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Electronic Supplementary Information

Dicyclopentadithienothiophene based non-fullerene acceptors for ternary blend organic photovoltaics

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Experimental Section

Characterization

^{1}H and ^{13}C NMR spectra were recorded using a Bruker 500 or a 300 instrument, with reference to solvent signals. Differential scanning calorimetry (DSC) was carried out on a Mettler DSC 822 instrument at a scan rate of 10 K/min. Thermo gravimetric analysis (TGA) was performed on a Perkin Elmer TGA-7 thermal analysis system using dry nitrogen as a carrier gas at a flow rate of 40 mL/min. UV–Vis absorption and fluorescence spectra were obtained in the indicated solvents at room temperature using JASCO V-530 and Hitachi F-4500 spectrometers, respectively. Differential pulse voltammetry experiments were performed with a conventional three electrode configuration (a platinum disk working electrode, an auxiliary platinum wire electrode, and a non-aqueous Ag reference electrode) with a supporting electrolyte of 0.1 M tetrabutylammonium hexafluorophosphate (dry $TBAPF_6$) in the specified dry solvent, using a CHI621C Electrochemical Analyzer (CH Instruments). Under N_2, the anhydrous OSC material was dissolved in above 0.1 M o-$C_6H_4Cl_2$ solution to prepare a 10^{-3} M test solution. In each DPV experiment, 5 mL of the test solution is scanned together with Fc/Fc$^+$ (also 10^{-3} M; as internal standard) under N_2. Electrochemical potentials were referenced to an Fc$^+$/Fc internal standard (at +0.64 V). Mass spectrometric data were obtained with a JMS-700 HRMS instrument. Grazing incidence XRD data were collected in the 2θ range of 5−50 degree on a Bruker powder diffractometer (D8 Discover) using Cu Kα1 radiation equipped with a 2D detector.

Fabrication and Characterization of OPVs

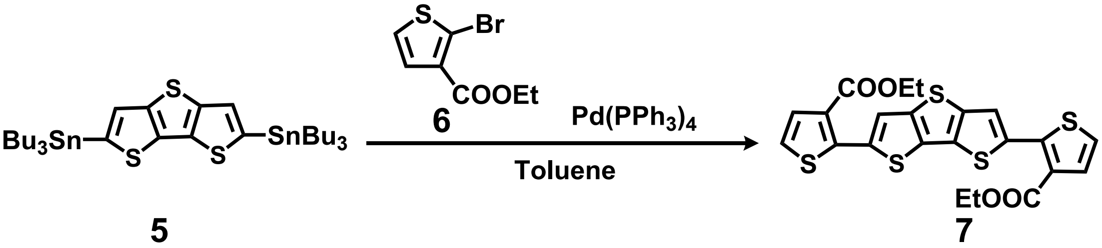
The device architecture for the OPVs consisted of a sandwich configuration: glass/ITO/ZnO/active layer/MoO_3/Ag. The ITO glass (6.4 Ω square^{-1}) from Sanyo, Japan, was used and patterned using laser ablation. The ITO glass was then cleaned sequentially with detergent, ultrasonicated in DI water, acetone, and isopropyl alcohol for 20 minutes, and dried in an oven at 120 °C for 30 minutes. To prepare the sol-gel ZnO precursor solution, zinc acetate (3.15 g), ethanolamine (0.9 mL), and 2-methoxyethanol (29.1 mL) were mixed and stirred at 25 °C for 3 days. Before the ZnO layer deposition, the surface of the glass/ITO substrate was treated with oxygen plasma (Harrick Plasma, PDC-32G) for 5 minutes. The ZnO precursor solution, filtered through a 0.45-μm filter, was then spin-coated onto the glass/ITO substrate. The coated substrate was heated at 160 °C for 10 minutes in ambient air, resulting in the formation of a ZnO layer with a thickness of approximately 30 nm. For the PM6:Y6 binary active layer, the precursor solution was prepared by dissolving PM6 and Y6 in a solvent of chloroform (CF) at a concentration of 7.3 mg/ml for the donor, with 0.5% 1-chloronaphthalene (CN). For the Y6:guest acceptor blend film, the precursor solution was prepared by dissolving the guest acceptor and Y6 in a solvent of CF at a concentration of 15 mg/ml. For the ternary active layer, the precursor solution was prepared by dissolving PM6, Y6, and the guest acceptor in a solvent of CF at a concentration of 7.3 mg/ml for the donor, with 0.5% CN. The solution was stirred overnight in an argon-filled glove box. The precursor solution was then spin-coated onto the glass/ITO/ZnO substrate at room temperature. The thickness of the active layer was optimized by controlling the spin rate and the concentration of the precursor solution. A MoO_3 layer with a thickness of 3 nm and an Ag layer with a thickness of 100 nm were sequentially deposited onto the active layer using an evaporation equipment with pressures below 10^{-6} Torr. The active area of the device was 0.1 cm^2, determined by the overlapping area between the ITO and Ag layers.

The UV–Vis absorption spectra of the thin films were recorded using a Jasco V-650 UV–Vis spectrophotometer. The photoelectronic properties of the OPVs, including the J–V, Jph–Veff, JSC–light intensity, and VOC–light intensity curves, were measured using a computer-controlled Keithley 2400 source measurement system. The measurements were conducted under AAA Class Solar Simulators from Enli Technology Co., Ltd., Taiwan, which allowed for controlling the light intensities ranging from 10 to 100 mW/cm^2. The EQE spectrum was measured using a QE-R Solar Cell Spectral Response Measurement System from Enli Technology Co., Ltd., Taiwan. The measurements were performed with the use of two certified photodetectors (Si and Ge) for monochromatic light calibration. The surface morphologies of the blend films were observed using an atomic force microscope (Bruker Dimension Edge) operating in tapping mode at room temperature. The GIWAXS spectra of the blend films were recorded at the TPS25A beamline of the National Synchrotron Radiation Research Center, Taiwan. The X-ray wavelength used was 1.8602 Å, and the incident angle was set to 0.05°. The photoelectric properties of OPDs, including photo-CELIV, TPC, and TPV measurements, were determined using the all-in-one characterization platform Paios from Fluxim AG. The photo-CELIV measurement was used to record the transient photocurrent of the OPV, allowing for the determination of the faster charge carrier mobility (μ) using the following equation.

$$\mu = \frac{2\,d^2}{3\,A\,t_{max}^2} \times \frac{1}{1 + 0.36\frac{\Delta j}{j_0}}$$

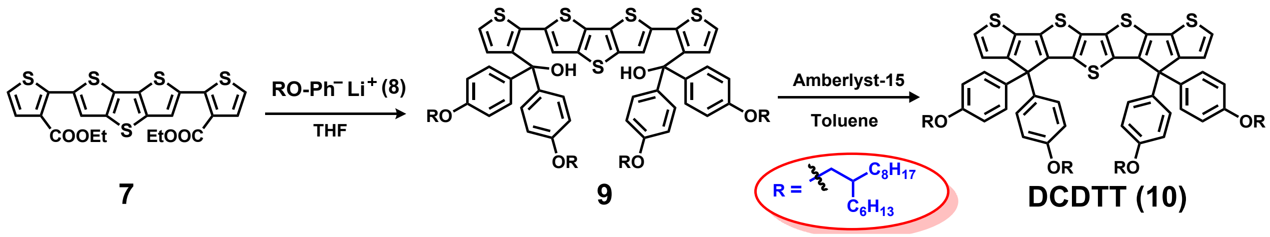
where *d, A,* $t_{\max}$, $j_{\max}$ are the film thickness of the active layer (m), the increasing rate of applied voltage (V s^{-1}), the time corresponding to the maximum of extraction peak (s), and the displacement current (A), respectively.

Synthesis conditions:



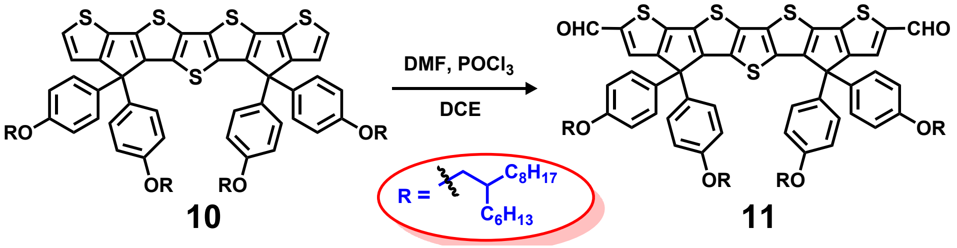
Scheme S1. Synthesis of compound **7**.

Synthesis of diethyl 2,2'-(dithieno[3,2-b:2',3'-d]thiophene-2,6-diyl)bis(thiophene-3-carboxylate) (6): Under anhydrous and deoxygenated conditions $Pd(PPh_3)_4$ (150 mg, 0.13 mmol) was added to the solution of bis(tributylstannyl)dithieno[3,2-b:2',3'-d]thiophene (**5**) (2.0 g, 2.7 mmol), ethyl 2-bromothiophene-3-carboxylate (**6**) (1.88 g, 8.1 mmol), and toluene (20 ml). The resulting mixture was refluxed for two days under nitrogen. After cooling to room temperature, the solvent was evaporated, the crude material was purified by column chromatography (15% EA/Hexane) to give product **7** as yellow solid, (1.0 g, 80%). ^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm) 7.74 (s, 2H), 7.52 (d, *J* = 5.4 Hz, 2H), 7.23 (d, *J* = 5.4 Hz, 2H), 4.32 (q, *J* = 7.2 Hz, 4H), 1.33 (t, *J* = 7.2 Hz, 6H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 163.06, 142.96, 141.58, 135.00, 132.32, 130.75, 128.22, 124.24, 122.60, 60.90, 14.25. HRMS (MALDI, $[M]^+$) calcd for $C_{22}H_{16}O_4S_5$, 503.9652; Found: 503.9647.



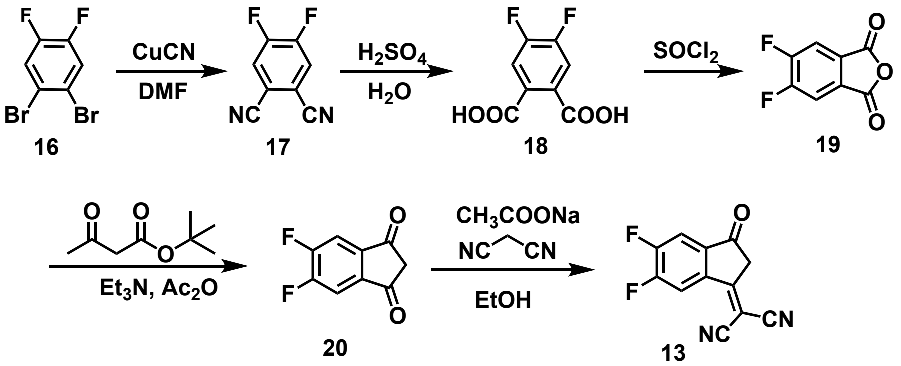
Scheme S2. Synthesis of **DCDTT** (**10**).

Synthesis of DCDTT (**10**)**:** 2.5 M *n*-BuLi (3.3 mL in Hexanes, 8.3 mmol) was slowly added to 1-bromo-4-((2-ethylhexyl)oxy)benzene (3.15 g, 8 mmol) at -78 °C in THF (30 ml) under anhydrous condition, the mixture was stirred for one hour and then it was warmed to 0 °C to remove the formed C_4H_9Br in the reaction by vacuum, then THF (30 mL) was added and transferred anion (**8**) slowly to reaction flask containing to solution of diethyl 2,2'-(dithieno[3,2-b:2',3'-d]thiophene-2,6-diyl)bis(thiophene-3-carboxylate (**7**) (0.5 g, 1 mmol) (70 mL) in THF (70 mL) under anhydrous condition at -78 ℃. Further, reaction mixture was slowly warmed to room temperature and heated to reflux for 2 hours. Further, reaction mixture was slowly warmed to room temperature and reaction was quenched by slow addition of deionized water and, THF was removed by rotary evaporator and reaction mixture was extracted by ether. Organic layer was dried over $MgSO_4$ and concentrated to give crude reaction mixture of benzylic alcohol **9** which was confirmed by ^1H NMR ((^1H NMR (500 MHz, $CDCl_3$): δ (ppm) 7.15-7.12 (m,10H), 6.82-6.80 (m,10H), 6.49 (d, *J* = 5.5 Hz, 2H), 3.83 (d, *J* = 5.5 Hz, 8H), 3.23 (s, 2H) (Note. benzylic alcohol **9** is not enough stable to collect useful ^{13}C NMR spectrum) and used for next step without further purification. To this crude reaction mixture toluene 30 ml followed by Amberlyst-15 was (0.5 g) was added under N_2 atmosphere and reaction mixture was refluxed for 4 hours. Further, reaction mixture was cool down to room temperature. toluene was removed under rotary evaporator and extracted with ethyl acetate and organic layer was dried over $MgSO_4$ and concentrated to give crude reaction mixture which is purified by column chromatography using DCM/Hexane (20:80) to give product **10** as orange liquid (0.5 g, 41%). ^1H NMR (500 MHz, $CDCl_3$)**:** δ (ppm) 7.19 (d, *J* = 5 Hz, 2H), 7.12 (d, *J* = 8.5 Hz, 8H), 7.01 (d, *J* = 5 Hz, 2H), 6.74 (d, *J* = 9 Hz, 8H), 3.76 (m, 8H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 158.56, 157.97, 149.33, 136.46, 136.27, 135.44, 134.17, 132.24, 128.91, 125.71, 123.16, 114.51, 70.81, 61.54, 38.10, 31.97, 31.46, 30.11, 29.77, 29.68, 29.41, 26.94, 22.74, 14.15; HRMS (MALDI, [M]$^+$) calcd for $C_{10}6H_{152}O_4S_5$, 1649.0294; Found: 1649.0289.



