Electronic Supplementary Information

Effect of the π-linker on the performance of organic photovoltaic devices based on push-pull D-π-A molecules

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Table S1. Thermal properties of **3T** and **DTT**

Material	TGA[a] (°C)	T_m[b] (°C)
3T	309	170
DTT	305	208

[a] temperature at 5% weight loss under nitrogen. [b] determined by DSC under nitrogen.

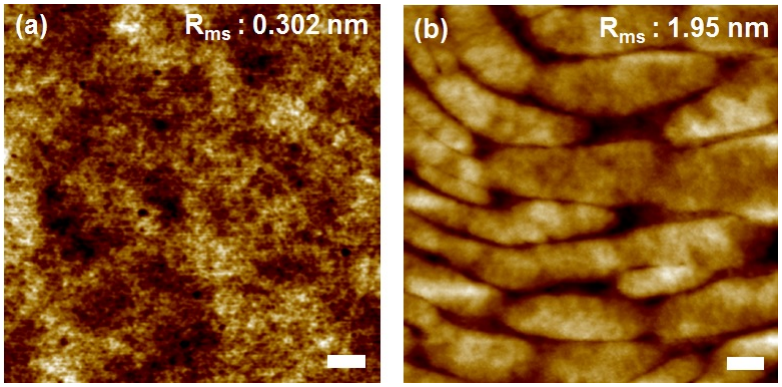

Fig. S1. Tapping mode AFM images of the thin films of (a) **3T** and (b) **DTT**. All scale bars are 200 nm.

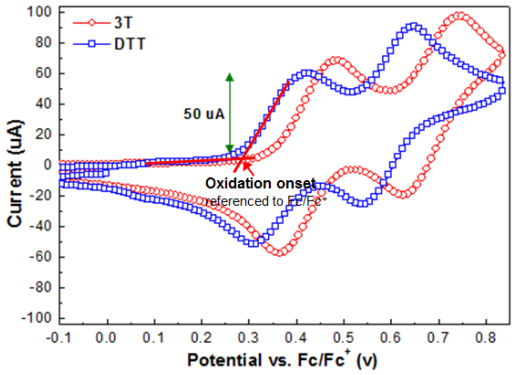

Fig. S2. Cyclic voltammograms of **3T** (red circle) and **DTT** (blue circle) in dichloromethane solution with tetrabutylammonium hexafluorophosphate (0.1 M $TBAPF_6$) as a supporting electrolyte at a scan rate of 0.05 V/s.

Table S2. Photovoltaic parameters of OPVs

Molecule of active layer	D:A ratio (w/w)	V_{oc} (V)	J_{sc} (mAcm^{-2})	FF (%)	PCE (%)
3T:$PC_{71}BM$	1:1	0.85	6.76	31	1.78
3T:$PC_{71}BM$	1:1.5	0.81	8.49	33	2.27
3T:$PC_{71}BM$	1:1.75	0.82	9.05	33	2.45
3T:$PC_{71}BM$	1:1.75[a]	0.85	9.19	33	2.58
3T:$PC_{71}BM$	1:2	0.77	9.90	32	2.44
3T:$PC_{71}BM$	1:3	0.57	9.74	32	1.77
DTT:$PC_{71}BM$	1:1.5	0.61	4.88	34	1.01
DTT:$PC_{71}BM$	1:1.75	0.72	8.11	31	1.81
DTT:$PC_{71}BM$	1:1.75[b]	0.76	9.50	33	2.38
DTT:$PC_{71}BM$	1:2	0.72	7.79	30	1.68

All thin films were made by spin-cast method using 2 *wt*% of **3T** or **DTT**:$PC_{71}BM$ active layer in chlorobenzene with varying weight ratios, [a]in chlorobenzene and chloroform solution (1:0.2 v/v), [b]with thermal annealing treatment at 150 °C for 10 min. All devices consist of ITO/PEDOT:PSS/**3T** or **DTT**:$PC_{71}BM$ (2 *wt*%)/LiF/Al.

