

## Supporting Information

### Electron Transport and Ultrafast Spectroscopic Studies of New

### Methanofullerenes bearing Heteroatom in exohedral chain

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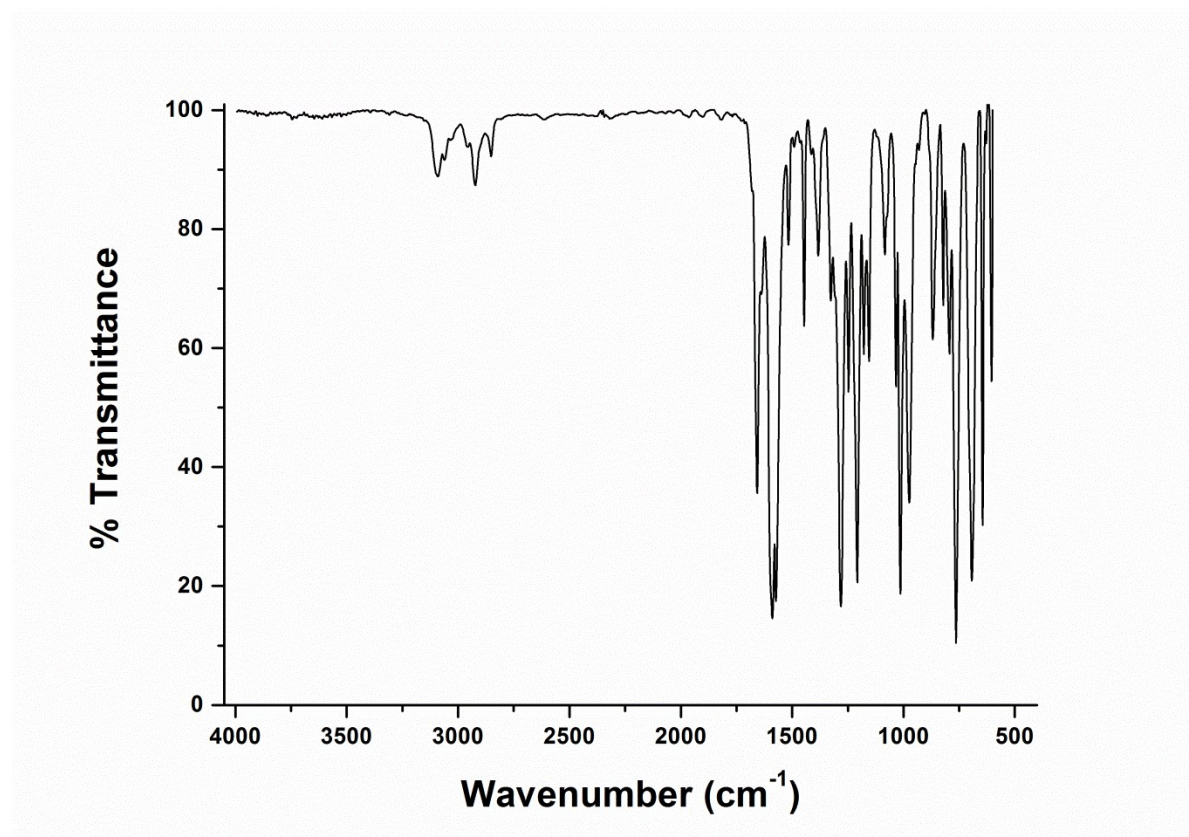


Figure S1. FTIR spectra of Chalcone 1a.

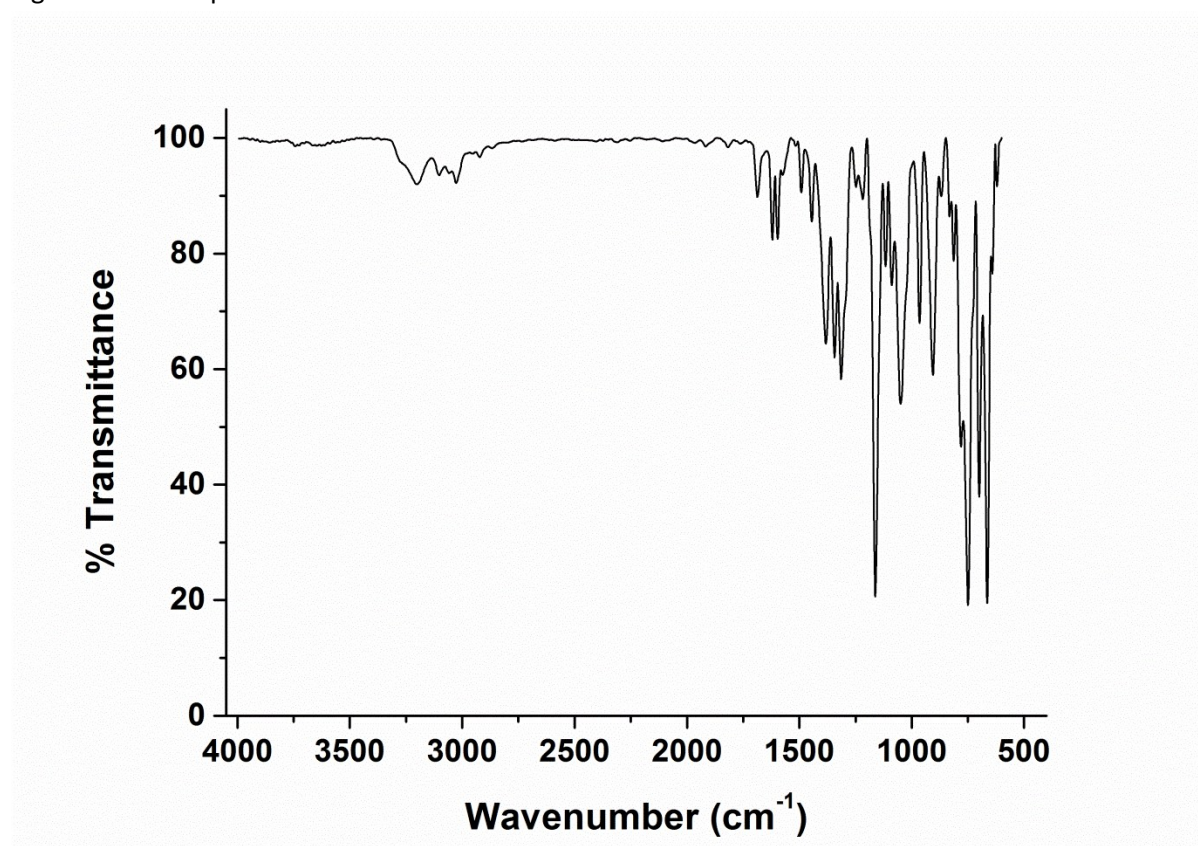


Figure S2. FTIR Spectra of hydrazone 1b.