Scheme S3. Synthesis of compound **11**.

Synthesis of compound 11: Slowly $POCl_3$ (3 mL) was added to DMF (2 mL) in 30 mL DCE at 0°C and stirred for 30 min at same temperature. To this solution, **DCDTT** (**10**) (0.5 g, 0.19 mmol) was added 0°C and refluxed for 20 hours. Reaction mixture was cooled to room temperature and slowly saturated solution of $NaHCO_3$ was added at 0°C and warmed to RT. Reaction mixture was extracted with ethyl acetate, organic layer was concentrated, and crude residue was purified by column chromatography (EA/Hexane 15:85) to obtain compound **11** as orange liquid (0.3 g 58%). ^1H NMR (500 MHz, $CDCl_3$): δ (ppm) 9.80 (s, 2H), 7.62 (s, 2H), 7.10 (d, J = 8.5 Hz, 8H), 6.77 (d, J = 9 Hz, 8H), 3.76 (m, 8H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 182.25, 158.87, 158.39, 153.13, 146.46, 144.25, 136.74, 136.29, 135.22, 132.55, 131.27, 128.63, 114.68, 70.79, 61.78, 37.94, 31.87, 31.83, 30.30, 30.00, 29.65, 29.57, 29.30, 26.82, 22.63, 14.06. HRMS (MALDI, [M]$^+$) calcd for $C_{76}H_{88}O_6S_5$, 1705.0192 Found: 1705.0187.



Scheme S4: Synthesis of compound **13.**

***Synthesis of 4,5-difluorophthalonitrile* (17):** Under anhydrous condition mixture of 1,2-difluoro-4,5-dibromobenzene (**16**) (5 g, 18.4 mmol), copper(I) cyanide (3.458 g, 38.6 mmol), and 80 ml of dry dimethylformamide was heated to 130 °C for 24 hours. After the reaction was completed, 200 ml of 0.066 M $FeSO_{4\ (aq)}$ was added and further stirred for 10 minutes. The suspension was filtered and extracted with ethyl acetate. The organic layer was dried over $MgSO_4$ and concentrated. Dimethylformamide was distilled by vacuum. The residual was purified by column chromatography using ethyl acetate/hexane (15:85) to give white solid of compound **17** (0.7 g, 23.2%). ^1H NMR (500 MHz, $CDCl_3$): δ (ppm) 7.67 (t, *J* = 8.00 Hz, 2H).

Synthesis of 4,5-difluorophthalic acid (18): To the mixture of 4 ml deionized water, and 2 ml of conc. H_2SO_4 in the 20 ml flask, 4,5-difluorophthalonitrile (**17**) (0.7 g) was added and heated to 125 °C for 16 hours. Next, the reaction mixture was cooled to room temperature and poured into 100 ml deionized water. Then, reaction mixture was extracted with ethyl acetate, organic layer was dried over $MgSO_4$, and concentrated to obtain compound **18** as white solid (0.732 g, 85%). ^1H NMR (500 MHz, d-DMSO): δ (ppm) 7.82 (*t*, *J* = 9.15 Hz, 2H).

Synthesis of 5,6-difluoroisobenzofuran-1,3-dione (19): Under anhydrous conditions, 0.732 g of 4,5 difluorophthalic acid (**18**) was added in reaction flask at RT. Next, warmed up the flask to 60 °C, and to this slowly added 15 ml of $SOCl_2$. The reaction mixture was heated to 90 °C, and refluxed for 16 hours. Next, the reaction mixture was concentrated to remove $SOCl_2$, and extracted with ethyl acetate and water. The organic layer was dried over $MgSO_4$, and concentrated to obtain compound **19** as yellow solid (0.6 g, 90%). ^1H NMR (500 MHz, $CDCl_3$): δ (ppm) 7.83 (t, *J* = 6.90 Hz, 2 H).

Synthesis of 5,6-difluoro-1H-indene-1,3(2H)-dione (20): 5,6-difluoroisobenzofuran-1,3-dione (**19**) (0.6 g, 3.25 mmol), acetic anhydride (3.6 ml), and triethylamine (1.8 ml) were sequentially added under an inert atmosphere. Then, tert-butyl acetoacetate (0.6 g, 3.79 mmol) was added to the reaction. The reaction was stirred at 35 °C for 24 hours. Then, a mixture of ice-water (10 ml) and concentrated HCl (10 ml) were added into reaction flask sequentially. The mixture was heated to 75 °C for 1.5 hours. Reaction mixture was cooled to room temperature and poured into 100 ml deionized water. Then, reaction mixture was extracted with ethyl acetate. The organic layer was dried over $MgSO_4$ and concentrated to obtain compound **20** as yellow solid (0.374 g, 63%). ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) 7.75 (t, *J* = 7.35 Hz, 2 H), 3.26 (s, 2 H).

Synthesis of 2-(5,6-difluoro-3-oxo-2,3-dihydro-1H-inden-1-ylidene)malononitrile (13): 5,6-difluoro-1H-indene-1,3(2H)-dione (**20**) (0.374 g, 2.05 mmol), malononitrile (0.271 g, 4.10 mmol), and anhydrous sodium acetate (0.253 g, 3.075 mmol) were sequentially added to absolute ethanol (10 mL) in a reaction flask at room temperature. After 1 hour of reaction at room temperature, the mixture was heated at 70 °C for two hours to complete the reaction. Then, 50 ml deionized water was added into flask and acidified to PH 1-2 with HCl. The precipitate was filtered and washed with water and petroleum ether to obtain compound **13** as gray solid (265 mg, 56%). ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm): 8.47 (q, 1H), 7.76 (t, J = 7.5 Hz, 1H), 3.76 (s, 2H); ^{19}F NMR (282 MHz, $CDCl_3$): δ (ppm) -119.82 （*d*, *J* = 18.89 Hz, 1F） -120.29 （(d, *J* = 18.89 Hz, 1F).

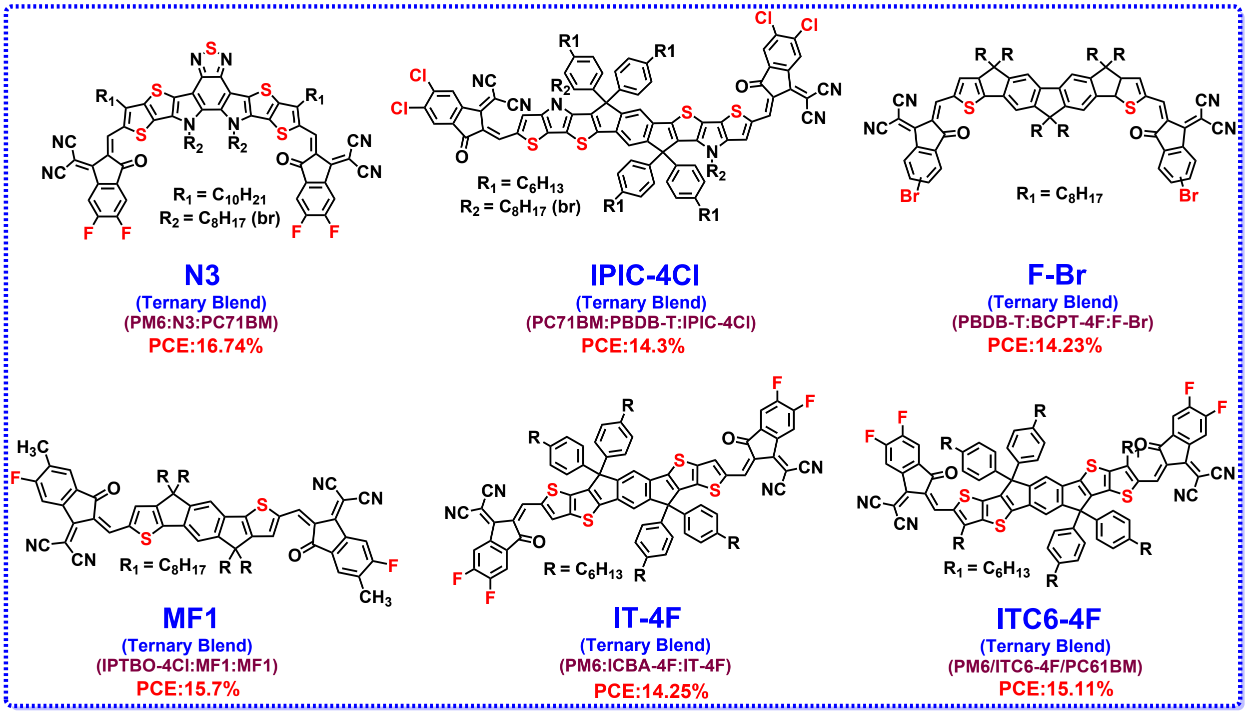


Figure S1. Chemical structures of non-fullerene acceptors used in the reported ternary blend OPVs.

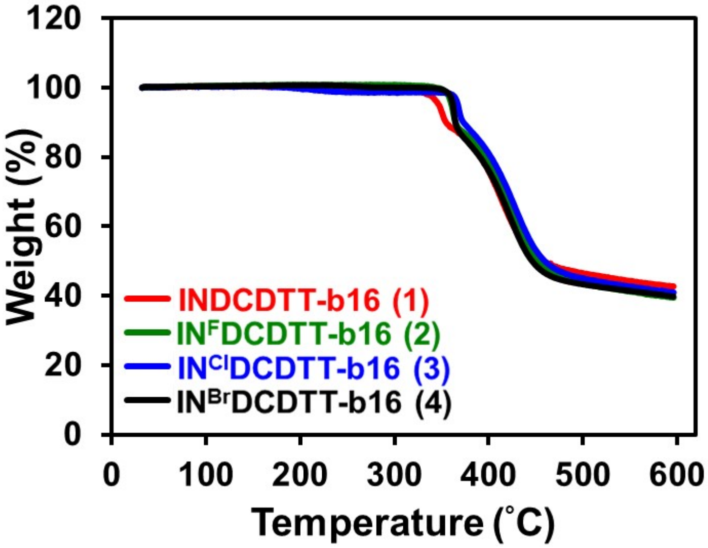


Figure S2. TGA curves of the studied compounds **1-4**.

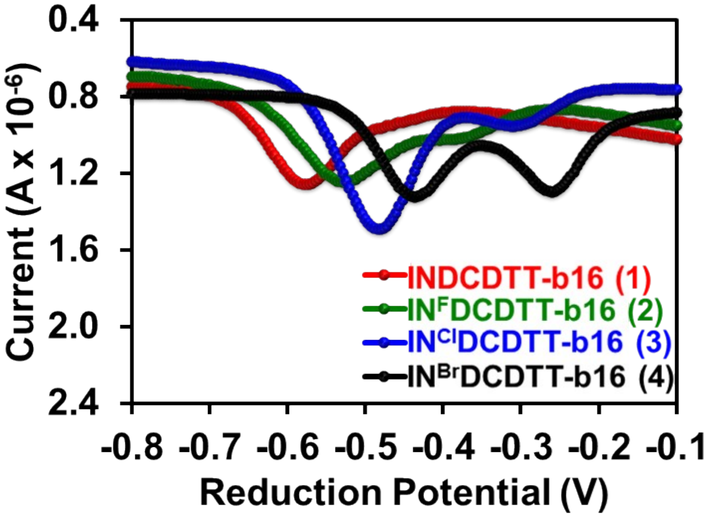


Figure S3. DPV response curves of the studied compounds **1-4**.

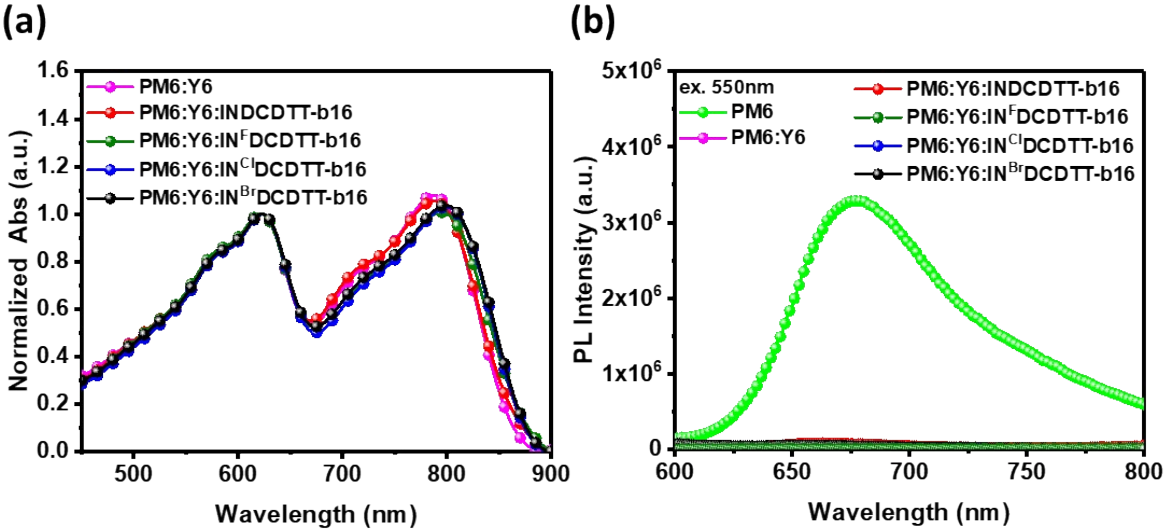


Figure S4. (a) UV–Vis spectra of binary and ternary blend films. (b) PL spectra of the neat and blend films.

