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Enhanced Photovoltaic Effect from Naphtho[2,3-c]thiophene-4,9-dione-based Polymer through Alkyl Side Chain Induced Backbone Distortion

Xiaoman Bi,[ab] Tao Zhang,[b] Cunbin An,*[b] Pengqing Bi,[b] Kangqiao Ma,[ab] Sunsun Li,[b] Kaihu Xian,[b] Qianglong Lv,[b] Shaoqing Zhang,[bc] Huifeng Yao,[b] Bowei Xu,[b] Jianqi Zhang,*[e] Shaokui Cao,*[a] Jianhui Hou*[bd]

[a]School of Materials Science and Engineering, Zhengzhou University, Zhengzhou 450001, China. E-mail: caoshaokui@zzu.edu.cn.

[b]Beijing National Laboratory for Molecular Sciences, State Key Laboratory of Polymer Physics and Chemistry, Institute of Chemistry, Chinese Academy of Sciences, Beijing 100190, China. E-mail: ancunbin@iccas.ac.cn; hjhzlz@iccas.ac.cn; Tel.: +86-10-82615900.

[c]School of Chemistry and Biological Engineering, University of Science and Technology Beijing, Beijing 100083, China.

[d]University of Chinese Academy of Sciences, Beijing 100049, China.

[e]Key Laboratory ofNanosystem and Hierarchical Fabrication, National Center for Nanoscience and Technology, Beijing 100190. E-mail: zhangjq@nanoctr.cn.

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1. Instruments

^{1}H and ^{13}C NMR spectra were carried out on a Bruker AVANCE 300 spectrometer at room temperature. MALDI-TOF mass spectra were recorded on a Bruker Reflex II-TOF Spectrometer using 337 nm nitrogen laser with tetracyanoquinodimethane (TCNQ) as matrix. Elementary analysis was conducted on an instrument of Flash EA 1112. Gel permeation chromatography (GPC) was performed on HLC-8321GPC/HT at 145 °C with linear polystyrene as references and o-dichlorobenzene as eluent. Thermogravimetric analysis (TGA) was carried out with a heating rate of 10 °C min^{-1} from 20 to 600 ^{o}C under an inert atmosphere on TGA-2050 from TA Instruments, Inc. The current density-voltage (*J–V*) measurements were performed via the solar simulator (SS-F5-3A, Enlitech) along with AM 1.5G spectra whose intensity was calibrated by the certified standard silicon solar cell (SRC-2020, Enlitech) at 100 mW/cm^2. The EQE spectrum was measured through the Solar Cell Spectral Response Measurement System QE-R3011 (Enli Technology Co., Ltd., Taiwan). Silicon diode was used as reference cell in both *J-V* and EQE.

2. Measurements

Single crystal structure: X-ray crystallographic data for compound **3a** and **3b** was measured on a XtaLAB AFC10 (RCD3): fixed-chi single diffractometer. The crystal was kept at 170.00(10) K during data collection. Using Olex2, the structure was solved with the ShelXT structure solution program using Intrinsic Phasing and refined with the ShelXL refinement package using Least Squares minimisation.

Optical characterizations: UV-vis absorption spectra of polymers in solution and in films were measured on a Hitachi U-3100 UV–vis spectrophotometer. The film samples were spin-coated onto quartz plates (1×1 cm^2).

Cyclic Voltammetry (CV): The cyclic voltammetry was conducted on a CHI650D electrochemical workstation, where the tetrabutylammonium hexafluorophosphate acetonitrile (Bu_4NPF_6 in anhydrous acetonitrile) solution was used as the electrolyte while the scan rate was 100 mV s^{-1} under argon at room temperature. Silver wire, Pt wire, and glassy carbon electrode were used as the reference electrode, counter electrode and working electrode, respectively. The Fc/Fc^+ redox couple was used as an external standard.

Density functional theory (DFT) calculation: The molecular modeling calculations were conducted using the Gaussian 09 program based on the DFT method using B3LYP/6-31G (d, p) level.

Fabrication and measurement of OPV cells. PBTN-*p*- and **PBTN-*o*-**based PSCs were fabricated with the conventional device architecture of ITO/poly(3,4-ethylenedioxythiophene):poly(styrenesulfonate) (PEDOT:PSS)/BHJ/PFN-Br/Al. Pre-patterned indium tin oxide (ITO)-coated glass with a sheet resistance of 10−15 ohm/square was cleaned sequential sonication in deionized water, acetone and isopropanol twice for 15 min. Then it was transferred to oven and dried at 150 °C for 15 min. After ultraviolet-ozone treatment for 20 min, the 10 nm layer of PEDOT:PSS (Heraeus Materials, 4083) was spin-coated on ITO. The substrates were annealed for 15 min at 150 °C, and transferred to the nitrogen-filled glovebox. The photoactive layer of polymer donor:BO-4Cl were fully dissolved in chloroform (CF) at 40 °C for 1 hour. Before the spin-coating, 0.5% volume 1,8-diiodoctane (DIO) was used as the solvent additive. The active layer thicknesses were controlled at 100 ± 10 nm. The blend films were treated with the thermal annealing at 100 °C for 10 min followed by spin coating of PFN-Br as anode interfacial layer. Finally, Al (100 nm) was evaporated onto the devices under high vacuum to acquire an area of 4 mm^2 cell.

AFM characterizations. AFM images were recorded on a Nanoscope V AFM microscope (Bruker), where the tapping mode was used.

3 Synthetic detail

All reagents and chemicals were used as received from commercial sources without further purification. The monomer of (4,8-bis(5-(2-ethylhexyl)-4-fluorothiophen-2-yl)benzo[1,2-b:4,5-b']dithiophene-2,6-diyl)bis(trimethylstannane) was purchased from Organtec solar Materials Inc.

Synthesis of 1,2-bis(2-ethylhexyl)benzene (1a) and 1,4-bis(2-ethylhexyl)benzene (1b):

Under Argon, dichlorobenzene (1equiv.), Ni(dppp)Cl2 (dppp = 1,3-bis(disphenyphosphino)propane) (0.1-1 mol%) and (2-ethylhexyl)magnesium bromide (2.5 equiv. 1M in ethyl ether) were slowly added to a 250 mL two-neck flask with 50 mL of dry ethyl ether. The reaction mixture was refluxed for 3 days. The mixture is poured onto ice, neutralized by diluted HCl, and extracted with DCM (3 x 100 mL). The combined organic layers were dried over MgSO4. Evaporation of solvent furnished viscous liquid which was purified by column chromatography with petroleum ether as eluent to get colorless oil product. Compound **1a**: Application of the general procedure to 1,2-dichlorobenzene (4.567 g, 31.07 mmol), Ni(dppp)Cl_2 (0.0673 g, 0.12 mmol), and (2-ethylhexyl)magnesium bromide in 1M ethyl ether solution (77.67 mL, 77.67 mmol). 75.36% yield. ^{1}H NMR (300 MHz, CDCl3) δ 7.54 (dd, J = 9.2, 5.6 Hz, 2H), 7.52 – 7.46 (m, 2H), 3.16 – 2.95 (m, 4H), 2.06 (s, 2H), 1.87 – 1.69 (m, 16H), 1.34 (t, J = 7.2 Hz, 12H). ^{13}C NMR (75 MHz, CDCl3) δ 140.05 (s), 130.22 (s), 125.42 (s), 40.60 (s), 37.26 (s), 32.67 (s), 29.04 (s), 25.73 (s), 23.23 (s), 14.21 (s), 10.98 (s). TOF MS EI+, C22H38: m/z 302. Compound **1b**: Application of the general procedure to 1,4-dichlorobenzene (4.567 g, 31.07 mmol), Ni(dppp)Cl_2 (0.0673 g, 0.12 mmol), and (2-ethylhexyl)magnesium bromide in 1M ethyl ether solution (77.67 mL, 77.67 mmol). 69.30% yield. ^{1}H NMR (300 MHz, CDCl3) δ 7.03 (s, 4H), 2.50 (s, 4H), 1.55 (s, 2H), 1.26 (s, 16H), 0.84 (s, 12H). ^{13}C NMR (75 MHz, CDCl3) δ 138.93 (s), 128.97 (s), 77.50 (s), 77.08 (s), 76.65 (s), 41.22 (s), 39.88 (s), 32.49 (s), 29.00 (s), 25.60 (s), 23.16 (s), 14.20 (s), 10.89 (s). TOF MS EI+, C22H38: m/z 302.

