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Supporting Information

Enhancing the performance of polymer solar cells by tuning the drying process of blend films via changing side chains and using solvent additive

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1.1 Measurements and characterization

Unless otherwise noted, all reactions were carried out under a nitrogen atmosphere and monitored by thin layer chromatography (TLC) on silica gel plates. ^{1}H and ^{13}C NMR spectra were recorded on a Bruker AV 400 spectrometer. UV-visible absorption spectra were measured on a PerkinElmer UV-vis spectrometer model Lambda 750. Thermal gravimetric analysis (TGA) and differential scanning calorimetry (DSC) were performed on TA2100 and Perkin-Elmer Diamond differential scanning calorimetry (DSC) instrument, respectively, under an atmosphere of nitrogen at a heating rate of 10 ^{o}C/min. Atomic force microscopy (AFM) measurements were carried out under ambient conditions using a Digital Instrument Multimode Nanoscope IIIA using the tapping mode. The thickness of blend films was measured by a Dektak 6 M surface profilometer. XRD experiments were carried out by X' Pert PRO MPD instrument. The electrochemical behavior of polymers was studied using cyclic voltammetry (CHI 630A Electrochemical Analyzer) with a three-electrode electrochemical cell in a 0.1 M Bu_4NPF_6 CH_3CN solution under an atmosphere of nitrogen with a scanning rate of 0.1 V/S. A Pt plate working electrode, a Pt wire counter electrode, and an $Ag/AgNO_3$ (0.01 M in CH_3CN) reference electrode were used.

1.2 Polymer Solar Cells Fabrication and Characterization

PSCs were fabricated with the device configuration of ITO/PEDOT:PSS (40 nm)/**P1-3**:$PC_{71}BM$/LiF (0.5 nm)/Al (100 nm). The conductivity of ITO is 20 Ω. PEDOT:PSS (Baytron Al 4083 from H.C. Starck) was filtered with a 0.45 mm polyvinylidene difluoride (PVDF) film before use. A PEDOT:PSS thin layer was spin-coated on top of the cleaned ITO substrate at 3000 rpm/s for 60 s and dried subsequently at 130 ^{o}C for 20 min on a hotplate. The thickness of the PEDOT:PSS layer is about 30 nm. A mixture of **P1-3** and $PC_{71}BM$ in 1,2-dichlorobenzene (DCB) was stirred at dissolving temperature overnight to ensure sufficient dissolution and then the blend solution was spin-coated onto PEDOT:PSS layer to form active layer. Thermal annealing was carried out after the spin-coating process on a hotplate. A top electrode of 0.5 nm LiF and 100 nm of aluminum was thermally evaporated at a pressure of 10^{-4} Pa through a shadow mask. On one substrate five cells with an effective area of 0.04 cm^2 for each were fabricated. Current-voltage (I-V) and external quantum efficiency (EQE) measurements were conducted in air without encapsulation. I-V characteristics were recorded at room temperature using an Agilent B2902A Source Meter under the illumination of an AM1.5G AAA class solar simulator (model XES-301S, SAN-EI) with an intensity of 100 mW cm^{-2} and the white light intensity was calibrated with a standard single-crystal Si solar cell.

1.3 Space-Charge Limited Current Measurement

Hole-only devices with a structure of ITO/PEDOT:PSS (30 nm)/ **P1-3**:$PC_{71}BM$ /Au (100 nm) were fabricated. The blend solution of **P1-3** and $PC_{71}BM$ in 1,2-dichlorobenzene (DCB) was spin-coated onto PEDOT:PSS layer to form active layer like PSC devices, and 100 nm of Au was thermally evaporated at a pressure of 10^{-4} Pa through a shadow mask. Dark J–V curves of the hole-only devices were measured by the space-charge limited current (SCLC) method.

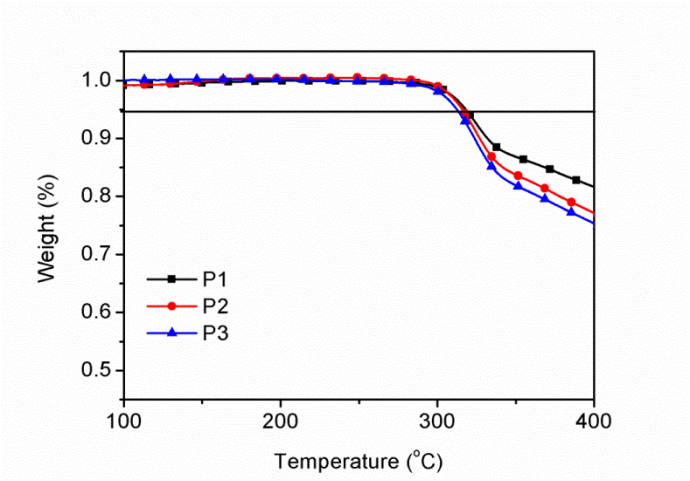

Fig. S1 TGA curves of **P1-3**.

