

SUPPORTING INFORMATION

Design, Synthesis, and Characterization of α,ω -Disubstituted Indeno[1,2-b]fluorene-6,12-dione-Thiophene Molecular Semiconductors. Enhancement of Ambipolar Charge Transport Through Synthetic Tailoring of Alkyl Substituents.

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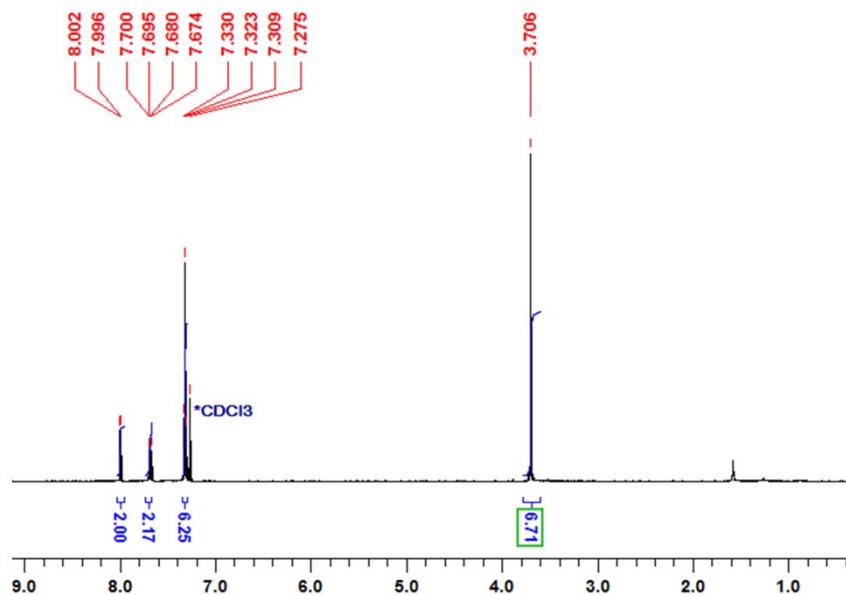


Figure S1. ¹H NMR spectra of compound **1** in CDCl₃ at room temperature.

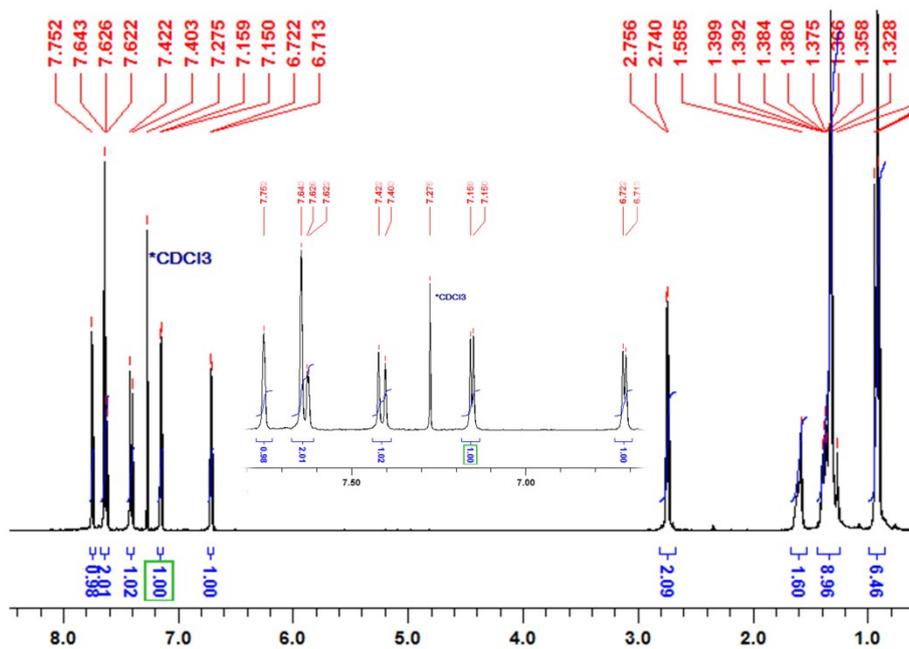


Figure S2. ¹H NMR spectra of **2EH-TIFDKT** in CDCl₃ at room temperature.

