



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

Suang Siri Arunlimsawat, Patteera Funchien, Pongsakorn Chasing, Atthapon Saenubol, Taweesak Sudyoasuk and Vinich Promarak

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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, ^{13}C NMR, and HRMS spectra of the synthesized compounds

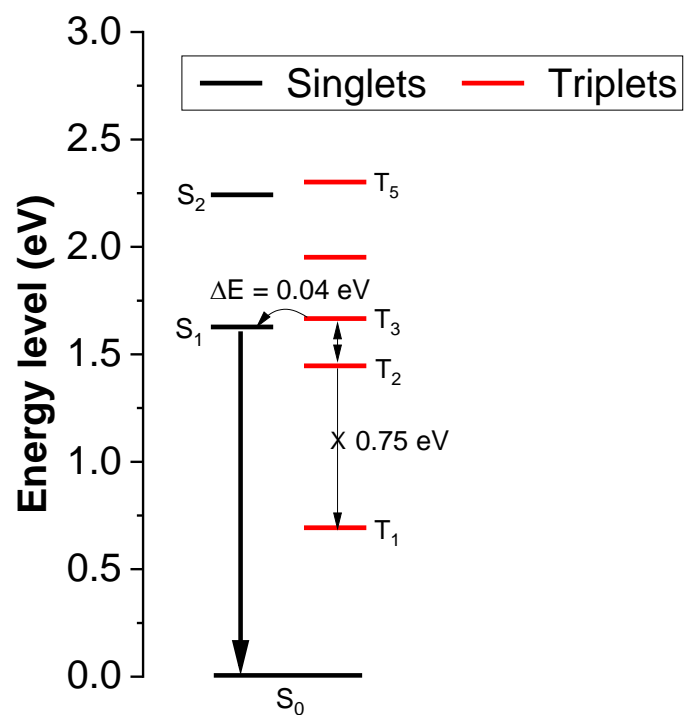


Figure S1: The energy diagram of singlet and triplet excited states of the compound estimated by CAM-B3LYP/6-31G(d,p) calculations.

