

# Electron acceptors with a truxene core and perylene diimide branches for organic solar cells: the effect of ring-fusion

Kaiwen Lin<sup>‡</sup>, Shiliang Wang<sup>‡</sup>, Zhenfeng Wang, Qingwu Yin, Xi Liu, Jianchao Jia, Xiao'e Jia, Peng Luo, Xiaofang Jiang, Chunhui Duan\*, Fei Huang\* and Yong Cao

<sup>‡</sup>*These authors contributed equally to this work.*

*\*Corresponding author. Institute of Polymer Optoelectronic Materials and Devices, State Key Laboratory of Luminescent Materials and Devices, South China University of Technology, Guangzhou 510640, P. R. China.*

*E-mail: duanchunhui@scut.edu.cn; msfhuang@scut.edu.cn*

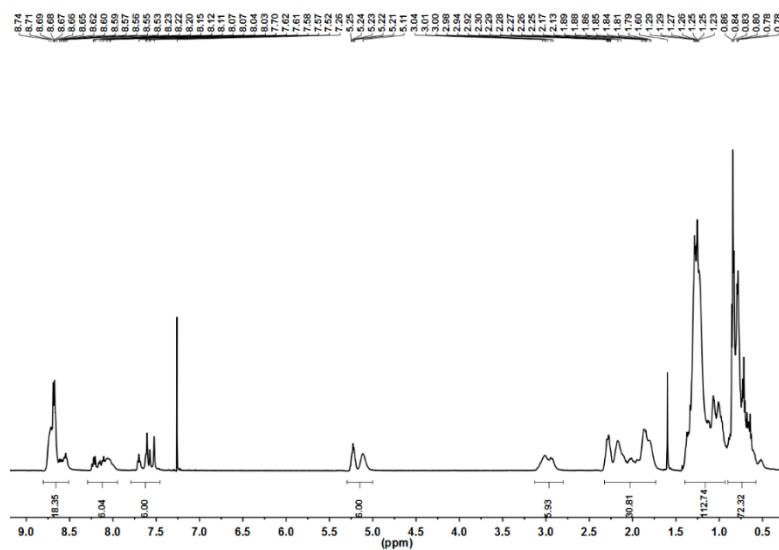


FIGURE S1  $^1\text{H}$  NMR spectrum of Tr-3PDI.

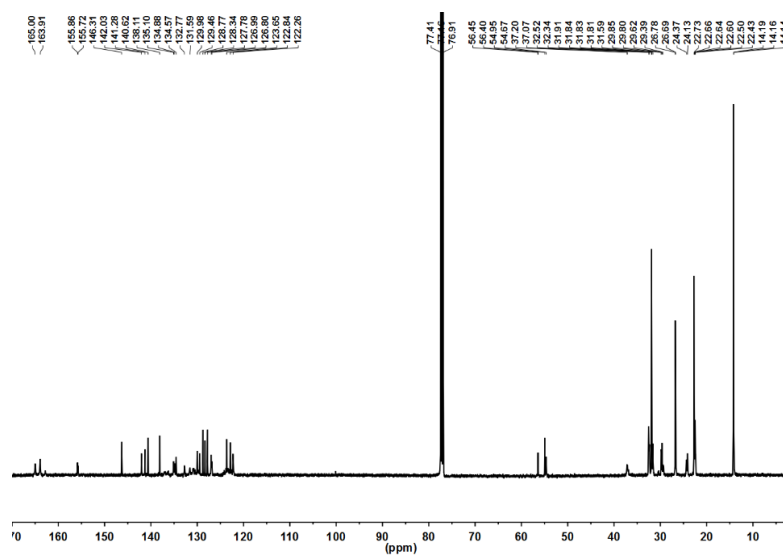


FIGURE S2  $^{13}\text{C}$  NMR spectrum of Tr-3PDI.

