Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supporting Information

Naphthalimide-arylamine Derivatives with Aggregation Induced Delayed Fluorescence for Realizing Efficient Green to Red Electroluminescence

Shuo Chen,[a] Pengju Zeng,[a] Weigao Wang,[a] Xuedong Wang,[b] Yukun Wu,[c] Pengju Lin,[a] Zhengchun Peng*,[a]

[a] *Key Laboratory of Optoelectronic Devices and Systems of Ministry of Education and Guangdong Province, College of Optoelectronic Engineering, Shenzhen University, Shenzhen, Guangdong, 518060, P.R. China*

[b] *Jiangsu Key Laboratory for Carbon-Based Functional Materials & Devices, Institute of Functional Nano & Soft Materials (FUNSOM) & Collaborative, Innovation Center of Suzhou Nano Science and Technology, Soochow University, Suzhou, Jiangsu, 215123, P.R. China*

[c] *Key Lab of Advanced Transducers and Intelligent Control System, College of Physics and Optoelectronics, Taiyuan University of Technology, Taiyuan, Shanxi, 030024, P.R. China*

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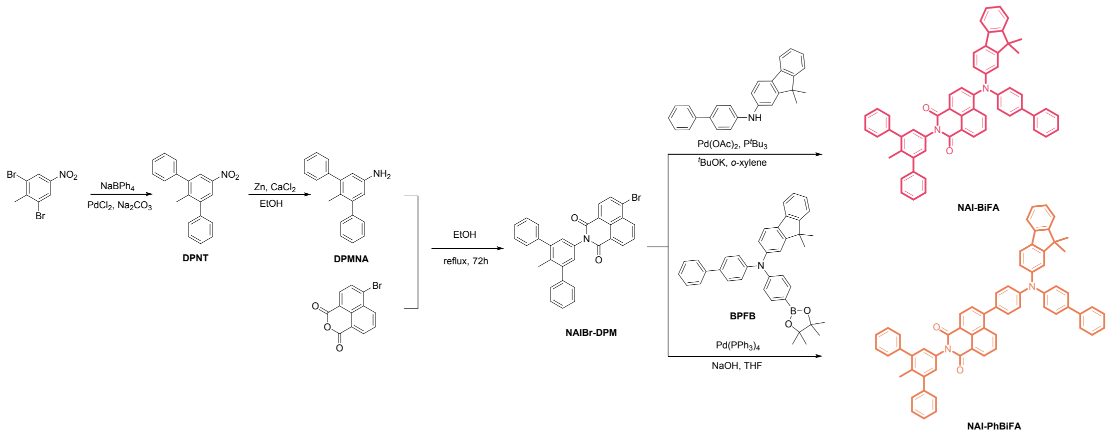


Scheme S1. Synthetic routes of the investigated compounds **NAI-BiFA** and **NAI-PhBiFA**.

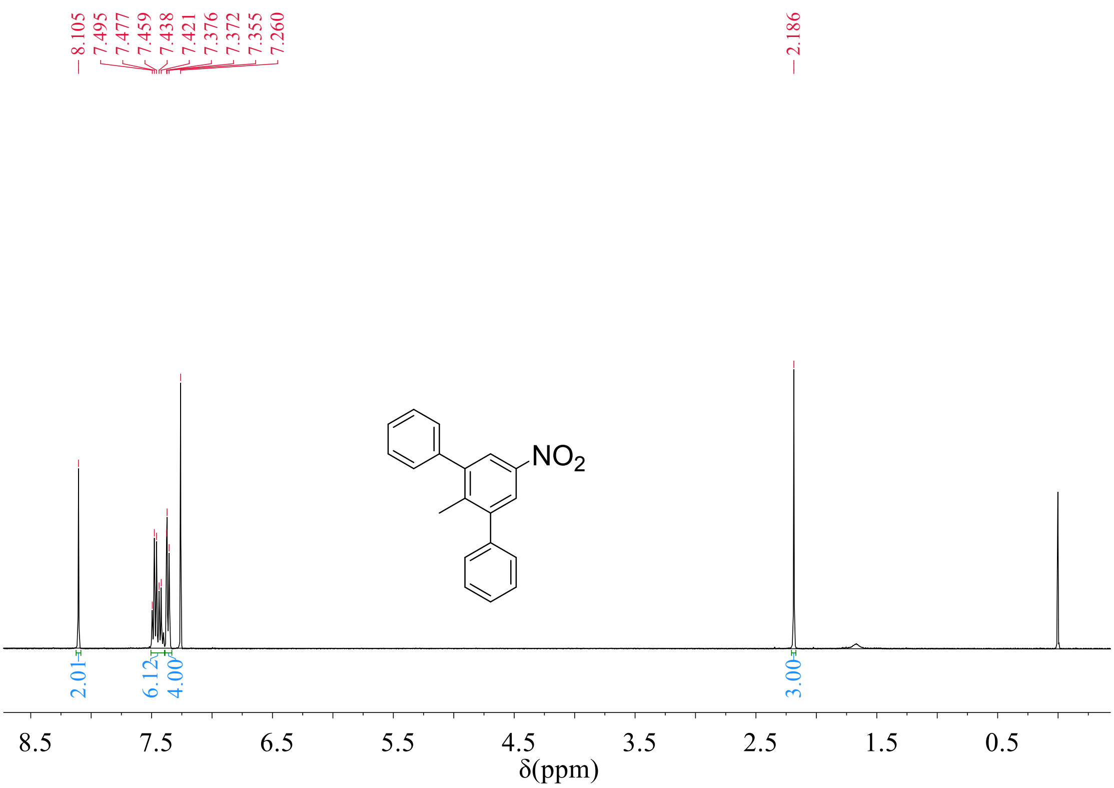


Figure S1. ^{1}H NMR spectrum of compound **DPNT**.

