

## Impact of fluorine substituted $\pi$ -bridge on the photovoltaic performance of small-molecule donor materials

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### 1. Experimental section

#### Materials synthesis

##### 5,5'-(2,5-difluoro-1,4-phenylene)bis(3-decylthiophene) (2a)

Compound **1a** (1 g, 3.7 mmol), (4-decylthiophen-2-yl)trimethylstannane (3.6 g), Pd(PPh<sub>3</sub>)<sub>4</sub> (247 mg), and 40 mL of toluene were added into a two necks round bottom flask. The mixture was stirred at 110 °C for 48 hours under argon protection. After removal of solvent, the crude reaction mixture was subjected to column chromatography on silica gel using petroleum ether as eluent to afford compound **2a** (1.5 g, yield 72%) as colorless solid.

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  (ppm) 7.42–7.30 (m, 4H), 6.98 (s, 2H), 2.63 (s, 4H), 1.61 (d, 10H), 1.27 (s, 22H), 0.88 (s, 6H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):  $\delta$  (ppm) 155.68, 144.25, 135.45, 128.28, 121.90, 121.21, 114.96, 31.92, 30.54, 30.47, 29.63, 29.60, 29.47, 29.34, 29.32, 22.70, 14.13. MS (MALDI-TOF): calcd. for C<sub>34</sub>H<sub>48</sub>F<sub>2</sub>S<sub>2</sub>  $m/z$  = 558.32; found 558.27.

##### 5,5'-(perfluoro-1,4-phenylene)bis(3-decylthiophene) (2b)

Compound **2b** was synthesized according to the same procedure of compound **2a**. The purified product (1.42 g, yield 65%) was a colorless solid.

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 7.48 (s, 2H), 7.13 (s, 2H), 2.65 (t, 4H), 1.64 (dd, 4H), 1.30 (d, 28H), 0.88 (t, 6H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 143.67, 143.61, 131.56, 131.53, 131.50, 127.53, 123.16, 31.92, 30.49, 30.38, 29.63, 29.60, 29.46, 29.34, 29.29, 22.70, 14.13. MS (MALDI-TOF): calcd. for  $\text{C}_{34}\text{H}_{46}\text{F}_4\text{S}_2$   $m/z$  = 594.30; found 593.42.

### **2-bromo-3-decyl-5-(4-(4-decylthiophen-2-yl)-2,5-difluorophenyl)thiophene (3a)**

Compound **2a** (1.5 g, 2.7 mmol) and *N*-Bromosuccinimide (534 mg, 3.0 mmol) were dissolved in 50 mL  $\text{CHCl}_3$  under an argon atmosphere and dark against light. After being stirred for 8 hours at room temperature, the reaction mixture was poured into water and extracted with  $\text{CH}_2\text{Cl}_2$ . The organic layer was washed with water three times and dried over  $\text{MgSO}_4$ . After removal of the solvent, the crude reaction mixture was subjected to column chromatography on silica gel using petroleum ether as eluent to afford compound **3a** (1.54 g, yield 90%) as colorless solid.

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 7.38–7.32 (m, 2H), 7.27 (dd, 1H), 7.16 (s, 1H), 6.98 (s, 1H), 2.71–2.54 (m, 4H), 1.68–1.52 (m, 6H), 1.27 (s, 26H), 0.88 (t, 6H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 144.30, 142.93, 128.43, 128.37, 127.46, 127.40, 121.44, 121.40, 115.26, 115.00, 114.68, 114.42, 110.66, 110.60, 31.92, 30.53, 30.47, 30.38, 29.72, 29.63, 29.61, 29.60, 29.58, 29.47, 29.42, 29.35, 29.33, 29.24, 24.15, 23.32, 21.59, 21.06, 15.12, 14.13. MS (MALDI-TOF): calcd. for  $\text{C}_{34}\text{H}_{47}\text{F}_2\text{S}_2\text{Br}$   $m/z$  = 636.23; found 637.15.

### **2-bromo-3-decyl-5-(4-(4-decylthiophen-2-yl)-2,3,5,6-tetrafluorophenyl)thiophene (3b)**

Compound **3b** (1.41 g, yield 88%) was synthesized similarly as described above for compound **3a** except that compound **2b** (1.42 g, 2.4 mmol) was used instead of compound **2a**.

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 7.49 (s, 1H), 7.35 (s, 1H), 7.15 (s, 1H), 2.63 (dt, 4H), 1.63 (dd, 4H), 1.27 (s, 25H), 0.88 (t, 9H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 145.13, 143.65, 142.49, 141.99, 131.71, 131.07, 128.24, 127.64, 127.38, 125.11,

124.41, 123.45, 113.06, 111.59, 31.93, 30.48, 30.37, 29.75, 29.70, 29.64, 29.62, 29.59, 29.48, 29.41, 29.36, 29.31, 29.21, 23.03, 22.71, 22.56, 14.43, 14.29, 14.13, 13.95. MS (MALDI-TOF): calcd. for C<sub>34</sub>H<sub>45</sub>F<sub>4</sub>S<sub>2</sub>Br  $m/z$  =672.21; found 673.20.

**5-(4-(5-bromo-4-decylthiophen-2-yl)-2,5-difluorophenyl)-3-decylthiophene-2-carbaldehyde (4a)**

Anhydrous *N,N*-Dimethylformamide (1 mL) and POCl<sub>3</sub> (0.9 mL) were added to a two necks round bottom flask and the mixture was stirred at 0 °C for 20 minutes. Subsequently, 1.54 g of compound **3a** (1.54 g, 2.4 mmol) in 1,2-dichloroethane (40 mL) was added to the mixture. Then the mixture was stirred at 90 °C for 8 hours. After cooling to ambient temperature, the reaction mixture was poured into ice water (60 mL) and neutralized with NaHCO<sub>3</sub>, and then extracted with CH<sub>2</sub>Cl<sub>2</sub>. The organic layer was washed with water three times and dried over MgSO<sub>4</sub>. After removing the solvent, the residue was subjected to column chromatography on silica gel using a mixture of CH<sub>2</sub>Cl<sub>2</sub> and petroleum ether (1:4, v/v) as the eluent to afford compound **4a** (1.53 g, yield 95%) as pale-yellow solid.

