

## Electronic Supplementary Information (ESI)

# DPP-based small molecule, non-fullerene acceptors for “channel II” charge generation in OPVs and their improved performance in ternary cells

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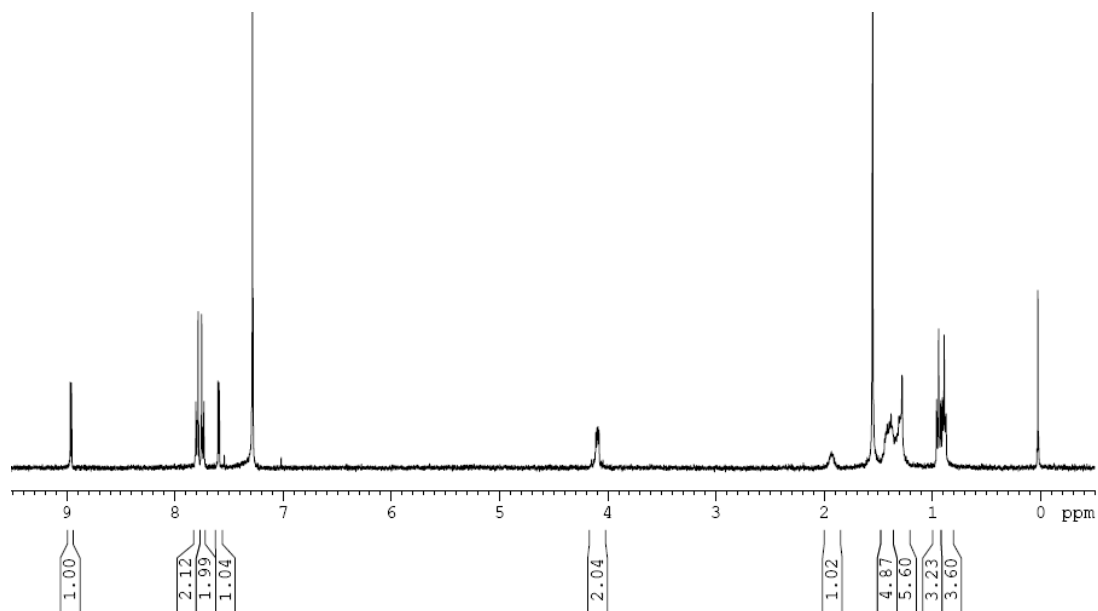
