Electronic Supplementary Information

Functionalized phenylimidazole-based *facial*-homoleptic iridium(III) complexes and their excellent performance in blue phosphorescent organic light-emitting diodes

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Table S1 Crystallographic data and parameters for **FIr** and **CNIr**

Compound	**FIr**·(*n*-hexane)	**CNIr**
Formula	$C_{69}H_{80}F_3IrN_6$	$C_{66}H_{66}IrN_9$
Fomula weight	1242.59	1177.47
Crystal system	Monoclinic,	Monoclinic
Space group	*P2(1)/n*	*P2(1)/n*
a (Å)	13.994(3)	14.985(3)
b (Å)	21.759(4)	26.651(5)
c (Å)	23.610(5)	17.246(3)
α (°)	90	90
β (°)	97.437(8)	102.60(3)
γ (°)	90	90
V (Å^3)	7129(2)	6721(2)
Z	4	4
ρ_{calc}(g cm^{-3})	1.158	1.164
μ (mm^{-1})	1.920	2.028
F(000)	2560	2408
T (K)	223(2)	293(2) K 2.068 to 28.356°.
Scan mode	*multi*	*multi*
hkl range	–18 → +18, –29 → +28, –31 → +31	–20→+20, –35→+35, –23→+21
Measd reflns	235130	247154
Unique reflns [R_{int}]	17785 [0.0807]	16757 [0.1033]
Reflns used for refinement	17785	16757
Refined parameters	726	697
R_1[a] (I>2σ(I))	0.0429	0.0463
wR_2[b] all data	0.1081	0.1544
GOF on F^2	1.025	1.021
ρ_{fin} (max/min) (e Å^{-3})	0.683, –0.353	0.810, –0.715

[a] $R_1 = \sum||Fo| - |Fc||/\sum|Fo|$. [b] $wR_2 = \{[\sum w(Fo^2 - Fc^2)^2]/[\sum w(Fo^2)^2]\}^{1/2}$.

Table S2 Selected bond lengths (Å) and angles (°) for **FIr** and **CNIr**

FIr		**CNIr**	
lengths (Å)			
Ir–C1	2.020(3)	Ir–C1	2.017(5)
Ir–C22	2.009(3)	Ir–C22	2.011(5)
Ir–C43	2.017(3)	Ir–C43	2.013(5)
Ir–N1	2.111(3)	Ir–N1	2.125(4)
Ir–N3	2.114(3)	Ir–N3	2.116(4)
Ir–N5	2.108(3)	Ir–N5	2.094(4)
angles (°)			
C1–Ir–C22	94.78(12)	C1–Ir–C22	96.21(18)
C1–Ir–C43	93.87(12)	C1–Ir–C43	95.03(18)
C22–Ir–C43	94.53(13)	C22–Ir–C43	94.64(19)
C1–Ir–N5	171.27(11)	C1–Ir–N5	88.56(17)
C22–Ir–N5	91.40(11)	C22–Ir–N5	172.86(17)
C43–Ir–N5	79.47(11)	C43–Ir–N5	79.61(18)
C1–Ir–N1	79.13(11)	C1–Ir–N1	79.28(17)
C22–Ir–N1	173.26(11)	C22–Ir–N1	94.17(17)
C43–Ir–N1	88.82(12)	C43–Ir–N1	169.98(18)
C1–Ir–N3	93.38(11)	C1–Ir–N3	174.31(18)
C22–Ir–N3	79.14(11)	C22–Ir–N3	79.22(17)
C43–Ir–N3	170.74(11)	C43–Ir–N3	88.76(18)
N1–Ir–N3	98.19(10)	N1–Ir–N3	97.56(16)
N1–Ir–N5	94.96(10)	N1–Ir–N5	91.93(16)
N3–Ir–N5	93.83(10)	N3–Ir–N5	96.31(17)

