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S U P P L E M E N T A R Y M A T E R I A L

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B E L O N G I N G TO T H E P A P E R

Regenerable Chain-Breaking 2,3-Dihydrobenzo[b]selenophene-5-ol Antioxidants

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RECEIVED DATE (to be automatically inserted after your manuscript is accepted if required according to the journal that you are submitting your paper to)

Contents:

General Experimental Details

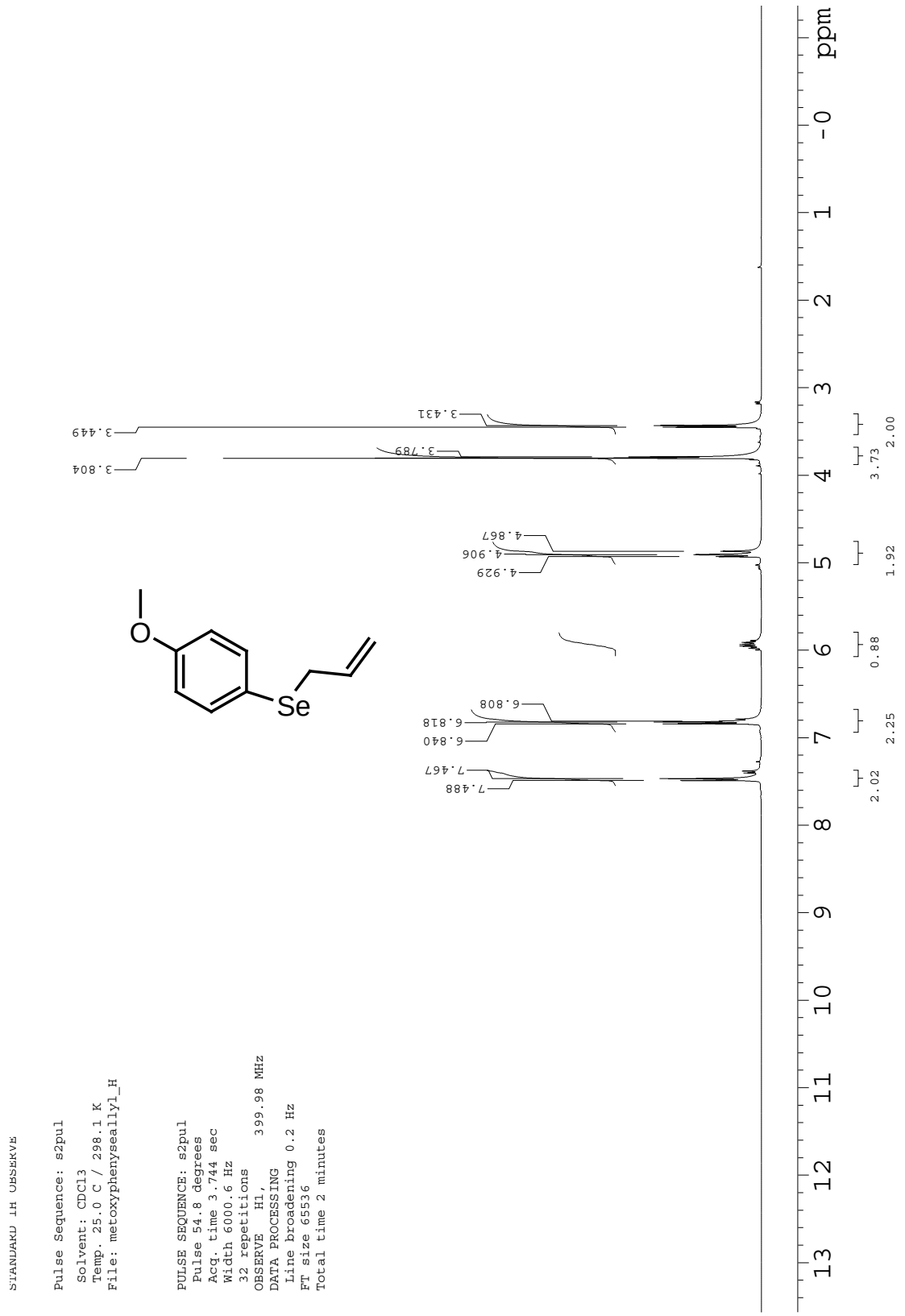
All NMR experiments were carried out on a 400 MHz spectrometer (400 MHz for ^{1}H and 100 MHz for ^{13}C) in $CDCl_3$. NMR chemical shifts are reported in ppm referenced to the solvent peak of $CDCl_3$ (7.26 ppm for ^{1}H and 77.16 ppm for ^{13}C, respectively). The ^{77}Se NMR spectra were obtained at 95.35 MHz, respectively, in $CDCl_3$ using diphenyl diselenide as external standard. Chemical shifts are reported relative to dimethyl selenide (^{77}Se) (0 ppm) by assuming that the chemical shift of the standard is 461 ppm. Mass spectra reported are for ions of ^{80}Se. Microwave reactions were carried out in a Biotage Initiator 60 EXP focused microwave reactor equipped with an IR sensor for continuous monitoring of the reaction temperature. Melting points are uncorrected. clogP value of compounds was calculated by BioByte corporation software together SYbYL v.7.2.4. THF was dried by distillation over sodium/benzophenone. 4-Methoxy-2,3,5-trimethylbromobenzene,[1] 2-bromo-5-methoxybenzyl bromide,[2] and compound **10**[2]were prepared according to literature procedures.

References:

1. Shanks, D.; Amorati, R.; Fumo, M. G.; Pedulli, G. F.; Valgimigli, L.; Engman, L. *J. Org. Chem.* **2006**, *71*, 1033.

2. Al-Maharik, N.; Engman, L.; Malmström, J.; Schiesser, C. H. *J. Org. Chem.* **2001**, 66, 6286.

^{1}H NMR spectrum of **3a**.



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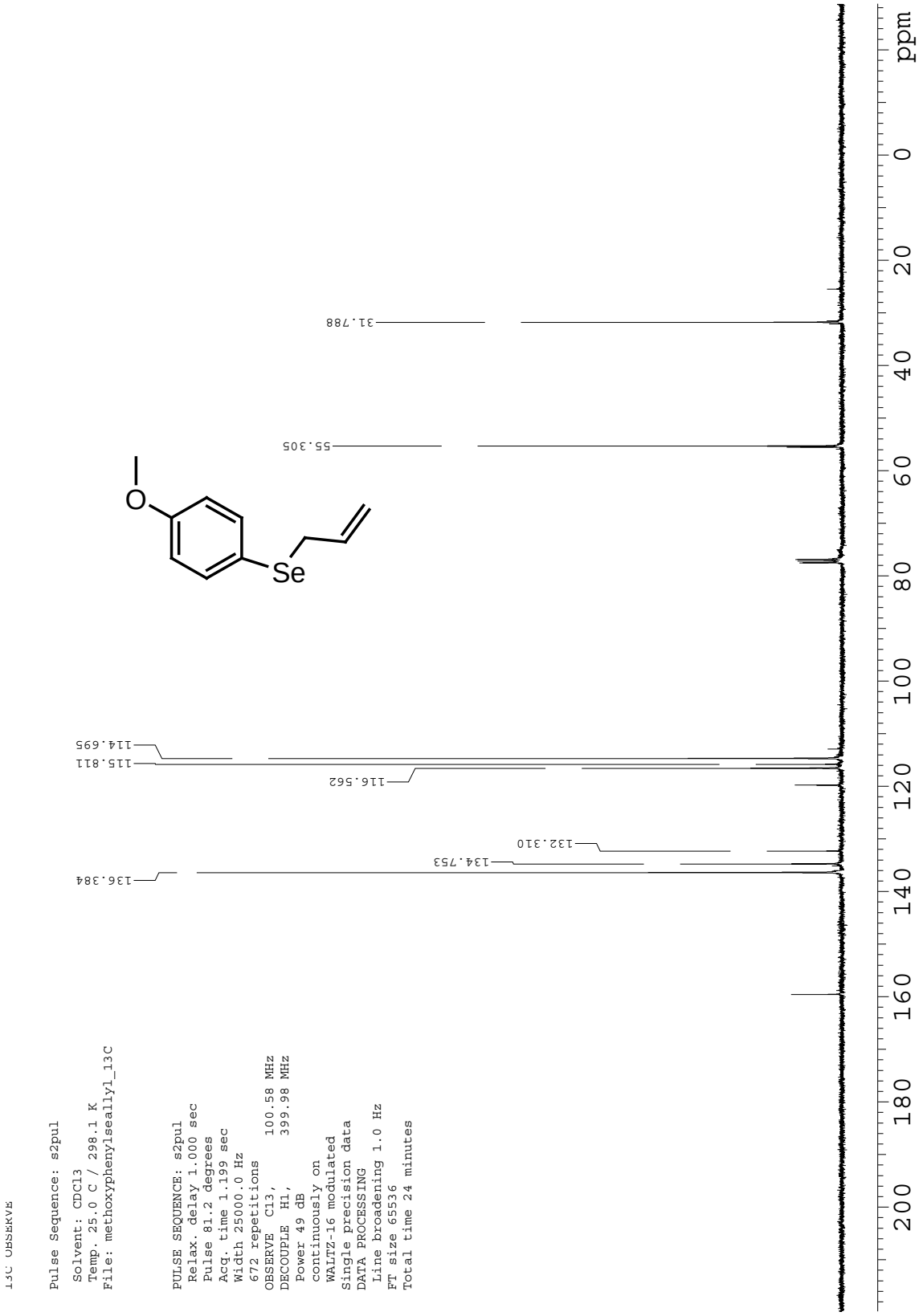

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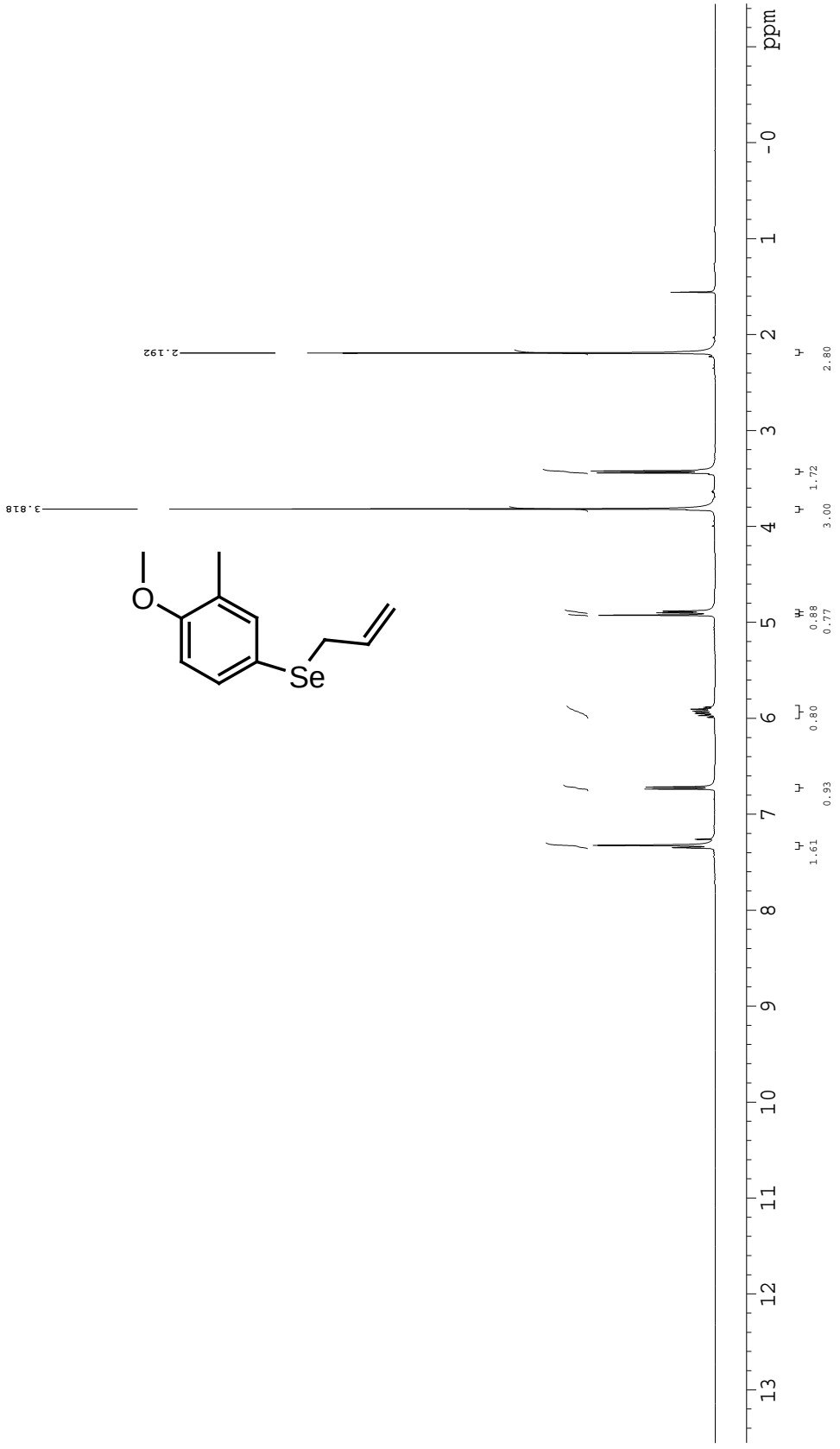

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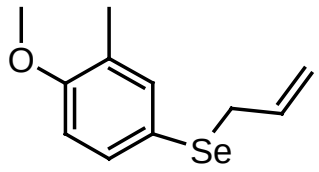

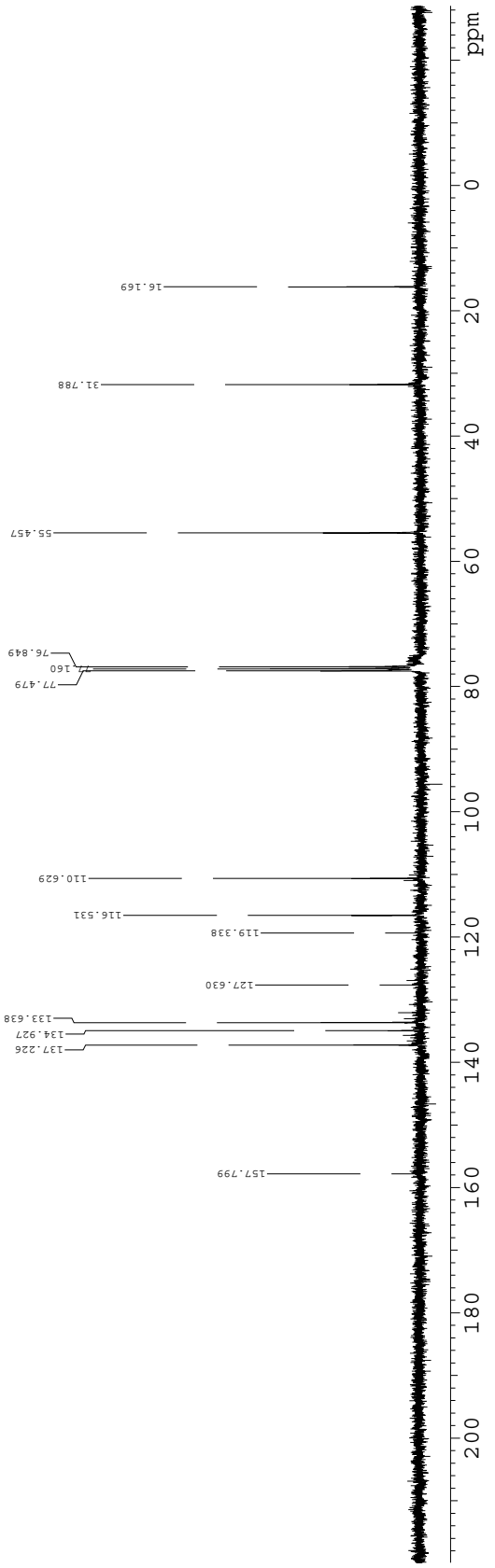

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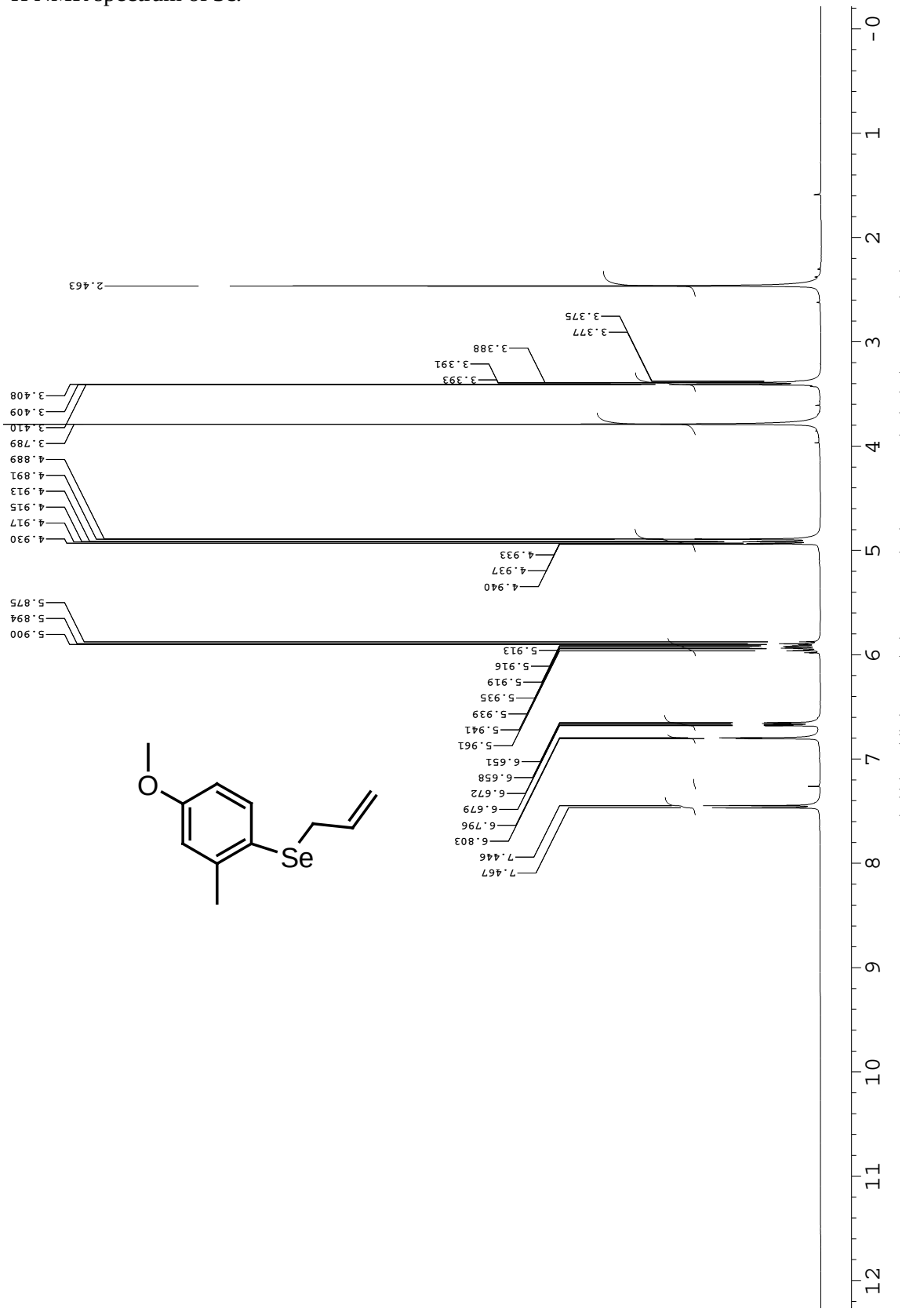

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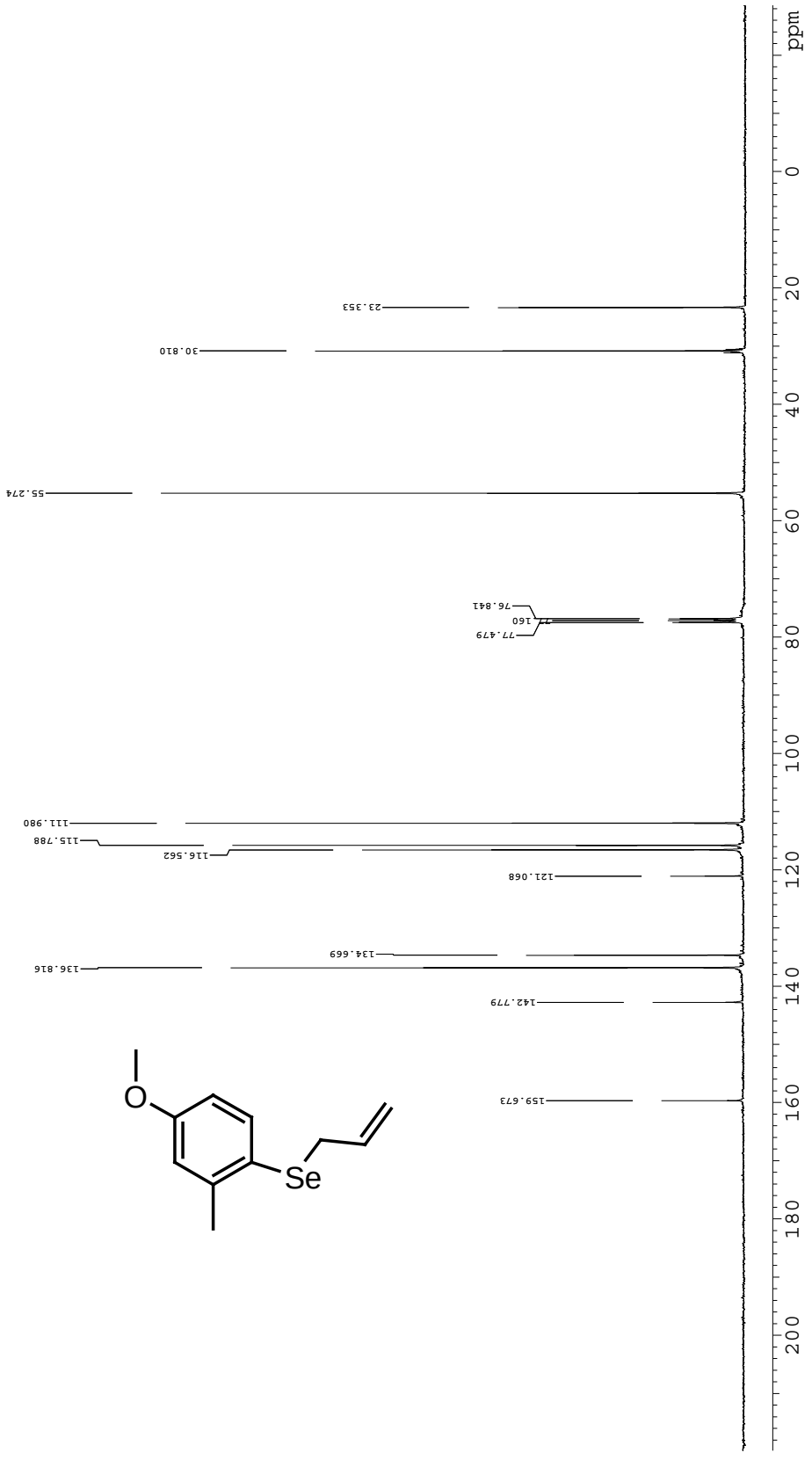

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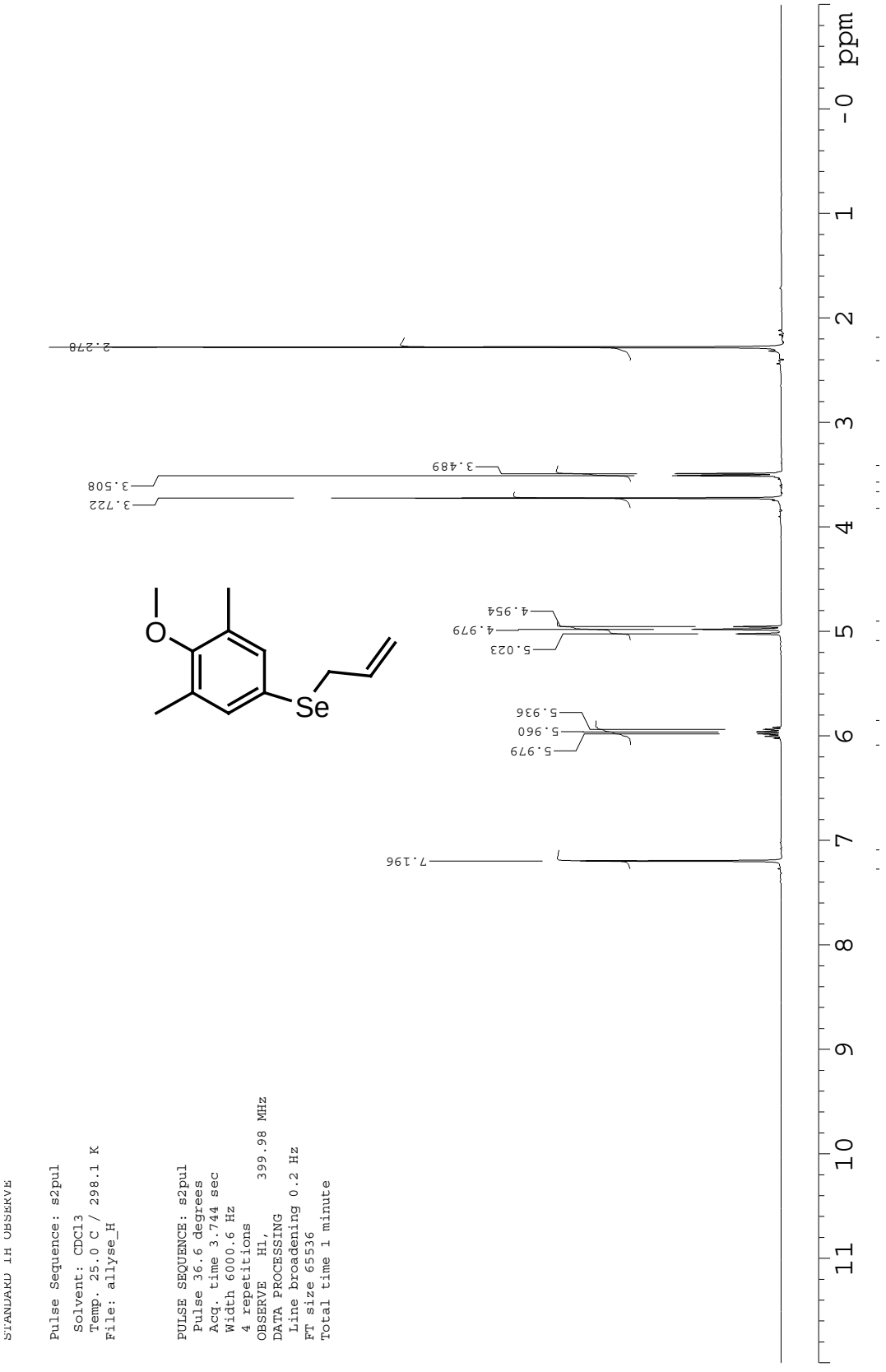

