

Supporting Information

Effect of Dye End Groups in Non-Fullerene Fluorene- and Carbazole-Based Small Molecule Acceptors on Photovoltaic Performance

Yujeong Kim,^a Chang Eun Song,^b Sang-Jin Moon,^b Eunhee Lim^{a,†}

^aDepartment of Chemistry, Kyonggi University, San 94-6, Iui-dong, Yeongtong-gu, Suwon-si, Gyeonggi 443-760, Republic of Korea

^bKorea Research Institute of Chemical Technology (KRICT), 100 Jang-dong, Yuseong-gu, Daejeon 305-600, Republic of Korea

* Corresponding author: Tel. +82-31-249-9663; E-mail address: ehlim@kyonggi.ac.kr

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1. ^1H and ^{13}C NMR spectra

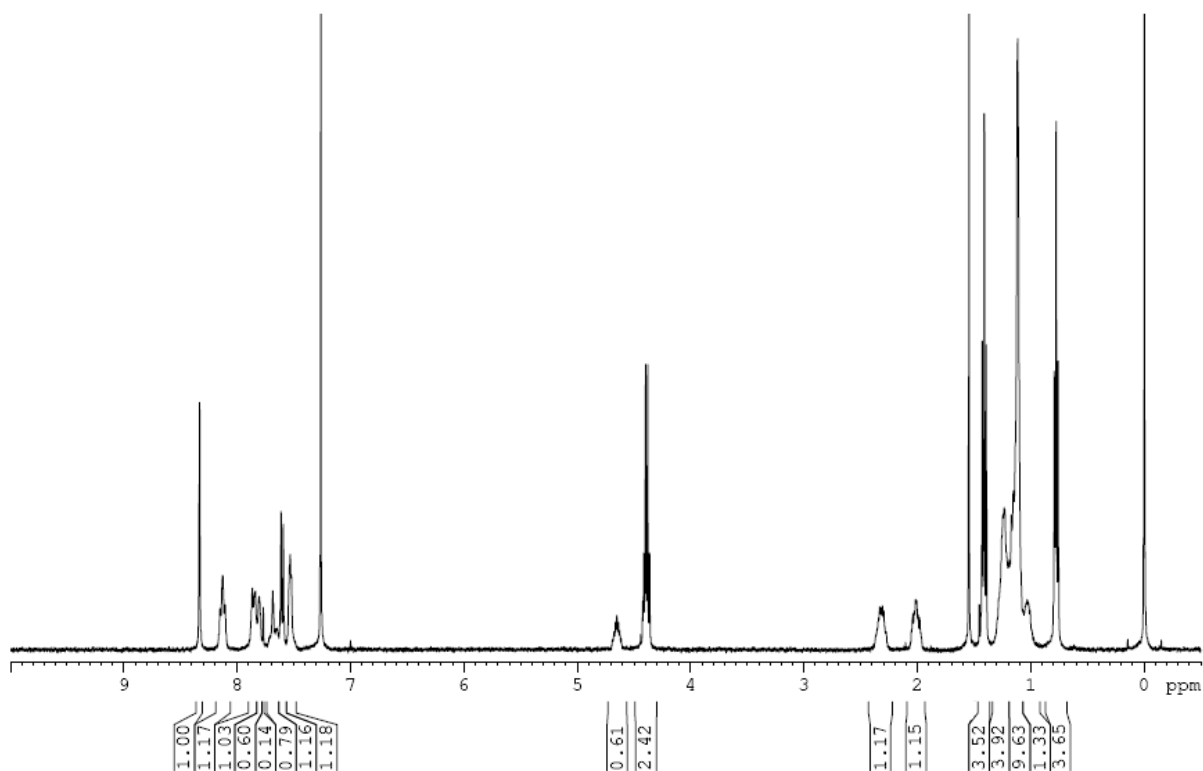


Figure S1. ^1H NMR spectra of Cz-ECA.

