Supplementary Materials

Regio- and Stereoselective Synthesis of (*Z*,*Z*)-Bis(3-amino-3-oxo-1-propenyl) Selenides and Diselenides Based on 2-Propynamides: A Novel Family of Diselenides with High Glutathione Peroxidase-Like Activity

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Experimental (General Information)

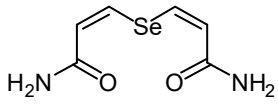
The ^{1}H (400.1 MHz), ^{13}C (100.6 MHz), ^{77}Se (76.3 MHz), and ^{15}N (40.6 MHz) NMR spectra (the spectra can be find in Supplementary Materials) were recorded on a Bruker DPX-400 spectrometer (Bruker BioSpin GmbH, Rheinstetten, Germany) in $CDCl_3$ or DMSO-d_6 5–10% solutions and referred to TMS (^{1}H, ^{13}C), nitromethane (^{15}N) and dimethyl selenide (^{77}Se).

Elemental analysis was performed on a Thermo Scientific Flash 2000 Elemental Analyzer. Melting points were determined on the Kofler apparatus. The organic solvents were dried and distilled according to standard procedures.

Crystal data were collected on a Bruker D8 Venture diffractometer with MoKa radiation (λ = 0.71073) using the φ and ω scans. The structures were solved and refined by direct methods using the SHELX programs set [1]. Data were corrected for absorption effects using the multi-scan method (SADABS). Non-hydrogen atoms were refined anisotropically using SHELX programs set [1]. Supplementary Materials contain the crystallographic data for compounds CCDC 1834087 (**2a**), 1834088 (**2d**), 1834089 (**2f**) and 1841340 (**2i**). These data can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif

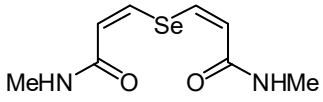
^{1}H, ^{13}C, ^{77}Se, and ^{15}N NMR spectra of products 2a-i

(Z,Z)-Bis(3-amino-3-oxo-1-propenyl) selenide (2a):



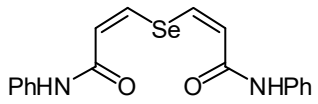
The product was prepared according to the general procedure. The pure sample was obtained by extraction from the residue by acetone. Acetone was removed under reduced pressure to give **2a** (48 mg, 91%); white powder; mp 183–184 °C. ^{1}H NMR (400 MHz, d_6-DMSO): δ 6.38 (d, ^{3}J = 9.5 Hz, 2H, =CHCO), 7.11, 7.50 (br s, 4H, NH_2), 7.65 (d, ^{3}J = 9.5 Hz, 2H, SeCH=). ^{13}C NMR (100 MHz, d_6-DMSO): δ 120.6 (=CCO), 145.3 (SeC=, $^{1}J_{Se–C}$ = 128.2 Hz), 168.1 (C=O). ^{77}Se NMR (76 MHz, d_6-DMSO): δ 507.4. ^{15}N NMR (40 MHz, d_6-DMSO): δ –269.5 ($^{1}J_{N–H}$ = 88.4, 89.2 Hz); The 2D ^{15}N NMR HMBC {^{1}H–^{15}N} spectrum contain cross-peaks of N-atom with protons of NH_2.

(Z,Z)-Bis(*N*-methyl-3-amino-3-oxo-1-propenyl) selenide (2b):



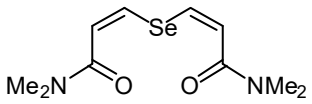
The product was prepared according to the general procedure. After removing the solvent, the product did not require further purification (58 mg 97%); white powder; mp 215–216 °C. ^{1}H NMR (400 MHz, d_6-DMSO): δ 2.63 (d, ^{3}J = 4.4 Hz, 6H, CH_3), 6.35 (d, ^{3}J = 9.6 Hz, 2H, =CHCO), 7.59 (d, ^{3}J = 9.6 Hz, 2H, SeCH=), 8.01 (q, ^{3}J = 4.4 Hz, 2H, NH). ^{13}C NMR (100 MHz, d_6-DMSO): δ 25.5 (CH_3), 120.4 (=CCO), 144.0 (SeC=, $^{1}J_{Se–C}$ = 127.4 Hz), 166.8 (C=O). ^{77}Se NMR (76 MHz, d_6-DMSO): δ 502.7. ^{15}N NMR (40 MHz, d_6-DMSO): δ –272.9 ($^{1}J_{N–H}$ = 91.9 Hz); The 2D ^{15}N NMR HMBC {^{1}H–^{15}N} spectrum contain cross-peaks of N-atom with protons of NH and CH_3.

(Z,Z)-Bis(*N*-phenyl-3-amino-3-oxo-1-propenyl) selenide (2c):



The product was prepared according to the general procedure. After removing the solvent, the residue was dissolved in THF and precipitated with cold hexane (76 mg 85%); yellowish powder; mp 219–220 °C. ^{1}H NMR (400 MHz, d_6-DMSO): δ 6.65 (d, ^{3}J = 9.6 Hz, 2H, =CHCO), 7.06 (t, ^{3}J = 7.7 Hz, 2H, H^{p}), 7.33 (dd, ^{3}J = 7.7 Hz, 4H, H^{m}), 7.66 (d, ^{3}J = 7.7 Hz, 4H, H^{o}), 7.94 (d, ^{3}J = 9.6 Hz, 2H, SeCH=), 10.23 (s, 2H, NH). ^{13}C NMR (100 MHz, d_6-DMSO): δ 119.0 (=CCO), 121.0 (C^{o}), 123.4 (C^{p}), 128.9 (C^{m}), 139.1 (C^{i}), 146.7 (SeC=, $^{1}J_{Se–C}$ = 129.0 Hz), 164.9 (C=O). ^{77}Se NMR (76 MHz, d_6-DMSO): δ 518.8. ^{15}N NMR (40 MHz, d_6-DMSO): δ –243.1 ($^{3}J_{N–H}$ = 6.6 Hz); The 2D ^{15}N NMR HMBC {^{1}H–^{15}N} spectrum contain cross-peaks of N-atom with protons of H^{o}.

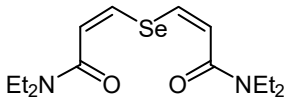
(Z,Z)-Bis(*N*,*N*-dimethyl-3-amino-3-oxo-1-propenyl) selenide (2d):



The product was prepared according to the general procedure. After removing the solvent, the residue was dissolved in $CHCl_3$ and precipitated with cold hexane (55 mg, 84%); white powder; mp 181–182 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 3.94, 3.00 (s, 12H, CH_3), 6.68 (d, ^{3}J = 9.7 Hz, 2H, =CHCO), 7.47 (d, ^{3}J = 9.7 Hz, 2H, SeCH=). ^{13}C NMR

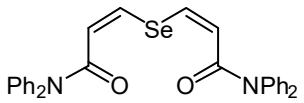
(100 MHz, $CDCl_3$): δ 35.4, 37.2 (CH_3), 116.8 (=<u>C</u>CO), 147.6 (SeC=, $^1J_{Se-C}$ = 132.6 Hz), 166.9 (C=O). ^{77}Se NMR (76 MHz, $CDCl_3$): δ 516.8. ^{15}N NMR (40 MHz, $CDCl_3$): δ –281.5; The 2D ^{15}N NMR HMBC {^{1}H–^{15}N} spectrum contain cross-peaks of N-atom with protons of CH_3 and =CHCO.

(Z,Z)-Bis(*N,N*-diethyl-3-amino-3-oxo-1-propenyl) selenide (2e):



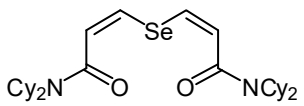
The product was prepared according to the general procedure. After removing the solvent, the residue was dissolved in $CHCl_3$, cold hexane was added and the mixture was placed in the refrigerator (–18 °C) for crystallization. Obtained solid was dried in vacuum (65 mg, 82%); pale yellow viscous solid; mp 56–57 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.14 (t, ^3J = 6.8 Hz, 12H, CH_3), 3.33, 3.41 (q, ^3J = 6.8 Hz, 8H, CH_2), 6.66 (d, ^3J = 9.7 Hz, 2H, =CHCO), 7.48 (d, ^3J = 9.7 Hz, 2H, SeCH=). ^{13}C NMR (100 MHz, $CDCl_3$): δ 13.2, 14.8 (CH_3), 40.6, 42.1 (CH_2), 117.1 (=<u>C</u>CO), 147.5 (SeC=, $^1J_{Se-C}$ = 131.9 Hz), 166 (C=O). ^{77}Se NMR (76 MHz, $CDCl_3$): δ 519.4. ^{15}N NMR (40 MHz, $CDCl_3$): δ –251.5; The 2D ^{15}N NMR HMBC {^{1}H–^{15}N} spectrum contain cross-peaks of N-atom with all protons.

(Z,Z)-Bis(*N,N*-diphenyl-3-amino-3-oxo-1-propenyl) selenide (2f):



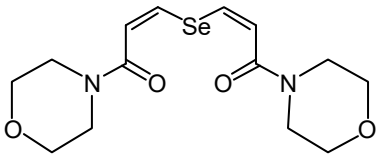
The product was prepared according to the general procedure for 8 h. After removing the solvent, the residue was dissolved in $CHCl_3$ and precipitated with cold hexane. Yield: (111 mg, 88%); beige powder; mp 201–203 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 6.35 (d, ^3J = 9.7 Hz, 2H, =CHCO), 7.23–7.30 (m, 12H, $H^{o,p}$), 7.32–7.40 (m, 8H, H^m), 7.48 (d, ^3J = 9.7 Hz, 2H, SeCH=). =). ^{13}C NMR (100 MHz, $CDCl_3$): δ 119.6 (=<u>C</u>CO), 125.1–128.6 ($C^{o,p}$), 129.2 (C^m), 142.6 (C^i), 149.2 (SeC=, $^1J_{Se-C}$ = 133.9 Hz), 166.3 (C=O). ^{77}Se NMR (76 MHz, $CDCl_3$): δ 533.3. ^{15}N NMR (40 MHz, $CDCl_3$): δ –232.3; The 2D ^{15}N NMR HMBC {^{1}H–^{15}N} spectrum contain cross-peaks of N-atom with protons of =CHCO, SeCH= and H^o.

(Z,Z)-Bis(*N,N*-dicyclohexyl-3-amino-3-oxo-1-propenyl) selenide (2g):



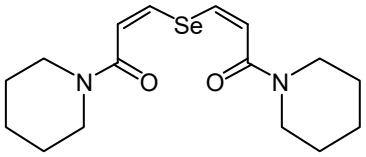
The product was prepared according to the general procedure. After removing the solvent, the residue was recrystallized from benzene (77 mg, 66%); white powder; mp 127–129 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.03–1.38, 1.44–1.90 (m, 36H, H^{2-6}), 2.19 (br m, 4H, $H^{2,6}$), 3.45 (br m, 4H, H^1), 6.70 (d, ^3J = 9.7 Hz, 2H, =CHCO), 7.39 (d, ^3J = 9.7 Hz, 2H, SeCH=). ^{13}C NMR (100 MHz, $CDCl_3$): δ 24.4 ($C^{3,4,5}$), 25.4 ($C^{3,5}$), 29.4, 30.6, 31.0 ($C^{2,6}$), 54.5, 56.0 (C^1), 118.8 (=<u>C</u>CO), 145.0 (SeC=, $^1J_{Se-C}$ = 130.6 Hz), 165.4 (C=O). ^{77}Se NMR (76 MHz, $CDCl_3$): δ 508.7. ^{15}N NMR (40 MHz, $CDCl_3$): δ –233.4; The 2D ^{15}N NMR HMBC {^{1}H–^{15}N} spectrum contain cross-peaks of N-atom with protons of =CHCO and SeCH=.

(Z,Z)-Bis(3-morpholino-3-oxo-1-propenyl) selenide (2h):



The product was prepared according to the general procedure. After removing the solvent, the residue was dissolved in $CHCl_3$ and precipitated with cold hexane (72 mg, 84%); white powder; mp 196–197 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 3.52 (br m, 4H, $H^{3,5}$), 3.65 (br m, 12H, $H^{3,5}$, $H^{2,6}$), 6.70 (d, ^3J = 9.7 Hz, 2H, =CHCO), 7.56 (d, ^3J = 9.7 Hz, 2H, SeCH=). ^{77}Se NMR (76 MHz, $CDCl_3$): δ 520.2. ^{15}N NMR (40 MHz, $CDCl_3$): δ –264.5; The 2D ^{15}N NMR HMBC {^{1}H–^{15}N} ($CDCl_3$) spectrum contain cross-peaks of N-atom with proton of =CHCO.

(Z,Z)-Bis(3-piperidino-3-oxo-1-propenyl) selenide (2i):



The product was prepared according to the general procedure. After removing the solvent, the residue was dissolved in $CHCl_3$ and precipitated with cold hexane (72 mg, 85%); beige powder; mp 208–209 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.53–1.61 (m, 8H, $H^{3,5}$), 1.61–1.70 (m, 4H, H^4), 3.49, 3.61 (br m, 8H, $H^{2,6}$), 6.75 (d, ^3J = 9.8 Hz, 2H, =CHCO), 7.49 (d, ^3J = 9.8 Hz, 2H, SeCH=). ^{13}C NMR (100 MHz, $CDCl_3$): δ 24.7 (C^4), 25.6, 26.7 ($C^{3,5}$), 42.9, 46.8 ($C^{2,6}$), 117.0 (=CCO), 147.1 (SeC=, $^1J_{Se-C}$ = 131.0 Hz), 165.5 (C=O). ^{77}Se NMR (76 MHz, $CDCl_3$): δ 508.7. ^{15}N NMR (40 MHz, $CDCl_3$): δ –258.2; The 2D ^{15}N NMR HMBC {^{1}H–^{15}N} spectrum contain cross-peaks of N-atom with protons of =CHCO and SeCH=.

Crystal data and structural refinement

Crystal data were collected on a Bruker D8 Venture diffractometer with MoKa radiation (λ = 0.71073) using the φ and ω scans. The structures were solved and refined by direct methods using the SHELX programs set [1]. Data were corrected for absorption effects using the multi-scan method (SADABS). Nonhydrogen atoms were refined anisotropically using SHELX programs set [1]. Crystallographic CCDC data: **1834087 (2a), 1834088 (2d), 1834089 (2f)** and **1841340 (2i).** These data can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

The molecular structures are depicted in Figures S1-S4. Principal bond distances, bond angles and torsion angles are presented in Table S1.

Reference

1. Sheldrick, G.M. *Acta Crystallogr.* **2008**, *D64*, 112.

(Z,Z)-Bis(3-amino-3-oxo-1-propenyl) selenide (2a)

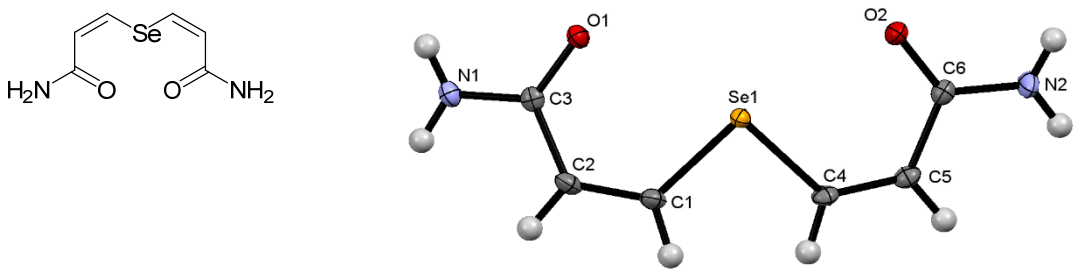


Figure S1. Molecular structure of compound **2a** (ORTEP, 50% probability ellipsoids).

Single crystal of **2a** was grown at room temperature by slow evaporation from THF–CCl_4 solution, mounted in inert oil and transferred to the cold gas stream of the diffractometer.

Crystal data. $C_6H_8N_2O_2Se$, M = 219.10, orthorhombic, a = 5.0919(2), b = 10.2345(3), c = 15.4229(5) Å, V = 803.7(1) Å^3, T = 100 K, space group $P2_12_12_1$ (no.19), Z = 4, 7904 reflections measured, 2318 unique (R^{int} = 0.020), which were used in all calculations. The final w$R(F^2)$ was 0.045 (all data).