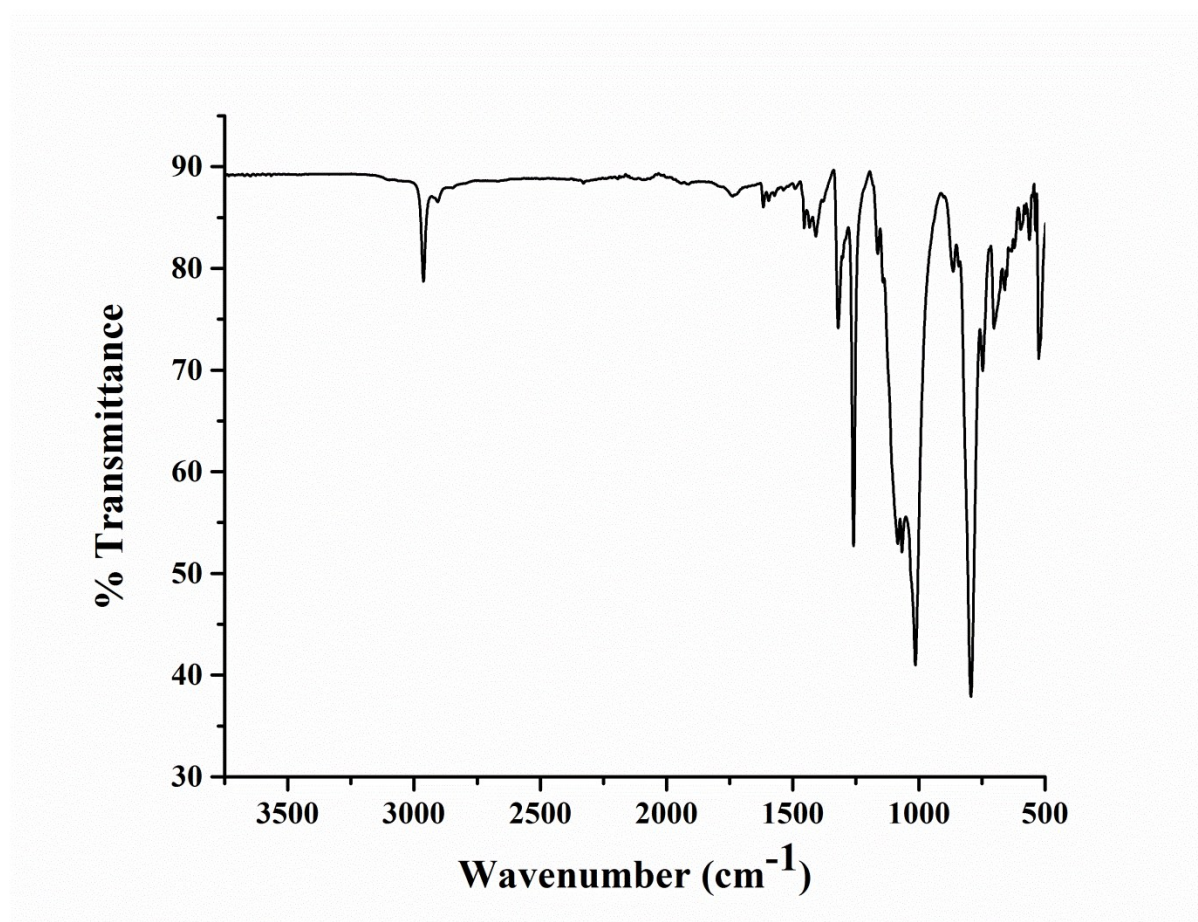
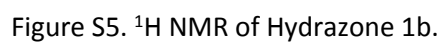


Figure S3. FTIR spectra of Product 1 (C60-Thio3CA).





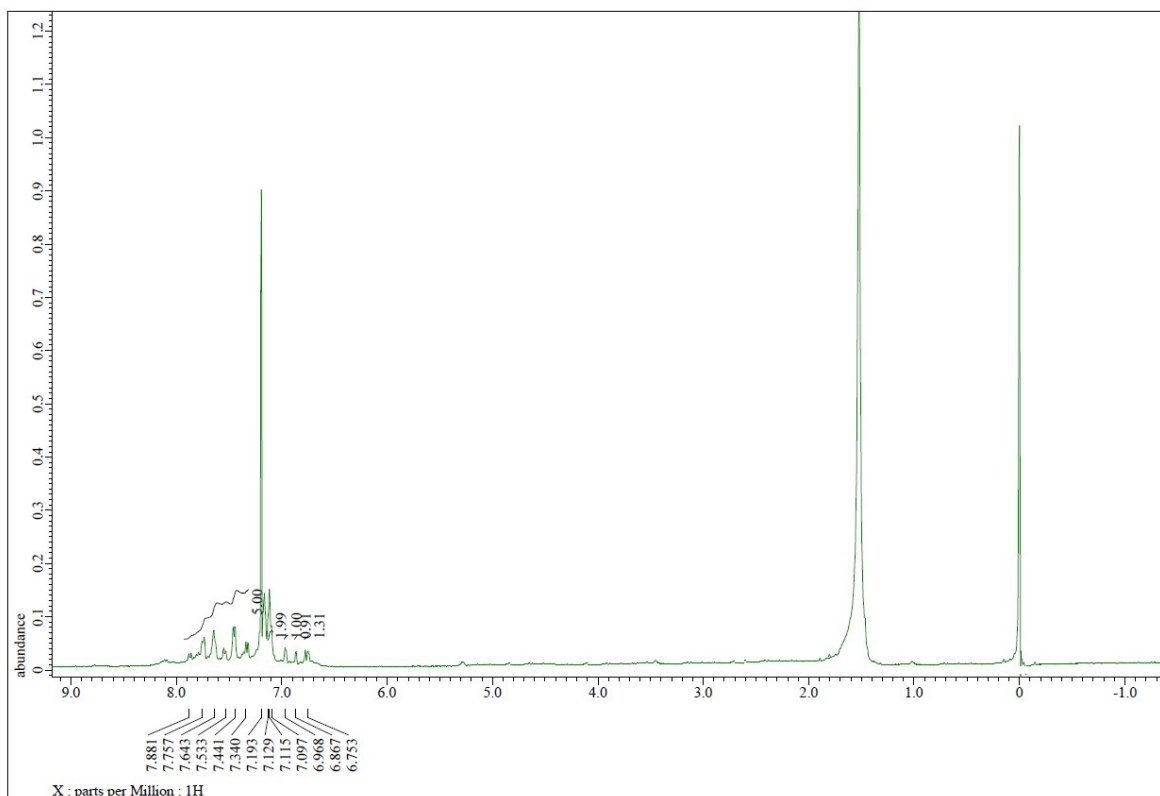


Figure S6.  $^1\text{H}$  NMR Spectra of Product 1 (C60-Thio3CA)

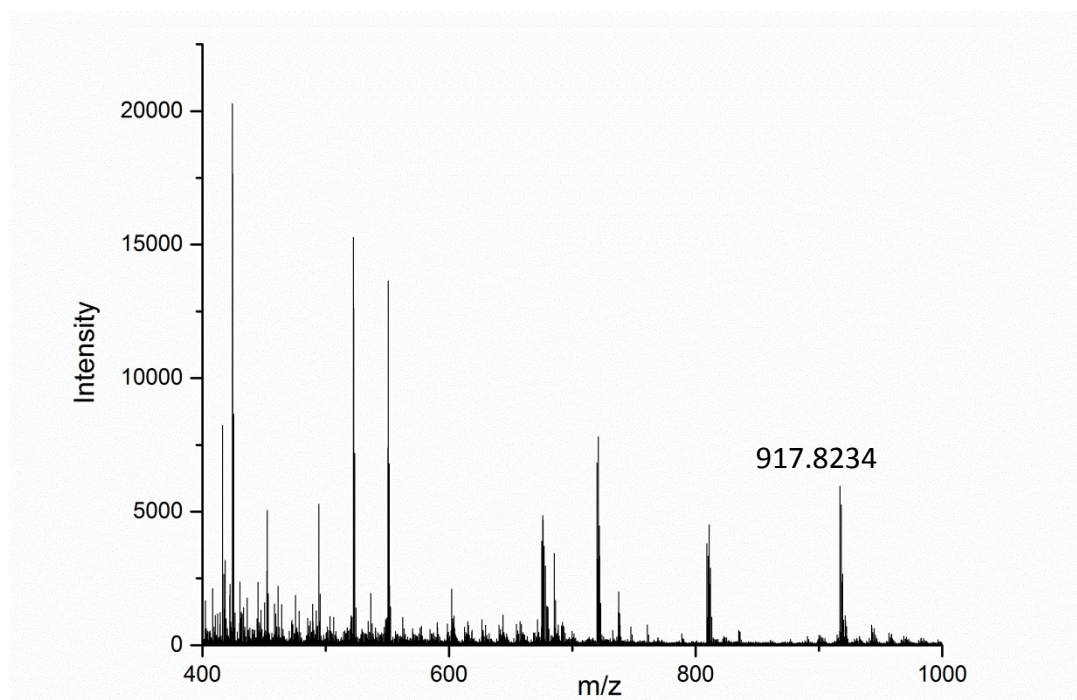


Figure S7. MALDI-TOF HRMS of Product 1.

