Supporting information

Highly Efficient Dual-Core Derivatives with EQEs as high as 8.38% at High Brightness for OLED Blue Emitters

Seokwoo Kang, Hyocheol Jung, Hayoon Lee, Sunwoo Park, Joonghan Kim, and Jongwook Park[a]*

General information

Reagents and solvents were purchased as reagent grade and used without further purification. Analytical TLC was carried out on Merck 60 F254 silica gel plate, and column chromatography was performed on Merck 60 silica gel (230-400 mesh). The ^{1}H-NMR spectra were recorded on Bruker Avance 300 spectrometers. The FAB+-mass and EI+-spectra were recorded on a JMS-600W, JMS-700, 6890 Series and Flash1112, Flash2000. The optical UV-Vis absorption spectra were obtained using a Lambda 1050 UV/Vis/NIR spectrometer (Perkin Elmer). A Perkin-Elmer luminescence spectrometer LS55 (Xenon flash tube) was used to perform PL spectroscopy. The transient PL was measured with a Quantaurus-Tau fluorescence life time measurement system. The glass transition temperatures (T_g) of the compounds were DSC under a nitrogen atmosphere using a DSC 4000 (Perkin Elmer). T_d of the compounds were measured with TGA using a TGA4000 (Perkin Elmer). The HOMO energy levels were determined with ultraviolet photoelectron yield spectroscopy (Riken Keiki AC-2). The LUMO energy levels were derived from the HOMO energy levels and the band gaps. For the EL devices, all organic layers were deposited under 10^{-6} torr, with a rate of deposition of 1 Å/s to give an emitting area of 4 mm^2. The LiF and aluminum layers were continuously deposited under the same vacuum conditions. The current-voltage-luminance (I-V-L) characteristics of the fabricated EL devices were obtained with a Keithley 2400 electrometer. Light intensities were obtained with a Minolta CS-1000A. To calibrate the EQE values considering the angular dependence, emission angular distributions were also measured. The operational stabilities of the devices were measured under encapsulation in a glovebox.
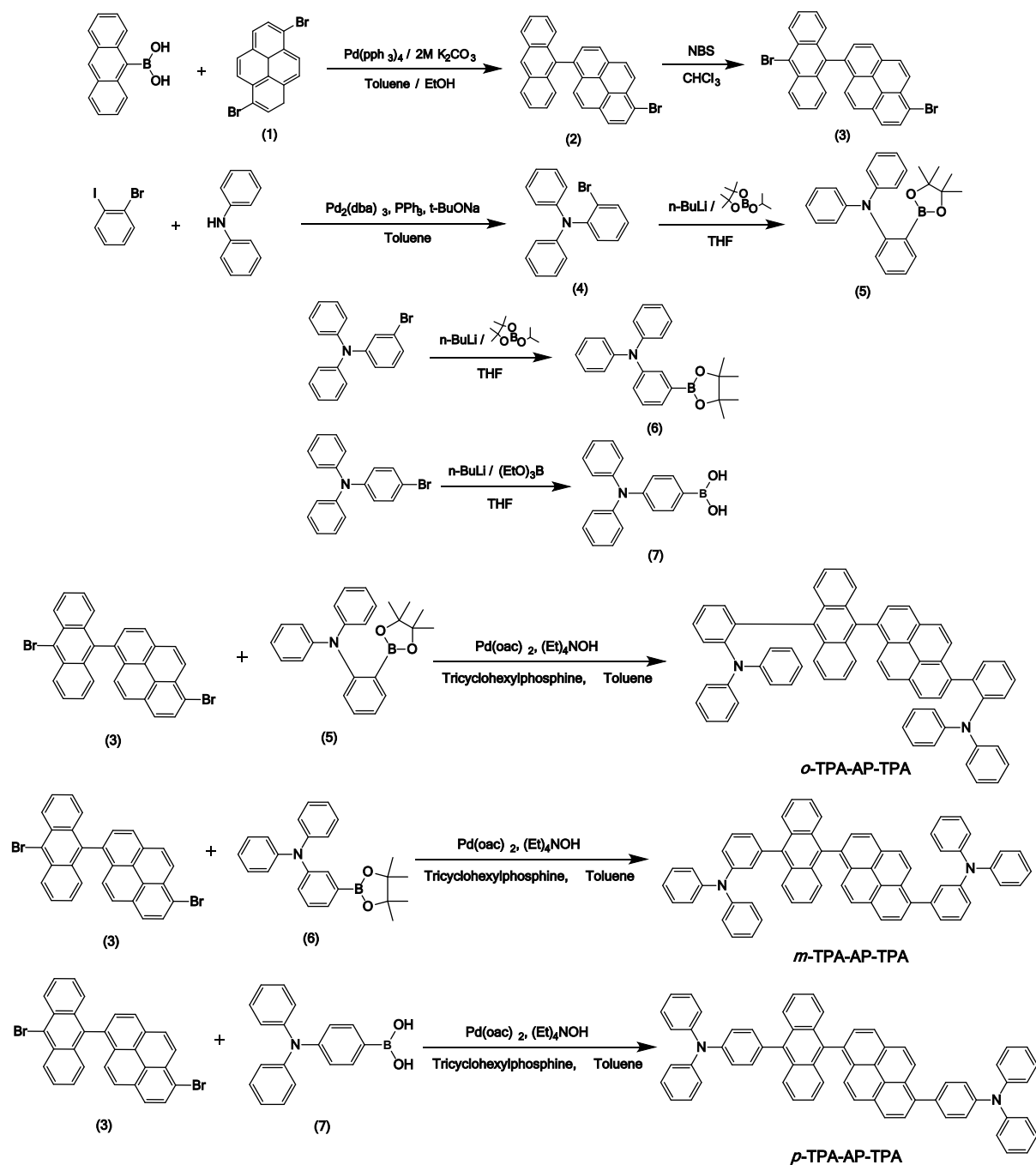
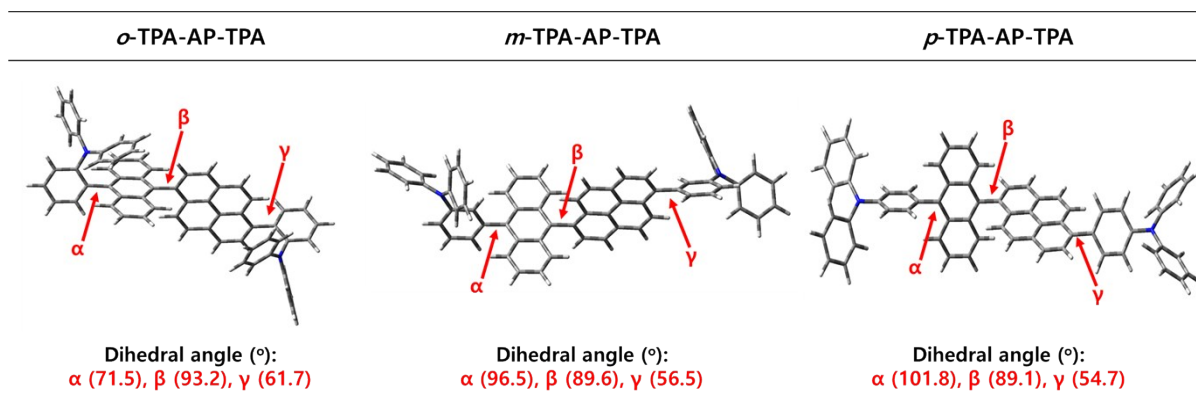**Fig. S1** Synthetic routes of newly synthesized compounds

