Electronic Supplementary Information

Low bandgap copolymers based on monofluorinated isoindigo towards efficient polymer solar cells

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1. Solar cell optimization tables

Table S1. Overview of the solar cell optimization studies for copolymer **PIID-5T**.

PIID-5T:$PC_{71}BM$ (w/w)	Total conc. (mg/mL)	Solvent	DIO (% v/v)	Annealing (°C-min)	V_{oc} (V)	J_{sc} (mA/cm^2)	FF (%)	PCE (%)
1:1	20	odCB	-	-	0.69	8.88	43	2.61
1:1	20	odCB	-	140-30	0.71	6.28	50	2.24
1:1	20	$CHCl_3$:odCB (1:1)	-	-	0.67	8.18	37	2.01
1:1	20	$CHCl_3$:odCB (1:1)	-	120-10	0.70	6.69	40	1.88
1:2	25	odCB	-	-	0.70	6.95	47	2.30
1:2	25	odCB	-	120-10	0.71	4.64	56	1.83
1:3	**25**	**odCB**	-	-	**0.70**	**6.51**	**58**	**2.64**
1:3	25	odCB	-	120-2	0.72	5.37	64	2.45
1:3	**25**	**odCB**	-	**120-5**	**0.71**	**6.19**	**64**	**2.83**
1:3	25	odCB	3	-	0.67	8.03	39	2.12
1:3	25	odCB	3	120-5	0.69	5.11	53	1.85

Table S2. Overview of the solar cell optimization studies for copolymer **PFIID-5T**.

PFIID-5T:$PC_{71}BM$ (w/w)	Total conc. (mg/mL)	Solvent	DIO (% v/v)	Annealing (°C-min)	V_{oc} (V)	J_{sc} (mA/cm^2)	FF (%)	PCE (%)
1:1	25	odCB	-	-	0.60	7.94	44	2.10
1:1	25	odCB	-	120-2	0.64	6.74	44	1.94
1:1	25	odCB	-	120-5	0.64	7.41	49	2.33
1:2	25	odCB	-		0.62	7.59	66	3.13
1:2	25	odCB	-	120-2	-	-	-	-
1:2	25	odCB	-	120-5	-	-	-	-
1:3	**25**	**odCB**	-	-	**0.61**	**9.88**	**60**	**3.64**
1:3	25	odCB	-	120-2	0.65	9.08	63	3.68
1:3	**25**	**odCB**	-	**120-5**	**0.65**	**8.93**	**64**	**3.72**
1:3	25	odCB	1	-	0.58	9.39	55	3.00
1:3	25	odCB	1	120-5	0.61	8.28	61	3.08
1:3	25	odCB	2	-	0.58	9.64	54	3.03
1:3	25	odCB	2	120-5	0.64	7.96	59	3.03
1:3	25	odCB	3	-	0.58	9.79	48	2.73
1:3	25	odCB	3	120-5	0.64	7.32	59	2.78
1:4	25	odCB	-	-	0.59	9.47	53	2.97
1:4	25	odCB	-	120-2	0.63	9.88	58	3.64
1:4	25	odCB	-	120-5	0.63	9.69	60	3.64

Table S3. Overview of the solar cell optimization studies for copolymer **PFIID-5T_H**.

PFIID-5T_H:$PC_{71}BM$ (w/w)	Total conc. (mg/mL)	Solvent	DIO (% v/v)	Annealing (°C-min)	V_{oc} (V)	J_{sc} (mA/cm^2)	FF (%)	PCE (%)
1:1	12	odCB	-	-	0.61	8.52	57	2.96
1:1	12	odCB	-	120-5	0.64	7.06	57	2.55
1:2	15	odCB	-	-	0.59	9.60	60	3.44
1:2	15	odCB	-	120-5	0.63	9.27	56	3.30
1:2	12	odCB	-	-	0.58	4.84	61	1.72
1:2	12	odCB	-	120-5	0.61	5.04	58	1.78
1:3	**16**	**odCB**	**-**	**-**	**0.59**	**13.88**	**61**	**5.04**
1:3	16	odCB	-	-	0.62	10.99	60	4.13
1:4	12	odCB	-	-	0.59	5.94	65	2.25
1:4	12	odCB	-	120-5	0.62	6.34	64	2.52

Table S4. Overview of the solar cell optimization study for the mixed **PFIID-5T:PFIID-5T_H** blend.

