

**Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.
This journal is © The Royal Society of Chemistry 2021**

Supporting Information

Selenium-containing two-dimensional conjugated fused-ring electron acceptor for enhanced crystal packing, charge transport, and photovoltaic performance

Shi-Sheng Wan,^{a,d,†} Qiaoqiao Zhao,^{b,†} Zhao Jiang,^{a,†} Gui-Zhou Yuan,^a Lu Yan,^a Hwa Sook Ryu,^c Asif Mahmood,^a Yan-Qiang Liu,^a Heng Li,^b Han Young Woo,^c Feng He,^{*,b} and Jin-Liang Wang^{*,a}

^aKey Laboratory of Cluster Science of Ministry of Education, Beijing Key Laboratory of Photoelectronic/Electrophotonic Conversion Materials, School of Chemistry and Chemical Engineering, Beijing Institute of Technology, Beijing, 100081, China.

E-mail: jinliwang@bit.edu.cn

^bShenzhen Grubbs Institute, Department of Chemistry and Guangdong Provincial Key Laboratory of Catalysis, Southern University of Science and Technology, Shenzhen, 518055, China. E-mail: hef@sustech.edu.cn

^cDepartment of Chemistry, Korea University, Seoul, Republic of Korea.

^dBeijing National Laboratory for Molecular Sciences

†These authors contributed equally to this work.

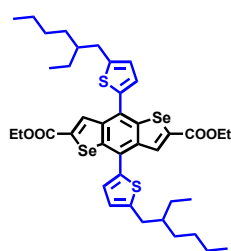
Experimental Section

Materials and Characterization: All air and water-sensitive reactions were carried out under N₂. Toluene and THF were dried by Na and then freshly distilled before to use. The other precursors were used as the common commercial level. ¹H and ¹³C NMR spectra were carried out on a Bruker Ascend-400 and 700 NMR spectrometer. All chemical shifts were reported in ppm. Chemical shifts in ¹H NMR were referenced to TMS and in ¹³C NMR were referenced to CDCl₃. MALDI-TOF-MS was recorded on a Bruker BIFLEX III mass spectrometer. Thermogravimetric analysis (TGA) was performed using a TA Instrument Q600 analyzer under nitrogen gas flow with a heating rate of 10 °C min⁻¹. UV-vis absorption spectra were taken on a 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 (Bu₄NPF₆) acetonitrile solution. During CV measurements, the films were drop-cast on the glass carbon working electrode from THF solution. The film morphology was conducted by atomic force microscopy (AFM, Veeco Metrology Group/Digital Instruments) with tapping mode. Transmission electron microscopy (TEM) images were acquired using a HITACHI H-7650 electron microscope operating at an acceleration voltage of 100 kV. 2D Grazing-Incidence Wide-Angle X-ray Scattering (GIWAXS) measurements were carried out at the PLSII 9A U-SAXS beam line of Pohang Accelerator Laboratory, Korea. GIWAXS samples were prepared on PEDOT:PSS covered Si wafers in a similar manner to the devices of PSCs.

Single crystal analysis: Single crystals of **C8T-BDSe4Cl** or **C8T-BDT4Cl** were

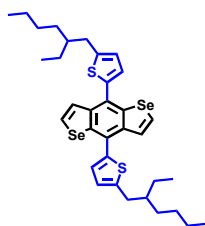
obtained by slow diffusion of ethanol into its chloroform solution and crystals were precipitated after the solvent evaporation in one week at room temperature. Single crystals data collection was performed on a Bruker SMART CCD area detector, using graphite-monochromated Mo K α radiation ($\lambda=0.71073$ Å). The software package SHELXL-2018 was used to solve and refine the crystal structure. Refinement of accurate structure of side groups has traditionally been prohibited by involving disorder. Fortunately, it is sufficient to analyze the stacking patterns of molecular backbones.

BHJ-OSC Fabrication and Characterization: The device structure was Glass/ITO/ZnO/active layer/MoO₃/Ag. The hole-only devices structure was ITO/PEDOT:PSS/activelayer/MoO₃/Ag and the electron-only device structure was ITO/ZnO/activelayer/PNDIT-F3N/Al. The ITO substrates were sonicated sequentially in Me₂CO, detergent, deionized water and i-PrOH to clean the ITO surface, followed by drying overnight at 90 °C in a vacuum oven. A PEDOT:PSS interlayer from a precursor solution was spin-coated onto the pre-cleaned and UV-treated ITO substrates, then heated at 150 °C for 10 min. The device structures of Glass/ITO/ZnO/active layer/MoO₃/Ag. were fabricated. A blend film of PM6: FREAs (**C8T-BDSe4Cl** or **C8T-BDT4Cl**) (1:1, w/w) was prepared by spin-coating its hot solution (80 °C) of chlorobenzene/1,8-diiodooctane (99.5:0.5, total concentration: 18 mg mL⁻¹) at 3000 rpm for 30 s. The substrates were then thermal annealed at 80 °C for 10 min. A thin layer (10 nm) of MoO₃ and Ag cathode (100 nm) were deposited by thermal evaporation in a high vacuum chamber ($\sim 10^{-6}$ mbar). 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 mm². 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 external quantum efficiency (EQE) was measured by a solar cell photodetector measurement system(Enlitech, Inc).

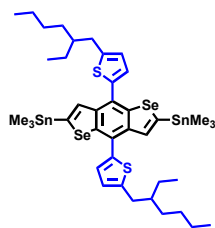


Compound 2: In a 200 mL two-neck round-bottom flask, compound **1** (0.18 g, 0.30 mmol), tributyl(5-(2-ethylhexyl)thiophen-2-yl)stannane (0.70 g, 1.22 mmol), and Pd(PPh₃)₄ (35 mg, 0.030 mmol) was added. The flask was evacuated and back-filled with N₂ three times, and then freshly distilled toluene (30 mL) was injected into the reaction mixture. The resulting mixture was refluxed for 12 h under the N₂ atmosphere. After being cooled to room temperature, the solvents were then removed under reduced pressure. The crude product was purified by silica gel column chromatography, eluting with dichloromethane/petroleum ether (1:4) to obtain compound **2** as yellow solid (0.22 g, 87%). ¹H NMR (CDCl₃, 400 MHz, ppm): δ 8.52 (s, 2H, Se-H), 7.22-7.23 (d, *J* = 4.0 Hz, 2H, Th-H), 6.89-6.90 (d, *J* = 4.0 Hz, 2H, Th-H), 4.33-4.38 (q, *J* = 6.8 Hz, 4H, CH₂), 2.85-2.87 (d, *J* = 6.8 Hz, 4H, CH₂), 1.69-1.76 (m, 8H, CH, CH₃), 1.31-1.41 (m, 16H,

CH₂), 0.91-0.96 (m, 12H, CH₃). ¹³C NMR (CDCl₃, 100 MHz, ppm): δ 163.8, 146.5, 144.3, 138.9, 137.9, 137.4, 133.9, 131.1, 128.1, 125.7, 61.7, 41.5, 34.2, 32.5, 28.9, 25.7, 22.9, 14.3, 14.1, 10.9. HR-ESI-MS (*m/z*): calcd for: C₄₀H₅₁O₄S₂Se₂: 819.1554. Found: 819.1542.

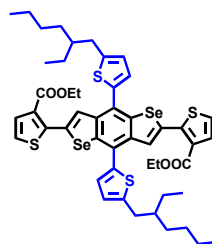


Compound 3: In a 200 mL two-neck round-bottom flask, compound **2** (1.23 g, 1.56 mmol), LiOH·H₂O (1.05 g, 25.0 mmol) was added and then THF (30 mL) and H₂O (30 mL) was injected into the reaction mixture. The resulting mixture was refluxed for 12 h. After being cooled to room temperature, the reaction mixture was acidified by HCl (pH = 1) and the reaction mixture was then extracted with ethyl acetate (3 × 30 mL). The organic layers were combined and washed with saturated brine solution and dried over anhydrous Na₂SO₄. Then the solvents were then removed under reduced pressure to obtain crude compound for next step without further purification. To a solution of crude compound in dry quinoline (20 mL) was added copper powder (0.28 g, 2.96 mmol). After addition, the mixture was refluxed for 1 h. After the mixture was cooled to room temperature, the quinoline was removed by dilute hydrochloric acid. Then the mixture was extracted with petroleum ether (3 × 30 mL). The organic layers were combined and washed with saturated brine solution and dried over anhydrous Na₂SO₄. The solvents were then removed under reduced pressure and the crude product was purified by silica gel column chromatography, eluting with petroleum ether to obtain compound **3** as pale-yellow solid (0.51 g, 50%). ¹H NMR (CDCl₃, 400 MHz, ppm): δ 7.95-7.97 (d, *J* = 8.0 Hz, 2H, Se-H), 7.83-7.85 (d, *J* = 8.0 Hz, 2H, Se-H), 7.22-7.23 (d, *J* = 3.6 Hz, 2H, Th-H), 6.87-6.88 (d, *J* = 3.6 Hz, 2H, Th-H), 2.86-2.88 (d, *J* = 6.8 Hz, 4H, CH₂), 1.66-1.71 (m, 2H, CH), 1.33-1.49 (m, 16H, CH₂), 0.92-0.99 (m, 12H, CH₃). ¹³C NMR (CDCl₃, 100 MHz, ppm): δ 145.5, 142.0, 139.2, 138.3, 129.5, 128.7, 127.4, 127.3, 125.3, 41.5, 34.2, 32.5, 28.9, 25.7, 23.0, 14.1, 10.9. HR-ESI-MS (*m/z*): calcd for: C₃₄H₄₂S₂Se₂: 674.1058. Found: 675.1145 ([M+H]⁺).

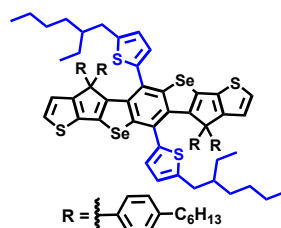


Compound 4: In 250 mL round-bottom flask, compound **3** (0.32 g, 0.48 mmol) was added and backfilled with N₂ three times, and freshly distilled THF (50 mL) was added. Then *n*-BuLi (2.4 M, 1.2 mL, 2.85 mmol) was added dropwise into slowly and stirred at -78 °C for 1 h. After that, the mixture was stirred at room temperature for another 1 h. After being cooled to -78 °C, the solution of trimethyltin chloride (3.12 mL, 3.12 mmol) in THF was added into the reaction mixture. Then the mixture was stirred at room temperature for 12 h. The mixture was quenched by water, and extracted with dichloromethane (3 × 30 mL). The organic layers were combined and washed with saturated brine solution and dried over anhydrous Na₂SO₄. After removal of the solvent, the yellow solid was obtained (0.45 g, 95%). The crude product was used for next step

without further purification.

