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Supporting information

Acceptor-donor-acceptor molecule solution processable by polar non-halogenated solvents for organic field-effect transistors

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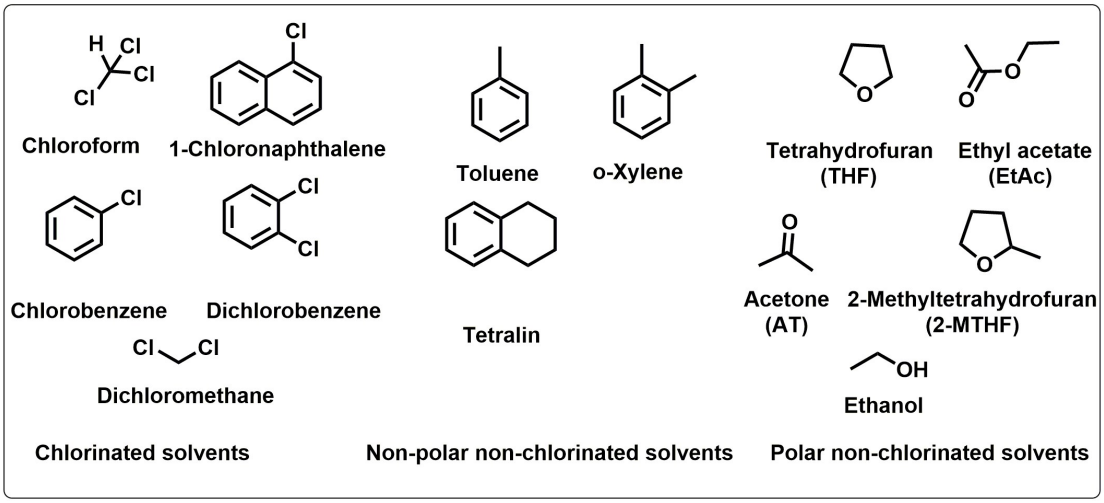


Fig. S1. The structures of solvents for solution-processed OFETs.

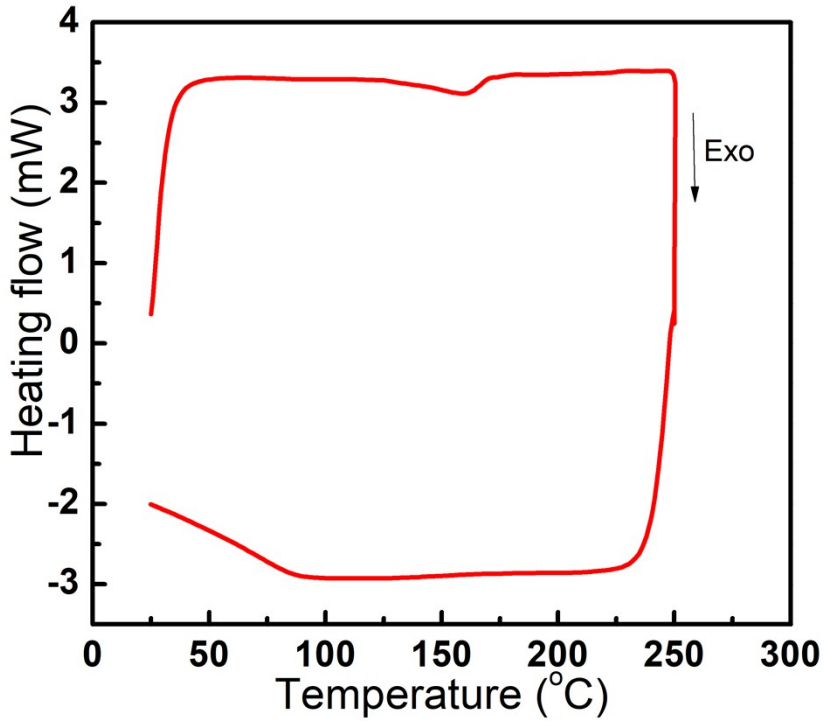


Fig. S2. The DSC curve of **IDTT-IDD-N**. An exothermic transition characteristic of crystallization was observed at about 165 °C, indicating that the semiconductor forms a crystalline structure. The DSC was referenced from our previous work.[S1]

