Supplementary Information (SI) for Journal of Materials Chemistry C.

Supporting Information

Dithienopyrrolothiophene (DTPT) Based Acceptors for Fine-Tuning Molecular Packing and Enhancing Ternary Organic Photovoltaic Performance

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Experimental Section

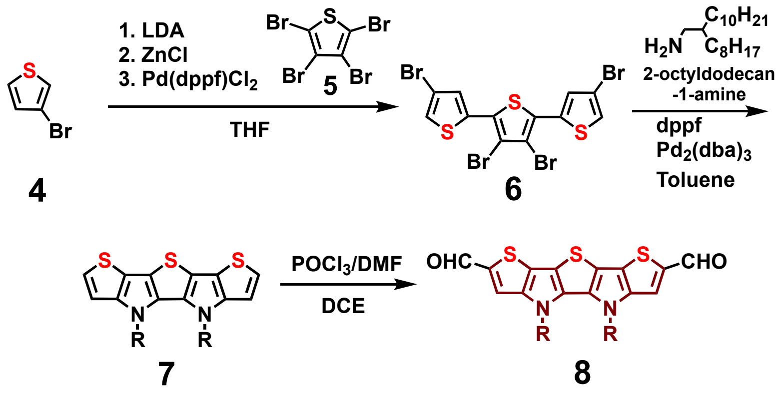
Characterization

^{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$_6$H$_4$Cl$_2$ 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

Commercially available chemicals and reagents were used without further purification. OPVs were fabricated using a sandwich configuration consisting of glass/ITO/ZnO/active layer/MoO3/Ag. Initially, the glass/ITO substrate with a sheet resistance of 6.4 Ω/sq was thoroughly cleaned and sonicated in deionized water, acetone, and isopropanol for 20 minutes in an ultrasonic bath (DELTA, DC200H). A sol–gel ZnO precursor solution was then prepared by stirring zinc acetate (3.15 g), ethanolamine (0.9 mL), and 2-methoxyethanol (29.1 mL) at 25 °C for 3 days. Before depositing the ZnO layer, the glass/ITO substrate was treated with oxygen plasma for 5 minutes using a Harrick Plasma cleaner (PDC-32G). The precursor solution was filtered through a 0.45-μm filter and spin-coated onto the glass/ITO substrate, followed by annealing at 170 °C for 10 minutes to form a ZnO layer with a thickness of approximately 30 nm. The binary precursor solution for the active layer was prepared by dissolving PM6 (donor) and Y6 (host acceptor) in chloroform (CF) with 0.5% 1-chloronaphthalene (CN) at a weight ratio of 1:1.2. The solution was stirred at 60 °C for one hour in an argon-filled glovebox. For the ternary active layer, the precursor solution consisted of PM6 (donor), Y6 (host acceptor), and **IN-DTPT**-derivative (guest acceptor) in chloroform (CF) with 0.5% 1-chloronaphthalene (CN) at a weight ratio of 1:1.2:0.1. The solution was stirred for one hour at 60 °C in an argon-filled glovebox. Both precursor solutions were deposited onto the glass/ITO/ZnO substrate at room temperature. The thickness of the active layer was optimized by controlling the spin rate and precursor solution concentration. Using evaporation equipment under vacuum (pressures < 10^{-6} torr), a 3 nm MoO3 layer and a 100 nm Ag layer were deposited onto the active layer to complete the device. The active area (0.1 cm^2) was defined by the overlap between the ITO and Ag electrodes.

The photocurrent–voltage (J–V) characteristics of the devices were measured using a computer-controlled Keithley 2400 source measure unit (SMU) and an Enlitech solar simulator (AAA Class) under AM 1.5G illumination (1000 W m^{-2}). The photovoltaic parameters (Voc, Jsc, FF, and PCE) as functions of light illumination intensity were measured under AM 1.5G solar simulator illumination. The illumination intensity was calibrated using a standard silicon (Si) reference cell and a KG-5 filter. External quantum efficiencies (EQEs) were measured using an Enlitech QE-R spectral response measurement system to calibrate the current densities of the devices. The UV–Vis absorption spectra of the thin films were recorded using a Jasco V-650 UV–Vis spectrophotometer. The PL spectra of the thin films were recorded using a Edinburgh FLS1000 Photoluminescence Spectrometer. The topographical and phase images of the active layers fabricated under various conditions were obtained using atomic force microscopy (AFM) (Bruker Dimension Edge) operated in tapping mode. Grazing-incidence wide-angle X-ray scattering (GIWAXS) spectra of the blend films were recorded at the TPS25A beamline (National Synchrotron Radiation Research Center, Taiwan) using an X-ray wavelength of 1.8602 Å and an incident angle of 0.05°. The all-in-one characterization platform Paios (Fluxim AG) was used to determine the photoelectric properties of OPVs, including photo-CELIV, TPC, and TPV measurements.



Scheme S1. Synthesis of key intermediatess **7** and **8**.

Synthesis of compound 6: 2.5 M LDA (7.58 mL, 15.2 mmol) was slowly added to 3-bromothiophene (**4**) (3.15 g, 8 mmol) at -78 °C in THF (80 ml) under the anhydrous condition at 0 °C and continued stirring for one hour at the same temperature. Then $ZnCl_2$ (2.01 g, 15.2 mmol) was added to the reaction mixture at 0 °C and stirred for another 1 hour. Afterward, $Pd(dppf)Cl_2$ (0.2 g, 0.3 mmol) and tetrabromothiophene (**5**) (2 g, 5 mmol) were added and the reaction mixture was refluxed for 24 hours. After completion of the reaction, deionized water was added to terminate the reaction, and a crude reaction mixture was extracted with ethyl acetate. The organic layer was concentrated by rotary evaporator, and purified by column chromatography using n-hexane as eluent to get a white solid (1.2 g, 60%). ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.45 (d, J = 5 Hz, 2 H), 7.10 (d, J = 5 Hz, 2H).

Synthesis of compound 7: Under anhydrous and oxygen-free conditions, the catalyst $Pd_2(dba)_3$ (0.13 g, 0.14 mmol) and the ligand dppf (0.3 g, 0.57 mmol) were added to toluene. Next, sodium t-butoxide (2.1 g, 22.88 mmol) and 3,3',3',4'-tetrabromo-2,2':5',2'-terthiophene (**6**) (0.72 g, 1.43 mmol), were added at room temperature and kept stirring for 20 minutes, finally, 2-octyldodecan-1-amine (0.54 g, 3.43 mmol) was added to the reaction mixture and refluxed overnight. After the reaction was complete, deionized water was added to terminate the reaction and extracted with diethyl ether. The organic layer was collected and concentrated on rotavapor and the crude reaction mixture was purified by column chromatography to give compound **7** (0.4 g, 55%). ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.08 (d, J = 5 Hz, 2 H), 7.00 (d, J = 5 Hz, 2 H), 4.35 (t, J = 7.5 Hz, 4 H), 0.87 (t, J = 7.5 Hz, 6 H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 144.18, 130.11, 121.92, 116.69, 115.96, 111.14, 48.99, 31.95, 31.42, 29.49, 29.34, 27.02, 22.65, 14.08，

Synthesis of compound 8: Slowly $POCl_3$ (4.5 mL) was added to DMF (3.7 mL) in 30 mL DCE at 0°C and stirred for 30 min at the same temperature. To this solution, compound **7** (DTPT-b20) (0.4 g, 0.47mmol) was added at 0°C and refluxed for 20 hours. The reaction mixture was cooled to room temperature and a slowly saturated solution of $NaHCO_3$ was added at 0°C and warmed to RT. The reaction mixture was extracted with ethyl acetate, the organic layer was concentrated and the crude residue was purified by column chromatography (EA/Hexane 15:85) to obtain compound **8** (diCHO-DTPT-b20) as orange liquid ((0.38 g, 90%). ^{1}H NMR (300 MHz, $CDCl_3$): δ 9.89 (s, 2 H), 7.63 (s, 2 H), 4.30 (d, J = 7.5 Hz, 4 H) 0.88 (m, 12 H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 82.63, 145.12, 140.73, 133.72, 124.64, 119.92, 119.62, 53.72, 39.24, 31.90, 31.82, 31.43, 31.15, 30.33, 30.19, 29.82, 29.70, 29.58, 29.43, 29.37, 29.32, 29.21, 26.19, 22.68, 22.63, 14.11.