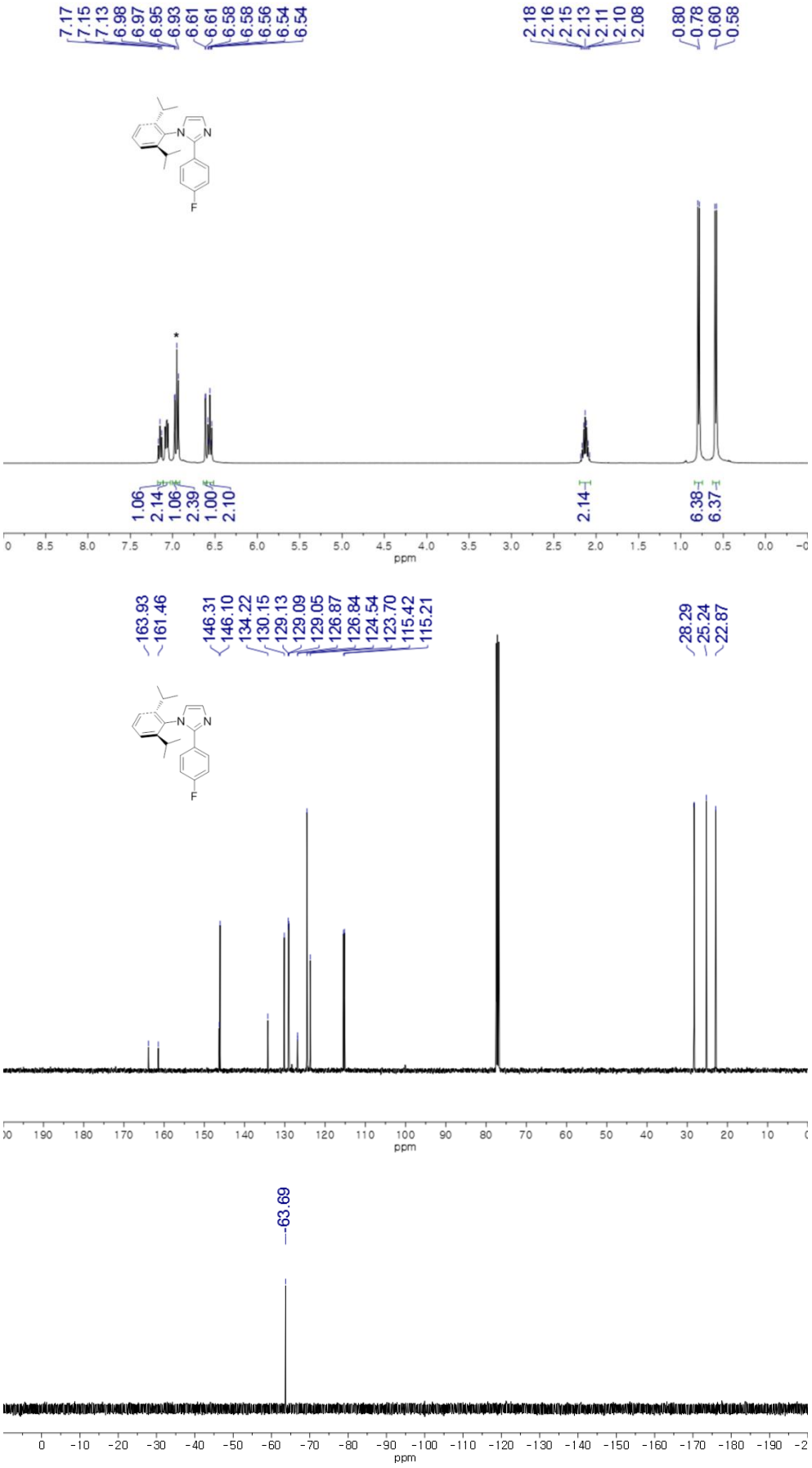

Fig. S1 ^{1}H (top), ^{13}C (middle) and ^{19}F NMR spectrum of **FL** (∗ from residual $CHCl_3$ in $CDCl_3$).

