Statistical copolymers of thiophene-3-carboxylates and selenophene-3-carboxylates; ^{77}Se NMR as a tool to examine copolymer sequence in selenophene-based conjugated polymers

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Supporting Information

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Materials and Methods. All reactions and manipulations of air and water sensitive compounds were carried out under a dry N_2 atmosphere using an mBraun glovebox or standard Schlenk techniques with dried and degassed solvents. All solvents and chemicals used for extraction and column chromatography were used as received. Flash chromatography was completed using a Biotage Isolera One Flash Chromatography System with 250-400 mesh silica gel (grade 60). The 2,2,6,6-tetramethylpiperidinylmagnesium chloride lithium chloride complex solution (TMPMgCl·LiCl) and 2-isopropoxy-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (*i*PrO-Bpin) were purchased from Sigma-Aldrich. All other chemicals were obtained from commercial sources and used as received. 3-bromoselenophene was prepared according to a literature procedure,[1] and this was used to prepare selenophene 3-carboxylic acid using a palladium catalyzed hydroxycarbonylation,[2] and chemical shifts were compared against a previous report.[3] The 2-bromothiophene 3-carboxylic acid were prepared according to a literature procedure.[4]

NMR Analysis. All NMR experiments were collected at 300 K on either a two-channel Bruker Avance III NMR instrument equipped with a Broad Band Inverse (BBI) probe, or a Bruker NEO 500 NMR spectrometer equipped with the multinuclear BBO Prodigy cryoprobe. Both instruments operate at 500 MHz for ^{1}H (160.5 for ^{11}B{^{1}H}, 125.7 MHz for ^{13}C{^{1}H}, and 95.36 MHz for ^{77}Se). The ^{1}H NMR spectra are referenced to residual protio solvents (7.26 ppm for $CDCl_3$ and 5.32 ppm for CD_2Cl_2) and the ^{13}C{^{1}H} NMR spectra are referenced to $CDCl_3$ (77.2 ppm). ^{11}B{^{1}H} spectra were referenced to the lock signal. In all ^{13}C{^{1}H} NMR spectra collected for the borylated monomers; no signal is observed for the carbon atom directly attached to the boron due to quadrupolar relaxation.

^{77}Se coupling was observed in ^{1}H and ^{13}C{^{1}H} NMR in some cases though it is not explicitly noted in the experimental sections. ^{1}H-^{13}C HMBC experiments were run with the hmbcetgpl3nd pulse program, optimized for long-range ^{1}H-^{13}C coupling constants (cnst13 = 8 Hz, d6=0.625s). ^{1}H-^{77}Se HSQC experiments were run with the hsqcetgp pulse program, optimized for long-range coupling (cnst2 = 10 Hz). Number average degree of polymerization (DP_n) was calculated by integration of tail-to-tail (TT) defect from catalyst initiation to main chain signal. The TT signal was set to 2 to account for both protons and DP_n was equal to the integration of the signal for the main chain plus 1 for the end group.

A minor impurity was observed in the NMR spectra for selenophene-3-carboxylic acid and 2-ethylhexyl 2-bromoselenophene-3-carboxylate (Figures S1 and S2) that was difficult to remove during purification.

Gel-Permeation Chromatography. GPC measurements were performed on a Waters Instrument equipped with a 717 plus autosampler, a Waters 2414 refractive index (RI) detector and two SDV columns (Porosity 1000 and 100000 Å; Polymer Standard Services) with THF as the eluent (flow rate 1 mL/min, 40 °C). A 10-point calibration based on polystyrene standards (Polystyrene, ReadyCal Kit, Polymer Standard Services) was applied for determination of molecular weights. For P3(2EH)ES, some early peaks were observed in the chromatograms (near 11 and 14 min) which were not included in molecular weight determination as they were attributed to aggregation (Figure S16). If the polymer samples are left to sit for a period, precipitates are observed.

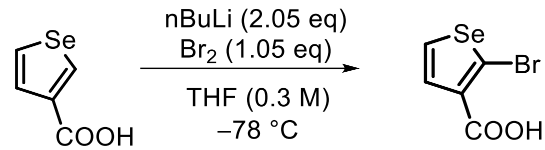
Mass Spectrometry. DART-MS measurements were performed on a Thermo Scientific Exactive Plus EMR Orbitrap Mass Spectrometer (temperature and positive/negative mode specified in sample names) with He as the carrier gas. Samples in the form of 0.2 mg/mL solutions (in ether or ethyl acetate) were introduced to the system via glass capillaries. In some cases, $[2M + H]^+$ and $[M + H_2O + H]^+$ species were also observed.

UV-Vis Spectroscopy. UV-Vis spectra of all polymers were recorded on a Varian Cary 5000 spectrophotometer. Prior to recording the spectra for all polymers, a 100% transmittance sample was taken of the cuvette (quartz, 10 mm × 10 mm). The "blank" of the solvent ($CHCl_3$) was then collected for baseline subtraction during analysis. Solution measurements were completed using $CHCl_3$ as the solvent at concentrations of ~0.0075 mg/mL. Thin film samples were prepared by drop-casting from $CHCl_3$ in the dark. Prior to sample preparation, 22 × 22 mm glass cover slips were cleaned by washing with acetone, isopropanol, and hexane. After that, the cover glass slips were dried under a stream of dry N_2. 2 mg of the polymer was dissolved in 1 mL of $CHCl_3$ by warming with a heat-gun in a glass vial, and the hot polymer solution was cast onto the glass cover slip which was placed on a petri-dish. The glass cover slips were left on the dark with the cover until evaporation. The films were annealed at 150 °C for 40 min under a N_2 environment in a glovebox prior to analysis.

Cyclic Voltammetry. Electrochemical potentials were determined using a Bio-Logic SP-150 potentiostat. 100 mV/s sweep rates were used for all samples. A 1 mm^2 glassy carbon working electrode, a platinum coil counter electrode, and a silver wire pseudo-reference electrode were employed for the measurements. For solid-state measurements, the sample was drop cast onto the working electrode from a 5 mg/mL solution in $CHCl_3$, and the electrochemical studies were completed in degassed acetonitrile [0.40 V ($E_{Fc/Fc+}$) vs. SCE for MeCN.[5]

Computational Studies. Density functional theory (DFT) calculations were performed using Gaussian 16.[6] The dimers discussed in Figure 2 are defined by the relevant heterocycle with an E suffix for the ester group (e.g. TETE corresponds to [2,2'-bithiophene]-3,4'-dicarboxylate). Torsional potential energy scans for all compounds in the main text were performed at the ωB97XD/6-31G(d,p) level, while for the triads and pentads geometries for NMR analysis were optimized at the B3LYP/cc-pVDZ level of theory following the most stable orientation of ester side chain. The shielding tensor for Se atoms for all studied triads and pentads were also computed at the B3LYP/cc-pVDZ level of theory. The cartesian coordinates for dimers, triads and pentads are available below as well as shielding tensor values for relevant structures.

Experimental section for monomers and monomer precursors

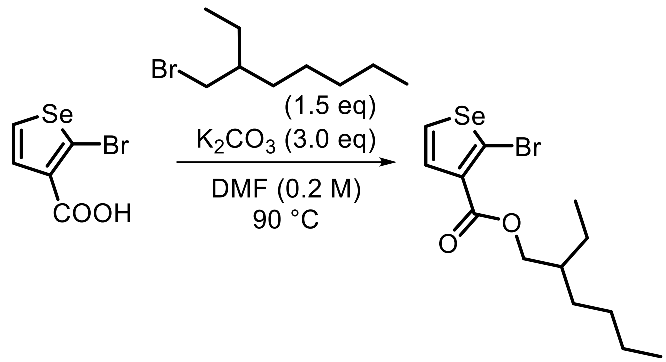


2-bromoselenophene-3-carboxylic acid. To a solution of selenophene 3-carboxylic acid (2.80 g, 16.00 mmol) in THF (53 mL) under N_2, was added *n*BuLi (2.5 M hexane solution, 13.1 mL, 32.8 mmol) at −78 °C dropwise over 15 min by syringe. The reaction mixture was stirred for 1.5 h at −78 °C and then Br_2 (0.87 mL, 17.0 mmol) was added dropwise over 5 min. After being stirred for an additional 1 h at −78 °C, the reaction mixture was quenched with 1 M aqueous HCl. The mixture was concentrated under reduced pressure, diluted with water, and extracted with Et_2O (3 × 100 mL). The combined organic extracts were washed with brine, dried over Na_2SO_4, filtered, and concentrated under reduced pressure. The crude product was purified by column chromatography on silica gel (gradient conditions from hexane:Et_2O = 3:10 to 100 % Et_2O) to afford a brown solid (3.2 g, 79%).

^{1}H-NMR (500 MHz, $CDCl_3$): δ 7.91 (d, *J* = 6.3 Hz, 1H), 7.68 (d, *J* = 6.3 Hz, 1H)

^{13}C-NMR (125 MHz, $CDCl_3$): δ167.3, 133.1, 132.0, 131.3, 127.5.

HR-EIMS (m/z): $[M-H]^-$ calculated for $C_5H_2BrO_2Se$ 252.8409.; found 252.8410.

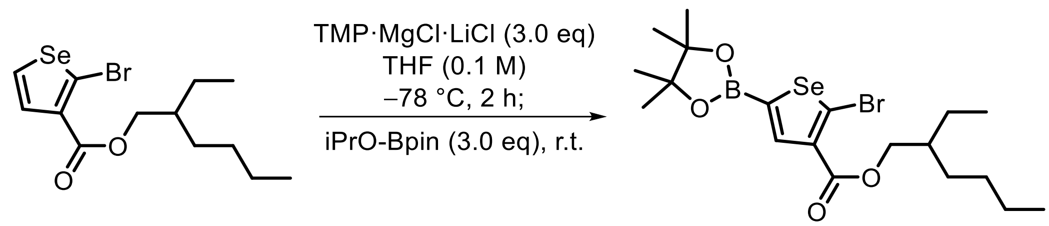


2-ethylhexyl 2-bromoselenophene-3-carboxylate. To a solution of 2-bromoselenophene-3-carboxylic acid (1.70 g, 6.69 mmol) in DMF (33 mL), was added K_2CO_3 (2.77 g, 20.0 mmol). After being heated at 90°C for 1 h, 2-ethylhexylbromide (1.80 mL, 10.1 mmol) was added, and the resultant reaction mixture was stirred at 90 °C for 30 min. Upon cooling to room temperature, the mixture was quenched with water. The contents of the reaction flask were transferred to a separatory funnel and extracted with Et_2O (3 × 100 mL). The combined organic extracts were washed with brine, dried over Na_2SO_4, filtered, and concentrated under reduced pressure. The crude product was purified by column chromatography on silica gel (gradient conditions from 100% hexane to a 7:3 mixture of hexane:CH_2Cl_2) to afford a yellow oil (1.42 g, 58%).

^{1}H-NMR (500 MHz, $CDCl_3$): δ 7.87 (d, *J* = 6.3 Hz, 1H), 7.60 (d, *J* = 6.3 Hz, 1H), 4.20 (t, *J* = 5.4 Hz, 2H), 1.73 – 1.64 (m, 1H), 1.51–1.27 (m, 8H), 0.95–0.86 (m, 6H).

^{13}C{^{1}H7-NMR (125 MHz, $CDCl_3$): δ 163.0, 134.3, 131.9, 130.9, 124.6, 67.5, 39.0, 30.7, 29.2, 24.1, 23.2, 14.2, 11.3.

HR-EIMS (m/z): $[M+H]^+$ calculated for $C_{13}H_{20}BrO_2Se$ 366.9806.; found 366.9807.



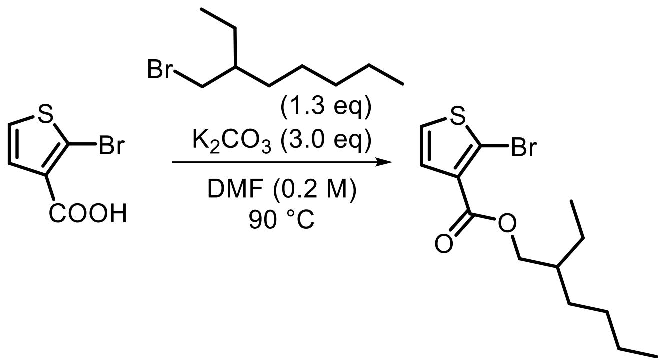
2-ethylhexyl 2-bromo-5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)selenophene-3-carboxylate. To a solution of 2-ethylhexyl 2-bromoselenophene-3-carboxylate (1.42 g, 3.88 mmol) in THF (35 mL) under N_2, TMP·MgCl·LiCl (1.0 M in THF/PhMe, 11.6 mL, 11.6 mmol) was added at −78 °C dropwise by syringe over 10 min. The reaction mixture was stirred for 2.5 h at −78 °C at which time, *i*PrO-Bpin (2.4 mL, 11.6 mmol) was added. Upon warming to room temperature and stirring for 2.5 h, the solvent was removed *in vacuo*. The residue was filtered through a plug of silica gel with a 1:4 ethyl acetate:pentane solution to elute the crude product. Fractional distillation was used to obtain the title compound in 76% yield (1.45 g). Impurities were separated from the product under full vacuum at 130 °C (oil bath temperature), and the desired product was distilled at 170 °C (oil bath temperature). The title compound was obtained as a yellow solid at room temperature.

^{1}H-NMR (500 MHz, $CDCl_3$): δ 8.13 (s, 1H), 4.20 (dd, *J* = 5.8, 2.0 Hz, 2H), 1.74 – 1.65 (m, 1H), 1.51 – 1.24 (m, 20H), 0.94–0.86 (m, 6H).

^{11}B-NMR (160 MHz, $CDCl_3$): δ 29.6.

^{13}C{^{1}H}-NMR (125 MHz, $CDCl_3$): δ 163.0, 141.3, 135.8, 131.0, 84.8, 67.6, 39.0, 30.7, 29.2, 24.9, 24.0, 23.2, 14.3, 11.2.

HR-EIMS (m/z): $[M+H]^+$ calculated for $C_{19}H_{31}BBrO_4Se$ 493.0659.; found 493.0661.

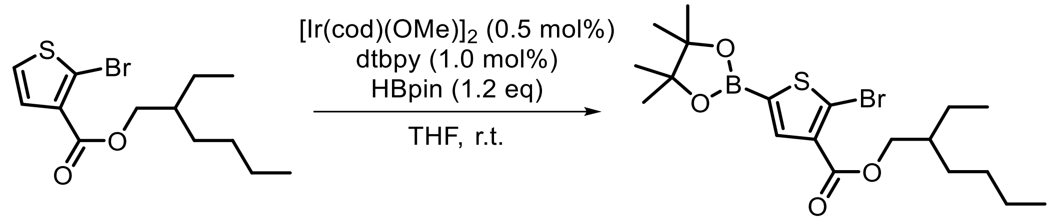


2-ethylhexyl 2-bromothiophene-3-carboxylate. To a solution of 2-bromothiophene-3-carboxylic acid (1.50 g, 7.24 mmol) in DMF (36 mL), was added K_2CO_3 (2.99 g, 21.6 mmol). After being heated at 90°C for 1 h, 2-ethylhexylbromide (1.68 mL, 9.4 mmol) was added, and the resultant reaction mixture was stirred at 90 °C for 16 h. Upon cooling to room temperature, the mixture was quenched with water. The contents of the reaction flask were transferred to a separatory funnel and extracted with Et_2O (3 × 100 mL). The combined organic extracts were washed with brine, dried over Na_2SO_4, filtered, and concentrated under reduced pressure. The crude product was purified by column chromatography on silica gel (gradient conditions from 100% hexane to a 7:3 mixture of hexane:CH_2Cl_2) to afford a colorless oil (2.26 g, 98%).

^{1}H-NMR (500 MHz, $CDCl_3$): δ 7.37 (d, *J* = 5.8 Hz, 1H), 7.22 (d, *J* = 5.8 Hz, 1H), 4.22 (t, *J* = 5.3 Hz, 2H), 1.74 – 1.65 (m, 1H), 1.50 – 1.37 (m, 4H), 1.36 – 1.26 (m, 4H), 0.95 – 0.86 (m, 6H).

^{13}C-NMR (126 MHz, $CDCl_3$): δ 162.4, 131.6, 129.7, 126.0, 119.7, 67.5, 39.0, 30.7, 29.2, 24.1, 23.2, 14.3, 11.3.

HR-EIMS (m/z): $[M+H]^+$ calculated for $C_{13}H_{20}BrO_2S$ 319.0362.; found 319.0361.



2-ethylhexyl 2-bromo-5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)thiophene-3-carboxylate. In a N_2 filled glovebox, a 20 mL scintillation vial was charged with (1,5-cyclooctadiene)(methoxy)iridium(I) dimer (11.0 mg, 0.017 mmol), 4,4'-di-tert-butyl-2,2'-dipyridyl or dtbpy (9.0 mg, 0.033 mmol), and 2 mL of THF. The reaction mixture was stirred for 30 min at room temperature, at which time pinacolborane (0.7 mL, 4.8 mmol) was added. The mixture turned dark red-brown over 30 min. Then, 2-ethylhexyl 2-bromothiophene-3-carboxylate (1.31 g, 4.1 mmol) dissolved in 2 mL of THF was added dropwise to the reaction mixture (caution: H_2 gas evolves in this step). The solution was stirred overnight in in the glovebox. The scintillation vial was removed from the glovebox and the reaction mixture was concentrated using rotary evaporation. The crude product was purified using column chromatography (gradient from 1:0 to 1:3 hexanes:CH_2Cl_2). The final product was collected as a yellow solid (1.16 g, 64%).

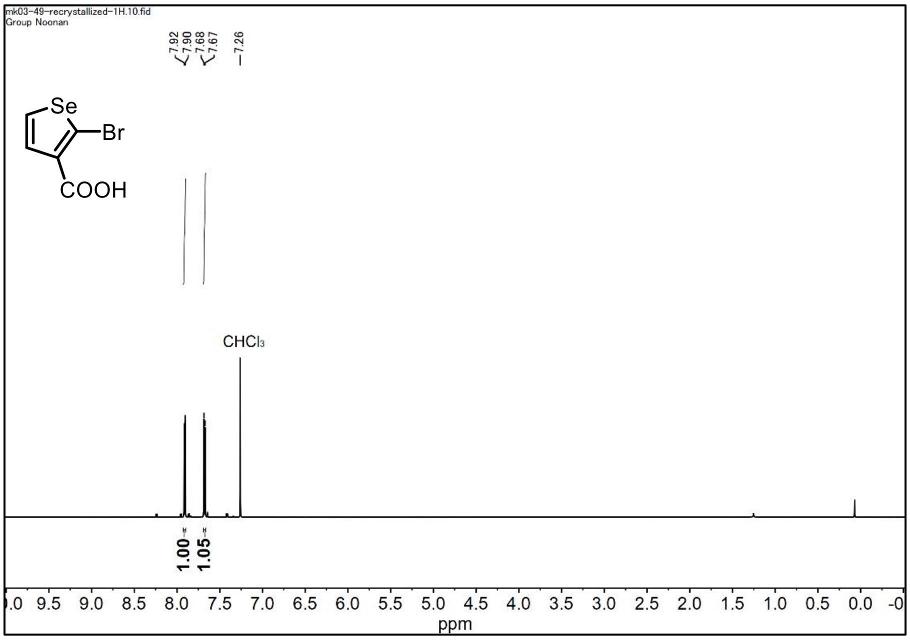
^{1}H-NMR (500 MHz, $CDCl_3$): δ 7.83 (s, 1H), 4.20 (dd, *J* = 5.7, 4.3 Hz, 2H), 1.74 – 1.65 (m, 1H), 1.49 – 1.37 (m, 4H), 1.35 – 1.28 (m, 16H), 0.95 – 0.87 (m, 6H).

^{11}B-NMR (160 MHz, $CDCl_3$): δ 28.9.

^{13}C{^{1}H}-NMR (125 MHz, $CDCl_3$): δ 162.3, 139.2, 132.7, 126.1, 84.8, 67.5, 39.0, 30.6, 29.2, 24.9, 24.0, 23.2, 14.3, 11.2.

HR-EIMS (m/z): $[M+H]^+$ calculated for $C_{19}H_{31}BBrO_4S$ 445.1214.; found 445.1214

NMR spectra for monomers and monomer precursors



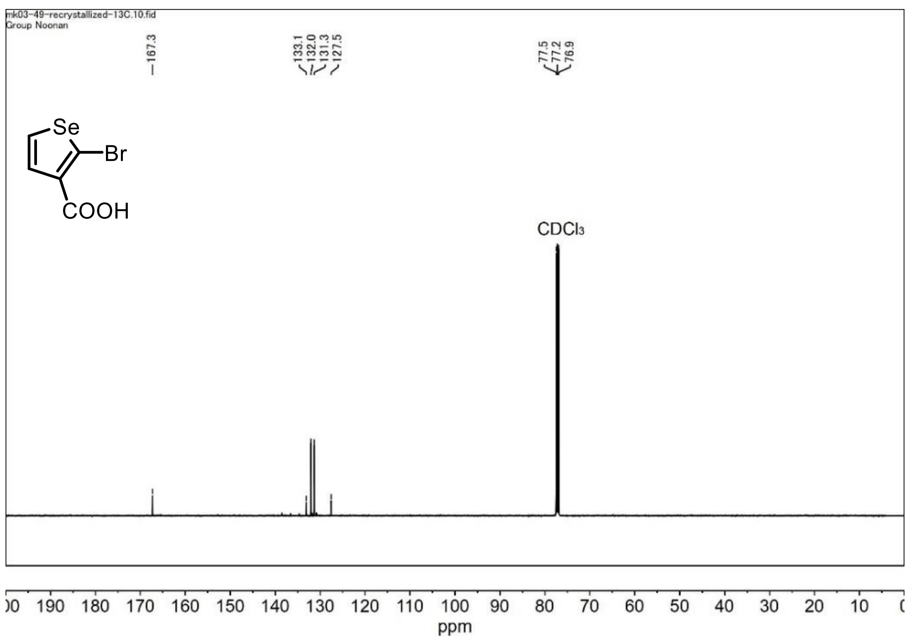
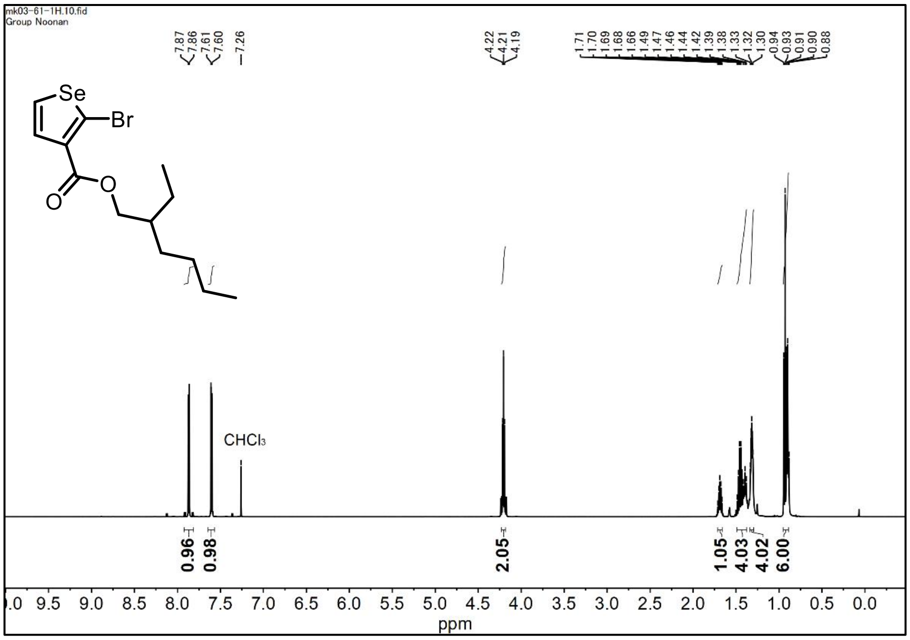


Figure S1. ^{1}H NMR spectrum (top, 500 MHz) and ^{13}C{^{1}H} NMR spectrum (bottom, 126 MHz) of 2-bromoselenophene-3-carboxylic acid collected in $CDCl_3$ (25 °C).



