Thin film morphology and efficiency of organic solar cells based on a diketopyrrolopyrrole polymer

Supplementary Information

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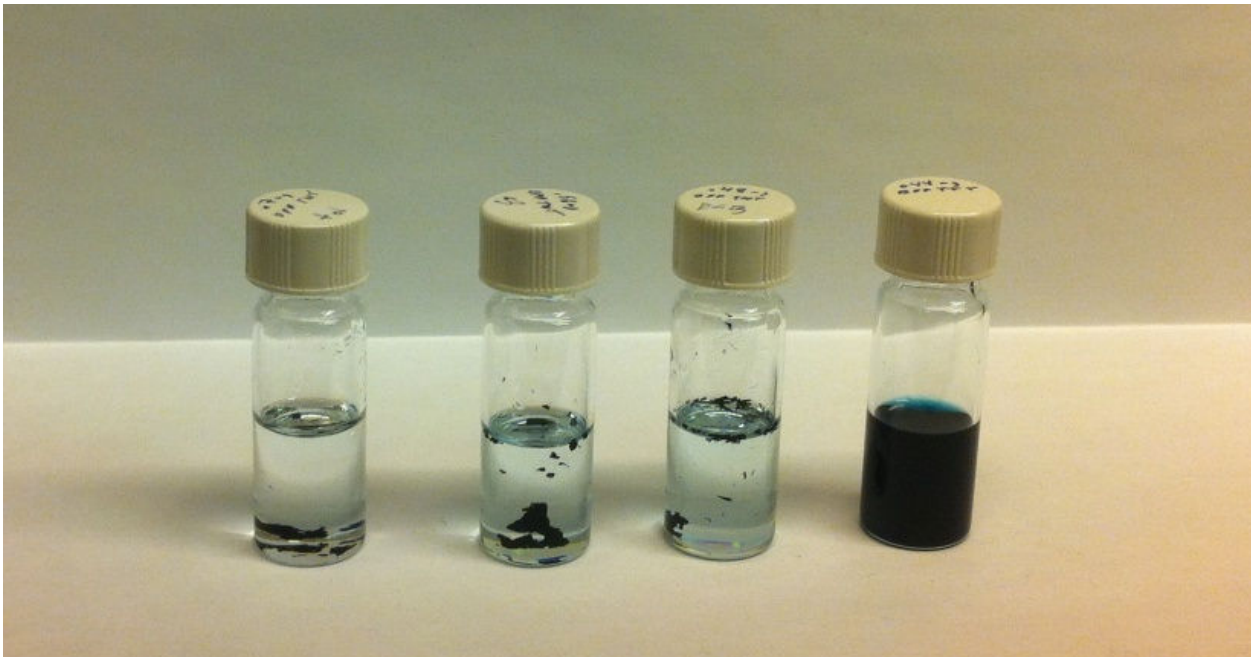

Figure S1. pDPP-TNT is insoluble in most common solvents. Chloroform is a rare solvent in which pDPP-TNT is soluble in. pDPP-TNT in toluene, chlorobenzene, dichlorobenzene, and chloroform (left to right) (0.25 mg/mL) after 68 hours at room temperature (pDPP-TNT was fully dissolved in chloroform in less than 1 hour).

