

Supplementary Information

Facile preparation of small molecules for bulk heterojunction solar cells

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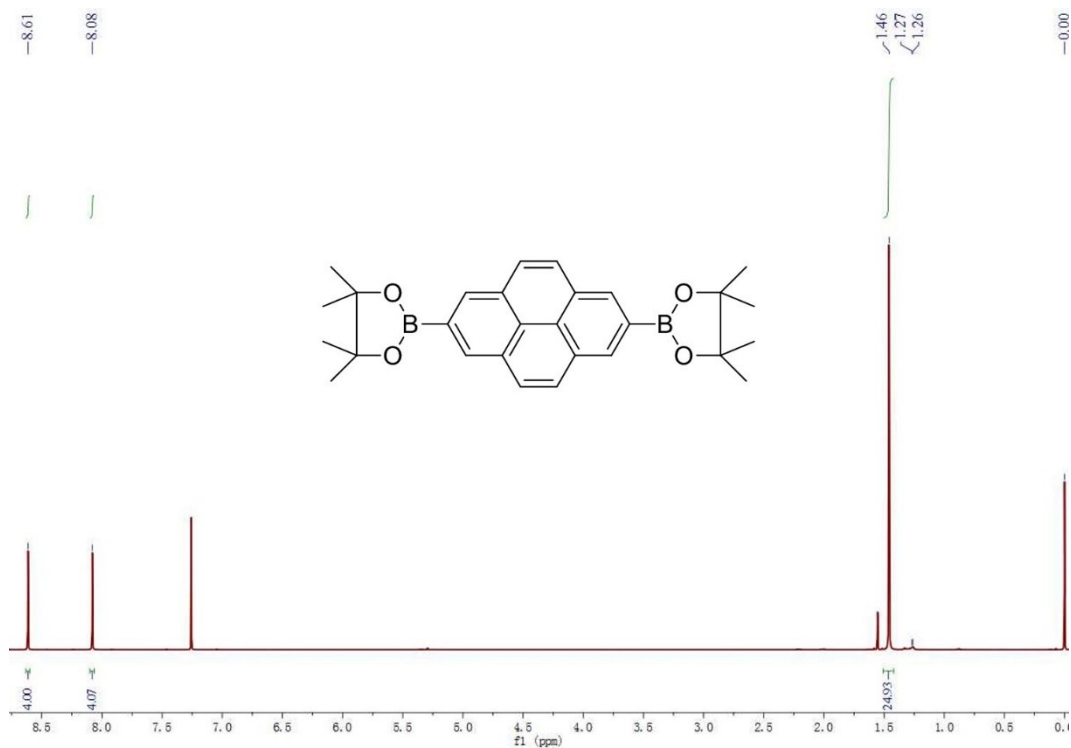


Fig. S1. ¹H NMR spectrum (500MHz, CDCl₃) of **1**.

