Supplementary Information

Synthesis, characterization, and air stability study of pyrimido[4,5-*g*]quinazoline-4,9-dione-based polymers for organic thin-film transistors

Jesse Quinn, Yinghui He, Daid A. Khan, Jonathan Rasmussen, Haritosh Patel, Fezza Haider, Wassim Kapadia and Yuning Li*

Department of Chemical Engineering and Waterloo Institute of Nanotechnology, (WIN), University of Waterloo, 200 University Ave West, Waterloo, N2L 3G1, Canada

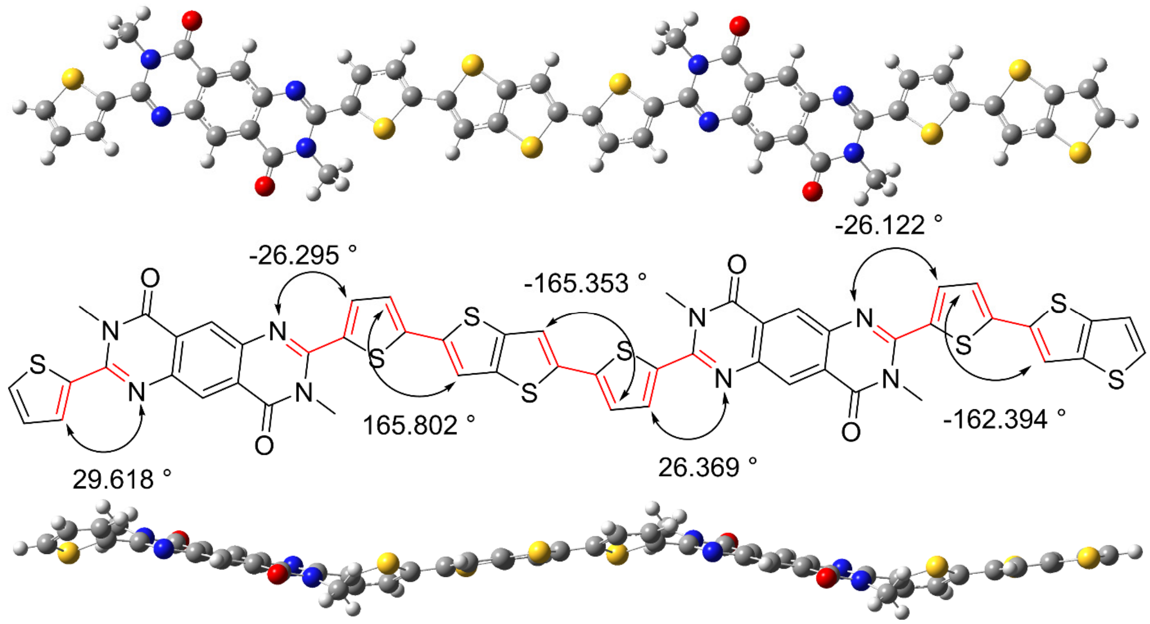

Figure S1. The optimized geometry and dihedral angles of the PQ2T-TT-Me dimer using Gaussian 09 Revision D.01[1] with the B3LYP/6-31G(d) level of theory under tight convergence.

