Supplementary Information

Non-Fullerene Polymer Solar Cells based on Selenophene-Containing Fused-Ring Acceptor with Photovoltaic Performance of 8.6%

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Keywords: Nonfullerene Electron Acceptor, Ladder-Type, Organic Photovoltaics, Indacenodithiophene, Conjugated Molecules.

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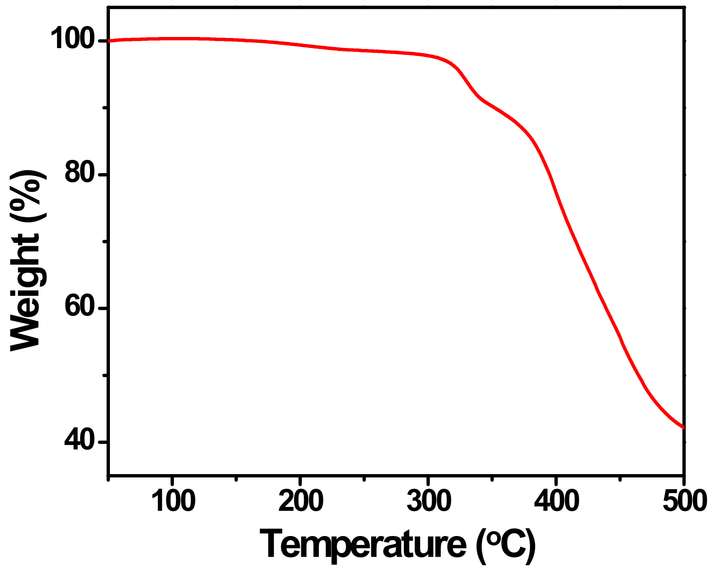


Fig. S1. TGA plot of IDSe-T-IC with a heating rate of 10 ºC min^{-1} under an inert atmosphere.

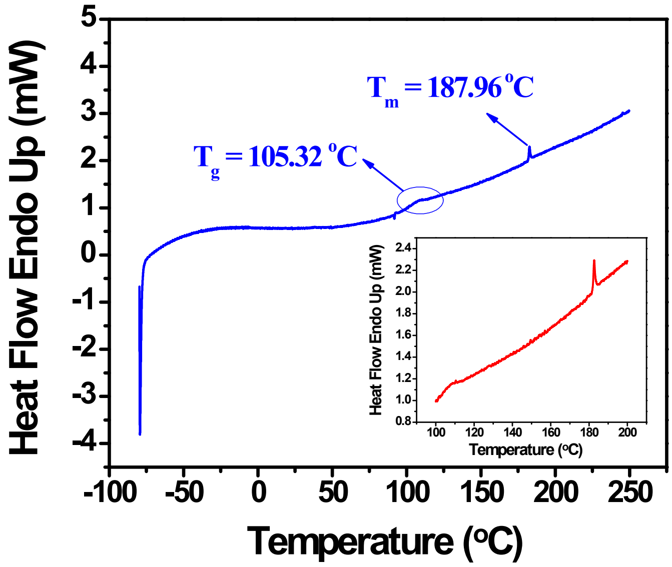
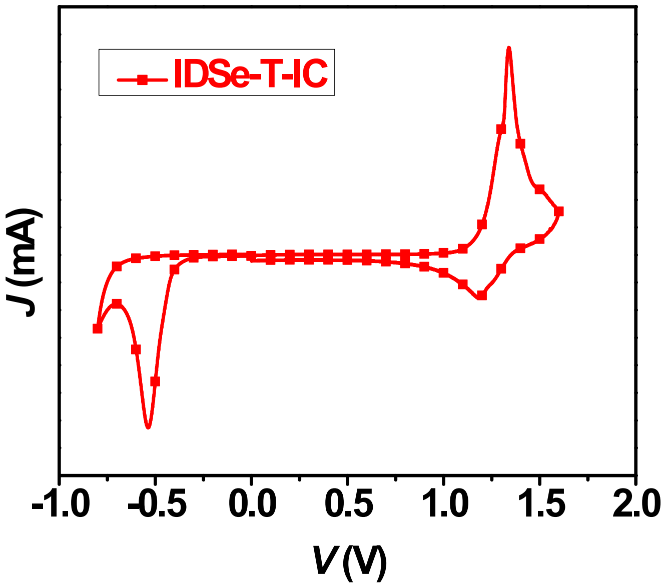


Fig. S2. DSC plot of IDSe-T-IC with a heating rate of 10 ºC min^{-1} under an inert atmosphere.



