Supplementary Information

Naphthyridinedione-based multifunctional small molecules for both photovoltaics and transistors application

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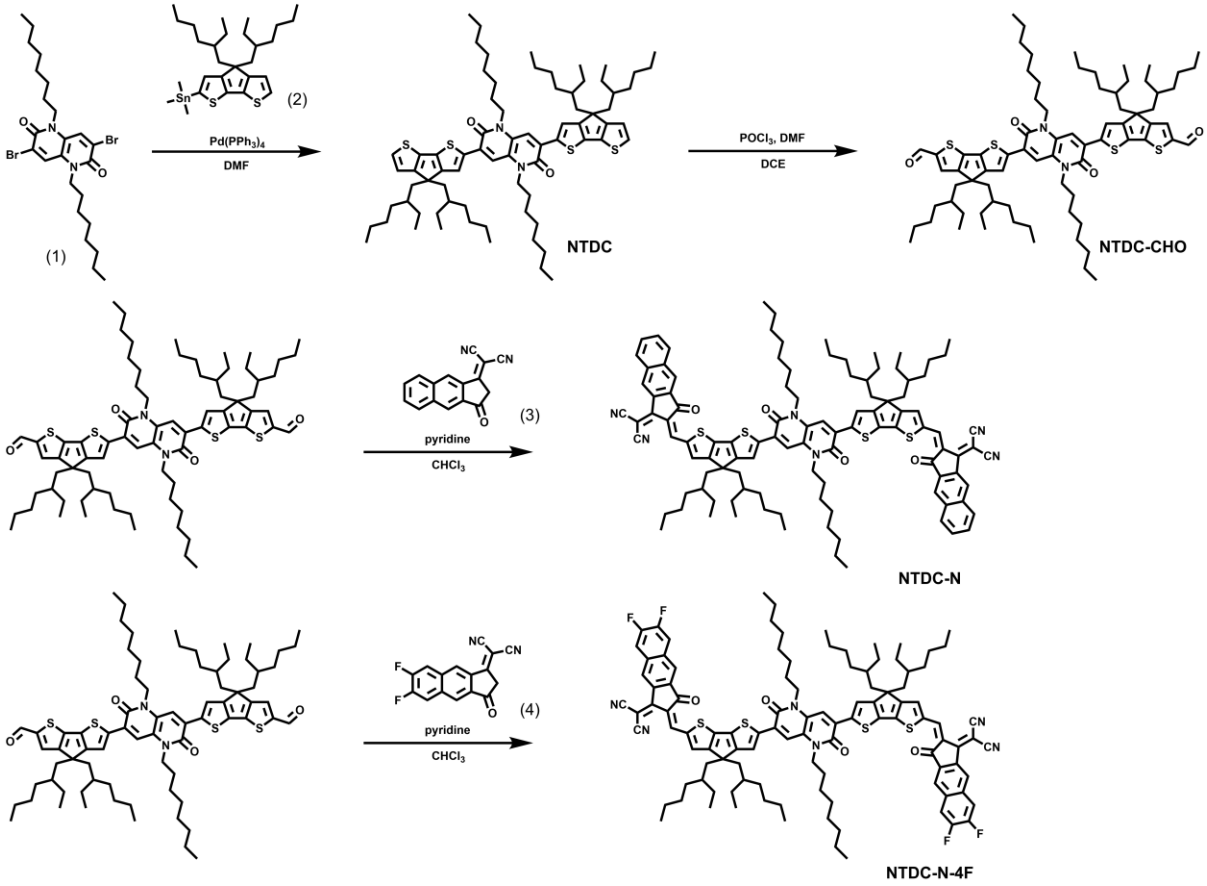

Scheme S1 Synthetic route of NTDC-N and NTDC-N-4F.