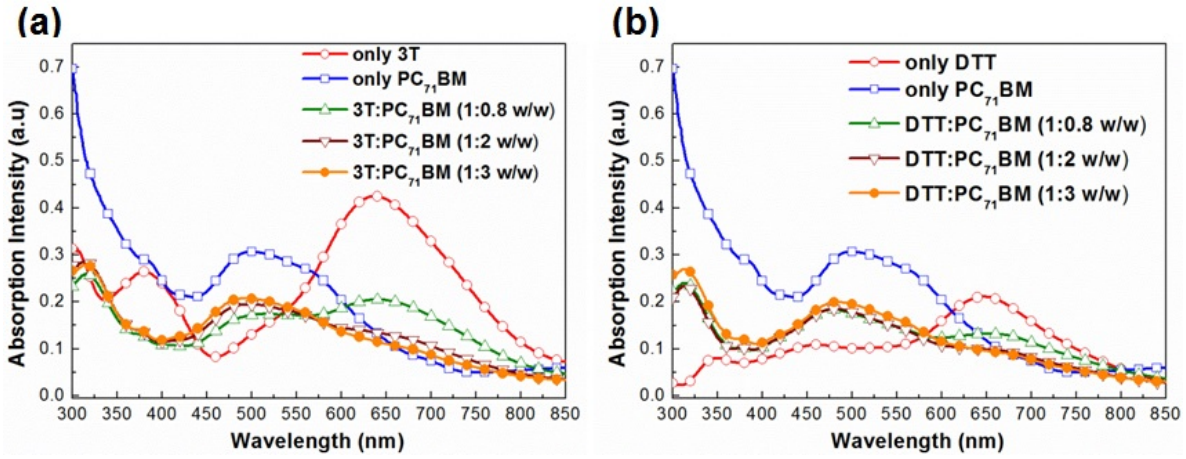

Fig. S3. UV/vis absorption spectra of (a) **3T** and (b) **DTT** thin films with various $PC_{71}BM$ concentrations

Table S3. Photovoltaic parameters of OPVs based on the **DTT**:$PC_{71}BM$ active layer

Molecules of active layer	D:A ratio (w/w)	Thermal annealing condition (°C)	V_{oc} (V)	J_{sc} ($mAcm^{-2}$)	FF (%)	PCE (%)
DTT:$PC_{71}BM$	1:1.75	120 °C, 10 min	0.74	9.04	31	2.07
		140 °C, 10 min	0.76	9.16	31	2.16
		150 °C, 10 min	0.76	9.50	33	2.38
		160 °C, 10 min	0.75	9.49	32	2.28
		180 °C, 10 min	0.66	9.26	32	1.96
		200 °C, 10 min	0.58	8.96	31	1.61

All thin films were spin-cast by 2 *wt*% of **DTT**:$PC_{71}BM$ active layer in chlorobenzene and chloroform (1:0.2 v/v) with thermal annealing treatment at 150 °C for 10 min. All devices consist of ITO/PEDOT:PSS/ **DTT**:$PC_{71}BM$ (2 *wt*%)/LiF/Al.

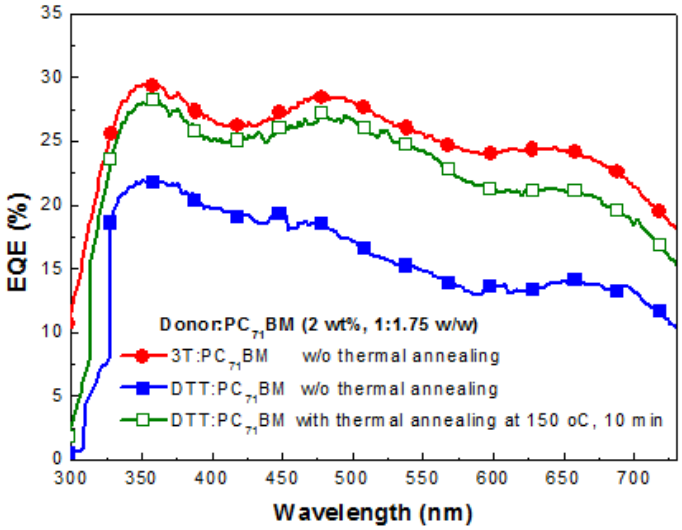

Fig. S4. EQE plots for BHJ devices (donor: $PC_{71}BM$ (2 wt%, 1:1.75 w/w))

