

Article

# Attachment of Chiral Functional Groups to Modify the Activity of New GPx Mimetics

## Supplemental Information

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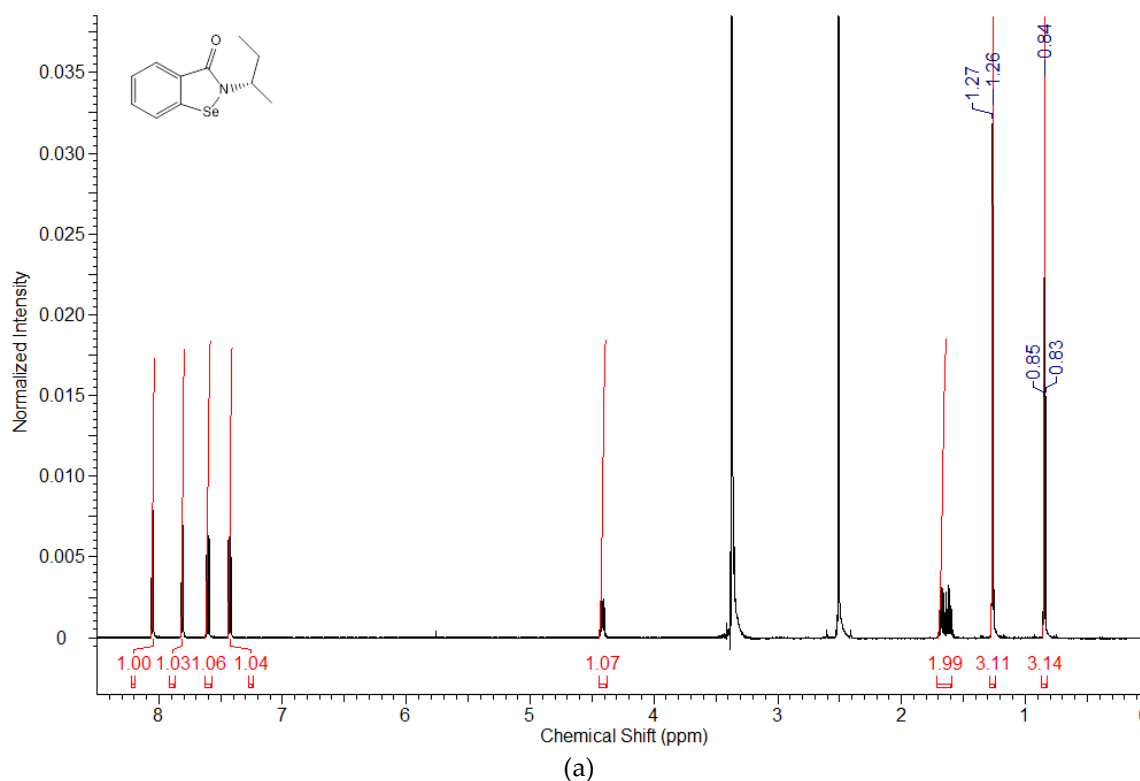
<sup>3</sup> Department of Crystallochemistry and Biocrystallography, Faculty of Chemistry, Nicolaus Copernicus University in Toruń, 7 Gagarin Street, 87-100 Toruń, Poland; awojt@umk.pl

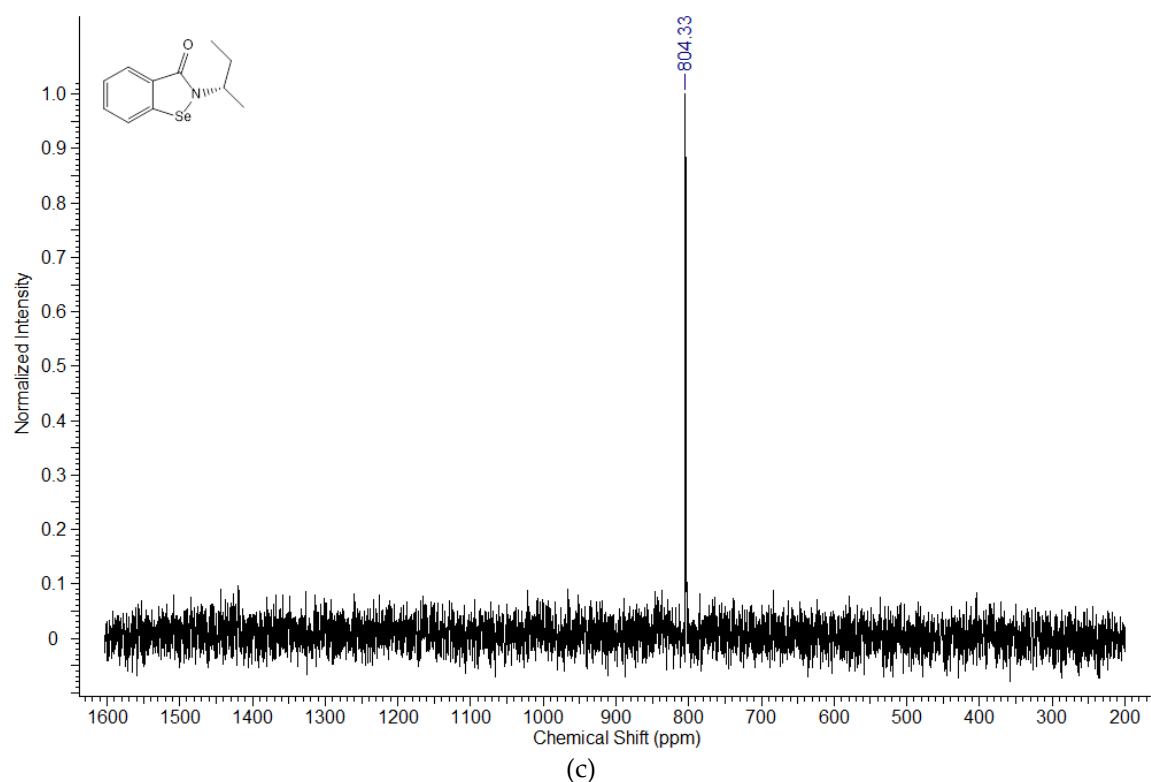
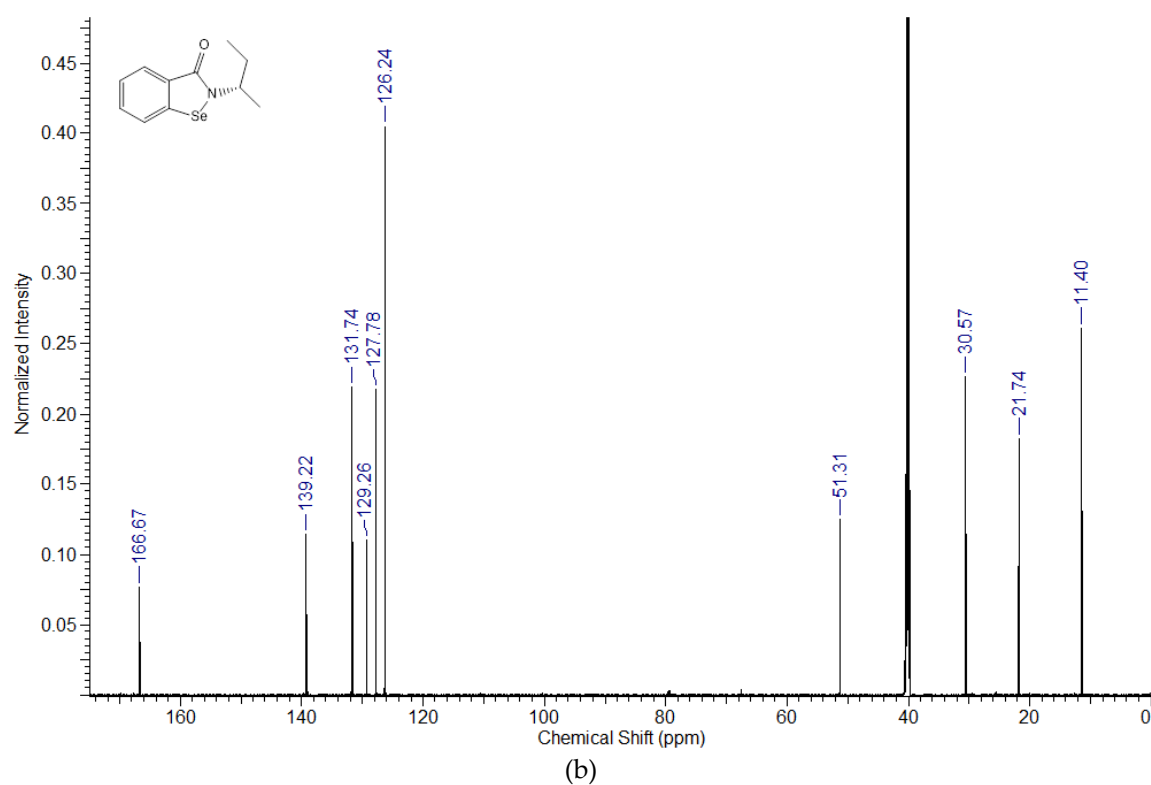
\* Correspondence: jsch@umk.pl

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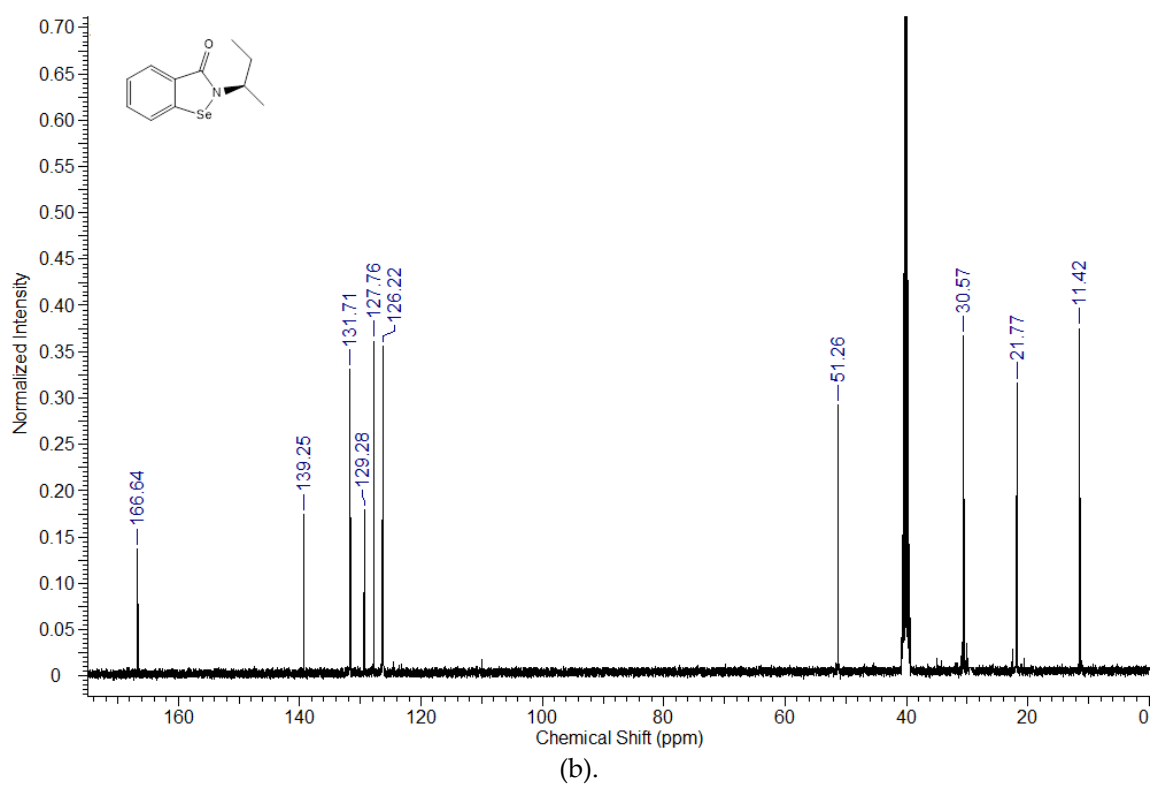
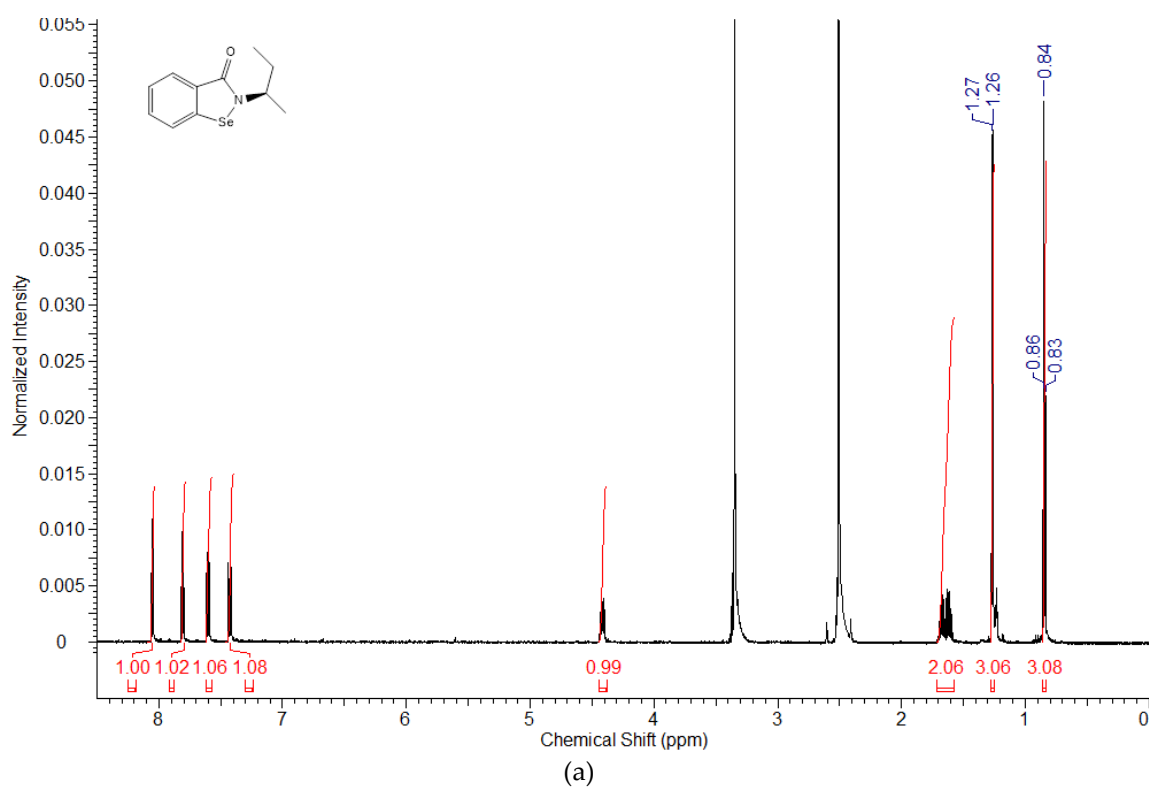
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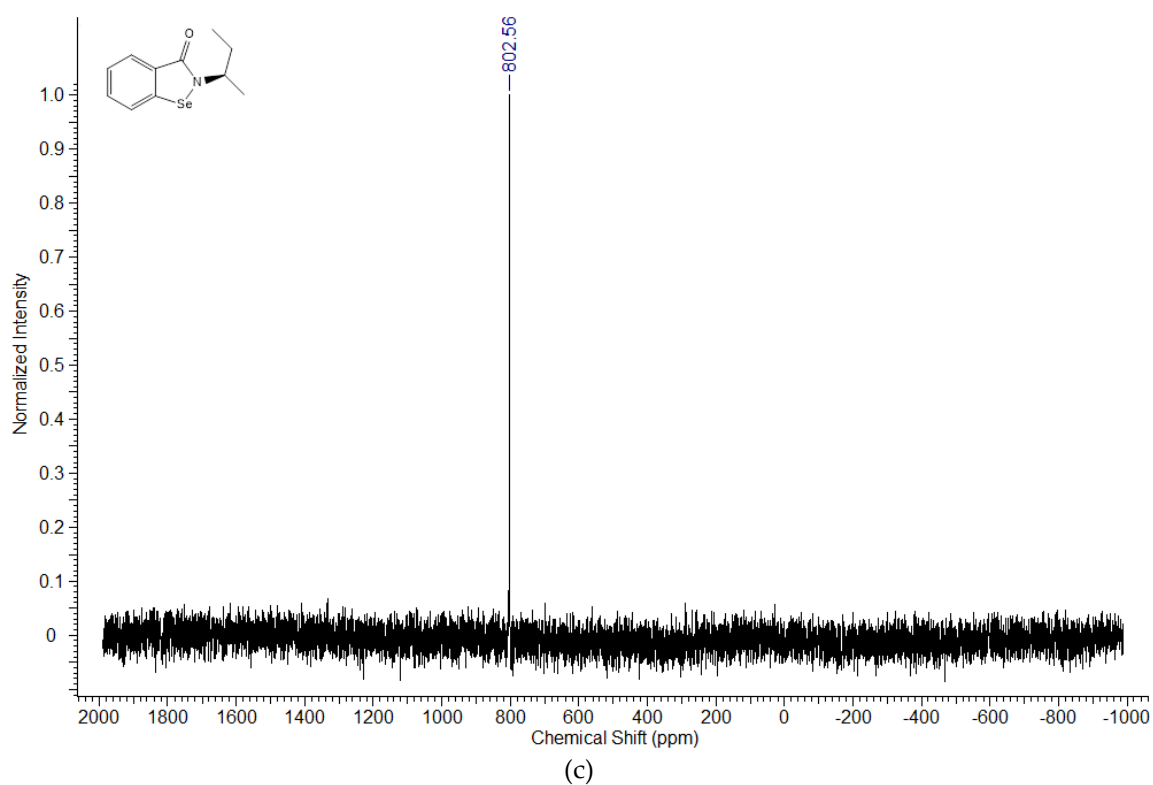
### 1. NMR spectra of benzoselenazol-3(2H)-ones 18a-31a



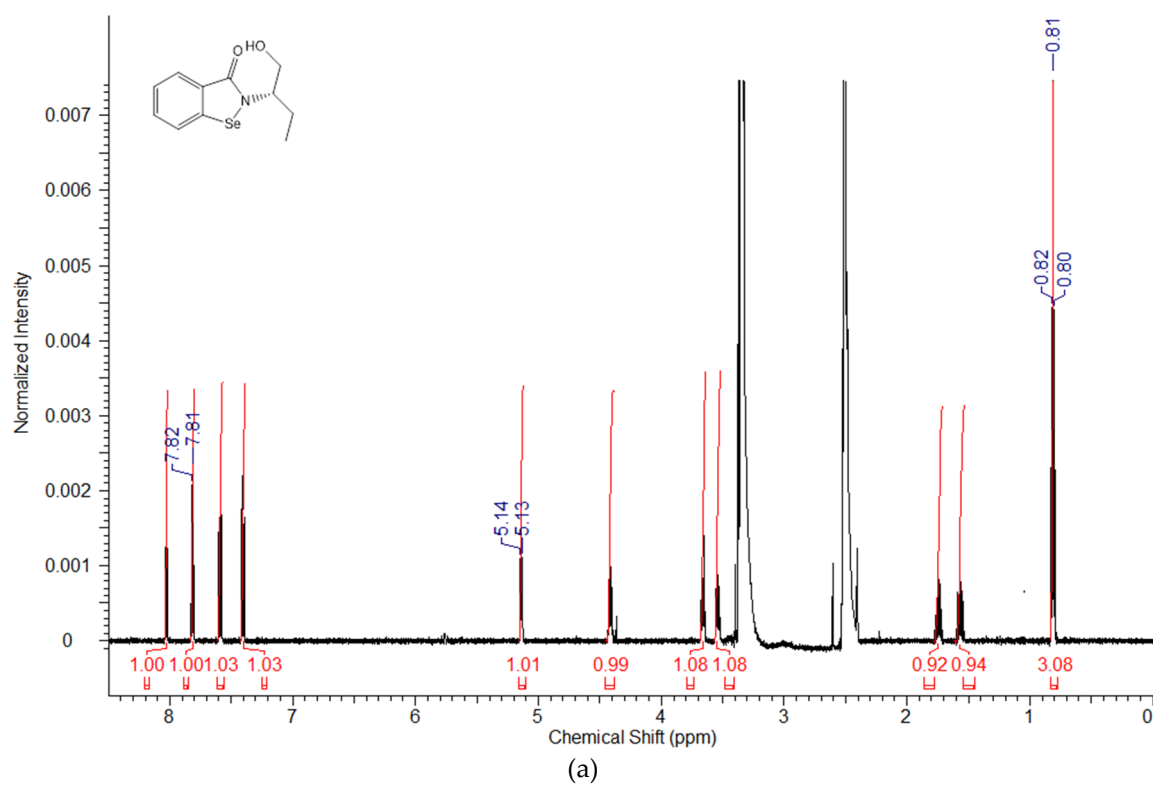


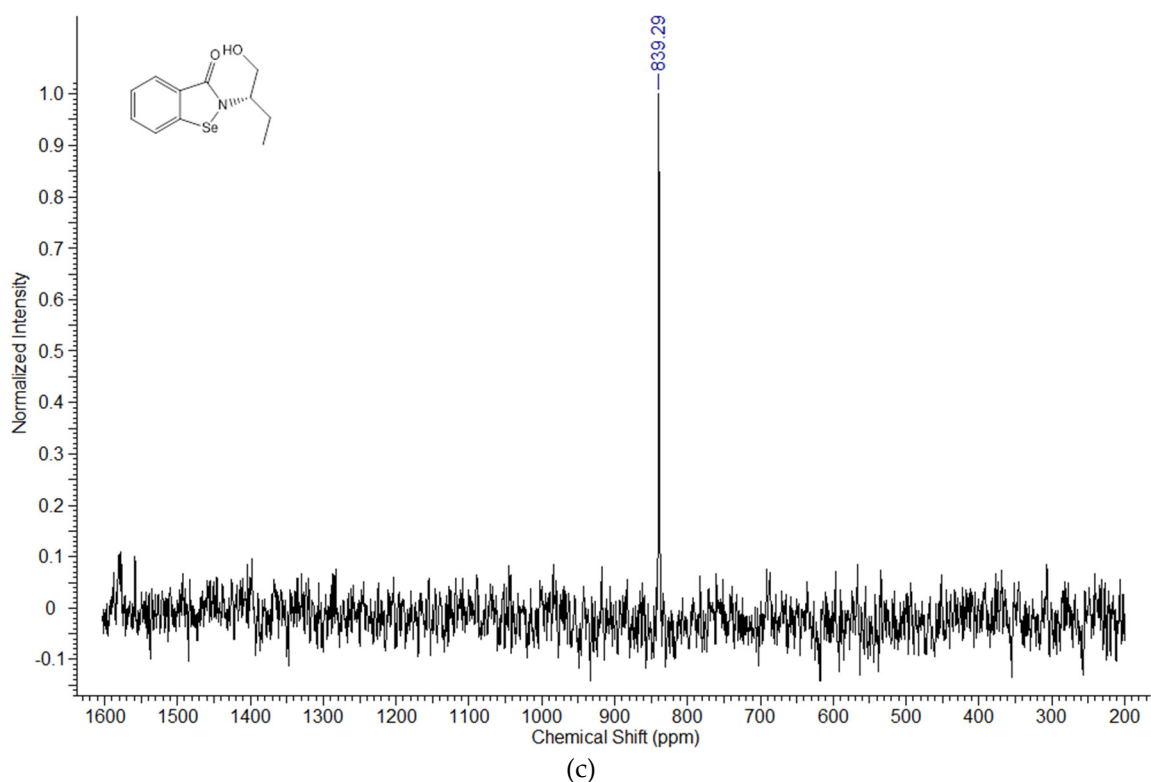
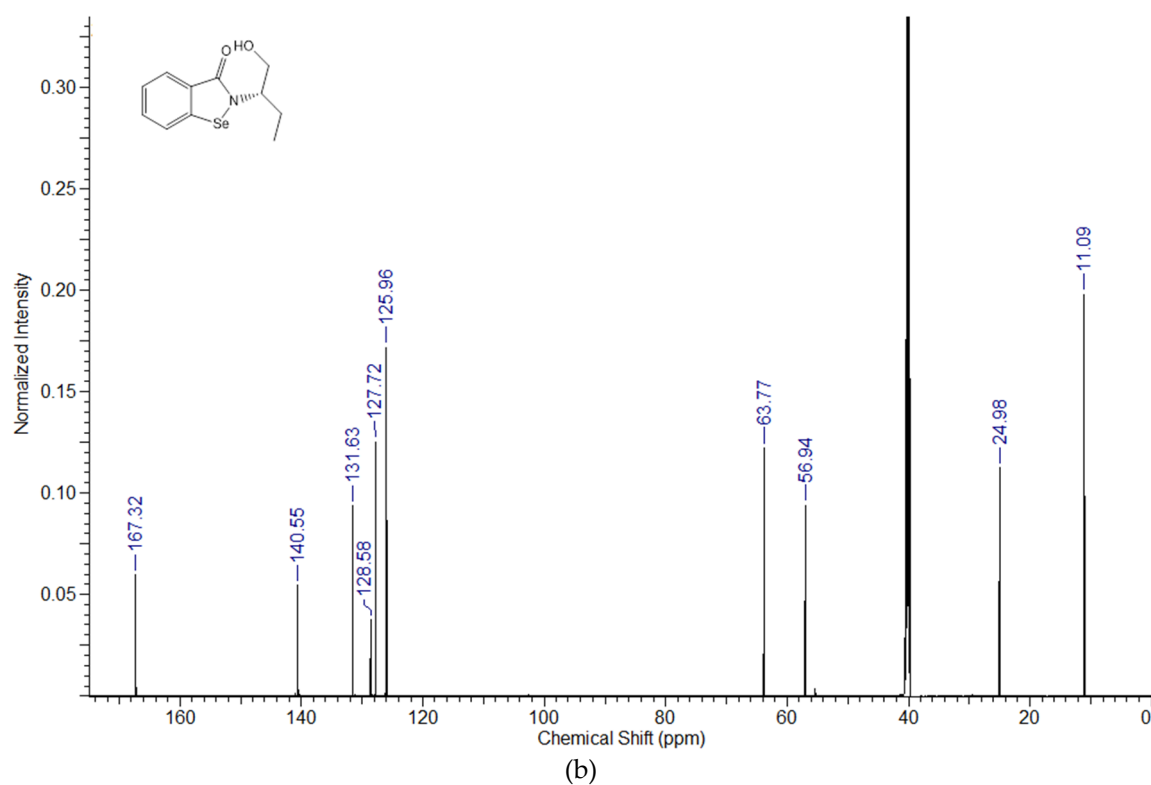
**Figure S1.** (a)  $^1\text{H}$  NMR, (b)  $^{13}\text{C}$  NMR, and (c)  $^{77}\text{Se}$  NMR spectra of *N*-[(*S*)(+)-*sec*-butyl]-1,2-benziselenazol-3(2*H*)-one **18a**.



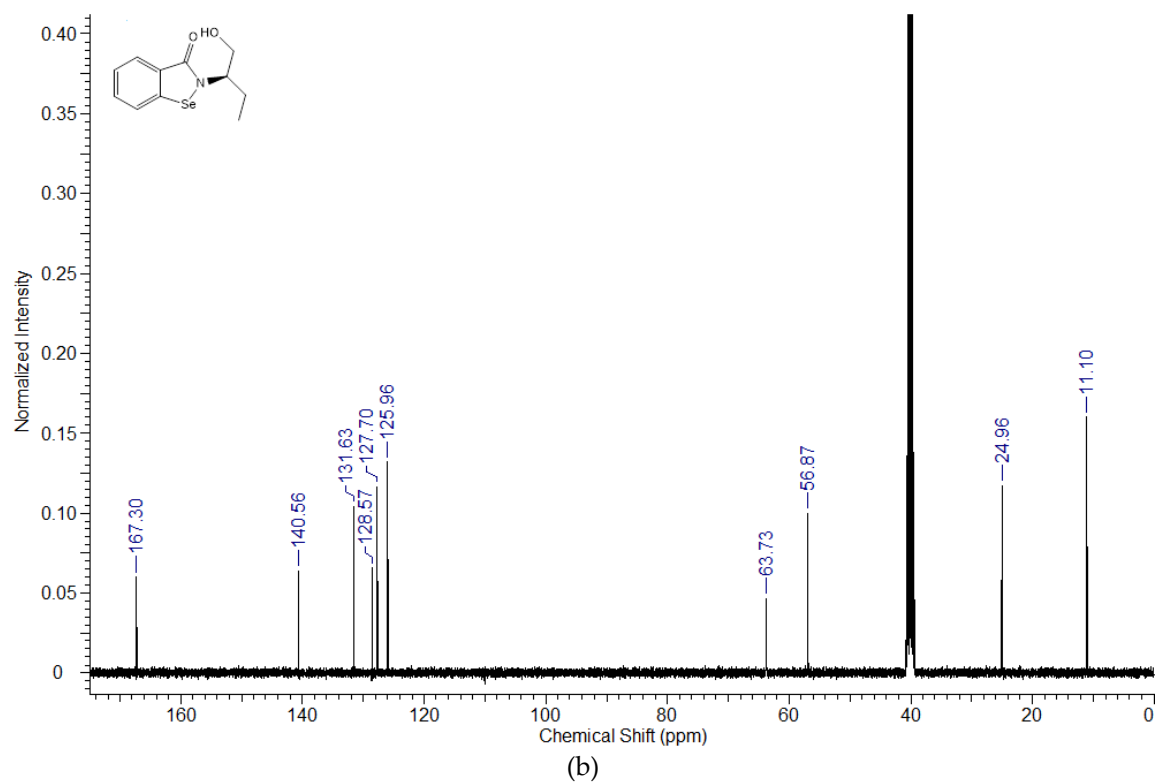
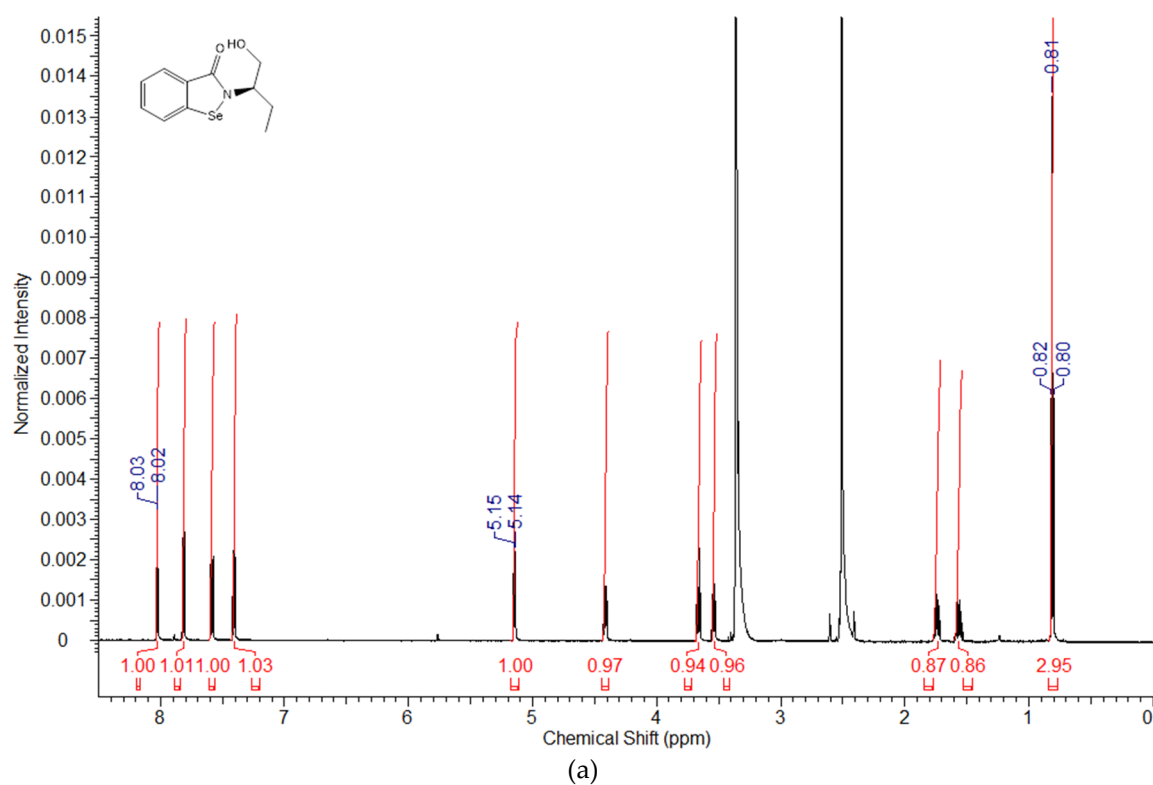


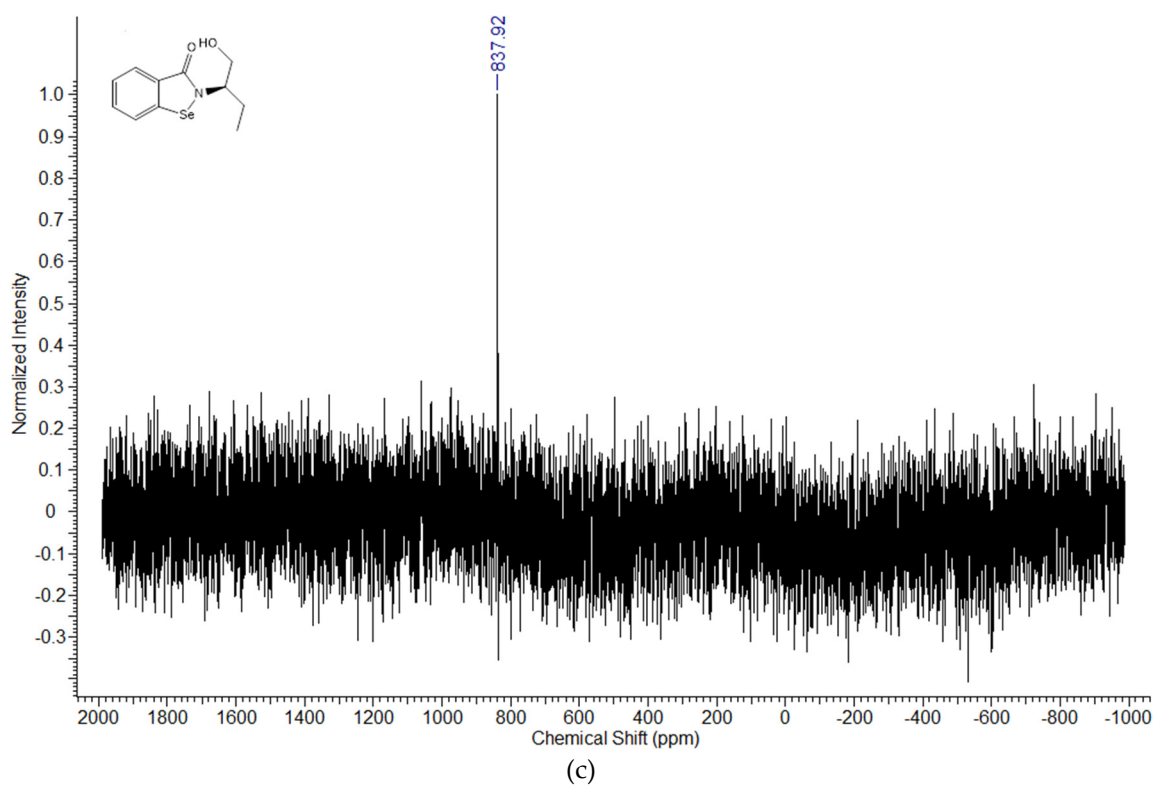
**Figure S2.** (a)  $^1\text{H}$  NMR, (b)  $^{13}\text{C}$  NMR, and (c)  $^{77}\text{Se}$  NMR spectra of *N*-[(*R*)-(-)-*sec*-butyl]-1,2-benziselenazol-3(2*H*)-one **19a**.



