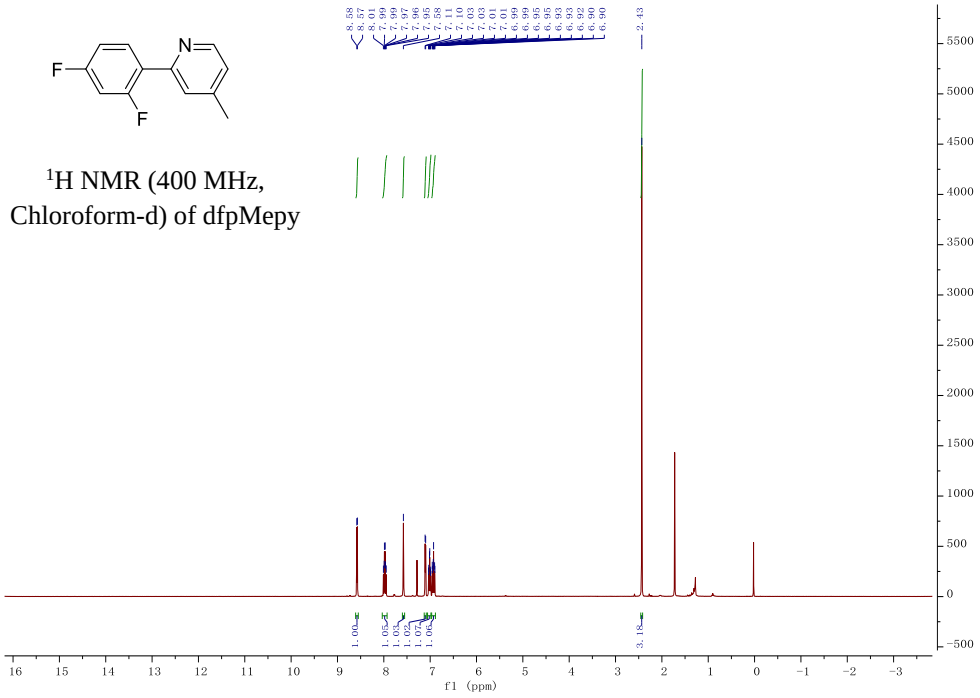
Supplementary Material

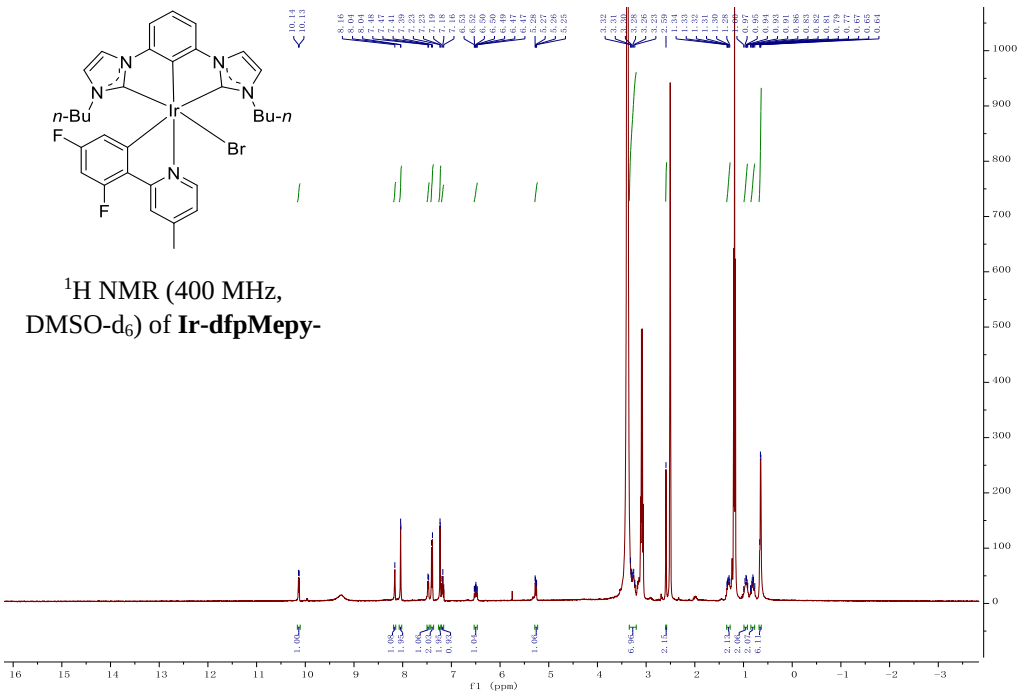
The detailed procedure of measuring absolute quantum efficiency: 0.35 mg **Ir-dfpMepy-CN** was added into a 1ml glass bottle with 500 μl DCM. After the solution is evenly mixed, 100 μl mixed solution was transferred to a 5 ml volumetric flask DCM was then added into the 5 ml volumetric flask to get a 2×10^{-5} mol/L **Ir-dfpMepy-CN** solution. A cuvette with 2×10^{-5} mol/L **Ir-dfpMepy-CN** solution and reference cuvette are prepared for the quantum efficiency test by the absolute PL quantum yield spectrometer C11345 (Quantum-QY Hamamastu).