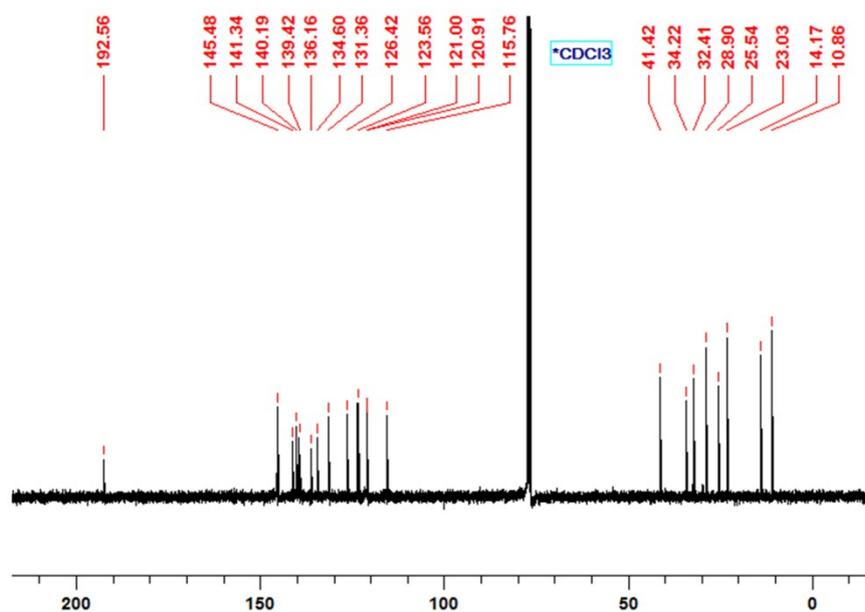


Figure S3. ¹³C NMR spectra of **2EH-TIFDKT** in CDCl₃ at room temperature.

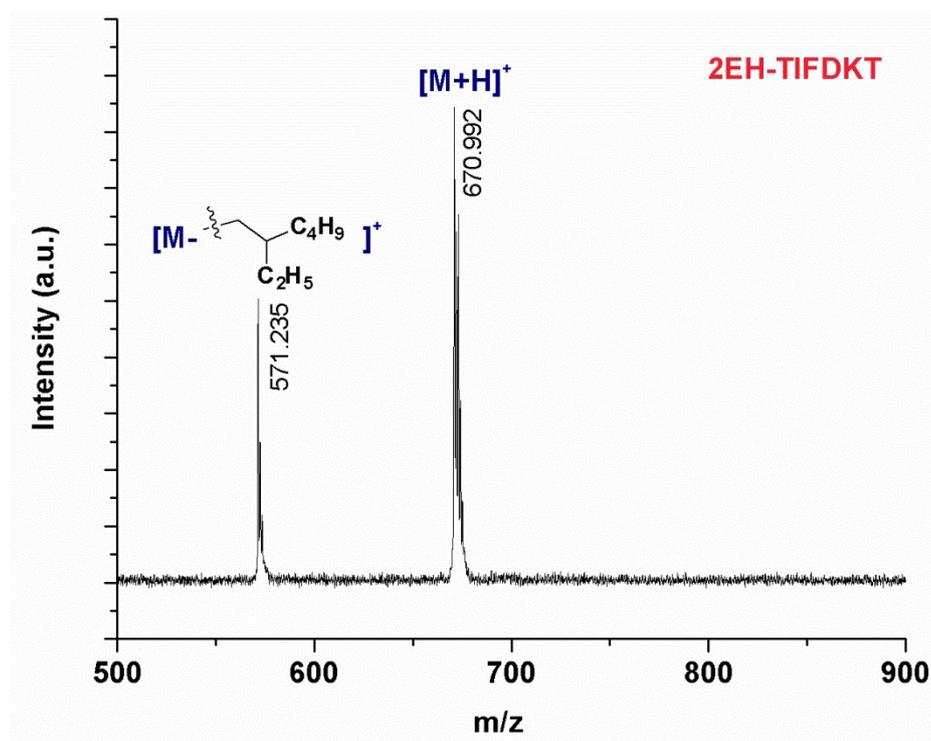


Figure S4. Positive ion and linear mode MALDI TOF-MS spectrum of **2EH-TIFDKT**.