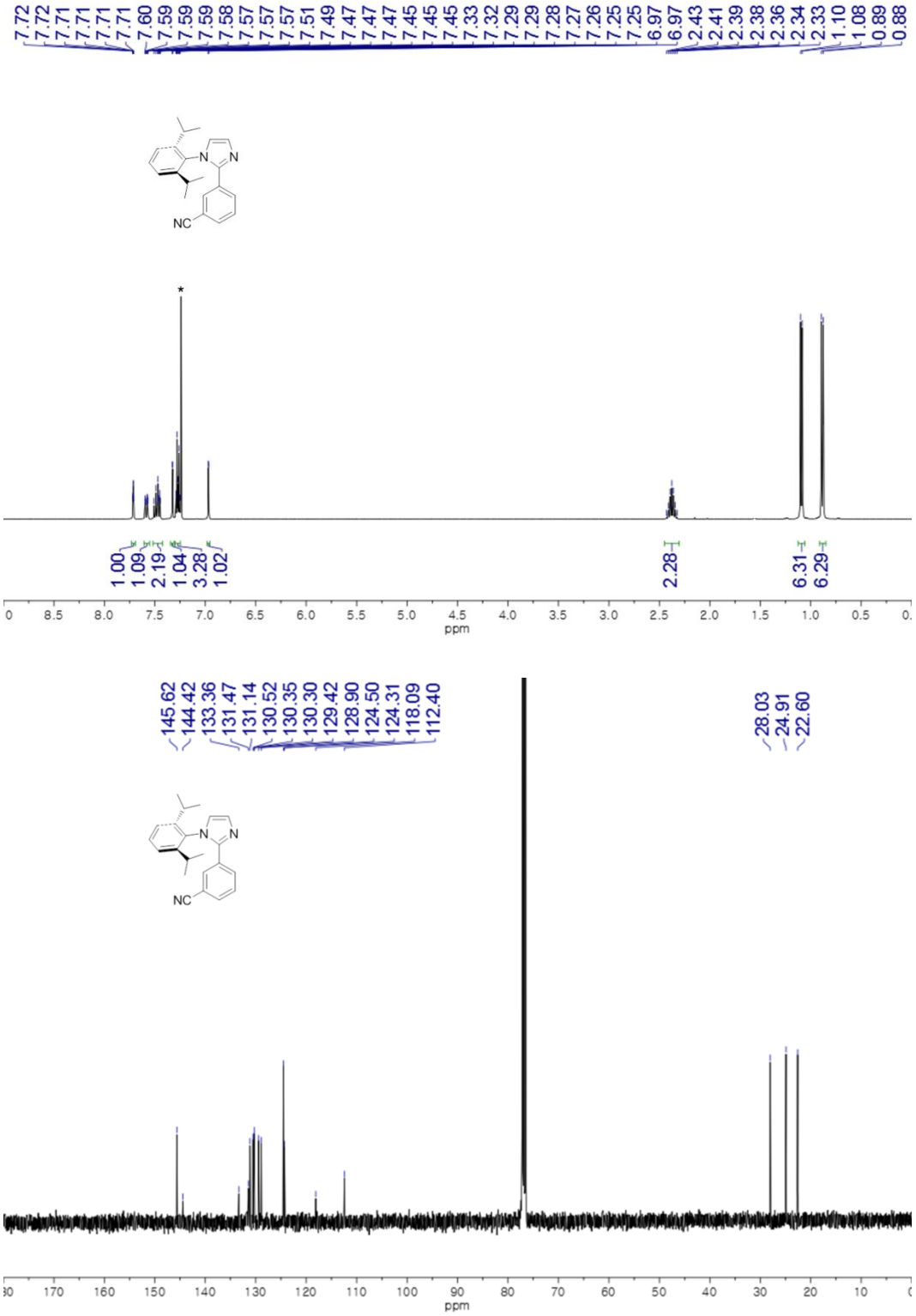

Fig. S2 ^{1}H (top) and ^{13}C (bottom) NMR spectrum of **CNL** (∗ from residual $CHCl_3$ in $CDCl_3$).