Synthesis IN-DPTP-b20 (1): Under anhydrous conditions, compound **8** (diCHO-DTPT-b20) (0.06 g, 0.07 mmol) and 2-(3-oxo-2,3-dihydro-1H-inden-1-ylidene)-Malononitrile (x) (60 mg, 0.31 mmol) were dissolved in 30 mL $CHCl_3$, 1 mL pyridine, and then heated to reflux for 24 hours. The reaction mixture was cooled to room temperature, and extracted with dichloromethane. The organic layer was dried over $MgSO_4$, concentrated, and purified by column chromatography (50:50 DCM/Hexane) to give **IN-DPTP-b20** (**1**) as a blue-green solid (0.04 g, 40%). ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.74 (s, 2 H), 8.58 (d, J = 5 Hz, 2 H), 7.95 (d, J = 10 Hz, 2 H), 7.79 (m, 4 H), 7.70 (s, 2 H), 4.38 (d, J = 10 Hz, 4 H), 0.82 (m, 12 H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 187.80, 159.80, 147.91, 139.82, 138.06, 136.76, 135.61, 135.17, 134.31, 133.09, 125.72, 125.06, 123.58, 123.20, 121.30, 114.95, 114.79, 102.7695. HRMS (HR-MALDI [M]$^+$) calcd for $C_{78}H_{94}N_6O_2S_3$: 1242. 6600. Found: 1242.6595.

Synthesis of IN^F-DPTP-b20 (2) Under anhydrous conditions, compound **8** (diCHO-DTPT-b20) (100 mg, 0.076 mmol) and 2-(5,6-difluoro-3-oxo-2,3-dihydro-1H-inden-1-ylidene)malononitrile (52 mg, 0.22 mmol) was dissolved in 30 mL $CHCl_3$, 1 mL pyridine, and then heated to reflux for 24 hours. The reaction mixture was cooled to room temperature, and extracted with dichloromethane. The organic layer was dried over $MgSO_4$, concentrated, and purified by column chromatography (50:50 DCM/Hexane) to give **IN^F-DPTP-b20** (**2**) as a blue-green solid (80 mg, 67%); ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.82 (s, 2H), 8.77 (d, J = 5 Hz, 2H), 8.47 (d, J = 10 Hz, 2H), 7.74 (m, 4 H), 7.65 (s, 2H), 4.32 (d, *J* = 10 Hz, 4 H), 0.82 (m, 12 H); ^{13}C NMR (125 MHz, CDCl$_3$): 185.50, 157.76, 155.41, 153.42, 153.31, 148.19, 137.79, 136.49, 135.96, 134.39, 133.35, 125.88, 123.48, 120.69, 114.91, 114.74, 114.51, 114.42, 112.56, 112.41, 68.47, 54.00, 39.88, 31.94, 31.87, 31.36, 30.10, 29.65, 29.57, 29.51, 29.36, 29.29, 26.39, 22.68, 14.10; HRMS (HR-MALDI [M]$^+$) calcd for $C_{78}H_{90}F_4N_6O_2S_3$: 1314.6224. Found: 1314.6230.

Synthesis of IN^{Cl}-DPTP-b20 (3): Under anhydrous conditions, compound **8** (diCHO-DTPT-b20) (0.06 g, 0.07 mmol) and 2-(5,6-dichloro-3-oxo-2,3-dihydro-1H-inden-1-ylidene)malononitrile (x) (80 mg, 0.31 mmol) were dissolved in 30 mL CHCl$_3$, 1 mL pyridine, and then heated to reflux for 24 hours. The reaction mixture was cooled to room temperature, and extracted with dichloromethane. The organic layer was dried over MgSO$_4$, concentrated, and purified by column chromatography (50:50 DCM/Hexane) to give **IN^{Cl}-DPTP-b20** (**3**) as a blue-green solid (0.04 g, 40%). ^{1}H NMR (500 MHz, CDCl$_3$): δ 8.76 (s, 2 H), 8.65 (s, 2 H), 7.87 (s, 2 H), 7.78 (s, 2 H), 4.34 (d, *J* = 7.5 Hz, 4 H), 0.84 (t, *J* = 5 Hz, 6 H); ^{13}C NMR (125 MHz, CDCl$_3$): δ 185.54, 157.71, 148.48, 139.58, 139.28, 138.58, 138.23, 138.08, 136.03, 135.90, 133.53, 126.76, 125.82, 124.93, 123.65, 120.84, 114.61, 114.40, 104.12. HRMS (HR-MALDI [M]$^+$) calcd for $C_{78}H_{90}Cl_4N_6O_2S_3$: 1378.5041. Found: 1378.5036.

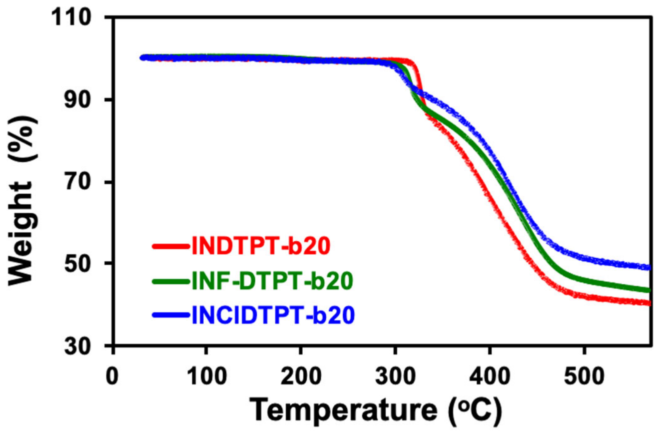


Figure S1. TGA curves of the studied compounds **1-3**.

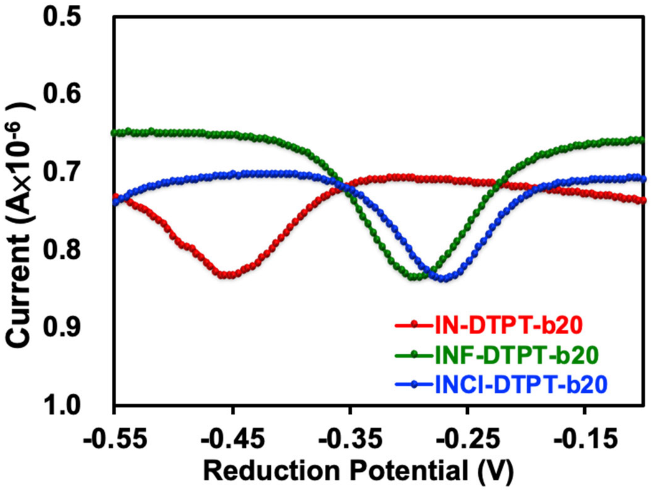


Figure S2. DPV response curves of the studied compounds **1-3**.

Table S1. *J–V* characteristics of the **IN-DTPT-b20**-containing ternary OPVs with vary blend ratio.

Blend ratio of PM6:Y6: NFA (1)	J_{SC} (mA/cm^2)	V_{OC} (V)	FF (%)	PCE (%)
1:1.2:0	25.27	0.857	71.6	15.50
1:1.2:0.05	25.22	0.869	72.6	15.92
1:1.2:0.10	25.37	0.872	75.2	16.63
1:1.2:0.20	22.33	0.897	70.1	14.04