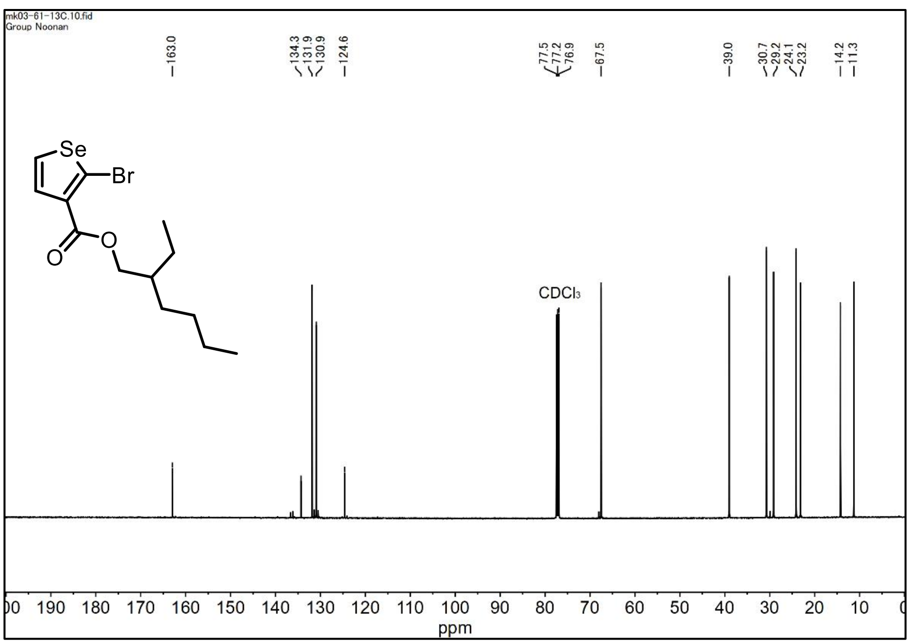


Figure S2. ^{1}H NMR spectrum (top, 500 MHz) and ^{13}C{^{1}H} NMR spectrum (bottom, 126 MHz) of 2-ethylhexyl 2-bromoselenophene-3-carboxylate collected in $CDCl_3$ (25 °C).

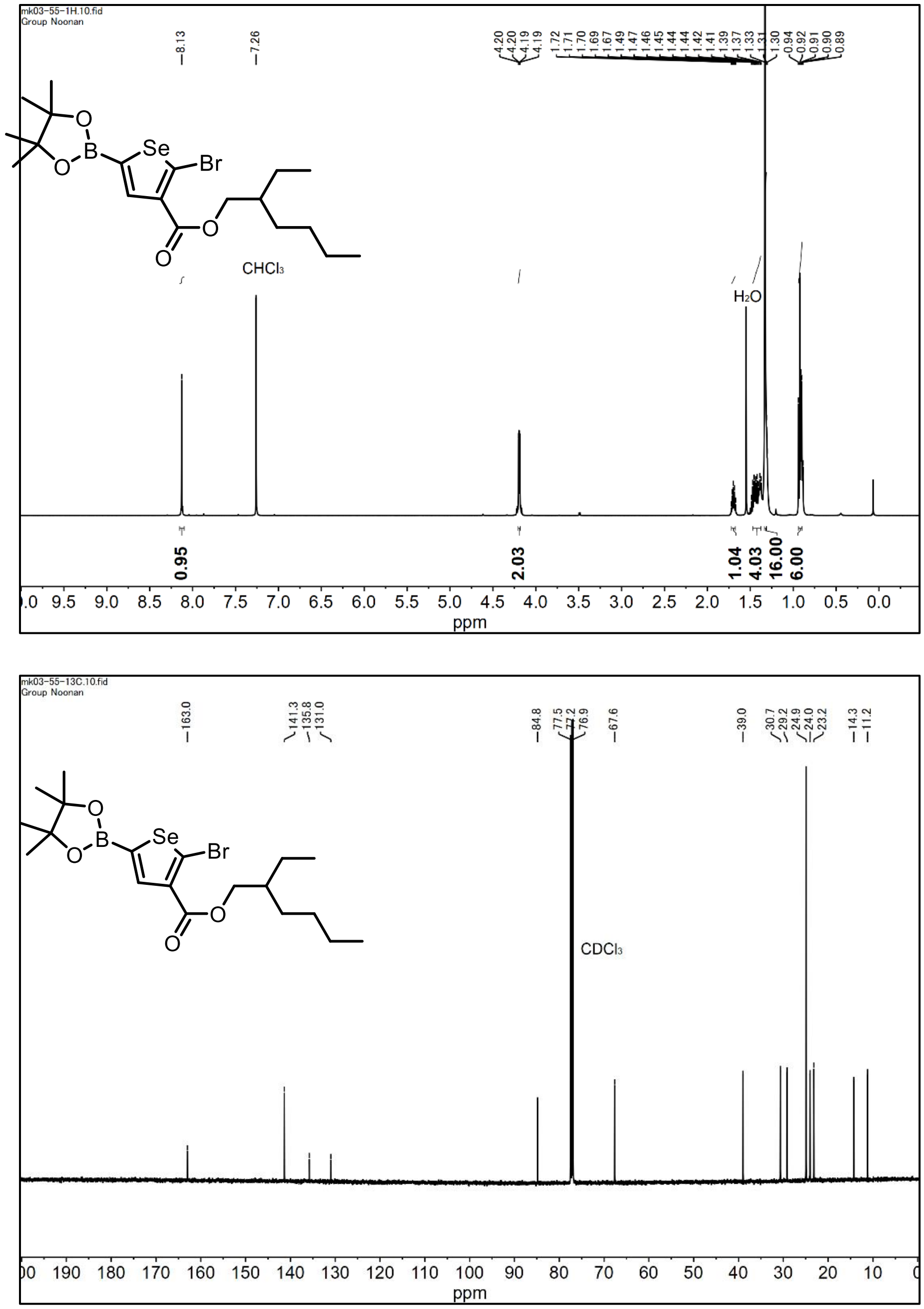


Figure S3a. ^{1}H NMR spectrum (top, 500 MHz) and $^{13}C\{^{1}H\}$ NMR spectrum (bottom, 126 MHz) of 2-ethylhexyl 2-bromo-5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)selenophene-3-carboxylate collected in $CDCl_3$ (25 °C).

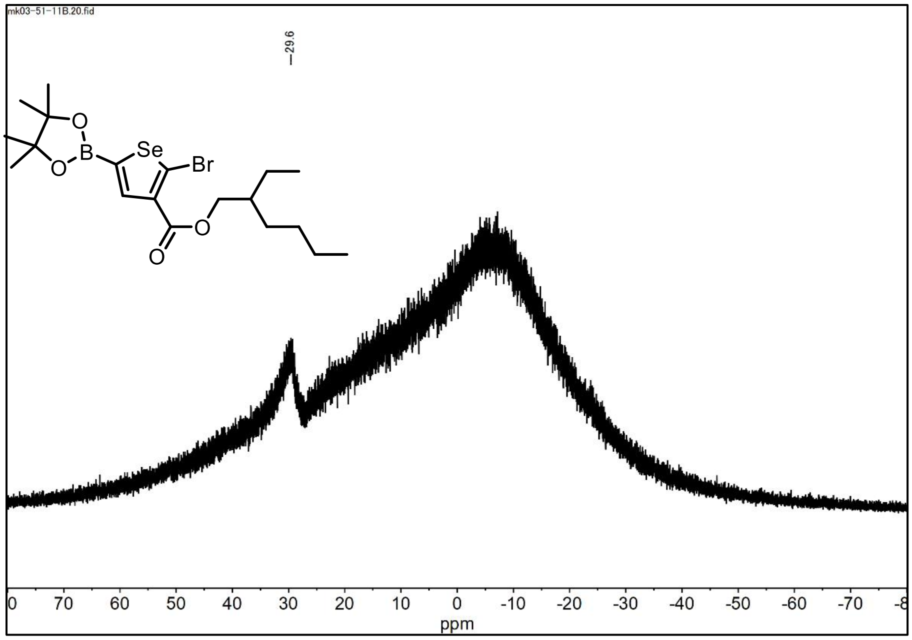
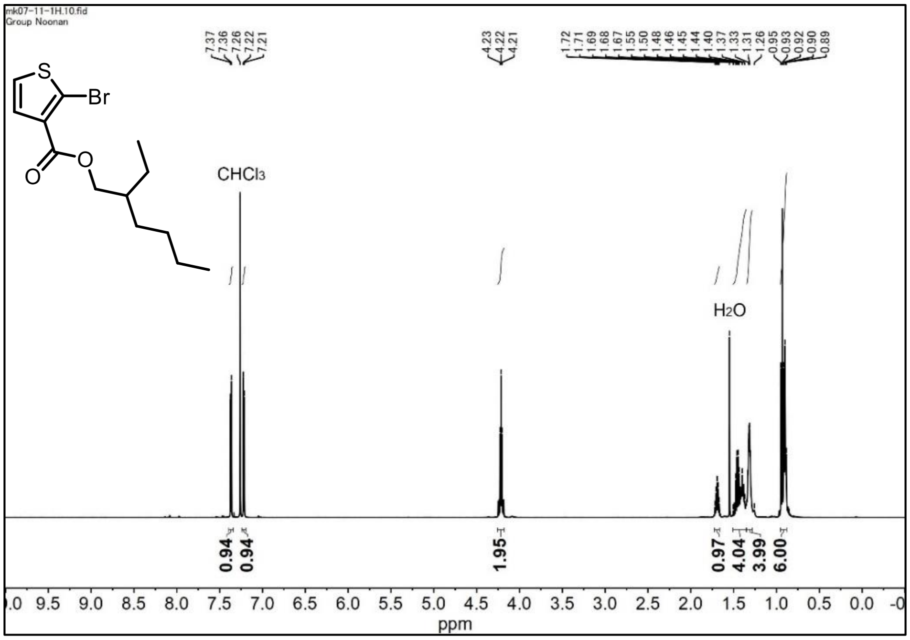


Figure S3b. $^{11}B\{^{1}H\}$ spectrum (160 MHz) of 2-ethylhexyl 2-bromo-5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)selenophene-3-carboxylate collected in $CDCl_3$ (25 °C).



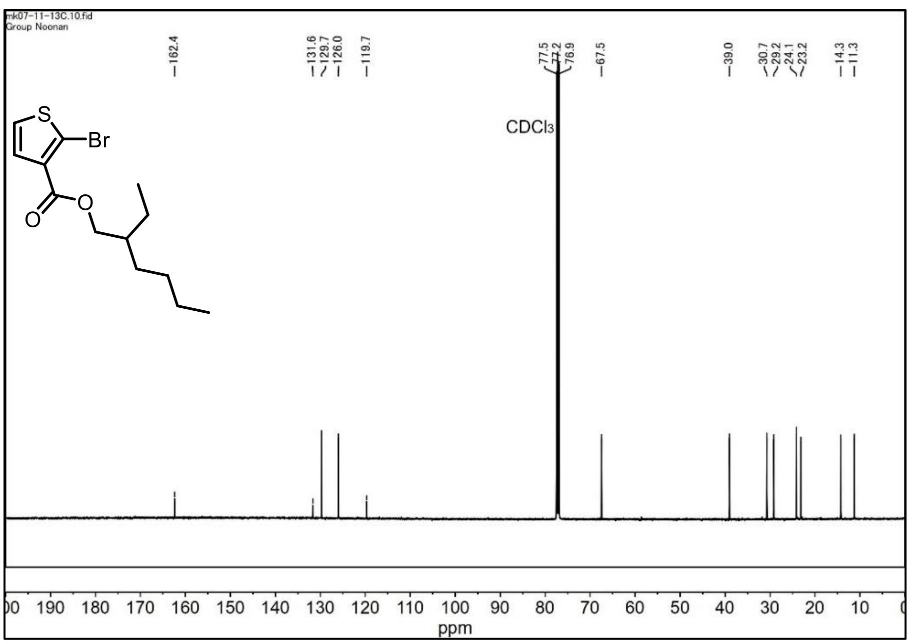
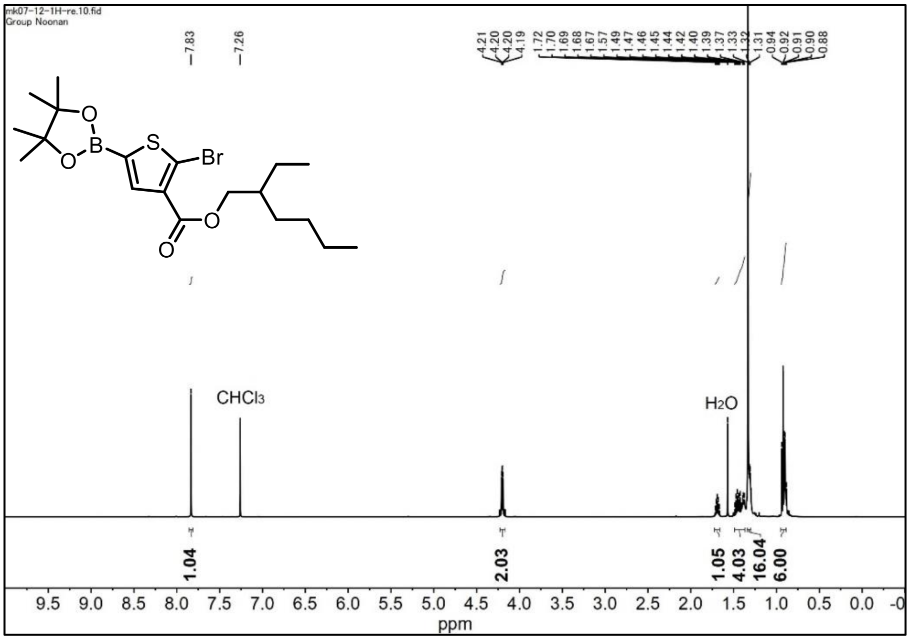


Figure S4. ^{1}H NMR spectrum (top, 500 MHz) and $^{13}C\{^{1}H\}$ NMR spectrum (bottom, 126 MHz) of 2-ethylhexyl 2-bromothiophene-3-carboxylate collected in $CDCl_3$ (25 °C).



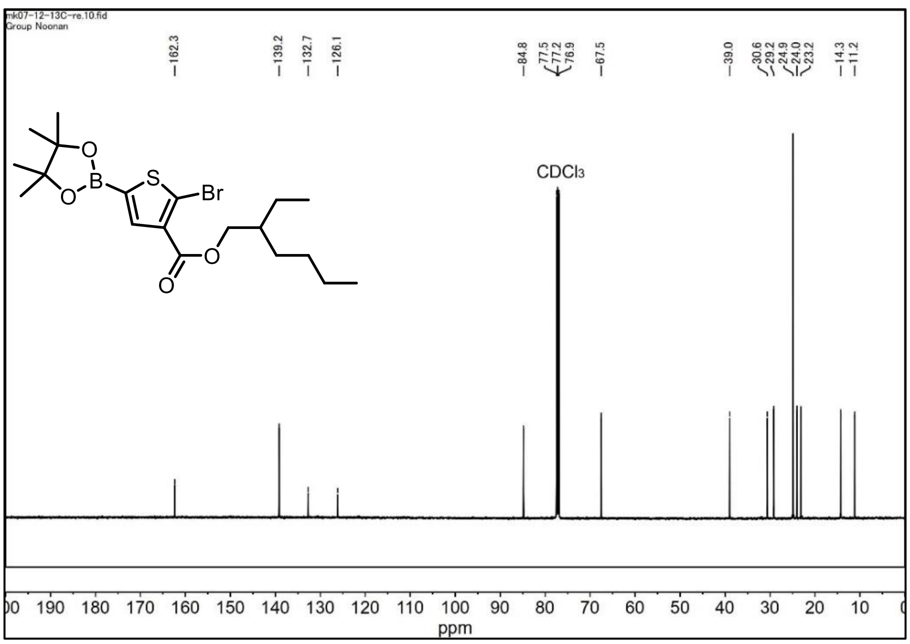


Figure S5a. ^{1}H NMR spectrum (top, 500 MHz) and $^{13}C\{^{1}H\}$ NMR spectrum (bottom, 126 MHz) of 2-ethylhexyl 2-bromo-5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)thiophene-3-carboxylate collected in $CDCl_3$ (25 °C).

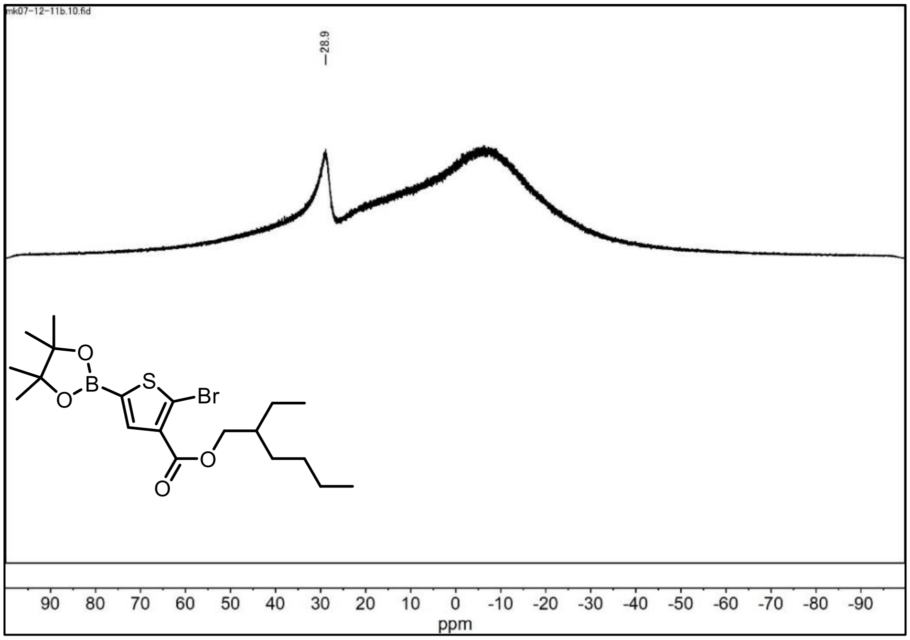


Figure S5b. $^{11}B\{^{1}H\}$ spectrum (160 MHz) of 2-ethylhexyl 2-bromo-5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)thiophene-3-carboxylate collected in $CDCl_3$ (25 °C).

HRMS for monomers and monomer precursors

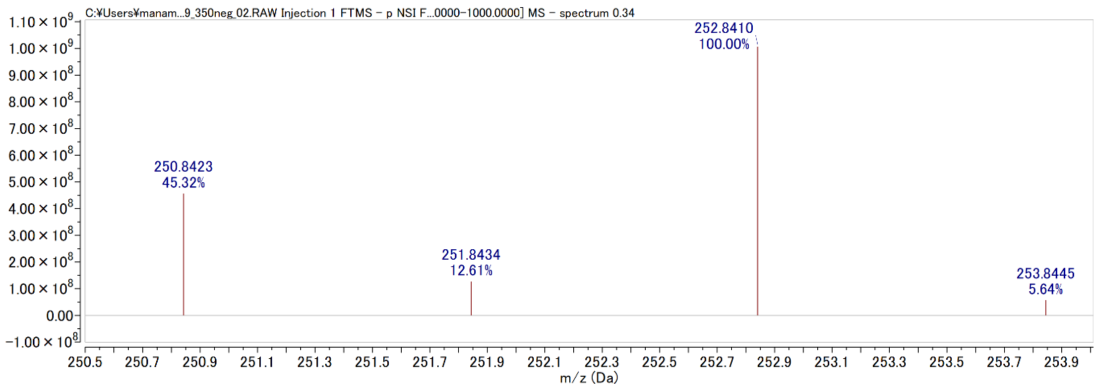


Figure S6. DART-MS of 2-bromoselenophene-3-carboxylic acid.

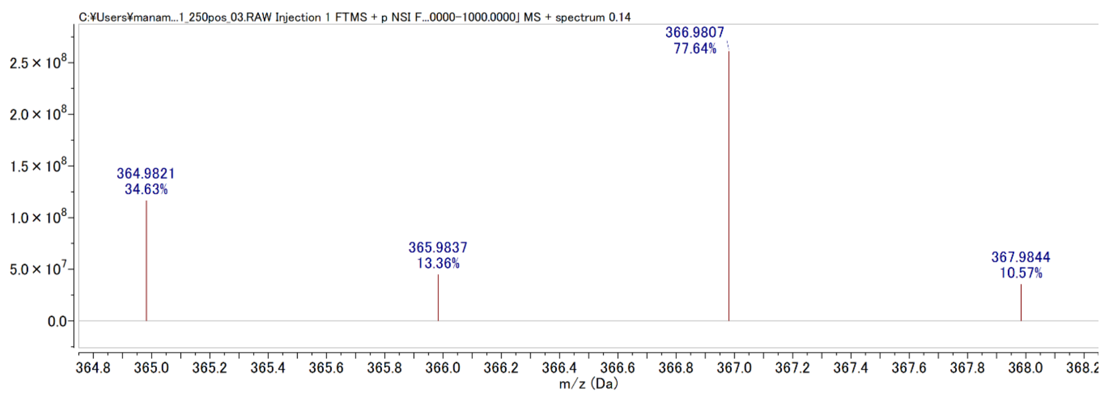


Figure S7. DART-MS of 2-ethylhexyl 2-bromoselenophene-3-carboxylate.

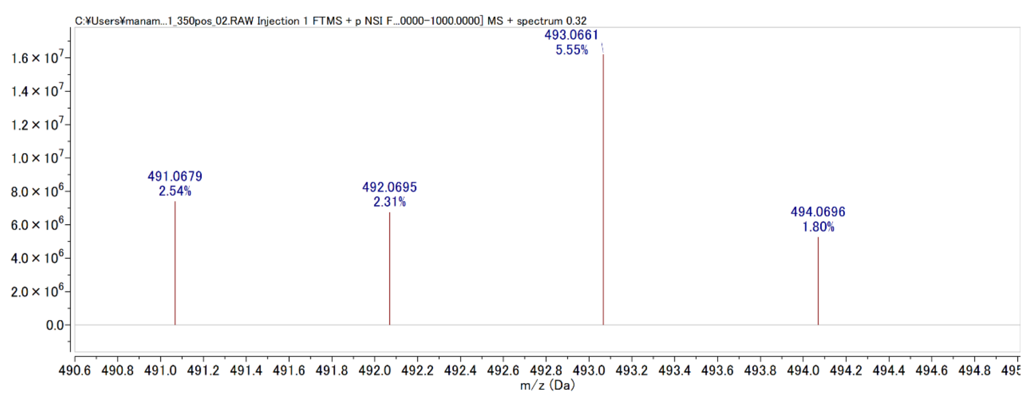


Figure S8. DART-MS of 2-ethylhexyl 2-bromo-5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)selenophene-3-carboxylate.

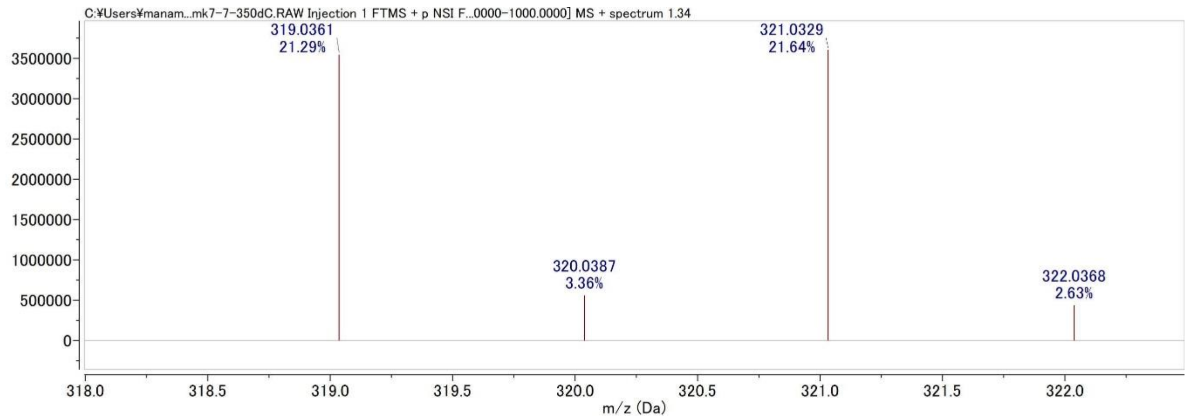


Figure S9. DART-MS of 2-ethylhexyl 2-bromothiophene-3-carboxylate.

