

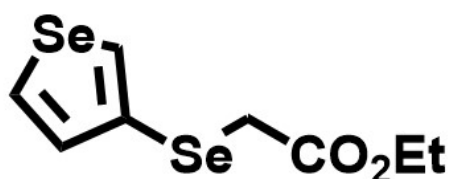
Extending Se Substitution to the Limit: from 5S to 5Se in High-Efficiency Non-Fullerene Acceptors

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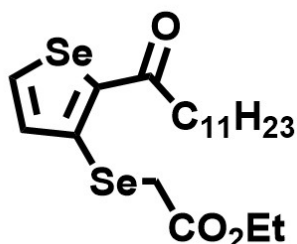
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Materials and synthesis. All the starting materials were purchased from commercial suppliers and used without further purification unless indicated otherwise. Polymeric donor **PM6** was purchased from Solarmer Material (Beijing) Inc and **5Se** acceptor was synthesized based on our previously reported methods. All reactions and manipulations were carried out under argon atmosphere with the use of standard Schlenk techniques.

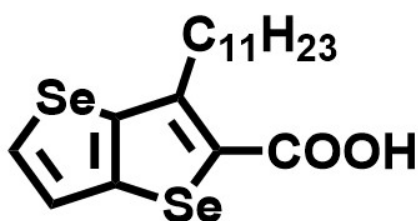


Synthesis of Compound 2 To a stirred solution of 3-bromoselenophene (2 g, 9.5 mmol) in dry diethyl ether (500 mL) was dropwise added n-BuLi (2.5 M in hexanes, 10.5 mL) at -78°C over 30 minutes. The mixture was kept at -78°C for one hour, after which selenium powder (0.83 g, 10.48 mmol) was added in small portions. The mixture was kept at -78°C for one more hour, and was slowly warmed to -40°C . As soon as the black selenium powder was fully consumed and a transparent solution with light yellow color was obtained, ethyl 2-bromoacetate (1.91g, 11.43 mmol) was added dropwise and the solution was gradually warmed to room temperature overnight. The reaction was

then quenched by addition of saturated aqueous ammonium chloride solution and extracted with diethyl ether. The combined organic layer was dried over anhydrous MgSO_4 and purified by silica gel, yielding a yellow oil (0.67 g, 24%). ^1H NMR (400 MHz, CHCl_3) δ 8.22 – 8.06 (m, 1H), 7.98 (dd, $J = 5.5, 2.5$ Hz, 1H), 7.44 – 7.36 (m, 1H), 4.12 (q, $J = 7.2$ Hz, 2H), 3.43 (s, 2H), 1.21 (t, $J = 7.2$ Hz, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 170.83, 135.60, 134.16, 132.26, 130.55, 61.33, 28.03, 13.52.

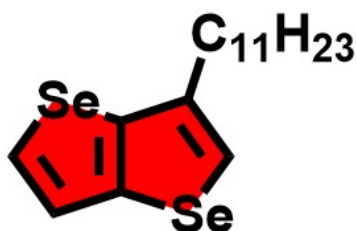


Synthesis of Compound 3 To a stirred solution of *Compound 2* (6 g, 20.26 mmol) and lauroyl chloride (5.31g, 24.32 mmol) in dry toluene (20 mL) was dropwise added a solution of tin(IV) chloride (6.5g, 25.0 mmol) in dry toluene (30 mL) at -10°C . The mixture was kept at -10°C for 30 minutes, and then stirred at room temperature overnight. The reaction was quenched by addition of 10% HCl in aqueous solution and extracted with CH_2Cl_2 . The combined extracts were washed with brine, dried over anhydrous MgSO_4 , and then filtered. The crude product was purified by silica gel, yielding a yellow oil (3.0g, 31%). ^1H NMR (400 MHz, CDCl_3) δ 7.87 (d, $J = 5.8$ Hz, 1H), 7.27 (d, $J = 5.7$ Hz, 1H), 3.79 (q, $J = 7.1$ Hz, 2H), 3.22 (s, 2H), 2.41 (t, $J = 7.4$ Hz, 2H), 1.41 – 1.32 (m, 2H), 0.95 – 0.82 (m, 19H), 0.50 (t, $J = 6.7$ Hz, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 194.57, 171.44, 137.91, 136.04, 132.77, 131.07, 61.68, 42.23, 30.87, 29.83, 29.62, 28.44, 27.55, 26.33, 26.13, 25.06, 24.71, 23.81, 14.91, 13.64.

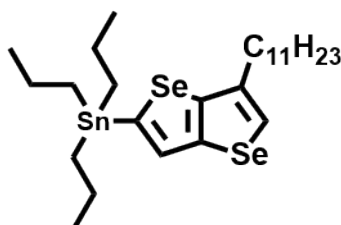


Synthesis of Compound 4 At room temperature, a solution of *Compound 3* (2.9 g, 6.61 mmol) in absolute ethanol (10 mL) was dropwise added into a solution of NaOEt, which was freshly prepared from sodium (0.46 g, 19.83 mmol) and absolute ethanol (20 mL), under an argon atmosphere to form a thick yellow slurry. The mixture was then refluxed overnight, after which the solvents were removed by rotary evaporation. The residue was dissolved in water and acidified with 10% HCl in aqueous solution, followed by extraction using ethyl acetate. The combined extracts were washed with brine, dried over anhydrous MgSO_4 , and then filtered. The solvent was removed by rotary evaporation to give the crude product as a brown solid, which was further purified by column chromatography on silica gel with CH_2Cl_2 as eluent to afford 4 as a white solid (2.4 g, 84%). ^1H NMR (400 MHz, DMSO) δ 14.26 (s, 1H), 9.65 (d, $J = 5.6$ Hz, 1H),

9.01 (d, $J = 5.6$ Hz, 1H), 4.35 (t, $J = 7.7$ Hz, 2H), 2.97 – 2.86 (m, 2H), 2.59 – 2.49 (m, 16H), 2.13 (t, $J = 6.7$ Hz, 3H). ^{13}C NMR (101 MHz, DMSO) δ 164.85, 146.64, 143.77, 141.50, 135.25, 131.09, 126.49, 31.32, 30.96, 29.03, 28.96, 28.92, 28.74, 22.13, 13.98.

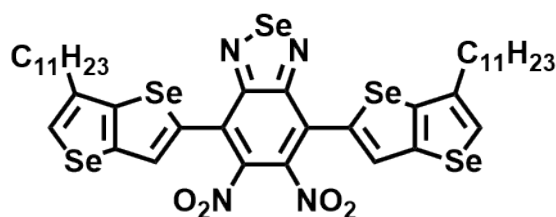


Synthesis of Compound 5 A mixture of *Compound 4* (2.2 g, 5.1 mmol) and silver carbonate (150 mg, 0.41 mmol) in DMSO (15 mL) was added acetic acid (50 μL), and then heated at 120°C overnight. The reaction mixture was then cooled to room temperature and passed through a celite pad to remove the inorganic residues. The celite pad was rinsed with diethyl ether for several times, and the combined filtrates were extracted with water. The combined extracts were washed with brine, dried over anhydrous MgSO_4 , and then filtered. The solvent was removed by rotary evaporation to give the crude product as a light brown oil, which was further purified by column chromatography on silica gel with hexanes as eluent to afford 4 as a colorless oil (1.2 g, 51%). ^1H NMR (400 MHz, CDCl_3) δ 7.97 (dd, $J = 5.6, 1.7$ Hz, 1H), 7.70 – 7.47 (m, 2H), 2.79 (t, $J = 7.7$ Hz, 2H), 1.85 (q, $J = 7.1$ Hz, 2H), 1.55 – 1.35 (m, 16H), 1.01 (t, $J = 6.9$ Hz, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 142.44, 139.69, 138.86, 129.52, 125.65, 123.85, 32.69, 32.09, 29.89, 29.84, 29.81, 29.75, 29.59, 29.53, 28.69, 22.86, 14.30.

