

Supporting Information

Benzonitrile-based AIE polymer host with simple synthesis process for high-efficiency solution-processable green and blue TADF organic light emitting diodes

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General method

The ¹H were recorded on the BRUKER AMX instrument. The optimized structure was calculated by Gaussian09 at the B3LYP functional with 6-31G basis sets. Use Netzsch simultaneous thermal analyzer (STA) system (STA 409PC) and DSC 2910 Modulation Calorimeter to record thermogravimetric analysis (TGA) and differential scanning calorimetry (DSC) curves at a heating rate of 10°C min⁻¹. The UV-Vis absorption spectrum of the compound was measured by SHIMADZU UV-2450. The photoluminescence emission spectra were recorded with HORIBA FLUOROMAX-4. The PL quantum efficiency was measured with an integrating sphere at an excitation wavelength of 330 nm. Cyclic voltammetry (CV) is performed on the CHI750C voltammetry analyzer in a typical three-electrode cell, which has a platinum plate working electrode, a platinum wire counter electrode and a silver wire reference electrode.

Device manufacturing and measurement

The glass substrate with ITO coating were rinsed in deionized water, sonicated in acetone, ethanol and isopropanol in sequence. Before device fabrication, the ITO substrate was treated in a UV-

ozone oven for 20 minutes. Then PEDOT:PSS was spin-coated on the ITO substrate and dried at 150°C for 10 minutes. Then put the substrate in a nitrogen glove box, spin-coated the emission layer on the PEDOT:PSS layer, and annealed at 80°C for 15 minutes. After that, TPBi was vacuum deposited as the electron transport layer, and Cs₂CO₃ and Al were vacuum deposited as the cathode. EL spectra, device brightness and current density-voltage characteristics are recorded using a combination of Photo-Research PR-655 SpectraScan and Keithley 2400 Sourcemeter. The device is tested under atmospheric conditions without a protective package.

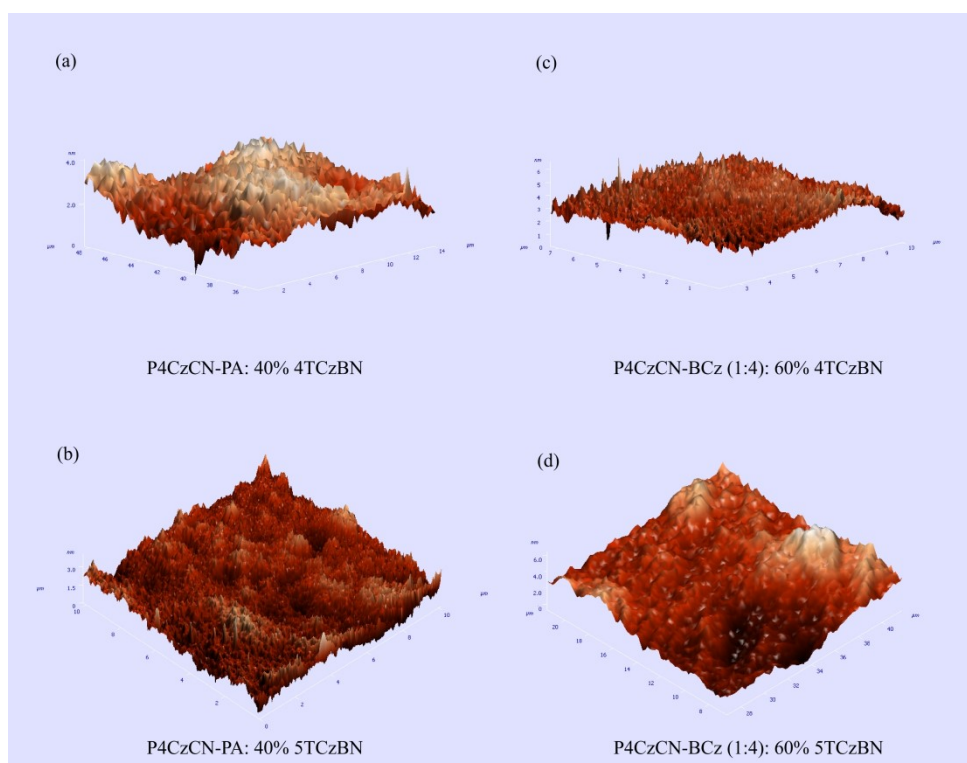
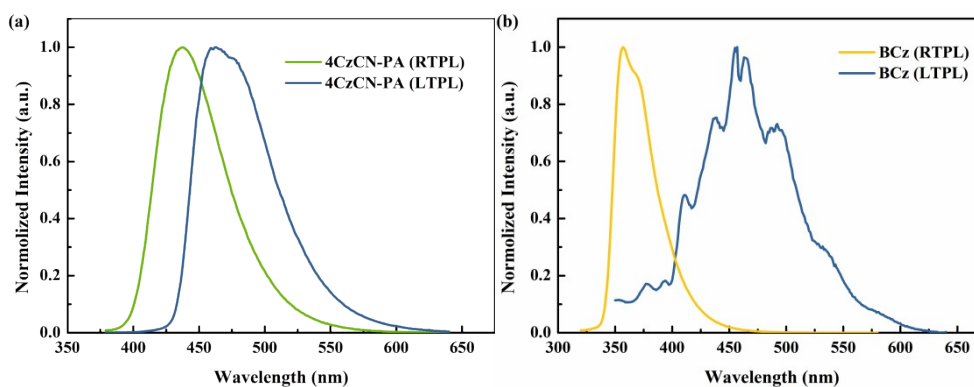


Figure S1. AFM topographic images of P4CzCN-PA: 40% 4TCzBN (a), P4CzCN-PA: 40% 5TCzBN (b), P4CzCN-BCz (1:4): 60% 4TCzBN (c) and P4CzCN-BCz (1:4): 60% 5TCzBN (d).



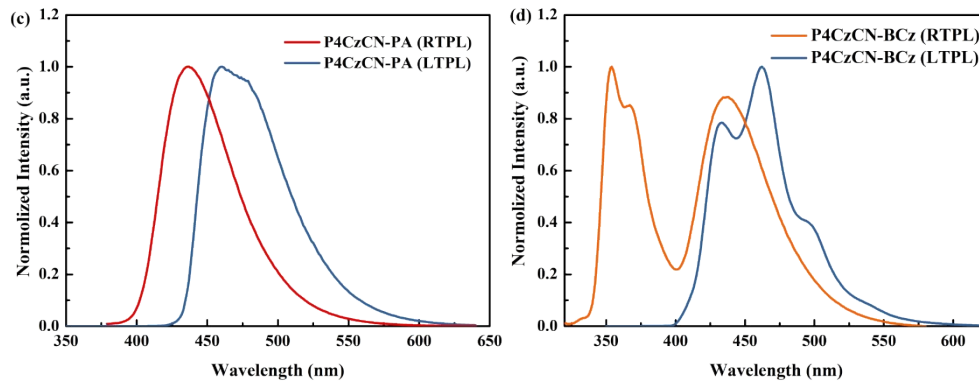


Figure S2. Fluorescence (measured at room temperature) and phosphorescence spectra (measured at 77K) in toluene solution of 4CzCN-PA (a), BCz (b), P4CzCN-PA (c) and P4CzCN-BCz (1:4) (d).

