Electronic Supplementary Information

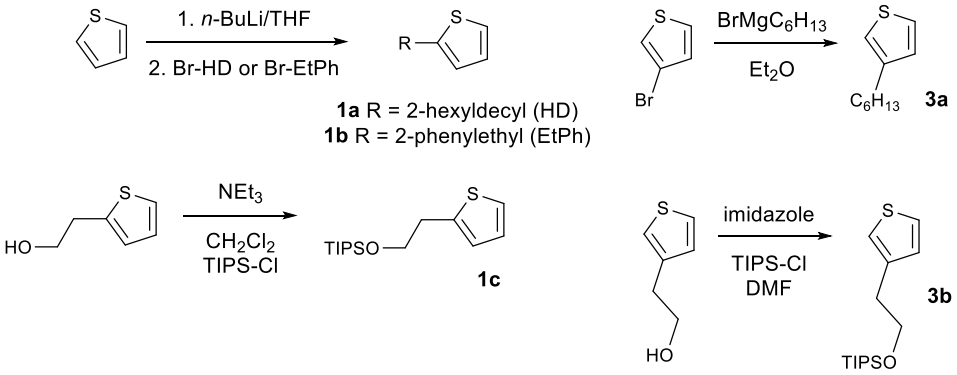
A stability study of polymer solar cells using conjugated polymers with different donor or acceptor side chain patterns

Ilona M. Heckler,[a] Jurgen Kesters,[b] Maxime Defour,[c] Huguette Penxten,[b] Bruno Van Mele,[c] Wouter Maes[b] and Eva Bundgaard*[a]

[a] *Technical University of Denmark, Department of Energy Conversion and Storage, Frederiksborgvej 399, 4000 Roskilde, Denmark.*
[b] *Hasselt University, Institute for Materials Research (IMO-IMOMEC), Design & Synthesis of Organic Semiconductors (DSOS), Agoralaan 1 - Building D, 3590 Diepenbeek.*
[c] *Physical Chemistry and Polymer Science (FYSC), Vrije Universiteit Brussels (VUB), Pleinlaan 2, 1050 Brussels, Belgium.*
**corresponding author: evbu@dtu.dk*

Table of contents

1. Additional information to the synthesized compounds



Scheme S1. *Synthetic procedures yielding monomers* ***1a–c*** *and* ***3a–b****.*