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ (ppm) 10.05 (s, 1H), 7.42 (s, 1H), 7.38 (s, 1H), 7.32 (s, 1H), 7.22 (s, 1H), 2.97 (t, 2H), 2.58 (t, 2H), 1.80–1.53 (m, 4H), 1.30 (d, 28H), 0.88 (t, 6H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ (ppm) 182.02, 153.28, 143.18, 137.51, 134.51, 130.14, 129.79, 128.17, 123.26, 120.43, 115.88, 115.46, 114.92, 114.56, 111.75, 31.91, 31.89, 31.47, 29.70, 29.61, 29.58, 29.52, 29.40, 29.38, 29.34, 29.31, 29.22, 28.59, 23.14, 22.68, 22.40, 14.39, 14.12, 13.94, 13.76. MS (MALDI-TOF): calcd. for C<sub>35</sub>H<sub>47</sub>F<sub>2</sub>OS<sub>2</sub>Br  $m/z$  =664.22; found 665.39.

**5-(4-(5-bromo-4-decylthiophen-2-yl)-2,3,5,6-tetrafluorophenyl)-3-decylthiophene-2-carbaldehyde (4b)**

Compound **4b** (1.32 g, yield 90%) was synthesized similarly as described above for compound **4a** except that compound **3b** (1.41 g, 2.1 mmol) was used instead of compound **3a**.

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ (ppm) 10.11 (s, 1H), 7.52 (s, 1H), 7.41 (s, 1H), 3.01 (t, 2H), 2.62 (t, 2H), 2.13–1.49 (m, 38H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ (ppm) 182.31, 152.17, 144.01, 142.97, 142.73, 138.94, 138.76, 135.90, 133.34, 132.21, 131.70,

127.30, 124.88, 124.10, 113.84, 31.91, 31.47, 30.48, 30.34, 30.32, 29.71, 29.67, 29.60, 29.57, 29.52, 29.47, 29.39, 29.36, 29.34, 29.31, 29.29, 29.18, 28.47, 22.68, 14.12. MS (MALDI-TOF): calcd. for C<sub>35</sub>H<sub>45</sub>F<sub>4</sub>OS<sub>2</sub>Br  $m/z$  = 700.20; found 701.25.

**5,5'-(((4,8-bis(5-(2-ethylhexyl)thiophen-2-yl)benzo[1,2-b:4,5-b']dithiophene-2,6-diyl)bis(4-decylthiophene-5,2-diyl))bis(2,5-difluoro-4,1-phenylene))bis(3-decylthiophene-2-carbaldehyde) (5a)**

(4,8-Bis(5-(2-ethylhexyl)thiophen-2-yl)benzo[1,2-b:4,5-b']dithiophene-2,6-diyl)bis(trimethylstannane) (200 mg, 0.22 mmol), compound **4a** (366 mg, 0.55 mmol), Pd(PPh<sub>3</sub>)<sub>4</sub> (15 mg), and 40 mL of toluene were added into a two necks round bottom flask and stirred at 110 °C for 48 hours under argon protection. After removing solvent, the crude reaction mixture was subjected to column chromatography on silica gel using a mixture of CH<sub>2</sub>Cl<sub>2</sub> and petroleum ether (4:5, v/v) as eluent to afford compound **5a** (347 mg, yield 90%) as red solid.

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ (ppm) 10.07 (s, 2H), 7.72 (s, 2H), 7.38 (d, 10H), 6.93 (s, 2H), 3.00–2.83 (m, 12H), 1.61 (s, 40H), 1.27 (s, 56H), 0.87 (d, 10H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ (ppm) 181.97, 154.15, 153.64, 153.26, 145.98, 144.04, 141.85, 139.01, 137.44, 136.90, 136.81, 136.59, 134.04, 134.00, 132.96, 132.91, 130.85, 130.77, 129.97, 129.90, 127.85, 125.51, 123.43, 121.84, 41.52, 34.33, 32.56, 31.95, 31.90, 31.47, 30.59, 29.93, 29.88, 29.71, 29.64, 29.59, 29.54, 29.41, 29.39, 29.35, 29.32, 29.26, 29.15, 28.96, 28.59, 25.75, 23.07, 22.71, 22.69, 14.19, 14.13, 10.94. MS (MALDI-TOF): calcd. for C<sub>104</sub>H<sub>134</sub>F<sub>4</sub>O<sub>2</sub>S<sub>8</sub>  $m/z$  = 1747.81; found 1747.07.

**5,5'-(((4,8-bis(5-(2-ethylhexyl)thiophen-2-yl)benzo[1,2-b:4,5-b']dithiophene-2,6-diyl)bis(4-decylthiophene-5,2-diyl))bis(2,3,5,6-tetrafluoro-4,1-phenylene))bis(3-decylthiophene-2-carbaldehyde) (5b)**

Compound **5b** (353 mg, yield 88%) was synthesized similarly as described above for compound **5a** except that compound **4b** (385 mg, 0.55 mmol) was used instead of compound **4a**.

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ (ppm) 10.04 (s, 2H), 7.68 (s, 2H), 7.50 (s, 2H), 7.46 (s, 2H), 7.30 (s, 2H), 6.86 (s, 2H), 2.93 (t, 4H), 2.81 (s, 8H), 1.53 (s, 30H), 1.23 (d, 60H), 0.86 – 0.79 (m, 16H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ (ppm) 182.24, 152.17, 150.00,

147.76, 146.13, 141.24, 139.25, 137.16, 136.99, 136.69, 136.24, 136.12, 133.29, 129.69, 128.44, 127.89, 125.56, 124.47, 123.99, 123.73, 123.65, 122.41, 120.21, 119.11, 41.51, 34.92, 34.88, 34.57, 34.29, 32.55, 31.94, 31.89, 31.45, 30.61, 30.20, 29.71, 29.68, 29.57, 29.52, 29.49, 29.37, 29.31, 29.27, 28.95, 28.48, 27.10, 25.75, 24.60, 23.05, 22.70, 14.12, 10.92. MS (MALDI-TOF): calcd. for C<sub>104</sub>H<sub>130</sub>F<sub>8</sub>O<sub>2</sub>S<sub>8</sub> *m/z* =1819.77; found 1818.88.

#### **BDTP-2F**

Compound **5a** (347 mg, 0.2 mmol) was dissolved in a solution of anhydrous CHCl<sub>3</sub> (40 mL) and piperidine (1 mL). After adding 3-ethylrhodanine (640 mg, 4 mmol), mixture was stirred and refluxed for 8 hours under argon. Then the reaction mixture was extracted with CHCl<sub>3</sub> and dried over MgSO<sub>4</sub>. After removal of the solvent, the residue was subjected to column chromatography on silica gel using a mixture of CH<sub>2</sub>Cl<sub>2</sub> and petroleum ether (3:5, v/v) as the eluent to afford BDTP-2F as a dark red solid (343 mg, 85% yield).