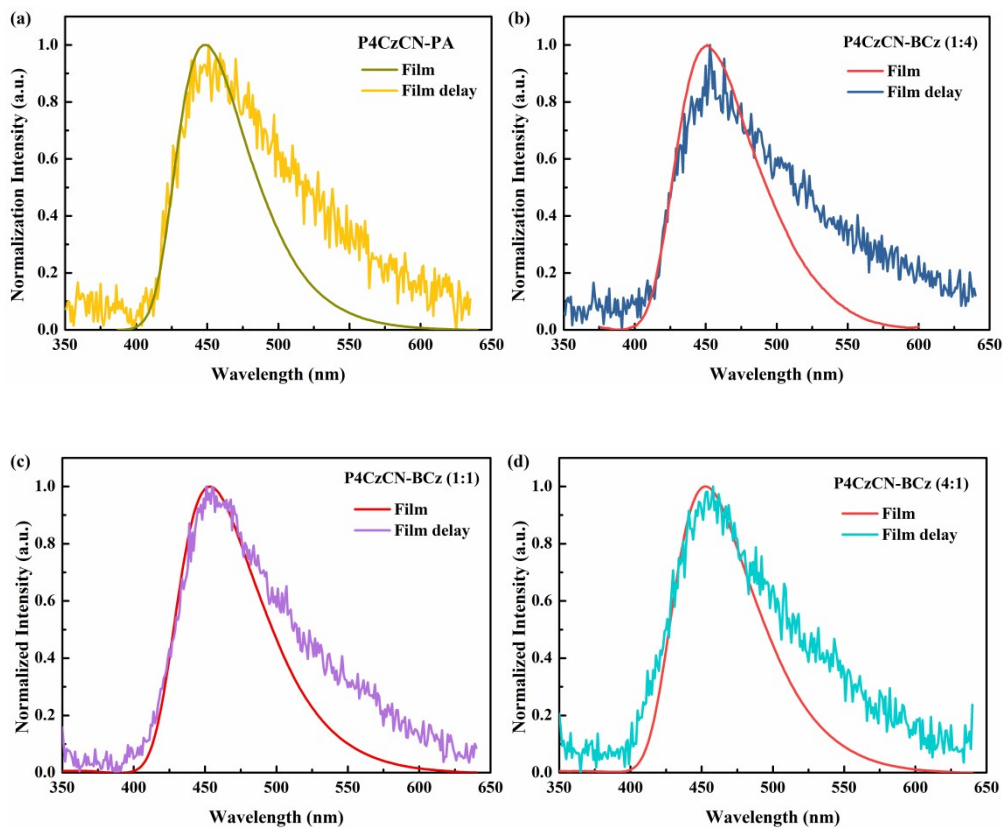


Figure S3. Fluorescence and delay Fluorescence spectra of P4CzCN-PA (a), P4CzCN-BCz (1:4) (b), P4CzCN-BCz (1:1) (c) and P4CzCN-BCz (4:1) (d) at room temperature

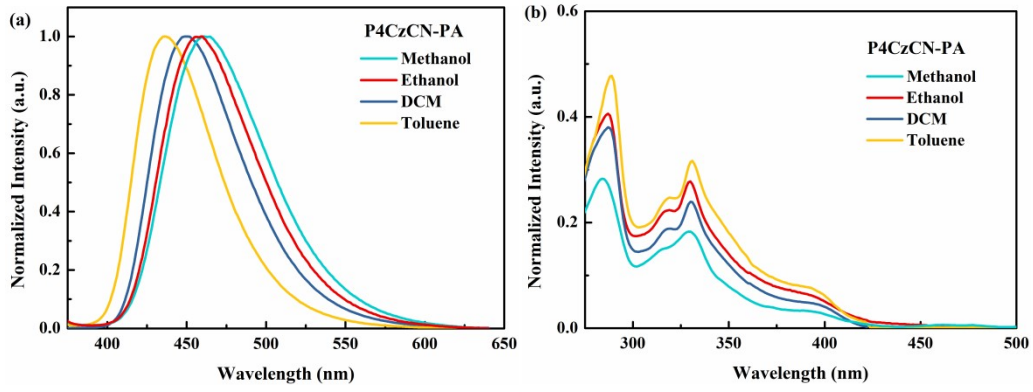
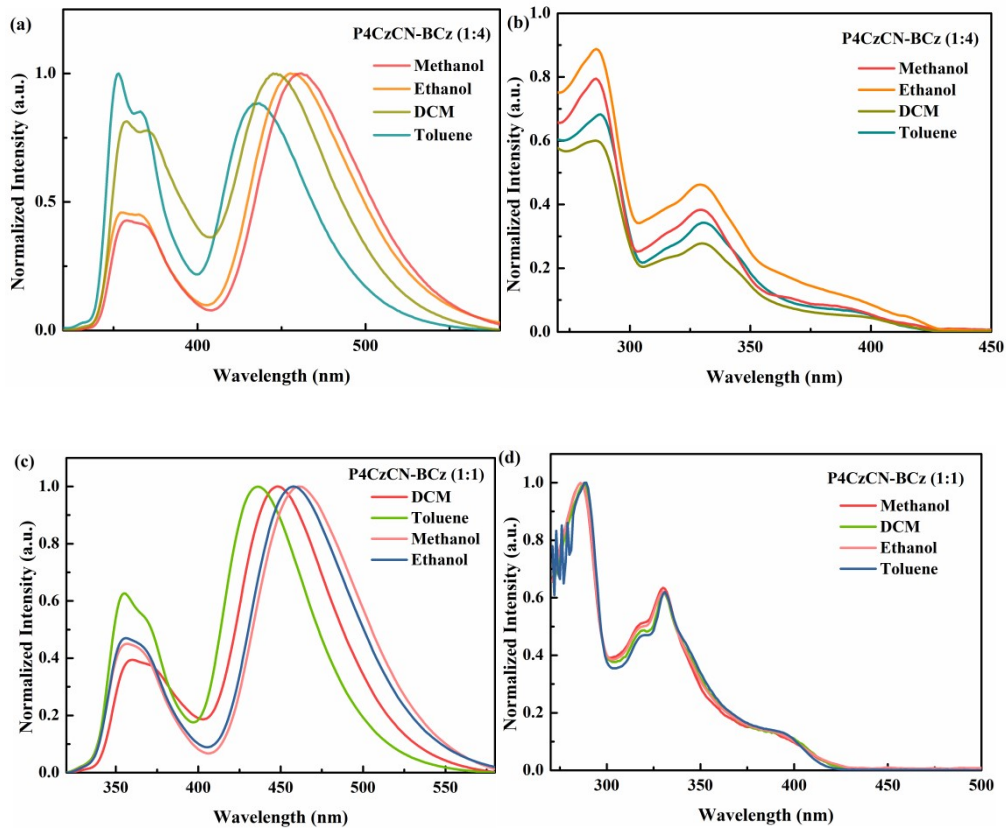


Figure S4. PL and UV spectra of P4CzCN-PA in different solvents.



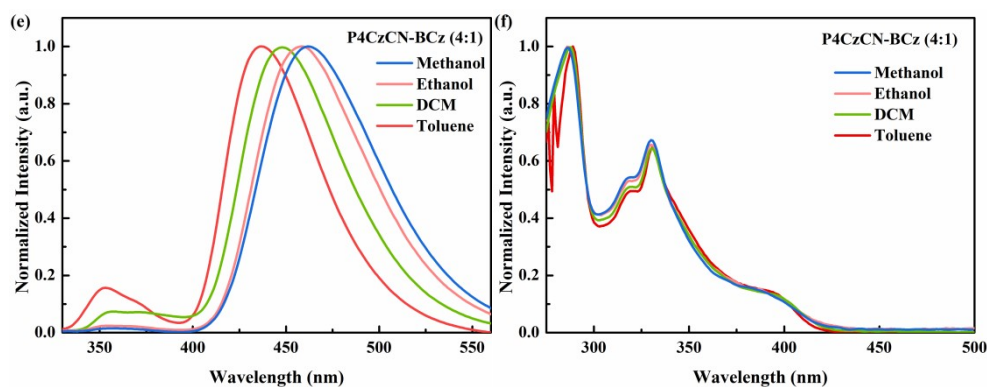


Figure S5. PL and UV spectra of P4CzCN-BCz (1:4) (a,b), P4CzCN-BCz (1:1) (c,d) and P4CzCN-BCz (4:1) (e,f) in different solvents.