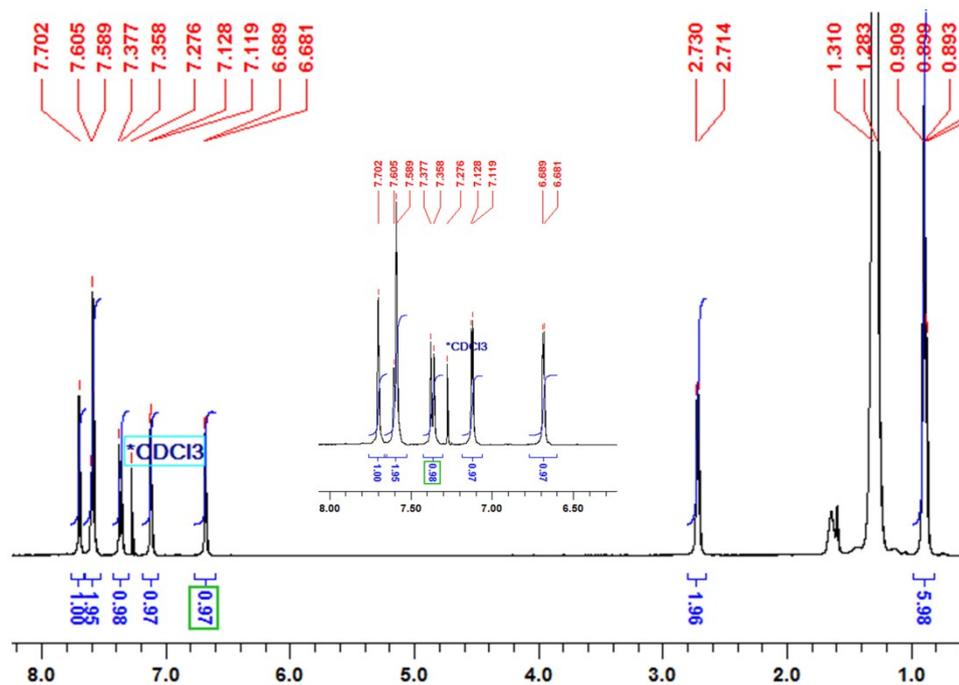


Figure S5. ¹H NMR spectra of **2OD-TIFDKT** in CDCl₃ at room temperature.

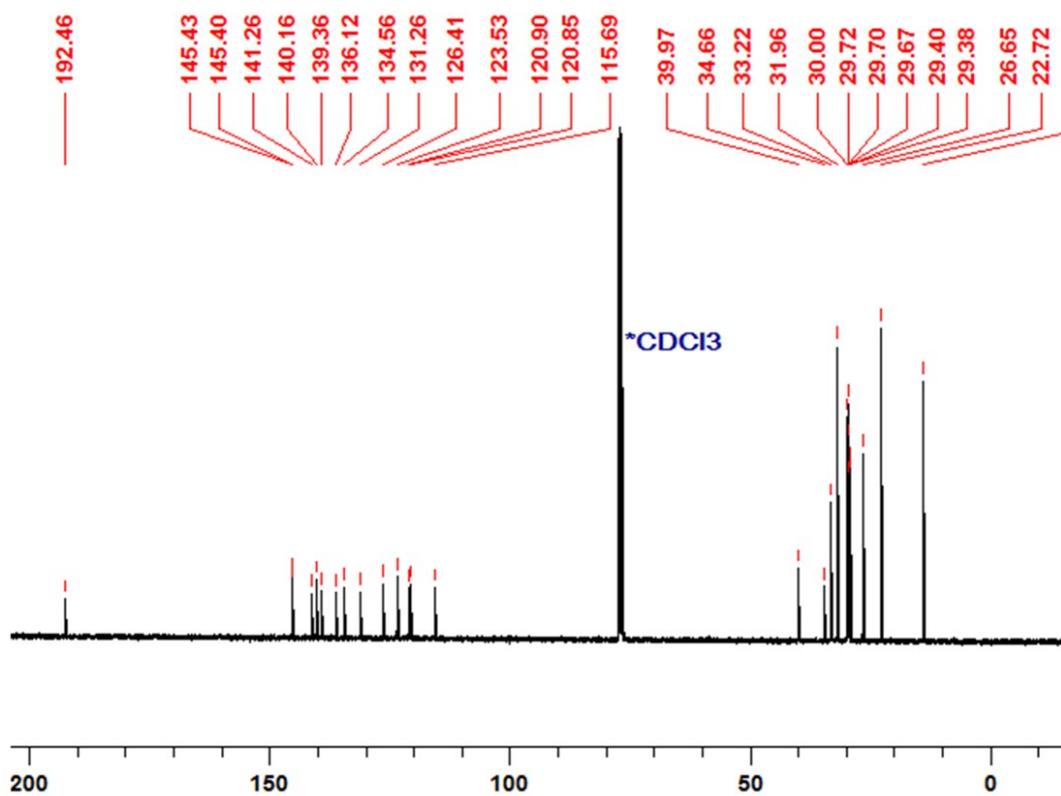


Figure S6. ¹³C NMR spectra of **2OD-TIFDKT** in CDCl₃ at room temperature.

