Supplementary Information

Indigo-based Highly Coplanar Semiconducting Polymer for N-Type Organic Thin Film Transistors

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Supplementary Information

1. Computer simulations

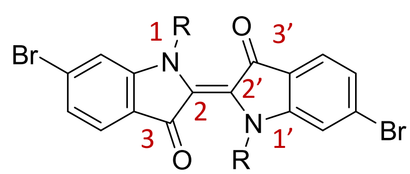
Geometry optimization of model compounds was performed based on the density functional theory (DFT) using the B3LYP hybrid function[1] and the 6-31G* basis set and the Gaussian 09W package[2] on the Shared Hierarchical Academic Research Computer Network (SHARCNET) of Canada.

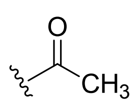
The route used for all calculations was the following:

opt=tight freq b3lyp/6-31g(d) guess=save geom=connectivity int=ultrafine

The obtained key dihedral angles of two model compounds, (*E*)-6,6'-dibromo-[2,2'-biindolinylidene]-3,3'-dione (or Tyrian Purple) (*trans*-IDBr) and (*E*)-1,1'-diacetyl-6,6'-dibromo-[2,2'-biindolinylidene]-3,3'-dione (*trans*-IDBrAc) are summarized in Table S1.

Table S1. Summary of computer simulation results of model compounds, *trans*-IDBr and *trans*-IDBrAc.



R = H (*trans*-IDBr), 

(*trans*-IDBrAc)

Model compound	Dihedral angle, °		
	N(1)-C(2)-C(2')-N(1')	N(1)-C(2)-C(2')-C(3')	C(3)-C(2)-C(2')-C(3')
trans-IDBr	180	0	180
trans-IDBrAc	173.3	22.6/24.5	139.5