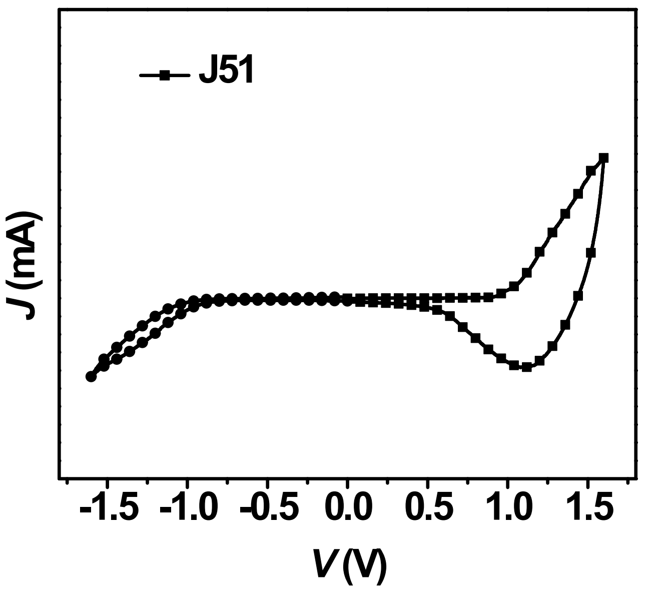


Fig. S3. The CV curves of IDSe-T-IC and J51 in CH_3CN /0.1 M $[nBu_4N]^+[PF_6]^-$ at 100 mV s^{-1}. The horizontal scale refers to the Ag/AgCl electrode.

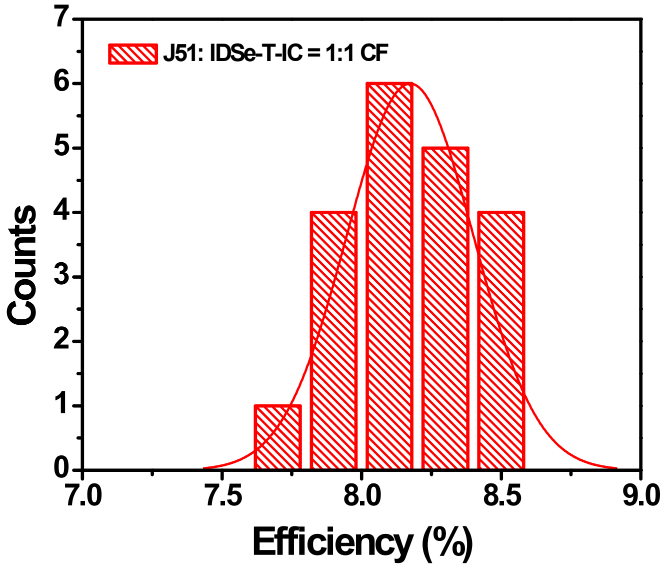


Fig. S4a. Statistical histogram of PCEs of PSCs based on J51: IDSe-T-IC (1:1, w/w) fabricated with chloroform solution.

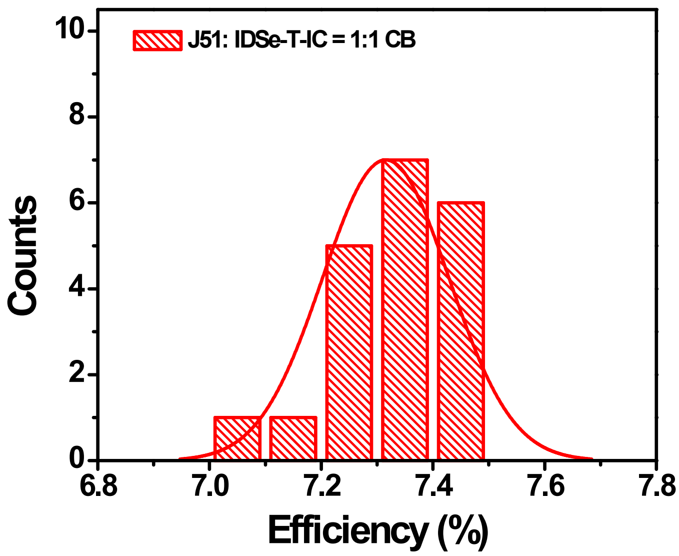


Fig S4b. Statistical histogram of PCEs of PSCs based on J51: IDSe-T-IC (1:1, w/w) fabricated with chlorobenzene solution.