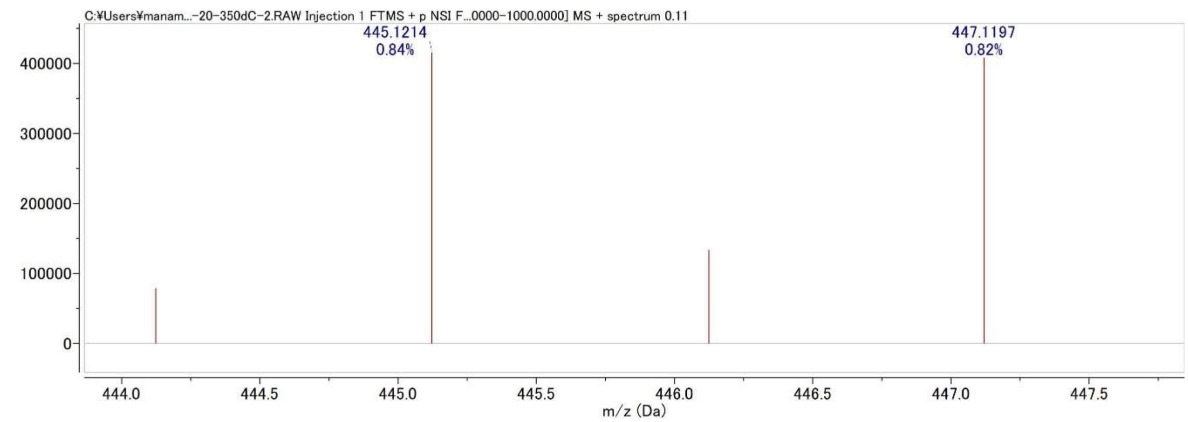


Figure S10. DART-MS of 2-ethylhexyl 2-bromo-5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)thiophene-3-carboxylate.

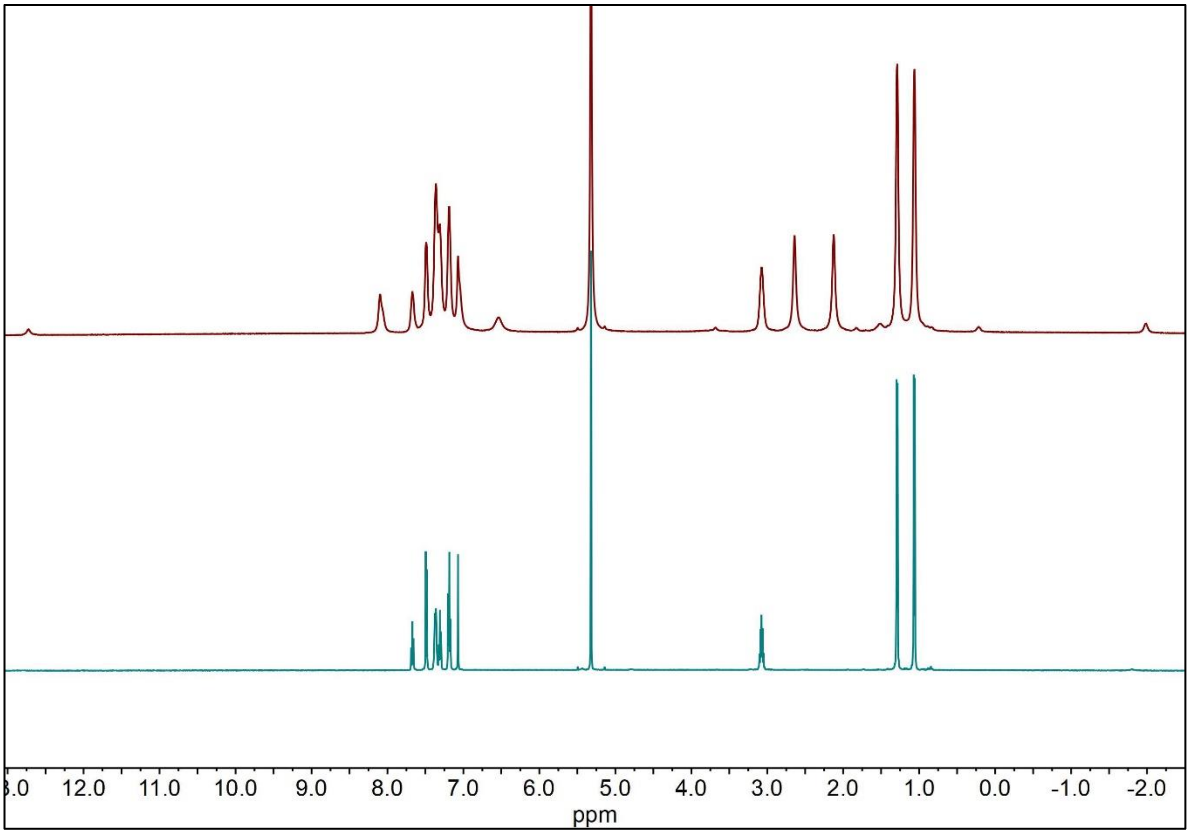
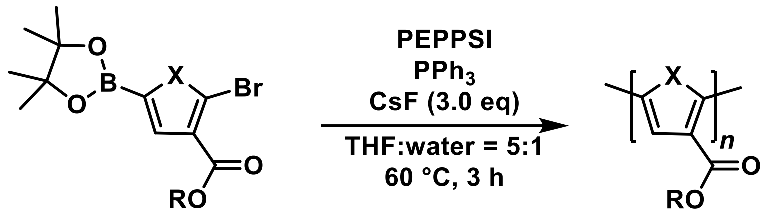


Figure S11. (Top) ^{1}H NMR spectrum (500 MHz) of commercial Ni(IPr)(PPh_3)Cl_2 (TCI, Lot # FJLZN-GK), (Bottom) ^{1}H NMR spectrum (500 MHz) of the synthesized Ni(IPr)(PPh_3)Cl_2.[7] Both spectra were collected in CD_2Cl_2 (25 °C).

General polymerization/copolymerization procedure



In a N_2 filled glovebox, a 20 mL scintillation vial equipped with a Teflon screw cap was charged with a calculated amount of PEPPSI catalyst (noted in Table 1), CsF (0.36 mmol, 54 mg), monomer(s) (0.12 mmol), and THF (3.3 mL for P3(2EH)ET, 6.7 mL for P3(2EH)ES, and 3.3 mL for the total monomer amounts in the cases of copolymerization). A calculated amount of PPh_3 in a THF stock solution was added to the reaction mixture. The reaction vial was promptly capped, removed from the glove box, and placed in a 60 °C oil bath. Immediately, a small amount of degassed H_2O (0.67 mL for P3(2EH)ET, 1.34 mL for P3(2EH)ES, and 0.67 mL for the total monomer amounts in the cases of copolymerization) was injected into the reaction with a N_2 purged syringe. At the noted time, the polymerization was quenched using 6 M methanolic HCl solution. The precipitate was collected using vacuum filtration, then washed with methanol, hot acetone, and water to remove any unreacted monomer/oligomers and salts, respectively. The resultant solid was dissolved in minimal amount of THF, and reprecipitated with methanol. The precipitate was collected using vacuum filtration. The final polymer was obtained as an orange solid for P3(2EH)ET and a dark purple solid for P3(2EH)ES. Yields are listed in Table 1.

P3(2EH)ES

^{1}H-NMR (500 MHz, $CDCl_3$): δ 8.08 (s, 1H), 4.26–4.20 (m, 2H), 1.78-1.67 (m, 1H), 1.51–1.27 (m, 8H), 0.99–0.87 (m, 6H).

$^{13}C\{^1H\}$-NMR (125 MHz, $CDCl_3$): δ 164.2, 155.1, 137.5, 134.4, 128.9, 68.0, 39.0, 30.7, 29.1, 24.1, 23.2, 14.3, 11.3.

P3(2EH)ET

^1H-NMR (500 MHz, $CDCl_3$): δ 7.83 (s, 1H), 4.27–4.15 (m, 2H), 1.73-1.63 (m, 1H), 1.43–1.20 (m, 8H), 0.95–0.85 (m, 6H).

$^{13}C\{^1H\}$-NMR (125 MHz, $CDCl_3$): δ 163.0, 142.9, 132.7, 132.3, 128.6, 67.8, 39.0, 30.6, 29.1, 24.0, 23.2, 14.3, 11.2.

NMR spectra of polymers

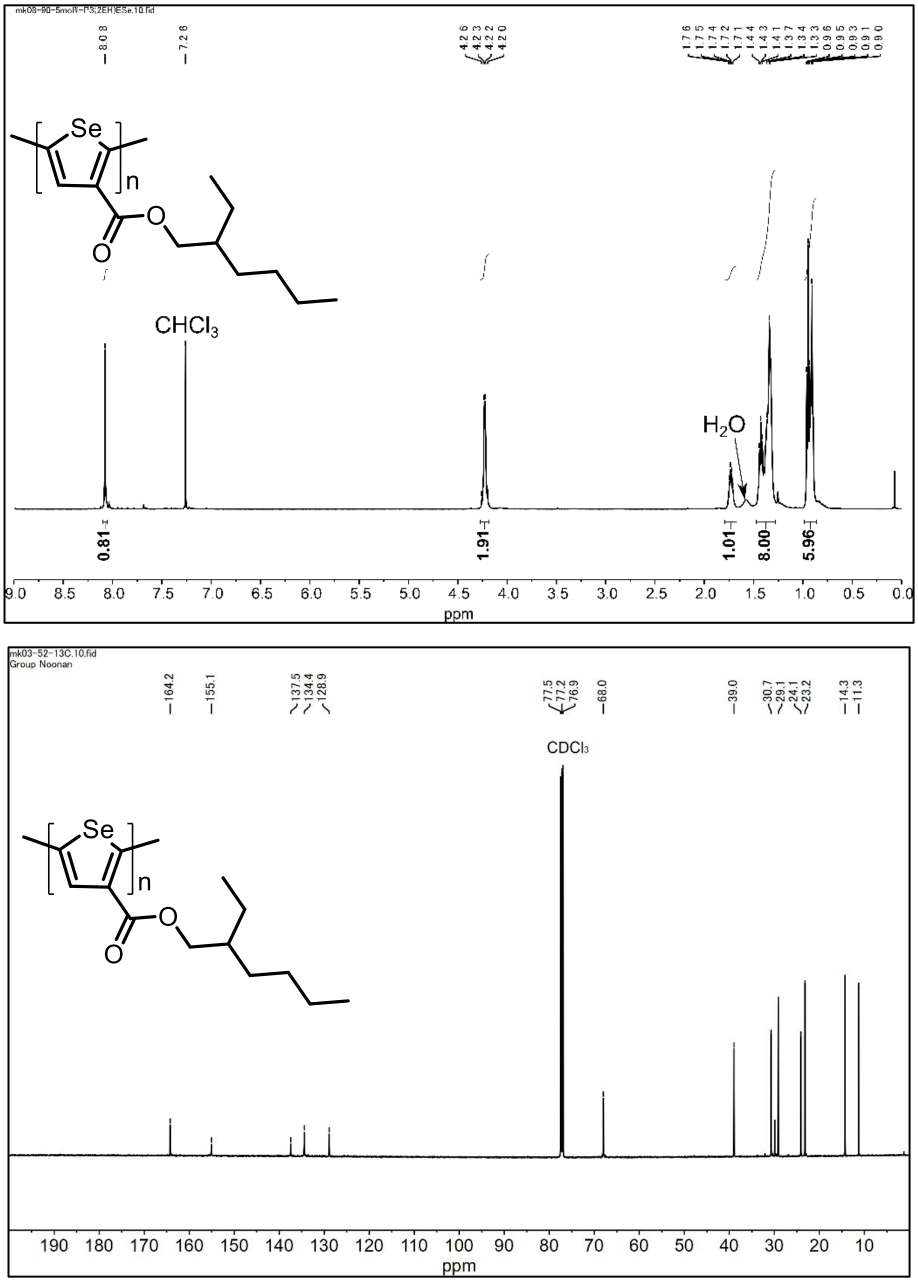
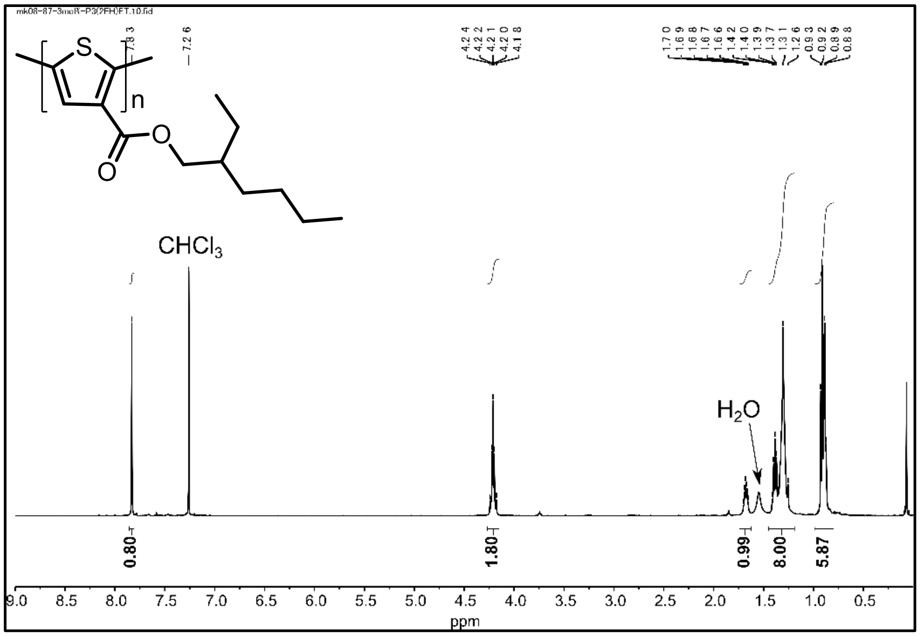


Figure S12. ^{1}H NMR spectrum (top, 500 MHz) and $^{13}C\{^{1}H\}$ NMR spectrum (bottom, 126 MHz) of P3(2EH)ES collected in $CDCl_3$ (25 °C),



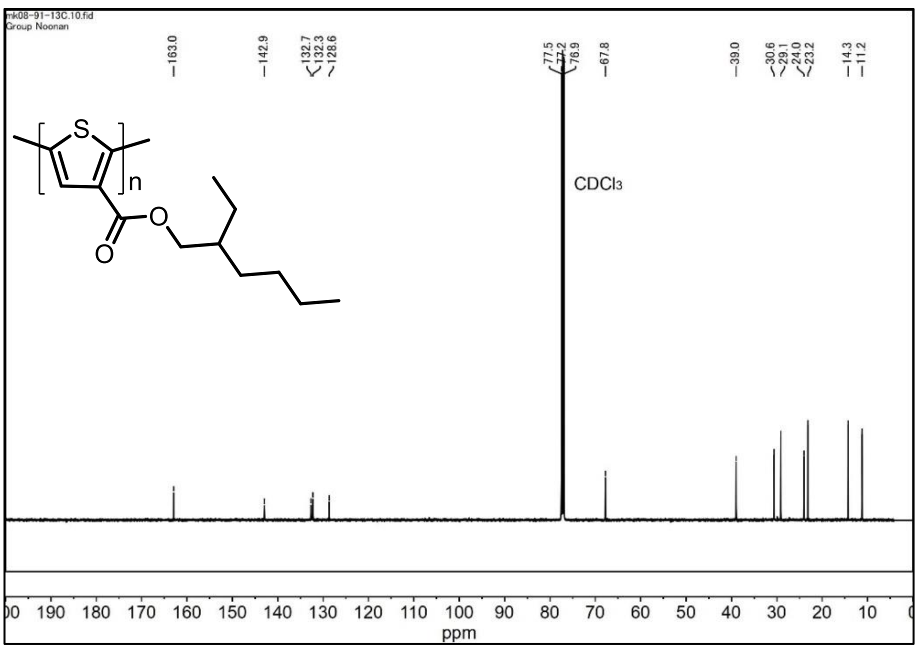


Figure S13. ^{1}H NMR spectrum (top, 500 MHz) and $^{13}C\{^{1}H\}$ NMR spectrum (bottom, 126 MHz) of P3(2EH)ET collected in $CDCl_3$ (25 °C).

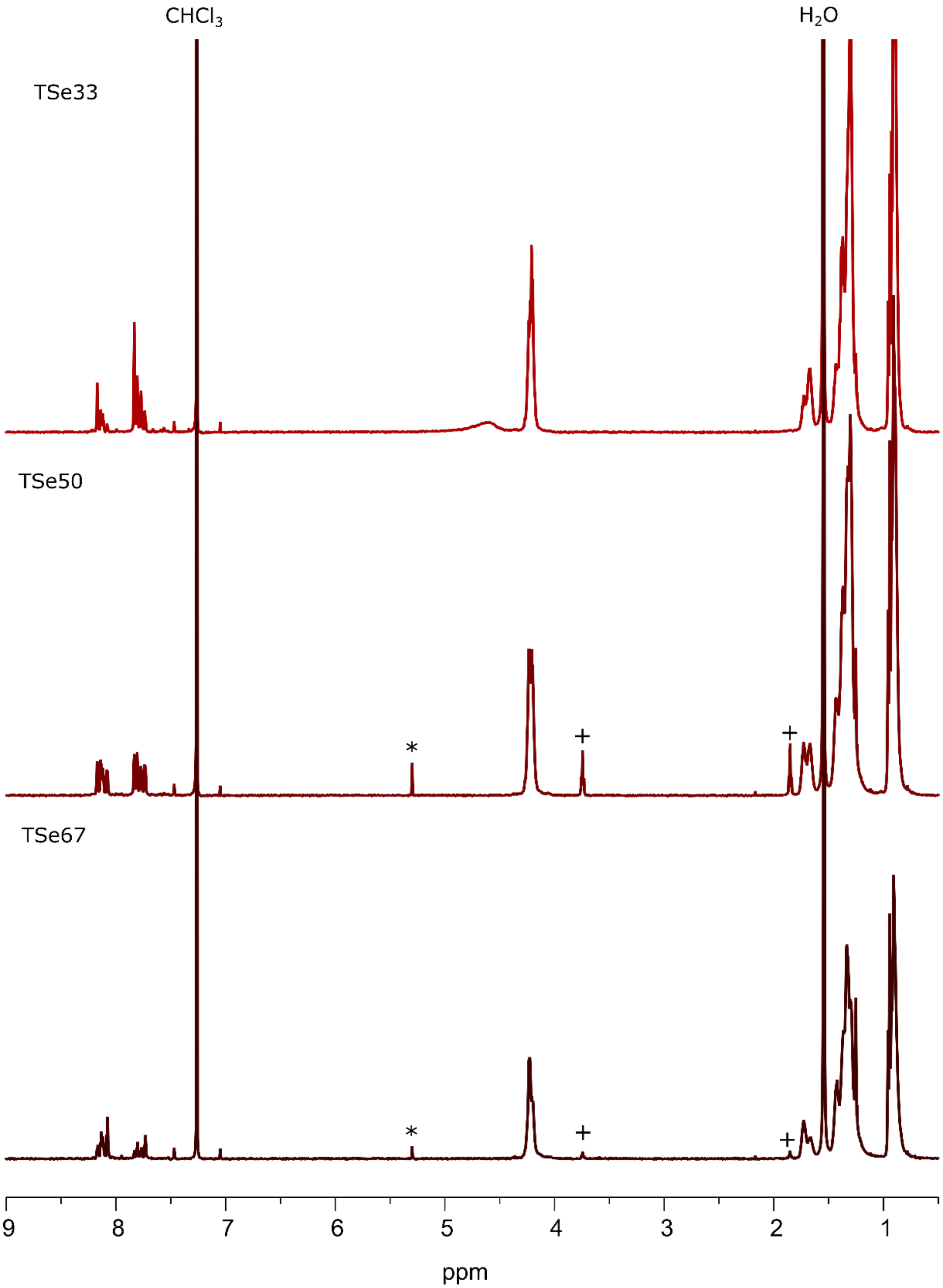


Figure S14. [1]H NMR spectra of *stat*-TSe copolymers collected in $CDCl_3$ (25 °C). Residual solvents are noted with * for CH_2Cl_2 and + for THF.

GPC data for P3(2EH)ET, P3(2EH)ES, and *stat*-TSe

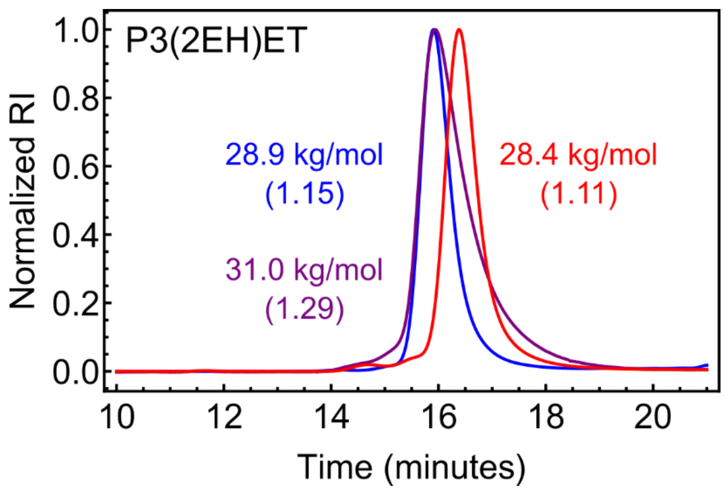


Figure S15. GPC chromatograms of P3(2EH)ET samples prepared using 3 mol % PEPPSI-IPent (Red), 3 mol% PEPPSI-IPent/PPh_3 (Purple), and 5 mol% PEPPSI-IPent/PPh_3 (Blue) . Entries 2 - 4, Table 1.

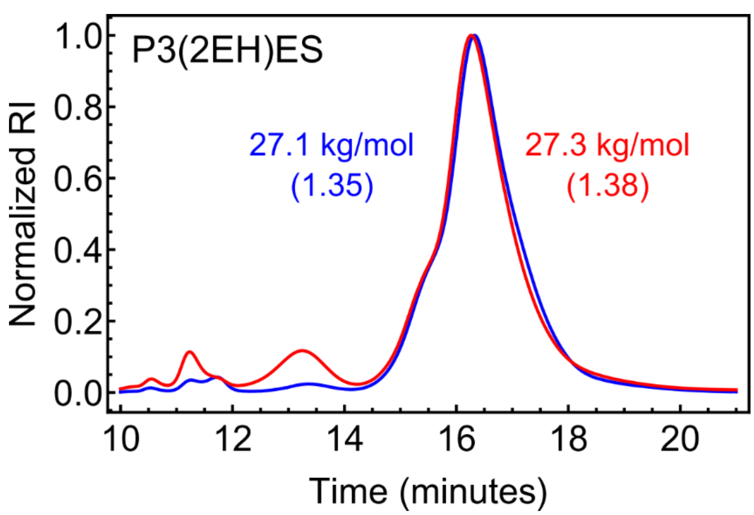


Figure S16. GPC chromatograms of P3(2EH)ES samples prepared using 3 mol% PEPPSI-IPent/PPh_3 (Blue), and 5 mol% PEPPSI-IPent/PPh_3 (Red) . Entries 5 and 6, Table 1. The peaks at 12 and 14 are believed to be due to aggregation.

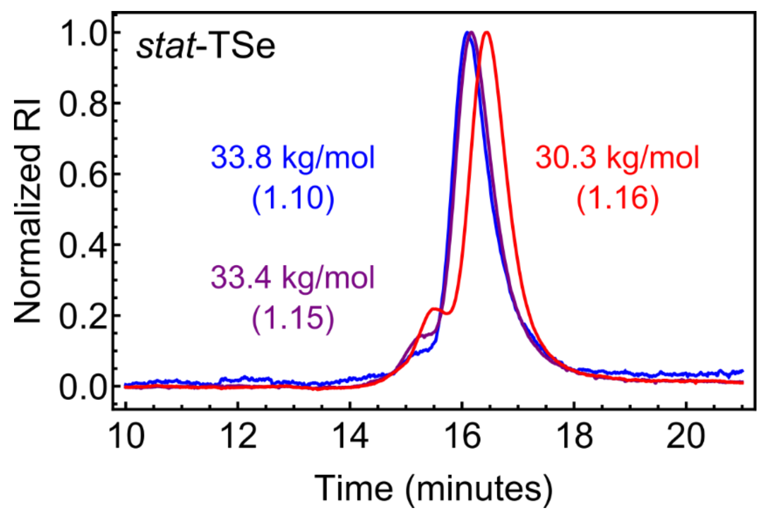


Figure S17. GPC chromatograms of *stat*-TSe_{67} (Red), *stat*-TSe_{50} (Purple), *stat*-TSe_{33} (Blue) from Table 2.

