Electronic Supplementary Information

Influence of moiety sequence on the performance of small molecular photovoltaic materials

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Table S1 Device optimization for the OSCs based on **BDT(ThBTTh)$_2$** and **BDT(BTTh$_2$)$_2$** [a]

Compound	Weight Ratio to $PC_{61}BM$	C_{total} (mg mL^{-1})	Additive [b] (amount)	$T_{annealing}$ (°C)	V_{OC} (V)	J_{SC} (mA cm^{-2})	FF (%)	PCE (%)
BDT(ThBTTh)$_2$	3:1	30	-	120	0.90	5.97	53.7	2.88
	1.5:1	30	-	120	0.91	7.94	56.8	4.10
	1:1	30	-	100	0.86	7.57	64.1	4.19
	1:1	**30**	**-**	**120**	**0.89**	**9.33**	**54.5**	**4.53**
	1:1	40	-	120	0.86	9.07	54.7	4.28
	1:1	30	-	140	0.87	3.85	45.9	1.53
	1:2	30	-	120	0.90	4.92	60.0	2.65
	1:3	30	-	120	0.87	2.24	65.2	1.27
	1:1	30	DIO (0.25% in v/v)	120	0.84	6.30	42.4	2.25
	1:1	30	DIO (0.5% in v/v)	120	0.21	3.77	26.1	0.21
	1:1	30	PDMS (0.2 mg mL^{-1})	120	0.88	8.57	55.7	4.19
BDT(BTTh$_2$)$_2$	3:1	30	-	120	0.53	3.36	36.7	0.65
	1.5:1	30	-	120	0.76	3.19	38.6	0.93
	1:1	30	-	80	0.74	1.96	38.0	0.55
	1:1	30	-	100	0.74	4.59	36.7	1.25
	1:1	20	-	120	0.63	4.52	35.8	1.02
	1:1	**30**	**-**	**120**	**0.82**	**4.74**	**40.5**	**1.58**
	1:1	40	-	120	0.76	3.73	37.9	1.08
	1:1	30	-	140	0.53	2.73	28.8	0.42
	1:2	30	-	120	0.62	2.81	33.7	0.59
	1:3	30	-	120	0.54	1.08	33.2	0.19
	1:1	30	DIO (0.25% in v/v)	120	0.51	3.45	33.2	0.59
	1:1	30	DIO (0.5% in v/v)	120	0.33	0.75	28.5	0.07
	1:1	30	PDMS (0.2 mg mL^{-1})	120	0.74	4.13	40.9	1.26

[a] Other conditions: annealing for 10 min, spin coated at 1000 rpm for 30 s

[b] DIO: 1,8-diiodoctane, PDMS: polydimethylsiloxane.

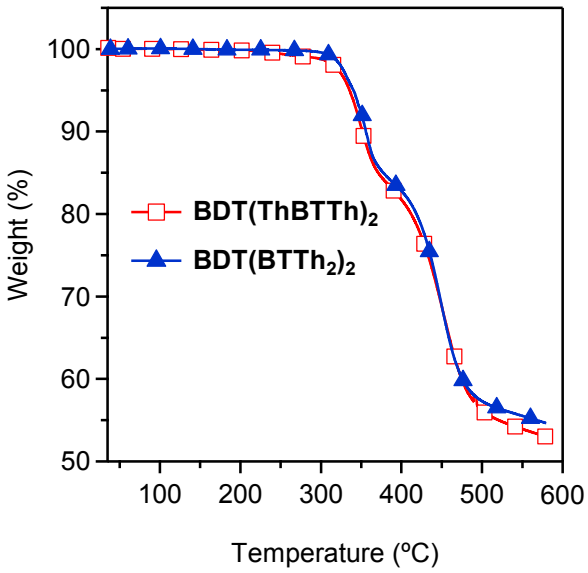

Fig. S1 TGA curves of **BDT(ThBTTh)$_2$** and **BDT(BTTh$_2$)$_2$**, at a heating rate of 10 °C min $^{-1}$ under N_2.

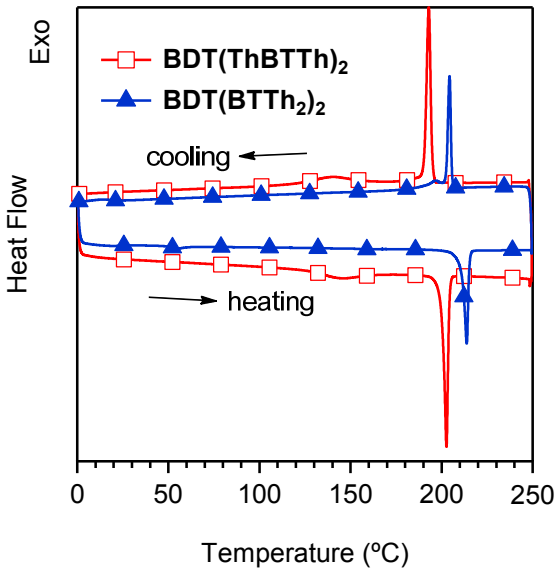

Fig. S2 The second heating and cooling DSC curves of **BDT(ThBTTh)$_2$** and **BDT(BTTh$_2$)$_2$**, at a heating and cooling rate of 10 ^{o}C min^{-1} under N_2.

