

Supporting Information

Wide-bandgap dithienobenzodithiophene-based π - conjugated polymers consisting of fluorinated benzotriazole and benzothiadiazole for polymer solar cells

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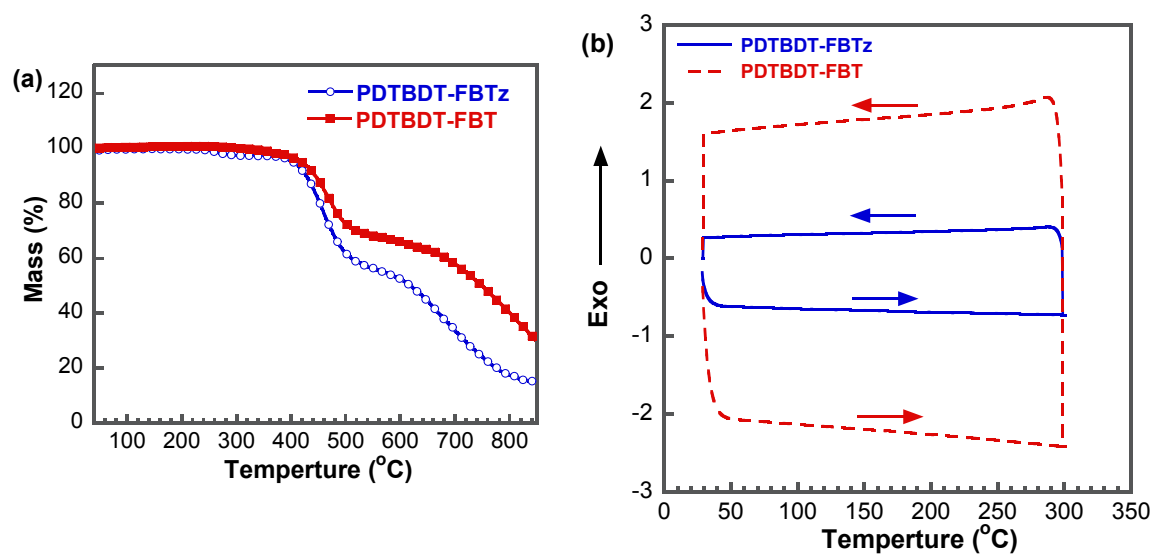


Fig. S1 TGA curves (a) and DSC (b) traces of copolymers.

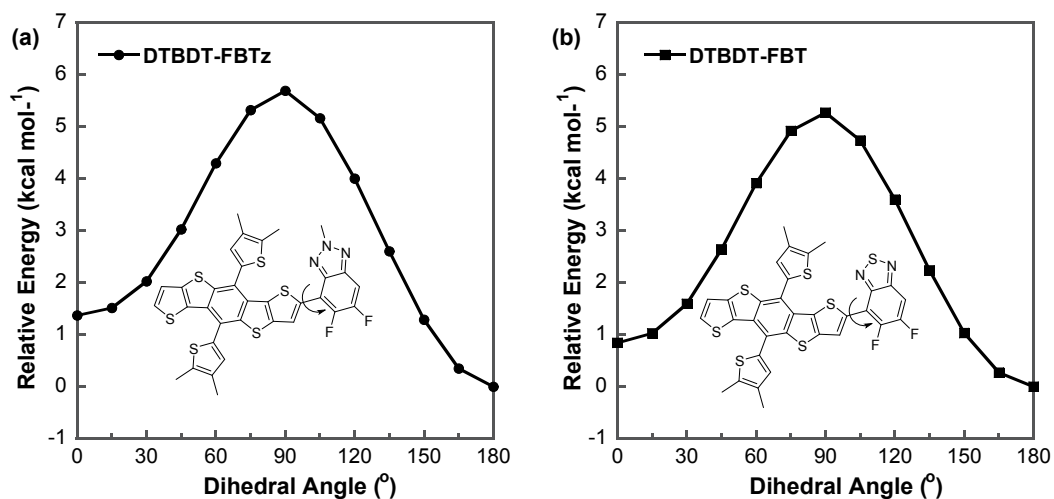


Fig. S2 PESs plot of relative energy as a function of dihedral angle for DTBBDT-FBTz (a) and DTBBDT-FBT (b).

