Supporting Information

Substituent effect on the electroluminescence efficiency of amidinate-ligated bis(pyridylphenyl) iridium(III) complexes

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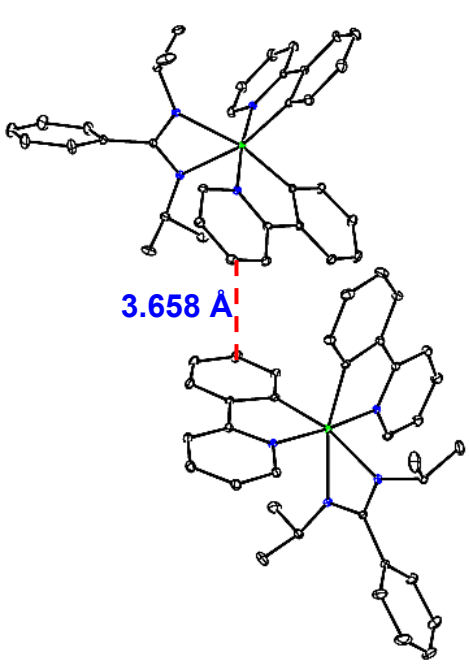
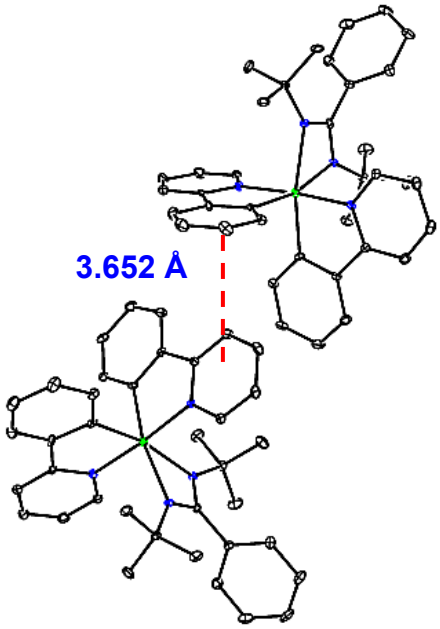
Table S1 Summary of crystal data of complexes (**1-4**)

	1	**2**	**3**·toluene	**4**
Empirical formula	$C_{35}H_{35}IrN_4$	$C_{37}H_{39}IrN_4$	$C_{35}H_{35}IrN_4$	$C_{36}H_{38}IrN_5$
fw	703.87	731.92	704.2491	732.91
Temp(k)-	293(2)	173	173	173(2)
Cryst syst	Orthorhombic	Orthorhombic	Monoclinic	Monoclinic
Space group	*P*na2$_1$	*P*na2$_1$	*P*2$_1$/n	*C*c
Unit cell dimens				
a (Å)	11.357(2)	11.3066(15)	11.359(5)	16.198(9)
b (Å)	8.6176(17)	32.677(4)	24.368(11)	18.410(10)
c (Å)	31.532(6)	8.6138(12)	23.379(11)	10.788(6)
α (o)	90	90	90	90
β [°]	90	90	97.568(8)	101.611(8)
γ [°]	90	90	90	90
V, (Å3)	3086.1(11)	3182.5(7)	6415(5)	3151(3)
Z	4	4	4	4
density(calcd), g/cm3	1.515	1.528	1.553	1.545
abs coeff, mm-1	4.355	4.227	4.196	4.27
F(000)-	1400	1464	3000	1464
θ range [°]	3.04 to 27.45	1.91-25.07	1.21- 25.08	1.69 to 25.08
reflns collected	29341	15868	33602	8105
indep reflns(Rint)	7032(0.0405)	4840(0.0457)	11290(0.0921)	4738 (0.0439)
data/restraints/params	7032 / 1 / 365	4840/1/385	11290 / 8 / 763	4738 / 2 / 379
GOF on F^2	1.027	1.018	0.798	0.814
Final R index [I > 2σ(I)]	0.0259	0.0296	0.0501	0.0425
Rw	0.0461	0.0599	0.0727	0.058