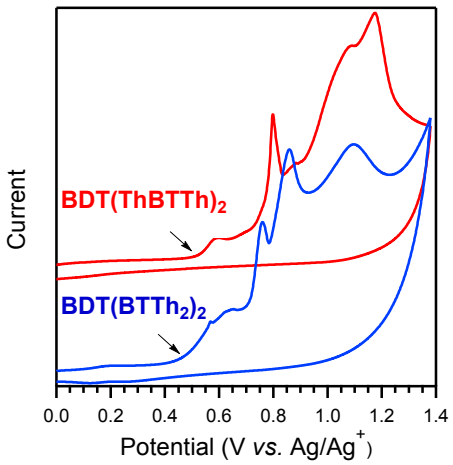

Fig. S3 Cyclic voltammograms of **BDT(ThBTTh)$_2$** and **BDT(BTTh$_2$)$_2$** films. The film samples were casted from chlorobenzene solutions onto glassy carbon electrodes and measured in CH_3CN containing 0.1 M Bu_4NPF_6 at a scan rate of 50 mV s^{-1}.

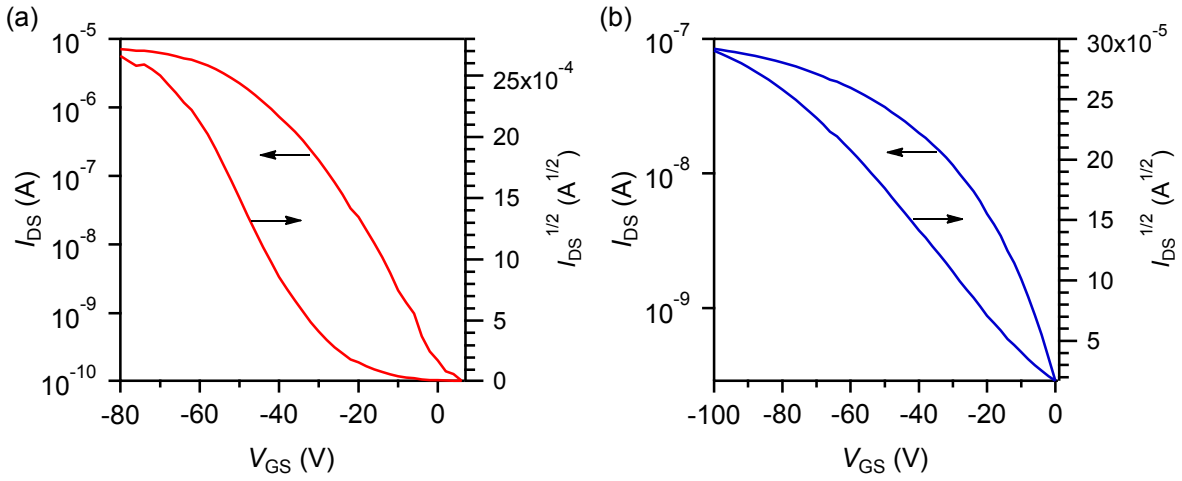

Fig. S4 The OFET transfer curves of (a) **BDT(ThBTTh)$_2$** and (b) **BDT(BTTh$_2$)$_2$** measured with a device structure of Si/SiO_2/OTS/active layer/Au.

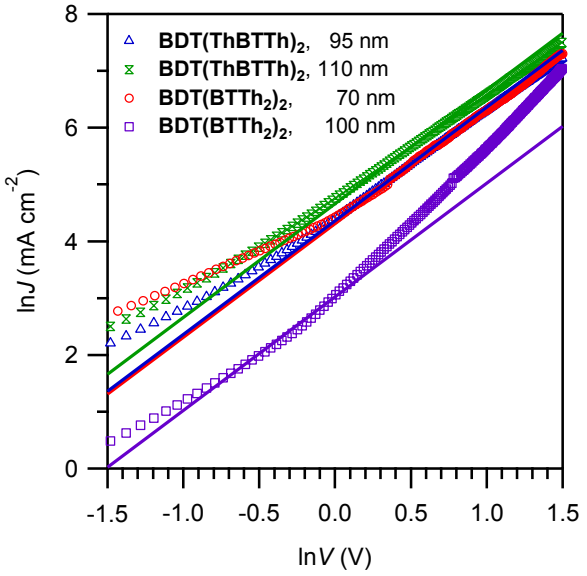

Fig. S5 ln*J*–ln*V* and their SCLC fitting curves of **BDT(ThBTTh)$_2$** and **BDT(BTTh$_2$)$_2$** blend films with $PC_{61}BM$ (1/1, w/w) under different thicknesses.