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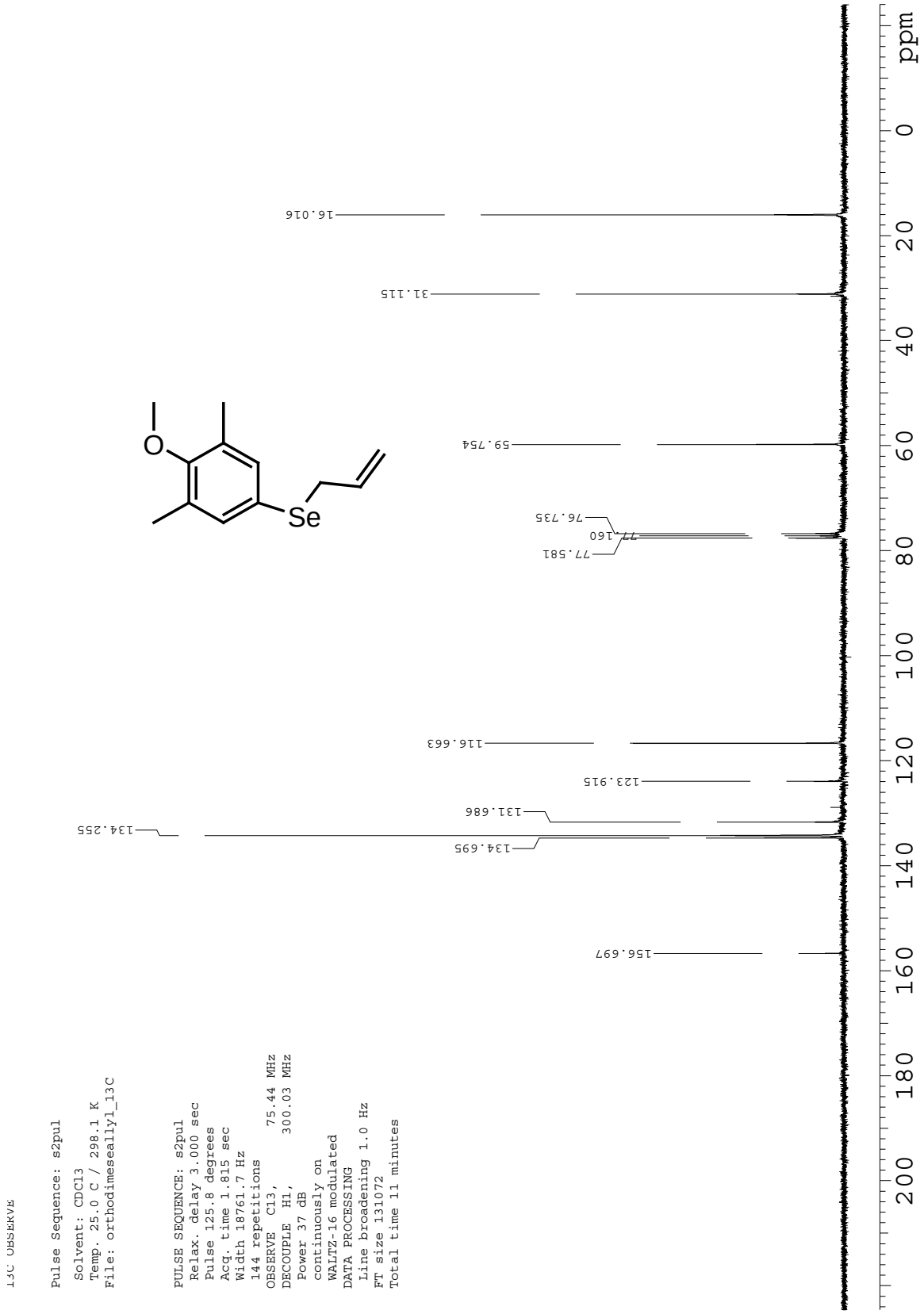

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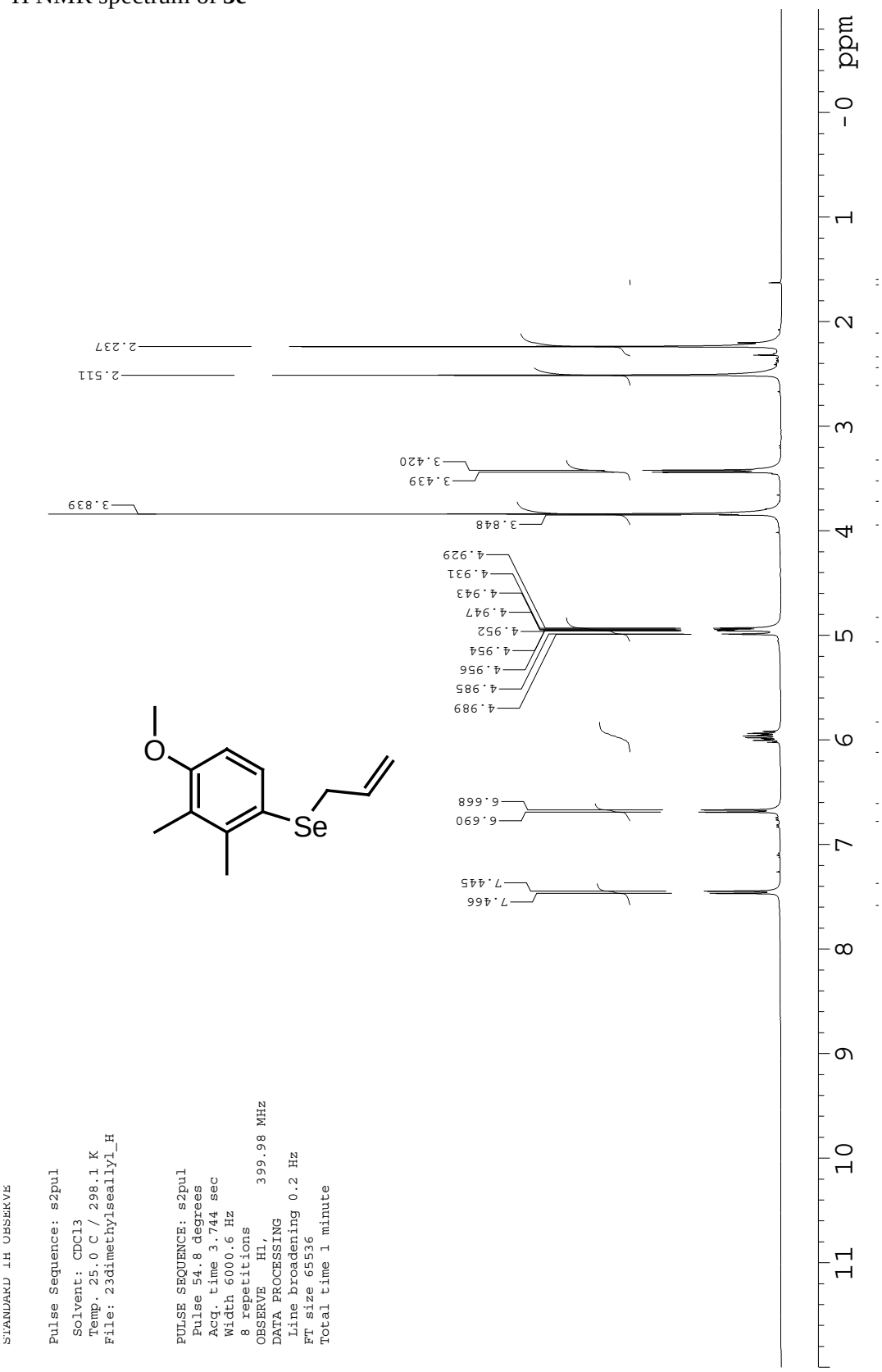

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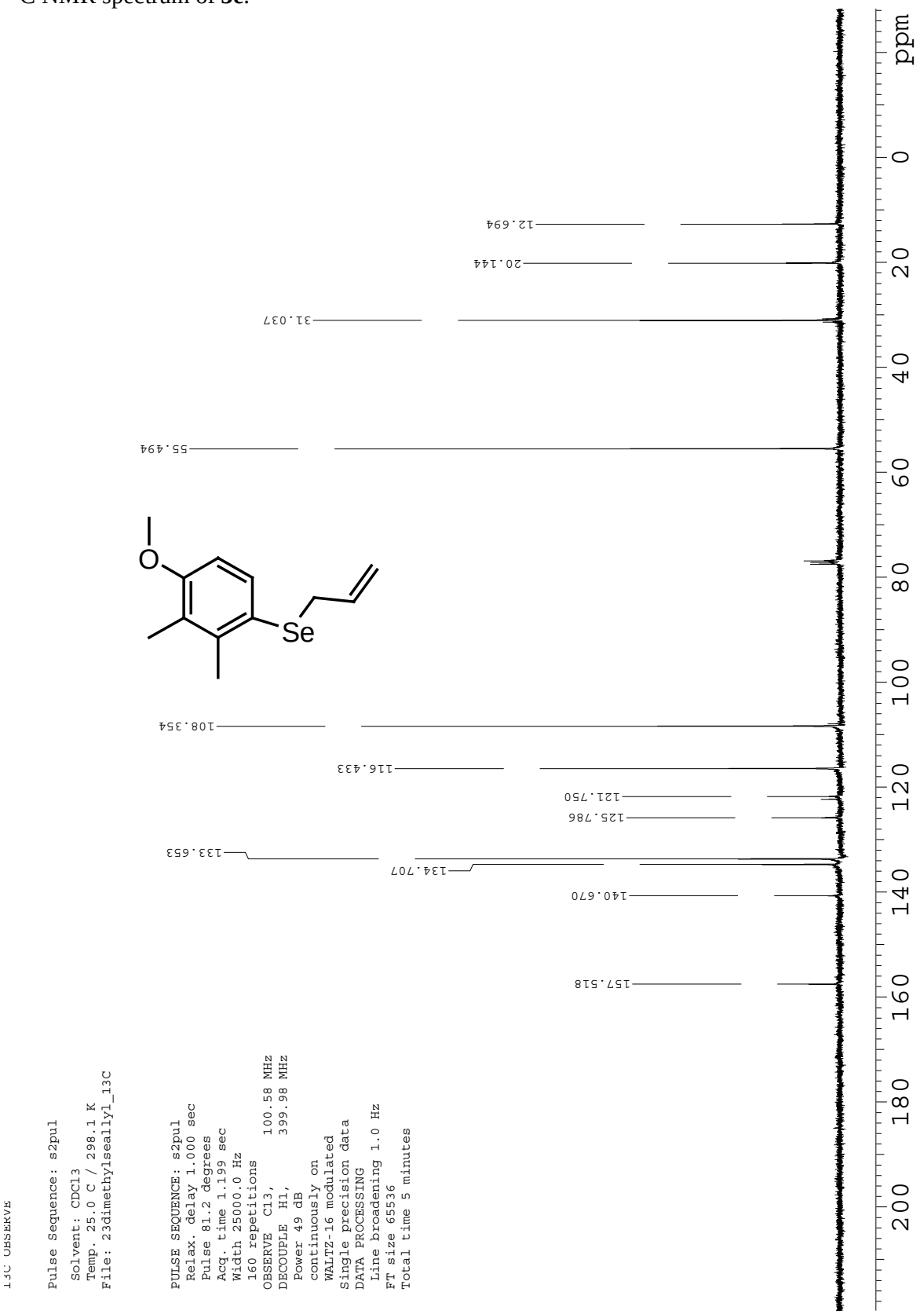

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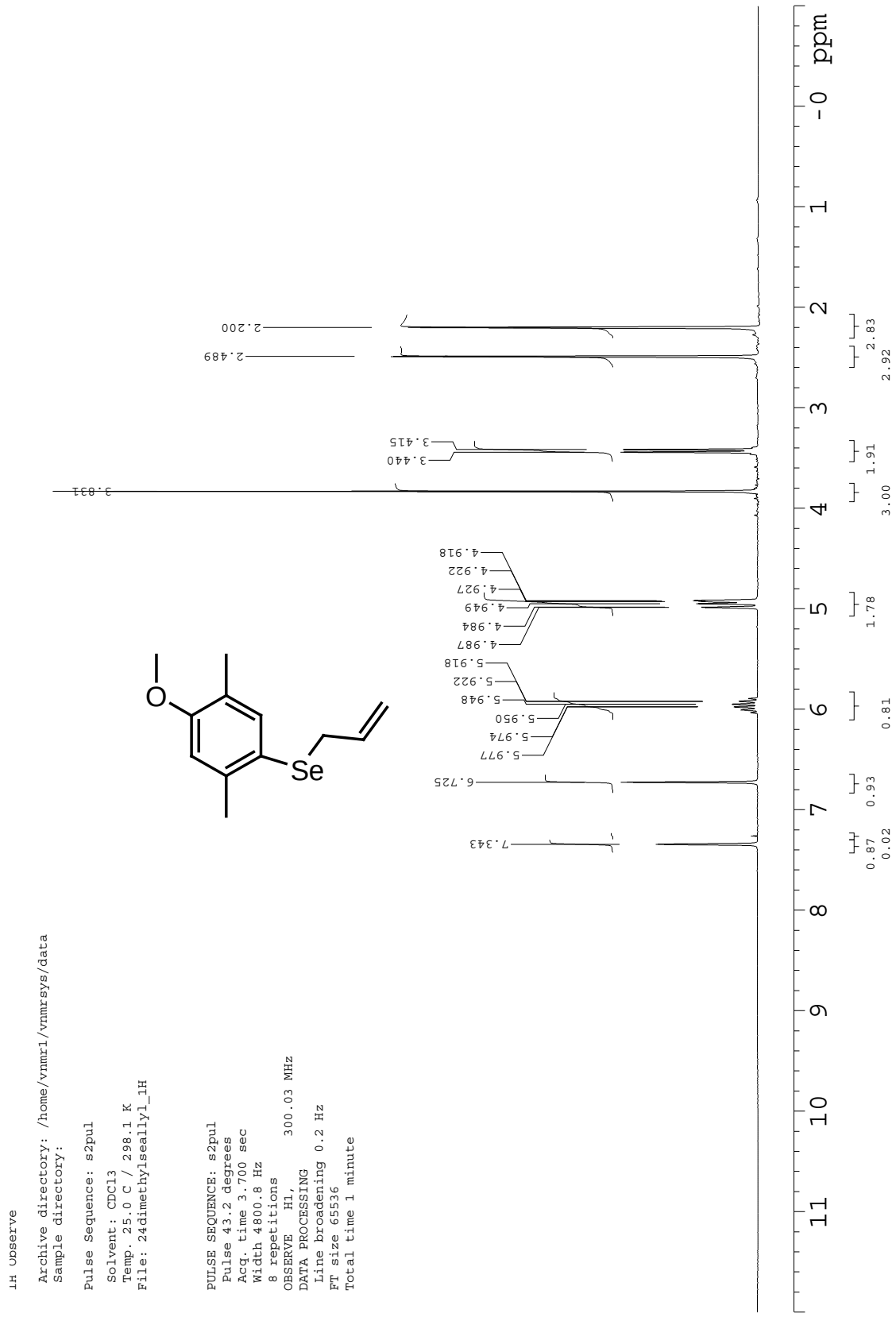

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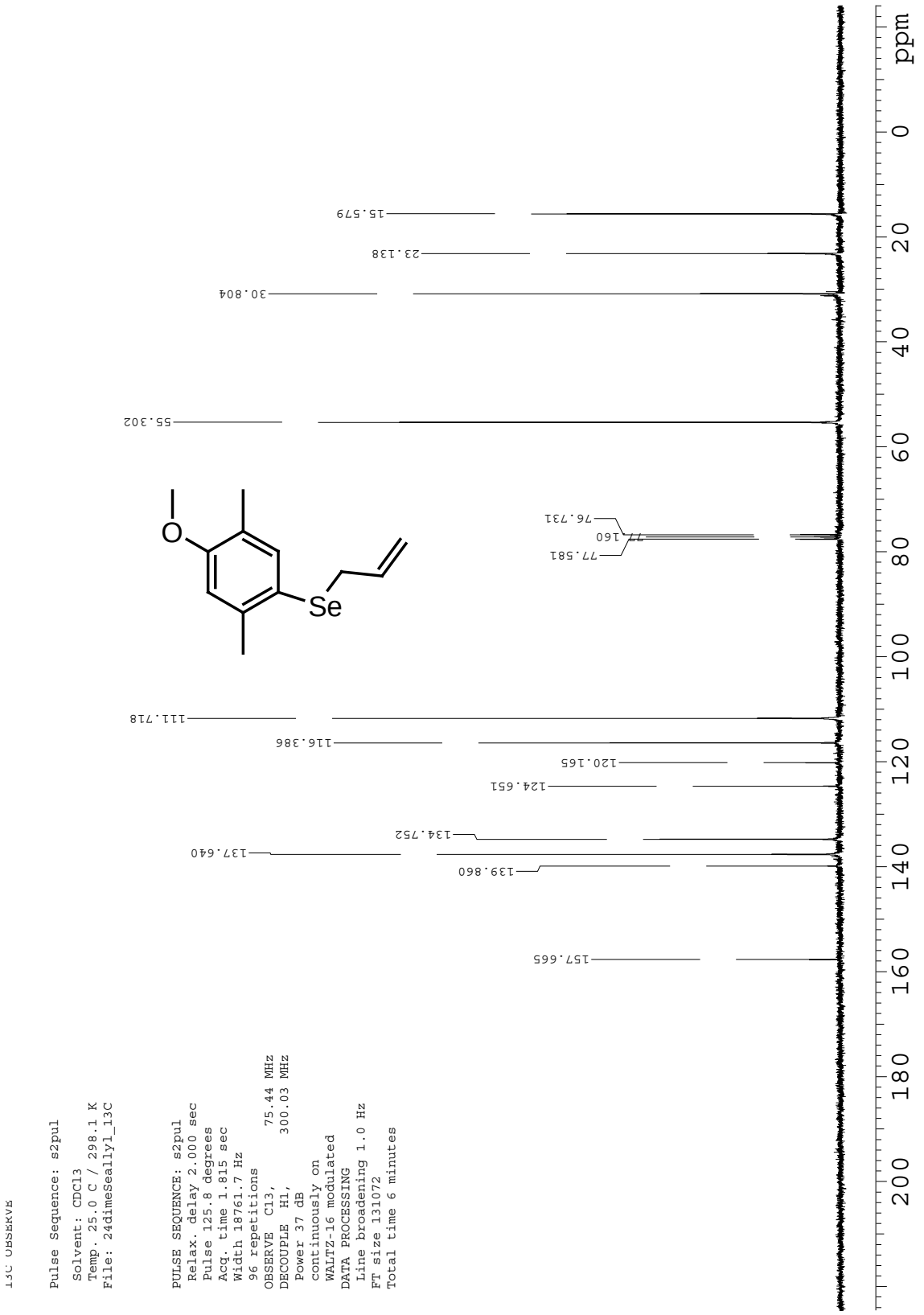

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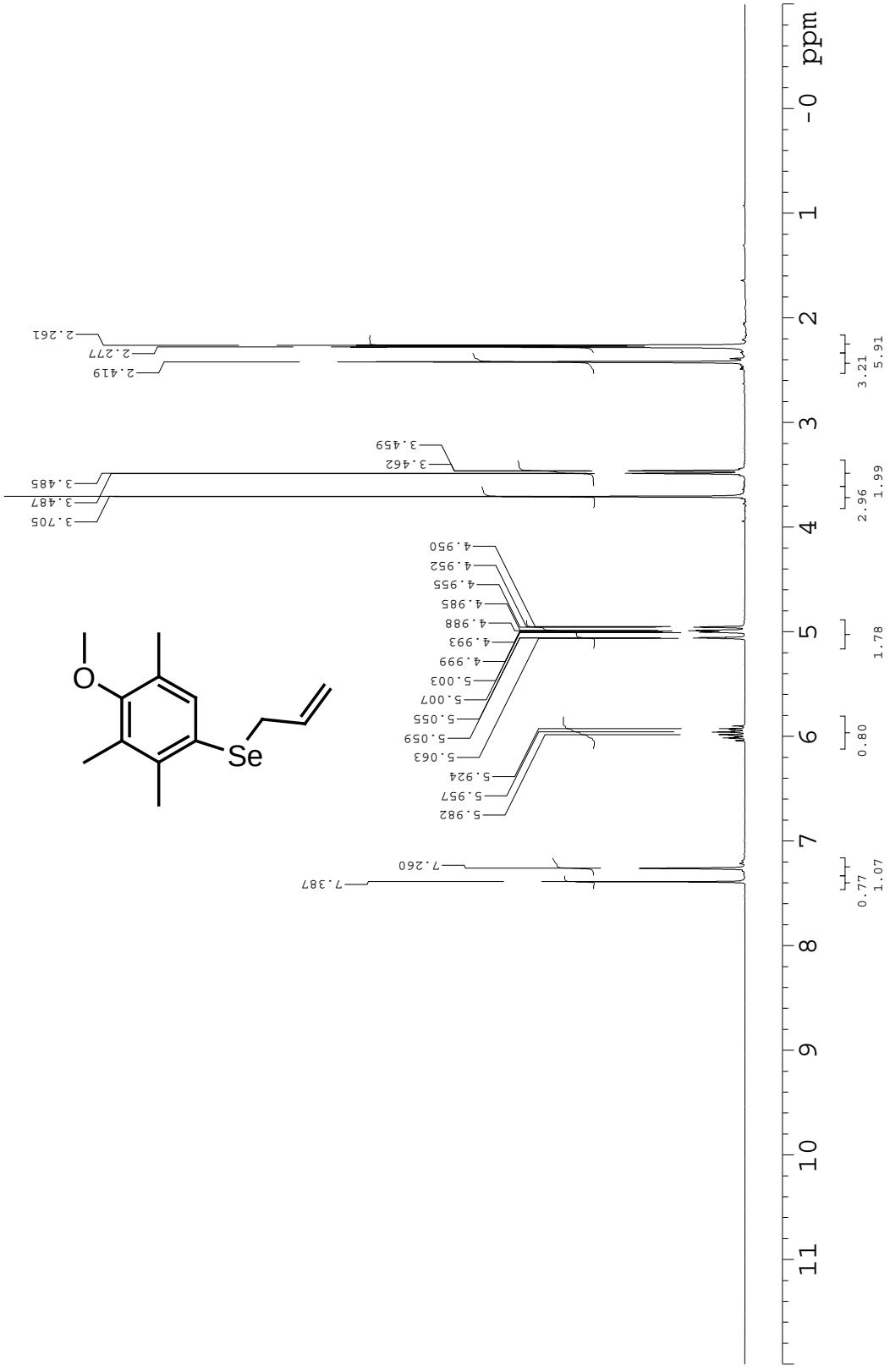

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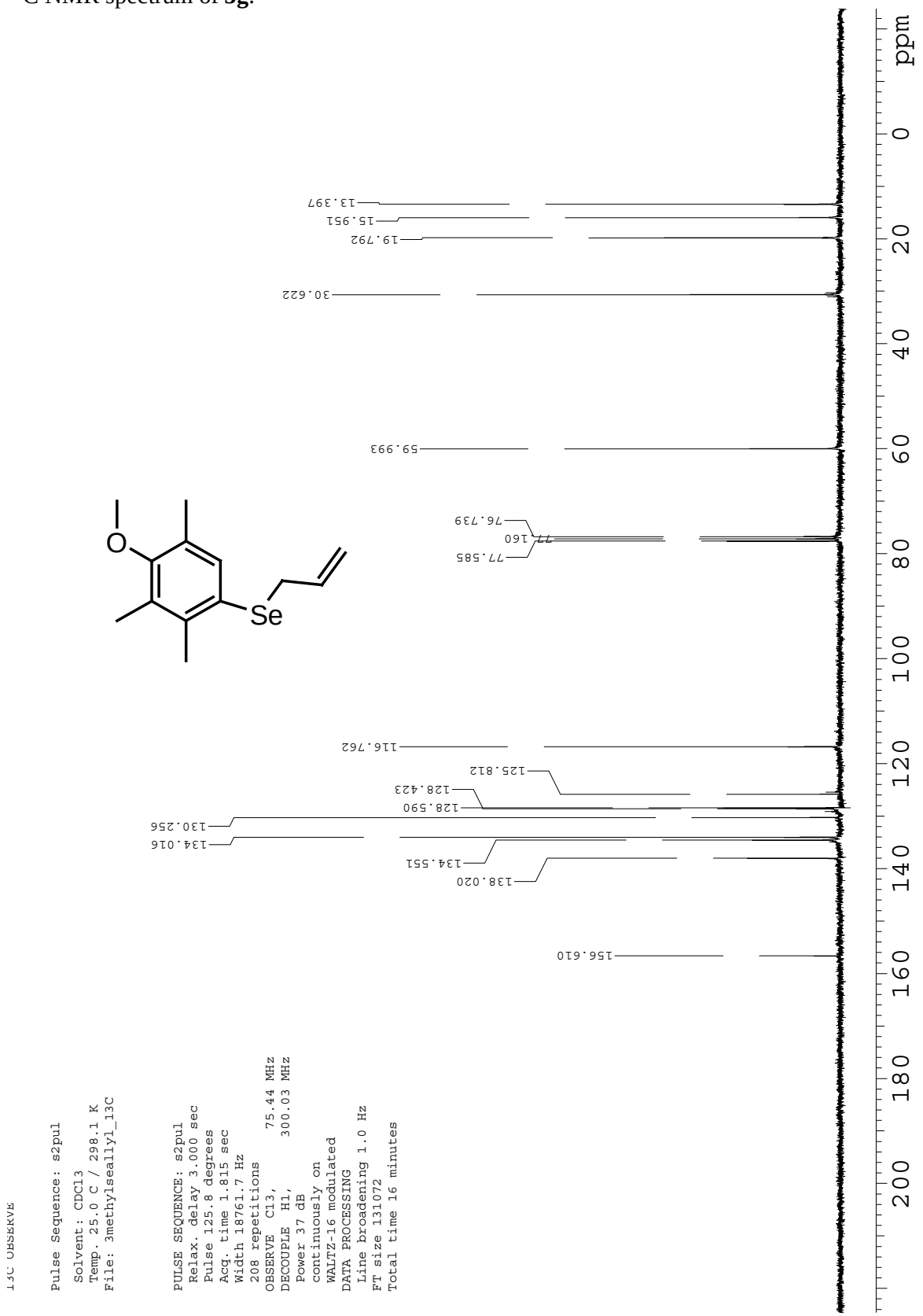
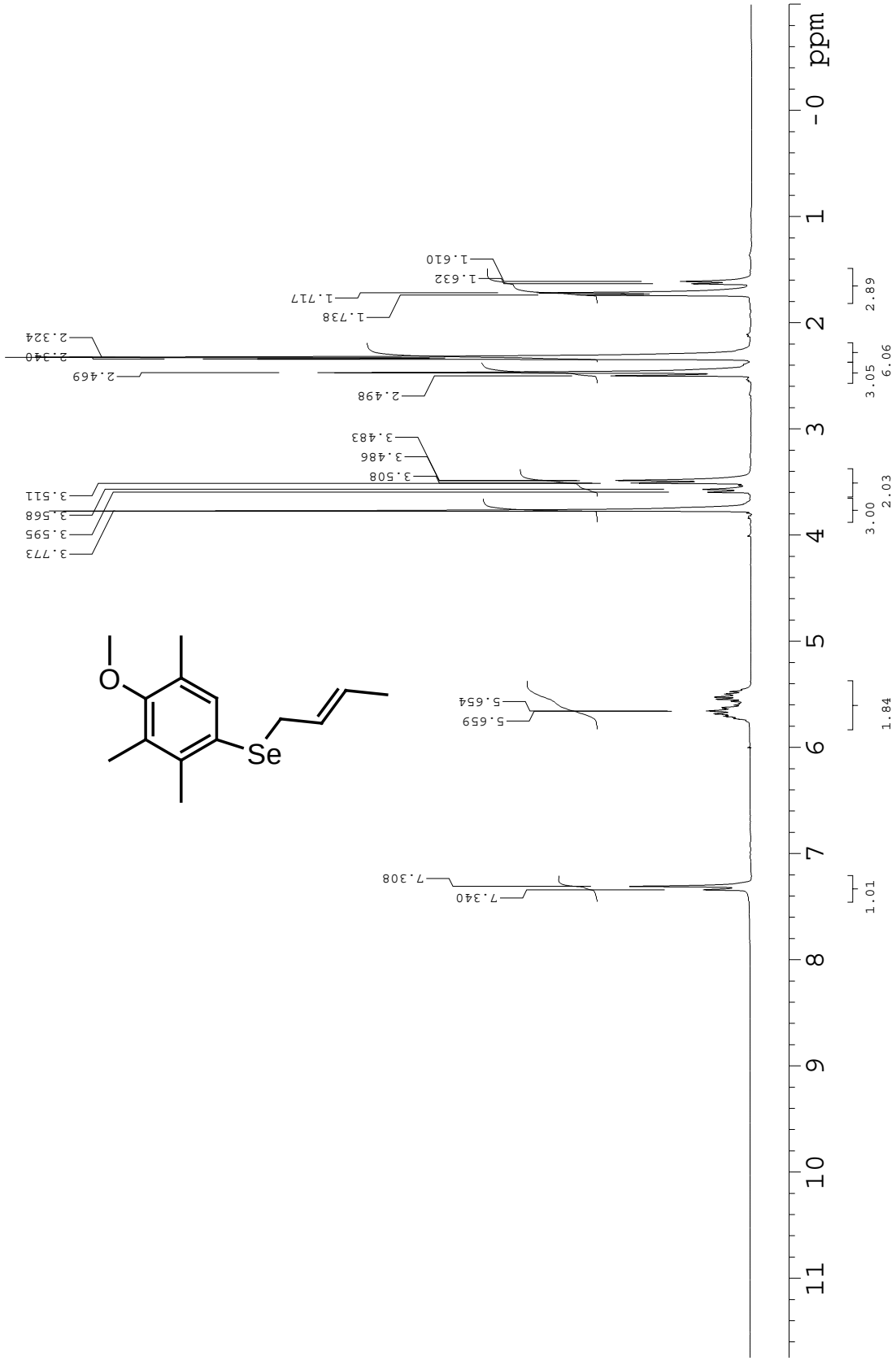
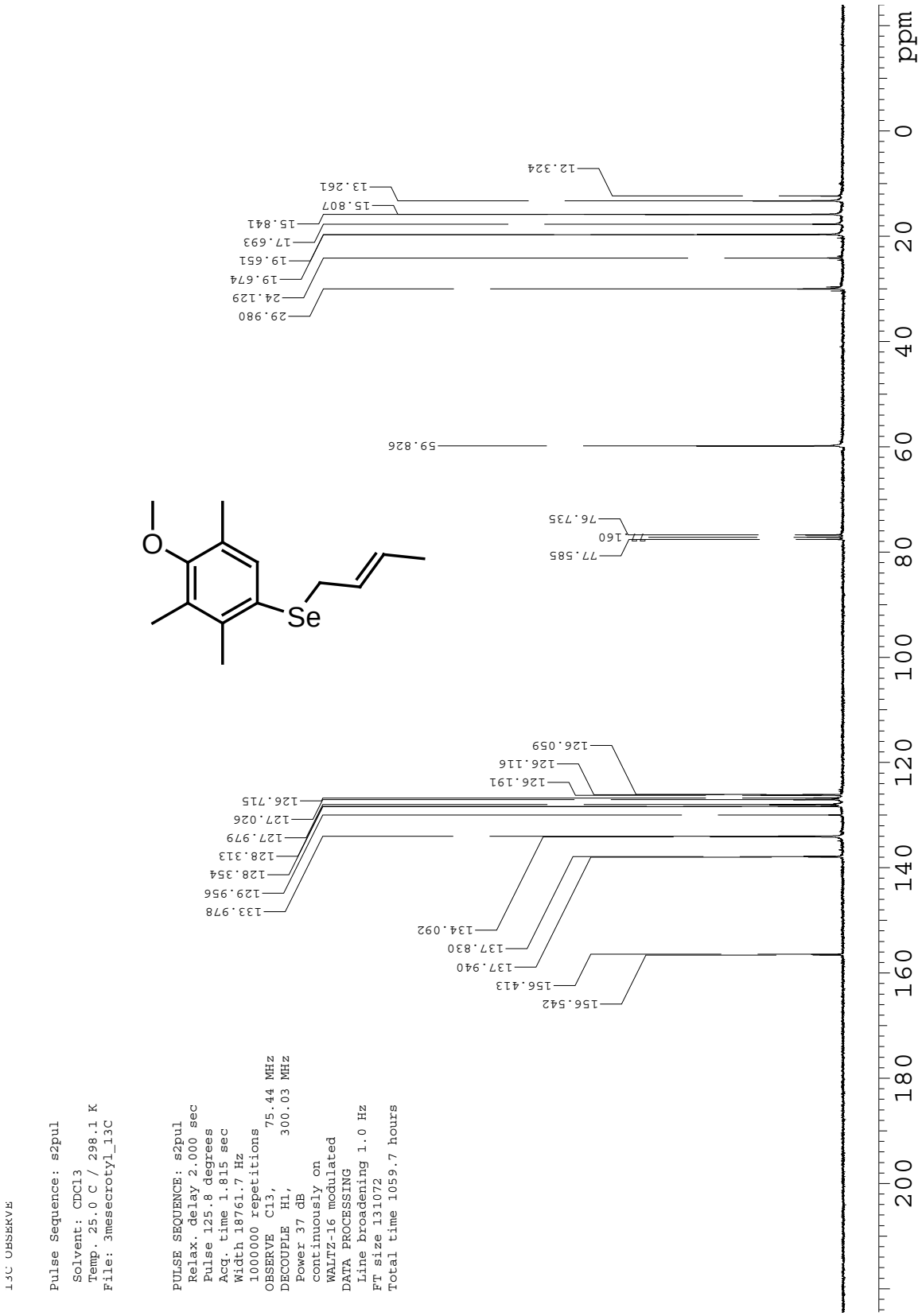