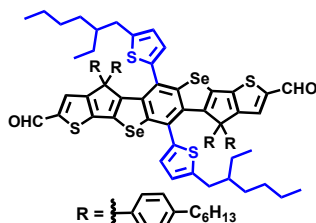


Compound 5: In a 200 mL two-neck round-bottom flask, compound 4 (0.48 g, 0.48 mmol), the ethyl 2-bromothiophene-3-carboxylate (0.56 g, 2.39 mmol), and Pd(PPh₃)₄ (0.05 g, 0.04 mmol) was added. The flask was evacuated and back-filled with N₂ three times, and then freshly distilled toluene was injected into the reaction mixture. The resulting mixture was refluxed for 12 h under the N₂ atmosphere. After being cooled to room temperature, the solvents were then removed under reduced pressure. The crude product was purified by silica gel column chromatography, eluting with dichloromethane/petroleum ether (1:1) to obtain the product as red solid (0.43 g, 91%). ¹H NMR (CDCl₃, 400 MHz, ppm): δ 8.06 (s, 2H, Se-H), 7.48-7.49 (d, *J* = 5.6 Hz, 2H, Th-H), 7.25-7.26 (d, *J* = 4.0 Hz, 2H, Th-H), 7.20-7.21 (d, *J* = 5.6 Hz, 2H, Th-H), 6.86-6.87 (d, *J* = 4.0 Hz, 2H, Th-H), 4.26-4.31 (q, *J* = 7.2 Hz, 4H, CH₂), 2.84-2.85 (d, *J* = 6.8 Hz, 4H, CH₂), 1.64-1.69 (m, 2H, CH), 1.32-1.45 (m, 16H, CH₂), 1.25-1.28 (t, *J* = 7.2 Hz, 6H, CH₃), 0.92-0.96 (m, 12H, CH₃). ¹³C NMR (CDCl₃, 100 MHz, ppm): 163.2, 145.8, 145.5, 143.5, 138.5, 138.3, 136.8, 130.7, 129.1, 128.4, 128.3, 127.6, 125.5, 124.5, 60.9, 41.4, 34.2, 32.5, 28.9, 25.7, 23.0, 14.2, 10.9. HR-ESI-MS (*m/z*): calcd for: C₄₈H₅₄O₄S₄Se₂ : 982.1235. Found: 983.1320 ([M+H]⁺).

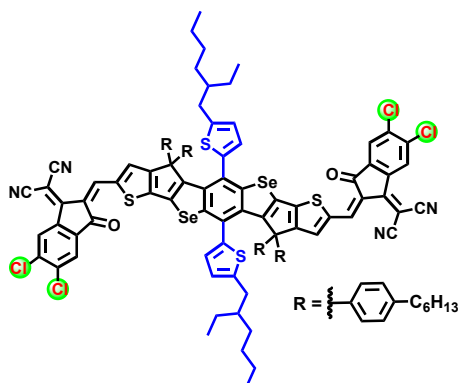


Compound 6: 1-bromo-4-hexylbenzene (0.98 g, 4.06 mmol) was dissolved in anhydrous THF (40 mL), *n*-BuLi in hexane (2.4 M, 1.48 mL, 3.57 mmol) was added slowly at -78 °C under N₂ atmosphere. The reaction mixture was stirred at -78 °C for 1 h, and then a solution of compound 6 (0.25 g, 0.25 mmol) in THF (30 mL) was added dropwise into the reaction mixture. The reaction mixture was then warmed to room temperature and was stirred for another 10 h. The reaction mixture was poured into water and extracted with dichloromethane (3 × 50 mL). The organic layer was washed with water, combined and dried over anhydrous Na₂SO₄. After removal of the solvent, the concentrated mixture (0.39 g, 0.24 mmol) and *p*-toluene sulfonic acid (0.090 g, 0.52 mmol) was charged into two-neck flask under nitrogen atmosphere. Then freshly distilled toluene was injected into the mixture. The resulting solution was stirred at 70 °C for 3 h. Then the mixture was poured into water, extracted with dichloromethane. Then the organic layers were combined, then washed with water and dried over anhydrous Na₂SO₄. After removal of the solvent, the crude product was purified by flash column chromatography (silica gel), eluting with dichloromethane/petroleum ether (1:10) to obtain the product as light yellow solid (0.23 g, 65%). ¹H NMR (CDCl₃, 400 MHz, ppm): δ 7.01-7.02 (d, *J* = 4.8 Hz, 2H, Th-H), 6.93-6.99 (m, 16H, Ph-H), 6.73-6.74 (d, *J* = 4.8 Hz, 2H, Th-H), 6.31-6.32 (d, *J* = 3.6 Hz, 2H, Th-H), 6.03-6.04 (d, *J* = 3.6 Hz, 2H, Th-H), 2.52-2.73 (m, 12H, CH₂), 1.57-1.62 (m, 10H, CH, CH₂), 1.27-

1.33 (m, 40H, CH₂), 0.87-0.97 (m, 24H, CH₃). ¹³C NMR (CDCl₃, 100 MHz, ppm): δ 164.2, 153.4, 153.1, 145.8, 141.4, 141.3, 140.7, 140.4, 140.3, 139.2, 139.1, 139.0, 136.9, 136.8, 136.54, 136.50, 136.4, 132.2, 129.9, 128.5, 128.4, 128.3, 127.9, 127.8, 127.3, 124.1, 123.9, 122.3, 64.4, 41.5, 41.3, 35.6, 35.5, 33.9, 33.8, 32.5, 32.4, 31.8, 31.7, 31.6, 31.5, 29.7, 29.3, 29.2, 29.1, 28.95, 28.90, 25.7, 25.5, 23.2, 23.1, 22.7, 22.6, 14.3, 14.2, 14.1, 10.84, 10.80. HR-ESI-MS (m/z): calcd for C₉₂H₁₁₀S₄Se₂: 1502.5821. Found: 1502.5830.



Compound 7: To a solution of compound **6** (0.18 g, 0.11 mmol) in dry 1,2-dichloroethane (30 mL) was added DMF (0.5 mL, 0.30 mmol) and POCl₃ (0.20 mL, 0.24 mmol) dropwise under N₂ atmosphere at 0 °C. After addition, the cooling bath was removed and the reaction mixture was refluxed for 12 h. The mixture was quenched with saturated aqueous solution of sodium acetate and then the mixture was stirred for another 1 h. The reaction mixture was then extracted with dichloromethane. The organic layers were combined and washed with saturated brine solution and dried over anhydrous Na₂SO₄. After removal of the solvent, the crude product was purified by flash column chromatography (silica gel), eluting with petroleum ether/dichloromethane (2:1) to obtain the product as red solid (0.16 g, 85%). ¹H NMR (CDCl₃, 400 MHz, ppm): δ 9.62 (s, 2H, CHO), 7.36 (s, 2H, Th-H), 6.93-6.98 (m, 16H, Ph-H), 6.32-6.33 (d, *J* = 3.6 Hz, 2H, Th-H), 6.02-6.03 (d, *J* = 3.6 Hz, 2H, Th-H), 2.53-2.69 (m, 12H, CH₂), 1.54-1.59 (m, 10H, CH, CH₂), 1.28-1.38 (m, 40H, CH₂), 0.87-0.98 (m, 24H, CH₃). ¹³C NMR (CDCl₃, 100 MHz, ppm): δ 182.5, 164.2, 157.34, 157.30, 155.0, 146.6, 145.7, 141.23, 141.20, 141.16, 141.14, 141.13, 135.5, 135.4, 130.6, 129.9, 128.31, 128.28, 128.22, 128.1, 128.0, 127.93, 127.88, 127.86, 127.81, 64.7, 41.5, 41.3, 35.6, 35.5, 33.9, 33.8, 32.5, 32.4, 31.8, 31.5, 31.4, 29.2, 29.1, 28.9, 28.8, 25.8, 25.7, 25.5, 23.2, 23.1, 22.7, 22.6, 14.3, 14.2, 14.1, 10.84, 10.81. HR-ESI-MS (m/z): calcd for C₉₄H₁₁₁O₂S₄Se₂: 1559.5792. Found: 1559.5815 ([M+H]⁺).



C8T-BDS₄Cl: In a 100 mL two-neck round-bottom flask, **7** (0.06 g, 0.05 mmol), **IC-2Cl** (0.11 g, 0.31 mmol) was added. The reaction mixture was evacuated and backfilled with N₂ three times, and then freshly degassed chloroform (50 mL) and pyridine (0.8 mL) were added into the reaction mixture. The reaction mixture was stirred at room temperature for 12 h. Then the solution was poured into methanol and

the precipitate was filtered off and washed with methanol. The crude product was purified by silica gel column chromatography, eluting with petroleum ether/dichloromethane (1:1) to give the product as purple solid (0.07 g, 93%). ^1H NMR (CDCl_3 , 400 MHz, ppm): δ 8.70 (s, 2H, C=CH), 8.69 (s, 2H, Ph-H), 7.86 (s, 2H, Ph-H), 7.35 (s, 2H, Th-H), 6.90-7.03 (m, 16H, Ph-H), 6.36-6.37 (d, $J = 3.6$ Hz, 2H, Th-H), 6.06-6.07 (d, $J = 3.6$ Hz, 2H, Th-H), 2.55-2.78 (m, 12H, CH_2), 1.54-1.62 (m, 10H, CH, CH_2), 1.30-1.40 (m, 40H, CH_2), 0.87-1.01 (m, 24H, CH_3). ^{13}C NMR (CDCl_3 , 175 MHz, ppm): δ 186.1, 157.9, 141.5, 141.2, 139.44, 139.42, 139.1, 138.8, 138.5, 135.9, 130.9, 130.3, 128.5, 128.4, 128.35, 128.33, 128.2, 127.8, 127.7, 126.8, 124.9, 120.28, 128.26, 114.4, 68.7, 64.7, 41.3, 41.19, 41.17, 35.6, 35.5, 33.7, 33.6, 32.6, 32.5, 32.4, 31.8, 31.7, 31.5, 31.4, 29.22, 29.21, 29.0, 28.94, 28.93, 25.7, 25.6, 25.3, 23.19, 23.17, 22.65, 22.63, 14.3, 14.2, 14.1, 10.9, 10.7. MALDI-TOF MS (m/z): calcd for $\text{C}_{118}\text{H}_{114}\text{Cl}_4\text{N}_4\text{O}_2\text{S}_4\text{Se}_2$: 2046.0 (100 %). Found: 2046.0. Elemental Analysis: calcd for $\text{C}_{118}\text{H}_{114}\text{Cl}_4\text{N}_4\text{O}_2\text{S}_4\text{Se}_2$: C, 69.20; H, 5.61; N, 2.74. Found: C, 65.50; H, 5.39; N, 2.42.