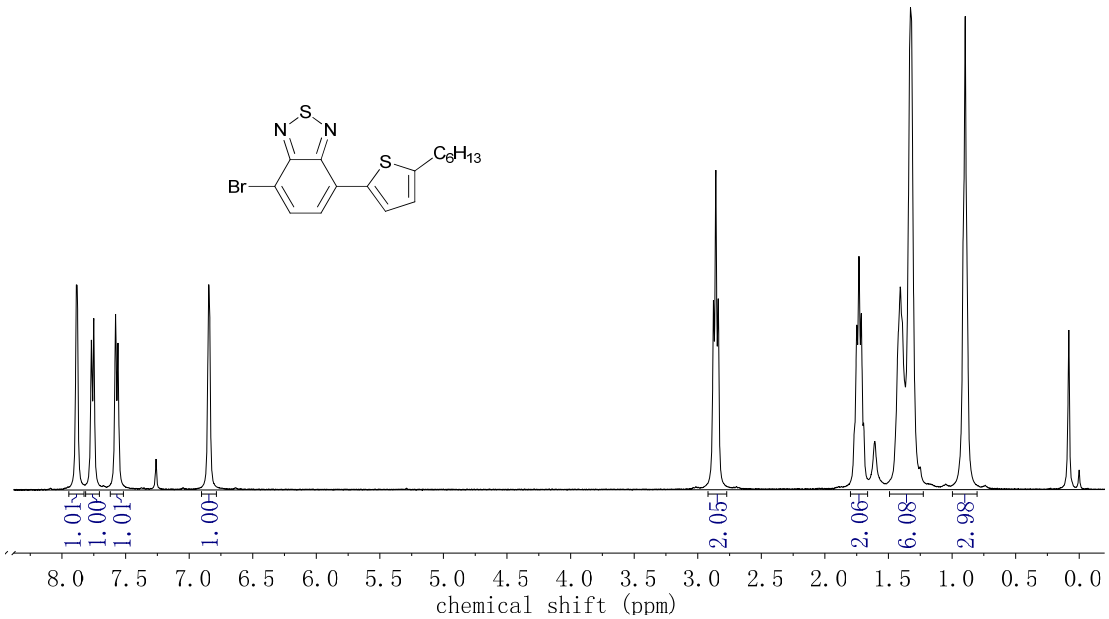

Fig. S6 ^{1}H NMR spectrum of compound **1** in $CDCl_3$ at room temperature.

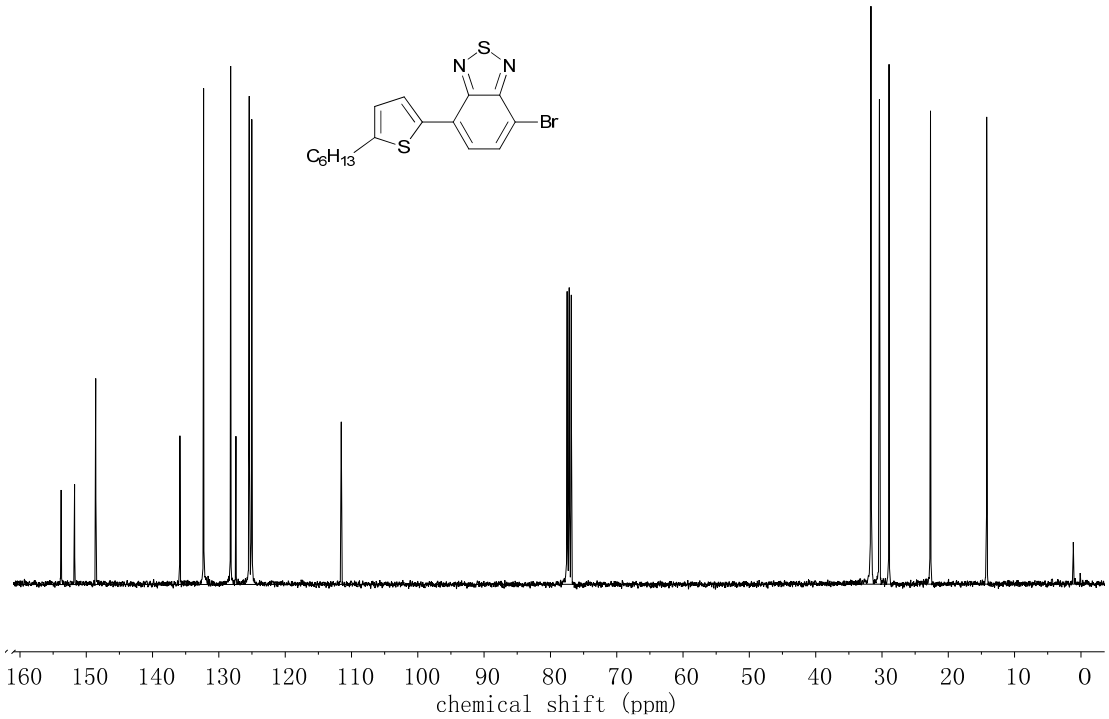

Fig. S7 ^{13}C NMR spectrum of compound **1** in $CDCl_3$ at room temperature.