2. Additional data

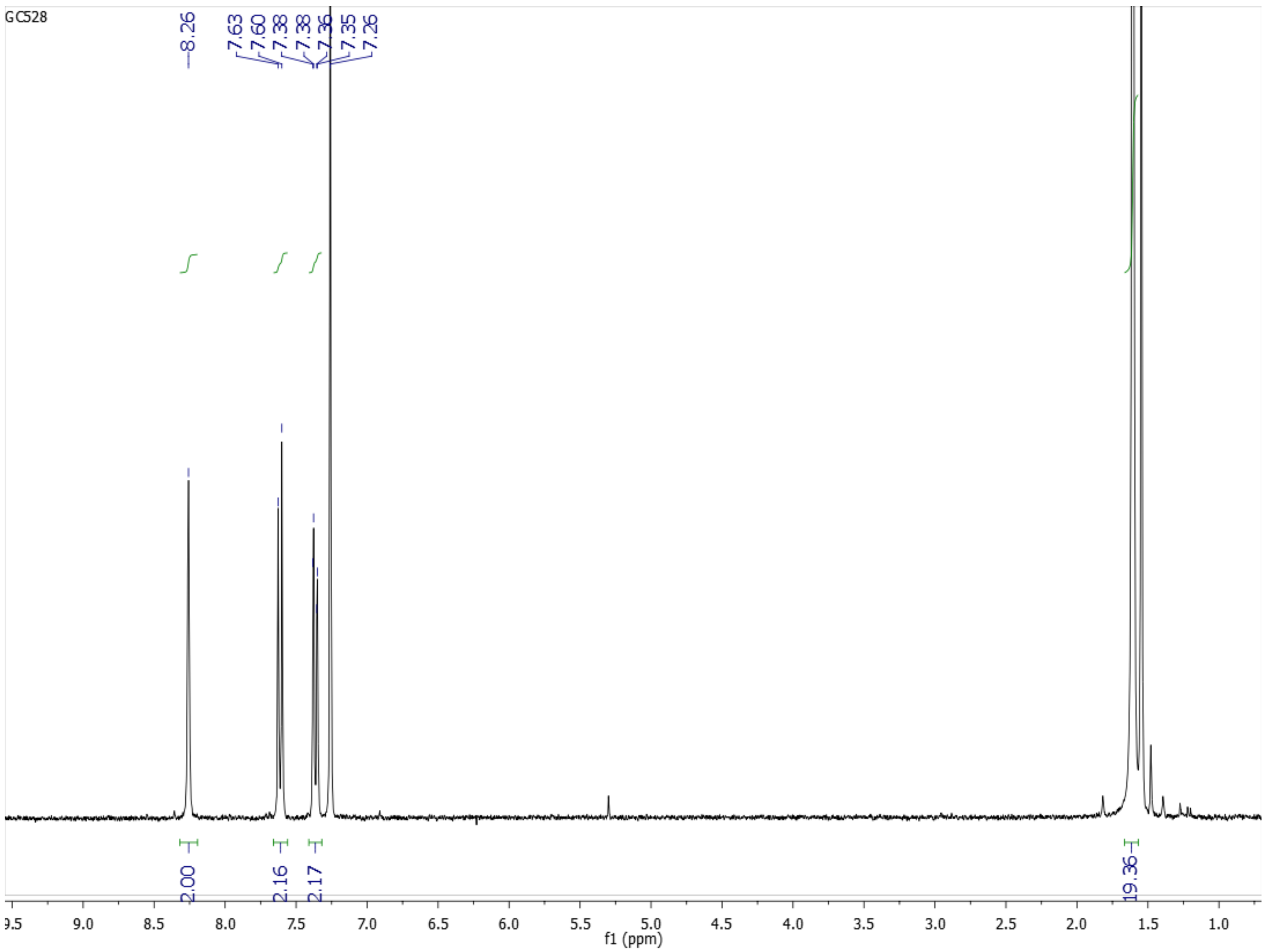


Fig. S1 The 300 MHz ^{1}H NMR spectrum of di-*tert*-butyl 6,6'-dibromo-3,3'-dioxo-[2,2'-biindolinylidene]-1,1'-dicarboxylate (compound **2**) measured in $CDCl_3$.