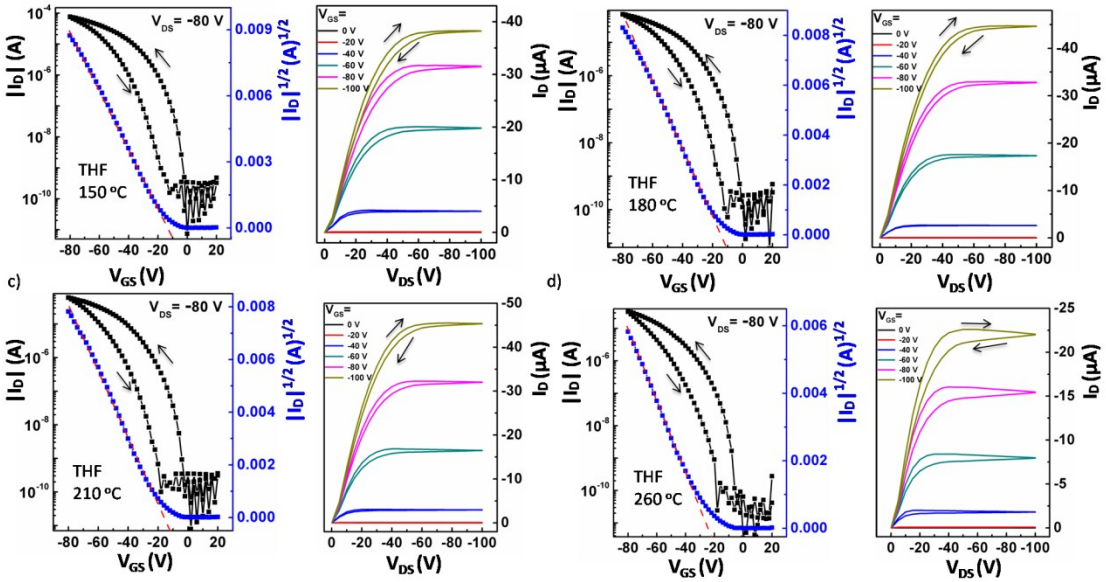


Fig. S3. The transfer and output curves of devices fabricated from THF solution.