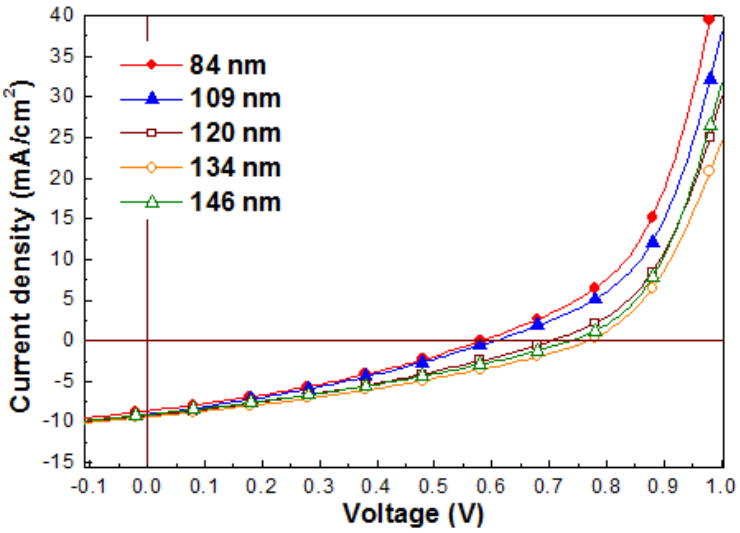

Fig. S5. Current density-voltage (J-V) characteristics of OPVs based on the **DTT**:$PC_{71}BM$ active layer according to the active layer thickness

Table S4. Photovoltaic parameters of OPVs based on the **DTT**:$PC_{71}BM$ active layer according to the active layer thickness

Active layer Thickness	V_{oc} (V)	J_{sc} ($mAcm^{-2}$)	FF (%)	PCE (%)
84 nm	0.58	8.59	33	1.62
109 nm	0.60	9.04	33	1.79
120 nm	0.70	9.18	32	2.08
132 nm	0.76	9.34	33	2.36
146 nm	0.73	9.03	32	2.14

All thin films were spin-cast by 2 *wt*% of the **DTT**:$PC_{71}BM$ active layer in chlorobenzene and chloroform (1:0.2 v/v) at various temperatures. All devices consist of ITO/PEDOT:PSS/ **DTT**:$PC_{71}BM$ (2 *wt*%)/LiF/Al.

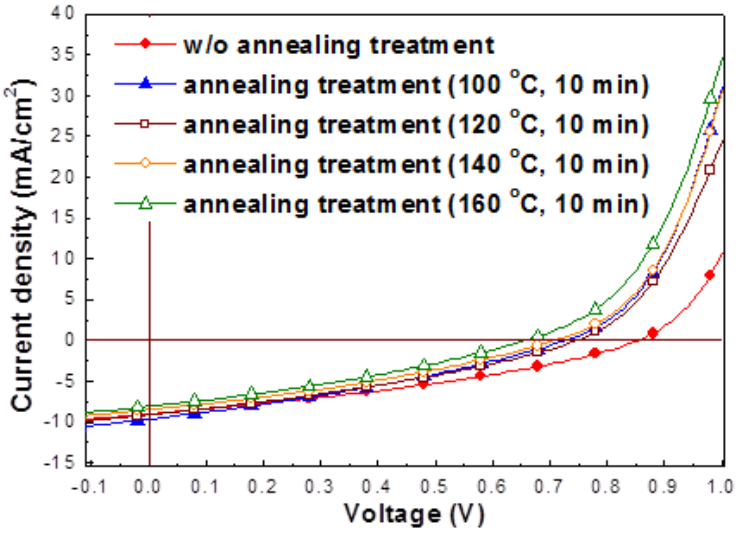

Fig. S6. Current density-voltage (J-V) characteristics of OPVs based on the **3T**:$PC_{71}BM$ active layer under various thermal annealing treatment conditions

Table S5. Photovoltaic parameters of OPVs based on the **3T**:$PC_{71}BM$ active layer under various thermal annealing treatment conditions