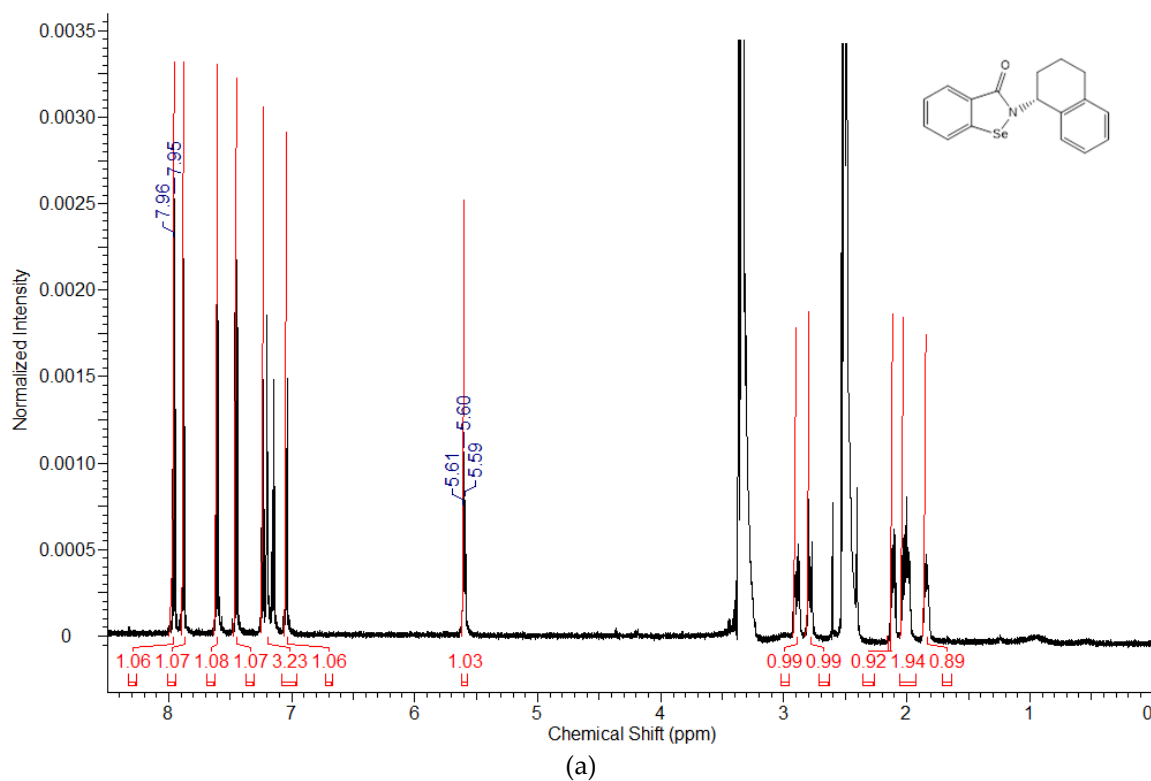


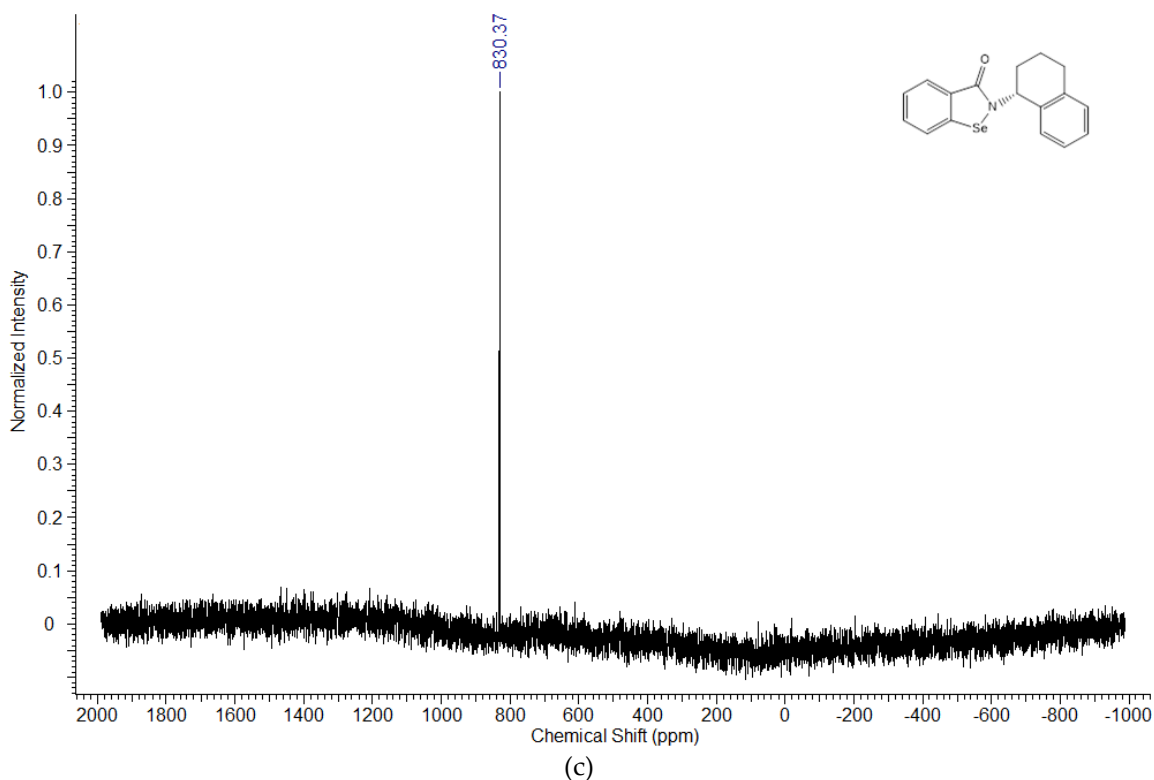
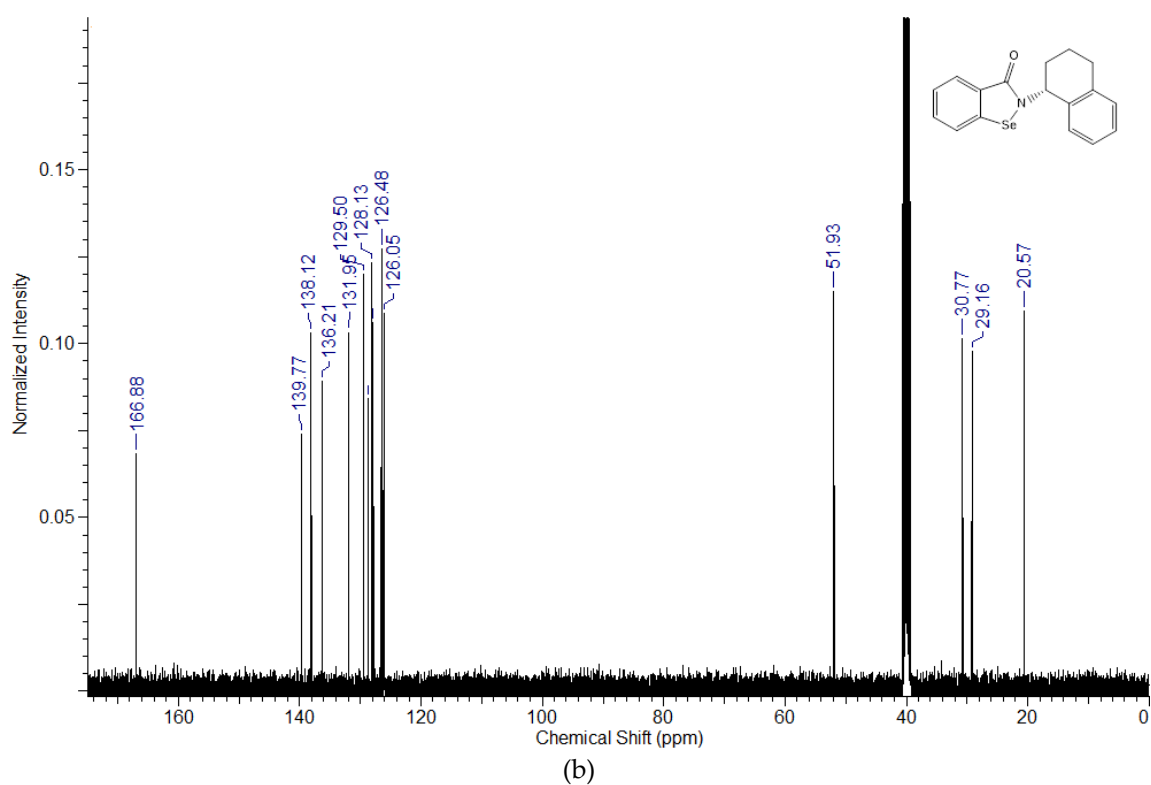
**Figure S3.** (a) <sup>1</sup>H NMR, (b) <sup>13</sup>C NMR, and (c) <sup>77</sup>Se NMR spectra of *N*-[(*S*)-(+)-1-hydroxy-2-butanyl]-1,2-benzisoselenazol-3(2*H*)-one **20a**.





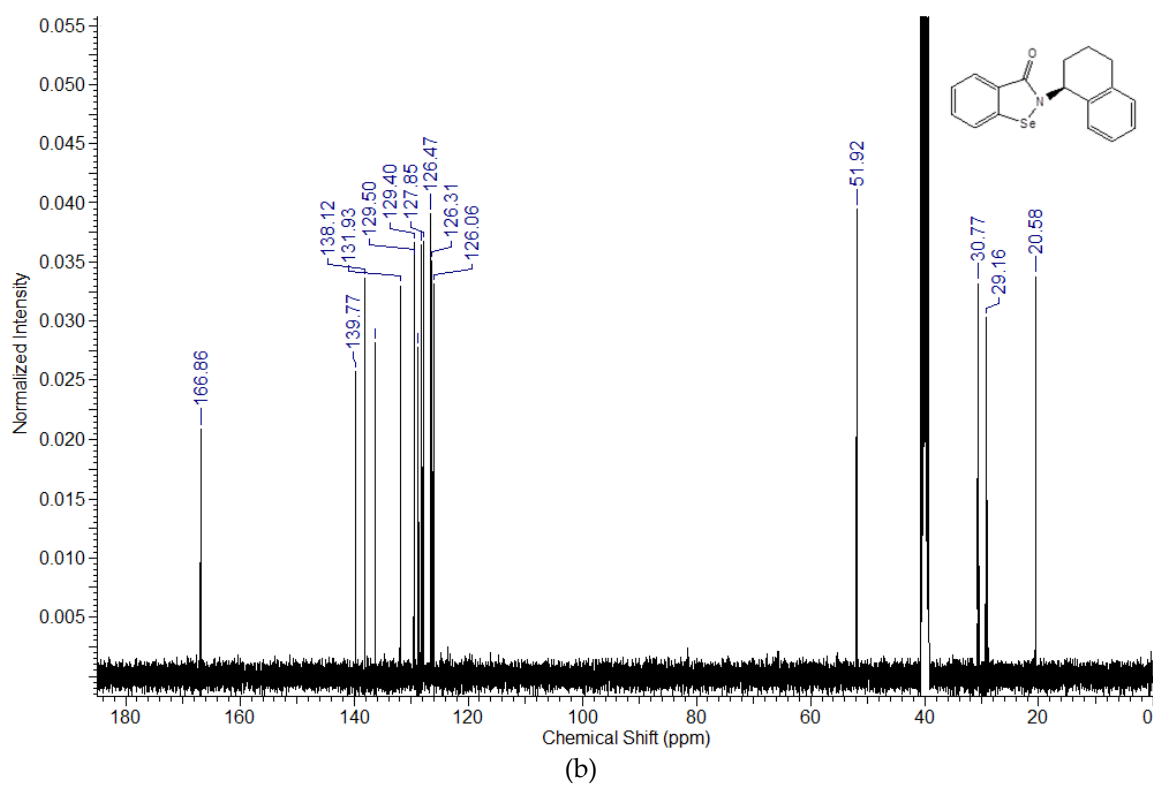
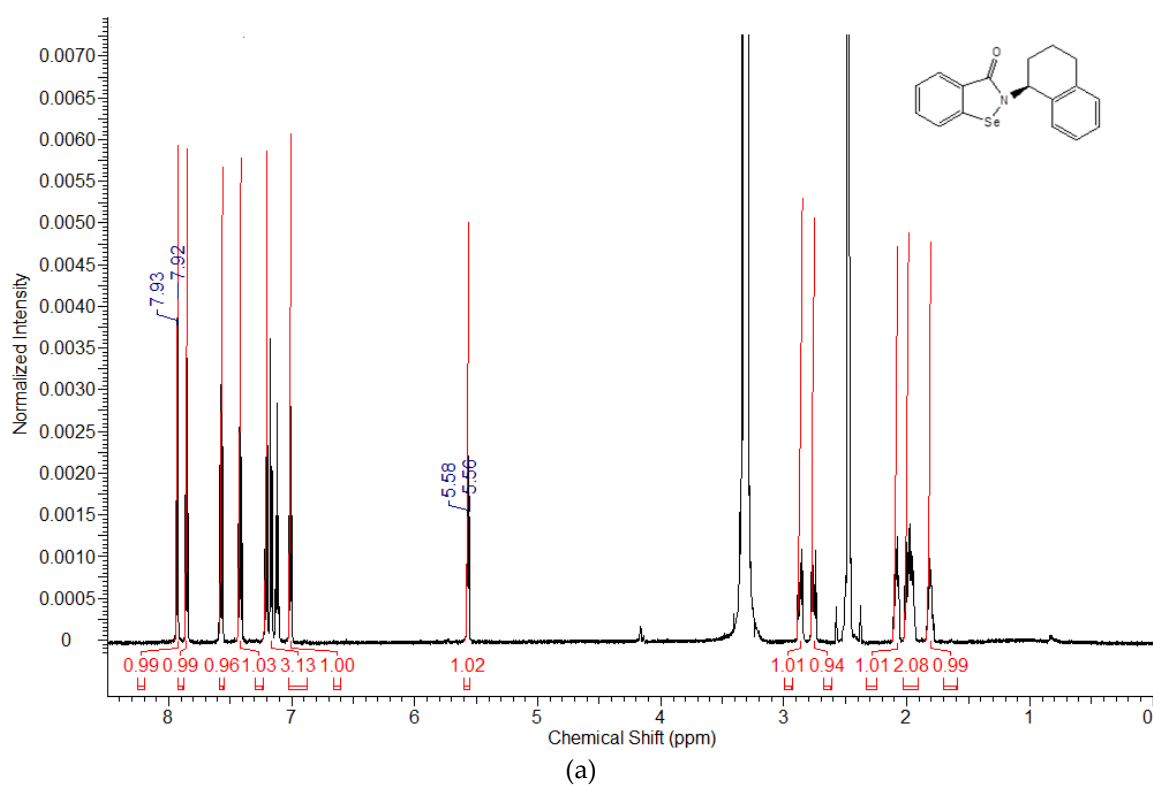
**Figure S4.** (a)  $^1\text{H}$  NMR, (b)  $^{13}\text{C}$  NMR, and (c)  $^{77}\text{Se}$  NMR spectra of *N*-[(*R*)-(-)-1-hydroxy-2-butanyl]-1,2-benzisoselenazol-3(2*H*)-one **21a**.

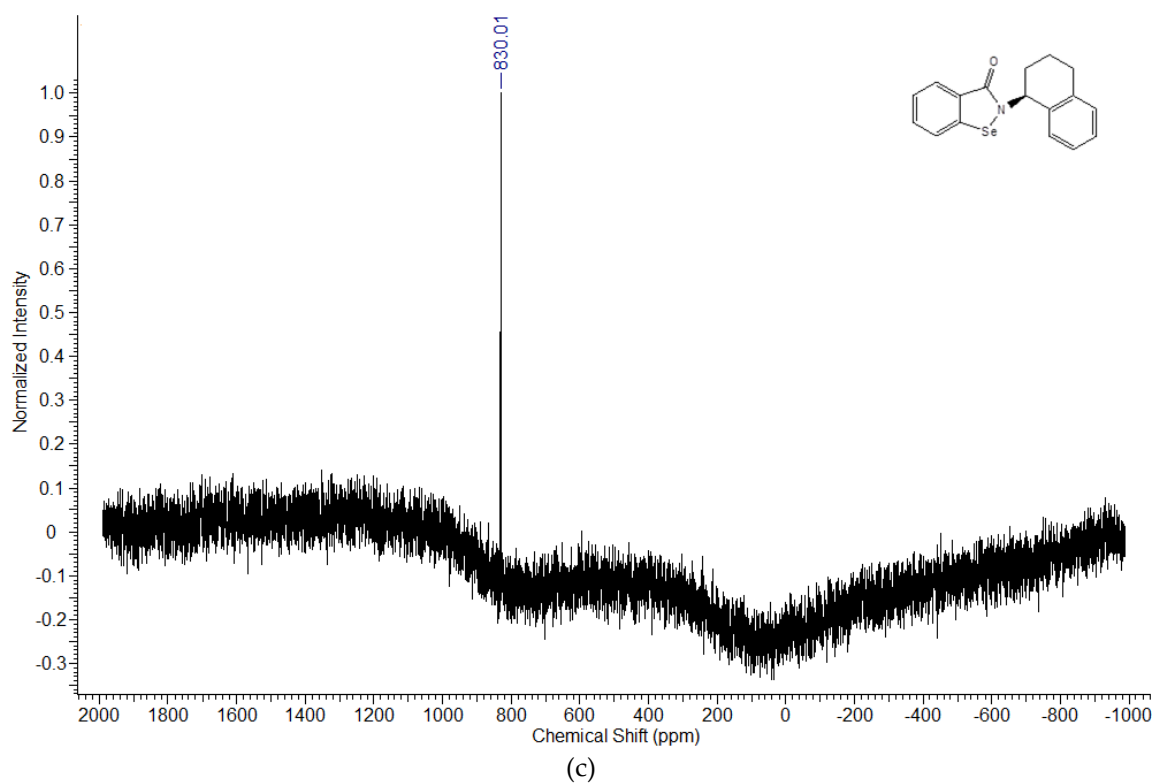




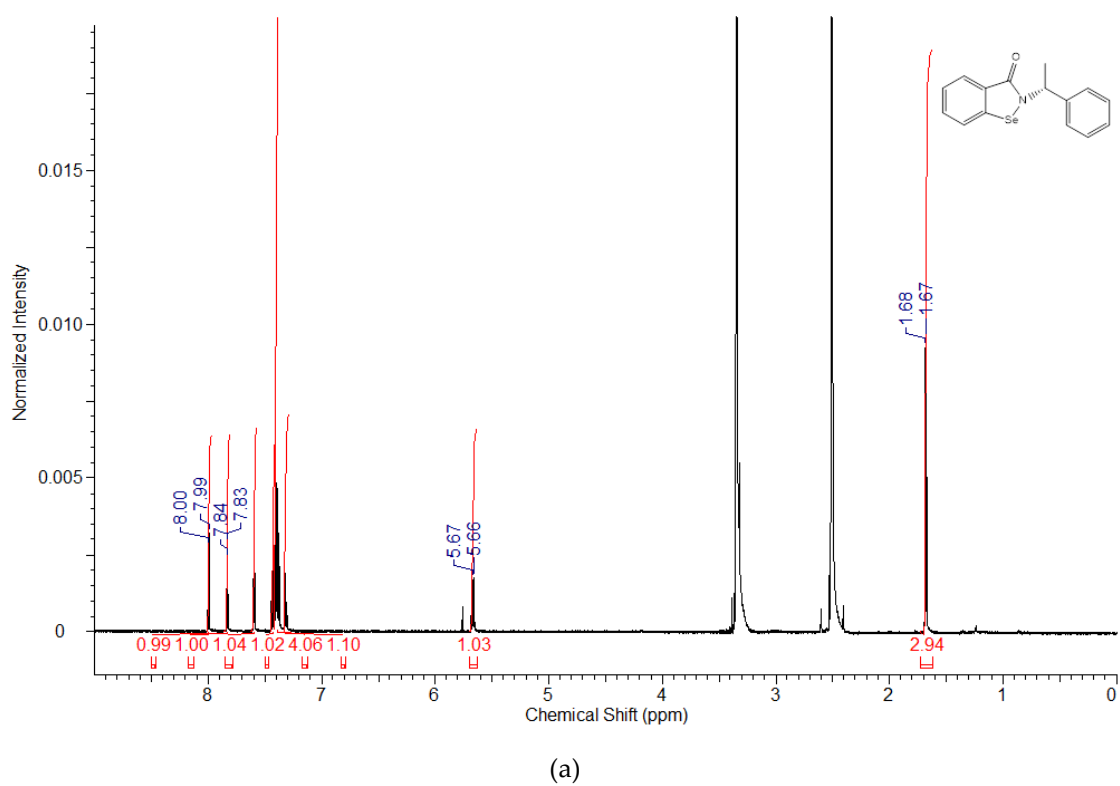
**Figure S5.** (a) <sup>1</sup>H NMR, (b) <sup>13</sup>C NMR, and (c) <sup>77</sup>Se NMR spectra of *N*-[(*R*)-(-)-1,2,3,4-tetrahydro-1-naphthyl]-1,2-benzisoselenazol-3(2*H*)-one **22a**.

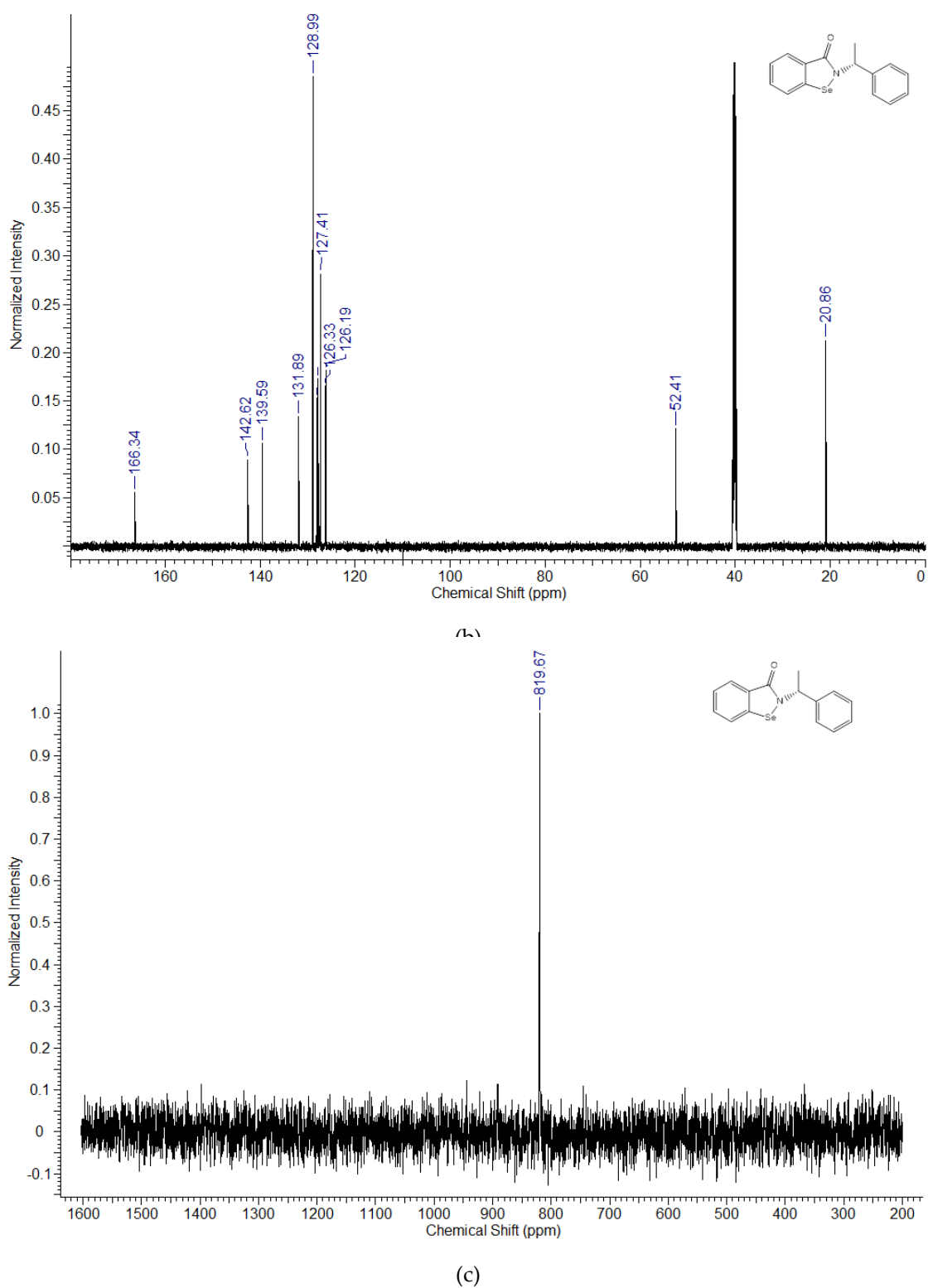




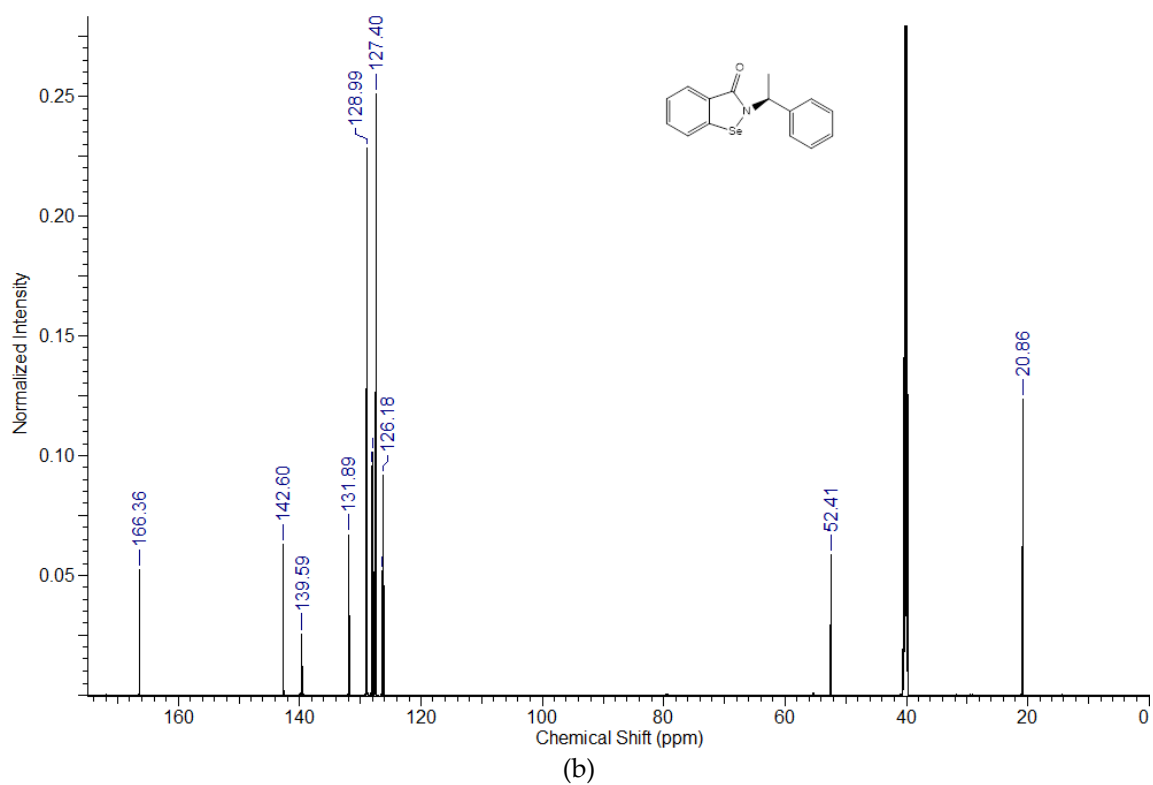
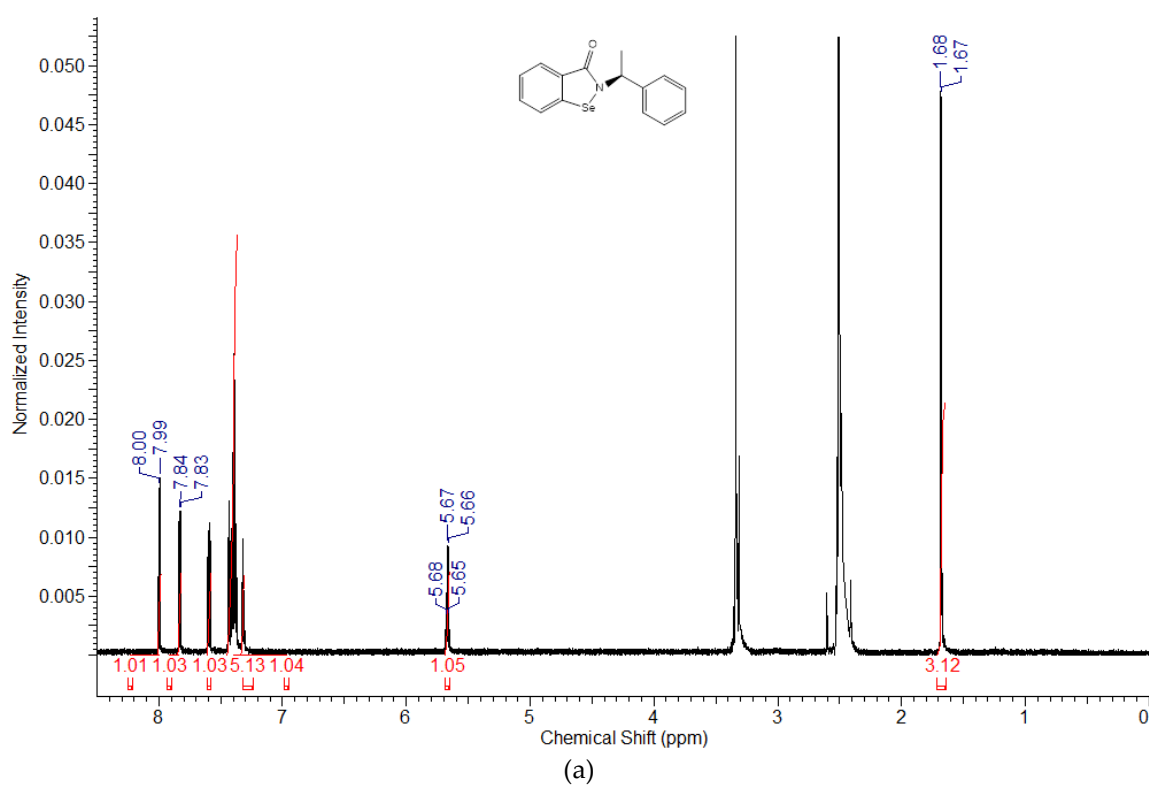


