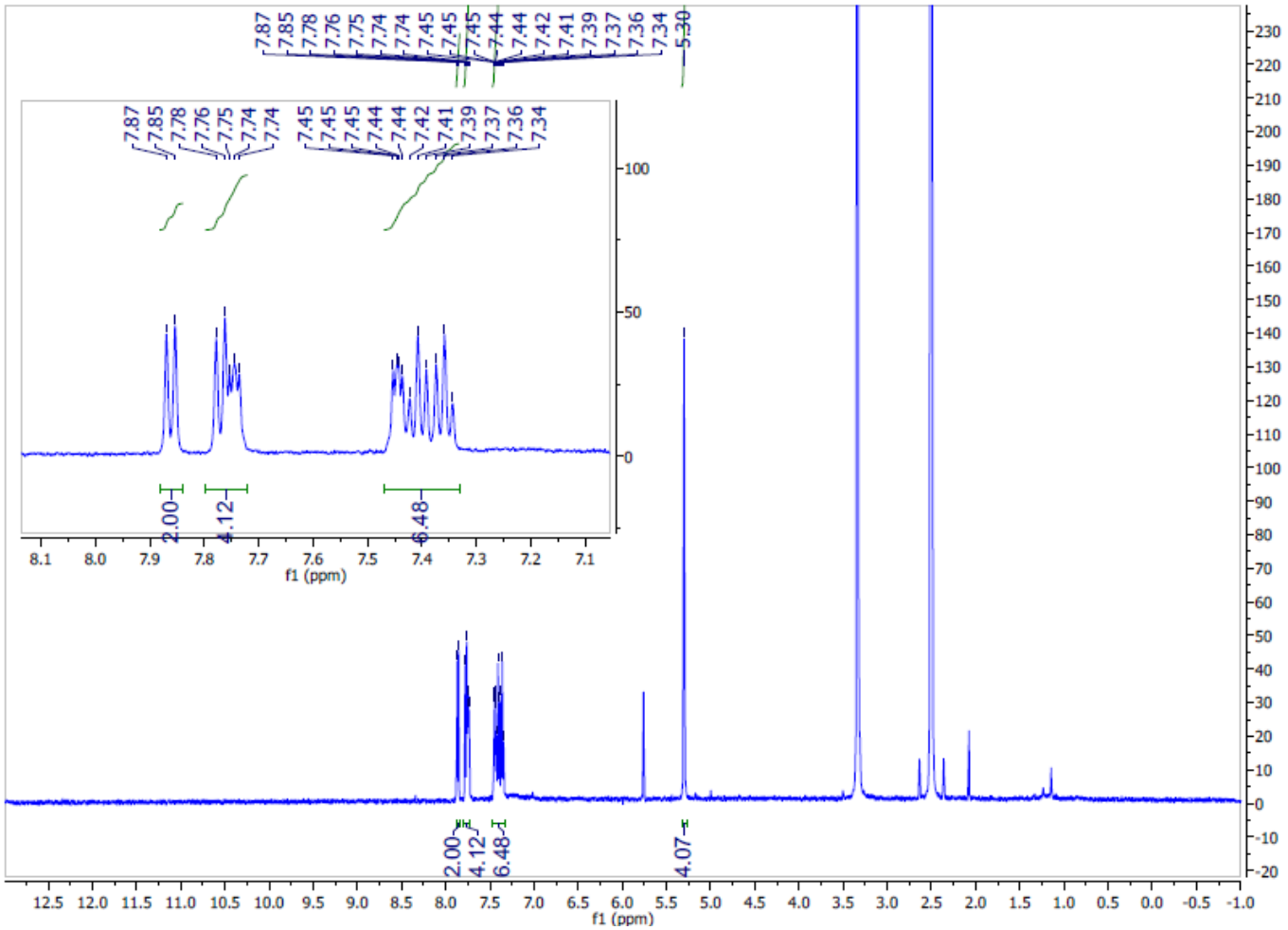
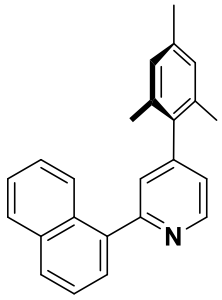


Figure **S3**. ^{1}H NMR spectrum of **1,1'-(α, α'-*o*-xylylene)-2,2'-bibenzimidazole** in DMSO-d_6.

4-Mesityl-2-(napthalen-1-yl)pyridine: Mesnpy.



2-Chloro-4-mesitylpyridine (0.250 g, 1.73 mmol, 1.0 equiv.) and 1,4-dioxane (12 mL) were added to a round bottom flask. The mixture was degassed by evacuating and purging the system with N_2 three times, $Pd(PPh_3)_4$ (0.037 g, 0.032 mmol, 3 mol%) was added under positive N_2 pressure and then the reaction mixture was sealed and heated to 50 °C for 1 h. 1-Naphthylboronic acid (0.297 g, 1.73 mmol, 1.6 equiv.), potassium carbonate (0.418 g, 3.02 mmol, 2.8 equiv.) and distilled water (3 mL) were added to the reaction mixture and it was degassed by three further N_2 purging cycles. The reaction mixture was then heated to reflux for 24 h, before cooling to room temperature. Distilled water was poured onto the reaction mixture before it was extracted multiple times with dichloromethane. The organic fractions were combined and washed with brine before drying over magnesium sulfate. Filtration and evaporation gave the crude product which was purified by flash column chromatography (silica, hexane/ethyl acetate gradient: 100:0 to 90:10) to afford the pure compound as a white crystalline solid (0.283 g). **Yield**: 68%. **Mp:** 151 – 153 °C. **R_f:** 0.12 (EtOAc/Hexanes 1:9 on silica). **^{1}H NMR (500 MHz, CD_2Cl_2) δ (ppm):** 8.82 (d, *J* = 5.0 Hz, 1H), 8.19 (d, *J* = 8.0 Hz, 1H), 7.93 (d, *J* = 8.0 Hz, 2H), 7.66 (d, *J* = 7.0 Hz, 1H), 7.60 – 7.55 (m, 1H), 7.54 – 7.47 (m, 2H), 7.41 (s, 1H), 7.17 (dd, *J* = 5.0, 1.5 Hz, 1H), 6.98 (s, 2H), 2.32 (s, 3H), 2.10 (s, 6H). **^{13}C {^{1}H} NMR (126 MHz, $CDCl_3$) δ (ppm):** 159.3, 149.9, 149.6, 138.7, 137.5, 136.4,

135.1, 133.9, 131.2, 128.7, 128.3, 127.5, 126.3, 126.0, 125.8, 125.7, 125.3, 123.2, 20.8, 20.5. **HR-MS (FTMS$^+$): [M + H]$^+$ Calculated:** ($C_{24}H_{21}NH$) 324.1717; **Found:** 324.1747.

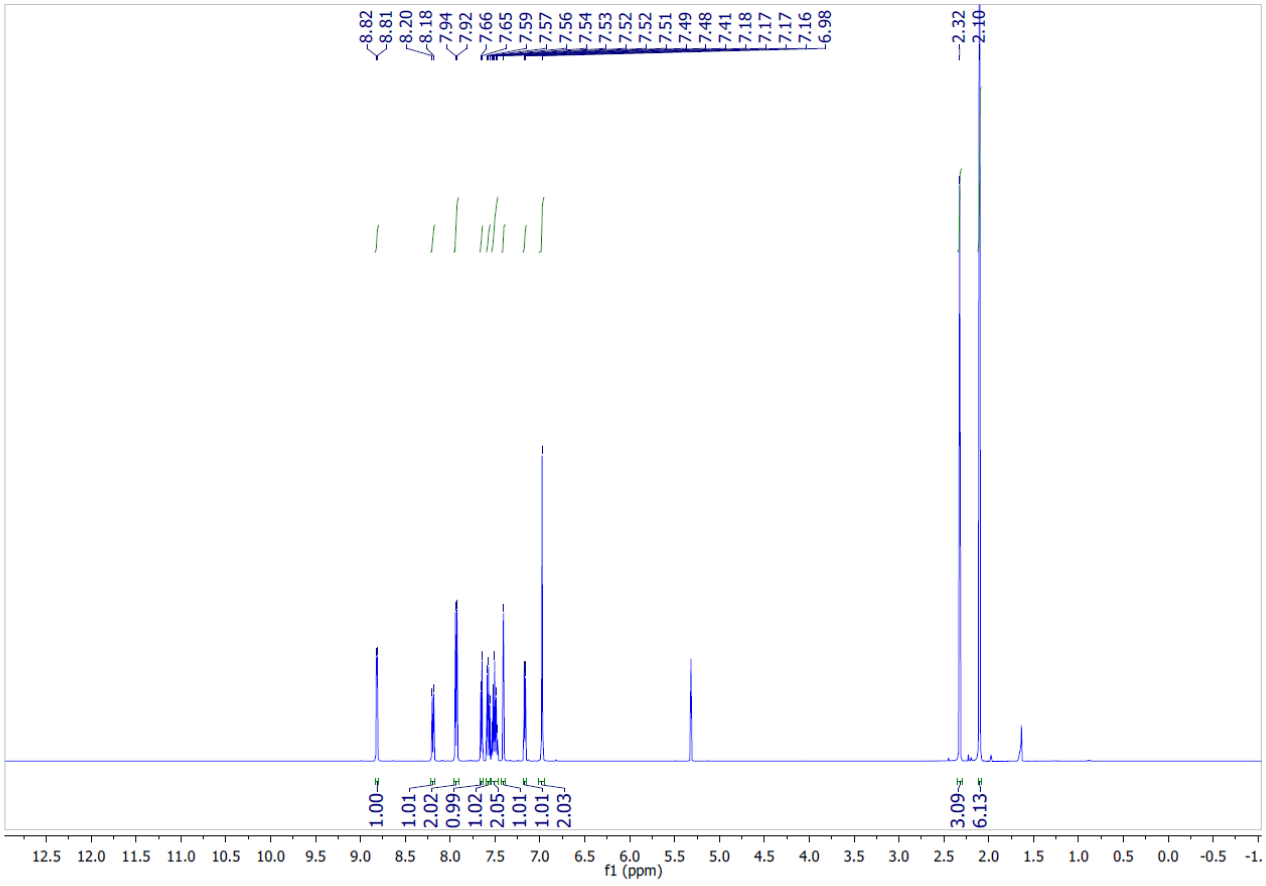


Figure **S4**. ^{1}H NMR spectrum of **4-mesityl-2-(naphthalen-1-yl)pyridine** in CD_2Cl_2.

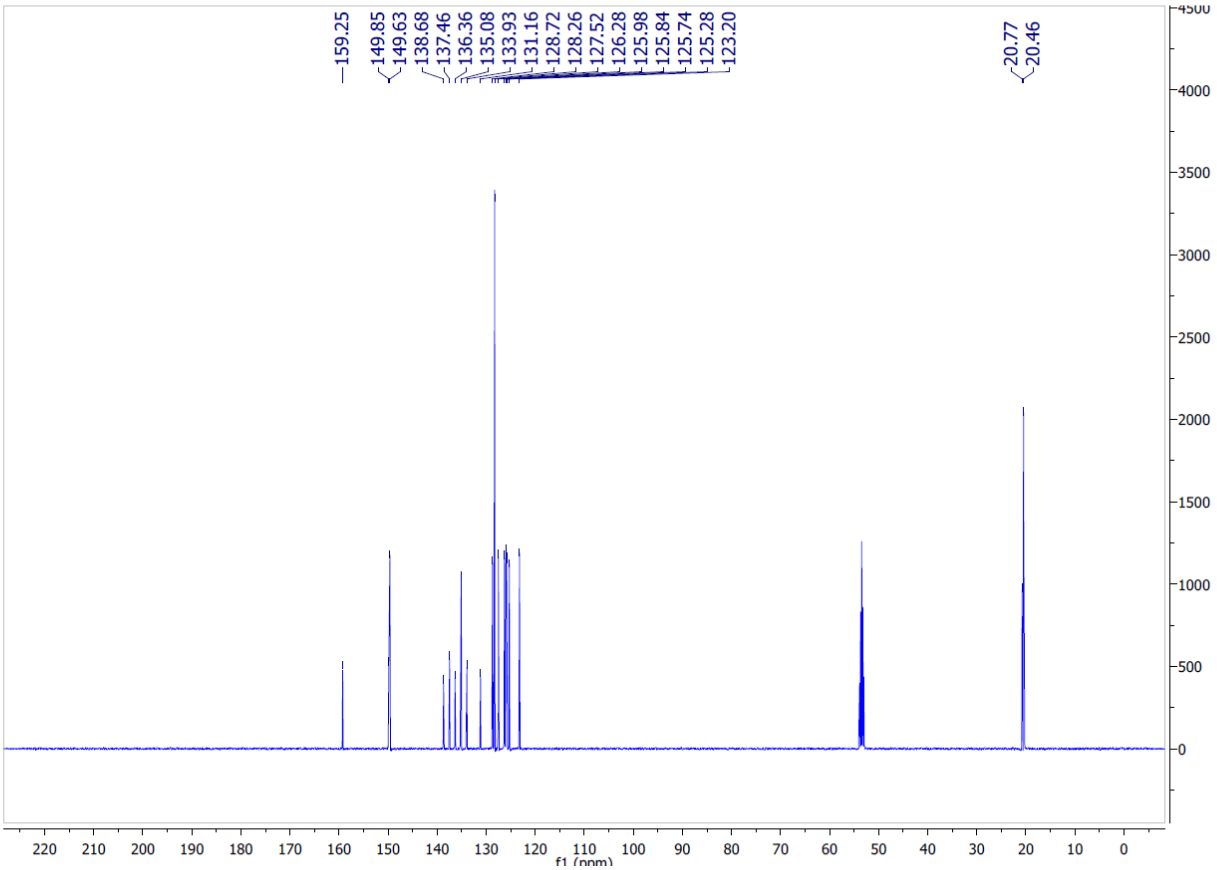
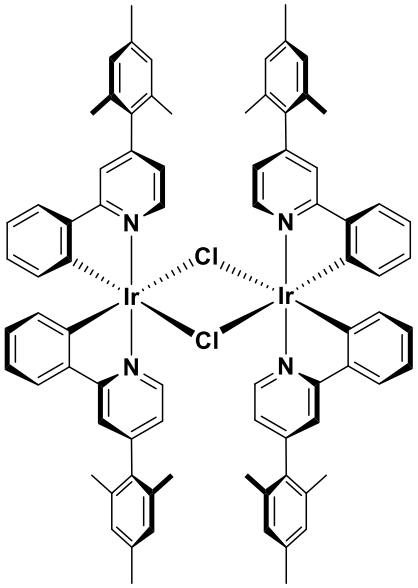


Figure **S5**. ^{13}C NMR spectrum of **4-mesityl-2-(naphthalen-1-yl)pyridine** in $CDCl_3$.