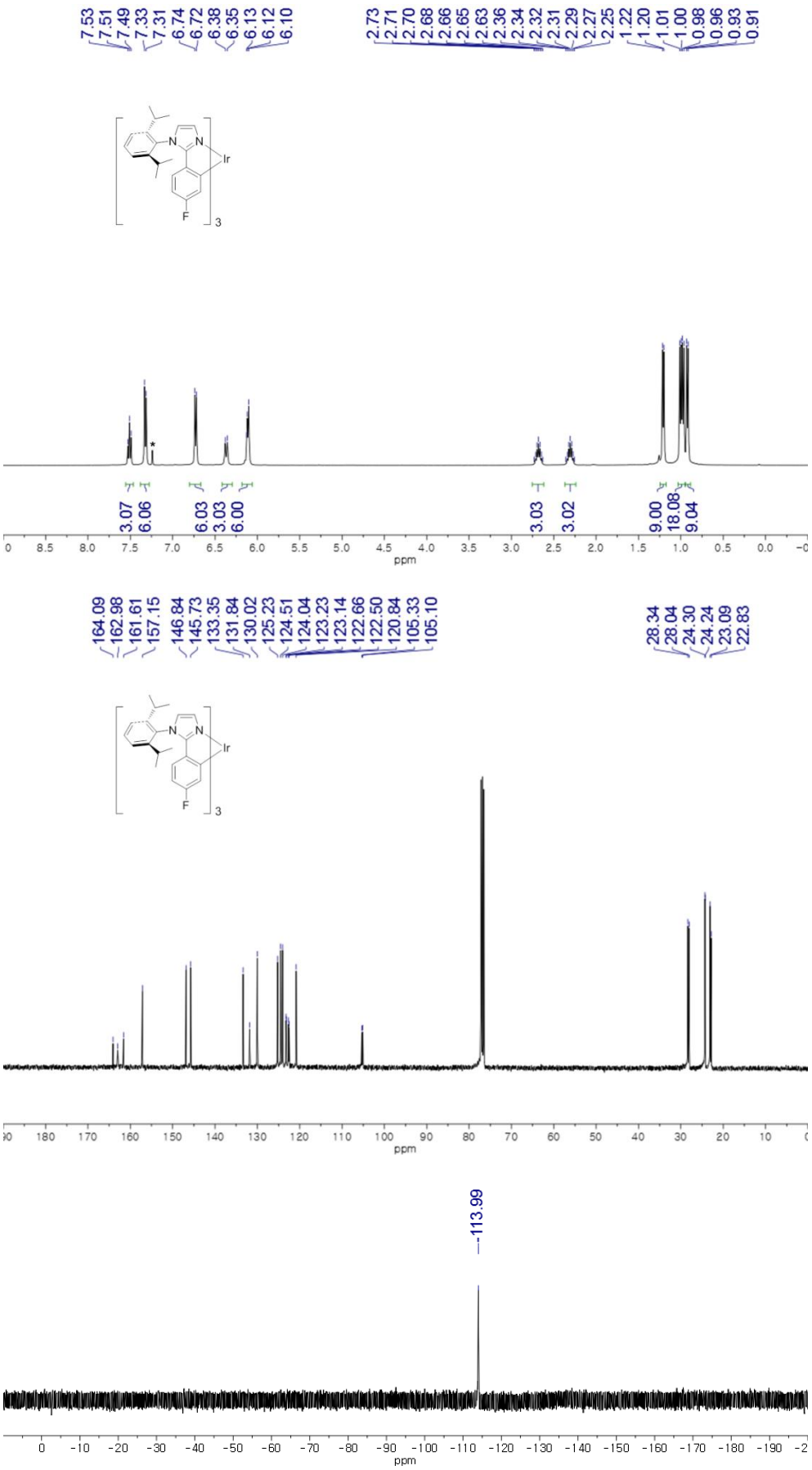

Fig. S3 ^{1}H (top), ^{13}C (middle) and ^{19}F NMR spectrum of *fac*-**FIr** (∗ from residual $CHCl_3$ in $CDCl_3$).