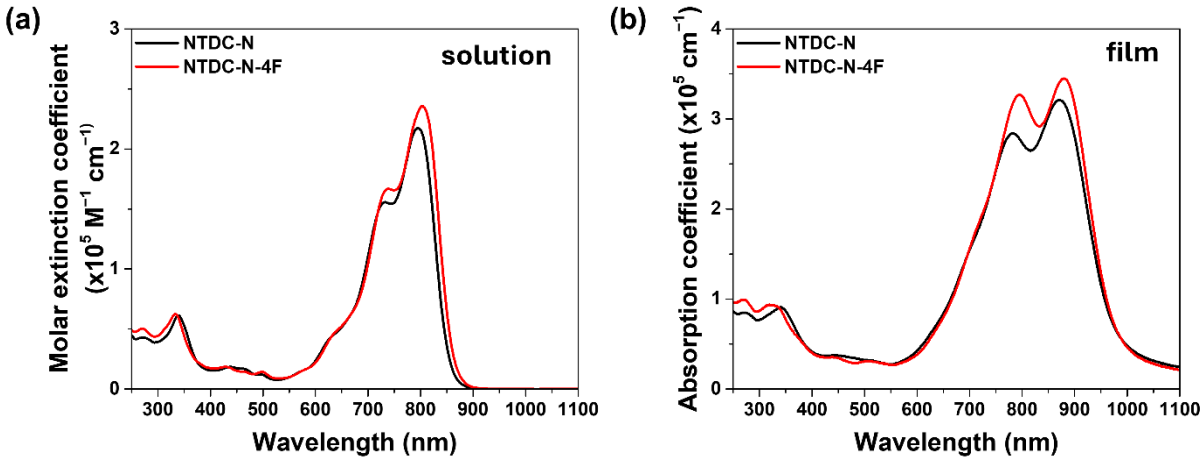

Fig. S1 (a) Molar extinction coefficients in 10 μM $CHCl_3$ solution and (b) Absorption coefficient in thin film of NTDC-N and NTDC-N-4F.

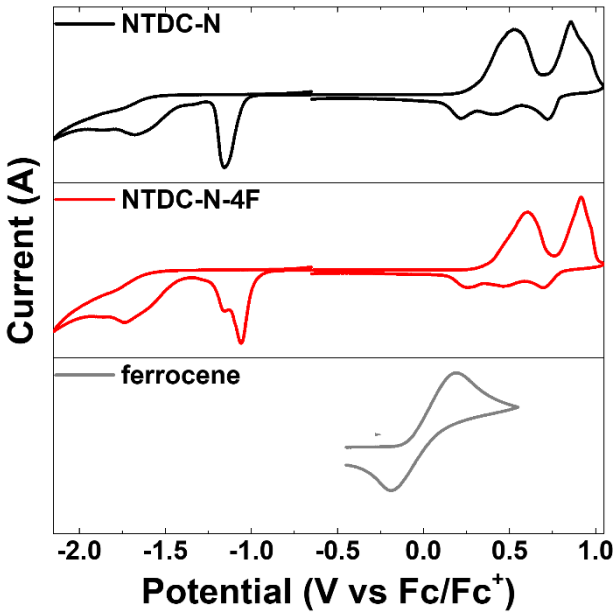

Fig. S2 Cyclic voltammograms of NTDC-N, NTDC-N-4F, and ferrocene.

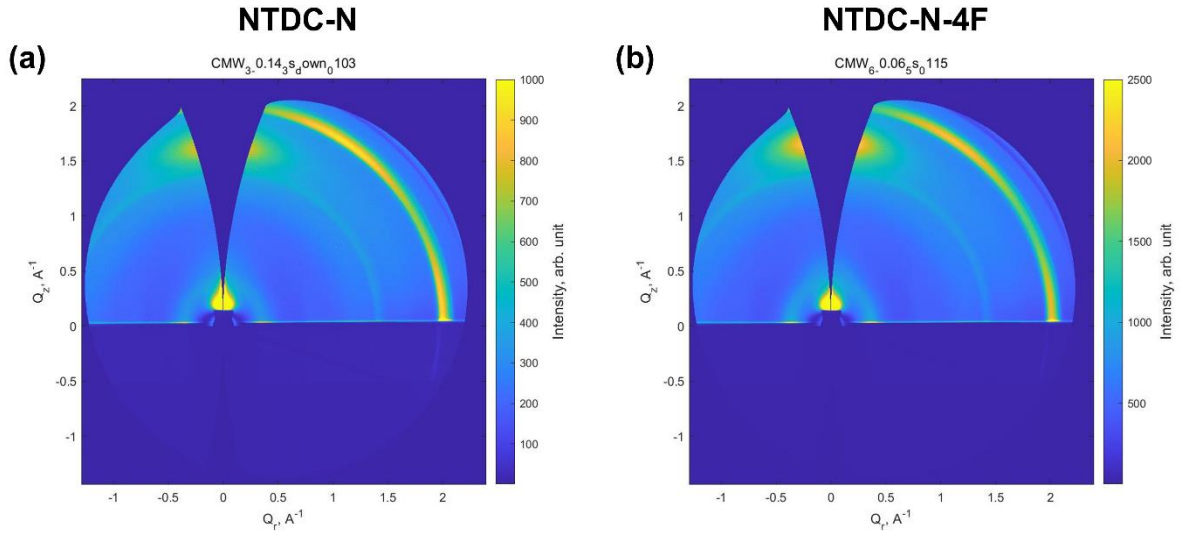

Fig. S3 2D GIWAXS patterns of (a) NTDC-N and (b) NTDC-N-4F neat films. The faint ring patterns around q = 1.5 $Å^{-1}$ and the bright ring patterns around q = 2 $Å^{-1}$ are originated from ITO substrates.