(Z,Z)-Bis(*N,N*-dimethyl-3-amino-3-oxo-1-propenyl) selenide (2d):

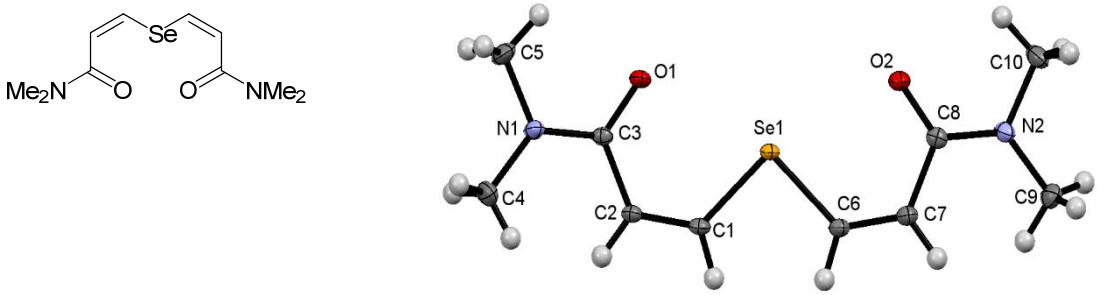


Figure S2. Molecular structure of compound **2d** (ORTEP, 50% probability ellipsoids).

Single crystal of **2d** was grown at room temperature by slow evaporation from THF–CCl_4 solution, mounted in inert oil and transferred to the cold gas stream of the diffractometer.

Crystal data. $C_{10}H_{16}N_2O_2Se$, M = 275.21, monoclinic, a = 7.7963(3), b = 13.5983(5), c = 11.9165(5) Å, β = 108.326(1), V = 1199.3(1) Å^3, T = 100 K, space group $P2_1/n$ (no.14), Z = 4, 38529 reflections measured, 3494 unique (R^{int} = 0.023), which were used in all calculations. The final w$R(F^2)$ was 0.057 (all data).

(Z,Z)-Bis(*N,N*-diphenyl-3-amino-3-oxo-1-propenyl) selenide (2f):

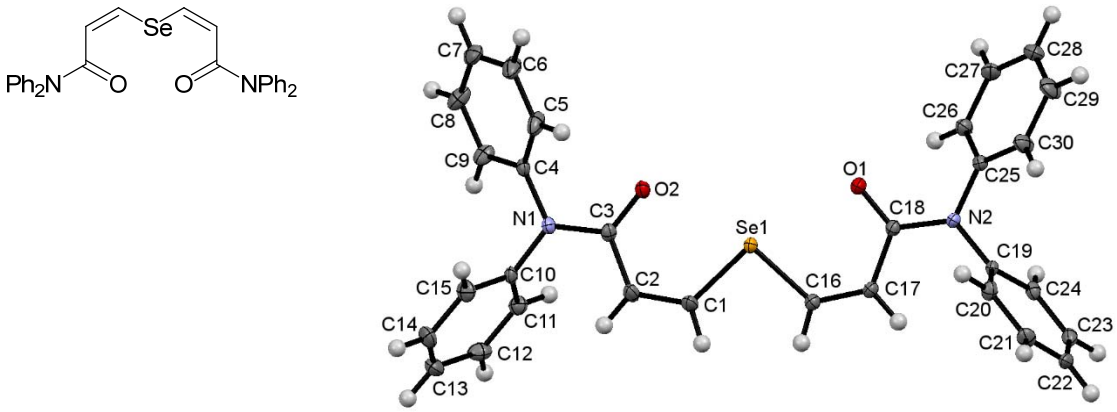


Figure S3. Molecular structure of compound **2f** (ORTEP, 50% probability ellipsoids).

Single crystal of **2f** was grown at room temperature by slow evaporation from THF–CCl_4 solution, mounted in inert oil and transferred to the cold gas stream of the diffractometer.

Crystal data. $C_{30}H_{24}N_2O_2Se$, M = 523.48, monoclinic, a = 11.2300(4), b = 14.5920(5), c = 18.5198(6) Å, β = 93.637(1), V = 3028.7(2) Å^3, T = 100 K, space group $P2_1/n$ (no.14), Z = 4, 85073 reflections measured, 8875 unique (R^{int} = 0.053), which were used in all calculations. The final w$R(F^2)$ was 0.141 (all data).

(Z)-3-[(Z)-3-oxo-3-piperidino-1-propenyl]selanyl-1-morpholino-2-propen-1-one (2i):

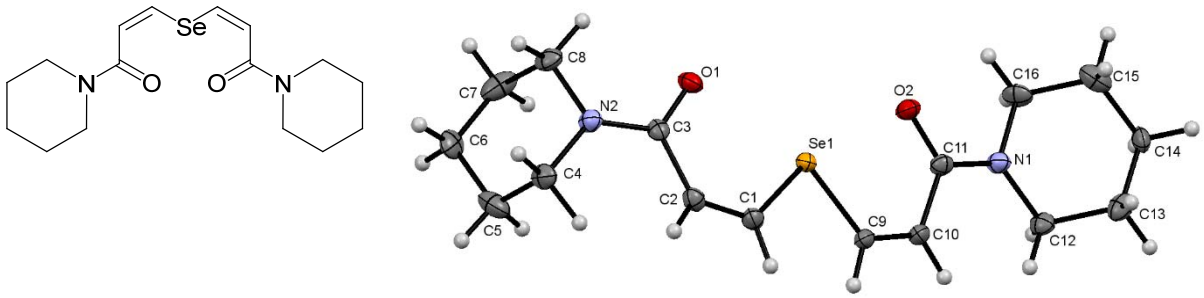


Figure S4. Molecular structure of compound **2i** (ORTEP, 50% probability ellipsoids).

Single crystal of **2i** was grown at room temperature by slow evaporation from CH_2Cl_2–CCl_4 solution, mounted in inert oil and transferred to the cold gas stream of the diffractometer.

Crystal data. $C_{16}H_{24}N_2O_2Se$, M = 355.30, orthorhombic, a = 9.2034(2), b = 10.3785(3), c =16.1407(5) Å, V = 1541.7(1) Å^3, T = 100 K, space group $P2_12_12_1$ (no.19), Z = 4, 19296 reflections measured, 4497 unique (R^{int} = 0.028), which were used in all calculations. The final w$R(F^2)$ was 0.068 (all data).

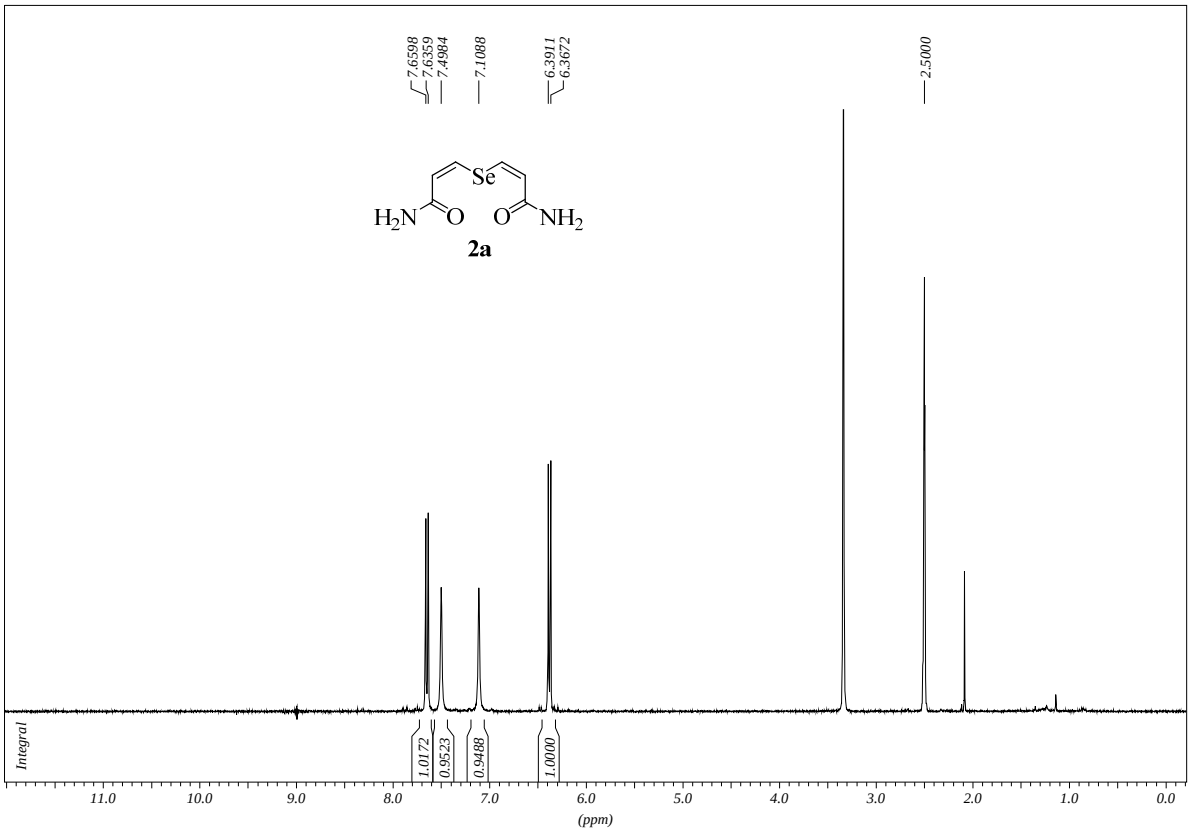
Table S1. Selected bond lengths, bond and torsion angles in compounds **2a, 2d, 2f, 2i.**

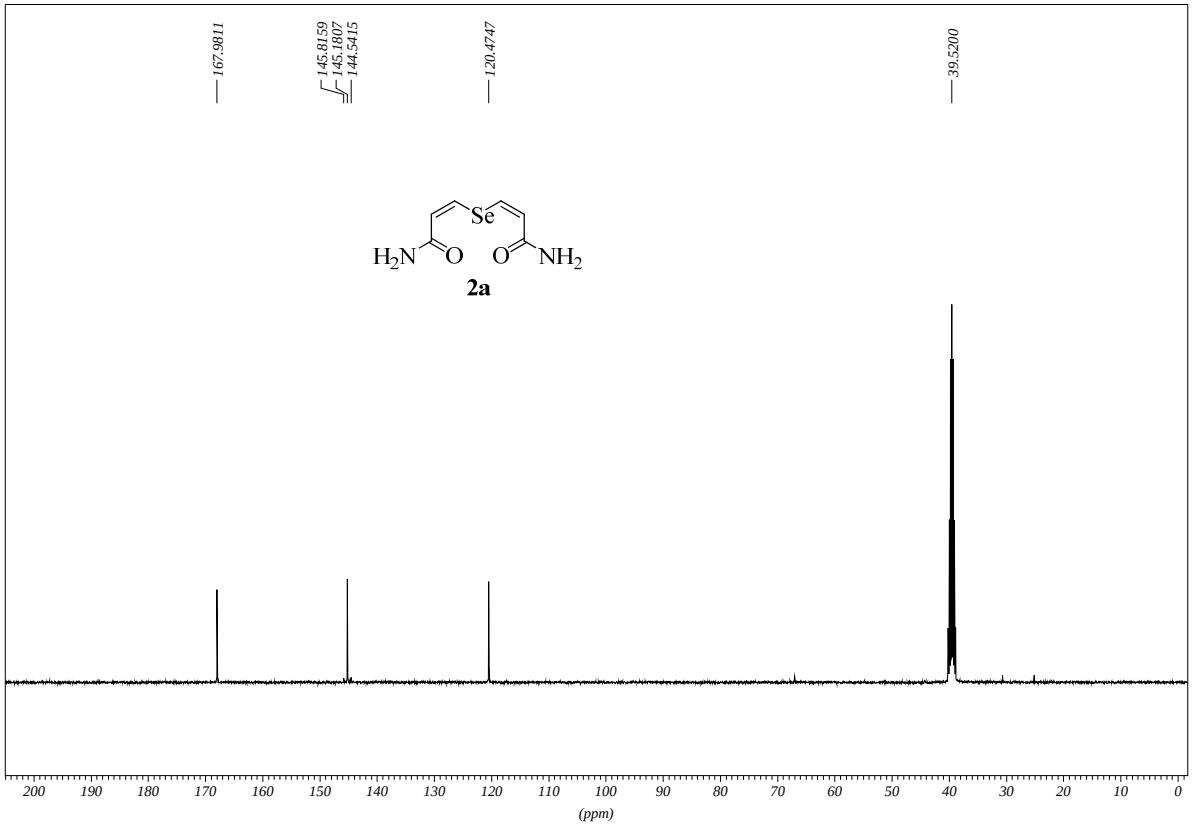
Amide	Bond	*l*, Å	Angle	φ, °	Angle	θ, °
2a	Se1-C4	1.893(2)	C4-Se1-C1	94.8(1)	C4-Se1-C1-C2	-162.4(2)
	Se1-C1	1.900(2)	C2-C1-Se1	125.4(2)	Se1-C1-C2-C3	3.6(3)
	O1-C3	1.243(3)	C1-C2-C3	122.3(2)	C1-C2-C3-O1	-22.1(4)
	O2-C6	1.241(3)	O1-C3-N1	122.0(2)	C1-C2-C3-N1	155.1(2)
	N1-C3	1.342(3)	O1-C3-C2	121.1(2)	C1-Se1-C4-C5	-177.2(2)

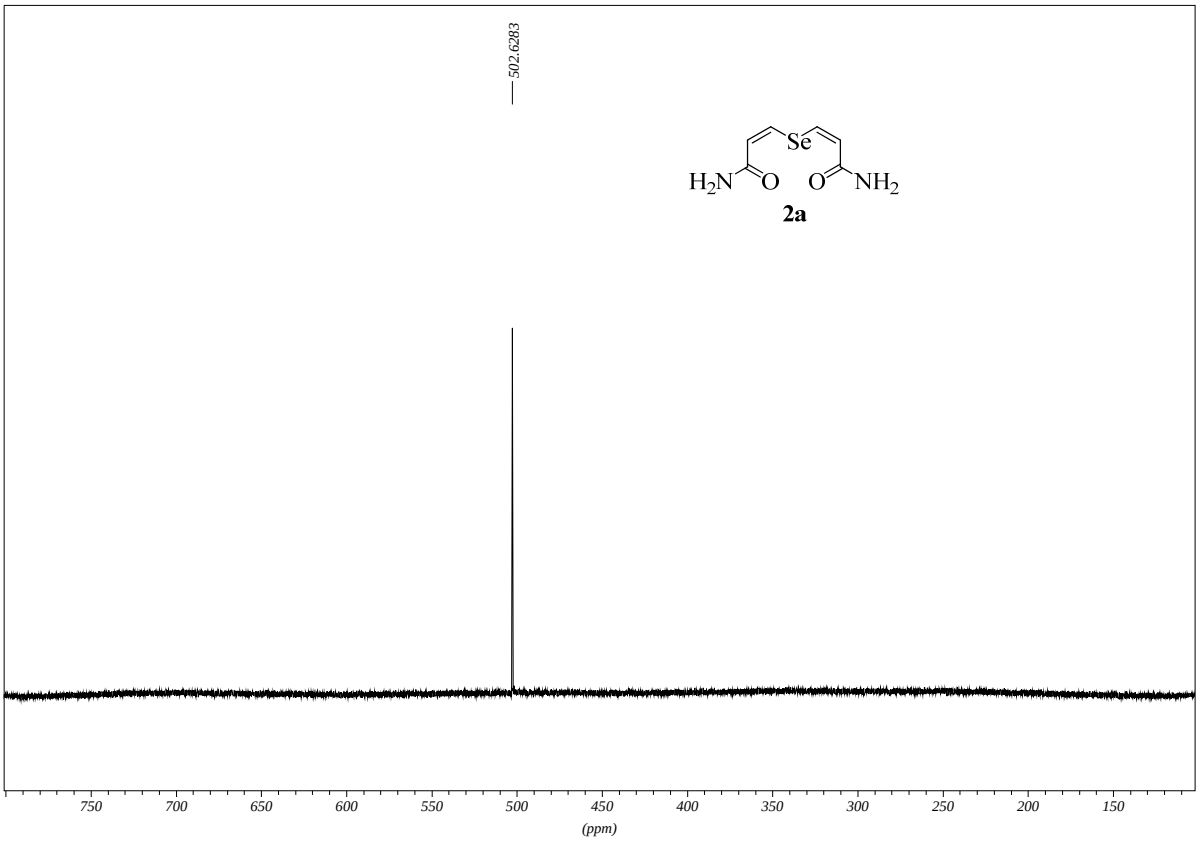
	N2-C6	1.335(3)	N1-C3-C2	116.8(2)	Se1-C4-C5-C6	4.1(4)
	C1-C2	1.335(3)	C5-C4-Se1	125.2(2)	C4-C5-C6-O2	-4.8(4)
	C2-C3	1.473(3)	C4-C5-C6	122.5(2)	C4-C5-C6-N2	172.3(2)
2d	Se1-C1	1.896(1)	C1-Se1-C6	92.5(1)	C6-Se1-C1-C2	173.8(1)
	Se1-C6	1.899(1)	C8-N2-C10	119.6(1)	Se1-C1-C2-C3	-1.7(2)
	O1-C3	1.245(2)	C8-N2-C9	125.3(1)	C1-C2-C3-O1	12.3(2)
	C4-N1	1.456(2)	C10-N2-C9	115.1(1)	C1-C2-C3-N1	-166.2(1)
	O2-C8	1.241(2)	C2-C1-Se1	127.0(1)	O1-C3-N1-C4	-174.1(1)
	N2-C8	1.353(2)	C1-C2-C3	122.1(1)	C2-C3-N1-C4	4.4(2)
	N2-C10	1.453(2)	O1-C3-N1	121.7(1)	O1-C3-N1-C5	3.9(2)
	N2-C9	1.458(2)	O1-C3-C2	120.0(1)	C2-C3-N1-C5	-177.6(1)
	C1-C2	1.338(2)	N1-C3-C2	118.3(1)	C1-Se1-C6-C7	172.0(1)
	C2-C3	1.473(2)	C3-N1-C4	125.3(1)	Se1-C6-C7-C8	0.0(2)
2f	Se1-C16	1.892(3)	C16-Se1-C1	93.7(1)	Se1-C1-C2-C3	-0.7(5)
	Se1-C1	1.898(3)	C3-N1-C4	120.8(2)	C4-N1-C3-O2	-3.2(4)
	O2-C3	1.234(3)	C3-N1-C10	121.8(2)	C10-N1-C3-O2	168.0(3)
	O1-C18	1.229(3)	C4-N1-C10	116.9(2)	C16-Se1-C1-C2	-174.9(3)
	N1-C3	1.378(3)	C2-C1-Se1	125.7(2)	C4-N1-C3-C2	175.8(2)
	N1-C4	1.434(3)	C1-C2-C3	120.7(3)	C1-C2-C3-O2	-7.7(4)
	C1-C2	1.342(4)	O2-C3-N1	121.7(2)	C10-N1-C3-C2	-13.1(4)
	C2-C3	1.465(4)	O2-C3-C2	120.5(2)	C1-C2-C3-N1	173.3(3)
2i	Se1-C1	1.892(3)	C9-Se1-C1	94.7(1)	C9-Se1-C1-C2	-169.5(3)
	Se1-C9	1.891(3)	N2-C4-C5	109.7(3)	Se1-C1-C2-C3	5.2(4)
	O1-C3	1.248(4)	C11-N1-C16	119.6(2)	C1-C2-C3-O1	-14.0(4)
	N1-C11	1.359(4)	C11-N1-C12	127.0(2)	C1-C2-C3-N2	163.9(3)
	N1-C16	1.461(4)	C16-N1-C12	113.2(2)	O1-C3-N2-C4	170.0(3)
	N1-C12	1.473(4)	C2-C1-Se1	126.5(2)	C2-C3-N2-C4	-7.8(4)
	C1-C2	1.330(4)	C1-C2-C3	122.0(3)	O1-C3-N2-C8	11.4(4)
	C2-C3	1.480(4)	O1-C3-C2	119.5(3)	C2-C3-N2-C8	-166.4(3)
	C3-N2	1.350(4)	N2-C3-C2	118.8(3)	C5-C4-N2-C3	-99.5(4)
	N2-C8	1.469(4)	C3-N2-C4	125.8(3)	C5-C4-N2-C8	60.5(3)