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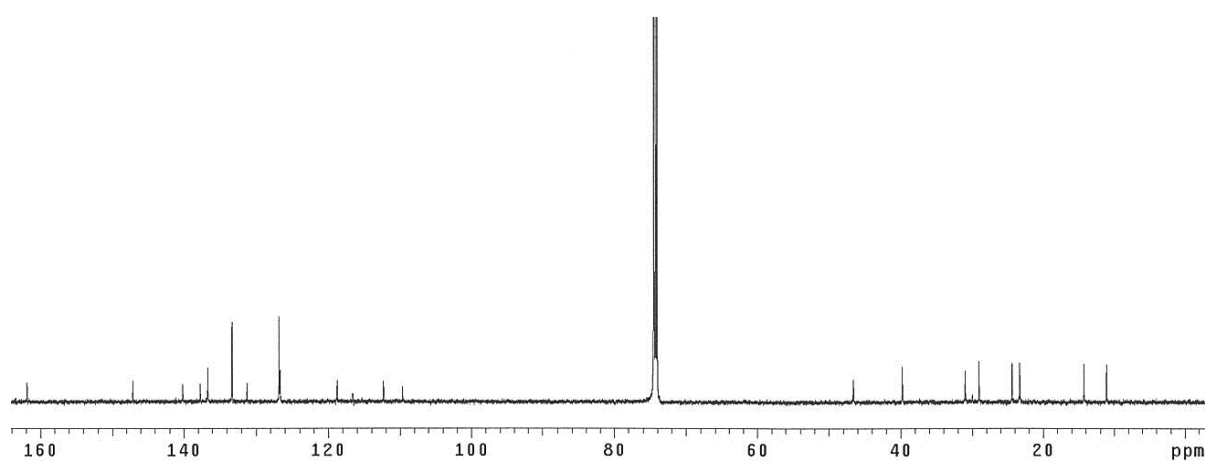
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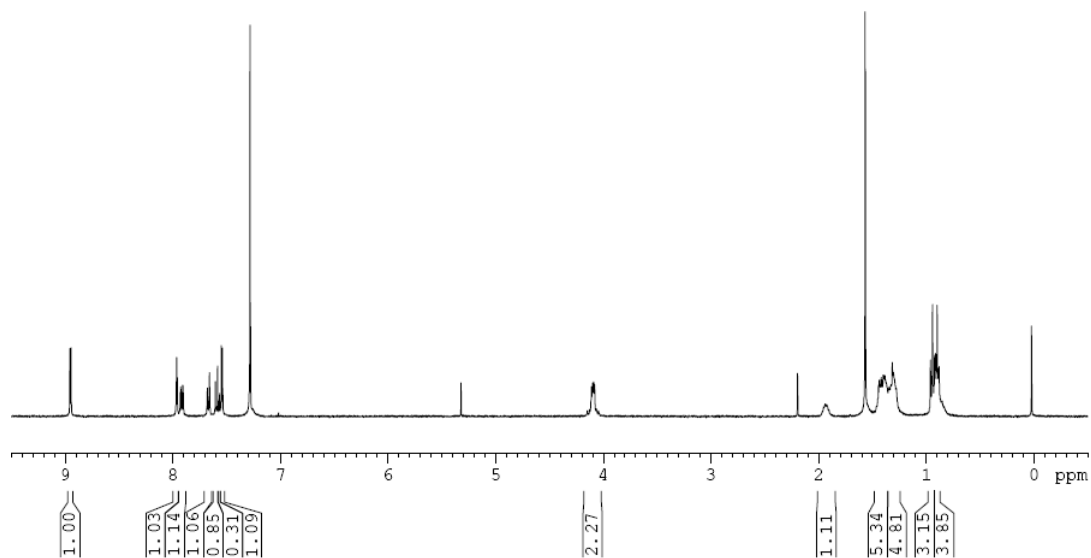
## 1. $^1\text{H}$ and $^{13}\text{C}$ NMR spectra