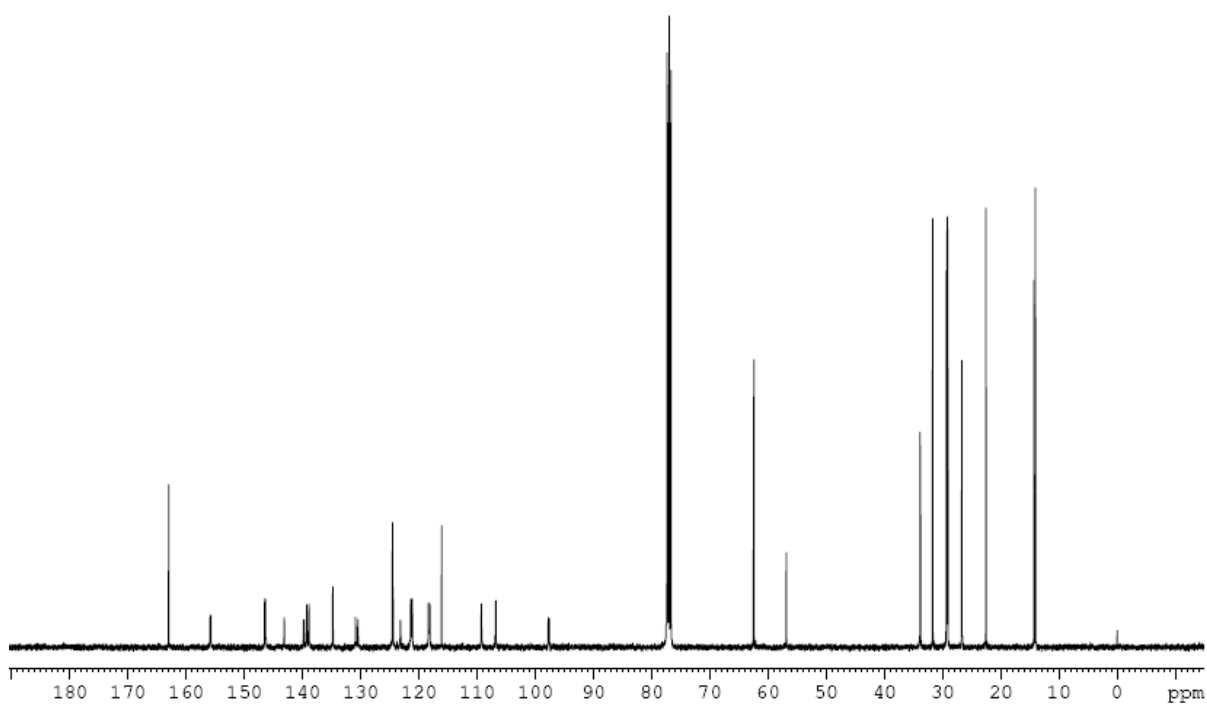


Figure S2. ^{13}C NMR spectra of Cz-ECA.

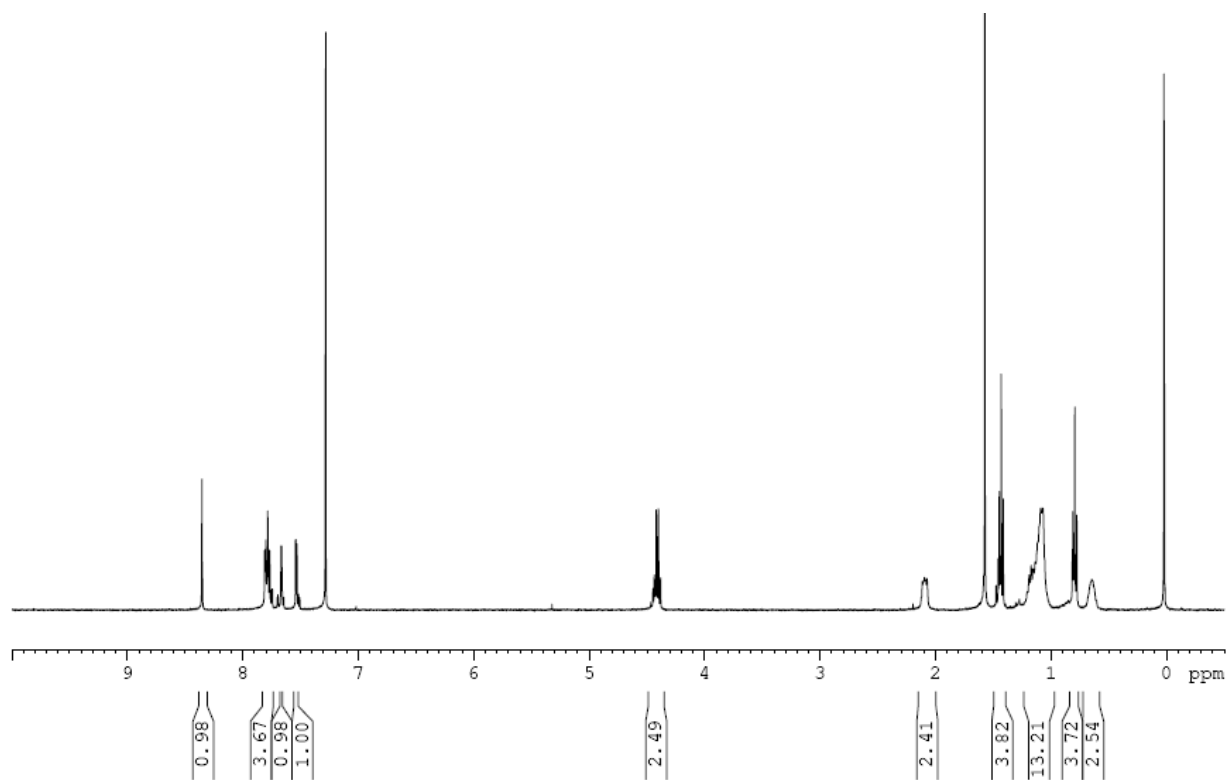


Figure S3. ^1H NMR spectra of **Flu-ECA**.

