

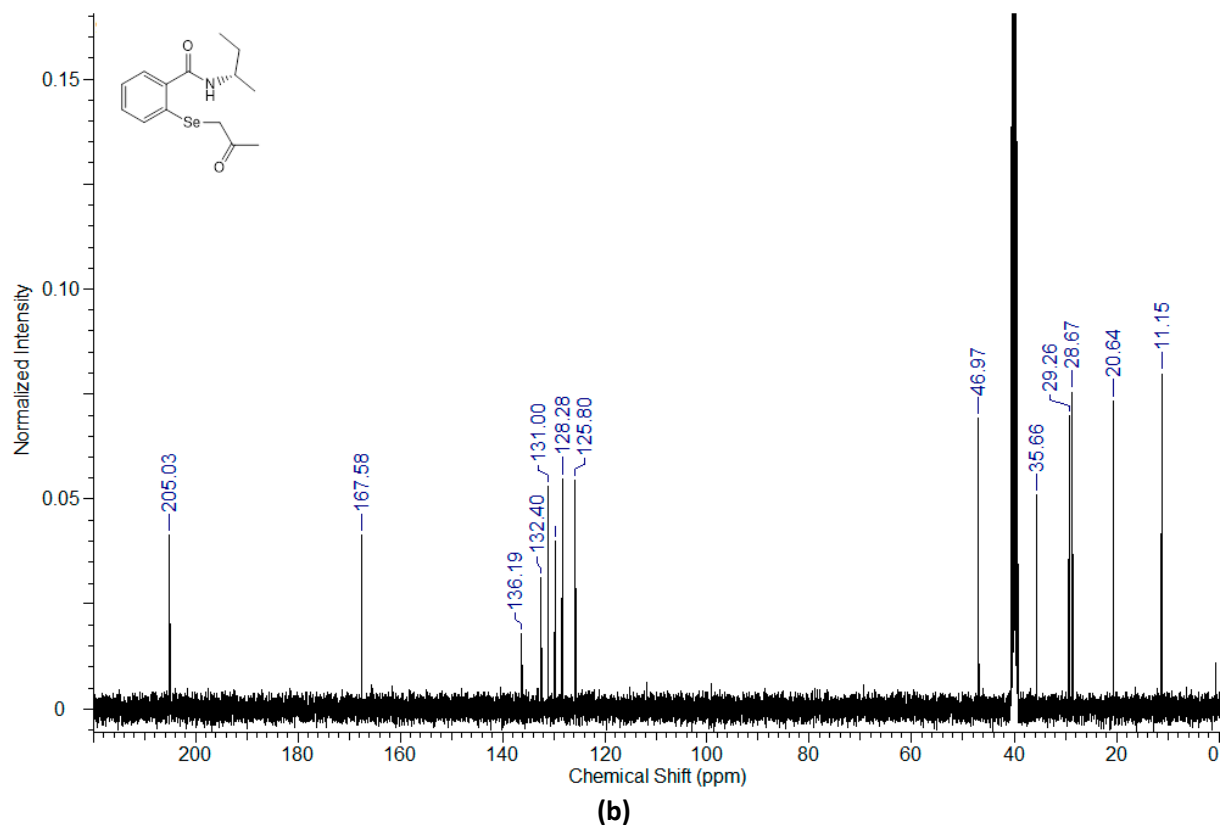
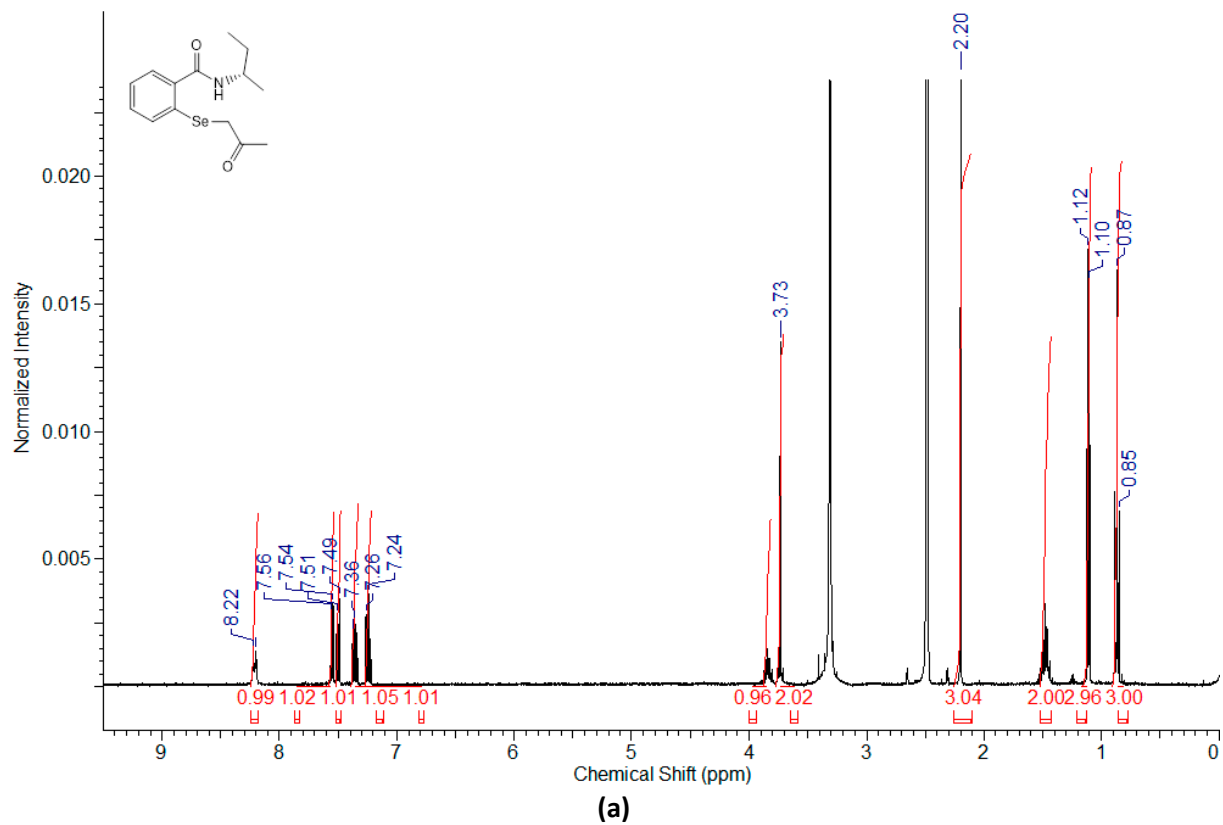
Supplementary Materials

Synthesis of New Chiral β -Carbonyl Selenides with Antioxidant and Anticancer Activity Evaluation—Part I

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1. NMR spectra of 2-((2-oxopropyl)selenanyl) benzamides 11-24



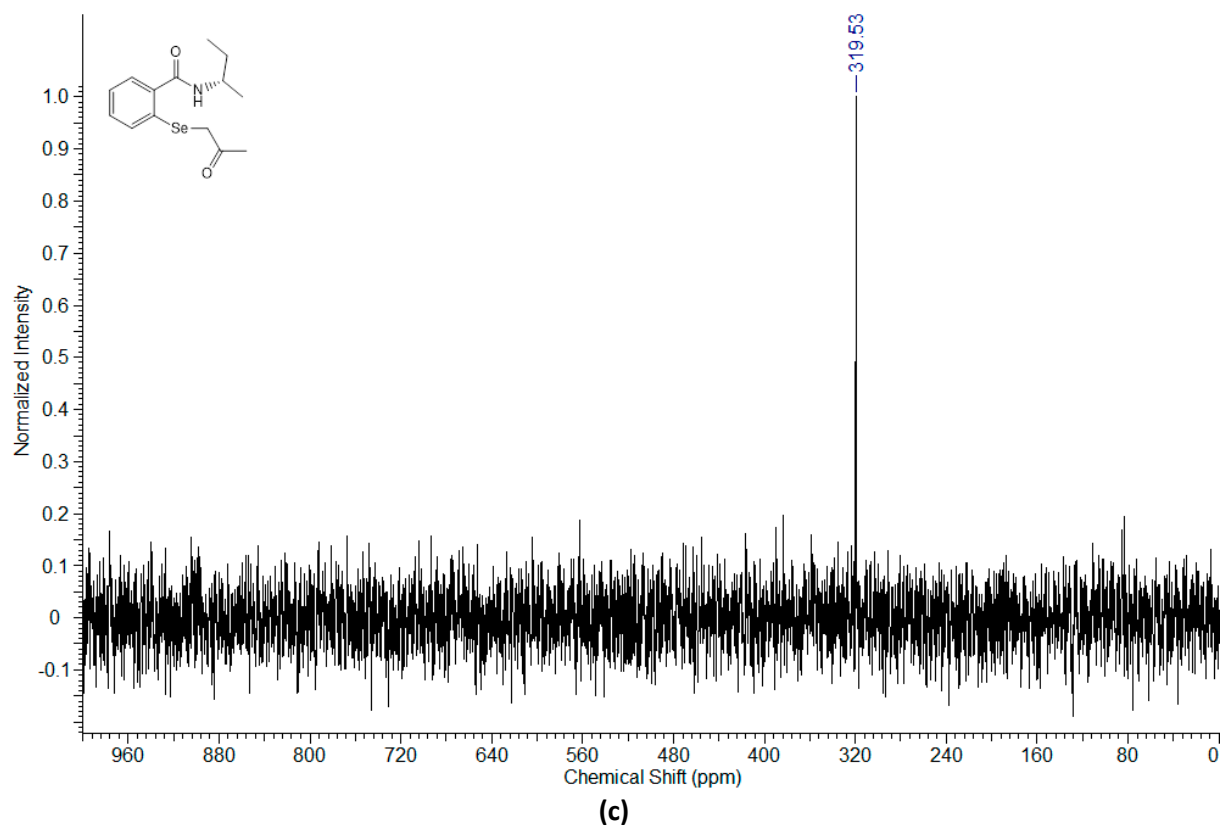
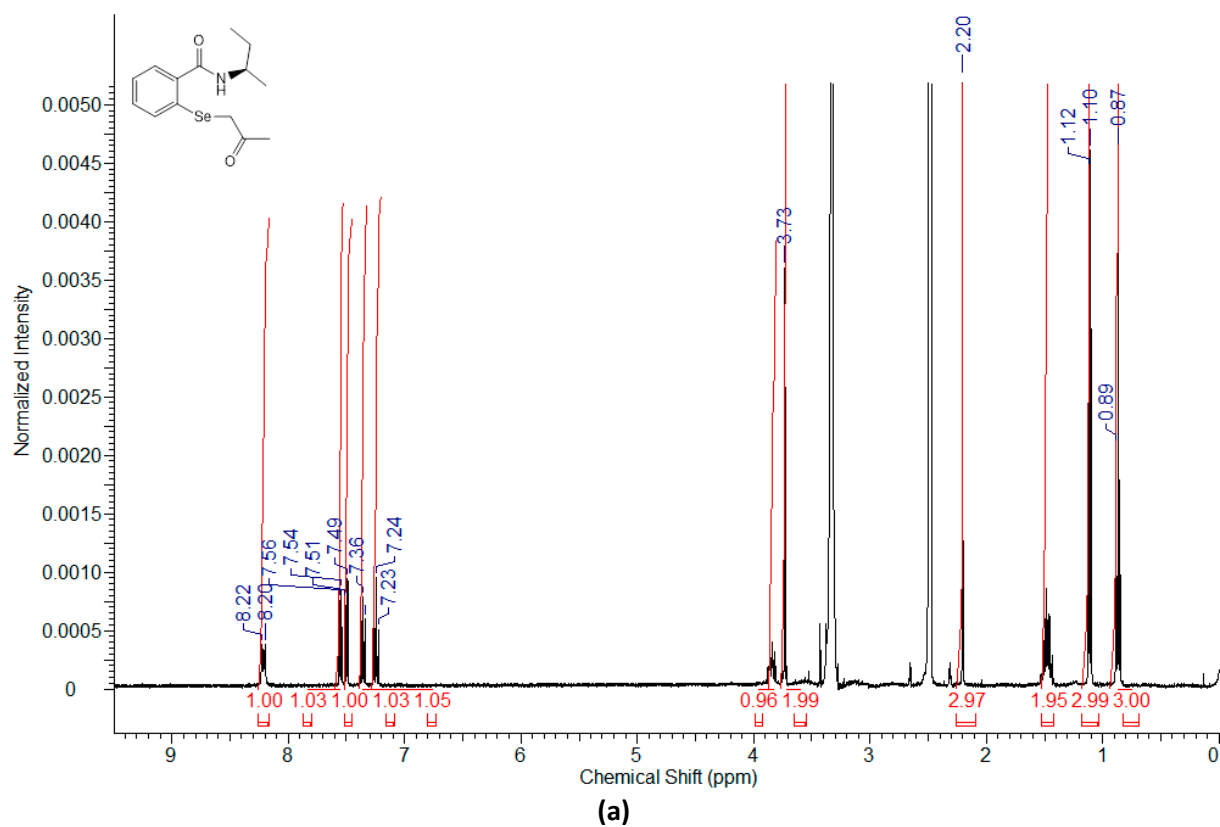


Figure S1. (a) ^1H NMR, (b) ^{13}C NMR, and (c) ^{77}Se NMR spectra of *N*-((*S*)-(+)-*sec*-butyl)-2-((2-oxopropyl)selanyl)benzamide **11**.



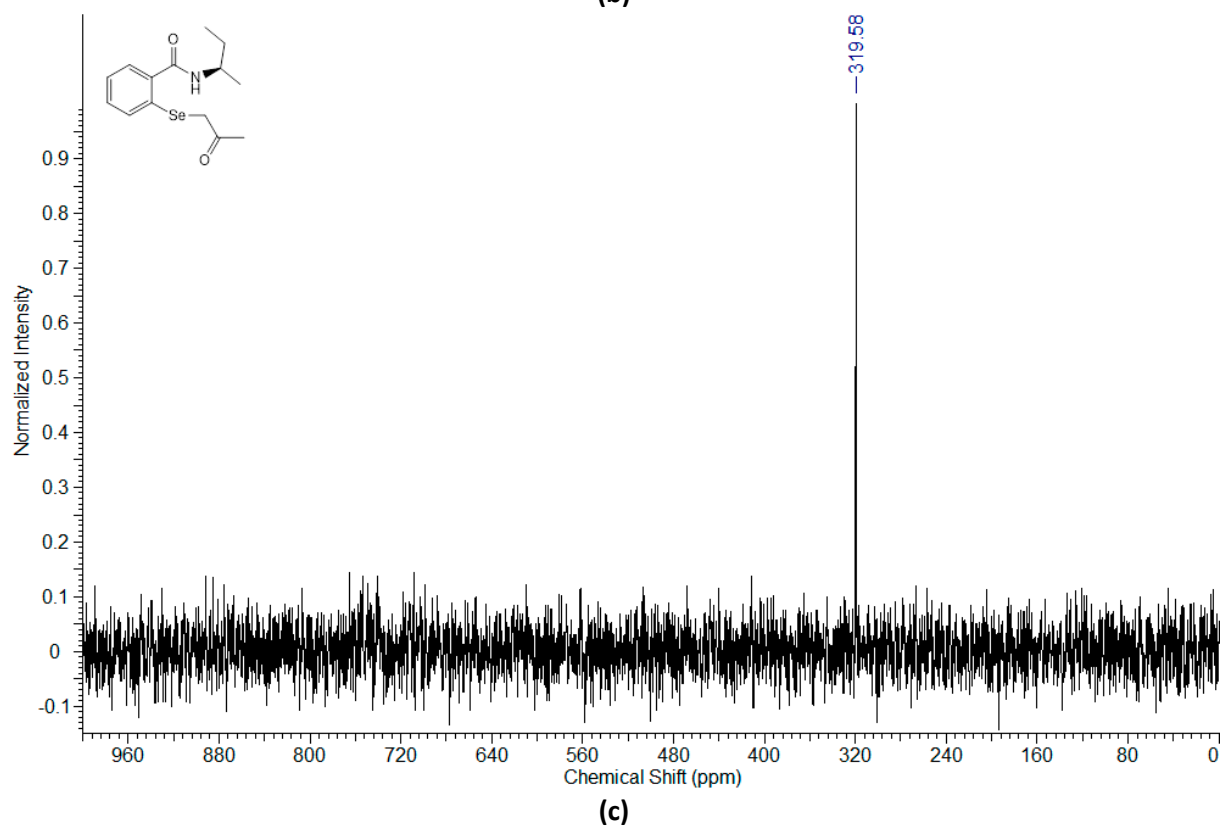
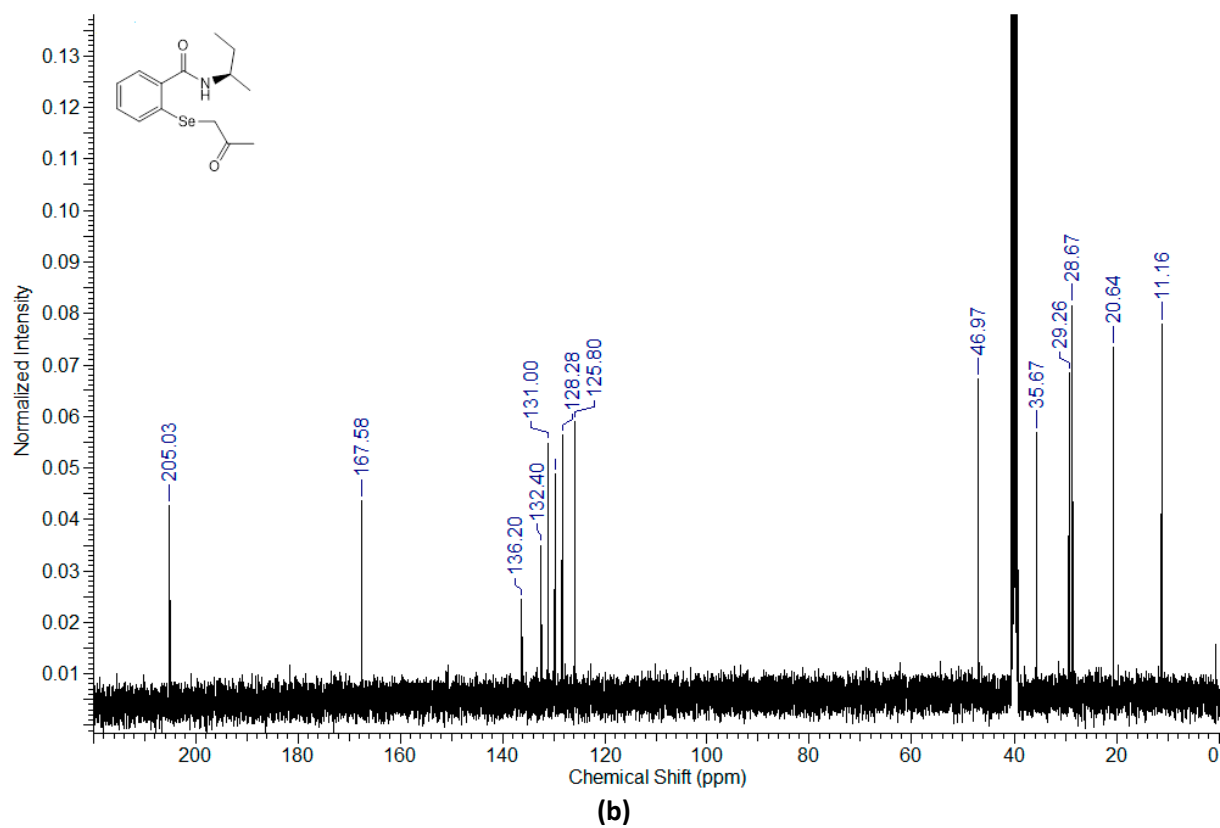
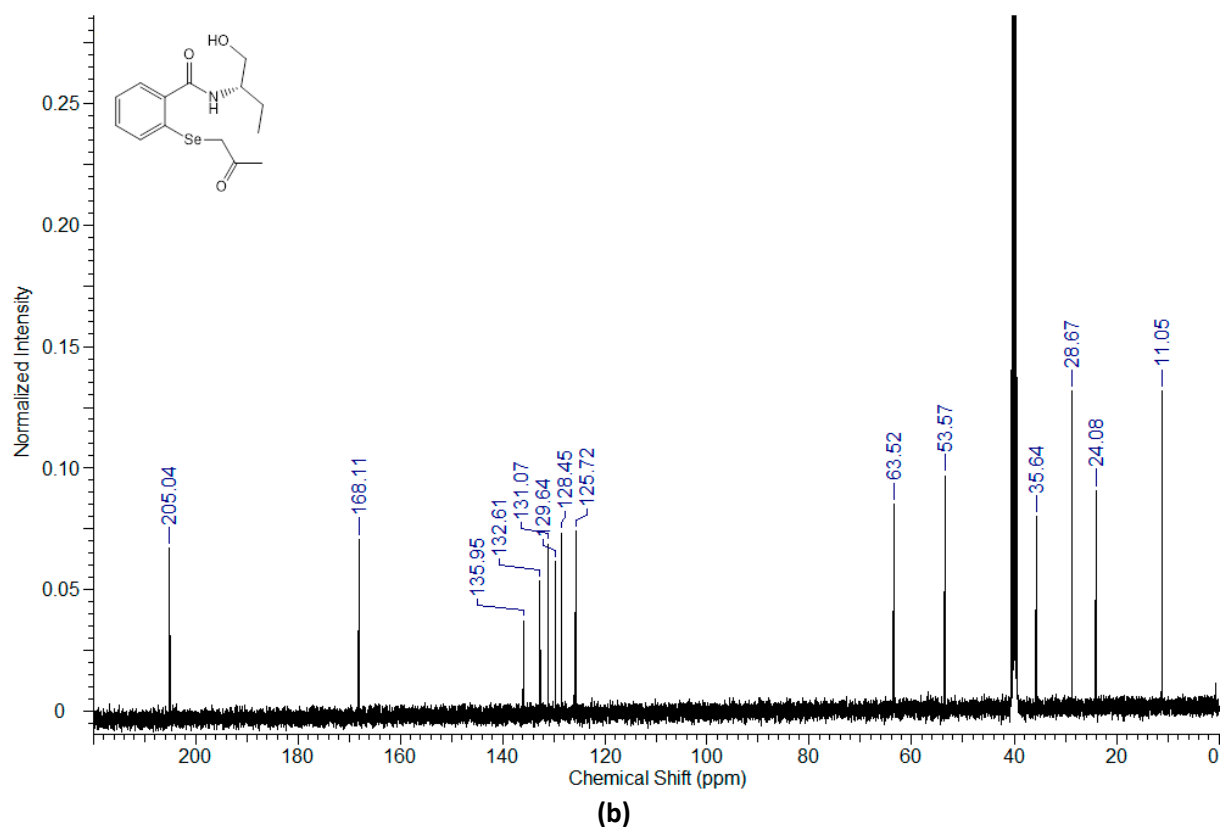
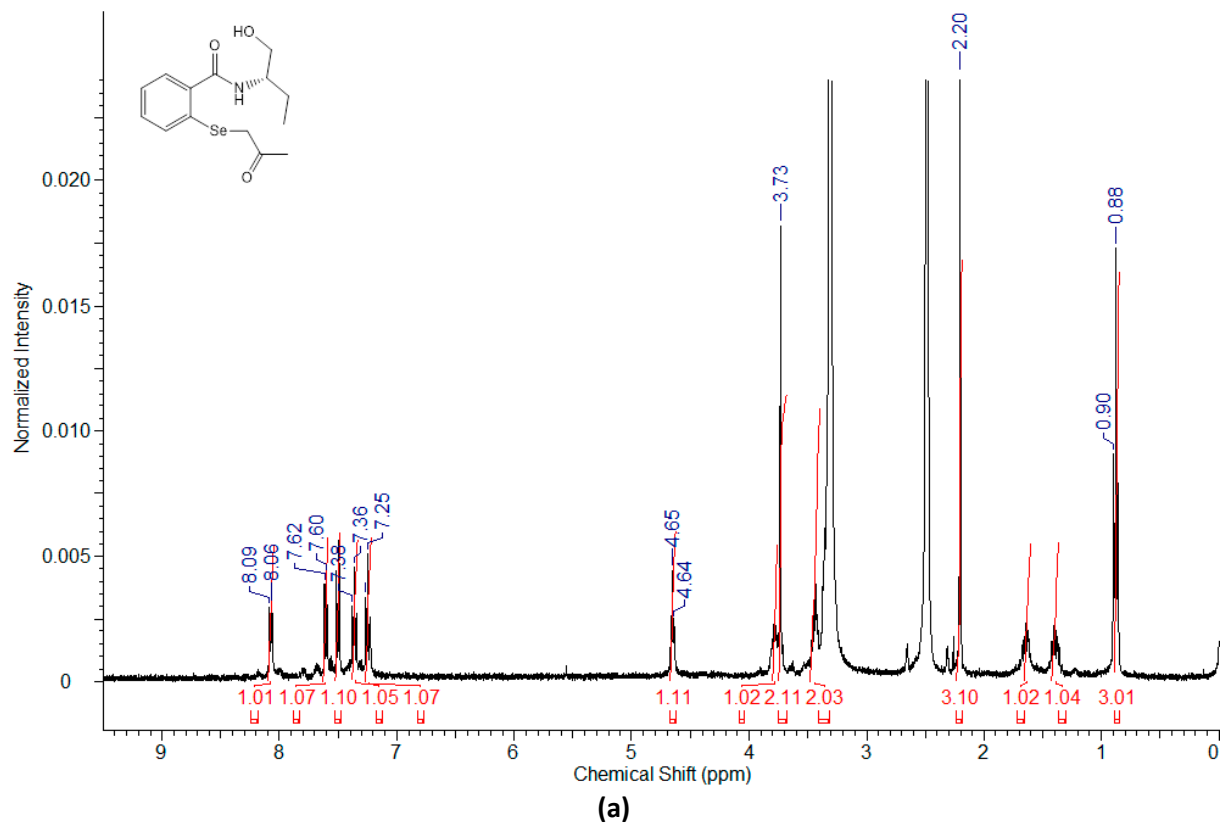


Figure S2. (a) ^1H NMR, (b) ^{13}C NMR, and (c) ^{77}Se NMR spectra of *N*-((*R*)-(-)-*sec*-butyl)-2-((2-oxopropyl)selanyl)benzamide **12**.