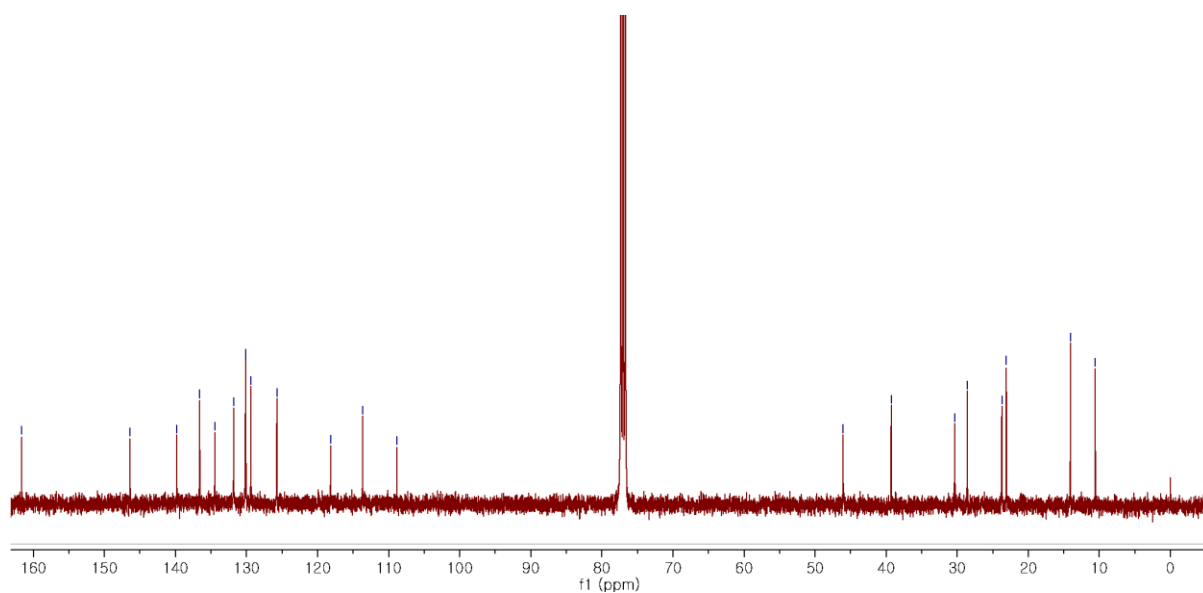
**Figure S1.**  $^1\text{H}$  NMR spectra of *p*-DPP-PhCN.



