

Electronic supplementary information (ESI)

DTBDT-TTPD: A new dithienobenzodithiophene-based small molecule for use in efficient photovoltaic devices

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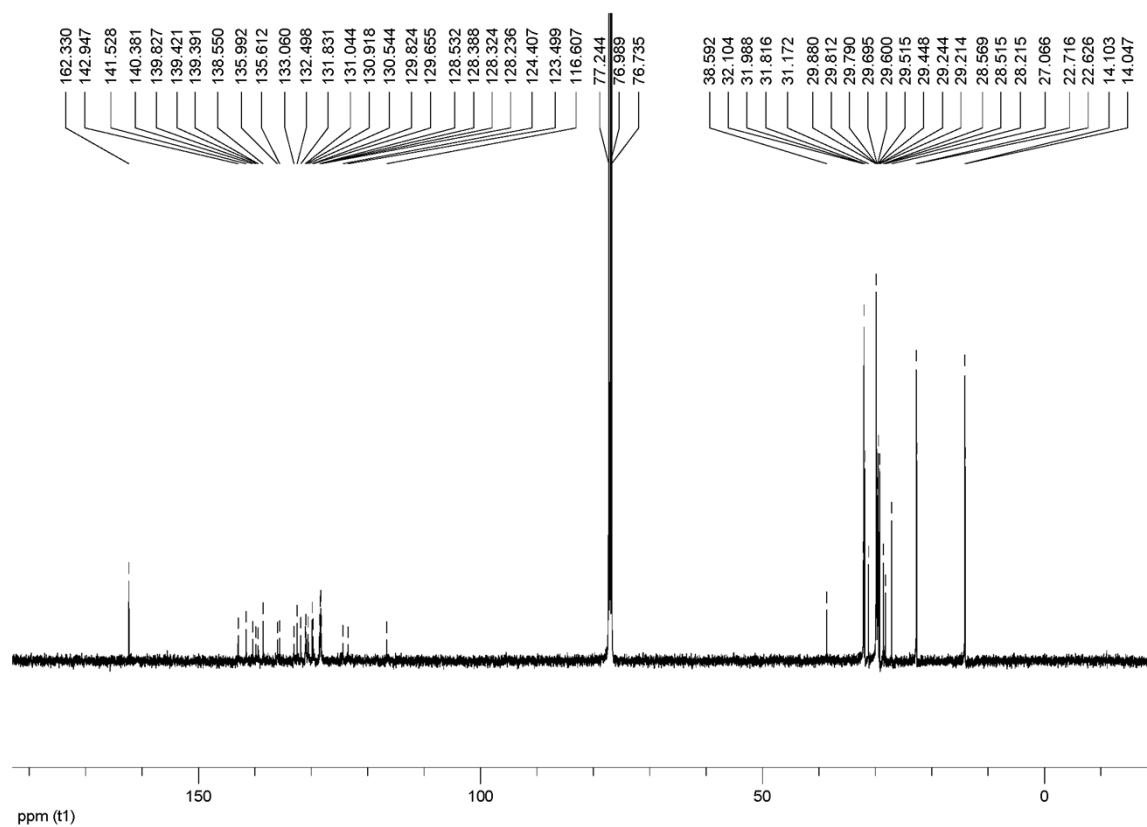
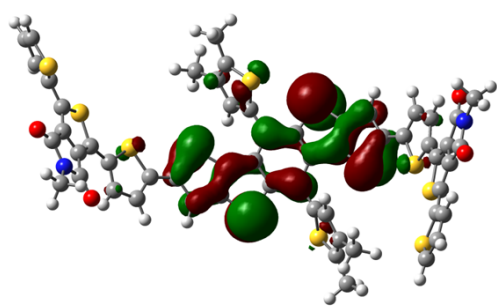
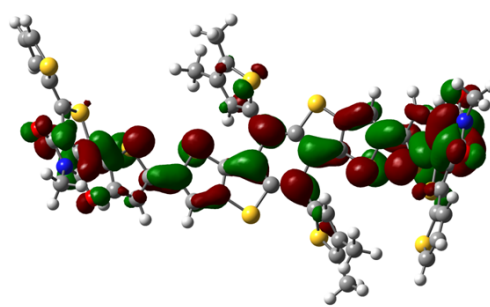


