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Supporting Information

Achieving high-performance non-halogenated nonfullerene acceptors-based organic solar cells with 13.7% efficiency through synergistic strategy of Indacenodithieno[3,2-b]selenophene core unit and non-halogenated thiophene-based terminal group

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Experimental Section

Materials and Characterization:

All air and water-sensitive reactions were carried out under N_2. Toluene and THF were dried by Na and then freshly distilled before to use. The other precursors were used as the common commercial level. ^{1}H and ^{13}C NMR spectra were carried out on a Bruker Ascend-400 and 700 NMR spectrometer. All chemical shifts were reported in ppm. Chemical shifts in ^{1}H NMR were referenced to TMS and in ^{13}C NMR were referenced to $CDCl_3$. The peaks positions of ^{13}C NMR were marked by groups. HR-MALDI-TOF-MS was recorded on a Bruker BIFLEX III mass spectrometer. HR-ESI-MS was recorded on a Bruker Solarix XR mass spectrometer. Thermogravimetric analysis (TGA) was performed using a TA Instrument Q600 analyzer under nitrogen gas flow with a heating rate of 10 ºC min^{-1}. UV-vis absorption spectra were taken on Hitachi UH5300 UV-vis spectrometer. The electrochemical cyclic voltammetry was carried out on CHI electrochemical workstation with glass carbon disk, Ag/Ag$^+$ electrode, and Pt wire, as working electrode, reference electrode, and counter electrode, respectively, in a 0.1 M tetrabutylammonium hexafluorophosphate (Bu_4NPF_6) acetonitrile solution. During CV measurements, the films were drop-cast on the glass carbon working electrode from THF solution. Atomic force microscopy (AFM) measurements were taken on a Bruker Inova atomic microscope in tapping mode. Transmission electron microscope (TEM) measurements were performed using a ZEISS LIBRA 200 FE instrument at 200 kV accelerating voltage. Grazing incidence X-ray scattering (GIXD) data were performed at beamline BL14B1 of the Shanghai Synchrotron Radiation Facility (SSRF).

BHJ-OSC Fabrication and Characterization:

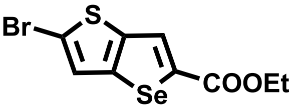
The device structure was glass/ITO/PEDOT:PSS/active layer/PNDI-F3N-Br/Al. A glass substrate with a pre-patterned ITO (sheet resistance = 15 Ω sq^{-1}) was ultrasonicated subsequently in detergent, deionized water, acetone, and isopropanol. After the plates were dried by high-pressure air flow, the substrates were cleaned by UV-ozone treatment for 30 min. PEDOT:PSS (Clevios P VP AI 4083) solution was spin-coated on the substrates at 5000 rpm for 60 s, which were then baked on a hot plate at 150 °C for about 15 min. After cooled to room temperature, the substrates were transferred to an argon filled glove box. The blend film of **PM6**: **TTTIC** or **TSeTIC**, (1:1, w/w) was prepared by spin-coating its mixed solution in CB/DIO (99.5:0.5 v/v) (20 mg mL^{-1}) at 2000 rpm for 60 s. Then the substrates were baked on a hot plate at 100 ^{o}C for 5 min. After cooled down to room temperature, PNDI-F3N-Br solution (0.5 mg/mL in MeOH) was spin-coated on the top of the active blend films at 4000 rpm for 60 s. Al cathode (100 nm) was finally deposited by using thermal evaporation in a high vacuum chamber (7×10^{-5} Pa). The optimal thickness of the active layer was typical 100 nm, which was measured using a Dektak 6 M surface profilometer. The device area was exactly fixed at 4.0 mm^{2}. The J-V characterization of the devices was carried out on a computer-controlled Keithley 2400 Source Measurement system with a solar simulator (XES-70S1, SAN EI Co., Ltd.) was used as the light source. The light intensity was monitored by using a standard Si solar cell (KONICA MINOLTA, INC.). The EQE values were tested with a Newport Model 77890 (Newport Co., Ltd.) during illumination with monochromatic light from a xenon lamp. For photocurrent behavior analysis, the photocurrent density (J_{ph}) is given by $J_{\mathrm{ph}} = J_{\mathrm{L}}$-$J_{\mathrm{D}}$, where J_{L} and J_{D} represent the light and dark current density, respectively. The effective voltage (V_{eff}) is given by the difference of compensation voltage (V_0, determined when the J_{ph} is zero) and applied voltage (V), and the saturation value of J_{ph} in the high V_{eff} region is the saturation photocurrent density (J_{sat}). The corresponding exciton dissociation probability (P_{diss}, defined as the ratio of J_{ph} to J_{sat}) can be determined under short circuit condition.

SCLC mobility measurement (SCLC)

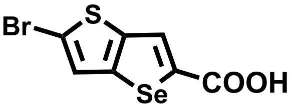
SCLC method was used to determine the hole and electron mobilities in a solar cell device by constructing different single-carrier-transporting device. The carrier mobility of the blend films were measured with the hole-only and electron-only device structure of ITO/PEDOT:PSS/**TTTIC:PM6** or **TSeTIC:PM6**/Au and Al/**TTTIC:PM6** or **TSeTIC:PM6**/Al, respectively. The active layers for the two devices are spin-coated under same condition as that of the real solar cell. The mobilities were determined by fitting the dark current to a SCLC model which is described as:

$$J = \frac{9\varepsilon_0\varepsilon_r\mu_0V^2}{8L^3}exp\left(0.89\beta\sqrt{\frac{V}{L}}\right)$$

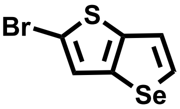
where J is the current density, L is the film thickness of the active layer, μ is the holeor electron mobility, ε_0 is the permittivity of free space (8.85 × 10^{-12} F m^{-1}), ε_{r} is the relative dielectric constant of the transport medium, V (= V_{appl} - V_{bi}) is the internal voltage in the device, where V_{appl} is the applied voltage and V_{bi} is the built-in voltage reflecting the difference of work functions of the two electrodes.



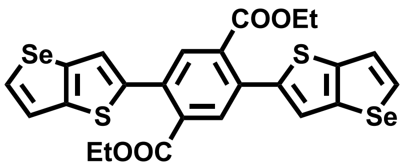
Compound 1: To a solution of ethyl selenopheno[3,2-b]thiophene-5-carboxylate (6.00 g, 23.2 mmol) in chloroform (50 mL) and acetic acid (30 mL), *N*-bromobutanimide (4.95 g, 27.8 mmol) was added. The reaction mixture was refluxed for 3 h under N_2 atmosphere, and then quenched by adding aqueous $NaHSO_3$. The reaction mixture was then extracted with dichloromethane. The organic layers were combined, and washed with saturated brine solution and dried over anhydrous Na_2SO_4. After removal of the solvent, the crude product was purified by gravity column chromatography (silica gel), eluting with petroleum ether/ethyl acetate (10:1) to afford light yellow solid (7.10 g, 91%). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ 8.11 (s, 1H, Se-*H*), 7.32 (s, 1H, Th-*H*), 4.44-4.33 (q, *J* = 7.2 Hz, 2H, C*H*$_2$), 1.40-1.37 (t, *J* = 7.2 Hz, 3H, C*H*$_3$). ^{13}C NMR (175 MHz, $CDCl_3$, ppm): δ 163.5, 142.7, 140.4, 138.1, 127.4, 125.6, 117.9, 61.5, 14.3. HR-ESI-MS (*m*/*z*): calcd for $C_9H_7O_2BrSSe$:337.8510. Found: 337.8508.



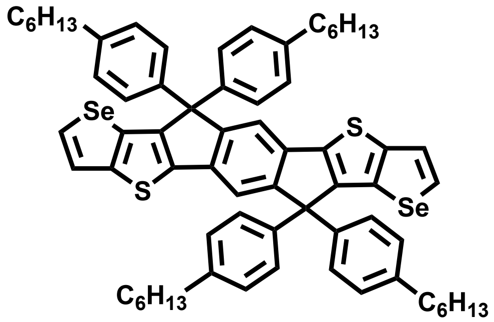
Compound 2: To a solution of compound **1** (6.00 g, 23.17 mmol) in THF (50 mL) and H_2O (50 mL), LiOH·H_2O (4.40 g, 105 mmol) was added. The reaction mixture was refluxed for 12 h and then THF was removed under reduced pressure. To the residue water, concentrated hydrochloric acid was added. The precipitate was collected by filtration and washed with water then dried in vacuo to afford light yellow solid (6.34 g, 97%). ^{1}H NMR (400 MHz, d_6-DMSO, ppm): δ 8.00 (s, 1H, Se-*H*), 7.63 (s, 1H, Th-*H*), 3.54 (s, 1H, COO-*H*). ^{13}C NMR (175 MHz, d_6-DMSO, ppm): δ 165.6, 145.7, 141.4, 140.3, 126.9, 125.9, 115.2. HR-ESI-MS (*m*/*z*): Calcd for $C_7H_3BrO_2SSe$: 308.8130, Found: 308.8122.



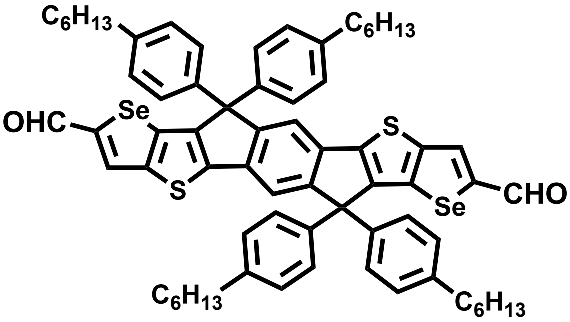
Compound 3: To a solution of compound **2** (3.20 g, 10.3 mmol) in quinoline (80 mL), copper (260 mg, 4.09 mmol) was added. The reaction mixture was refluxed for 2 h and then was cooled to room temperature. The reaction mixture was then extracted with dichloromethane. The organic layers were combined, and washed with 1 M HCl (aq.) and dried over anhydrous Na_2SO_4. After removal of the solvent, the crude product was purified by gravity column chromatography (silica gel), eluting with petroleum ether to afford white solid (2.30 g, 84%). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ 8.00-7.98 (d, *J* = 5.6 Hz, 1H, Se-*H*), 7.41-7.40 (d, *J* = 5.6 Hz, 1H, Se-*H*), 7.30 (s, 1H, Th-*H*). ^{13}C NMR (175 MHz, $CDCl_3$, ppm): δ 141.0, 137.3, 130.1, 125.1, 121.5, 113.1. HR-ESI-MS (*m*/*z*): calcd for C_6H_3BrSSe: 265.8299, Found: 265.8295.