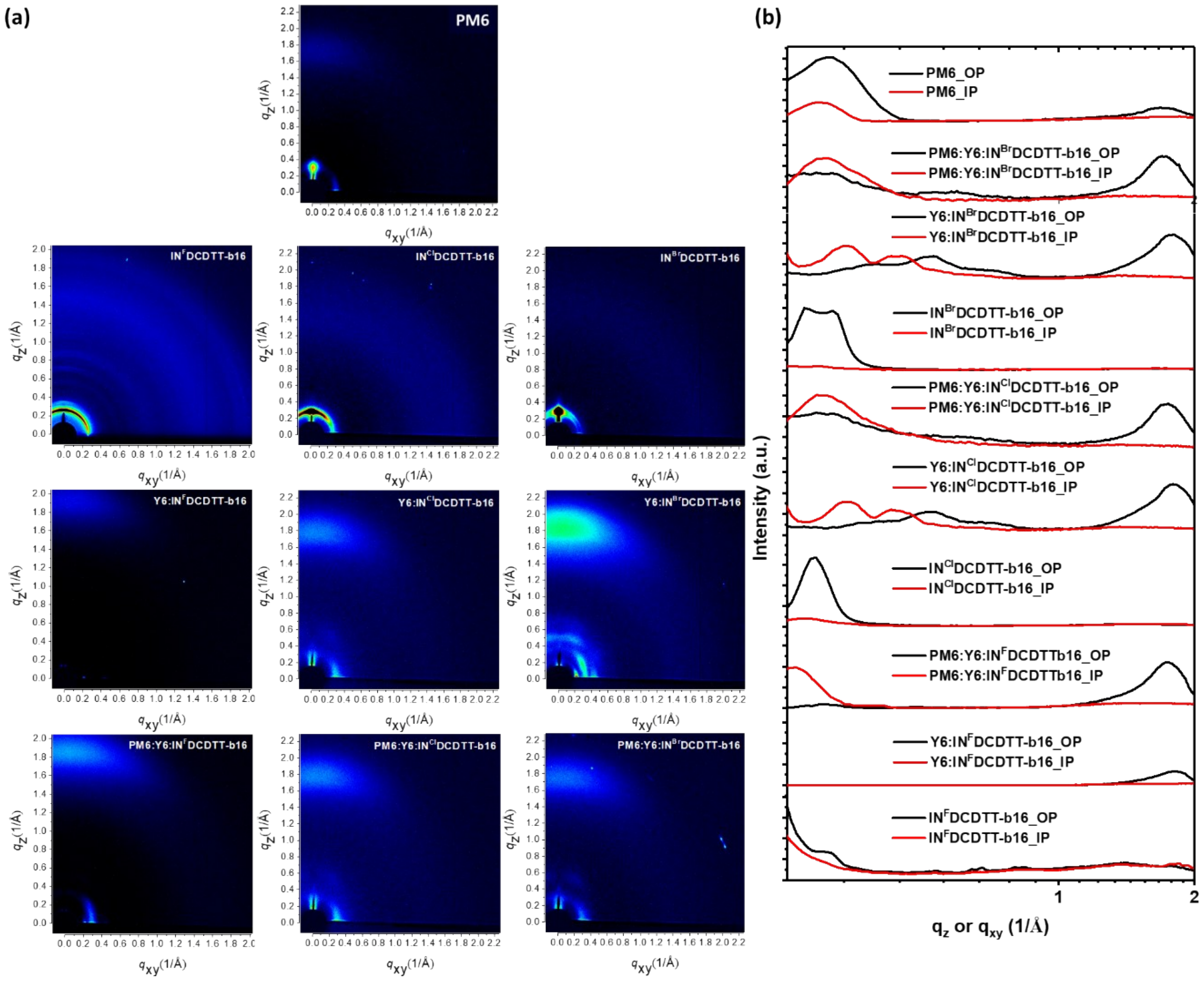
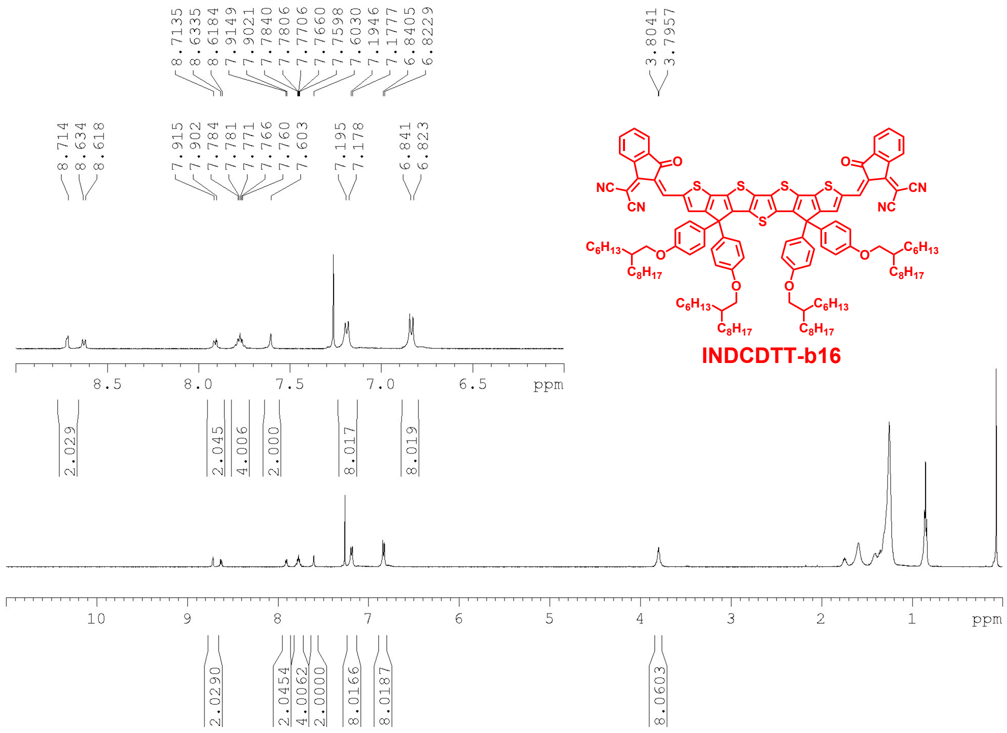


Figure S5. (a) 2D- and (b) 1D-GIWAXS profiles of neat and blend films.

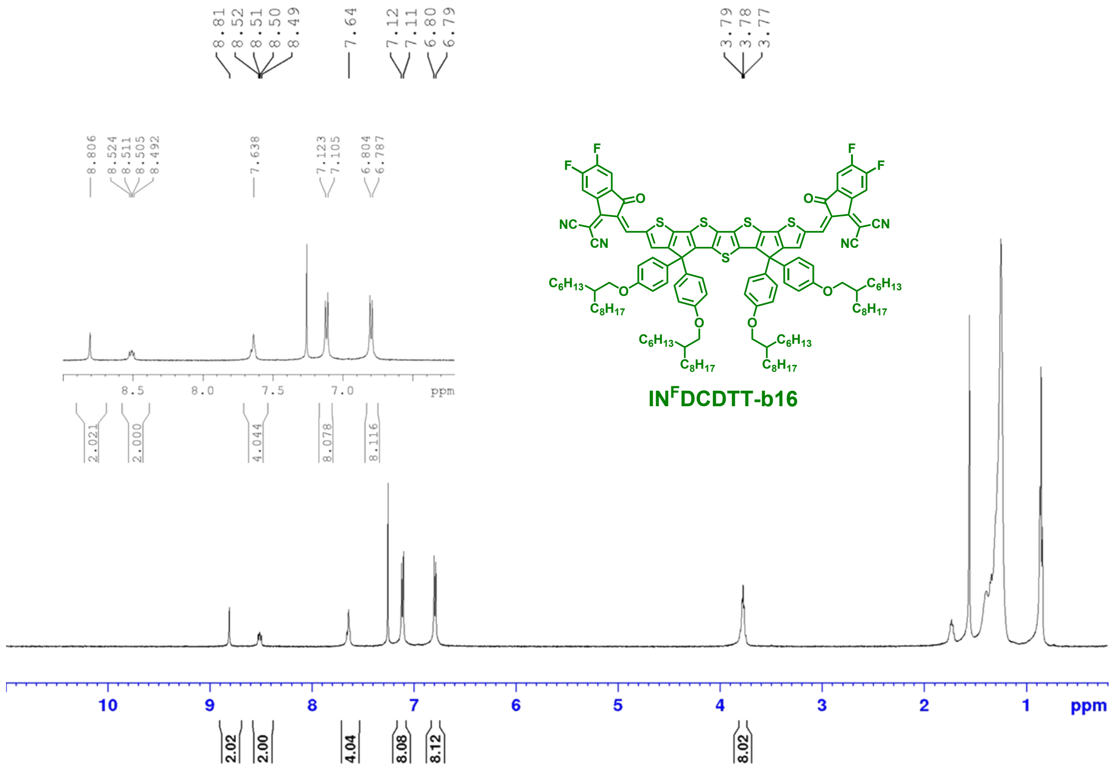
Table S1. The optimized conditions of PM6:Y6: **INDCDTT-b16**-based OPV.

Blend ratio	Additive	Thermal annealing	J_{SC} (mA/cm²)	V_{OC} (V)	FF (%)	PCE (%)
1:1.2:0.10	CN_0.5%	w/o	24.24	0.89	73.9	15.90
1:1.2:0.07	w/o	w/o	25.31	0.85	58.1	12.50
	CN_0.5%	w/o	24.70	0.87	75.8	16.27
	CN_0.5%	90℃_10min	24.50	0.85	71.0	14.71
1:1.2:0.05	CN_0.5%	w/o	24.20	0.86	74.2	15.43

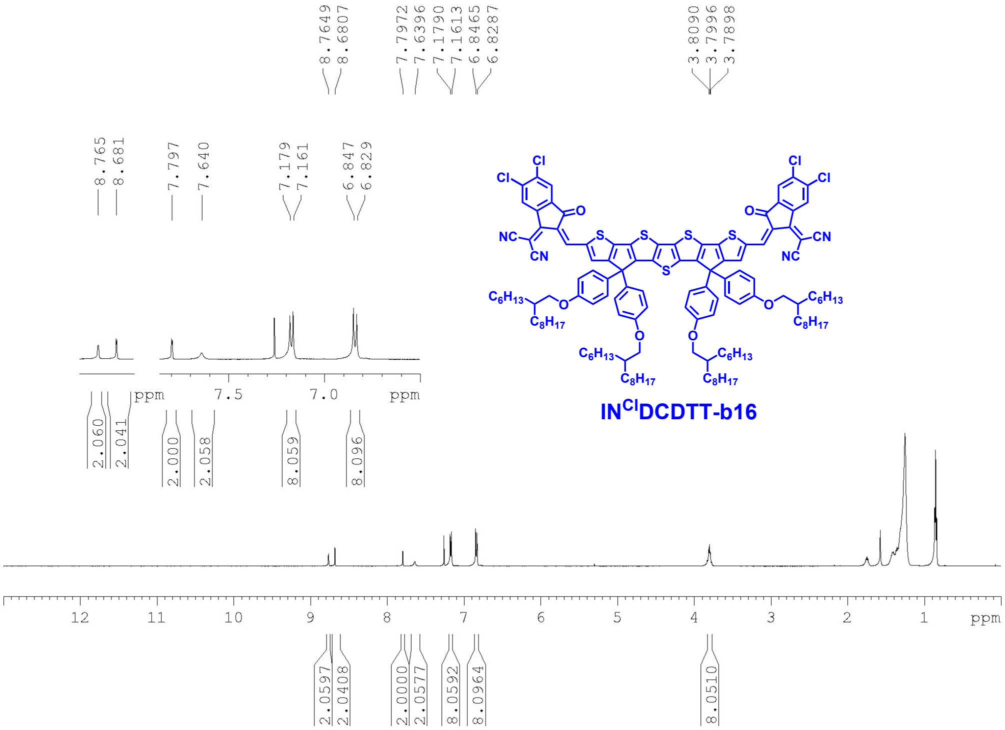
^{1}H NMR spectra of synthesized compounds