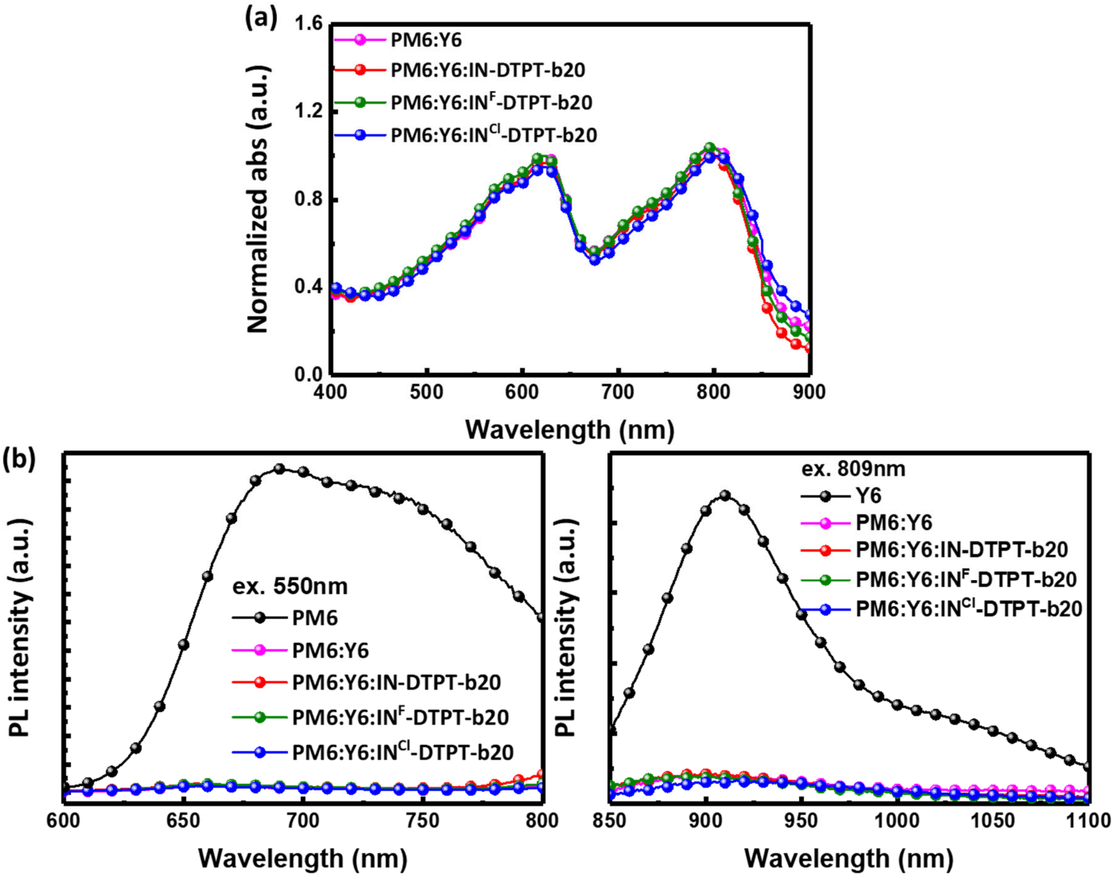


Figure S3. (a) UV–Vis spectra of binary and ternary blend films. (b) PL spectra of the neat and blend films.

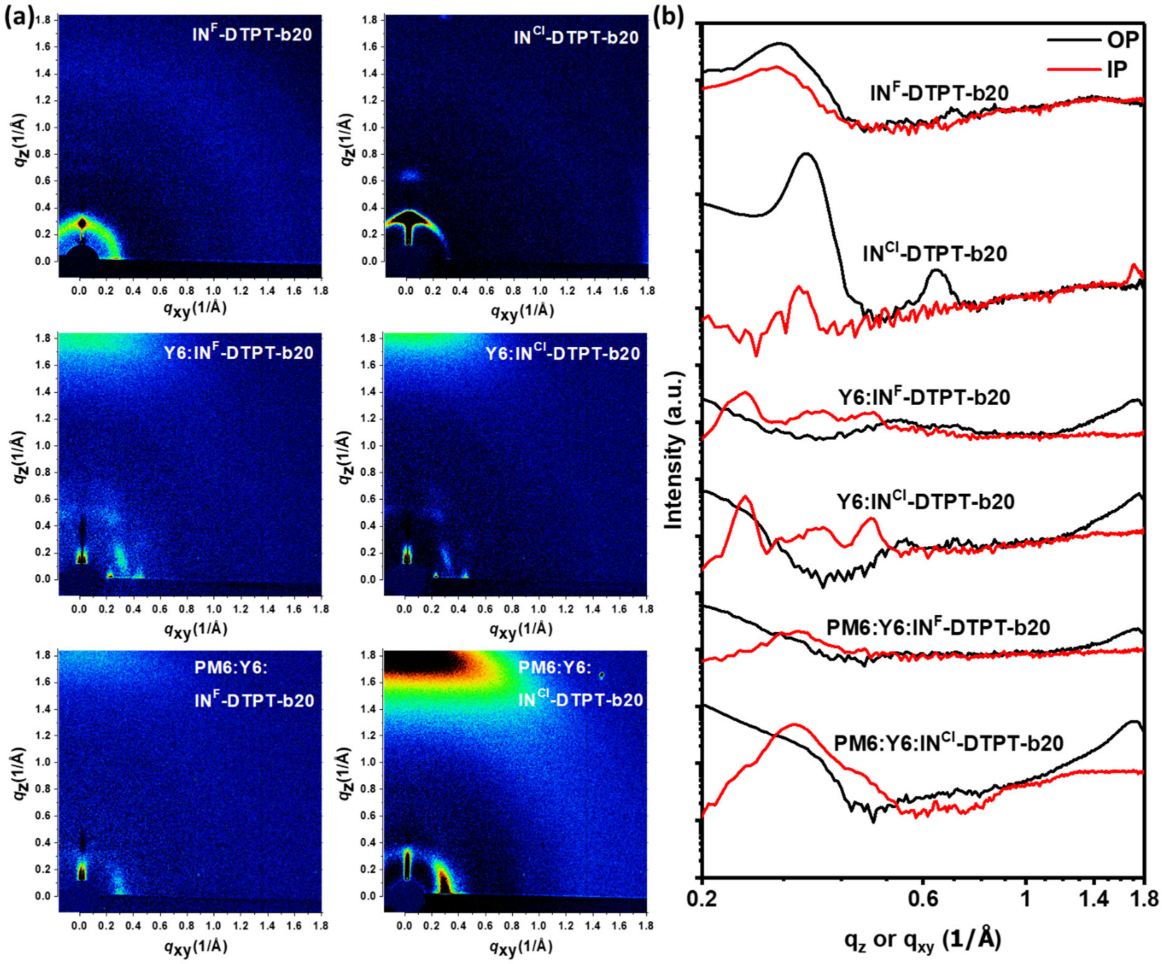


Figure S4. (a) 2D- and (b) 1D-GIWAXS profiles of neat and blend films.

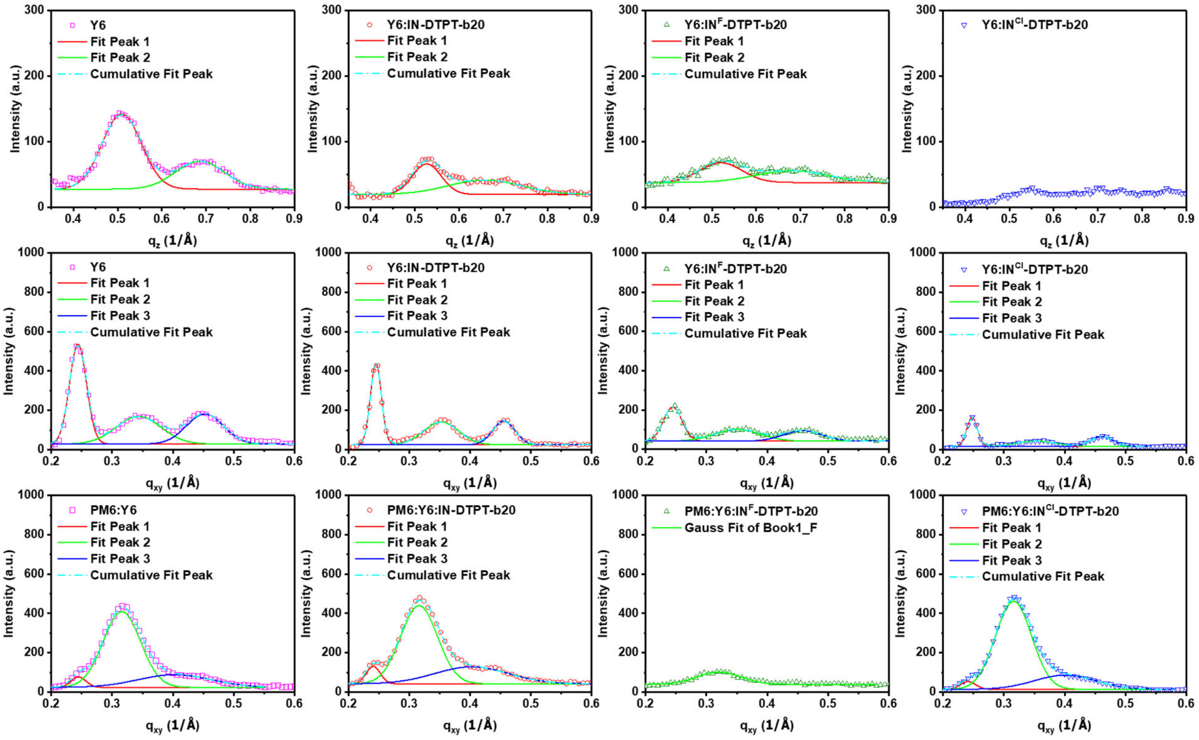


Figure S5. The zoom-in 1D GIWAXS profile can be fitted by using two or three Gaussian functions.

Table S2. GIWAXS characteristics, including peak position (q), stacking distance (d), full width at half-maximum (FWHM), and crystal coherence length (CCL), of Y6 and Y6:IN-DTPT blend films.