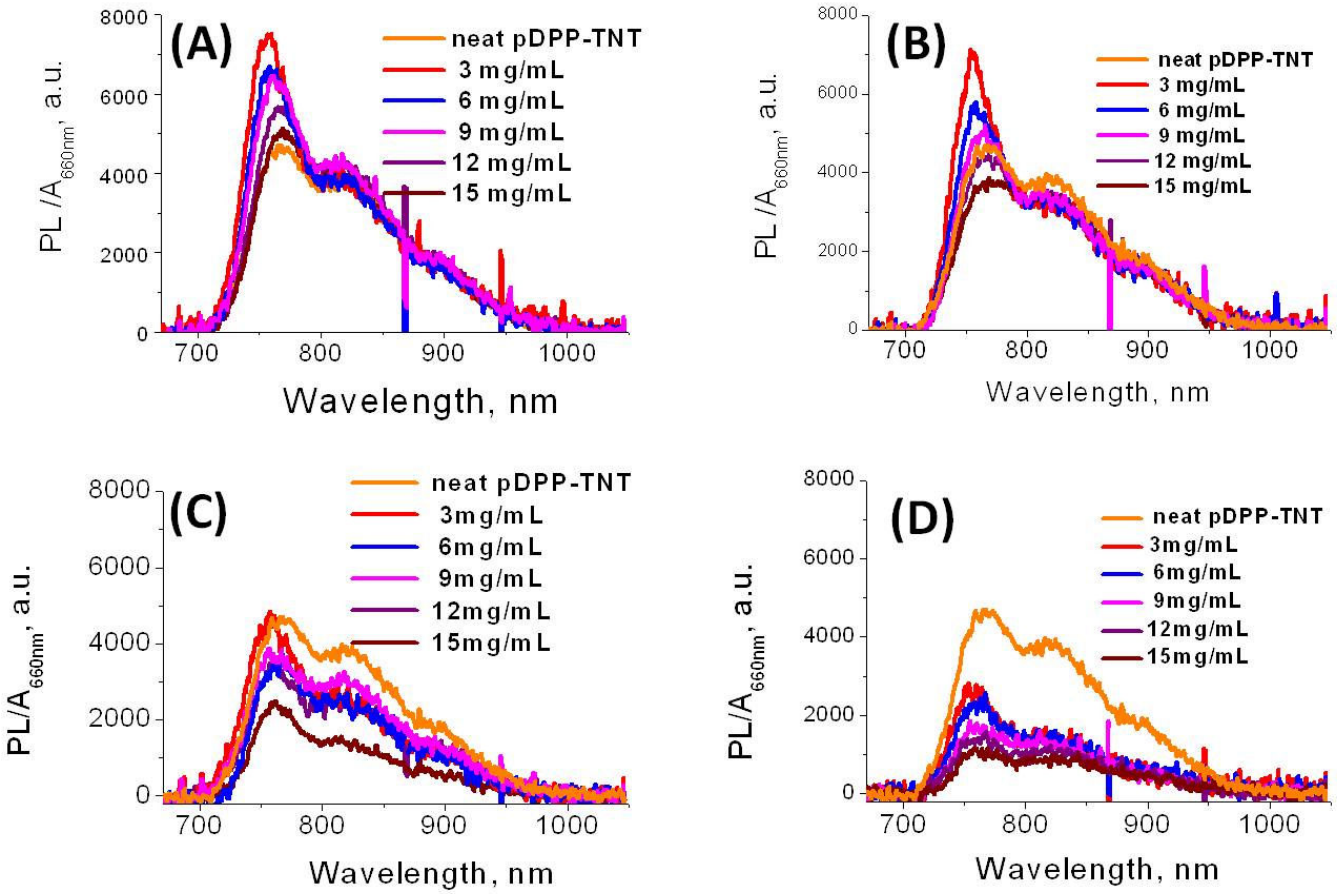

Figure S2. Actual PL spectra of films scaled to the corresponding film absorptance at the excitation wavelength (660nm).
(A) and (C): films of different thicknesses spin-coated from chloroform;
(B) and (D): films of different thicknesses spin-coated from mixed solvent.
(A) and (B): films rinsed in hexane to selectively remove [70]PCBM.
PL spectrum of a neat pDPP-TNT film scaled to its absorptance at 660nm is shown in all graphs.

	1:1 chloroform 9 mg/mL	1:1 chloroform 12 mg/mL	1:1 chloroform 15 mg/mL	1:1 mixed solvents 9 mg/mL	1:1 mixed solvents 12 mg/mL	1:1 mixed solvents 15 mg/mL
J_{sc} [mA/cm^2]	2.4	2.1	1.7	5.3	7.9	8.2
V_{oc} [V]	0.78	0.79	0.77	0.74	0.69	0.7
FF	46	47	47	50	43	40
PCE [%]	0.87	0.79	0.63	1.9	2.4	2.3

	1:3 chloroform 9 mg/mL	1:3 chloroform 12 mg/mL	1:3 chloroform 15 mg/mL	1:3 mixed solvents 9 mg/mL	1:3 mixed solvents 12 mg/mL	1:3 mixed solvents 15 mg/mL
J_{sc} [mA/cm^2]	3.1	3.3	3	4.4	7.4	9
V_{oc} [V]	0.75	0.76	0.79	0.57	0.58	0.62
FF	54	54	54	49	46	45
PCE [%]	1.3	1.4	1.3	1.2	2	2.5

Table S1. OPV performance of devices utilizing blend ratios 1:1 and 1:3 pDPP-TNT: [70]PCBM with the active layer spin-coated from either chloroform or a mixed solvent system of chloroform :DCB (4:1).

