

## **Supporting Information**

### **Facile synthesis and evaluation of electron transport and photophysical properties of photoluminescent PDI derivatives**

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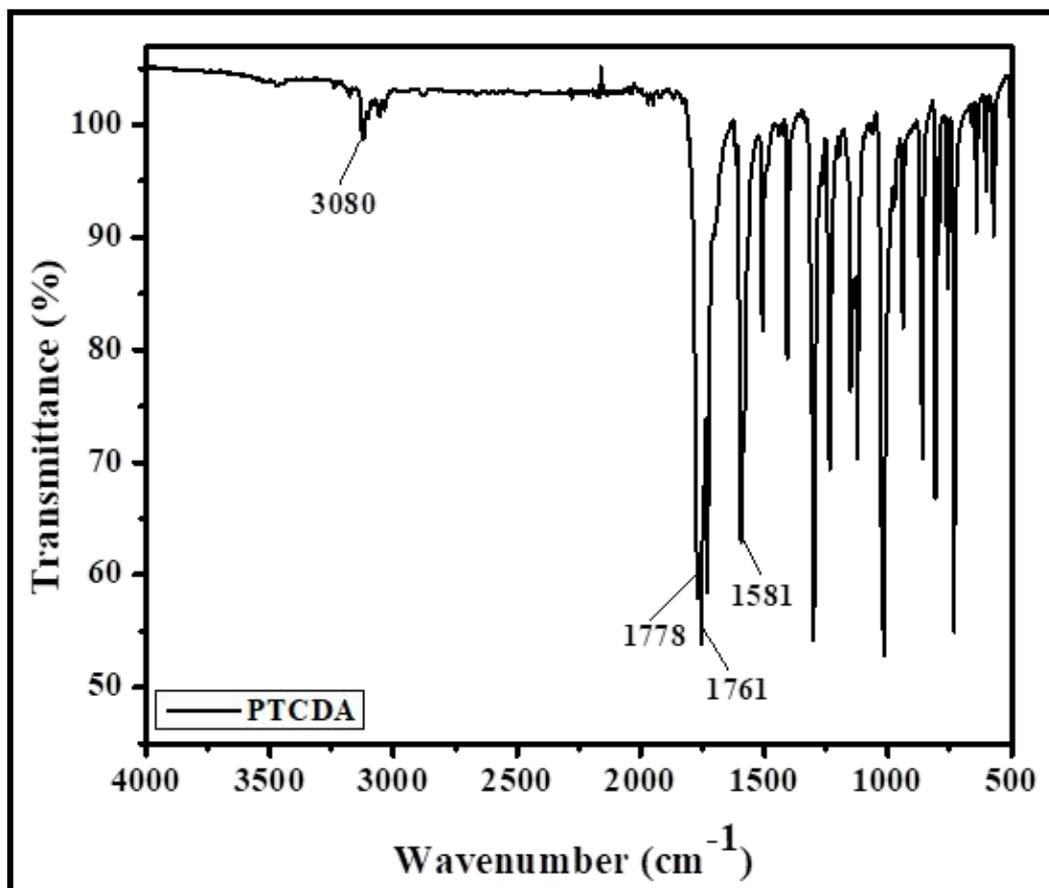


Figure S1. FT-IR spectra of Perylene-3,4,9,10 tetracarboxylic dianhydride (PTCDA).

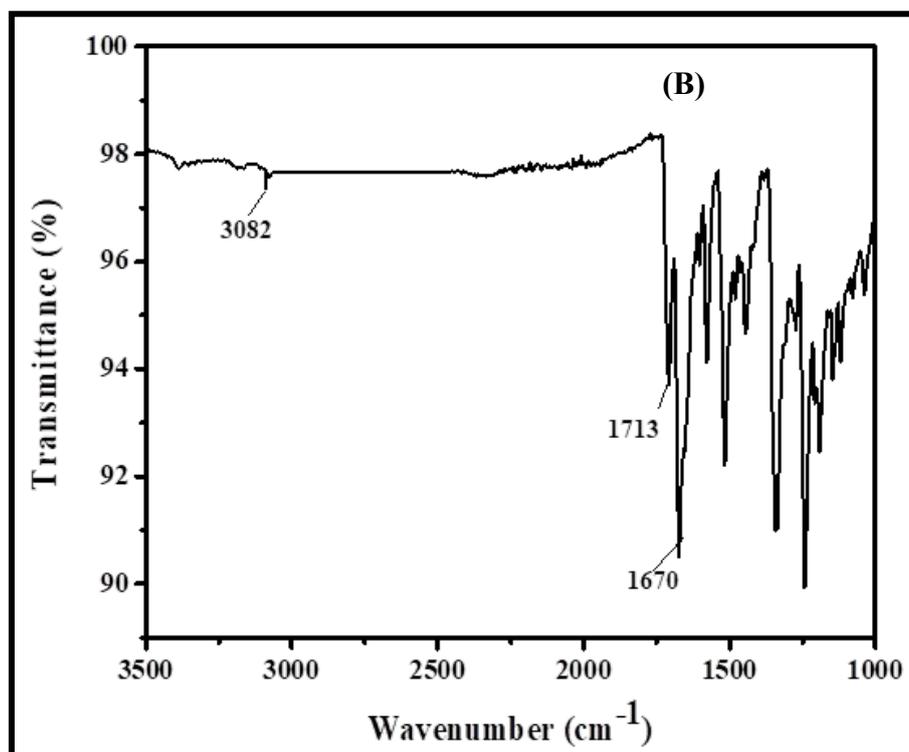
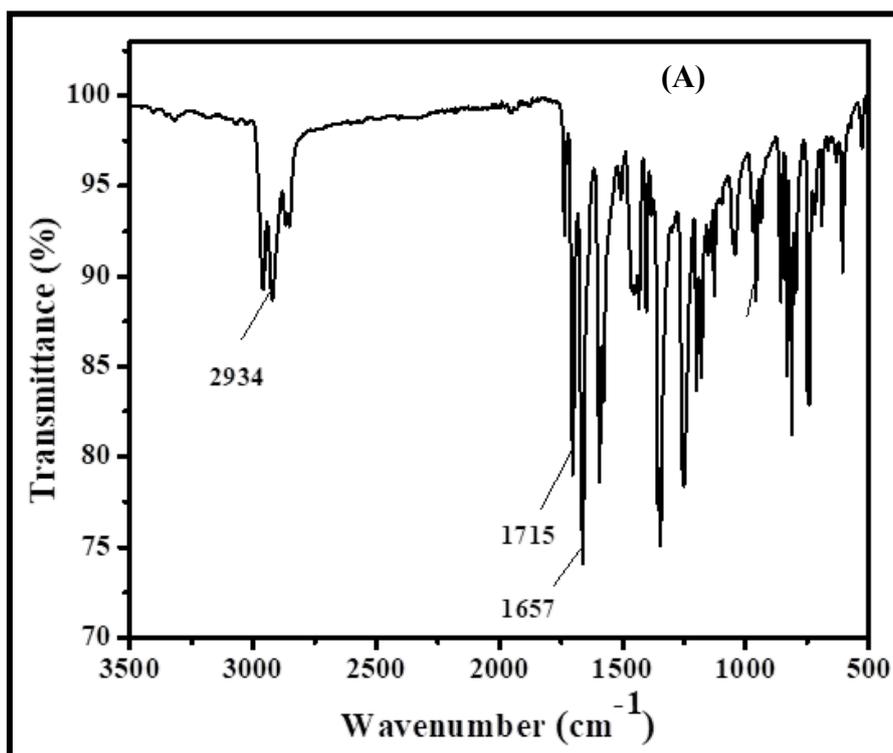


Figure S2. FT-IR spectra of (A) *i*PrP-PDI (1) and (B) NO<sub>2</sub>P-PDI (2).