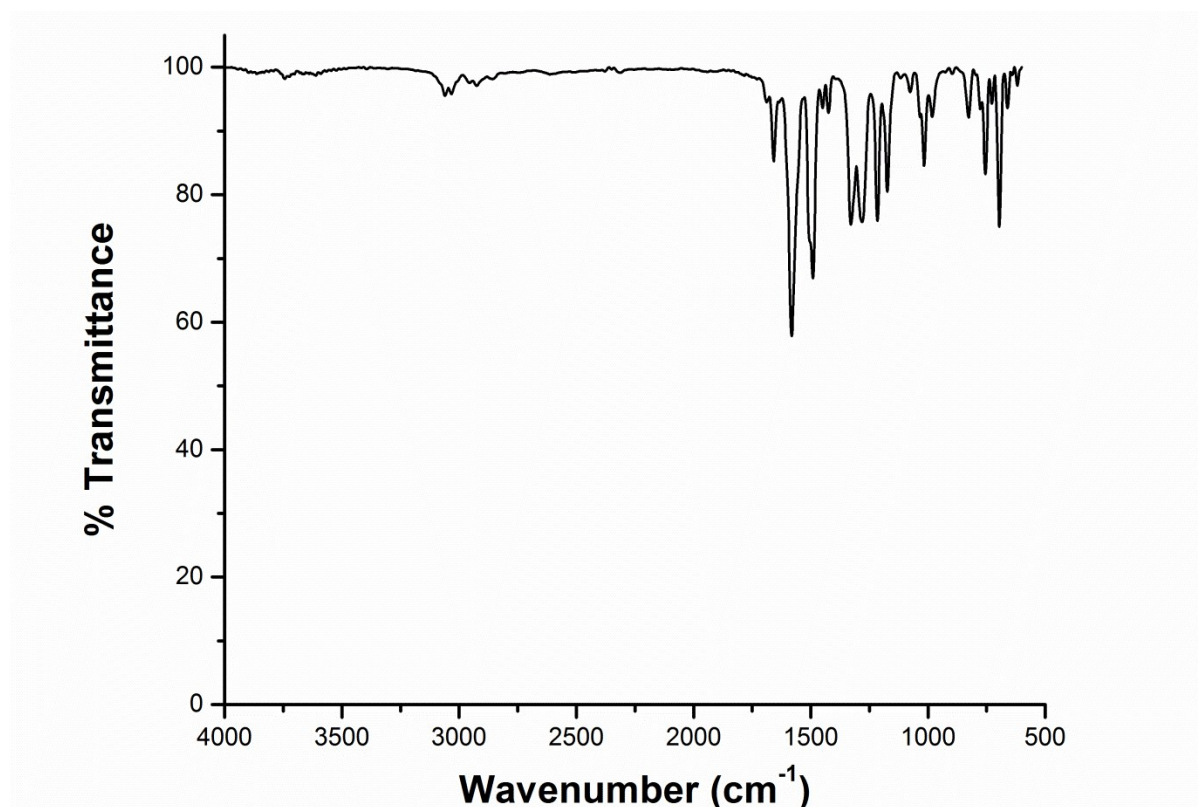


Figure S8. FTIR spectra of chalcone 2a.

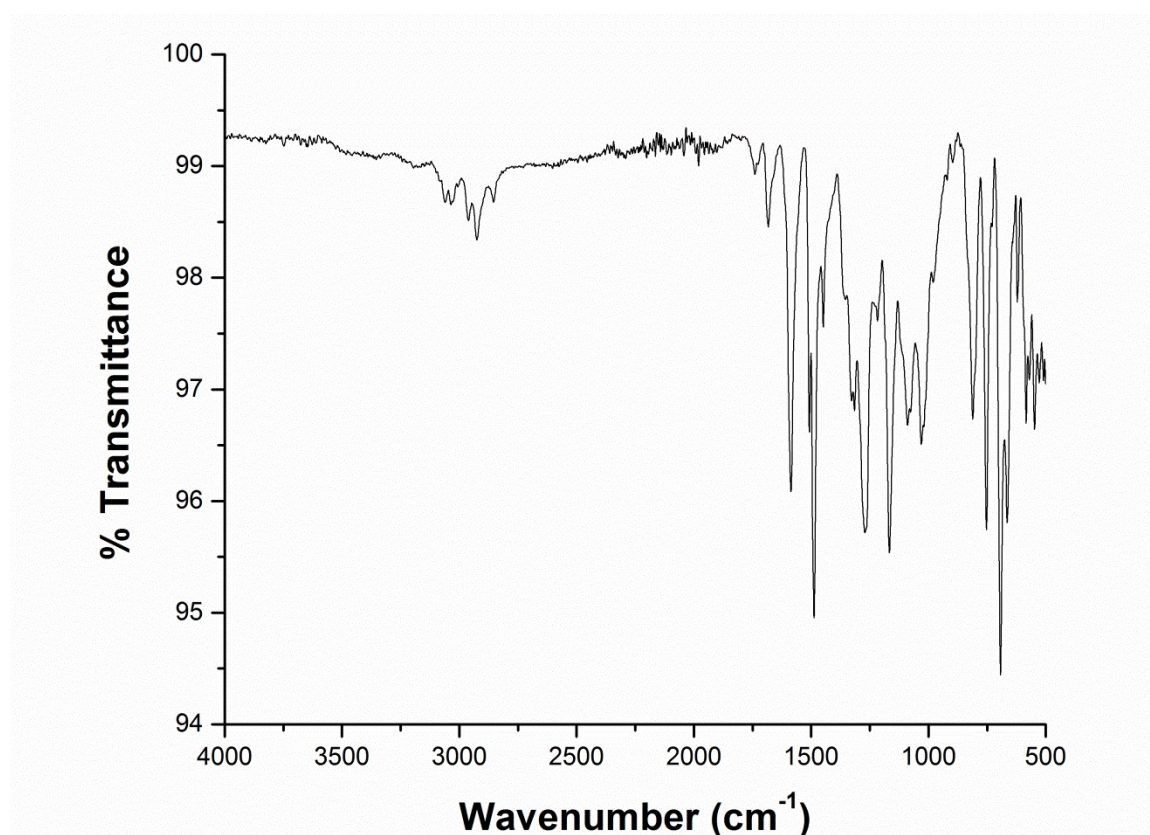


Figure S9. FTIR spectra of Hydrazone 2b.

