

Supporting Information

Alkoxyphenylthiophene Linked Benzodithiophene Based Medium Band Gap Polymers for Organic Photovoltaics: Efficiency Improvement upon Methanol Treatment Depends on the Planarity of Backbone

Kakaraparthi Kranthiraja,[†] Kumarasamy Gunasekar,[†] Woosum Cho,[†] Myungkwan Song,[‡] Young Geun Park,[§] Jin Yong Lee,[§] Yurim Shin,[±] In-Nam Kang,[±] Ajeong Kim,^{||} Hyunjung Kim,^{||} BongSoo Kim,^{⊥,¶,*} Sung-Ho Jin^{†,*}

[†]Department of Chemistry Education, Graduate Department of Chemical Materials, BK 21 PLUS Team for Advanced Chemical Materials, and Institute for Plastic Information and Energy Materials, Pusan National University, Busan, 609-735, Republic of Korea

[‡]Surface Technology Division, Korea Institute of Materials Science, Changwon 641-831, Republic of Korea

[§]Department of Chemistry, Sungkyunkwan University, Suwon 440-746, Republic of Korea

[±]Department of Chemistry, The Catholic University of Korea, Bucheon 420-743, Republic of Korea

^{||}Department of Physics, Sogang University, Seoul 121-742, Republic of Korea

[⊥]Photo-electronic Hybrids Research Center, Korea Institute of Science and Technology (KIST), Seoul, 136-791, Republic of Korea

Figure S1. ^1H -NMR and ^{13}C -NMR of compound 2	3
Figure S2. ^1H -NMR and ^{13}C -NMR of compound D	4
Figure S3. MALDI-TOF MS data of compound 2	5
Figure S4. MALDI-TOF MS data of compound D	6
Figure S5. ^1H -NMR of P1 and P2	7
Figure S6. TGA curves of P1 and P2	8
Figure S7. UV-visible absorption spectra of (a) P1 and (b) P2 polymers in solution with various concentration.	9
Figure S8. Cyclic voltammograms of P1 and P2	10
Figure S9. X-ray diffraction spectra: (a) glass/PEDOT:PSS, glass/PEDOT:PSS/ P1 , glass/PEDOT:PSS/ P1 :PC ₇₁ BM blend, and glass/PEDOT:PSS/ P1 :PC ₇₁ BM blend (MeOH), (b) glass/PEDOT:PSS, glass/PEDOT:PSS/ P2 , glass/PEDOT:PSS/ P2 :PC ₇₁ BM blend, and glass/PEDOT:PSS/ P2 :PC ₇₁ BM blend (MeOH)	11
Figure S10. Space charge limited current (SCLC) mobility data of the (a) P1 and P2 hole only devices (b) P1 and P2 electron only devices	12
Figure S11. In-depth compositional distributions taken from TOF-SIMS measurement: (a) P1 :PC ₇₁ BM blend, (b) P2 :PC ₇₁ BM blend, (c) P1 : PC ₇₁ BM blend (MeOH), and (d) P2 : PC ₇₁ BM blend (MeOH).	13
Table S1. Molecular weights and thermal decomposition temperatures of polymers	14
Table S2. Hole mobilities and electron mobilities of polymers: PC ₇₁ BM with and without methanol treatment	15