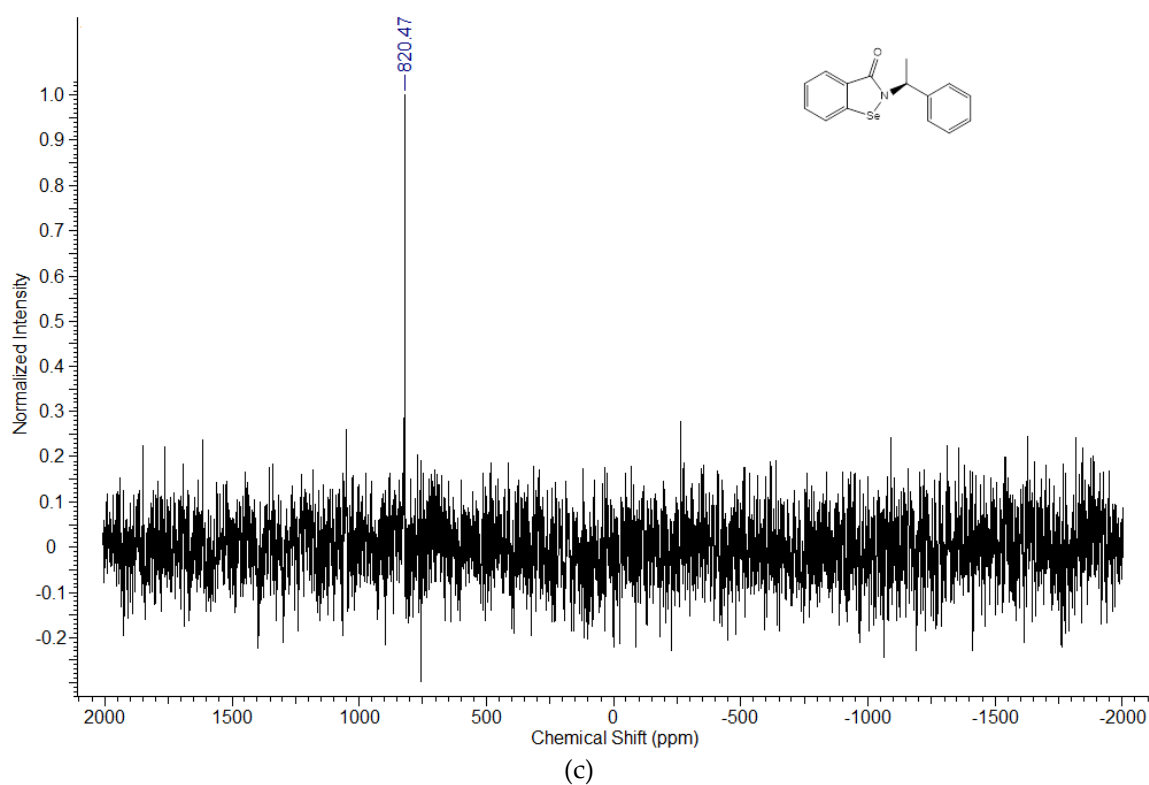
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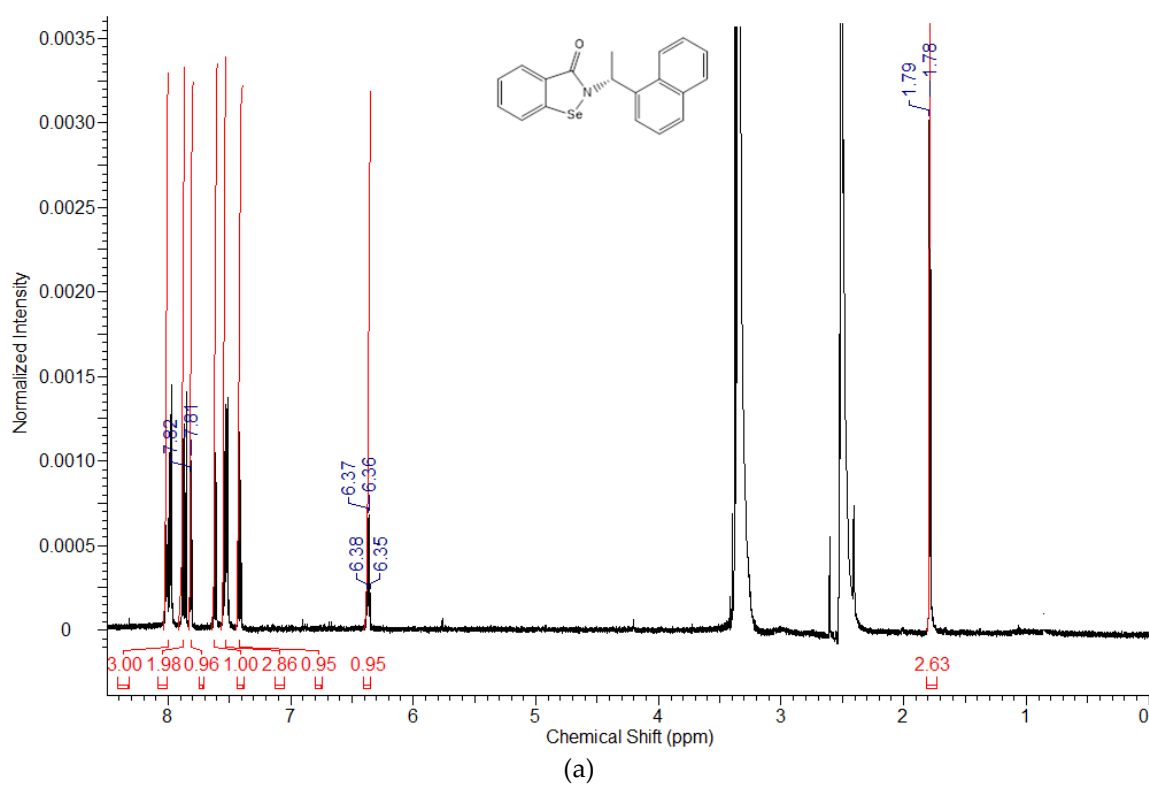


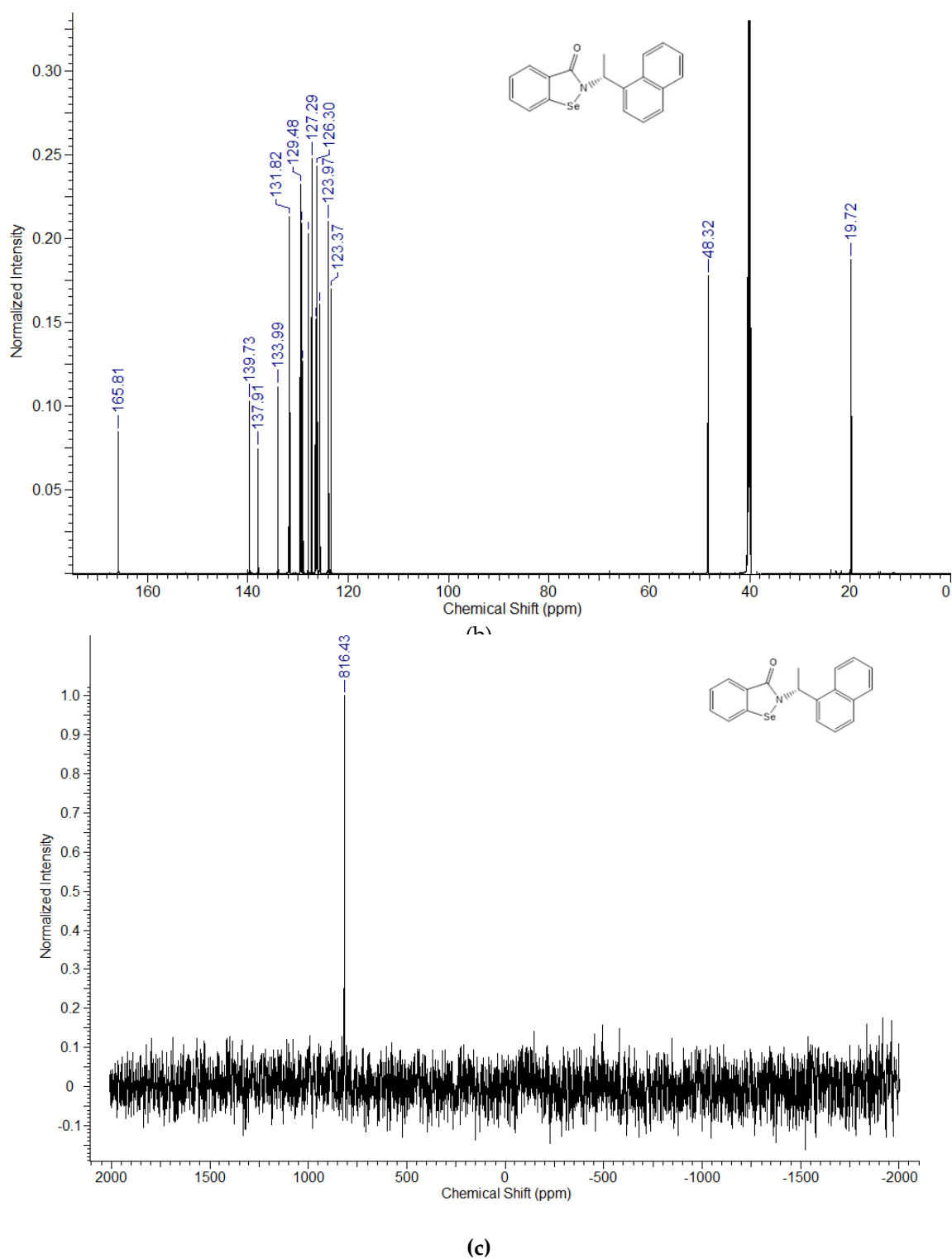
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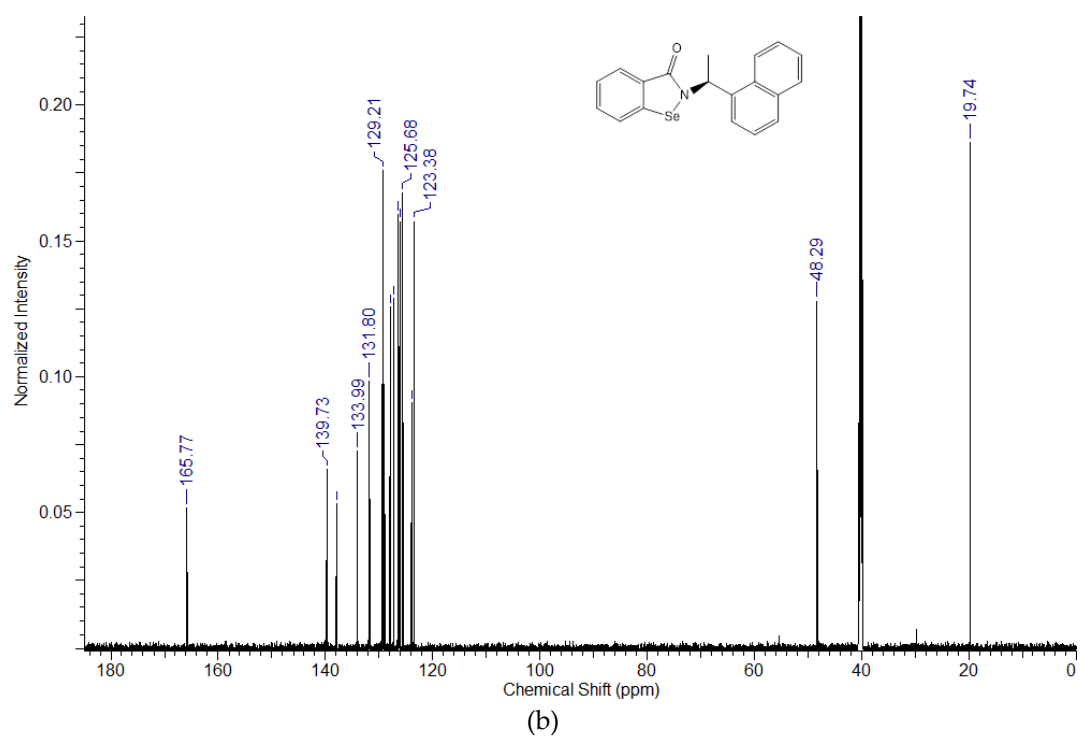
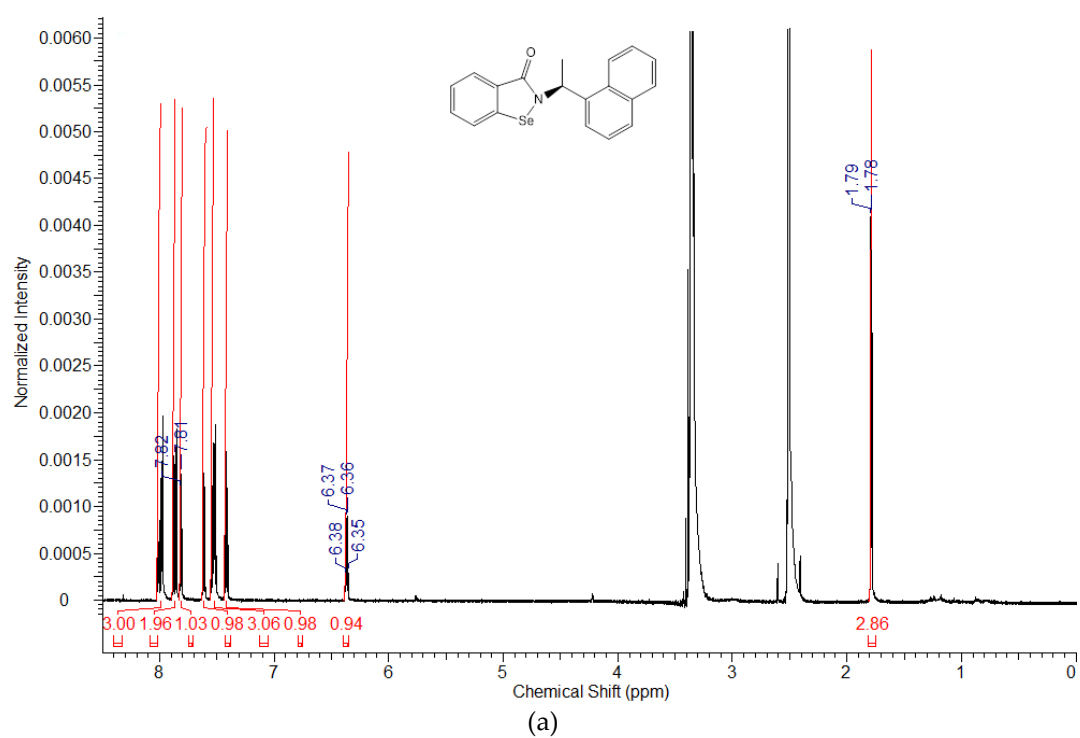


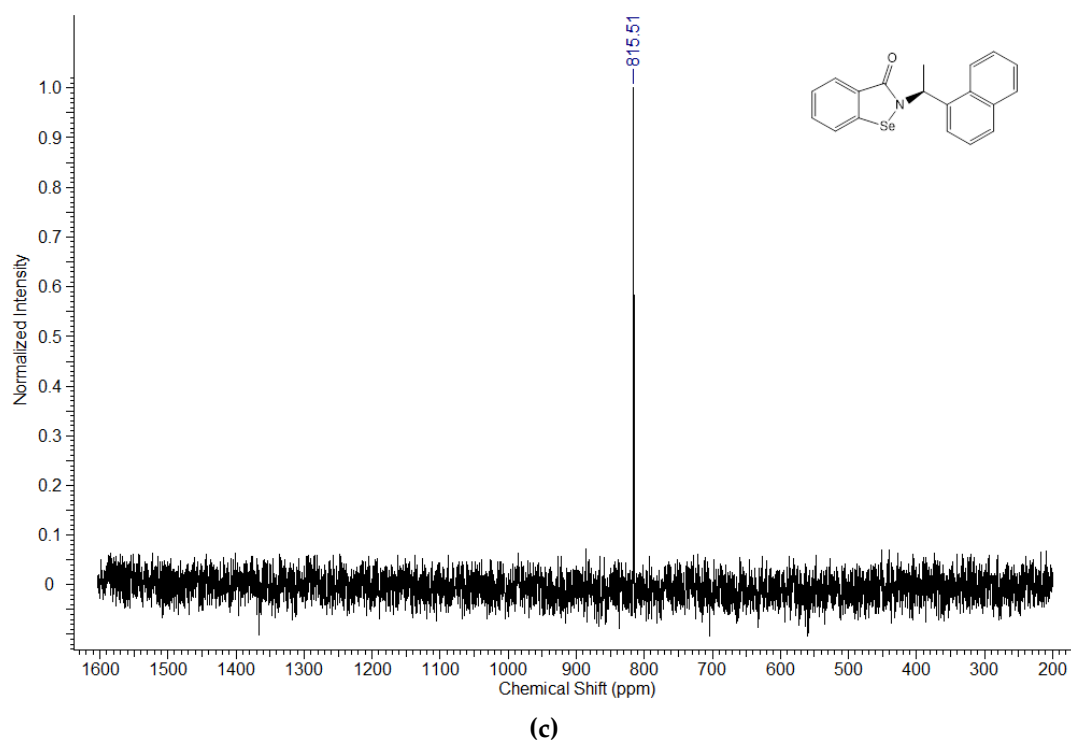
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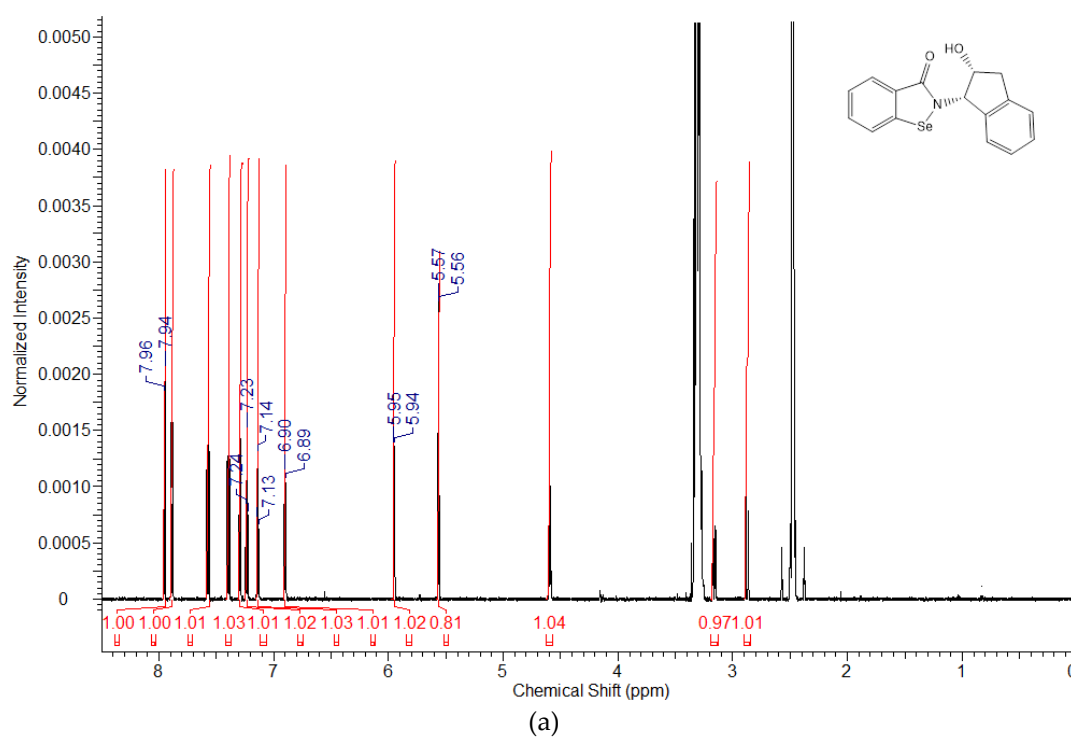


**Figure S9.** (a)  $^1\text{H}$  NMR, (b)  $^{13}\text{C}$  NMR, and (c)  $^{77}\text{Se}$  NMR spectra of *N*-[(*R*)-(-)-1-(1-naphthyl)ethyl]-1,2-benzisoselenazol-3(2*H*)-one **26a**

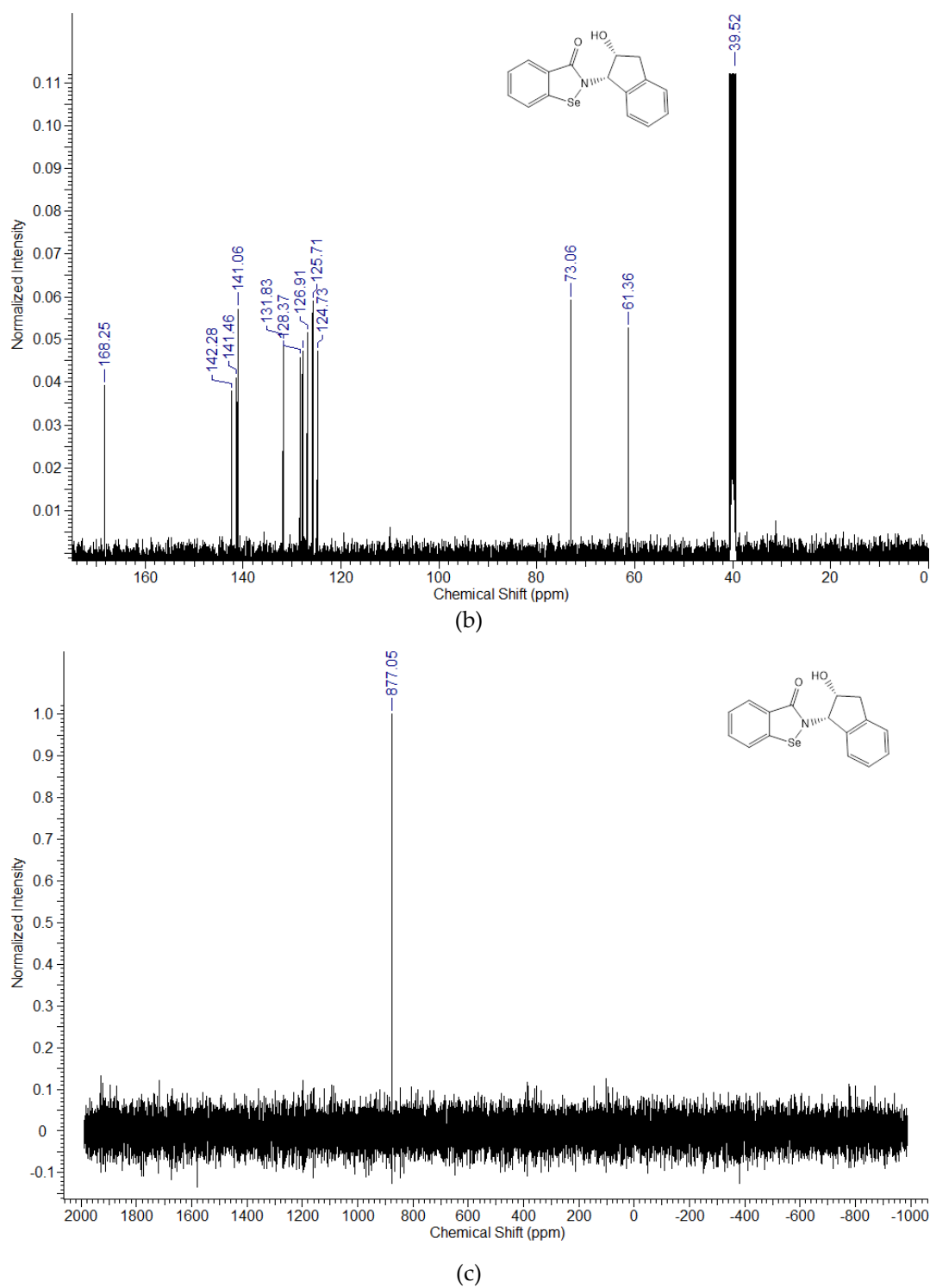




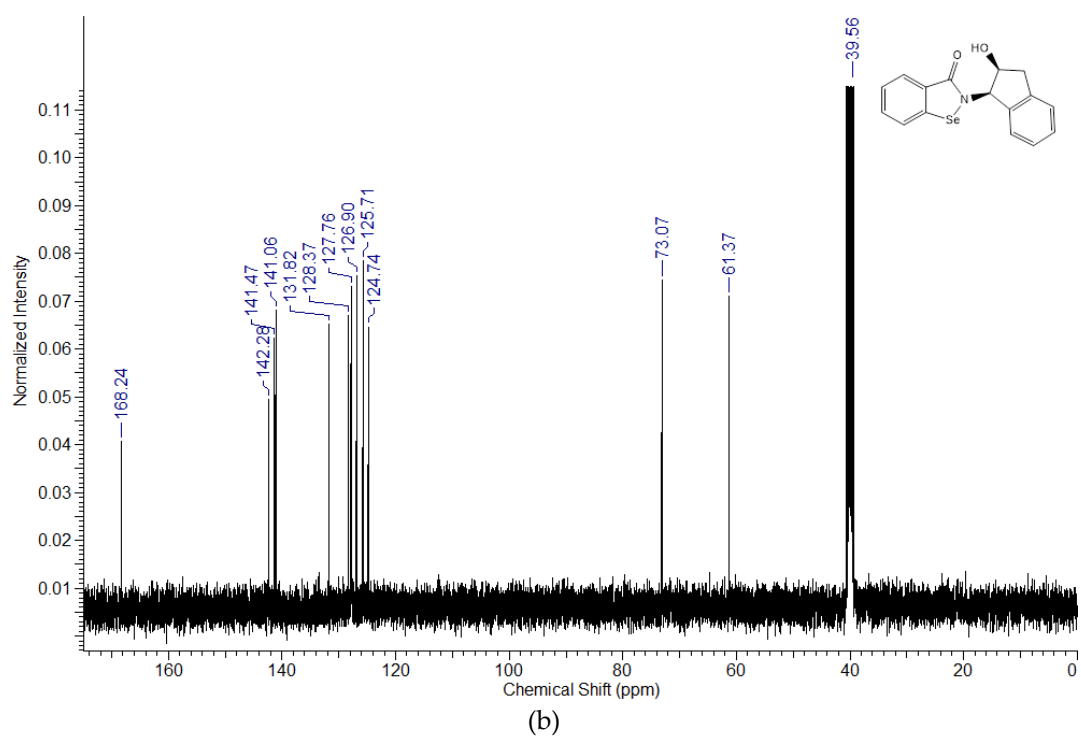
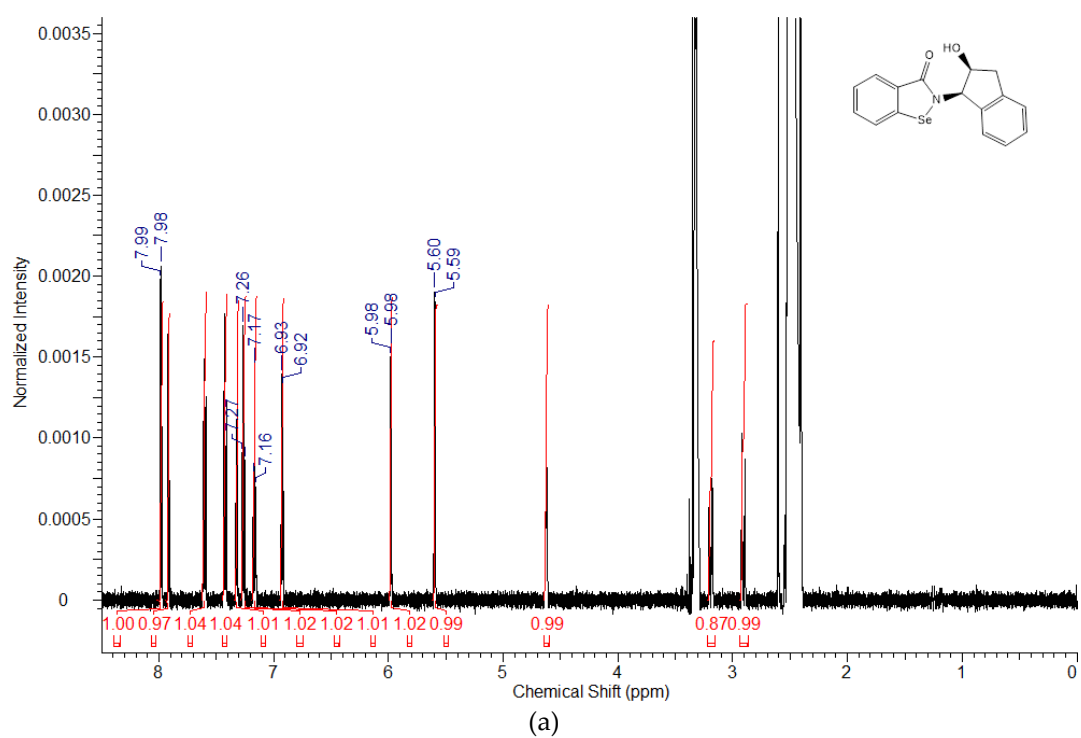
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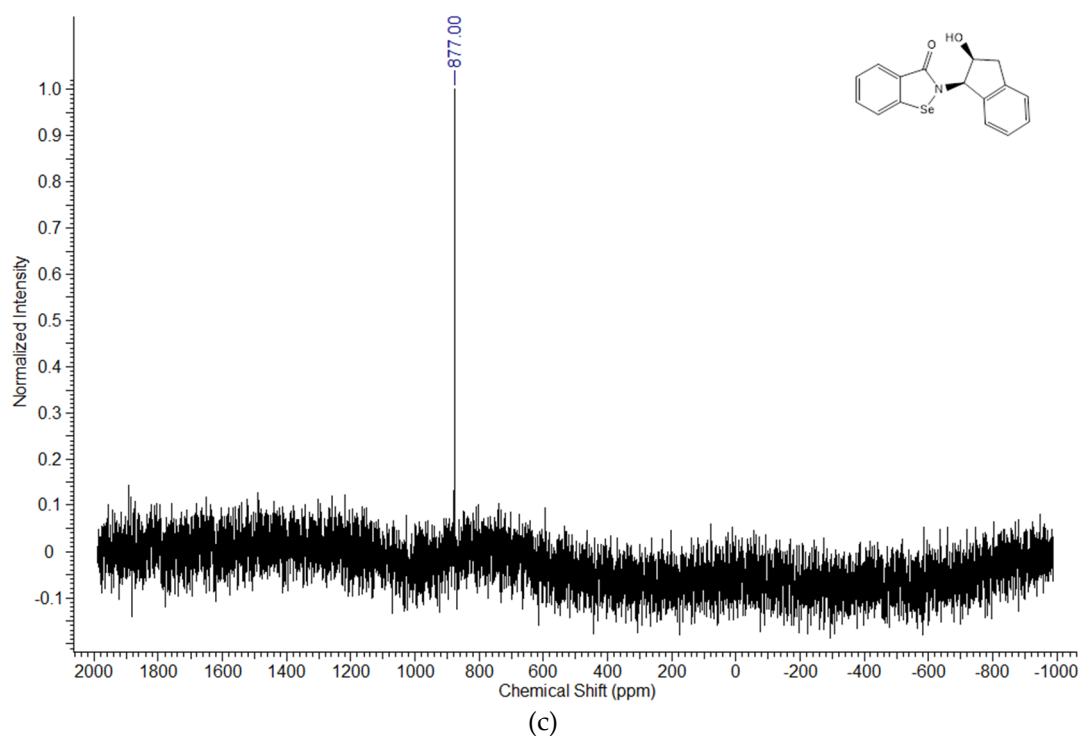




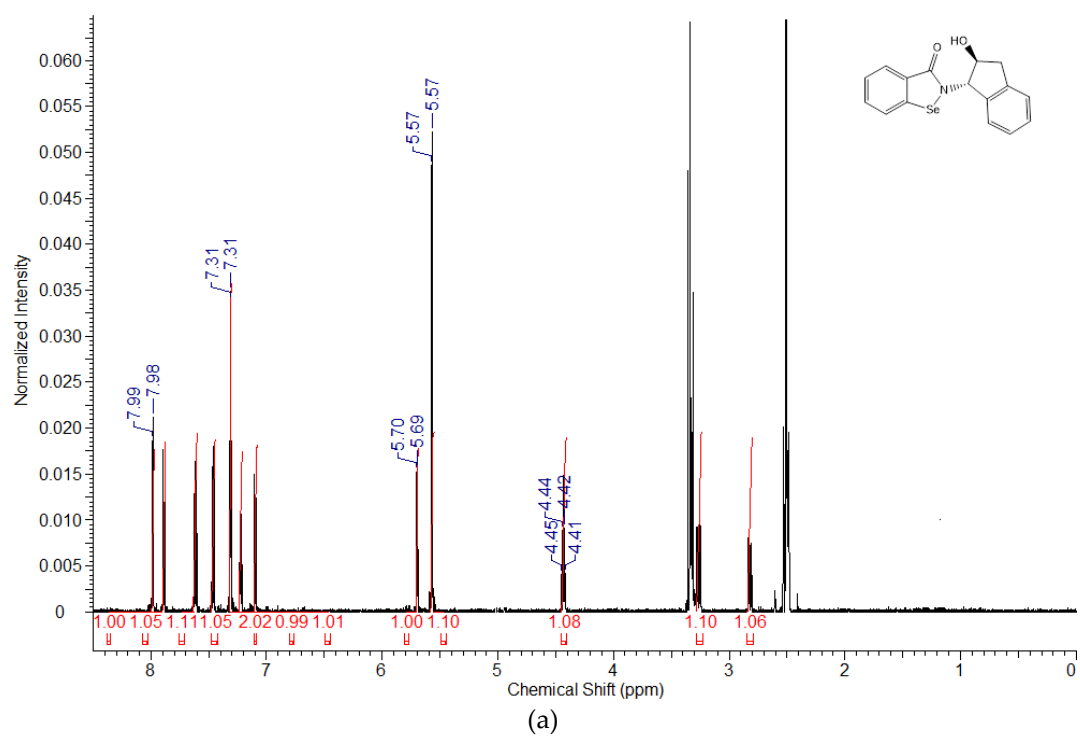


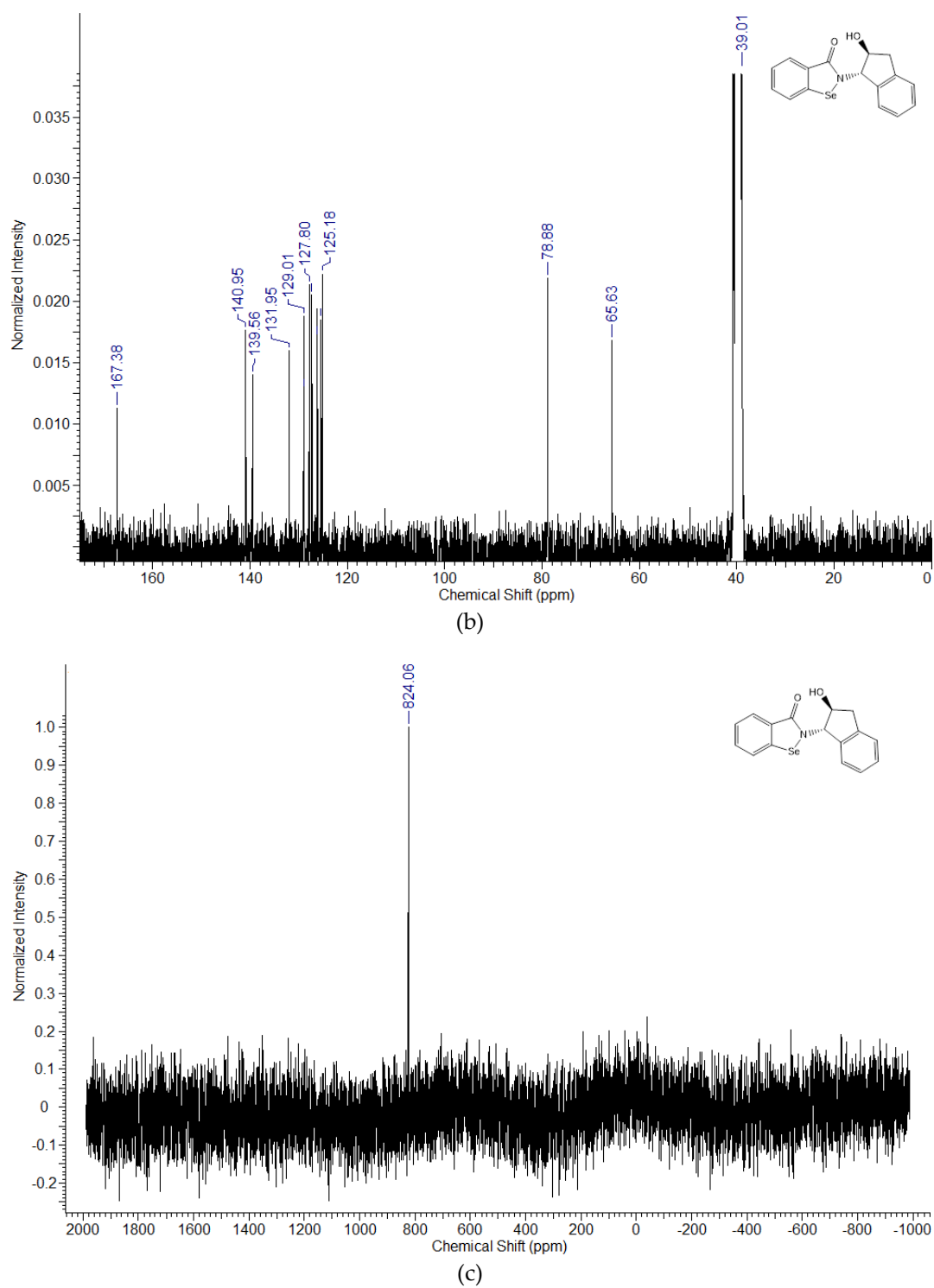
**Figure S11.** (a) <sup>1</sup>H NMR, (b) <sup>13</sup>C NMR, and (c) <sup>77</sup>Se NMR spectra of *N*-[(1*S*,2*R*)-(-)-*cis*-2-hydroxy-1-indanyl]-1,2-benzisoselenazol-3(2*H*)-one **28a**.