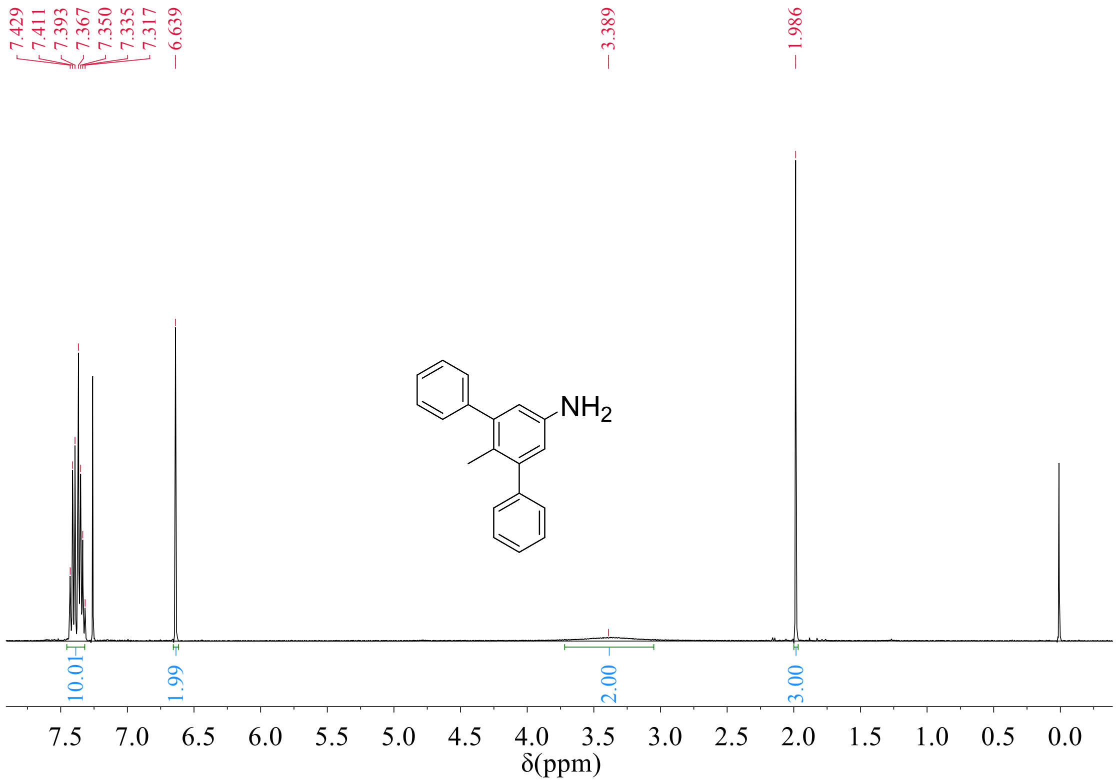


Figure S2. ^{1}H NMR spectrum of compound **DPMNA**.

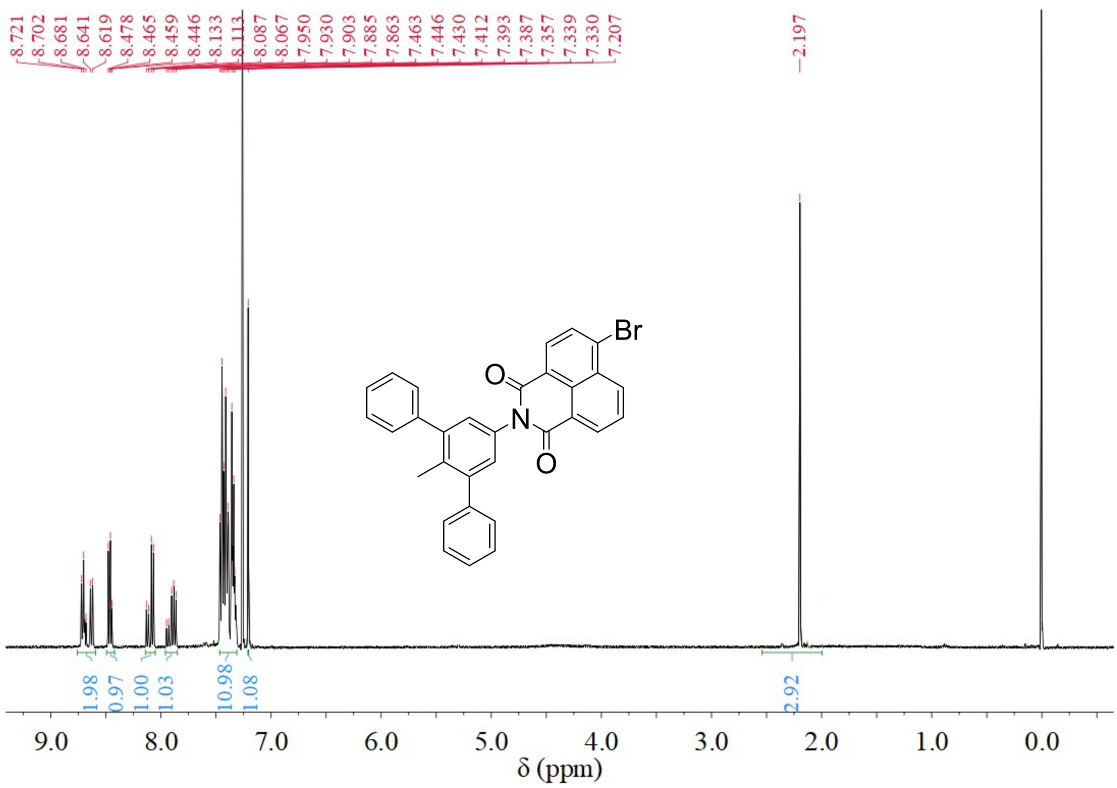


Figure S3. ^{1}H NMR spectrum of compound **NAIBr-DPM**.