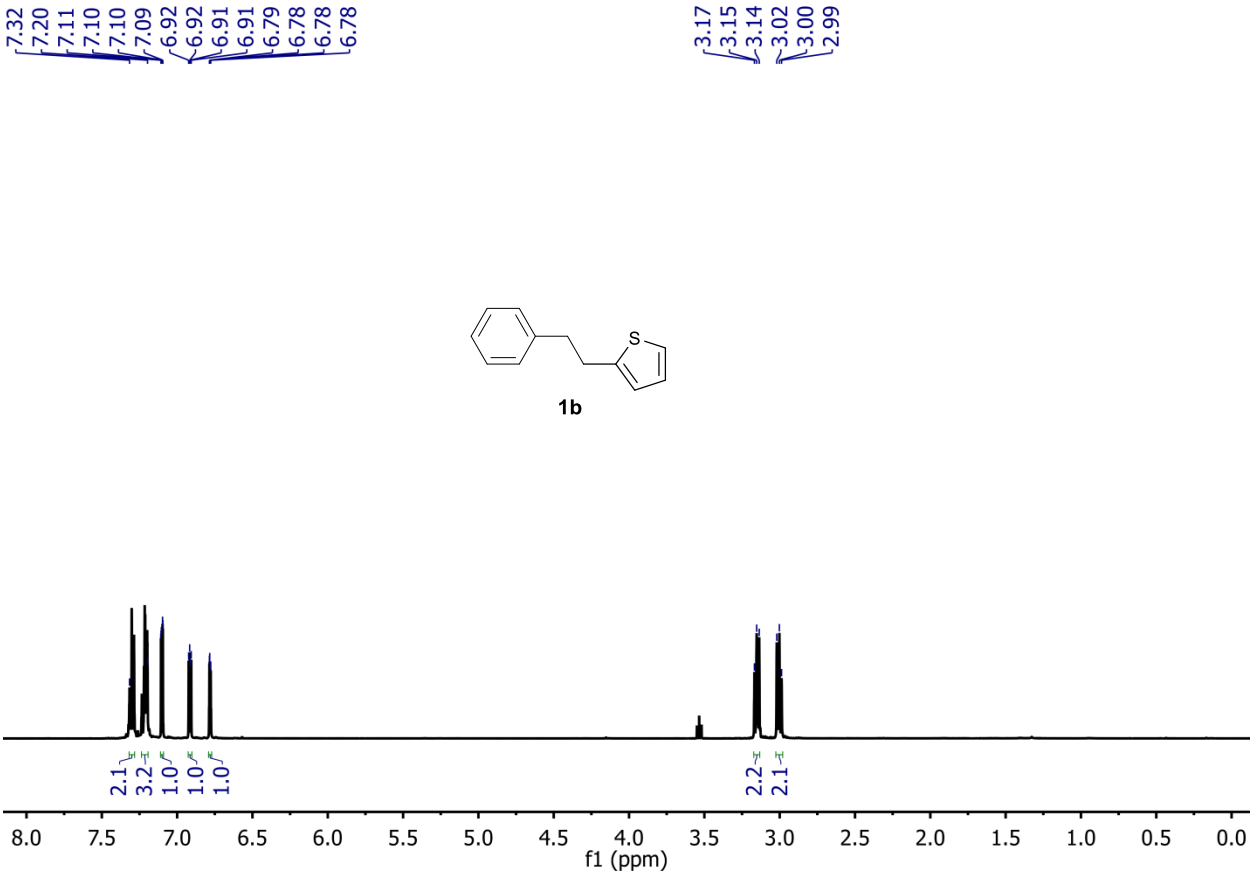


Fig. S1.1 *^{1}H NMR spectrum of compound* ***1b*** *in $CDCl_3$.*

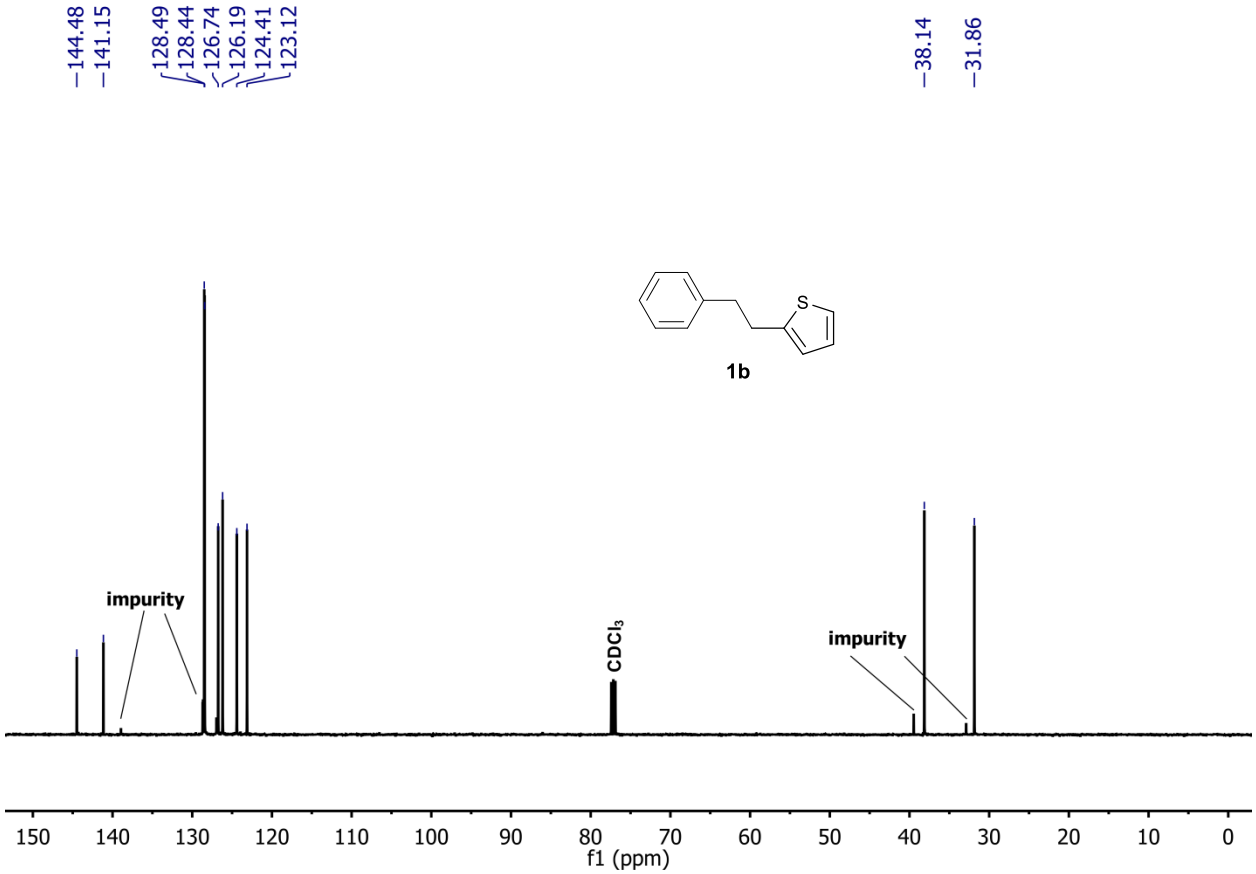


Fig. S1.2 *^{13}C NMR spectrum of compound **1b** in $CDCl_3$.*

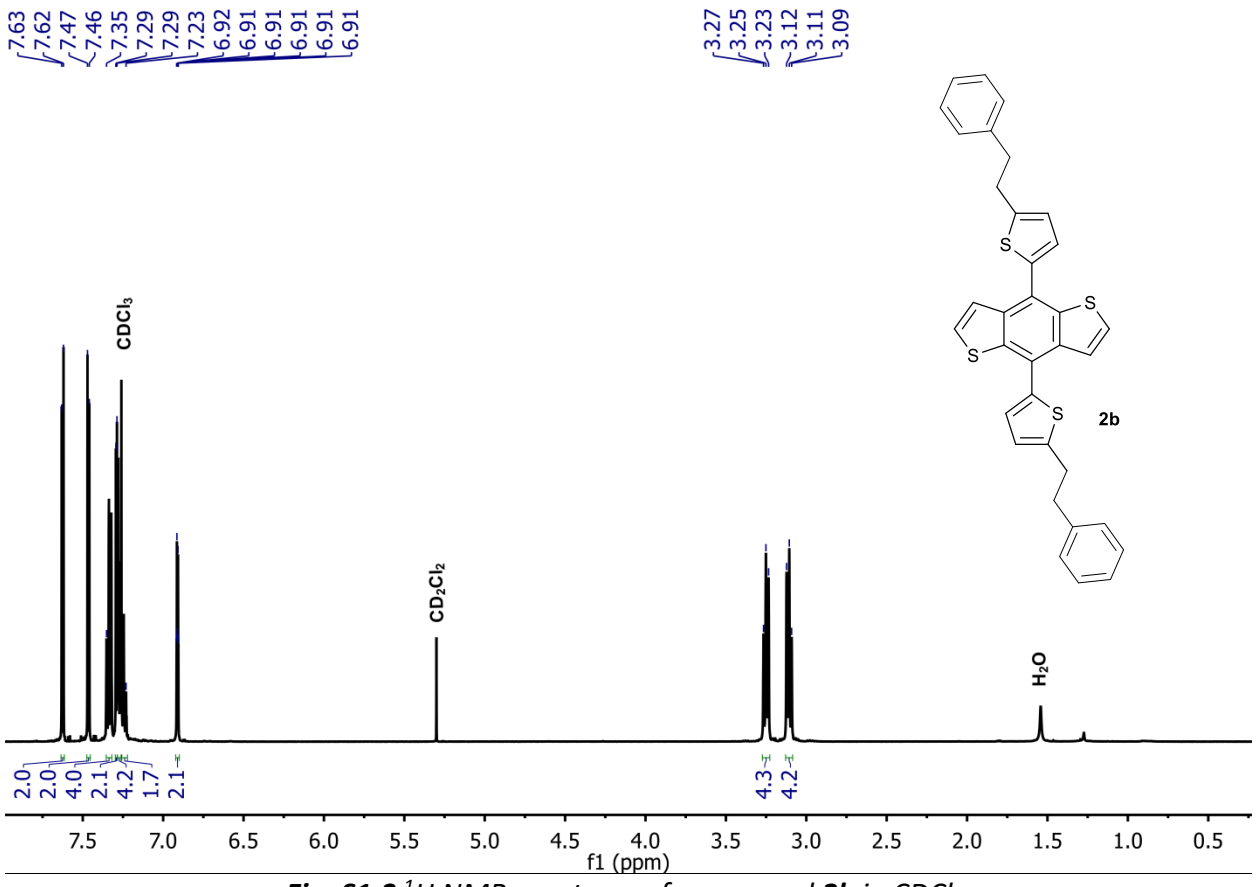


Fig. S1.3 *^{1}H NMR spectrum of compound **2b** in $CDCl_3$.*

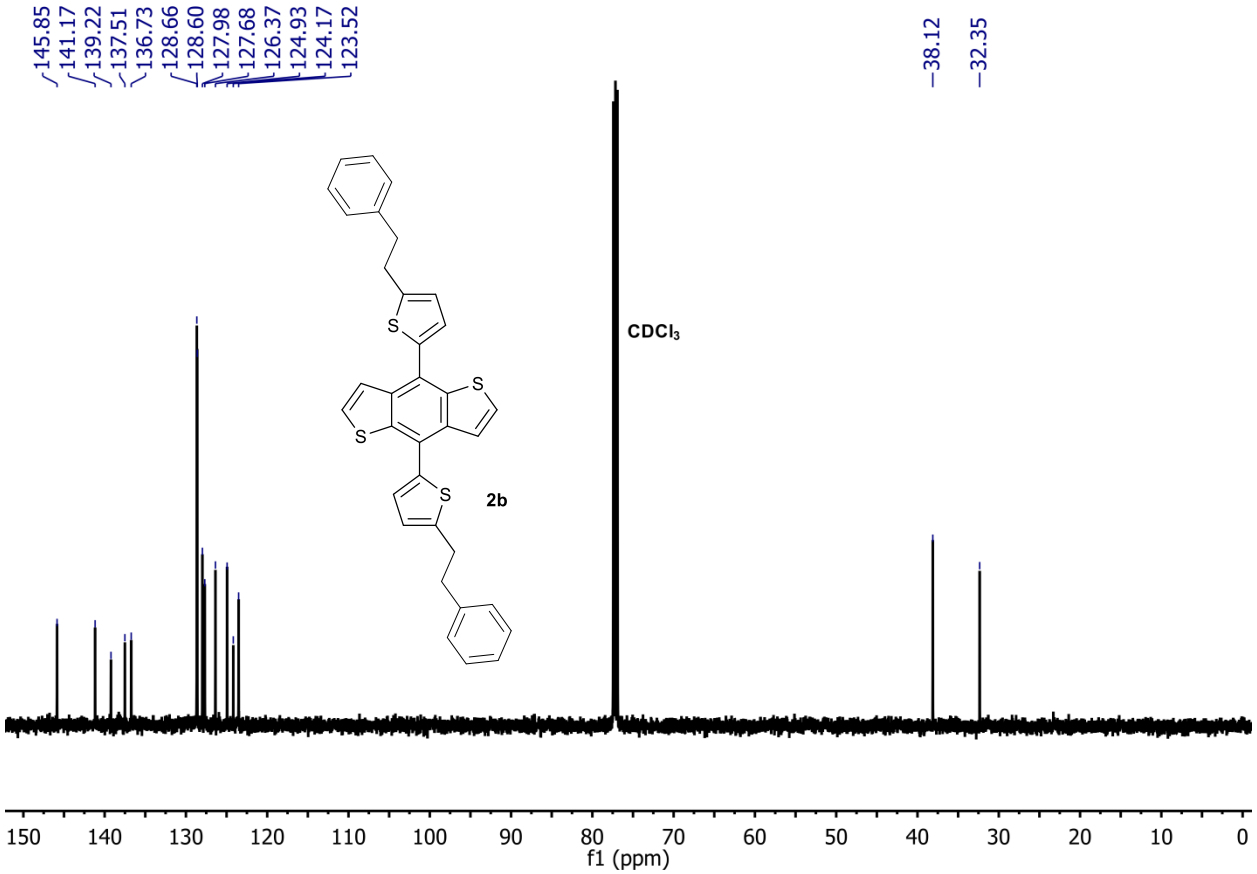


Fig. S1.4 *^{13}C NMR spectrum of compound **2b** in $CDCl_3$.*

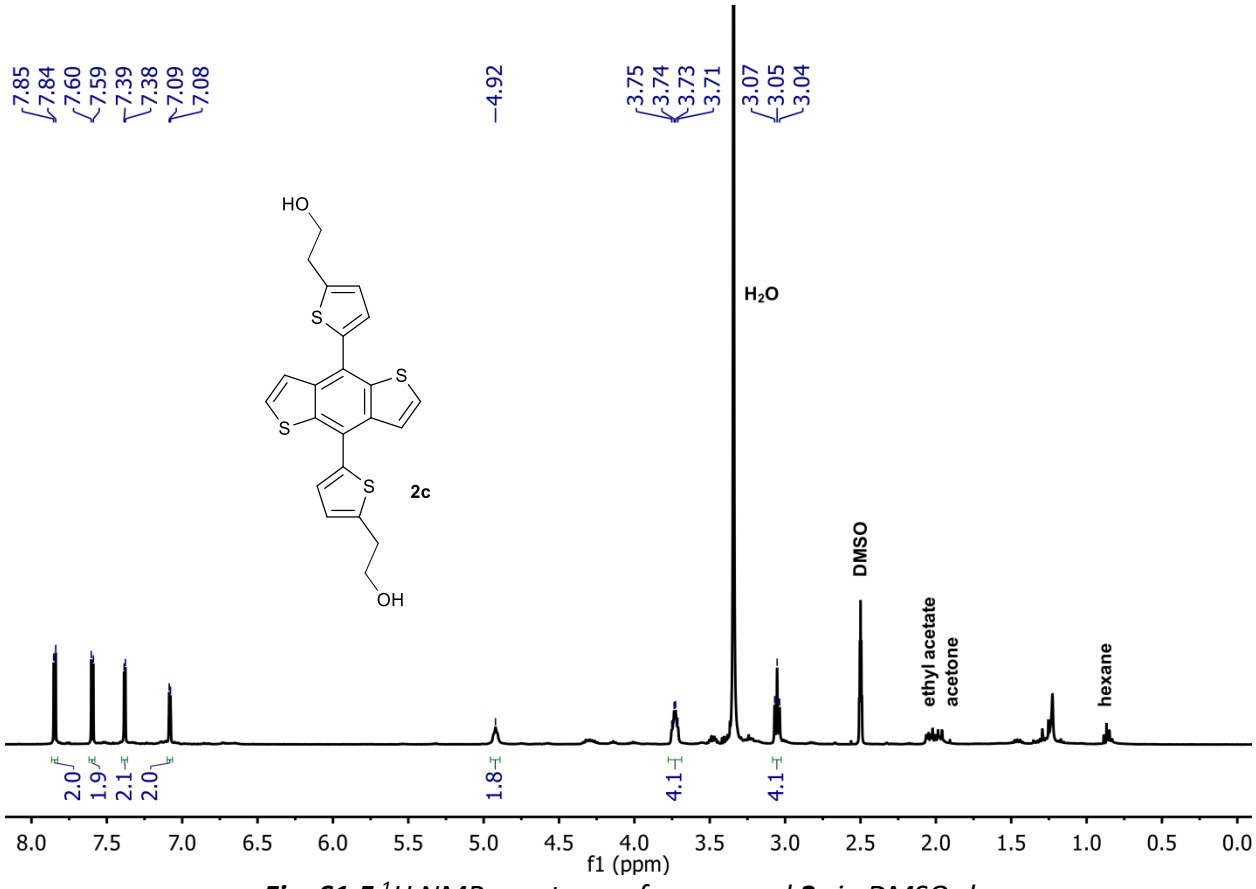


Fig. S1.5 *^{1}H NMR spectrum of compound **2c** in DMSO-d_6.*

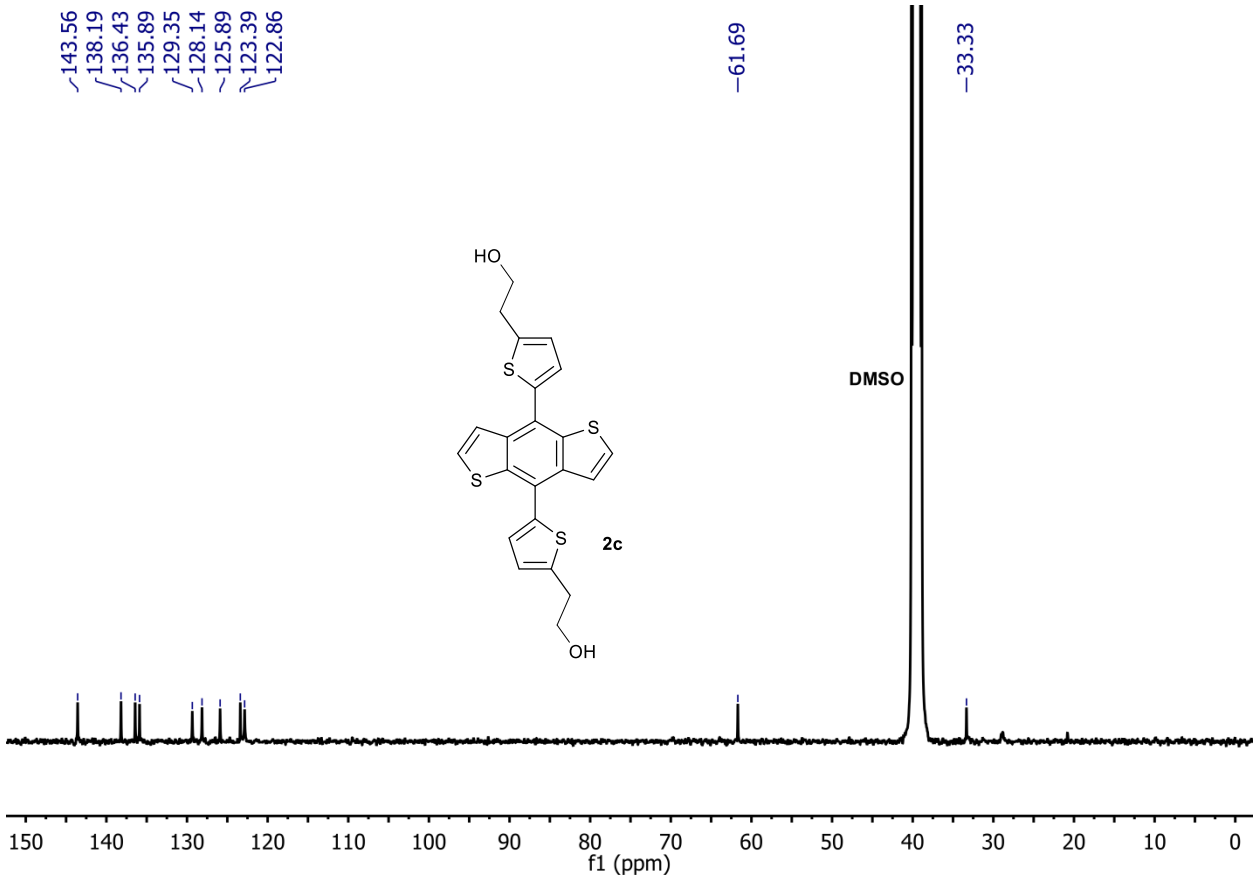


Fig. S1.6 *^{13}C NMR spectrum of compound **2c** in DMSO-d_6.*

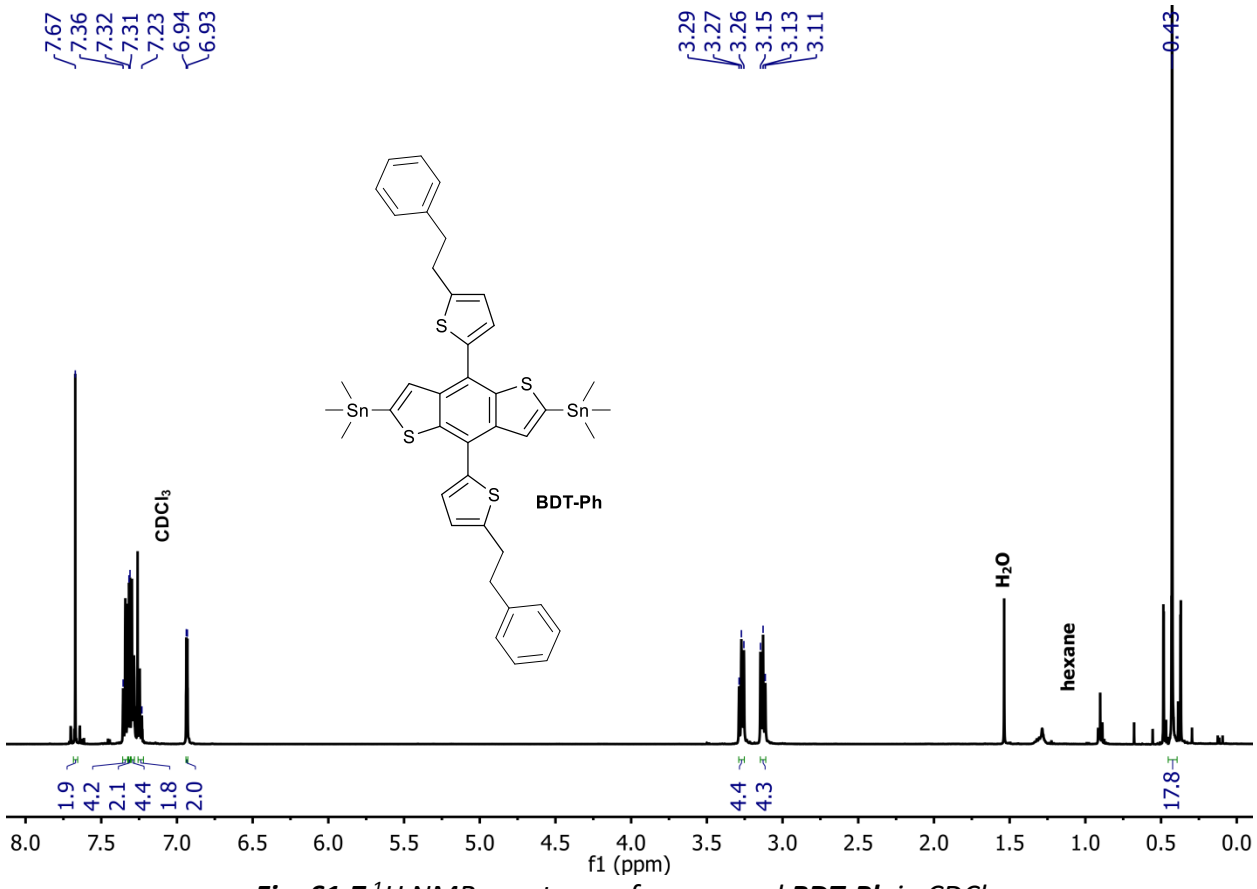


Fig. S1.7 *^{1}H NMR spectrum of compound **BDT-Ph** in $CDCl_3$.*

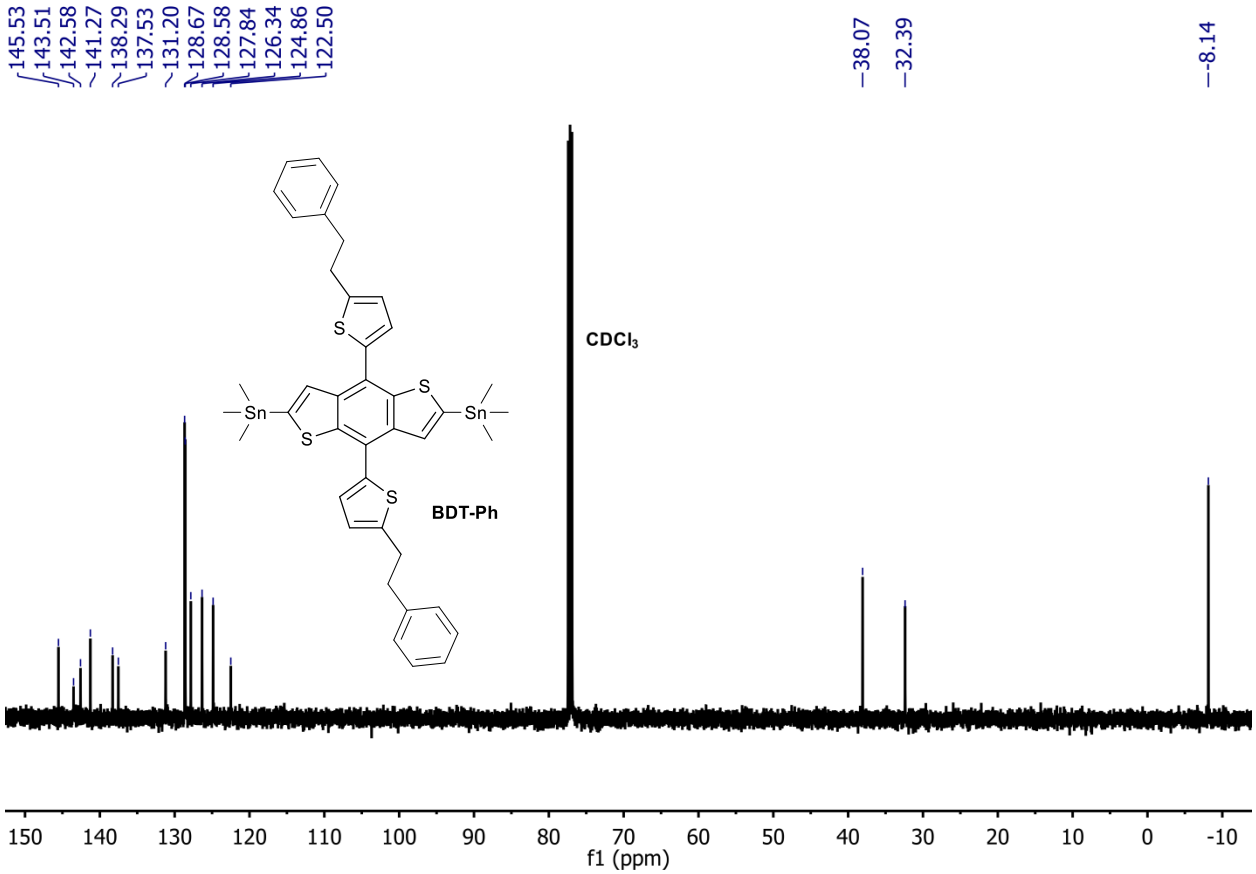


Fig. S1.8 *^{13}C NMR spectrum of compound **BDT-Ph** in $CDCl_3$.*

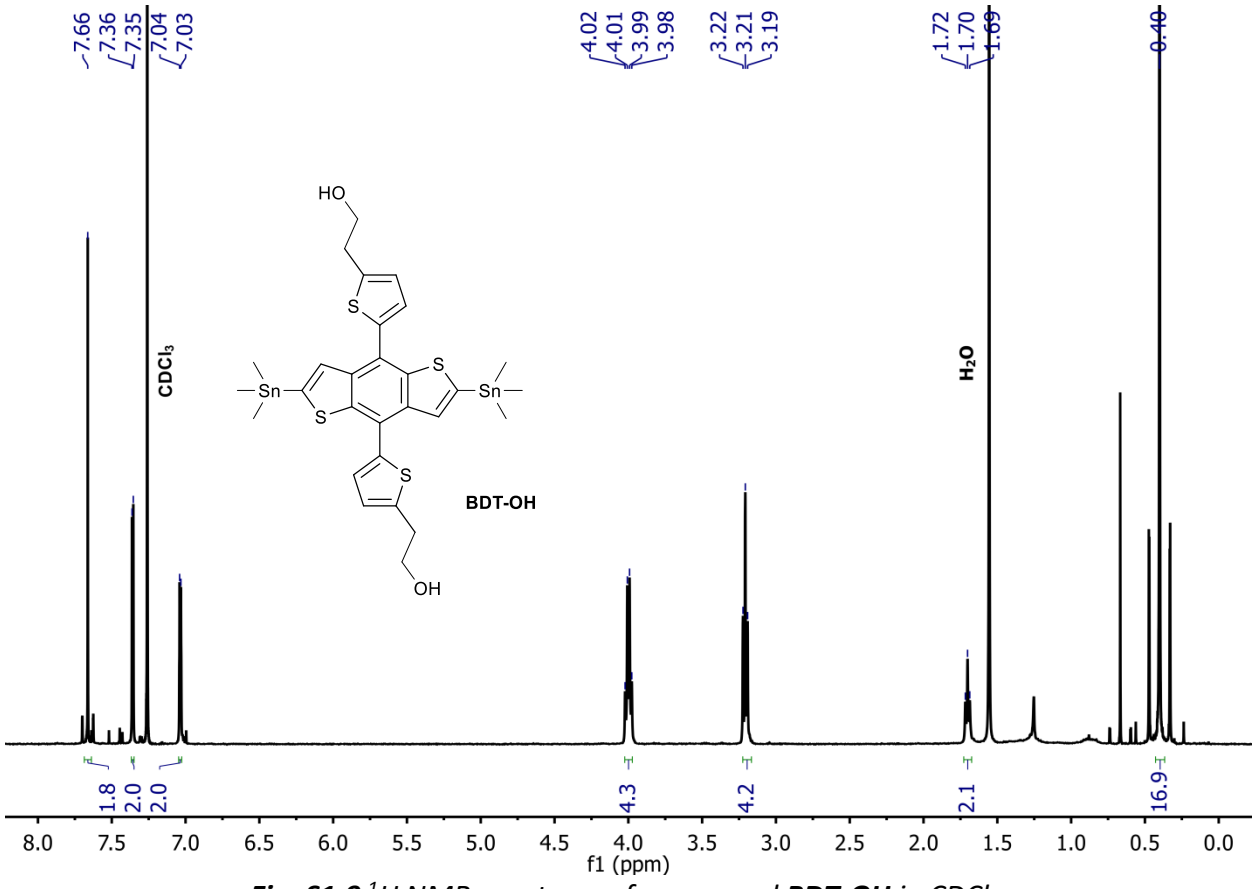


