

Electronic Supplementary Information (ESI) for New Journal of Chemistry

New Designed Isoindigo/Thiophene Medium-sized Molecule Containing π (D-A-D) Bridge with Unexpected Organic Photovoltaic Performance

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^1H and ^{13}C NMR spectra

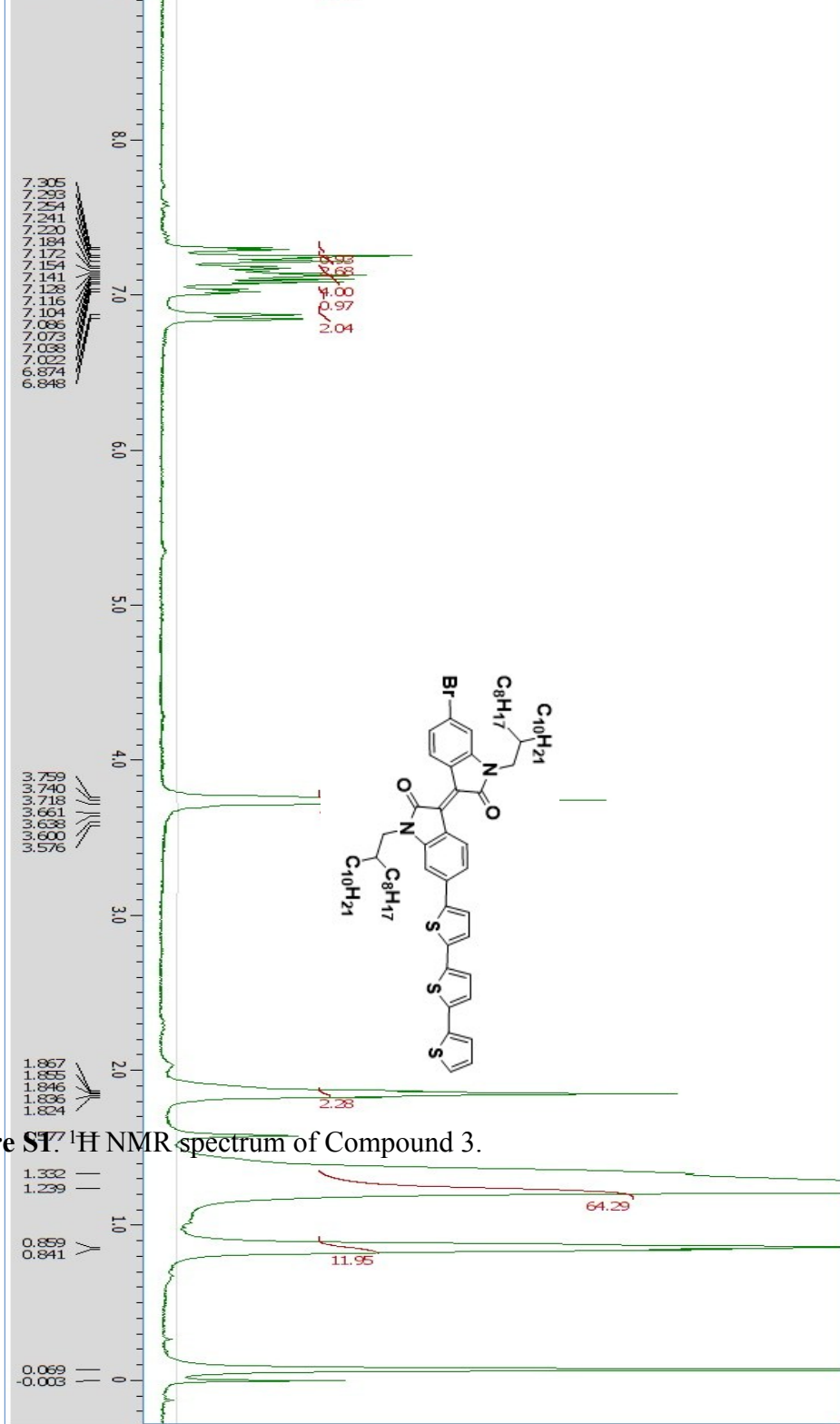


Figure S1. ^1H NMR spectrum of Compound 3.