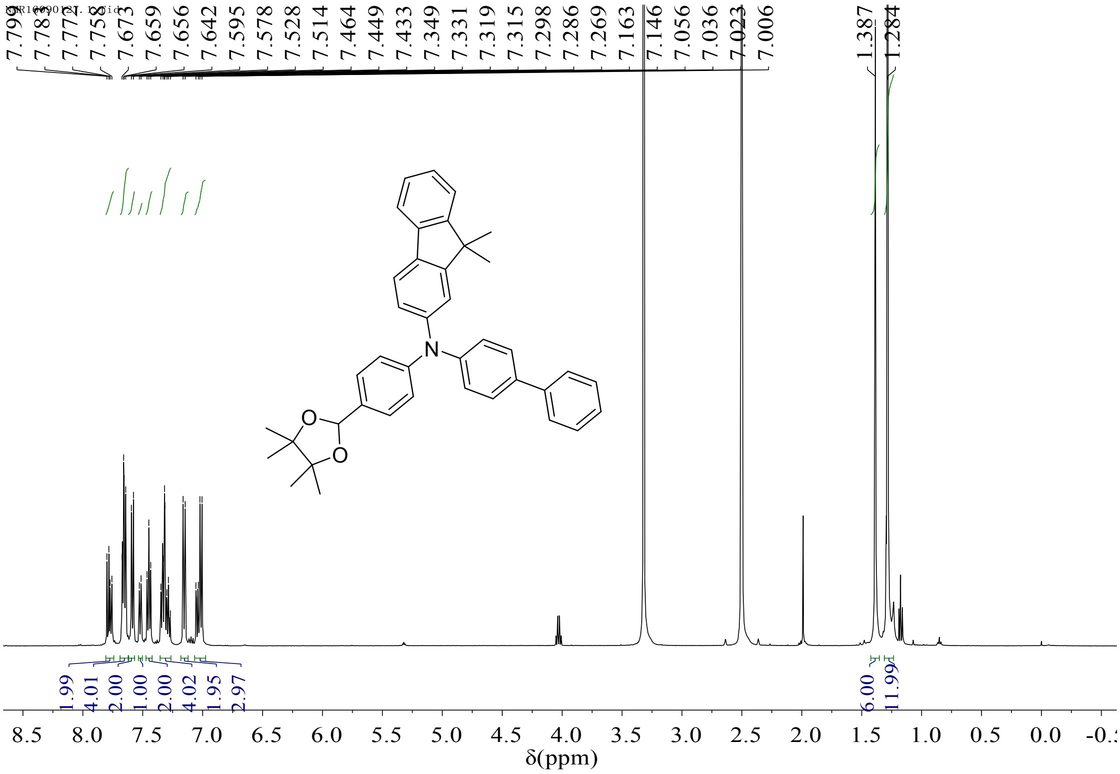


Figure S4. ^{1}H NMR spectrum of compound **BPFB**.

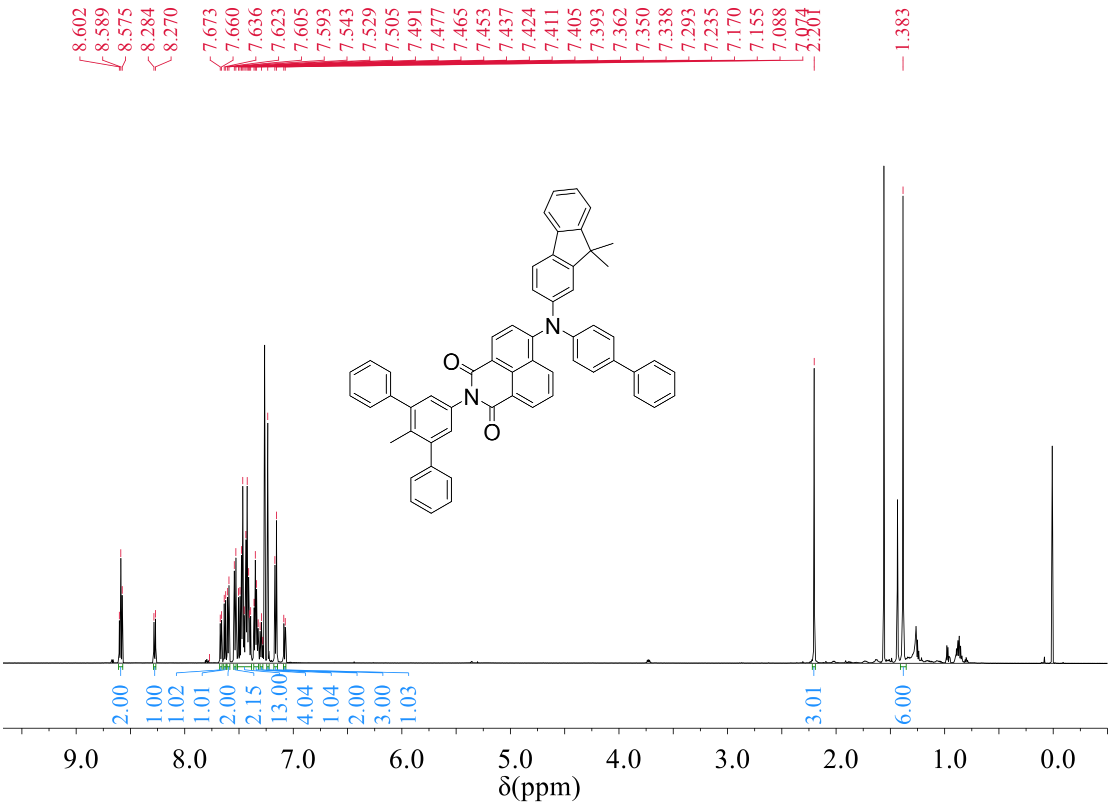


Figure S5. ^{1}H NMR spectrum of compound **NAI-BiFA**.