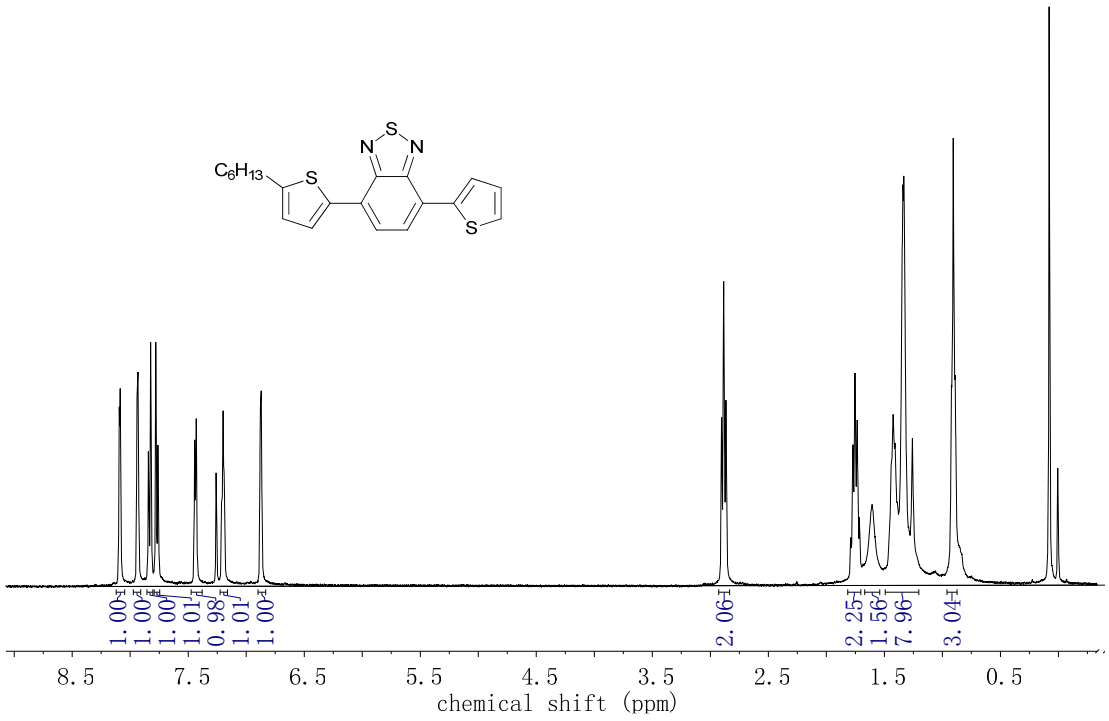

Fig. S8 ^{1}H NMR spectrum of compound **2** in $CDCl_3$ at room temperature.

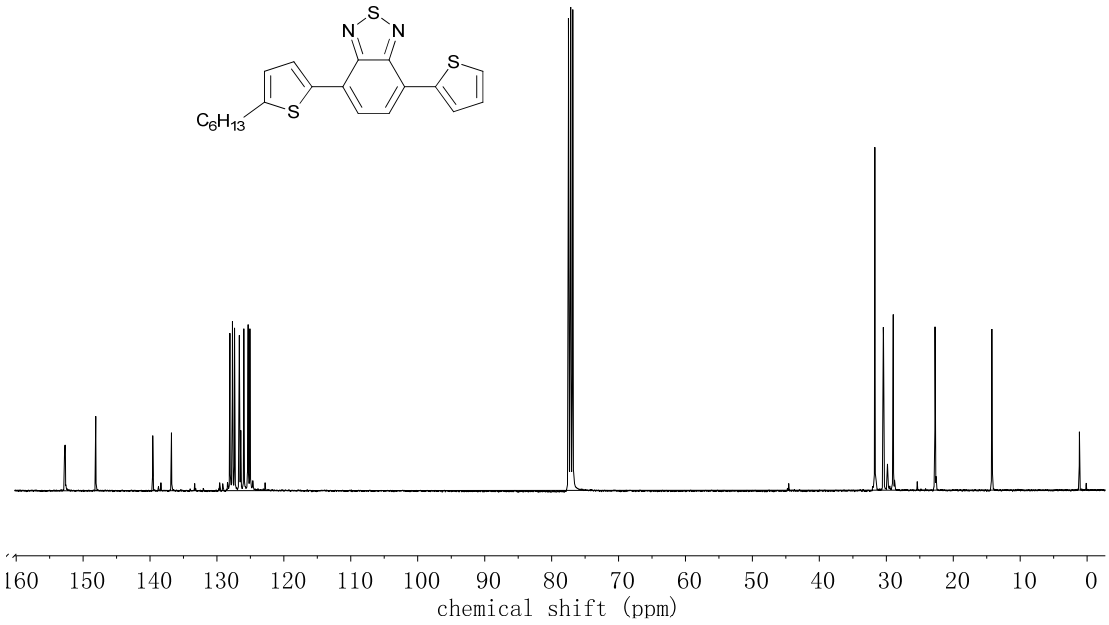

Fig. S9 ^{13}C NMR spectrum of compound **2** in $CDCl_3$ at room temperature.

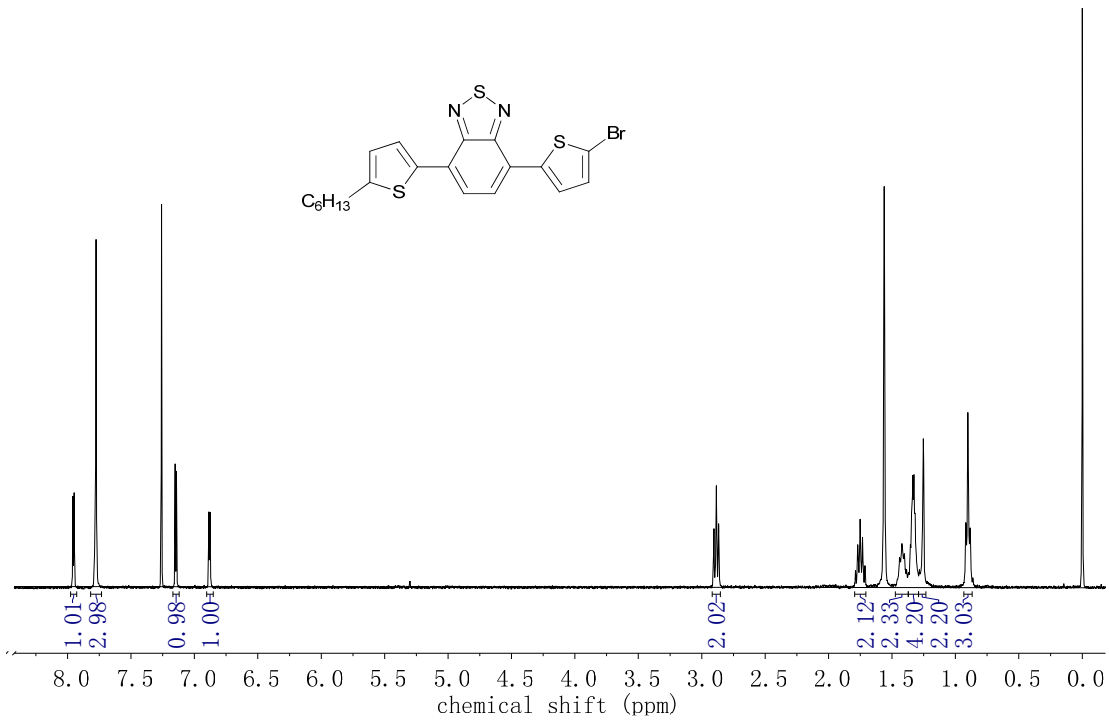

Fig. S10 ^{1}H NMR spectrum of compound **3** in $CDCl_3$ at room temperature.