Synthesis of 1,3-dibromo-6,7-bis(2-ethylhexyl)naphtho[2,3-c]thiophene-4,9-dione (2a) and 1,3-dibromo-5,8-bis(2-ethylhexyl)naphtho[2,3-c]thiophene-4,9-dione (2b):

2,5-dibromothiophene-3,4-dicarboxylic acid (1 equiv.) was dissolved in oxalyl chloride (＞4 equiv.) in a two-necked round-bottomed flask at 0 °C under Argon. The mixture was stirring for 10 min followed by addition of a few drops of DMF, then refluxed for 1 h. After cooling down, surplus oxalyl chloride was removed in vacuum to get solid residue which was further dissolved in dry DCM as solution I. $AlCl_3$ (4.5 equiv.) was dissolved in dry DCM at 0 °C in a two-necked flask under protection of Argon to make solution II. Solution I was added dropwise into solution II at 0 °C followed by stirring for 10 min. Then solution of compound **1a**/**1b** (1 equiv.) in dry DCM (5 mL) was added dropwise to the mixture mentioned above at 0 ^{o}C. After stirring the reaction mixture at 0 ^{o}C for 2 hours, it was poured into ice and extracted with DCM. The resulting organic layer was washed with water and dried with $MgSO_4$. After removal of solvent under reduced pressure, the residue was purified by column chromatography on silica gel to get solid product. Compound **2a**: Application of the general procedure to 2,5-dibromothiophene-3,4-dicarboxylic acid (3.25 g, 9.85 mmol), oxalyl chloride (6 mL), compound **1a** (2.98 g, 9.85 mmol), $AlCl_3$ (5.91 g, 44.33 mmol). 63.32% yield. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.99 (s, 2H), 2.69 (d, *J* = 7.0 Hz, 4H), 1.68 (s, 2H), 1.33 (dd, *J* = 15.3, 7.5 Hz, 16H), 0.98 – 0.78 (m, 12H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 177.93 (s), 148.30 (s), 133.14 (s), 131.89 (s), 129.05 (s), 120.42 (s), 40.48 (s), 37.49 (s), 32.56 (s), 28.88 (s), 25.69 (s), 23.00 (s), 14.09 (s), 10.88 (s). MALDI-TOF [-H$^+$], $C_{28}H_{36}Br_2O_2S$: m/z 596.9. Compound **2b**: Application of the general procedure to 2,5-dibromothiophene-3,4-dicarboxylic acid (1.33 g, 4.03 mmol), oxalyl chloride (6 mL), compound **1b** (1.22 g, 4.03 mmol), $AlCl_3$ (2.42 g, 18.14 mmol). 31.32% yield. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.33 (s, 2H), 3.09 (s, 4H), 1.63 (s, 2H), 1.26 (s, 16H), 0.85 (s, 12H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 180.54 (s), 144.22 (s), 137.30 (s), 134.56 (s), 134.06 (s), 117.73 (s), 77.57 (s), 77.14 (s), 76.72 (s), 40.42 (s), 40.05 (d), 32.53 (s), 28.64 (s), 25.77 (s), 23.12 (s), 14.18 (s), 10.77 (s). MALDI-TOF [-H$^+$], $C_{28}H_{36}Br_2O_2S$: m/z 594.7.

Synthesis of 6,7-bis(2-ethylhexyl)-1,3-di(thiophen-2-yl)naphtho[2,3-c]thiophene-4,9-dione (3a) and 5,8-bis(2-ethylhexyl)-1,3-di(thiophen-2-yl)naphtho[2,3-c]thiophene-4,9-dione (3b):

$Pd(PPh_3)_4$ (59 mg, 0.051 mmol) was added to the solution of compound **2a** or **2b** (1.02 g, 1.71 mmol) and tributyl(thiophen-2-yl)stannane (1.404 g, 3.76 mmol) in toluene (30 mL). The mixture was stirred and heated to 110 ^{o}C for 30 hours under argon protection. After removal of the solvent toluene, the crude product was purified via column chromatography on a silica gel using hexane/CH_2Cl_2 (5:1) as eluent to give compound **3a** or **3b** as orange solid (yield ~70%). Compound **3a**: ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.05 (s, 2H), 7.83 (s, 2H), 7.54 (s, 2H), 7.16 (s, 2H), 2.68 (d, *J* = 6.9 Hz, 4H), 1.66 (s, 2H), 1.42 – 1.11 (m, 16H), 0.88 (t, *J* = 6.4 Hz, 12H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 180.15 (s), 147.66 (s), 143.58 (s), 133.06 (s), 132.22 (s), 131.01 (s), 130.31 (s), 129.70 (s), 128.87 (s), 127.34 (s), 40.59 (s), 37.57 (s), 32.62 (s), 28.95 (s), 25.72 (s), 23.04 (s), 14.11 (s), 10.92 (s). MALDI-TOF [-H$^+$], $C_{36}H_{42}O_2S_3$: m/z 603.0. **Compound 3b**: ^{1}H NMR (300 MHz, $CDCl_3$)

δ 7.79 (s, 2H), 7.48 (s, 2H), 7.30 (s, 2H), 7.12 (s, 2H), 3.10 (s, 4H), 1.65 (s, 2H), 1.27 (s, 16H), 0.86 (s, 12H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 184.00 (s), 142.82 (s), 140.37 (s), 136.51 (s), 135.28 (s), 133.14 (s), 132.08 (s), 130.06 (s), 128.98 (s), 127.40 (s), 40.61 (s), 39.22 (s), 32.63 (s), 28.75 (s), 25.71 (s), 23.14 (s), 14.15 (s), 10.65 (s). MALDI-TOF [-H$^+$], $C_{36}H_{42}O_2S_3$: m/z 600.9.

Synthesis of 1,3-bis(5-bromothiophen-2-yl)-6,7-bis(2-ethylhexyl)naphtho[2,3-c]thiophene-4,9-dione (4a) and 1,3-bis(5-bromothiophen-2-yl)-5,8-bis(2-ethylhexyl)naphtho[2,3-c]thiophene-4,9-dione (4b):

Compound **3a** or **3b** (0.85 g, 1.41 mmol) was dissolved in 20 mL dry THF in a 50 mL two-necked flask. After being flushed by a gentle stream of argon for 5 min, *N*-bromosuccinimide (0.53 g, 2.96 mmol) was added in one portion at 0 ^{o}C. The mixture was stirred at room temperature until TLC showed the reaction end, and then was poured into 20 mL water. The mixture was extracted with DCM (3 × 50 mL). After removal of the solvent from organic layer, the crude product was purified via column chromatography on silica gel using hexane/CH_2Cl_2 (5:1) as eluent to give compound **4a** or **4b** as yellow solid (yield ~80%). Compound **4a**: ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.05 (s, 2H), 7.51 (s, 2H), 7.10 (s, 2H), 2.70 (s, 4H), 1.67 (s, 2H), 1.27 (s, 16H), 0.86 (s, 12H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 180.15 (s), 148.08 (s), 142.57 (s), 134.29 (s), 131.88 (s), 130.84 (s), 129.88 (d), 128.94 (s), 118.63 (s), 40.62 (s), 37.64 (s), 32.62 (s), 28.95 (s), 25.73 (s), 23.04 (s), 14.10 (s), 10.92 (s). MALDI-TOF [-H$^+$], $C_{36}H_{40}Br_2O_2S_3$: m/z 762.0. Compound **4b**: ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.37 (s, 2H), 7.27 (s, 2H), 7.00 (s, 2H), 3.13 (s, 2H), 2.97 (s, 2H), 1.64 (s, 2H), 1.30 (s, 16H), 0.88 (s, 12H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 183.70 (s), 143.43 (s), 139.74 (s), 137.04 (s), 134.55 (d), 133.84 – 133.66 (m), 131.53 (s), 130.00 (d), 117.56 (s), 40.54 (s), 39.54 (s), 32.75 (s), 28.84 (s), 25.70 (s), 23.21 (s), 14.24 (s), 10.66 (s). MALDI-TOF [-H$^+$], $C_{36}H_{40}Br_2O_2S_3$: m/z 758.9.

Synthesis of PBTN-*p* or PBTN-*o*

In a 25 mL flask, compound **4a** or **4b** (188.108 mg, 0.20 mmol) and **5** (152.14 mg, 0.20 mmol) were dissolved in 7 mL chlorobenzene, and the flask was flushed with argon for 10 min. Then 20 mg of $Pd(PPh_3)_4$ was added into the solution, and the mixture was flushed with argon for another 15 min. The solution was heated to reflux under argon protection for 10 h or 6h, respectively. After cooling to ambient temperature, the polymer was precipitated in 200 mL of methanol, filtered through a Soxhlet thimble. The precipitate was then subjected to Soxhlet extraction with methanol, hexane, and chloroform. The polymer was precipitated from 100 mL of methanol. The precipitates were collected and dried under vacuum overnight to get polymer as solid. **PBTN-*p***: Molecular weight by GPC (145 °C): M_n = 15.7 kg mol^{-1}, Đ= 1.7. Elemental analysis: Calcd. for $C_{70}H_{80}F_2O_2S_7$: C 69.15, H 6.63; found: C 68.47, H 6.46. **PBTN-*o***: Molecular weight by GPC (145 °C):M_n = 18.7 kg mol^{-1}, Đ= 2.1. Elemental analysis: Calcd. For $C_{70}H_{80}F_2O_2S_7$: C 69.15, H 6.63; found: C 68.79, H 6.50.