1 Supplementary Figures and Tables



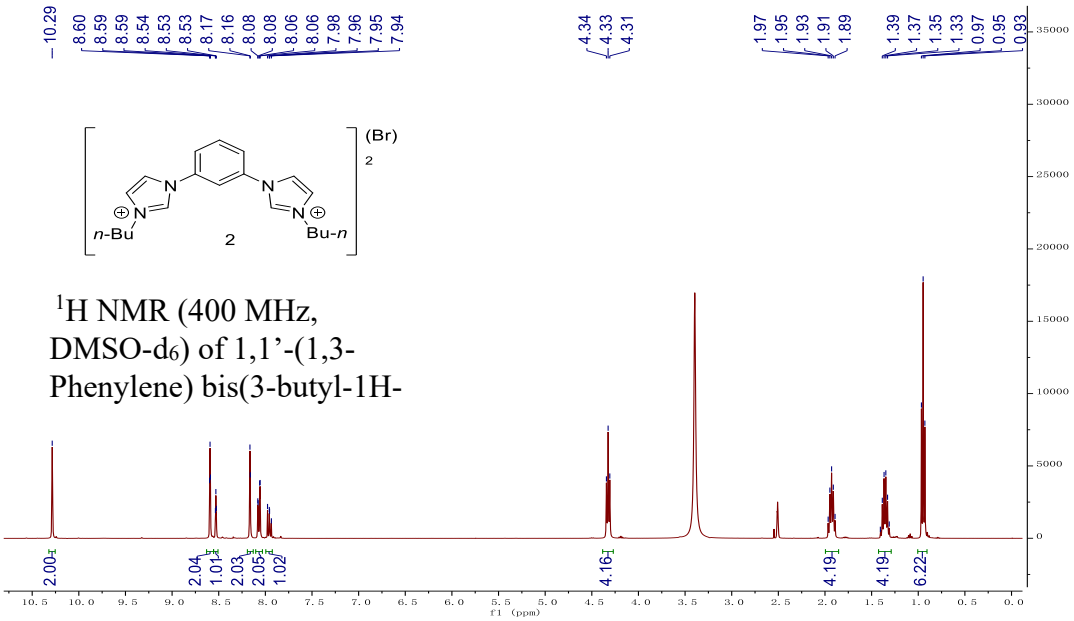
^{1}H NMR (400 MHz, Chloroform-d) of dfpMepy

Supplementary figure 1. ^{1}H NMR of 2-(2,4-difluorophenyl)-4-methylpyridine(dfpMepy) in $CDCl_3$.



