Supporting Info

Molecularly Engineered Thienyl-Triphenylamine Substituted Zinc Phthalocyanine as Dopant Free Hole Transporting Materials in Perovskite Solar Cells

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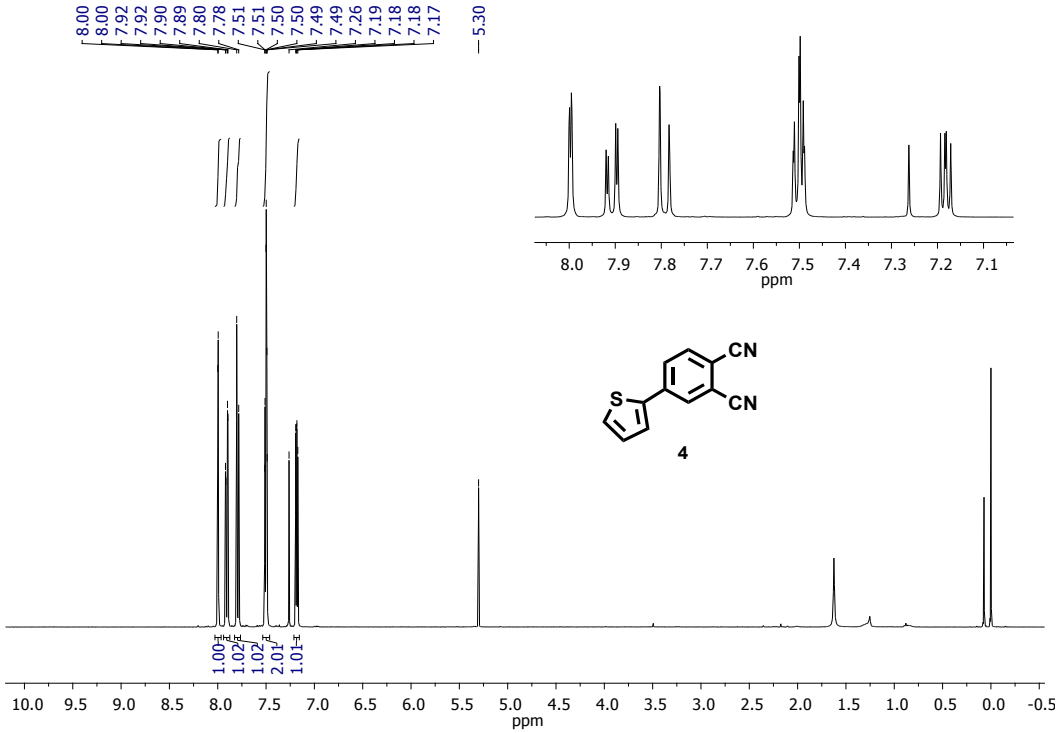

Fig. S1. ^{1}H NMR spectrum of phthalonitrile **4** in $CDCl_3$.