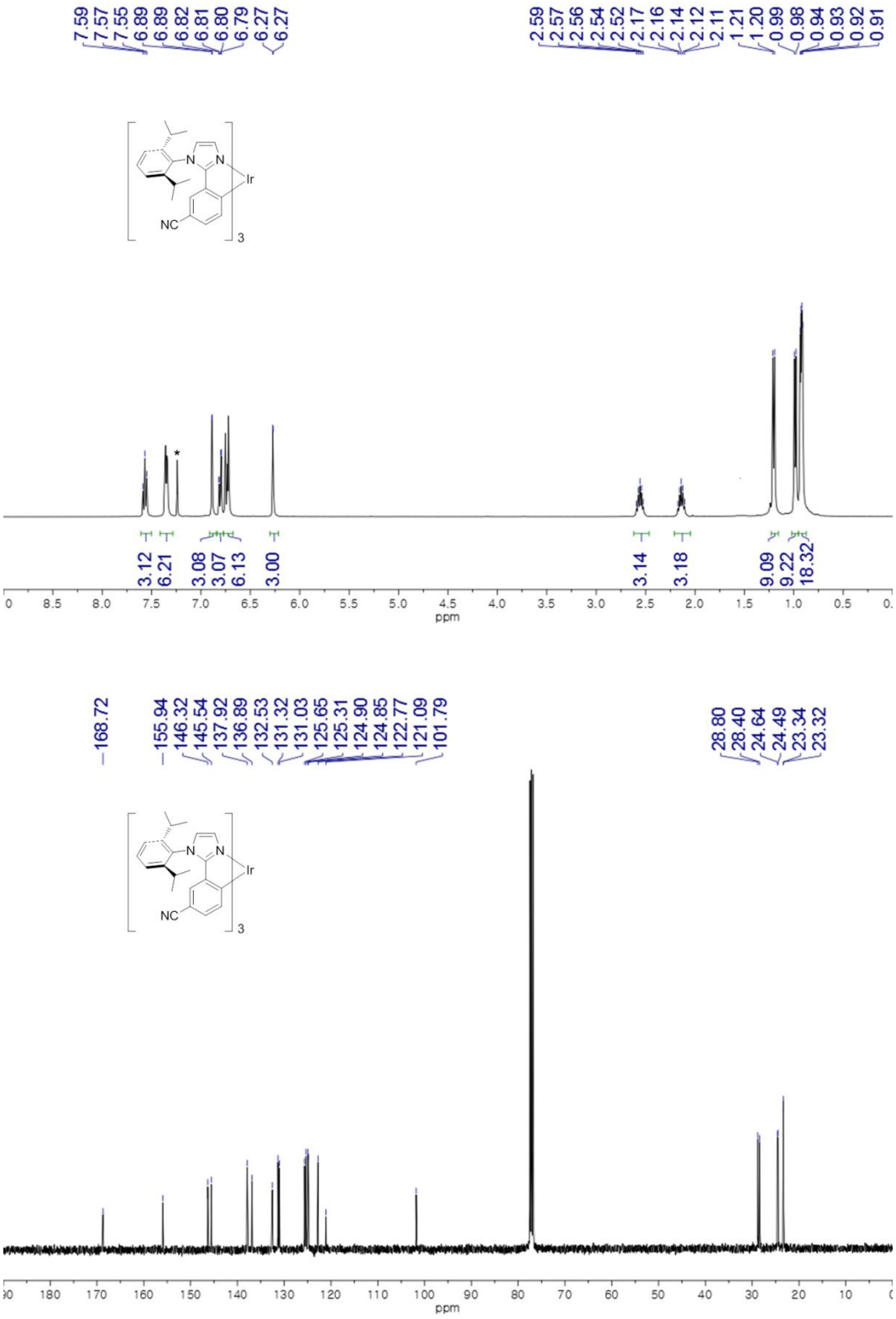

Fig. S4 ^{1}H (top) and ^{13}C (bottom) NMR spectrum of *fac*-**CNIr** (∗ from residual $CHCl_3$ in $CDCl_3$).

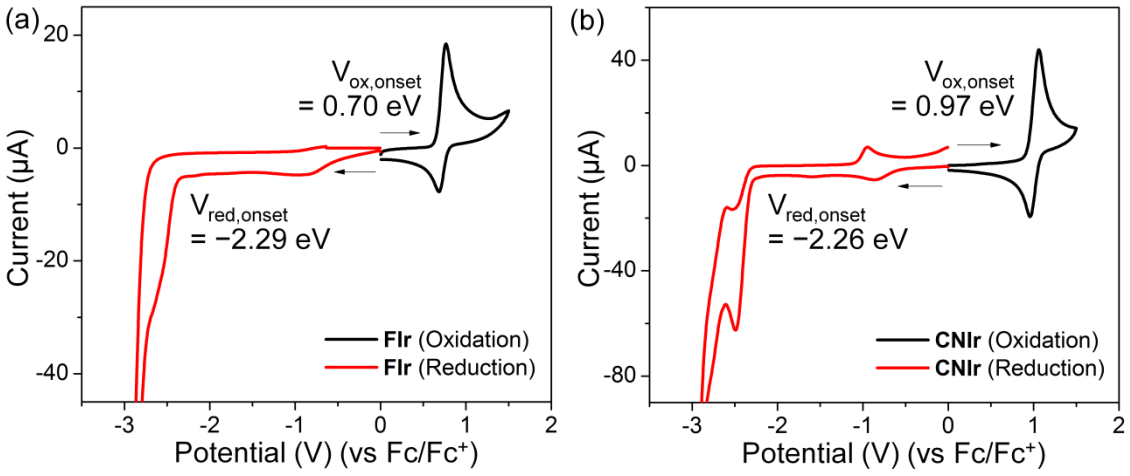

Fig. S5 Cyclic voltammograms (CV) of (a) **FIr** and (b) **CNIr** showing oxidation and reduction (5×10^{-4} M in DCM, scan rate: 100mV/s).

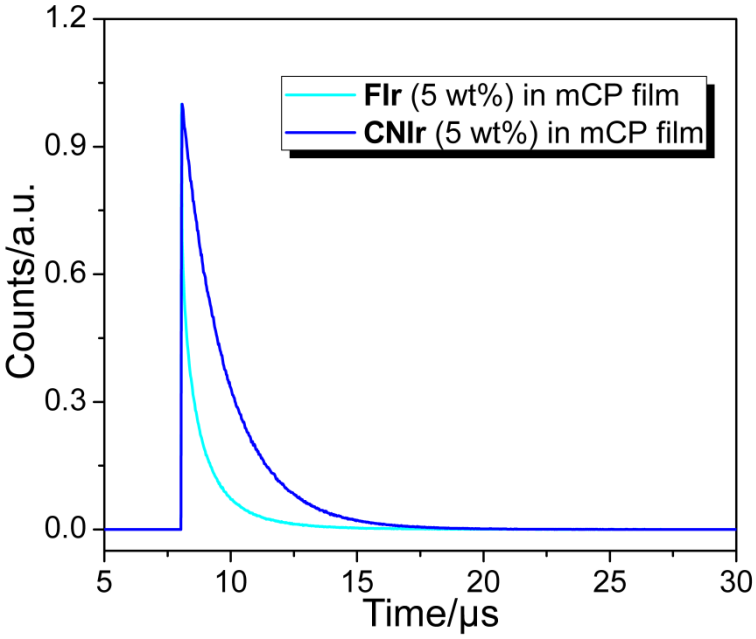

Fig. S6 Emission decay curves of **FIr** and **CNIr** (5 wt% doped in mCP film)