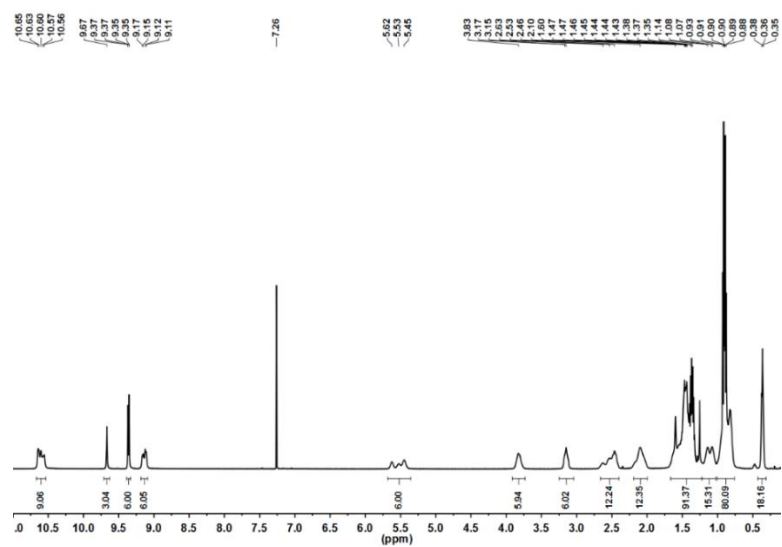


FIGURE S3  $^1\text{H}$  NMR spectrum of FTr-3PDI.

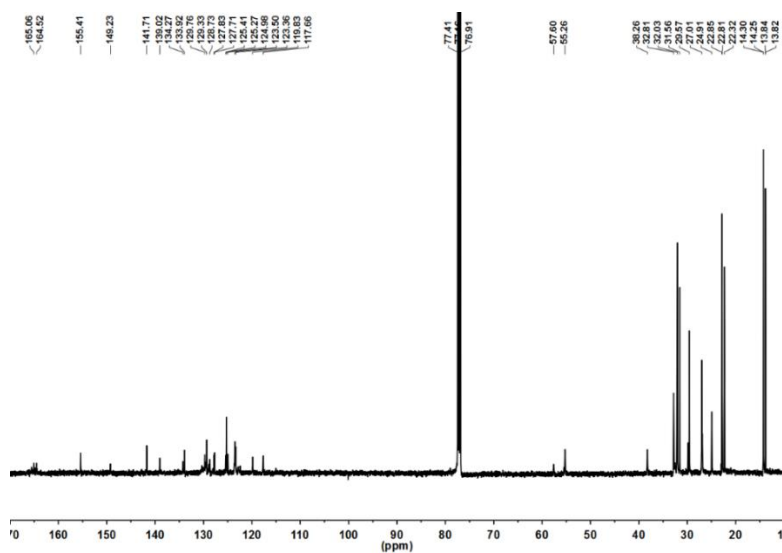
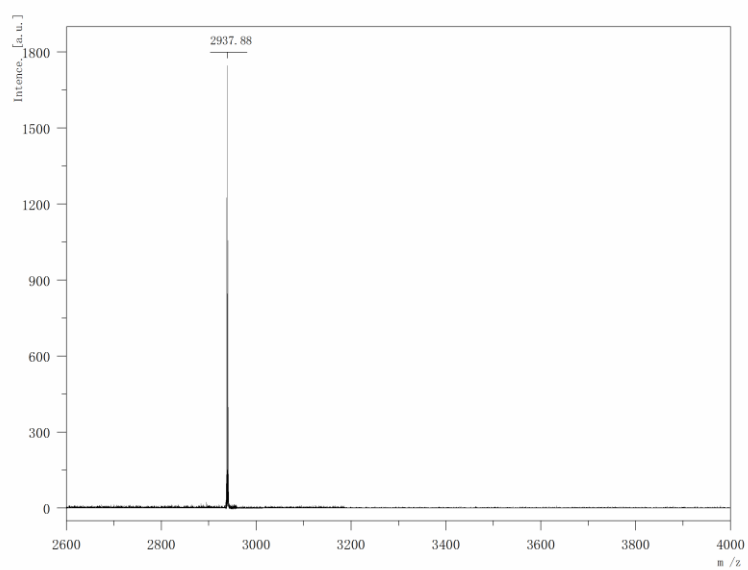
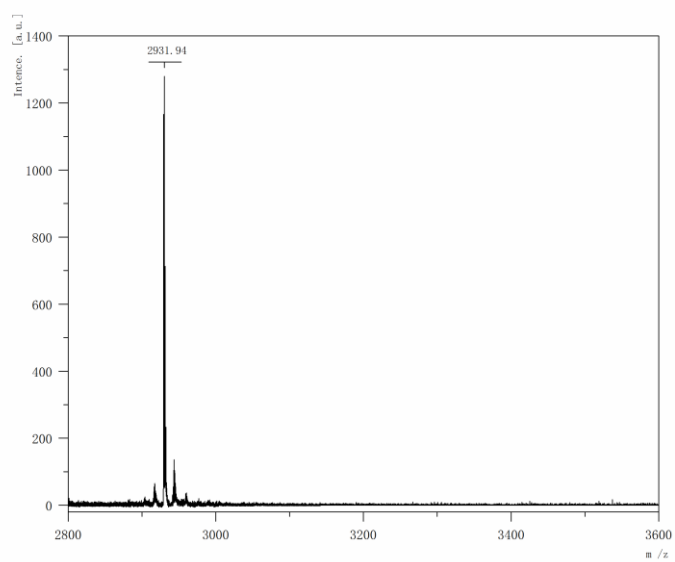