o-TPA-AP-TPA	*m*-TPA-AP-TPA	*p*-TPA-AP-TPA

Dihedral angle (°):
α (71.5), β (93.2), γ (61.7)

Dihedral angle (°):
α (96.5), β (89.6), γ (56.5)

Dihedral angle (°):
α (101.8), β (89.1), γ (54.7)

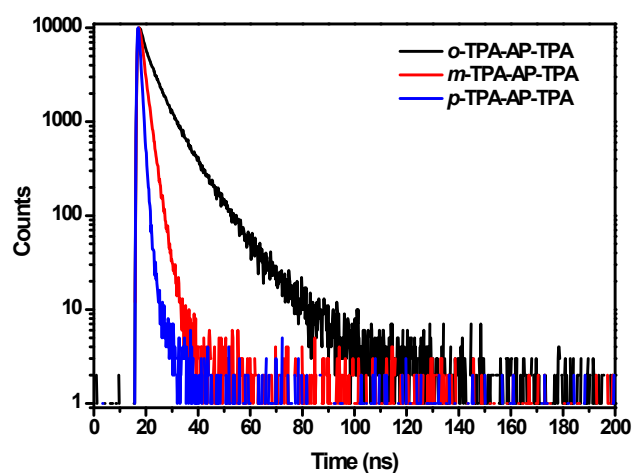**Fig. S2** Optimization structure and dihedral angle of synthesized compounds

