Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A

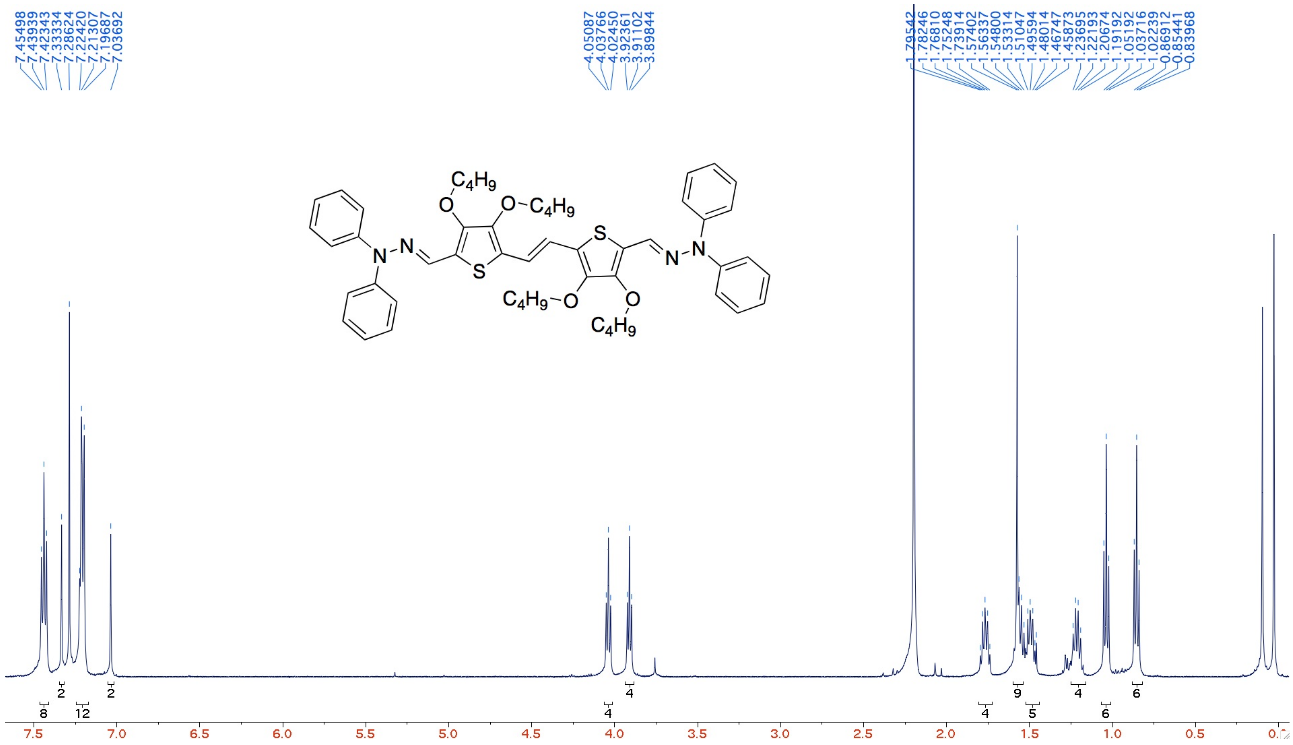
Hydrazone end capped molecular donors for Bulk Heterojunction solar cells. Open Circuit Voltage tuning through molecular design.

Mauro Sassi,[a] Maurizio Crippa,[a] Riccardo Ruffo,[a] Riccardo Turrisi,[a] Martin Drees,[b] Upendra K. Pandey,[c] Roberto Termine,[c] Attilio Golemme,[c] Antonio Facchetti[b] and Luca Beverina[a]*

[a] Department of Materials Science and INSTM, University of Milano-Bicocca, Via Cozzi 53, I-20125 Milano, Italy. [b] Polyera Corporation, 8045 Lamon Avenue, Suite 140 ,Skokie, IL 60077. [c] Centro di Eccellenza CEMIF.CAL, LASCAMM CR-INSTM, CNR-IPCF UOS CS - LiCryL, Dipartimento di Chimica, Università della Calabria, 87036 Rende, Italy.