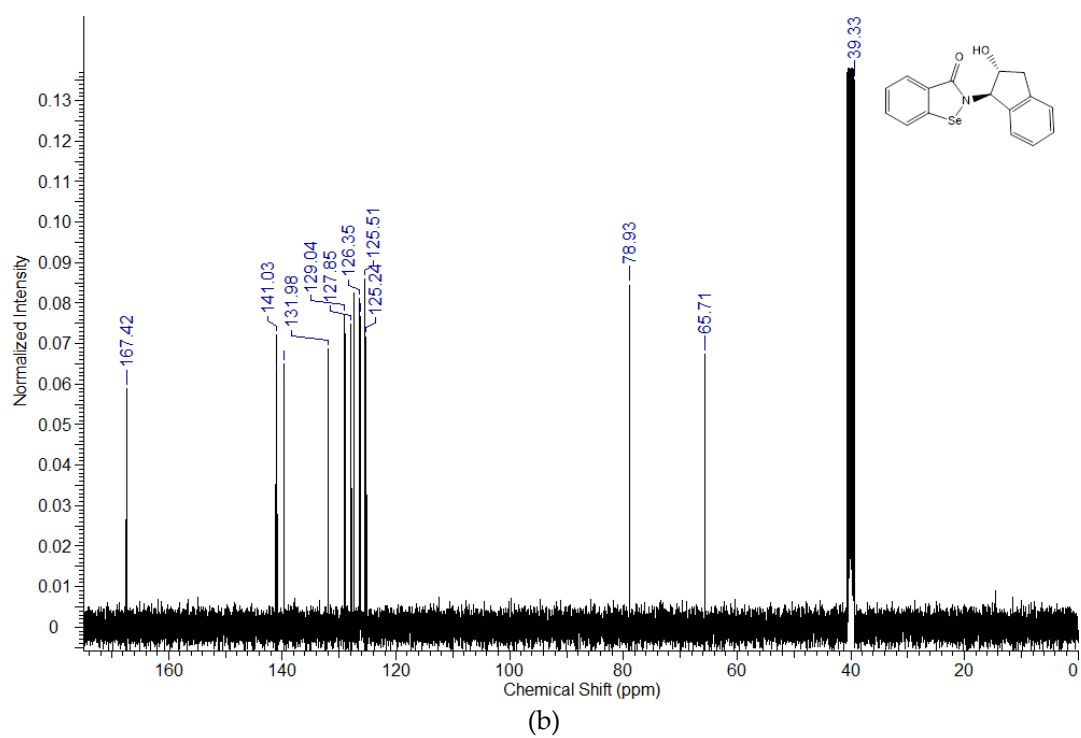
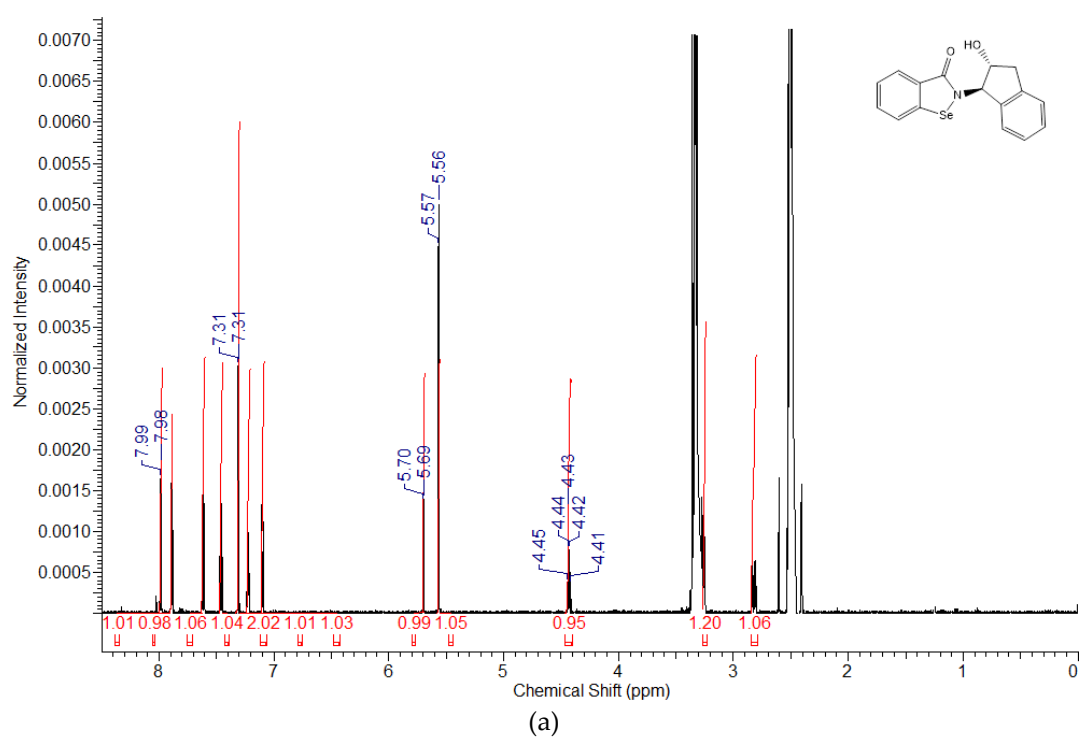


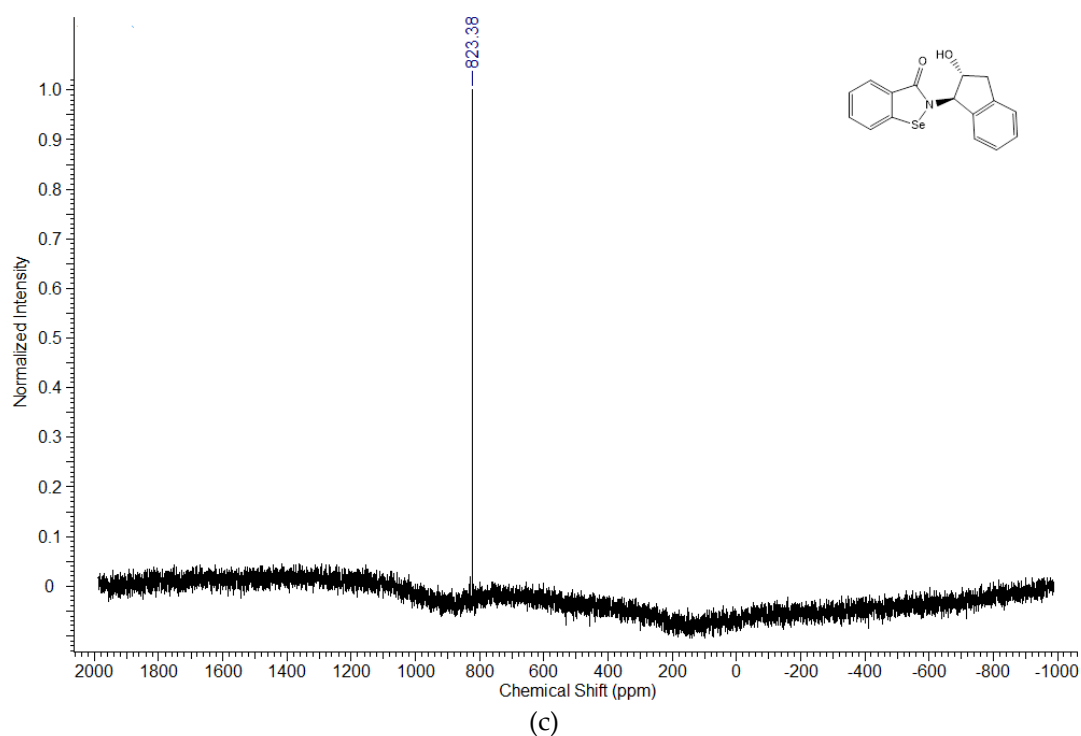
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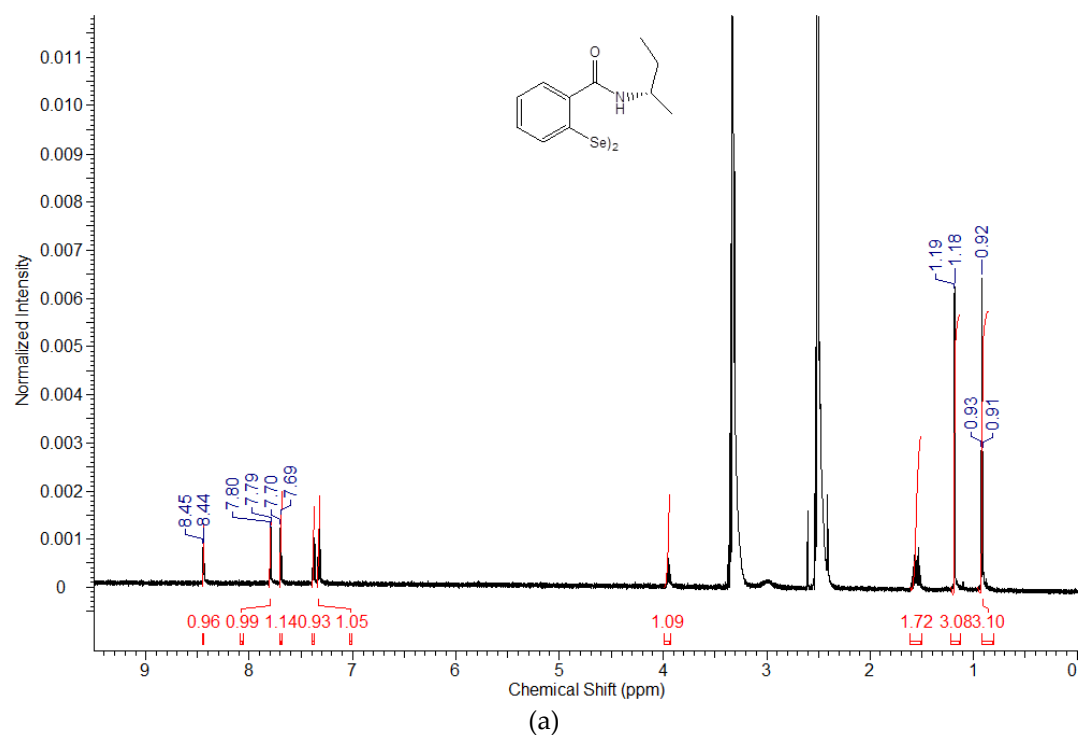
**Figure S13.** (a) <sup>1</sup>H NMR, (b) <sup>13</sup>C NMR, and (c) <sup>77</sup>Se NMR spectra of *N*-[(1*S*,2*S*)-(+)-*trans*-2-hydroxy-1-indanyl]-1,2-benzisoselenazol-3(2*H*)-one **30a**

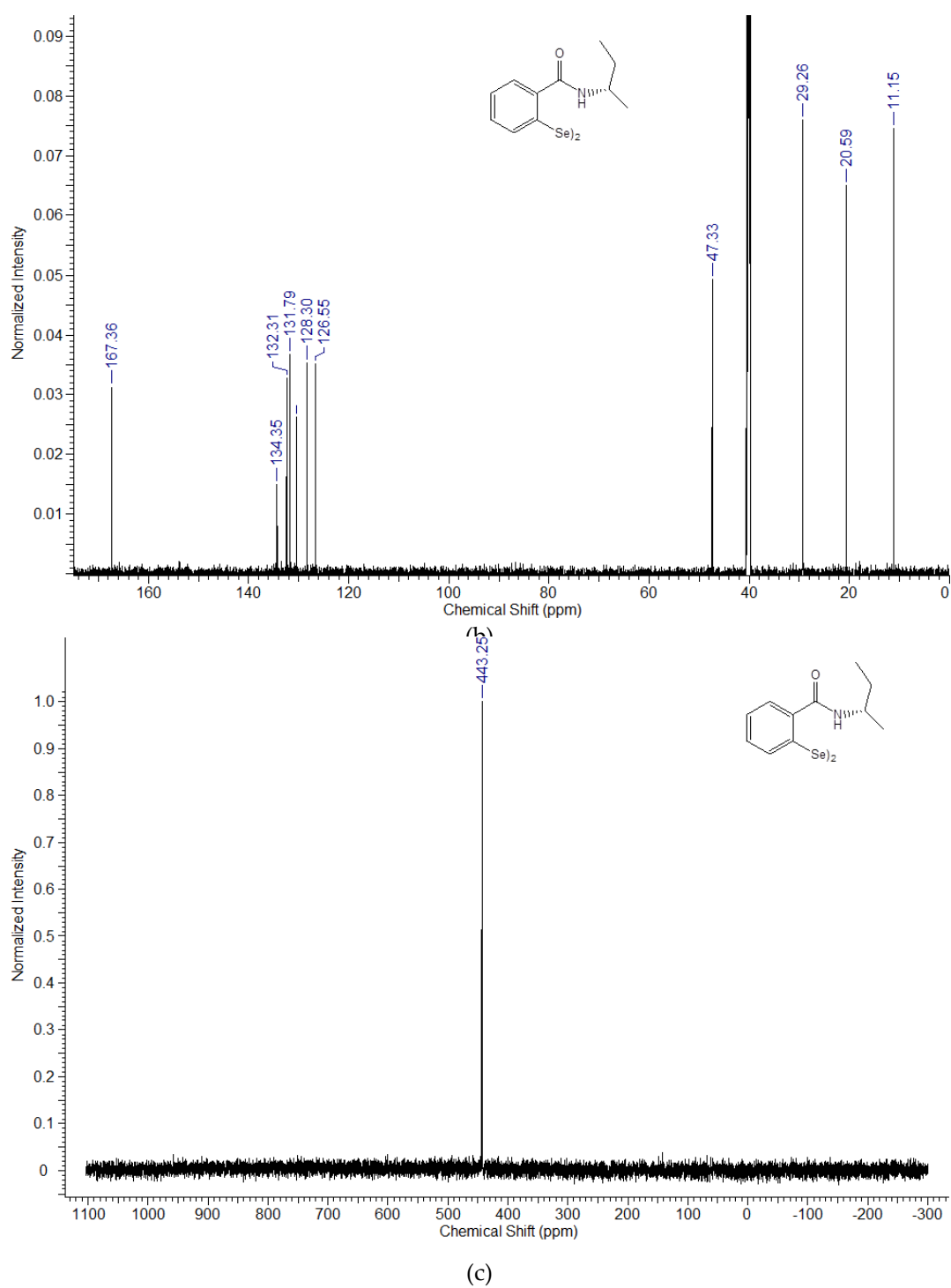




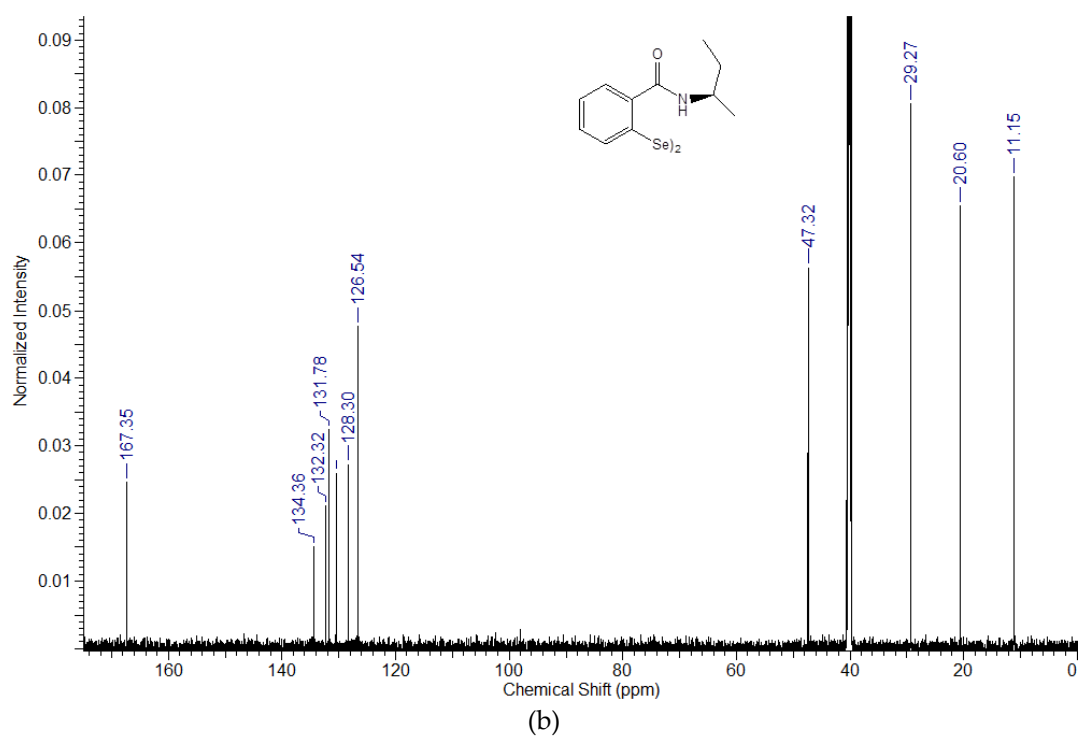
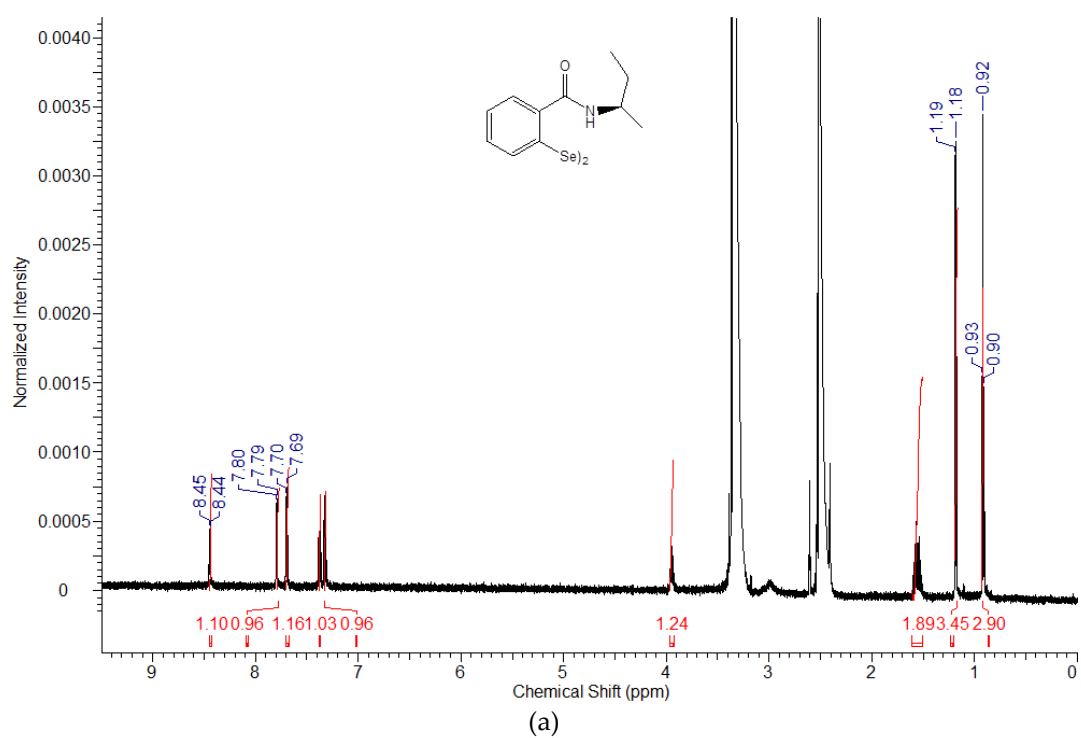
**Figure S14.** (a)  $^1\text{H}$  NMR, (b)  $^{13}\text{C}$  NMR, and (c)  $^{77}\text{Se}$  NMR spectra of *N*-[(1*R*,2*R*)-(-)-*trans*-2-hydroxy-1-indanyl]-1,2-benzisoselenazol-3(2*H*)-one **31a**.

## 2. NMR spectra of diselenides 18b-31b

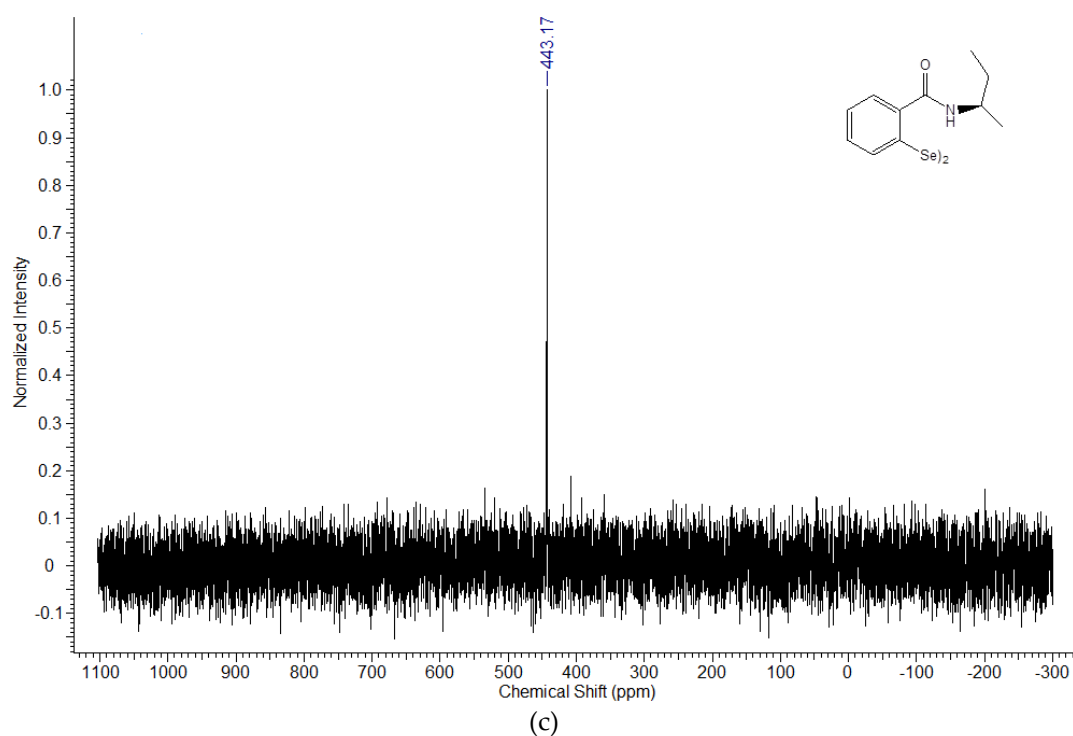




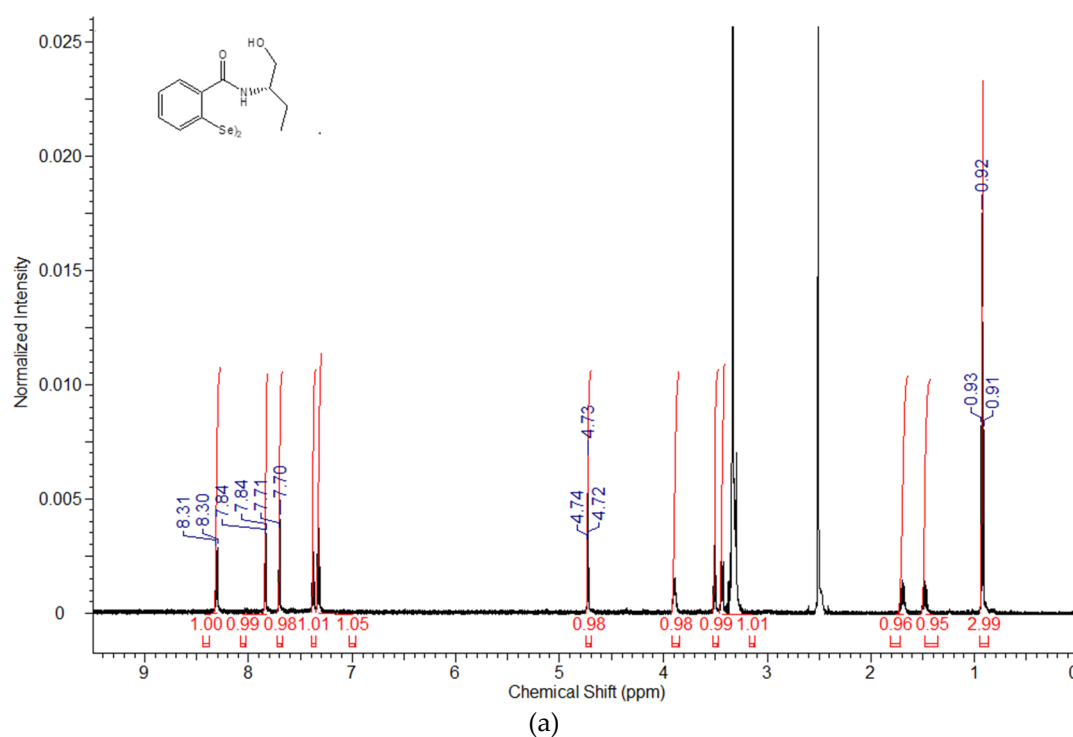
**Figure S15.** (a) <sup>1</sup>H NMR, (b) <sup>13</sup>C NMR, and (c) <sup>77</sup>Se NMR spectra of 2,2'-diselenobis[N-(S)-(+)-sec-butylbezamide] **18b**

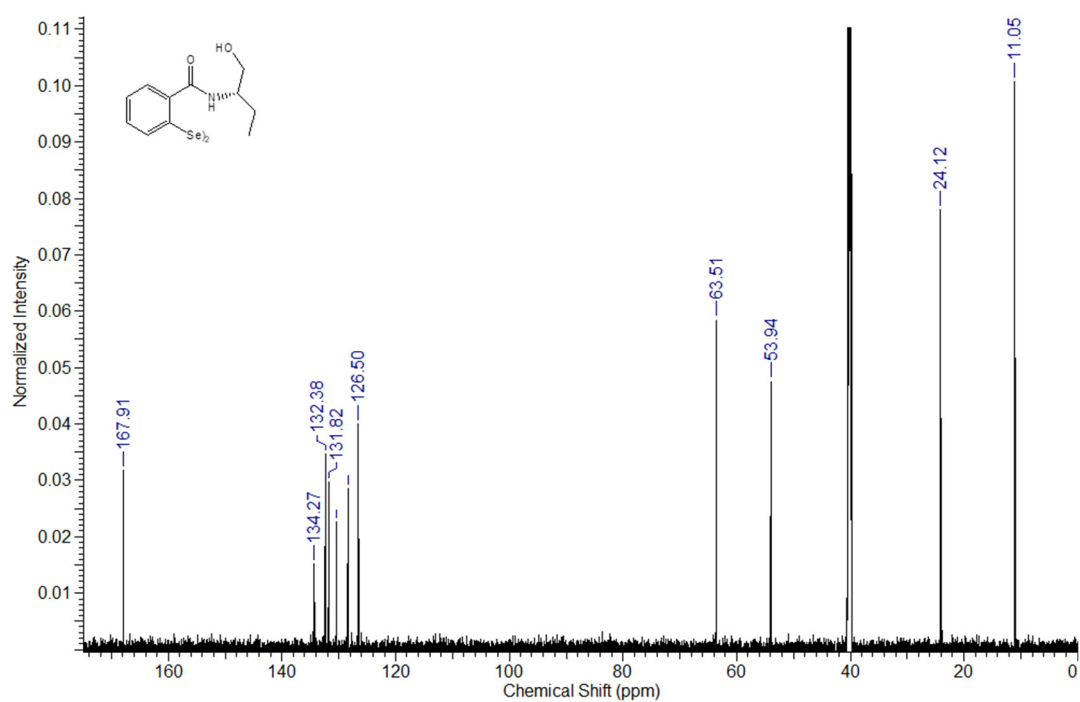




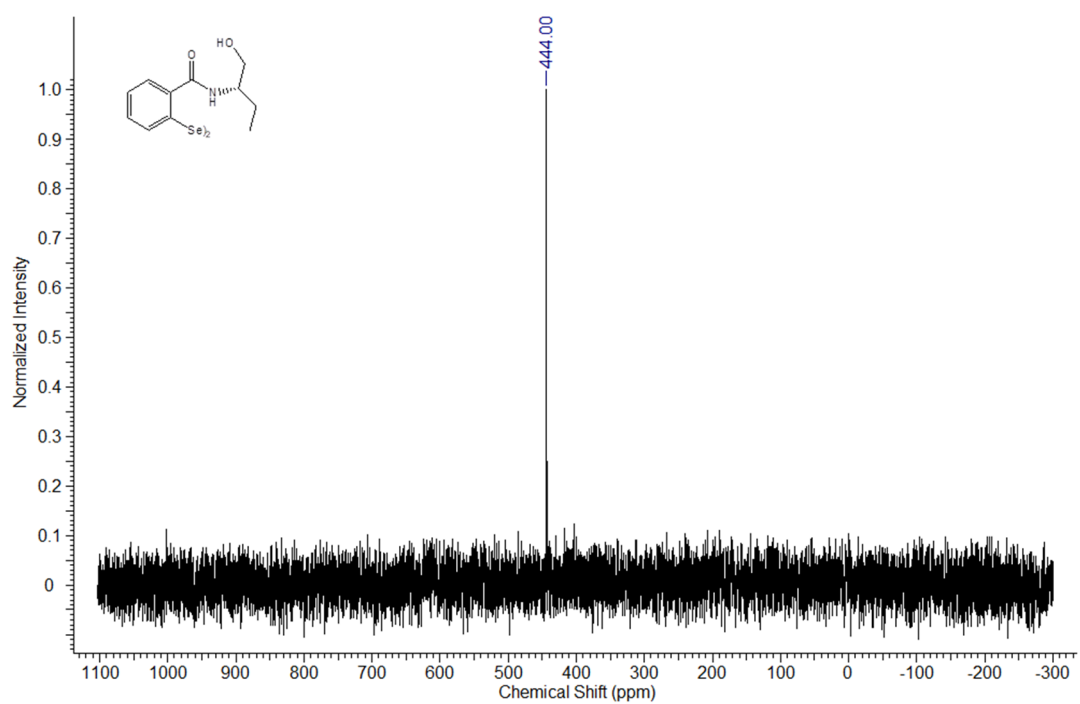


**Figure S16.** (a)  $^1\text{H}$  NMR, (b)  $^{13}\text{C}$  NMR, and (c)  $^{77}\text{Se}$  NMR spectra of 2,2'-diselenobis[*N*-(*R*)-(-)-*sec*-butylbenzamide] **19b**