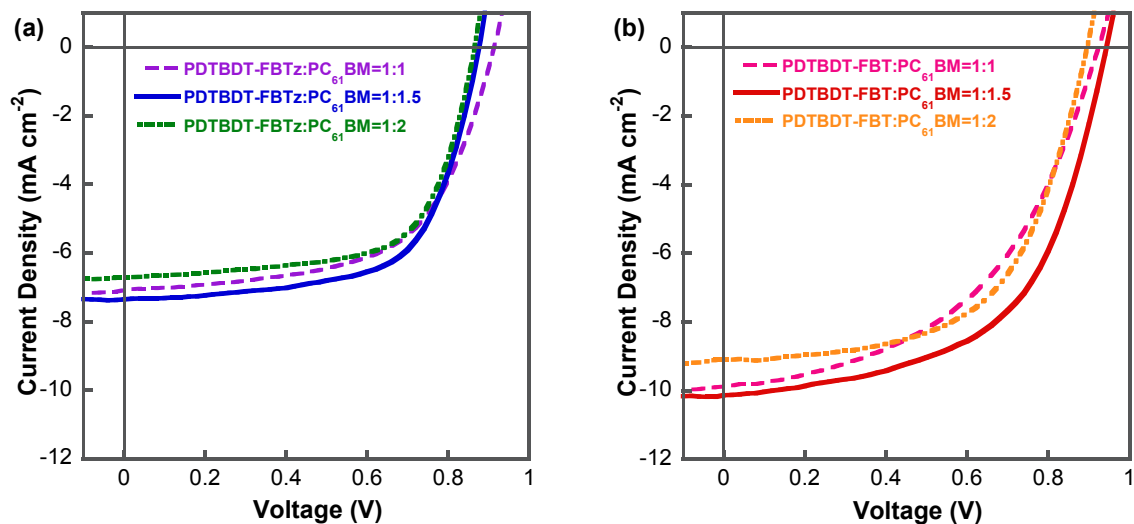


Fig. S3 J - V curves of photovoltaic devices based on polymer:PC₆₁BM blend films with different D/A ratios (a: PDTBDT-FBTz:PC₆₁BM; b: PDTBDT-FBT:PC₆₁BM) under the illumination of AM 1.5 G, 100 mW cm⁻².

Table S1. Photovoltaic properties of the PSCs based on copolymers with different blend ratios. Device structure: ITO/PEDOT:PSS/polymer:PC₆₁BM/Ca/Al.

polymer	polymer/PC ₆₁ BM (wt:wt)	J_{sc} (mA cm ⁻²)	V_{oc} (V)	FF (%)	PCE (%)
PDTBDT-FBTz	1:1	7.08	0.91	59.5	3.83
	1:1.5	7.35	0.88	64.5	4.17
	1:2	6.71	0.86	65.5	3.78
PDTBDT-FBT	1:1	9.88	0.92	48.4	4.40
	1:1.5	10.14	0.94	56.2	5.36
	1:2	9.11	0.90	58.1	4.76

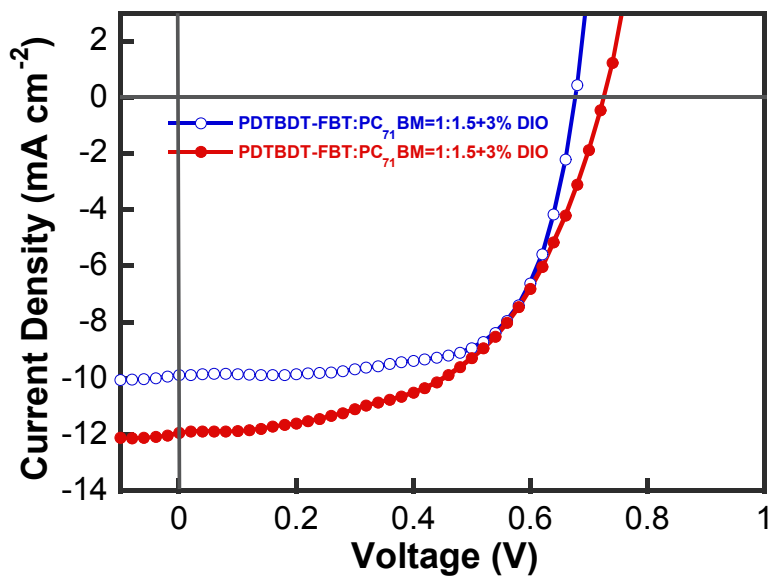


Fig. S4 J - V curves of devices based on polymer:PC₇₁BM (1:1.5, wt:wt) with 3% DIO additive under the illumination of AM 1.5 G, 100 mW cm⁻².