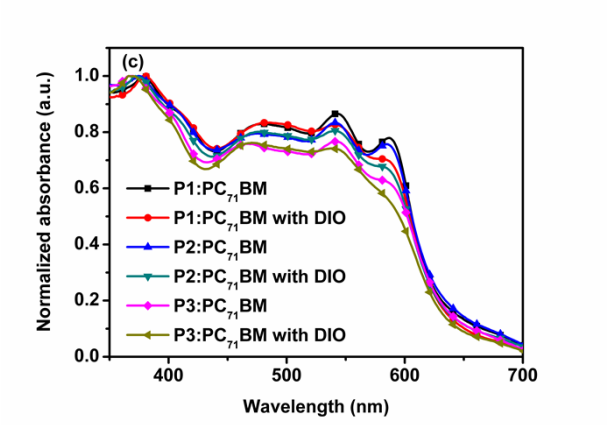

Fig. S2 UV-vis absorption spectra of **P1-3** based blend films without and with 2% DIO.

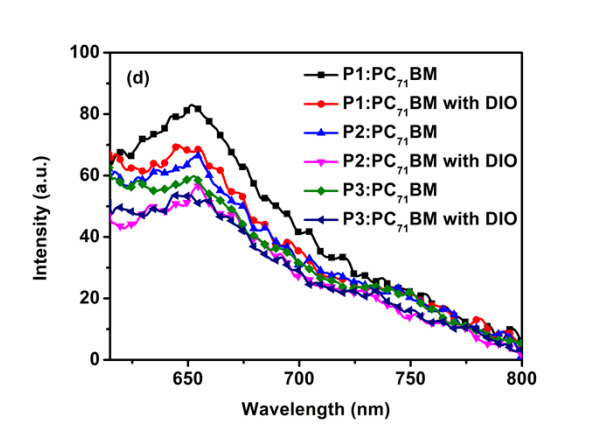

Fig. S3 Fluorescence spectra of **P1-3** based blend films without and with 2% DIO.

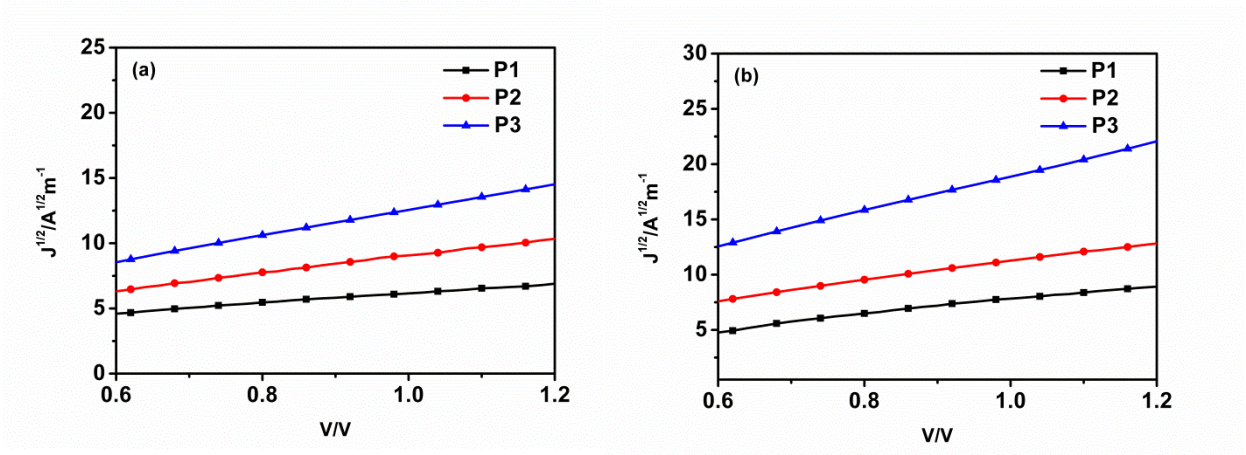

Fig. S4 Hole mobility of **P1-3**:$PC_{71}BM$ based devices without (a) and with 2% DIO (b) by SCLC.

