

Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

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Electronic Supplementary information (ESI):

New π -Conjugated Polymers as Acceptors Designed for all Polymer Solar Cells based on Imide/Amide-Derivatives

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1. The TGA and DSC curves of P1 and P2

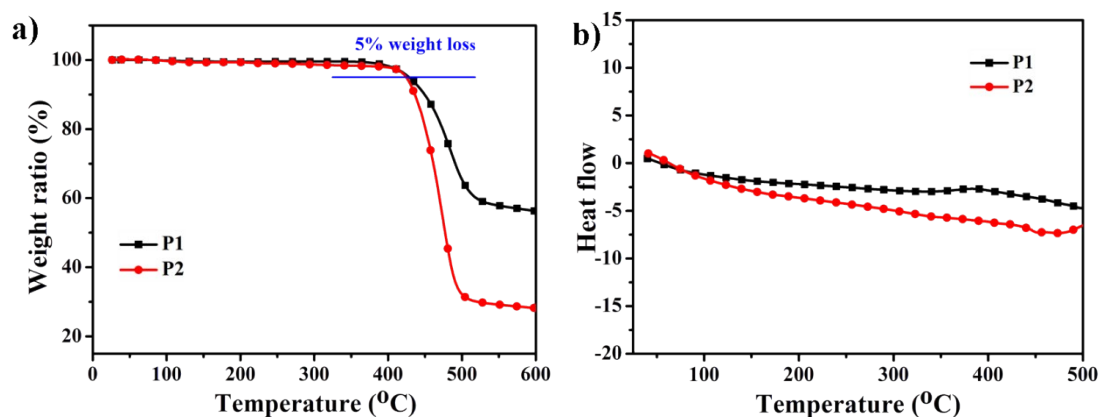


Fig. S1 The TGA curves (a) and DSC curves (b) of **P1** and **P2** (at a heating rate of $10\text{ }^{\circ}\text{C min}^{-1}$ under nitrogen atmosphere).

2. The calculated absorption profiles and molecular conformations of dimers of P1 and P2

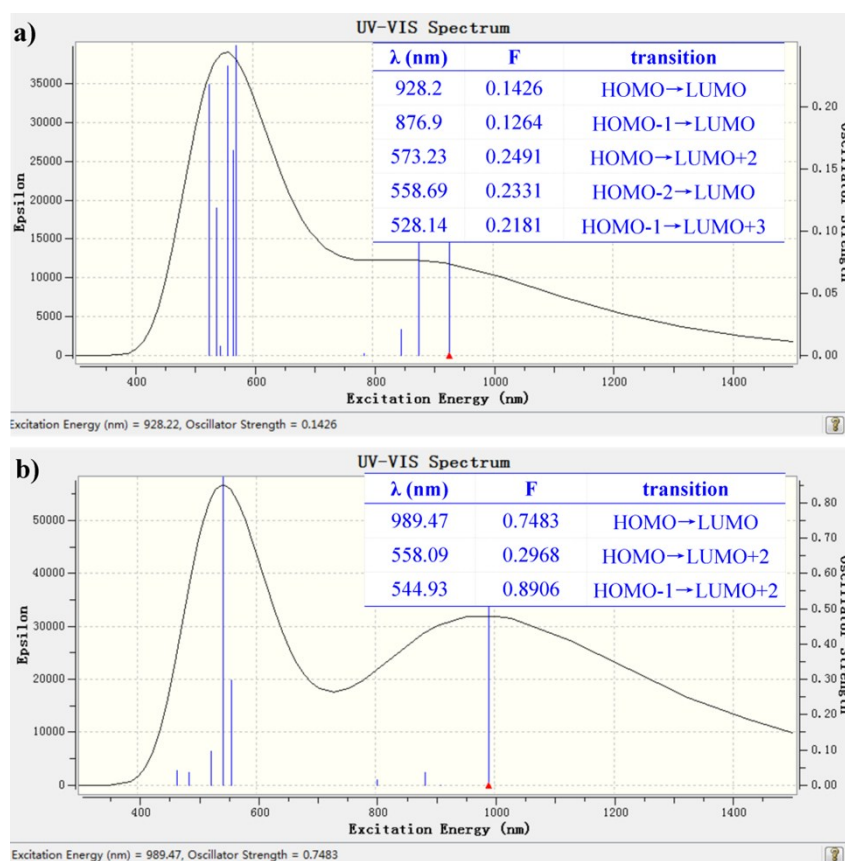


Fig. S2 The absorption profiles of dimers of **P1** (a) and **P2** (b) by quantum-chemical calculations (B3LYP/6-31G).