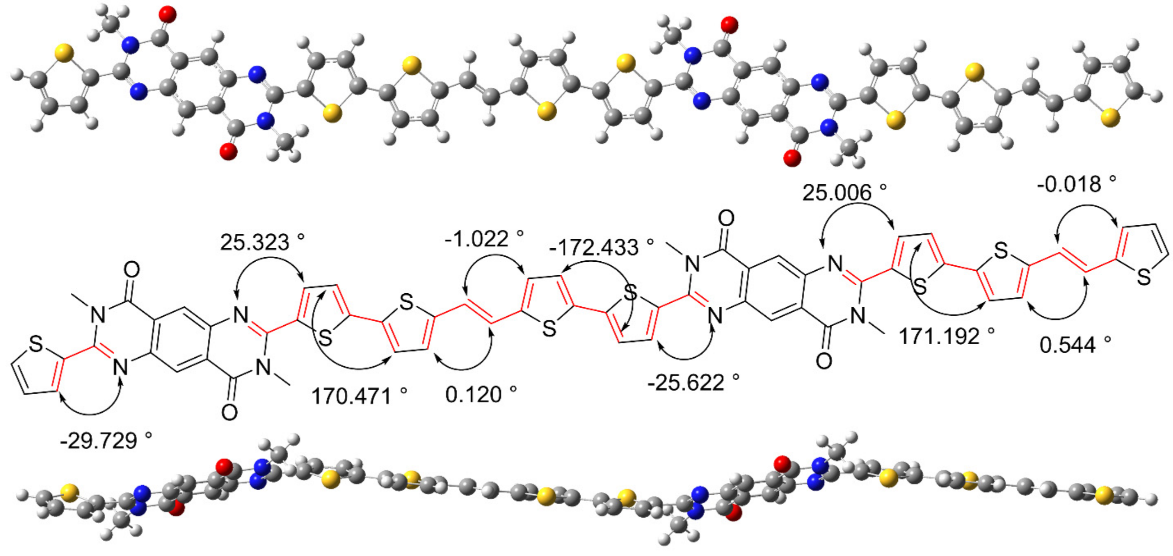

Figure S2. The optimized geometry and dihedral angles of the PQ2T-TVT-Me dimer using Gaussian 09 Revision D.01[1] with the B3LYP/6-31G(d) level of theory under tight convergence.

