# Supporting Information

**Photoresponsive Dynamic Covalent Bond Based on Addition-Fragmentation Chain Transfer of Allyl Selenides**

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## 1. Experimental Procedures

### 1.1 Instruments

*NMR*

$^{1}$H-NMR and $^{13}$C-NMR spectra were recorded in DMSO-$d_6$ or $CDCl_3$ on a Bruker Avance 300 at 300/75 MHz or on a Bruker Avance 400 at 400/100 MHz. $^{77}$Se-NMR spectra were recorded in DMSO-$d_6$ or $CDCl_3$ on Agilent 600 MHz. Chemical shifts are presented in parts per million (δ) relative to $CDCl_3$ (7.26 ppm in $^{1}$H- and 77.00 ppm in $^{13}$C-NMR respectively) as internal standard or relative to diphenyl selenide (416.00 ppm) in $^{77}$Se NMR. Coupling constants (*J*) in $^{1}$H-NMR are given in Hz. The resonance multiplicities are described as *s* (single), *d* (doublet), *t* (triplet), q (quartets) or *m* (multiplet).

*LC-MS*

LC-MS spectra were carried out on a Bruker micro TOF-QIII, the samples were dissolved in HPLC methanol.

*ESR*

ESR experiments were carried out on a JEOL JES-X3 Series ESR spectrometer (Shanghai, China) at room temperature. General instrument parameters are as follows: microwave power, 0.998 mW, modulation frequency, 100 kHz, macrowave frequency, 9150 MHz, modulation amplitude, 100 G, center field, 3260 G.

*GPC*

Both the number-average molecular weight ($M_{n,GPC}$) and molecular weight distribution ($Đ$) of all the polymers were determined by TOSOH HLC-8320 gel permeation chromatograph (GPC) equipped with a refractive-index detector (DMF), using TSK gel Multi pore HZ-N (3) 4.6 × 150 mm column and a RI detector at 40℃. DMF (containing LiBr) was used as the eluent at a flow rate of 0.60 mL $min^{-1}$. All the GPC samples were injected using a TOSOH plus auto sampler and the molar masses were calibrated with narrow polydispersity using polystyrene standards followed by a universal calibration.

*UV*

UV spectra were recorded on a Shimadzu UV-3150 spectrophotometer (Shimadzu China, Shanghai, China), and $CHCl_3$ was chose as solvent.

*TGA*

Thermogravimetric analysis was carried out on a TG/DTA 6300 Instruments with a heating rate of 10 ℃ $min^{-1}$ from the room temperature to 800 ℃ under nitrogen atmosphere.

*DSC*

Differential scanning calorimeter was carried out on a DSC2010 Instruments with a heating rate of 10 ℃ $min^{-1}$ from -70 ℃ to 40 ℃

*DMA*

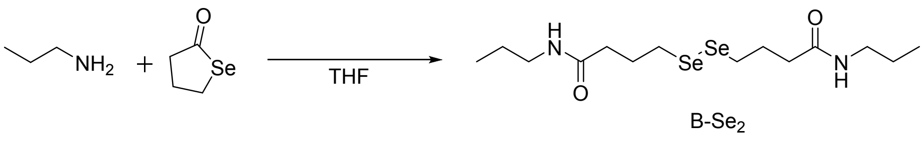
Dynamic thermal mechanical analysis was carried out on a TA Instrument DMA Q800 analyzer. According to the GB/T2941 standard, the dumbbell-shaped specimens were obtained by using the type 3 cutter, and the thickness was about 1 mm.

### 1.2 Materials

Propylamine (98%), phenyl disulfide (99%), poly(propylene glycol) ($M_w$ = 2000 g $mol^{-1}$ ) were purchased from Macklin Co., Ltd. (Shanghai China). Tributylphosphine (95%) and 4-aminobenzylamine (98%) were purchased from Aladdin Co., Ltd. (Shanghai China). 1,8-Diazabicyclo[5.4.0]undec-7-ene (98%) and 3-chloro-2-chloromethyl-1-propene (97%) were purchased from Energy chemical Co., Ltd. (Shanghai China). Sodium thiophenoxide (97%), isophorone diisocyanate (99%), dibutyltin dilaurate (95%) and poly(propylene glycol) ($M_w$ = 3000 g $mol^{-1}$ ) were purchased from Adamas-beta Co., Ltd. (Shanghai China). Triethylamine (99%) was purchased from Yonghua chemical Co., Ltd. (Jiangsu China). Tetrahydrofuran (THF, 99.9%) and dimethylformamide (DMF, 99.9%) were purchased from Oceanpak Co., Ltd. (Sweden). Chloroform ($CHCl_3$) was purchased from Enox Co., Ltd. (Jiangsu China).

### 1.3. Synthetic procedures of compounds

#### *1.3.1 Synthesis of 4,4'-diselanediylbis(N-propylbutanamide) (**B-Se₂**)*

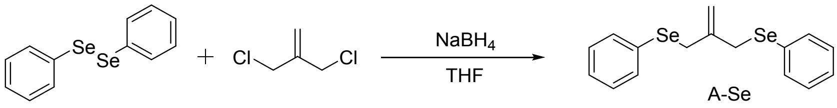



**Scheme S1.** Synthesis of **$B\text{-}Se_2$**.

Into a 25 mL round bottom flask equipped with a magnetic stir bar was added a THF solution (3 mL) of propylamine (0.355 g, 6.0 mmol), then a THF solution (3 mL) of γ-butyroselenolactone (1.080 g, 7.2 mmol) was added slowly. The solution was stirred for 24 h at room temperature. The reaction mixture was filtered and the solids got.

Characterization data for **$B\text{-}Se_2$** (Figure S18-21): A light yellow solid was obtained in 83% yield. $^{1}H$ NMR (300 MHz, $CDCl_3$) δ 6.14 (brs, 2H), 3.19 (q, $J$ = 13.1, 6.8 Hz, 4H), 2.93 (t, $J$ = 7.1 Hz, 4H), 2.31 (t, $J$ = 7.2 Hz, 4H), 2.08 (m, $J$ = 7.1 Hz, 4H), 1.63- 1.37 (m, 4H), 0.91 (t, $J$ = 7.4 Hz, 6H). $^{13}C$ NMR (75 MHz, $CDCl_3$) δ 172.29, 41.34, 35.83, 29.09, 26.73, 22.86, 11.43. $^{77}Se$ NMR (114 MHz, $CDCl_3$) δ 299.88. HRMS (EI) m/z calcd for $C_{14}H_{28}N_2O_2Se_2$ (M + $Na^+$): 439.0373, found 439.0374.

### *1.3.2 Synthesis of (2-methylenepropane-1,3-diyl)bis(phenylselane) (**A-Se**)*

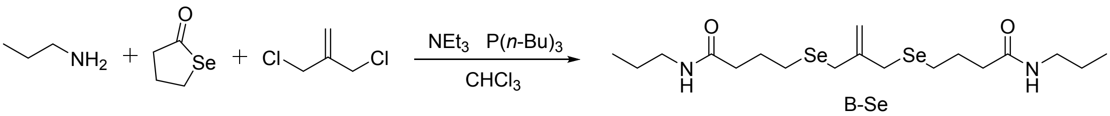



**Scheme S2.** Synthesis of **A-Se**.

Into a 50 mL three-necked flask equipped with a magnetic stir bar was added a THF solution (20 mL) of diphenyl diselenide (1.405 g, 4.5 mmol). Under argon atmosphere, an aqueous solution (10 mL) of $NaBH_4$ (0.340 g, 9 mmol) was added slowly. Then a THF solution (10 mL) of 3-chloro-2-chloromethyl-1-propene (0.188 g, 1.5 mmol) was added into the flask. The solution was stirred for 24h at room temperature. The reaction mixture was filtered and extracted with $CHCl_3$. The organic phase was dried with anhydrous $NaSO_4$. Then the solvent was evaporated, and the crude product was purified by silica gel column chromatography.

Characterization data for **A-Se** (Figure S22-25): A light yellow liquid was obtained in 66% yield. $^1H$ NMR (300 MHz, $CDCl_3$) δ 7.59 - 7.38 (m, 4H), 7.32 - 7.12 (m, 6H), 4.71 (s, 2H), 3.72 (s, 4H). $^{13}C$ NMR (75 MHz, $CDCl_3$) δ 141.84, 133.58, 130.21, 129.00, 127.30, 115.61, 32.79. $^{77}Se$ NMR (114 MHz, $CDCl_3$) δ 318.47. HRMS (EI) m/z calcd for $C_{16}H_{16}Se_2$ (M + $Na^+$): 390.9475, found 390.9474.

### *1.3.3 Synthesis of 4,4'-((2-methylenepropane-1,3-diyl)bis(selanediyl))bis(N-propylbutanamide) (**B-Se**)*

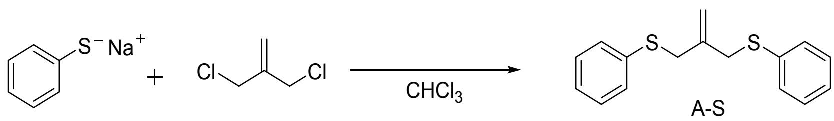



**Scheme S3.** Synthesis of **B-Se**.

Into a 25 mL Schlenk tube equipped with a magnetic stir bar was added a $CHCl_3$ solution (3 mL) of propylamine (0.398 g, 6.6 mmol), $NEt_3$ (0.671 g, 6.6 mmol) and P(n-Bu)$_3$ (0.472 g, 2.2 mmol). Under argon atmosphere, γ-butyroselenolactone (0.995 g, 6.3 mmol) was added slowly. Then a $CHCl_3$ solution (2 mL) of 3-chloro-2-chloromethyl-1-propene (0.383 g, 3 mmol) was added into the tube. The solution was stirred for 24h at room temperature. The reaction mixture was filtered, and the solids were treated with sodium borohydride in aqueous solution. Finally, the reaction mixture was filtered and the solids got.

Characterization data for **B-Se** (Figure S26-29): A white solid was obtained in 52% yield. $^1H$ NMR (300 MHz, $CDCl_3$) δ 5.81 (brs, 2H), 4.91 (s, 2H), 3.36 (s, 4H), 3.19 (q, $J$ = 13.1, 6.8 Hz, 4H), 2.51 (t, $J$ = 7.1 Hz, 4H), 2.27 (t, $J$ = 7.3 Hz, 5H), 1.96 (m, $J$ = 7.1 Hz, 4H), 1.62 - 1.38 (m, 4H), 0.90 (t, $J$ = 7.4 Hz, 6H). $^{13}C$ NMR (75 MHz, $CDCl_3$) δ 171.92, 142.26, 114.45, 41.27, 36.35, 27.29, 25.83, 23.50, 22.88, 11.32. $^{77}Se$ NMR (114 MHz, $CDCl_3$) δ 170.32. HRMS (EI) m/z calcd for $C_{18}H_{34}N_2O_2Se_2$ (M + $Na^+$): 493.0843, found 493.0866.

### *1.3.4 Synthesis of (2-methylenepropane-1,3-diyl)bis(phenylsulfane) (**A-S**)*

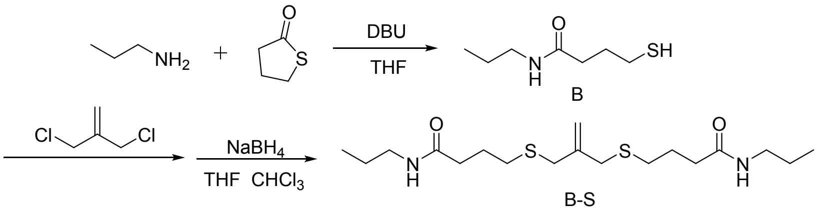



**Scheme S4.** Synthesis of **A-S**.

Into a 50 mL three-necked flask equipped with a magnetic stir bar was added a CHCl3 solution (20 mL) of sodium thiophenoxide (1.4538 g, 11 mmol). Under argon atmosphere, a $CHCl_3$ solution (10 mL) of 3-chloro-2-chloromethyl-1-propene (0.625 g, 5 mmol) was added into the flask. The solution was stirred for 24h at room temperature. The reaction mixture was filtered and extracted with $CHCl_3$. The organic phase was dried with anhydrous $NaSO_4$. Then the solvent was evaporated, and the crude product was purified by silica gel column chromatography.

Characterization data for **A-S** (Figure S30-32): A light yellow liquid was obtained in 28% yield. $^1H$ NMR (300 MHz, $CDCl_3$) δ 7.41 - 7.10 (m, 10H), 4.91 (s, 2H), 3.70 (s, 4H). $^{13}C$ NMR (75 MHz, $CDCl_3$) δ 139.93, 135.75, 130.29, 128.83, 126.38, 116.82, 38.57. HRMS (EI) m/z calcd for $C_{16}H_{16}S_2$ (M + $Na^+$): 295.0586, found 295.0580.

### *1.3.5 Synthesis of 4,4'-((2-methylenepropane-1,3-diyl)bis(sulfanediyl))bis(N-propylbutanamide) (**B-S**)*



**Scheme S5.** Synthesis of **B-S**.

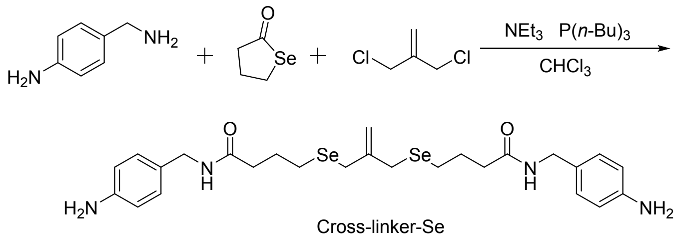
Into a 50 mL round bottom flask equipped with a magnetic stir bar was added a THF solution (20 mL) of propylamine (5.911 g, 100 mmol), DBU (1.522 g, 2 mmol). Under argon atmosphere, a THF solution (20 mL) of γ-butyrothiolactone (2.247 g, 110 mmol) was added slowly. The solution was stirred for 24 h at room temperature. Then the solvent was evaporated, and the crude product was purified by silica gel column chromatography.

Characterization data for product **B** (Figure S33-34): A yellow liquid was obtained in 88% yield. $^1$H NMR (300 MHz, $CDCl_3$) δ 6.06 (brs, 1H), 3.14 (q, *J* = 13.6, 6.5 Hz, 2H), 2.52 (q, *J* = 14.9, 7.0 Hz, 2H), 2.26 (t, *J* = 7.3 Hz, 2H), 1.88 (m, *J* = 7.1 Hz, 2H), 1.59 – 1.37 (m, 2H), 1.31 (t, *J* = 8.0 Hz, 1H), 0.86 (t, *J* = 7.4 Hz, 3H). $^{13}$C NMR (75 MHz, $CDCl_3$) δ 172.20, 41.23, 34.73, 29.66, 24.12, 22.81, 11.37.

Into a 50 mL three-necked flask equipped with a magnetic stir bar was added a $CHCl_3$ solution (3 mL) of product B **(**6.600 g, 40.9 mmol) and $NEt_3$ (0.253 g, 44.2 mmol). Under argon atmosphere, $NaBH_4$ (1.500 g, 40.9 mmol) was added slowly. Then a $CHCl_3$ solution (5 mL) of 3-chloro-2-chloromethyl-1-propene (2.212g, 17.7 mmol) was added into the flask. The solution was stirred for 24h at room temperature. The reaction mixture was filtered, and the solids were treated with sodium borohydride in aqueous solution. Finally, the reaction mixture was filtered and the solids got.

Characterization data for **B-S** (Figure S35-37): A white solid was obtained in 23% yield. $^1$H NMR (300 MHz, $CDCl_3$) δ 5.86 (brs, 2H), 5.00 (s, 2H), 3.36 - 3.11 (m, 8H), 2.47 (t, *J* = 7.0 Hz, 5H), 2.30 (t, *J* = 7.3 Hz, 4H), 1.92 (m, *J* = 7.1 Hz, 4H), 1.66 - 1.38 (m, 4H), 0.92 (t, *J* = 7.4 Hz, 6H). $^{13}$C NMR (75 MHz, $CDCl_3$) δ 172.35, 140.69, 115.64, 41.31, 35.26, 35.17, 30.58, 24.83, 22.86, 11.39. HRMS (EI) m/z calcd for $C_{18}H_{34}N_2O_2S_2$ (M + $Na^+$): 397.1954, found 397.1964.

