ELECTRONIC SUPPORTING INFORMATION

Pyrene-1,5,6,10-Tetracarboxyl Diimide: A New Building Block for High-Performance Electron-Transporting Polymers

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Table of Contents

1. Materials and Measurements

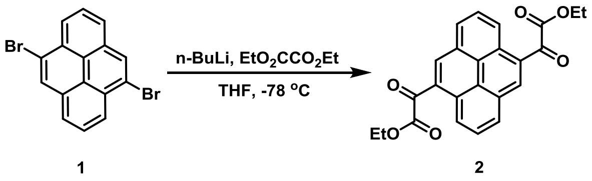
All reagents were purchased from commercial suppliers and used without further purification unless otherwise noted. All oxygen or moisture sensitive reactions were performed under nitrogen atmosphere using the standard Schlenk method. Toluene and tetrahydrofuran (THF) were distilled over sodium and benzophenone prior to use. ^{1}H and ^{13}C NMR spectra were recorded on a Bruker Avance 400, operating at 400 MHz (^{1}H) and 101 MHz (^{13}C), or Bruker-500, operating at 500 MHz (^{1}H) using $CDCl_3$ as the solvent unless otherwise noted. Chemical shifts are reported in parts per million (ppm) with TMS (0 ppm) as the reference for ^{1}H NMR spectra and $CDCl_3$ (77.04 ppm) as the reference for ^{13}C NMR spectra. The MALDI-TOF mass spectra (MS) were recorded on a Bruker BIFLEX III time-of-flight (TOF) mass spectrometer using a 337 nm nitrogen laser as the matrix, and the high-resolution (HR) MS were recorded on Bruker Fourier Transform Ion Cyclotron Resonance Mass Spectrometer Solarix XR.

The absorption spectra were recorded with a Hitachi U-4100 spectrophotometer, and the emission spectra were obtained with a Horiba Jobin Yvon FluoroMax-4P spectrofluorimeter equipped with an R928 photomultiplier tube and a 150 W ozone-free xenon arc lamp used as the excitation light source. The cyclic voltammetry was carried out on a Gamry Interface 1000 electrochemical workstation with the three-electrode configuration, using Ag/AgCl as the reference electrode, a Pt plate as the counter electrode, and a glassy carbon as the working electrode. The polymer thin-film was dropped on the working electrode and n-Bu_4NPF_6 (0.1 mol L^{-1}) was dissolved in $CHCl_3$. The potentials were referenced to the Fc^+/Fc couple by using ferrocene as the external standard in $CHCl_3$ solution. The scan rate is 100 mV s^{-1}. The thermal gravity analyses (TGA) were performed on a TA Instrument Q600 analyzer under N_2 (10 ^{o}C min^{-1}) atmosphere and the differential scanning calorimetry (DSC) analyses were performed on a METTLER TOLEDO Instrument DSC822 calorimeter.

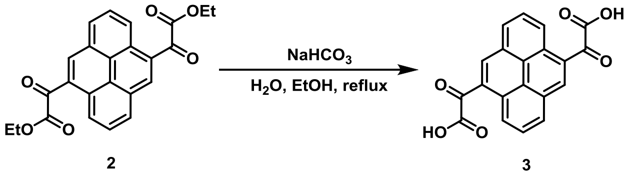
The single-crystal data were collected at the SSRF BL17U beamline, with the graphite-monochromated Mo Kα radiation (0.71073 Å). Using Olex2, the structure was solved with ShelXS and refined with the ShelXL-97 refinement package using Least Squares minimization.

2. Synthetic Procedures

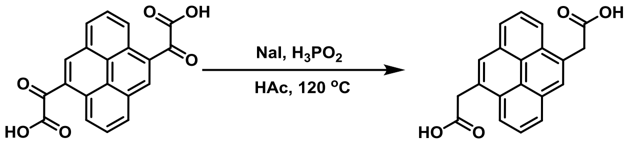
Compound 4,9-dibromopyrene, polymers **N2200** (M_n=41.8 kDa, PDI=2.97) and **PDI-TT** (M_n=10.4 kDa, PDI=2.07) are synthesized according to the literature procedures.[1, 2]



Compound 2.[3] A solution of butyllithium in hexane (2.4 M, 3.7 mL, 8.8 mmol) was added dropwise to a stirred suspension of **1** (800 mg, 2.2 mmol) in dry THF (25 mL) under nitrogen atmosphere at -78 ^{o}C, and the mixture was stirred for 1 h at -78 ^{o}C. The cooling bath was removed and stirring was continued for another 1 h at room temperature. Then, the mixture was cooled to -78 ^{o}C again, and a solution of diethyl oxalate (1.5 mL, 1.077 g/mL, 11 mmol) was quickly added, and the mixture was stirred for 1 h. Next, the cooling bath was removed and stirring was continued for one more hour at room temperature. The mixture was then poured into 2 M aqueous hydrochloric acid (20 mL), extracted with CH_2Cl_2 three times, and the combined organic layers were dried over sodium sulfate and then concentrated. The crude product was purified via recrystallization in ethanol to afford compound **2** (625 mg, 70%) as a light-yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.60 (d, 2H), 8.71 (s, 2H), 8.41 (d, 2H), 8.20 (t, 2H), 4.60 (q, 4H), 1.52 (t, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 188.37, 164.32, 139.07, 129.30, 128.60, 128.25, 127.88, 127.14, 127.04, 126.71, 62.72, 14.22. ESI MS: Calcd. for $C_{24}H_{19}O_6$ ($[M+H]^+$): 403.1180; Found: 403.1176 (m/z).



Compound 3. A aqueous solution of sodium bicarbonate (4.2 g, 50 mmol, 45 mL) was added to a stirred solution of **2** (670 mg, 1.7 mmol) in ethanol (18 mL), and the mixture was stirred at reflux for 16 h. The homogenous solution was cooled to room temperature and poured cautiously into 2 M aqueous hydrochloric acid (45 mL). The precipitate was filtered and washed with water. The crude product was dissolved in acetone to the filter off the insoluble salts, and the solution was evaporated to afford compound **3** (547 mg, 95%) as a light-yellow solid, which was used in the subsequent step without further purification. ^{1}H NMR (400 MHz, acetone-d_6) δ 9.57 (dd, J = 8.1, 2H), 9.01 (s, 2H), 8.70 (dd, J =7.7, 2H), 8.32 (t, 2H). ^{13}C NMR (151 MHz, Acetone-d_6) δ 191.67, 166.82, 140.66, 131.37, 130.81, 129.81, 129.52, 129.02, 128.94, 128.25. MALDI HRMS: Calcd. for $C_{20}H_{10}O_6$ (M$^-$): 346.0479; Found: 346.0482 (m/z).



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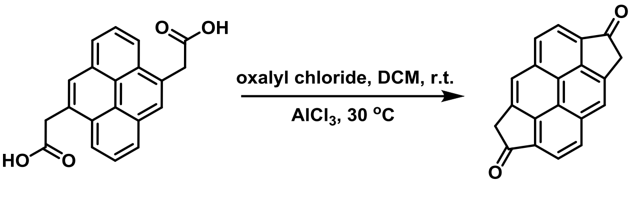
Compound 4.[4] Hypophosphorous acid (50% aqueous solution, 0.58 mL, 1.225 g /mL, 5.4 mmol) was added to a mixture of **3** (670 mg, 1.9 mmol) and sodium iodide (255 mg, 1.7 mmol) in acetic acid (6.7 mL) under nitrogen atmosphere. The mixture was heated at reflux for 16 h. The yellow solution was cooled to room temperature and water (6 mL) was added. The mixture was then filtered and the precipitate was washed with a small amount of ethanol to afford **4** (554 mg, 90%) as a light-yellow solid, which was used in the subsequent step without further purification. ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.53 (br, 2H), 8.44–8.22 (m, 4H), 8.21–8.01 (m, 4H), 4.27 (s, 4H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 173.25, 131.51, 131.09, 130.50, 129.31, 126.77, 125.52, 124.03, 122.20. ESI MS: Calcd. for $C_{20}H_{15}O_4$ ([M+H]$^+$) : 319.0963 ; Found: 319.0964 (m/z).



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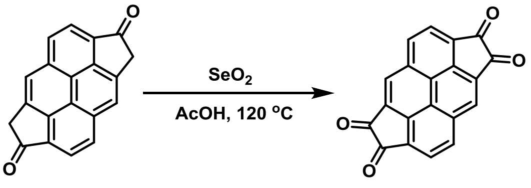
Compound 5. Oxalyl chloride (1.3 mL, 1.5 g/mL, 15.3 mmol) was charged to a stirred solution of **4** (500 mg, 1.5 mmol) in anhydrous CH_2Cl_2 (50 mL). A few drops of anhydrous *N*,*N*-dimethylformamide was added and the mixture was stirred for an hour at room temperature. The solvent was then evaporated to afford a dark yellow solid. To remove the residual oxalyl chloride, additional CH_2Cl_2 (50 mL) was added and then evaporated under reduced pressure. The acid chloride intermediate in anhydrous CH_2Cl_2 (50 mL) was added with $AlCl_3$ (1.2 g, 9.4 mmol) in small portions. After stirring for 3 h at 30 ^{o}C, the reaction mixture was poured over ice. Once the ice was melted, the mixture was filtered. The precipitate was applied to Soxhlet extraction with chloroform overnight. The filtrate was combined with the extracting solution and extracted with chloroform three times. The combined organic layers were dried over anhydrous sodium sulfate and concentrated to afford **5** (266 mg, 60%) as a yellow solid. ^{1}H NMR (500 MHz, $C_2D_2Cl_4$, 363 K) δ 8.45 (q, 4H), 8.14 (s, 2H), 4.12 (s, 4H). ^{13}C NMR spectrum could not be obtained. ESI MS: Calcd. for $C_{20}H_{11}O_2$ ($[M+H]^+$) : 283.0753 ; Found: 283.0756 (m/z).



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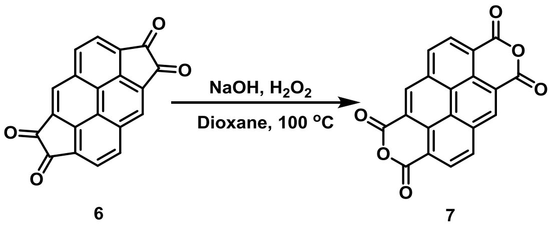
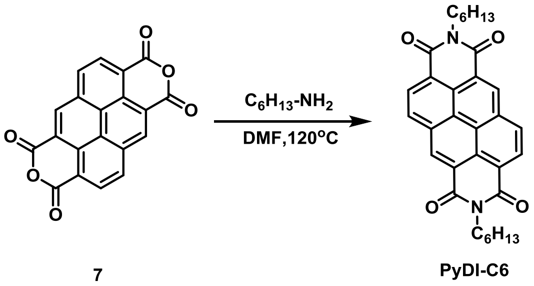
Compound 6. Selenium dioxide (2.3 g, 21 mmol) was added to a stirred solution of **5** (600 mg, 2.1 mmol) in acetic acid (40 mL). The mixture was heated at reflux for 16 h. The solution was cooled to room temperature with water (120 mL) added to it, and the mixture was then filtered. The precipitate was washed with a small amount of ethanol to afford **6** (593 mg) as a dark red solid, which was applied to the subsequent step without further purification. The compound is insoluble in common organic solvents, so the NMR data are not available.

