

Supporting information for:

Dynamic Diselenide Containing Polyester from Alcoholysis/Oxidation of γ -Butyroselenolactone

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diethyl γ , γ' -diselenodibutyrate (1): Yellow liquid, yield >99%. ¹H NMR (300 MHz, CDCl₃) δ 4.15 (q, J = 7.1 Hz, 4H), 2.93 (t, J = 7.2 Hz, 4H), 2.43 (t, J = 7.3 Hz, 4H), 2.14-2.00 (m, 4H), 1.26 (t, J = 7.1 Hz, 6H). ¹³C NMR (75 MHz, CDCl₃) δ 173.53, 61.09, 34.39, 29.44, 26.69, 14.91. ⁷⁷Se NMR (114 MHz, CDCl₃) δ 302.81. HR-ESI-MS: *calculated m/z* C₁₂H₂₂NaO₄Se₂ [M+Na⁺]: 412.9746; *experimental m/z* [M+Na⁺]: 412.9807.

dimethyl γ , γ' -diselenodibutyrate (2): Yellow liquid, yield >99%; ¹H NMR (300 MHz, CDCl₃) δ 3.68 (s, 6H), 2.93 (t, J = 7.2 Hz, 4H), 2.45 (t, J = 7.3 Hz, 4H), 2.13-2.01 (m, 4H). ¹³C NMR (75 MHz, CDCl₃) δ 173.95, 52.29, 34.08, 29.35, 26.61. ⁷⁷Se NMR (114 MHz, CDCl₃) δ 302.09. HR-ESI-MS: *calculated m/z* C₁₀H₁₈NaO₄Se₂ [M+Na⁺]: 384.9433; *experimental m/z* [M+Na⁺]: 384.9515.

dipropyl γ , γ' -diselenodibutyrate (3): Yellow liquid, yield 99%; ¹H NMR (300 MHz, CDCl₃) δ 4.04 (t, J = 6.7 Hz, 4H), 2.94 (t, J = 7.2 Hz, 4H), 2.44 (t, J = 7.3 Hz, 4H), 2.13-2.00 (m, 4H), 1.72-1.58 (m, 4H), 0.94 (t, J = 7.4 Hz, 6H). ¹³C NMR (75 MHz, CDCl₃) δ 173.60, 66.73, 34.37, 29.44, 26.71, 22.64, 11.06. ⁷⁷Se NMR (114 MHz, CDCl₃) δ 302.58. HR-ESI-MS: *calculated m/z* C₁₄H₂₆NaO₄Se₂ [M+Na⁺]: 441.0059; *experimental m/z* [M+Na⁺]: 441.0039.

dibutyl γ , γ' -diselenodibutyrate (4): Yellow liquid, yield 91%; ¹H NMR (300 MHz, CDCl₃) δ 4.08 (t, J = 6.7 Hz, 4H), 2.93 (t, J = 7.2 Hz, 4H), 2.43 (t, J = 7.3 Hz, 4H), 2.13-2.00 (m, 4H), 1.67-1.54 (m, 4H), 1.45-1.30 (m, 4H), 0.93 (t, J = 7.3 Hz, 6H). ¹³C NMR (75 MHz, CDCl₃) δ 173.61, 65.03, 43.39, 31.33, 29.44, 26.71, 19.81, 14.37. ⁷⁷Se NMR (114 MHz, CDCl₃) δ 302.60. HR-ESI-MS: *calculated m/z* C₁₆H₃₀NaO₄Se₂ [M+Na⁺]: 469.0372; *experimental m/z* [M+Na⁺]:

469.0364.

dihexyl γ , γ' -diselenodibutyrate (5): Yellow liquid, yield 90%, ^1H NMR (300 MHz, CDCl_3) δ 4.07 (t, J = 6.7 Hz, 4H), 2.93 (t, J = 7.2 Hz, 4H), 2.43 (t, J = 7.3 Hz, 4H), 2.13-1.99 (m, 4H), 1.68-1.54 (m, 4H), 1.41-1.23 (m, 12H), 0.89 (t, J = 6.8 Hz, 6H). ^{13}C NMR (75 MHz, CDCl_3) δ 173.64, 65.36, 34.41, 32.11, 29.46, 29.27, 26.73, 26.28, 23.22, 14.68. ^{77}Se NMR (114 MHz, CDCl_3) δ 302.49. HR-ESI-MS: *calculated* m/z $\text{C}_{20}\text{H}_{38}\text{NaO}_4\text{Se}_2[\text{M}+\text{Na}^+]$: 525.0998; *experimental* m/z $[\text{M}+\text{Na}^+]$: 525.0866.

di(2-methylallyl) γ , γ' -diselenodibutyrate (6): Yellow liquid, yield 91%; ^1H NMR (300 MHz, CDCl_3) δ 4.97 (d, J = 12.8 Hz, 4H), 4.51 (s, 4H), 2.94 (t, J = 7.2 Hz, 4H), 2.49 (t, J = 7.3 Hz, 4H), 2.16-2.02 (m, 4H), 1.76 (s, 6H). ^{13}C NMR (75 MHz, CDCl_3) δ 173.18, 140.55, 113.64, 68.70, 34.29, 29.35, 26.66, 20.20. ^{77}Se NMR (144 MHz, CDCl_3) δ 302.09. HR-ESI-MS: *calculated* m/z $\text{C}_{16}\text{H}_{26}\text{NaO}_4\text{Se}_2[\text{M}+\text{Na}^+]$: 465.0059; *experimental* m/z $[\text{M}+\text{Na}^+]$: 464.9926.

diisopropyl γ , γ' -diselenodibutyrate (7): Yellow liquid, yield 24%; ^1H NMR (300 MHz, CDCl_3) δ 5.08-4.92 (m, 2H), 2.93 (t, J = 7.3 Hz, 4H), 2.39 (t, J = 7.3 Hz, 4H), 2.12-1.99 (m, 4H), δ 1.22 (d, J = 6.3 Hz, 12H). ^{13}C NMR (75 MHz, CDCl_3) δ 173.03, 68.37, 34.74, 29.48, 26.77, 22.52. ^{77}Se NMR (114 MHz, CDCl_3) δ 303.68. HR-ESI-MS: *calculated* m/z $\text{C}_{14}\text{H}_{26}\text{NaO}_4\text{Se}_2[\text{M}+\text{Na}^+]$: 441.0059; *experimental* m/z $[\text{M}+\text{Na}^+]$: 441.0116.

di(prop-2-yn-1-yl) γ , γ' -diselenodibutyrate (8): Yellow liquid, yield 83%; ^1H NMR (300 MHz, CDCl_3) 4.68 (d, J = 2.5 Hz, 4H), 2.93 (t, J = 7.2 Hz, 4H), 2.50 (m, 6H), 2.16-2.01 (m, 4H). ^{13}C NMR (75 MHz, CDCl_3) δ 172.67, 78.29, 75.59, 52.62, 33.99, 29.15, 26.48. ^{77}Se NMR (114 MHz, CDCl_3) δ 302.45. HR-ESI-MS: *calculated* m/z $\text{C}_{14}\text{H}_{18}\text{NaO}_4\text{Se}_2[\text{M}+\text{Na}^+]$: 432.9433; *experimental* m/z $[\text{M}+\text{Na}^+]$: 432.9455.

dibenzyl γ , γ' -diselenodibutyrate (9): Yellow liquid, yield 98%; ^1H NMR (300 MHz, CDCl_3) δ 7.40-7.30 (m, J = 9.08 Hz, 10H), 5.12 (s, 4H), 2.91 (t, J = 7.2 Hz, 4H), 2.48 (t, J = 7.3 Hz, 4H), 2.15-2.01 (m, 4H). ^{13}C NMR (75 MHz, CDCl_3) δ 173.34, 136.57, 129.24, 128.90, 127.64, 66.98, 34.33, 29.33, 26.63. ^{77}Se NMR (114 MHz, CDCl_3) δ 320.55. HR-ESI-MS: *calculated* m/z $\text{C}_{22}\text{H}_{26}\text{NaO}_4\text{Se}_2[\text{M}+\text{Na}^+]$: 537.0059; *experimental* m/z $[\text{M}+\text{Na}^+]$: 537.0039.

dicyclohexyl γ , γ' -diselenodibutyrate (10): Yellow liquid, yield 15%; ^1H NMR (300 MHz, CDCl_3) δ 4.80-4.69 (m, J = 8.9 Hz, 2H), 2.93 (t, J = 7.3 Hz, 4H), 2.41 (t, J = 7.3 Hz, 4H), 2.13-1.99 (m, 4H), 1.90-1.15 (m, 20H). ^{13}C NMR (75 MHz, CDCl_3) δ 172.98, 73.36, 34.82, 32.32, 29.52, 26.86, 26.04, 24.42. ^{77}Se NMR (114 MHz, CDCl_3) δ 303.60. HR-ESI-MS: *calculated* m/z $\text{C}_{20}\text{H}_{34}\text{NaO}_4\text{Se}_2[\text{M}+\text{Na}^+]$: 521.0685; *experimental* m/z $[\text{M}+\text{Na}^+]$: 521.0708.