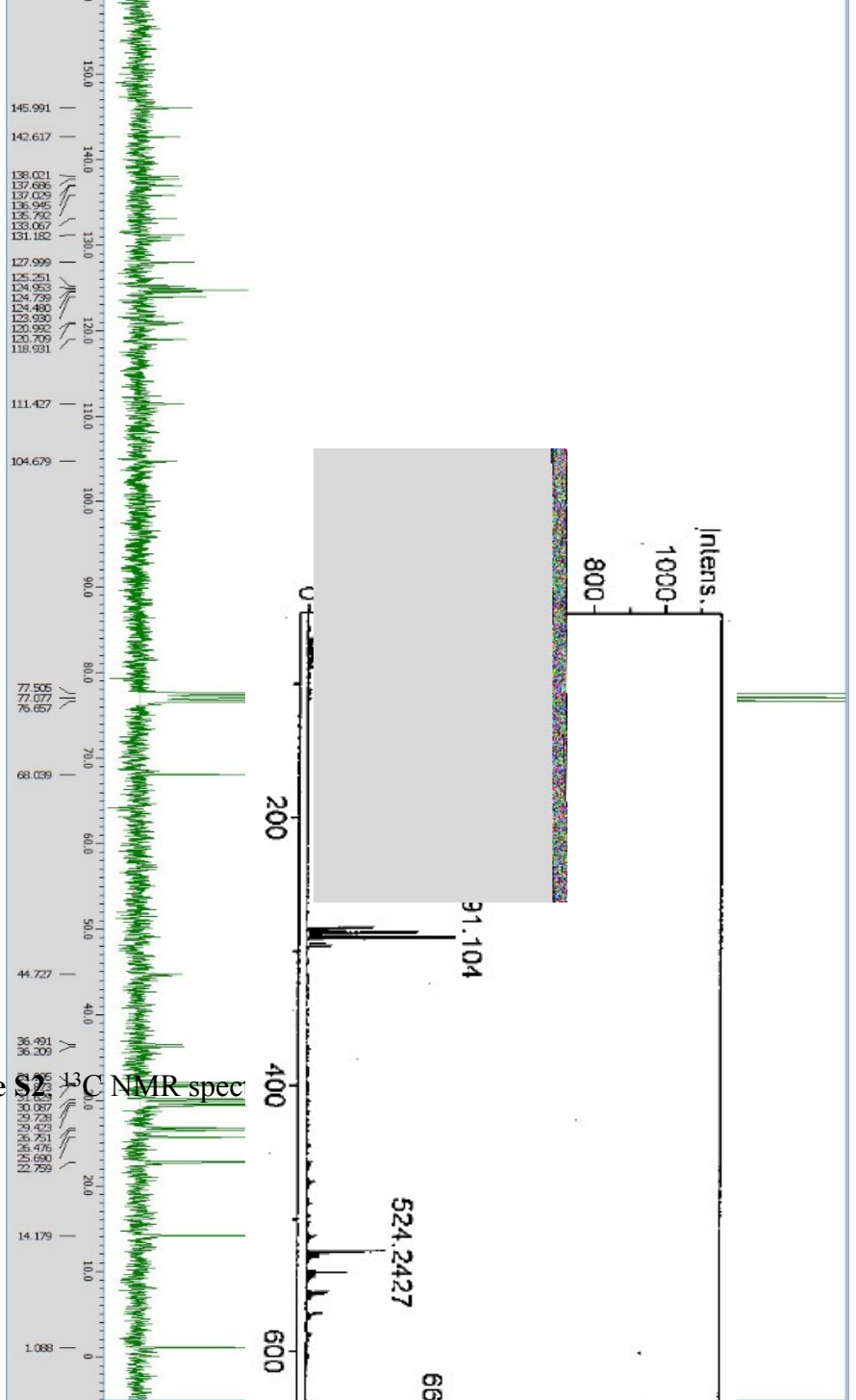


Figure S2. ^{13}C NMR spec

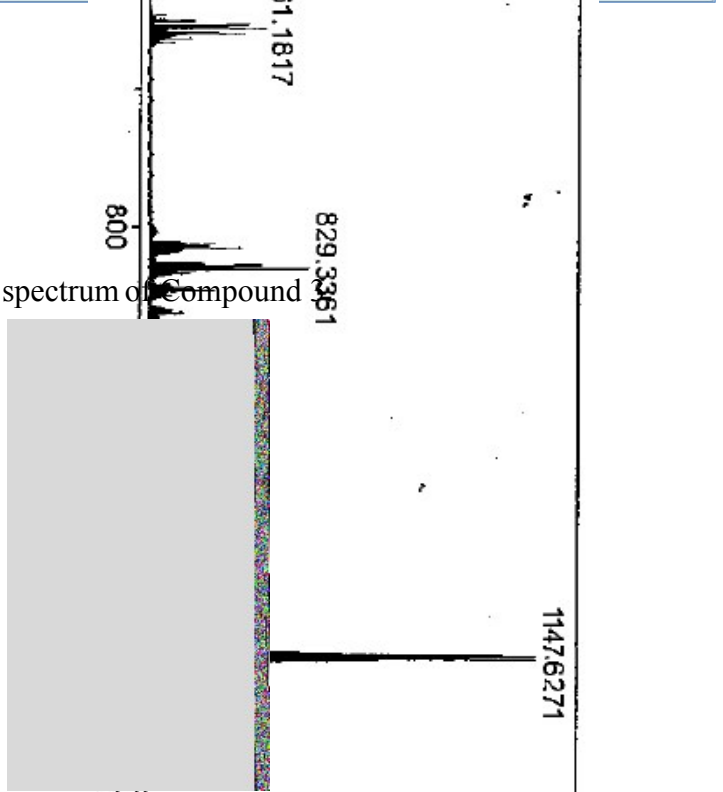


Figure S3. Mass spectrum of Compound