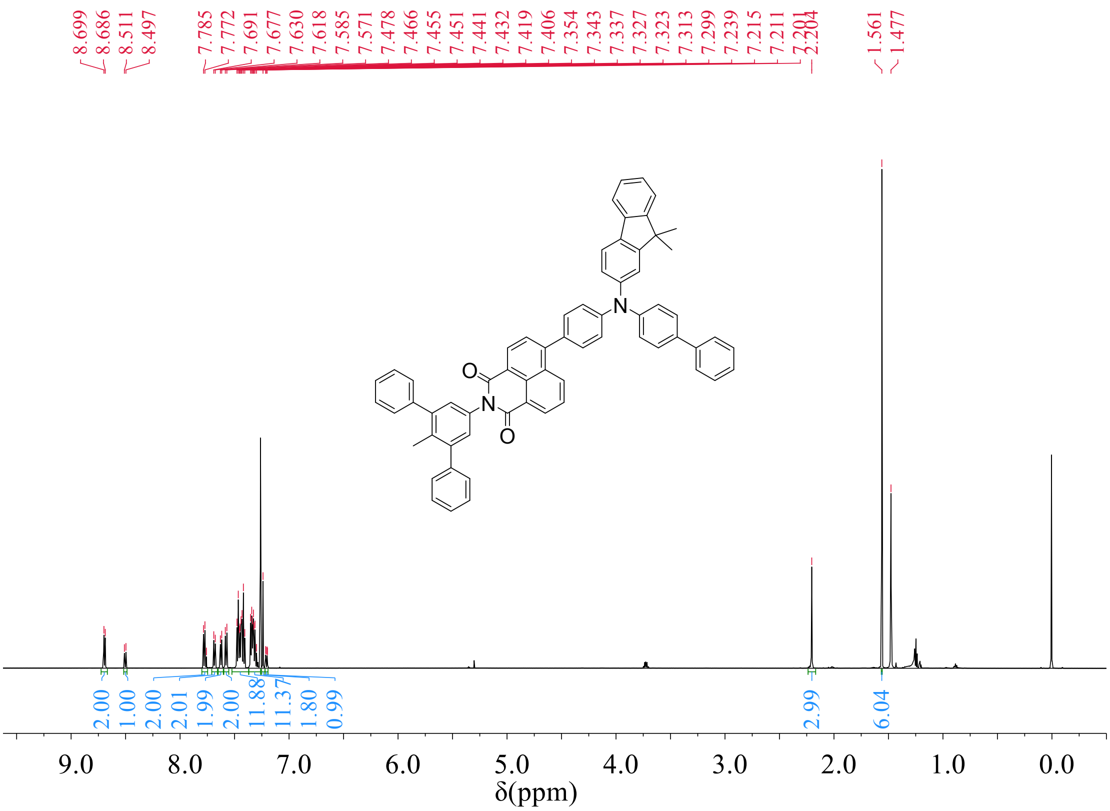


Figure S6. ^{1}H NMR spectrum of compound **NAI-PhBiFA**.

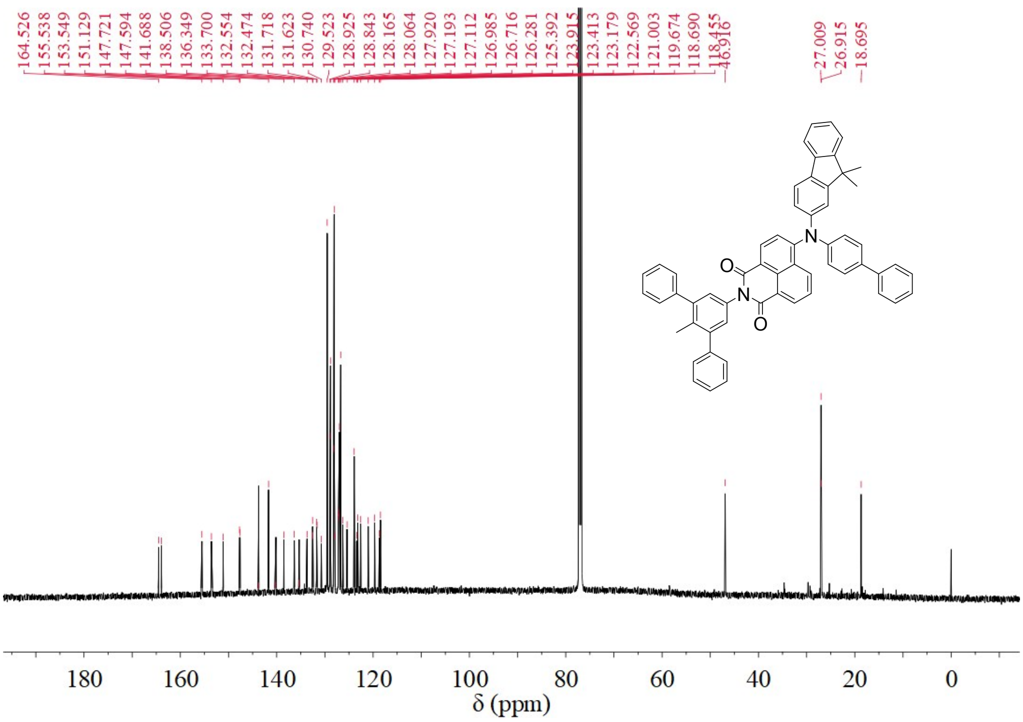


Figure S7. ^{13}C NMR spectrum of compound **NAI-BiFA**.