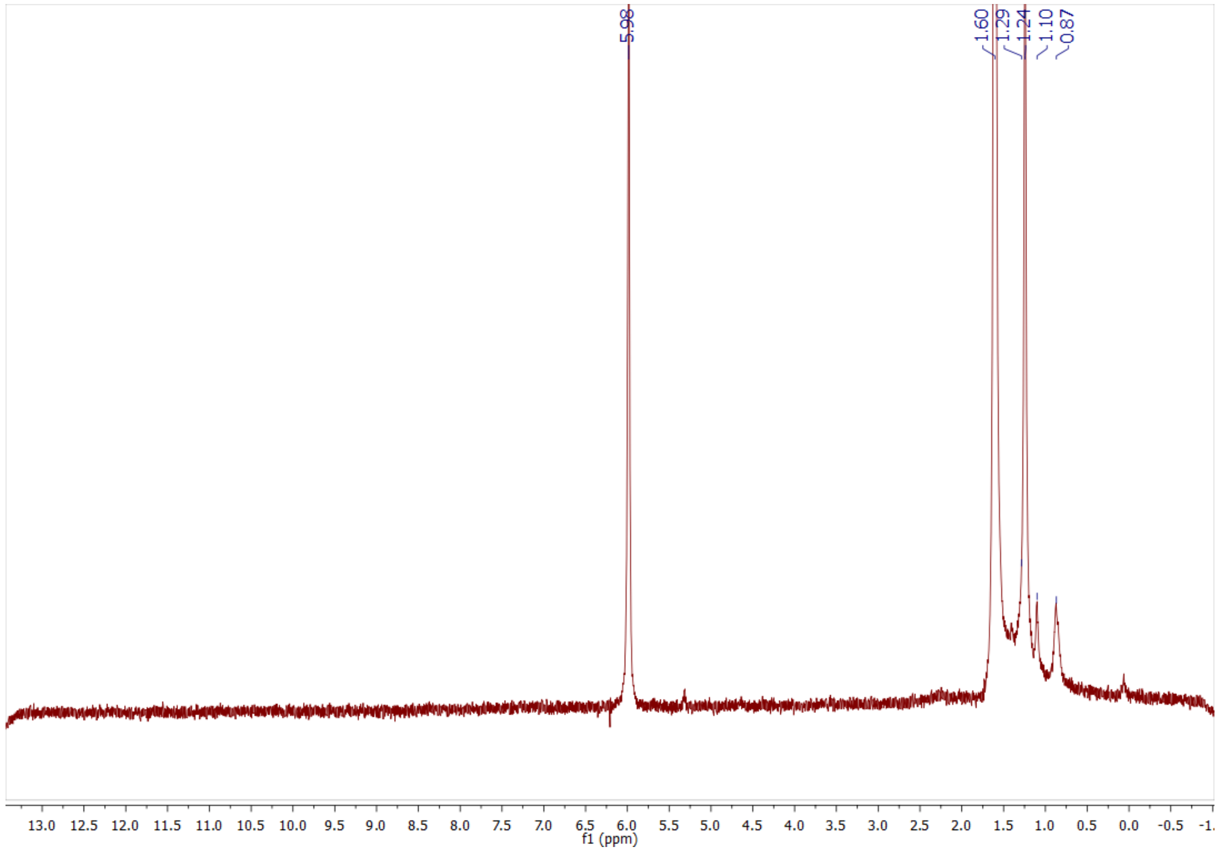

Figure S3. 300 MHz ^{1}H NMR spectrum for PPQ2T-TT-24 in 1,1,2,2-tetrachloroethane-d_2.

