Wide bandgap copolymers with vertical benzodithiophene dicarboxylate for high-performance polymer solar cells with efficiency up to 7.49%

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Captions of Figures

Table S1 Dihedral angles between donor BDT, thiophene space and acceptor V- BDTC units in PV-BDTC1 and PV-BDTC2

Table S2 Photovoltaic parameters of the polymer/$PC_{71}BM$-based PSCs at different polymer/$PC_{71}BM$ weight ratios from 1:1 to 1:2.5

Table S3 Photovoltaic parameters of PV-BDTC2/$PC_{71}BM$-based PSCs at different DIO concentrations from 2 wt% to 4 wt%.

Fig. S1 Abpsorption spectrum of the PV-BDTC2/$PC_{71}BM$ blend film at a weight ratio of 1:2.

Fig. S2 *J* – *V* curves of the optimized polymer/$PC_{61}BM$-based solar cells under a simulated AM 1.5 G irradiation (100 mW cm^{-2}); (b) *EQE* curves of the optimized polymer/$PC_{61}BM$-based solar cells under illumination of monochromatic light.

Fig. S3 AFM morphology images (2 um × 2 um). (a), (d) PV-BDTC2purefilm, RMS: 0.629 nm; (b), (e) PV-BDTC2:$PC_{71}BM$ blendfilm without DIO,RMS: 0.440 nm; (c), (f) PV-BDTC2:$PC_{71}BM$ blendfilm with 3% DIO, RMS:0.783 nm.

Fig. S4 ^{1}H NMR and ^{13}C NMR spectra of compound **1-6** and monomer M1.

Fig. S5 MALDI-TOF MS spectrum of compound **6**.

Table S1

polymer	ɵ1	ɵ2	ɵ3	ɵ4
PV-BDTC1	20.39	47.98	41.30	24.13
PV-BDTC2	27.36	47.99	41.39	25.76

ɵ1, ɵ4 dihedral angles between donor BDT and thiophene space; ɵ2, ɵ3 dihedral angles between V-BDTC unit and thiophene space.

Table S2

polymer	D/A ratio	V_{oc} (V)	J_{sc} (mA cm^{-2})	*FF* (%)	PCE (%)
PV-BDTC1	1:1	0.94	6.08	36.00	2.06
	1:1.5	0.89	5.13	44.35	2.02
	1:2	0.93	5.90	59.39	3.25
	1:2.5	0.88	6.12	43.58	2.34
PV-	1:2	0.89	4.89	43.96	1.90
PV-BDTC2	1:1	1.06	7.18	38.99	2.96
	1:1.5	1.02	8.23	46.94	3.94
	1:2	1.04	8.93	60.8	5.61
	1:2.5	0.95	6.90	35.36	2.32

Table S3

PV-BDTC2: $PC_{71}BM$	V_{oc} (V)	J_{sc} (mA cm^{-2})	*FF* (%)	PCE (%)	PCE_{max} (%)
(1:1, 3% DIO)	1.033±0.005	9.083±0.121	0.605±0.006	5.677±0.105	5.791

(1:2, 3% DIO)	1.031±0.004	10.15±0.102	0.700±0.005	7.326±0.112	7.491
(1:3, 3% DIO)	1.010±0.006	9.412±0.098	0.565±0.004	5.371±0.097	5.473
(1:2, 0% DIO)	1.035±0.004	8.775±0.103	0.605±0.004	5.495±0.104	5.616
(1:2, 2% DIO)	1.033±0.003	9.881±0.114	0.651±0.003	6.645±0.126	6.763
(1:2, 4% DIO)	1.008±0.005	9.255±0.096	0.571±0.005	5.327±0.094	5.466

Figure S1

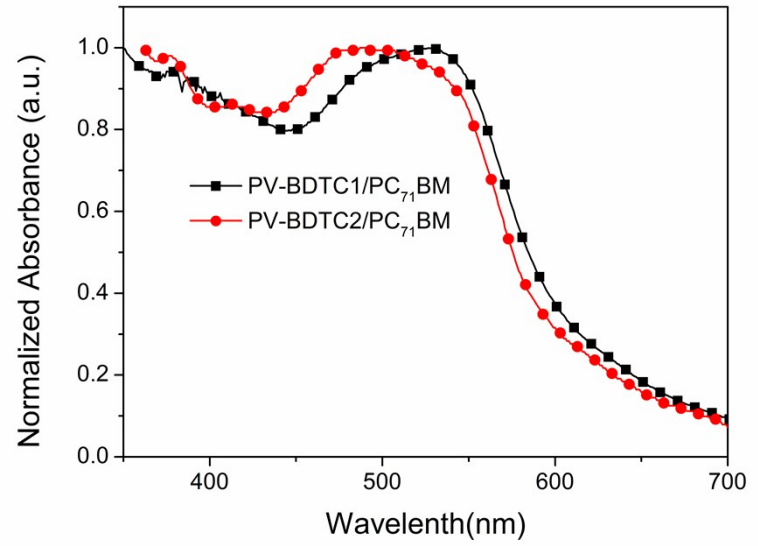
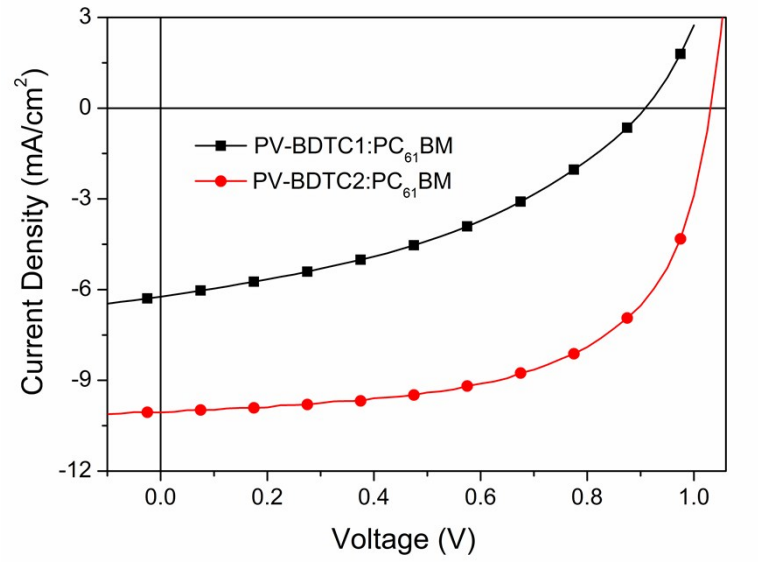