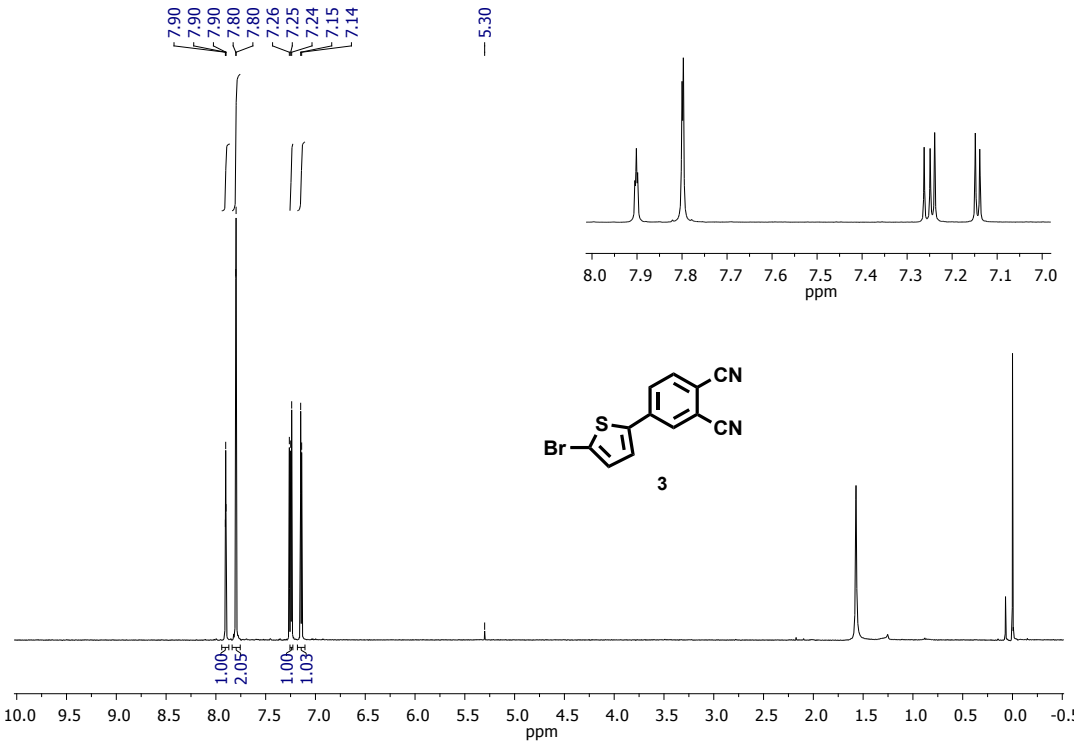

Fig. S2. ^{1}H NMR spectrum of phthalonitrile **3** in $CDCl_3$.

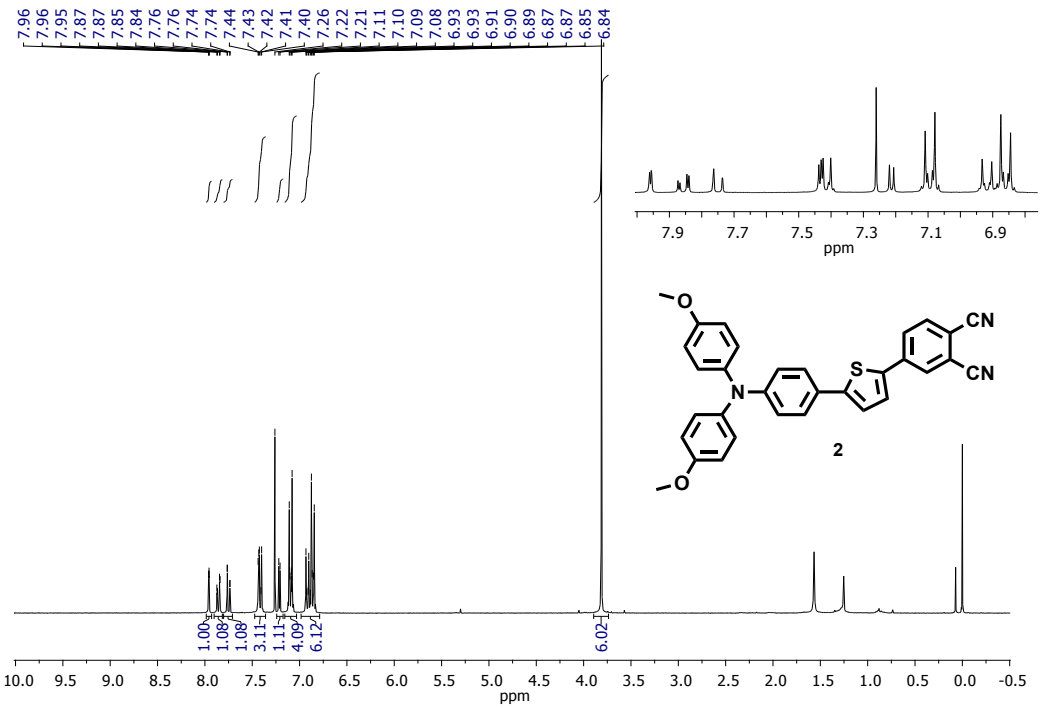

Fig. S3. ^{1}H NMR spectrum of phthalonitrile **2** in $CDCl_3$.