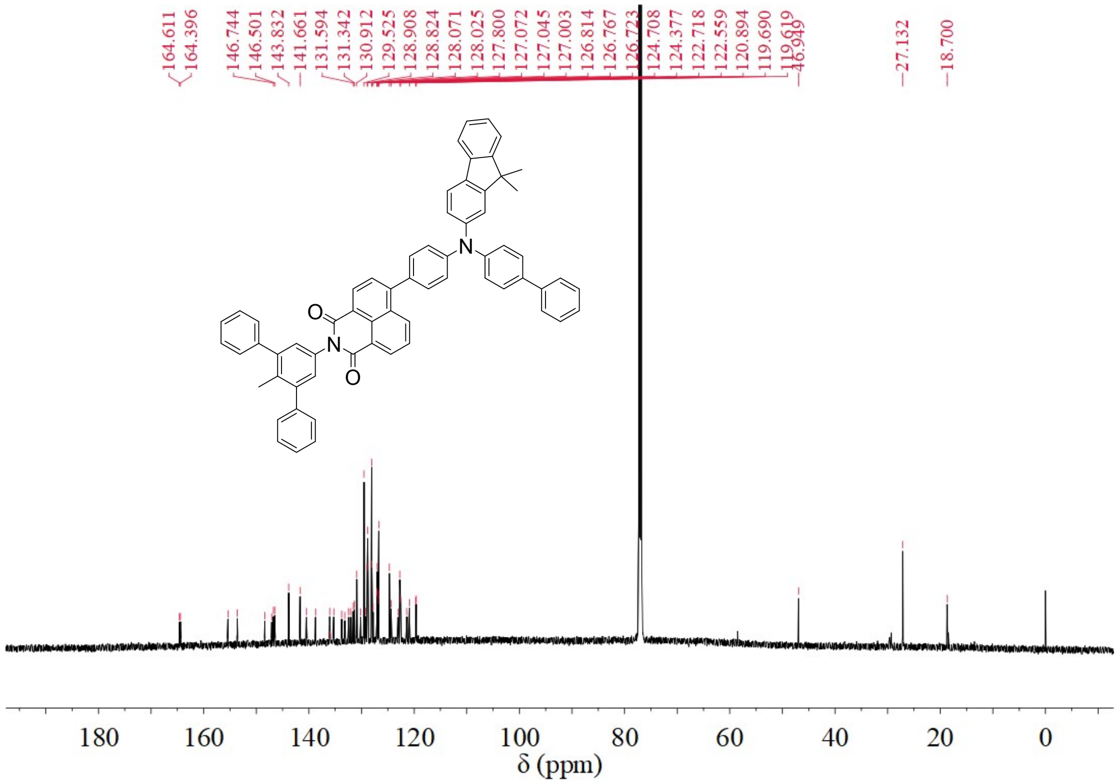


Figure S8. ^{13}C NMR spectrum of compound **NAI-PhBiFA**.

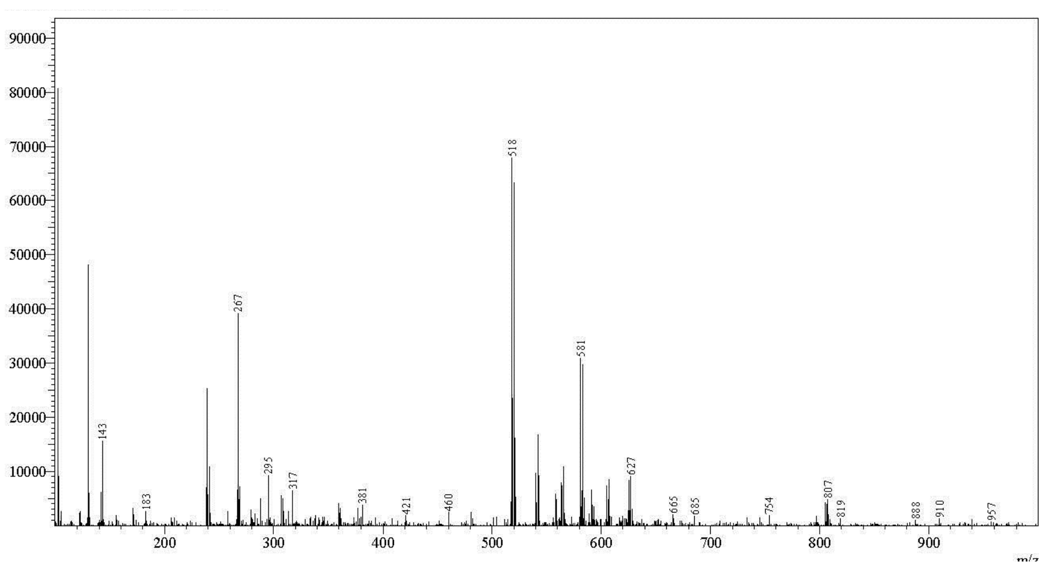
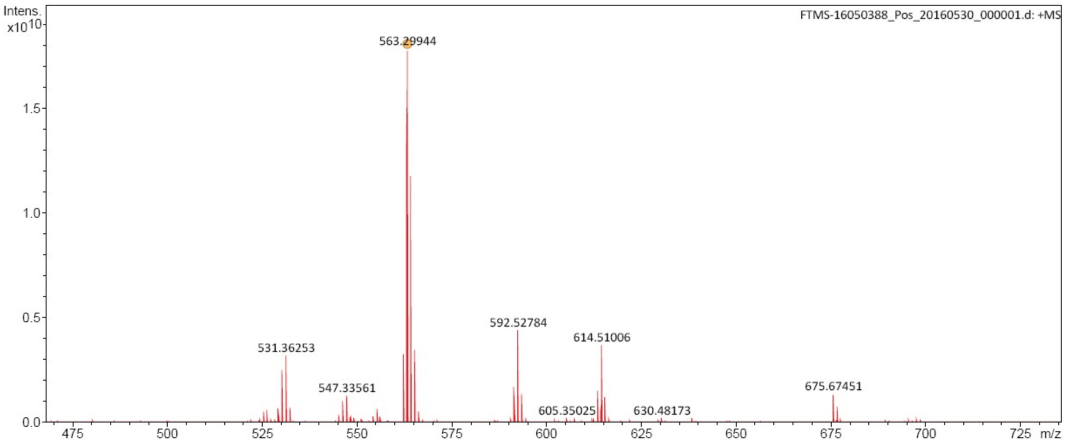


Figure S9. MS spectrum of compound **NAIBr-DPM**.



Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
563.299440	1	C39H38BNO2	100.00	563.299011	0.4	-0.6	136.7	22.0	odd	ok

Figure S10. HR-MS spectrum of compound **BPFB**.