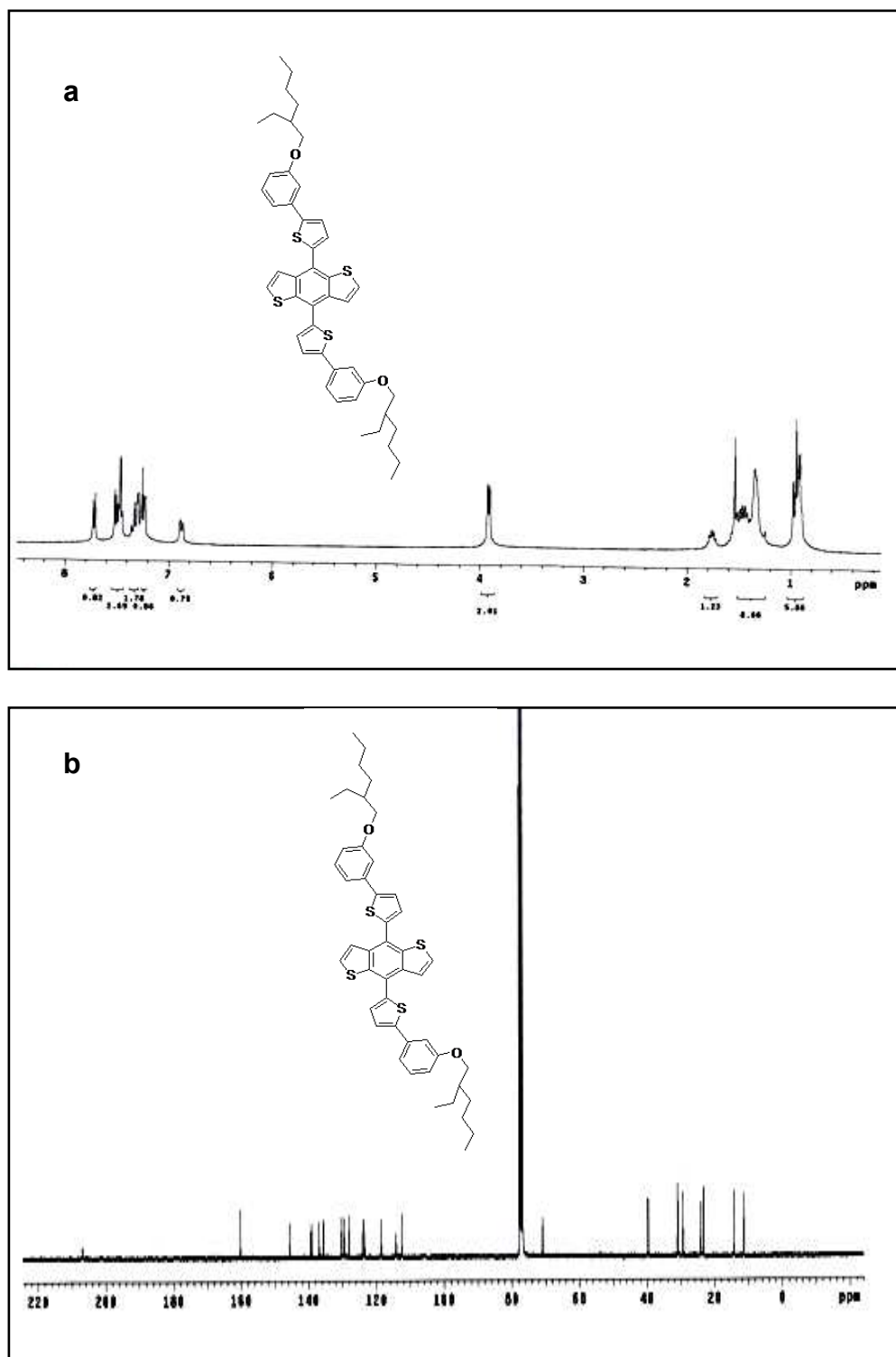


Figure S1

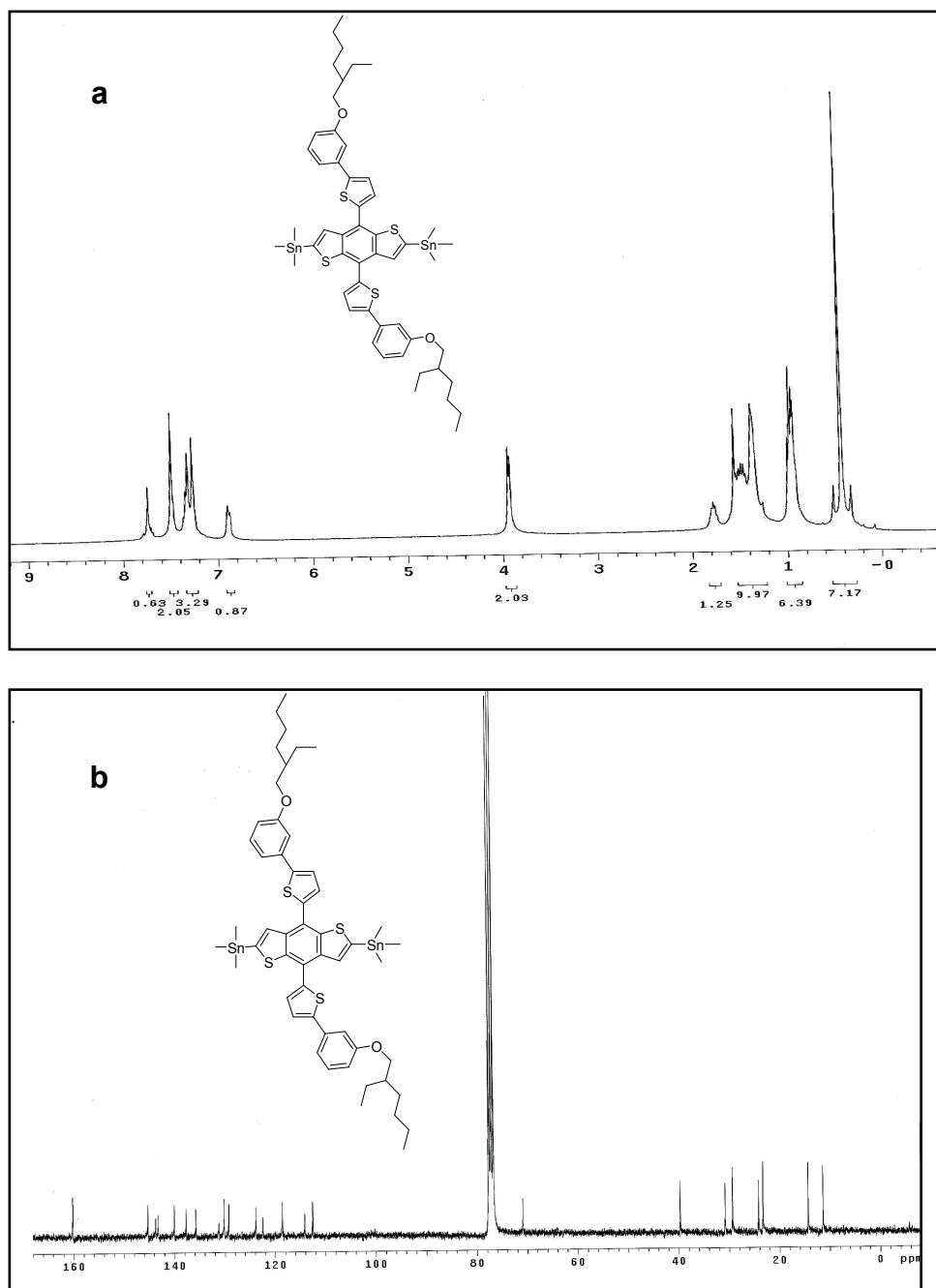