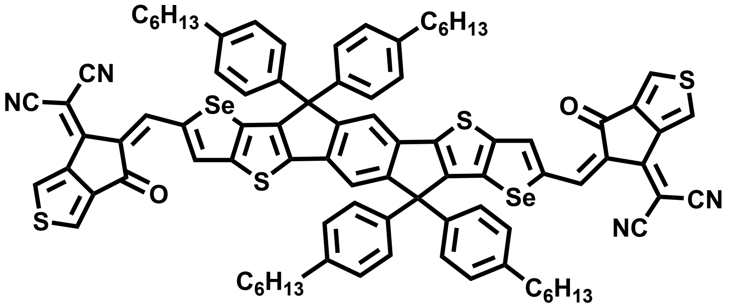
Compound 5: To a solution of diethyl 2,5-bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl) terephthalate (**4**) (0.84 g, 1.78 mmol), compound **3** (1.42 g , 5.44 mmol) in degassed THF (60 mL), 30 mL aqueous $NaHCO_3$ (3.36 g, 40 mmol) and $Pd(PPh_3)_4$ (0.11 g, 0.096 mmol) were added. The reaction mixture was refluxed for 12 h under N_2, and then quenched by adding a saturated aqueous solution of ammonium chloride. The reaction mixture was then extracted with dichloromethane. The organic layers were combined, and washed with saturated brine solution and dried over anhydrous Na_2SO_4. After removal of the solvent, the crude product was purified by gravity column chromatography (silica gel), eluting with petroleum ether/dichloromethane (5:1) to afford the product as yellow solid (0.69 g, 65%). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ 7.99-7.98 (d, *J* = 5.6 Hz, 2H, Se-*H*), 7.89 (s, 2H, Th-*H*), 7.51-7.50 (d, *J* = 5.6 Hz, 2H, Se-*H*), 7.34 (s, 2H, Ph-*H*), 4.27-4.22 (q, *J* = 7.2 Hz, 4H, CH_2), 1.15-1.12 (t, *J* = 7.2 Hz, 6H, CH_3). ^{13}C NMR (175 MHz, $CDCl_3$, ppm): δ 167.5, 141.6, 141.5, 138.7, 134.0, 133.6, 132.0, 130.8, 122.4, 122.0, 61.8, 13.8. HR-ESI-MS (*m*/*z*): calcd for $C_{24}H_{18}O_4S_2Se_2$: 593.9049, Found: 594.9045 ($[M+H]^+$).



IDTSe: To a solution of 4-hexyl-1-bromobenzene (3.20 g, 13.4 mmol) in THF (20 mL) at –78 °C was added *n*-BuLi (4.0 mL, 9.55 mmol, 2.4 M in hexane) and the mixture was kept at –78 °C for 1 h. A solution of compound **5** (0.57 g, 0.96 mmol) in THF (10 mL) was then added slowly. After this addition, the mixture was stirred at room temperature for 2 h and then the reaction was quenched by adding a saturated aqueous solution of ammonium chloride. The reaction mixture was then extracted with dichloromethane. The combined organic layers were dried over anhydrous Na_2SO_4. After removing the solvent, the crude product was charged into three-neck flask. Acetic acid (40 mL) and concentrated H_2SO_4 (1.0 mL) were added and the reaction mixture was stirred at 80°C for 3 h. Then the mixture was poured into water and extracted with dichloromethane. The combined organic layers were washed with saturated brine solution and dried over anhydrous Na_2SO_4. The resulting crude was purified by silica gel column chromatography using a mixture of petroleum ether/dichloromethane (10:1) as the eluent to give light yellow solid (0.76 g, 71%). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ 7.84-7.83 (d, *J* = 5.6 Hz, 2H, Se-*H*), 7.53 (s, 2H, Ph-*H*), 7.52-7.51 (d, *J* = 5.6 Hz, 2H, Se-*H*), 7.19-7.17 (d, *J* = 8.4 Hz, 8H, Ph-*H*), 7.10-7.07 (d, *J* = 8.4 Hz, 8H, Ph-*H*), 2.58-2.54 (t, *J* = 8.0 Hz, 8H, CH_2), 1.62-1.55 (m, 8H, CH_2), 1.35-1.28 (m, 12H, CH_2), 0.89-0.85 (t, *J* = 6.8 Hz, 12H, CH_3). ^{13}C NMR (175 MHz, $CDCl_3$, ppm): δ 153.5, 149.1, 142.8, 142.6, 141.7, 140.3, 136.0, 133.6, 129.7, 128.4, 128.1, 122.8, 116.9, 62.9, 35.6, 31.7, 31.2, 29.1, 22.6, 14.1. HR-ESI-MS (*m/z*): calcd for $C_{68}H_{74}S_2Se_2$: 1114.3635, Found: 1115.3618 ($[M+H]^+$).



IDTSe-CHO: To a solution of **IDTSe** (0.30 g, 0.27 mmol) in 1,2-dichloroethane (35 mL) at 0 °C was added DMF (1.0 mL) and $POCl_3$ (0.8 mL) dropwise under N_2 atmosphere. After addition, the cooling bath was removed and the reaction mixture was refluxed for 6 h. The reaction mixture was quenched by adding an ice-cold saturated aqueous solution of sodium acetate and then the mixture was stirred for another 1 h. The reaction mixture was then extracted with chloroform. The combined organic layers were washed with saturated brine solution and dried over anhydrous Na_2SO_4. After removal of solvent, the crude product was purified by column chromatography (silica gel), eluting with petroleum ether/dichloromethane (1:1) to yield the product as yellow solid (0.29 g, 91%). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ 9.77 (s, 2H, CHO), 8.18 (s, 2H, Se-*H*), 7.64 (s, 2H, Ph-*H*), 7.15-7.10 (d, *J* = 8.4 Hz, 16H, Ph-*H*), 2.58-2.54 (t, *J* = 8.0 Hz, 8H, CH_2), 1.62-1.55 (m, 8H, CH_2), 1.32-1.28 (m, 24H, CH_2), 0.88-0.85 (t, *J* = 6.8 Hz, 12H, CH_3). ^{13}C NMR (175 MHz, $CDCl_3$, ppm): δ 183.8, 154.9, 150.1, 148.8, 148.6, 142.6, 142.3, 140.1, 139.2, 136.4, 132.8, 128.7, 127.8, 118.0, 63.1, 35.5, 31.6, 31.2, 29.1, 22.5, 14.1. HR-ESI-MS (*m/z*): calcd for $C_{70}H_{74}O_2S_2Se_2$: 1170.3533, Found: 1171.3570 ($[M+H^+]^+$).



TSeTIC: In a 100 mL round-bottomed flask, **IDTSe-CHO** (0.20 g, 0.17 mmol) and 2-(6-oxo-5,6-dihydro-4H-cyclopenta[c]thiophen-4-ylidene)malononitrile (0.21 g, 1.03 mmol) was added. The reaction mixture was evacuated and backfilled with N_2 three times. Then freshly degassed chloroform (40 mL) and pyridine (1 mL) were added into the reaction mixture. The reaction mixture was refluxed for 12 h. After cooling to room temperature, the reaction mixture was poured into methanol (250 mL) and the precipitate was filtered off and washed with methanol. The crude product was purified by column chromatography (silica gel), eluting with petroleum ether/dichloromethane (1:2) to obtain the product as dark green solid (0.24 g, 90%). ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 8.94 (s, 2H, CH=C), 8.344-8.339 (d, *J* = 2 Hz, 2H, Th-*H*), 8.23 (s, 2H, Se-*H*), 7.89-7.88 (d, *J* = 2 Hz, 2H, Th-*H*), 7.68 (s, 2H, Ph-*H*), 7.20-7.18 (d, *J* = 8.4 Hz, 8H, Ph-*H*), 7.15-7.12 (d, *J* = 8.4 Hz, 8H, Ph-*H*), 2.58-2.55 (t, *J* = 8.0 Hz, 8H, CH_2), 1.63-

1.59 (m, 8H, CH_2), 1.31-1.28 (m, 24H, CH_2), 0.88-0.84 (m, 12H, CH_3). ^{13}C NMR ($CDCl_3$, 175 MHz, ppm): δ 182.1, 156.2, 155.9, 153.1, 151.7, 150.8, 145.0, 142.5, 142.4, 142.0, 141.1, 140.5, 138.9, 137.1, 128.9, 127.9, 127.7, 127.6, 125.5, 118.8, 115.0, 114.3, 67.5, 63.1, 35.6, 31.7, 31.2, 29.1, 22.6, 14.1. HR-MALDI-TOF MS (m/z): calcd for $C_{90}H_{78}N_4O_2S_4Se_2$: 1535.3700. Found:1535.3724 ($[M]^+$).