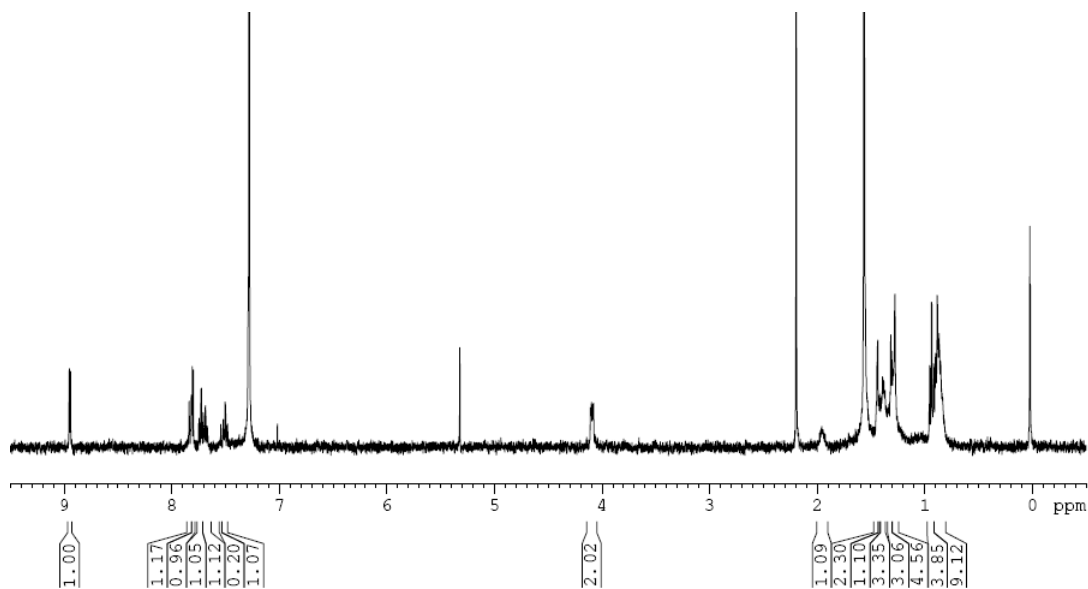
**Figure S2.**  $^{13}\text{C}$  NMR spectra of *p*-DPP-PhCN.



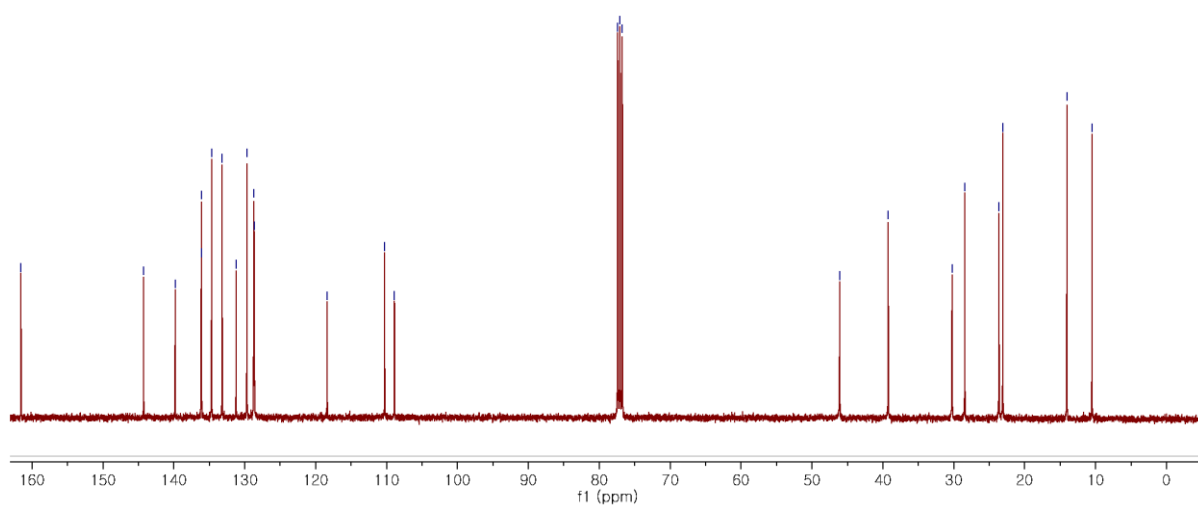
**Figure S3.**  $^1\text{H}$  NMR spectra of *m*-DPP-PhCN.