### *1.3.6 Synthesis of **cross-linker***

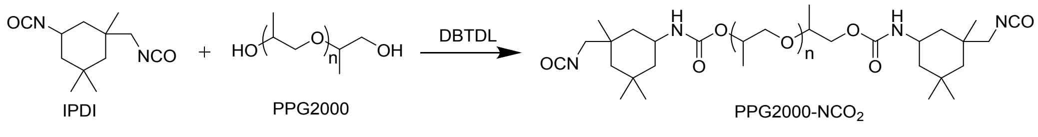


**Scheme S6.** Synthesis of **Cross-linker-Se**.

Into a 250 mL three-necked flask equipped with a magnetic stir bar was added a $CHCl_3$ solution (75 mL) of 4-aminobenzylamine (16.13 g, 132 mmol), $NEt_3$ (13.36 g, 132 mmol)and P(*n*-Bu)$_3$ (4.04 g, 20 mmol). Under argon atmosphere, a $CHCl_3$ solution (75 mL) of γ-Butyroselenolactone (18.89 g, 126 mmol) and 3-chloro-2-chloromethyl-1-propene 7.50 g, 60 mmol) was added slowly into the flask. The solution was stirred for 24h at room temperature. The reaction mixture was filtered, and the solids were treated with sodium borohydride in aqueous solution. Finally, the reaction mixture was filtered and the solids got.

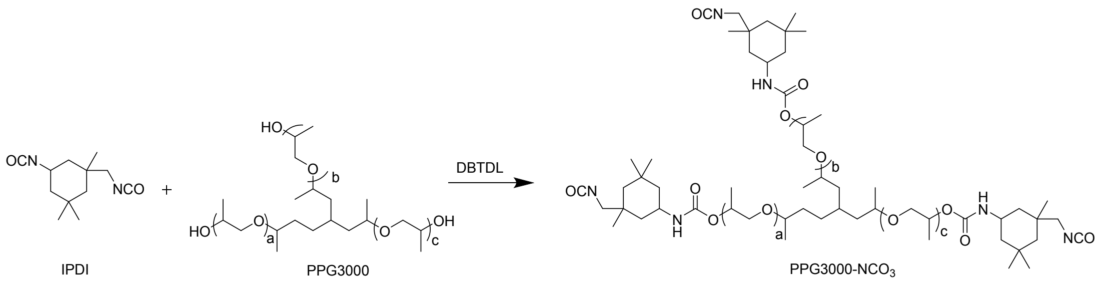
Characterization data for **Cross-linker-Se** (Figure S38-41): A white solid was obtained in 43% yield. $^1$H NMR (300 MHz, DMSO) δ 8.11 (brs, 2H), 6.89 (d, *J* = 8.2 Hz, 4H), 6.49 (d, *J* = 8.3 Hz, 4H), 4.93 (d, *J* = 3.2 Hz, 6H), 4.06 (d, *J* = 5.7 Hz, 4H), 3.33 (s, 4H), 2.44 (t, *J* = 7.3 Hz, 4H), 2.18 (t, *J* = 7.2 Hz, 4H), 1.94 - 1.68 (m, 4H). $^{13}$C NMR (101 MHz, DMSO) δ 171.65, 147.93, 142.81, 128.71, 126.90, 114.69, 114.16, 42.29, 35.84, 27.22, 26.40, 23.49. $^{77}$Se NMR (114 MHz, DMSO) δ 171.76. HRMS (EI) m/z calcd for $C_{26}H_{36}N_2O_2Se_2$ (M + $H^+$): 597.1241, found 597.1269.

### *1.3.7 Synthesis of PPG2000-$NCO_2$ and PPG3000-$NCO_3$*



**Scheme S7.** Synthesis of PPG2000-$NCO_2$.

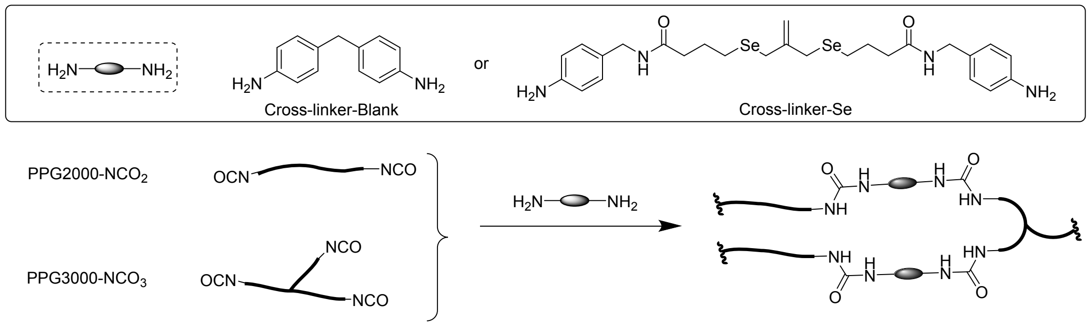
PPG2000-$NCO_2$ was synthesized following a literature procedure.[1] PPG2000 (30 g, 15 mmol) was added into a 500 mL glass reactor equipped with a mechanical stirrer and vacuum inlet, then was degassed by stirring under vacuum while heating at 90 °C for 60 min. Dibutyltin dilaurate (DBTDL) (50 ppm) and IPDI (6.66 g, 30 mmol) was added and the mixture was further stirred under vacuum at 70 °C for 50 min. The reaction was monitored by FT-IR spectroscopy (Figure S42), where the appearance of new bands corresponded to the carbonyl group of the urethane moiety at 1719 $cm^{-1}$ and amide can be observed at 3333 $cm^{-1}$. Moreover, the disappearance of the hydroxyl stretching band at 3489 $cm^{-1}$ can be observed, which was used as criteria to establish that the reaction was finished.




**Scheme S8.** Synthesis of PPG3000-$NCO_3$.

PPG3000-$NCO_3$ was synthesized following a literature procedure.[1] PPG3000 (30 g, 10 mmol) was added into a 500 mL glass reactor equipped with a mechanical stirrer and vacuum inlet, then was degassed by stirring under vacuum while heating at 90 °C for 60 min. Dibutyltin dilaurate (DBTDL) (50 ppm) and IPDI (6.66 g, 30 mmol) was added and the mixture was further stirred under vacuum at 70 °C for 50 min. The reaction was monitored by FT-IR spectroscopy (Figure S43), where the appearance of new bands corresponded to the carbonyl group of the urethane moiety at 1719 $cm^{-1}$ and amide can be observed at 3333 $cm^{-1}$. Moreover, the disappearance of the hydroxyl stretching band at 3489 $cm^{-1}$ can be observed, which was used as criteria to establish that the reaction was finished.

### *1.3.8 Synthesis of **PU-Blank** and **PU-Se***




**Scheme S9.** Synthesis of **PU-Blank** and **PU-Se**.

PPG2000-$NCO_2$ and PPG3000-$NCO_3$ were mixed in an open FTFE mold with an area of 90 $cm^2$. A solution of Cross-linker-Blank or Cross-linker-Se in THF/DMF (v/v = 1/1) was added into the mold and then degassed in vacuum for 0.5 h. The overall NCO/$NH_2$ ratio of the mixture kept at 1.0. The curing was carried out for 24 h at 60 °C and the process could be easily monitored by FT-IR spectroscopy, the results of which are shown in Figures S44. Moreover, the disappearance of the NCO stretching band at 2266 $cm^{-1}$ can be observed, which was used as criteria to establish that the reaction was finished. In order to remove the remaining solvent, the polyurethane elastomer **PU-Blank** with Cross-linker-blank as the crosslinker and **PU-Se** with **Cross-linker-Se** as the crosslinker can be obtained by placing them in a constant temperature oven at 60 °C for 48 h (Figure S45).

## 2. Results and Discussion

### 2.1 UV spectra A-Se and B-Se

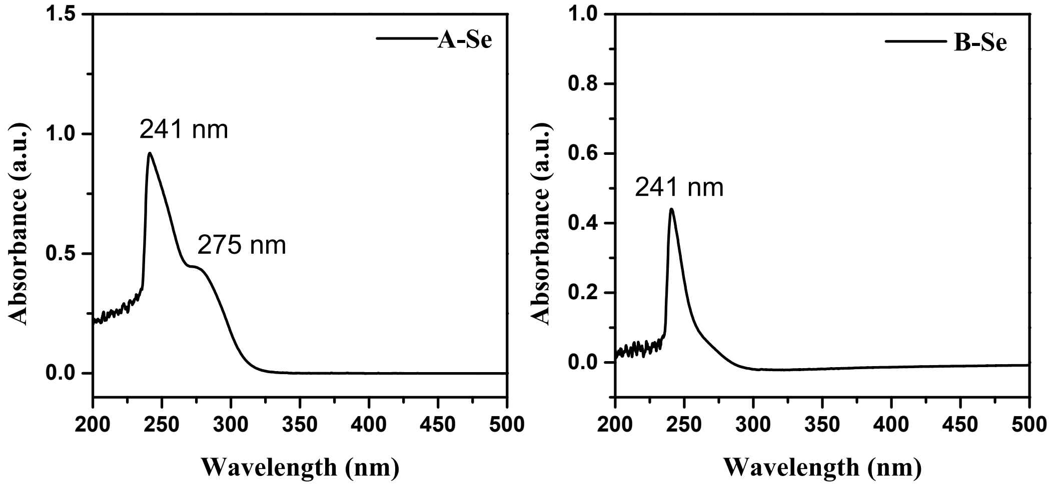



**Figure S1**. UV spectra of A-Se and B-Se.

## 2.2 The structure characterization of the exchange product AB-Se

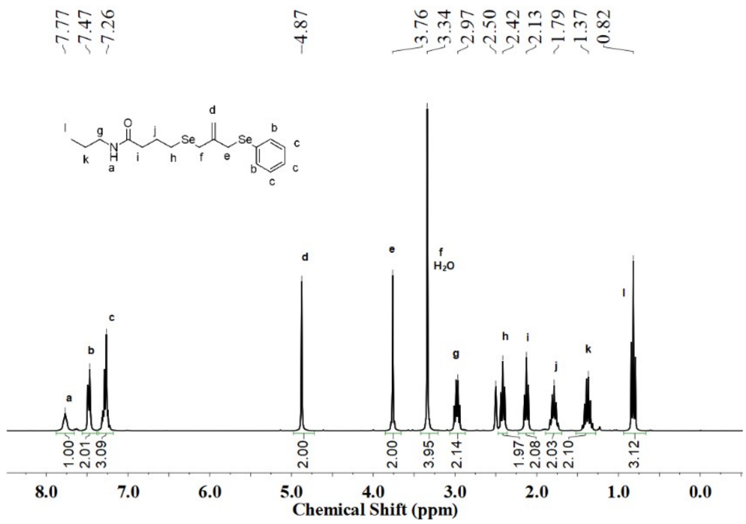



**Figure S2.** [1]H NMR spectrum of **AB-Se** in DMSO-$d_6$.

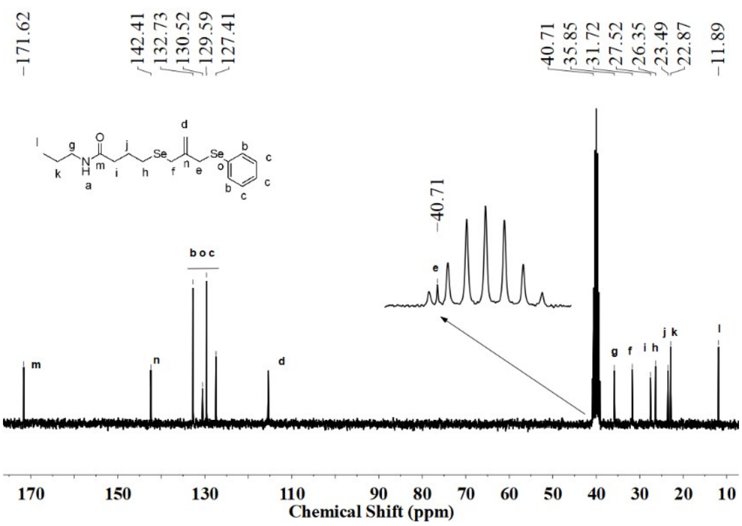



**Figure S3.** [13]C NMR spectrum of **AB-Se** in DMSO-$d_6$.

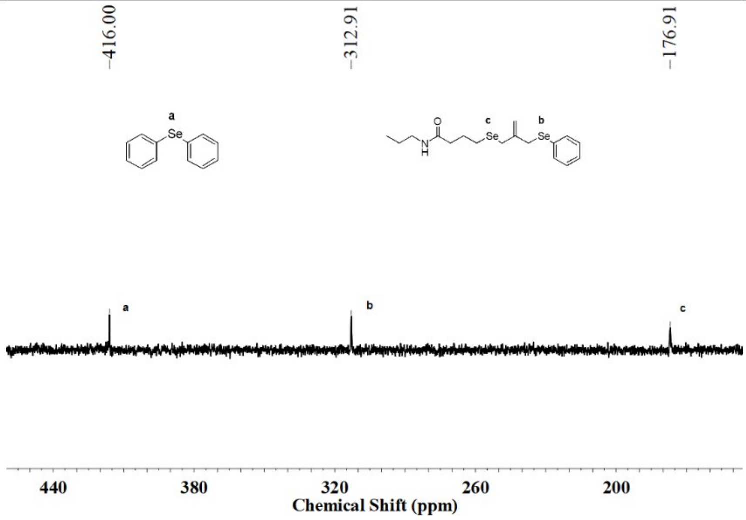



**Figure S4.** $^{77}$Se NMR spectrum of **AB-Se** in DMSO-$d_6$.

**$C_{17}H_{25}NOSe_2$ : 419.0267, found 419.0268.**

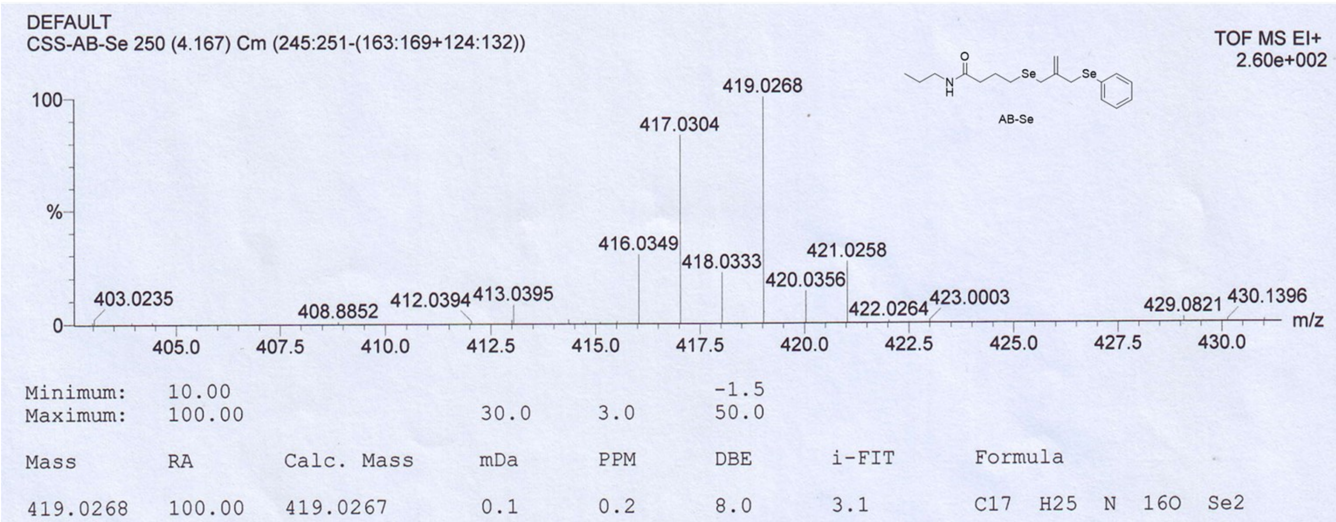



**Figure S5.** LC-MS spectrum of **AB-Se**.

### 2.3 Exchange reaction of allyl sulfides

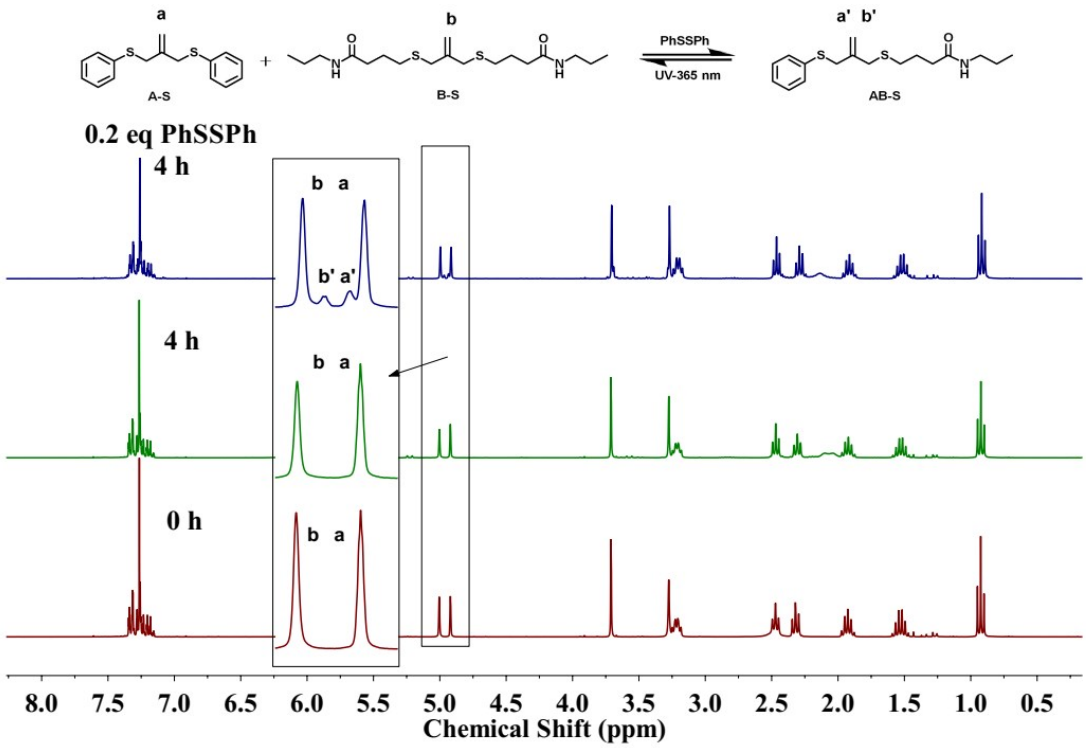



**Figure S6.** Exchange reaction of allyl sulfides in $CDCl_3$ at room temperature with the concentrations both of **A-S** and **B-S** at 0.02 M.