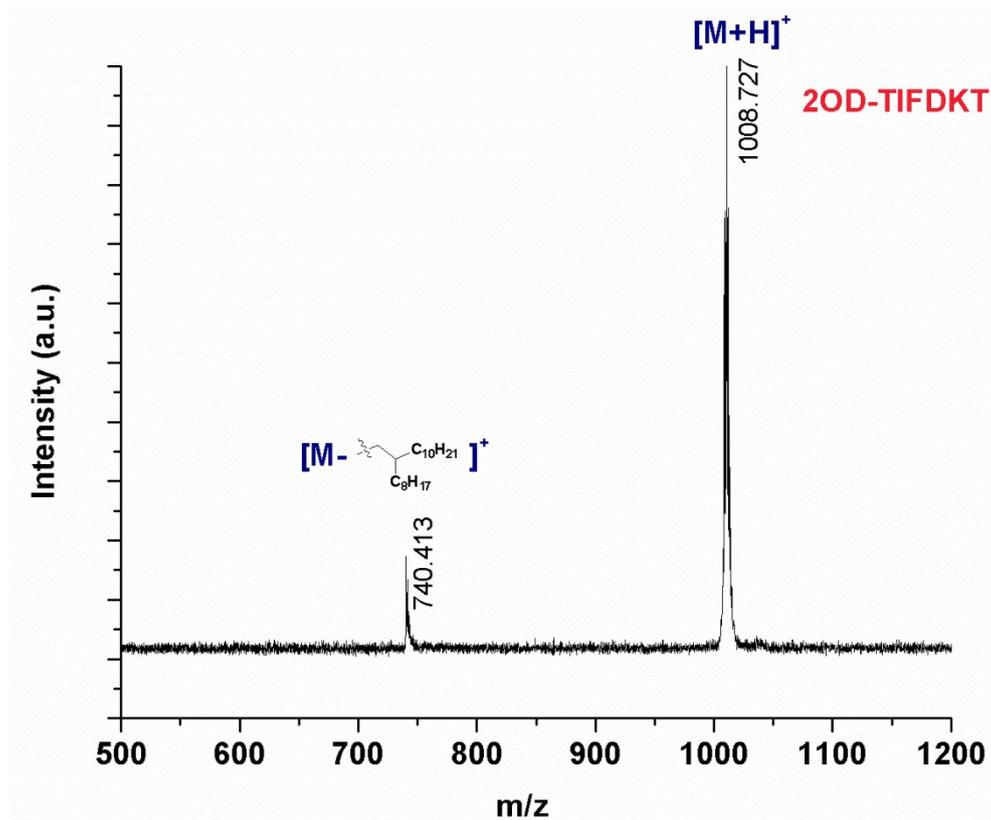


Figure S7. Positive ion and linear mode MALDI TOF-MS spectrum of 2OD-TIFDKT.

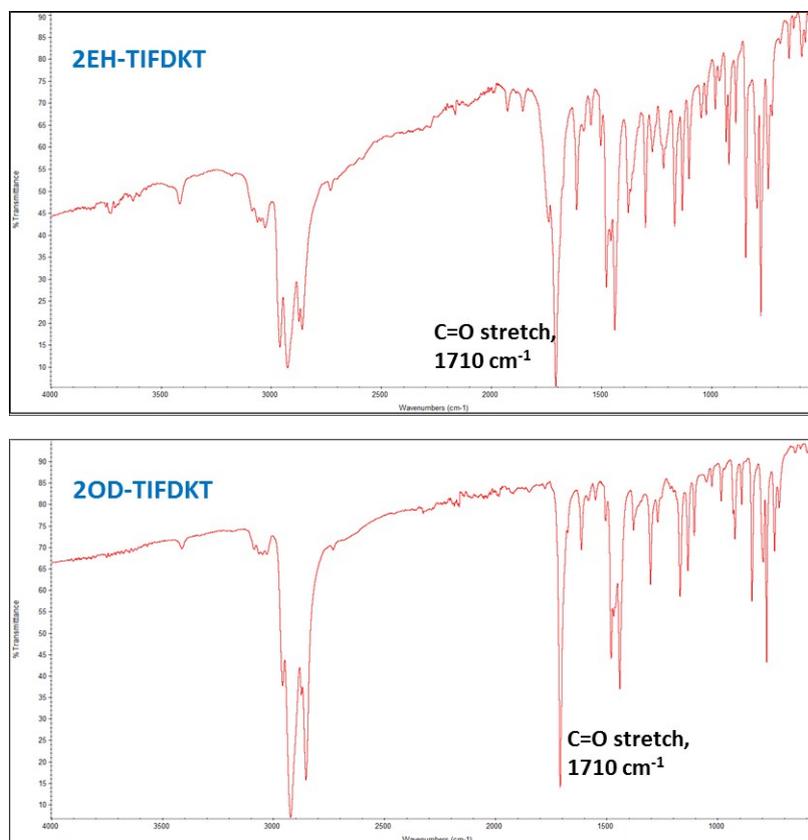


Figure S8. FTIR spectra of 2EH-TIFDKT and 2OD-TIFDKT.