Fig. S1. ^{13}C NMR spectra of DTBDT-TTPD



HOMO: -5.25 eV



LUMO: -2.74 eV

Fig. S2. HOMO and LUMO surface plots for **DTBDT-TTPD**

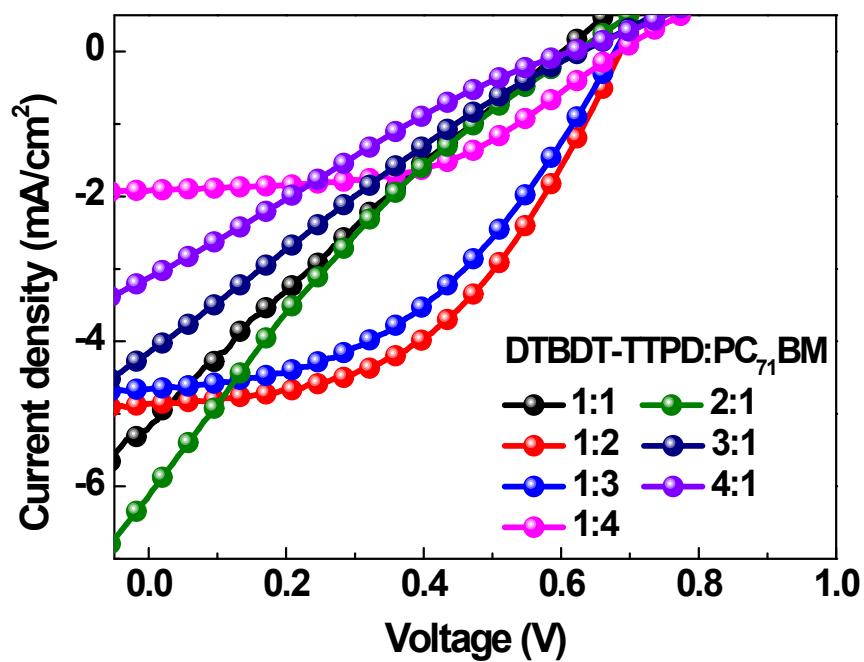


Fig. S3. J - V curves for DTBDT-TTPD:PC₇₁BM devices at various ratios in chloroform under an illumination of AM 1.5G, 100mW/cm²

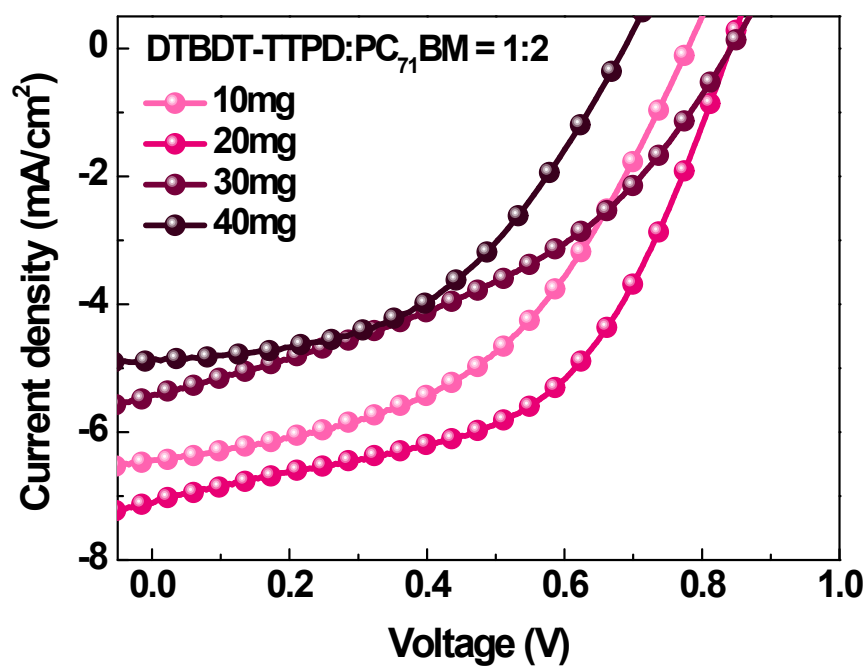


Fig. S4. *J-V* characteristics of the DTBDT-TTPD based solar cells with different material concentrations (DTBDT-TTPD:PC₇₁BM = 1:2 w/w).