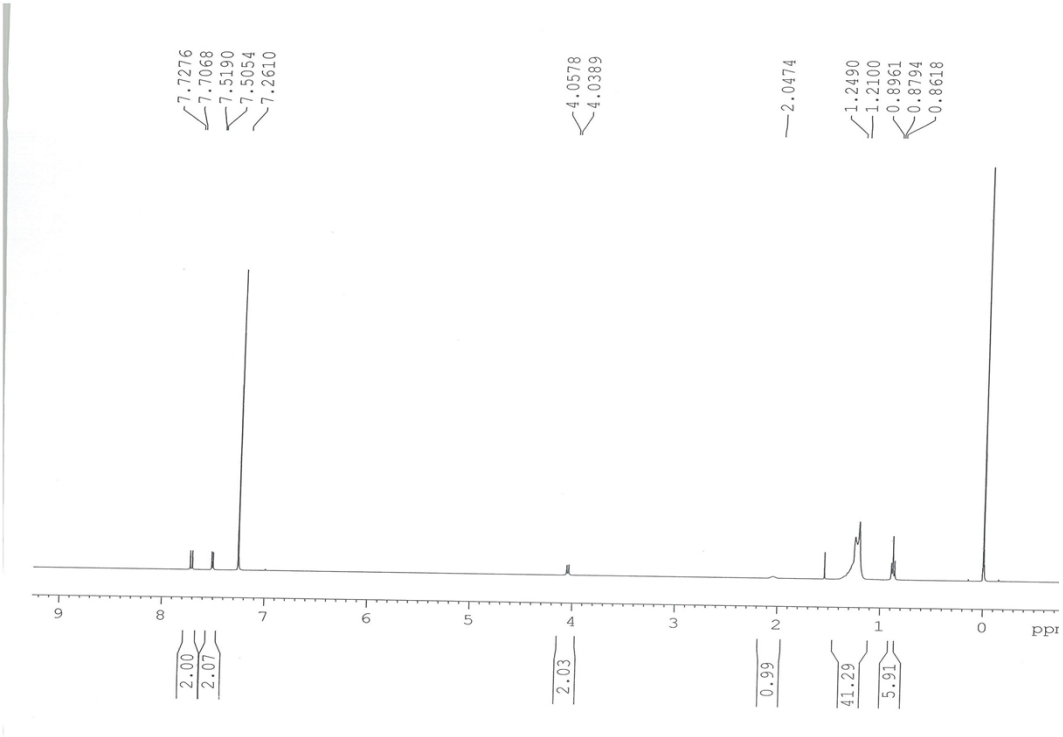

Fig. S5 ^{1}H NMR spectrum of **compound 2b** (measured in $CDCl_3$).