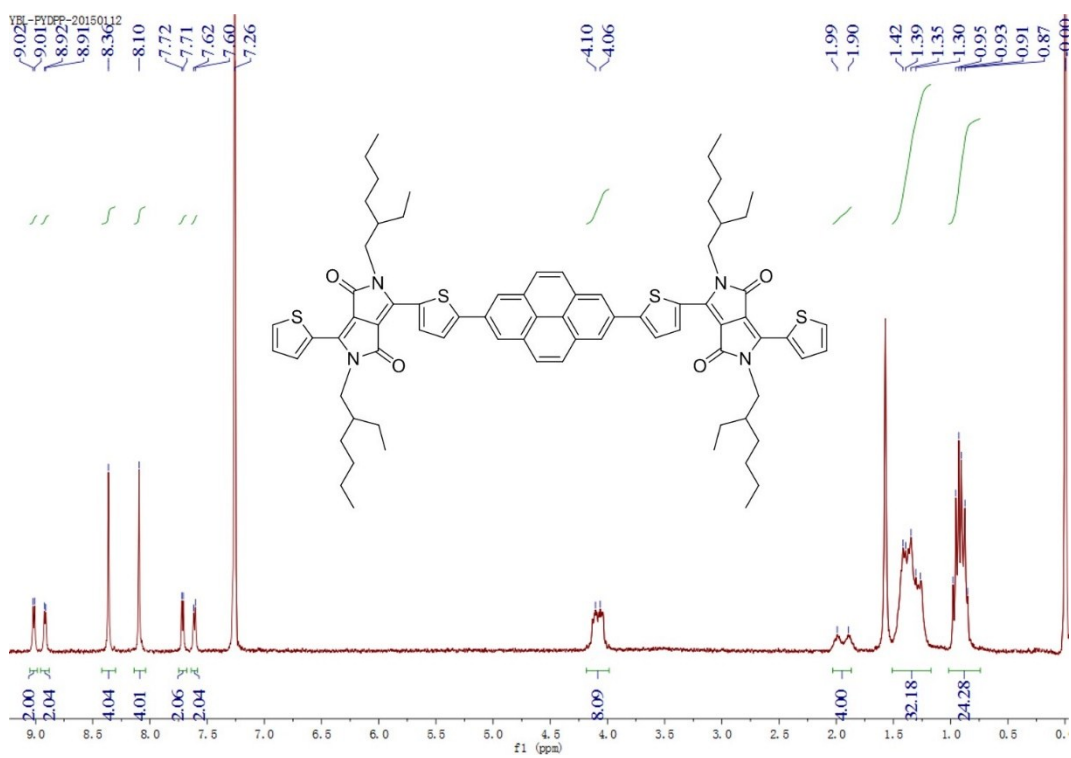


Fig. S2. ¹H NMR spectrum (500MHz, CDCl₃) of **3a**.

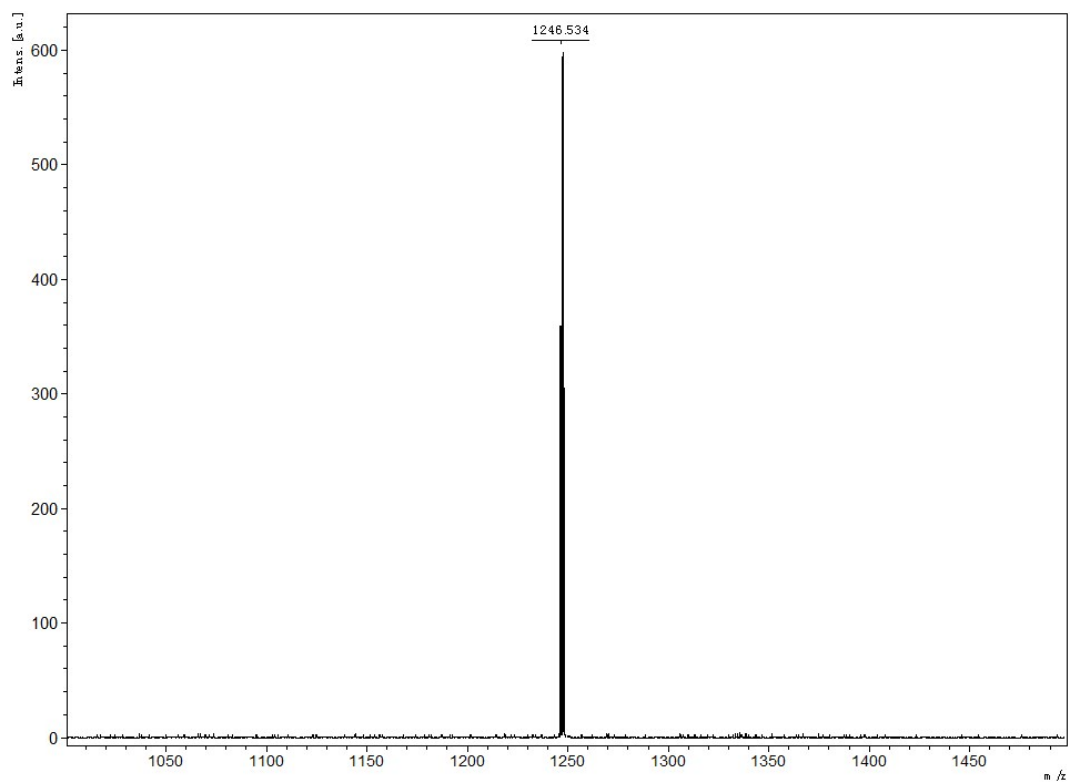


Fig. S3. Mass (MALDI-TOF) spectrum of **3a**.