Fig. S1.9 *^{1}H NMR spectrum of compound **BDT-OH** in $CDCl_3$.*

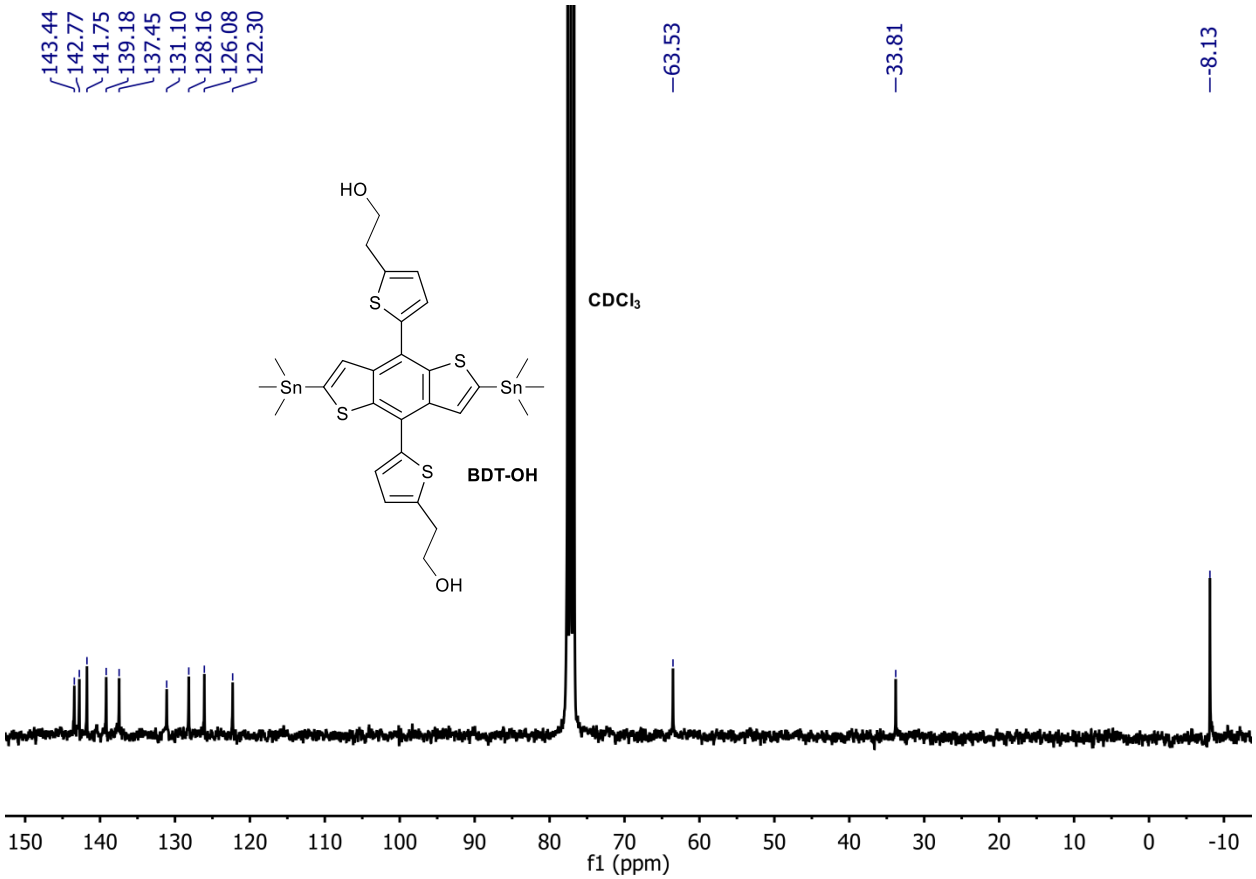


Fig. S1.10 *^{13}C NMR spectrum of compound **BDT-OH** in $CDCl_3$.*

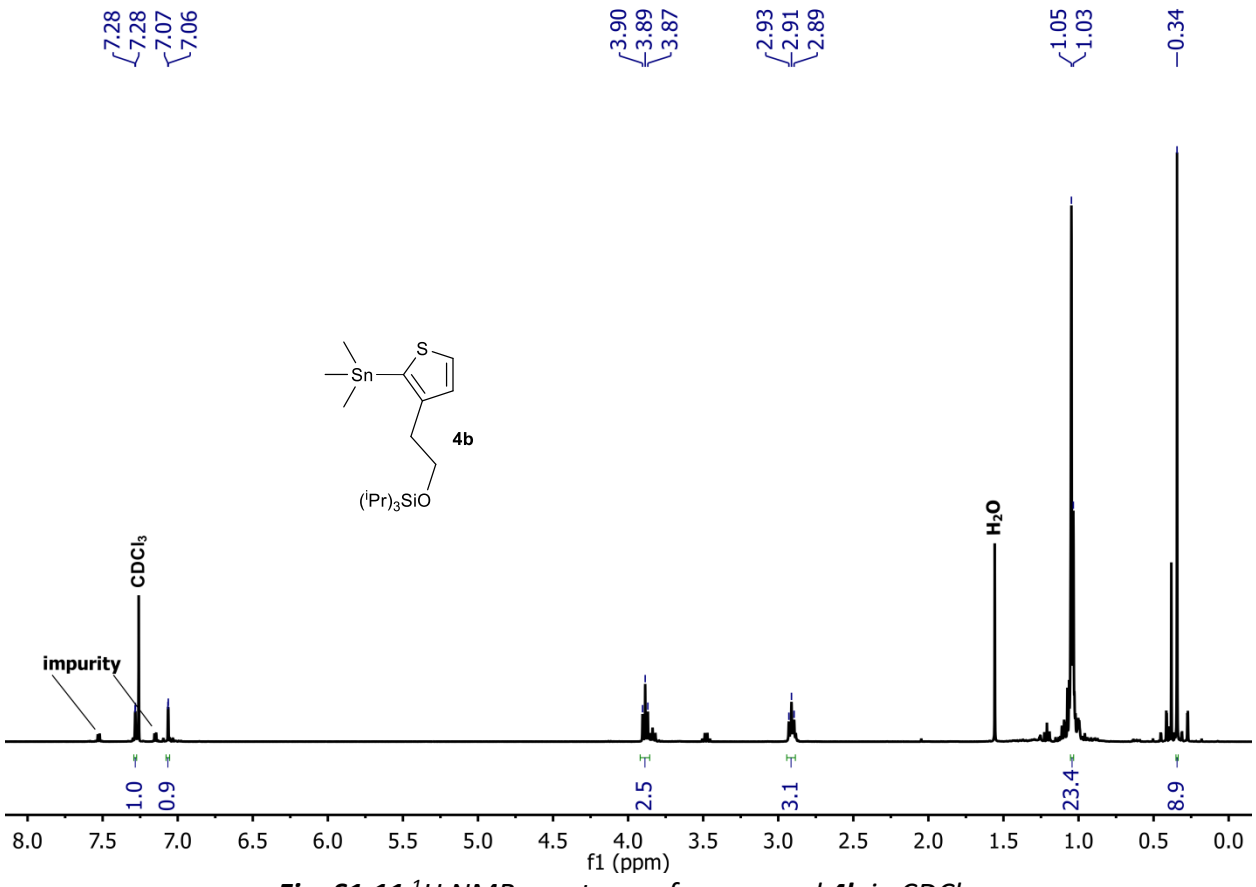


Fig. S1.11 *^{1}H NMR spectrum of compound **4b** in $CDCl_3$.*

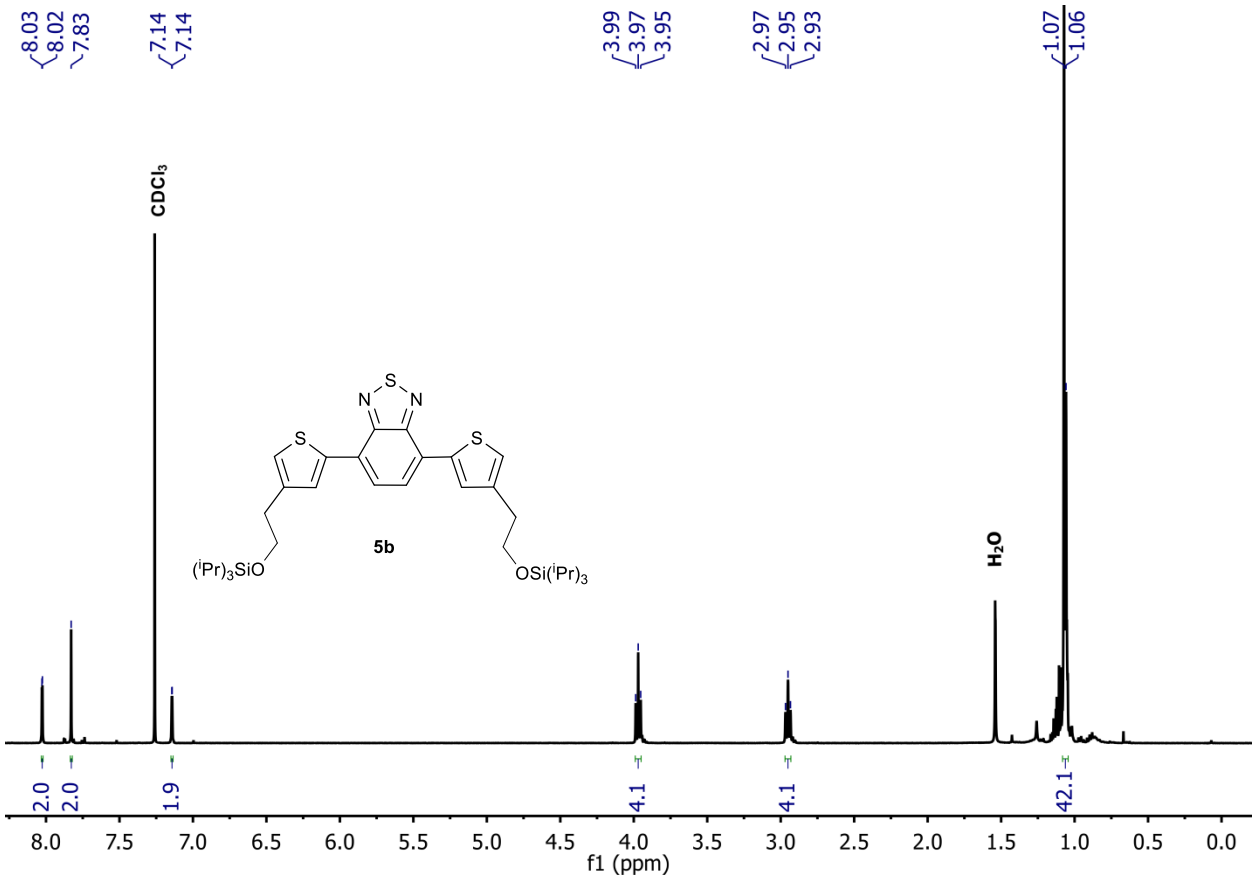


Fig. S1.12 *^{1}H NMR spectrum of compound **5b** in $CDCl_3$.*

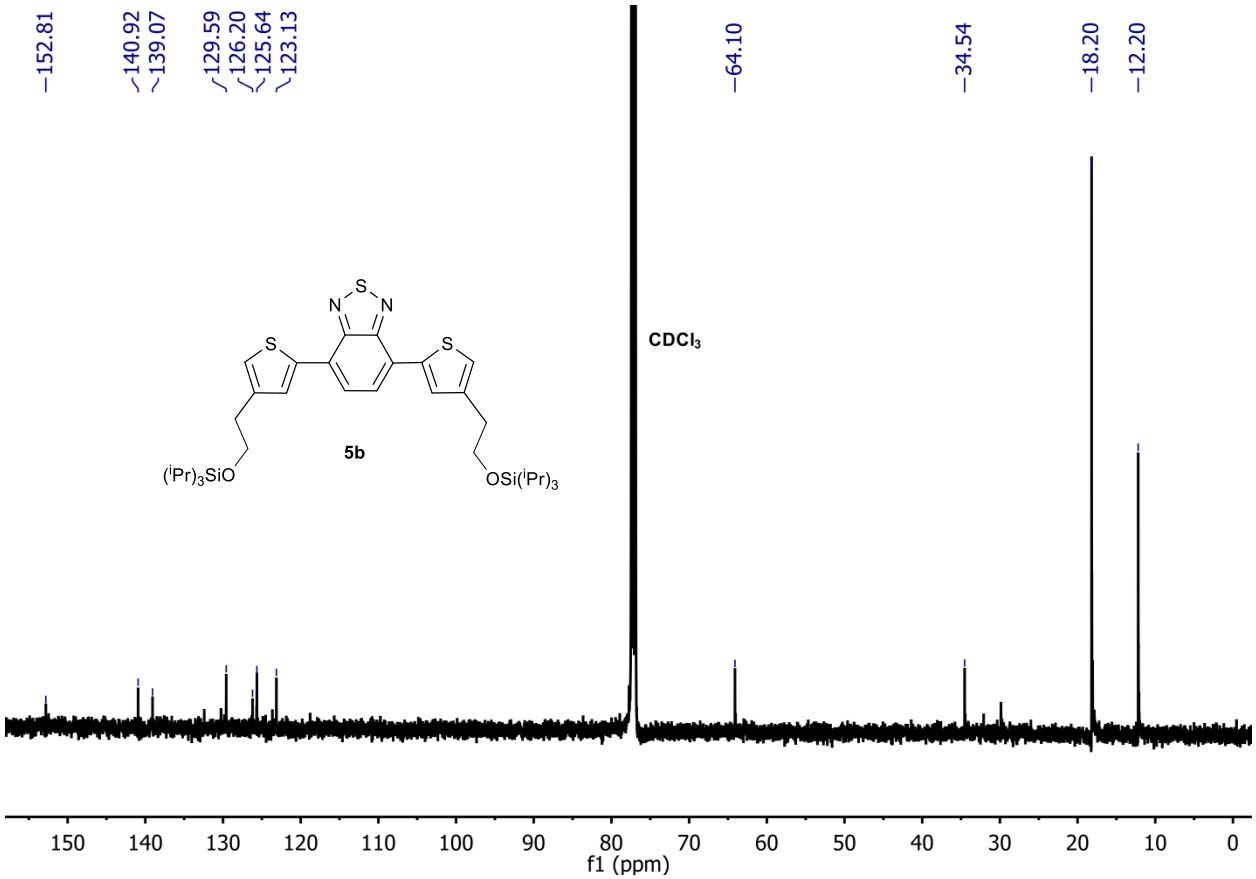


Fig. S1.13 *^{13}C NMR spectrum of compound **5b** in $CDCl_3$.*

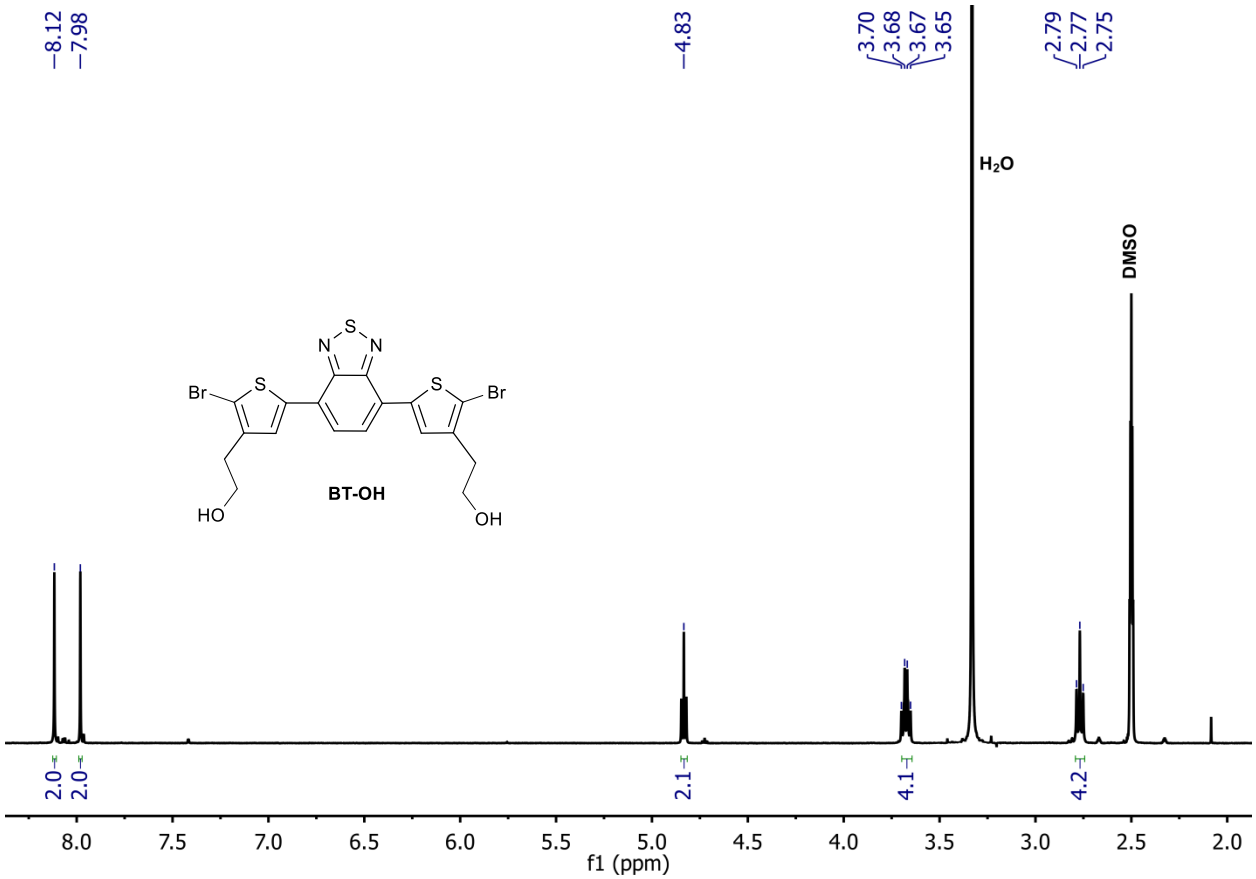


Fig. S1.14 *^{1}H NMR spectrum of compound **BT-OH** in DMSO-d_6.*

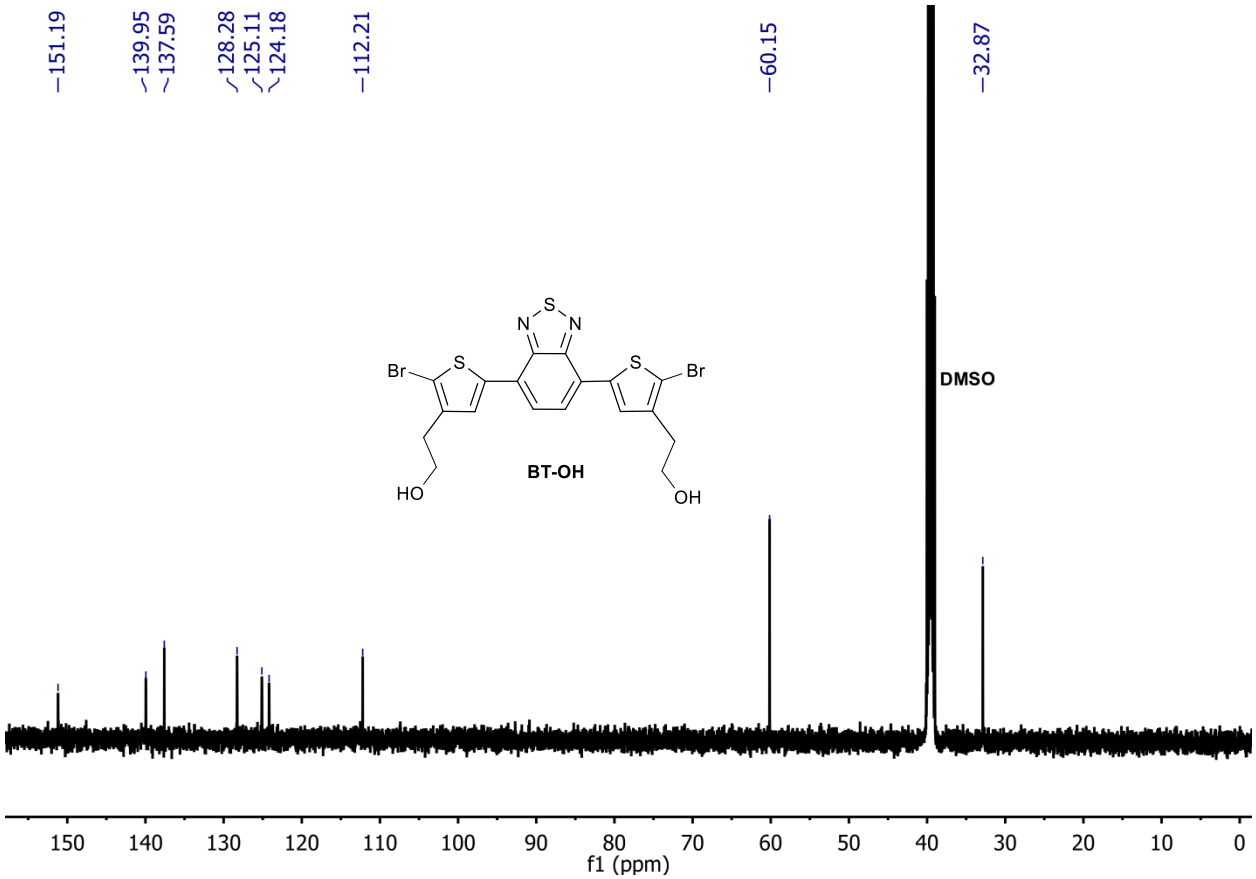


Fig. S1.15 *^{13}C NMR spectrum of compound **BT-OH** in DMSO-d_6.*

2. Additional information to polymer characterization

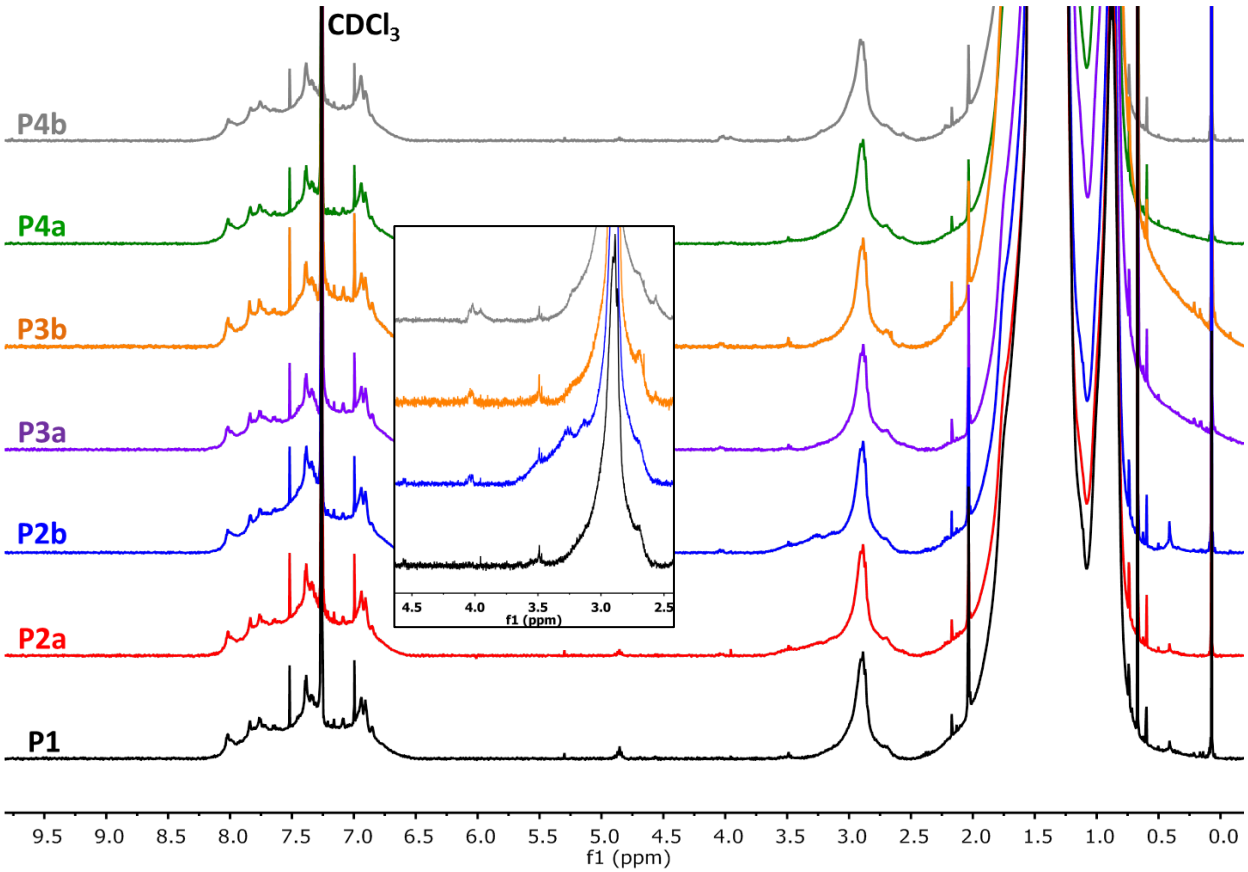


Fig. S1.16 *^{1}H NMR spectra of* ***P1–P4b*** *in $CDCl_3$.*

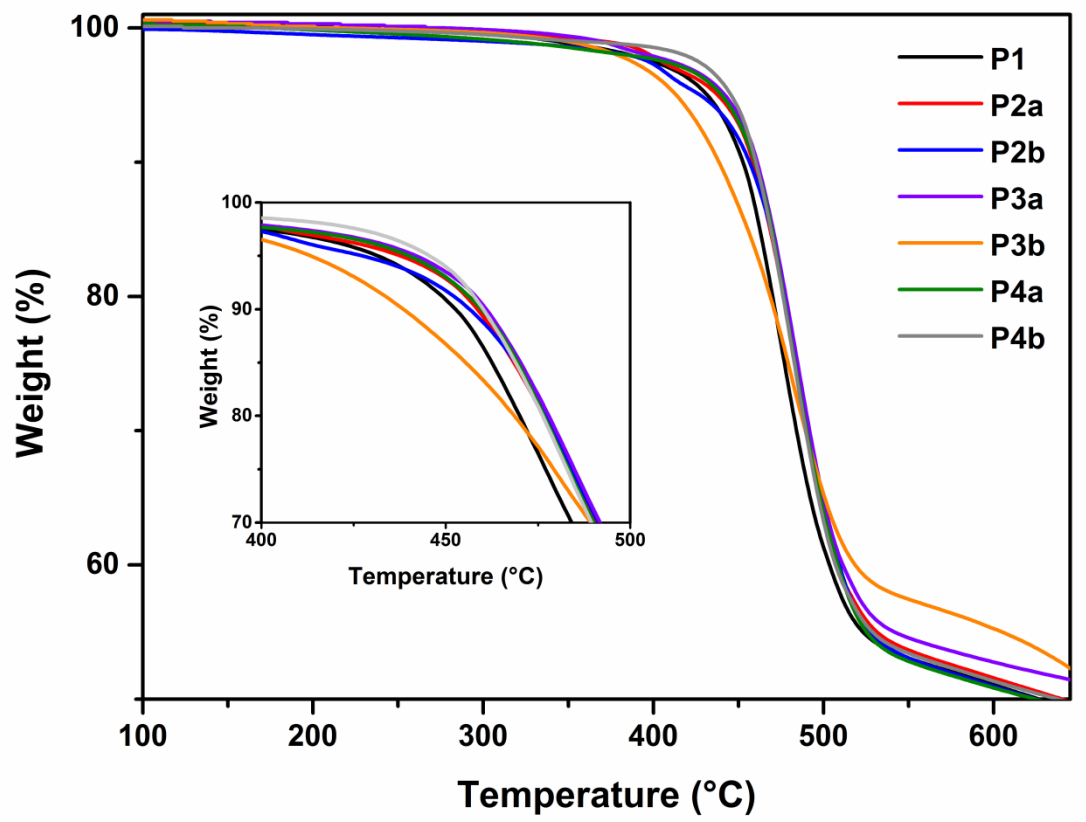