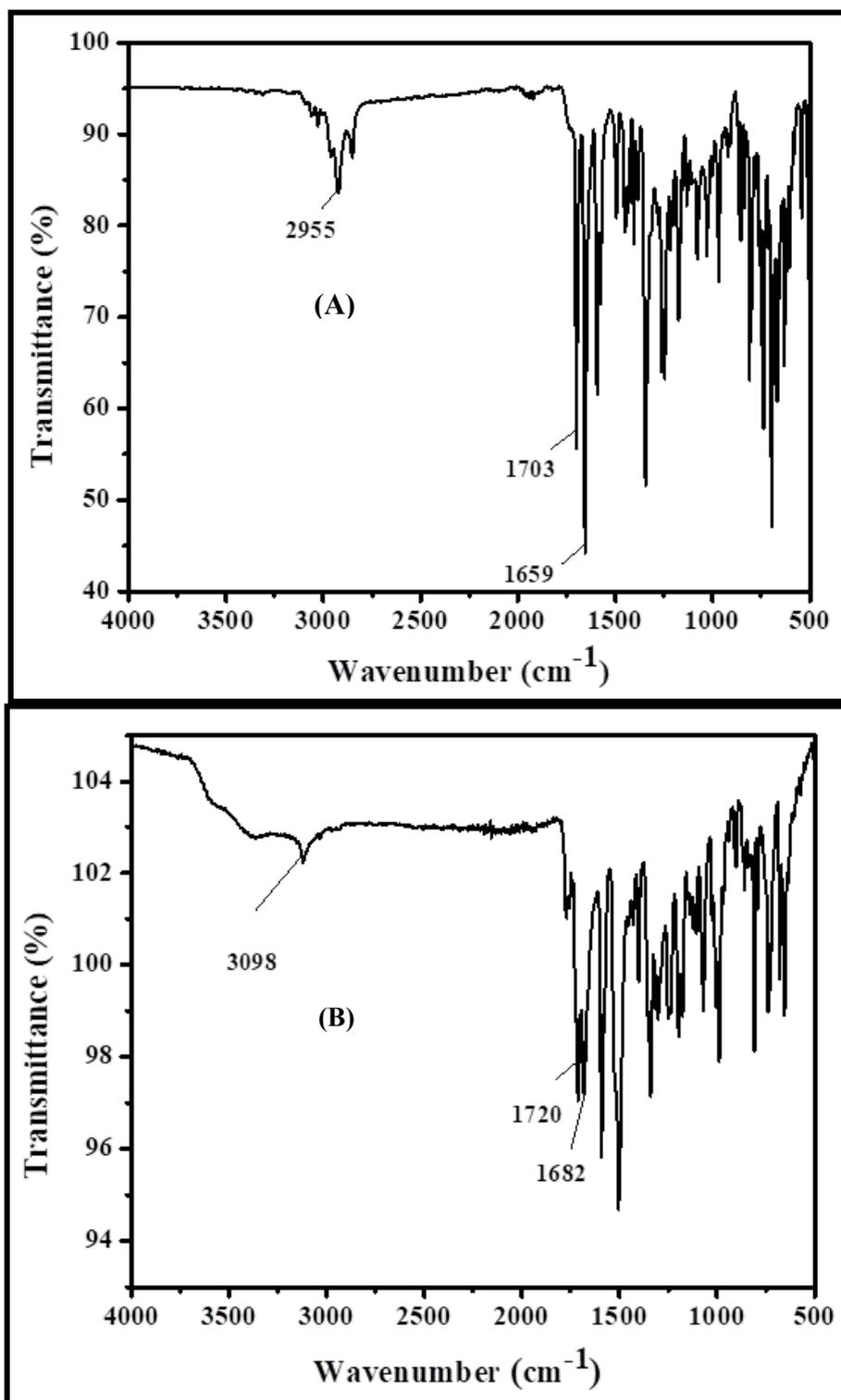
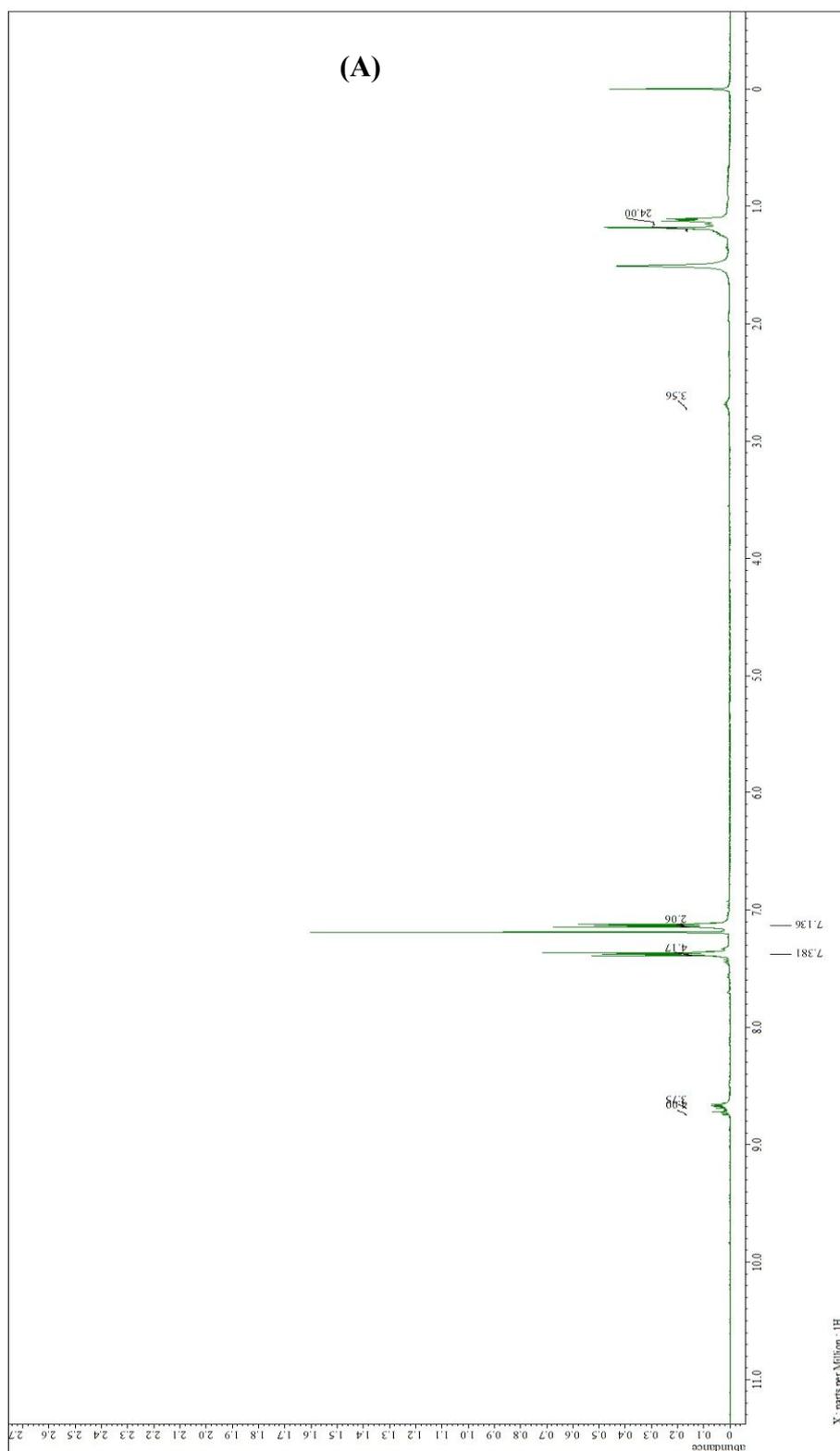


Figure S3. FT-IR spectra of (A) DPM-PDI (3) and (B) PFP-PDI (4).