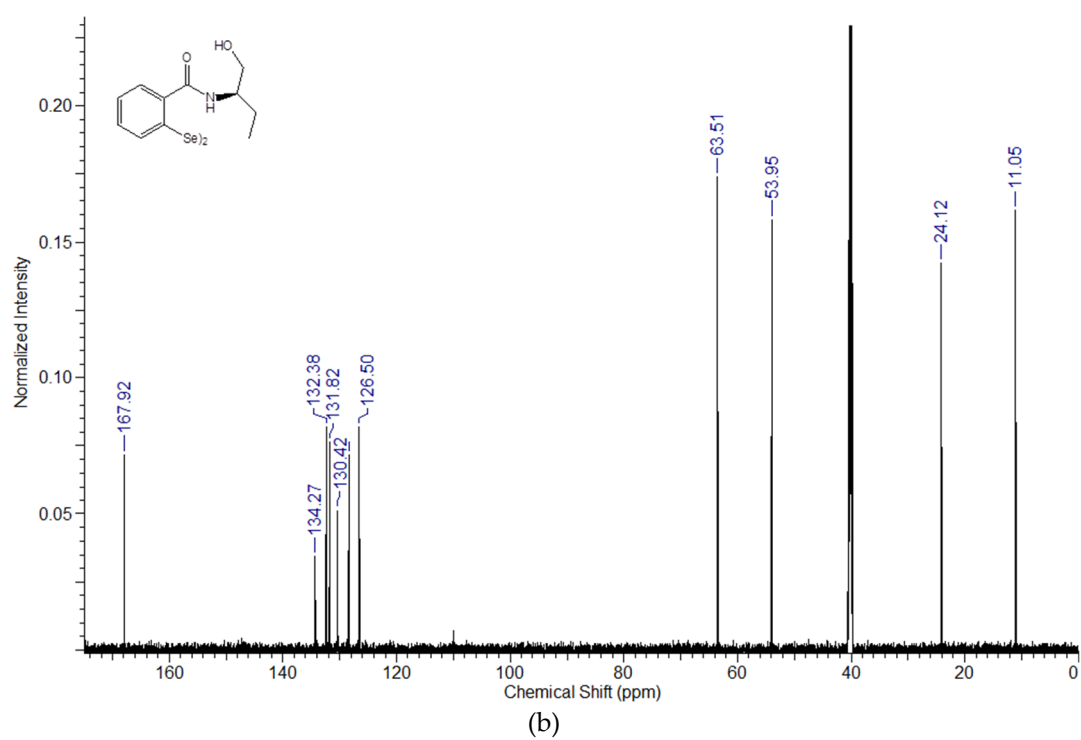
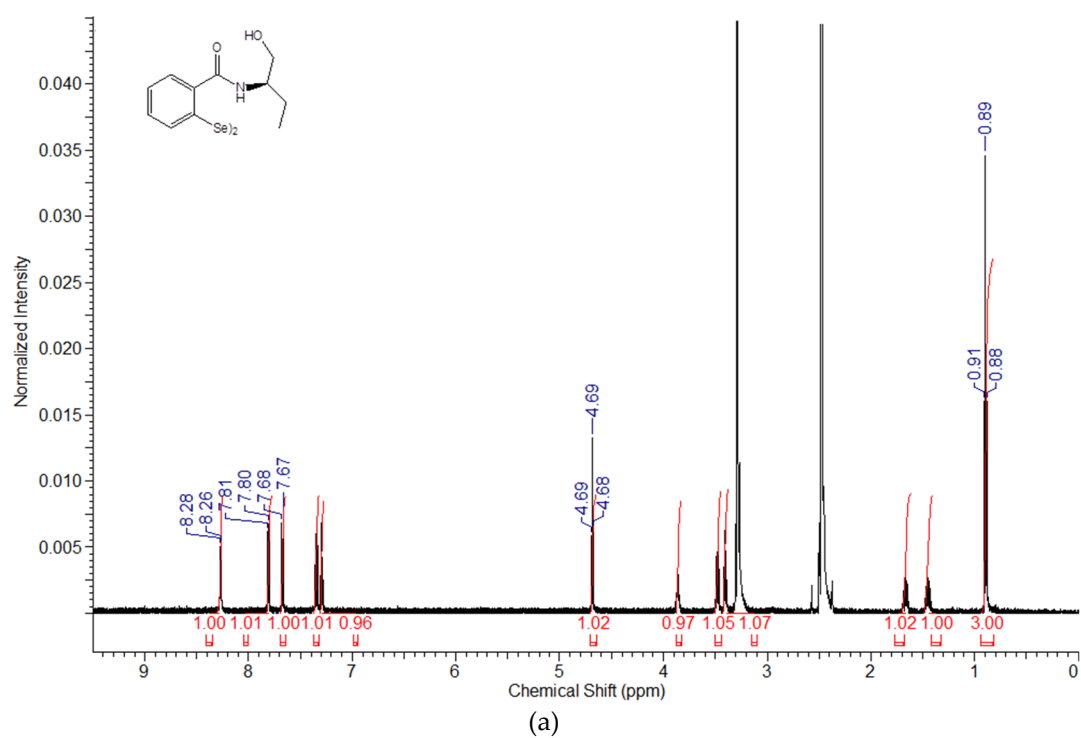


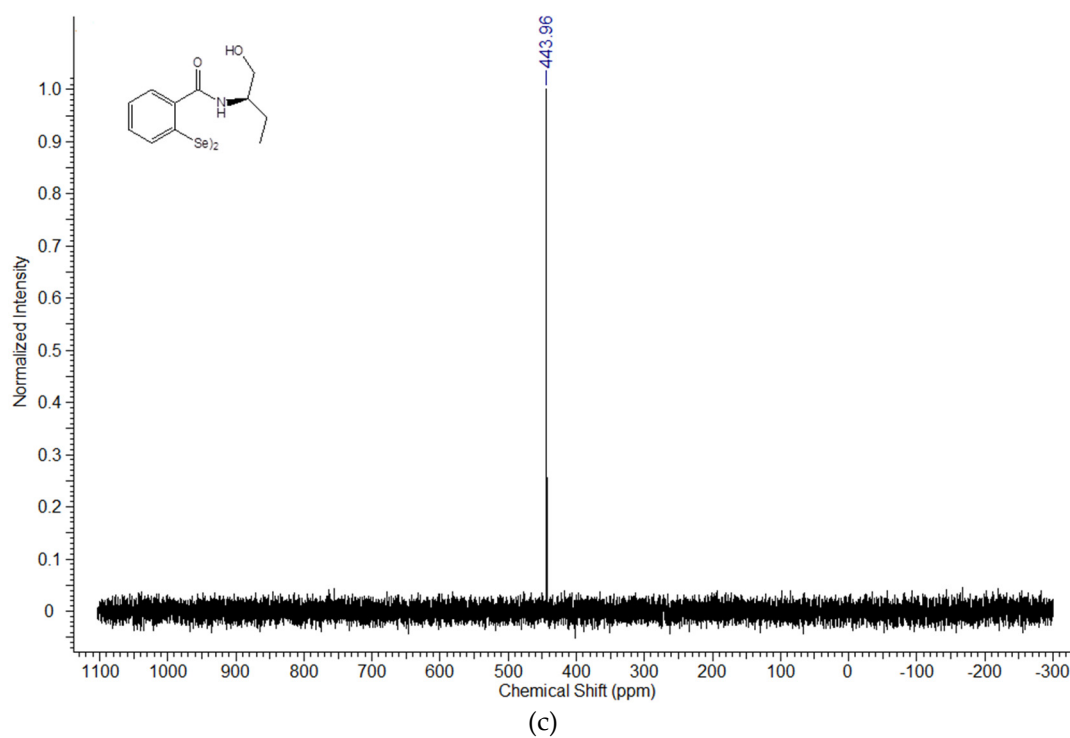
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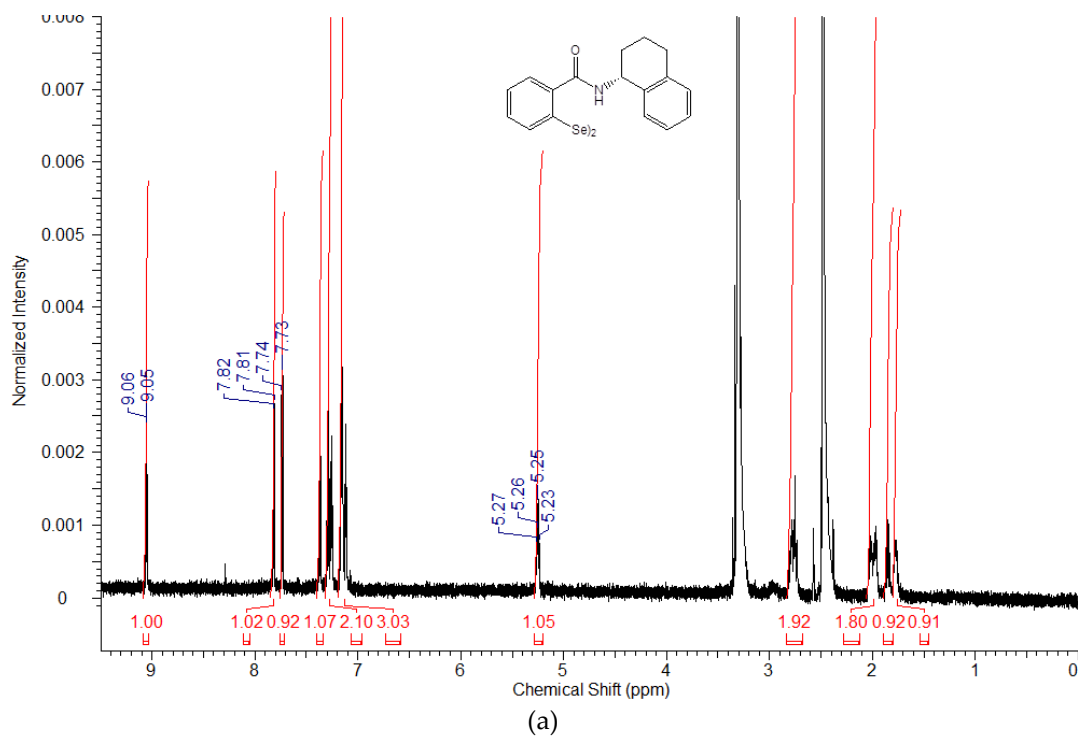
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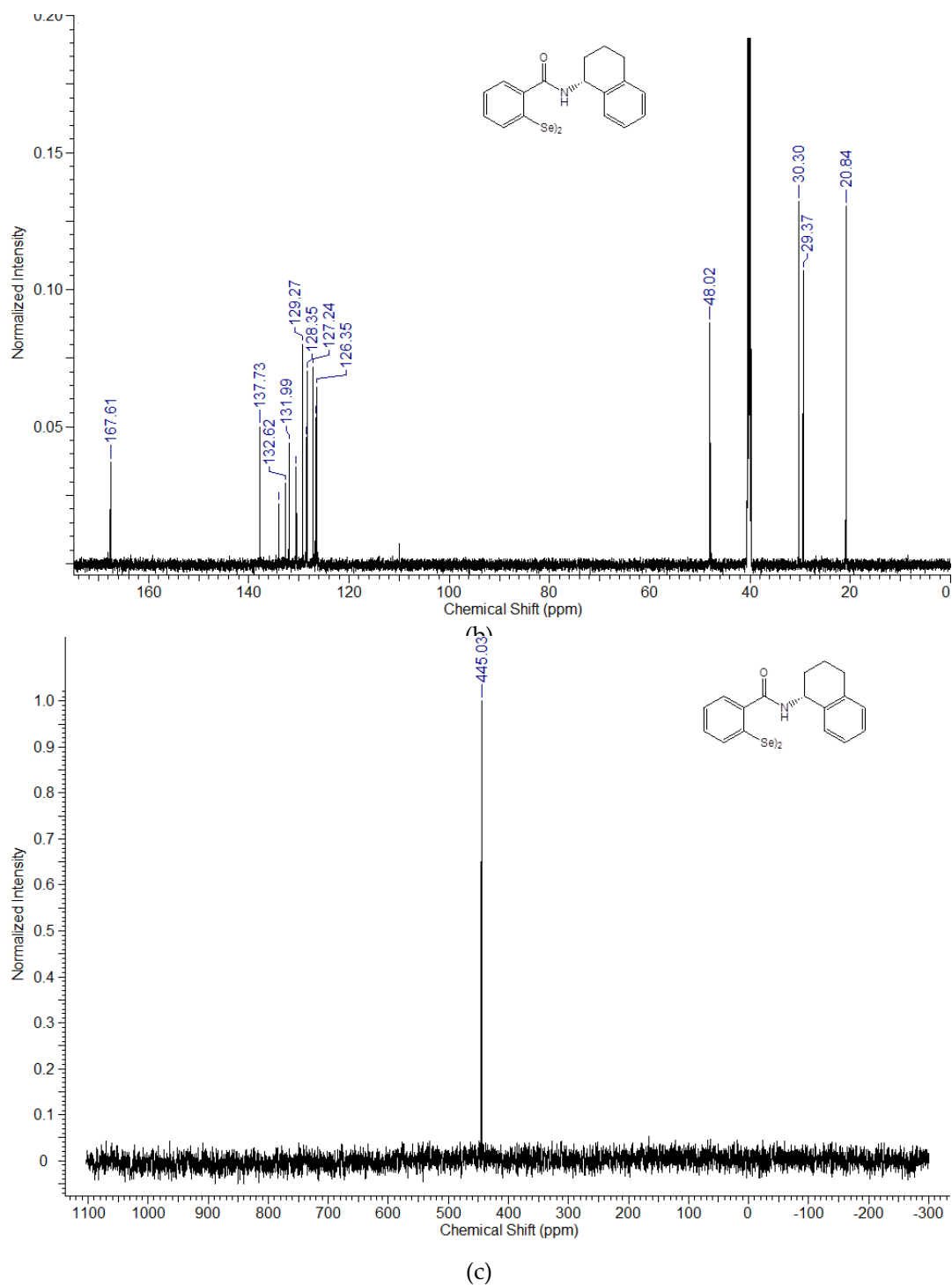
**Figure S17.** (a) <sup>1</sup>H NMR, (b) <sup>13</sup>C NMR, and (c) <sup>77</sup>Se NMR spectra of 2,2'-diselenobis[*N*-(*S*)-(+)-1-hydroxy-2-butanylbezamide] **20b**



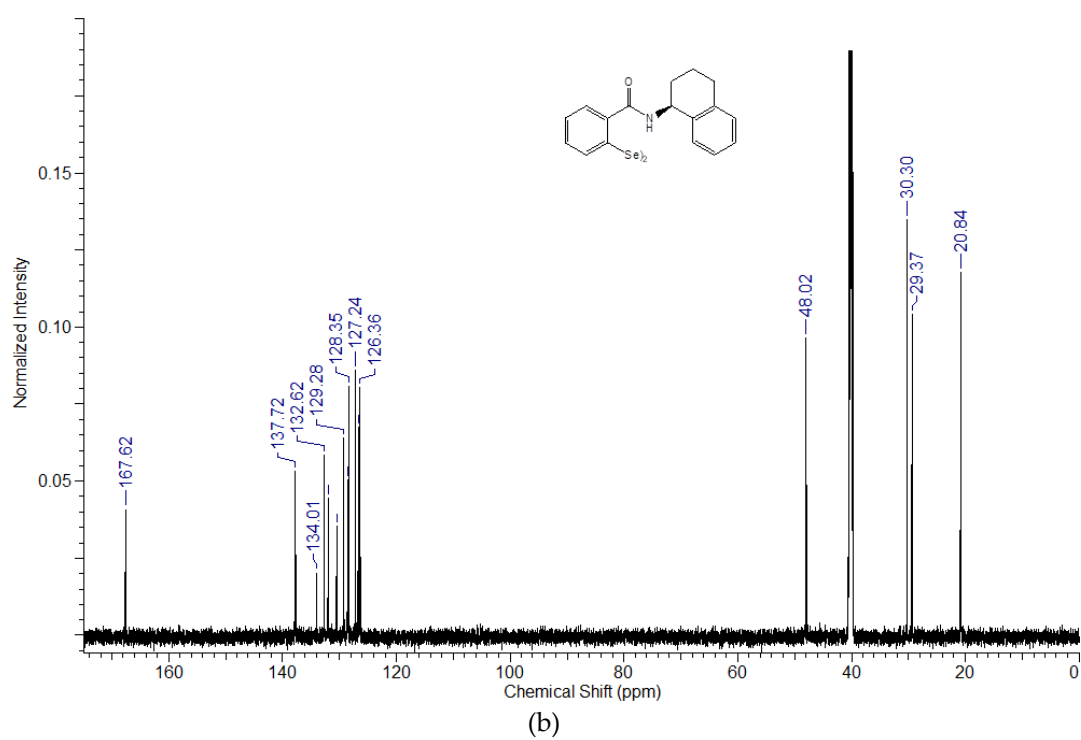
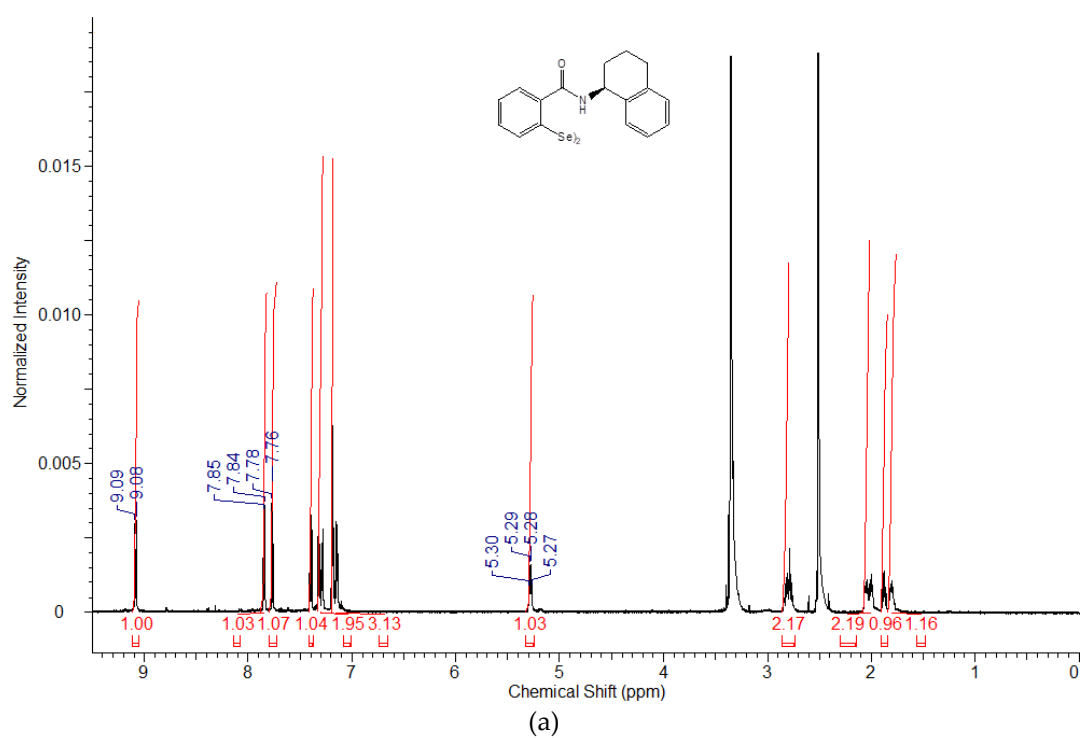


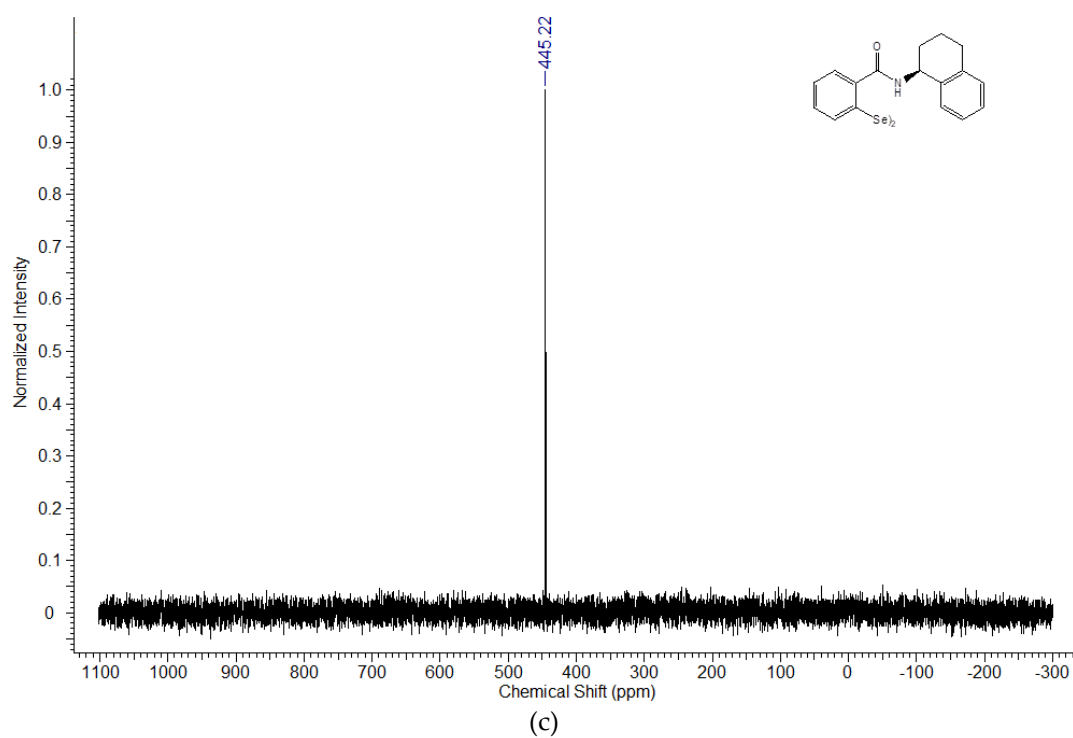
**Figure S18.** (a)  $^1\text{H}$  NMR, (b)  $^{13}\text{C}$  NMR, and (c)  $^{77}\text{Se}$  NMR spectra of 2,2'-diselenobis[*N*-(*R*)-(-)-1-hydroxy-2-butanylbezamide] **21b**.



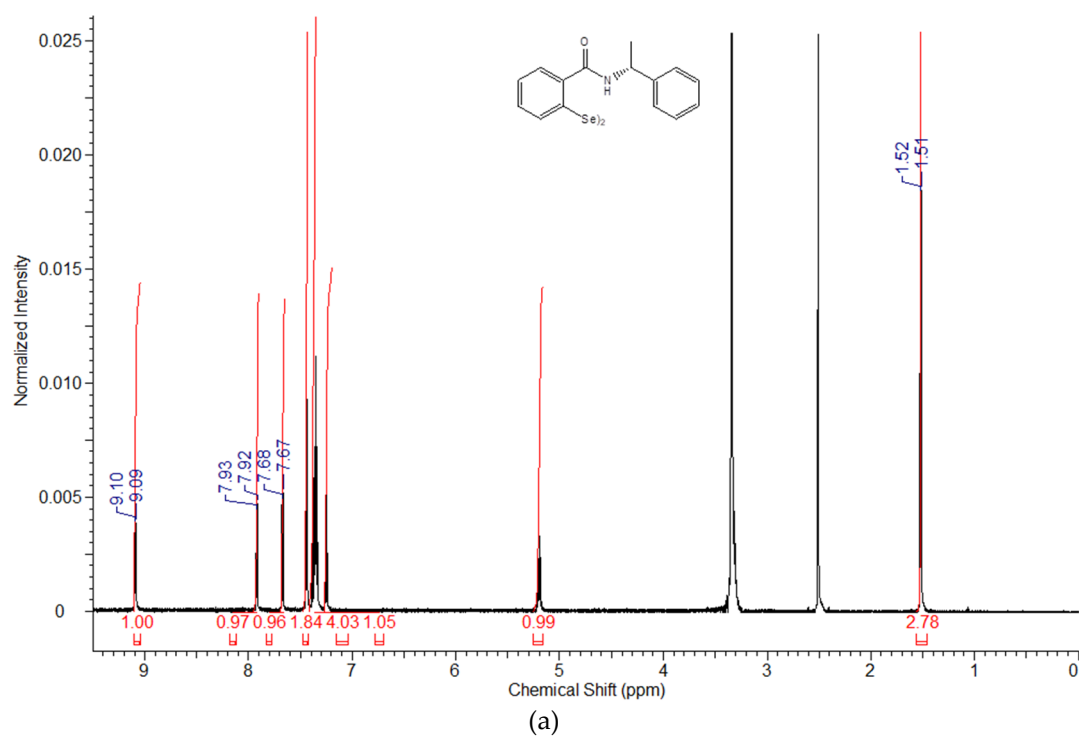


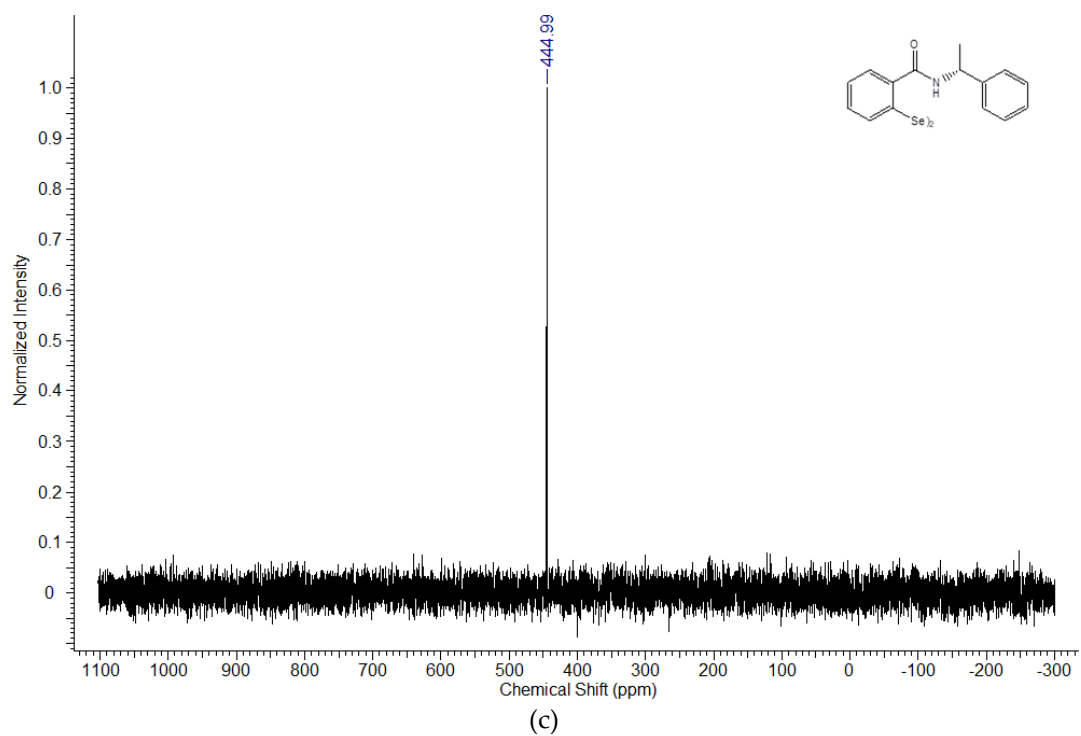
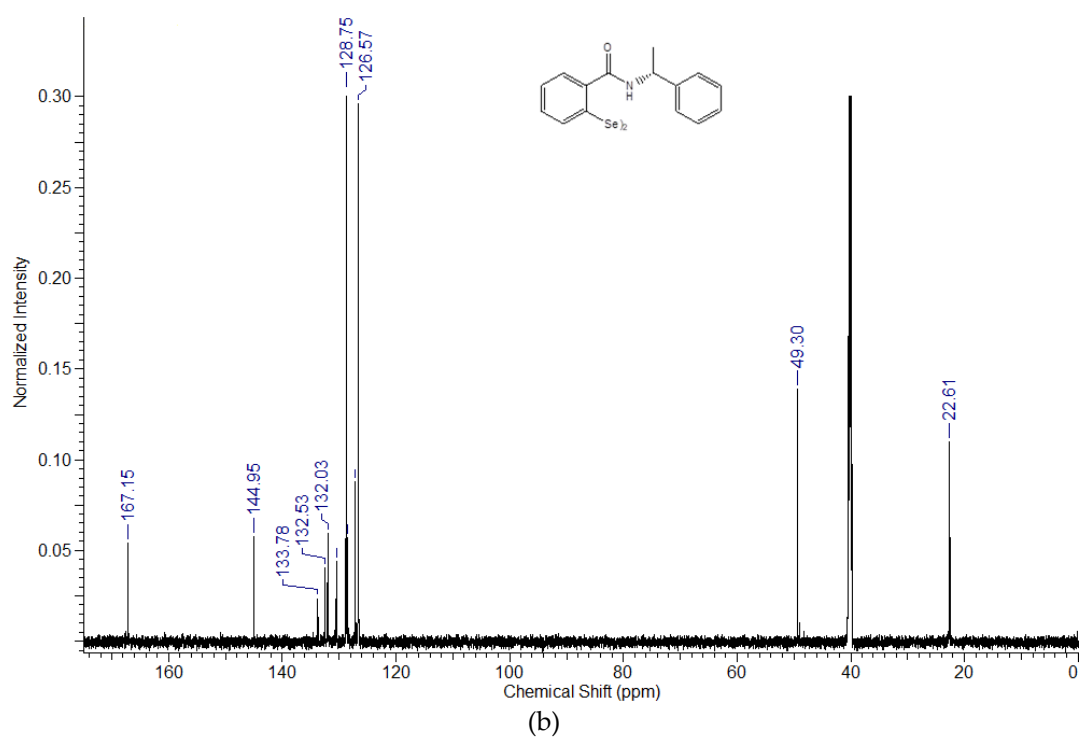
**Figure S19.** (a)  $^1\text{H}$  NMR, (b)  $^{13}\text{C}$  NMR, and (c)  $^{77}\text{Se}$  NMR spectra of 2,2'-diselenobis[N-(R)-(-)-1,2,3,4-tetrahydro-1-naphylbenzamide] 22b





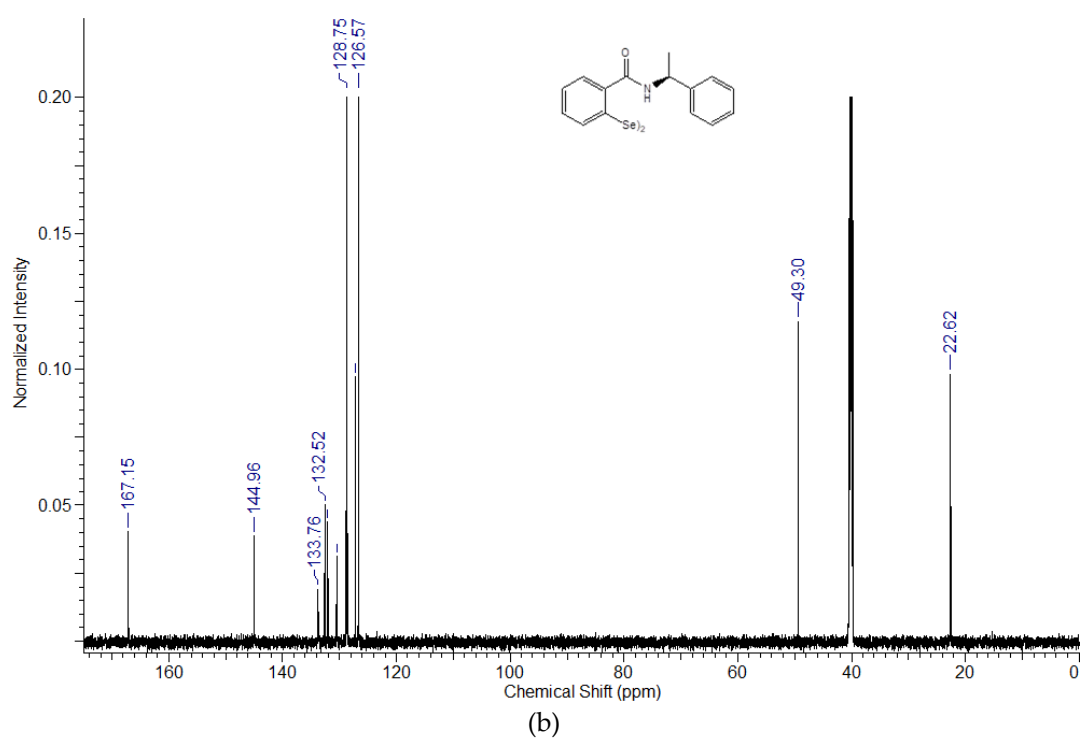
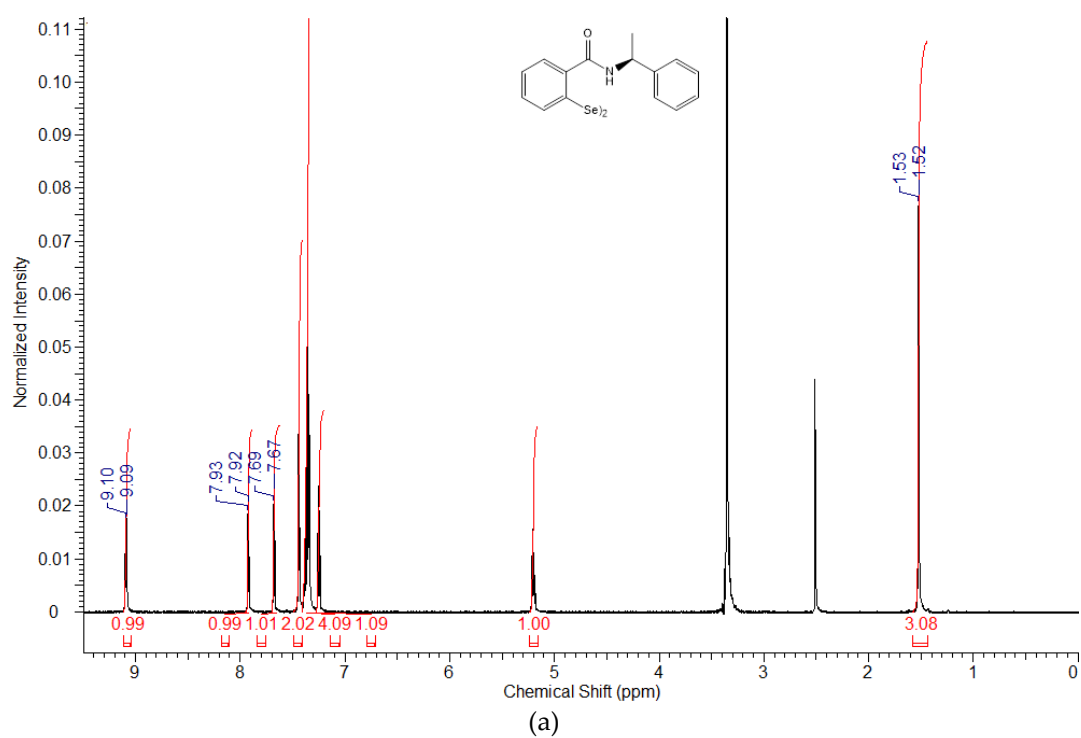
**Figure S20.** (a)  $^1\text{H}$  NMR, (b)  $^{13}\text{C}$  NMR, and (c)  $^{77}\text{Se}$  NMR spectra of 2,2'-diselenobis[*N*-(*S*)-(+)-1,2,3,4-tetrahydro-1-naphthylbezamide] **23b**

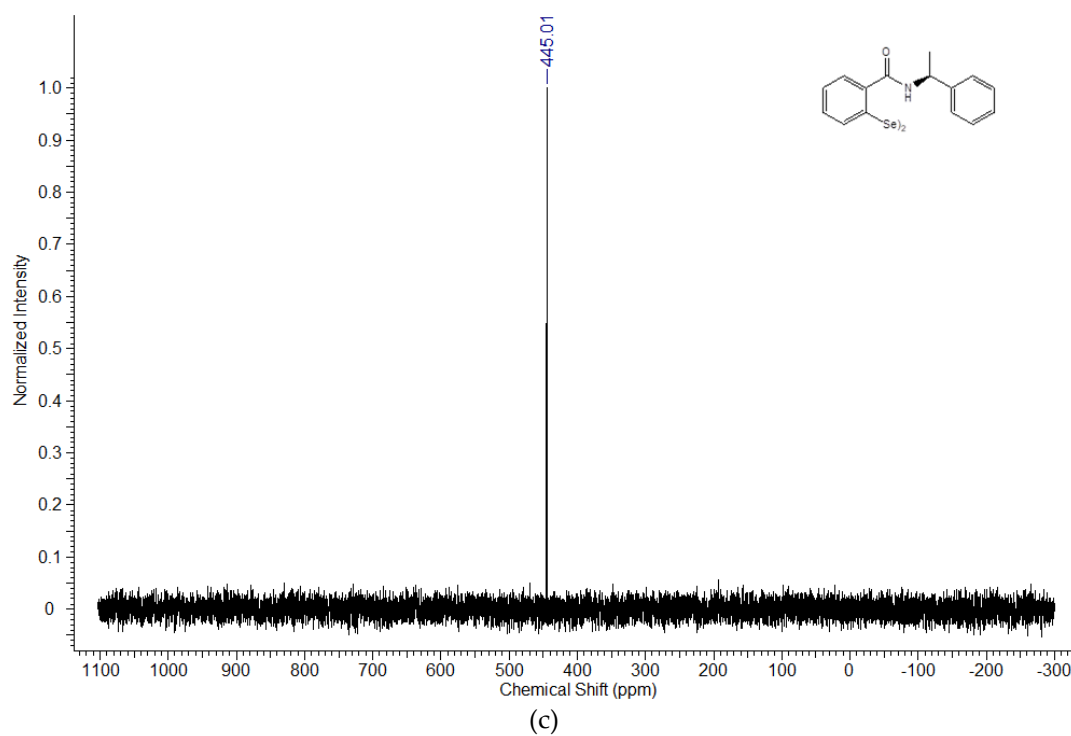




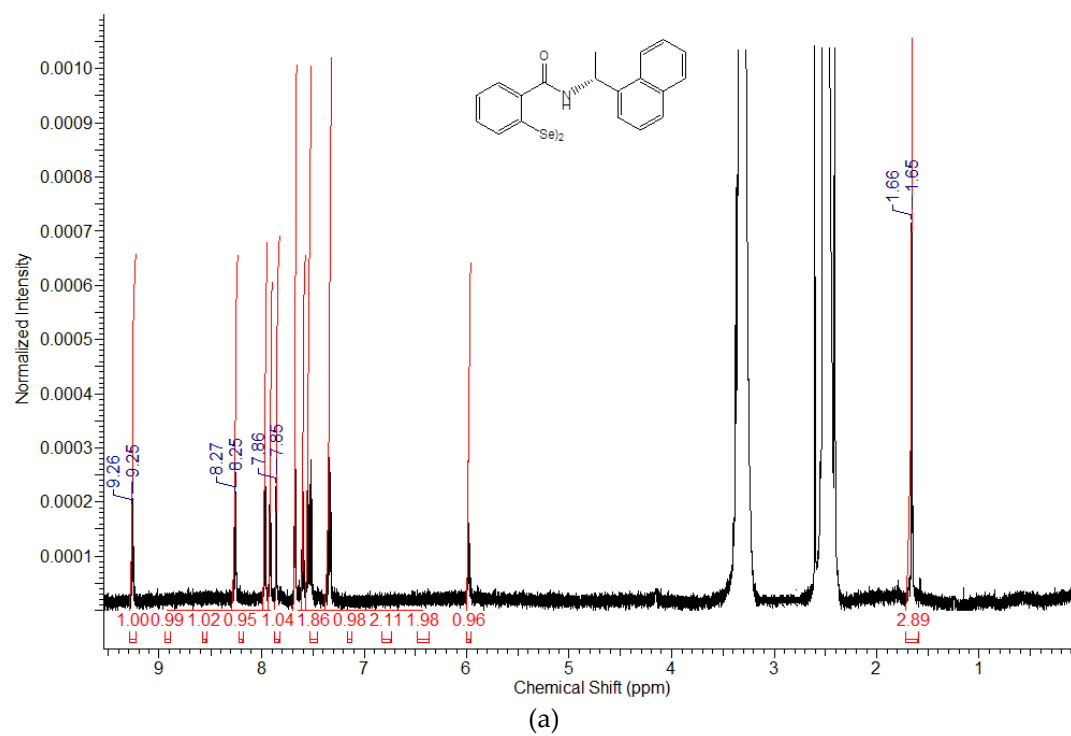
**Figure S21.** (a)  $^1\text{H}$  NMR, (b)  $^{13}\text{C}$  NMR, and (c)  $^{77}\text{Se}$  NMR spectra of 2,2'-diselenobis[N-(R)-(+)- $\alpha$ -methylbenzylbezamide] **24b**.