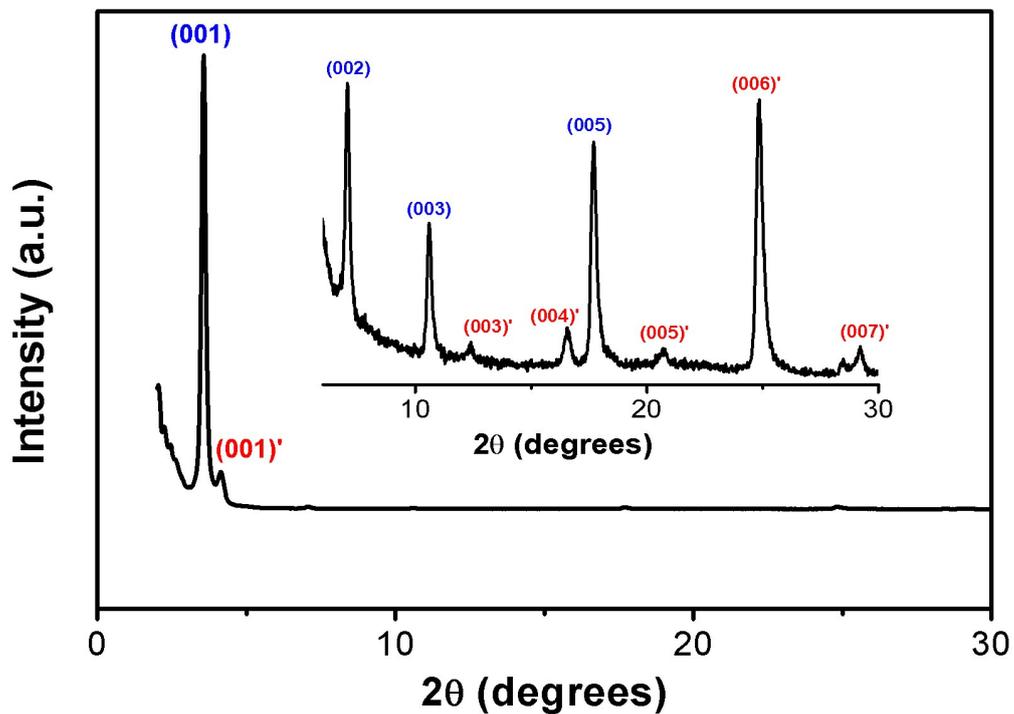


Figure S9. θ - 2θ X-ray diffraction (XRD) scans of films fabricated by drop-casting of **2EH-TIFDKT**.

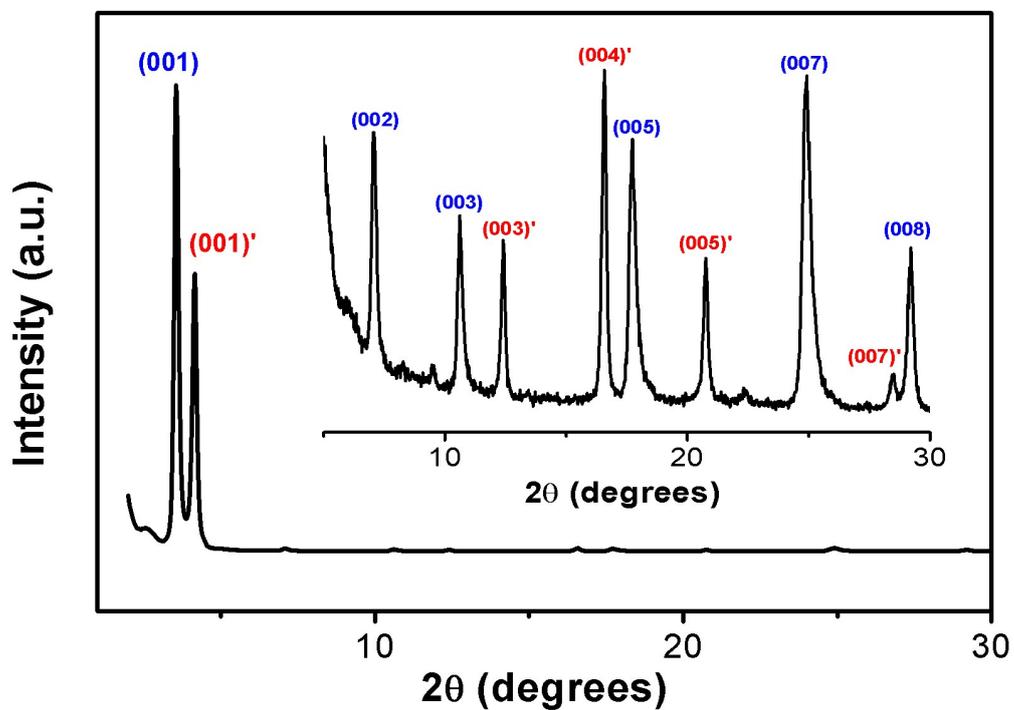


Figure S10. θ - 2θ X-ray diffraction (XRD) scans of films fabricated by droplet-pinned crystallization of **2EH-TIFDKT**.