Examples of ^{1}H, ^{13}C, and ^{77}Se NMR spectra of products

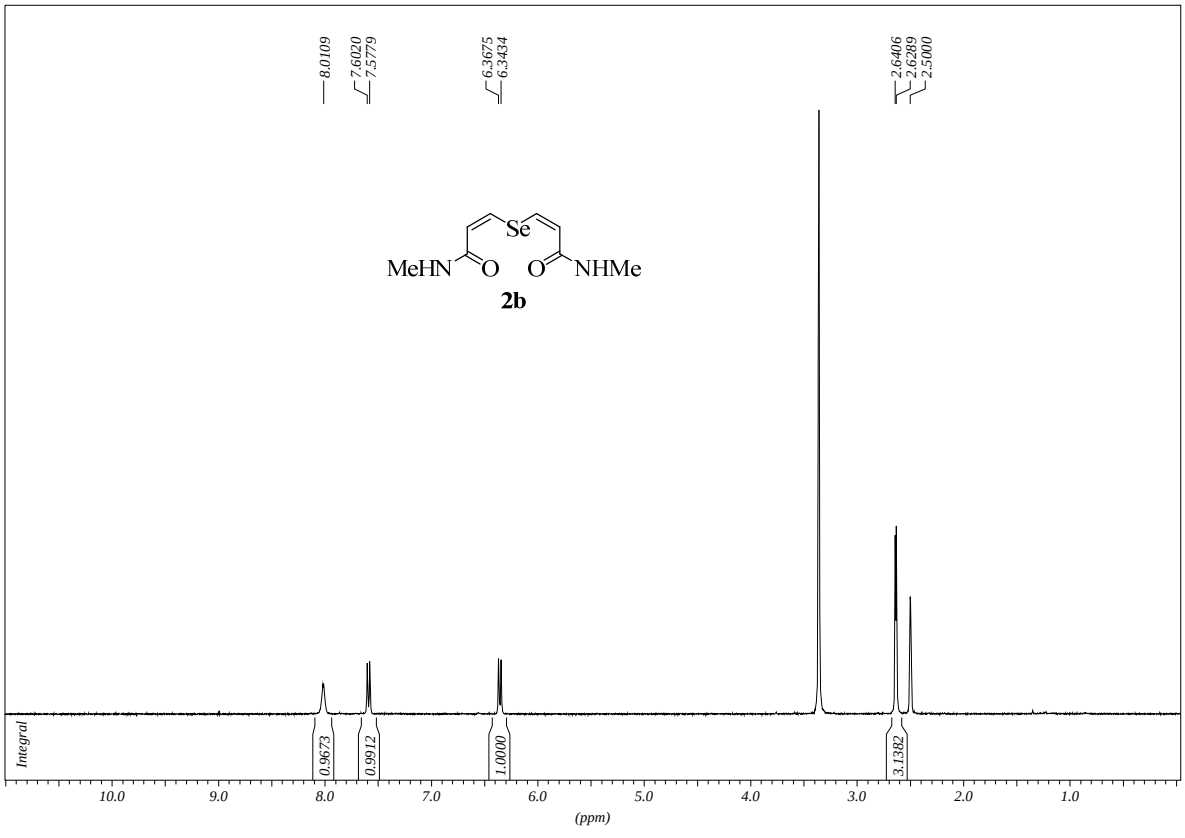
^{1}H, ^{13}C, and ^{77}Se NMR spectra of product 2a

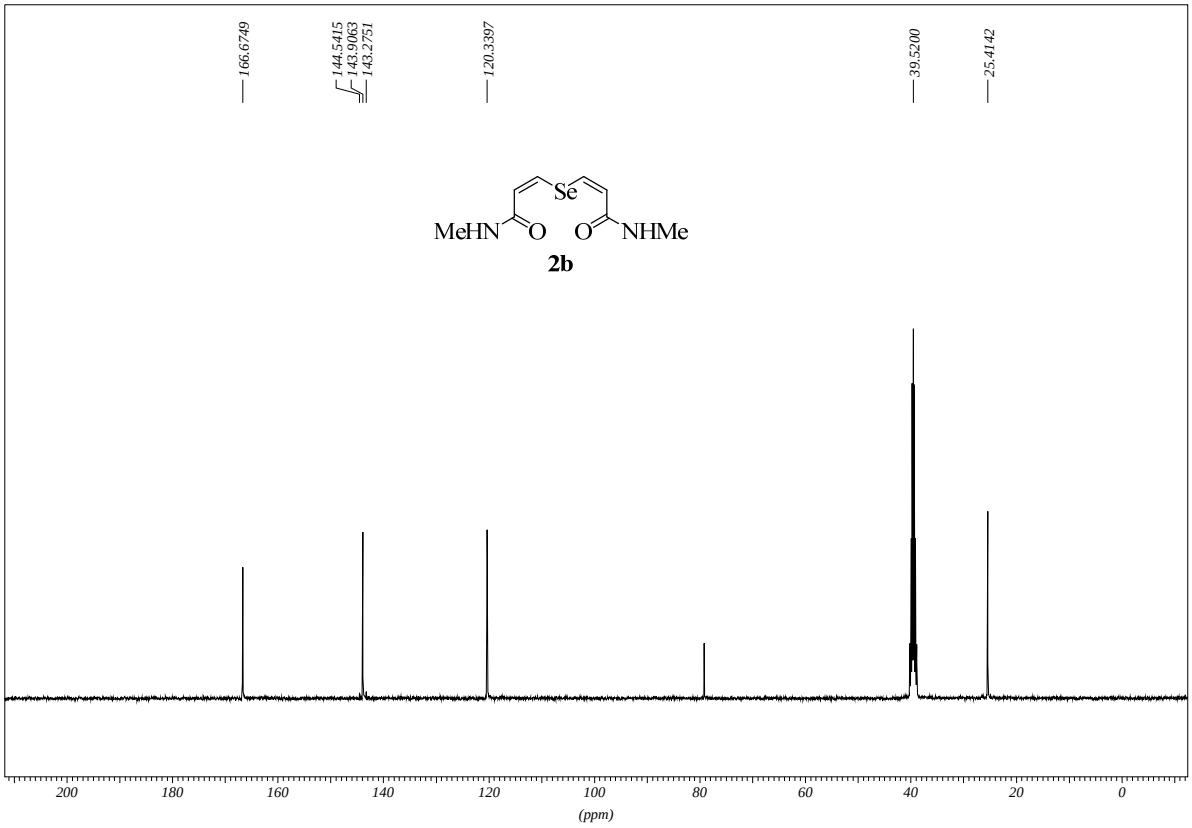

7.6598
7.6359
7.4984
7.1088
6.3911
6.3672
2.5000
Se
H2N
O
O
NH2
2a
Integral
1.0172
0.9523
0.9488
1.0000
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
(ppm)

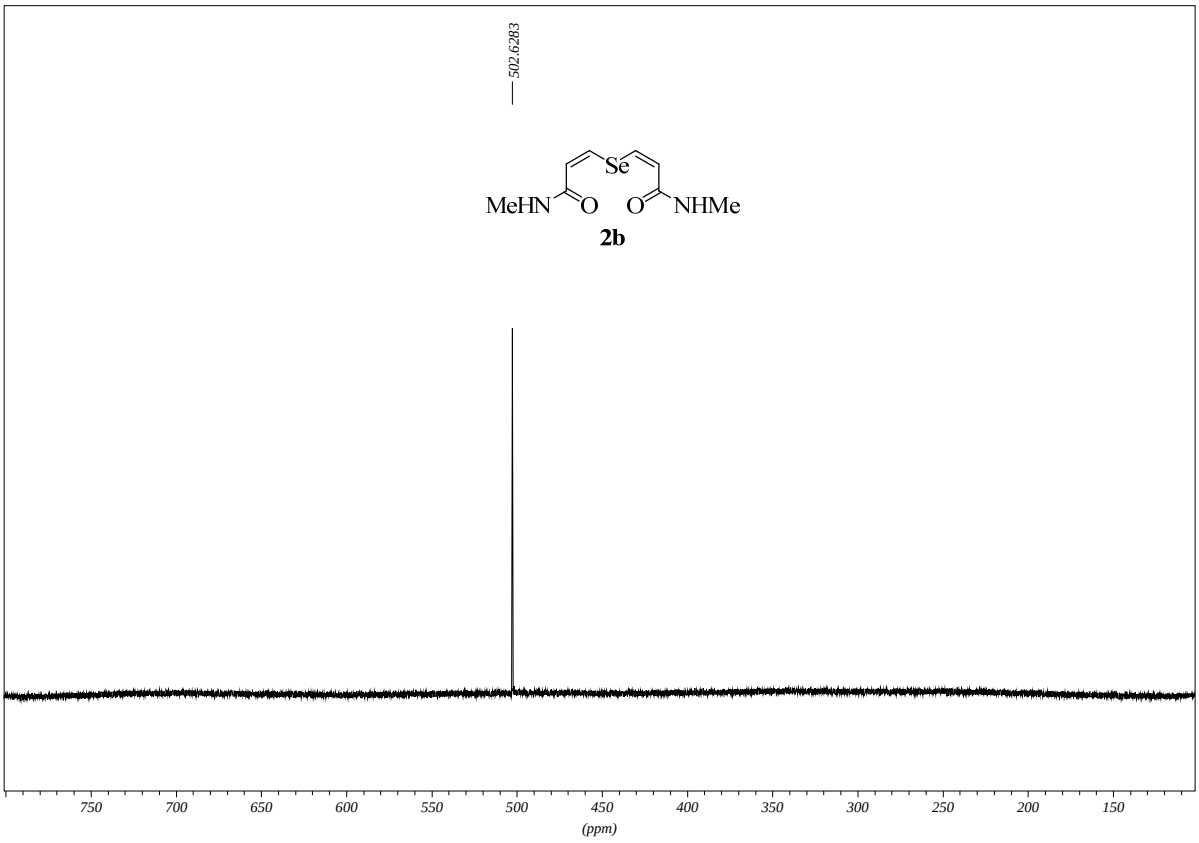

167.9811
145.8159
145.1807
144.5415
120.4747
39.5200
Se
H2N
O
O
NH2
2a
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
(ppm)



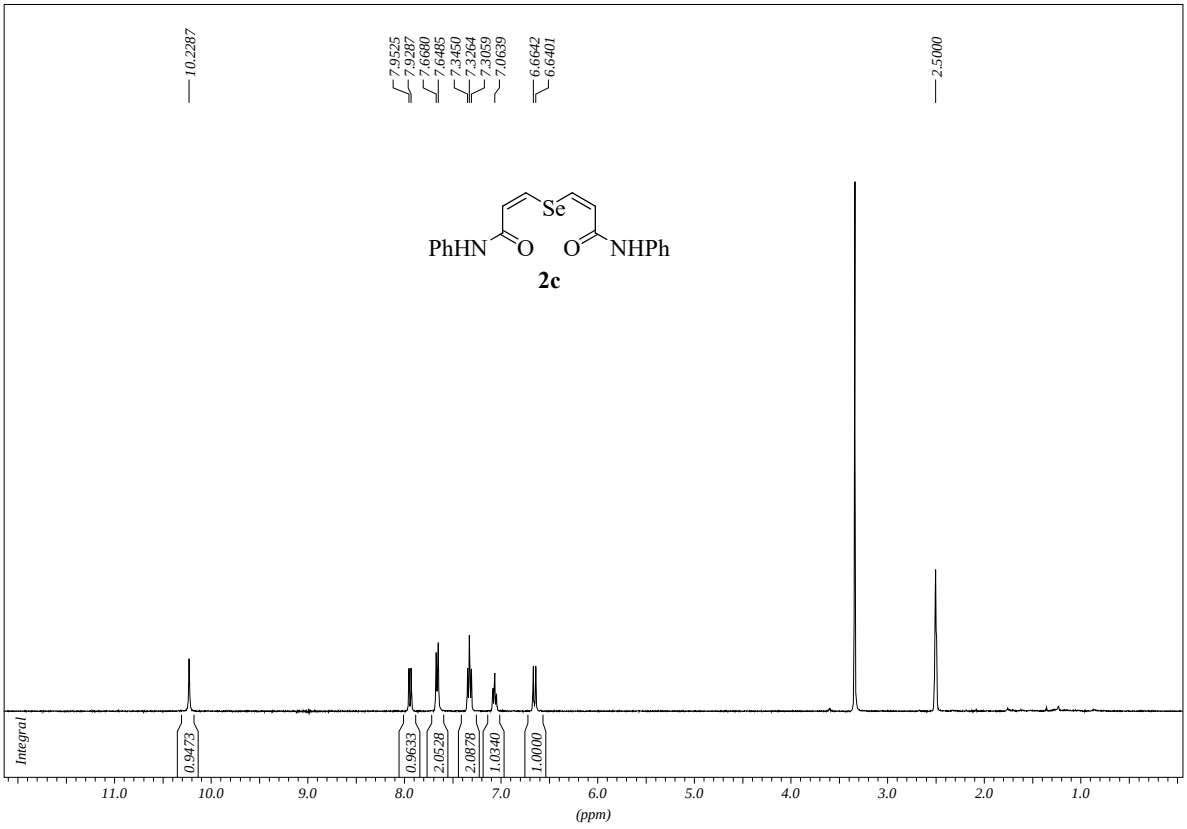
^{1}H, ^{13}C, and ^{77}Se NMR spectra of product 2b