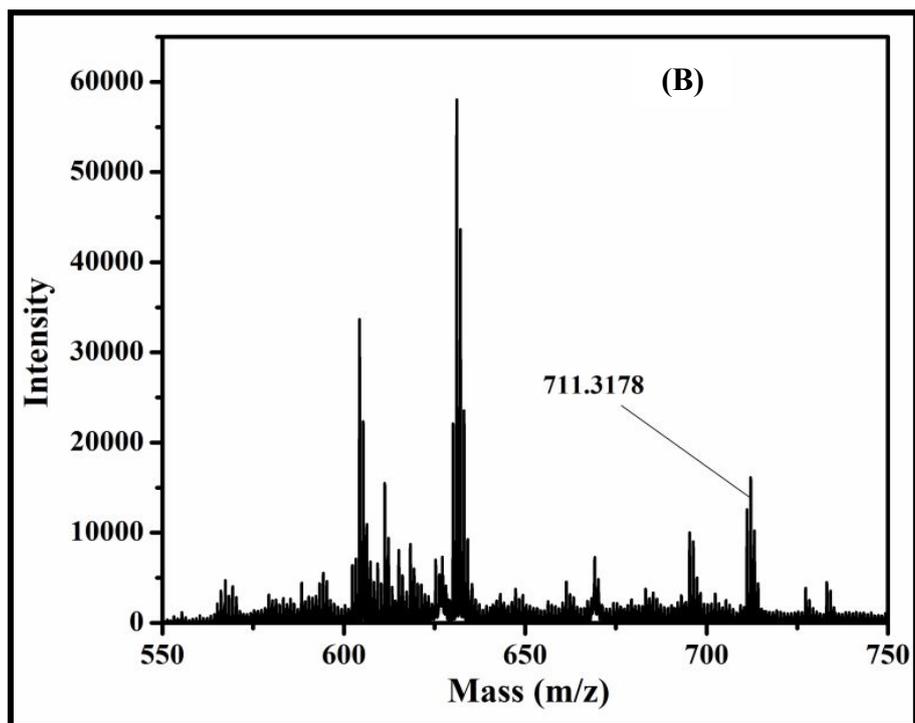
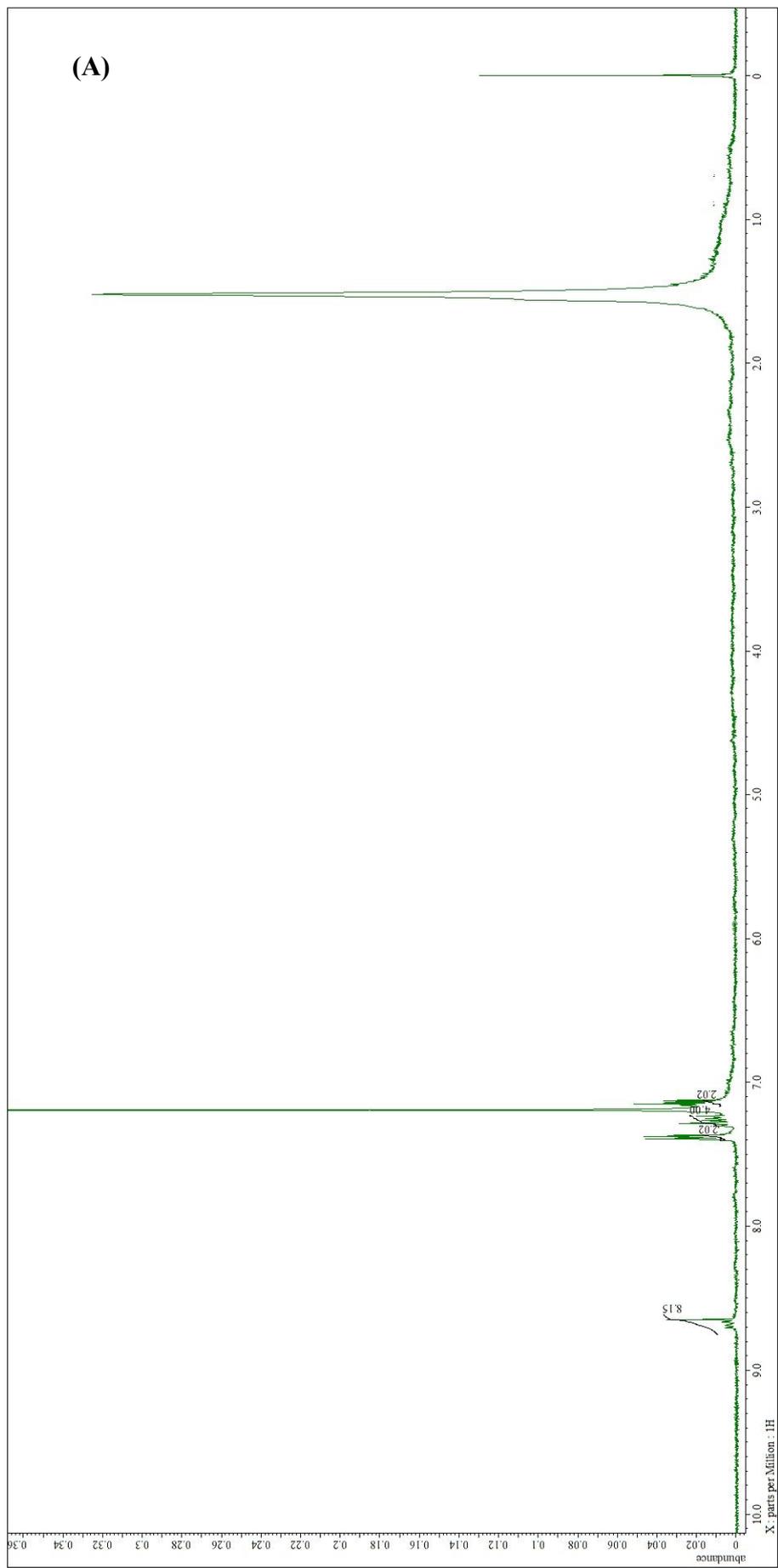


Figure S4. (A)  $^1\text{H}$  NMR, and (B) HR-MS spectra of *iPrP*-PDI.



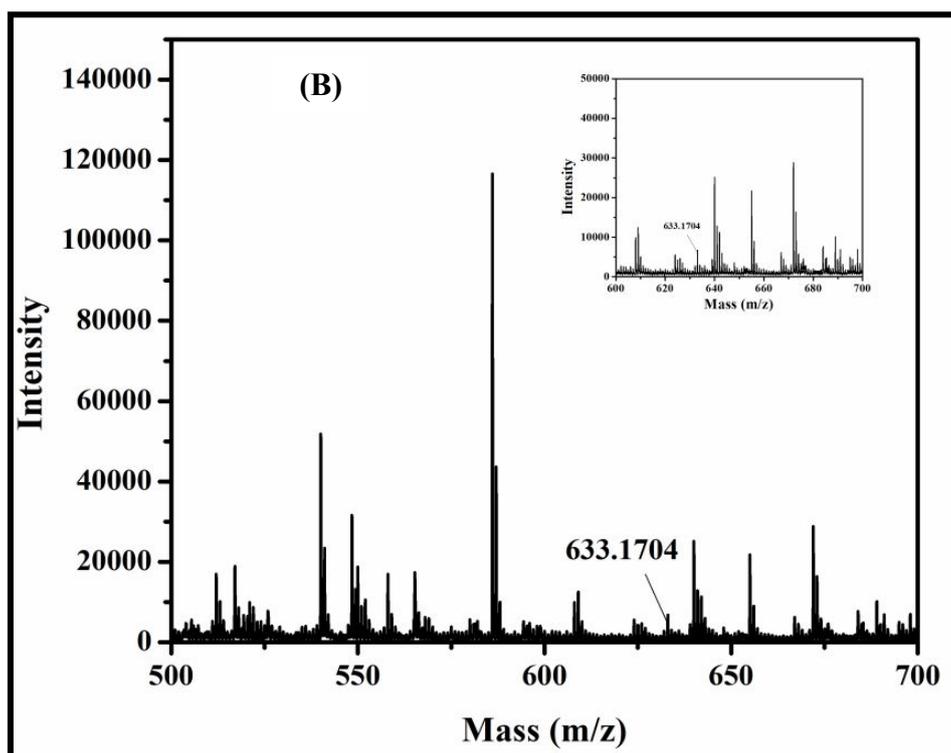
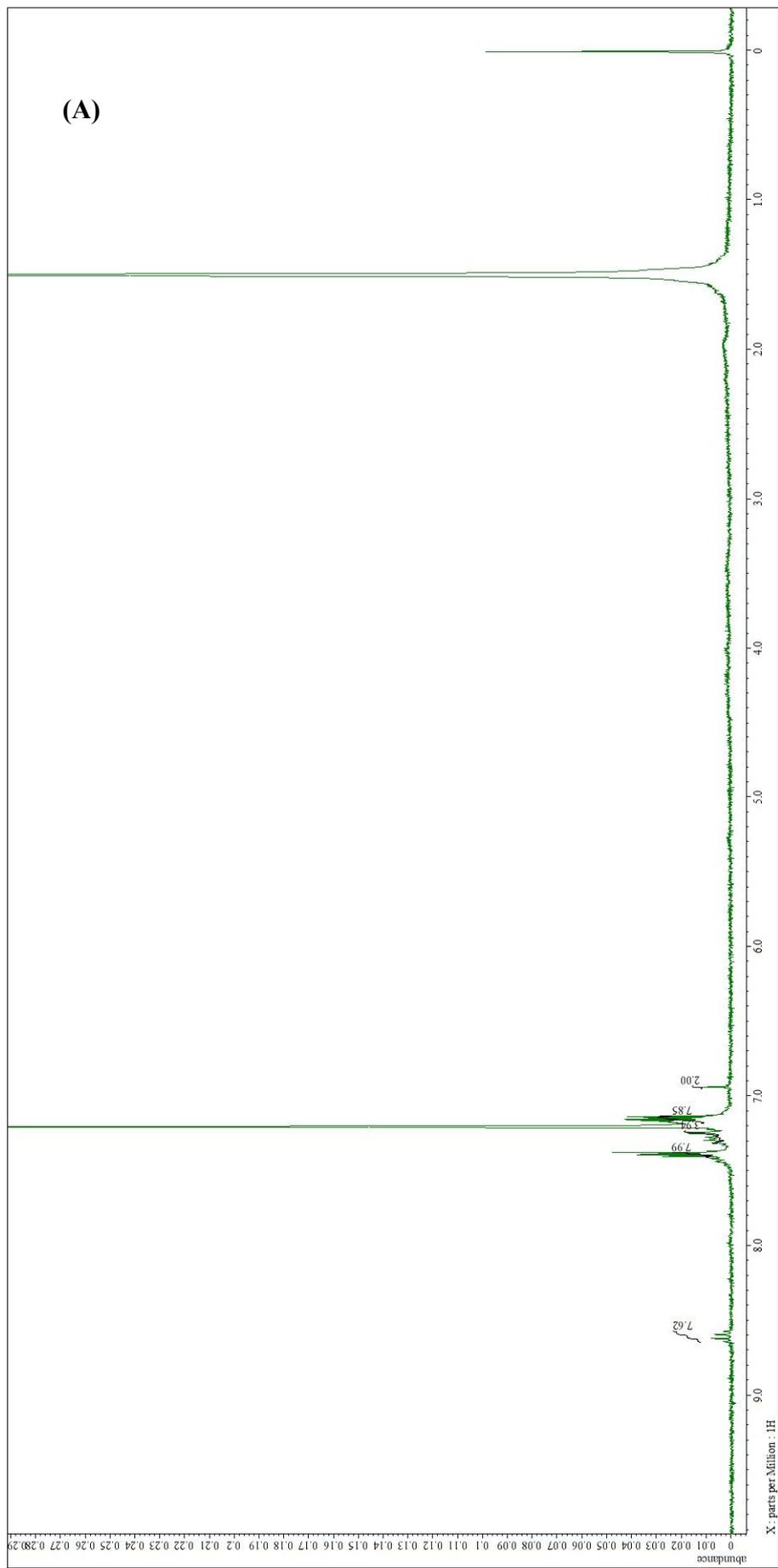


Figure S5. (A)  $^1\text{H}$  NMR and (B) HR-MS spectra of  $\text{NO}_2\text{P-PDI}$ .



