Supporting Information

Directly coupled dual emitting core based molecular design of thermally activated delayed fluorescent emitters

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Keywords: thermally activated delayed fluorescence·dopant engineering·quantum efficiency·electroluminescence

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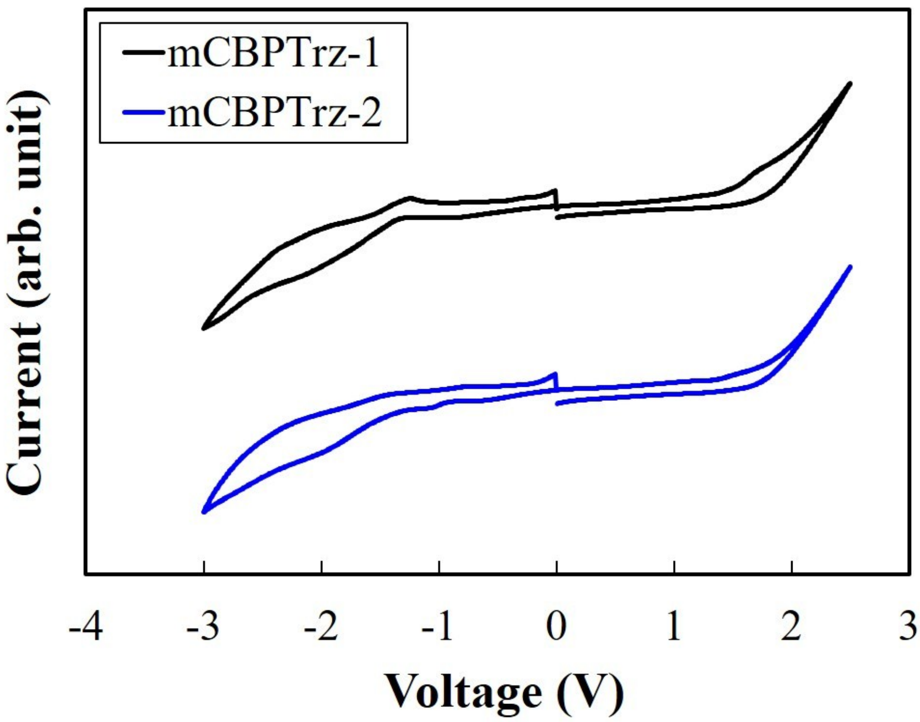


Figure S1. Cyclic voltammograms of mCBPTrz-1 and mCBPTrz-2.

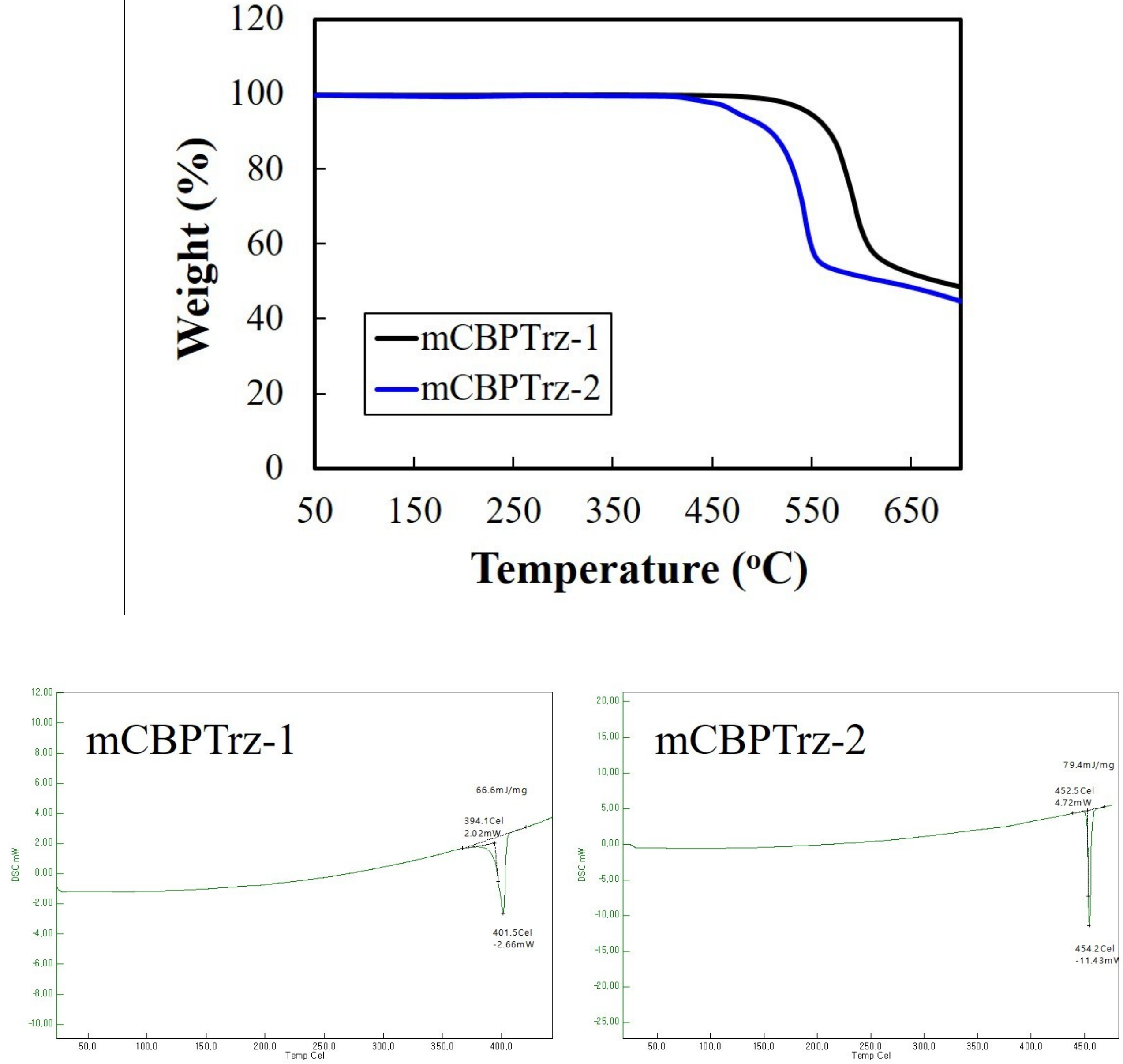


Figure S2. TGA and DSC curves of mCBPTrz-1 and mCBPTrz-2.

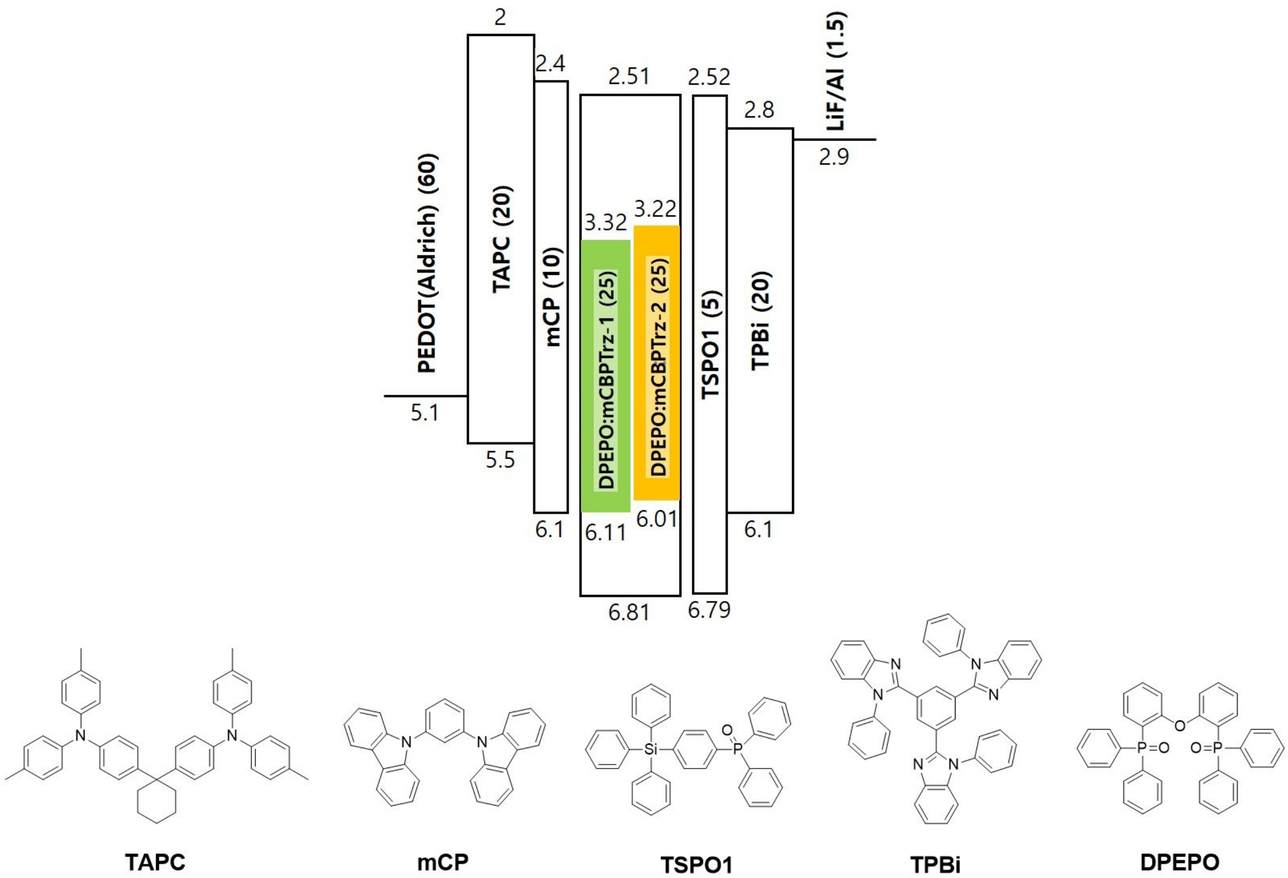


Figure S3. Energy level diagram and chemical structure of materials.