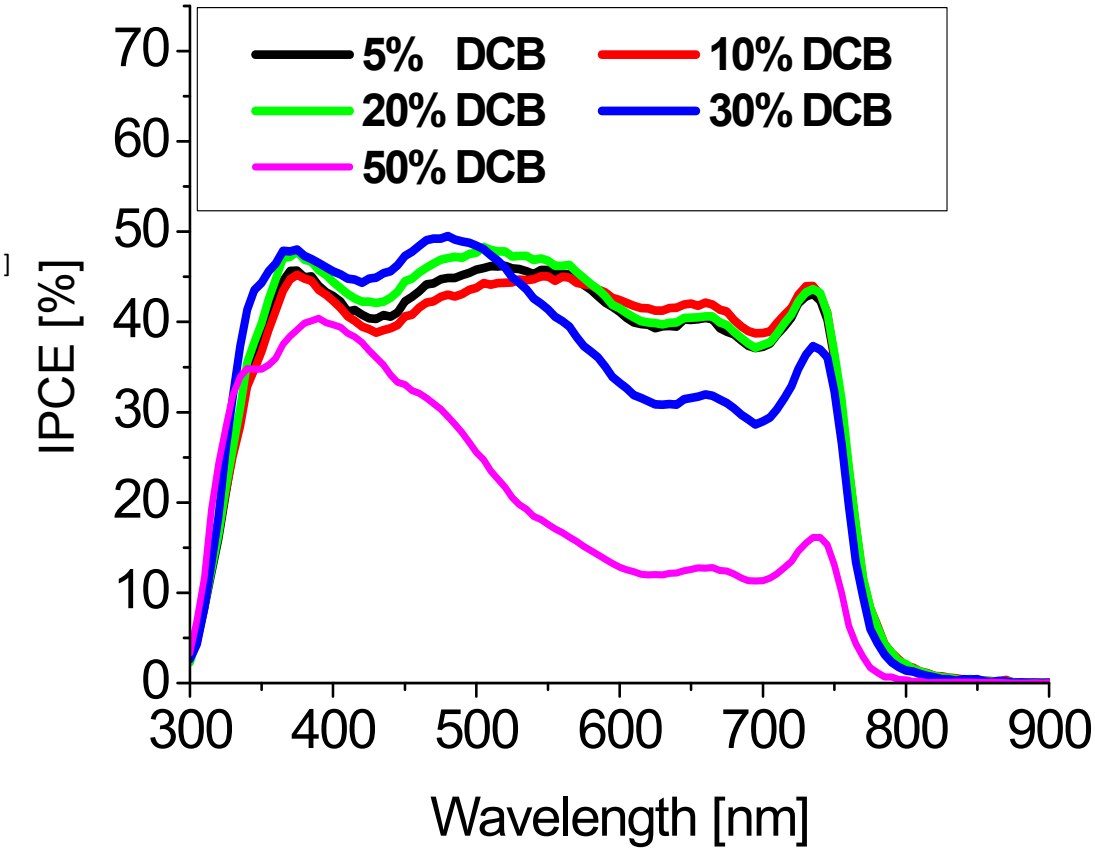

Figure S3. IPCE spectra for devices fabricated from the mixed solvent system with various ratios of chloroform and DCB. Very similar current generation is shown for a range of solvent ratios. Investigated ratios of DCB in the solution were 5 %, 10 %, 20 %, 30 %, and 50 %. The reduction in IPCE for devices utilizing higher concentrations of DCB can be attributed to a reduced film thickness.