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>), as shown in **Fig. S6**: δ (ppm) 7.85 (s, 2H), 7.59 (s, 2H), 7.36 (d, 4H), 7.29 (d, 4H), 7.23 (s, 2H), 6.96 (d, 2H), 4.14 (q, 4H), 2.94 (d, 4H), 2.76 (dd, 8H), 1.65 (d, 8H), 1.57 (s, 4H), 1.44–1.23 (m, 76H), 0.99 (dt, 12H), 0.89 (dd, 12H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>), as shown in **Fig. S7**: δ (ppm) 191.97, 167.19, 156.10, 155.85, 153.64, 153.38, 150.50, 145.56, 141.95, 141.92, 141.22, 138.24, 136.92, 136.52, 136.42, 133.56, 133.51, 132.88, 132.83, 130.54, 129.37, 127.92, 125.40, 122.82, 122.41, 120.81, 120.29, 41.53, 39.78, 34.39, 32.66, 32.03, 31.94, 31.11, 30.34, 30.16, 29.97, 29.92, 29.85, 29.79, 29.72, 29.66, 29.56, 29.53, 29.51, 29.39, 29.34, 29.02, 25.73, 23.17, 22.77, 22.72, 14.28, 14.17, 14.15, 12.30, 10.98. MS (MALDI-TOF) as shown in **Fig. S8**: calcd. for C<sub>114</sub>H<sub>144</sub>F<sub>4</sub>N<sub>2</sub>O<sub>2</sub>S<sub>12</sub> *m/z* =2033.78; found 2034.32.

#### **BDTP-4F**

**BDTP-4F** (327 mg, yield 80%) was synthesized similarly as described above for **BDTP-2F** except that compound **5b** (353 mg, 0.2 mmol) was used instead of compound **5a**.

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ), as shown in **Fig. S9**:  $\delta$  (ppm) 7.87 (s, 2H), 7.64 (s, 2H), 7.55 (s, 2H), 7.49 (s, 2H), 7.38 (d, 2H), 6.99 (d, 2H), 4.17 (q, 4H), 2.95 (d, 4H), 2.87–2.70 (m, 8H), 1.85–1.51 (m, 18H), 1.46–1.29 (dd, 68H), 1.09–0.84 (m, 26H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ), as shown in **Fig. S10**:  $\delta$  (ppm) 191.91, 167.19, 149.38, 145.80, 145.27, 145.04, 144.80, 142.47, 140.66, 138.46, 136.69, 136.56, 136.11, 134.60, 134.37, 134.31, 133.80, 132.53, 132.49, 128.02, 126.41, 125.47, 123.11, 122.42, 121.41, 112.69, 110.42, 41.52, 39.87, 34.38, 32.64, 32.01, 31.93, 31.09, 30.33, 29.91, 29.87, 29.82, 29.72, 29.66, 29.64, 29.51, 29.48, 29.37, 29.04, 29.00, 28.90, 28.85, 25.71, 23.13, 22.76, 22.72, 14.23, 14.16, 14.14, 12.28, 10.93. MS (MALDI-TOF) as shown in **Fig. S11**: calcd. for  $\text{C}_{114}\text{H}_{140}\text{F}_8\text{N}_2\text{O}_2\text{S}_{12}$   $m/z = 2107.09$ ; found 2105.36.

## 2. Materials characterization

NMR spectra were recorded in  $\text{CDCl}_3$  on a Bruker AV 400 MHz FT-NMR spectrometer and chemical shifts are quoted relative to tetramethylsilane for  $^1\text{H}$  and  $^{13}\text{C}$  nuclei. The molecular mass was confirmed by using an Ultraflex extreme matrix-assisted laser desorption ionization mass spectrometer (MALDI-TOF-MS).

UV-Vis absorption spectra were recorded on the Cary 5000 UV-Vis-NIR Spectrophotometer. For the solid-state measurements, two small-molecule solutions in chloroform were spin-coated on quartz plates.

A Cyclic voltammetry was performed on a Zahner IM6e electrochemical workstation with a three-electrode system in a solution of 0.1 M  $[\text{Bu}_4\text{N}]\text{PF}_6$  acetonitrile solution at a scan rate of  $100 \text{ mV s}^{-1}$ . Glassy carbon disc coated with small-molecule film was used as the working electrode. A Pt wire was used as the counter electrode and  $\text{Ag}/\text{Ag}^+$  was used as the reference electrode. Ferrocene/ferrocenium redox couple was used as the external standard and its redox potential is 0.06 V versus  $\text{Ag}/\text{Ag}^+$ . The HOMO and LUMO energy levels were calculated from the onset of the oxidation and reduction potential of small-molecule using the following equations:  $\text{HOMO} = -e(\varphi_{\text{ox}} + 4.74)$  (eV);  $\text{LUMO} = -e(\varphi_{\text{red}} + 4.74)$  (eV), respectively.

DSC traces were recorded on the Discovery DSC2500 in nitrogen at a rate of  $10 \text{ }^\circ\text{C min}^{-1}$ .

### 3. Device fabrication and characterization

The device was fabricated with a conventional architecture of glass/ITO/PEDOT:PSS/active layer/PDINO/Al. The ITO-coated glass was pre-cleaned and modified by a thin layer of PEDOT:PSS which was spin-cast from a PEDOT:PSS aqueous solution (Baytron PVP Al4083 from H.C. Stark) at 5000 rpm for 40 s, and then dried at 150 °C for 15 min in air. The thickness of the PEDOT:PSS layer is 30 nm. Then the devices were transferred to a nitrogen-filled glove-box, where the active layer was spin-coated from chloroform solution onto the PEDOT:PSS layer. The PDINO which serves as the electron-transporting layer is spin-coated onto the active layer at 4000 rpm for 30 s. Finally, top 100 nm Al electrode was deposited in vacuum onto the PDINO layer at a pressure of  $3.0 \times 10^{-4}$  Pa. The active area defined by an aperture mask with area of  $10.00 \text{ mm}^2$  ( $2.00 \text{ mm} \times 5.00 \text{ mm}$ ) for determining the active area of the solar cells.

The current density-voltage ( $J$ - $V$ ) measurement of the OSCs were measured under a illumination of AM 1.5G ( $100 \text{ mW cm}^{-2}$ ) using a SS-F5-3A solar simulator (AAA grade,  $50 \times 50 \text{ mm}^2$  photobeam size) of Enli Technology CO., Ltd.. The EQE was measured by using a Solar Cell Spectral Response Measurement System QE-R3011 (Enli Technology Co., Ltd.). The light intensity at each wavelength was calibrated by a standard single-crystal Si solar cell.