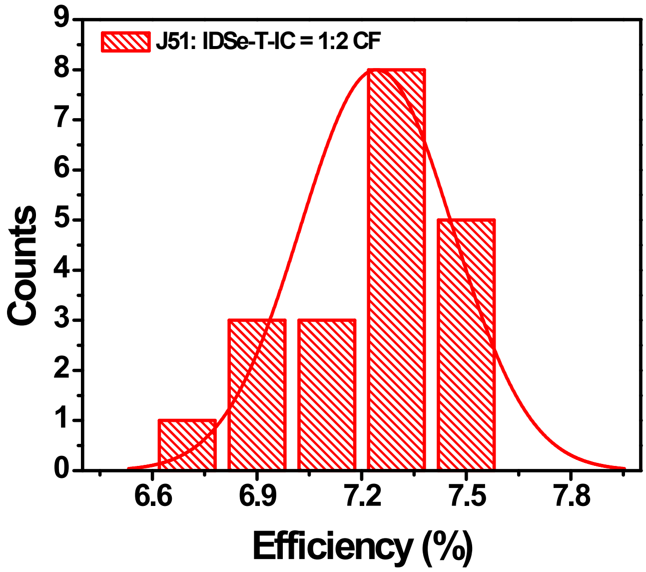


Fig. S4c. Statistical histogram of PCEs of PSCs based on J51: IDSe-T-IC (1:2, w/w) fabricated with chloroform solution.

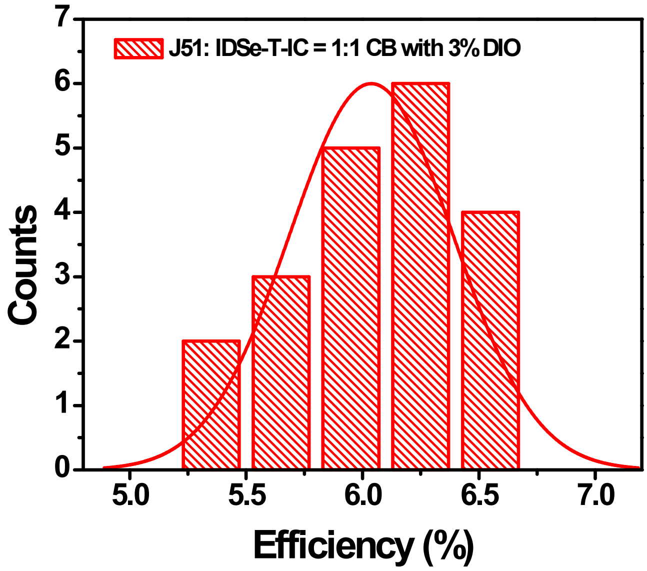


Fig. S4d. Statistical histogram of PCEs of PSCs based on J51: IDSe-T-IC (1:1, w/w) fabricated with chlorobenzene solution with 3% DIO.

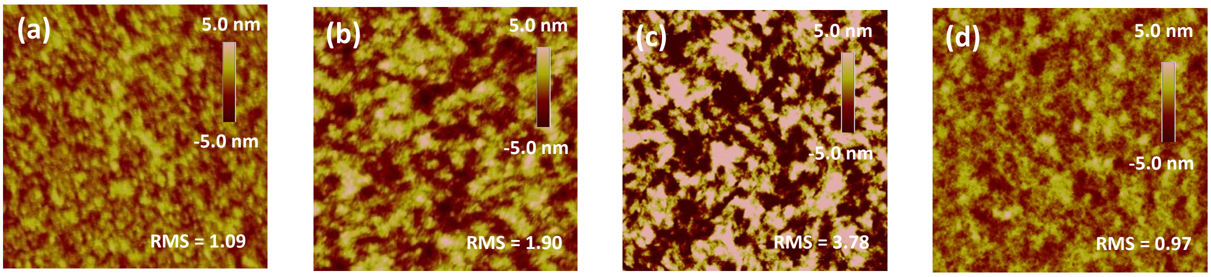


Fig. S5. AFM topography images (5 × 5 μm) of J51:IDSe-T-IC (1 : 1 w/w) blend films from CB (a), o-DCB (b), CB with 3% DIO (c) and CF (d).