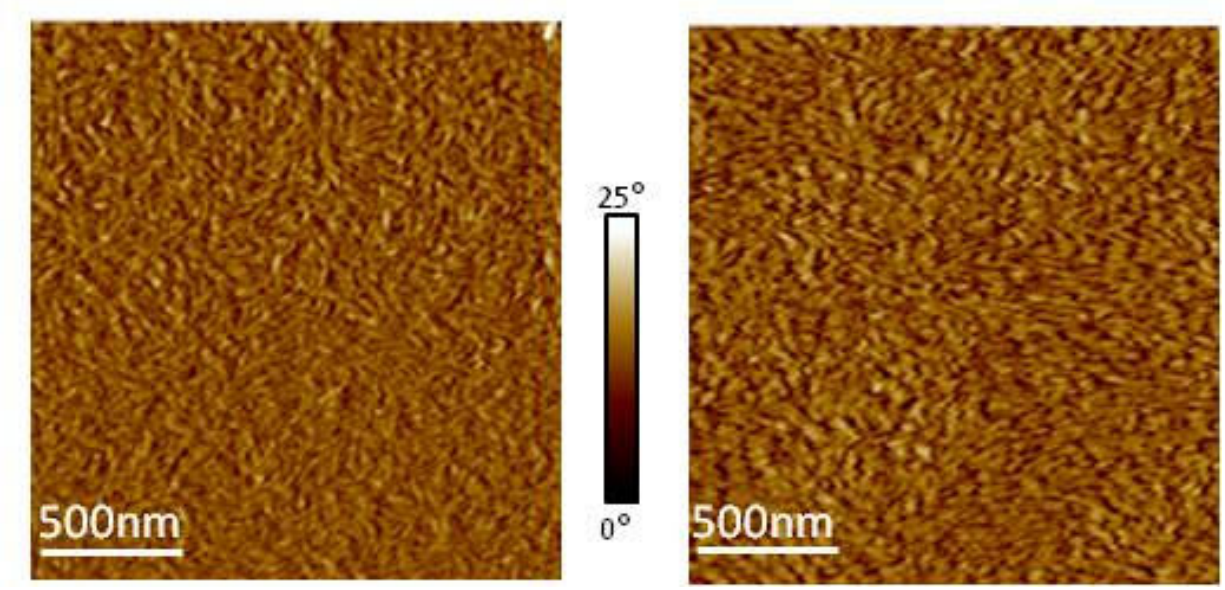

Figure S4. AFM phase images of neat pDPP-TNT films spin coated from chloroform (left) and chloroform:DCB (4:1) mixed solvent system (right).