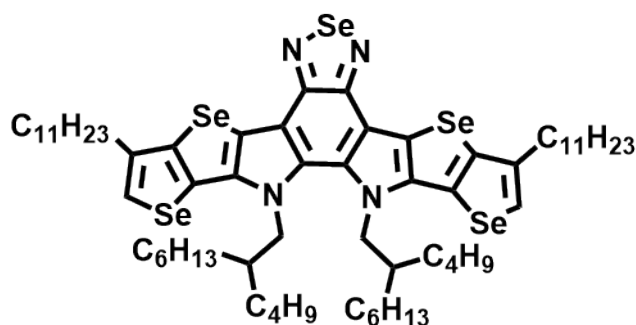


Synthesis of Compound 6 To a stirred solution of *Compound 1* (1.6 g, 4.1 mmol) in dry THF (15 mL) was added LDA (2 M in hexanes, 2.1 mL), at -40°C (dry ice/ACN) under an argon atmosphere. After stirring at -40°C for 1 hour, tributyltin chloride (4.5 mmol) was added in one portion under -40°C . The reaction mixture was slowly warmed to room temperature overnight, quenched by addition of water and extracted with hexanes. The combined extracts were washed with brine, dried over anhydrous MgSO_4 , and then filtered. The solvent was removed by rotary evaporation to give the

stannylated compound **2** as a light yellow oil, which was used without further purification.

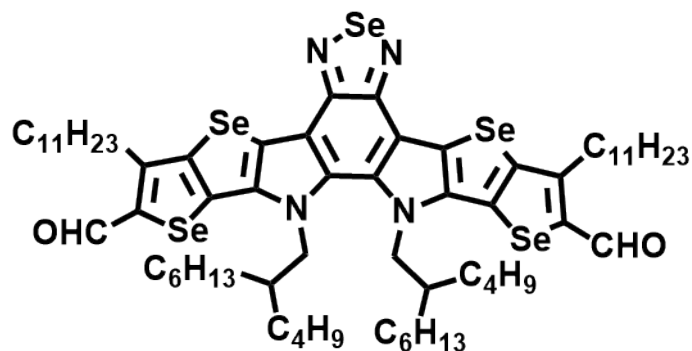


Synthesis of Compound 7b A mixture of *Compound 2b* (0.8 g, 2.26 mmol), 4,7-dibromo-5,6-dinitro[2,1,3] benzothiadiazole (0.2g, 1.03 mmol), Pd₂(dba)₃ (9 mg, 2 mol%) and tri(*o*-tolyl)phosphine (25 mg, 10 mol%) in dry toluene (5 mL) was stirred under protection of argon at room temperature for 3 days. The solvents were then removed by rotary evaporation, and the residue was subjected onto a silica gel column then eluted with hexanes/CH₂Cl₂ (v/v = 4:1) to afford *3b* as a dark red solid (0.81 g, 67%). ¹H NMR (400 MHz, CDCl₃) δ 7.84 (s, 2H), 7.70 (s, 2H), 2.74 (t, *J* = 7.7 Hz, 4H), 1.77 (q, *J* = 7.7 Hz, 4H), 1.28 (d, *J* = 7.2 Hz, 32H), 0.90 – 0.86 (m, 6H). ¹³C NMR (101 MHz, CDCl₃) δ 156.66, 149.07, 141.07, 140.07, 139.03, 133.06, 129.00, 127.76, 123.30, 32.56, 32.06, 32.03, 29.81, 29.78, 29.74, 29.54, 29.50, 28.69, 22.84, 14.28.

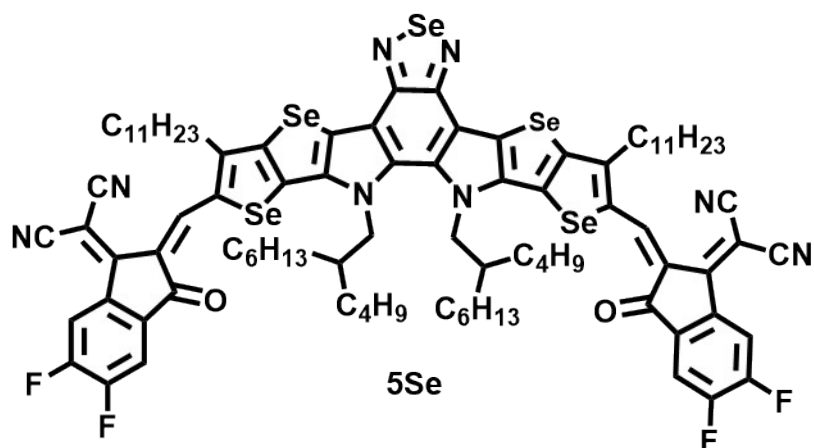


Synthesis of Compound 8b To a solution of *Compound 3b* (0.1 g, 1.01 mmol) in degassed 1,2-dichlorobenzene (4 mL) was added freshly distilled P(OEt)₃ (3.45 mL, 20.2 mmol) under protection of argon. The reaction mixture was then refluxed

overnight, cooled to room temperature and precipitated with cold methanol. The crude product was collected by filtration as a bright orange solid, which was then dissolved in anhydrous DMF (16 mL) and added 2-butyloctyl iodide (1.81 g, 6.02 mmol) and freshly ground sodium hydroxide (321 mg, 8 mmol) under an argon atmosphere. The reaction mixture was then heated at 70°C for 1 day, quenched by addition of water and extracted with CH₂Cl₂. The combined extracts were washed with brine, dried over anhydrous MgSO₄, and then filtered. The solvent was removed by rotary evaporation to give the crude product as an orange oil, which was further purified by column chromatography on silica gel with hexanes/CH₂Cl₂ (v/v = 8:1) as eluent to afford *4b* as a yellowish orange solid (270 mg, 23 %). ¹H NMR (400 MHz, CDCl₃) δ 7.50 (s, 2H), 4.51 (d, *J* = 7.9 Hz, 4H), 2.77 (t, *J* = 7.7 Hz, 4H), 2.15 – 2.04 (m, 2H), 1.82 (q, *J* = 7.8 Hz, 4H), 1.26 m, 38H), 0.88 (m, 32H), 0.67 – 0.58 (m, 12H). ¹³C NMR (101 MHz, CDCl₃) δ 161.42, 154.24, 142.09, 141.06, 140.67, 131.68, 123.88, 123.59, 121.10, 120.72, 115.92, 66.74, 54.91, 38.91, 37.36, 37.25, 34.55, 32.08, 32.00, 31.94, 31.77, 31.62, 31.27, 30.95, 30.53, 30.31, 30.25, 29.85, 29.81, 29.73, 29.64, 29.57, 29.52, 29.05, 29.00, 28.11, 26.77, 25.19, 23.09, 22.95, 22.91, 22.84, 22.78, 22.61, 14.24, 14.20, 14.15, 14.10, 13.91, 13.87.



Synthesis of Compound 9b. POCl₃ (0.28 mL) was added drop by drop to DMF (2.5 mL) at 0°C under the protection of argon and then stirred at room temperature for 5 h to gain the Vilsmerier reagent. The Vilsmerier reagent was added into a 1,2-dichloroethane (50 mL) solution of compound 4b (0.5 g, 0.39 mmol). The above reaction mixture was stirred at 0 °C for 4 h. The mixture was quenched with CH₃COONa (aq), and then extracted with CH₂Cl₂ (50 mL×3). The combined organic layer was dried over anhydrous MgSO₄ and purified by silica gel, yielding a orange solid (0.18 g, 30%). ¹H NMR (400 MHz, CDCl₃) δ 10.02 (s, 2H), 4.55 (d, *J* = 8.0 Hz, 4H), 3.15 (t, *J* = 7.8 Hz, 4H), 2.04 (s, 2H), 1.90 (m, 4H), 1.26 (d, *J* = 5.5 Hz, 38H), 0.89 (m, 30H), 0.65 (m, 12H).