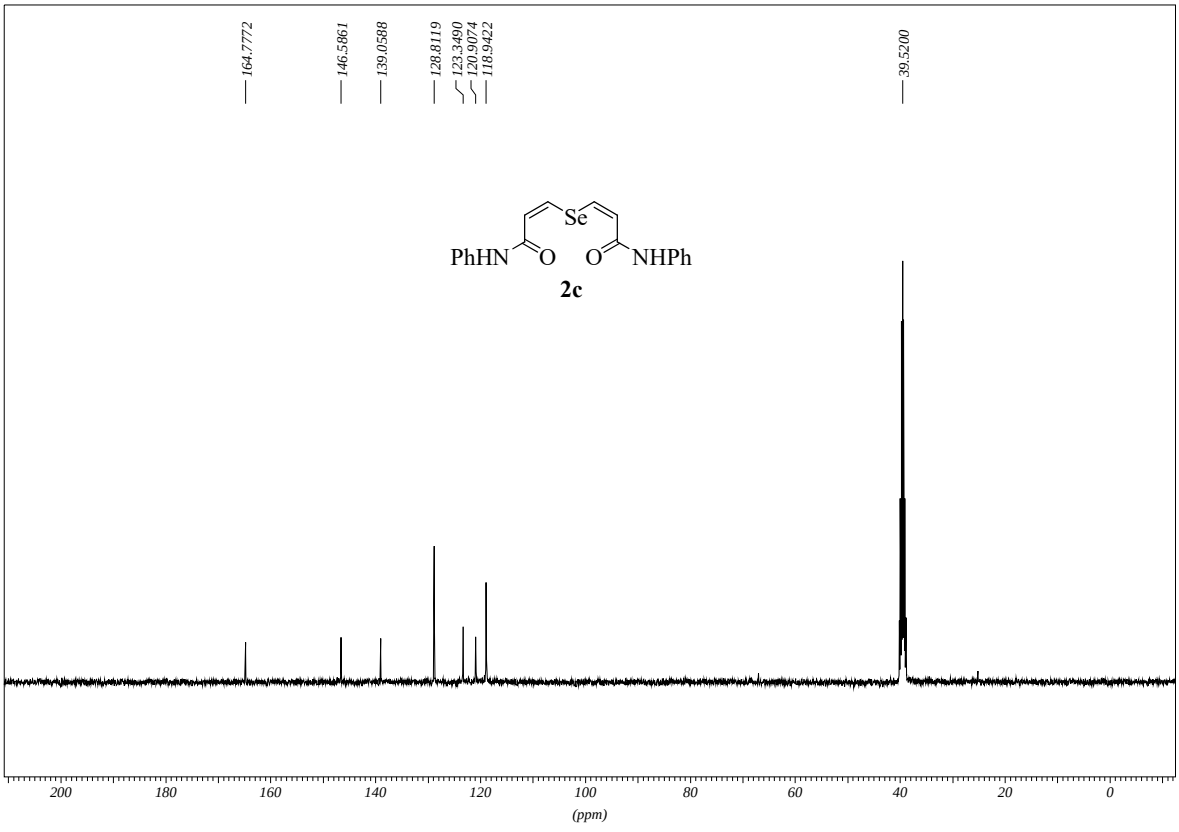


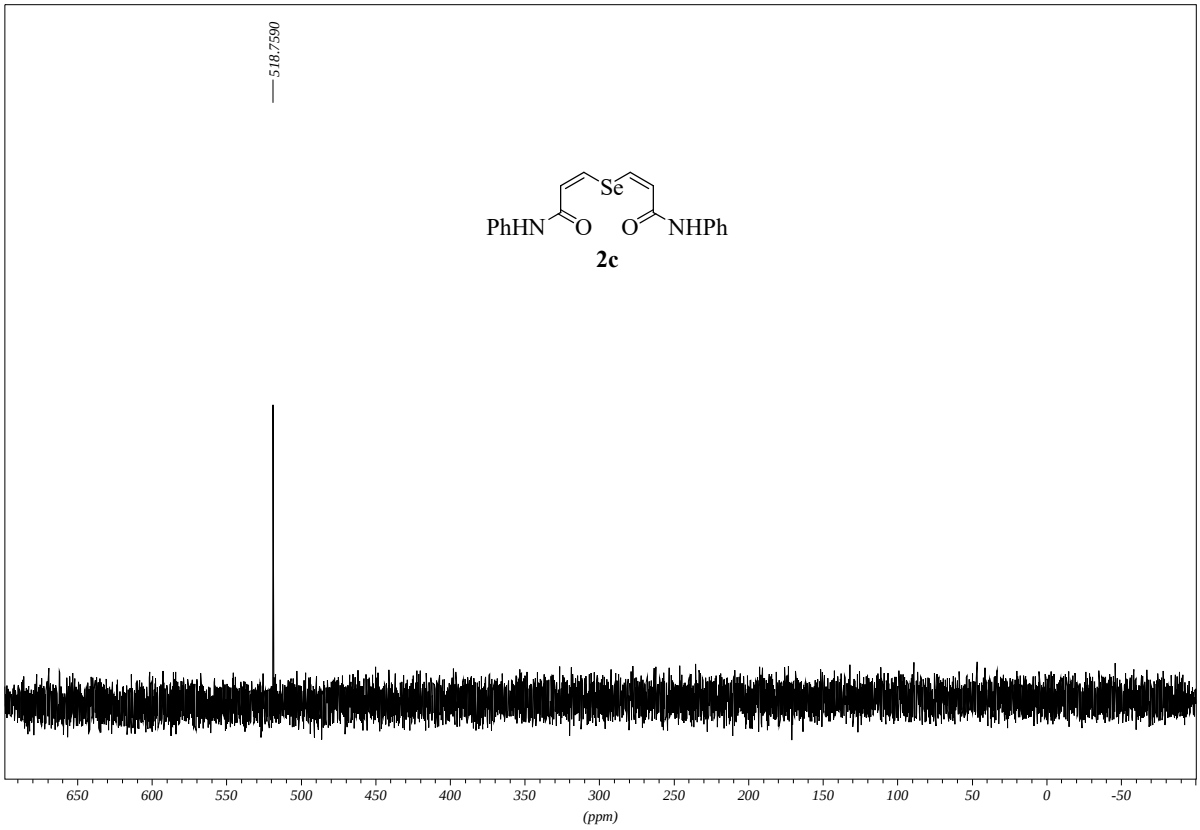

166.6749
144.5415
143.9063
143.2751
120.3397
39.5200
25.4142
Se
MeHN
O
O
NHMe
2b
200
180
160
140
120
100
80
60
40
20
0
(ppm)