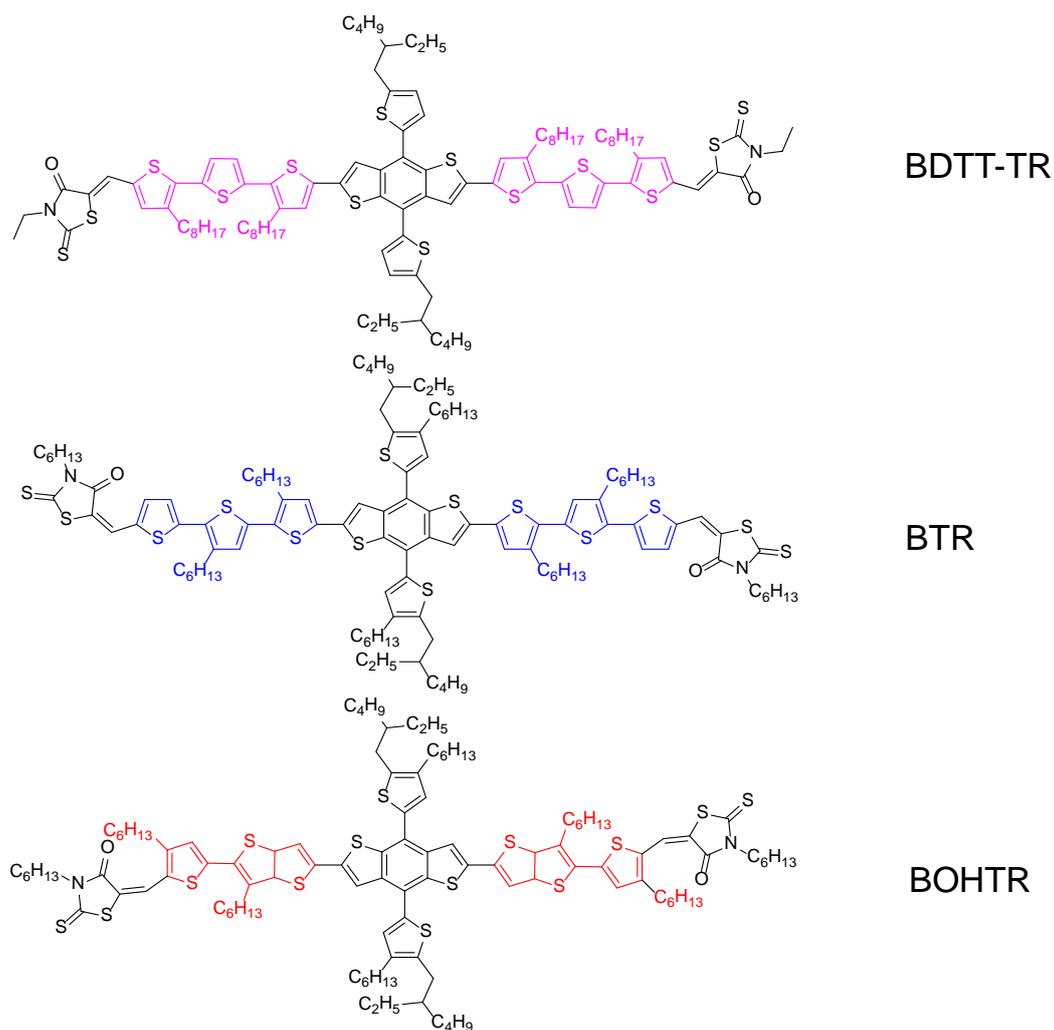
### 4. Mobility measurement.

The devices with a structure of glass/ITO/PDEOT:PSS/active layer/MoO<sub>3</sub>/Al and a structure of glass/ITO/ZnO/active layer/PDINO/Al were fabricated to measure the hole and electron mobilities, respectively. The devices were protected from light with tin foil during the measurements. The hole and electron mobilities were calculated by using the space-charge-limited current method. The statistical values for the hole and electron mobilities were calculated from four devices, respectively.

$$J \cong (9/8)\varepsilon\varepsilon_0\mu_0V^2 \exp(0.89\sqrt{V/E_0L})/L^3$$

where  $\varepsilon$  is the dielectric constant of the polymers,  $\varepsilon_0$  is the permittivity of the vacuum,  $\mu_0$  is the zero-field mobility,  $E_0$  is the characteristic field,  $J$  is the current density, and

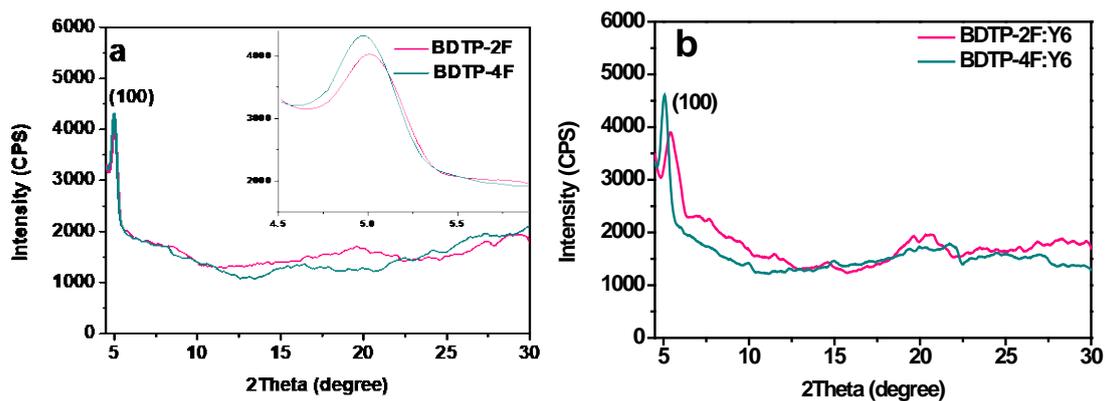
$L$  is the thickness of the film.



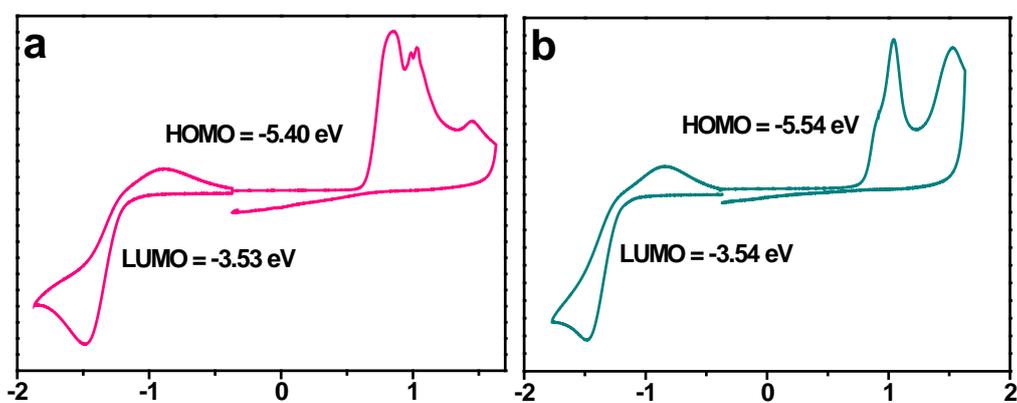
**Fig. S1** The chemical structures of BDTT-TR, BTR and BOHTR.