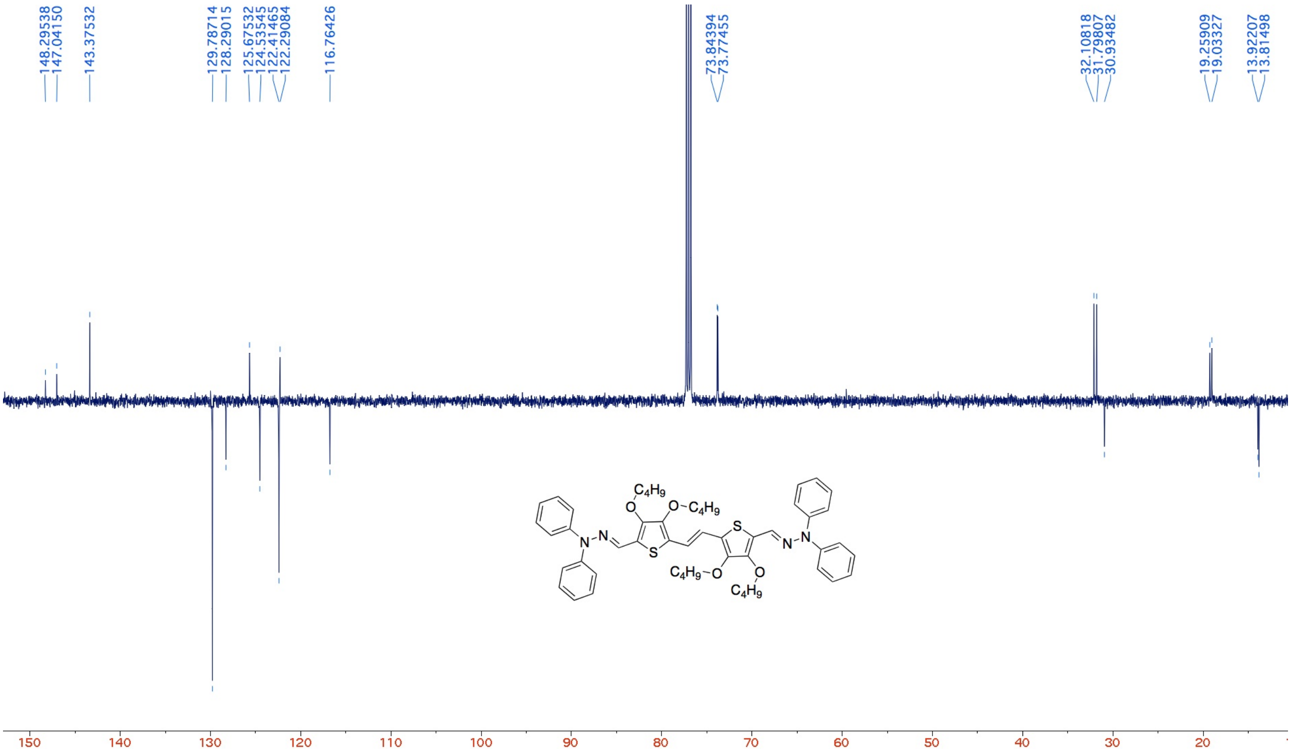
Supporting information.

1. ^{1}H NMR of Derivative **1** (500 MHz, $CDCl_3$)