502.6283
Se
MeHN
O
O
NHMe
2b
750
700
650
600
550
500
450
400
350
300
250
200
150
(ppm)

^{1}H, ^{13}C, and ^{77}Se NMR spectra of product 2c

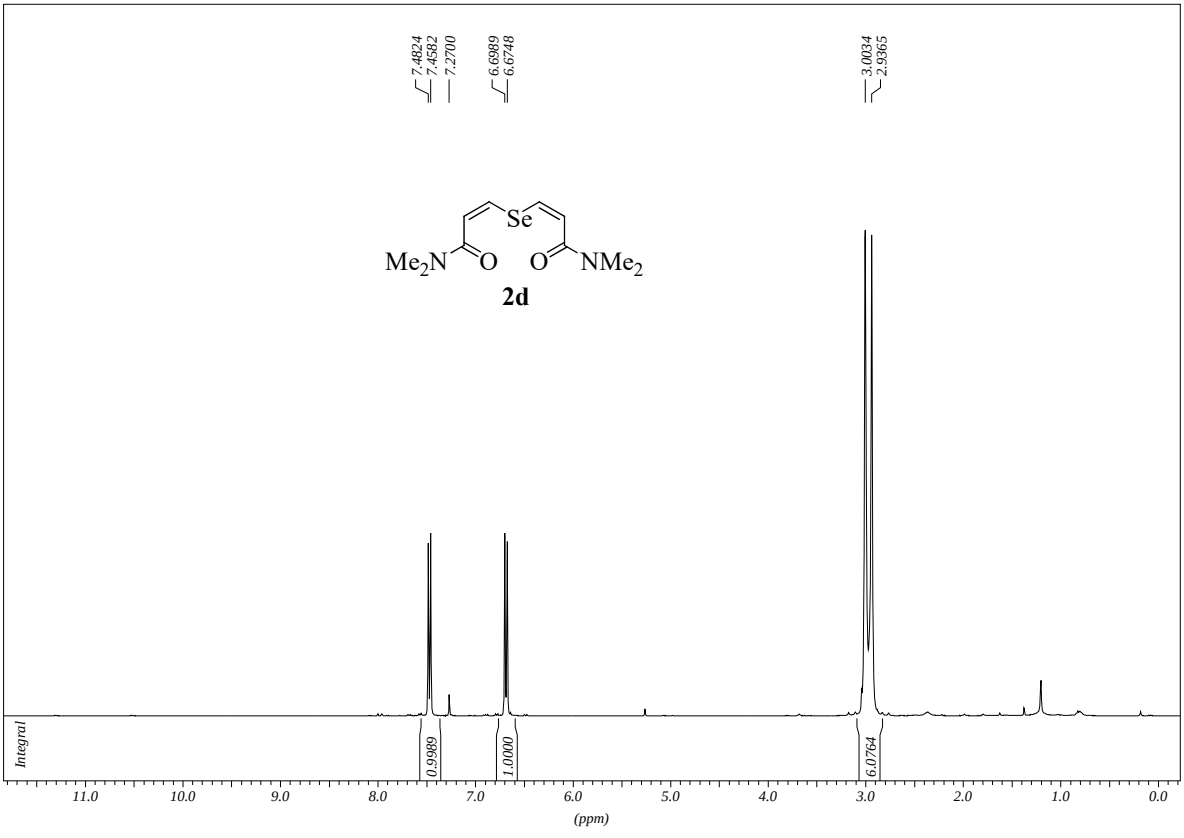




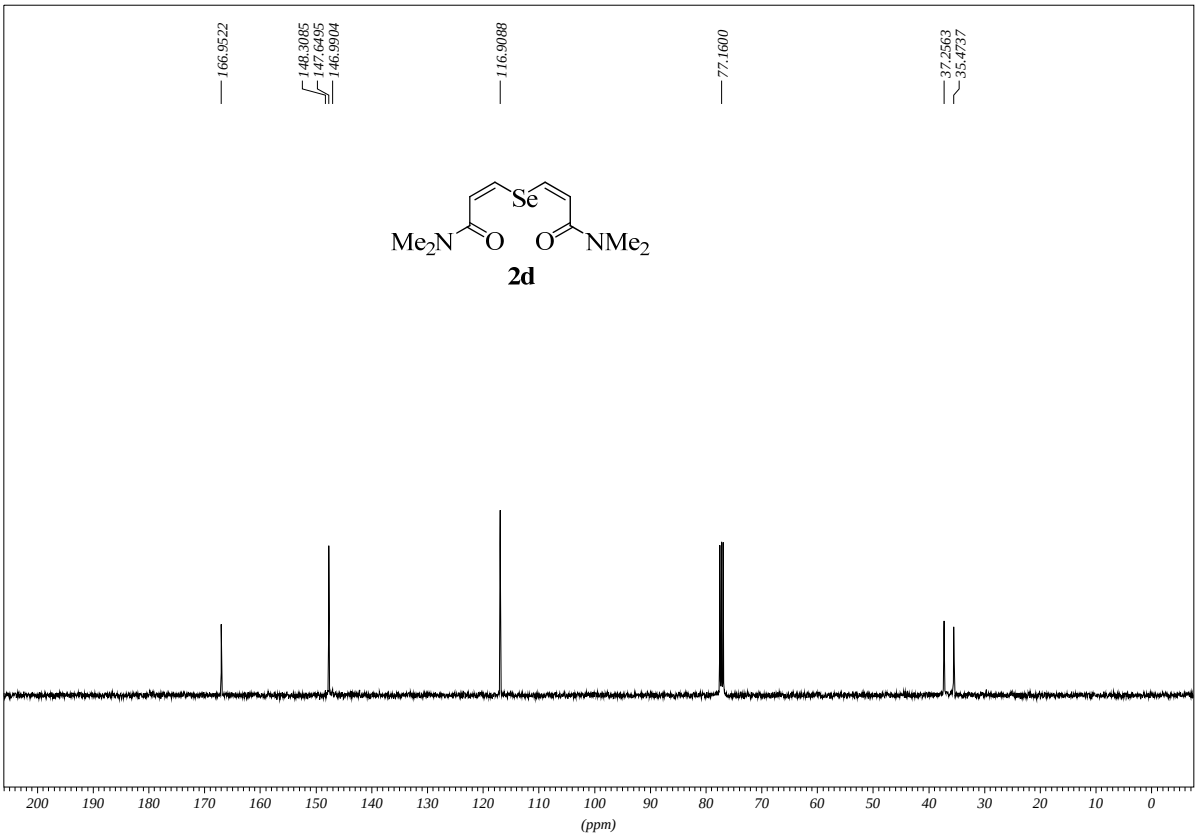


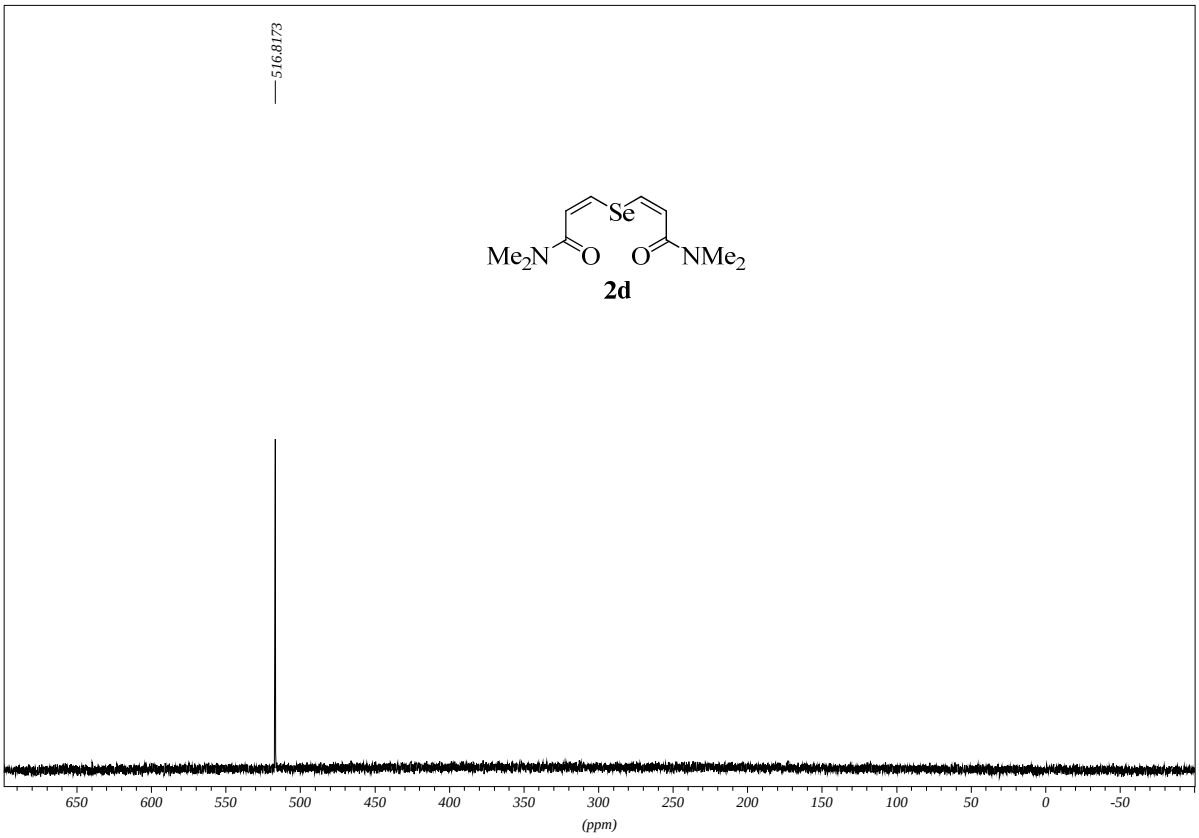
2c

^{1}H, ^{13}C, and ^{77}Se NMR spectra of product 2d

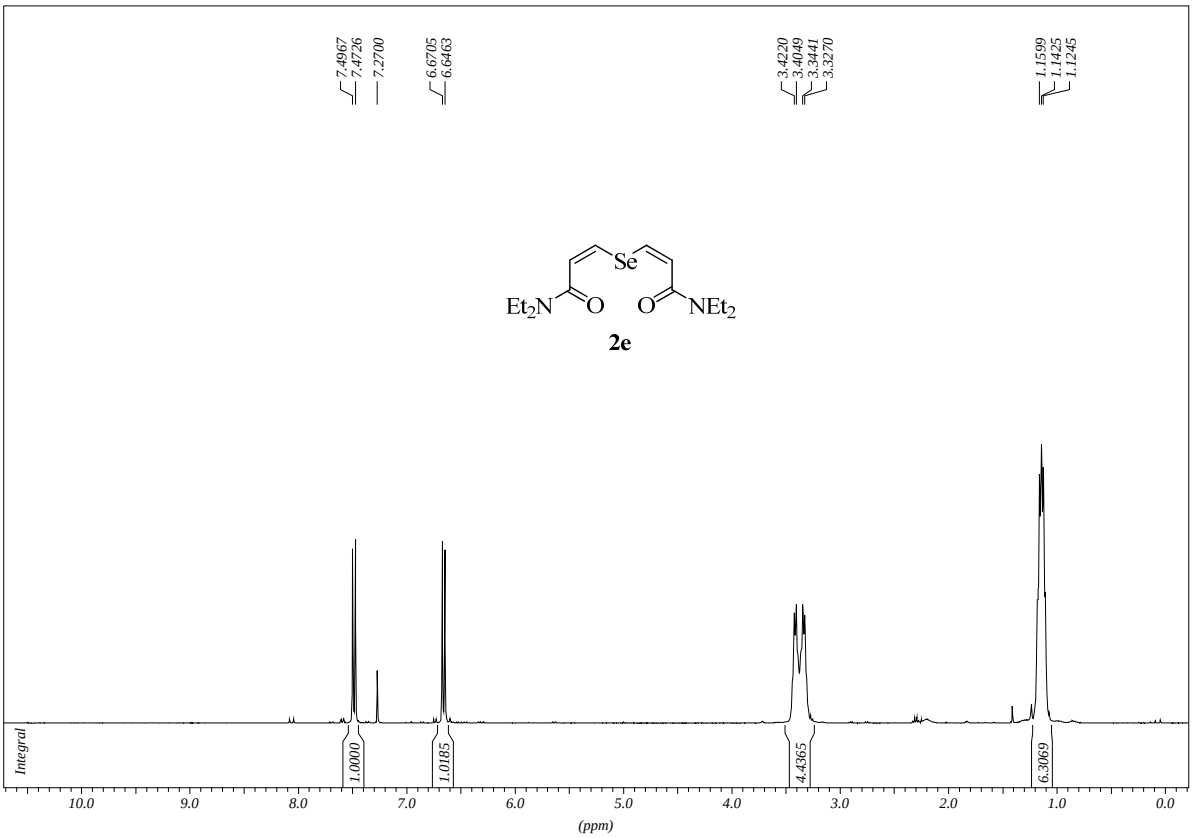


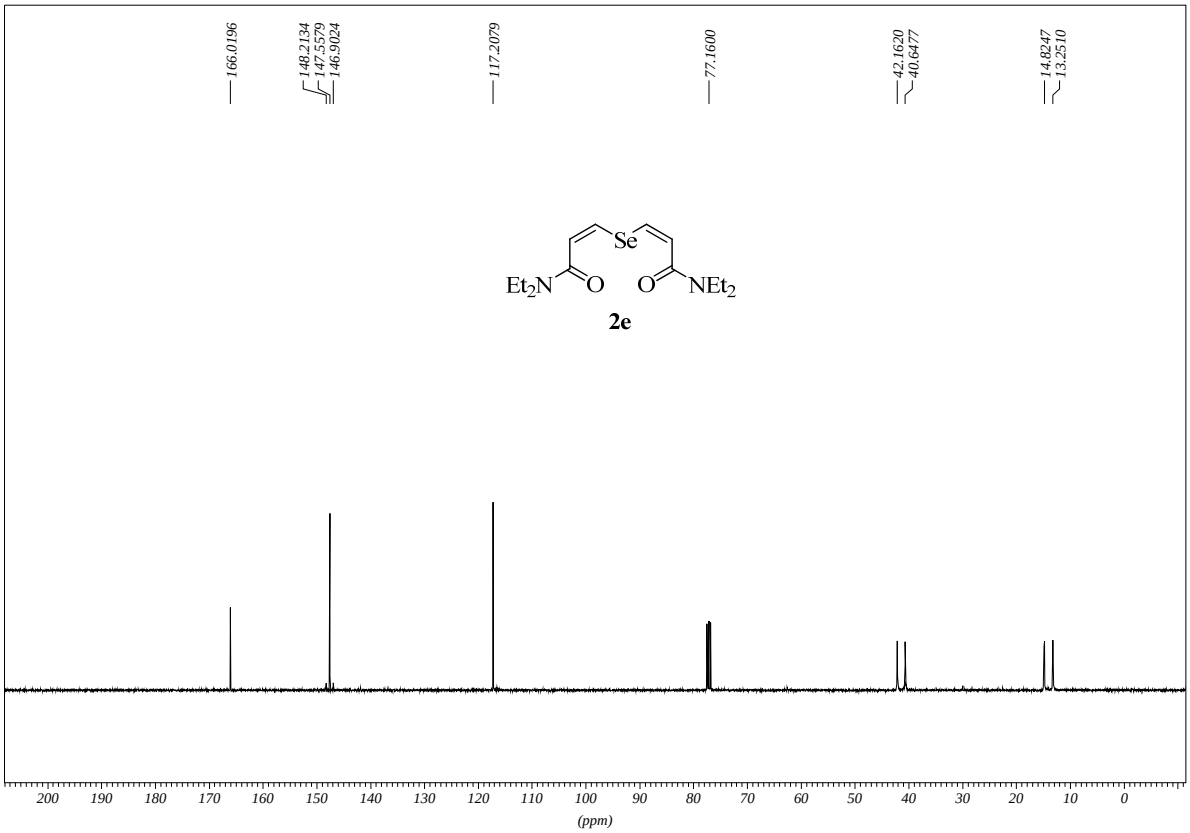
2d

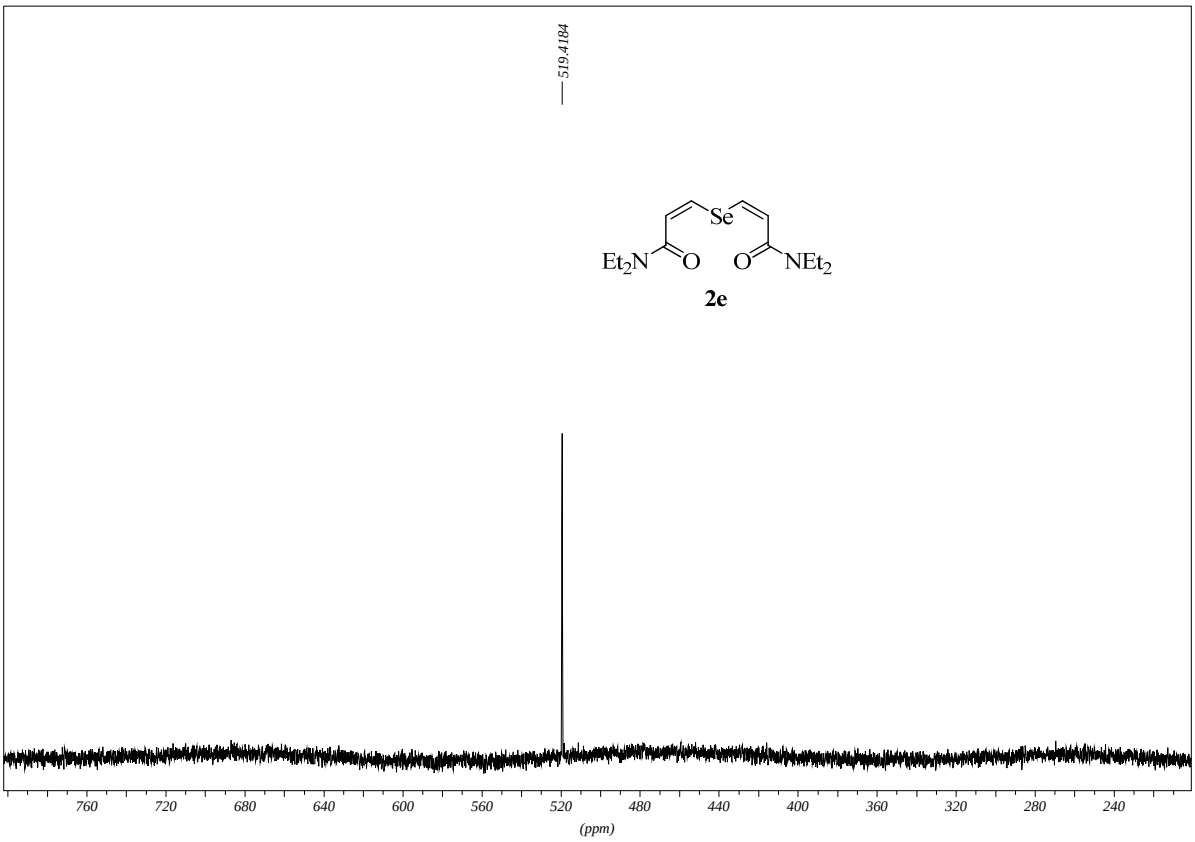

166.9522
148.3085
147.6495
146.9904
116.9088
77.1600
37.2563
35.4737
Se
Me2N
O
O
NMe2
2d
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
(ppm)


516.8173
Se
Me2N
O
O
NMe2
2d
650 600 550 500 450 400 350 300 250 200 150 100 50 0 -50
(ppm)

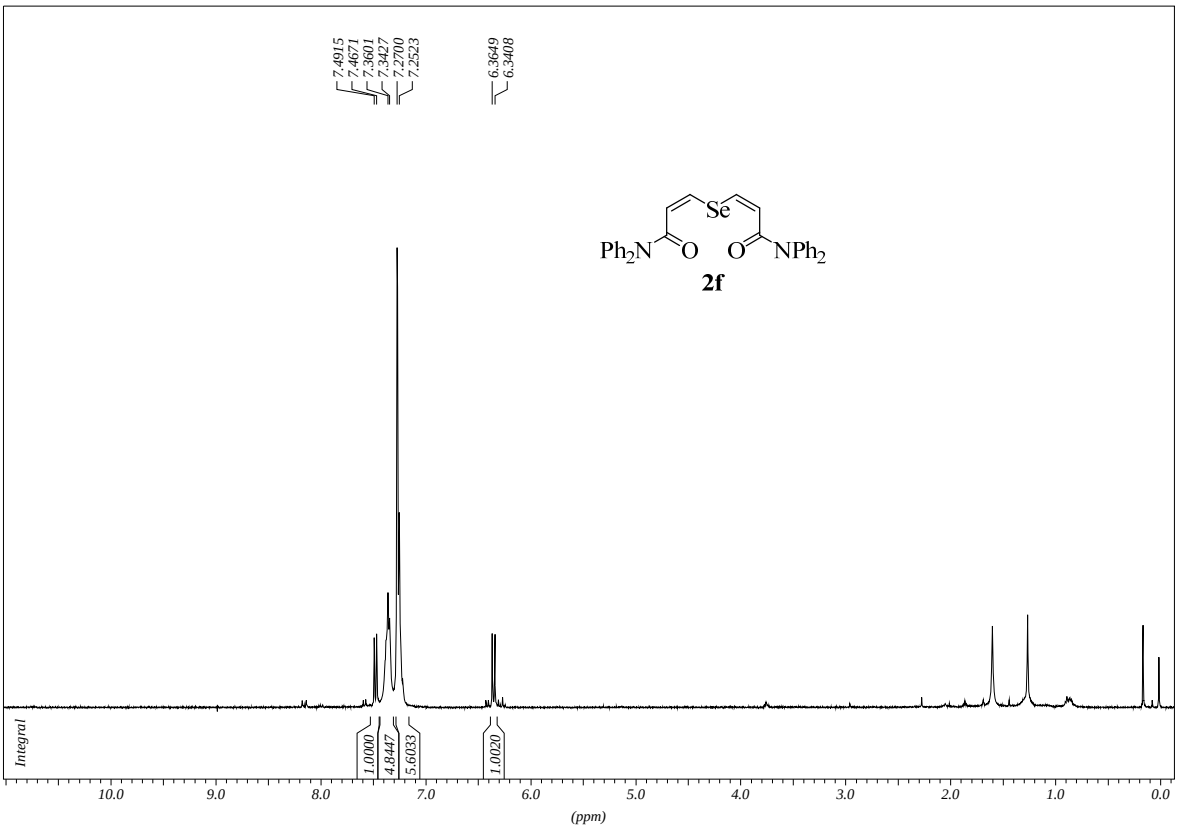
^{1}H, ^{13}C, and ^{77}Se NMR spectra of product 2e