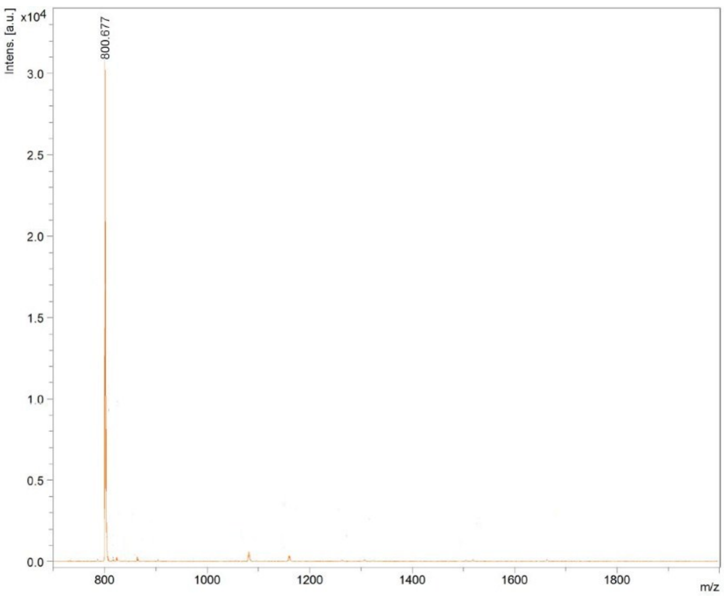


Figure S11. HR-MS spectrum of compound **NAI-BiFA**.

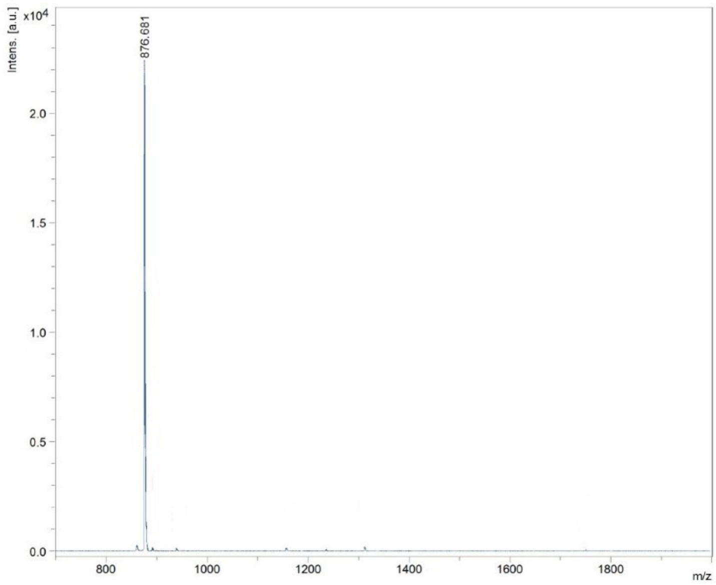


Figure S12. HR-MS spectrum of compound **NAI-PhBiFA**.

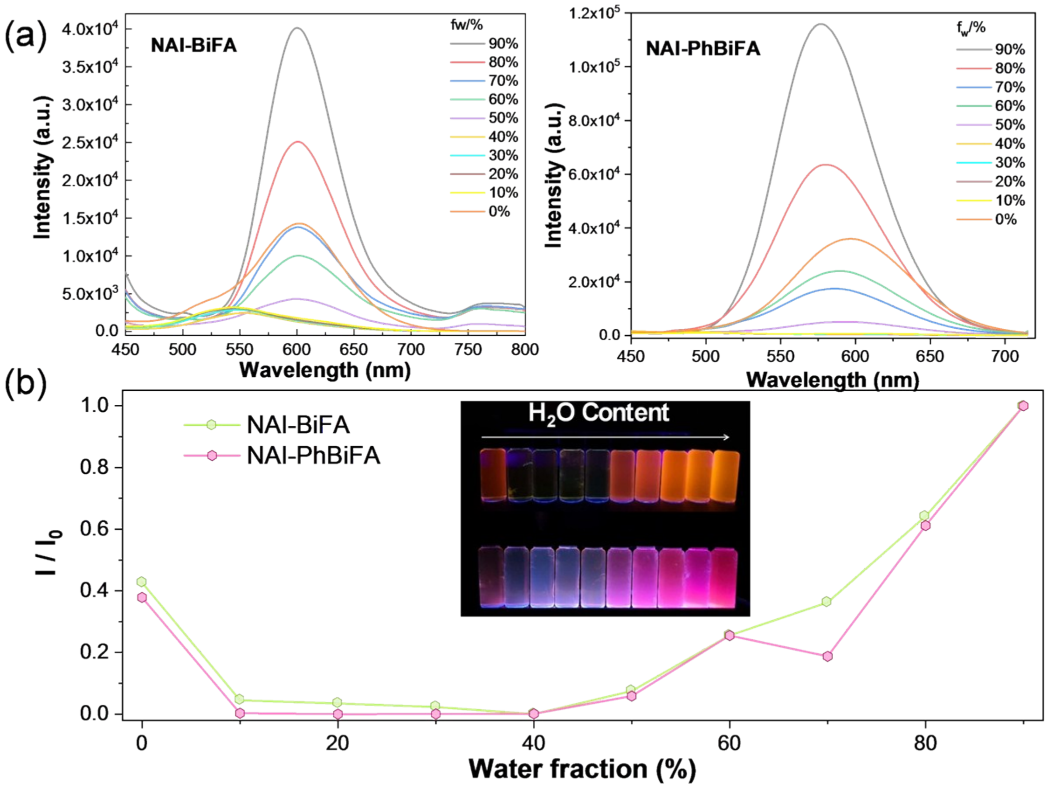
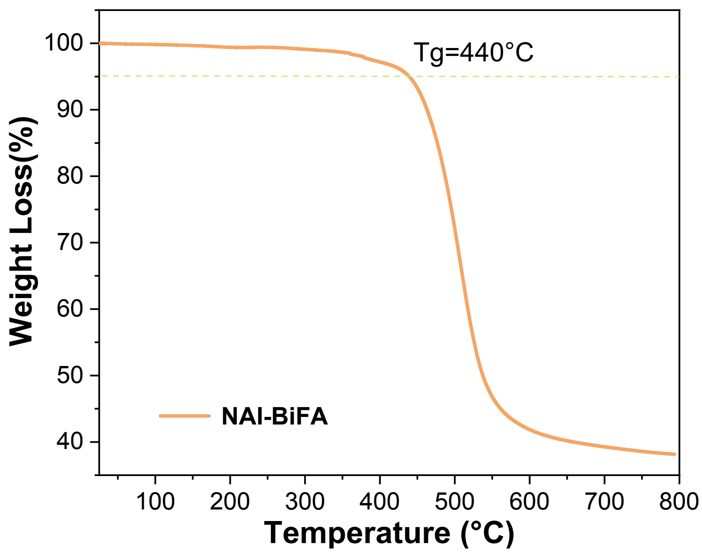