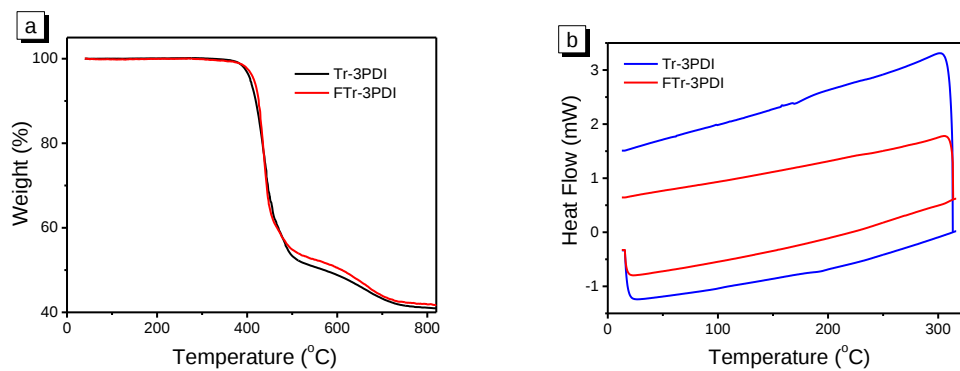
FIGURE S4  $^{13}\text{C}$  NMR spectrum of FTr-3PDI.



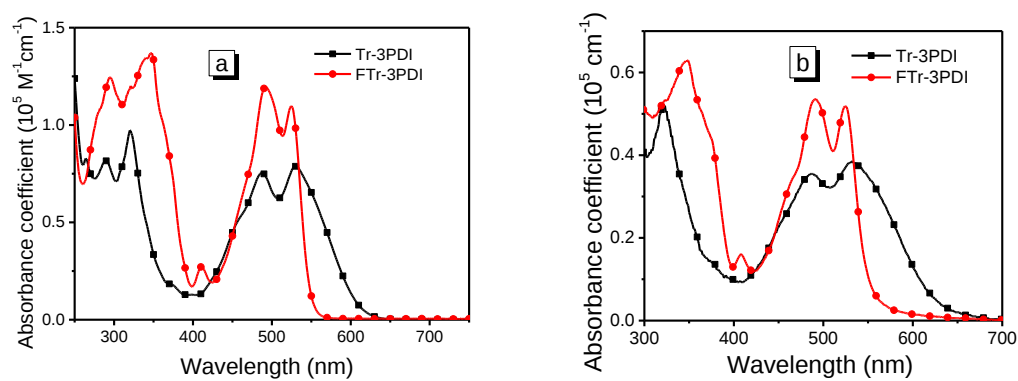
**FIGURE S5** Maldi-TOF of Tr-3PDI.