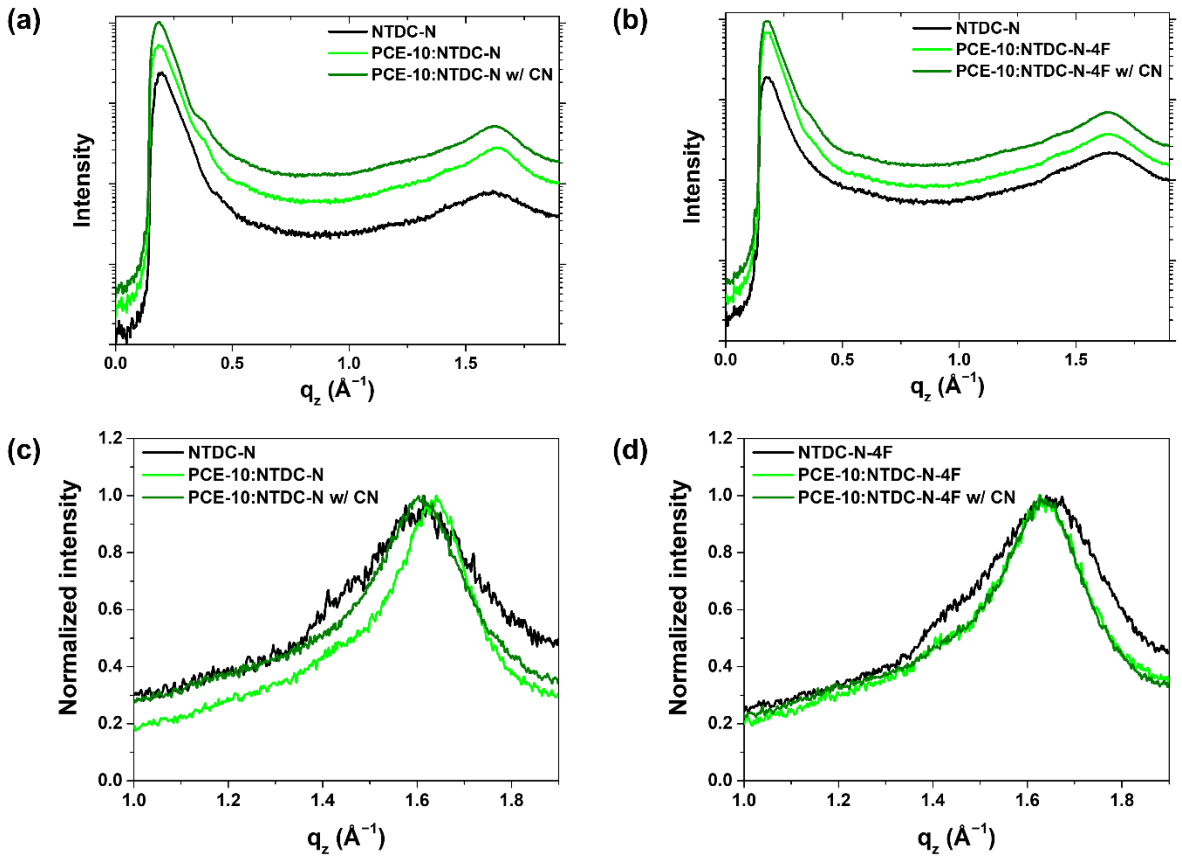

Fig. S4 Out-of-plane linecuts of GIWAXS patterns of pristine acceptor films, polymer:acceptor blend films, and polymer:acceptor blend films w/ CN. (a and c) NTDC-N and (b and d) NTDC-N-4F. Normalized peaks near π- π stacking pattern of films are described on (c) NTDC-N and (d) NTDC-N-4F.

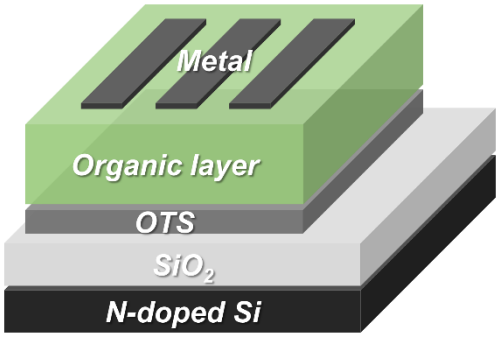

Fig. S5 Device structure of OFET devices.

