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Electronic Supporting Information

The kinetics of alkyl radical ring closures at selenium: formation of selenane.

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General procedures for the preparation of **5**, **7** and **10** (R ≠ Bn). Table S1. Gaussian Archive Entries for all transition structures **11** calculated in this work. ^{1}H, ^{13}C and ^{77}Se NMR spectra of **5**, **7** and **10** (R ≠ Bn). (35 pages).

General procedures for the preparation of 5, 7 and 10 (R ≠ Bn).

Materials and Instrumentation: Chemicals and HPLC grade solvents were used as received and reactions were performed under argon unless otherwise stated. Dry ethanol was attained by distillation over magnesium. Dichloromethane, diethyl ether and tetrahydrofuran were dried using Glass Contour© solvent system. ^{1}H NMR spectra were collected using a Varian INOVA 400 or 500 MHz NMR.^{13}C and ^{77}Se NMR spectra were recorded on a Varian INOVA 500 mHz NMR. ^{1}H and ^{13}C NMR chemical shifts are given in ppm relative to internally referenced $CHCl_3$. ^{77}Se NMR chemical shifts are given in ppm relative to externally referenced diphenyl diselenide (δ 464). High resolution mass spectra were collected on a Finnigan LTQ FT by Thermo Electron Corporation. Infrared spectra were obtained using a Perkin Elmer Spectrum One FTIR spectrometer. Gas chromatography analysis was performed using Schimadzu GC-17A (column: CYDEX-B, 50m × 0.22mm, film thickness 0.25μm.

General procedure for the preparation of ethyl 5-(alkylseleno)hexanoates 7 and alkyl hexyl selenides 10.

Sodium borohydride was added portion wise to a solution of the dialkyl diselenide[S1-S3] (0.55 equiv) in anhydrous ethanol (5 mL per mmol diselenide) at 0° until the yellow colour has disappeared. Ethyl 5-bromohexanoate or 1-bromohexane (1.0 equiv) was added and the solution was stirred at RT overnight. The solvent was removed *in vacuo* and residue taken up in water. The resultant mixture was extracted with ether (3 x), the combined organic phases were dried ($MgSO_4$ or Na_2SO_4) and concentrated *in vacuo*. The residue was separated by flash chromatography (petroleum spirts : ethyl acetate) to yield the required product as a yellow oil.

General procedure for the hydrolysis of esters 7.

Aqueous sodium hydroxide (ca. 1.0 equiv) was added to a solution of the required ester **7** (1.0 equiv) in ethanol (3.0 mL per mmol ester) and the resultant solution heated as reflux for 1 h. After cooling to RT, the ethanol was removed *in vacuo*, the residue dissolved in water and the aqueous solution washed with ether (3 x). After acidification with 10% hydrochloric acid, the solution was extracted with ether (3 x), the combined organic phases dried (Na_2SO_4) and the solvent removed *in vacuo* to afford the required 6-(alkylseleno)hexanoic acid as a pale solid which was converted to the corresponding Kim ester **5** without further purification.

General procedure for the preparation of Kim esters 5.

A solution of *N,S*-dimethyl-*N*-hydroxydithiocarbamate (1.5 equiv) in dichloromethane (1.0 mL per 1.5 mmol carbamate) was added drop wise to a solution of *N,N'*-dicyclohexylcarbodiimide (1.0 equiv) and the required 6-(alkylseleno)hexanoic acid (1.0 equiv) in dichloromethane (2.0 mL per mmol acid). The reaction mixture was stirred at RT overnight and then filtered through celite. The filtrate was washed with $NaHCO_3$ and satd NaCl. The organic phase was dried (Na_2SO_4) and concentrated *in vacuo* to afford a grey-green oil that was separated by flash chromatography (petroleum spirts : ethyl acetate) to yield the required product as a yellow/green oil.

References.

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S2 A. Krief, C. Delmotte and W. Dumont, *Tetrahedron,* 1997, **53**, 12147 – 12158.

S3 E. Block, M. Birringer, W. Jiang, T. Nakahodo, H. J. Thompson, P. J. Tuscanp, H. Uzar, X. Zhang and Z. Zhu, *J. Agric, Food Chem.,* 2001, **49**, 458 – 470.

S4 H. J. Reich and C. P. Jasperse, *J. Org. Chem.,* 1986, **51**, 2981 – 2988.

Table S1.

Alkyl group (R)	Temp. (°C)	[**9**] / [**10**][a]	k_H[b] ($M^{-1}s^{-1}$)	k_c (s^{-1})
2-octyl	23	8.6×10^{-3}	7.8×10^{6}	6.7×10^{3}
	35	1.06×10^{-2}	8.9×10^{6}	9.5×10^{3}
	45	1.06×10^{-2}	9.9×10^{6}	1.2×10^{4}
	55	1.77×10^{-2}	1.09×10^{7}	1.9×10^{4}
	65	2.79×10^{-2}	1.19×10^{6}	3.3×10^{4}
	70	2.79×10^{-2}	1.24×10^{7}	3.5×10^{4}
	75	2.75×10^{-2}	1.30×10^{7}	3.6×10^{4}
tert-butyl	25	2.19×10^{-2}	8.0×10^{6}	1.8×10^{4}
	38	3.53×10^{-3}	9.2×10^{6}	3.3×10^{4}
	45	3.95×10^{-2}	9.9×10^{6}	3.9×10^{4}
	58	4.52×10^{-3}	1.12×10^{6}	5.1×10^{4}
	63	5.46×10^{-2}	1.17×10^{6}	6.4×10^{4}
	72	7.25×10^{-2}	1.27×10^{7}	9.2×10^{4}
benzyl	70	1.39×10^{-1}	1.24×10^{7}	1.7×10^{5}
	75	1.61×10^{-1}	1.30×10^{7}	2.1×10^{5}
	80	1.89×10^{-1}	1.35×10^{7}	2.6×10^{5}
	90	1.54×10^{-1}	1.49×10^{7}	2.3×10^{5}
	100	1.87×10^{-1}	1.58×10^{7}	3.0×10^{5}
	105	1.90×10^{-1}	1.63×10^{7}	3.1×10^{5}
	110	2.21×10^{-1}	1.69×10^{7}	3.7×10^{5}
	116	2.52×10^{-2}	1.76×10^{7}	4.4×10^{5}

[a]Average of three experiments. [b]Taken from ref. 36.

Table S1. Rate data for the ring closure of the 5-(alkylseleno)pentyl radical 4 (R ≠ *n*-octyl). Reaction performed under pseudo-first-order conditions in 0.1M *tert*-dodecanethiol.

B3LYP/6-31G(d) Gaussian Archive Entries for the transition states 11 involved in the cyclization of radicals 4, and single-point energies.

Transition state 11, R = Me.