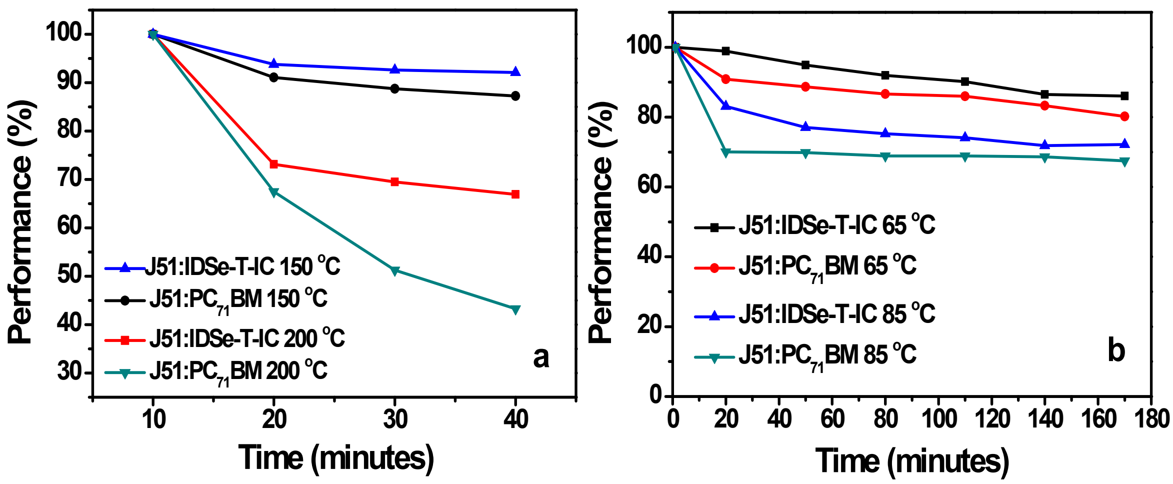


Fig. S6. (a) The stability of the PCEs for the devices based on J51: IDSe-T-IC (1:1, w/w) and J51:$PC_{71}BM$ (1:2, w/w) blended films after thermal treatment at 150 ^{o}C and 200 ^{o}C for different time; (b) The stability of the PCEs for the final devices based on J51: IDSe-T-IC and J51:$PC_{71}BM$ after thermal treatment at 65 ^{o}C and 85 ^{o}C for different time.

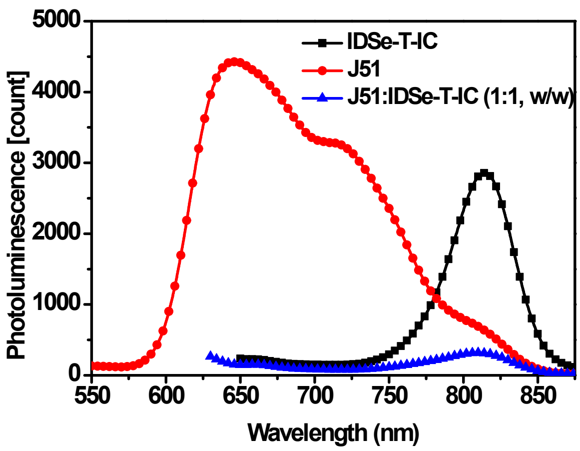


Fig. S7. Photoluminescence spectra of J51 (excitation at 500 nm), J51:IDSe-T-IC (1 : 1, w/w) (excitation at 600 nm) and IDSe-T-IC (excitation at 600 nm) in the thin film.