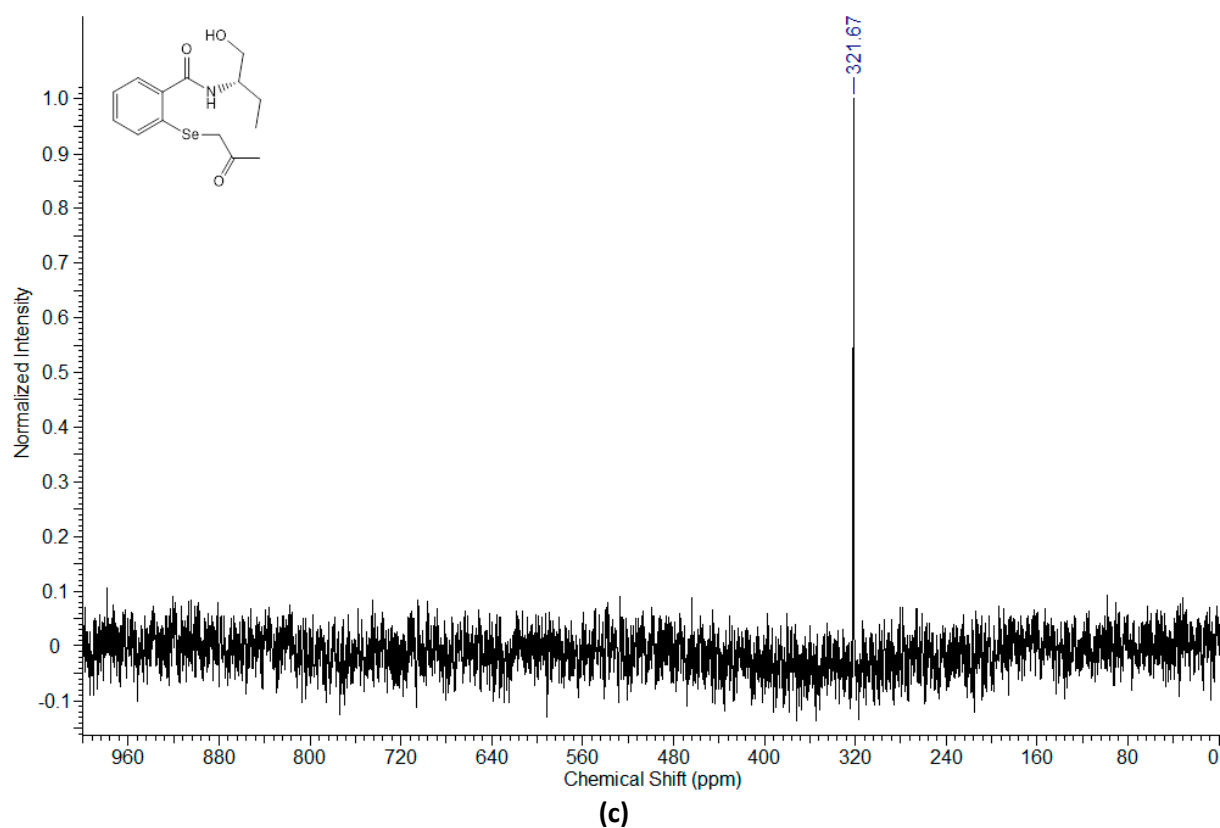
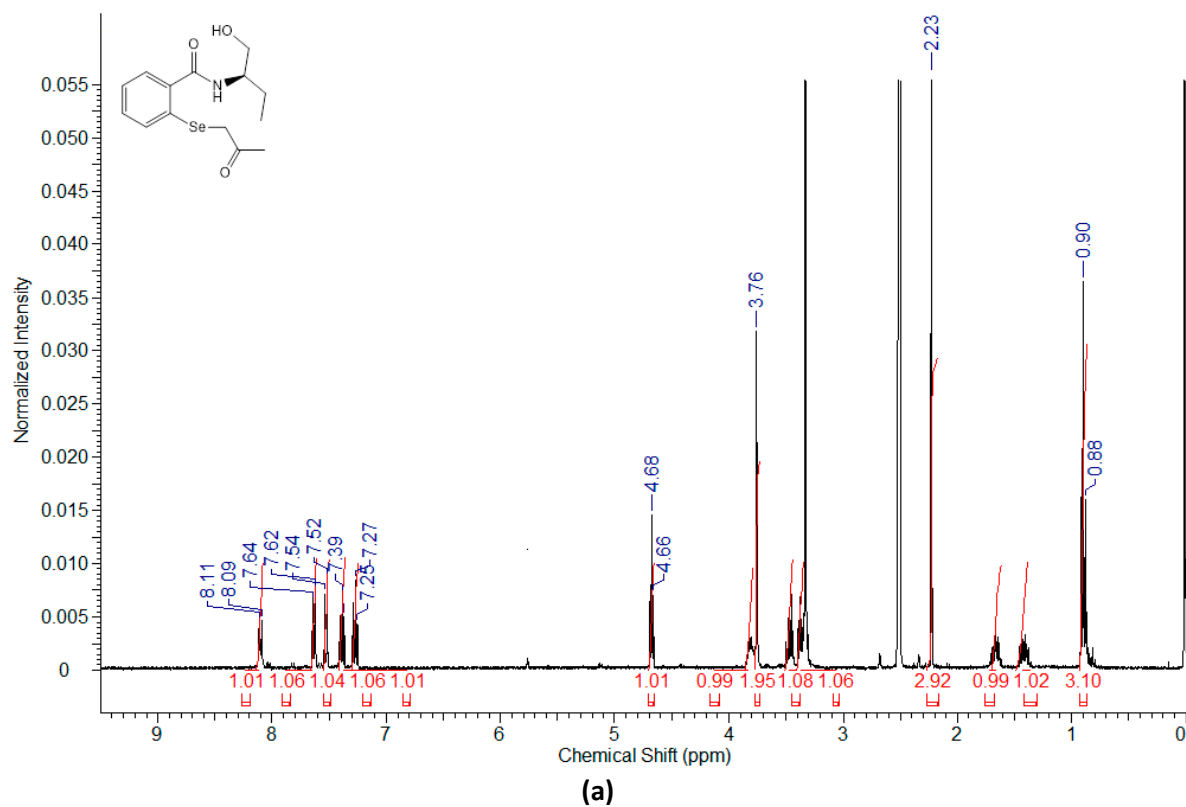


Figure S3. (a) ^1H NMR, (b) ^{13}C NMR, and (c) ^{77}Se NMR spectra of *N*-((*S*)-(+)-1-hydroxy-2-butanyl)-2-((2-oxopropyl)selanyl)benzamide **13**.



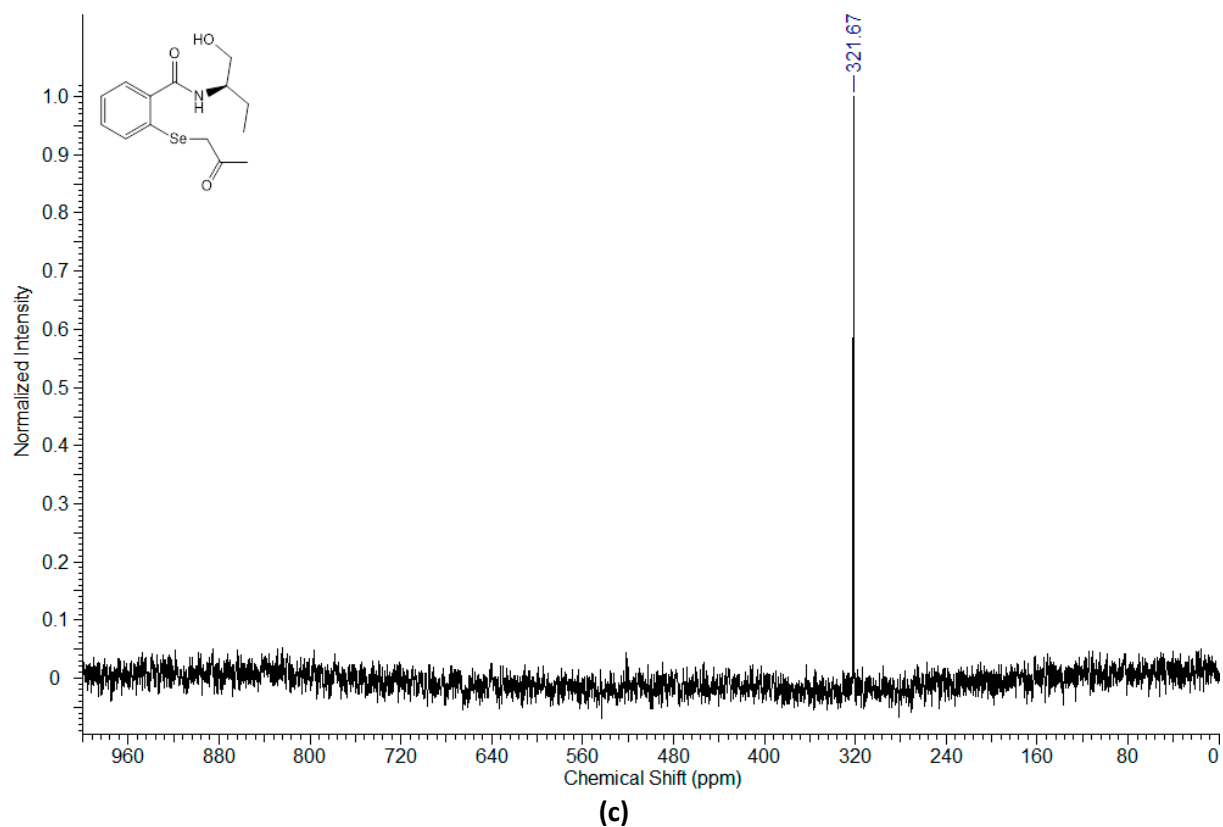
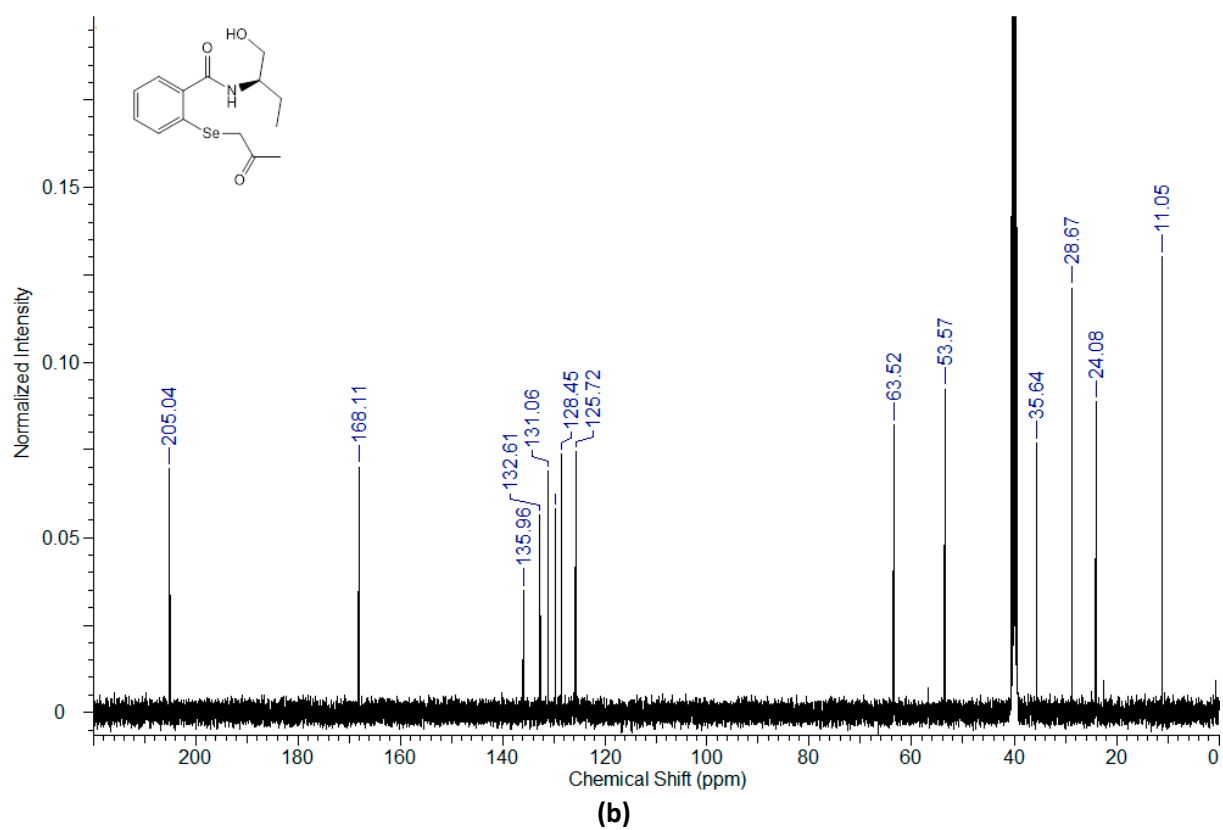
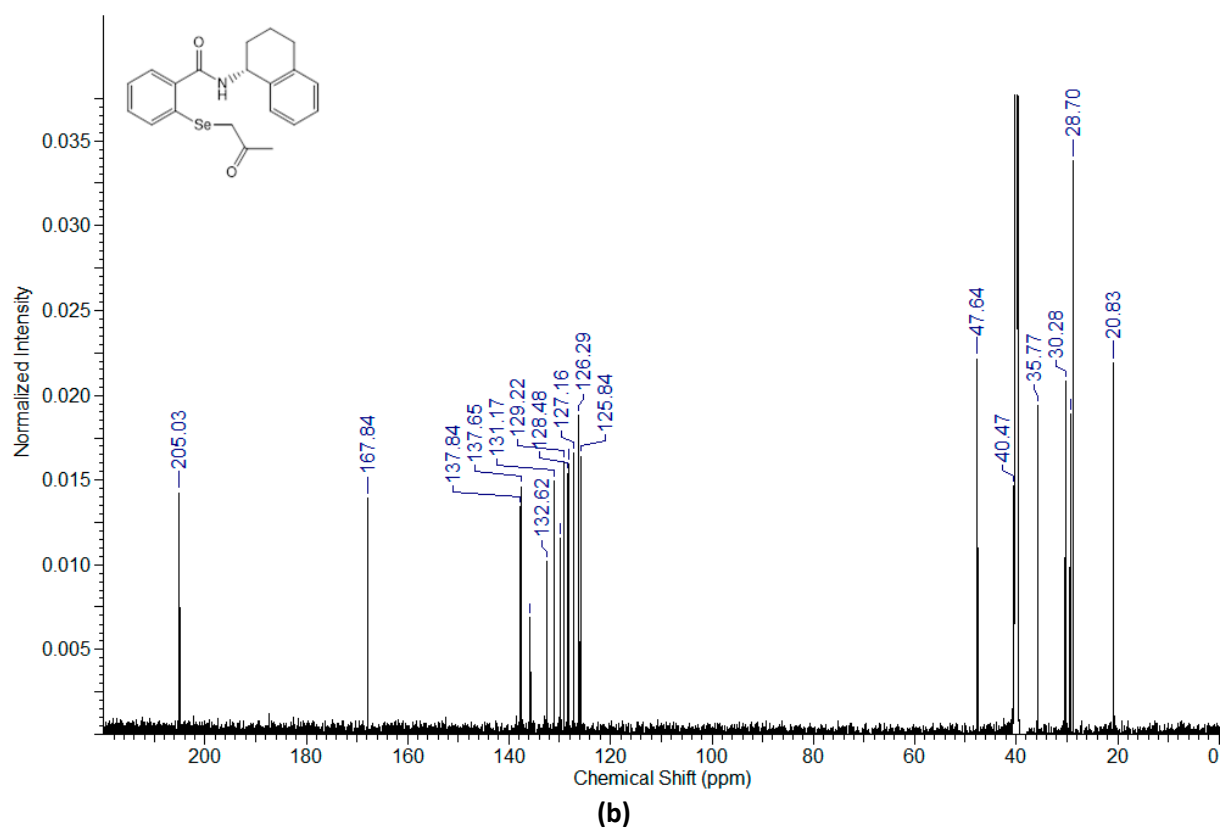
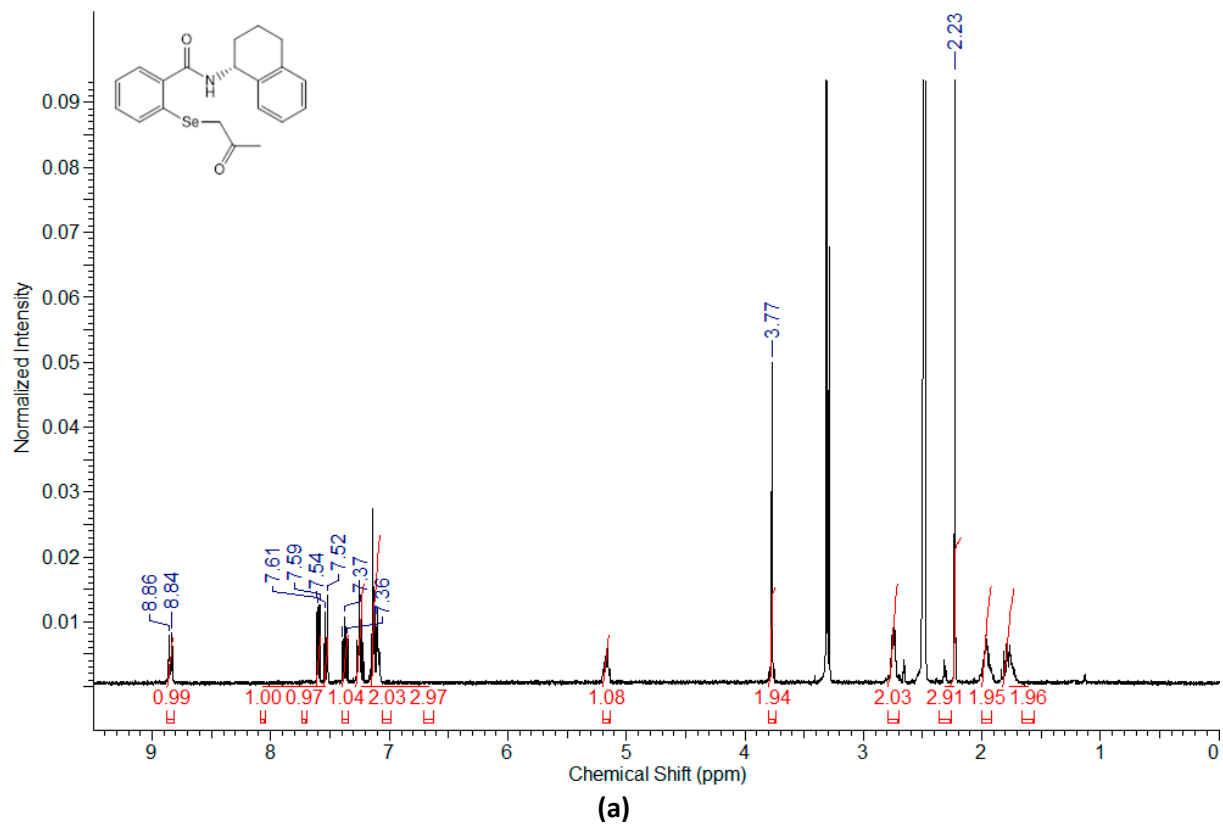


Figure S4. (a) ^1H NMR, (b) ^{13}C NMR, and (c) ^{77}Se NMR spectra of *N*-((*R*)-(-)-1-hydroxy-2-butanyl)-2-((2-oxopropyl)selanyl)benzamide **14**.