1\1\GINC-MERRI014\FTS\UB3LYP\6-31G(d)\C6H13Se1(2)\ROOT\21-Feb-2014\0\\
B3LYP/6-31G(d) opt=(noeigentest,calcfc,ts) freq=noraman maxdisk=100g
b\\freq\\0,2\Se,0.,0.,0.\C,0.,0.,1.98270465\C,1.4122175438,0.,2.571369
0351\C,2.2229471276,-1.2763499189,2.2959219327\C,-1.9004574472,1.18476
95847,-0.0639350375\H,-1.631342966,2.1651495805,0.3301207009\H,-2.1565
646961,1.2122388297,-1.1219486641\H,-2.6427025377,0.6589168763,0.53452
98853\H,-0.573299327,-0.8737341068,2.3097602992\H,-0.5437249826,0.9000
742625,2.277873533\H,1.3286651964,0.1371701737,3.6595235764\H,1.955181
2575,0.8720173037,2.1834206733\H,1.697384086,-2.1377221368,2.735016130
8\H,3.1843319827,-1.2037178776,2.8205525827\C,2.4819821634,-1.55401227
37,0.806647539\H,3.0417205798,-0.7165533656,0.367679742\H,3.1363293638
,-2.4382174794,0.7222512179\C,1.2149614395,-1.7908264398,0.0033430833\
H,0.5763503844,-2.5801234581,0.4079771733\H,1.3946220819,-1.956202865,
-1.0607675057\\Version=AM64L-G09RevC.01\State=2-A\HF=-2635.7756654\S2=
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022371,-0.1761625,0.4682977\Polar=0.,0.,0.,0.,0.,0.\Quadrupole=-0.1934
109,-0.2714404,0.4648512,-0.7171195,-0.3260569,0.5953485\PG=C01 [X(C6H
13Se1)]\\@

ROMP2/GTMP2large//B3LYP/6-31G(d)=-2636.0158068

ROCCSDT/GT1Bas//B3LYP/6-31G(d)=-2635.3807755

Transition state 11, R = Et.

1\1\GINC-R2530\FTS\UB3LYP\6-31G(d)\C7H15Se1(2)\ROOT\23-Feb-2014\1\\# B
3LYP/6-31G(d) opt=(grad,noeigentest,ts,calcfc) freq=noraman\\ts\\0,2\S
e\C,1,B1\C,2,B2,1,A1\C,3,B3,2,A2,1,D1,0\C,1,B4,2,A3,3,D2,0\H,5,B5,1,A4
,2,D3,0\H,5,B6,1,A5,2,D4,0\H,2,B7,1,A6,5,D5,0\H,2,B8,1,A7,5,D6,0\H,3,B
9,2,A8,1,D7,0\H,3,B10,2,A9,1,D8,0\H,4,B11,3,A10,2,D9,0\H,4,B12,3,A11,2
,D10,0\C,4,B13,3,A12,2,D11,0\H,14,B14,4,A13,3,D12,0\H,14,B15,4,A14,3,D
13,0\C,14,B16,4,A15,3,D14,0\H,17,B17,14,A16,4,D15,0\H,17,B18,14,A17,4,
D16,0\C,5,B19,1,A18,2,D17,0\H,20,B20,5,A19,1,D18,0\H,20,B21,5,A20,1,D1
9,0\H,20,B22,5,A21,1,D20,0\\B1=1.98357611\B2=1.53053957\B3=1.53711985\
B4=2.19528759\B5=1.09293372\B6=1.09188704\B7=1.0946688\B8=1.09274811\B
9=1.10013758\B10=1.09782104\B11=1.10048987\B12=1.09773829\B13=1.537287
37\B14=1.09886743\B15=1.1040403\B16=1.51459663\B17=1.0921212\B18=1.090
74542\B19=1.51200429\B20=1.09562789\B21=1.09638499\B22=1.10072844\A1=1
12.45790499\A2=114.72038387\A3=93.81350229\A4=103.41862558\A5=100.8761
004\A6=107.83371235\A7=105.94138377\A8=108.12502536\A9=108.66963671\A1
0=108.98808052\A11=108.68381511\A12=114.61612826\A13=109.60694024\A14=
108.4458586\A15=113.74626058\A16=114.86702608\A17=114.49780827\A18=111
.86310319\A19=110.89117432\A20=111.64638015\A21=111.6006087\D1=-67.788
03687\D2=-142.13428337\D3=50.90445126\D4=-194.80127705\D5=94.77499162\

D6=-21.1604428\D7=170.9422902\D8=55.38749993\D9=-60.43532198\D10=-175.
7462527\D11=61.94475639\D12=59.4362328\D13=174.79367446\D14=-63.357106
61\D15=-52.26316106\D16=177.14296257\D17=-73.49982397\D18=-56.72517854
\D19=63.23803913\D20=-176.81787217\\Version=ES64L-G09RevD.01\State=2-A
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=4.198e-05\Dipole=-0.0280221,-0.0735532,0.4313791\Quadrupole=0.011633,
-0.3074555,0.2958225,-1.3155403,0.2864416,0.2994241\PG=C01 [X(C7H15Se1
)]\\@

ROMP2/GTMP2large//B3LYP/6-31G(d)=-2675.2368084

ROCCSDT/GT1Bas//B3LYP/6-31G(d)=-2674.5645816

Transition state 11, R = *iso*-Propyl.

1\1\GINC-R2506\FTS\UB3LYP\6-31G(d)\C8H17Se1(2)\ROOT\23-Feb-2014\1\\# B
3LYP/6-31G(d) opt=(ts,noeigentest,calcfc,grad) freq=noraman\\ts ipr\\0
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1,A4,2,D3,0\H,2,B6,1,A5,5,D4,0\H,2,B7,1,A6,5,D5,0\H,3,B8,2,A7,1,D6,0\H
,3,B9,2,A8,1,D7,0\H,4,B10,3,A9,2,D8,0\H,4,B11,3,A10,2,D9,0\C,4,B12,3,A
11,2,D10,0\H,13,B13,4,A12,3,D11,0\H,13,B14,4,A13,3,D12,0\C,13,B15,4,A1
4,3,D13,0\H,16,B16,13,A15,4,D14,0\H,16,B17,13,A16,4,D15,0\C,5,B18,1,A1
7,2,D16,0\H,19,B19,5,A18,1,D17,0\H,19,B20,5,A19,1,D18,0\H,19,B21,5,A20
,1,D19,0\C,5,B22,1,A21,2,D20,0\H,23,B23,5,A22,1,D21,0\H,23,B24,5,A23,1
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5\B4=2.16069228\B5=1.09477737\B6=1.09438927\B7=1.09313237\B8=1.1003002
4\B9=1.09768072\B10=1.10054563\B11=1.09778302\B12=1.53791246\B13=1.098
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1.5166175\B19=1.09621864\B20=1.09556182\B21=1.1013778\B22=1.51789433\B
23=1.09503483\B24=1.09748984\B25=1.0999485\A1=112.38249669\A2=114.7745
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125503\A16=115.59011698\A17=109.88212878\A18=110.77764004\A19=111.9455
0717\A20=111.10769854\A21=105.36991605\A22=111.4986793\A23=111.01486\A
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3=-64.11031577\D14=-49.9120787\D15=175.41793965\D16=-73.18210081\D17=-
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9\RMSF=5.312e-05\Dipole=-0.0517568,0.0301837,0.3962697\Quadrupole=-0.2
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C8H17Se1)]\\@