Thermal annealing condition (°C)	V_{oc} (V)	J_{sc} ($mAcm^{-2}$)	FF (%)	PCE (%)
w/o annealing treatment	0.85	9.02	34	2.63
100 °C, 10 min	0.72	9.65	32	2.21
120 °C, 10 min	0.73	9.03	33	2.17
140 °C, 10 min	0.69	8.40	33	1.90
160 °C, 10 min	0.64	7.99	32	1.66

All thin films were spin-cast by 2 *wt*% of the **3T**:$PC_{71}BM$ active layer in chlorobenzene and chloroform (1:0.2 v/v) under various thermal annealing treatment conditions. All devices consist of ITO/PEDOT:PSS/ **DTT**:$PC_{71}BM$ (2 *wt*%)/LiF/Al.

Fig. S7. ^{13}C NMR spectrum of **3T** in $CDCl_3$

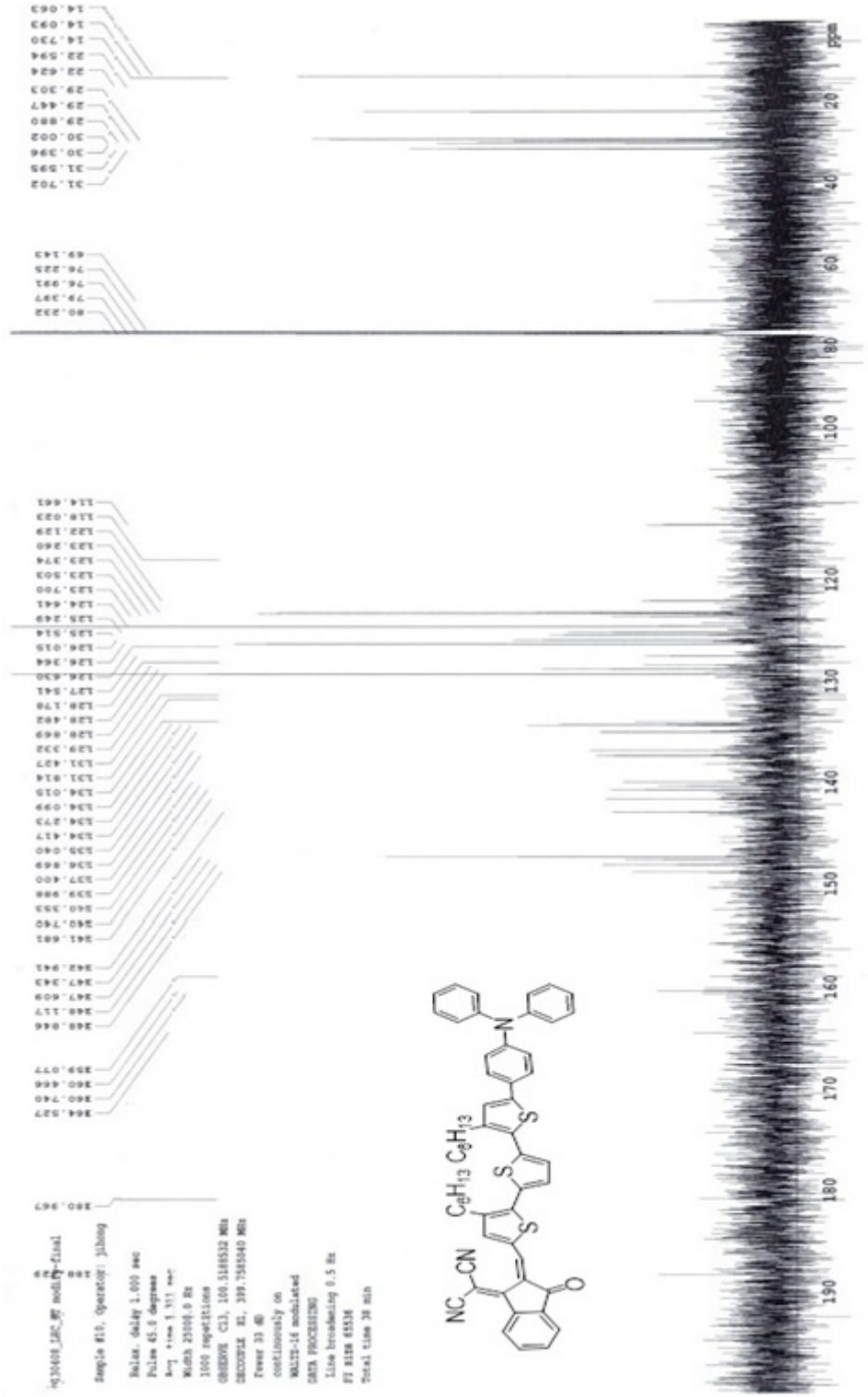