PFIID-5T:PFIID-5T_H:$PC_{71}BM$ (w/w)	Total conc. (mg/mL)	Solvent	V_{oc} (V)	J_{sc} (mA/cm^2)	FF (%)	PCE (%)
0.5:0.5:3	16	odCB	0.59	10.81	62	4.00

Table S5. Overview of the solar cell optimization studies for copolymer **PFIID-T-BDT-T**.

PFIID-T-BDT-T:$PC_{71}BM$ (w/w)	Total conc. (mg/ml)	Solvent	DIO (% v/v)	Annealing (°C-min)	V_{oc} (V)	J_{sc} (mA/cm^2)	FF (%)	PCE (%)
1:1	25	odCB	-	-	0.86	1.43	45	0.55
1:1	25	odCB	-	120-5	0.88	1.45	50	0.64
1:2	25	odCB	-	-	0.86	2.32	54	1.08
1:2	25	odCB	-	120-5	0.88	1.92	59	0.99
1:3	**25**	**odCB**	-	-	**0.86**	**2.66**	**57**	**1.30**
1:3	25	odCB	-	120-2	0.88	2.42	60	1.28
1:3	**25**	**odCB**	-	**120-5**	**0.87**	**2.32**	**60**	**1.22**
1:3	25	odCB	3	-	0.78	1.56	46	0.56
1:3	25	odCB	3	-	0.71	0.38	44	0.12
1:3	12	$CHCl_3$	-	-	0.84	1.00	60	0.51
1:3	12	$CHCl_3$	-	120-5	0.86	1.06	59	0.54
1:3	20	CB	-	-	0.84	1.49	63	0.79
1:3	20	CB	-	120-5	0.85	1.26	61	0.66
1:4	25	odCB	-	-	0.85	2.62	57	1.27
1:4	25	odCB	-	120-5	0.86	2.57	58	1.28

Table S6. Overview of the solar cell optimization studies for copolymer **PFIID-2T-BDT-2T**.

PFIID-2T-BDT-2T:$PC_{71}BM$ (w/w)	Total conc. (mg/mL)	Solvent	DIO (% v/v)	Annealing (°C-min)	V_{oc} (V)	J_{sc} (mA/cm^2)	FF (%)	PCE (%)
1:3	**25**	**odCB**	-	-	**0.68**	**6.33**	**57**	**2.45**
1:3	25	odCB	-	120-2	0.75	5.53	63	2.62
1:3	**25**	**odCB**	-	**120-5**	**0.74**	**4.68**	**64**	**2.23**
1:3	25	odCB	3	-	0.61	4.76	29	0.85
1:3	25	odCB	3	120-2	0.72	5.00	46	1.66
1:3	12	$CHCl_3$	-	-	0.74	1.42	68	0.72
1:3	12	$CHCl_3$	-	120-5	0.76	1.62	66	0.81
1:3	20	CB	-	-	0.64	2.47	43	0.68
1:3	20	CB	-	120-5	0.22	2.64	34	0.20
1:3	20	odCB	-	100-5	0.73	5.71	46	1.91
1:3	20	odCB	-	120-5	0.76	5.98	49	2.22

2. ^{1}H NMR spectra of monomers and polymers

Figure S1. ^{1}H NMR spectrum of monomer **6** ($CDCl_3$).