ROMP2/GTMP2large//B3LYP/6-31G(d)=-2714.4534379

ROCCSDT/GT1Bas//B3LYP/6-31G(d)=-2713.7510934

Transition state 11, R = *tert*-Bu

1\1\GINC-MERRI012\FTS\UB3LYP\6-31G(d)\C9H19Se1(2)\ROOT\21-Feb-2014\0\\
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6,-0.2156321444,2.0862849518\C,1.3823245558,-0.0231281761,2.5445388441
\C,2.3250529437,-1.1986729589,2.2377280562\C,-1.9349453464,1.184292020
4,-0.0386001105\H,-0.4685960247,-1.1736394213,2.4294268666\H,-0.698938
2362,0.5807606539,2.4847023208\H,1.3785642691,0.1378907689,3.633089603
3\H,1.7749800039,0.8951210282,2.089149572\H,1.9486684257,-2.0998719195
,2.7449604896\H,3.3045336763,-0.9840198269,2.6846891223\C,2.5179755787
,-1.5134288224,0.7444255735\H,2.9053694282,-0.6259081629,0.2248910597\
H,3.3070841496,-2.2826415812,0.6548465402\C,1.2711903023,-1.9953541031
,0.0525353765\H,0.6971772897,-2.774293377,0.5546153866\H,1.3348563542,
-2.1337018351,-1.0251519601\C,-3.1168101397,0.5699199115,0.6982940592\
H,-3.3520120656,-0.424614086,0.3056674562\H,-2.926091146,0.4718125909,
1.7728646464\H,-4.0133982786,1.200248619,0.5855672624\C,-2.1644155806,
1.237117659,-1.5456004026\H,-1.2798808167,1.6133424908,-2.0724888288\H
,-2.4039037095,0.2461435925,-1.9475003654\H,-3.004303443,1.9071952994,
-1.7819107703\C,-1.5072686968,2.53570644,0.5184833286\H,-1.2765643281,
2.4898349817,1.5889402946\H,-0.6230898438,2.9183213413,-0.001631634\H,
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19Se1)]\\@

ROMP2/GTMP2large//B3LYP/6-31G(d)=-2753.6763773

ROCCSDT/GT1Bas//B3LYP/6-31G(d)=-2752.9377168

Transition state 11, R = Bn.

1\1\GINC-R2800\FTS\UB3LYP\6-31G(d)\C12H17Se1(2)\ROOT\11-Mar-2014\1\\#
B3LYP/6-31G(d) opt=(ts,noeigentest,calcfc,grad) freq=noraman\\ts bn\\0
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1,A4,5,D3,0\H,2,B6,1,A5,5,D4,0\H,3,B7,2,A6,1,D5,0\H,3,B8,2,A7,1,D6,0\H
,4,B9,3,A8,2,D7,0\H,4,B10,3,A9,2,D8,0\C,4,B11,3,A10,2,D9,0\H,12,B12,4,
A11,3,D10,0\H,12,B13,4,A12,3,D11,0\C,12,B14,4,A13,3,D12,0\H,15,B15,12,
A14,4,D13,0\H,15,B16,12,A15,4,D14,0\C,5,B17,1,A16,2,D15,0\C,18,B18,5,A
17,1,D16,0\C,18,B19,5,A18,1,D17,0\C,19,B20,18,A19,5,D18,0\H,19,B21,18,
A20,5,D19,0\C,20,B22,18,A21,5,D20,0\H,20,B23,18,A22,5,D21,0\C,23,B24,2
0,A23,18,D22,0\H,21,B25,19,A24,18,D23,0\H,23,B26,20,A25,18,D24,0\H,25,
B27,23,A26,20,D25,0\H,5,B28,1,A27,2,D26,0\H,5,B29,1,A28,2,D27,0\\B1=1.
98845666\B2=1.5310481\B3=1.53740422\B4=2.12160862\B5=1.09429415\B6=1.0
9344259\B7=1.10031302\B8=1.09788376\B9=1.10040677\B10=1.0977744\B11=1.
53828084\B12=1.09903899\B13=1.10588495\B14=1.50372305\B15=1.08956668\B
16=1.08802576\B17=1.48229223\B18=1.4041659\B19=1.40554405\B20=1.394305
39\B21=1.08763863\B22=1.39295084\B23=1.08755035\B24=1.39753506\B25=1.0
8707795\B26=1.08706774\B27=1.08672985\B28=1.09010842\B29=1.09155771\A1
=112.98926298\A2=115.29596911\A3=95.03642837\A4=107.74492494\A5=105.85
148529\A6=107.95861521\A7=108.68255045\A8=109.04446107\A9=108.38080192
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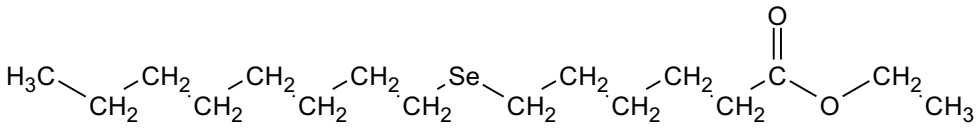
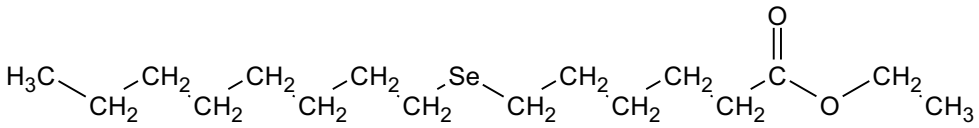
20.55309533\A19=120.85161411\A20=119.24070811\A21=120.86407102\A22=119
.10148407\A23=120.19152791\A24=119.7387706\A25=119.7610697\A26=120.223
45412\A27=105.99790939\A28=103.40043184\D1=-69.92732134\D2=-136.751410
35\D3=99.69082162\D4=-15.87285919\D5=169.04670775\D6=53.70340256\D7=-5
9.91420531\D8=-175.00523438\D9=62.8467998\D10=56.69646054\D11=171.5499
4541\D12=-66.77668857\D13=-46.44849842\D14=173.27800062\D15=-185.86324
418\D16=96.78499584\D17=-80.53794102\D18=-178.47232672\D19=1.82341013\
D20=-181.40552904\D21=-1.29696156\D22=-0.61357393\D23=180.47446895\D24
=179.45905535\D25=-180.03980707\D26=-63.66928291\D27=53.5529728\\Versi
on=ES64L-G09RevD.01\State=2-A\HF=-2866.8344166\S2=0.764549\S2-1=0.\S2A
=0.750093\RMSD=6.301e-09\RMSF=2.292e-05\Dipole=0.0898083,-0.0952522,0.
5184119\Quadrupole=-0.8798374,-1.7134914,2.5933289,0.9179507,1.0537099
,-1.1826249\PG=C01 [X(C12H17Se1)]\\@