General procedure for the synthesis of [Ir(C^N)$_2$(μ-Cl)]$_2$ dimer intermediates. The dimers were prepared according to the method reported by Nonoyama.[6] $IrCl_3.3H_2O$ (1.0 equiv.), C^N ligand (2.2 equiv.) and a 5:1 v/v mixture of 2-ethoxyethanol and water were added to a round bottom flask to give a suspension with a concentration of 0.20 M. This mixture was degassed via vigorously bubbling with N_2. The reaction mixture was heated to reflux for 19 h whereupon a yellow or orange precipitate formed. After cooling to room temperature, the precipitate was filtered, washed with water, diethyl ether and hexane to give the title compound.

Tetrakis[2-phenyl-4-(2,4,6-trimethylphenyl)pyridinato-*N*,$C^{2'}$]-bis(μ-chloro)diiridium(III), Ir(Mesppy)$_2$(μ-Cl)$_2$



Yellow powder. **Yield**: 72%. **^{1}H NMR (500 MHz, CD_2Cl_2) δ (ppm):** 9.66 (d, *J* = 5.8 Hz, 4H), 7.74 (d, *J* = 1.8 Hz, 4H), 7.50 (dd, *J* = 7.8, 1.3 Hz, 4H), 7.01 (d, *J* = 14.0 Hz, 8H), 6.84 – 6.80 (m, 8H), 6.67 (ddd, *J* = 8.3, 7.1, 1.4, 4H), 5.91 (dd, *J* = 7.9, 1.1 Hz, 4H), 2.38 (s, 12H), 2.12 (s, 12H), 2.11 (s, 12H). Characterisation matches that previously reported.[1]

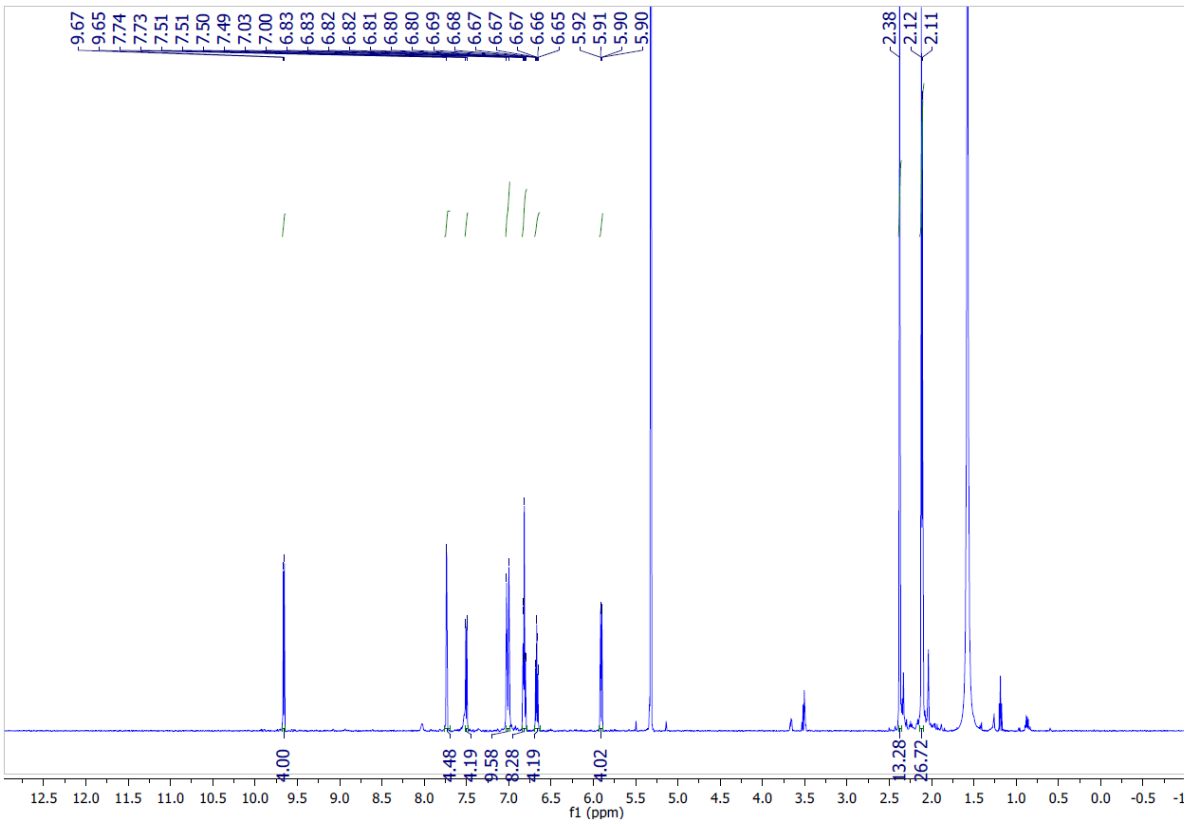
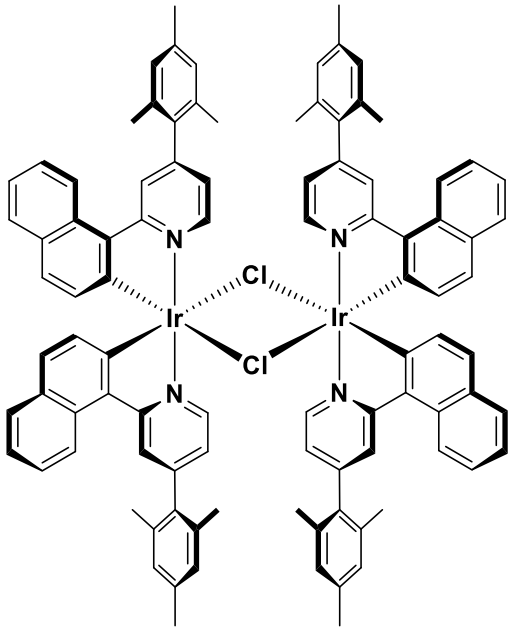


Figure **S6**. ^{1}H NMR spectrum of **Tetrakis[2-phenyl-4-(2,4,6-trimethylphenyl)pyridinato-*N*,*C*$^{2'}$]-bis(μ-chloro)diiridium(III)** (**Ir(Mesppy)$_2$(μ-Cl]$_2$**) in CD_2Cl_2.

Tetrakis[2-(naphthalen-1-yl)-4-(2,4,6-trimethylphenyl)pyridinato-*N*,$C^{2'}$]-bis(μ-chloro)diiridium(III), Ir(Mesnpy)$_2$(μ-Cl)$_2$



Orange powder. **Yield**: 70%. **^{1}H NMR (500 MHz, CD_2Cl_2) δ (ppm):** 9.76 (d, *J* = 5.7 Hz, 4H), 8.46 (d, *J* = 5.7 Hz, 4H), 8.35 (s, 4H), 7.59 (d, *J* = 7.9 Hz, 4H), 7.39 (t, *J* = 7.8 Hz, 4H), 7.22 (t, *J* = 7.4 Hz, 4H), 7.11 (s, 4H), 7.05 (s, 4H), 7.00 (d, *J* = 8.6 Hz, 4H), 6.93 (d, *J* = 5.8 Hz, 4H), 5.85 (d, *J* = 8.6 Hz, 4H), 2.41 (s, 12H), 2.35 (s, 12H), 2.14 (s, 12H).

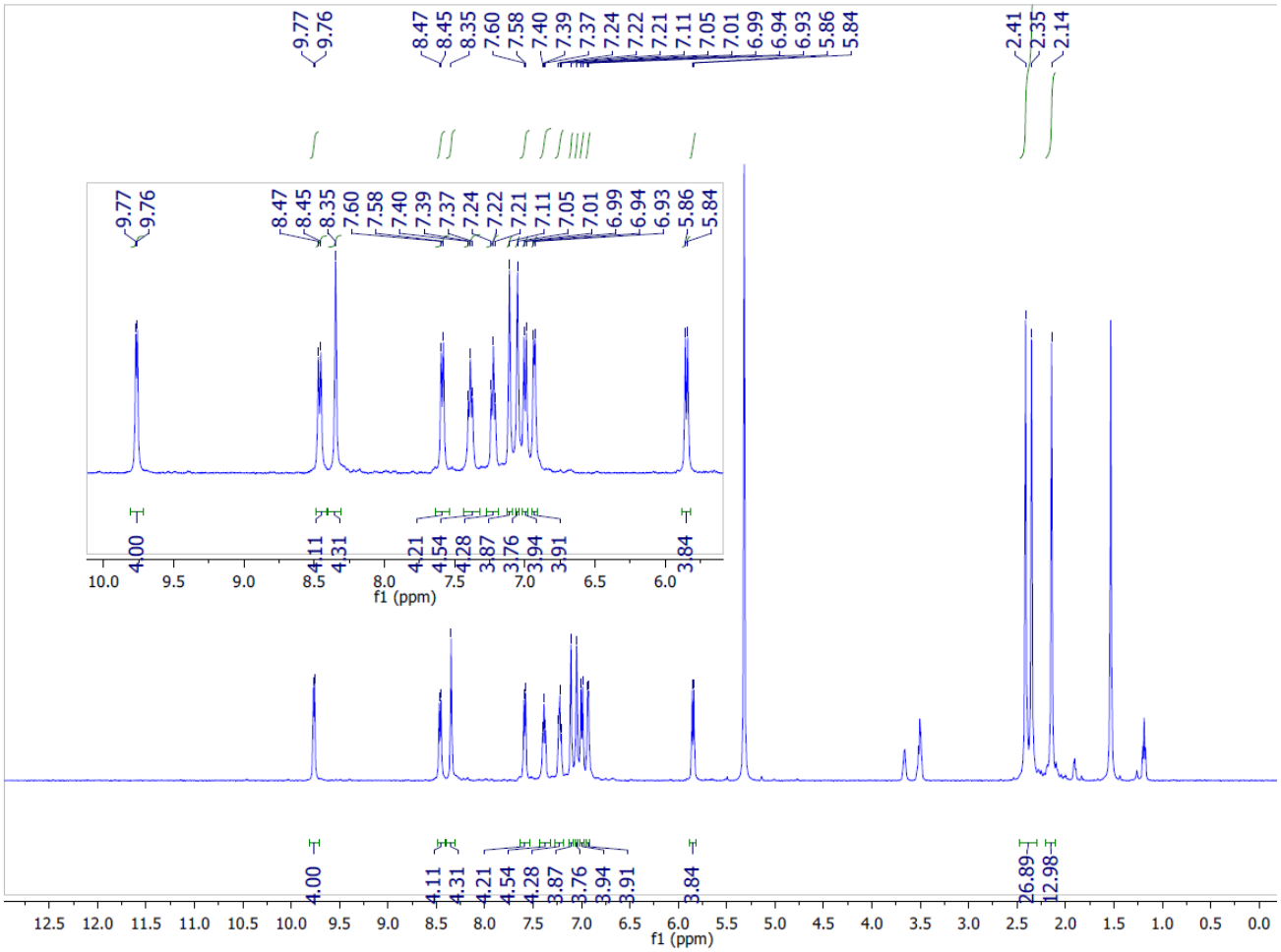
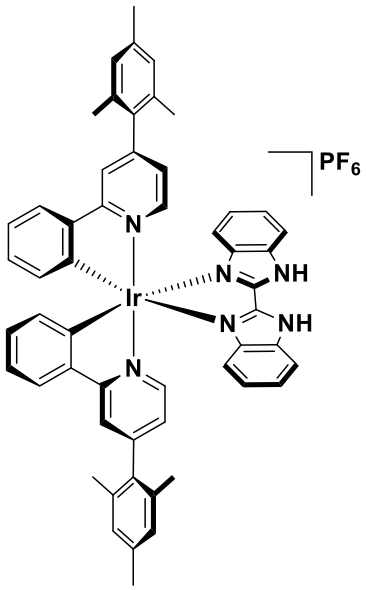


Figure **S7**. ^{1}H NMR spectrum of **Tetrakis[2-(naphthalen-1-yl)-4-(2,4,6-trimethylphenyl)-pyridinato-*N*,*C*$^{2'}$]-bis(μ-chloro)diiridium(III)** (**Ir(Mesnpy)$_2$(μ-Cl]$_2$**) in CD_2Cl_2.

General procedure for the synthesis of [Ir(C^N)$_2$(N^N)](PF$_6$) complexes. [Ir(C^N)$_2$(μ-Cl)]$_2$ dimer (1.0 equiv.) and N^N ligand (2.2 equiv.) were added to a round bottom flask. DCM and MeOH (1:1) were added to the flask to give a reaction mixture with a concentration of ca. 0.50 M. This mixture was degassed via vigorously bubbling with N_2, and then refluxed for 24 h. The reaction mixture was cooled to room temperature and then evaporated to dryness before purification by column chromatography. The fractions were combined, evaporated to dryness and then MeOH was added. The MeOH solution was added to aqueous ammonium hexafluorophosphate (0.500 g in 5 mL) to reprecipitate the compound as its hexafluorophosphate salt. The mixture was stirred for 1 h then filtered, and washed with water and hexane. The compound may be purified further by dissolving in the minimum volume of methanol, and adding dropwise to excess hexane. The product was filtered and washed with hexane to give the pure product.

Iridium (III) bis[2-(phenyl)-4-(2,4,6-trimethylphenyl)pyridinato-N,C$^{2'}$]-*N,N'*-(1*H*,1'*H*-2,2'-bibenzimidazole)hexafluorophosphate: [Ir(Mesppy)$_2$(H$_2$bibenz)](PF$_6$).



