Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Replacing Cyano (−C≡N) Group to Design Environmentally Friendly Fused-Ring Electron Acceptors

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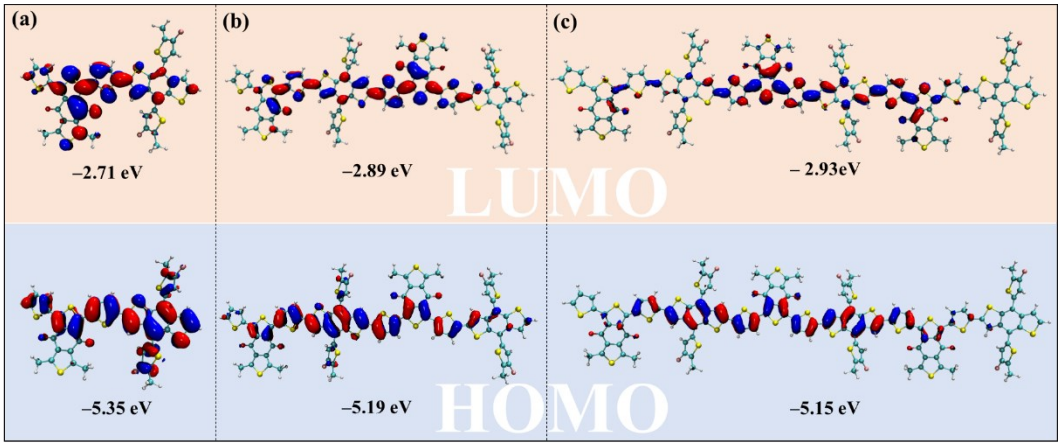

Figure S1. Spatial distribution and energy levels of HOMO and LUMO for one repeating unit (a), two repeating units (b), and three repeating units of PBDB-TF.

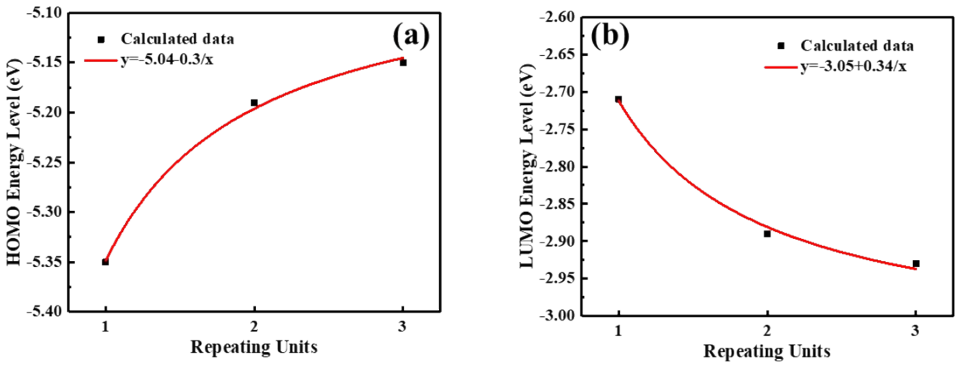

Figure S2. Evolution of the energy levels of HOMO (a) and LUMO (b) for one, two, and three repeating units of PBDB-TF. The red line represents the data fitting curve.

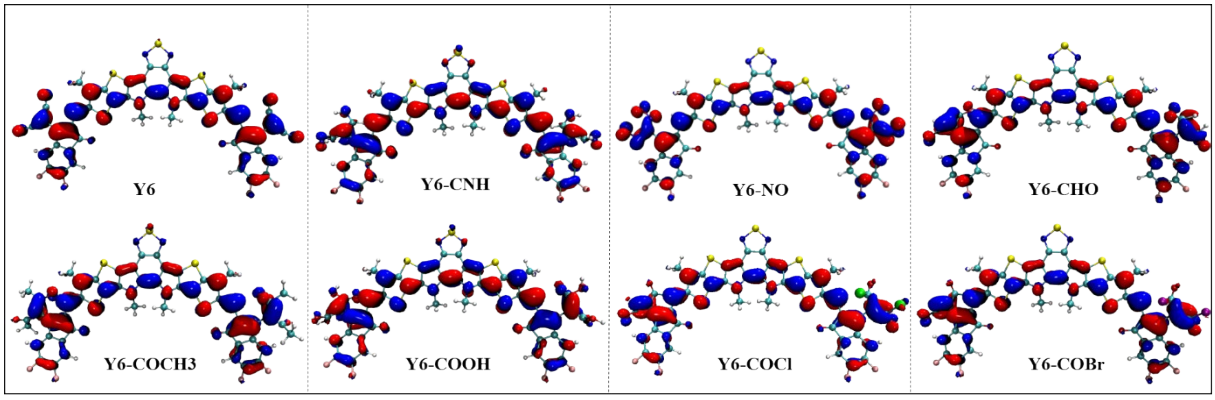

Figure S3 Spatial distribution of LUMO for Y6, Y6-CNH, Y6-NO, Y6-CHO, Y6-COCH3, Y6-COOH, Y6-COCl, and Y6-COBr.