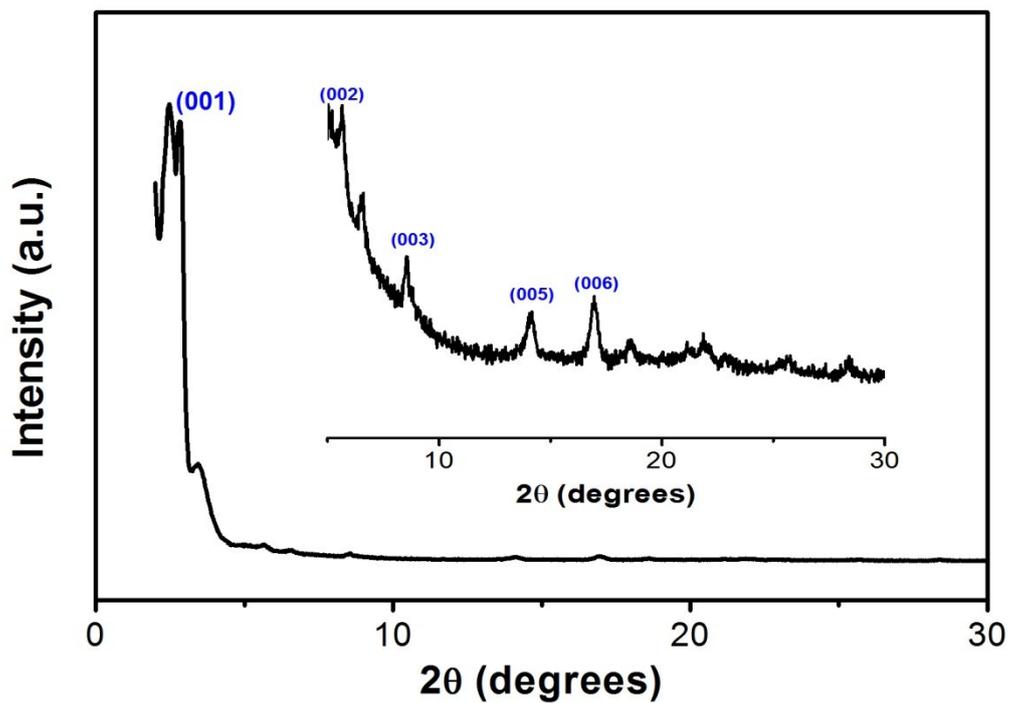


Figure S11. θ - 2θ X-ray diffraction (XRD) scans of films fabricated by drop-casting of **2OD-TIFDKT**.

