

Supporting Information

for

A deep-red fluorophore based on naphthothiadiazole as emitter with hybridized local and charge transfer and ambipolar transporting properties for electroluminescent devices

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Energy diagram of singlet and triplet excited states estimated by CAM-B3LYP/6-31G(d,p) calculations and copies of ¹H NMR, ¹³C NMR, and HRMS spectra of the synthesized compounds

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Figure S1: The energy diagram of singlet and triplet excited states of the compound estimated by CAM-B3LYP/6-31G(d,p) calculations.



Figure S2: ¹H NMR spectrum of 2 in CDCl₃ (600 MHz) @ 25 °C.



Figure S3: ¹³C NMR spectrum of **2** in CDCl₃ (151 MHz) @ 25 °C.



Figure S4: APCI–TOF mass spectrum $[M + H]^+$ of **2**.



Figure S5: APCI–TOF mass spectrum $[M + H]^+$ of the crude product mixute from the NBS bromination in the synthesis of compound **3**.



Figure S7: ¹³C NMR spectrum of **3** in CDCl₃ (151 MHz) @ 25 °C.



Figure S8: APCI–TOF mass spectrum $[M + H]^+$ of **3**.



Figure S9: ¹H NMR spectrum of TPECNz in CDCl₃ (600 MHz) @ 25 °C.





Figure S11: MALDI–TOF mass spectrum [M]⁺ of TPECNz.