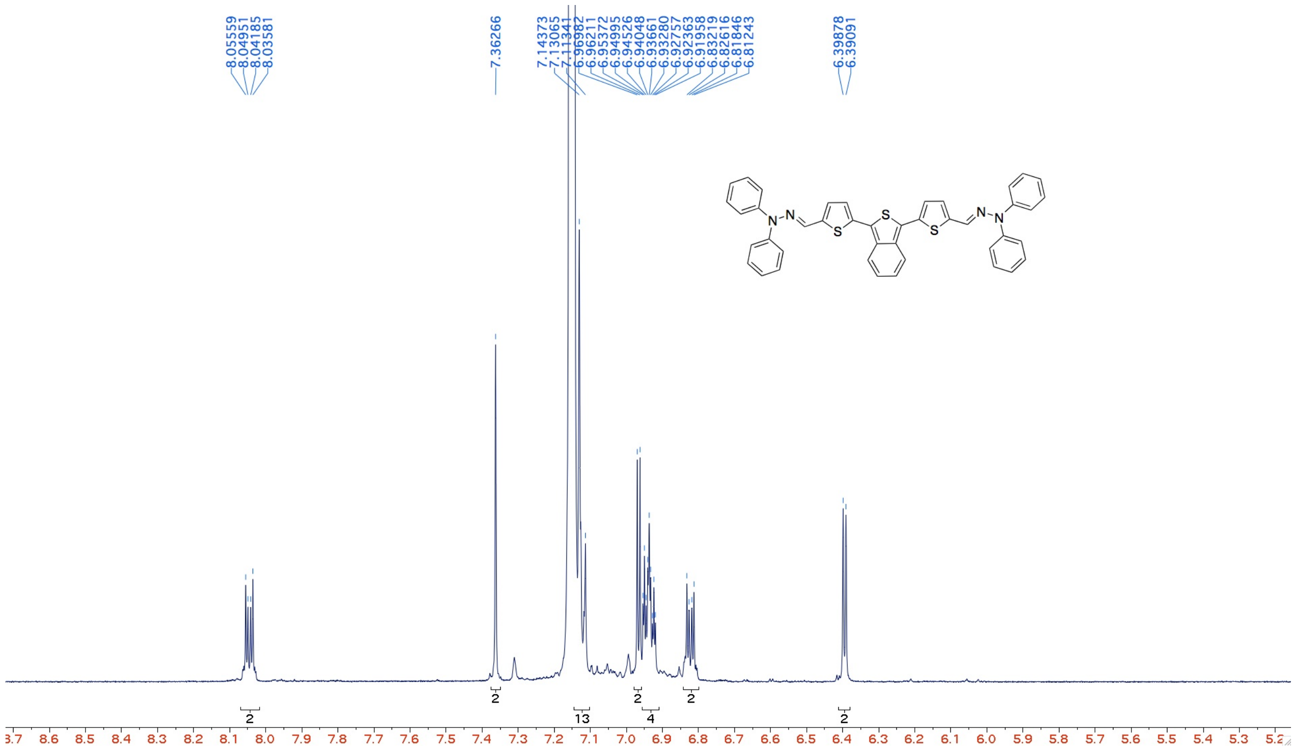
Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A
This journal is © The Royal Society of Chemistry 2012

2. ^{13}C NMR of Derivative **1** (125.70 MHz, $CDCl_3$)