Fig. S8. ^{1}H NMR spectrum of **3T** in $CDCl_3$

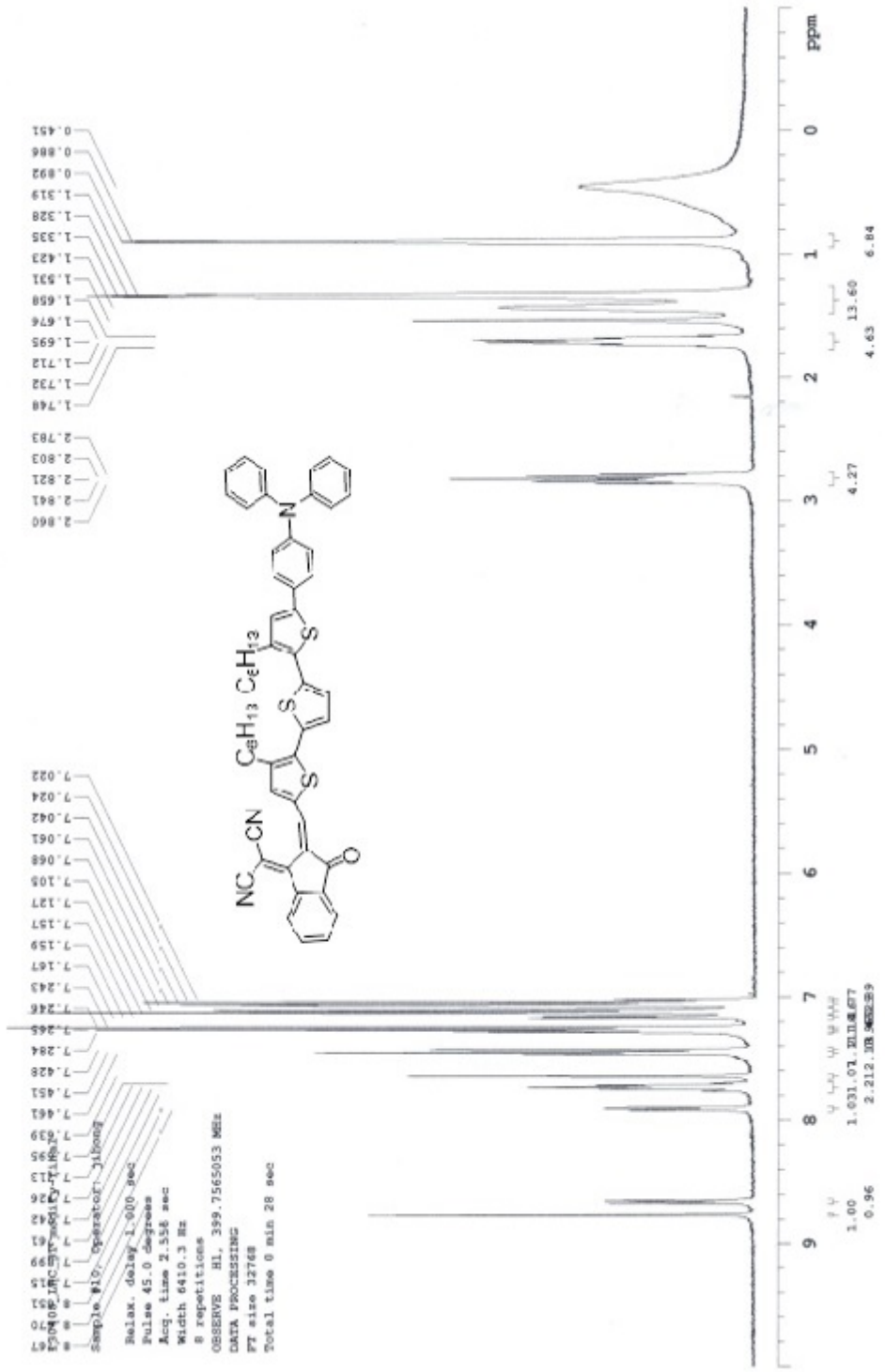

Fig. S9. ^{13}C NMR spectrum of **DTT** in $CDCl_3$

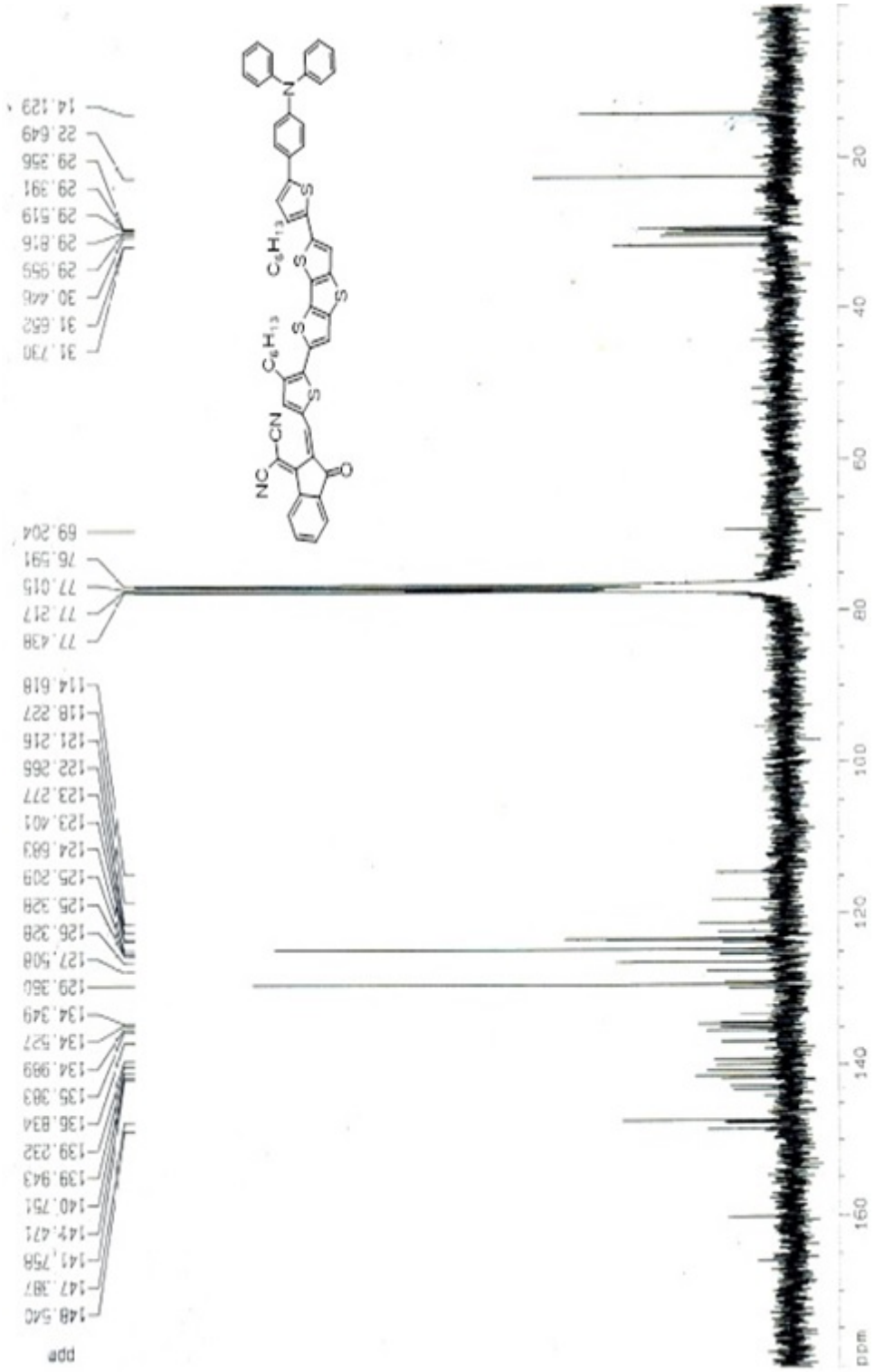

