Supporting information for:

Pyrazolium Based Electrolyte for Solid-State Dye-Sensitized Solar Cells with High Fill Factor and Open-Circuit Voltage

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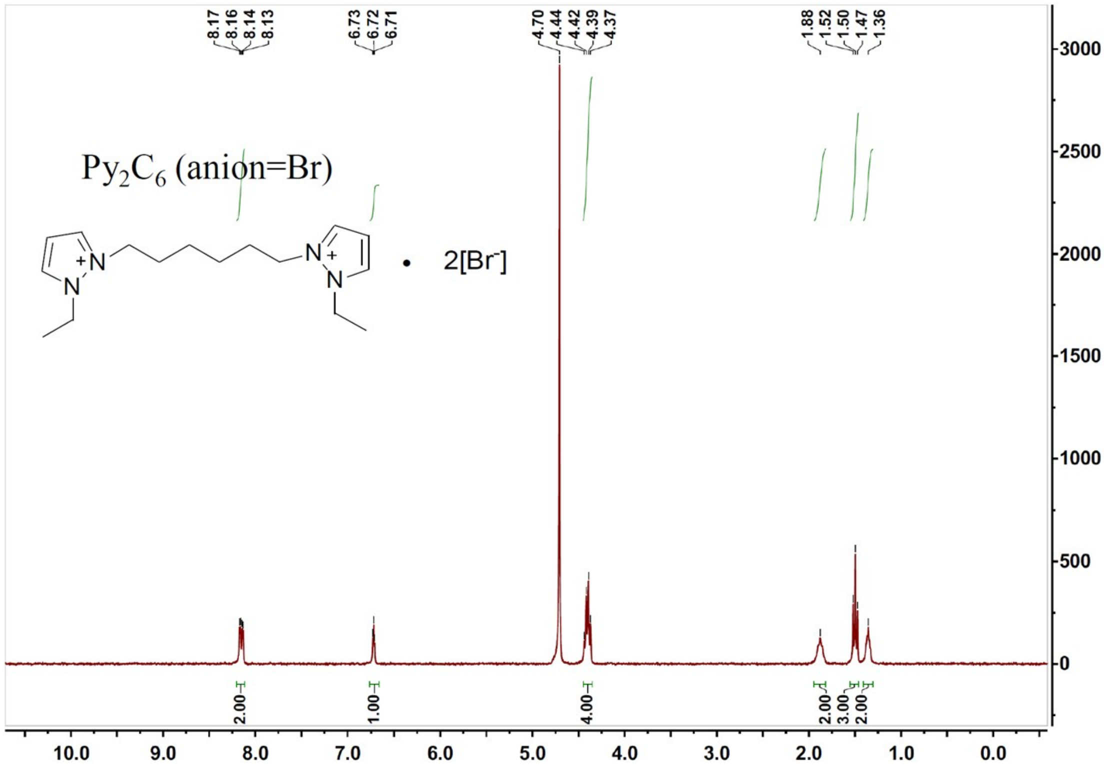
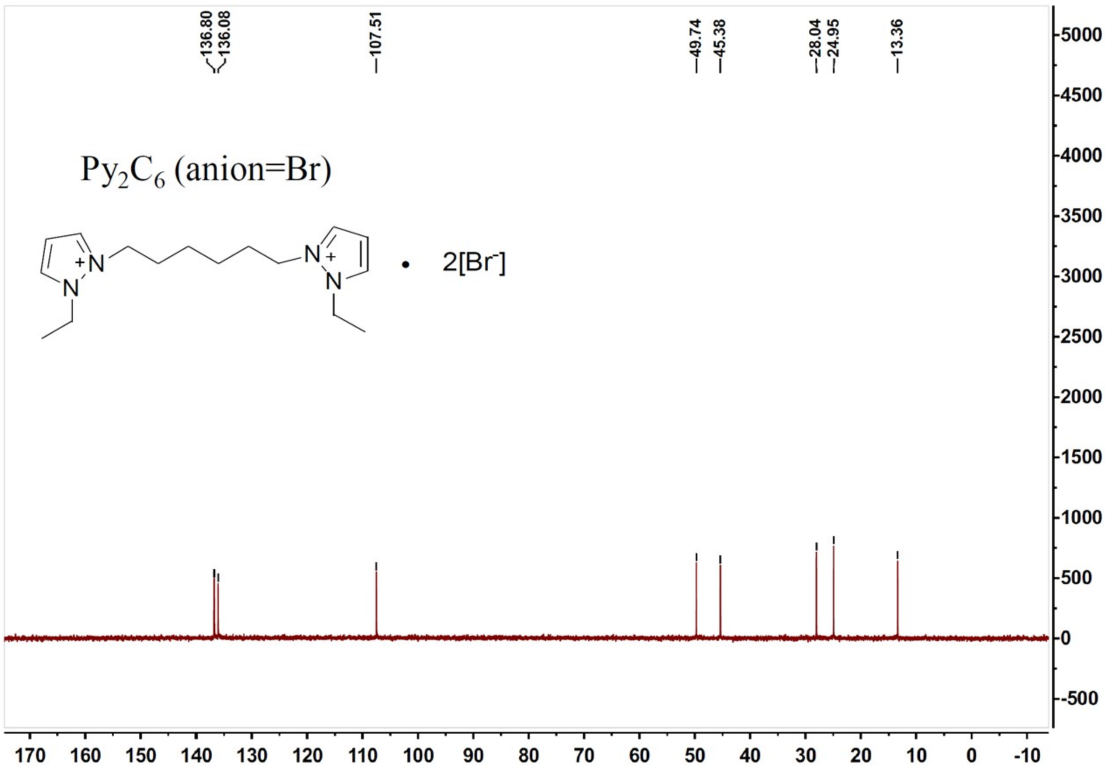
Part 1 ^{1}H NMR, ^{13}C NMR and ESI - MS of Py_nC_6 (*n* = 2, 1; anion = Br) (Fig. S1 – S2).

