Electronic Supplementary Material (ESI) for RSC Advances.

Electronic Supplementary Information

Organic solar cells based on bowl-shape small-molecules

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Homepage: http://www.ucm.es/info/fullerene/

Experimental Section

Instrumentation

Solvents were purchased from Sigma-Aldrich and were used without further purification. TruxTTF and truxTTF-CO were were prepared according to previously reported synthetic procedures (ref 37 and 38). Absorption studies were performed using a Cary 5000 UV-Vis-NIR spectrometer from Varian. The thickness of blends were measured by employing a KLA-Tencor Alpha-Step D-120 stylus profilometer. Atomic Force Microscopy was performed on a SPM Nanoscope Illa multimode microscope working in tapping mode under ambient conditions.

Solar cell fabrication

$PC_{61}BM$ and $PC_{71}BM$ were purchased from American Dye Source and used as received. The ITO-coated glasses (Delta technologies, 5-15 Ω) were pre-cleaned stepwise by ultracentrifugation 15 minutes in detergent, deionized water, methanol, acetone and iso-propanol and then by a 20 minutes UV-ozone treatment (Jelight Company, USA). A thin layer of PEDOT:PSS (Clevios P VP AI 4083, 5000 rpm, 30 seconds, ≈ 30 nm) was spin-coated onto the ITO glass and baked at 150 ºC for 15 minutes in air. Subsequently, the active layer with varying weight ratios (1:6, 1:4 and 1:2 w/w) was spin-coated at 900 rpm from chlorobenzene:*o*-DCB (1:3 v/v) solutions. TruxTTF or truxTTF-CO:$PC_{61}BM$ or $PC_{71}BM$ (1:6, 1:4 and 1:2 w/w) was spin-coated at 900 rpm. Then the devices were transferred to a N_2 filled glove box (< 0.1 ppm O_2 and < 0.1 ppm H_2O) for further processing. The photoactive layer was annealed at 70 ºC for 10 minutes followed by thermal evaporation 60 nm of aluminum (1 x 10^{-6} mbar) as negative electrode with a shadow mask of 4 mm^2. The current-voltage characteristics of the devices were measured by using a computer-controlled Keithley 2420 source unit under 1 sun, AM1.5G spectrum from a solar simulator (Photo Emission Tech CT100) by using a Xenon-lamp at 100 mW cm^{-2} as light source and calibrated with a Si-reference cell. The incident photon to current efficiency was recorded using a Bentham PVE300 model.

