## **Supporting Information**

## Efficient carbazole-based small-molecule organic solar cells with an

## improved fill factor

Yongtao Liu<sup>a</sup>, Yanna Sun<sup>a</sup>, Miaomiao Li<sup>a</sup>, Huanran Feng<sup>a</sup>, Wang Ni<sup>a</sup>, Hongtao Zhang<sup>a,\*</sup>, Xiangjian Wan<sup>a</sup>, and Yongsheng Chen<sup>a,\*</sup>

State Key Laboratory and Institute of Elemento-Organic Chemistry, The Centre of Nanoscale Science and Technology and Key Laboratory of Functional Polymer Materials, Collaborative Innovation Center of Chemical Science and Engineering (Tianjin), College of Chemistry, Nankai University, Tianjin, 300071, China. Email: htzhang@nankai.edu.cn; yschen99@nankai.edu.cn; Fax: +86 22 2349 9992.



Scheme S1. Synthetic routes for DI3TCz.



Figure S1. TGA curve of DI3TCz with a heating rate of 10°C min<sup>-1</sup> under  $N_2$  atmosphere.



Figure S2. Uv-vis absorption spectral of DI3TCz:PC<sub>71</sub>BM blend films.



**Figure S3.** Cyclic voltammograms of DI3TCz in  $CH_2Cl_2$  with 0.1M  $Bu_4NPF_6$  with a scan rate of 100 mV s<sup>-1</sup>.



**Figure S4.** J-V characteristics for electron-only (a) and hole-only (b) devices fabricated from DI3TCz:PC<sub>71</sub>BM (1:0.8). The solid lines represent the fit using a model of single carrier SCLC with field-independent mobility. The JD-V characteristics are corrected for the built-in voltage Vbi that arises from the work function difference between the contacts.



Figure S5. <sup>1</sup>H NMR spectral of compound DI3TCz at 300K in CDCl<sub>3</sub>.



Figure S6. <sup>13</sup>C NMR spectral of compound DI3TCz at 300K in CDCl<sub>3</sub>.



Figure S7. The MALDI-TOF plot of compound DI3TCz.



**Figure S8.** The chemical structure of PrC60MA. (Li, C. Z.; Chueh, C. C.; Yip, H. L.; O'Malley, K. M.; Chen, W. C.; Jen, A. K. Y. *J. Mater. Chem.* **2012**, *22*, 8574)