Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supporting Information

Synthesis and Properties of Air-stable n-Channel Semiconductors Based on MEH-PPV Derivatives Containing Benzo[*c*]cinnoline Moieties

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Structural Identification by NMR Spectroscopy

Monomer

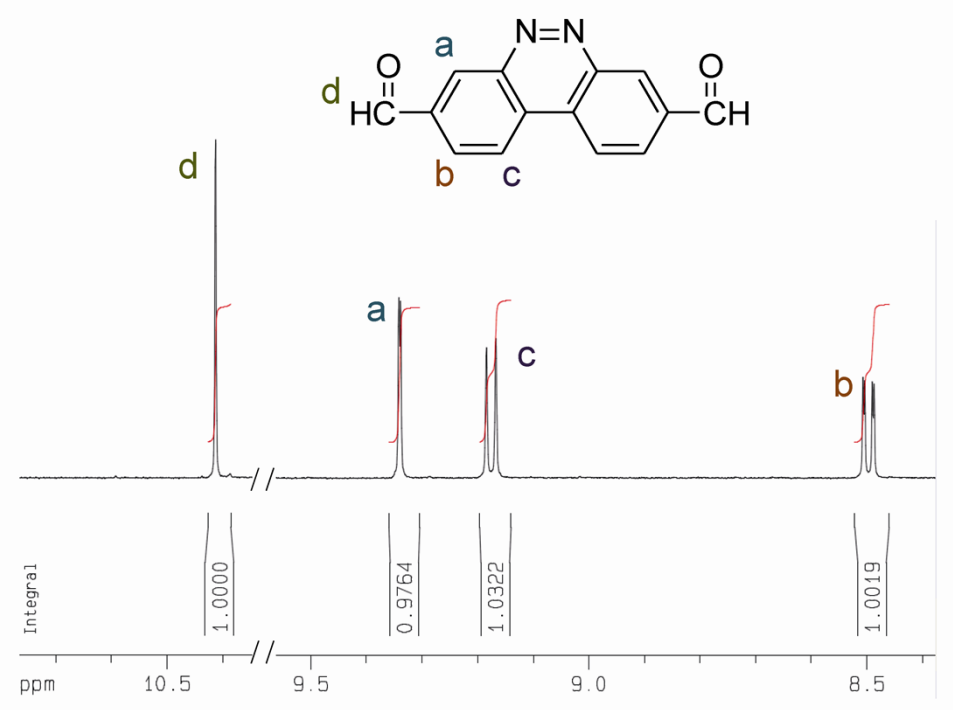

Fig. S1 ^{1}H NMR spectrum of compound **4** in DMSO-d_6.

Polymers

Several *d*-solvents, such as $CDCl_3$, THF-d_8, and DMSO-d_6, were used to prepare NMR samples. Quality NMR spectra can not be obtained due to the poor solubility except **P10** in $CDCl_3$. The ^{1}H and ^{13}C NMR spectra of **P10** in $CDCl_3$ were shown in Fig. S2 and S3, respectively. Due to the limited solubility of **P10** in $CDCl_3$, these spectra were obtained after 128 scans (^{1}H NMR spectrum) and 18135 scans (^{13}C NMR spectrum). The peaks at 6.6~7.7 ppm in Fig. S2 were attributed to the hydrogens on vinylene linkages and phenyl rings of the MEH-PPV segments. The peaks of hydrogens on the benzo[*c*]cinnilone segments appeared at 8.77, 8.53, and 8.13 ppm. By comparing the ^{13}C NMR spectra of MEH-PPV and **P10**, several new peaks appearing at 129.03, 128.22, and 125.29 ppm were assigned to the carbons on benzo[*c*]cinnoline segments (Fig. S3). The peaks of the quaternary carbons (B, E, and F in

Fig. S3) were too weak to be identified due to their nature and the limited solubility of **P10** in $CDCl_3$.