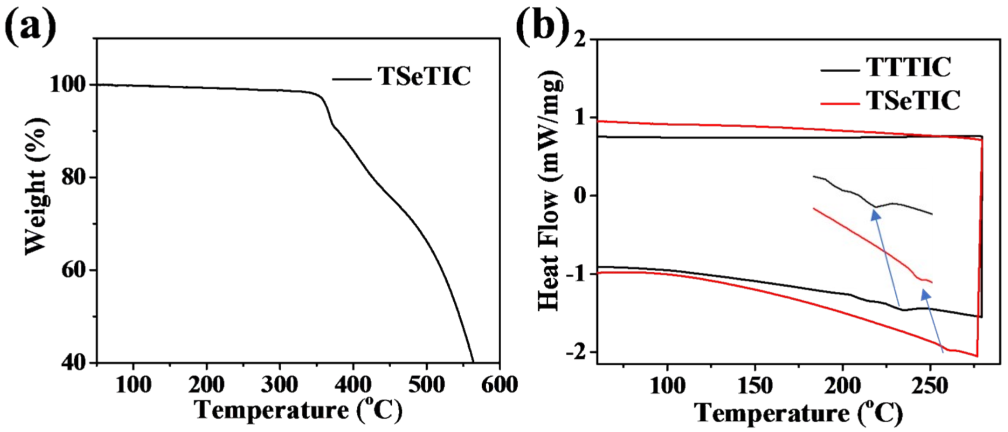


Figure S1. (a) Thermal gravimetric analysis (TGA) of **TSeTIC** with a heating rate of 10 °C/min under N_2 atmosphere; (b) DSC traces of **TTTIC** and **TSeTIC** with a heating/cooling circle under N_2 atmosphere.

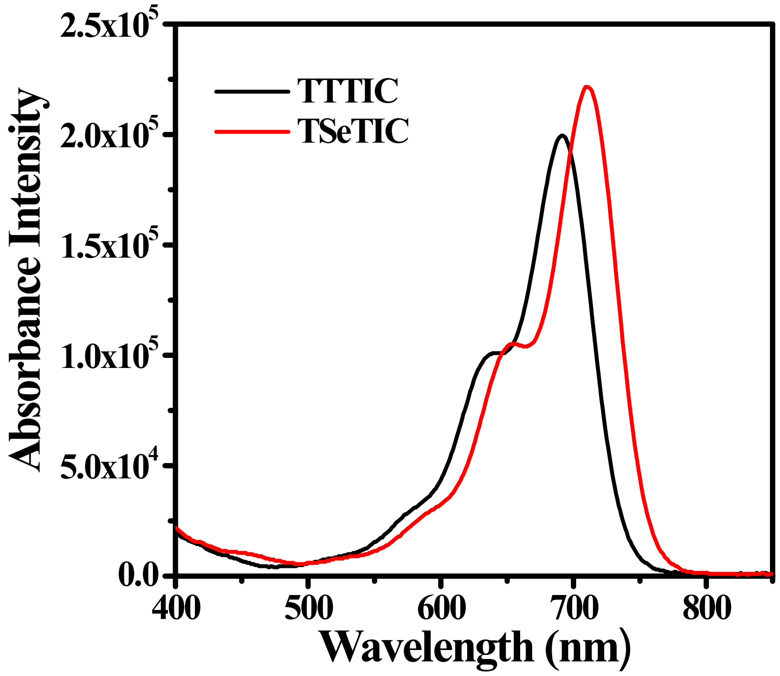


Figure S2. The absorption spectra of **TTTIC** and **TSeTIC** in chloroform solutions (2×10^{-6} M).

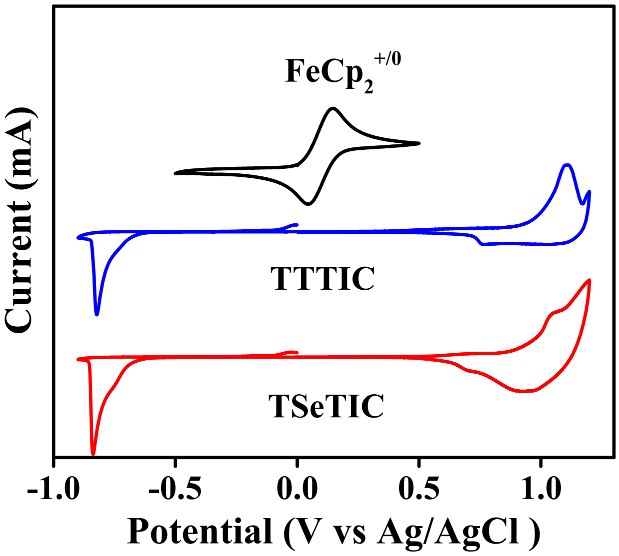


Figure S3. Cyclic voltammograms for **TTTIC** and **TSeTIC** films in CH_3CN/0.1 M $[^nBu_4N]^+$ $[PF6]^-$ at 100 mV s^{-1}, the potential was referred to the Ag/AgCl reference electrode.

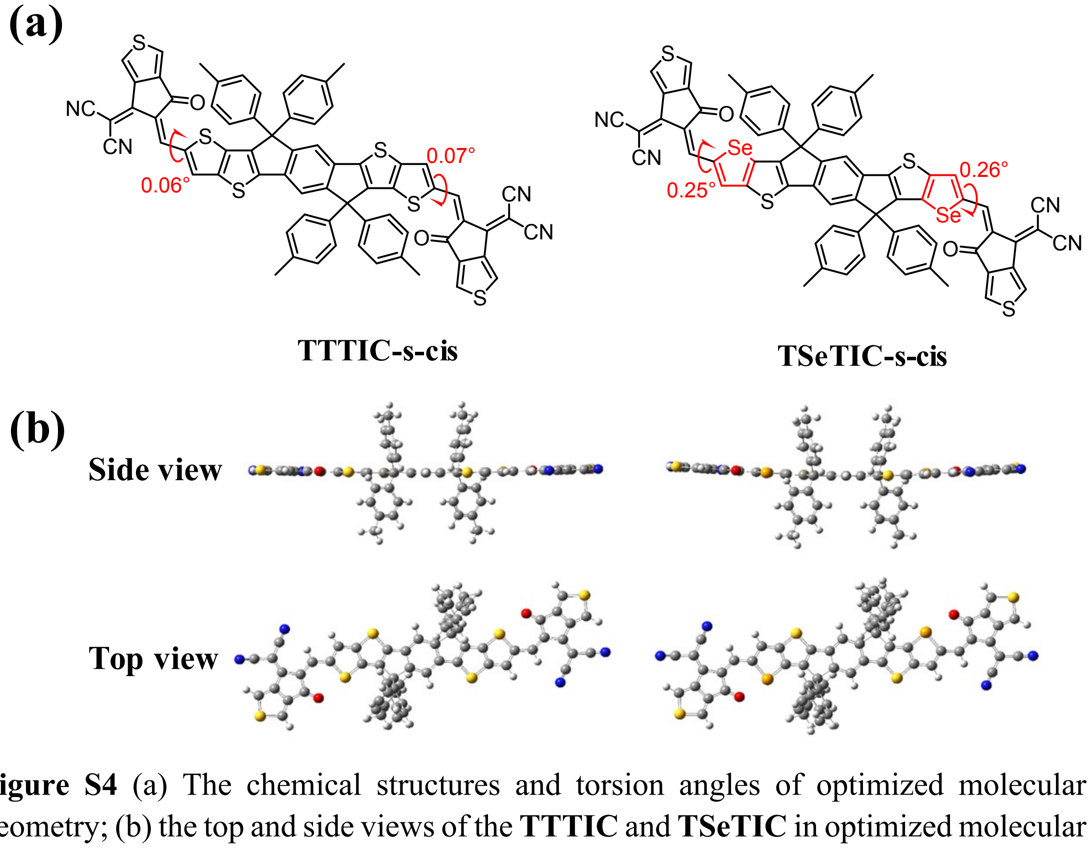


Figure S4 (a) The chemical structures and torsion angles of optimized molecular geometry; (b) the top and side views of the **TTTIC** and **TSeTIC** in optimized molecular geometry.

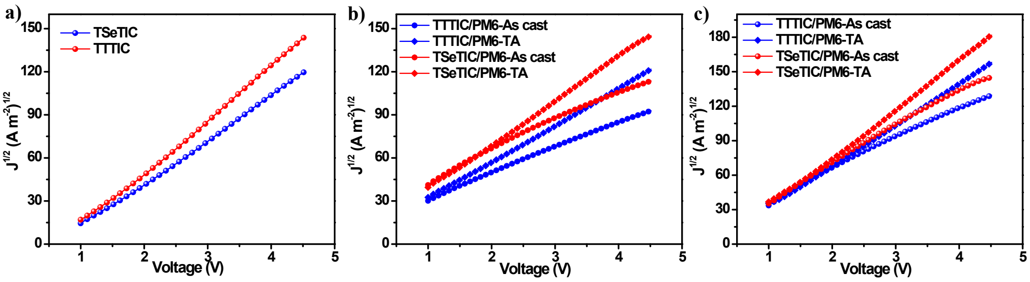


Figure S5. a) Space-charge-limited current (SCLC) *J-V* characteristics for electron-only devices based on neat **TTTIC** and **TSeTIC** films under dark condition; Space-charge-limited current (SCLC) *J-V* characteristics for b) electron-only and c) hole-only of **PM6:TTTIC** and **PM6:TSeTIC** with/without TA under dark condition.

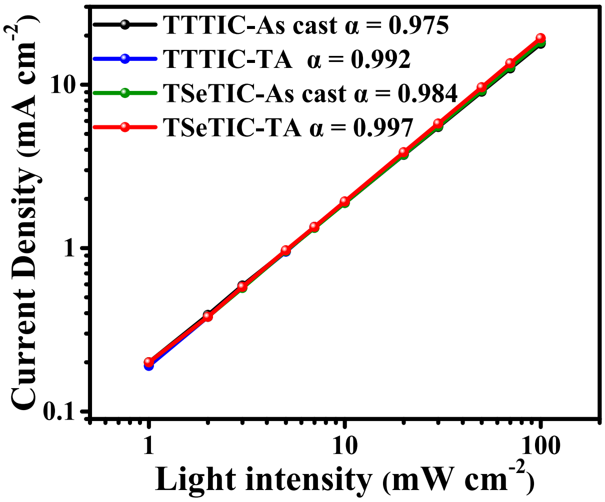


Figure S6. J_{SC} versus light intensity (P) of the devices based on **TTTIC/PM6** and **TSeTIC/PM6** with/without thermal annealing.