Yellow solid. **Yield**: 60%. **Mp:** 331 – 333 °C (decomp.). **R$_f$:** 0.63 (DCM/MeOH 9:1 on silica). **^{1}H NMR (500 MHz, CD$_2$Cl$_2$) δ (ppm):** 11.55 (s, br 2H), 7.75 – 7.68 (m, 8H), 7.42 (t, *J* = 7.7 Hz, 2H), 7.08 – 7.15 (m, 4H), 7.01 (t, *J* = 7.4 Hz, 2H), 6.97 (s, 2H), 6.91 (s, 2H), 6.75 (dd, *J* = 5.9, 1.6 Hz, 2H), 6.55 (d, *J* = 7.4 Hz, 2H), 6.42 (d, *J* = 8.4 Hz, 1H), 2.30 (s, 6H), 2.10 (s, 6H), 1.87 (s, 6H). **^{13}C {^{1}H} NMR (126 MHz, CDCl$_3$) δ (ppm):** 168.5, 151.9, 149.8, 147.8, 145.4, 144.3, 141.0, 138.5, 135.5, 135.5, 135.4, 134.6, 132.5, 130.3, 128.8, 128.7, 126.9, 125.0, 124.9, 122.7, 121.0, 118.4, 113.8, 21.1, 20.7. **HR-MS (FTMS$^+$): [M – PF$_6$]$^+$ Calculated:** ($C_{54}H_{46}IrN_6$) 971.3412; **Found:** 971.3408. **Anal.** Calcd for $C_{54}H_{46}F_6IrN_6P$ (MW 1116.19): C, 58.11; H, 4.15; N, 7.53. Found: C, 57.98; H, 4.16; N, 7.51 (average of two runs).

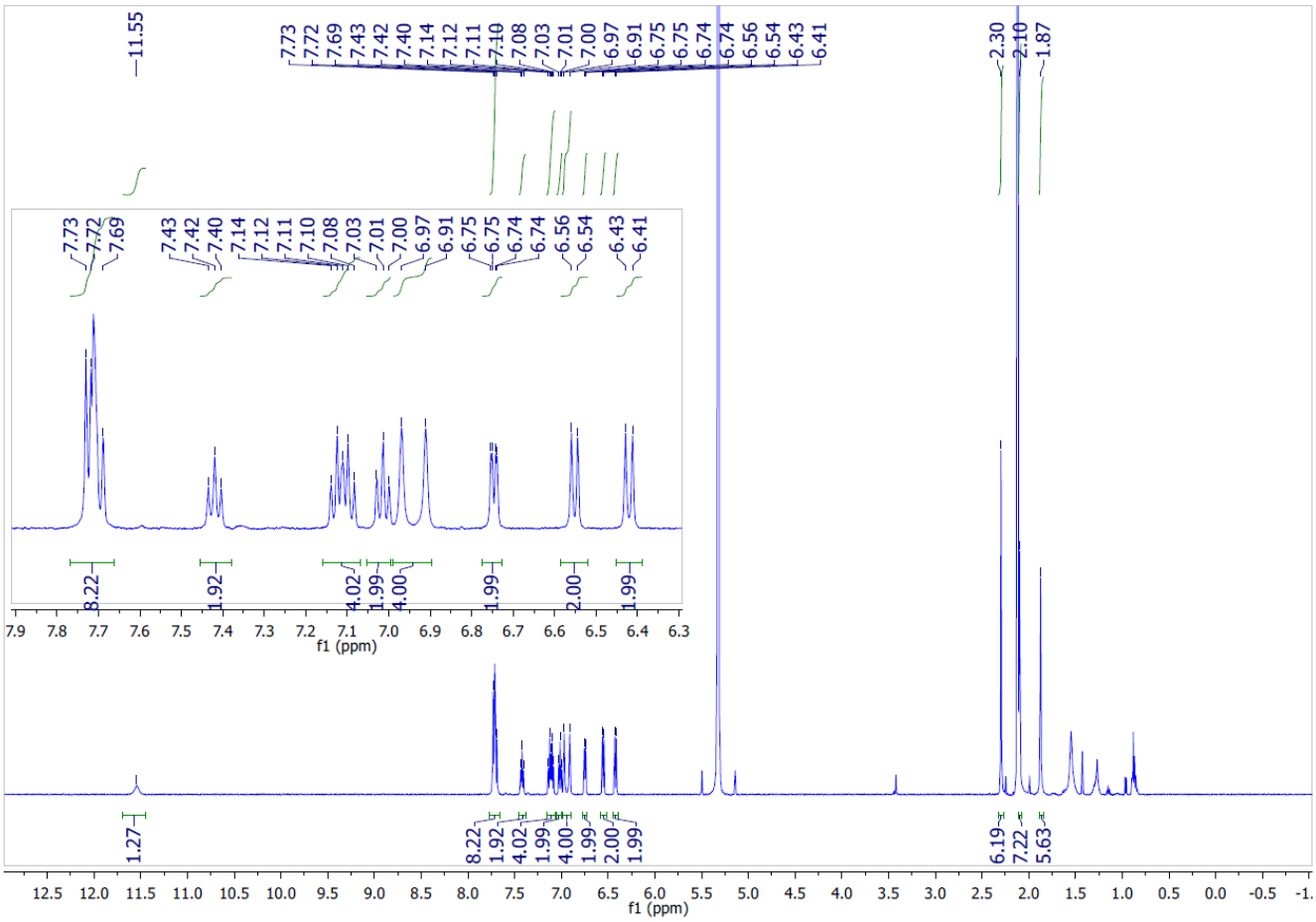


Figure **S8**. ^{1}H NMR spectrum of **Iridium (III) bis[2-(phenyl)-4-(2,4,6-trimethylphenyl)pyridinato-N,C$^{2'}$]-*N,N'*-(1*H*,1'*H*-2,2'-bibenzimidazole) hexafluorophosphate ([Ir(Mesppy)$_2$(H$_2$bibenz)](PF$_6$))** in CD_2Cl_2.

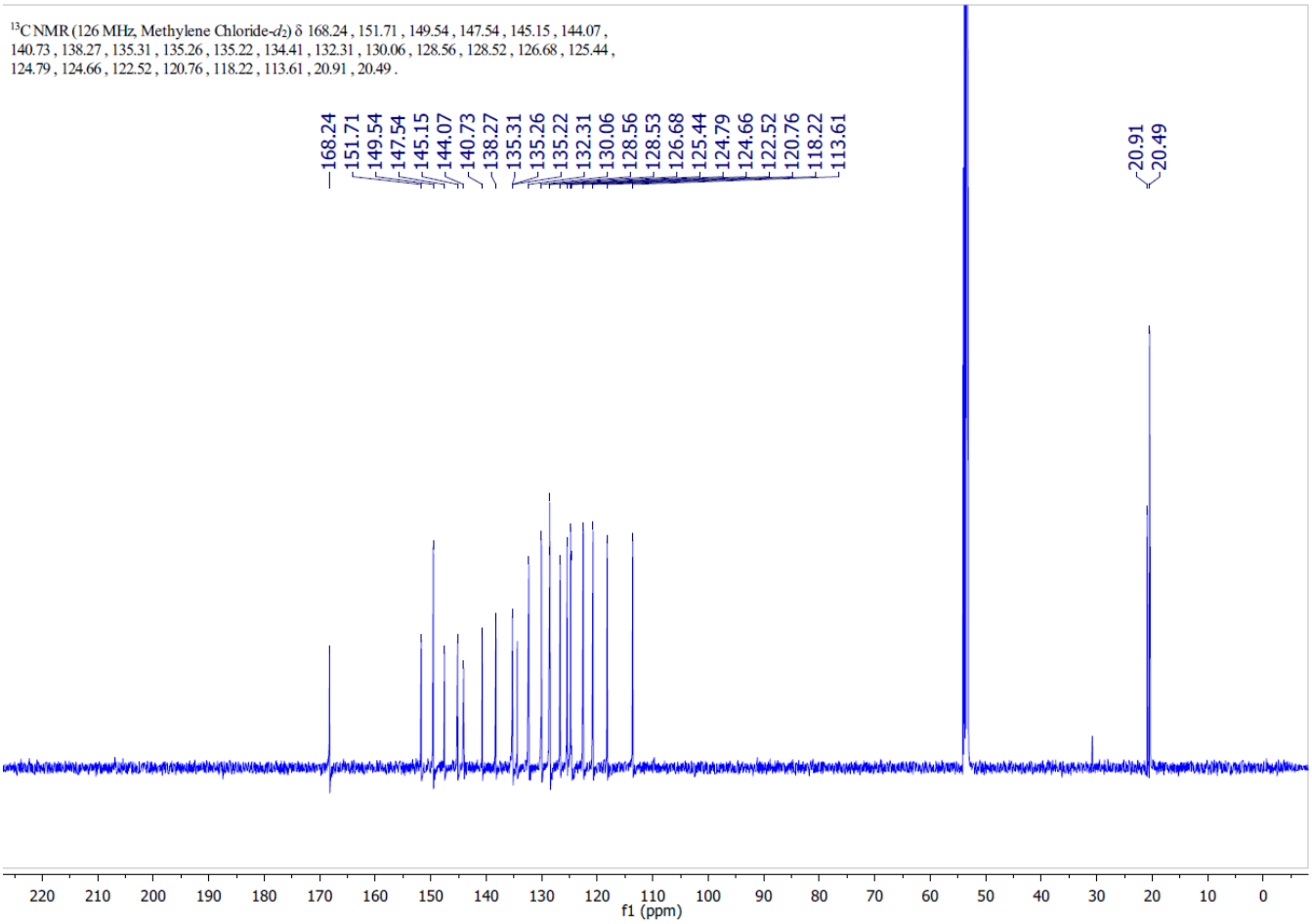
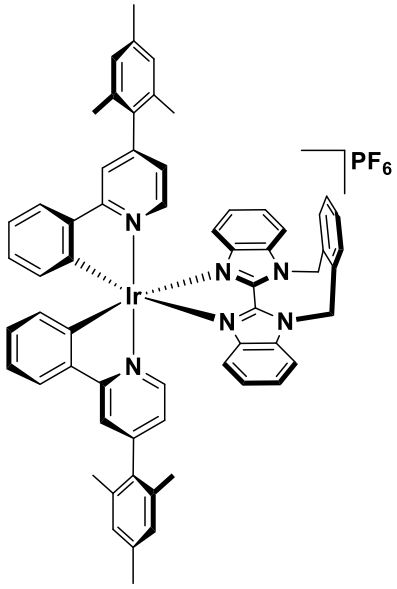


Figure **S9**. ^{13}C NMR spectrum of **Iridium (III) bis[2-(phenyl)-4-(2,4,6-trimethylphenyl)pyridinato-N,C$^{2'}$]-*N,N'*-(1*H*,1'*H*-2,2'-bibenzimidazole) hexafluorophosphate** (**[Ir(Mesppy)$_2$(H$_2$bibenz)](PF$_6$)**) in $CDCl_3$.

Iridium (III) bis[2-(phenyl)-4-(2,4,6-trimethylphenyl)pyridinato-N,C$^{2'}$]-*N,N′*-(1,1'-(a,a'-*o*-xylyl)-2,2'-bibenzimidazole)hexafluorophosphate: [Ir(Mesppy)$_2$(*o*-Xylbibenz)](PF$_6$).



Yellow solid. **Yield**: 62%. **Mp:** 264 – 267 °C (decomp.). **R$_f$:** 0.57 (DCM/MeOH 9:1 on silica). **^{1}H NMR (500 MHz, DMSO-*d*$_6$, 372 K) δ (ppm):** 8.36 (d, *J* = 8.5 Hz, 2H), 7.92 – 7.88 (m, 4H), 7.71 (dd, *J* = 5.6, 3.4 Hz, 2H), 7.57 – 7.50 (m, 4H), 7.45 (dd, *J* = 5.7, 3.3 Hz, 2H), 7.10 (t, *J* = 8.0 Hz, 2H), 7.05 (t, *J* = 8.0 Hz, 2H), 6.98 – 6.89 (m, 6H), 6.75 (dd, *J* = 6.0, 1.9 Hz, 2H), 6.40 (dd, *J* = 7.6, 1.2 Hz, 2H), 6.36 (d, *J* = 8.4 Hz, 2H), 6.24 (d, *J* = 3.0 Hz, 2H), 2.28 (s, 3H), 1.89 (br s, 12H). **^{13}C {^{1}H} NMR (126 MHz, CD_2Cl_2) δ (ppm):** 168.3, 151.8, 149.6, 149.0, 145.1, 144.9, 140.6, 138.5, 136.2, 135.5, 135.3, 134.5, 132.3, 131.3, 131.3, 130.3, 128.8, 128.7, 127.1, 126.0, 124.9, 122.7, 121.0, 119.2, 111.6, 47.5, 21.1, 20.7, 20.6. **HR-MS (FTMS$^+$): [M – PF$_6$]$^+$ Calculated:** ($C_{62}H_{52}IrN_6$) 1073.3882; **Found:** 1073.3873. **Anal.** Calcd for $C_{62}H_{52}F_6IrN_6P$ (MW 1218.32): C, 61.12; H, 4.39; N, 6.90. Found: C, 61.14; H, 4.03; N, 6.84 (average of two runs).