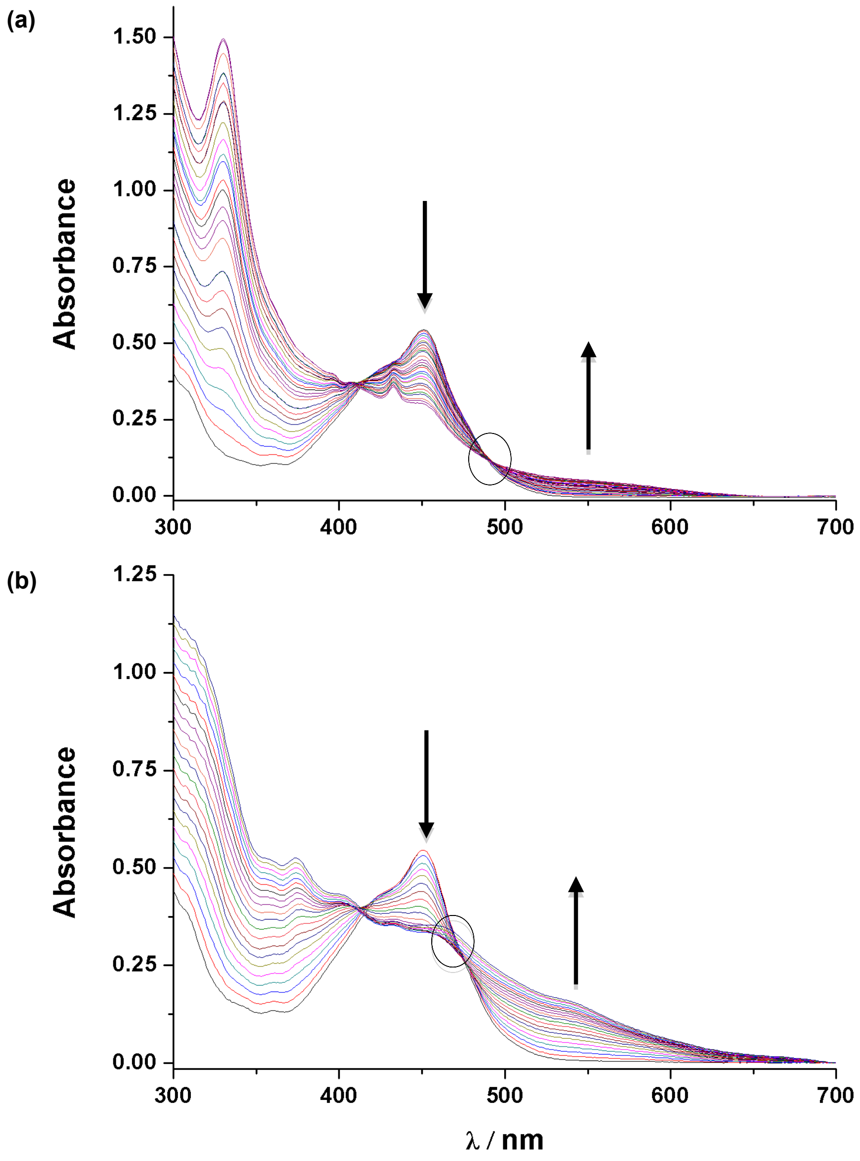
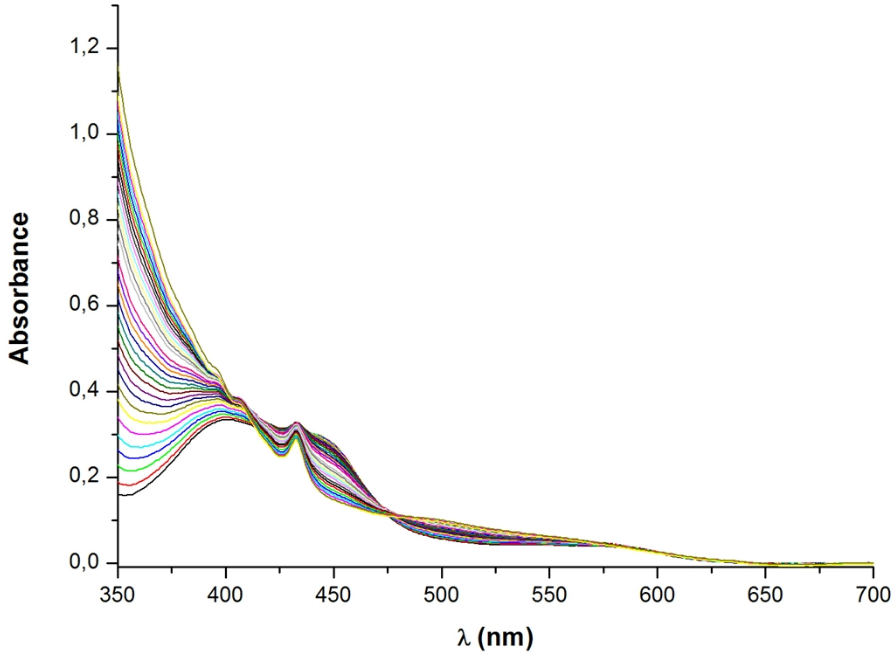


Figure S1. UV/ vis spectra as obtained during the titration of (a) truxTTF (1.15×10^{-4} M) with $PC_{61}BM$ (4.9×10^{-4} M) and (b) truxTTF (1.15×10^{-4} M) with $PC_{71}BM$ (4.37×10^{-4} M), in chlorobenzene at room temperature. Each addition corresponds to 0.1 equiv.