Figure S2



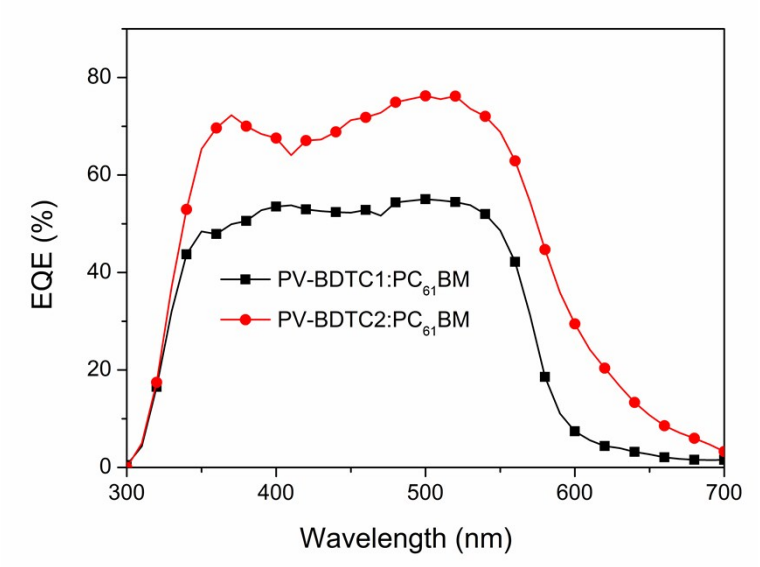


Figure S3

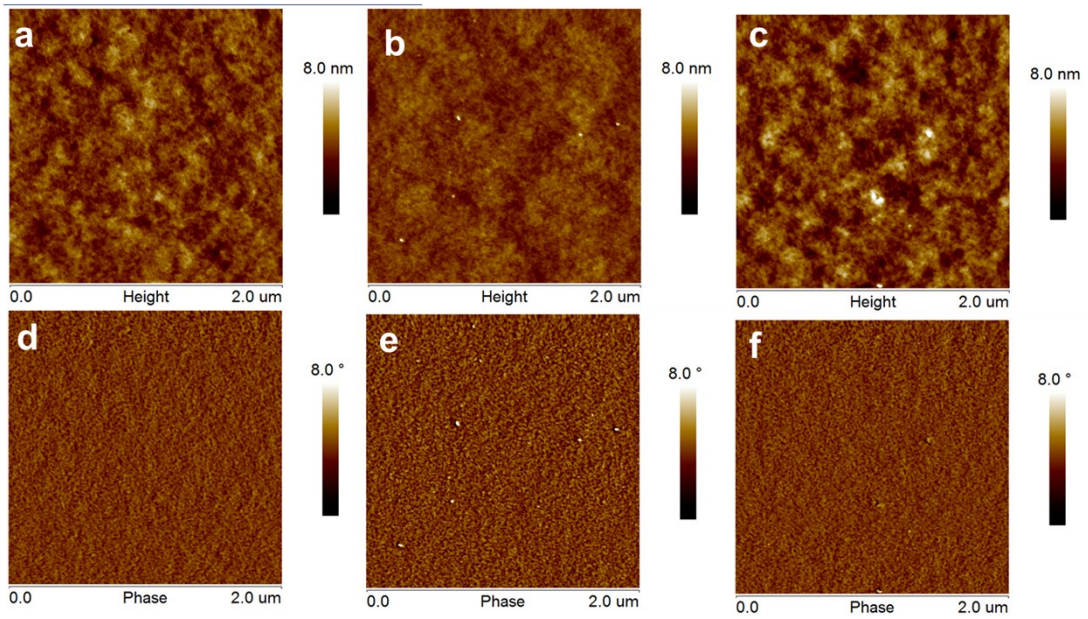
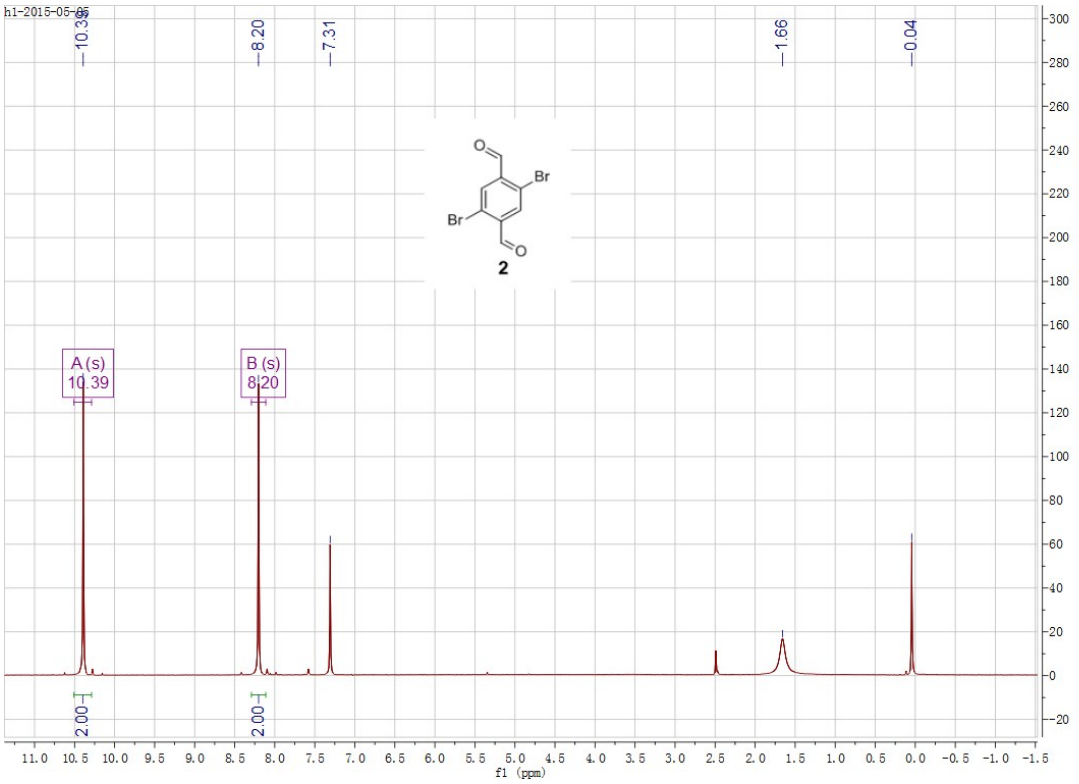