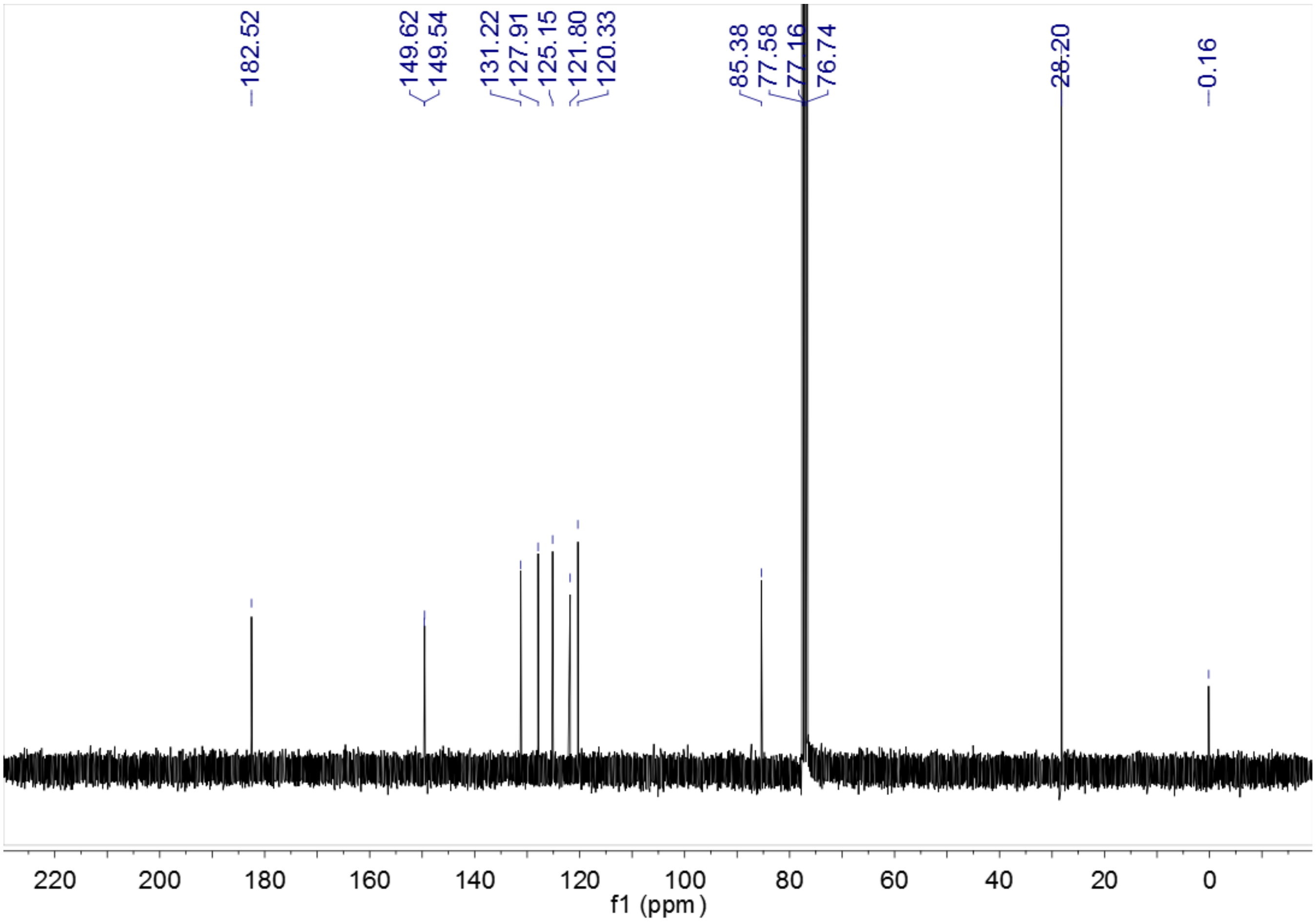


Fig. S2 The 75 MHz ^{1}C NMR spectrum of di-*tert*-butyl 6,6'-dibromo-3,3'-dioxo-[2,2'-biindolinylidene]-1,1'-dicarboxylate (compound **2**) measured in $CDCl_3$.