## 2.4 Exchange reaction of allyl selenides with TEMPO

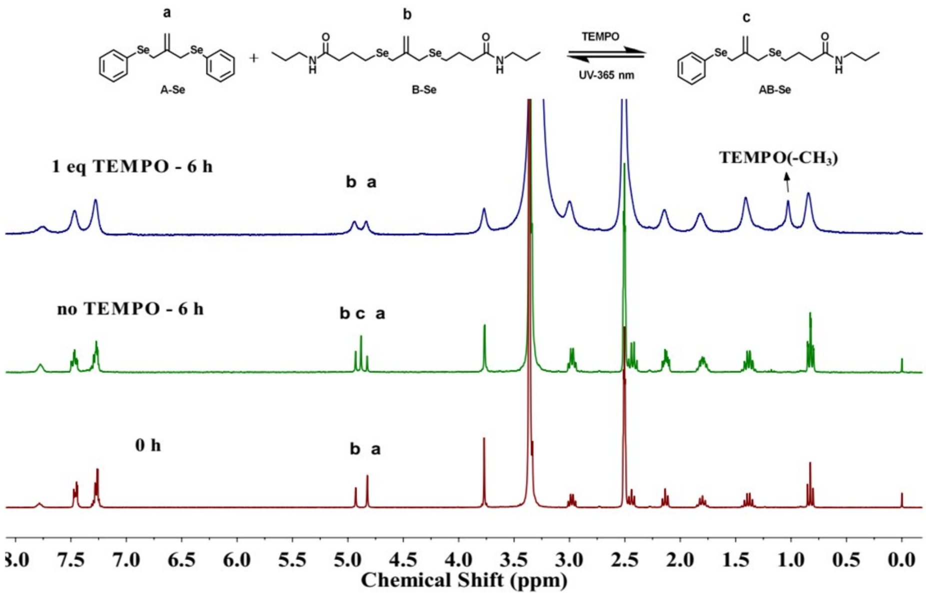



**Figure S7.** Exchange reaction of allyl selenides in DMSO-$d_6$ with TEMPO at room temperature, and the concentrations of **A-Se** and **B-Se** are both 0.005 M.

## 2.5 ESR spectra of B-Se and B-Se$_2$

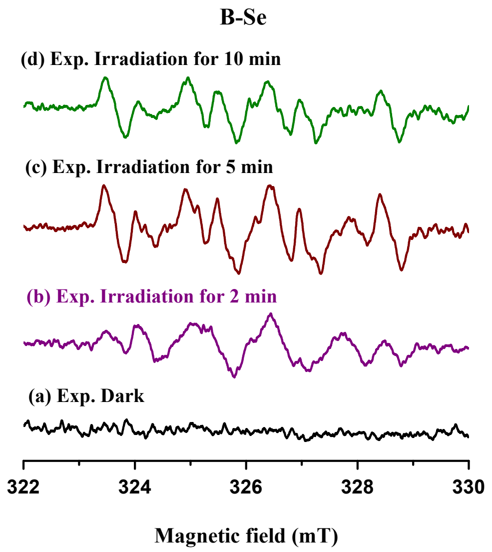



**Figure S8.** ESR spectra of **B-Se** and DMPO under darkness (a), irradiation (305-390 nm) for 2 min (b), 5 min (c) and 10 min (d) in DMSO, [**B-Se**]$_0$ : [DMPO]$_0$ = 1.0 : 6.7, [**B-Se**]$_0$ = 0.03 M.

## 2.6 ESR spectra of B-Se$_2$

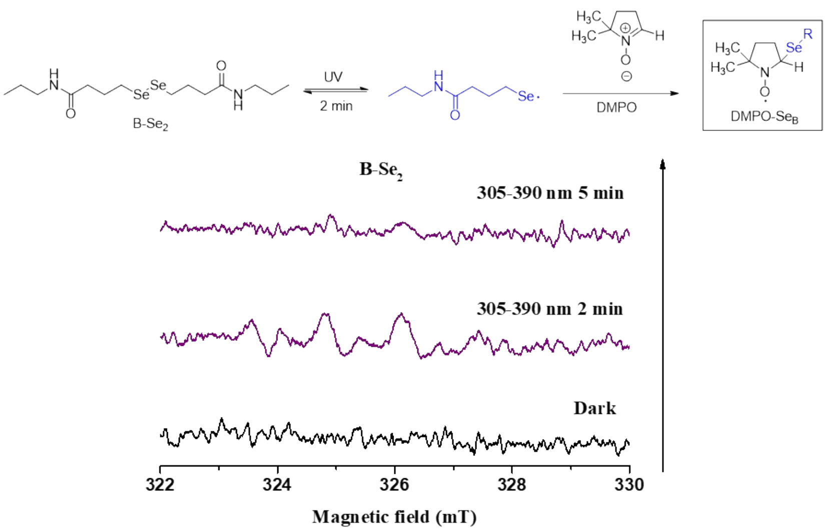



**Figure S9.** ESR spectra of **B-Se$_2$** and DMPO under irradiation in DMSO, [**B-Se$_2$**]$_0$:[DMPO]$_0$ = 1.0 : 3.3, [**B-Se$_2$**]$_0$ = 0.015 M.

## 2.7 $^{77}$Se NMR spectra

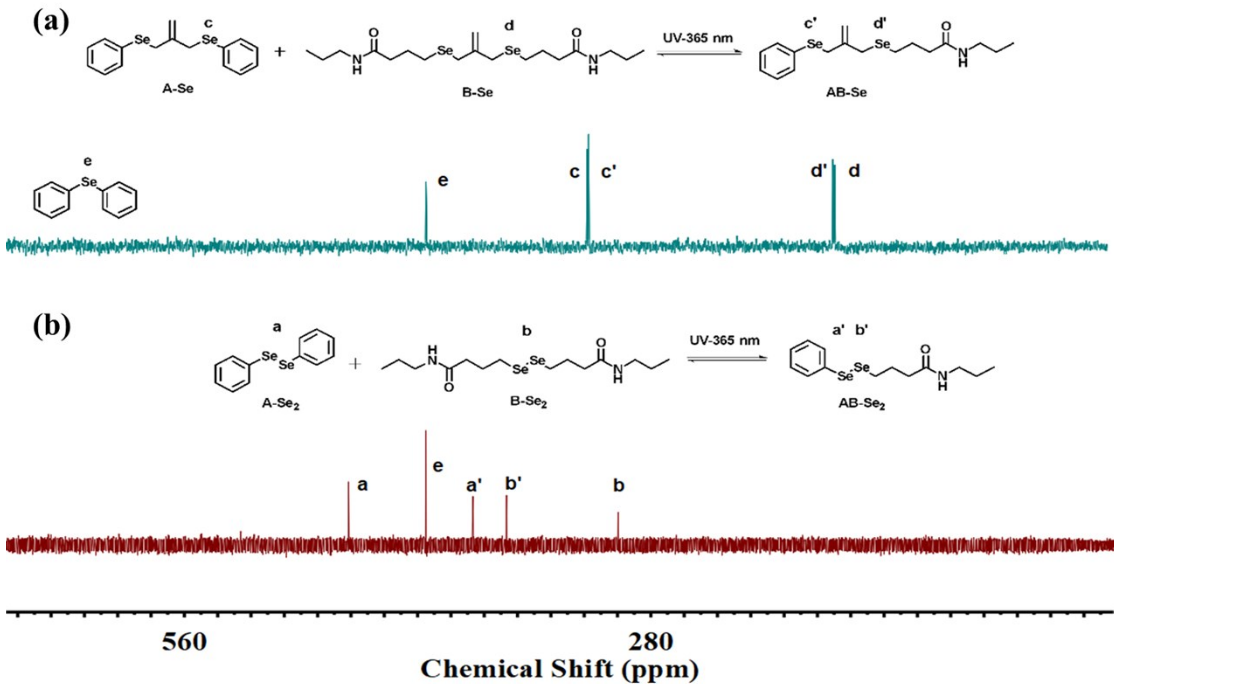



**Figure S10.** $^{77}$Se NMR spectra of compounds in equilibrium in $CDCl_3$. (a) **A-Se**, **B-Se** and **AB-Se**. (b) **A-Se$_2$**, **B-Se$_2$** and **AB-Se$_2$**. There were no diselenides in this system.

### 2.8 DFT calculations

Free energy surface

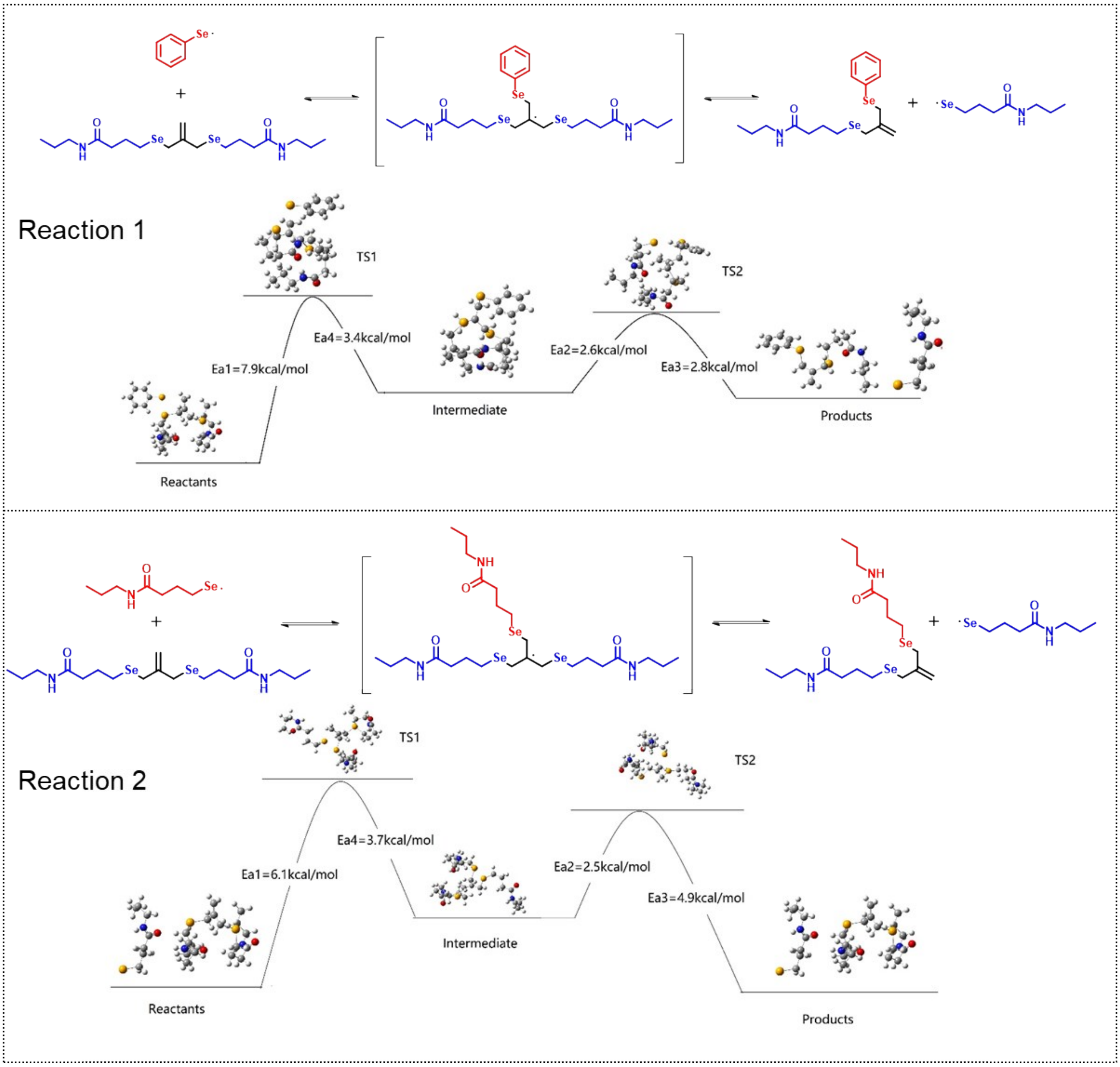
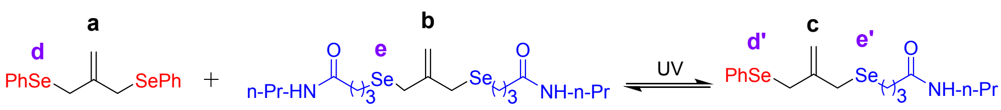



**Figure S11.** DFT calculations of exchange reaction of aryl (top) and alkyl (bottom) selenium with **B-Se**. Molecular geometries were optimized using a DFT method of three-parameter Becke-style hybrid functional (B3LYP) with the Pople basis set 6-31G(d). All the calculations were performed using the GAUSSIAN16.

## 2.9 Kinetics study




**A-Se** **B-Se** **AB-Se**

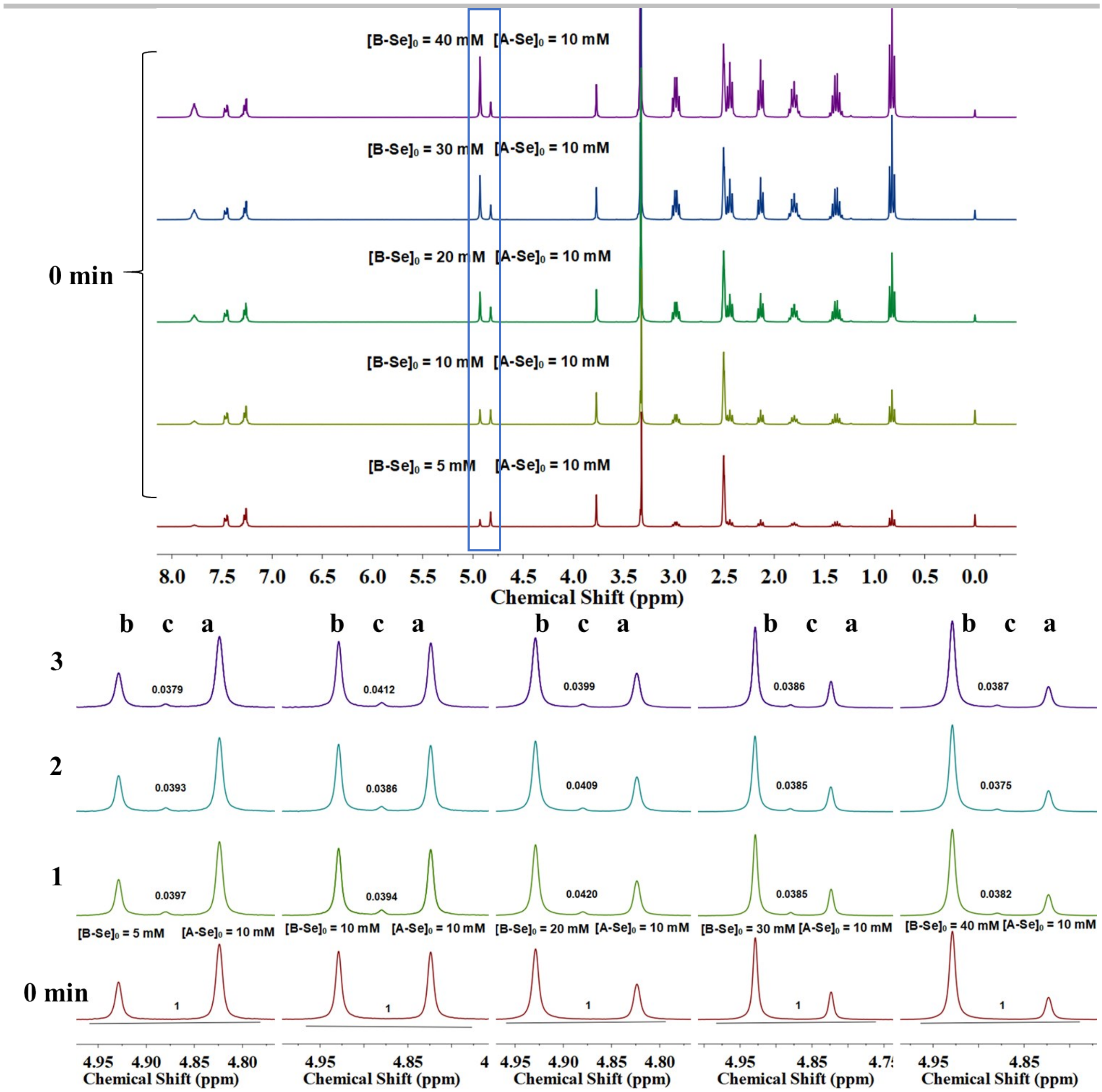



**Figure S12.** Kinetics of the exchange reaction, which was tracked by $^1$H NMR in DMSO-$d_6$ under 365 nm UV light (2 mW cm$^{-2}$). Then, the initial reaction generation ratio of AB-Se (three parallel experiments at each concentration) was determined by $^1$H NMR until it reached around 0.04. The initial reaction rate of AB-Se was obtained from the reaction time and generation ratio {$v_{0(AB\text{-}Se)}$ = ([A-Se]$_0$+[B-Se]$_0$)×[$I_c$/($I_a$+$I_b$+$I_c$)]/t}.