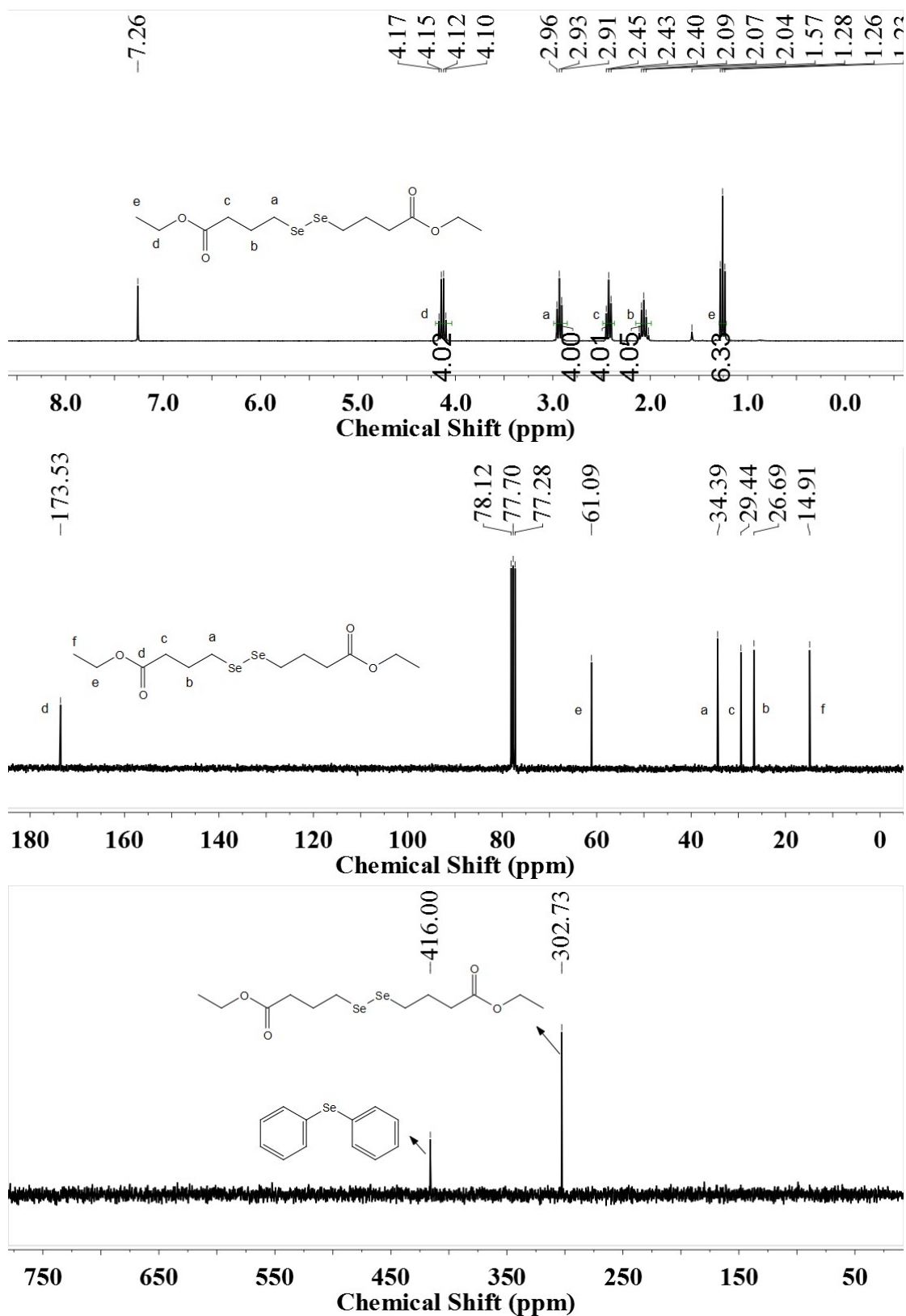


Figure S1. ¹H, ¹³C, and ⁷⁷Se NMR spectra of diethyl γ, γ'-diselenodibutyrate.

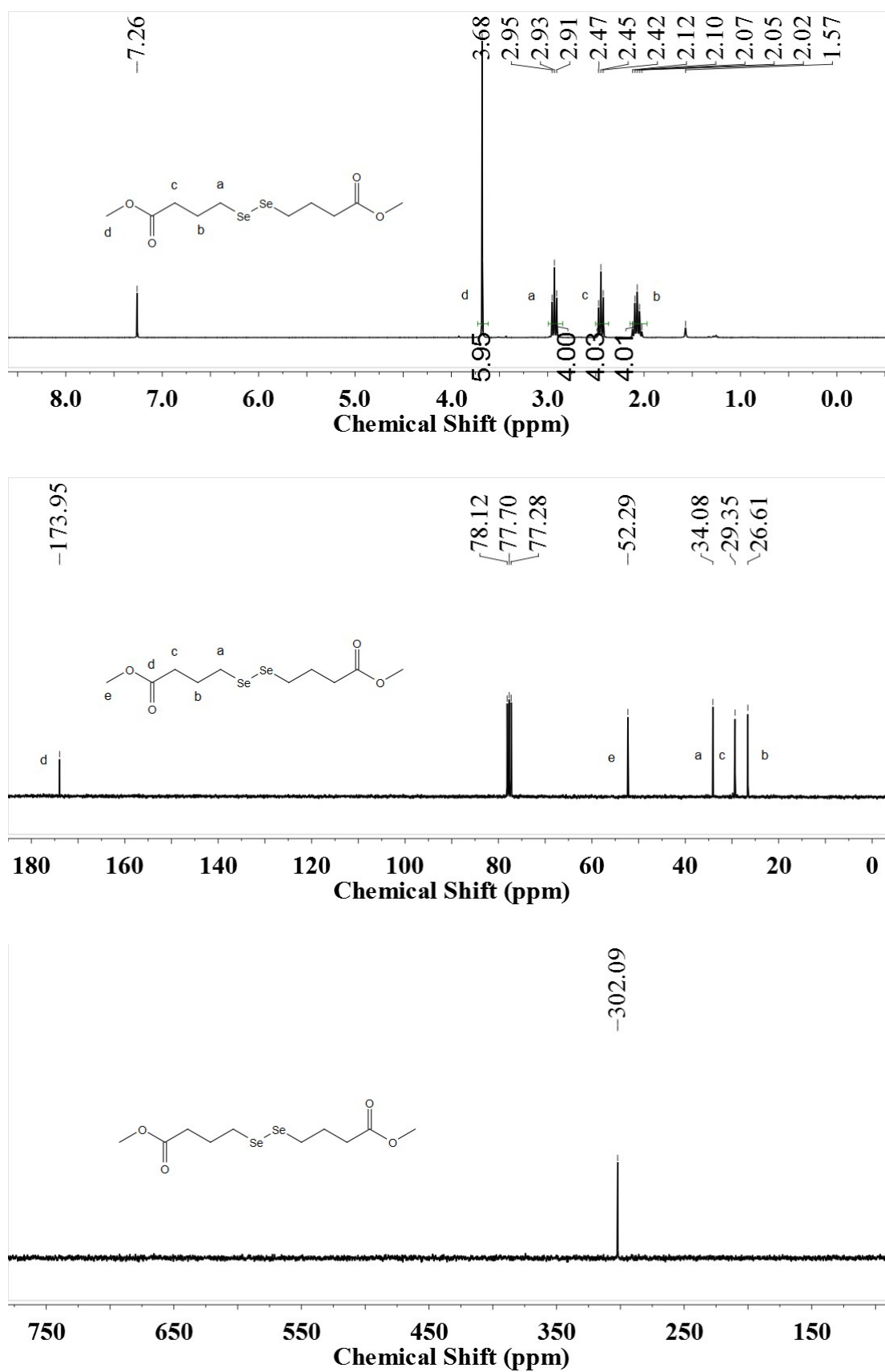


Figure S2. ^1H , ^{13}C , and ^{77}Se NMR spectra of dimethyl γ , γ' -diselenodibutyrate.

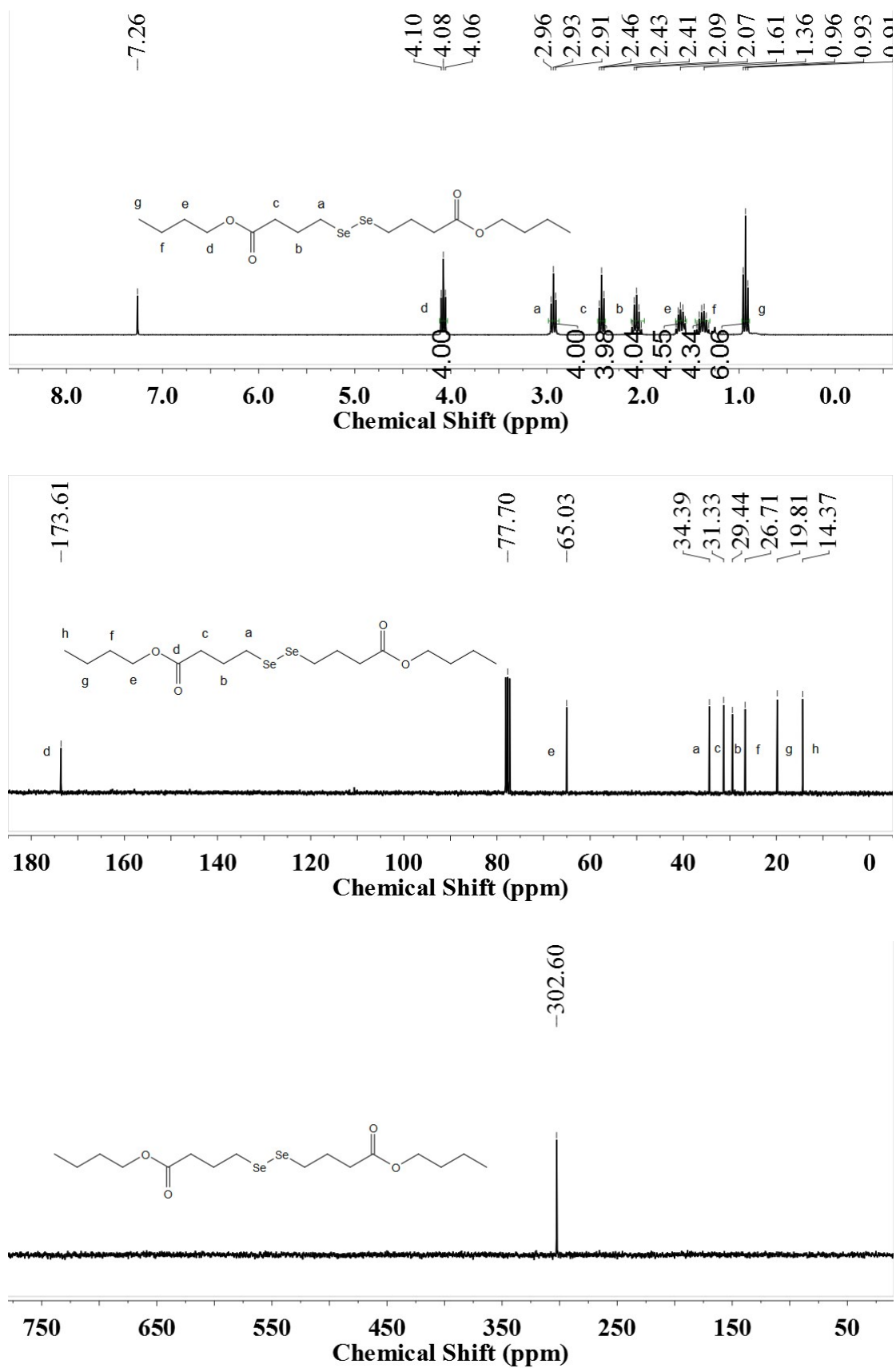


Figure S4. ¹H, ¹³C, and ⁷⁷Se NMR spectra of dibutyl γ, γ'-diselenodibutyrate.

