# Significant Improvement of Semiconducting Performance of the Diketopyrrolopyrrole-Quaterthiophene Conjugated Polymer through Side-Chain Engineering via Hydrogen-Bonding

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## 1. Thermogravimetric Analysis (TGA) and Differential Scanning Calorimetry (DSC) Curves

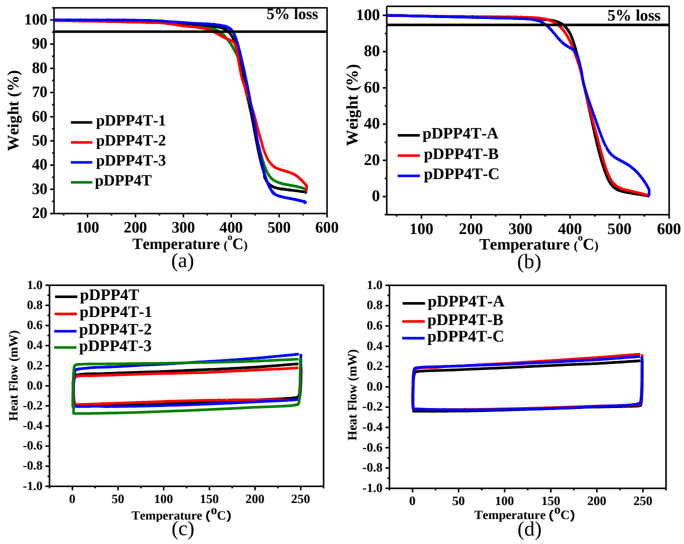



**Figure S1**. (a-b) TGA curves of **pDPP4T-1**, **pDPP4T-2**, **pDPP4T-3**, **pDPP4T**, **pDPP4T-A**, **pDPP4T-B** and **pDPP4T-C**: heating rate: 10 °C/min. From 25 °C to 550 °C under nitrogen atmosphere; (c-d) DSC curves (endo up) of **pDPP4T-1**, **pDPP4T-2**, **pDPP4T-3**, **pDPP4T**, **pDPP4T-A**, **pDPP4T-B** and **pDPP4T-C** recorded at a heating and cooling rate (0-250 °C) of 10 °C/min under nitrogen.

## 2. Cyclic Voltammograms

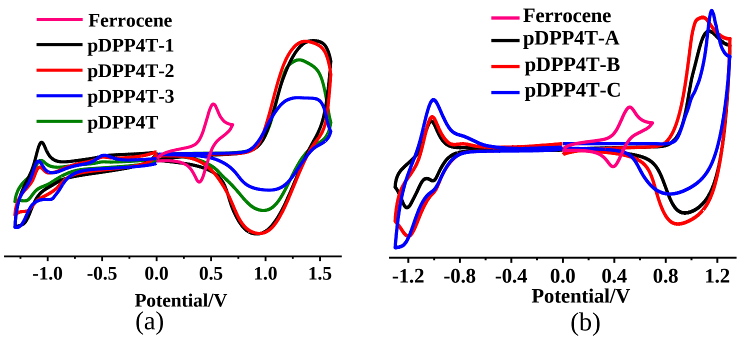
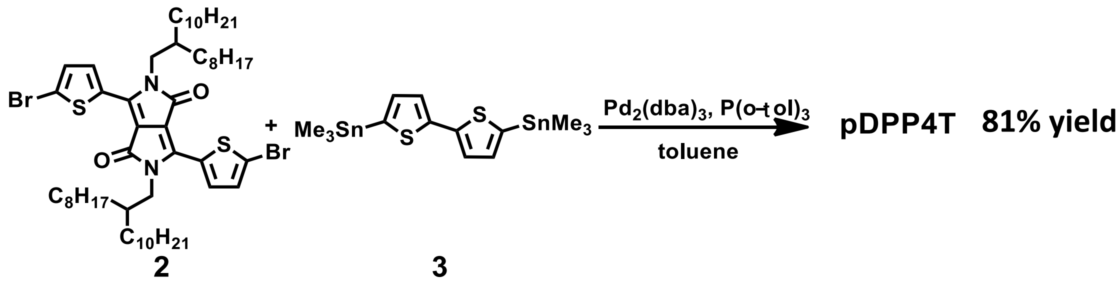
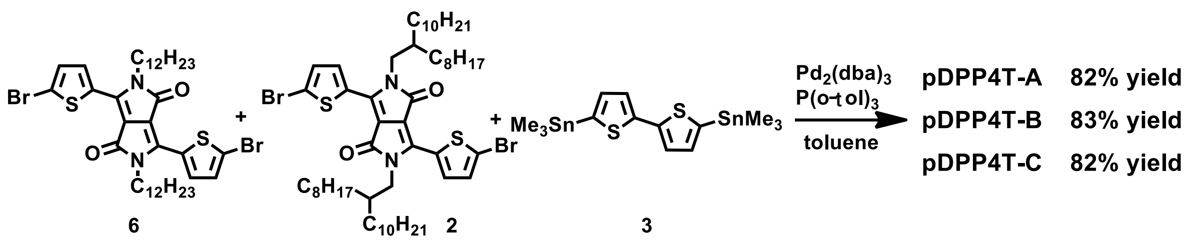



**Figure S2.** Cyclic voltammograms of **pDPP4T-1**, **pDPP4T-2**, **pDPP4T-3**, **pDPP4T**, **pDPP4T-A**, **pDPP4T-B** and **pDPP4T-C** films at a scan rate of 100 $mVs^{-1}$. Pt was used as working electrode and counter electrode and Ag/AgCl (saturated KCl) as reference electrode; *n*-$Bu_4NPF_6$ (0.1 M) in $CH_3CN$ as supporting electrolyte. For calibration, the redox potential of ferrocene/ferrocenium ($Fc/Fc^+$) was measured under the same conditions.

### 3. Synthesis and Characterization of pDPP4T, pDPP4T-A, pDPP4T-B and pDPP4T-C




***Synthesis of pDPP4T.*** Compound **2** (101.9 mg, 0.10 mmol), compound **3** (49.2 mg, 0.10 mmol), P($o$-tol)$_3$ (4.9 mg, 0.016mmol) and $Pd_2(dba)_3$ (1.8 mg, 0.0020 mmol) were used. The purified polymer was collected to give deep green solid (83.3 mg, 81% yield). $^1$H NMR (500 MHz, 1,1,2,2-tetrachloroethane-$d_2$, 100 $^o$C): $\delta$ 8.98-8.92 (m, br, 2H), 7.31-6.94 (m, br, 6H), 4.09-4.02 (m, br, 4H), 2.18-2.03 (m, br, 10H), 1.30 (s, 56H),0.92 (s, 12H); $^{13}$C NMR (100 MHz, solid): $\delta$ 160.09, 140.33, 136.05, 128.04, 123.69, 107.94, 45.24, 38.36, 32.08, 30.09, 23.05, 14.41; $M_w/M_n$ (GPC) = 40.2/18.8 kg mol$^{-1}$. Anal. calcd for $(C_{62}H_{90}N_2O_2S_4)_n$: C, 72.75; H, 8.86; N, 2.74; S, 12.53. Found: C, 72.50; H, 8.92; N, 2.78; S, 12.39.




***Synthesis of pDPP4T-A.*** Compound **6** (2.6 mg, 0.0033 mmol), compound **2** (101.9 mg, 0.10 mmol), compound **3** (50.7 mg, 0.10 mmol), P($o$-tol)$_3$ (5.0 mg, 0.016 mmol) and $Pd_2(dba)_3$ (1.9 mg, 0.0021 mmol) were used. The purified polymer was collected to give deep green solid (86.7 mg, 82% yield). $^1$H NMR (500 MHz, 1,1,2,2-tetrachloroethane-$d_2$, 100 $^o$C): $\delta$ 8.85 (s, br, 2H), 7.07-6.91 (m, br, 6H), 4.09 (s, br, 4H), 2.25-2.08 (m, br, 10H), 1.67-1.32 (m, br, 56H), 0.93 (s, 12H); $^{13}$C NMR (100 MHz, solid): $\delta$ 160.91, 140.94, 137.32, 129.00, 124.76, 108.64, 45.08, 38.79, 37.63, 32.66, 30.58, 23.56, 14.88. $M_w/M_n$ (GPC) = 211.6/74.0 kg mol$^{-1}$. Anal. calcd. for $(C_{1936}H_{2878}N_{62}O_{62}S_{124})_n$: C, 72.69; H, 9.07; N, 2.71; S, 12.43. Found: C, 72.27; H, 8.57; N, 2.82; S, 12.51.

***Synthesis of pDPP4T-B.*** Compound **6** (4.0 mg, 0.0050 mmol), compound **2** (101.9 mg, 0.10 mmol), compound **3** (51.8 mg, 0.11 mmol), P(*o*-tol)$_3$ (5.1 mg, 0.017 mmol) and $Pd_2(dba)_3$ (1.9 mg, 0.0021 mmol) were used. The purified polymer was collected to give deep green solid (88.7 mg, 83% yield). $^1$H NMR (500 MHz, 1,1,2,2-tetrachloroethane-$d_2$, 100 ºC): $\delta$ 8.89 (s, br, 2H), 7.08-6.93 (m, br, 6H), 4.09 (s, br, 4H), 2.25-2.07 (m, br, 10H), 1.69-1.32 (m, br, 56H), 0.93 (s, 12H); $^{13}$C NMR (100 MHz, solid): $\delta$ 160.87, 141.25, 136.74, 128.59, 124.29, 108.37, 45.46, 38.73, 32.67, 30.72, 23.62, 14.94. $M_w/M_n$ (GPC) = 190.9/91.5 kg mol$^{-1}$. Anal. calcd. for $(C_{1306}H_{1938}N_{42}O_{42}S_{84})_n$: C, 72.64; H, 9.05; N, 2.72; S, 12.47. Found: C, 71.89; H, 8.68; N, 2.80; S, 12.49.

***Synthesis of pDPP4T-C.*** Compound **6** (8.0 mg, 0.010 mmol), compound **2** (101.9 mg, 0.10 mmol), compound **3** (54.1 mg, 0.11 mmol), P(*o*-tol)$_3$ (5.4 mg, 0.018mmol) and $Pd_2(dba)_3$ (2.0 mg, 0.0022 mmol) were used. The purified polymer was collected to give deep green solid (92.2 mg, 82% yield). $^1$H NMR (500 MHz, 1,1,2,2-tetrachloroethane-$d_2$, 100 ºC): $\delta$ 8.99-8.90 (m, br, 2H), 7.14-6.97 (m, br, 6H), 4.11-4.00 (s, br, 4H), 2.10-2.06 (m, br, 10H), 1.47-1.33 (m, br, 56H), 0.92 (s, 12H); $^{13}$C NMR (100 MHz, solid): $\delta$ 160.21, 140.49, 136.35, 128.20, 123.69, 108.09, 45.09, 38.55, 31.93, 30.14, 23.05, 14.39. $M_w/M_n$

(GPC) = 207.8/94.6 kg mol$^{-1}$. Anal. calcd. for $(C_{666}H_{958}N_{22}O_{22}S_{44})_n$: C, 72.48; H, 8.75; N, 2.79; S, 12.78. Found: C, 72.46; H, 8.75; N, 2.50; S, 12.88.

## 4. HOMO/LUMO Energies and Band Gaps of pDPP4T-A, pDPP4T-B and pDPP4T-C

**Table S1. Absorption, Onset Redox Potentials, HOMO/LUMO Energies and Band Gaps of pDPP4T-A, pDPP4T-B and pDPP4T-C.**

| polymer | $\lambda_{max}{}^{a}$ (nm) ($\varepsilon_{max}$, M$^{-1}$ cm$^{-1}$)$^{b}$ | | $E_{redl}{}^{onset}$ (V)$^{c}$ | $E_{LUMO}$ (eV)$^{d}$ | $E_{oxl}{}^{onset}$ (V)$^{c}$ | $E_{HOMO}$ (eV)$^{d}$ | $E_g{}^{cv}$ (eV)$^{e}$ | $E_g{}^{opt}$ (eV)$^{f}$ |
|---|---|---|---|---|---|---|---|---|
| | solution | film | | | | | | |
| **pDPP4T-A** | 784(80000) | 726,784 | -1.28 | -3.52 | 0.47 | -5.27 | 1.75 | 1.33 |
| **pDPP4T-B** | 788(82000) | 726,790 | -1.26 | -3.54 | 0.46 | -5.26 | 1.71 | 1.32 |
| **pDPP4T-C** | 800(83000) | 726,790 | -1.26 | -3.54 | 0.46 | -5.26 | 1.72 | 1.32 |

$^{a}$ Absorption maxima in $CHCl_3$ solution ($1.0\times10^{-5}$ M for each polymer) and the spin-coated thin film; $^{b}$ Molar extinction coefficient ($\varepsilon_{max}$, M$^{-1}$ cm$^{-1}$); $^{c}$ Onset potentials (V vs Fc/Fc$^{+}$) for reduction ($E_{redl}{}^{onset}$) and oxidation ($E_{oxl}{}^{onset}$); $^{d}$ Estimated with the following equation: $E_{HOMO} = -(E_{oxl}{}^{onset} + 4.8)$ eV, $E_{LUMO} = -(E_{redl}{}^{onset} + 4.8)$ eV; $^{e}$ Based on redox potentials; $^{f}$ Based on the absorption spectral data.