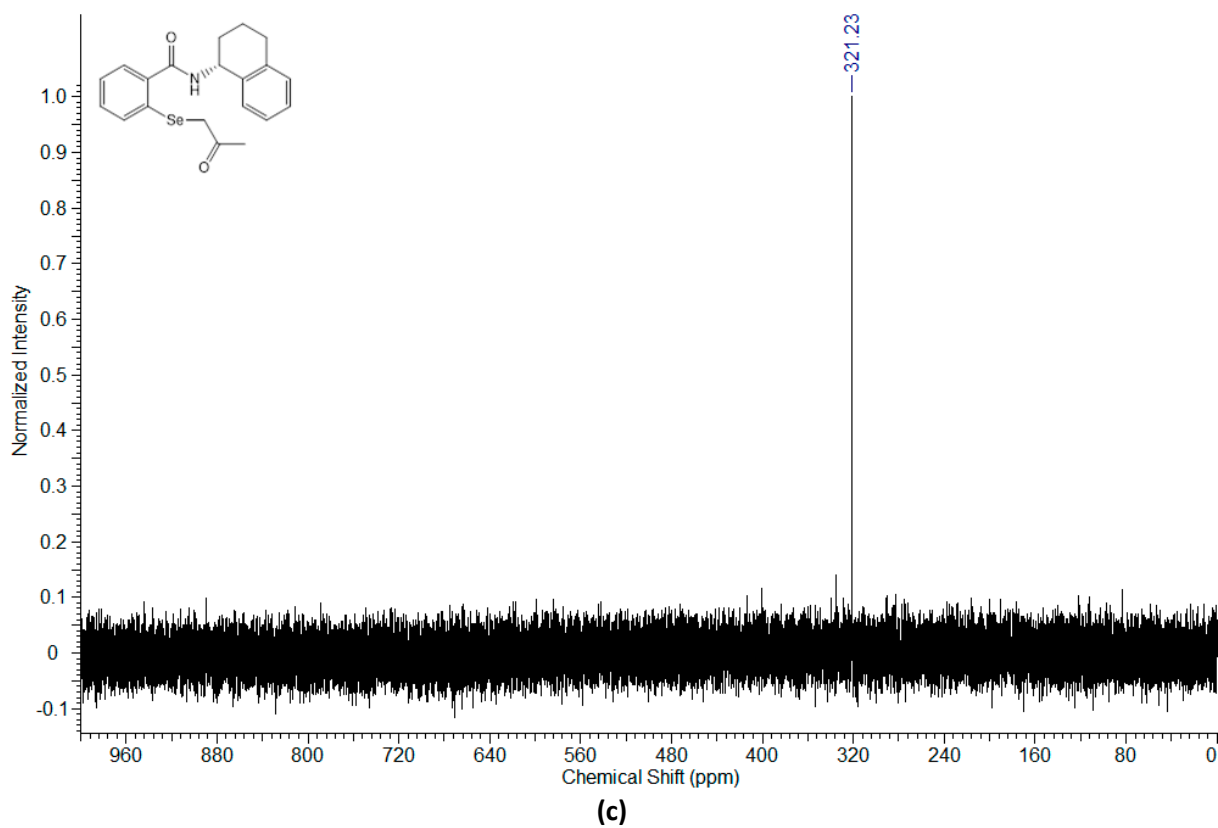
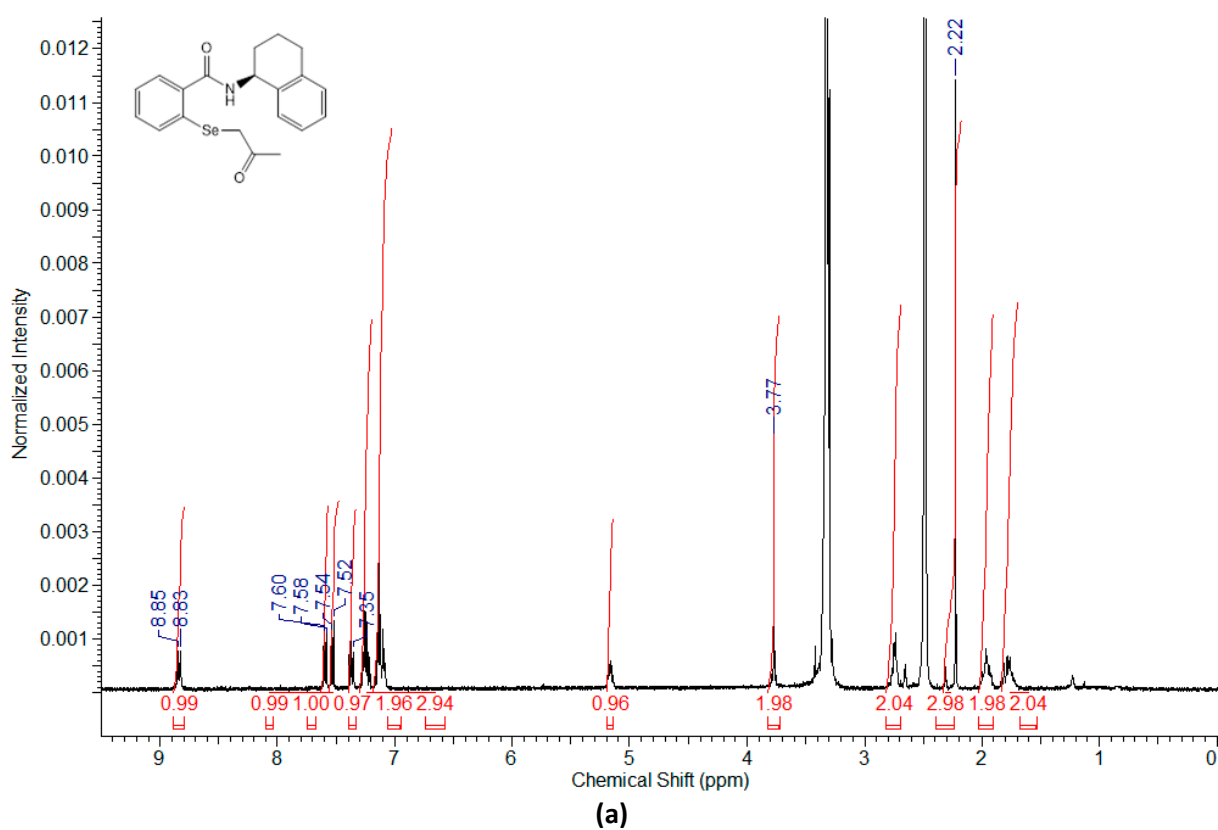


Figure S5. (a) ^1H NMR, (b) ^{13}C NMR, and (c) ^{77}Se NMR spectra of *N*-((*R*)-(-)-1,2,3,4-tetrahydro-1-naphthyl) 2-((2-oxopropyl)selanyl)benzamide **15**.



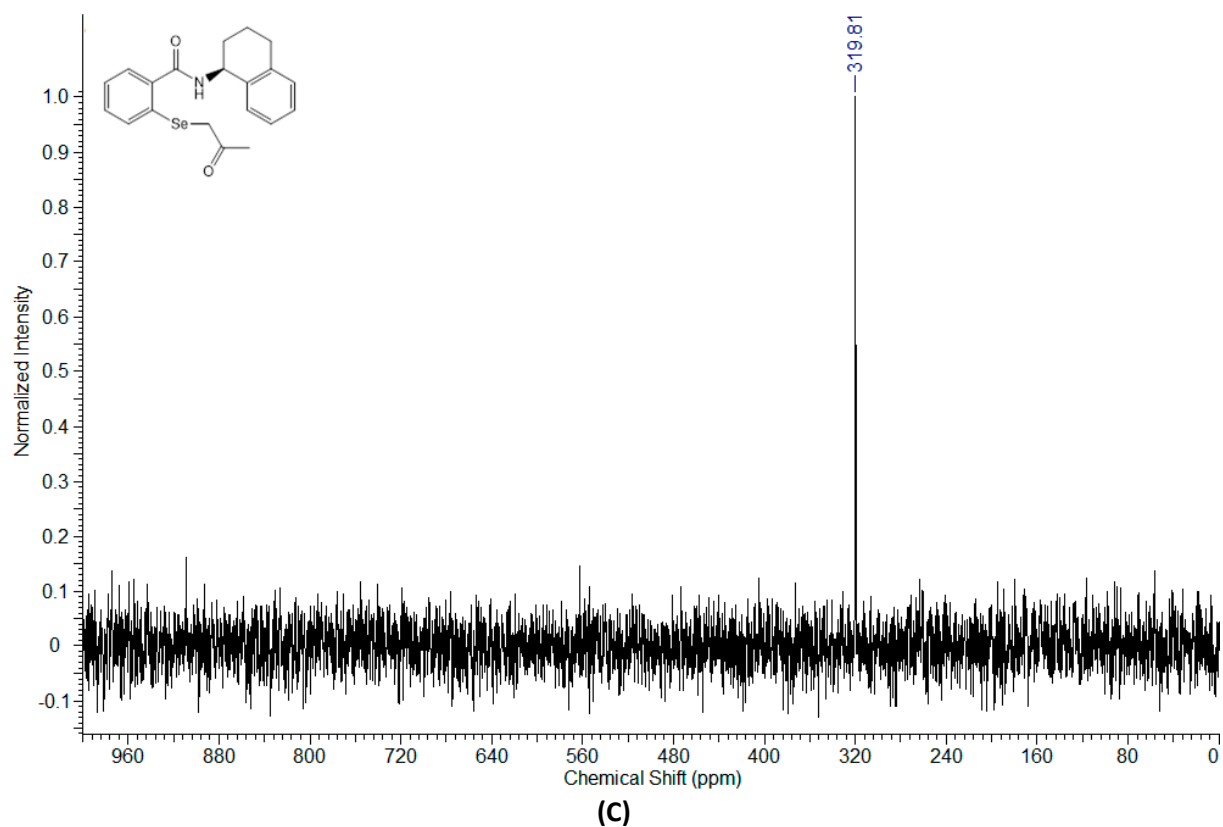
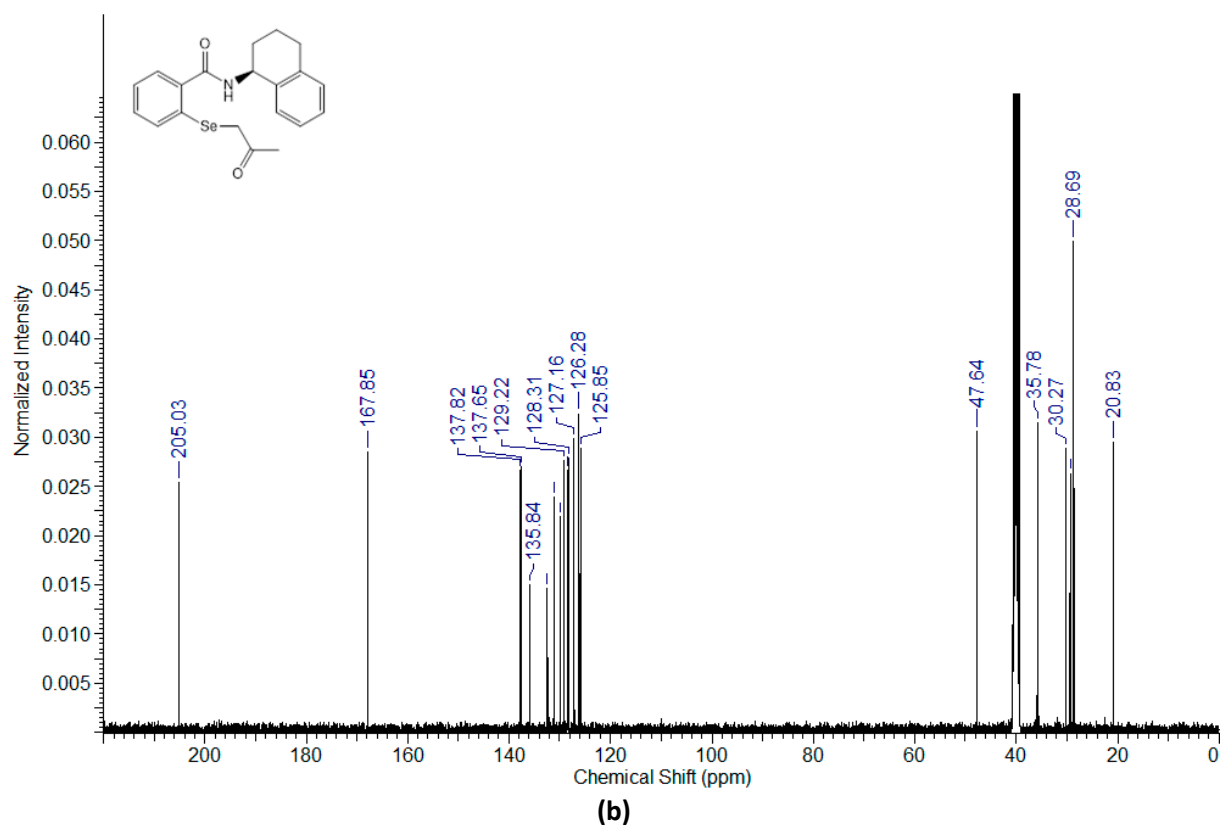
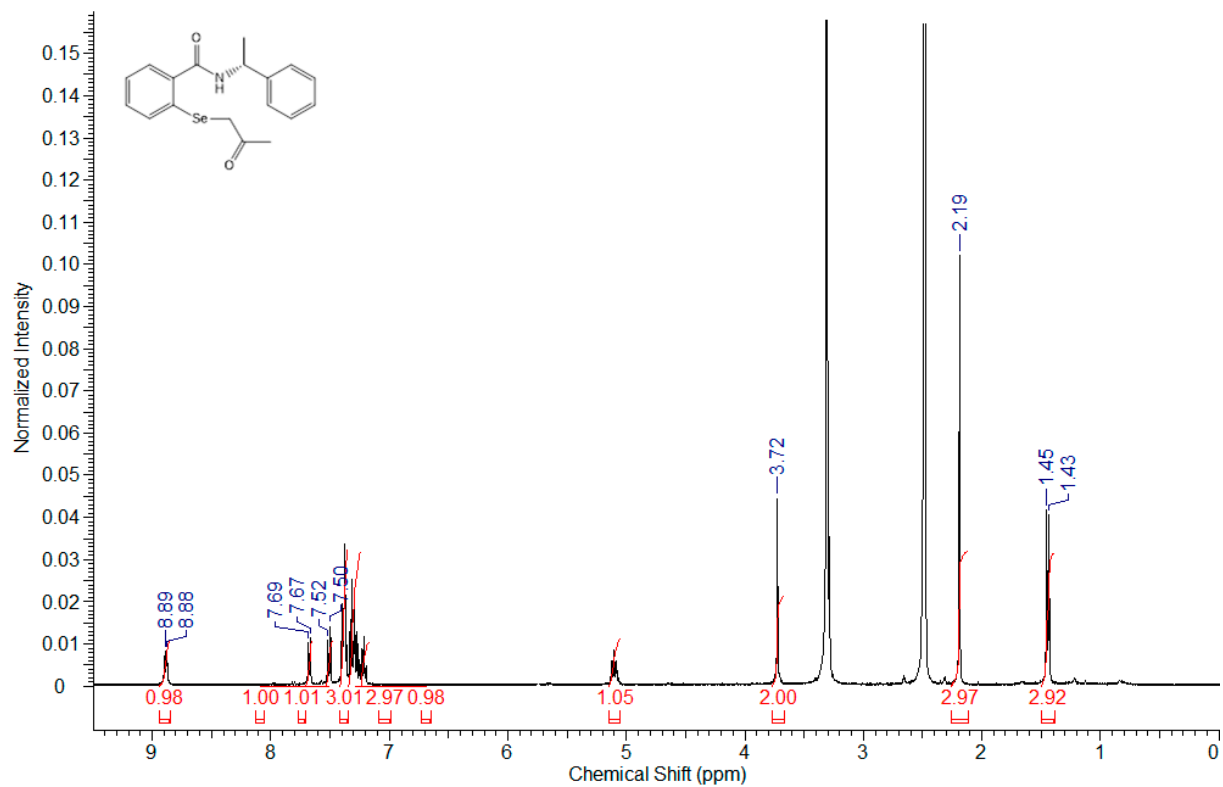
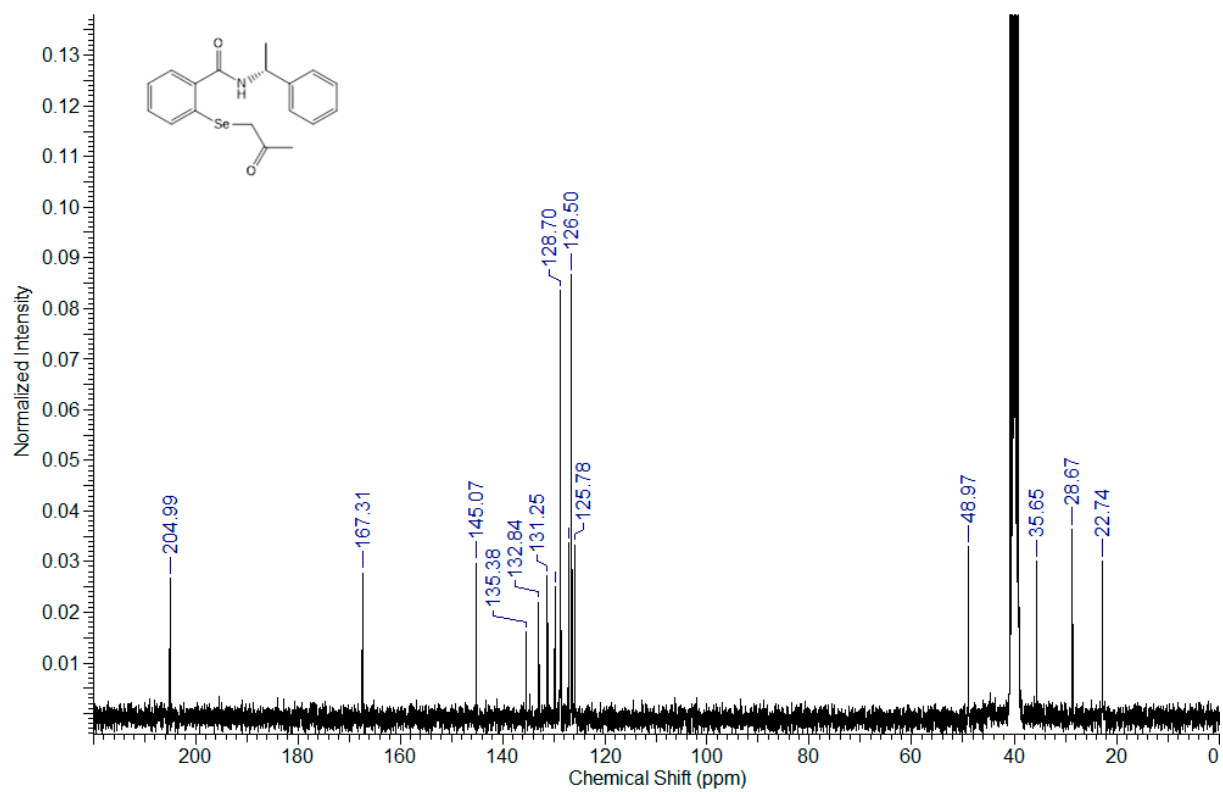


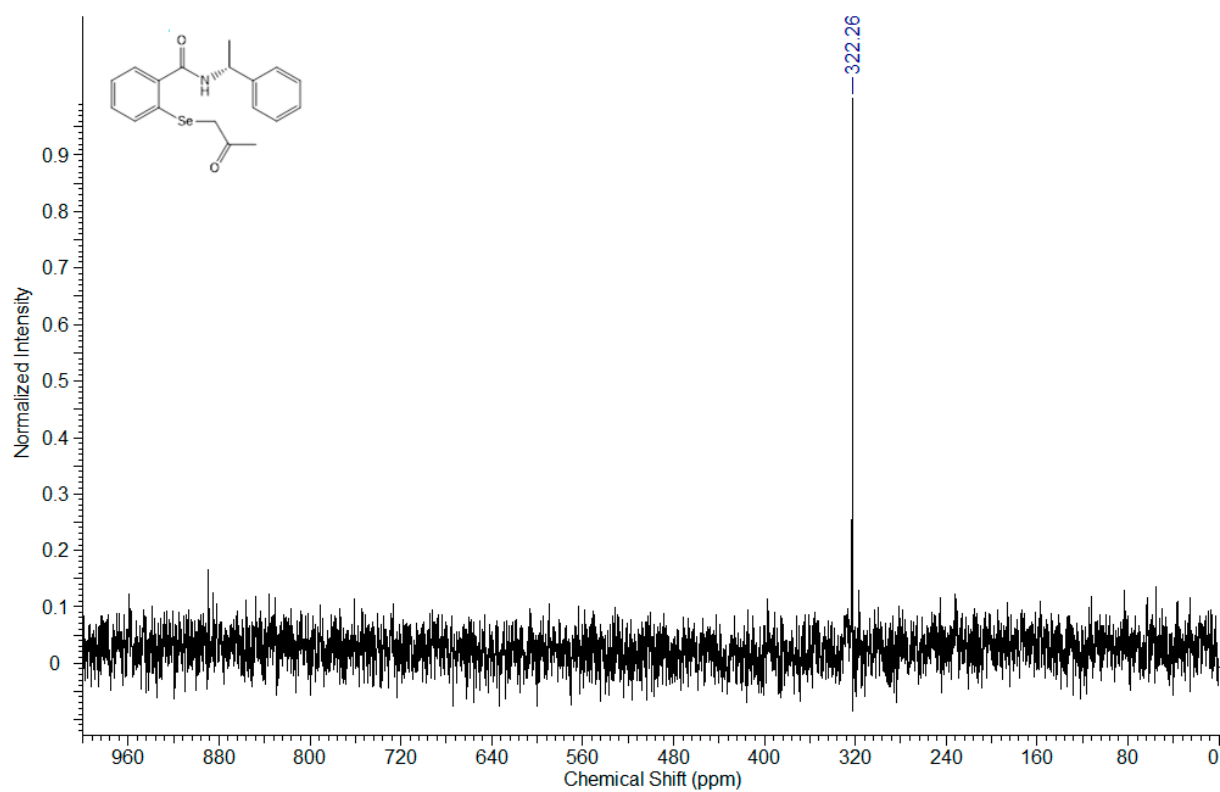
Figure S6. (a) ¹H NMR, (b) ¹³C NMR, and (c) ⁷⁷Se NMR spectra of *N*-((*S*)-(+)-1,2,3,4-tetrahydro-1-naphthyl) 2-((2-oxopropyl)selanyl)benzamide **16**.