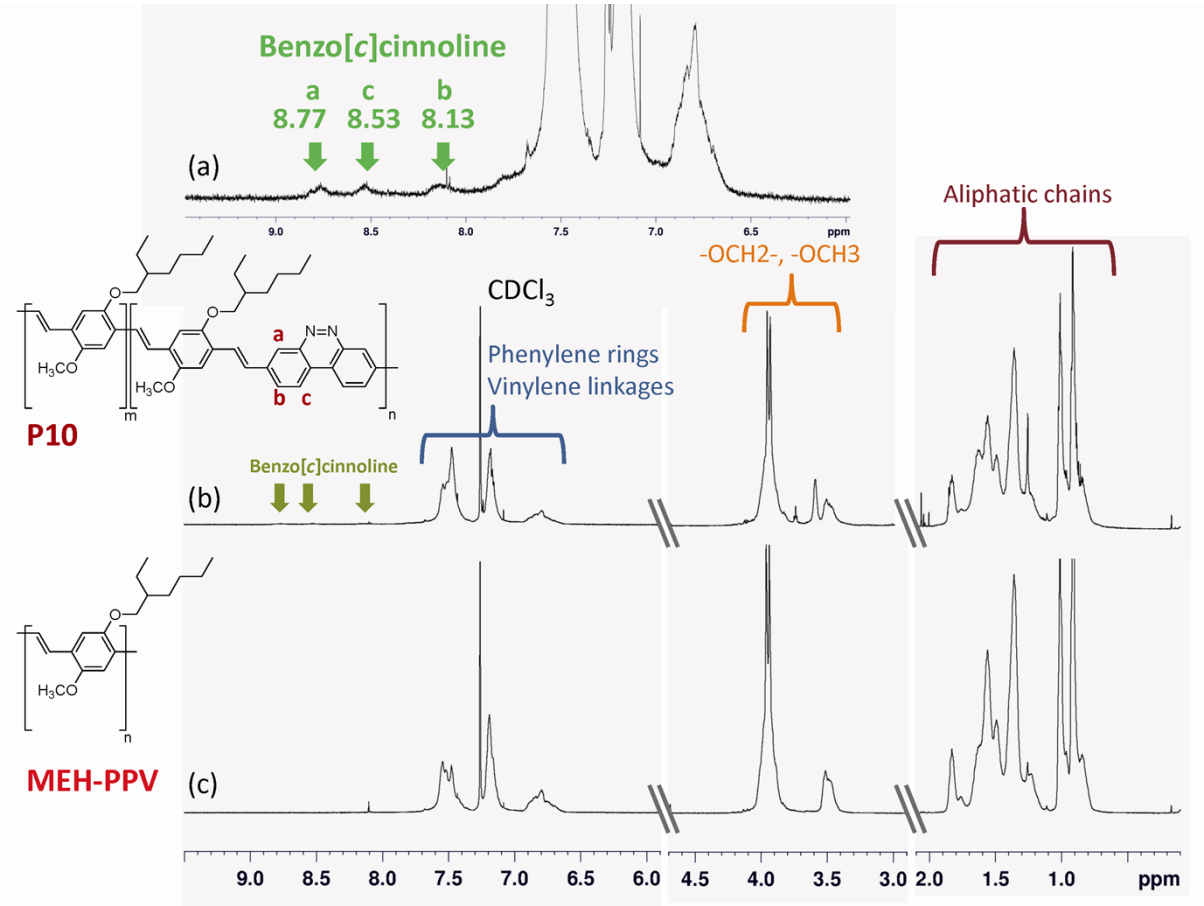

Fig. S2 ^{1}H NMR spectra of **P10** (a), (b) and MEH-PPV (c) in $CDCl_3$.