Fig. S2. *TGA profiles for polymers* ***P1–P4b****.*

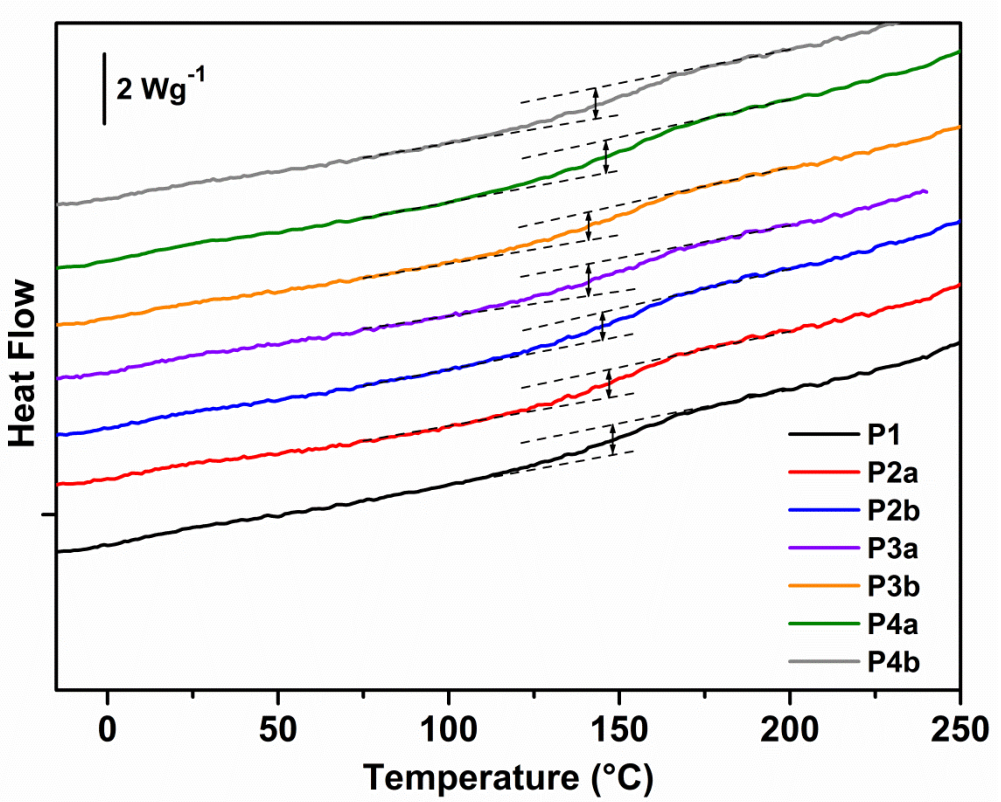


Fig. S3. *RHC heating profiles, obtained at 500 K/min after cooling at 20 K/min (2nd heating), for polymers* ***P1–P4b*** *(curves shifted vertically for clarity).*

3. Additional information to device preparation and characterization

Table S1. *Averaged current-voltage (I-V) parameters for the solvent (and fullerene) screening of SC PSCs based on* ***P1****.*

Active layer[a]	Solvent	*Voc*[c]	*Jsc*[c]	FF[c]	PCE (best)[c]
P1:$PC_{61}BM$	ODCB[b]	0.76	8.90	53	3.59 (3.84)
P1:$PC_{61}BM$	CF[b]	0.75	9.74	61	4.50 (5.27)
P1:$PC_{71}BM$	ODCB[b]	0.74	10.70	56	4.45 (4.60)
P1:$PC_{71}BM$	CF[b]	0.75	9.59	56	3.98 (4.26)

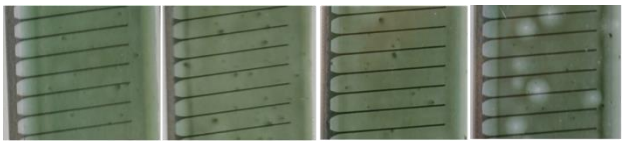
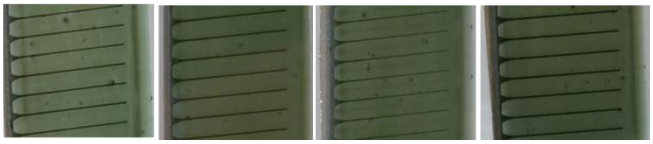