(a)

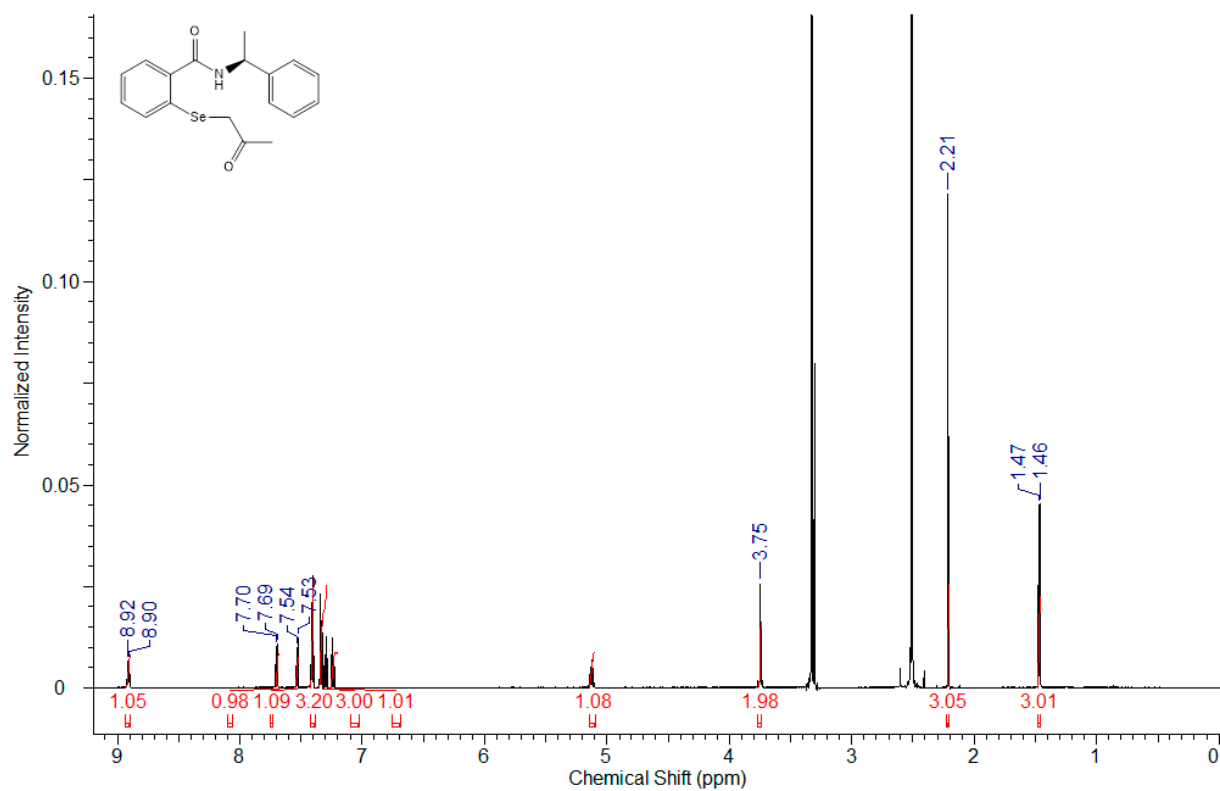


(b)



(c)

Figure S7. (a) ^1H NMR, (b) ^{13}C NMR, and (c) ^{77}Se NMR spectra of *N*-((*R*)-(+)- α -methylbenzyl)-2-((2-oxopropyl)selanyl)benzamide **17**.



(a)

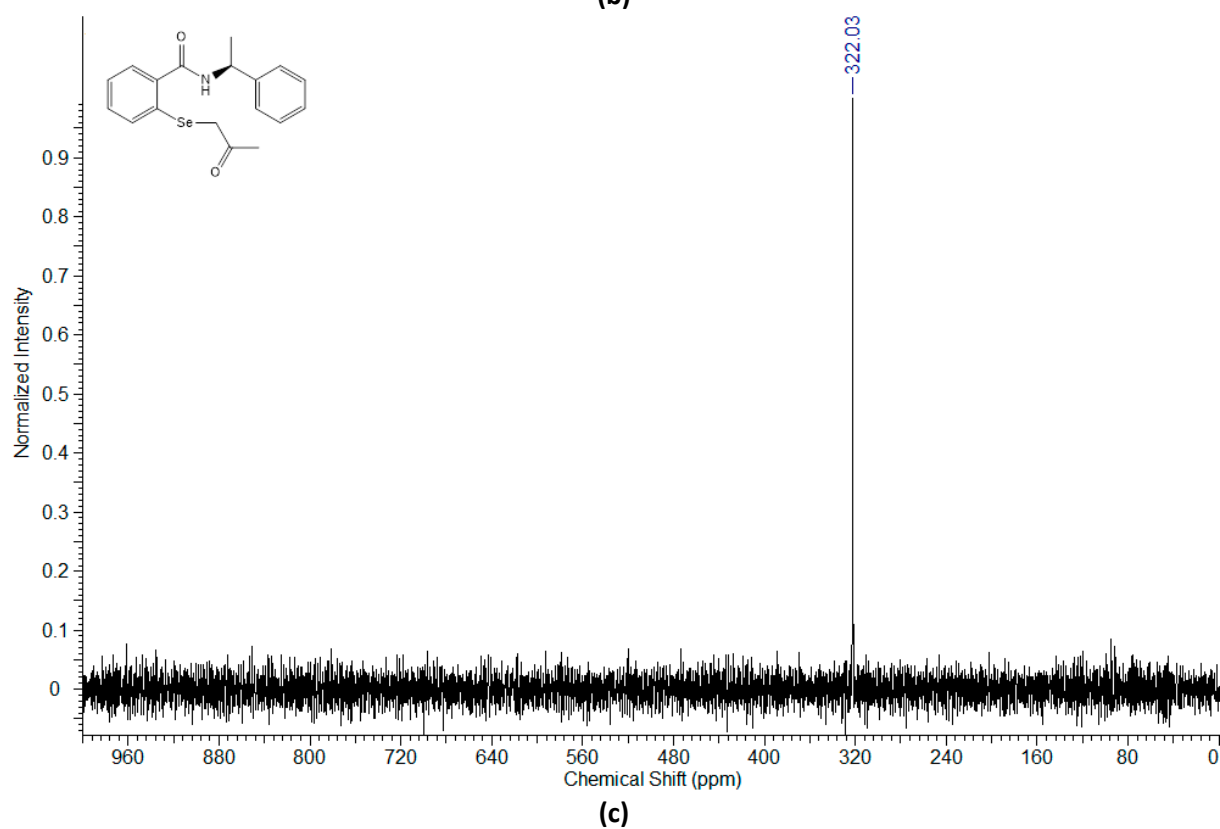
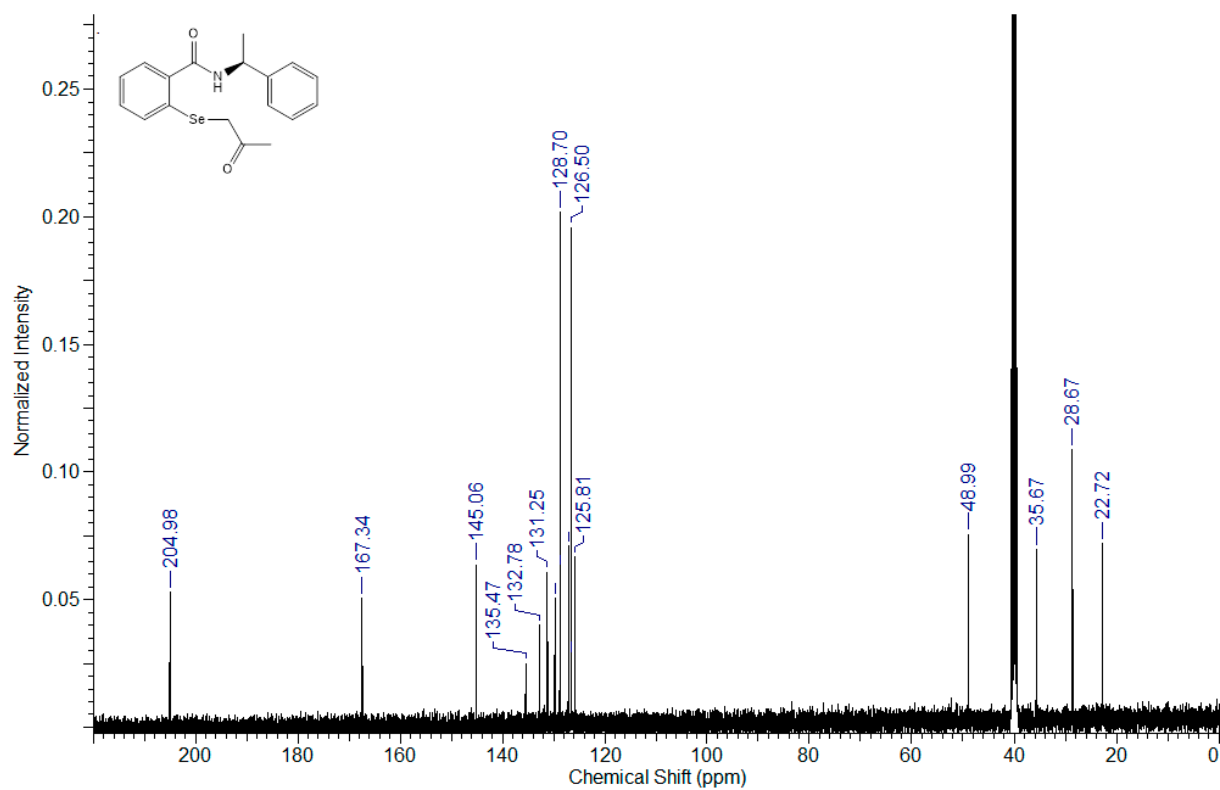
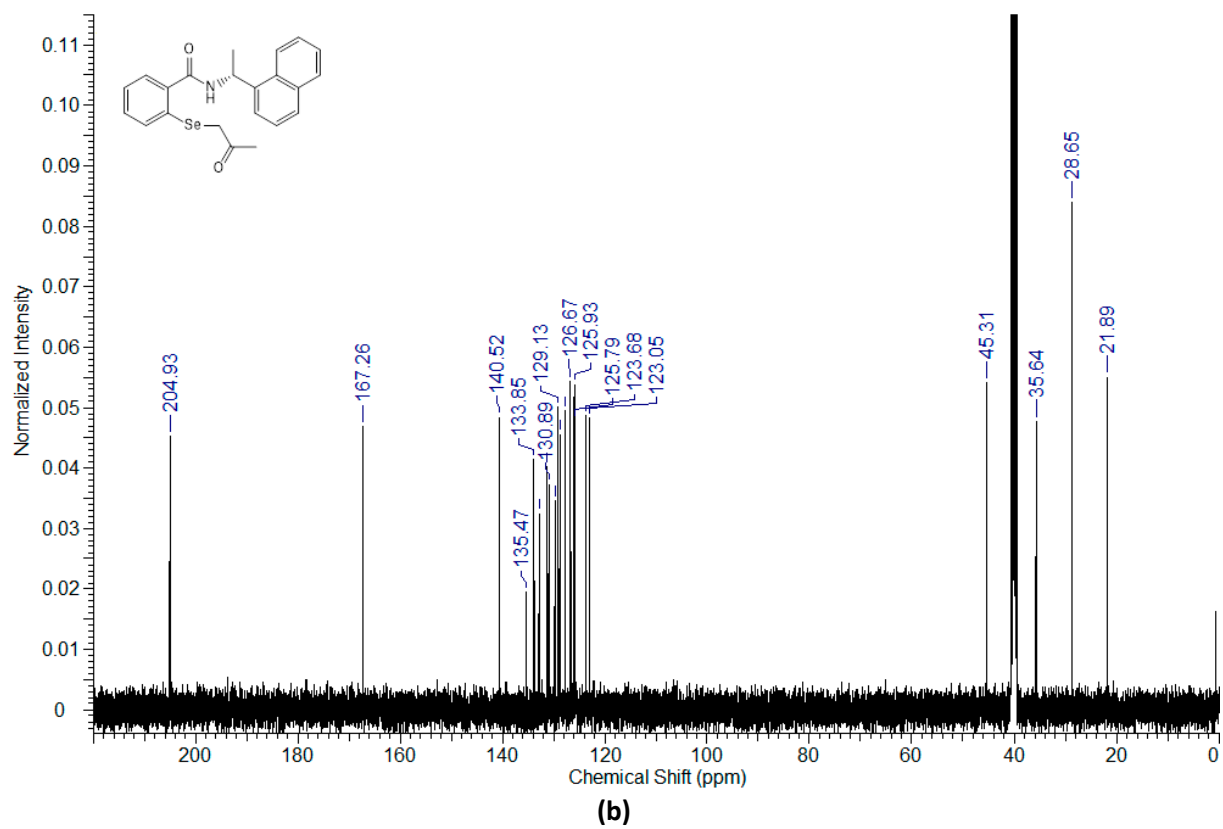
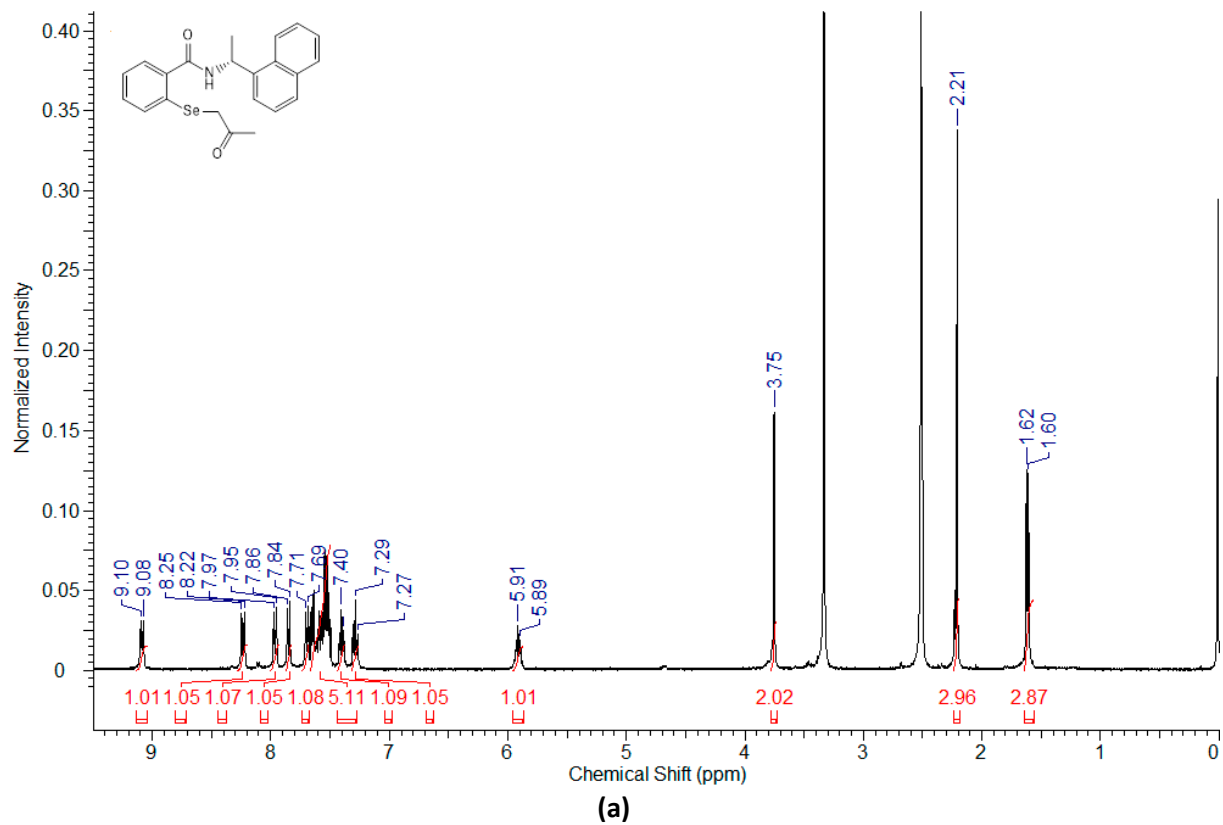


Figure S8. (a) ¹H NMR, (b) ¹³C NMR, and (c) ⁷⁷Se NMR spectra of *N*-((*S*)-(-)-α-methylbenzyl)-2-((2-oxopropyl)selanyl)benzamide **18**.



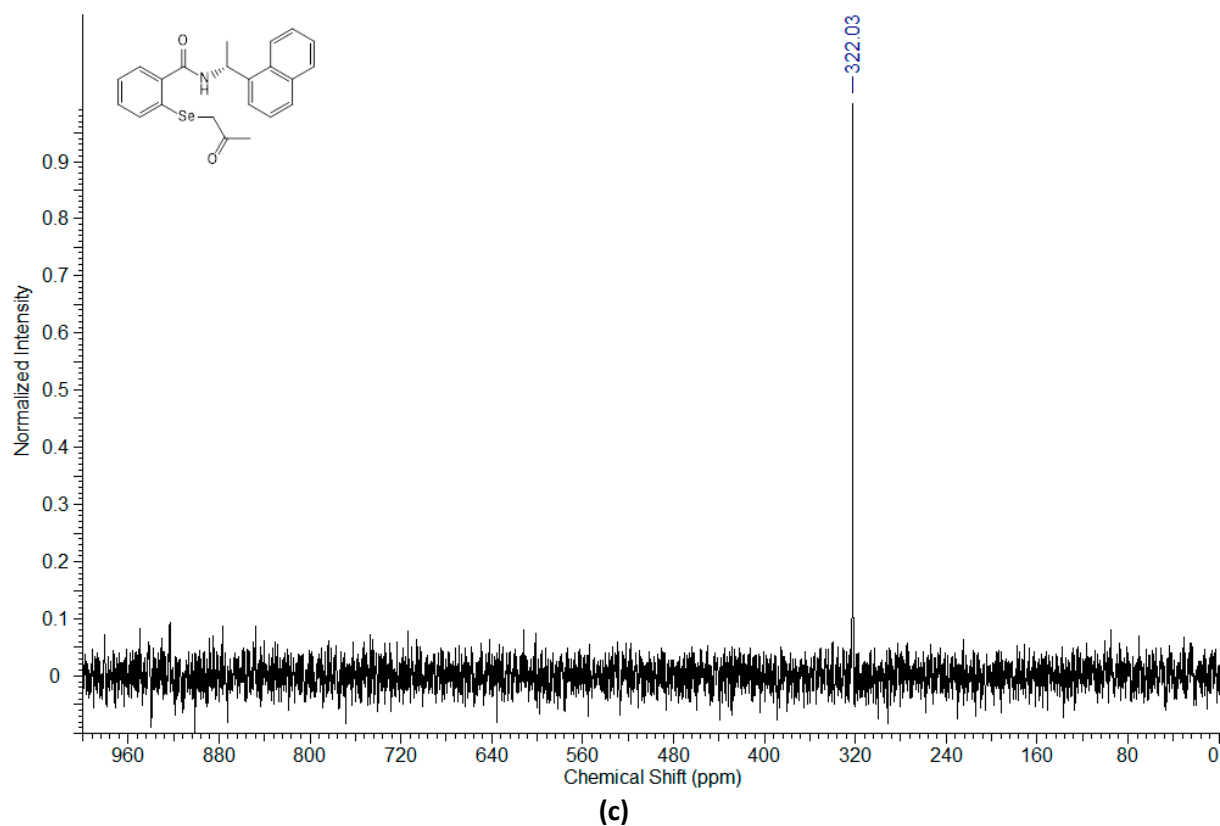
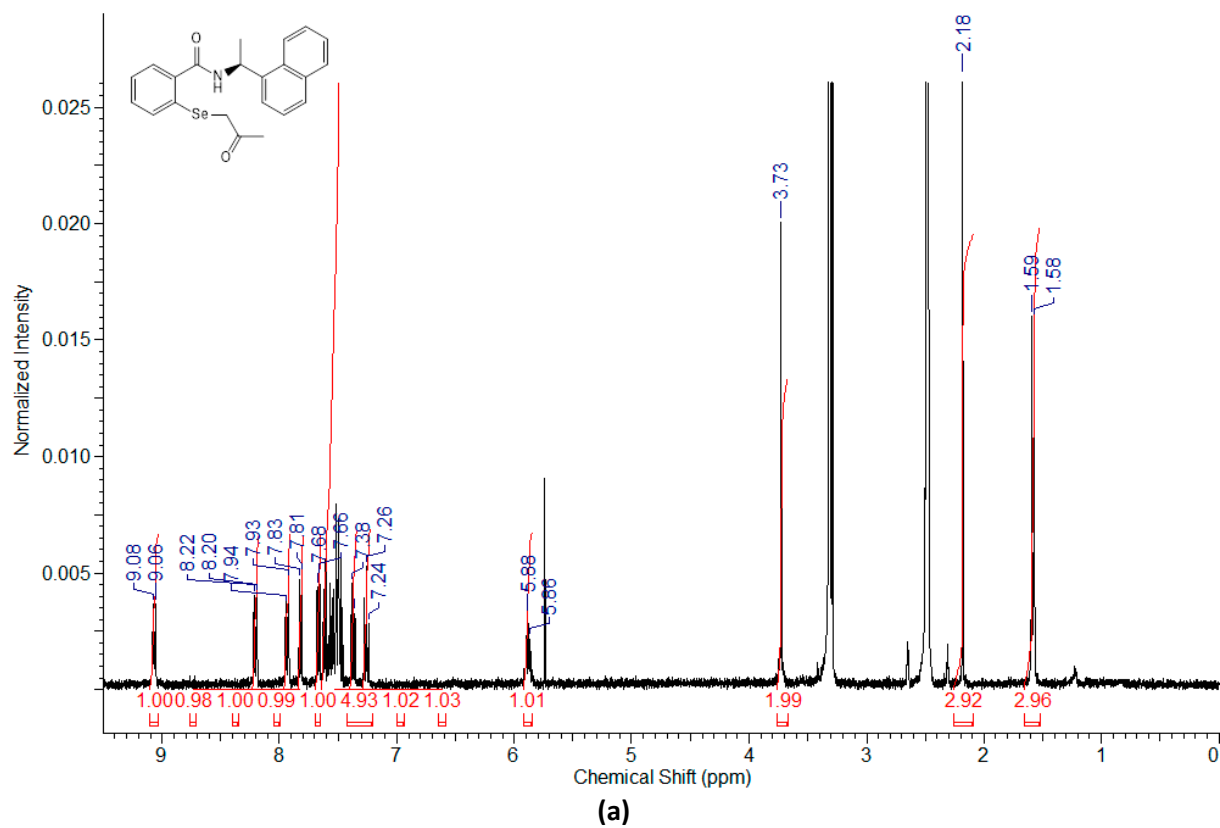


Figure S9. (a) ^1H NMR, (b) ^{13}C NMR, and (c) ^{77}Se NMR spectra of *N*-((*S*)-(-)-1-(1-naphthyl)ethyl)-2-((2-oxopropyl)selanyl)benzamide **19**.