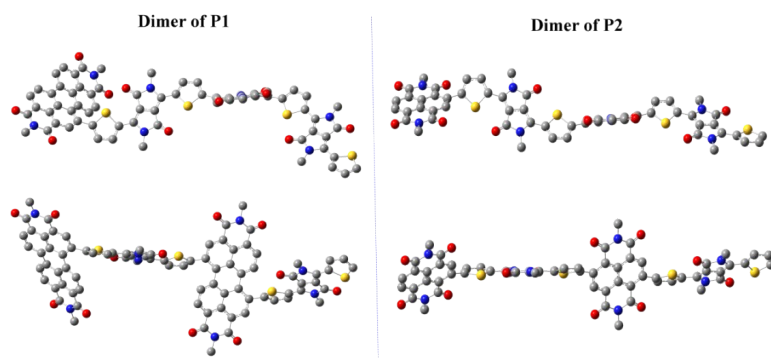


Fig. S3 The diagram of molecular conformations of dimers of **P1** and **P2** by quantum-chemical calculations.

3. UV-vis-NIR absorption spectra of donor, acceptors and blending films

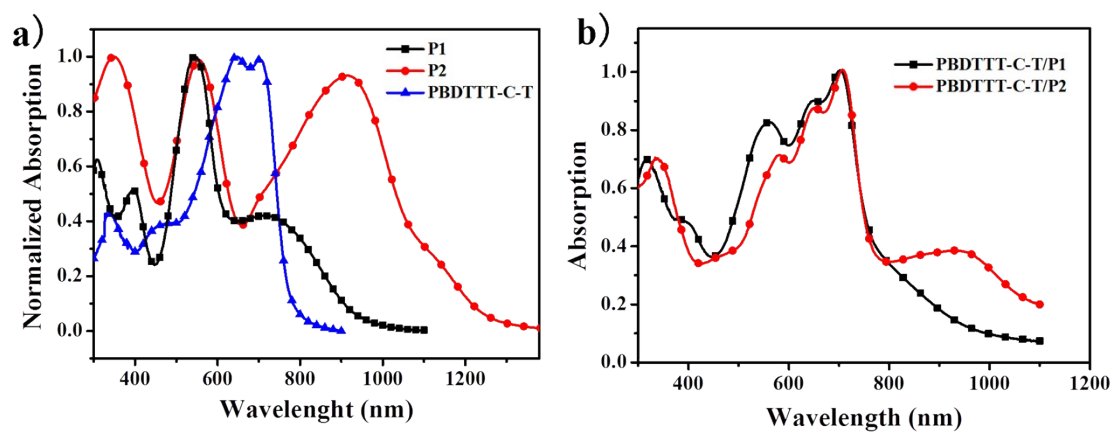


Fig. S4 a) Normalized UV-vis-NIR absorption spectra of thin films for **P1**, **P2** and PBDTTT-C-T; b) Absorptions of the blend thin films of PBDTTT-C-T:**P1** ($w/w = 1/1$) and PBDTTT-C-T:**P2** ($w/w = 1/1$).