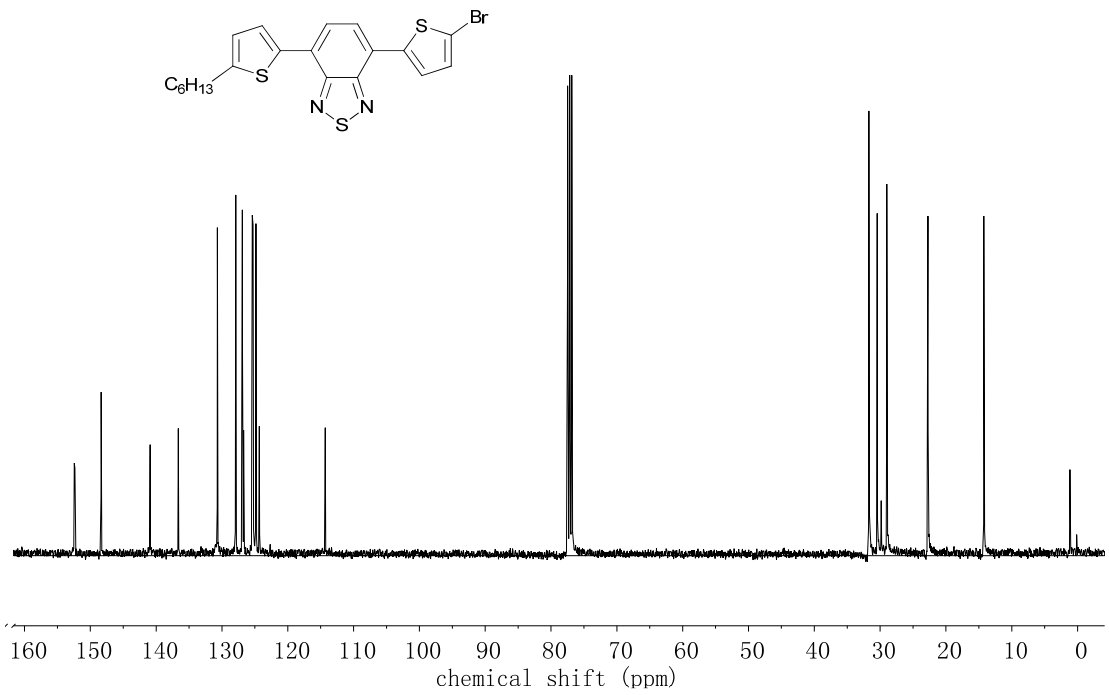

Fig. S11 ^{13}C NMR spectrum of compound **3** in $CDCl_3$ at room temperature.

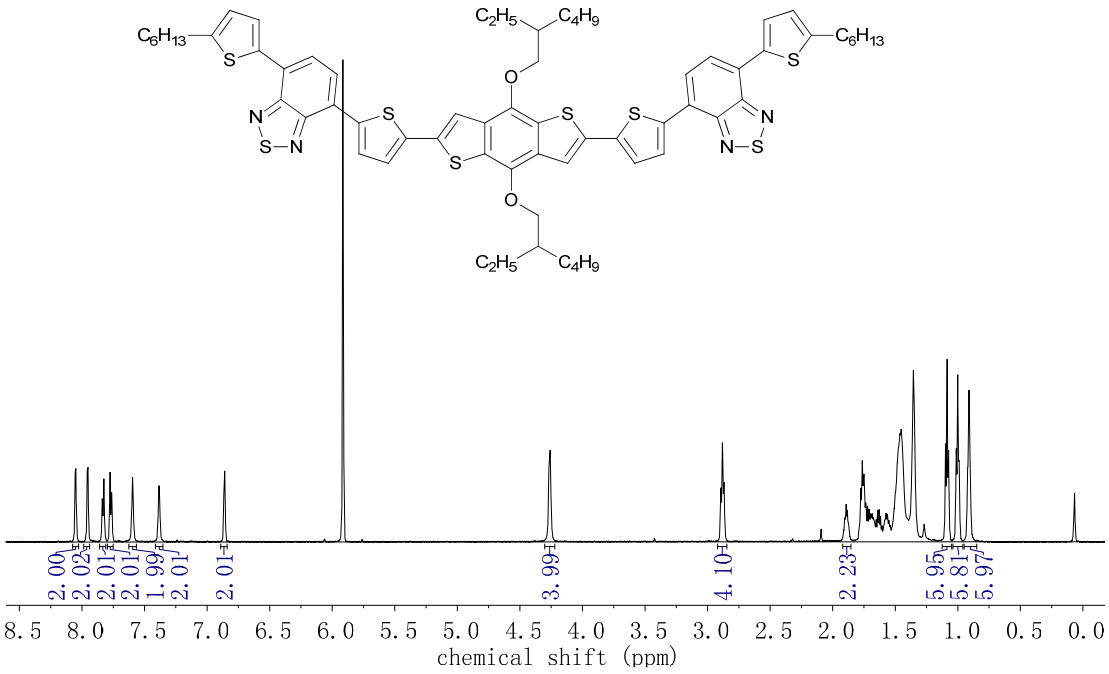

Fig. S12 ^{1}H NMR spectrum of **BDT(ThBTTh)$_2$** in CD_2Cl_4 at 110 ^{o}C.