Figure S2

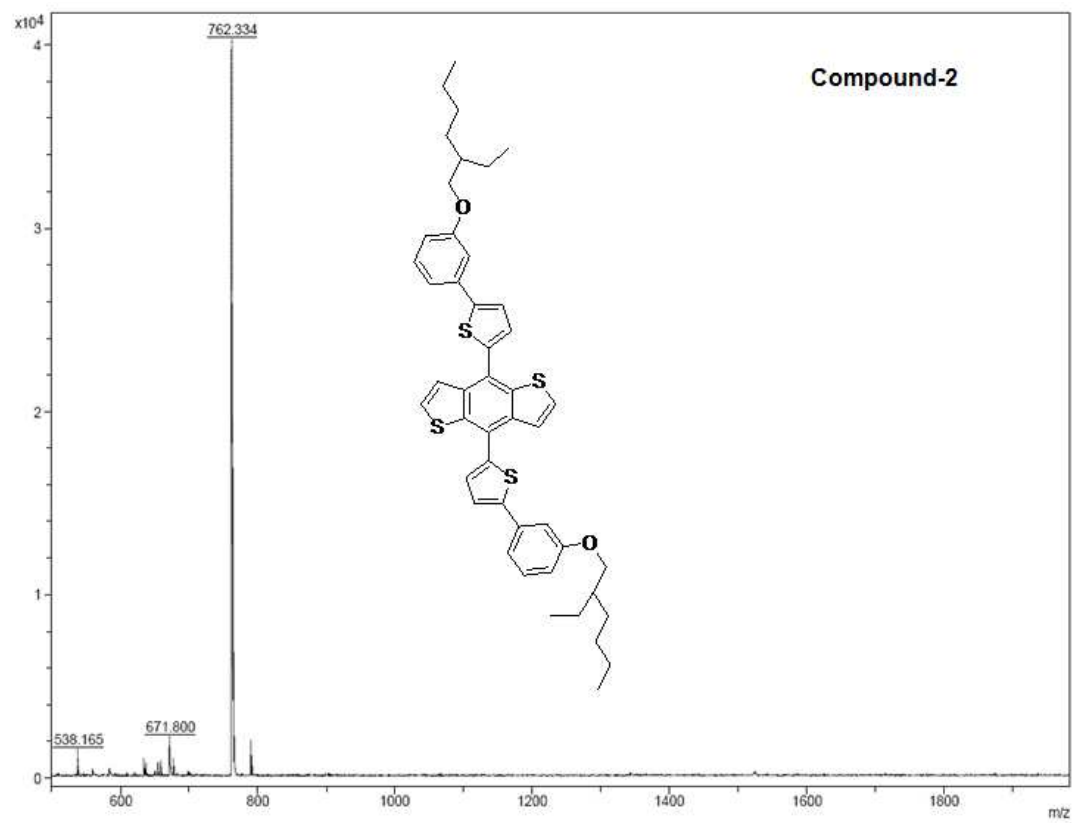