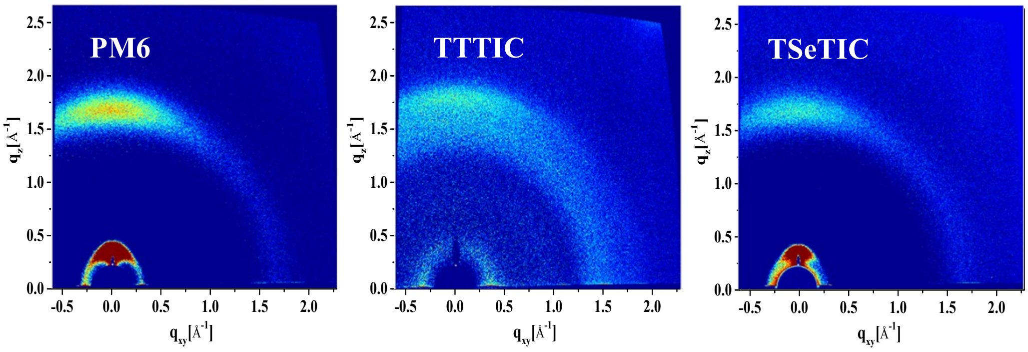


Figure S7. 2D GIXD patterns of **PM6**, **TTTIC**, and **TSeTIC** pure films.

Table S1. The key photovoltaic parameters of OSCs based on thiophene-containing IC terminal group functionalized A-D-A type NF-SMAs/polymer donor in binary organic solar cells in comparison with our **PM6/TSeTIC**-based devices.

Active layer (D/A)	**E_{g} [eV]**	**V_{oc} [V]**	**J_{sc} [mA/cm^2]**	**FF [%]**	**PCE$_{\mathrm{max}}$ [%]**	**$E_{\mathrm{loss}}{}^{\mathrm{a}}$ [eV]**	**Ref.**
PBT1-EH:ITCPTC	1.58	0.95	16.5	75.1	11.8	0.65	[S1]
J71: ITCPTC	1.58	0.896	17.52	74.1	11.63	0.684	[S2]
J71: MeIC	1.58	0.918	18.41	74.2	12.54	0.662	[S2]
J71: m-MeIC	1.54	0.922	18.56	70.6	12.08	0.62	[S3]
PBDB-T: m-MeIC	1.54	0.847	18.11	71.3	10.93	0.69	[S3]
PCE-10: m-MeIC	1.54	0.798	16.51	63.3	8.34	0.74	[S3]
PBDB-T:BTTIC-Th	1.467	0.902	19.45	73.6	12.91	0.565	[S4]
PBDB-T:BTTIC-TT	1.474	0.924	19.61	74.2	13.44	0.55	[S4]
PBDB-T:BTTIC-Ph	1.455	0.930	16.47	59.7	9.14	0.525	[S4]
PBDB-T:IDTCN	1.67	0.85	12.06	62.48	6.40	0.82	[S5]
PBDB-T:ITCPTC	1.58	0.84	17.53	72.77	10.74	0.74	[S5]
PBDB-T:IDT6CN	1.63	0.83	15.14	73.77	9.27	0.80	[S5]
PBDB-T:IDT6CN-Th	1.61	0.81	16.75	76.72	10.41	0.80	[S5]
PBDB-T:IDT6CN-M	1.65	0.91	16.02	76.83	11.20	0.74	[S5]
PM6:T6Me	1.38	0.87	21.33	65.13	12.09	0.51	[S6]
PM6:T7Me	1.36	0.89	17.12	58.79	8.96	0.47	[S6]
PM6:T8Me	1.35	0.90	10.54	64.21	6.09	0.45	[S6]
PTQ10:IDTCN	1.67	0.98	13.9	54.0	7.4	0.69	[S7]
PTQ10:IDTPC	1.52	0.93	17.5	74.6	12.2	0.59	[S7]
PBDB-T:MeIC	1.53	0.896	18.07	74.3	12.03	0.634	[S8]
PBDB-T:MeIC1	1.54	0.927	18.32	74.1	12.58	0.613	[S8]
PBDB-T:BTTIC	1.47	0.904	19.52	74.7	13.18	0.566	[S9]
PBDB-T:BTOIC	1.39	0.862	18.60	68.4	10.96	0.528	[S9]
PBT1-C-LW:ITCPTC	1.58	0.92	15.9	74.0	10.8	0.66	[S10]
PBT1-C-MW:ITCPTC	1.58	0.94	17.2	79.0	12.8	0.64	[S10]
PBT1-C-MW2:ITCPTC	1.58	0.93	17.1	78.0	12.4	0.65	[S10]
PBT1-C-HW:ITCPTC	1.58	0.93	16.8	77.0	12.0	0.65	[S10]
PBDB-T:ITCT-DM	1.58	0.904	17.4	65.0	10.56	0.676	[S11]
PBDB-T:ITCPTC-Th	1.60	0.856	17.05	72.7	10.61	0.744	[S12]
PBDB-T:ITCPTC-Se	1.59	0.869	15.2	68.3	9.02	0.721	[S12]
PBDB-T: IDTC	1.51	0.917	16.56	61.61	9.35	0.583	[S13]
PBDB-T: IDTO	1.53	0.943	16.25	65.41	10.02	0.587	[S13]
PM6:ITCPTC	1.65	0.95	17.6	73.4	12.3	0.73	[S14]
PM6:ITC-2Cl	1.58	0.91	20.1	74.1	13.6	0.67	[S14]
PTQ10:IDTPC	1.53	0.93	17.5	74.6	12.2	0.60	[S15]
PTQ10:IDTPC-Me	1.55	0.95	13.8	70.3	9.2	0.60	[S15]
PTQ10:IDTPC-DMe	1.57	1.02	13.5	68.0	9.3	0.55	[S15]
PBDB-T:BTTIC-0M	1.47	0.86	18.95	72.9	11.87	0.61	[S16]
PBDB-T:BTTIC-2M	1.47	0.90	19.39	75.3	13.15	0.57	[S16]
PBDB-T:BTTIC-4M	1.49	0.968	15.67	63.7	9.60	0.522	[S16]
PBT1-EH:IDTCN	1.67	0.93	13.31	70.2	8.69	0.74	[S17]
J71: ITIC5	1.53	0.897	18.48	75.5	12.5	0.633	[S18]

HFQx:ITTC	1.61	0.88	16.49	71.0	10.4	0.73	[S19]
PBT1-C-2Cl:IDTT-2F-Th	1.55	0.912	17.82	73.9	12.01	0.638	[S20]
PBDB-T:Y2	1.40	0.82	23.56	69.4	13.4	0.58	[S21]
PBDBTF:C8-ITCC	1.66	1.04	16.1	63.0	10.5	0.62	[S22]
PBDBTF:C8-ITCC-Cl	1.58	0.95	17.9	73.0	12.4	0.63	[S22]
PM7:BDSeThCl	1.62	0.97	17.85	68.8	11.91	0.65	[S23]
PBDB-T:ITCC	1.67	1.01	15.9	71.0	11.4	0.66	[S24]
PTB7-Th:ITCT	1.67	0.95	15.13	72.0	10.42	0.72	[S25]
PBDB-T:BDCPDT-TTC	1.58	0.94	17.72	61.78	10.29	0.64	[S26]
PBDB-T:ITBTC	1.61	0.941	16.37	71.3	10.99	0.63	[S27]
PM6:TSeTIC	**1.53**	**0.93**	**19.42**	**75.9**	**13.71**	**0.60**	**This work**

$^{a}E_{\mathrm{loss}} = E_{\mathrm{g}} - eV_{\mathrm{oc}}$, where E_{g} is the lowest energy bandgap of acceptor components.

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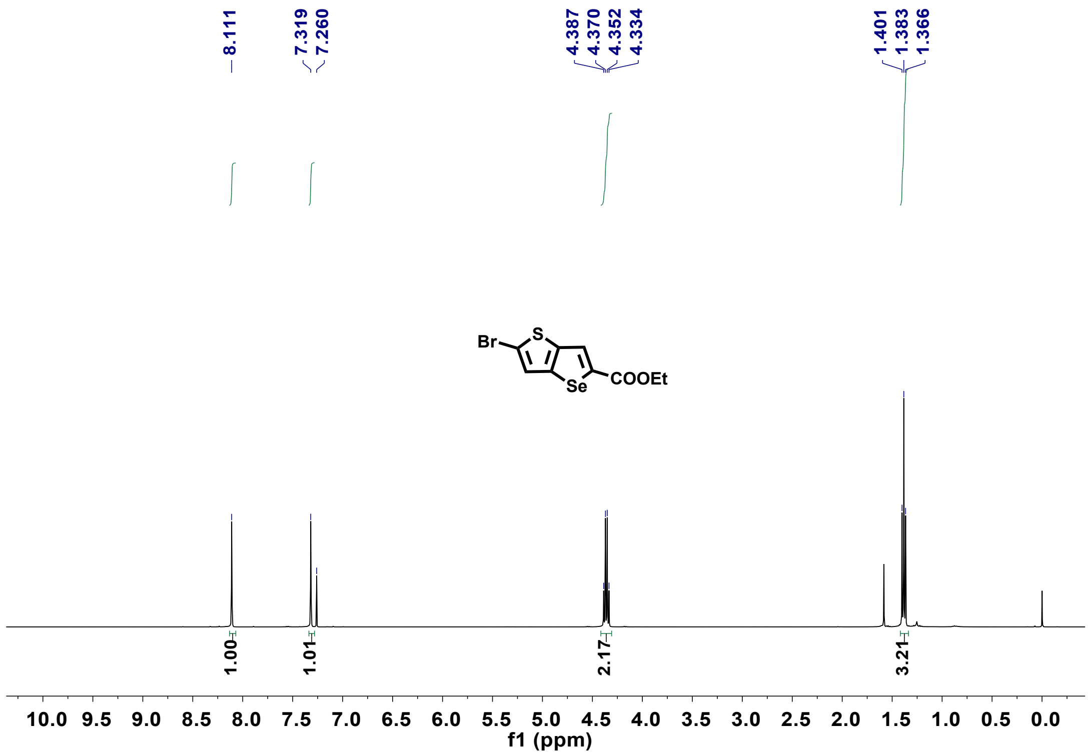
Copies of ^{1}H NMR and ^{13}C NMR, and HR-MALDI-TOF MS Spectra