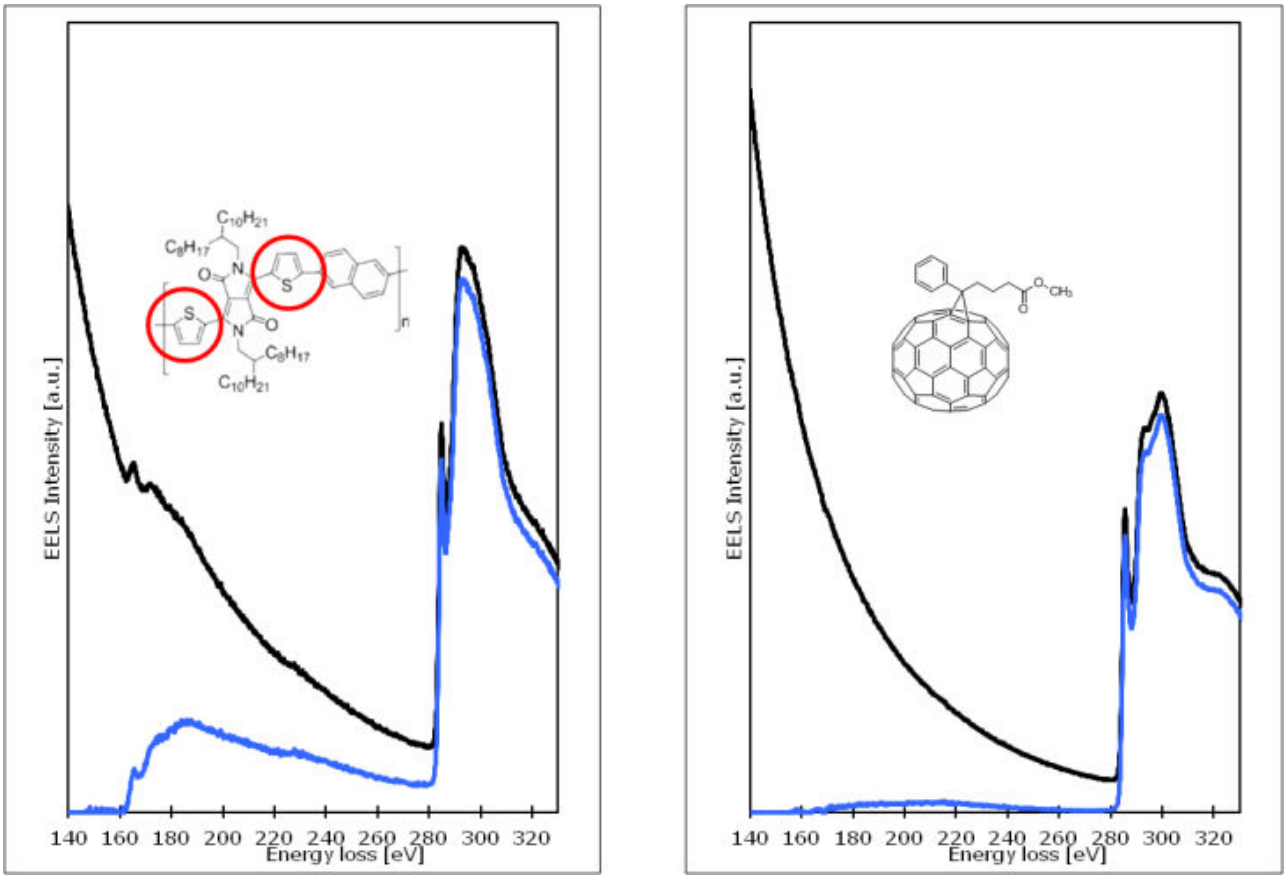

Figure S5. EELS (electron energy loss spectroscopy) spectra of p-DPP-TNT (left) and [70]PCBM (right). Black line – raw data, blue line – after background subtraction. Sulfur signal is observed at ~180-200 eV (position of peak maximum).

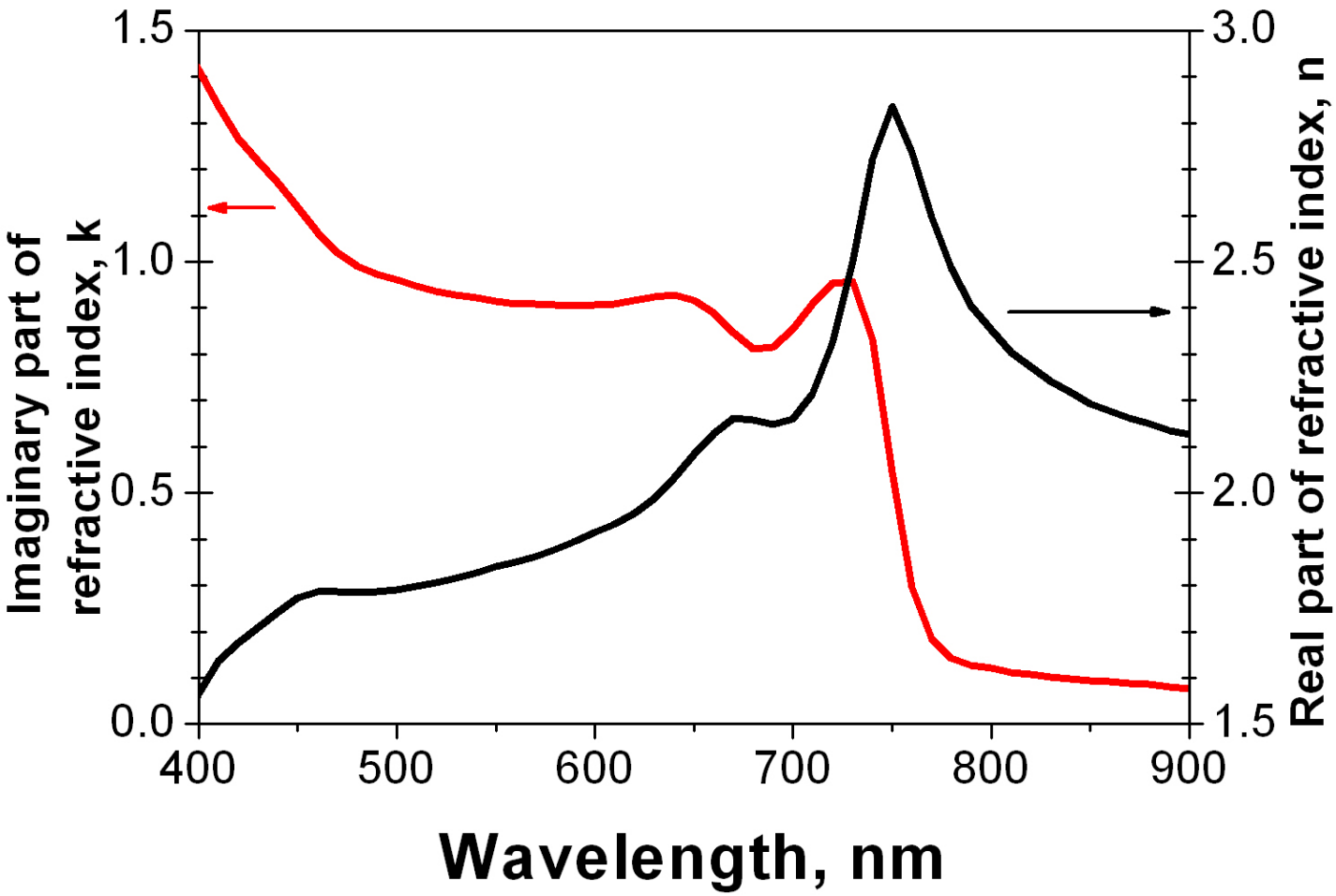

Figure S6. Real (black) and imaginary (red) parts of refractive index for pDPP-TNT BHJ film spin-coated from mixture of chloroform:DCB (4:1) on silicon wafer with native oxide. Thickness of the film determined by ellipsometry is 24.5nm.