OP directions	(010)				(110)				(011)			
	q [Å^{-1}]	D [Å]	FWHM [Å^{-1}]	CCL [Å]	q [Å^{-1}]	D [Å]	FWHM [Å^{-1}]	CCL [Å]	q [Å^{-1}]	D [Å]	FWHM [Å^{-1}]	CCL [Å]
Y6	1.72	3.65	0.269	21.02	0.69	9.11	0.131	43.17	0.51	12.32	0.105	53.86
Y6:IN-DTPT-b20	1.75	3.59	0.254	22.26	0.66	9.52	0.182	31.07	0.53	11.86	0.075	75.40
Y6: IN^{F}-DTPT-b20	1.72	3.65	0.307	18.42	0.68	9.24	0.168	33.66	0.52	12.08	0.112	50.49
Y6: IN^{Cl}-DTPT-b20	1.74	3.61	0.271	20.87	-	-	-	-	-	-	-	-

IP directions	(002)				(101)				(001)			
	q [Å^{-1}]	D [Å]	FWHM [Å^{-1}]	CCL [Å]	q [Å^{-1}]	D [Å]	FWHM [Å^{-1}]	CCL [Å]	q [Å^{-1}]	D [Å]	FWHM [Å^{-1}]	CCL [Å]
Y6	0.45	13.96	0.071	79.65	0.34	18.48	0.087	65.00	0.24	26.18	0.033	171.36
Y6: IN-DTPT-b20	0.46	13.66	0.043	131.51	0.35	17.95	0.068	83.16	0.25	25.13	0.021	269.28
Y6: IN^{F}-DTPT-b20	0.46	13.66	0.074	76.42	0.35	17.95	0.088	64.26	0.25	25.13	0.036	157.08
Y6: IN^{Cl}-DTPT-b20	0.46	13.66	0.043	131.51	0.35	17.95	0.073	77.46	0.25	25.13	0.020	282.74

Table S3. GIWAXS characteristics, including peak position (q), stacking distance (d), full width at half-maximum (FWHM), and crystal coherence length (CCL), of binary and ternary blend film.

OP directions	**(010)**				**-**			
	q [Å^{-1}]	**D [Å]**	**FWHM [Å^{-1}]**	**CCL [Å]**	-	-	-	-
PM6:Y6	1.70	3.70	0.278	20.32	-	-	-	-
PM6:Y6:IN-DTPT-b20	1.71	3.67	0.271	20.87	-	-	-	-
PM6:Y6: IN^{F}-DTPT-b20	1.72	3.65	0.298	18.97	-	-	-	-
PM6:Y6: IN^{Cl}-DTPT-b20	1.71	3.67	0.267	21.20	-	-	-	-
IP directions	**(001)**				**Lamellar peak**			
	q [Å^{-1}]	**D [Å]**	**FWHM [Å^{-1}]**	**CCL [Å]**	**q [Å^{-1}]**	**D [Å]**	**FWHM [Å^{-1}]**	**CCL [Å]**
PM6:Y6	0.24	26.18	0.029	195.00	0.32	19.63	0.072	78.54
PM6:Y6: IN-DTPT-b20	0.24	26.18	0.024	235.62	0.32	19.63	0.071	79.65
PM6:Y6: IN^{F}-DTPT-b20	-	-	-	-	0.32	19.63	0.084	67.32
PM6:Y6: IN^{Cl}-DTPT-b20	0.24	26.18	0.03	188.50	0.32	19.63	0.07	80.78

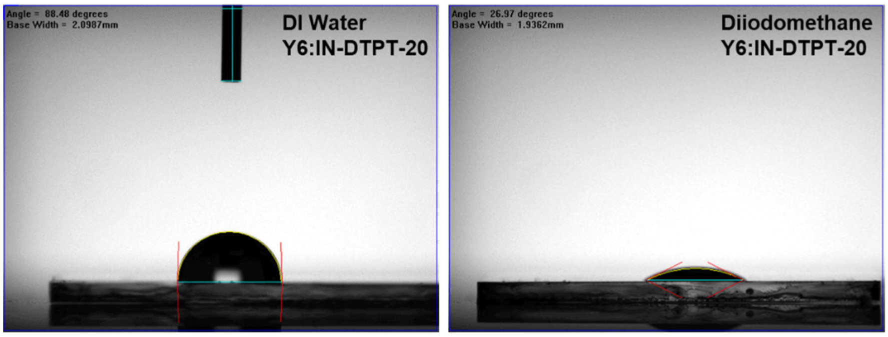


Figure S6. Contact angles of drops of water and diiodomethane for Y6:**IN-DTPT-b20** blend film.

Table S4. Surface energies and the Flory–Huggins parameters of PM6, Y6, and Y6:**IN-DTPT-b20**.

Sample	Polar ($mJ\ m^{-2}$)	Dispersive ($mJ\ m^{-2}$)	Surface energy ($mJ\ m^{-2}$)	χ PM6-X	Ref.
PM6	2.04	36.21	38.26	-	1
Y6	3.62	44.31	47.92	0.54	1
Y6:**IN-DTPT-b20**	4.27	45.56	49.83	0.76	-

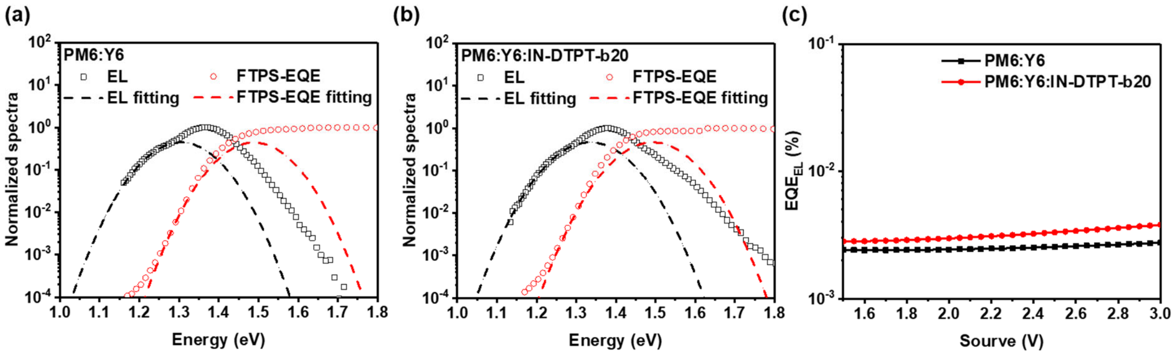
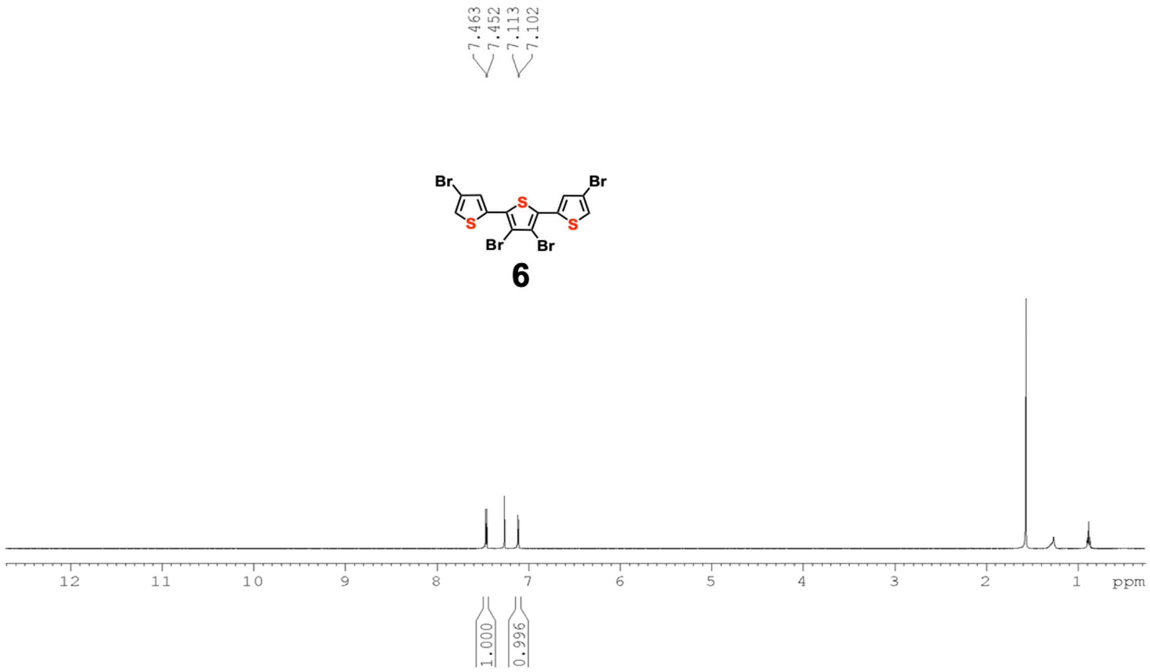


Figure S7. The normalized and fitted FTPS-EQE and EL curves of (a) PM6:Y6- and (b) PM6:Y6:**IN-DTPT-b20** -based OPVs. (c) The EQE_{EL} spectra of the binary and ternary OPVs

Table S5. Detailed Energy loss parameters of the binary and ternary OPVs.