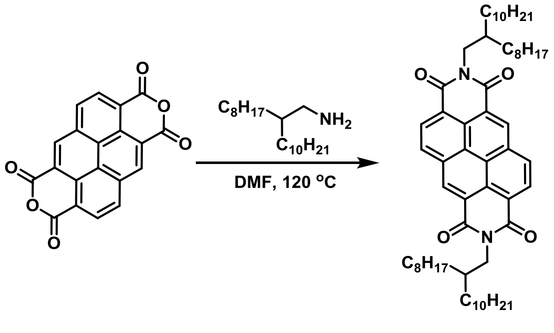


Compound 7. A solution of **6** (600 mg, 1.9 mmol) in dioxane (60 mL) was added with an aqueous solution of sodium hydroxide (4.8 g, 120 mmol) with stirring and then heated to 100 ^{o}C. An aqueous solution of hydrogen peroxide (30%, 44 mL, 1.11 g/mL, 1.43 mol) was added dropwise to the stirred mixture at 100 ^{o}C over 30 min. Aqueous hydrochloric acid (40 mL) was then added at room temperature until the red precipitates were no longer produced. The mixture was filtered and the precipitate was dried to afford a red solid of **7** (595 mg), which was applied to the subsequent step without further purification.



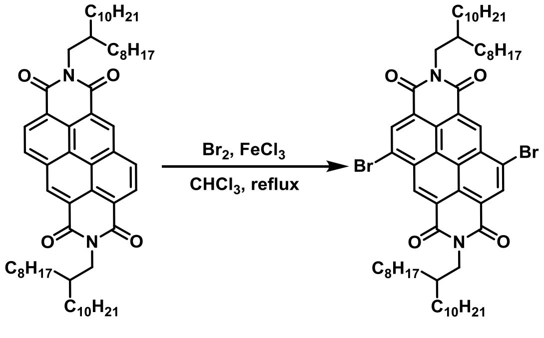
PyDI-C6. A solution of hexylamine (0.2 mL, 0.76 g/mL, 1.5 mmol) in *N*,*N*-dimethylformamide (DMF, 2 mL) was added to the solution of **7** (50 mg, 0.15 mmol) in DMF (2 mL) under a nitrogen atmosphere. The reaction mixture was heated at 120 ^{o}C overnight, and then cooled and diluted with water. The mixture was extracted with chloroform three times. The combined organic layers were washed with water and dried over anhydrous sodium sulfate. After concentrated under reduced pressure, the residue was purified with column chromatography of silica gel eluted with dichloromethane to offer **PyDI-C6** (30 mg, **5** to **PyDI-C6** yield 30%) as a yellow solid. ^{1}H NMR (500 MHz, $C_2D_2Cl_4$, 363 K) δ 9.39 (s, 2H), 9.09 (d, 2H), 8.74 (d, 2H), 4.35 (t, 4H), 1.88–1.91 (m, 4H), 1.54–1.59 (m, 4H), 1.48–1.39 (m, 8H), 0.98

(t, 6H). ^{13}C NMR spectrum could not be obtained due to the low solubility of the compound. MALDI HRMS: Calcd. for $C_{32}H_{33}N_2O_4$ ($[M+H]^+$): 509.2434; Found: 509.2414 (m/z).



7 PyDI-C8,12

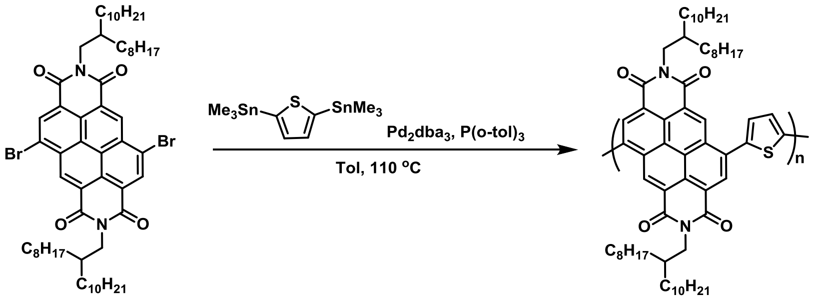
PyDI-C8,12. A similar procedure for **PyDI-C6** was followed, with 2-octyldodecan-1-amine replacing hexylamine. The column chromatography was eluted with dichloromethane/hexane (v/v=2:3) to give **PyDI-C8,12** (434 mg, **5** to **PyDI-C8,12** yield 30%) as a yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.33 (s, 2H), 9.03 (d, 2H), 8.69 (d, 2H), 4.24 (t, 4H), 2.13–2.01 (m, 2H), 1.49–1.10 (m, 64H), 0.80-0.86 (m, 12H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 164.20, 164.02, 134.10, 132.96, 130.07, 128.41, 126.39, 124.08, 123.62, 122.92, 45.02, 36.73, 31.89, 31.77, 30.05, 29.64, 29.33, 29.32, 29.30, 26.53, 22.68, 22.65, 14.11. MALDI HRMS: Calcd. for $C_{60}H_{89}N_2O_4$ ($[M+H]^+$): 901.6779; Found: 901.6816 (m/z). Elem. Anal.: Calcd. for $C_{60}H_{88}N_2O_4$: C, 79.95; H, 9.84; N, 3.11; O, 7.10. Found: C, 79.60; H, 10.16; N, 2.92; O, 7.32



PyDI-C8,12 diBr-PyDI

diBr-PyDI. To a solution of mixed Br_2 (0.34 mL, 3.12 g/mL, 6.6 mmol) and **PyDI-C8,12** (300 mg, 0.33 mmol) in chloroform (4 ml) was added ferric chloride (5 mg, 0.033 mmol). After stirring for 16 hours at 85 ℃, the reaction was quenched at 0

^{o}C by adding aqueous sodium thiosulfate (10 ml). The mixture was extracted with dichloromethane three times, and the combined organic layers were washed with water and dried over anhydrous sodium sulfate. After concentrated under reduced pressure, the residue was purified with column chromatography of silica gel eluted with dichloromethane/hexane (v/v=1:2) to afford **diBr-PyDI** (211 mg, 60%) as a red solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.57 (s, 2H), 9.21 (s, 2H), 4.23 (d, 4H), 2.04–2.06 (m, 2H), 1.46–1.17 (m, 64H), 0.82-0.86 (m, 12H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 163.04, 162.76, 132.93, 132.81, 132.22, 126.54, 125.22, 124.73, 124.33, 123.21, 45.27, 36.75, 31.89, 31.87, 31.79, 30.02, 29.63, 29.61, 29.56, 29.31, 29.29, 26.52, 22.65, 22.64, 14.07. MALDI HRMS: Calcd. for $C_{60}H_{87}Br_2N_2O_4$ ($[M+H]^+$): 1057.4931; Found: 1057.5027 (m/z).

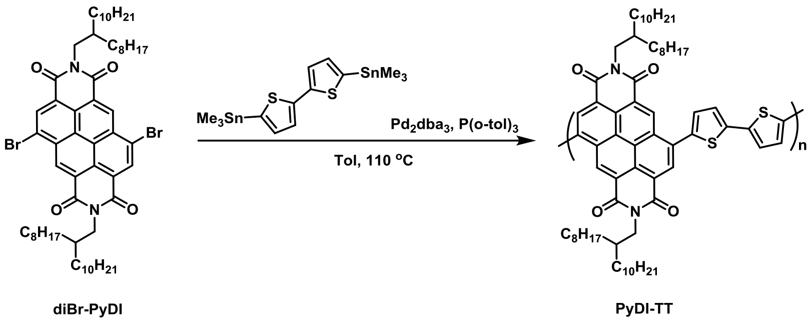


diBr-PyDI

PyDI-T

PyDI-T. A Schlenk tube charged with **diBr-PyDI** (50 mg, 0.047 mmol), 2,5-bis(trimethylstannyl)thiophene (19 mg, 0.047 mmol), $Pd_2(dba)_3$ (2.1 mg, 0.0023 mmol), and P(*o*-tol)$_3$ (2.9 mg, 0.0094 mmol) was evacuated and back-filled with nitrogen three times, and then toluene (2 mL) was added via a syringe under nitrogen atmosphere. The reaction vessel was sealed and stirred at 110 ^{o}C for 96 h. Upon cooling to room temperature, the polymer was precipitated by dispersing in methanol (50 mL). The obtained deep red solid was purified by eluting from size exclusion chromatography column filled with Bio-Beads S-X1 Beads. After concentrated under reduced pressure, the solid residue was re-dissolved in chloroform (2 mL) and dispersed slowly into methanol (50 mL). The precipitates were collected by filtration, washed with methanol, and dried under reduced pressure to give **PyDI-T** (38 mg, 80%) as a deep red solid. M_n = 44.8 kDa, M_w = 151.0 kDa, PDI = 3.38. ^{1}H NMR (500

MHz, $CDCl_3$) δ 9.36 (br, 4H), 8.29 (br, 2H), 4.06 (br, 4H), 1.99 (br, 2H), 1.51–0.97 (m, 64H), 0.81 (br, 12H).



PyDI-TT. A Schlenk tube charged with **diBr-PyDI** (50 mg, 0.047mmol), 5,5'-bis(trimethylstannyl)-2,2'-bithiophene (23 mg, 0.047mmol), $Pd_2(dba)_3$ (2.1 mg, 0.0023 mmol), and P(*o*-tol)$_3$ (2.9 mg, 0.0094 mmol) was evacuated and back-filled with nitrogen three times, and then toluene (2 mL) was added via a syringe under nitrogen atmosphere. The reaction mixture was sealed and stirred at 110 ℃ for 96 h. Upon cooling to room temperature, the reaction mixture was dispersed in methanol (50 mL). The deep red precipitates were eluted from a size exclusion chromatography column filled with Bio-Beads S-X1 Beads, and then concentrated under reduced pressure. The solid residue was re-dissolved in chloroform (2 mL) and dispersed slowly into methanol (50 mL). The precipitates were collected by filtration, washed with methanol, and dried under reduced pressure to offer **PyDI-TT** (41 mg, 80%) as a deep green solid. M_n = 52.4 kDa, M_w = 151.9 kDa, PDI = 2.89. ^1H NMR (500 MHz, $CDCl_3$) δ 9.44 (br, 2H), 8.95 (br, 2H), 8.06–7.38 (m, 4H), 4.31 (br, 4H), 2.14 (br, 2H), 1.46–1.04 (m, 64H), 0.97–0.62 (m, 12H).