Figure S3

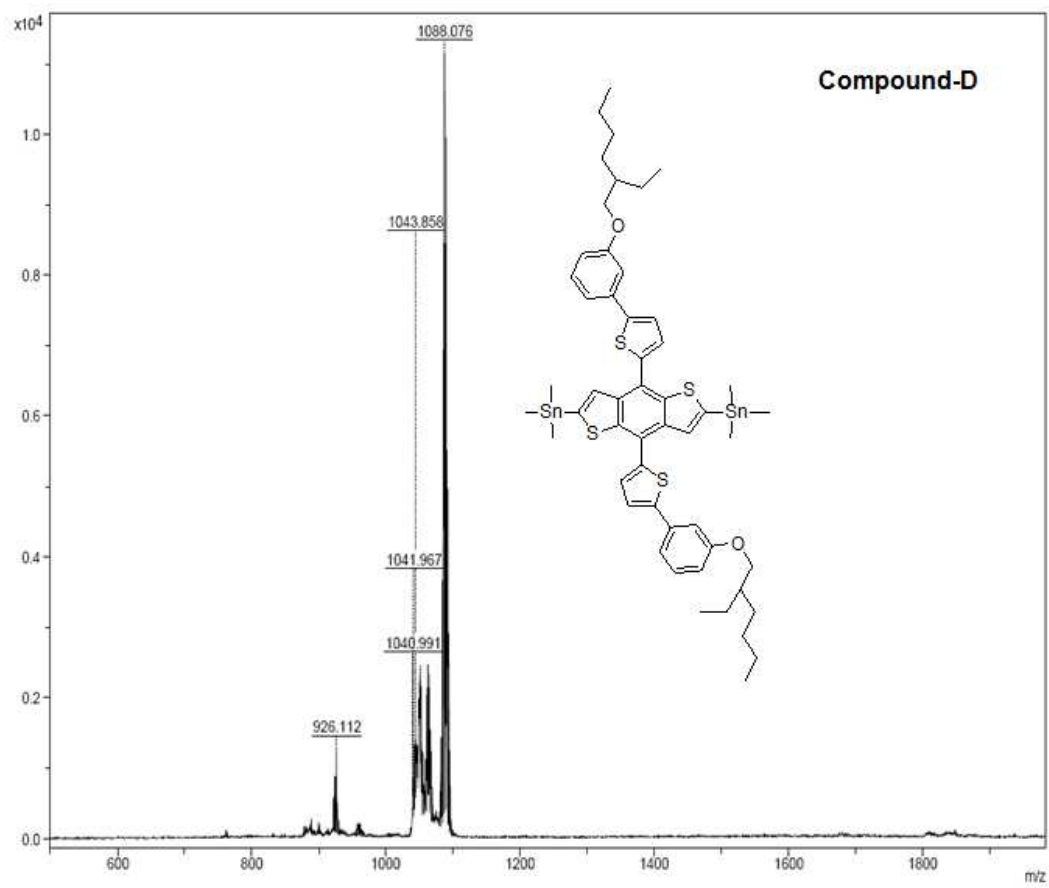


Figure S4