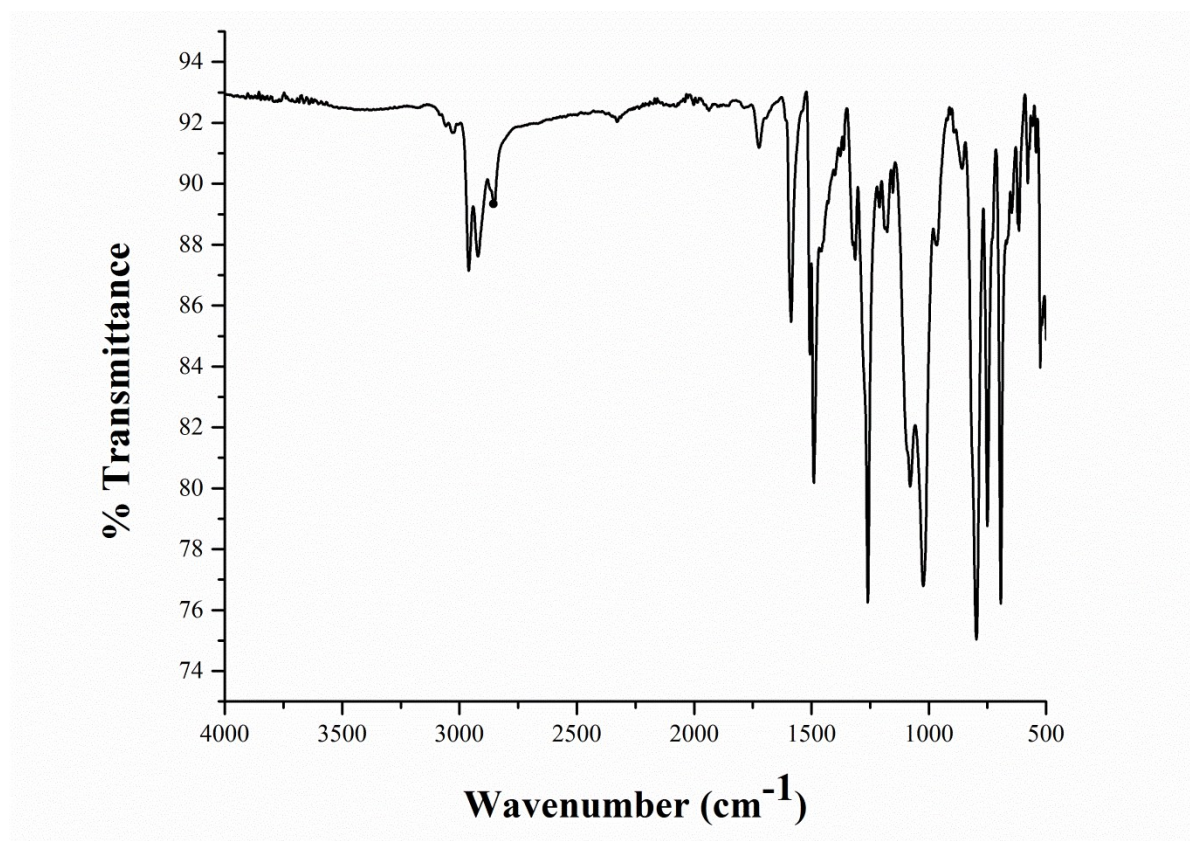


Figure S10. FTIR spectra of product 2.

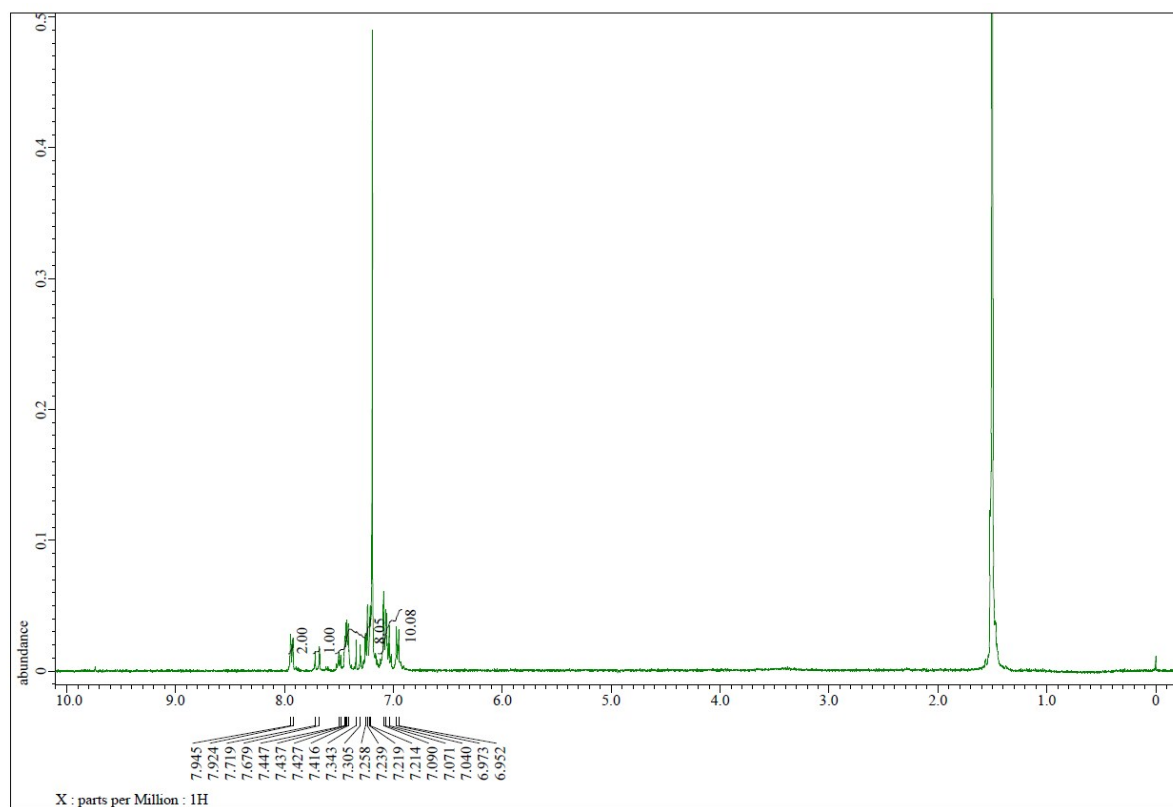


Figure S11. <sup>1</sup>H NMR spectra of Chalcone 2a.

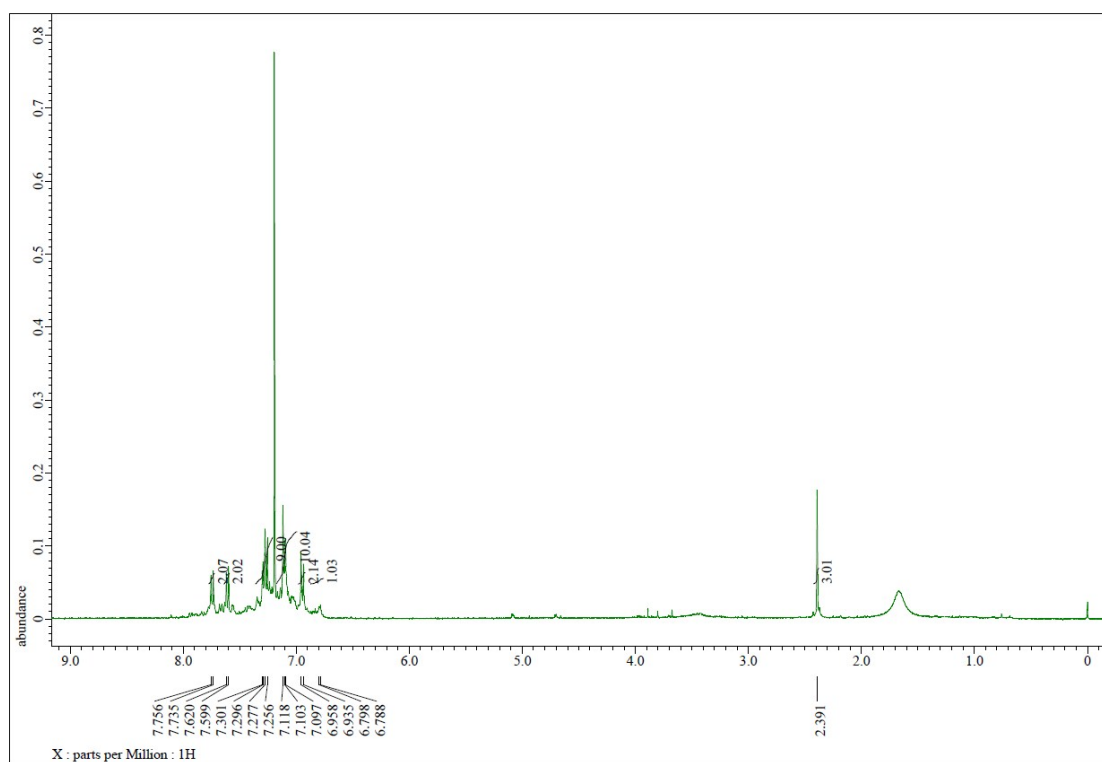


Figure S12.  $^1\text{H}$  NMR spectra of hydrazone 2b.