3. Single-Crystal X-Ray Analysis

Table S1 Crystal Data and Structure Refinement for PyDI-C6

Empirical formula	$C_{32}H_{32}N_2O_4$
Formula weight	508.59
Temperature/K	169.99(10)
Crystal system	triclinic
Space group	P-1
a/Å	4.7923(10)
b/Å	9.0337(12)
c/Å	14.831(2)
α /°	101.002(11)
β /°	94.467(15)
γ /°	96.830(14)
Volume/$Å^3$	622.44(18)
Z	1
$\rho_{calc}g/cm^3$	1.357
μ/mm^{-1}	0.716
F(000)	270.0
Crystal size/mm^3	0.25 × 0.09 × 0.08
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	6.104 to 151.946
Index ranges	$-6 \leqslant h \leqslant 5, -11 \leqslant k \leqslant 11, -13 \leqslant l \leqslant 18$
Reflections collected	6435
Independent reflections	2402 [R_{int} = 0.0520, R_{sigma} = 0.0438]
Data/restraints/parameters	2402/102/202
Goodness-of-fit on F^2	1.065
Final R indexes [I>=2σ (I)]	R_1 = 0.0809, wR_2 = 0.2237
Final R indexes [all data]	R_1 = 0.0998, wR_2 = 0.2426
Largest diff. peak/hole / e $Å^{-3}$	0.37/-0.34

4. Electrochemical Characterizations

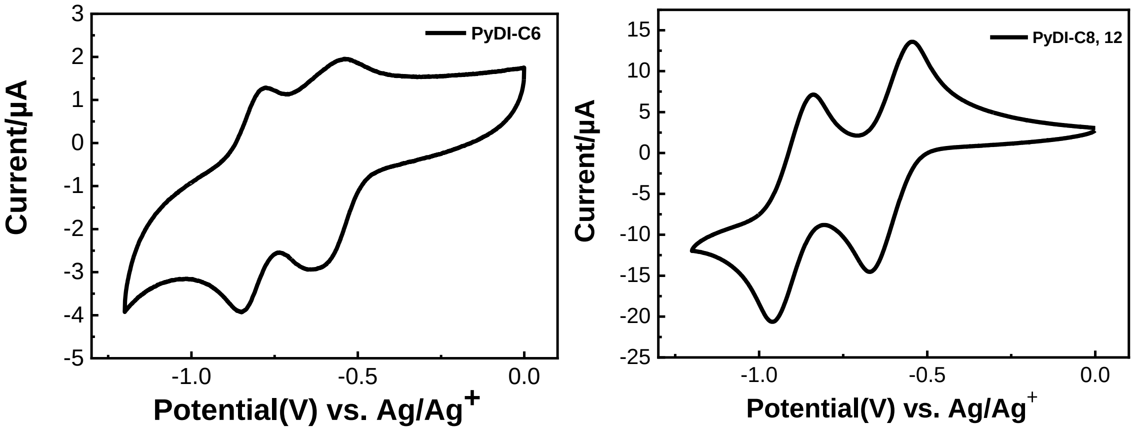


Figure S1. Cyclic voltammograms of **PyDI-C6** and **PyDI-C8,12.**

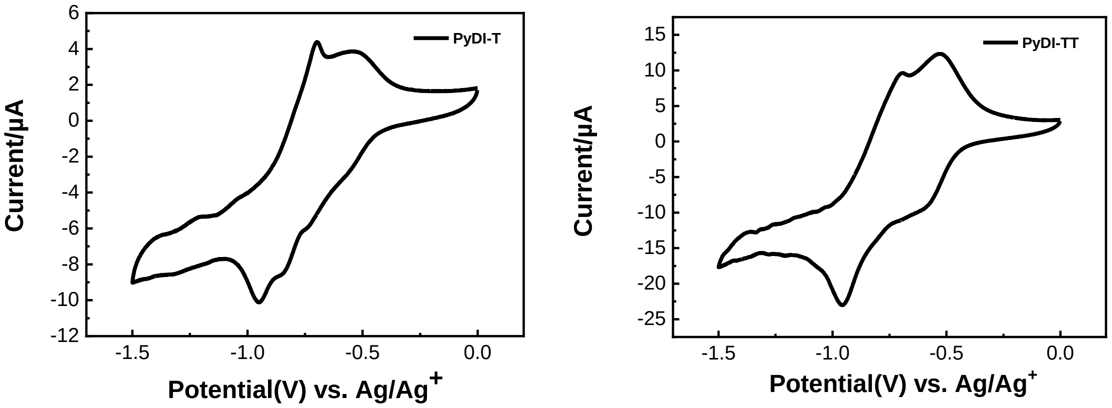


Figure S2. Cyclic voltammograms of **PyDI-T** and **PyDI-TT.**

5. Thermal Properties

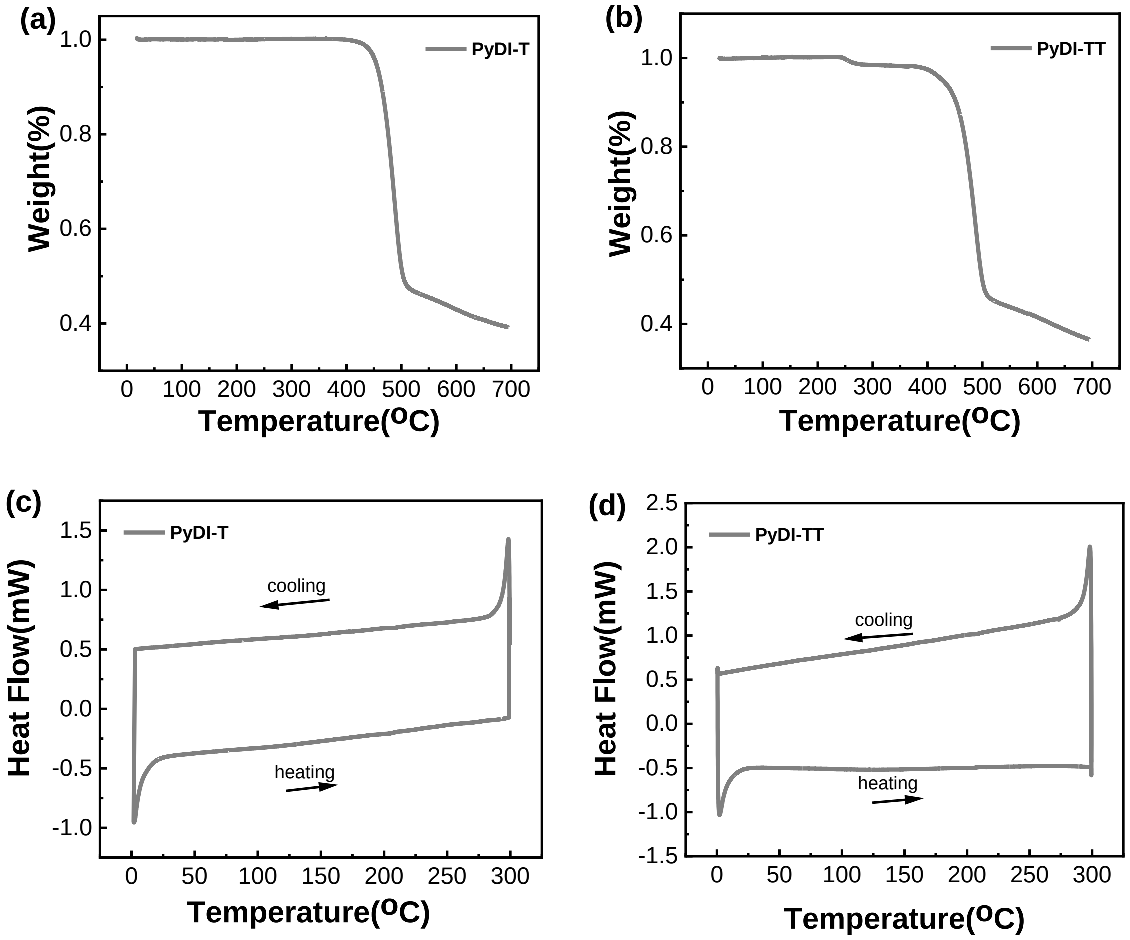


Figure S3. TGA (a and b) DSC (c and d) profiles for **PyDI-T** (a/c) and **PyDI-TT** (b/d).

6. Absorption Spectra

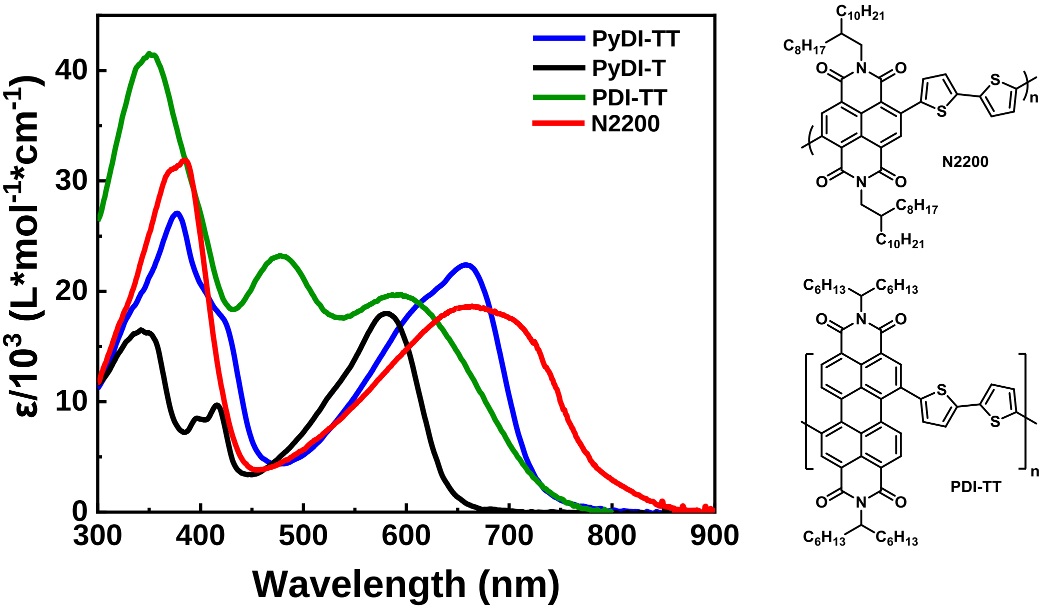


Figure S4. Absorption spectra of **PyDI-T** and **PyDI-TT** in chloroform solution (1×10^{-5} M), in comparison to those of **N2200** and **PDI-TT**.

7. Theoretical Calculations

Density functional theory (DFT) calculations at the B3LYP/6-31G(d,p) level[5] were performed with **PyDI**, **PyDI-T**, **PyDI-TT**. For comparison, corresponding calculations were also performed with **N2200** and **PDI-TT** using the same method, and the results of **N2200** and **PDI-TT** were in agreement with previous studies with similar backbones.[6-8] Time-dependent DFT (TD-DFT) calculations were performed with **PyDI-T** and **PyDI-TT** using Gaussian 09 program with CAM-B3LYP/6-31G(d,p). The orbital pictures were prepared using Gaussview, the hole and electron distributions were calculated with Multiwfn.[9,10] All long alkyl substituents were replaced with methyl groups in the calculations.