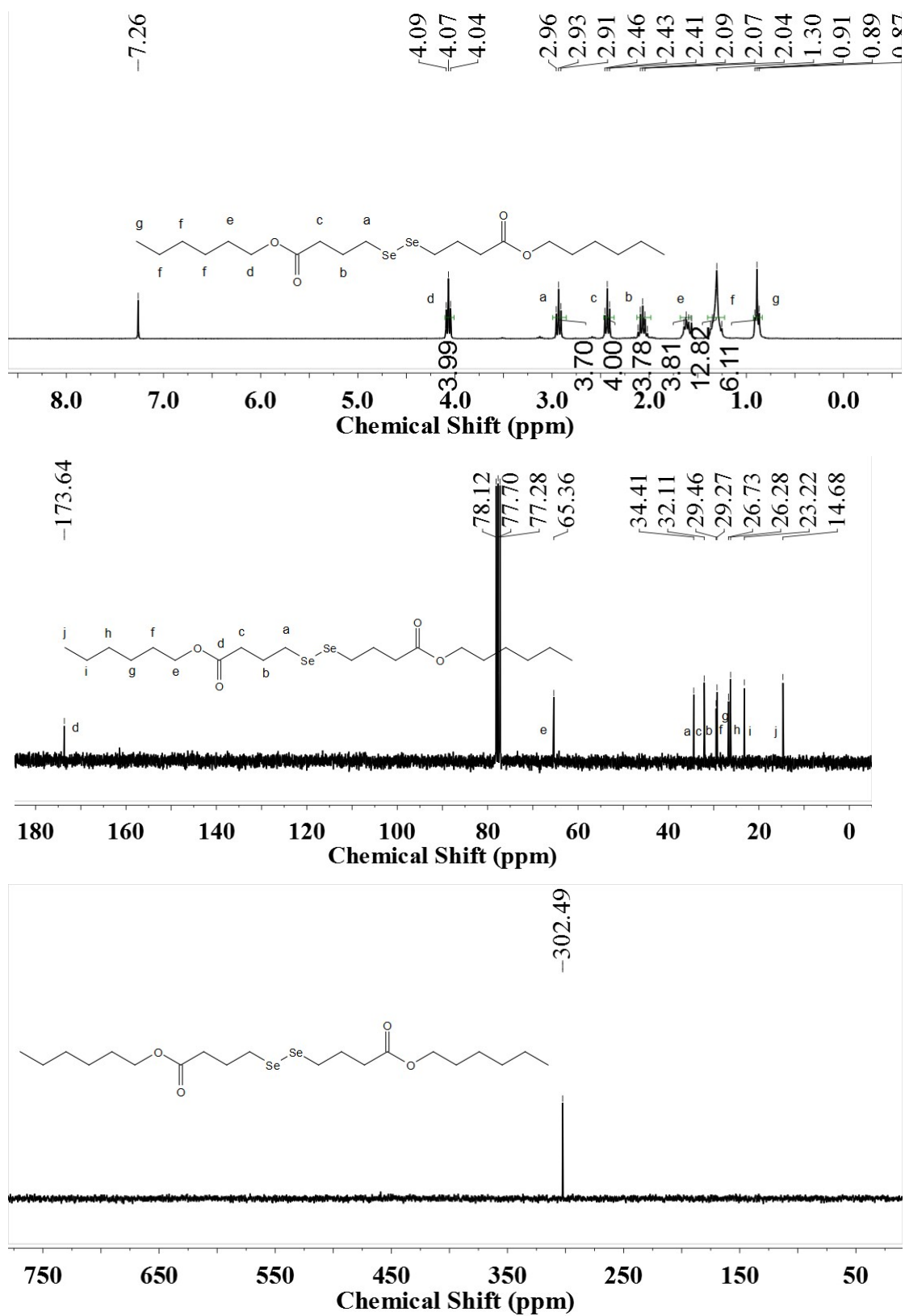


Figure S5. ^1H , ^{13}C , and ^{77}Se NMR spectra of dihexyl γ , γ' -diselenodibutyrate.

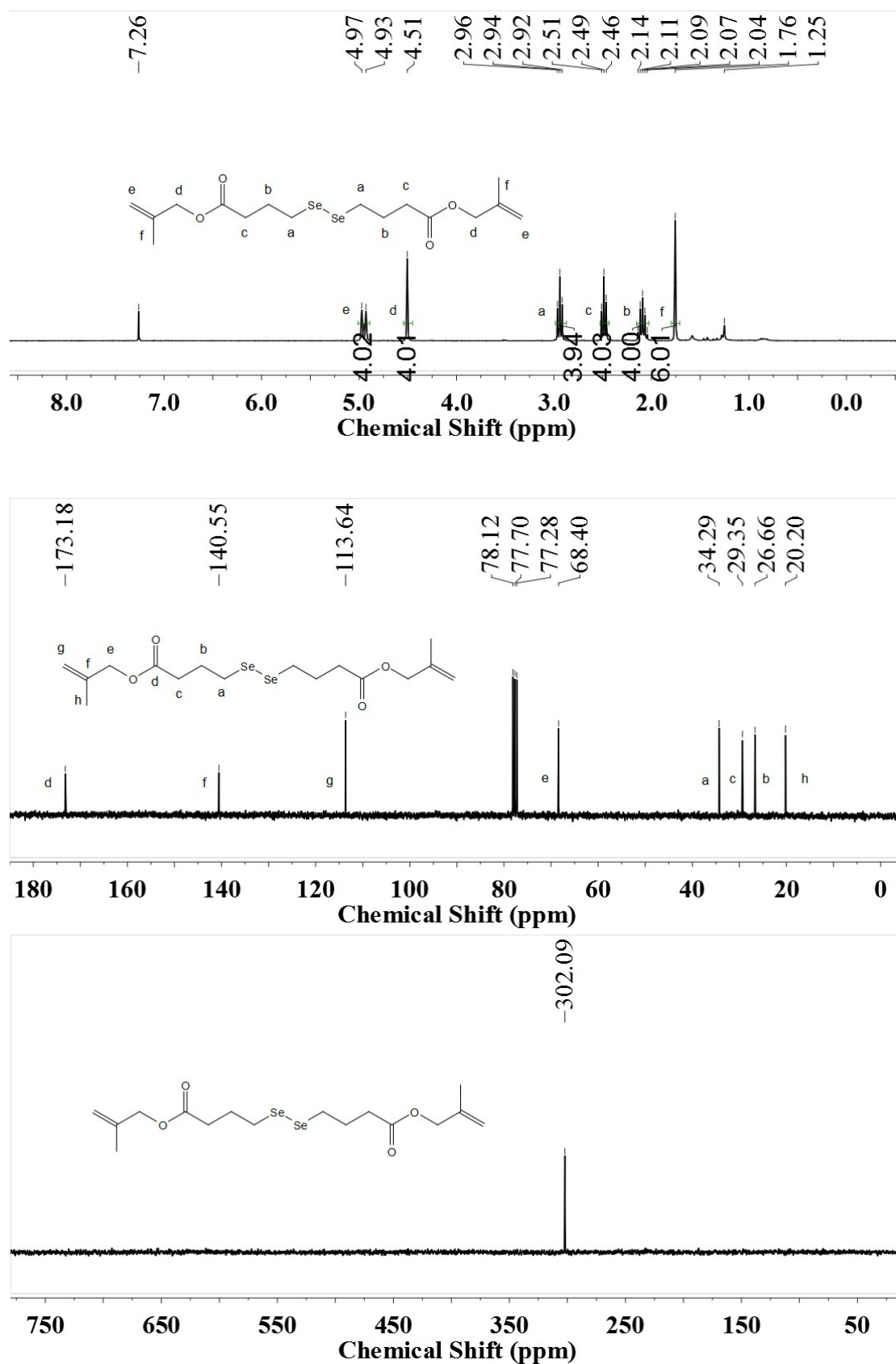


Figure S6. ¹H, ¹³C, and ⁷⁷Se NMR spectra of di(2-methylallyl) γ, γ'-diselenodibutyrate.