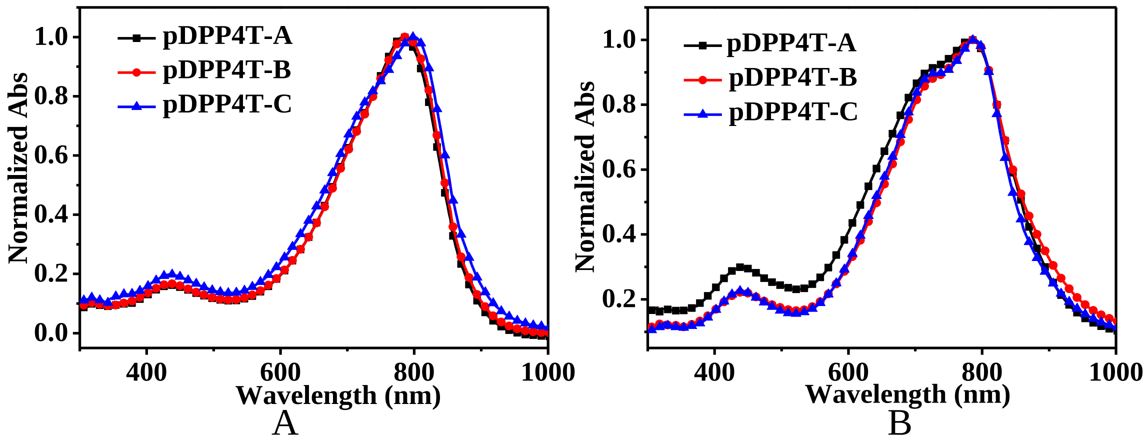



**Figure S3.** Normalized UV-vis absorption spectra of **pDPP4T-A**, **pDPP4T-B** and **pDPP4T-C** in $CHCl_3$ ($1.0\times10^{-5}$ M) (A) and their thin films (B).

## 5. Fabrication of FET Devices

Solutions of conjugated polymers were prepared by dissolving the copolymers in chloroform at a concentration of 7.0 mg/mL except **pDPP4T-C** (3.0 mg/mL in 1,1,2,2-tetrachloroethane). The typical polymer film thickness (around 40-45 nm) was measured on profilometer (Ambios Tech. XP-2). Bottom-Gate/Bottom-Contact FETs were fabricated. A heavily doped *n*-type Si wafer and a layer of dry oxidized $SiO_2$ (300 nm, with roughness lower than 0.1 nm and capacitance of 11 nF $cm^{-2}$) were used as a gate electrode and gate dielectric layer, respectively. The drain-source (*D*-*S*) gold contacts (28 nm) were fabricated by photo-lithography. The substrates were first cleaned by sonication in acetone and water for 5.0 min and immersed in Piranha solution (2:1 mixture of sulfuric acid and 30% hydrogen peroxide) for 20 min. This was followed by rinsing with deionized water and isopropyl alcohol for several times, and it was blow-dried with nitrogen. Then, the surface was modified with *n*-octadecyltrichlorosilane (OTS). After that, the substrates were cleaned in *n*-hexane, $CHCl_3$ and isopropyl alcohol. The films of conjugated polymers were fabricated by spin-coating their solutions at 3000 rpm. The annealing process was carried out in vacuum for 1.0 h at each temperature.

The bottom-gate/top-contact devices with fabricated similarly except Au source/drain electrodes (50 nm) were deposited via thermal vacuum evaporation through a shadow mask after spin coating the semiconductor solution and then annealed at different temperatures in vacuum for 1.0 h. Field-effect characteristics of the devices were determined in nitrogen using a Keithley 4200 SCS semiconductor parameter analyzer.

Linear mobility was calculated according to the equation below:

$$\boldsymbol{I_{DS} = (W/L)C_i\mu(V_{GS} - V_{Th})V_{DS} \quad V_{DS} \ll V_{GS} - V_{Th}} \qquad \textbf{(1)}$$

The mobility of the OFETs in the saturation region was extracted from the following equation:

$$I_{DS}=\frac{W}{2L}\mu C_i(V_{GS}-V_{Th})^2 \qquad (2)$$

Where $I_{DS}$ is the drain electrode collected current; $L$ and $W$ are the channel length and width, respectively; $\mu$ is the mobility of the device; $C_i$ is the capacitance per unit area of the gate dielectric layer; $V_{GS}$ is the gate voltage, and $V_{Th}$ is the threshold voltage. The $V_{Th}$ of the device was determined by extrapolating the $(I_{DS,sat})^{1/2}$ vs. $V_{GS}$ plot to $I_{DS} = 0$.

The contact resistance was determined in the following way (a. Luan, S.; Neudeck, G. W. *J. Appl. Phys.* **1992**, *72*, 766; b. Lefenfeld, M.; Blanchet, G.; Rogers, J. A. *Adv. Mater.* **2003**, *15*, 1188.). For a BGBC FET, the ON resistance, $R_{ON}$, in the linear operation regime (source-drain voltage <<gate voltage), can be expressed as follows:

$$R_{\mathrm{on}} = \frac{\partial V_{\mathrm{DS}}}{\partial I_{\mathrm{DS}}}\int_{V_{\mathrm{DS}}\to 0}^{V_{\mathrm{GS}}} = R_{ch} + R_p = \frac{L}{W\mu_i C_i(V_{GS} - \mathrm{V}_{\mathrm{T}h})} + R_p \qquad (3)$$

where $R_{ch}$ is the channel resistance, $R_p$ is the parasitic resistance, and $V_{GS}$ is the gate voltage. The parasitic resistance, $R_p$, which is associated with the contacts between *S-D* electrode and semiconductor layer, can be extracted by measuring the ON resistance, $R_{ON}$, from the linear region of the FET output characteristics. We got a plot of $R_{ON}$ as a function of $L$ at the gate voltage of -30 V, and found that the relationship of $R_{ON}$ vs $L$ gives straight lines, indicating that the ON resistance is well expressed by Eq. (3). By extrapolating the relationship of $R_{ON}$ vs $L$ to $L$= 0, the contact resistance values can be determined. The contact resistances for BGBC devices with thin films of **pDPP4T-1**, **pDPP4T-2**, **pDPP4T-3**, **pDPP4T**, **pDPP4T-A**, **pDPP4T-B** and **pDPP4T-C** were determined to be 0.82 MΩ, 0.21 MΩ, 0.11 MΩ, 1.40 MΩ, 0.71 MΩ, 0.53 MΩ and 0.52 MΩ, respectively.

## 6. Transfer and Output Curves of BGBC and BGTC Devices with Thin Films of pDPP4T-1, pDPP4T-2, pDPP4T-3, pDPP4T, pDPP4T-A, pDPP4T-B and pDPP4T-C

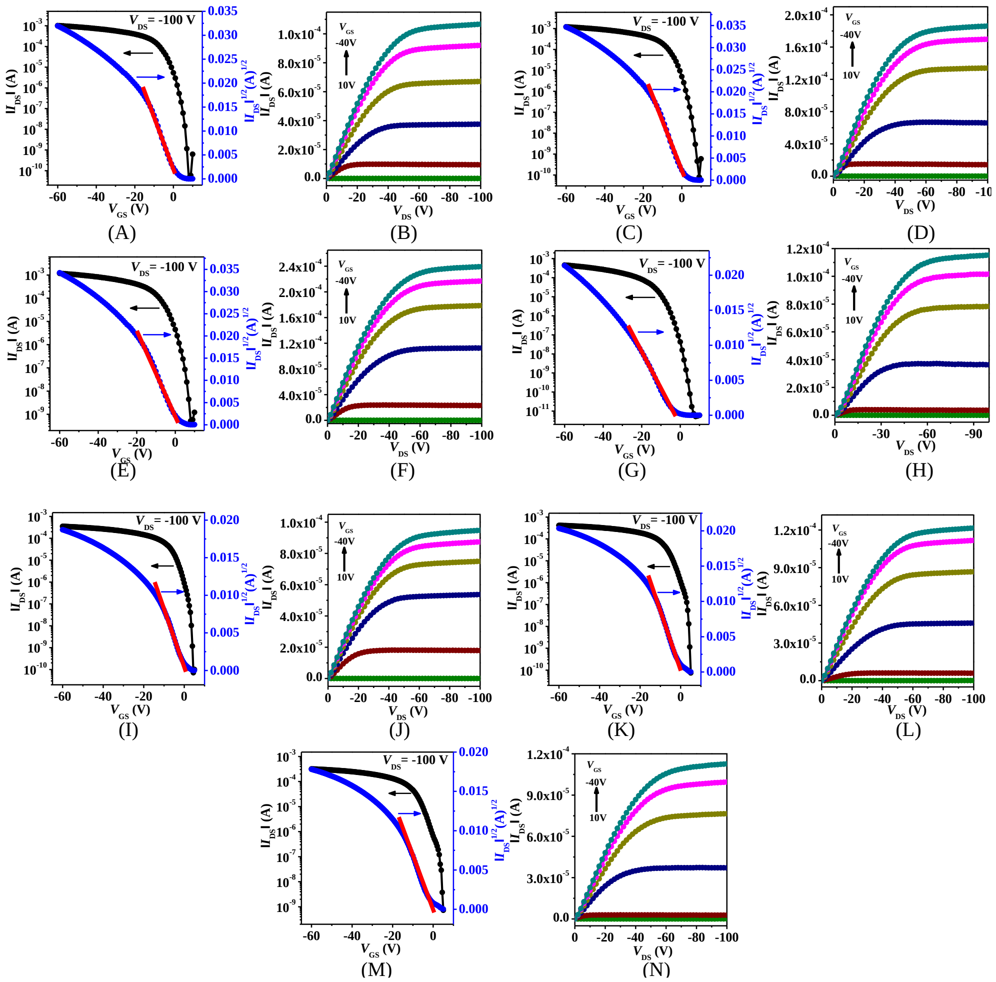



**Figure S4.** The transfer and output curves of BGBC FETs with thin films of **pDPP4T-1** (A, B), **pDPP4T-2** (C, D), **pDPP4T-3** (E, F), **pDPP4T** (G, H), **pDPP4T-A** (I, J), **pDPP4T-B** (K, L) and **pDPP4T-C** (M, N) after thermal annealing at 100 °C; the channel width ($W$) and length ($L$) were 1440 $\mu$m and 50 $\mu$m, respectively.