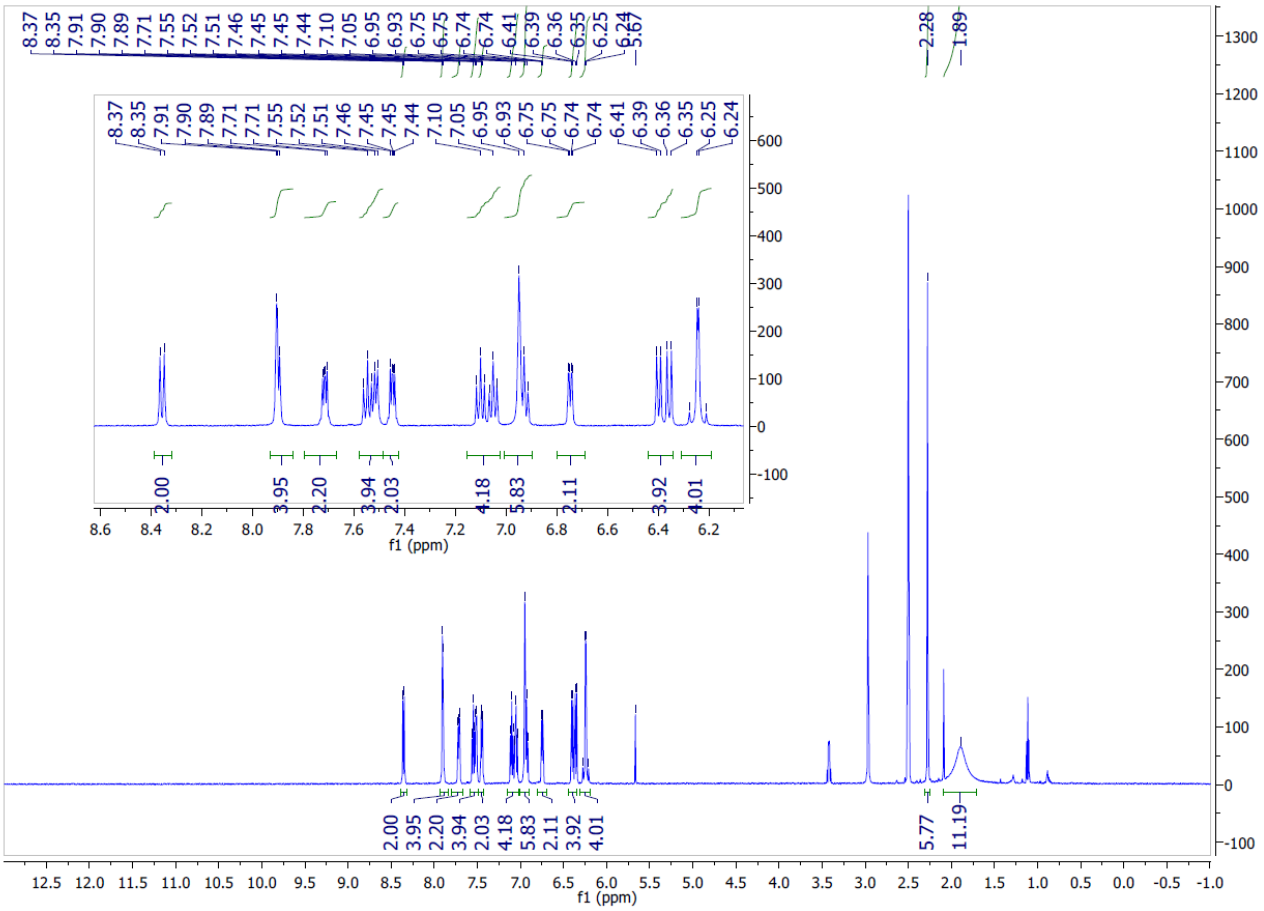


Figure **S10**. ^{1}H NMR spectrum of **Iridium (III) bis[2-(phenyl)-4-(2,4,6-trimethylphenyl)pyridinato-N,C$^{2'}$]-*N,N'*-(1,1'-(a,a'-*o*-xylyl)-2,2'-bibenzimidazole) hexafluorophosphate** (**[Ir(Mesppy)$_2$(*o*-Xylbibenz)](PF$_6$)**) in DMSO-d_6 at 372 K.

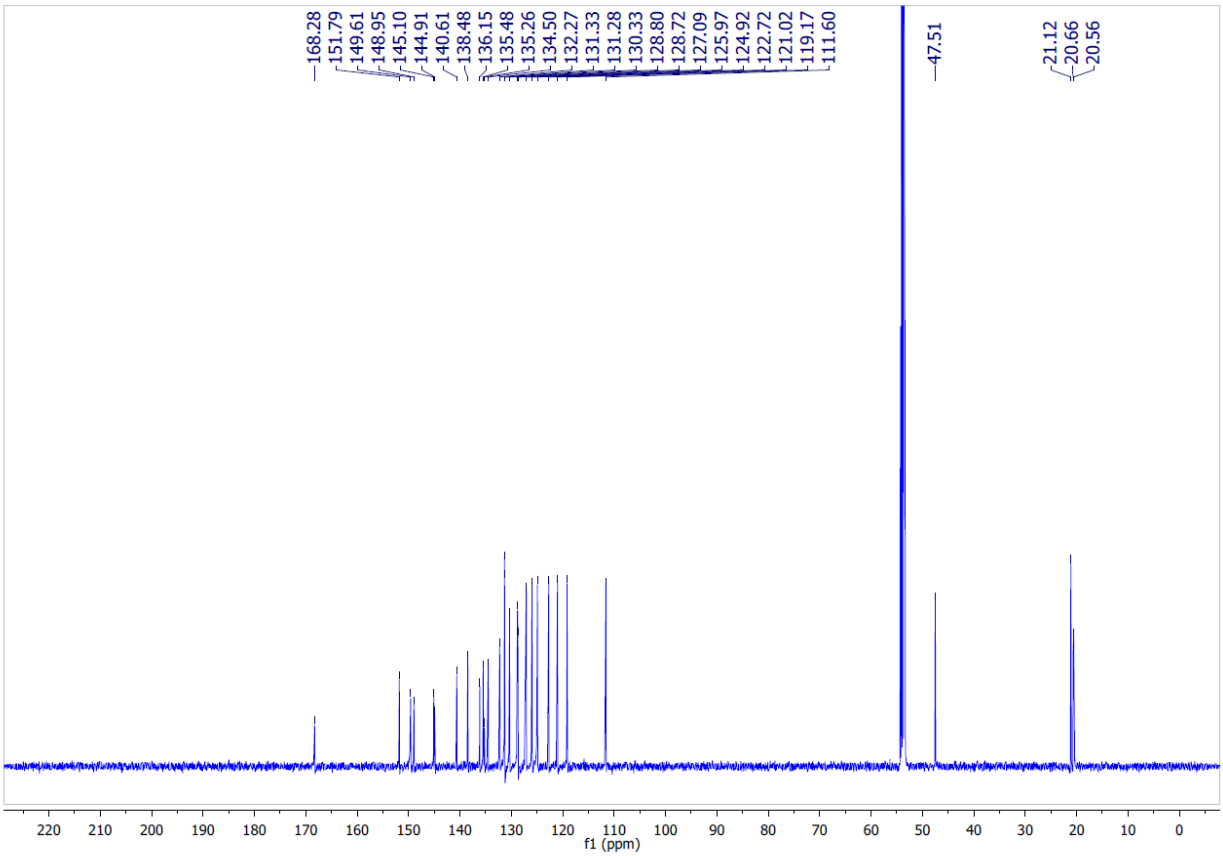


Figure **S11**. ^{13}C NMR spectrum of **Iridium (III) bis[2-(phenyl)-4-(2,4,6-trimethylphenyl)pyridinato-N,C$^{2'}$]-*N,N'*-(1,1'-(a,a'-*o*-xylyl)-2,2'-bibenzimidazole) hexafluorophosphate** (**[Ir(Mesppy)$_2$(*o*-Xylbibenz)](PF$_6$)**) in CD_2Cl_2.

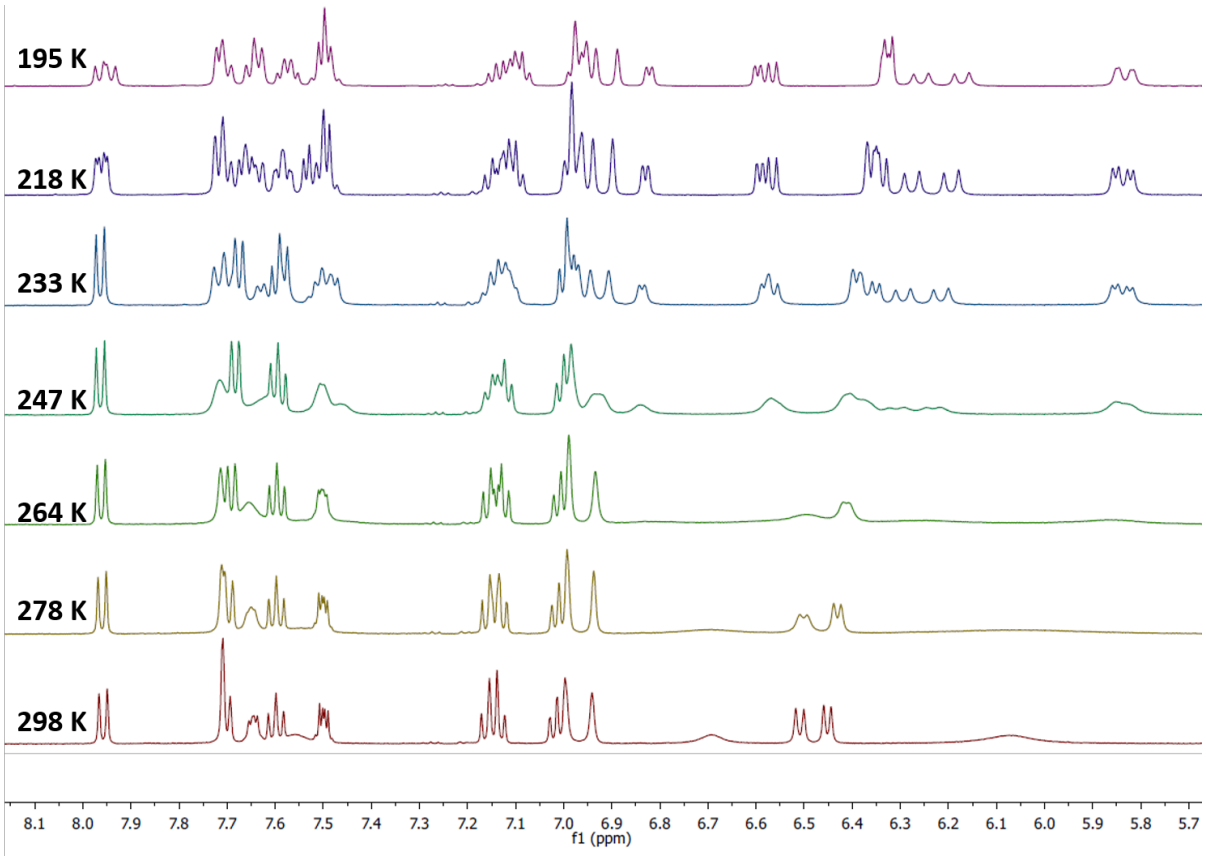
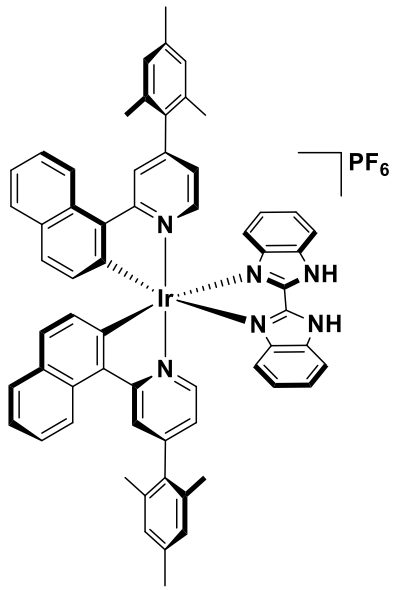


Figure **S12**. ^{1}H NMR temperature study of **Iridium (III) bis[2-(phenyl)-4-(2,4,6-trimethylphenyl)pyridinato-N,C$^{2'}$]-*N,N'*-(1,1'-(a,a'-*o*-xylyl)-2,2'-bibenzimidazole) hexafluorophosphate ([Ir(Mesppy)$_2$(*o*-Xylbibenz)](PF$_6$))** in CD_2Cl_2.

Iridium (III) bis[2-(naphthalen-1-yl)-4-(2,4,6-trimethylphenyl)-pyridinato-*N*,$C^{2'}$]-*N*,*N*′-(1*H*,1'*H*-2,2'-bibenzimidazole)hexafluorophosphate: [Ir(Mesnpy)$_2$(H_2bibenz)](PF_6).



Orange solid. **Yield**: 31%. **Mp:** 281 – 283 °C (decomp.). **R_f:** 0.60 (DCM/MeOH 9:1 on silica). **^{1}H NMR (500 MHz, CD_2Cl_2) δ (ppm):** 8.40 (d, *J* = 8.7 Hz, 2H), 8.30 (s, 2H), 7.91 (d, *J* = 5.9 Hz, 2H), 7.83 (d, *J* = 8.0 Hz, 2H), 7.70 (d, *J* = 8.3 Hz, 2H), 7.47 (t, *J* = 7.8 Hz, 2H), 7.41 – 7.36 (m, 4H), 7.33 (t, *J* = 7.0 Hz, 2H), 6.98 (d, *J* = 13.2 Hz, 4H), 6.82 (t, *J* = 7.8 Hz, 2H), 6.78 (d, *J* = 5.5 Hz, 2H), 6.51 (d, *J* = 8.4 Hz, 2H), 6.04 (d, *J* = 8.4 Hz, 2H), 2.32 (s, 6H), 2.16 (s, 6H), 1.98 (s, 6H). **^{13}C {^{1}H} NMR (126 MHz, CD_2Cl_2) δ (ppm):** 169.4, 151.9, 150.5, 140.9, 139.2, 138.5, 135.9, 135.6, 135.4, 131.9, 131.6, 130.7, 130.1, 130.0, 128.8, 128.8, 127.6, 126.7, 125.5, 125.1, 124.0, 123.7, 122.0, 118.1, 113.9, 21.2, 20.8, 20.7. **HR-MS (FTMS$^+$): $[M - PF_6]^+$ Calculated:** ($C_{62}H_{50}IrN_6$) 1071.3726; **Found:** 1071.3722. **Anal.** Calcd for $C_{62}H_{52}F_6IrN_6P$ (MW 1216.31): C, 61.22; H, 4.14; N, 6.99. Found: C, 61.65; H, 4.25; N, 6.96 (average of two runs).

