Supporting Information

The Effect of Single Atom Replacement on Organic Thin Film Transistors: Case of Thieno[3,2-b]pyrrole vs Furo[3,2-b]pyrrole

Chandima Bulumulla, Ruwan Gunawardhana, Sang Ha Yoo, Cody R. Mills, Ruvanthi N. Kularatne, Thomas N. Jackson, Michael C. Biewer, Enrique D. Gomez, and Mihaela C. Stefan

The Department of Chemistry & Biochemistry and Department of Bioengineering, The University of Texas at Dallas, Richardson, TX, 75080, United States

The Department of Chemical Engineering, Department of Electrical Engineering and Materials Research Institute, The Pennsylvania State University, University Park, PA 16802, United States
Contents

1. NMR spectra........................................................................................................................................S3-S12

2. MALDI-TOF MS spectra of TP-FBT2T-TP and FP-FBT2T-FP.............................................................S13

3. GIWAXS spectra of TP-FBT2T-TP and FP-FBT2T-FP before and after annealing...................S13-S14

4. TMAFM images of TP-FBT2T-TP and FP-FBT2T-FP......................................................................S14
Fig S1 $^1$H NMR spectrum of ethyl-2-azido-3-(thiophen-2-yl)acrylate

Fig S2 $^{13}$C NMR spectrum of ethyl-2-azido-3-(thiophen-2-yl)acrylate
Fig S3 \(^1\)H NMR spectrum of ethyl-2-azido-3-(furan-2-yl)acrylate

Fig S4 \(^{13}\)C NMR spectrum of ethyl-2-azido-3-(furan-2-yl)acrylate
Fig S5 $^1$H NMR spectrum of ethyl 4$H$-thieno[3,2-$b$]pyrrole-5-carboxylate

Fig S6 $^{13}$C NMR spectrum of ethyl 4$H$-thieno[3,2-$b$]pyrrole-5-carboxylate
**Fig S7** $^1$H NMR spectrum of ethyl 4$H$-furo[3,2-$b$]pyrrole-5-carboxylate

**Fig S8** $^{13}$C NMR spectrum of ethyl 4$H$-furo[3,2-$b$]pyrrole-5-carboxylate
Fig S9 ¹H NMR spectrum of ethyl 4-dodecyl-4H-thieno[3,2-b]pyrrole-5-carboxylate

Fig S10 ¹³C NMR spectrum of ethyl 4-dodecyl-4H-thieno[3,2-b]pyrrole-5-carboxylate
Fig S11 $^1$H NMR spectrum of ethyl 4-dodecyl-4$H$-furo[3,2-$b$]pyrrole-5-carboxylate

Fig S12 $^{13}$C NMR spectrum of ethyl 4-dodecyl-4$H$-furo[3,2-$b$]pyrrole-5-carboxylate
Fig S13 $^1$H NMR spectrum of ethyl 4-dodecyl-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-4$H$-thieno[3,2-$b$]pyrrole-5-carboxylate

Fig S14 $^{13}$C NMR spectrum of ethyl 4-dodecyl-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-4$H$-thieno[3,2-$b$]pyrrole-5-carboxylate
Fig S15 $^1$H NMR spectrum of ethyl 4-dodecyl-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-4H-furo[3,2-b]pyrrole-5-carboxylate

Fig S16 $^{13}$C NMR spectrum of ethyl 4-dodecyl-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-4H-furo[3,2-b]pyrrole-5-carboxylate
Fig S17 $^1$H NMR spectrum of TP-FBT2T-TP

Fig S18 $^{13}$C NMR spectrum of TP-FBT2T-TP
Fig S19 $^1$H NMR spectrum of FP-FBT2T-FP

Fig S20 $^{13}$C NMR spectrum of FP-FBT2T-FP
**Fig S21** MALDI-TOF spectrum of TP-FBT2T-TP

**Fig S22** MALDI-TOF spectrum of FP-FBT2T-FP

**Fig S23** (a) GIWAXS spectrum, (c) out-of-plane cut, (d) in-plane cut of TP-FBT2T-TP film before annealing. (b) GIWAXS spectrum (e) out-of-plane cut, (f) in-plane cut of TP-FBT2T-TP film after annealing
**Fig S24** (a) GIWAXS spectrum, (c) out-of-plane cut, (d) in-plane cut of FP-FBT2T-FP film before annealing. (b) GIWAXS spectrum (e) out-of-plane cut, (f) in-plane cut of FP-FBT2T-FP film after annealing.

**Fig S25** TMAFM (a) height image, (b) phase image of TP-FBT2T-TP thin film annealed at 120 °C. TMAFM (a) height image, (b) phase image of FP-FBT2T-FP thin film annealed at 100 °C