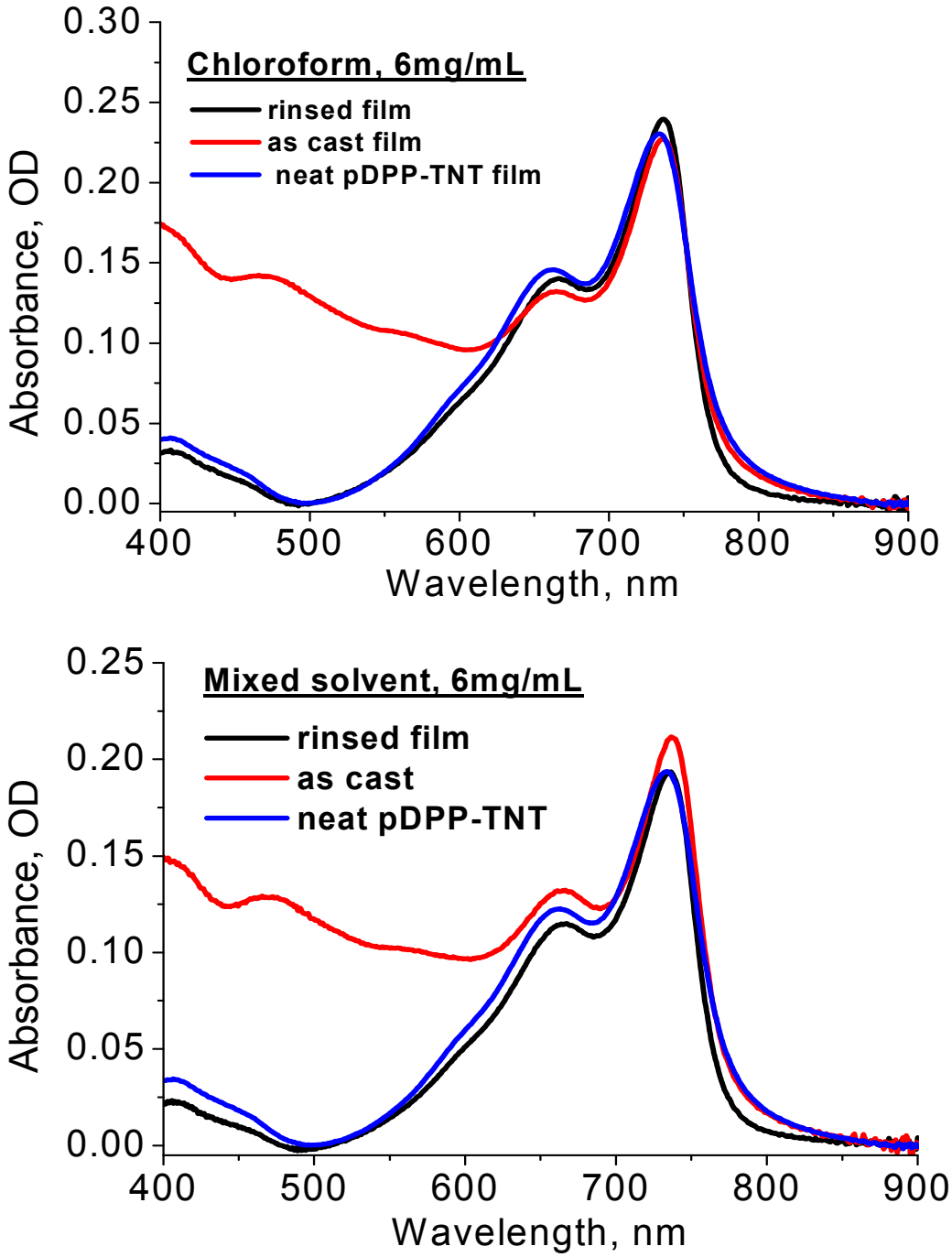

Figure S7. Typical UV-vis spectra of the pDPP-TNT: [70]PCBM blend films rinsed in hexane to selectively remove [70]PCBM. Spectra of the same films before rinsing are shown as well as the spectrum of neat pDPP-TNT film rescaled to match corresponding rinsed film absorbance maxima.