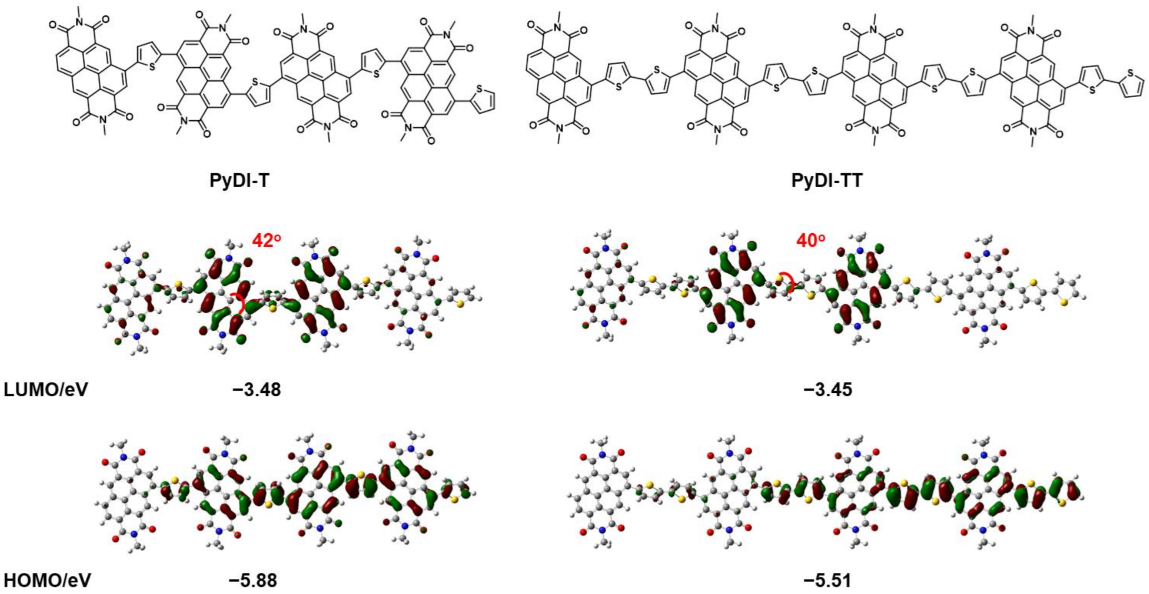


Figure S5. DFT-optimized molecular geometries of **PyDI-T** and **PyDI-TT** with frontier molecular orbitals and energy levels

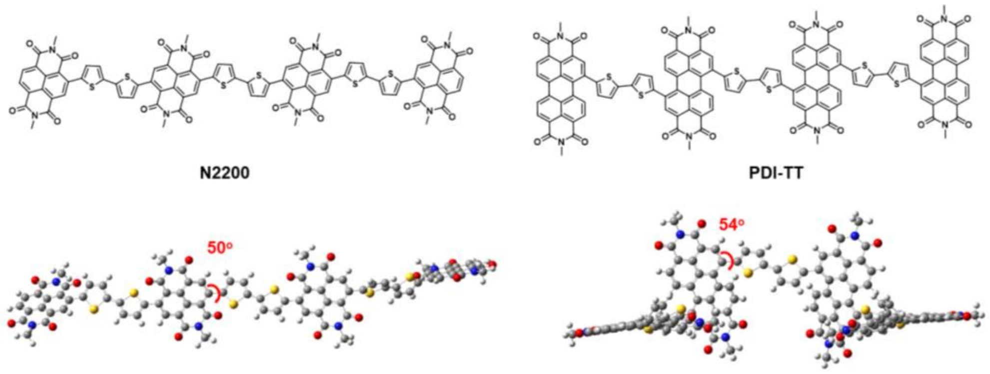
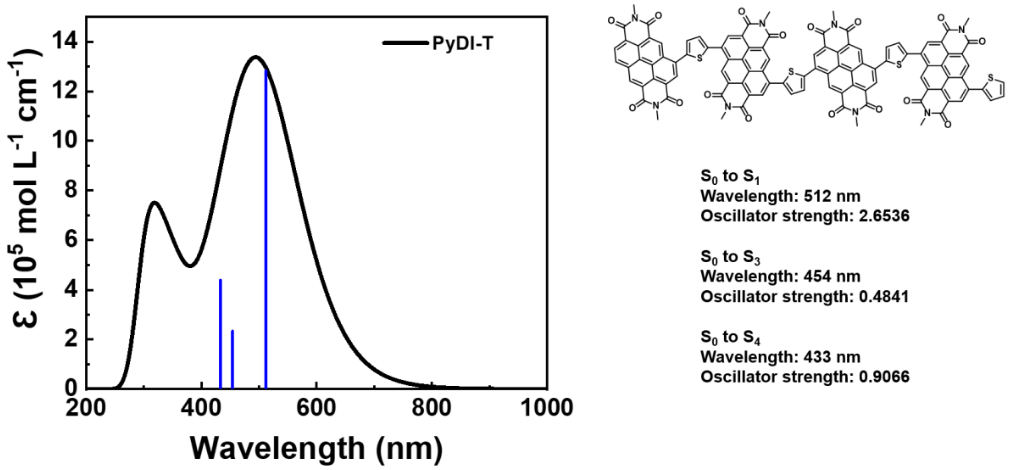


Figure S6. DFT-optimized molecular geometries of **N2200** and **PDI-TT**.



S_0 to S_1
Wavelength: 512 nm
Oscillator strength: 2.6536

S_0 to S_3
Wavelength: 454 nm
Oscillator strength: 0.4841

S_0 to S_4
Wavelength: 433 nm
Oscillator strength: 0.9066

Figure S7. TD-DFT (CAM- B3LYP/6-31G(d,p)) calculations of **PyDI-T**

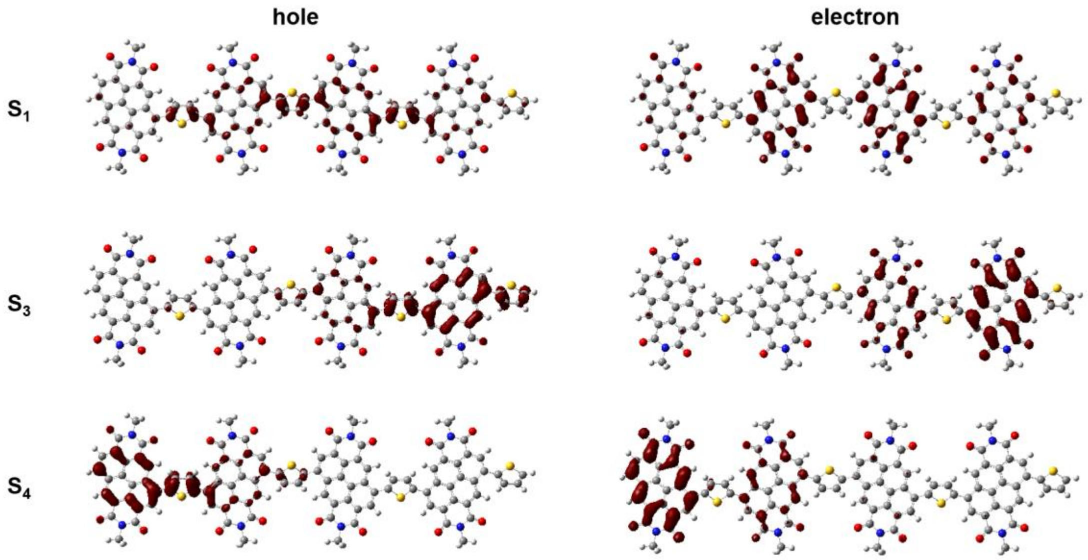
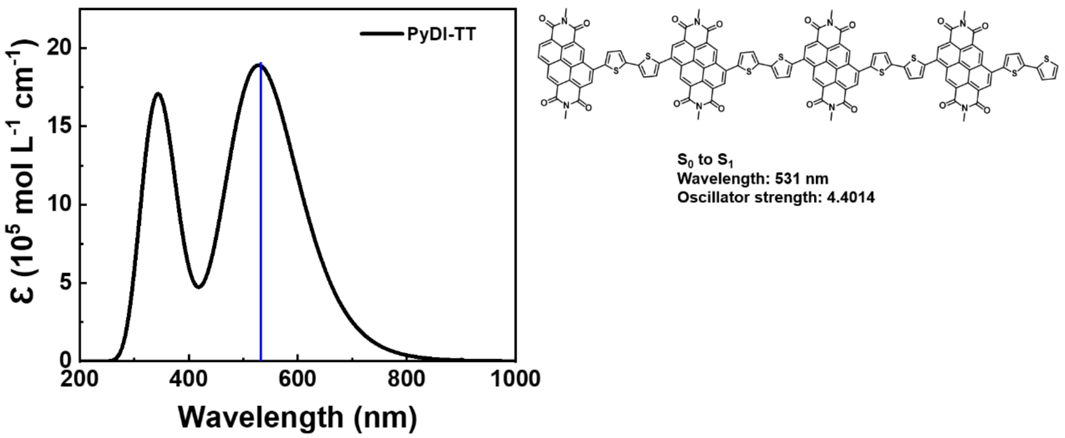


Figure S8. The hole and electron distributions of **PyDI-T** in the corresponding excited states.



S_0 to S_1
Wavelength: 531 nm
Oscillator strength: 4.4014

Figure S9. TD-DFT (CAM- B3LYP/6-31G(d,p)) calculations of **PyDI-TT**

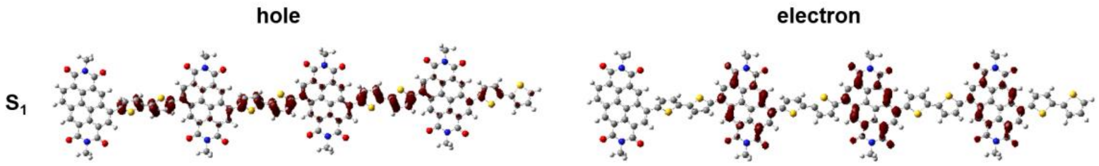


Figure S10. The hole and electron distributions of **PyDI-TT** in the excited state.

8. OFET Device Fabrication and Characterizations

PyDI-T and **PyDI-TT** were dissolved in *o*-chlorobenzene (ODCB) and heated at 80 ^{o}C overnight, and then the solution (4 mg/mL in ODCB) was filter through a 0.45 μm aperture. All wafers were sequentially cleaned with acetone, detergent, deionized water (three times) and isopropyl alcohol using ultra sonication and then dried under vacuum at 80 ^{o}C.

For n-channel FETs, a top-gate/bottom-contact (TG/BC) device configuration was used. The patterned Au/SiO_2/Si substrates were immersed in a phenylethanethiol solution (5 mM in anhydrous toluene) for 4 h to construct the self-assembled monolayers, followed by washing with anhydrous toluene and isopropyl alcohol. The semiconducting layer was deposited by spin-coating the polymer solution onto the patterned Au/SiO_2/Si substrate with SAM at 1500 rpm/min, followed by thermal annealing at 180 ^{o}C for 5 min. A CYTOP solution was spin-coated as the dielectric layer. Before thermal annealing at 100 ^{o}C for 1 h, an aluminum layer was thermally evaporated as the gate electrode. The devices were characterized in the air with an Agilent B2912A Semiconductor Analyzer. The electron mobility in the saturation region was calculated according to the following equation: $I_D = (W/2L)C_i\mu(V_G - V_T)^2$ Where ID is the drain current, W and L are the device channel width and length, C_i is the gate dielectric layer capacitance per unit area, μ is the carrier mobility, V_G and V_T are gate voltage and threshold voltage.