^{1}H NMR spectrum of 3-methyl-2-propen-1-yl 4-methoxy-2,3,5-trimethylphenyl selenide.



^{13}C NMR spectrum of 3-methyl-2-propen-1-yl 4-methoxy-2,3,5-trimethylphenyl selenide.



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Power 37 dB
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DATA PROCESSING
Line broadening 1.0 Hz
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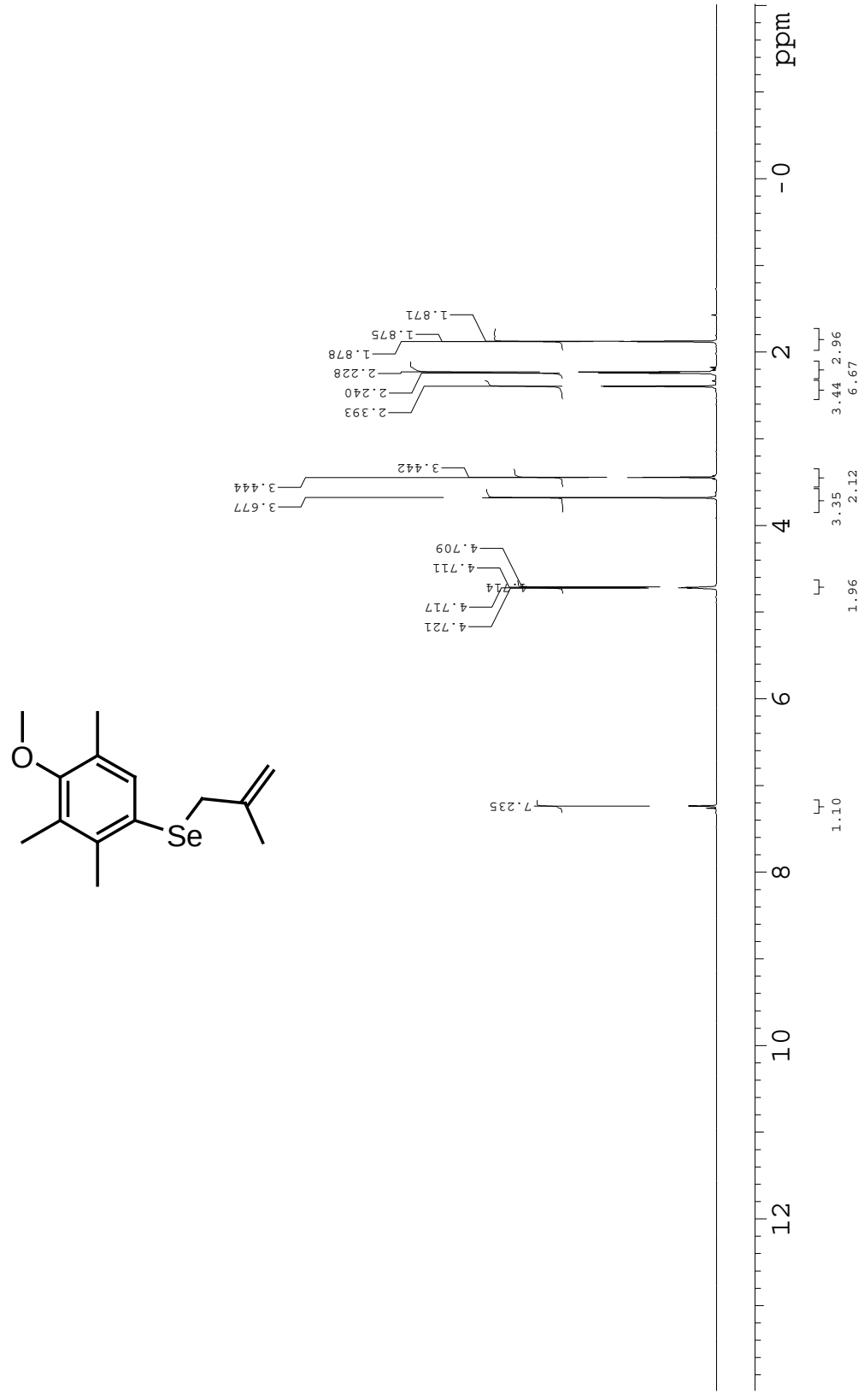
^{1}H NMR spectrum of 2-methyl-2-propen-1-yl 4-methoxy-2,3,5-trimethylphenyl selenides.



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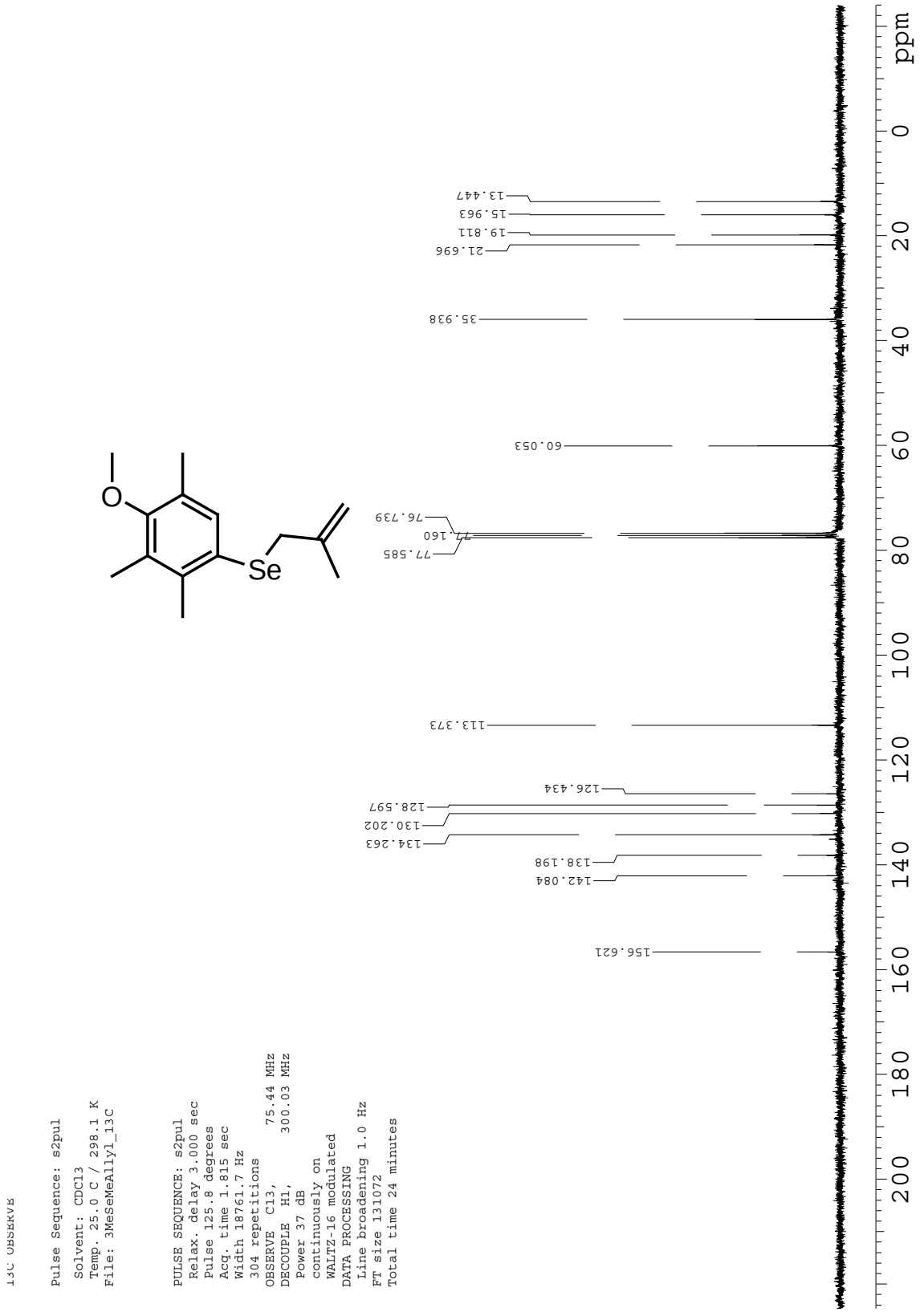
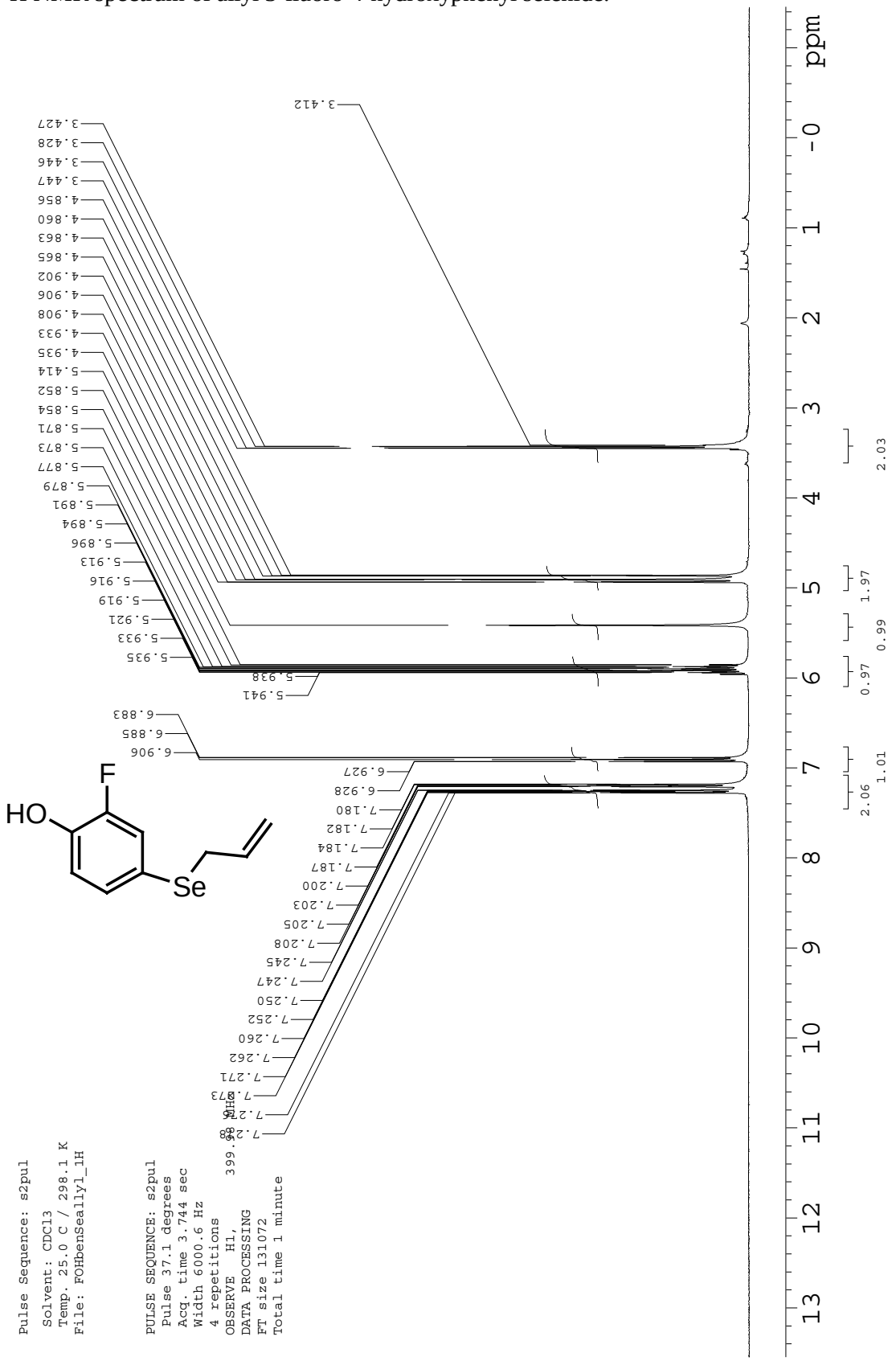
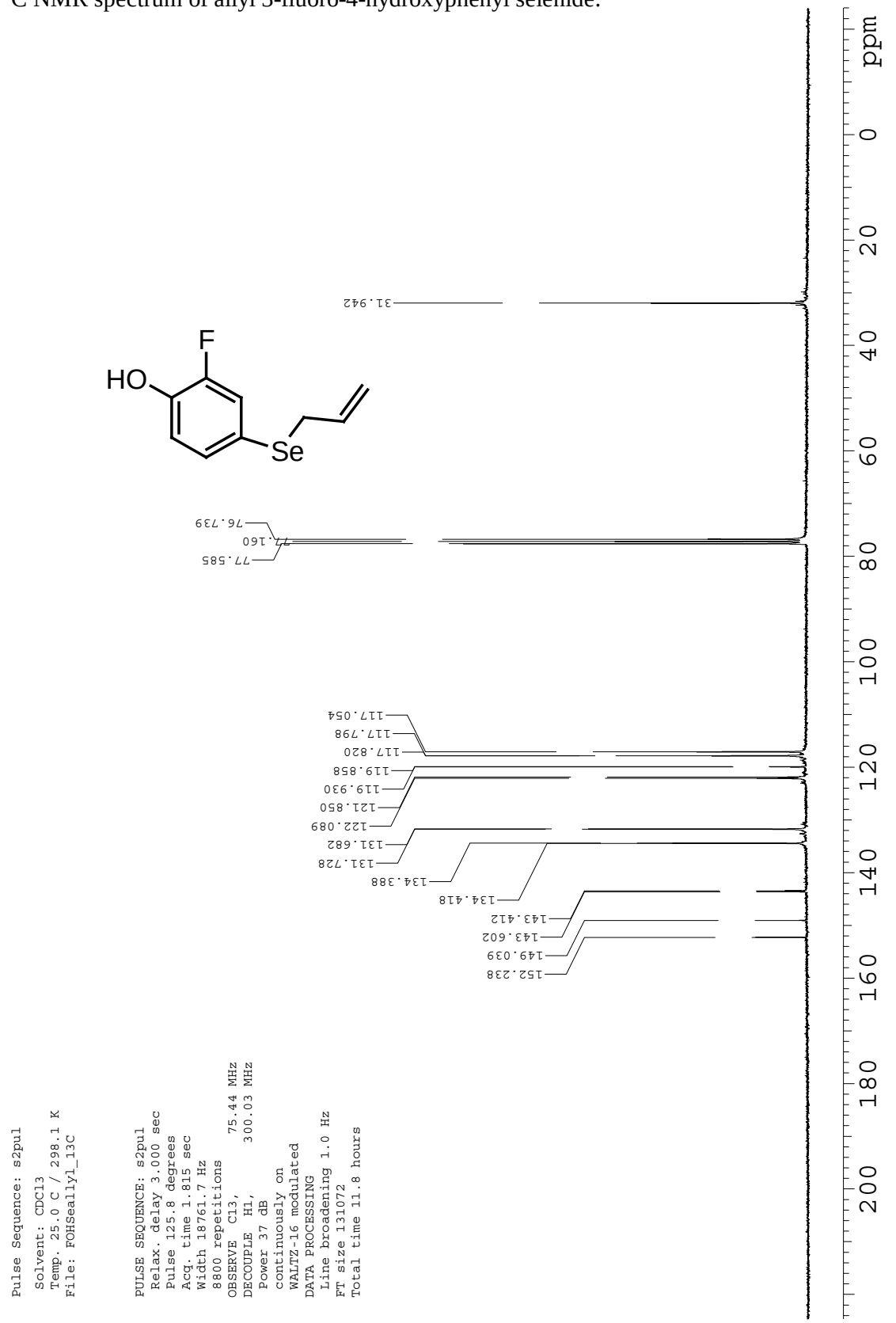


^{1}H NMR spectrum of allyl 3-fluoro-4-hydroxyphenyl selenide.



^{13}C NMR spectrum of allyl 3-fluoro-4-hydroxyphenyl selenide.



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Temp. 25.0 C / 298.1 K
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Relax. delay 3.000 sec
Pulse 125.8 degrees
Acq. time 1.815 sec
Width 18761.7 Hz
8800 repetitions
OBSERVE C13, 75.44 MHz
DECOUPLE H1, 300.03 MHz
Power 37 dB
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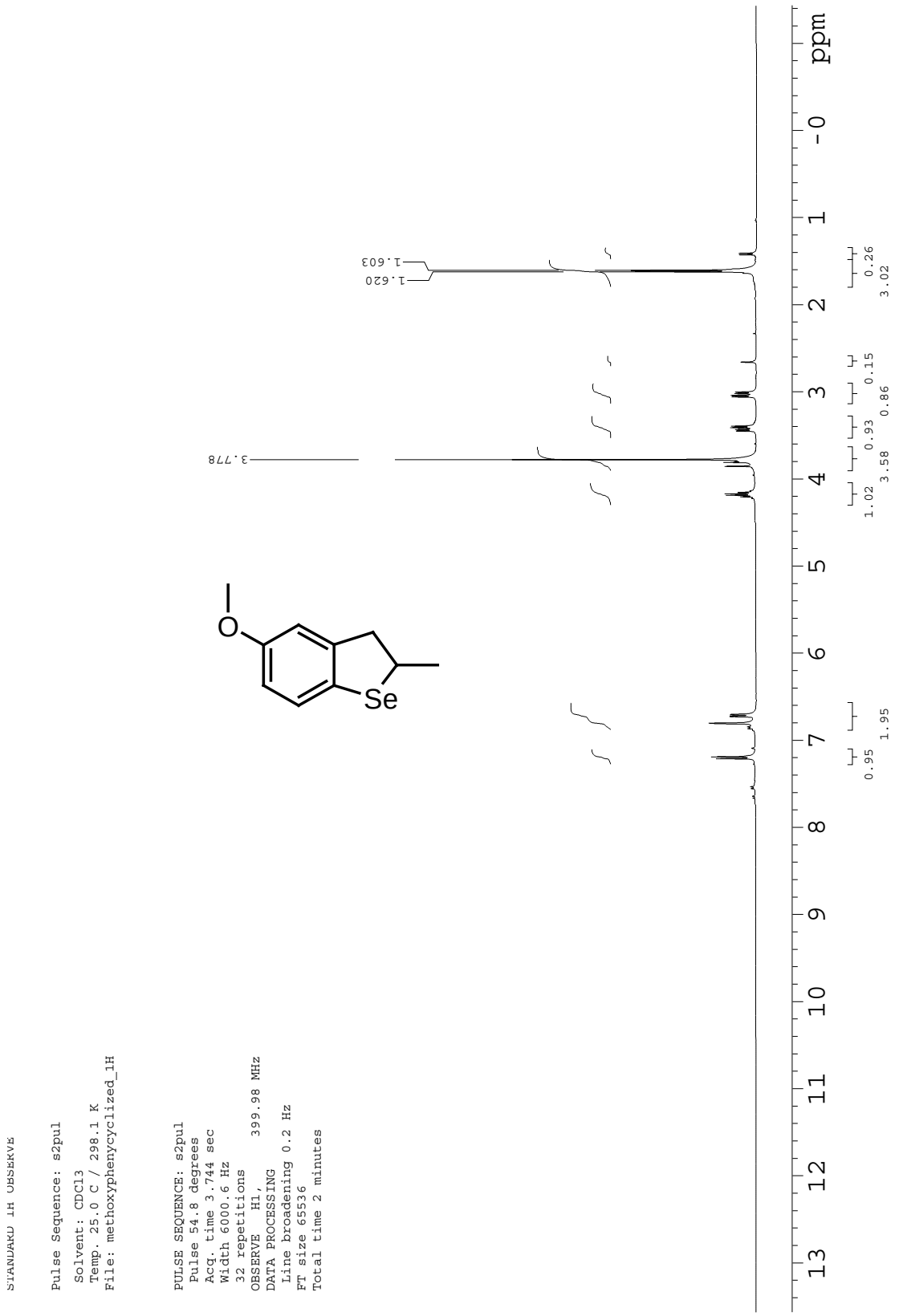
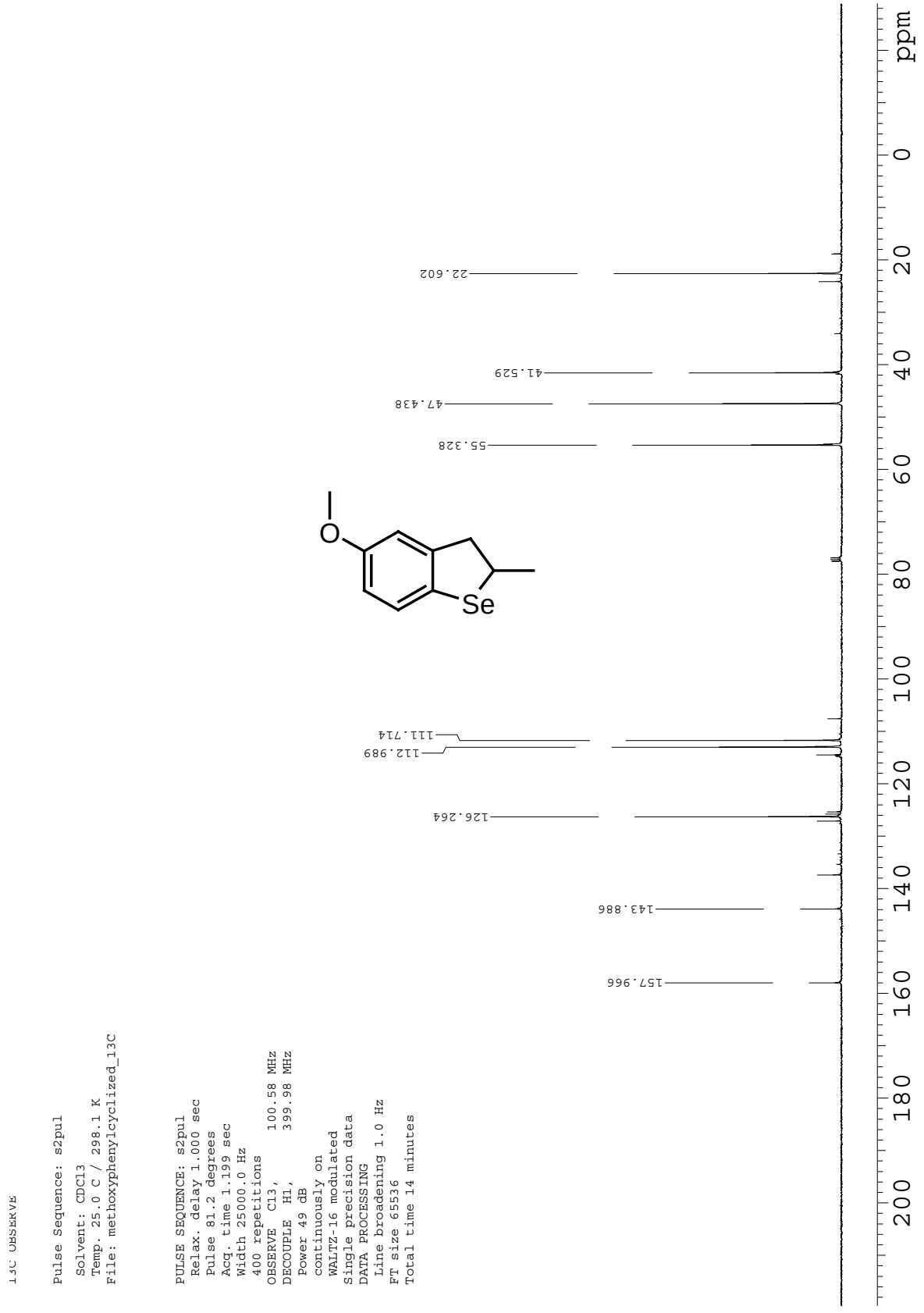
^{1}H NMR spectrum of **4a**.