Active layer	**E_{gap} [eV]**	**qV_{OC} [eV]**	**E_{loss} [eV]**	**E_{CT} [eV]**	**ΔE_{CT} [eV]**	**ΔE_{rad} [eV]**	**$\Delta E_{non\text{-}rad}$ [eV]**	**EQE_{EL}**
PM6:Y6	1.436	0.854	0.582	1.404	0.032	0.278	0.272	2.6×10^{-5}
PM6:Y6 :**IN-DTPT-b20**	1.437	0.871	0.566	1.414	0.023	0.278	0.265	3.3×10^{-5}

^{1}H NMR of synthesized compounds



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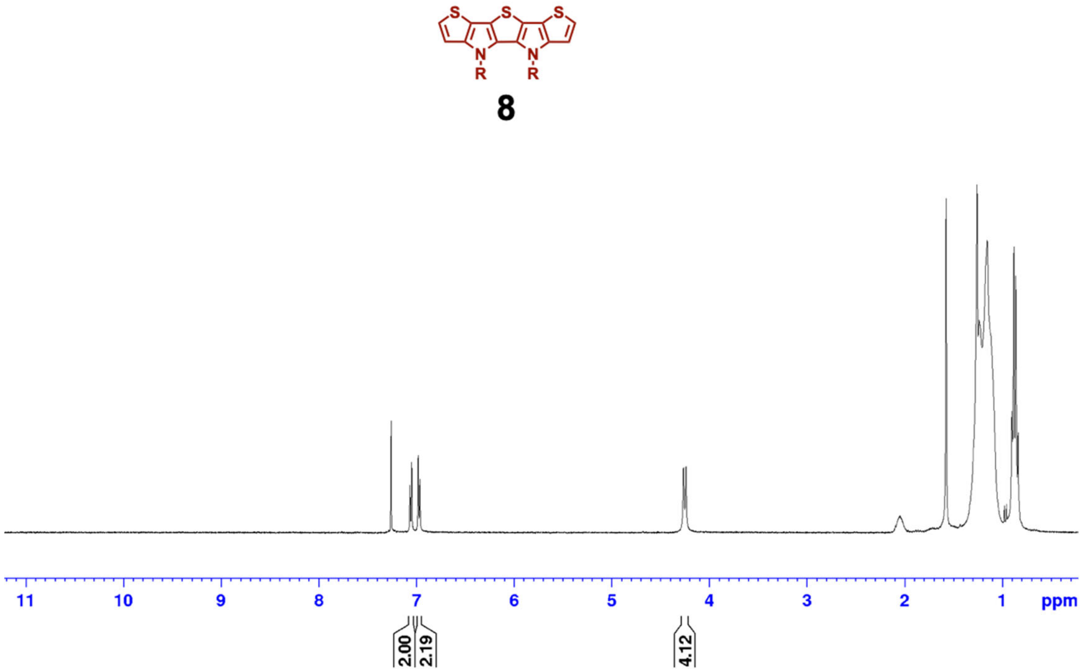