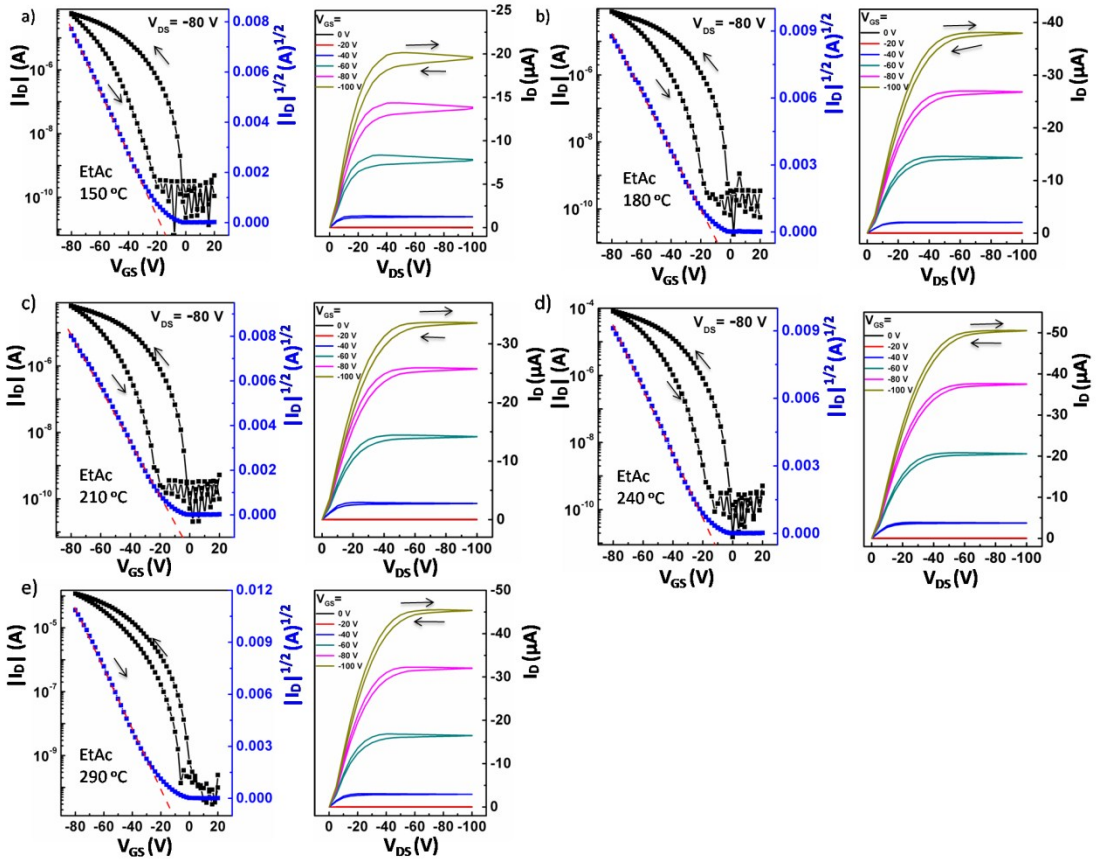


Fig. S4. The transfer and output curves of devices fabricated from EtAc solution.

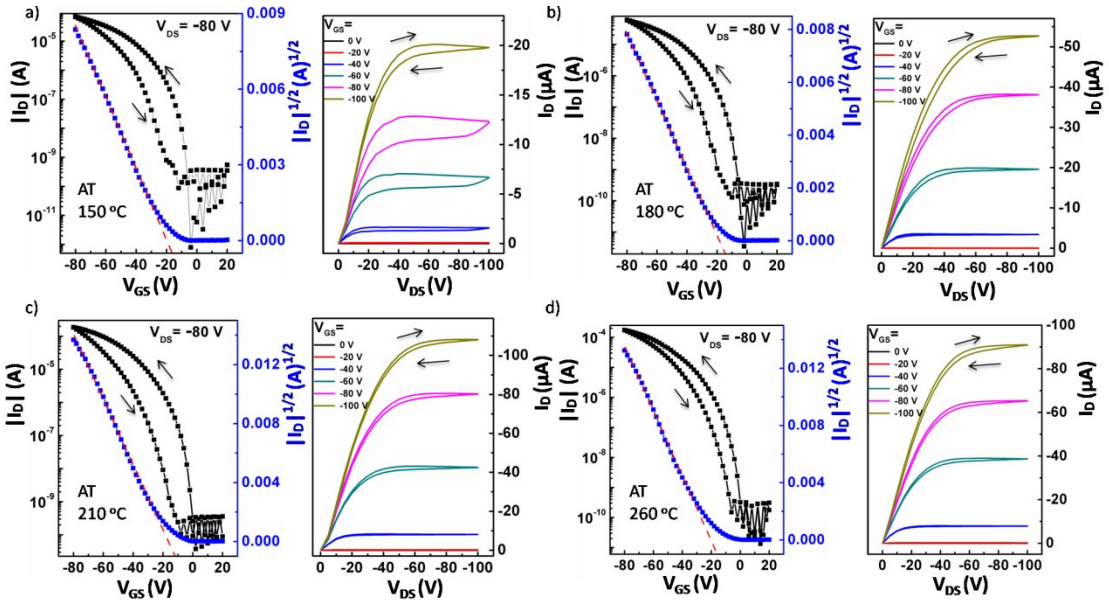


Fig. S5. The transfer and output curves of devices fabricated from AT solution.