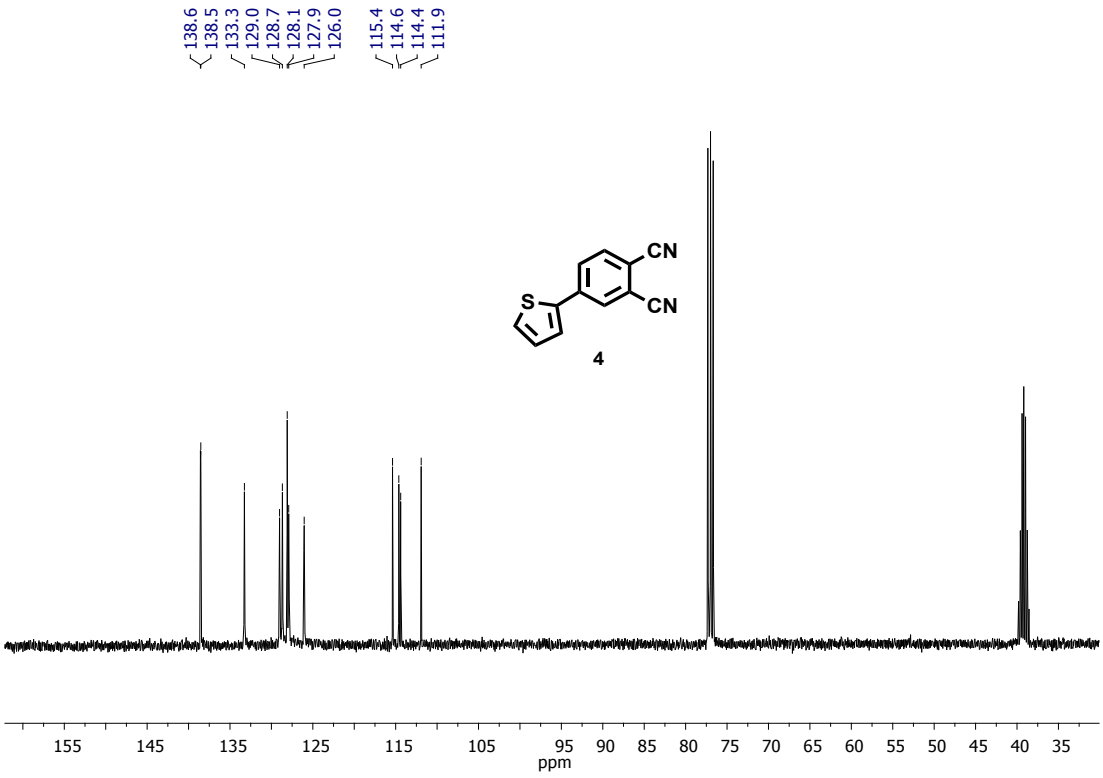

Fig. S4. ^{13}C NMR spectrum of phthalonitrile **4** in $CDCl_3$ + DMSO-d_6.