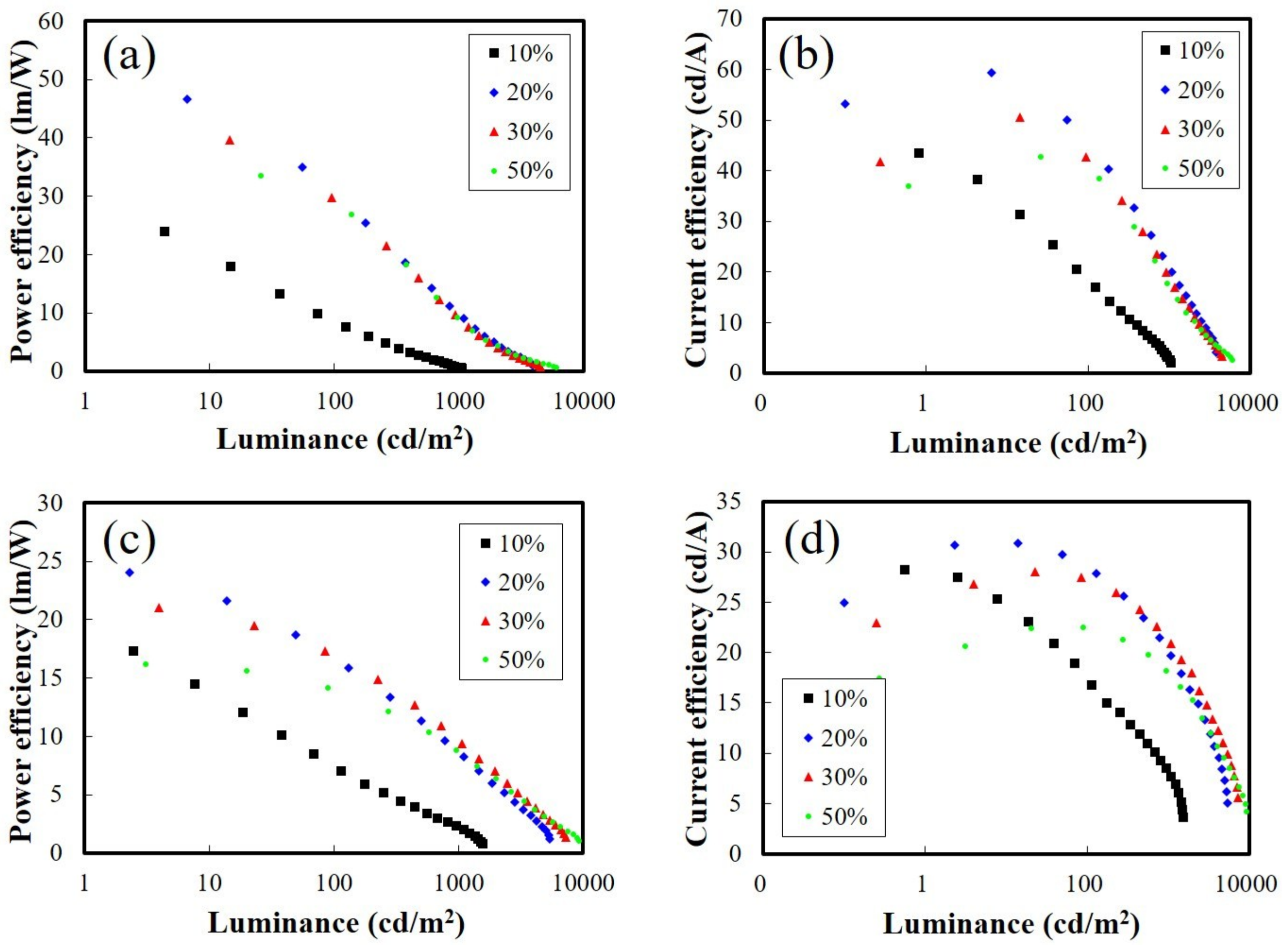


Figure S4. Power and current efficiencies (a), (b) for mCBPTrz-1 and (c), (d) for mCBPTrz-2.

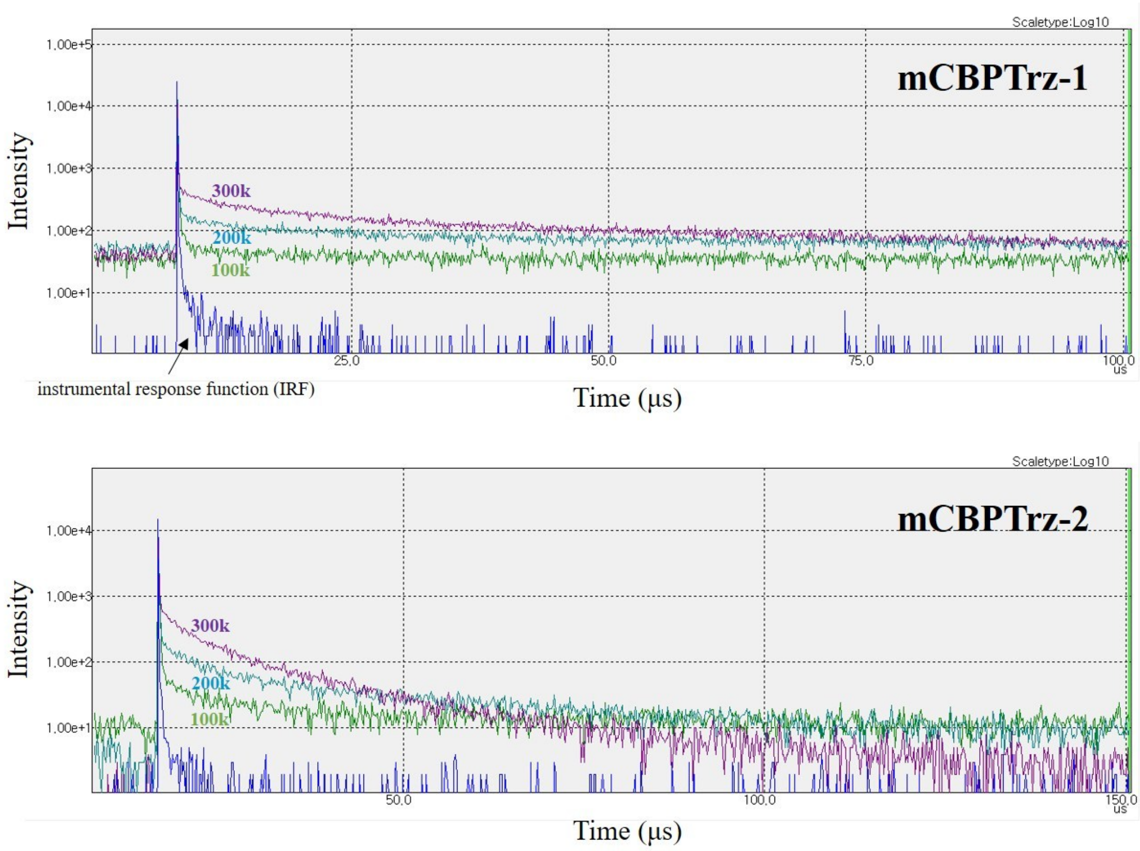


Figure S5. PL decay curves of mCBPTrz-1 and mCBPTrz-2 measured at various temperatures.