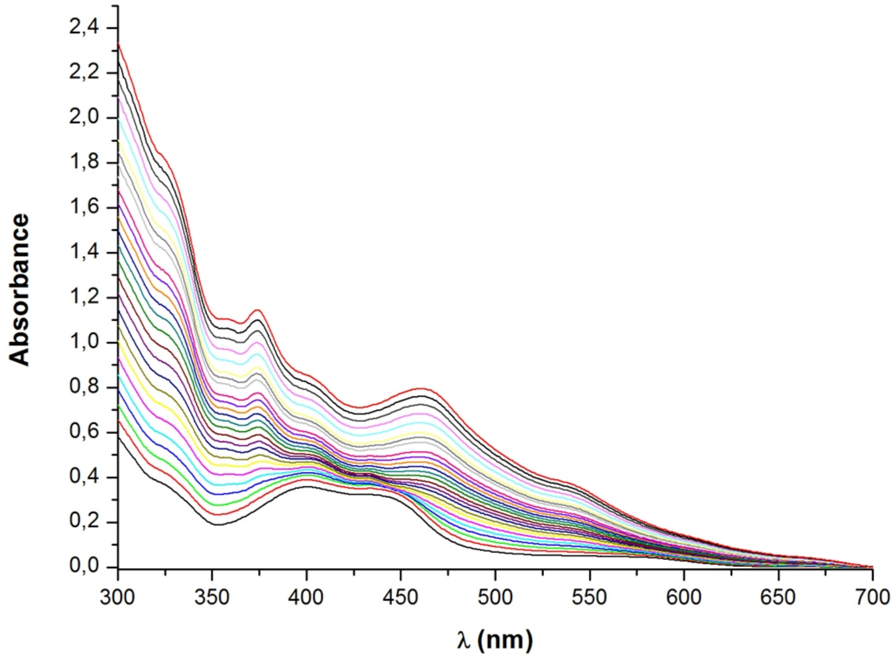


Figure S2. UV/ vis spectra as obtained during the titration of (a) truxTTF-CO (1.44 x 10^{-4} M) with $PC_{61}BM$ (7.14 x 10^{-4} M). Each addition corresponds to 0.2 equiv. (b) truxTTF (1.15 x 10^{-4} M) with $PC_{71}BM$ (7.48 x 10^{-4} M), in chlorobenzene at room temperature. Each addition corresponds to 0.24 equiv.

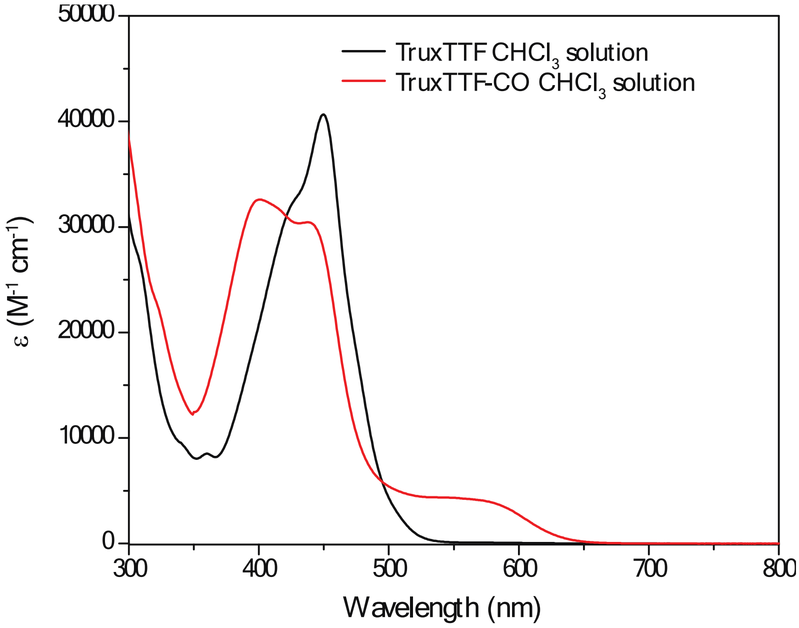


Figure S3. UV-vis absorption spectra of truxTTF and truxTTF-CO in diluted chloroform solutions.