Figure S4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7.31
1.66
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B (s)
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2.00
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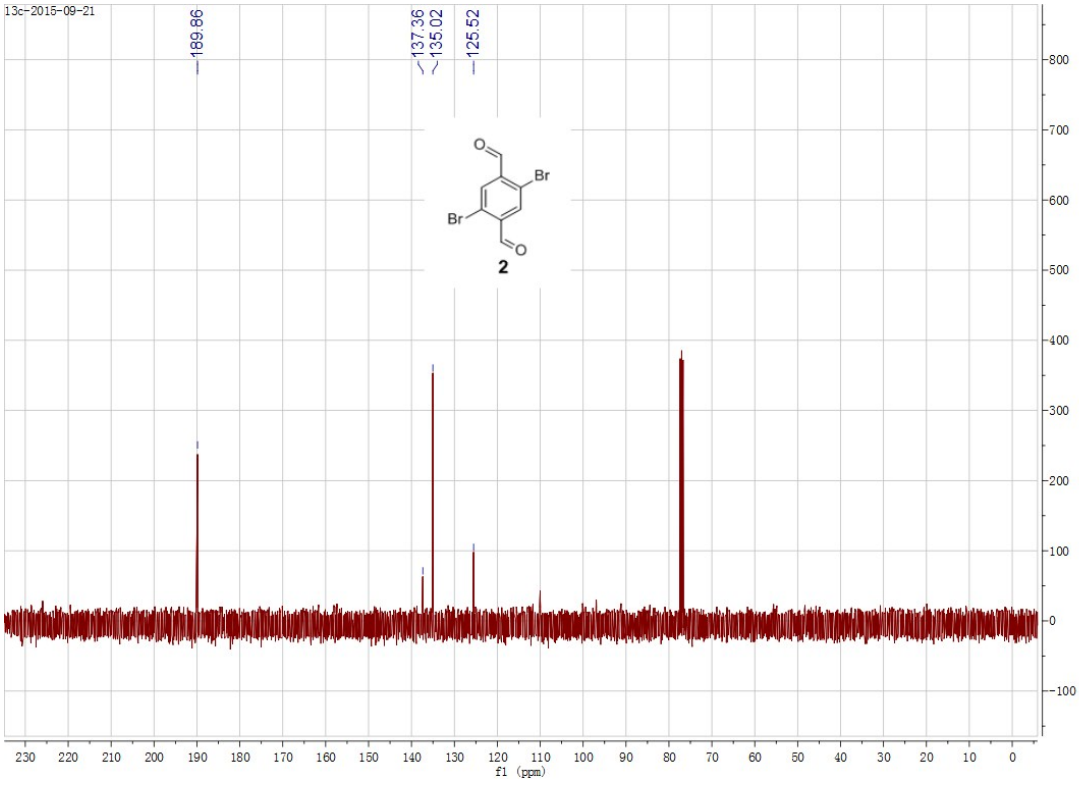
Br
O
O
2
f1 (ppm)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Br
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O
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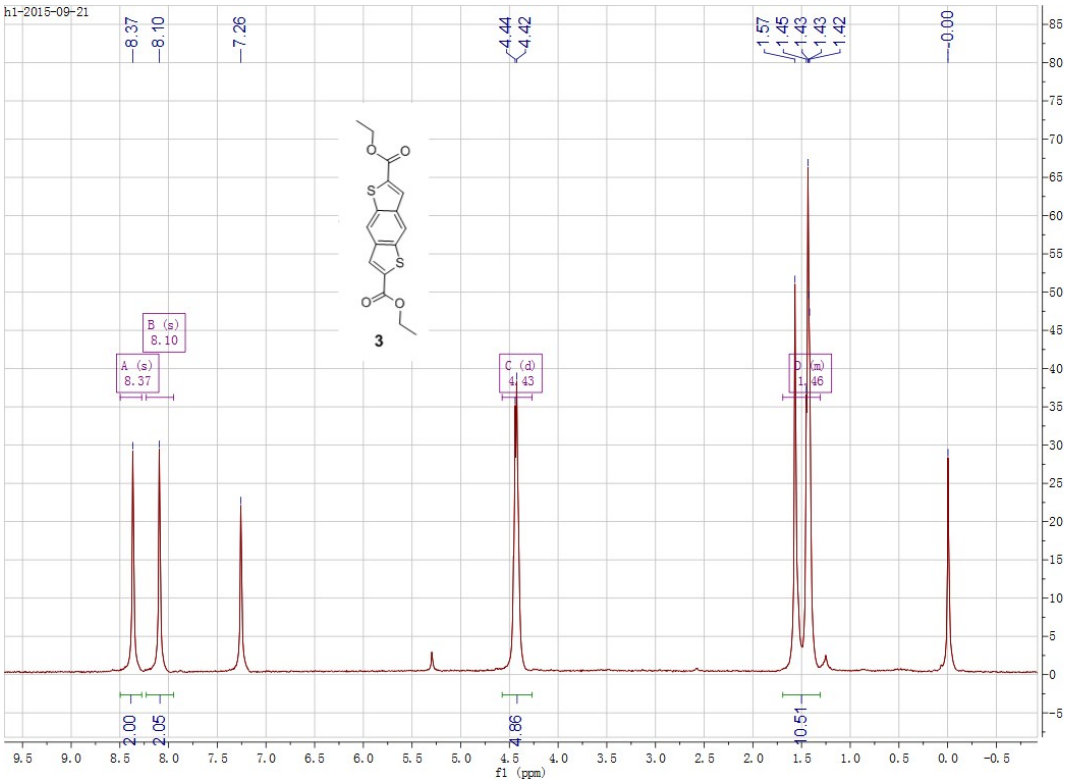