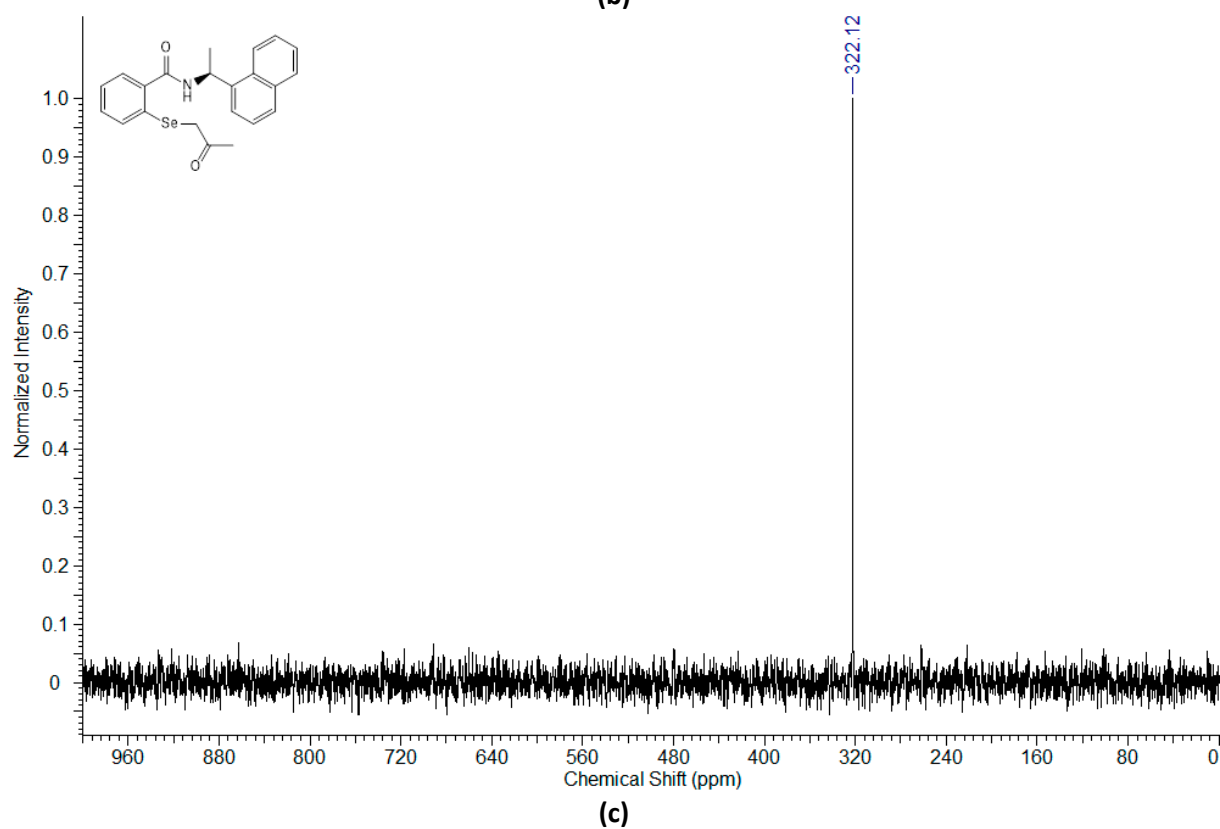
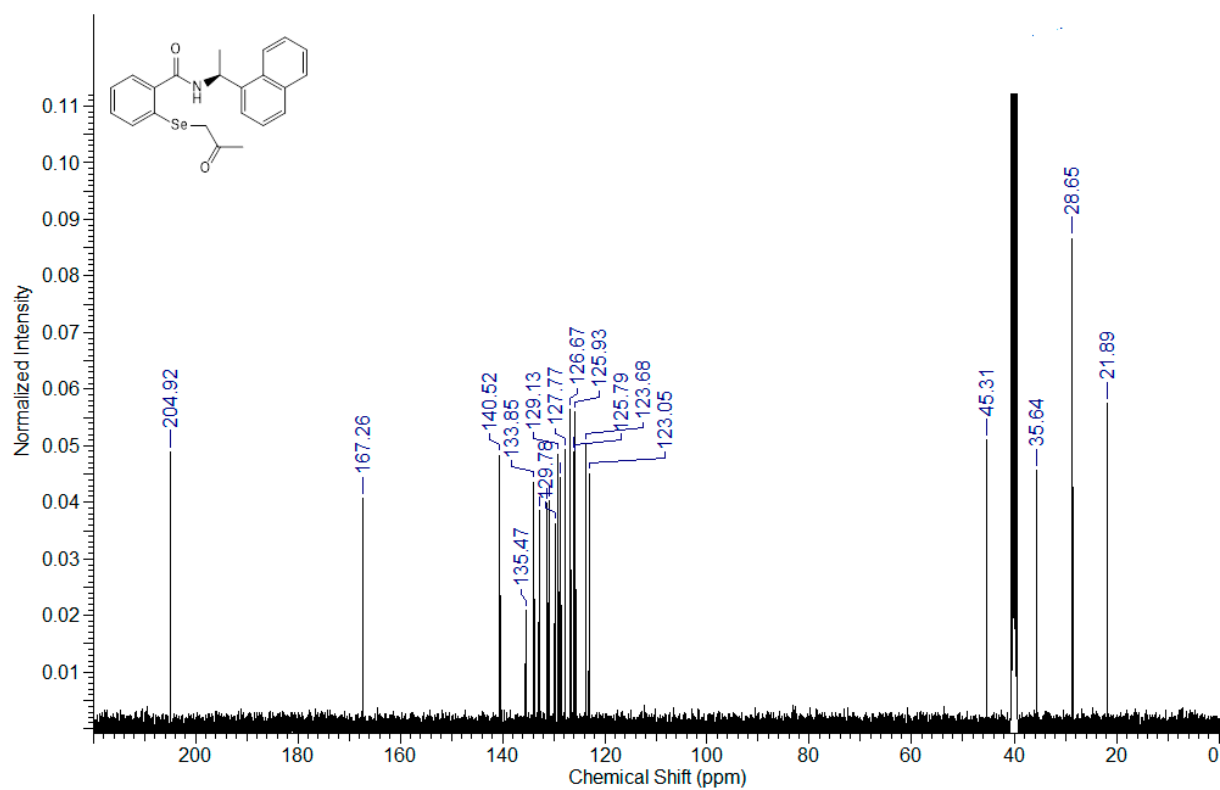
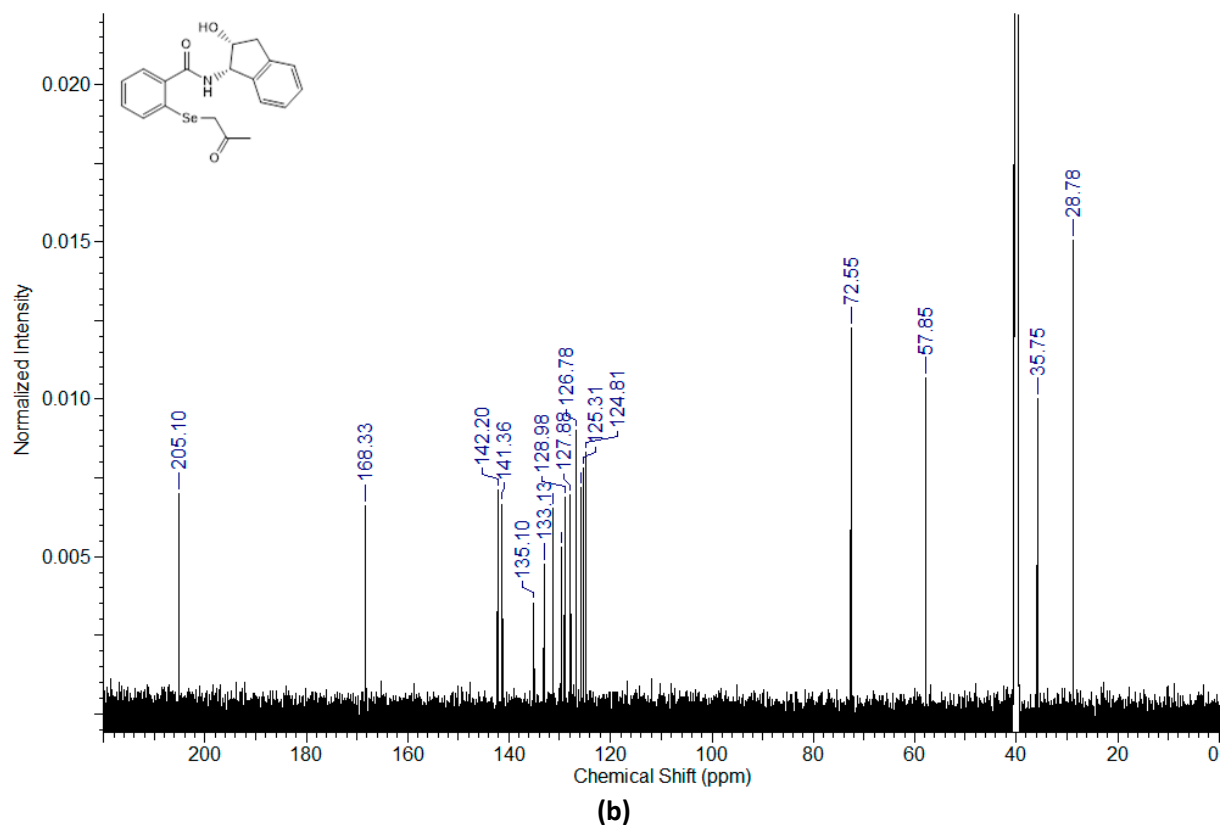
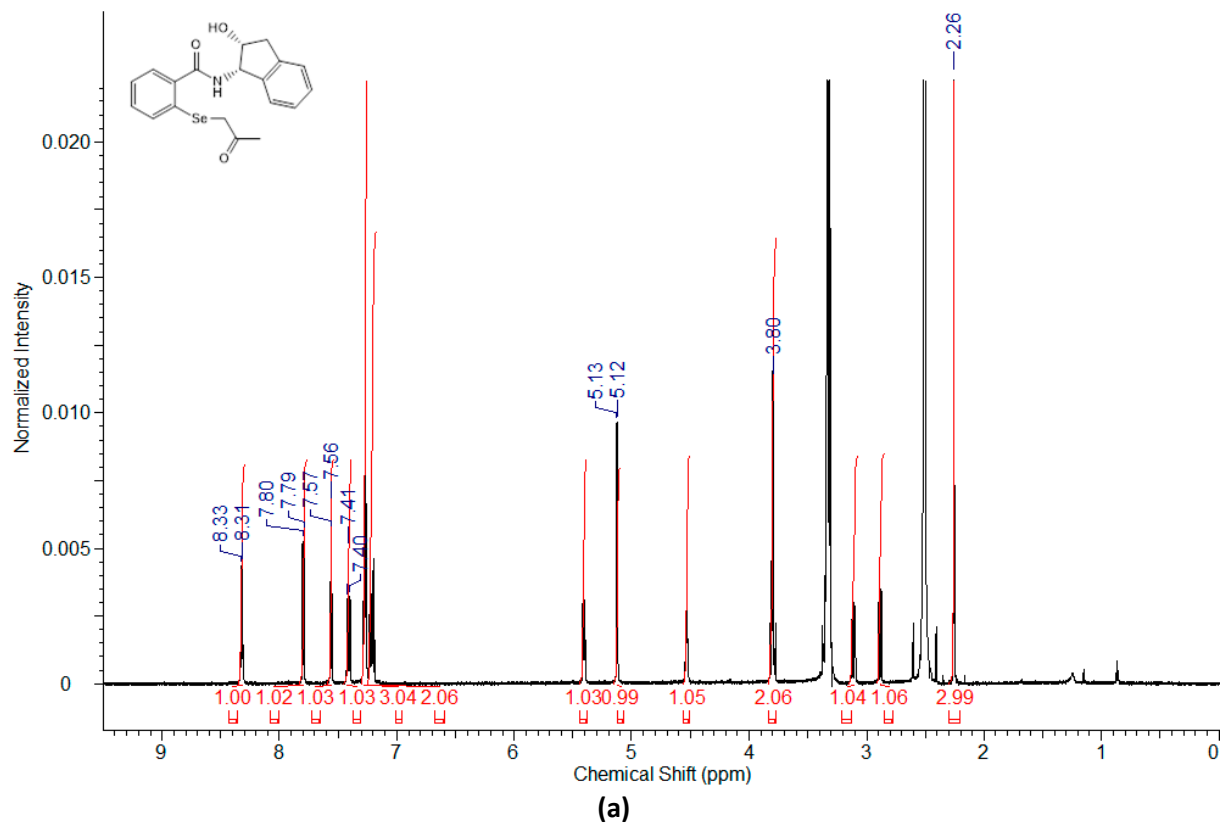


Figure S10. (a) ¹H NMR, (b) ¹³C NMR, and (c) ⁷⁷Se NMR spectra of *N*-((*R*)-(+)-1-(1-naphthyl)ethyl)-2-((2-oxopropyl)selanyl)benzamide **20**.



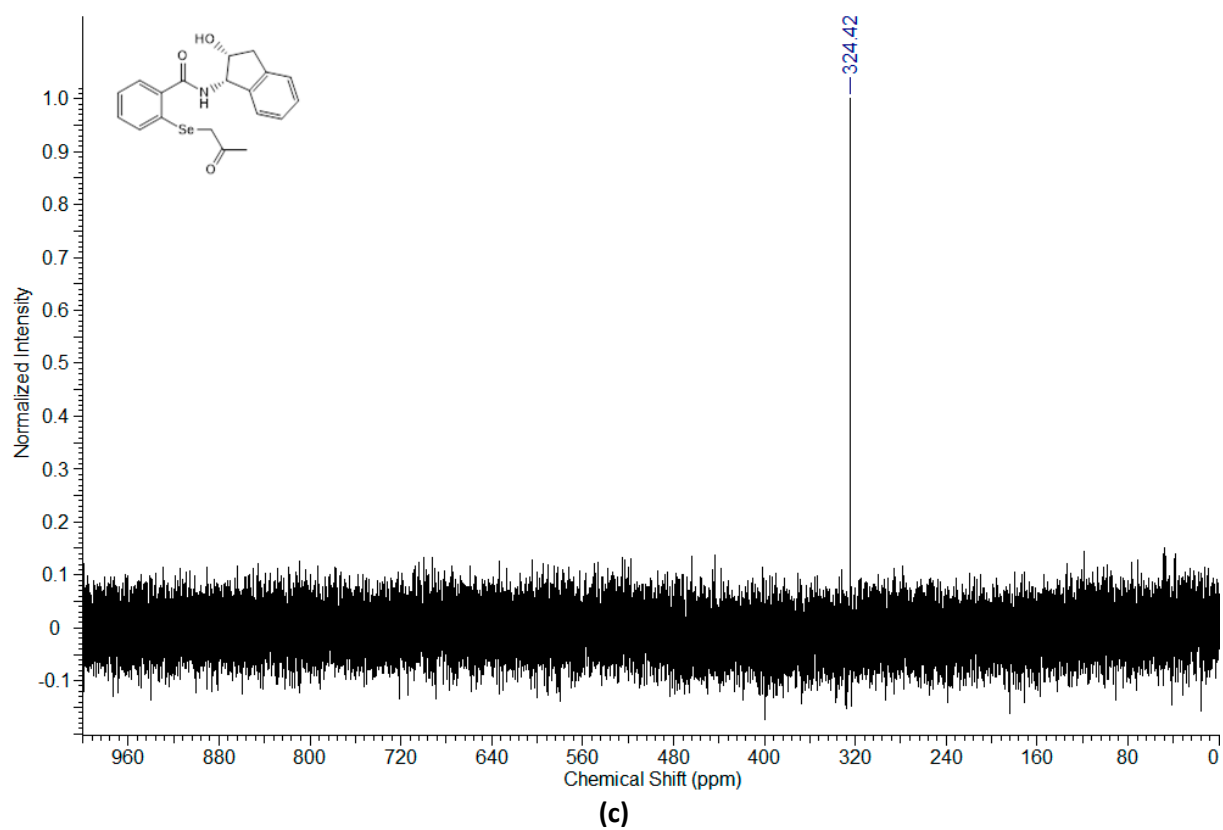
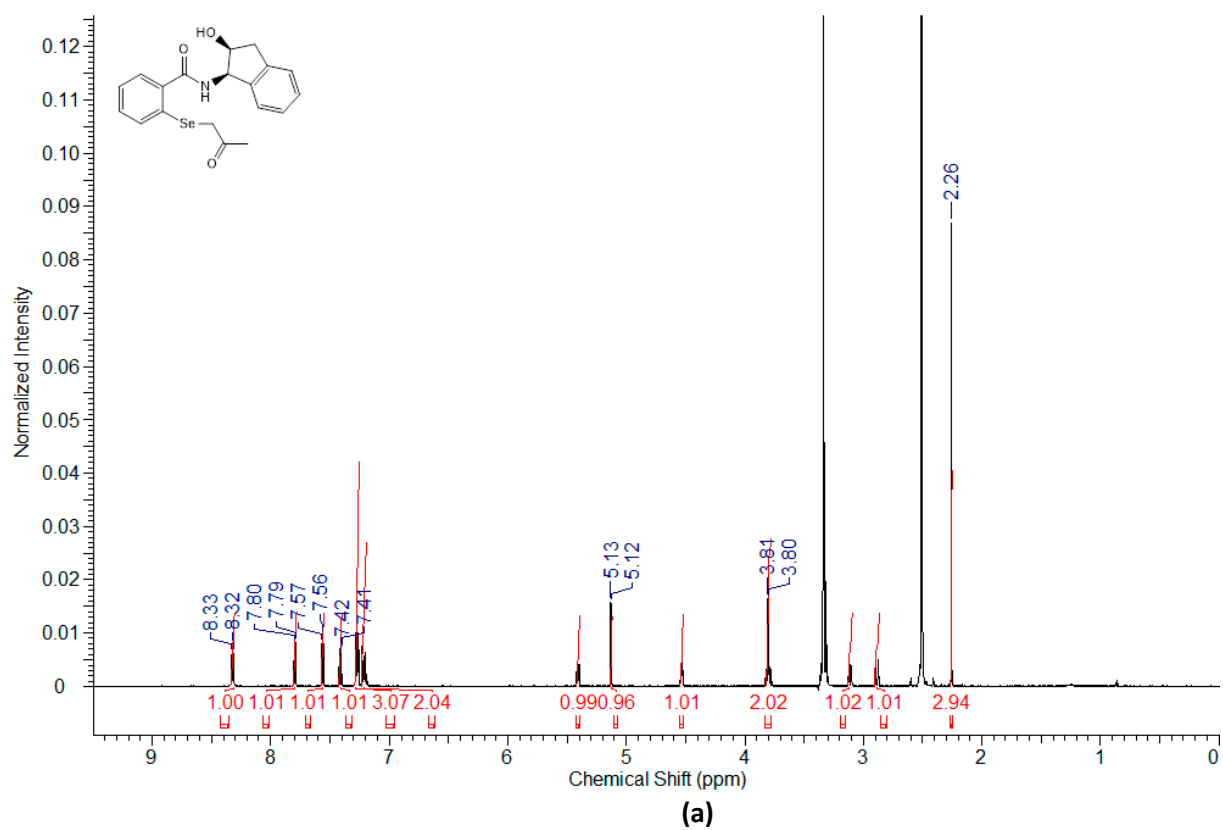
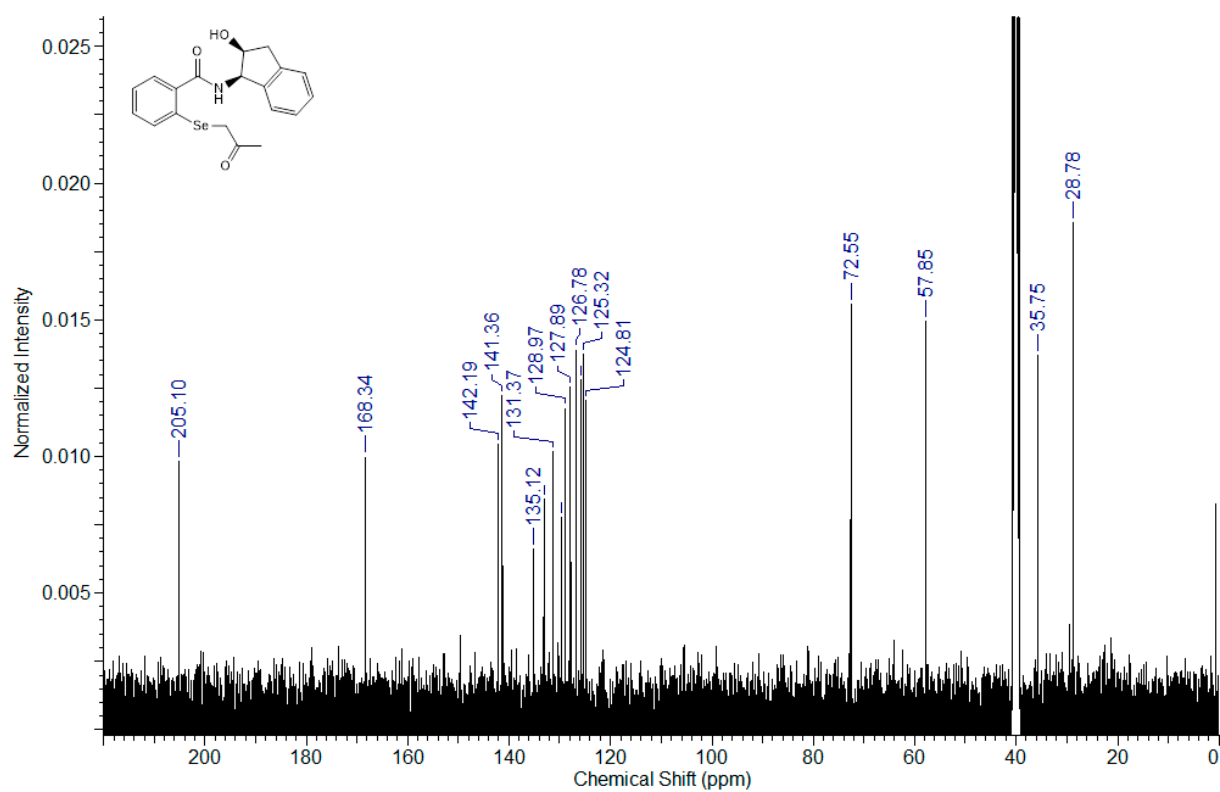
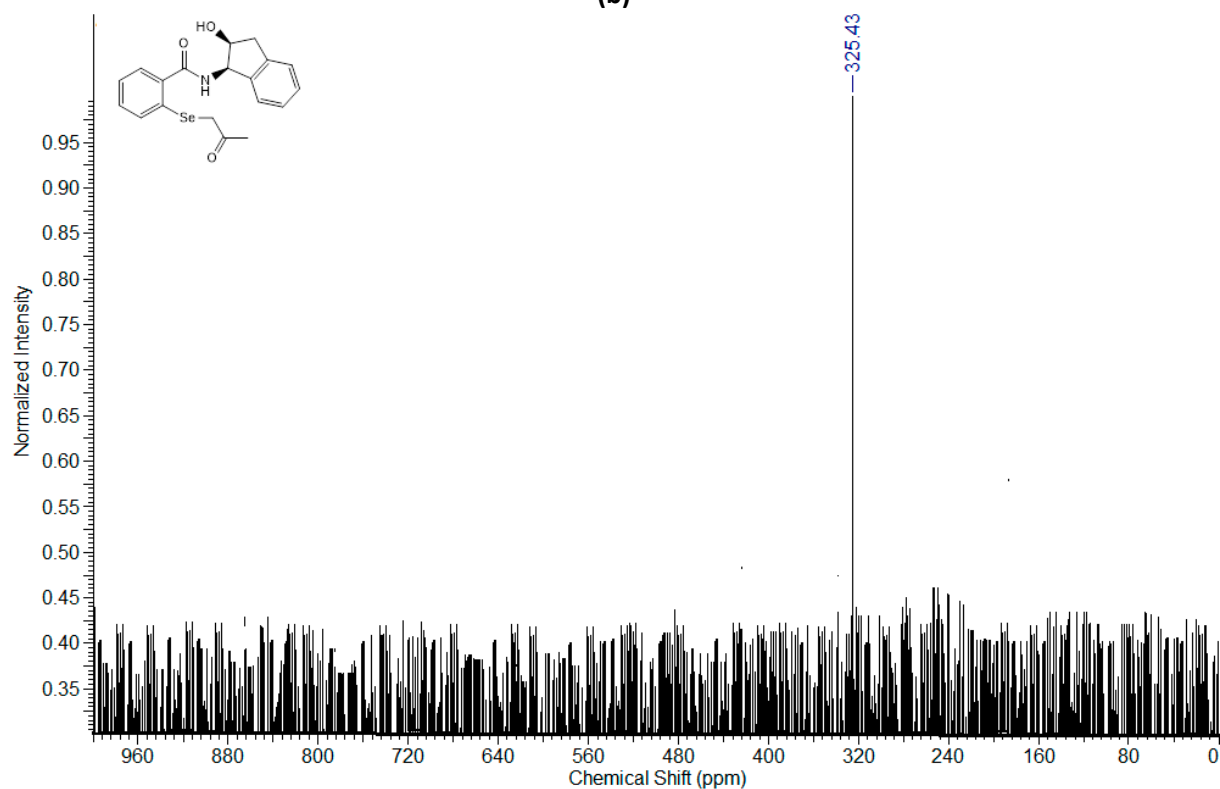


Figure S11. (a) ^1H NMR, (b) ^{13}C NMR, and (c) ^{77}Se NMR spectra of *N*-((1*S*,2*R*)-(-)-*cis*-2-hydroxy-1-indanyl)- 2-((2-oxopropyl)selanyl)benzamide **21**.