DP estimation from 1H-NMR spectrum for P3(2EH)ES and P3(2EH)ET

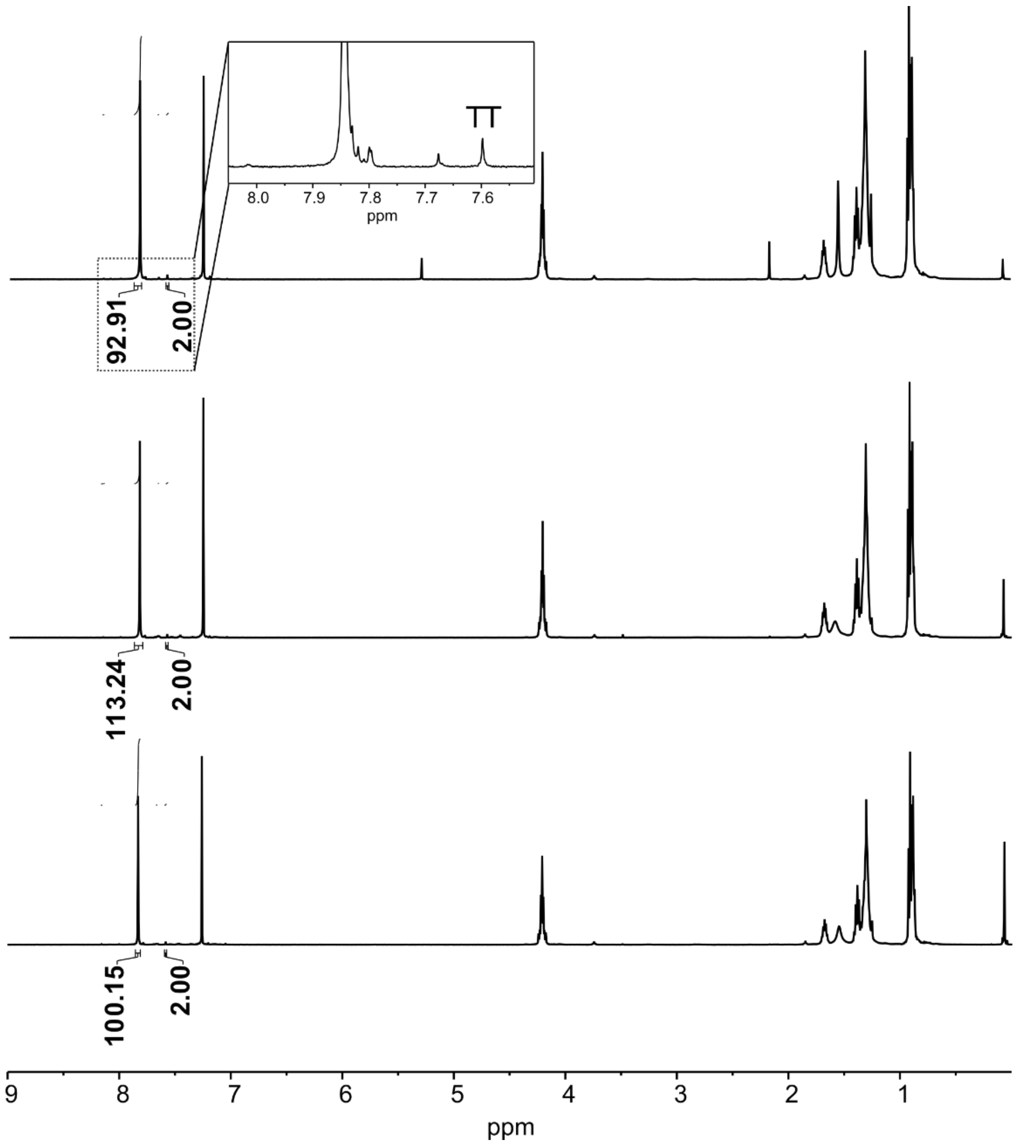


Figure S18. ^{1}H-NMR spectrum and DP estimation (compared to TT signal) of P3(2EH)ET samples prepared using 3 mol % PEPPSI-IPent (top), 3 mol% PEPPSI-IPent/PPh_3 (middle), and 5 mol% PEPPSI-IPent/PPh_3 (bottom) . Entries 2 - 4, Table 1, collected in $CDCl_3$ (500 MHz).

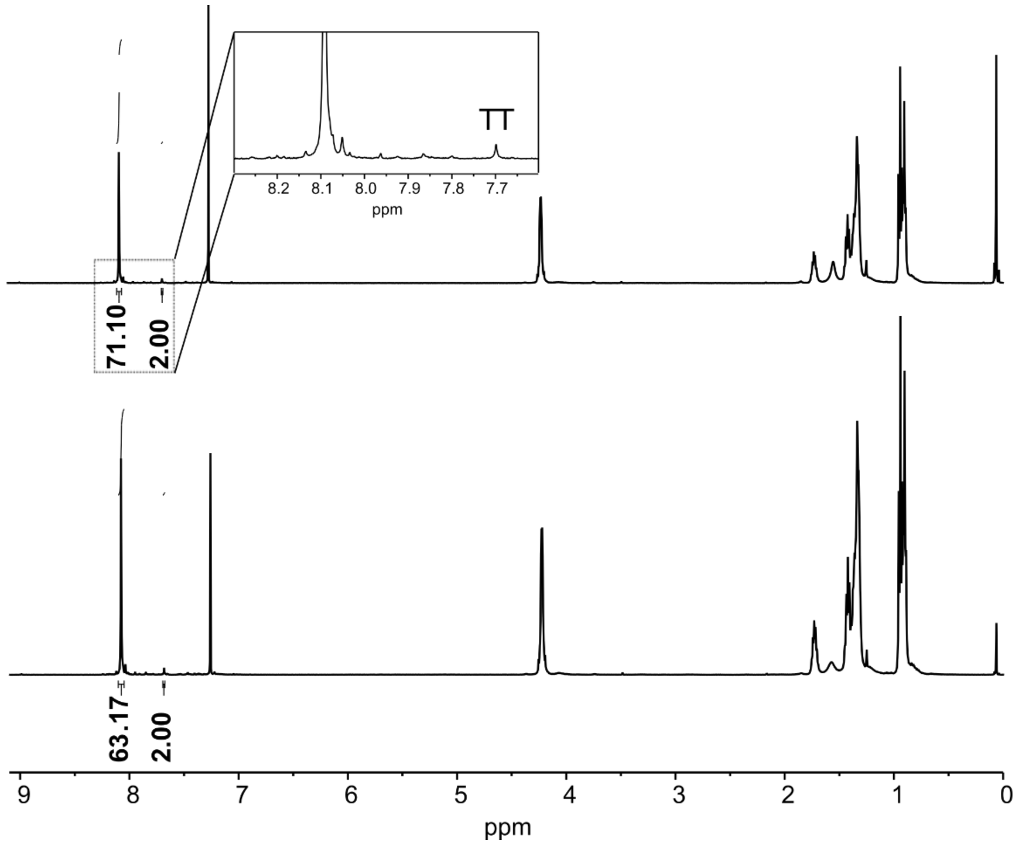


Figure S19. [1]H-NMR spectrum and DP estimation (compared to TT signal) of P3(2EH)ES samples prepared using 3 mol% PEPPSI-IPent/PPh_3 (top), and 5 mol% PEPPSI-IPent/PPh_3 (bottom) . Entries 5 and 6, Table 1, collected in $CDCl_3$ (500 MHz).

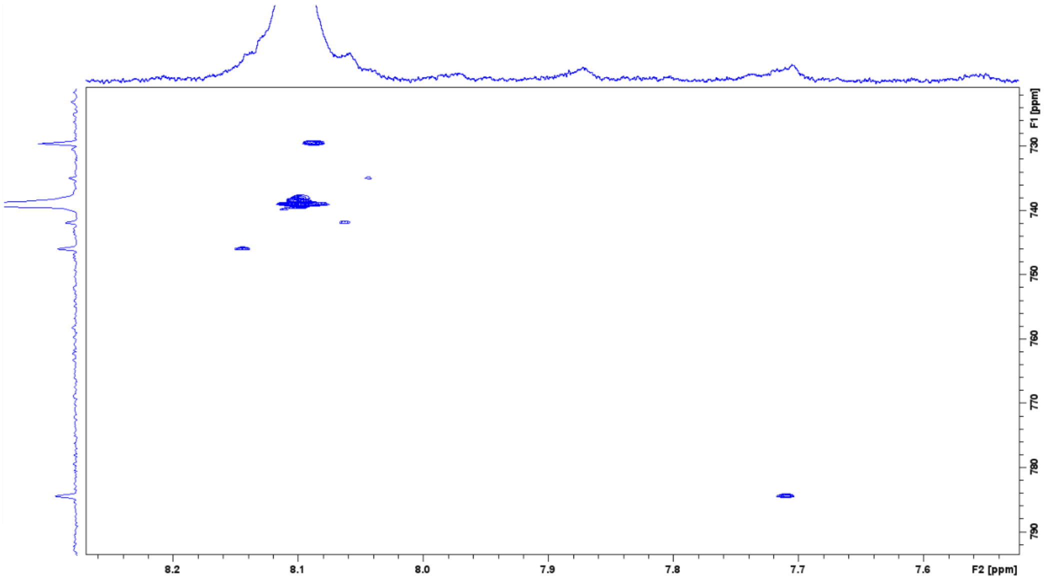


Figure S20. $J_{H,Se}$-optimized HSQC 2D NMR spectrum of P3(2EH)ES sample illustrating the differences of Se chemical shifts affected by end-groups, collected in $CDCl_3$ (500 MHz).

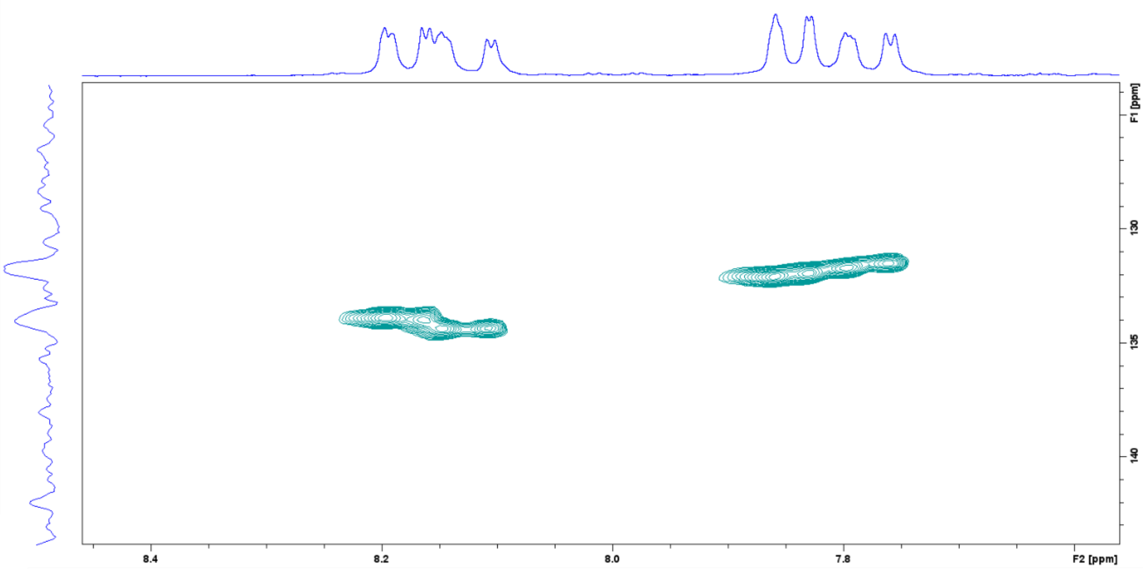


Figure S21. ^{1}H, ^{13}C-HSQC NMR spectrum of *stat*-TSe_{50} sample illustrating the 8 direct proton-carbon correlations for the configurational triads. Collected in $CDCl_3$ (500 MHz, 25 °C).

λ_{max} (solution and solid-state), the solid-state absorption edge(ν_{edge}), and oxidation potential onset of P3(2EH)ET (M_n = 38.4 kg/mol), *stat*-TSe33 (M_n = 33.8 kg/mol), *stat*-TSe50 (M_n = 33.4 kg/mol), *stat*- TSe67 (M_n = 30.3 kg/mol), and P3(2EH)ES (M_n = 31.8 kg/mol). The two homopolymers were obtained from polymerization with 1 mol % PEPPSI-IPent.

Polymer	λ_{max} (nm, $CHCl_3$)	λ_{max} (nm, film)	λ_{onset} (nm, film)	ν_{edge} (eV)	$E^{ox}_{onset}{}^{cv}$ (V)
P3(2EH)ET	423	474	589	2.11	1.04
stat-TSe33	450	525	648	1.91	0.99
stat-TSe50	461	550	661	1.88	0.95
stat-TSe67	474	559	676	1.83	0.91
P3(2EH)ES	503	600	709	1.75	0.89

Determination of Onset Potentials for Oxidation in the solid-state in CV

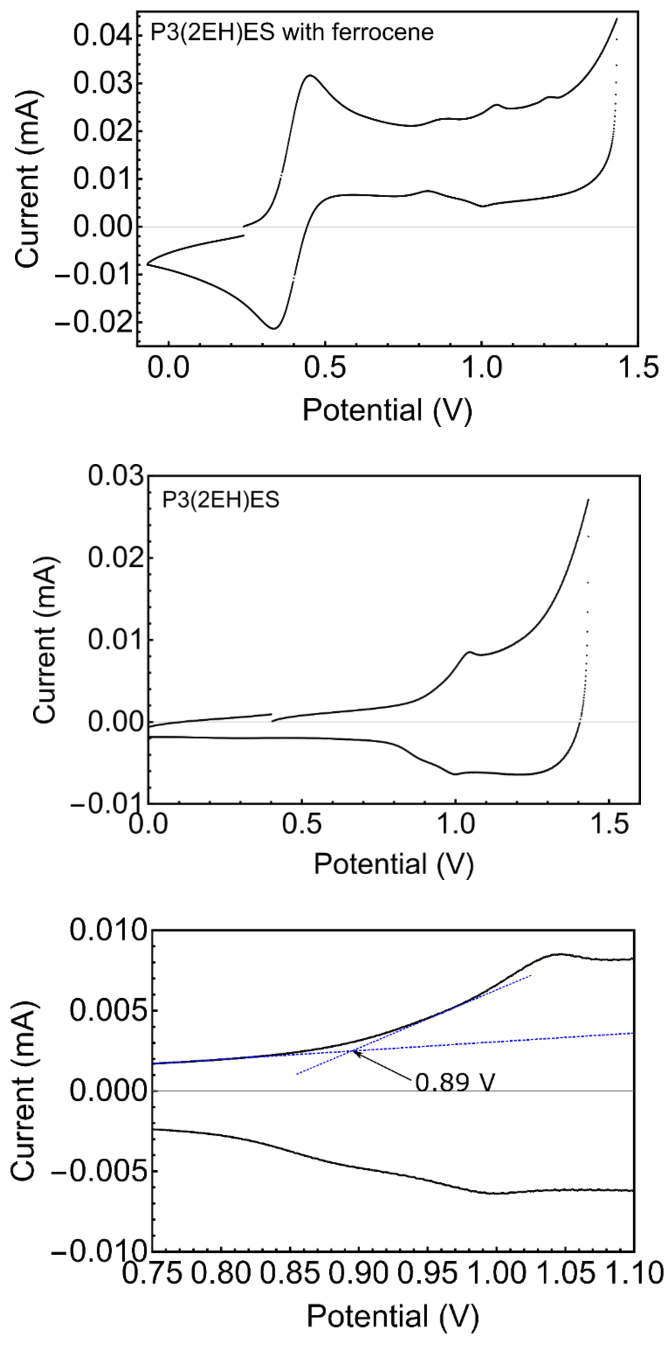


Figure S22. CV of P3(2EH)ES in the solid state with ferrocene (top), P3(2EH)ES in the solid state (middle), and determination of onset potentials for oxidation (bottom).

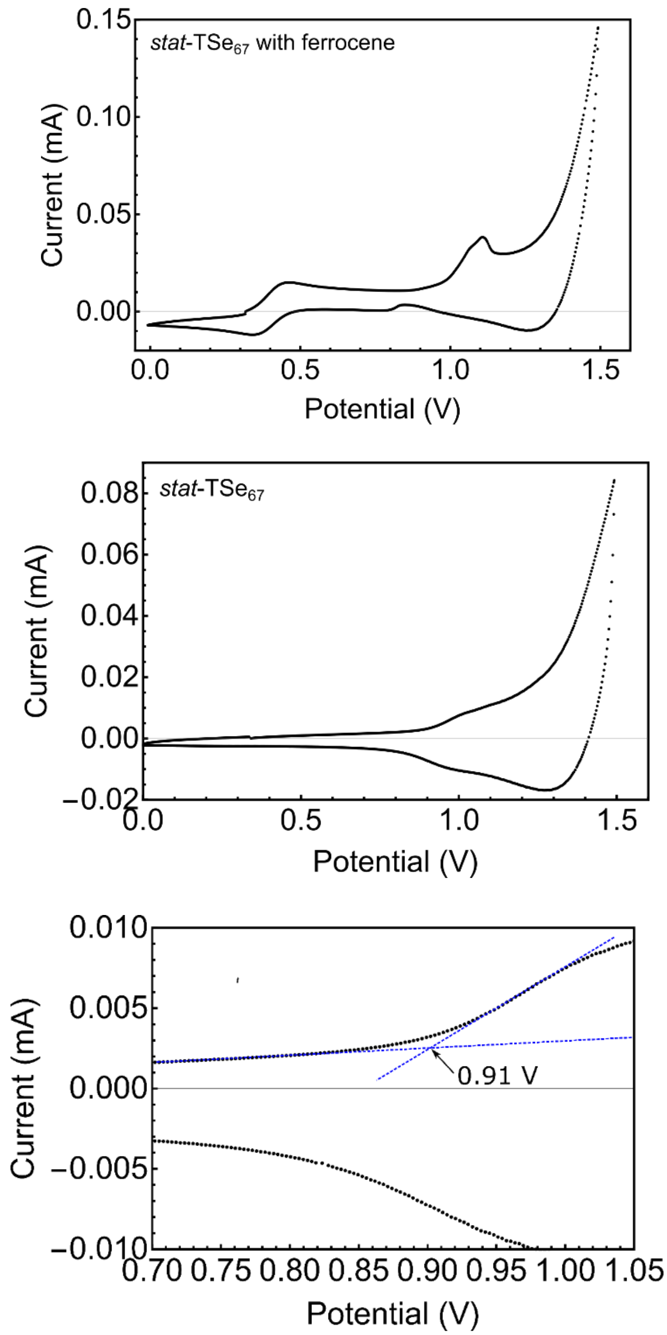


Figure S23. CV of *stat*-TSe_{67} in the solid state with ferrocene (top), *stat*-TSe_{67} in the solid state (middle), and determination of onset potential for oxidation (bottom).

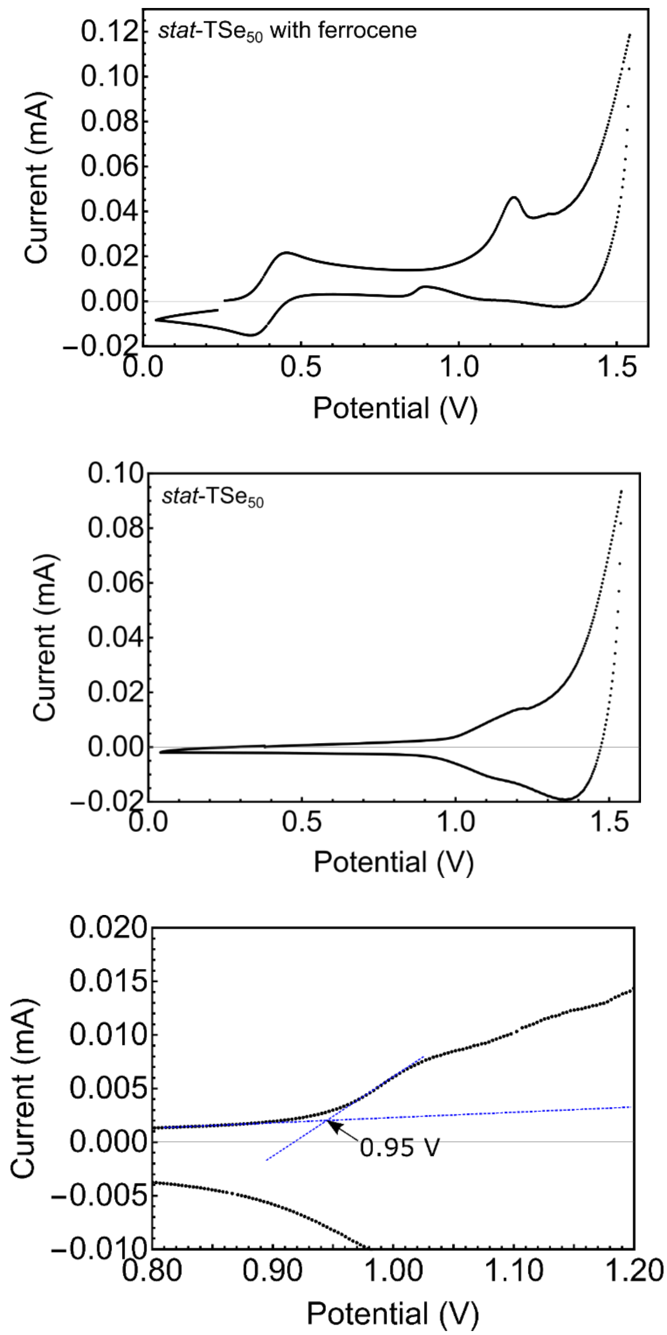


Figure S24. CV of *stat*-TSe_{50} in the solid state with ferrocene (top), *stat*-TSe_{50} in the solid state (middle), and determination of onset potential for oxidation (bottom).

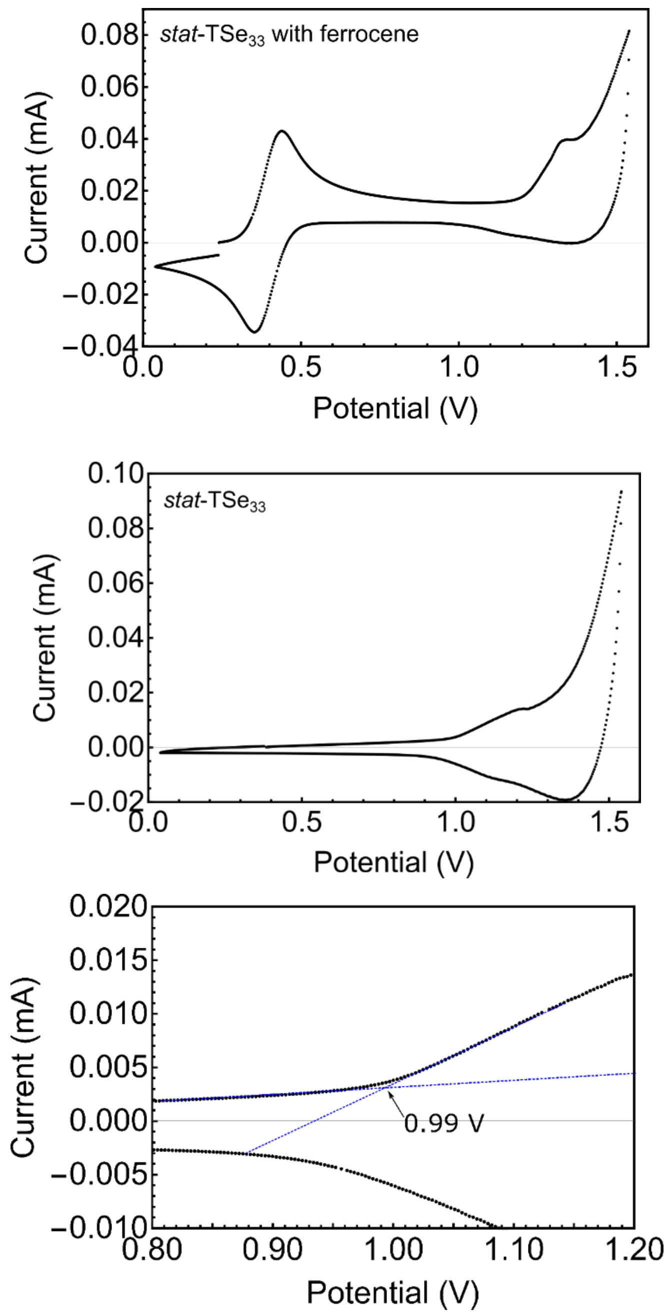
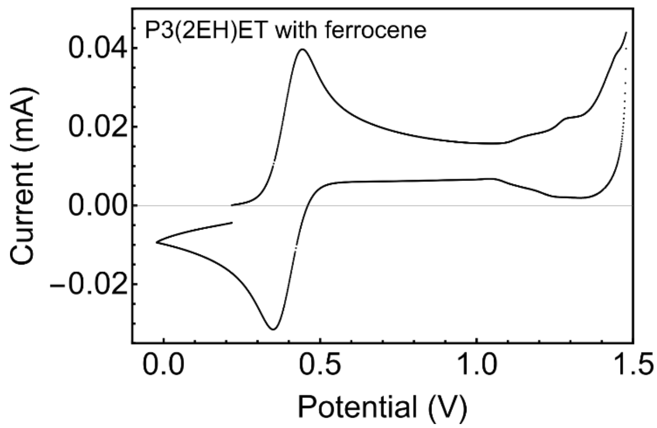
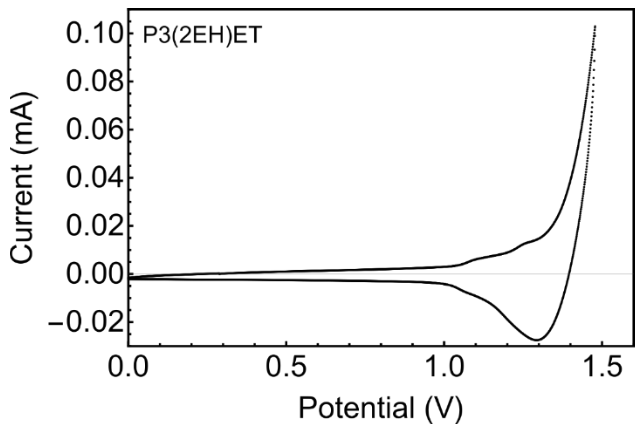


Figure S25. CV of *stat*-TSe_{33} in the solid state with ferrocene (top), *stat*-TSe_{33} in the solid state (middle), and determination of onset potential for oxidation (bottom).