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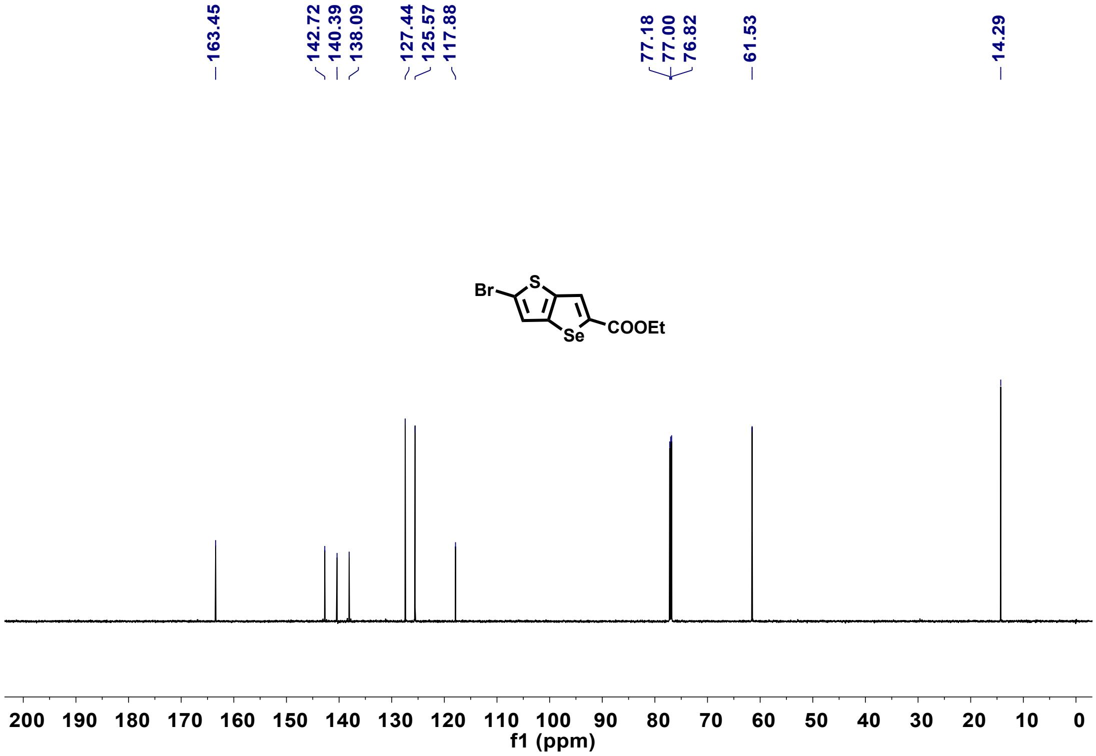

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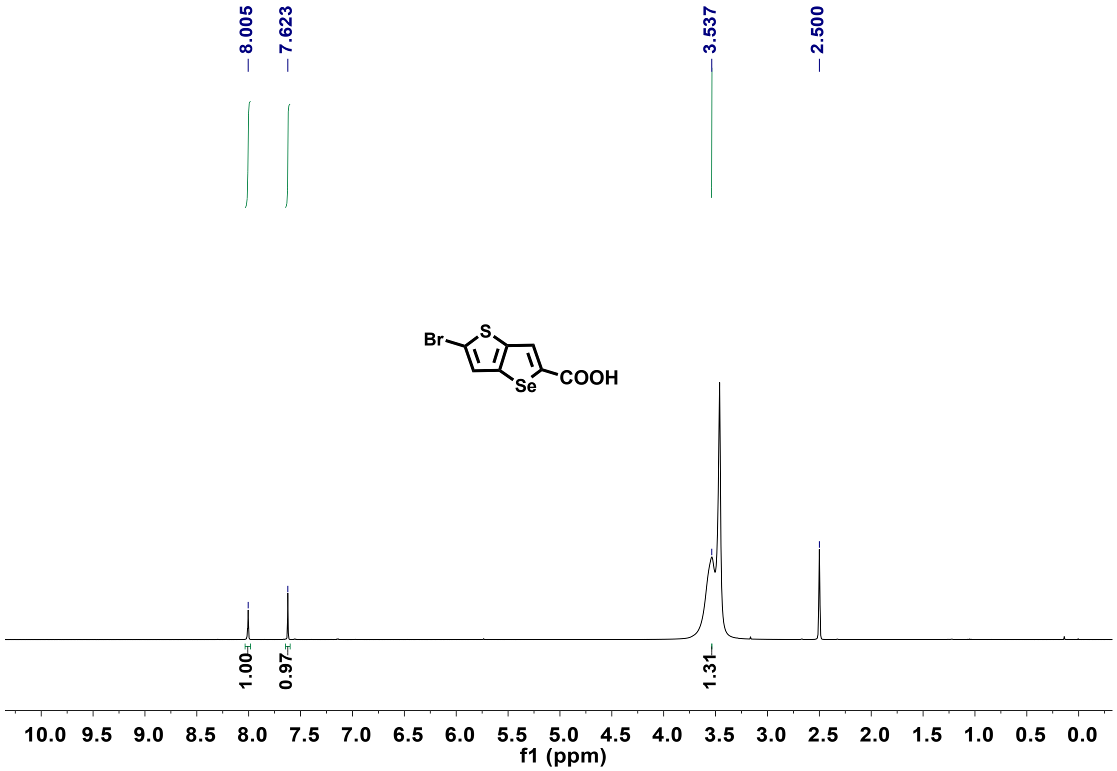

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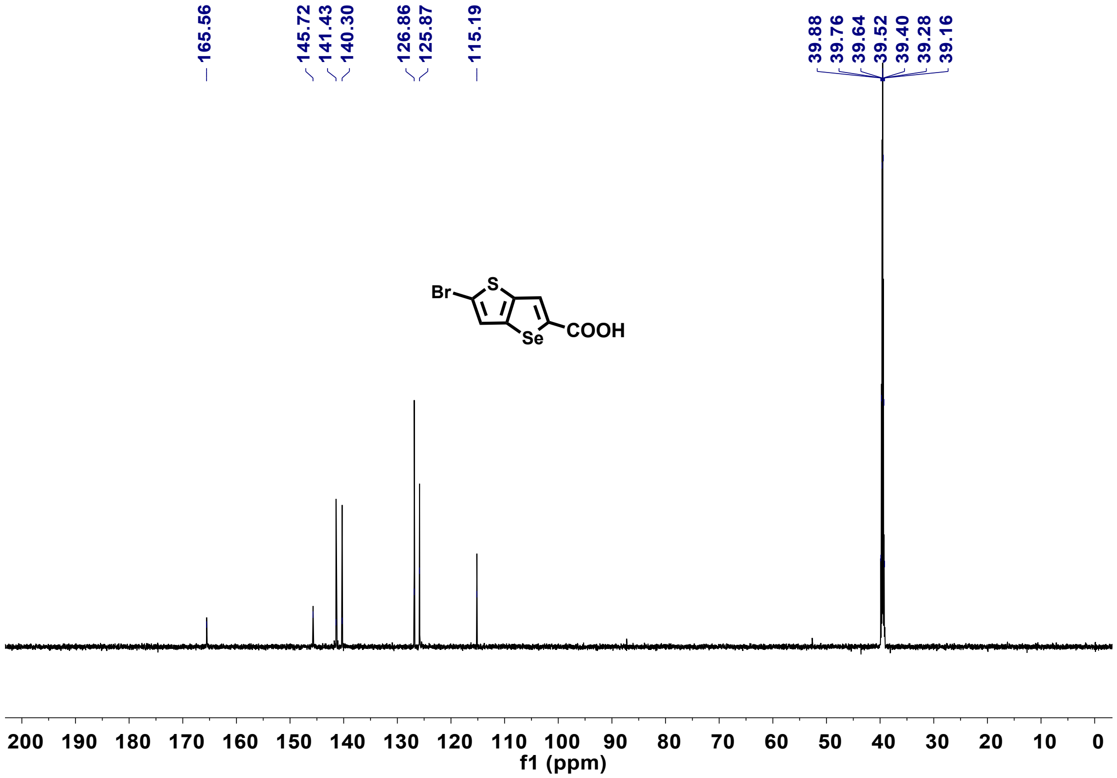

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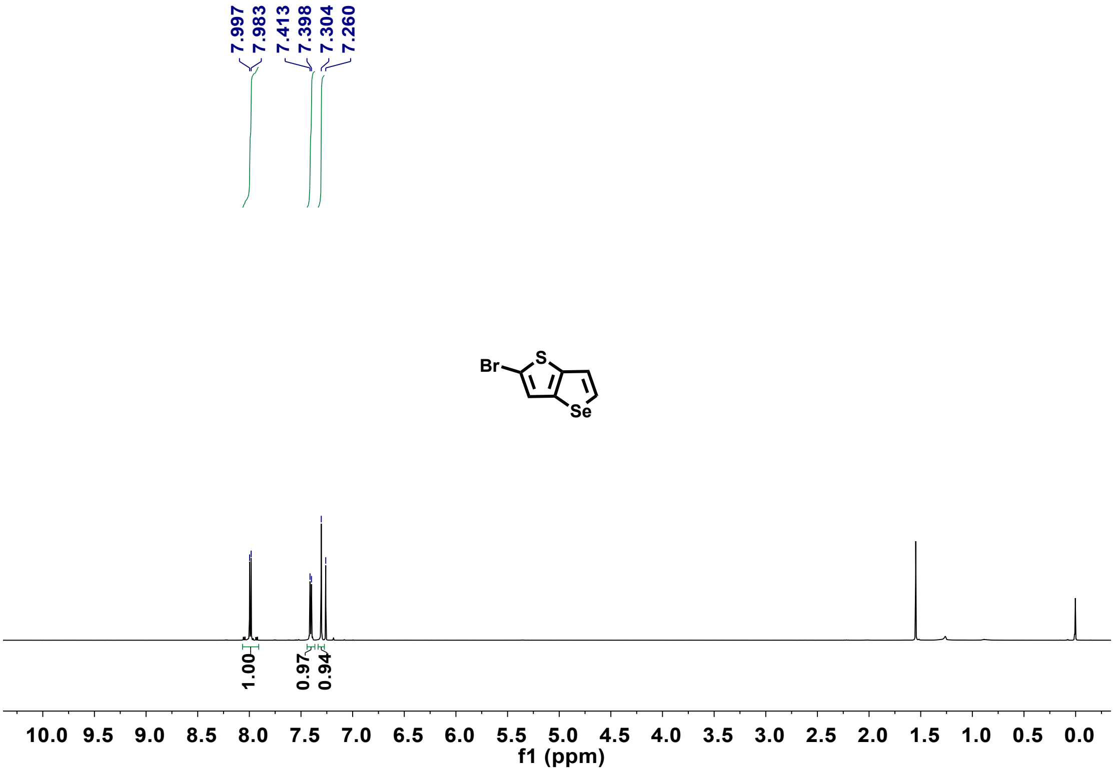