ROMP2/GTMP2large//B3LYP/6-31G(d)=-2866.5547094

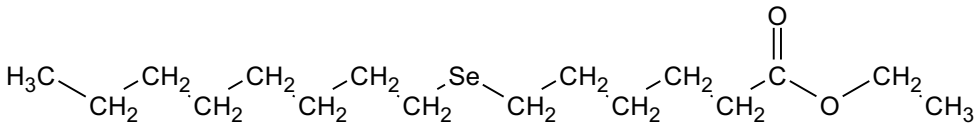
ROCCSDT/GT1Bas//B3LYP/6-31G(d)=-2865.7533212


H3C
CH2
CH2
CH2
CH2
CH2
CH2
Se
CH2
CH2
CH2
CH2
C
O
O
CH2
CH3

2400
2300
2200
2100
2000
1900
1800
1700
1600
1500
1400
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
-100
-200
)0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
f1 (ppm)


H3C
CH2
CH2
CH2
CH2
CH2
CH2
Se
CH2
CH2
CH2
CH2
C
O
O
CH2
CH3

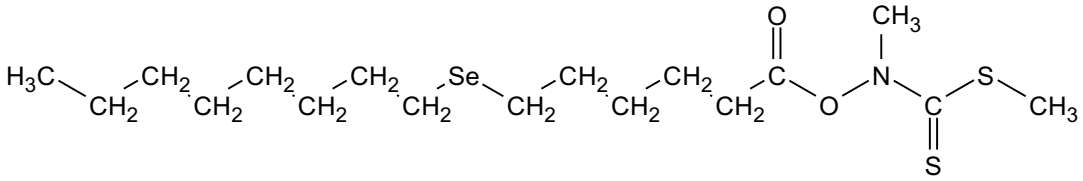
70
65
60
55
50
45
40
35
30
25
20
15
10
5
0
-5
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)



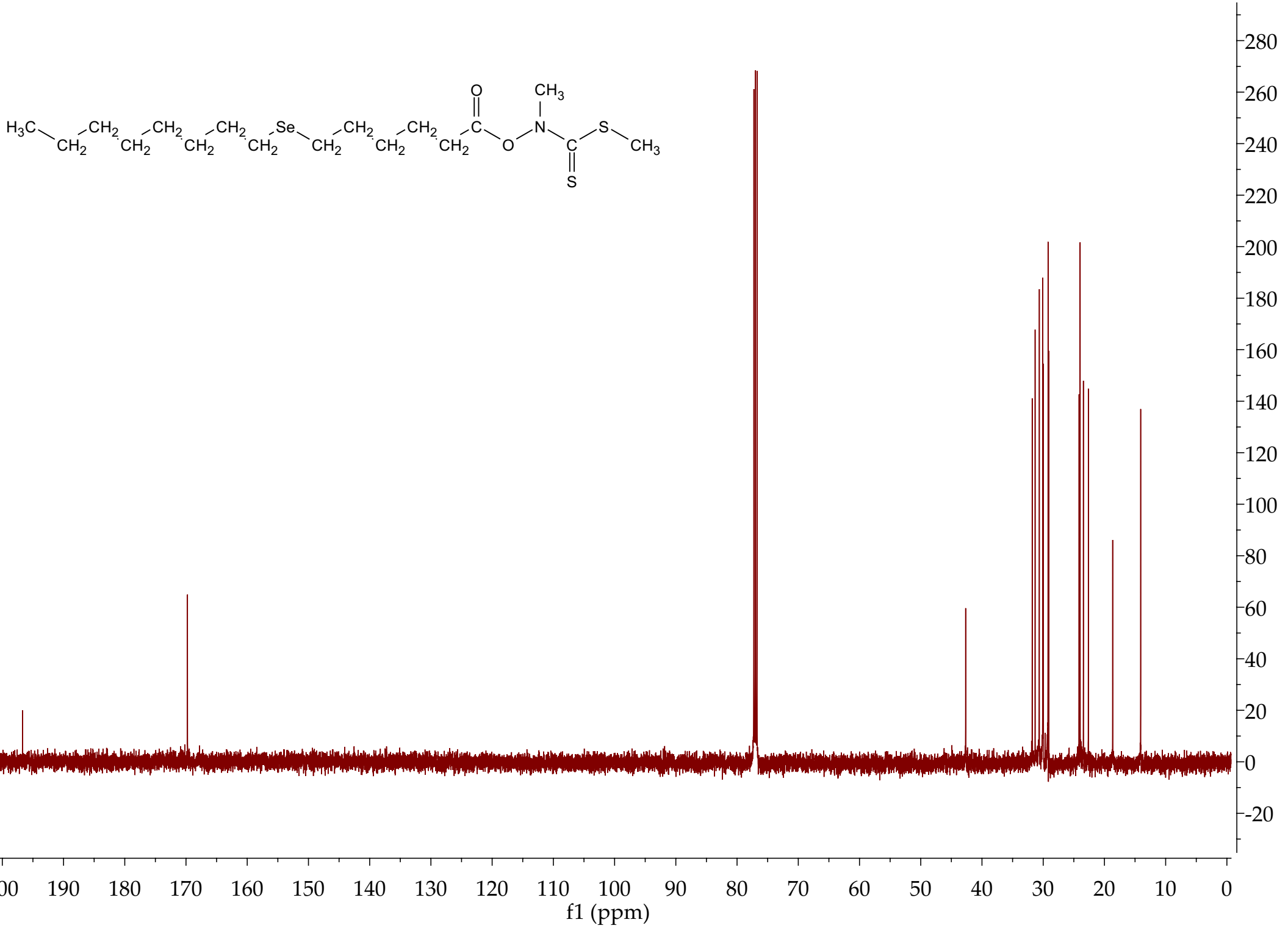
1500
1400
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
-100

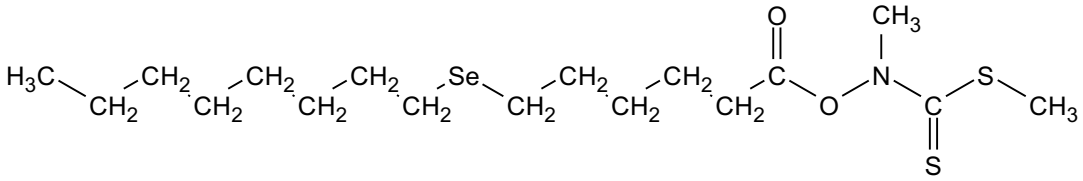
660 620 580 540 500 460 420 380 340 300 260 220 180

f1 (ppm)