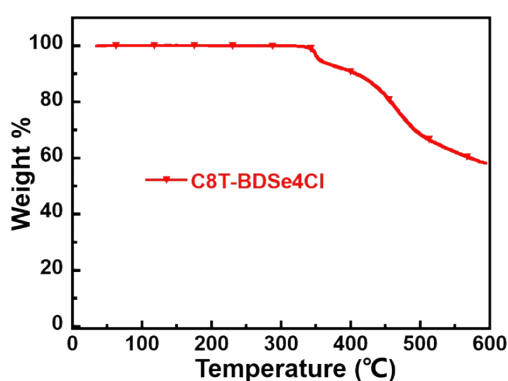


Figure S1. Thermal gravity analyses (TGA) of **C8T-BDSe4Cl** with a heating rate of $10\text{ }^\circ\text{C}/\text{min}$ under N_2 atmosphere.

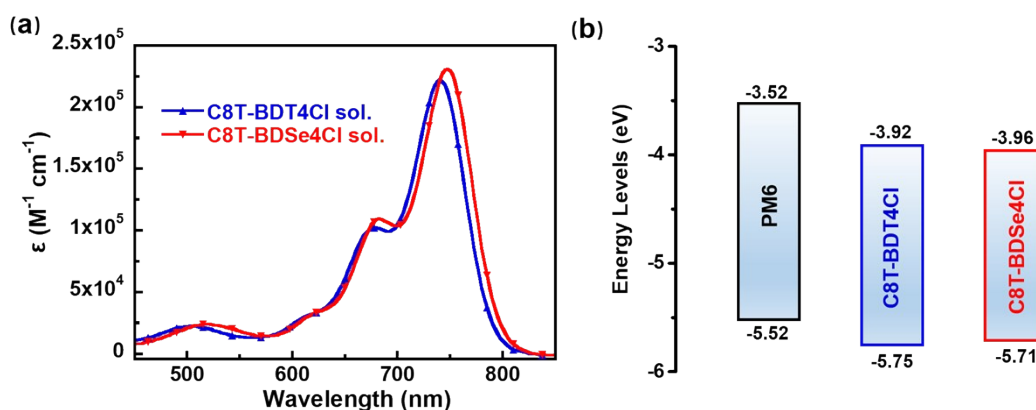


Figure S2. (a) Absorption spectrum of **C8T-BDT4Cl** and **C8T-BDSe4Cl** in chloroform solutions (2.0×10^{-5} M). (b) The energy levels alignment of **C8T-BDT4Cl** and **C8T-BDSe4Cl**.

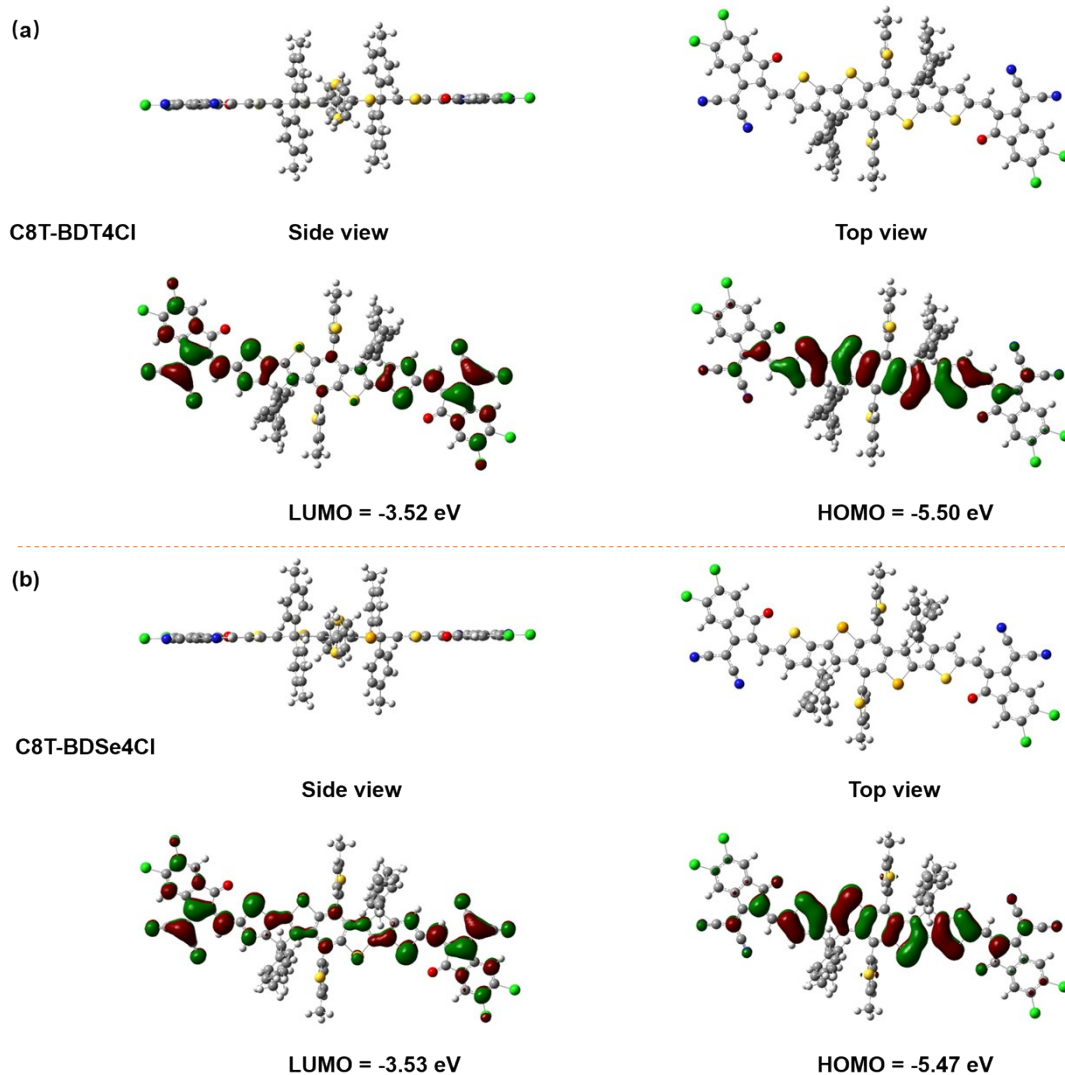


Figure S3. Molecular geometry and calculated energy levels for the **C8T-BDT4Cl** (a) and for the **C8T-BDSe4Cl** (b) by DFT.

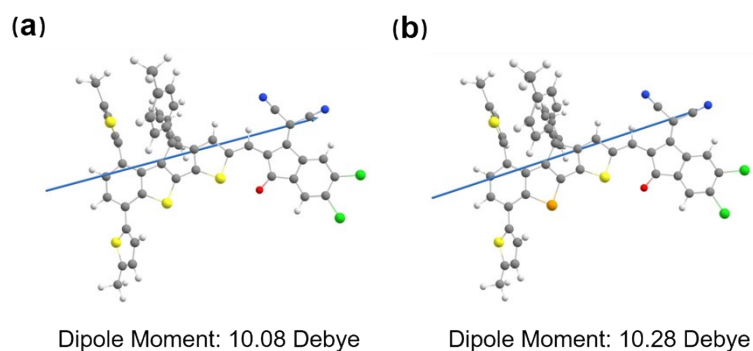


Figure S4. Calculated half molecular dipole moments of **C8T-BDT4Cl** (a) and **C8T-BDSe4Cl** (b) by DFT.

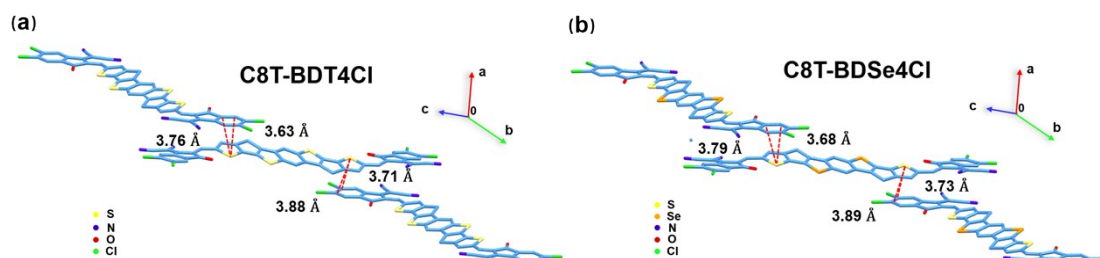


Figure S5. The relevant intermolecular interaction of multiple intermolecular S $\cdots\pi$ interactions between the central electron-rich core moiety and the end groups of **C8T-BDT4Cl** (a) and **C8T-BDSe4Cl** (b) in molecular slipped stacking direction.

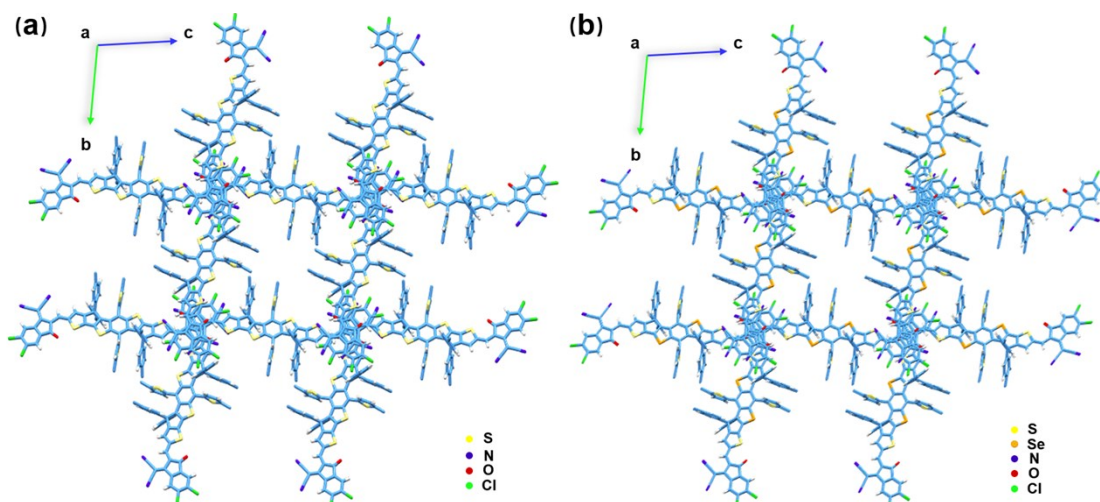


Figure S6. The top view of reticular architecture with 3D π - π stacking for crystal **C8T-BDT4Cl** (a), of **C8T-BDSe4Cl** (b). All of the alkyl side chain on the thiophene and phenyl are simplified to methyl groups.