Figure S13. (a) PL spectra of **NAI-BiFA** and **NAI-PhBiFA** in THF/H_2O mixtures with different water fractions (f_w) and (b) Changes in the emission intensity of **NAI-BiFA** and **NAI-PhBiFA** in THF–H_2O mixtures with various volume fractions of water (0–90%). Inset: Photographs of **NAI-BiFA** (top) and **NAI-PhBiFA** (bottom) in solvents with increased f_w under 365 nm hand lamp irradiation.



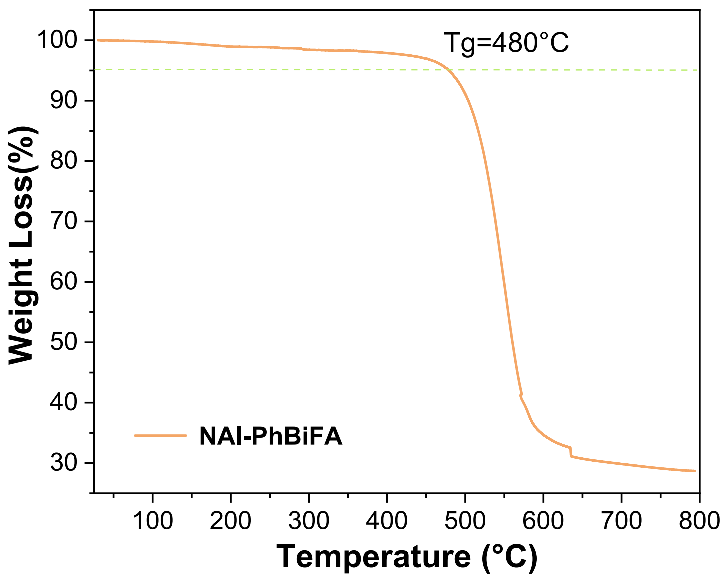


Figure S14. TGA diagram for **NAI-BiFA** and **NAI-PhBiFA** recorded at a heating rate of 10 °C min^{-1} under nitrogen flushing.

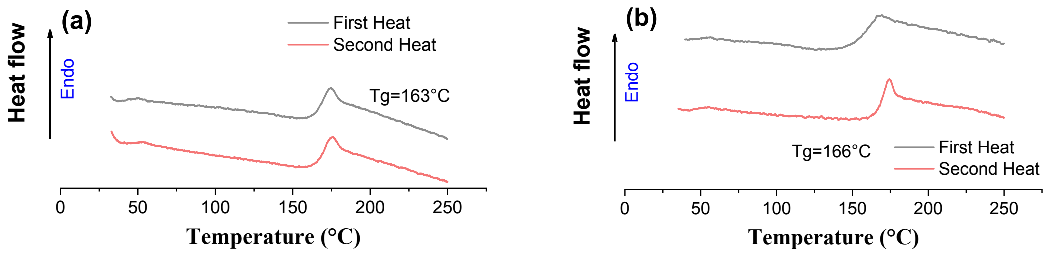


Figure S15. DSC spectra of the first and second heating cyclings for **NAI-BiFA** (a) and **NAI-PhBiFA** (b), at a heating rate of 10 °C min^{-1} under nitrogen flushing.

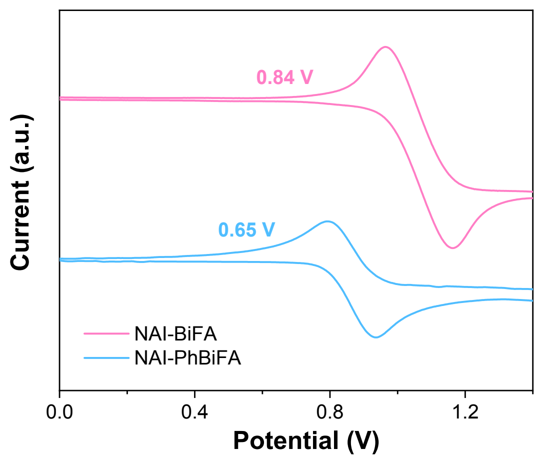


Figure S16. Cyclic voltammogram of compouds **NAI-BiFA** and **NAI-PhBiFA** in the anode scan.

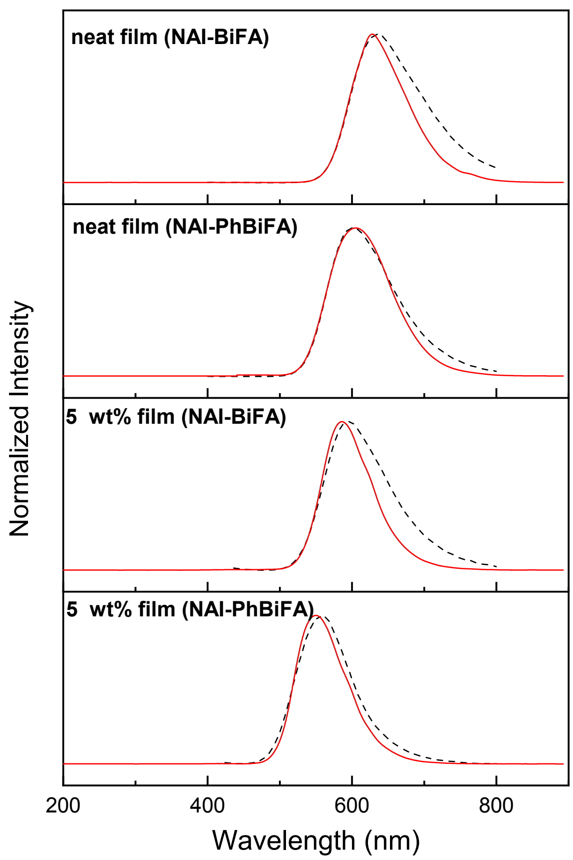


Figure S17. Comparison of the electroluminescence spectra of OLEDs (solid line) and the photoluminescence spectra of the thin films (dash line).