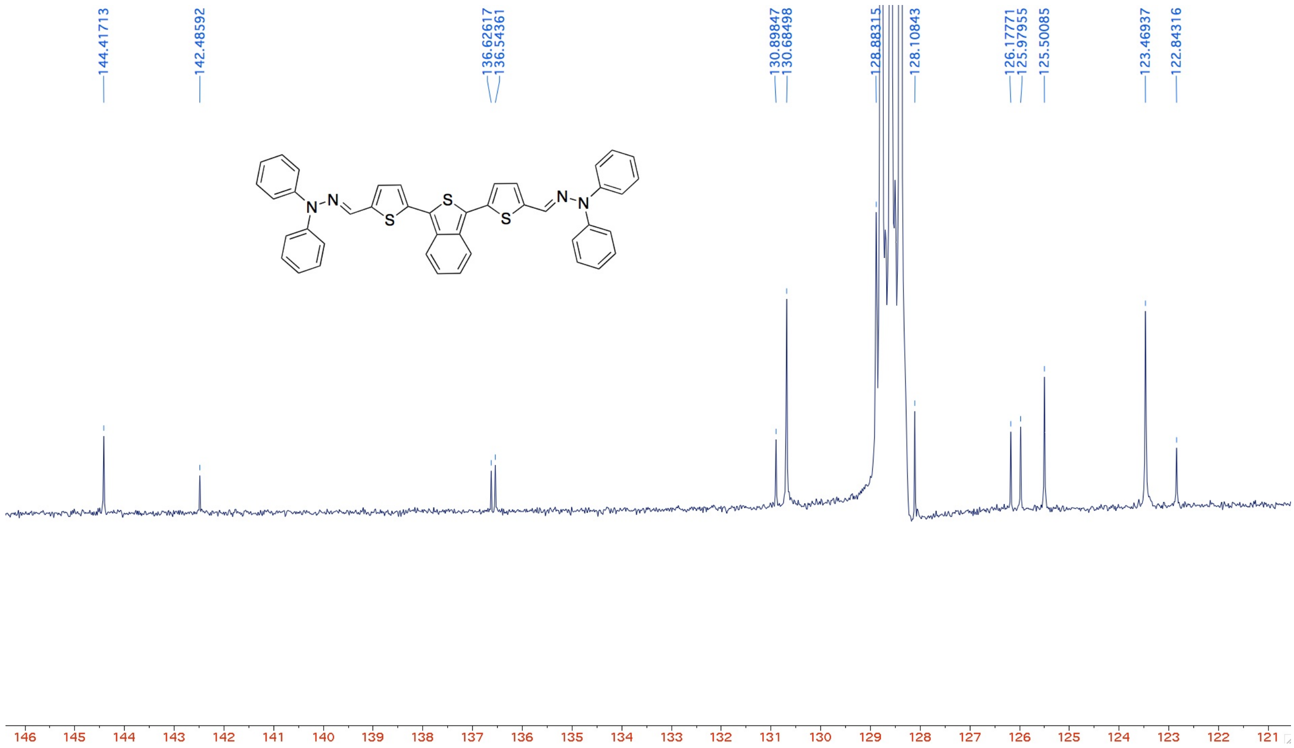


Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A

3. ^{1}H NMR of Derivative **2** (500 MHz, C_6D_6)



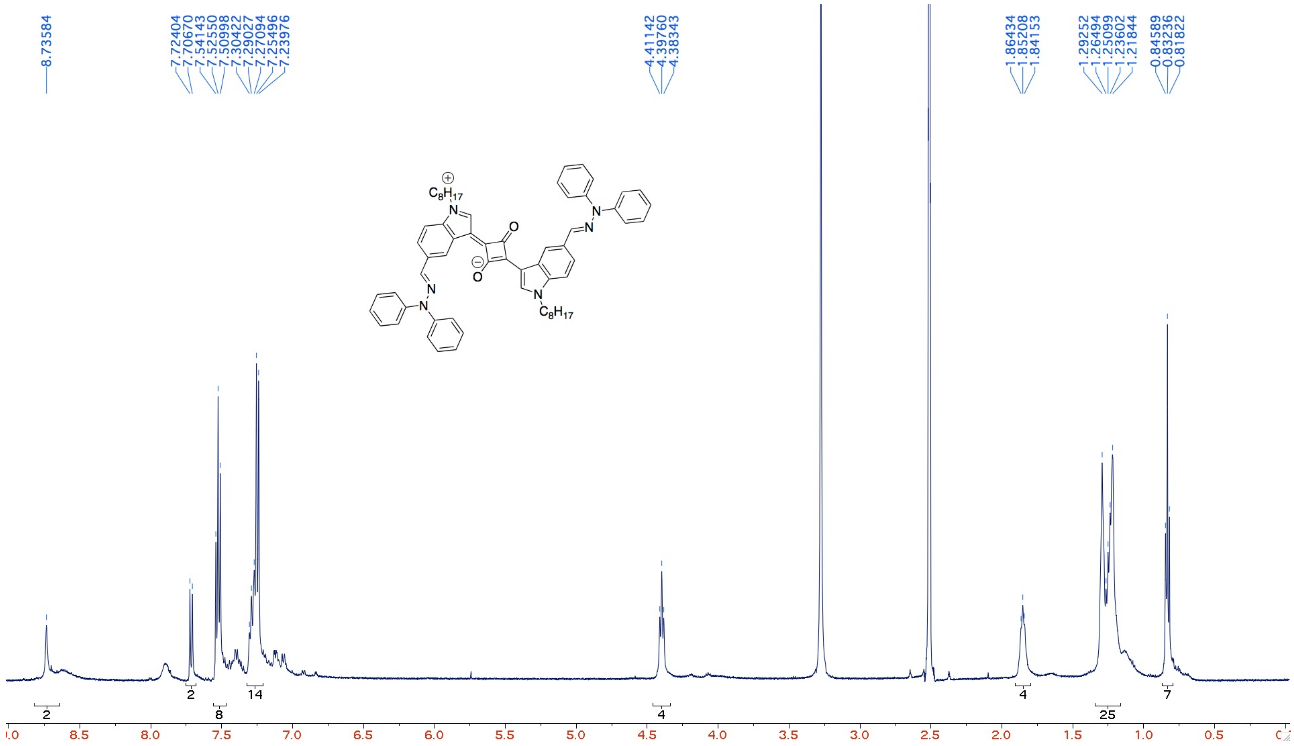
4. ^{13}C NMR of Derivative **2** (125.70 MHz, C_6D_6)



Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A
This journal is © The Royal Society of Chemistry 2012

5. ^{1}H NMR of Derivative **3** (500 MHz, DMSO-d_6)

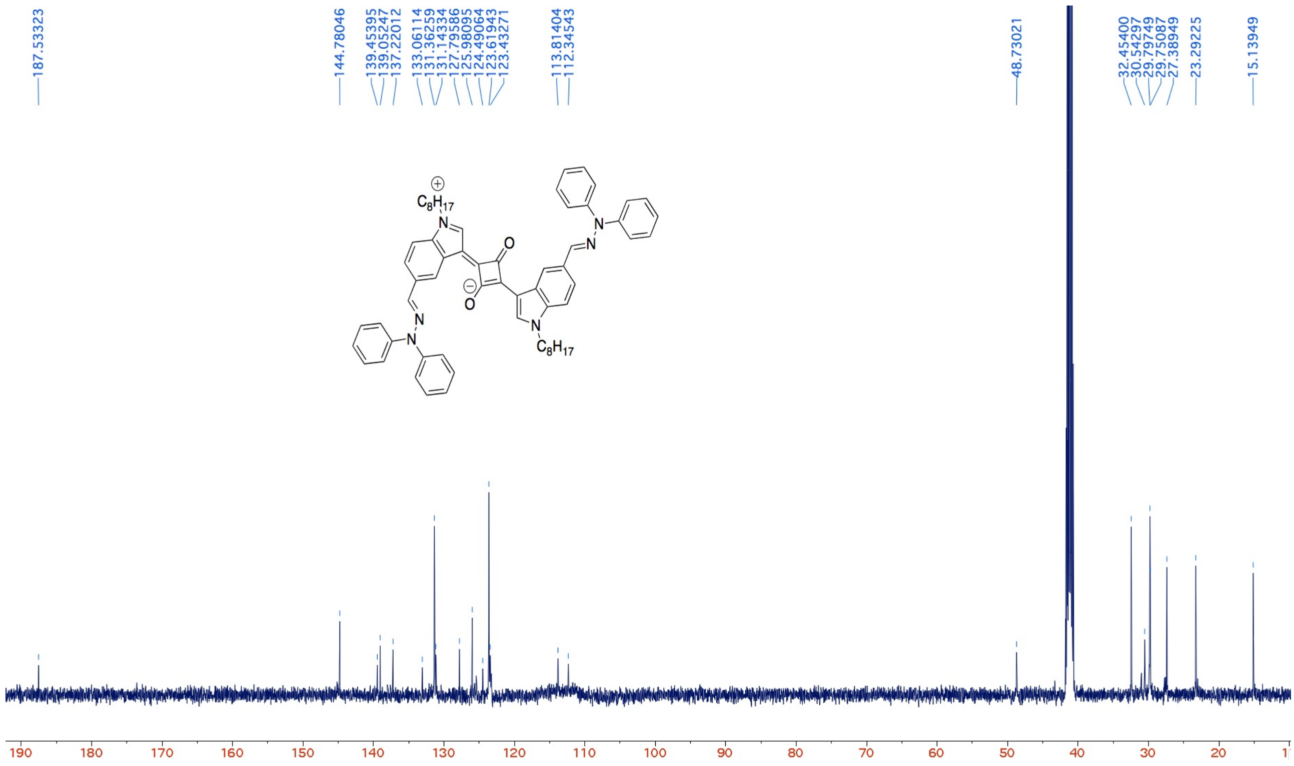
Note that derivative 3 is not fully stable in DMSO, however the NMR soectra in $CDCl_3$, CD_2Cl_2 and C_6D_6 are broad and without any interpretable splitting pattern due to aggregation.