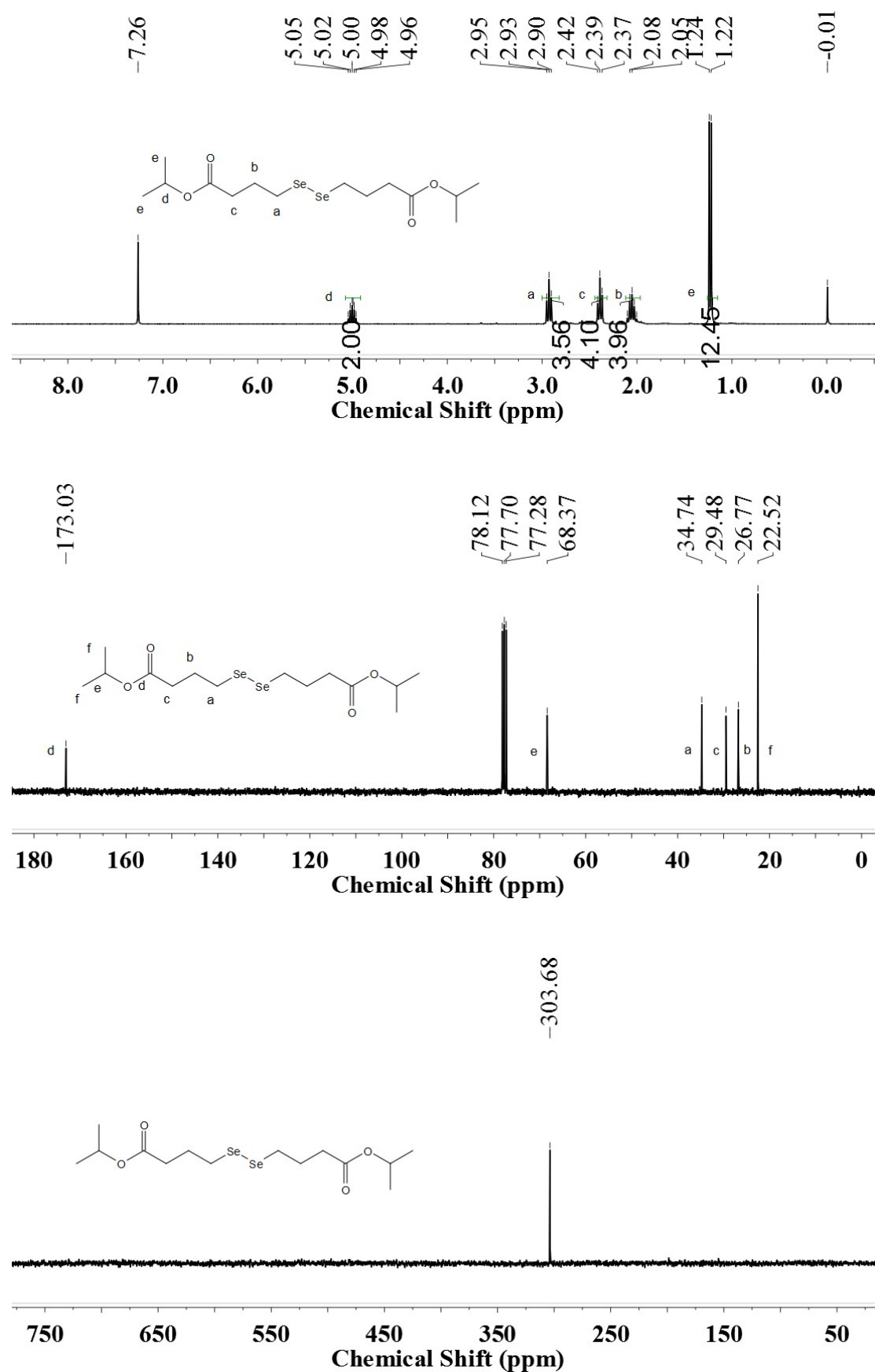


Figure S7. ¹H, ¹³C, and ⁷⁷Se NMR spectra of diisopropyl γ, γ'-diselenobutyrate.

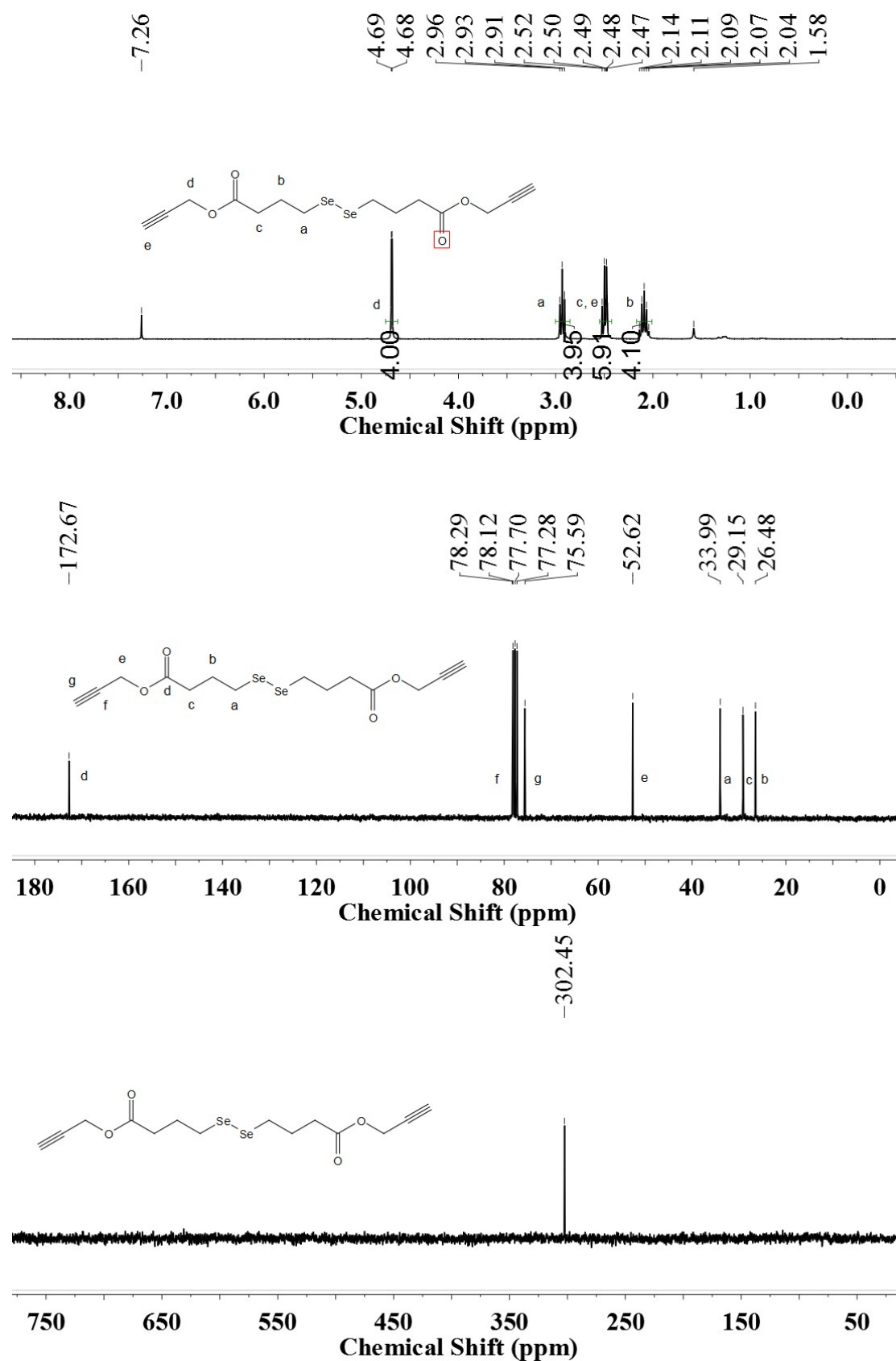


Figure S8. ¹H, ¹³C, and ⁷⁷Se NMR spectra of di(prop-2-yn-1-yl) γ , γ' -diselenodibutyrate.

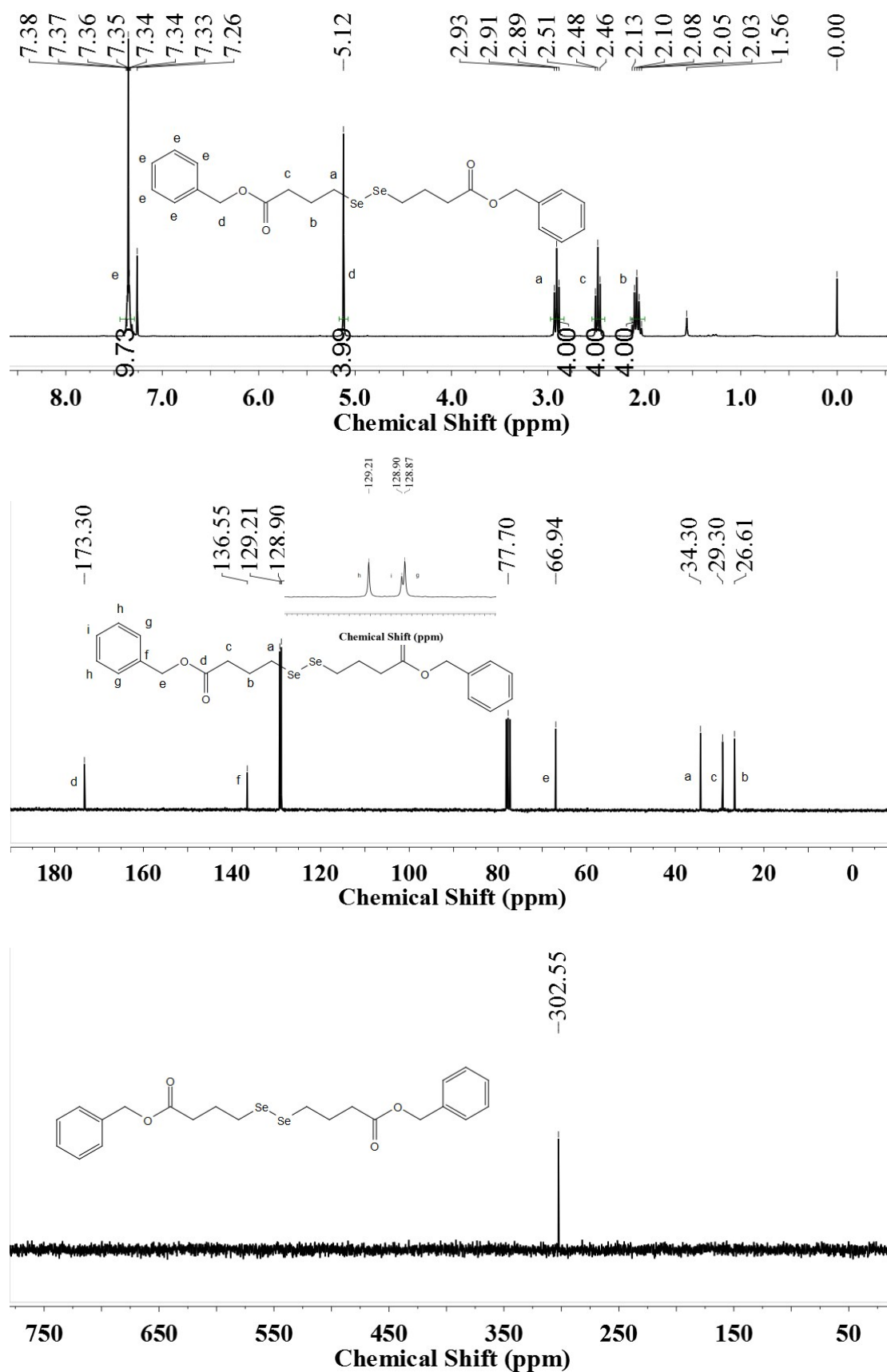


Figure S9. ¹H, ¹³C, and ⁷⁷Se NMR spectra of dibenzyl γ, γ'-diselenodibutyrate.