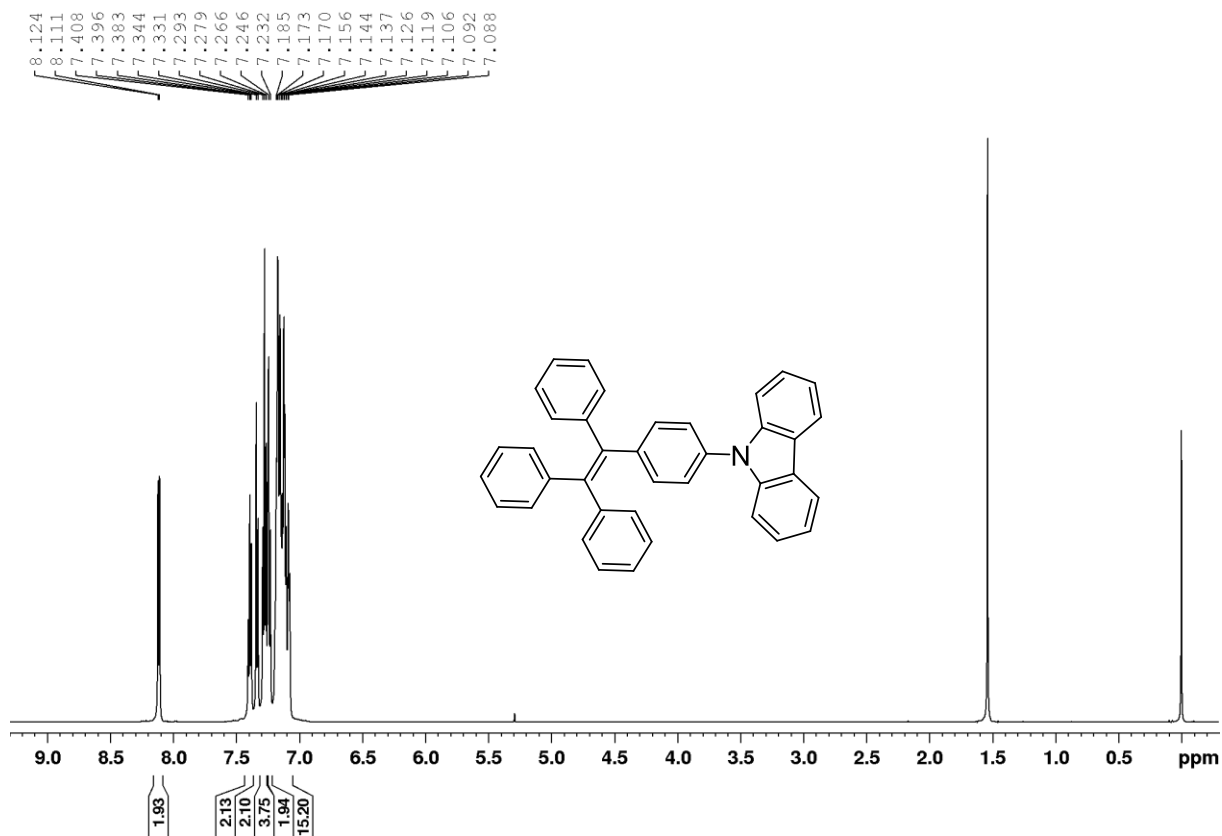


Figure S2: ¹H NMR spectrum of **2** in CDCl₃ (600 MHz) @ 25 °C.

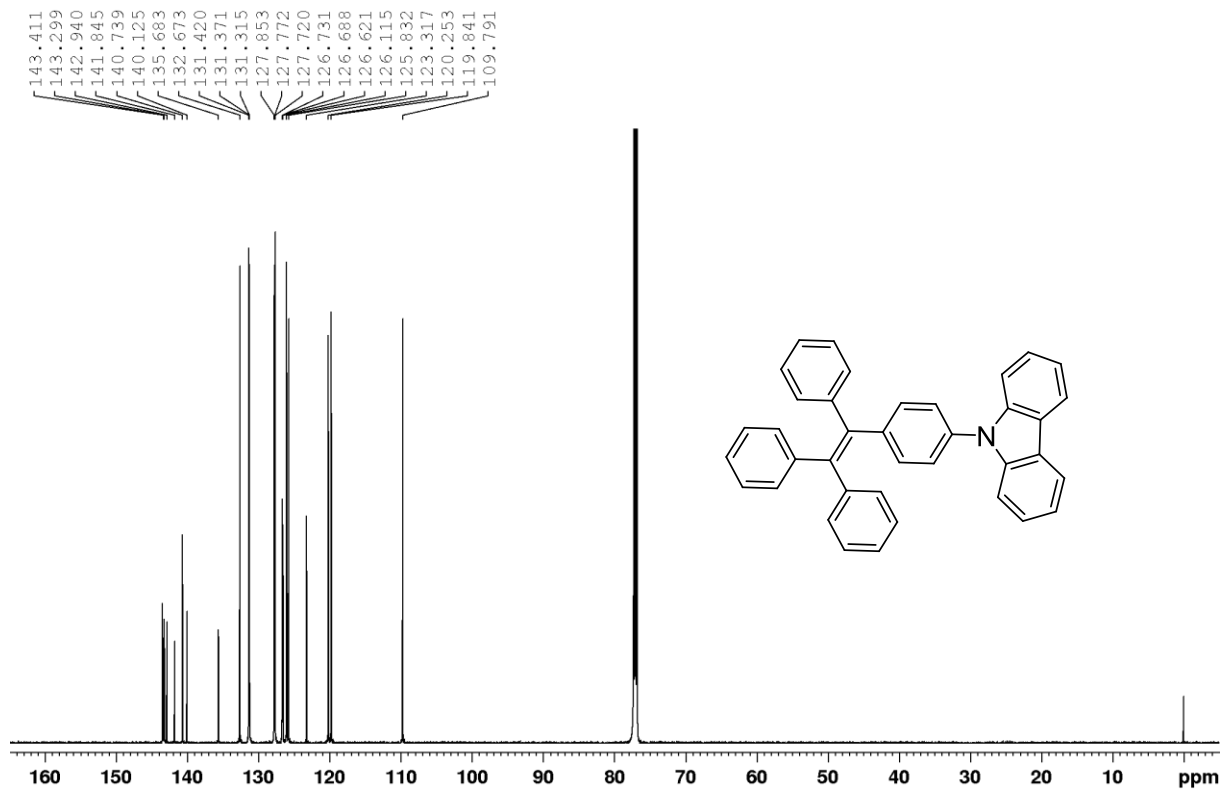


Figure S3: ¹³C NMR spectrum of **2** in CDCl₃ (151 MHz) @ 25 °C.