4. The calculated HOMO/LUMO energy levels of DPP, NDI and PDI moieties by DFT

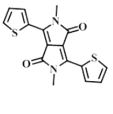
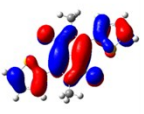
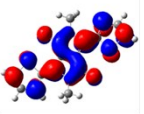
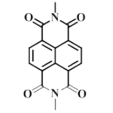
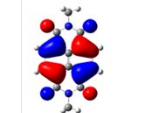
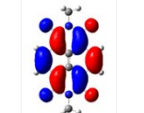
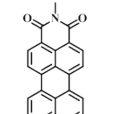
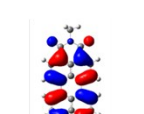
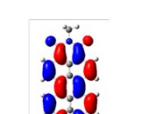
	HOMO	LUMO	E _g
 DPP	 -4.980	 -2.467	2.512
 NDI	 -7.032	 -3.407	3.625
 PDI	 -5.997	 -3.462	2.535

Fig. S5 The diagram of HOMO/LUMO energy levels of DPP, NDI and PDI moieties calculated by DFT (the alkyl chains in *N*-positions were replaced by methyl group).

5. Characteristics of all-PSCs

Table S1 Characteristics of all-PSCs based on blend films of PTB7-Th/**P1** and PTB7-Th/**P2**,

PBDTTT-C-T/**P1** and PBDTTT-C-T/**P2**

Donor:Acceptor	w/w	V_{OC} (V)	J_{SC} (mA cm ⁻²)	FF (%)	PCE (%) ^b
PTB7-Th: P1 ^a	1:1	0.67	6.24	43.75	1.83 (1.78)
PBDTTT-C-T: P1	1:1	0.68	7.06	41.78	2.01 (1.96)
PTB7-Th: P2 ^a	1:1	0.57	0.93	43.03	0.23 (0.20)
PBDTTT-C-T: P2	1:1	0.58	1.16	44.32	0.30 (0.27)

^a The data were based on 40 devices. ^b Data were provided in “highest (average)” format.

6. Energy level diagrams of the materials in all-PSCs

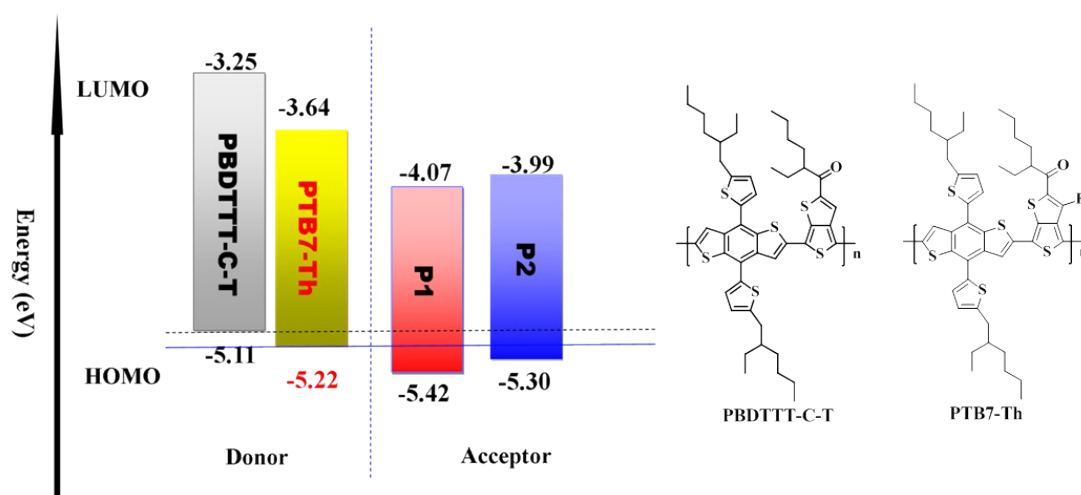
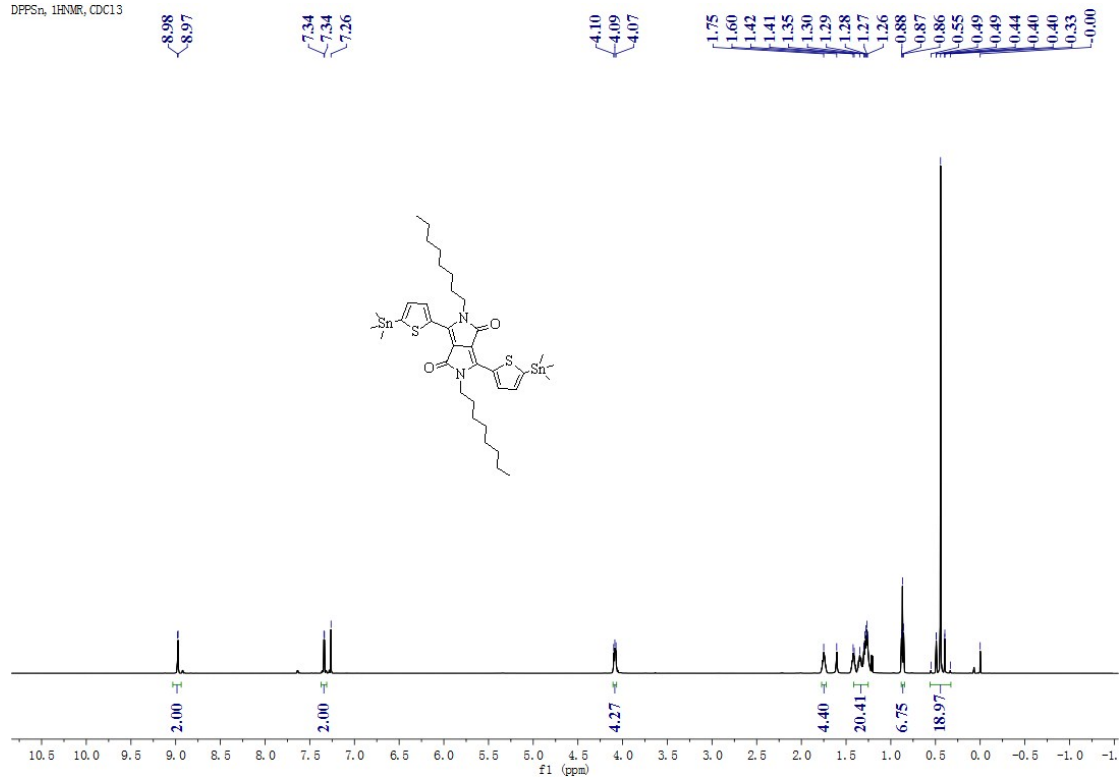