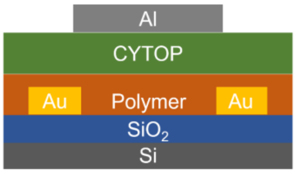


Figure S11. The TG/BC OFET device architecture.

9. GIWAXS Measurements

The GIWAXS data were obtained at beamline BL14B1 of the Shanghai Synchrotron Radiation Facility at a wavelength of 1.2398 Å. BL14B1 is a beamline based on bending magnet and a Si(111) double crystal monochromator was employed to monochromatize the beam. The size of the focus spot is about 0.5 mm and the end station was equipped with a Huber 5021 diffractometer. NaI scintillation detector was used for data collection.

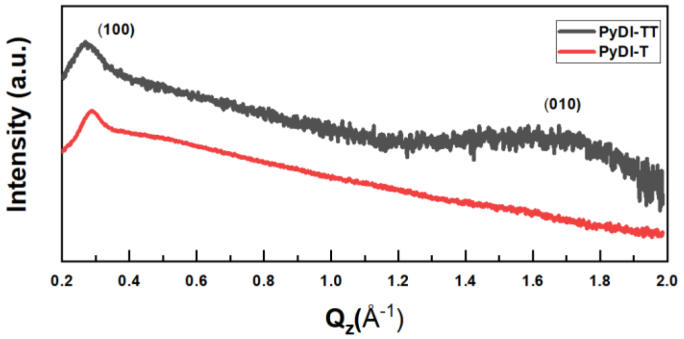


Figure S12. Out-of-plane scattering profiles of **PyDI-T** and **PyDI-TT** films

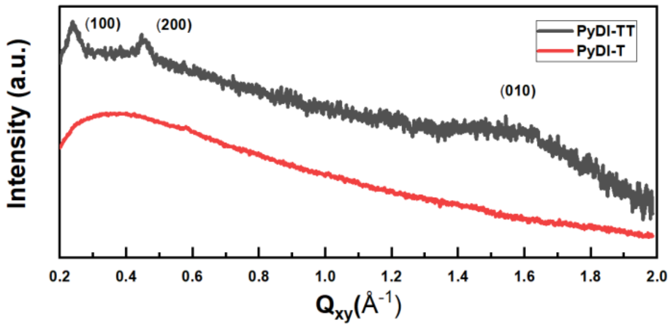
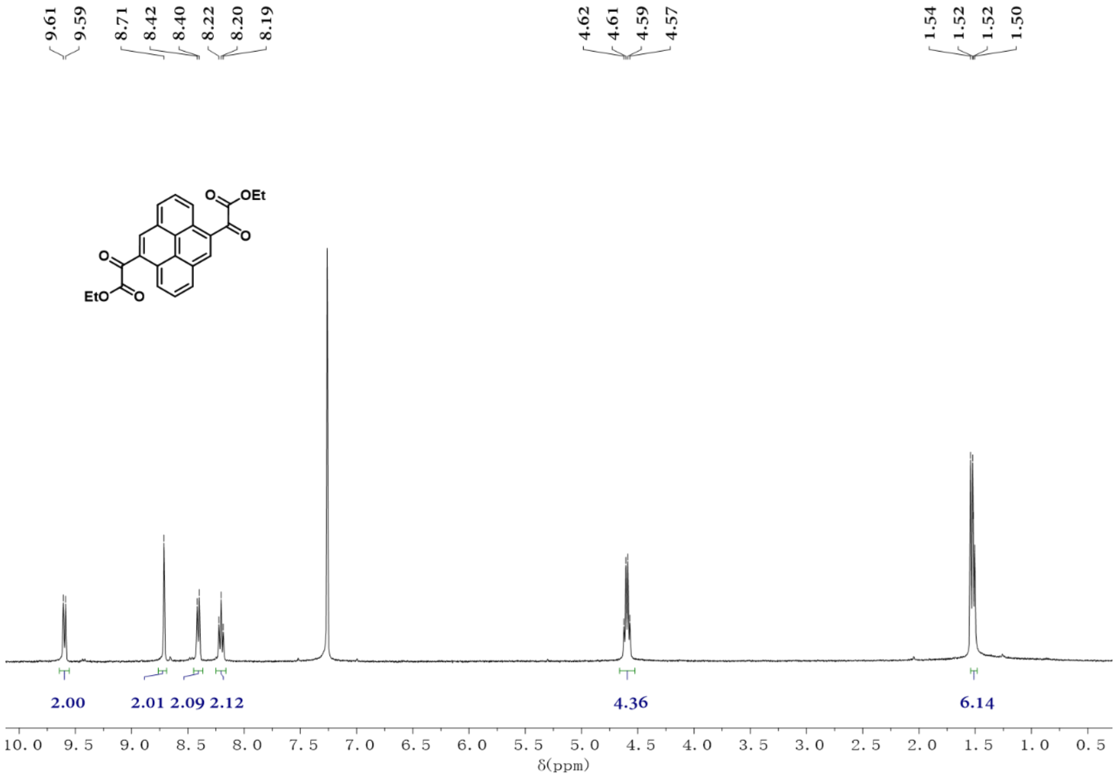


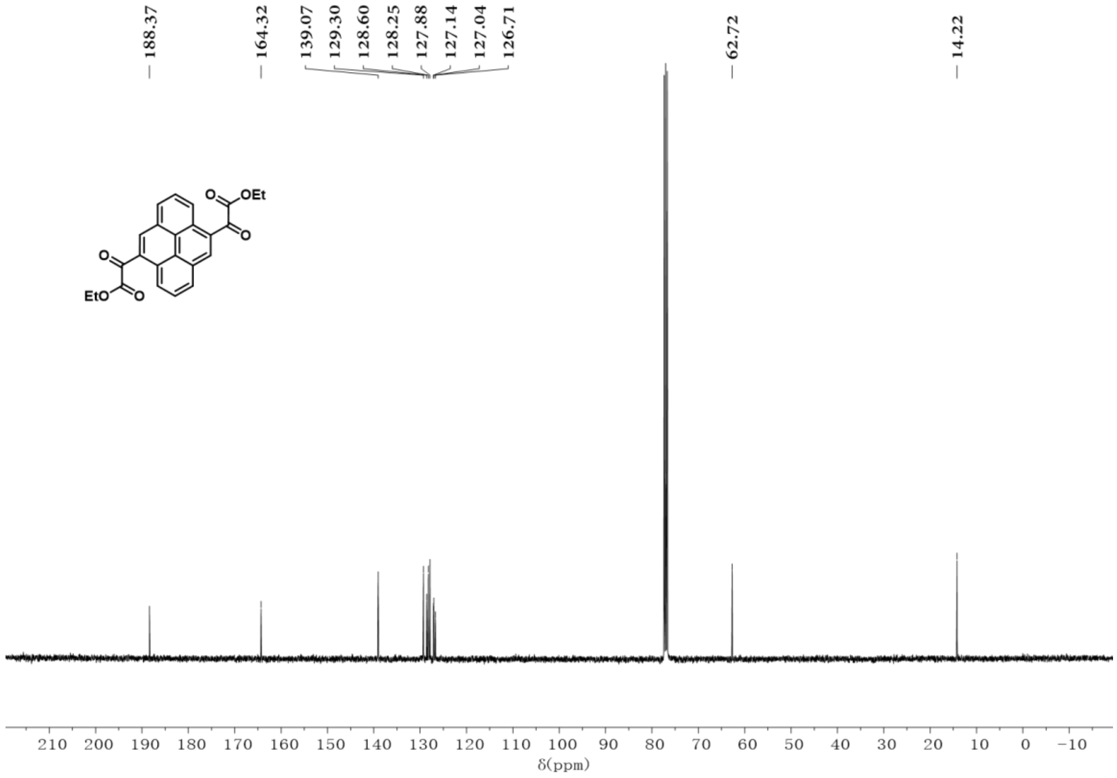
Figure S13. In-plane scattering profiles of **PyDI-T** and **PyDI-TT** films

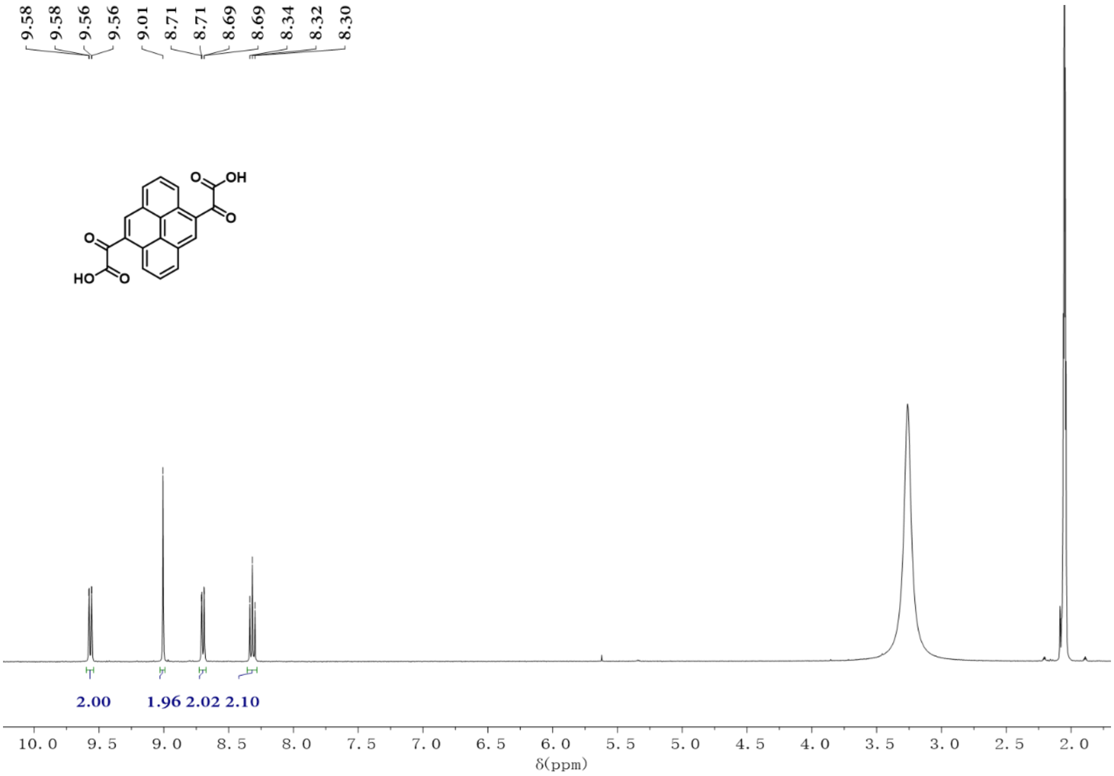
Table S2. Data from GIWAXS of **PyDI-T** and **PyDI-TT** Films