Table S2 Photovoltaic Properties of devices based on polymer:PC₇₁BM (1:1.5, wt:wt) with 3% DIO additive under the illumination of AM 1.5 G, 100 mW cm⁻².

polymer	polymer/PC ₇₁ BM (wt:wt)	DIO	J_{sc} (mA cm ⁻²)	V_{oc} (V)	FF (%)	PCE (%)
PDTBDT-FBTz	1:1.5	3%	9.88	0.68	67.7	4.55
PDTBDT-FBT	1:1.5	3%	11.93	0.72	53.6	4.60

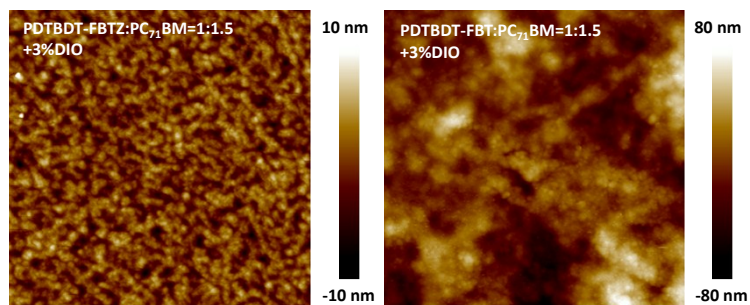


Fig. S5 AFM topography images (5 μm × 5 μm) of polymer:PC₇₁BM (1:1.5, wt:wt) blend films with 3% DIO additive spin-coated on ITO/PEDOT:PSS substrates.