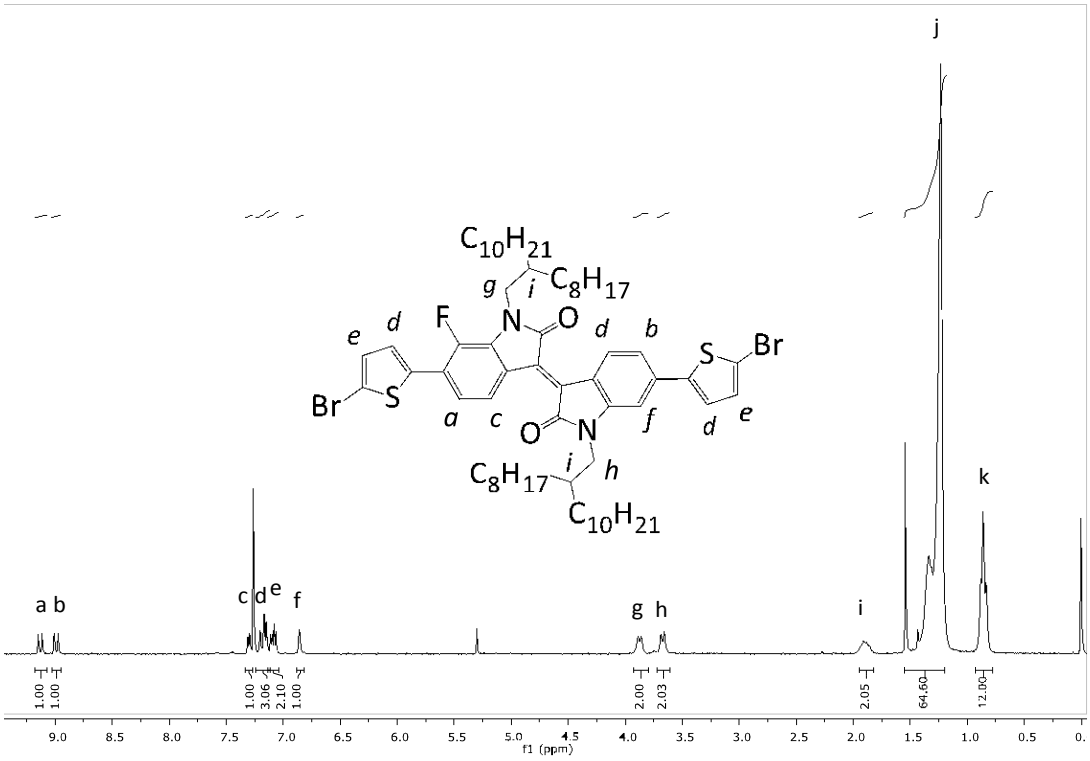
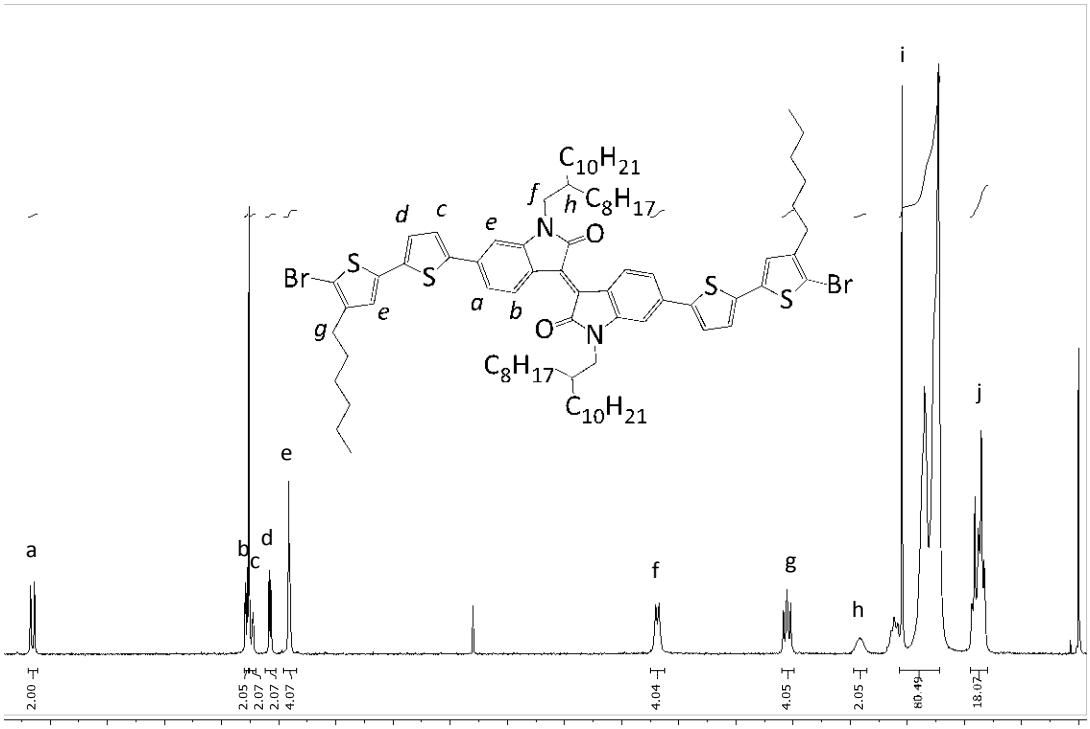


Figure S2. ^{1}H NMR spectrum of monomer **9** ($CDCl_3$).