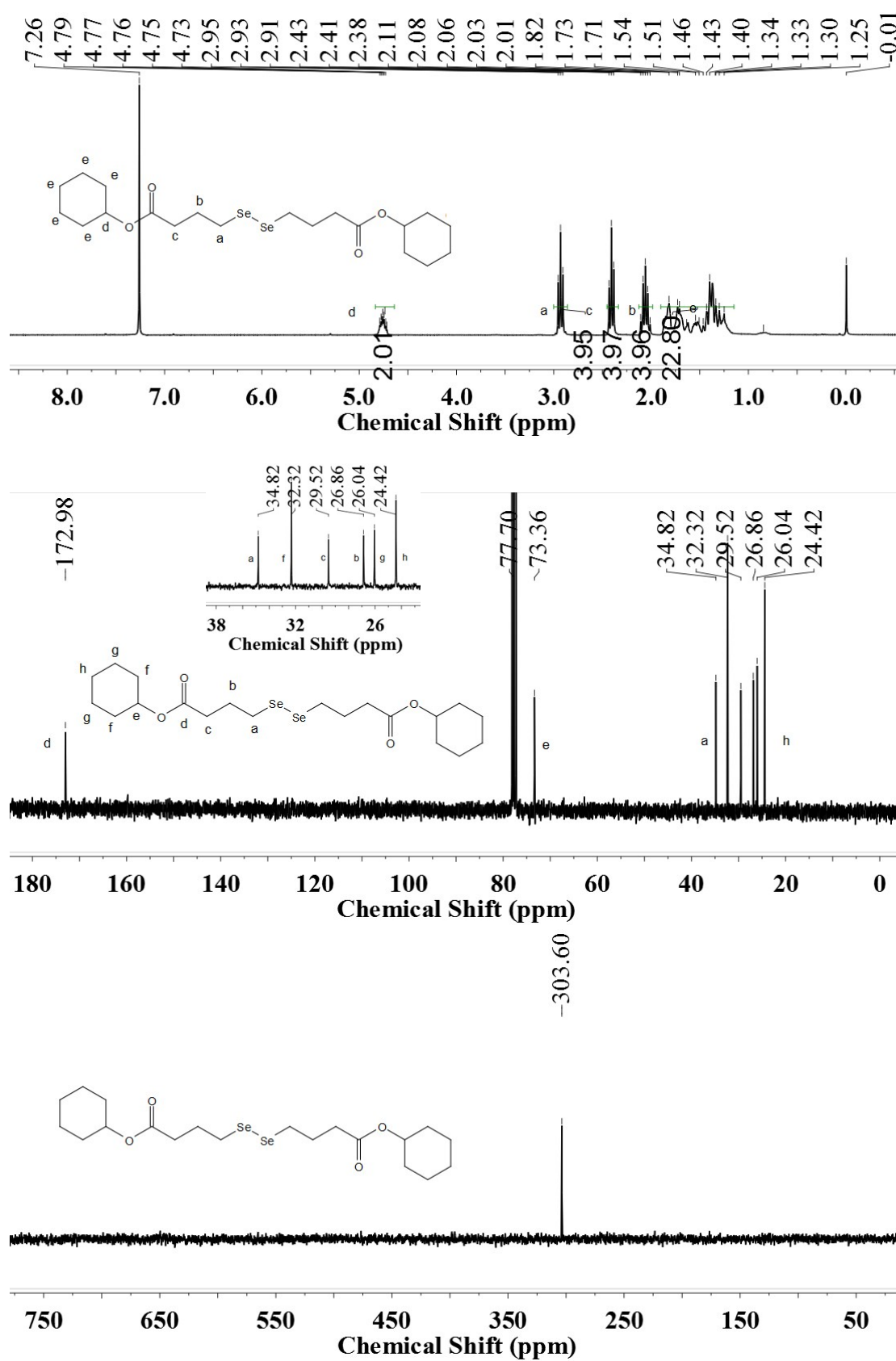


Figure S10. ¹H, ¹³C, and ⁷⁷Se NMR spectra of dicyclohexyl γ, γ'-diselenodibutyrate.

Diselenide Containing Polyester:

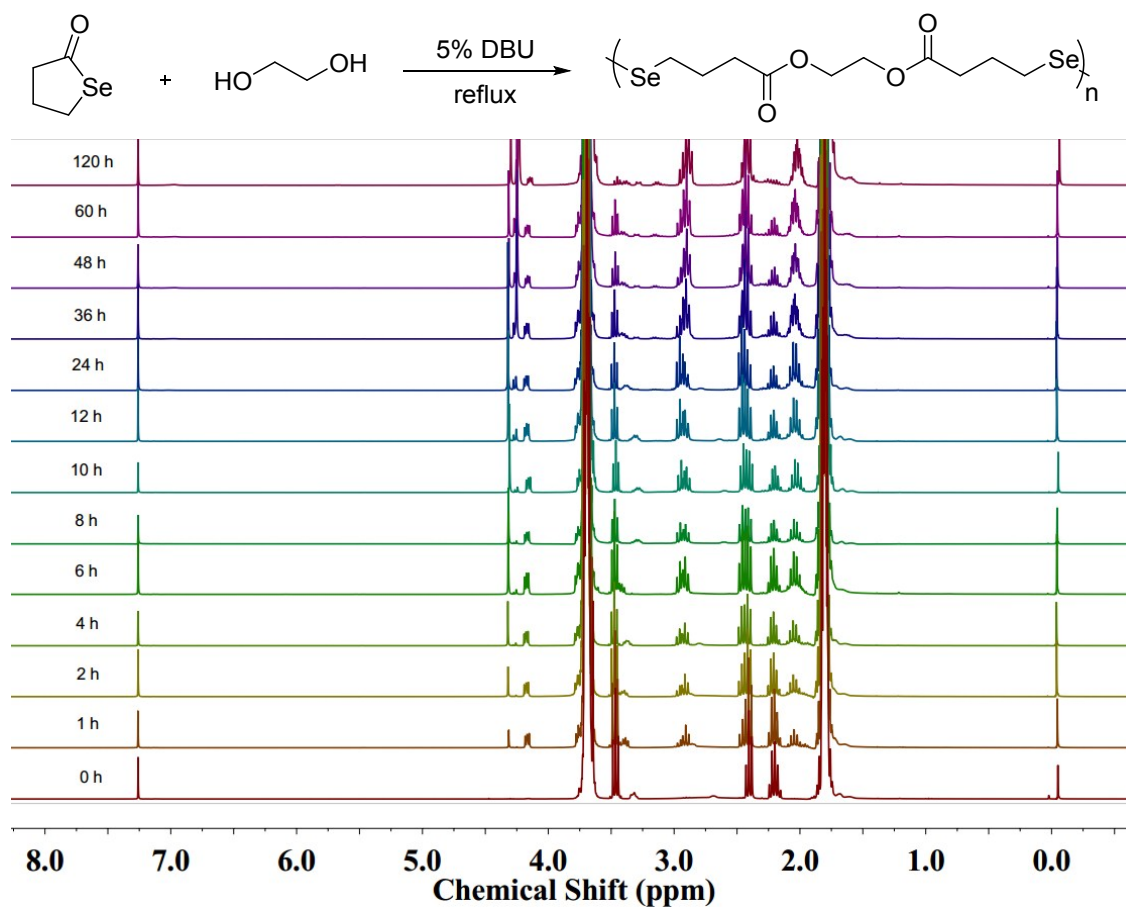


Figure S11. ^1H NMR spectra of the reaction solution of γ -butyroselenolactone with ethylene glycol.

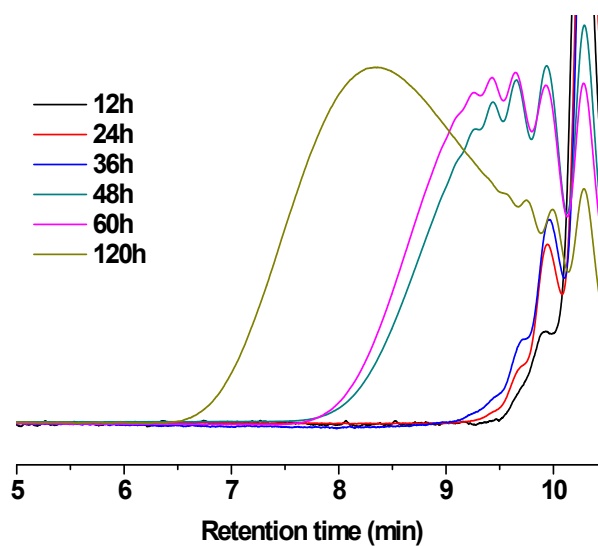


Figure S12. SEC curves of polymers from the reaction of ethylene glycol and γ -butyroselenolactone in THF (EGSe_2) ($1 \times 10^{-3} \text{ mol L}^{-1}$).

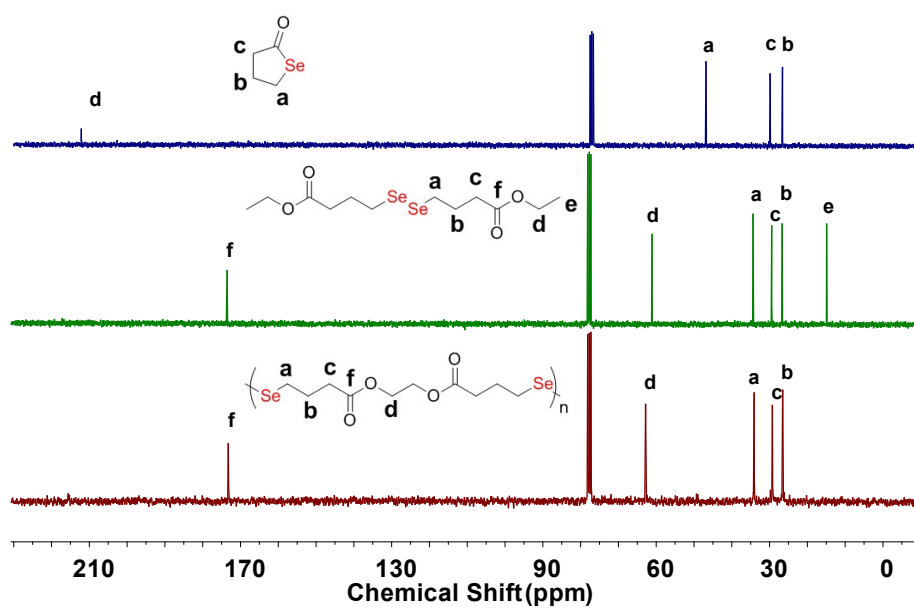


Figure S13 ^{13}C NMR spectra of γ -butyroselenolactone, diethyl γ,γ' -diselenodibutyrate and polyester (EGSe₂).