Fig. S10. ^{1}H NMR spectrum of **DTT** in $CDCl_3$

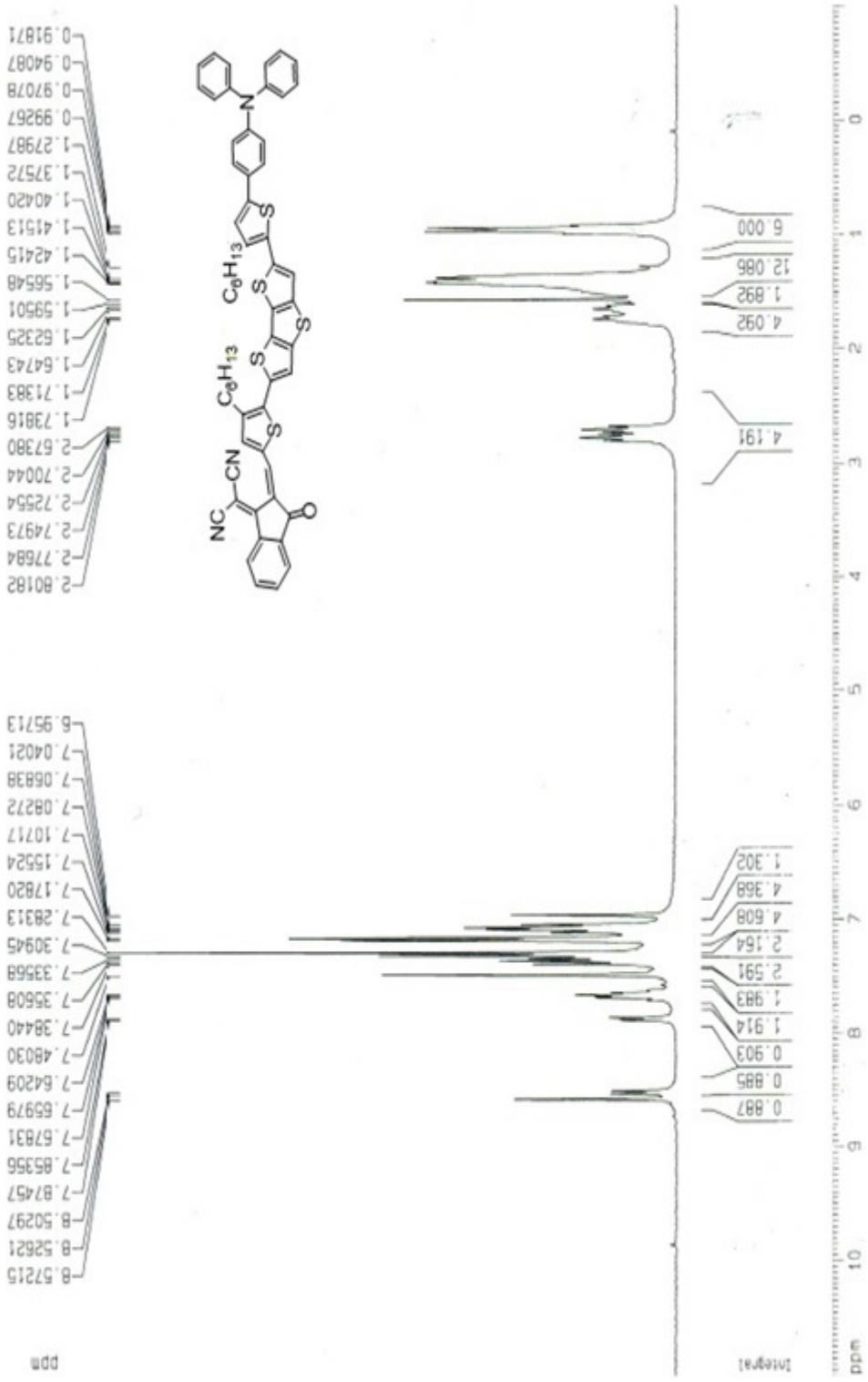

Fig. S11. Mass spectrum of **3T**

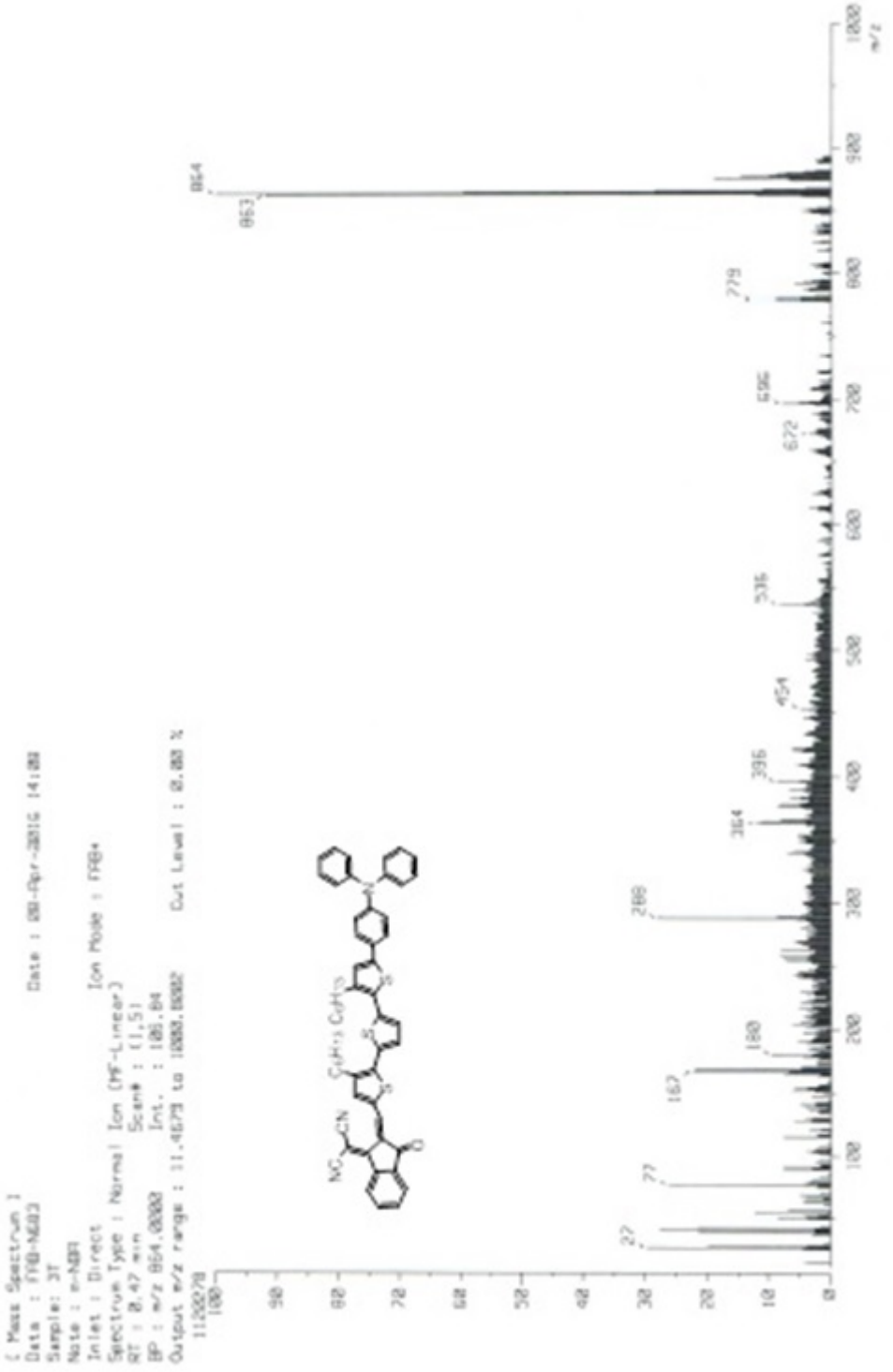

Fig. S12. Mass spectrum of **DTT**