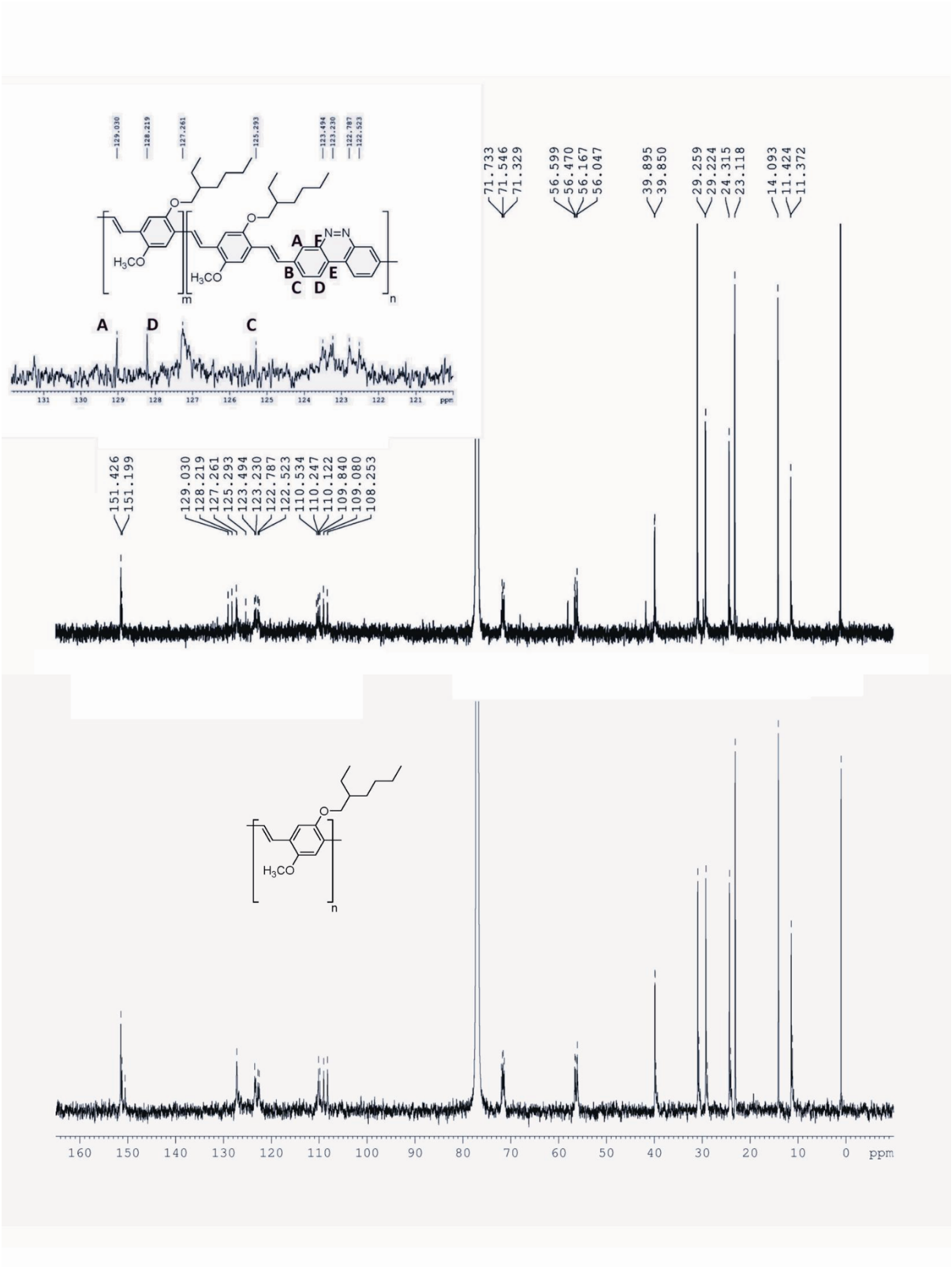

Fig. S3 ^{13}C NMR spectra of **P10** and MEH-PPV in $CDCl_3$.

Redox Behavior Characterized by Cyclic Voltammetry

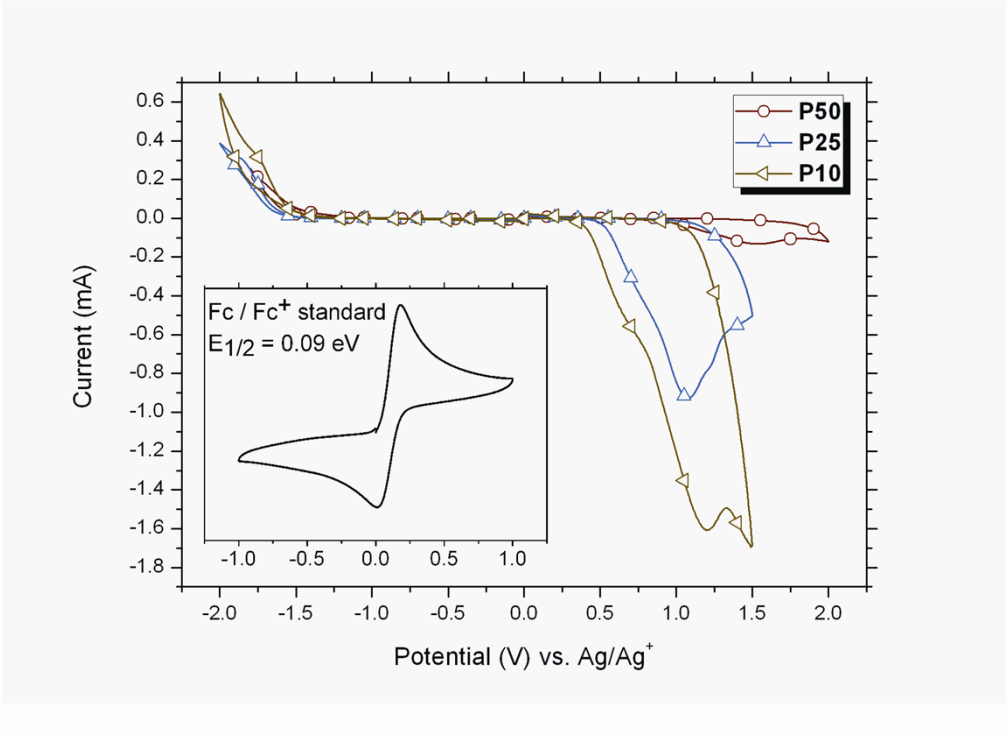

Fig. S4 Cyclic voltammograms of polymer films on an ITO-coated glass substrate in CH_3CN containing 0.1M TBAP.

Simulation methods

The theoretical calculations were carried out with the Maestro graphical interface of Schrodinger molecular modeling suite. (Maestro 9.4.047; Schrodinger, LLC: New York, www.schrodinger.com) The repeating units of MEH-PPV and **P50** were employed in the molecular simulation. The monomer structures were initially minimized using the OPLS_2005 (MacroModel, Version 9.9.2; Schrodinger, LLC: New York, www.schrodinger.com) force field with a dielectric constant of 1.0. Full geometry optimization was then carried out using density functional theory (DFT) within Jaguar module of Schrodinger molecular modeling suite. (Jaguar 8.0; Schrodinger, LLC: New York, 2010) The hybrid functional of the DFT method B3LYP is combined with 6-31G** basis set. SCF and convergence criteria were set at 5e-5 Hartree or RMS density matrix change of 5e-6,

whichever is met first. Single point electronic energy calculation on the optimized geometries were performed at the B3LYP/6-31G** level of theory. All computation was executed on a 16 CPU Intel Xeon workstation running Red Hat Linux.