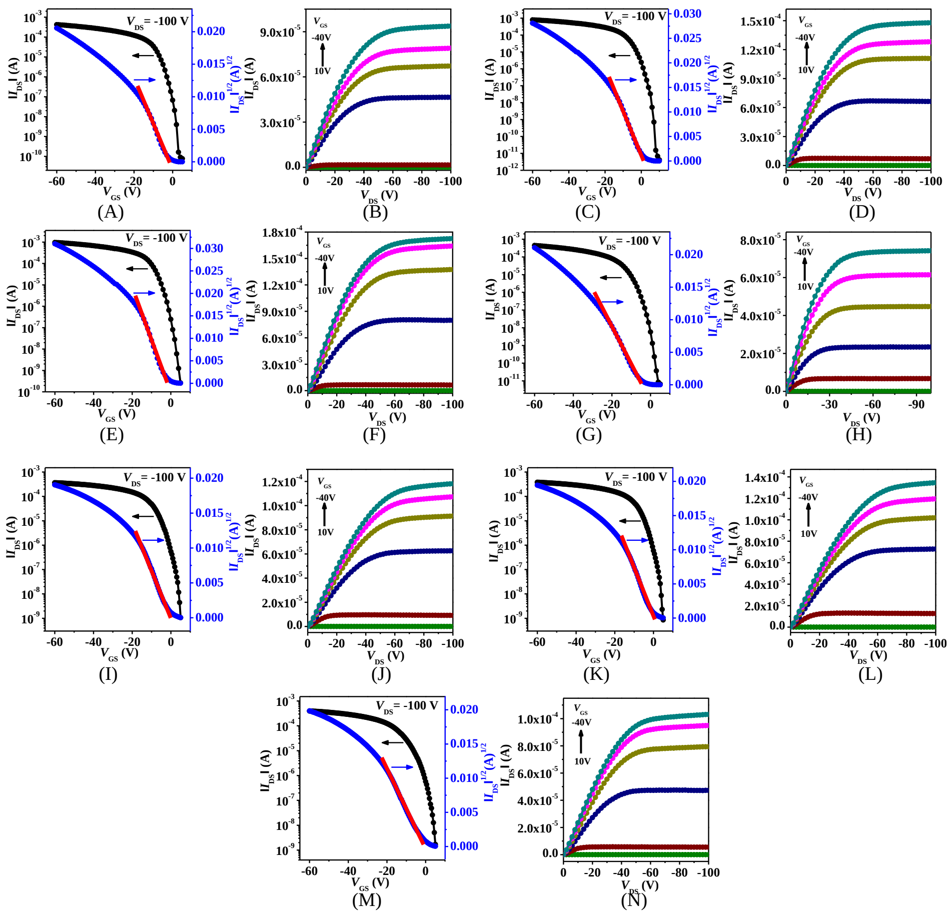



**Figure S5.** The transfer and output curves of BGTC FETs with thin films of **pDPP4T-1** (A, B), **pDPP4T-2** (C, D), **pDPP4T-3** (E, F), **pDPP4T** (G, H), **pDPP4T-A** (I, J), **pDPP4T-B** (K, L) and **pDPP4T-C** (M, N) after thermal annealing at 100 °C; the channel width (*W*) and length (*L*) were 3000 $\mu$m and 100 $\mu$m, respectively.

**Table S2. Hole Mobilities ($\mu_h$), Threshold Voltages ($V_{Th}$) and $I_{on}/I_{off}$ Ratios for BGTC FETs with thin films of pDPP4T-1, pDPP4T-2, pDPP4T-3, pDPP4T, pDPP4T-A, pDPP4T-B and pDPP4T-C after Annealing at 100 °C.**

| polymer | $\mu_h^a$ /cm$^2$ V$^{-1}$ s$^{-1}$ | $V_{Th,\ h}$/V | $I_{on}/I_{off}$ |
|---|---|---|---|
| **pDPP4T-1** | 4.8/4.4 | -3 - 10 | $10^6$ - $10^7$ |
| **pDPP4T-2** | 6.4/5.9 | 0 - 9 | $10^7$ - $10^8$ |
| **pDPP4T-3** | 8.8/7.1 | -5 - 10 | $10^6$ - $10^7$ |
| **pDPP4T-A** | 3.7/3.1 | -5 - 8 | $10^5$ - $10^6$ |
| **pDPP4T-B** | 4.1/3.5 | -4 – 9 | $10^5$ - $10^6$ |
| **pDPP4T-C** | 2.6/2.1 | -3 – 10 | $10^5$ - $10^6$ |
| **pDPP4T** | 2.6/2.2 | -5 - 11 | $10^7$ - $10^8$ |

[a] The mobilities were provided in "highest/average" form, and the performance data were obtained based on more than 10 different FETs.

## 7. Devices Stability Data

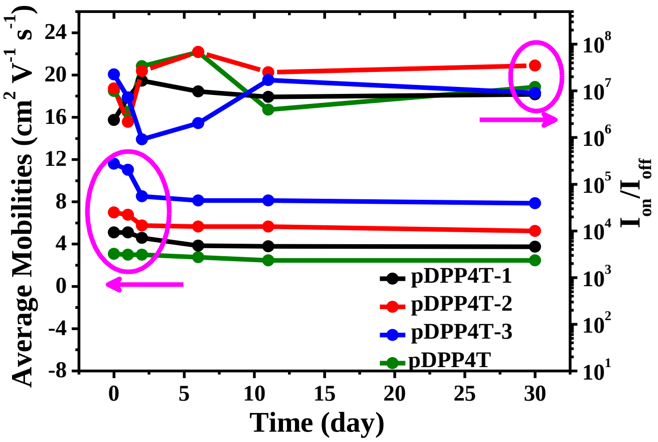



**Figure S6.** Variation of hole mobilities and $I_{on}/I_{off}$ ratios for BGBC FETs of **pDPP4T-1**, **pDPP4T-2**, **pDPP4T-3** and **pDPP4T** after being left in air for 30 days.

## 8. 1-D GIXRD Patterns

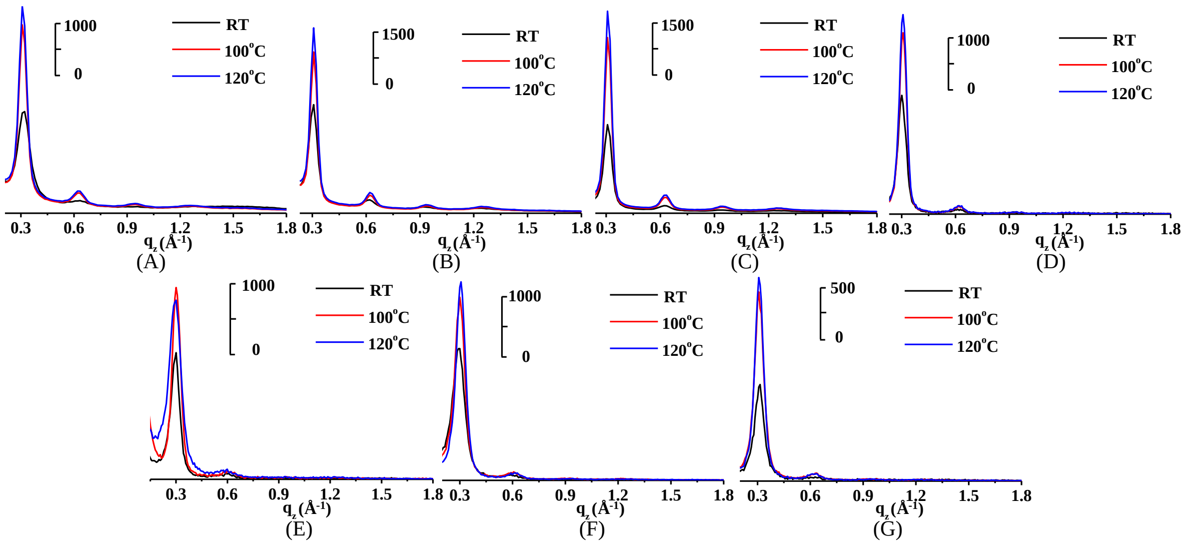



**Figure S7.** 1-D GIXRD patterns in the *out-of-plane* direction for **pDPP4T-1** (A), **pDPP4T-2** (B), **pDPP4T-3** (C), **pDPP4T** (D) and **pDPP4T-A** (E), **pDPP4T-B** (F) and **pDPP4T-C** (G) deposited on OTS-modified $SiO_2$/Si substrates after thermal annealing at different temperatures.

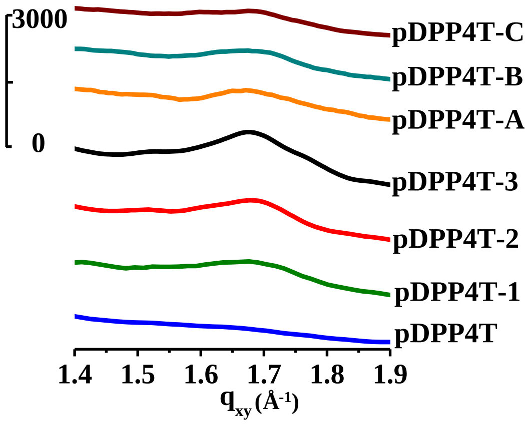



**Figure S8.** 1-D GIXRD patterns in the *in-plane* direction for **pDPP4T-1**, **pDPP4T-2**, **pDPP4T-3**, **pDPP4T**, **pDPP4T-A**, **pDPP4T-B**, and **pDPP4T-C** deposited on OTS-modified $SiO_2$/Si substrates after thermal annealing at 100 °C.

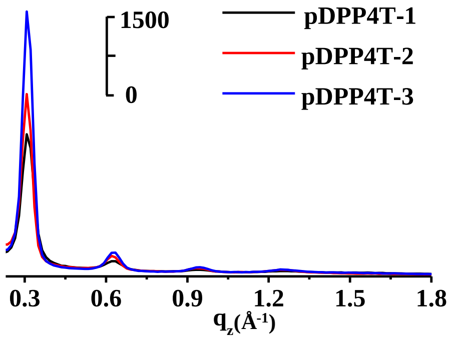



**Figure S9.** 1-D *out-of-plane* X-ray diffraction patterns of **pDPP4T-1**, **pDPP4T-2** and **pDPP4T-3** after thermal annealing at 100 °C.

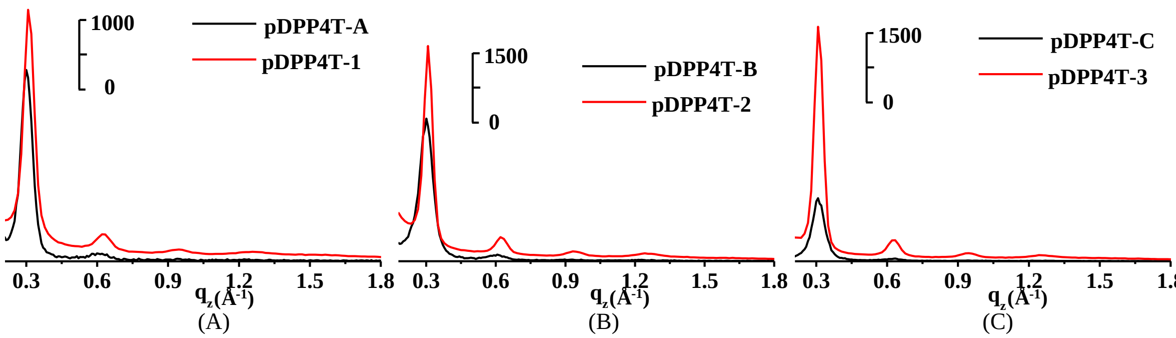



**Figure S10.** 1-D *out-of-plane* X-ray diffraction patterns of **pDPP4T-1** and **pDPP4T-A** (A), **pDPP4T-2** and **pDPP4T-B** (B) and **pDPP4T-3** and **pDPP4T-C** (C) after thermal annealing at 100 °C.

## 9. AFM Images of pDPP4T-A, pDPP4T-B and pDPP4T-C

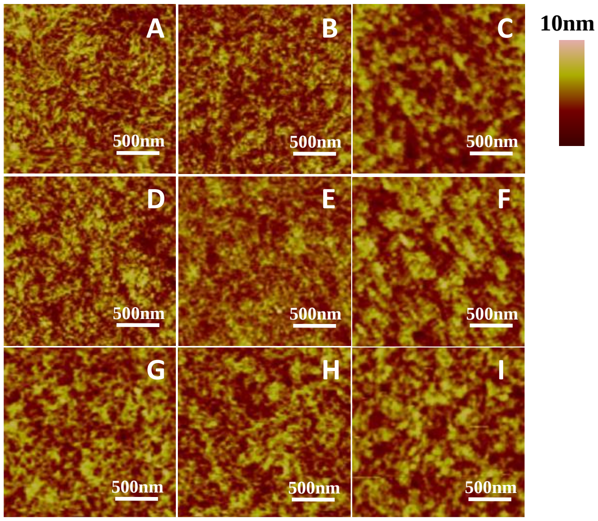


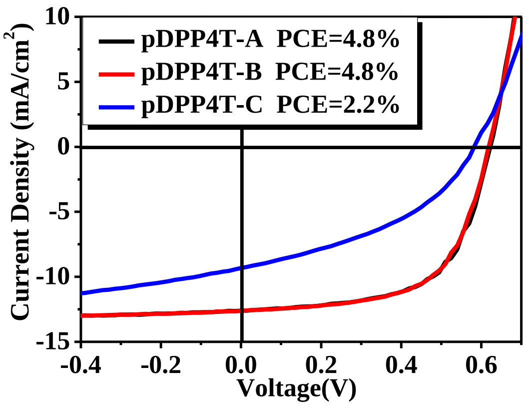

**Figure S11.** AFM height images of thin films of **pDPP4T-A** (A, D, G), **pDPP4T-B** (B, E, H) and **pDPP4T-C** (C, F, I) deposited on OTS-modified $SiO_2$/Si substrates at room temperature (*up*) and after thermal annealing at 100 $^oC$ (*middle*) and 120 $^oC$ (*down*).