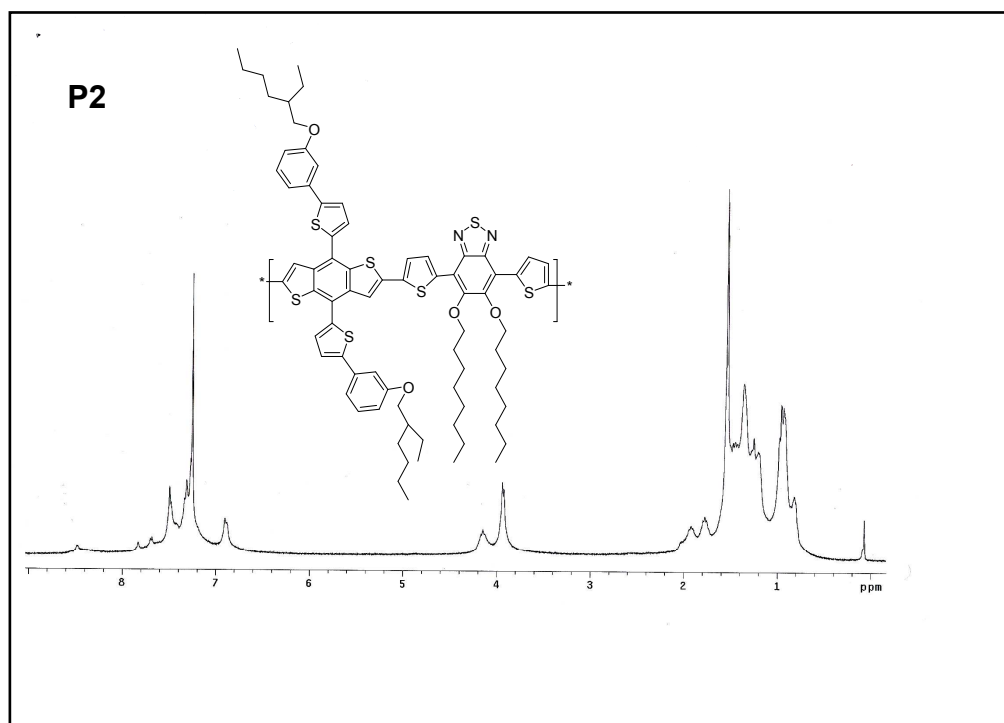
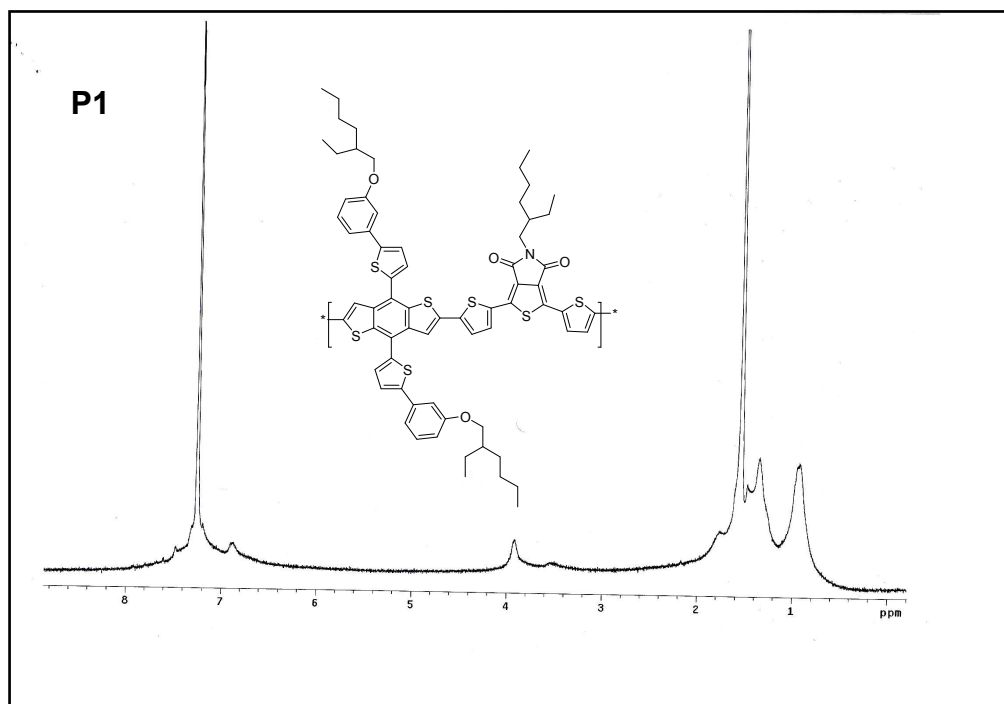


Figure S5.