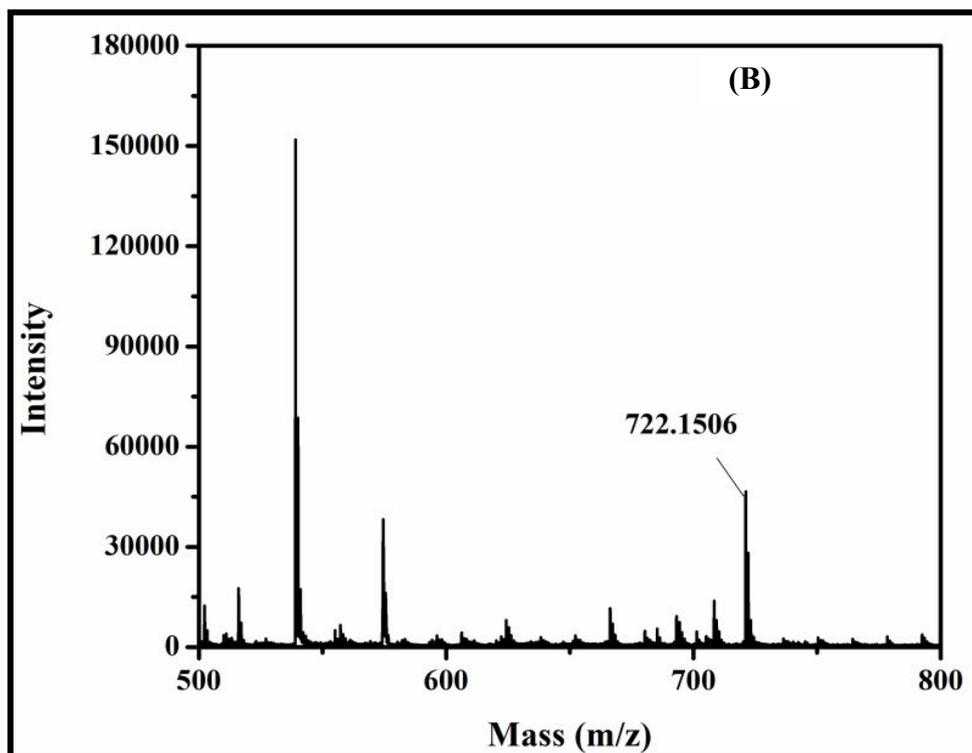
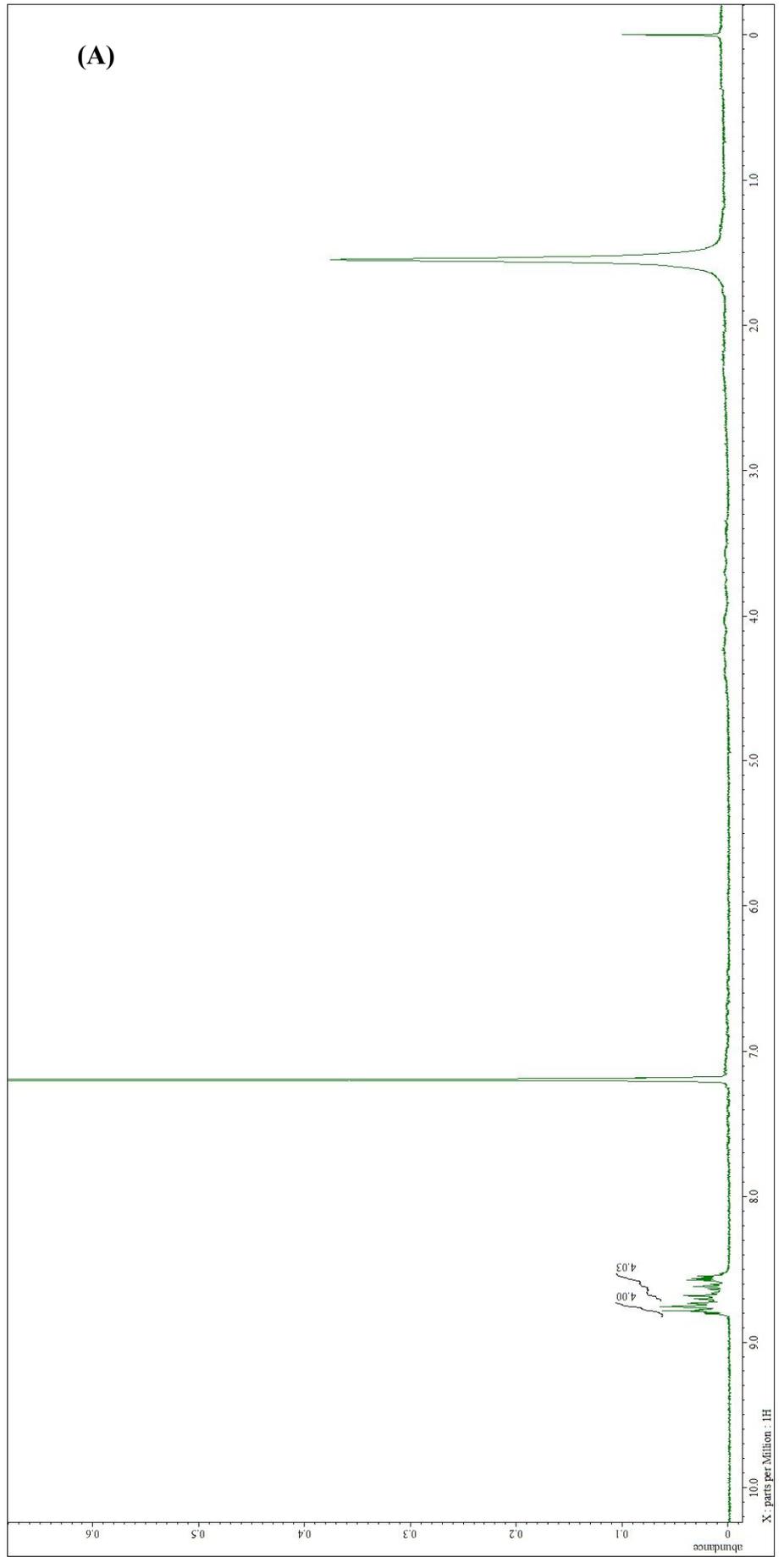


Figure S6. (A)  $^1\text{H}$  NMR, and (B) HR-MS spectra of DPM-PDI.