## 10. Fabrication of Organic Photovoltaic Cells

OPVs were fabricated with ITO as the positive electrode and Al as the negative electrode. The patterned indium tin oxide (ITO) glass (sheet resistance = 15 Ω/square) was precleaned in an ultrasonic bath in detergent, deionized water, acetone and isopropyl alcohol, then treated in an ultraviolet-ozone chamber (Jelight Company, USA) for 30 min. A thin layer (30 nm) of poly(3,4-ethylenedioxythi-ophene):poly(styrenesulfonate) (PEDOT:PSS, Baytron PVP AI 4083, Germany) was spin-coated onto the ITO glass and baked at 150 $^oC$ for 15 min. Blend solution were prepared in different solvents at a total concentration of 15-18 mg/ml (donor/acceptor weight ratio:1/2 or 1/1) and stirred 2 hours for complete dissolution. Then, the **pDPP4T**, **pDPP4T-1**, **pDPP4T-2**, **pDPP4T-3, pDPP4T-A**, **pDPP4T-B** and **pDPP4T-C**/$PC_{71}BM$ blend solution was spin-coated. The thickness (ca.

100-120 nm) of the active layer was measured using an Ambios Technology XP-2 profilometer. Ca (ca. 20 nm) and aluminum layer (ca. 70 nm) were then evaporated onto the surface of the active layer under vacuum (ca. $10^{-5}$ Pa) to form the negative electrode respectively. The active area of the device was 5.0 mm$^2$. The *J–V* curves were measured with a computer-controlled Keithley 236 Source Measure Unit. A xenon lamp coupled with AM 1.5 solar spectrum filters was used as the light source, and the optical power at the sample was 100 mW cm$^{-2}$. The incident photon to converted current efficiency (IPCE) spectra were performed at Solar Cell Spectral Response Measurement System QE-R3011 (EnliTechnololy Co. Ltd).

## 11. *J-V* Curves and IPCE Spectra of pDPP4T-A, pDPP4T-B and pDPP4T-C with $PC_{71}BM$



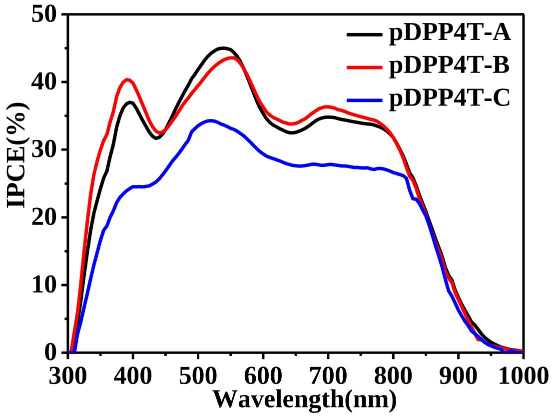
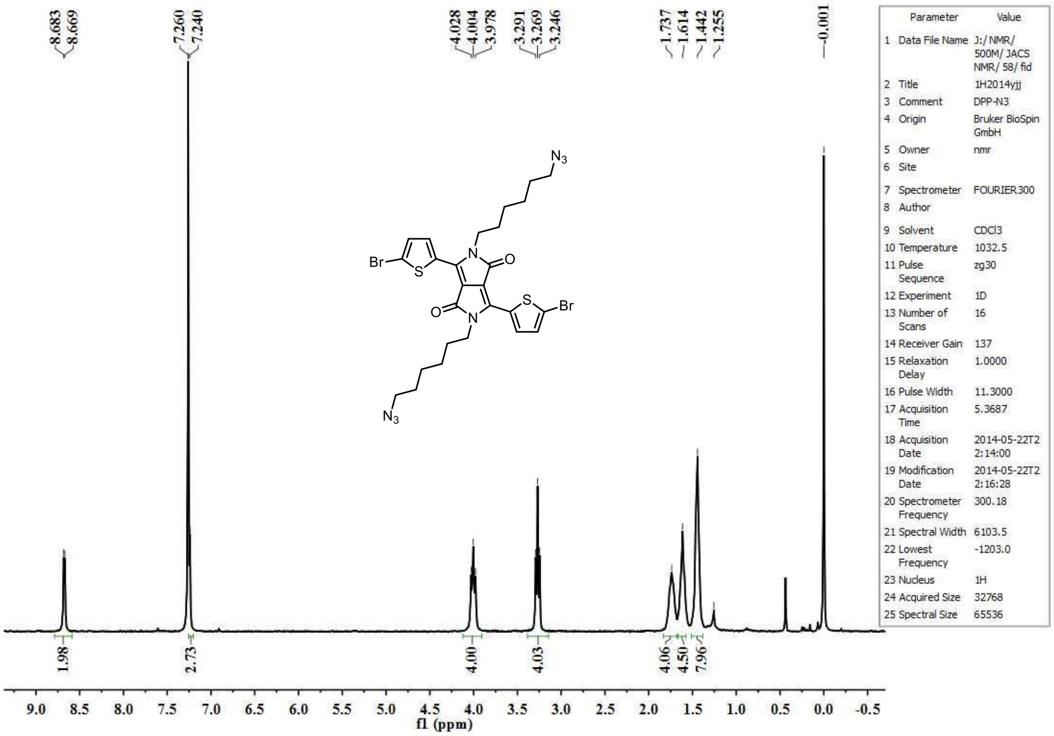
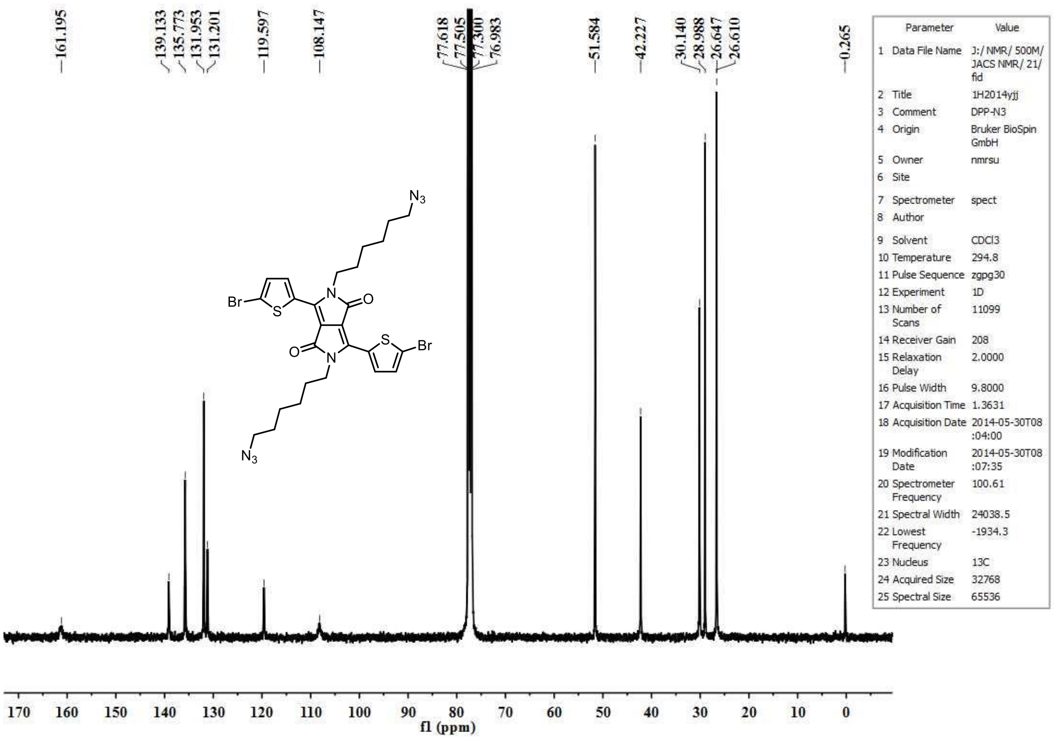




**Figure S12.** *J-V* curves (*left*) and IPCE spectra (*right*) of photovoltaic cells with the respective blend films of **pDPP4T-A**, **pDPP4T-B** and **pDPP4T-C** with $PC_{71}BM$ at 1:2 weight ratio under AM 1.5 illumination (100 mW/cm$^2$).

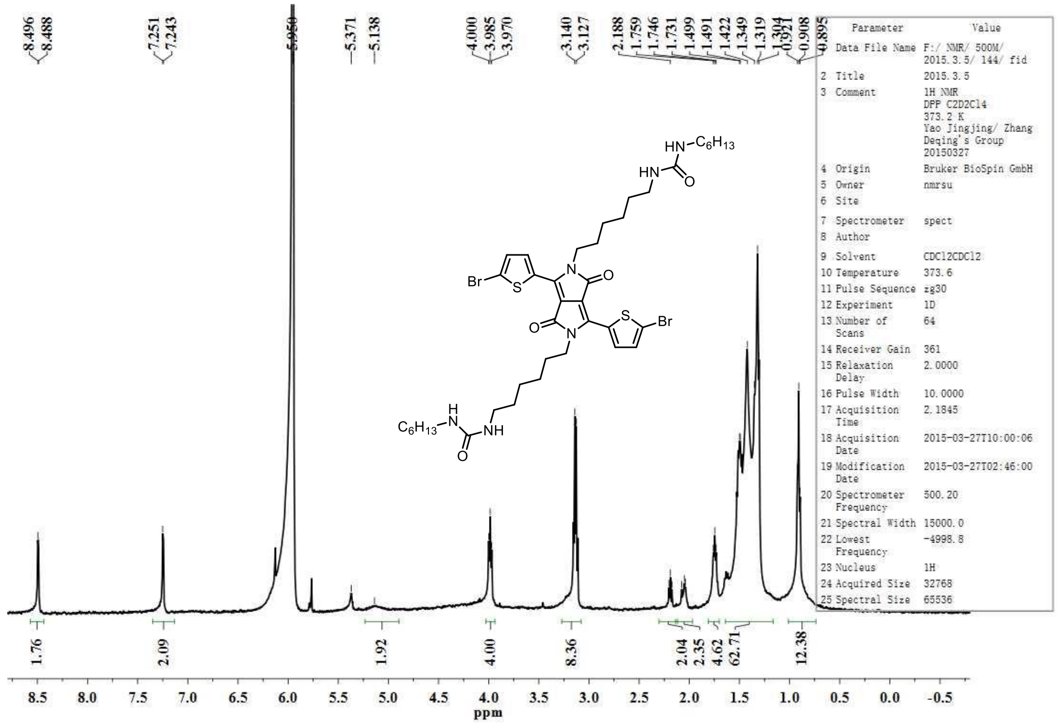
## 12. $^{1}$HNMR and $^{13}$CNMR Spectra