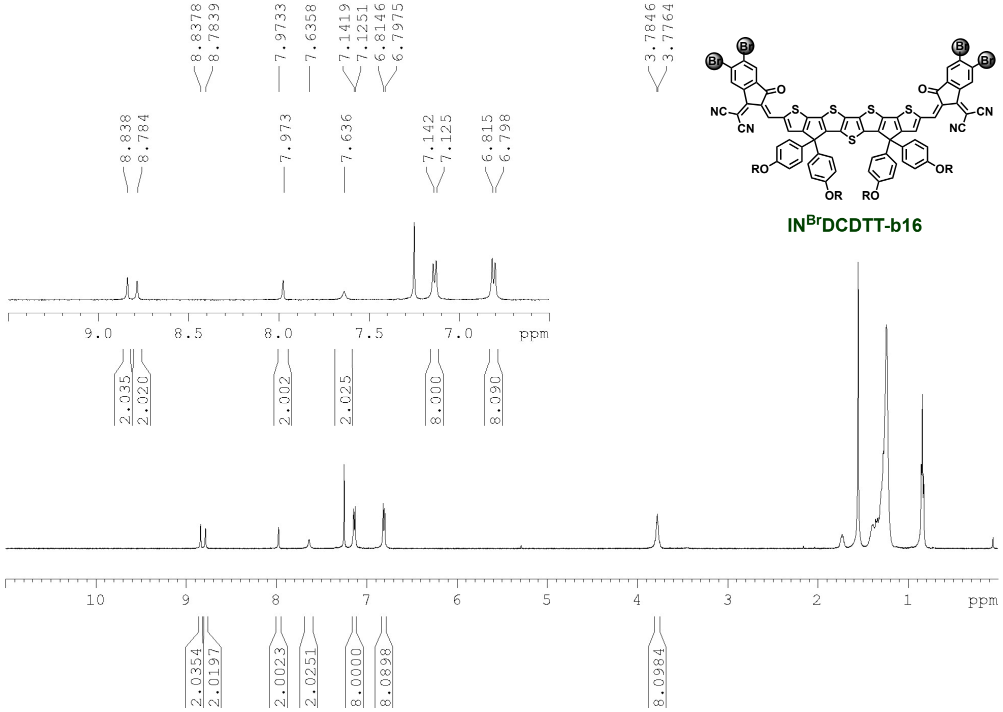
INDCDTT-b16



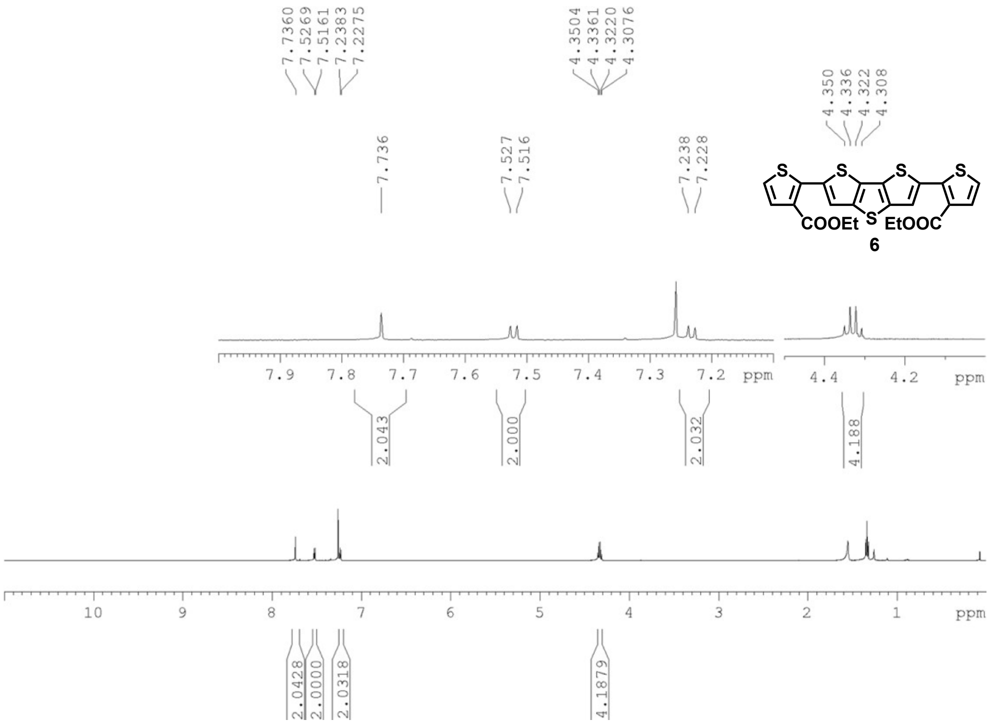
IN^{F}DCDTT-b16



$IN^{Cl}DCDTT$-b16



$IN^{Br}DCDTT$-b16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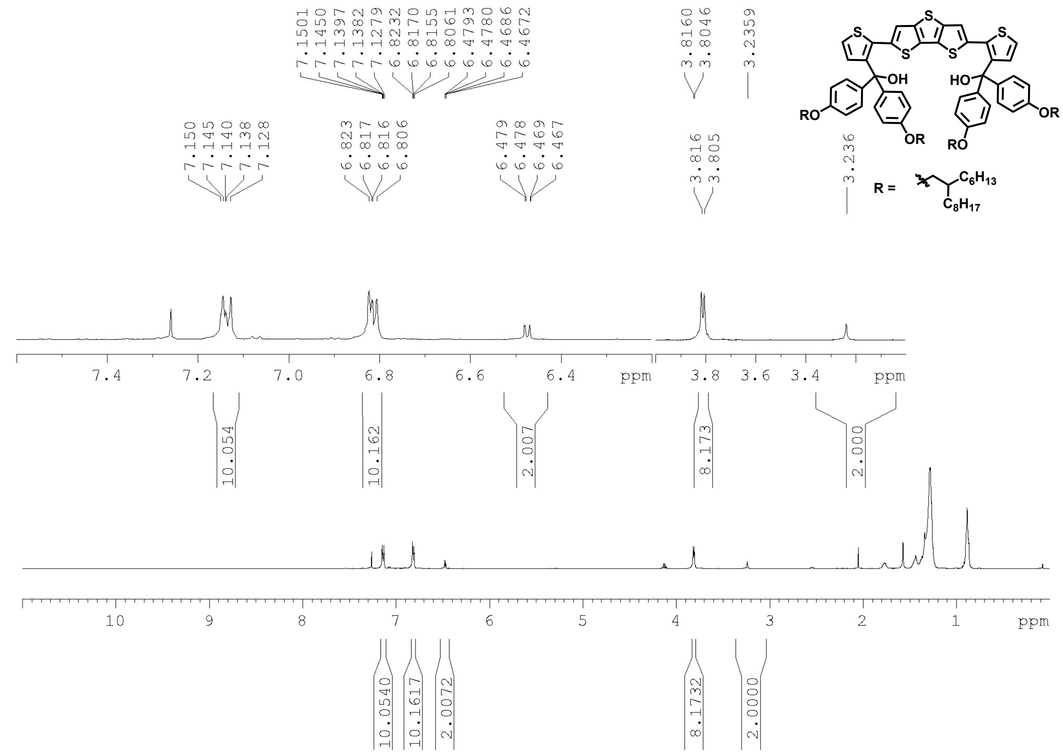
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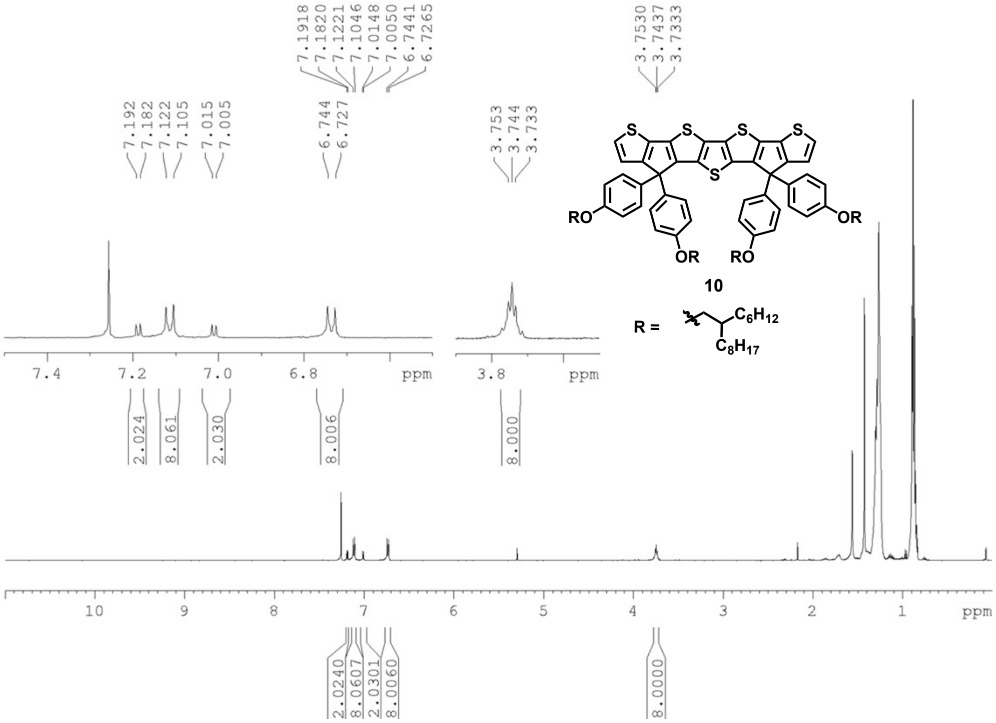

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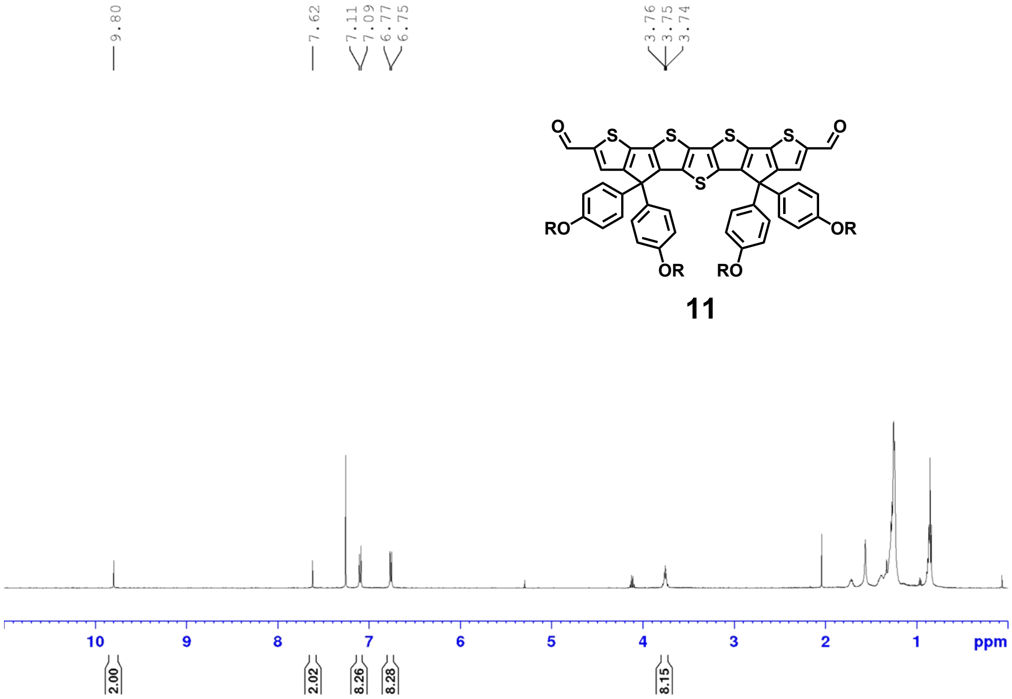