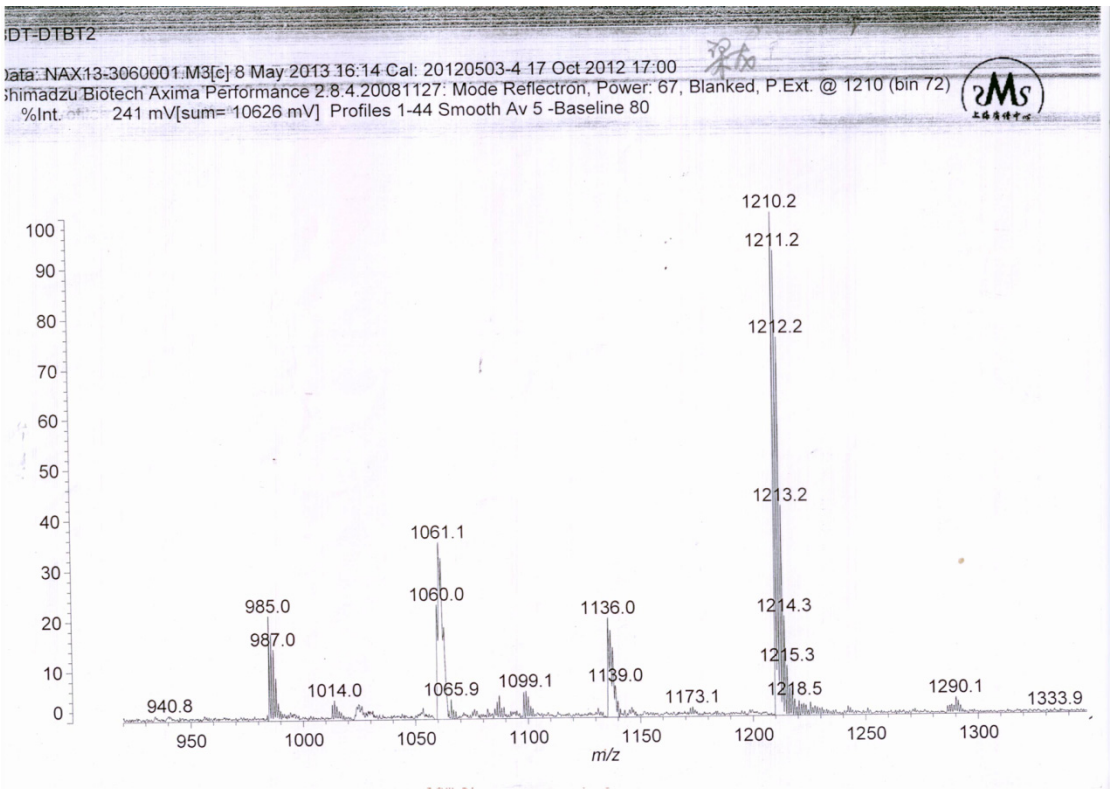

Fig. S13 MALDI-TOF mass spectrum of **BDT(ThBTTh)$_2$**.

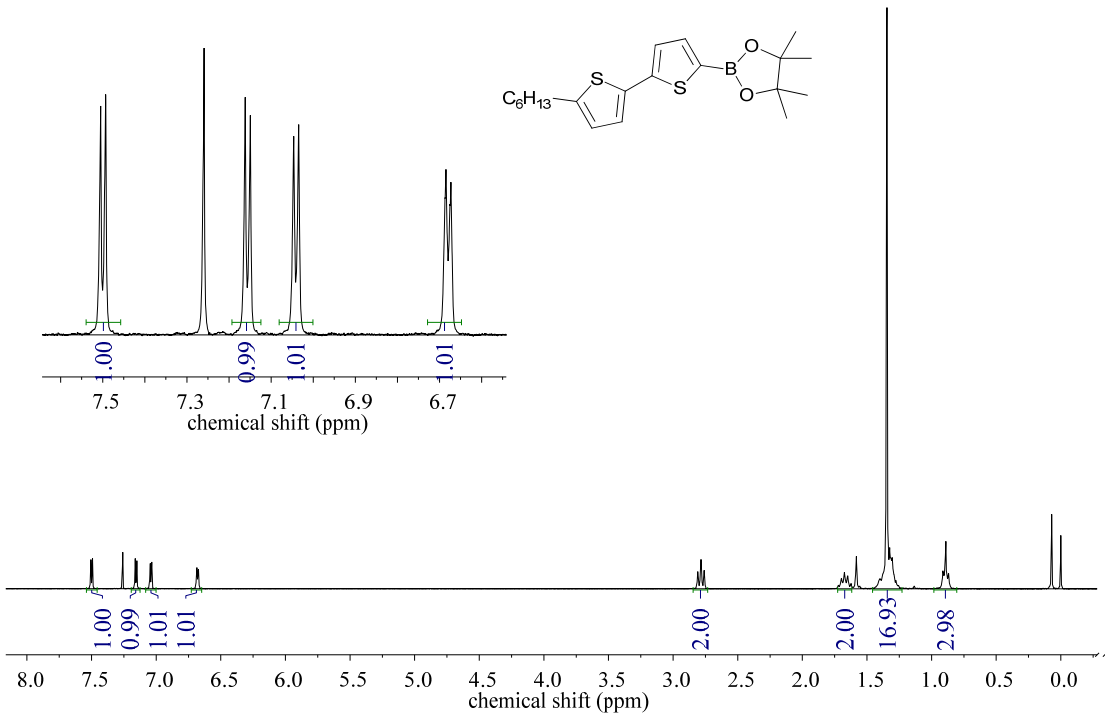

Fig. S14 ^{1}H NMR spectrum of compound **4** in $CDCl_3$ at room temperature.