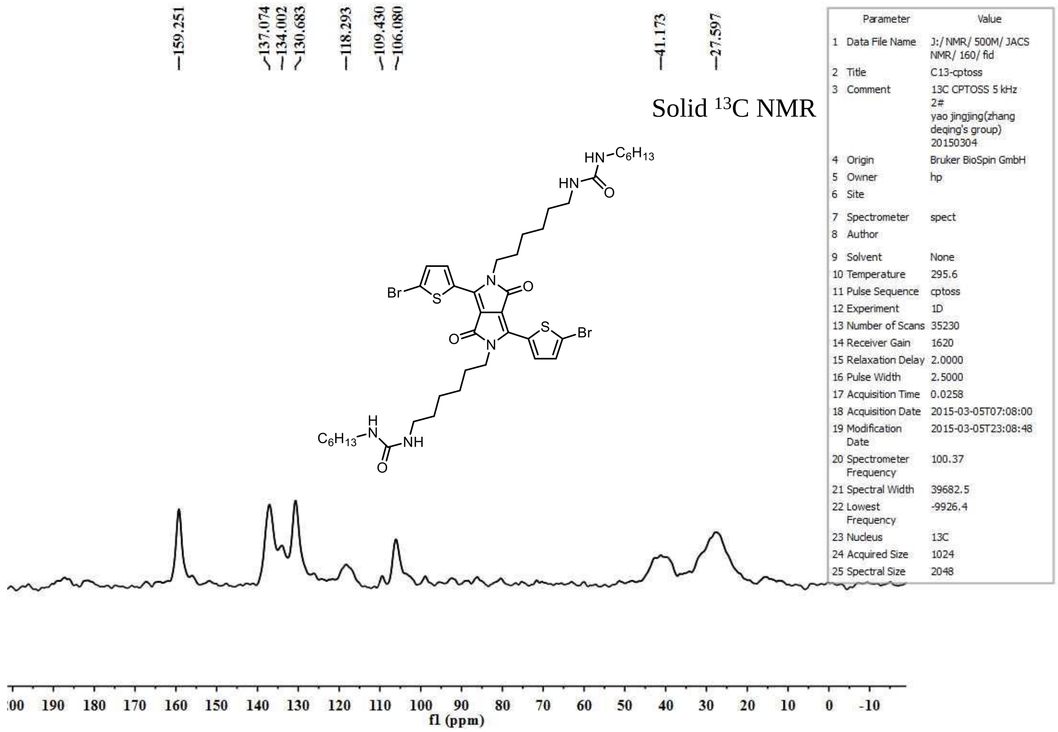
Compound **5**



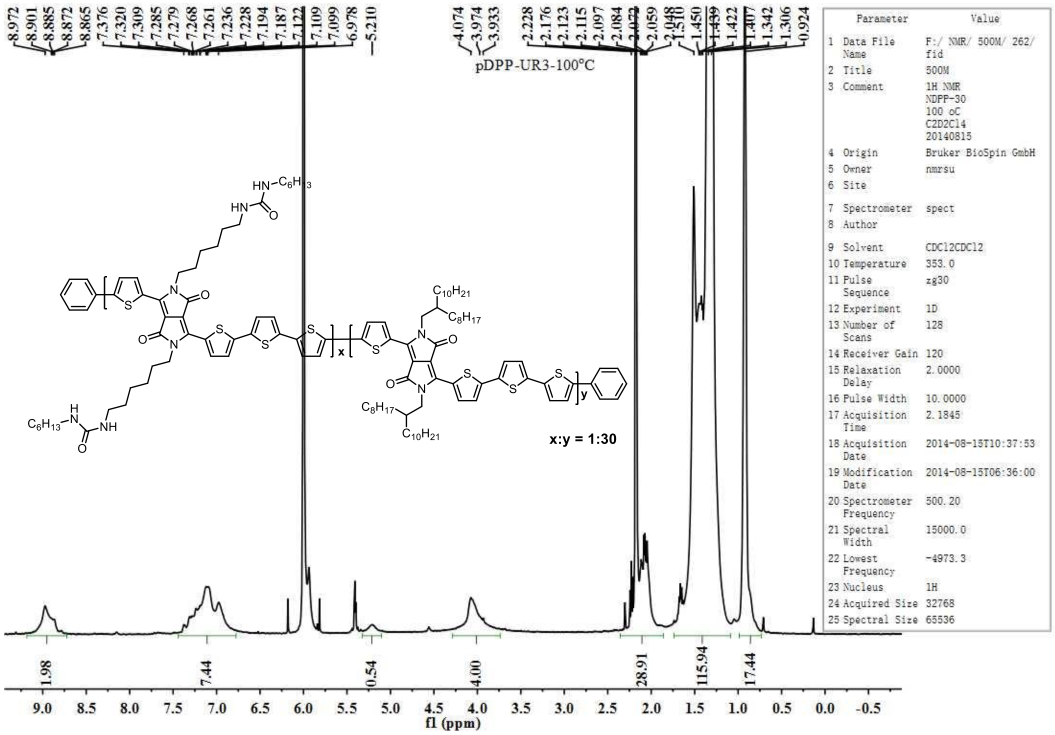



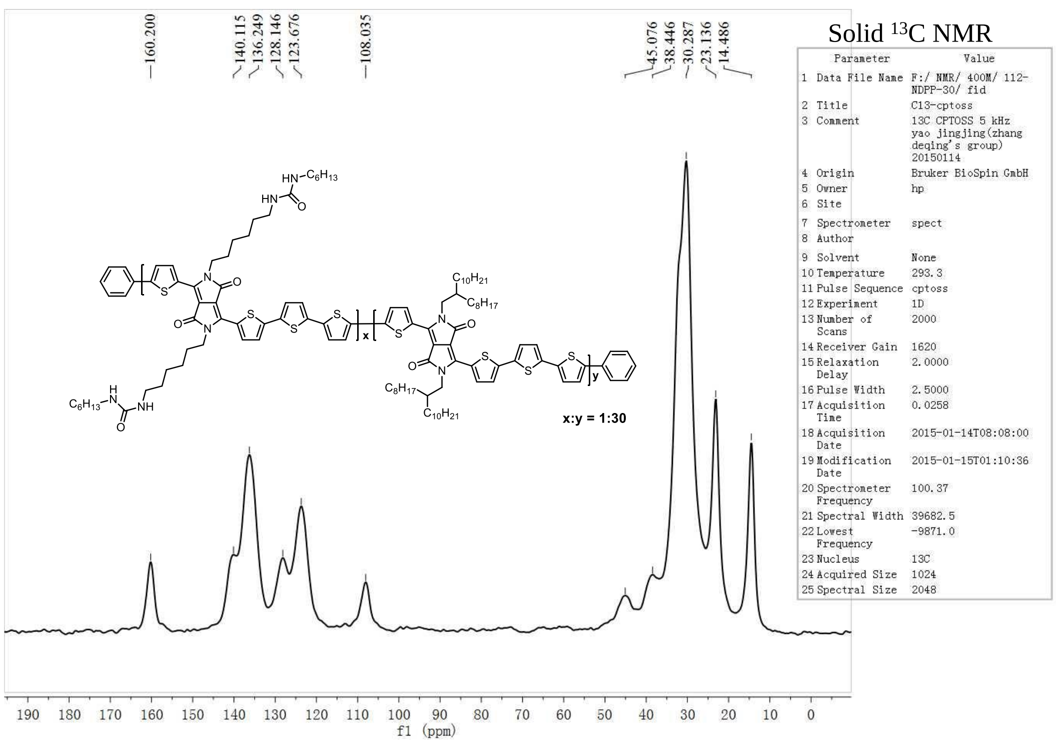
Compound **1**


8.496
8.488
7.251
7.243
5.950
5.371
5.138
4.000
3.985
3.970
3.140
3.127
2.188
1.759
1.746
1.731
1.499
1.491
1.422
1.349
1.319
1.304
0.921
0.908
0.895
Parameter Value
1 Data File Name F:/ NMR/ 500M/ 2015.3.5/ 144/ fid
2 Title 2015.3.5
3 Comment 1H NMR DPP C2D2Cl4 373.2 K Yao Jingjing/ Zhang Deqing's Group 20150327
4 Origin Bruker BioSpin GmbH
5 Owner nmrsu
6 Site
7 Spectrometer spect
8 Author
9 Solvent CDCl2CDCl2
10 Temperature 373.6
11 Pulse Sequence zg30
12 Experiment 1D
13 Number of Scans 64
14 Receiver Gain 361
15 Relaxation Delay 2.0000
16 Pulse Width 10.0000
17 Acquisition Time 2.1845
18 Acquisition Date 2015-03-27T10:00:06
19 Modification Date 2015-03-27T02:46:00
20 Spectrometer Frequency 500.20
21 Spectral Width 15000.0
22 Lowest Frequency -4998.8
23 Nucleus 1H
24 Acquired Size 32768
25 Spectral Size 65536
HN–C6H13
HN
O
Br
S
N
O
O
N
S
Br
C6H13–N
H
NH
O
1.76
2.09
1.92
4.00
8.36
2.04
2.35
4.62
62.71
12.38
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 0.5 0.0 -0.5
ppm

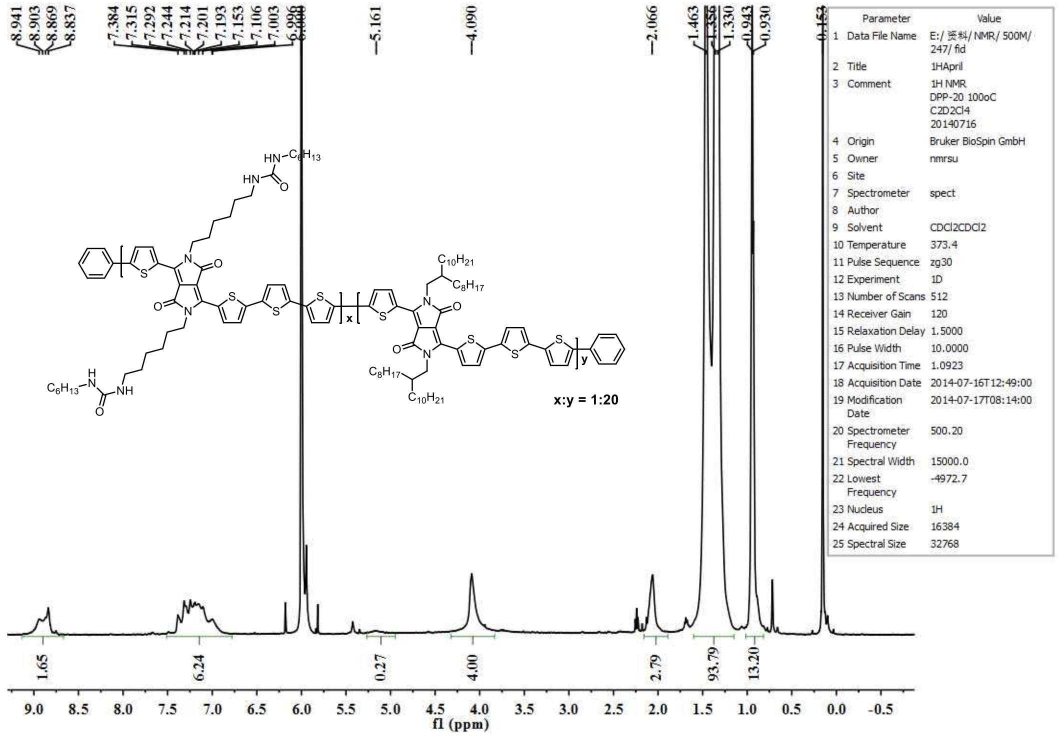

159.251
137.074
134.002
130.683
118.293
109.430
106.080
41.173
27.597
Solid 13C NMR
Parameter Value
1 Data File Name J:/ NMR/ 500M/ JACS NMR/ 160/ fid
2 Title C13-cptoss
3 Comment 13C CPTOSS 5 kHz 2# yao jingjing(zhang deqing's group) 20150304
4 Origin Bruker BioSpin GmbH
5 Owner hp
6 Site
7 Spectrometer spect
8 Author
9 Solvent None
10 Temperature 295.6
11 Pulse Sequence cptoss
12 Experiment 1D
13 Number of Scans 35230
14 Receiver Gain 1620
15 Relaxation Delay 2.0000
16 Pulse Width 2.5000
17 Acquisition Time 0.0258
18 Acquisition Date 2015-03-05T07:08:00
19 Modification Date 2015-03-05T23:08:48
20 Spectrometer Frequency 100.37
21 Spectral Width 39682.5
22 Lowest Frequency -9926.4
23 Nucleus 13C
24 Acquired Size 1024
25 Spectral Size 2048
HN–C6H13
HN
O
Br
S
N
O
O
N
S
Br
C6H13–N
H
NH
O
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