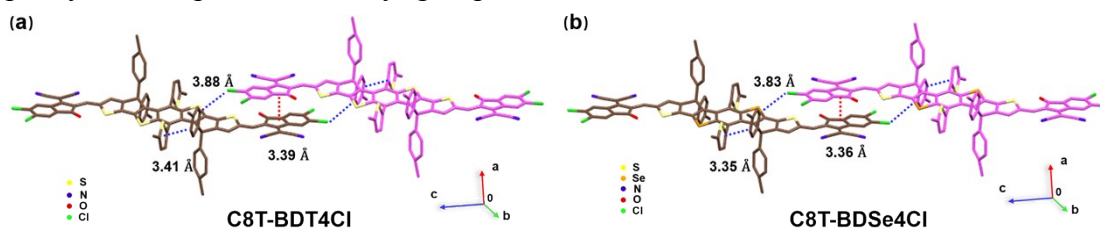


Figure S7. A special intermolecular interaction channel for **C8T-BDT4Cl** (a) and **C8T-BDSe4Cl** (b). All of the alkyl side chain on the thiophene and phenyl are simplified to methyl groups.

Table S1 Check CIF report of XRD data of single crystal of **C8T-BDT4Cl** (CCDC 2004058) and **C8T-BDSe4Cl** (CCDC 2004060).

Compound	C8T-BDT4Cl	C8T-BDSe4Cl
Temperature	293 K	180 K
Bond precision	C-C = 0.0114 Å	C-C = 0.0095 Å
	Wavelength = 0.71073 Å	Wavelength = 0.71073 Å
Cell		
	a (Å)	13.9260 (6)
	b (Å)	20.4965 (8)
	c (Å)	21.8458 (5)
	a (Å)	14.0457 (3)
	b (Å)	20.5912 (4)
	c (Å)	22.0365 (3)

α (°)	95.706 (2)	96.290 (1)
β (°)	93.685 (2)	91.577 (1)
γ (°)	108.330 (4)	109.722 (2)
Volume	5859.6 (4)	5949.2 (2)
Crystal system	Triclinic	Triclinic
Space group	P -1	P -1
Hall group	-P 1	-P 1
Formula	$C_{118}H_{114}Cl_4N_4O_2S_6$	$C_{118}H_{114}Cl_4N_4O_2S_4Se_2$
Molecular Weight	1953.60	2046.49
Dx, g cm ⁻³	1.175	1.143
Z	2	4
μ (mm ⁻¹)	0.325	0.828
F000	2174.0	2132.0
h, k, lmax	18, 28, 30	16, 24, 26
Data completeness	0.844	0.999
Theta(max)	30.777	25.027
R(reflections)	0.1482 (12447)	0.0816 (15285)
wR2(reflections)	0.4161 (30918)	0.2020 (21016)
S	1.178	1.078
Npar	1062	1207

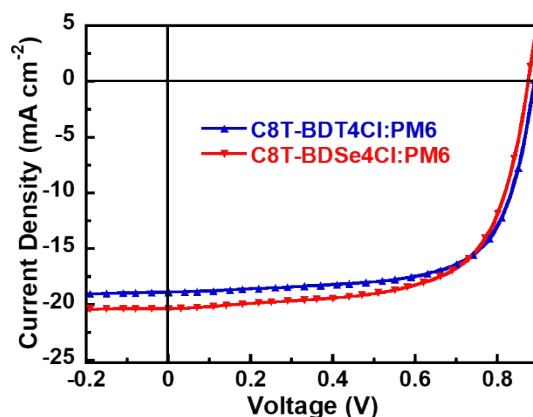


Figure S8. Characteristic J - V curves of **PM6:C8T-BDT4Cl** and **PM6:C8T-BDSe4Cl** without DIO additive, under the irradiation of AM 1.5G, 100 mW cm⁻².

Table S2. Photovoltaic parameters based on **PM6: C8T-BDT4Cl** and **PM6:C8T-BDSe4Cl** without DIO additive, under the irradiation of AM 1.5G, 100 mW cm⁻².

Acceptors	J_{sc} (mA cm ⁻²)	V_{oc} (V)	FF (%)	PCE (%)
C8T-BDT4Cl	18.88	0.889	68.6	11.51
C8T-BDSe4Cl	20.36	0.874	65.7	11.70

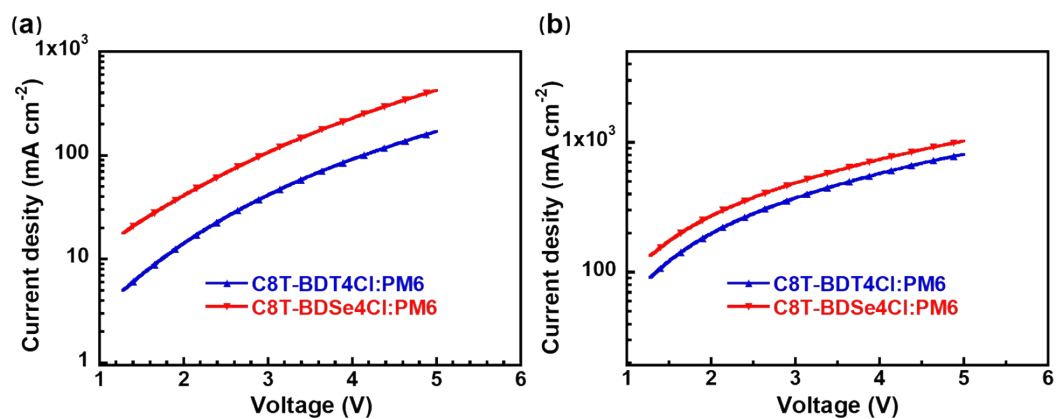
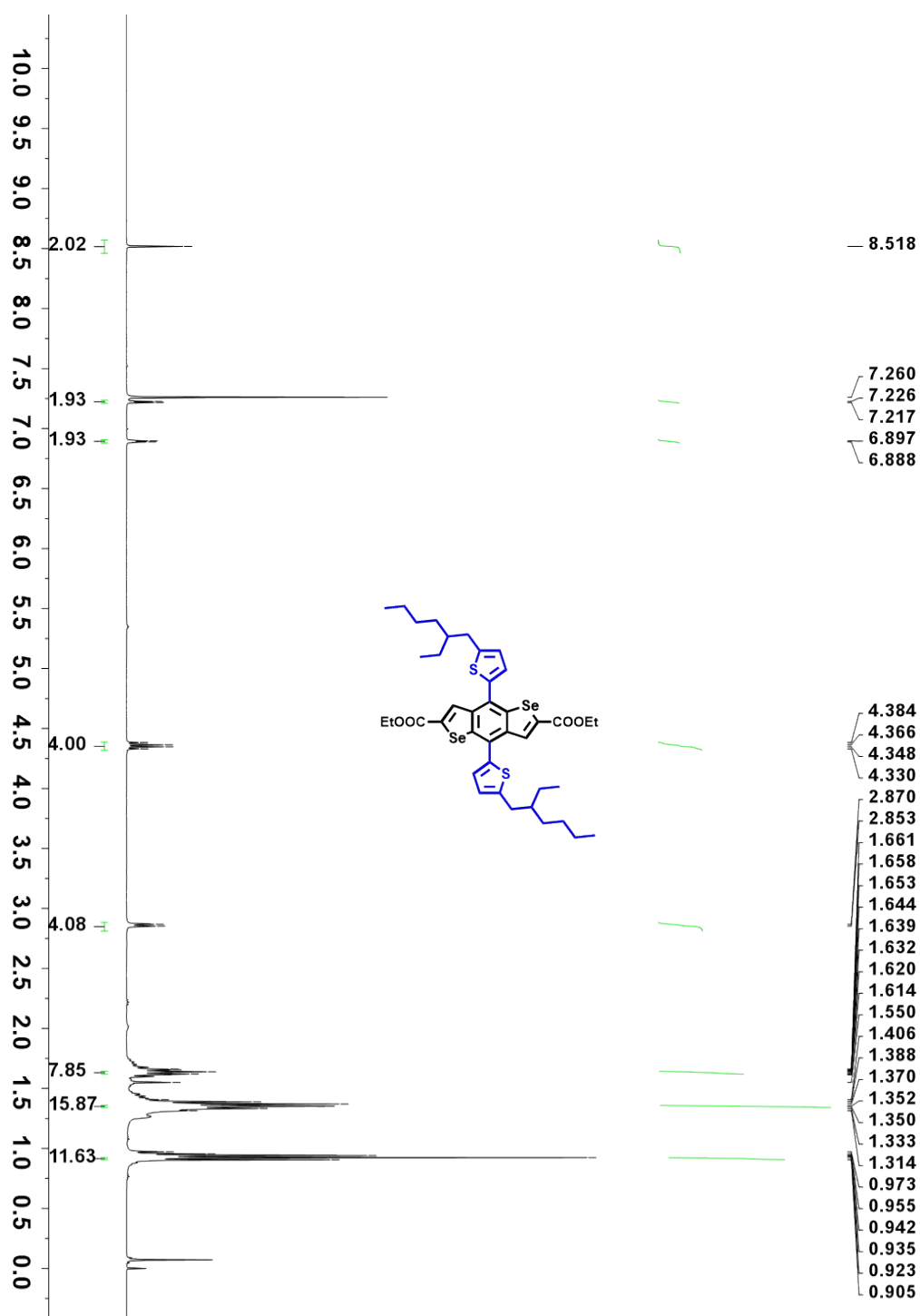
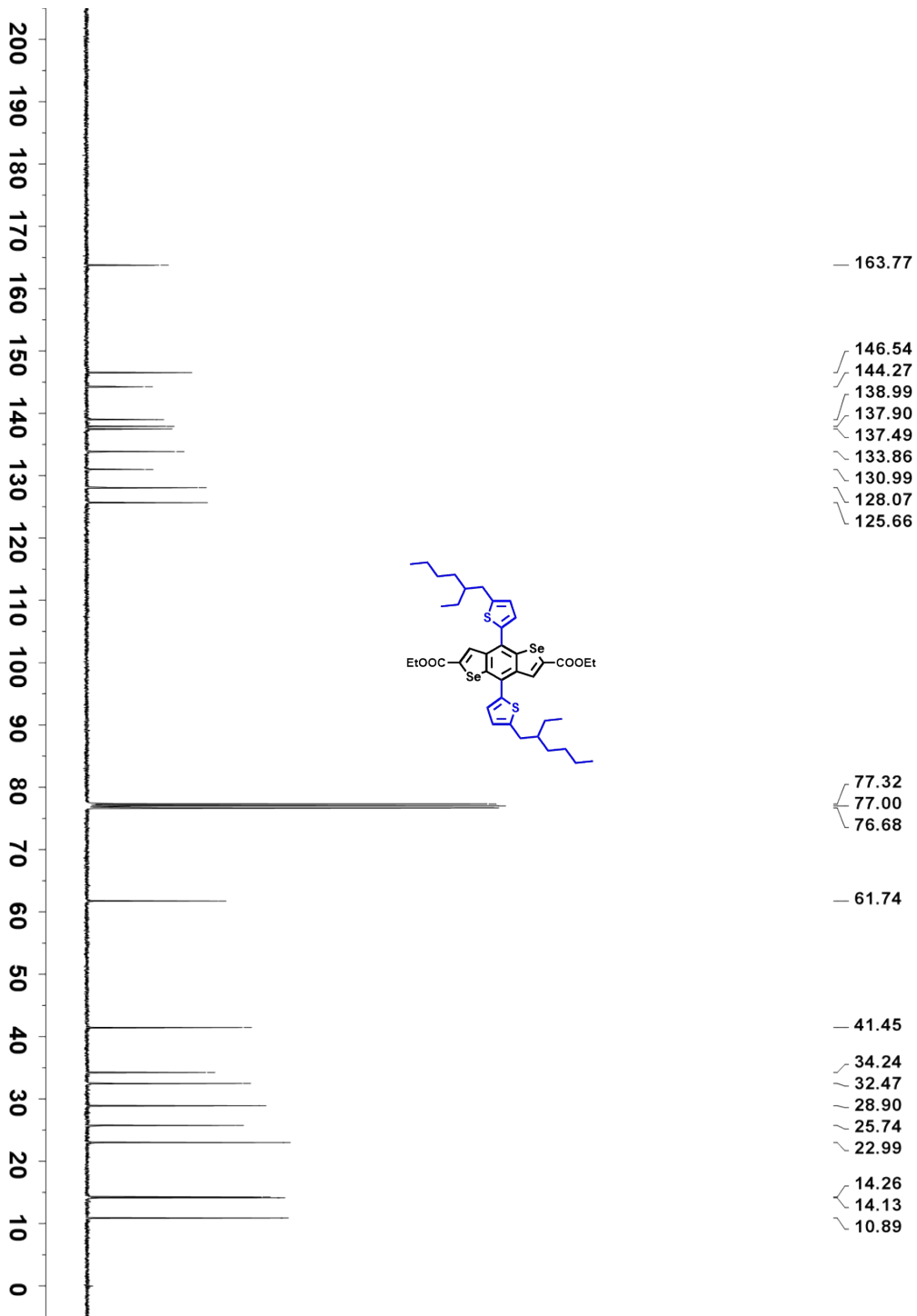