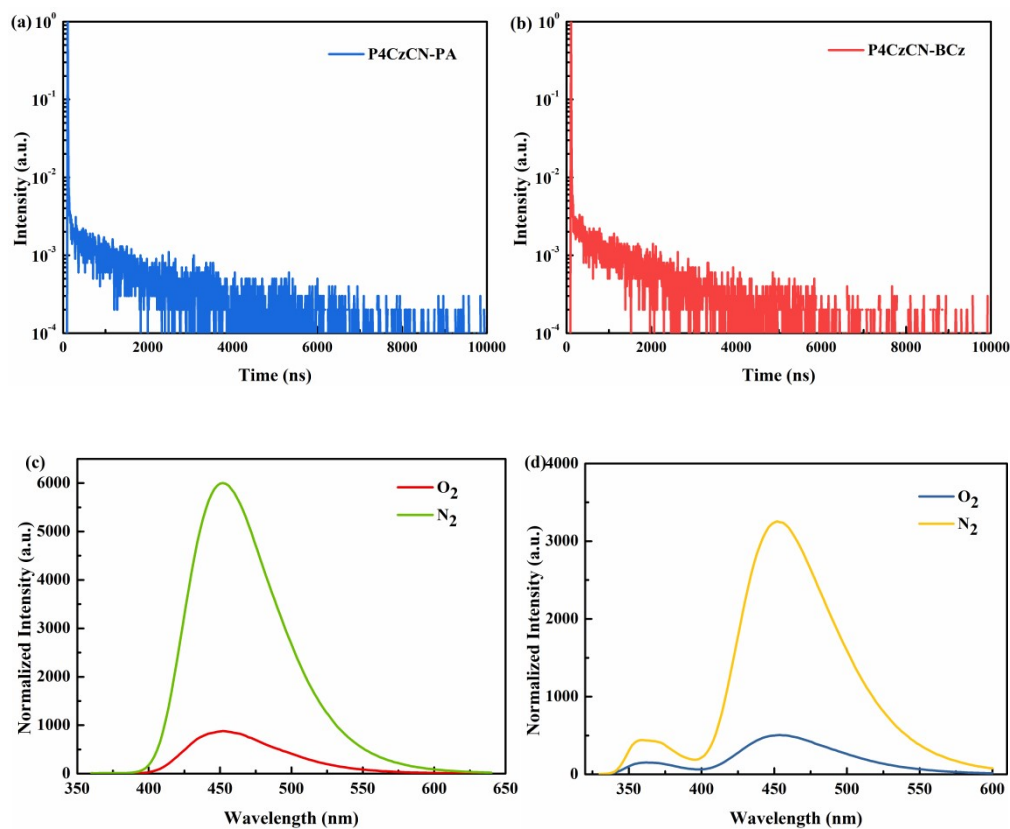


Figure S6. Transient photoluminescence decay curves of P4CzCN-PA (a), P4CzCN-BCz (b) and fluorescence spectra of P4CzCN-PA (c), P4CzCN-BCz (d) in O₂/N₂.

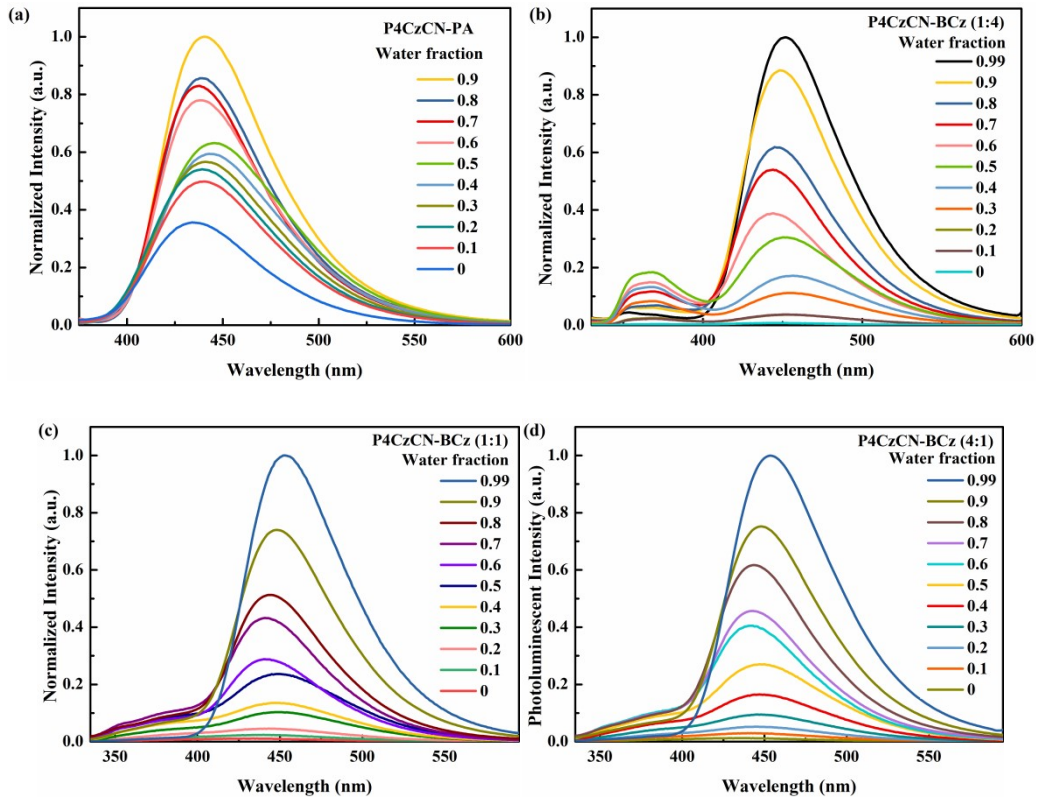


Figure S7. PL spectra of P4CzCN-PA (a), P4CzCN-BCz (1:4) (b), P4CzCN-BCz (1:1) (c), and P4CzCN-BCz (4:1) (d) in mixed solvents with different volume ratios of acetone and water.

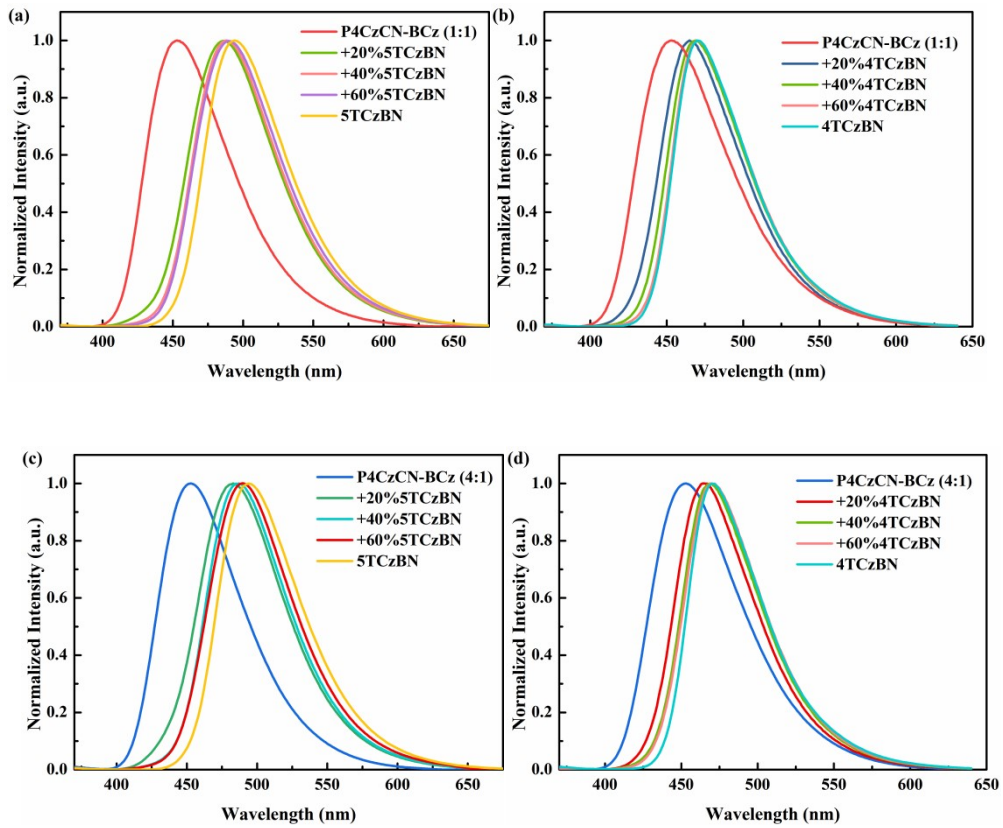


Figure S8 PL spectra of P4CzCN-BCz(1:1) (a,b) and P4CzCN-BCz(4:1) (c,d) films at different guest materials and doping concentration.

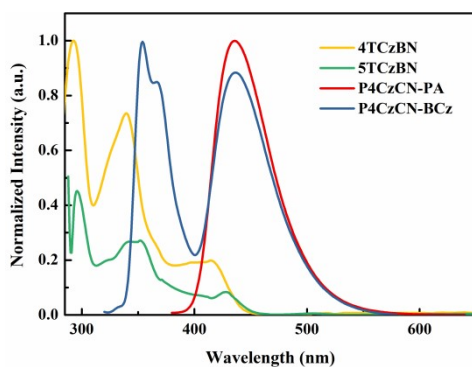


Figure S9 UV-vis absorption of 5TCzBN, 4TCzBN and PL emission of P4CzCN-PA, P4CzCN-BCz (1:4) in toluene solution.

