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Supporting Information

Molecular Design Approach Managing Molecular Orbital Superposition for High Efficiency without Color Shift in Thermally Activated Delayed Fluorescent Organic Light-Emitting Diodes

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Table S1. Summary of the TD-DFT calculation of the three TADF molecules at the B3LYP/6-311+G** level.

Emitters	HOMO (eV)	LUMO (eV)	B.G (eV)	S_1 (eV), CI description	T_1 (eV), CI description	ΔE_{ST} (eV)
o-CNPhe	-5.30	-2.31	2.99	2.28, H→L 99%	2.26, H→L 99%	0.02
m-CNPhe	-5.40	-2.39	3.01	2.36, H→L 99%	2.33, H→L 99%	0.03
o-CNPheAm	-5.12	-1.96	3.16	2.50, H→L 98%	2.48, H→L 98%	0.02

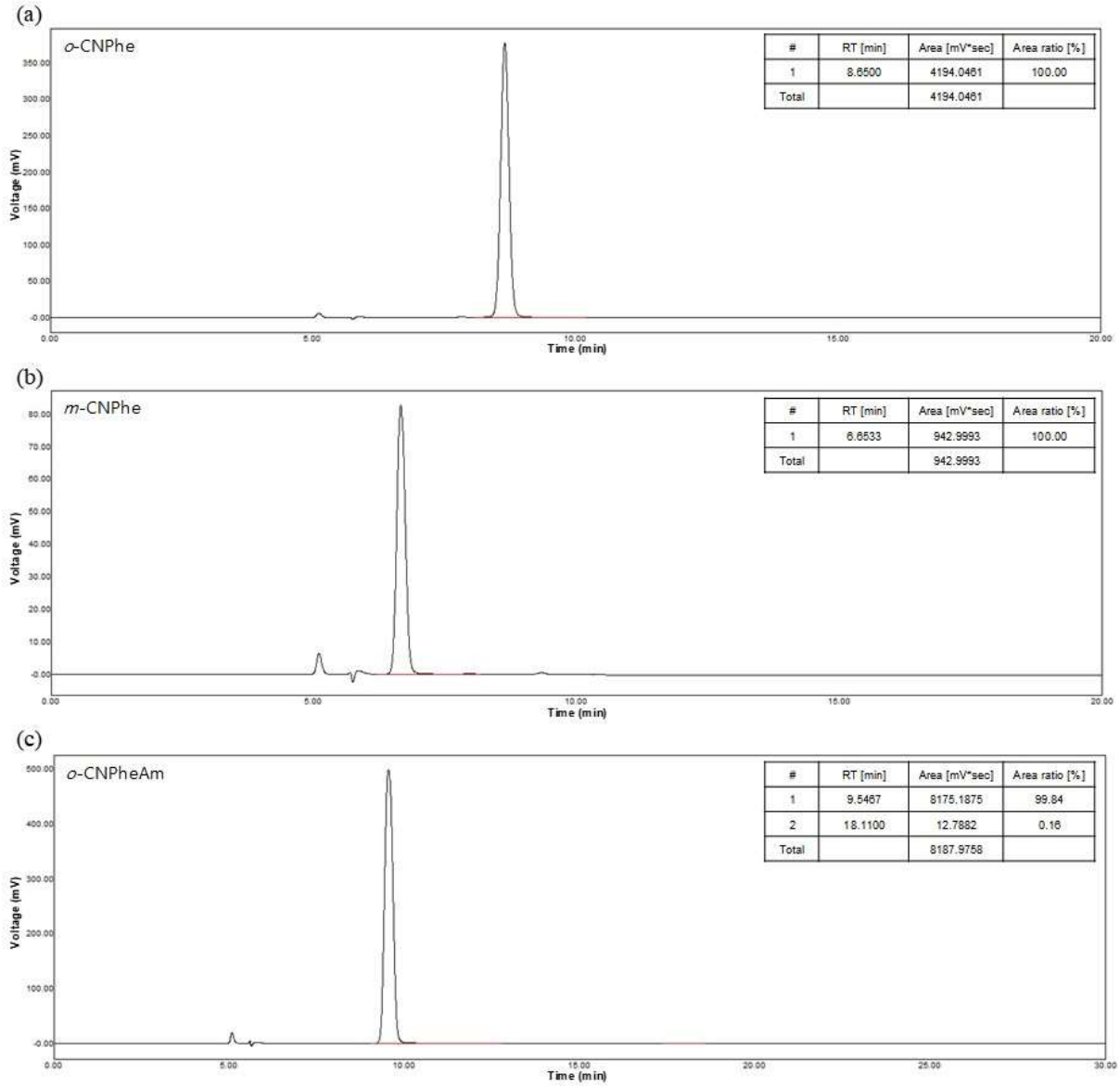

Figure S1. High performance liquid chromatography data of o-CNPhe, m-CNPhe, and o-CNPheAm for the purity confirmation.

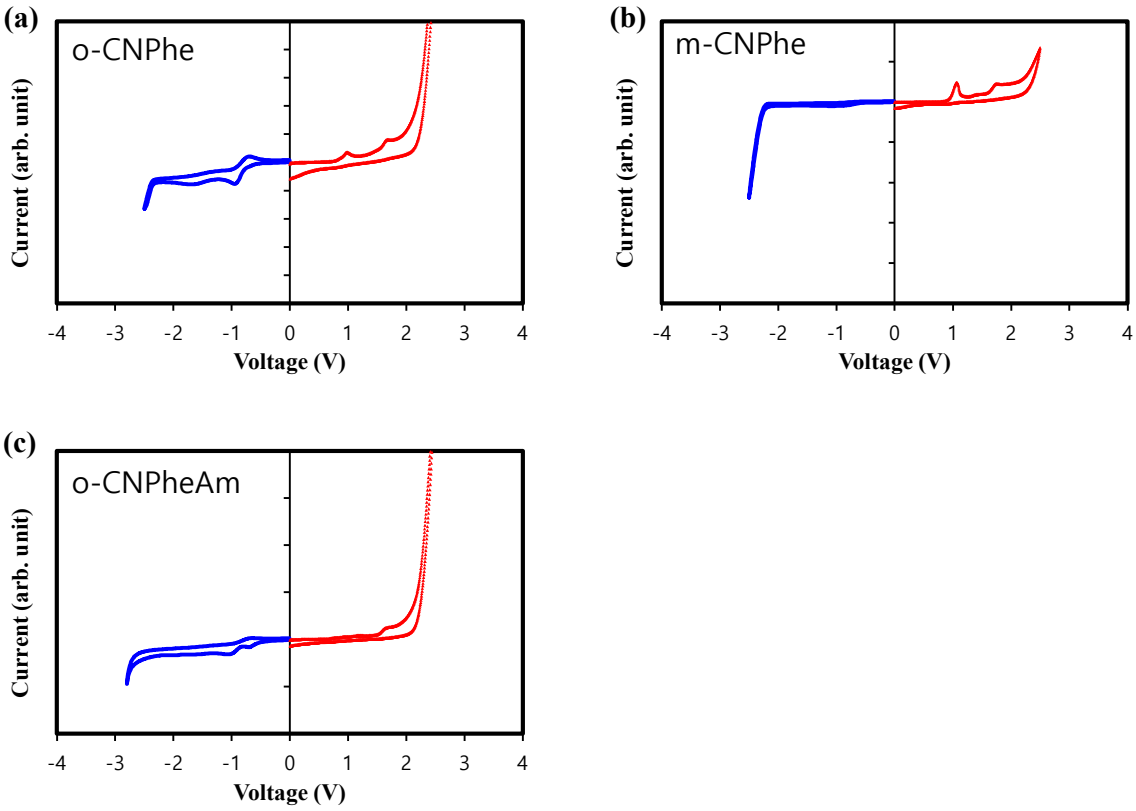

Figure S2. CV curves of o-CNPhe, m-CNPhe, and o-CNPheAm.