^{13}C NMR spectrum of **4a**.



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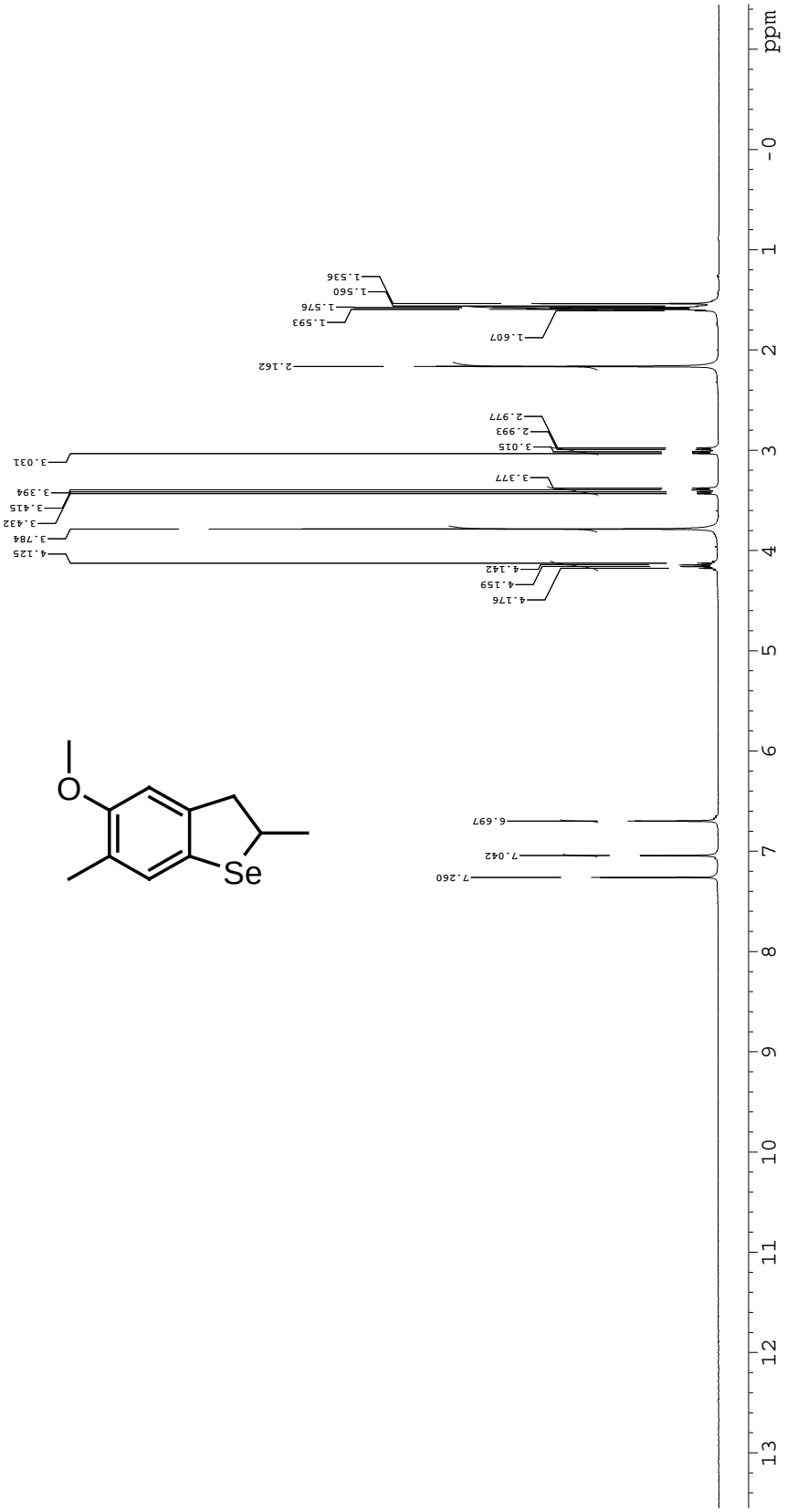

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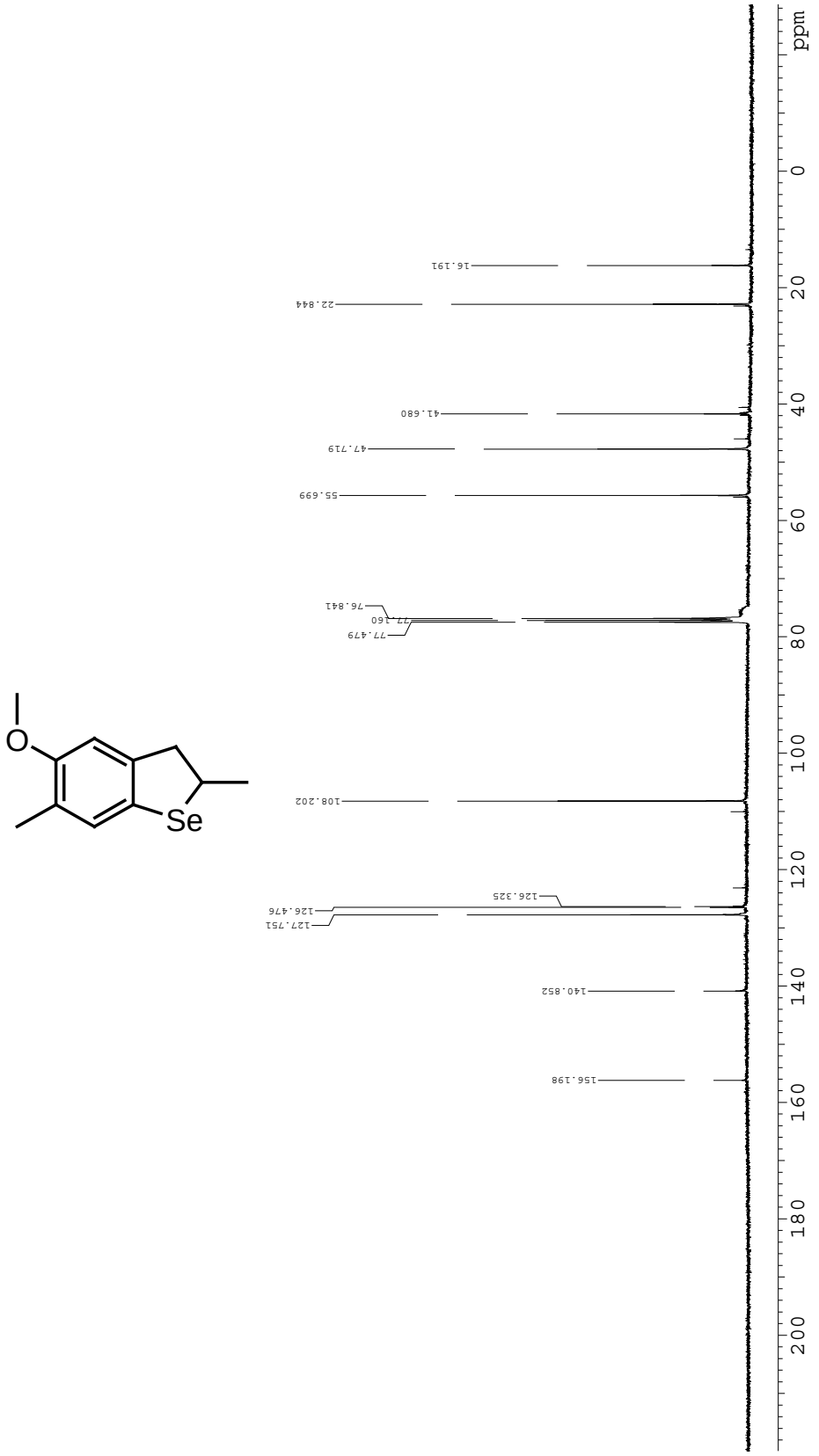

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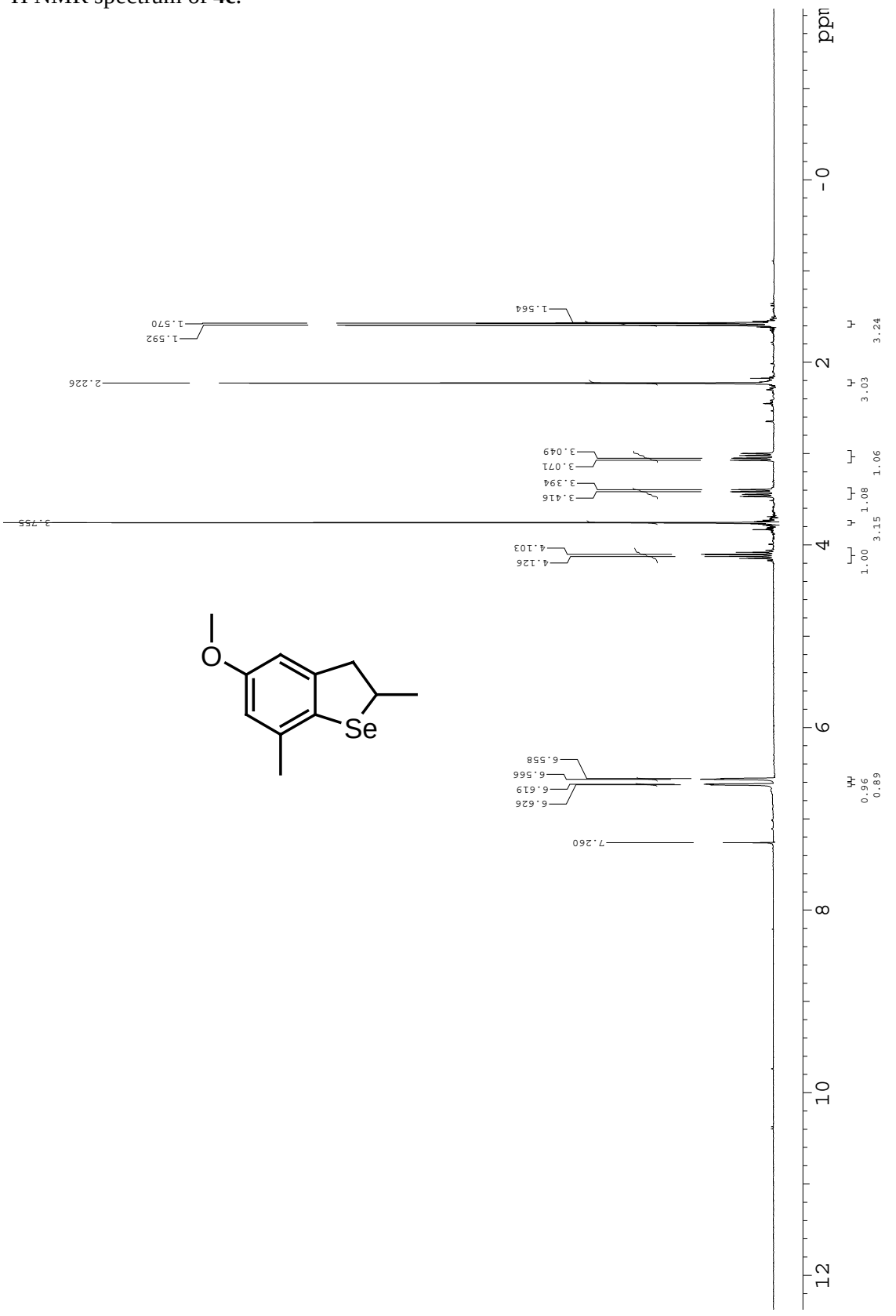

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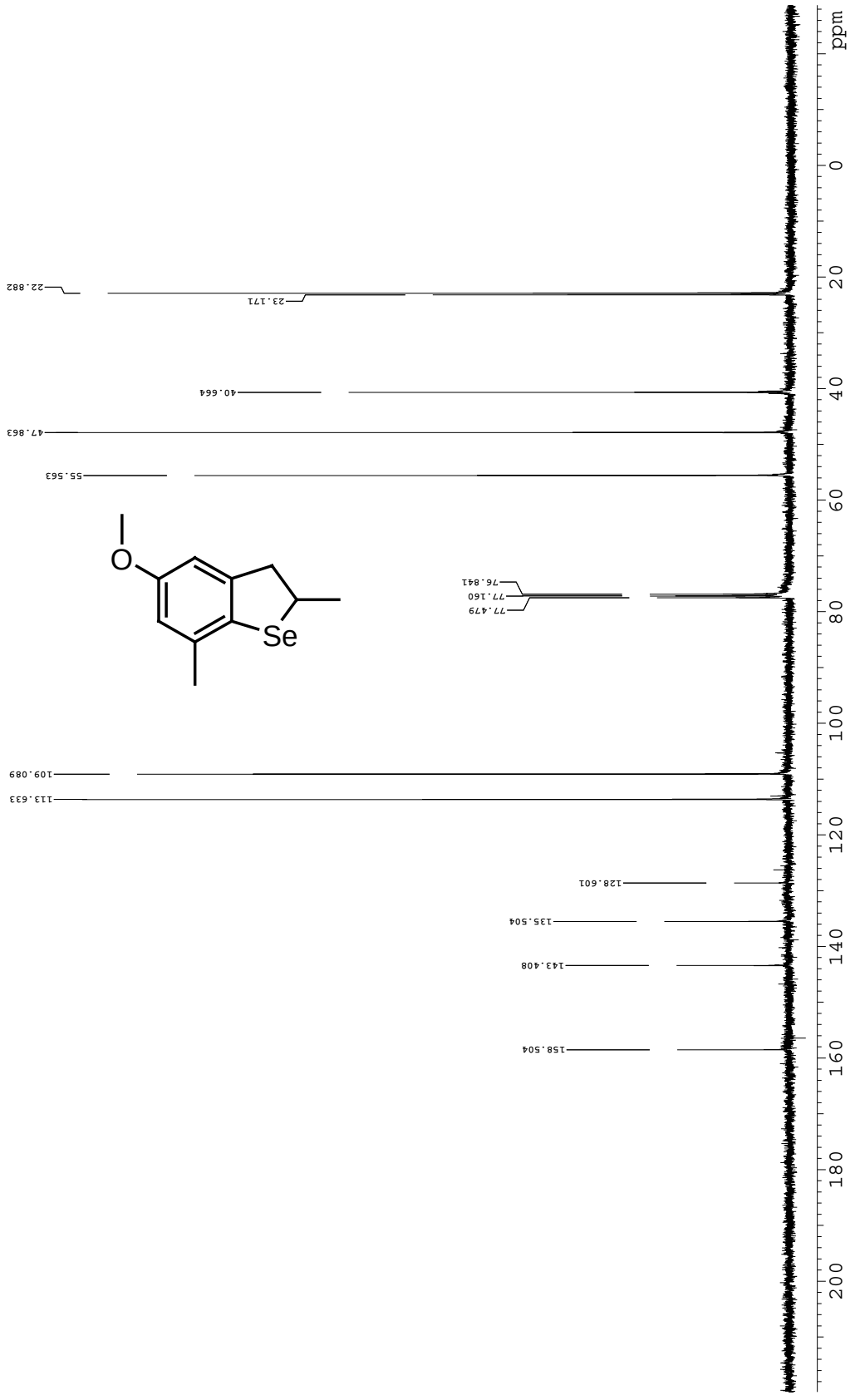

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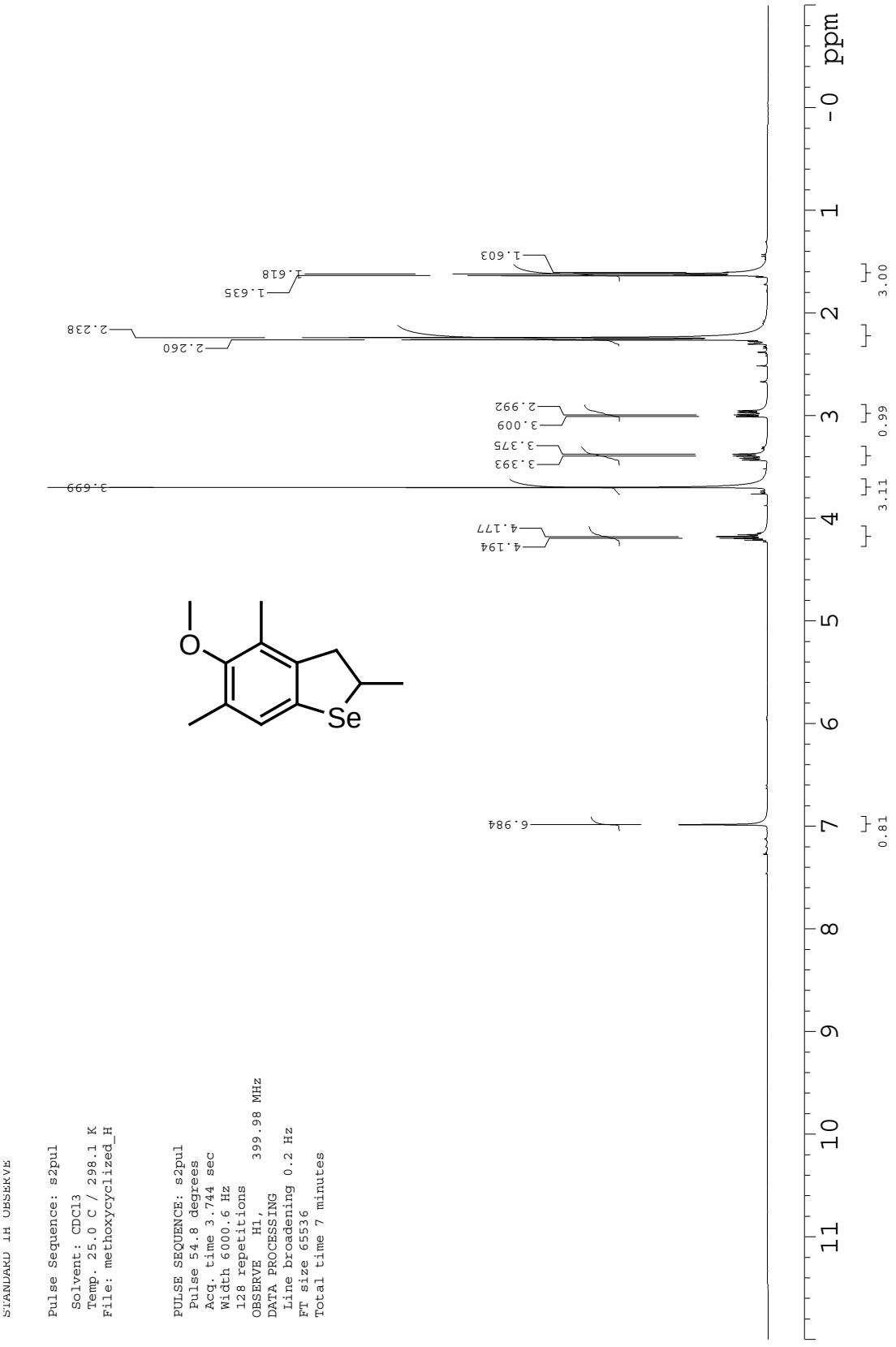

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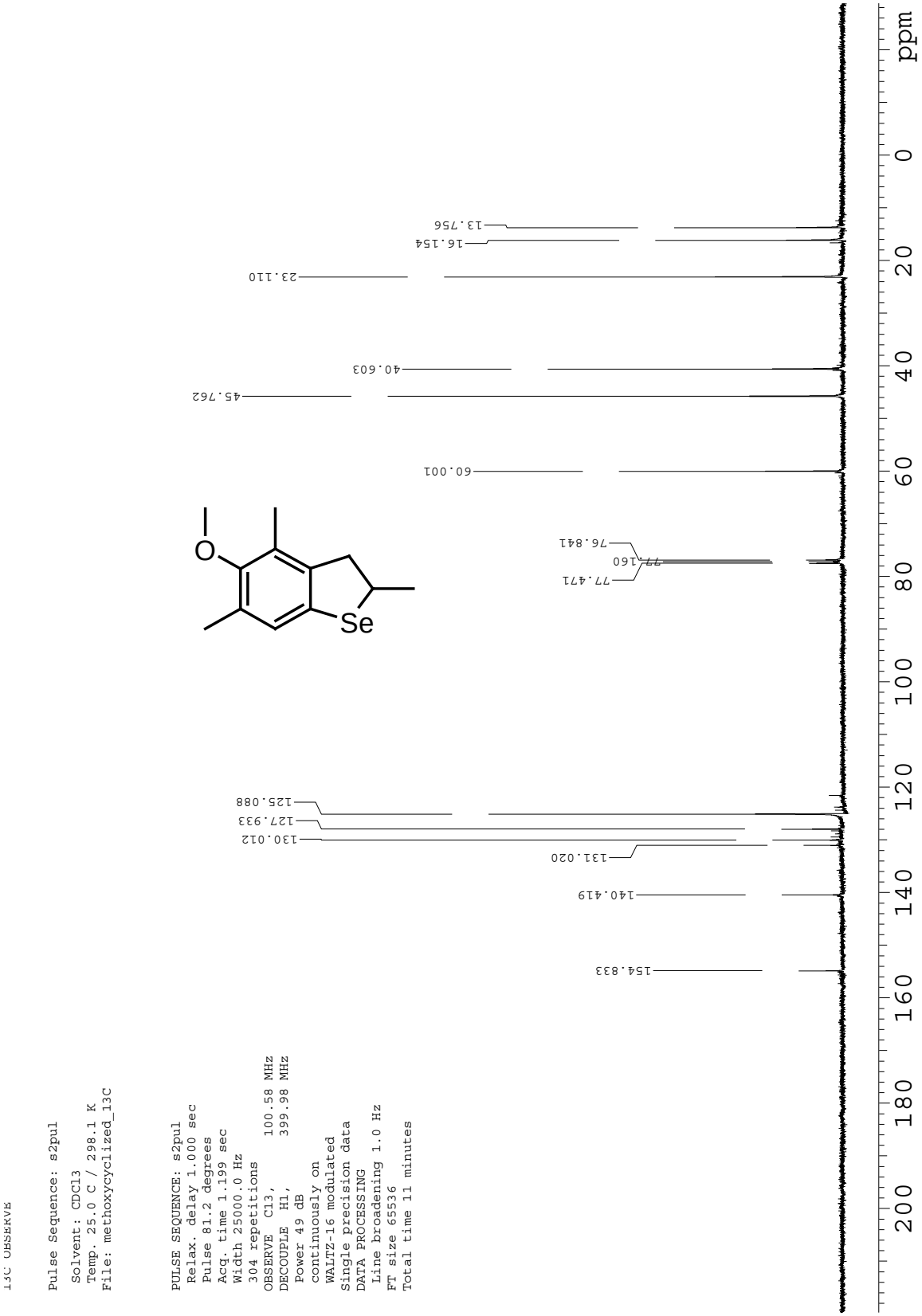

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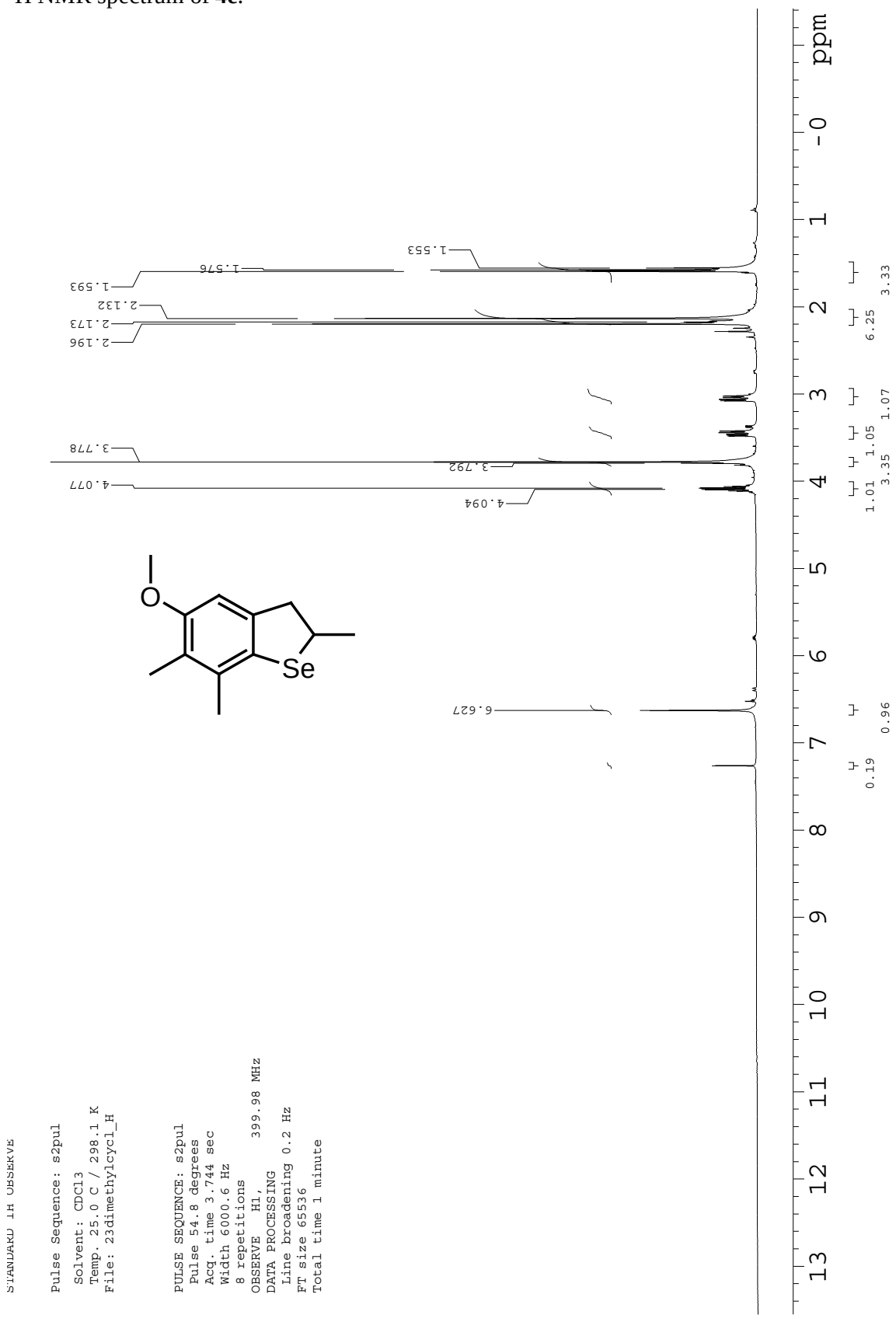