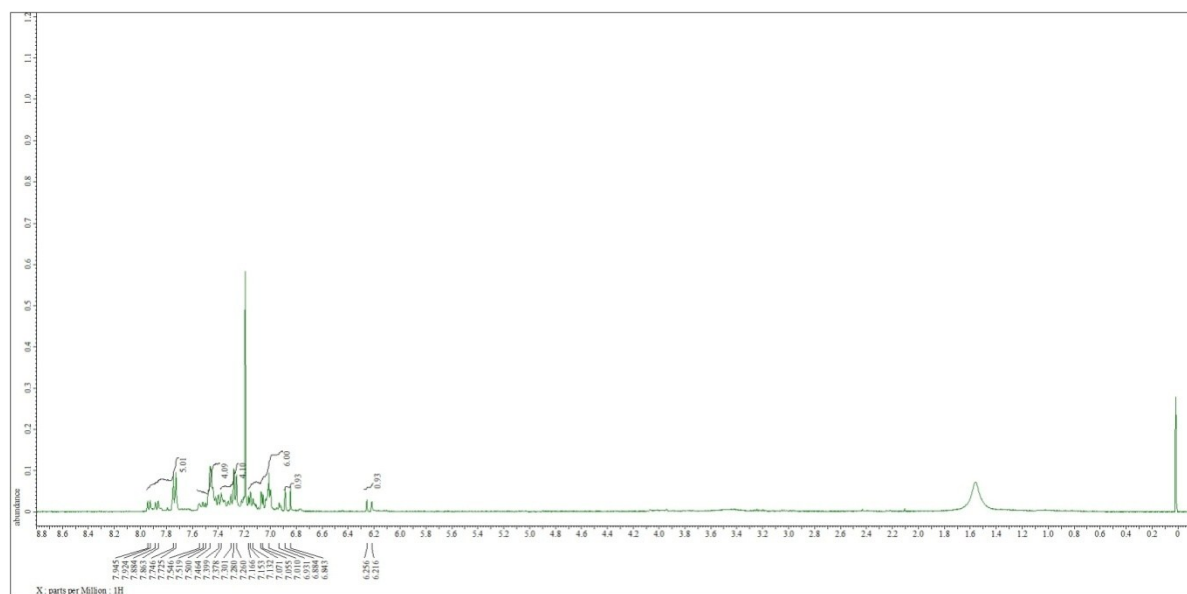


Figure S13.  $^1\text{H}$  NMR spectra of Product 2 (C60-DPAB).



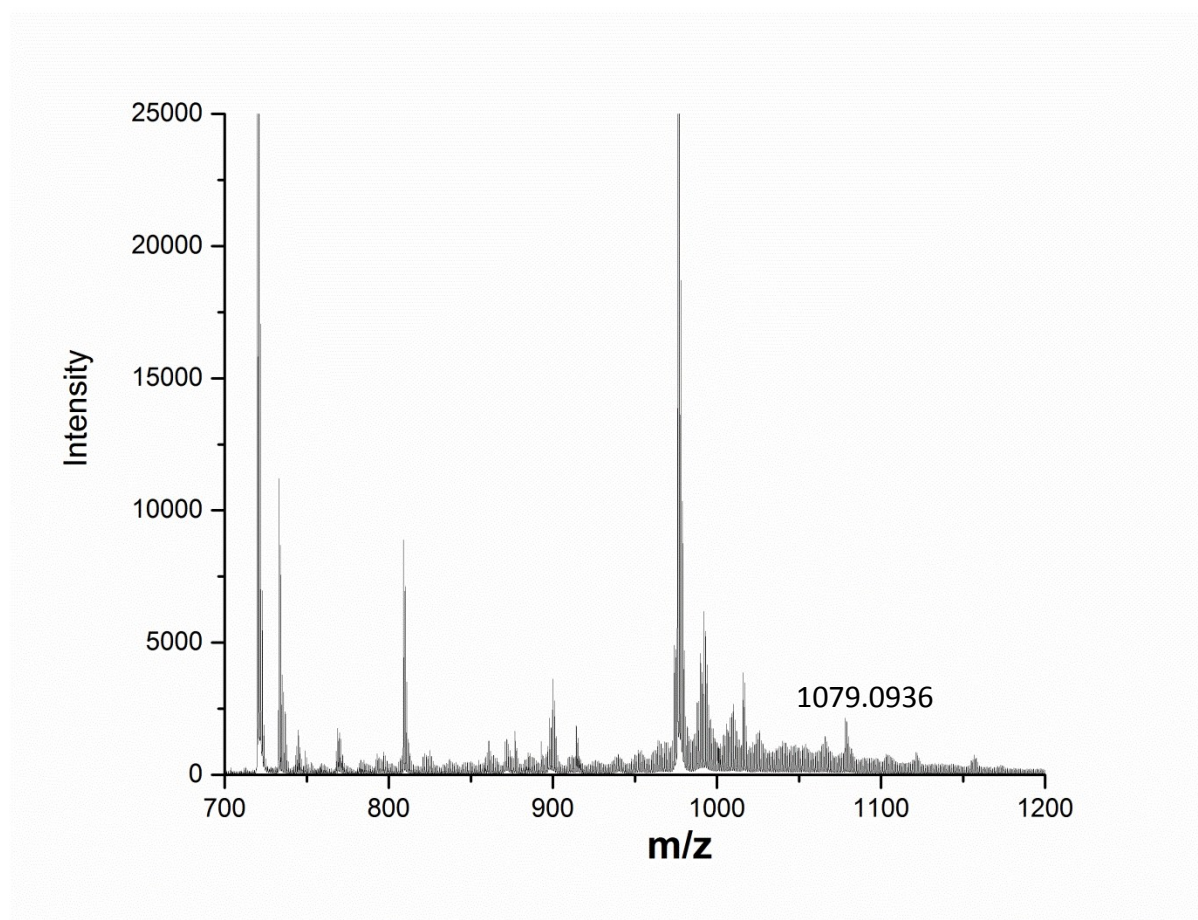


Figure S14. MALDI-TOF HRMS of Product 2.

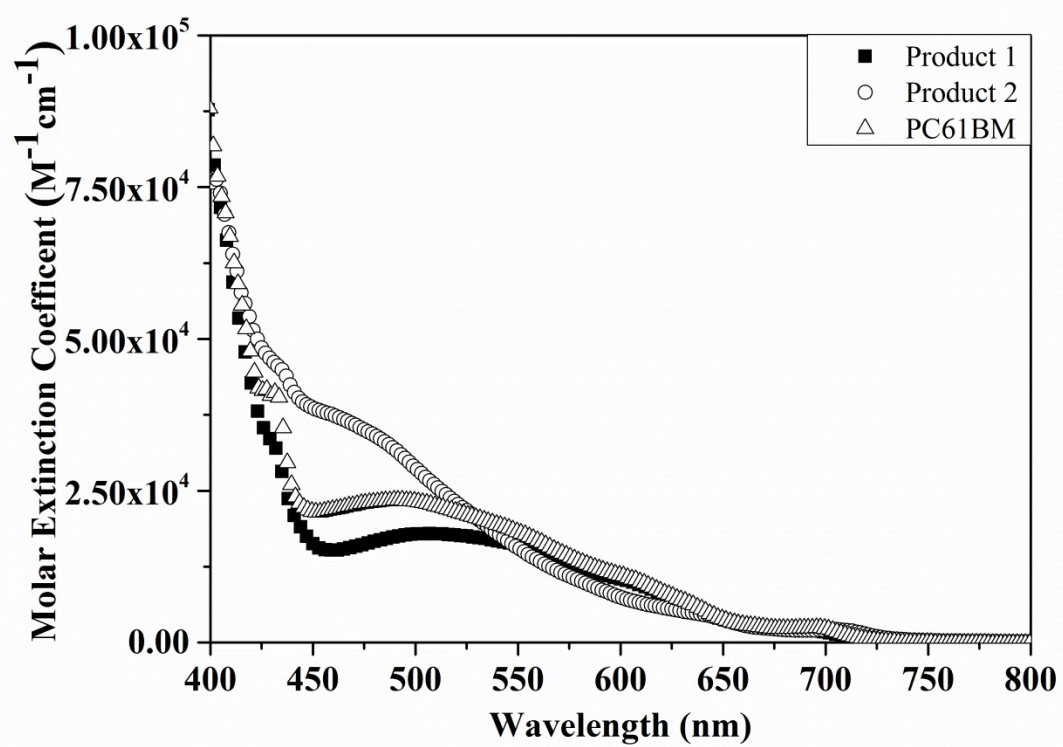


Figure S15. Absorption coefficient vs. wavelength plot for Product 1 (Thio-C60) and Product 2 (DPAB-C60) in chloroform solution.