Figure S9. (a) The dark $J-V$ plots of electron-only devices based on **C8T-BDT4Cl:PM6** and **C8T-BDSe4Cl:PM6** blend films, respectively. (b) The dark $J-V$ plots of hole-only devices based on **C8T-BDT4Cl:PM6** and **C8T-BDSe4Cl:PM6** blend films, respectively.

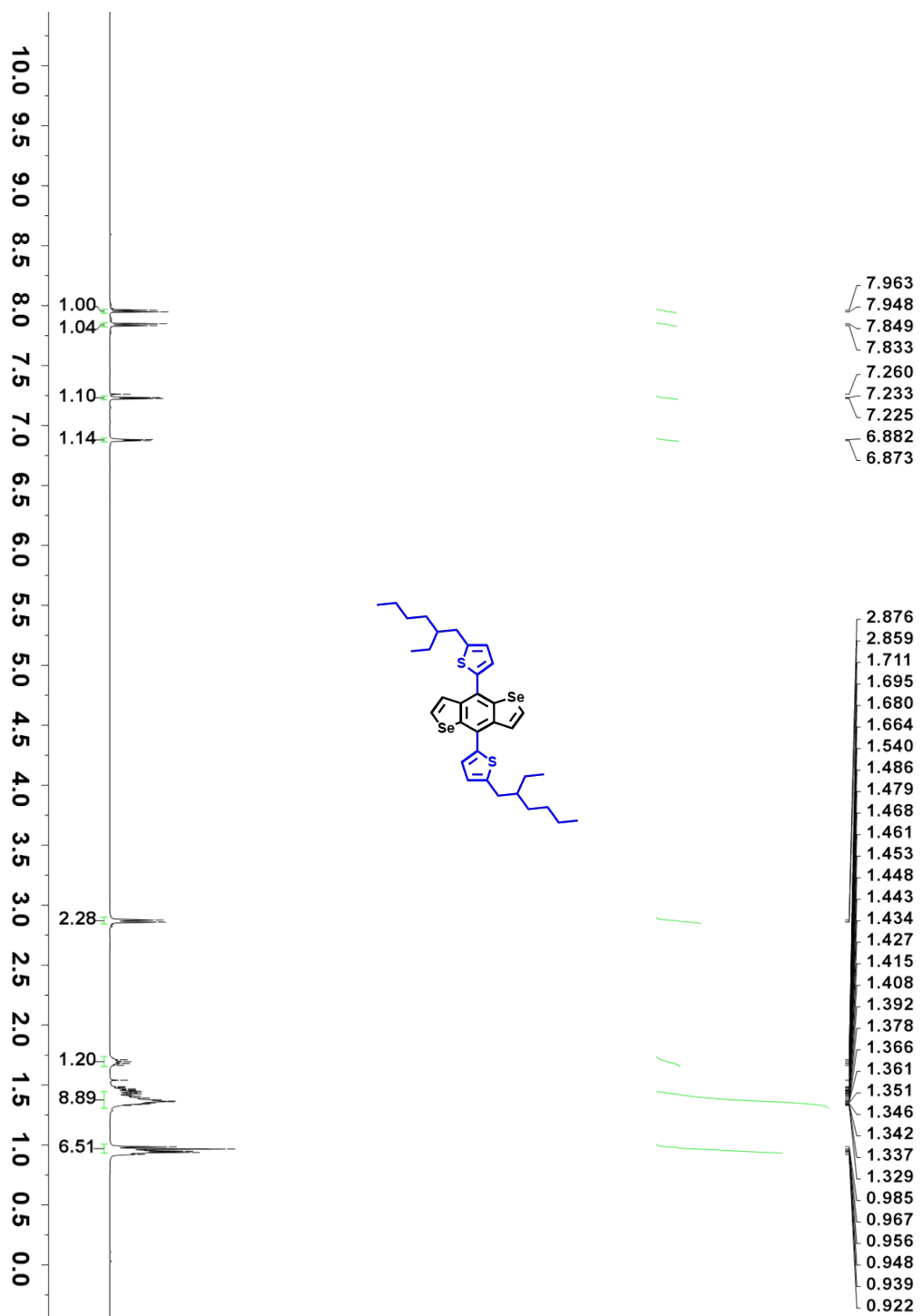
¹H NMR, ¹³C NMR, and MALDI-TOF-MS spectrum of new compounds