Polymer	**In plane (nm)**		**Out of plane (nm)**	
	lamellar	**π-π**	**lamellar**	**π-π**
PyDI-T	N.A.	N.A.	2.23	N.A.
PyDI-TT	2.62	0.39	2.35	0.37

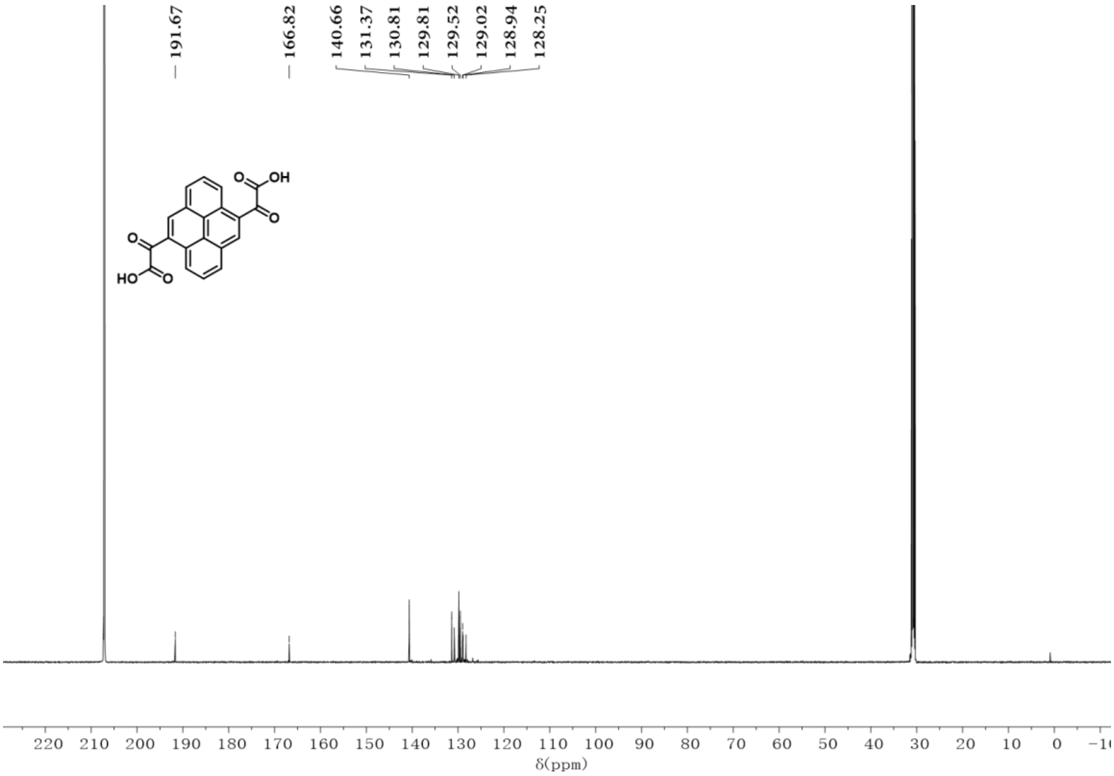
10. Copies of ^{1}H and ^{13}C NMR Spectra







9.58
9.58
9.56
9.56
9.01
8.71
8.71
8.69
8.69
8.34
8.32
8.30
O
OH
O
O
HO
O
2.00
1.96
2.02
2.10
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
δ(ppm)