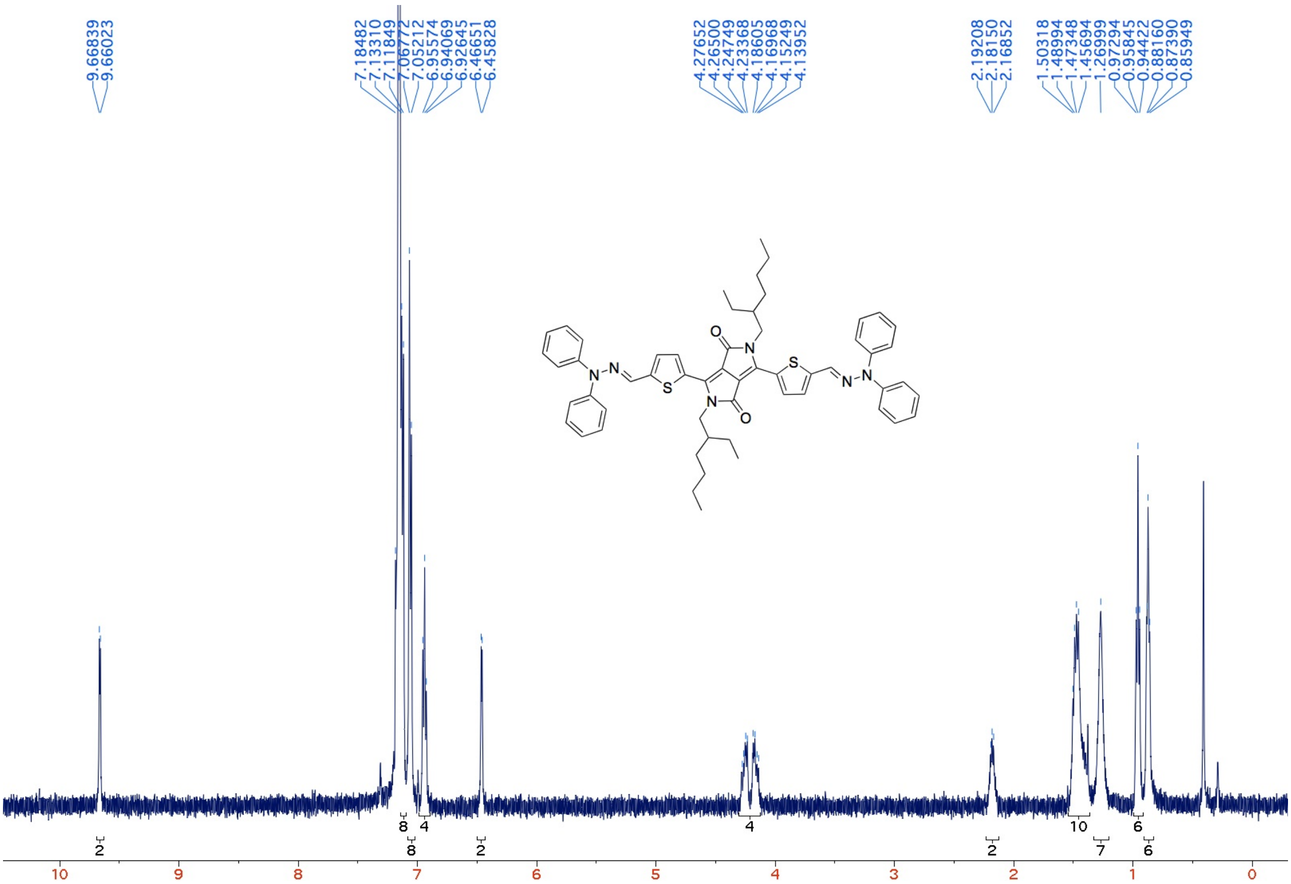
Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A

6. ^{13}C NMR of Derivative **3** (125.70 MHz, DMSO-d_6)