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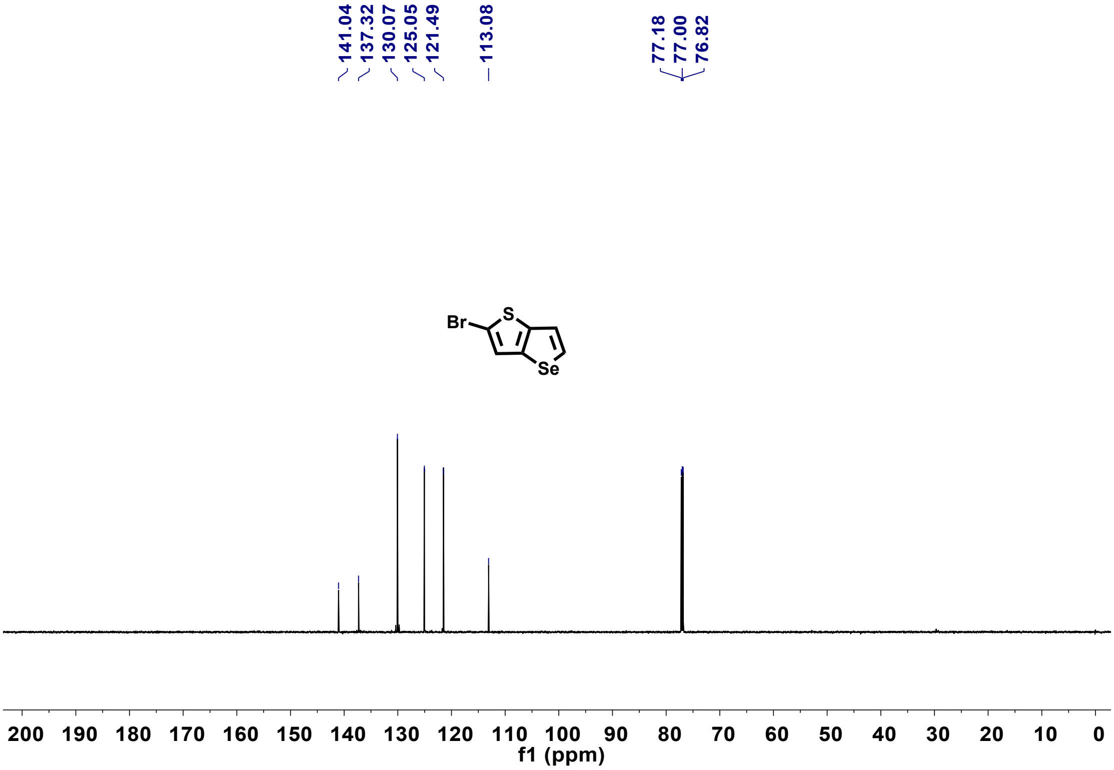

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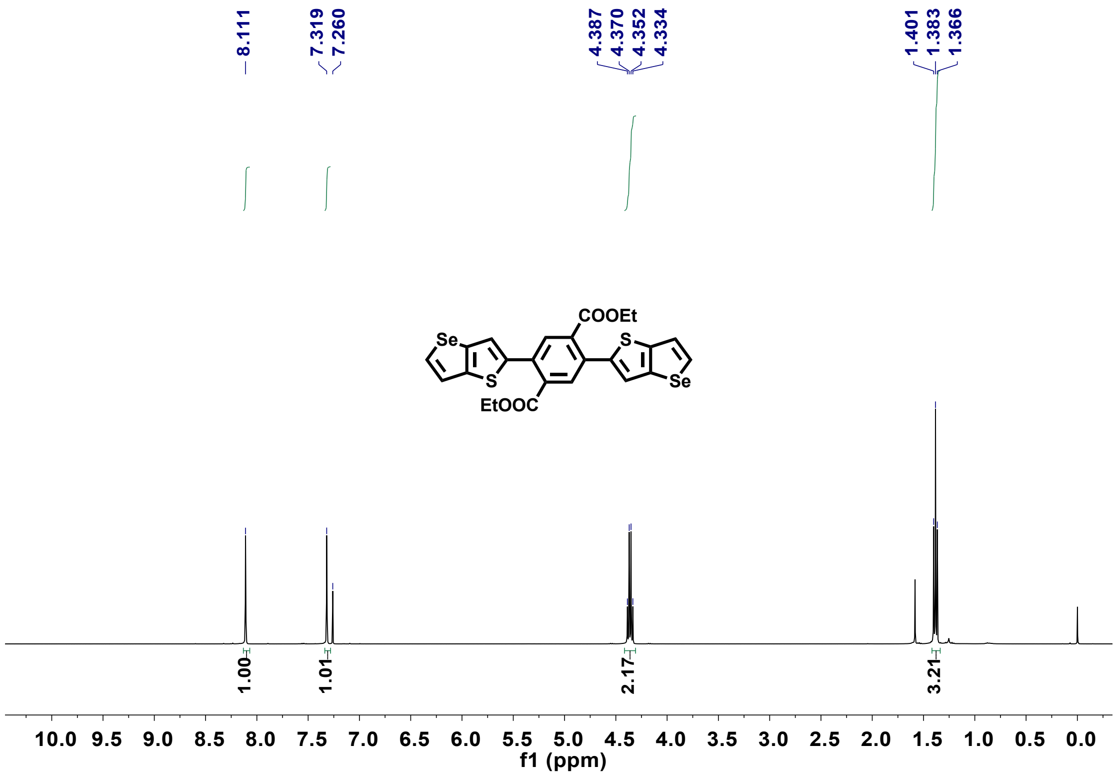

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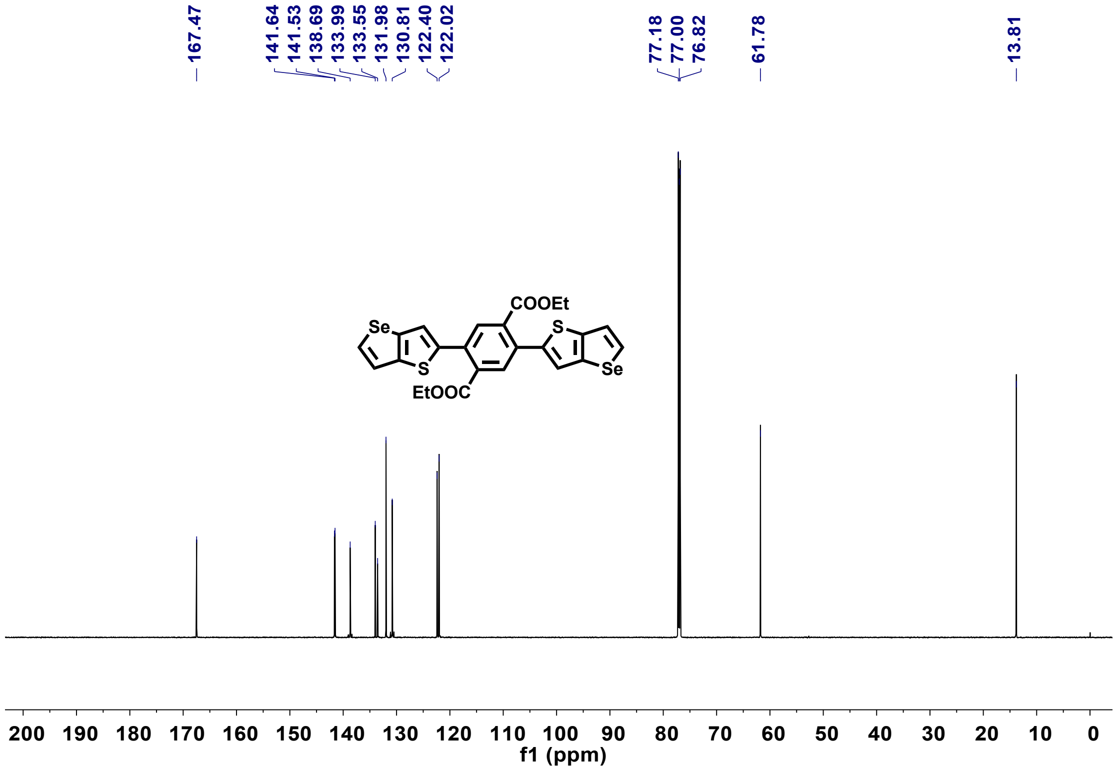