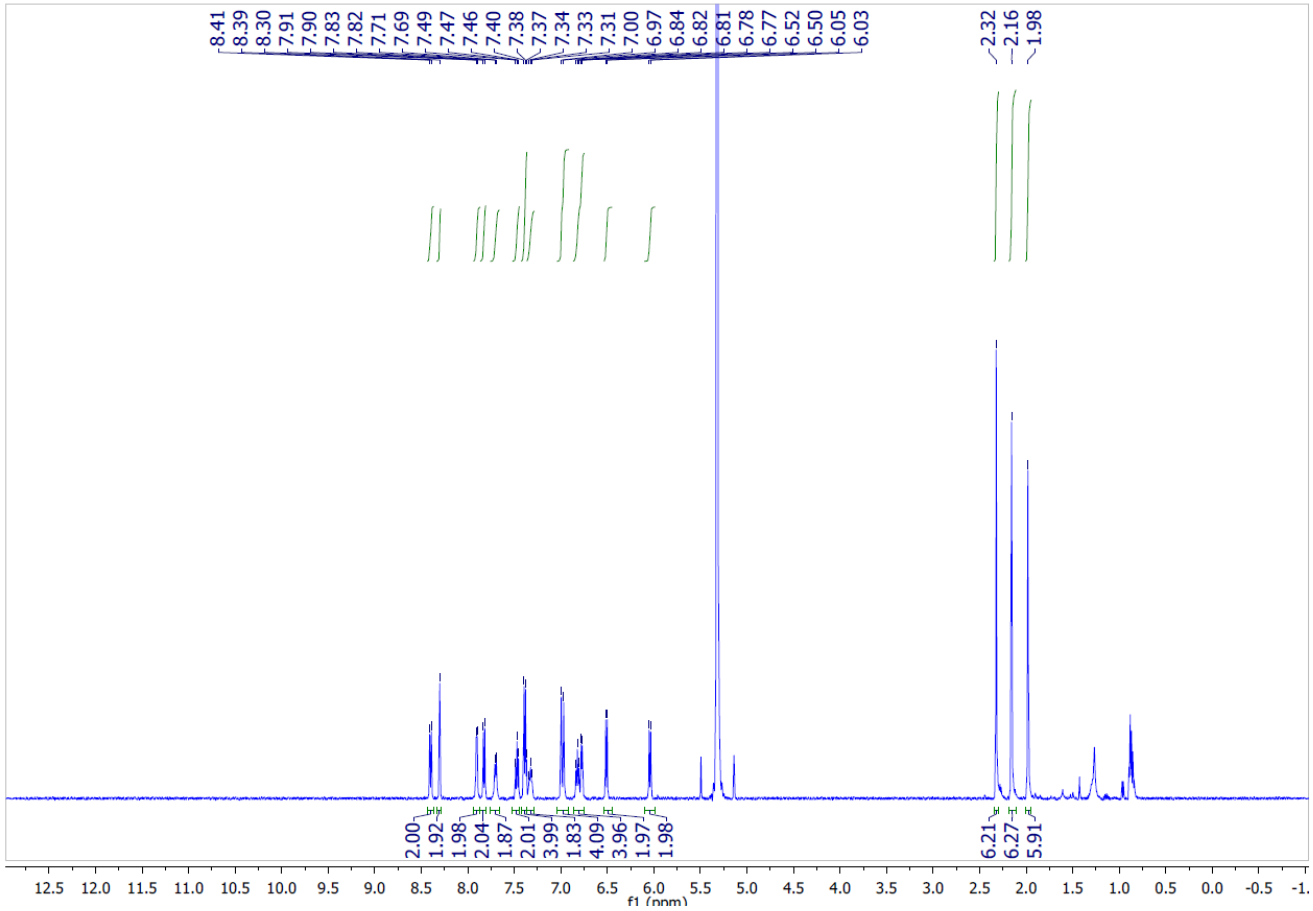


Figure **S13**. ^{1}H NMR spectrum of **Iridium (III) bis[2-(naphthalen-1-yl)-4-(2,4,6-trimethylphenyl)-pyridinato-*N*,*C*$^{2'}$]-*N*,*N*′-(1*H*,1'*H*-2,2'-bibenzimidazole) hexafluorophosphate ([Ir(Mesnpy)$_2$(H$_2$bibenz)](PF$_6$))** in CD_2Cl_2.

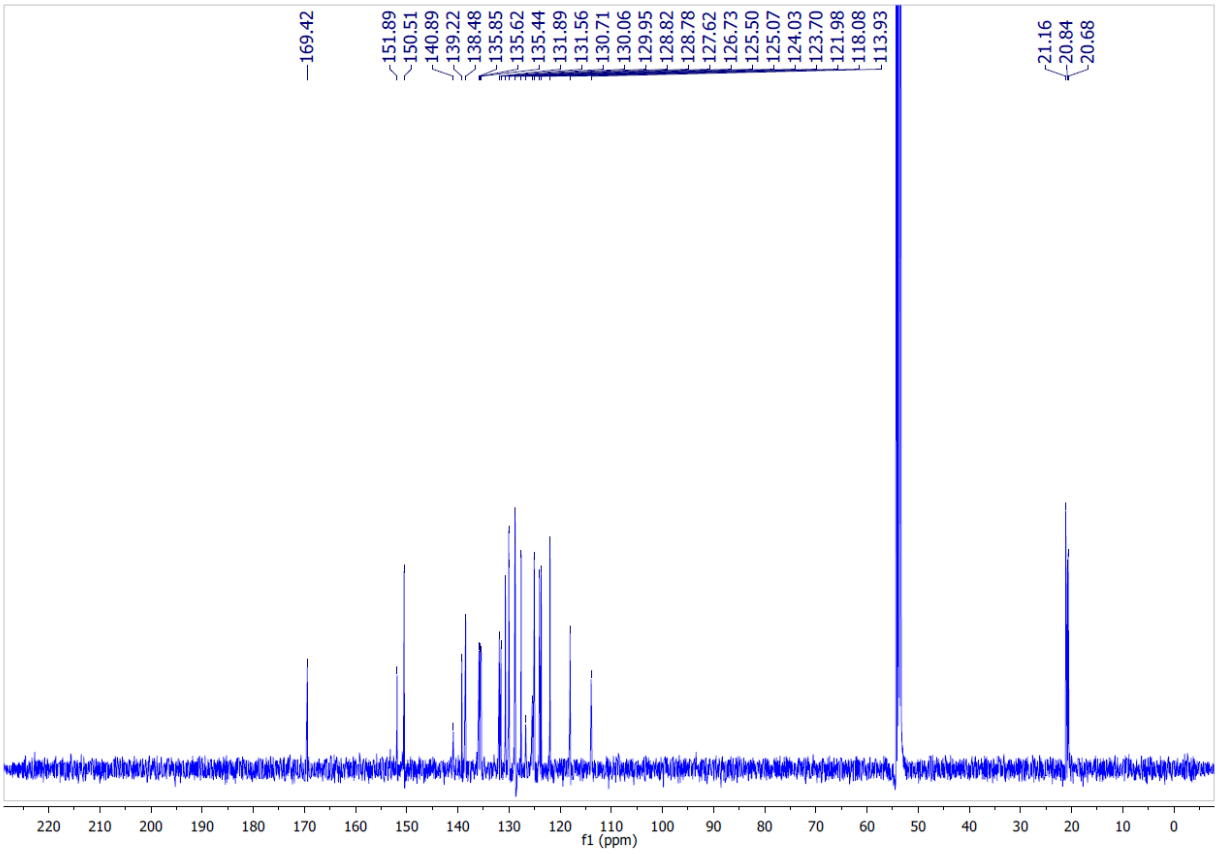
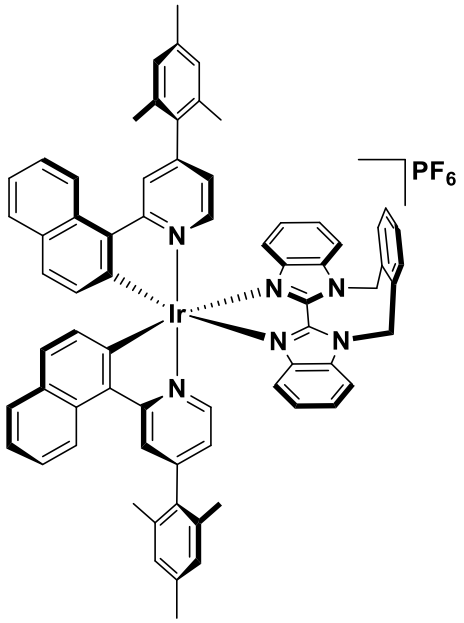


Figure **S14**. ^{13}C NMR spectrum of **Iridium (III) bis[2-(naphthalen-1-yl)-4-(2,4,6-trimethylphenyl)-pyridinato-*N*,*C*$^{2'}$]-*N*,*N*′-(1*H*,1'*H*-2,2'-bibenzimidazole) hexafluorophosphate ([Ir(Mesnpy)$_2$(H$_2$bibenz)](PF$_6$))** in CD_2Cl_2.

Iridium (III) bis[2-(naphthalen-1-yl)-4-(2,4,6-trimethylphenyl)pyridinato-N,C$^{2'}$]-*N,N′*-(1,1'-(a,a'-*o*-xylyl)-2,2-bibenzimidazole)hexafluorophosphate: [Ir(Mesnpy)$_2$(*o*-Xylbibenz)](PF$_6$).



Orange solid. **Yield**: 36%. **Mp:** 337 – 340 °C (decomp.). **R$_f$:** 0.57 (DCM/MeOH 9:1 on silica). **^{1}H NMR (500 MHz, DMSO-*d*$_6$, 372 K) δ (ppm):** 8.36 (dd, *J* = 8.6, 3.7 Hz, 4H), 8.16 (d, *J* = 1.8 Hz, 2H), 7.86 (d, *J* = 8.0 Hz, 2H), 7.77 – 7.70 (m, 4H), 7.53 (t, *J* = 8.5 Hz, 2H), 7.50 – 7.35 (m, 8H), 6.99 (s, 4H), 6.86 – 6.77 (m, 4H), 6.50 (d, *J* = 8.4 Hz, 2H), 6.26 (s, 4H), 6.06 (d, *J* = 8.4 Hz, 2H), 2.30 (s, 6H), 1.94 (br s, 12H). **^{13}C {^{1}H} NMR (126 MHz, CD_2Cl_2) δ (ppm):** 169.2, 153.9, 151.8, 150.5, 144.9, 140.4, 139.0, 138.5, 136.1, 135.8, 135.5, 135.4, 134.5, 131.9, 131.5, 131.4, 131.3, 130.5, 130.0, 128.8, 128.8, 127.7, 127.1, 125.9, 125.2, 124.1, 123.7, 121.9, 118.9, 111.6, 47.5, 21.2, 20.7, 20.7. **HR-MS (FTMS$^+$): [M – PF$_6$]$^+$ Calculated:** ($C_{70}H_{56}IrN_6$) 1173.4196; **Found:** 1173.4182. **Anal.** Calcd for $C_{70}H_{56}F_6IrN_6P$ (MW 1318.44): C, 63.77; H, 4.28; N, 6.37. Found: C, 63.55; H, 4.40; N, 6.25 (average of two runs).

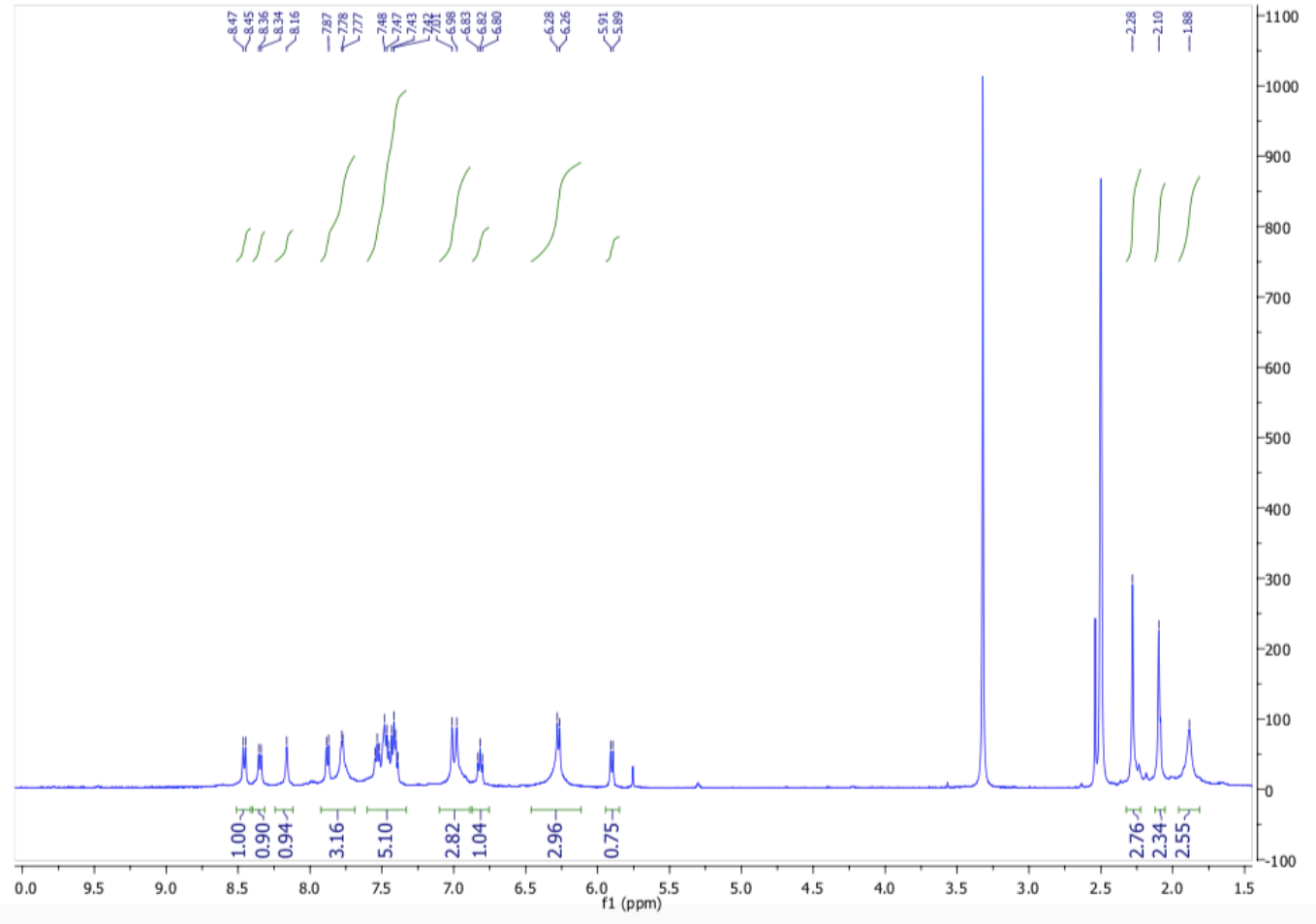


Figure **S15**. ^{1}H NMR spectrum of **Iridium (III) bis[2-(naphthalen-1-yl)-4-(2,4,6-trimethylphenyl)pyridinato-N,C$^{2'}$]-*N,N'*-(1,1'-(a,a'-*o*-xylyl)-2,2-bibenzimidazole) hexafluorophosphate: [Ir(Mesnpy)$_2$(*o*-Xylbibenz)](PF$_6$).** in DMSO-d_6.