# pDPP4T-1

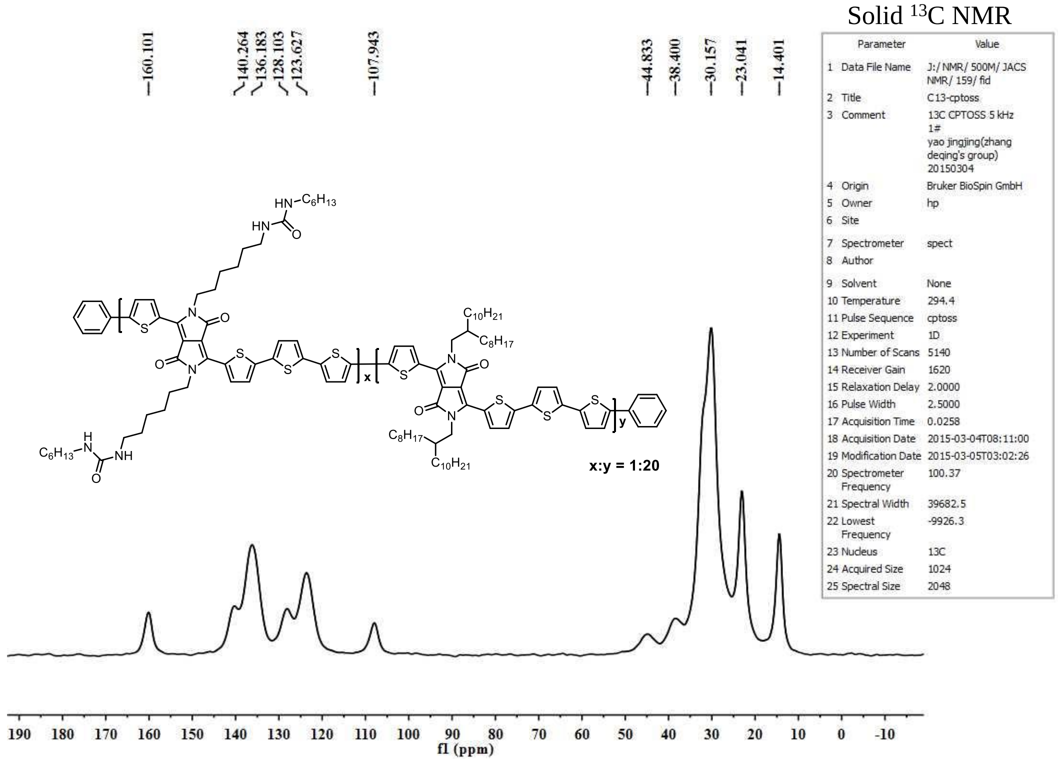

8.972
8.901
8.885
8.872
8.865
7.376
7.320
7.309
7.285
7.279
7.268
7.261
7.236
7.228
7.194
7.187
7.122
7.109
7.099
6.978
5.210
4.074
3.974
3.933
2.228
2.176
2.123
2.115
2.097
2.084
2.072
2.059
2.048
1.510
1.450
1.439
1.422
1.407
1.342
1.306
0.924
pDPP-UR3-100°C
x:y = 1:30
1.98
7.44
0.54
4.00
28.91
115.94
17.44
f1 (ppm)
Parameter Value
1 Data File Name F:/ NMR/ 500M/ 262/ fid
2 Title 500M
3 Comment 1H NMR NDPP-30 100 oC C2D2Cl4 20140815
4 Origin Bruker BioSpin GmbH
5 Owner nmrsu
6 Site
7 Spectrometer spect
8 Author
9 Solvent CDCl2CDCl2
10 Temperature 353.0
11 Pulse Sequence zg30
12 Experiment 1D
13 Number of Scans 128
14 Receiver Gain 120
15 Relaxation Delay 2.0000
16 Pulse Width 10.0000
17 Acquisition Time 2.1845
18 Acquisition Date 2014-08-15T10:37:53
19 Modification Date 2014-08-15T06:36:00
20 Spectrometer Frequency 500.20
21 Spectral Width 15000.0
22 Lowest Frequency -4973.3
23 Nucleus 1H
24 Acquired Size 32768
25 Spectral Size 65536


Solid 13C NMR
160.200
140.115
136.249
128.146
123.676
108.035
45.076
38.446
30.287
23.136
14.486
x:y = 1:30
f1 (ppm)
Parameter Value
1 Data File Name F:/ NMR/ 400M/ 112-NDPP-30/ fid
2 Title C13-cptoss
3 Comment 13C CPTOSS 5 kHz yao jingjing(zhang deqing's group) 20150114
4 Origin Bruker BioSpin GmbH
5 Owner hp
6 Site
7 Spectrometer spect
8 Author
9 Solvent None
10 Temperature 293.3
11 Pulse Sequence cptoss
12 Experiment 1D
13 Number of Scans 2000
14 Receiver Gain 1620
15 Relaxation Delay 2.0000
16 Pulse Width 2.5000
17 Acquisition Time 0.0258
18 Acquisition Date 2015-01-14T08:08:00
19 Modification Date 2015-01-15T01:10:36
20 Spectrometer Frequency 100.37
21 Spectral Width 39682.5
22 Lowest Frequency -9871.0
23 Nucleus 13C
24 Acquired Size 1024
25 Spectral Size 2048