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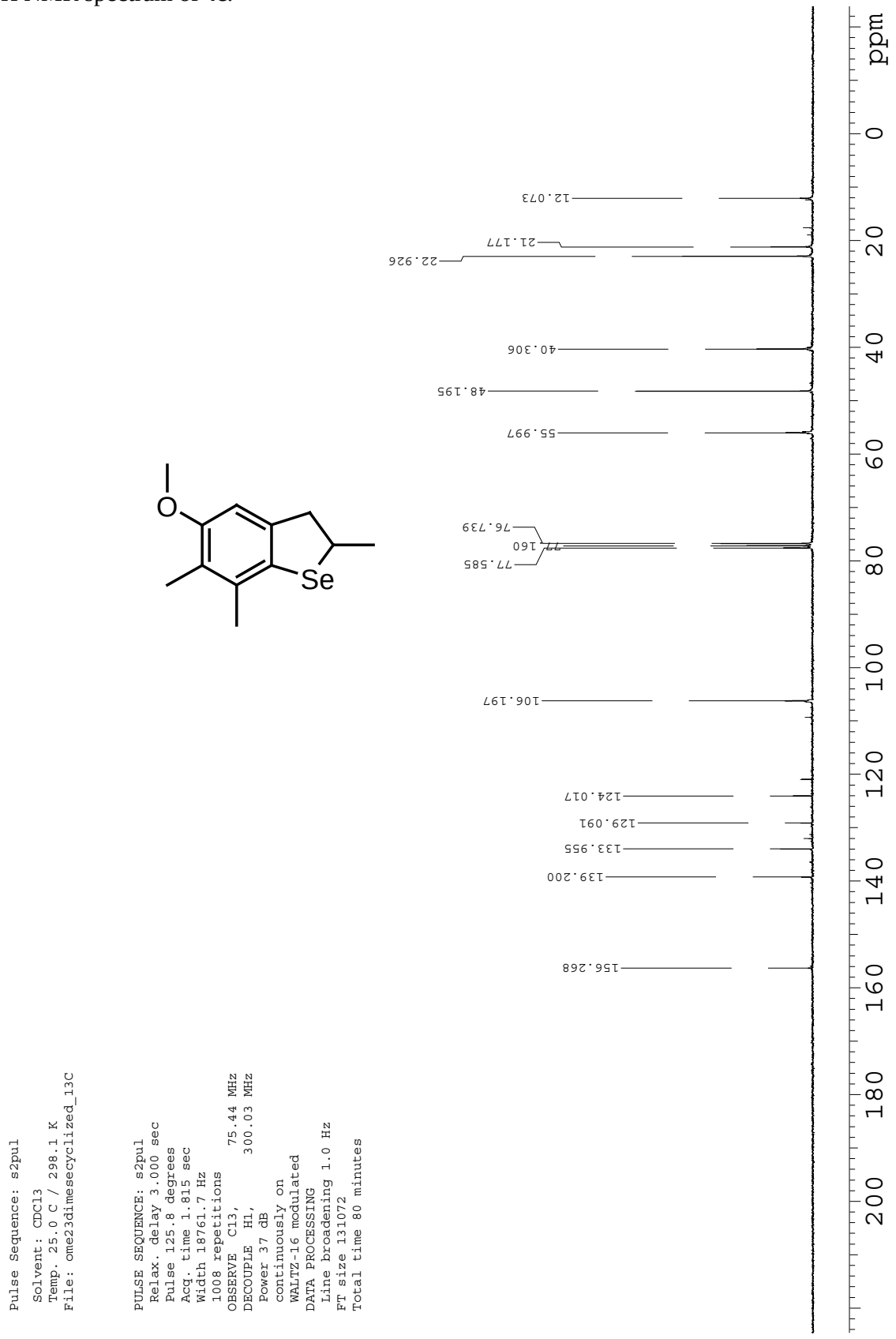

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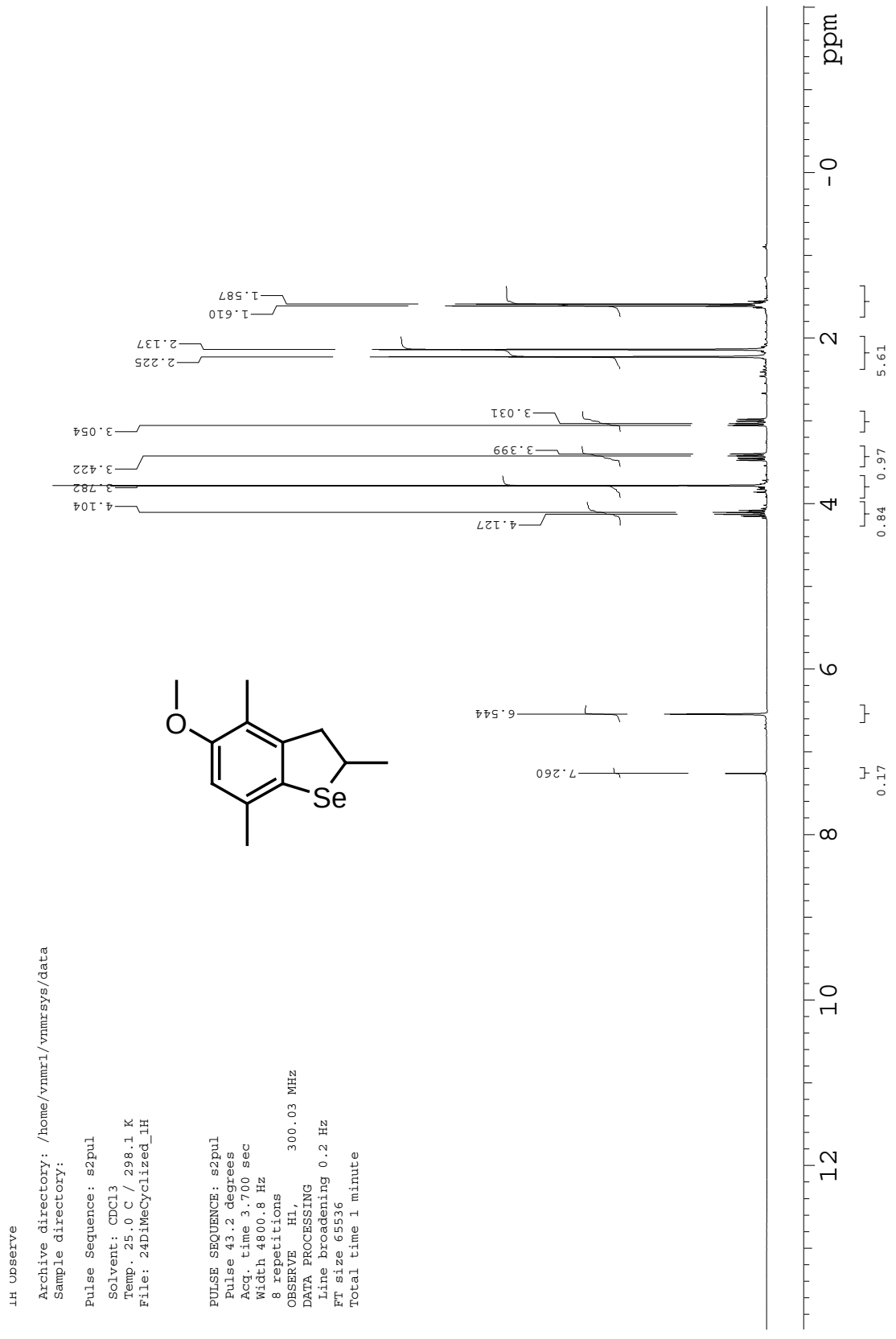

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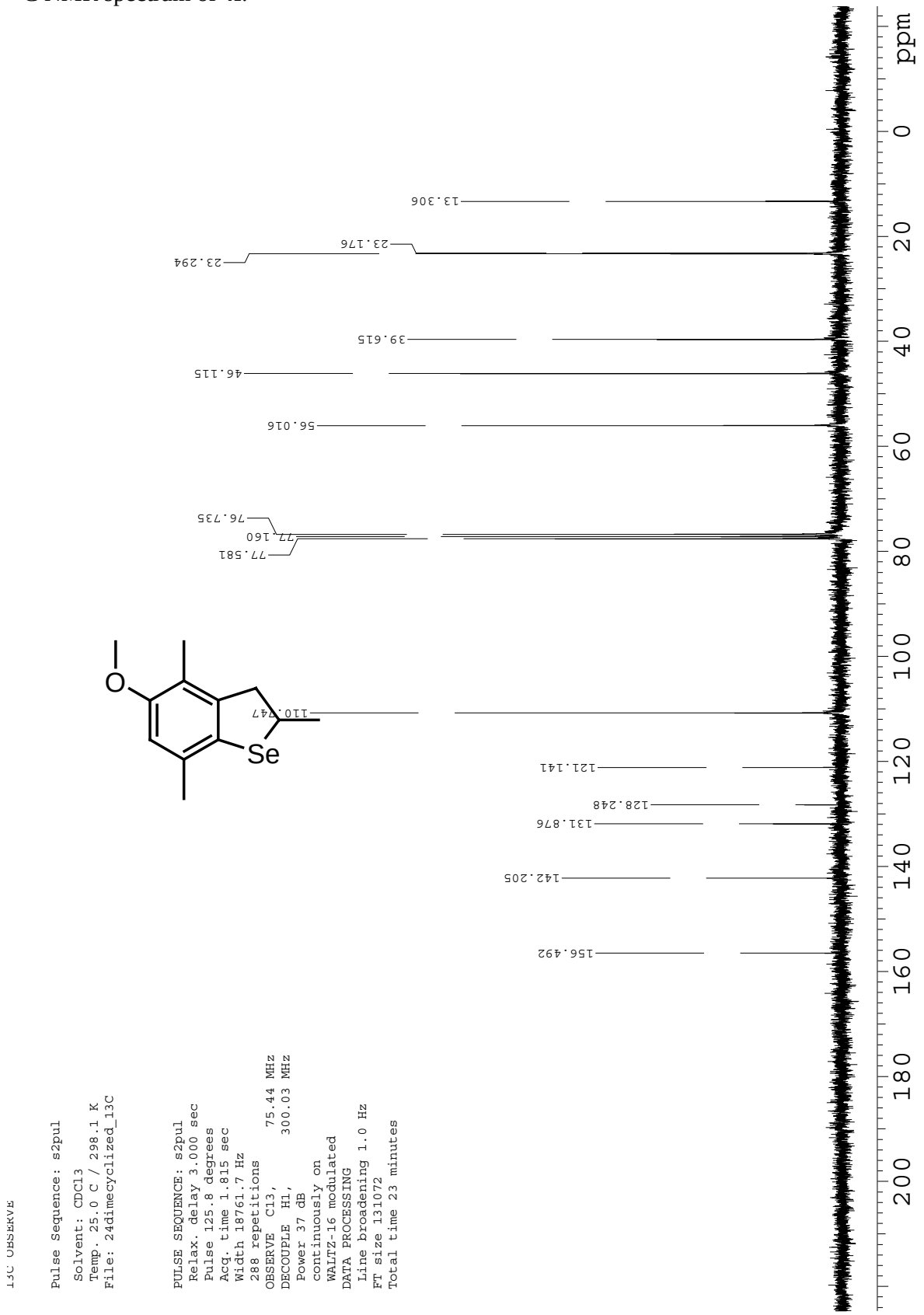

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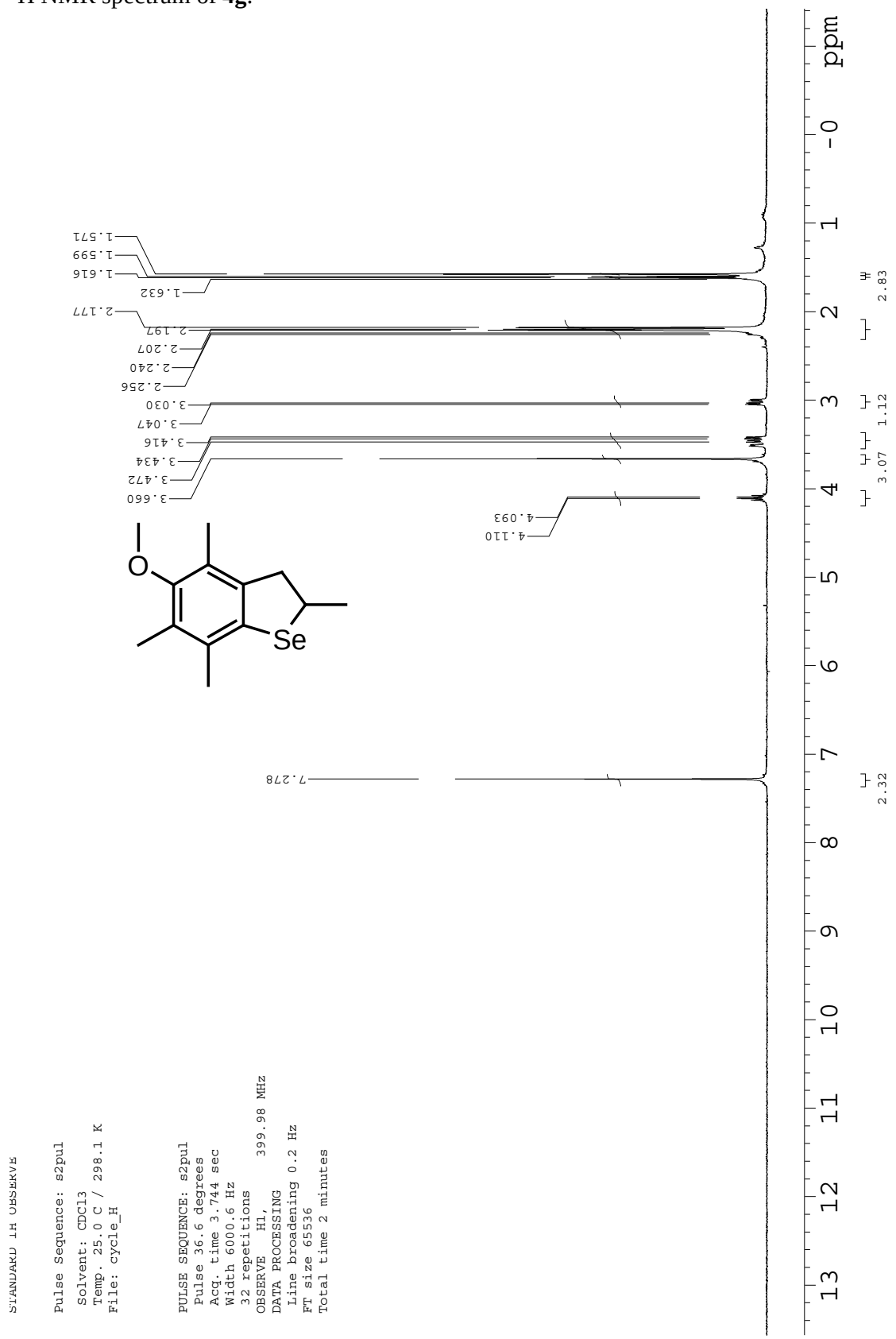

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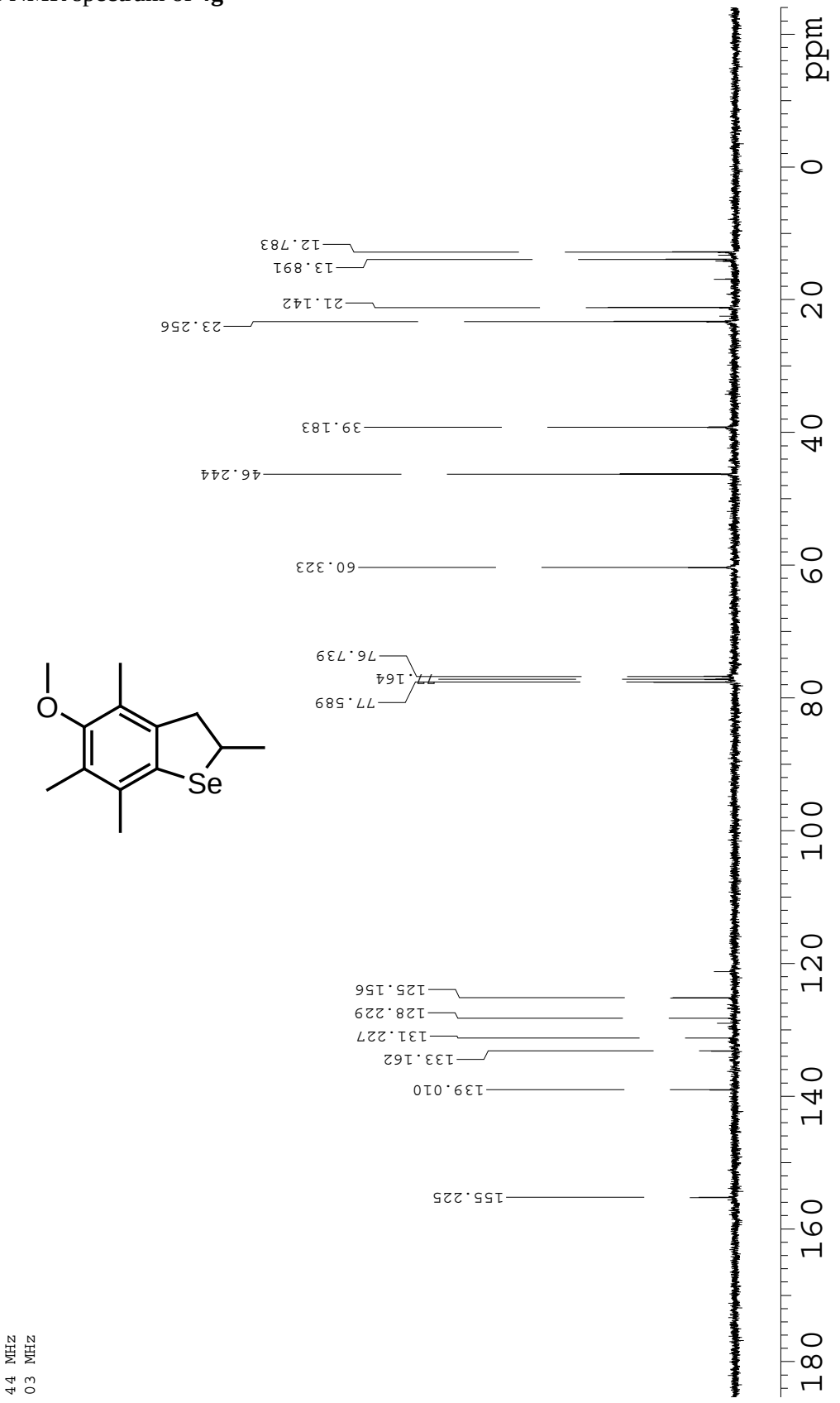

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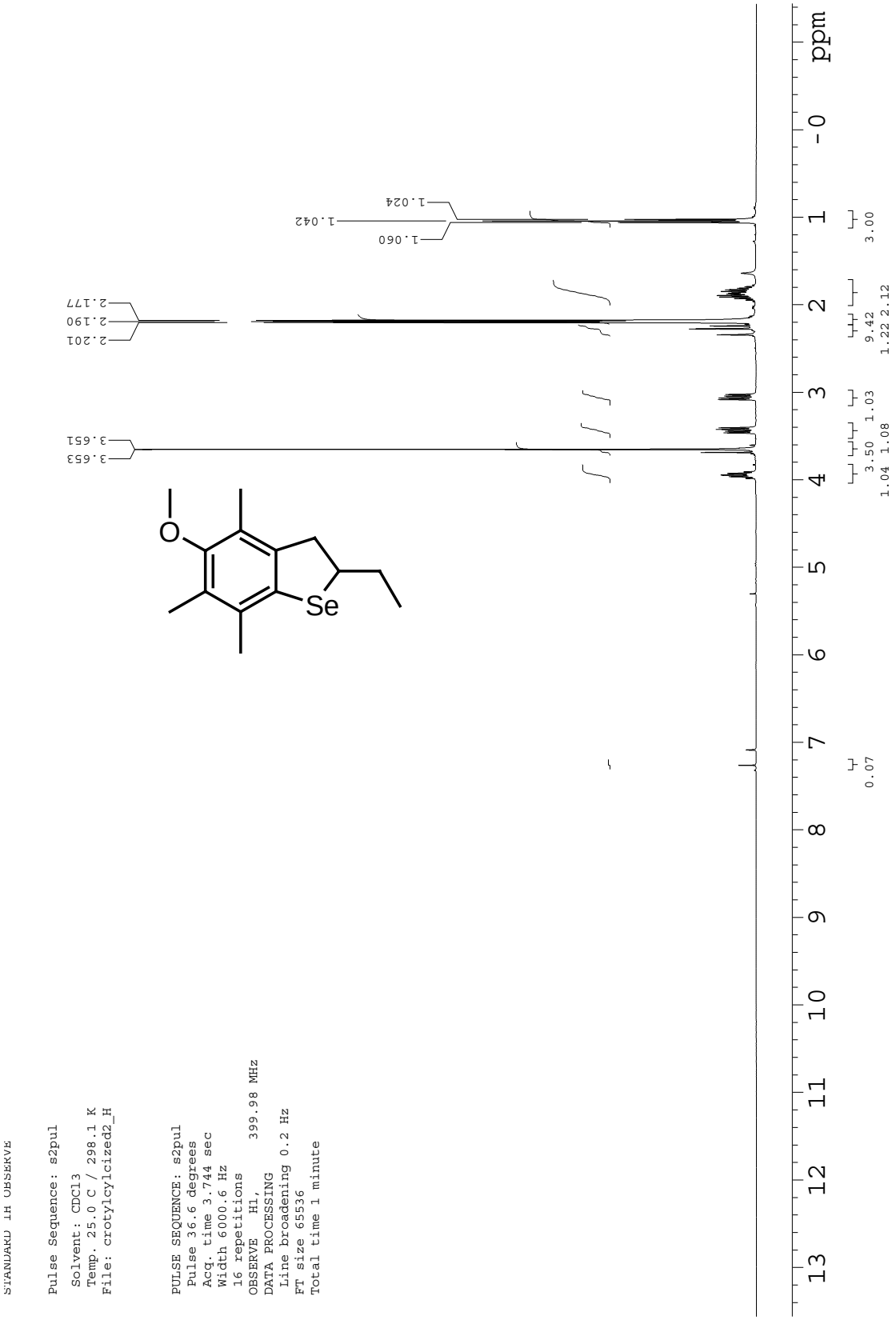
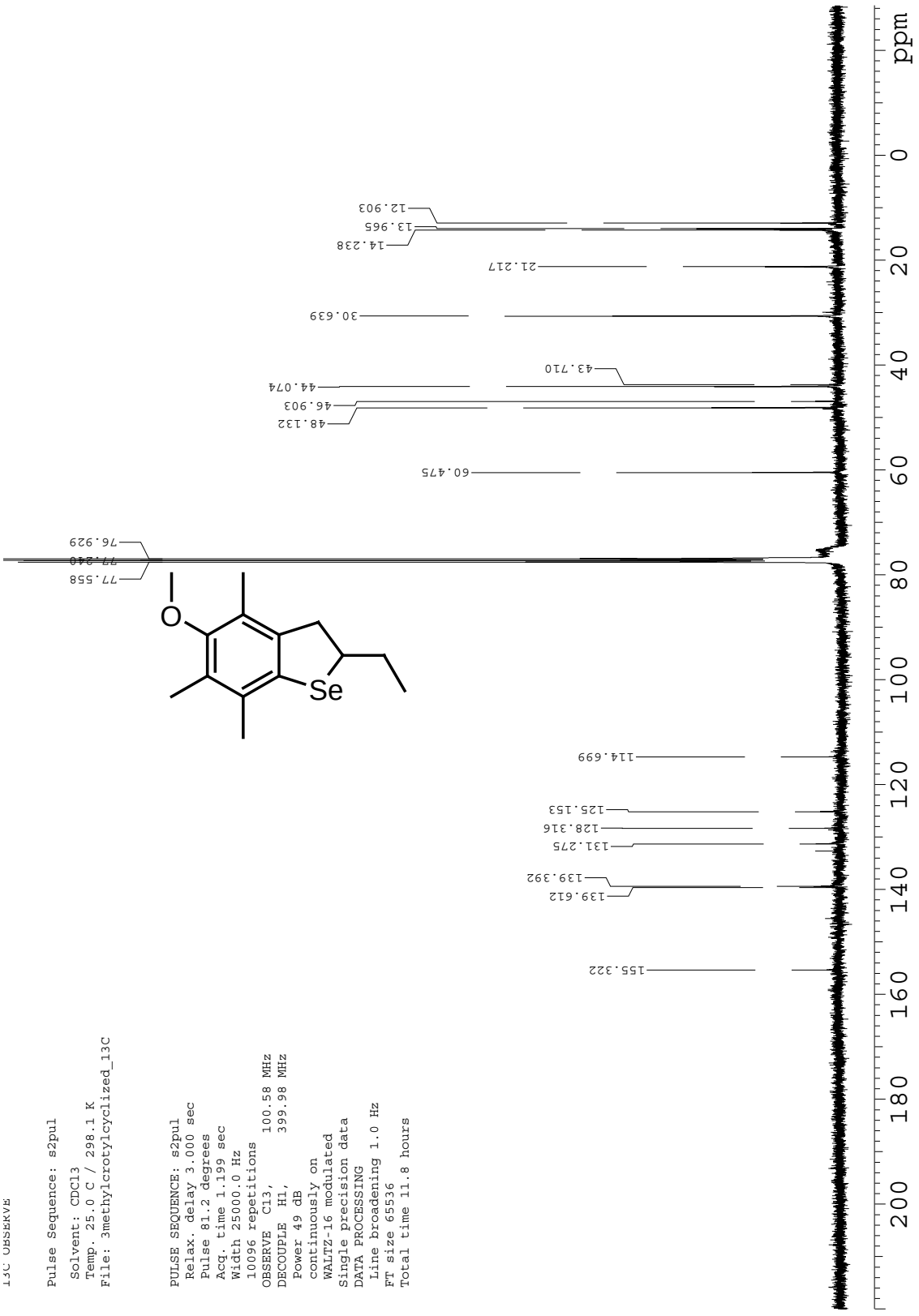


^{13}C NMR spectrum of 2-ethyl-5-methoxy-4,6,7-trimethyl-2,3-dihydrobenzo[*b*]selenophene.