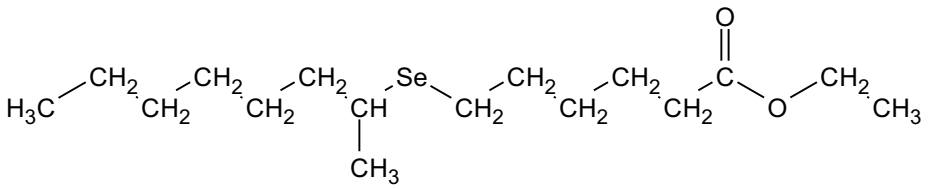

H3C
CH2
CH2
CH2
CH2
CH2
CH2
Se
CH2
CH2
CH2
CH2
CH2
O
C
O
N
CH3
C
S
S
CH3

2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
400
200
0
-200
0.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

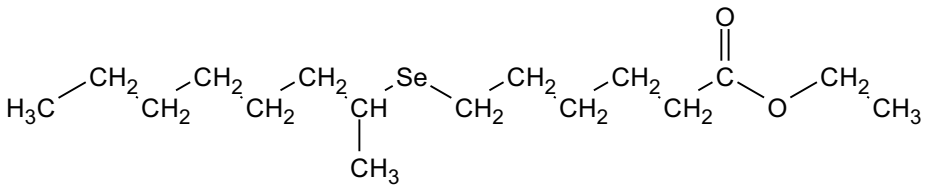

f1 (ppm)


H3C
CH2
CH2
CH2
CH2
CH2
CH2
Se
CH2
CH2
CH2
CH2
O
C
O
N
CH3
C
S
S
CH3

90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
5
0
-5
650
600
550
500
450
400
350
300
250
200
150
100
50
f1 (ppm)


O
H3C
CH2
CH2
CH2
CH2
CH2
CH2
CH
CH3
Se
CH2
CH2
CH2
CH2
CH2
C
O
CH2
CH3

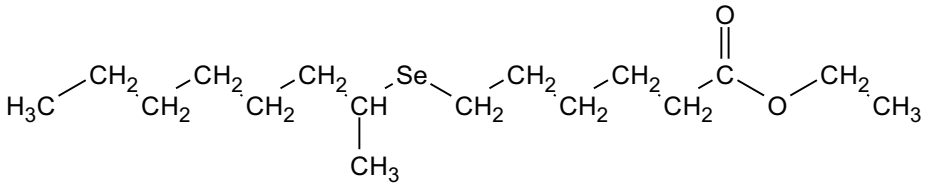
900
800
700
600
500
400
300
200
100
0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)



110
100
90
80
70
60
50
40
30
20
10
0
-10

200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

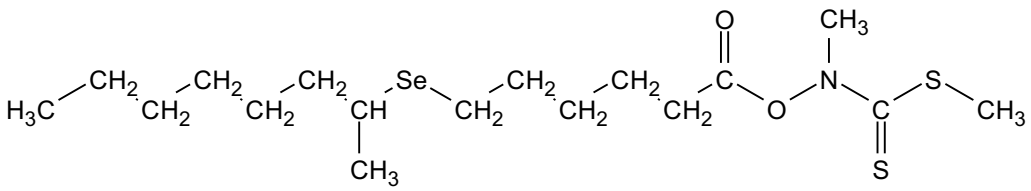
f1 (ppm)



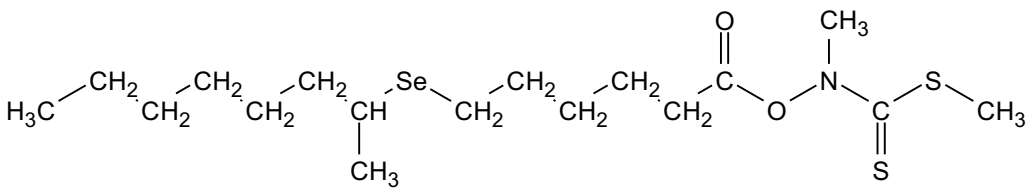
400
350
300
250
200
150
100
50
0

640 620 600 580 560 540 520 500 480 460 440 420 400 380 360 340 320 300 280 260 240

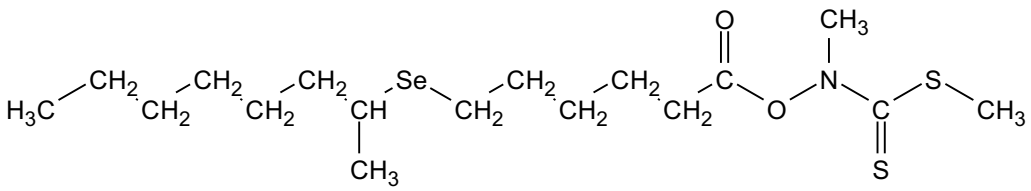
f1 (ppm)


O
CH3
H3C
CH2
CH2
CH2
CH2
CH2
CH
Se
CH2
CH2
CH2
CH2
C
O
N
C
S
S
CH3
CH3

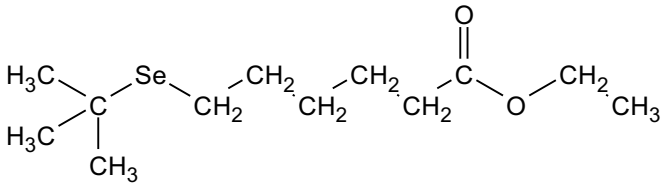
2500
2400
2300
2200
2100
2000
1900
1800
1700
1600
1500
1400
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
-100
-200
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)



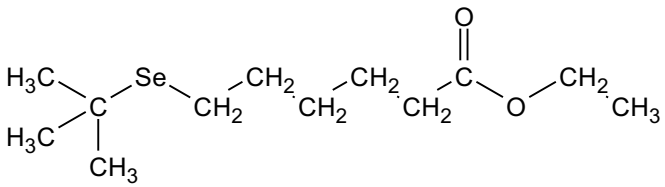
110
100
90
80
70
60
50
40
30
20
10
0
-10
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


O
CH3
H3C
CH2
CH2
CH2
CH2
CH2
CH
CH3
Se
CH2
CH2
CH2
CH2
C
O
N
C
S
S
CH3

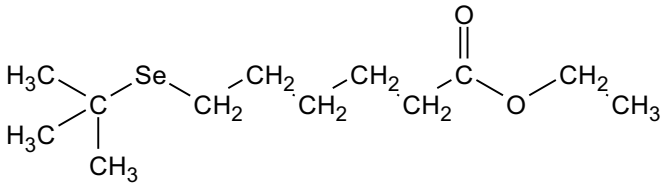
450
400
350
300
250
200
150
100
50
0
460
420
380
340
300
260
220
180
140
f1 (ppm)


H3C
C
H3C
CH3
Se
CH2
CH2
CH2
CH2
CH2
C
O
O
CH2
CH3

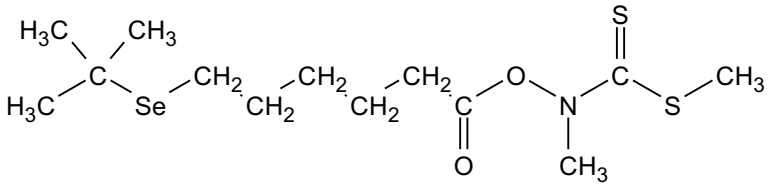
1000
900
800
700
600
500
400
300
200
100
0
0.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)