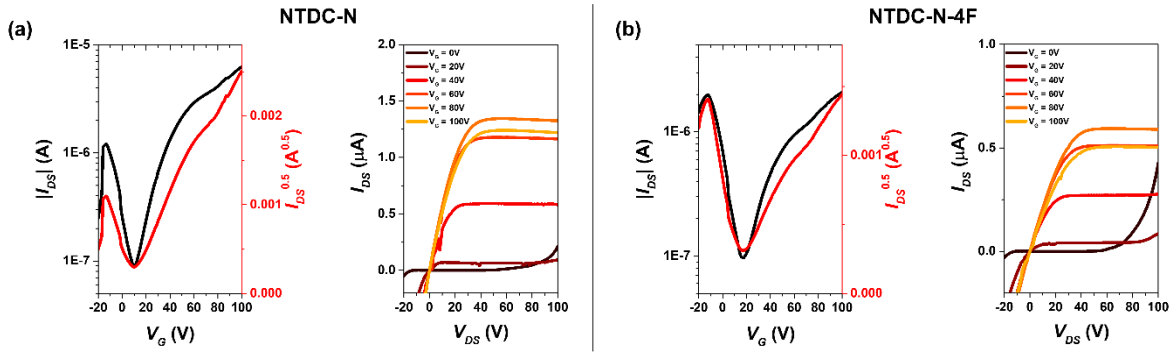

Fig. S6 Representative transfer (left side of (a and b), V_{DS} = 100 V) and output curves (right side of (a and b), V_G = −100 V) for top-contact bottom-gate *n*-channel mode OFETs with Al electrode of (a) NTDC-N and (b) NTDC-N-4F. Substrate temperature is 110°C. Channel width (W) and length (L) are 100 μm and 1 mm, respectively.

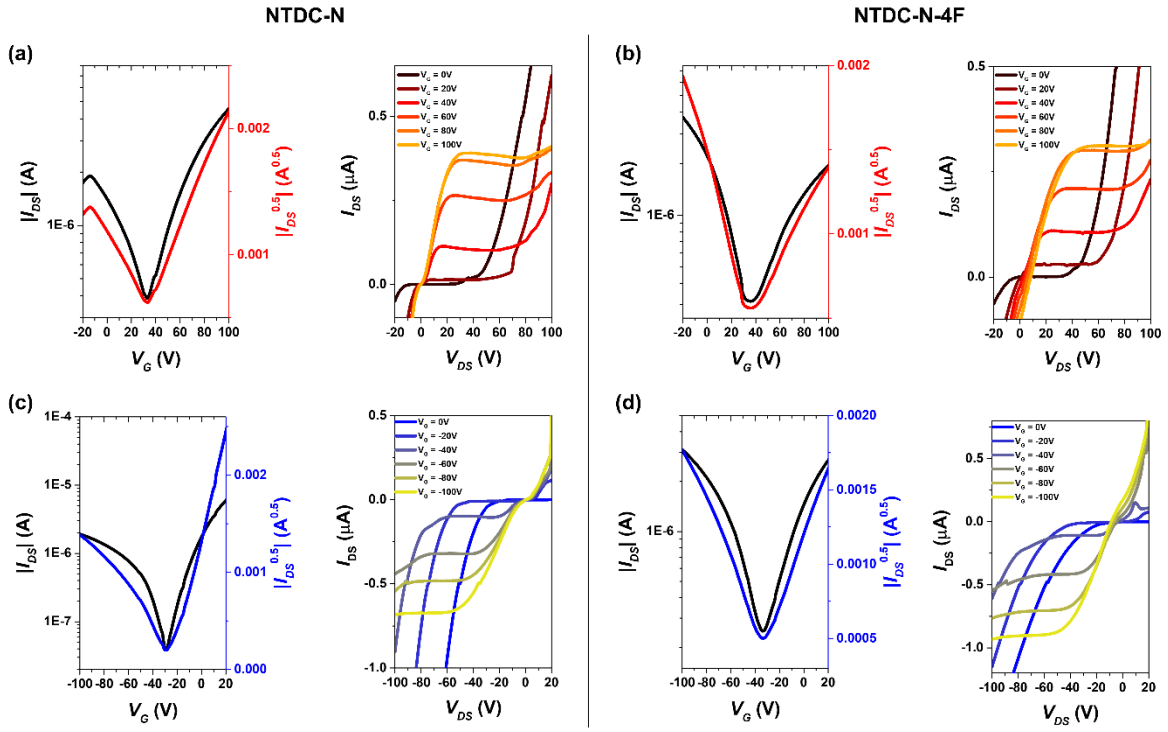

Fig. S7 Representative transfer (left, V_{DS} = 100 V for *n*-channel mode and V_{DS} = −100 V for *p*-channel mode) and output curves (right, V_G = −100 V *n*-channel mode and V_G = 100 V for *p*-channel mode) for top-contact bottom-gate OFETs with Al electrode of (a and c) NTDC-N and (b and d) NTDC-N-4F. *n*-Channel mode and *p*-channel mode OFET characteristics are on the top (a and b) and the bottom (c and d), respectively. Channel width (W) and length (L) are 100 μm and 1 mm, respectively.