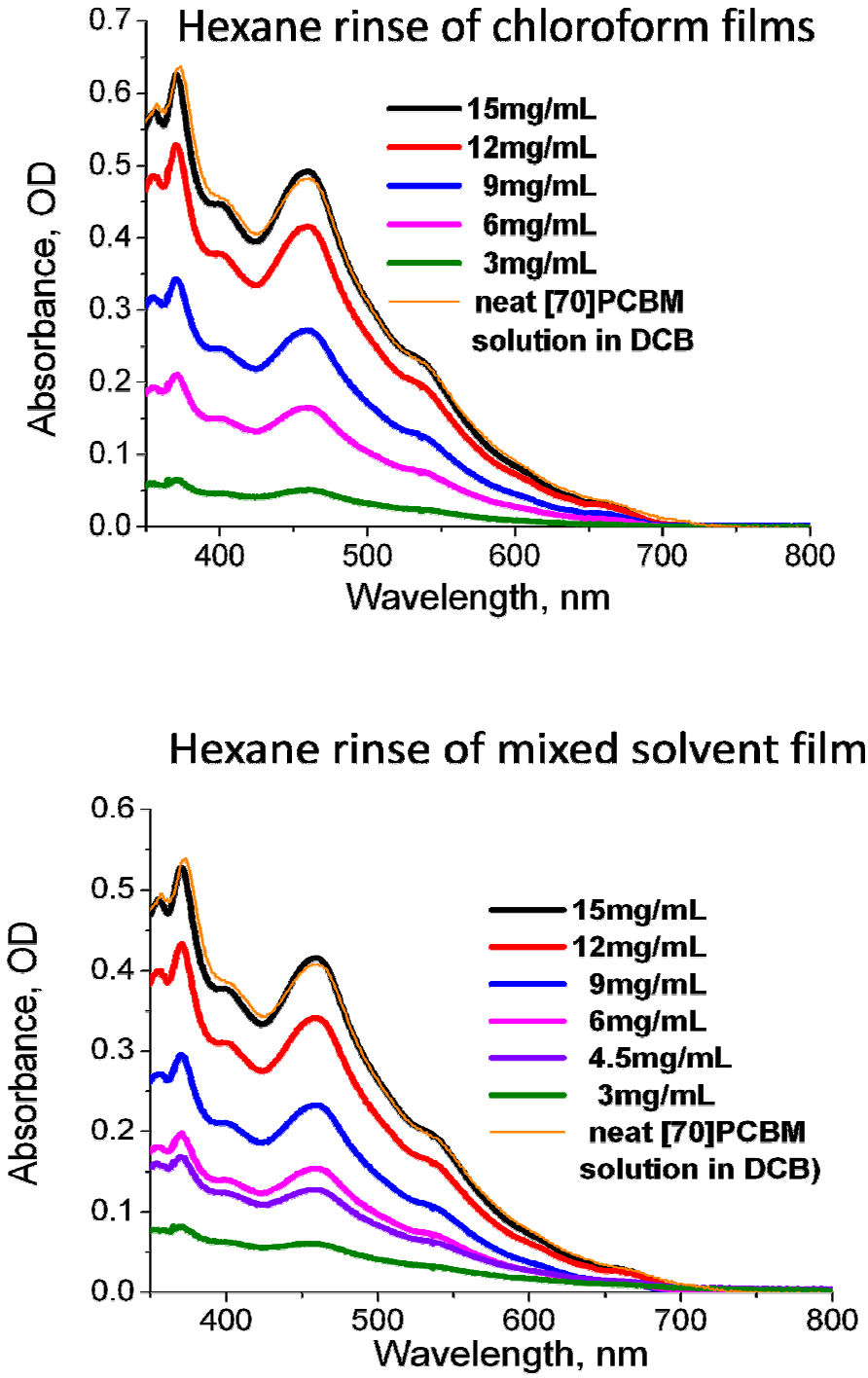

Figure S8. UV-vis spectra of hexane rinses of all the films. For comparison, neat [70]PCBM solution spectrum is shown as well (rescaled in both graphs to match approximately the rinse of 15mg/mL film) .