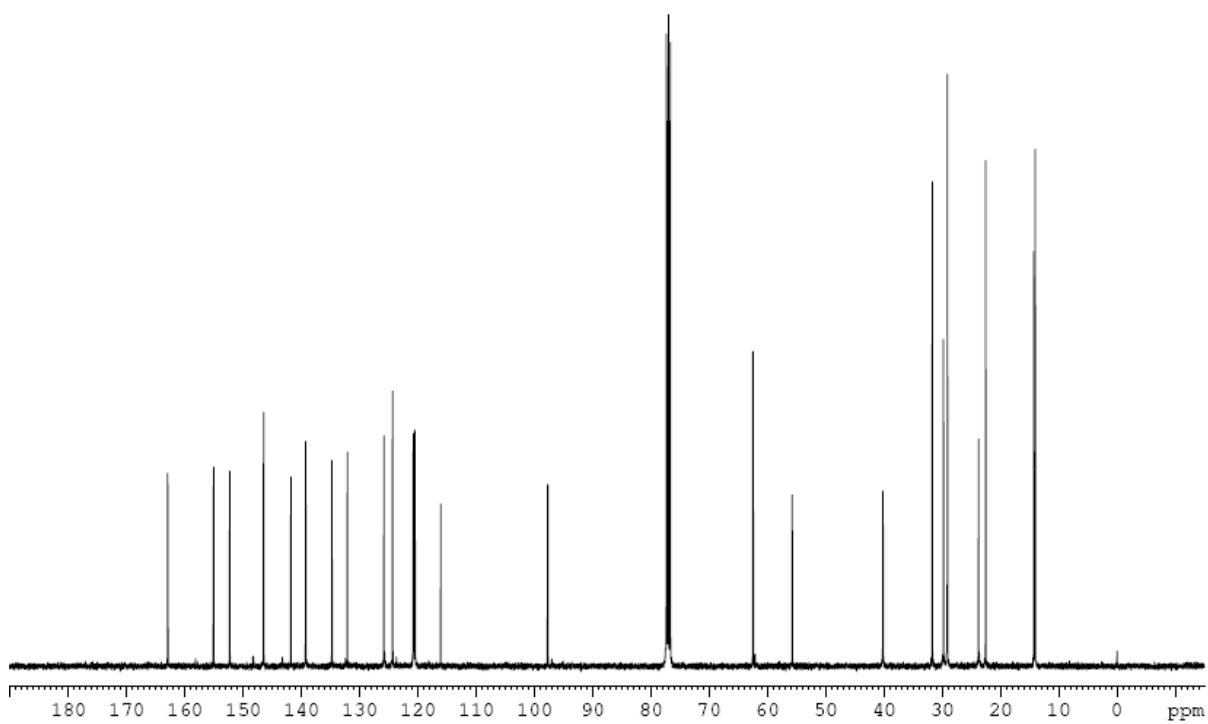


Figure S4. ^{13}C NMR spectra of **Flu-ECA**.