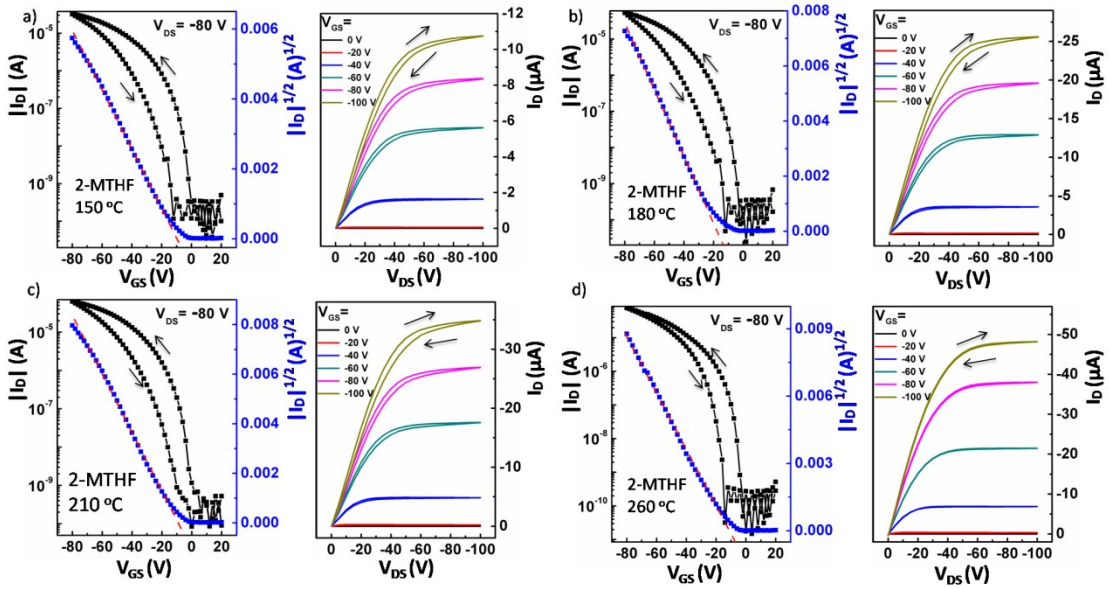


Fig. S6. The transfer and output curves of devices fabricated from 2-MTHF solution.