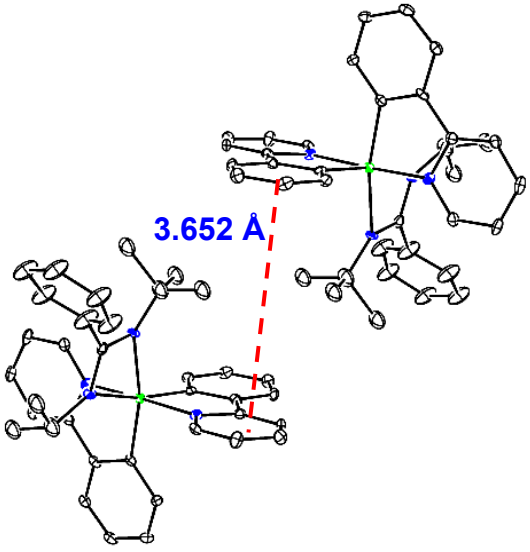
Figure S1 The distances between two nearest parallel *ppy* planes in complexes (**1-4**):



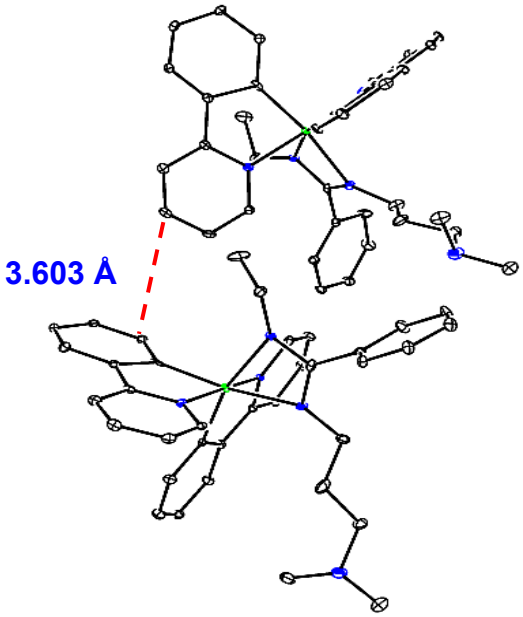
1