Fig. S1 Py_2C_6 (anion = Br) ^{1}H NMR (300 MHz, D_2O) δ 8.15 (dd, *J* = 8.4, 2.8 Hz, 2H), 6.72 (t, *J* = 2.9 Hz, 1H), 4.40 (dd, *J* = 13.8, 6.7 Hz, 4H), 1.88 (s, 2H), 1.50 (t, *J* = 7.3 Hz, 3H), 1.36 (s, 2H). ^{13}C NMR (101 MHz, D_2O) δ 136.80, 136.08, 107.51, 49.74, 45.38, 28.04, 24.95, 13.36. MS Calculated for $C_{16}H_{28}BrN_4$ (m/z): 355.1493, Found: 355.1492.





Display Report

Analysis Info

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Sample Name	hetong	Instrument	maXis 10103
Comment			

Acquisition Parameter

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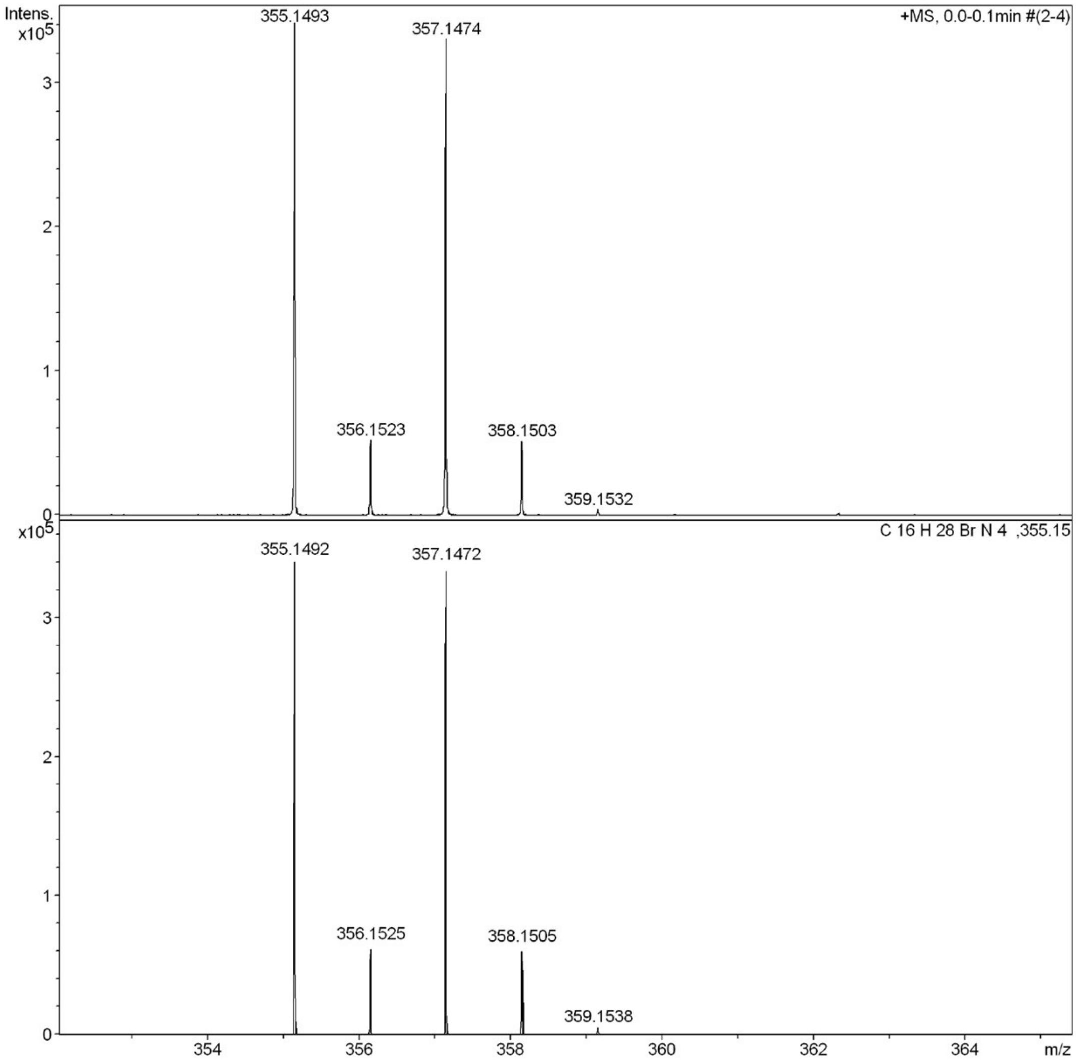
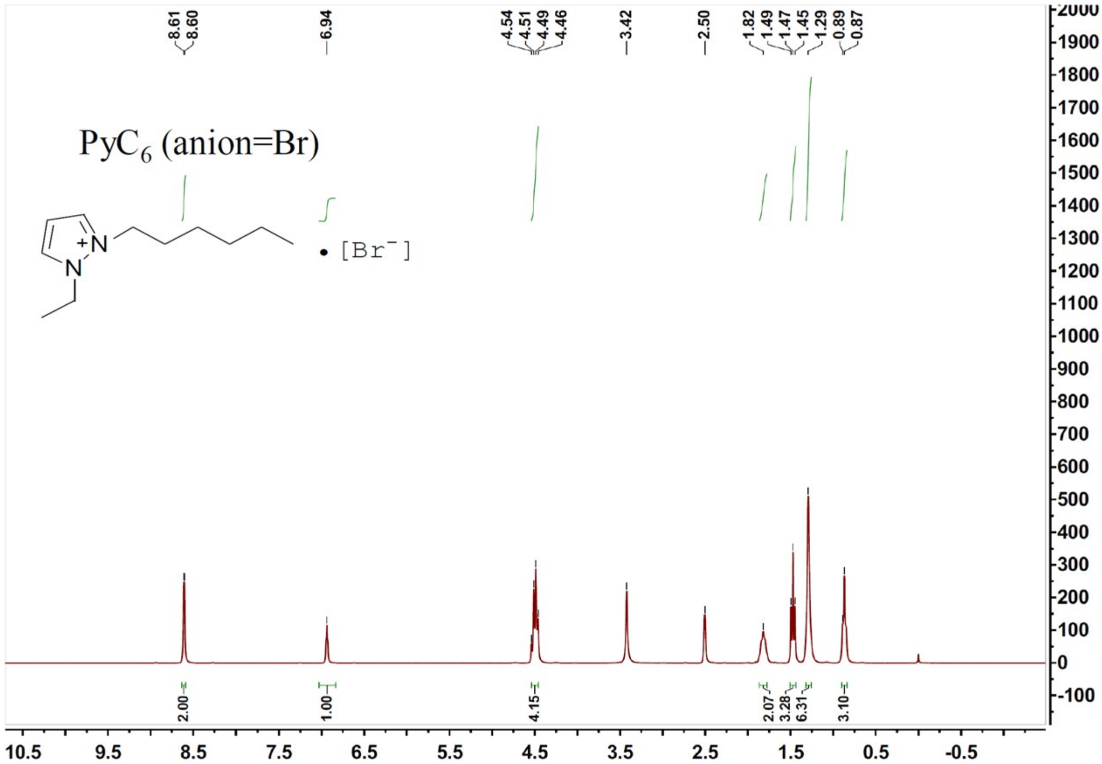
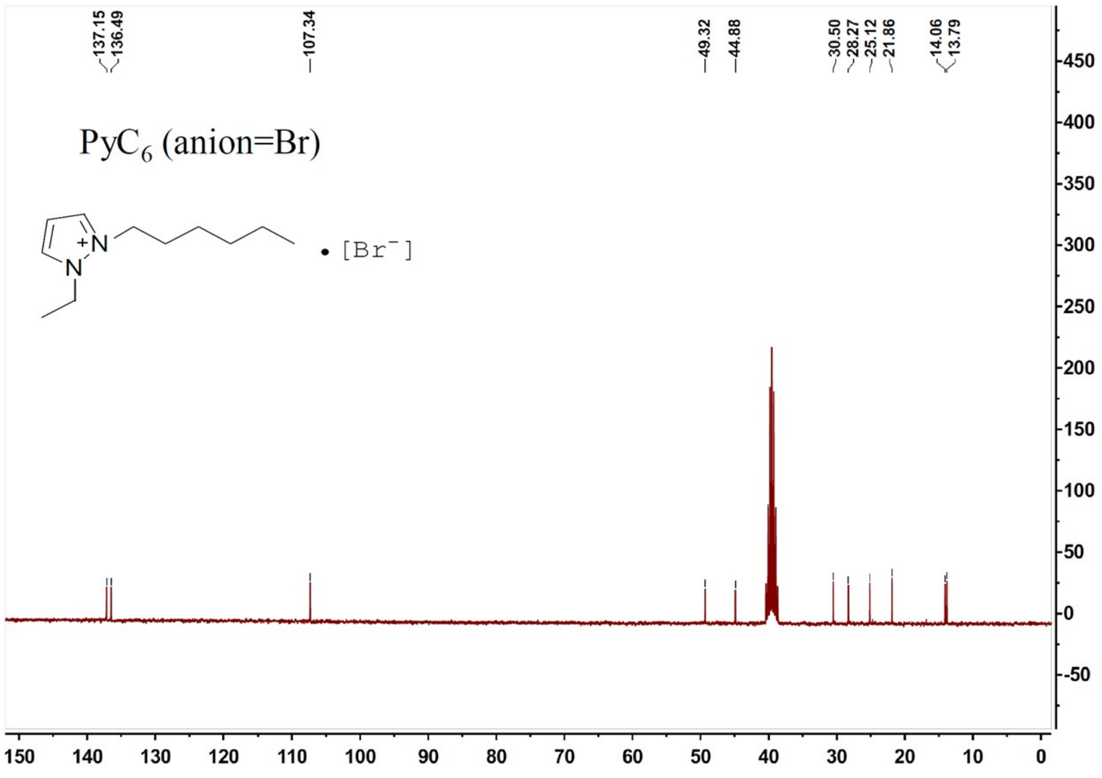