**Figure S4.**  $^{13}\text{C}$  NMR spectra of *m*-DPP-PhCN.

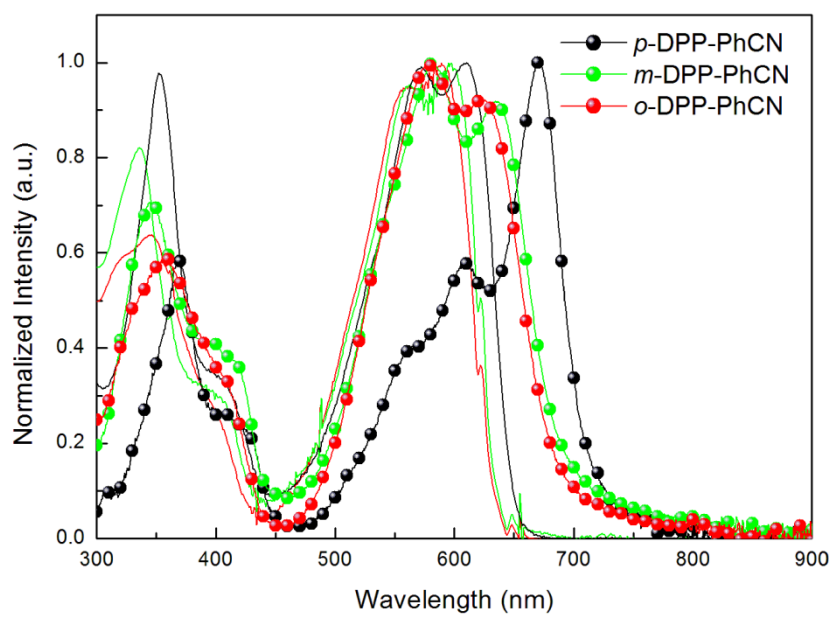


**Figure S5.**  $^1\text{H}$  NMR spectra of *o*-DPP-PhCN.



**Figure S6.**  $^{13}\text{C}$  NMR spectra of *o*-DPP-PhCN.

## 2. Normalized UV absorption spectra



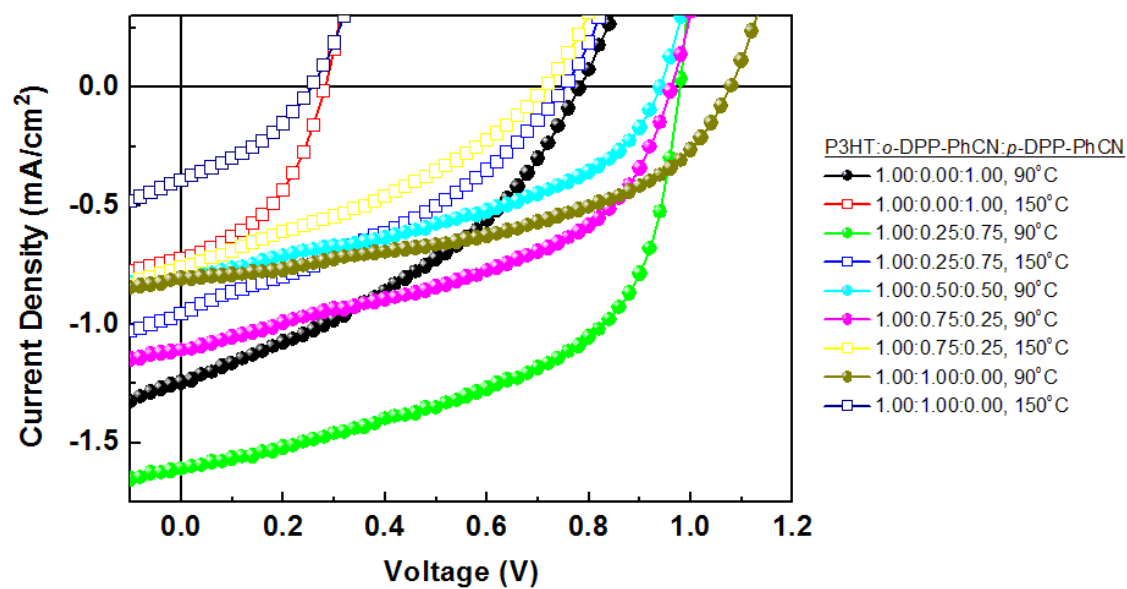
**Figure S7.** Normalized UV absorption spectra of **DPP-PhCN** acceptors in solution (solid lines) and film (symbols).

### 3. OPV characteristics

**Table S1.** Photovoltaic performances with various blend ratios and annealing temperatures <sup>a</sup>

Active layer	D/A ratio	Annealing Temp (°C)	V <sub>OC</sub> (V)	J <sub>SC</sub> (mA/cm <sup>2</sup> )	FF (%)	PCE (%)
P3HT: <i>p</i> -DPP-PhCN	1:2	90	0.59	1.52	40	0.35
		120	0.38	1.44	40	0.22
		150	0.15	0.78	37	0.04
	1:1	90	0.78	1.24	37	0.36
		120	0.56	1.64	50	0.47
		150	0.28	0.73	43	0.09
	2:1	90	0.47	1.01	49	0.23
		120	0.44	1.48	54	0.35
		150	0.24	1.18	46	0.13
P3HT: <i>m</i> -DPP-PhCN	1:2	90	0.51	0.43	29	0.06
		120	0.55	0.58	32	0.10
		150	0.32	0.30	29	0.03
	1:1	90	0.43	0.47	30	0.06
		120	0.45	0.56	31	0.08
		150	0.28	0.29	36	0.03
	2:1	90	0.45	0.36	33	0.05
		120	0.51	0.33	27	0.05
		150	0.26	0.18	35	0.02
P3HT: <i>o</i> -DPP-PhCN	1:2	90	1.09	1.14	34	0.43
		120	1.07	1.22	28	0.37
		150	0.12	0.42	32	0.02
	1:1	90	1.08	0.81	46	0.40
		120	1.09	1.19	35	0.46
		150	0.25	0.39	36	0.04
	2:1	90	1.09	0.92	44	0.44
		120	1.09	1.17	36	0.46
		150	0.58	0.82	45	0.22