2



3



4

Figure S2. Phosphorescent life-times of complexes (**1-4**) in toluene solution

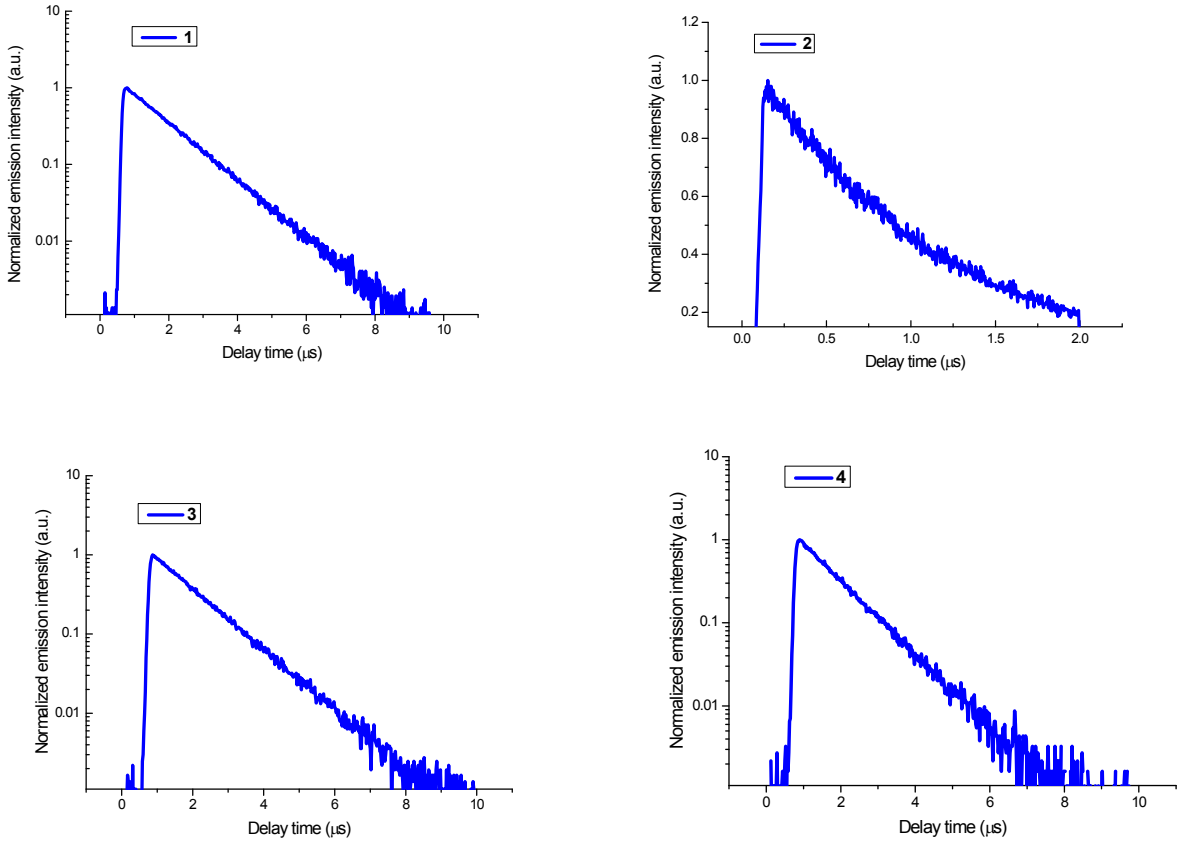
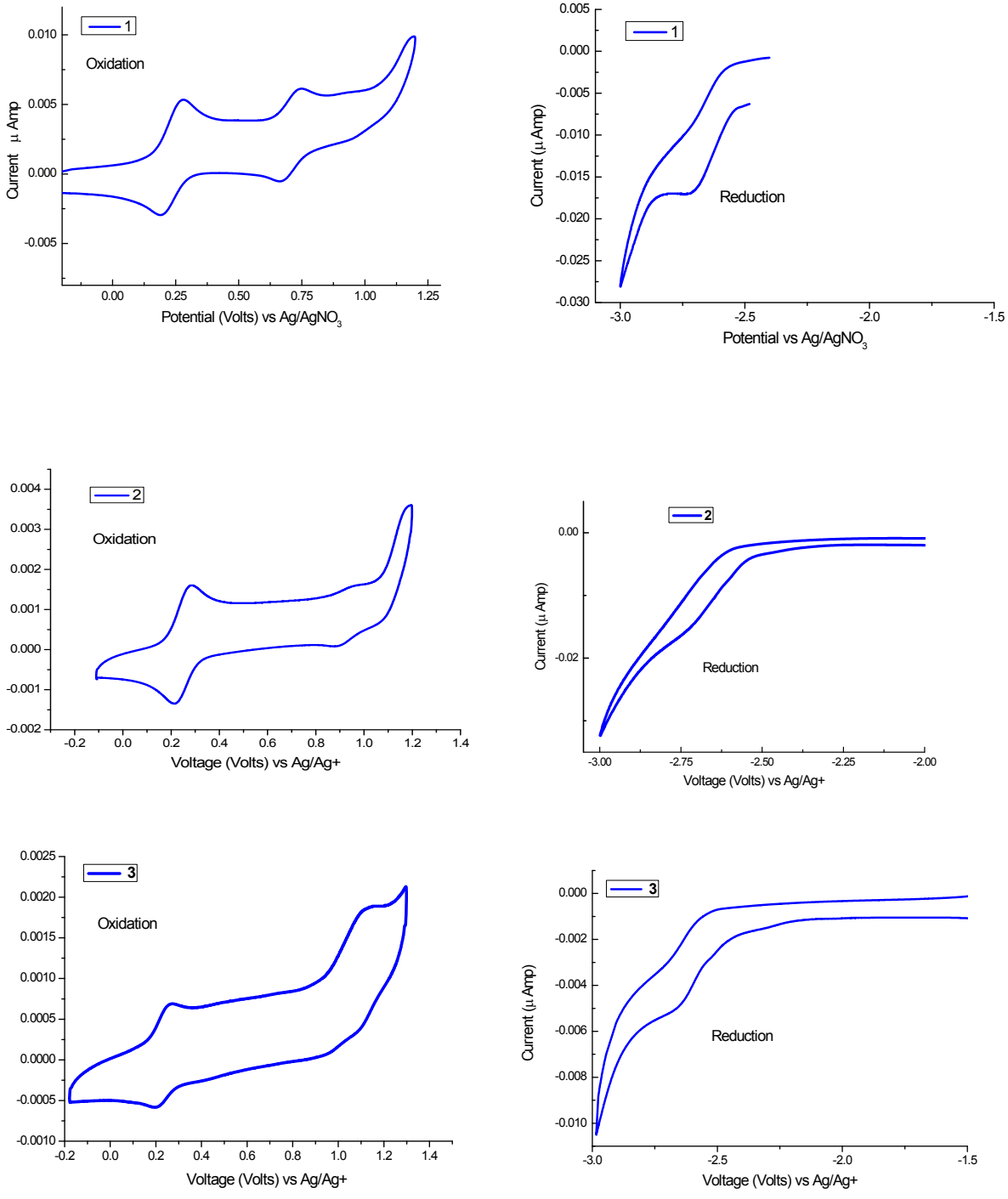