Fig. S6 Energy level diagrams of the materials in PTB7-Th/**(P1 or P2)** and PBDTTT-C-T/**(P1 or P2)** based photovoltaic devices.

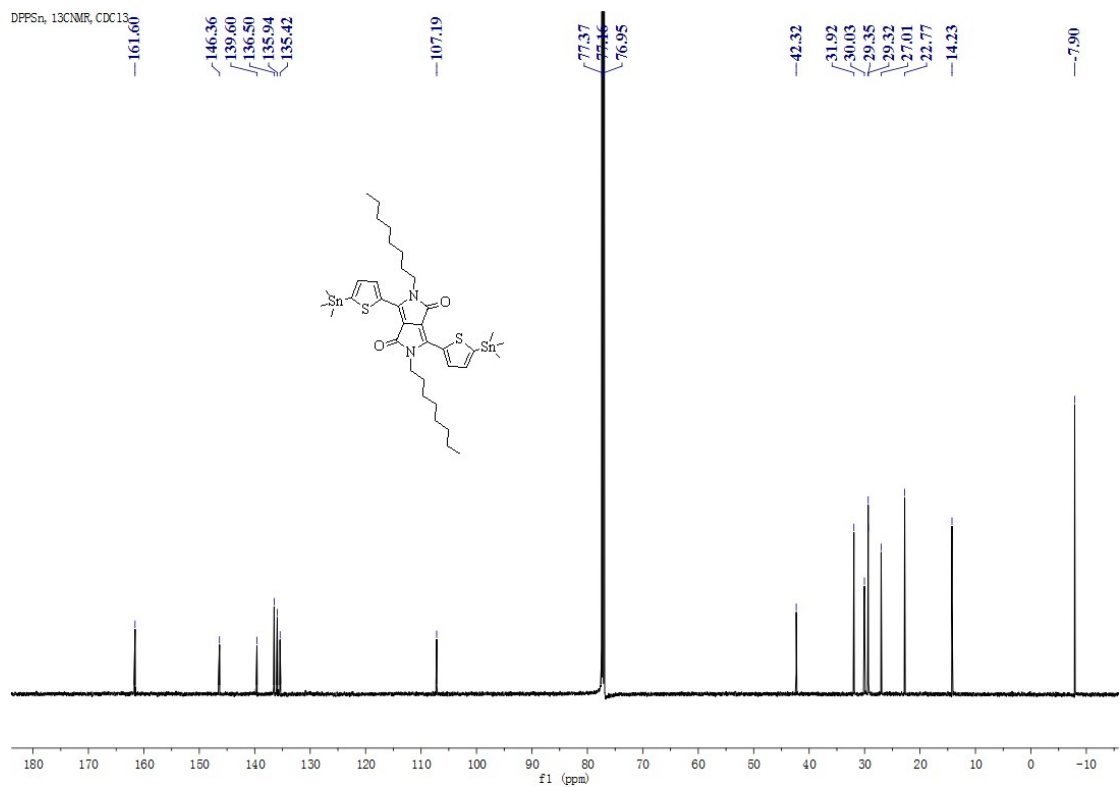
^a L. Ye, C. Zhou, H. Meng, H. Wu, C. Lin, H. Liao, S. Zhang and J. Hou, *J. Mater. Chem. C*, 2015, 3, 564-569.