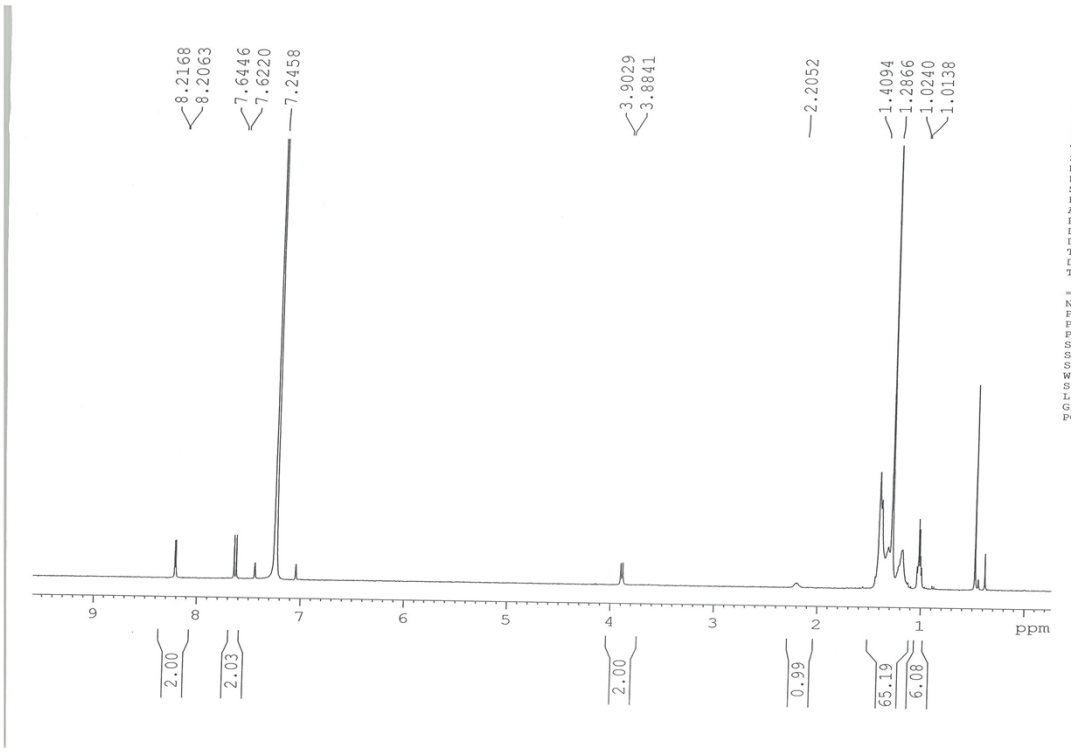

Fig. S6 ^{1}H NMR spectrum of **compound 3b** (measured in $CDCl_3$).

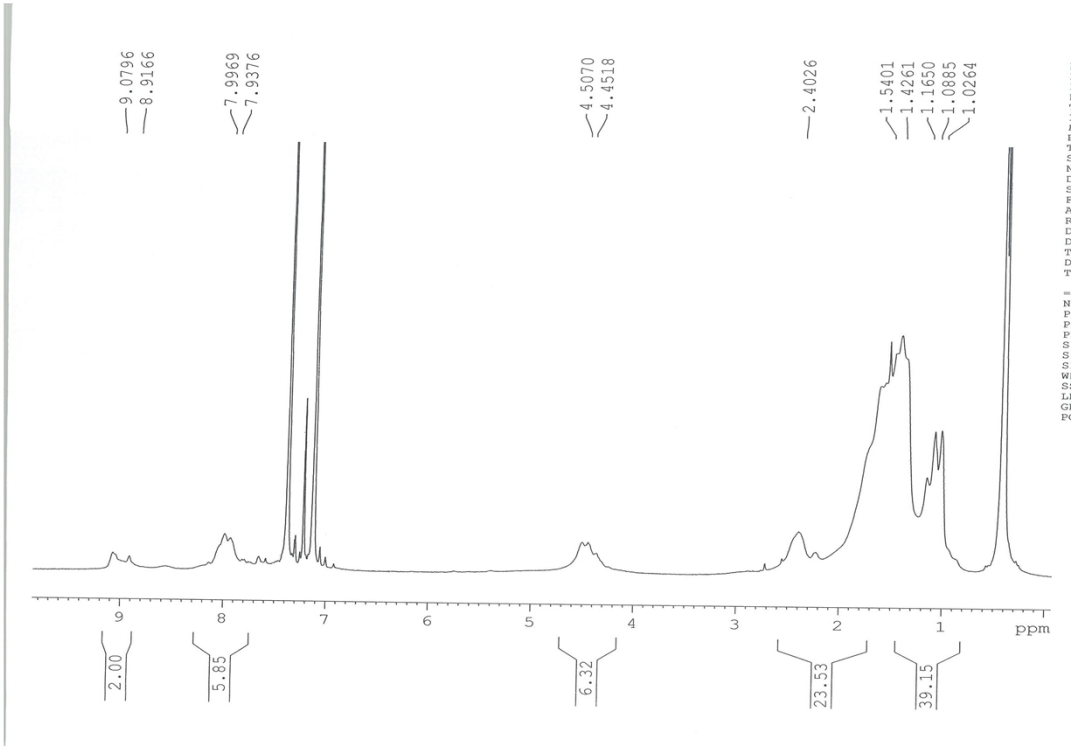

Fig. S7 ^{1}H NMR spectrum of **P1** (measured in 1,2-dichlorobenzene-d4).