Figure S3. Cyclic voltammograms of complexes (**1-4**) in acetonitrile solution



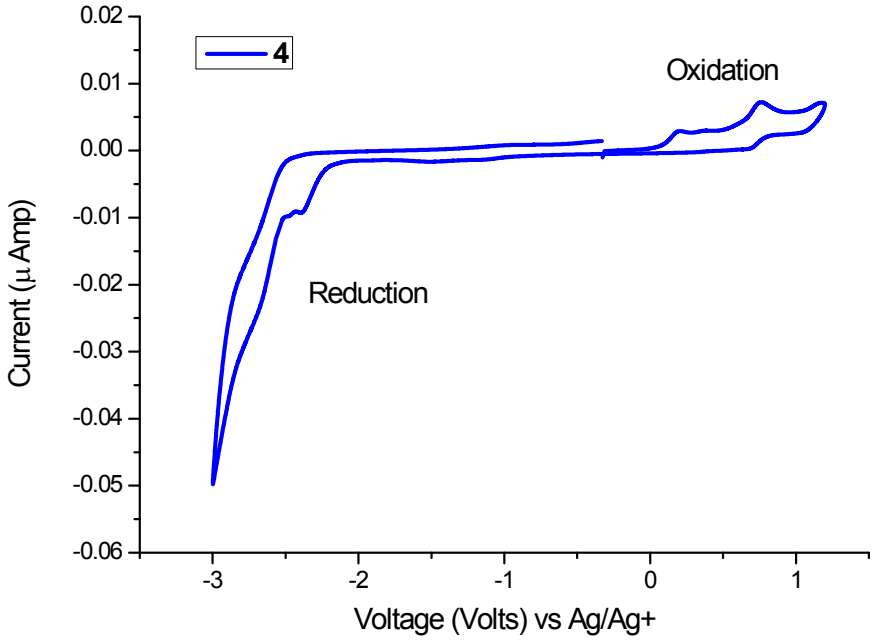

4
Oxidation
Reduction
Current (μ Amp)
Voltage (Volts) vs Ag/Ag+
0.02
0.01
0.00
-0.01
-0.02
-0.03
-0.04
-0.05
-0.06
-3
-2
-1
0
1

Figure S4. Electroluminescence spectra of complex (**1**) at different doping concentration: inset: Photograph of OLED device at 9 V.