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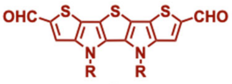
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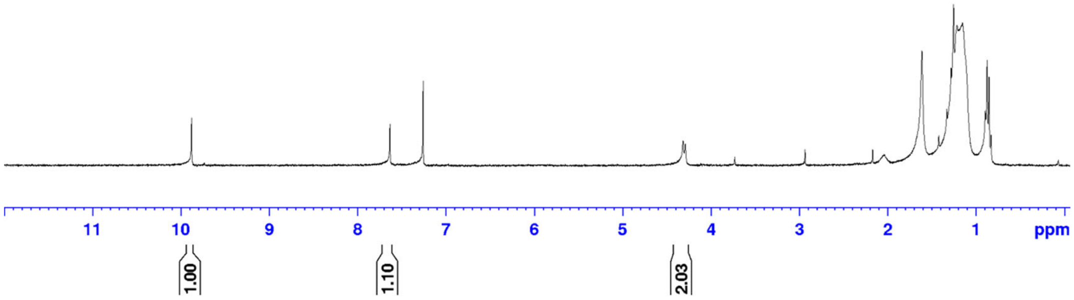
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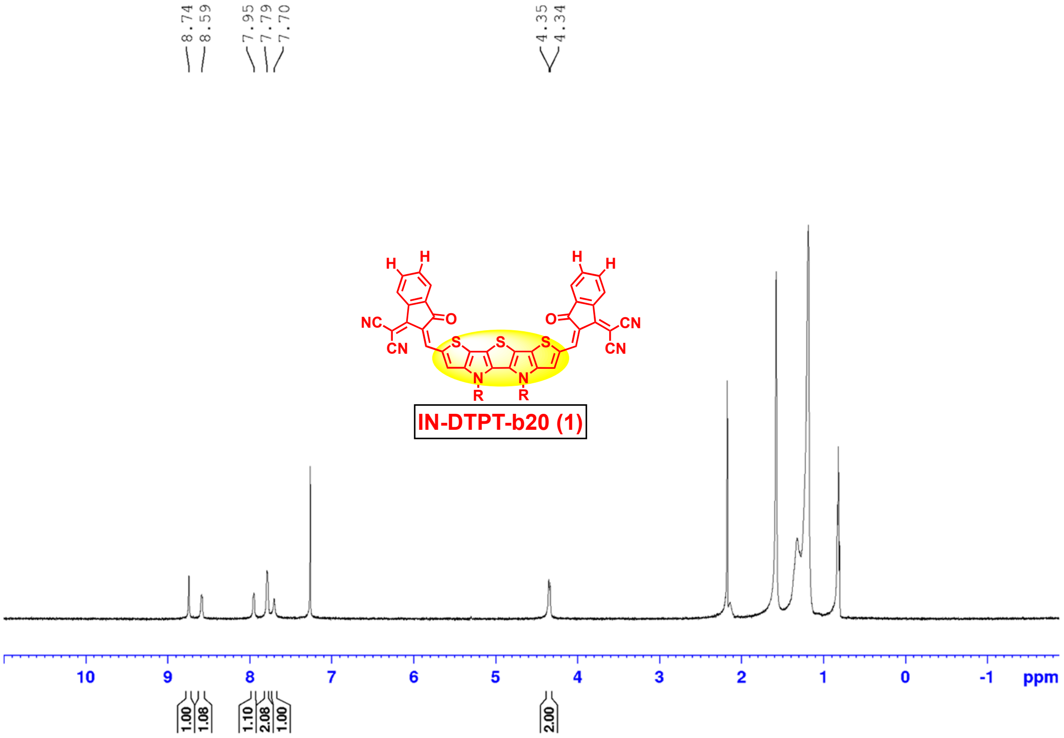
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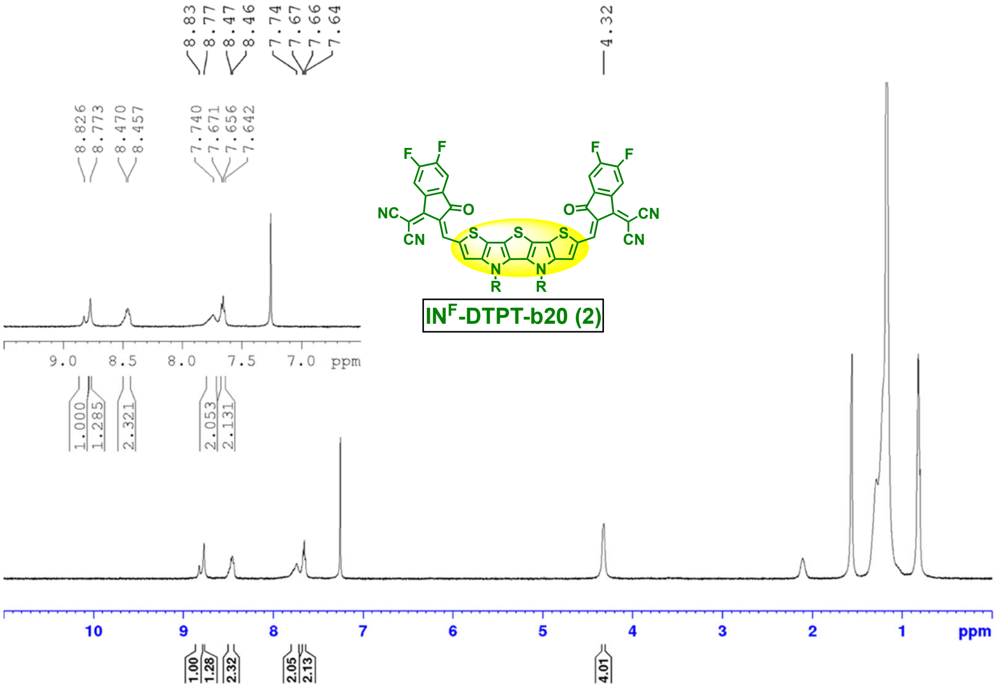
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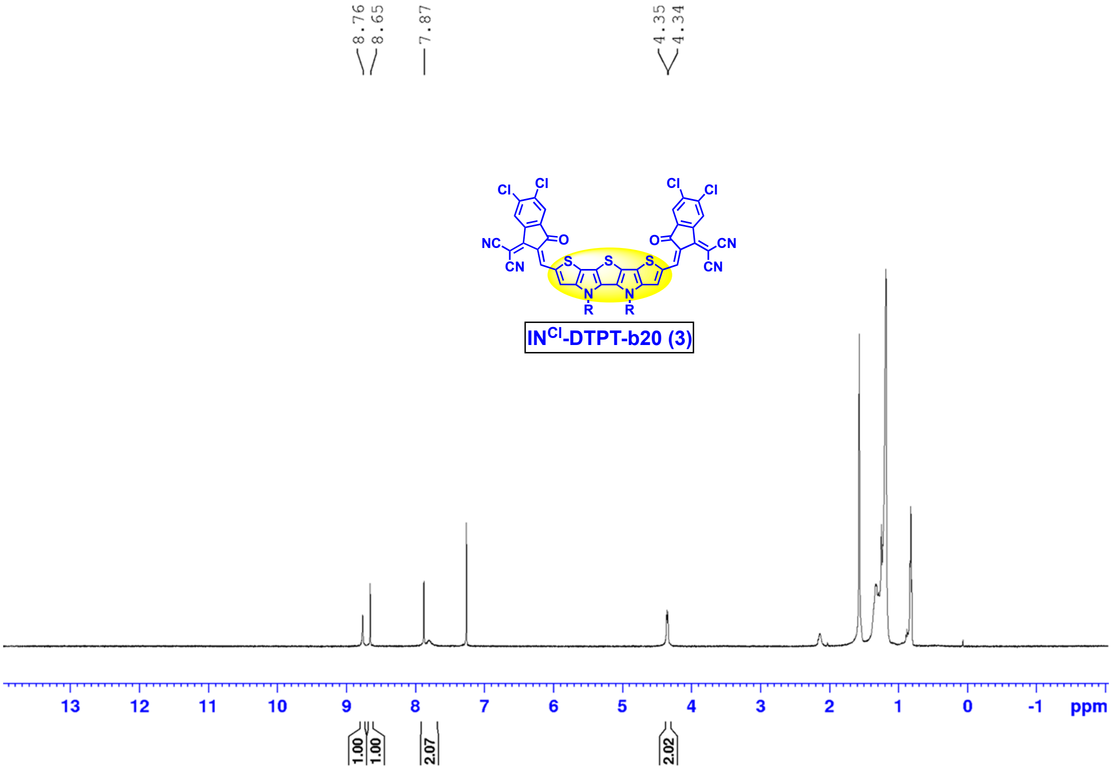
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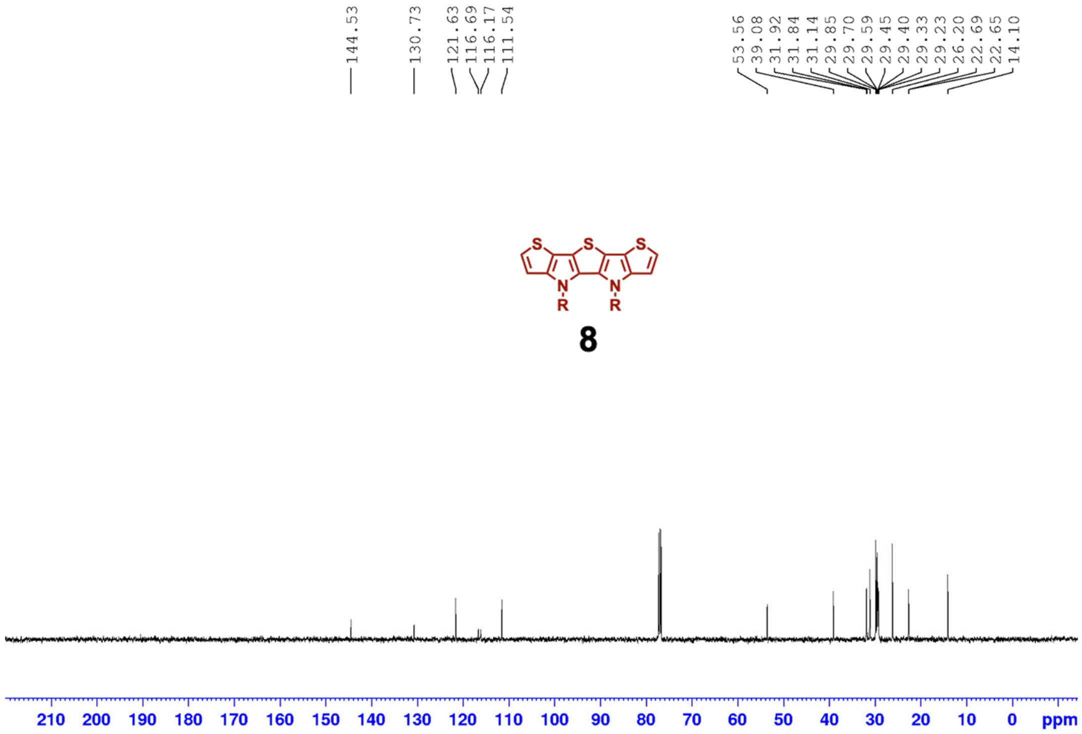
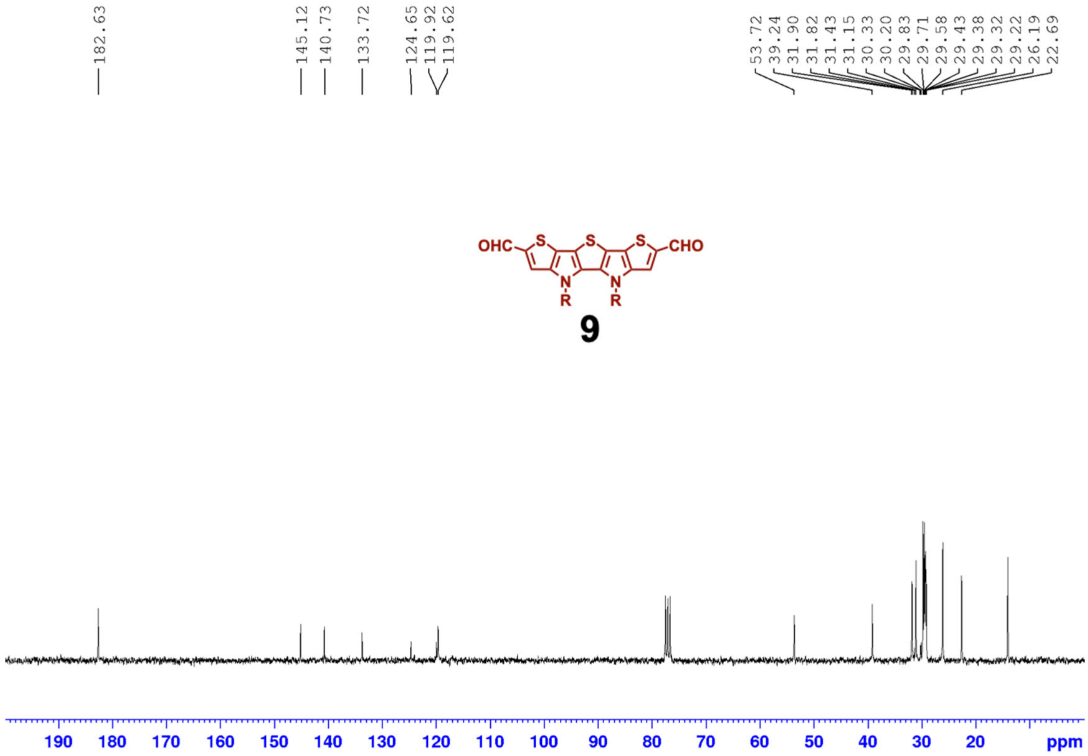
4.35
4.34
Cl
Cl
NC
CN
O
S
S
S
N
N
R
R
CN
CN
IN^{Cl}-DTPT-b20 (3)
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
ppm
1.00
1.00
2.07
2.02