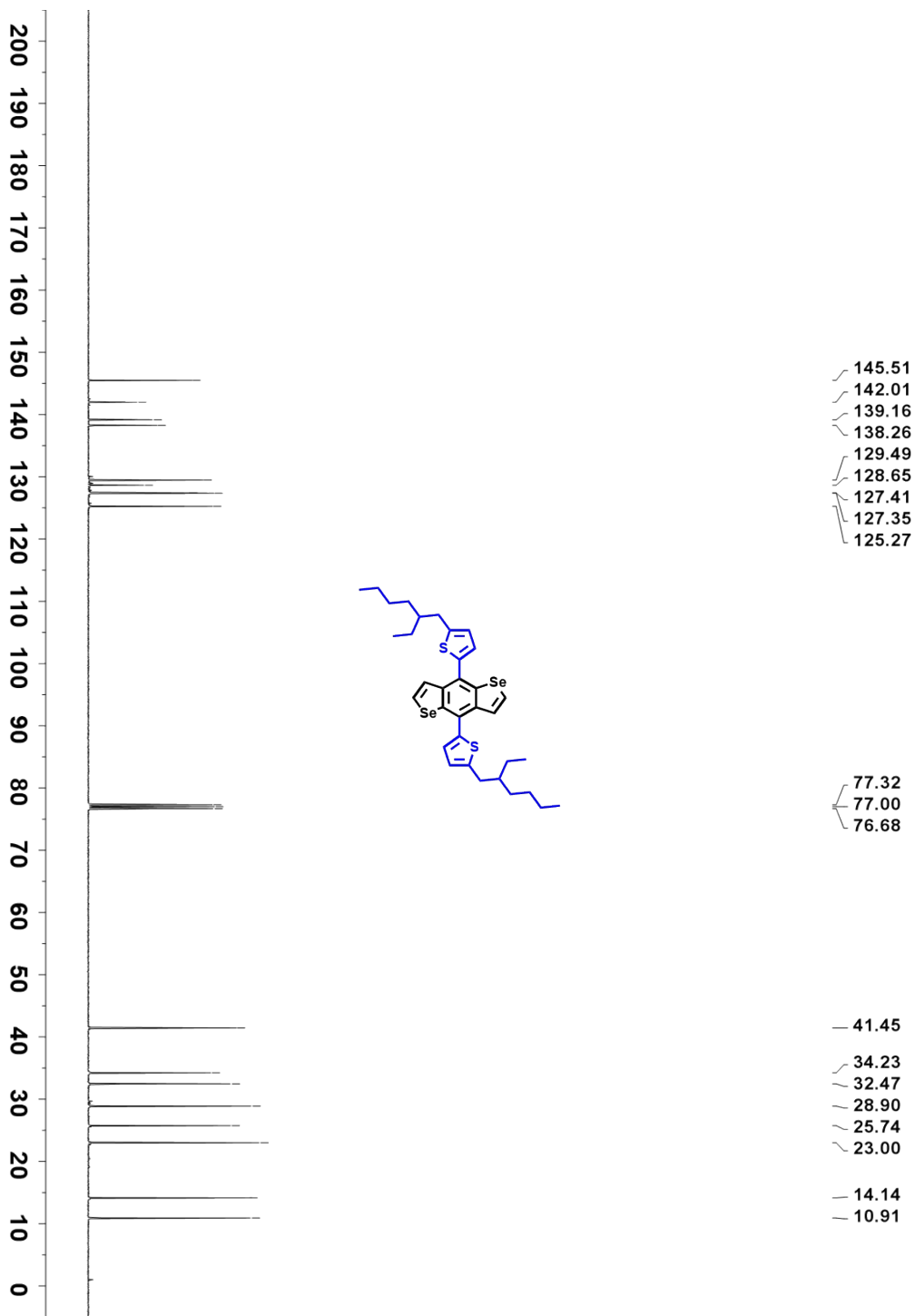
¹H NMR spectrum for **2**



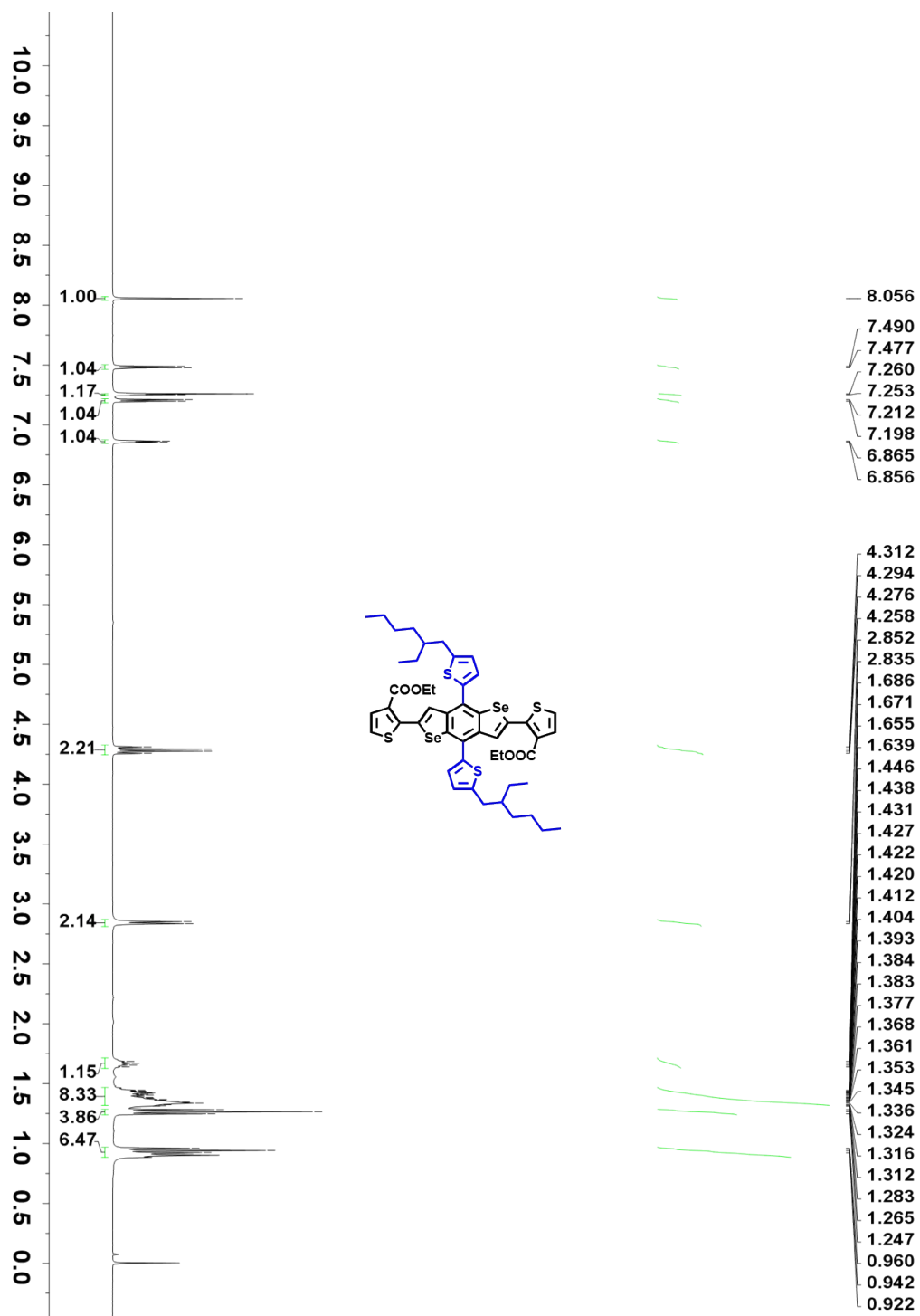
¹³C NMR spectrum for **2**



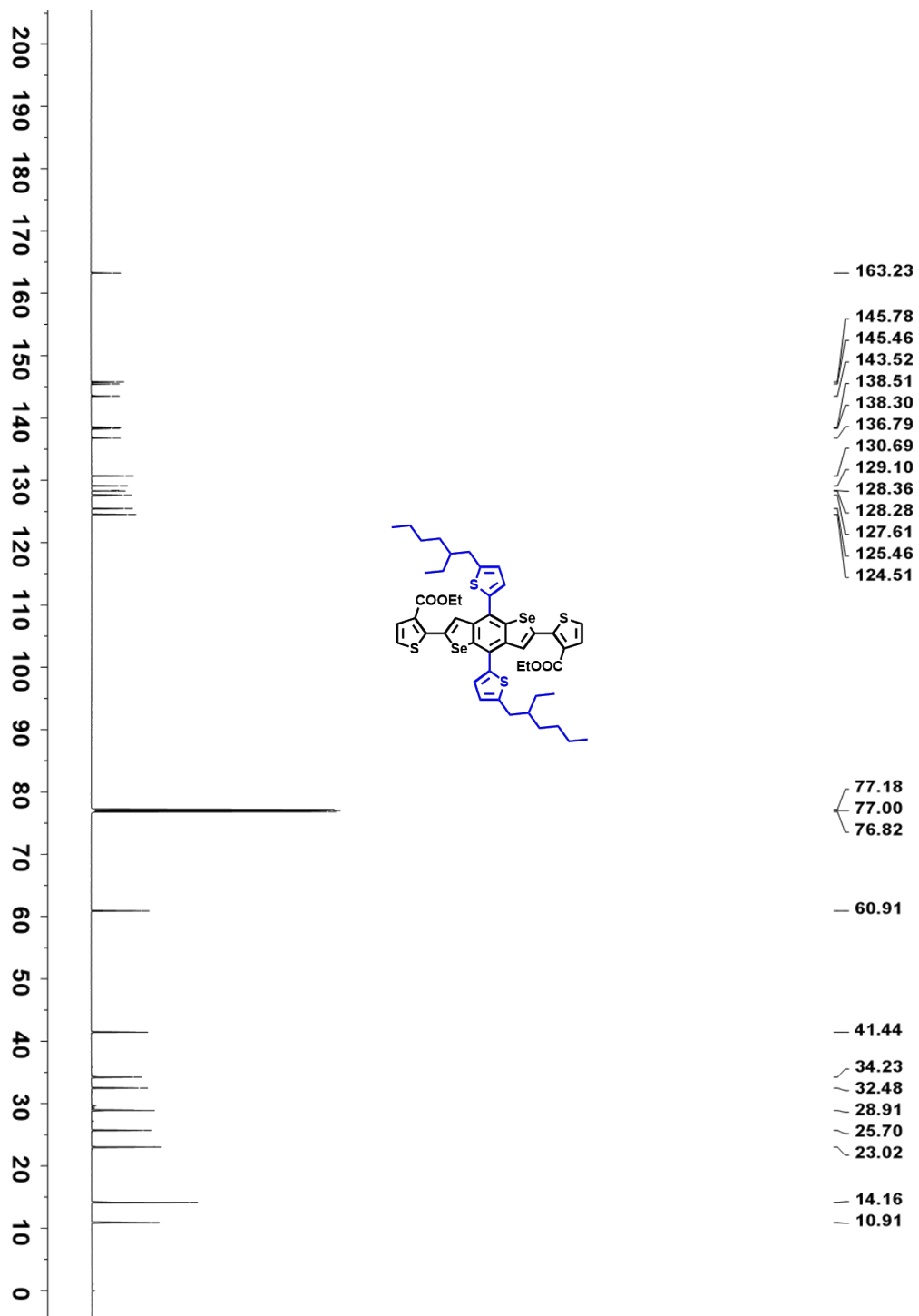
^1H NMR spectrum for **3**



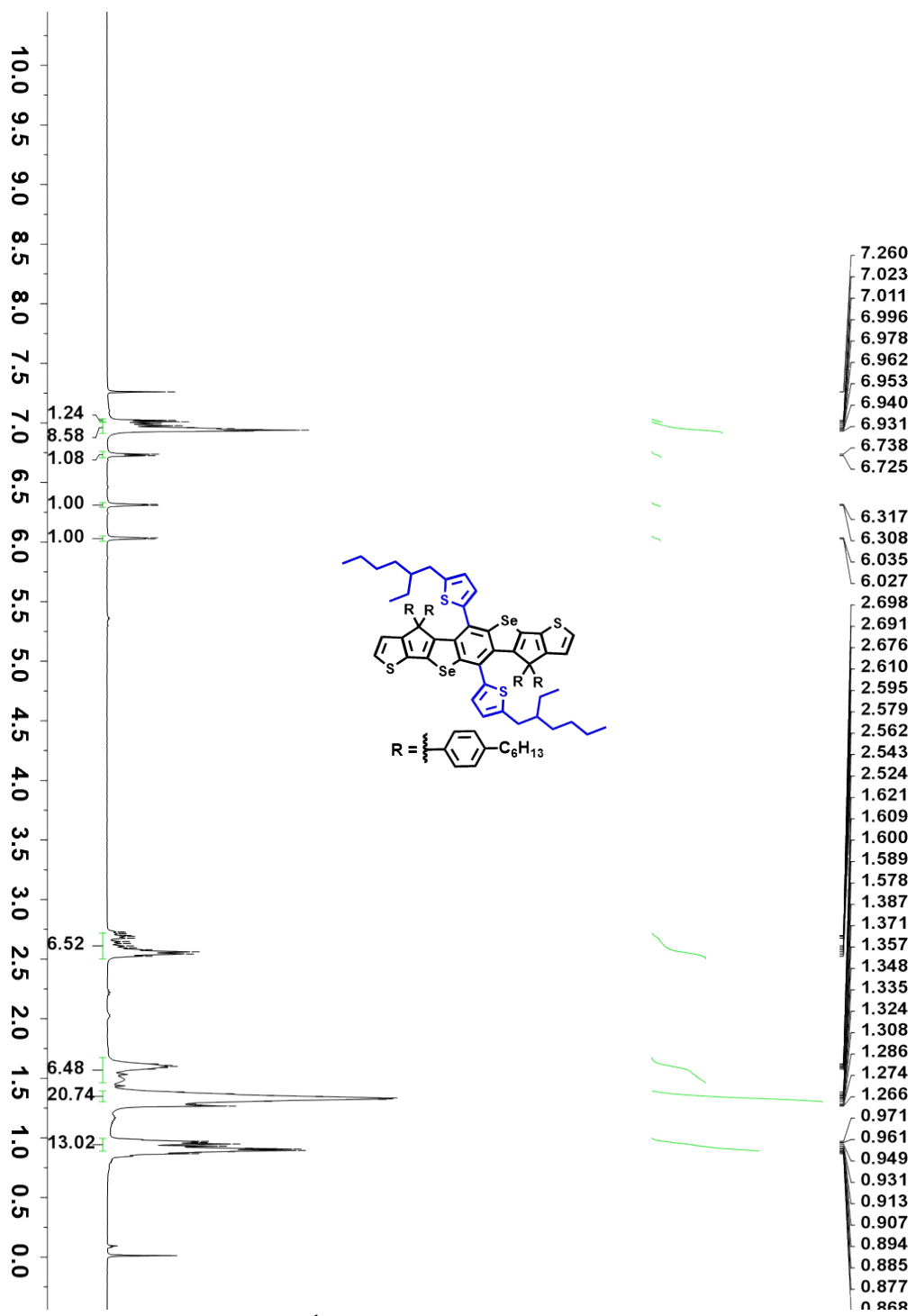
¹³C NMR spectrum for **3**