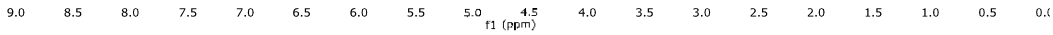

9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

Figure S3. ^{1}H NMR spectrum of monomer **10** ($CDCl_3$).

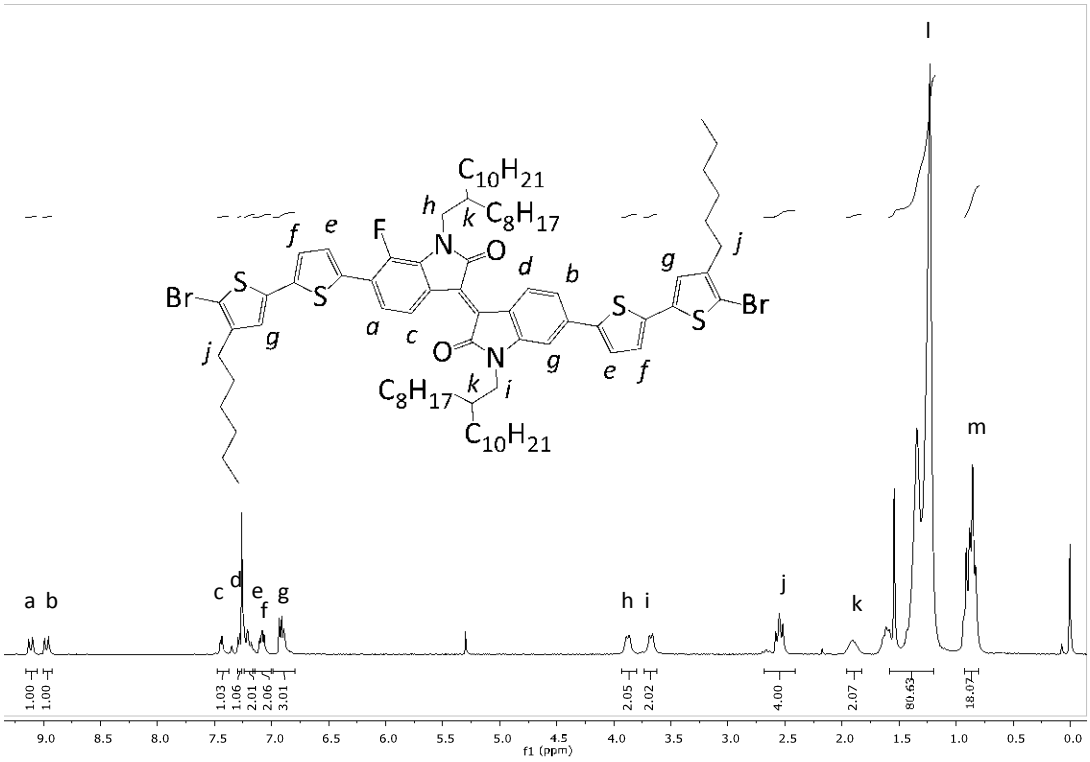


Figure S4. ^{1}H NMR spectrum of **PIID-5T** ($C_2D_2Cl_4$, 100 °C).

Figure S5. ^{1}H NMR spectrum of **PFIID-5T** ($C_2D_2Cl_4$, 100 °C).