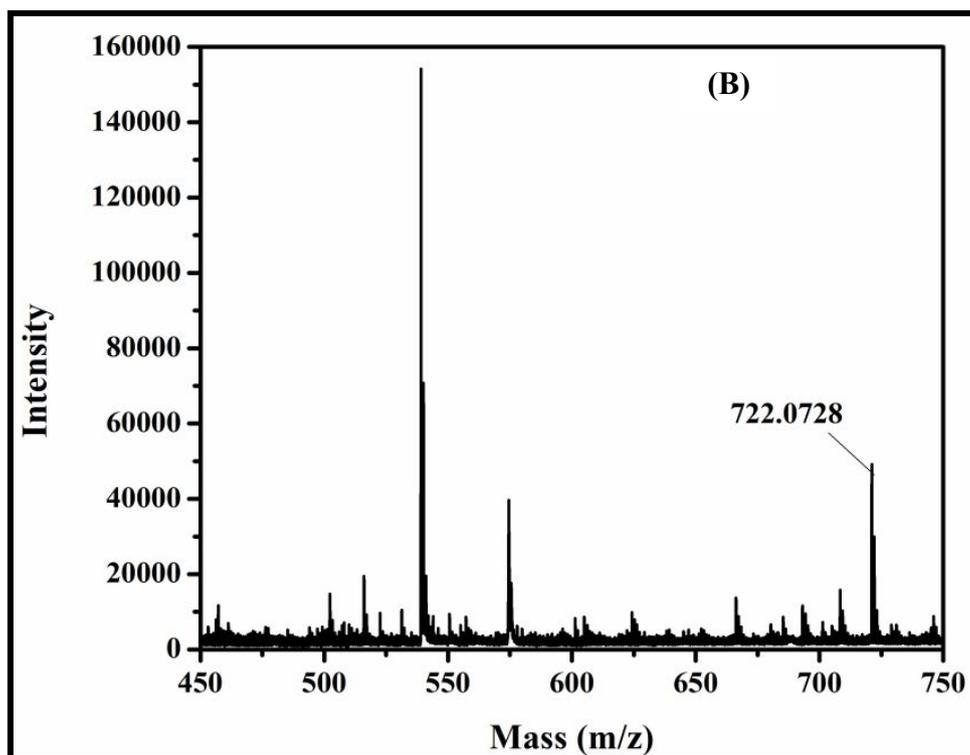
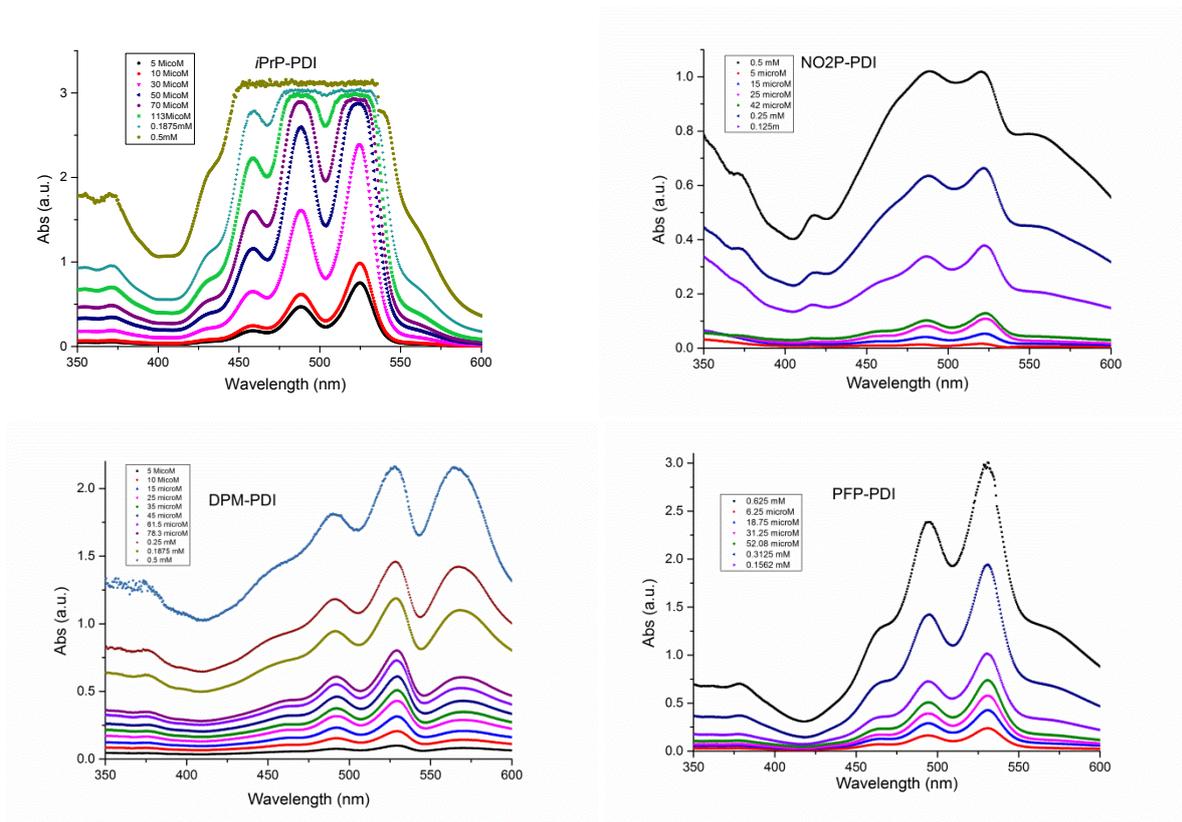
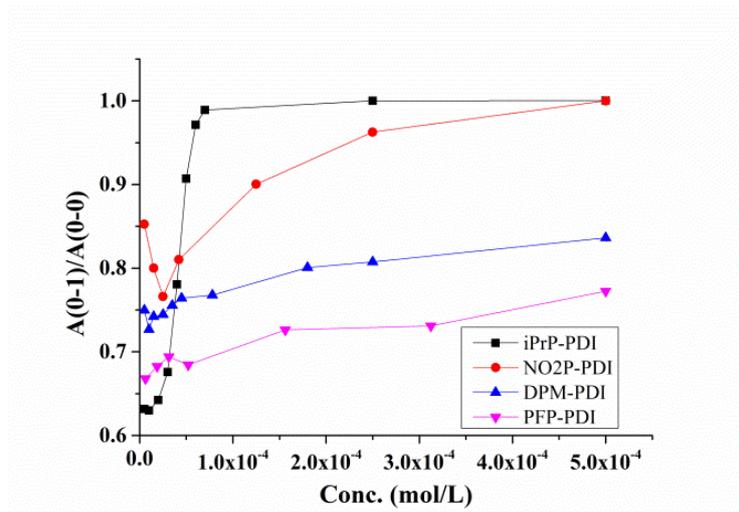


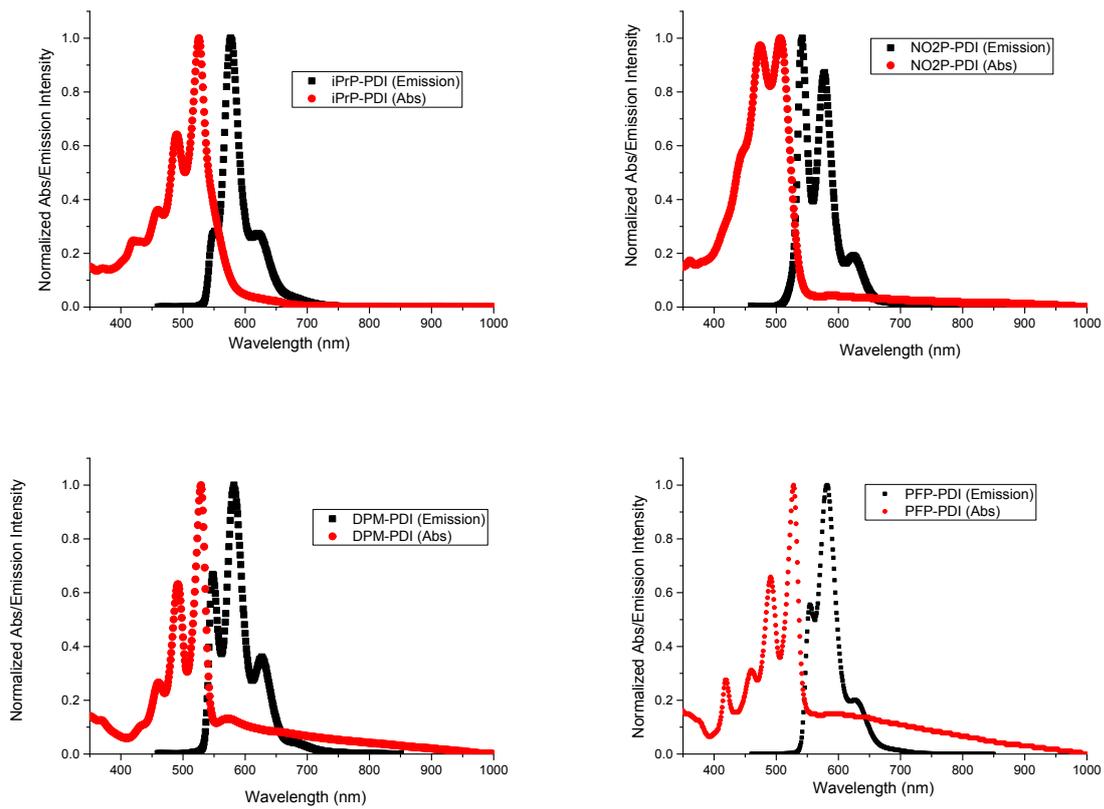
Figure S7. (A)  $^1\text{H}$  NMR, and (B) HR-MS spectra of PFP-PDI.