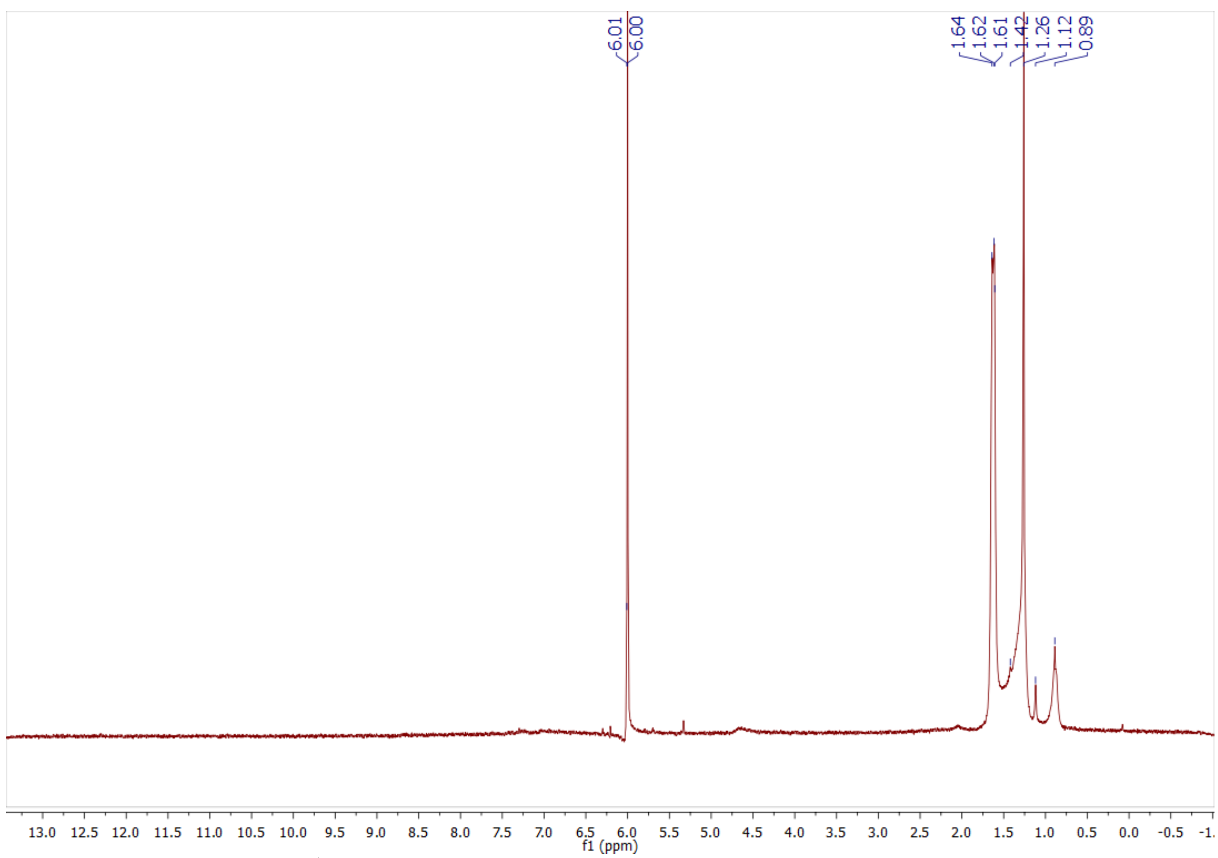

Figure S4. 300 MHz ^{1}H NMR spectrum for PPQ2T-TVT-24 in 1,1,2,2-tetrachloroethane-d_2.

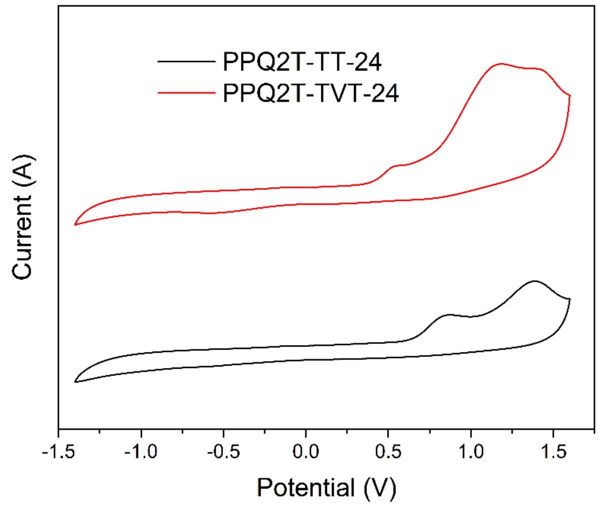

Figure S5. Cyclic voltammograms of the PPQ2T-TT-24 and PPQ2T-TVT-24 thin-films on a platinum electrode in 0.1 M Bu_4NPF_6 acetonitrile solution at a scanning rate of 50 mV s^{-1}.

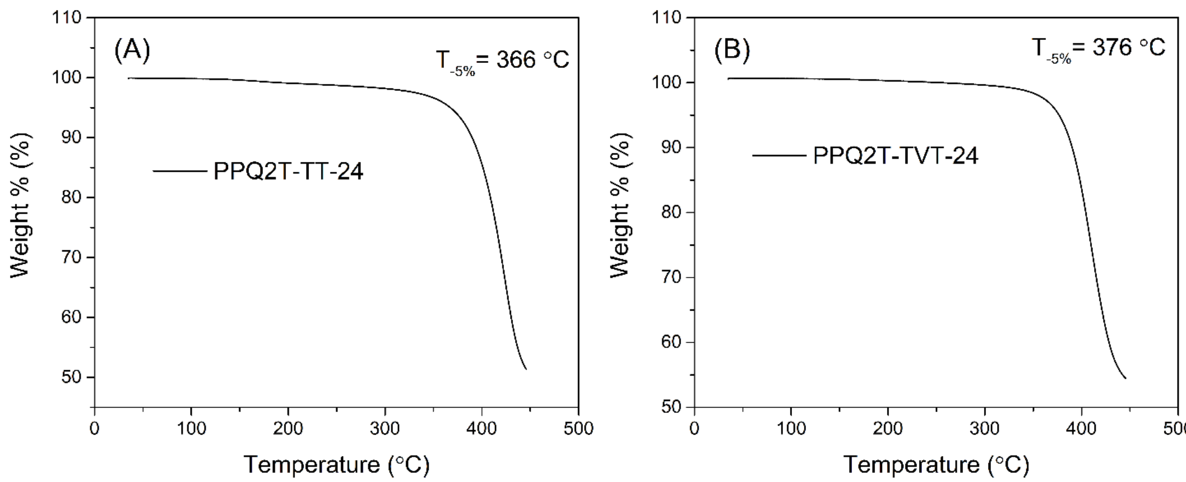

Figure S6. TGA thermograms of PPQ2T-TT-24 (A) and PPQ2T-TVT-24 (B) with a heating rate of 10 °C min^{-1} under nitrogen.