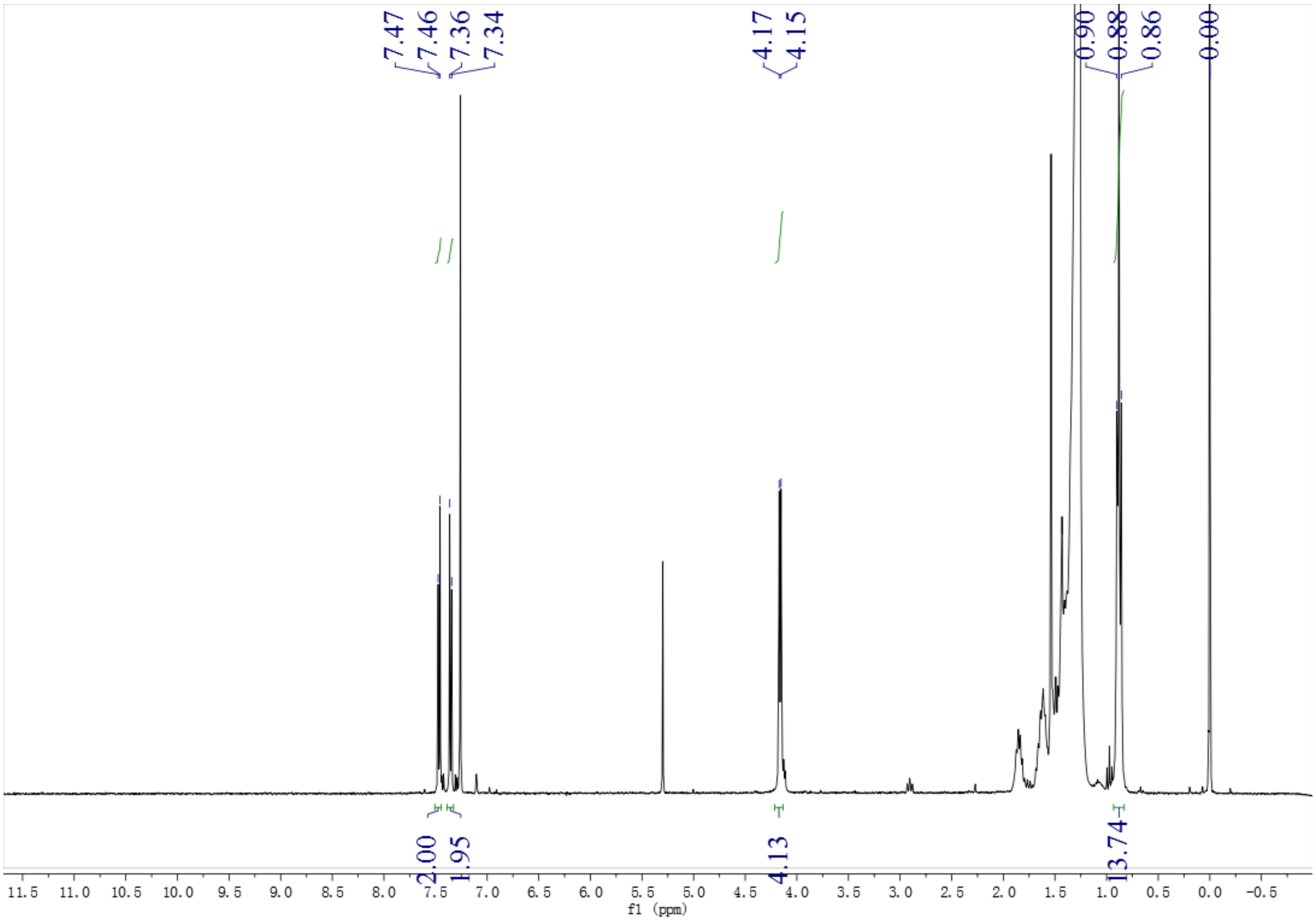


Fig. S3 The 300 MHz ^{1}H NMR spectrum of 4,8-bis((2-decyltetradecyl)oxy)benzo[1,2-*b*:4,5-*b*']dithiophene (compound **3**) measured in $CDCl_3$.