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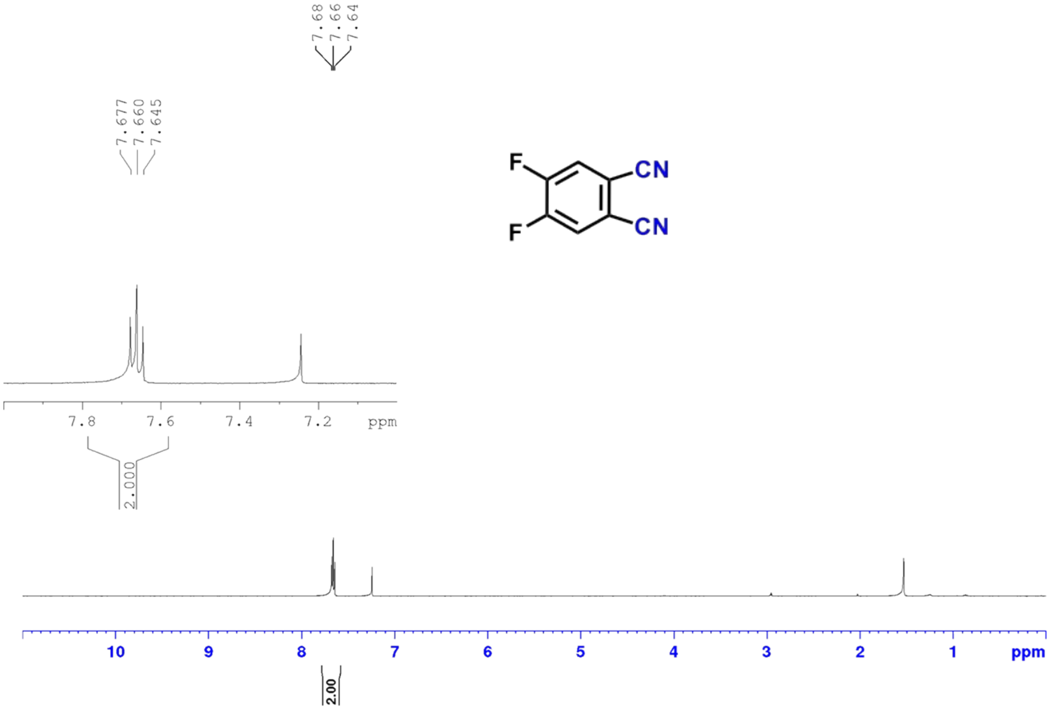
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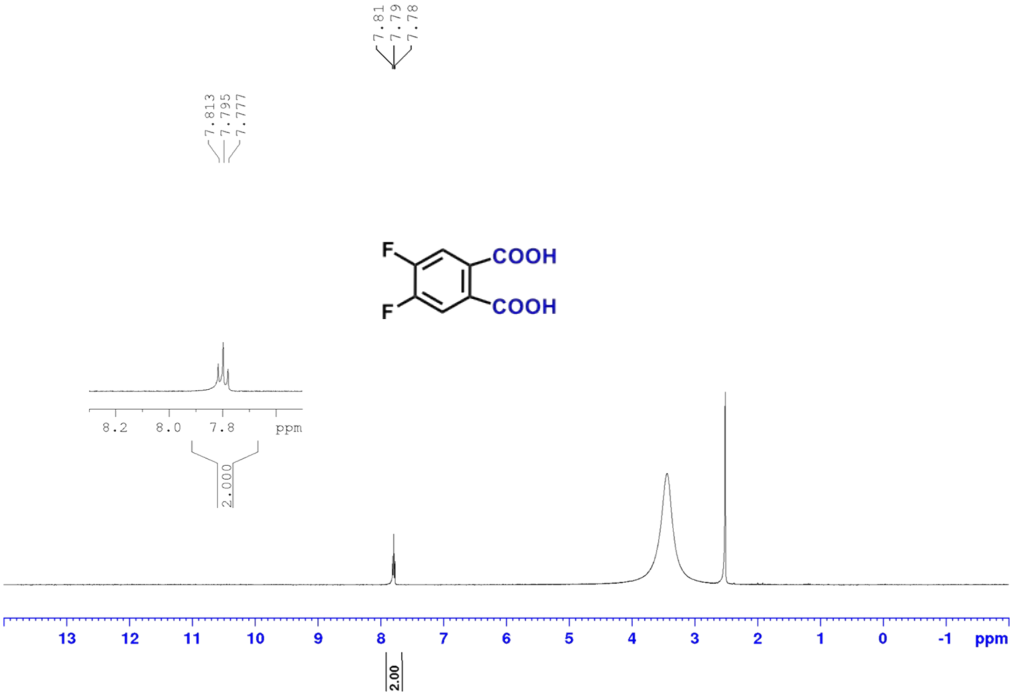
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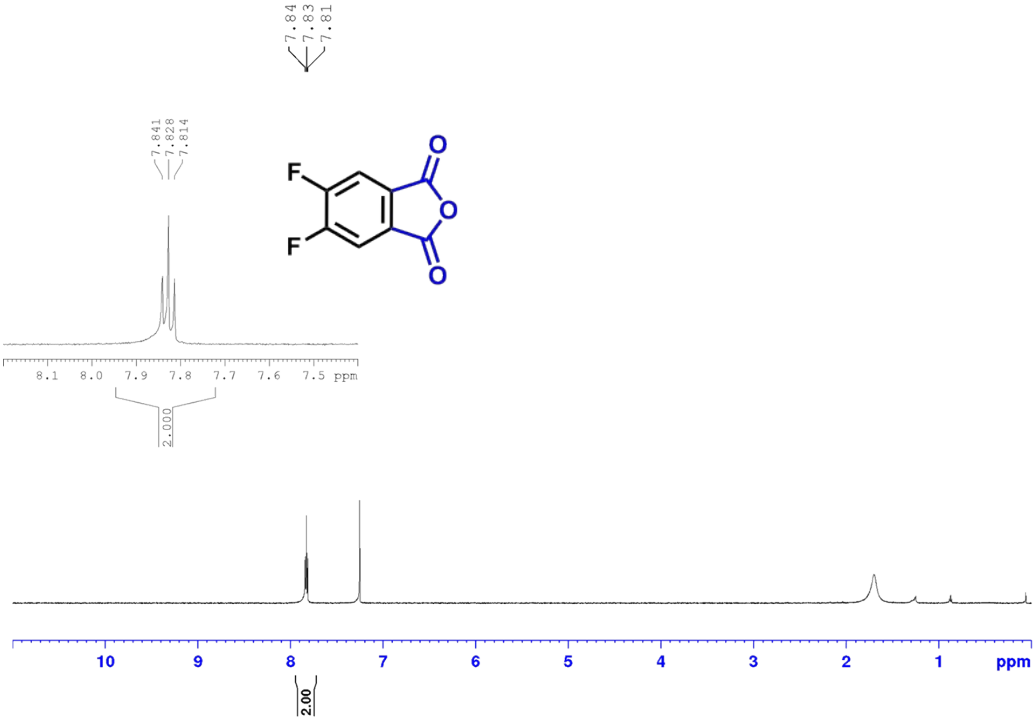
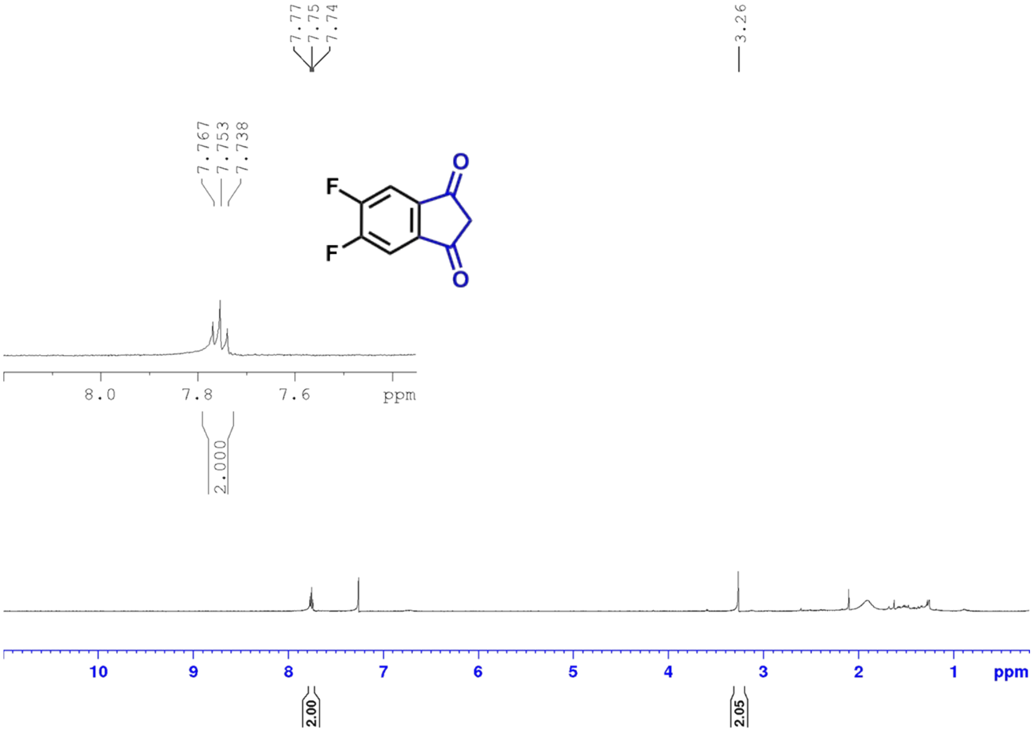
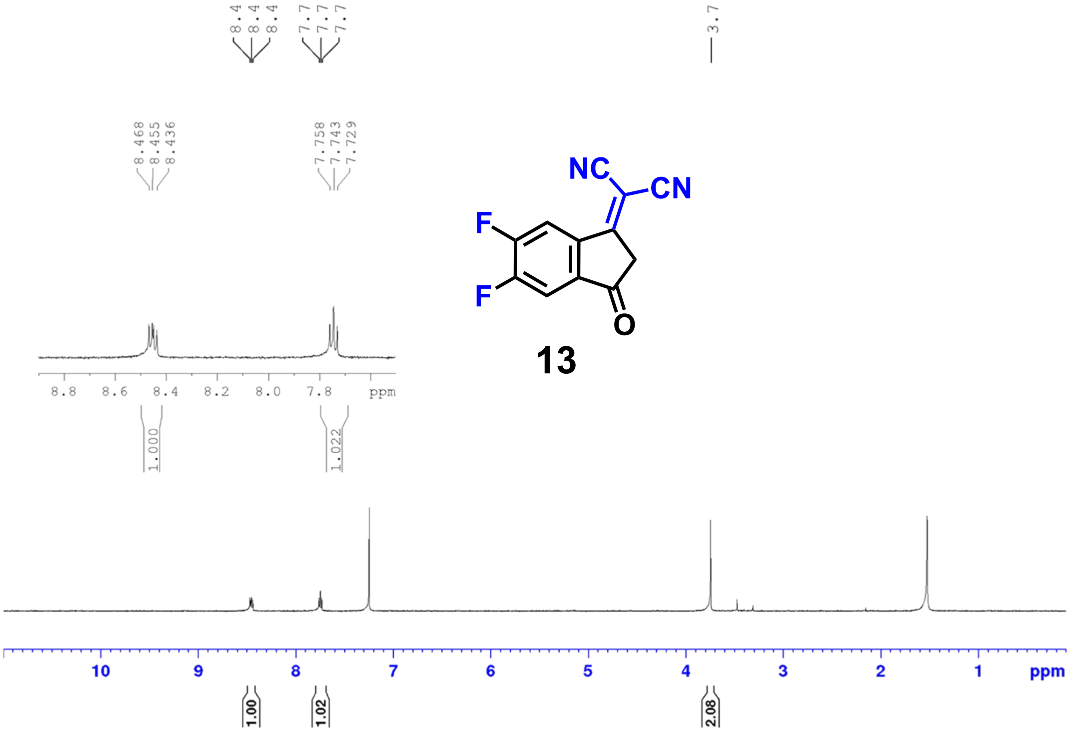
7.79
7.78
7.813
7.795
7.777
F
F
COOH
COOH
8.2
8.0
7.8
ppm
2.000
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
ppm
2.00



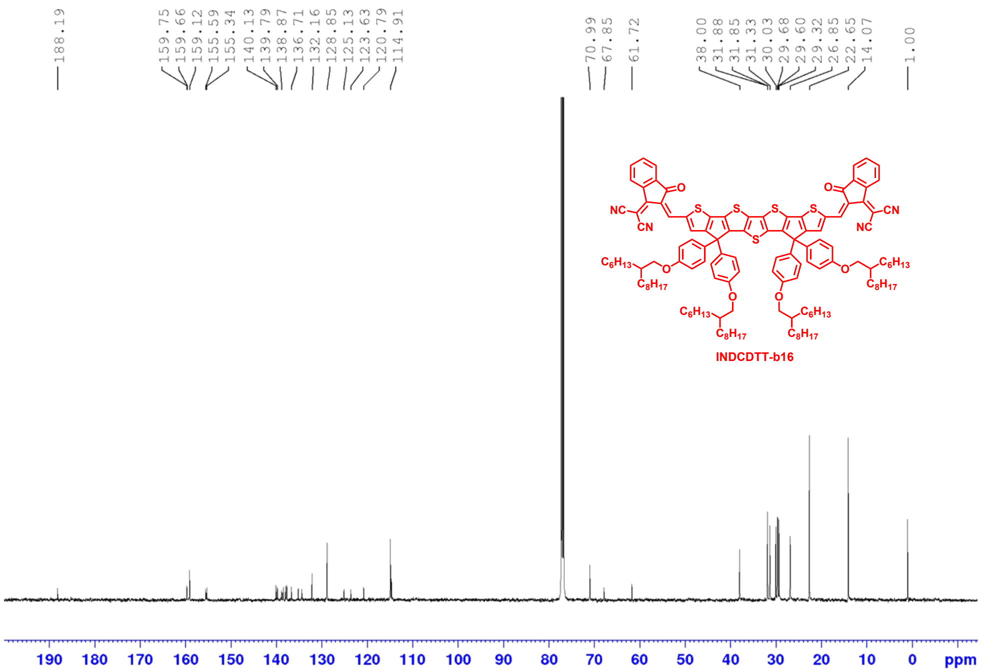
7.84
7.83
7.81
7.841
7.828
7.814
F
F
O
O
O
8.1
8.0
7.9
7.8
7.7
7.6
7.5
ppm
2.000
10
9
8
7
6
5
4
3
2
1
ppm
2.00

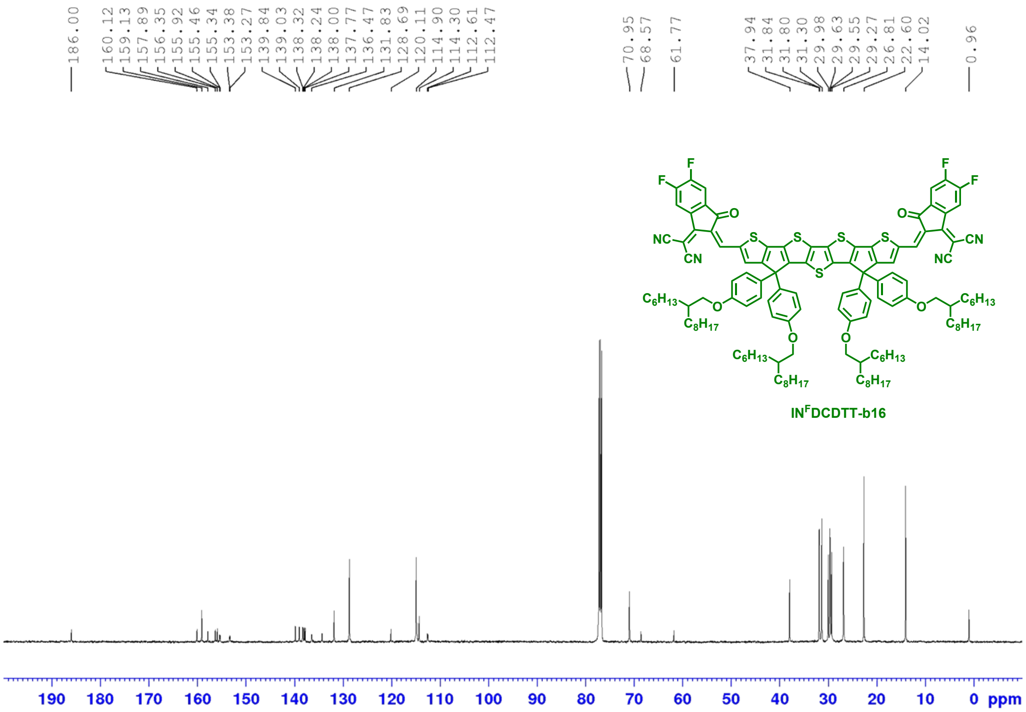


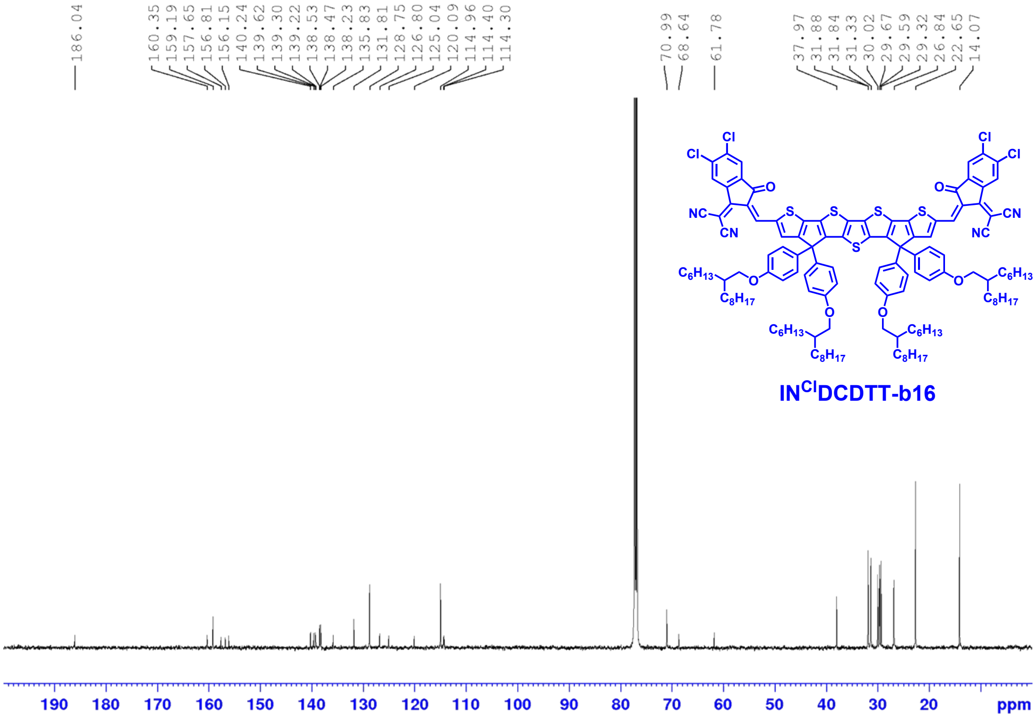
7.77
7.75
7.74
3.26
7.767
7.753
7.738
F
F
O
O
8.0
7.8
7.6
ppm
2.000
10
9
8
7
6
5
4
3
2
1
ppm
2.00
2.05