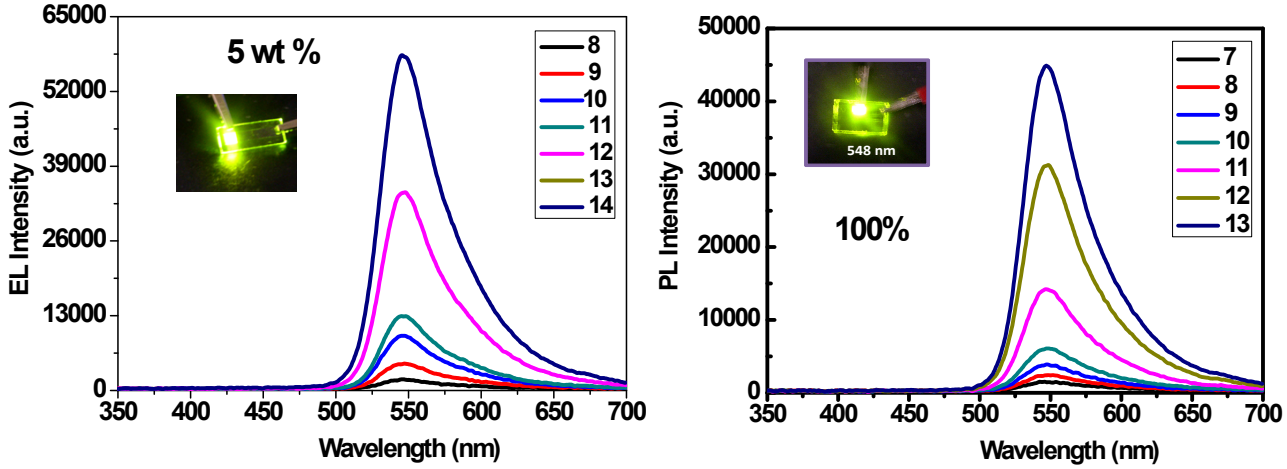


Figure S5. Current-density (*J*), voltage (*V*) and luminance (*L*) characteristics of OLEDs based on complex (**1**).

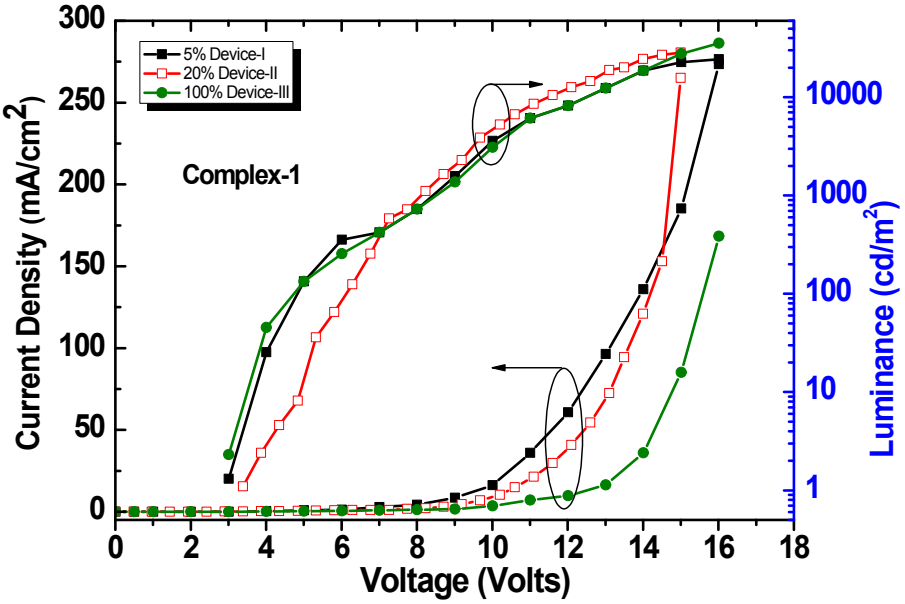
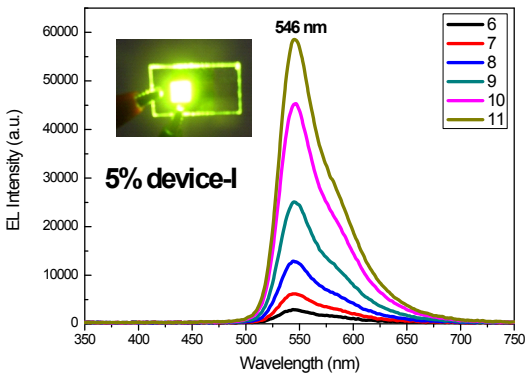
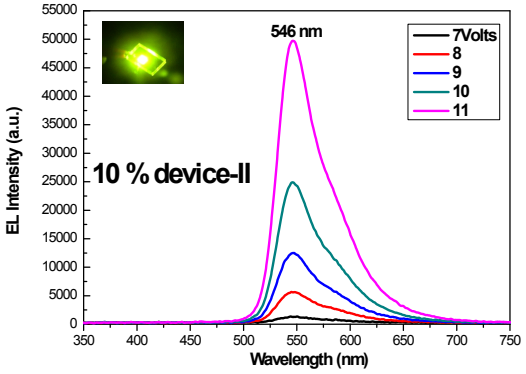
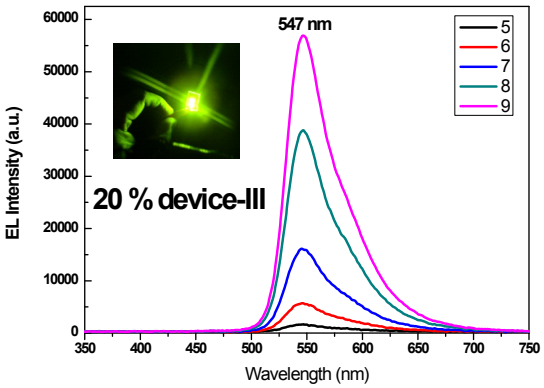
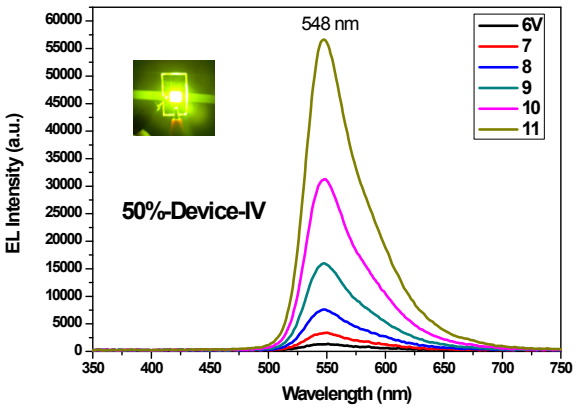