f1 (ppm)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1.57
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1.42
0.00
B (s)
8.10
A (s)
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C (d)
4.43
D (m)
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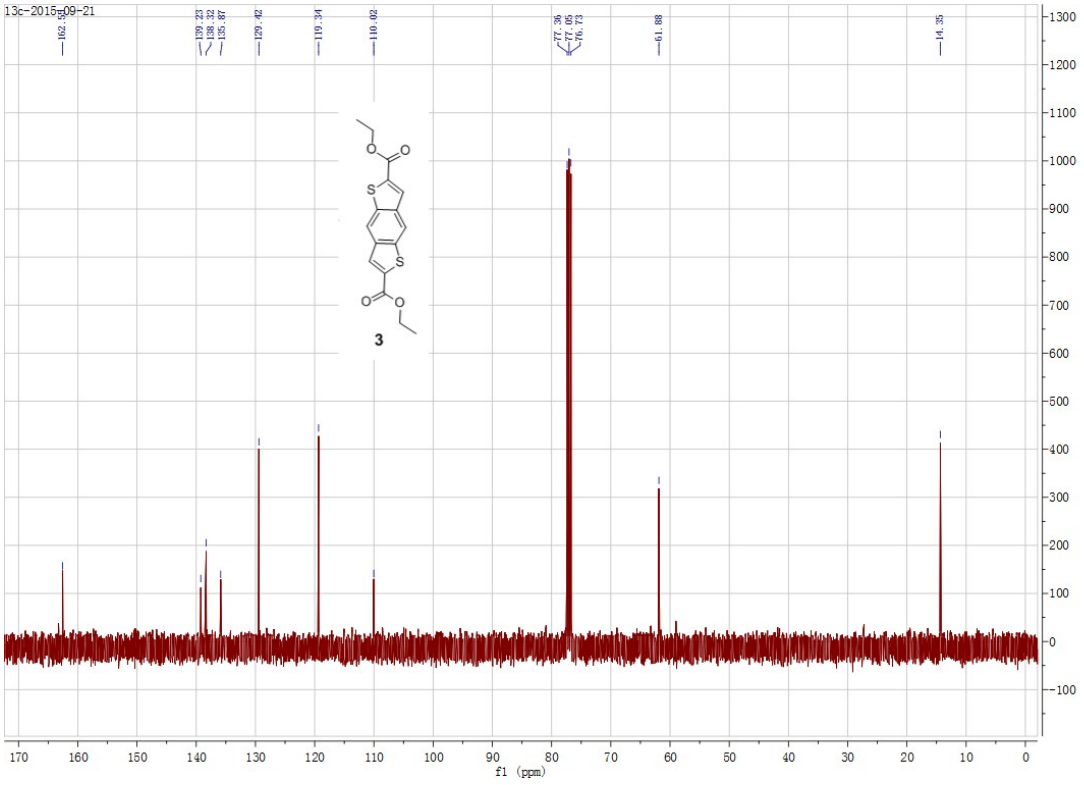
10.51
f1 (ppm)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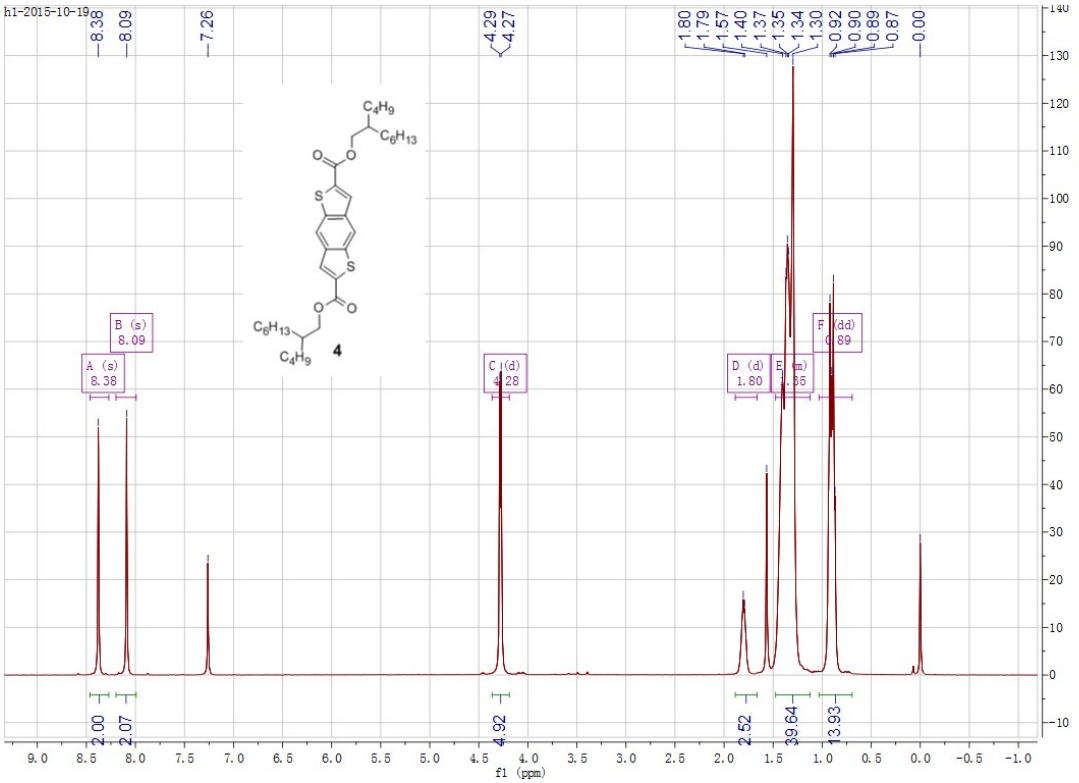
61.88
14.35
3
f1 (ppm)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1.35