**Table S1** the HOMO energy levels of donors and their selected device performances

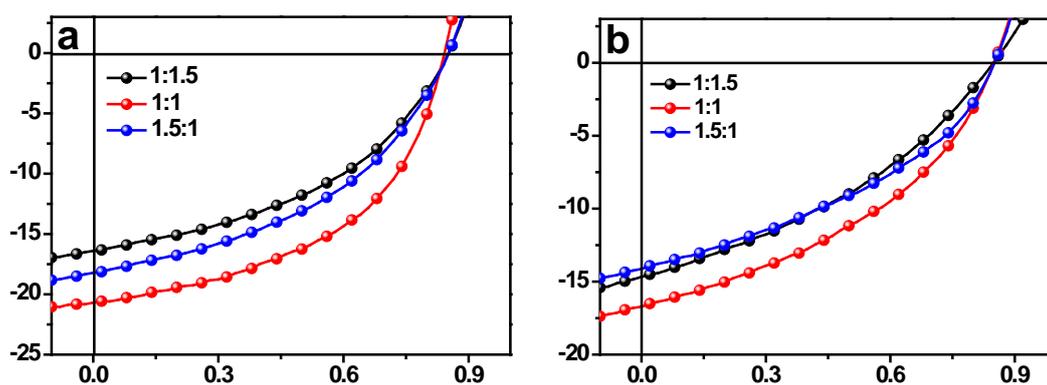
Donor	HOMO	Acceptor	$V_{oc}$ [V]	$J_{sc}$ [ $\text{mA cm}^{-2}$ ]	FF	PCE [%]	Reference
BDTT-TR	-5.17	Y6	0.780	23.64	0.661	12.18	1
BOHTR	-5.36	Y6	0.830	23.1	0.562	10.80	2
BTR	-5.34	Y6	0.850	22.25	0.564	10.67	3
BDTP-2F	-5.40	Y6	0.859	23.24	0.512	10.21	This work
BDTP-4F	-5.54	Y6	0.850	16.72	0.404	5.76	This work

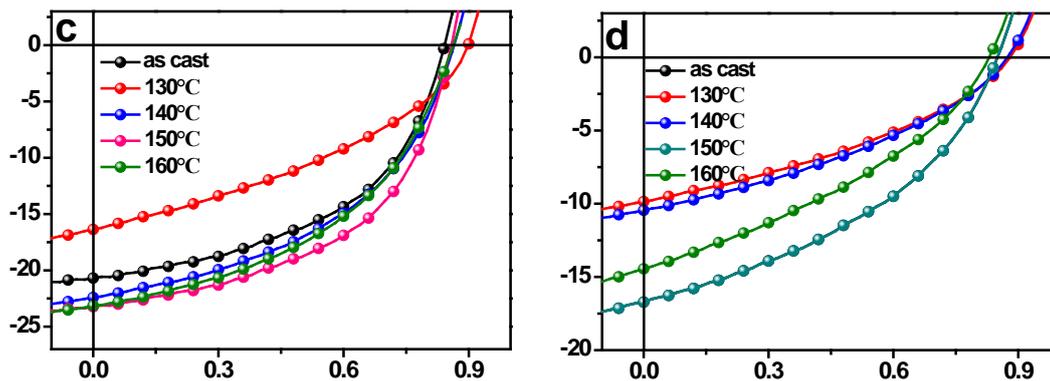


**Fig. S2** X-ray diffraction patterns of BDTP-2F, BDTP-4F, BDTP-2F:Y6 and BDTP-4F:Y6 films cast from  $\text{CHCl}_3$  on Si substrates.



**Fig. S3** Cyclic voltammograms of BDTP-2F (a) and BDTP-4F (b).

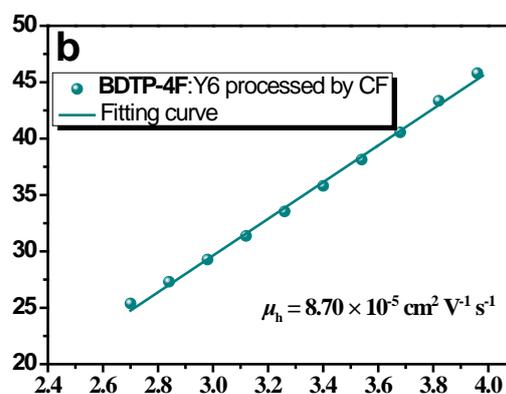
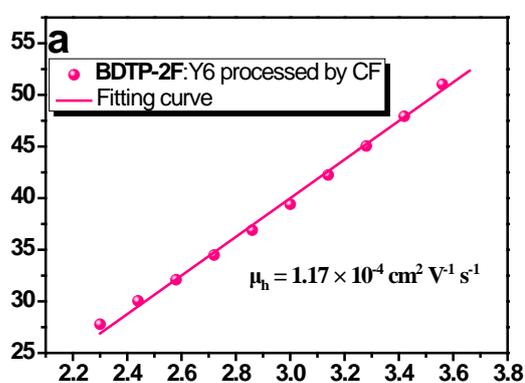