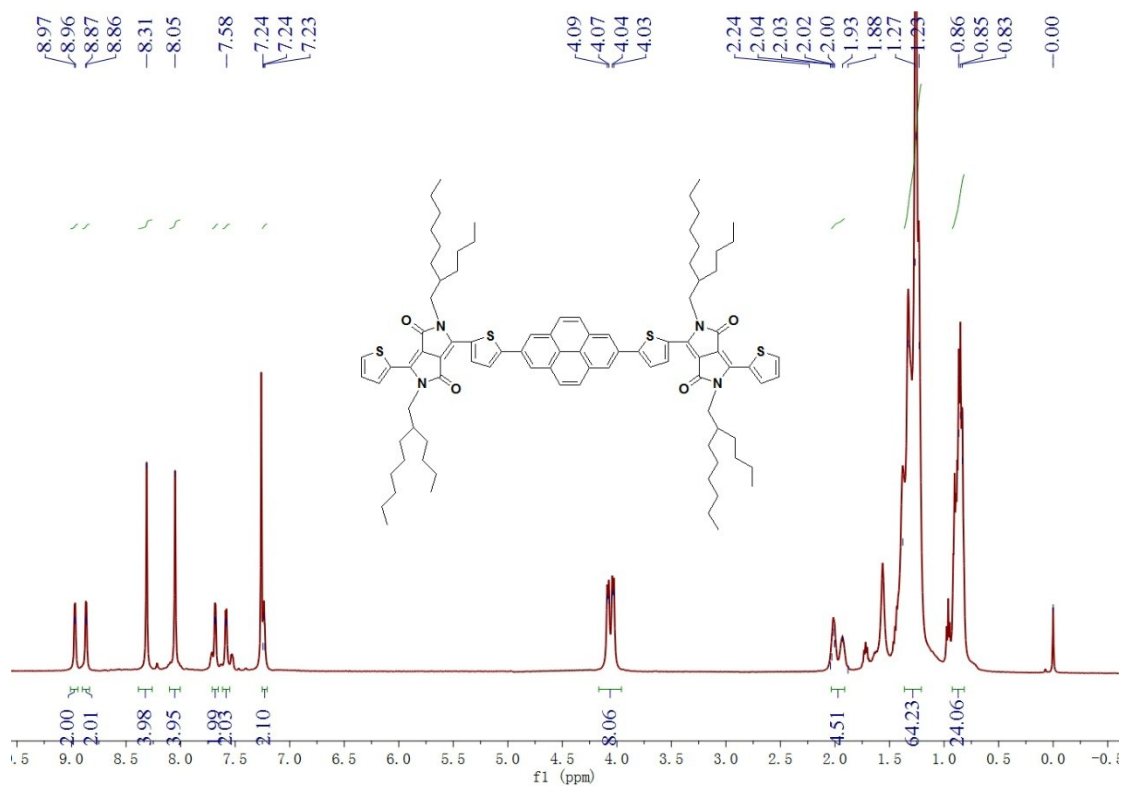


Fig. S4. ^1H NMR spectrum (500MHz, CDCl_3) of **3b**.