Synthesis of Compound 5Se. Under the protection of argon, Compound 9 (100 mg,

0.07 mmol) and 2-(5,6-difluoro-3-oxo-2,3-dihydro-1H-inden-1-ylidene) malononitrile (64.4 mg, 0.28 mmol) was dissolved in dry chloroform (30 mL), followed by the addition of pyridine (0.5 mL). After stirring at room temperature for 12 h, the mixture was poured into water and then extracted with CHCl₃ (30 mL×2), the organic layer was dried over anhydrous MgSO₄ for 3 h. After removal of solvent, the crude product was purified by silica gel, and then recrystallized from CHCl₃ and methanol to give *5Se* as a dark blue solid (106 mg, 87%). ¹H NMR (600 MHz, CDCl₃) δ 9.25 (s, 2H), 8.56 (q, *J* = 9.9, 6.4 Hz, 2H), 7.68 (t, *J* = 7.4 Hz, 2H), 4.68 (d, *J* = 8.1 Hz, 4H), 3.21 (m, 4H), 2.14 (m, 2H), 1.86 (m, 4H), 1.54 – 1.17 (m, 44H), 1.06 – 0.83 (m, 32H), 0.71 – 0.64 (m, 12H). ¹³C NMR (151 MHz, CDCl₃) δ 186.92, 159.14, 158.79, 153.52, 146.16, 142.69, 140.68, 137.45, 136.53, 134.34, 134.08, 133.41, 129.03, 118.94, 118.53, 115.06, 114.92, 114.69, 112.43, 112.31, 68.27, 55.61, 39.09, 32.41, 31.93, 31.71, 31.61, 30.41, 30.27, 30.14, 29.96, 29.66, 29.63, 29.52, 29.47, 29.41, 29.35, 28.00, 22.83, 22.79, 22.70, 22.49, 14.14, 14.05, 13.80, 13.77.

Measurements and Instruments. The ¹H and ¹³C nuclear magnetic resonance (NMR) spectra were taken on a Bruker AV400 Spectrometer. Matrix assisted laser desorption/ionization time-of-flight (MALDI-TOF) mass spectrometry were performed on a Bruker Autoflex III instrument. Varian 7.0T FTMS was used to achieve the HR-MS data. UV-vis spectra were obtained with a Cary 5000 Spectrophotometers. Cyclic voltammogram (CV) was performed with a LK2010 Microcomputer based Electrochemical Analyzer at a scan rate of 100 mV/s. The *J-V* characteristics were recorded using a Keithley 2400 source measure unit under AM 1.5 G (100 mW cm⁻²)

(Enli SS-F5-3A solar simulator). The light intensity was calibrated using a standard Si diode with Si filter (Newport) to bring spectral mismatch to unity. Device area is approximately 4 mm². A mask with 2.58 mm² area was used to measure the J - V characteristics. EQE were measured using an Enlitech QE-R EQE system equipped with a standard Si diode in air. EQE_{EL} measurements were performed by applying external voltage/current sources through the devices (REPS, Enlitech). The FTPS-EQE measurement was carried out on an Enlitech FTPS PECT-600 instrument. The GIWAXS data were obtained at 1W1A Diffuse X-ray Scattering Station, Beijing Synchrotron Radiation Facility (BSRF-1W1A). Samples were prepared on Si/PEDOT:PSS substrates under the same conditions as those used for device fabrication. SCLC was used to measure hole and electron mobilities, using a diode configuration of ITO/PEDOT:PSS/active layer/MoO_x/Ag for hole and glass/ZnO/active layer/PDINO/Ag for electron by taking the dark current density in the range of 0–8 V and fitting the results to a space charge limited form.

Fabrication of OPV devices. The photovoltaic devices were fabricated with a structure of indium tin oxide ITO/PEDOT:PSS/Active layer/PDINO/Ag. The ITO-coated glass substrates were cleaned by ultrasonic treatment in detergent, deionized water, acetone, and isopropyl alcohol under ultrasonication for 15 minutes each time and subsequently dried by a nitrogen flow. A thin layer of PEDOT:PSS (CLEVIOS P VP AI 4083) was spin-coated on the substrates with 4500 rpm and baked at 150 °C for 15 min in air. Then the substrates were transferred into an argon-filled glove box. The active layer was spin

coated from 15.6 mg/mL chloroform solution (D:A = 1:1.4, 0.3% Diiodomethane) at 2200 rpm for 30 s to form an active layer of around 120 nm. A thin layer of PDINO was spin-coated from 2 mg/mL methanol solution at 3000 rpm for 20 s on the top of active layer. Ag (150 nm) was successively evaporated onto the active layer through a shadow mask.

The calculation of ΔE_1 , ΔE_2 and ΔE_3 .

The detailed components of E_{loss} can be categorized into three parts based on the detailed balance theory, as shown in Equation (1):

$$E_{loss} = (E_{gap} - qV_{OC}^{SQ}) + (qV_{OC}^{SQ} - qV_{OC}^{rad}) + (qV_{OC}^{rad} - qV_{OC})$$

Where

$$V_{OC}^{SQ} = \frac{kT}{q} \ln \left(\frac{J_{SC}^{SQ}}{J_0^{SQ}} + 1 \right) \cong \frac{kT}{q} \ln \left(\frac{q \cdot \int_{E_g}^{+\infty} \phi_{AM1.5G}(E) dE}{q \cdot \int_{E_g}^{+\infty} \phi_{BB}(E) dE} \right)$$

Where $\phi_{BB}(E)$ is black body emission at room temperature.

Thus, for the unavoidable radiative recombination ΔE_1

$$\Delta E_1 = E_{gap} - qV_{OC}^{SQ}$$

$$V_{OC}^{rad} = \frac{kT}{q} \ln \left(\frac{J_{SC}}{J_0^{rad}} + 1 \right) \cong \frac{kT}{q} \ln \left(\frac{q \cdot \int_0^{+\infty} EQE(E) \phi_{AM1.5G}(E) dE}{q \cdot \int_0^{+\infty} EQE(E) \phi_{BB}(E) dE} \right)$$

Thus, for the additional radiative recombination ΔE_2

$$\Delta E_2 = qV_{OC}^{SQ} - qV_{OC}^{rad}$$

Finally, for the non-radiative recombination loss ΔE_3

$$\Delta E_3 = qV_{OC}^{rad} - qV_{OC}$$

Where V_{oc} is the open circuit voltage.

For the two devices, we chose the corresponding EQE_{EL} value (2.95×10^{-4} of 4Se, 4.43×10^{-4} of 5Se) at the injected current density value equal to the integrated current density value (25.73 mA cm^{-2} of 4Se, 24.96 mA cm^{-2} of 5Se).

ΔV_{nr} is the voltage loss by non-radiative recombination and is calculated by the following equation: $\Delta V_{nr} = (kT/q) \ln(1/EQE_{EL})$.”

Table S1. Optical properties and electronic energy levels of **4Se** and **5Se**.

| Comp. | λ_{MAX}^{Sol} | λ_{MAX}^{Film} | HOMO | LUMO | E_g^{CV} | λ_{onset} | E_g^{Opt} |
|------------|-----------------------|------------------------|-------|-------|-------------------|-------------------|-------------------|
| | [nm] | [nm] | [eV] | [eV] | [eV] ^a | [nm] | [eV] ^b |
| 4Se | 767 | 852 | -5.63 | -3.86 | 1.94 | 945 | 1.31 |
| 5Se | 778 | 865 | -5.59 | -3.86 | 1.83 | 962 | 1.29 |

^aThe energy gap derived from CVs. ^b The optical bandgap estimated from the absorption onset.