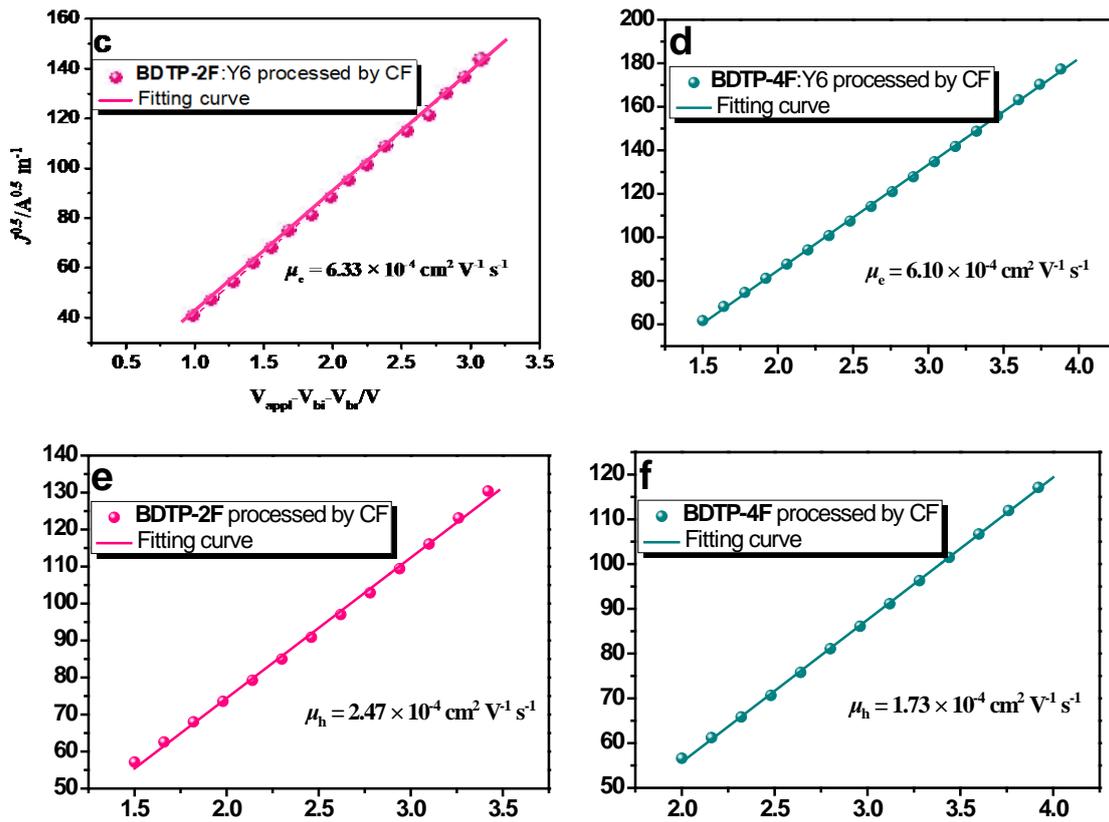


**Fig. S4** The  $J$ - $V$  curves of the devices based BDTP-2F (a) and BDTP-4F (b) with different D/A ratio. The  $J$ - $V$  curves of the devices based BDTP-2F (c) and BDTP-4F (d) with different TA temperature.

**Table S1** Photovoltaic parameters of device based on BDTP-2F:Y6 and BDTP-4F:Y6 blended films with different donor: acceptor under one sun illumination.

donor	D/A ratio	$V_{oc}$ [V]	$J_{sc}$ [ $\text{mA cm}^{-2}$ ]	FF	PCE [%]
BDTP-2F	1:1.5	0.853	16.40	0.352	4.93
	1:1	0.851	20.69	0.387	6.82
	1.5:1	0.850	18.21	0.372	5.74
BDTP-4F	1:1.5	0.848	14.68	0.361	4.51
	1:1	0.850	16.72	0.387	5.50
	1.5:1	0.851	14.13	0.386	4.66





**Fig. S5** (a) Hole-only and (c) electron only device of BDTP-2F:Y6 blend film; (b) Hole-only and (d) electron only device of BDTP-4F:Y6 blend film; hole-only device of pristine (e) BDTP-2F and (f) BDTP-4F films.

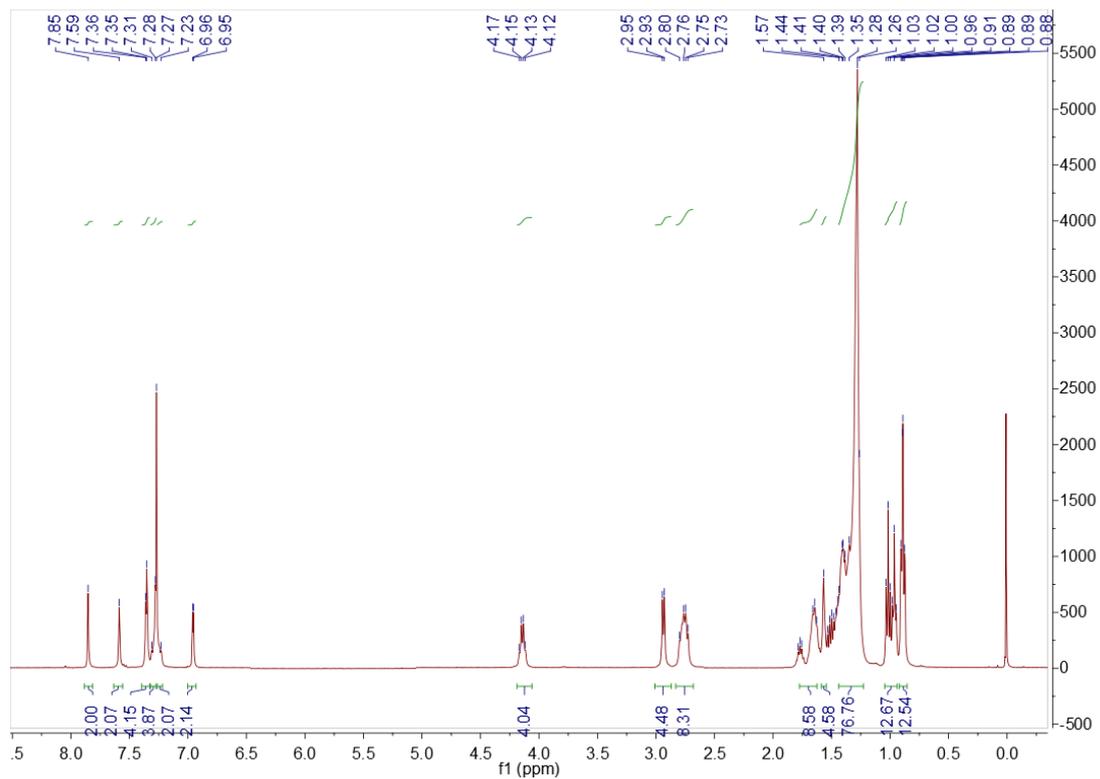


Fig. S6 The  $^1\text{H}$  NMR spectrum of BDTP-2F in  $\text{CDCl}_3$ .