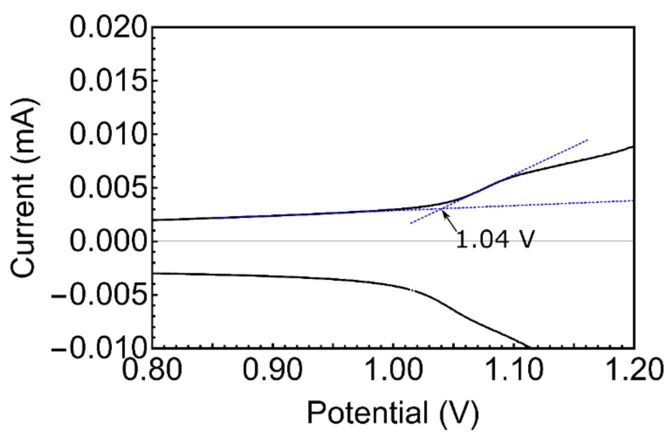


Figure S26. CV of P3(2EH)ET in the solid-state with ferrocene (top), P3(2EH)ET in the solid-state (middle), and determination of oxidation onset potential (bottom).

Determination of Onset Potentials in the solid-state UV-Vis

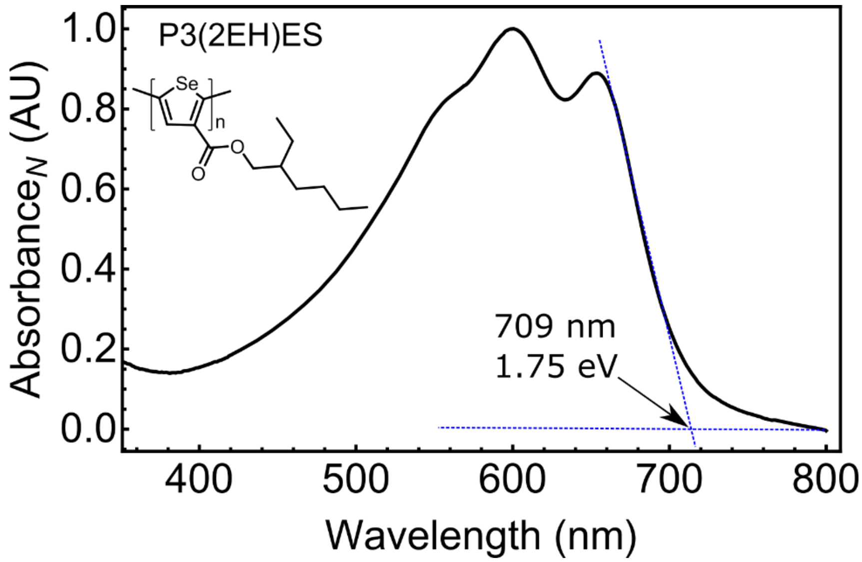


Figure S27. Determination of onset wavelength for band gap determination from solid-state UV-vis spectrum of P3(2EH)ES in solid-state (cast from $CHCl_3$).

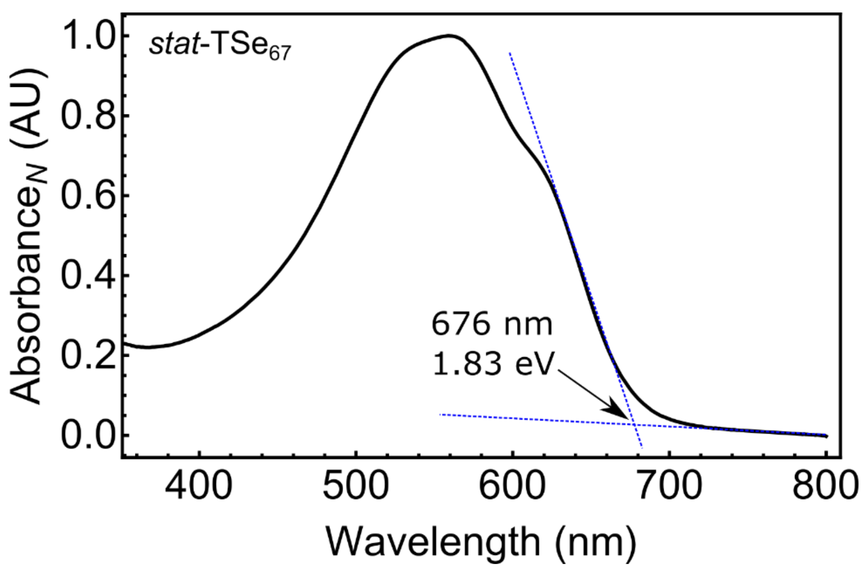


Figure S28. Determination of onset wavelength for band gap determination from solid-state UV-vis spectrum of *stat*-TSe$_{67}$ in solid-state (cast from $CHCl_3$).

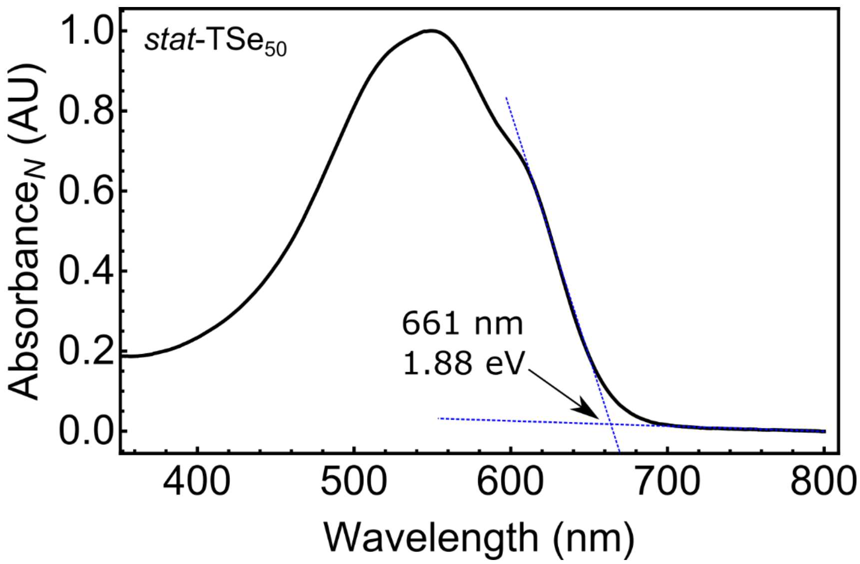


Figure S29. Determination of onset wavelength for band gap determination from solid-state UV-vis spectrum of *stat*-TSe_{50} in solid-state (cast from $CHCl_3$).

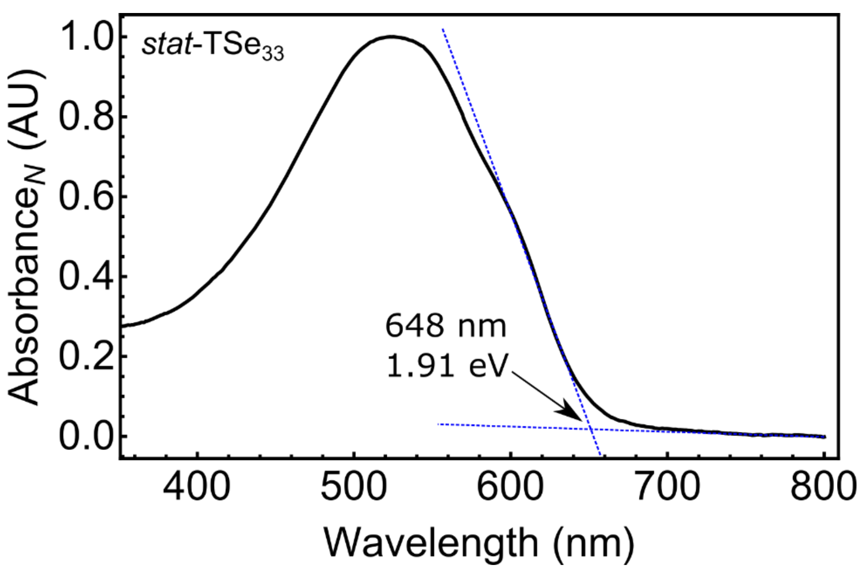


Figure S30. Determination of onset wavelength for band gap determination from solid-state UV-vis spectrum of *stat*-TSe_{33} in solid-state (cast from $CHCl_3$).

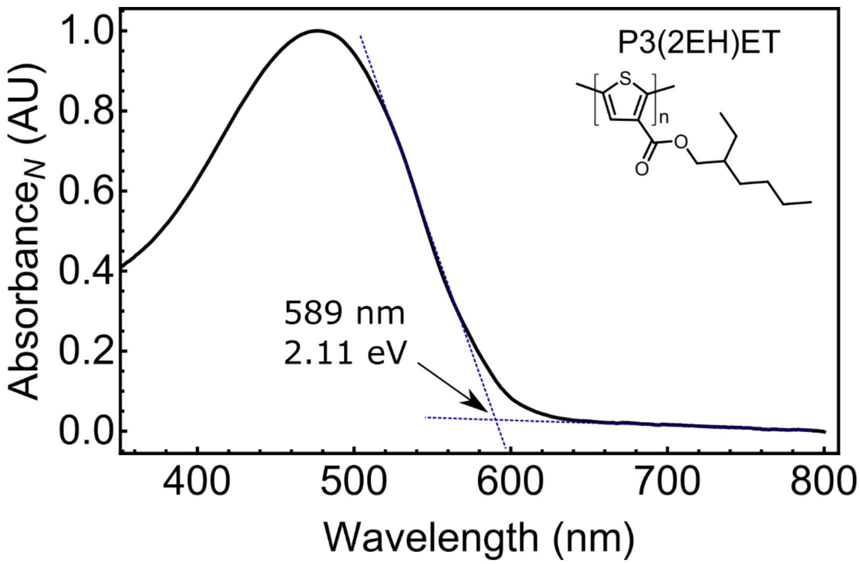


Figure S31. Determination of onset wavelength for band gap determination from solid-state UV-vis spectrum of P3(2EH)ET in solid-state (cast from $CHCl_3$).

Molecular Weight Versus Conversion Procedure.

In a N_2 filled glovebox, a 20 mL scintillation vial equipped with a Teflon screw cap was charged with 3(2EH)ET (27.1 mg, 0.061 mmol), 3(2EH)ESe (30.0 mg, 0.061 mmol), PEPPSI-IPent catalyst (2.9 mg, 0.0037 mmol), CsF (55.6 mg, 0.37 mmol), 1,3,5-trimethoxybenzene (6.2 mg, 0.037 mmol) , and 3 mL of THF. PPh_3 (5.6 mg, 0.012 mmol) was weighed into a separate vial, dissolved in 2.8 mL THF. 0.48 mL of this PPh_3 stock solution was taken, and added to the catalyst solution. The reaction vial was promptly capped, removed from the glove box, and placed in a 60 °C oil bath. 0.68 mL of degassed H_2O was injected into the reaction with a N_2 purged syringe. An aliquot (0.05 mL) was removed from the reaction mixture and diluted with dry, degassed ether (4 mL), filtered through a 0.22 μm syringe filter, and submitted for GC-MS analysis (designated as the 0 min time point). Aliquots (0.35 mL) were taken at specified intervals (the time refers to elapsed time after water addition). For each aliquot, 0.3 mL was quenched with 6 M methanolic HCl (2 mL), filtered through a 0.22 μm syringe filter, washed with methanol and acetone, dried under vacuum, dissolved in THF, and analyzed by GPC. The remaining 0.05 mL was diluted with dry, degassed ether (4 mL), filtered through a 0.22 μm syringe filter, and submitted for GC-MS analysis.

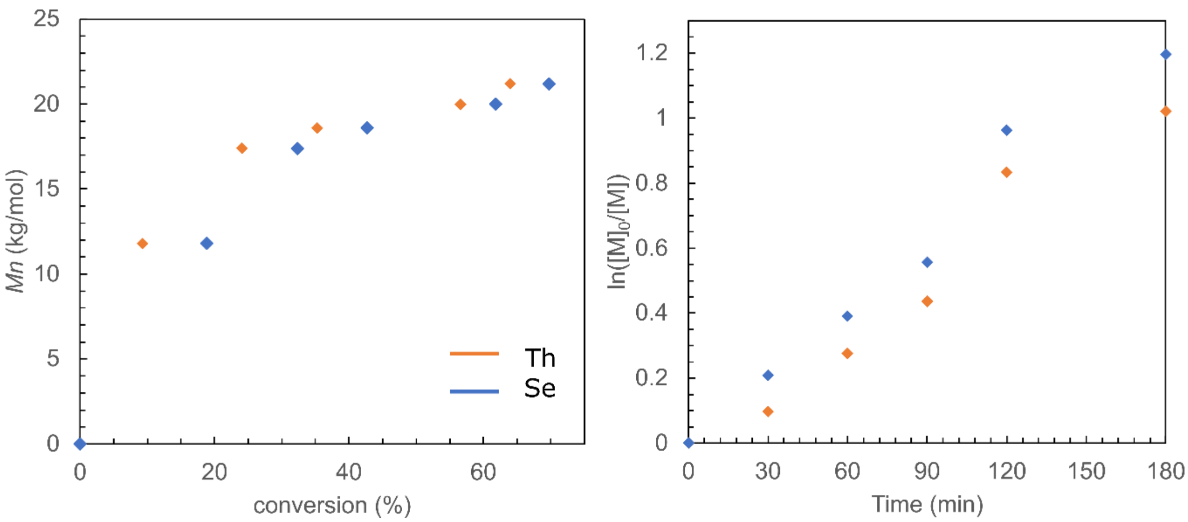


Figure S32. (Left) number-average molecular weight versus conversion. (Right) semilogarithmic plot of conversion versus time. Orange square corresponds to 3(2EH)ET and blue square corresponds to 3(2EH)ESe.

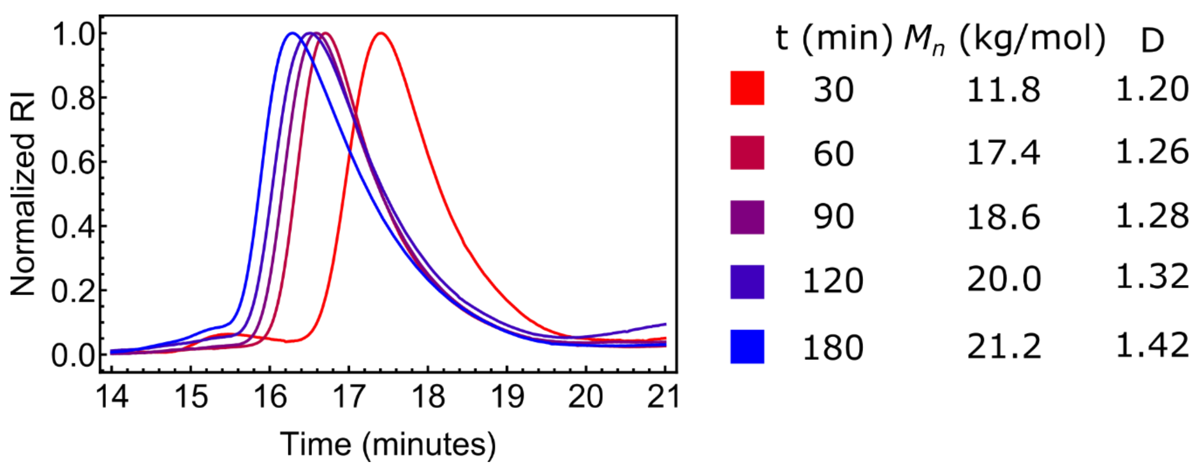


Figure S33. GPC data for conversion versus molecular weight experiment.

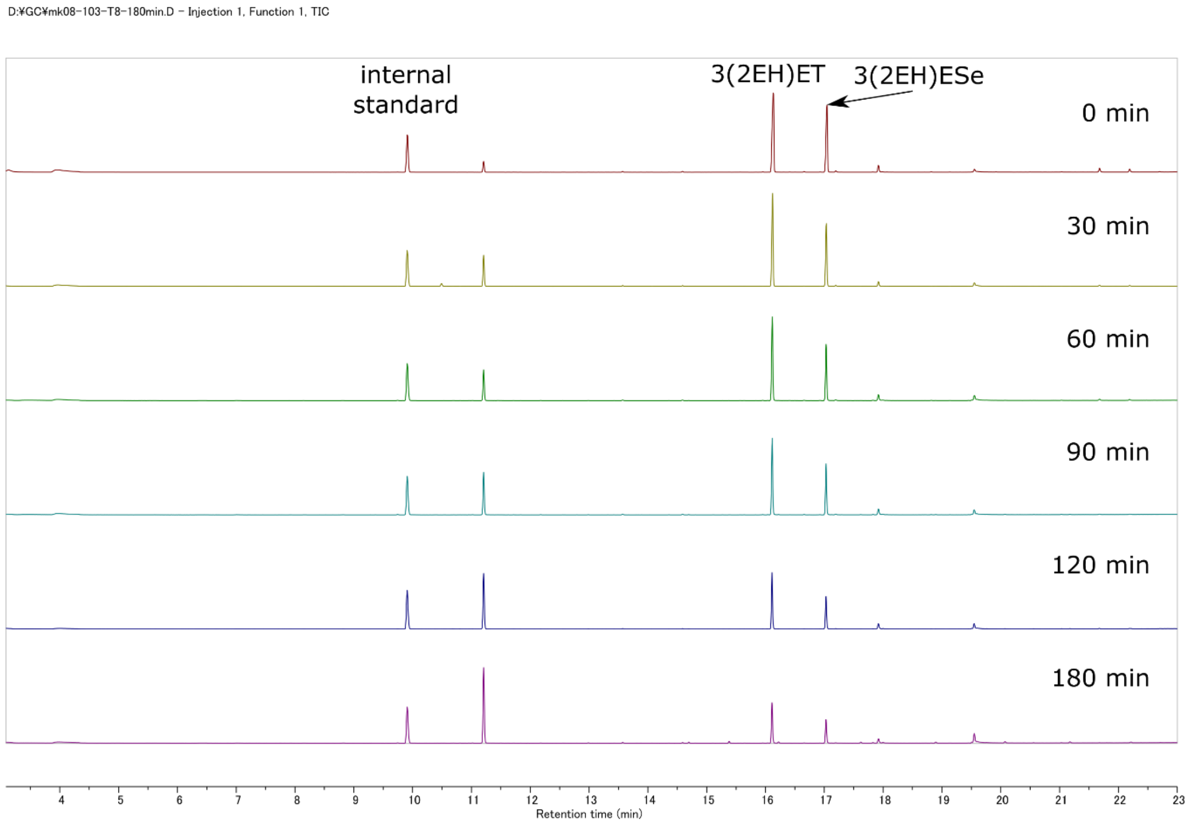


Figure S34. Stack plot of GC-MS data collected for molecular weight versus conversion experiment.

Cartesian coordinates and total energies for optimized dimers (*anti* orientation)

2,2’-bithiophene

Energy: -1104.681014 Hartrees

C	-3.1954670000	0.1294470000	0.0000050000
C	-2.8010530000	-1.1740790000	-0.0000280000
C	-1.3851400000	-1.3186460000	-0.0000420000
C	-0.7177540000	-0.1213160000	0.0000320000
S	-1.8465110000	1.2028950000	0.0000160000
H	-4.2007160000	0.5253180000	0.0000210000
H	-3.4925110000	-2.0072460000	-0.0000630000
H	-0.8798120000	-2.2774600000	0.0000190000
C	0.7178680000	0.1211130000	0.0000040000
C	1.3850590000	1.3186060000	-0.0000390000
S	1.8465510000	-1.2028260000	0.0000210000
C	2.8009340000	1.1741180000	-0.0000330000
H	0.8795680000	2.2773400000	0.0000520000
C	3.1955010000	-0.1294190000	-0.0000070000
H	3.4923800000	2.0072900000	-0.0000300000
H	4.2007510000	-0.5252910000	0.0000520000

2,2’-biselenophene

Energy: -5107.126938 Hartrees

C	-3.2246380000	0.6776620000	0.0000860000
C	-2.4682520000	1.8067210000	0.0000820000
C	-1.0607580000	1.5788510000	-0.0000140000
C	-0.6749270000	0.2670200000	-0.0000410000
H	-4.3029820000	0.6140510000	0.0001440000
H	-2.8984540000	2.8013850000	0.0001410000
H	-0.3407070000	2.3910770000	-0.0000320000
C	0.6749390000	-0.2670060000	-0.0000170000
C	1.0607280000	-1.5788470000	0.0000090000
C	2.4682150000	-1.8067190000	0.0000870000
H	0.3406340000	-2.3910280000	-0.0000570000
C	3.2246240000	-0.6776860000	0.0000720000
H	2.8984120000	-2.8013870000	0.0000850000
H	4.3029660000	-0.6140900000	0.0001470000
Se	-2.1739920000	-0.8465590000	-0.0000300000
Se	2.1740080000	0.8465590000	-0.0000290000

2-(selenophen-2-yl)thiophene

Energy: -3105.903864 Hartrees

C	-3.5686590000	-0.0253980000	0.0000190000
C	-3.0370690000	-1.2795010000	0.0000100000
C	-1.6142830000	-1.2700810000	0.0000050000
C	-1.0774260000	-0.0085460000	0.0000070000
H	-4.6106440000	0.2603290000	-0.0000100000
H	-3.6352170000	-2.1819720000	0.0000430000
H	-1.0074130000	-2.1687480000	-0.0000570000
C	0.3234080000	0.3802830000	-0.0000230000
C	0.8497230000	1.6420780000	-0.0000180000
C	2.2743800000	1.7117870000	0.0000070000
H	0.2252760000	2.5291500000	0.0000050000
C	2.9016510000	0.5063560000	0.0000290000
H	2.8120290000	2.6527710000	0.0000490000
H	3.9663080000	0.3237870000	0.0000380000
Se	1.6890560000	-0.8924110000	-0.0000050000
S	-2.3430370000	1.1865490000	0.0000070000

dimethyl [2,2'-bithiophene]-3,4'-dicarboxylate

Energy: -1560.30107 Hartrees

C	-2.3055600000	-2.9335240000	-0.0000460000
C	-3.0973400000	-1.8357320000	-0.0001550000
S	-0.6397800000	-2.5058130000	0.0001200000
C	-2.3584510000	-0.6072580000	-0.0000960000
H	-4.1776980000	-1.8647560000	-0.0002360000
C	-0.9831380000	-0.7958000000	0.0000190000
C	-3.0554900000	0.6915430000	0.0000350000
C	0.1829980000	0.0914740000	0.0000660000
O	-2.5321530000	1.7854260000	0.0002810000
O	-4.3902460000	0.5353410000	-0.0001470000
C	1.4838830000	-0.3577130000	-0.0000100000
S	0.1626340000	1.8427390000	-0.0000160000
C	-5.1428340000	1.7474900000	0.0000100000
C	2.4479810000	0.6819900000	-0.0000710000
H	1.7648420000	-1.4032080000	-0.0000720000
C	1.8652230000	1.9205380000	-0.0000960000
H	-4.9158810000	2.3414020000	-0.8880220000
H	-6.1884520000	1.4435140000	-0.0002890000
H	-4.9162380000	2.3409700000	0.8884200000
C	3.9155940000	0.5124490000	-0.0000420000
O	4.7142400000	1.4218620000	-0.0000130000
O	4.2673390000	-0.7851730000	-0.0000460000
C	5.6723530000	-1.0311200000	0.0000510000
H	6.1386670000	-0.5984310000	0.8880310000
H	5.7828870000	-2.1145130000	0.0001680000
H	6.1387080000	-0.5986370000	-0.8880060000
H	-2.5993130000	-3.9731130000	-0.0001070000
H	2.3820620000	2.8702810000	-0.0001450000

methyl 5-(3-(methoxycarbonyl)selenophen-2-yl)thiophene-3-carboxylate (SETE)