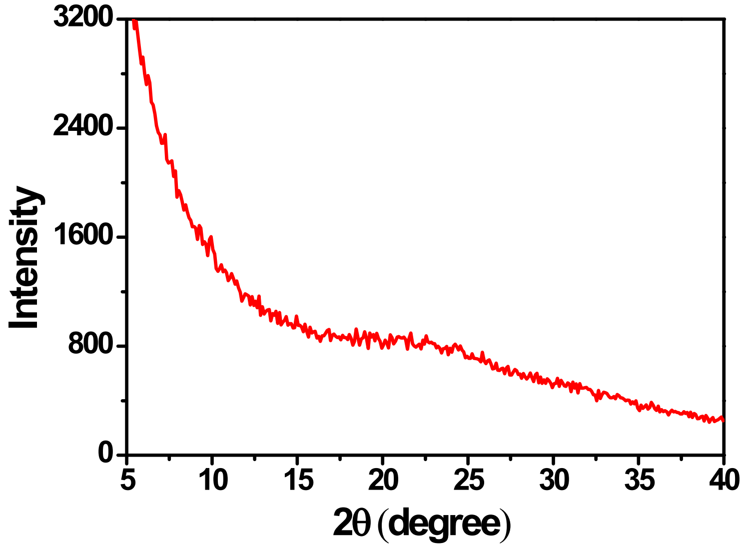


Fig. S8. The XRD pattern of the IDSe-T-IC film spin-coated on an ITO/PEDOT:PSS substrate.

Hole and electron mobility were measured using the space charge limited current（SCLC）method. ITO/PEDOT:PSS/ J51: IDSe-T-IC/Au for hole-only devices and ITO/ZnO/ J51: IDSe-T-IC /PDINO/Al for electron-only devices. The SCLC mobilities were calculated by MOTT-Gurney equation:

$$J = \frac{9\varepsilon_r\varepsilon_0\mu V^2}{8L^3}$$

Where J is the current density, εr is the relative dielectric constant of active layer material usually 2-4 for organic semiconductor, herein we use a relative dielectric constant of 4, ε0 is the permittivity of empty space, μ is the mobility of hole or electron and L is the thickness of the active layer (114 nm), V is the internal voltage in the device, and $V=V_{app} - V_{bi}$, where V_{app} is the voltage applied to the device, and V_{bi} is the built-in voltage resulting from the relative work function difference between the two electrodes. As shown n Figure S8, the hole and electron mobilities of J51 : IDSe-T-IC (1:1,w/w) are estimated as 8.25×10^{-5} and 7.72×10^{-5} $cm^2\ V^{-1}\ s^{-1}$ respectively, corresponding to nearly balanced charge transport ($\mu_h/\mu_e = 1.1$).

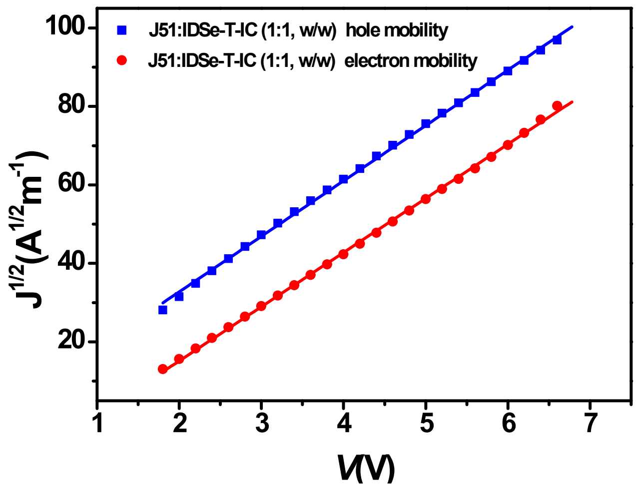


Fig. S9. J-V plots for electron-only (a) and hole-only (b) devices based on J51:IDSe-T-IC (1:1, w/w) blended films.

Table S1. The LUMO/HOMO energy levels and torsional angles of IDT-T-IC and IDSe-T-IC.

Compound	HOMO (eV)	LUMO (eV)	E_g (eV)	θ_1 (°)	θ_2 (°)	θ_3 (°)	θ_4 (°)
IDT-T-IC	-5.21	-3.24	1.97	0.1	11.8	0.1	11.7
IDSe-T-IC	-5.18	-3.27	1.91	0.1	0.7	0.1	0.2

Table S2. E_{loss} vs PCE of recent high performance narrow band gap polymers.