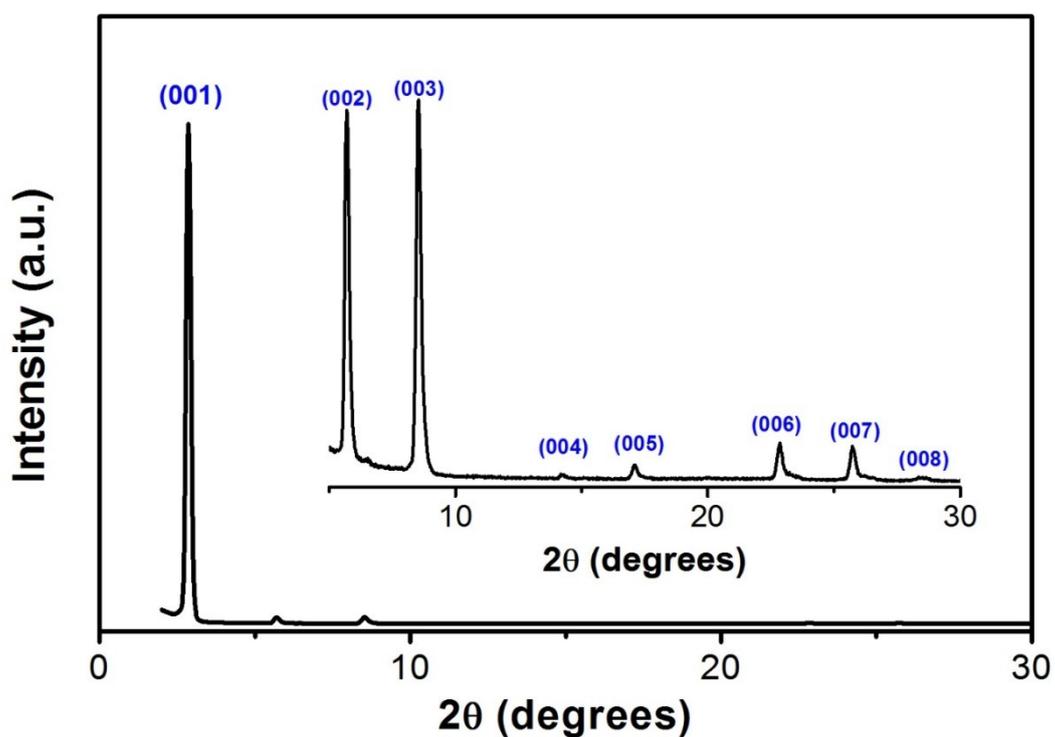


Figure S12. θ - 2θ X-ray diffraction (XRD) scans of films fabricated by droplet-pinned crystallization of **2OD-TIFDKT**.

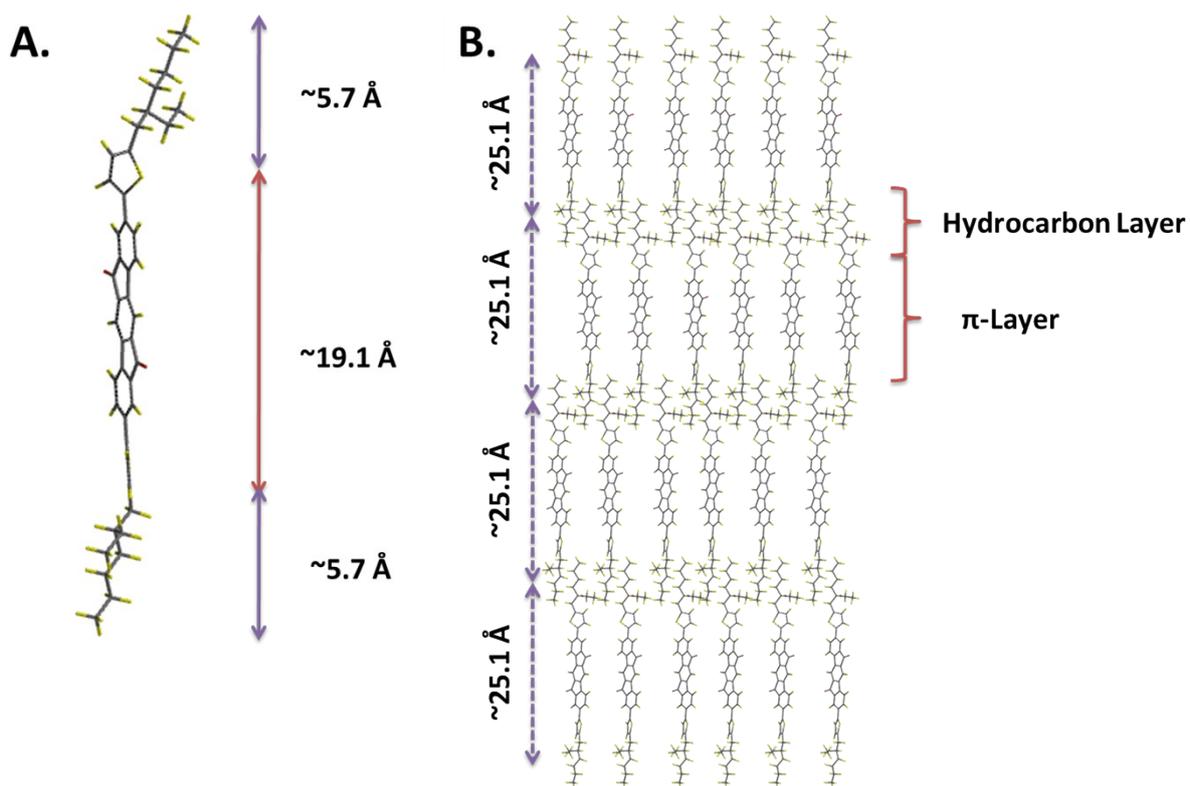


Figure S13. A. The computed molecular dimensions, and B. Proposed thin-film phase packing motif for **2EH-TIFDKT**.