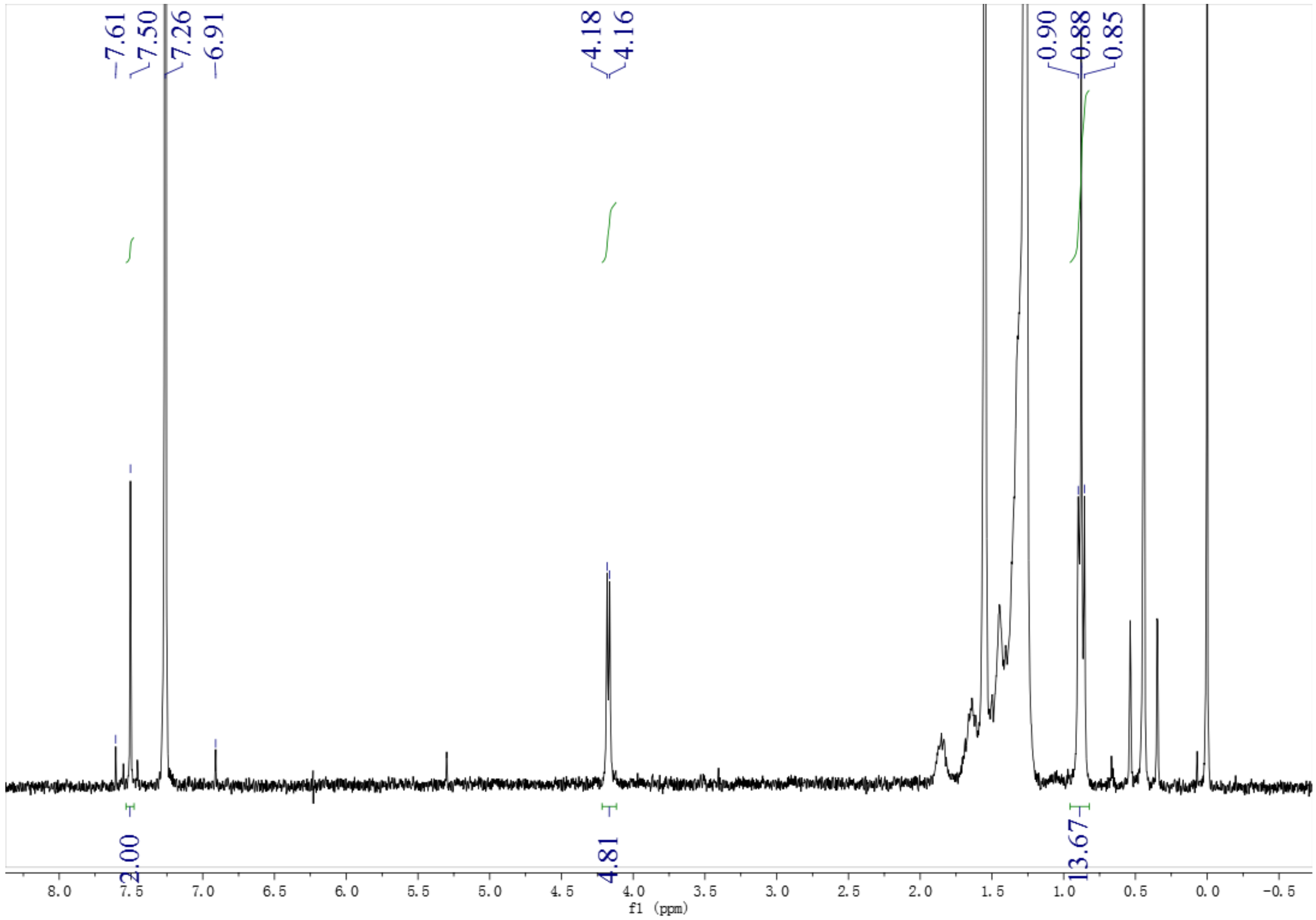


Fig. S4 The 300 MHz ^{1}H NMR spectrum of (4,8-bis((2-decyltetradecyl)oxy)benzo[1,2-*b*:4,5-*b*']dithiophene-2,6-diyl)bis(trimethylstannane) (compound **4**) measured in $CDCl_3$.