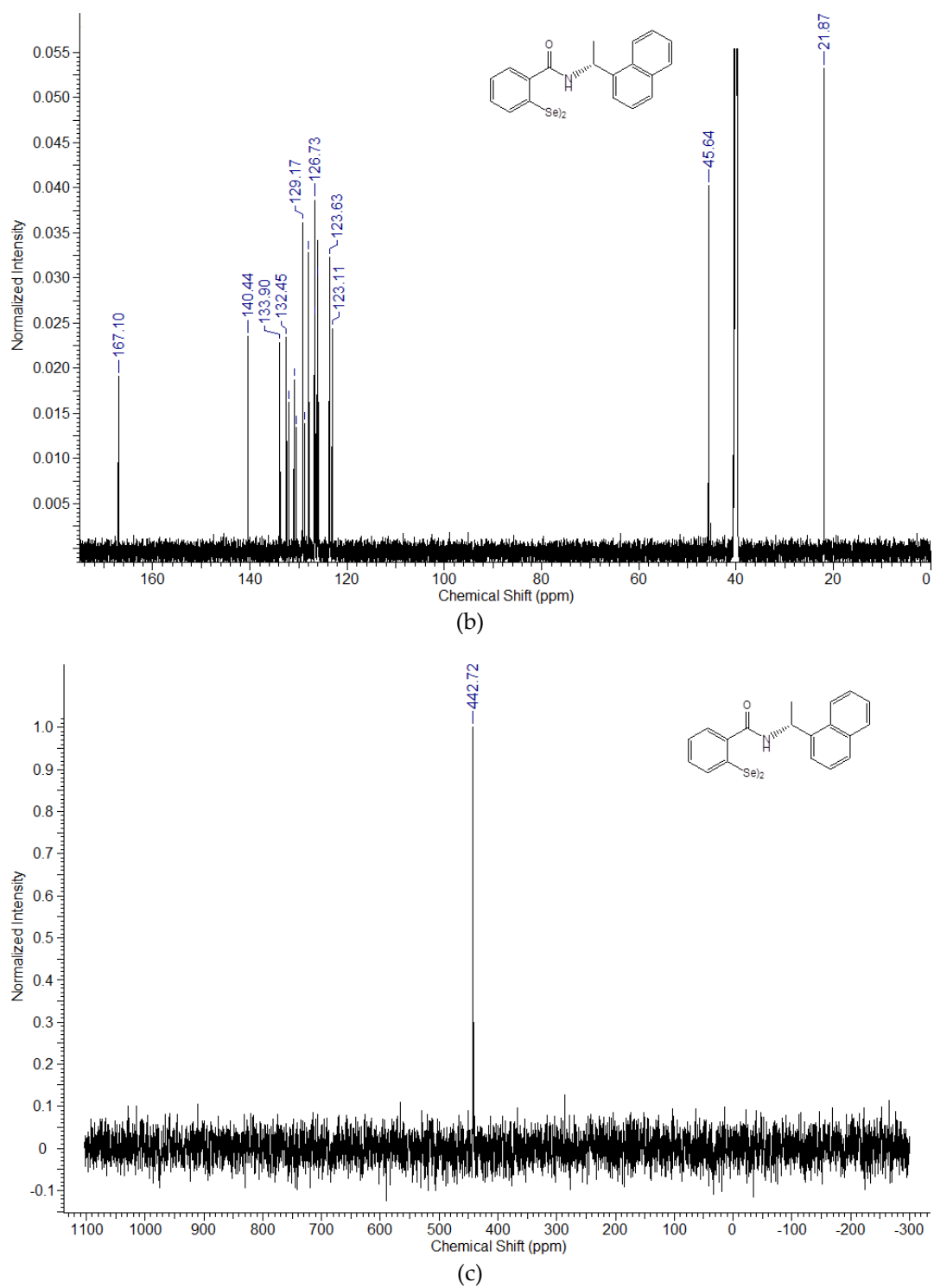




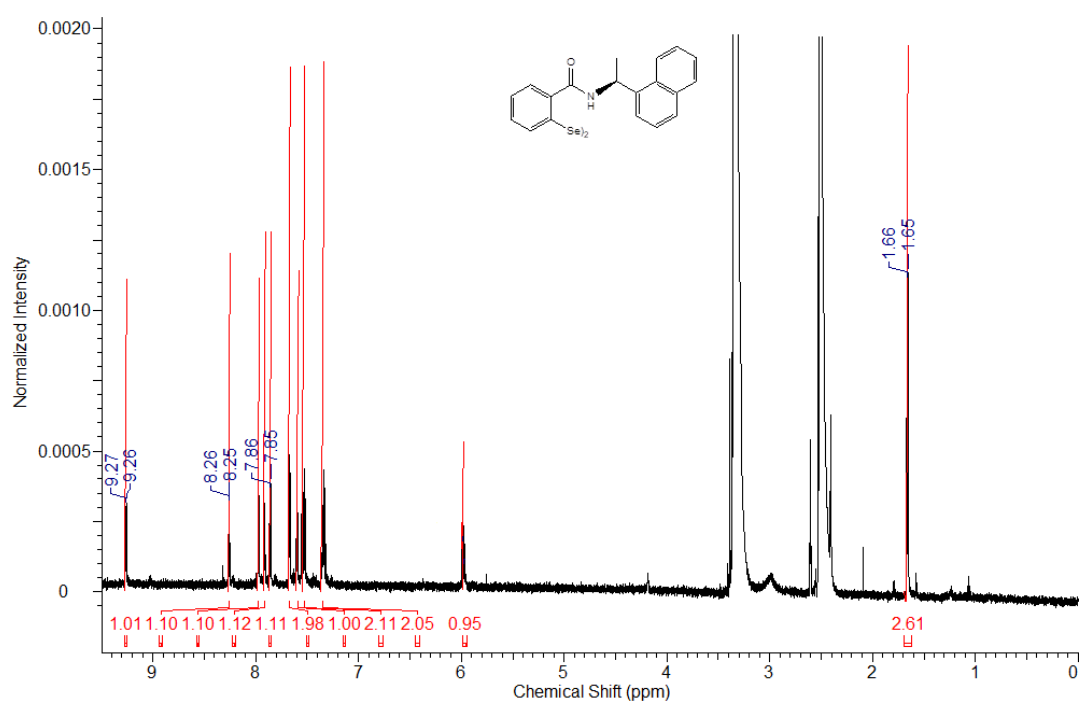


**Figure S22.** (a)  $^1\text{H}$  NMR, (b)  $^{13}\text{C}$  NMR, and (c)  $^{77}\text{Se}$  NMR spectra of 2,2'-diselenobis[N-(S)-(-)- $\alpha$ -methylbenzylbezamide] **25b**.

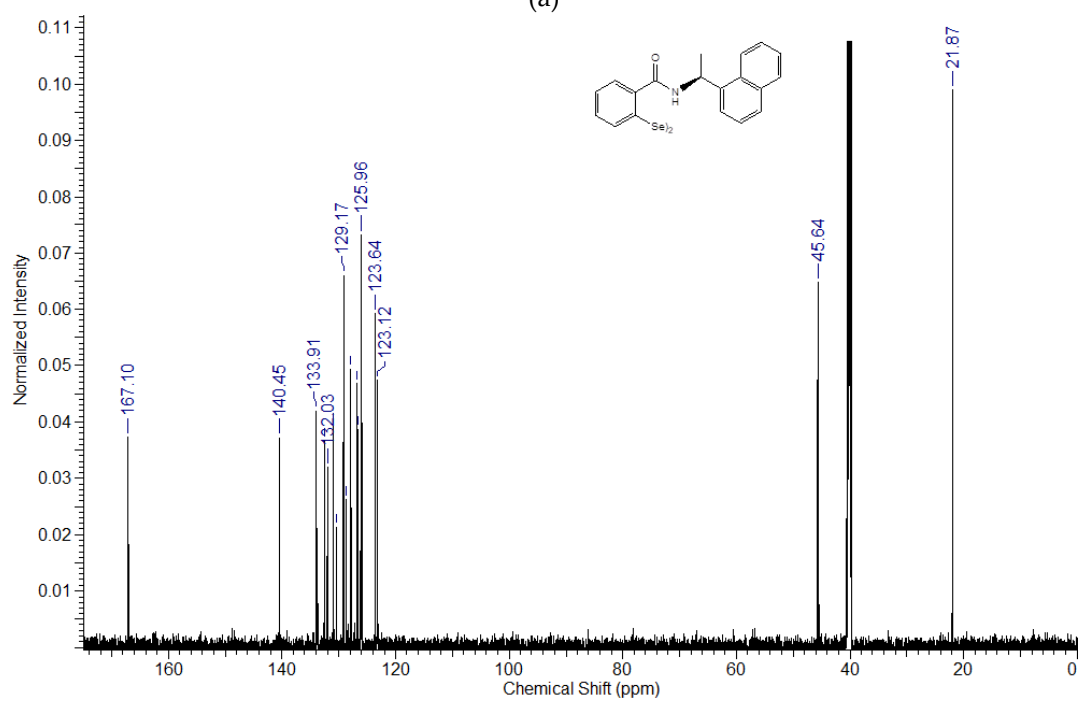




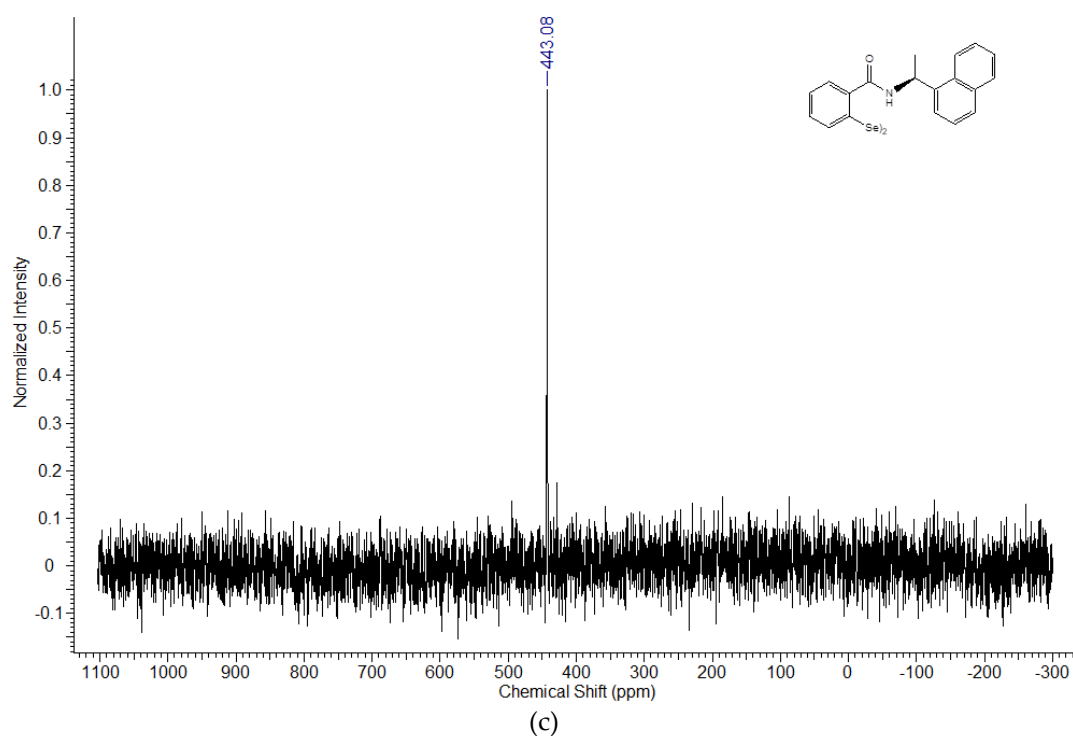
**Figure S23.** (a) <sup>1</sup>H NMR, (b) <sup>13</sup>C NMR, and (c) <sup>77</sup>Se NMR spectra of 2,2'-diselenobis[*N*-(*S*)-(-)-1-(1-naphthyl)ethyl]benzamide] **26b**.



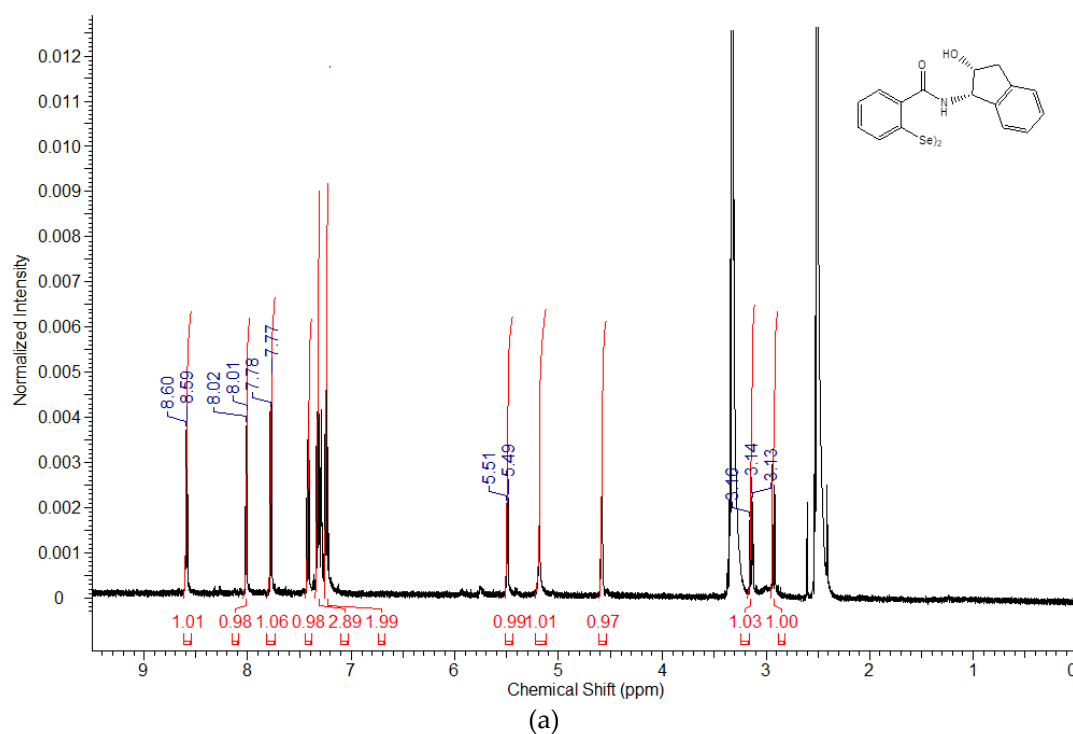
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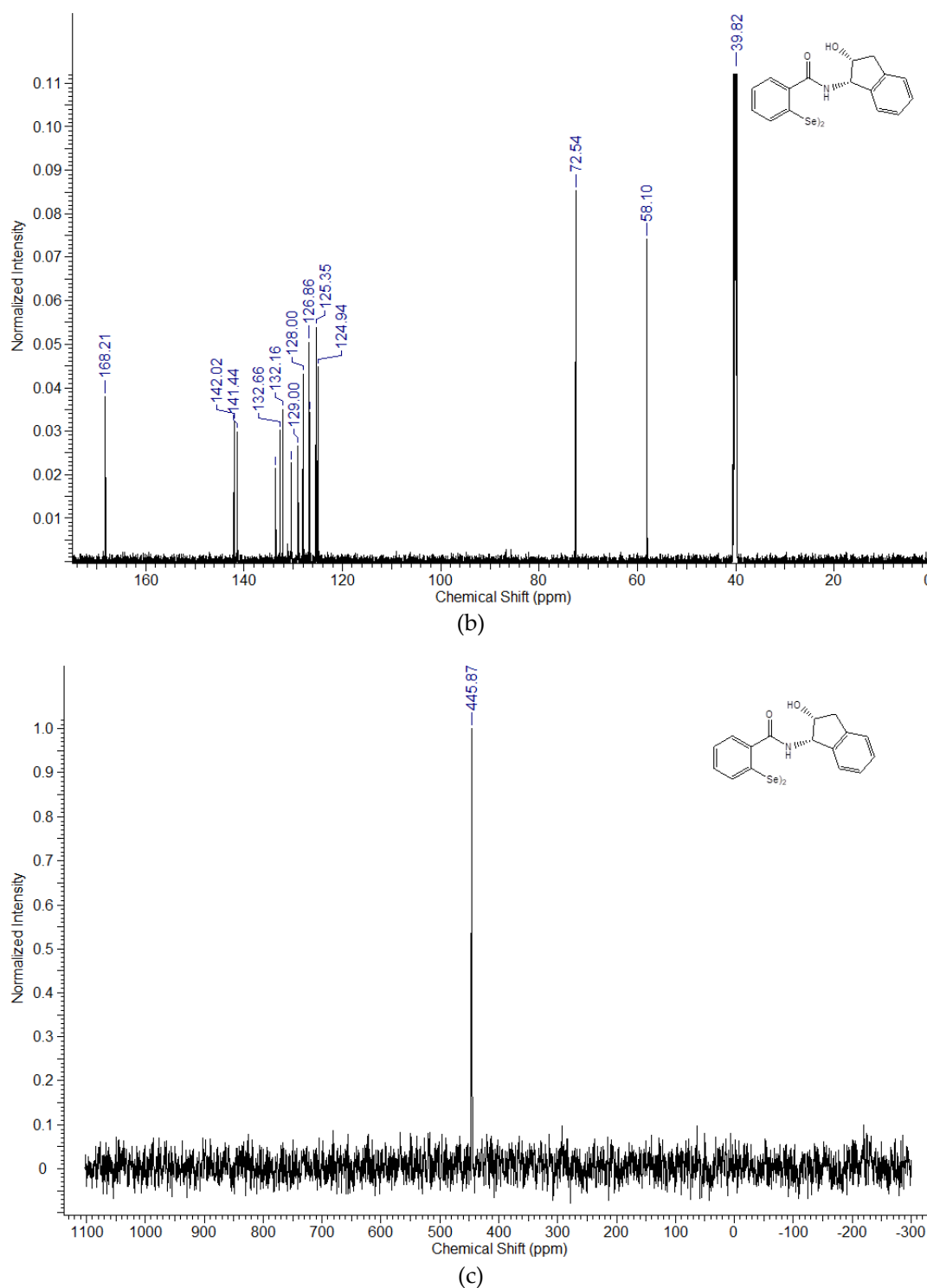


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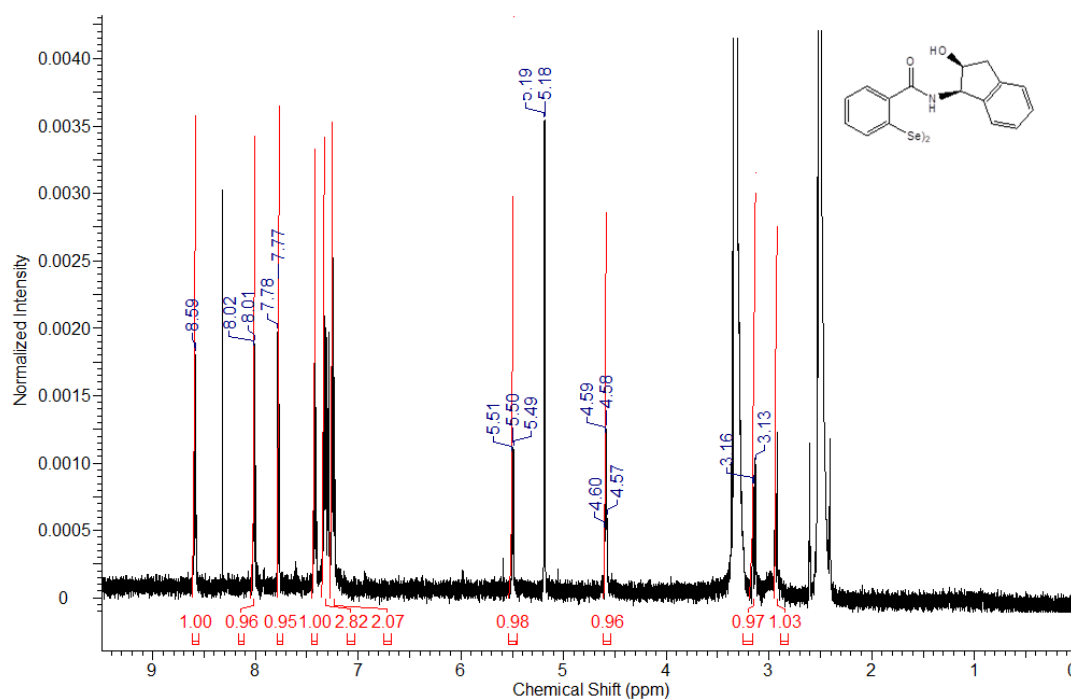


**Figure S24.** (a)  $^1\text{H}$  NMR, (b)  $^{13}\text{C}$  NMR, and (c)  $^{77}\text{Se}$  NMR spectra of 2,2'-diselenobis[N-(R)-(+)-1-(1-naphthyl)ethyl]benzamide **27b**.

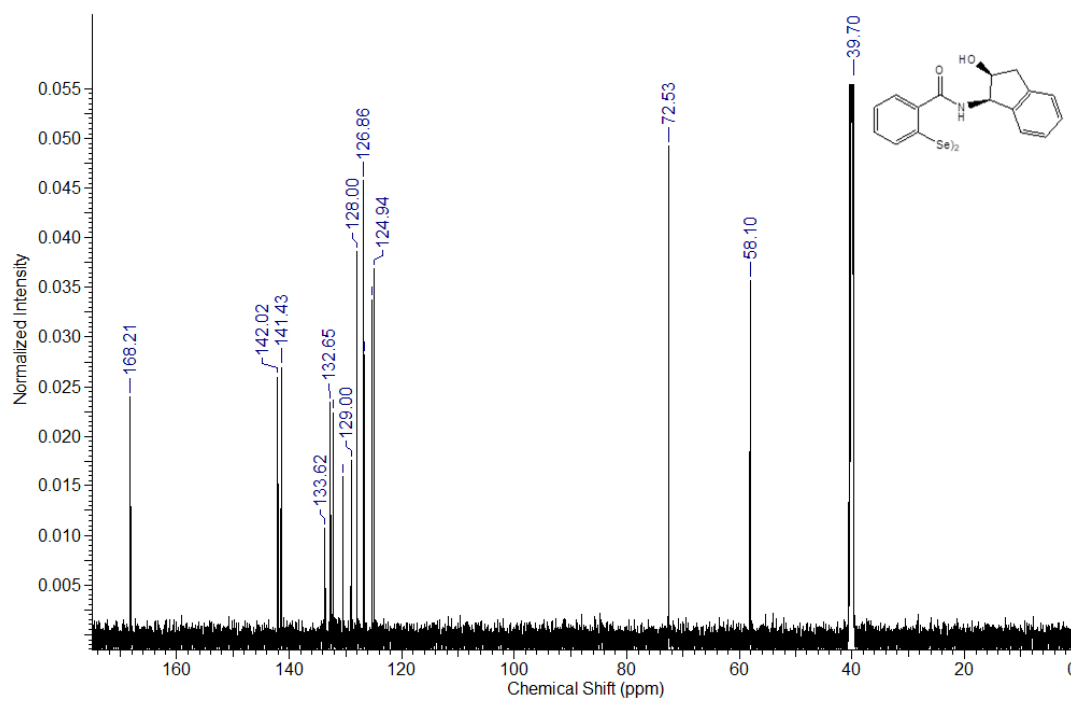




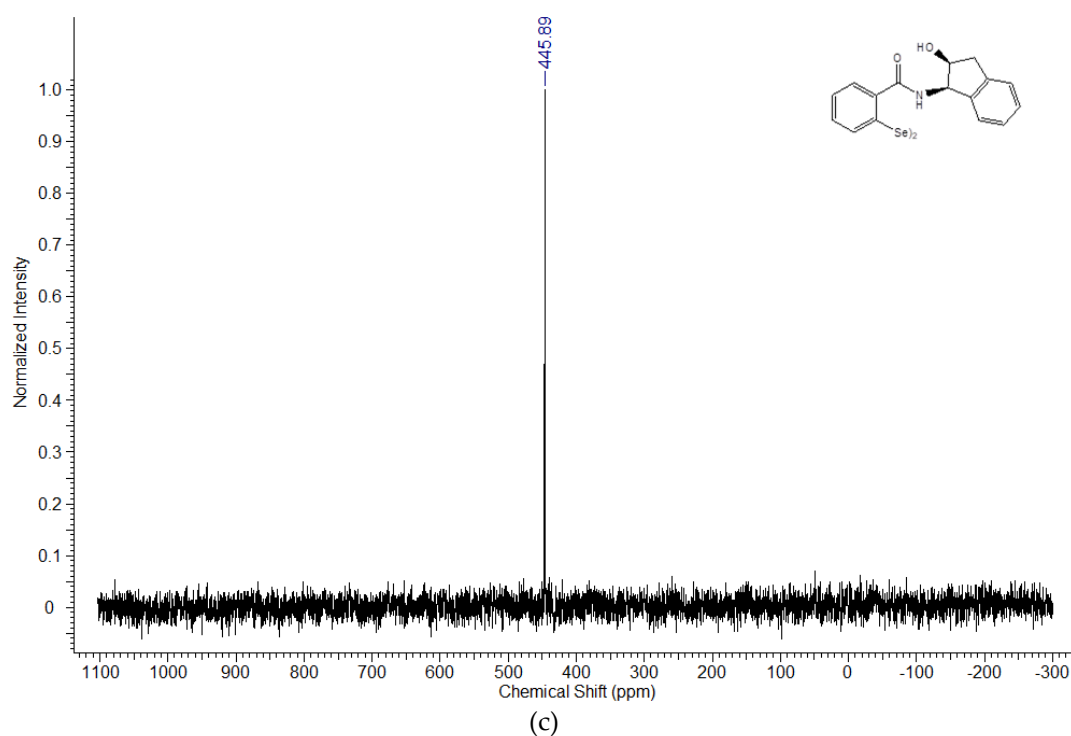
**Figure S25.** (a)  $^1\text{H}$  NMR, (b)  $^{13}\text{C}$  NMR, and (c)  $^{77}\text{Se}$  NMR spectra of 2,2'-diselenobis[N-(1S,2R)-(-)-cis-2-hydroxy-1-indanyl]benzamide **28b**.