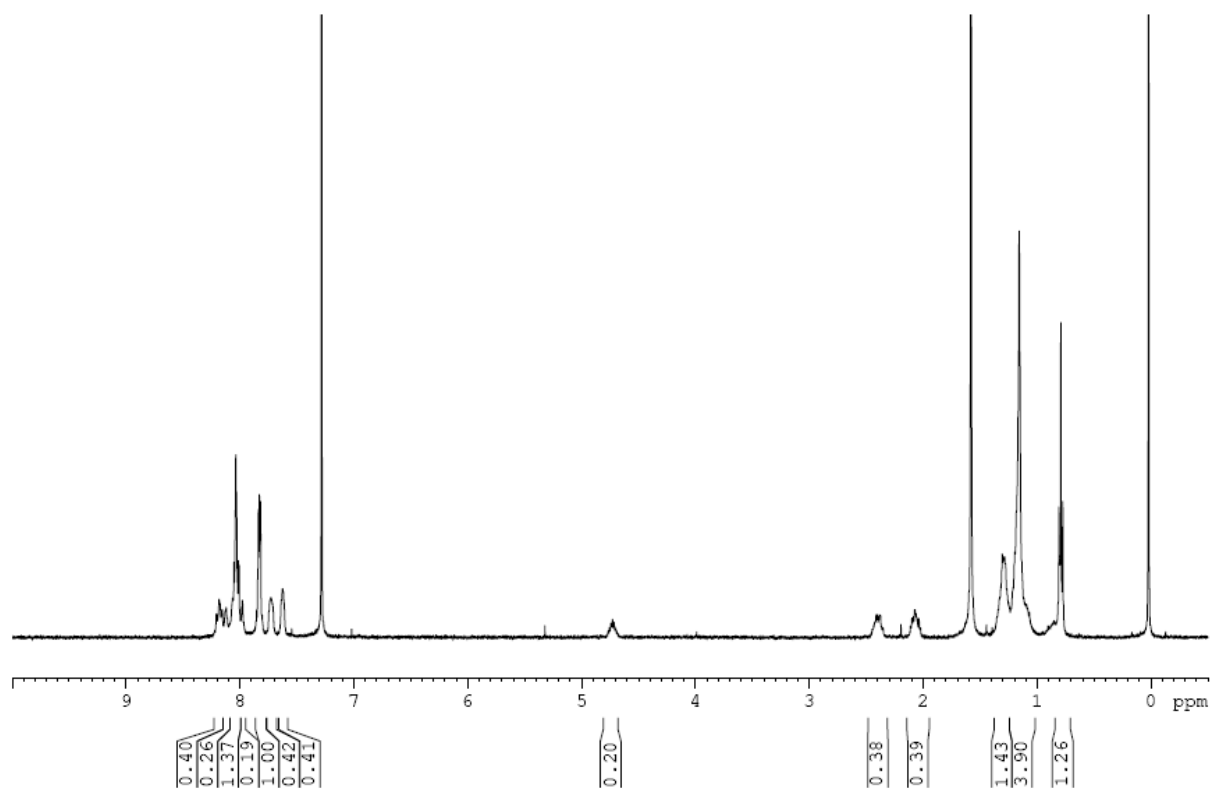


Figure S5. ^1H NMR spectra of Cz-IN.

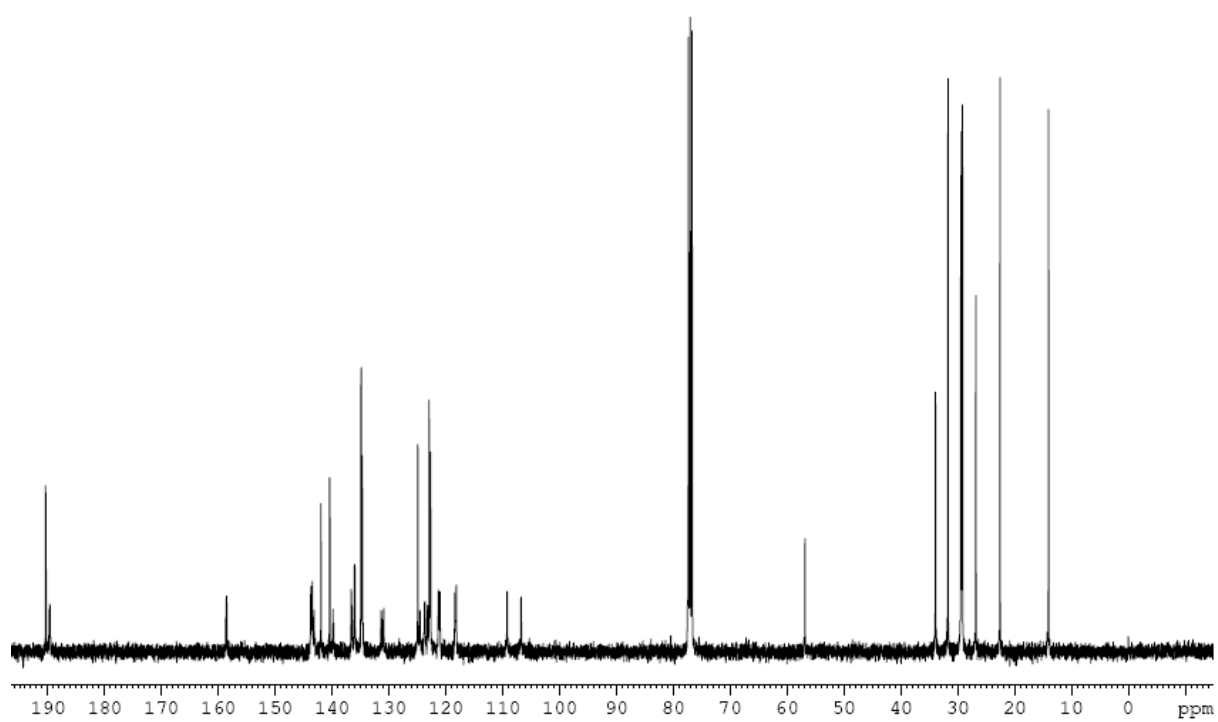


Figure S6. ^{13}C NMR spectra of Cz-IN.