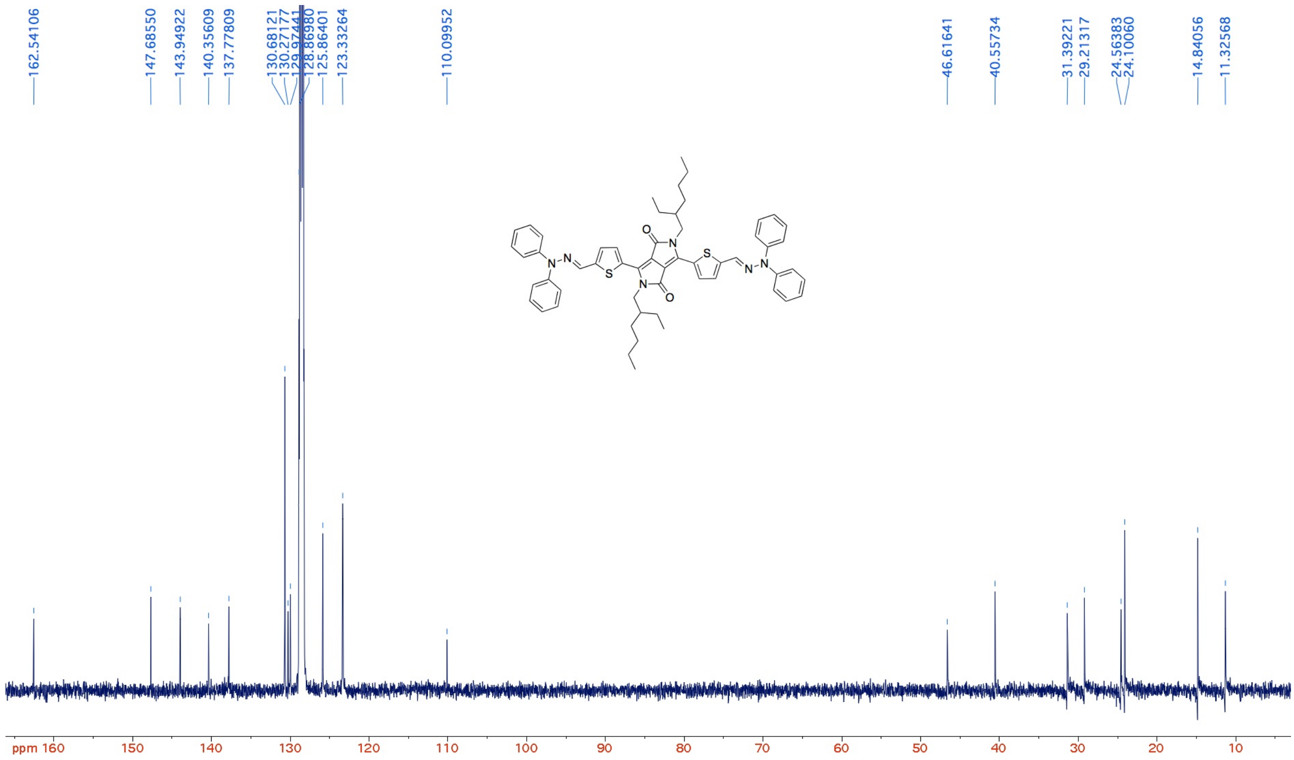
Note that derivative 3 is not fully stable in DMSO, however the NMR soectra in $CDCl_3$, CD_2Cl_2 and C_6D_6 are broad and without any interpretable splitting pattern due to aggregation.



7. ^{1}H NMR of Derivative **5** (500 MHz, C_6D_6)



8. ^{13}C NMR of Derivative **5** (125.70 MHz, C_6D_6).



9. Table S1. Data for Solution-Processed Hydrazones:$PC_{71}BM$ BHJ Photovoltaic Cells.

Blend	Active Layer (nm)	V_{oc} (Volts)	I_{sc} (mA/cm^2)	Efficiency (η)	Fill Factor (FF)	Cathode Composition
1:$PC_{61}BM$	50	0.54	1.67	0.29	0.32	LiF/Al
1:$PC_{71}BM$	50	0.57	2.66	0.48	0.32	LiF/Al
1:$PC_{71}BM$	50	0.62	2.69	0.59	0.35	Ca/Al
2:$PC_{71}BM$	70	0.58	1.90	0.36	0.33	Ca/Al
(1:3) 3:$PC_{71}BM$	50	0.68	4.70	1.16	0.36	LiF/Al
(1:3) 4:$PC_{71}BM$	50	0.56	7.16	1.49	0.37	LiF/Al
(1:1) 5:$PC_{71}BM$	50	0.77	2.50	0.6	0.30	LiF/Al
(1:2) 5:$PC_{71}BM$	50	0.74	5.10	1.20	0.33	LiF/Al
(1:3) 5:$PC_{71}BM$	75	0.71	6.17	1.53	0.35	LiF/Al