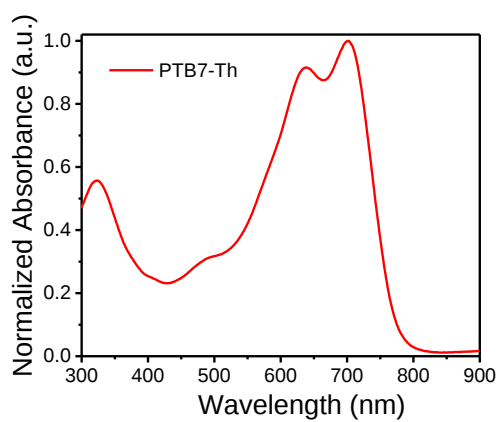
**FIGURE S6** Maldi-TOF of FTr-3PDI.



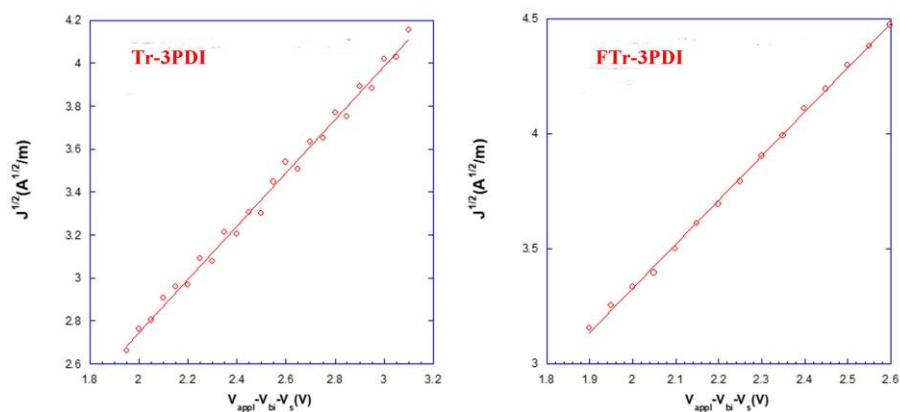
**FIGURE S7** (a) TGA and (b) DSC spectra of Tr-3PDI and FTr-3PDI.



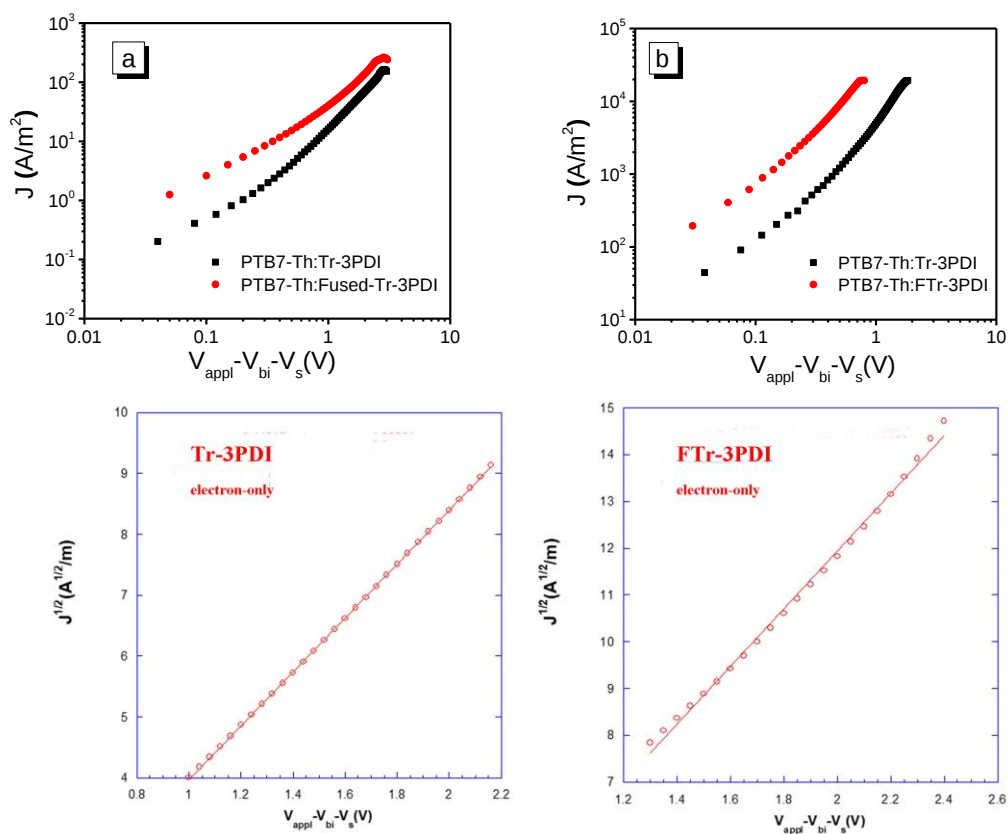
**FIGURE S8** UV-vis absorption spectra of Tr-3PDI and FTr-3PDI in chloroform solution ( $1.0 \times 10^{-5}$  M) (a) and as thin film (b).