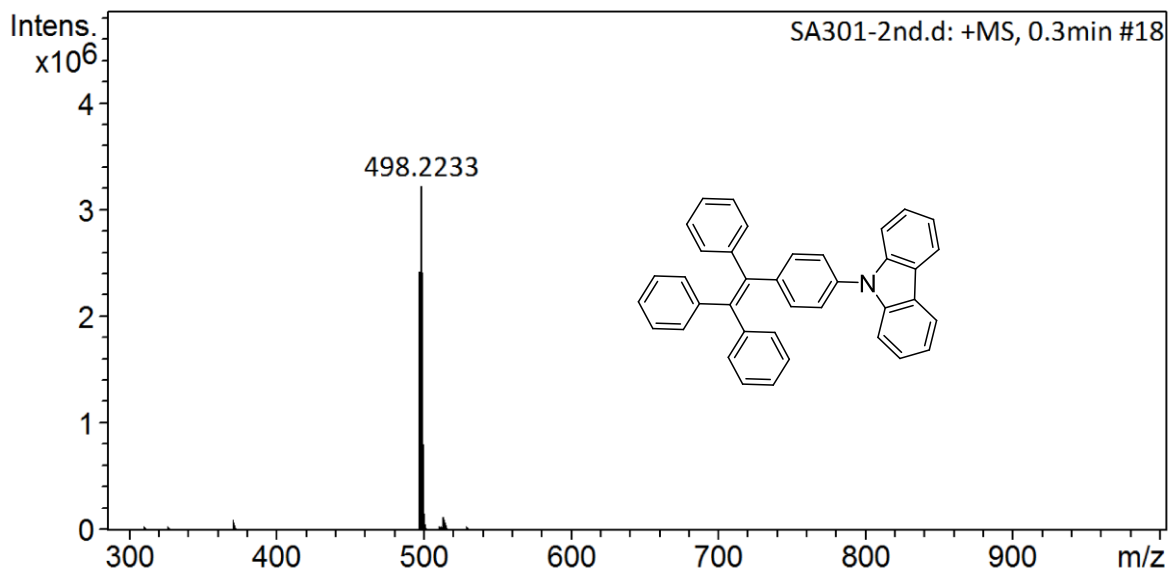


Figure S4: APCI-TOF mass spectrum $[M + H]^+$ of **2**.

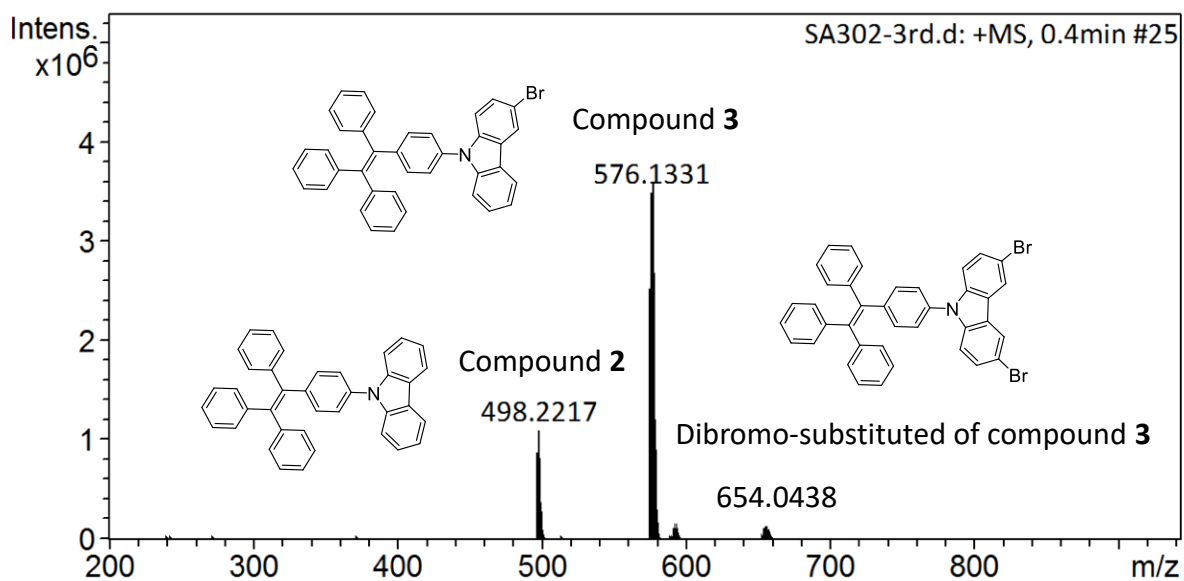


Figure S5: APCI-TOF mass spectrum $[M + H]^+$ of the crude product mixture from the NBS bromination in the synthesis of compound **3**.