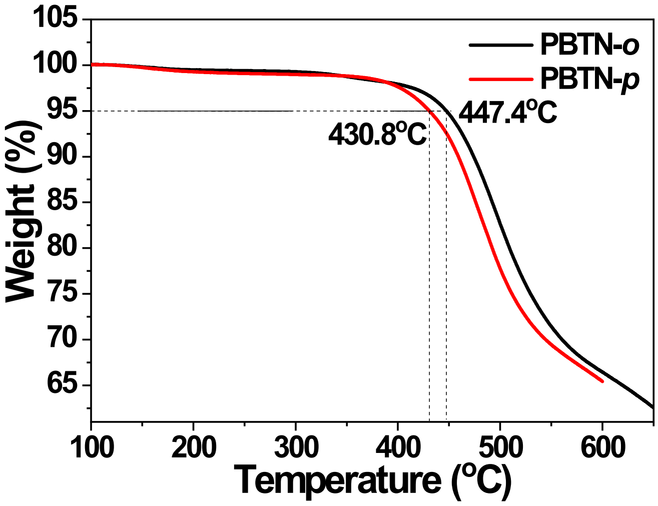

Fig. S1 Thermogravimetric analysis plots of the polymers under a nitrogen atmosphere with a heating rate of 10 °C/min.

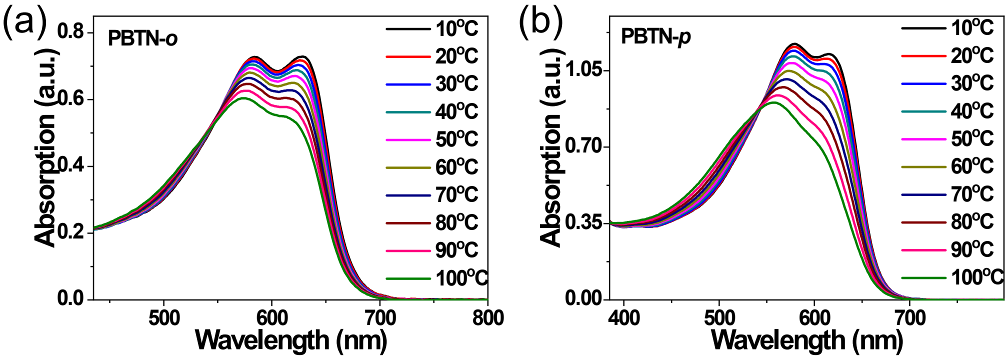

Fig. S2 The temperature-dependent UV-vis absorption spectra of (a) **PBTN-*o*** and (b) **PBTN-*p***.

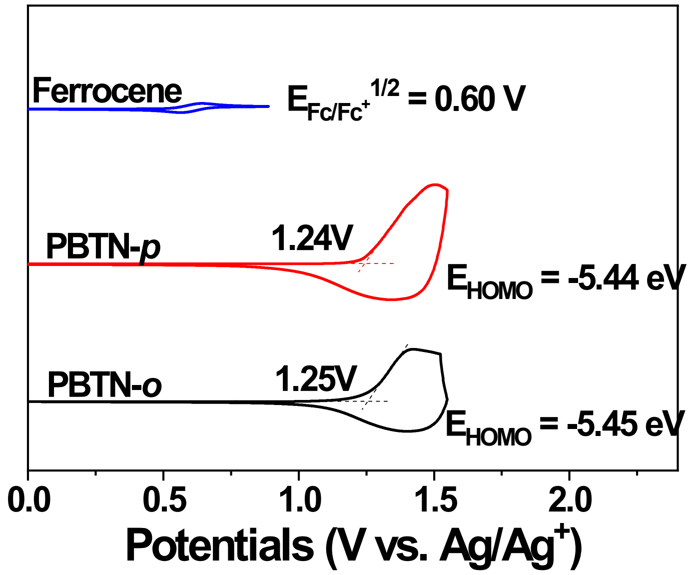

Fig. S3 The cyclic voltammetry plots for **PBTN-*p*** and **PBTN-*o*** films.

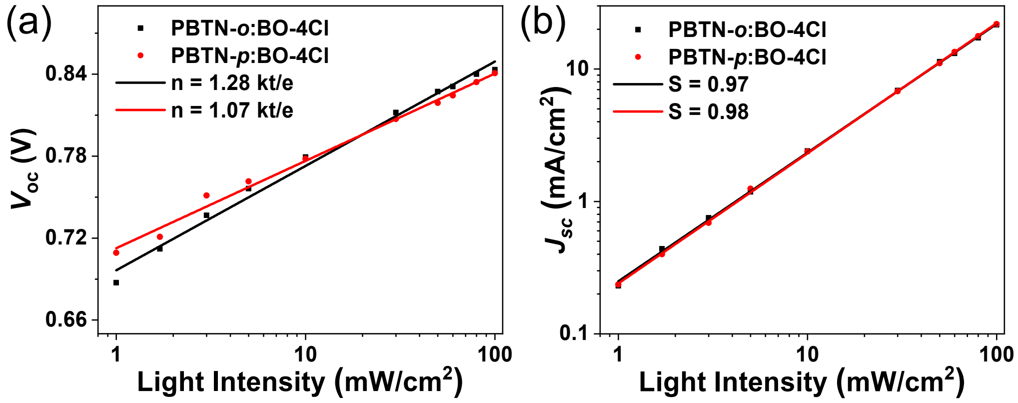

Fig. S4 Light intensity dependences of the (a) V_{OC} and (b) J_{SC} for the **PBTN-*o***:BO-4Cl- and **PBTN-*p***:BO-4Cl-based devices.

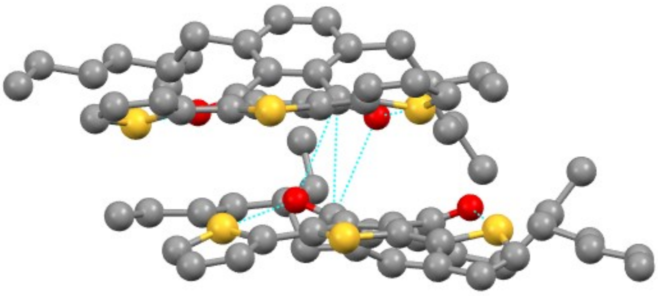

Fig. S5 The dimer feature of molecule **3b**.

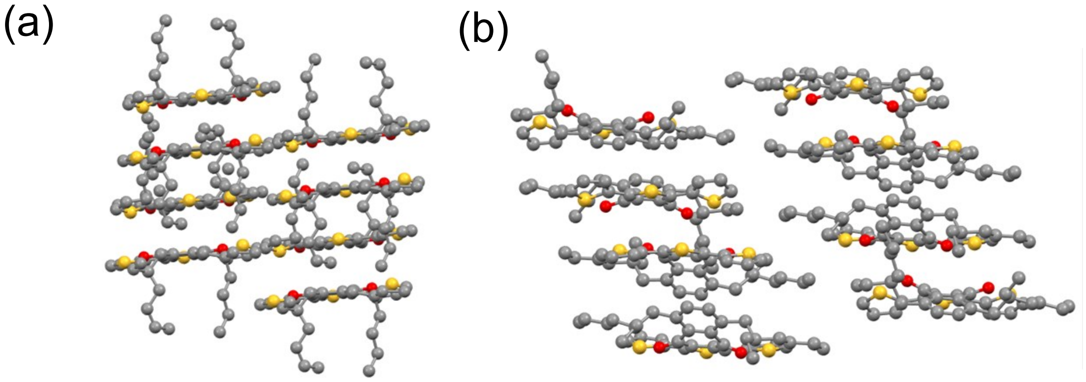

Fig. S6 The molecular arrangements of molecule (a) 3a and (b) **3b**.

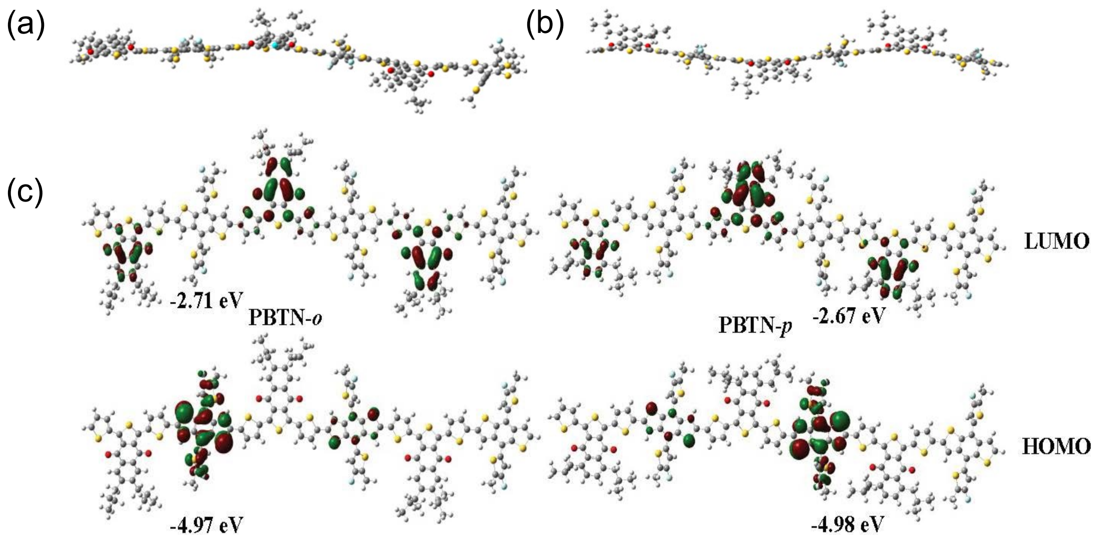

Fig. S7 The side views of trimers of (a) **PBTN-*o*** and (b) **PBTN-*p***（c）DFT calculation of geometries and molecular energy levels for the PBTN-*o* (left) and PBTN-*p* (right) models.