H3C
C
Se
CH2
CH2
CH2
CH2
C
O
CH2
CH3
H3C
CH3
O

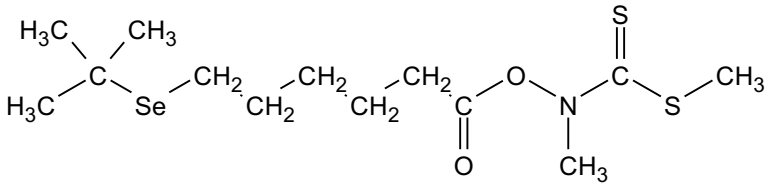
450
400
350
300
250
200
150
100
50
0
230
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


O
H3C
Se
CH2
CH2
CH2
C
CH2
C
H3C
CH2
CH2
CH2
O
CH3
CH3

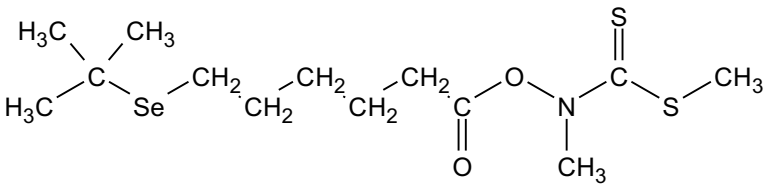
1500
1400
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
490
470
450
430
410
390
370
350
330
310
290
270
250
230
210
f1 (ppm)


H3C
CH3
C
H3C
Se
CH2
CH2
CH2
CH2
C
O
O
N
CH3
C
S
S
CH3

2100
2000
1900
1800
1700
1600
1500
1400
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
-100
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)


H3C
CH3
C
H3C
Se
CH2
CH2
CH2
CH2
C
O
O
N
CH3
C
S
S
CH3

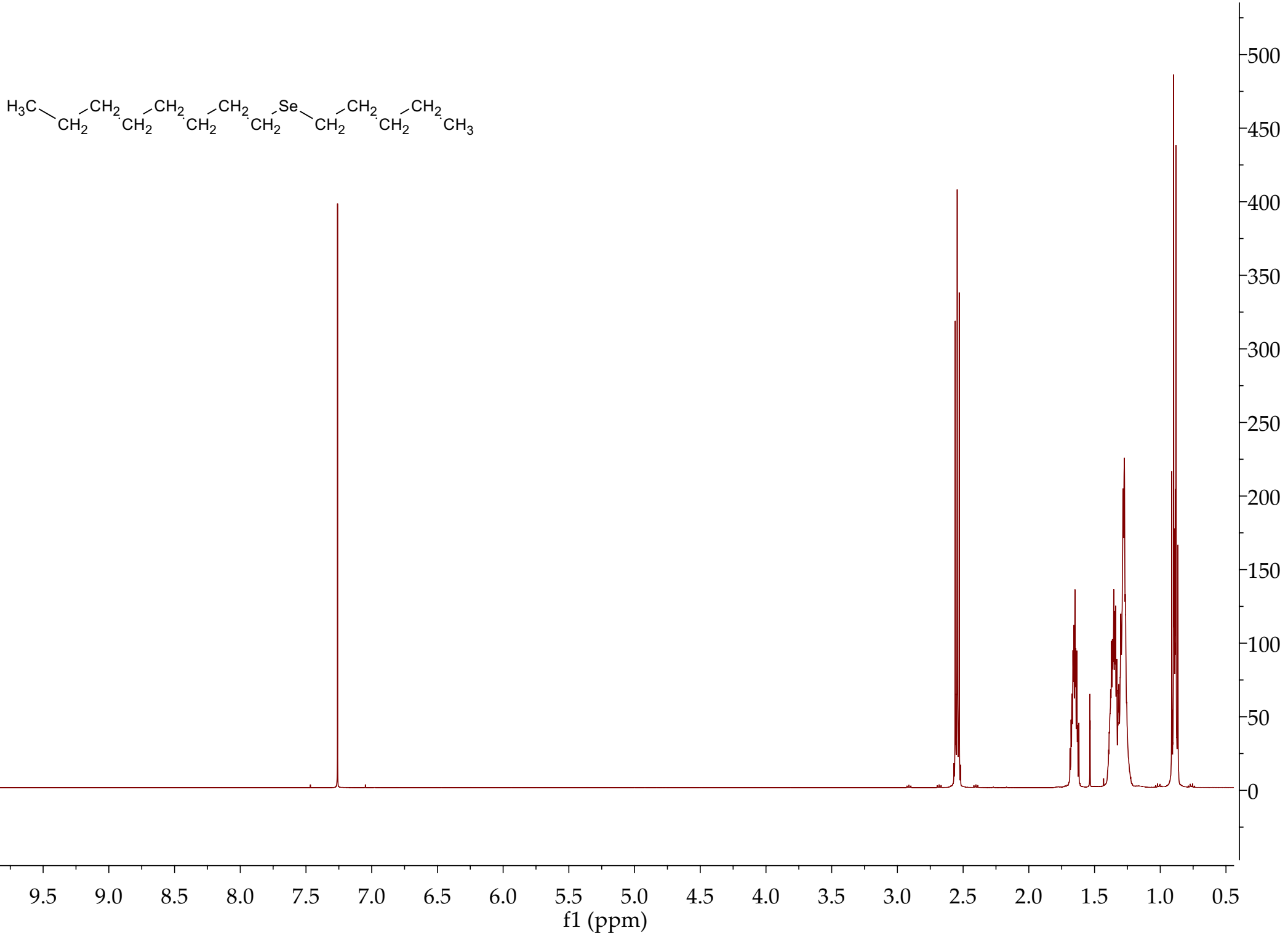
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
10
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