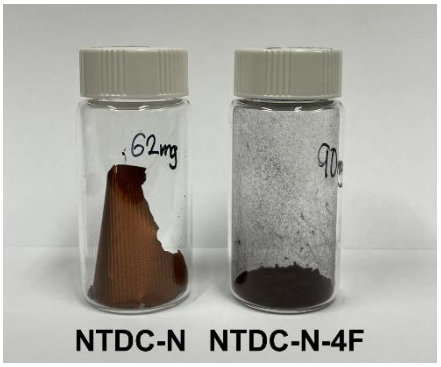

Fig. S8 An image of NTDC-N and NTDC-N-4F.

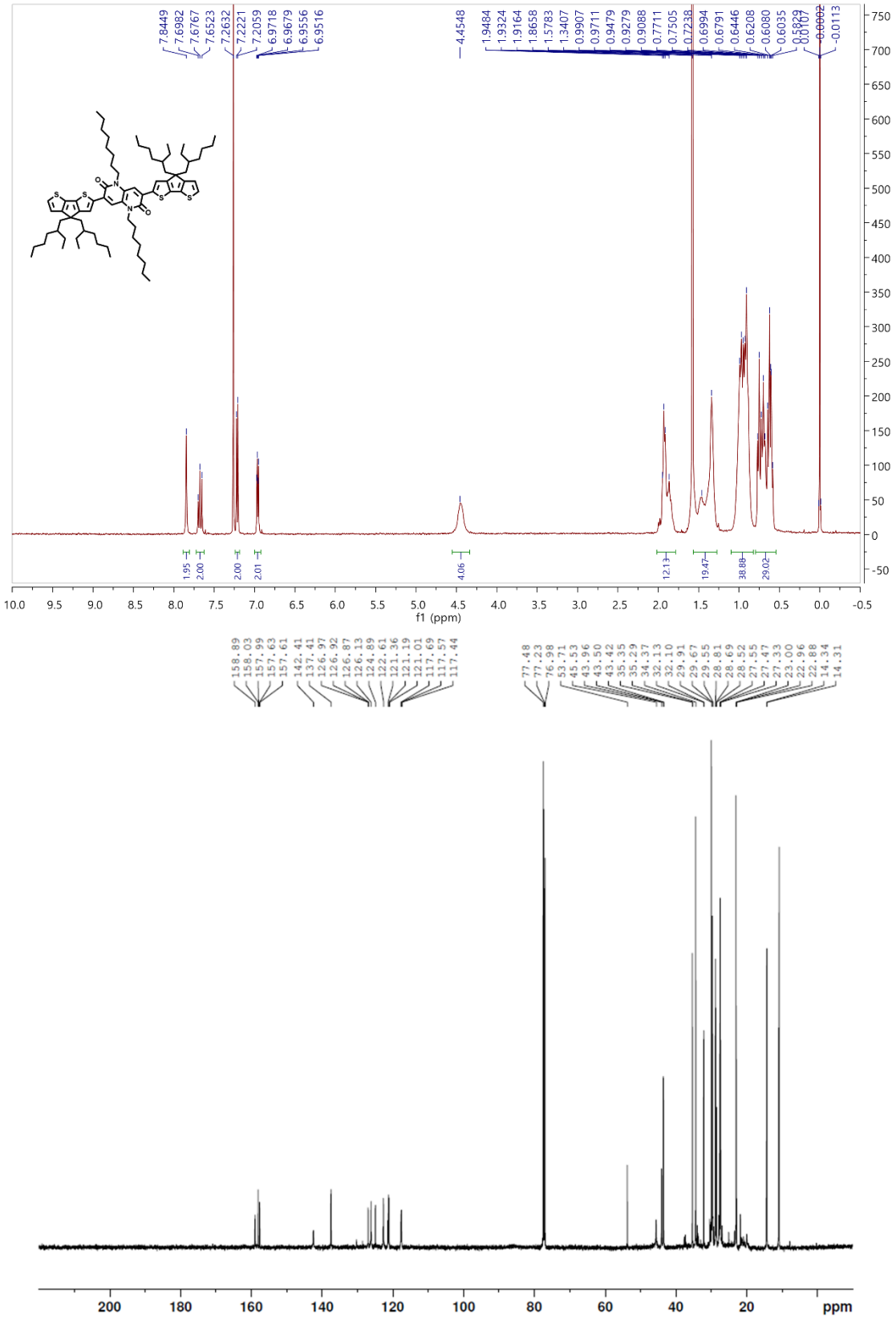

Fig. S9 ^{1}H NMR and ^{13}C NMR spectra of **NTDC** ($CDCl_3$).