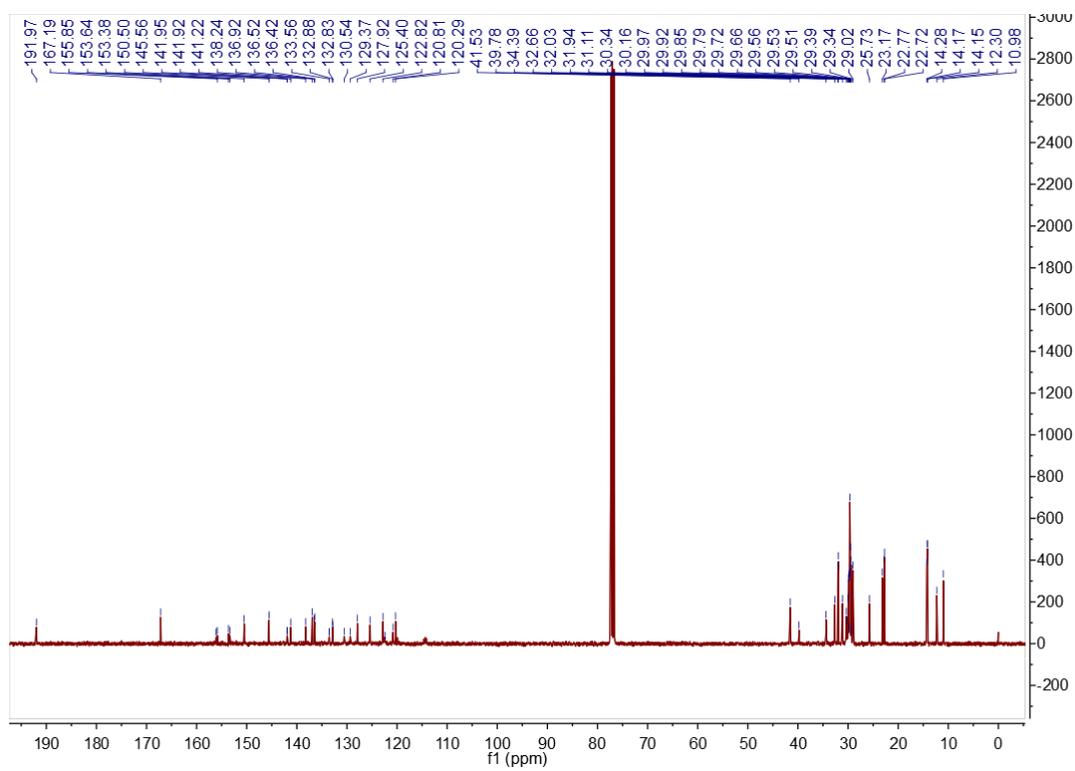
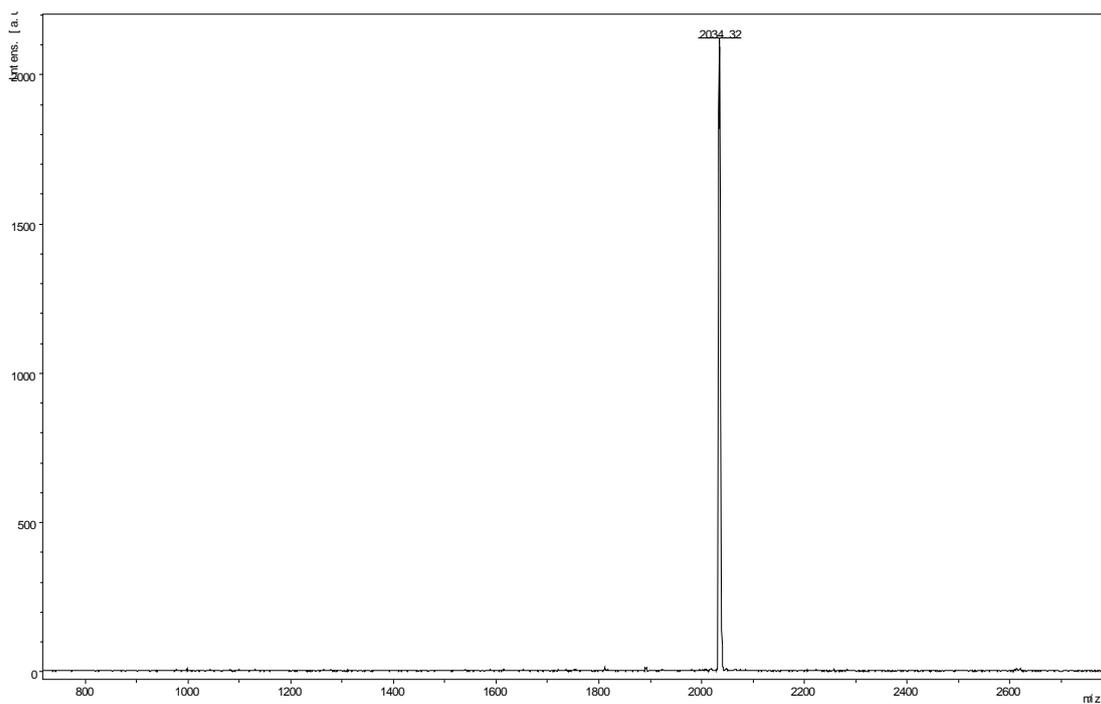
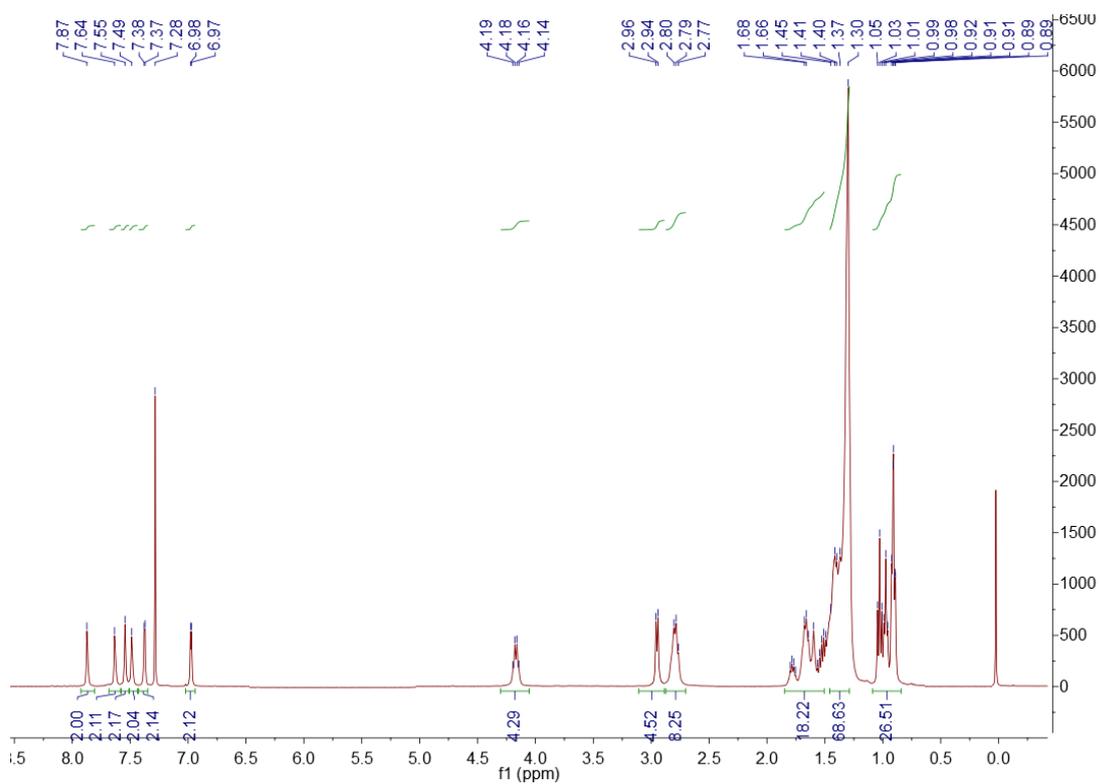