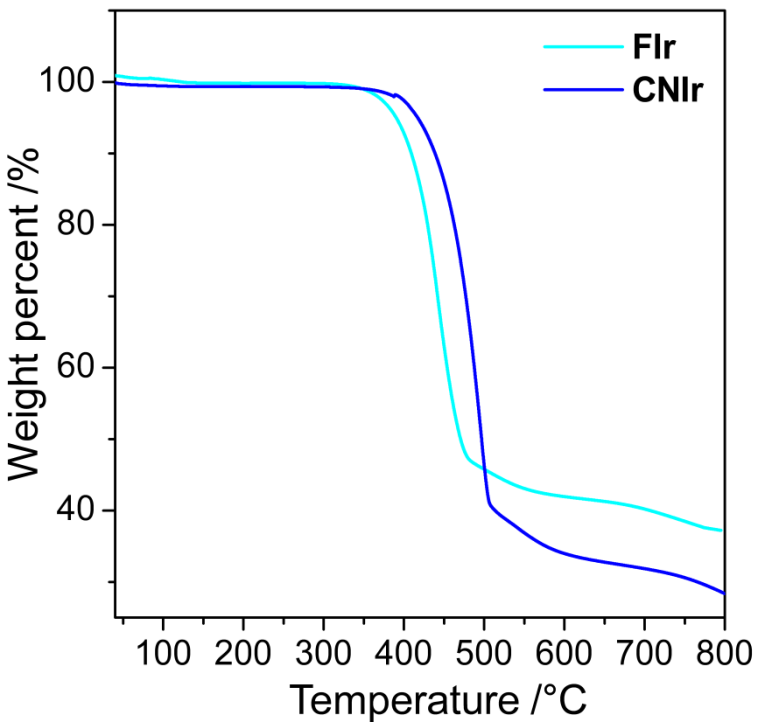

Fig. S7 TGA curves of **FIr** and **CNIr**

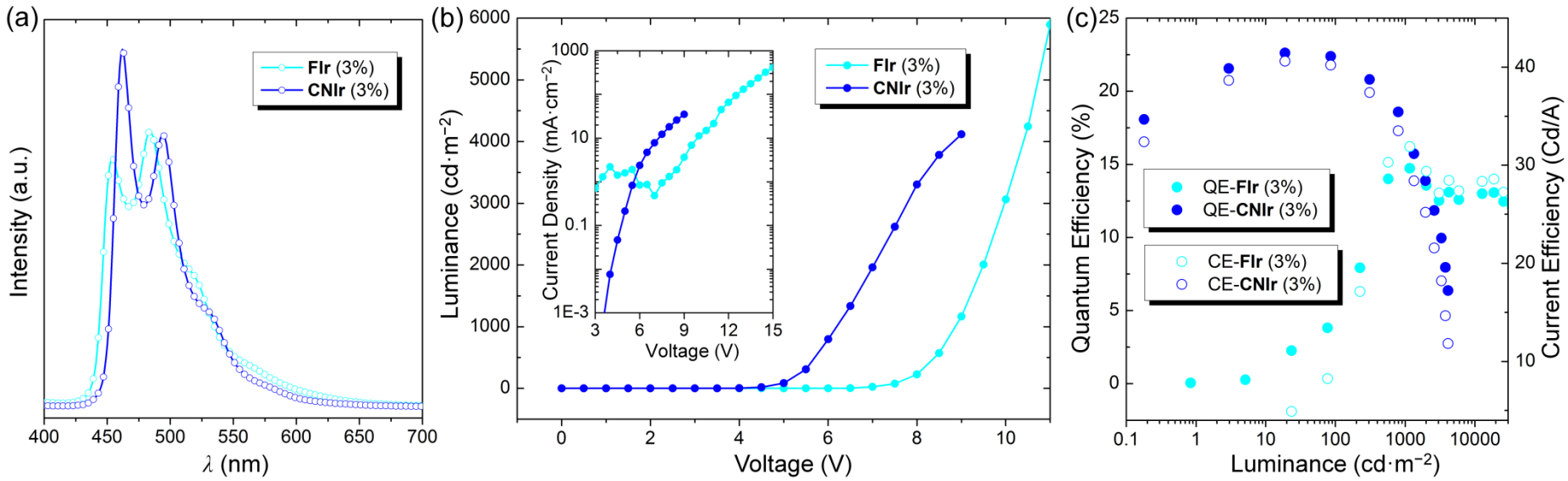

Fig. S8 (a) EL spectra of the OLEDs using **FIr** and **CNIr** (3%) with mCP, (b) luminance(*L*)–voltage(*V*) characteristics (the inset shows current density(*J*)–voltage(*V*) characteristics) and (c) external quantum efficiency–current efficiency–luminance(*L*) characteristics of the devices.