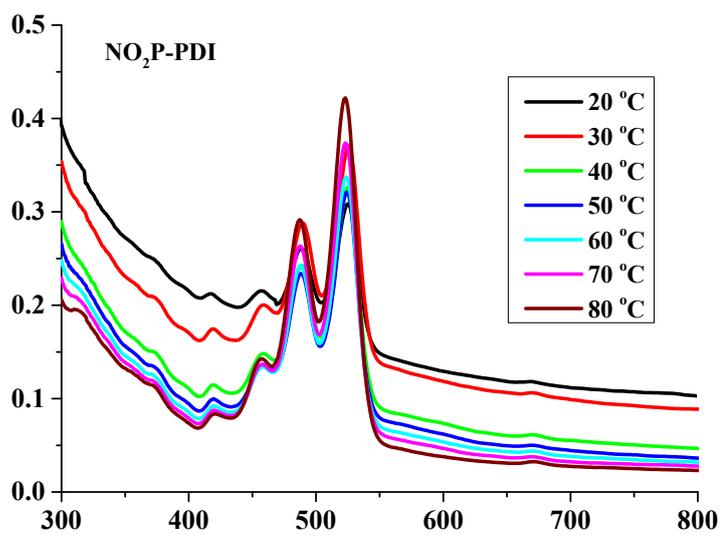
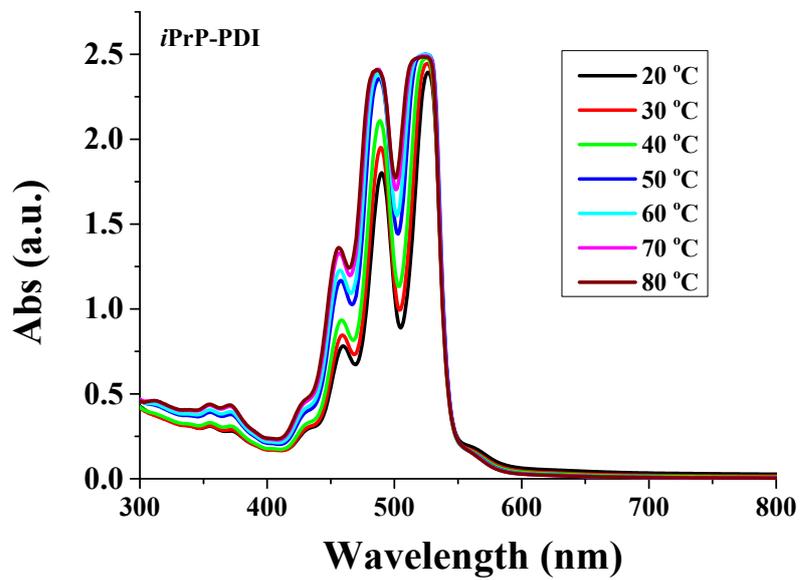
**Figure S8.** Concentration variable absorption spectra of PDIs in toluene.



**Figure S9.** Comparative  $A_{(0-1)}/A_{(0-0)}$  transition with change in concentration for PDIs.



**Figure S10.** Comparative absorption emission spectra of the PDIs in chloroform solution.



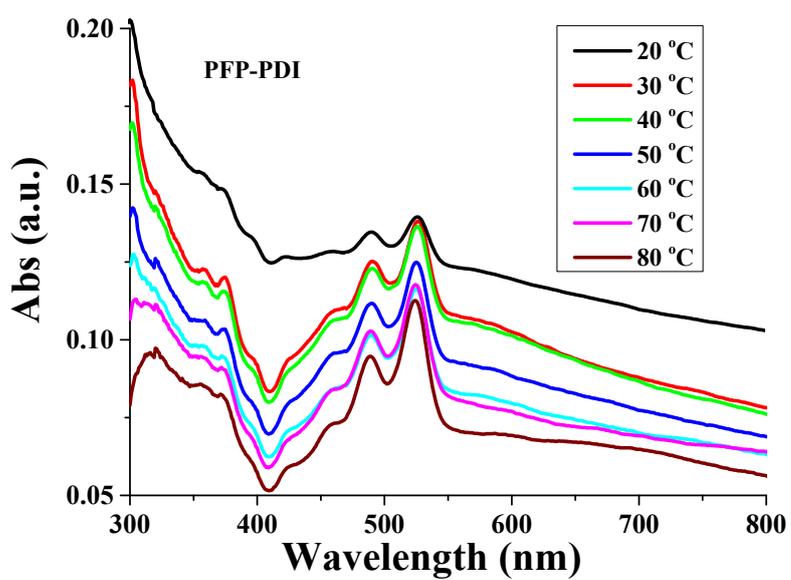
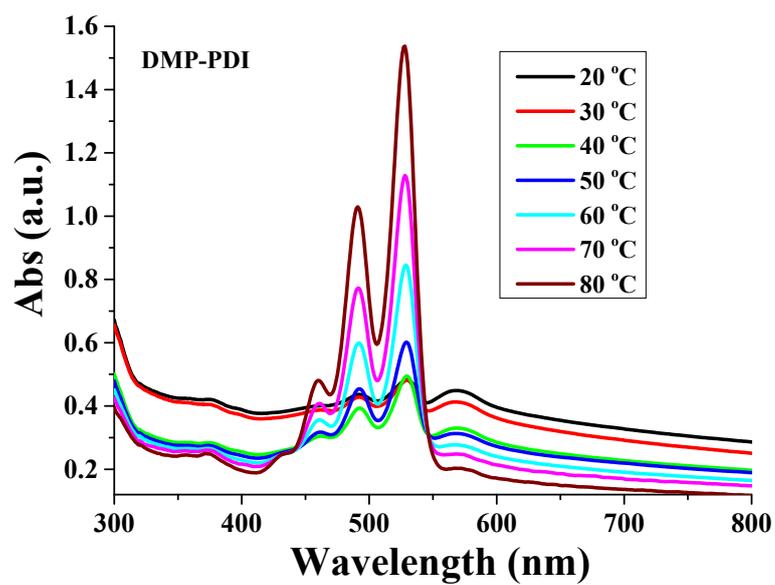
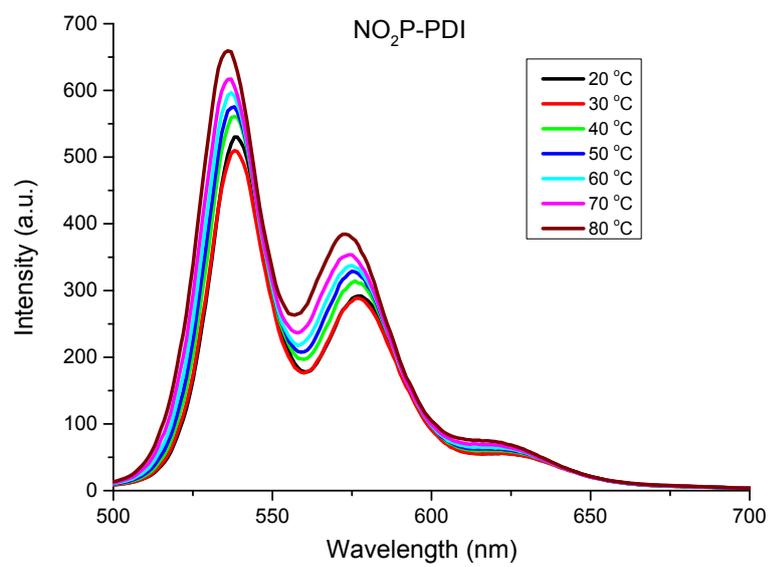
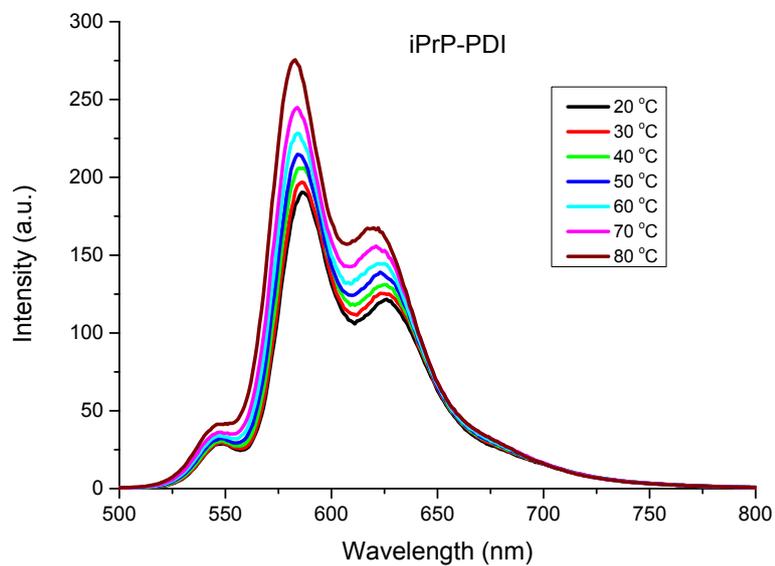


Figure S11. Temperature variable (20-80 °C) absorption spectra of PDI derivatives in toluene solution (diluted).