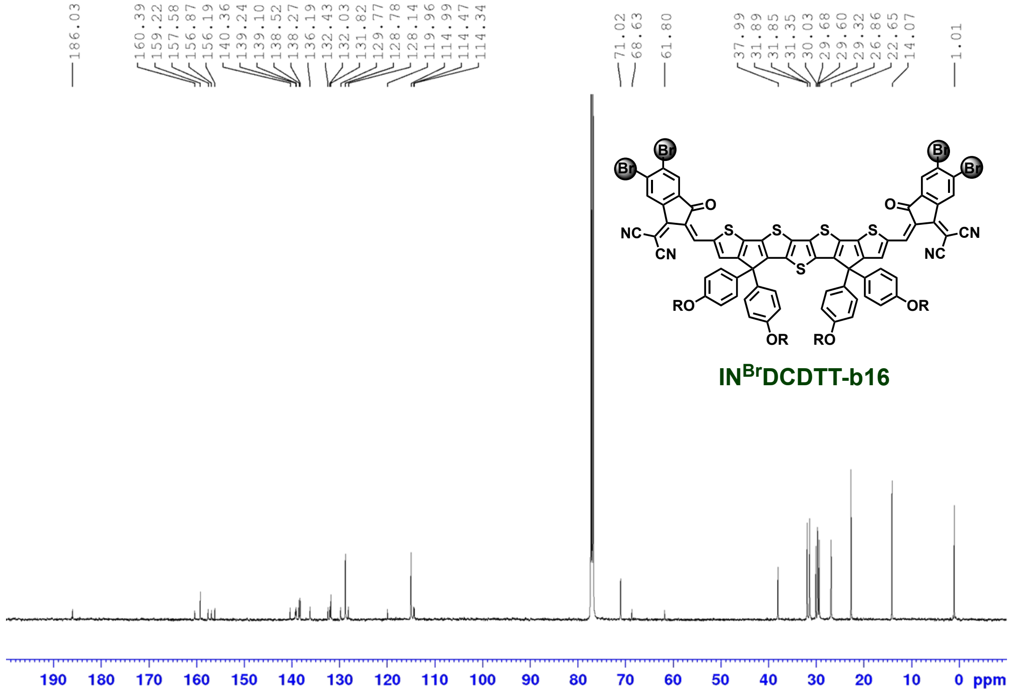

13
8.4
8.4
8.4
7.7
7.7
7.7
3.7
8.468
8.455
8.436
7.758
7.743
7.729
NC
CN
F
F
O
8.8
8.6
8.4
8.2
8.0
7.8
ppm
1.000
1.022
10
9
8
7
6
5
4
3
2
1
ppm
1.00
1.02
2.08

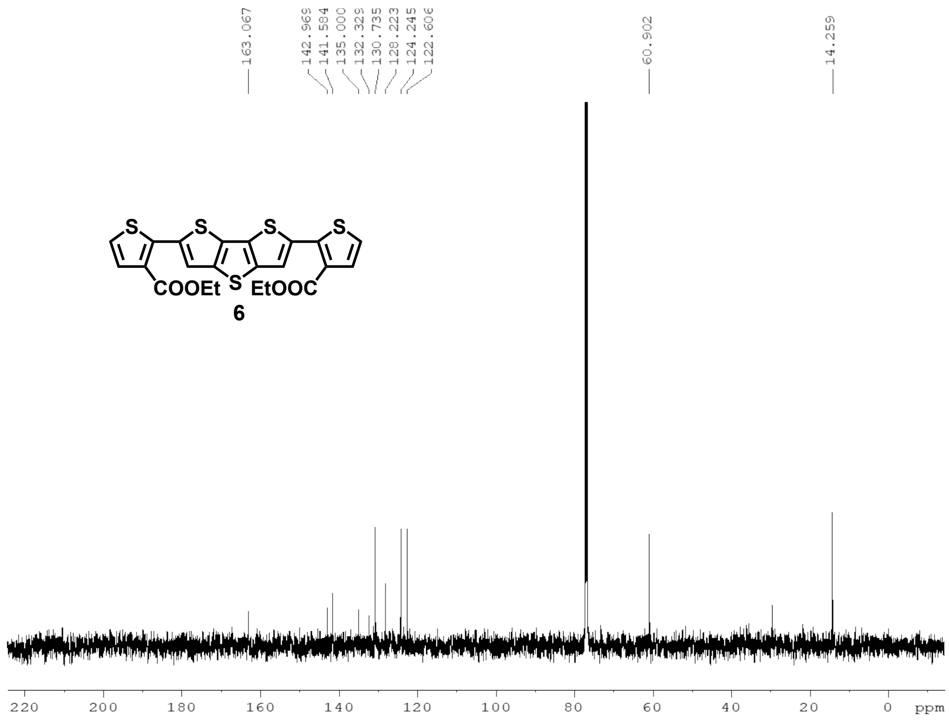
^{13}C NMR of synthesized compounds


INDCDTT-b16

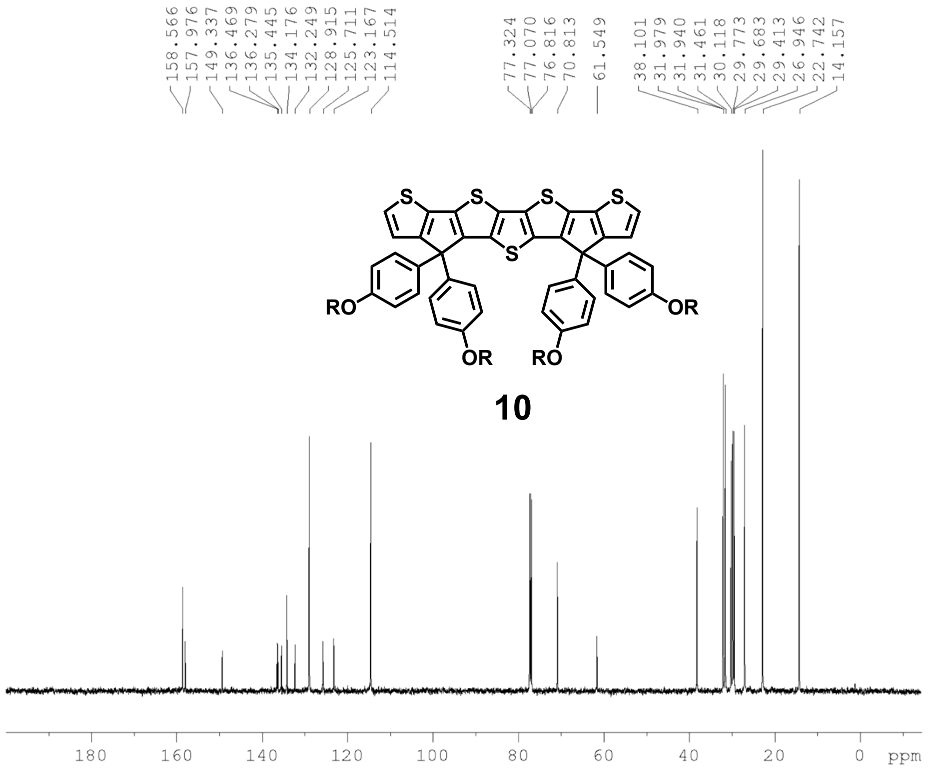

IN^{F}DCDTT-b16


186.04
160.35
159.19
157.65
156.81
156.15
140.24
139.62
139.30
139.22
138.53
138.47
138.23
135.83
131.81
128.75
126.80
125.04
120.09
114.96
114.40
114.30
70.99
68.64
61.78
37.97
31.88
31.84
31.33
30.02
29.67
29.59
29.32
26.84
22.65
14.07
Cl
Cl
O
NC
CN
S
S
S
S
S
S
C_6H_{13}
C_8H_{17}
O
IN^{Cl}DCDTT-b16
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

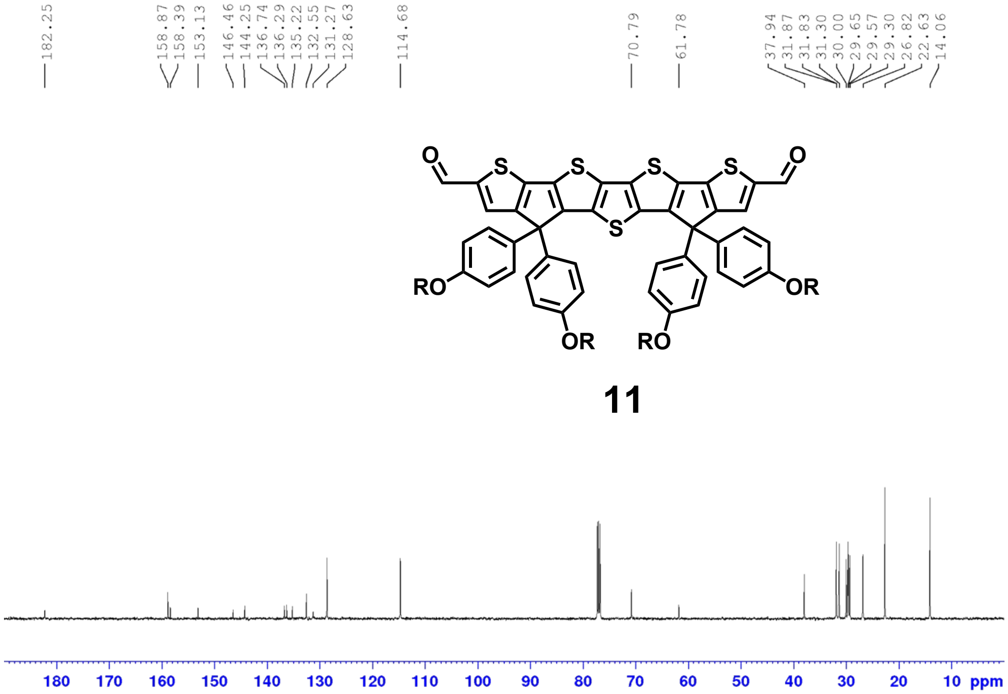

186.03
160.39
159.22
157.58
156.87
156.19
140.36
139.24
139.10
138.52
138.27
136.19
132.43
132.03
131.82
129.77
128.78
128.14
119.96
114.99
114.47
114.34
71.02
68.63
61.80
37.99
31.89
31.85
31.35
30.03
29.68
29.60
29.32
26.86
22.65
14.07
1.01
Br
Br
O
NC
CN
S
S
S
S
S
S
RO
OR
IN^{Br}DCDTT-b16
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


163.067
142.969
141.584
135.000
132.329
130.735
128.223
124.245
122.606
60.902
14.259
S
S
S
S
S
COOEt
EtOOC
220
200
180
160
140
120
100
80
60
40
20
0
ppm