7. ^1H NMR and ^{13}C NMR spectra

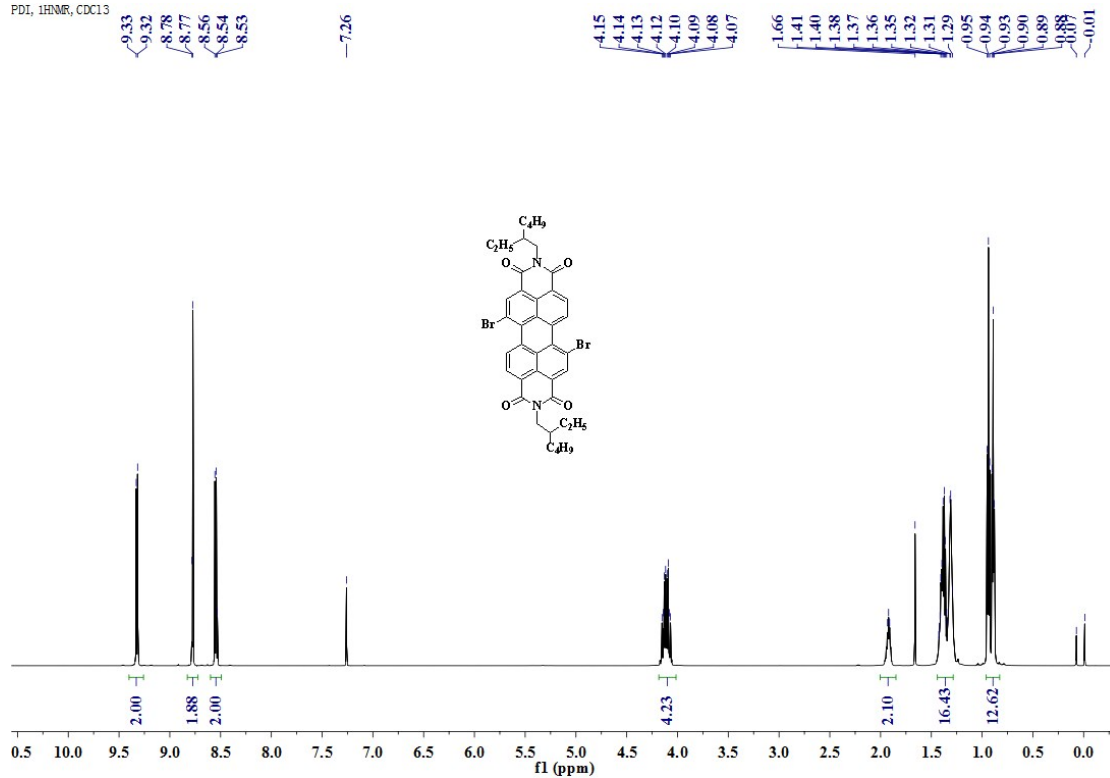
DPPS_n, ^1H NMR, CDCl₃