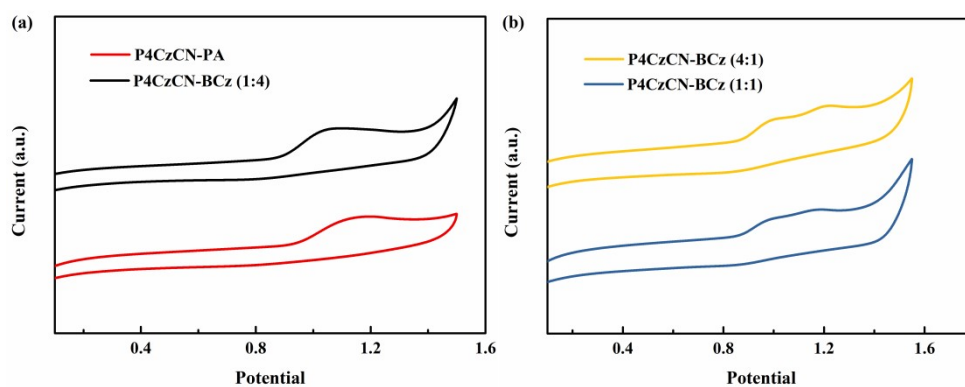
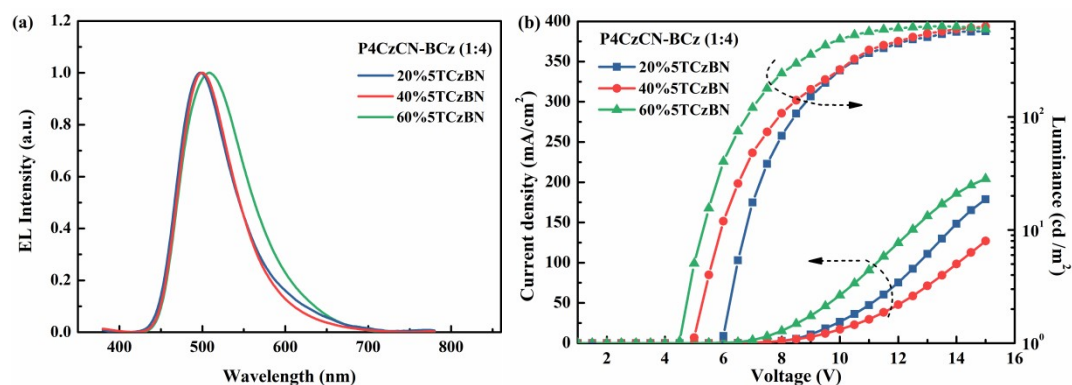


Figure S10. Cyclic voltammetry (CV) curves of P4CzCN-PA, P4CzCN-BCz(1:4) (a) and P4CzCN-BCz(1:1), P4CzCN-BCz(4:1) (b) measured at room temperature in CH_2Cl_2 .



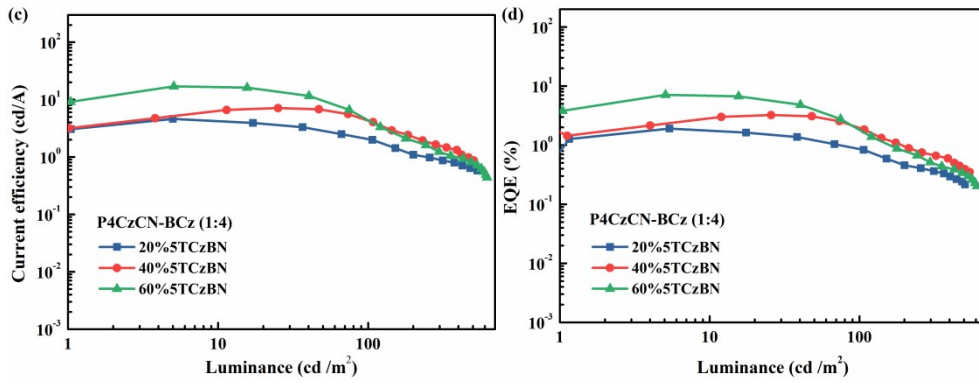


Figure S11 (a) The electroluminescence spectra, (b) current density-voltage-luminance (J-V-L) curves, (c) the curves of current efficiency (CE) versus luminance, (d) the curves of external quantum efficiency (EQE) versus luminance.

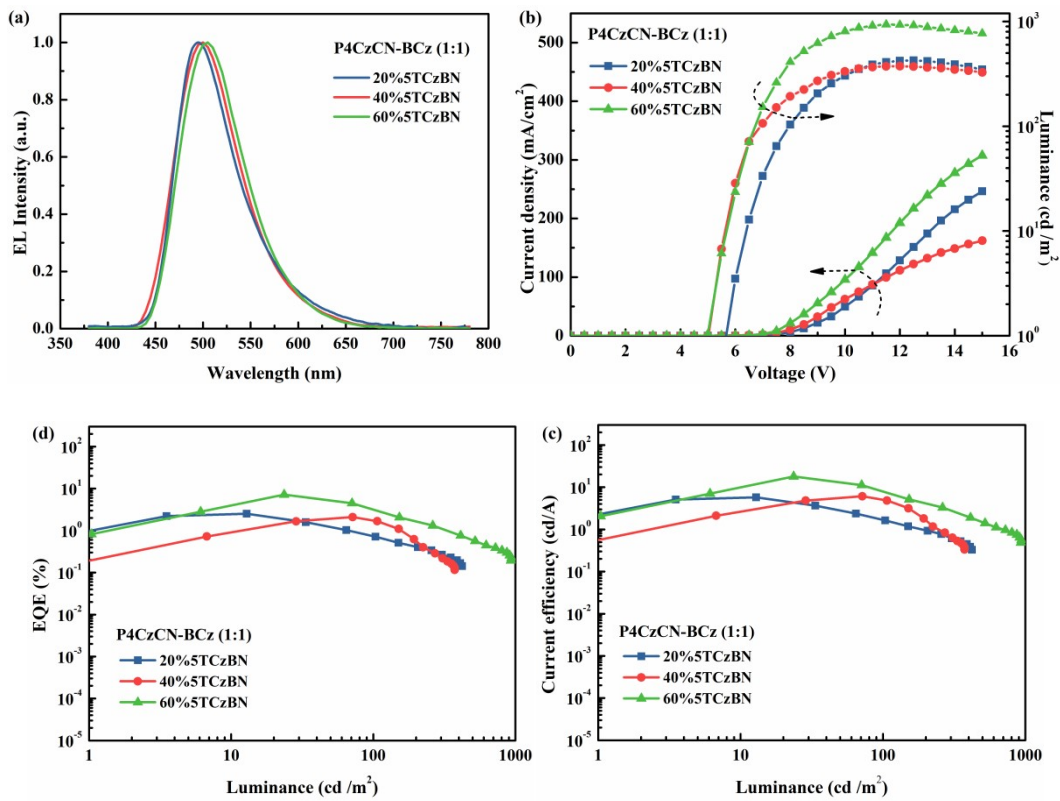


Figure S12 (a) The electroluminescence spectra, (b) current density-voltage-luminance (J-V-L) curves, (c) the curves of current efficiency (CE) versus luminance, (d) the curves of external quantum efficiency (EQE) versus luminance.