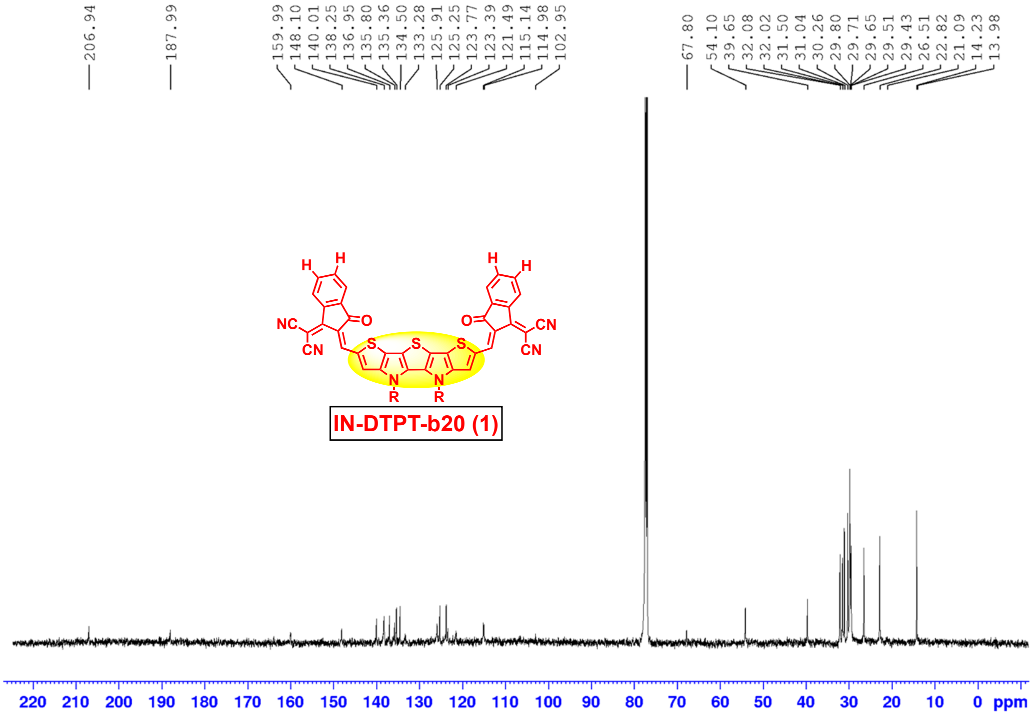
^{13}C NMR of synthesized compounds

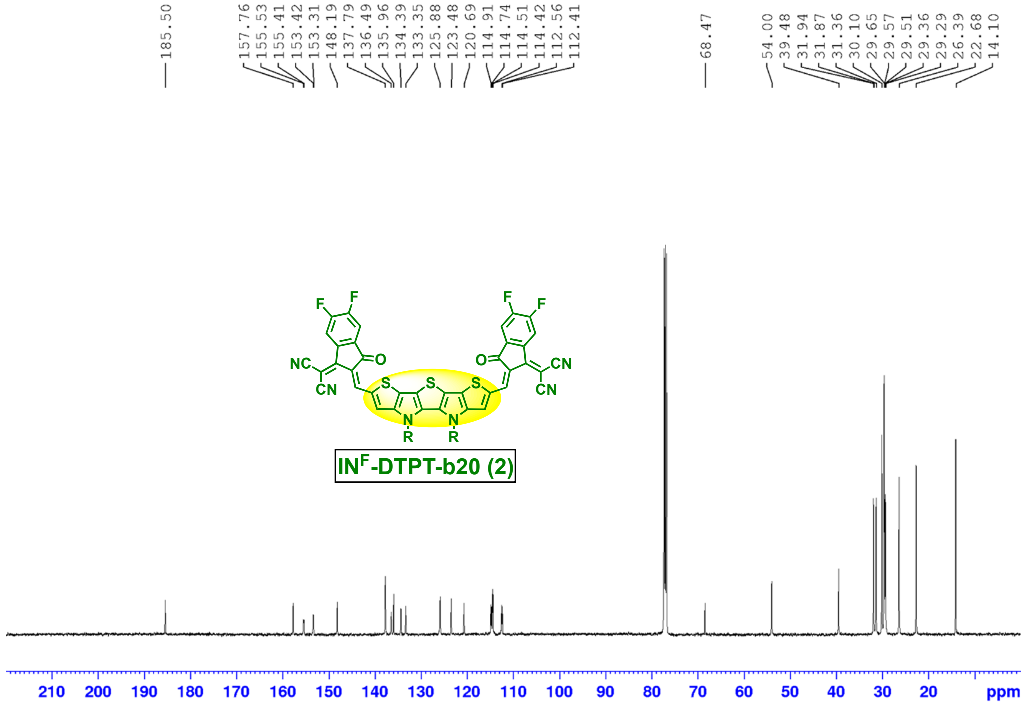


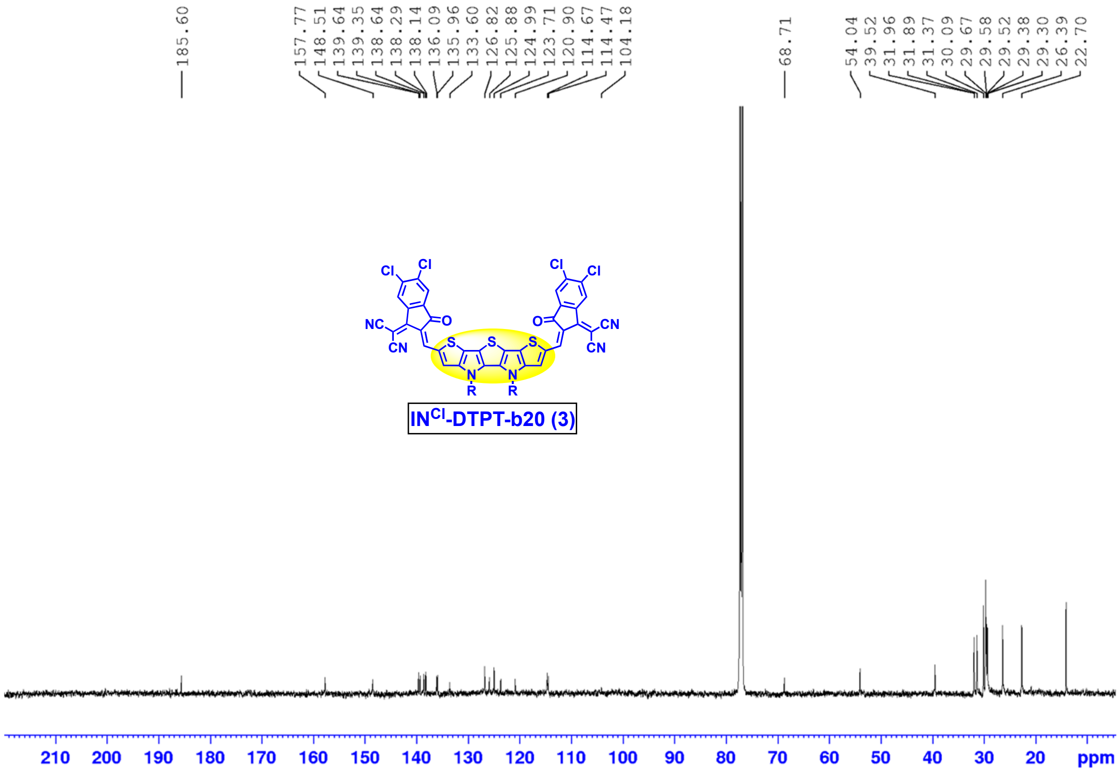
8



9


206.94
187.99
159.99
148.10
140.01
138.25
136.95
135.80
135.36
134.50
133.28
125.91
125.25
123.77
123.39
121.49
115.14
114.98
102.95
67.80
54.10
39.65
32.08
32.02
31.50
31.04
30.26
29.80
29.71
29.65
29.51
29.43
26.51
22.82
21.09
14.23
13.98
H
H
H
H
NC
CN
O
O
CN
CN
S
S
S
N
N
R
R
IN-DTPT-b20 (1)
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