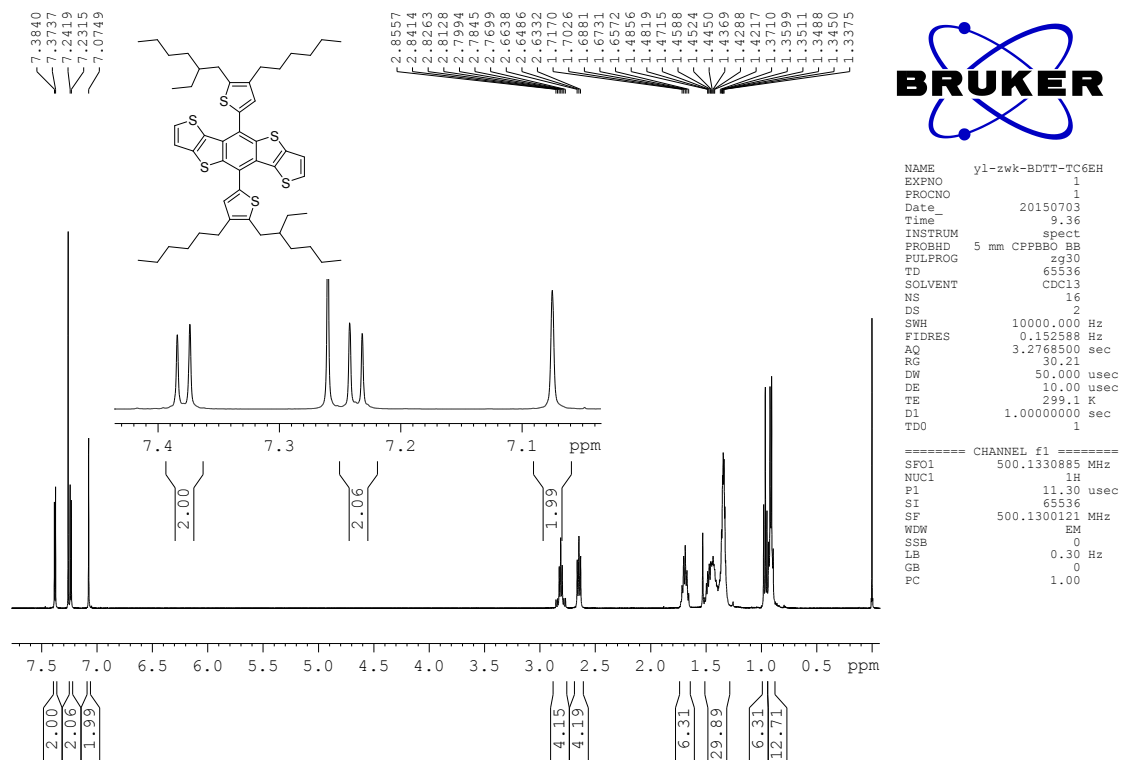


Fig. S6 ¹H NMR spectra of compound 2.

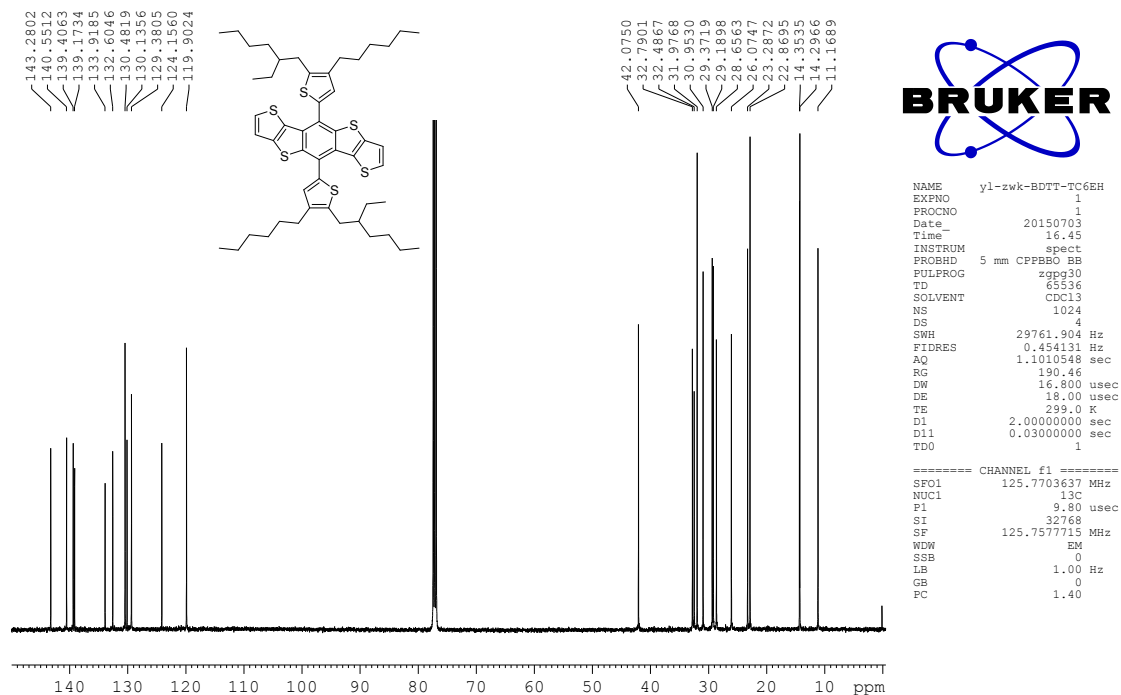
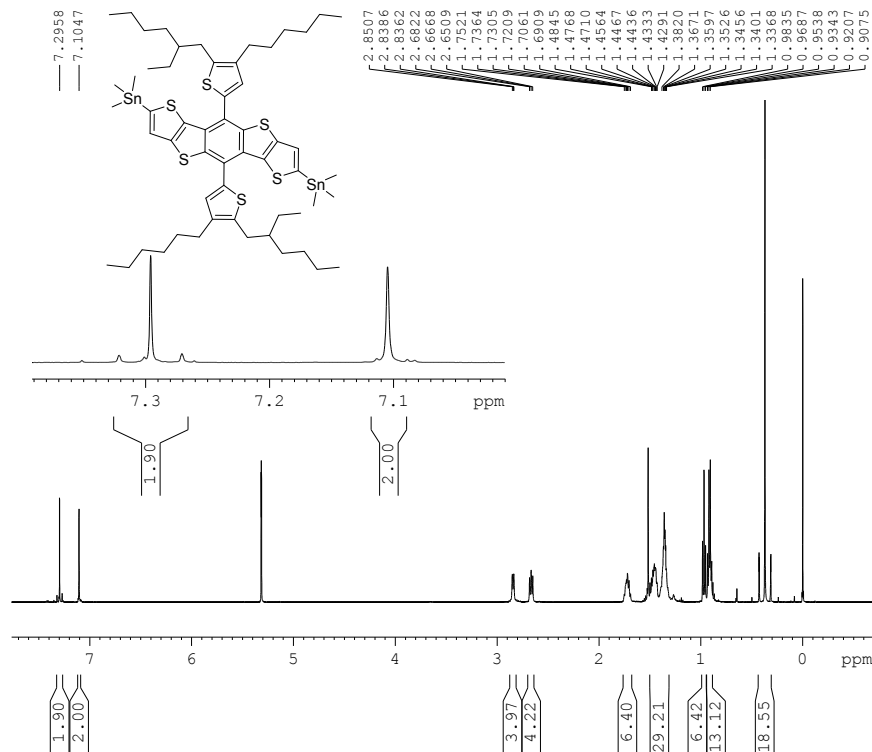