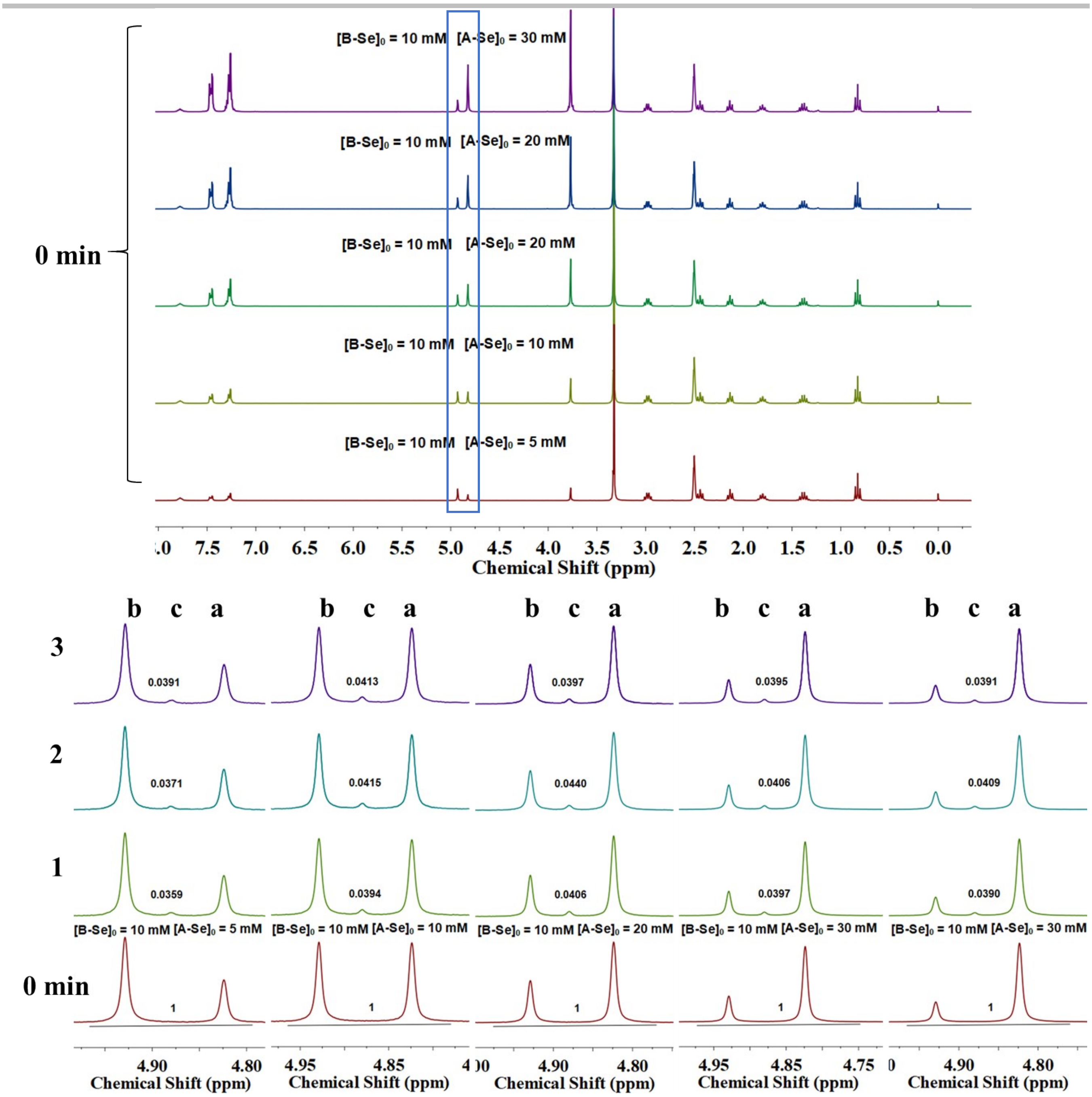



**Figure S13.** Kinetics of the exchange reaction, which was tracked by $^1$H NMR in DMSO-$d_6$ under 365 nm UV light (2 mW cm$^{-2}$). Then, the initial reaction generation ratio of AB-Se (three parallel experiments at each concentration) was determined by $^1$H NMR until it reached around 0.04. The initial reaction rate of AB-Se was obtained from the reaction time and generation ratio {$v_{0(AB\text{-}Se)}$ = ([A-Se]$_0$+[B-Se]$_0$)×[$I_c$/($I_a$+$I_b$+$I_c$)]/t}.

### 2.10 Stress strain curves of PU-Blank and PU-Se

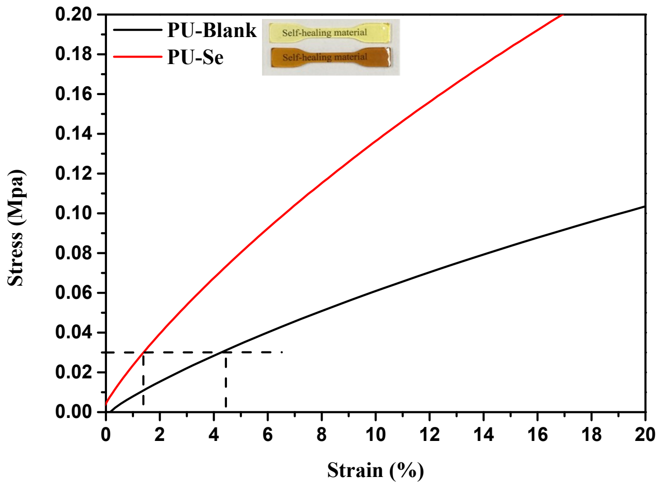



**Figure S14.** Stress strain curves of polyurethane elastomer **PU-Blank** and **PU-Se** at room temperature.

## 2.11 The content of AB-Se change with time under 100 °C or UV-365 nm

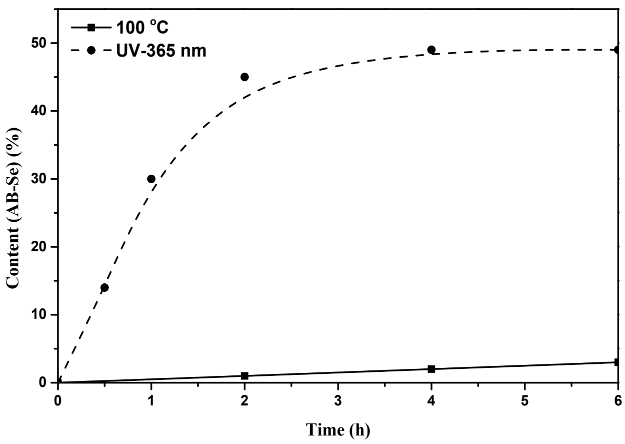



**Figure S15.** The content of **AB-Se** change with time in DMSO-$d_6$ under 100 °C or in $CDCl_3$ under UV-365 nm.

## 2.12 Thermal properties of PU-Se and PU-Blank

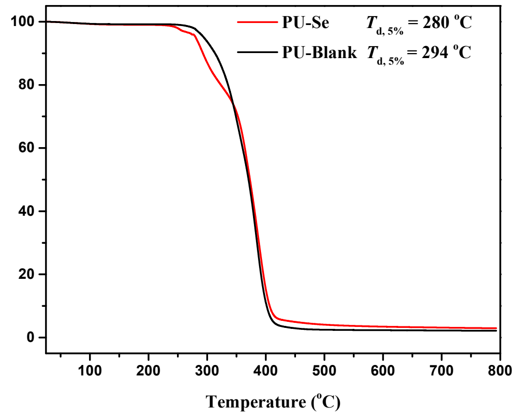



**Figure S16.** TGA curves of **PU-Se** and **PU-Blank**.

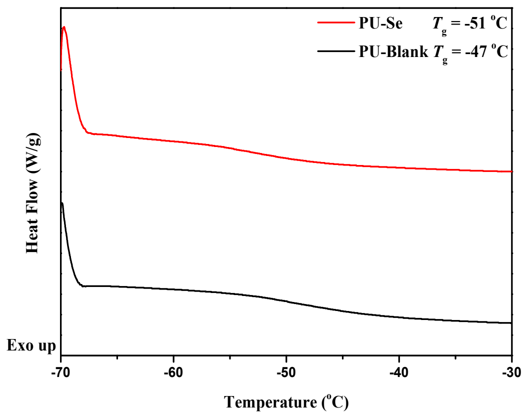



**Figure S17.** DSC curves of **PU-Se** and **PU-Blank**.

## 2.13 NMR and LC-MS of compounds

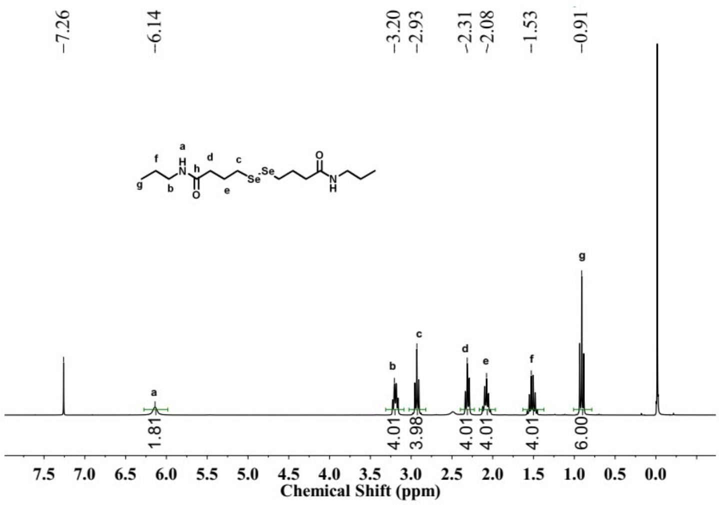



**Figure S18.** $^1$H NMR spectrum of **B-Se$_2$** in $CDCl_3$.

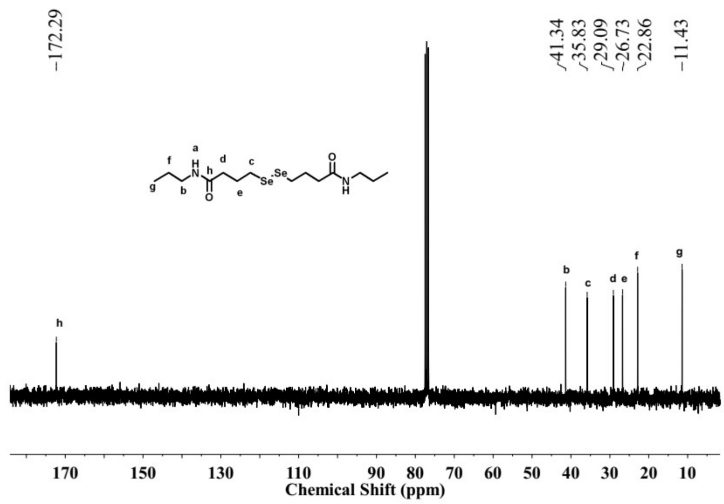



**Figure S19.** $^{13}C$ NMR spectrum of **B-Se$_2$** in $CDCl_3$

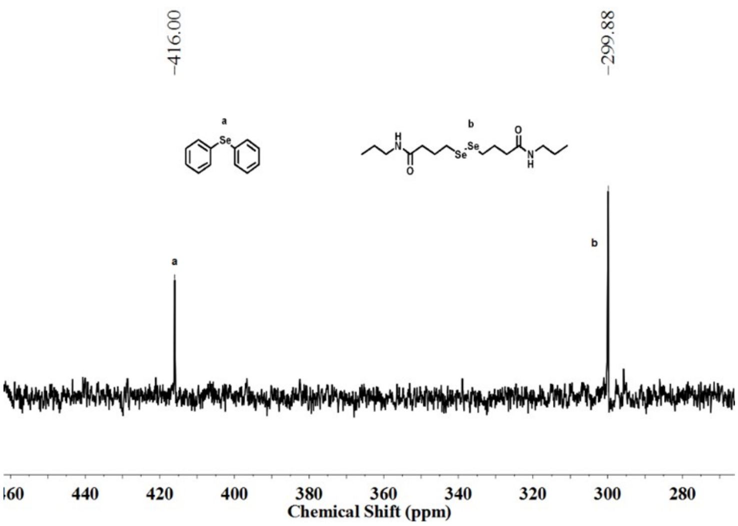



**Figure S20.** $^{77}Se$ NMR spectrum of **B-Se$_2$** in $CDCl_3$.

$C_{14}H_{28}N_2O_2Se_2$ (M + Na$^+$): 439.0373, found 439.0394.