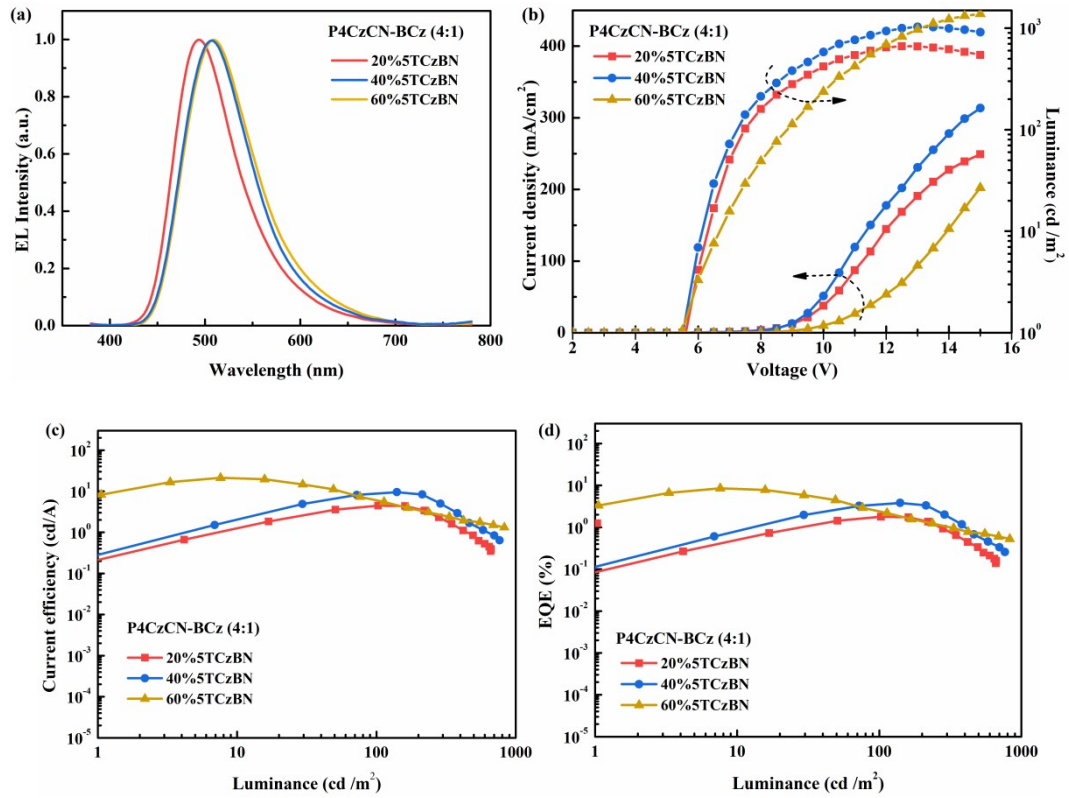


Figure S13 (a) The electroluminescence spectra, (b) current density-voltage-luminance (J-V-L) curves, (c) the curves of current efficiency (CE) versus luminance, (d) the curves of external quantum efficiency (EQE) versus luminance.

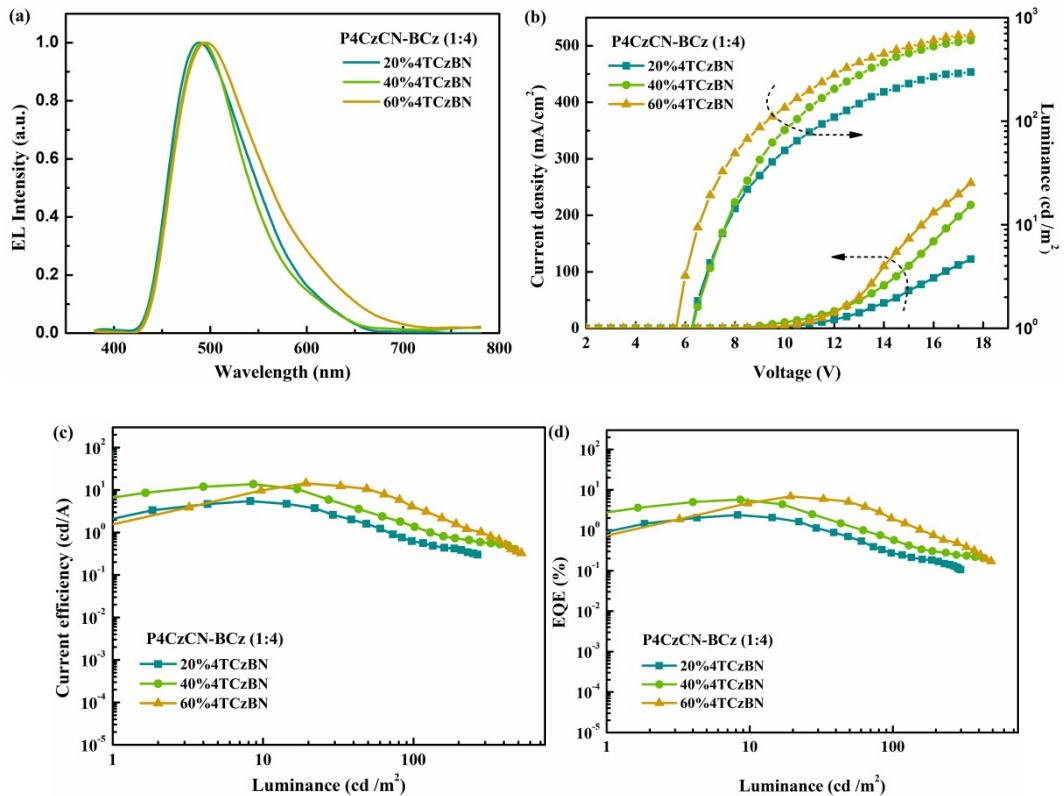


Figure S14 (a) The electroluminescence spectra, (b) current density-voltage-luminance (J-V-L) curves, (c) the curves of current efficiency (CE) versus luminance, (d) the curves of external quantum efficiency (EQE) versus luminance.

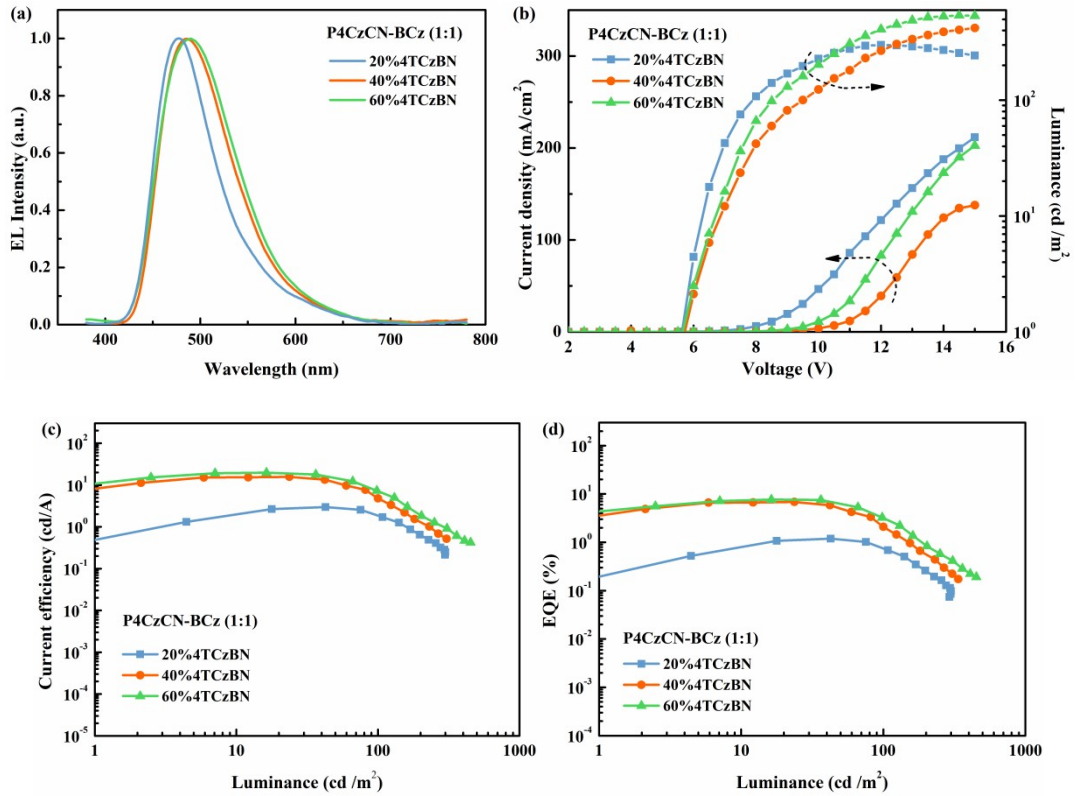
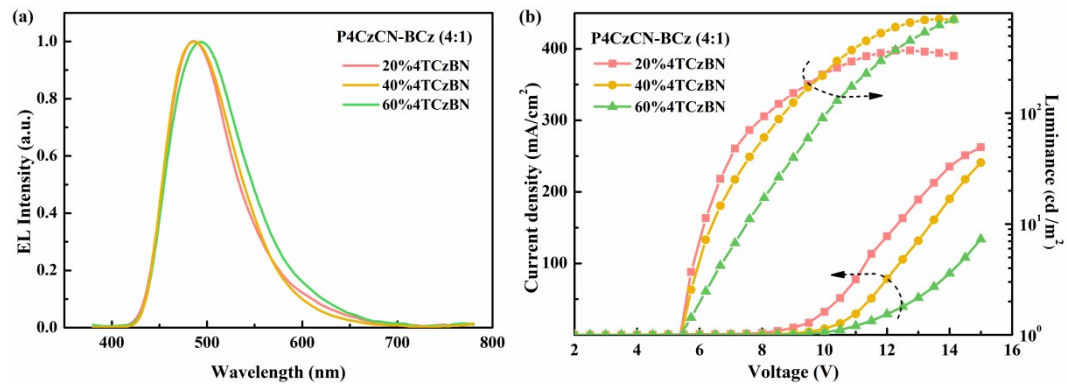


Figure S15 (a) The electroluminescence spectra, (b) current density-voltage-luminance (J-V-L) curves, (c) the curves of current efficiency (CE) versus luminance, (d) the curves of external quantum efficiency (EQE) versus luminance.