191.67
166.82
140.66
131.37
130.81
129.81
129.52
129.02
128.94
128.25
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O
O
HO
O
220
210
200
190
180
170
160
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120
110
100
90
80
70
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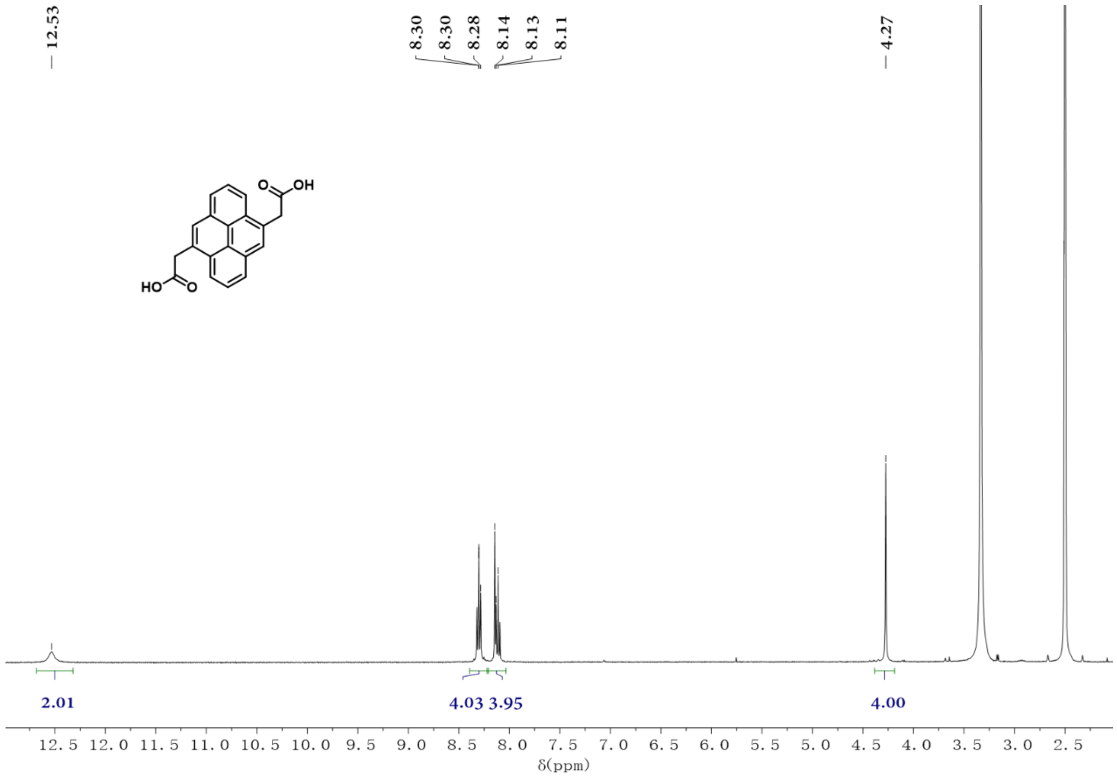
50
40
30
20
10
0
−1
δ(ppm)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8.28
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8.13
8.11
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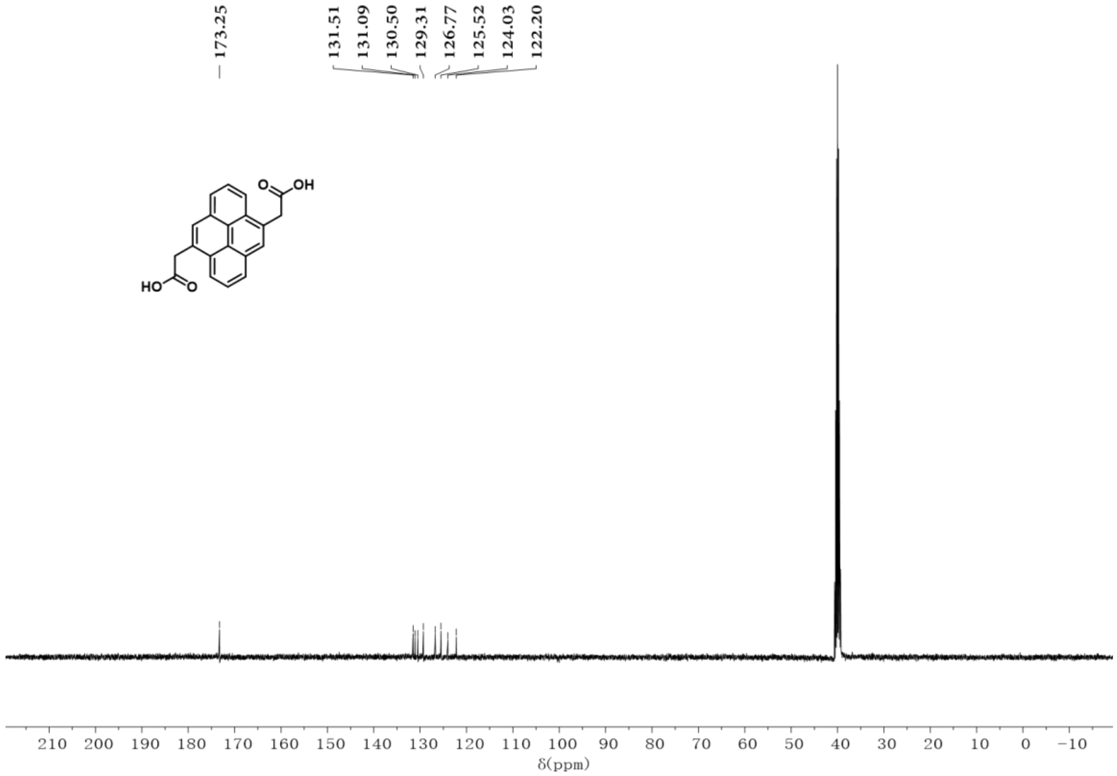
OH
HO
O
2.01
4.03
3.95
4.00
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5
δ(ppm)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131.09
130.50
129.31
126.77
125.52
124.03
122.20
O
OH
HO
O
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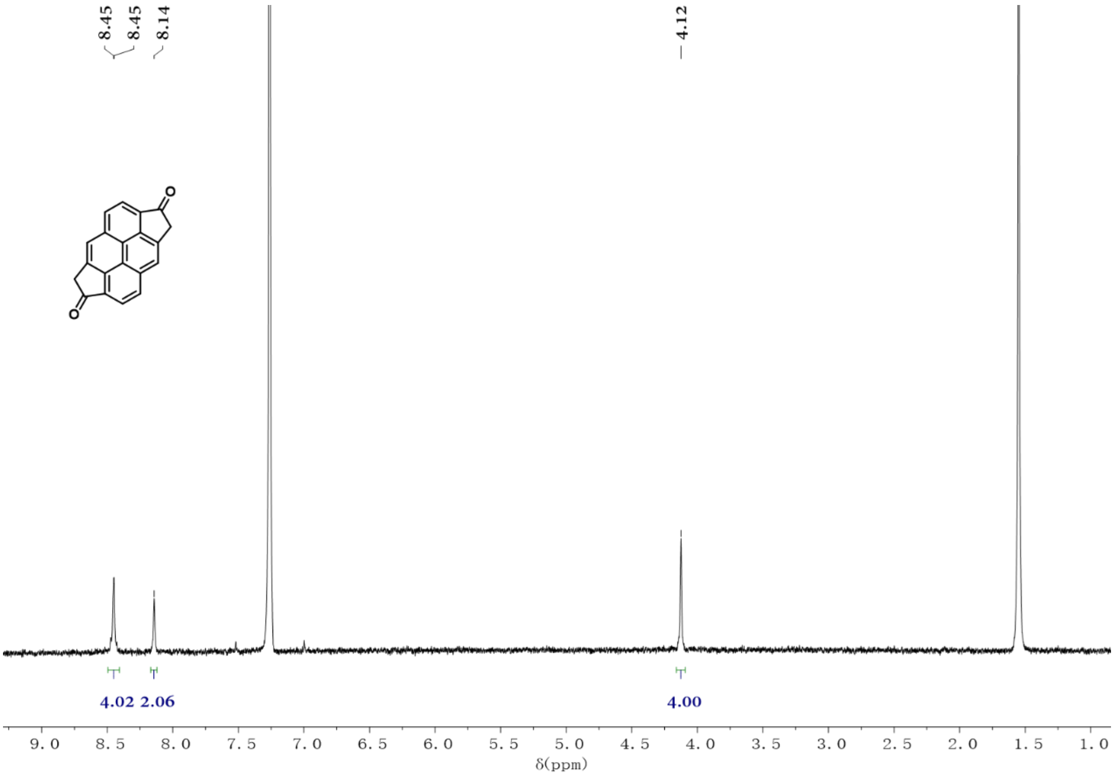
δ(ppm)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8.45
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4.12
O
O
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2.06
4.00
9.0
8.5
8.0
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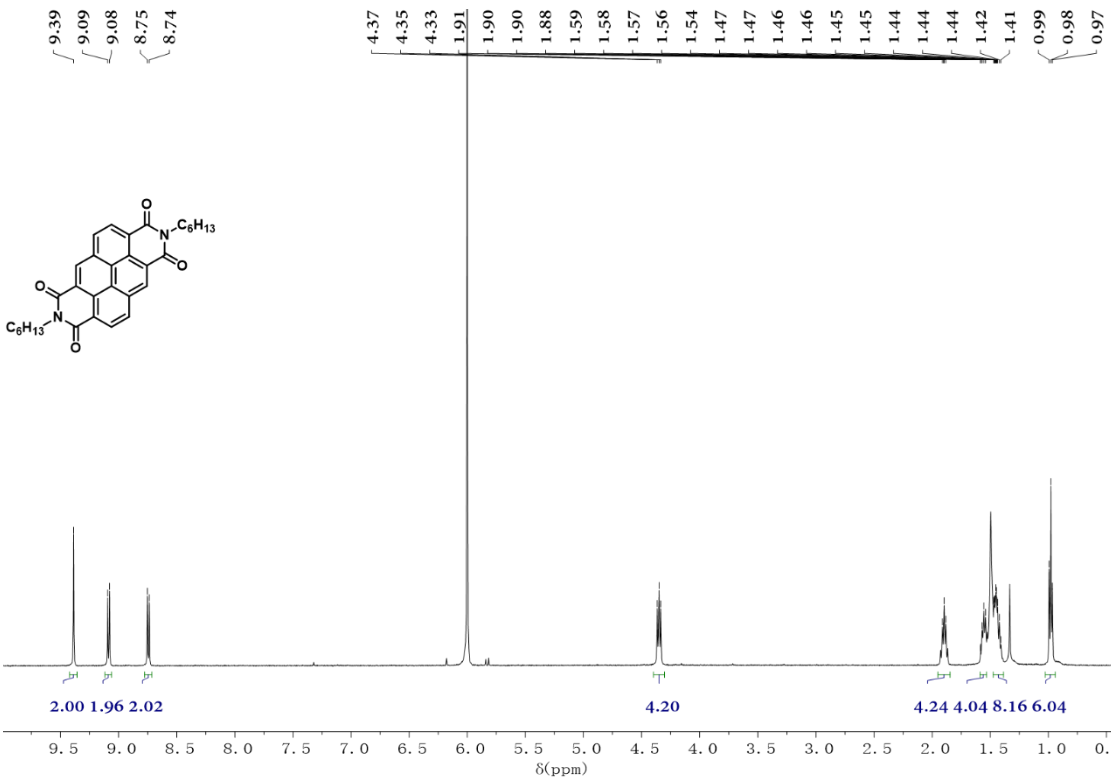
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
δ(ppm)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1.58
1.57
1.56
1.54
1.47
1.47
1.46
1.46
1.45
1.45
1.44
1.44
1.44
1.42
1.41
0.99
0.98
0.97
O
O
O
O
N
N
C6H13
C6H13
2.00
1.96
2.02
4.20
4.24
4.04
8.16
6.04
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
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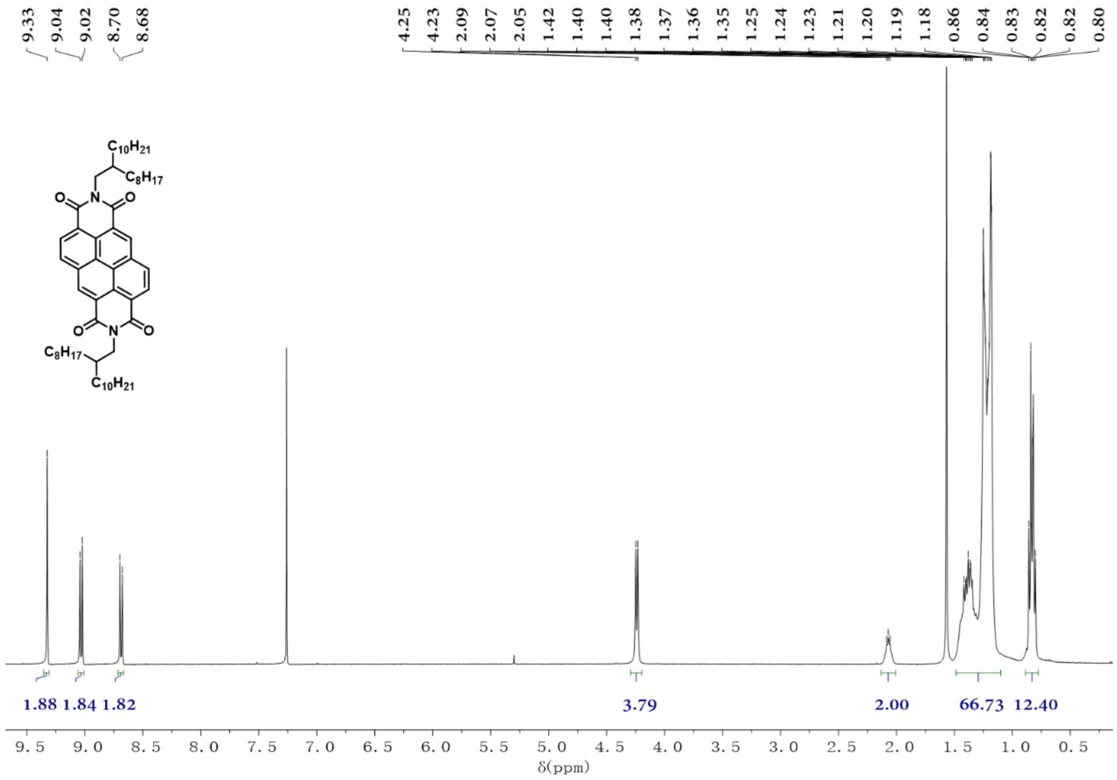
1.0
0.
δ(ppm)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1.38
1.37
1.36
1.35
1.25
1.24
1.23
1.21
1.20
1.19
1.18
0.86
0.84
0.83
0.82
0.82
0.80
C10H21
C8H17
O
N
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3.79