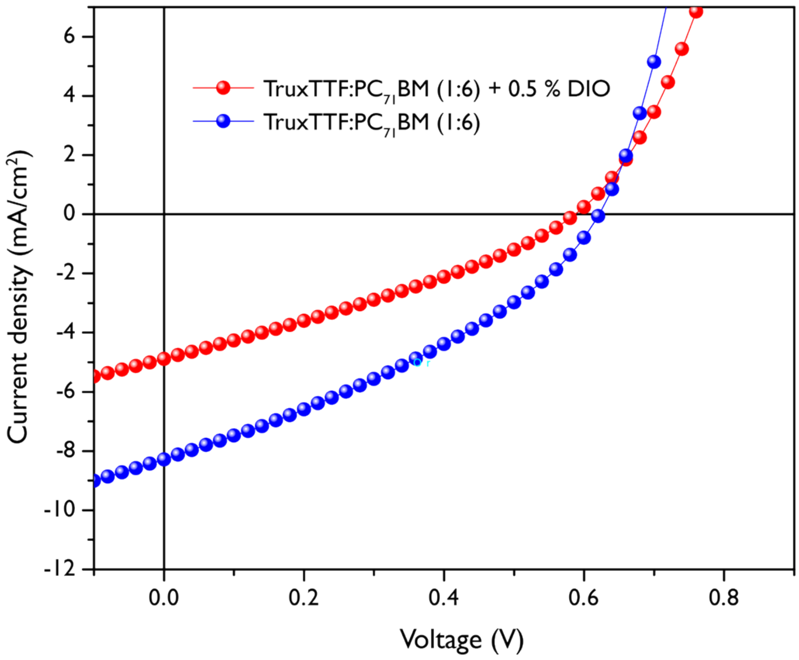


Figure S4. Current density-voltage (*J-V*) curves of the blend truxTTF:$PC_{71}BM$ (1:6) w/w with and without DIO.

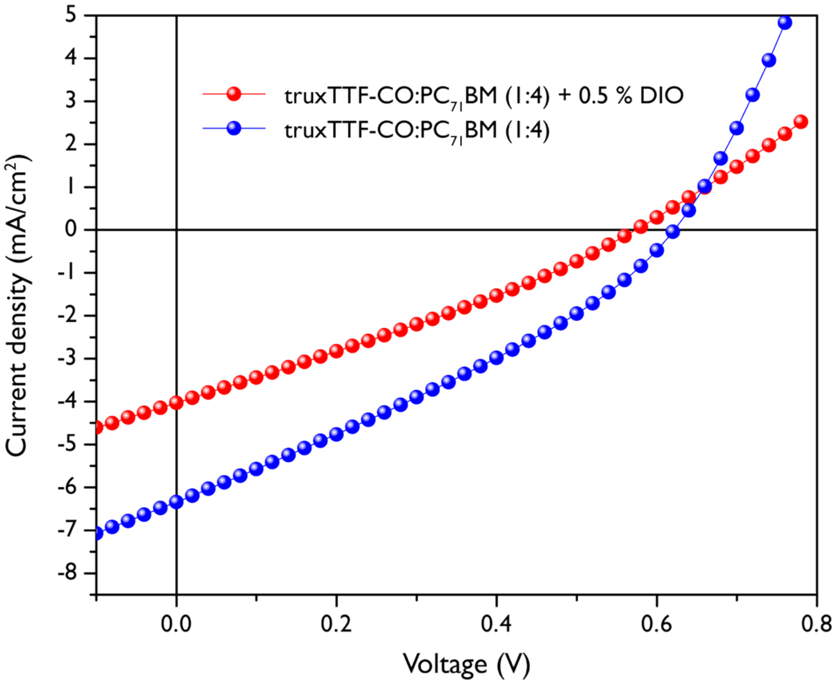


Figure S5. Current density-voltage (*J*-*V*) curves of the blend truxTTF-CO:PC$_{71}$BM (1:4) w/w with and without DIO.