[a] Polymer solar cells prepared by spin-coating with a polymer:fullerene ratio of 1:2. [b] ODCB = *o*-dichlorobenzene, CF = chloroform. [c] Open-circuit voltage (in V), short-circuit current density (in mA/cm^2), fill factor (in %), power conversion efficiency (average over 4 devices, in %).

Table S2. *Averaged current-voltage (I-V) parameters for PSCs based on* ***P1****:*$PC_{61}BM$*, roll coated from different solvents and using different polymer:*$PC_{61}BM$ *ratios and processing temperatures.*

Solvent[a]	**P1**:$PC_{61}BM$[b]	*T*[c]	d[d]	*Voc*[e]	*Jsc*[e]	FF[e]	PCE (best)[e]
ODCB	1:2	**60**	450	0.70	5.68	57	2.07 (2.26)
ODCB	1:2	**80**	450	0.70	5.23	61	2.79 (2.81)
ODCB	**1:2**	**70**	450	0.71	7.59	61	3.07 (3.31)
ODCB	**1:1.5**	70	450	0.71	7.22	62	2.95 (3.15)
ODCB	**1:1**	70	450	0.69	6.68	56	2.34 (2.59)
CF	1:2	70	450	[f]	[f]	[f]	[f]
CB/3%CN	1:2	70	450	0.72	5.71	61	2.46 (2.51)
ODCB/CB 4/1	1:2	70	**450**	0.73	7.79	60	**3.43 (3.60)**
ODCB/CB 4/1	1:2	70	**390**	0.72	7.46	62	3.34 (3.49)