1.34
1.30
0.92
0.90
0.89
0.87
0.00
B (s)
8.09
A (s)
8.38
C (d)
4.28
D (d)
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2.52
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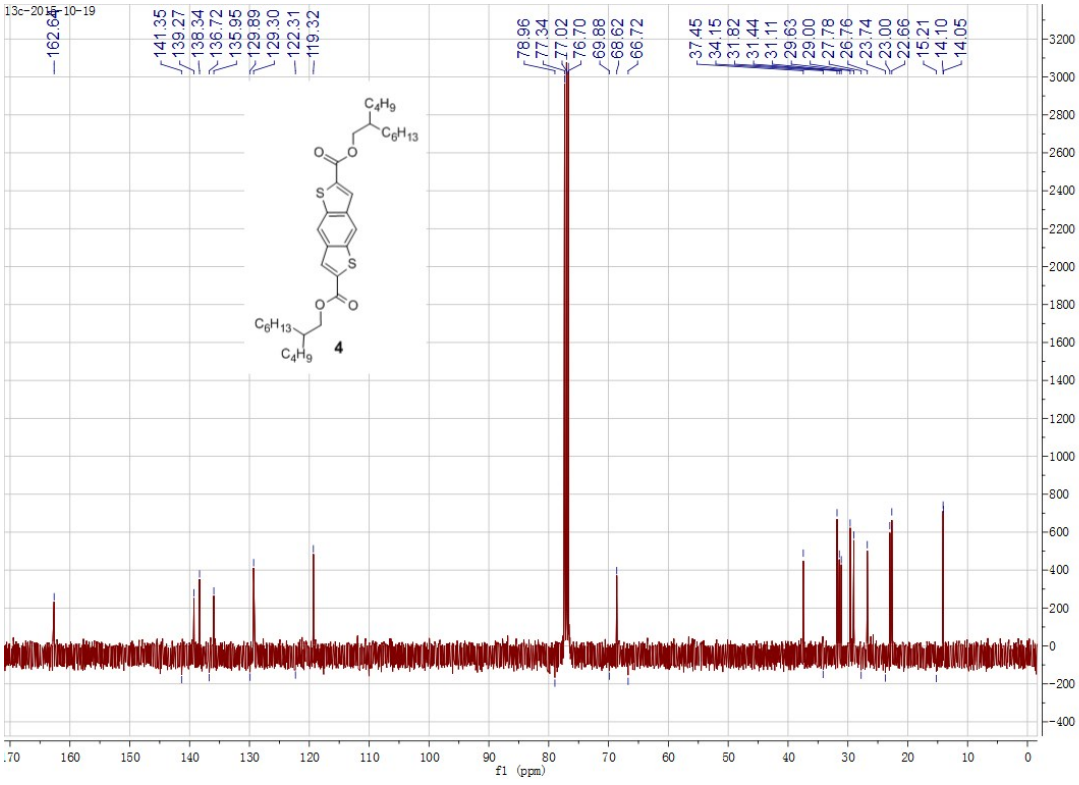
4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77.34
77.02
76.70
69.88
68.62
66.72
37.45
34.15
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31.44
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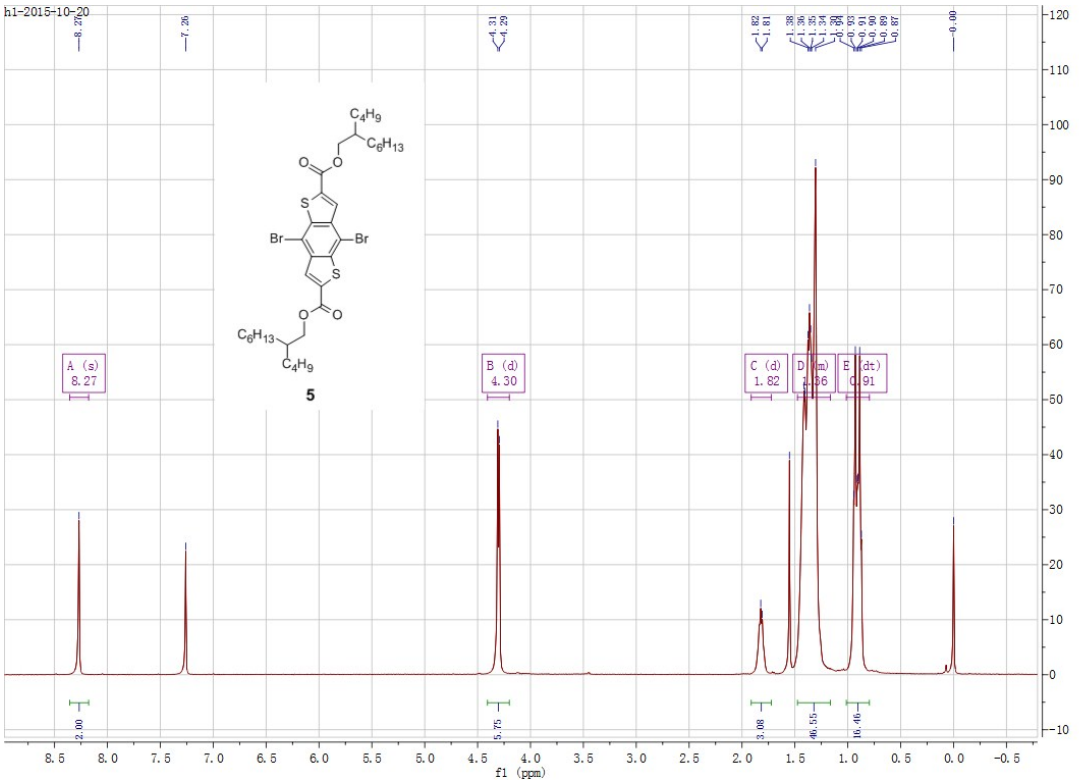