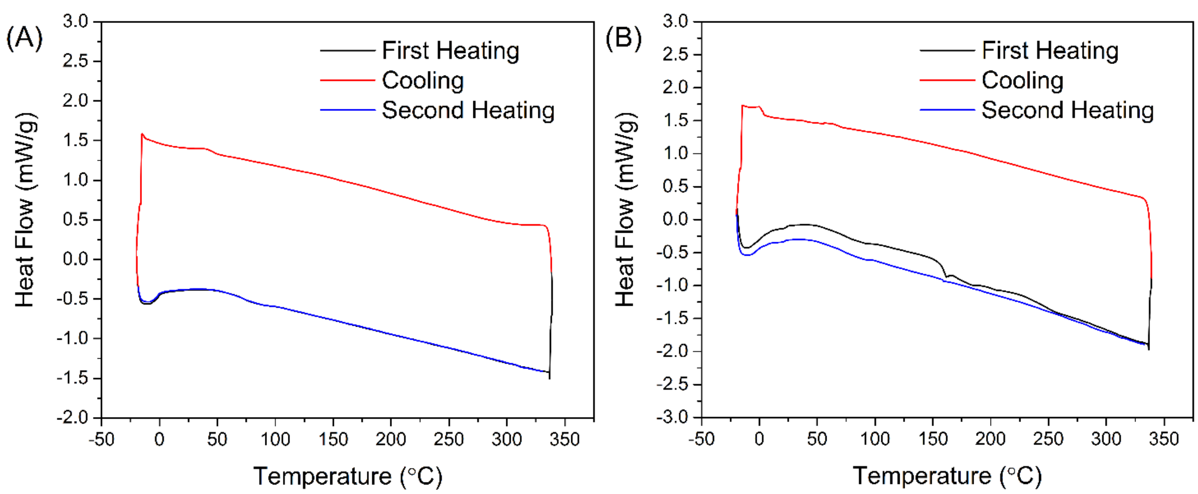

Figure S7. DSC thermograms of PPQ2T-TT-24 (A) and PPQ2T-TVT-24 (B) with a temperature ramp of 20 °C min^{-1}.

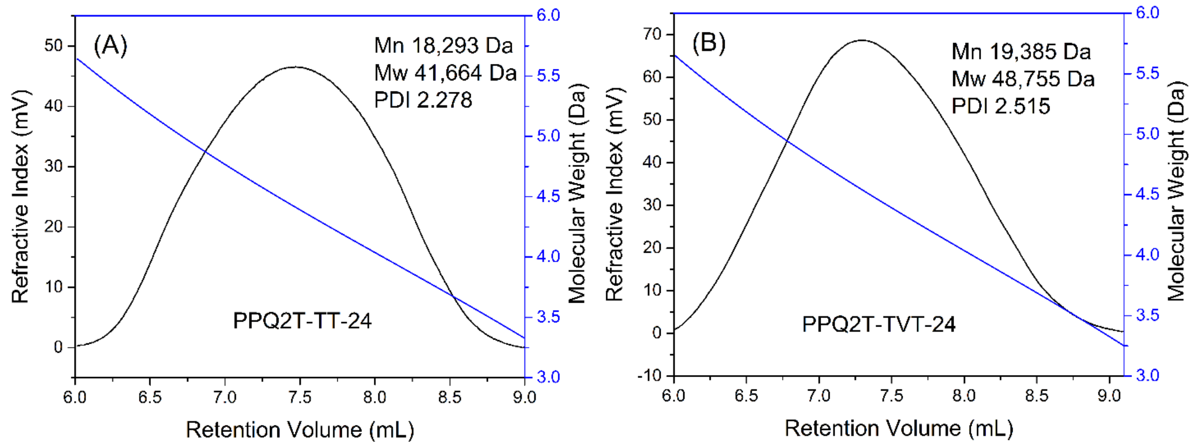

Figure S8. High temperature GPC traces of **PPQ2T-TT-24** (A) and **PPQ2T-TVT-24** (B) with refractive index detector measured at 140 °C.