[a] *Ortho*-dichlorobenzene (ODCB), chloroform (CF), chlorobenzene (CB), 2-chloronaphthalene (CN). [b] Donor:acceptor ratio of the photoactive layer blend. [c] Processing temperature (°C). [d] Active layer thickness (in nm) [e] Open-circuit voltage (in V), short-circuit current density (in mA/cm^2), fill factor (in %), power conversion efficiency (average over 5-6 devices, in %). [f] No *I-V* characteristics could be obtained due to an inhomogeneous photoactive layer.

Table S3. *Photographs of different roll-coated polymer:$PC_{61}BM$ films using different solvent ratios.*[a]

ODCB/CB[b]	**P1**	**P2a**	**P2b**	**P3a**[c]	**P3b**[c]	**P4a**	**P4b**
4/1					-[d]		-[d]
3/2	-[d]	-[d]	-[d]				

[a] Films were coated at 70 °C with a PAL thickness of 450 nm (polymer:$PC_{61}BM$ ratio of 1:2, 40 mg/mL), the scale bar of the pictures: the distance between two silver electrode fingers is 1.0 mm. [b]*Ortho*-dichlorobenzene (ODCB)/chlorobenzene (CB) in different ratios. [c] White spots on the film due to dewetting during the coating. [d] Coating was not performed due to the irrelevance of the experiment.