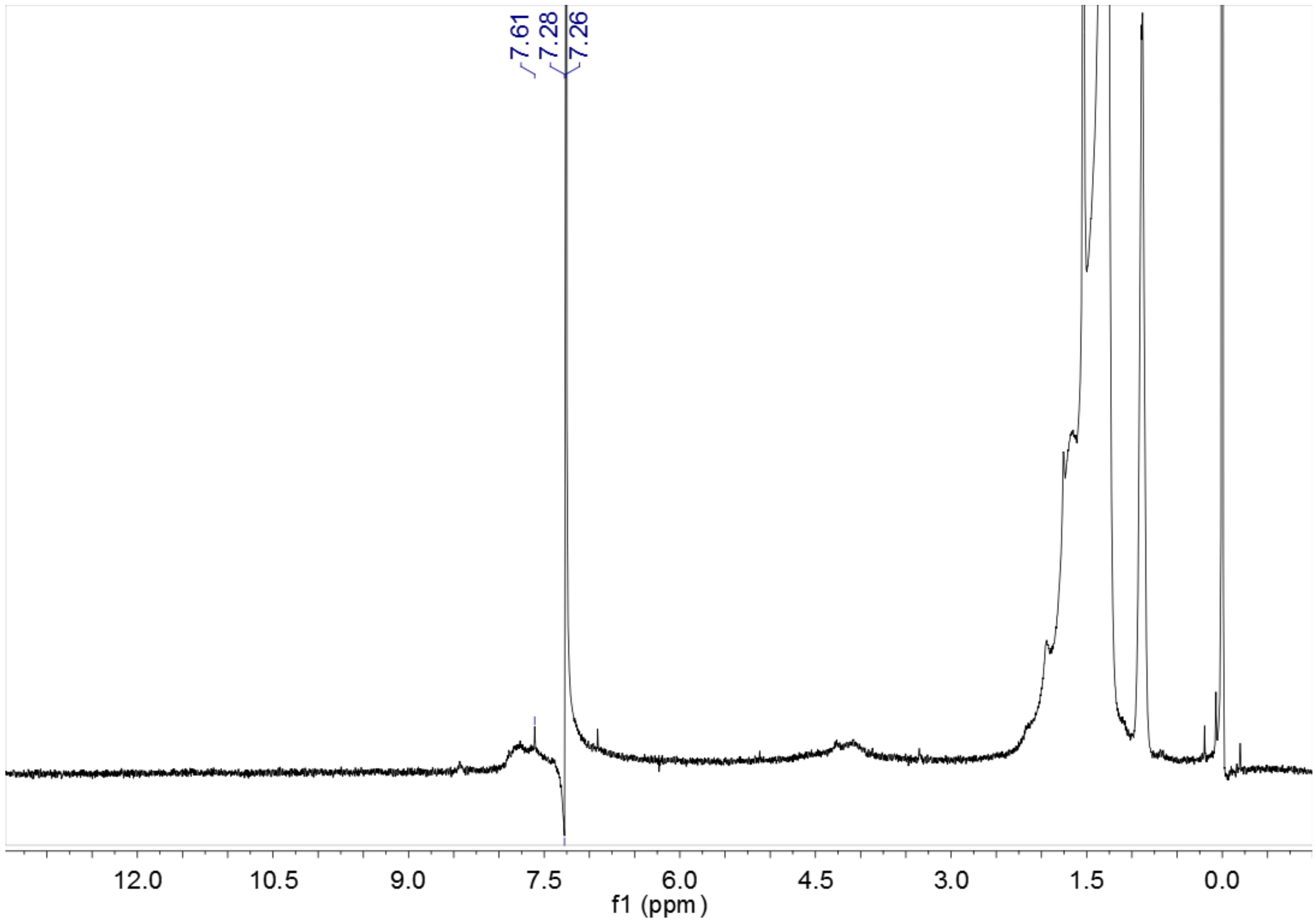


Fig. S5 The 300 MHz ^{1}H NMR spectrum of **PIDBDT** measured in $CDCl_3$.