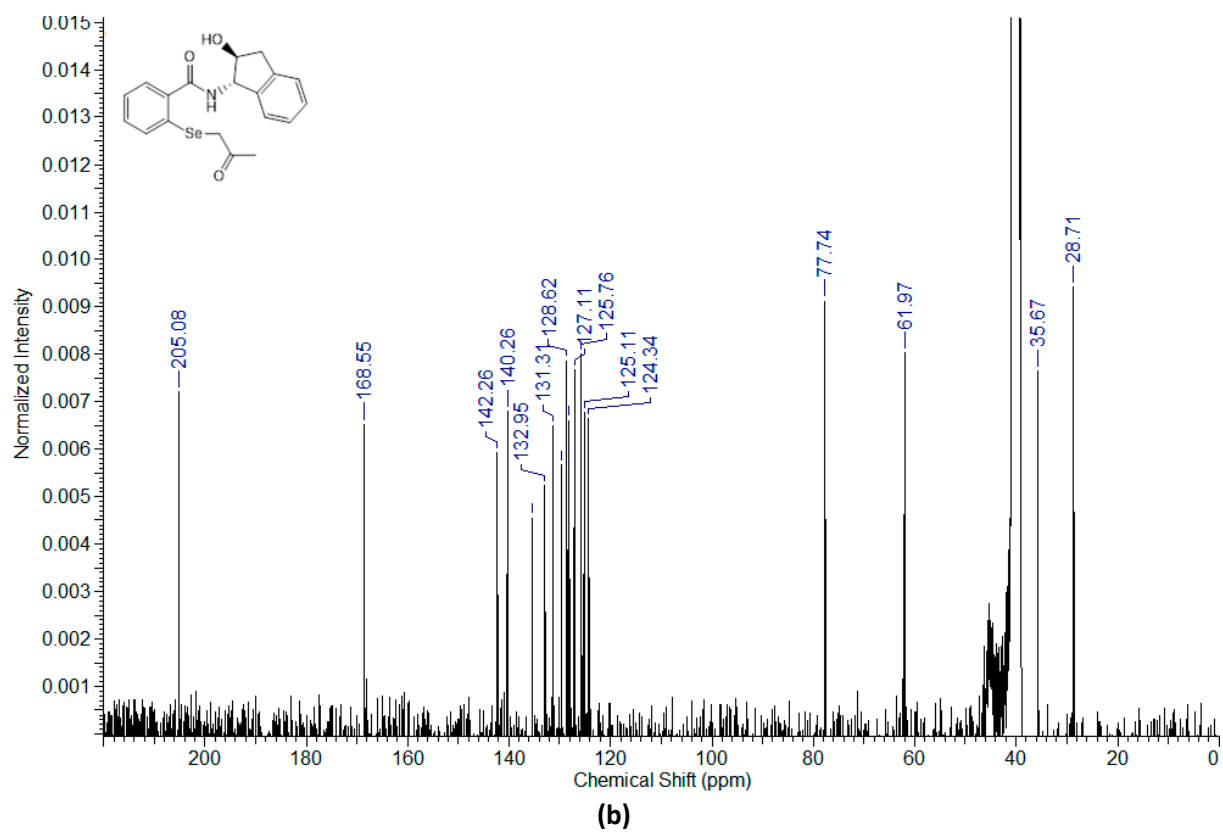
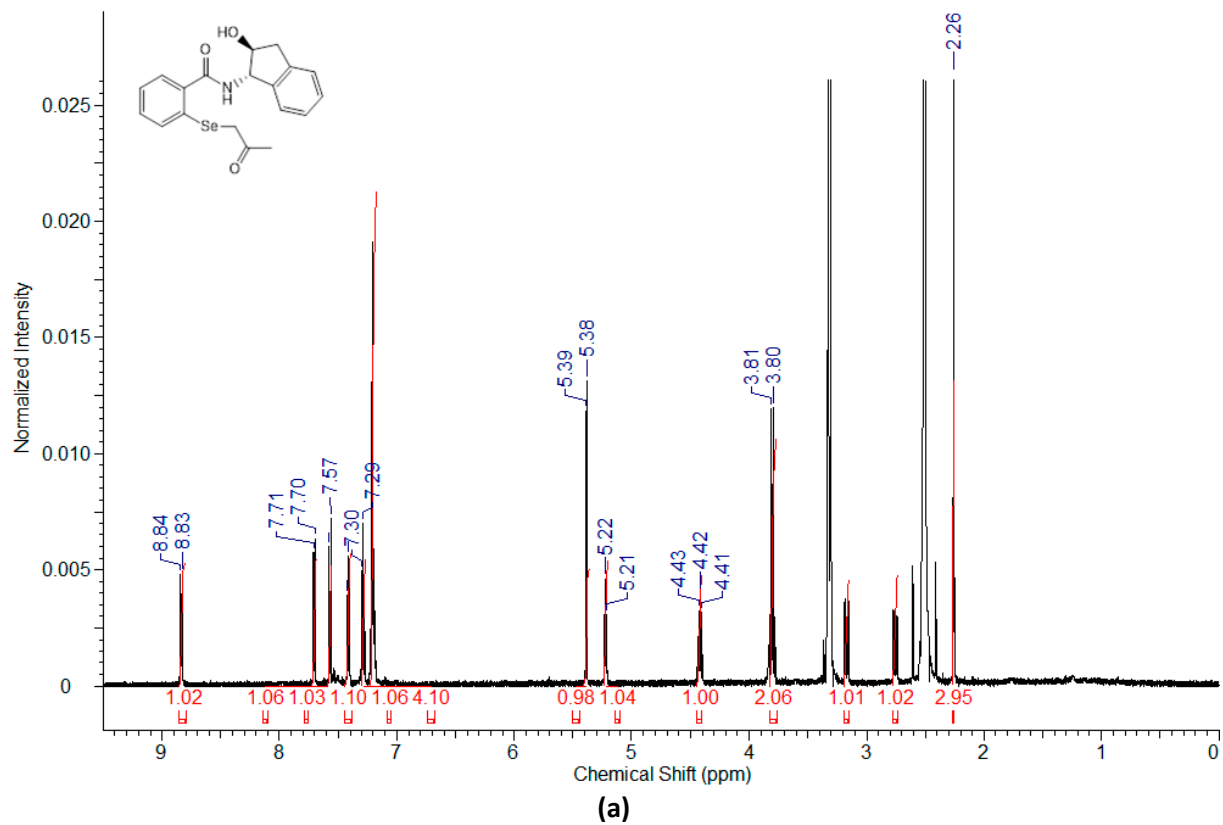


(b)



(c)

Figure S12. (a) ¹H NMR, (b) ¹³C NMR, and (c) ⁷⁷Se NMR spectra of *N*-((1*R*,2*S*)-(+)-*cis*-2-hydroxy-1-indanyl)- 2-((2-oxopropyl)selanyl)benzamide **22**.



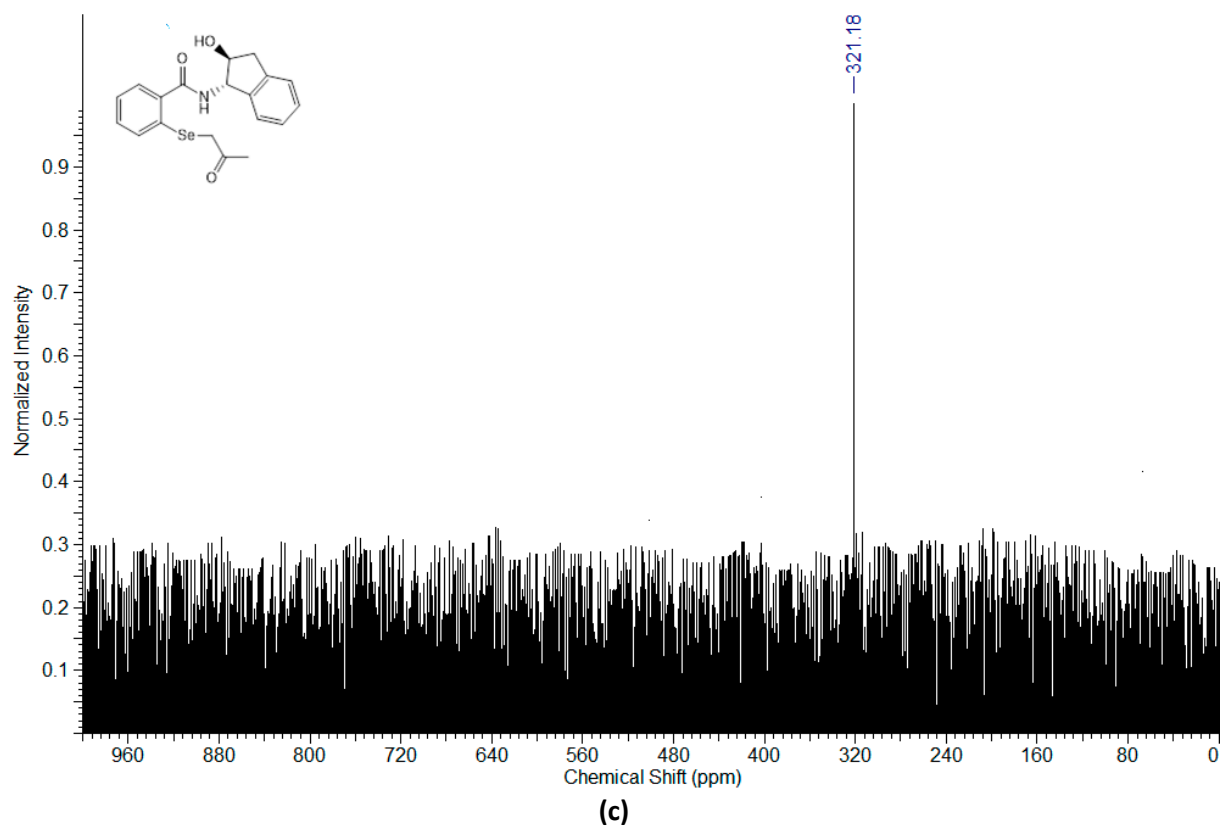
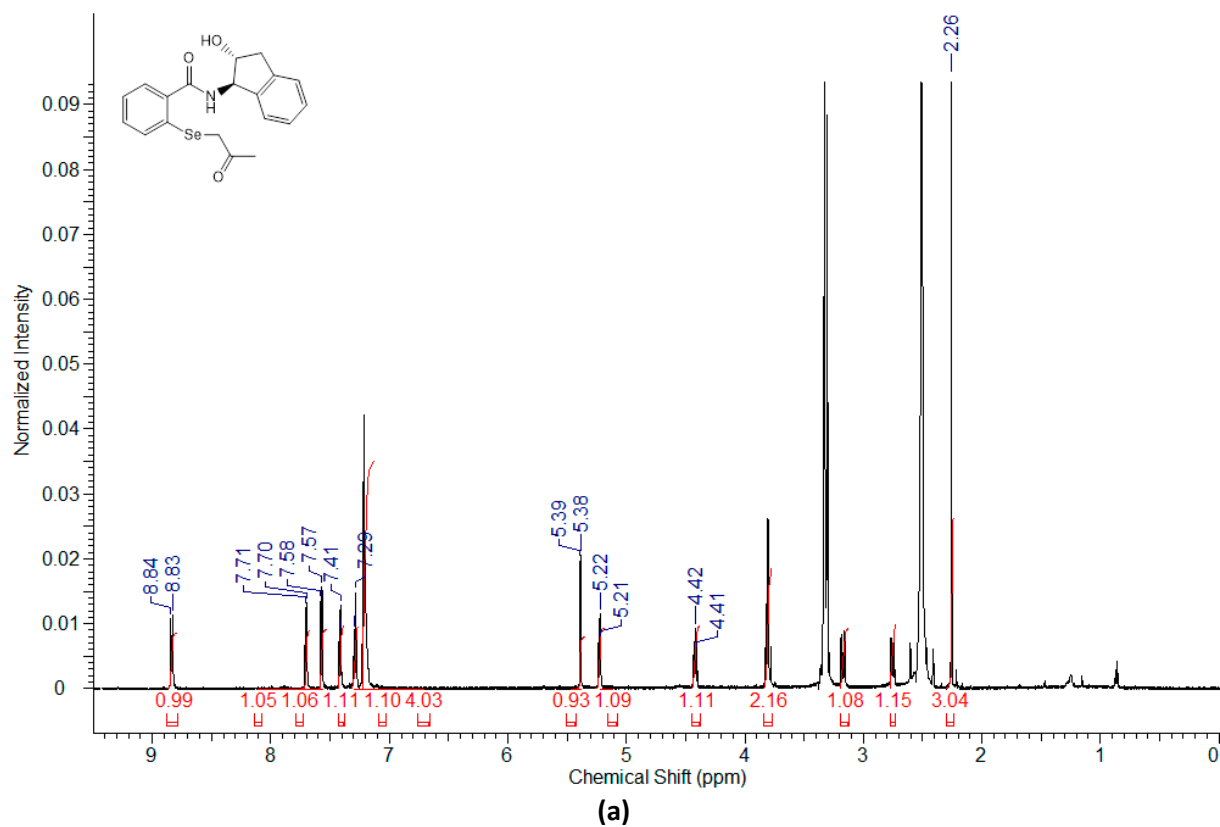
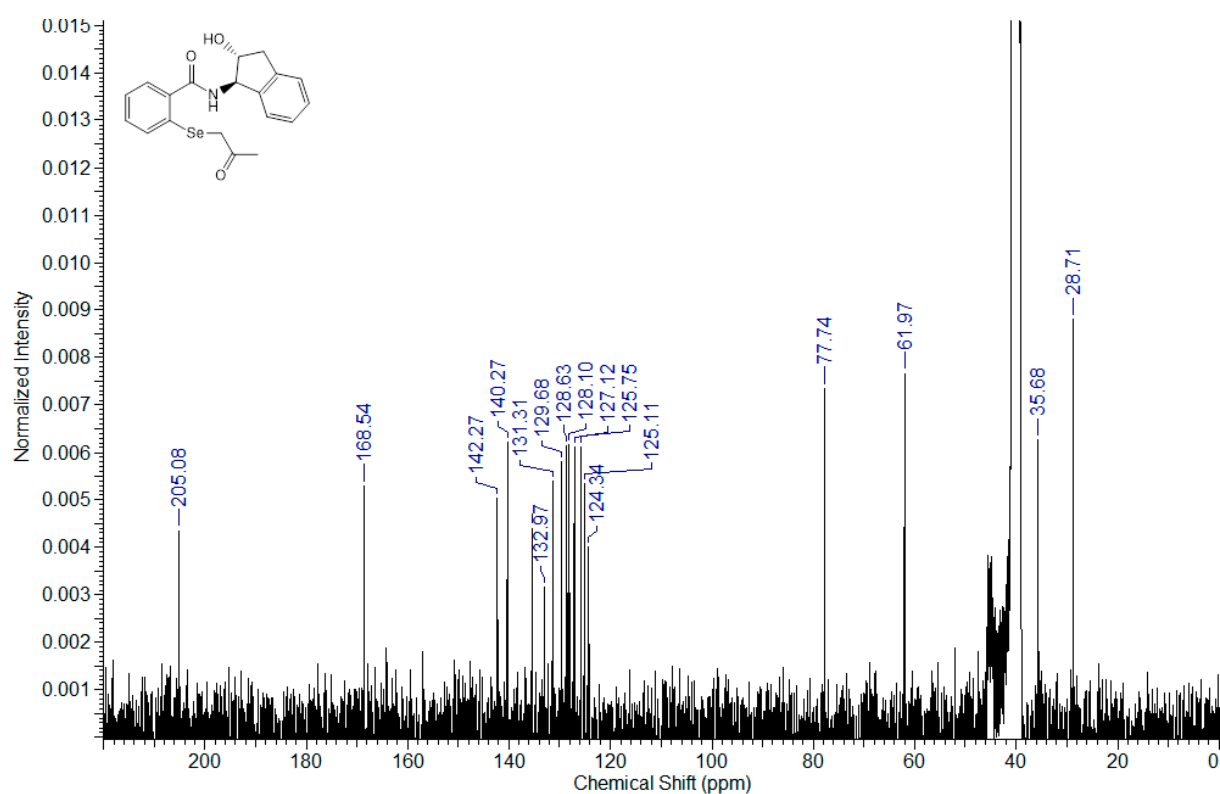
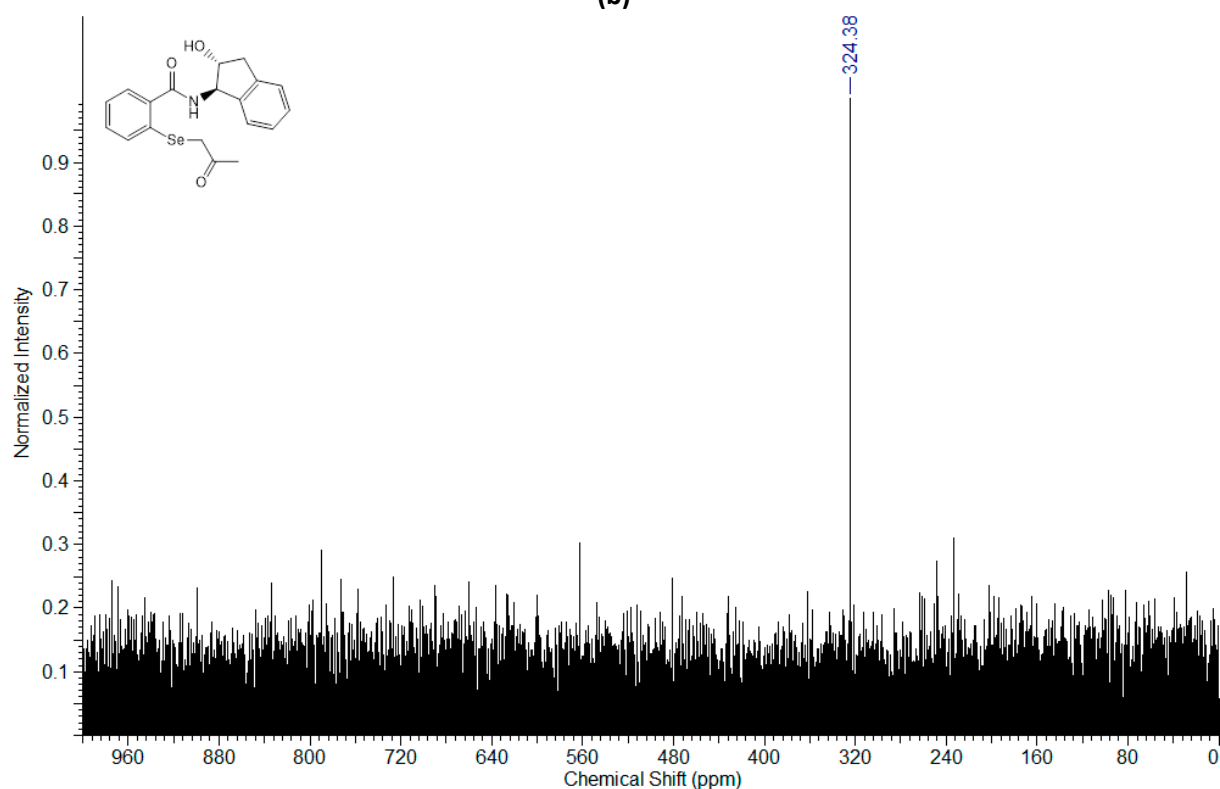


Figure S13. (a) ^1H NMR, (b) ^{13}C NMR, and (c) ^{77}Se NMR spectra of *N*-((1*S*,2*S*)-(+)-*trans*-2-hydroxy-1-indanyl)-2-((2-oxopropyl)selanyl)benzamide **23**.





(b)



(c)

Figure S14. (a) ^1H NMR, (b) ^{13}C NMR, and (c) ^{77}Se NMR spectra of *N*-((1*R*,2*R*)-(-)-*trans*-2-hydroxy-1-indanyl)-2-((2-oxopropyl)selanyl)benzamide **24**.