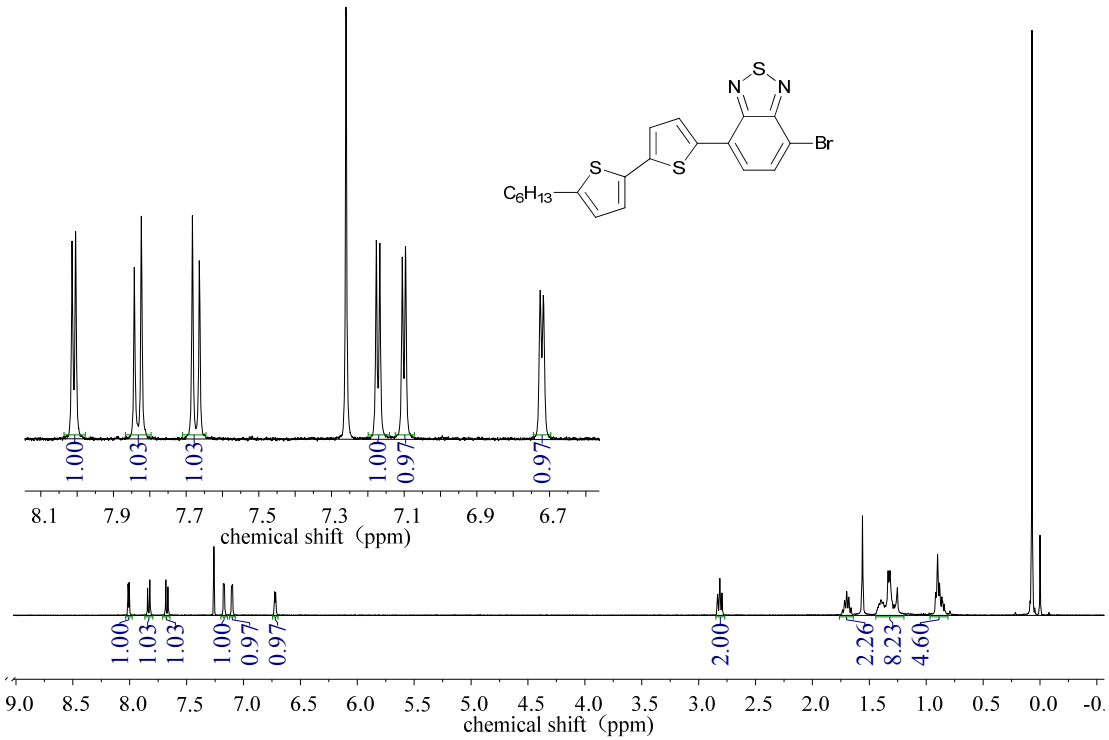

Fig. S15 ^{1}H NMR spectrum of compound **5** in $CDCl_3$ at room temperature.

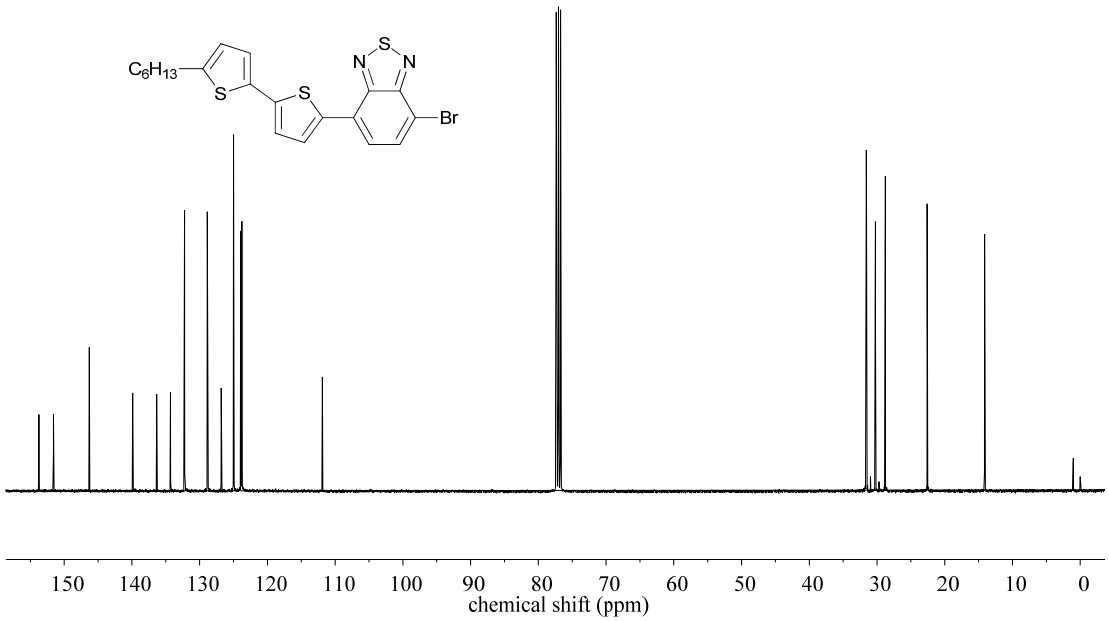

Fig. S16 ^{13}C NMR spectrum of compound **5** in $CDCl_3$ at room temperature.