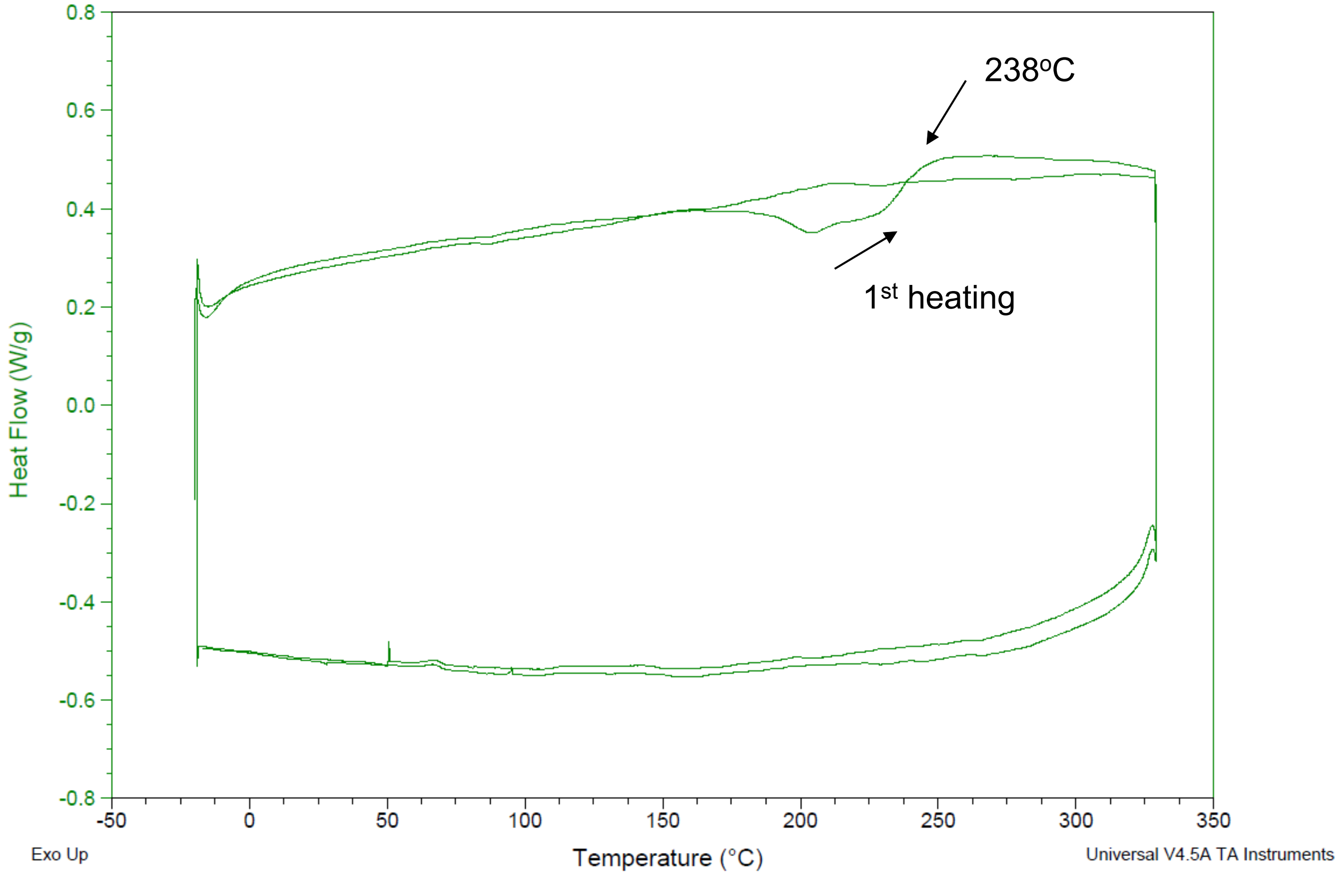


Fig. S6 DSC curves of **PIDBDT** with a heating rate of 10 °C·min^{-1} under N_2.

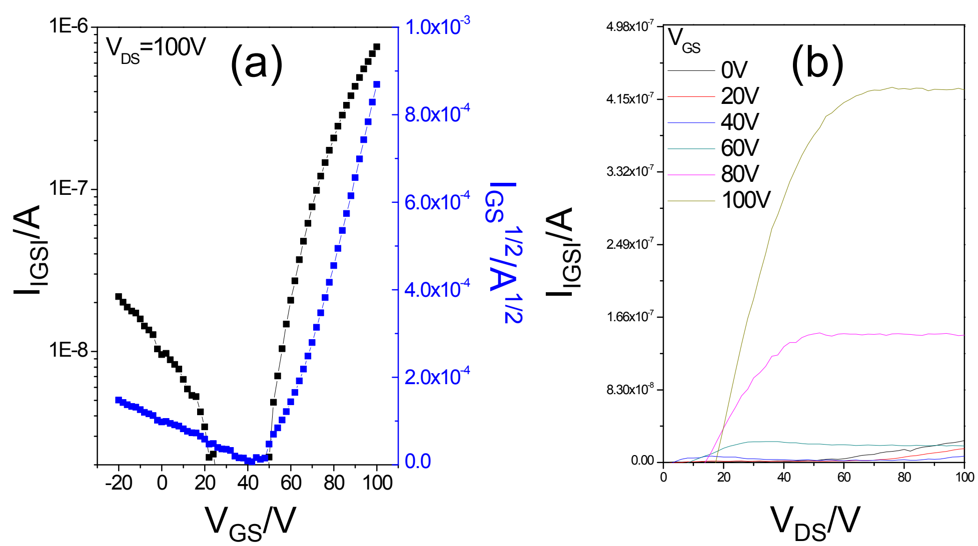


Fig. S7 Transfer and output curves of OTFT devices with **PIDBDT** thin films annealed at 250 °C for 1 h. Device dimensions: channel width (*W*) = 1 mm; channel length (*L*) = 30 μm.