Energy: -3561.523722 Hartrees

C	-2.4301260000	-2.6029540000	0.0000080000
C	-3.1087290000	-1.4352290000	0.0000290000
C	-2.2955580000	-0.2492480000	0.0000280000
H	-4.1885610000	-1.3765370000	0.0000470000
C	-0.9283040000	-0.4719370000	0.0000140000
C	-2.9429020000	1.0765530000	0.0000180000
C	0.2572000000	0.3869970000	0.0000110000
O	-2.3781810000	2.1499810000	0.0000740000
O	-4.2833900000	0.9777090000	-0.0000650000
C	1.5465910000	-0.0967740000	-0.0000120000
S	0.2914050000	2.1396140000	0.0000120000
C	-4.9829920000	2.2208710000	-0.0000780000
C	2.5412240000	0.9120050000	0.0000030000
H	1.8024110000	-1.1492000000	-0.0000760000
C	1.9951340000	2.1673210000	0.0000180000
H	-4.7310390000	2.8044640000	-0.8882050000
H	-6.0407170000	1.9620520000	-0.0000850000
H	-4.7310520000	2.8044810000	0.8880430000
C	4.0025220000	0.6964160000	-0.0000010000
O	4.8298150000	1.5797260000	0.0000340000
O	4.3125500000	-0.6121040000	-0.0000480000
C	5.7090480000	-0.9027160000	-0.0000450000
H	6.1888590000	-0.4851870000	0.8879940000
H	5.7851280000	-1.9890780000	-0.0000870000
H	6.1888800000	-0.4851170000	-0.8880390000
H	-2.8463250000	-3.5995120000	0.0000280000
H	2.5399870000	3.1013490000	0.0000370000
Se	-0.6075010000	-2.3174080000	0.0000070000

methyl 2-(4-(methoxycarbonyl)selenophen-2-yl)thiophene-3-carboxylate (TESE)

Energy: -3561.529199 Hartrees

C	2.2810640000	-3.1739560000	0.0000450000
C	3.0890390000	-2.0881270000	0.0001140000
S	0.6200990000	-2.7233280000	-0.0000720000
C	2.3658420000	-0.8505350000	0.0000830000
H	4.1689390000	-2.1329990000	0.0001710000
C	0.9874290000	-1.0184590000	0.0000390000
C	3.0691520000	0.4401860000	-0.0000270000
C	-0.1519320000	-0.1037490000	-0.0000300000
O	2.5489310000	1.5386540000	-0.0001690000
O	4.4015930000	0.2842540000	0.0000330000
C	-1.4578860000	-0.5279190000	-0.0000060000
C	5.1575000000	1.4949070000	-0.0000850000
C	-2.4452200000	0.4937620000	-0.0000100000
H	-1.7398700000	-1.5740570000	0.0000680000
C	-1.9303440000	1.7598480000	0.0000340000
H	4.9323070000	2.0887910000	0.8883190000
H	6.2020710000	1.1877210000	-0.0000890000
H	4.9322450000	2.0886680000	-0.8885550000
C	-3.9063480000	0.2646460000	-0.0000210000
O	-4.7417890000	1.1407980000	-0.0000390000
O	-4.2092290000	-1.0458640000	-0.0000140000
C	-5.6036440000	-1.3443280000	-0.0000150000
H	-6.0861770000	-0.9295540000	-0.8879220000
H	-5.6736190000	-2.4311620000	-0.0000350000
H	-6.0861920000	-0.9295790000	0.8878950000
H	2.5601160000	-4.2176030000	0.0000770000
H	-2.5253360000	2.6628020000	0.0000450000
Se	-0.0979420000	1.7747010000	0.0000580000

dimethyl [2,2'-biselenophene]-3,4'-dicarboxylate

Energy: -5562.752282 Hartrees

C	2.4365640000	-2.8408940000	0.0000540000
C	3.1255740000	-1.6793560000	0.0000650000
C	2.3203740000	-0.4883710000	-0.0000140000
H	4.2059530000	-1.6293420000	0.0001100000
C	0.9506630000	-0.6984850000	-0.0000320000
C	2.9670730000	0.8328120000	-0.0000530000
C	-0.2122550000	0.1830860000	-0.0000630000
O	2.3998320000	1.9082380000	-0.0003590000
O	4.3056840000	0.7411550000	0.0002700000
C	-1.5050810000	-0.2818870000	0.0000070000
C	5.0024290000	1.9864400000	0.0002240000
C	-2.5273080000	0.7031260000	-0.0000140000
H	-1.7570170000	-1.3361620000	0.0001600000
C	-2.0563620000	1.9863120000	-0.0000200000
H	4.7491270000	2.5690240000	0.8885360000
H	6.0605520000	1.7296820000	0.0002690000
H	4.7491460000	2.5689020000	-0.8881690000
C	-3.9787590000	0.4204480000	0.0000290000
O	-4.8463340000	1.2646440000	0.0000250000
O	-4.2324080000	-0.9008190000	0.0000850000
C	-5.6147530000	-1.2510320000	0.0001540000
H	-6.1123860000	-0.8546060000	-0.8877960000
H	-5.6443740000	-2.3397240000	0.0002910000
H	-6.1123470000	-0.8543790000	0.8880220000
H	2.8443390000	-3.8409530000	0.0000630000
H	-2.6825650000	2.8679930000	-0.0000340000
Se	0.6148280000	-2.5407820000	-0.0000770000
Se	-0.2255210000	2.0637410000	-0.0000300000

Cartesian coordinates (xyz) and shielding tensor for the proposed triads

Triad-I

Energy = -4343.736490 hartree

C -5.71840400 0.37462200 0.63070000

C -5.35794700 -0.89188500 0.28496800

C -3.94928600 -1.03923600 0.04443200

C -3.23050800 0.15277800 0.20190700

S -4.34483300 1.43589700 0.67921600

H -6.70886000 0.75728800 0.86740600

H -6.05349800 -1.72313300 0.19718300

C -1.83277000 0.52560800 0.04520300

C -1.37472200 1.82665600 0.06358100

C 0.03123600 2.04014300 -0.04113700

H -2.04621400 2.67937900 0.15130000

C 0.79269200 0.87173500 -0.12294600

C 2.22157700 0.59724200 -0.18372900

C 2.81128000 -0.58943400 0.22523800

S 3.45179100 1.64608400 -0.91019800

C 4.20481300 -0.67045700 -0.04911000

H 2.26558700 -1.38507100 0.72968200

C 4.67571500 0.46337100 -0.67892700

H 5.70580500 0.65142400 -0.97491900

C -3.36842200 -2.33840100 -0.32856700

O -2.17997100 -2.58533300 -0.45650400

O -4.31898600 -3.28217700 -0.51570700

C 0.58261200 3.41323400 -0.04185400

O 1.72420400 3.72535300 -0.32232400

O -0.35386700 4.33231500 0.30245200

C 5.10088600 -1.79888800 0.28772800

O 6.28891900 -1.84082900 0.04208300

O 4.43153900 -2.79949100 0.91135900

C -3.83154300 -4.58686000 -0.86763300

H -4.72469300 -5.21391500 -0.97515400

H -3.26838500 -4.54958300 -1.81190100

H -3.17299900 -4.98178000 -0.07973600

C 0.09567600 5.69567400 0.29489600

H 0.91604000 5.83863500 1.01392400

H 0.45186100 5.98350500 -0.70566900

H -0.77705300 6.29478400 0.58170400

C 5.23069000 -3.93549200 1.27243400

H 4.54316000 -4.63875500 1.75796900

H 5.68474900 -4.39204800 0.37998500

H 6.03547400 -3.64204000 1.96329000

Se -0.34701400 -0.64857500 -0.15627400

Shielding = σSe41 = 1129.0 ppm

Triad-II

Energy = -6347.078272 hartree

C -5.50399100 -0.20685400 0.56178400

C -4.96964100 -1.39444400 0.17512300

C -3.54799800 -1.39729600 -0.06325900

C -2.90664800 -0.16848700 0.11579600

H -6.54544900 0.01052400 0.79139800

H -5.56081000 -2.29973000 0.05017900

C -1.53976100 0.29656200 -0.04425400

C -1.17265100 1.62698300 -0.05884300

C 0.21541400 1.93939100 -0.14482600

H -1.90424300 2.43276800 -0.01441900

C 1.06073400 0.82711000 -0.17539800

C 2.50647100 0.65578900 -0.20139300

C 3.17089100 -0.47337600 0.25354900

C 4.57219500 -0.46090000 0.00927700

H 2.67281000 -1.29211300 0.77011700

C 4.97409100 0.68626000 -0.64388200

H 5.99424500 0.94001800 -0.92489900

C -2.86665400 -2.64022900 -0.46731600

O -1.66026300 -2.80227400 -0.55899900

O -3.74059700 -3.63951400 -0.72733300

C 0.66554300 3.34833900 -0.18047300

O 1.78771600 3.73421800 -0.44698600

O -0.34305400 4.20723900 0.11267600

C 5.53938500 -1.51185200 0.39650600

O 6.73245800 -1.47431700 0.17591400

O 4.92999100 -2.54071700 1.03530800

C -3.14923800 -4.89235000 -1.10705200

H -3.99122100 -5.57494600 -1.27331900

H -2.55521000 -4.77880600 -2.02593900

H -2.49425500 -5.27152900 -0.30850200

C 0.00668000 5.59891300 0.06783400

H 0.79732000 5.82492600 0.79873900

H 0.36457200 5.87911400 -0.93426900

H -0.91364500 6.14169600 0.31532700

C 5.80035800 -3.60571000 1.44502500

H 5.15436100 -4.34346700 1.93636000

H 6.30591400 -4.05217900 0.57546200

H 6.56627400 -3.23615100 2.14350400

Se 0.03357900 -0.77139100 -0.19026900

Se -4.19399000 1.12572900 0.68101400

S 3.67388700 1.77051100 -0.93368100

Shielding = σSe39 = 1127.2 ppm; σSe40 = 1197.9 ppm

Triad-III

Energy = -6347.081406 hartree

C 5.94284400 0.69028400 0.56497900

C 5.66698400 -0.59695700 0.21783100

C 4.26728000 -0.84545800 0.01070500

C 3.46780900 0.29007300 0.19462700

S 4.49720000 1.64796000 0.65603700

H 6.90840100 1.14256300 0.78086500

H 6.41885400 -1.37462200 0.10650900

C 2.04368800 0.56195000 0.07398200

C 1.49511800 1.82622000 0.10244300

C 0.07500500 1.93878300 0.03391000

H 2.10654600 2.72486400 0.16697600

C -0.60953100 0.71920700 -0.02325600

C -2.01513900 0.35319800 -0.04482000

C -2.48917100 -0.91408900 0.24855200

C -3.88848100 -1.12837700 0.08076600

H -1.83989100 -1.71296400 0.60631400

C -4.57986100 -0.02204100 -0.36010600

H -5.65546300 0.01238900 -0.52737500

C 3.77372500 -2.18182800 -0.35737000

O 2.60392800 -2.51573000 -0.45434100

O 4.78630600 -3.05102100 -0.57857300

C -0.56190500 3.26982600 0.01920700

O -1.73107600 3.50227900 -0.23830600

O 0.31485100 4.25948900 0.31242000

C -4.59225900 -2.40458500 0.35476800

O -5.78386300 -2.58667600 0.21229300

O -3.73948500 -3.36566000 0.78949300

C 4.38729500 -4.38614700 -0.92747000

H 5.32111100 -4.94416600 -1.06567800

H 3.78310600 -4.83409600 -0.12450800

H 3.79572200 -4.38506800 -1.85495100

C -0.22567900 5.58955800 0.28173900

H -0.62117300 5.82662600 -0.71728300

H -1.03783400 5.69594600 1.01609500

H 0.61120400 6.25211500 0.53333700

C -4.34526200 -4.63430500 1.07655100

H -3.52706100 -5.28470600 1.40915300

H -5.10489400 -4.53368800 1.86646300

H -4.82765800 -5.04806500 0.17810400

Se 0.64130700 -0.71675900 -0.08554700

Se -3.48737200 1.46388200 -0.57612200

Shielding = σSe40 = 1133.0 ppm; σSe41 = 1165.2 ppm

Triad-IV

Energy = -8350.423188 hartree

C 5.76974200 0.03767800 0.49197100

C 5.30170300 -1.17781700 0.10591500
C 3.87749700 -1.26890700 -0.09696400
C 3.16461200 -0.08474100 0.11054900
H 6.80089700 0.31842400 0.69813700
H 5.94553600 -2.04259200 -0.04332100
C 1.76807700 0.29527000 -0.01125300
C 1.31951500 1.59955700 -0.01076000
C -0.08720300 1.82578300 -0.06026900
H 2.00106600 2.44880600 0.01402600
C -0.86894300 0.66437600 -0.07072800
C -2.29954900 0.41379300 -0.05891400
C -2.86863300 -0.80210300 0.27979500
C -4.28343600 -0.90692600 0.14103500
H -2.27915000 -1.64026700 0.65090000
C -4.89147100 0.23885800 -0.32154100
H -5.96374100 0.35558500 -0.47223200
C 3.26615300 -2.54940900 -0.49628000
O 2.07076800 -2.78804400 -0.55741500
O 4.19520800 -3.48800200 -0.79013600
C -0.61426200 3.20329000 -0.10489000
O -1.76560000 3.52287700 -0.34868300
O 0.34564000 4.12650500 0.14219800
C -5.08268000 -2.11347000 0.46456400
O -6.28751800 -2.20213000 0.34683400
O -4.30228200 -3.12769200 0.91407500
C 3.67519900 -4.77285800 -1.16705500
H 4.55428600 -5.39799400 -1.36442300
H 3.06920300 -5.20109400 -0.35472400
H 3.04891900 -4.68952400 -2.06757500
C -0.08587500 5.49479400 0.07910900
H -0.48098000 5.73320100 -0.91973000
H -0.87166300 5.68913200 0.82405400
H 0.80684900 6.09415400 0.29471300
C -5.00294400 -4.33426300 1.24902400
H -4.23386700 -5.03884100 1.58839900

H -5.73763100 -4.14952400 2.04728200

H -5.53318100 -4.73348900 0.37120100

Se 0.26096600 -0.86863300 -0.11997700

Se 4.38146900 1.28307900 0.65865000

Se -3.68717900 1.62462600 -0.59930700

Shielding =σSe39 = 1130.4 ppm; σSe40 = 1197.0 ppm; σSe41 = 1165.4 ppm;

Cartesian coordinates (xyz) and Shielding tensor for the proposed pentads

Pentad-I

Energy = -13916.579435 hartree

C 6.38235100 0.20500800 -0.16177400

C 6.90887400 -0.87371800 0.52846100

C 8.32483400 -1.03195200 0.48514100

C 8.97778900 -0.07064500 -0.25388400

H 6.28533500 -1.56559400 1.09424900

H 10.05748700 -0.01545700 -0.38545500

C 4.95975800 0.46179300 -0.30155300

C 4.20754900 1.58958300 -0.65507800

C 2.79527900 1.40897200 -0.59972000

C 2.31241600 0.16486100 -0.24369300

H 2.13385300 2.23728200 -0.84919200

C 0.90476700 -0.13493500 -0.06918800

C 0.17322100 -1.32773500 0.01824000

C -1.23578100 -1.15947800 0.14058100

C -1.73520200 0.12741300 0.18758900

H -1.88097700 -2.03416700 0.20700700

C -3.14940400 0.44348600 0.22655800

C -3.87404900 1.60133700 0.53925100

C -5.29034600 1.45039100 0.49919900

C -5.80332900 0.22149000 0.13925300

H -5.92921800 2.29890500 0.74012300

C -7.22030800 -0.09613800 0.12689600

C -7.98355700 -1.14319000 -0.39775200

C -9.40765600 -1.02622400 -0.20863400

C -9.82803400 0.07248300 0.47084600

H -10.08813800 -1.78429900 -0.59185200

H -10.85058200 0.34884600 0.72108200

Se 7.81891000 1.19640700 -0.96098700

Se 3.79356700 -1.00453000 0.04095500

Se -0.27388600 1.35226800 0.11100400

Se -4.35418400 -0.95515400 -0.25208000

Se -8.38669400 1.15082400 0.98570100
C 9.08129200 -2.10910600 1.16792500
O 10.28717000 -2.24391900 1.13137000
O 8.25994600 -2.94524100 1.85084500
C 4.77132700 2.88756500 -1.07329800
O 5.93882100 3.10672000 -1.35046300
O 3.82768900 3.85602000 -1.14368600
C 0.75783400 -2.68184900 -0.00140600
O 1.94699400 -2.95057200 0.05108100
O -0.18750200 -3.64756400 -0.07143800
C -3.27833800 2.90525600 0.88619300
O -2.09705700 3.19891700 0.80299000
O -4.20493100 3.79574600 1.31160300
C -7.42375300 -2.30955700 -1.10433300
O -6.24022900 -2.59130400 -1.20304100
O -8.38800600 -3.08616100 -1.64913200
C 8.91755000 -4.01775700 2.54044300
H 9.46963300 -4.65536200 1.83344800
H 9.62687600 -3.62568900 3.28496300
H 8.11929400 -4.58778300 3.03135100
C 4.29509100 5.14115600 -1.58085200
H 5.05841800 5.53215200 -0.89181900
H 4.73158400 5.07511400 -2.58875100
H 3.41031700 5.78907800 -1.58454100
C 0.30635200 -4.99601100 -0.06697100
H -0.58374000 -5.63395900 -0.12426100
H 0.96502000 -5.17132300 -0.93046200
H 0.87155600 -5.20064600 0.85457300
C -3.70083400 5.09950700 1.64202900
H -4.57561200 5.68063900 1.95762200
H -2.96374200 5.03598000 2.45612800
H -3.22130100 5.56453200 0.76779000
C -7.92096900 -4.25709000 -2.33783900
H -7.36345000 -4.91433200 -1.65397100
H -8.82341100 -4.75916500 -2.70662500

H -7.26296000 -3.97906100 -3.17439200

Shielding = σSe28 = 1166.8 ppm; σSe29 = 1130.4 ppm; σSe30 = 1131.5 ppm; σSe31 = 1131.2 ppm; σSe32 = 1195.8 ppm

Pentad-II

Energy = -11913.237656 hartree

C 6.03194100 0.15913600 -0.18568200

C 6.54738400 -0.94169500 0.47746700

C 7.95982900 -1.12326300 0.41483200

C 8.62107200 -0.15899400 -0.31286700

H 5.91833200 -1.63381300 1.03682200

H 9.70003000 -0.11973400 -0.45573000

C 4.61251700 0.44288400 -0.30419100

C 3.87604800 1.58976300 -0.62813800

C 2.46152600 1.43227300 -0.56015600

C 1.96117000 0.19018800 -0.22175500

H 1.81185100 2.27629800 -0.78677700

C 0.55049300 -0.08888700 -0.03728100

C -0.20040900 -1.27040000 0.03710000

C -1.60505800 -1.08045600 0.17761600

C -2.08178700 0.21358300 0.25259400

H -2.26422600 -1.94529400 0.23551600

C -3.48991900 0.55369400 0.31149400

C -4.19132600 1.71755900 0.65212900

C -5.61100600 1.59251200 0.62290200

C -6.14402800 0.37836300 0.24563700

H -6.23466300 2.44459000 0.88828400

C -7.56896800 0.08682100 0.22496700

C -8.34661800 -0.96561100 -0.27558100

C -9.75698900 -0.77491100 -0.08090200

C -10.06281500 0.38506000 0.56307000

H -10.49436600 -1.49898300 -0.41917500

H -11.04230200 0.77024400 0.83821700

Se 7.47649200 1.14130600 -0.98191500

Se 3.42494700 -1.00938000 0.02460400

Se -0.60068200 1.41465600 0.18176900

Se -4.72301200 -0.81851700 -0.17263200

C 8.70506800 -2.22636000 1.06786000

O 9.90795800 -2.38102000 1.01493600

O 7.87703200 -3.06157200 1.74383300

C 4.45748400 2.88556500 -1.02851100

O 5.62556100 3.09009700 -1.31431200

O 3.52989100 3.87102300 -1.07073900

C 0.36051600 -2.63368200 -0.01281200

O 1.54536400 -2.92361100 0.02134400

O -0.60204500 -3.58182800 -0.08888600

C -3.56927600 3.00397100 1.01810500

O -2.38398600 3.27887500 0.92728100

O -4.47553000 3.90122500 1.47136300

C -7.82241600 -2.16836700 -0.94175900

O -6.64579500 -2.46884000 -1.06340500

O -8.81425200 -2.95316900 -1.42070100

C 8.52364700 -4.15841700 2.40493500

H 9.05679700 -4.79136100 1.67945900

H 9.24784100 -3.79314000 3.14877300

H 7.72117900 -4.72428700 2.89378500

C 4.01461600 5.15596100 -1.48913100

H 4.79167800 5.52111200 -0.80126500

H 4.43937200 5.10133200 -2.50271600

H 3.14107300 5.81872000 -1.47134800

C -0.13139500 -4.93829500 -0.11383100

H -1.03289800 -5.55996400 -0.17172100

H 0.51414300 -5.10947400 -0.98800700

H 0.44086400 -5.16874500 0.79720700

C -3.94563900 5.18917500 1.82256300

H -4.80693000 5.77838300 2.15953100

H -3.20109800 5.09654400 2.62704600

H -3.46752000 5.66382400 0.95271700

C -8.38586300 -4.15911200 -2.07330000

H -7.81525700 -4.79494000 -1.38006900

H -9.30651600 -4.66299800 -2.39100100

H -7.75188600 -3.92668400 -2.94174600

S -8.63382600 1.28790000 0.96001100

Shielding = σSe28 = 1166.9 ppm; σSe29 = 1130.4 ppm; σSe30 = 1131.2 ppm; σSe31 = 1133.4 ppm

Pentad-III

Energy = -11913.233977 hartree

C -6.15814500 0.17250900 0.12748500

C -6.66895100 -0.92117800 -0.55088100

C -8.08415100 -1.08913800 -0.52097900

C -8.75240500 -0.12076600 0.19476400

H -6.03404600 -1.61763200 -1.09811600

H -9.83390300 -0.07141400 0.31319500

C -4.73911800 0.44199400 0.27928800

C -3.99911400 1.58075100 0.62304700

C -2.58496700 1.40948800 0.58694200

C -2.08937600 0.16332900 0.25685900

H -1.93263000 2.24672700 0.83059100

C -0.67790900 -0.12976000 0.10164600

C 0.06298000 -1.31789900 0.04258700

C 1.47226400 -1.14185400 -0.06971900

C 1.95830200 0.14816500 -0.13441600

H 2.12607100 -2.01147700 -0.10786600

C 3.37144600 0.47939900 -0.19188300

C 4.08357100 1.66070300 -0.45284600

C 5.49253400 1.47059400 -0.43455300

C 5.91046400 0.18566700 -0.14979600

H 6.17857500 2.29444800 -0.61958400

C 7.29718500 -0.25731000 -0.17872800

C 8.00167500 -1.31395000 0.39917700

C 9.41822500 -1.32355000 0.13637400

C 9.88296600 -0.32147600 -0.65638800

H 10.06056600 -2.09600800 0.55536900

H 10.90904500 -0.14724300 -0.97483400

Se -7.61082700 1.16616700 0.89406800

Se -3.55864600 -1.02129900 -0.02538800

Se 0.49223800 1.36430100 -0.08086500

Se 8.49818700 0.81483400 -1.19954400

C -8.82501600 -2.18284000 -1.19450200

O -10.03023300 -2.32590900 -1.16934200

O -7.98995100 -3.02395800 -1.85426200

C -4.57687200 2.88123700 1.01338900

O -5.74906900 3.09654200 1.27312900

O -3.64088100 3.85747700 1.07913500

C -0.51204200 -2.67593300 0.08302300

O -1.69868300 -2.95402100 0.02206600

O 0.43926600 -3.63233400 0.18327800

C 3.49412100 2.98367400 -0.71476200

O 2.30945200 3.26819800 -0.65035200

O 4.43358500 3.90160500 -1.04001900

C 7.38999500 -2.36451200 1.24094000

O 6.19837600 -2.57075900 1.37651400

O 8.32855600 -3.11831100 1.86308100

C -8.63192100 -4.11245600 -2.53347700

H -9.18728400 -4.74254300 -1.82232200

H -9.33564500 -3.73787600 -3.29218300

H -7.82405800 -4.68445100 -3.00603300

C -4.12246400 5.14610500 1.48975400

H -4.88023400 5.52040100 0.78547900

H -4.57049000 5.09327700 2.49336600

H -3.24236500 5.80036800 1.49335500

C -0.04388300 -4.98451400 0.20194400

H 0.85058500 -5.61373800 0.28228000

H -0.71046200 -5.14684900 1.06189500

H -0.59747200 -5.21291800 -0.72107300

C 3.93950600 5.22649900 -1.29289500

H 4.82398400 5.82778300 -1.53503500

H 3.23111500 5.22288400 -2.13451900

H 3.42956100 5.62767000 -0.40438600

C 7.81624200 -4.18053300 2.68249200

H 7.21659000 -4.88113500 2.08222900

H 8.69839700 -4.68330300 3.09686500

H 7.18485200 -3.77917600 3.48905900

S 4.49829300 -0.83042400 0.14136800

Shielding = σSe28 = 1166.8 ppm; σSe29 = 1129.6 ppm; σSe30 = 1133.1 ppm; σSe31 = 1190.0 ppm