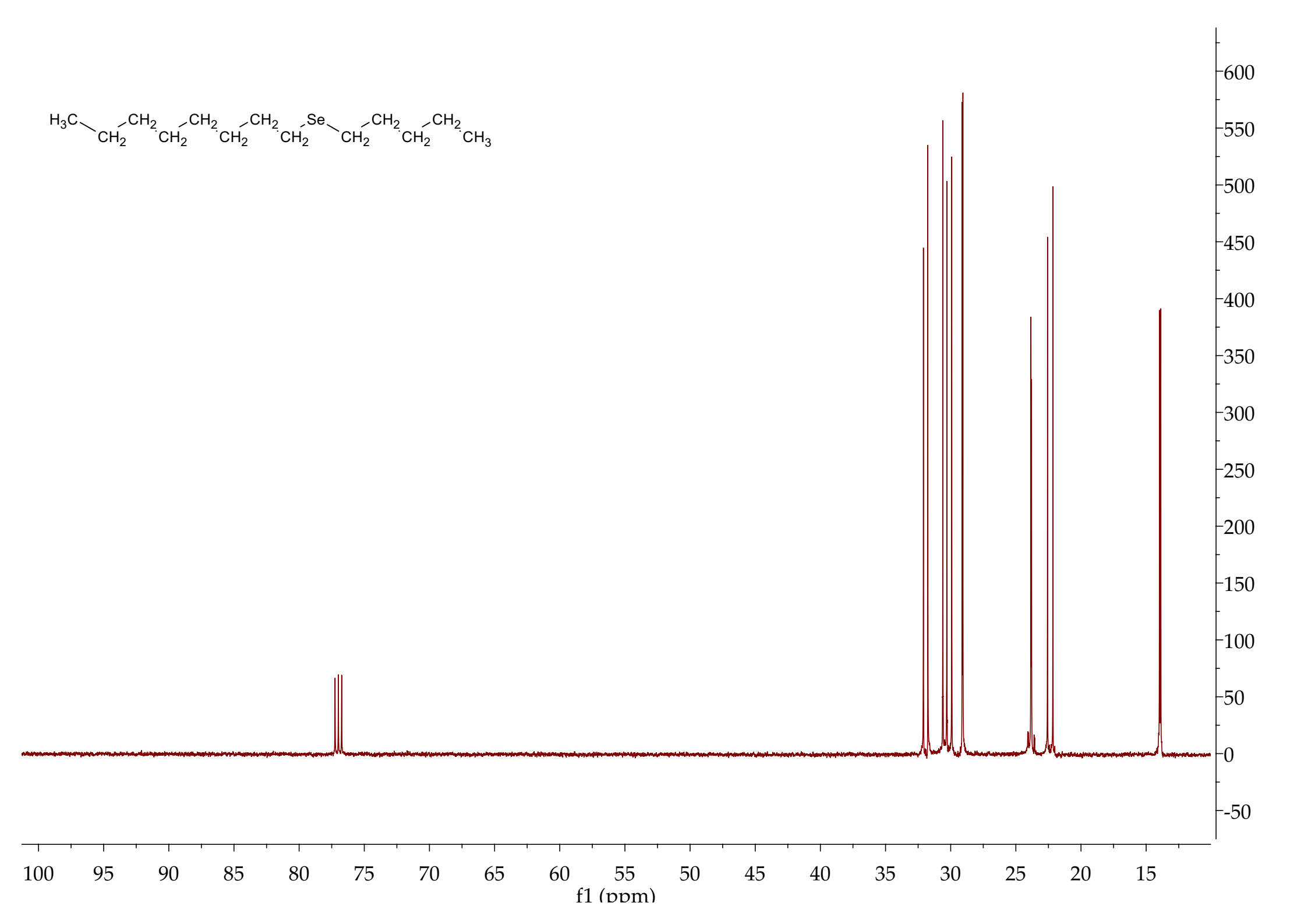


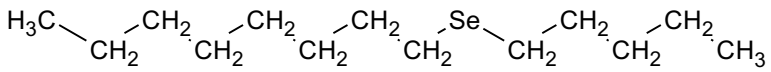
55
50
45
40
35
30
25
20
15
10
5
0

640 620 600 580 560 540 520 500 480 460 440 420 400 380 360 340 320 300 280 260 240

f1 (ppm)


H3C
CH2
CH2
CH2
CH2
CH2
CH2
Se
CH2
CH2
CH2
CH3
500
450
400
350
300
250
200
150
100
50
0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

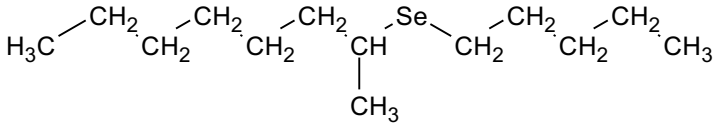

H3C
CH2
CH2
CH2
CH2
CH2
CH2
Se
CH2
CH2
CH2
CH2
CH3
600
550
500
450
400
350
300
250
200
150
100
50
0
-50
100
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
f1 (ppm)



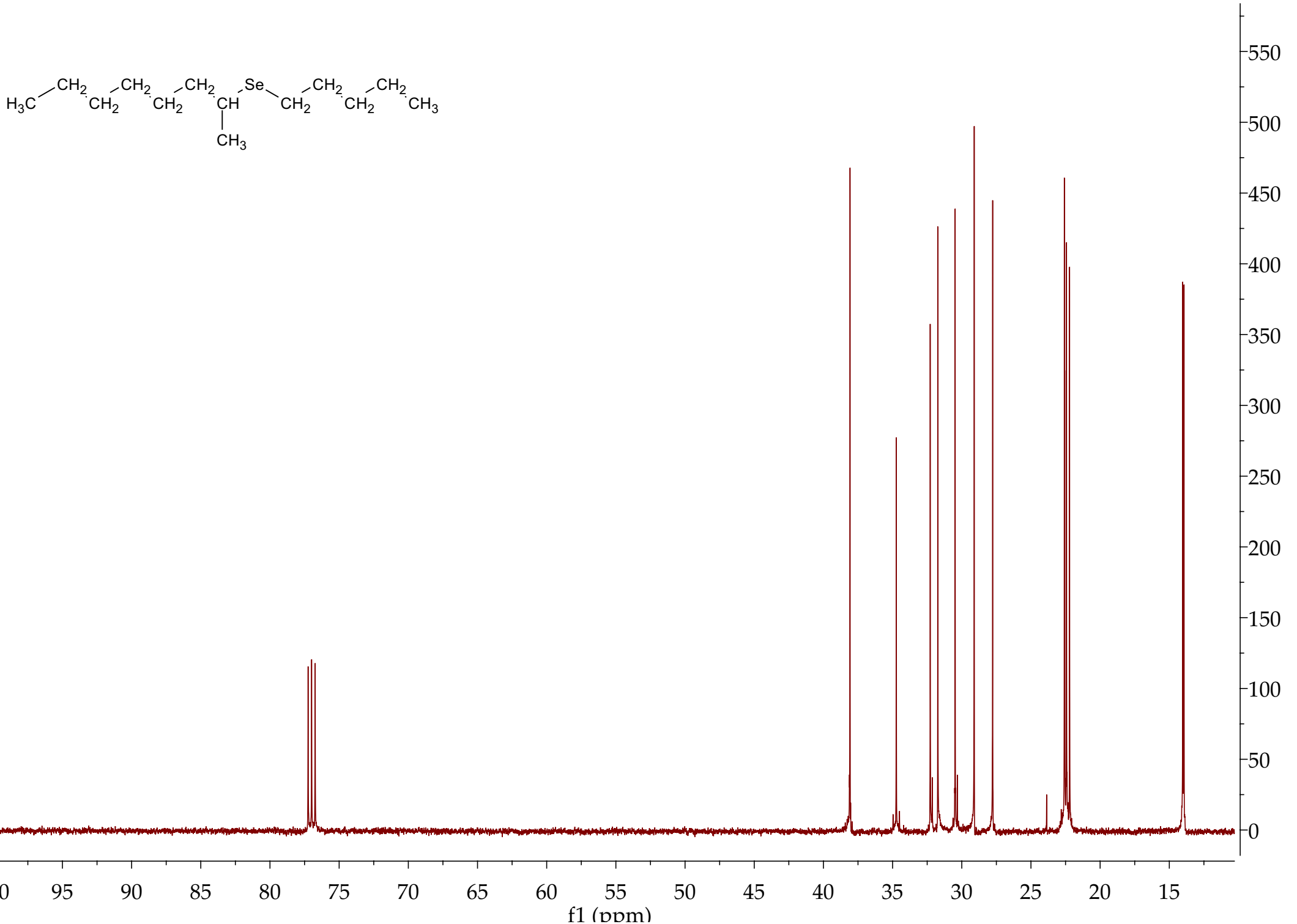
400
380
360
340
320
300
280
260
240
220
200
180
160
140
120
100
80
60
40
20
0
-20