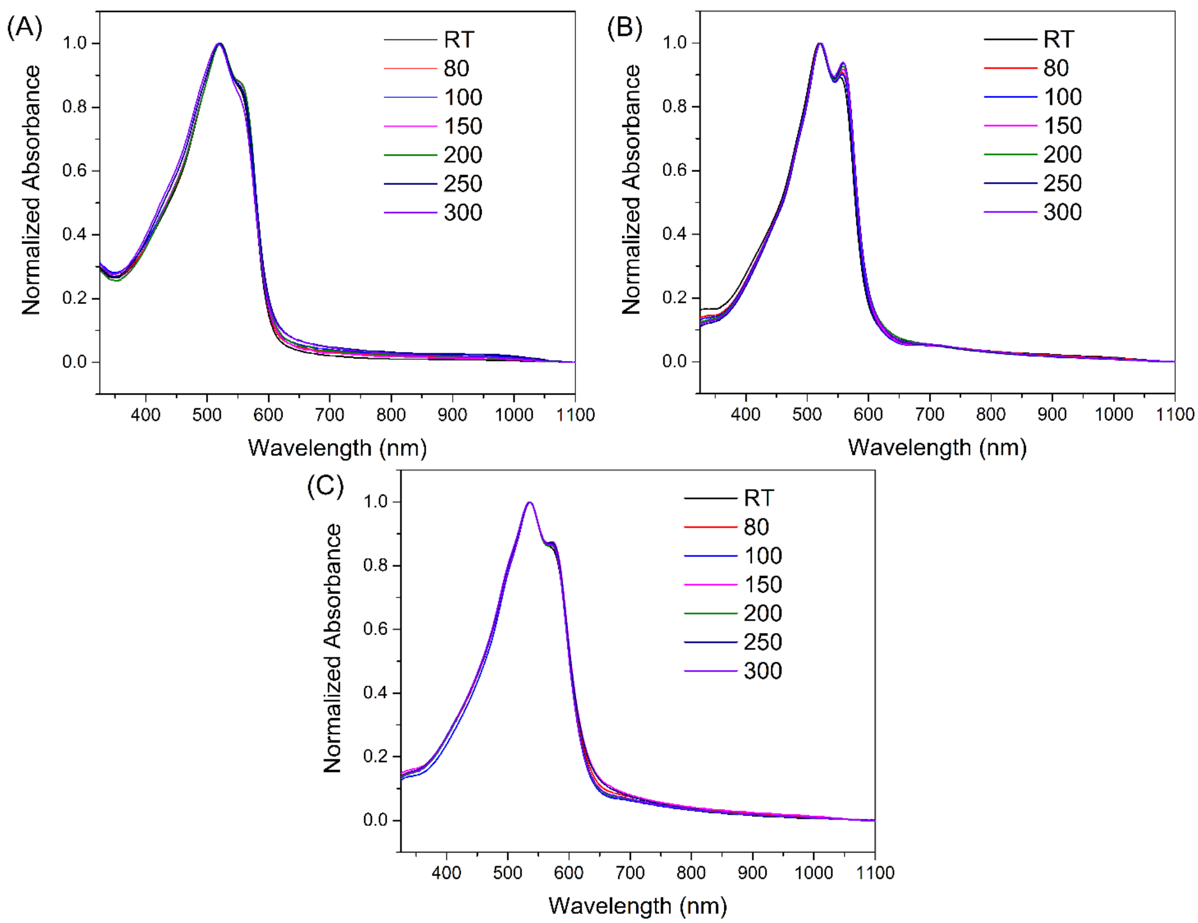

Figure S9. UV-Vis spectra of **PPQ2T-BT-24** (A), **PPQ2T-TT-24** (B), and **PPQ2T-TVT-24** (C) thin films spin coated on quartz substrates and annealed at different temperatures.