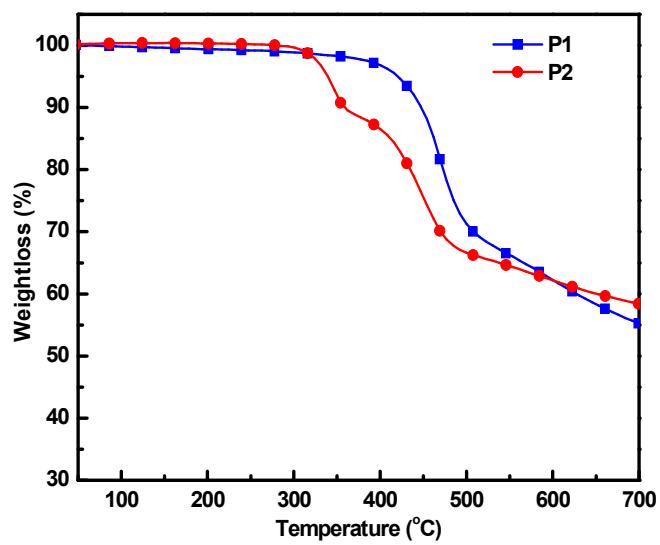


Figure S6

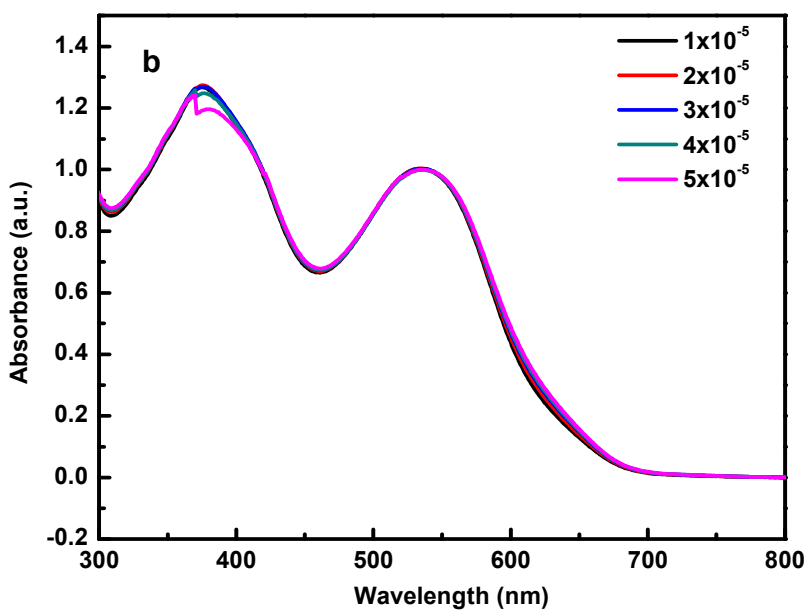
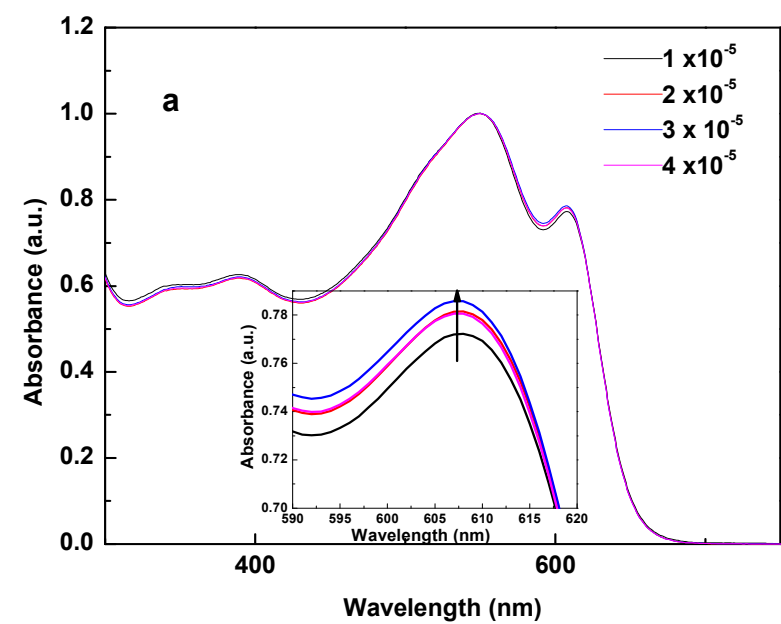