Fig. S7 ¹³C NMR spectra of compound 2.

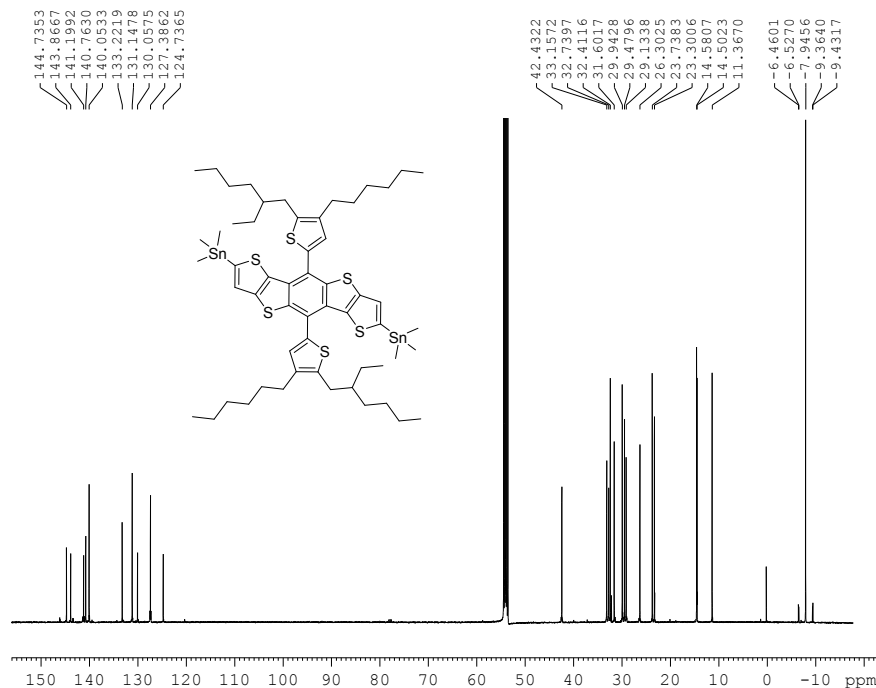


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PROCNO    1
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Time      12.55
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PULPROG   zg30
TD         65536
SOLVENT   CD2Cl2
NS         16
DS         2
SWH       10000.000 Hz
FIDRES    0.152588 Hz
AQ         3.2768500 sec
RG         30.21
DW         50.000 usec
DE         10.00 usec
TE         299.1 K
D1         1.00000000 sec
TDO        1

===== CHANNEL f1 =====
SF01      500.1330885 MHz
NUC1       1H
P1         11.14 usec
SI         65536
SF         500.13300212 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
  
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Fig. S8 ¹H NMR spectra of M1.



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NAME      yl-zwk-01C-Me3SnDTBDT
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PROCNO    1
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INSTRUM   spect
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PULPROG   zgpg30
TD         65536
SOLVENT   CD2Cl2
NS         5000
DS         4
SWH       29761.904 Hz
FIDRES    0.454131 Hz
AQ         1.1010548 sec
RG         190.46
DW         16.800 usec
DE         18.00 usec
TE         299.2 K
D1         2.00000000 sec
D11        0.03000000 sec
TDO        1

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NUC1      13C
P1         9.80 usec
SI         32768
SF         125.7577141 MHz
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Fig. S9 ¹³C NMR spectra of M1.