2. HPLC analyses of selenides 11-24

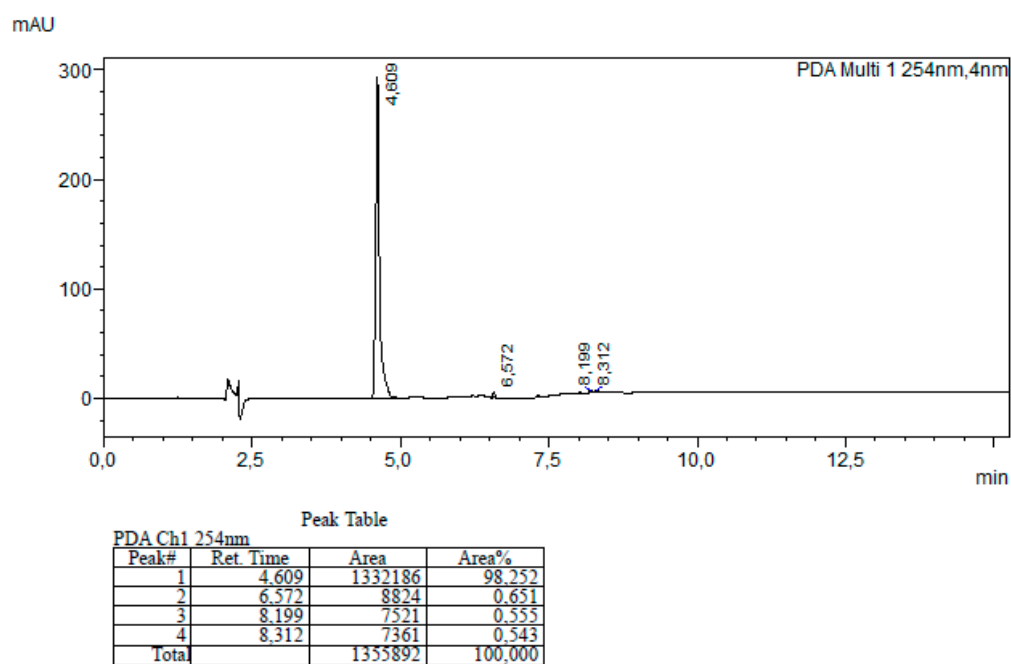


Figure S15. Chromatograph of *N*-((*S*)-(+)-*sec*-butyl)- 2-((2-oxopropyl)selanyl)benzamide **11**.

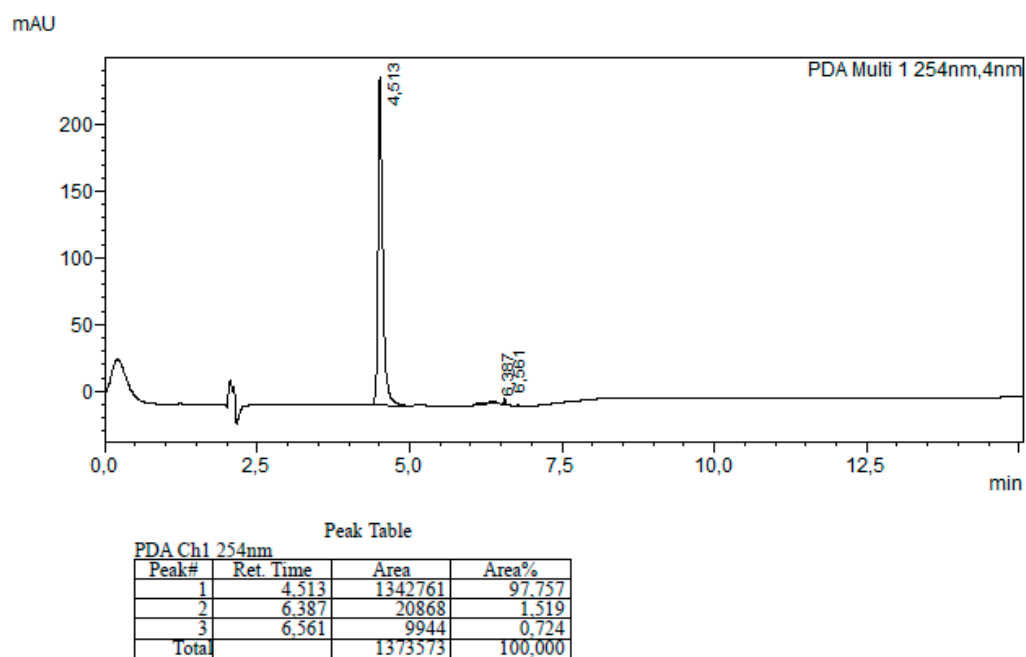


Figure S16. Chromatograph of *N*-((*R*)-(-)-*sec*-butyl)- 2-((2-oxopropyl)selanyl)benzamide **12**.

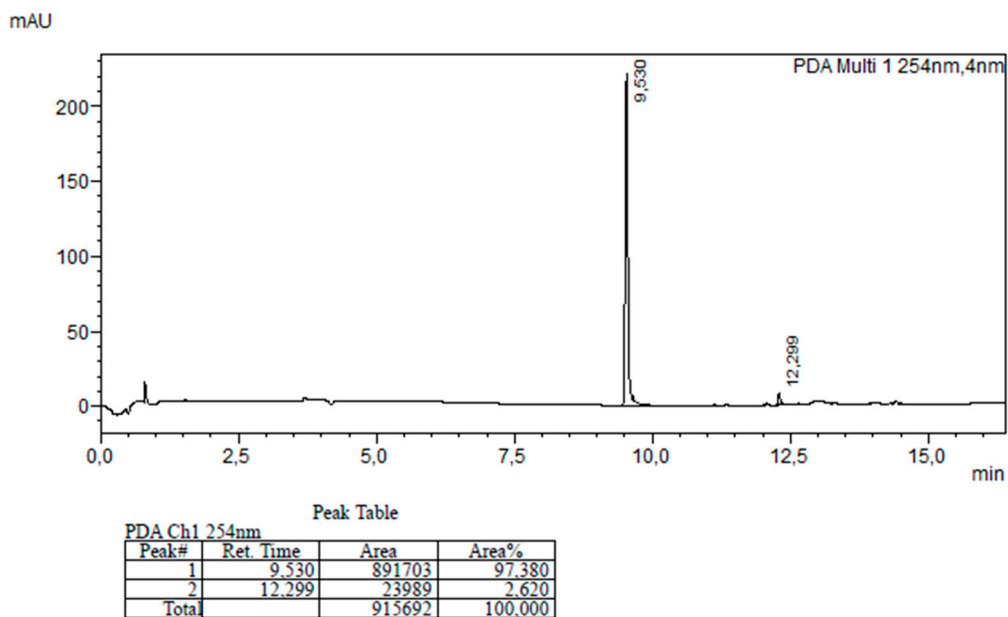


Figure S17. Chromatograph of *N*-((*S*)-(+)-1-hydroksy-2-butanyl)- 2-((2-oxopropyl)selanyl)benzamide
13.

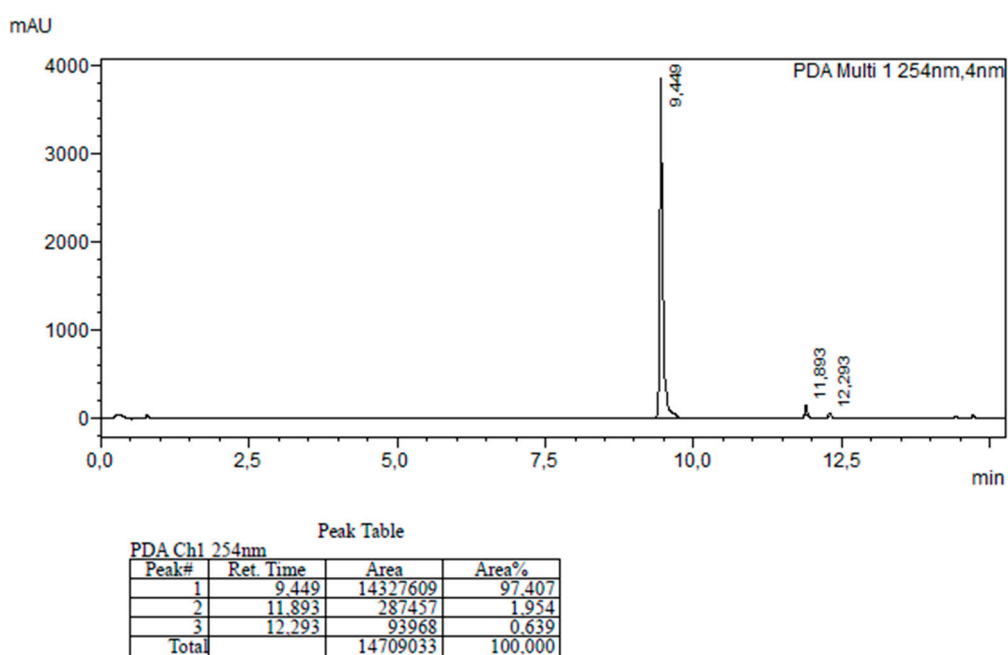
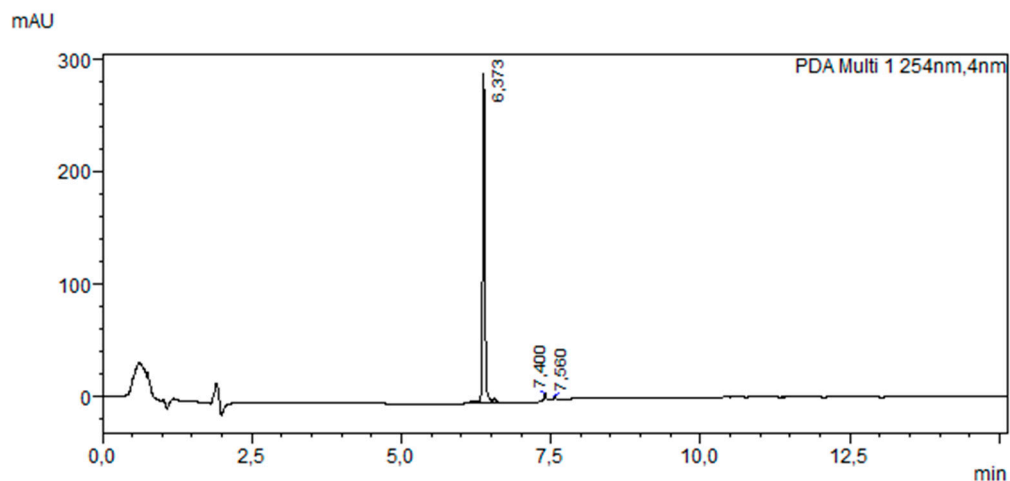


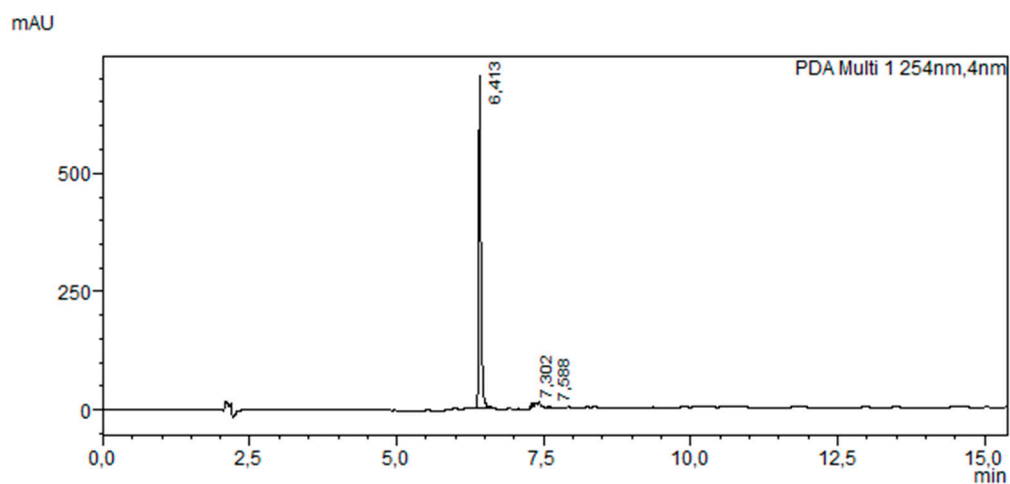
Figure S18. Chromatograph of *N*-((*R*)-(-)-1-hydroksy-2-butanyl)- 2-((2-oxopropyl)selanyl)benzamide
14.



Peak Table

Peak#	Ret. Time	Area	Area%
1	6.373	837632	98.578
2	7.400	9905	1.166
3	7.560	2180	0.257
Total		849717	100.000

Figure S19. Chromatograph of *N*-((*R*)-(-)-1,2,3,4-tetrahydro-1-naphthyl) 2-((2-oxopropyl)selanyl)benzamide **15**.



Peak Table

Peak#	Ret. Time	Area	Area%
1	6.413	1968918	98.553
2	7.302	15652	0.783
3	7.588	13263	0.664
Total		1997833	100.000

Figure S20. Chromatograph of *N*-((*S*)-(+)-1,2,3,4-tetrahydro-1-naphthyl) 2-((2-oxopropyl)selanyl)benzamide **16**.

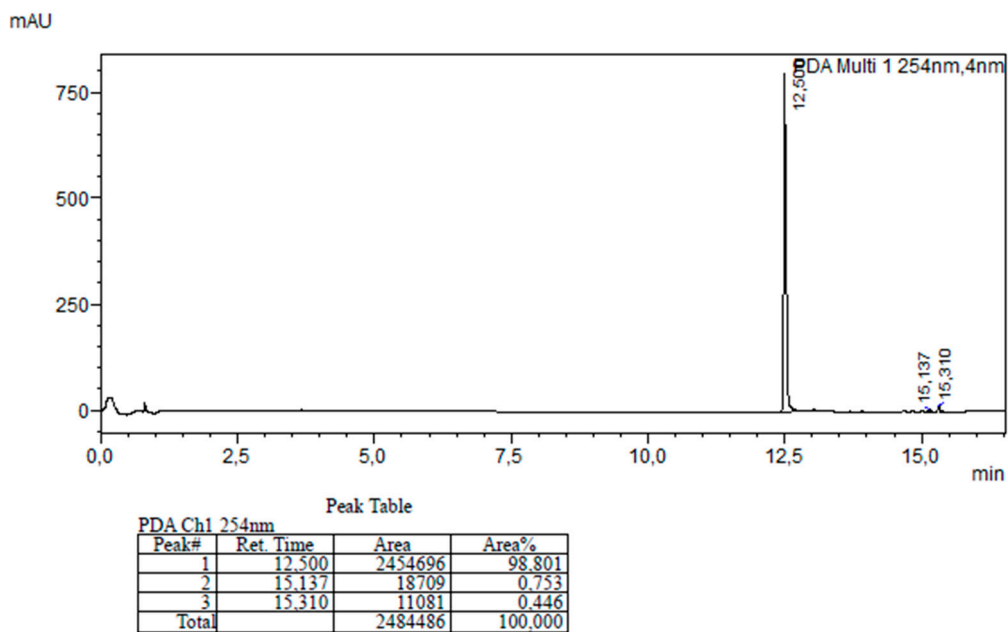


Figure S21. Chromatogram of *N*-((*R*)-(+)- α -methylbenzyl)-2-((2-oxopropyl)selanyl)benzamide **17**.

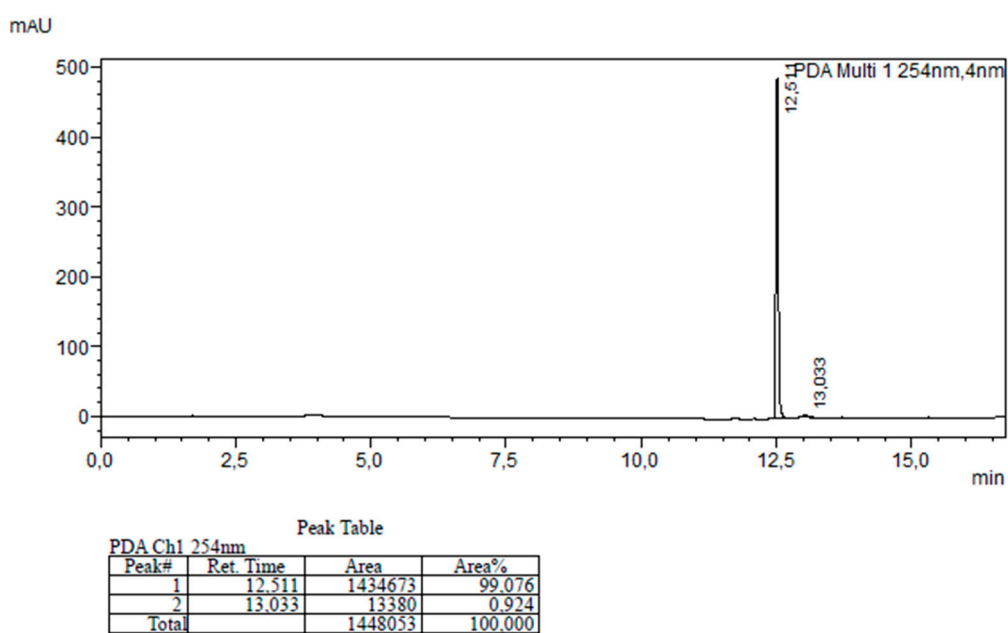


Figure S22. Chromatogram of *N*-((*S*)-(-)- α -methylbenzyl)-2-((2-oxopropyl)selanyl)benzamide **18**.

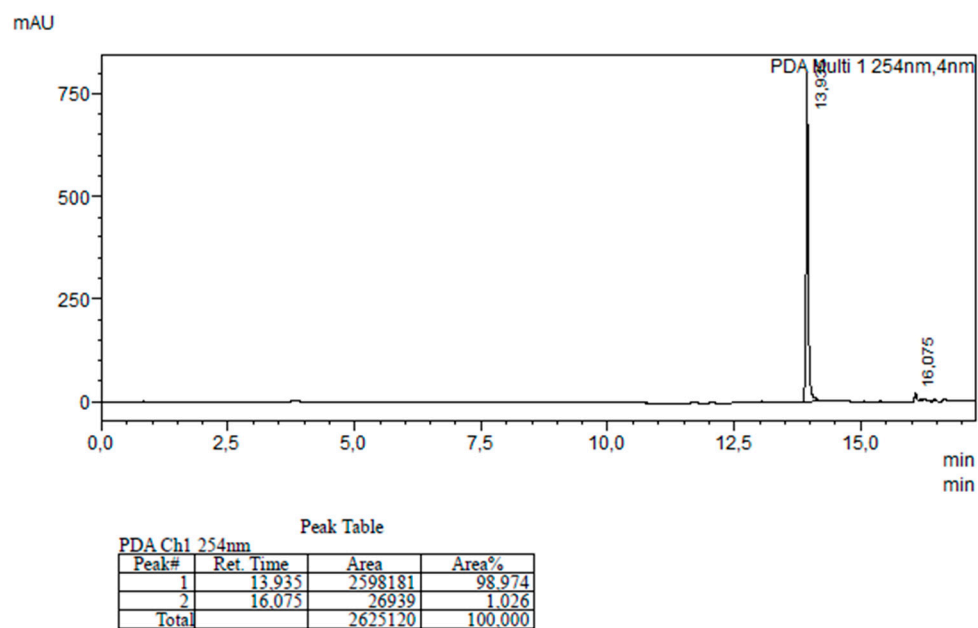


Figure S23. Chromatograph of *N*-((*S*)-(-)-1-(1-naphthyl)ethyl)- 2-((2-oxopropyl)selanyl)benzamide **19**.

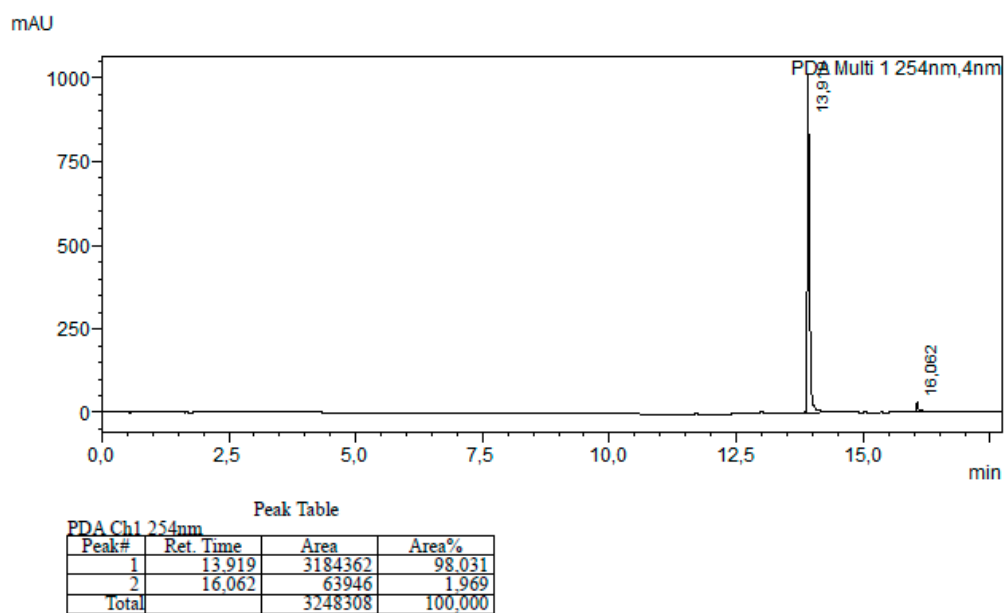
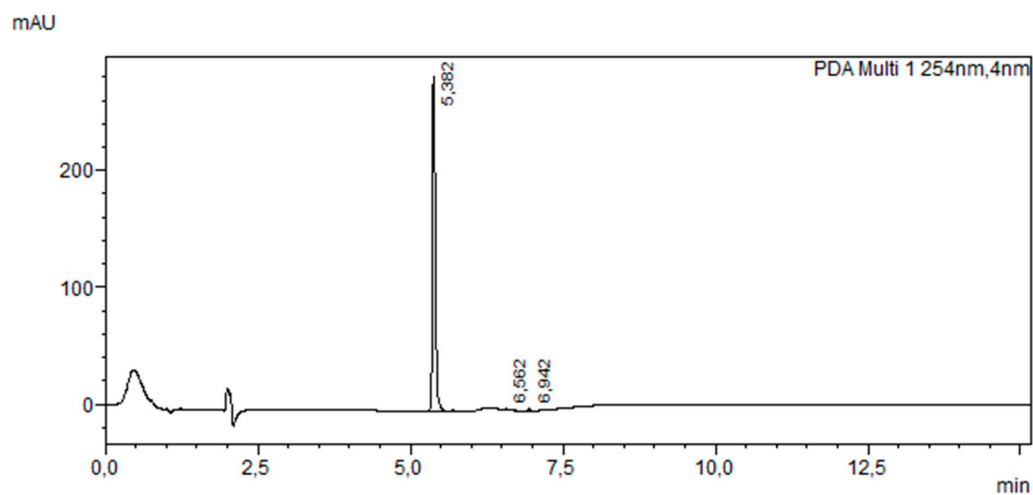


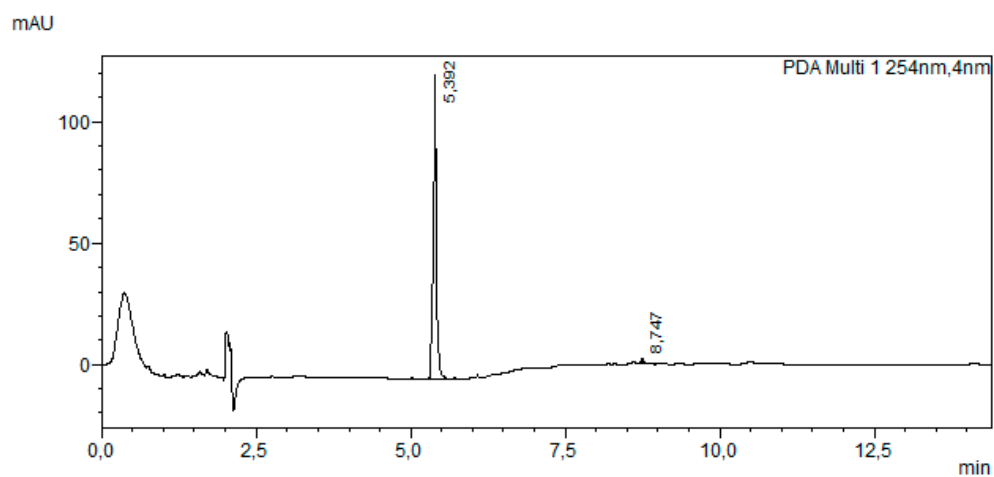
Figure S24. Chromatograph of *N*-((*S*)-(-)-1-(1-naphthyl)ethyl)- 2-((2-oxopropyl)selanyl)benzamide **20**.