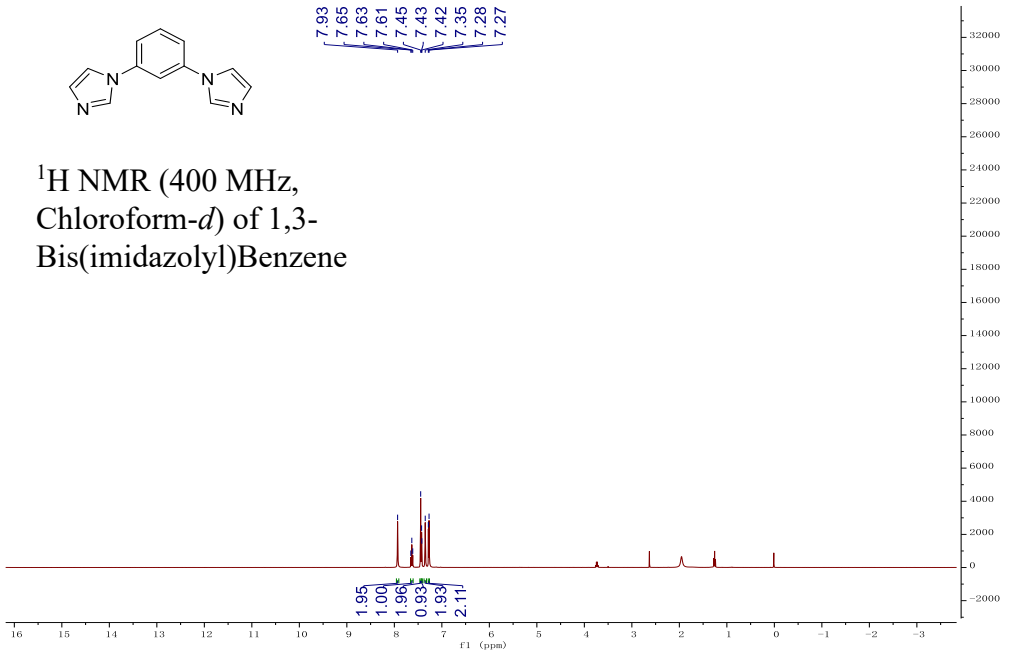
^{1}H NMR (400 MHz, DMSO-d$_6$) of **Ir-dfpMepy-Br**

Supplementary figure 2. ^{1}H NMR of **Ir-dfpMepy-Br** in DMSO-d$_6$.



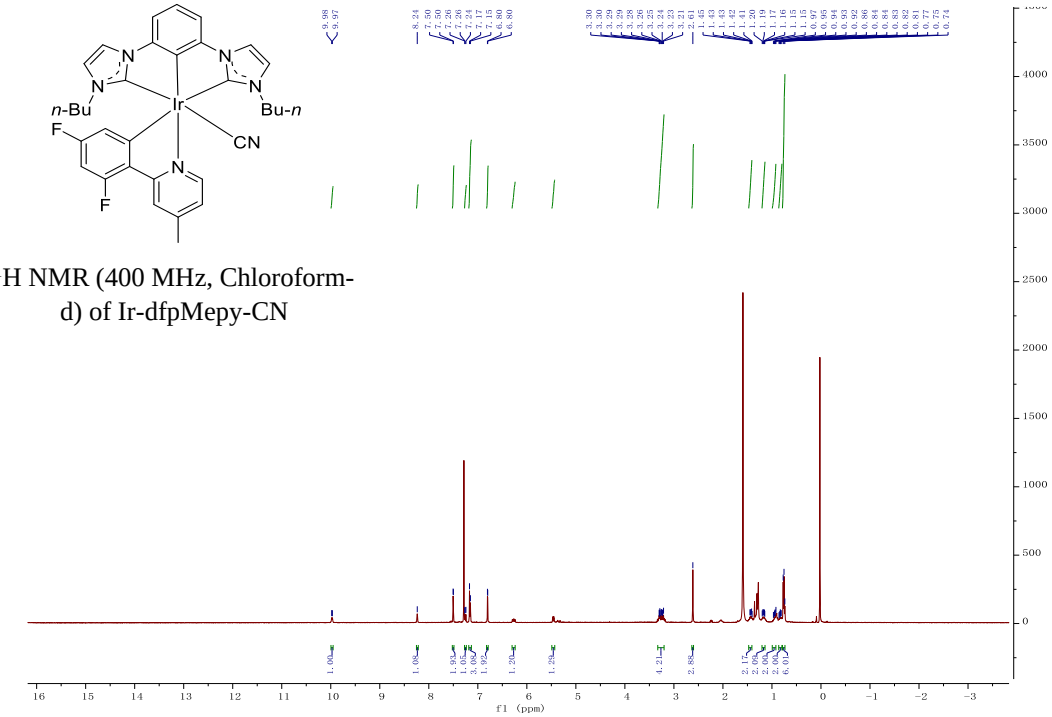
^{1}H NMR (400 MHz, DMSO-d$_6$) of 1,1'-(1,3-Phenylene) bis(3-butyl-1H-

