

Electronic Supporting Information (ESI) for:

## **Synthesis of Cyano-Substituted Conjugated Polymers for Photovoltaic Applications**

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**Table S1.** The best photovoltaic parameters of the PSCs. The average and deviation (10 devices are averaged) for the photovoltaic parameters of each device are given in parentheses.

| Donor    | Blend ratio <sup>a</sup> | $J_{sc}$<br>(mA/cm <sup>2</sup> ) | $V_{oc}$<br>(V)              | FF<br>(%)                    | PCE<br>(%)                   | $R_s$<br>( $\Omega$ cm <sup>2</sup> ) <sup>b</sup> |
|----------|--------------------------|-----------------------------------|------------------------------|------------------------------|------------------------------|----------------------------------------------------|
| PB-BtCN  | 3:3                      | 6.26<br>(6.01)                    | 0.94<br>(0.94)               | 66.8<br>(65.2)               | 3.93<br>(3.69)               | 3.75                                               |
|          |                          | 6.92<br>(6.65)                    | 0.94<br>(0.94)               | 62.1<br>(61.8)               | 4.04<br>(3.84)               |                                                    |
|          | 3:4                      | 6.39<br>(6.24)                    | 0.94<br>(0.94)               | 67.8<br>(68.0)               | 4.07<br>(3.99)               |                                                    |
|          |                          | <b>7.36</b><br><b>(7.24)</b>      | <b>0.93</b><br><b>(0.94)</b> | <b>67.1</b><br><b>(65.1)</b> | <b>4.59</b><br><b>(4.40)</b> |                                                    |
|          | 3:5                      | 6.99<br>(6.87)                    | 0.93<br>(0.93)               | 64.0<br>(63.4)               | 4.16<br>(4.06)               |                                                    |
|          |                          |                                   |                              |                              |                              |                                                    |
| PB-DPQCN | 3:2                      | 2.76<br>(2.59)                    | 0.76<br>(0.72)               | 50.9<br>(49.0±)              | 1.07<br>(0.92)               | 4.34                                               |
|          |                          | 5.02<br>(4.71)                    | 0.90<br>(0.88)               | 58.2<br>(56.9)               | 2.63<br>(2.36)               |                                                    |
|          | 3:4                      | 5.75<br>(5.63)                    | 0.95<br>(0.94)               | 58.6<br>(57.4)               | 3.20<br>(3.08)               |                                                    |
|          |                          | <b>5.89</b><br><b>(5.83)</b>      | <b>0.95</b><br><b>(0.95)</b> | <b>58.8</b><br><b>(57.4)</b> | <b>3.29</b><br><b>(3.16)</b> |                                                    |
|          | 3:5                      | 5.83<br>(5.79)                    | 0.96<br>(0.96)               | 57.2<br>(54.3)               | 3.20<br>(3.01)               |                                                    |
|          |                          |                                   |                              |                              |                              |                                                    |
| PB-DBPCN | 3:3                      | 3.71<br>(3.63)                    | 0.89<br>(0.89)               | 55.4<br>(56.0)               | 1.83<br>(1.81)               | 9.96                                               |
|          |                          | <b>4.19</b><br><b>(3.84)</b>      | <b>0.89</b><br><b>(0.89)</b> | <b>58.3</b><br><b>(56.1)</b> | <b>2.17</b><br><b>(1.91)</b> |                                                    |
|          | 3:4                      | 3.08<br>(2.95)                    | 0.89<br>(0.89)               | 51.3<br>(49.1)               | 1.41<br>(1.30)               |                                                    |
|          |                          | 2.71<br>(2.64)                    | 0.90<br>(0.89)               | 50.0<br>(49.6)               | 1.22<br>(1.17)               |                                                    |
|          | 3:5                      |                                   |                              |                              |                              |                                                    |
|          |                          |                                   |                              |                              |                              |                                                    |

<sup>a</sup>Mass ratio of polymer donor to PC<sub>71</sub>BM. <sup>b</sup>Series resistance (estimated from the corresponding best device).

**Table S2.** The photovoltaic parameters of the devices based on PB-BtCN with diverse concentrations of DIO additive and different type of acceptors. The averages of the photovoltaic parameters of each device are shown in parentheses.

| Polymer                          | Blend ratio | DIO amount | $J_{sc}$ (mA/cm <sup>2</sup> ) | $V_{oc}$ (V)        | FF (%)              | PCE (%)             |
|----------------------------------|-------------|------------|--------------------------------|---------------------|---------------------|---------------------|
| PB-BtCN :<br>PC <sub>71</sub> BM | 3:6         | 2%         | 8.73<br>(8.51±0.21)            | 0.90<br>(0.89±0.01) | 53.7<br>(51.6±0.82) | 4.22<br>(3.91±0.25) |
|                                  |             |            | 7.36<br>(7.24±0.11)            | 0.93<br>(0.94±0.01) | 67.1<br>(65.1±0.95) | 4.59<br>(4.40±0.15) |
| PB-BtCN :<br>PC <sub>71</sub> BM | 3:6         | 3%         | 6.97<br>(6.96±0.09)            | 0.90<br>(0.90±0.01) | 59.0<br>(56.9±1.24) | 3.70<br>(3.56±0.17) |
|                                  |             |            | 4.28<br>(4.01±0.26)            | 0.88<br>(0.88±0.01) | 55.7<br>(54.3±1.49) | 2.10<br>(2.03±0.12) |