Peak Table

Peak#	Ret. Time	Area	Area%
1	5.382	895176	99.004
2	6.562	2353	0.260
3	6.942	6653	0.736
Total		904183	100.000

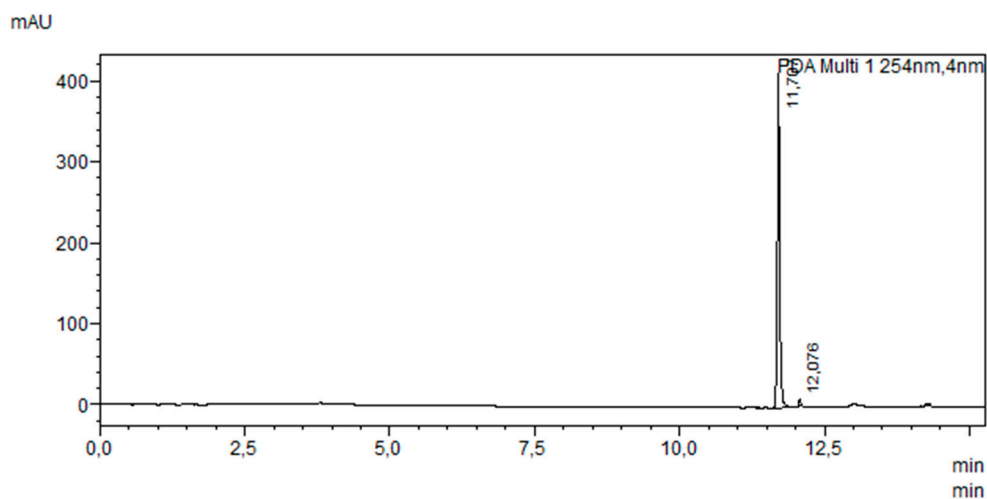
Figure S25. Chromatograph of *N*-((1*S*,2*R*)-(-)-*cis*-2-hydroxy-1-indanyl)-2-((2-oxopropyl)selanyl)benzamide **21**.



Peak Table

Peak#	Ret. Time	Area	Area%
1	5.392	454208	98.380
2	8.747	7481	1.620
Total		461689	100.000

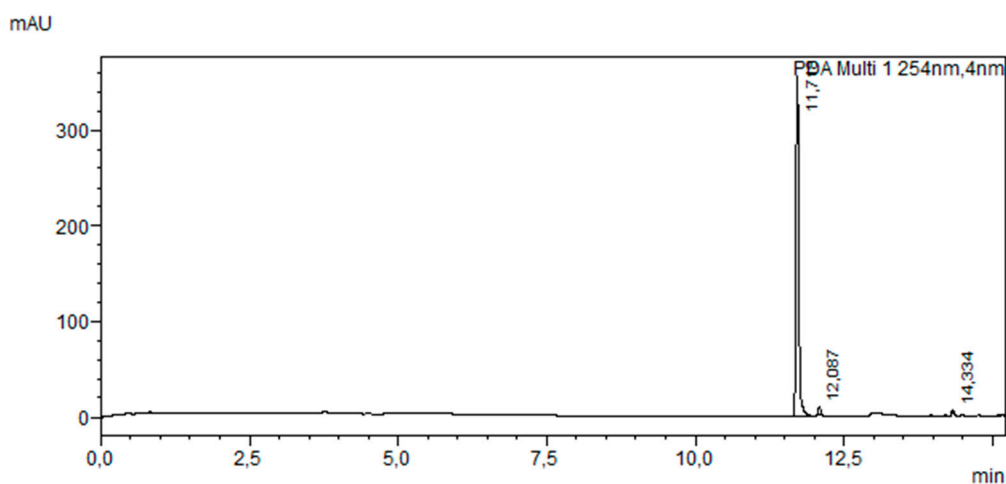
Figure S26. Chromatograph of *N*-((1*S*,2*R*)-(-)-*cis*-2-hydroxy-1-indanyl)-2-((2-oxopropyl)selanyl)benzamide **22**.



Peak Table

Peak#	Ret. Time	Area	Area%
1	11.707	1234832	98.252
2	12.076	21963	1.748
Total		1256796	100.000

Figure S27. Chromatograph of *N*-((1*S*,2*S*)-(+)-*trans*-2-hydroksy-1-indanyl)-2-((2-oxopropyl)selanyl)benzamide **23**.



Peak Table

Peak#	Ret. Time	Area	Area%
1	11.718	1105112	97.421
2	12.087	20992	1.851
3	14.334	8268	0.729
Total		1134373	100.000

Figure S28. Chromatograph of *N*-((1*R*,2*R*)-(-)-*trans*-2-hydroksy-1-indanyl)-2-((2-oxopropyl)selanyl)benzamide **24**.

3. Antioxidant activity measurement

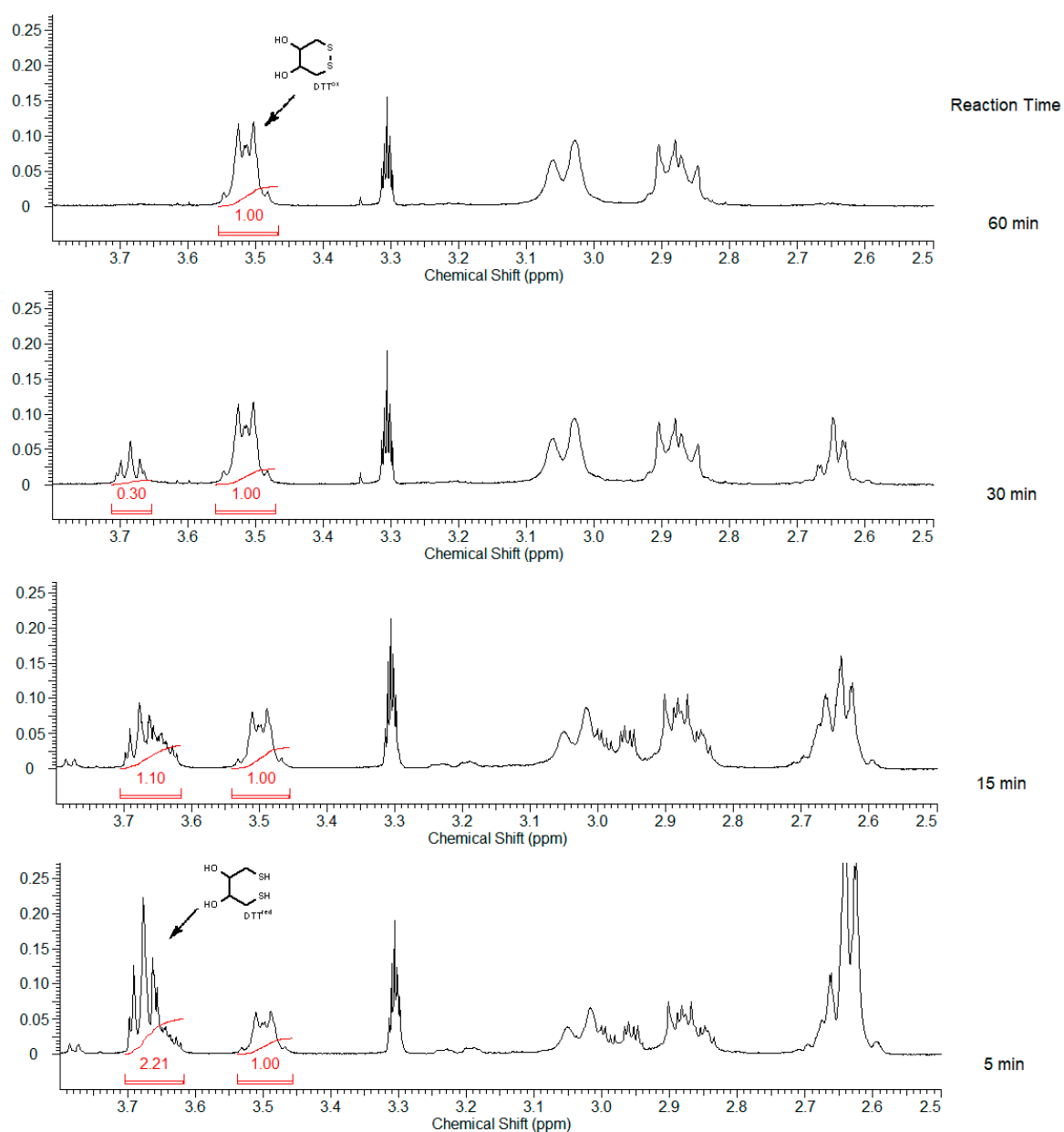


Figure S29. Example of ¹H NMR spectra for antioxidant Iwaoka test after reaction time 5 min, 15 min, 30 min, 60 min for compound 23.

Compound	5 min			15 min		
	Integration DTT ^{red}	Integration DTT ^{ox}	Remaining DTT ^{red} [%]	Integration DTT ^{red}	Integration DTT ^{ox}	Remaining DTT ^{red} [%]
11/12	5,301	1	84,13	1,945	1	66,04
11/12	2,751	1	73,34	1,293	1	56,39
13/14	3,843	1	79,35	2,06	1	67,32
13/14	1,827	1	64,63	1,231	1	55,18
15/16	5,999	1	85,71	3,536	1	77,95
15/16	5,886	1	85,48	3,618	1	78,35
17/18	12,895	1	92,80	8,566	1	89,55

17/18	7,569	1	88,33	9,945	1	90,86
19/20	13,786	1	93,24	8,491	1	89,46
19/20	13,322	1	93,02	9,703	1	90,66
21/22	3,136	1	75,82	1,077	1	51,85
21/22	2,205	1	68,80	1,096	1	52,29
21/22	2,684	1	72,86	1,105	1	52,49
23/24	3,844	1	79,36	1,052	1	51,27
23/24	3,721	1	78,82	1,622	1	61,86

Figure S30. Results of antioxidant activity measurement of integration from ^1H NMR spectra after reaction time 5 min and 15 min for all samples and compound 11-24.

Compound	5 min			15 min		
	Integration DTT ^{red}	Integration DTT ^{ox}	Remaining DTT ^{red} [%]	Integration DTT ^{red}	Integral DTT ^{ox}	Remaining DTT ^{red} [%]
11/12	0,705	1	41,35	0,197	1	16,46
11/12	0,886	1	46,98	0,1	1	9,09
13/14	1,104	1	52,47	0,307	1	23,49
13/14	0,823	1	45,15	0,25	1	20,00
15/16	2,273	1	69,45	1,267	1	55,89
15/16	2,245	1	69,18	1,322	1	56,93
17/18	4,373	1	81,39	2,733	1	73,21
17/18	5,331	1	84,20	2,869	1	74,15
19/20	4,904	1	83,06	2,422	1	70,78
19/20	5,509	1	84,64	2,468	1	71,16
21/22	0,451	1	31,08	0,134	1	11,82
21/22	0,301	1	23,14	0	1	0,00
21/22	0,375	1	27,27	0,079	1	7,32
23/24	0,368	1	26,90	0,09	1	8,26
23/24	0,502	1	33,42	0,15	1	13,04

Figure S31. Results of antioxidant activity measurement of integration from ^1H NMR spectra after reaction time 30 min and 60 min for all samples and compound 11-24.

4. DPPH test calibration curves

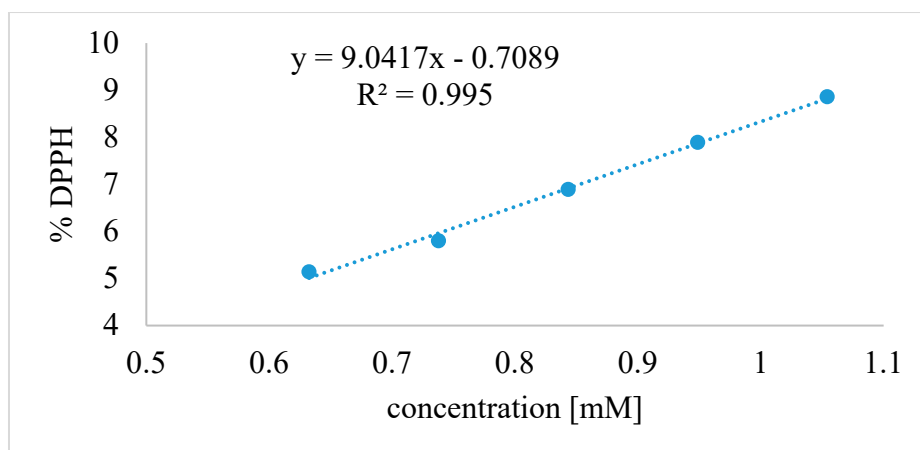


Figure S32. Compound 11/12—calibration curve.

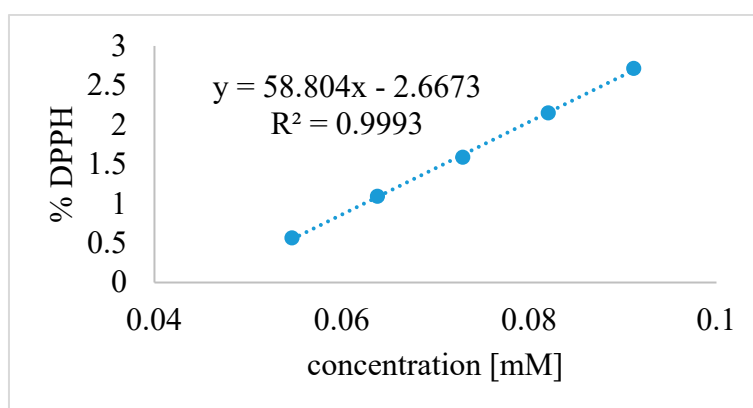


Figure S33. Compound 13/14—calibration curve.

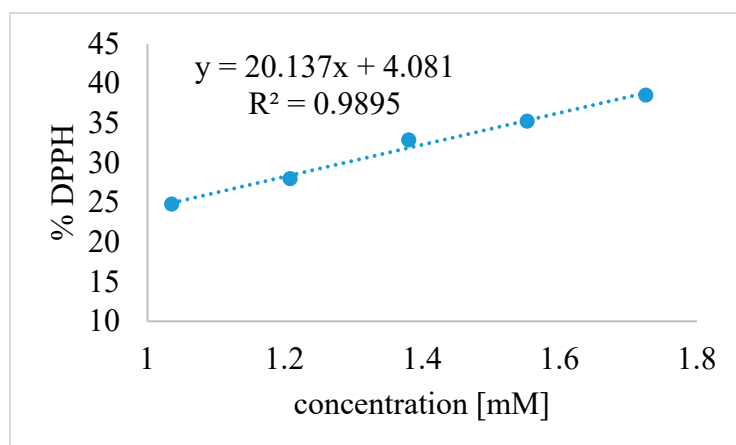


Figure S34. Compound 15/16—calibration curve.

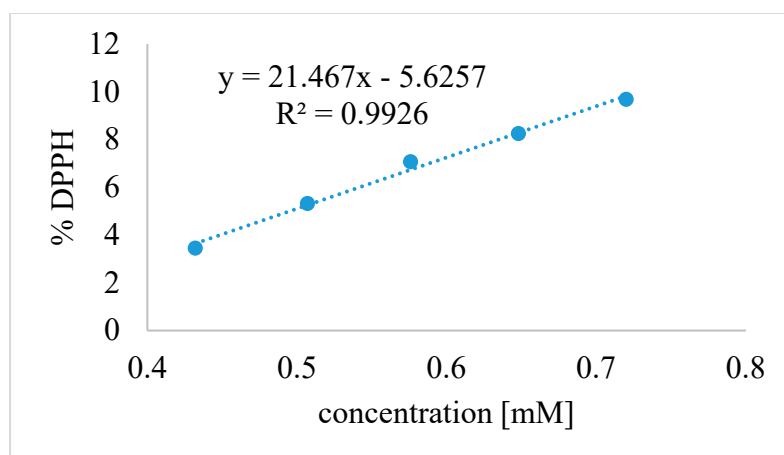


Figure S35. Compound 17/18—calibration curve.

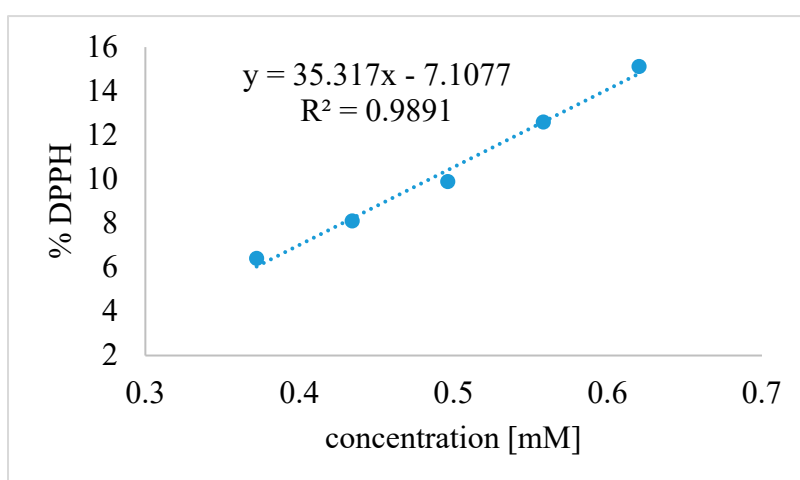


Figure S36. Compound 19/20—calibration curve.

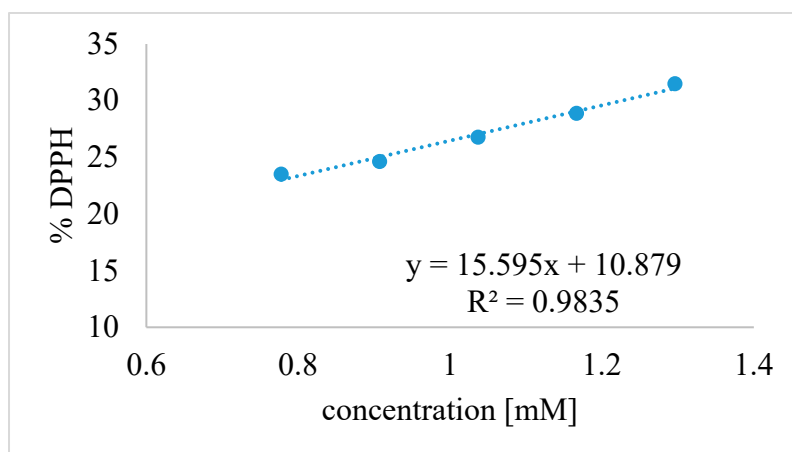


Figure S37. Compound 21/22—calibration curve.

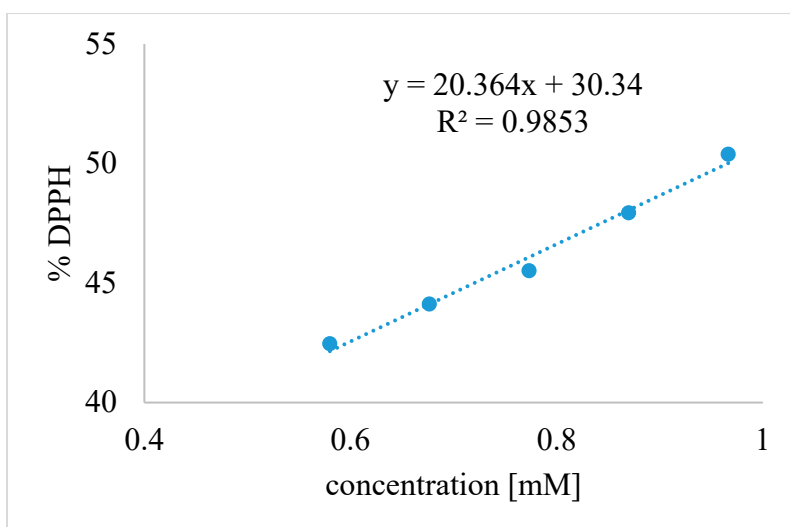
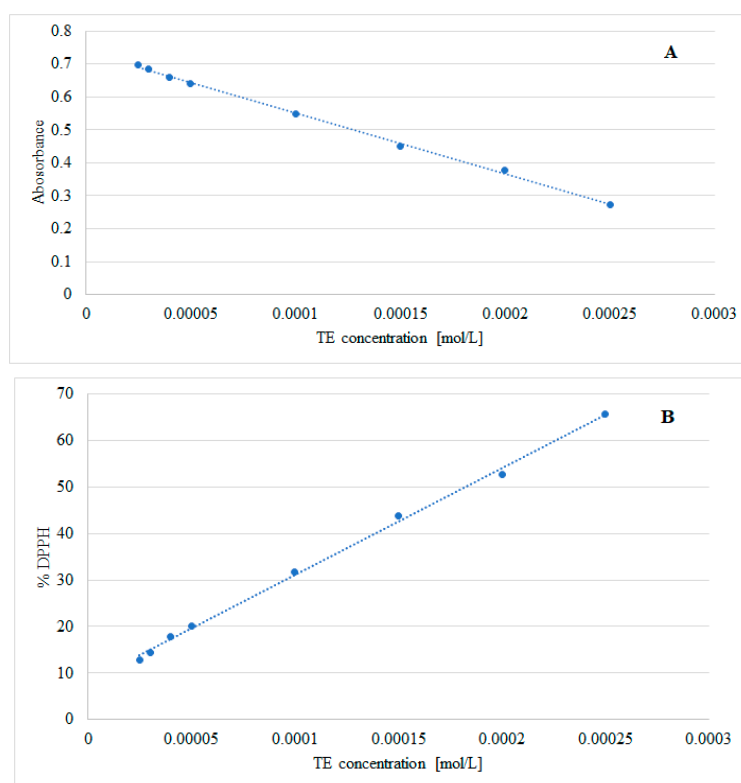


Figure S38. Compound 23/24—calibration curve.



Concentration range	$0.025 \cdot 10^{-3} - 0.25 \cdot 10^{-3} \text{ M}$
slope	304119
intercept	0.7493
R^2	0.998

Figure S39. Standard curves for the relationship: absorbance = function (concentration TE) (A), % DPPH = function (concentration of TE) (B).