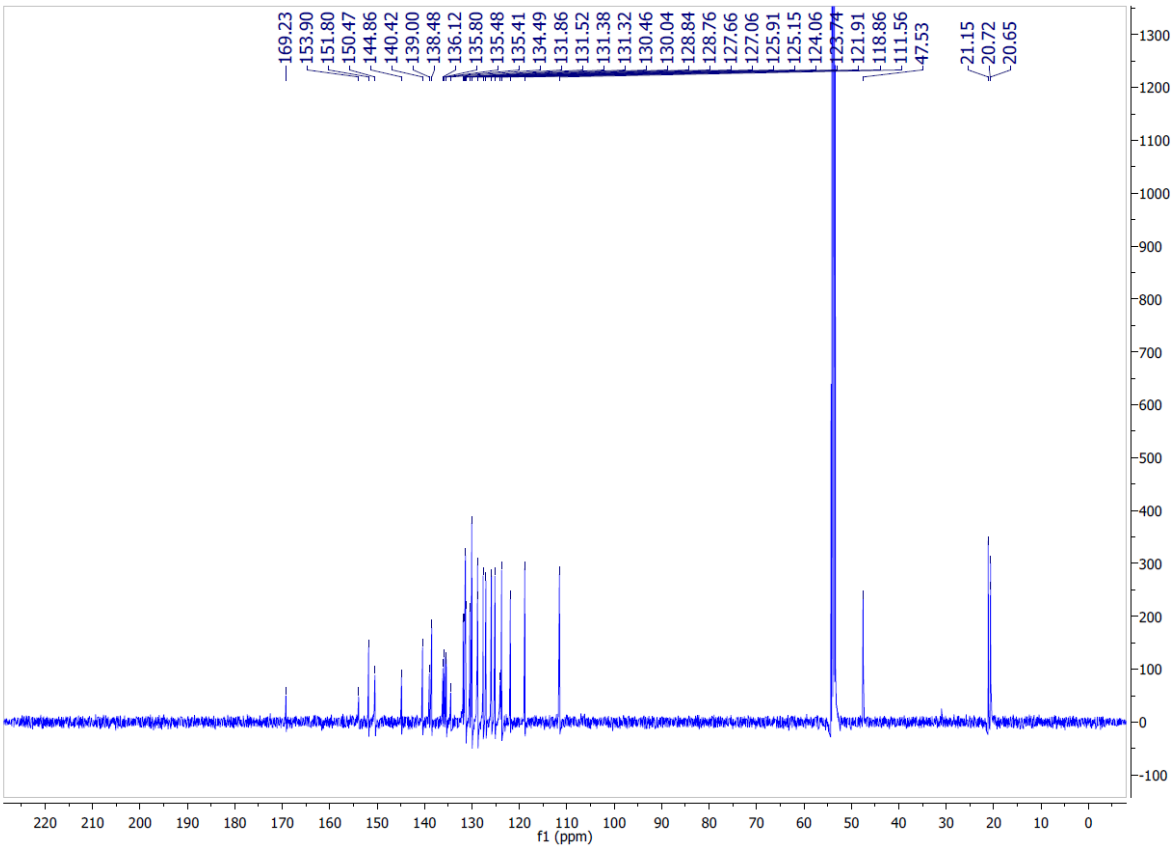


Figure **S16**. ^{13}C NMR spectrum of **Iridium (III) bis[2-(naphthalen-1-yl)-4-(2,4,6-trimethylphenyl)pyridinato-N,C$^{2'}$]-*N,N'*-(1,1'-(a,a'-*o*-xylyl)-2,2-bibenzimidazole) hexafluorophosphate: [Ir(Mesnpy)$_2$(*o*-Xylbibenz)](PF$_6$).** in CD_2Cl_2.

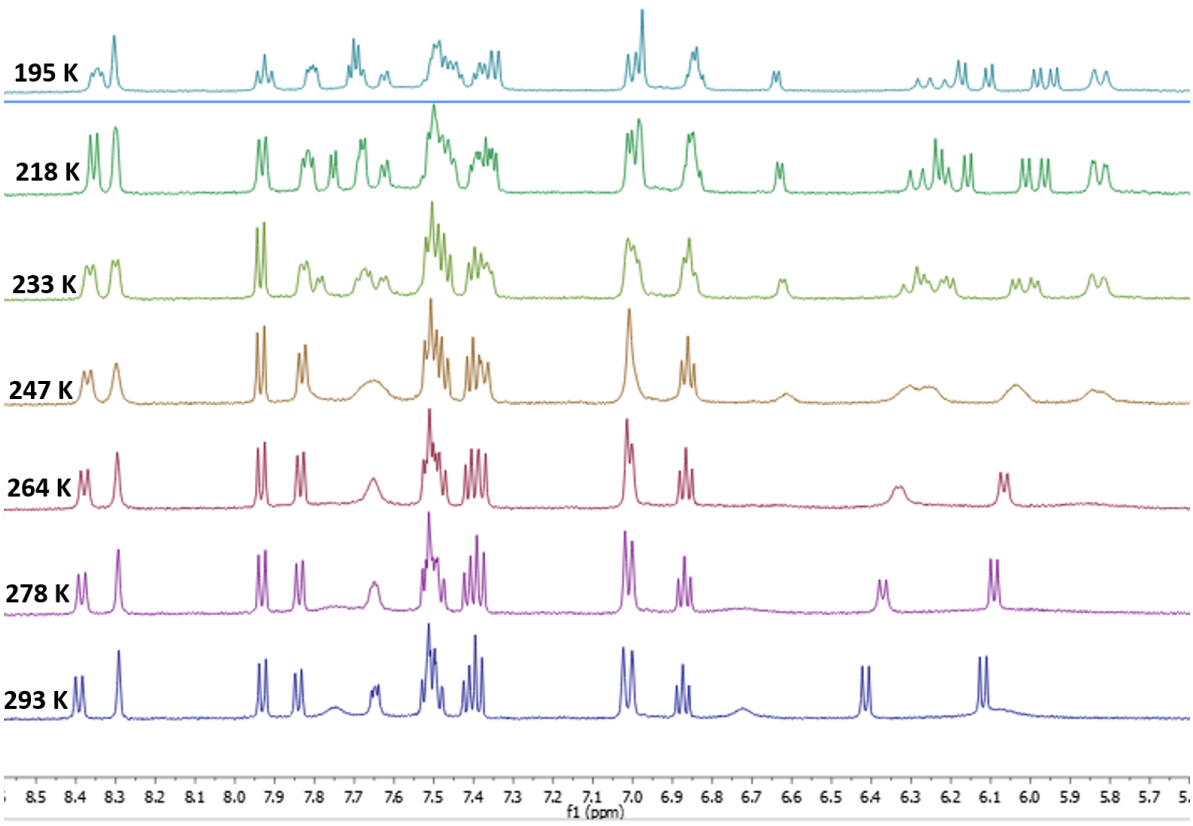
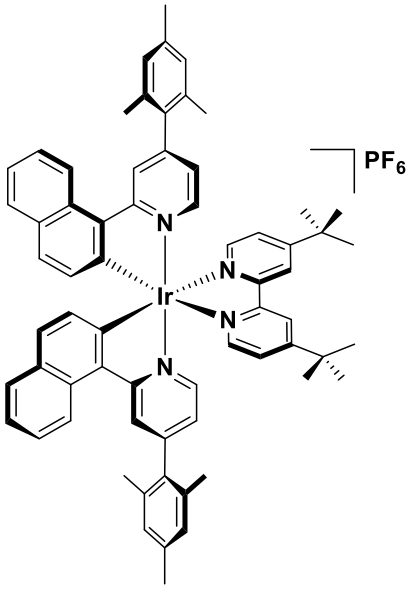


Figure **S17**. ^{1}H NMR temperature study of **Iridium (III) bis[2-(naphthalen-1-yl)-4-(2,4,6-trimethylphenyl)pyridinato-N,C$^{2'}$]-*N,N'*-(1,1'-(a,a'-*o*-xylyl)-2,2-bibenzimidazole) hexafluorophosphate: [Ir(Mesnpy)$_2$(*o*-Xylbibenz)](PF$_6$)** in CD_2Cl_2.

Iridium (III) bis[2-(naphthalen-1-yl)-4-(2,4,6-trimethylphenyl)-pyridinato-*N*,$C^{2'}$]-*N*,*N*′-(4,4'-di-*tert*-butyl-2,2'-bipyridine)hexafluorophosphate: Ir(Mesnpy)$_2$(dtbubpy)](PF$_6$).



Red solid. **Yield**: 62%. **Mp:** 372 – 374 °C (decomp.). **R$_f$:** 0.30 (DCM/MeOH 9:1 on silica). **^{1}H NMR (500 MHz, CD_2Cl_2) δ (ppm):** 8.45 (d, *J* = 8.7 Hz, 2H), 8.36 (dd, *J* = 7.4, 1.8 Hz, 4H), 7.88 (d, *J* = 5.9 Hz, 2H), 7.78 (dd, *J* = 8.1, 1.4, 2H), 7.72 (d, *J* = 5.8 Hz, 2H), 7.5 (ddd, *J* = 8.5, 6.8, 1.5 Hz, 2H), 7.42 (dd, *J* = 5.9 1.9 Hz, 2H), 7.38 (ddd, *J* = 8.0, 6.9, 1.0 Hz, 2H), 7.35 (d, *J* = 8.4 Hz, 2H), 7.03 (d, *J* = 9.0 Hz, 4H), 6.88 (dd, *J* = 5.9, 1.8 Hz, 2H), 6.39 (d, *J* = 8.3 Hz, 1H), 2.35 (s, 6H), 2.19 (s, 6H), 2.06 (s, 6H). **^{13}C {^{1}H} NMR (126 MHz, CD_2Cl_2) δ (ppm):** 168.9, 164.5, 155.9, 155.7, 155.3, 150.7, 149.4, 138.5, 137.7, 135.4, 135.2, 135.1, 131.8, 131.6, 130.5, 130.0, 129.9, 128.8, 128.7, 127.6, 125.8, 125.4, 124.0, 123.8, 121.7, 121.2, 35.8, 30.2, 21.0, 20.5. **HR-MS (FTMS$^+$): [M – PF$_6$]$^+$ Calculated:** ($C_{66}H_{64}IrN_4$) 1105.4760; **Found:** 1105.4743. **Anal.** Calcd for $C_{66}H_{64}F_6IrN_4P$ (MW 1250.45): C, 63.40; H, 5.16; N, 4.48. Found: C, 63.05; H, 5.19; N, 4.51 (average of two runs).

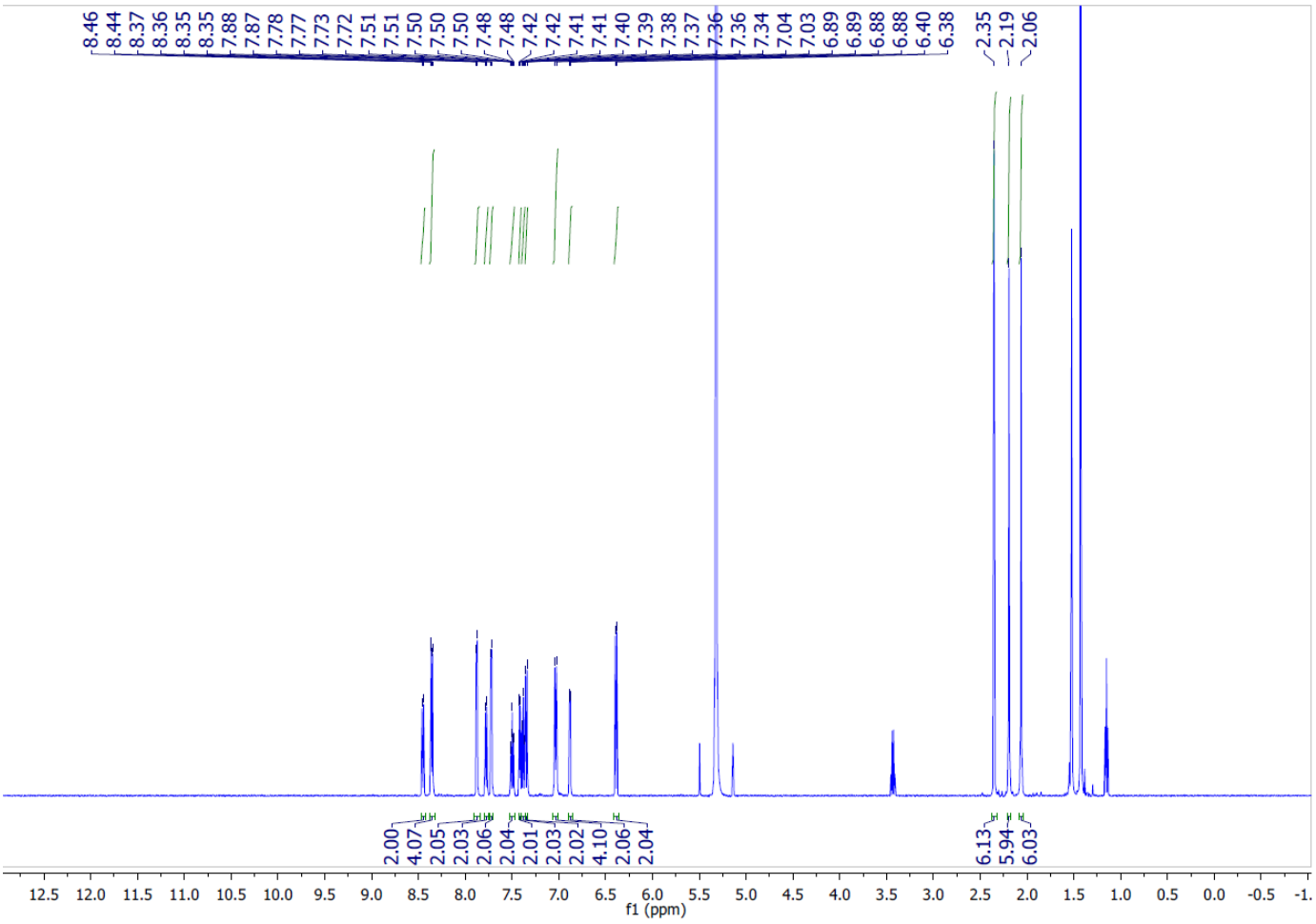


Figure **S18**. ^{1}H NMR spectrum of **Iridium (III) bis[2-(naphthalen-1-yl)-4-(2,4,6-trimethylphenyl)-pyridinato-*N*,*C*$^{2'}$]-*N*,*N*'-(4,4'-di-*tert*-butyl-2,2'-bipyridine) hexafluorophosphate (Ir(Mesnpy)$_2$(dtbubpy)](PF$_6$))** in CD_2Cl_2.