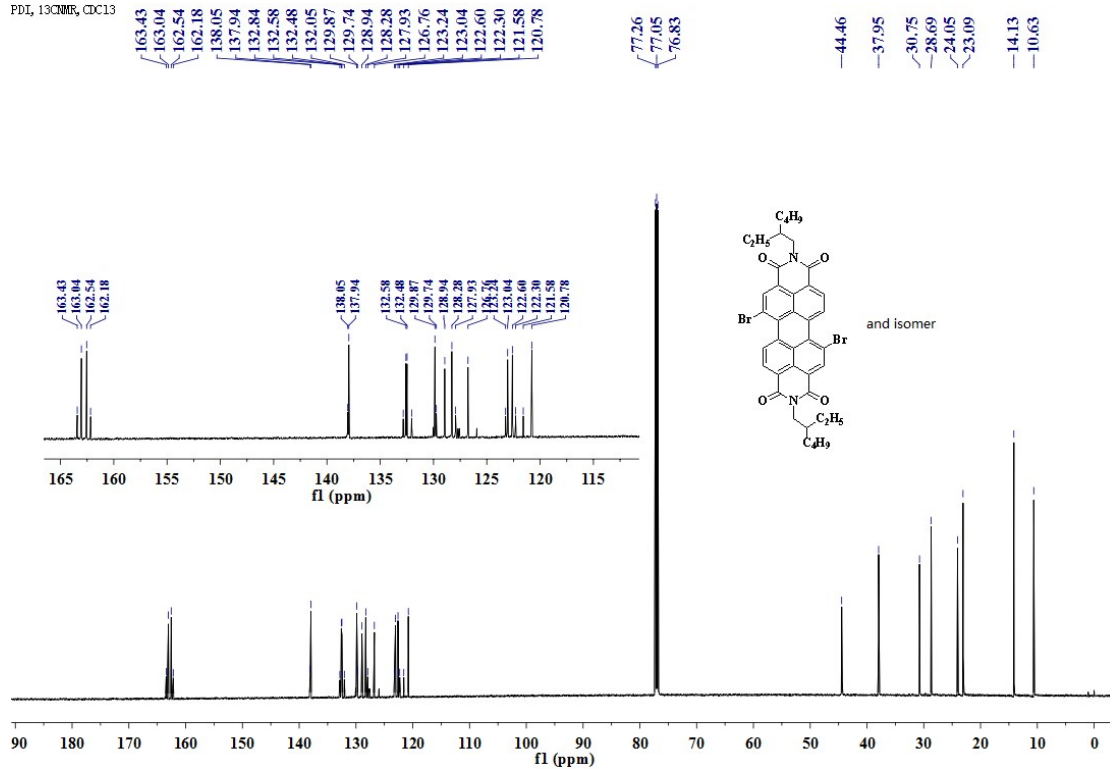
DPPS_n, ^{13}C NMR, CDCl₃



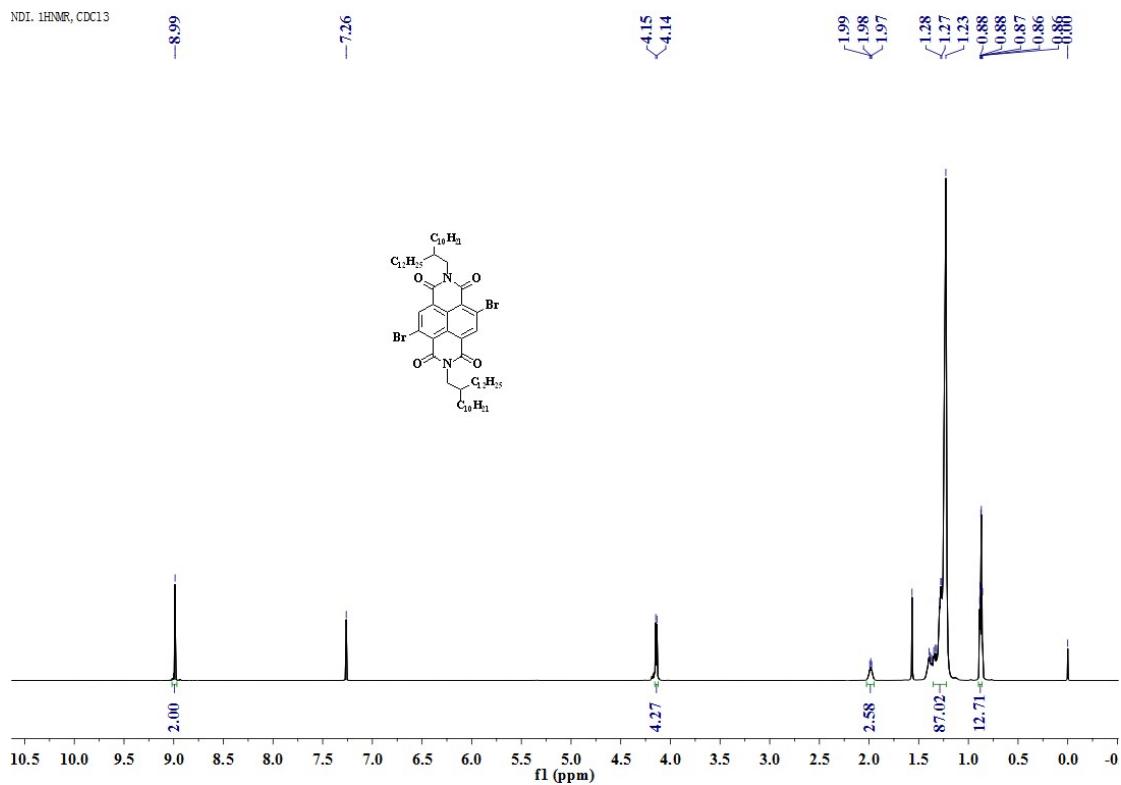