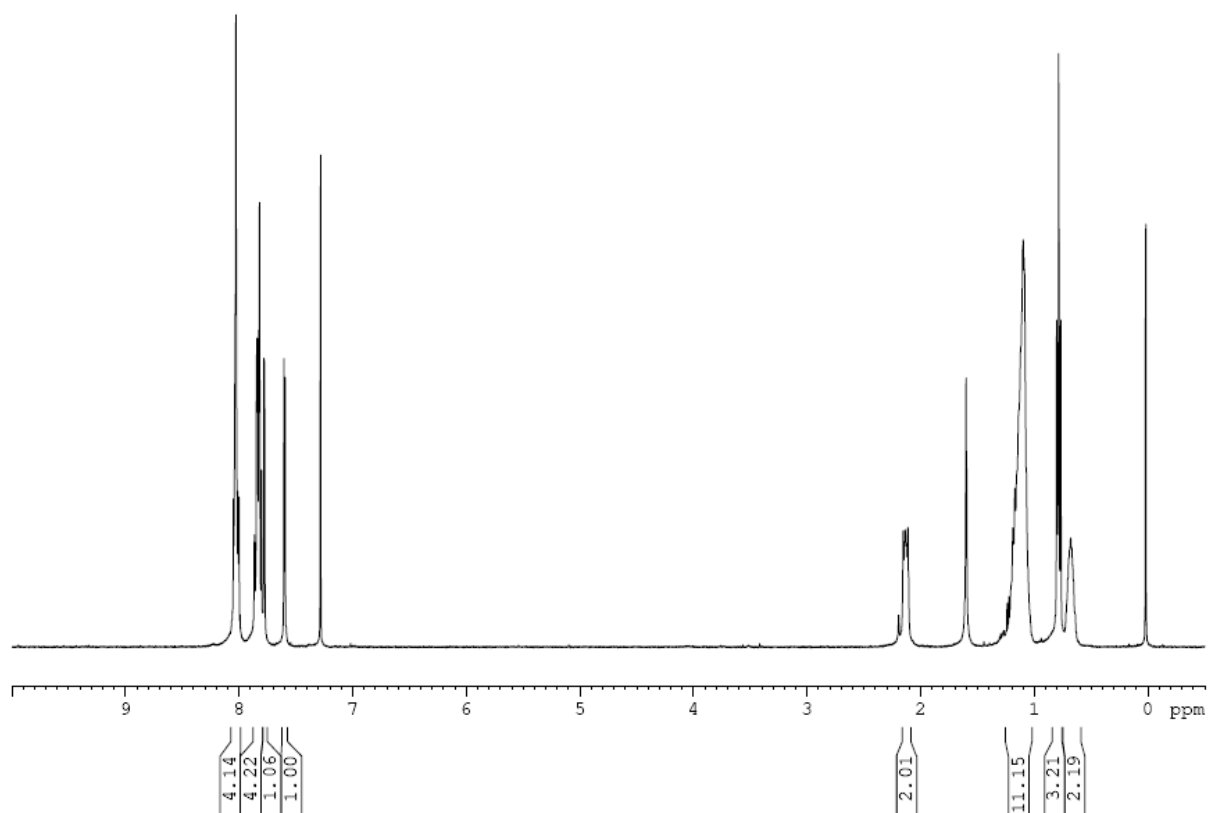


Figure S7. ^1H NMR spectra of **Flu-IN**.

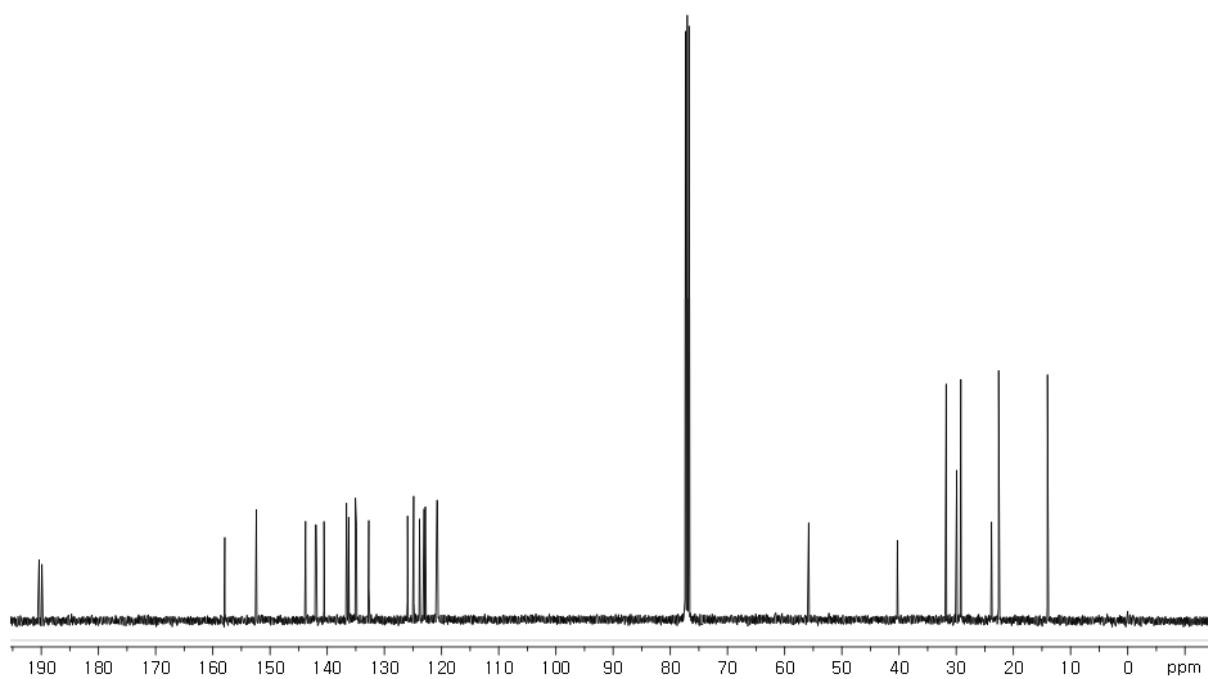


Figure S8. ^{13}C NMR spectra of **Flu-IN**.