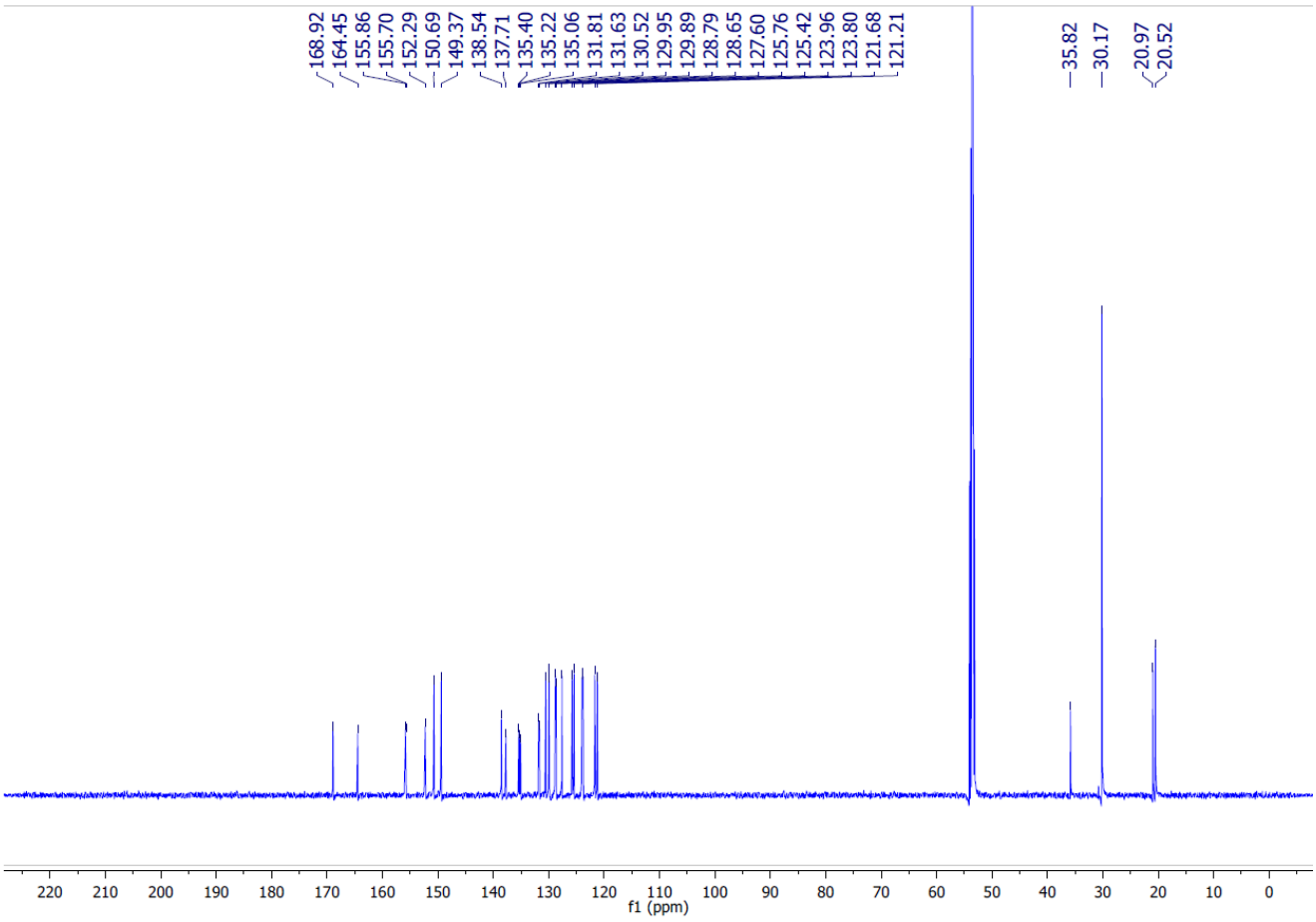
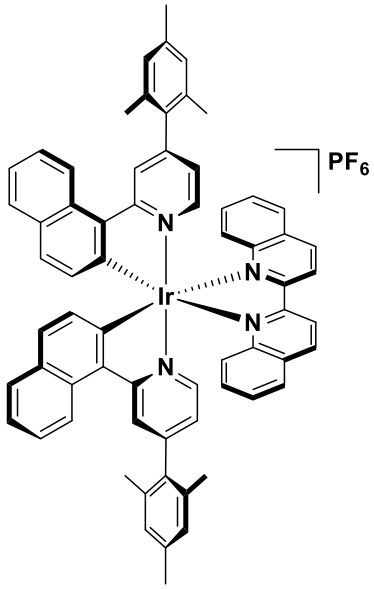


Figure **S19**. ^{13}C NMR spectrum of **Iridium (III) bis[2-(naphthalen-1-yl)-4-(2,4,6-trimethylphenyl)-pyridinato-*N*,*C*$^{2'}$]-*N*,*N*′-(4,4'-di-*tert*-butyl-2,2'-bipyridine) hexafluorophosphate (Ir(Mesnpy)$_2$(dtbubpy)](PF$_6$))** in CD_2Cl_2.

Iridium (III) bis[2-(naphthalen-1-yl)-4-(2,4,6-trimethylphenyl)-pyridinato-*N*,$C^{2'}$]-*N*,*N*′-(2,2'-biquinoline)hexafluorophosphate: Ir(Mesnpy)$_2$(biq)](PF$_6$).



Brick red solid. **Yield**: 37%. **Mp:** 231 – 232 °C (decomp.). **R$_f$:** 0.37 (DCM/MeOH 9:1 on silica). **^{1}H NMR (500 MHz, CD$_2$Cl$_2$) δ (ppm):** 8.76 – 8.69 (m, 4H), 8.28 (d, *J* = 8.6 Hz, 2H), 8.22 (d, *J* = 1.7 Hz, 2H), 7.98 – 7.86 (m, 6H), 7.75 (dd, *J* = 8.1, 1.4 Hz, 2H), 7.44 (t, *J* = 7.0 Hz, 4H), 7.38 – 7.31 (m, 4H), 7.02 – 6.90 (m, 6H), 6.72 (dd, *J* = 5.9, 1.7 Hz, 2H), 6.63 (d, *J* = 8.4 Hz, 4H), 2.31 (s, 6H), 2.19 (s, 6H), 1.75 (s, 6H). **^{13}C {^{1}H} NMR (126 MHz, CD$_2$Cl$_2$) δ (ppm):** 168.6, 160.0, 153.3, 152.5, 150.9, 148.5, 141.8, 138.7, 137.1, 135.4, 135.2, 135.2, 131.9, 131.8, 131.6, 130.7, 130.2, 130.0, 129.9, 129.5, 128.9, 128.9, 128.8, 128.3, 127.8, 125.4, 124.1, 123.1, 122.1, 121.8, 21.2, 20.8, 20.5. **HR-MS (FTMS$^+$): [M – PF$_6$]$^+$ Calculated:** ($C_{66}H_{52}IrN_4$) 1093.3821; **Found:** 1093.3809. **Anal.** Calcd for $C_{66}H_{52}F_6IrN_4P$ (MW 1238.35): C, 64.01; H, 4.23; N, 4.52. Found: C, 63.89; H, 4.13; N, 4.65 (average of two runs).

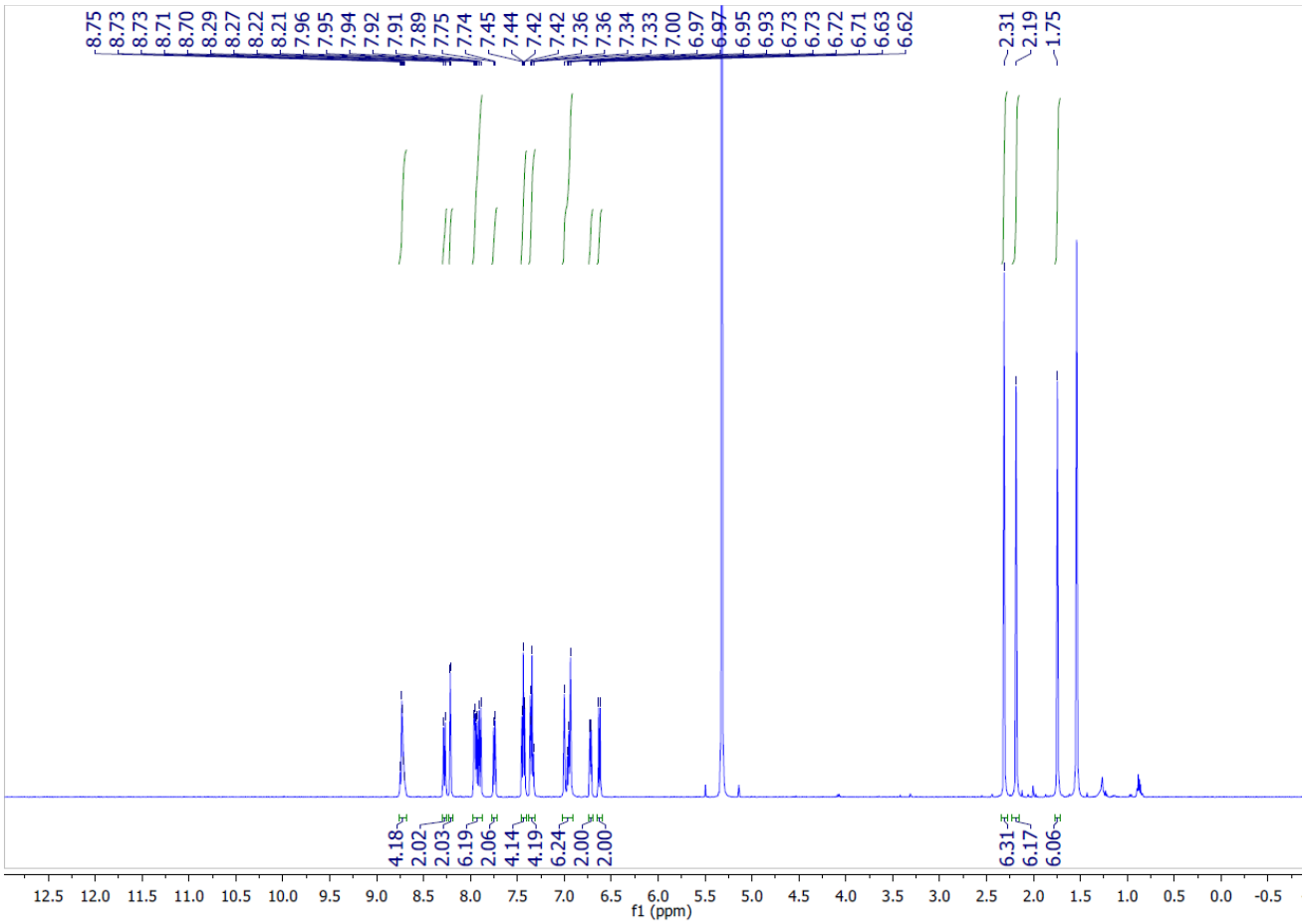


Figure **S20**. ^{1}H NMR spectrum of **Iridium (III) bis[2-(naphthalen-1-yl)-4-(2,4,6-trimethylphenyl)-pyridinato-*N*,*C*$^{2'}$]-*N*,*N*′-(2,2'-biquinoline) hexafluorophosphate (Ir(Mesnpy)$_2$(biq)](PF$_6$))** in CD_2Cl_2.

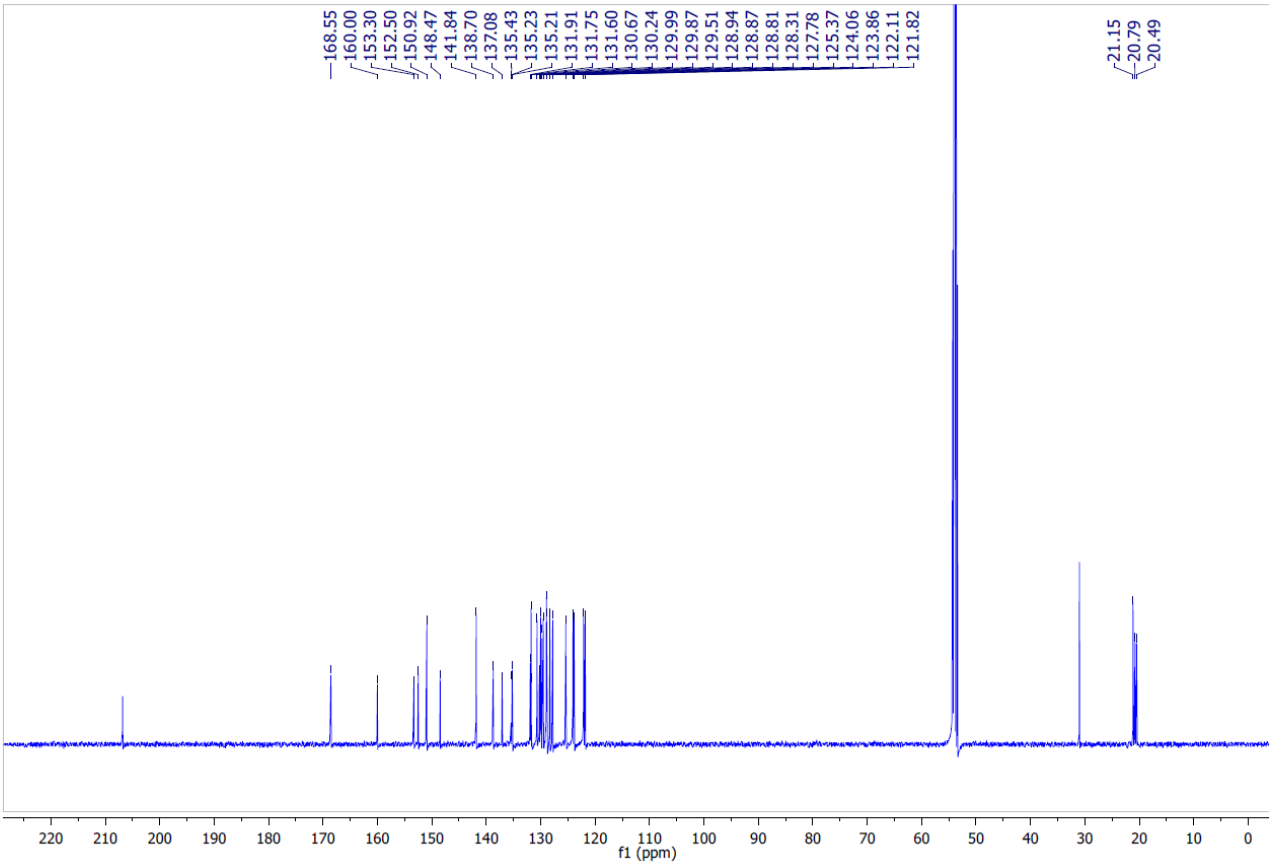


Figure **S21**. ^{13}C NMR spectrum of **Iridium (III) bis[2-(naphthalen-1-yl)-4-(2,4,6-trimethylphenyl)-pyridinato-*N*,*C*$^{2'}$]-*N*,*N*′-(2,2'-biquinoline) hexafluorophosphate (Ir(Mesnpy)$_2$(biq)](PF$_6$))** in CD_2Cl_2.