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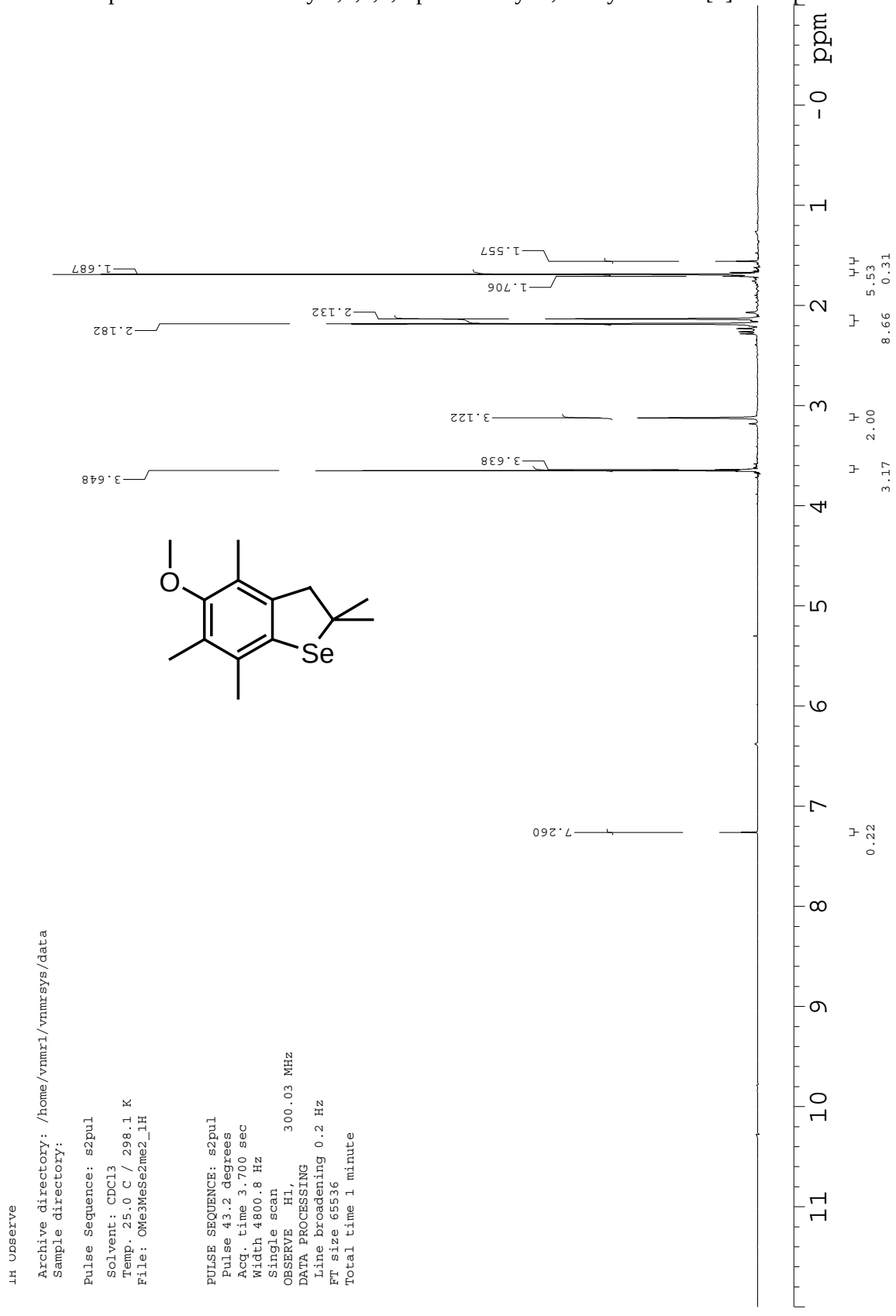
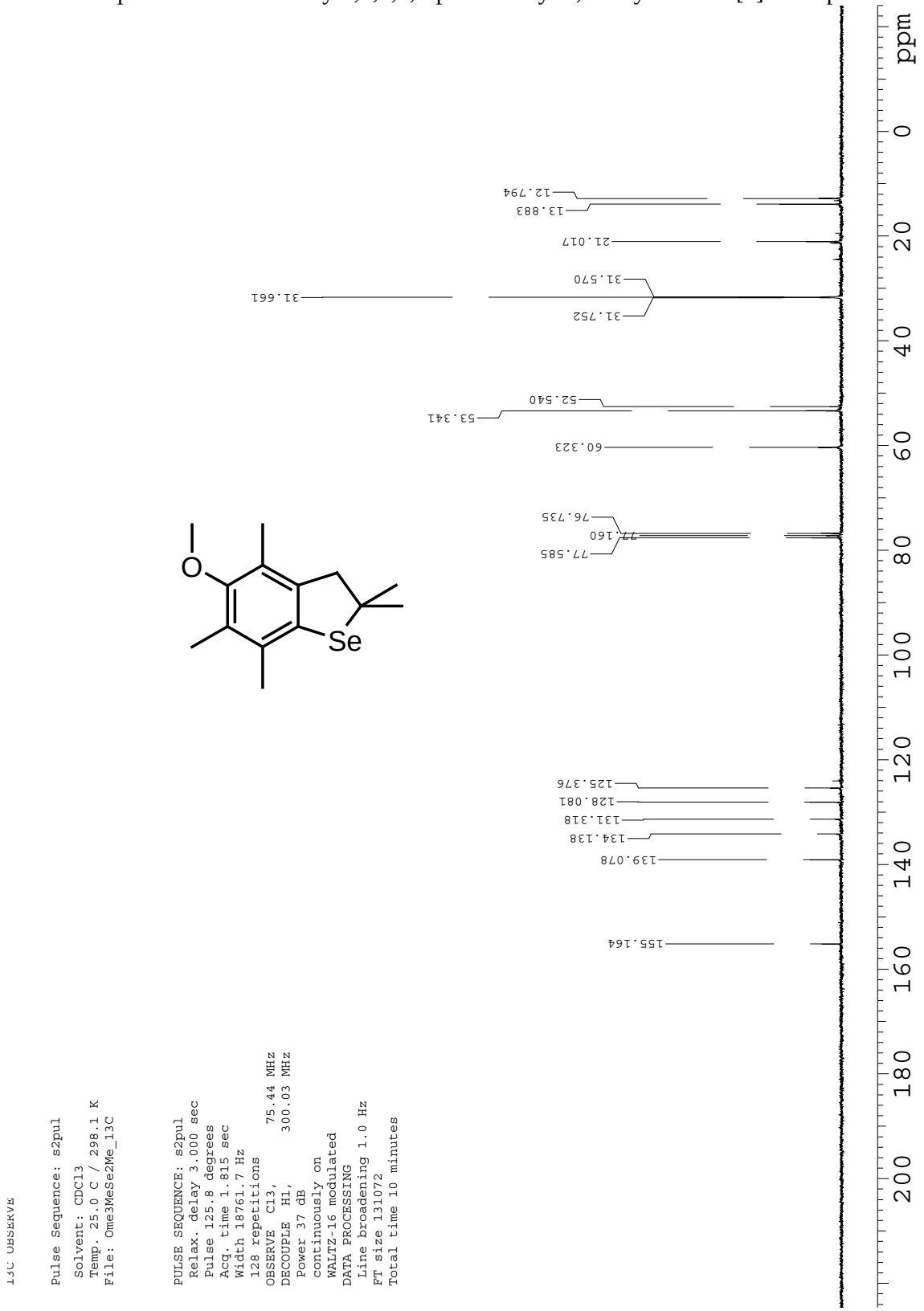


^{13}C NMR spectrum of 5-methoxy-2,2,4,6,7-pentamethyl-2,3-dihydrobenzo[*b*]selenophene



13C Observe

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Temp. 25.0 C / 298.1 K
File: Ome3MeSe2Me_13C

PULSE SEQUENCE: s2pul
Relax. delay 3.000 sec
Pulse 125.8 degrees
Acq. time 1.815 sec
Width 18761.7 Hz
128 repetitions
OBSERVE C13, 75.44 MHz
DECOUPLE H1, 300.03 MHz
Power 37 dB
continuously on
WALTZ-16 modulated
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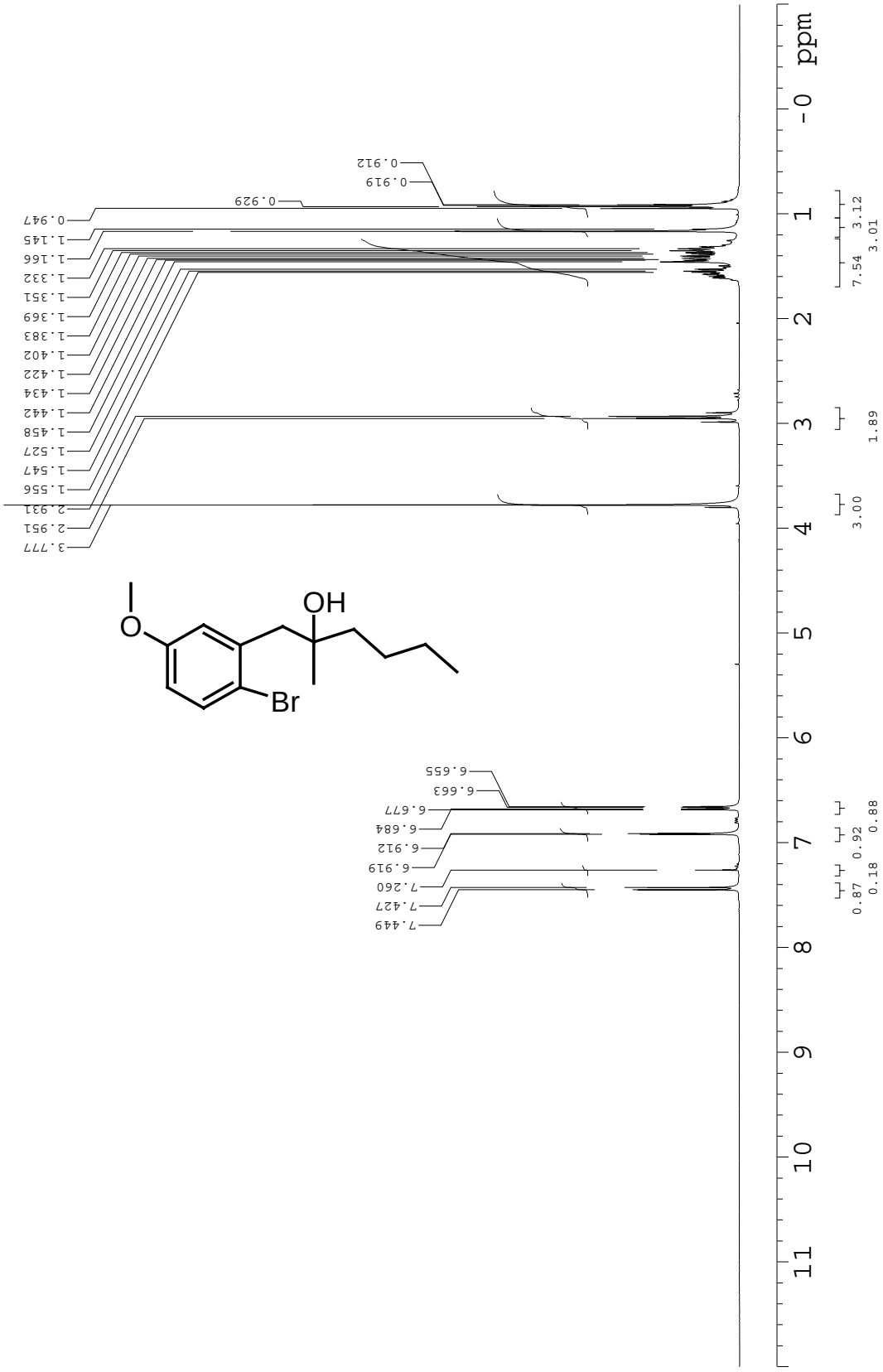
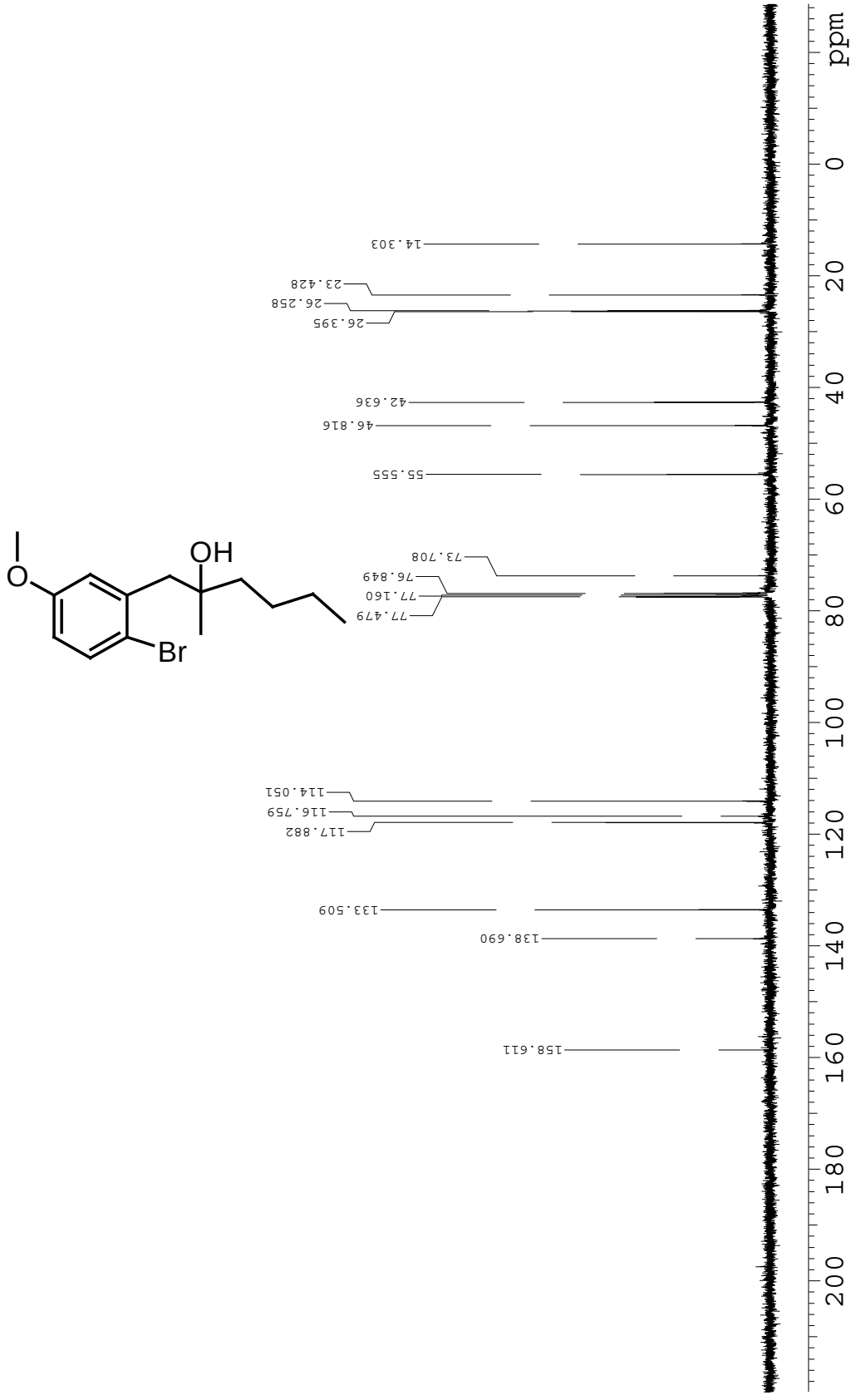
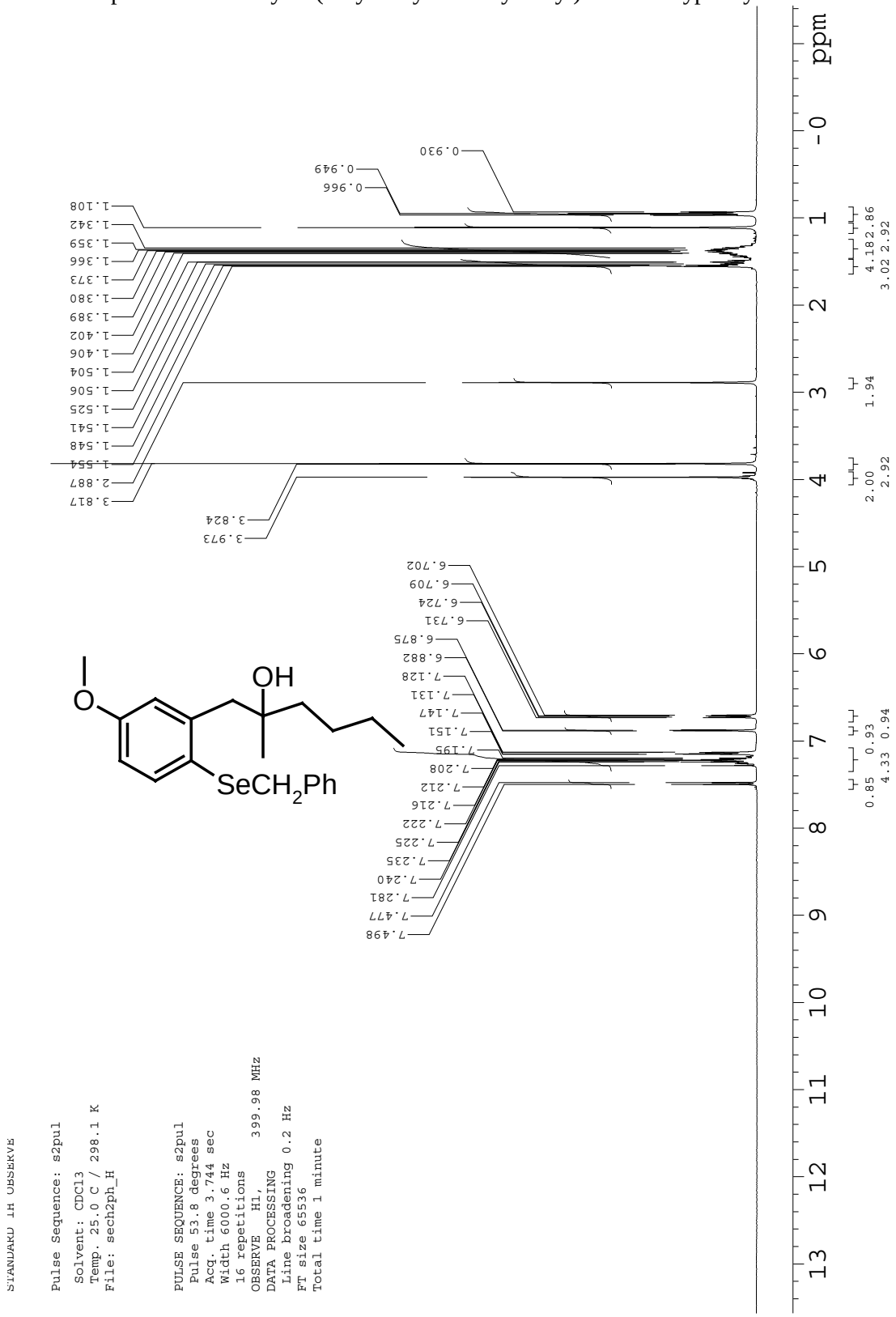
^{1}H NMR spectrum of 1-(2-bromo-5-methoxyphenyl)-2-methyl-2-hexanol.



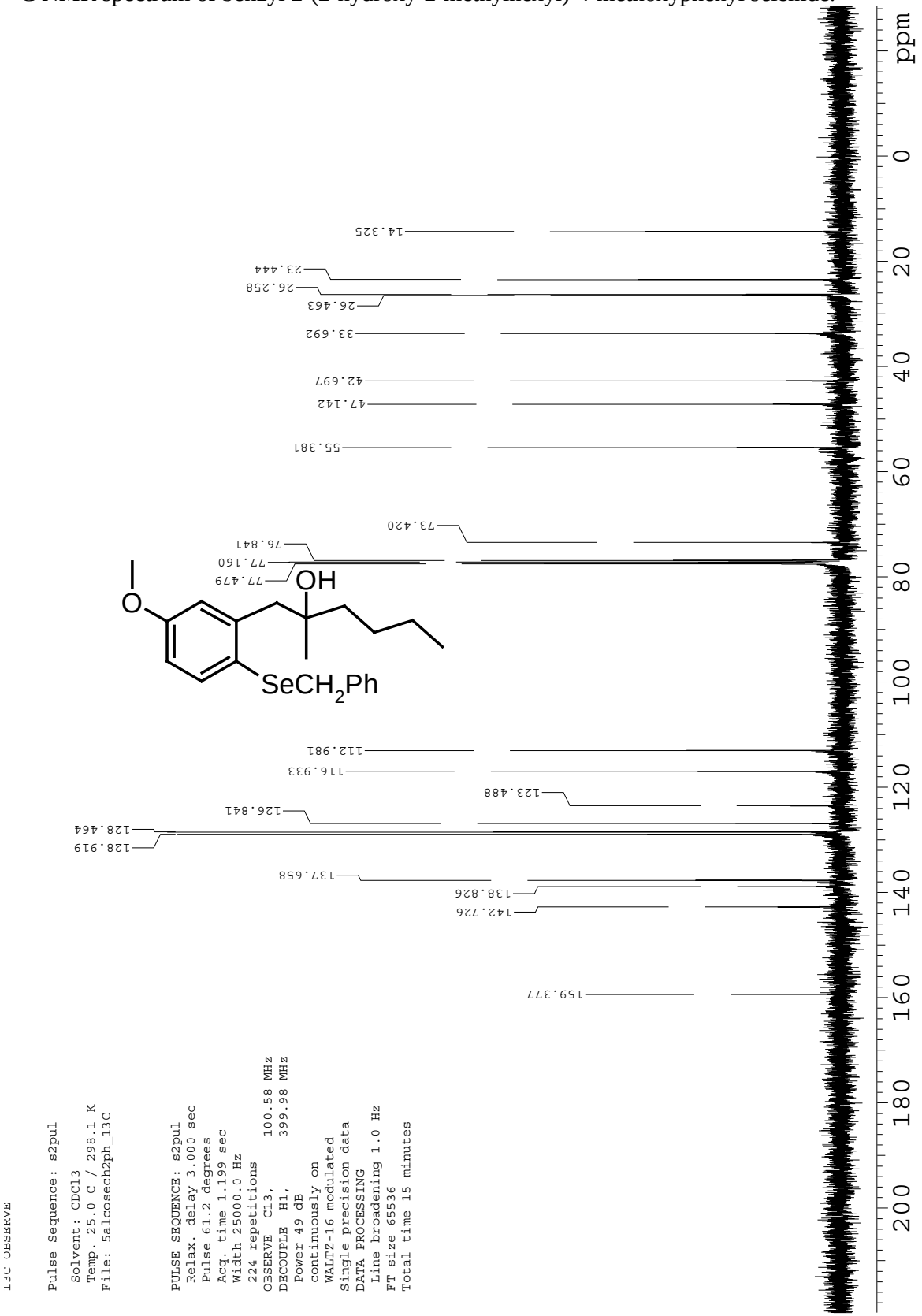
^{13}C NMR spectrum of 1-(2-bromo-5-methoxyphenyl)-2-methyl-2-hexanol.



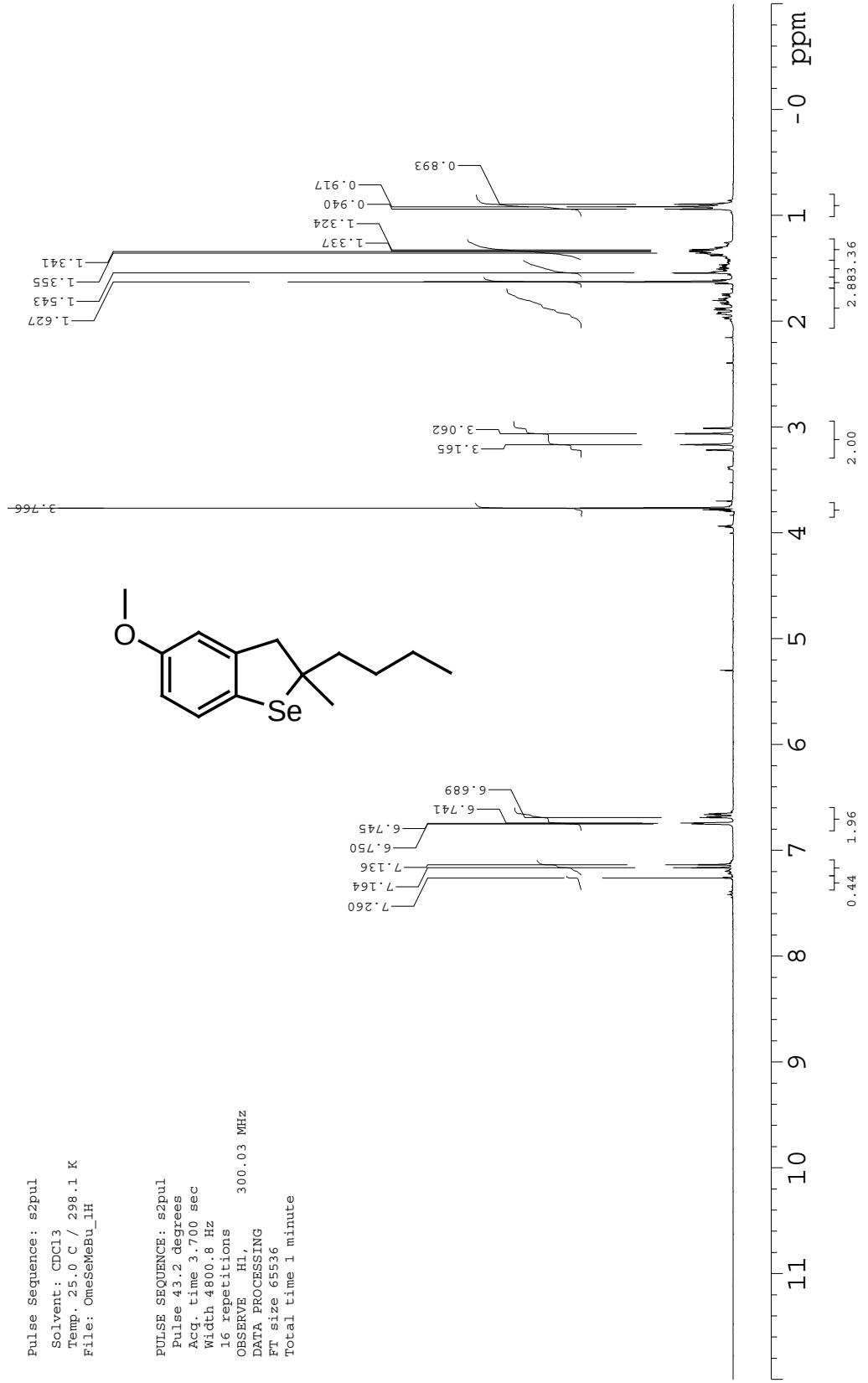
^{1}H NMR spectrum of benzyl 2-(2-hydroxy-2-methylhexyl)-4-methoxyphenyl selenide.



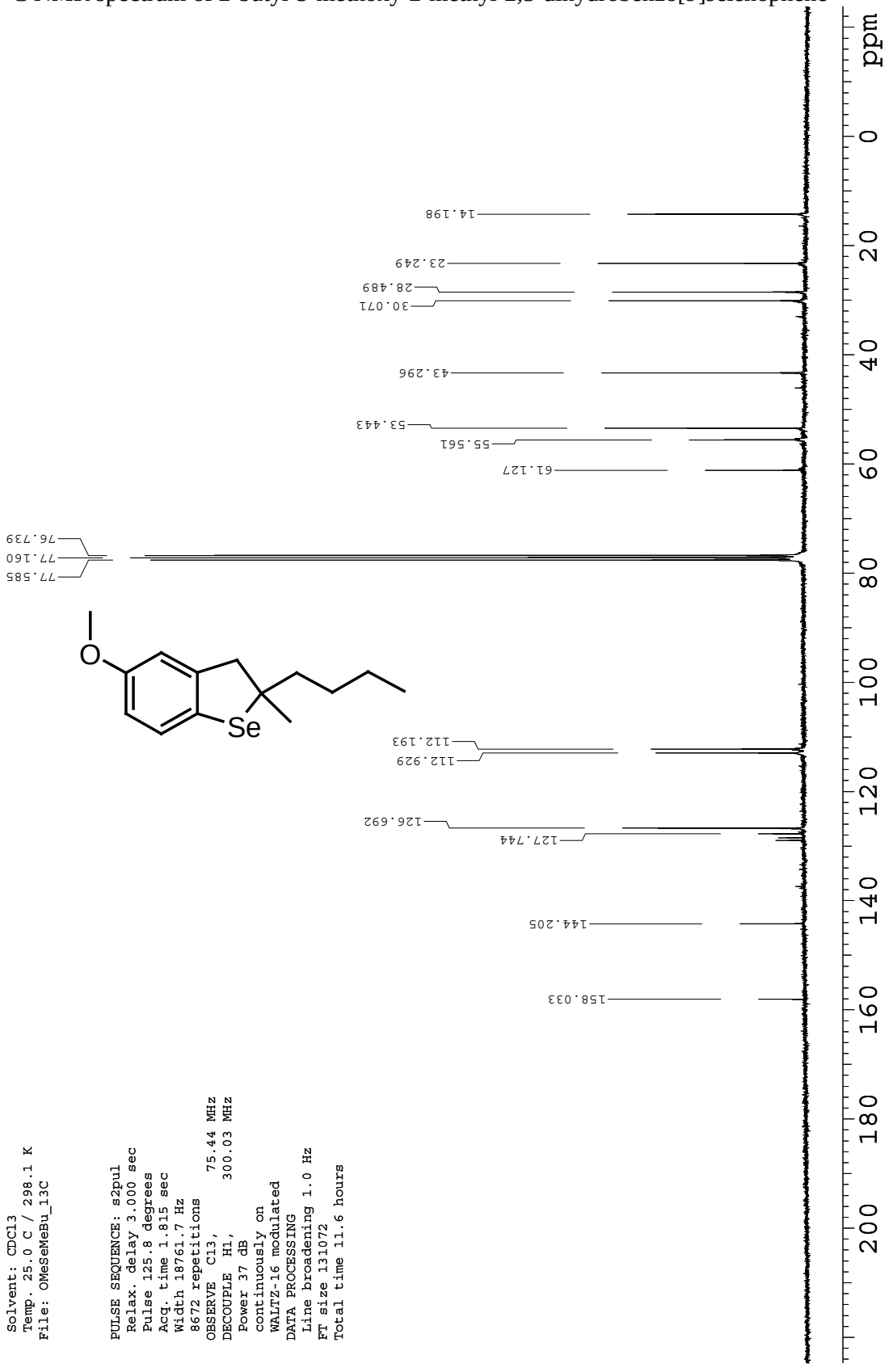
^{13}C NMR spectrum of benzyl 2-(2-hydroxy-2-methylhexyl)-4-methoxyphenyl selenide.