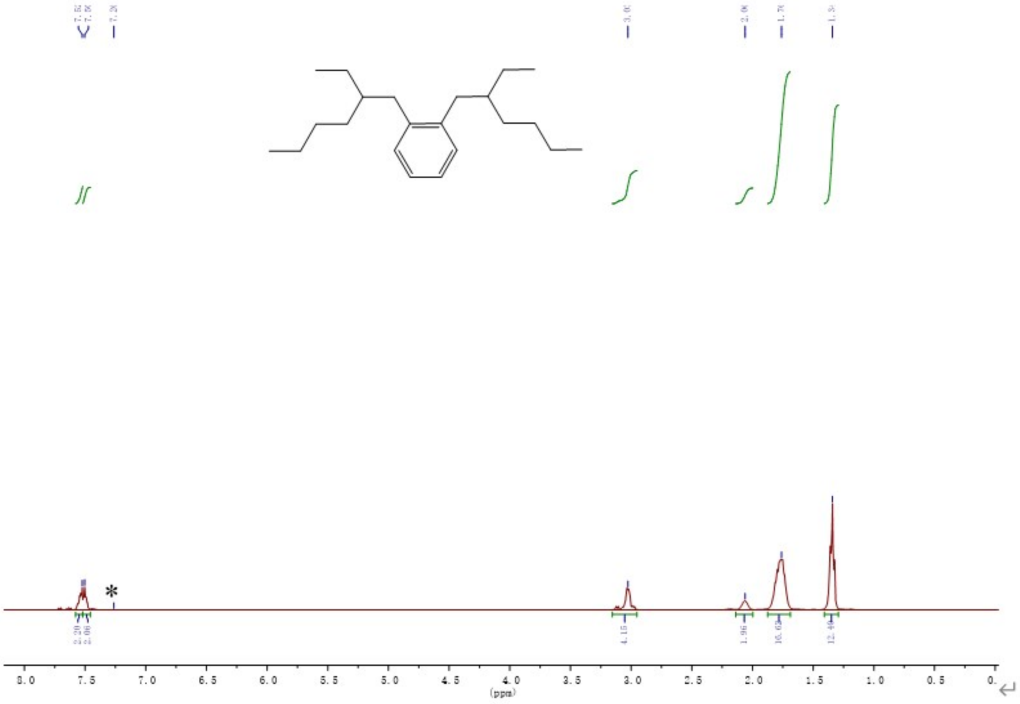

Figure S8. ^{1}H-NMR spectra of compound **1a** in $CDCl_3$.

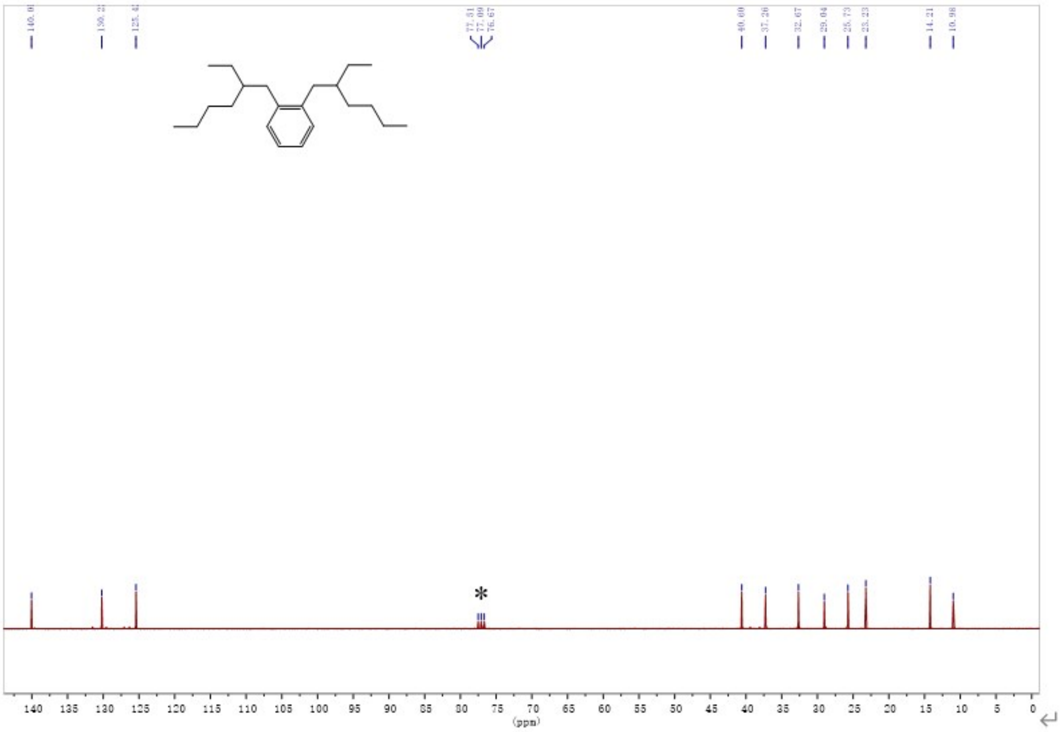

Figure S9. ^{13}C-NMR spectra of compound **1a** in CDCl$_3$.

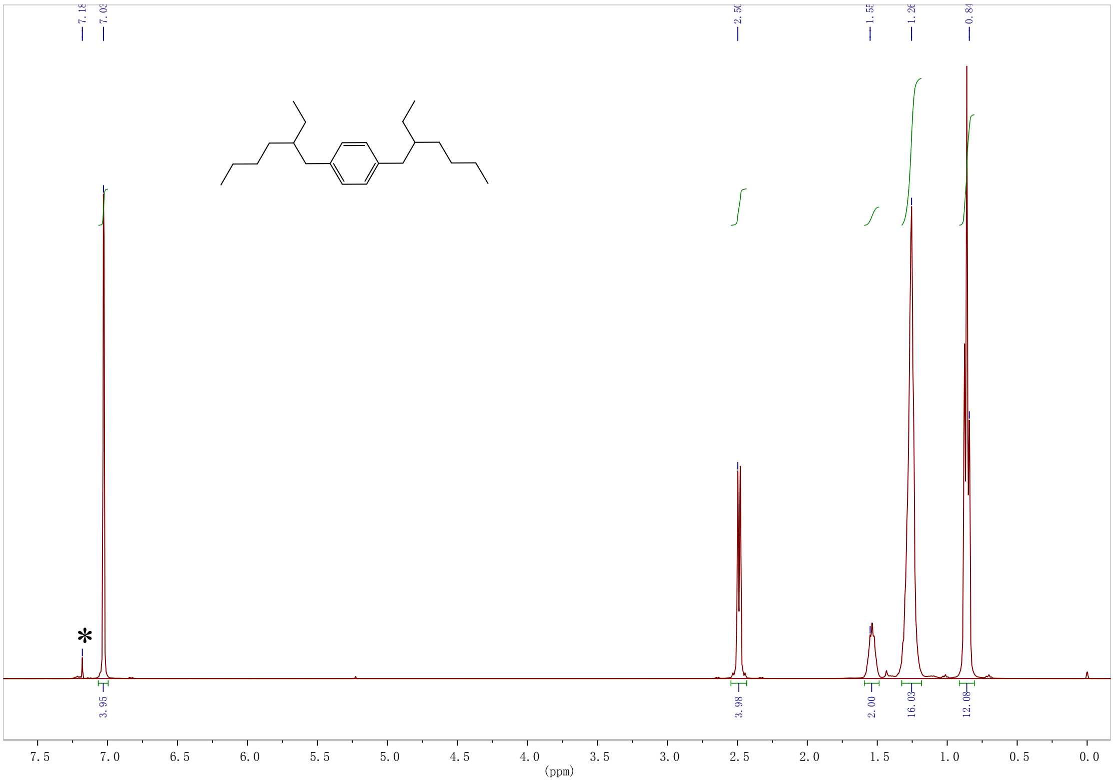

Figure S10. ^{1}H-NMR spectra of compound **1b** in CDCl$_3$.