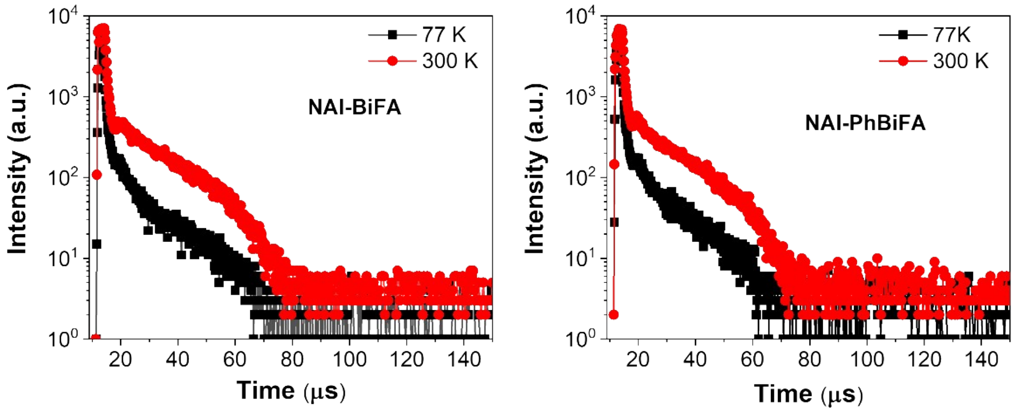


Figure S18. PL transient decay spectra at 77 K and 300 K for 5 wt%-doped thin films of **NAI-BiFA** and **NAI-PhBiFA** in a CBP host.

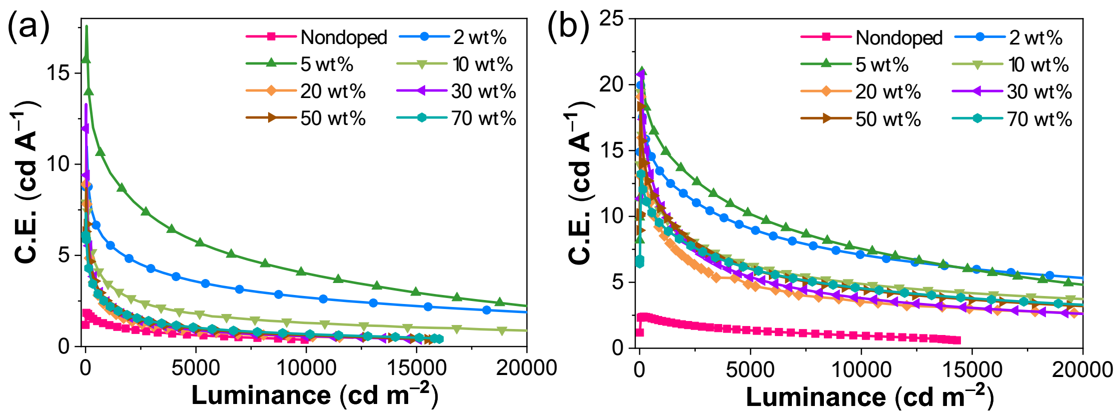


Figure S19. Power efficiency-luminance characteristics of OLEDs based on **NAI-BiFA** (a) and **NAI-PhBiFA** (b).

Calculation of Rate Constants

The rate constants were calculated according to following equation:

$$k_r(S_1 \rightarrow S_0) = \frac{\Phi_p}{\tau_p} \qquad \textbf{S1}$$

$$k_{nr}(S_1 \rightarrow S_0) = k_r \frac{1 - \Phi_{PL}}{\Phi_{PL}} \qquad \textbf{S2}$$

$$k_{ISC}(S_1 \rightarrow T_1) = k_r \left(\frac{1}{\Phi_p} - \frac{1}{\Phi_{PL}} \right) \qquad \textbf{S3}$$

$$k_{RISC}(T_1 \rightarrow S_1) = \frac{\Phi_{PL}}{k_r \tau_p \tau_d} \qquad \textbf{S4}$$

Where $\boldsymbol{\tau_p}$ and $\boldsymbol{\tau_d}$ represent lifetimes of the prompt and delayed decay components, respectively. $\boldsymbol{\Phi_{PL}}$, $\boldsymbol{\Phi_p}$ and $\boldsymbol{\Phi_d}$ represent PL quantum yield, quantum yields for prompt fluorescence and delayed fluorescence, respectively ($\boldsymbol{\Phi_{PL} = \Phi_p + \Phi_d}$). $\boldsymbol{k_r}$, $\boldsymbol{k_{nr}}$, $\boldsymbol{k_{ISC}}$ and $\boldsymbol{k_{RISC}}$ represent the rate constant for fluorescence radiative decay, nonradiative internal conversion, intersystem crossing (ISC) and reverse intersystem crossing (RISC), respectively.

$\boldsymbol{\Phi_p}$ and $\boldsymbol{\Phi_d}$ can be calculated by Equations S5 and S6

$$\Phi_p = \frac{A_1 \cdot \tau_p}{A_1 \cdot \tau_p + A_2 \cdot \tau_d} \Phi_{PL} \qquad \textbf{S5}$$

$$\Phi_d = \frac{A_2 \cdot \tau_d}{A_1 \cdot \tau_p + A_2 \cdot \tau_d} \Phi_{PL} \qquad \textbf{S6}$$

Where **A_1 and A_2** represent frequency factors. Transient PL curves could be fitted with a biexponential model as: $I(t) = A_1 \cdot \exp\left(-\frac{t_1}{\tau_p}\right) + A_2 \cdot \exp\left(-\frac{t_2}{\tau_d}\right)$