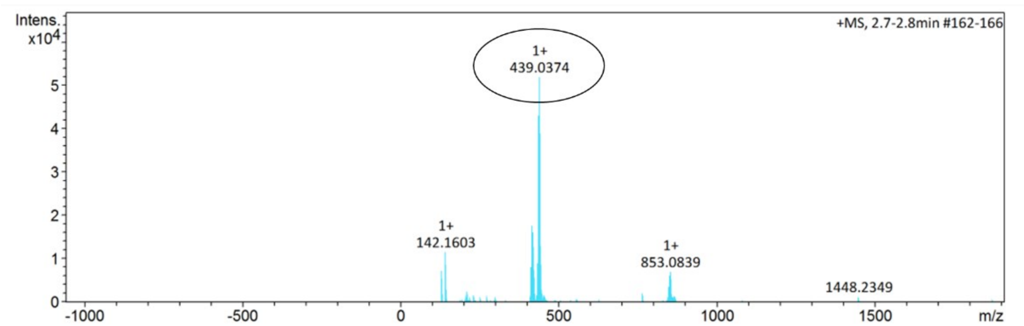



**Figure S21.** LC-MS spectrum of **B-Se$_2$**.

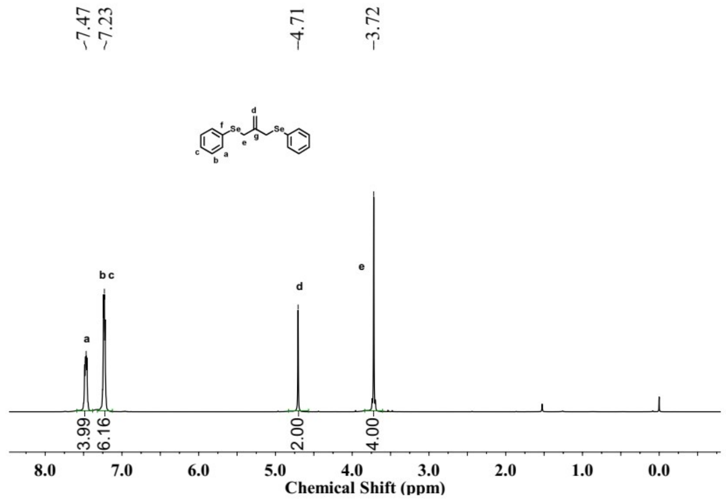



**Figure S22.** $^{1}H$ NMR spectrum of **A-Se** in $CDCl_3$.

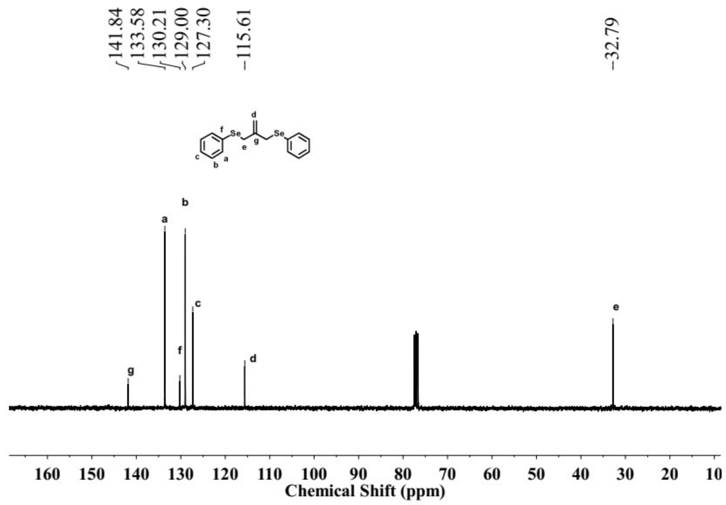



**Figure S23.** $^{13}C$ NMR spectrum of **A-Se** in $CDCl_3$.

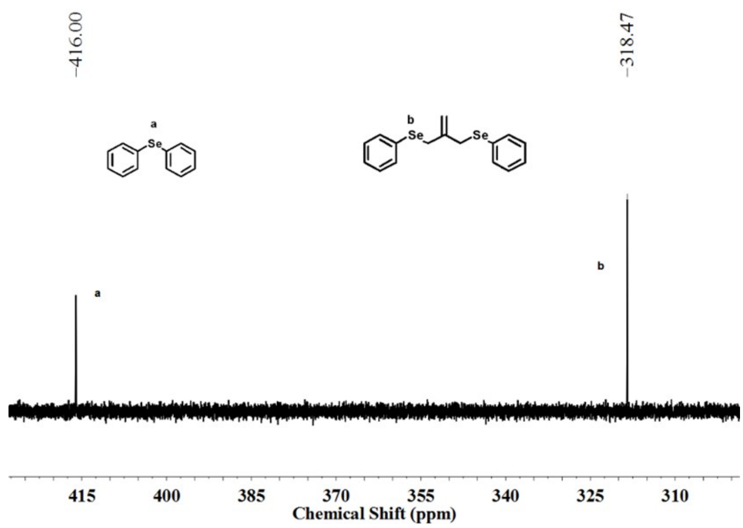



**Figure S24.** $^{77}Se$ NMR spectrum of **A-Se** in $CDCl_3$.

$C_{16}H_{16}Se_2$ (M + $Na^+$): 390.9475, found 390.9474.

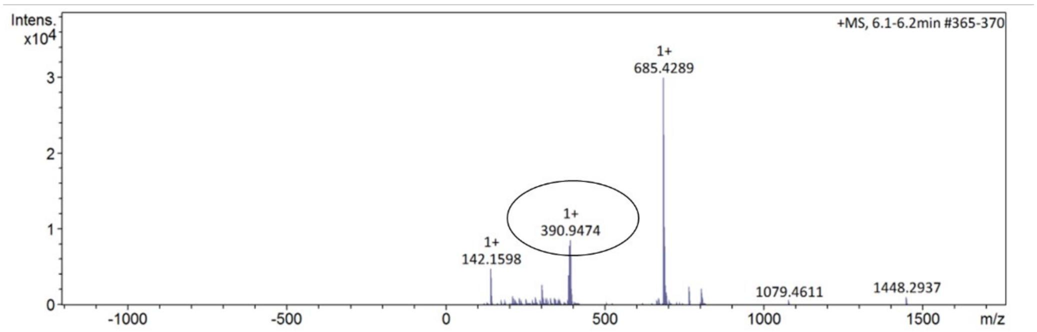



**Figure S25.** LC-MS spectrum of **A-Se**.

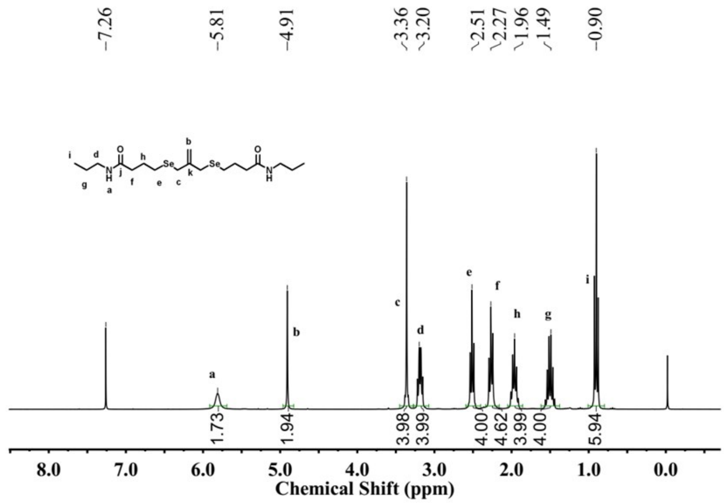



**Figure S26.** $^1$H NMR spectrum of **B-Se** in $CDCl_3$.

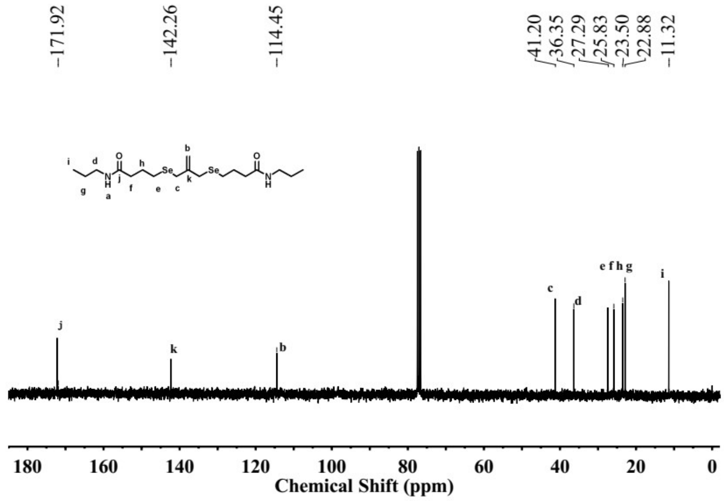



**Figure S27.** $^{13}$C NMR spectrum of **B-Se** in $CDCl_3$.

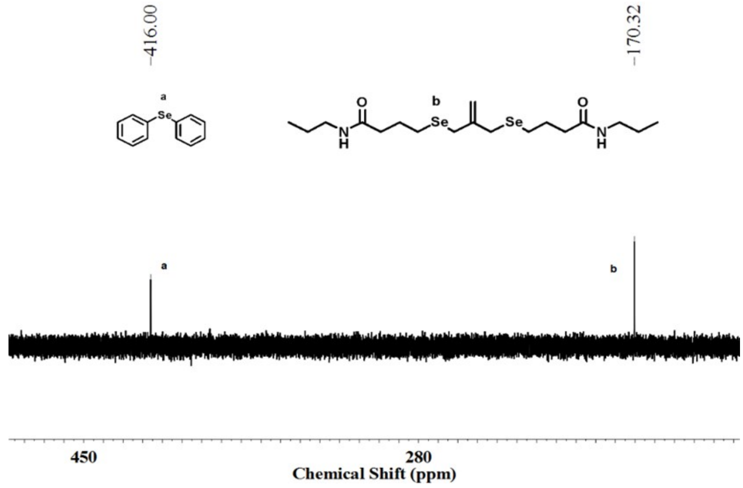



**Figure S28.** $^{77}$Se NMR spectrum of **B-Se** in $CDCl_3$.

$C_{18}H_{34}N_2O_2Se_2$ $(M + Na^+)$: 493.0843, found 493.0866.

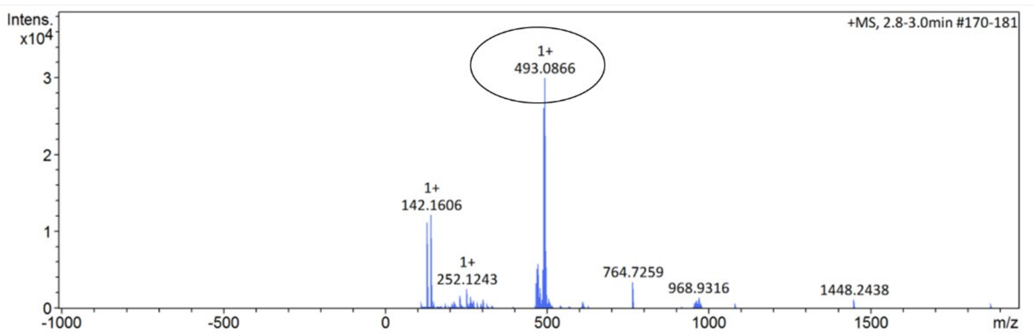



**Figure S29.** LC-MS spectrum of **B-Se**.

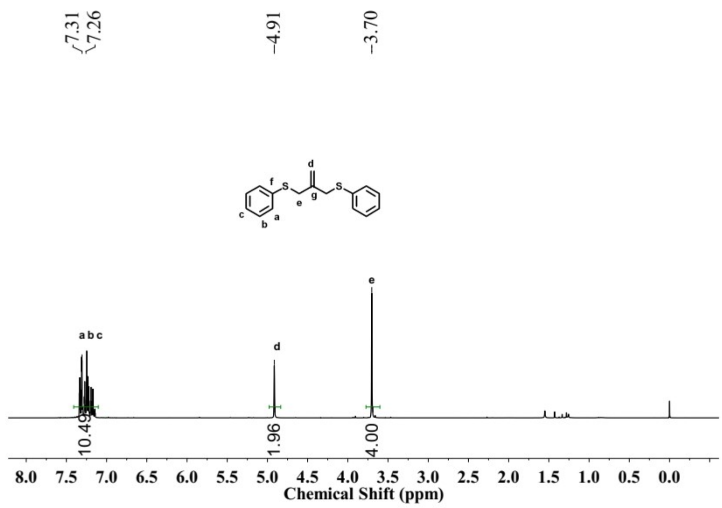



**Figure S30.** $^1$H NMR spectrum of **A-S** in $CDCl_3$.

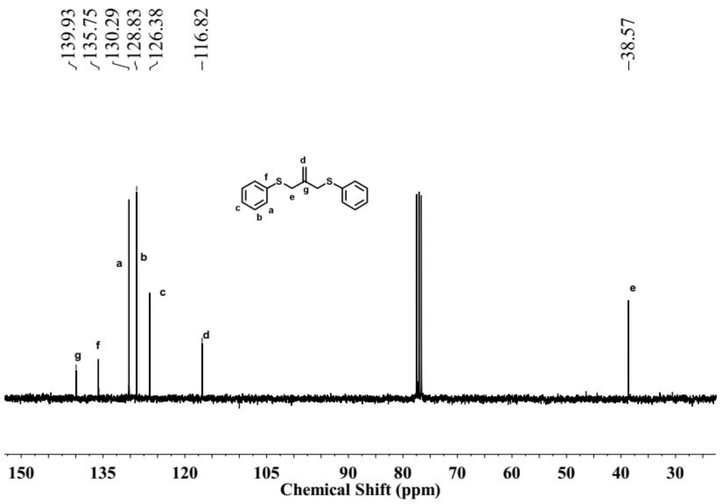


**Figure S31.** $^{13}C$ NMR spectrum of **A-S** in $CDCl_3$.

$C_{16}H_{16}S_2$ $(M + Na^+)$: 295.0586, found 295.0580.

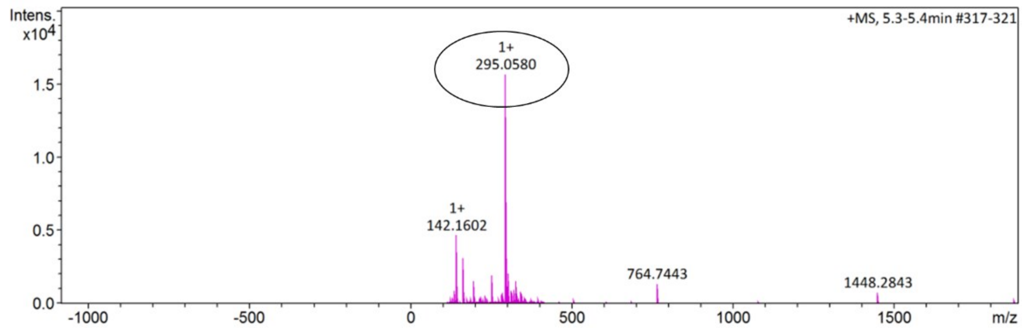


**Figure S32.** LC-MS spectrum of **A-S**.

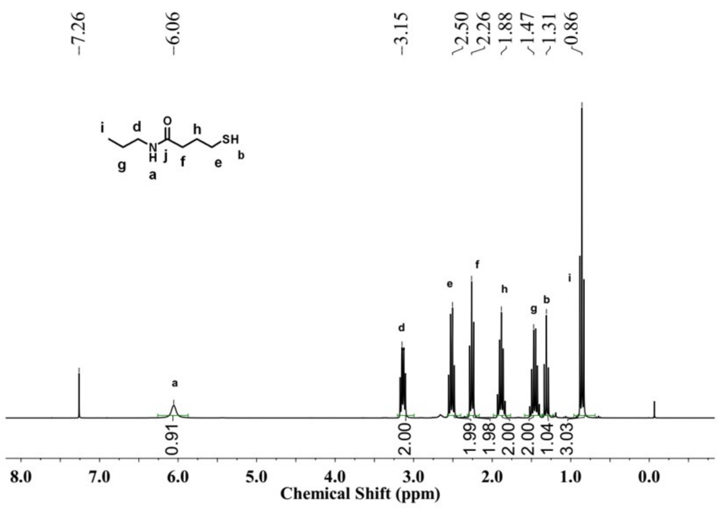


**Figure S33.** $^1H$ NMR spectrum of **B** in $CDCl_3$.

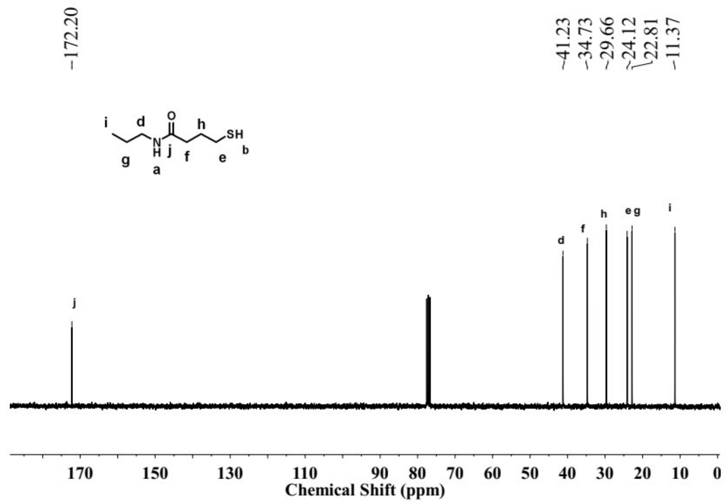



**Figure S34.** $^{13}C$ NMR spectrum of **B** in $CDCl_3$.

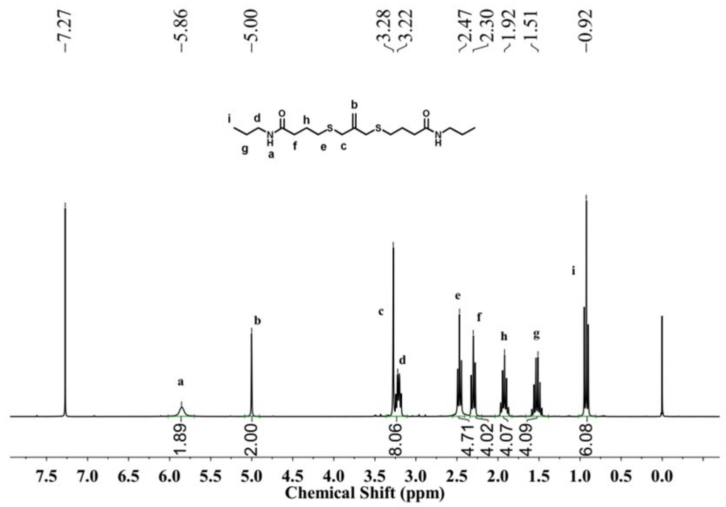



**Figure S35.** $^{1}H$ NMR spectrum of **B-S** in $CDCl_3$.

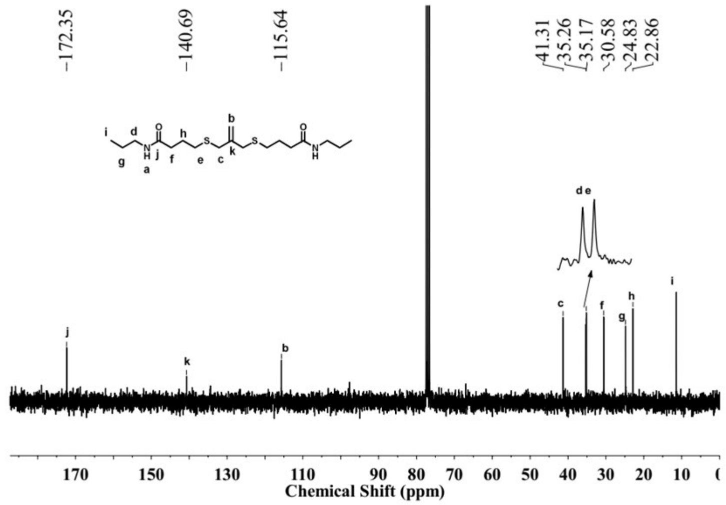



**Figure S36.** $^{13}C$ NMR spectrum of **B-S** in $CDCl_3$.

$C_{18}H_{34}N_2O_2S_2$ ($M + Na^+$): 397.1954, found 397.1964.