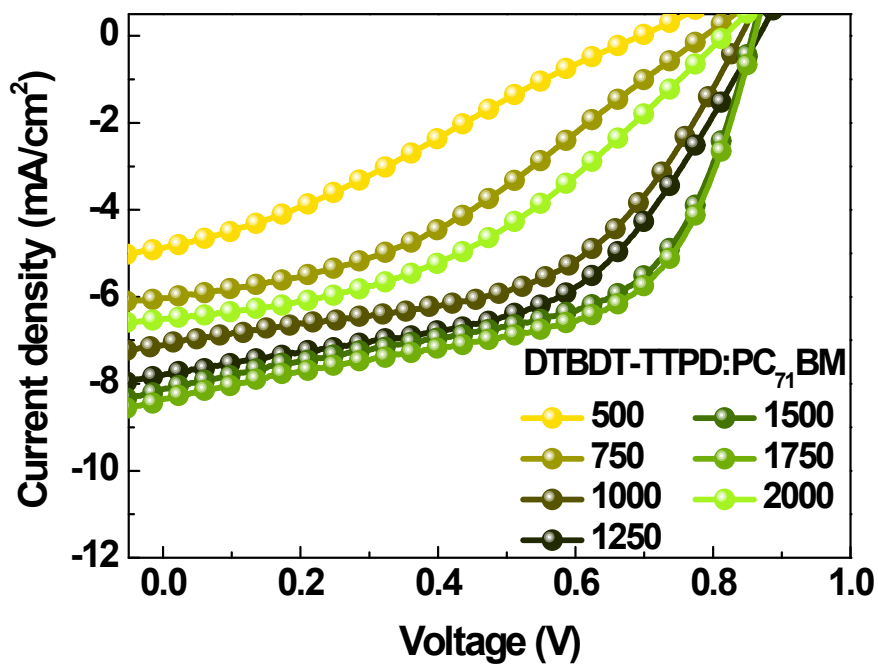


Fig. S5. Photocurrent-voltage (J - V) curves (AM 1.5G, 100mW cm⁻²) of the **DTBDT-TTPD:PC₇₁BM** (1:2 w/w) blend photovoltaic cells as a function of the active layer thickness.

Table S1. Summary of device parameters at various **DTBDT-TTPD/PC₇₁BM** compositions blended in chloroform.

Small molecule : PCBM	Blend ratios	V_{oc} (V)	J_{sc} (mA / cm ²)	FF (%)	PCE (%)
	1:1	0.60	5.2	23.3	0.73
	1:2	0.68	4.9	48.4	1.61
	1:3	0.67	4.7	44.8	1.34
DTBDT-TTPD:PC₇₁BM	1:4	0.68	1.9	50.3	0.67
	2:1	0.62	6.2	20.1	0.77
	3:1	0.63	4.2	22.8	0.60
	4:1	0.62	3.1	22.7	0.43

Table S2. Photovoltaic data of the **DTBDT-TTPD/PC₇₁BM** (1:2 w/w) at various material concentration conditions

Small molecule : PCBM	Total concentration (mg/ml)	V_{oc} (V)	J_{sc} (mA / cm ²)	FF (%)	PCE (%)
	10	0.78	6.4	47.5	2.38
DTBDT-TTPD:PC₇₁BM	20	0.84	7.1	52.0	3.10
	30	0.84	5.4	40.6	1.85
	40	0.68	4.9	48.4	1.61

Table S3. Summary of the photovoltaic properties of **DTBDT-TTPD:PC₇₁BM** BHJ solar cells as a function of active layer thickness.

Small molecule : PCBM	Active layer Thickness (nm)	V_{oc} (V)	J_{sc} (mA / cm ²)	FF (%)	PCE (%)
	160	0.70	4.9	28.9	0.97
	145	0.80	6.0	37.8	1.80
	125	0.84	7.1	52.0	3.10
DTBDT-TTPD:PC₇₁BM	100	0.87	7.8	51.3	3.47
	92	0.86	8.0	55.3	3.81
	85	0.86	8.4	54.8	3.95
	60	0.82	6.5	41.4	2.20