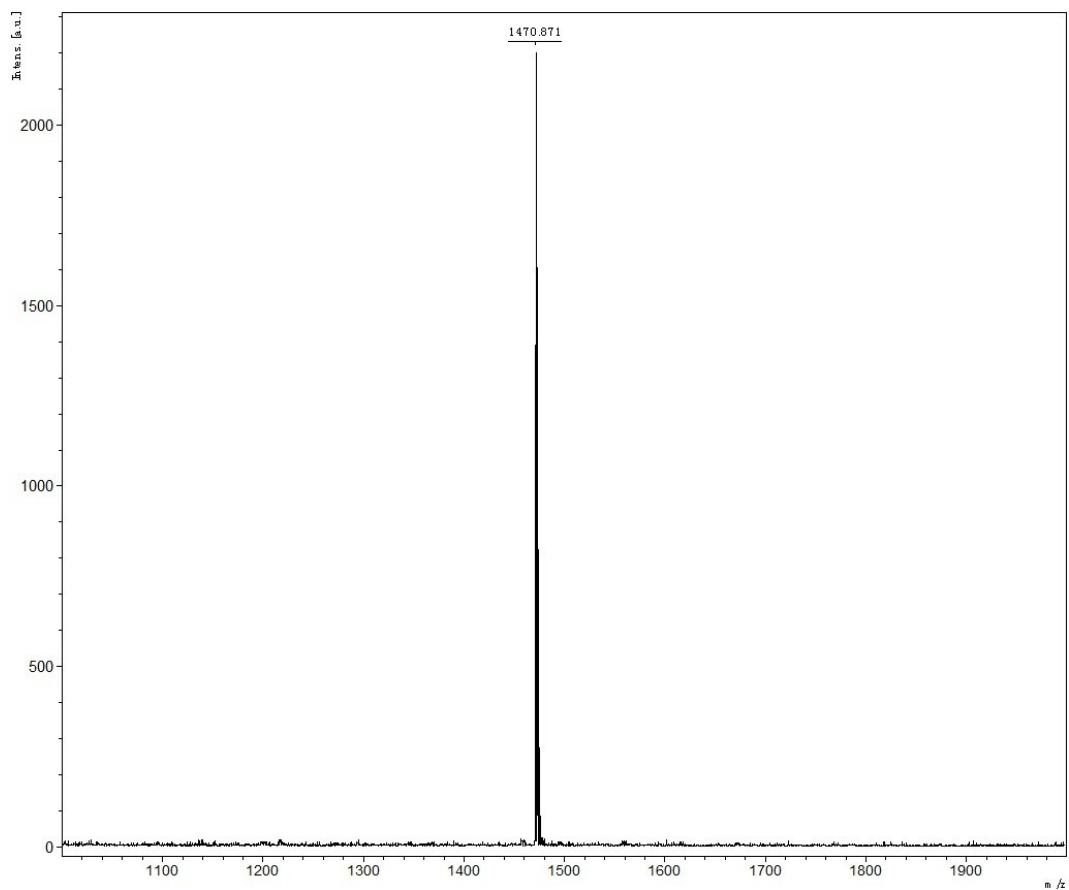


Fig. S5. Mass (MALDI-TOF) spectrum of **3b**.

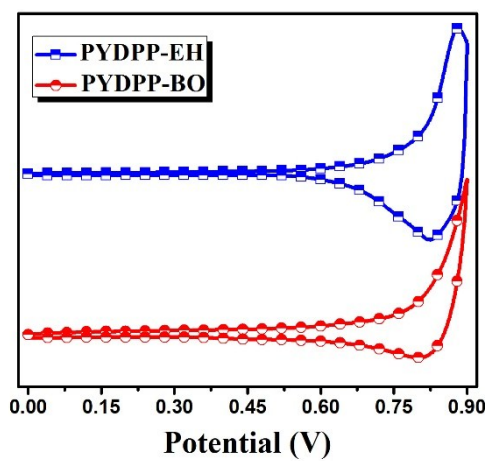


Fig. S6. Cyclic voltage curves of **3a** and **3b**.