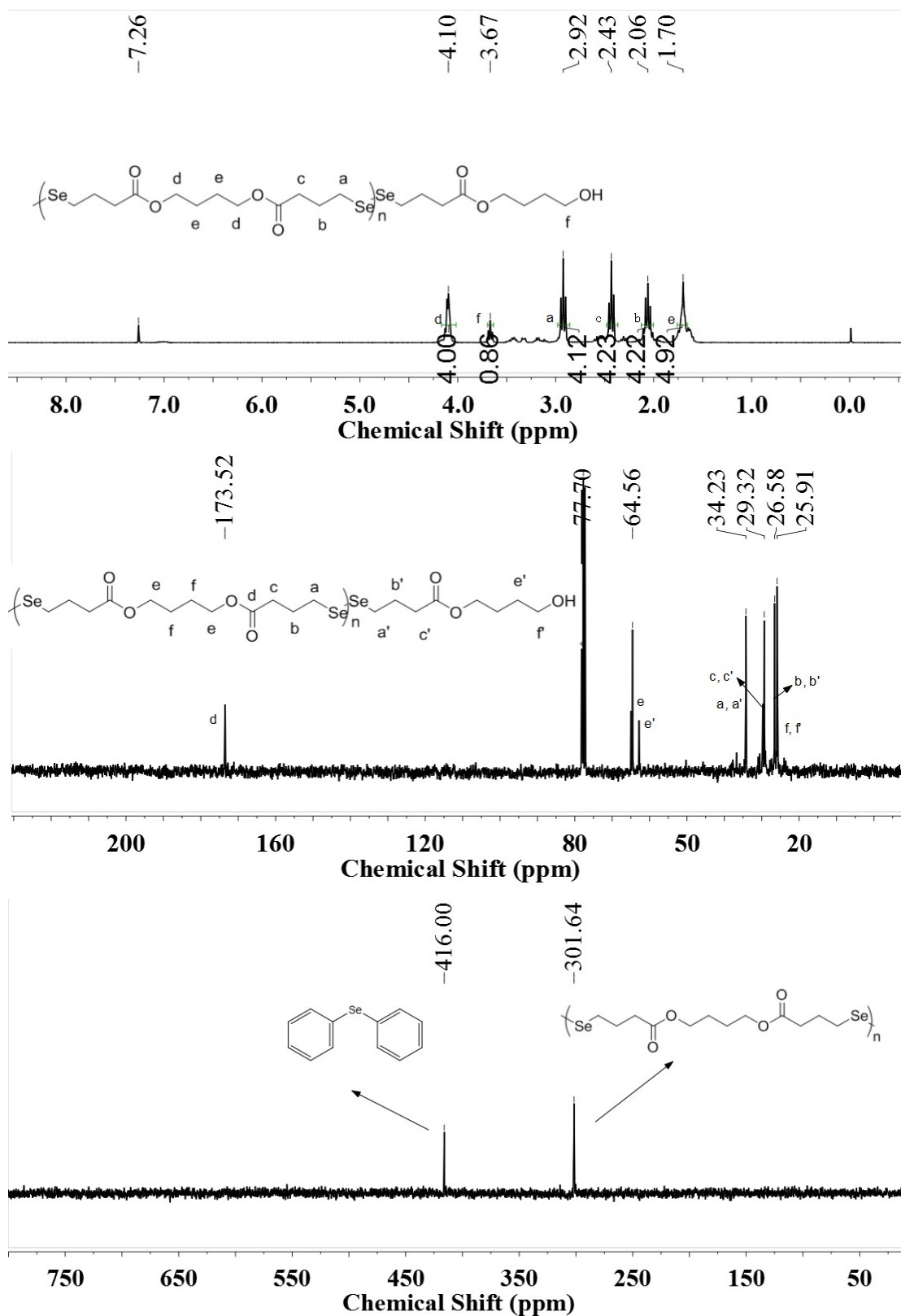


Figure S15. ^1H , ^{13}C , and ^{77}Se NMR spectra of BDOSe₂.

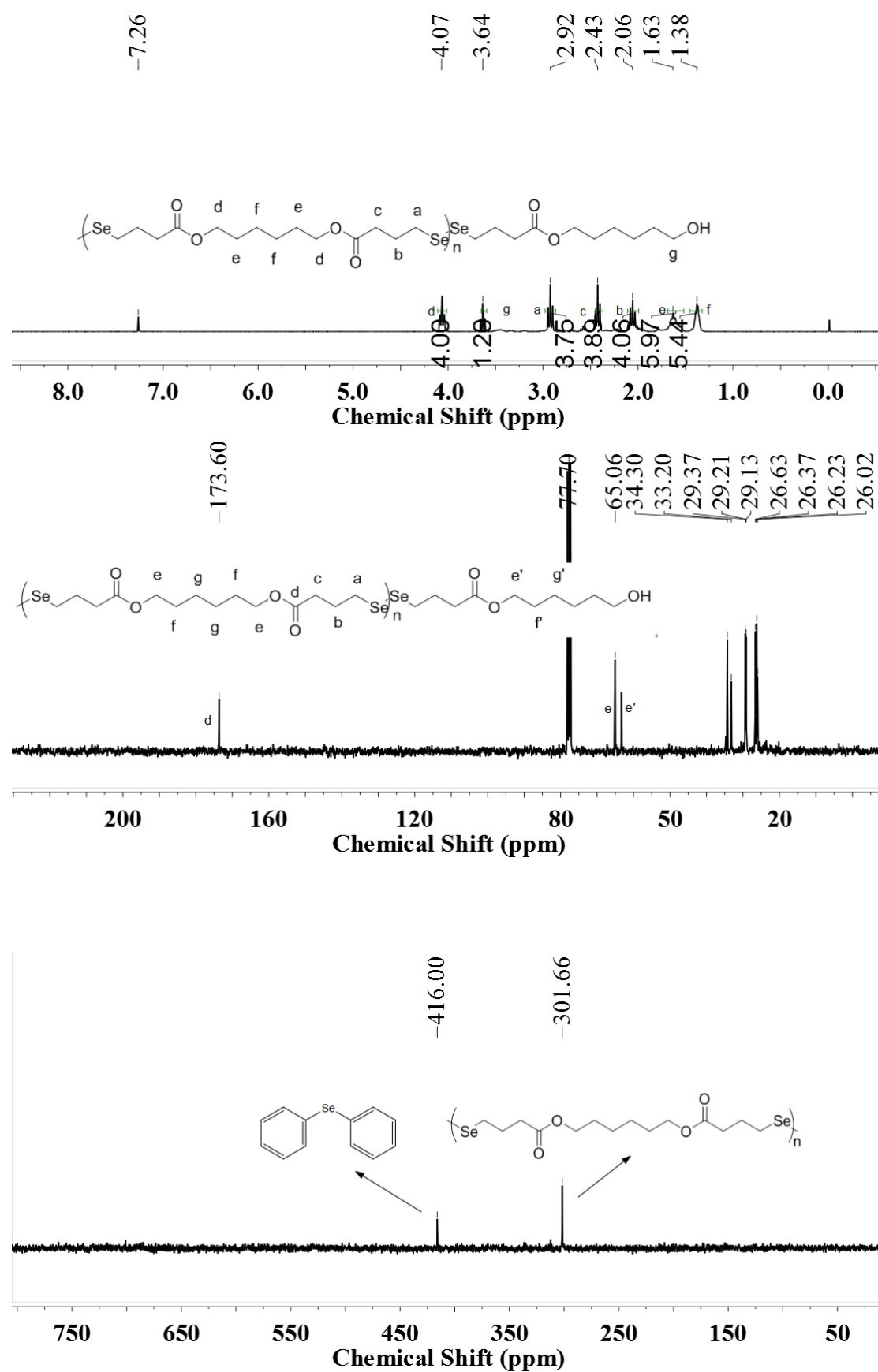


Figure S16. ¹H, ¹³C, and ⁷⁷Se NMR spectra of HDSe₂.

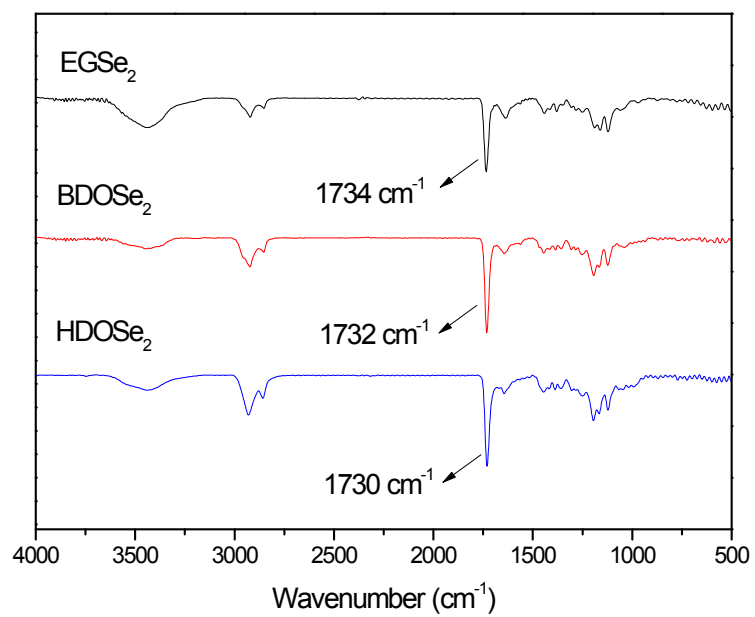


Figure S17. IR spectra of EGSe₂, BDOSe₂, HDOSe₂.