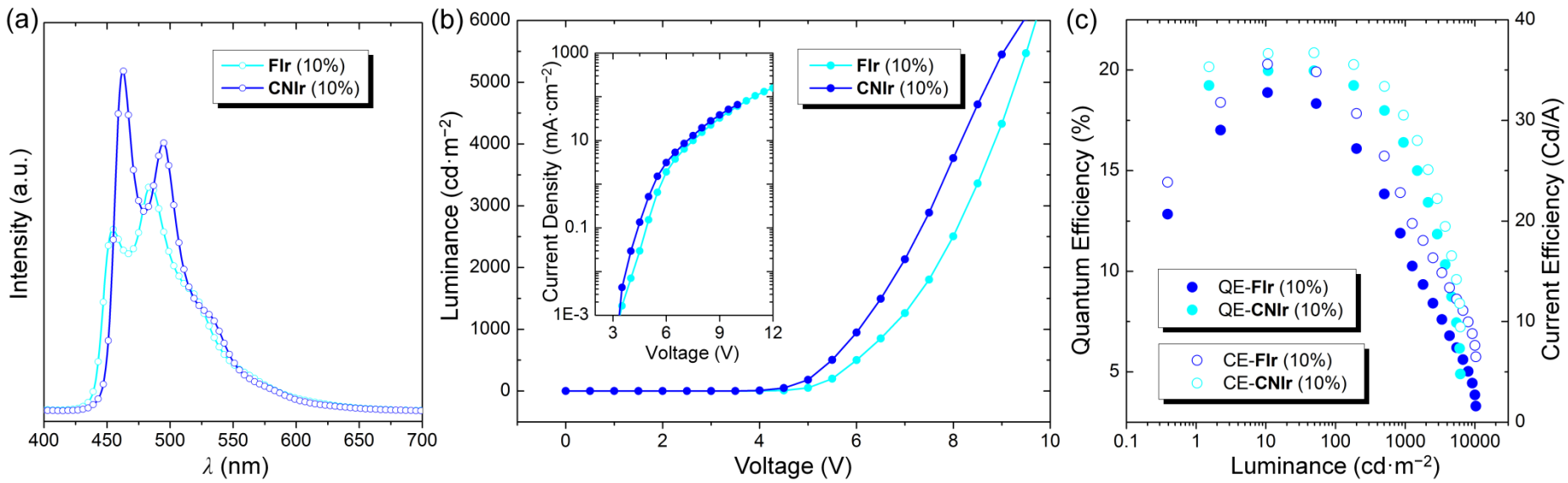

Fig. S9 (a) EL spectra of the OLEDs using **FIr** and **CNIr** (10%) with mCP, (b) luminance(*L*)–voltage(*V*) characteristics (the inset shows current density(*J*)–voltage(*V*) characteristics) and (c) external quantum efficiency–current efficiency–luminance(*L*) characteristics of the devices.