Table S2. Summary of the GIWAXS parameters for **PM6:4Se** and **PM6:5Se** films.

| | blend | out-of-plane | | | |
|----------------|----------------|-------------------------|--------------------|----------------------------|----------------------|
| | | q (\AA^{-1}) | d (\AA) | FWHM (\AA^{-1}) | CCL (\AA) |
| 4Se | (010) stacking | 1.70 | 3.71 | 0.32 | 17.93 |
| 5Se | (010) stacking | 1.67 | 3.75 | 0.29 | 19.40 |
| PM6:4Se | (010) stacking | 1.72 | 3.64 | 0.24 | 23.24 |
| PM6:5Se | (010) stacking | 1.71 | 3.68 | 0.21 | 26.67 |

Table S3. Measured energy losses for **PM6:4Se** and **PM6:5Se** based devices.

| Devices | E_g | V_{OC}^{SQ} | ΔE_1 | V_{OC}^{rad} | ΔE_2 | ΔE_3 | qV_{oc} | $\Delta E_3^{(b)}$ | E_{loss} |
|----------------|-------|---------------|--------------|----------------|--------------|-------------------|-----------|--------------------|------------|
| | [eV] | [V] | [eV] | [V] | [eV] | [eV] ^a | [eV] | [eV] | [V] |
| PM6:4Se | 1.312 | 1.056 | 0.256 | 0.989 | 0.067 | 0.167 | 0.822 | 0.214 | 0.490 |
| PM6:5Se | 1.289 | 1.035 | 0.254 | 0.962 | 0.073 | 0.152 | 0.812 | 0.198 | 0.477 |

^a The derived non-radiative energy loss from EQE_{EL} .

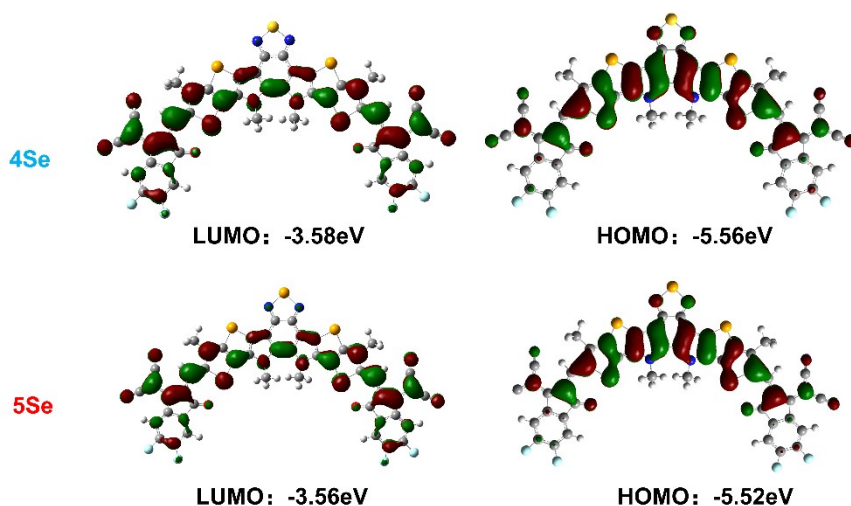


Figure.S1 Theoretical electron distribution calculated by the DFT for 4Se and 5Se.

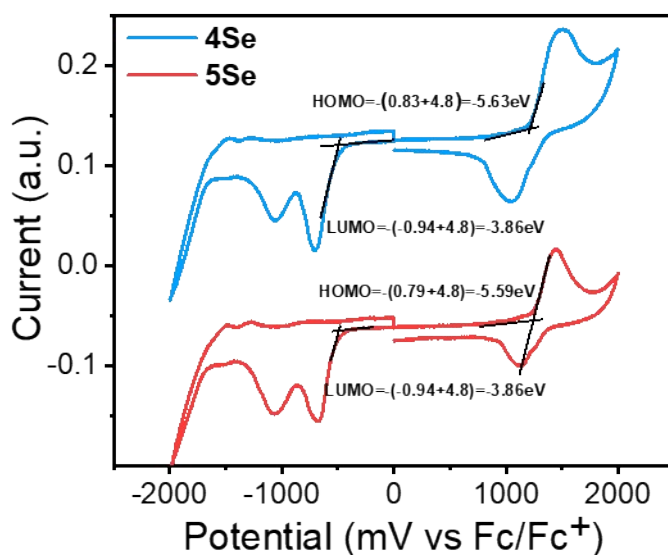


Figure. S2 Cyclic voltammogram of 4Se and 5Se film in acetonitrile solution with 0.1 mol L⁻¹ *n*-Bu₄NPF₆ at a scan rate of 100 mV s⁻¹. The HOMO/LUMO energy levels were calculated from the onset oxidation potential and the onset reduction potential vs FC/FC⁺, using the equation $E_{\text{HOMO}} = -(4.80 + E_{\text{onset vs FC/FC}^{\text{ox}}})$, $E_{\text{LUMO}} = -(4.80 + E_{\text{onset vs FC/FC}^{\text{re}}})$.

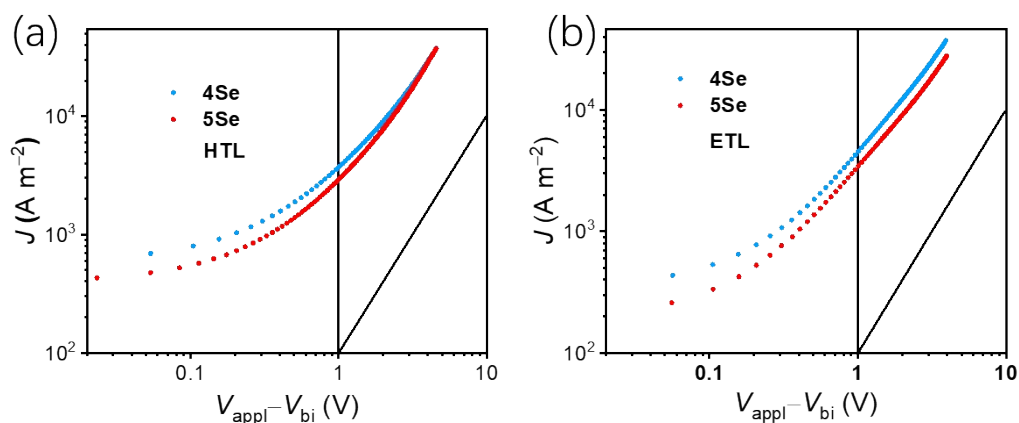


Figure. S3 The (a) hole (μ_h) and (b) electron (μ_e) mobilities of **PM6:4Se** and **PM6:5Se** devices. The lines are the fitting results according to Mott-Gurney law.

Table S4: The hole (μ_h) and electron (μ_e) mobilities of **PM6:4Se** and **PM6:5Se** devices, and average values with standard deviations obtained from 10 devices.

| Active layer | μ_h | μ_e |
|--------------|-------------------|-------------------|
| PM6:4Se | 6.09 5.44±0.41 | 7.20 6.45±0.50 |
| PM6:5Se | 5.99 5.42±0.39 | 5.77 4.99±0.45 |

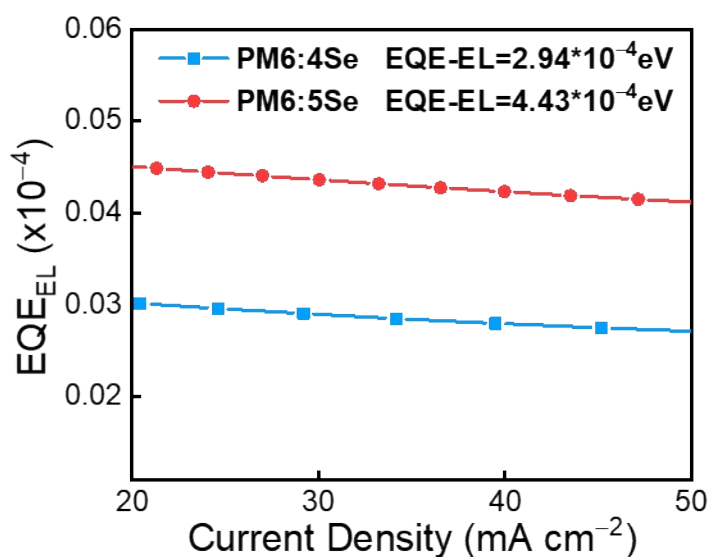


Figure. S4 EQE_{EL} of the devices based on the as-cast **PM6:4Se** and **PM6:5Se** blended films.