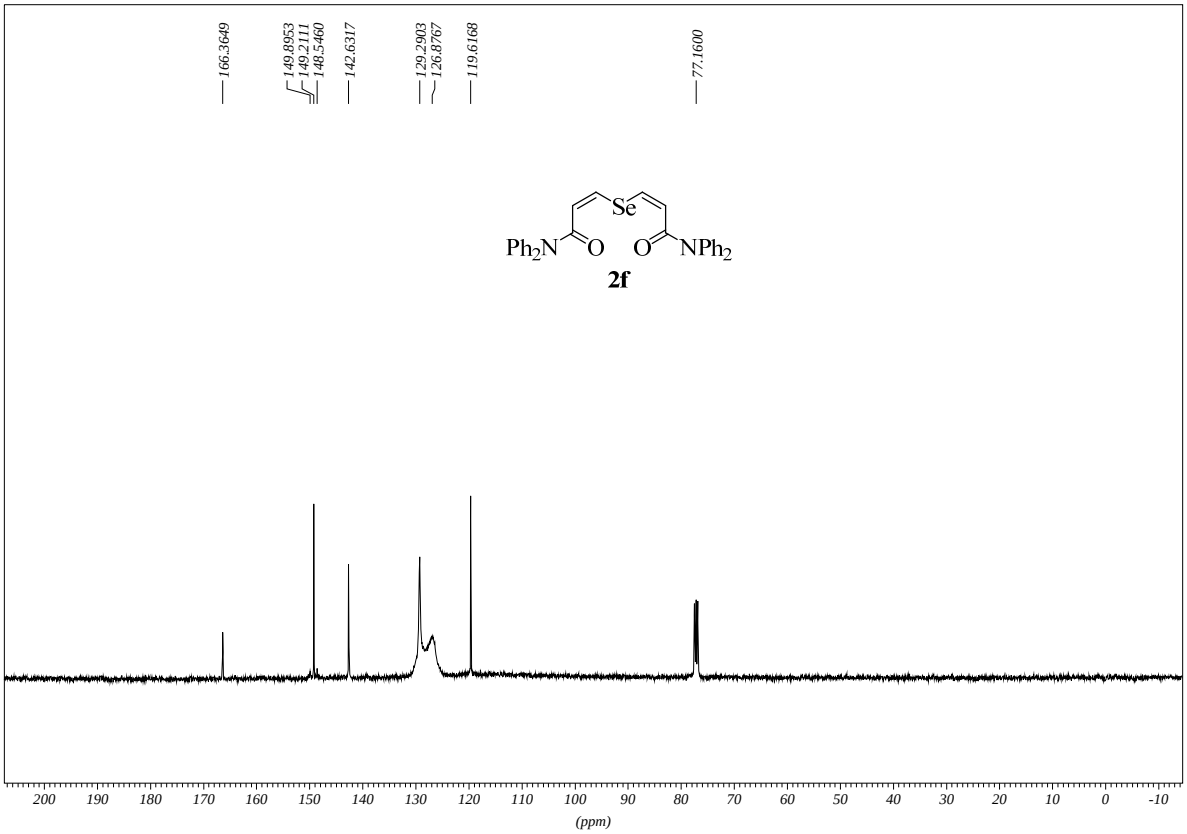


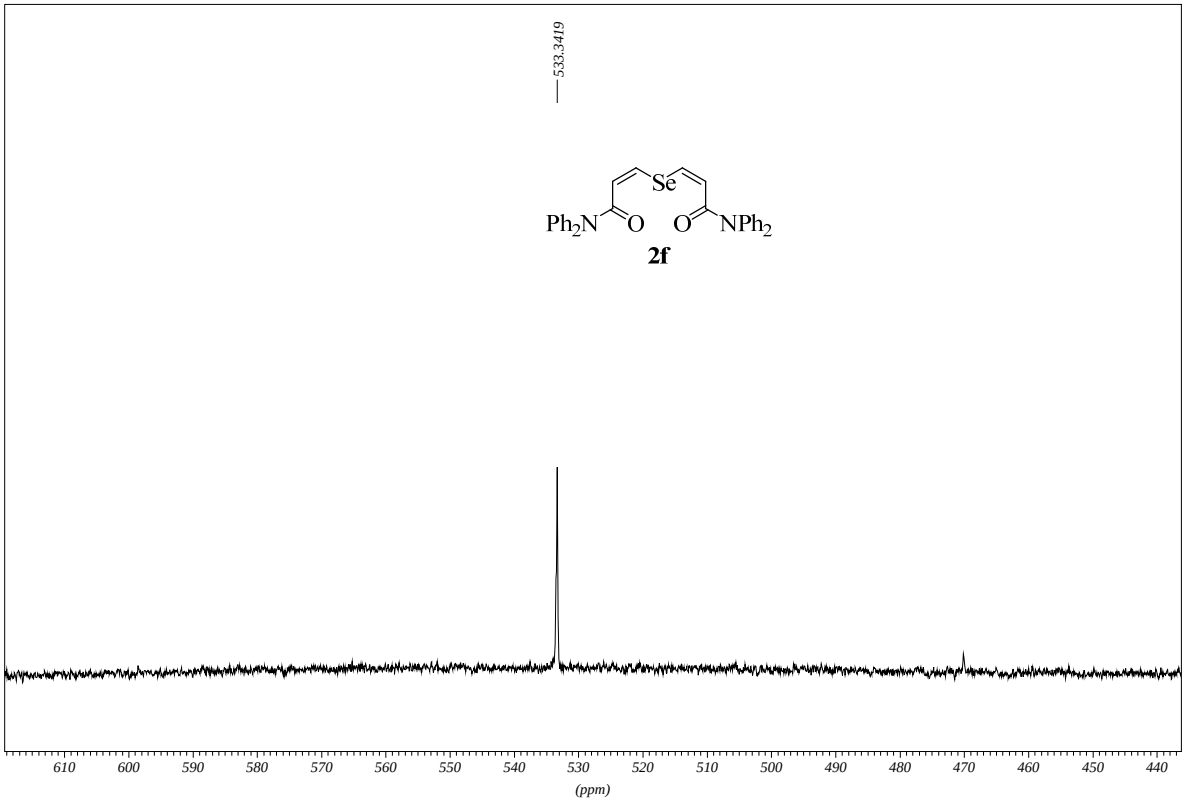




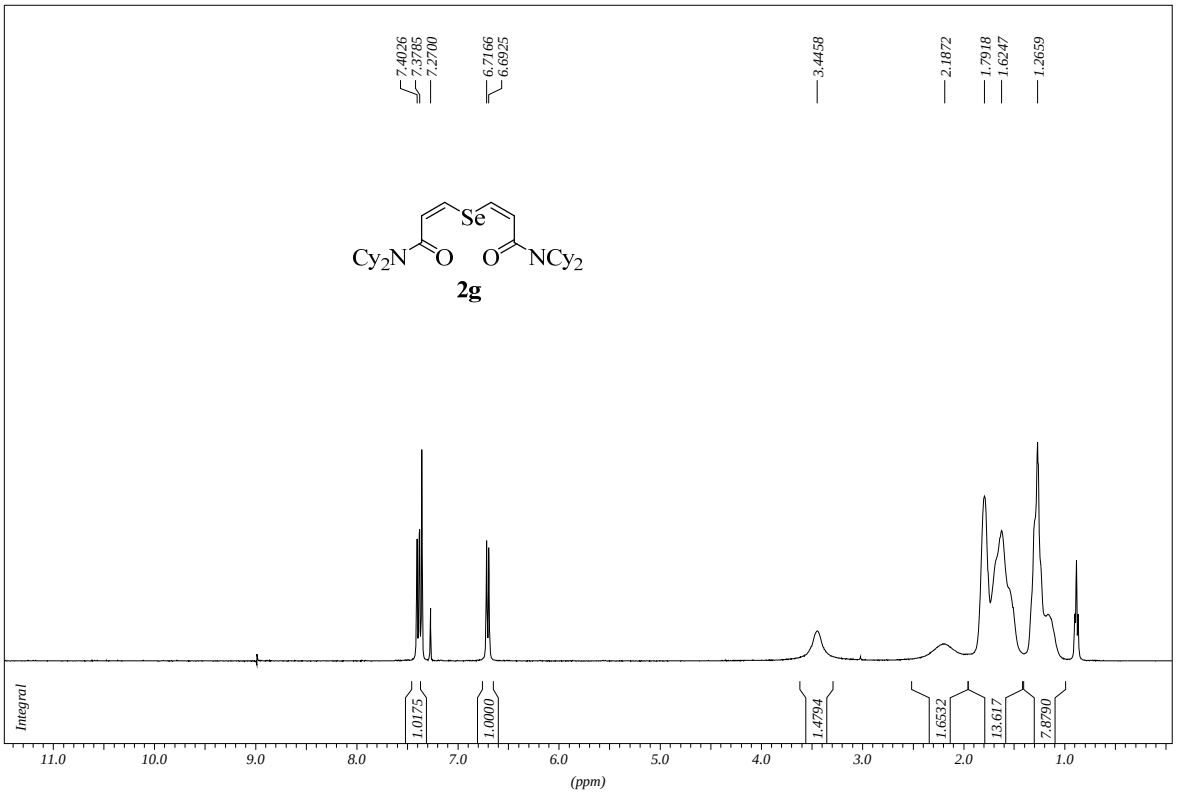
^{1}H, ^{13}C, and ^{77}Se NMR spectra of product 2f

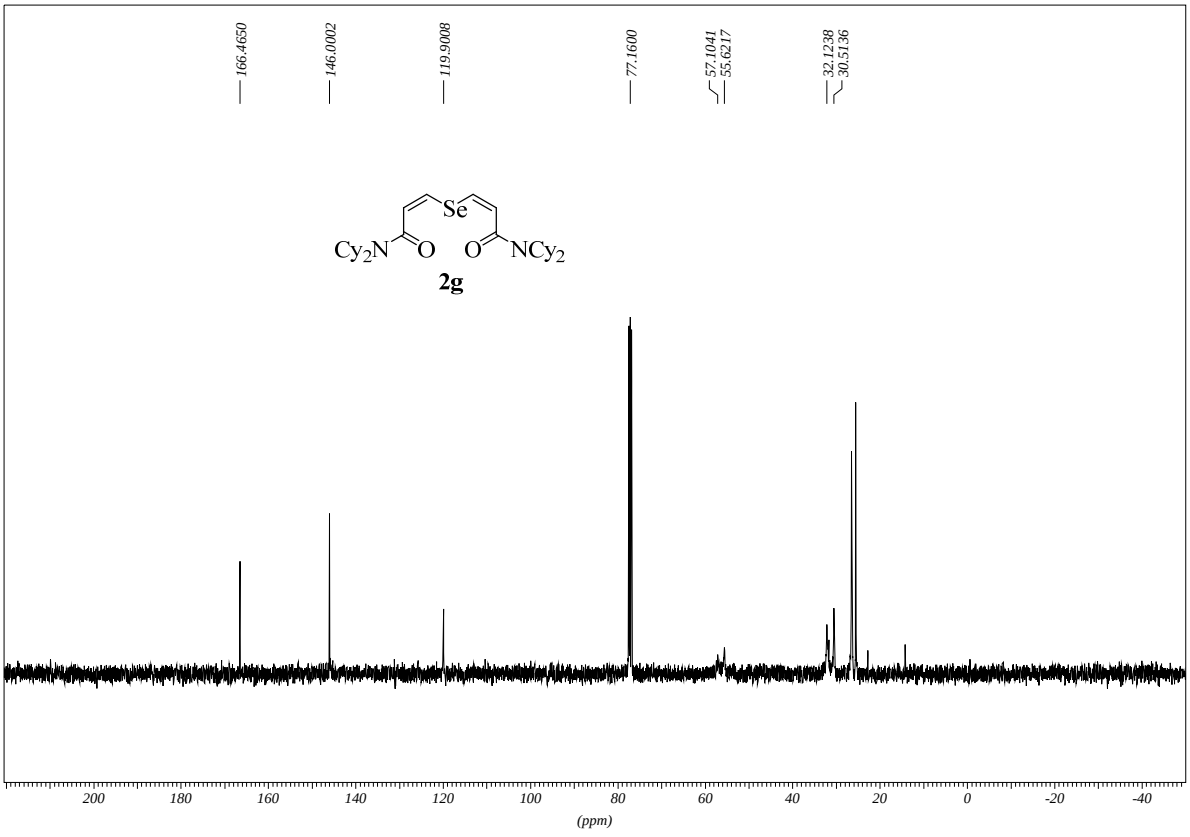


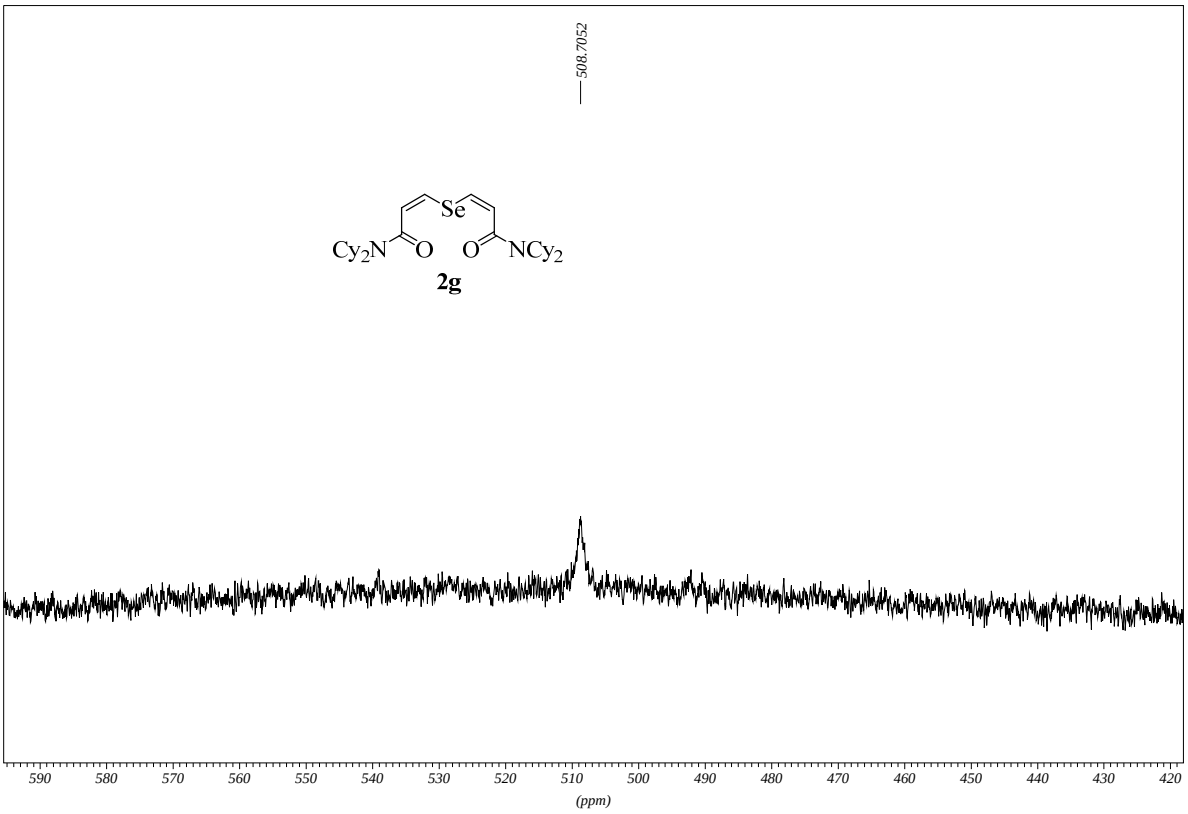

166.3649
149.8953
149.2111
148.5460
142.6317
129.2903
126.8767
119.6168
77.1600
Se
Ph2N
O
O
NPh2
2f
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
(ppm)


533.3419
Se
Ph2N
O
O
NPh2
2f
610 600 590 580 570 560 550 540 530 520 510 500 490 480 470 460 450 440
(ppm)

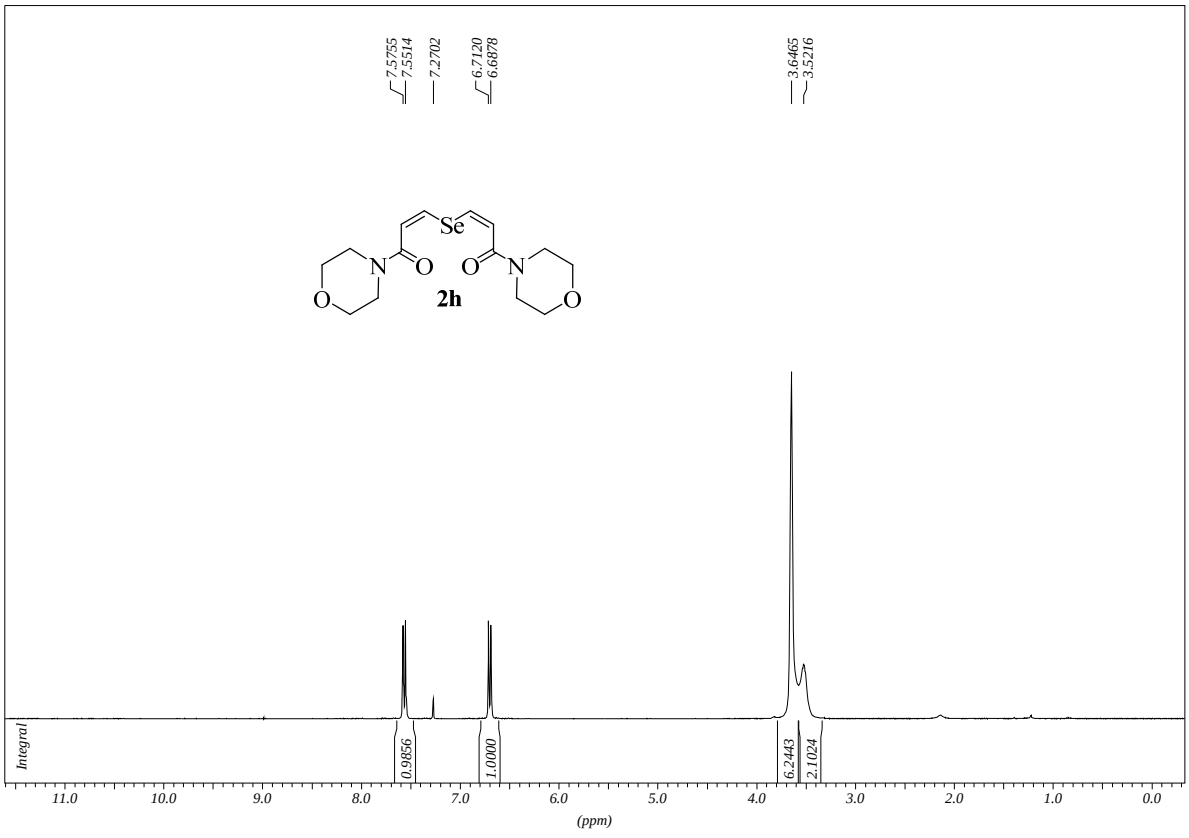
^{1}H, ^{13}C, and ^{77}Se NMR spectra of product 2g