6

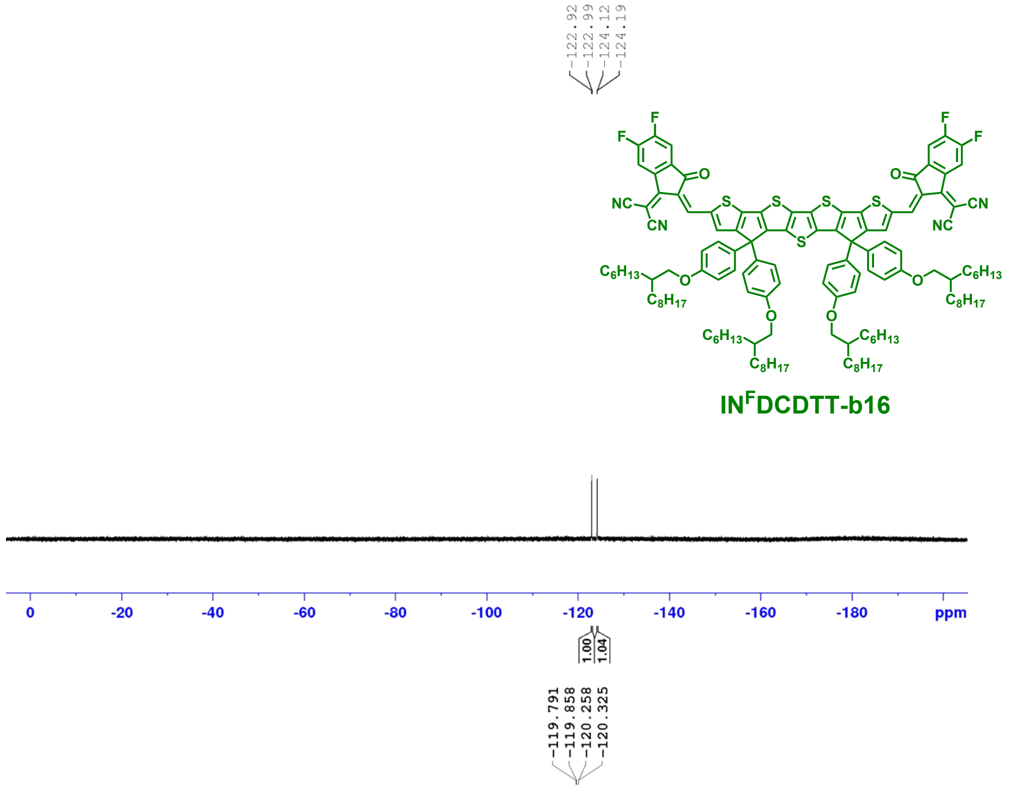

158.566
157.976
149.337
136.469
136.279
135.445
134.176
132.249
128.915
125.711
123.167
114.514
77.324
77.070
76.816
70.813
61.549
38.101
31.979
31.940
31.461
30.118
29.773
29.683
29.413
26.946
22.742
14.157
S
S
S
S
S
RO
OR
OR
RO
180
160
140
120
100
80
60
40
20
0
ppm

10

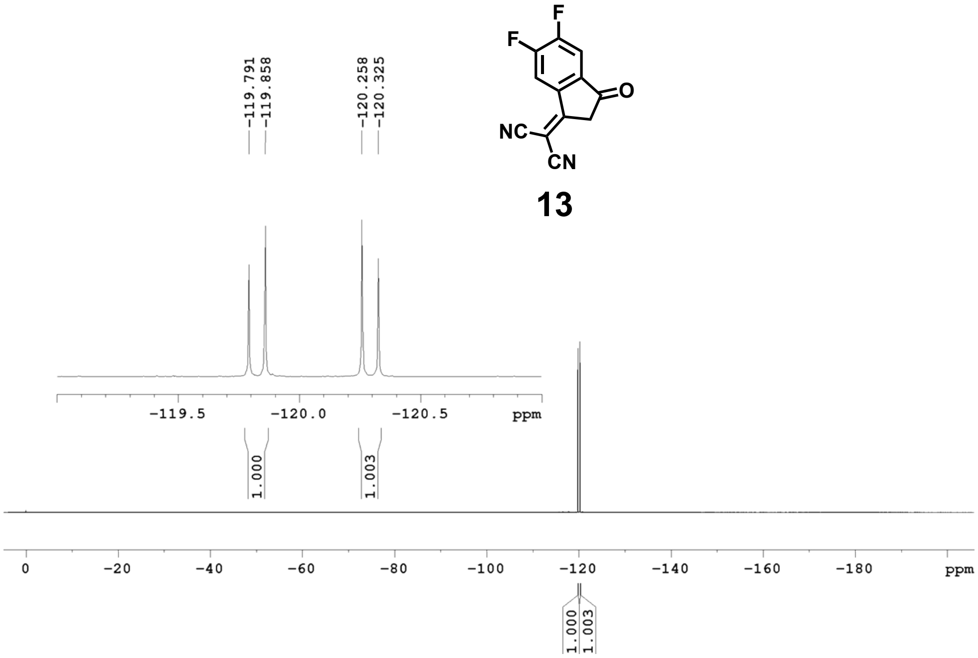

182.25
158.87
158.39
153.13
146.46
144.25
136.74
136.29
135.22
132.55
131.27
128.63
114.68
70.79
61.78
37.94
31.87
31.83
31.30
30.00
29.65
29.57
29.30
26.82
22.63
14.06
O
S
S
S
S
S
O
RO
OR
OR
RO
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