Supplementary figure 3. ^{1}H NMR of 1,1'-(1,3-Phenylene) bis(3-butyl-1H-imidazolium) Bromide in DMSO-d$_6$.



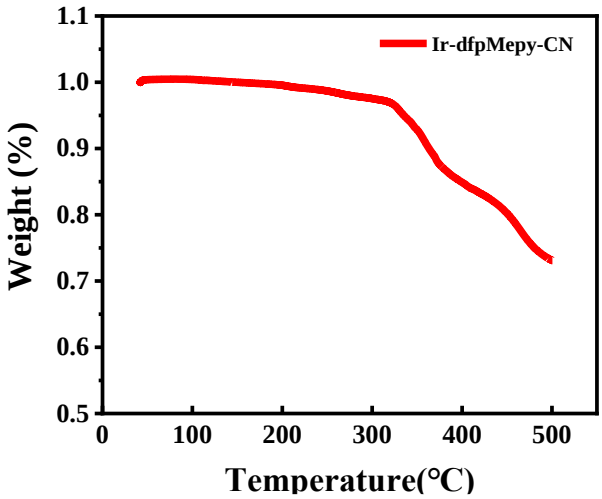
^{1}H NMR (400 MHz, Chloroform-*d*) of 1,3-Bis(imidazolyl)Benzene

Supplementary figure 4. ^{1}H NMR of 1,3-Bis(imidazolyl)Benzene in $CDCl_3$.