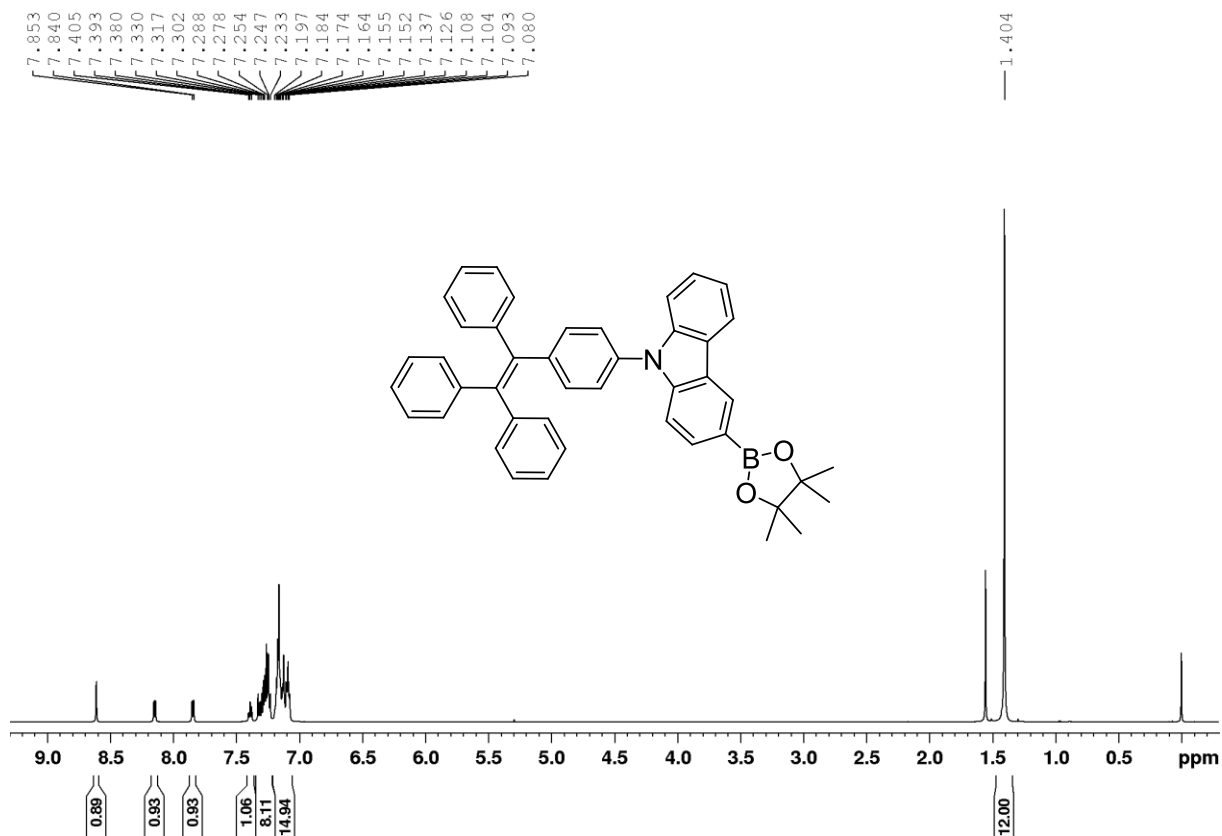


Figure S6: ¹H NMR spectrum of **3** in CDCl₃ (600 MHz) @ 25 °C.