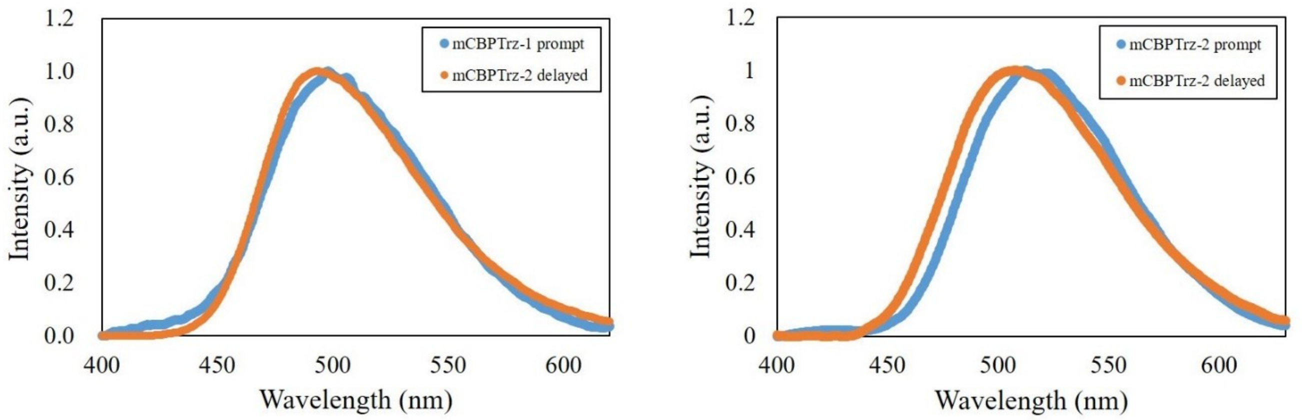
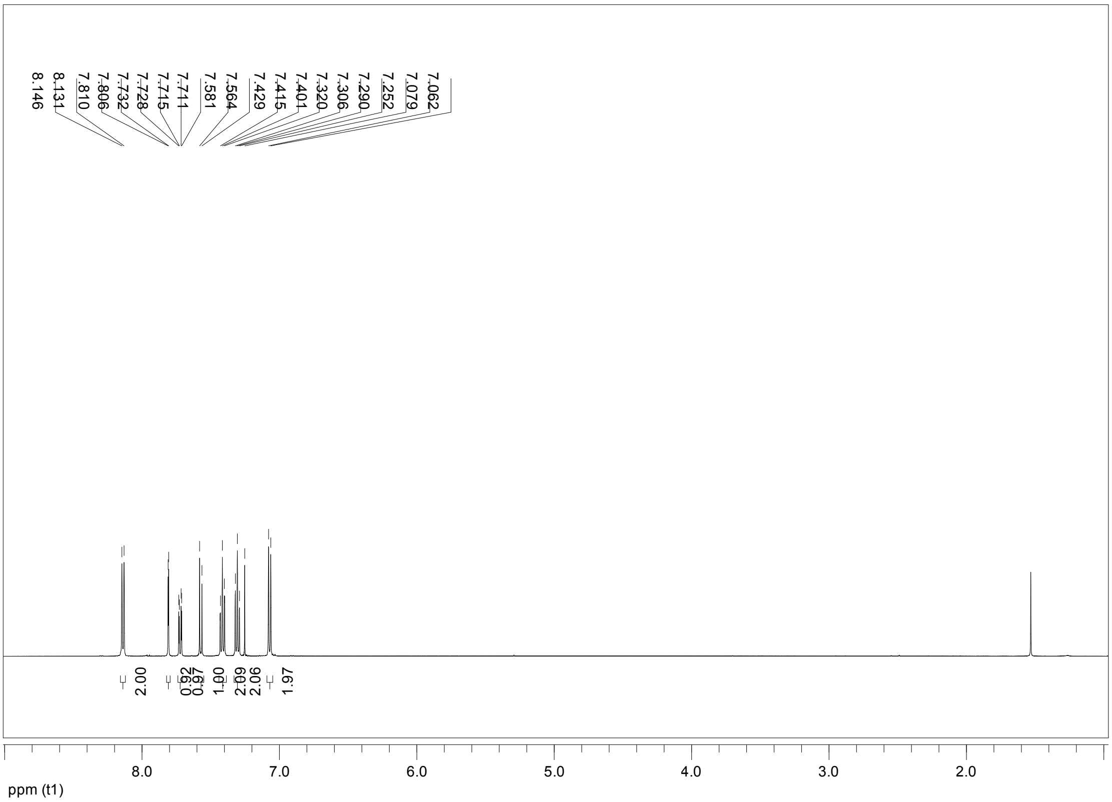


Figure S6. The PL emission spectra at prompt and delayed time.

(left: mCBPTrz-1, right: mCBPTrz-2)



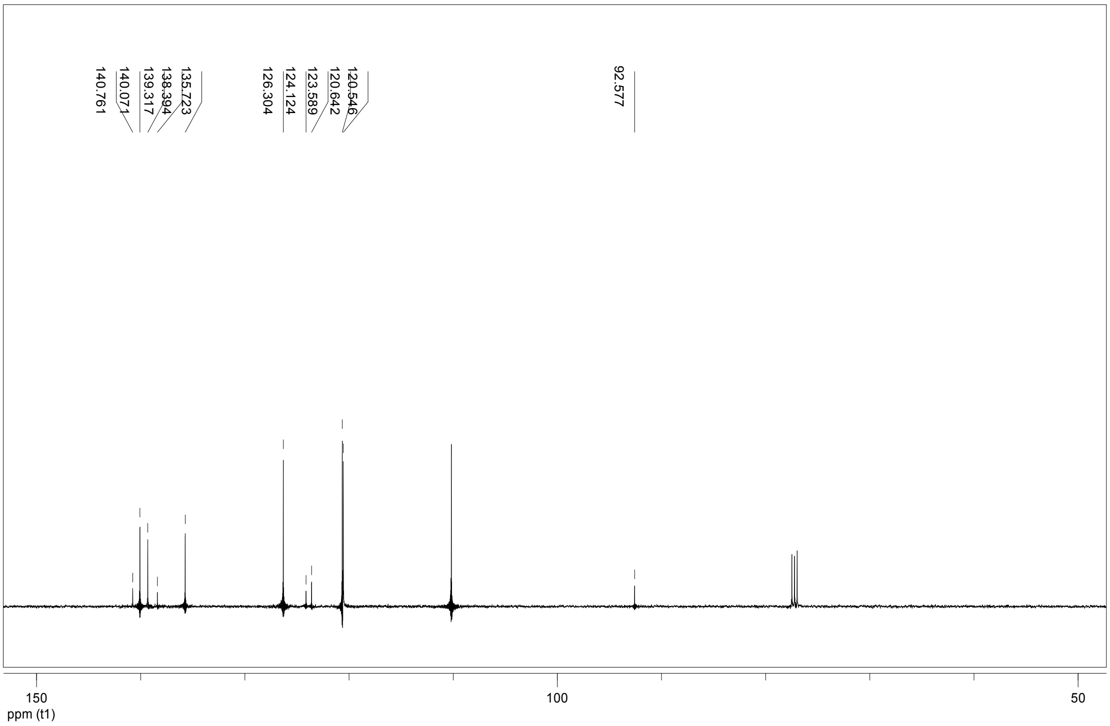
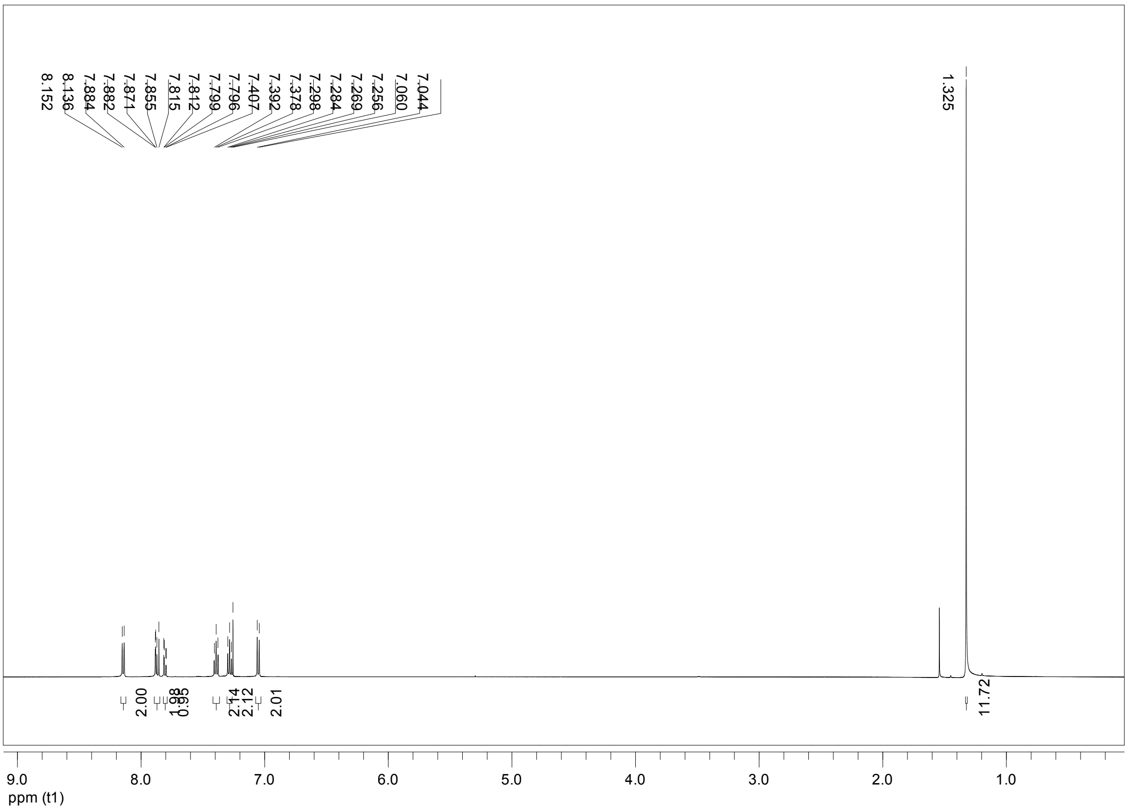


Figure S7. ^{1}H and ^{13}C NMR spectra of **A1**.