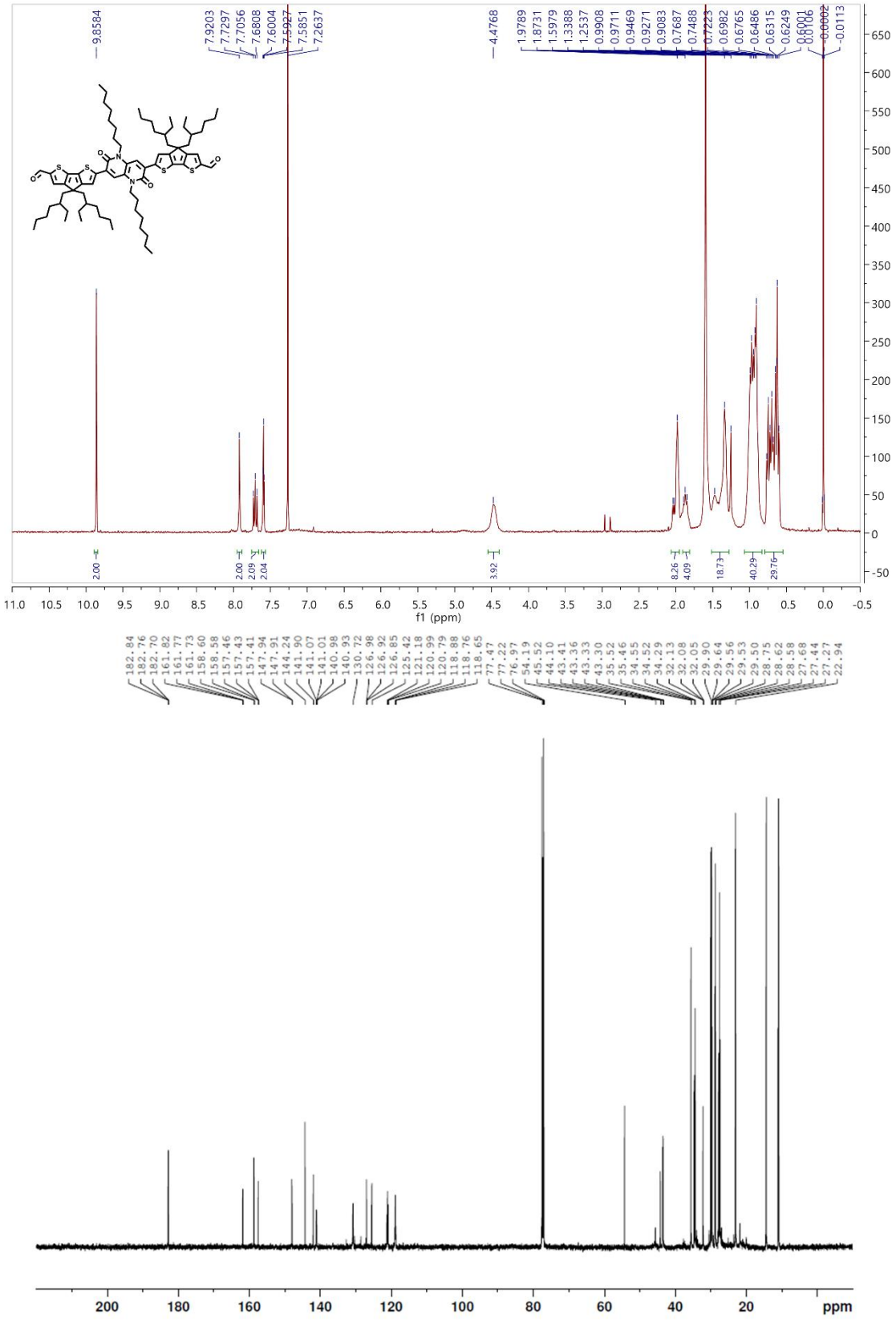

Fig. S10 ^{1}H NMR and ^{13}C NMR spectra of **NTDC-CHO** ($CDCl_3$).