Table S5 Photovoltaic parameters for OSCs with low $\Delta E_3(\leq 0.16 \text{ V})$.

| Devices | V_{OC} [V] | J_{SC} [mA cm ⁻²] | FF [%] | PCE [%] | ΔE_3 [eV] | ref |
|------------------------|-----------------|------------------------------------|-----------|------------|----------------------|-----------|
| PBT1-C-2Cl:BTA3 | 1.30 | 6.42 | 46.5 | 3.9 | 0.16 | 24 |
| PBDB-T:SM16-R | 0.977 | 19.00 | 60.02 | 11.14 | 0.145 | 25 |
| PM6:SN | 0.82 | 25.14 | 68.9 | 14.3 | 0.15 | 26 |
| E18:BTA3 | 1.32 | 6.39 | 58.98 | 4.98 | 0.124 | 27 |
| PM6:BTP-C9-ICT | 1.00 | 13.62 | 56.98 | 7.76 | 0.153 | 28 |
| PM6:4Se | 0.822 | 25.96 | 71.08 | 15.17 | 0.167 | this work |
| PM6:5Se | 0.812 | 25.73 | 72.93 | 15.23 | 0.152 | this work |

NMR and MS spectra

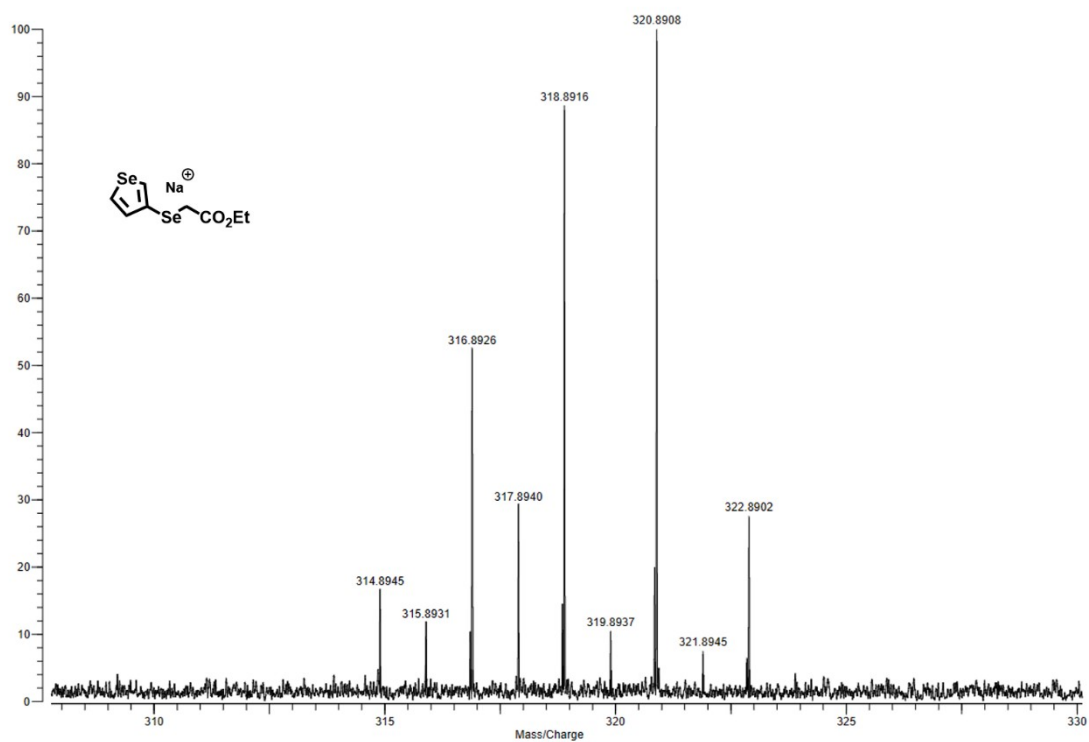


Figure S5. MS spectra of *compound 2* in CDCl₃.

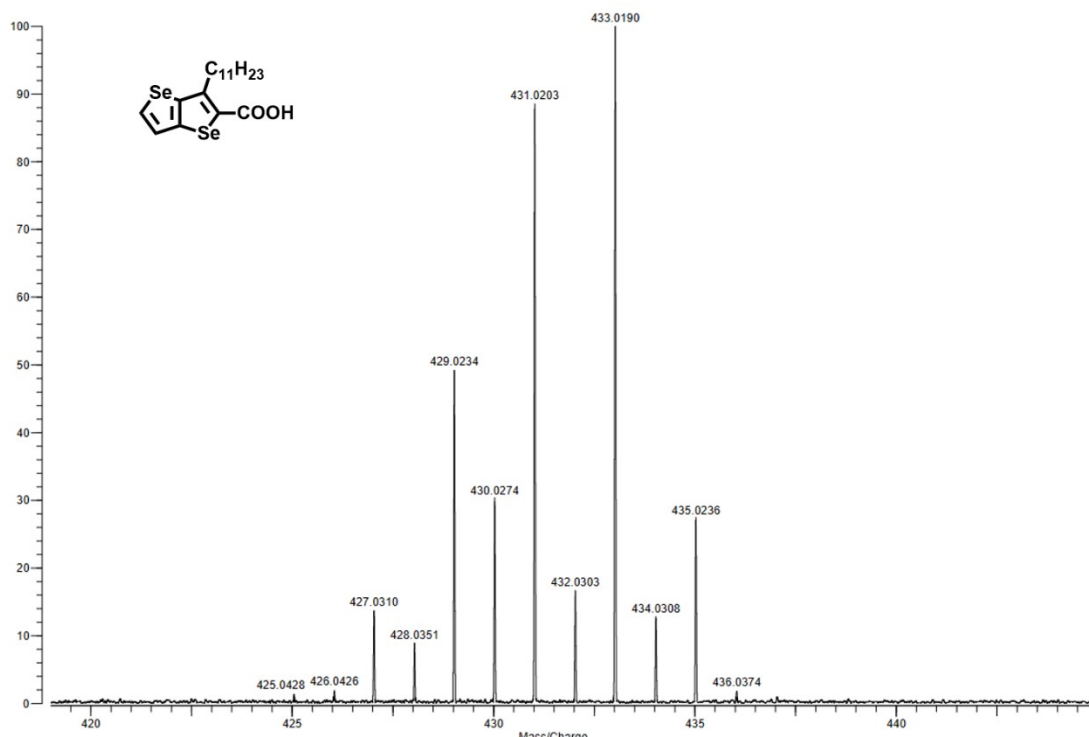


Figure S6. MS spectra of *compound 4* in CDCl₃.