Fig. S2 PyC_6·(anion = Br) [1]H NMR (400 MHz, DMSO) δ 8.61 (d, J = 2.2 Hz, 2H), 6.94 (s, 1H), 4.50 (q, J = 8.0 Hz, 4H), 1.82 (s, 2H), 1.47 (t, J = 7.1 Hz, 3H), 1.29 (s, 6H), 0.88 (d, J = 6.0 Hz, 3H). ^{13}C NMR (101 MHz, DMSO) δ 137.15, 136.49, 107.34, 49.32, 44.88, 30.50, 28.27, 25.12, 21.86, 14.06, 13.79. MS Calculated for $C_{11}H_{21}N_2$ (m/z): 181.1698, Found: 181.1699.





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Sample Name	hetong	Instrument	maXis 10103
Comment			

Acquisition Parameter

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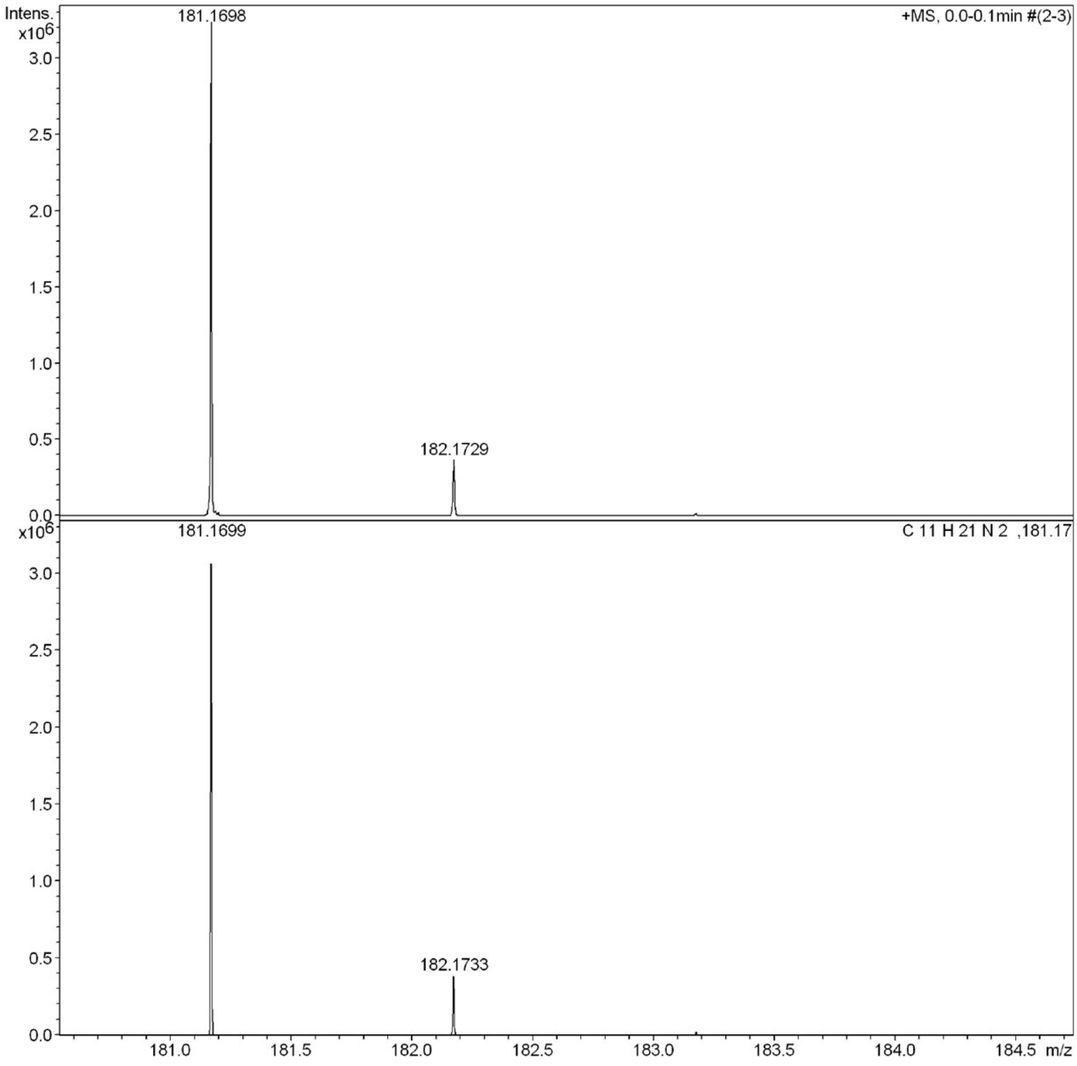
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	200.0 Vpp	Set Divert Valve	Waste



Part 2 ^{1}H NMR of Py_nC_6 (n = 2, 1) (Fig. S3 – S4).

Fig. S3 Py_2C_6 ^{1}H NMR (400 MHz, D_2O) δ 8.14 (dd, J = 8.2, 2.7 Hz, 2H), 6.71 (t, J = 3.0 Hz, 1H), 4.39 (dd, J = 13.8, 6.6 Hz, 4H), 1.87 (s, 2H), 1.49 (t, J = 7.3 Hz, 3H), 1.35 (t, J = 7.4 Hz, 2H).