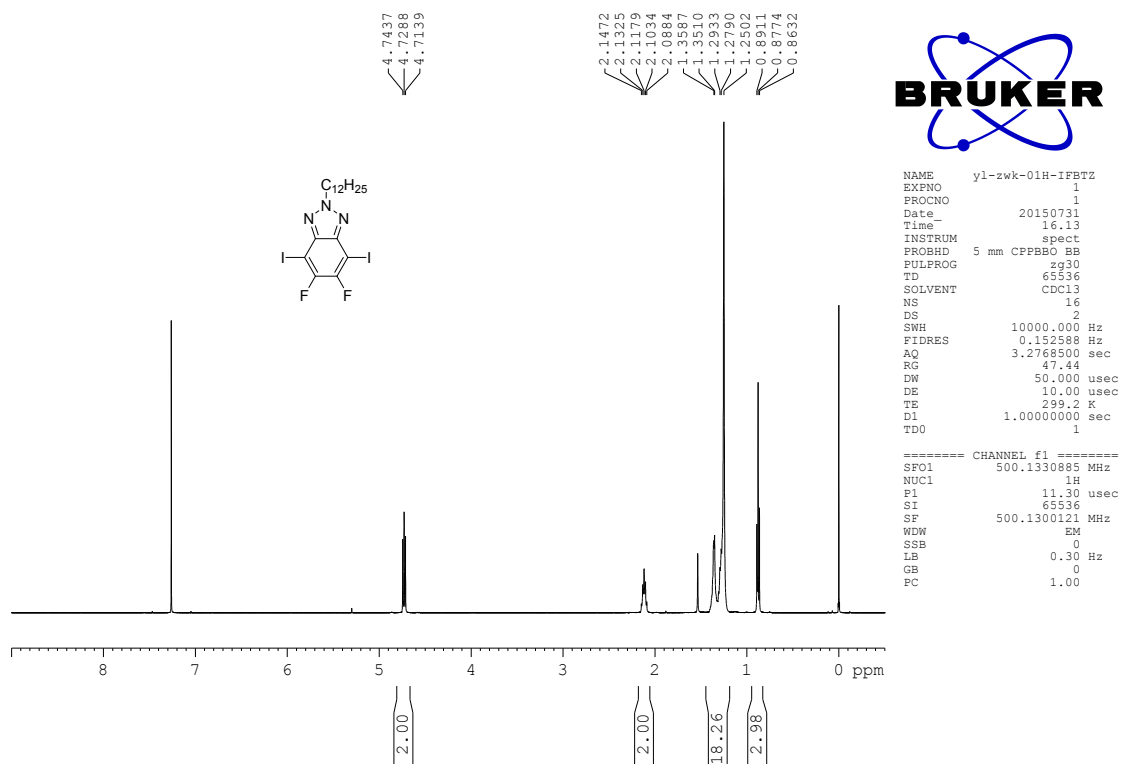


Fig. S10 ^1H NMR spectra of **M2**.