PDI, ¹H NMR, CDCl₃



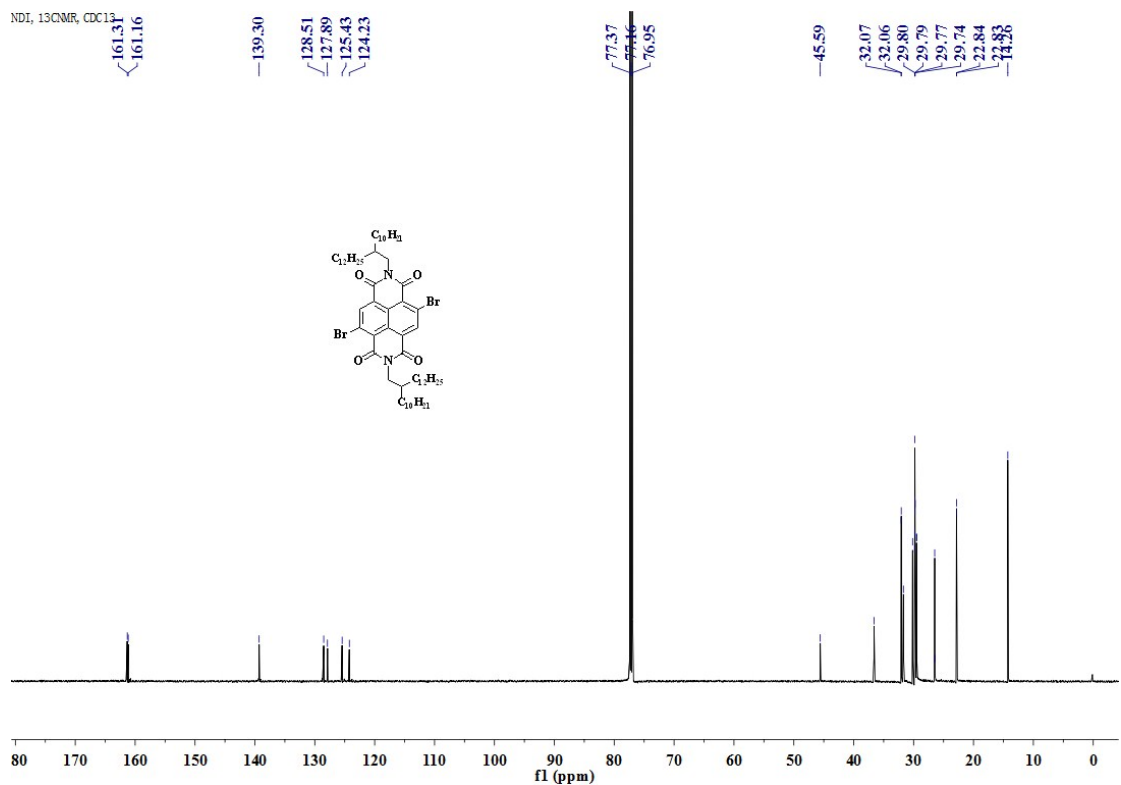
PDI, ¹³C NMR, CDCl₃