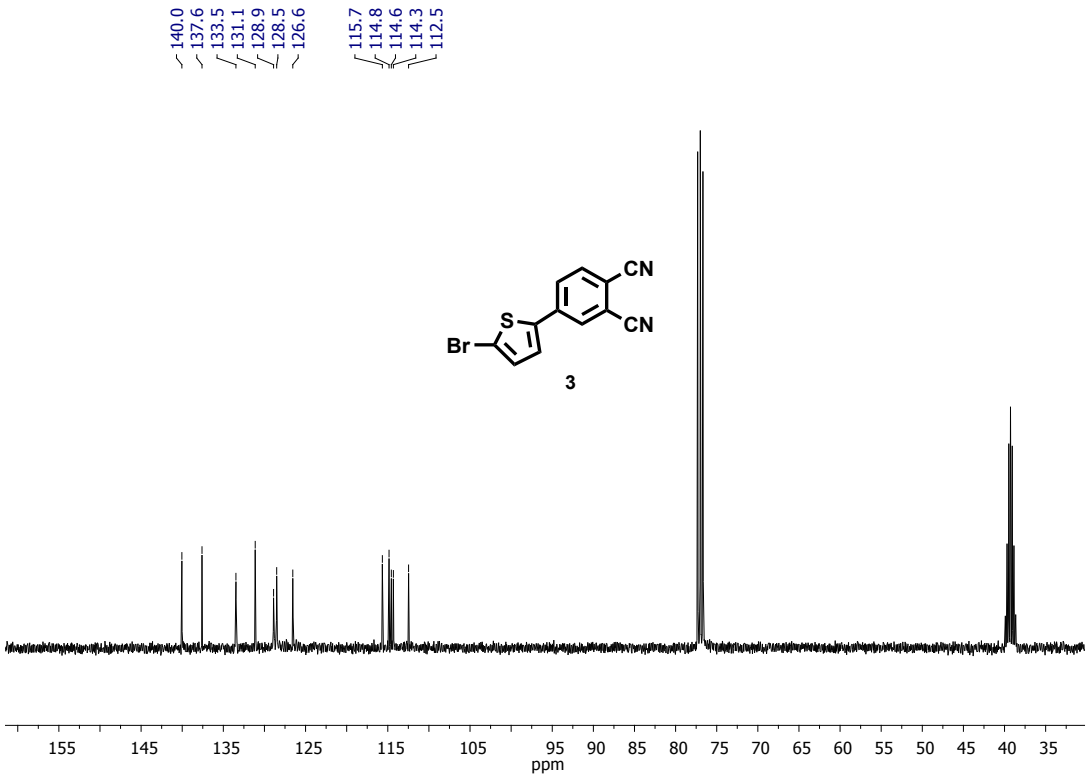

Fig. S5. ^{13}C NMR spectrum of phthalonitrile **3** in $CDCl_3$ + DMSO-d_6.

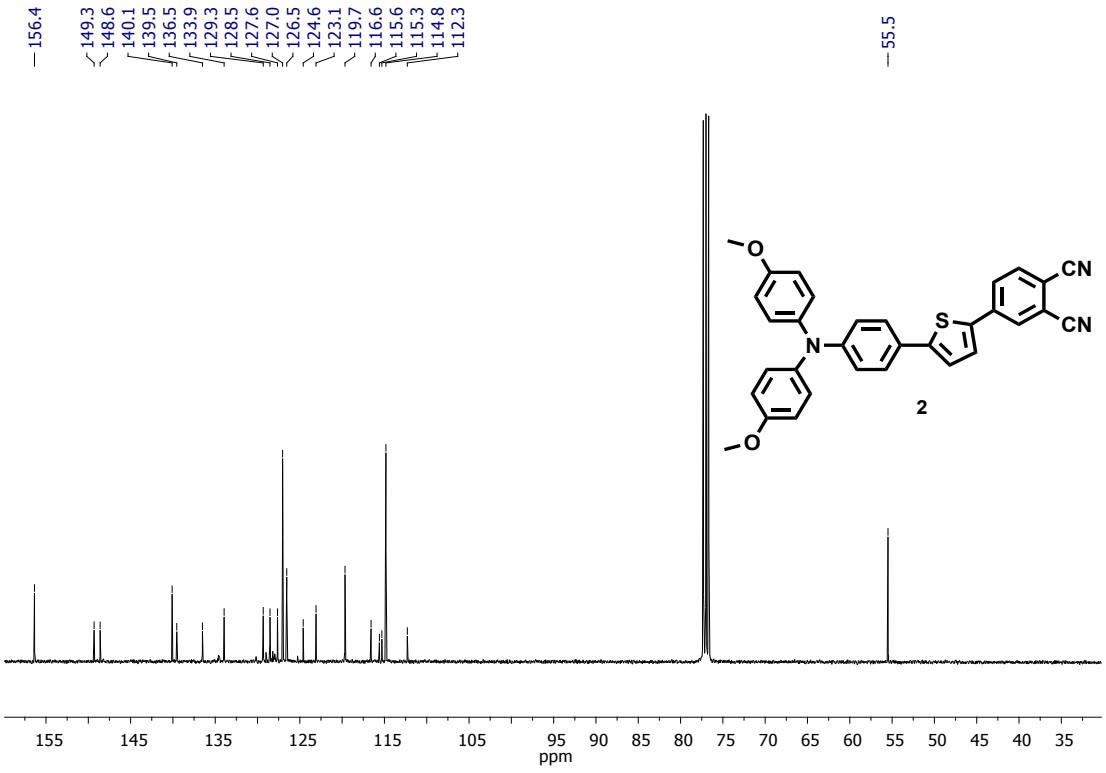

Fig. S6. ^{13}C NMR spectrum of phthalonitrile **2** in $CDCl_3$.