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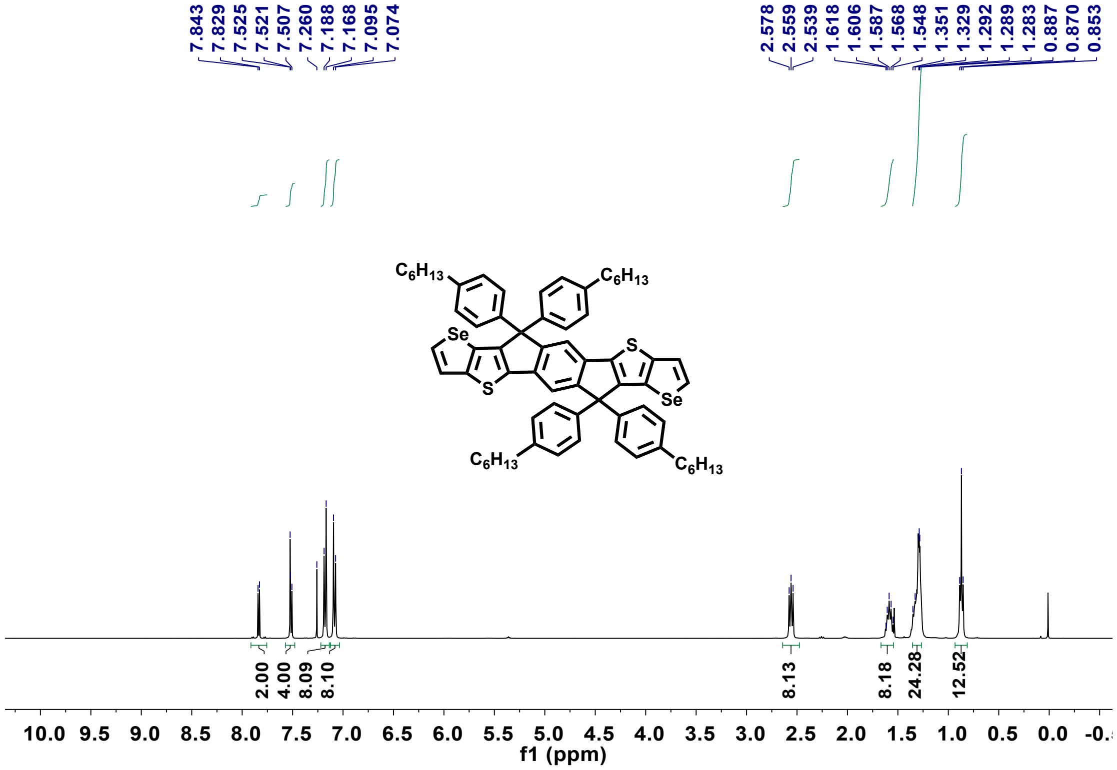

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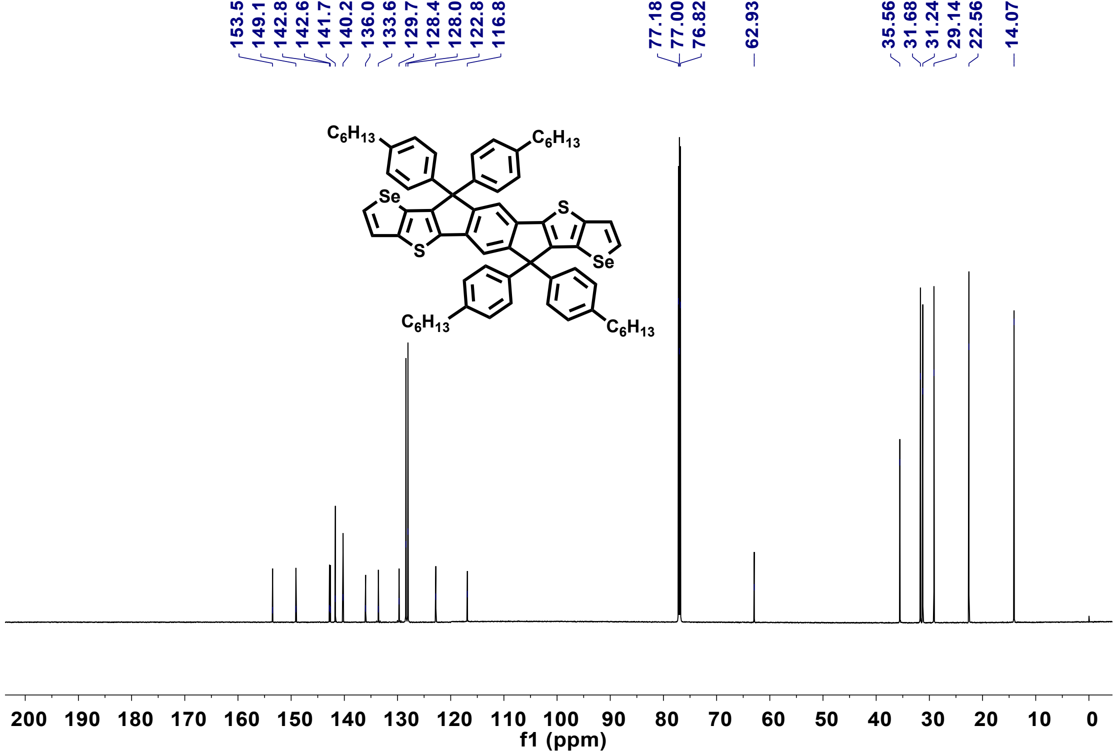

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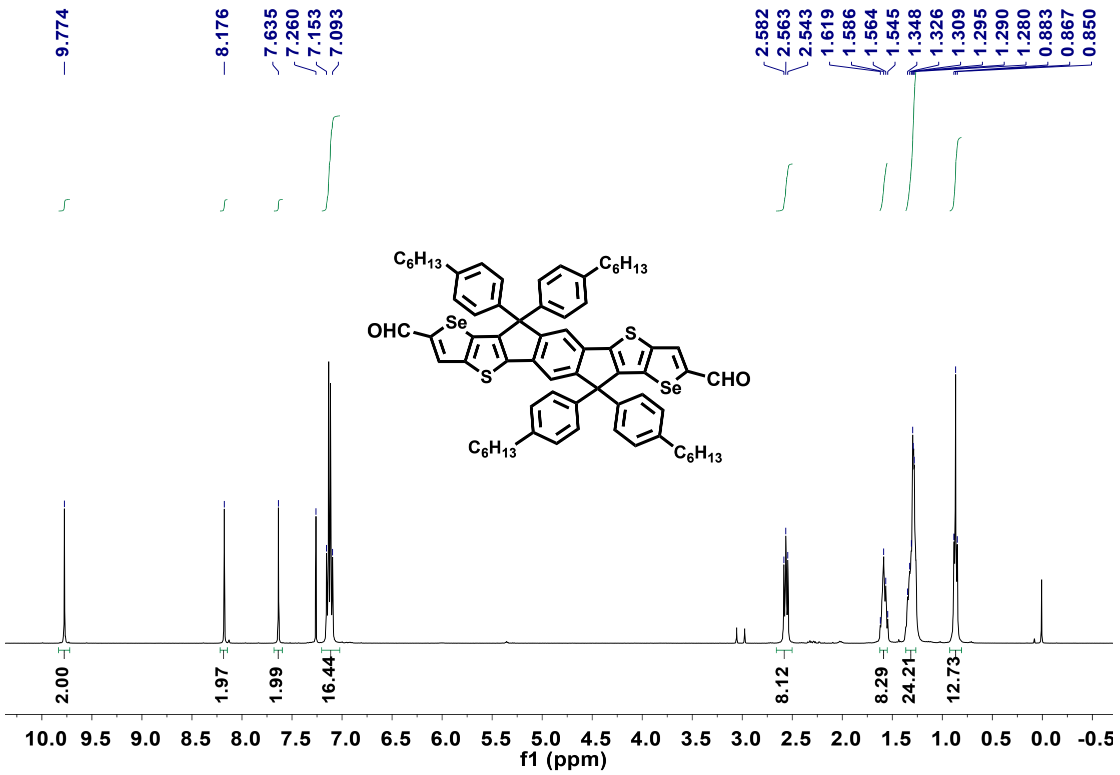
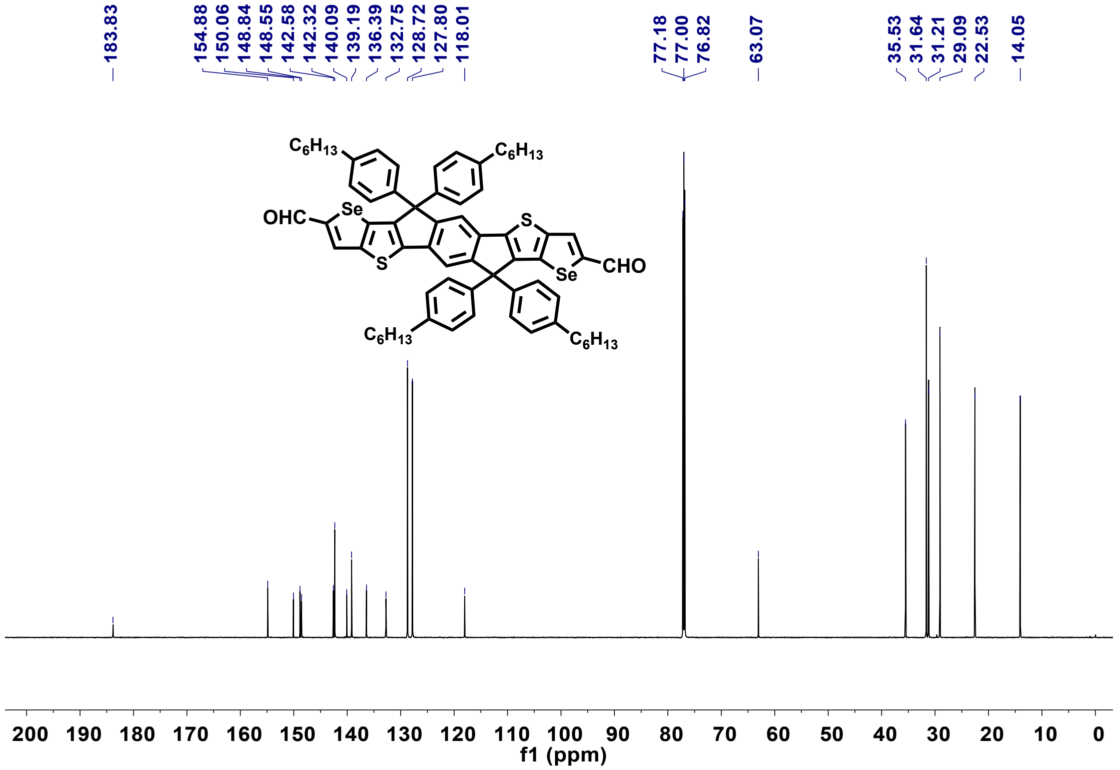