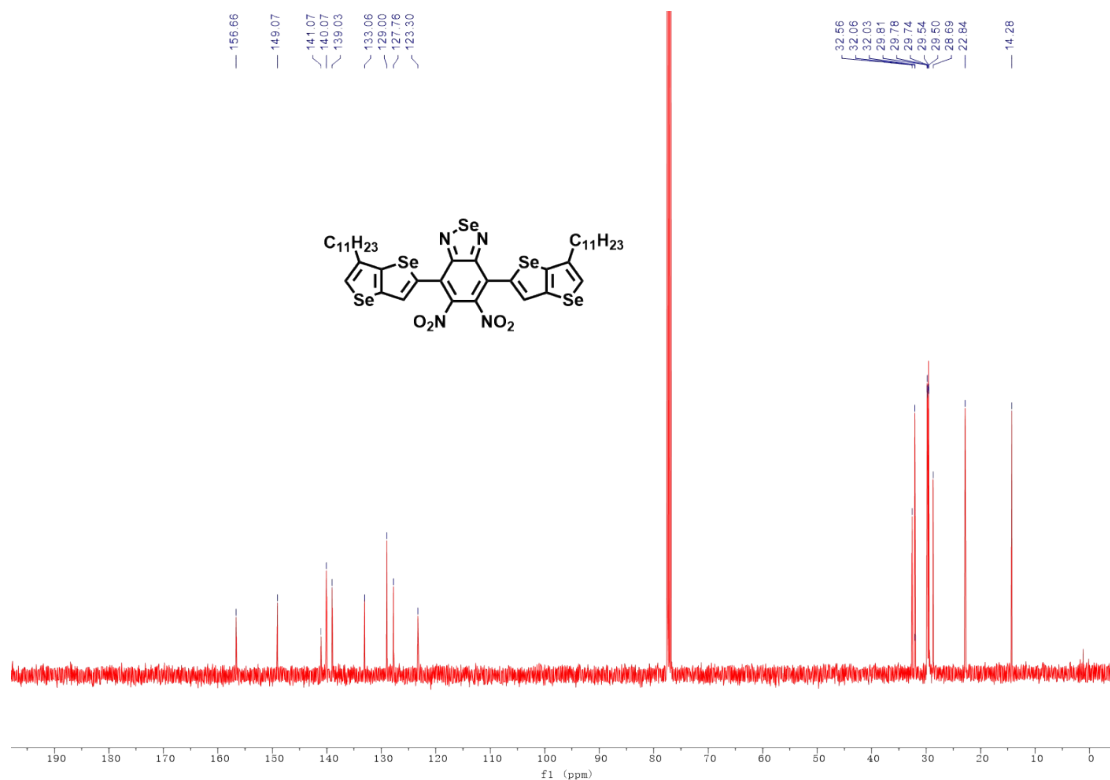


Fig. S7 ¹H NMR spectra of *compound 3b* in CDCl₃.

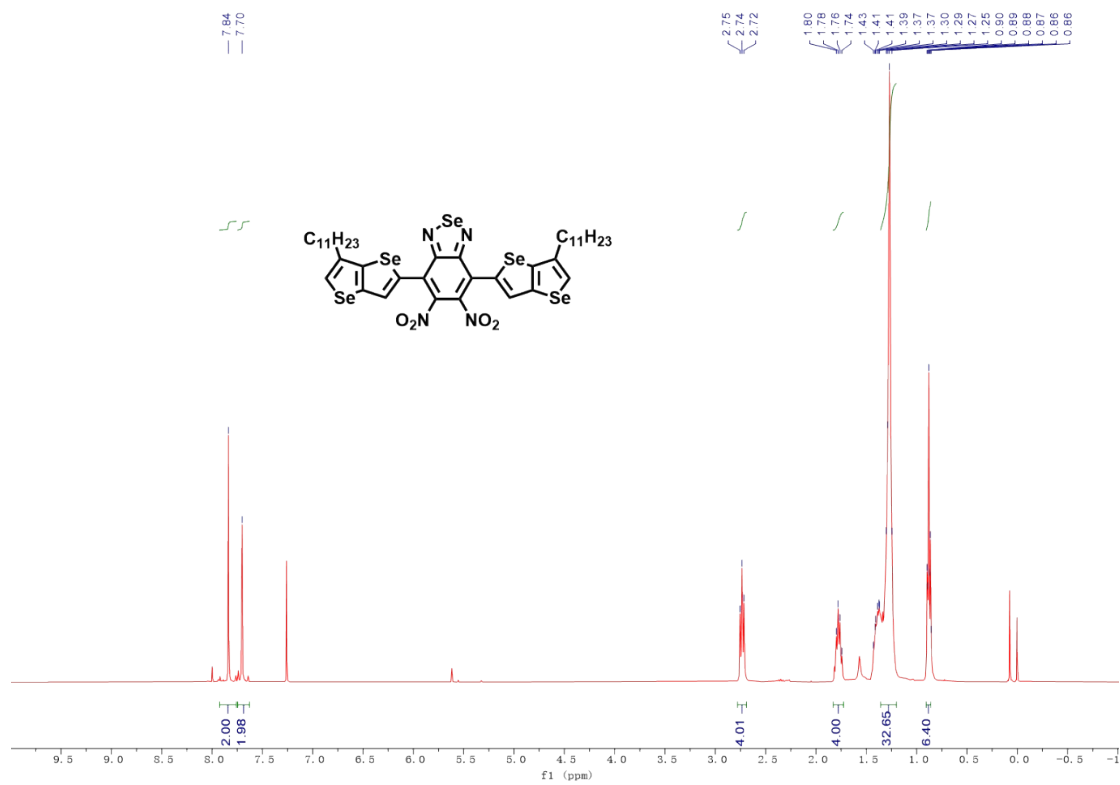


Fig. S8 ¹³C NMR spectra of *compound 3b* in CDCl₃.

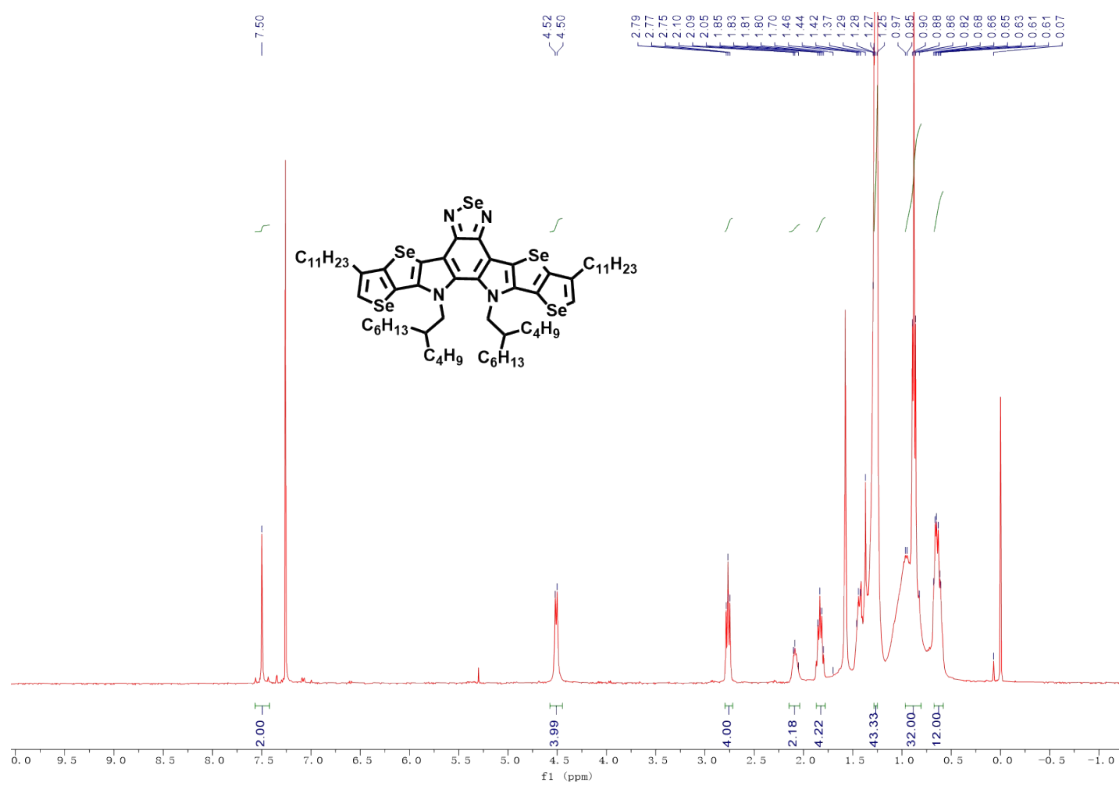


Fig. S9 ¹H NMR spectra of *compound 4b* in CDCl₃.