2. OPV characteristics

Table S1. Photovoltaic properties of the small molecules fabricated under various conditions

Acceptor	D:A ratio	T_a (°C) ^a	V_{OC} (V)	J_{SC} (mA/cm ²)	FF (%)	PCE (%)
Cz-ECA	1.0:1.5	80	0.98	2.31	42	0.96
	1.0:1.5	100	1.00	2.34	44	1.03
	1.0:1.5	120	1.00	2.32	43	1.00
Cz-IN	1.0:1.5	80	0.54	0.11	27	0.02
	1.0:1.5	100	0.61	0.13	26	0.02
	1.0:1.5	120	0.49	0.13	26	0.02
Cz-RH^b	1.0:1.5	80	1.03	4.82	50	2.50
	1.0:1.5	100	1.03	4.69	53	2.56
	1.0:1.5	120	1.03	4.63	50	2.40
PC₆₁BM	1.0:1.0	W/O	0.57	9.04	60	3.14
	1.0:1.0	120	0.59	8.59	63	3.16
	1.0:1.0	150	0.60	9.08	61	3.34

^aThe films were annealed at the annealing temperature (T_a) for 10 min. ^bTaken from ref. 35.

Table S2. Photovoltaic properties of the small molecules fabricated under various conditions

Acceptor	D:A ratio	T_a ($^{\circ}\text{C}$) ^a	V_{OC} (V)	J_{SC} (mA/cm ²)	FF (%)	PCE (%)
Flu-ECA	1.0:0.5	80	1.01	2.31	40	0.94
	1.0:0.5	100	1.01	2.22	41	0.94
	1.0:0.5	120	1.00	2.48	43	1.07
	1.0:1.0	80	1.04	2.86	41	1.23
	1.0:1.0	100	1.03	2.82	44	1.26
	1.0:1.0	120	1.02	2.65	41	1.10
	1.0:1.5	80	1.03	2.96	41	1.25
	1.0:1.5	100	1.04	2.87	42	1.25
	1.0:1.5	120	1.03	2.91	42	1.25
Flu-IN	1.0:0.5	80	0.83	2.74	43	0.98
	1.0:0.5	100	0.83	2.63	43	0.95
	1.0:0.5	120	0.54	1.45	39	0.31
	1.0:1.0	80	0.92	3.40	42	1.32
	1.0:1.0	100	0.92	3.20	44	1.28
	1.0:1.0	120	0.52	2.05	35	0.38
	1.0:1.5	80	0.91	2.90	42	1.14
	1.0:1.5	100	0.91	2.86	42	1.11
	1.0:1.5	120	0.43	1.17	40	0.20
Flu-RH ^b	1.0:1.0	90	1.01	5.22	48	2.53
	1.0:1.0	120	1.04	5.44	51	2.89
	1.0:1.0	150	1.04	5.29	50	2.78
	1.0:1.5	80	1.03	5.61	51	2.95
	1.0:1.5	120	1.03	5.52	53	3.00
	1.0:1.5	150	1.05	4.71	53	2.60

^aThe films were annealed at the annealing temperature (T_a) for 10 min. ^bTaken from ref. 35.