10. Figure S1. AFM images of representative devices made with derivatives 1-5 as the Donor compound.

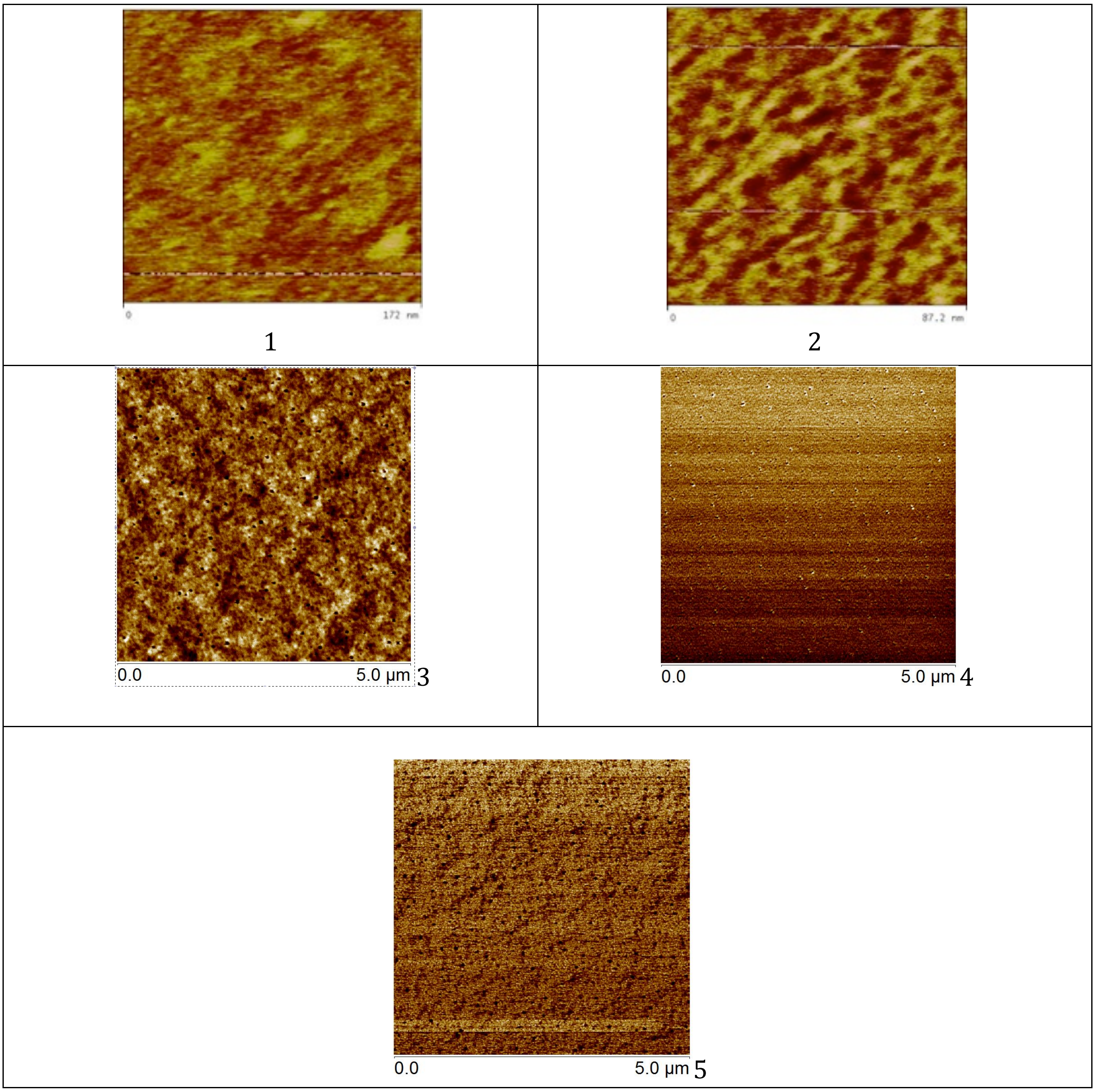


Figure S1. AFM images of the active layer of Derivatives **1-5** based OPV devices. Phase contrast.

Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A
This journal is © The Royal Society of Chemistry 2012

11. Figure S2. DPV plots of derivatives **3** and **5**.