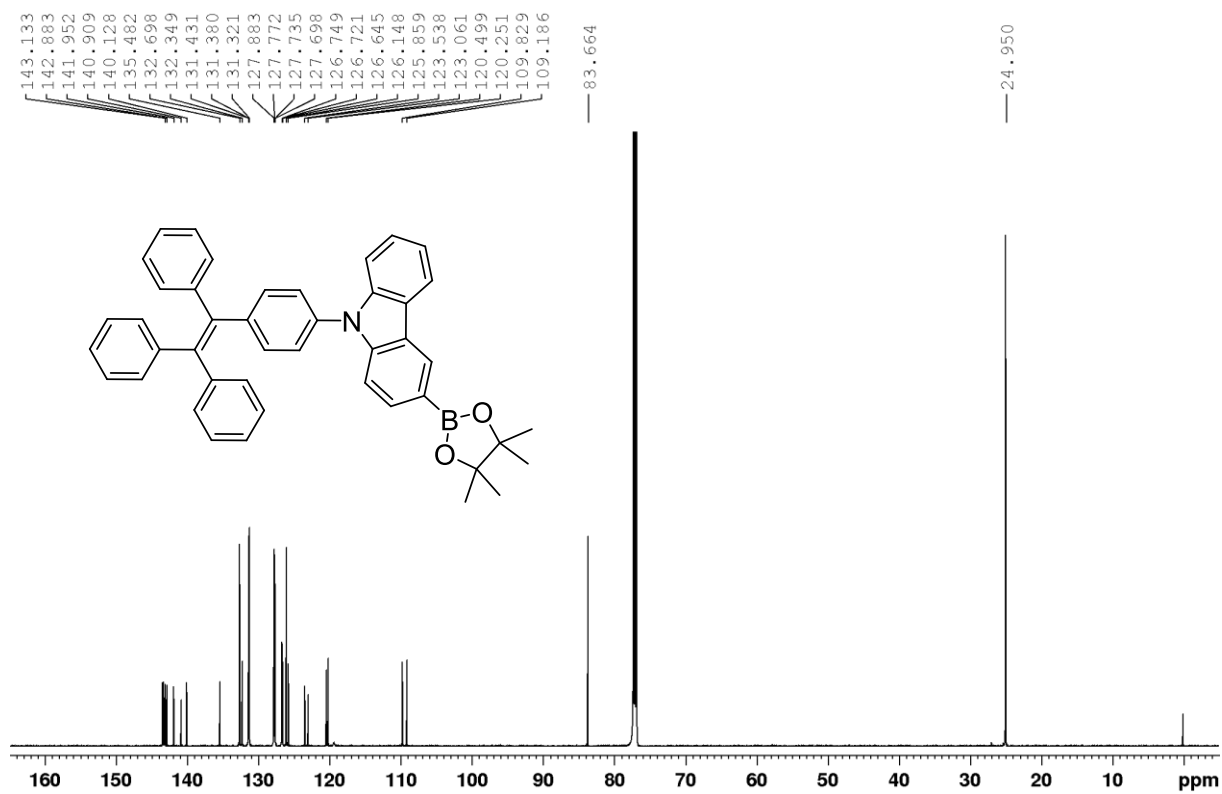


Figure S7: ¹³C NMR spectrum of **3** in CDCl₃ (151 MHz) @ 25 °C.