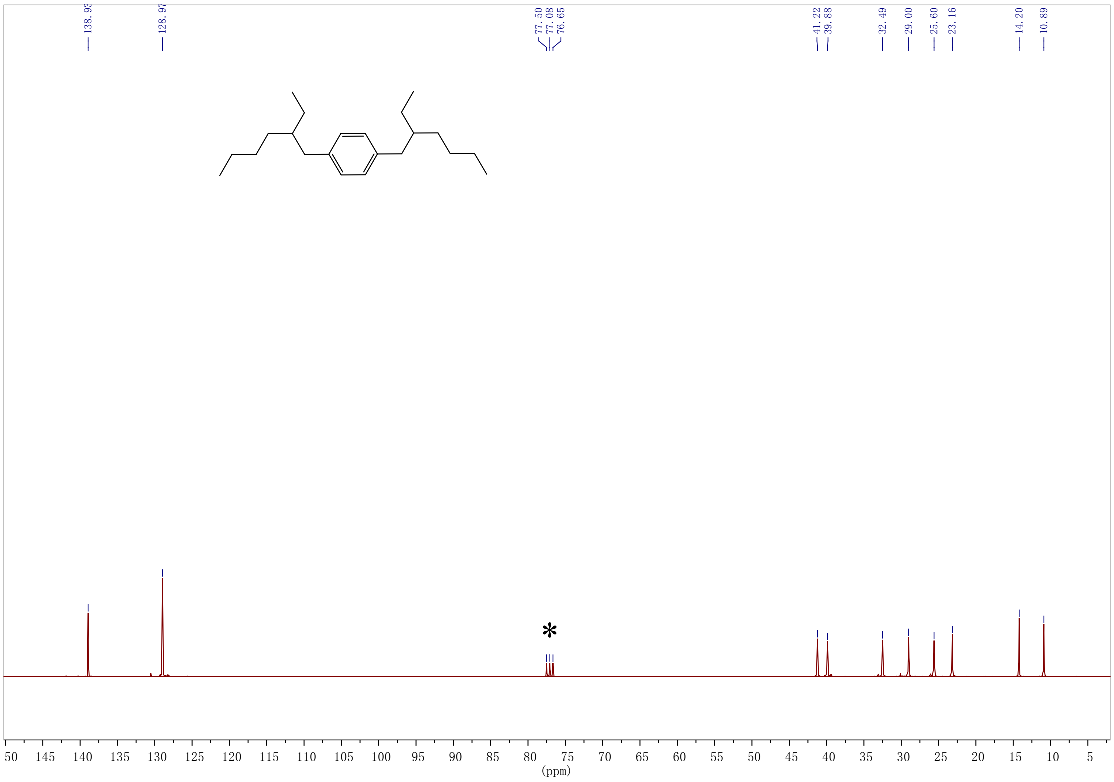

Figure S11. ^{13}C-NMR spectra of compound **1b** in CDCl$_3$.

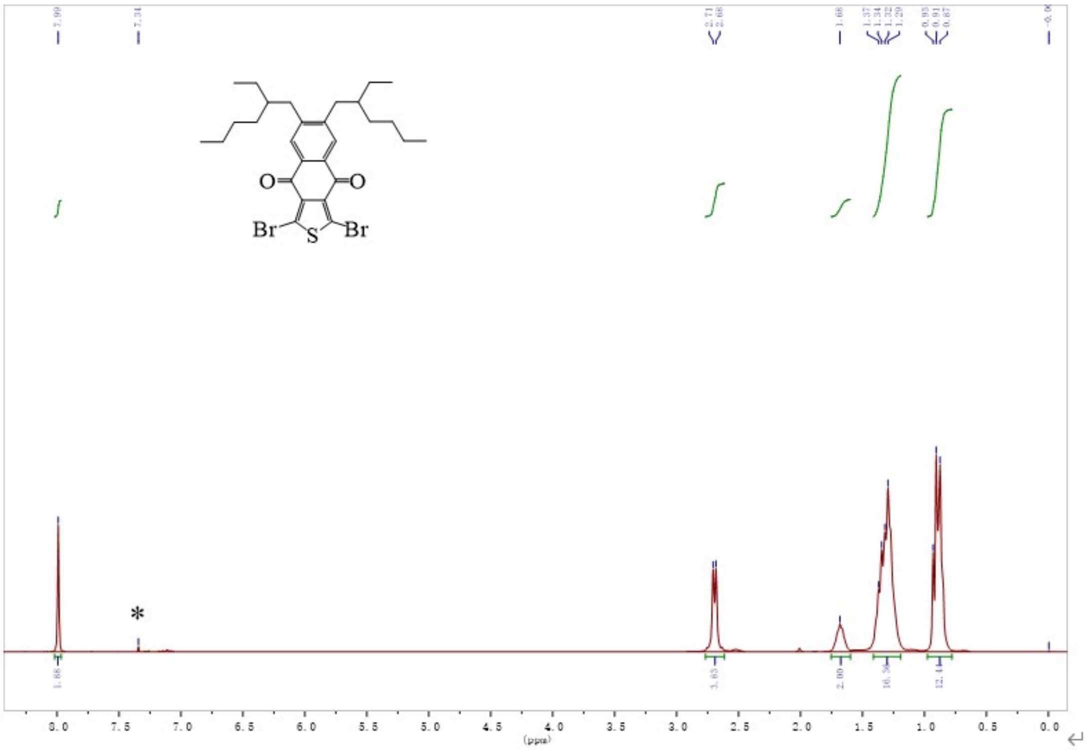

Figure S12. ^{1}H-NMR spectra of compound **2a** in CDCl$_3$.

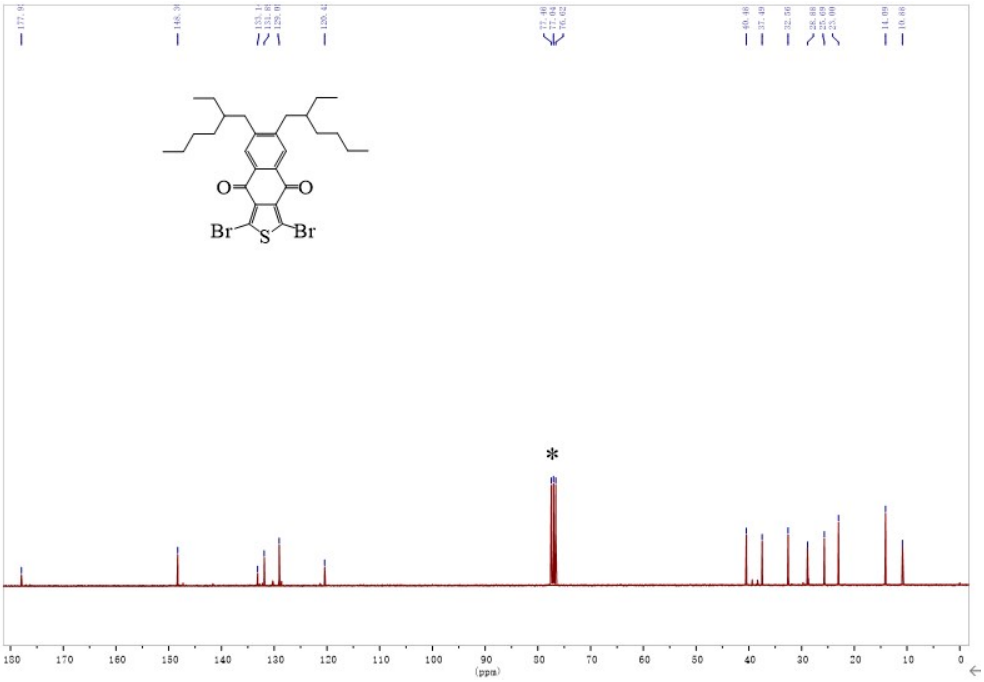

Figure S13. ^{13}C-NMR spectra of compound **2a** in $CDCl_3$.

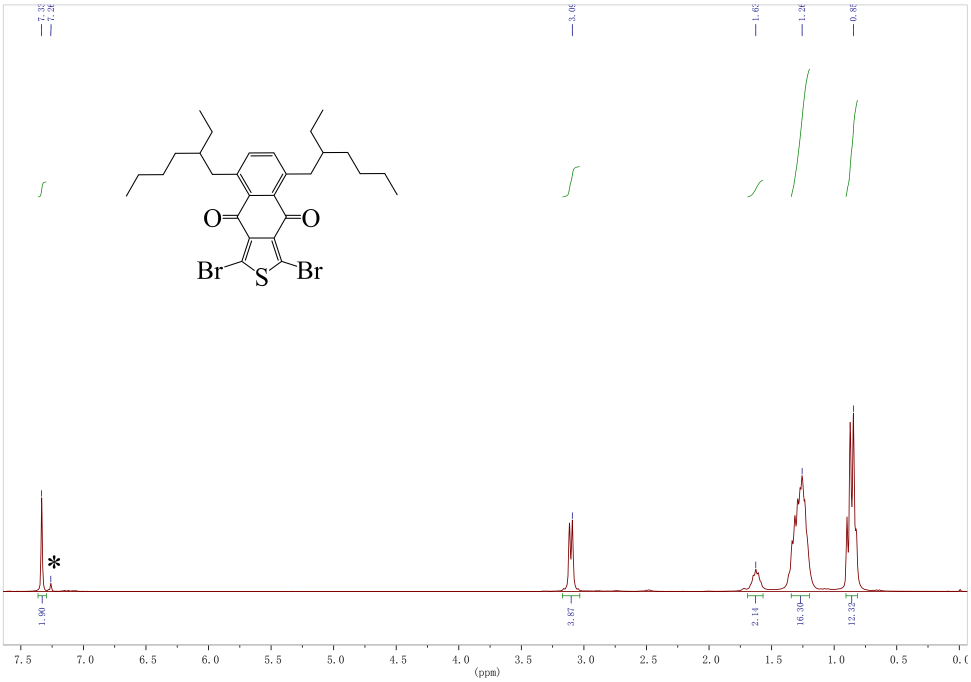

Figure S14. ^{1}H-NMR spectra of compound **2b** in $CDCl_3$.