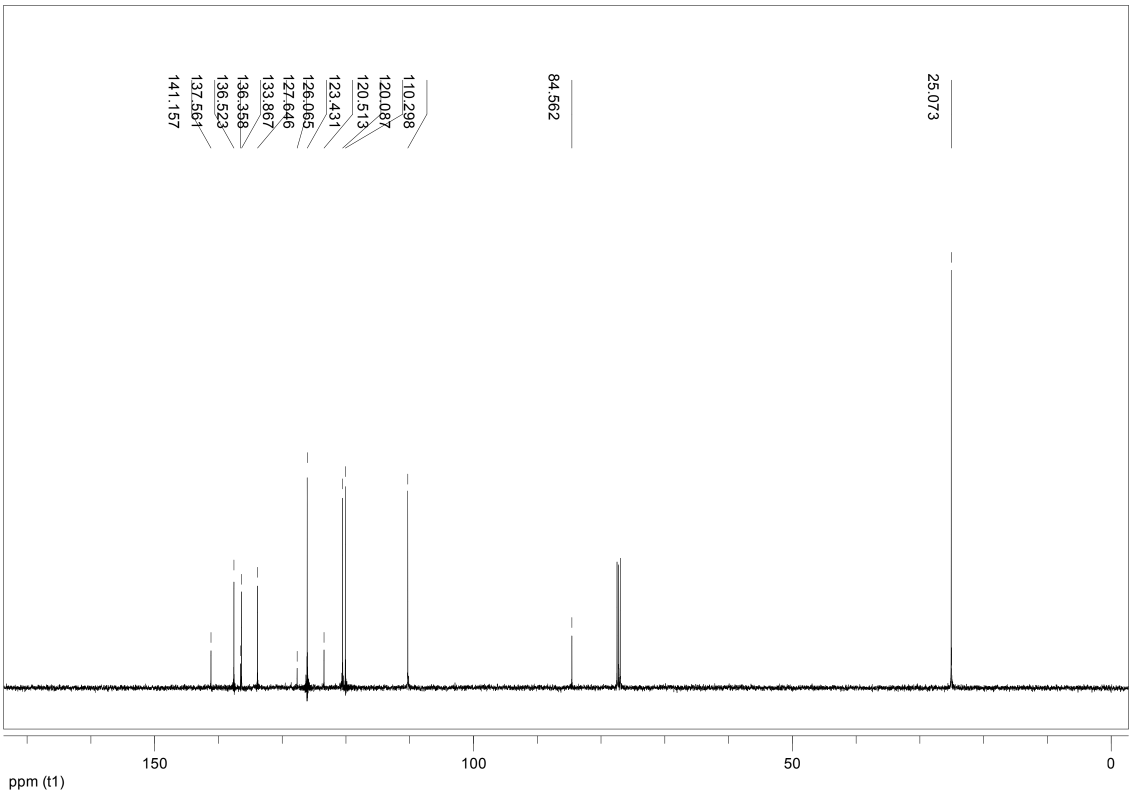
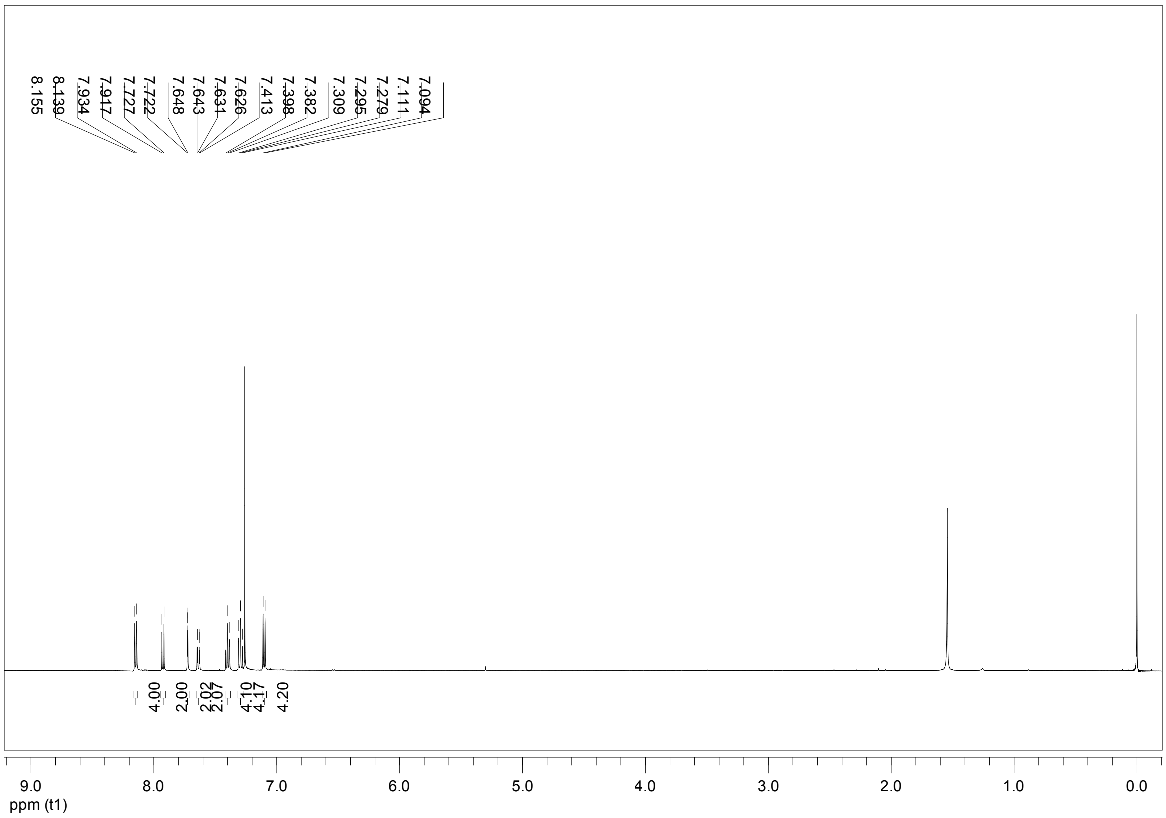


Figure S8. ^1H and ^{13}C NMR spectra of **A2**.



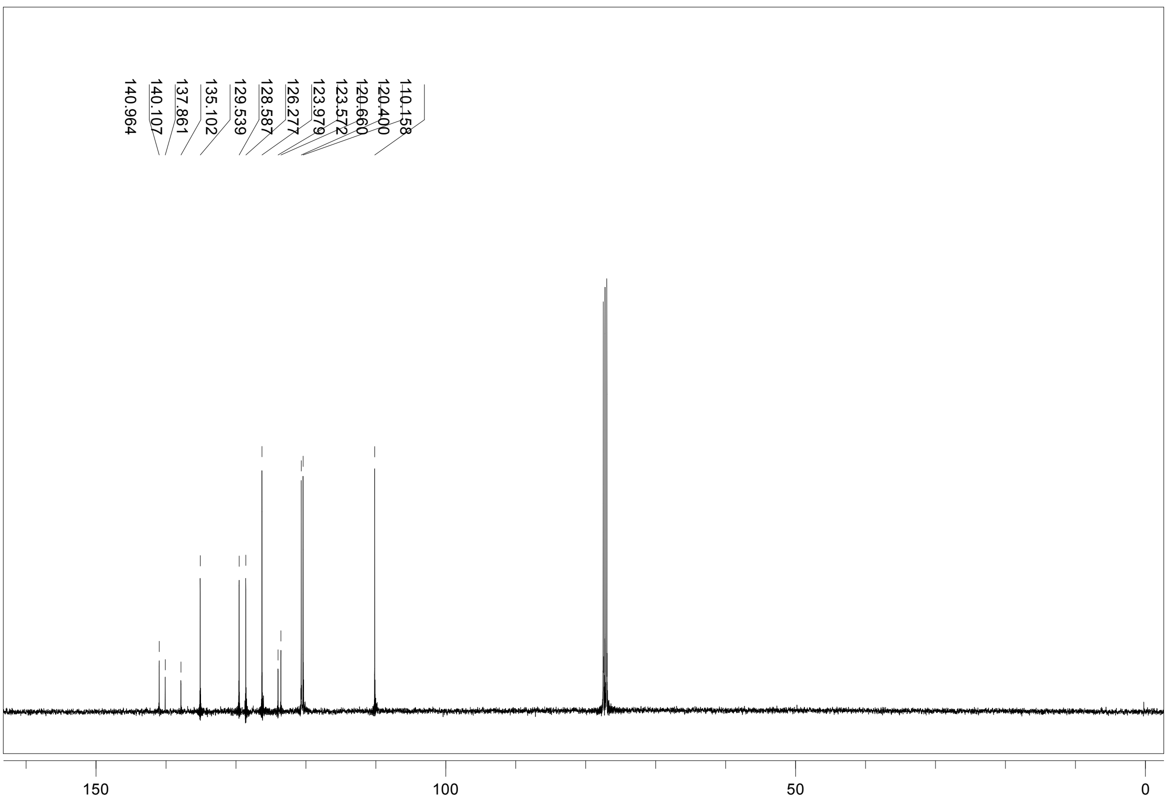


Figure S9. [1]H and [13]C NMR spectra of **A3**.