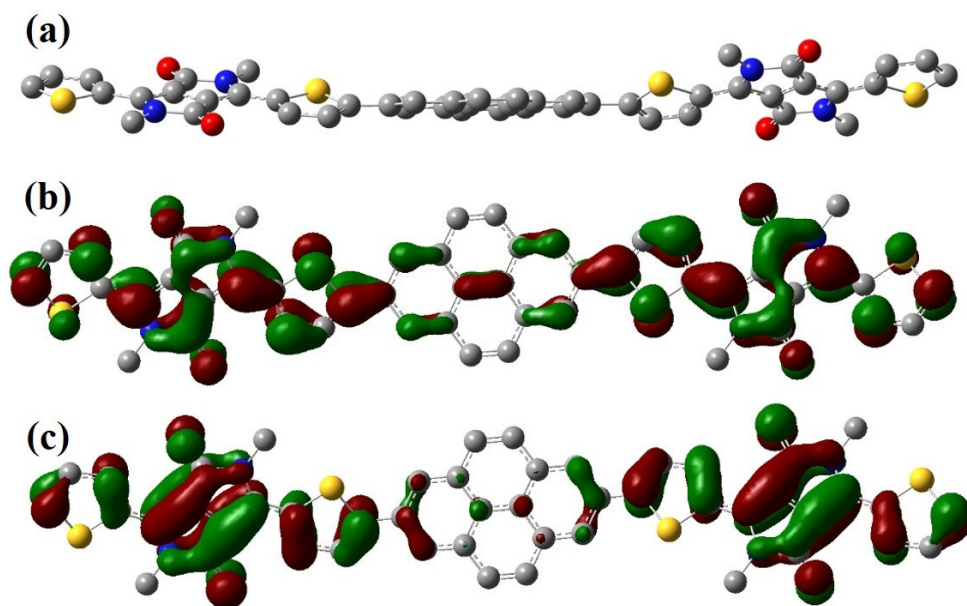


Fig. S7. The optimum geometry and electron-state-density distribution of PYDPP regardless of the *N*-alkyl substitutes: (a) geometry, (b) LUMO and (c) HOMO.

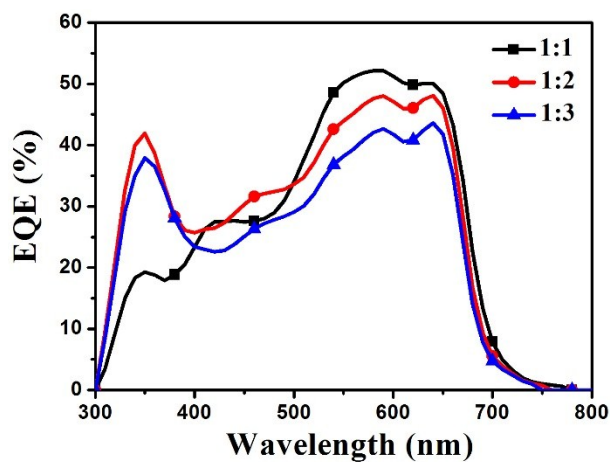


Figure S8. EQE response of PYDPP-EH based BHJ solar cells with different D/A ratio.

Table S1. Photovoltaic properties of BHJ solar cell devices having the configuration of ITO/PEDOT:PSS/PYDPP-EH:PC₆₁BM/PFN/Al.

Processing	D:A	$J_{SC}/\text{mA cm}^{-2}$	V_{OC}/V	FF/%	PCE/%
CF+0.4 vol%	1:1	9.66	0.87	55.17	4.64 ± 0.15
	1:2	8.49	0.87	57.94	4.28 ± 0.08
DIO	1:3	7.69	0.86	59.41	3.93 ± 0.11

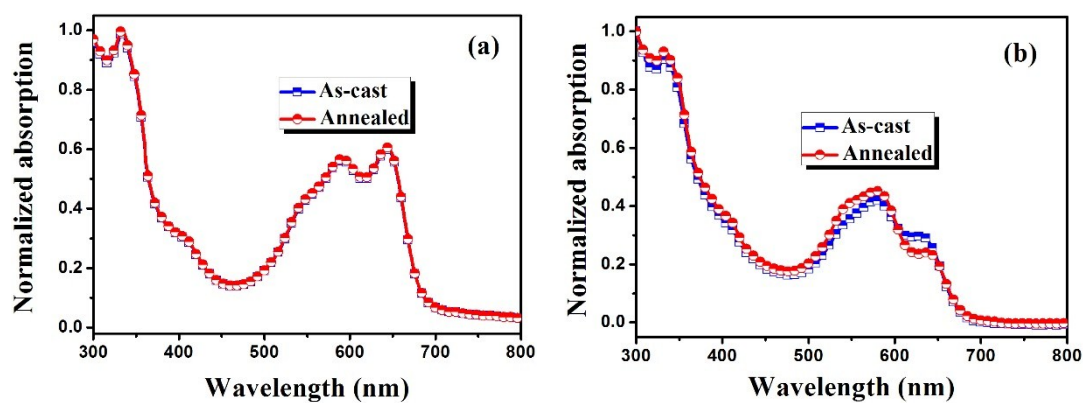


Figure S9. UV-vis absorption spectra of the as-cast and annealed blend films of (a) PYDPP-EH:PC₆₁BM and (b) PYDPP-BO:PC₆₁BM (1:1 w/w).