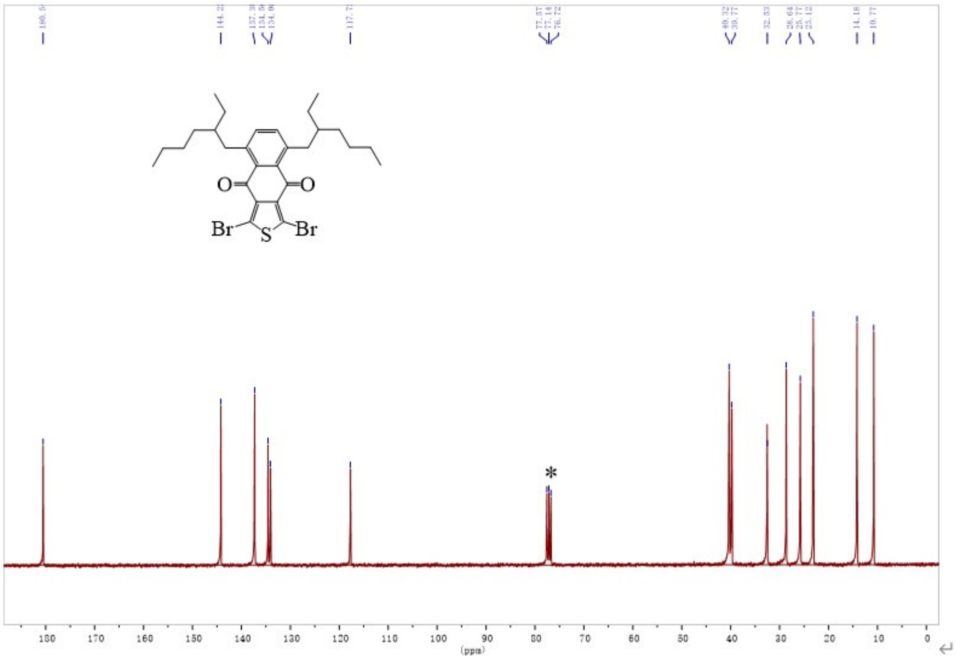

Figure S15. ^{13}C-NMR spectra of compound **2b** in $CDCl_3$.

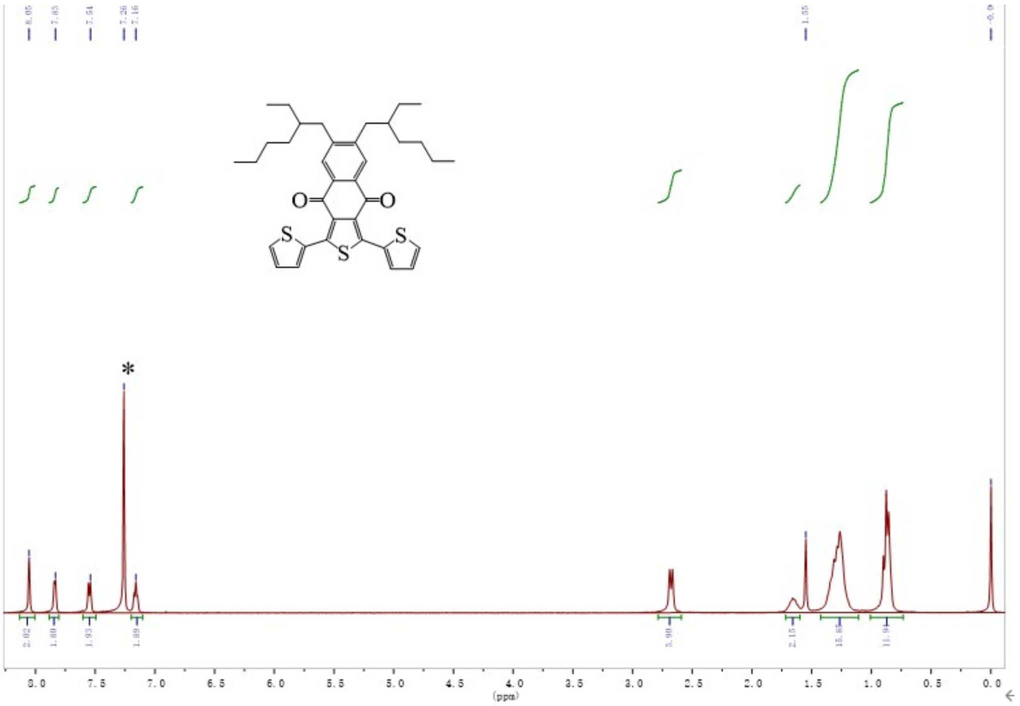

Figure S16. ^{1}H-NMR spectra of compound **3a** in $CDCl_3$.

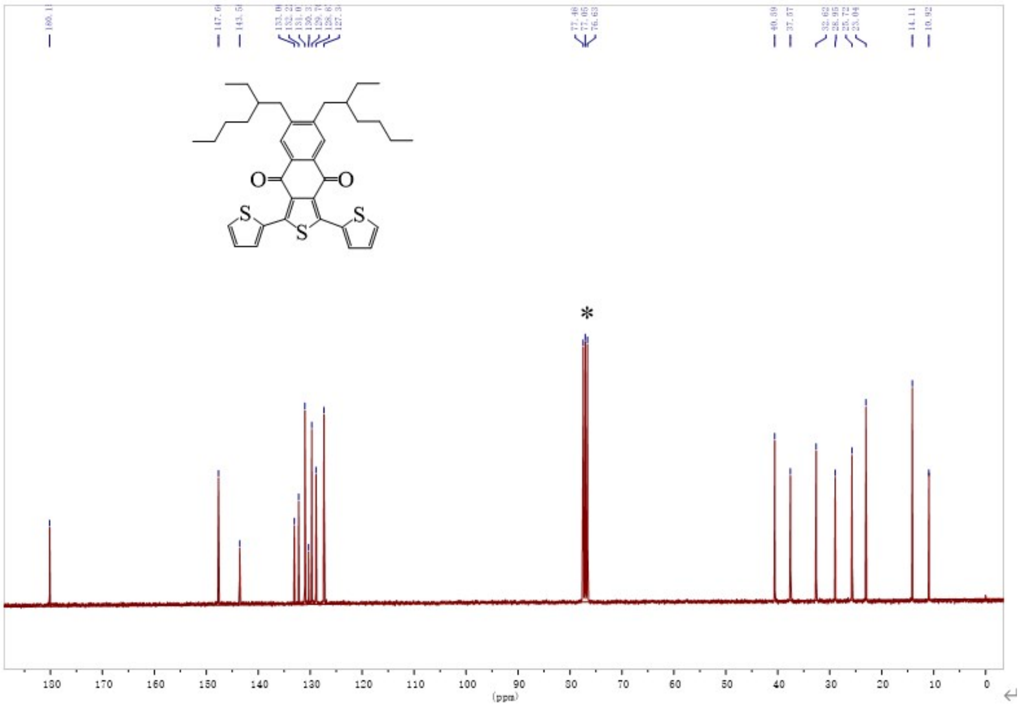

Figure S17. ^{13}C-NMR spectra of compound **3a** in CDCl$_3$.