4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1.81
1.38
1.36
1.35
1.34
1.33
1.32
0.93
0.91
0.90
0.89
0.87
0.00
A (s)
8.27
B (d)
4.30
C (d)
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E (dt)
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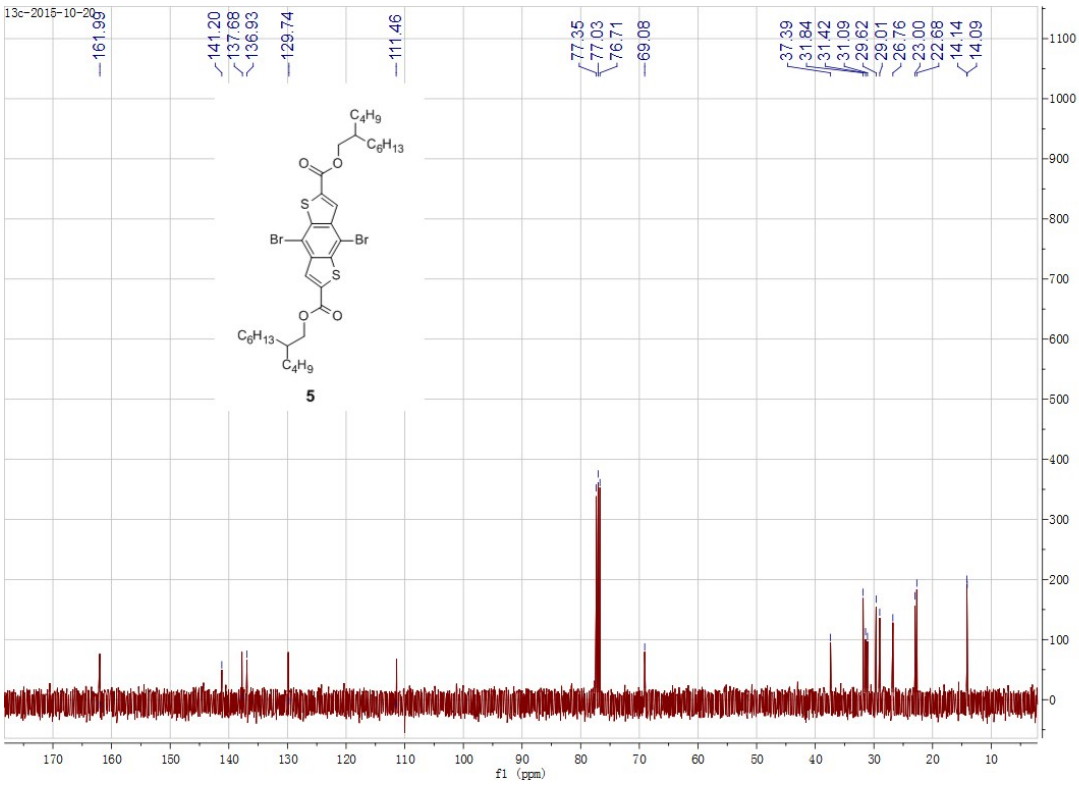
16.46
f1 (ppm)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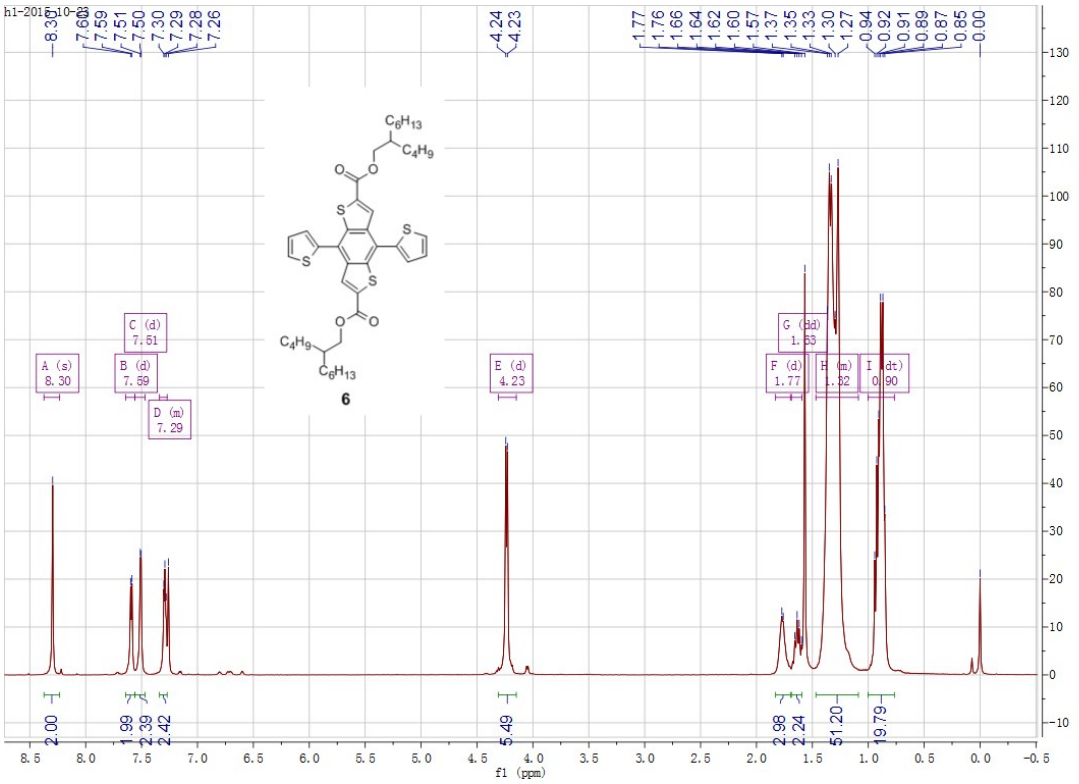
f1 (ppm)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4.23
1.77
1.76
1.66
1.64
1.62
1.60
1.57
1.37
1.35