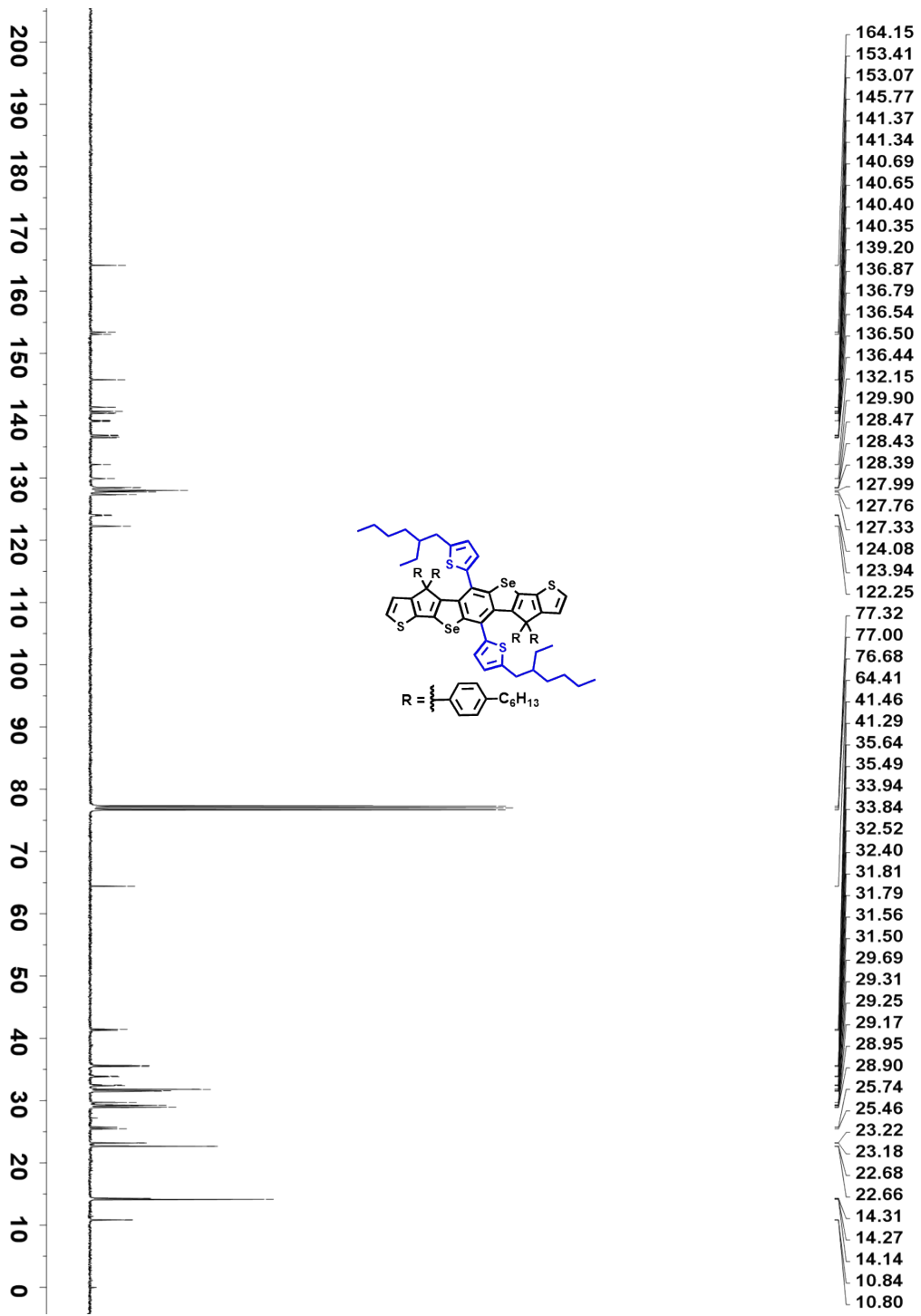
^1H NMR spectrum for 5



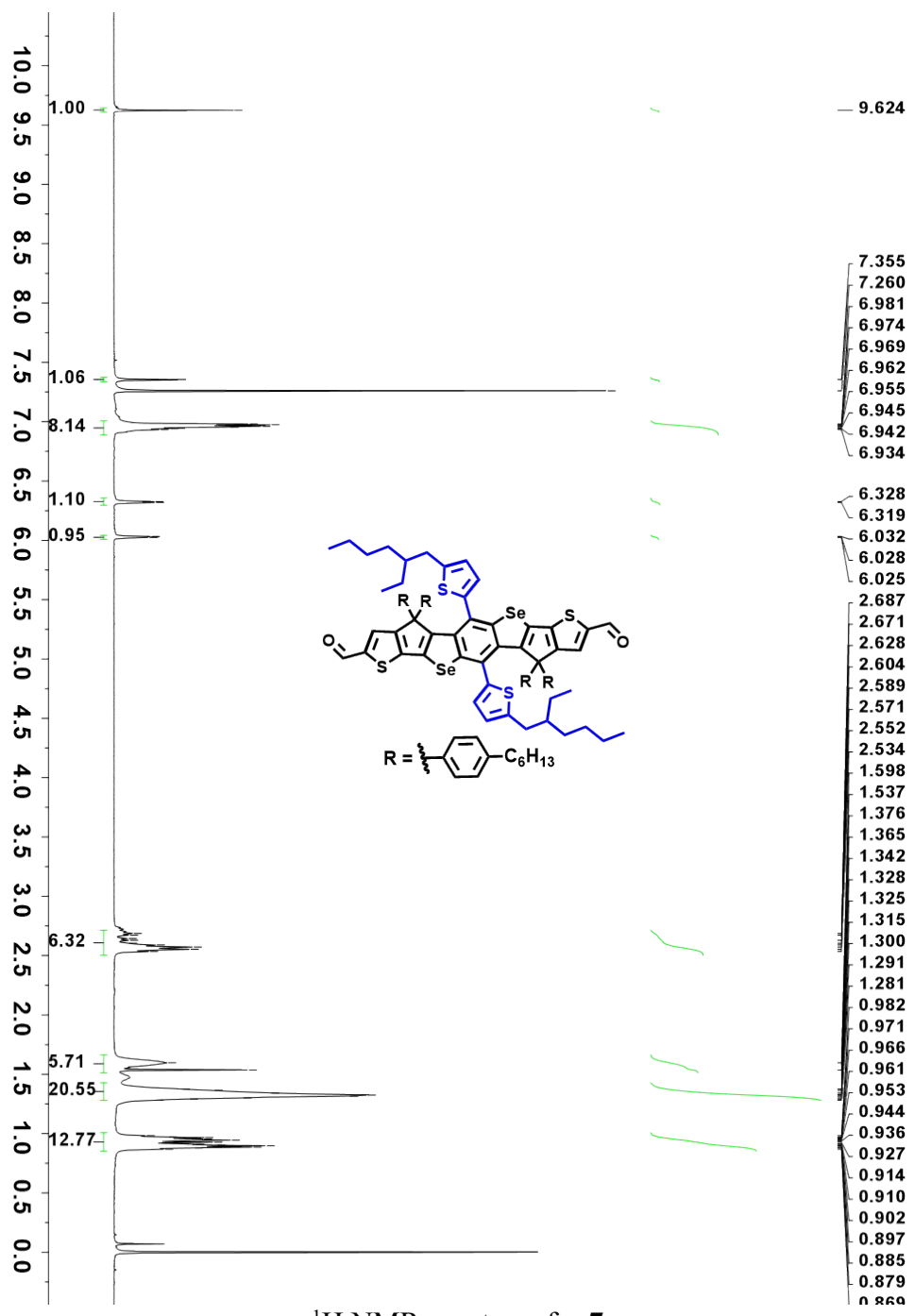
¹³C NMR spectrum for 5



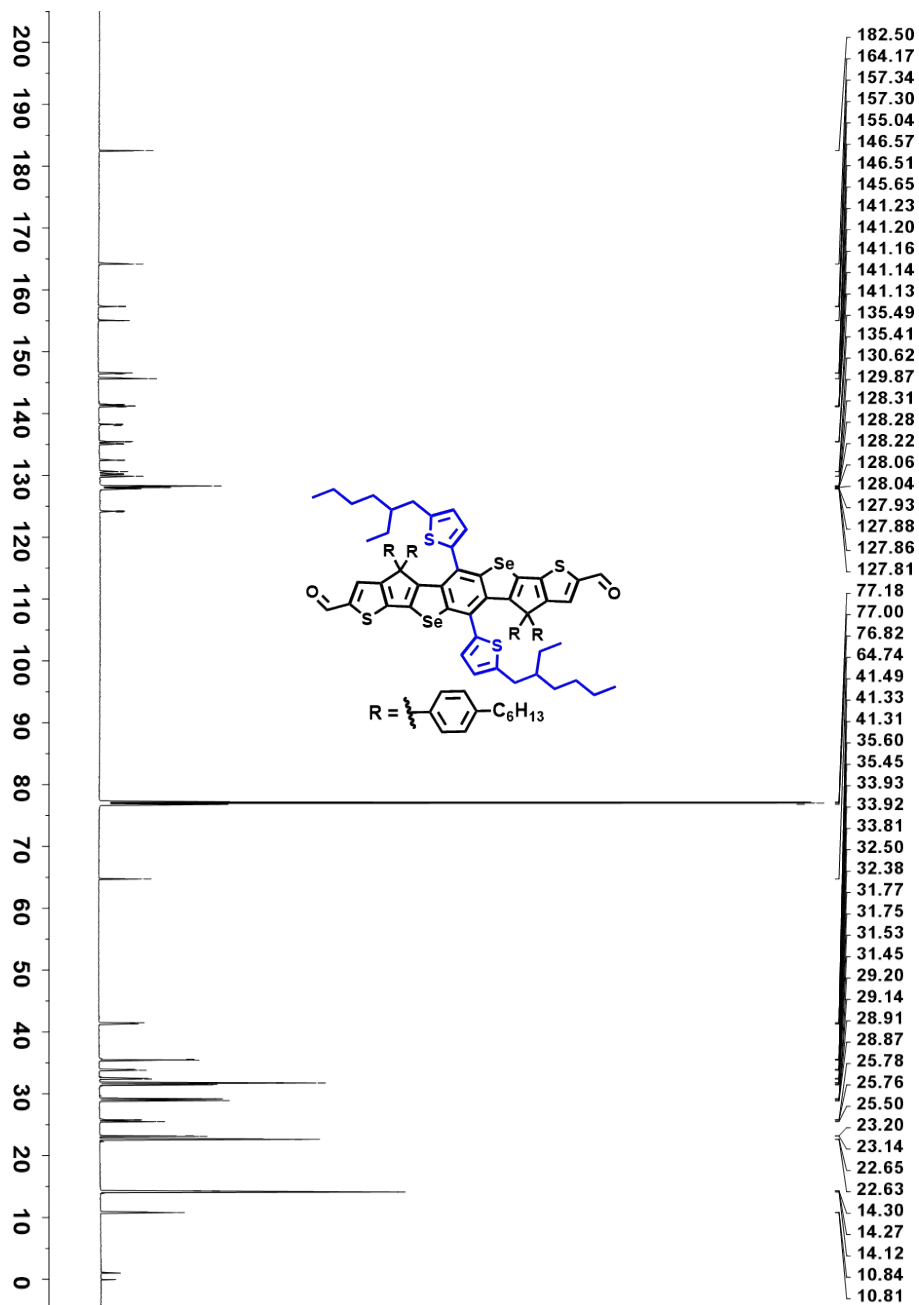
^1H NMR spectrum for **6**



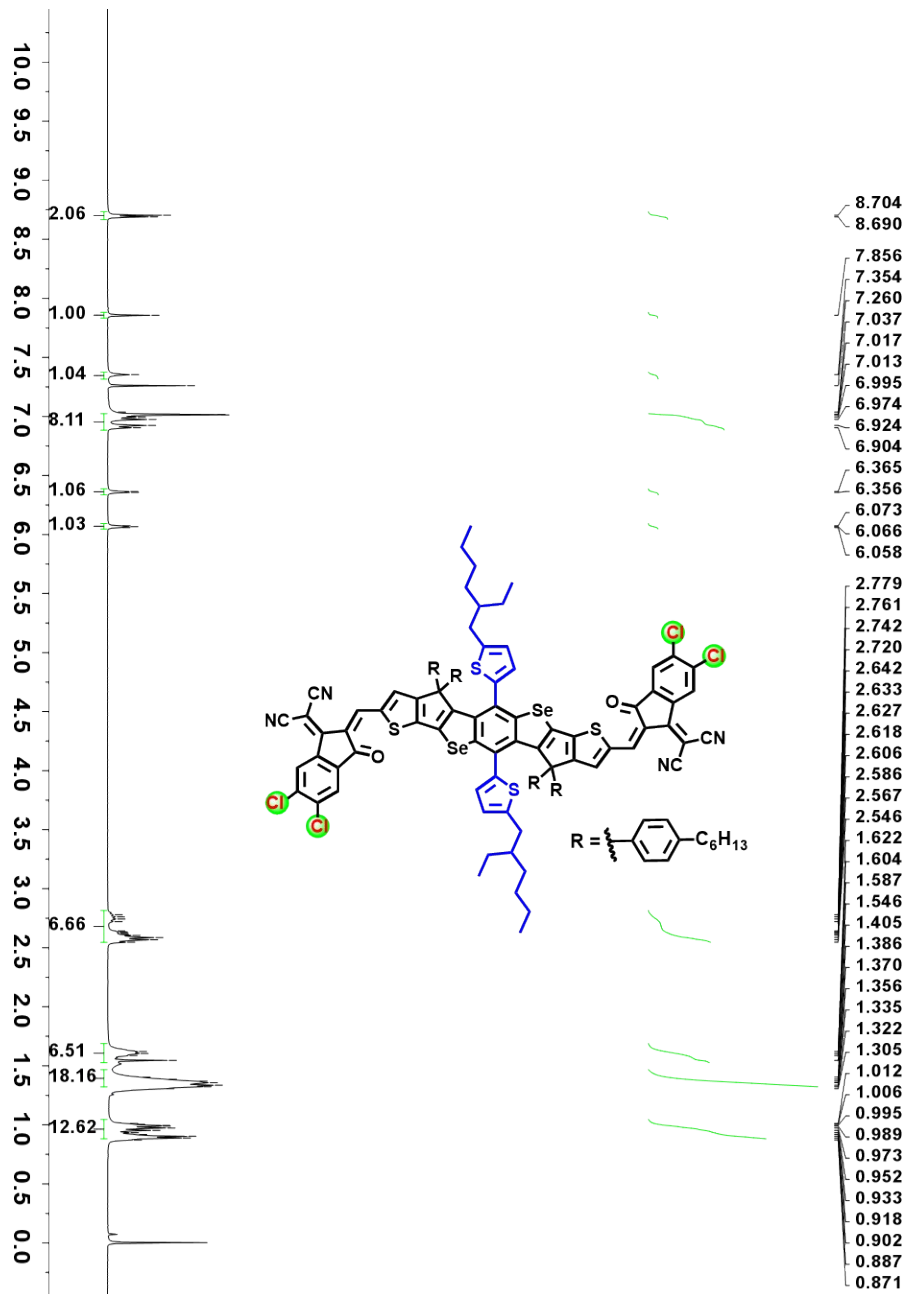