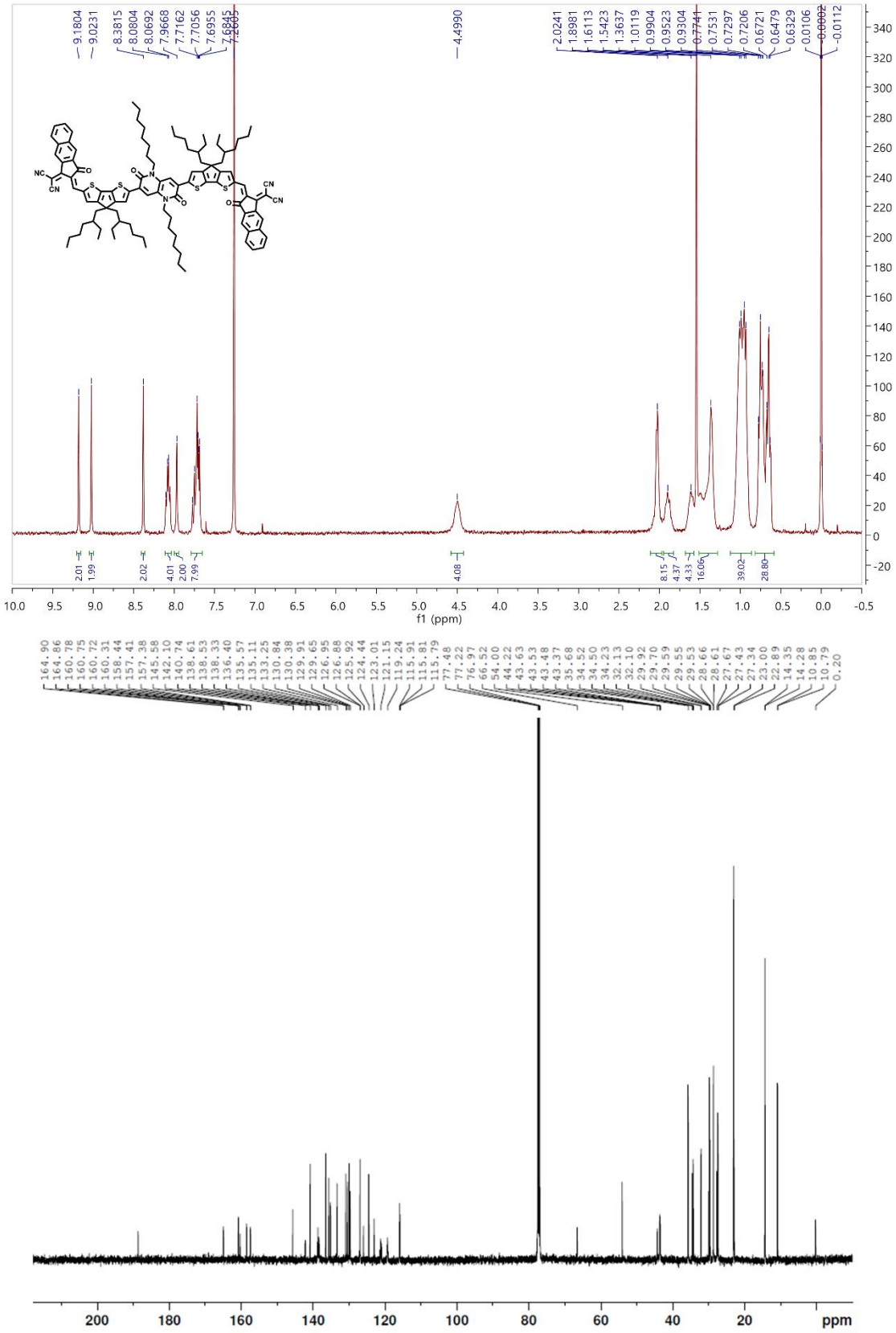

Fig. S11 ^{1}H NMR and ^{13}C NMR spectra of **NTDC-N** ($CDCl_3$).