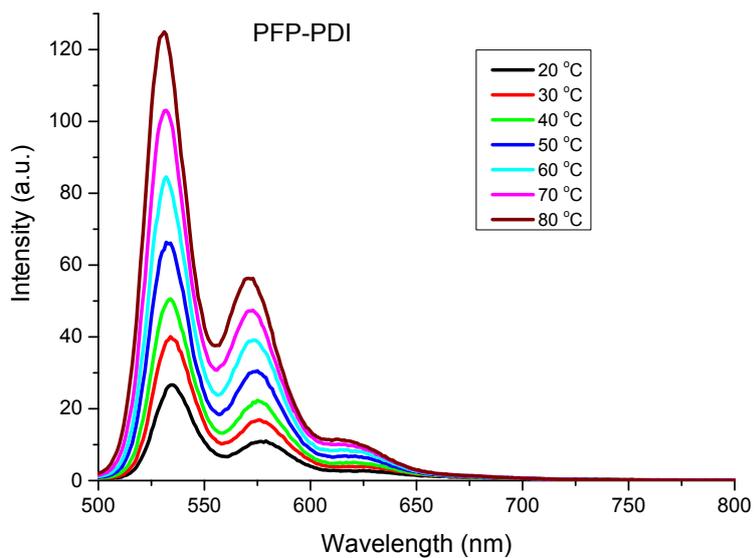
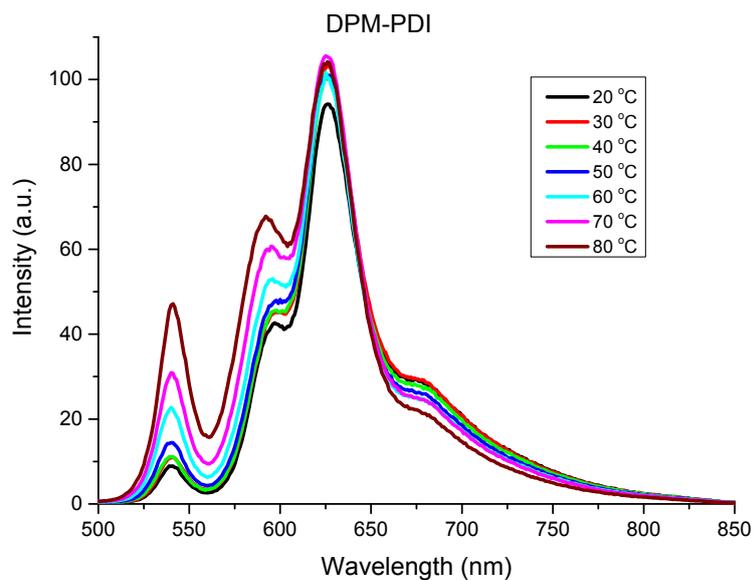
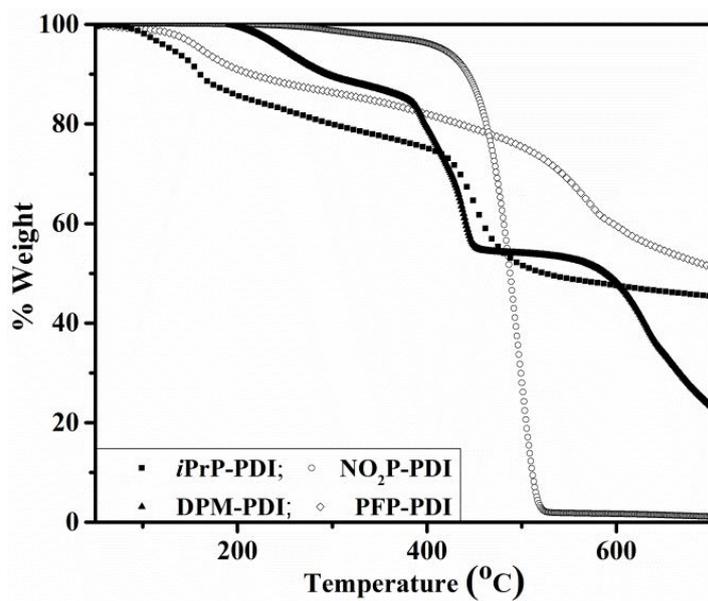


Figure S12. Temperature variable (20-80 °C) fluorescence spectra of PDI derivatives in toluene solution (0.5 mM) using 450 nm excitation wavelength.



**Figure S13.** TGA of *i*PrP-PDI (1), NO<sub>2</sub>P-PDI (2), DPM-PDI (3) and PFP-PDI (4) under N<sub>2</sub> flow of 20 mL min<sup>-1</sup> at 10 °C min<sup>-1</sup> temperature ramping.

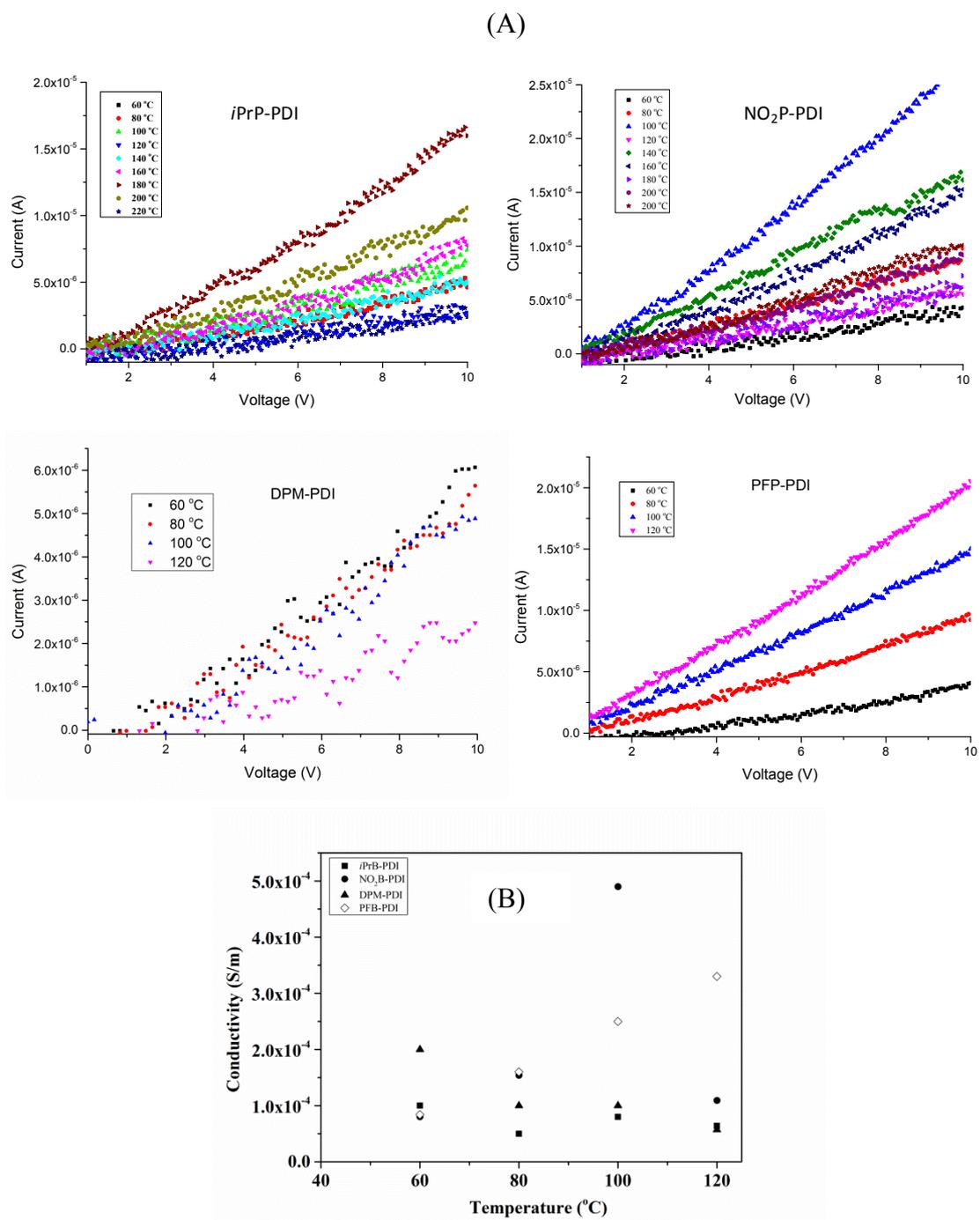


Figure S14. Electrical conductivity data (A) I vs V (B) Electrical conductivity at different temperatures for all the four PDIs.