Fig. S3 Time-resolved PL of the synthesized compounds (film states in which the synthesized material in PMMA was dispersed at 1wt%).
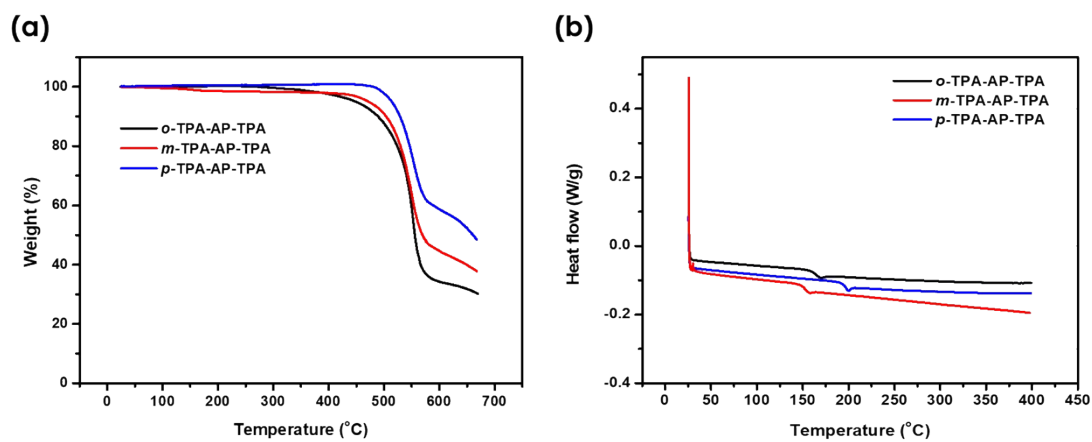

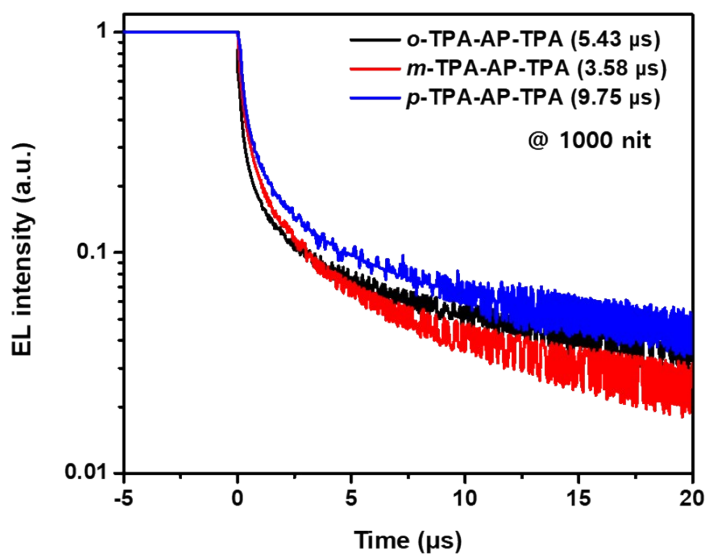**Fig. S4** (a) TGA and (b) DSC curves of synthesized compounds

Fig. S5 Transient electroluminescence (EL) responses of an ITO/2-TNATA (60 nm)/NPB (15 nm)/α,β-ADN: synthesized material 4% (30 nm)/TPBi (30 nm)/LiF (1 nm)/Al (200 nm)

Table S1 Photophysical properties of synthesized compounds.

Compounds	Φ_F[a]	τ_F (ns)[b]	k_{rad}[c] x 10^8/s	k_{nr}[c] x 10^7/s	k_{rad}/k_{nr}
o-TPA-AP-TPA	0.45	6.78	0.66	8.14	0.81
m-TPA-AP-TPA	0.74	1.89	3.91	13.8	2.83
p-TPA-AP-TPA	0.85	0.78	10.9	19.3	5.64

[a,b] Film states in which the synthesized material in PMMA was dispersed at 1wt%, [c] Values of k_{rad} and k_{nr} were calculated according to the equations $k_{rad} = \Phi_F/\tau_F$ and $k_{nr} = (1/\tau_F) - k_{rad.}$

Table S2 Absorption frequencies and oscillator strengths for the synthesized compounds calculated using TD-DFT (B3LYP/6-311G(d) method).

Compounds	λ_{abs} (nm) (oscillator strength, f)	Characteristic transition	Distribution of character[a]	Contribution (%)[b]
o-TPA-AP-TPA	419 (0.136)	HOMO → LUMO+1	P + TPA → P	88
		HOMO → LUMO	P + TPA → A	5
	406 (0.223)	HOMO−2 → LUMO	A + TPA → A	68
		HOMO−2 → LUMO+1	A + TPA → P	10
		HOMO−1 → LUMO	A + TPA → A	7
m-TPA-AP-TPA	399 (0.370)	HOMO−2 → LUMO	A → A	93

	358 (0.503)	HOMO−2 → LUMO	A → A	4
p-TPA-AP-TPA	424 (0.204)	HOMO−1 → LUMO	A + TPA → A	93
		HOMO → LUMO+1	P + TPA → P	6
	414 (0.526)	HOMO → LUMO+1	P + TPA → P	83
		HOMO−2 → LUMO	A + TPA → A	9
		HOMO−1 → LUMO	A + TPA → A	4
	396 (0.117)	HOMO−2 → LUMO	A + TPA → A	86
		HOMO → LUMO+1	P + TPA → P	7

[a] A: anthracene, P: pyrene, TPA: triphenylamine. [b] Where the sums of the contributions are less than 100%, the remaining contributions are from various minor transitions that are not listed.