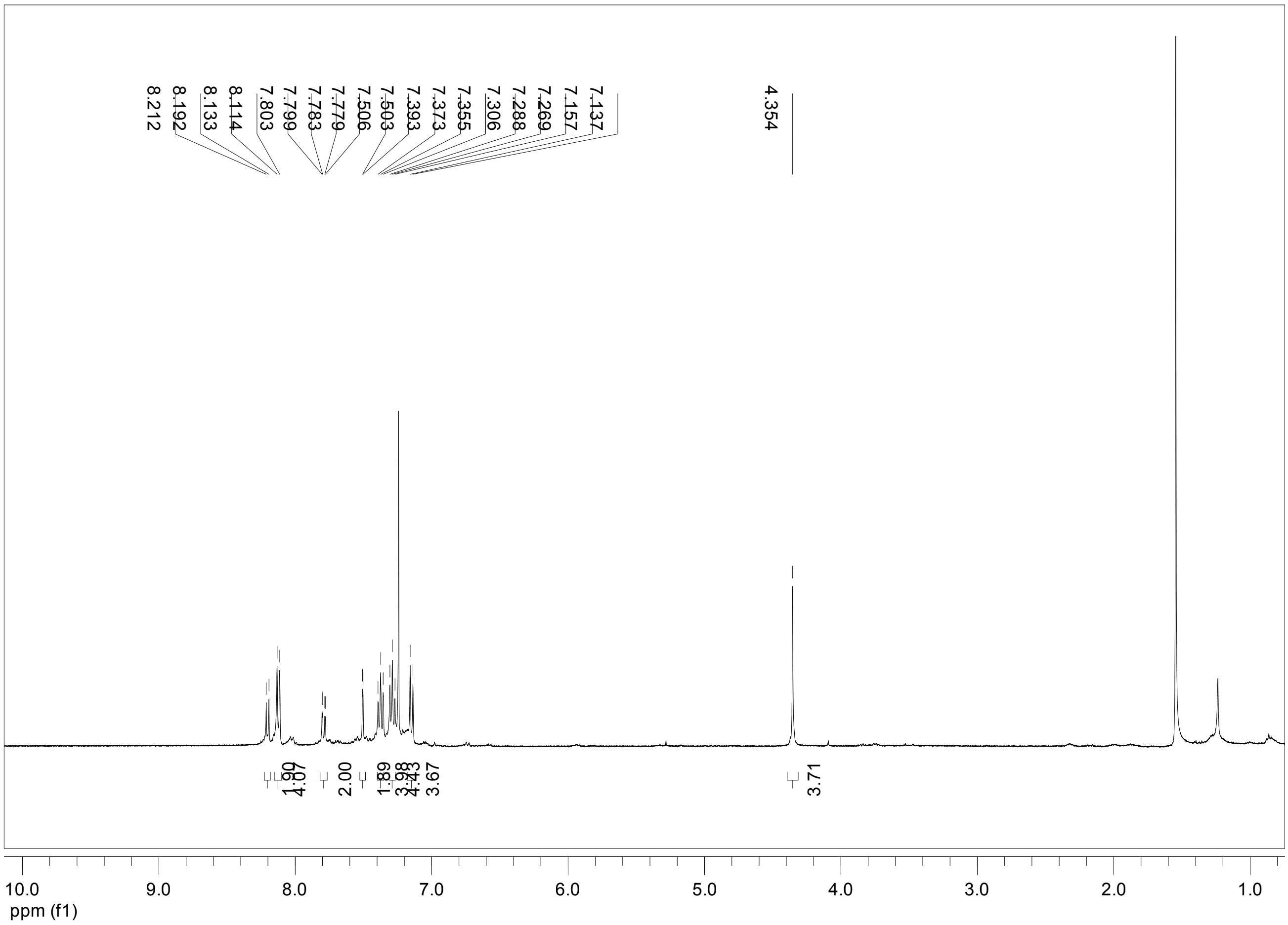
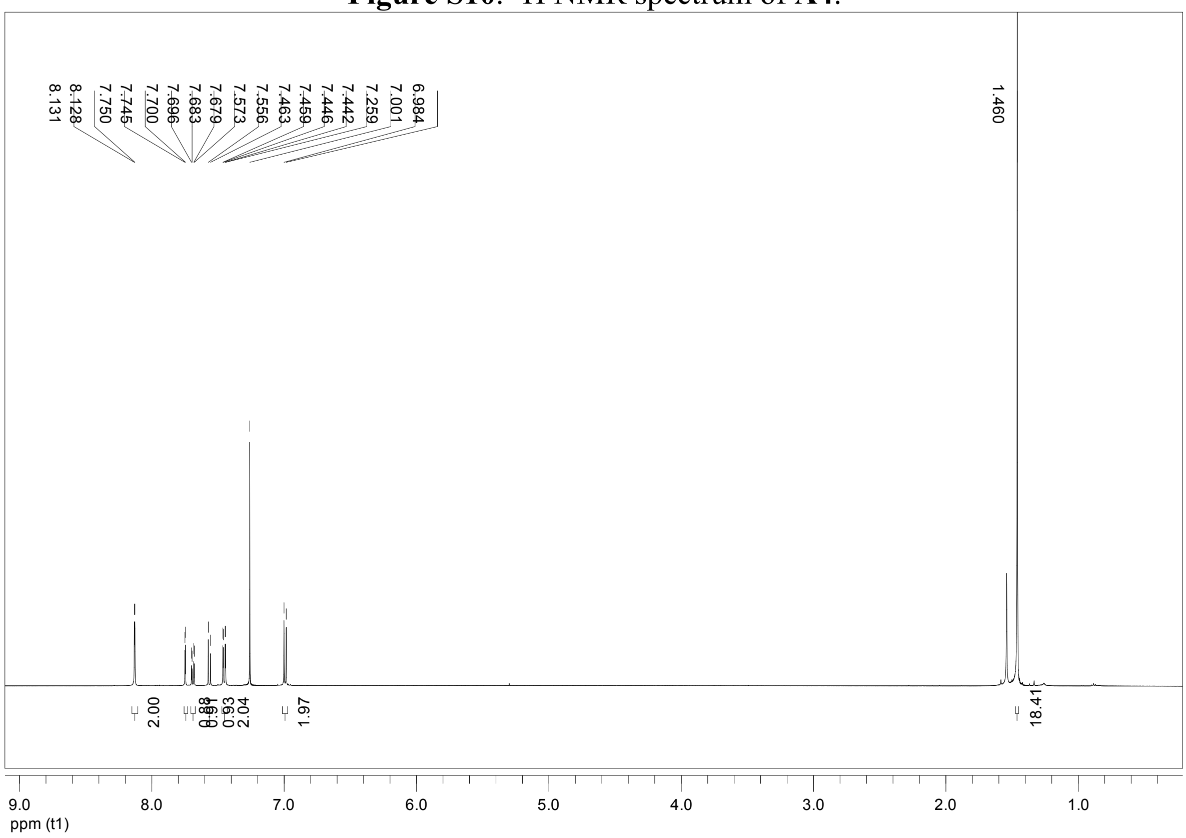


Figure S10. ¹H NMR spectrum of **A4**.



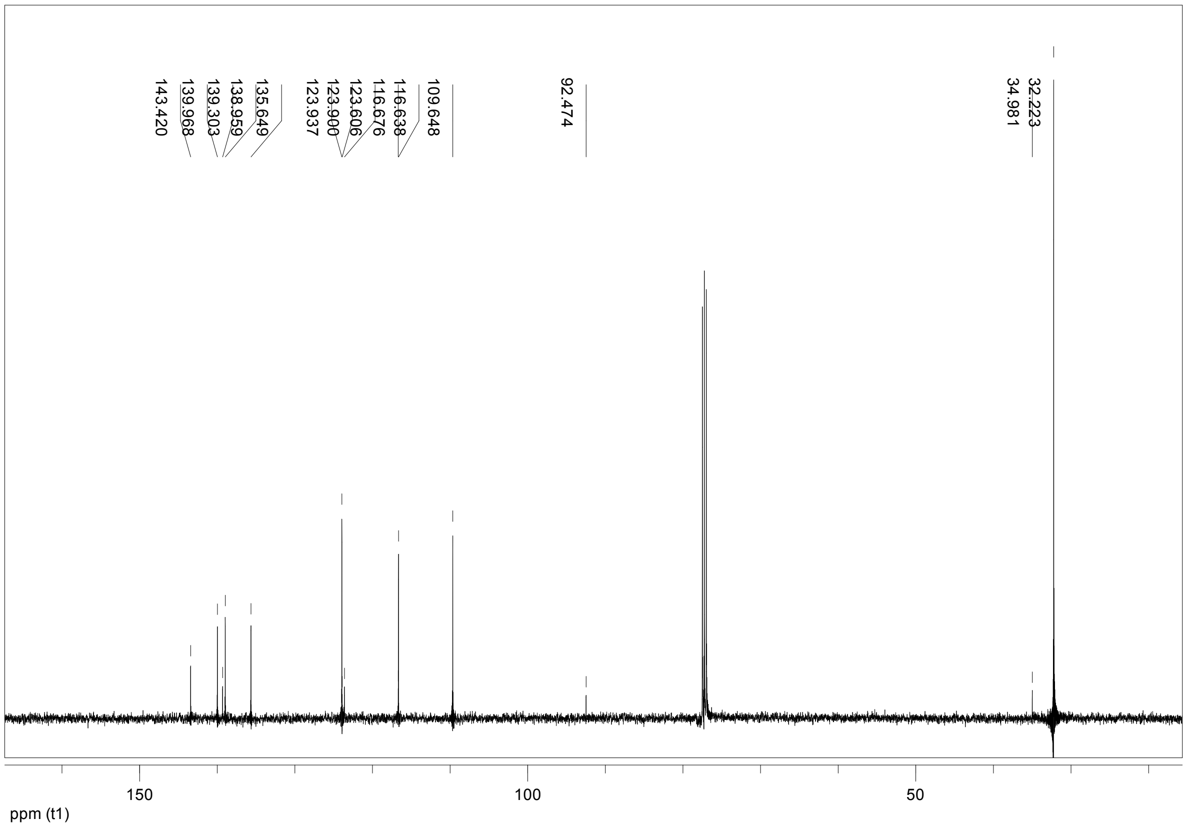
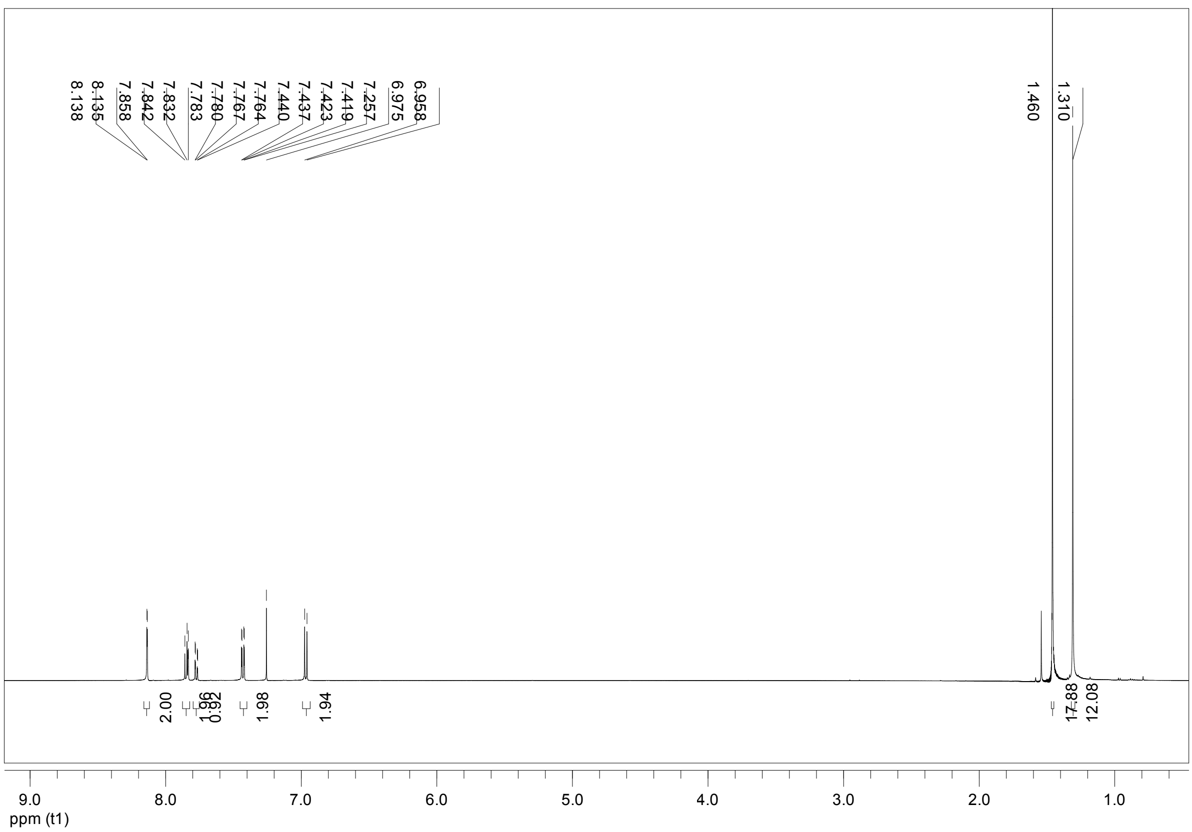