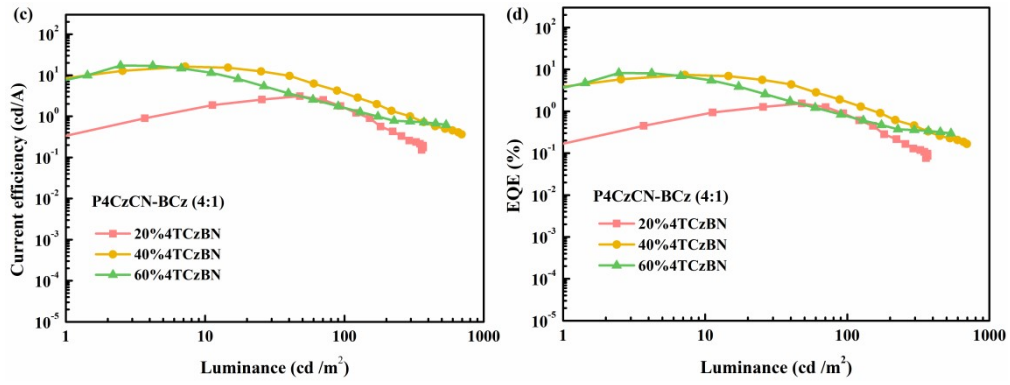


Figure S16 (a) The electroluminescence spectra, (b) current density-voltage-luminance (J-V-L) curves, (c) the curves of current efficiency (CE) versus luminance, (d) the curves of external quantum efficiency (EQE) versus luminance.

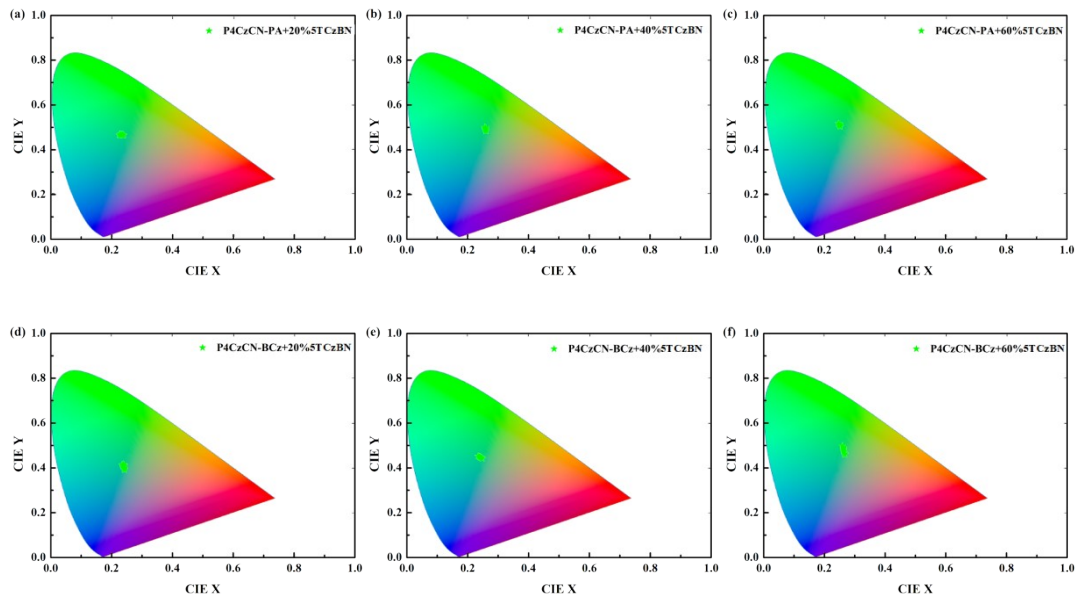
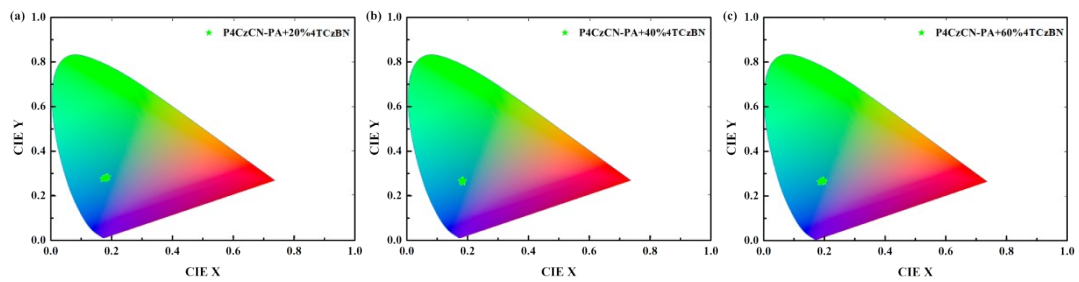


Figure S17 The green CIE of P4CzCN-PA and P4CzCN-BCz (1:4) in different doping concentration.



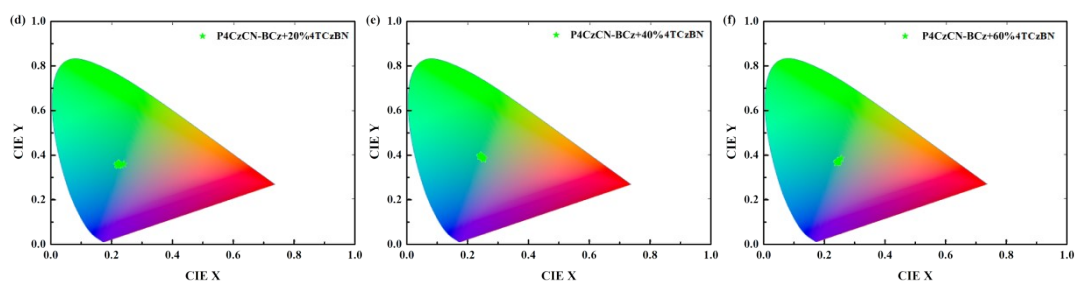


Figure S18 The blue CIE of P4CzCN-PA and P4CzCN-BCz (1:4) in different doping concentration.

Table S1. Device performance data of solution-processed TADF-OLEDs

| host | gust | Dopant conc. (wt.%) | EL peak [nm] | V_{on}^a [V] | CE_{max}^b [cd A ⁻¹] | PE_{max}^c [lm W ⁻¹] | EQE_{max}^d | CIE [x,y] ^e |
|---------------------|--------|------------------------|-----------------|-------------------|---------------------------------------|---------------------------------------|---------------|------------------------|
| P4CzCN-BCz (1:4) | 5tCzCN | 20 | 498 | 6 | 4.6 | 2.2 | 1.9 | (0.24, 0.40) |
| | | 40 | 500 | 5 | 6.8 | 3.6 | 3.2 | (0.25, 0.45) |
| | | 60 | 508 | 4.5 | 17.0 | 9.7 | 7.1 | (0.27, 0.49) |
| | 4tCzCN | 20 | 488 | 6.4 | 4.7 | 2.3 | 2.4 | (0.23, 0.36) |
| | | 40 | 492 | 6.3 | 13.7 | 5.7 | 5.7 | (0.24, 0.38) |
| | | 60 | 495 | 5.8 | 14.4 | 6.5 | 6.9 | (0.25, 0.37) |
| P4CzCN-BCz (1:1) | 5tCzCN | 20 | 495 | 5.8 | 5.8 | 2.8 | 2.5 | (0.24, 0.39) |
| | | 40 | 500 | 5.1 | 6.1 | 2.9 | 2.1 | (0.25, 0.40) |
| | | 60 | 504 | 5 | 17.9 | 9.4 | 7.2 | (0.25, 0.43) |
| | 4tCzCN | 20 | 477 | 5.7 | 3.0 | 1.3 | 1.2 | (0.21, 0.26) |
| | | 40 | 485 | 5.8 | 15.7 | 7.3 | 6.8 | (0.24, 0.38) |
| | | 60 | 490 | 5.7 | 19.8 | 7.6 | 7.6 | (0.24, 0.39) |

^aTurn on voltage at luminance of 1 cd m⁻². ^bMaximum current efficiency. ^cMaximum power efficiency.