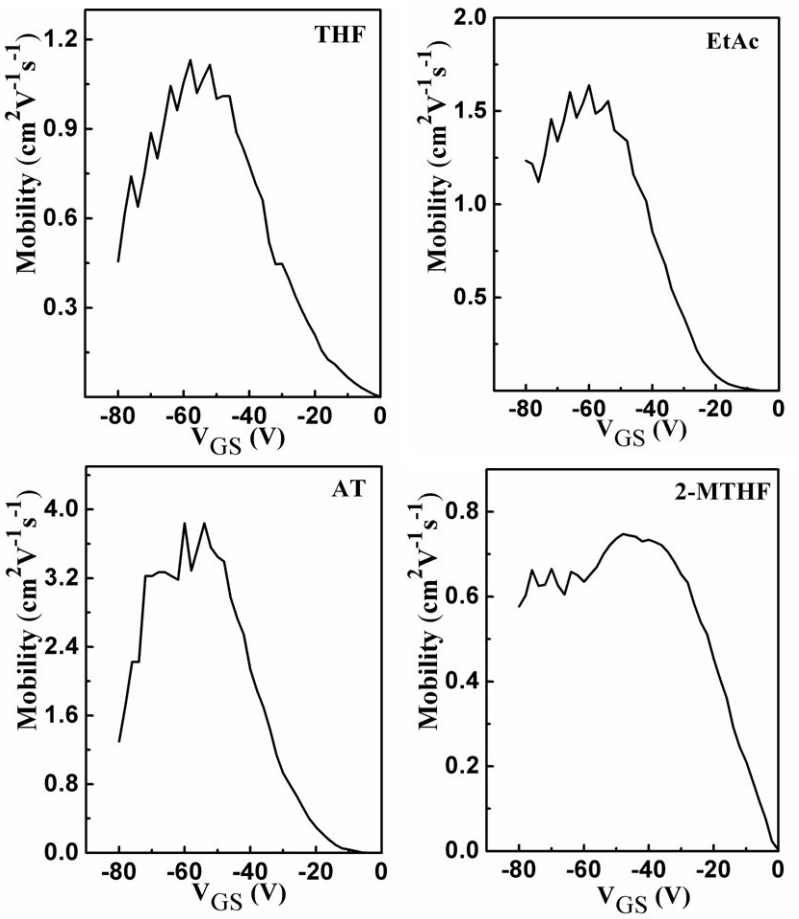


Fig. S7. Hole mobilities as a function of gate voltage for the devices processed from different solvents.

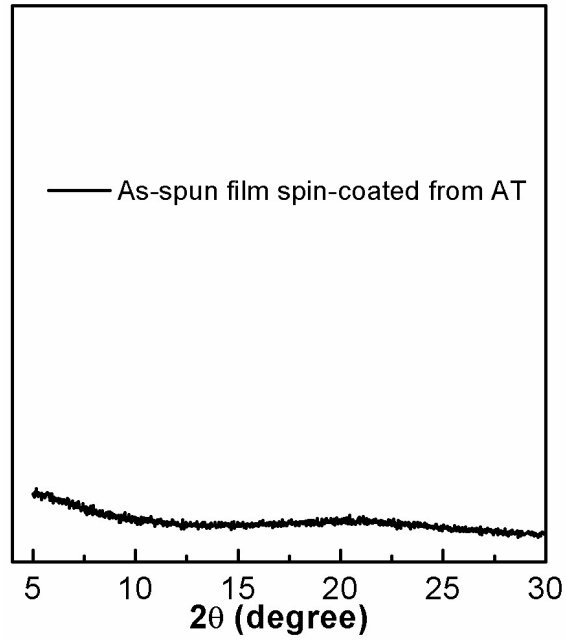


Fig. S8. The XRD pattern of the as-spun film spin-coated from AT solution. The as-spun film exhibited amorphous structure, which was in accordance with the result of the film processed from chloroform solution.[S1]

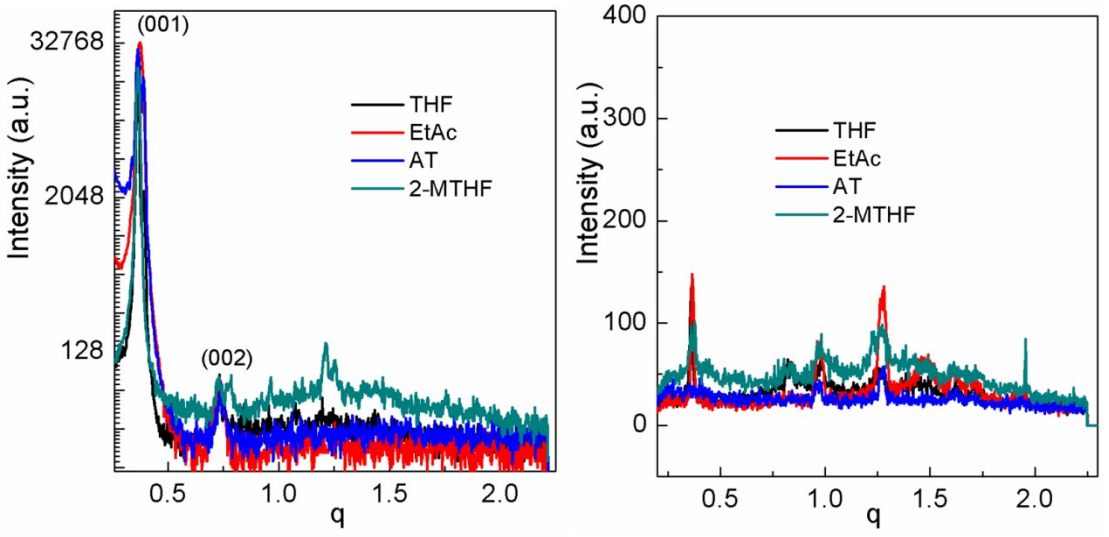


Fig. S9. Out-of-plane (left) and in-plane (right) line cuts of GIXD.