Figure S11. ^{1}H and ^{13}C NMR spectra of **B1**.



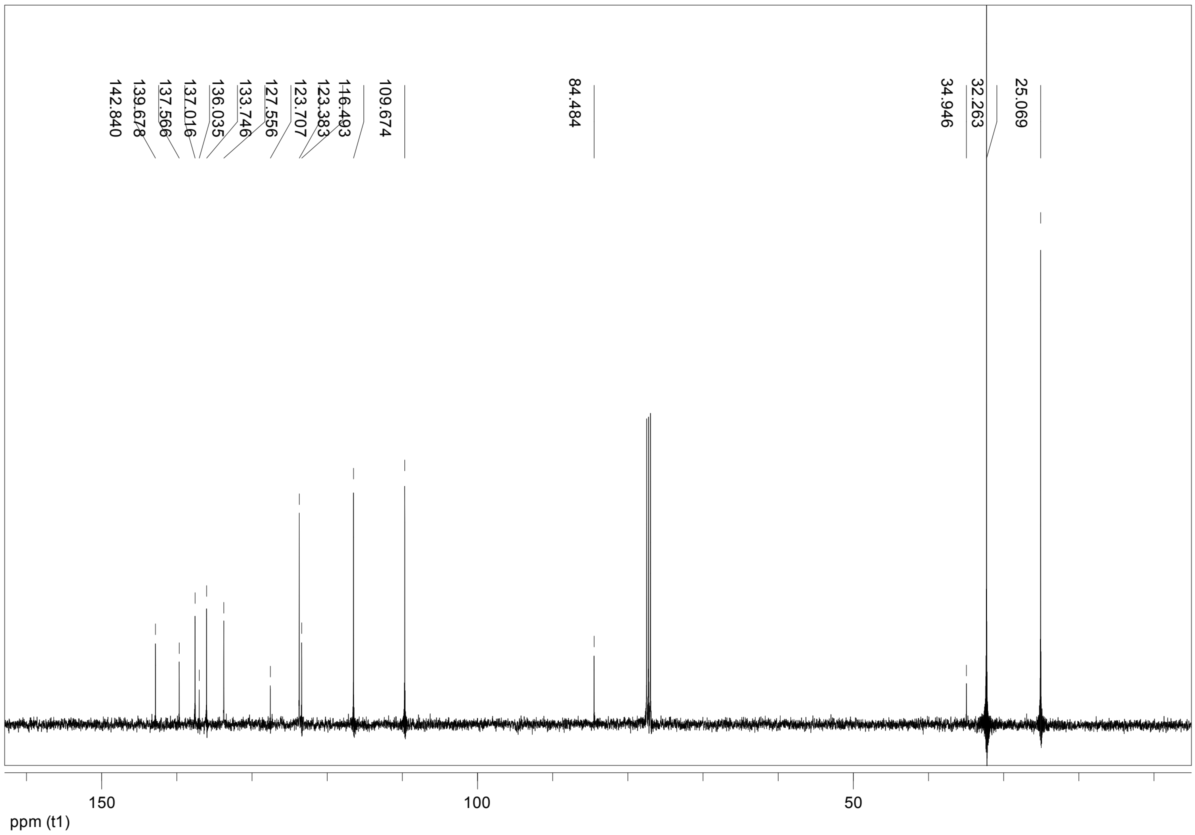
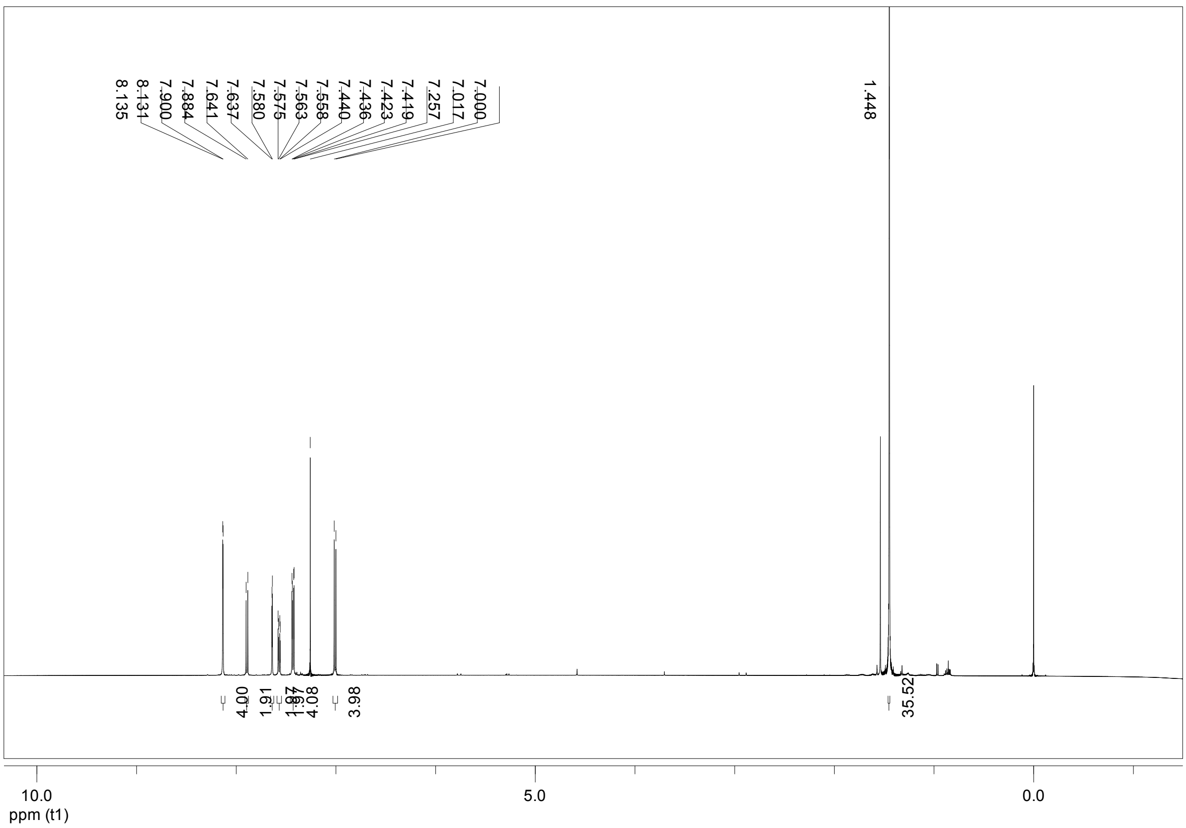


Figure S12. ^{1}H and ^{13}C NMR spectra of **B2**.