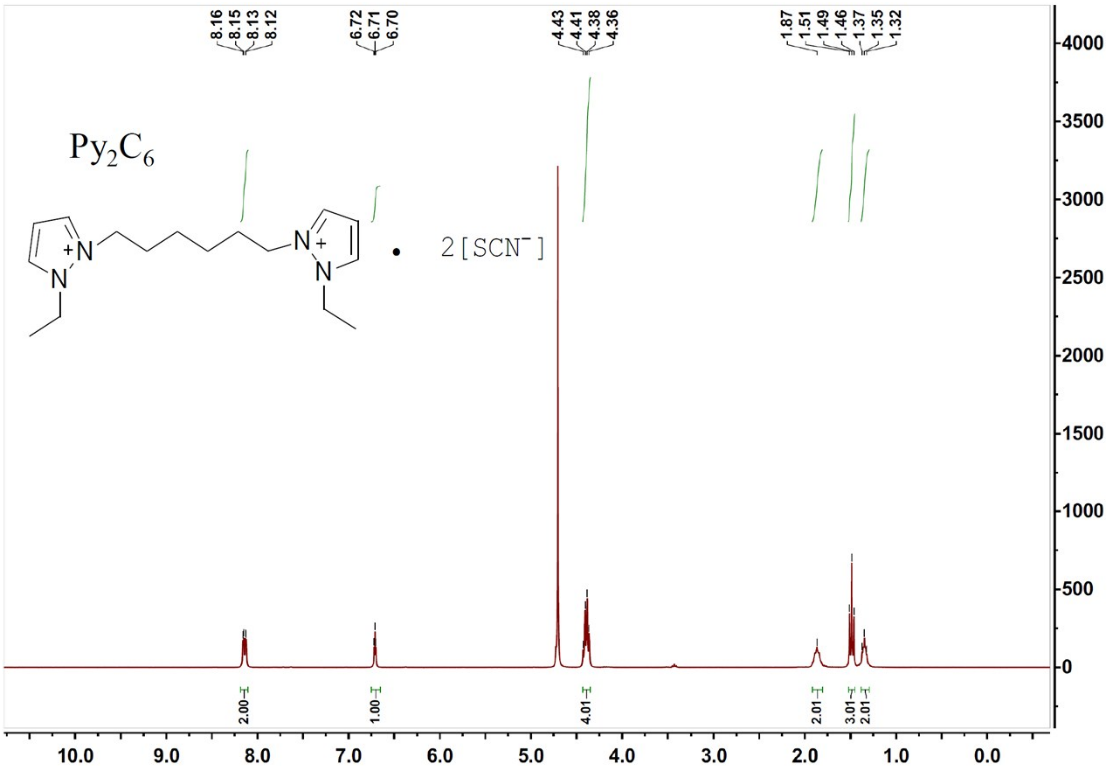
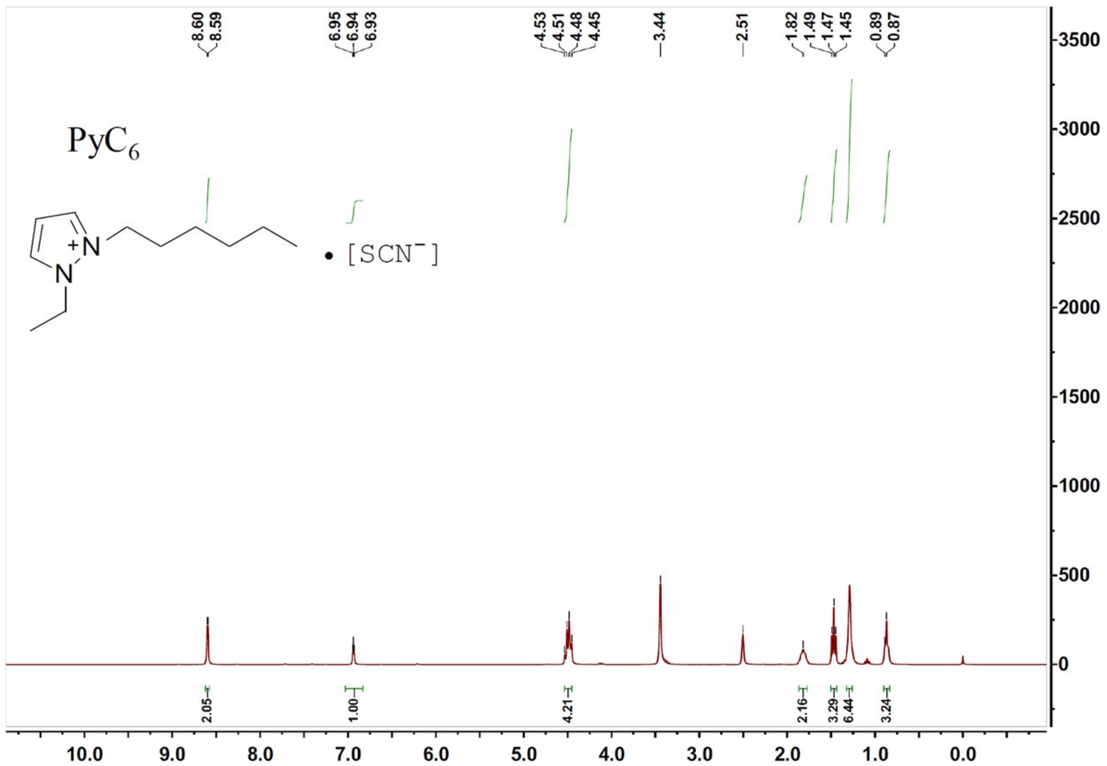


Fig. S4 PyC_6 ^{1}H NMR (400 MHz, DMSO) δ 8.60 (d, J = 2.5 Hz, 2H), 6.94 (t, J = 2.6 Hz, 1H), 4.53 – 4.45 (m, 4H), 1.82 (s, 2H), 1.47 (t, J = 7.2 Hz, 3H), 1.29 (s, 6H), 0.88 (d, J = 6.3 Hz, 3H).



Part3 IR spectra for Py_nC_6 (n = 2, 1; anion = Br) and Py_nC_6 (n = 2, 1) (Fig. S5).

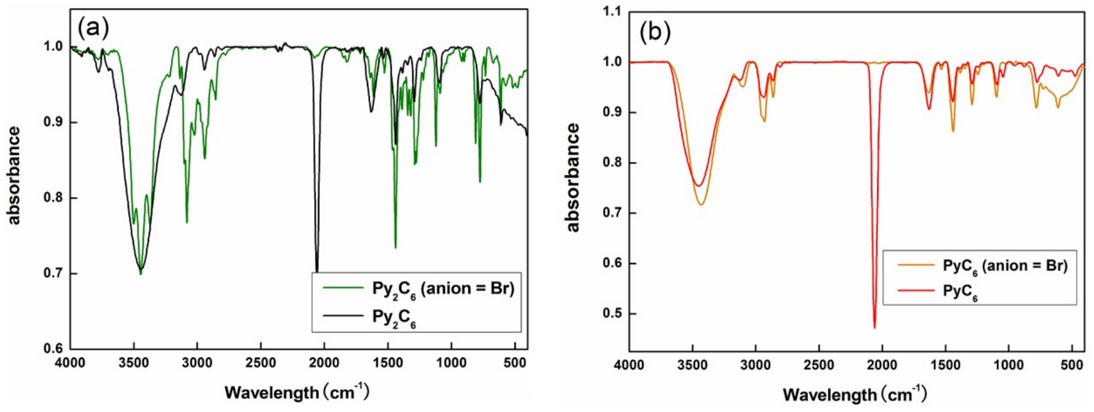


Fig. S5 IR spectra for (a) Py_2C_6 (anion = Br) and Py_2C_6, (b) PyC_6 (anion = Br) and PyC_6, In the IR spectra, 2070cm^{-1} is the characteristics absorption peak of the stretching vibration for SCN^-.[1]This suggests the success of the anion exchange.