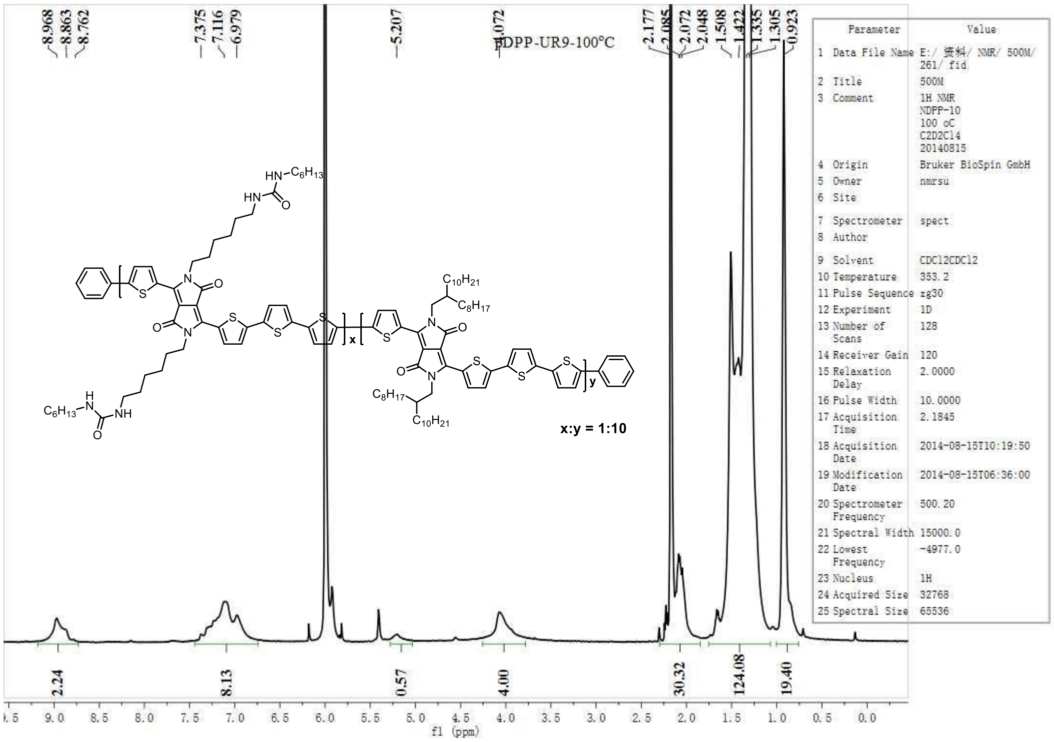
## pDPP4T-2

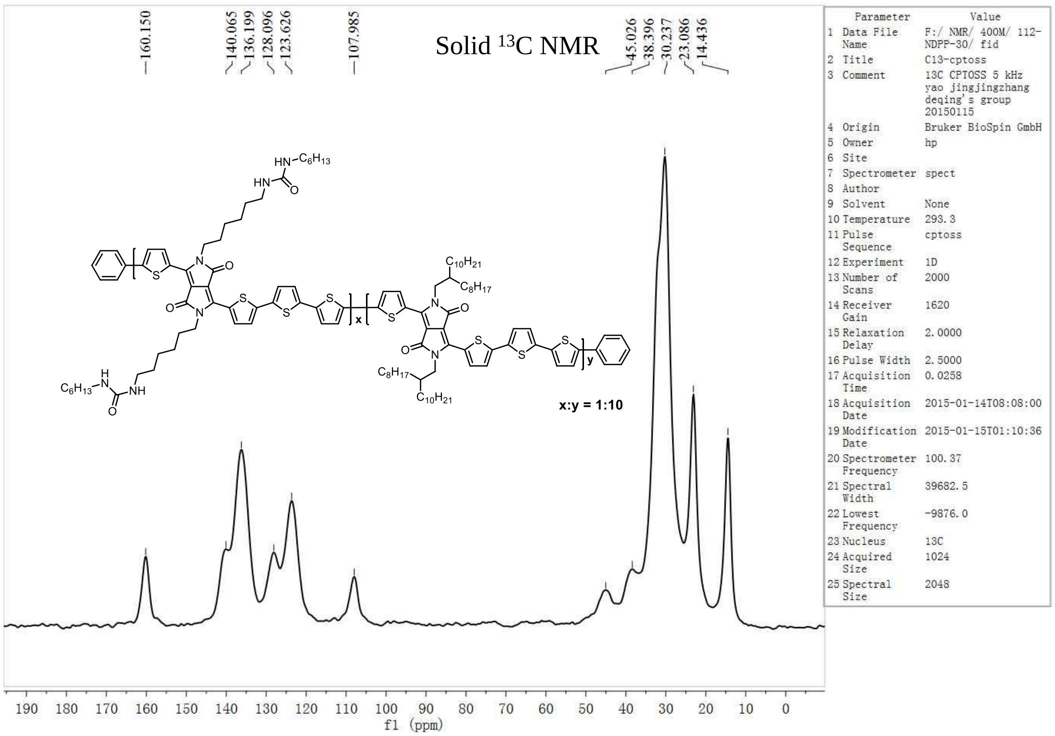



Solid $^{13}$C NMR

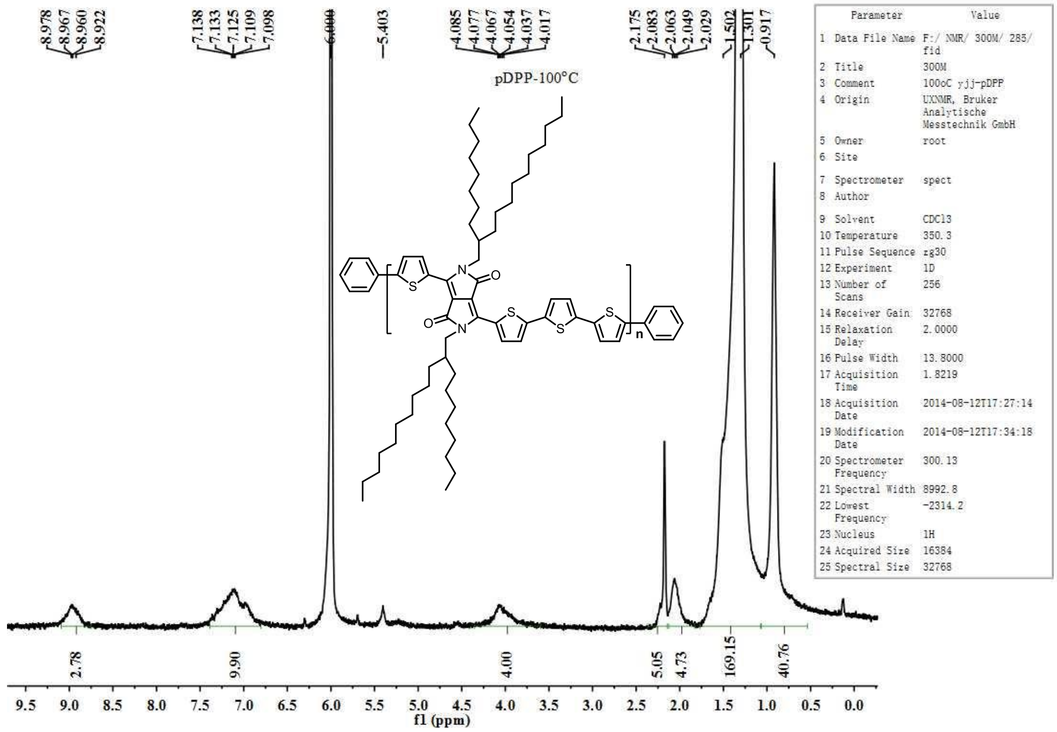


# pDPP4T-3

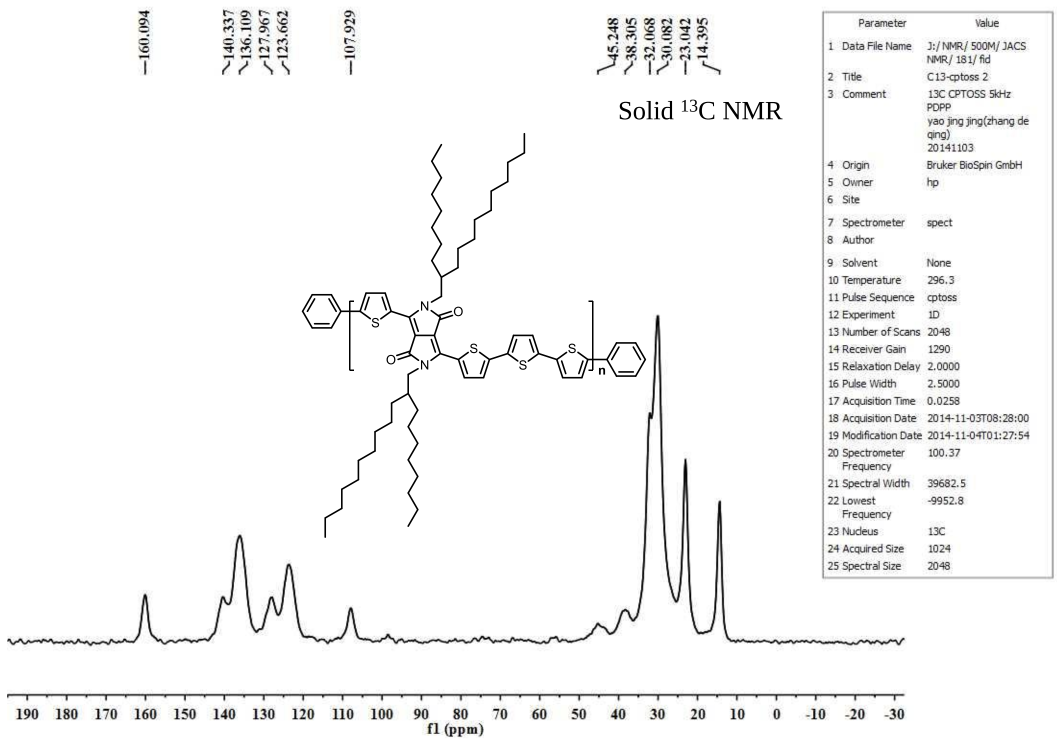


# pDPP4T

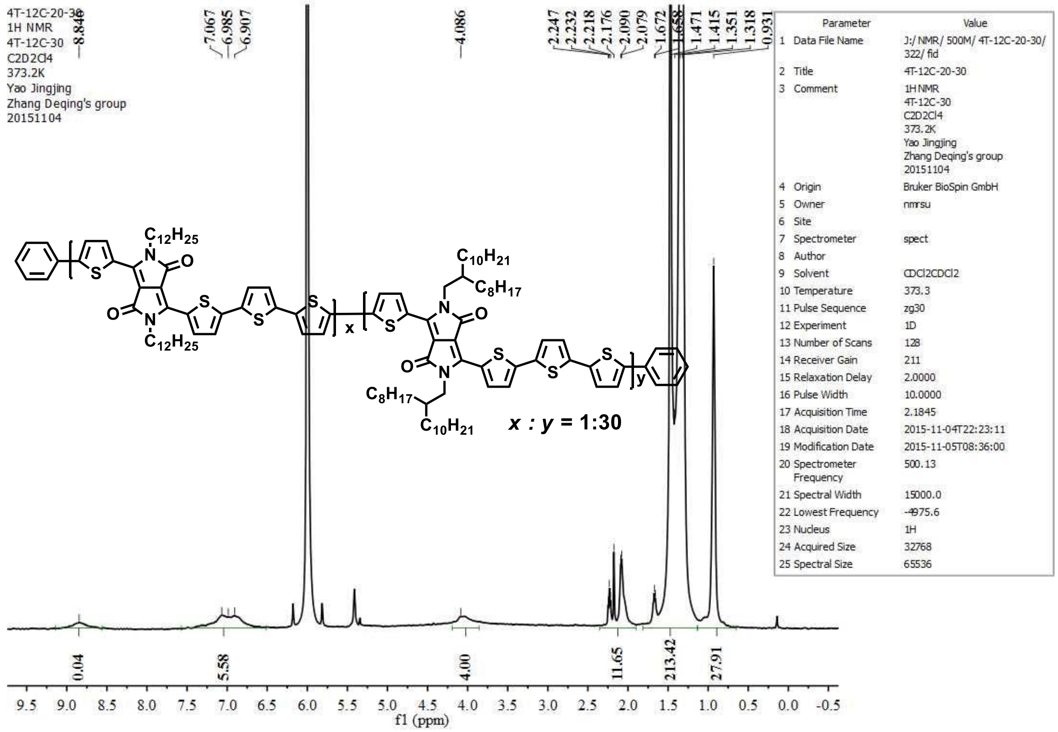


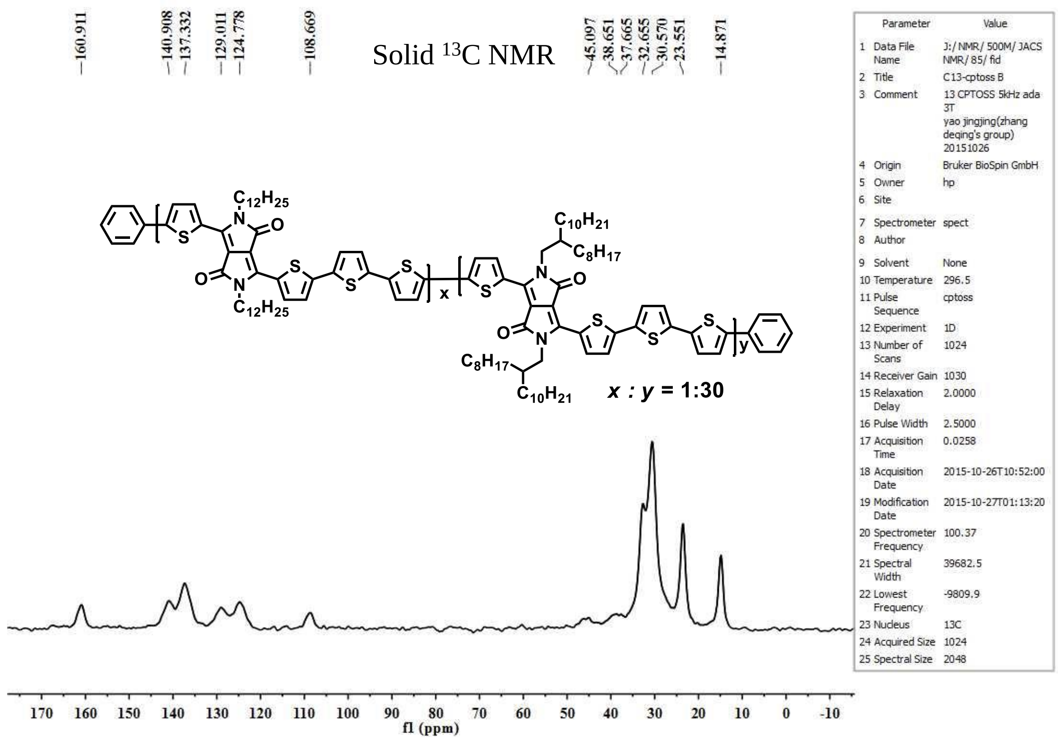
8.978
8.967
8.960
8.922
7.138
7.133
7.125
7.109
7.098
6.000
5.403
4.085
4.077
4.067
4.054
4.037
4.017
2.175
2.083
2.063
2.049
2.029
1.502
1.301
0.917
pDPP-100°C
S
N
O
n
2.78
9.90
4.00
5.05
4.73
169.15
40.76
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)
Parameter Value
1 Data File Name F:/ NMR/ 300M/ 285/ fid
2 Title 300M
3 Comment 100oC yjj-pDPP
4 Origin UXNMR, Bruker Analytische Messtechnik GmbH
5 Owner root
6 Site
7 Spectrometer spect
8 Author
9 Solvent CDCl3
10 Temperature 350.3
11 Pulse Sequence zg30
12 Experiment 1D
13 Number of Scans 256
14 Receiver Gain 32768
15 Relaxation Delay 2.0000
16 Pulse Width 13.8000
17 Acquisition Time 1.8219
18 Acquisition Date 2014-08-12T17:27:14
19 Modification Date 2014-08-12T17:34:18
20 Spectrometer Frequency 300.13
21 Spectral Width 8992.8
22 Lowest Frequency -2314.2
23 Nucleus 1H
24 Acquired Size 16384
25 Spectral Size 32768

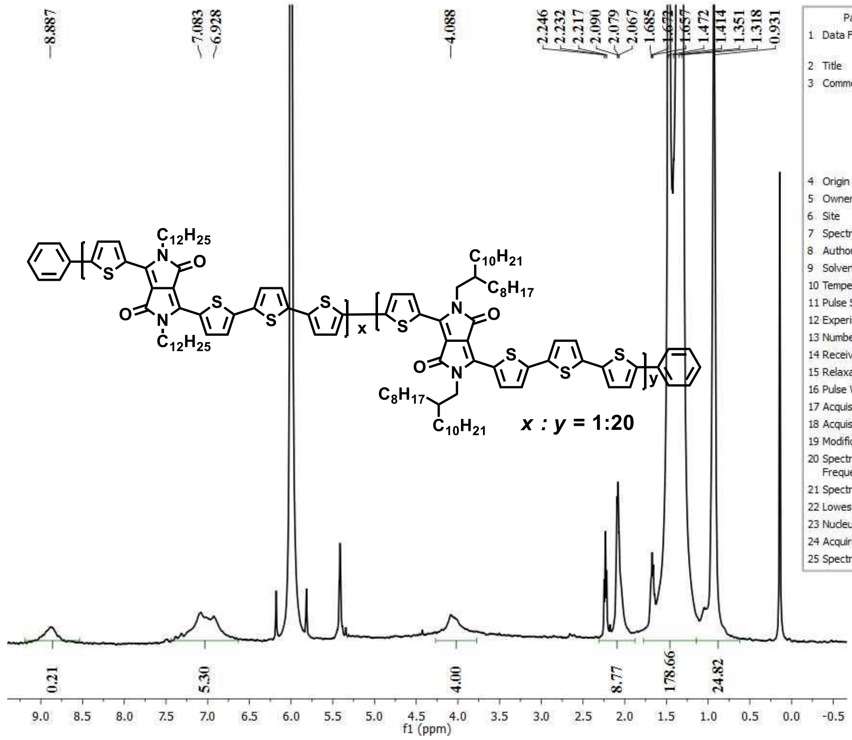
160.094
140.337
136.109
127.967
123.662
107.929
45.248
38.305
32.068
30.082
23.042
14.395
Solid 13C NMR
S
N
O
n
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30
f1 (ppm)
Parameter Value
1 Data File Name J:/ NMR/ 500M/ JACS NMR/ 181/ fid
2 Title C13-cptoss 2
3 Comment 13C CPTOSS 5kHz PDPP yao jing jing(zhang de qing) 20141103
4 Origin Bruker BioSpin GmbH
5 Owner hp
6 Site
7 Spectrometer spect
8 Author
9 Solvent None
10 Temperature 296.3
11 Pulse Sequence cptoss
12 Experiment 1D
13 Number of Scans 2048
14 Receiver Gain 1290
15 Relaxation Delay 2.0000
16 Pulse Width 2.5000
17 Acquisition Time 0.0258
18 Acquisition Date 2014-11-03T08:28:00
19 Modification Date 2014-11-04T01:27:54
20 Spectrometer Frequency 100.37
21 Spectral Width 39682.5
22 Lowest Frequency -9952.8
23 Nucleus 13C
24 Acquired Size 1024
25 Spectral Size 2048

# pDPP4T-A


4T-12C-20-30
1H NMR
4T-12C-30
C2D2Cl4
373.2K
Yao Jingjing
Zhang Deqing's group
20151104
8.840
7.067
6.985
6.907
4.086
2.247
2.232
2.218
2.176
2.090
2.079
1.672
1.658
1.471
1.415
1.351
1.318
0.931
C12H25
C10H21
C8H17
x : y = 1:30
0.04
5.58
4.00
11.65
213.42
27.91
f1 (ppm)
Parameter | Value
1 Data File Name | J:/ NMR/ 500M/ 4T-12C-20-30/ 322/ fid
2 Title | 4T-12C-20-30
3 Comment | 1H NMR 4T-12C-30 C2D2Cl4 373.2K Yao Jingjing Zhang Deqing's group 20151104
4 Origin | Bruker BioSpin GmbH
5 Owner | nmrsu
6 Site
7 Spectrometer | spect
8 Author
9 Solvent | CDCl2CDCl2
10 Temperature | 373.3
11 Pulse Sequence | zg30
12 Experiment | 1D
13 Number of Scans | 128
14 Receiver Gain | 211
15 Relaxation Delay | 2.0000
16 Pulse Width | 10.0000
17 Acquisition Time | 2.1845
18 Acquisition Date | 2015-11-04T22:23:11
19 Modification Date | 2015-11-05T08:36:00
20 Spectrometer Frequency | 500.13
21 Spectral Width | 15000.0
22 Lowest Frequency | -4975.6
23 Nucleus | 1H
24 Acquired Size | 32768
25 Spectral Size | 65536