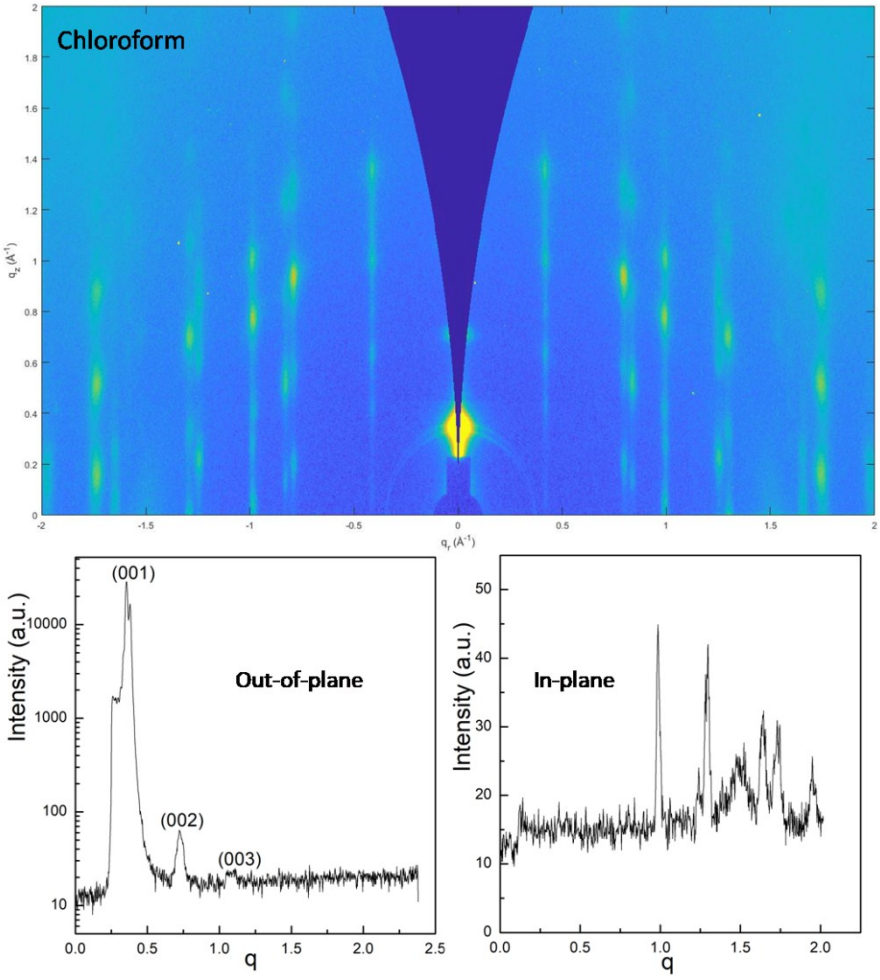


Fig. S10. GIXD pattern and line cuts of the sample processed from chloroform solution.

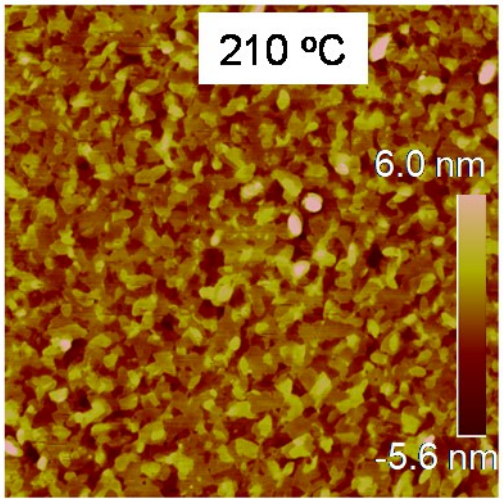


Fig. S11. The AFM height image (5 μm× 5 μm) of IDTT-IDD-N film spin-coated from chloroform solution. The AFM image was referenced from our previous work.[S1] The film processed from chloroform solution exhibited uniform and compact nanosheets that were well interconnected within the thin film.