1.33
1.30
1.27
0.94
0.92
0.91
0.89
0.87
0.85
0.00
A (s) 8.30
B (d) 7.69
C (d) 7.51
D (m) 7.29
E (d) 4.23
F (d) 1.77
G (dd) 1.83
H (m) 1.32
I (dt) 0.90
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2.39
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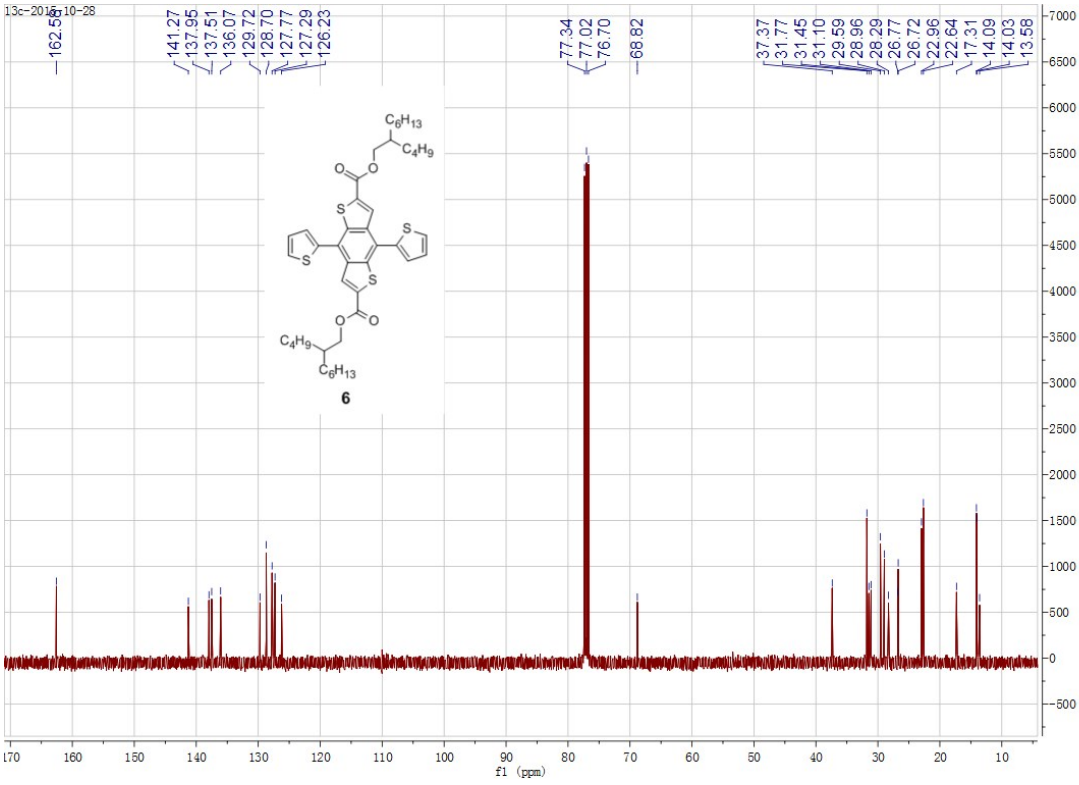
5.49
2.98
2.24
51.20
19.79
f1 (ppm)
6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76.70
68.82
37.37
31.77
31.45
31.10
29.59
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f1 (ppm)
6