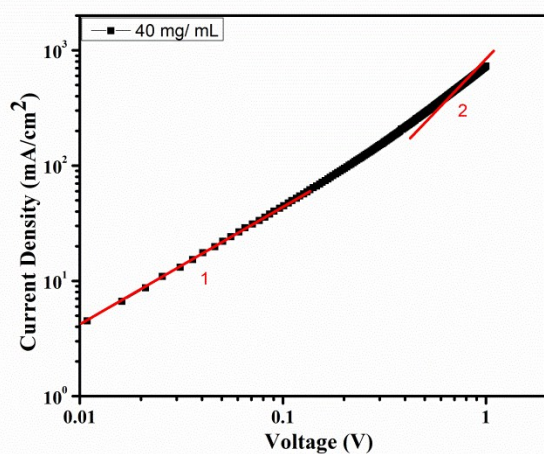
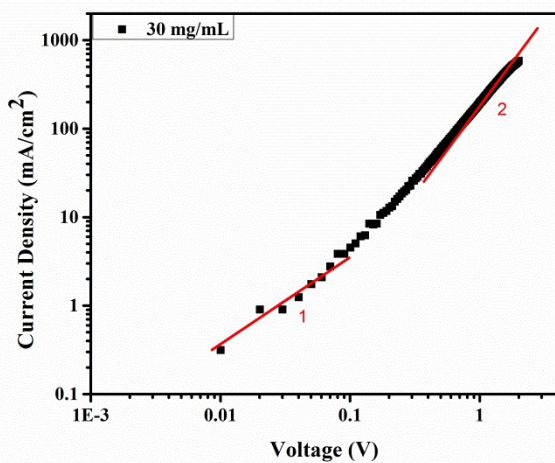
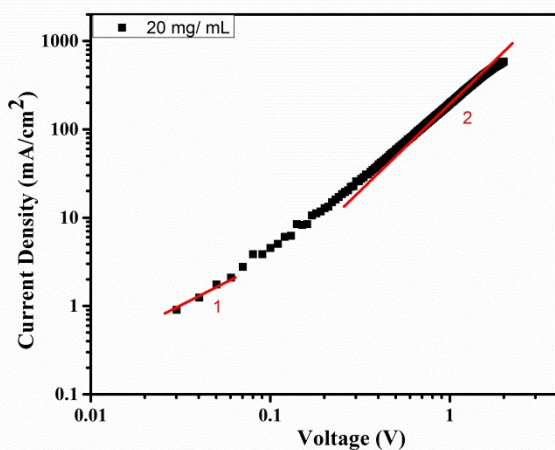


Figure S16. Log plot of J-V characteristics of Thio-C60 (Product 1) electron only devices (ITO/ZnO/Product/Al) for 20mg/mL, 30mg/mL and 40 mg/mL concentrations for calculation of electron mobility. Slope 1 and 2 show the Ohmic and SCLC regions respectively.

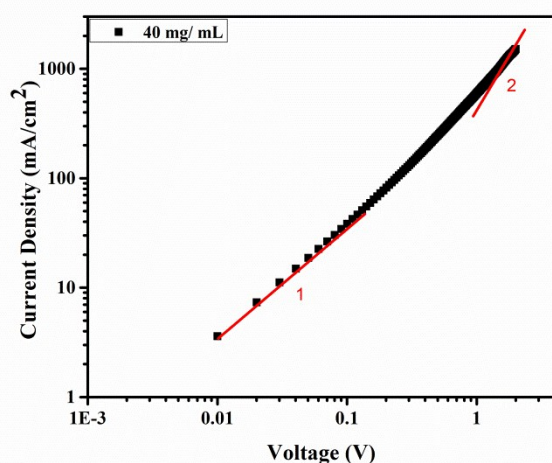
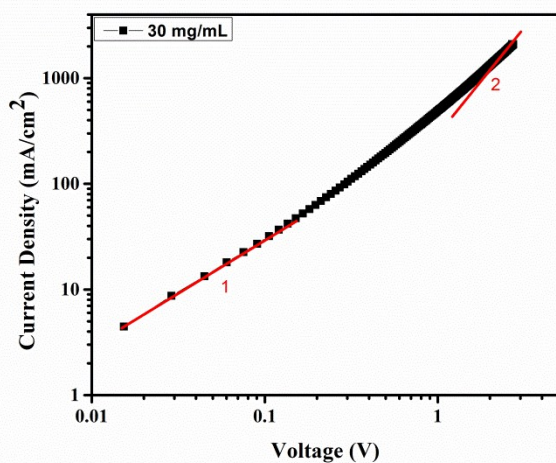
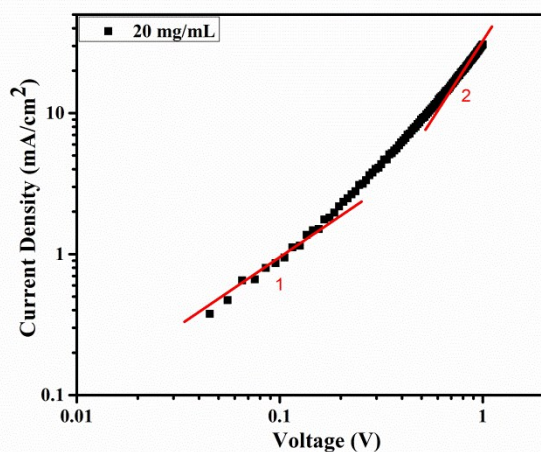


Figure S17. Log plot of J-V characteristics of DPAB-C60 (Product 2) electron only devices (ITO/ZnO/Product/Al) for 20mg/mL, 30mg/mL and 40 mg/mL concentrations for calculation of electron mobility. Slope 1 and 2 show the Ohmic and SCLC regions respectively.



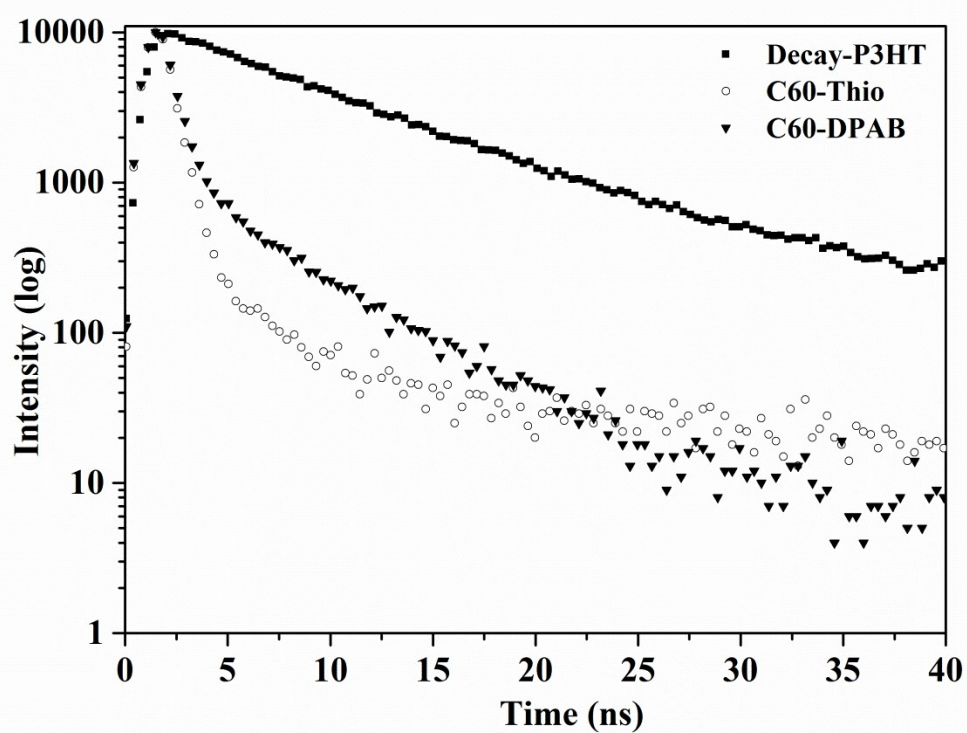


Figure S18. Time correlated single photon spectroscopy performed at 584 nm to study the decay kinetics of singlet excited state of P3HT in neat and in mixture with products 1 & 2.