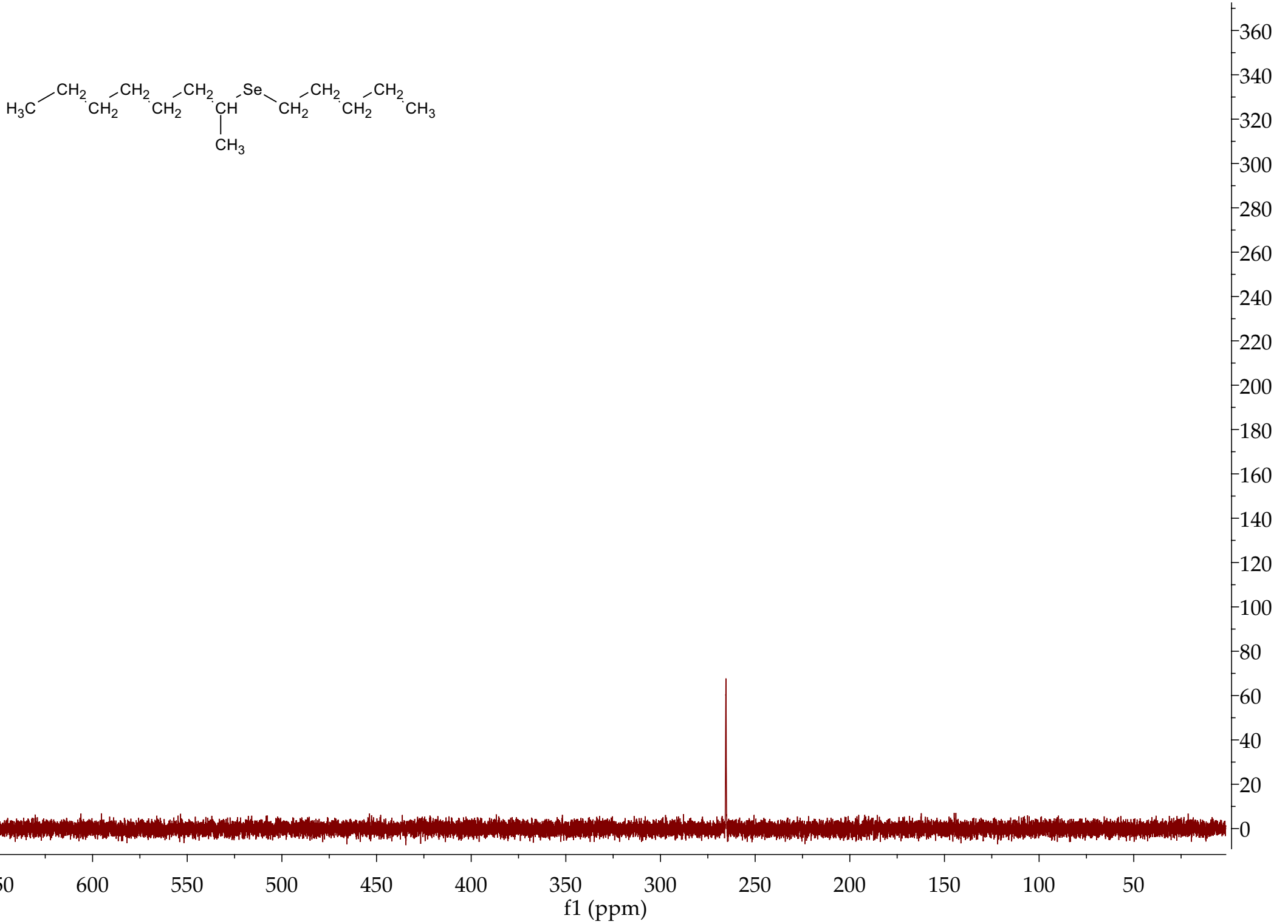
30
450
420
390
360
330
300
270
240
210
180

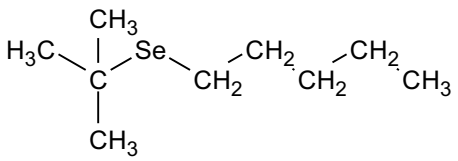
f1 (ppm)


H3C
CH2
CH2
CH2
CH2
CH2
CH
CH3
Se
CH2
CH2
CH2
CH2
CH3

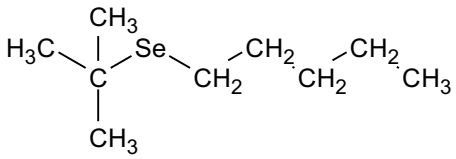
1000
900
800
700
600
500
400
300
200
100
0
-100
6.0
5.6
5.2
4.8
4.4
4.0
3.6
3.2
2.8
2.4
2.0
1.6
1.2
0.8
0.4
0.0
f1 (ppm)


H3C
CH2
CH2
CH2
CH2
CH
CH3
Se
CH2
CH2
CH2
CH3
550
500
450
400
350
300
250
200
150
100
50
0
00
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
f1 (ppm)

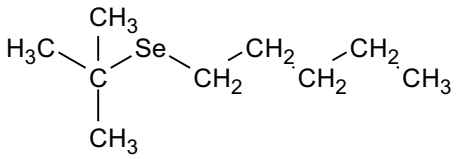

H3C
CH2
CH2
CH2
CH2
CH
CH3
Se
CH2
CH2
CH2
CH3
360
340
320
300
280
260
240
220
200
180
160
140
120
100
80
60
40
20
0
650
600
550
500
450
400
350
300
250
200
150
100
50
f1 (ppm)


CH3
H3C
C
Se
CH2
CH2
CH2
CH2
CH3
CH3

2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
400
200
0
-200
0.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)


CH3
H3C
C
Se
CH2
CH2
CH2
CH2
CH3
CH3

190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
f1 (ppm)


CH3
H3C
Se
CH2
CH2
CH2
C
CH2
CH2
CH3
CH3

120
110
100
90
80
70
60
50
40
30
20
10
0
650
600
550
500
450
400
350
300
250
200
150
100
50
f1 (ppm)