Figure S7

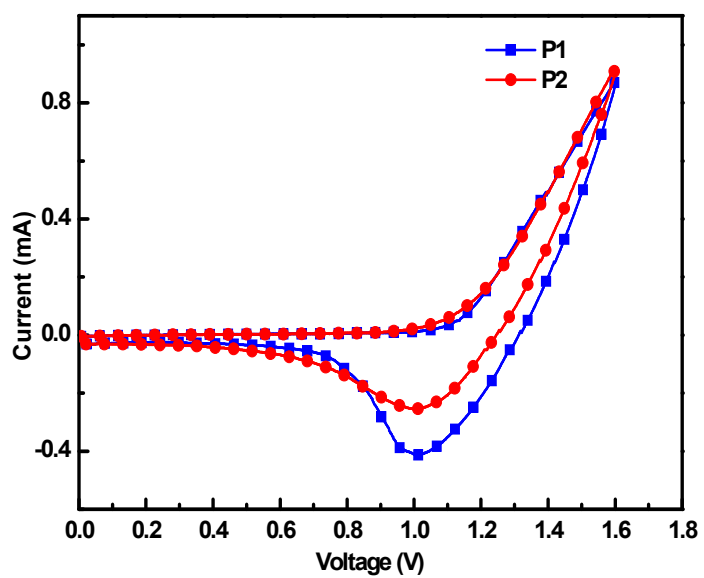


Figure S8

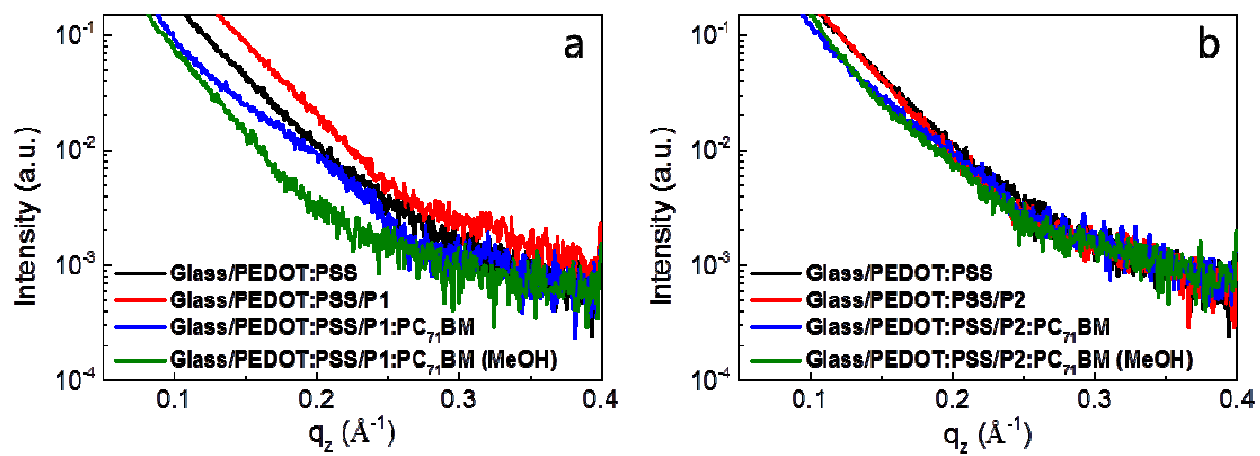


Figure S9

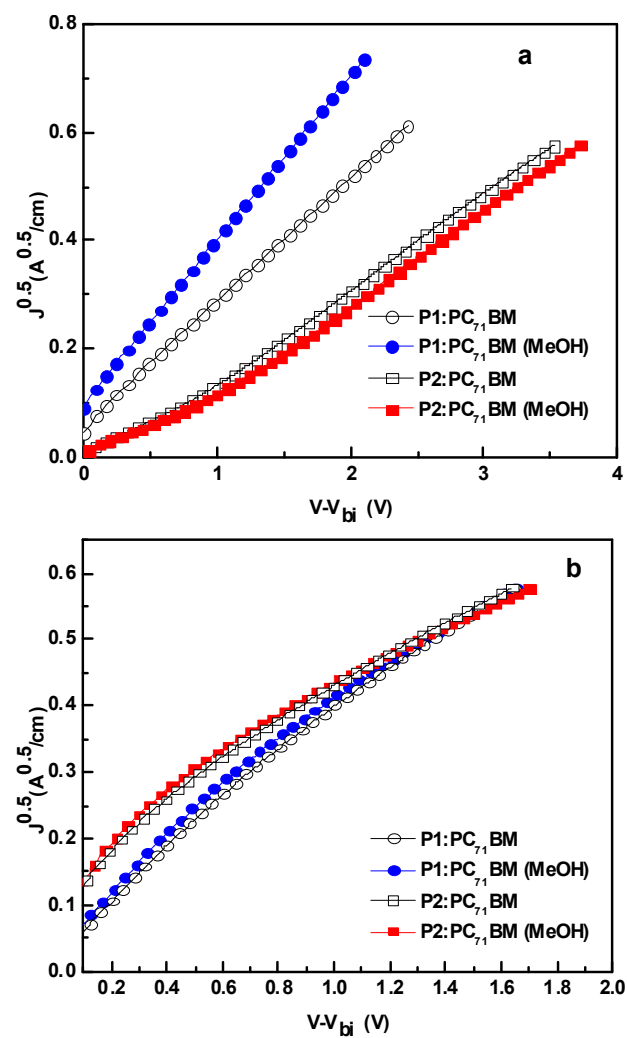


Figure S10

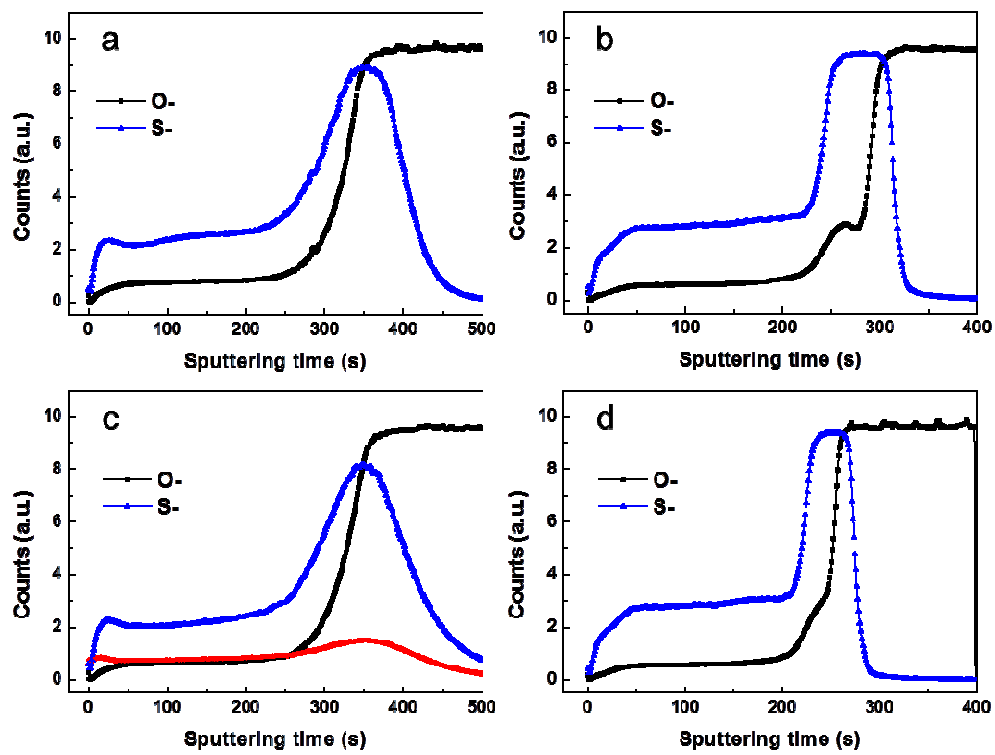


Figure S11

Table S1. Molecular Weights and Thermal Decomposition Temperatures of Polymers				
polymer	M_w (g/mol) ^a	M_n (g/mol) ^a	PDI	T_d (°C) ^b
P1	36000	30000	1.2	417
P2	32000	24000	1.3	337

^a M_w , M_n and polydispersity index were determined by gel permeation chromatography (GPC) in THF. ^bDecomposition temperature at 5% weight loss.

Table S2. Hole Mobilities and Electron Mobilities of Polymers: PC₇₁BM With and Without Methanol Treatment			
polymer	treatment	hole mobility (cm ² V ⁻¹ s ⁻¹)	electron mobility (cm ² V ⁻¹ s ⁻¹)
P1	none	1.62×10 ⁻⁴	3.65×10 ⁻⁴
P1	methanol	3.01×10 ⁻⁴	3.80×10 ⁻⁴
P2	none	9.45×10 ⁻⁵	2.82×10 ⁻⁴
P2	methanol	8.62×10 ⁻⁵	2.62×10 ⁻⁴