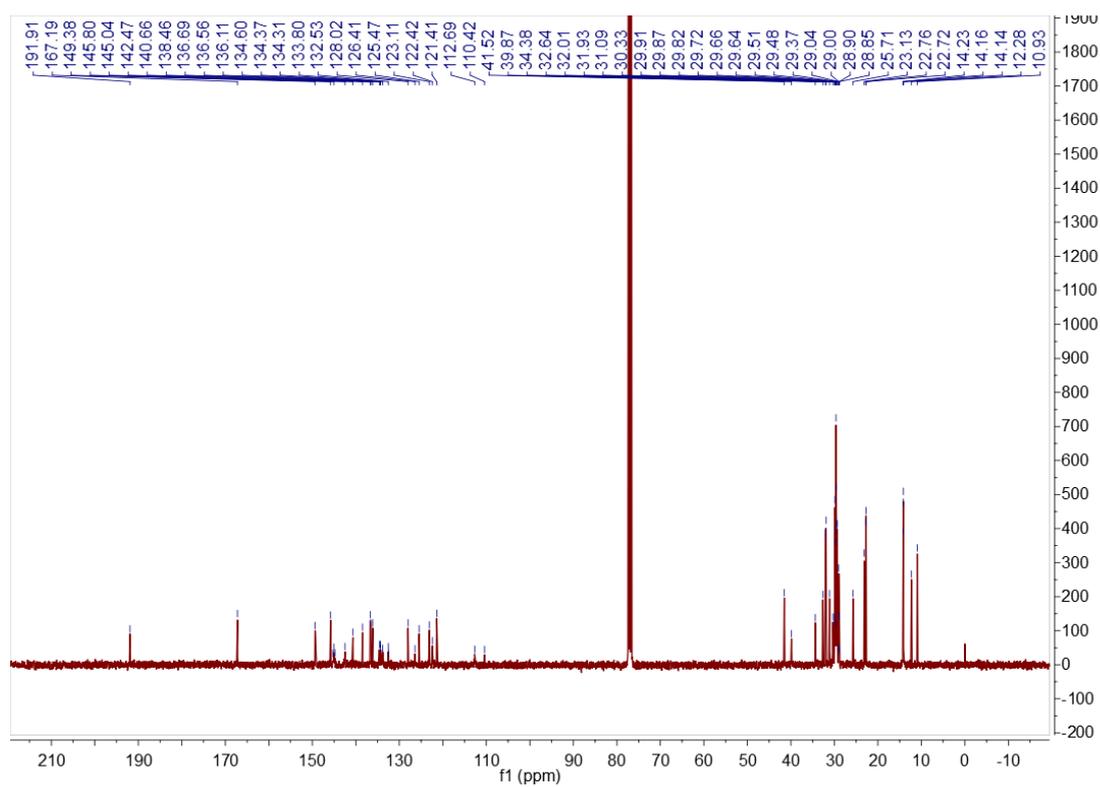
Fig. S7 The  $^{13}\text{C}$  NMR spectrum of BDTP-2F in  $\text{CDCl}_3$ .



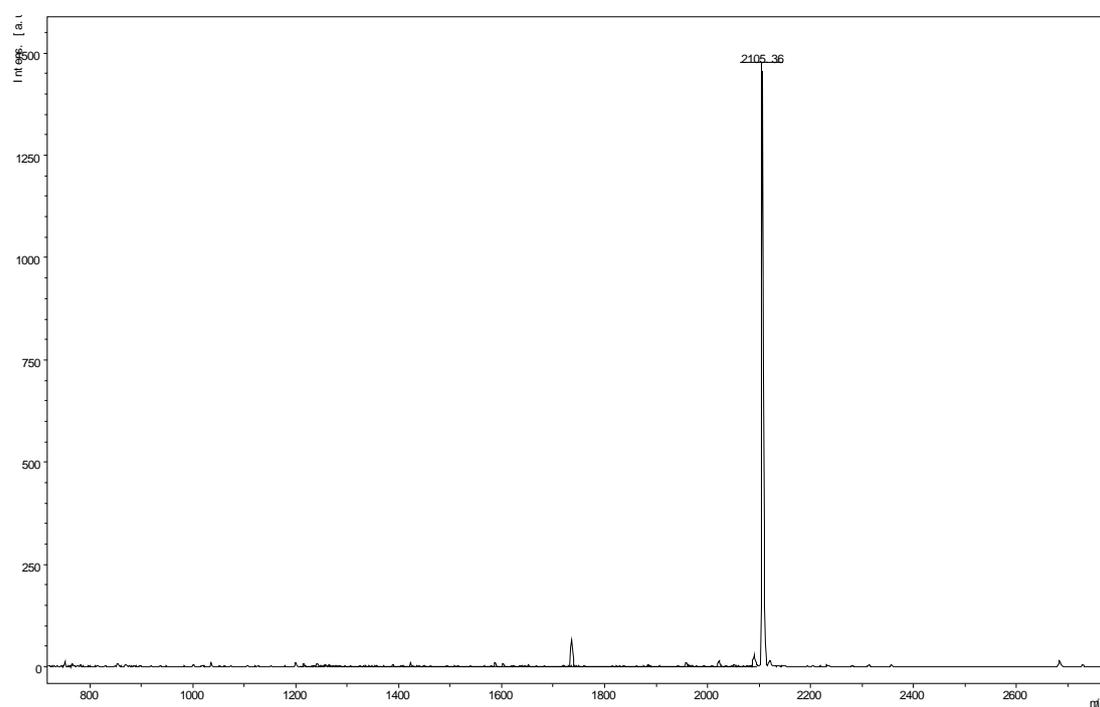
**Figure S8** Mass spectrum of BDTP-2F.



**Fig. S9** The  $^1\text{H}$  NMR spectrum of BDTP-4F in  $\text{CDCl}_3$ .



**Fig. S10** The  $^{13}\text{C}$  NMR spectrum of BDTP-4F in  $\text{CDCl}_3$ .



**Figure S11** Mass spectrum of BDTP-4F.

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