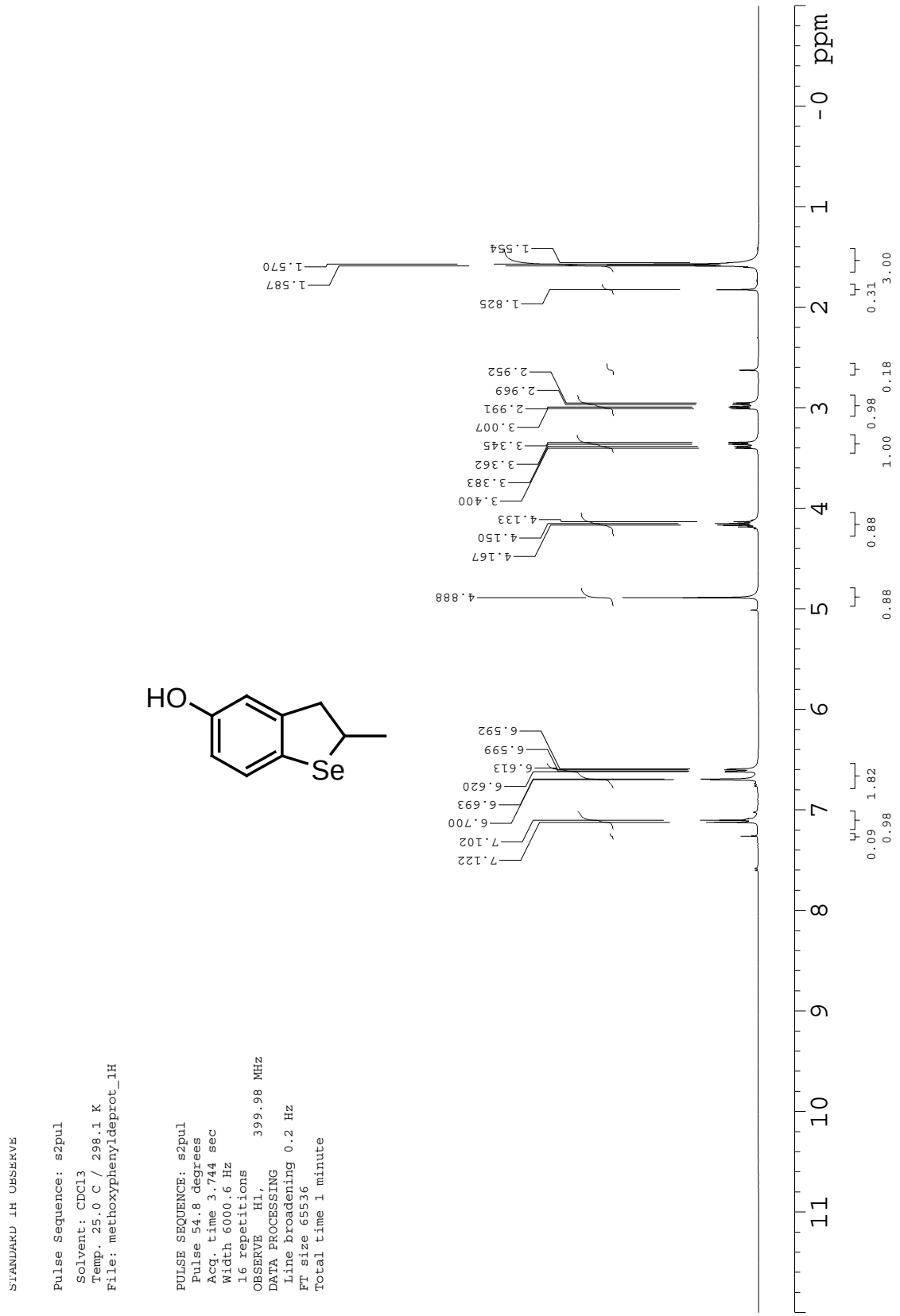
^{1}H NMR spectrum of 2-butyl-5-methoxy-2-methyl-2,3-dihydrobenzo[*b*]selenophene



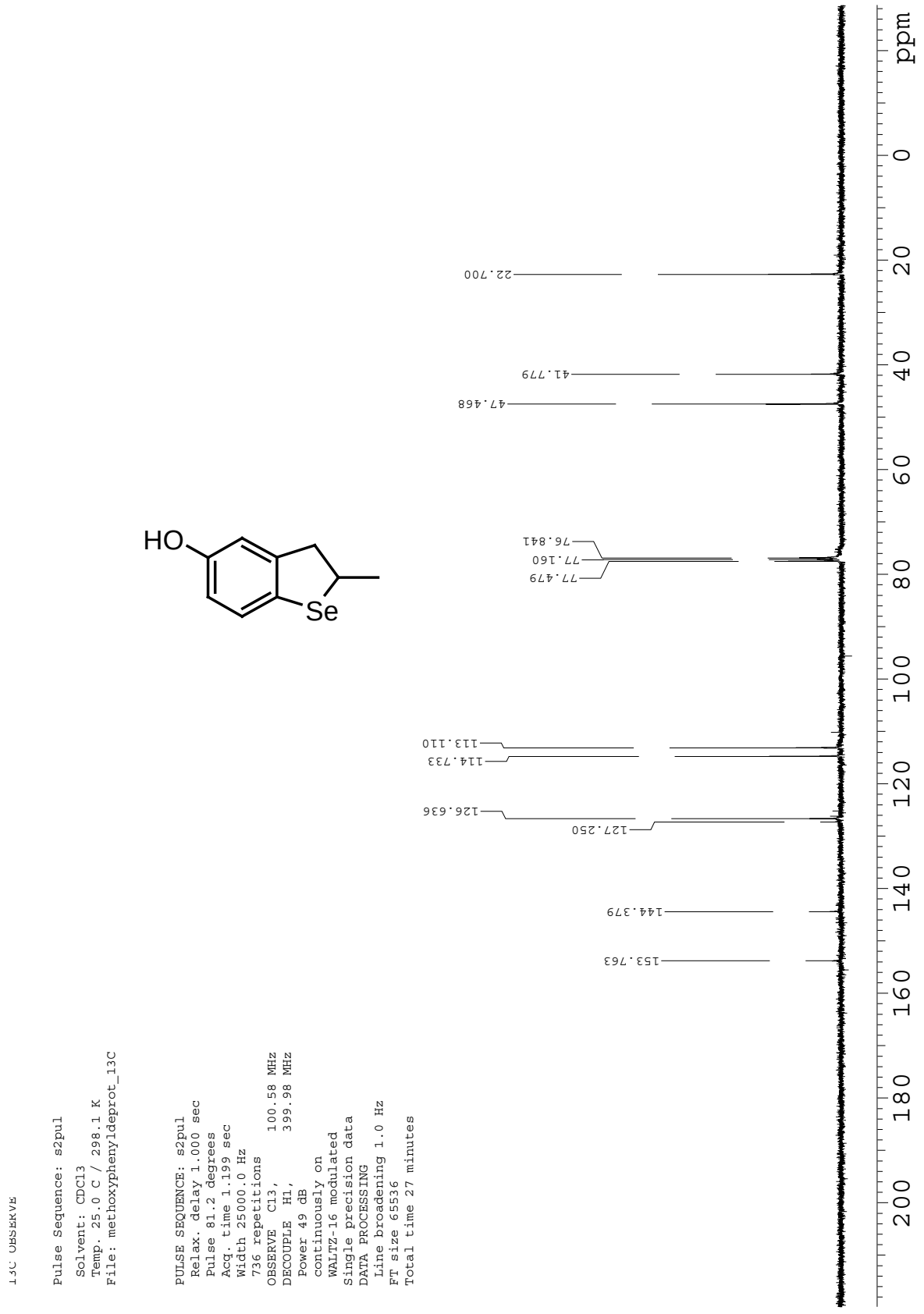
^{13}C NMR spectrum of 2-butyl-5-methoxy-2-methyl-2,3-dihydrobenzo[*b*]selenophene



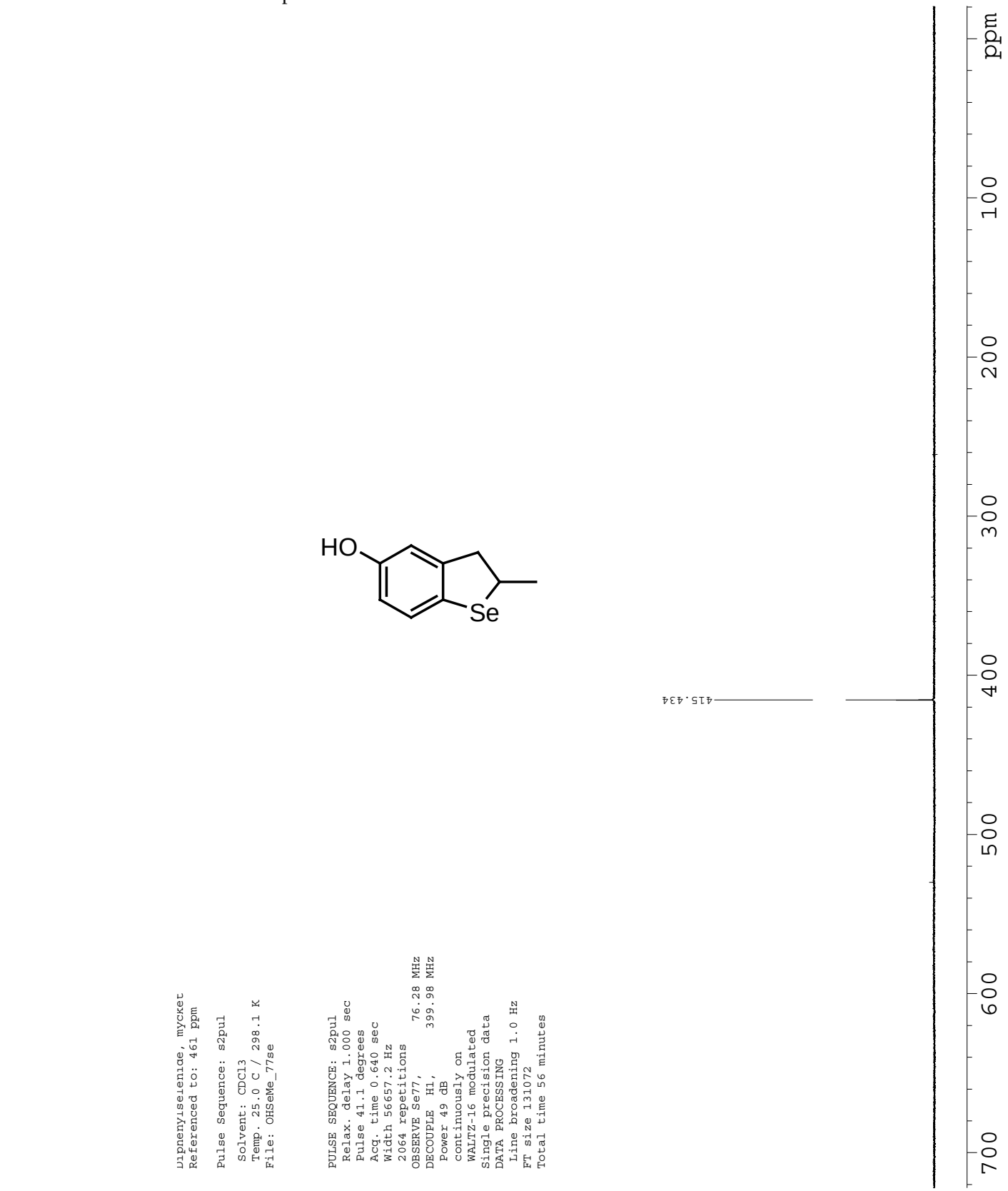
^{1}H NMR spectrum of **5a**.



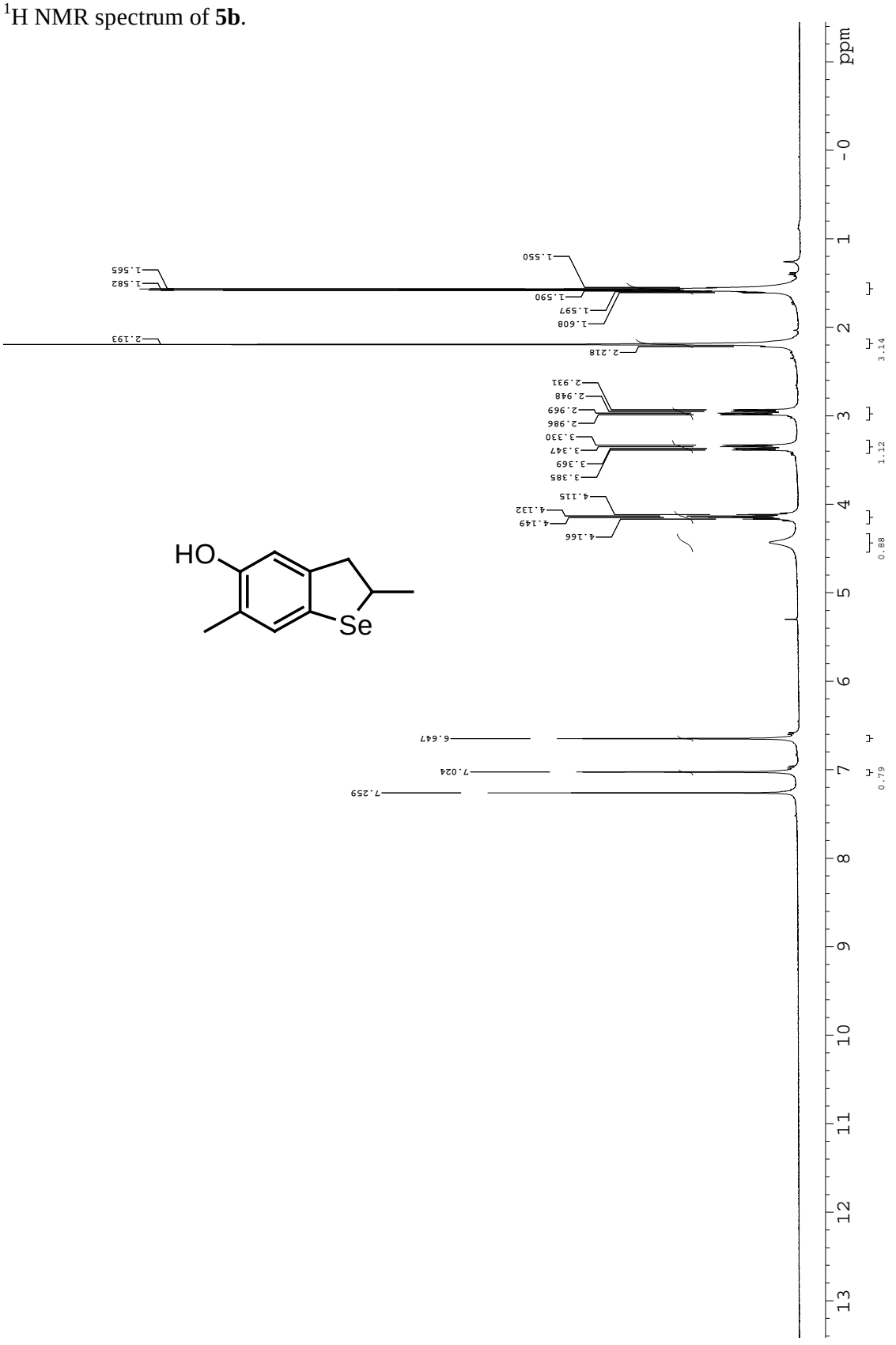
^{13}C NMR spectrum of **5a**.



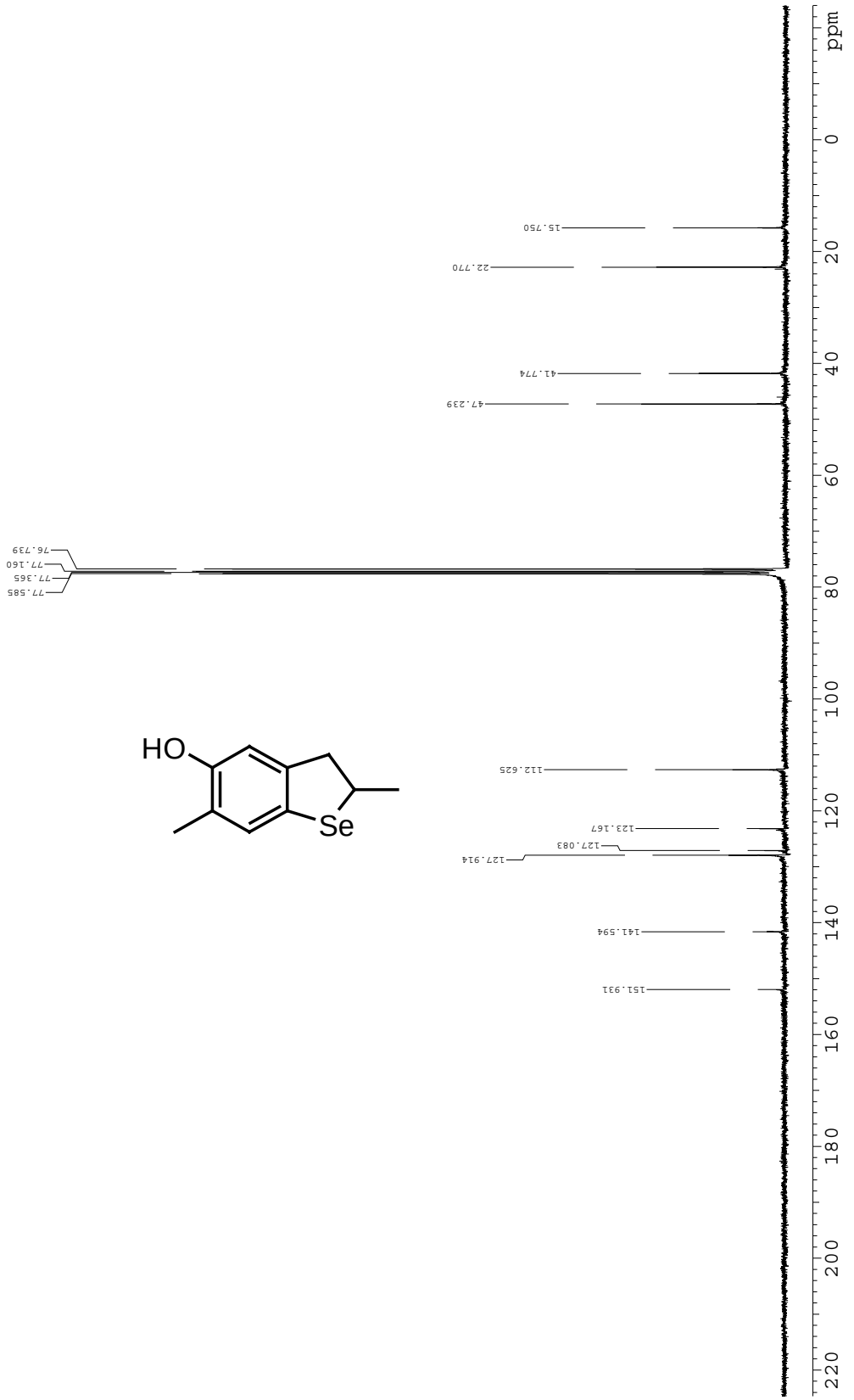
^{77}Se NMR spectrum of **5a**.



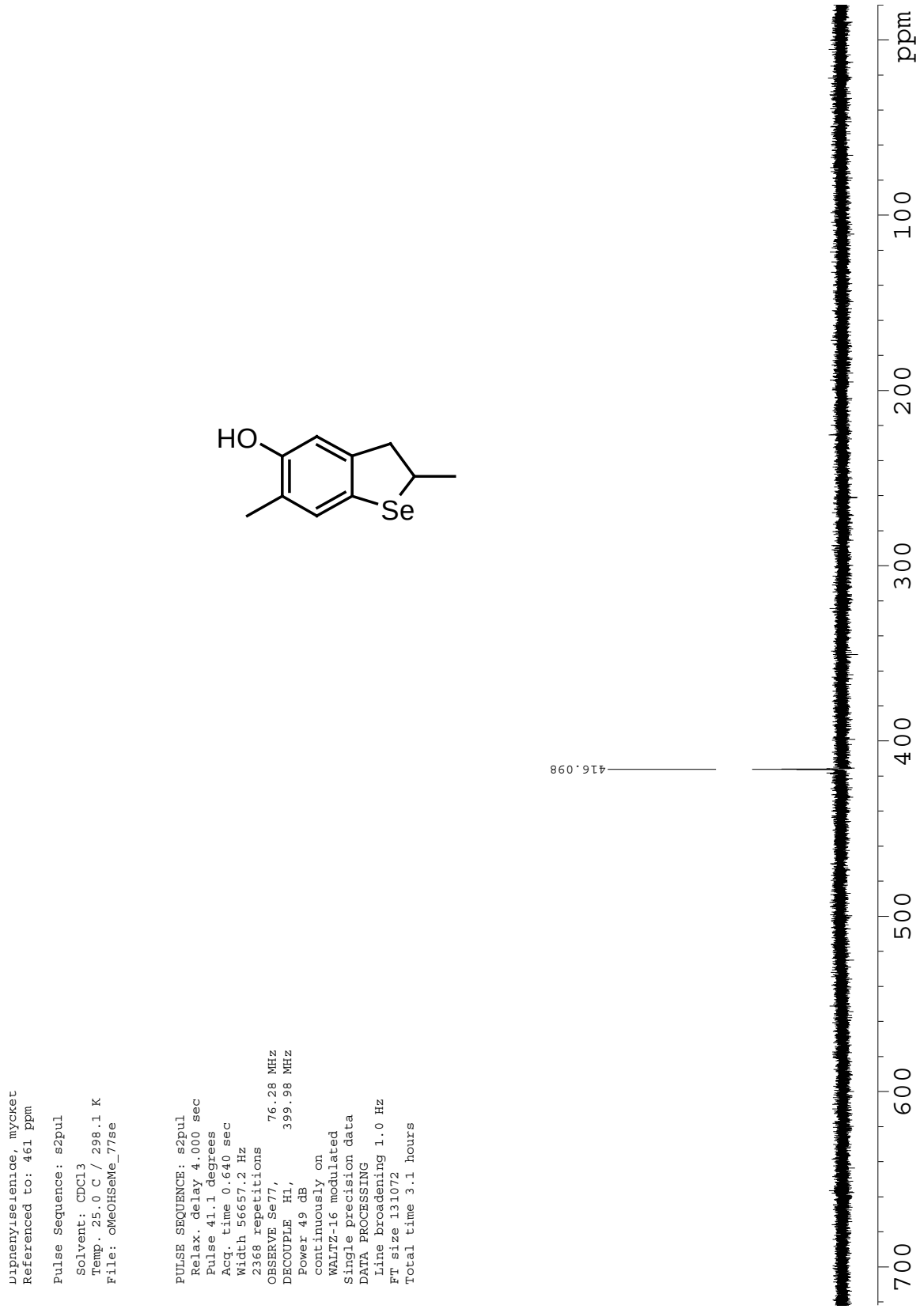
^{1}H NMR spectrum of **5b**.



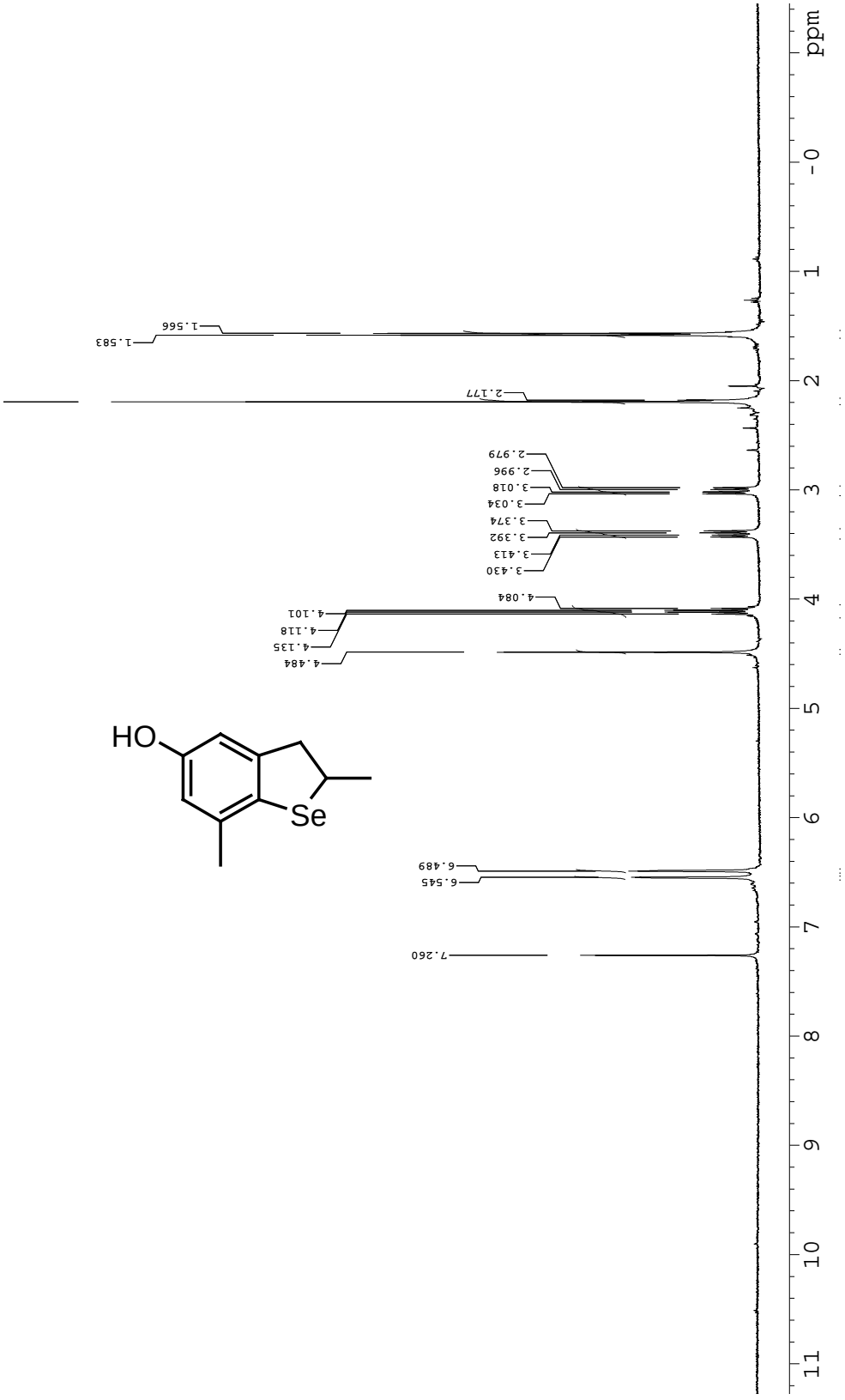
^{13}C NMR spectrum of **5b**.



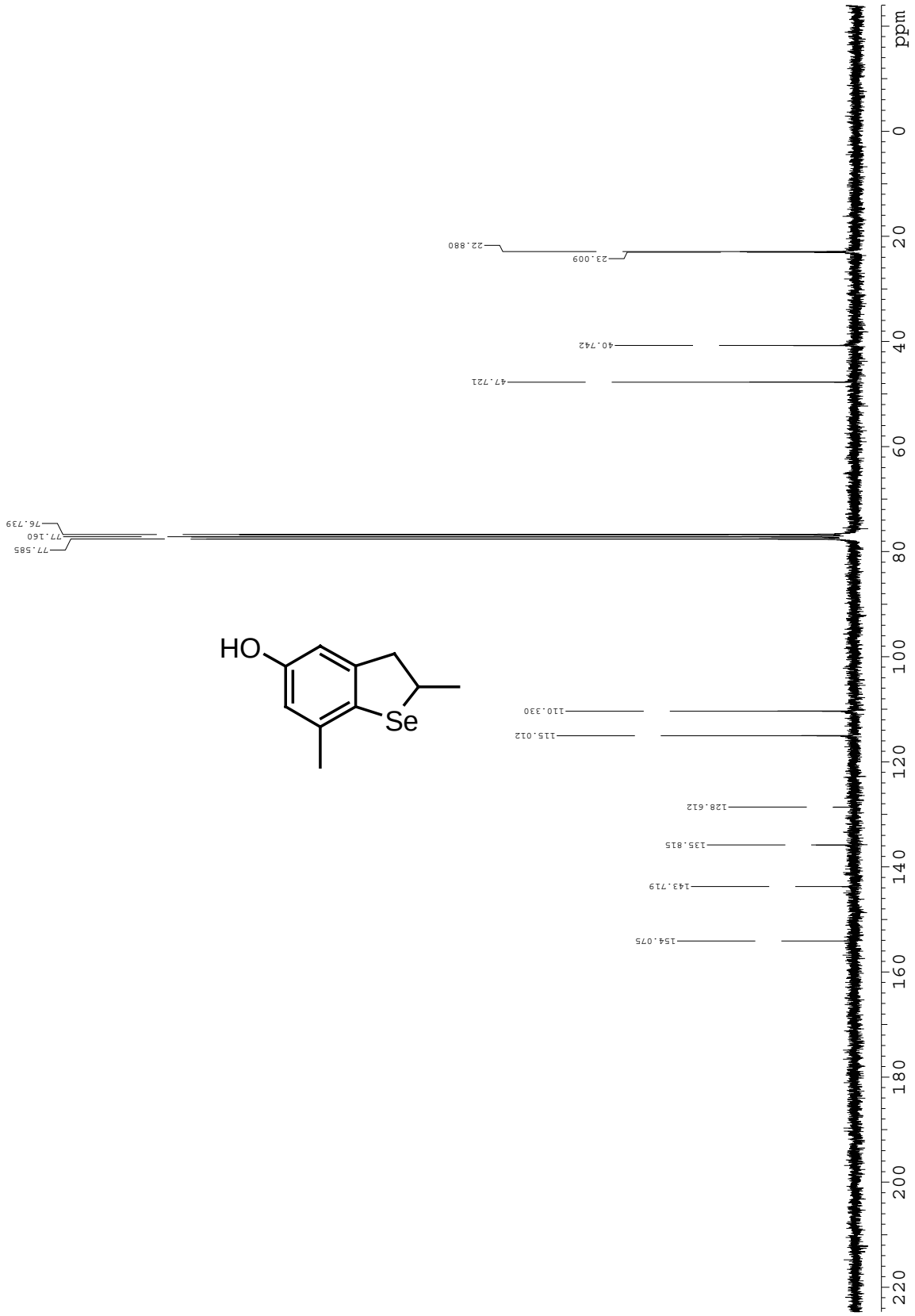
^{77}Se NMR spectrum of **5b**.