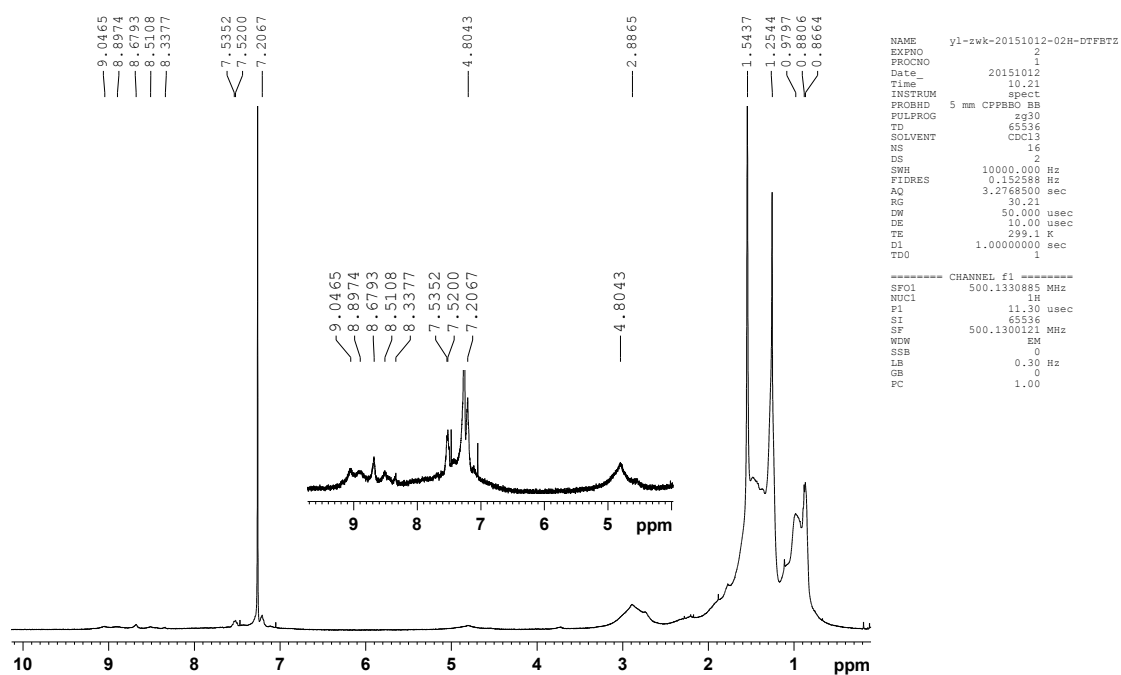


Fig. S11 ^1H NMR spectra of **PDTBDT-FBTz**.

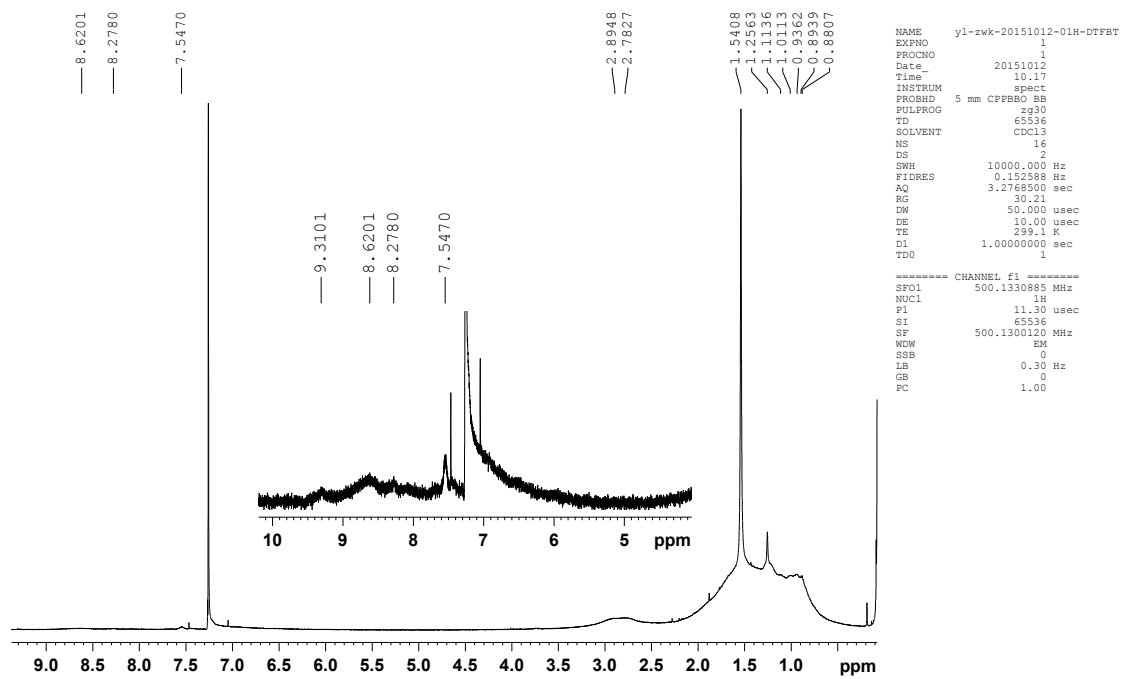


Fig. S12 ^1H NMR spectra of PDTBDT-FBT.