Supporting Information

Extending π-Conjugation System with Benzene: An Effective Method to Improve the Properties of Benzodithiophene-Based Polymer for Highly Efficient Organic Solar Cells

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Figure S1. XRD spectrum of PBDTBzT-DTffBT as film.



Figure S2. The energies and distributions of the frontier molecular orbitals of the

polymers.1

Table S1. Photovoltaic properties of the PSCs with different D/A ratios under AM 1.5G illumination (100 mW/cm²). D/A ratio $V_{\rm oc}$ (V) $J_{\rm sc} \,({\rm mA/cm}^2)$ FF (%) PCE_{max} (PCE_{ave})^a (%) Polymer

12.10

12.93

11.90

9.14

10.00

9.83

8.37

57.11

62.73

65.81

64.47

40.07

57.91

57.57

6.22 (5.95)

7.30 (7.16)

6.89 (6.84)

5.19 (5.00)

3.85 (3.76)

5.35 (5.32)

4.48 (4.39)

0.90

0.90

0.88

0.88

0.96

0.94

0.93

^aThe average PCE is obtained from 5 devices.

2:1

1.5:1

1:1

1:2

1.5:1

1:1

1:1.5

PBDTBzT-DTffBT

(With 1% DIO)

PBDTT-DTffBT

(Without DIO)



Figure S3. *J-V* curves of the PSCs based on (a) PBDTBzT-DTffBT and (b)

PBDTT-DTffBT with different D/A ratios.



Figure S4. ¹H NMR spectrum of compound 2.



Figure S5. ¹H NMR spectrum of compound 3.



Figure S6. ¹H NMR spectrum of BDTBzT.



Figure S7. ¹H NMR spectrum of DTffBT.



Figure S8. ¹H NMR spectrum of polymer PBDTBzT-DTffBT.



Figure S9. ¹H NMR spectrum of BDTT.



Figure S10. ¹H NMR spectrum of polymer PBDTT-DTffBT.

References

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