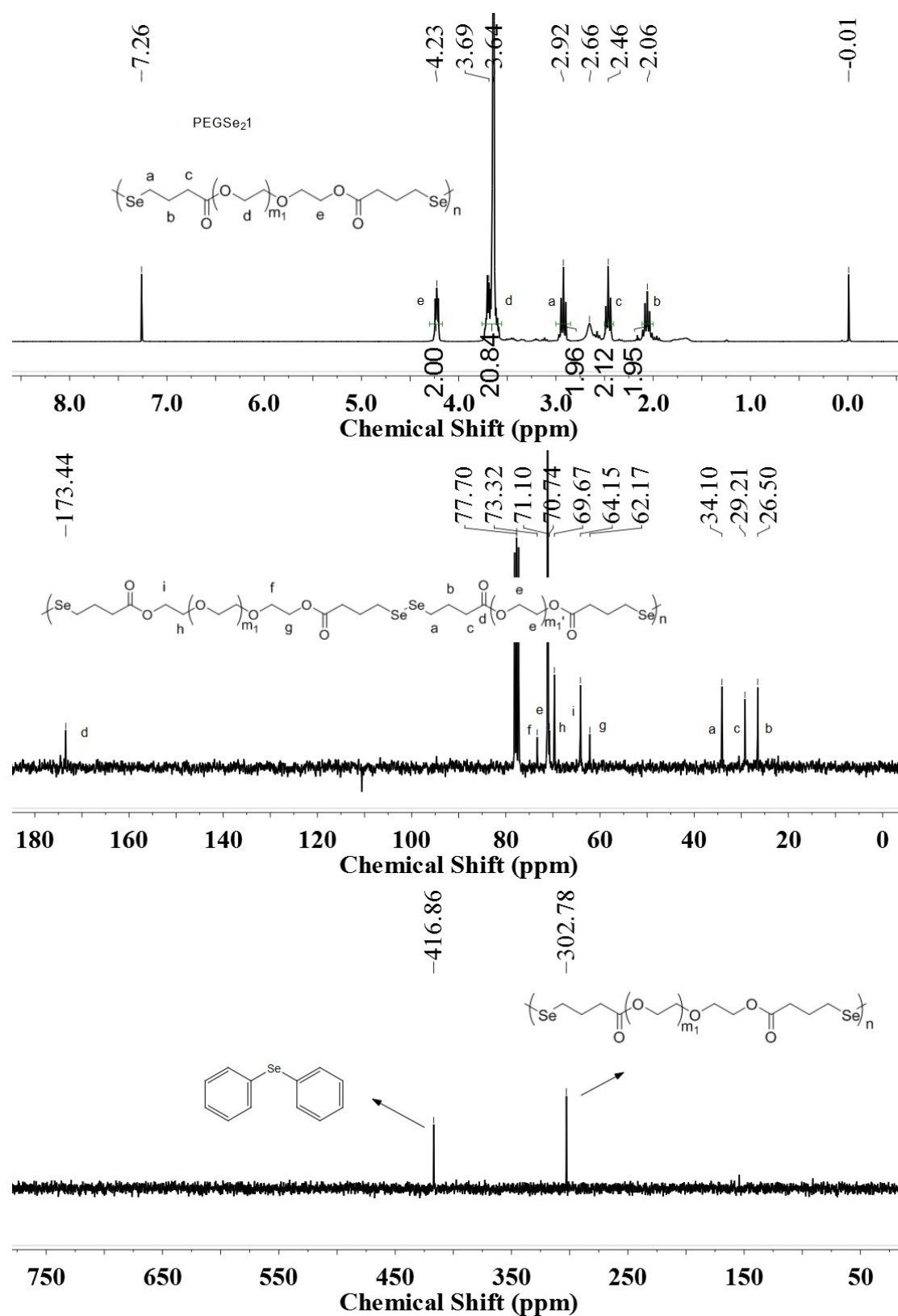


Figure S18. ^1H , ^{13}C , and ^{77}Se NMR spectra of PEGSe₂1.

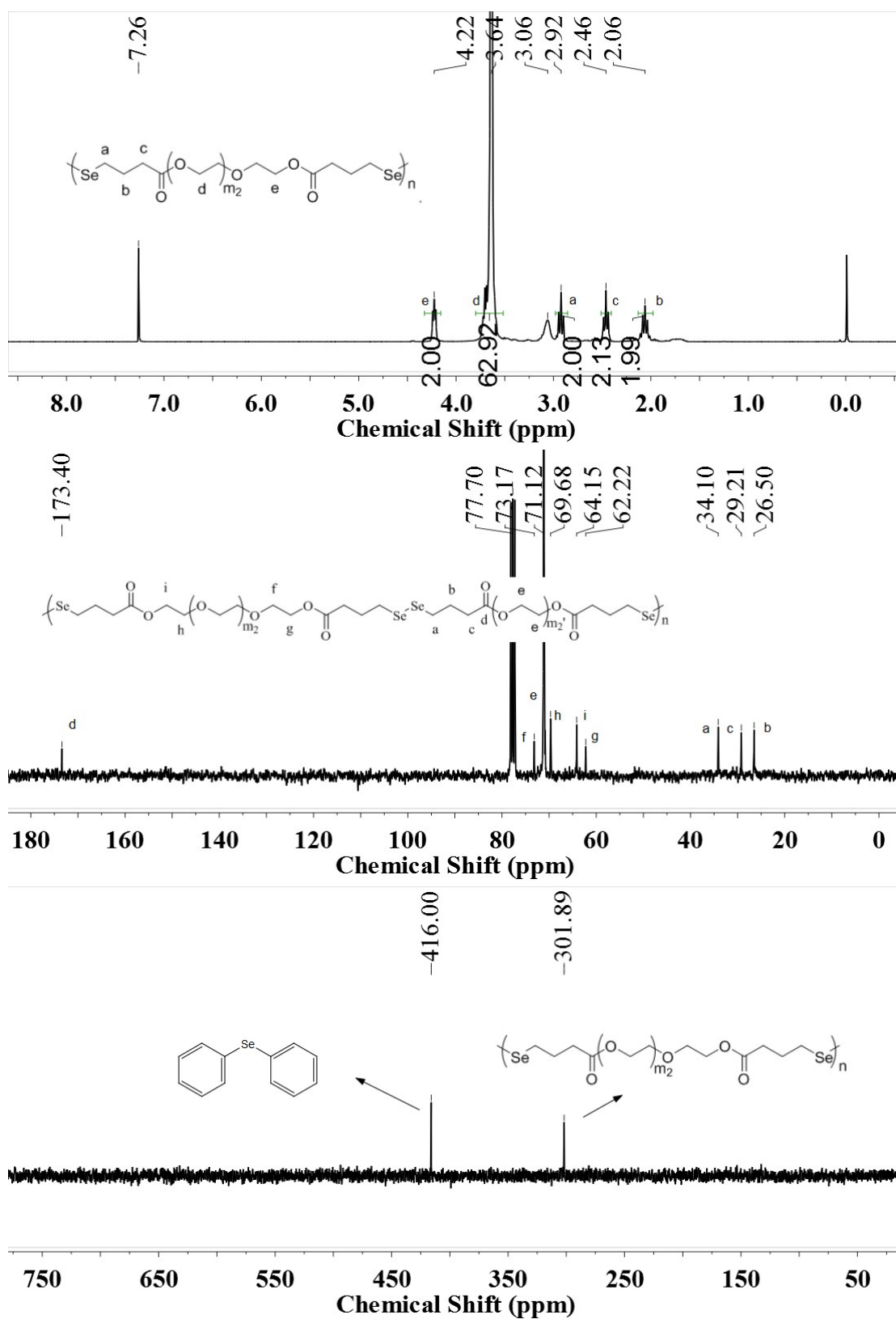


Figure S19. ¹H, ¹³C, and ⁷⁷Se NMR spectra of PEGSe_{2.2}.

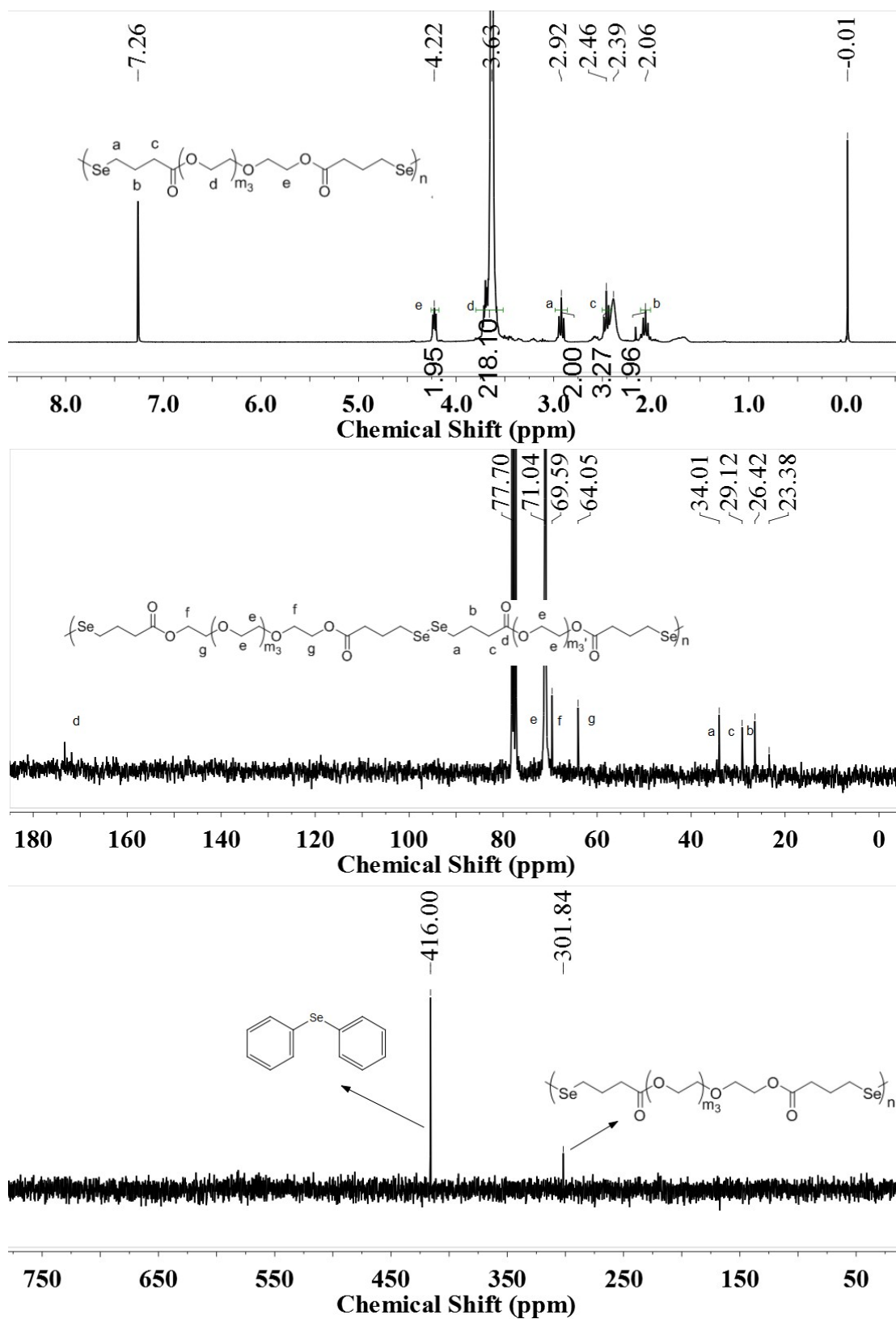


Figure S20. ^1H , ^{13}C , and ^{77}Se NMR spectra of PEGSe₂₃.