^dMaximum external quantum efficiency. ^eCIE = the Commission Internationale de L'Eclairage coordinates

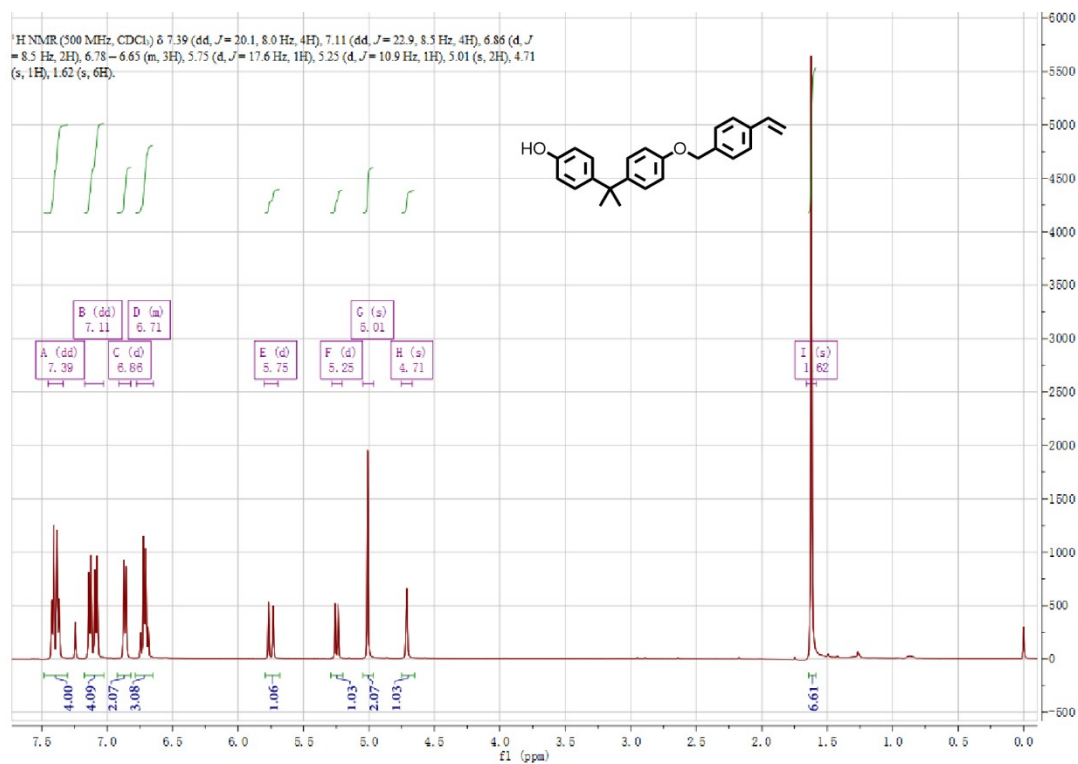


Figure S19. ¹H NMR spectra of 4-(2-(4-((4-vinylbenzyl)oxy)phenyl)propan-2-yl)phenol.

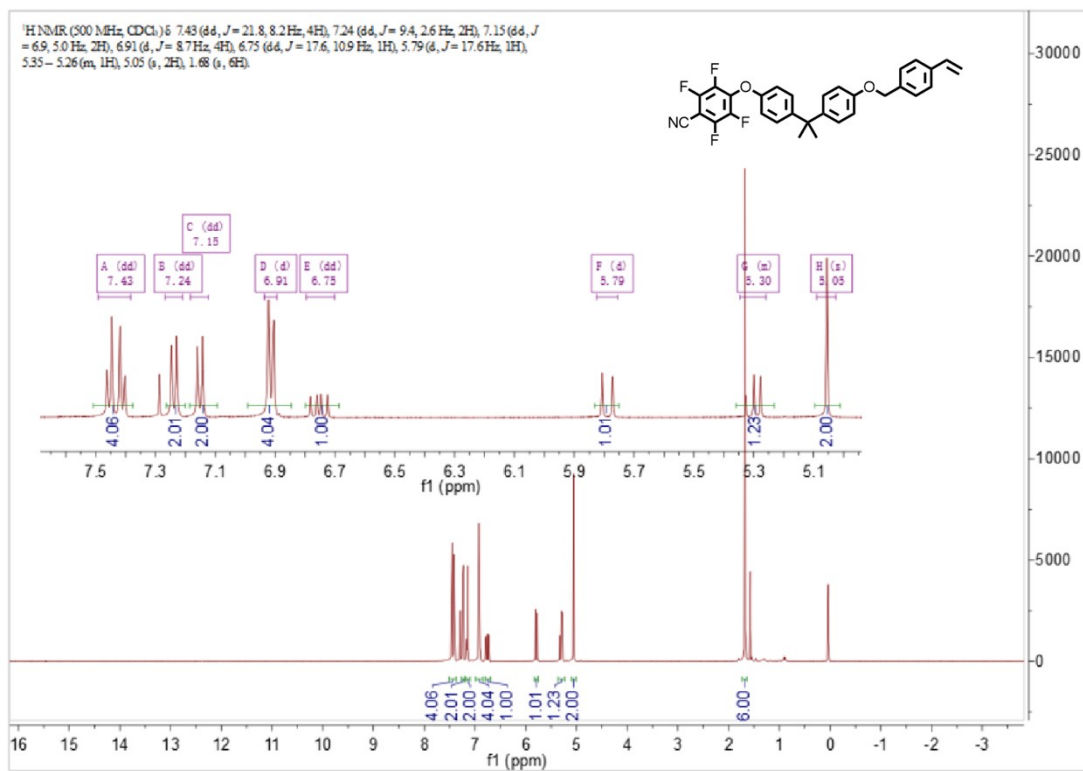


Figure S20. ¹H NMR spectra of 4FCN-PA.

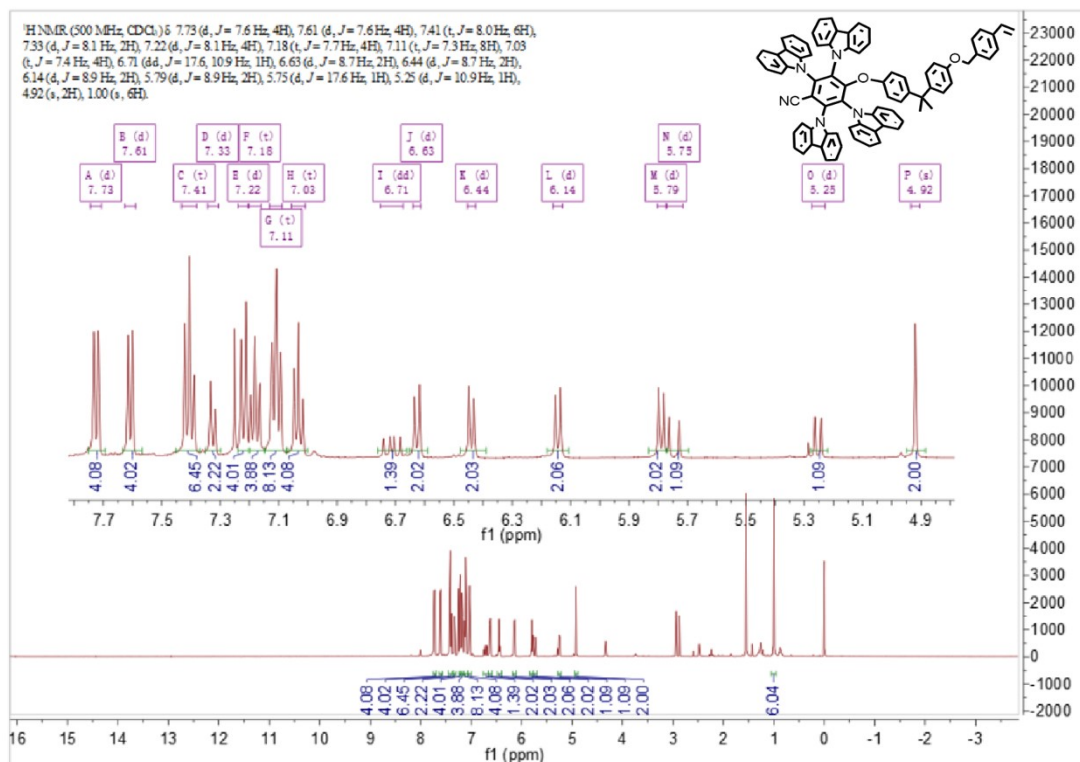


Figure S21. ¹H NMR spectra of M1.