Table S4. *Averaged current-voltage (I-V) parameters for RC PSCs based on* ***P3a*** *and* ***P4a****.*[a]

Polymer	ODCB/CB[b]	*Voc*[c]	*Jsc*[c]	FF[c]	PCE (best)[c]
P3a	4/1	0.72	7.64	57	3.13 (3.25)
P3a	3/2	0.72	7.63	57	3.17 (3.38)
P4a	4/1	0.72	7.79	52	2.94 (3.11)
P4a	3/2	0.72	7.99	55	3.16 (3.41)

[a] Polymer solar cells prepared by roll-coating with a polymer:$PC_{61}BM$ ratio of 1:2 at 70 °C, 450 nm active layer thickness. [b] *Ortho*-dichlorobenzene (ODCB)/chlorobenzene (CB) ratio. [c] Open-circuit voltage (in V), short-circuit current density (in mA/cm^2), fill factor (in %), power conversion efficiency (average over 5-6 devices, in %).

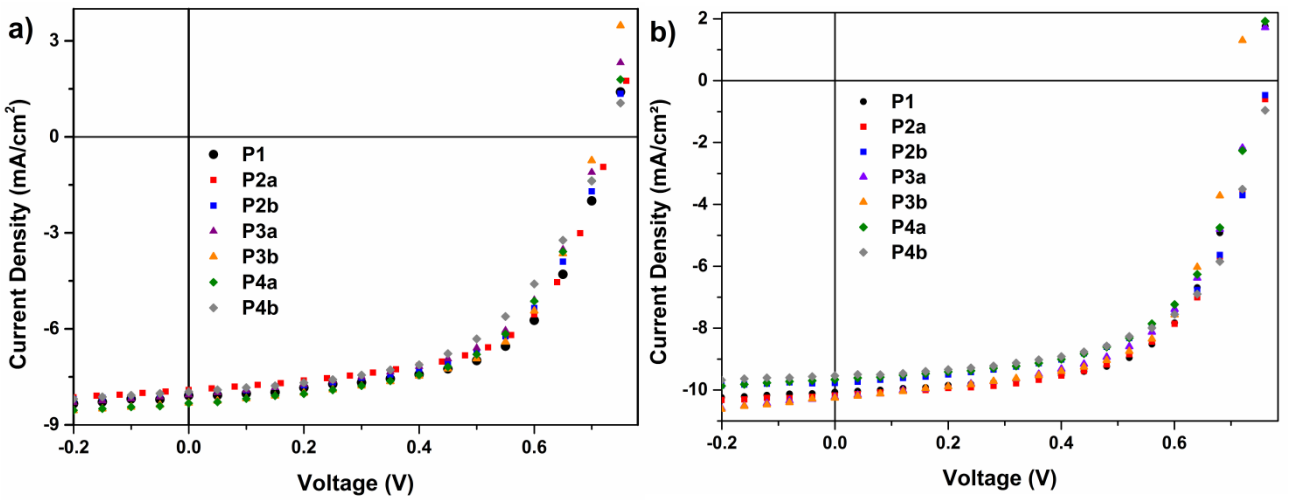


Fig. S4. *I-V curves for the best RC (a) and SC (b) PSCs based on* ***P1*****–*****P4b****.*