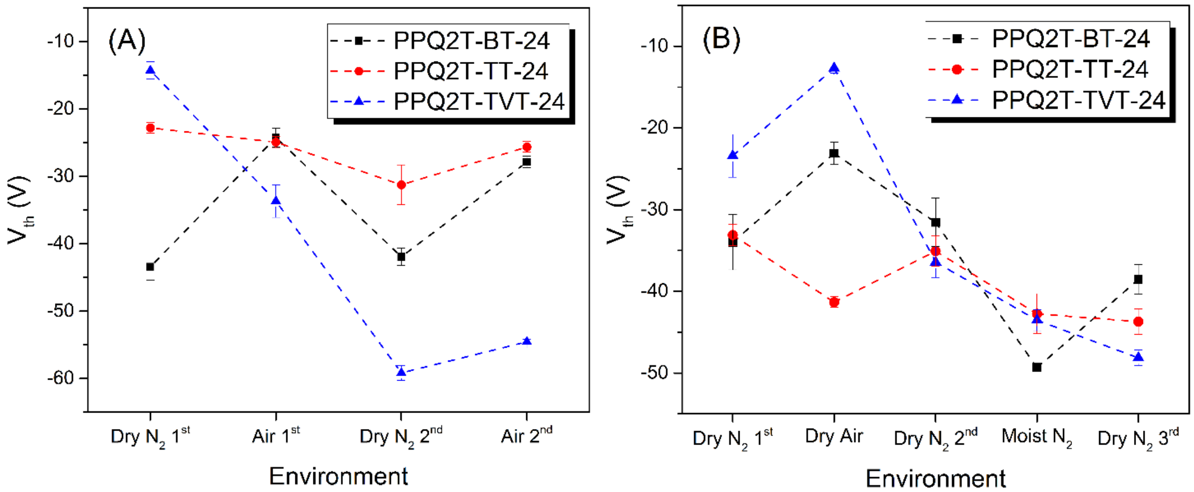

Figure S10. Threshold voltages of OTFTs of polymers measued in (A) dry nitrogen, ambient air, dry nitrogen, and ambient air and (B) dry nitrogen, dry air, dry nitrogen, moist nitrogen, and dry nitrogen. The ambient air had a relative humidity of 52% and a temperature of 24 °C. The dry nitrgen (inside a glove box) contained < 1ppm of H_2O and O_2. The moist nitrogen was a nitrogen gas saturated with H_2O vapour at 24 °C.

Table S1. The summary of OTFT performance of **PPQ2T-TT-24** and **PPQ2T-TVT-24** thin films annealed at different temperatures and characterized under dry nitrogen atmosphere.

Polymer	Annealing temperature (°C)	Hole mobility[a] (10^{-3} $cm^2V^{-1}s^{-1}$)	Average V_{th} (V)	I_{on}/I_{off}
PPQ2T-TT-24	80	1.92 (1.59 ± 0.26)	-22.08	~10^4
	100	1.90 (1.77 ± 0.18)	-6.31	~10^4
	150	2.27 (2.11 ± 0.16)	-9.28	~10^4
	200	2.27 (2.19 ± 0.05)	-25.05	~10^4
	250	2.63 (2.13 ± 0.48)	-29.59	~10^4
	300	3.08 (2.33 ± 0.58)	-13.43	~10^4
PPQ2T-TVT-24	80	3.80 (3.58 ± 0.18)	-6.50	~10^4
	100	4.96 (4.39 ± 0.46)	-7.70	~10^4
	150	5.34 (4.81 ± 0.39)	-3.32	~10^4
	200	5.26 (4.85 ± 0.40)	-7.88	~10^4
	250	3.99 (3.62 ± 0.35)	-4.60	~10^4
	300	3.81 (3.53 ± 0.32)	-3.93	~10^4

[a] The maximum (average ± standard deviation) mobility was calculated from the saturated regime of at least five devices for each condition.

References

1. Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M. J.; Heyd, J.; Brothers, E. N.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A. P.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. *Gaussian 09 Revision D.01*; Gaussian, Inc.: Wallingford, CT, USA, 2009.