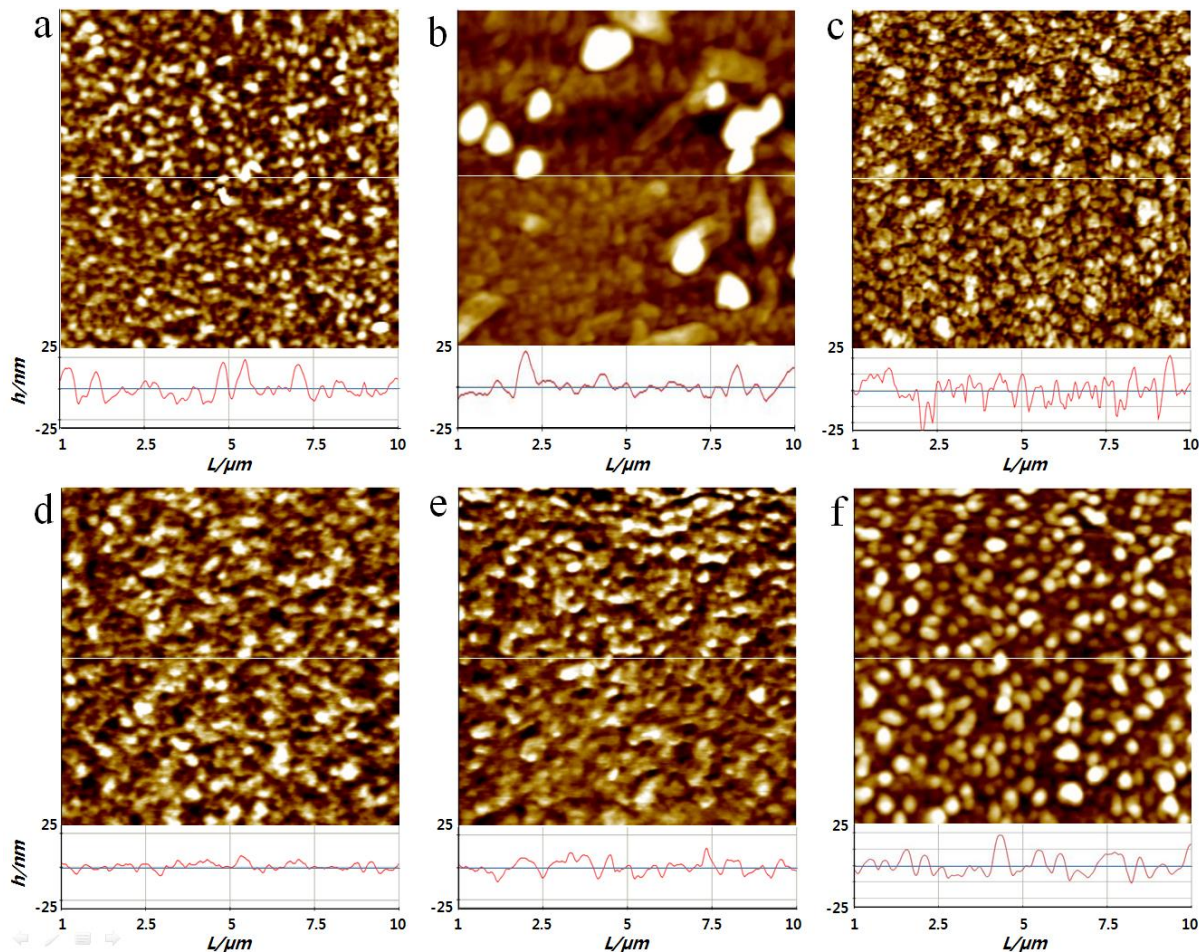
<sup>a</sup> Devices are spin-coated from a chloroform solution and annealed for 10 min



**Figure S8.**  $J$ - $V$  curves of OPV devices using chloroform as a solvent with various blend ratios and annealing temperatures.



#### 4. Atomic force microscopy (AFM) images



**Figure S9.** AFM images (10 × 10 μm) of the (a) Device I (P3HT:*p*-DPP-PhCN = 1:1, rms = 4.97 nm), (b) Device II (P3HT:*o*-DPP-PhCN:*p*-DPP-PhCN = 1:0.25:0.75, rms = 11.49 nm), (c) Device III (P3HT:*o*-DPP-PhCN:*p*-DPP-PhCN = 1:0.5:0.5, rms = 8.20 nm), (d) Device IV (P3HT:*o*-DPP-PhCN:*p*-DPP-PhCN = 1:0.75:0.25, rms = 2.95 nm), (e) Device V (P3HT:*o*-DPP-PhCN = 1:1, rms = 4.71 nm), and (f) P3HT:*o*-DPP-PhCN:*p*-DPP-PhCN = 1:0.25:0.75 (rms = 6.26 nm). The films were annealed at 120 °C (a–e) or 90 °C (f).