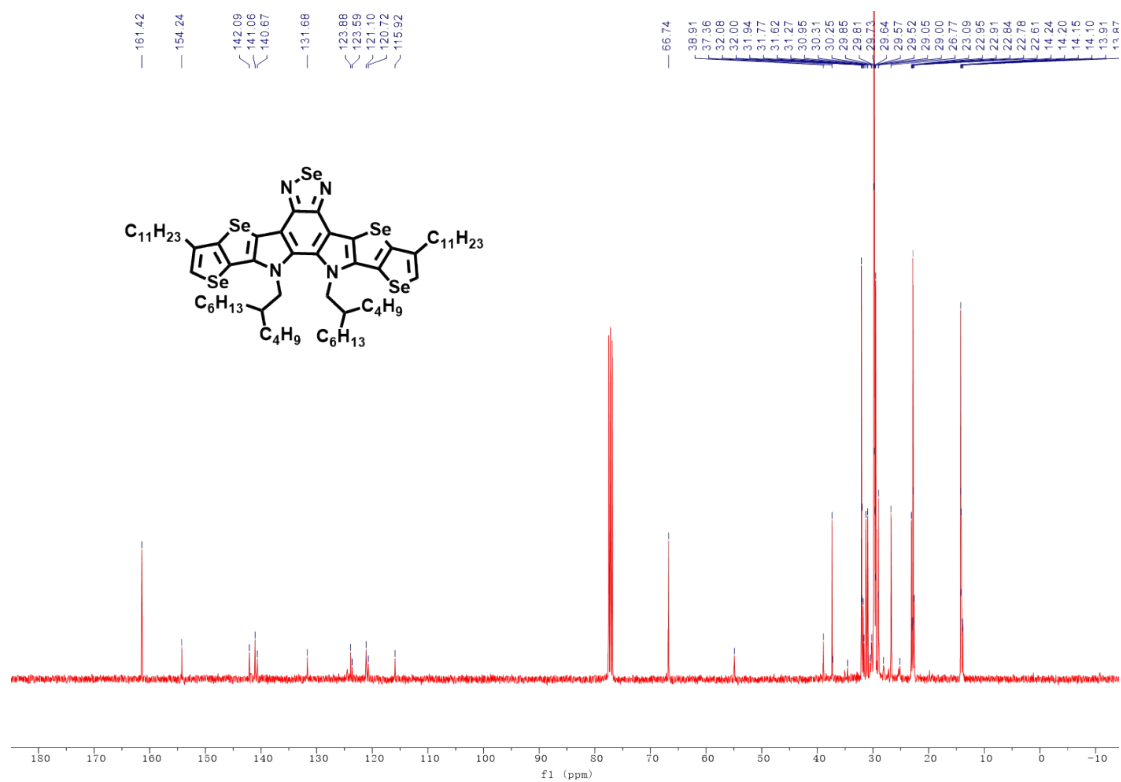


Fig. S10 ¹³C NMR spectra of *compound 4b* in CDCl₃.

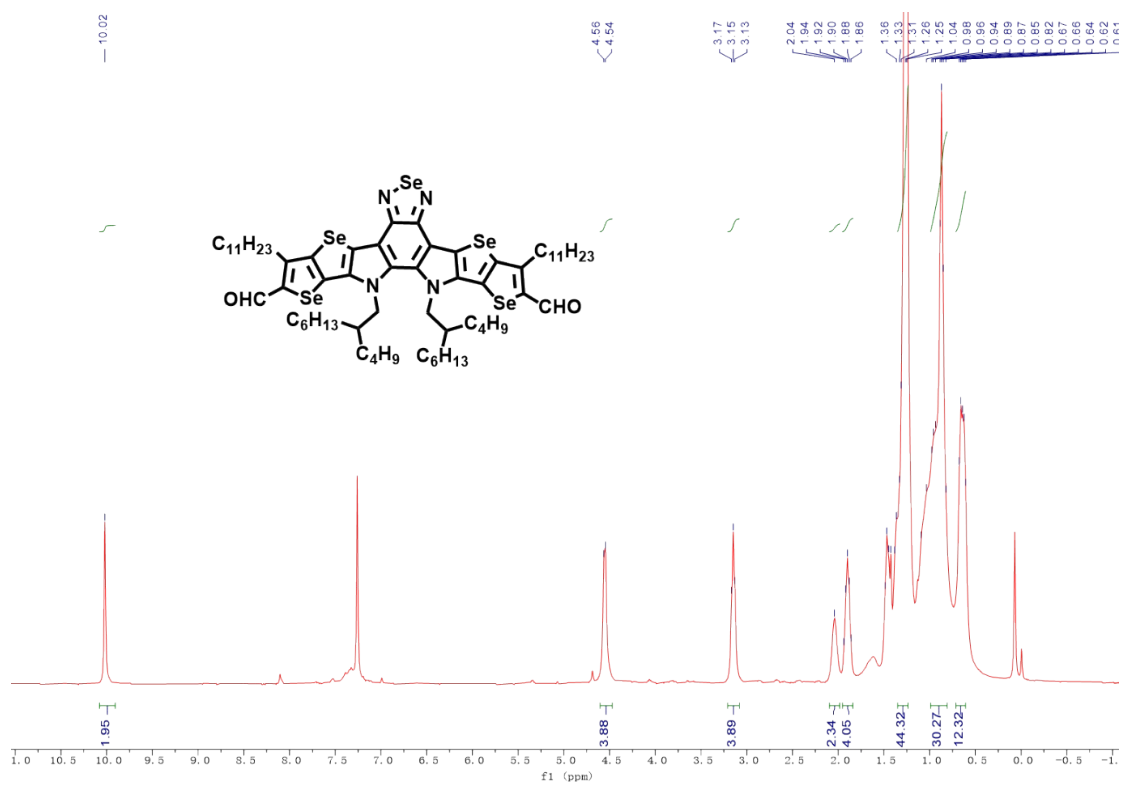


Fig. S11 ¹H NMR spectra of *compound 5b* in CDCl₃.

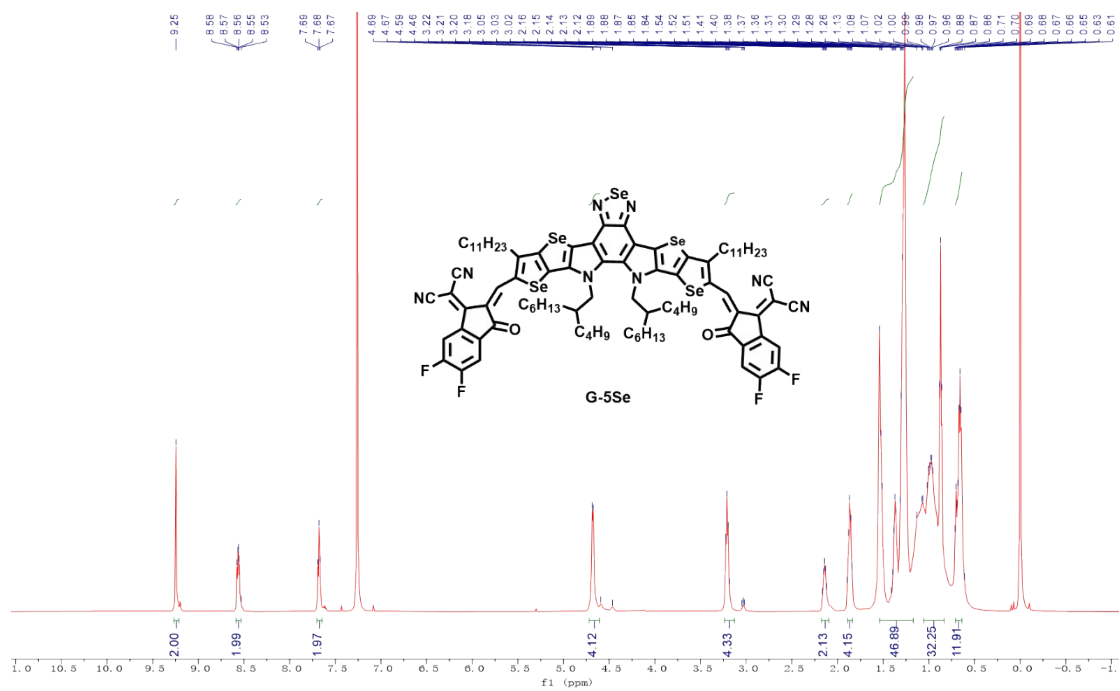


Fig. S12 ¹H NMR spectra of 5Se in CDCl₃.