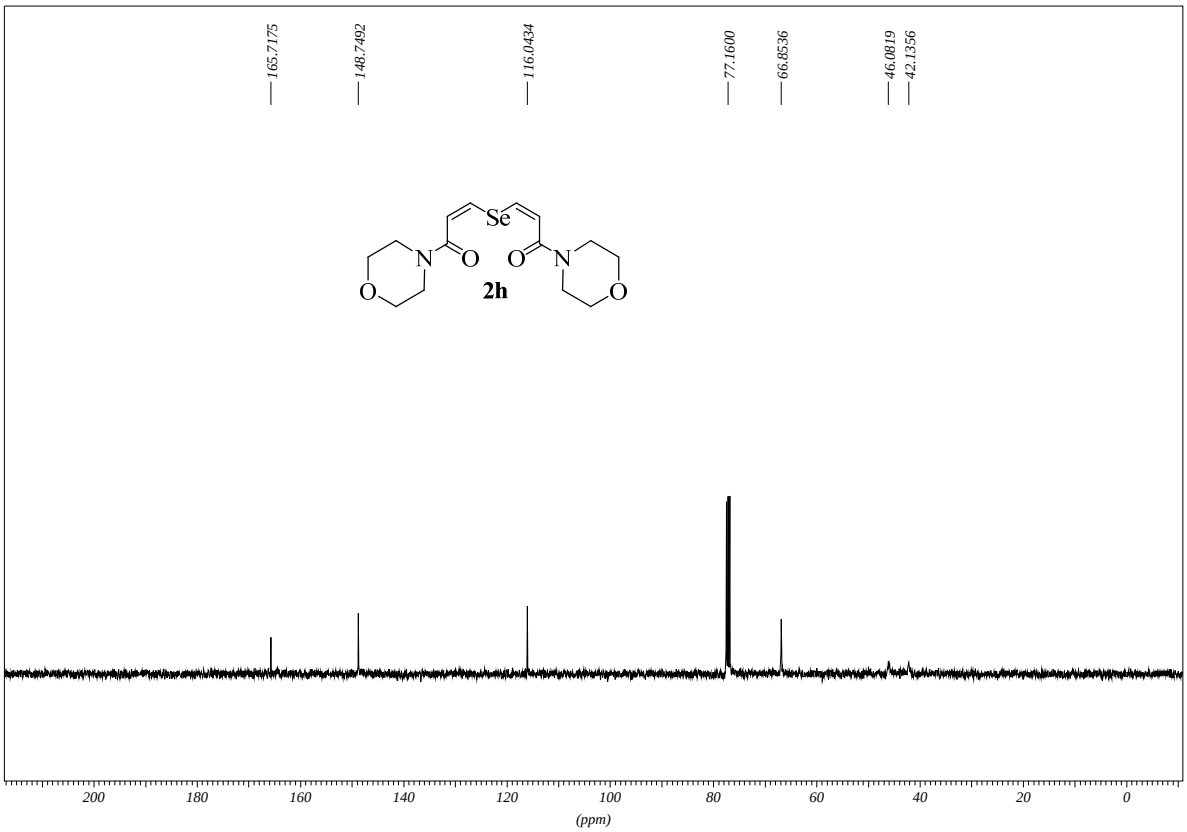


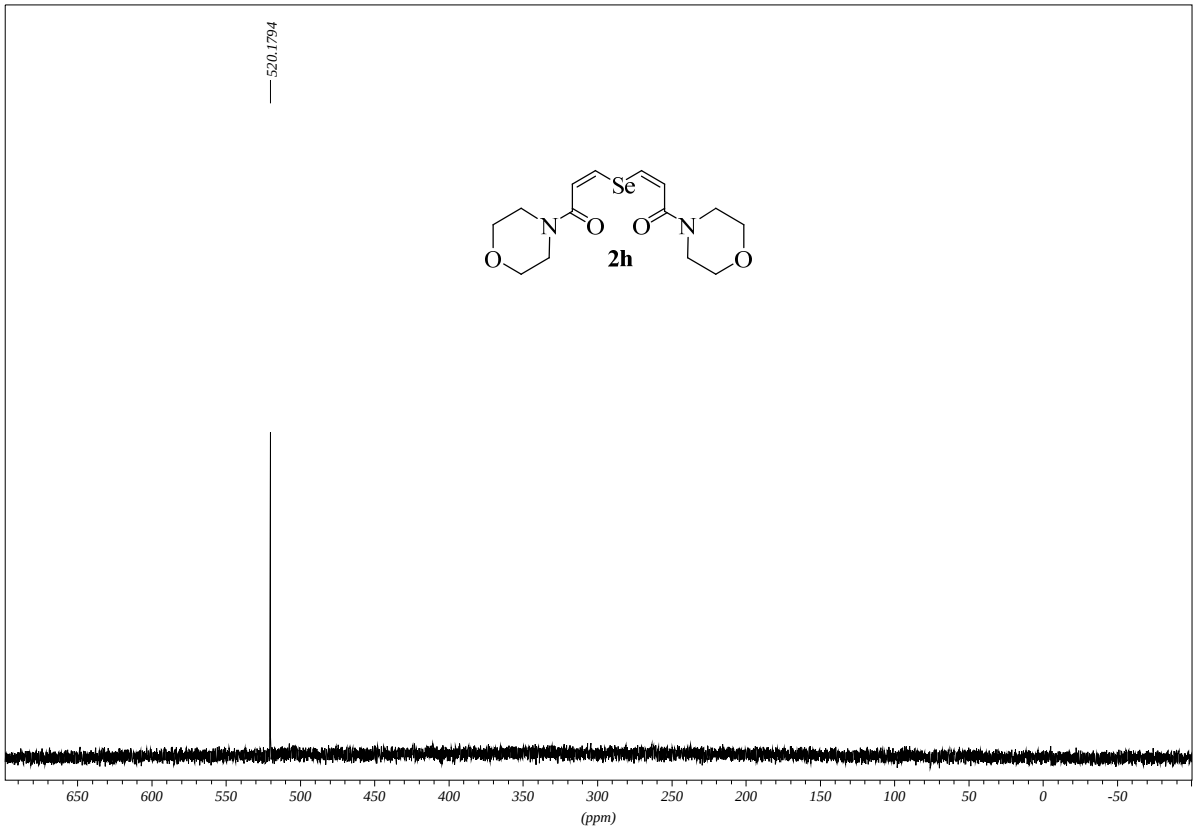




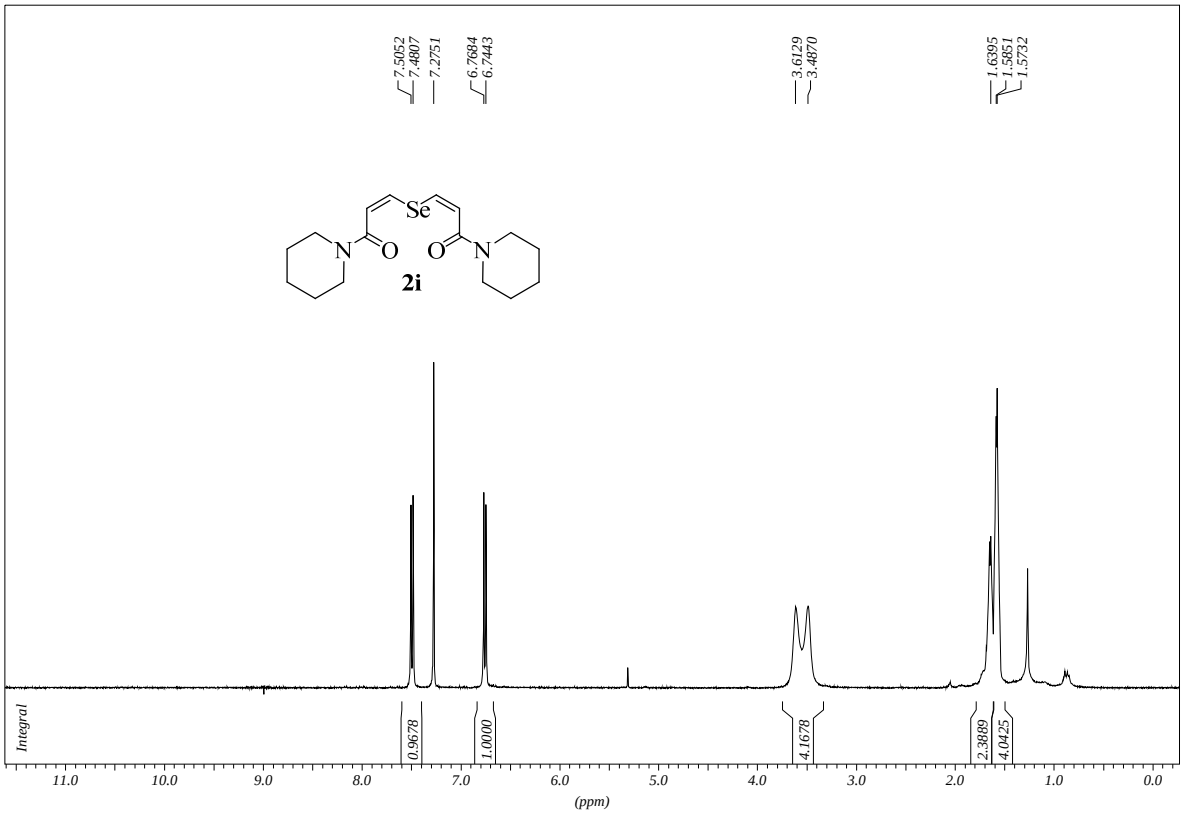
^{1}H, ^{13}C, and ^{77}Se NMR spectra of product 2h

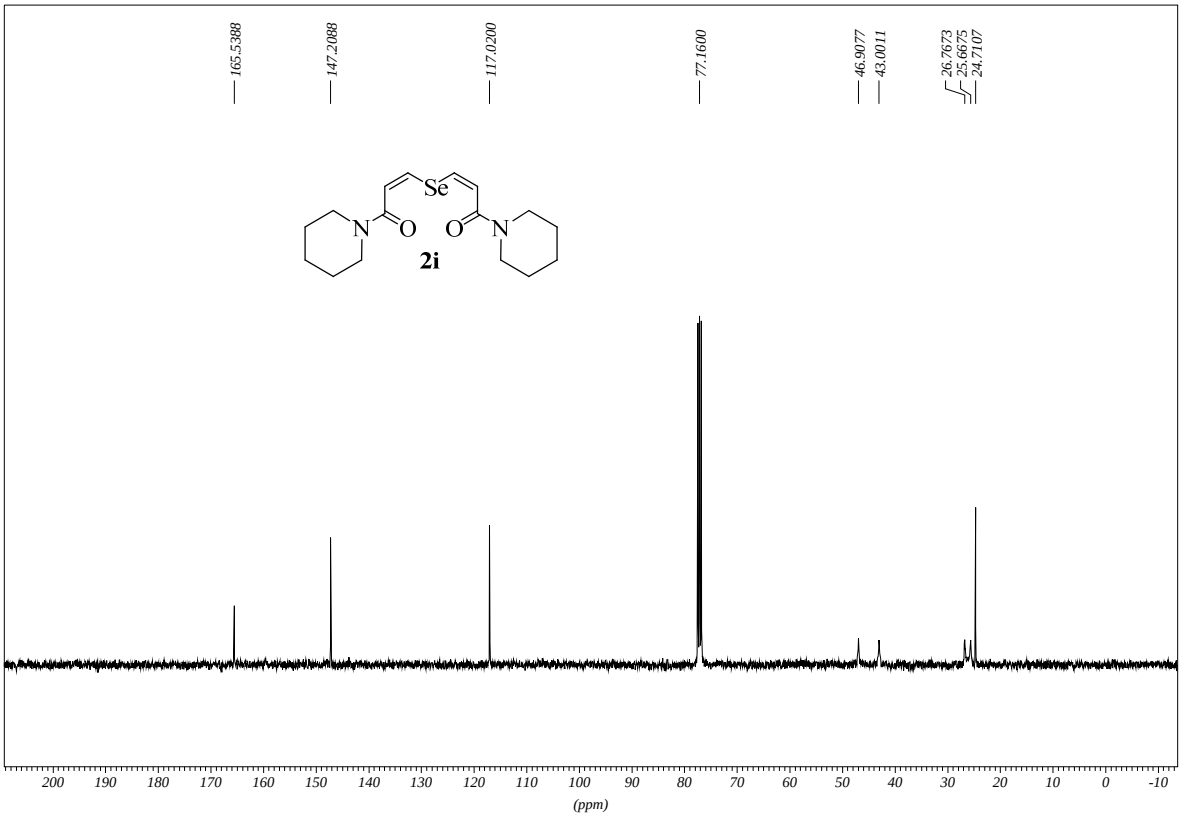


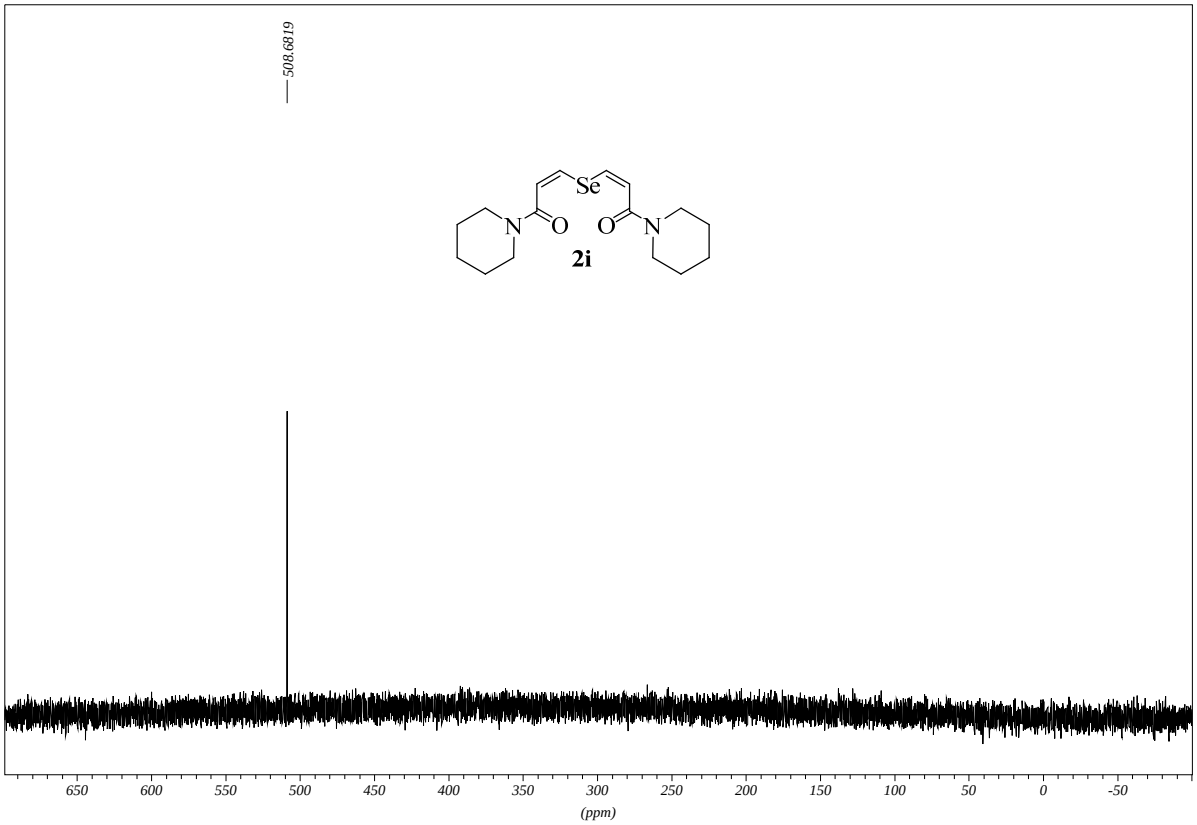

165.7175
148.7492
116.0434
77.1600
66.8536
46.0819
42.1356
Se
N
O
O
N
O
O
2h
200
180
160
140
120
100
80
60
40
20
0
(ppm)


520.1794
Se
N
O
O
N
O
O
2h
650
600
550
500
450
400
350
300
250
200
150
100
50
0
-50
(ppm)

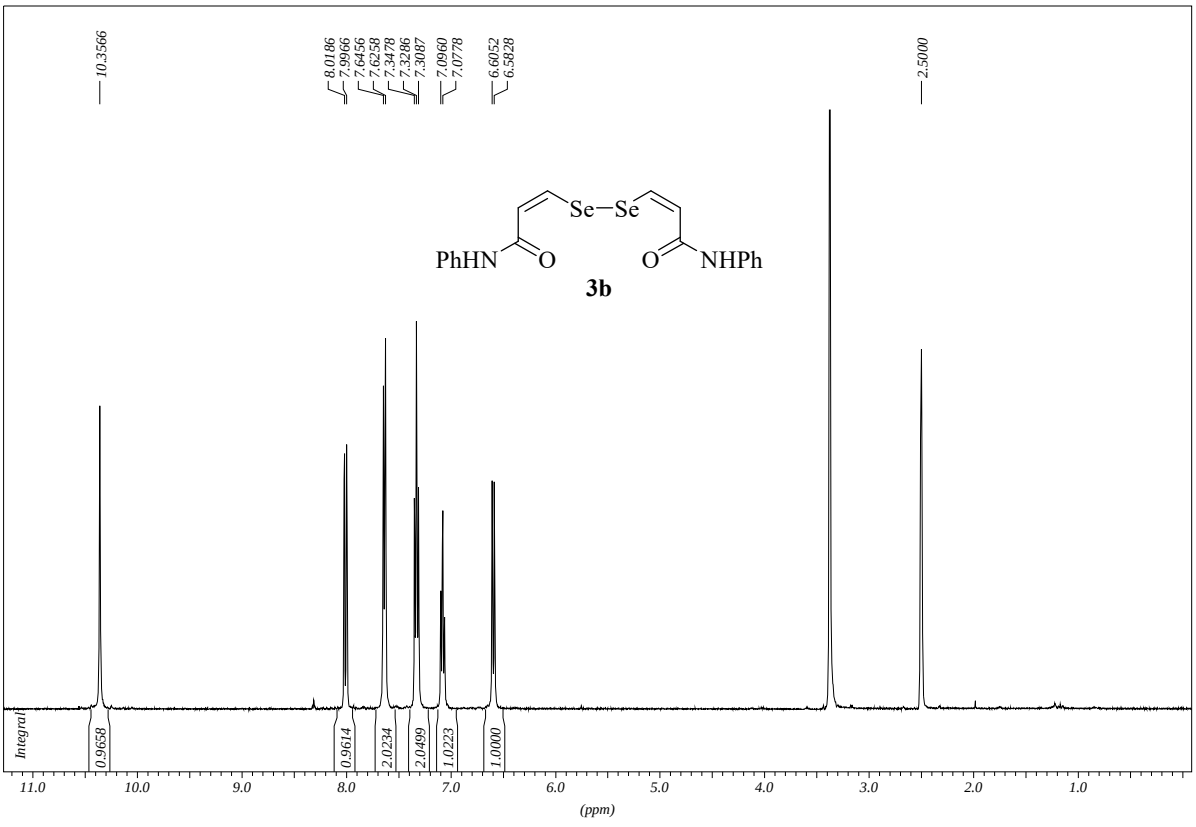
^{1}H, ^{13}C, and ^{77}Se NMR spectra of product 2i