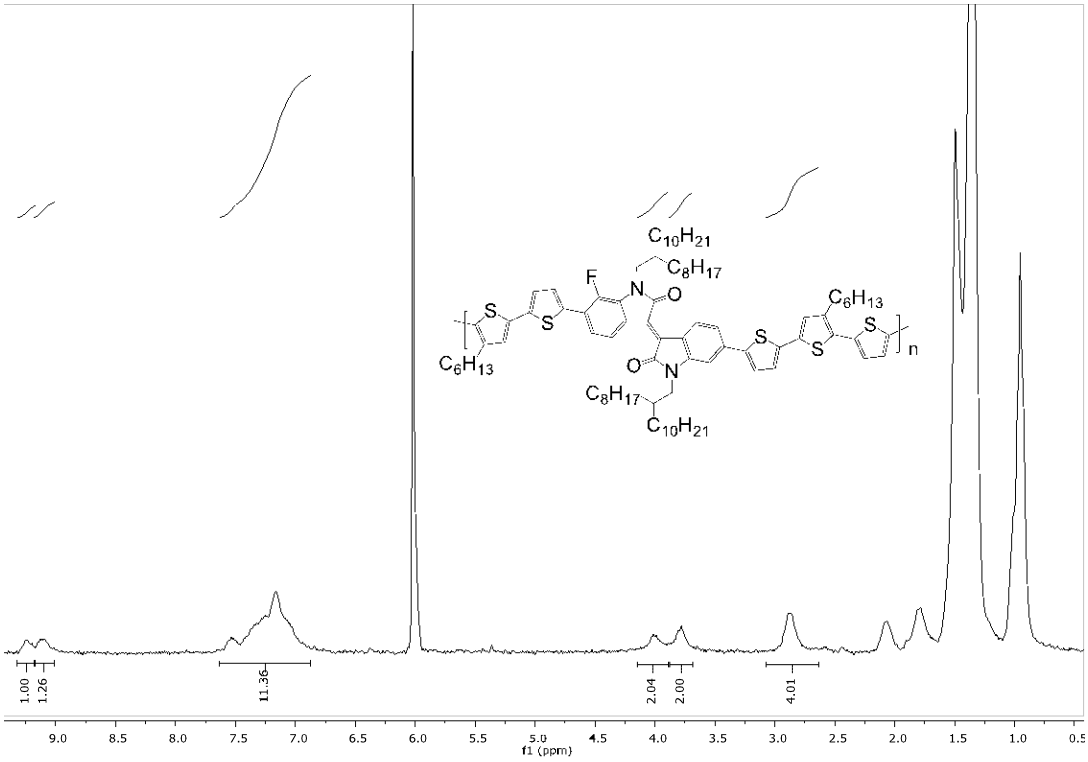


Figure S6. ^{1}H NMR spectrum of **PFIID-T-BDT-T** ($C_2D_2Cl_4$, 100 °C).