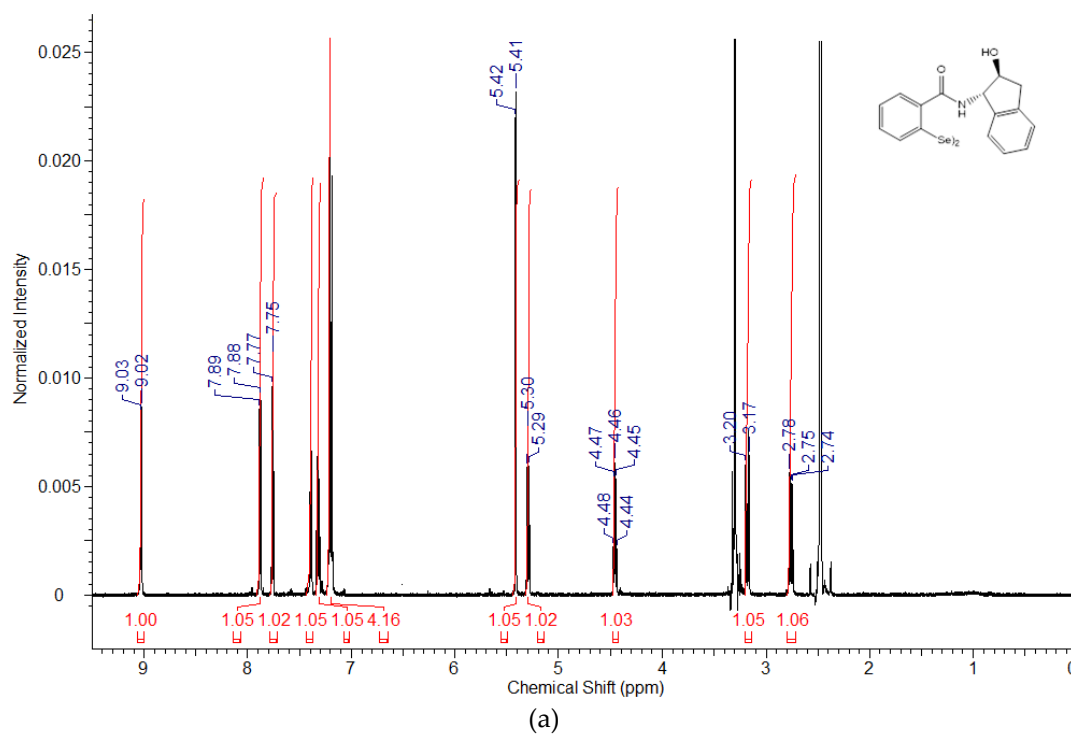
(a)



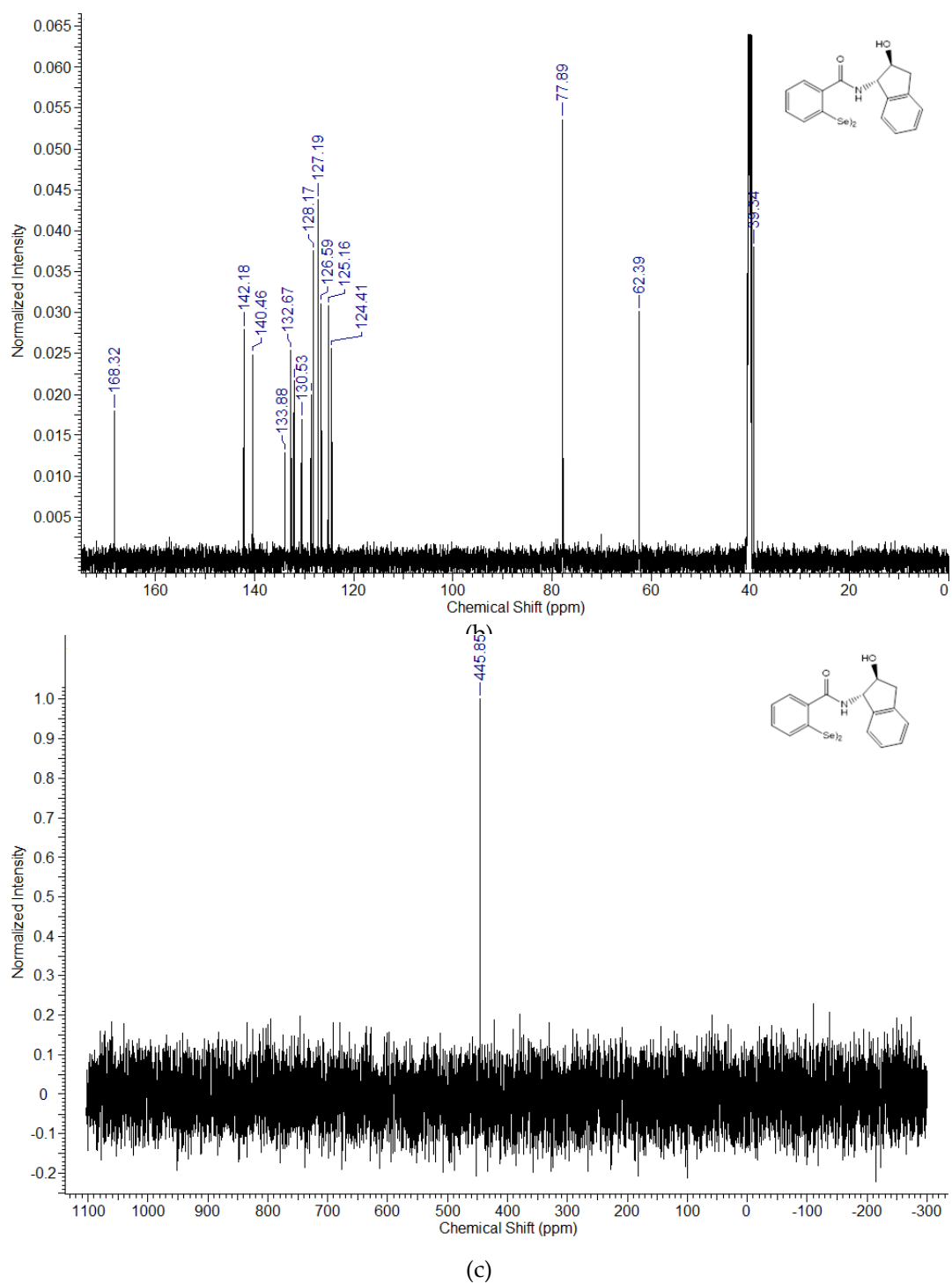
(b)



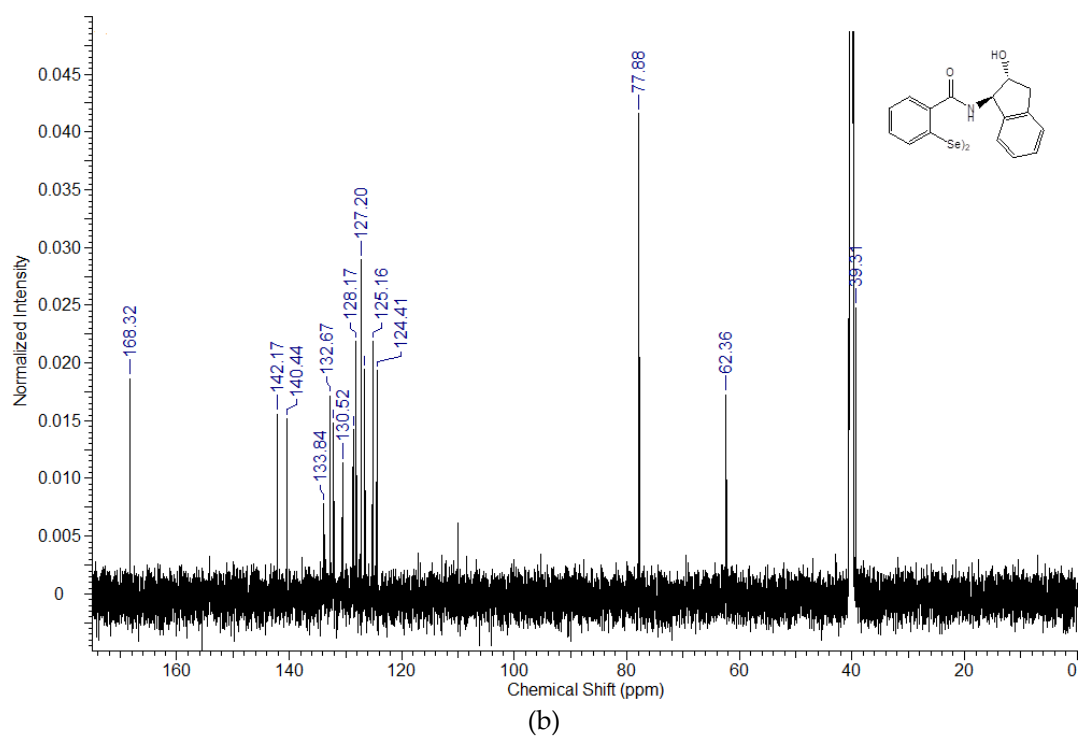
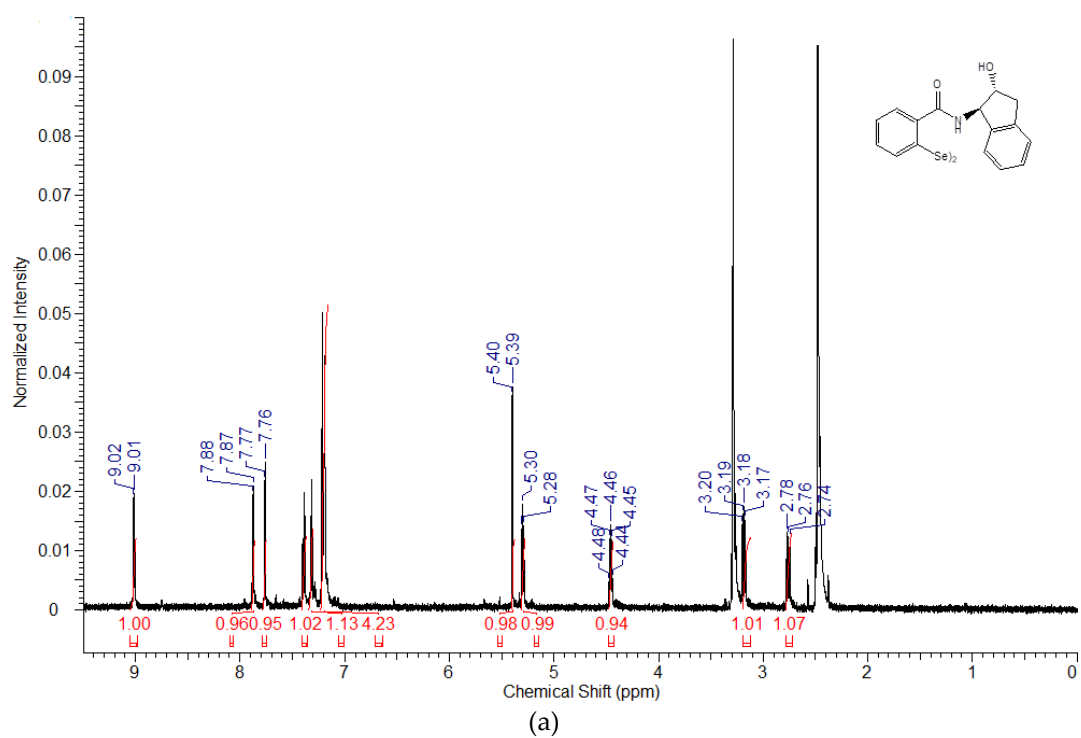
**Figure S26.** (a)  $^1\text{H}$  NMR, (b)  $^{13}\text{C}$  NMR, and (c)  $^{77}\text{Se}$  NMR spectra of 2,2'-diselenobis[*N*-(1*R*,2*S*)-(+)-*cis*-2-hydroxy-1-indanylbezamide] **29b**.

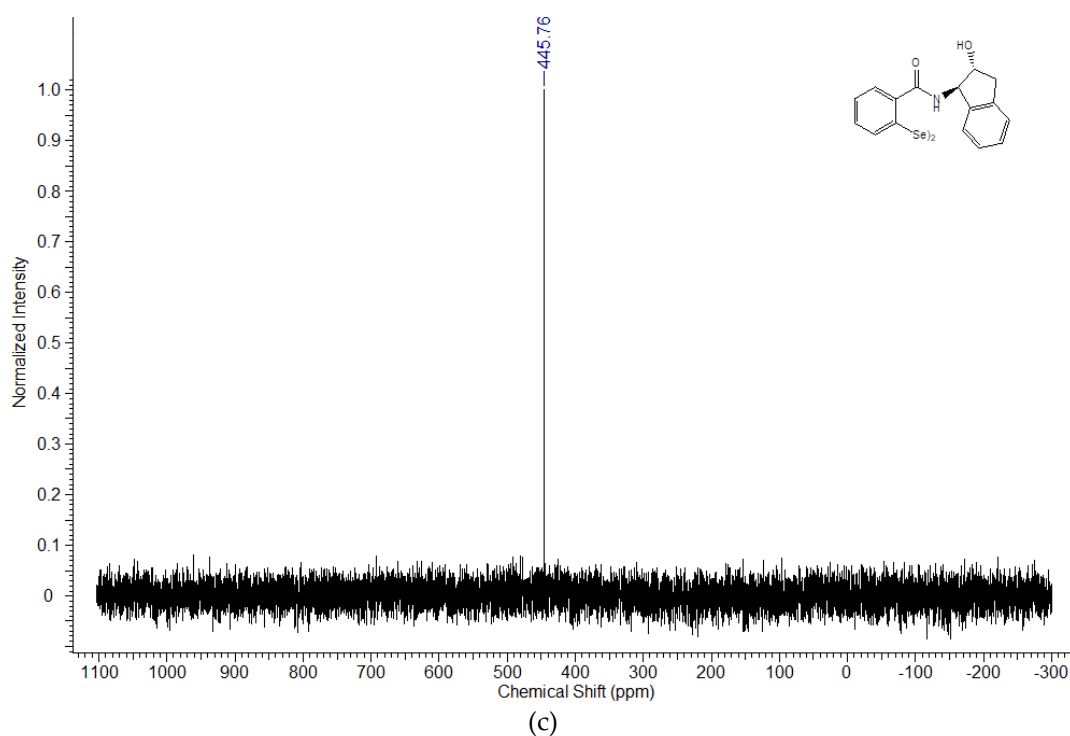






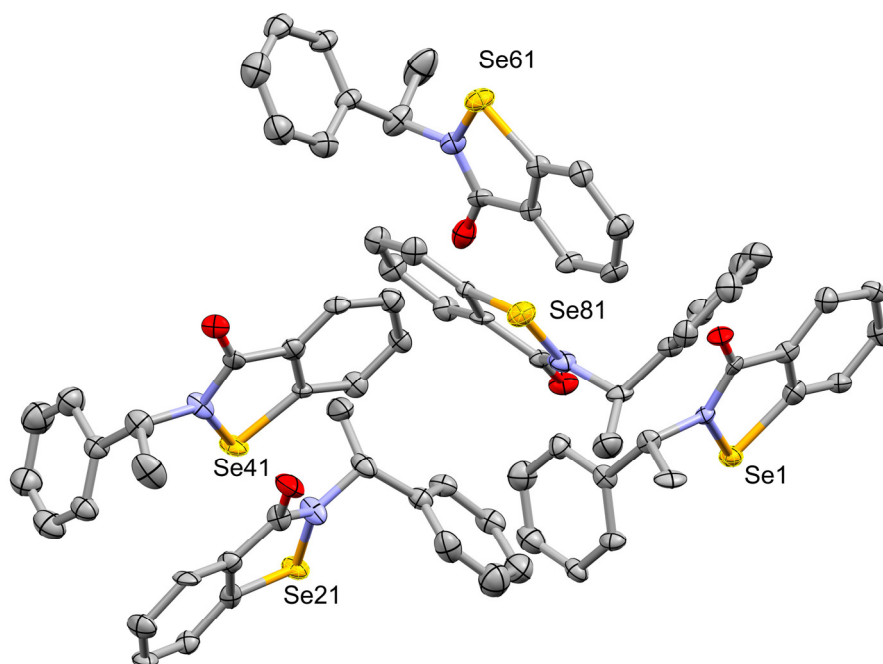
**Figure S27.** (a)  $^1\text{H}$  NMR, (b)  $^{13}\text{C}$  NMR, and (c)  $^{77}\text{Se}$  NMR spectra of 2,2'-diselenobis[N-(1*S*,2*S*)-(-)-*trans*-2-hydroxy-1-indanyl]benzamide] **30b**.



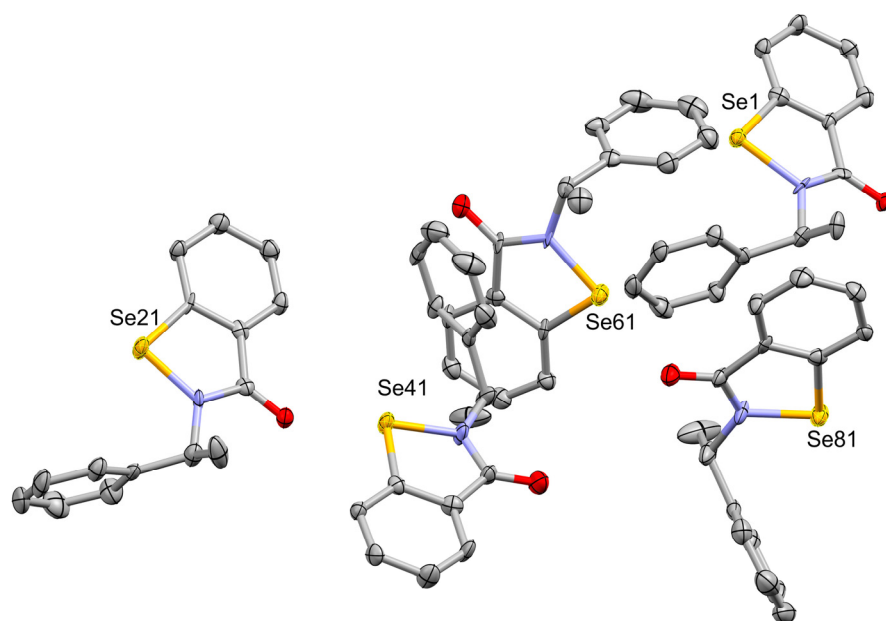


**Figure S28.** (a)  $^1\text{H}$  NMR, (b)  $^{13}\text{C}$  NMR, and (c)  $^{77}\text{Se}$  NMR spectra of 2,2'-diselenobis[*N*-(1*R*,2*R*)-(-)-*trans*-2-hydroxy-1-indanylbezamide] **31b**.

### 3. Crystallographic data of benzoselenazolo-3(2H)-ones **24a** and **25a**



**Figure S29.** Asymmetric part of the structure **24a**. Selenium atoms are labelled to identify molecules 1-5. ADPs are plotted at 50% probability level. Hydrogen atoms are omitted for clarity.



**Figure S30.** Asymmetric part of the structure **25a**. Selenium atoms are labelled to identify molecules 1-5. ADPs are plotted at 50% probability level. Hydrogen atoms are omitted for clarity.

**Table S1.** Crystal data and structure refinement for **24a**.

Identification code	<b>24a</b>
Empirical formula	C15 H13 N O Se
Formula weight	302.22
Temperature	100(2) K
Wavelength	1.54184 Å
Crystal system	Orthorhombic
Space group	P2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>
Unit cell dimensions	a = 10.0996(2) Å b = 52.3461(11) Å c = 12.6231(3) Å
Volume	6673.5(2) Å <sup>3</sup>
Z	20
Density (calculated)	1.504 Mg/m <sup>3</sup>
Absorption coefficient	3.696 mm <sup>-1</sup>
F(000)	3040
Crystal size	0.138 x 0.110 x 0.065 mm <sup>3</sup>
Theta range for data collection	3.377 to 77.944°.
Index ranges	-12 ≤ h ≤ 12, -66 ≤ k ≤ 47, -15 ≤ l ≤ 15
Reflections collected	85045
Independent reflections	13902 [R(int) = 0.0918]
Completeness to theta = 67.684°	99.9 %
Absorption correction	Semi-empirical from equivalents

Max. and min. transmission	1.00000 and 0.62936
Refinement method	Full-matrix least-squares on $F^2$
Data / restraints / parameters	13902 / 540 / 811
Goodness-of-fit on $F^2$	1.140
Final R indices [ $I > 2\sigma(I)$ ]	$R1 = 0.1055$ , $wR2 = 0.2987$
R indices (all data)	$R1 = 0.1079$ , $wR2 = 0.3013$
Absolute structure parameter	0.042(10)
Extinction coefficient	n/a
Largest diff. peak and hole	3.609 and -2.148 e. $\text{\AA}^{-3}$

**Table S2.** Bond lengths [ $\text{\AA}$ ] and angles [ $^\circ$ ] for **24a**.

Se(1)-C(10)	1.91(2)
Se(1)-N(2)	1.932(14)
N(2)-C(3)	1.31(2)
N(2)-C(11)	1.51(2)
C(3)-O(4)	1.19(2)
C(3)-C(5)	1.52(3)
C(5)-C(10)	1.39(3)
C(5)-C(6)	1.40(3)
C(6)-C(7)	1.39(3)
C(7)-C(8)	1.39(3)
C(8)-C(9)	1.40(3)
C(9)-C(10)	1.37(3)
C(11)-C(12)	1.53(3)
C(11)-C(13)	1.54(3)
C(13)-C(14)	1.37(3)
C(13)-C(18)	1.40(3)
C(14)-C(15)	1.40(3)
C(15)-C(16)	1.40(3)
C(16)-C(17)	1.35(3)
C(17)-C(18)	1.37(3)
Se(21)-C(30)	1.882(19)
Se(21)-N(22)	1.900(15)
N(22)-C(23)	1.36(2)
N(22)-C(31)	1.47(3)
C(23)-O(24)	1.23(3)
C(23)-C(25)	1.43(3)
C(25)-C(26)	1.31(3)
C(25)-C(30)	1.47(3)
C(26)-C(27)	1.42(3)
C(27)-C(28)	1.39(3)
C(28)-C(29)	1.38(3)
C(29)-C(30)	1.38(3)
C(31)-C(32)	1.52(4)
C(31)-C(33)	1.52(3)
C(33)-C(34)	1.36(3)
C(33)-C(38)	1.39(3)

C(34)-C(35)	1.40(3)
C(35)-C(36)	1.39(4)
C(36)-C(37)	1.39(4)
C(37)-C(38)	1.33(4)
Se(41)-N(42)	1.858(17)
Se(41)-C(50)	1.887(17)
N(42)-C(43)	1.33(2)
N(42)-C(51)	1.48(3)
C(43)-O(44)	1.26(2)
C(43)-C(45)	1.46(3)
C(45)-C(46)	1.36(3)
C(45)-C(50)	1.44(3)
C(46)-C(47)	1.40(3)
C(47)-C(48)	1.40(3)
C(48)-C(49)	1.39(3)
C(49)-C(50)	1.38(2)
C(51)-C(52)	1.50(3)
C(51)-C(53)	1.55(3)
C(53)-C(54)	1.38(3)
C(53)-C(58)	1.40(3)
C(54)-C(55)	1.38(3)
C(55)-C(56)	1.35(4)
C(56)-C(57)	1.39(4)
C(57)-C(58)	1.35(4)
Se(61)-N(62)	1.891(16)
Se(61)-C(70)	1.905(18)
N(62)-C(63)	1.33(2)
N(62)-C(71)	1.47(3)
C(63)-O(64)	1.23(2)
C(63)-C(65)	1.49(2)
C(65)-C(70)	1.35(2)
C(65)-C(66)	1.38(3)
C(66)-C(67)	1.41(3)
C(67)-C(68)	1.39(3)
C(68)-C(69)	1.41(3)
C(69)-C(70)	1.40(3)
C(71)-C(73)	1.50(3)
C(71)-C(72)	1.55(4)
C(73)-C(74)	1.36(3)
C(73)-C(78)	1.40(3)
C(74)-C(75)	1.39(3)
C(75)-C(76)	1.35(4)
C(76)-C(77)	1.37(4)
C(77)-C(78)	1.37(3)
Se(81)-C(90)	1.877(17)
Se(81)-N(82)	1.879(17)
N(82)-C(83)	1.34(2)
N(82)-C(91)	1.44(3)
C(83)-O(84)	1.27(2)

C(83)-C(85)	1.51(2)
C(85)-C(86)	1.38(3)
C(85)-C(90)	1.45(2)
C(86)-C(87)	1.45(3)
C(87)-C(88)	1.36(3)
C(88)-C(89)	1.40(3)
C(89)-C(90)	1.37(3)
C(91)-C(92)	1.52(3)
C(91)-C(93)	1.53(3)
C(93)-C(98)	1.39(3)
C(93)-C(94)	1.40(3)
C(94)-C(95)	1.38(3)
C(95)-C(96)	1.37(3)
C(96)-C(97)	1.40(4)
C(97)-C(98)	1.35(3)
C(10)-Se(1)-N(2)	83.0(8)
C(3)-N(2)-C(11)	121.2(15)
C(3)-N(2)-Se(1)	120.6(13)
C(11)-N(2)-Se(1)	118.3(11)
O(4)-C(3)-N(2)	125.1(19)
O(4)-C(3)-C(5)	127.7(18)
N(2)-C(3)-C(5)	107.1(16)
C(10)-C(5)-C(6)	120.7(19)
C(10)-C(5)-C(3)	117.6(18)
C(6)-C(5)-C(3)	121.7(17)
C(7)-C(6)-C(5)	118(2)
C(8)-C(7)-C(6)	121(2)
C(7)-C(8)-C(9)	120(2)
C(10)-C(9)-C(8)	119(2)
C(9)-C(10)-C(5)	121(2)
C(9)-C(10)-Se(1)	127.0(17)
C(5)-C(10)-Se(1)	111.6(16)
N(2)-C(11)-C(12)	110.4(16)
N(2)-C(11)-C(13)	111.0(14)
C(12)-C(11)-C(13)	114.0(16)
C(14)-C(13)-C(18)	118.6(18)
C(14)-C(13)-C(11)	119.9(18)
C(18)-C(13)-C(11)	121.5(17)
C(13)-C(14)-C(15)	121(2)
C(16)-C(15)-C(14)	118(2)
C(17)-C(16)-C(15)	120(2)
C(16)-C(17)-C(18)	121(2)
C(17)-C(18)-C(13)	120.5(19)
C(30)-Se(21)-N(22)	84.8(8)
C(23)-N(22)-C(31)	125.1(16)
C(23)-N(22)-Se(21)	116.3(13)
C(31)-N(22)-Se(21)	118.5(12)
O(24)-C(23)-N(22)	121.6(19)
O(24)-C(23)-C(25)	125.6(18)

N(22)-C(23)-C(25)	112.8(17)
C(26)-C(25)-C(23)	129(2)
C(26)-C(25)-C(30)	117.5(19)
C(23)-C(25)-C(30)	113.5(17)
C(25)-C(26)-C(27)	123(2)
C(28)-C(27)-C(26)	119(2)
C(29)-C(28)-C(27)	120.3(19)
C(30)-C(29)-C(28)	120.0(19)
C(29)-C(30)-C(25)	120.1(17)
C(29)-C(30)-Se(21)	127.6(15)
C(25)-C(30)-Se(21)	112.3(14)
N(22)-C(31)-C(32)	110.5(19)
N(22)-C(31)-C(33)	109.0(17)
C(32)-C(31)-C(33)	115.5(19)
C(34)-C(33)-C(38)	118(2)
C(34)-C(33)-C(31)	123.2(19)
C(38)-C(33)-C(31)	118(2)
C(33)-C(34)-C(35)	121(2)
C(36)-C(35)-C(34)	119(2)
C(37)-C(36)-C(35)	118(2)
C(38)-C(37)-C(36)	122(3)
C(37)-C(38)-C(33)	121(2)
N(42)-Se(41)-C(50)	85.4(7)
C(43)-N(42)-C(51)	120.7(17)
C(43)-N(42)-Se(41)	117.2(14)
C(51)-N(42)-Se(41)	122.1(13)
O(44)-C(43)-N(42)	124.1(18)
O(44)-C(43)-C(45)	123.1(18)
N(42)-C(43)-C(45)	112.6(18)
C(46)-C(45)-C(50)	119.0(18)
C(46)-C(45)-C(43)	127.4(19)
C(50)-C(45)-C(43)	113.5(17)
C(45)-C(46)-C(47)	120.6(18)
C(46)-C(47)-C(48)	119.8(19)
C(49)-C(48)-C(47)	120.7(19)
C(50)-C(49)-C(48)	118.8(18)
C(49)-C(50)-C(45)	120.9(17)
C(49)-C(50)-Se(41)	127.8(14)
C(45)-C(50)-Se(41)	111.2(13)
N(42)-C(51)-C(52)	109.7(19)
N(42)-C(51)-C(53)	107.7(16)
C(52)-C(51)-C(53)	115(2)
C(54)-C(53)-C(58)	118(2)
C(54)-C(53)-C(51)	124(2)
C(58)-C(53)-C(51)	118.1(19)
C(53)-C(54)-C(55)	120(2)
C(56)-C(55)-C(54)	122(2)
C(55)-C(56)-C(57)	119(2)
C(55)-C(56)-H(56A)	120.3



C(57)-C(56)-H(56A)	120.3
C(58)-C(57)-C(56)	120(3)
C(57)-C(58)-C(53)	121(2)
N(62)-Se(61)-C(70)	83.7(7)
C(63)-N(62)-C(71)	122.0(17)
C(63)-N(62)-Se(61)	118.3(13)
C(71)-N(62)-Se(61)	119.0(13)
O(64)-C(63)-N(62)	125.6(18)
O(64)-C(63)-C(65)	125.6(17)
N(62)-C(63)-C(65)	108.7(16)
C(70)-C(65)-C(66)	118.9(17)
C(70)-C(65)-C(63)	117.0(17)
C(66)-C(65)-C(63)	124.1(17)
C(65)-C(66)-C(67)	120.6(18)
C(68)-C(67)-C(66)	119.0(19)
C(67)-C(68)-C(69)	121(2)
C(70)-C(69)-C(68)	117.1(19)
C(65)-C(70)-C(69)	123.5(18)
C(65)-C(70)-Se(61)	112.2(13)
C(69)-C(70)-Se(61)	124.1(14)
N(62)-C(71)-C(73)	110.3(17)
N(62)-C(71)-C(72)	107(2)
C(73)-C(71)-C(72)	114(2)
C(74)-C(73)-C(78)	118(2)
C(74)-C(73)-C(71)	125(2)
C(78)-C(73)-C(71)	117.4(19)
C(73)-C(74)-C(75)	120(2)
C(76)-C(75)-C(74)	123(2)
C(75)-C(76)-C(77)	118(2)
C(76)-C(77)-C(78)	120(3)
C(77)-C(78)-C(73)	121(2)
C(90)-Se(81)-N(82)	86.5(7)
C(83)-N(82)-C(91)	122.6(16)
C(83)-N(82)-Se(81)	117.7(13)
C(91)-N(82)-Se(81)	119.5(13)
O(84)-C(83)-N(82)	126.6(16)
O(84)-C(83)-C(85)	122.9(15)
N(82)-C(83)-C(85)	110.4(15)
C(86)-C(85)-C(90)	121.8(17)
C(86)-C(85)-C(83)	124.0(16)
C(90)-C(85)-C(83)	114.2(15)
C(85)-C(86)-C(87)	115.0(18)
C(88)-C(87)-C(86)	123(2)
C(87)-C(88)-C(89)	121(2)
C(90)-C(89)-C(88)	119.0(19)
C(89)-C(90)-C(85)	120.3(17)
C(89)-C(90)-Se(81)	128.6(14)
C(85)-C(90)-Se(81)	111.1(12)
N(82)-C(91)-C(92)	111.1(18)

N(82)-C(91)-C(93)	109.8(15)
C(92)-C(91)-C(93)	114.3(18)
C(98)-C(93)-C(94)	117.7(19)
C(98)-C(93)-C(91)	118.6(19)
C(94)-C(93)-C(91)	123.5(18)
C(95)-C(94)-C(93)	121(2)
C(96)-C(95)-C(94)	118(2)
C(95)-C(96)-C(97)	122(2)
C(98)-C(97)-C(96)	119(2)
C(97)-C(98)-C(93)	122(2)

**Table S3.** Torsion angles [°] for **24a**.

C(11)-N(2)-C(3)-O(4)	-3(3)
Se(1)-N(2)-C(3)-O(4)	176.7(15)
C(11)-N(2)-C(3)-C(5)	-179.0(14)
Se(1)-N(2)-C(3)-C(5)	0.5(19)
O(4)-C(3)-C(5)-C(10)	-178.6(19)
N(2)-C(3)-C(5)-C(10)	-3(2)
O(4)-C(3)-C(5)-C(6)	2(3)
N(2)-C(3)-C(5)-C(6)	177.9(17)
C(10)-C(5)-C(6)-C(7)	-1(3)
C(3)-C(5)-C(6)-C(7)	178.8(17)
C(5)-C(6)-C(7)-C(8)	2(3)
C(6)-C(7)-C(8)-C(9)	0(3)
C(7)-C(8)-C(9)-C(10)	-2(3)
C(8)-C(9)-C(10)-C(5)	3(3)
C(8)-C(9)-C(10)-Se(1)	177.8(16)
C(6)-C(5)-C(10)-C(9)	-2(3)
C(3)-C(5)-C(10)-C(9)	178.7(17)
C(6)-C(5)-C(10)-Se(1)	-177.1(14)
C(3)-C(5)-C(10)-Se(1)	3(2)
C(3)-N(2)-C(11)-C(12)	-78(2)
Se(1)-N(2)-C(11)-C(12)	102.1(15)
C(3)-N(2)-C(11)-C(13)	154.3(16)
Se(1)-N(2)-C(11)-C(13)	-25.3(19)
N(2)-C(11)-C(13)-C(14)	-86(2)
C(12)-C(11)-C(13)-C(14)	148.5(19)
N(2)-C(11)-C(13)-C(18)	90(2)
C(12)-C(11)-C(13)-C(18)	-35(2)
C(18)-C(13)-C(14)-C(15)	-1(3)
C(11)-C(13)-C(14)-C(15)	175.5(19)
C(13)-C(14)-C(15)-C(16)	1(3)
C(14)-C(15)-C(16)-C(17)	-2(3)
C(15)-C(16)-C(17)-C(18)	2(3)
C(16)-C(17)-C(18)-C(13)	-2(3)
C(14)-C(13)-C(18)-C(17)	1(3)
C(11)-C(13)-C(18)-C(17)	-174.9(18)
C(31)-N(22)-C(23)-O(24)	-3(3)
Se(21)-N(22)-C(23)-O(24)	175.0(17)

C(31)-N(22)-C(23)-C(25)	176(2)
Se(21)-N(22)-C(23)-C(25)	-7(2)
O(24)-C(23)-C(25)-C(26)	1(4)
N(22)-C(23)-C(25)-C(26)	-177(2)
O(24)-C(23)-C(25)-C(30)	-177(2)
N(22)-C(23)-C(25)-C(30)	5(3)
C(23)-C(25)-C(26)-C(27)	-177(2)
C(30)-C(25)-C(26)-C(27)	1(3)
C(25)-C(26)-C(27)-C(28)	2(4)
C(26)-C(27)-C(28)-C(29)	-5(3)
C(27)-C(28)-C(29)-C(30)	5(3)
C(28)-C(29)-C(30)-C(25)	-1(3)
C(28)-C(29)-C(30)-Se(21)	176.3(15)
C(26)-C(25)-C(30)-C(29)	-1(3)
C(23)-C(25)-C(30)-C(29)	177.1(18)
C(26)-C(25)-C(30)-Se(21)	-179.5(16)
C(23)-C(25)-C(30)-Se(21)	-1(2)
N(22)-Se(21)-C(30)-C(29)	180.0(19)
N(22)-Se(21)-C(30)-C(25)	-2.1(14)
C(23)-N(22)-C(31)-C(32)	-100(3)
Se(21)-N(22)-C(31)-C(32)	83(2)
C(23)-N(22)-C(31)-C(33)	132(2)
Se(21)-N(22)-C(31)-C(33)	-45(2)
N(22)-C(31)-C(33)-C(34)	115(2)
C(32)-C(31)-C(33)-C(34)	-10(3)
N(22)-C(31)-C(33)-C(38)	-60(3)
C(32)-C(31)-C(33)-C(38)	175(2)
C(38)-C(33)-C(34)-C(35)	3(3)
C(31)-C(33)-C(34)-C(35)	-173(2)
C(33)-C(34)-C(35)-C(36)	-4(3)
C(34)-C(35)-C(36)-C(37)	4(4)
C(35)-C(36)-C(37)-C(38)	-2(4)
C(36)-C(37)-C(38)-C(33)	1(4)
C(34)-C(33)-C(38)-C(37)	-1(3)
C(31)-C(33)-C(38)-C(37)	175(2)
C(50)-Se(41)-N(42)-C(43)	0.6(15)
C(50)-Se(41)-N(42)-C(51)	-179.3(16)
C(51)-N(42)-C(43)-O(44)	-5(3)
Se(41)-N(42)-C(43)-O(44)	175.2(15)
C(51)-N(42)-C(43)-C(45)	179.4(18)
Se(41)-N(42)-C(43)-C(45)	0(2)
O(44)-C(43)-C(45)-C(46)	3(3)
N(42)-C(43)-C(45)-C(46)	178.8(19)
O(44)-C(43)-C(45)-C(50)	-175.7(17)
N(42)-C(43)-C(45)-C(50)	0(2)
C(50)-C(45)-C(46)-C(47)	-1(3)
C(43)-C(45)-C(46)-C(47)	-179.4(19)
C(45)-C(46)-C(47)-C(48)	1(3)
C(46)-C(47)-C(48)-C(49)	1(3)