11

^{19}F NMR of compound IN^{F}DCDTT-b16 (2), and 13

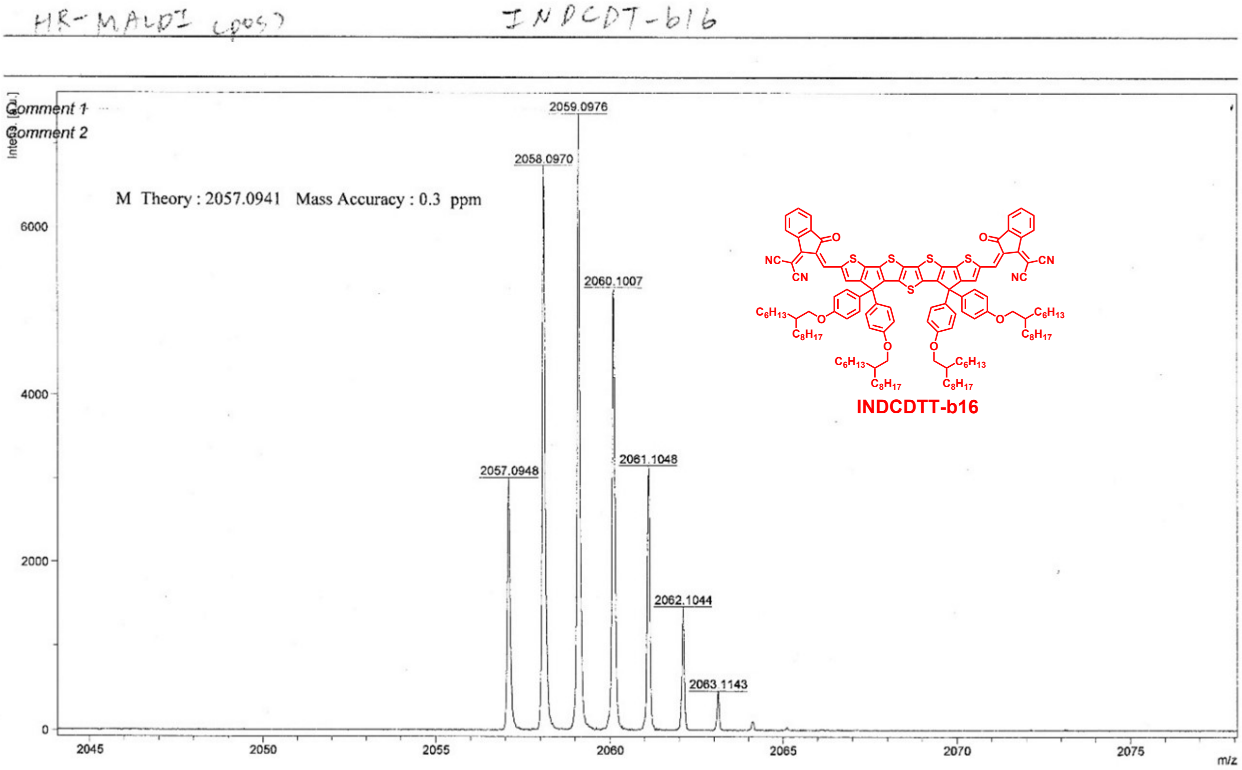


IN^{F}DCDTT-b16

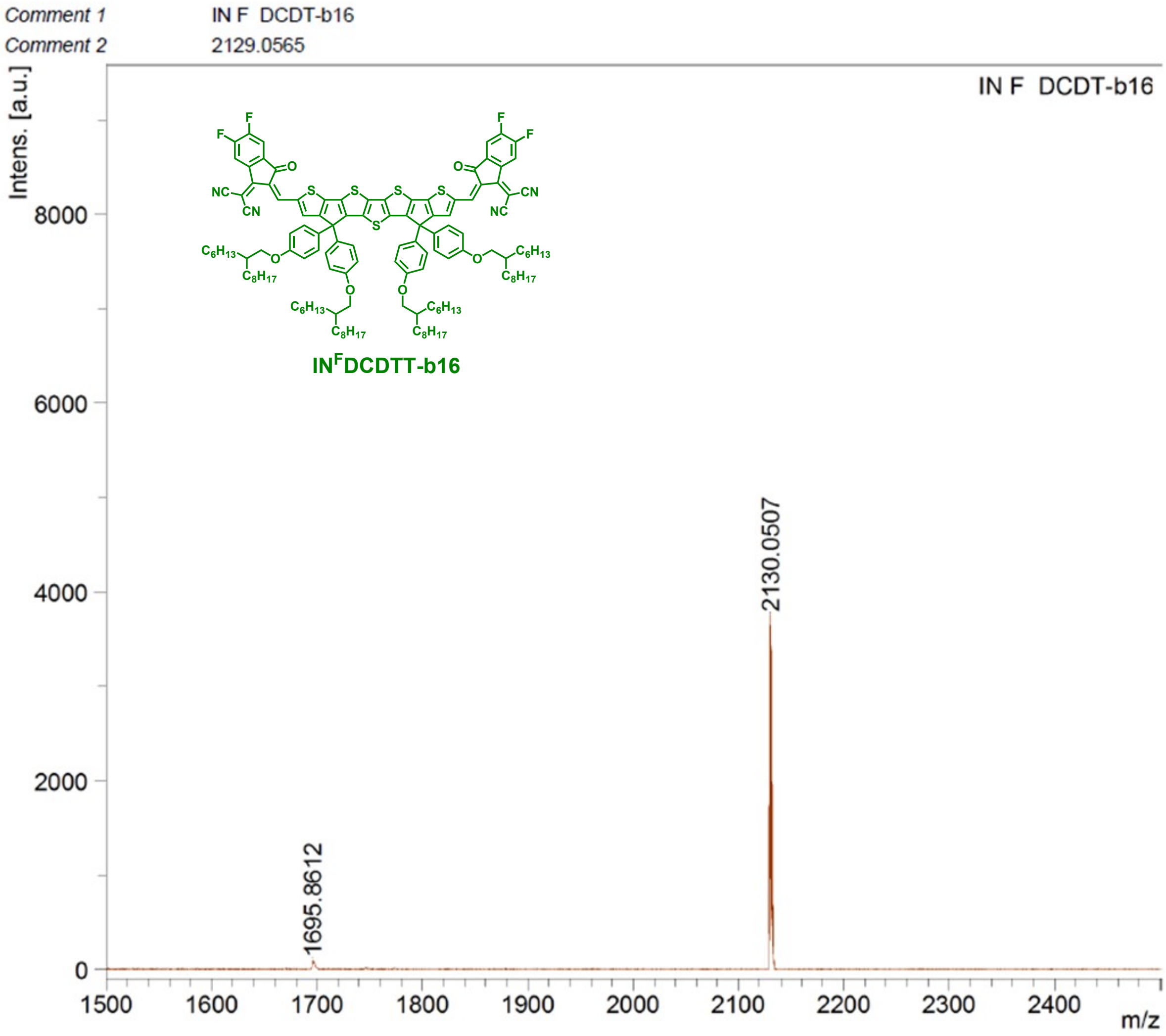


13

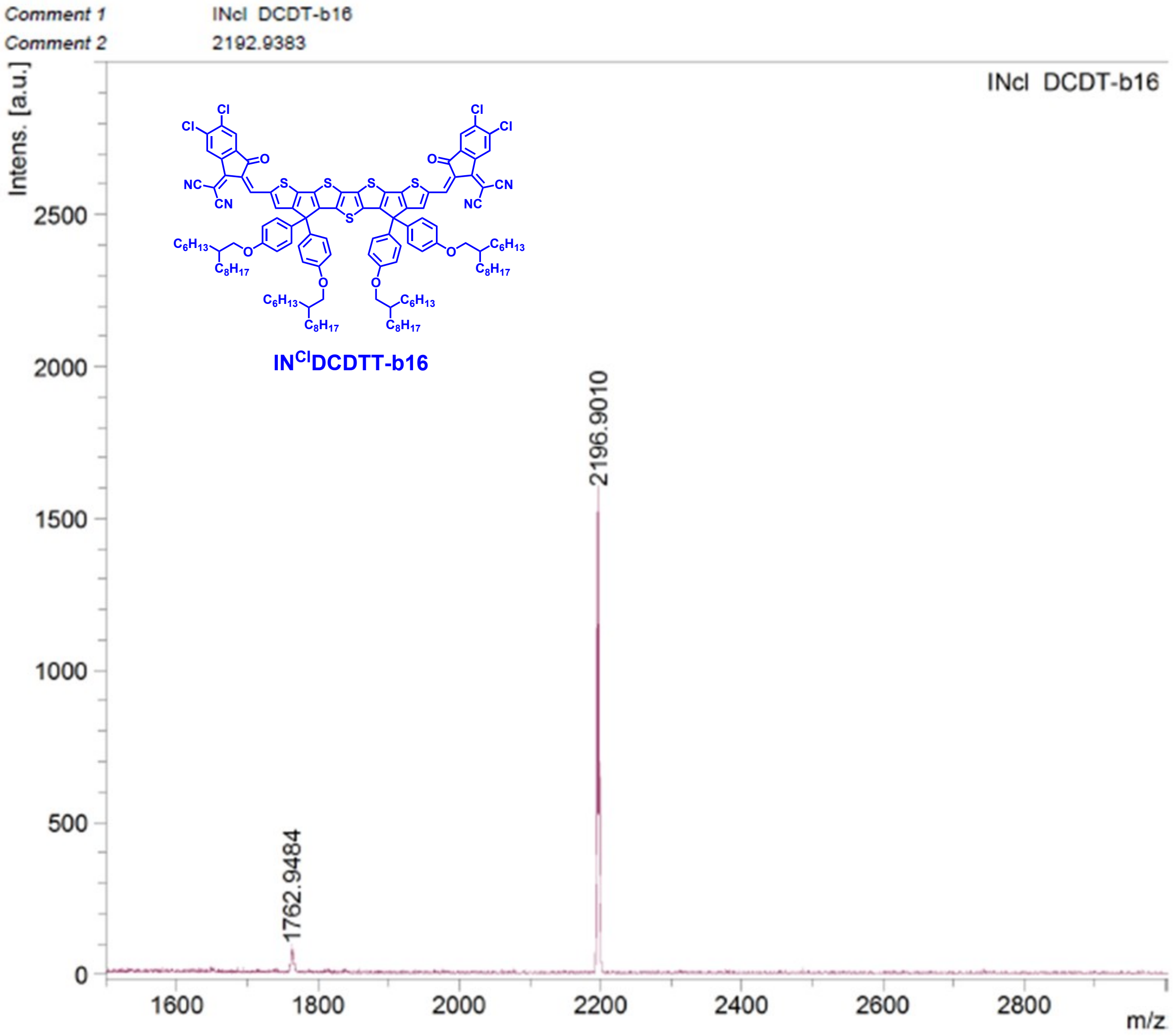
HRMS spectra of synthesized compounds



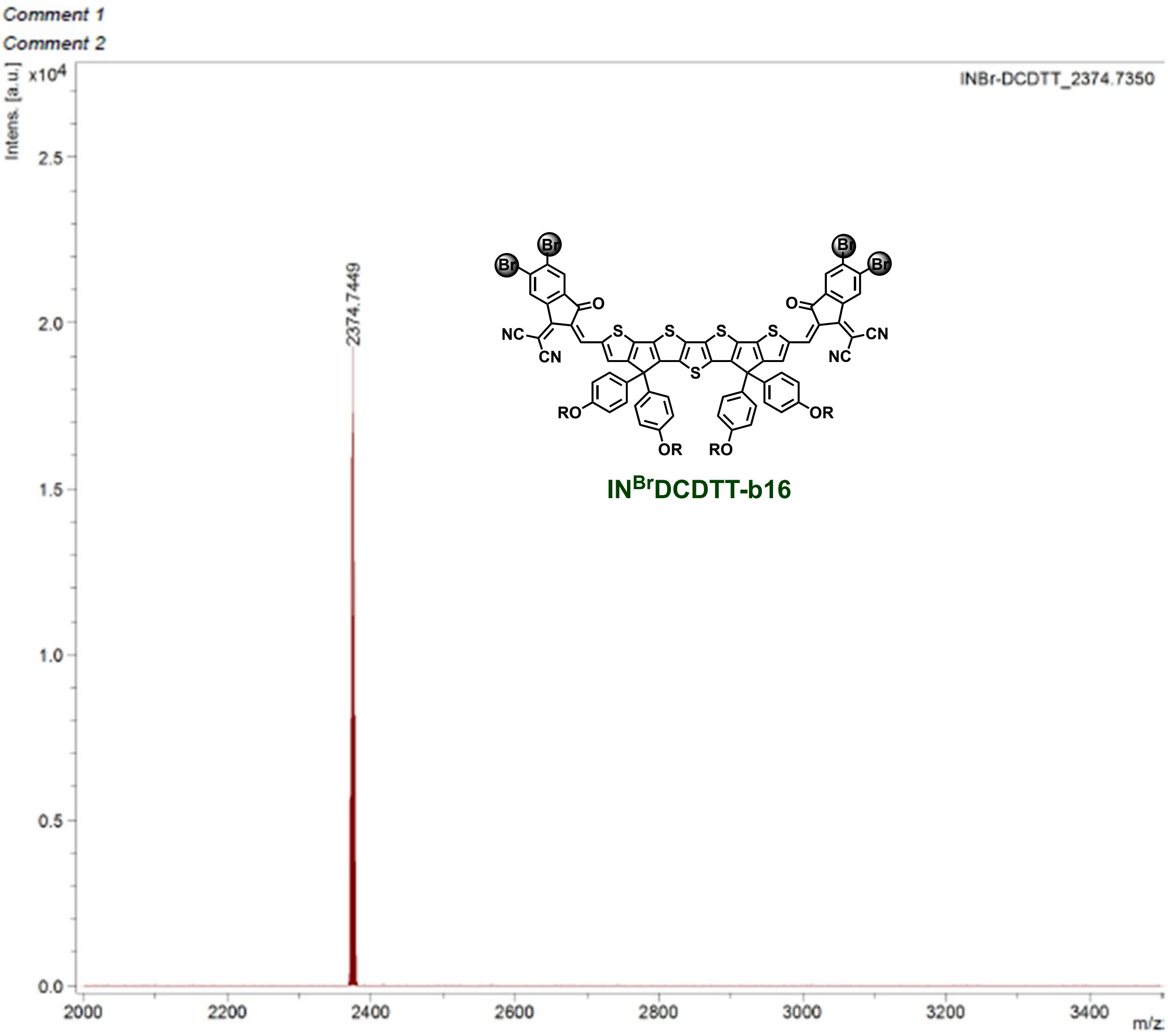
Formula	Mass	Error	mSigma	DblEq	N rule	Electron Configuration
C 132 H 156 F 4 N 4 O 6 S 5	2,129.0559	2.1876	96.4448	55.00	ok	odd



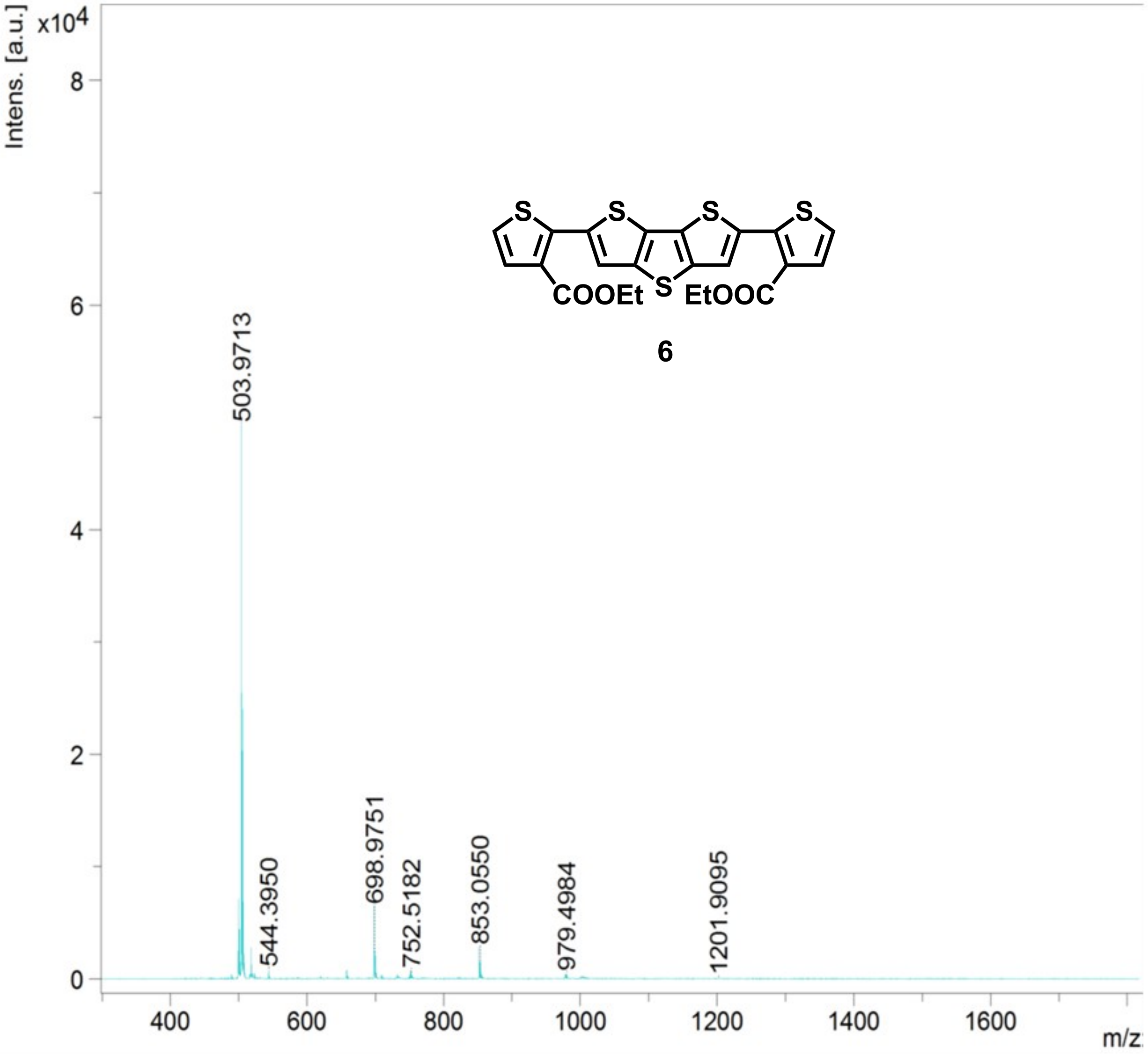
Formula	Mass	Error	mSigma	DblEq	N rule	Electron Configuration
C 132 H 157 Cl 4 N 4 O 6 S 5	2,193.9455	2.2299	229.2290	54.50	ok	even



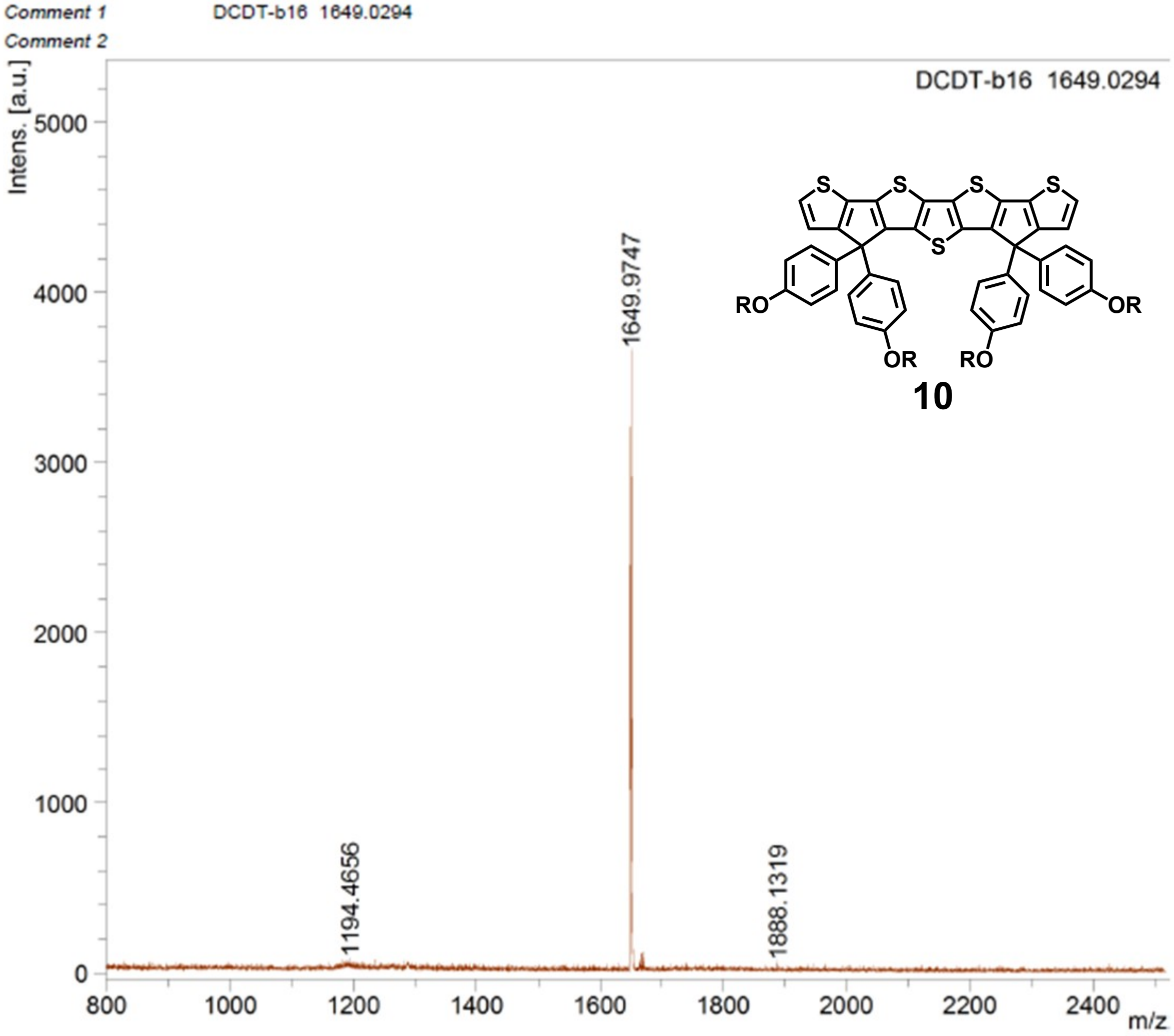
Formula	Mass	Error	mSigma	DblEq	N rule	Electron Configuration
C 132 H 156 Br 4 N 4 O 6 S 5	2,368.7356	0.2717	57.3512	55.00	ok	odd



Formula	Mass	Error	mSigma	DblEq	N rule	Electron Configuration
C 22 H 16 O 4 S 5	503.9647	13.1081	800.7537	15.00	ok	odd



Formula	Mass	Error	mSigma	DblEq	N rule	Electron Configuration
C 106 H 152 O 4 S 5	1,649.0289	1.8616	76.2139	31.00	ok	odd



Formula	Mass	Error	mSigma	DblEq	N rule	Electron Configuration
C 108 H 152 O 6 S 5	1,705.0187	16.0220	224.8814	33.00	ok	odd

Comment 1 DCDT-CHO-b16 1705.0192

Comment 2