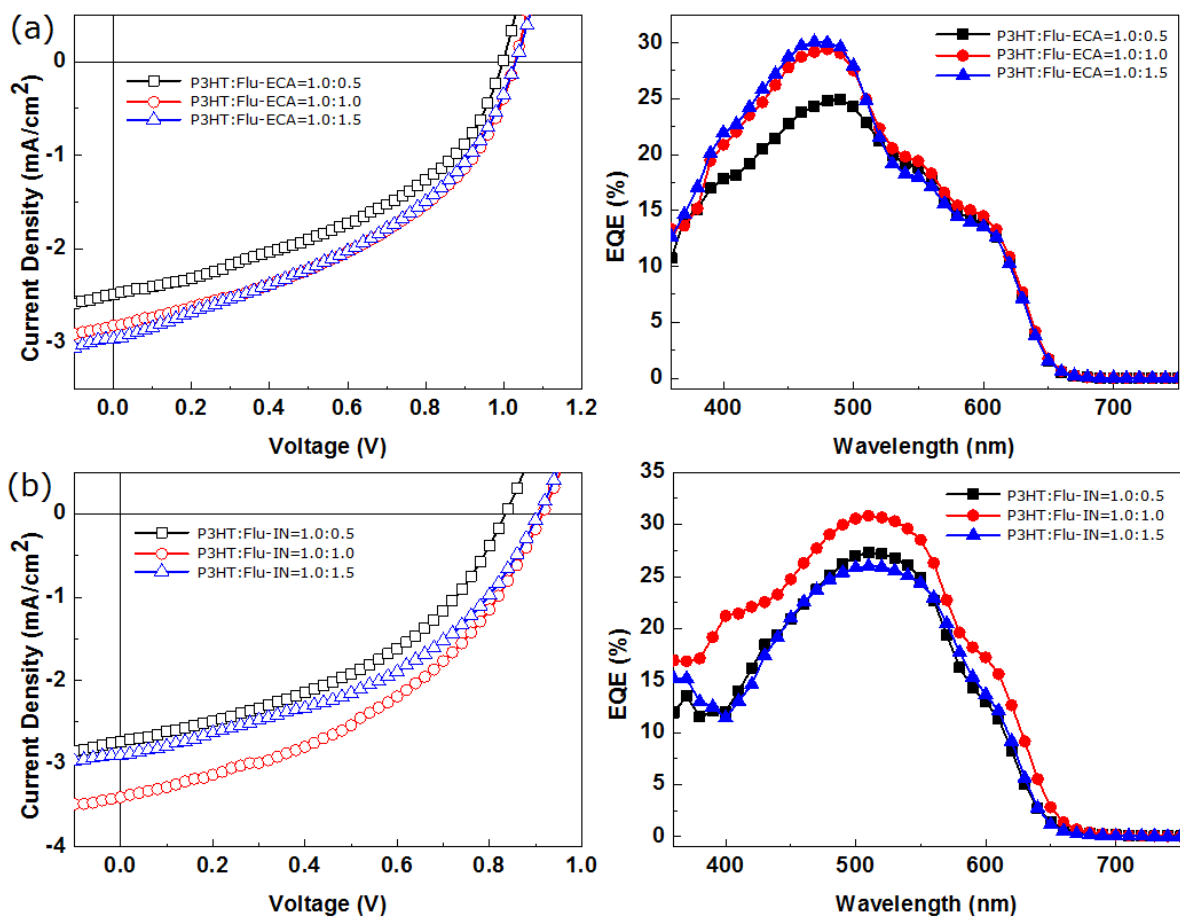


Figure S9. $J-V$ (left) and EQE (right) curves of OPV devices using (a) **Flu-ECA** and (b) **Flu-IN** as acceptors with various blend ratios (D:A).

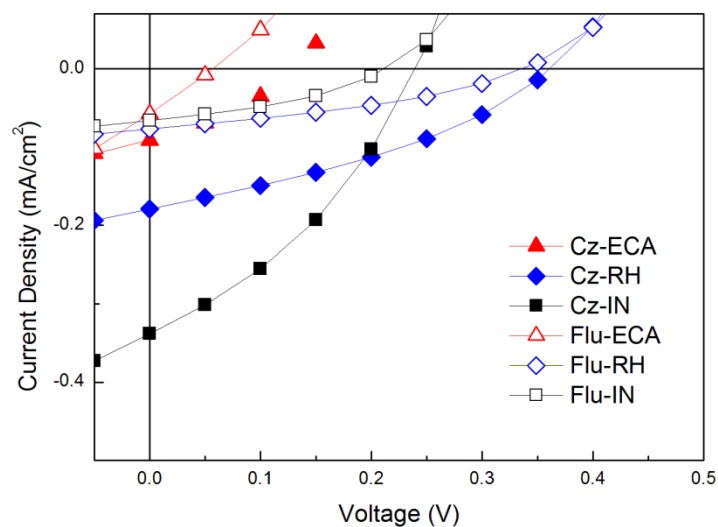


Figure S10. J - V curves of OPV devices using small molecules as donors.

Table S3. OPV devices using small molecules as donors^a

Donor	T_a (°C) ^b	V_{OC} (V)	J_{SC} (mA/cm ²)	FF (%)	PCE (%)
Cz-ECA	100	0.13	0.08	34	0.00
Cz-RH	100	0.36	0.18	35	0.02
Cz-IN	100	0.24	0.34	36	0.03
Flu-ECA	100	0.06	0.06	13	0.00
Flu-RH	100	0.35	0.09	34	0.01
Flu-IN	80	0.21	0.07	38	0.01

^a ITO/PEDOT:PSS/small molecule:PC₇₁BM (1:1)/LiF/Al. ^b The films were annealed at T_a for 10 min.