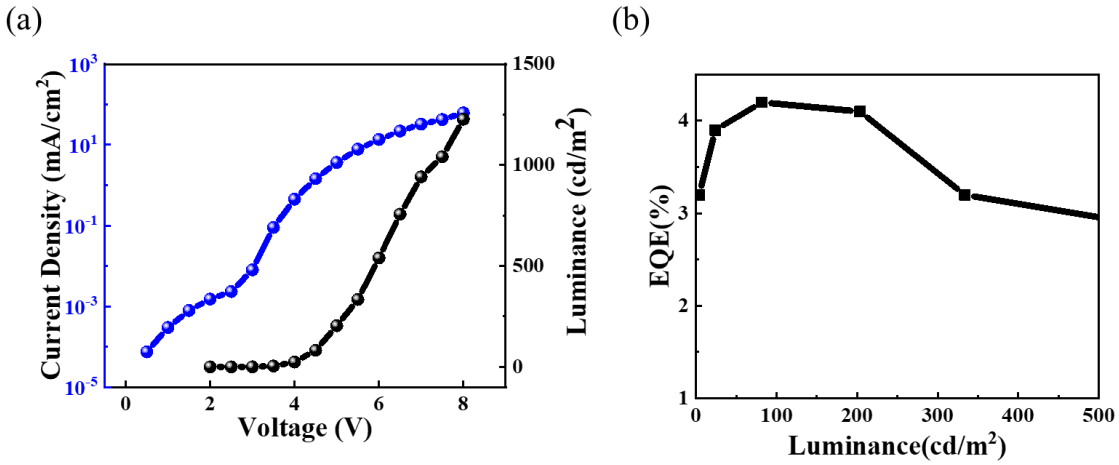


^{1}H NMR (400 MHz, Chloroform-d) of Ir-dfpMepy-CN

Supplementary figure 5. ^{1}H NMR of **Ir-dfpMepy-CN** in $CDCl_3$.



Supplementary figure 6. Thermogravimetric analysis of the **Ir-dfMeppy-CN.**

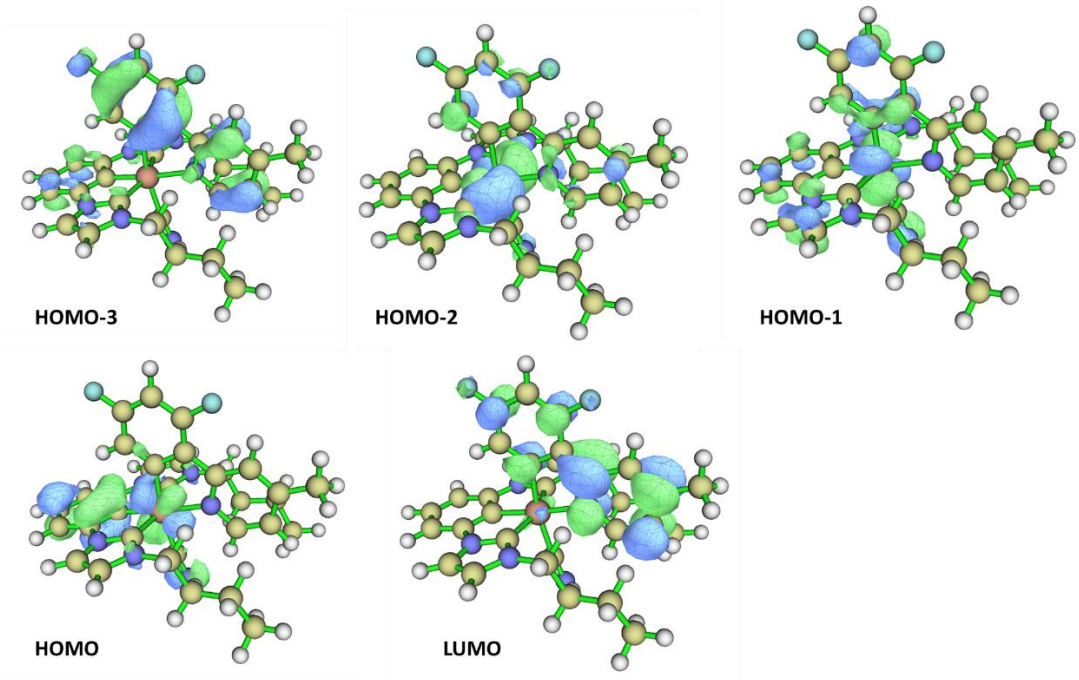


Supplementary figure 7. (a) J-Vand L-V curves and (b) External quantum efficiency of the device.

2 TD-DFT simulation results

Table S1 The calculated wavelength and charge transfer character of the optical transitions

	State	Energy(eV)	λ (nm)	Assignments
1	T1	2.8695	432	HOMO-3→LUMO 44.6% (LLCT & LC) HOMO-2 → LUMO 12.5% (MLCT) HOMO-1 → LUMO 21.8% (MLCT &LC)



Supplementary figure 8. The frontier molecular orbitals calculated at T_1 geometries.