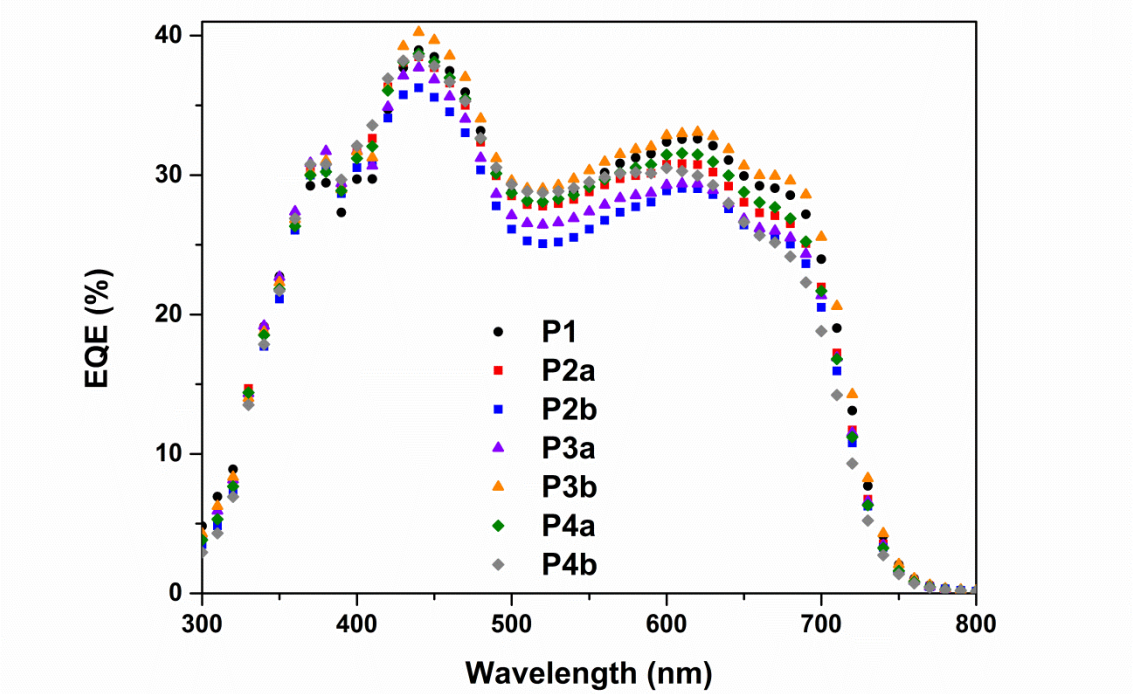


Fig. S5. *EQE spectra for the best RC PSCs based on* ***P1*****–*****P4b***.

4. Additional information to stability testing

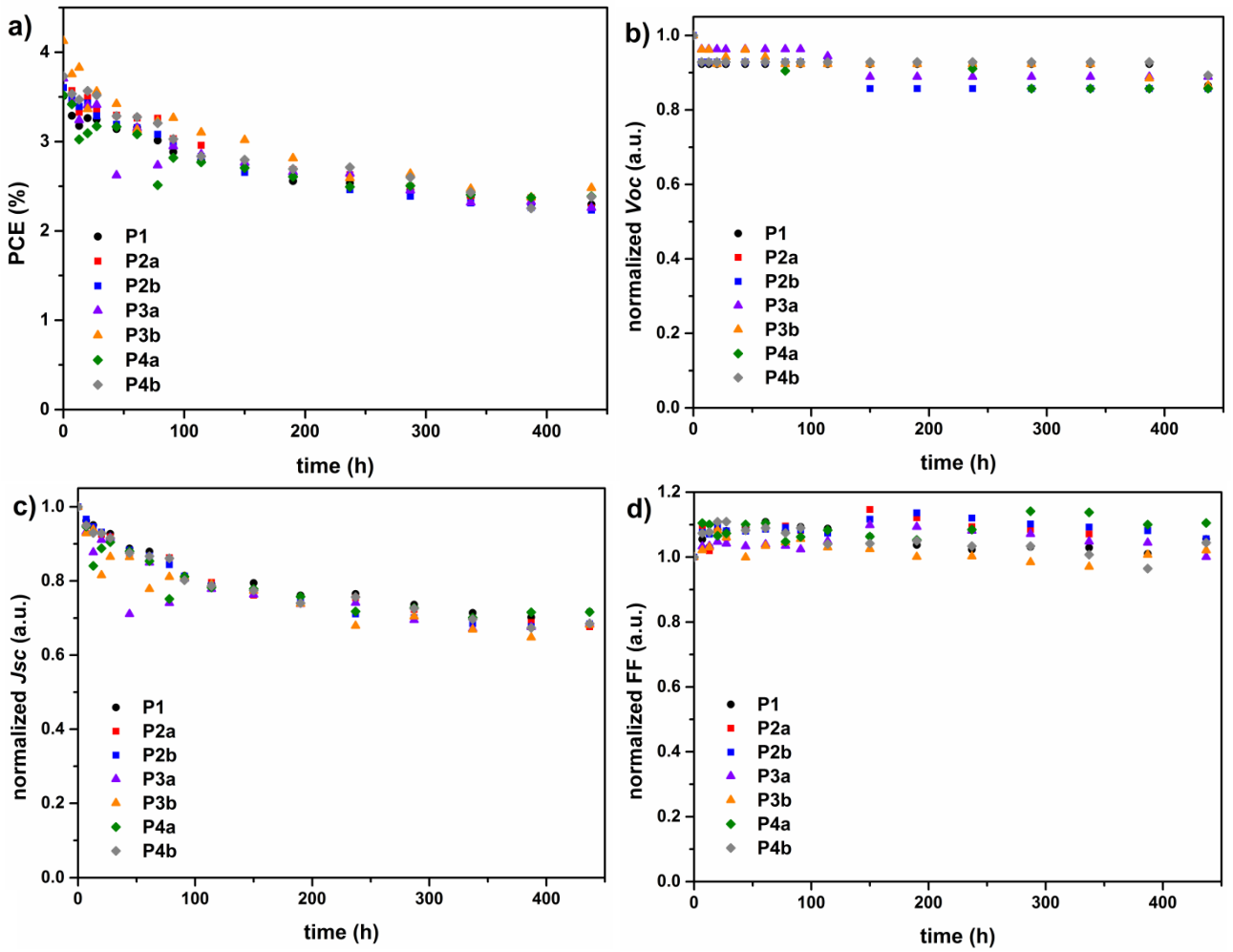


Fig. S6. *Stability measurements of SC PSCs based on* ***P1*****–*****P4b*** *under thermal stress (85 °C; ISOS-D-2) in terms of the averaged absolute PCE (a) and normalized Voc (b), Jsc (c) and FF (d).*

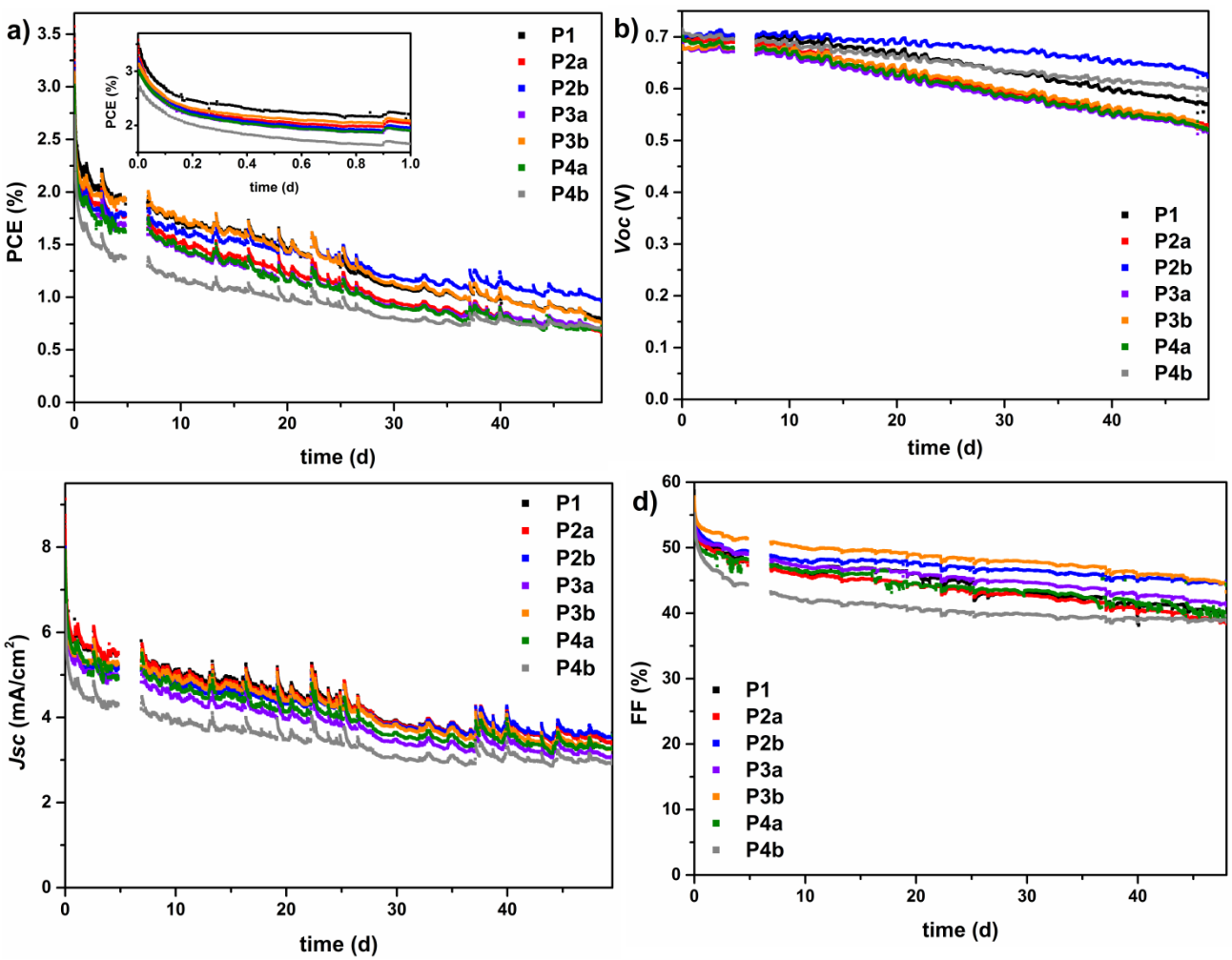


Fig. S7. *Stability measurements of RC PSCs based on* ***P1*****–*****P4b*** *under constant sun irradiance (AM 1.5) in terms of the averaged PCE (a), Voc (b), Jsc (c) and FF (d) (no data could be gathered between 5 and 7 days due to a software error).*