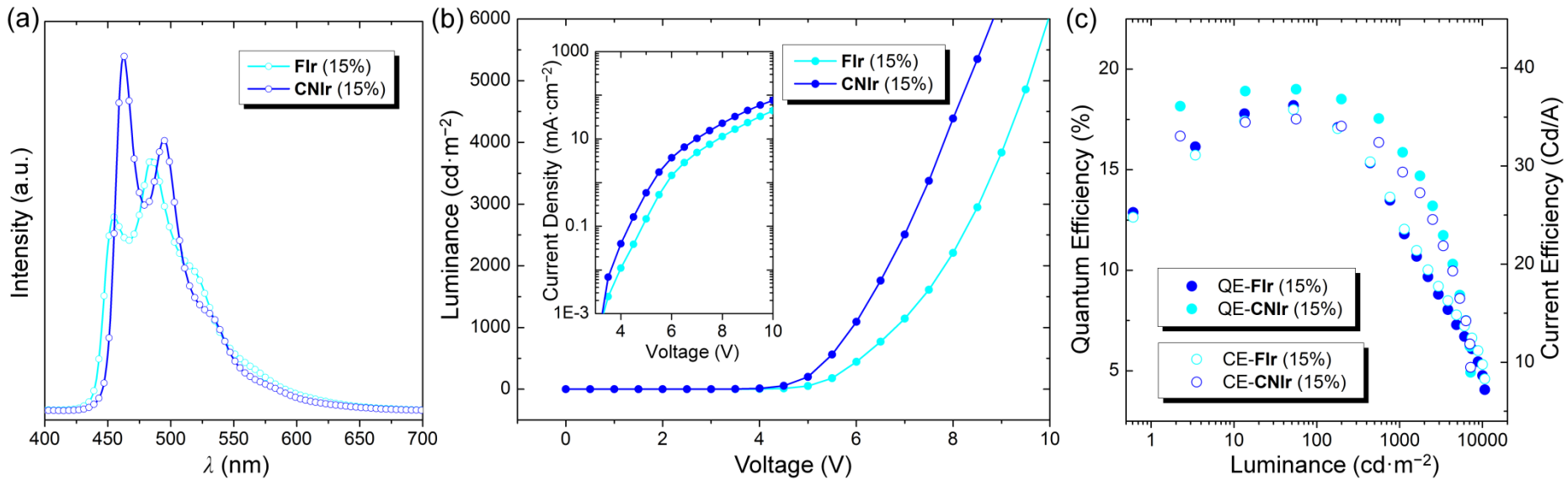

Fig. S10 (a) EL spectra of the OLEDs using **FIr** and **CNIr** (15%) with mCP, (b) luminance(*L*)–voltage(*V*) characteristics (the inset shows current density(*J*)–voltage(*V*) characteristics) and (c) external quantum efficiency–current efficiency–luminance(*L*) characteristics of the devices.

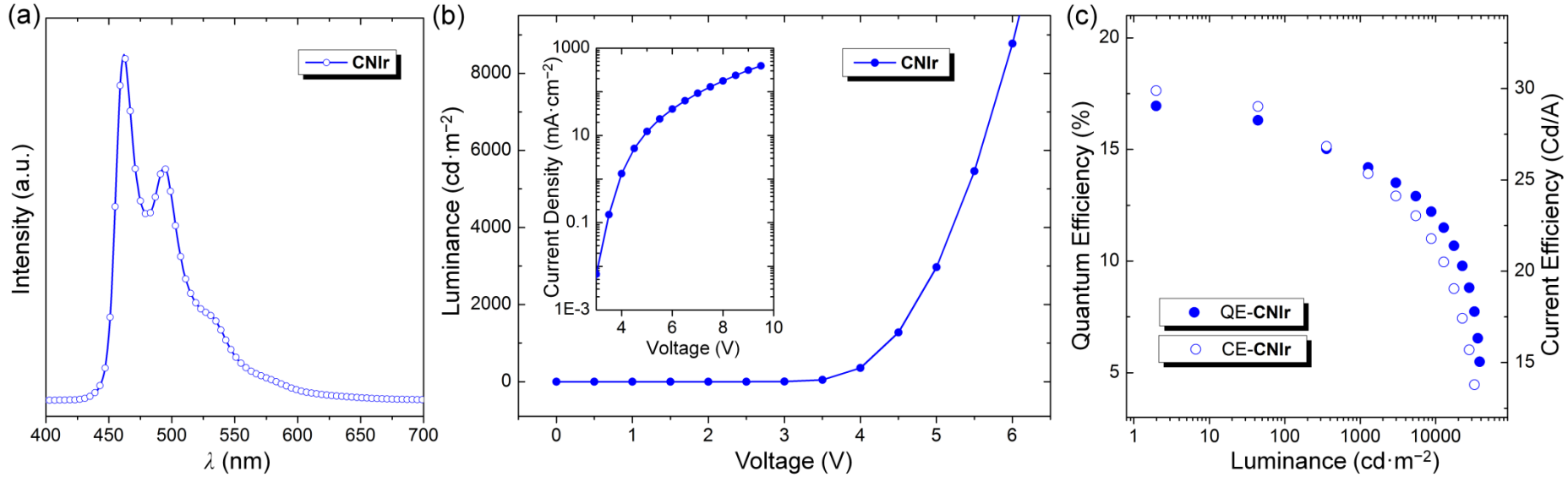

Fig. S11 (a) EL spectra, (b) luminance(*L*)–voltage(*V*) characteristics (the inset shows current density(*J*)–voltage(*V*) characteristics) and (c) external quantum efficiency–current efficiency–luminance(*L*) characteristics of the **CNIr** based device structure: ITO (50 nm)/BPBPA:HATCN (40 nm:30 wt%)/BPBPA (10 nm)/PCZAC (10 nm)/(mCBP:DBFTrz):**CNIr** ((50:50%):20 wt%) (30 nm)/DBFTrz (5 nm)/ZADN (20 nm)/LiF (1.5 nm)/Al (200 nm).