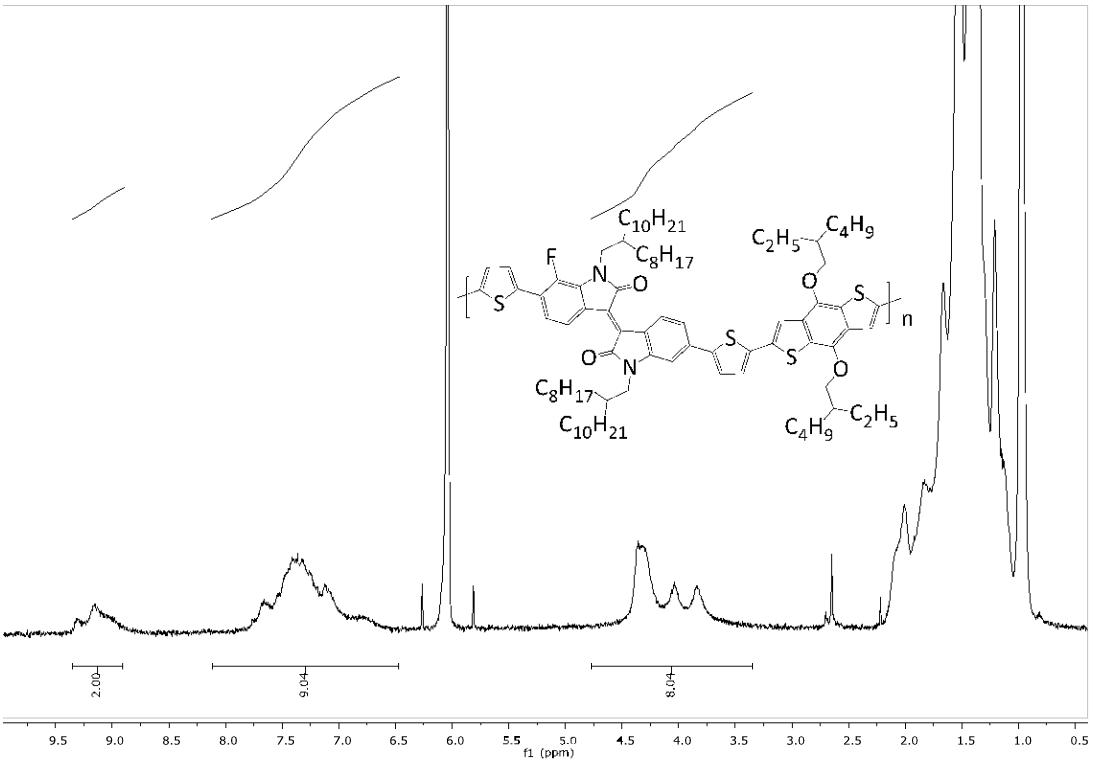
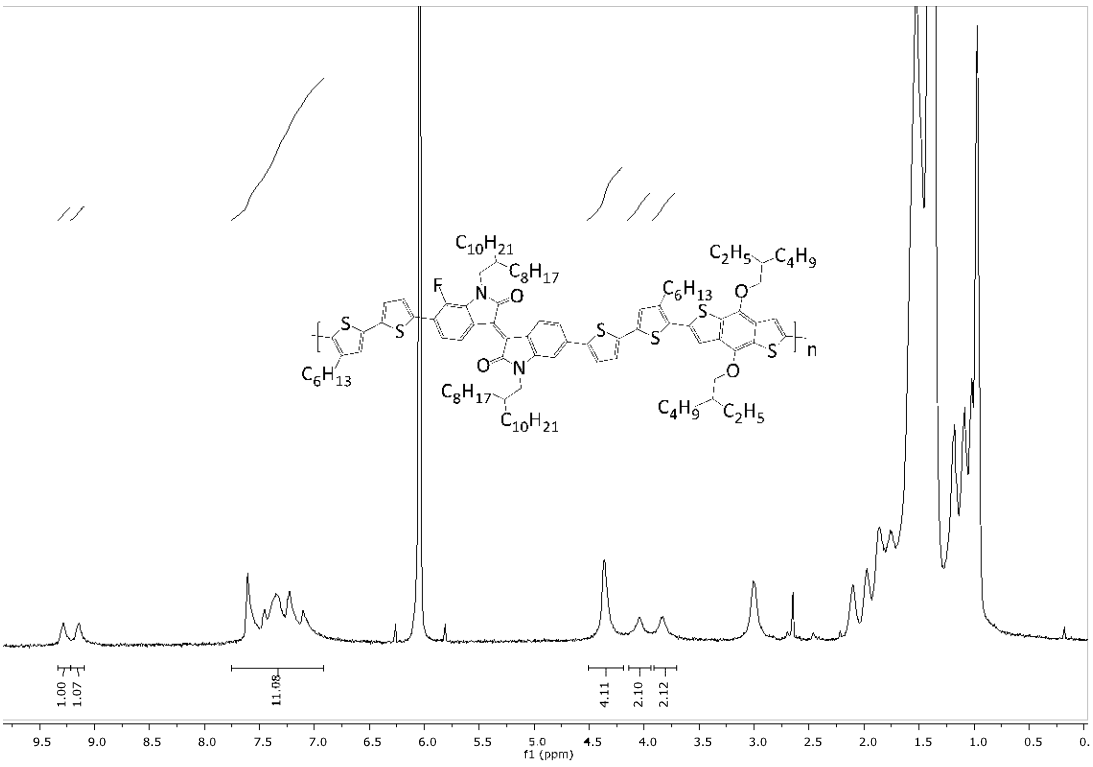
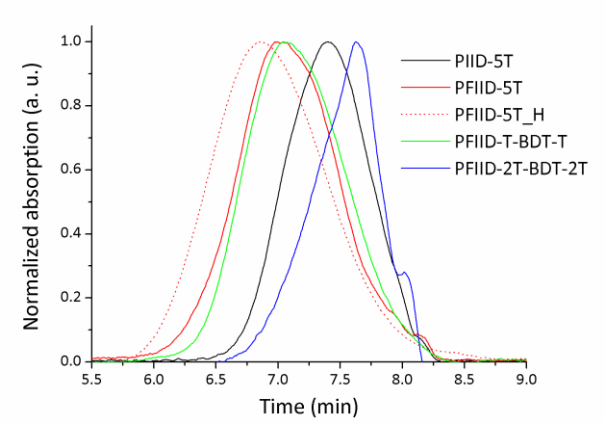


Figure S7. ^{1}H NMR spectrum of **PFIID-2T-BDT-2T** ($C_2D_2Cl_4$, 100 °C).



3. Gel permeation chromatograms and data

Figure S8. Gel permeation chromatograms for the copolymers (using *ortho*-dichlorobenzene at 140 °C as an eluent).



Copolymer	M_n (kg/mol)	D
PIID-5T	20.8	2.0
PFIID-5T	36.1	3.2
PFIID-5T_H	45.3	4.4
PFIID-T-BDT-T	32.8	2.8
PFIID-2T-BDT-2T	15.8	1.9