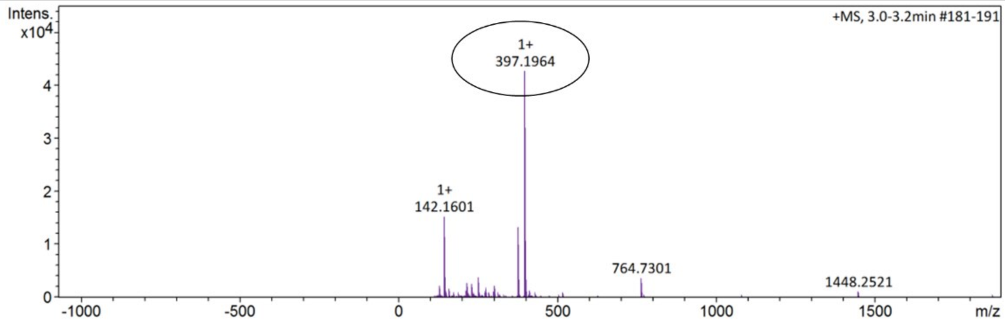



**Figure S37.** LC-MS spectrum of **B-S**.

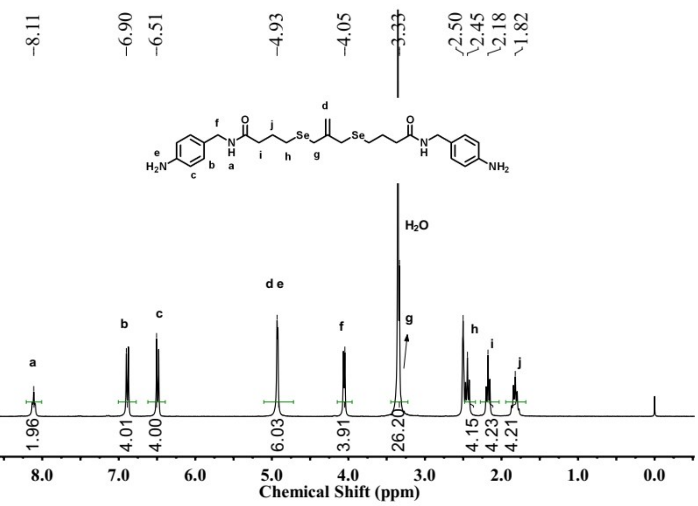



**Figure S38.** [1]H NMR spectrum of **Cross-linker-Se** in DMSO-$d_6$.

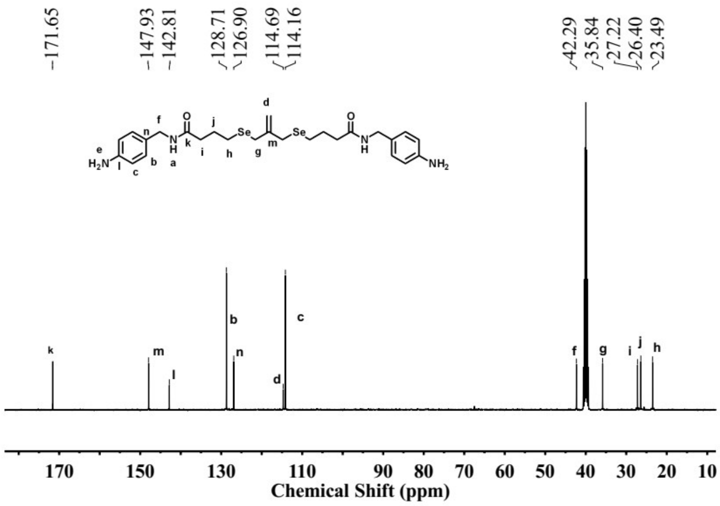



**Figure S39.** [13]C NMR spectrum of **Cross-linker-Se** in DMSO-$d_6$.

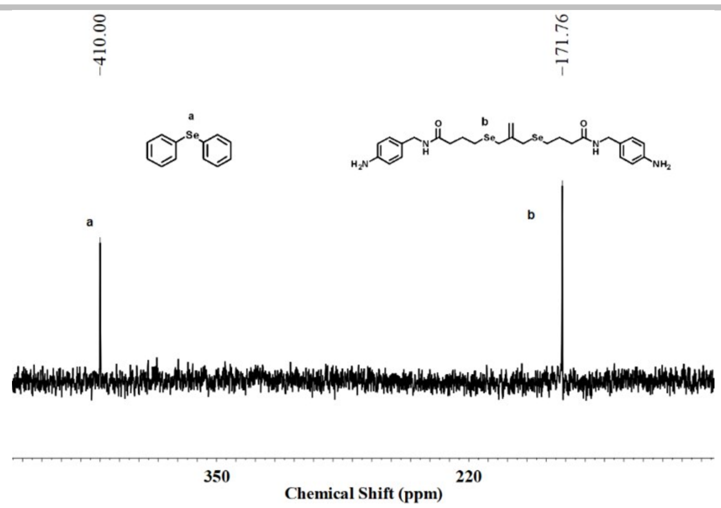



**Figure S40.** $^{77}$Se NMR spectrum of **Cross-linker-Se** in DMSO-$d_6$.

$C_{26}H_{36}N_2O_2Se_2$ ($M + H^+$): 597.1241, found 597.1269.

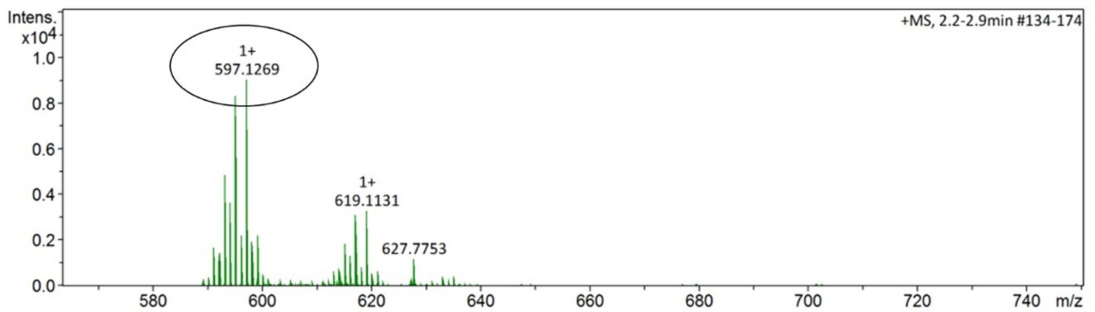



**Figure S41.** LC-MS spectrum of **Cross-linker-Se**.

### 2.14 FT-IR of polymer

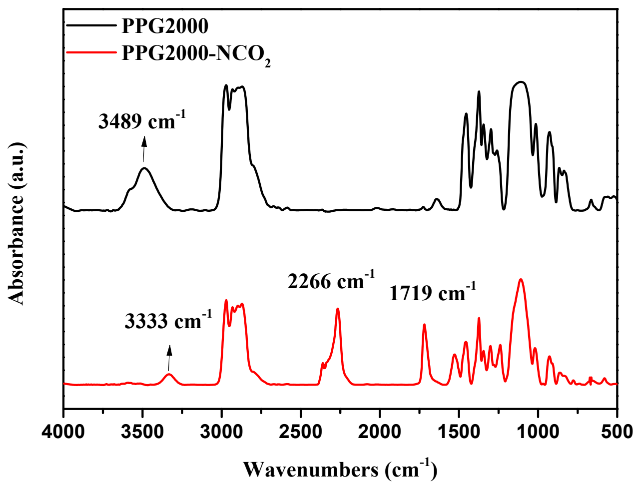



**Figure S42.** FT-IR spectra recorded for the synthesis of PPG2000-$NCO_2$.

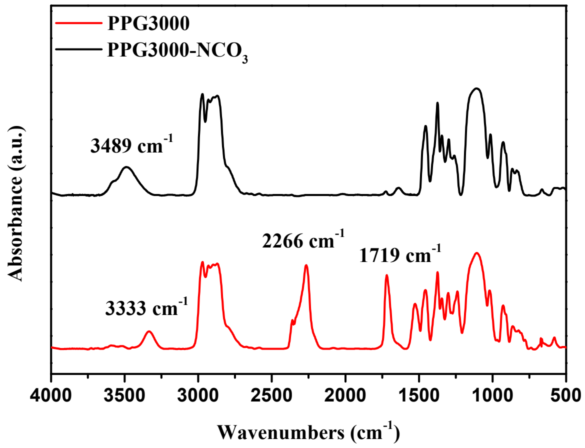



**Figure S43.** FT-IR spectra recorded for the synthesis of PPG3000-$NCO_3$.

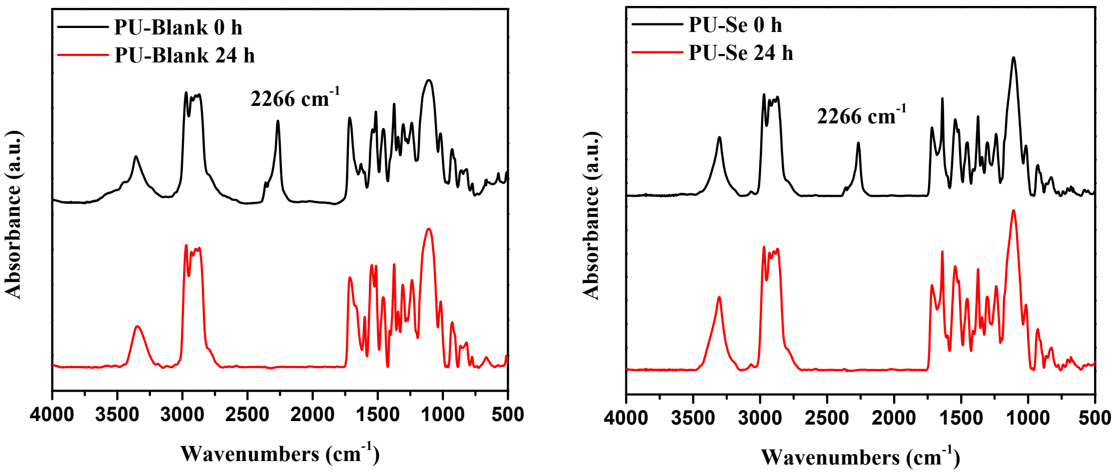



**Figure S44.** FT-IR spectra recorded for the synthesis of **PU-Blank** and **PU-Se**.

## 2.15 Photograph of PU-Blank and PU-Se

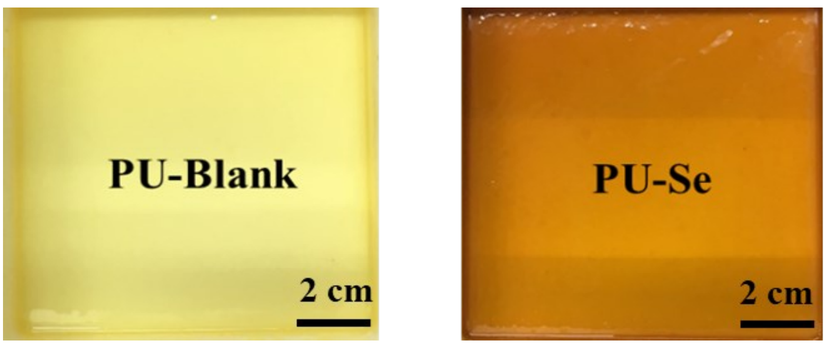
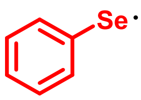



**Figure S45.** Photograph of **PU-Blank** and **PU-Se**.

## 2.16 Computational Details

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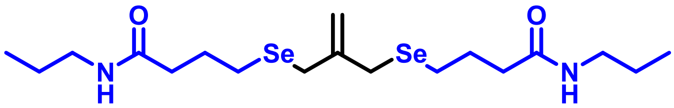


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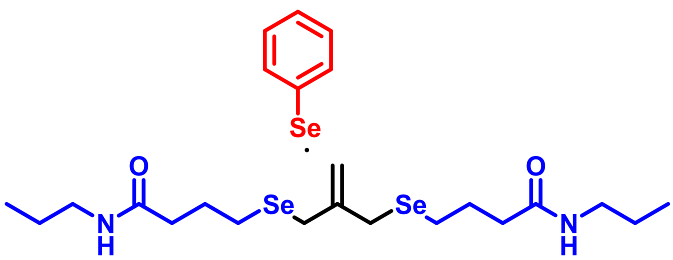
**Reaction 1-TS1**

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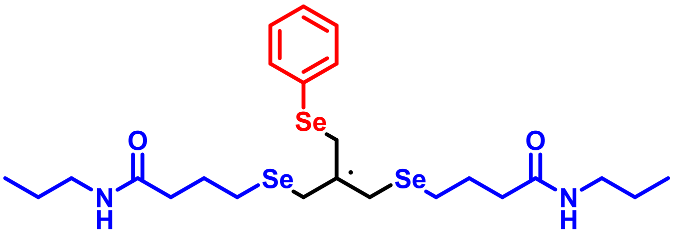
1.3277002584,-0.1237435593,3.7596722339\H,-1.3141403532,0.1930805268 ,2.0360055286\H,-1.3989917795,-2.6739469684,3.1502835386\H,0.128520506
2,-1.7998155443,2.9351341566\Se,1.200778477,1.2907273034,-2.2993679858 \C,-0.1651635658,2.2005145536,-3.4280538453\C,-1.54271147,2.4277511055
,-2.8038006349\C,-1.5695965828,3.4390932764,-1.6464799343\C,-1.1787537 392,2.8624437269,-0.2882351868\O,-1.7078936291,1.8401768757,0.16041134
35\N,-0.2894823042,3.5932648225,0.428986759\H,0.1199469837,4.406600505 2,-0.0058307784\C,0.1330220452,3.2397916756,1.781717193\C,-0.813832704

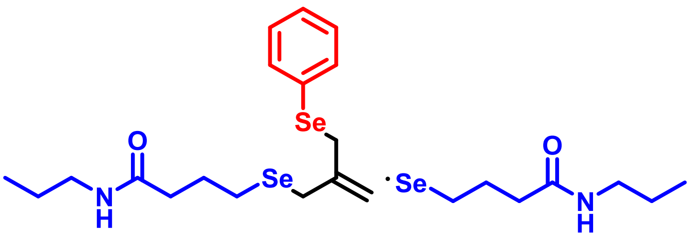
6,3.75279205,2.8766740105\C,-0.911376177,5.2793725342,2.9442299963\H,- 1.2887964995,5.6962055433,2.0031232453\H,0.067196927,5.7340621625,3.14 54078343\H,-1.5933598296,5.5960080256,3.7405096469\H,-0.4580865305,3.3 598607815,3.8386711078\H,-1.8053743681,3.3166539116,2.7075334889\H,0.2 09282813,2.1506158707,1.8308413151\H,1.1387440204,3.6521174439,1.92560 99332\H,-2.5996717032,3.797312817,-1.5211177903\H,-0.9603310256,4.3177 2929,-1.895892127\H,-2.2123785096,2.7958331741,-3.5938225171\H,-1.9729 876274,1.4847235331,-2.4497770012\H,-0.2425304978,1.6180056797,-4.3504 556728\H,0.3060152445,3.1548270462,-3.6883370475\C,1.8541693375,-2.322 7909547,-1.3580852306\H,2.2505017178,-2.6719579174,-2.306215171\H,2.05 20262827,-2.9463389614,-0.4922078147\Se,3.8736911035,-0.7618334175,-1. 150674698\C,3.812455598,-0.4650369282,0.7226662649\C,3.1541521509,0.66 24845797,1.249210676\C,4.4557752963,-1.3511346451,1.6048310487\C,3.154 4879101,0.897700376,2.6237752022\H,2.6293635297,1.3284464291,0.5699300 216\C,4.4525351293,-1.111416984,2.9774939591\H,4.9611210786,- 2.2221211 117,1.1990527345\C,3.804152234,0.0151789831,3.4913030029\H,2.647312316 5,1.7730009525,3.0215441962\H,4.9566652329,- 1.8031260488,3.6473510482\ H,3.8048634352,0.2038746752,4.5615041736\\Version=ES64L-G16RevA.03\Sta te=2-A\HF=-8396.1668652\S2=0.767137\S2- 1=0.\S2A=0.750171\RMSD=9.621e-0 9\RMSF=8.890e-07\ZeroPoint=0.5995562\