**FIGURE S9** UV-vis absorption spectra of PTB7-Th.



**FIGURE S10**  $J$ - $V$  characteristics of the pure truxene-PDI acceptors in electron-only devices.



**FIGURE S11**  $J$ - $V$  characteristics of the blend films of PTB7-Th:truxene-PDI acceptors in electron-only devices (a) and hole-only devices (b).

**TABLE S1** The optimization of host solvents (the thickness of active layers is 90 nm±5nm; donor/acceptor weight ratios is 1:1).

| Sample          | solvent      | $V_{oc}$ (V) | $J_{sc}$ (mA cm <sup>-2</sup> ) | $J_{sc}$ (mA cm <sup>-2</sup> )<br>(%) | PCE (%)     |
|-----------------|--------------|--------------|---------------------------------|----------------------------------------|-------------|
| PTB7-Th:Tr-3PDI | CF           | 0.89         | 4.65                            | 32.78                                  | 1.36        |
|                 | <b>o-DCB</b> | 0.90         | 6.18                            | 34.81                                  | <b>1.95</b> |
|                 | CB           | 0.89         | 6.00                            | 32.78                                  | 1.74        |
| PTB7-Th:        | CF           | 0.99         | 6.22                            | 35.29                                  | 2.17        |
| FTr-3PDI        | <b>o-DCB</b> | 1.02         | 5.91                            | 44.75                                  | <b>2.65</b> |
|                 | CB           | 1.02         | 5.44                            | 45.12                                  | 2.50        |

**TABLE S2** The optimization of donor/acceptor (D/A) weight ratios (the host solvents is o-DCB; the thickness of active layers is 90 nm±5nm).

| Sample               | D/A Ratio    | $V_{oc}$ (V) | $J_{sc}$ (mA cm <sup>-2</sup> ) | FF (%)       | PCE (%)     |
|----------------------|--------------|--------------|---------------------------------|--------------|-------------|
| PTB7-Th:Tr-3PDI      | 1:1          | 0.89         | 5.89                            | 34.96        | 1.88        |
|                      | <b>1:1.5</b> | <b>0.89</b>  | <b>6.14</b>                     | <b>35.12</b> | <b>1.96</b> |
|                      | 1:2          | 0.89         | 6.13                            | 34.83        | 1.91        |
|                      | 1:2.5        | 0.89         | 5.92                            | 34.5         | 1.82        |
| PTB7-Th:<br>FTr-3PDI | 1:1          | 1.03         | 4.48                            | 45.21        | 2.49        |
|                      | 1:1.5        | 1.02         | 5.78                            | 42.81        | 2.52        |
|                      | <b>1:2</b>   | <b>1.02</b>  | <b>5.91</b>                     | <b>45.75</b> | <b>2.85</b> |
|                      | 1:2.5        | 1.02         | 5.58                            | 43.56        | 2.44        |