Photophysical measurements. All samples were prepared in HPLC grade acetonitrile (MeCN) with varying concentrations on the order of μM. Absorption spectra were recorded at RT using a Shimadzu UV-1800 double beam spectrophotometer. Molar absorptivity determination was verified by linear least-squares fit of values obtained from at least three independent solutions at varying concentrations ranging from 1.19×10^{-4} to 1.12×10^{-5} M.

The sample solutions for the emission spectra were degassed by vigorous bubbling for 10 minutes. Steady-state emission and time-resolved emission spectra were recorded at 298 K using an Edinburgh Instruments F980 Fluorimeter or a Gilden Photonics Fluorimeter. All samples for steady-state measurements were excited at 420 nm using a xenon lamp while samples for time-resolved measurements were excited at 378 nm using a PDL 800-D pulsed diode laser. Emission quantum yields were determined using the optically dilute method.[7] A stock solution with absorbance of ca. 1.0 was prepared and then four dilutions were prepared with dilution factors of 5, 6.6, 10 and 20 to obtain solutions with absorbances of ca. 0.100, 0.075, 0.050, and 0.025, respectively. The Beer-Lambert law was found to be linear at the concentrations of the solutions. The emission spectra were then measured after the solutions were degassed by nitrogen purging for fifteen minutes per sample prior to spectrum acquisition. For each sample, linearity between absorption and emission intensity was verified through linear regression analysis and additional measurements were acquired until the Pearson regression factor (R^2) for the linear fit of the data set surpassed 0.9. Individual relative quantum yield values were calculated for each solution and the values reported represent the slope value. The equation $\Phi_s = \Phi_r(A_r/A_s)(I_s/I_r)(n_s/n_r)^2$ was used to calculate the relative quantum yield of each of the sample, where Φ_r is the absolute quantum yield of the reference, n is the refractive index of the solvent, A is the absorbance at the excitation

wavelength, and *I* is the integrated area under the corrected emission curve. The subscripts s and r refer to the sample and reference, respectively. A solution of $[Ru(bpy)_3]Cl_2$ in aerated water (Φ_r = 4.0%) was used as the external reference.[8]

Electrochemistry measurements. Cyclic voltammetry (CV) measurements were performed on an Electrochemical Analyzer potentiostat model 600D from CH Instruments. Solutions for cyclic voltammetry were prepared in MeCN and degassed with MeCN-saturated nitrogen bubbling for about 10 min prior to scanning. Tetra(*n*-butyl)ammoniumhexafluorophosphate ($TBAPF_6$; ca. 0.1 M in MeCN) was used as the supporting electrolyte. An Ag/Ag^+ electrode (silver wire in a solution of 0.1 M KCl in H_2O) was used as the pseudo-reference electrode; a Pt electrode was used as the counter electrode and a glassy carbon electrode was used for the working electrode. The redox potentials are reported relative to a saturated calomel electrode (SCE) electrode with a ferrocenium/ferrocene (Fc^+/Fc) redox couple as an internal reference (0.38 V vs SCE).[9]

X-ray crystallography

Single crystals were grown by slow evaporation of a hexane/ethyl acetate solution (Mesnpy), or by vapour diffusion of hexane into concentrated dichloromethane solution (**1**, **3** and **6**), or by vapour diffusion of diethyl ether into concentrated solutions of either THF (**4**) or acetonitrile (**5**). Data were collected at either 173 K (Mesnpy, **1**, **3**, **4** and **6**) or 90 K (**5**) using a Rigaku FR-X Ultrahigh brilliance Microfocus RA generator/confocal optics with Rigaku XtaLAB P200 diffractometer [Mo Kα radiation (λ = 0.71075 Å)]. Intensity data for were collected using ω steps accumulating area detector images spanning at least a hemisphere of reciprocal space. Data for all compounds analysed were collected and processed (including correction for Lorentz, polarization

and absorption) using CrystalClear.[10] Structures were solved by either direct (SIR2011),[11] Patterson (PATTY)[12] or dual-space (SHELXT)[13] methods and refined by full-matrix least-squares against F^2 (SHELXL-2014/7).[14] Non-hydrogen atoms were refined anisotropically, and carbon-bound hydrogen atoms were refined using a riding model. Nitrogen-bound hydrogen atoms in **3** were located from the difference Fourier map and refined subject to a distance restraint; however, the equivalent hydrogens in **1** could not be located, and were refined using a riding model. All calculations were performed using the CrystalStructure interface.[15] Selected crystallographic data are presented in Table **S1**. CCDC 1892241-1892246 contains the supplementary crystallographic data for this paper. The data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/structures.

Table S1. Crystal Data and Structure Refinement.

	Mesnpy	**1**	**3**	**4**	**5**	**6**
empirical formula	$C_{24}H_{21}N$	$C_{54}H_{46}F_6IrN_6P$	$C_{62.5}H_{51}ClF_6IrN_6P$	$C_{78}H_{72}F_6IrN_6O_2P$	$C_{66}H_{64}F_6IrN_4P$	$C_{68}H_{56}Cl_4F_6IrN_4P$
fw	323.44	1116.18	1258.77	1462.65	1250.44	1408.21
crystal description	colourless, prism	yellow, rod	orange, platelet	orange, chip	yellow, prism	red, prism
crystal size [mm^3]	0.15×0.15×0.10	0.18×0.02×0.02	0.09×0.05×0.02	0.05×0.03×0.01	0.16×0.05×0.03	0.22×0.12×0.10
temp [K]	173	173	173	173	93	173
space group	$P\bar{1}$	$P2_1/c$	$P\bar{1}$	$P\bar{1}$	$I2/a$	$P\bar{1}$
a [Å]	8.7072(12)	21.578(3)	12.3645(11)	15.0646(12)	11.0605(19)	15.06730(10)
b [Å]	8.7165(11)	34.277(5)	14.9064(13)	16.5639(16)	21.638(4)	15.4210(7)
c [Å]	11.9416(17)	17.791(3)	20.2905(16)	16.7149(9)	23.462(4)	16.2666(9)
α [°]	81.214(11)		101.2340(15)	62.602(8)		82.424(8)
β [°]	84.274(12)	108.335(4)	103.1960(15)	72.285(11)	97.585(7)	69.360(7)
γ [°]	80.451(11)		107.5530(14)	83.776(13)		63.442(6)
vol [$Å^3$]	880.7(2)	12491(3)	3328.5(5)	3525.0(6)	5565.8(16)	3162.3(3)
Z	2	8	2	2	4	2
ρ (calc) [g/cm^3]	1.220	1.187	1.256	1.378	1.492	1.479
μ [mm^{-1}]	0.070	2.221	2.130	1.988	2.500	2.373
F(000)	344	4464	1262	1488	2536	1412
reflns collected	13987	223017	54379	43181	36107	76370
independent reflns (R_{int})	3204 (0.0448)	22888 (0.1966)	12073 (0.0328)	12798 (0.0847)	5029 (0.0562)	11594 (0.0529)
data/restraints/params	3204/0/229	22888/333/1274	12073/13/726	12798/35/853	5029/0/360	11594/30/782
GOF on F^2	1.025	1.098	1.166	1.070	1.097	1.103
R_1 [$I > 2\sigma(I)$]	0.0426	0.1169	0.0353	0.0753	0.0224	0.0432
wR_2 (all data)	0.1253	0.3398	0.1068	0.2075	0.0659	0.1252
largest diff. peak/hole [$e/Å^3$]	0.21/-0.24	3.22/-3.09	1.57/-0.47	2.62/-0.67	1.28/-0/65	2.83/-1.66

DFT and TD-DFT calculations

Geometries were optimised at the PBE0 level[16] of density functional theory, employing the Stuttgart-Dresden relativistically adjusted pseudopotential along with its associated 6s5p3d valence basis for Ir[17] and 6-31G* basis[18] for all other atoms. Where available, the structures found in the solid were used as starting points for the optimizations (without counterions or co-crystallates). Harmonic vibrational frequencies were evaluated to ensure that all stationary points correspond to true minima. This level has performed well for the description of structures of 5d-metal complexes.[19] Single point energy calculations were performed on these optimized structures using the B3LYP/6-31G* functional and basis set,[20] the double-ζ quality SBKJC VDZ ECP basis set[21] with an effective core potential for the Ir(III) ion. In these energy calculations, bulk solvation effects have been included through a polarisable continuum model (PCM) in the integral equation formalism,[22] employing the parameters of acetonitrile. Energy calculations were performed for the lowest singlet and triplet states, as well as for the doublet states resulting from adding or removing an electron (doublets and triplets were described using the unrestricted Kohn-Sham formalism, which showed negligible spin contamination). Absorption spectra were modeled in the polarizable continuum using time-dependent DFT (TD-B3LYP),[23] solving for the lowest 60 states (each singlet and triplet, i.e. 120 in total). In our previous work this level has proven suitable for describing electronic excitations in related Ir complexes.[24] All computations were performed using the Gaussian 09 program.[25]

Table S2. HOMO and LUMO energies (ε), as well as negative vertical ionization potentials (IP) and electron affinities (EA) [in eV] of the complexes of this study (B3LYP/PCM(acetonitrile) level on PBE0 optimized structures).

Complex	ε^{LUMO}	-EA	ε^{HOMO}	-IP
1	-2.27	-2.36	-5.58	-5.45
2	-2.31	-2.41	-5.59	-5.46
3	-2.28	-2.38	-5.39	-5.27
4	-2.32	-2.43	-5.40	-5.27
5	-2.23	-2.30	-5.43	-5.29
6	-2.82	-2.94	-5.52	-5.39

Table S3: HOMO-LUMO gaps ΔE_{H-L}, vertical singlet-triplet splittings ΔE_{S-T}, key absorptions from TD-B3LYP computations, along with oscillator strengths *f*,[a] as well as vertical singlet-triplet splittings ΔE_{T-S} for the triplet state.

Comp	ΔE_{H-L} [eV]	ΔE_{S-T} [eV]	ΔE_{exc} [eV]	ΔE_{exc} [nm] calc	*(expt)*	Excitation[b]	*f*	ΔE_{T-S}[c] [eV/ (nm)]
1	3.31	2.70	2.56	482	*(479)*	H→L (T)	0.0	2.06/ (602)
			2.63	471	*(449)*	H→L	0.0005	
			2.7-2.9	461-422[d]	*(431)*	(T)[d]	0.0	
			3.15	394	*(402)*	H→L+1	0.084	
			3.71	334	*(361)*	H-6→L	0.180	
			3.85	324	*(340)*	H-9→L	0.373	
			3.88	319	*(322)*	H-2→L+2	0.220	
			4.56	272	*(282)*	H-2→L+4	0.420	
			4.74	262	*(263)*	H-11→L+1	0.166	
2	3.29	2.64	2.52	493	*(517)*	H→L; H-1→L (T)	0.0	2.05/ (605)
			2.60	476	*(471)*	H→L	0.0006	
			2.6-3.1	469-398[d]	*(442, 425)*	(T)[d]	0.0	
			3.16	392	*(386)*	H→L+1	0.071	
			3.65	340	*(352)*	H-4→L	0.255	
			3.74	332	*(335)*	H-9→L; H-7→L	0.300	
			4.07	304	*(289)*	H-1→L+3	0.184	
			4.55	273	*(270)*	H-2→L+4; H-3→L+4	0.220	
3	3.11	2.55	2.24	552	*(559)*	H→L+1 (T)	0.0	1.80/ (689)
			2.51	494	*(517)*	H→L	0.003	
			2.3-2.7	548-467[d]	*(463)*	(T)[d]	0.0	
			2.90	428	*(436)*	H→L+1	0.140	
			3.41	363	*(361)*	H-4→L	0.104	
			3.73	332		H-4→L+2	0.234	
			3.85	322	*(339)*	H-10→L,H-5→L	0.183	
			3.81	326	*(325)*	H-5→L	0.675	
			4.36	284	*(295)*	H→L+6	0.131	
			4.52	274	*(264)*	H-11→L+1;H→L+8	0.243	
4	3.08	2.53	2.25	550	(*556)*	H→L+1 (T)	0.0	1.80/ (689)
			2.48	501	*(519)*	H→L	0.002	
			2.3-2.9	546-431[d]	*(458)*	(T)[d]	0.0	
			2.91	427	*(427)*	H→L+1	0.130	
			3.18	390	*(391)*	H-2→L	0.057	
			3.35	370	*(374)*	H-4→L	0.217	
			3.71	335	*(351)*	H-8→L	0.387	
			3.73	332	*(337)*	H-4→L+2	0.217	
			3.76	330	*(319)*	H-4→L+1,H-3→L+1	0.234	
			4.37	284	*(291)*	H→L+8	0.112	
			4.54	274	*(263)*	H-3→L+4	0.327	

5	3.20	2.58	2.25	551	*(555)*	H→L+1 (T)	0.0	1.75/
			2.3,2.6	545,481[d]	*(517)*	H→L+2.H→L+1 (T)[d]	0.0	(708)
			2.60	478	*(454)*	H→L	0.001	
			2.89	429	*(422)*	H→L+1	0.117	
			3.40	364	*(391)*	H-1→L+2	0.100	
			3.56	348	*(358)*	H-6→L	0.116	
			3.69	336	*(339)*	H-2→L+5	0.133	
			3.89	319	*(310)*	H-6→L+3,H-5→L	0.100	
			4.21	294	*(294)*	H-3→L+3	0.065	
			4.42	281	*(285)*	H-7→L+3	0.131	
			4.59	270		H→L+11	0.184	
			4.65	267	*(266)*	H-6→L+4	0.478	
6	2.70	2.15	2.06	602		H→L (T)	0.0	1.68/
			2.11	588	(539)	H→L	0.010	(738)
			2.2-2.9	554-430[d]	(443)	(T)[d]	0.0	
			2.92	424	(420)	H→L+1	0.067	
			3.31	374	(370)	H-1→L+2	0.081	
			3.66	338	(354)	H-11→L	0.217	
			3.74	331	(294)	H-4→L+2; H-2→L+2	0.224	
			4.44	279	(265)	H-3→L+5; H→L+10	0.203	

[a]Unless otherwise noted, single point calculations on the ground-state singlet geometry. [b]Leading MO contributions to the excited state; H and L denote HOMO and LUMO, respectively (T in parentheses denotes singlet-triplet transition). [c]Single point calculation on the triplet-state geometry. [d]Several dark triplet states computed in this area.

Cartesian coordinates of complexes in xyz format (in Å), PBE0/ECP1 optimized

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107
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119
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133
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