**Reaction 1-Intermediate**




1\1\GINC-LOCALHOST\Freq\UB3LYP\6-31G(d)\C24H39N2O2Se3(2)\GAUSS\06-Oct- 2020\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk UB3LYP/6-31G(d ) Freq\\Title Card Required\\0,2\C,1.9384816941,0.4834341178,3.1025706 193\C,2.8253802148,1.5833982087,2.6915264638\H,3.3898358499,1.34515264 79,1.787825966\H,3.494543025,1.9257625267,3.4825319703\C,1.1498356915, -0.2216347662,2.0623374533\H,0.0844349681,-0.2203021993,2.3152944624\H ,1.2907400654,0.218360516,1.0760098884\Se,1.6323209991,-2.1654093379,1 .9762666735\C,-0.0424432107,-2.7810045732,1.112455975\C,-0.3370394631, -2.1619170986,-0.2586754397\C,0.4333758113,-2.771065103,-1.4449544458\ C,1.9631219914,-2.7564032861,-1.3629872401\O,2.5956950144,-3.793087508 3,-1.1800206128\N,2.5595010329,-1.5475724841,-1.5942341158\H,1.9959884 918,-0.7029844769,-1.5765931323\C,4.0068453506,-1.4031957064,-1.531622 6906\C,4.5212971133,-0.8138722399,-0.2111973396\C,6.0494456731,-0.8330 520266,-0.1207679602\H,6.5077530517,-0.269672433,-0.9439839815\H,6.432 8910592,-1.8591921677,-0.169161338\H,6.4007737795,-0.3915089746,0.8189 03001\H,4.070030725,-1.3767854102,0.6124420506\H,4.1580606301,0.219502 0463,-0.1164131588\H,4.4172075601,-2.406407656,-1.6727310115\H,4.33905 48805,-0.7826423024,-2.3756978456\H,0.159598425,-3.8246149269,-1.55762 53757\H,0.1218532491,-2.2484495586,-2.3590054291\H,-1.4087778703,-2.30 40514284,-0.4641130181\H,-0.1772750099,-1.0787718861,-0.2321088046\H,0 .0775361281,-3.8665684251,1.0421741874\H,-0.8496228138,-2.5707491745,1 .8196206034\Se,1.7100718569,3.2154094921,2.1596244722\C,2.9723286512,3 .9689916737,0.8175856432\C,3.0164858521,3.289063478,-0.5514025441\C,1. 7241393968,3.4094044541,-1.3746158436\C,0.682601155,2.32968645,-1.0901 38173\O,0.9789569946,1.1312598768,-1.0466438269\N,-0.5998132044,2.7619 295181,-0.9954570743\H,-0.7700379125,3.7563341317,-1.0134759795\C,-1.7 384909527,1.8623475663,-0.8298517586\C,-2.2458460443,1.2601064484,-2.1 484163015\C,-2.7826487283,2.2994826959,-3.136322577\H,-2.006879207,3.0 226466289,-3.4137545874\H,-3.626262729,2.8578446614,-2.7103371196\H,-3 .1329558219,1.8231926876,-4.0582247639\H,-3.0347806305,0.5359561363,-1 .9045241968\H,-1.4276578768,0.6906013921,-2.604434183\H,-1.438230088,1 .065814877,-0.1439282591\H,-2.5362156014,2.4372363022,-0.3449452386\H, 1.9741501628,3.2908642045,-2.43731516\H,1.2933883723,4.4132401333,-1.2 650971689\H,3.8346160787,3.7467690229,-1.1252348779\H,3.265568491,2.22 70179081,-0.4538412606\H,3.9604650996,3.9702071873,1.2866456571\H,2.65 94730953,5.0146678743,0.7219182636\C,1.5900009515,0.3145578927,4.51488 43359\H,2.4362131628,0.4322642367,5.196679045\H,1.0585137705,- 0.613545 2664,4.7272739725\Se,0.3767757183,1.8602088989,5.1464835144\C,-1.31448 30046,1.2246277067,4.4897635535\C,- 1.7944900385,1.6234838498,3.2348020 884\C,-2.0999716512,0.3968041776,5.3017071533\C,-3.0521883536,1.194980 6528,2.805073343\H,- 1.1723039322,2.2468485397,2.5985165418\C,-3.353630 968,-0.0326864373,4.8649289318\H,-1.7241186922,0.0992089622,6.27595313 89\C,- 3.8328697511,0.3685705354,3.6163205903\H,-3.4243710503,1.5076611 967,1.8330220035\H,-3.9562610537,-0.6754191425,5.5012250052\H,-4.81205 31044,0.0405377625,3.2777047062\\Version=ES64L-G16RevA.03\State=2-A\HF =-8396.1728064\S2=0.75777\S2-1=0.\S2A=0.750045\RMSD=5.795e- 09\RMSF=1.9 95e-06\ZeroPoint=0.6002043

**Reaction 1-TS2**




1\1\GINC-LOCALHOST\Freq\UB3LYP\6-31G(d)\C24H39N2O2Se3(2)\GAUSS\07-Oct- 2020\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk UB3LYP/6-31G(d ) Freq\\Title Card Required\\0,2\C,0.8131825778,-1.4619775621,-1.85993 12094\C,0.4678883171,-0.81488235,-3.0088453534\H,- 0.3501097341,-0.1018 837006,-3.0219026972\H,0.8637730352,-1.1203630667,-3.9722342536\C,0.26 49071466,-1.0288792799,- 0.5391116507\H,1.0907449668,-0.8197605797,0.14 6547905\H,-0.3669813049,-0.1442739985,-0.6159064487\Se,-0.7787507885,- 2.4855956732,0.3293249928\C,-0.150472947,-2.160910725,2.180143799\C,-0 .5045878686,-0.7815856017,2.7488569858\C,-1.9410034213,-0.638306996,3. 2895580109\C,-3.0578803628,-1.0040052621,2.3079240852\O,-3.5915333758, -2.1106342634,2.3405222073\N,-3.4314183167,-0.0051578644,1.4549100377\ H,-2.8233169946,0.8040491953,1.3646495344\C,-4.3848571524,-0.237016615 2,0.3784522145\C,-3.7185447457,-0.3169156917,-1.0016217914\C,-4.714079 4573,-0.644809957,-2.1171902984\H,-5.5058681974,0.1125985149,-2.182965 0334\H,-5.1974650631,-1.6138416804,-1.9438085401\H,-4.2190894926,-0.69 09671162,-3.0940717907\H,-2.9313533973,-1.0764514078,-0.9418964592\H,- 3.2193380062,0.6392901595,-1.2124799154\H,-4.8892442184,-1.1778484005,

0.6134695699\H,-5.1416876746,0.5606362199,0.3873280937\H,-2.0745305718 ,-1.3009376793,4.1505386474\H,-2.0762946189,0.3932500153,3.6395460518\
H,0.1814550325,-0.5780202965,3.5840694905\H,-0.3111341129,-0.000357221 1,2.0051622479\H,-0.6196399929,-2.9618000772,2.7592504507\H,0.93055309
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7,-2.0290278731\C,0.3087344379,3.2448537817,-0.626675897\C,-0.77652148 32,3.1349323323,0.4312800514\O,-1.4102444057,2.0859643031,0.5952558811
\N,-0.9951896011,4.240160211,1.1913371544\H,-0.4726902079,5.0768461252 ,0.9768651696\C,-2.009039549,4.2994316888,2.2418123997\C,-3.3955693025
,4.7328593499,1.7432734466\C,-3.4305434901,6.1505162201,1.1654121454\H ,-2.7681237973,6.2450828683,0.2966727404\H,-3.1182125176,6.8938017231,
1.9102388071\H,-4.440544692,6.4166041911,0.8361761849\H,-4.0930766401, 4.6588813769,2.5881306096\H,-3.7351003175,4.0094566582,0.992398853\H,-
2.0679641179,3.3033273225,2.6879775574\H,-1.6474113806,4.990979099,3.0 121797245\H,0.7714438536,4.2405234797,-0.6270220731\H,1.0918906413,2.5
196507532,-0.3718385691\H,-0.8845820461,3.6844199694,-2.3845224838\H,- 0.8131023998,1.9814013414,-1.952960978\H,0.494150025,2.507511,-4.05182
08726\H,1.5374136958,3.5919961672,-3.1309156761\C,1.8603496792,-2.5265 012465,-1.8479971485\H,1.8850128193,-3.0953458675,-2.7799155925\H,1.73
23836362,-3.2095776418,-1.0071522373\Se,3.7247616398,-1.7763800024,-1. 7422477429\C,3.8470635137,-1.4534642204,0.1527369786\C,3.6987999949,-0
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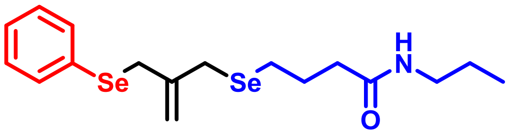
6359175\C,4.2736895259,-2.2781201955,2.3903388282\H,4.2780959708,-3.51 04198672,0.6160222099\C,4.1262618301,-0.9836091182,2.8960356048\H,3.73
04128802,1.0826226385,2.4198503676\H,4.5007973445,-3.1037333643,3.0596 357649\H,4.2371171754,-0.8007385952,3.9615817896\\Version=ES64L-
G16Rev A.03\State=2-A\HF=-8396.168514\S2=0.76113\S2-1=0.\S2A=0.750042\RMSD=2. 377e-09\RMSF=6.758e-07\ZeroPoint=0.5998674\




1\1\GINC-LOCALHOST\Freq\UB3LYP\6-31G(d)\C17H25N1O1Se2\GAUSS\08-Oct-202 0\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk
UB3LYP/6-31G(d) F req\\Title Card Required\\0,1\C,1.9599301435,-0.1867838277,-1.72803871 77\C,2.4693846383,0.1557393981,-
2.9182251308\H,1.8342074731,0.48518289 35,-3.7367108291\H,3.5367184807,0.1135548894,-3.1183858472\C,0.4803755 505,-0.105979162,-
1.4588889401\H,0.2538802339,0.6046578301,-0.65745624 71\H,-0.0552780195,0.2064684958,-2.3572229138\Se,-0.3268604222,-1.8444 702744,-
0.899200569\C,-0.5557913528,-1.4405842961,1.0291624283\C,-1.83 86682559,-0.6741375913,1.3732971104\C,-3.0856508057,-1.5633758405,1.58
02766421\C,-3.3792541906,-2.4653038873,0.3859279754\O,-2.7927403554,-3 .5330239465,0.2282716817\N,-4.3167295508,-1.9875765691,-0.4889272682\H
,-4.6673160576,-1.0524438298,-0.3288032392\C,-4.4817398023,-2.53785279 63,-1.8293410606\C,-3.785834496,-1.6789395681,-2.8946336048\C,-3.85931
75145,-2.2991898415,-4.2922301654\H,-4.8986017082,-2.4374265236,-4.616 1964419\H,-3.3710776249,-3.2806935569,-4.3139864458\H,-3.3630135431,-1
.6640412079,-5.0342371849\H,-2.7448182997,-1.5457114259,-2.5769450183\ H,-4.2439107056,-0.6783261024,-2.9098603695\H,-4.0453370989,-3.5392559
658,-1.7994189083\H,-5.5523918461,-2.6429517775,-2.0493553568\H,-2.918 6455245,-2.2226922102,2.4384177399\H,-3.9475865036,-0.9260777624,1.816
2473996\H,-1.6773030135,-0.1168618686,2.3067879736\H,-2.0403499097,0.0 746507027,0.596971377\H,-0.5344316643,-2.4202672043,1.512318234\H,0.33
59131956,-0.8796371989,1.3182107929\C,2.8408661296,-0.6826283363,-0.61 90765535\H,3.8874355416,-0.7201957881,-0.9218810313\H,2.5072989418,-1.
6640810558,-0.2729272768\Se,2.7393086355,0.5314750102,0.9697937541\C,3 .8570376718,-0.5179890051,2.1393238744\C,3.3016689683,-1.4917423794,2.
9765853038\C,5.237478494,-0.2894397625,2.1624806361\C,4.1238402099,-2. 234120173,3.8262927301\H,2.2305704617,-1.6684366132,2.9645776337\C,6.0
572376386,-1.032650953,3.0131348779\H,5.6626909648,0.472758462,1.51633 14839\C,5.5012416132,-2.0062982555,3.8452840684\H,3.6872105557,-2.9901
678624,4.4735386041\H,7.1284632297,-0.8495869705,3.0259678426\H,6.1392 464932,-2.5841652923,4.5085619562\\Version=ES64L-G16RevA.03\State=1-A\
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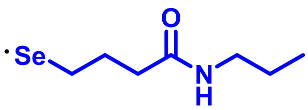
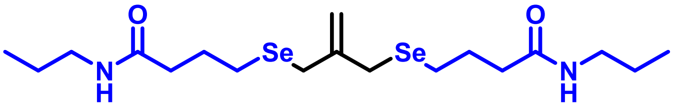



1\1\GINC-LOCALHOST\Freq\UB3LYP\6-31G(d)\C7H14N1O1Se1(2)\GAUSS\30-Sep-2 020\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk
UB3LYP/6-31G(d) Freq\\Title Card Required\\0,2\Se,-3.2711183874,-0.6156557986,0.02830 21964\C,-2.4968261253,1.1419472669,0.4649327526\C,-
0.9849292031,1.1513 718068,0.6749319072\C,-0.2000913655,0.7805658244,-0.5881856616\C,1.306 6754699,0.9209788563,-
0.3770096993\O,1.7883611642,1.875341492,0.224578 3389\N,2.06545624,-0.0743148978,-0.9273758126\H,1.5923459628,-0.845416 605,-
1.3775051171\C,3.5206686756,-0.1057951068,-0.8526466924\C,4.06619 49823,-1.2255839642,0.0463491497\C,3.6565903751,-1.0931526159,1.515547
6037\H,3.9986752615,-0.1409035943,1.9363024164\H,4.0831288226,-1.90382 14117,2.116732161\H,2.5676933742,-1.1299265343,1.627910566\H,5.1613769
739,-1.216945971,-0.0394220431\H,3.7388009297,-2.1993779544,-0.3466282 612\H,3.926931978,-0.2114053818,-1.8673516563\H,3.8223288627,0.8729988
796,-0.4710611017\H,-0.4780654395,1.4636825492,-1.4039669011\H,-0.4724 095176,-0.2321286164,-0.9124535629\H,-0.6682172412,2.150467311,0.99769
1146\H,-0.7258507136,0.45848188,1.484712633\H,-3.0332055312,1.46417543 89,1.3652654805\H,-2.8065515482,1.8123921471,-0.3452178424\\Version=ES
64L-G16RevA.03\State=2-A\HF=-2804.5228976\S2=0.752231\S2-1=0.\S2A=0.75 0002\RMSD=1.143e-10\RMSF=4.488e-06\ZeroPoint=0.2071859\




1\1\GINC-LOCALHOST\Freq\UB3LYP\6-31G(d)\C18H34N2O2Se2\GAUSS\05-Oct-202 0\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk
UB3LYP/6-31G(d) F req\\Title Card Required\\0,1\C,-1.237733721,-0.9833055886,0.218983643 2\C,0.034095134,-
0.5709729902,0.1317549829\C,0.8125127494,-0.147492968 8,1.3488002762\H,1.883143884,-0.2457936183,1.1612944775\H,0.5332305419 ,-
0.7175222981,2.2363403104\C,0.7755776477,-0.4982746999,-1.169440316\ H,0.1051680661,-0.5939834858,-2.024827137\H,1.3634097715,0.4205759844, -
1.2382480679\Se,2.0865396402,-2.0116405509,-1.2534948497\C,3.52673597 17,-1.1069363107,-2.2850499699\C,4.6912292321,-0.5938310631,-1.4320237
356\C,5.7574192539,-1.6567650634,-1.0817665129\C,5.1893559461,-2.92828 53513,-0.4606426873\O,4.6389039257,-3.7869065268,-1.1474495206\N,5.341
5613922,-3.0505130035,0.8932497718\H,5.6942704417,-2.2511385144,1.4015 792293\C,4.6696553263,-4.097540216,1.6538694635\C,3.3175724641,-3.6490
899608,2.2259545671\C,2.588710414,-4.7800345897,2.9566757349\H,3.18208 39286,-5.1652724503,3.7958138627\H,2.3853336639,-5.6191239586,2.280743
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1754,-4.9313985733,0.9620034135\H,5.3389618715,-4.4355226568,2.4557404 05\H,6.2627835266,-1.9707489108,-2.0018955141\H,6.5167827064,-1.204245