Pentad-IV

Energy = -11913.234167 hartree

C -6.44946900 -0.10407800 -0.11008700

C -6.87969300 1.00346600 0.59888400

C -8.28815000 1.21914500 0.64899700

C -9.02804700 0.27682900 -0.02923700

H -6.19052100 1.67897600 1.10456100

H -10.11533600 0.26499200 -0.08910000

C -5.04948500 -0.43800100 -0.32561200

C -4.37950000 -1.58475500 -0.77995600

C -2.96545900 -1.43923300 -0.76478400

C -2.50262500 -0.20915800 -0.33572100

H -2.30799700 -2.24283300 -1.08922700

C -1.09888400 0.11769000 -0.14844800

C -0.37790000 1.31636100 -0.10004000

C 1.02955700 1.15802100 0.04868400

C 1.53284100 -0.12462300 0.15560200

H 1.67099500 2.03728600 0.08524400

C 2.94753600 -0.43354200 0.22810600

C 3.67022900 -1.57743400 0.59223200

C 5.08669400 -1.42380100 0.56865100

C 5.60182000 -0.20645000 0.17447000

H 5.72397200 -2.26152200 0.84842900

C 7.01802100 0.11528700 0.17333300

C 7.78667800 1.14511900 -0.37674300

C 9.20788200 1.03968700 -0.16103800

C 9.62028300 -0.03230600 0.56447500

H 9.89235100 1.78559800 -0.56068400
H 10.63943400 -0.29605500 0.84082100
Se -7.97172900 -1.04025500 -0.80360800
Se 0.07608100 -1.35583100 0.10968200
Se 8.17376100 -1.09584400 1.09529600
C -8.95242800 2.33612000 1.36358800
O -10.15166400 2.51978700 1.40578300
O -8.05369400 3.14608700 1.97611500
C -5.01421600 -2.82725700 -1.25034000
O -6.20719400 -2.99891700 -1.43816900
O -4.10546800 -3.80383500 -1.47961900
C -0.97018900 2.66803100 -0.19924900
O -2.15681900 2.93379700 -0.15593300
O -0.02146200 3.62670000 -0.33622700
C 3.07217300 -2.86978500 0.97556000
O 1.89218400 -3.16798000 0.88759100
O 3.99406800 -3.74380000 1.44276900
C 7.23495900 2.28346900 -1.13369100
O 6.05243700 2.55814700 -1.26005700
O 8.20555100 3.04227800 -1.69205400
C -8.61848500 4.25507400 2.68985100
H -9.19012300 4.90538900 2.01052000
H -9.29160900 3.90385500 3.48655600
H -7.76604200 4.79762700 3.11652700
C -4.64228100 -5.04227000 -1.96908800
H -5.35133800 -5.47163000 -1.24572800
H -5.16426900 -4.88972600 -2.92560300
H -3.77806800 -5.70416800 -2.10177700
C -0.51626700 4.97213000 -0.41159000
H 0.37258500 5.60684800 -0.51064700
H -1.17843600 5.09470800 -1.28161400
H -1.07916400 5.23204400 0.49748000
C 3.48729800 -5.03626600 1.81149900
H 4.35870700 -5.60476800 2.15789000
H 2.73992700 -4.94593200 2.61359500

H 3.01941700 -5.53182700 0.94779800

C 7.74631100 4.18633600 -2.42951300

H 7.17725100 4.86633900 -1.77818700

H 8.65308400 4.67715700 -2.80278800

H 7.10144000 3.87649000 -3.26511200

S -3.88330900 0.82669900 0.03535200

Se 4.15594500 0.95172300 -0.27898700

Shielding = σSe28 = 1167.5 ppm; σSe29 = 1127.9 ppm; ; σSe30 = 1195.6 ppm; σSe67 = 1131.9 ppm

Pentad-V

Energy = -11913.234479

C 6.69084900 0.29538000 -0.31188900

C 7.24760600 -0.68984200 0.49005200

C 8.65675100 -0.82533400 0.35113500

C 9.17416500 0.06158100 -0.57074600

H 6.66527400 -1.29665300 1.18130800

H 10.22322000 0.16722300 -0.83980100

C 5.26196900 0.54668500 -0.43458300

C 4.49955900 1.66474000 -0.78657800

C 3.09033600 1.47093400 -0.70850200

C 2.62479100 0.22553400 -0.33104300

H 2.41740000 2.29133200 -0.95359100

C 1.22260900 -0.08599200 -0.13223100

C 0.50613600 -1.28507100 -0.01276300

C -0.90306800 -1.13067200 0.12583500

C -1.41650500 0.15110300 0.15525500

H -1.53713300 -2.01116900 0.21776300

C -2.83370200 0.45204600 0.20696500

C -3.56739400 1.60695200 0.50895900

C -4.98228600 1.43954000 0.48976000

C -5.48570500 0.19892200 0.15755900

H -5.62770600 2.28490700 0.72420800

C -6.89900800 -0.13478700 0.16899200

C -7.65692300 -1.19866900 -0.32880200

C -9.07972000 -1.09452200 -0.12319400

C -9.50381700 0.01030300 0.54396300

H -9.75640500 -1.86621500 -0.48538000

H -10.52615900 0.27926100 0.80295700

Se 0.02920100 1.39079500 0.03498400

Se -8.06833600 1.11274500 1.02286800

C 9.52358100 -1.77172800 1.08749700

O 10.72603200 -1.86575200 0.94941500

O 8.80915500 -2.53747200 1.94869300

C 5.05335800 2.97204800 -1.20293200

O 6.21289500 3.19846000 -1.49301900

O 4.09781900 3.93366600 -1.24504900

C 1.10626200 -2.63231000 -0.01528700

O 2.29941400 -2.88603300 0.02366600

O 0.17190700 -3.61026500 -0.05206100

C -2.98211600 2.92331900 0.82556300

O -1.80550900 3.22868500 0.72133400

O -3.91313000 3.81047200 1.24816100

C -7.09288600 -2.37008600 -1.02358800

O -5.90759100 -2.64040900 -1.13246000

O -8.05504300 -3.16589000 -1.54378800

C 9.57760500 -3.48506600 2.70401300

H 10.09236400 -4.19121300 2.03504300

H 10.33246700 -2.97263200 3.31942200

H 8.85560600 -4.01238900 3.33939000

C 4.54947700 5.22716600 -1.67241000

H 5.31806500 5.61655400 -0.98815900

H 4.97517400 5.17668900 -2.68591100

H 3.65997400 5.86858800 -1.65829100

C 0.68196100 -4.95252800 -0.02977400

H -0.20119900 -5.60181400 -0.06081800

H 1.32909000 -5.13664700 -0.90012300

H 1.26390300 -5.13276800 0.88642500

C -3.41977800 5.12552400 1.54890900

H -4.29687900 5.70204000 1.86650600

H -2.67090800 5.08465100 2.35364900

H -2.95773000 5.58059100 0.66014100

C -7.58351100 -4.34266100 -2.21936800

H -7.01036600 -4.98261800 -1.53203000

H -8.48478600 -4.86045400 -2.56875800

H -6.93896300 -4.07106300 -3.06841700

Se -4.02833600 -0.96797800 -0.23226800

Se 4.12211500 -0.92543400 -0.05673800

S 7.97291600 1.08629600 -1.24687600

Shielding = σSe66 = 1126.2 ppm; σSe28 = 1132.3 ppm; σSe65 = 1131.0 ppm; σSe29 = 1195.8 ppm

Pentad-VI

Energy = -9909.892313 hartree

C 5.78616500 0.13841200 -0.15772600

C 6.29146600 -0.97294800 0.49557800

C 7.70366100 -1.15952000 0.44264600

C 8.37497500 -0.18875500 -0.26695900

H 5.65487300 -1.66960600 1.04058800

H 9.45526400 -0.15211600 -0.40011600

C 4.36895100 0.42946800 -0.28473600

C 3.63981700 1.58332500 -0.60020100

C 2.22409100 1.43062600 -0.54636000

C 1.71616300 0.18631300 -0.22833500

H 1.57993500 2.28029900 -0.76769300

C 0.30311900 -0.09012000 -0.05748200

C -0.45304700 -1.26887800 -0.00562000

C -1.85814500 -1.07557800 0.12927500

C -2.32553200 0.21972000 0.22004000

H -2.52303700 -1.93693600 0.16366900

C -3.73305100 0.56950300 0.30216200

C -4.42542100 1.75633500 0.58852900

C -5.83744200 1.58639200 0.58530700

C -6.27320600 0.31074600 0.28946200

H -6.51050400 2.41517000 0.79279000

C -7.66766600 -0.11311700 0.31870100

C -8.38316700 -1.18040200 -0.23416300

C -9.79116500 -1.11922900 0.04058800

C -10.15044800 -0.04562600 0.79892100

H -10.48856500 -1.86818900 -0.32729700

H -11.14064400 0.23416100 1.15204300

Se 7.24140600 1.12469600 -0.92900000

Se 3.17289800 -1.02225700 0.01456600

Se -0.84389600 1.41664700 0.16378100

C 8.43887100 -2.27395100 1.08776900

O 9.64154000 -2.43284600 1.04305600

O 7.60175000 -3.11436400 1.74584000

C 4.22971500 2.88182800 -0.97876400

O 5.40101100 3.08544200 -1.25170100

O 3.30628300 3.87143400 -1.01636700

C 0.10266100 -2.63375500 -0.07457000

O 1.28611500 -2.92879000 -0.03490400

O -0.86301100 -3.57564500 -0.17534500

C -3.81409400 3.06717400 0.86173500

O -2.62636200 3.33591800 0.78616200

O -4.73621700 3.99312200 1.21200300

C -7.80066700 -2.27502900 -1.03441800

O -6.61434400 -2.49855800 -1.18795700

O -8.76220300 -3.04795500 -1.59433600

C 8.23828100 -4.22229800 2.39820000

H 8.77499900 -4.84807600 1.66914800

H 8.95760300 -3.86960900 3.15276100

H 7.42940400 -4.79105800 2.87292200

C 3.79963700 5.15969600 -1.41391800

H 4.57204300 5.51288400 -0.71465500

H 4.23305900 5.11641500 -2.42437700

H 2.92854900 5.82565700 -1.39521500

C -0.39871000 -4.93373600 -0.22123700

H -1.30275500 -5.54958900 -0.29793900

H 0.25318000 -5.09199900 -1.09313000

H 0.16491500 -5.18353000 0.69009400

C -4.22039400 5.30692300 1.47875300

H -5.09324200 5.91659800 1.74122400

H -3.50173900 5.28044500 2.31121600

H -3.71587800 5.71460600 0.59009700

C -8.28196200 -4.15417200 -2.37406500

H -7.67380600 -4.83152500 -1.75596100

H -9.17949100 -4.66668300 -2.74068900

H -7.66801300 -3.79937300 -3.21520600

S -8.77416800 0.92828800 1.21061200

S -4.88190900 -0.72235300 -0.02863400

Shielding = σSe28 = 1166.9 ppm; σSe29 = 1129.6 ppm; σSe30 = 1133.1 ppm

Pentad-VII

Energy = -9909.892388 hartree

C 6.09189100 0.05872000 -0.13762800

C 6.51163900 -1.07186500 0.54059100

C 7.91672700 -1.31216500 0.56852800

C 8.66444100 -0.36698100 -0.09701800

H 5.81715100 -1.74724600 1.03910900

H 9.75098700 -0.37197000 -0.16993800

C 4.69530900 0.42092500 -0.32818300

C 4.03960300 1.58848100 -0.74910800

C 2.62355800 1.46644500 -0.71970500

C 2.14488700 0.23530000 -0.31160200

H 1.97615200 2.28793300 -1.01856300

C 0.73806700 -0.07196300 -0.11446400

C -0.00242300 -1.25915900 -0.08156900

C -1.40528500 -1.08044400 0.08681400

C -1.88570100 0.20787100 0.22511600

H -2.06069800 -1.94972600 0.11316400

C -3.29410500 0.53943200 0.32028600

C -3.99314900 1.68835000 0.71251100

C -5.41284600 1.55969200 0.70239400

C -5.94846700 0.35715700 0.29327100

H -6.03437900 2.40023100 1.00667700

C -7.37281500 0.06170200 0.28602700

C -8.15553200 -0.97662400 -0.23557500

C -9.56308000 -0.79700400 -0.01205800

C -9.86165000 0.34057500 0.67387800

H -10.30382700 -1.51227800 -0.36149900

H -10.83761600 0.71338100 0.97714500

Se 7.62153900 0.98498400 -0.82823800

Se -0.40911700 1.41540800 0.18643000

Se -4.53119400 -0.82034700 -0.18798300

C 8.57030900 -2.45631900 1.24915200

O 9.76666900 -2.66092800 1.27258500

O 7.66521400 -3.26520100 1.85372200

C 4.68971600 2.83027400 -1.19989500

O 5.88317300 2.98621300 -1.39814200

O 3.79498400 3.82663300 -1.39700700

C 0.56559800 -2.61824600 -0.21493100

O 1.74794900 -2.90479300 -0.19134100

O -0.40084100 -3.55798400 -0.35958000

C -3.36858800 2.96306100 1.11259500

O -2.18461100 3.24263600 1.01644400

O -4.26990700 3.84362400 1.60617800

C -7.63889400 -2.15563300 -0.94853800

O -6.46357100 -2.44775500 -1.09936100

O -8.63620600 -2.92837000 -1.43559000

C 8.21944400 -4.39972700 2.53482200

H 8.77219100 -5.04340100 1.83387600

H 8.90752500 -4.07839900 3.33137300

H 7.36296700 -4.93789400 2.95897000

C 4.34693900 5.06649100 -1.86555000

H 5.07150700 5.46786000 -1.14148500

H 4.85513900 4.92653300 -2.83137100

H 3.49255900 5.74546400 -1.97331200

C 0.07016800 -4.90965200 -0.46798300

H -0.83042000 -5.52731500 -0.56888300

H 0.71976800 -5.02562300 -1.34833200

H 0.63937800 -5.19733200 0.42871300

C -3.73701300 5.11993200 1.99364900

H -4.59470300 5.69628500 2.36067000

H -2.98250600 5.00156600 2.78536100

H -3.27020000 5.62402200 1.13429900

C -8.21510000 -4.11148500 -2.13323000

H -7.63101700 -4.76689500 -1.47012500

H -9.13940200 -4.60834000 -2.45140400

H -7.59646900 -3.84933900 -3.00427200

S -8.42896200 1.23494000 1.07651200

S 3.51205100 -0.83147100 0.01997900

Shielding = σSe28 = 1167.6 ppm; σSe29 = 1127.8 ppm; σSe30 = 1134.2 ppm

Pentad-VIII

Energy = -9909.892701 hartree

C 6.33845600 0.24715900 -0.33962100

C 6.88758500 -0.76354300 0.43543900

C 8.29231300 -0.92070500 0.27605400

C 8.81394100 -0.02448900 -0.63439200

H 6.30315200 -1.37400600 1.12169100

H 9.86130100 0.06825100 -0.91457200

C 4.91279600 0.52549700 -0.43940700

C 4.16586800 1.66333800 -0.75974000

C 2.75448300 1.49228600 -0.66828400

C 2.27178300 0.24779600 -0.30991500

H 2.09313100 2.32890700 -0.88882000

C 0.86678200 -0.04359900 -0.10051600

C 0.13112900 -1.23226800 0.00479000

C -1.27362100 -1.05649300 0.16279400

C -1.76441800 0.23297600 0.22229500

H -1.92154300 -1.92778900 0.24543400

C -3.17558700 0.55785000 0.29527300

C -3.88576200 1.71880200 0.62725600

C -5.30416200 1.57705000 0.61960500

C -5.82801400 0.35105300 0.26870000

H -5.93405700 2.42603000 0.88013800

C -7.24959700 0.04281800 0.27228700

C -8.02169100 -1.02567500 -0.20211900

C -9.43138800 -0.84828800 0.00927300

C -9.74184300 0.31736100 0.64066200

H -10.16487300 -1.58557400 -0.30829600

H -10.72190500 0.69525800 0.92375200

Se 3.75195400 -0.93396400 -0.07660300

Se -0.29907900 1.44987300 0.10856300

Se -4.39892600 -0.83579200 -0.15057500

C 9.15126800 -1.89679000 0.98225200

O 10.35007000 -2.00903100 0.82704300

O 8.43407200 -2.66723000 1.83695700

C 4.73742400 2.96902300 -1.15671300

O 5.89724600 3.18126800 -1.45628000

O 3.79837300 3.94759400 -1.16818300

C 0.70768000 -2.58926600 -0.03032300

O 1.89660800 -2.86421000 -0.01097500

O -0.24392500 -3.55025700 -0.07363300

C -3.27372800 3.01796200 0.96414200

O -2.09320800 3.30501800 0.85169500

O -4.18389500 3.91165700 1.41648700

C -7.49260000 -2.23195800 -0.85796500

O -6.31431500 -2.52093200 -0.99087700

O -8.48160700 -3.03468300 -1.31240700

C 9.19489100 -3.64321100 2.56327600

H 9.68866100 -4.34460100 1.87379100

H 9.96634500 -3.15663900 3.17910100

H 8.47159200 -4.17054700 3.19716400

C 4.26746300 5.24143800 -1.57519500

H 5.05050800 5.60386300 -0.89252100

H 4.68054600 5.20394000 -2.59446300

H 3.38944600 5.89758600 -1.53784600

C 0.24304300 -4.90118500 -0.08287400

H -0.65153700 -5.53460400 -0.11490800

H 0.87614400 -5.07986400 -0.96460400

H 0.83301400 -5.10864900 0.82236800

C -3.66430300 5.21120600 1.73934600

H -4.52755200 5.79564000 2.07959100

H -2.90706000 5.14017100 2.53410500

H -3.20460000 5.67734800 0.85509700

C -8.04807700 -4.24506200 -1.95329900

H -7.46117200 -4.86432700 -1.25868500

H -8.96700700 -4.76381500 -2.25146100

H -7.42827800 -4.01811400 -2.83335000

S -8.31816700 1.24216000 1.00471100

S 7.62275900 1.03456000 -1.27451600

Shielding = σSe28 = 1126.3 ppm; σSe29 = 1132.1 ppm; σSe30 = 1133.3 ppm

Pentad-IX

Energy = -9909.888709 hartree

C -6.22169800 0.06759400 0.07766100

C -6.63441500 -1.05444000 -0.61878400

C -8.04045000 -1.28197600 -0.68305700

C -8.79604600 -0.33483700 -0.02932800

H -5.93379000 -1.73253100 -1.10488700

H -9.88406600 -0.33061900 0.01673800

C -4.82709700 0.41589400 0.30518800

C -4.17162100 1.57482700 0.74953300

C -2.75630600 1.44014600 0.75419000

C -2.27905800 0.20708100 0.35056800

H -2.10917100 2.25390800 1.07412200

C -0.87096700 -0.11234400 0.18304500

C -0.13987400 -1.30508800 0.16746100

C 1.26795600 -1.13866000 0.02776300

C 1.75702100 0.14614800 -0.10244900
H 1.91881800 -2.01139200 0.02300200
C 3.17021000 0.46968900 -0.19644500
C 3.88067400 1.63798500 -0.51408300
C 5.28941900 1.44479500 -0.51143000
C 5.70872900 0.17035800 -0.18503000
H 5.97434300 2.25891100 -0.73885300
C 7.09357900 -0.27819100 -0.22083400
C 7.80545900 -1.31283700 0.38684800
C 9.21693600 -1.33813800 0.09907700
C 9.66992800 -0.37077900 -0.74216200
H 9.86465500 -2.09516200 0.53751200
H 10.69052000 -0.21329000 -1.08595800
Se -7.75970800 1.00263000 0.73708500
Se 0.29463500 1.36716500 -0.08436000
Se 8.27862800 0.74729100 -1.30604500
C -8.68701700 -2.41543800 -1.38787600
O -9.88417900 -2.60916300 -1.44221500
O -7.77437600 -3.22803200 -1.97584400
C -4.82161900 2.81953300 1.19229500
O -6.01813300 2.98491700 1.36239300
O -3.92320700 3.80659200 1.41766800
C -0.72232000 -2.65913800 0.29323000
O -1.90618300 -2.93550800 0.24069500
O 0.23232300 -3.60519900 0.46655400
C 3.28944000 2.95102900 -0.81729300
O 2.10567600 3.23910700 -0.74858700
O 4.22504700 3.85511000 -1.18853400
C 7.20610500 -2.32583800 1.28195600
O 6.01656900 -2.52203400 1.44718900
O 8.15366200 -3.05669700 1.91763400
C -8.32147600 -4.35281800 -2.67856600
H -8.89679400 -4.99652200 -1.99605600
H -8.98698200 -4.01982100 -3.48937200
H -7.45950600 -4.89549100 -3.08548800