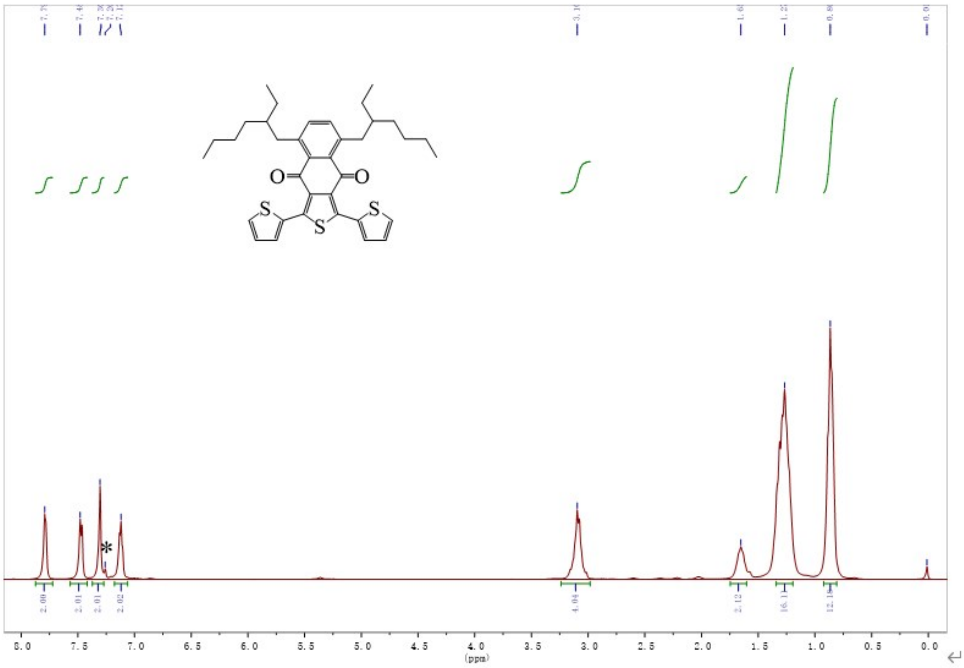

Figure S18. ^{1}H-NMR spectra of compound **3b** in CDCl$_3$.

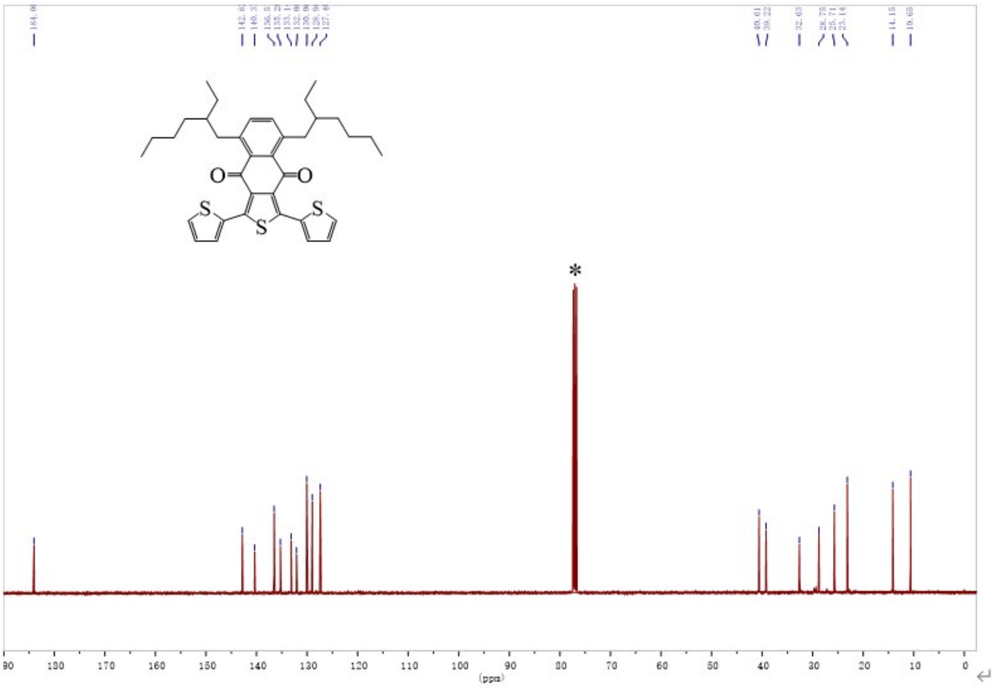

Figure S19. ^{13}C-NMR spectra of compound **3b** in $CDCl_3$.

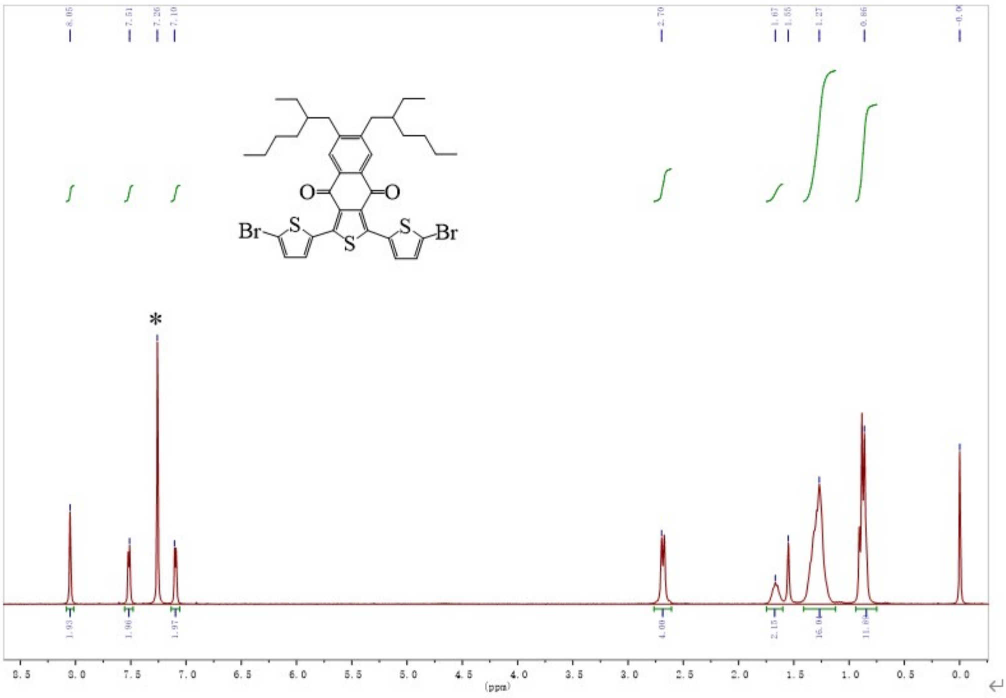

Figure S20. ^{1}H-NMR spectra of compound **4a** in $CDCl_3$.

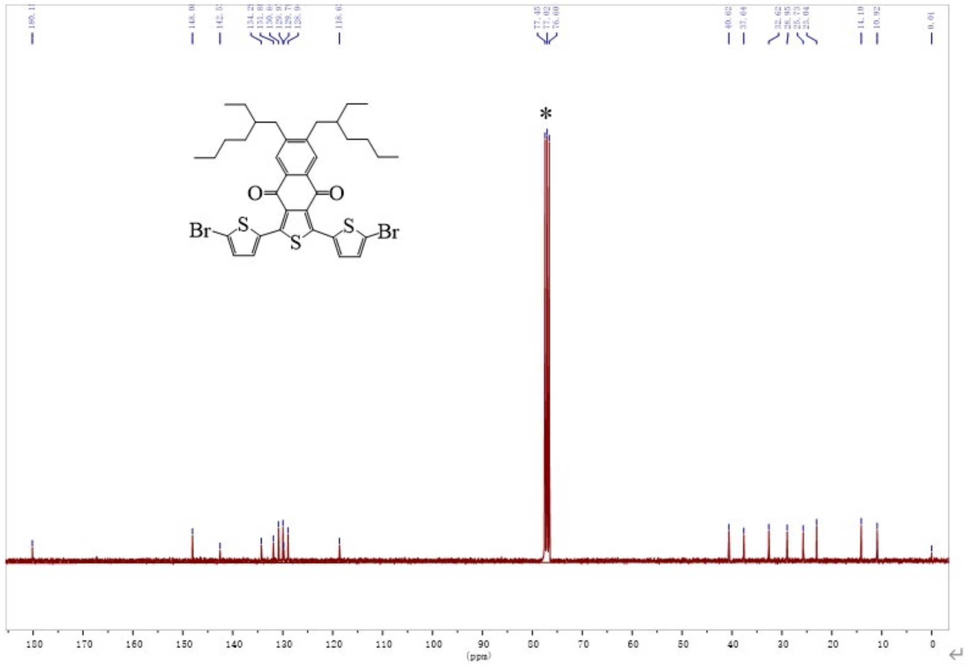

Figure S21. ^{13}C-NMR spectra of compound **4a** in CDCl$_3$.