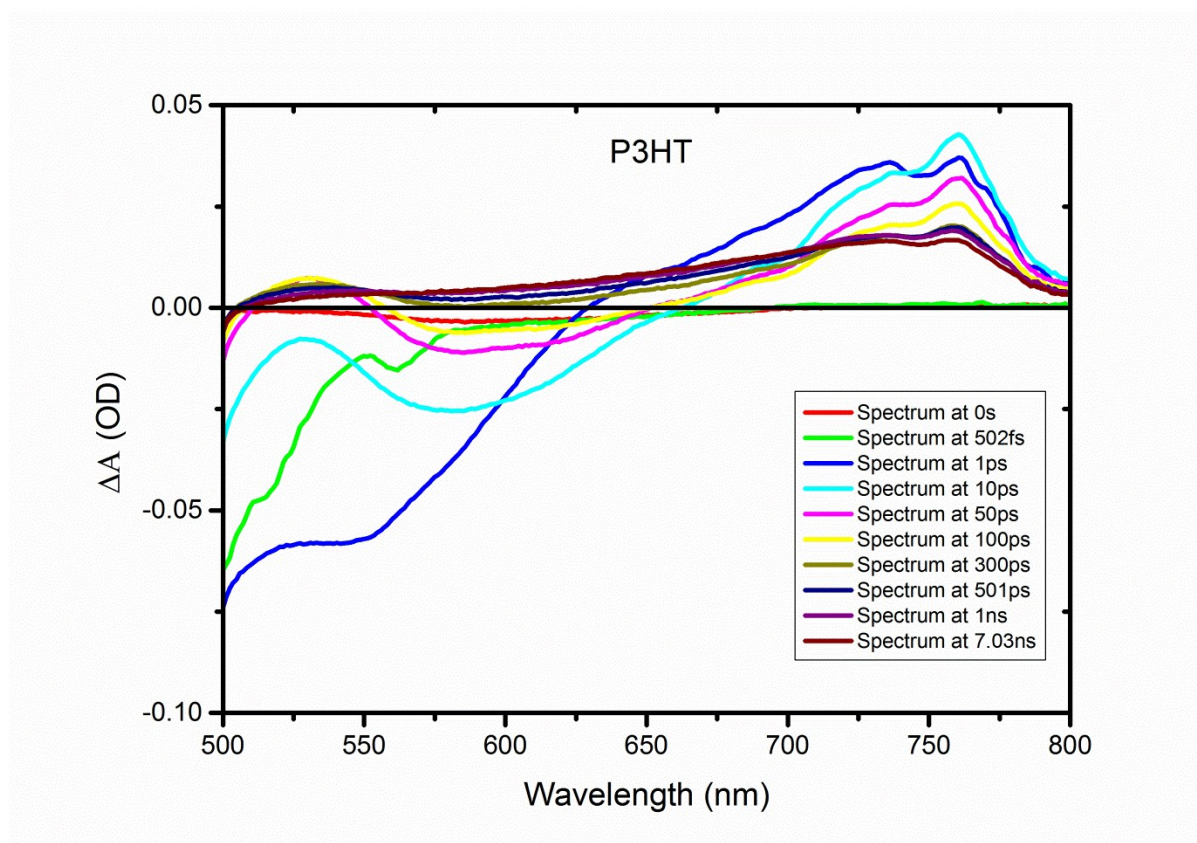


Figure S19. Transient absorption spectra of P3HT polymer in chloroform using 480 nm pump wavelength in visible range.

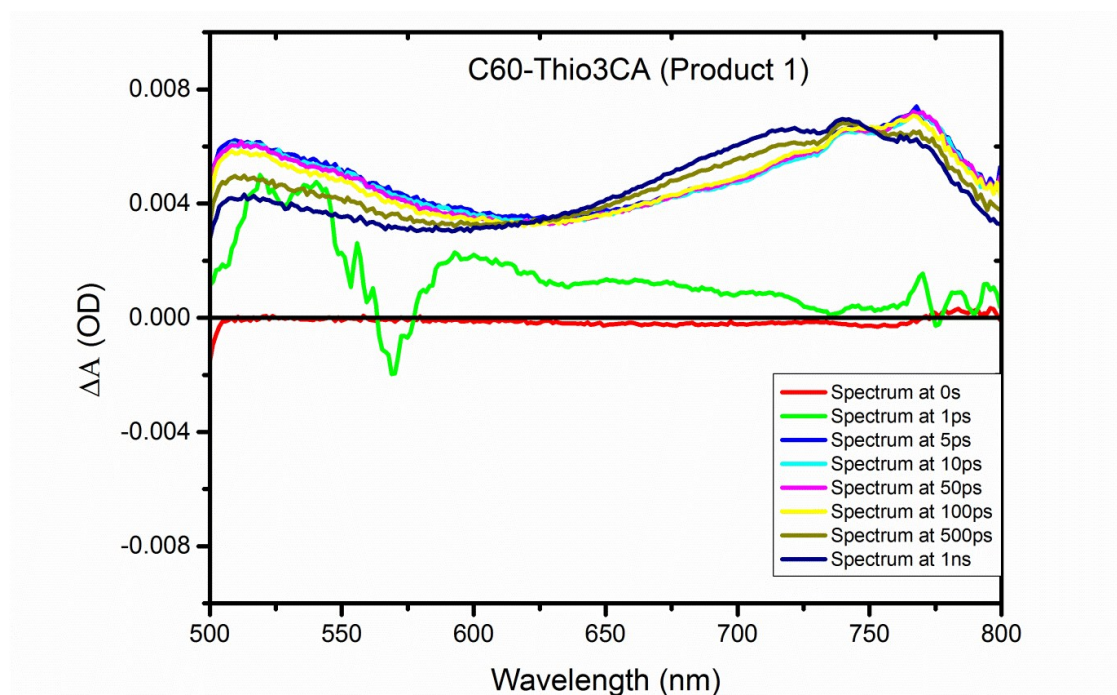


Figure S20. Transient absorption spectra of neat Product 1 in chloroform using 480 nm pump wavelength in visible region.