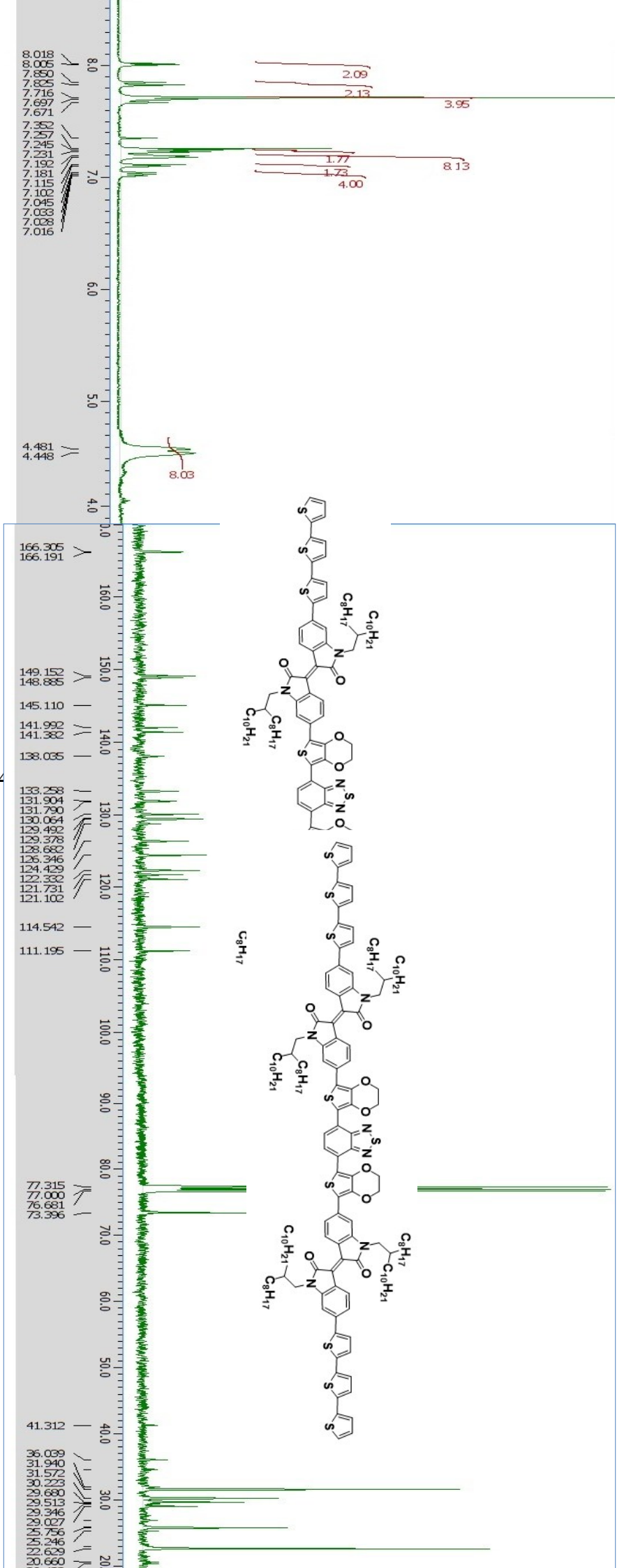


Figure S4

Figure S5. ^{13}C NMR spectrum of Compound 5.

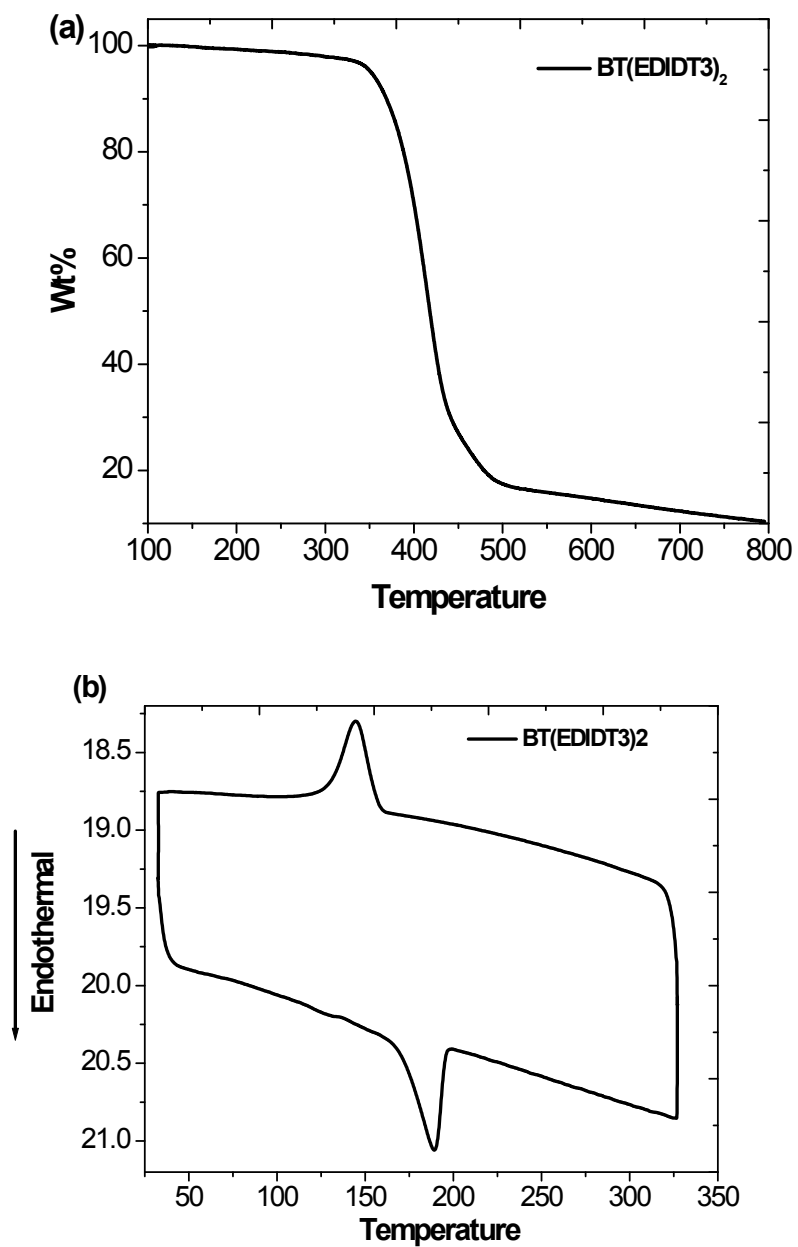


Figure S6. (a) TGA thermogram of BT(EDIDT3)₂ and (b) differential scanning calorimetry (DSC) under a nitrogen atmosphere at a heating rate of 10⁰C min⁻¹.