Part 4 XRD patterns for Py_nC_6 (n = 2, 1; anion = Br) and Py_nC_6 (n = 2, 1) (Fig. S6).

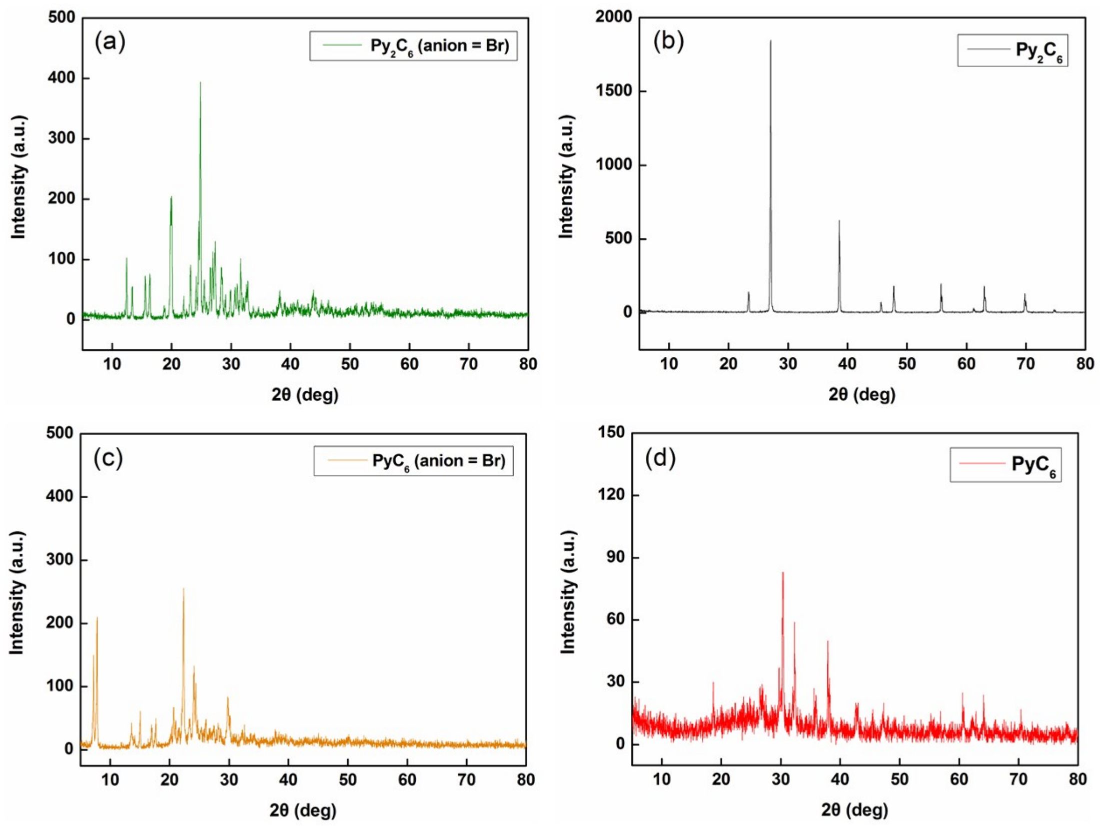


Fig. S6 XRD patterns for (a) Py_2C_6 (anion = Br), (b) Py_2C_6, (c) PyC_6 (anion = Br) and (d) PyC_6.

Part 5 The thermal gravimetric analysis (TGA, 5% weight loss) and differential scanning calorimeter (DSC) for Py_nC_6 (n = 2, 1; anion = Br) and Py_nC_6 (n = 2, 1) (Fig. S7 – S8).

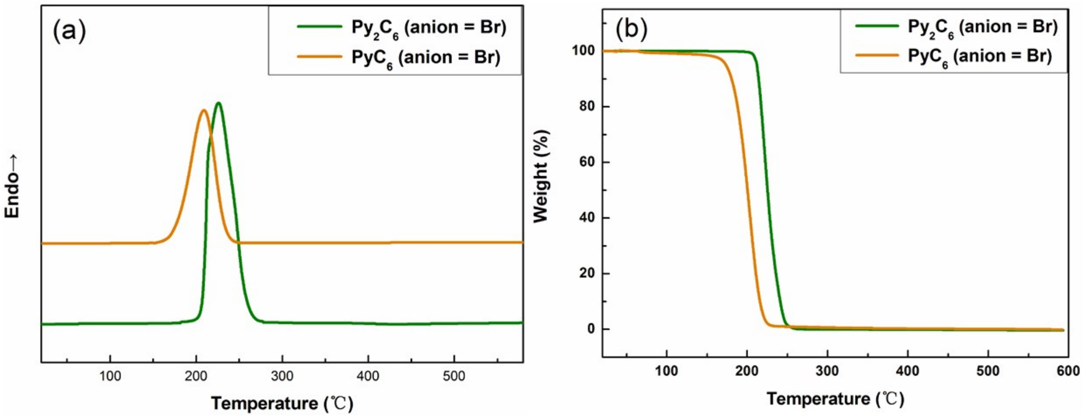


Fig. S7 (a) DSC curves and (b) TGA curves of a series of Py_nC_6 (n = 2, 1; anion = Br).