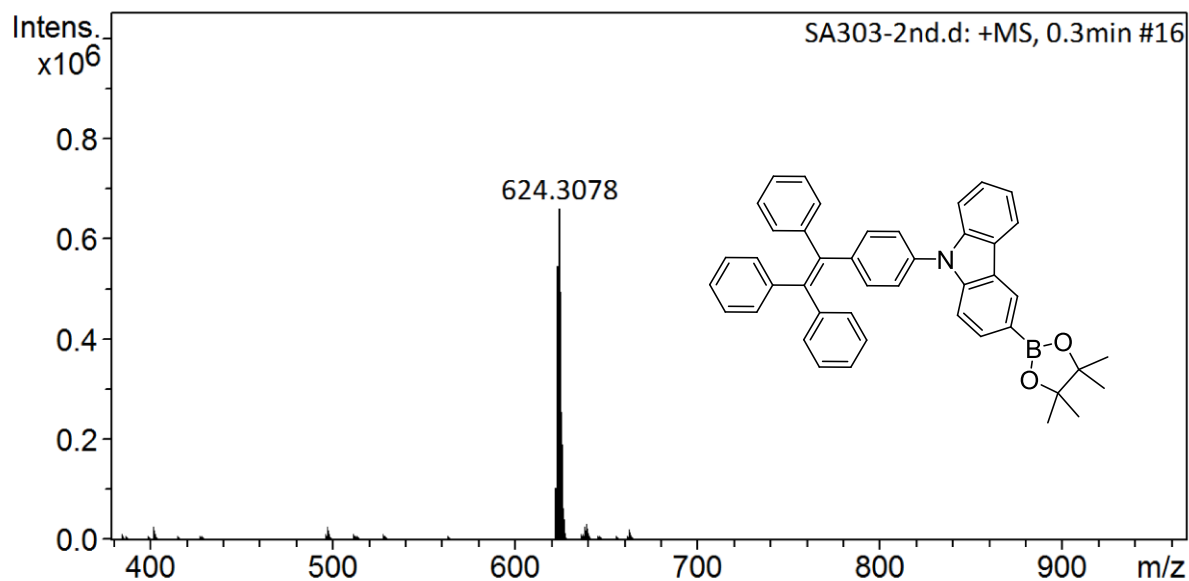


Figure S8: APCI-TOF mass spectrum $[M + H]^+$ of **3**.

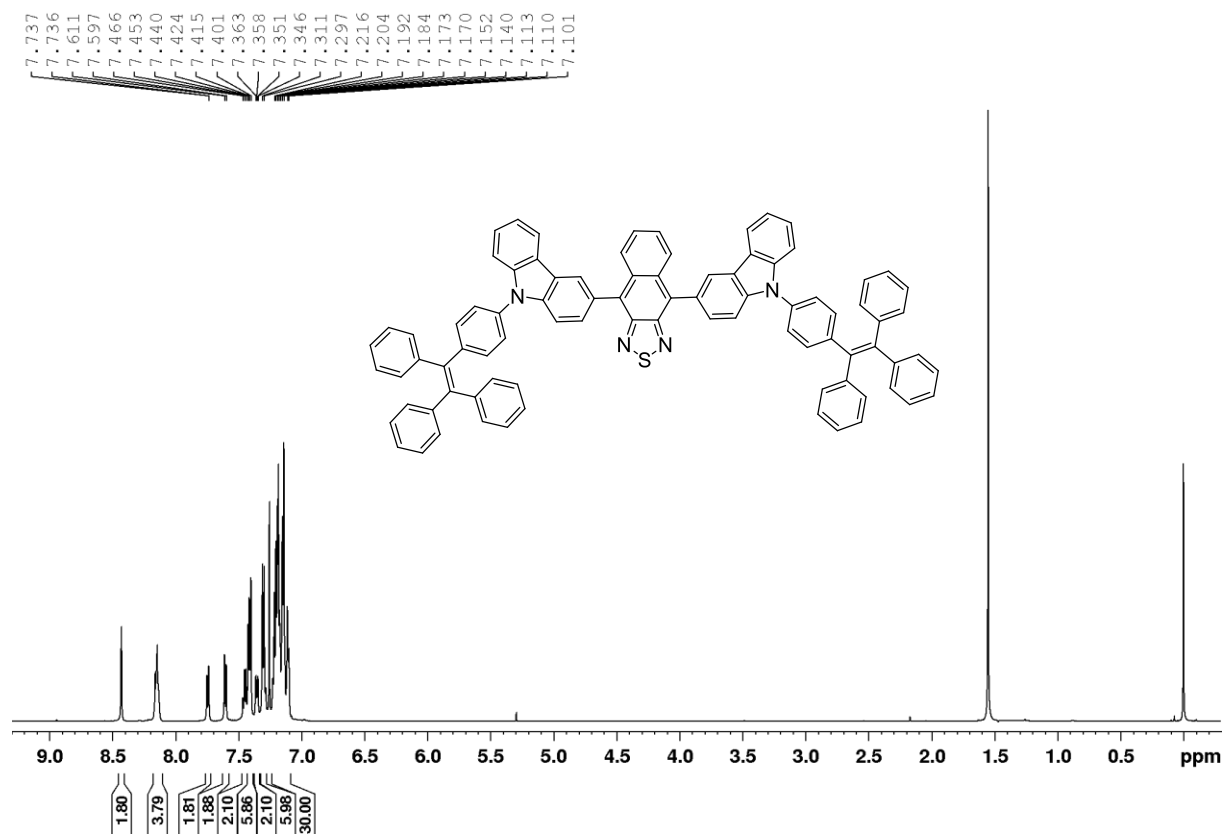


Figure S9: ^1H NMR spectrum of **TPECNz** in CDCl_3 (600 MHz) @ 25 °C.