Table S1. The previous works related to OFETs processed from polar non-chlorinated solvents.

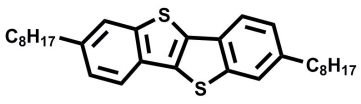
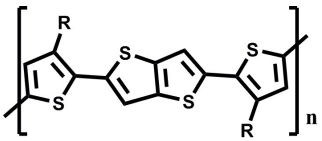
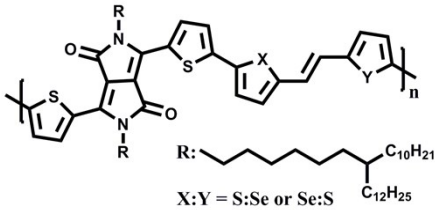
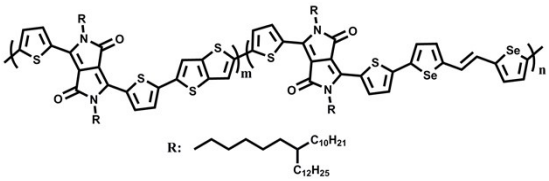
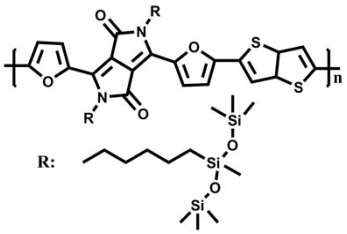
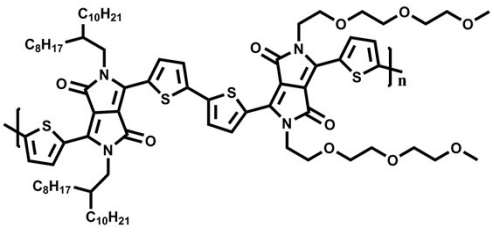
Structure	Solvent	μ ($cm^2V^{-1}s^{-1}$)	Ref.
	Cyclohexanone	3.5	*Organic Electronics*, 2019, 69, 181-189.
 R: $CH2(CH_2)_{12}CH_3$	Ethyl acetate	0.039	*Organic Electronics*, 2016, 30, 18-29.
 X:Y = S:Se or Se:S	Tetrahydrofuran	6.4	*Adv. Mater.,* 2015, 27, 3626-3631.
	Butanol	0.83	*Adv. Funct. Mater.*, 2015, 25, 4844-4850
	Ethanol	0.25	
	Tetrahydrofuran	0.8	*ACS Appl. Mater. Interfaces,* 2017, 9, 15652−15661.
	Tetrahydrofuran	3	*J. Am. Chem. Soc.*, 2012, 134, 16532−16535

Table S2. The optical properties of **IDTT-IDD-N** processed from different polar non-chlorinated solvents.

Solvent	λ_{max} [nm]		
	Solution	Film	Annealed
Tetrahydrofuran (THF)	548	600	609
Ethyl acetate (EtAc)	552	601	611
Acetone (AT)	548	601	609
2-Methyltetrahydrofuran (2-MTHF)	561	578	587
Chloroform [a]	588	598	610

[a] The data were referred from the previous work[S1]

Table S3. The field-effect performances of **IDTT-IDD-N**-based devices fabricated from different polar non-chlorinated solvents.