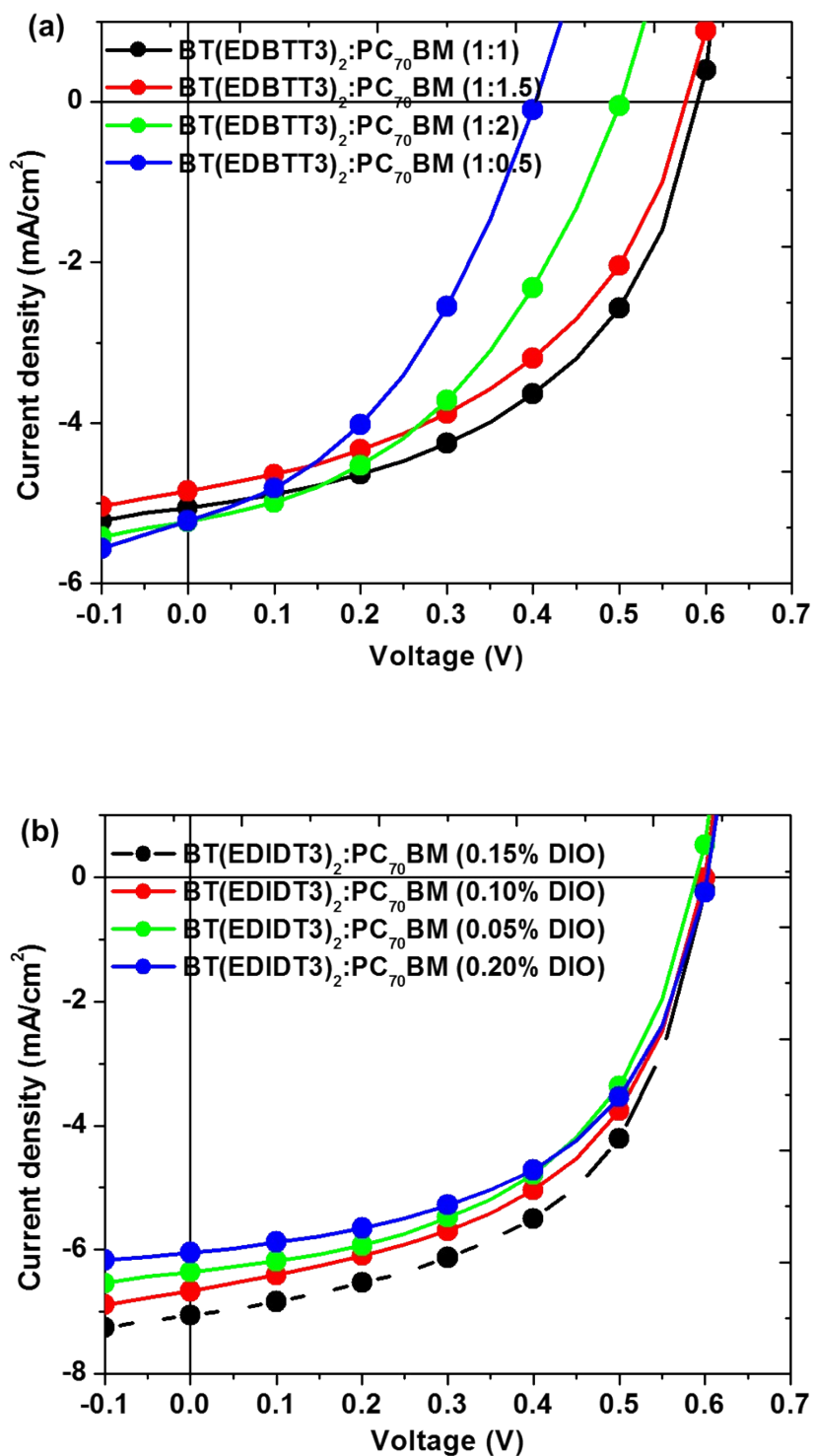


Fig. S7. (a) Current density versus voltage characteristics of ITO/PEDOT:PSS/BT(EDIDT3)₂:PC₇₀BM/Ca/Al organic photovoltaic devices with different donor and acceptor ratio without DIO. (b) Current density versus voltage characteristics of TO/PEDOT:PSS/BT(EDIDT3)₂:PC₇₀BM/Ca/Al (1:1) organic photovoltaic devices with different DIO content.