Donor	Acceptor	V_{oc}	J_{sc}	FF	PCE	E_g	E_{loss}	EQE_{max}
		(V)	(mA cm^{-2})	(%)	(%)	(eV)	(V)	(%)
PBDTTS-TTDffBT	PC71BM	0.85	15.43	72.0	9.4	1.59	0.74	90
P3HT	ICBA	0.84	12.10	72.3	7.3	1.91	1.07	85
PBnDT-FTAZ	PCBM	0.79	11.80	73.0	6.8	1.91	1.12	75
PBDTPD	PC71BM	0.92	13.10	61.0	7.3	1.84	0.92	70
PFDCTBT-C8	PC71BM	0.83	12.60	66.8	7.0	1.75	0.92	70
PTB7	PC71BM	0.76	15.80	70.2	8.4	1.65	0.89	70
PBnDT-DTffBT	PCBM	0.91	12.90	61.2	7.2	1.71	0.80	64
PIDTT-DFBT	PC71BM	0.96	12.20	61.0	7.0	1.76	0.80	65
PDTG-TPD	PC71BM	0.86	14.00	67.3	8.1	1.65	0.79	65
PBDT-DTNT	PC71BM	0.80	11.70	61.0	6.0	1.55	0.75	65
PDPP2FT-C14	PC71BM	0.65	14.80	64.0	6.2	1.36	0.71	50
PCPDT-FBT	PC71BM	0.77	15.60	50.0	5.8	1.46	0.69	65
PBDTDPP	PC71BM	0.82	10.50	60.0	5.2	1.31	0.49	45
pDPP5T-2	PC71BM	0.56	15.90	64.0	5.7	1.41	0.85	
PR2	PC71BM	0.77	13.50	58.0	6.0	1.40	0.63	55

PBDTP-DPP	PC71BM	0.76	13.60	60.0	6.2	1.46	0.70	50
PDPT-DFBT	PC71BM	0.70	18.00	63.0	8.0	1.38	0.68	63
PDPP2Tz2T	PC71BM	0.92	8.80	63.0	5.1	1.47	0.55	40
PDPP2TzDTP	PC71BM	0.69	14.90	54.0	5.6	1.28	0.59	52
PDPP5T	PCBM	0.58	14.00	65.0	5.3	1.46	0.88	65
C2	PC71BM	0.61	18.60	64.0	7.3	1.40	0.79	70
PIPCP	PC71BM	0.86	13.00	55.0	6.2	1.47	0.61	60
PNOz4T	PC71BM	0.96	14.5	64.0	8.9	1.52	0.56	63
PBDF-T1	PC71BM	0.92	13.3	75.5	9.4	1.83	0.91	77
TBTIT-h	PC71BM	0.72	17.7	71.0	9.1	1.60	0.88	76
PM6	PC71BM	0.98	12.7	74.0	9.2	1.80	0.82	80
PffBT-T3	PC71BM	0.82	18.7	68.3	10.5	1.63	0.81	80
PBDTT-FTTE	PNDIS-HD	0.81	18.80	51.0	7.7	1.59	0.78	90
PBDTT-TT	PDI1	0.80	13.30	55.0	6.1	1.59	0.79	61
PBDTT-TT-F	P(NDIDT-FT2)	0.81	13.53	62.0	6.7	1.59	0.78	65
PSEHTT	DBFI- DMT	0.92	12.56	55.0	6.4	1.82	0.90	80
PTB7-Th	HPDI4	0.80	15.10	68.0	8.3	1.59	0.79	80
PDBT-T1	SdiPBI-S	0.90	11.98	66.1	7.2	1.82	0.92	70
PBDTT-F-TT	tetra-PDI	0.86	8.25	48.1	3.5	1.59	0.73	45
PTB7-TH	ITIC	0.81	14.21	59.1	6.8	1.59	0.78	70
PBDTT-F-TT	TPE-PDI4	0.91	11.70	52.0	5.5	1.59	0.68	55
PBDT-TS1	PPDI	0.82	12.51	53.0	5.4	1.55	0.73	65
PffBT4T-2DT	SF-PDI2	0.98	10.70	57.0	6.0	1.65	0.67	55
P3HT	SF(DPPB)4	1.14	8.29	55.0	5.2	1.77	0.63	48
PDBT-T1	SdiPBI-Se	0.95	12.48	69.7	8.2	1.80	0.85	70
PPDT2FBT	NIDCS-HO	1.03	11.88	63.0	7.6	1.80	0.67	72
PffT2-FTAZ-2DT	IEIC	1.0	12.20	59.0	7.3	1.57	0.57	56
PDBT-T1	SdiPBI-Se	0.95	12.48	69.7	8.4	1.77	0.82	73
J51	N2200	0.83	14.18	70.2	8.3	1.48	0.65	75
PBDTT-F-TT	di-PBI	0.80	11.68	55.0	5.3	1.59	0.79	50

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