**TABLE S3** The optimization of thickness for PTB7-Th:Tr-3PDI (the host solvents is o-DCB; D/A) weight ratio is 1:1.5).

| Thickness(nm) | $V_{oc}$ (V) | $J_{sc}$ (mA cm <sup>-2</sup> ) | FF (%)       | PCE (%)     |
|---------------|--------------|---------------------------------|--------------|-------------|
| 162           | 0.88         | 4.96                            | 33.21        | 1.45        |
| 152           | 0.88         | 5.03                            | 32.78        | 1.46        |
| 138           | 0.86         | 5.42                            | 31.45        | 1.47        |
| 120           | 0.90         | 5.61                            | 34.00        | 1.72        |
| 113           | 0.90         | 5.99                            | 35.18        | 1.91        |
| <b>102</b>    | <b>0.91</b>  | <b>5.89</b>                     | <b>37.21</b> | <b>1.96</b> |
| 92            | 0.91         | 5.68                            | 37.42        | 1.93        |
| 76            | 0.90         | 4.90                            | 38.52        | 1.69        |

**TABLE S4** The optimization of thickness for PTB7-Th:FTr-3PDI (the host solvents is o-DCB; D/A) weight ratio is 1:2).

| Thickness(nm) | V <sub>oc</sub> (V) | J <sub>sc</sub> (mA cm <sup>-2</sup> ) | FF (%)       | PCE (%)     |
|---------------|---------------------|----------------------------------------|--------------|-------------|
| 49            | 0.98                | 3.38                                   | 34.91        | 1.16        |
| 68            | 1.00                | 5.46                                   | 39.63        | 2.17        |
| 76            | 1.01                | 5.91                                   | 40.94        | 2.43        |
| 85            | 1.02                | 5.81                                   | 42.19        | 2.71        |
| <b>96</b>     | <b>1.01</b>         | <b>7.16</b>                            | <b>44.17</b> | <b>3.20</b> |
| 112           | 1.02                | 5.54                                   | 42.1         | 2.45        |
| 125           | 1.02                | 4.88                                   | 41.95        | 2.09        |
| 136           | 1.02                | 4.62                                   | 43.78        | 2.07        |
| 150           | 1.00                | 4.12                                   | 40.30        | 1.66        |

**TABLE S5** The optimization of thermal annealing (TA) for PTB7-Th:FTr-3PDI (the host solvents is o-DCB; D/A weight ratio is 1:2; the thickness of active layers is 100 nm±5nm).

| Sample            | V <sub>oc</sub> (V) | J <sub>sc</sub> (mA cm <sup>-2</sup> ) | FF (%)       | PCE (%)     |
|-------------------|---------------------|----------------------------------------|--------------|-------------|
| N/A               | 0.96                | 7.00                                   | 37.53        | 2.53        |
|                   | 1.01                | 6.55                                   | 41.89        | 2.78        |
| 80°C 5min         | 1.00                | 6.87                                   | 42.47        | 2.88        |
|                   | 1.01                | 6.55                                   | 40.41        | 2.67        |
| 100°C 5min        | 1.01                | 5.99                                   | 41.35        | 2.51        |
|                   | 1.02                | 5.60                                   | 43.81        | 2.51        |
| <b>120°C 5min</b> | <b>1.02</b>         | <b>6.91</b>                            | <b>44.07</b> | <b>3.05</b> |
|                   | <b>1.03</b>         | <b>7.15</b>                            | <b>45.12</b> | <b>3.33</b> |
| 140°C 5min        | 1.01                | 6.63                                   | 40.61        | 2.73        |
|                   | 0.98                | 6.63                                   | 37.19        | 2.41        |