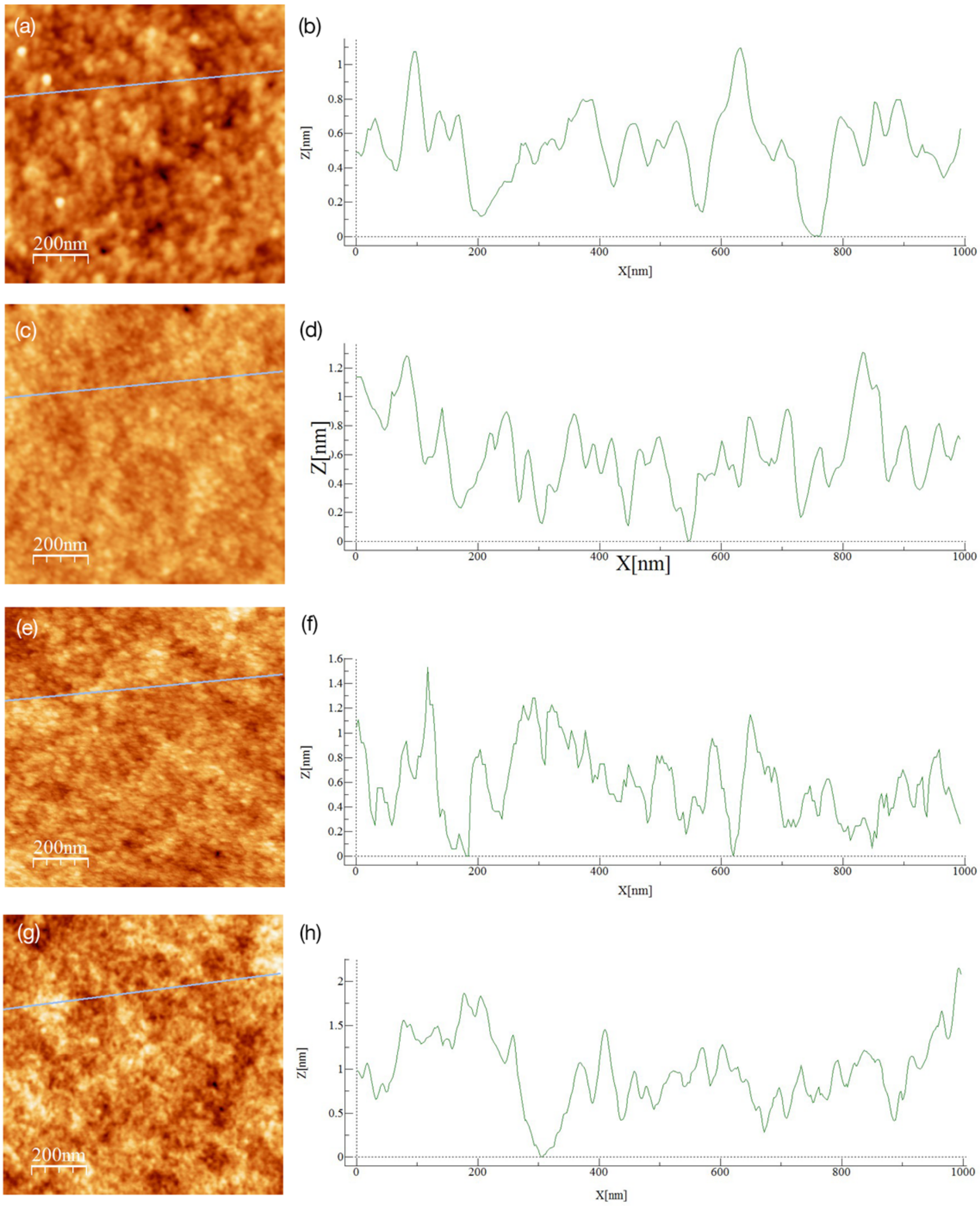


Figure S6. Tapping mode AFM height and their profile roughness (1 μm x 1μm) of blends films spin-coated from chlorobenzene:o-DCB of (a and b) truxTTF:$PC_{61}BM$ (1:6), (c and d) truxTTF:$PC_{71}BM$ (1: 6), (e and f) truxTTF-CO:$PC_{61}BM$ (1:4) and (g and h) truxTTF-CO:$PC_{71}BM$ (1:4).