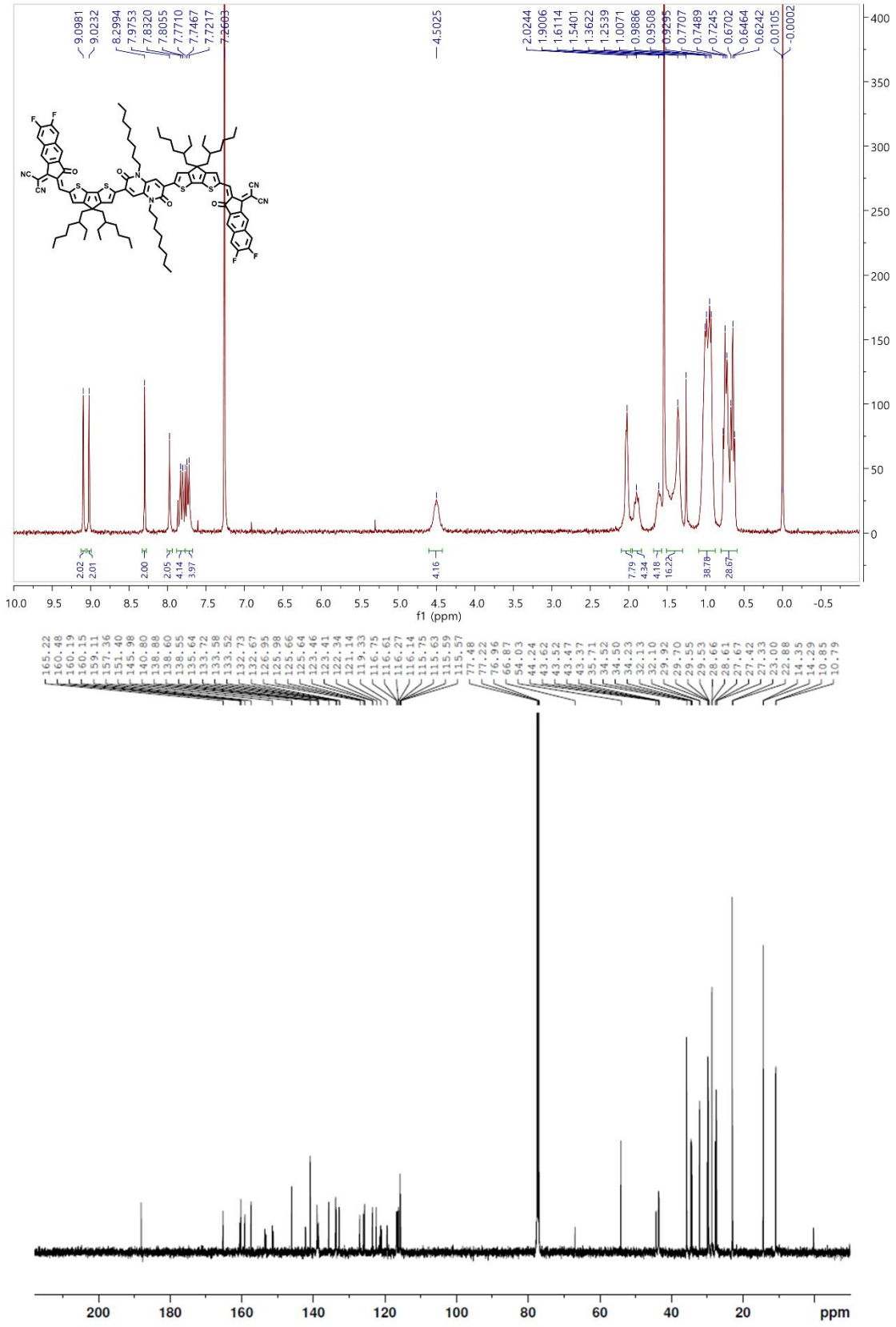

Fig. S12 ^{1}H NMR and ^{13}C NMR spectra of **NTDC-N-4F** ($CDCl_3$).

Table S1 Device performances of OPV devices using different additives.

BHJ	Additive	V_{oc} [V]	J_{sc} [mA cm^{-2}]	FF	PCE [%]
PCE-10:NTDC-N	-	0.71	18.97	0.51	6.85
	DPE 0.5 vol%	0.71	13.97	0.57	5.70
	DIO 0.5 vol%	0.70	9.26	0.58	3.79
	CN 0.5 vol%	0.71	19.52	0.54	7.51
PCE-10:NTDC-N-4F	-	0.65	20.49	0.59	7.83
	DPE 0.5 vol%	0.63	19.87	0.61	7.61
	DIO 0.5 vol%	0.64	17.60	0.59	6.60
	CN 0.5 vol%	0.64	20.08	0.61	8.16

Table S2 GIWAXS parameters of acceptors and blend films.

Film	q_z (Å^{-1})	π-π stacking (Å)	FWHM (Å^{-1})	CCL (Å)
NTDC-N	1.6102	3.90	0.2840	22.12
PCE-10:NTDC-N	1.6406	3.83	0.1876	33.49
PCE-10:NTDC-N w/ CN	1.6048	3.91	0.2209	28.44
NTDC-N-4F	1.6485	3.81	0.2702	23.25
PCE-10:NTDC-N-4F	1.6349	3.84	0.2021	31.09
PCE-10:NTDC-N-4F w/ CN	1.6349	3.84	0.2082	30.18

Table S3 Summary of OFET device performances according to substrate temperatures.

Material	Substrate temperature	$\mu_{e.avg}$ [a)] [$cm^2\ V^{-1}\ s^{-1}$]	$\mu_{e.max}$ [b)] [$cm^2\ V^{-1}\ s^{-1}$]
NTDC-N	25℃	$(1.67 \pm 0.25) \times 10^{-3}$	2.32×10^{-3}
	70℃	$(2.34 \pm 0.51) \times 10^{-3}$	3.14×10^{-3}
	110℃	$(1.05 \pm 0.17) \times 10^{-2}$	1.31×10^{-2}
NTDC-N-4F	25℃	$(1.20 \pm 0.09) \times 10^{-3}$	1.31×10^{-3}
	70℃	$(1.79 \pm 0.17) \times 10^{-3}$	2.19×10^{-3}
	110℃	$(3.48 \pm 0.35) \times 10^{-3}$	4.21×10^{-3}

[a)] Average electron mobility. [b)] Maximum electron mobility.