Solvent	Annealing temperature (°C)	$\mu_{h,max}$ ($cm^2V^{-1}s^{-1}$)	$\mu_{h,avg}$ ($cm^2V^{-1}s^{-1}$)	V_{th}(V)	I_{on}/I_{off}
EtAc	N/A	/	/	/	/
	150	0.54	0.52	-14.2	3.13×10^6
	180	0.55	0.53	-18.2	4.37×10^6
	210	0.61	0.59	-14.9	4.68×10^6
	240	0.78	0.73	-16.9	5.44×10^6
	260	1.49	1.15	-29.5	2.48×10^7
	290	1.09	0.97	-18.4	4.01×10^6
THF	N/A	/	/	/	/
	150	0.64	0.61	-13.3	1.04×10^7
	180	0.72	0.67	-16.2	2.39×10^7
	210	0.83	0.60	-28.1	3.32×10^7
	240	1.01	0.71	-22.1	4.43×10^7
	260	0.46	0.37	-27.1	9.81×10^6
AT	N/A	/	/	/	/
	150	0.33	0.31	-21.8	2.94×10^6
	180	0.70	0.61	-20.2	1.92×10^7
	210	1.88	1.63	-18.8	5.01×10^6
	240	2.40	2.15	-23.5	7.95×10^6
	260	1.85	1.42	-20.7	1.32×10^7
2-MTHF	N/A	/	/	/	/
	150	0.25	0.23	-9.89	8.65×10^5
	180	0.50	0.45	-17.6	2.16×10^6
	210	0.54	0.47	-7.82	7.41×10^5
	240	0.81	0.72	-11.5	1.09×10^6
	260	0.62	0.51	-13.7	5.19×10^6

Experimental section

All the available chemicals and regents were used as received without further purification. The small molecule (**IDTT-IDD-N**) was synthesized according to the previous literature.[S1]

Measurements and characterization

Absorption spectra were measured using solution in different polar non-chlorinated solvents and films cast onto quartz glass using Agilent Cary 5000 model spectrophotometer. X-ray diffraction (XRD) measurements were carried out in the reflection mode at room temperature using an 18-kW D/MAX2500 V XRD system. Grazing-incidence-X-ray diffraction (GIXD) measurements were performed using 3C beamlines at the Pohang Accelerator Laboratory (PAL) in Korea. The fabrication of GIXD samples was same as the devices (In the Section of Device Fabrication). The atomic force microscopy (AFM) images were obtained using a SPA300HV instrument.

Fabrication and characterization of OFET device

Bottom-gate/top-contact (BG/TC) OFET devices were fabricated on a gate of *n*-doped Si with a 300-nm-thick SiO_2 dielectric layer (capacitance: 10.8 nF cm^{-2}). The substrates were subjected to a piranha solution (70 vol% H_2SO_4 and 30 vol% H_2O_2), followed by UV-ozone treatment. The surface of the wafer was modified with octadecyltrimethoxysilane (OTS) self-assembled monolayers (SAM) according to the previous procedures.[S2] Then, the polar non-chlorinated solutions (~5 mg/mL) was dropped onto the OTS-treated Si/SiO_2 and spin-coated at 6000 rpm for 45 s in a glove box. The small molecule films were annealed at different temperatures (150–290 °C) in a glove box. The Au source-drain electrodes were prepared by thermal evaporation (~ 30 nm). The OFET devices had a channel length (L) of 130 μm and a channel width (W) of 760 μm. The devices were characterized under air condition using a Keithley 4200 semiconductor parametric analyzer. The saturation-regime mobility (μ) was obtained using the following equation: $I_d = (W/2L)C_i\mu\ (V_g\text{-}V_{th})^2$, where I_d is the drain current, C_i is the capacitance of the gate dielectric, V_g is the gate-source voltage, and V_{th} is the threshold voltage.

[s_1] Zhang, G.; Zhao, Y.; Kang, B.; Park S.; Ruan, J.; Lu, H.; Qiu, L.; Ding, Y.; Cho, K. Fused heptacyclic-based acceptor-donor-acceptor small molecules: N-substituted toward high-performance solution processable field-effect transistors. Chem. Mater. **2019**, 31, 2027-2035.

[s_2] Ito, Y.; Virkar, A. A.; Mannsfeld, S.; Oh, J. H.; Toney, M.; Locklin, J.; Bao, Z. Crystalline ultrasmooth self-assembled monolayers of alkylsilanes for organic field-effect transistors. *J. Am. Chem. Soc.* **2009**, 131, 9396-9404.