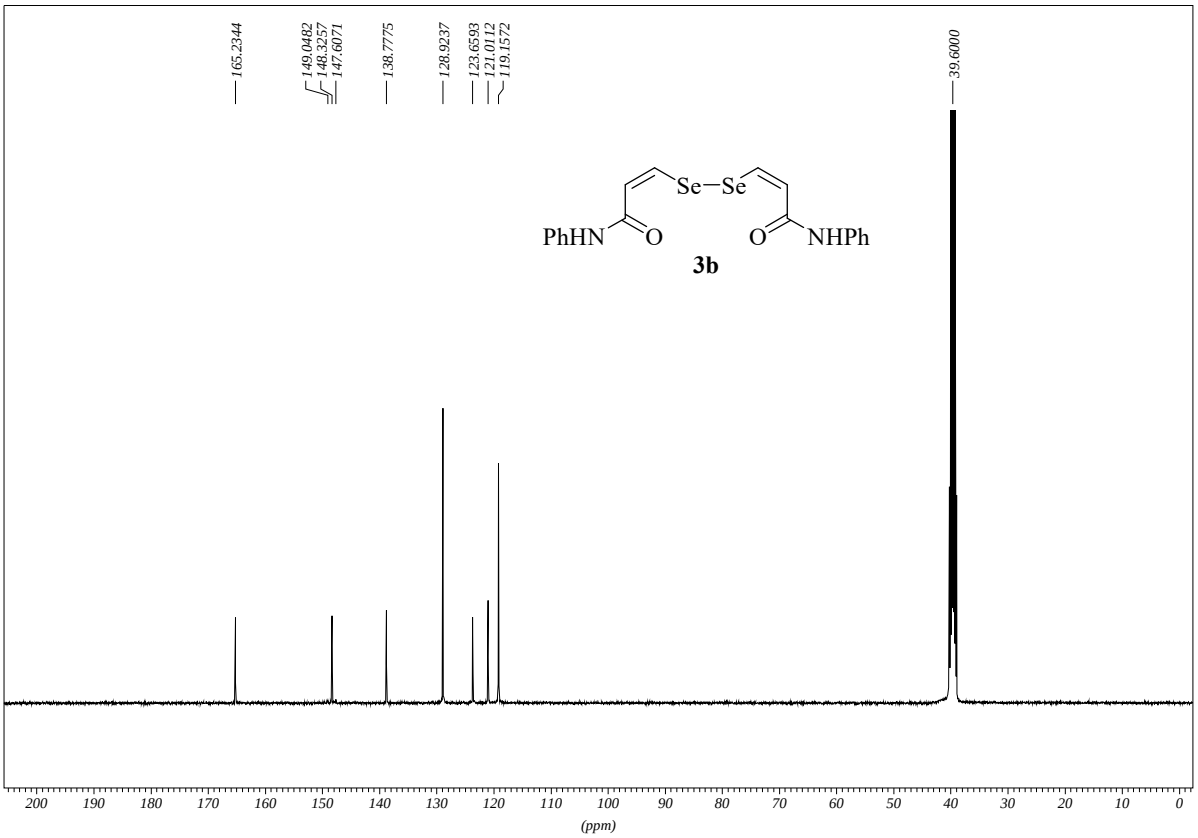


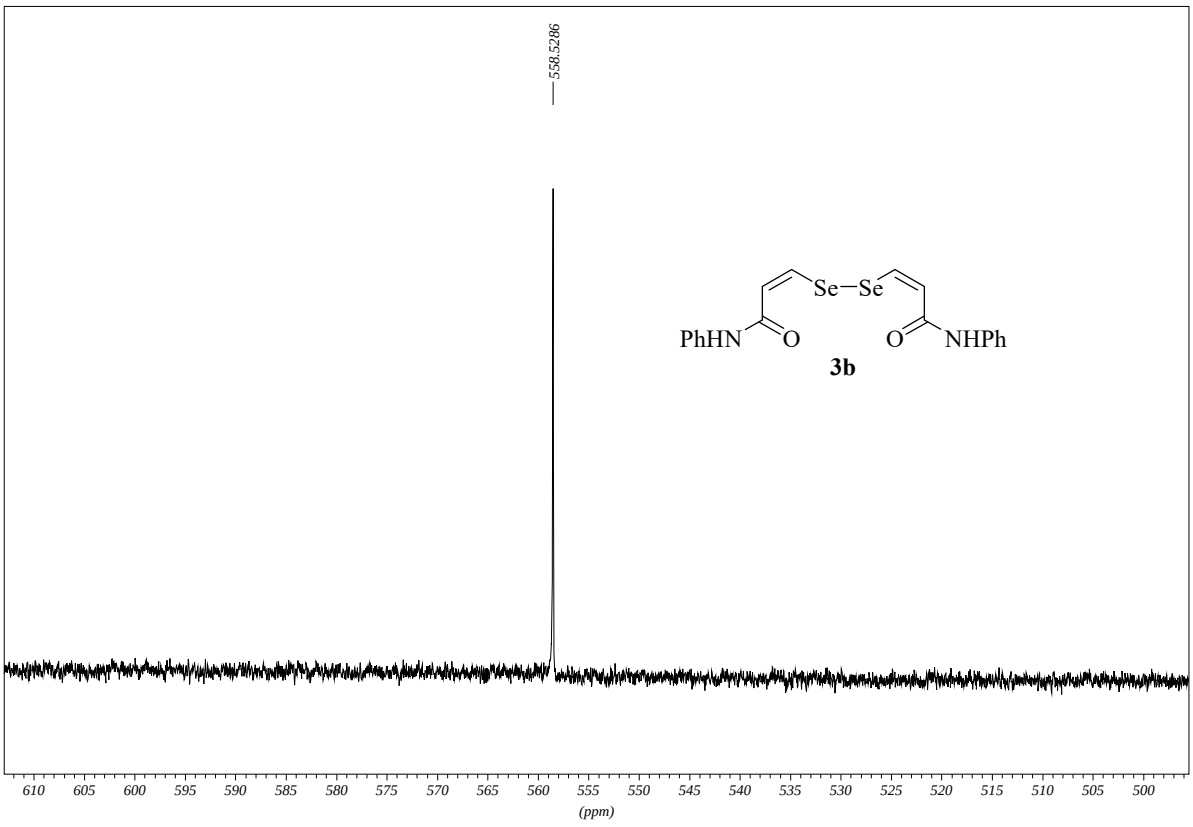




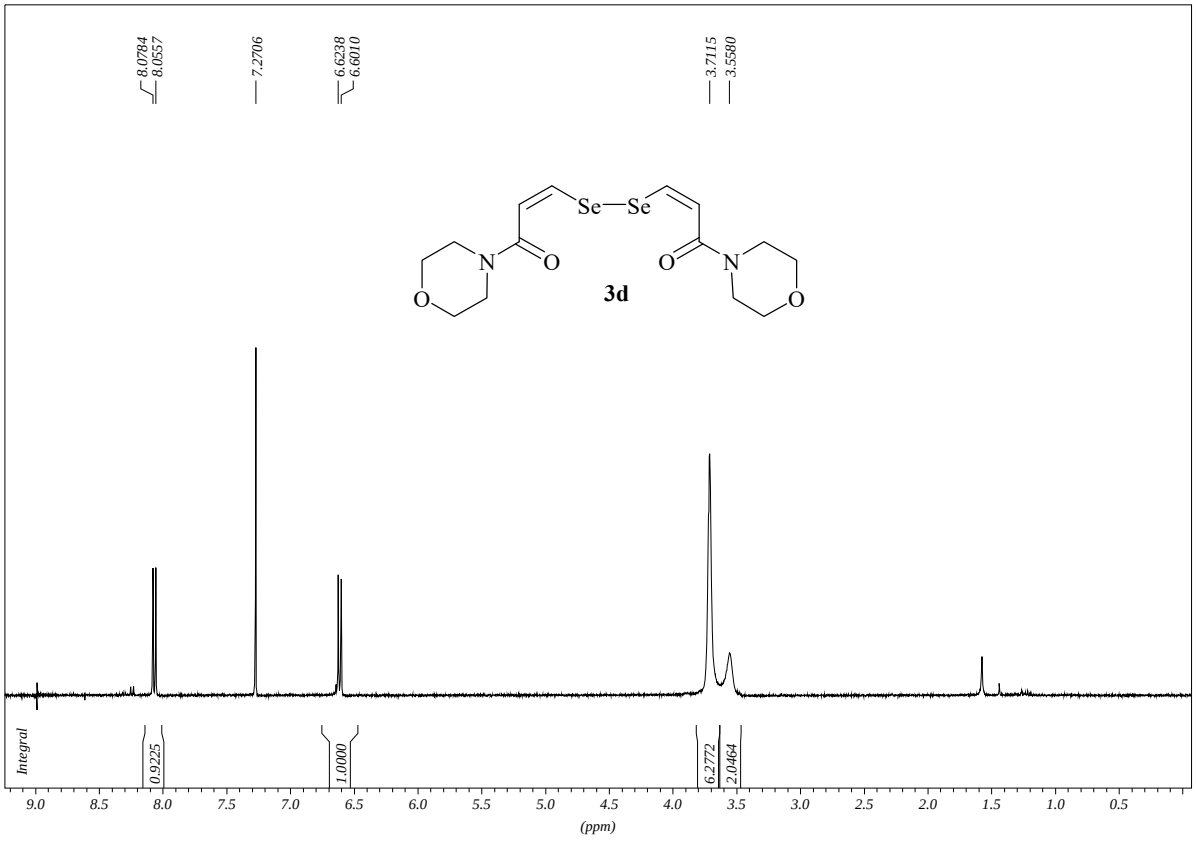
^{1}H, ^{13}C, and ^{77}Se NMR spectra of product 3b

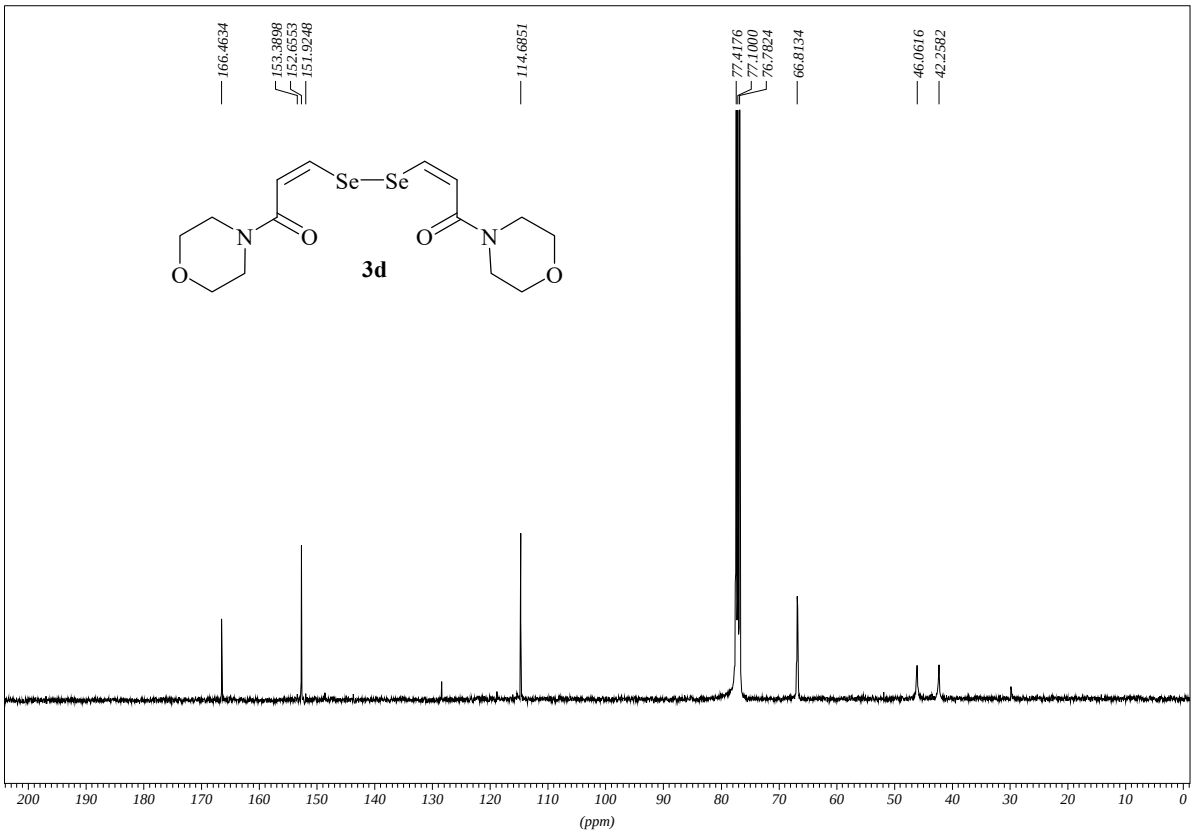


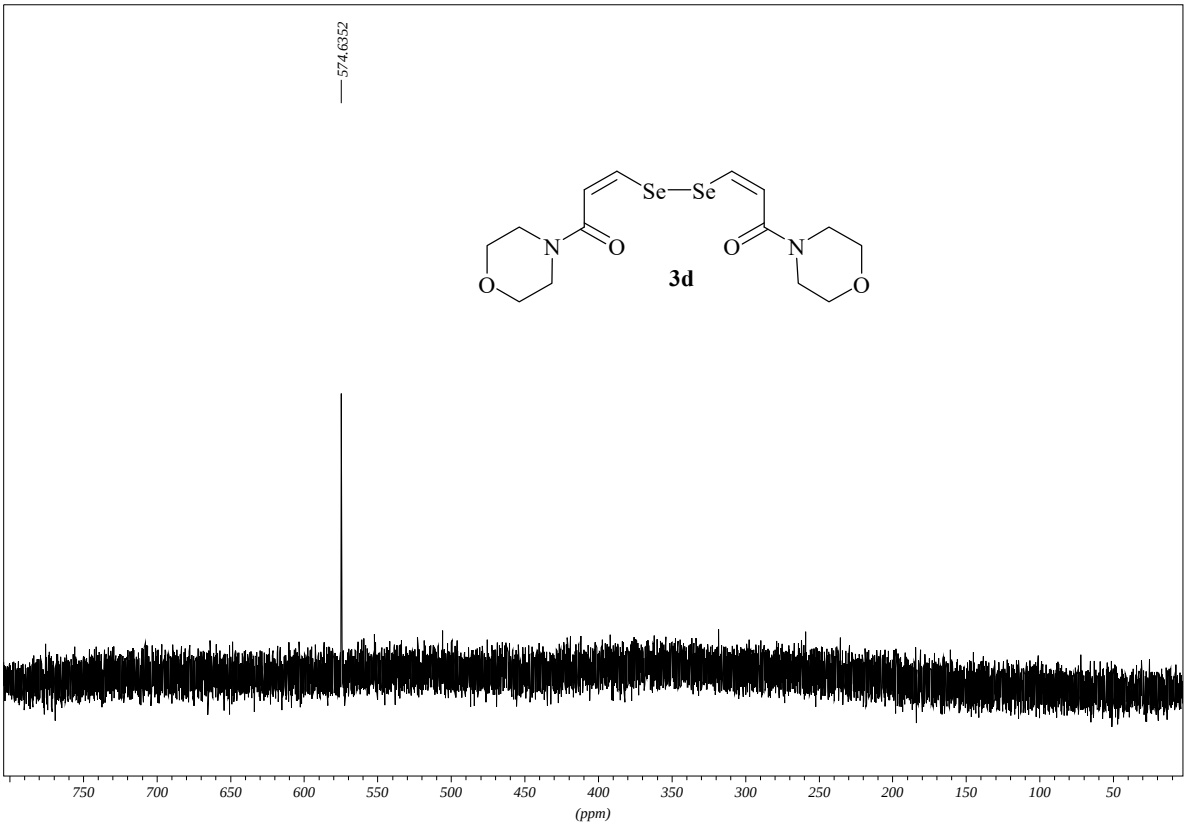

165.2344
149.0482
148.3257
147.6071
138.7775
128.9237
123.6593
121.0112
119.1572
39.6000
Se—Se
PhHN
O
O
NHPh
3b
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
(ppm)


558.5286
Se—Se
PhHN
O
O
NHPh
3b
610 605 600 595 590 585 580 575 570 565 560 555 550 545 540 535 530 525 520 515 510 505 500
(ppm)

^{1}H, ^{13}C, and ^{77}Se NMR spectra of product 3d






574.6352
Se—Se
N
O
O
N
O
O
3d
750
700
650
600
550
500
450
400
350
300
250
200
150
100
50
(ppm)