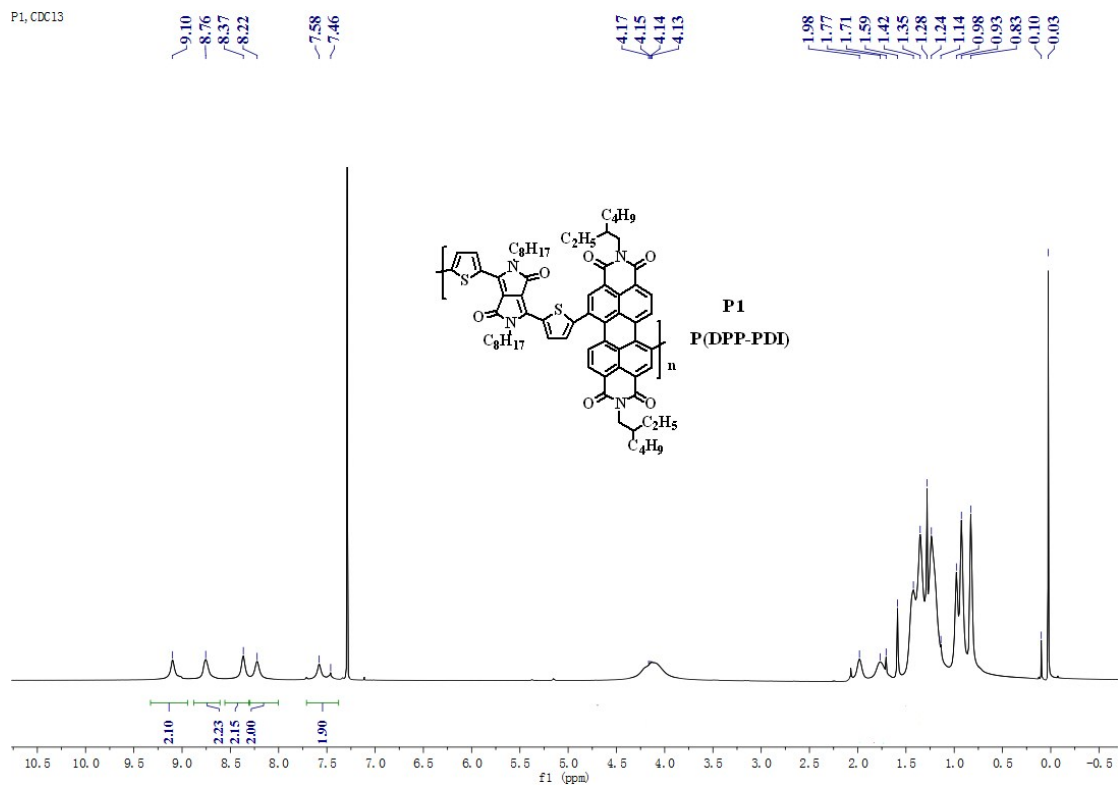
NDI, 1H NMR, CDC13



NDI, 13C NMR, CDC13



P1, CDC13



P2, CDC13