3. Atomic force microscopy (AFM) images

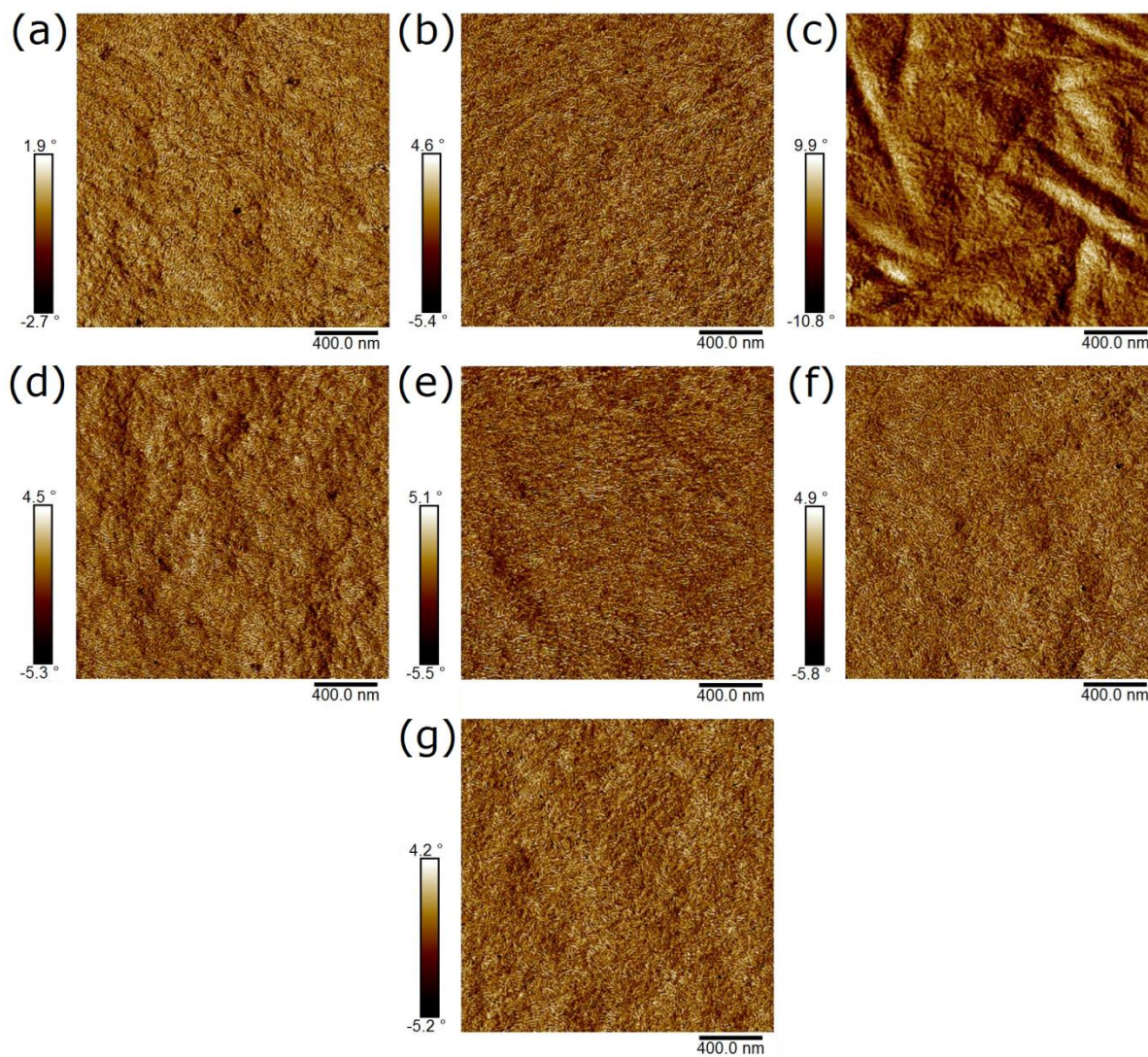


Figure S11. Phase images ($2 \times 2 \mu\text{m}$) of (a) P3HT:Cz-ECA, (b) P3HT:Cz-RH, (c) P3HT:Cz-IN, (d) P3HT:Flu-ECA, (e) P3HT:Flu-RH, (f) P3HT:Flu-IN, and (g) P3HT:PC₆₁BM films.

4. UV absorption spectra of the films

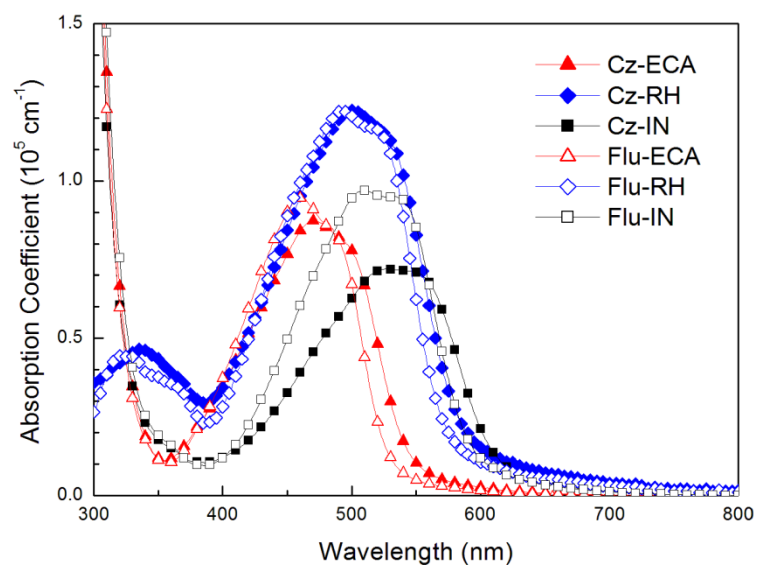


Figure S12. UV-visible absorption spectra of the films spin-coated from chloroform solution.