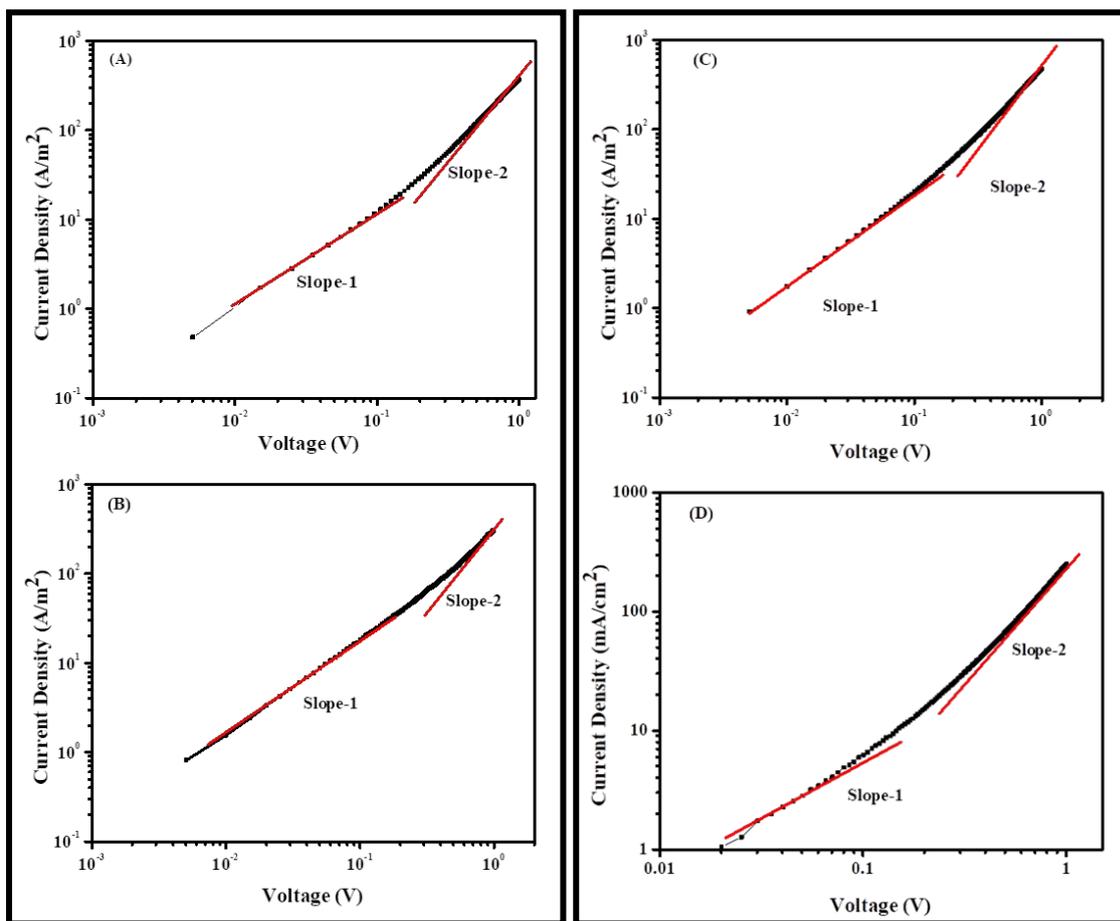


Figure S15. Electron transport J-V plots for (A) *i*PrP-PDI, (B) NO<sub>2</sub>P-PDI, (C) DPM-PDI and (D) PFP-PDI with slope.

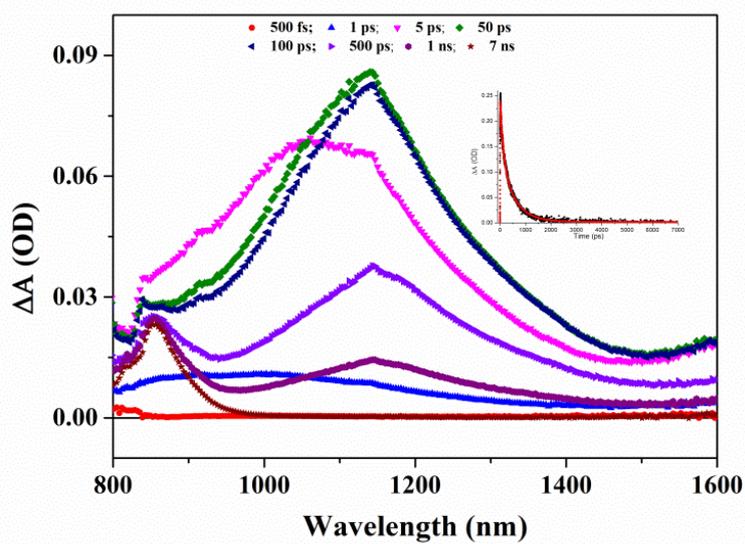
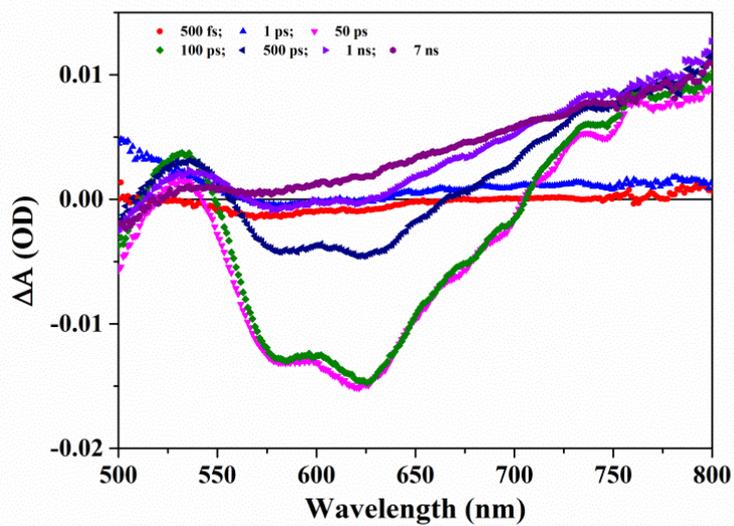
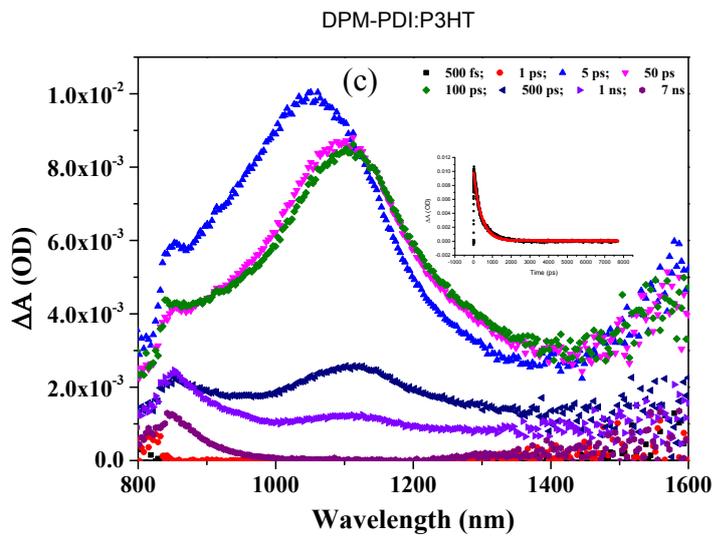
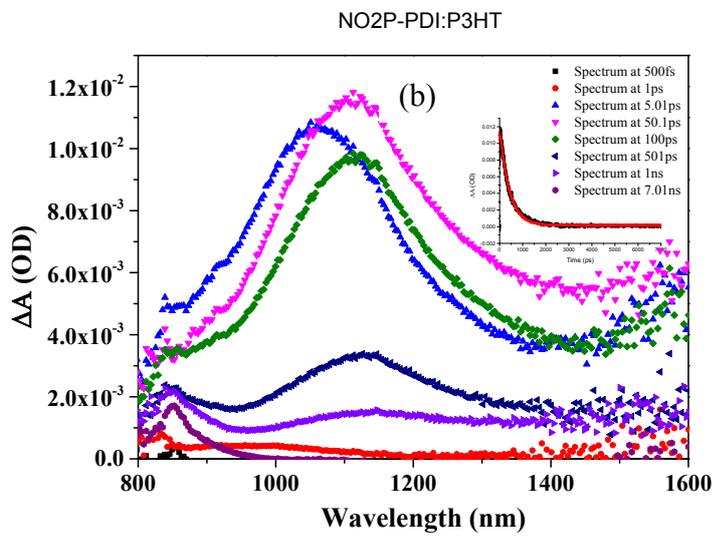
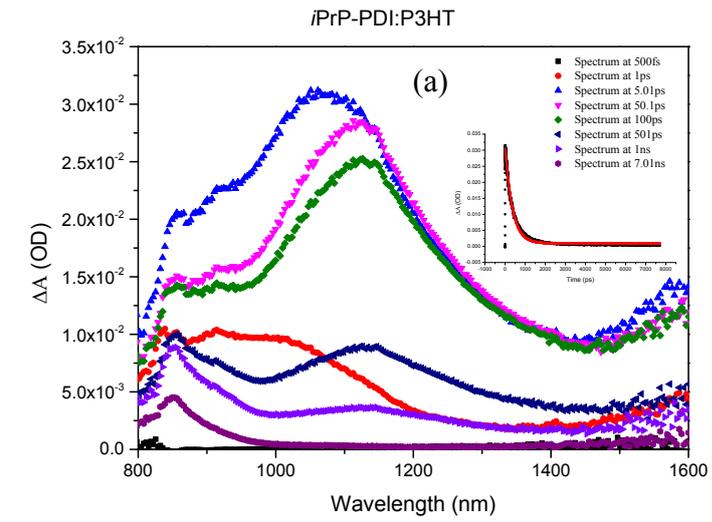


Figure S16. P3HT TAS spectra using 480 nm pump wavelength in visible and NIR region.



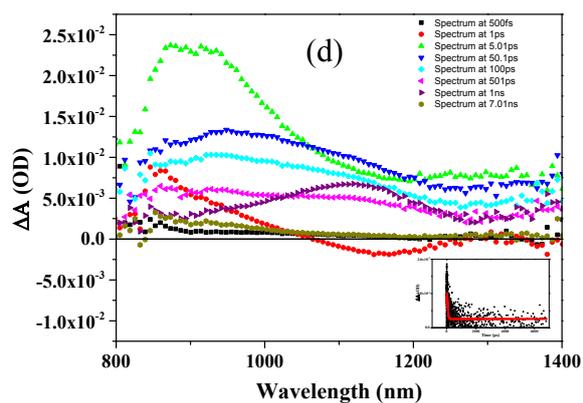


Figure S17. TAS spectra of P3HT mixture with (a) *i*PrP-PDI, (b) NO<sub>2</sub>P-PDI, (c) DPM-PDI and (d) PFP-PDI for NIR region using 480 nm pump wavelength. Inset shows the decay of  $\sim 1140$  nm transient absorption for P3HT singlet excited state.