^{13}C NMR spectrum for 6



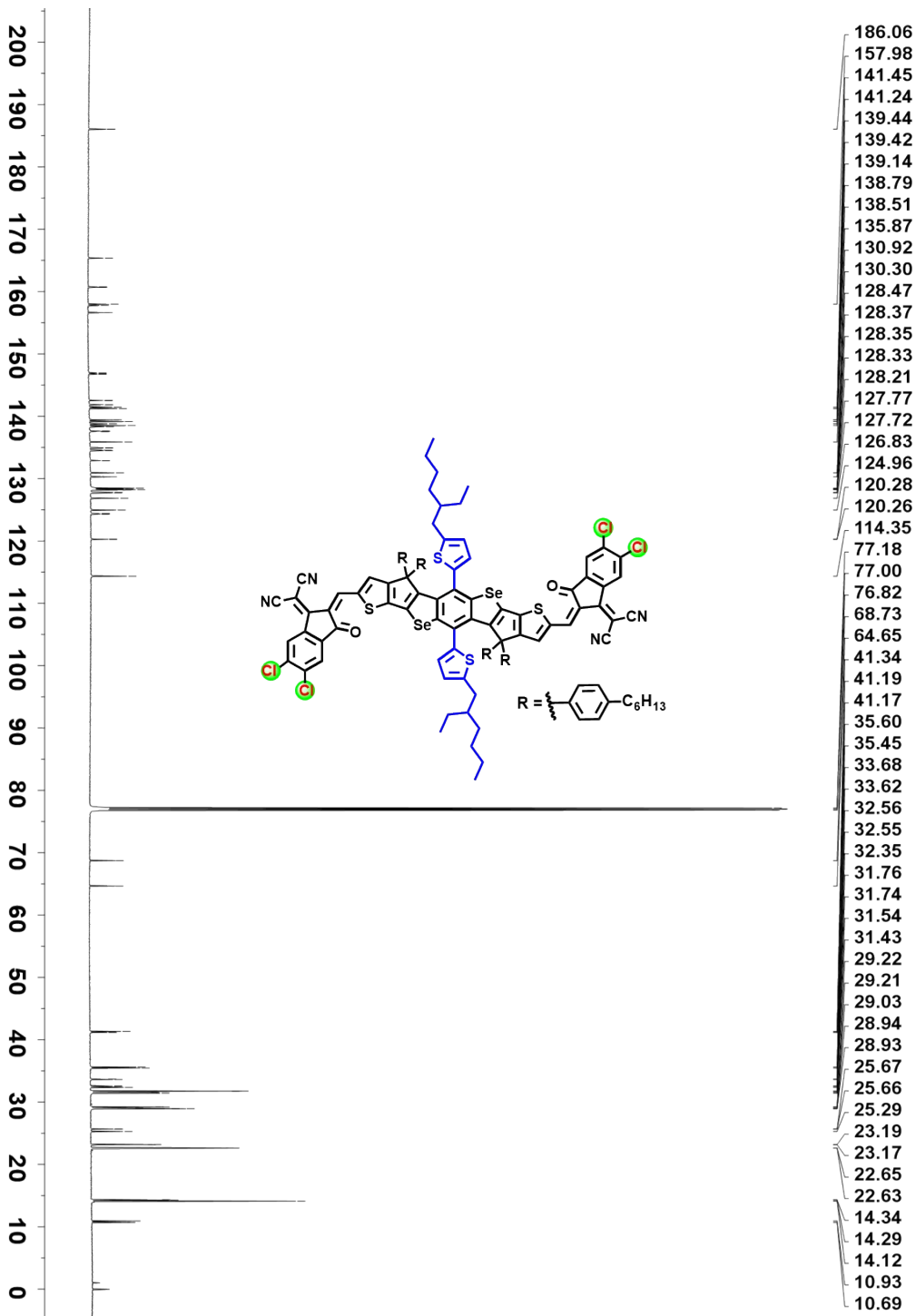
^1H NMR spectrum for 7



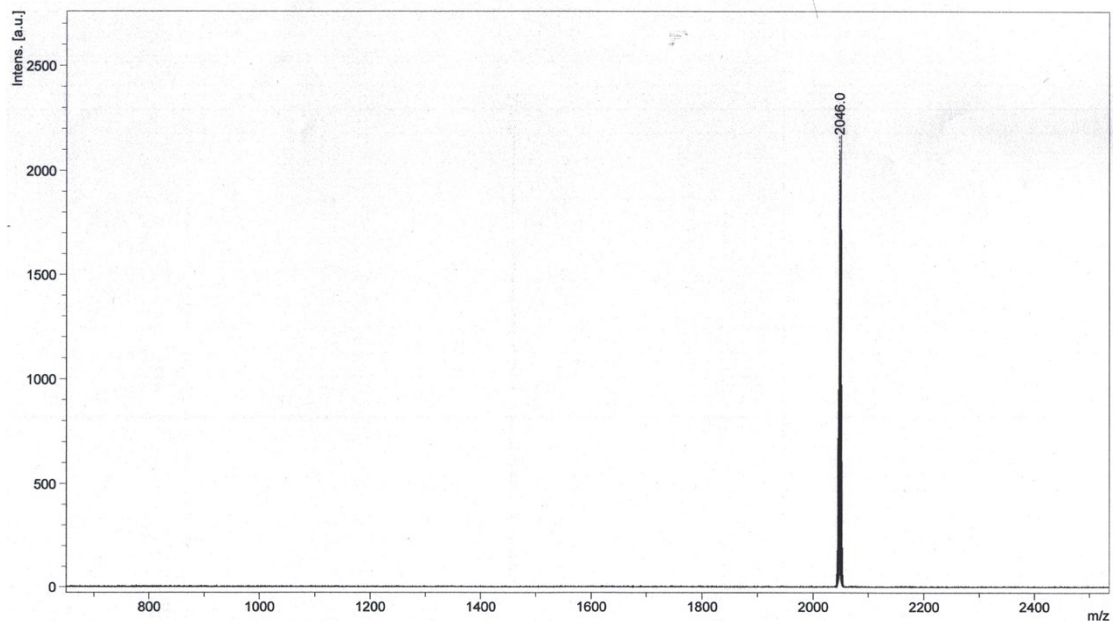
^{13}C NMR spectrum for 7



¹H NMR spectrum for C8T-BDS4Cl



¹³C NMR spectrum for C8T-BDSe4Cl



MALDI-TOF mass spectrum of **C8T-BDSe4Cl**