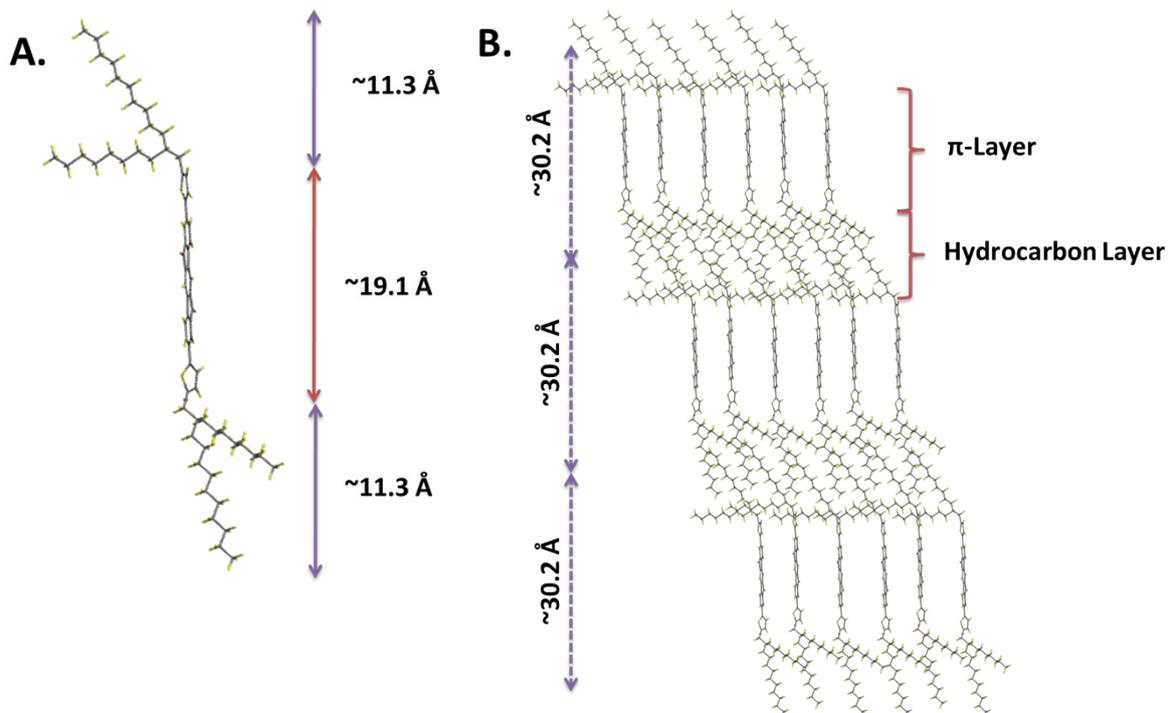


Figure S14. A. The computed molecular dimensions, and B. Proposed thin-film phase packing motif for **2OD-TIFDKT**.

Table S1. Electrical performances of OTFTs based on Indeno[1,2-b]fluorene-6,12-dione-thiophene derivatives, **2EH-TIFDKT** and **2OD-TIFDKT** measured under ambient condition.

Material	Method	N-channel			P-channel		
		μ_e (cm ² /Vs)	V _T (V)	I _{on} /I _{off}	μ_h (cm ² /Vs)	V _T (V)	I _{on} /I _{off}
2EH-TIFDKT	DC	-	-	-	2.7×10 ⁻⁴	-33	6.3×10 ⁶
	DPC	-	-	-	1.6×10 ⁻⁴	-38	2.6×10 ⁴
	SS	-	-	-	2.2×10 ⁻³	2.8	4.8×10 ²
2OD-TIFDKT	DC	-	-	-	2.9×10 ⁻⁴	-12	2.0×10 ⁵
	DPC	-	-	-	8.0×10 ⁻⁴	-14	8.1×10 ²
	SS	-	-	-	5.4×10 ⁻⁴	-9.7	5.2×10 ⁴

Supplementary crystallographic material.

CCDC 1420110 (for **Compound 2 (IFDK-BR2)**) contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Table S2. Crystal data and refinement parameters for **IFDK-BR2**.

Empirical Formula	C ₂₀ H ₈ Br ₂ O ₂
Formula weight (g. mol⁻¹)	440.08
Temperature (K)	300.(2)
Wavelength (Å)	0.71073
Crystal system	Monoclinic
Space group	<i>P</i> 2 ₁ /c
a (Å)	3.8828(3)
b (Å)	13.5879(11)
c (Å)	14.1314(13)
α(°)	90
β(°)	95.032(6)
γ(°)	90
Crystal size (mm)	0.139 x 0.146 x 0.525
V (Å³)	742.69(11)
Z	2
ρ_{calcd} (g. cm⁻³)	1.968
μ (mm⁻¹)	5.467
F(000)	428

θ range for data collection ($^\circ$)	3.00-25.68
h/k/l	-4/4, -15/16, -15/17
Reflections collected	5701
Independent reflections	1408 [R(int) = 0.0764]
Absorption correction	Multi-scan
Data/restraints/parameters	1408 / 0 / 109
Goodness-of-fit on F^2	1.009
Final R indices [$I > 2\sigma(I)$]	$R_1 = 0.0454$, $wR_2 = 0.1093$
R indices (all data)	$R_1 = 0.0566$, $wR_2 = 0.1159$
Largest diff. peak and hole ($e.\text{\AA}^{-3}$)	0.771 and -0.702