Figure S6. Electroluminescence spectra of complex (**2**): Devices I, II, III, IV and V at different voltages: Photographs of OLED device at 9 V.









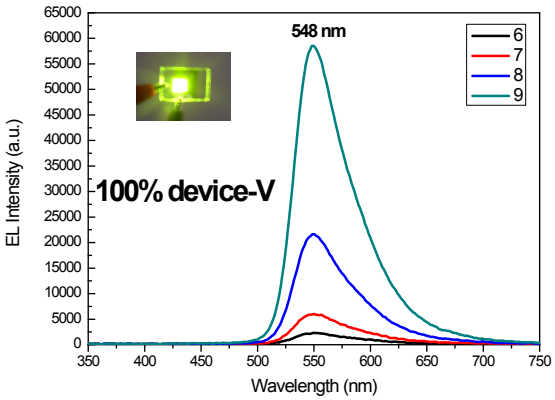


Figure S7. Electroluminescence spectra of complex (**3**) Devices I, II, III and IV at different voltages. Photograph of OLED device at 9 V.

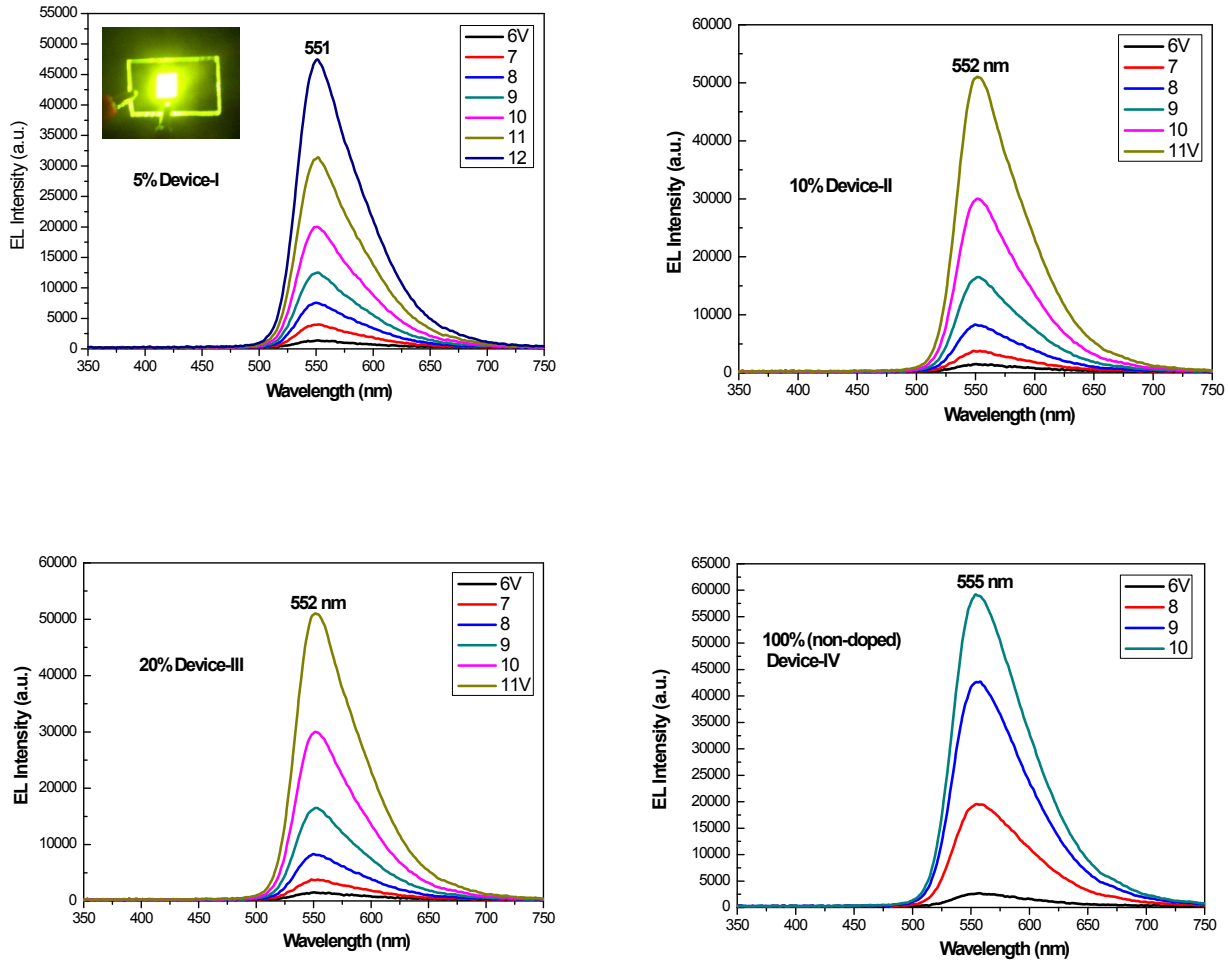


Figure S8. Current-density (*J*), voltage (*V*) and luminance (*L*) characteristics of OLEDs based on complex (**3**).

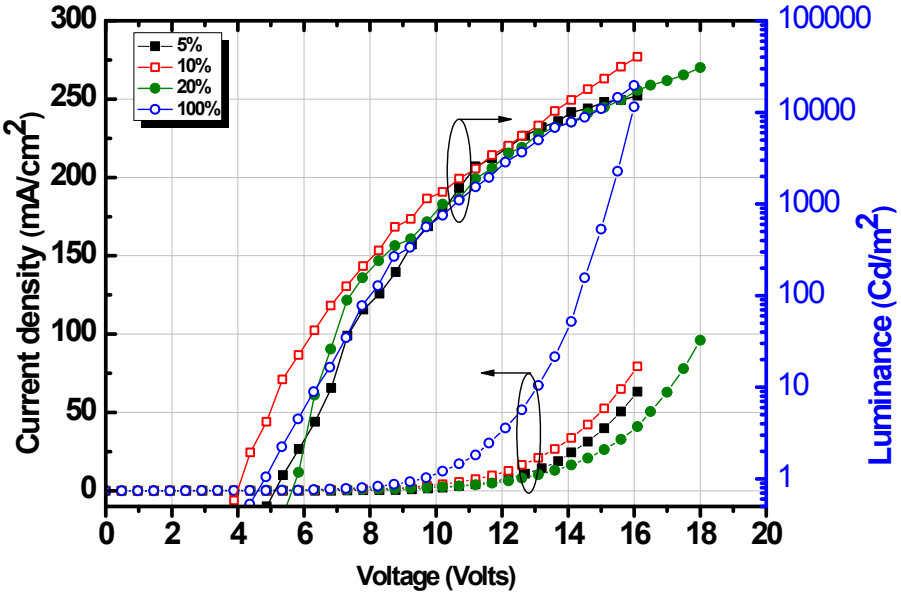


Figure S9. Electroluminescence spectra of complex (**4**) Devices I (5%) at different voltages.