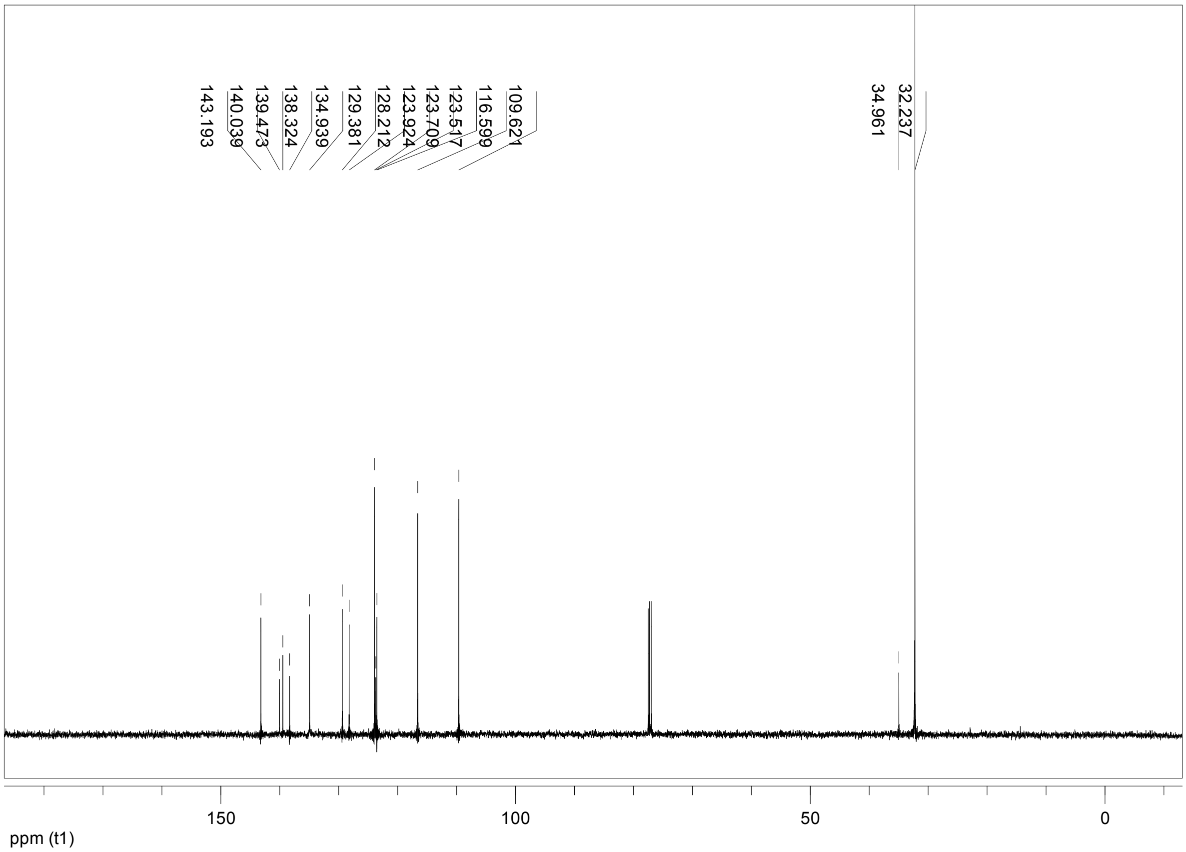


Figure S13. ^{1}H and ^{13}C NMR spectra of **B3**.

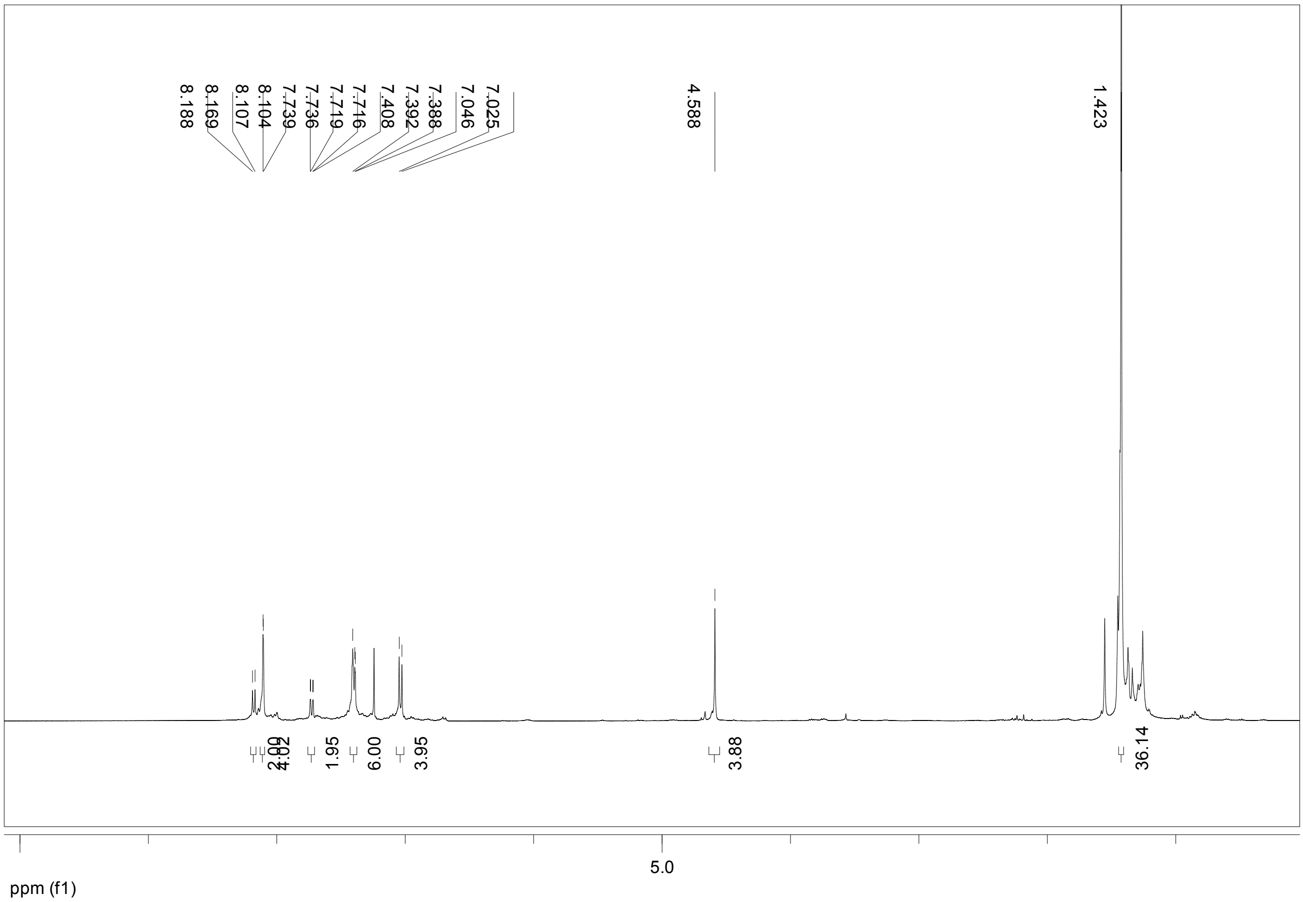


Figure S14. ^{1}H NMR spectrum of **B4**.

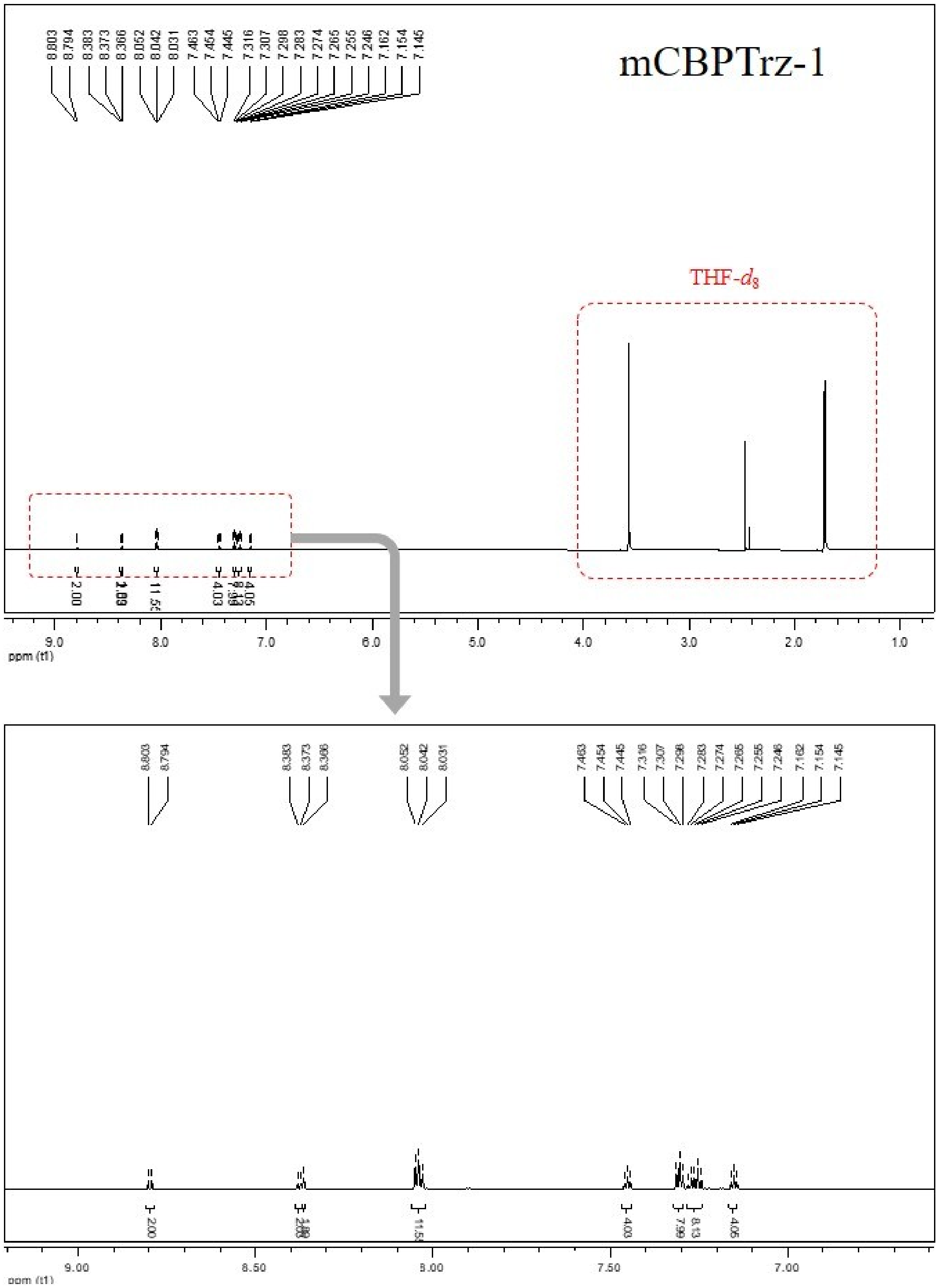


Figure S15. ^{1}H NMR spectrum of mCBPTrz-1.