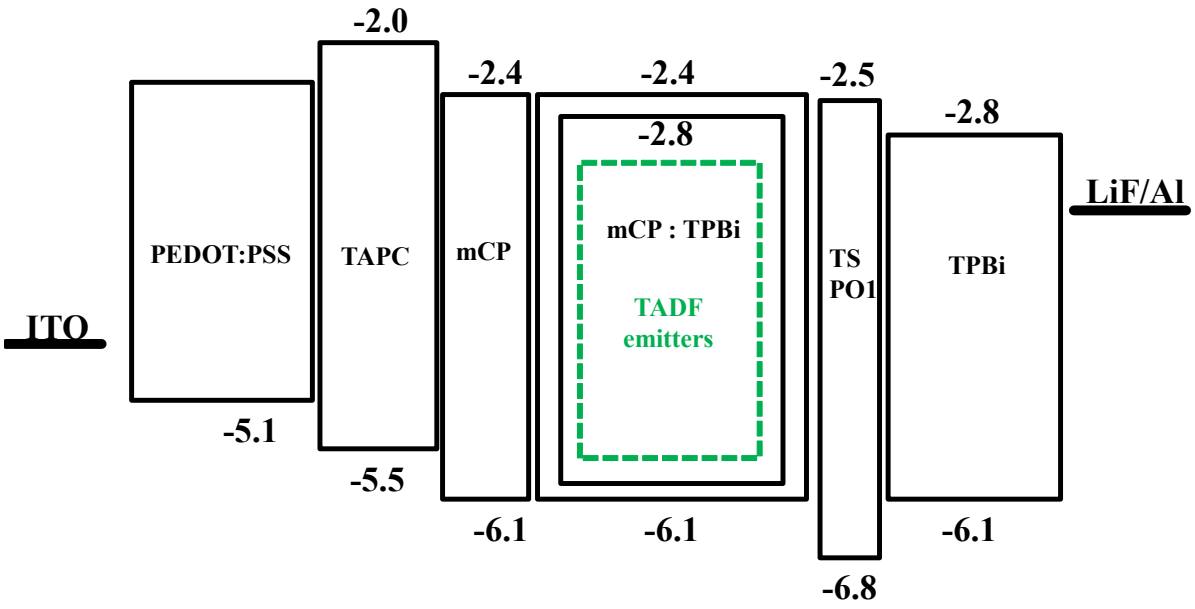

Figure S3. Device structure and energy diagram of TADF OLEDs .

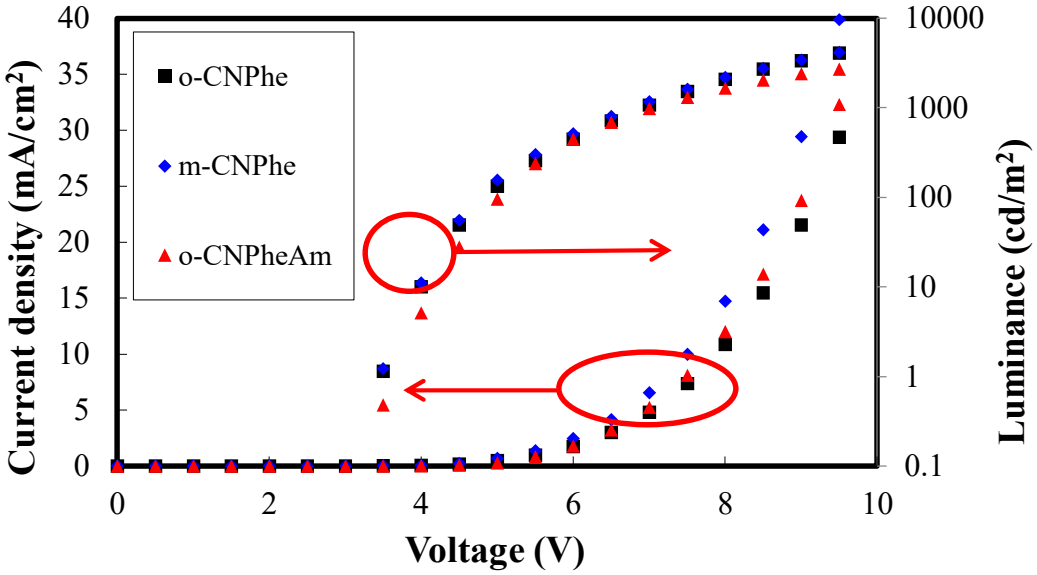

Figure S4. Current density, luminance, and voltage data of TADF emitters.