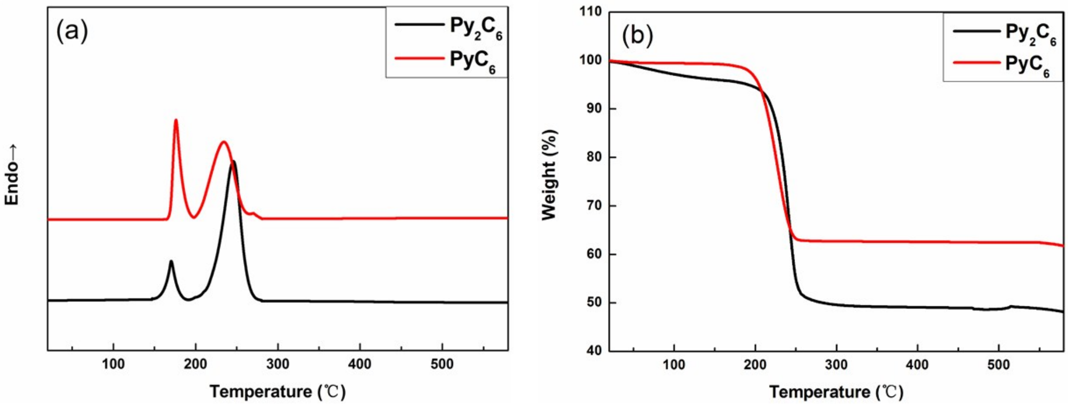


Fig. S8 (a) DSC curves and (b) TGA curves of a series of Py_nC_6 (n = 2, 1).

Part 5 Cyclic voltammetry (CV) for Py_2C_6, PyC_6 and PMII electrolytes using symmetrical Pt electrode.

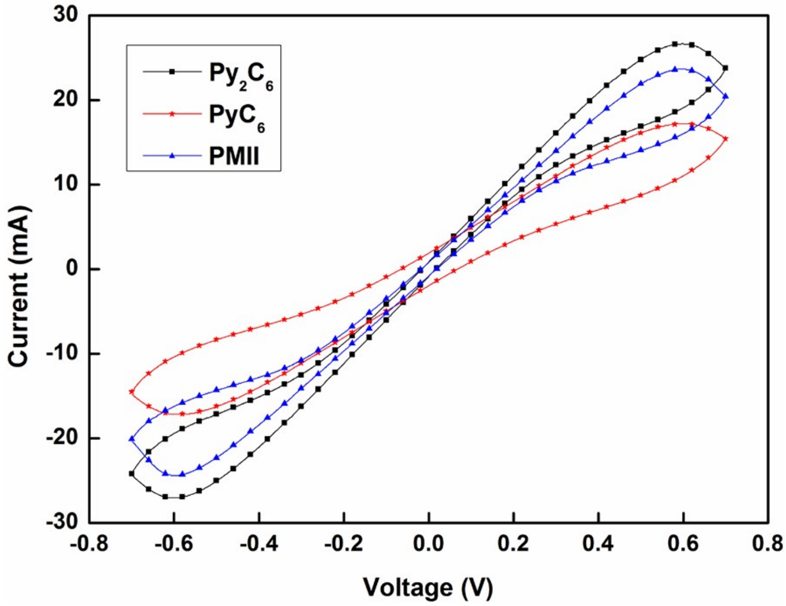


Fig. S9 Cyclic voltammetry (CV) using symmetrical Pt electrode sandwiched with Py_2C_6, PyC_6 and PMII electrolytes at a scan rate of 100mV/s.

Part 6 DSSC devices of equivalent circuit models

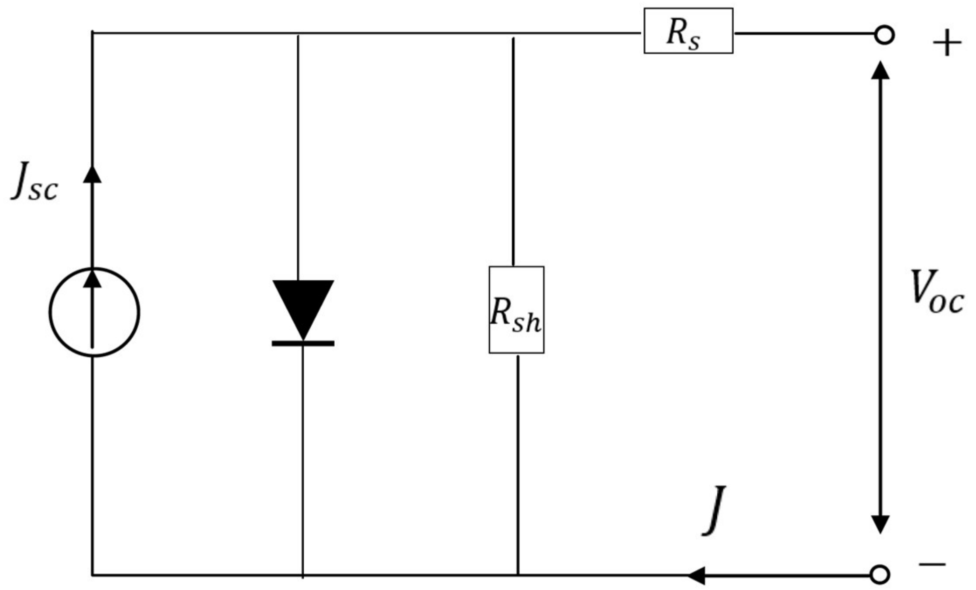


Fig. S10 DSSC devices were conducted by the equivalent circuit models, and a p-n junction solar cell can be simulated with an ideal diode, series resistance R_s, and shunt resistance R_{sh}.