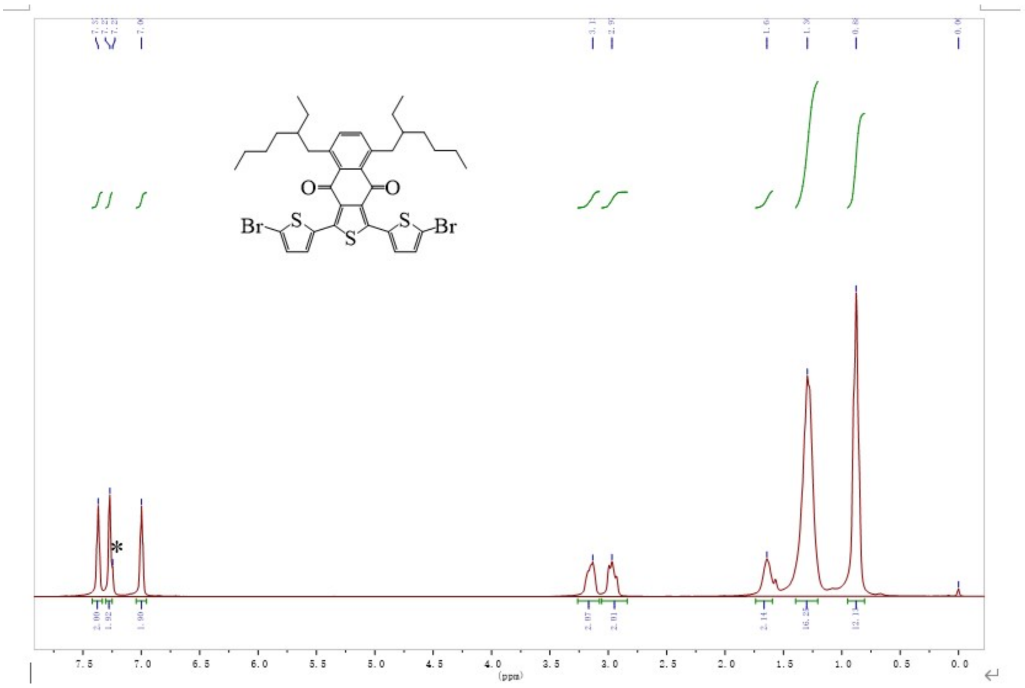

Figure S22. ^{1}H-NMR spectra of compound **4b** in CDCl$_3$.

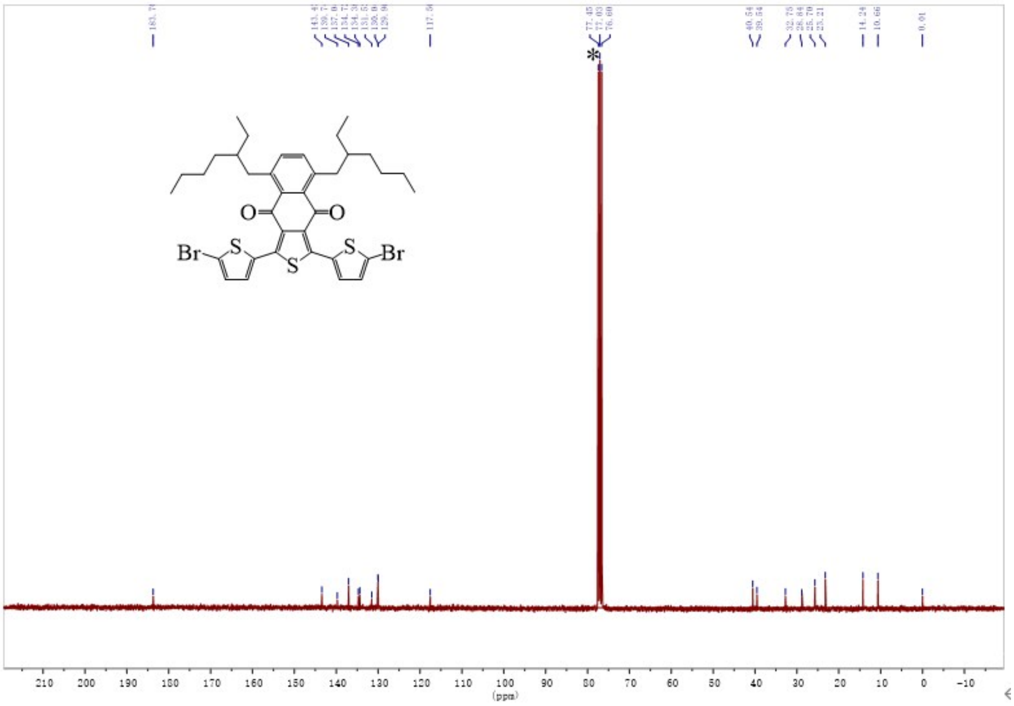

Figure S23. ^{13}C-NMR spectra of compound **4b** in CDCl$_3$.

Table S1. The photovoltaic parameters of the devices with varied **PBTN-*o***:BO-4Cl ratios. BHJ: PBTN-*o*:BO-4Cl**,** Conc. 10 mg/mL, solvent CB, DIO 0.5%**,** soluble temperature 80 ℃ 3 hrs, Rpm 60s, Annealing 100 ℃ (10 min).

D/A	R (rpm)	V_{oc} (V)	J_{sc} (mA cm^{-2})	FF	PCE (%)
1.5:1	2000	0.83	18.53	0.64	9.85
1:1	2500	0.84	22. 41	0.63	11.85
1:1.5	1800	0.82	22.76	0.52	9.53

Table S2. The photovoltaic parameters of the devices with varied solvent addictive (DIO) volume ratios. BHJ: PBTN-*o*:BO-4Cl**,** D/A 1:1, Conc. 10 mg/mL, solvent CB, soluble temperature 80 ℃ 3 hrs, Rpm 60 s, Annealing 100 ℃ (10 min).

DIO	V_{oc} (V)	J_{sc} (mA cm^{-2})	FF	PCE (%)
0	0.85	23.99	0.54	10.94
0.5	0.84	22. 41	0.63	11.85
1	0.82	20.6	0.65	10.91
2	0.78	17.64	0.63	8.82

Table S3. The photovoltaic parameters of devices with different annealing temperatures. BHJ: PBTN-*o*:BO-4Cl**,** D/A 1:1, Conc. 10 mg/mL, solvent CB, DIO 0.5%, soluble temperature 80 ℃ 3 hrs, 1800 Rpm 60 s, Annealing (10 min).

Annealing temperature (°C)	V_{oc} (V)	J_{sc} (mA cm^{-2})	FF	PCE (%)
80	0.85	22.76	0.59	11.54
100	0.84	22. 41	0.63	11.85
120	0.84	23.09	0.56	10.84
140	0.84	23.05	0.54	10.48
160	0.83	22.18	0.54	9.85

Table S4. The photovoltaic parameters of the devices with varied PBTN-*p*:BO-4Cl ratios. BHJ: PBTN-*p*:BO-4Cl**,** Conc. 6 mg/mL, solvent CB, DIO 0.5%**,** soluble temperature 80 ℃ 3 hrs, Rpm 60 s, Annealing 100℃ (10 min).

D/A	R (rpm)	V_{oc} (V)	J_{sc} (mA cm^{-2})	FF	PCE (%)
1.5:1	1600	0.84	23.32	0.68	13.42
1:1	1800	0.84	24.67	0.68	14.10
1:1.5	2000	0.84	24.09	0.62	12.52

Table S5. The photovoltaic parameters of the devices with varied solvent addictive (DIO) volume ratios. BHJ: PBTN-*p*:BO-4Cl**,** D/A 1:1, Conc. 6 mg/mL, solvent CB, soluble temperature 80 ℃ 3 hrs, Rpm 60 s, Annealing 100 ℃ (10 min).

DIO	V_{oc} (V)	J_{sc} (mA cm^{-2})	FF	PCE (%)
0	0.85	20.28	0.71	12.24
0.5	0.84	24.67	0.68	14.10

1	0.81	12.85	0.64	6.65
2	0.77	4.06	0.43	1.34

Table S6. The photovoltaic parameters of devices with different annealing temperatures. BHJ: PBTN-*p*:BO-4Cl, D/A 1:1, Conc. 6 mg/mL, solvent CB, DIO 0.5%, soluble temperature 80 ℃ 3 hrs, 1800 Rpm 60 s, Annealing (10 min).

Annealing temperature (^{o}C)	**V_{oc} (V)**	**J_{sc} (mA cm^{-2})**	**FF**	**PCE (%)**
80	0.84	24.02	0.68	13.69
100	0.84	24.67	0.68	14.10
120	0.84	24.09	0.68	13.65
140	0.83	22.58	0.68	12.79
160	0.83	23.48	0.54	10.38

Table S7. Crystal data of compound 3a and 3b.

Compound	**3a**	**3b**
Empirical formula	$C_{36}H_{42}O_2S_3$	$C_{36}H_{42}O_2S_3$
Formula weigh (g mol^{-1})	602.87	602.87
CCDC NO.	1989665	1989664
Temperature (K)	170.00(10)	170.00(10)
Crystal system	triclinic	triclinic
Space group	P-1	P-1
Crystal size (mm^3)	0.52 × 0.18 × 0.13	0.33 × 0.25 × 0.05
a (Å)	8.5152(2)	14.6922(4)

b (Å)	10.8053(3)	14.8833(5)
c (Å)	17.7226(4)	16.9828(5)
α (°)	83.121(2)	74.604(3)
β (°)	86.107(2)	70.817(3)
γ (°)	76.291(2)	68.089(3)
Z	2	4
Volume / Å^3	1571.47(7)	3210.50(19)
Absorption (mm^{-1})	0.267	0.262
Refinement method	ShelXL refinement package	ShelXL refinement package
No. of reflections measured	22906	42234
R_{int}	0.0158	0.0282
Goodness of fit on F^2	1.036	1.044