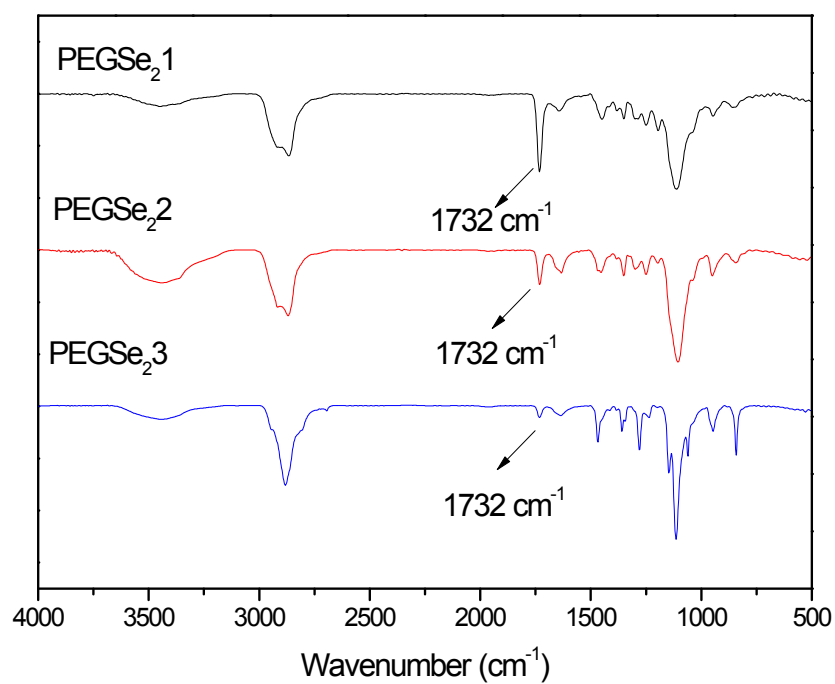


Figure S21. FTIR spectra of PEGSe₂1, PEGSe₂2, PEGSe₂3.

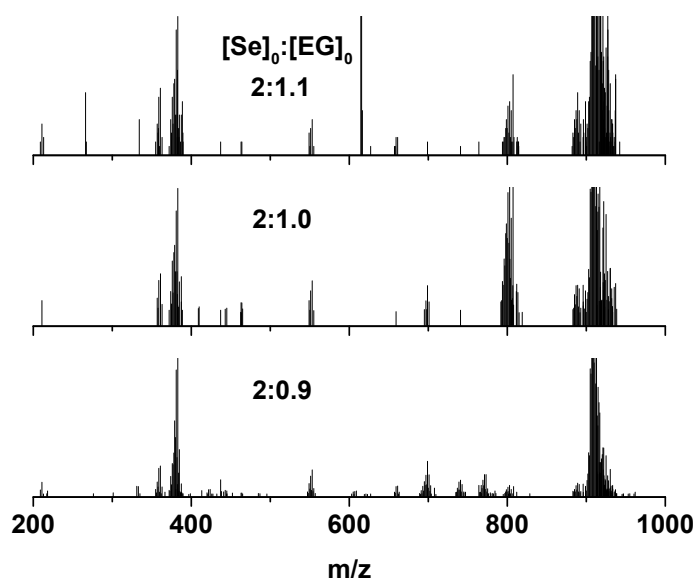
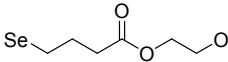
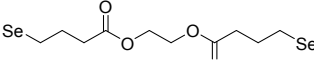
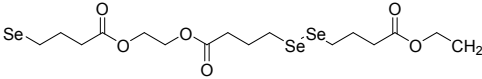
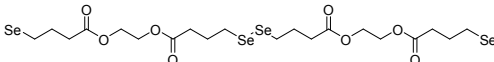
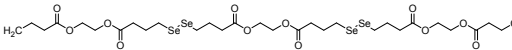
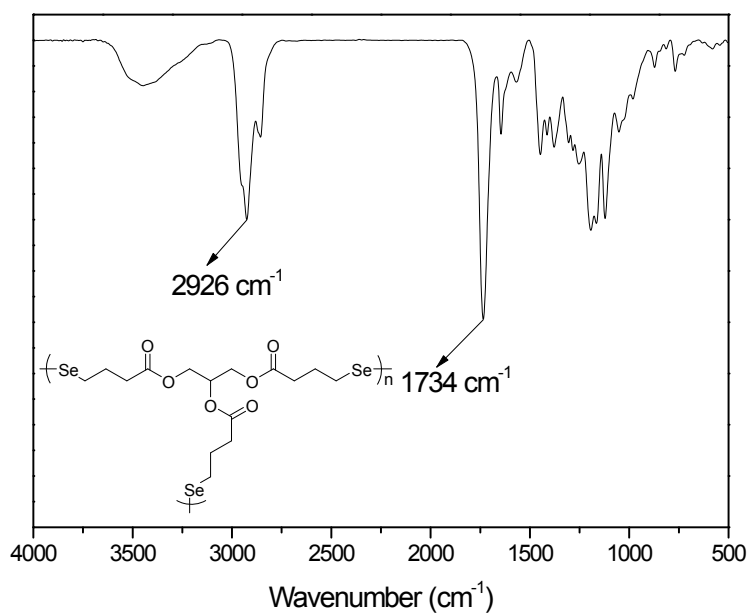


Figure S22. HRMS spectra of polyesters from the reaction of ethylene glycol and γ -butyroselenenolactone with a ratio of $[\text{Se}]_0:[\text{EG}]_0 = 2:0.9/2:1/2:1.1$ in THF.

Table S1. Mass Measurement of Different Chain Populations of Oligomers Detected by LC-MS.

Entry	Structure	Calculated m/z (+H)	Calculated m/z (+Na)	Experimental m/z
1	 Chemical Formula: C ₆ H ₁₀ O ₃ Se Exact Mass: 209.9795	210.9873	233.9771	210.9855
2	 Chemical Formula: C ₁₀ H ₁₆ O ₄ Se ₂ Exact Mass: 359.9379	360.9457	382.9277	360.9435
3	 Chemical Formula: C ₁₆ H ₂₆ O ₆ Se ₃ Exact Mass: 551.9233	552.9311	574.9131	553.0654
4	 Chemical Formula: C ₂₀ H ₃₂ O ₈ Se ₄ Exact Mass: 717.8766	720.8836	740.8664	740.8715
5	 Chemical Formula: C ₃₀ H ₄₈ O ₁₂ Se ₅ Exact Mass: 915.9822	916.9902	938.9720	917.0435

**Figure S23.** FTIR spectrum for the polyesters obtaining form reaction of γ -butyroselenolactone and glycerol in THF.

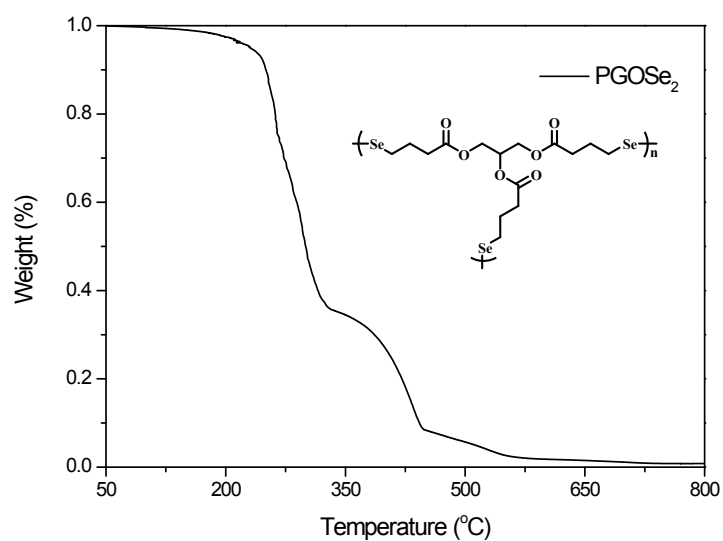


Figure S24. TGA spectrum for the polyesters obtained from reaction of γ -butyroselenolactone and glycerol in THF.

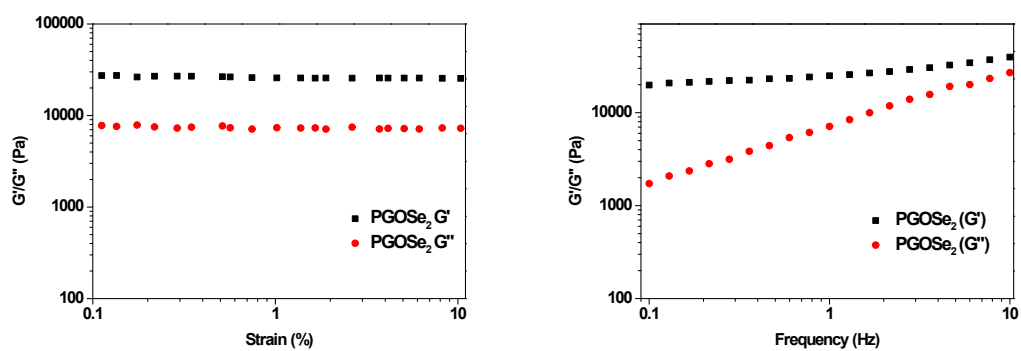


Figure S25. Rheological testing of polyester materials (PGOSe₂).

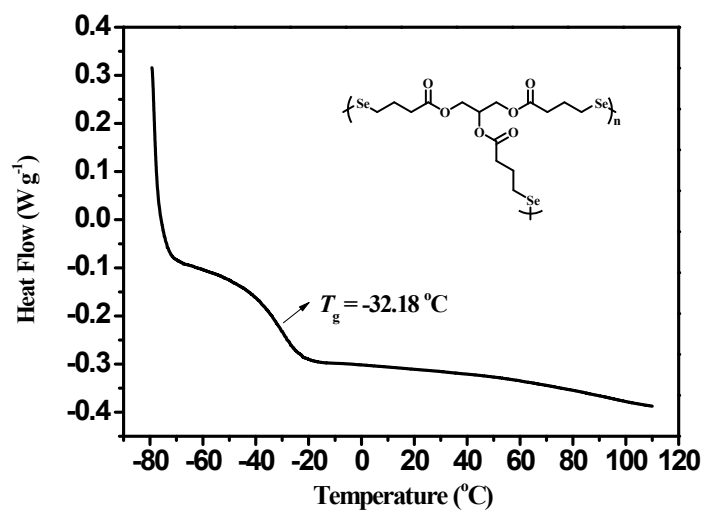


Figure S26. DSC curves of polyesters (PGOSe₂).