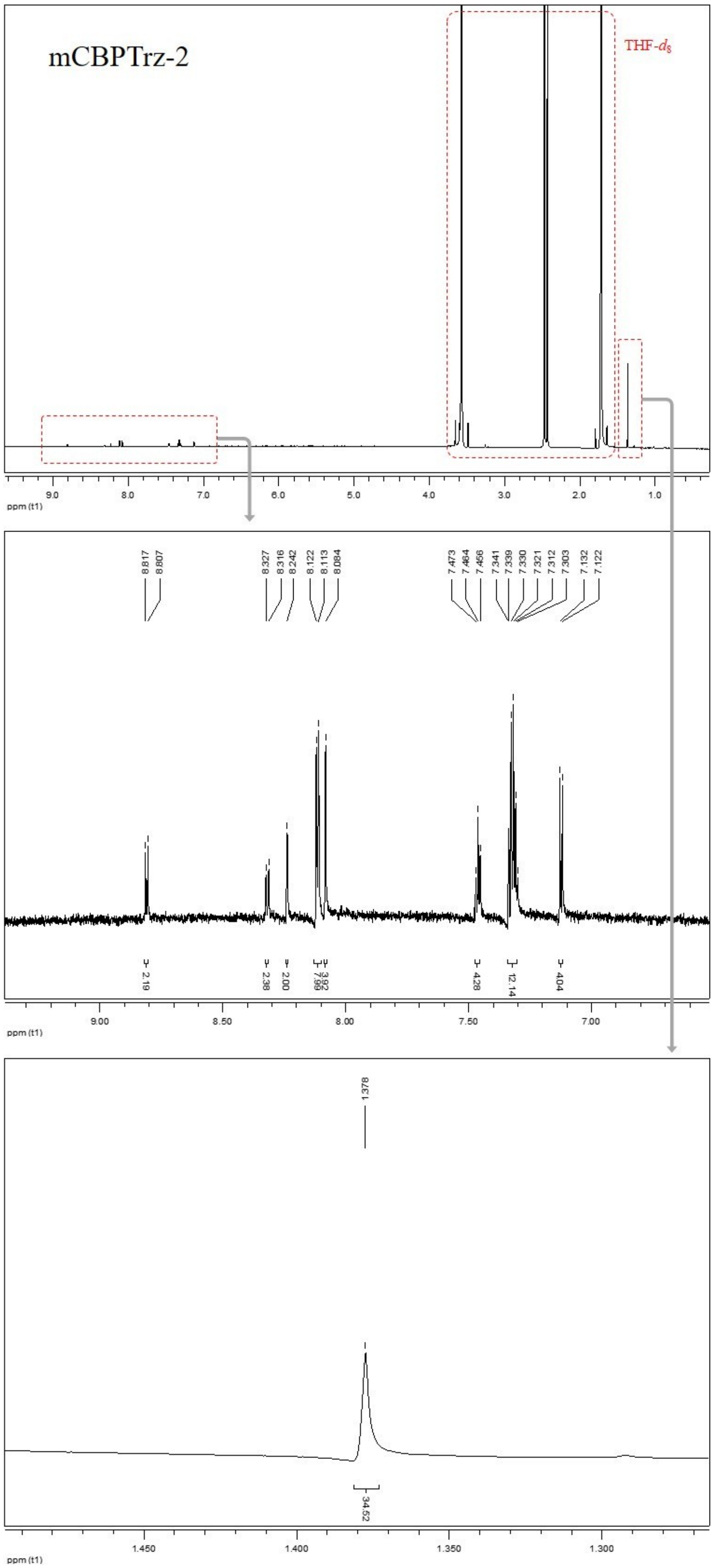
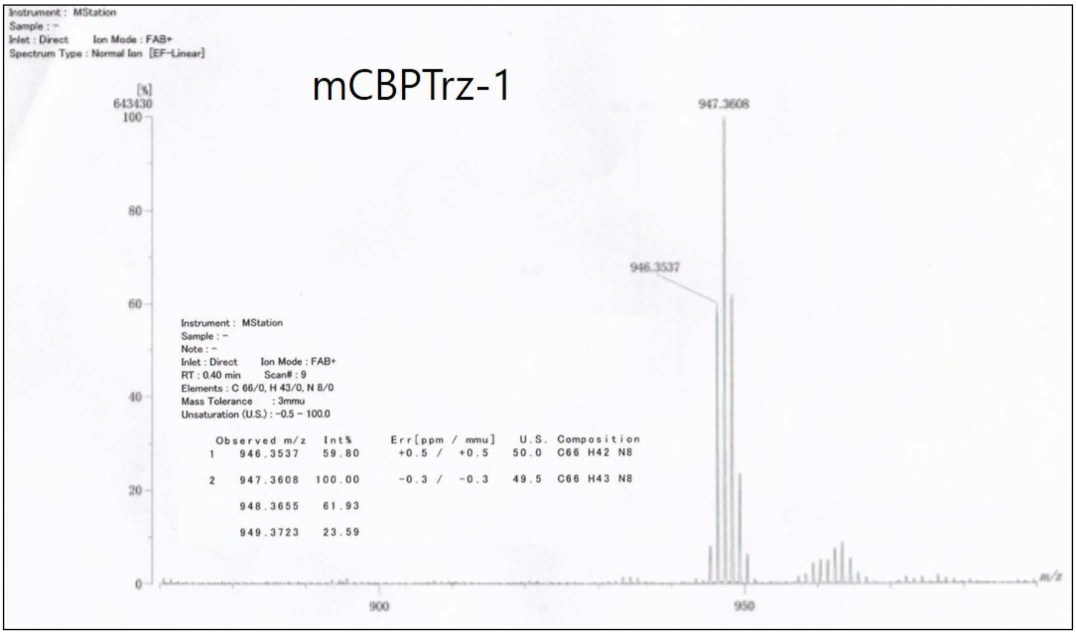


Figure S16. ^{1}H NMR spectrum of mCBPTrz-2.



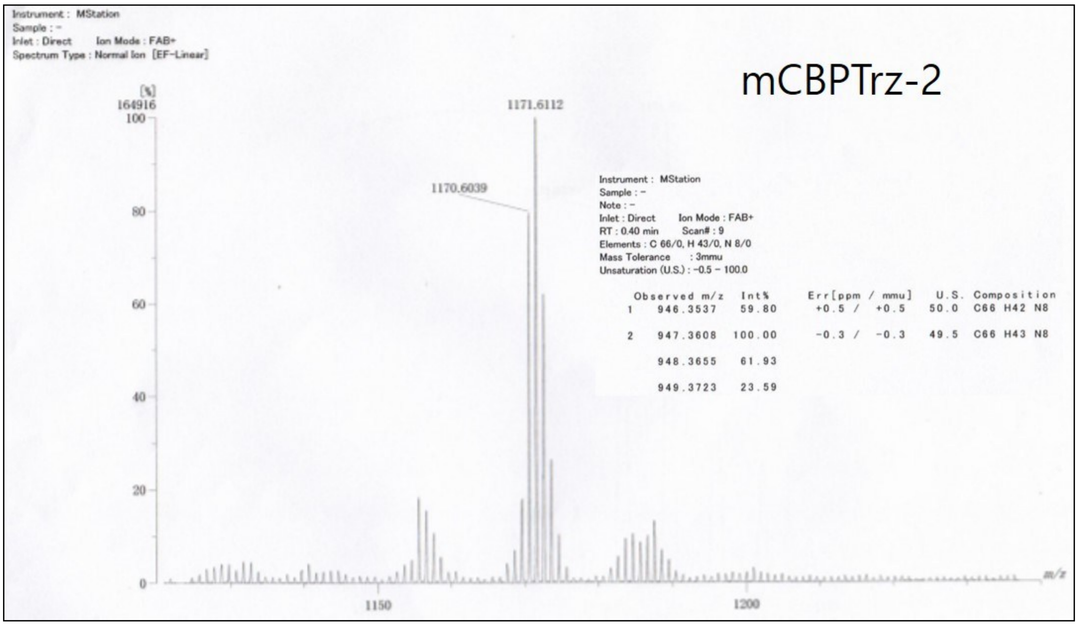


Figure S17. High resolution mass spectrometry (HRMS) data of mCBPTrz-1 and mCBPTrz-2.

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Eager 300 S/W Validation
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Operator ID: SNU-EA2000
Company name: Thermo Fisher

(Unit: wt%)

Sample name	Nitrogen	Carbon	Hydrogen
mCBP-Trz1	11.8677	83.7546	4.3393
mCBP-Trz2	9.5487	84.0477	6.2947

Figure S18. Elemental analysis data of mCBPTrz-1 and mCBPTrz-2.

$\tau_p = 1/k_p$

$\tau_d = 1/k_d$

$k_{ISC} = (1-\Phi_F) \times k_p$

$k_{RISC} = (k_p k_d / k_{ISC}) \times (\Phi_{TADF}/\Phi_F)$

$k_r^S = k_p \Phi_F$

$k_{nr}^T = k_d - k_{RISC}\Phi_F$

Equations for the calculation of rate constants