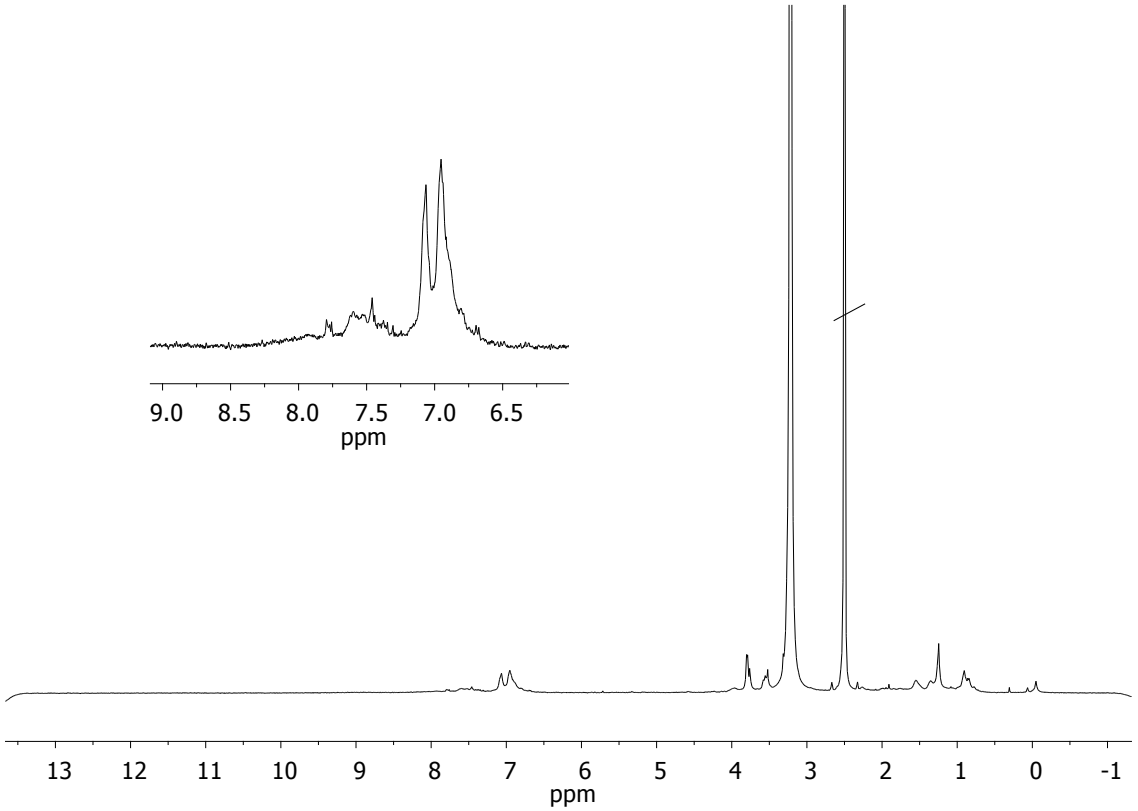

Fig. S7. ^{1}H NMR spectrum of **ZnTPPc** in DMSO-d_6

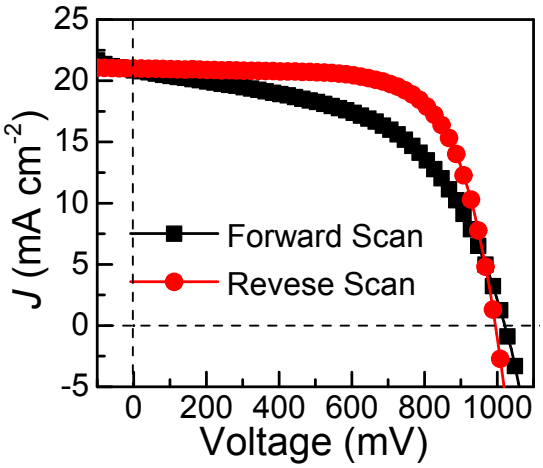

Fig. S8 *J-V* curves of forward and reverse scans under simulated AM 1.5G illumination for the ZnTPPc-based PSC.