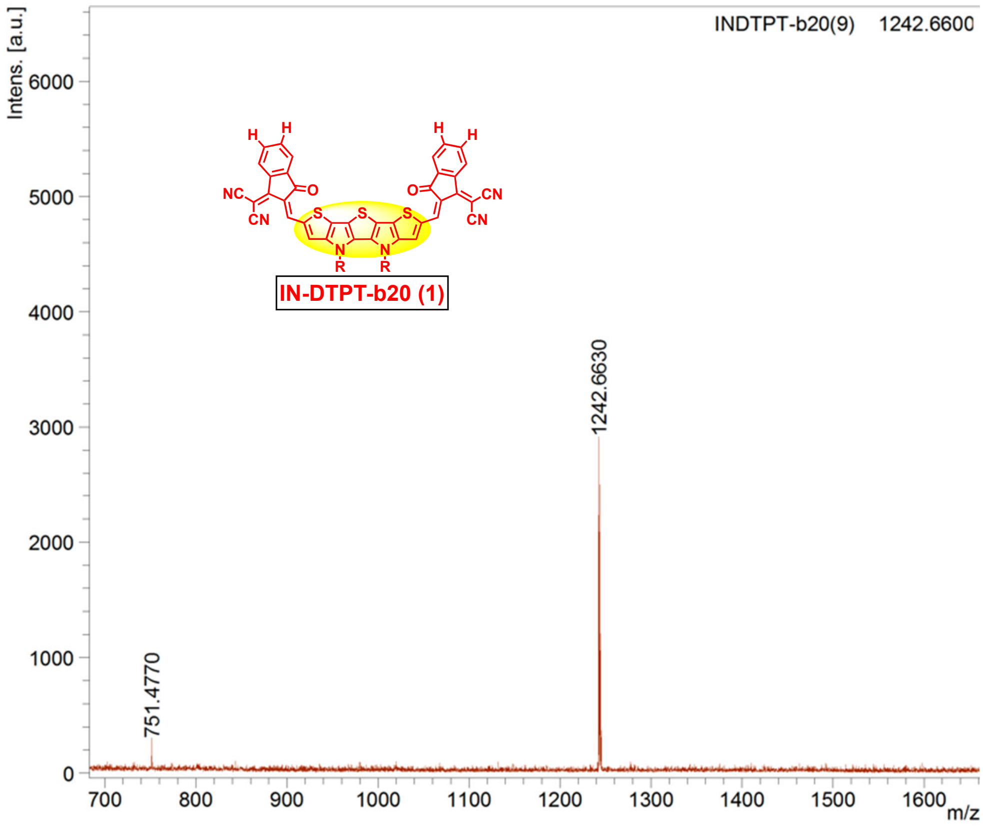

185.50
157.76
155.53
155.41
153.42
153.31
148.19
137.79
136.49
135.96
134.39
133.35
125.88
123.48
120.69
114.91
114.74
114.51
114.42
112.56
112.41
68.47
54.00
39.48
31.94
31.87
31.36
30.10
29.65
29.57
29.51
29.36
29.29
26.39
22.68
14.10
F
F
F
F
NC
CN
O
O
CN
CN
S
S
S
N
N
R
R
IN^F-DTPT-b20 (2)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


185.60
157.77
148.51
139.64
139.35
138.64
138.29
138.14
136.09
135.96
133.60
126.82
125.88
124.99
123.71
120.90
114.67
114.47
104.18
68.71
54.04
39.52
31.96
31.89
31.37
30.09
29.67
29.58
29.52
29.38
29.30
26.39
22.70
Cl
Cl
Cl
Cl
NC
CN
O
O
CN
CN
S
S
S
N
N
R
R
IN^{Cl}-DTPT-b20 (3)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

HRMS spectrum of synthesized compounds

SmartFormula

Formula	Mass	Error	mSigma	DblEq	N rule	Electron Configuration
C 78 H 94 N 6 O 2 S 3	1,242.6595	2.7907	76.5195	35.00	ok	odd

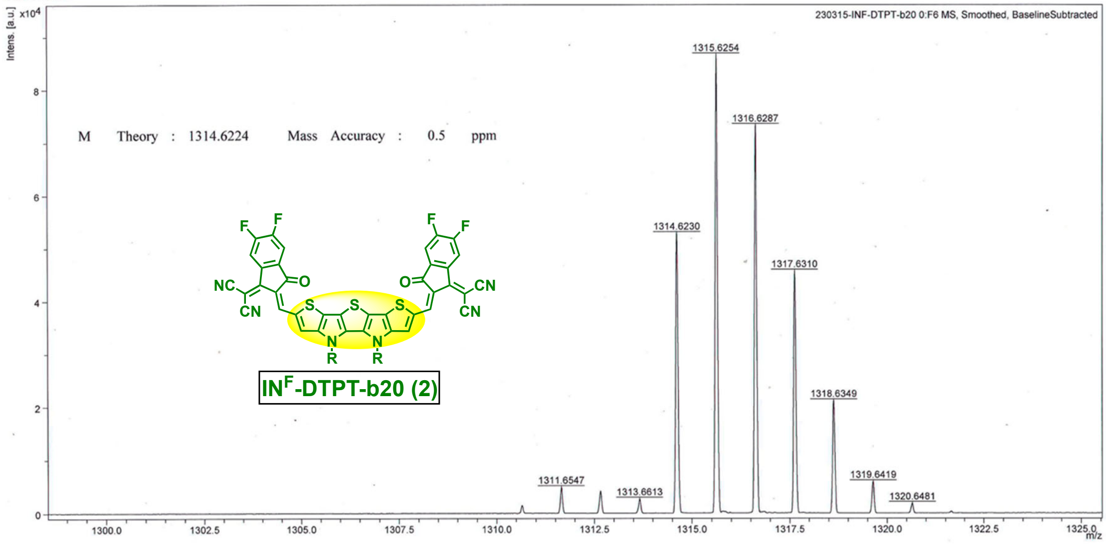


HR-MALDI (pos) INF-DTPT-b20

D:\service\MALDI-BRUKER\2023\23-0315\230315-INF-DTPT-b20\0_F6\1\1Ref

Comment 1

Comment 2

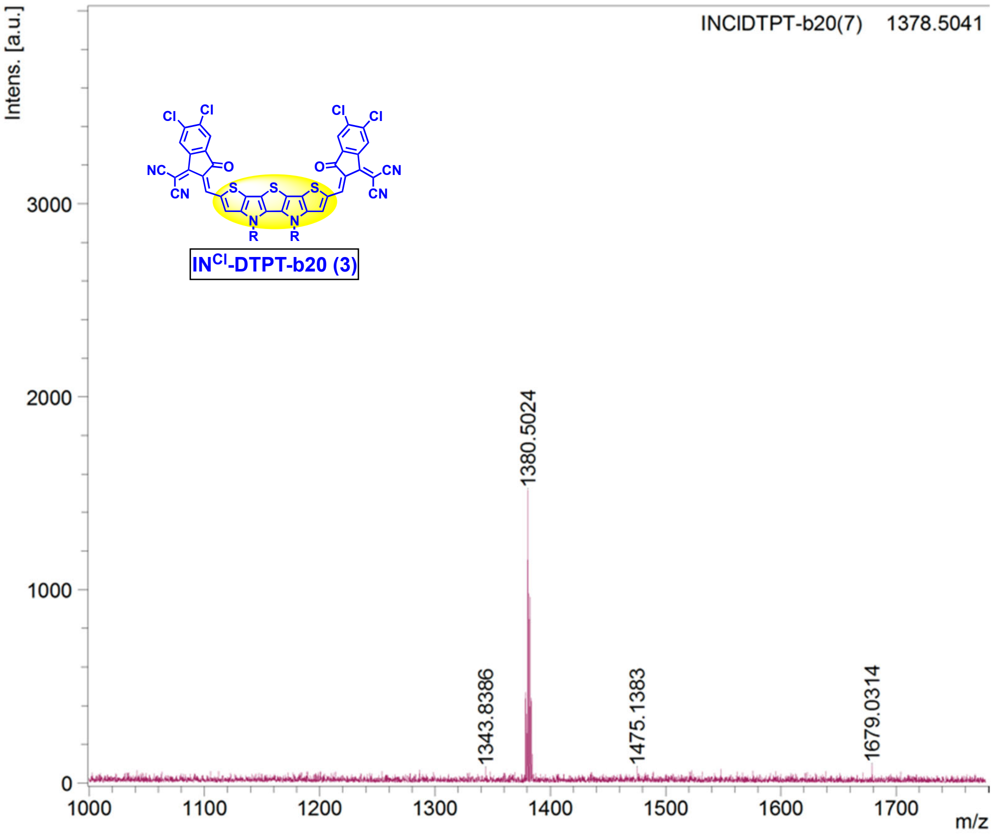


M Theory : 1314.6224 Mass Accuracy : 0.5 ppm

IN^F-DTPT-b20 (2)

SmartFormula

Formula	Mass	Error	mSigma	DblEq	N rule	Electron Configuration
C 78 H 90 Cl 4 N 6 O 2 S 3	1,378.5036	1.0679	152.6076	35.00	ok	odd



Reference

1. B.-H. Jiang, Y.-J. Peng, Y.-W. Su, J.-F. Chang, C.-C. Chueh, T.-S. Shieh, C.-I. Huang and C.-P. Chen, *Chemical Engineering Journal*, 2022, **431**, 133950.