C -4.47556000 5.04825800 1.88095600

H -5.17869000 5.46078500 1.14217900

H -5.00839400 4.90654000 2.83314700

H -3.61814800 5.71886400 2.01406900

C -0.25135000 -4.95276400 0.57044100

H 0.64188000 -5.57629200 0.69700100

H -0.92337100 -5.05894000 1.43504700

H -0.80033600 -5.24107900 -0.33858200

C 3.72856800 5.17008300 -1.48502700

H 4.61036400 5.76098500 -1.76021900

H 3.01008200 5.13550000 -2.31733400

H 3.22958400 5.60478600 -0.60613500

C 7.65326900 -4.08275600 2.78890600

H 7.04089800 -4.80515300 2.22866200

H 8.54137000 -4.57127800 3.20759400

H 7.03769000 -3.64653500 3.58956600

S 4.29922500 -0.82994900 0.16701500

S -3.64684500 -0.84531000 -0.02070400

Shielding = σSe28 = 1167.5 ppm; σSe29 = 1129.3 ppm; σSe30 = 1189.6 ppm

Pentad-X

Energy = -9909.889023 hartree

C 6.47261000 0.26332200 -0.27004400

C 7.01277400 -0.74189100 0.51834300

C 8.42242600 -0.88515700 0.39303300

C 8.95704300 0.01615000 -0.50475800

H 6.41799000 -1.35812200 1.19040500

H 10.00990500 0.11920600 -0.75956400

C 5.04710300 0.52754700 -0.40434600

C 4.29691400 1.65785500 -0.74308000

C 2.88546100 1.47280500 -0.68560200

C 2.40674400 0.22363700 -0.33855700

H 2.22163800 2.30304300 -0.92237600

C 1.00031200 -0.08219200 -0.16108500

C 0.27415500 -1.27757900 -0.07318100

C -1.13566100 -1.11608700 0.05451700

C -1.63583500 0.16909700 0.10366500

H -1.77862600 -1.99243900 0.11576700

C -3.05201300 0.48506700 0.17348200

C -3.77457200 1.66242000 0.42312100

C -5.18134000 1.45589200 0.42573400

C -5.58770500 0.16153200 0.16825900

H -5.87460300 2.27492700 0.60515300

C -6.96872800 -0.29671200 0.22193500

C -7.66785300 -1.37108700 -0.32914200

C -9.08092000 -1.39226700 -0.04885900

C -9.54760600 -0.38205700 0.73235400

H -9.71928700 -2.17906500 -0.44671300

H -10.57170800 -0.21406500 1.06037700

Se 3.89234300 -0.94344500 -0.06959400

Se -0.18509700 1.40103800 0.01022600

Se -8.16961800 0.77910000 1.23899700

C 9.27367000 -1.85272900 1.12001200

O 10.47693300 -1.95299500 0.99389900

O 8.54365400 -2.63032900 1.95716500

C 4.86487100 2.96911100 -1.12657300

O 6.02941600 3.19292100 -1.39800900

O 3.91661300 3.93826800 -1.16116400

C 0.86456700 -2.62913600 -0.09904400

O 2.05546300 -2.89210000 -0.05193800

O -0.07624500 -3.59841000 -0.16805900

C -3.19744000 2.99646100 0.65487000

O -2.01704500 3.29329400 0.57093500

O -4.14352000 3.90906700 0.97575300

C -7.05423000 -2.42902400 -1.16019400

O -5.86201900 -2.62429000 -1.30641800

O -7.99142300 -3.20375500 -1.75818900

C 9.29627900 -3.59884500 2.70181800

H 9.81358600 -4.29516000 2.02456100

H 10.04767000 -3.10473100 3.33616500

H 8.56307000 -4.13345200 3.31797800

C 4.38251800 5.23666700 -1.55719900

H 5.14524000 5.60692900 -0.85597700

H 4.82040300 5.20317000 -2.56620100

H 3.49738200 5.88406600 -1.54126100

C 0.42295500 -4.94490700 -0.17147400

H -0.46495800 -5.58594600 -0.22725800

H 1.07813400 -5.11392600 -1.03885700

H 0.99337000 -5.15096500 0.74653900

C -3.66192900 5.24385000 1.19920800

H -4.55041000 5.83915400 1.44146000

H -2.94352700 5.26328500 2.03208100

H -3.16736600 5.63494800 0.29761900

C -7.47678100 -4.27408800 -2.56550300

H -6.86240700 -4.95772300 -1.96058100

H -8.35799700 -4.79352000 -2.96088400

H -6.85932600 -3.87960900 -3.38612500

S -4.16747500 -0.84314000 -0.12316400

S 7.77129600 1.06333600 -1.17382200

Shielding = σSe28 = 1125.6 ppm; σSe29 = 1133.9 ppm; σSe30 = 1190.0 ppm

Pentad-XI

Energy = -9909.889242 hartree

C 6.77952100 0.18086200 -0.25597000

C 7.23503300 -0.82104800 0.58638800

C 8.64287000 -1.02023100 0.53937200

C 9.25811800 -0.16440400 -0.35073300

H 6.58121700 -1.39880600 1.23701200

H 10.32590200 -0.10668200 -0.55174800

C 5.37370200 0.50722600 -0.46462100

C 4.69287200 1.64559300 -0.91590700

C 3.28094600 1.48819700 -0.87784500

C 2.83449500 0.25624600 -0.43344800

H 2.61191400 2.28556900 -1.19420700

C 1.43609200 -0.08008800 -0.22205200

C 0.72679600 -1.28438700 -0.14935700

C -0.67976300 -1.13721300 0.01881500

C -1.19294200 0.14199400 0.11850300

H -1.31246800 -2.02174000 0.07526800

C -2.60922300 0.43927100 0.20836700

C -3.33669400 1.58053000 0.57101800

C -4.75192600 1.41424800 0.56966500

C -5.26179700 0.18832600 0.19571200

H -5.39253700 2.24927700 0.84987900

C -6.67496700 -0.14575800 0.21835600

C -7.44224400 -1.18800100 -0.30981700

C -8.86110500 -1.09263600 -0.07488100

C -9.27257500 -0.01664000 0.64521700

H -9.54459200 -1.84863600 -0.45685700

H -10.28997500 0.24116300 0.93337400

Se 0.25155300 1.38564300 0.03620300

Se -7.82809200 1.06496500 1.14410200

C 9.41705900 -1.99942000 1.33437400

O 10.62051500 -2.14736500 1.27461400

O 8.61498400 -2.72629100 2.15027800

C 5.31821300 2.89761800 -1.38590900

O 6.50181900 3.06796000 -1.60981600

O 4.39869100 3.87808200 -1.56274200

C 1.33035000 -2.63131600 -0.24188800

O 2.52024700 -2.88489700 -0.21383700

O 0.38941900 -3.60072100 -0.35307600

C -2.74463000 2.88208100 0.93205000

O -1.56882400 3.18968900 0.82328200

O -3.66729000 3.75271500 1.40397100

C -6.89130200 -2.32952000 -1.06255500

O -5.70830800 -2.59528900 -1.20282100

O -7.86297100 -3.10261300 -1.59898800

C 9.28910300 -3.70344600 2.95636900

H 9.81302300 -4.43597900 2.32390500

H 10.02535200 -3.22224300 3.61781900

H 8.50426300 -4.19379000 3.54508700

C 4.91883400 5.12497800 -2.04743700

H 5.65129100 5.54223000 -1.34035000

H 5.41008400 4.98999800 -3.02280300

H 4.05107300 5.78914400 -2.14042900

C 0.89635800 -4.94209600 -0.42066200

H 0.01242900 -5.58649900 -0.49899500

H 1.54650600 -5.06819200 -1.29919500

H 1.47541900 -5.18603100 0.48266200

C -3.16677300 5.05353100 1.75136700

H -4.03799800 5.61788500 2.10492600

H -2.40660700 4.97840700 2.54293500

H -2.71647800 5.54398900 0.87549600

C -7.40417000 -4.25044900 -2.33084000

H -6.82002600 -4.91855100 -1.68055100

H -8.31178400 -4.75301000 -2.68600800

H -6.77390900 -3.94395400 -3.17873100

S 4.22976700 -0.76594800 -0.08049600

Se -3.81234500 -0.96180200 -0.26665200

S 8.14974500 0.90423600 -1.11322400

Shielding = σSe28 = 1128.7ppm; σSe29 = 1195.7 ppm; σSe66 = 1131.9 ppm

Pentad-XII

Energy = -7906.547046 hartree

C 5.84190300 0.03477800 -0.11140100

C 6.25040200 -1.10406300 0.55977000

C 7.65412100 -1.35089400 0.59824100

C 8.41204000 -0.40279300 -0.05140700

H 5.54839300 -1.78101500 1.04546300

H 9.49918100 -0.41189100 -0.11436200

C 4.44872300 0.40495300 -0.31139000

C 3.80187300 1.57968200 -0.72582600

C 2.38498700 1.46344600 -0.71081100

C 1.89773300 0.22994000 -0.32073000

H 1.74389100 2.29091900 -1.00681600

C 0.48829300 -0.07418200 -0.13672400

C -0.25808000 -1.25741400 -0.12951600

C -1.66136300 -1.07517800 0.03463300

C -2.13151700 0.21343400 0.19344700

H -2.32327800 -1.93959300 0.03486800

C -3.53868800 0.55383800 0.31524100

C -4.22913200 1.72690000 0.65741500

C -5.64062000 1.55250500 0.67320200

C -6.07781700 0.28685600 0.33948000

H -6.31219100 2.37086500 0.92261100

C -7.47020400 -0.14321000 0.37933400

C -8.19287500 -1.19121100 -0.20025500

C -9.59542700 -1.14614400 0.10378600

C -9.94327700 -0.10382000 0.90963700

H -10.29744200 -1.88317000 -0.27913400

H -10.92731000 0.15827400 1.29231900

Se 7.38182000 0.96074100 -0.77914500

Se -0.65368100 1.41569300 0.17236400

C 8.29641400 -2.50431800 1.27397000

O 9.49160800 -2.71441700 1.30646400

O 7.38227000 -3.31473000 1.86263500

C 4.46143000 2.82329100 -1.15739200

O 5.65727000 2.97602300 -1.34334400

O 3.57283100 3.82571300 -1.35173300

C 0.30445500 -2.61657100 -0.28667800

O 1.48525600 -2.90905300 -0.25763700

O -0.66516500 -3.54727500 -0.46025900

C -3.61623400 3.02833200 0.96813500

O -2.42956800 3.30115800 0.88747200

O -4.53451400 3.94030400 1.36186600

C -7.62245500 -2.25187100 -1.05335800

O -6.43862200 -2.46494900 -1.23760100

O -8.59220600 -3.00574100 -1.62488400

C 7.92521200 -4.45807300 2.53809000
H 8.48155100 -5.09761400 1.83620800
H 8.60732800 -4.14730300 3.34390500
H 7.06250100 -4.99634000 2.94927700
C 4.13438700 5.06794500 -1.80223200
H 4.85427300 5.45839100 -1.06760200
H 4.65050900 4.93590000 -2.76496200
H 3.28399900 5.75186200 -1.91033300
C -0.20092300 -4.89900700 -0.59401800
H -1.10413900 -5.50878300 -0.71666700
H 0.45605700 -4.99939700 -1.47079500
H 0.35838400 -5.20952400 0.30130100
C -4.01648500 5.24452600 1.66864400
H -4.88668100 5.84365400 1.96231800
H -3.28833200 5.18959200 2.49140100
H -3.52247700 5.68363400 0.78912000
C -8.12359600 -4.07937500 -2.45566700
H -7.50212100 -4.77795500 -1.87562200
H -9.02643600 -4.58042200 -2.82507500
H -7.52647900 -3.69016600 -3.29369200
S 3.25702600 -0.84625400 0.01144200
S -8.56231400 0.85888100 1.33184900
S -4.68964100 -0.72942600 -0.04021200
Shielding = σSe28 = 1167.6 ppm; σSe29 = 1129.4 ppm

Pentad-XIII

Energy = -7906.547360 hartree
C 6.09741000 0.22783200 -0.30523400
C 6.63571200 -0.79795900 0.45749100
C 8.04116700 -0.95815400 0.30774200
C 8.57428600 -0.04893400 -0.58293700
H 6.04286200 -1.41744500 1.12826800
H 9.62442500 0.04422000 -0.85237600
C 4.67379200 0.51364400 -0.41286100

C 3.93419600 1.65965900 -0.72073600
C 2.52137000 1.49271000 -0.64464500
C 2.03077400 0.24438100 -0.31143000
H 1.86554400 2.33580300 -0.85701800
C 0.62308000 -0.04544900 -0.11773300
C -0.11791800 -1.23220400 -0.03764500
C -1.52339100 -1.05390300 0.11399700
C -2.00522400 0.23688100 0.19079900
H -2.17709000 -1.92257200 0.17124700
C -3.41574300 0.57107900 0.28673700
C -4.11863800 1.75393500 0.56353300
C -5.52839100 1.56702800 0.58222900
C -5.95244100 0.28163200 0.31273500
H -6.20866100 2.39093600 0.78554800
C -7.34112200 -0.15841200 0.36755200
C -8.05080400 -1.24308300 -0.15829600
C -9.45569100 -1.19427100 0.13427000
C -9.81797100 -0.11276100 0.87983500
H -10.14871900 -1.95743400 -0.21204700
H -10.80675700 0.16090000 1.24160100
Se -0.53944900 1.45062000 0.09458500
C 8.89006300 -1.94949500 1.00482700
O 10.08973100 -2.06392000 0.85822000
O 8.16235000 -2.73136400 1.84001600
C 4.51424800 2.96954200 -1.09056000
O 5.67756600 3.18232400 -1.37578500
O 3.57893900 3.95180700 -1.09431600
C 0.45347300 -2.59095600 -0.09393700
O 1.64125200 -2.87066400 -0.07012400
O -0.50147900 -3.54635400 -0.16289600
C -3.51977900 3.07634000 0.80732500
O -2.33654300 3.35798700 0.71136200
O -4.44840100 3.99671600 1.15495400
C -7.46561800 -2.34369300 -0.94833400
O -6.27879000 -2.55543200 -1.11417500

O -8.42496500 -3.13728400 -1.48249400

C 8.91288200 -3.72266300 2.55624500

H 9.40987000 -4.41429300 1.85925500

H 9.68084400 -3.24980000 3.18693400

H 8.18196100 -4.25768400 3.17476300

C 4.05663100 5.25043400 -1.47524100

H 4.83415500 5.59863500 -0.77898000

H 4.47967300 5.22824000 -2.49085900

H 3.18062900 5.90914500 -1.43565900

C -0.02079000 -4.89915100 -0.19547100

H -0.91812800 -5.52729900 -0.24700900

H 0.61818100 -5.06311500 -1.07582300

H 0.56128000 -5.12741100 0.70988900

C -3.94520600 5.32092000 1.39303100

H -4.82193600 5.92437900 1.65691300

H -3.21547800 5.31696900 2.21622000

H -3.45734200 5.71965700 0.49112600

C -7.94162900 -4.25036800 -2.25045300

H -7.31696400 -4.91000200 -1.62965400

H -8.83761200 -4.77967900 -2.59640300

H -7.34341400 -3.90214700 -3.10556400

S -8.44834600 0.88416900 1.25719000

S -4.55302500 -0.73965000 -0.00776500

S 7.39294100 1.02552200 -1.21556800

Se 3.50409400 -0.94704800 -0.08509000

Shielding = σSe28 = 1133.9 ppm; σSe67 = 1125.7 ppm

Pentad-XIV

Energy = -7906.547463 hartree

C 6.42047300 0.13309700 -0.28885600

C 6.86961600 -0.89668500 0.52278100

C 8.27307400 -1.11847300 0.45202800

C 8.89134200 -0.25163900 -0.42524800

H 6.21447000 -1.47905100 1.16793700

H 9.95724800 -0.20710300 -0.63918000
C 5.01788200 0.48826300 -0.47044600
C 4.35097800 1.64834200 -0.88580300
C 2.93715700 1.51416600 -0.83219300
C 2.47524300 0.27999300 -0.41035600
H 2.27801100 2.33005700 -1.12087600
C 1.07409900 -0.03743300 -0.18810100
C 0.34532900 -1.23088400 -0.13220400
C -1.05634200 -1.06379100 0.05741100
C -1.54637000 0.22127500 0.19124600
H -1.70300400 -1.93882400 0.10283400
C -2.95618600 0.54095000 0.30562400
C -3.65950700 1.68655700 0.69967400
C -5.07795500 1.54499700 0.71263900
C -5.60877500 0.33446700 0.32118000
H -5.70237800 2.38229000 1.01994700
C -7.03031800 0.02612200 0.33831400
C -7.81147600 -1.02305000 -0.16353600
C -9.21698700 -0.85445300 0.08044900
C -9.51527100 0.28542300 0.76270300
H -9.95652300 -1.57888100 -0.25230500
H -10.48980500 0.65165800 1.07833300
Se -0.08212500 1.44203100 0.11680100
C 9.04049100 -2.12990400 1.21247100
O 10.24033400 -2.29672500 1.13304900
O 8.23658700 -2.86302500 2.02096400
C 4.99159600 2.90024800 -1.33505200
O 6.17489800 3.05567500 -1.57116200
O 4.08695100 3.90012500 -1.47633600
C 0.92437400 -2.58544500 -0.26185600
O 2.10997600 -2.85978800 -0.25511900
O -0.03447700 -3.53621900 -0.38123600
C -3.04045600 2.97005600 1.07991600
O -1.86087900 3.25971900 0.96228800
O -3.94181500 3.84596200 1.58157900

C -7.29513300 -2.20256100 -0.87587300

O -6.11963700 -2.48527500 -1.04249500

O -8.29270600 -2.98764400 -1.34217600

C 8.90405800 -3.87108100 2.79382300

H 9.40710500 -4.59651400 2.13670600

H 9.65693600 -3.41894400 3.45706500

H 8.11851300 -4.36249800 3.38070800

C 4.62211600 5.14905600 -1.93890700

H 5.37083200 5.53716100 -1.23224600

H 5.09818500 5.02871400 -2.92367100

H 3.76478500 5.82981000 -2.00473500

C 0.44845800 -4.88412700 -0.48453000

H -0.44733900 -5.51171000 -0.56465700

H 1.08465100 -5.00206900 -1.37434600

H 1.03519600 -5.15737100 0.40535200

C -3.41470500 5.13023700 1.95029500

H -4.27166000 5.70144100 2.32694900

H -2.64619300 5.02516200 2.73032200

H -2.96686900 5.63181800 1.07946000

C -7.87158200 -4.17195100 -2.03778400

H -7.27156100 -4.81731000 -1.37906700

H -8.79608900 -4.67932800 -2.33826600

H -7.26868300 -3.91056700 -2.92001400

S 3.85715200 -0.77376800 -0.10008100

Se -4.18837500 -0.83387500 -0.17291600

S -8.08474300 1.19556500 1.13662700

S 7.79171300 0.85393100 -1.14667300

Shielding = σSe28 = 1128.6 ppm; σSe64 = 1134.1 ppm

Pentad-XV

Energy = -7906.543784 hartree

C 6.55830500 0.14275200 -0.21705200

C 6.99490800 -0.87782900 0.61279300

C 8.40164200 -1.08746500 0.58040300

C 9.03514900 -0.22069600 -0.28598500

H 6.32814100 -1.46199200 1.24427600

H 10.10588900 -0.16794400 -0.47210100

C 5.15790700 0.48417100 -0.43783300

C 4.49183800 1.63572300 -0.87744100

C 3.07823400 1.48897500 -0.86027200

C 2.61679700 0.25293900 -0.44371400

H 2.41965300 2.29719900 -1.17105600

C 1.21363600 -0.07660700 -0.25317600

C 0.49363200 -1.27548100 -0.21555100

C -0.91353500 -1.12053900 -0.05654400

C -1.41216900 0.16102400 0.06837500

H -1.55624300 -1.99900400 -0.03343100

C -2.82679300 0.47296600 0.17961300

C -3.54306700 1.63749600 0.49779000

C -4.94992900 1.43188000 0.51671700

C -5.36236800 0.15115000 0.20659100

H -5.63883200 2.24175800 0.74724000

C -6.74249700 -0.30937000 0.26566400

C -7.45361100 -1.35496500 -0.32388000

C -8.86059400 -1.39046500 -0.01591700

C -9.31026200 -0.42061200 0.82424500

H -9.50767200 -2.15655100 -0.43930500

H -10.32725500 -0.26944400 1.18128800

Se 0.03852000 1.39491400 0.01635100

Se -7.92114500 0.71402000 1.35973600

C 9.15763100 -2.08712300 1.36742600

O 10.36057200 -2.24362200 1.32068900

O 8.33916800 -2.82226900 2.15927000

C 5.13291400 2.89076300 -1.31712300

O 6.32070300 3.05585800 -1.52195900

O 4.22327700 3.88131600 -1.48914600

C 1.08695100 -2.62501000 -0.33660700

O 2.27434000 -2.88913800 -0.29994100

O 0.13938800 -3.58213400 -0.48515200

C -2.95928100 2.95818700 0.78184100

O -1.77931000 3.25614100 0.69332900

O -3.89743900 3.85684800 1.15964200

C -6.85787000 -2.36963400 -1.21951500

O -5.66905600 -2.55683400 -1.39970000

O -7.80769500 -3.11364000 -1.83625000

C 8.99483800 -3.81947700 2.95597000

H 9.52150700 -4.54437800 2.31703300

H 9.72584800 -3.35645800 3.63595400

H 8.19840500 -4.31431300 3.52502900

C 4.75941000 5.13230800 -1.94497500

H 5.48511700 5.53165900 -1.22079100

H 5.26310700 5.01036100 -2.91569600

H 3.89802800 5.80468000 -2.03833700

C 0.63482000 -4.92590800 -0.58319200

H -0.25402300 -5.55940300 -0.68945400

H 1.29425400 -5.03420500 -1.45716700

H 1.20079200 -5.19958100 0.31991600

C -3.40856800 5.17867100 1.43789200

H -4.29152500 5.76393600 1.72127900

H -2.67756700 5.15746800 2.25967900

H -2.92659100 5.61042300 0.54812600

C -7.31045700 -4.14210600 -2.70649700

H -6.68410900 -4.85480400 -2.14928900

H -8.19996200 -4.64152100 -3.10903900

H -6.70984700 -3.70683700 -3.51895500

S 3.99918700 -0.78654100 -0.09166500

S -3.94910900 -0.83945900 -0.15751400

S 7.94522600 0.87041800 -1.04324000

Shielding = σSe28 = 1130.0 ppm; σSe29 = 1189.6 ppm

Pentad-XVI

Energy = -5903.202121 hartree

C 6.17596700 0.10874000 -0.25725600

C 6.61275400 -0.93288800 0.54590600

C 8.01586100 -1.16005800 0.48585500

C 8.64631500 -0.28532700 -0.37473600

H 5.94891300 -1.52022400 1.17752700

H 9.71441500 -0.24289800 -0.57786500

C 4.77673700 0.47236000 -0.44797100

C 4.11877100 1.64047200 -0.85477700

C 2.70381500 1.51173200 -0.81655200

C 2.23299800 0.27417600 -0.41527500

H 2.05098600 2.33415000 -1.10111800

C 0.82894000 -0.04074900 -0.20733500

C 0.09399000 -1.23073100 -0.17907100

C -1.30825900 -1.06064900 0.00605700

C -1.78801300 0.22470500 0.16190500

H -1.96173500 -1.93127600 0.02402300

C -3.19635200 0.55299500 0.30286200

C -3.89240000 1.72196500 0.64753200

C -5.30177600 1.53463400 0.68621400

C -5.73214100 0.26267600 0.36788600

H -5.97709900 2.34845700 0.94029500

C -7.11964700 -0.18005100 0.43210200

C -7.84125200 -1.23878400 -0.12902800

C -9.23936400 -1.20450900 0.19612800

C -9.58460000 -0.15974200 0.99995000

H -9.94023900 -1.95067200 -0.17083900

H -10.56508200 0.09601200 1.39581400

Se -0.32237400 1.44069800 0.10724000

C 8.77148000 -2.18412000 1.24119500

O 9.97130600 -2.35529600 1.17131100

O 7.95659000 -2.92343600 2.03286000

C 4.76903800 2.89522000 -1.28160600

O 5.95532800 3.04878000 -1.50341300

O 3.86985500 3.90052800 -1.41973000

C 0.66739300 -2.58535200 -0.33416200

O 1.85163900 -2.86541600 -0.32231700

O -0.29504000 -3.52739800 -0.48377600

C -3.28696200 3.03122200 0.93968200

O -2.10434100 3.31442400 0.83842100

O -4.20748300 3.93729500 1.34159600

C -7.27397500 -2.30020000 -0.98327000

O -6.09115300 -2.50328900 -1.18452000

O -8.24518200 -3.06753300 -1.53404400

C 8.61209800 -3.94389600 2.79967500

H 9.11841900 -4.66339700 2.13856800

H 9.36038000 -3.50330500 3.47576500

H 7.81871800 -4.43900500 3.37275000

C 4.41484100 5.15290000 -1.86101200

H 5.15791600 5.52891300 -1.14196700

H 4.90041700 5.04296500 -2.84234800

H 3.56103900 5.83807100 -1.92693800

C 0.18097000 -4.87540700 -0.61417800

H -0.71777800 -5.49541000 -0.71666000

H 0.82423200 -4.97637200 -1.50099400

H 0.75832100 -5.17262500 0.27416800

C -3.69704900 5.24852200 1.63085700

H -4.56816700 5.84164400 1.93383300

H -2.95565500 5.20638700 2.44246900

H -3.22098100 5.68574100 0.74057200

C -7.77925300 -4.14261500 -2.36442100

H -7.14199200 -4.83096500 -1.78928800

H -8.68285300 -4.65500000 -2.71599100

H -7.19916100 -3.75382100 -3.21451300

S 3.60716800 -0.78953100 -0.10593900

S -4.34048300 -0.74326900 -0.02621000

S 7.55847400 0.83393300 -1.09294900

S -8.20641000 0.81862800 1.39425600

Shielding = σSe28 = 1130.1 ppm

References

1. P. H. Chen, K. Nakano, K. Suzuki, K. Hashimoto, T. Kikitsu, D. Hashizume, T. Koganezawa and K. Tajima, *ACS Appl. Mater. Inter.*, 2017, **9**, 4758-4768.
2. C. Shao, A. Lu, X. Wang, B. Zhou, X. Guan and Y. Zhang, *Org. Biomol. Chem.*, 2017, **15**, 5033-5040.
3. P. Franchetti, L. Cappellacci, G. Abu Sheikha, H. N. Jayaram, V. V. Gurudutt, T. Sint, B. P. Schneider, W. D. Jones, B. M. Goldstein, G. Perra, A. De Montis, A. G. Loi, P. La Colla and M. Grifantini, *J. Med. Chem.*, 1997, **40**, 1731-1737.
4. Y. Qiu, J. C. Worch, A. Fortney, C. Gayathri, R. R. Gil and K. J. T. Noonan, *Macromolecules*, 2016, **49**, 4757-4762.
5. N. G. Connelly and W. E. Geiger, *Chem. Rev.*, 1996, **96**, 877-910.
6. Gaussian 16, Revision C.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.
7. K. Matsubara, K. Ueno and Y. Shibata, *Organometallics*, 2006, **25**, 3422-3427.