^{1}H NMR spectrum for **IDTSe-CHO**



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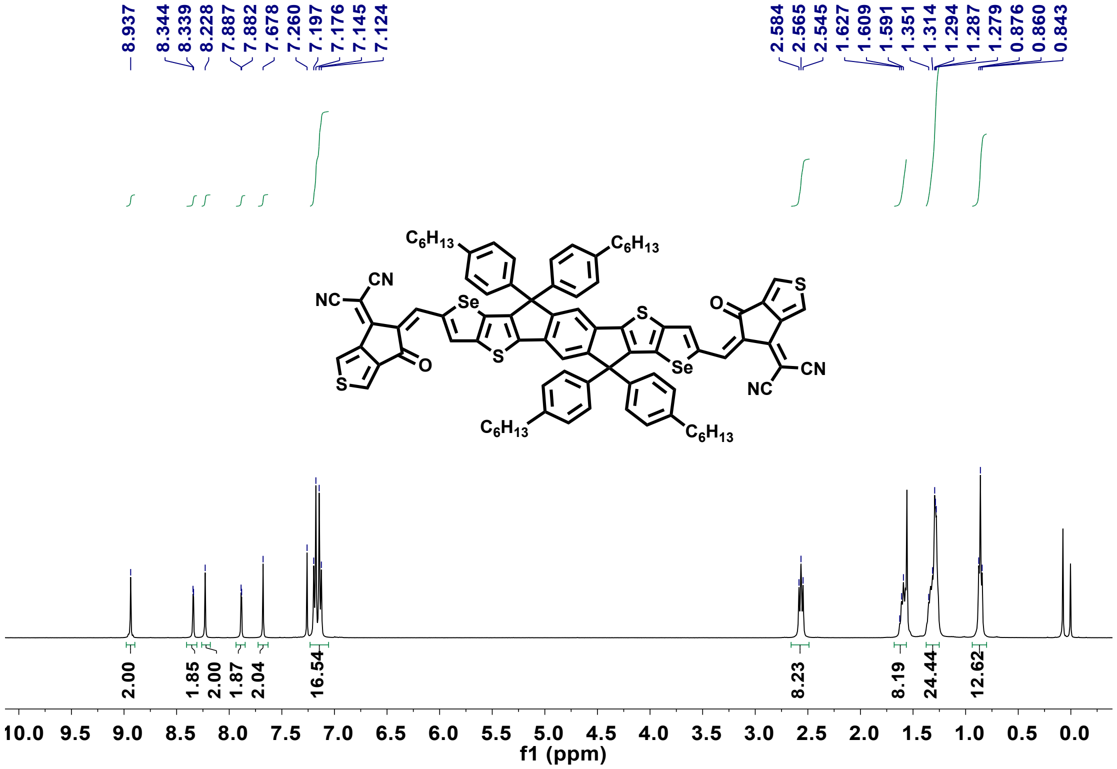
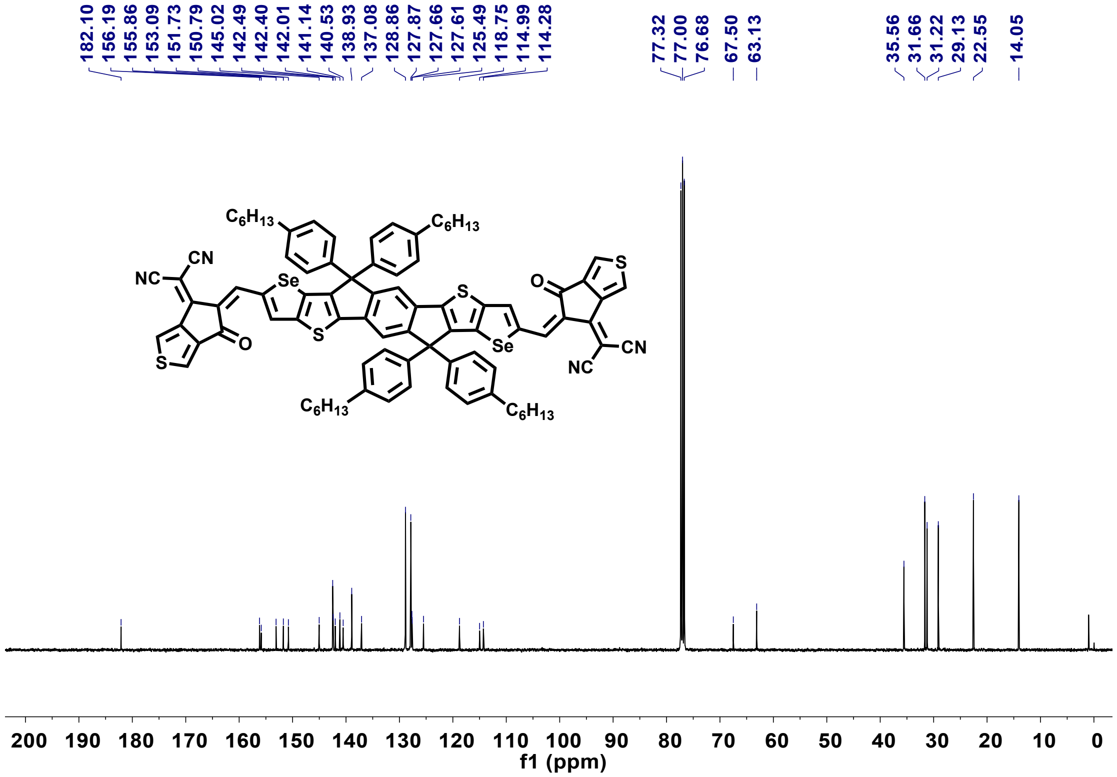


^{1}H NMR spectrum for **TSeTIC**



^{13}C NMR spectrum for **TSeTIC**

MALDI,IDTSE-THIC,20170920

Analysis Info

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Method	MALDI_P_100-3000	Operator	
Sample Name	MURU-N-ESI	Instrument	solariX
Comment			

Acquisition Parameter

Acquisition Mode	Single MS	Acquired Scans	2	Calibration Date	Mon Sep 11 06:44:42
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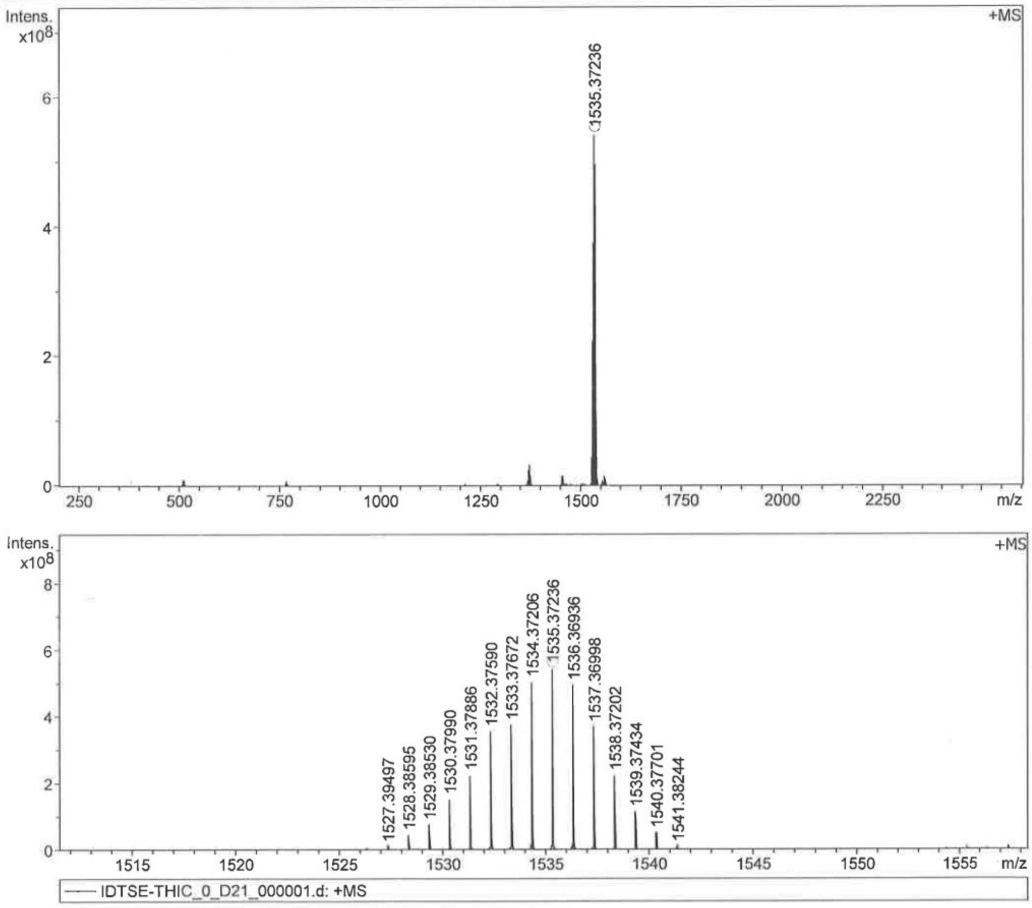
Broadband High Mass	2600.0 m/z	Laser Power	44.4 lp	Apodization	Sine-Bell Multiplication
Source Accumulation	0.001 sec	Laser Shot Frequency	0.020 sec		
Ion Accumulation Time	0.300 sec				



Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
1535.372357	1	$C_{90}H_{82}N_4O_2S_4Se_2$	100.00	1535.369964	-1.6	-2.5	359.8	52.0	odd	ok

HR-MALDI-TOF MS Spectra of **TSeTIC**