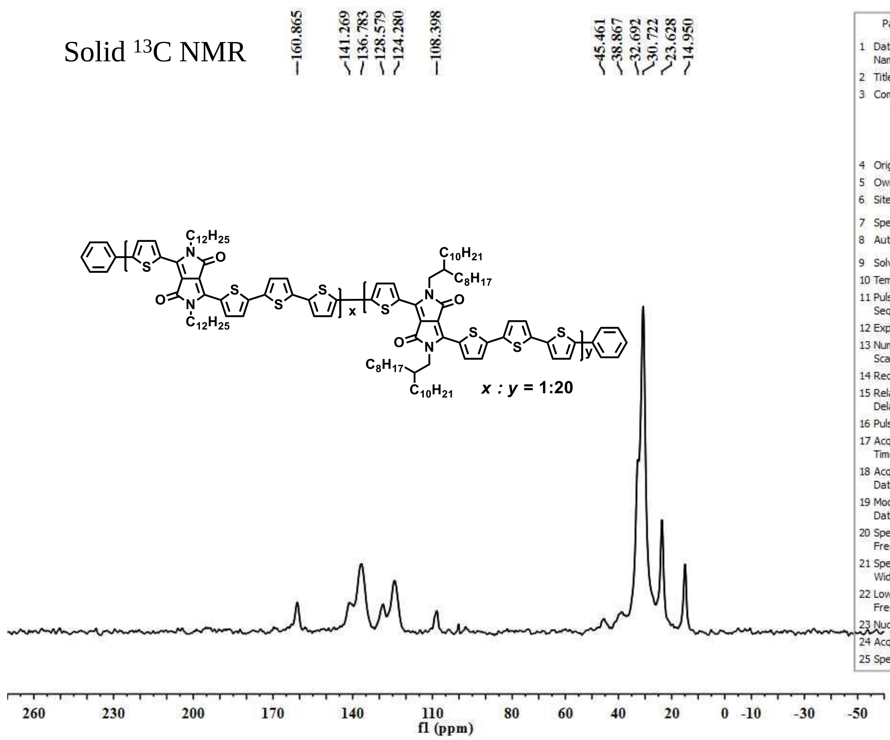

Solid 13C NMR
160.911
140.908
137.332
129.011
124.778
108.669
45.097
38.651
37.665
32.655
30.570
23.551
14.871
C12H25
C10H21
C8H17
x : y = 1:30
f1 (ppm)
Parameter | Value
1 Data File Name | J:/ NMR/ 500M/ JACS NMR/ 85/ fid
2 Title | C13-cptoss B
3 Comment | 13 CPTOSS 5kHz ada 3T yao jingjing(zhang deqing's group) 20151026
4 Origin | Bruker BioSpin GmbH
5 Owner | hp
6 Site
7 Spectrometer | spect
8 Author
9 Solvent | None
10 Temperature | 296.5
11 Pulse Sequence | cptoss
12 Experiment | 1D
13 Number of Scans | 1024
14 Receiver Gain | 1030
15 Relaxation Delay | 2.0000
16 Pulse Width | 2.5000
17 Acquisition Time | 0.0258
18 Acquisition Date | 2015-10-26T10:52:00
19 Modification Date | 2015-10-27T01:13:20
20 Spectrometer Frequency | 100.37
21 Spectral Width | 39682.5
22 Lowest Frequency | -9809.9
23 Nucleus | 13C
24 Acquired Size | 1024
25 Spectral Size | 2048

# pDPP4T-B



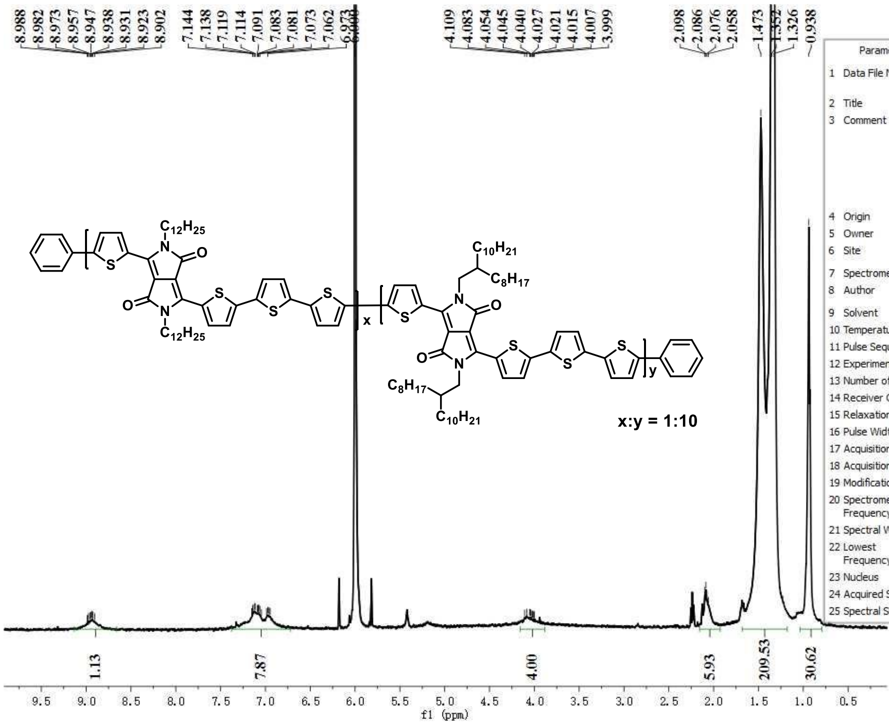

| Parameter | Value |
|---|---|
| 1 Data File Name | J:/ NMR/ 500M/ 4T-12C-20-30/ 321/ fid |
| 2 Title | 4T-12C-20-30 |
| 3 Comment | 1H NMR 4T-12C-20 C2D2Cl4 373.2K Yao Jingjing Zhang Deqing's group 20151104 |
| 4 Origin | Bruker BioSpin GmbH |
| 5 Owner | nmrsu |
| 6 Site | |
| 7 Spectrometer | spect |
| 8 Author | |
| 9 Solvent | CDCl2CDCl2 |
| 10 Temperature | 373.2 |
| 11 Pulse Sequence | zg30 |
| 12 Experiment | 1D |
| 13 Number of Scans | 128 |
| 14 Receiver Gain | 211 |
| 15 Relaxation Delay | 2.0000 |
| 16 Pulse Width | 10.0000 |
| 17 Acquisition Time | 2.1845 |
| 18 Acquisition Date | 2015-11-04T17:54:57 |
| 19 Modification Date | 2015-11-05T08:36:00 |
| 20 Spectrometer Frequency | 500.13 |
| 21 Spectral Width | 15000.0 |
| 22 Lowest Frequency | -4975.6 |
| 23 Nucleus | 1H |
| 24 Acquired Size | 32768 |
| 25 Spectral Size | 65536 |

Solid $^{13}$C NMR

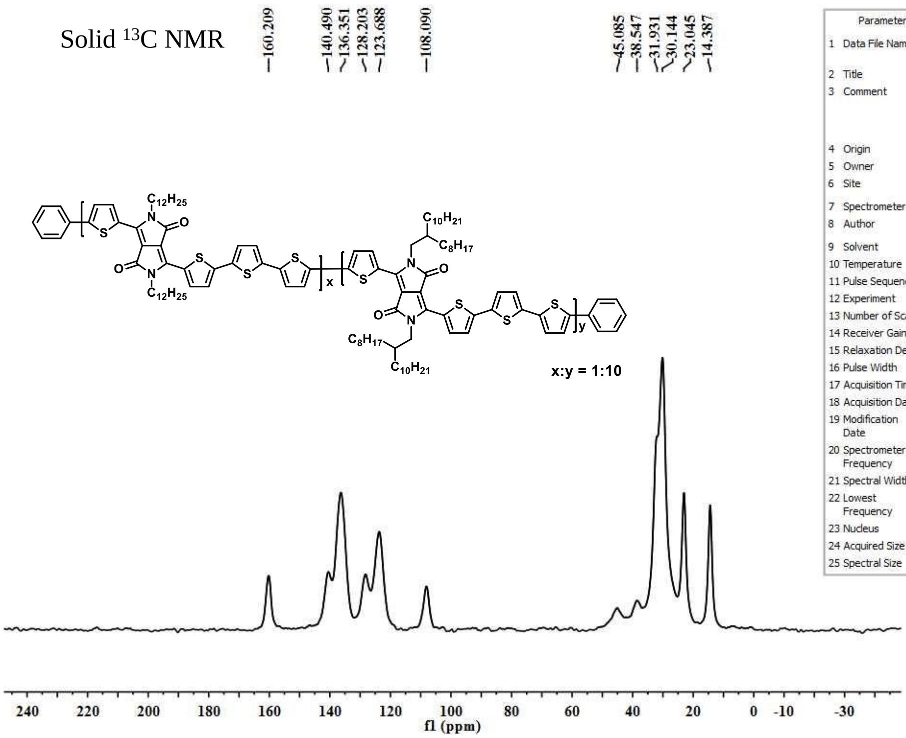



| Parameter | Value |
|---|---|
| 1 Data File Name | J:/ NMR/ 500M/ JACS NMR/ 86/ fid |
| 2 Title | C13-cptoss B |
| 3 Comment | 13 CPTOSS 5kHz ada 4T yao jingjing(zhang deqing's group) 20151026 |
| 4 Origin | Bruker BioSpin GmbH |
| 5 Owner | hp |
| 6 Site | |
| 7 Spectrometer | spect |
| 8 Author | |
| 9 Solvent | None |
| 10 Temperature | 296.4 |
| 11 Pulse Sequence | cptoss |
| 12 Experiment | 1D |
| 13 Number of Scans | 1024 |
| 14 Receiver Gain | 1030 |
| 15 Relaxation Delay | 2.0000 |
| 16 Pulse Width | 2.5000 |
| 17 Acquisition Time | 0.0258 |
| 18 Acquisition Date | 2015-10-26T11:31:00 |
| 19 Modification Date | 2015-10-27T01:59:10 |
| 20 Spectrometer Frequency | 100.37 |
| 21 Spectral Width | 39682.5 |
| 22 Lowest Frequency | -9808.1 |
| 23 Nucleus | 13C |
| 24 Acquired Size | 1024 |
| 25 Spectral Size | 2048 |

# pDPP4T-C




| | Parameter | Value |
|---|---|---|
| 1 | Data File Name | F:/ NMR/ 500M/ 101-DPP-12C-HNMR/ fid |
| 2 | Title | 500M |
| 3 | Comment | 1H NMR Juhewu C2D2Cl4 373.2 K Yao Jingjing Zhang Deqing's group 20150528 |
| 4 | Origin | Bruker BioSpin GmbH |
| 5 | Owner | nmrsu |
| 6 | Site | |
| 7 | Spectrometer | spect |
| 8 | Author | |
| 9 | Solvent | CDCl2CDCl2 |
| 10 | Temperature | 372.8 |
| 11 | Pulse Sequence | zg30 |
| 12 | Experiment | 1D |
| 13 | Number of Scans | 128 |
| 14 | Receiver Gain | 259 |
| 15 | Relaxation Delay | 2.0000 |
| 16 | Pulse Width | 10.0000 |
| 17 | Acquisition Time | 2.1845 |
| 18 | Acquisition Date | 2015-05-28T18:37:36 |
| 19 | Modification Date | 2015-05-29T01:46:00 |
| 20 | Spectrometer Frequency | 500.20 |
| 21 | Spectral Width | 15000.0 |
| 22 | Lowest Frequency | -4523.5 |
| 23 | Nucleus | 1H |
| 24 | Acquired Size | 32768 |
| 25 | Spectral Size | 65536 |




| | Parameter | Value |
|---|---|---|
| 1 | Data File Name | J:/ NMR/ 500M/ JACS NMR/ 7/ fid |
| 2 | Title | JACS NMR |
| 3 | Comment | 13C CPTOSS NMR 8kHz field :5667-5686 yao jingjing(zhang de qing's group) |
| 4 | Origin | Bruker BioSpin GmbH |
| 5 | Owner | hp |
| 6 | Site | |
| 7 | Spectrometer | spect |
| 8 | Author | |
| 9 | Solvent | None |
| 10 | Temperature | 295.1 |
| 11 | Pulse Sequence | cptoss |
| 12 | Experiment | 1D |
| 13 | Number of Scans | 1024 |
| 14 | Receiver Gain | 1030 |
| 15 | Relaxation Delay | 2.0000 |
| 16 | Pulse Width | 3.8000 |
| 17 | Acquisition Time | 0.0344 |
| 18 | Acquisition Date | 2015-12-16T02:27:16 |
| 19 | Modification Date | 2015-12-16T03:01:46 |
| 20 | Spectrometer Frequency | 100.37 |
| 21 | Spectral Width | 29761.9 |
| 22 | Lowest Frequency | -4902.3 |
| 23 | Nucleus | 13C |
| 24 | Acquired Size | 1024 |
| 25 | Spectral Size | 2048 |