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22905\H,3.0440592057,-0.2820970229,-2.8131362424\H,-1.801561504,-1.280 7482476,-0.6611400677\H,-1.7550047215,-1.0393678746,1.173589368\Se,0.4
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012,5.4139082306,-3.328817227\H,2.769309816,5.717965692,-2.6170552054\ H,1.1870076119,6.1572257859,-3.2834759507\H,2.4274420476,5.4569256129,
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7980688,2.9593213304\H,3.5378463297,1.3199706709,1.6699225975\H,1.9831
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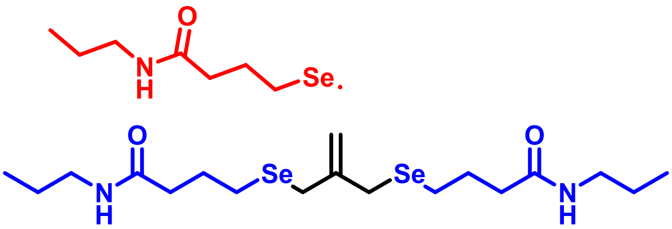
**Reaction 2-TS1**



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1.9661501675,-7.323478095 3,-5.9130727993\N,0.0360974756,-6.367709015,-6.4438539761\H,0.64879444 82,-5.5817642131,-
6.2774408953\C,0.4129207337,-7.3345922508,-7.4662251 428\C,0.3879343861,-6.7652844747,-8.8930037636\C,-1.0001303013,-6.3118 148587,-
9.353036505\H,-1.7175616629,-7.1393425184,-9.317540368\H,-0.96 87167634,-5.9316245717,-10.3802712359\H,-1.3882531896,-5.5132431041,-8
.711785287\H,0.7709120081,-7.5426201365,-9.5684087446\H,1.0966431237,- 5.9269229358,-8.9622616397\H,1.4147819517,-7.7220321825,-7.2379469483\
H,-0.2959623451,-8.1613064106,-7.3718675686\H,-1.2507272462,-5.7854043 015,-3.724830904\H,-0.5765934124,-4.5452321279,-4.7893537681\H,-3.4853
852393,-5.4805803791,-4.8198207981\H,-2.8157948192,-4.2055433843,-5.83 44633836\H,-4.0433760093,-3.2287157429,-3.9132812651\H,-3.0309918053,-
4.0828073288,-2.7581877024\C,-0.1271902497,-2.8811643679,-1.8847380579 \C,-0.5525610376,-2.0324820566,-0.9003665643\C,-1.6118496204,-2.426736
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.8867149377,-0.6362258632\C,-4.3525359516,-1.7591634185,1.1140306005\C ,-4.0415170968,-0.4987278414,1.9260065983\C,-4.5240663694,0.8213403308
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,4.0255869939,-2.6639172125\H,-4.5155207322,4.1255669831,-1.7041421166 \H,-4.7587550756,3.9224603716,-3.4472780166\H,-3.4549354226,4.95982680
3,-2.8496769456\H,-2.5314012304,2.7499657761,-3.6217104903\H,-2.266329 857,2.9684493331,-1.894232833\H,-3.040084009,0.6489805868,-2.495598005
7\H,-4.5279934902,1.3354903645,-3.1418435147\H,-4.4104000281,1.6210374 299,2.0355701127\H,-5.5943252229,0.7543670103,1.0569628827\H,-4.517693
1952,-0.5987522391,2.9121426205\H,-2.9634380128,-0.4212023755,2.107593 5726\H,-4.123133689,-2.6654726554,1.6817641474\H,-5.4140180479,-1.8015
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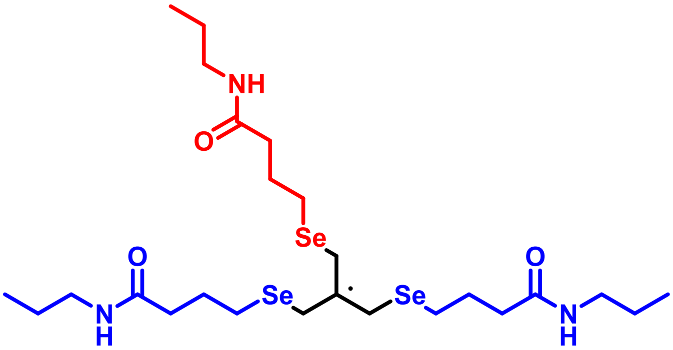
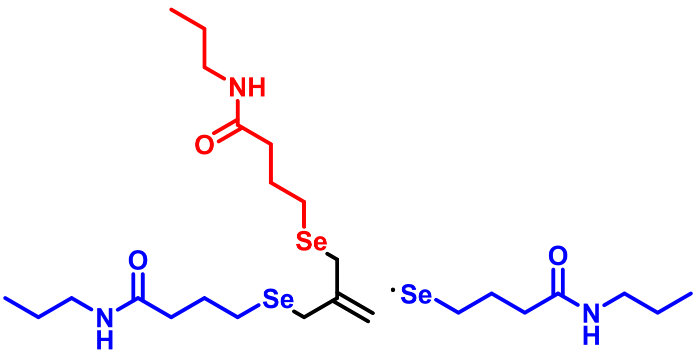
07\ZeroPo int=0.7163477\

**Reaction 2-Intermediate**




1\1\GINC-LOCALHOST\Freq\UB3LYP\6-31G(d)\C25H48N3O3Se3(2)\GAUSS\04-Oct- 2020\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk UB3LYP/6-31G(d ) Freq\\Title Card Required\\0,2\Se,-2.3736091644,-0.9571978049,0.0441 567876\C,-3.3524561632,-0.7172571359,-1.6673810848\C,-4.8179421795,-0. 3158807494,-1.5009992617\C,-5.0242955365,0.9792573342,-0.7176330558\C, -6.5013439778,1.3495571351,-0.5716688324\O,-7.4072297659,0.6610871244, -1.0275229533\N,-6.7246668303,2.5195821042,0.1048382872\H,-5.928050606 7,3.0108124076,0.4875253337\C,-8.0553698574,3.0397366546,0.3902447541\ C,-8.4429902049,2.9659762816,1.8749566582\C,-8.5156066998,1.5391125188 ,2.4251918138\H,-9.2419911396,0.93747144,1.8673012078\H,-8.812481831,1 .5394152393,3.4799530535\H,-7.5458538162,1.0353784416,2.3505848975\H,-9.4167826089,3.4615494927,1.9899360288\H,-7.7297449542,3.5586627232,2. 4666972769\H,-8.1143707947,4.0796592746,0.0421160891\H,-8.7447500172,2 .4454884962,-0.2150056376\H,-4.4959354938,1.8142492268,-1.2018726669\H ,-4.5765045014,0.8649281072,0.2793557676\H,-5.2696241956,-0.2169447377 ,-2.496722766\H,-5.3675895199,-1.1199178487,-1.0000373745\H,-3.2743961 959,-1.6898148118,-2.1603058821\H,-2.7705618598,-0.0087171881,-2.26443 19413\C,-1.4015271917,0.8454354857,0.1867645953\C,0.0442570278,0.60966 56624,0.1233810424\C,0.7282797774,0.5063919965,-1.1793039139\H,1.80687 70332,0.4360055097,-1.0397447296\H,0.4808799817,1.3291767126,-1.856270 1026\C,0.7921721571,0.2384761416,1.3463272083\H,0.1358735754,0.0762983 576,2.2037867835\H,1.4328160613,-0.6315567529,1.1754021033\Se,2.059874 5622,1.7365314628,1.8313721016\C,3.3480757779,0.6548927908,2.888130451 5\C,4.4731534799,0.0280213448,2.0565518502\C,5.6844177028,0.9586494327 ,1.8166667308\C,5.3161318436,2.3318347879,1.2644838693\O,4.8645822973, 3.2162506925,1.9896190273\N,5.5351524049,2.5119536341,-0.0737475315\H, 5.7880381356,1.7008570569,-0.6216306699\C,5.0498805525,3.6881540437,-0 .7847052168\C,3.6782854874,3.4693077081,-1.4380919227\C,3.1450339403,4 .7339384962,-2.1167685877\H,3.8247023791,5.0859449208,-2.9033194967\H, 3.024756206,5.5489719078,-1.3930967288\H,2.1681677421,4.5542344165,-2. 5795063682\H,2.9901947212,3.1219318681,-0.6591859193\H,3.7547157308,2. 6564650123,-2.1760362316\H,4.9887878256,4.4878814091,-0.0422039478\H,5 .7961110792,3.9806448185,-1.5350313601\H,6.1874914418,1.1443899105,2.7 721544846\H,6.4035460412,0.4498557599,1.1620823847\H,4.8530130441,-0.8 571692625,2.5867219162\H,4.0715349672,-0.3387367348,1.1067325135\H,3.7 317982785,1.3498514653,3.6378986439\H,2.7551786793,-0.1101926104,3.395 874369\H,-1.7273214355,1.2621862674,1.1407078032\H,-1.7955824353,1.440 8597509,-0.6404781992\Se,0.1678851138,-1.1585912787,-2.2074762917\C,1. 6287981979,-1.0885116417,-3.5598915038\C,3.030521275,-1.4100647628,-3. 0308541151\C,3.1763697044,-2.7958619166,-2.3785327156\C,2.5222981172,- 2.862427195,-0.9962201048\O,2.7845858794,-2.0264455888,-0.1299438875\N ,1.7018600303,-3.9281016054,-0.7746555332\H,1.4321187605,-4.4499316814 ,-1.5962763914\C,0.7414450435,-3.9372745337,0.3354320276\C,1.370178847 1,-4.2285931281,1.7021340965\C,2.0039975215,-5.6189324725,1.8009314114 \H,2.7968901392,-5.7433789755,1.0551569655\H,1.2609122194,-6.409654485 3,1.6342458787\H,2.4455973206,-5.7825950367,2.7903037155\H,0.578817606 9,-4.1259703268,2.4571742648\H,2.1160890447,-3.4569144021,1.9157324003 \H,0.2058279873,-2.9796703146,0.3340421912\H,0.0063997792,-4.715506223 3,0.0987144125\H,4.2440440782,-3.002713526,-2.2327124177\H,2.788728850 5,-3.5765668689,-3.046242409\H,3.7361143797,-1.3425008718,-3.871219189 3\H,3.3452385867,-0.6577484218,-2.2990783211\H,1.6036568508,-0.1025695 105,-4.0336792307\H,1.3191796289,-1.8236451802,-4.3112189849\\Version= ES64L-G16RevA.03\State=2-A\HF=-8569.6994403\S2=0.756896\S2-1=0.\S2A=0. 750036\RMSD=2.587e-09\RMSF=6.068e-07\ZeroPoint=0.7165918

**Reaction 2-TS2**




1\1\GINC-LOCALHOST\Freq\UB3LYP\6-31G(d)\C25H48N3O3Se3(2)\GAUSS\05-Oct- 2020\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk UB3LYP/6-31G(d ) Freq\\Title Card Required\\0,2\Se,-2.2382943432,-0.1015963392,-0.118 8888518\C,-3.2263604694,0.6057953326,1.4570734651\C,-4.6383704168,1.02 53052423,1.045708726\C,-5.5456351562,-0.1623472222,0.7078590193\C,-6.8 417332419,0.2729945327,0.0261580107\O,-6.9055023649,1.2704354643,-0.68 46135787\N,-7.9141407119,-0.5466539644,0.2539886625\H,-7.7777621039,-1 .364949123,0.8313300426\C,-9.2146705709,-0.3575916908,-0.3754600281\C, -9.5609120739,-1.4363143343,-1.4128456437\C,-8.6081943569,-1.470781318 9,-2.6109112051\H,-8.5947988119,-0.5070215308,-3.1323021514\H,-8.90793 43141,-2.2419778103,-3.3292421082\H,-7.5818920469,-1.68791025,-2.29564 60251\H,-10.5877434106,-1.2504671413,-1.7563482925\H,-9.5793883939,-2. 4205841933,-0.9218378408\H,-9.9875840791,-0.3297072209,0.40416301\H,-9 .1783270011,0.6287286796,-0.8450191517\H,-5.7620441836,-0.7510475241,1 .6101267374\H,-5.0064341006,-0.8303940445,0.0210894787\H,-5.0814775912

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4,-2.2340382386\C,3.1541685592,-1.19556431,-2.6556100838\C,4.673397959 3,-1.3803075111,-2.4851247604\C,5.1821959032,-1.6830019566,-1.07204163
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1195621642,2.0897084181\C,3.24401804,3.7498423545,0.7592531058\C,2.856 1849865,2.9382674619,-0.4736959802\O,3.3294065837,1.8164450376,-
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.0833989881,2.0646526799,2.0930134026\H,1.0873071993,2.9315568847,3.43 2068048\H,0.9725816829,4.299439667,2.3319698295\\Version=ES64L-
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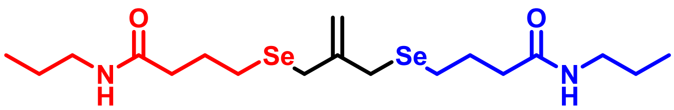


1\1\GINC-LOCALHOST\Freq\UB3LYP\6-31G(d)\C18H34N2O2Se2\GAUSS\05-Oct-202 0\0\\#N Geom=AllCheck Guess=TCheck SCRF=Check GenChk
UB3LYP/6-31G(d) F req\\Title Card Required\\0,1\C,-1.237733721,-0.9833055886,0.218983643 2\C,0.034095134,-
0.5709729902,0.1317549829\C,0.8125127494,-0.147492968 8,1.3488002762\H,1.883143884,-0.2457936183,1.1612944775\H,0.5332305419 ,-
0.7175222981,2.2363403104\C,0.7755776477,-0.4982746999,-1.169440316\ H,0.1051680661,-0.5939834858,-2.024827137\H,1.3634097715,0.4205759844, -
1.2382480679\Se,2.0865396402,-2.0116405509,-1.2534948497\C,3.52673597 17,-1.1069363107,-2.2850499699\C,4.6912292321,-0.5938310631,-1.4320237
356\C,5.7574192539,-1.6567650634,-1.0817665129\C,5.1893559461,-2.92828 53513,-0.4606426873\O,4.6389039257,-3.7869065268,-1.1474495206\N,5.341
5613922,-3.0505130035,0.8932497718\H,5.6942704417,-2.2511385144,1.4015 792293\C,4.6696553263,-4.097540216,1.6538694635\C,3.3175724641,-3.6490
899608,2.2259545671\C,2.588710414,-4.7800345897,2.9566757349\H,3.18208 39286,-5.1652724503,3.7958138627\H,2.3853336639,-5.6191239586,2.280743
8123\H,1.6286888434,-4.437928095,3.3585984749\H,2.7128686199,-3.266962 3135,1.3957571673\H,3.4774225753,-2.8052018588,2.9138577831\H,4.526479
1754,-4.9313985733,0.9620034135\H,5.3389618715,-4.4355226568,2.4557404 05\H,6.2627835266,-1.9707489108,-2.0018955141\H,6.5167827064,-1.204245
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22905\H,3.0440592057,-0.2820970229,-2.8131362424\H,-1.801561504,-1.280 7482476,-0.6611400677\H,-1.7550047215,-1.0393678746,1.173589368\Se,0.4
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900444\C,3.3160503888,2.2574845541,2.1919674682\C,3.4395976256,3.41219 51308,1.1831056313\C,2.6893852043,3.1422370586,-
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7980688,2.9593213304\H,3.5378463297,1.3199706709,1.6699225975\H,1.9831
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## References

1 Y. Qian; X. An; X. Huang; X. Pan; J. Zhu; X. Zhu, *Polymers* **2019,** *11*, 773.

## Author Contributions

S. S. Chen, Prof. X. Q. Pan and Prof. J. Zhu conceived the research idea and co-wrote the original draft. S. S. Chen, M. Liu performed the synthesis and characterization. J. D. Zhang performed DFT calculations. Prof. Z. B. Zhang and Prof. X.L. Zhu co-revised the manuscript.