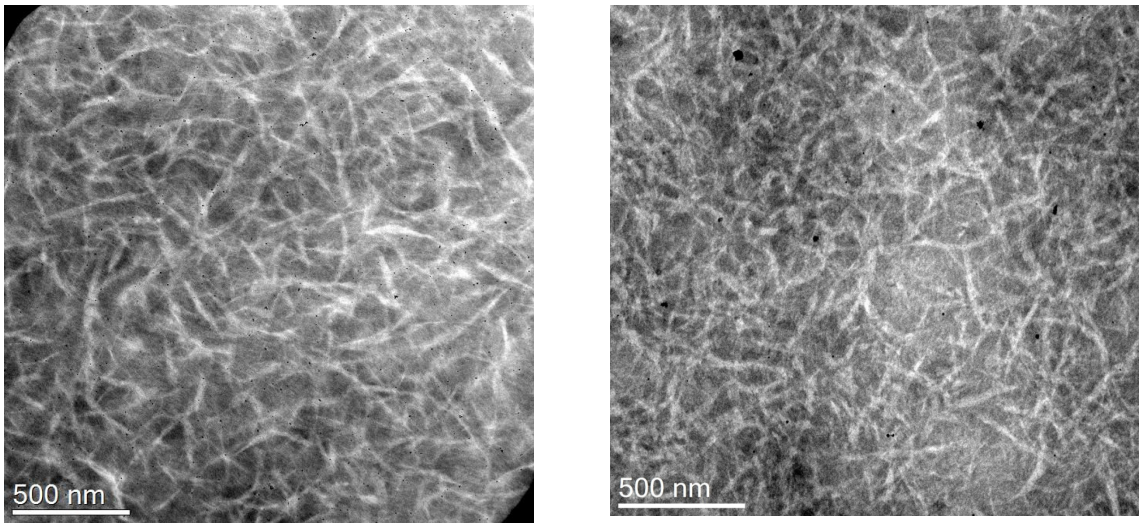

Figure S9. TEM images for mixed solvent films of different thicknesses. Corresponding initial solution concentrations were 4.5mg/mL (left) and 9mg/mL (right).

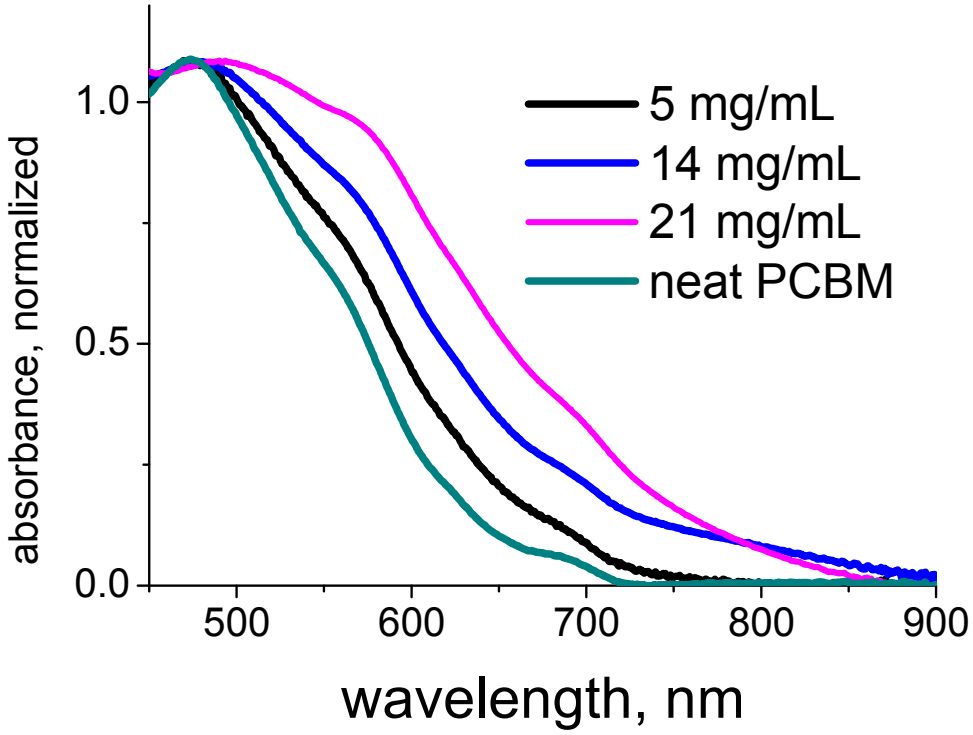

Figure S10. Normalized UV-vis spectra of 1:2 PMMA:[70]PCBM films of different thicknesses (spin-coated from chloroform using different initial solution concentrations) and neat [70]PCBM film. It is clearly seen that the long wavelength tail absorption increases significantly with film thickness.