Part 7 Long-term Stability of DSSC (Fig. S11), equivalent circuit (Fig. S12) (Table S1)

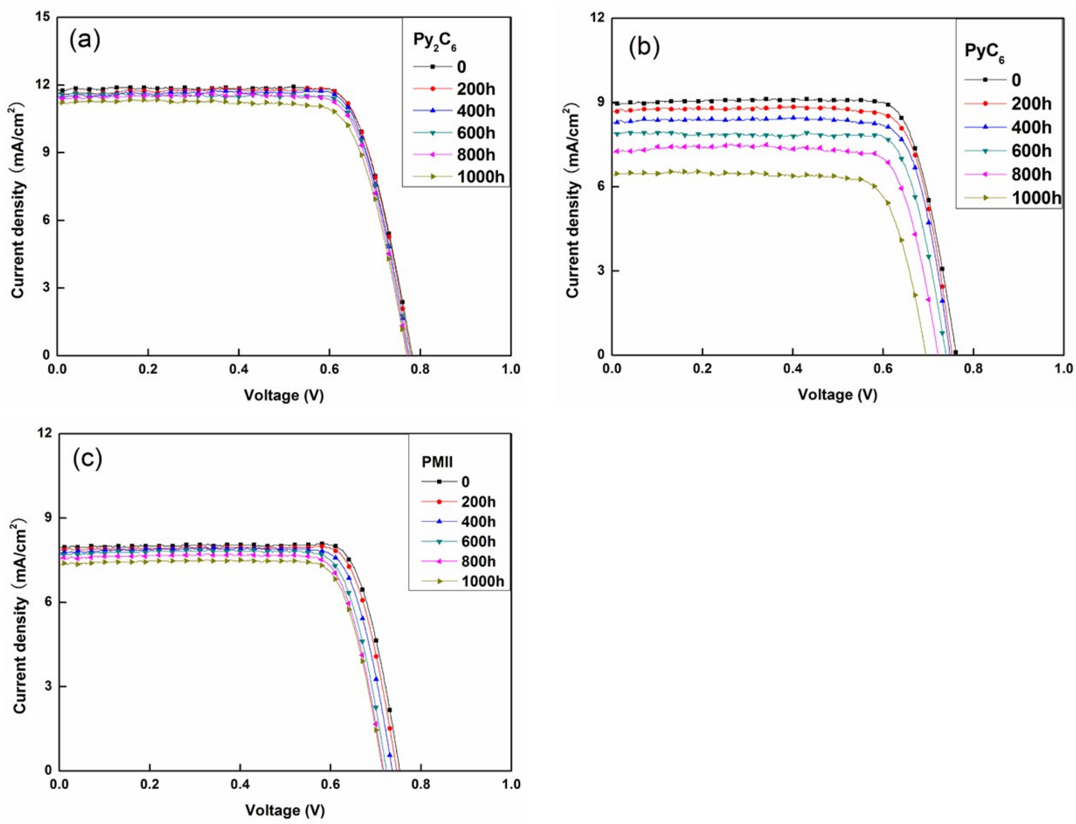


Fig. S11 *J-V* curves of part time based on (a) Py_2C_6, (b) PyC_6 and (c) PMII electrolytes.

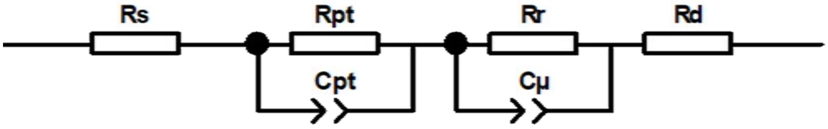


Fig. S12 Equivalent circuit deduced from EIS curves.

Table S1 Stability of DSSC based on (a) Py_2C_6, (b) PyC_6 and (c) PMII electrolytes.

	Time (h)	0	100	200	300	400	500	600	700	800	900	1000
Py_2C_6	J_{sc} (mA/cm^2)	11.78	11.76	11.64	11.63	11.60	11.61	11.61	11.44	11.43	11.36	11.24
	V_{oc} (V)	0.779	0.779	0.778	0.778	0.776	0.776	0.775	0.775	0.773	0.772	0.771
	FF (%)	79.55	79.36	79.40	79.35	79.21	78.70	78.58	78.28	78.21	78.22	77.20
	PCE (%)	7.30	7.27	7.19	7.18	7.13	7.09	7.07	6.94	6.91	6.86	6.69
PyC_6	J_{sc} (mA/cm^2)	8.99	8.89	8.74	8.54	8.32	8.26	7.98	7.47	7.36	7.08	6.52
	V_{oc} (V)	0.766	0.762	0.755	0.751	0.751	0.747	0.741	0.728	0.721	0.713	0.696
	FF (%)	79.43	80.16	79.86	79.36	79.22	79.09	79.15	79.07	78.58	77.46	77.35
	PCE (%)	5.47	5.43	5.27	5.09	4.95	4.88	4.68	4.30	4.17	3.91	3.51
PMII	J_{sc} (mA/cm^2)	7.97	7.97	7.89	7.82	7.80	7.75	7.72	7.66	7.57	7.49	7.38
	V_{oc} (V)	0.754	0.752	0.749	0.743	0.739	0.732	0.727	0.720	0.720	0.719	0.717
	FF (%)	81.71	81.59	81.39	80.89	80.67	80.56	80.36	79.78	80.54	79.85	79.75
	PCE (%)	4.91	4.89	4.81	4.70	4.65	4.57	4.51	4.40	4.39	4.30	4.22

Reference

1 Ganesan, K.; Ratke, L. Facile Preparation of Monolithic κ-Carrageenan Aerogels. *Soft Matter* **2014**, *10*, 3218-3224.