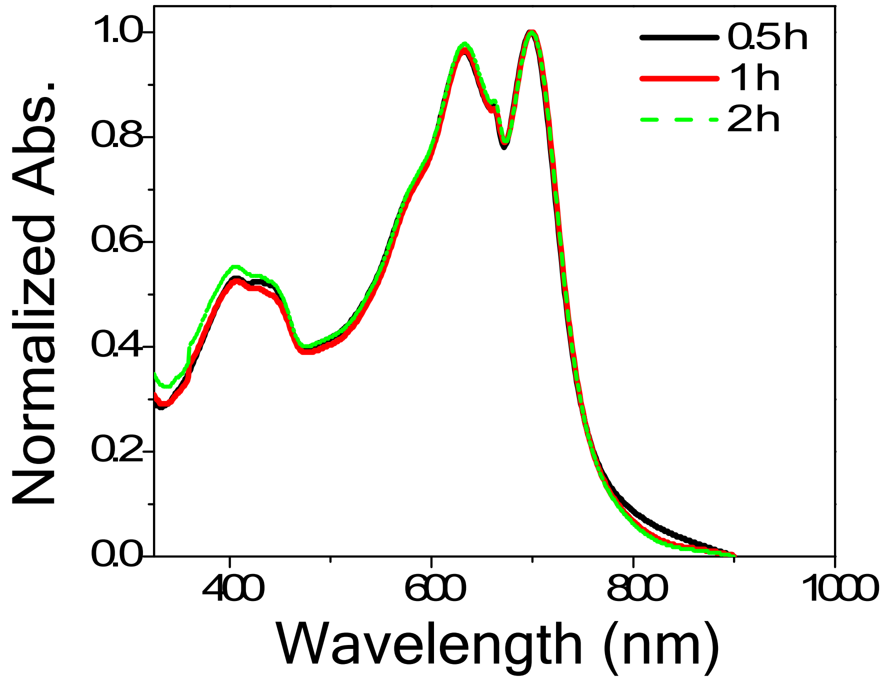


Fig. S8 UV-vis absorption spectra of **PIDBDT** films on glass substrates annealed at 200 °C for different periods of time.

Table S2. Performance of OTFT devices using PIDBDT annealed at 200 or 250 °C.[a]

Annealing temperature / time	Average electron mobility, μ_e ($cm^2V^{-1}s^{-1}$)	Maximum electron mobility, μ_e ($cm^2V^{-1}s^{-1}$)	Standard deviation ($cm^2V^{-1}s^{-1}$)	Threshold voltage, V_{th} (V)	Current on-to-off ratio, I_{on}/I_{off}	Drain voltage, V_{DS} (V)
200 °C / 0.5 h	3.1×10^{-3}	3.9×10^{-3}	4.5×10^{-4}	39.7-55.3	$\sim 10^3$	100
200 °C / 1 h	4.9×10^{-3}	5.7×10^{-3}	4.7×10^{-4}	32.2-57.5	$\sim 10^3$	100
200 °C / 3 h	4.1×10^{-3}	4.9×10^{-3}	4.2×10^{-4}	35.7-56.7	$\sim 10^3$	100
250 °C / 1 h	2.5×10^{-3}	3.1×10^{-3}	4.4×10^{-4}	42.2-57.6	$\sim 10^3$	100

[a] Data were collected from at least five devices for each condition.

3. References

1. (a) A. D. Becke, Phys. Rev. A, 1988, 38, 3098. (b) C. Lee, W. Yang and G. G. Parr, Phys. Rev. B, 1988, 37, 785.

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