C(47)-C(48)-C(49)-C(50)	-2(3)
C(48)-C(49)-C(50)-C(45)	3(3)
C(48)-C(49)-C(50)-Se(41)	179.6(15)
C(46)-C(45)-C(50)-C(49)	-1(3)
C(43)-C(45)-C(50)-C(49)	177.8(17)
C(46)-C(45)-C(50)-Se(41)	-178.5(14)
C(43)-C(45)-C(50)-Se(41)	0(2)
N(42)-Se(41)-C(50)-C(49)	-177.7(18)
N(42)-Se(41)-C(50)-C(45)	-0.5(14)
C(43)-N(42)-C(51)-C(52)	-86(3)
Se(41)-N(42)-C(51)-C(52)	94(2)
C(43)-N(42)-C(51)-C(53)	148.1(18)
Se(41)-N(42)-C(51)-C(53)	-32(2)
N(42)-C(51)-C(53)-C(54)	103(2)
C(52)-C(51)-C(53)-C(54)	-20(3)
N(42)-C(51)-C(53)-C(58)	-75(2)
C(52)-C(51)-C(53)-C(58)	162(2)
C(58)-C(53)-C(54)-C(55)	3(3)
C(51)-C(53)-C(54)-C(55)	-176(2)
C(53)-C(54)-C(55)-C(56)	-1(4)
C(54)-C(55)-C(56)-C(57)	0(4)
C(55)-C(56)-C(57)-C(58)	-2(4)
C(56)-C(57)-C(58)-C(53)	4(4)
C(54)-C(53)-C(58)-C(57)	-4(4)
C(51)-C(53)-C(58)-C(57)	174(2)
C(70)-Se(61)-N(62)-C(63)	3.7(15)
C(70)-Se(61)-N(62)-C(71)	174.7(17)
C(71)-N(62)-C(63)-O(64)	1(3)
Se(61)-N(62)-C(63)-O(64)	172.2(16)
C(71)-N(62)-C(63)-C(65)	-174.5(18)
Se(61)-N(62)-C(63)-C(65)	-4(2)
O(64)-C(63)-C(65)-C(70)	-174.3(19)
N(62)-C(63)-C(65)-C(70)	2(2)
O(64)-C(63)-C(65)-C(66)	5(3)
N(62)-C(63)-C(65)-C(66)	-179.0(18)
C(70)-C(65)-C(66)-C(67)	2(3)
C(63)-C(65)-C(66)-C(67)	-177.6(18)
C(65)-C(66)-C(67)-C(68)	0(3)
C(66)-C(67)-C(68)-C(69)	1(3)
C(67)-C(68)-C(69)-C(70)	-3(3)
C(66)-C(65)-C(70)-C(69)	-4(3)
C(63)-C(65)-C(70)-C(69)	175.8(17)
C(66)-C(65)-C(70)-Se(61)	-178.3(15)
C(63)-C(65)-C(70)-Se(61)	1(2)
C(68)-C(69)-C(70)-C(65)	4(3)
C(68)-C(69)-C(70)-Se(61)	178.0(15)
C(63)-N(62)-C(71)-C(73)	131(2)
Se(61)-N(62)-C(71)-C(73)	-40(2)
C(63)-N(62)-C(71)-C(72)	-105(2)

Se(61)-N(62)-C(71)-C(72)	85(2)
N(62)-C(71)-C(73)-C(74)	121(2)
C(72)-C(71)-C(73)-C(74)	0(3)
N(62)-C(71)-C(73)-C(78)	-61(3)
C(72)-C(71)-C(73)-C(78)	178(2)
C(78)-C(73)-C(74)-C(75)	3(3)
C(71)-C(73)-C(74)-C(75)	-179(2)
C(73)-C(74)-C(75)-C(76)	-2(4)
C(74)-C(75)-C(76)-C(77)	0(4)
C(75)-C(76)-C(77)-C(78)	-1(4)
C(76)-C(77)-C(78)-C(73)	2(4)
C(74)-C(73)-C(78)-C(77)	-3(3)
C(71)-C(73)-C(78)-C(77)	178(2)
C(90)-Se(81)-N(82)-C(83)	0.6(15)
C(90)-Se(81)-N(82)-C(91)	175.5(15)
C(91)-N(82)-C(83)-O(84)	1(3)
Se(81)-N(82)-C(83)-O(84)	175.5(15)
C(91)-N(82)-C(83)-C(85)	-176.4(16)
Se(81)-N(82)-C(83)-C(85)	-2(2)
O(84)-C(83)-C(85)-C(86)	6(3)
N(82)-C(83)-C(85)-C(86)	-176.4(18)
O(84)-C(83)-C(85)-C(90)	-175.0(16)
N(82)-C(83)-C(85)-C(90)	2(2)
C(90)-C(85)-C(86)-C(87)	2(3)
C(83)-C(85)-C(86)-C(87)	-179.8(17)
C(85)-C(86)-C(87)-C(88)	-2(3)
C(86)-C(87)-C(88)-C(89)	1(4)
C(87)-C(88)-C(89)-C(90)	0(3)
C(88)-C(89)-C(90)-C(85)	0(3)
C(88)-C(89)-C(90)-Se(81)	-177.4(15)
C(86)-C(85)-C(90)-C(89)	-1(3)
C(83)-C(85)-C(90)-C(89)	-179.5(16)
C(86)-C(85)-C(90)-Se(81)	176.8(15)
C(83)-C(85)-C(90)-Se(81)	-1.8(19)
N(82)-Se(81)-C(90)-C(89)	178.2(18)
N(82)-Se(81)-C(90)-C(85)	0.8(13)
C(83)-N(82)-C(91)-C(92)	-121(2)
Se(81)-N(82)-C(91)-C(92)	65(2)
C(83)-N(82)-C(91)-C(93)	112(2)
Se(81)-N(82)-C(91)-C(93)	-63(2)
N(82)-C(91)-C(93)-C(98)	-76(2)
C(92)-C(91)-C(93)-C(98)	158.4(19)
N(82)-C(91)-C(93)-C(94)	99(2)
C(92)-C(91)-C(93)-C(94)	-26(3)
C(98)-C(93)-C(94)-C(95)	0(3)
C(91)-C(93)-C(94)-C(95)	-176(2)
C(93)-C(94)-C(95)-C(96)	0(3)
C(94)-C(95)-C(96)-C(97)	-1(4)
C(95)-C(96)-C(97)-C(98)	3(4)

C(96)-C(97)-C(98)-C(93)	-3(4)
C(94)-C(93)-C(98)-C(97)	2(3)
C(91)-C(93)-C(98)-C(97)	178(2)

**Table S4.** Hydrogen bonds for **24a** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(9)-H(9A)...O(4)#1	0.95	2.27	2.95(2)	128.1
C(29)-H(29A)...O(44)#2	0.95	2.36	3.05(2)	128.5
C(49)-H(49A)...O(24)	0.95	2.35	3.03(3)	127.6
C(69)-H(69A)...O(84)#3	0.95	2.45	3.16(3)	131.6
C(89)-H(89A)...O(64)	0.95	2.44	3.11(3)	127.4

Symmetry transformations used to generate equivalent atoms:

#1 -x+3/2,-y+1,z+1/2 #2 x,y,z+1 #3 x,y,z-1 .

**Table S5.** Crystal data and structure refinement for **25a**.

Identification code	<b>25a</b>
Empirical formula	C15 H13 N O Se
Formula weight	302.22
Temperature	100(2) K
Wavelength	1.54184 Å
Crystal system	Orthorhombic
Space group	P2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>
Unit cell dimensions	a = 10.1164(3) Å b = 12.6176(4) Å c = 52.3764(15) Å
Volume	6685.6(3) Å <sup>3</sup>
Z	20
Density (calculated)	1.501 Mg/m <sup>3</sup>
Absorption coefficient	3.690 mm <sup>-1</sup>
F(000)	3040
Crystal size	0.175 x 0.102 x 0.051 mm <sup>3</sup>
Theta range for data collection	3.375 to 77.905°
Index ranges	-12 ≤ h ≤ 12, -15 ≤ k ≤ 13, -64 ≤ l ≤ 25
Reflections collected	31953
Independent reflections	12315 [R(int) = 0.0329]
Completeness to theta = 67.684°	99.6 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.87047
Refinement method	Full-matrix least-squares on F <sup>2</sup>
Data / restraints / parameters	12315 / 6 / 816
Goodness-of-fit on F <sup>2</sup>	1.096
Final R indices [I > 2σ(I)]	R1 = 0.0492, wR2 = 0.1213
R indices (all data)	R1 = 0.0502, wR2 = 0.1218
Absolute structure parameter	0.011(9)
Extinction coefficient	n/a

Largest diff. peak and hole	1.291 and -0.900 e.Å <sup>-3</sup>
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**Table S6.** Bond lengths [Å] and angles [°] for **25a**.

Se(1)-C(10)	1.900(8)
Se(1)-N(2)	1.922(6)
N(2)-C(3)	1.289(11)
N(2)-C(11)	1.492(10)
C(3)-O(4)	1.248(10)
C(3)-C(5)	1.493(11)
C(5)-C(10)	1.388(11)
C(5)-C(6)	1.401(11)
C(6)-C(7)	1.370(13)
C(7)-C(8)	1.396(13)
C(8)-C(9)	1.386(12)
C(9)-C(10)	1.391(12)
C(11)-C(13)	1.519(11)
C(11)-C(12)	1.531(11)
C(13)-C(14)	1.388(12)
C(13)-C(18)	1.397(12)
C(14)-C(15)	1.393(12)
C(15)-C(16)	1.393(14)
C(16)-C(17)	1.364(13)
C(17)-C(18)	1.388(12)
Se(21)-N(22)	1.877(7)
Se(21)-C(30)	1.895(8)
N(22)-C(23)	1.364(10)
N(22)-C(31)	1.478(11)
C(23)-O(24)	1.237(10)
C(23)-C(25)	1.461(11)
C(25)-C(26)	1.387(11)
C(25)-C(30)	1.409(11)
C(26)-C(27)	1.380(12)
C(27)-C(28)	1.399(13)
C(28)-C(29)	1.393(12)
C(29)-C(30)	1.392(11)
C(31)-C(32)	1.519(14)
C(31)-C(33)	1.525(12)
C(33)-C(38)	1.376(12)
C(33)-C(34)	1.398(13)
C(34)-C(35)	1.376(14)
C(35)-C(36)	1.371(16)
C(36)-C(37)	1.363(17)
C(37)-C(38)	1.396(14)
Se(41)-C(50)	1.882(8)
Se(41)-N(42)	1.890(7)
N(42)-C(43)	1.353(11)
N(42)-C(51)	1.483(11)

C(43)-O(44)	1.229(11)
C(43)-C(45)	1.451(12)
C(45)-C(46)	1.371(12)
C(45)-C(50)	1.423(12)
C(46)-C(47)	1.383(12)
C(47)-C(48)	1.390(13)
C(48)-C(49)	1.377(12)
C(49)-C(50)	1.389(11)
C(51)-C(53)	1.511(12)
C(51)-C(52)	1.528(17)
C(53)-C(58)	1.379(12)
C(53)-C(54)	1.392(13)
C(54)-C(55)	1.376(15)
C(55)-C(56)	1.384(16)
C(56)-C(57)	1.370(15)
C(57)-C(58)	1.412(13)
Se(61)-N(62)	1.882(6)
Se(61)-C(70)	1.887(8)
N(62)-C(63)	1.359(10)
N(62)-C(71)	1.454(11)
C(63)-O(64)	1.248(9)
C(63)-C(65)	1.488(11)
C(65)-C(66)	1.402(11)
C(65)-C(70)	1.403(11)
C(66)-C(67)	1.394(13)
C(67)-C(68)	1.388(14)
C(68)-C(69)	1.378(12)
C(69)-C(70)	1.387(11)
C(71)-C(73)	1.507(12)
C(71)-C(72)	1.527(13)
C(73)-C(78)	1.392(12)
C(73)-C(74)	1.407(13)
C(74)-C(75)	1.385(13)
C(75)-C(76)	1.362(15)
C(76)-C(77)	1.399(16)
C(77)-C(78)	1.365(14)
Se(81)-N(82)	1.882(7)
Se(81)-C(90)	1.905(8)
N(82)-C(83)	1.337(11)
N(82)-C(91)	1.469(11)
C(83)-O(84)	1.232(10)
C(83)-C(85)	1.484(11)
C(85)-C(90)	1.355(12)
C(85)-C(86)	1.399(12)
C(86)-C(87)	1.381(13)
C(87)-C(88)	1.386(14)
C(88)-C(89)	1.388(13)
C(89)-C(90)	1.404(11)
C(91)-C(93)	1.504(12)



C(91)-C(92)	1.527(17)
C(93)-C(98)	1.380(12)
C(93)-C(94)	1.391(14)
C(94)-C(95)	1.391(14)
C(95)-C(96)	1.374(17)
C(96)-C(97)	1.375(16)
C(97)-C(98)	1.387(14)
C(10)-Se(1)-N(2)	83.7(3)
C(3)-N(2)-C(11)	123.3(6)
C(3)-N(2)-Se(1)	117.6(5)
C(11)-N(2)-Se(1)	119.0(5)
O(4)-C(3)-N(2)	123.6(7)
O(4)-C(3)-C(5)	124.8(7)
N(2)-C(3)-C(5)	111.4(7)
C(10)-C(5)-C(6)	120.2(8)
C(10)-C(5)-C(3)	114.9(7)
C(6)-C(5)-C(3)	124.9(7)
C(7)-C(6)-C(5)	119.1(8)
C(6)-C(7)-C(8)	120.7(8)
C(9)-C(8)-C(7)	120.7(8)
C(8)-C(9)-C(10)	118.7(8)
C(5)-C(10)-C(9)	120.7(8)
C(5)-C(10)-Se(1)	112.2(6)
C(9)-C(10)-Se(1)	127.1(7)
N(2)-C(11)-C(13)	111.1(6)
N(2)-C(11)-C(12)	109.4(7)
C(13)-C(11)-C(12)	114.2(7)
C(14)-C(13)-C(18)	119.3(8)
C(14)-C(13)-C(11)	119.7(8)
C(18)-C(13)-C(11)	121.0(7)
C(13)-C(14)-C(15)	120.9(8)
C(16)-C(15)-C(14)	119.1(8)
C(17)-C(16)-C(15)	120.1(8)
C(16)-C(17)-C(18)	121.4(8)
C(17)-C(18)-C(13)	119.2(8)
N(22)-Se(21)-C(30)	84.8(3)
C(23)-N(22)-C(31)	121.4(7)
C(23)-N(22)-Se(21)	117.3(6)
C(31)-N(22)-Se(21)	121.3(5)
O(24)-C(23)-N(22)	123.5(7)
O(24)-C(23)-C(25)	126.1(7)
N(22)-C(23)-C(25)	110.4(7)
C(26)-C(25)-C(30)	119.0(8)
C(26)-C(25)-C(23)	125.4(8)
C(30)-C(25)-C(23)	115.5(7)
C(27)-C(26)-C(25)	119.5(8)
C(26)-C(27)-C(28)	121.2(8)
C(29)-C(28)-C(27)	120.3(8)
C(30)-C(29)-C(28)	117.9(8)

C(29)-C(30)-C(25)	121.9(7)
C(29)-C(30)-Se(21)	126.1(6)
C(25)-C(30)-Se(21)	111.9(6)
N(22)-C(31)-C(32)	110.3(8)
N(22)-C(31)-C(33)	108.2(7)
C(32)-C(31)-C(33)	115.3(8)
C(38)-C(33)-C(34)	118.1(8)
C(38)-C(33)-C(31)	123.3(9)
C(34)-C(33)-C(31)	118.6(8)
C(35)-C(34)-C(33)	121.2(10)
C(36)-C(35)-C(34)	119.9(10)
C(37)-C(36)-C(35)	119.9(9)
C(36)-C(37)-C(38)	120.7(9)
C(33)-C(38)-C(37)	120.1(9)
C(50)-Se(41)-N(42)	84.9(3)
C(43)-N(42)-C(51)	124.6(7)
C(43)-N(42)-Se(41)	116.6(6)
C(51)-N(42)-Se(41)	118.7(6)
O(44)-C(43)-N(42)	122.0(8)
O(44)-C(43)-C(45)	126.7(8)
N(42)-C(43)-C(45)	111.3(7)
C(46)-C(45)-C(50)	119.4(8)
C(46)-C(45)-C(43)	125.5(8)
C(50)-C(45)-C(43)	115.1(7)
C(45)-C(46)-C(47)	120.2(8)
C(46)-C(47)-C(48)	120.3(9)
C(49)-C(48)-C(47)	120.8(8)
C(48)-C(49)-C(50)	119.2(8)
C(49)-C(50)-C(45)	120.1(8)
C(49)-C(50)-Se(41)	128.0(6)
C(45)-C(50)-Se(41)	111.9(6)
N(42)-C(51)-C(53)	108.2(7)
N(42)-C(51)-C(52)	109.1(8)
C(53)-C(51)-C(52)	115.5(9)
C(58)-C(53)-C(54)	118.7(9)
C(58)-C(53)-C(51)	123.3(9)
C(54)-C(53)-C(51)	117.9(9)
C(55)-C(54)-C(53)	121.0(9)
C(54)-C(55)-C(56)	120.4(10)
C(57)-C(56)-C(55)	119.6(9)
C(56)-C(57)-C(58)	120.1(9)
C(53)-C(58)-C(57)	120.1(9)
N(62)-Se(61)-C(70)	85.8(3)
C(63)-N(62)-C(71)	123.9(7)
C(63)-N(62)-Se(61)	116.8(5)
C(71)-N(62)-Se(61)	118.8(5)
O(64)-C(63)-N(62)	124.9(7)
O(64)-C(63)-C(65)	125.1(7)
N(62)-C(63)-C(65)	110.0(6)

C(66)-C(65)-C(70)	120.2(8)
C(66)-C(65)-C(63)	123.9(7)
C(70)-C(65)-C(63)	115.8(7)
C(67)-C(66)-C(65)	117.8(8)
C(68)-C(67)-C(66)	121.2(9)
C(69)-C(68)-C(67)	121.2(9)
C(68)-C(69)-C(70)	118.5(8)
C(69)-C(70)-C(65)	121.1(8)
C(69)-C(70)-Se(61)	127.5(6)
C(65)-C(70)-Se(61)	111.5(6)
N(62)-C(71)-C(73)	110.2(7)
N(62)-C(71)-C(72)	111.1(8)
C(73)-C(71)-C(72)	114.8(8)
C(78)-C(73)-C(74)	117.4(8)
C(78)-C(73)-C(71)	119.3(8)
C(74)-C(73)-C(71)	123.2(8)
C(75)-C(74)-C(73)	121.2(9)
C(76)-C(75)-C(74)	119.3(10)
C(75)-C(76)-C(77)	121.1(10)
C(78)-C(77)-C(76)	119.1(9)
C(77)-C(78)-C(73)	121.8(9)
N(82)-Se(81)-C(90)	84.2(3)
C(83)-N(82)-C(91)	123.2(7)
C(83)-N(82)-Se(81)	117.4(6)
C(91)-N(82)-Se(81)	119.0(6)
O(84)-C(83)-N(82)	124.1(7)
O(84)-C(83)-C(85)	125.9(8)
N(82)-C(83)-C(85)	109.9(7)
C(90)-C(85)-C(86)	119.7(8)
C(90)-C(85)-C(83)	116.3(8)
C(86)-C(85)-C(83)	124.0(7)
C(87)-C(86)-C(85)	118.9(8)
C(86)-C(87)-C(88)	120.7(9)
C(87)-C(88)-C(89)	121.1(8)
C(88)-C(89)-C(90)	116.8(8)
C(85)-C(90)-C(89)	122.7(8)
C(85)-C(90)-Se(81)	112.2(6)
C(89)-C(90)-Se(81)	125.0(7)
N(82)-C(91)-C(93)	109.8(7)
N(82)-C(91)-C(92)	109.1(9)
C(93)-C(91)-C(92)	115.7(9)
C(98)-C(93)-C(94)	118.3(8)
C(98)-C(93)-C(91)	123.4(9)
C(94)-C(93)-C(91)	118.3(8)
C(95)-C(94)-C(93)	121.2(10)
C(96)-C(95)-C(94)	120.0(11)
C(95)-C(96)-C(97)	118.8(10)
C(96)-C(97)-C(98)	121.6(10)
C(93)-C(98)-C(97)	120.0(9)

**Table S7.** Torsion angles [°] for **25a**.

C(11)-N(2)-C(3)-O(4)	1.8(12)
Se(1)-N(2)-C(3)-O(4)	-176.7(6)
C(11)-N(2)-C(3)-C(5)	178.1(7)
Se(1)-N(2)-C(3)-C(5)	-0.5(9)
O(4)-C(3)-C(5)-C(10)	178.7(8)
N(2)-C(3)-C(5)-C(10)	2.5(10)
O(4)-C(3)-C(5)-C(6)	-2.9(13)
N(2)-C(3)-C(5)-C(6)	-179.1(7)
C(10)-C(5)-C(6)-C(7)	-0.7(13)
C(3)-C(5)-C(6)-C(7)	-179.0(8)
C(5)-C(6)-C(7)-C(8)	-0.2(13)
C(6)-C(7)-C(8)-C(9)	0.9(14)
C(7)-C(8)-C(9)-C(10)	-0.8(13)
C(6)-C(5)-C(10)-C(9)	0.9(13)
C(3)-C(5)-C(10)-C(9)	179.3(7)
C(6)-C(5)-C(10)-Se(1)	178.2(6)
C(3)-C(5)-C(10)-Se(1)	-3.3(9)
C(8)-C(9)-C(10)-C(5)	-0.1(13)
C(8)-C(9)-C(10)-Se(1)	-177.0(7)
N(2)-Se(1)-C(10)-C(5)	2.4(6)
N(2)-Se(1)-C(10)-C(9)	179.5(8)
C(3)-N(2)-C(11)-C(13)	-154.0(7)
Se(1)-N(2)-C(11)-C(13)	24.5(9)
C(3)-N(2)-C(11)-C(12)	79.0(9)
Se(1)-N(2)-C(11)-C(12)	-102.5(7)
N(2)-C(11)-C(13)-C(14)	87.1(9)
C(12)-C(11)-C(13)-C(14)	-148.5(8)
N(2)-C(11)-C(13)-C(18)	-89.6(9)
C(12)-C(11)-C(13)-C(18)	34.8(11)
C(18)-C(13)-C(14)-C(15)	1.4(13)
C(11)-C(13)-C(14)-C(15)	-175.4(8)
C(13)-C(14)-C(15)-C(16)	-1.2(14)
C(14)-C(15)-C(16)-C(17)	0.9(14)
C(15)-C(16)-C(17)-C(18)	-0.8(14)
C(16)-C(17)-C(18)-C(13)	0.9(13)
C(14)-C(13)-C(18)-C(17)	-1.2(12)
C(11)-C(13)-C(18)-C(17)	175.6(8)
C(30)-Se(21)-N(22)-C(23)	-1.3(6)
C(30)-Se(21)-N(22)-C(31)	179.5(7)
C(31)-N(22)-C(23)-O(24)	2.2(13)
Se(21)-N(22)-C(23)-O(24)	-177.0(6)
C(31)-N(22)-C(23)-C(25)	-178.8(8)
Se(21)-N(22)-C(23)-C(25)	2.1(9)
O(24)-C(23)-C(25)-C(26)	-0.7(14)
N(22)-C(23)-C(25)-C(26)	-179.8(8)
O(24)-C(23)-C(25)-C(30)	177.1(8)

N(22)-C(23)-C(25)-C(30)	-1.9(10)
C(30)-C(25)-C(26)-C(27)	0.9(13)
C(23)-C(25)-C(26)-C(27)	178.6(8)
C(25)-C(26)-C(27)-C(28)	-1.2(14)
C(26)-C(27)-C(28)-C(29)	0.8(15)
C(27)-C(28)-C(29)-C(30)	-0.1(13)
C(28)-C(29)-C(30)-C(25)	-0.2(13)
C(28)-C(29)-C(30)-Se(21)	-179.2(7)
C(26)-C(25)-C(30)-C(29)	-0.2(13)
C(23)-C(25)-C(30)-C(29)	-178.2(7)
C(26)-C(25)-C(30)-Se(21)	178.9(6)
C(23)-C(25)-C(30)-Se(21)	1.0(10)
N(22)-Se(21)-C(30)-C(29)	179.2(8)
N(22)-Se(21)-C(30)-C(25)	0.1(6)
C(23)-N(22)-C(31)-C(32)	86.4(10)
Se(21)-N(22)-C(31)-C(32)	-94.5(9)
C(23)-N(22)-C(31)-C(33)	-146.7(8)
Se(21)-N(22)-C(31)-C(33)	32.4(10)
N(22)-C(31)-C(33)-C(38)	-104.2(10)
C(32)-C(31)-C(33)-C(38)	19.7(13)
N(22)-C(31)-C(33)-C(34)	75.2(10)
C(32)-C(31)-C(33)-C(34)	-160.8(9)
C(38)-C(33)-C(34)-C(35)	3.3(14)
C(31)-C(33)-C(34)-C(35)	-176.2(9)
C(33)-C(34)-C(35)-C(36)	-1.5(16)
C(34)-C(35)-C(36)-C(37)	-0.9(17)
C(35)-C(36)-C(37)-C(38)	1.4(16)
C(34)-C(33)-C(38)-C(37)	-2.8(13)
C(31)-C(33)-C(38)-C(37)	176.7(9)
C(36)-C(37)-C(38)-C(33)	0.5(15)
C(50)-Se(41)-N(42)-C(43)	-3.6(7)
C(50)-Se(41)-N(42)-C(51)	177.6(8)
C(51)-N(42)-C(43)-O(44)	3.4(15)
Se(41)-N(42)-C(43)-O(44)	-175.3(7)
C(51)-N(42)-C(43)-C(45)	-176.7(9)
Se(41)-N(42)-C(43)-C(45)	4.6(10)
O(44)-C(43)-C(45)-C(46)	-3.2(16)
N(42)-C(43)-C(45)-C(46)	177.0(9)
O(44)-C(43)-C(45)-C(50)	176.7(9)
N(42)-C(43)-C(45)-C(50)	-3.1(11)
C(50)-C(45)-C(46)-C(47)	-1.7(14)
C(43)-C(45)-C(46)-C(47)	178.2(9)
C(45)-C(46)-C(47)-C(48)	-0.7(16)
C(46)-C(47)-C(48)-C(49)	3.2(16)
C(47)-C(48)-C(49)-C(50)	-3.1(14)
C(48)-C(49)-C(50)-C(45)	0.7(13)
C(48)-C(49)-C(50)-Se(41)	-177.6(7)
C(46)-C(45)-C(50)-C(49)	1.7(13)
C(43)-C(45)-C(50)-C(49)	-178.1(8)

C(46)-C(45)-C(50)-Se(41)	-179.8(7)
C(43)-C(45)-C(50)-Se(41)	0.4(10)
N(42)-Se(41)-C(50)-C(49)	-180.0(8)
N(42)-Se(41)-C(50)-C(45)	1.6(6)
C(43)-N(42)-C(51)-C(53)	-134.0(9)
Se(41)-N(42)-C(51)-C(53)	44.6(10)
C(43)-N(42)-C(51)-C(52)	99.6(12)
Se(41)-N(42)-C(51)-C(52)	-81.8(9)
N(42)-C(51)-C(53)-C(58)	-114.9(9)
C(52)-C(51)-C(53)-C(58)	7.7(13)
N(42)-C(51)-C(53)-C(54)	61.8(11)
C(52)-C(51)-C(53)-C(54)	-175.6(9)
C(58)-C(53)-C(54)-C(55)	0.5(14)
C(51)-C(53)-C(54)-C(55)	-176.3(9)
C(53)-C(54)-C(55)-C(56)	-0.4(16)
C(54)-C(55)-C(56)-C(57)	0.3(16)
C(55)-C(56)-C(57)-C(58)	-0.4(15)
C(54)-C(53)-C(58)-C(57)	-0.6(12)
C(51)-C(53)-C(58)-C(57)	176.0(8)
C(56)-C(57)-C(58)-C(53)	0.6(13)
C(70)-Se(61)-N(62)-C(63)	-2.6(6)
C(70)-Se(61)-N(62)-C(71)	-175.3(7)
C(71)-N(62)-C(63)-O(64)	-3.1(13)
Se(61)-N(62)-C(63)-O(64)	-175.3(6)
C(71)-N(62)-C(63)-C(65)	176.0(7)
Se(61)-N(62)-C(63)-C(65)	3.7(9)
O(64)-C(63)-C(65)-C(66)	-5.1(13)
N(62)-C(63)-C(65)-C(66)	175.9(8)
O(64)-C(63)-C(65)-C(70)	175.9(8)
N(62)-C(63)-C(65)-C(70)	-3.2(10)
C(70)-C(65)-C(66)-C(67)	-1.5(13)
C(63)-C(65)-C(66)-C(67)	179.4(8)
C(65)-C(66)-C(67)-C(68)	-0.4(14)
C(66)-C(67)-C(68)-C(69)	1.7(15)
C(67)-C(68)-C(69)-C(70)	-1.0(13)
C(68)-C(69)-C(70)-C(65)	-1.0(12)
C(68)-C(69)-C(70)-Se(61)	179.2(7)
C(66)-C(65)-C(70)-C(69)	2.3(12)
C(63)-C(65)-C(70)-C(69)	-178.6(7)
C(66)-C(65)-C(70)-Se(61)	-177.9(6)
C(63)-C(65)-C(70)-Se(61)	1.2(9)
N(62)-Se(61)-C(70)-C(69)	-179.5(8)
N(62)-Se(61)-C(70)-C(65)	0.6(6)
C(63)-N(62)-C(71)-C(73)	-109.3(9)
Se(61)-N(62)-C(71)-C(73)	62.8(9)
C(63)-N(62)-C(71)-C(72)	122.3(9)
Se(61)-N(62)-C(71)-C(72)	-65.6(9)
N(62)-C(71)-C(73)-C(78)	76.5(10)
C(72)-C(71)-C(73)-C(78)	-157.2(8)

N(62)-C(71)-C(73)-C(74)	-100.2(9)
C(72)-C(71)-C(73)-C(74)	26.1(12)
C(78)-C(73)-C(74)-C(75)	-0.2(13)
C(71)-C(73)-C(74)-C(75)	176.5(9)
C(73)-C(74)-C(75)-C(76)	0.7(14)
C(74)-C(75)-C(76)-C(77)	-0.1(15)
C(75)-C(76)-C(77)-C(78)	-0.9(16)
C(76)-C(77)-C(78)-C(73)	1.4(15)
C(74)-C(73)-C(78)-C(77)	-0.8(13)
C(71)-C(73)-C(78)-C(77)	-177.7(9)
C(90)-Se(81)-N(82)-C(83)	-2.7(7)
C(90)-Se(81)-N(82)-C(91)	-176.3(8)
C(91)-N(82)-C(83)-O(84)	-0.2(15)
Se(81)-N(82)-C(83)-O(84)	-173.5(7)
C(91)-N(82)-C(83)-C(85)	176.2(8)
Se(81)-N(82)-C(83)-C(85)	2.9(10)
O(84)-C(83)-C(85)-C(90)	174.9(8)
N(82)-C(83)-C(85)-C(90)	-1.5(11)
O(84)-C(83)-C(85)-C(86)	-4.0(14)
N(82)-C(83)-C(85)-C(86)	179.6(8)
C(90)-C(85)-C(86)-C(87)	-0.9(13)
C(83)-C(85)-C(86)-C(87)	178.0(8)
C(85)-C(86)-C(87)-C(88)	-0.6(14)
C(86)-C(87)-C(88)-C(89)	0.9(15)
C(87)-C(88)-C(89)-C(90)	0.3(14)
C(86)-C(85)-C(90)-C(89)	2.2(13)
C(83)-C(85)-C(90)-C(89)	-176.7(8)
C(86)-C(85)-C(90)-Se(81)	178.4(7)
C(83)-C(85)-C(90)-Se(81)	-0.5(10)
C(88)-C(89)-C(90)-C(85)	-1.9(13)
C(88)-C(89)-C(90)-Se(81)	-177.6(6)
C(83)-N(82)-C(91)-C(93)	-129.8(9)
Se(81)-N(82)-C(91)-C(93)	43.4(11)
C(83)-N(82)-C(91)-C(92)	102.5(12)
Se(81)-N(82)-C(91)-C(92)	-84.3(10)
N(82)-C(91)-C(93)-C(98)	-120.6(9)
C(92)-C(91)-C(93)-C(98)	3.4(14)
N(82)-C(91)-C(93)-C(94)	57.7(11)
C(92)-C(91)-C(93)-C(94)	-178.3(10)
C(98)-C(93)-C(94)-C(95)	1.1(13)
C(91)-C(93)-C(94)-C(95)	-177.3(8)
C(93)-C(94)-C(95)-C(96)	-1.3(15)
C(94)-C(95)-C(96)-C(97)	1.2(15)
C(95)-C(96)-C(97)-C(98)	-0.9(15)
C(94)-C(93)-C(98)-C(97)	-0.8(13)
C(91)-C(93)-C(98)-C(97)	177.5(8)
C(96)-C(97)-C(98)-C(93)	0.7(14)

**Table S8.** Hydrogen bonds for **25a** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(9)-H(9)...O(4)#1	0.95	2.28	2.953(10)	127.3
C(29)-H(29)...O(44)#2	0.95	2.36	3.037(10)	128.1
C(49)-H(49)...O(24)	0.95	2.35	3.020(10)	127.1
C(69)-H(69)...O(84)	0.95	2.45	3.125(10)	127.8
C(89)-H(89)...O(64)#3	0.95	2.50	3.200(11)	130.6

Symmetry transformations used to generate equivalent atoms:.

#1 -x+1,y-1/2,-z+1/2    #2 x,y-1,z    #3 x,y+1,z    .