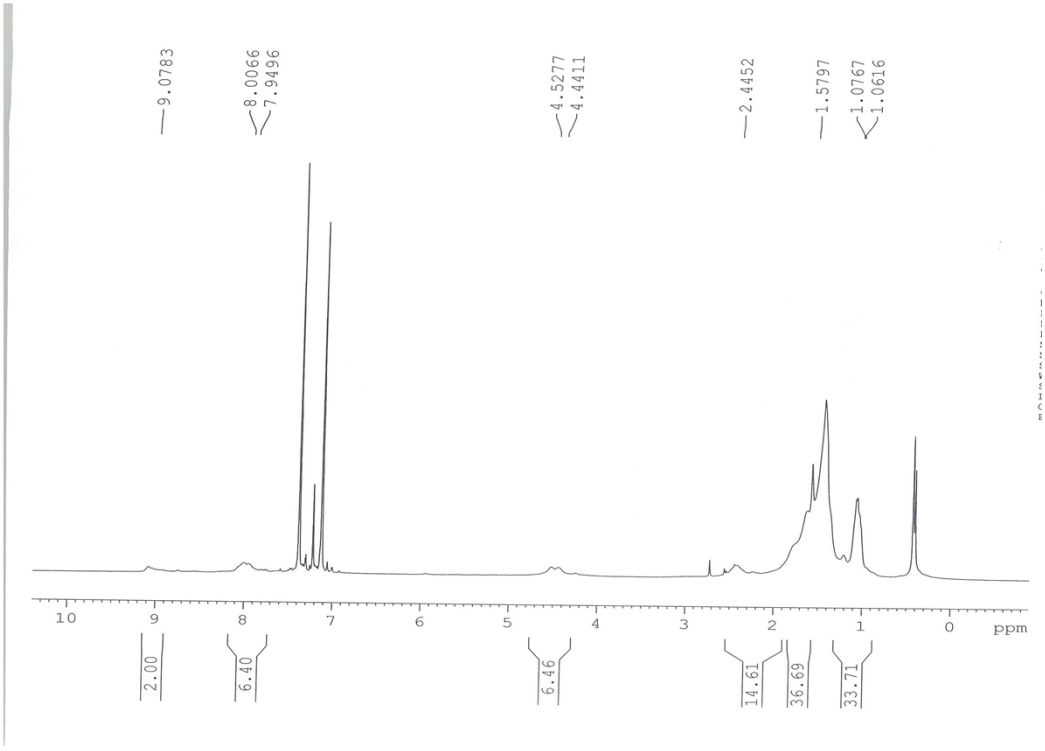

Fig. S8 ^{1}H NMR spectrum of **P2** (measured in 1,2-dichlorobenzene-d4).

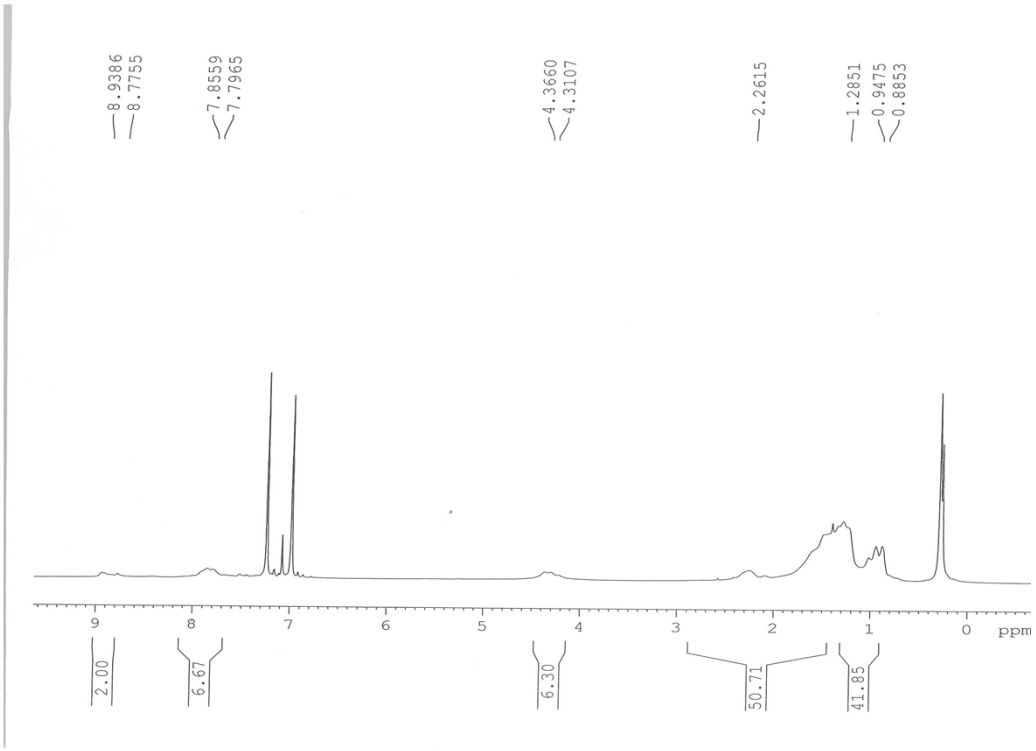

Fig. S9 ^{1}H NMR spectrum of **P3** (measured in 1,2-dichlorobenzene-d4).