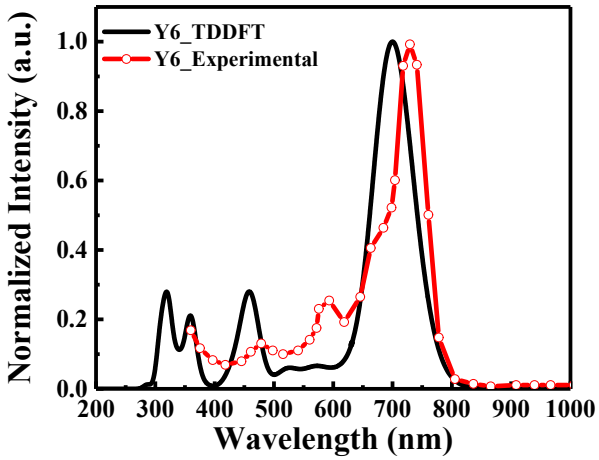

Figure S4. TD-DFT calculated normalized absorption spectrum and experimental result of Y6 in chloroform based on PBE0/def2-SVPD.

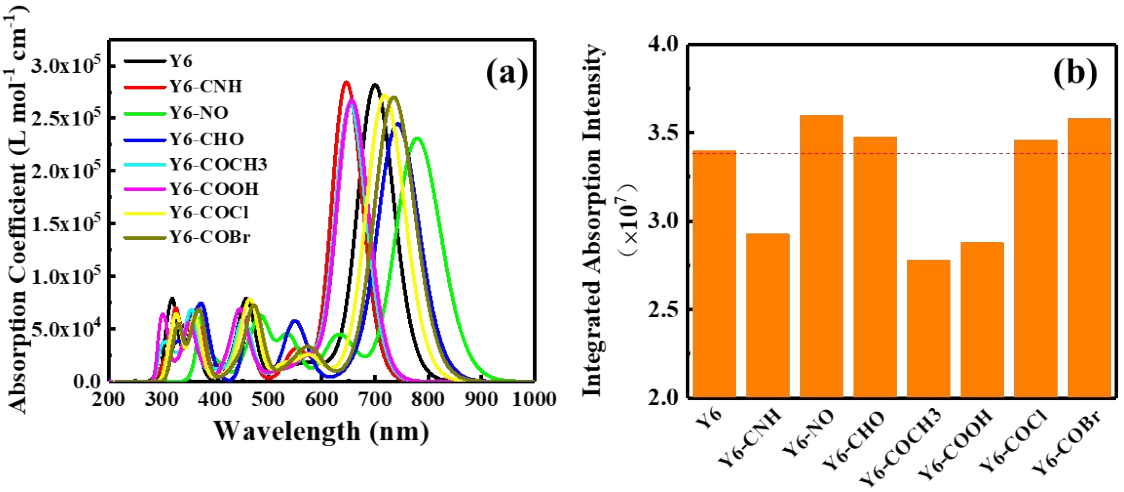

Figure S5 TD-DFT calculated absorption spectra (a) and integrated absorption intensity (b) of Y6, Y6-CNH, Y6-NO, Y6-CHO, Y6-COCH3, Y6-COOH, Y6-COCl, and Y6-COBr in chloroform based on PBE0/def2-SVPD.

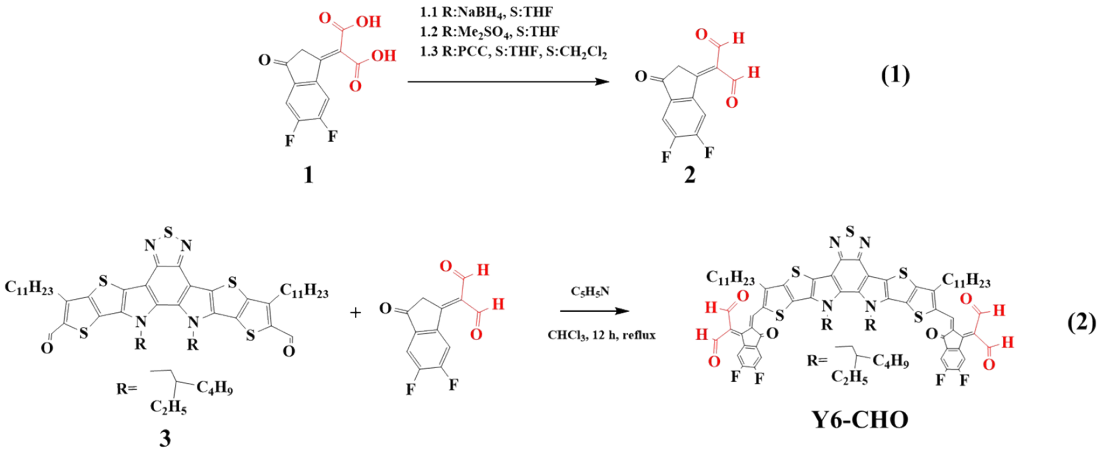

Figure S6 Possible synthetic routes of Y6-CHO.