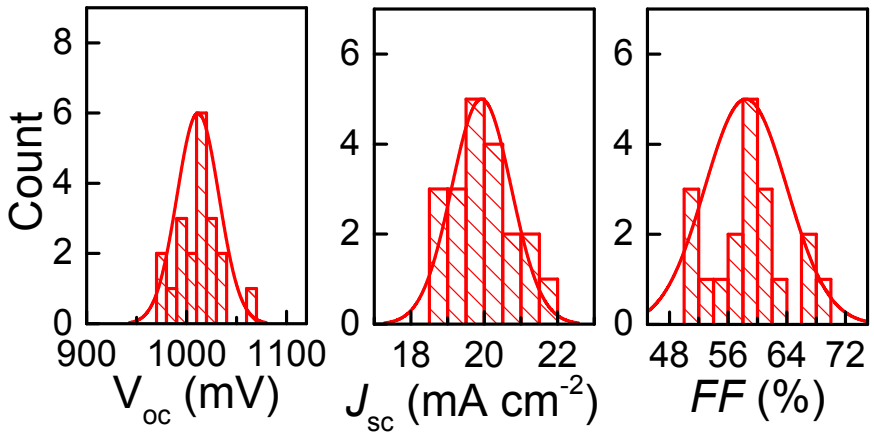

Fig. S9 Histograms of V_{OC}, J_{SC} and FF of PSCs with ZnTPPc as an HTM. The data was analysed from 20 cells.

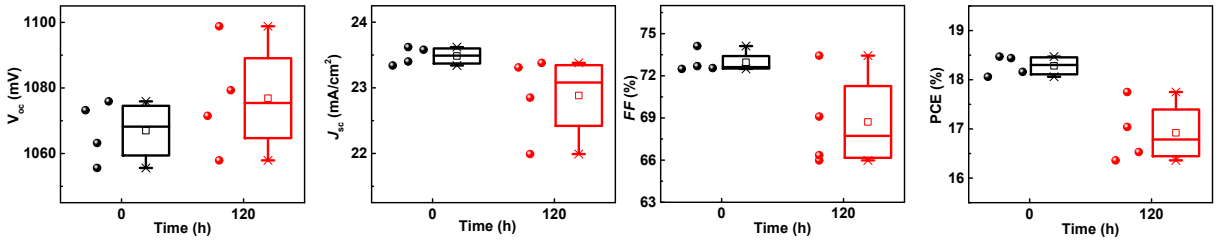

Fig. S10 Statistical box plots of the photovoltaic performance parameters of devices using doped Spiro-OMeTAD vs different storage time.

Table S1 Device performance parameters for the ZnTPPc-based PSC under forward and reverse scans.

Scan direction	V_{oc} (mV)	J_{sc} (mA cm^{-2})	FF (%)	PCE (%)
Forward	994.3	21.0	69.42	14.50
Reverse	1.020	20.91	53.18	11.34
Average	1006.9	20.96	61.3	12.92

Table S2 Average values of device performance parameters of PSCs with different HTMs measured at the different aging time. ZnPPC in its pristine form, while Spiro-OMeTAD is in doped state.

HTM	Time (h)	V_{oc} (mV)	J_{sc} (mA cm^{-2})	FF (%)	PCE (%)
ZnTPPc	0	1018.6±14.6	19.71±0.71	59.15±2.62	11.89±0.98
ZnTPPc	432	1032.2±16.6	19.74±0.94	58.99±2.24	11.92±0.88
Spiro-OMeTAD	0	1068.0±9.3	23.49±0. 14	72.96±0.78	18.28±0.21
Spiro-OMeTAD	120	1076.9±17.1	22.88±0.64	68.72±3.45	16.92±0.62

Table S3 Device performance parameters of PSCs with **ZnTTPc** measured at the different aging time.

Time (h)	No	V_{oc} (mV)	J_{sc} (mA cm^{-2})	FF (%)	PCE (%)
0	1	1027.2	20.99	60.00	12.94
0	2	1034.2	19.80	60.21	12.33
0	3	1041.9	20.29	60.85	12.86
360	1	1019.1	20.25	59.79	12.33
360	2	1018.1	19.37	60.17	11.87
360	3	1025.3	19.83	58.30	11.85
3360	1	1025.8	20.82	54.76	11.70
3360	2	986.8	19.07	57.14	10.75
3360	3	1008.6	20.52	54.38	11.26