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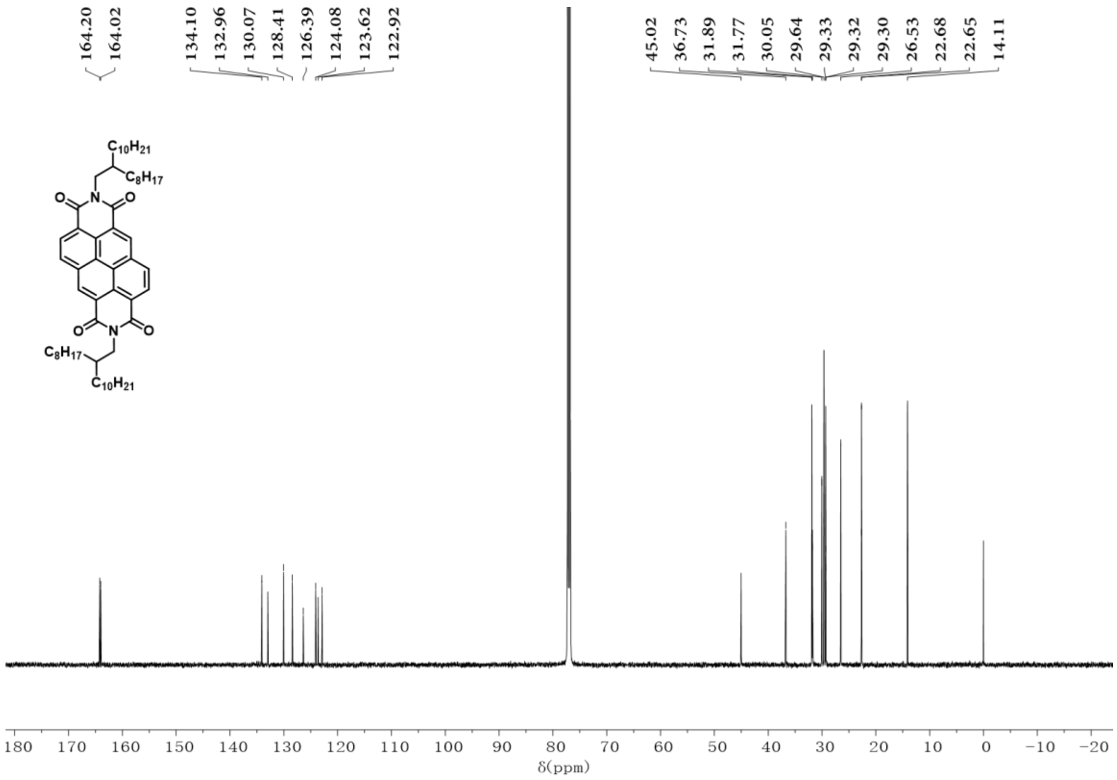
δ(ppm)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31.77
30.05
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29.33
29.32
29.30
26.53
22.68
22.65
14.11
C10H21
C8H17
O
N
180
170
160
150
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100
90
80
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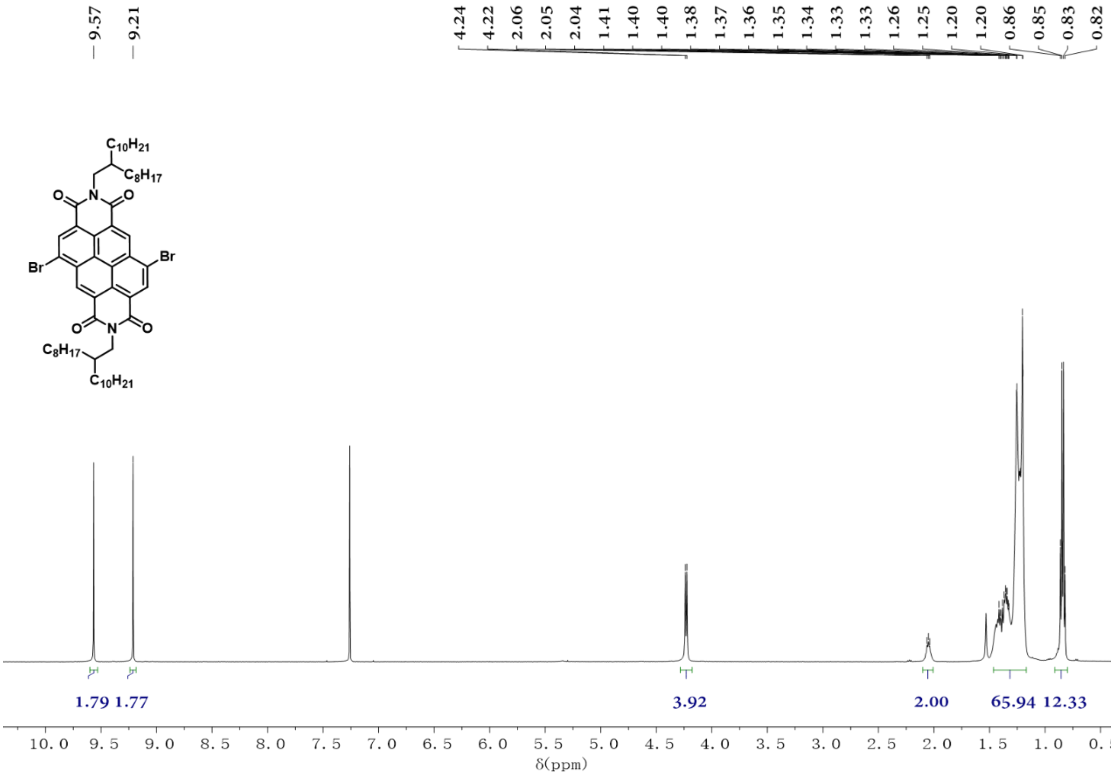
−20
δ(ppm)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1.35
1.34
1.33
1.33
1.26
1.25
1.20
1.20
0.86
0.85
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0.82
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C8H17
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N
Br
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2.00
65.94
12.33
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0
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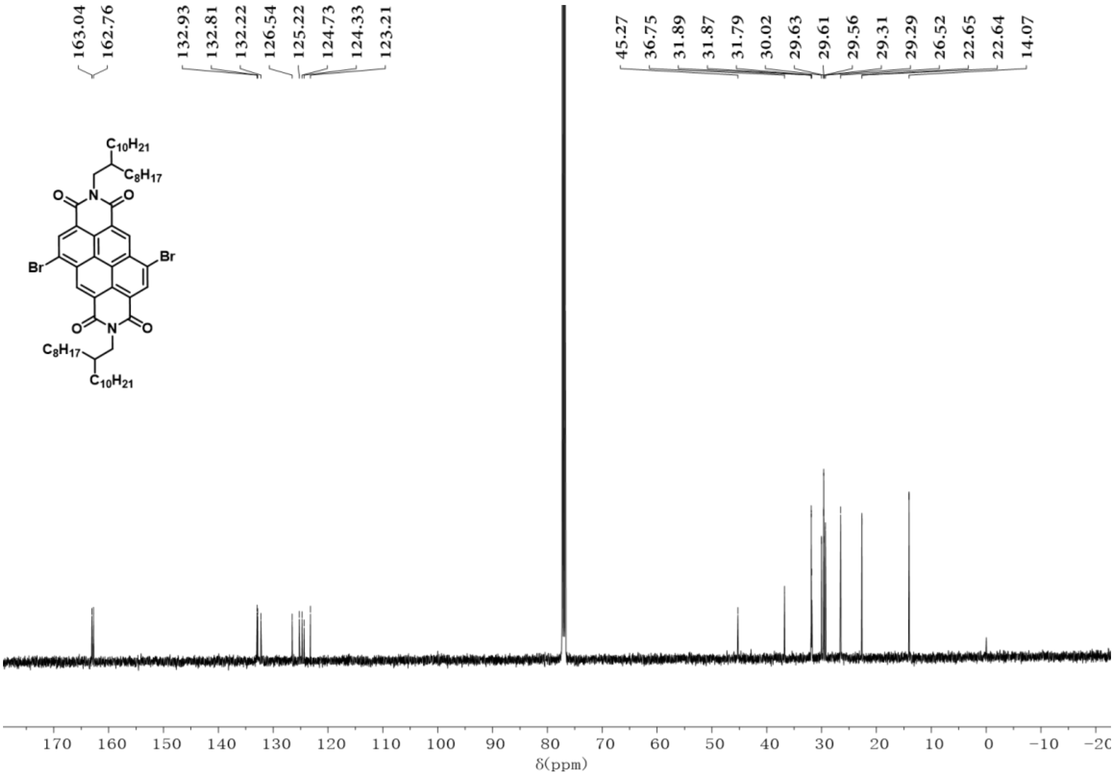
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29.63
29.61
29.56
29.31
29.29
26.52
22.65
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O
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Br
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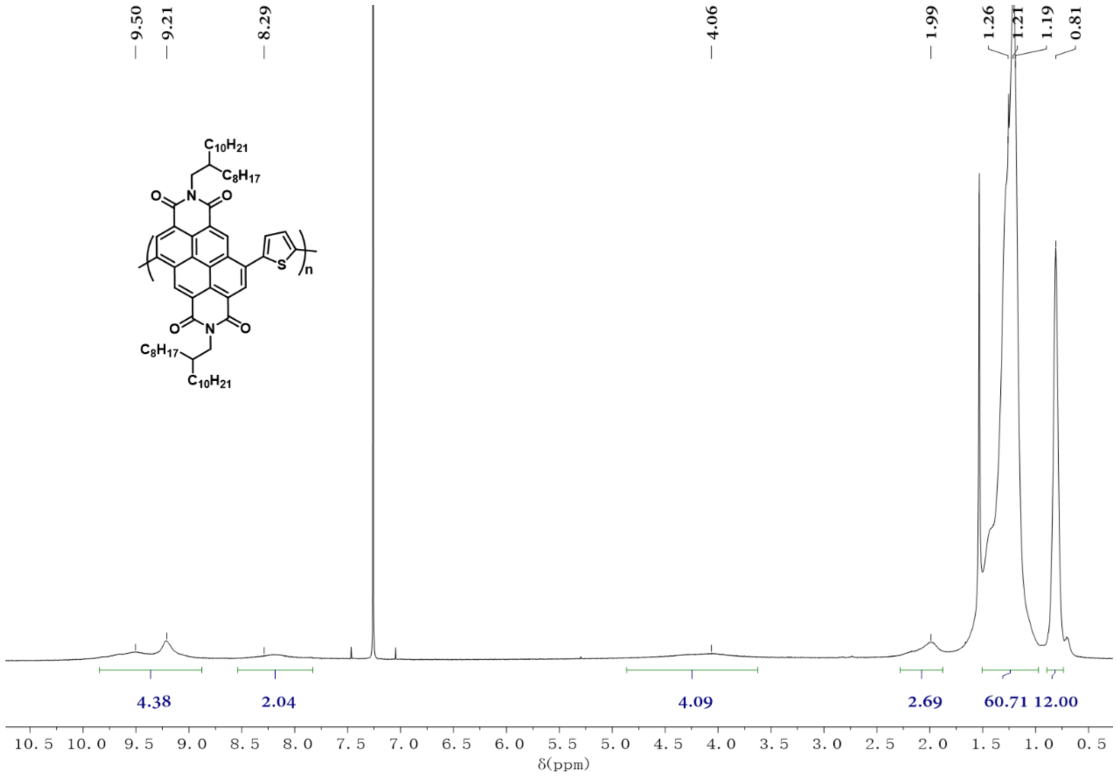
δ(ppm)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N
O
S
n
4.38
2.04
4.09
2.69
60.71
12.00
10.5
10.0
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9.0
8.5
8.0
7.5
7.0
6.5
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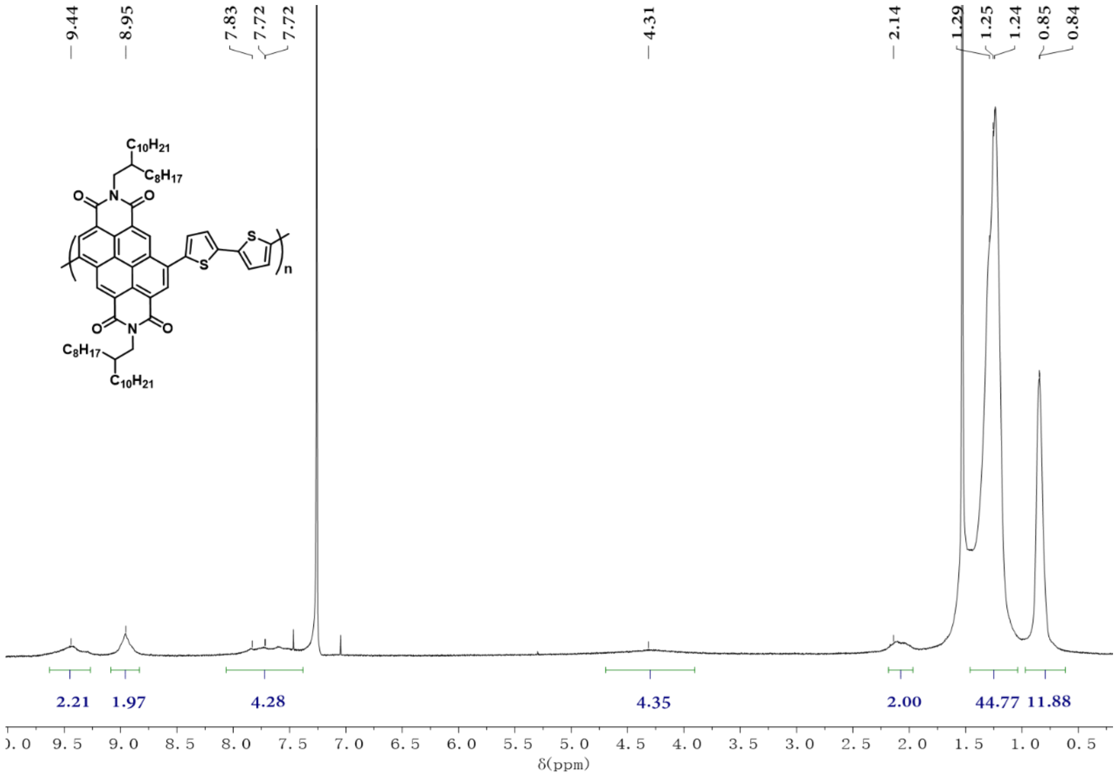
δ(ppm)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C8H17
O
N
O
S
S
n
2.21
1.97
4.28
4.35
2.00
44.77
11.88
9.5
9.0
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8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
δ(ppm)

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