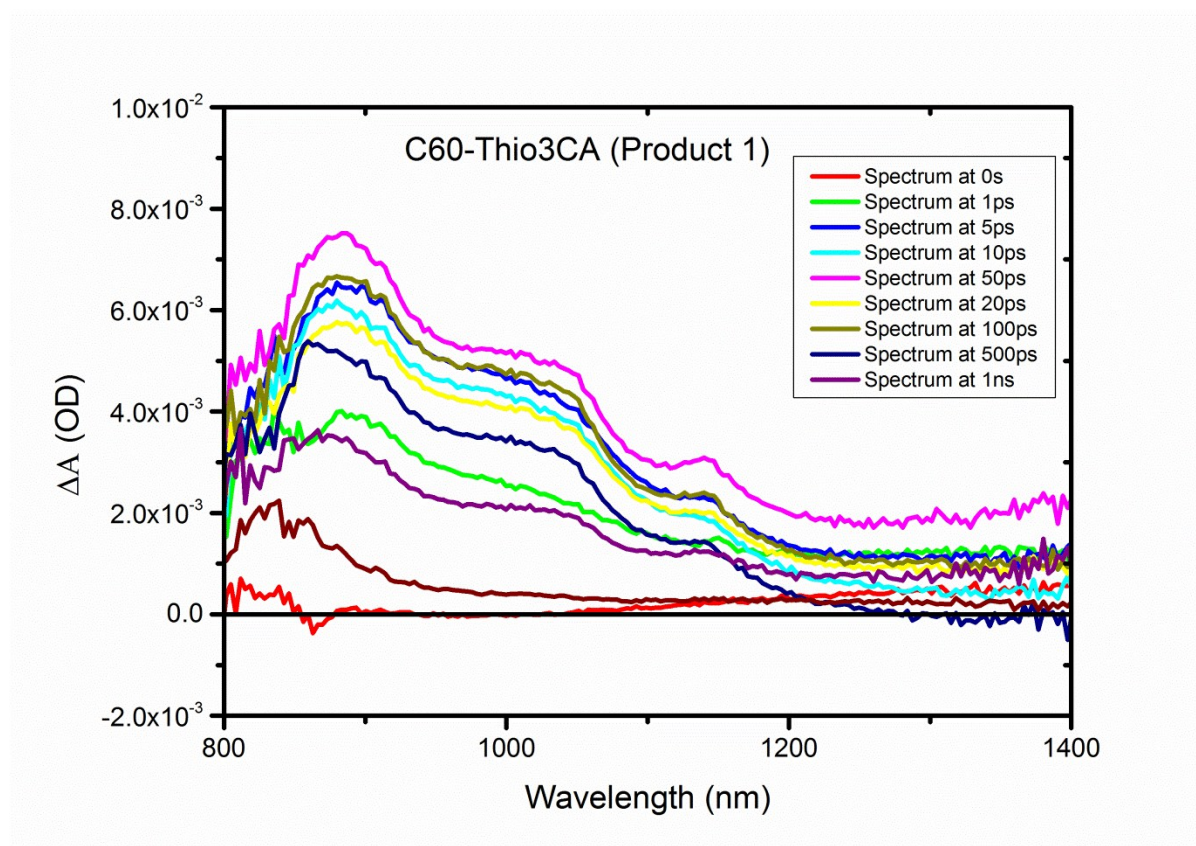


Figure S21. Transient absorption spectra of neat Product 1 in chloroform using 480 nm pump wavelength in NIR region.





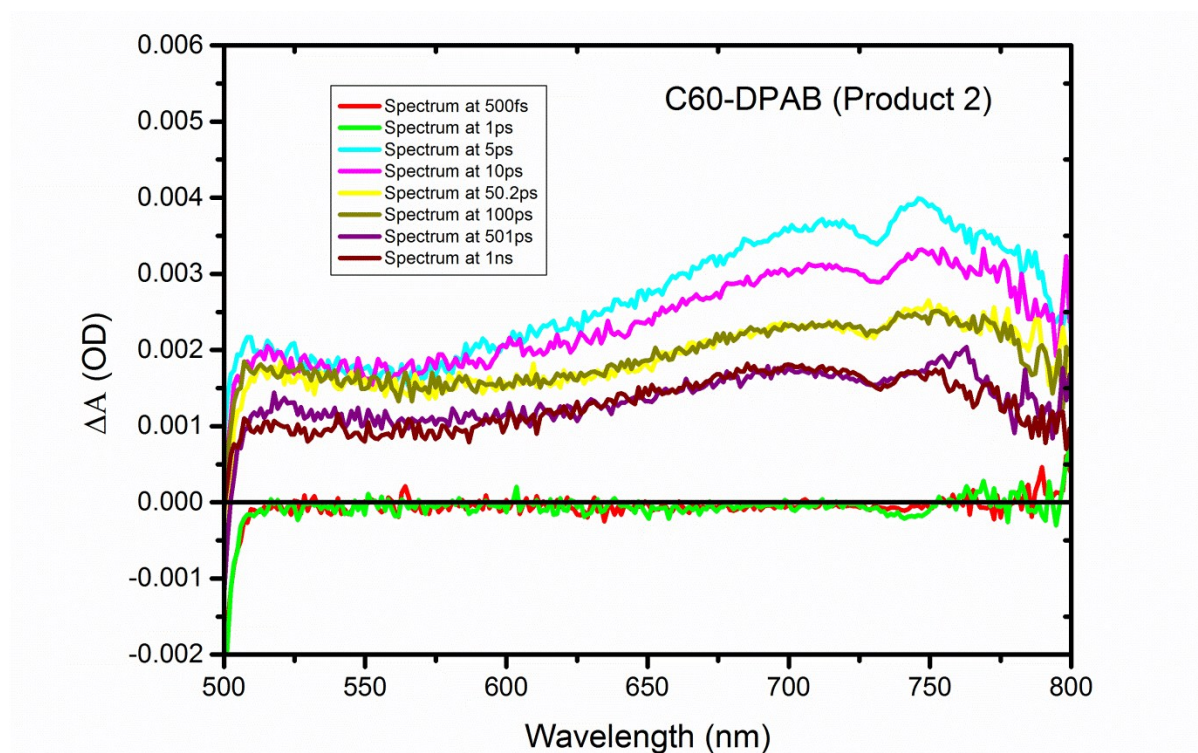


Figure S22. Transient absorption spectra of neat Product 2 in chloroform using 480 nm pump wavelength in visible region.

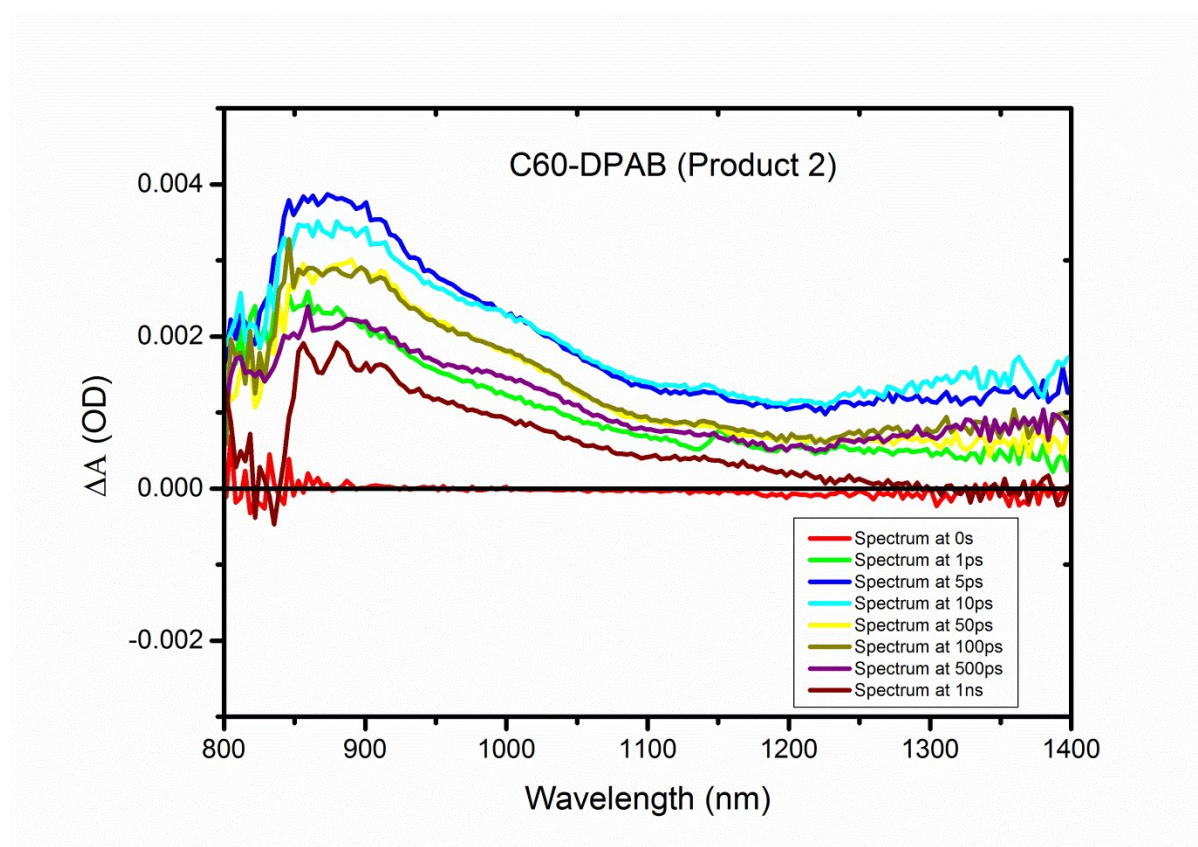


Figure S23. Transient absorption spectra of neat Product 2 in chloroform using 480 nm pump wavelength in NIR region.