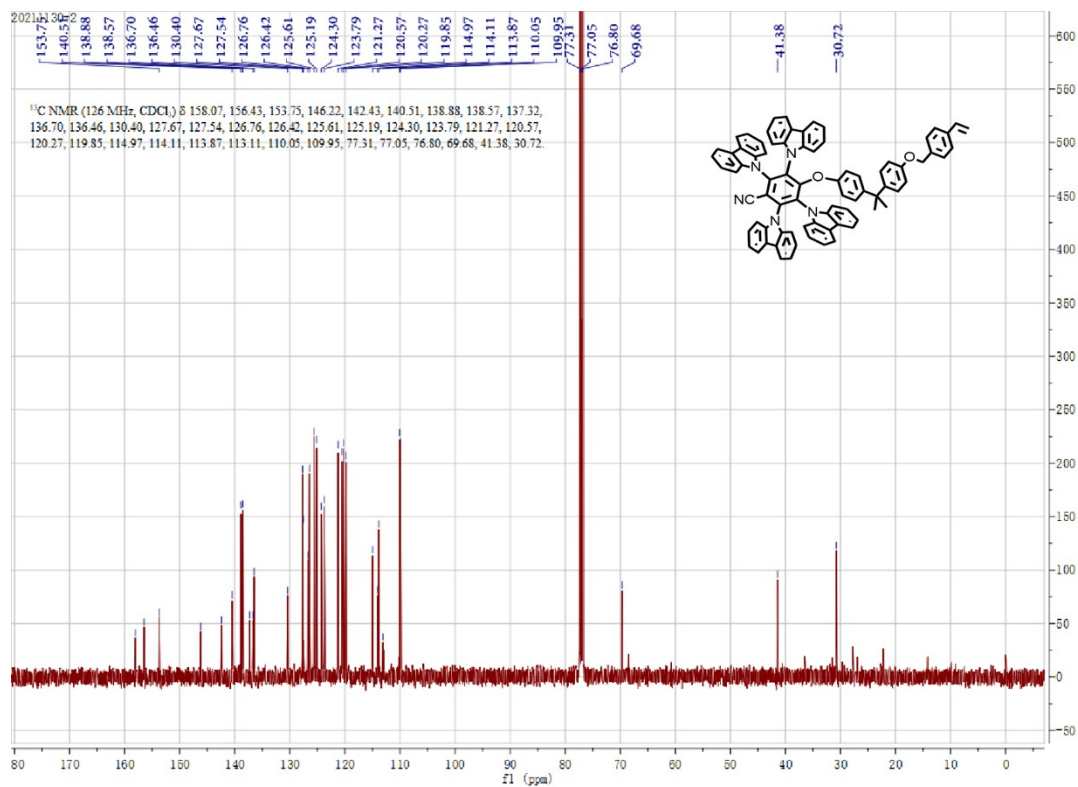


Figure S22. ¹³C NMR spectra of M1.

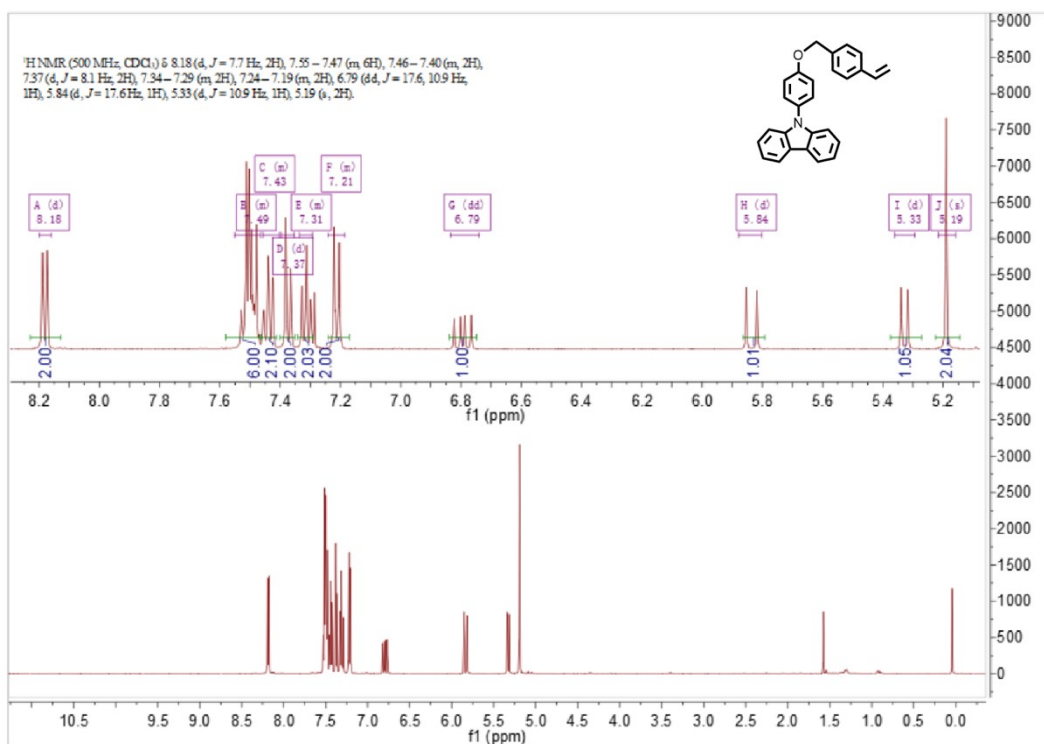


Figure S23. ¹H NMR spectra of M2.

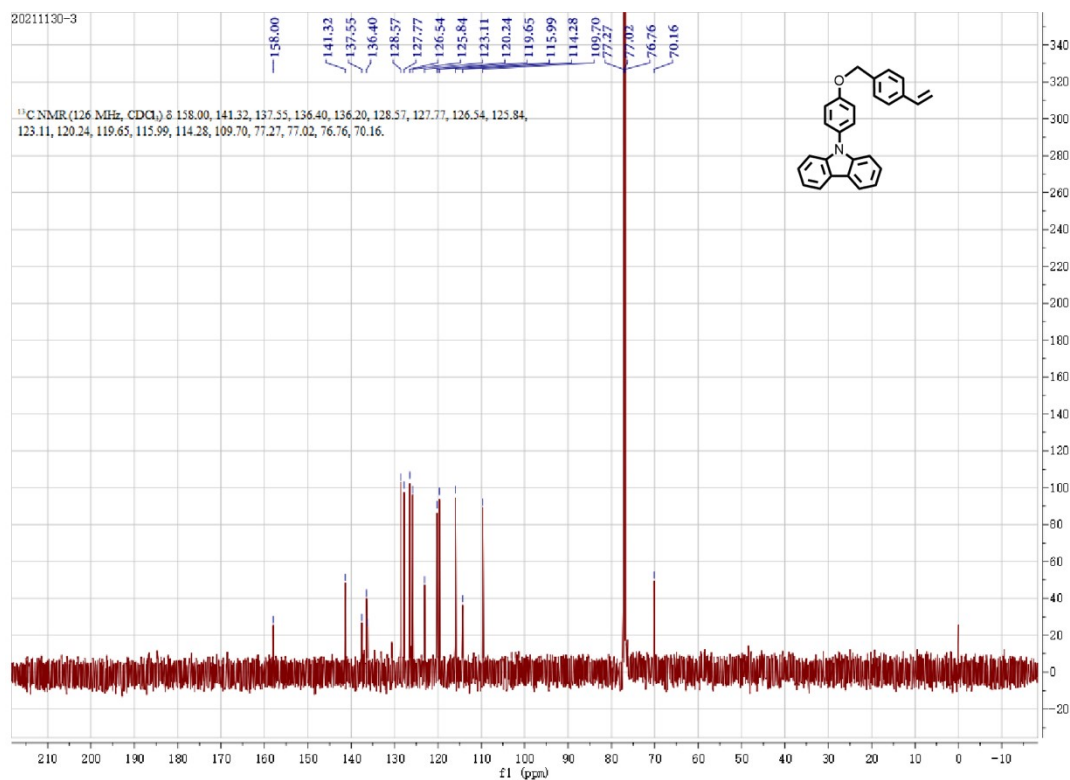


Figure S24. ^{13}C NMR spectra of M2.