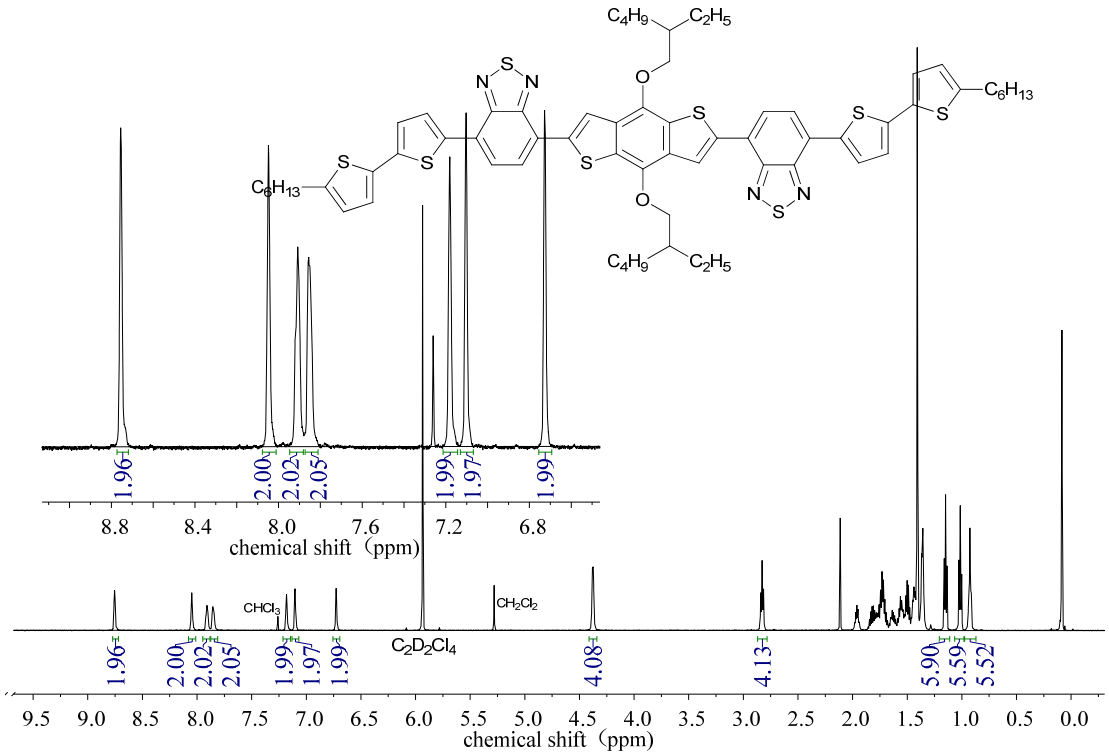

Fig. S17 ^{1}H NMR spectrum of compound **BDT(BTTh$_2$)$_2$** in CD_2Cl_4 at 110 ^{o}C.

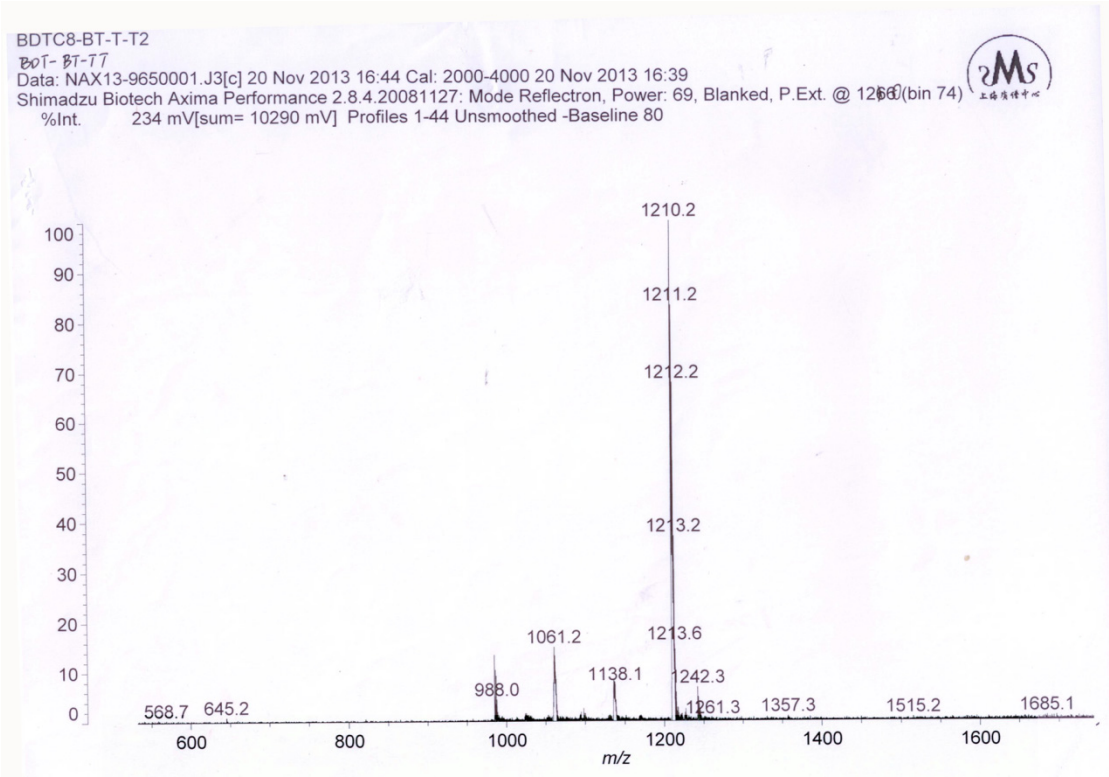

Fig. S18 MALDI-TOF mass spectrum of compound **BDT(BTTh$_2$)$_2$**.