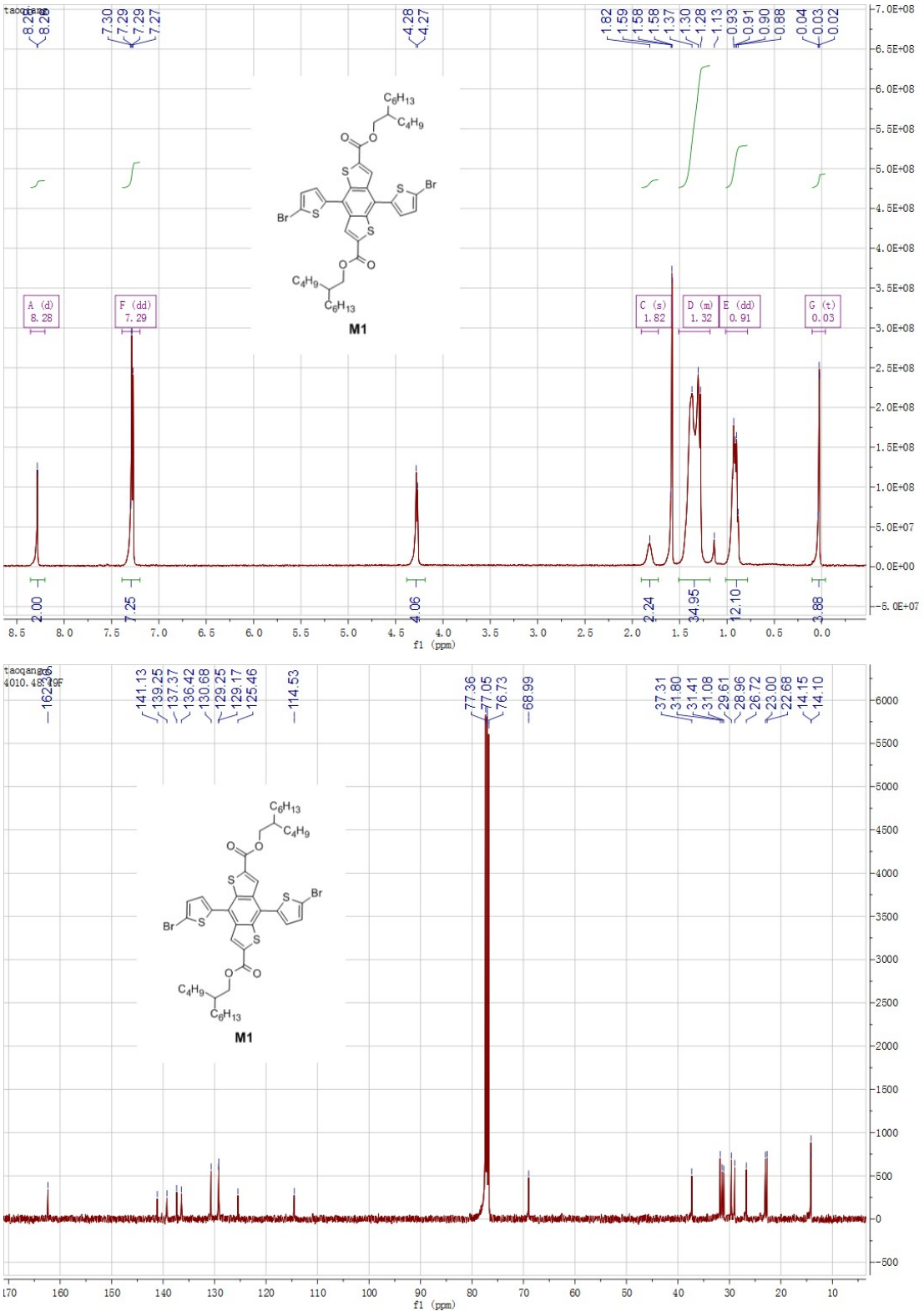
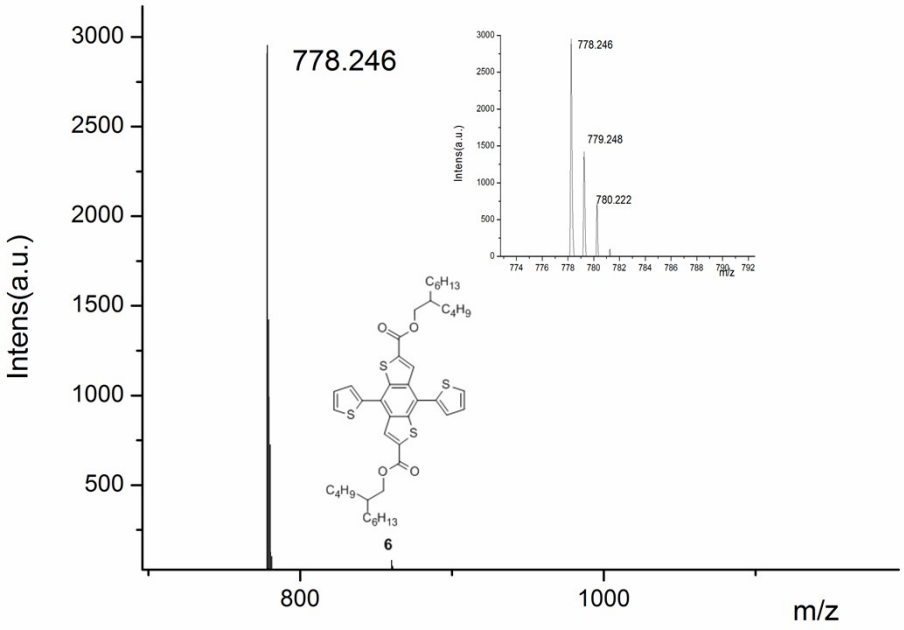


Figure S5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Intens(a.u.)
m/z
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1000
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2000
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1000
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6