**TABLE S6** The optimization of subsequent solvent annealing (SVA) for PTB7-Th:FTTr-3PDI (the host solvents is o-DCB; D/A weight ratio is 1:2; the thickness of active layers is 100 nm±5nm).

| Sample                 | $V_{oc}$ (V) | $J_{sc}$ (mA cm <sup>-2</sup> ) | FF (%)       | PCE (%)     |
|------------------------|--------------|---------------------------------|--------------|-------------|
| N/A                    | 1.02         | 5.41                            | 41.83        | 2.31        |
|                        | 1.02         | 5.64                            | 41.98        | 2.41        |
| 860rpm CF 15s          | 1.00         | 5.46                            | 39.93        | 2.17        |
| <b>860rpm CF 30s</b>   | <b>1.03</b>  | <b>5.82</b>                     | <b>44.07</b> | <b>2.63</b> |
| 860rpm CF 1min         | 1.01         | 5.95                            | 41.90        | 2.53        |
| 860rpm THF 15s         | 1.03         | 4.84                            | 45.04        | 2.26        |
| 860rpm THF 30s         | 1.01         | 5.99                            | 40.24        | 2.43        |
| <b>860rpm THF 1min</b> | <b>1.02</b>  | <b>6.04</b>                     | <b>43.67</b> | <b>2.70</b> |
| 860rpm N/A             | 1.02         | 5.79                            | 43.10        | 2.55        |

**TABLE S7** The optimization of solvent additives (the host solvents is o-DCB; D/A weight ratio is 1:1.5 for PTB7-Th:Tr-3PDI and 1:2 for PTB7-Th:FTTr-3PDI; the thickness of active layers is 100 nm±5nm).

| Sample                | solvent additives | $V_{oc}$ (V) | $J_{sc}$ (mA cm <sup>-2</sup> ) | FF (%)       | PCE (%)     |
|-----------------------|-------------------|--------------|---------------------------------|--------------|-------------|
| PTB7-Th:Tr-3PDI       | 2%DIO             | 0.93         | 5.40                            | 37.93        | 1.90        |
|                       | <b>2%CN</b>       | <b>0.92</b>  | <b>6.51</b>                     | <b>36.51</b> | <b>2.18</b> |
|                       | 1%DIO&1%CN        | 0.93         | 5.47                            | 37.84        | 1.92        |
| PTB7-Th:<br>FTTr-3PDI | 2%DIO             | 1.06         | 4.52                            | 47.91        | 2.29        |
|                       | <b>2%CN</b>       | <b>1.02</b>  | <b>8.09</b>                     | <b>45.63</b> | <b>3.77</b> |
|                       | 1%DIO&1%CN        | 1.02         | 6.10                            | 49.53        | 3.07        |

**TABLE S8** The optimization of solvent additives (CN) (the host solvents is o-DCB; D/A weight ratio is 1:1.5 for PTB7-Th:Tr-3PDI and 1:2 for PTB7-Th:FTTr-3PDI; the thickness of active layers is 100 nm±5nm).

| Sample                | solvent additives | $V_{oc}$ (V) | $J_{sc}$ (mA cm <sup>-2</sup> ) | FF (%)       | PCE (%)     |
|-----------------------|-------------------|--------------|---------------------------------|--------------|-------------|
| PTB7-Th:Tr-3PDI       | 1% CN             | 0.91         | 6.36                            | 37.23        | 2.15        |
|                       | <b>2%CN</b>       | <b>0.92</b>  | <b>6.51</b>                     | <b>36.51</b> | <b>2.18</b> |
|                       | 3%CN              | 0.93         | 5.40                            | 37.93        | 1.90        |
| PTB7-Th:<br>FTTr-3PDI | 1%CN              | 1.03         | 7.15                            | 45.10        | 3.32        |
|                       | <b>2%CN</b>       | <b>1.02</b>  | <b>8.09</b>                     | <b>45.63</b> | <b>3.77</b> |
|                       | 3%CN              | 1.02         | 6.10                            | 49.53        | 3.07        |