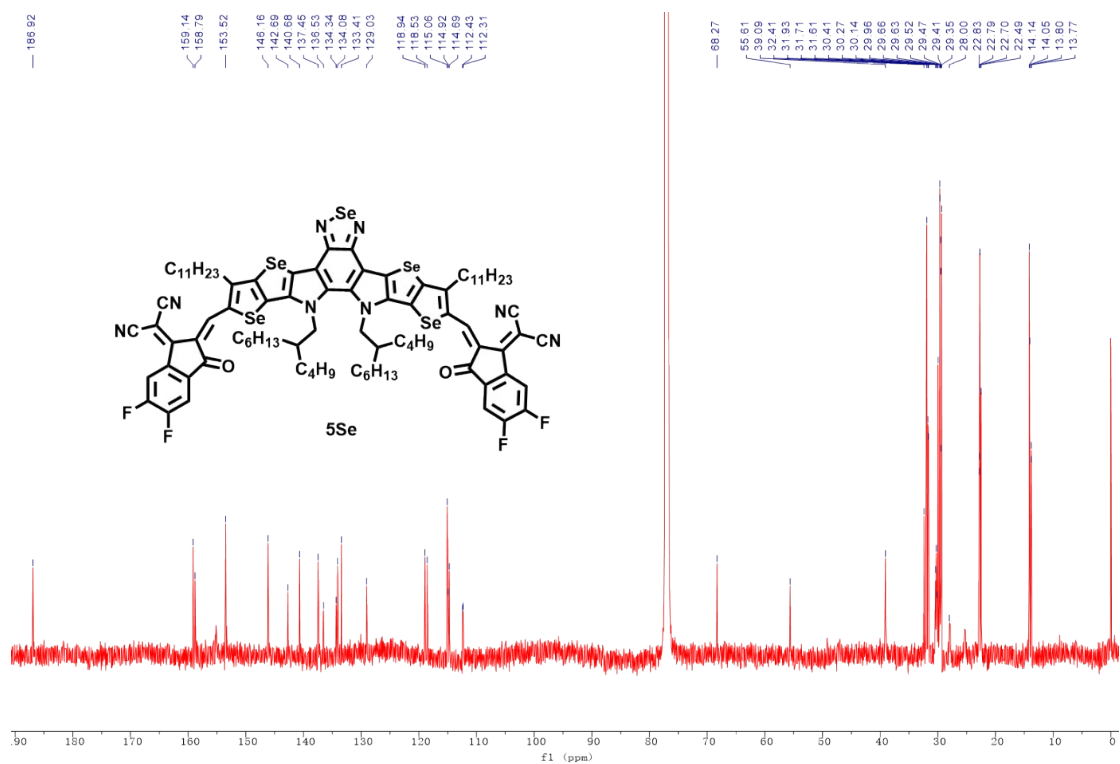


Fig. S13 ¹³C NMR spectra of 5Se in CDCl₃.

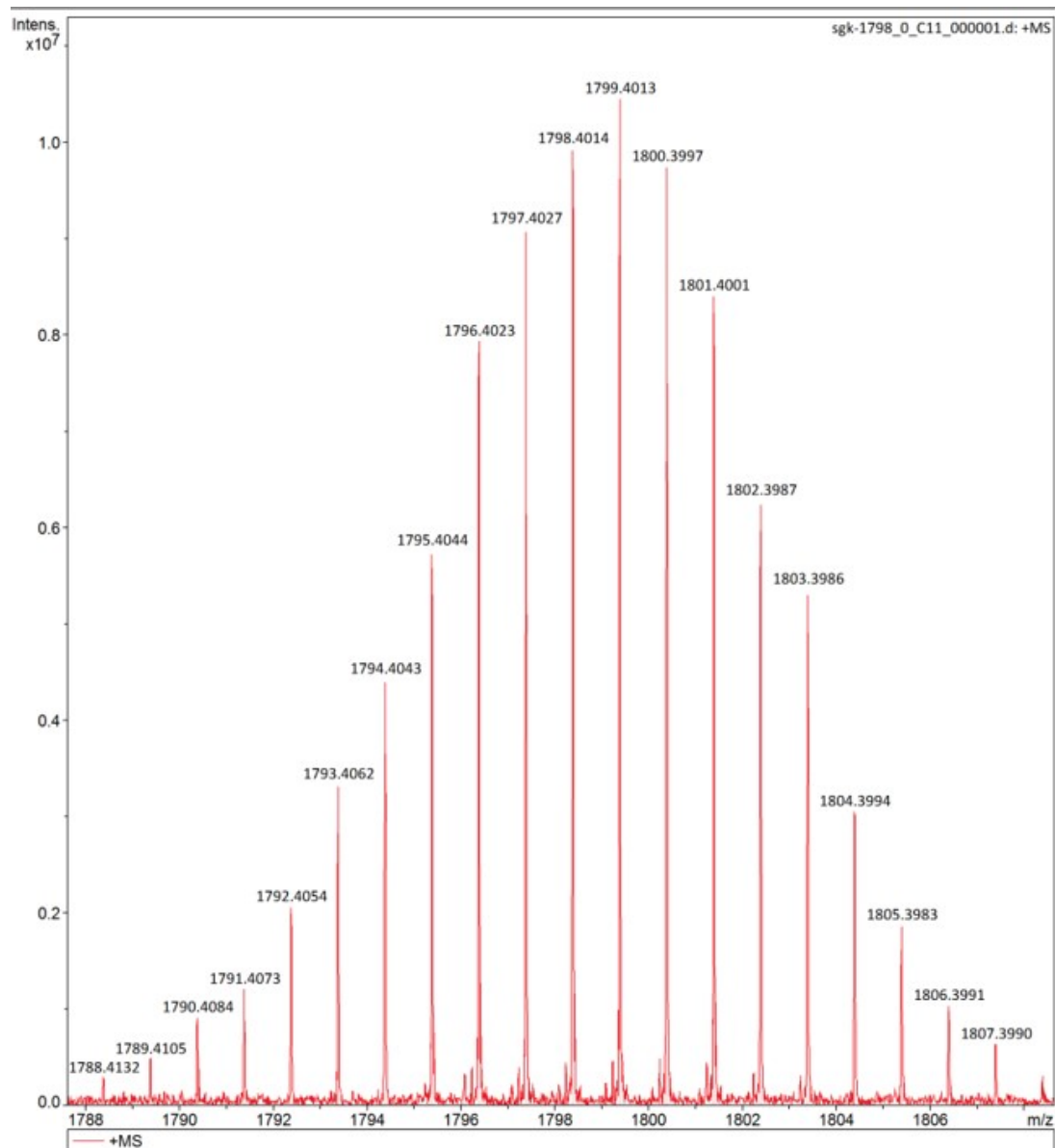


Fig. S14 HR-MS plots of compound 5Se.