Table S1. Photovoltaic performance of ITO/PEDOT:PSS/ BT(EDIDT3)₂:PC₇₀BM/Ca/Al organic photovoltaic devices with different donor and acceptor ratio (without DIO) and DIO content. The BT(EDIDT3)₂ and PC₇₀BM ratio was fixed with 1:1 in photovoltaic devices with different DIO content

(BT(EDIDT3) ₂ :PC ₇₀ BM (ratio))	J_{sc} (mA/cm ²)	V_{oc} (V)	FF (%)	PCE (%)
(1:1)	0.59	5.06	0.49	1.45
(1:1.5)	0.58	4.85	0.46	1.28
(1:2)	0.5	5.23	0.42	1.12
(1:0.5)	0.4	5.22	0.4	0.85
(BT(EDIDT3) ₂ :PC ₇₀ BM (1:1) DIO content (%)				
0.15	0.6	7.06	0.53	2.25
0.10	0.6	6.67	0.51	2.04
0.05	0.59	6.36	0.51	1.91
0.20	0.6	6.05	0.52	1.91

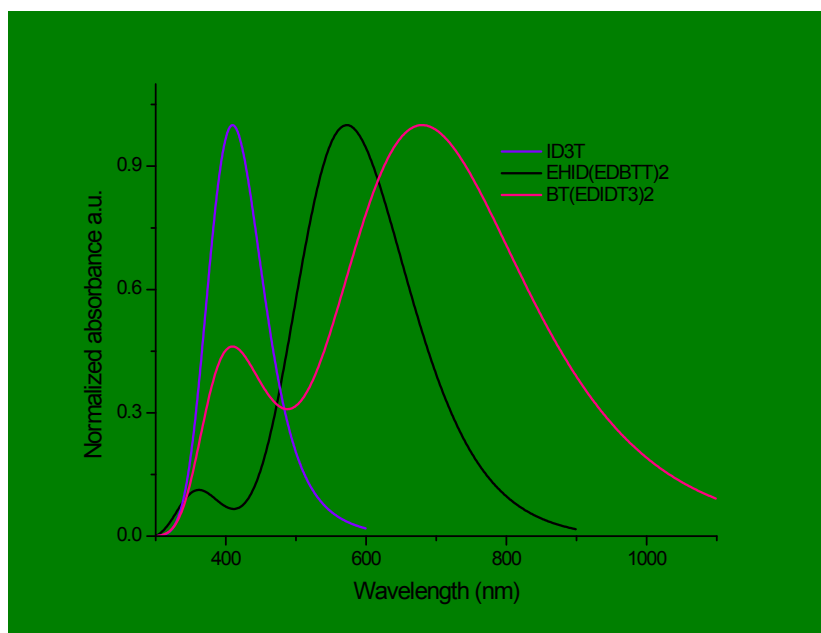


Figure S8. Simulated UV-Vis absorption spectra of the title compounds in CHCl₃ by TD-DFT/CAM-B3LYP/6-31G(d,p).

Table S2. Excited-state vertical transition energies (Cal λ_{\max} , nm), oscillator strengths and main electronic configuration of the first excited state and their percentage contribution (C%) of the title compounds using TD- CAM-B3LYP/6-31G(d,p)

	Cal λ_{\max} (nm)	f	Main configuration	C%	Exp λ_{\max} (nm)
BT(EDIDT3)2	679	2.60	H \rightarrow L; H-1 \rightarrow L+1	0.44; 0.24	662
EHID(EDBTT)2	571	2.11	H \rightarrow L	0.72	568
IDT3	407	1.66	H \rightarrow L; H-2 \rightarrow L	0.68; 0.25	401