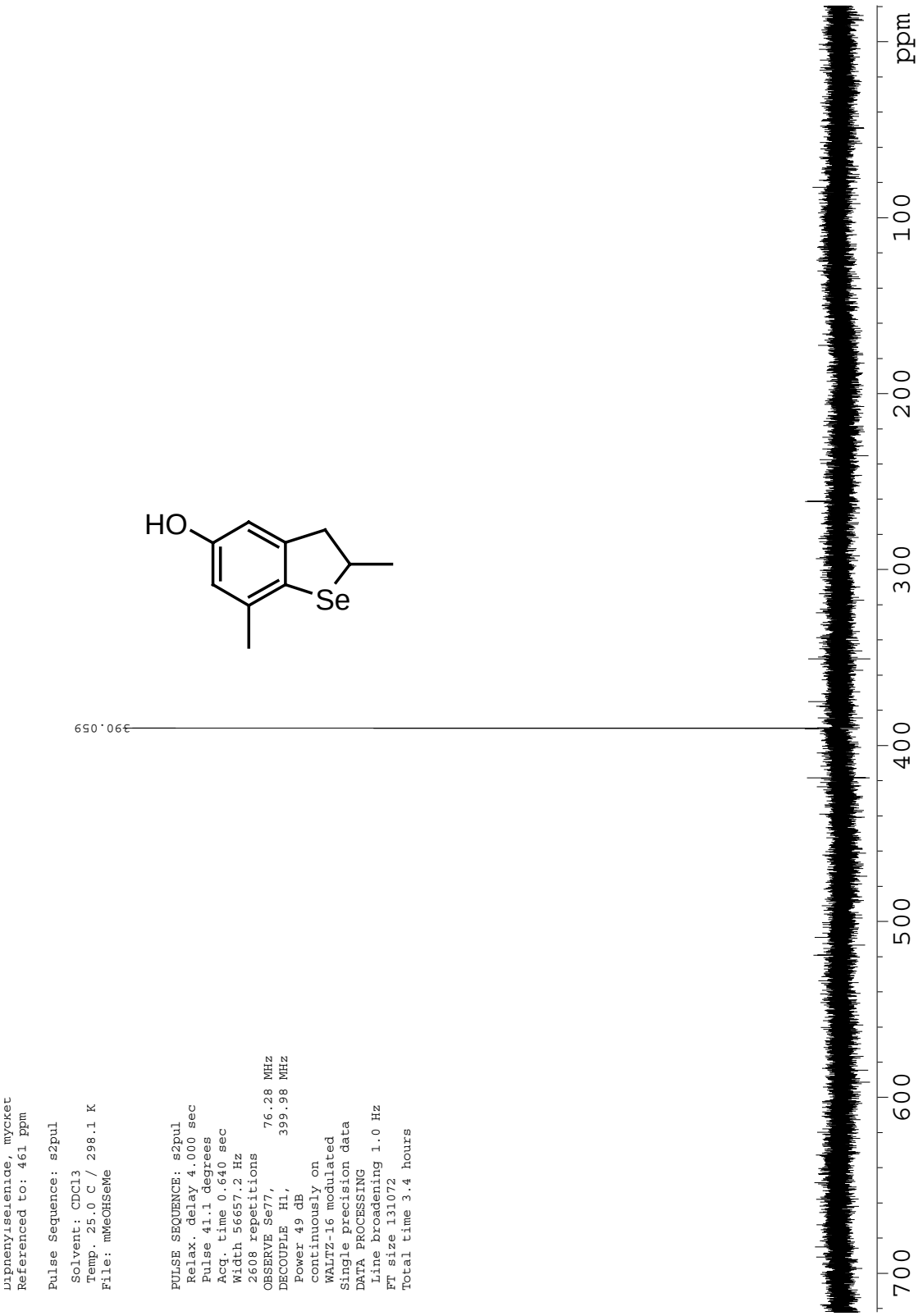
^{1}H NMR spectrum of **5c**.



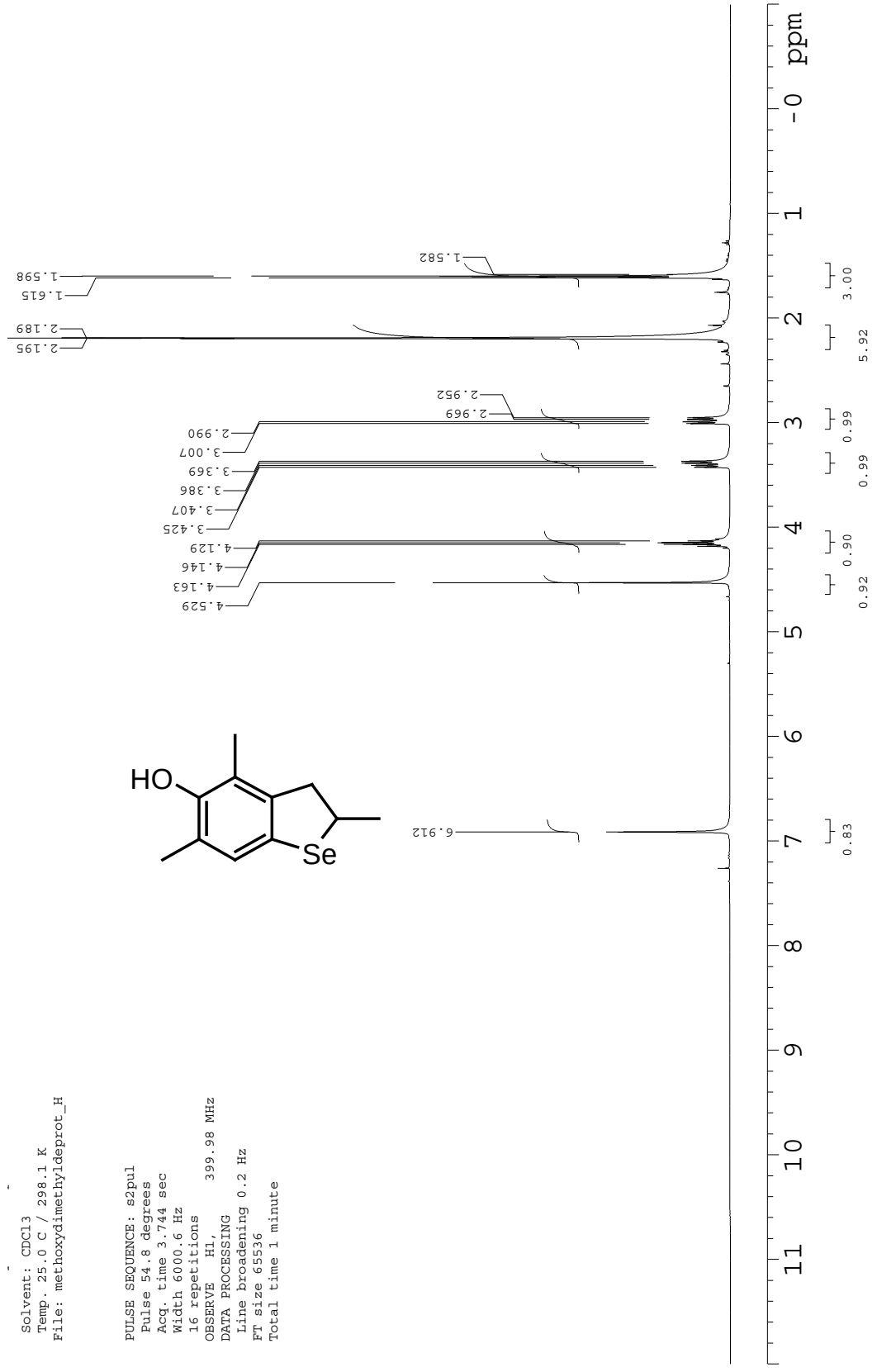
^{13}C NMR spectrum of **5c**.



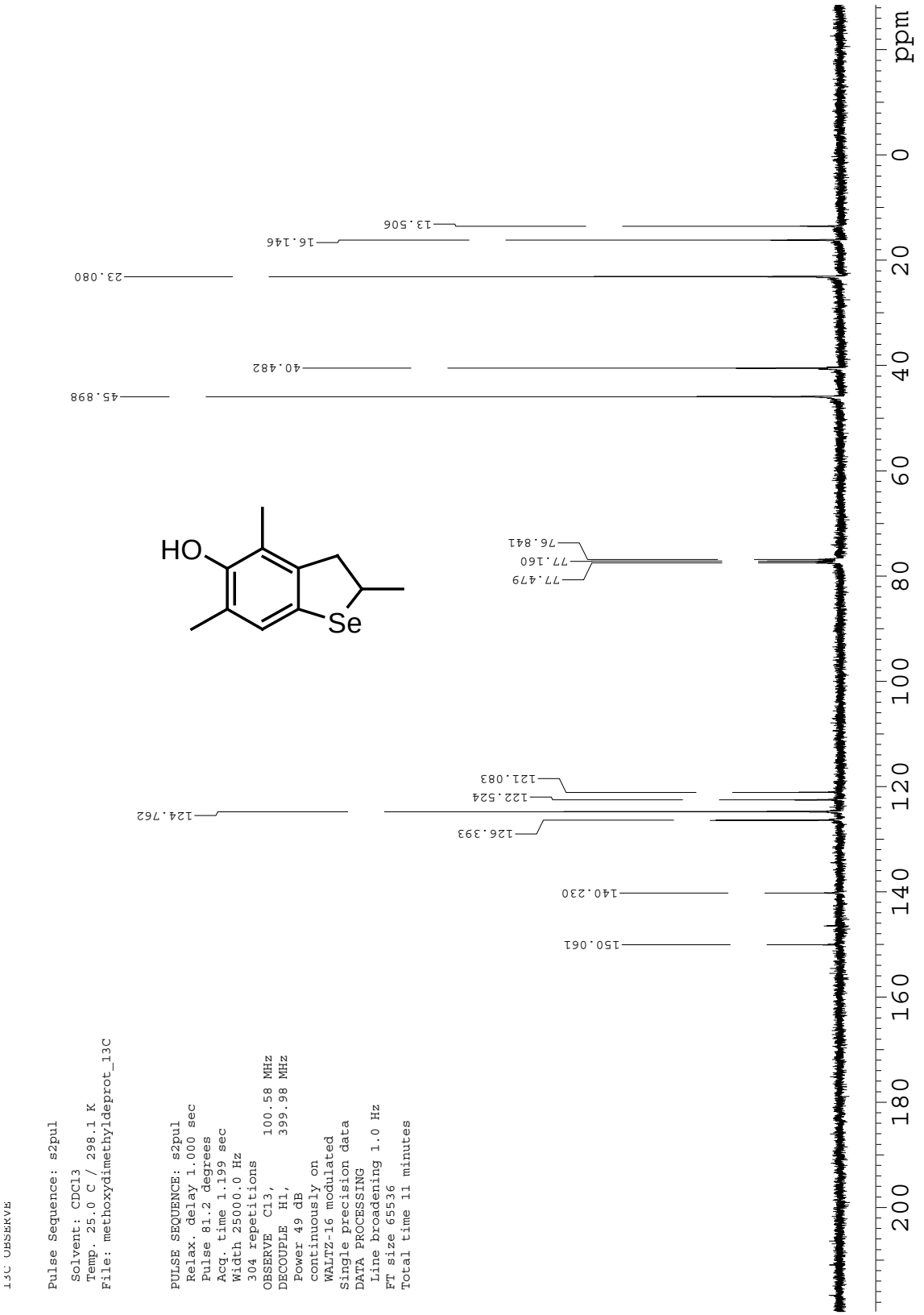
^{77}Se NMR spectrum of **5c**.



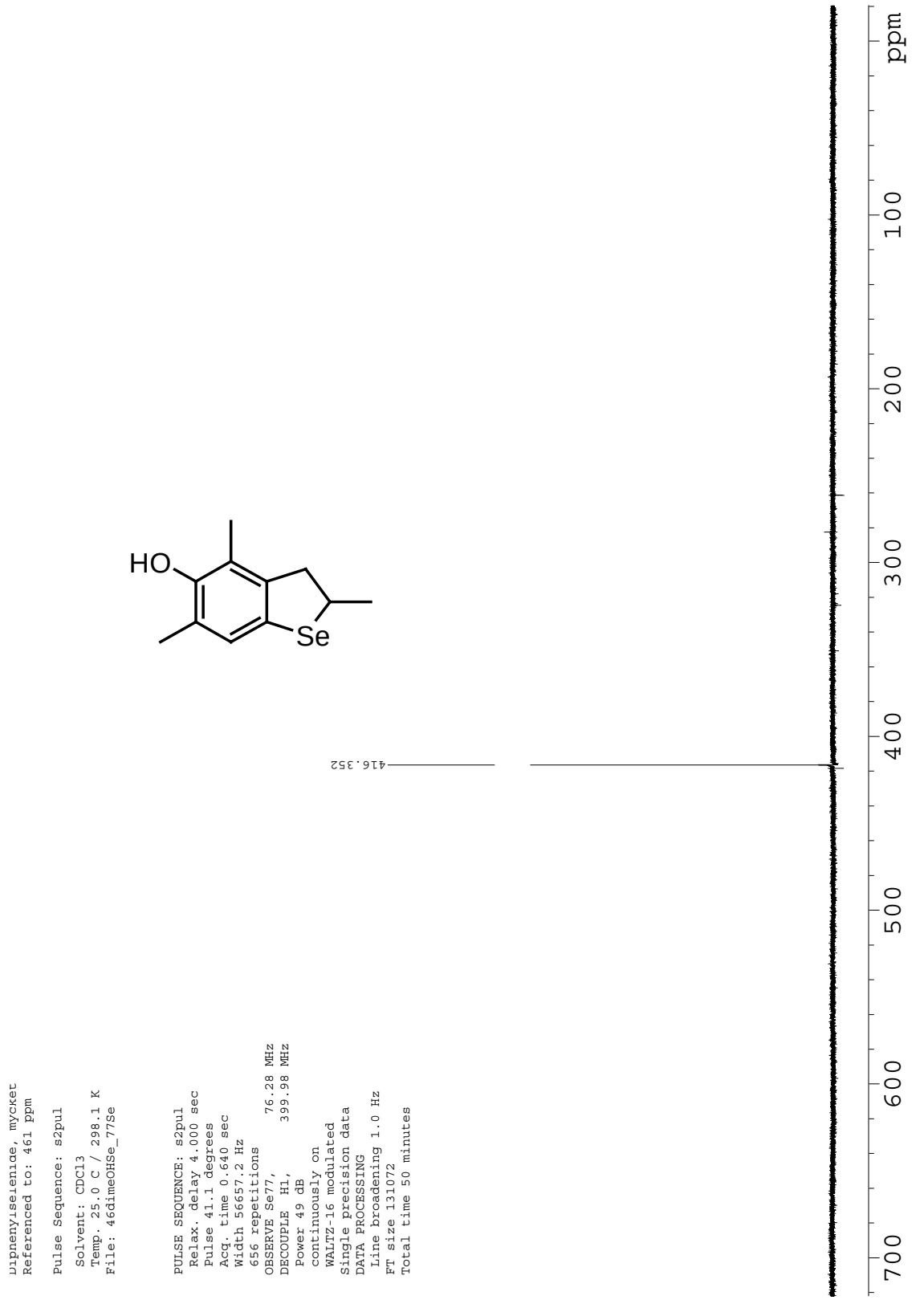
^{1}H NMR spectrum of **5d**.



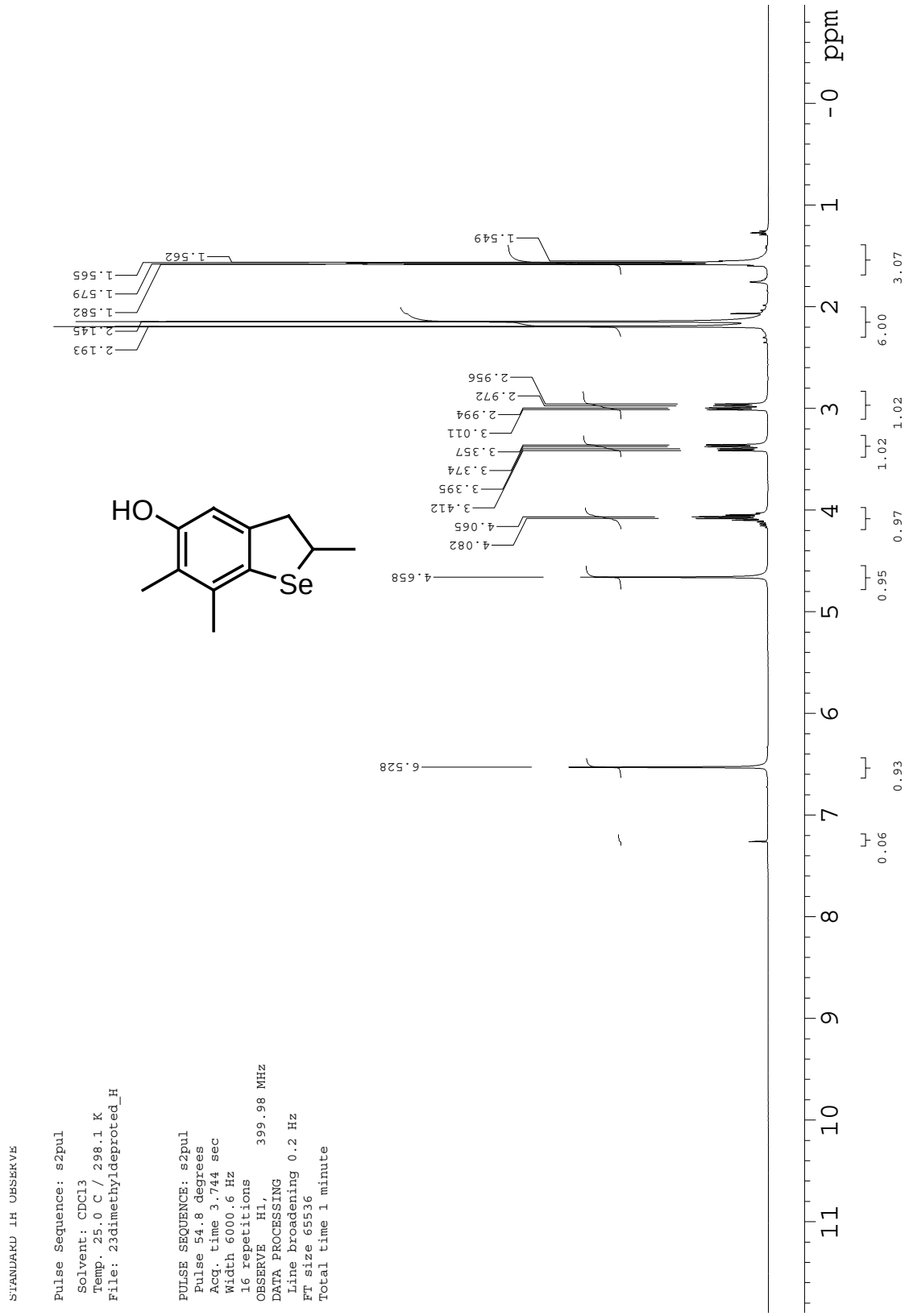
^{13}C NMR spectrum of **5d**.



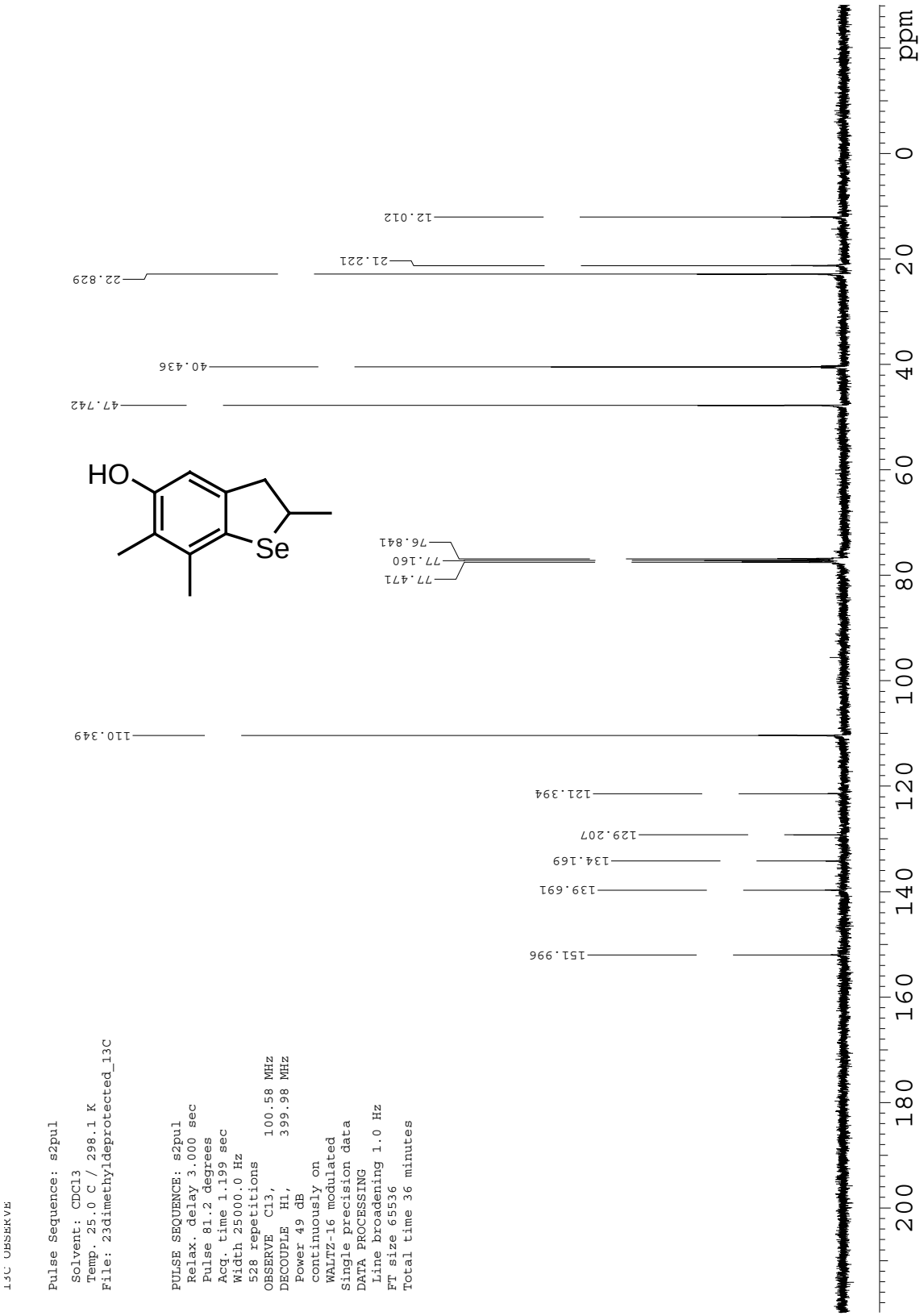
^{77}Se NMR spectrum of **5d**.



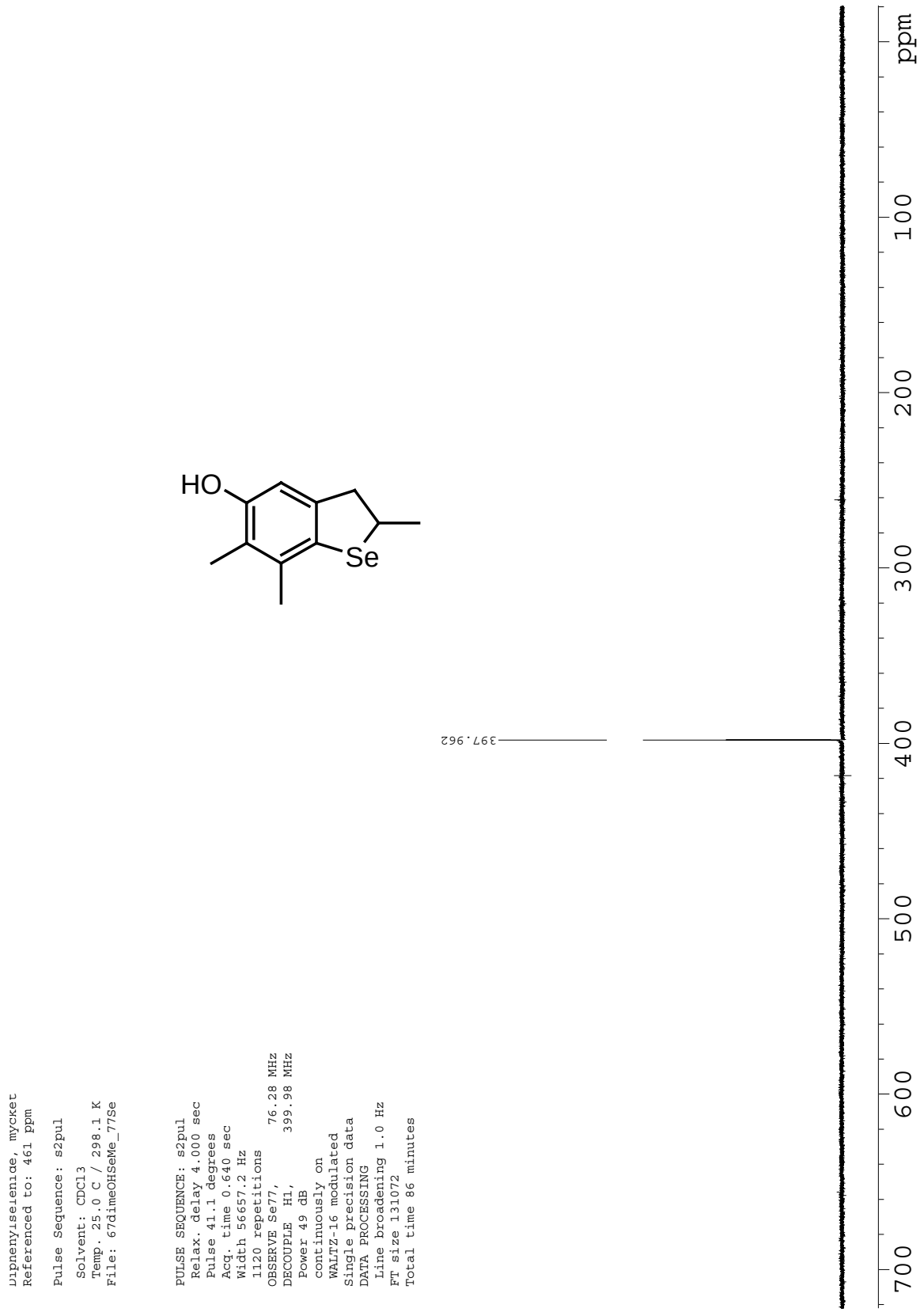
^{1}H NMR spectrum of **5e**.



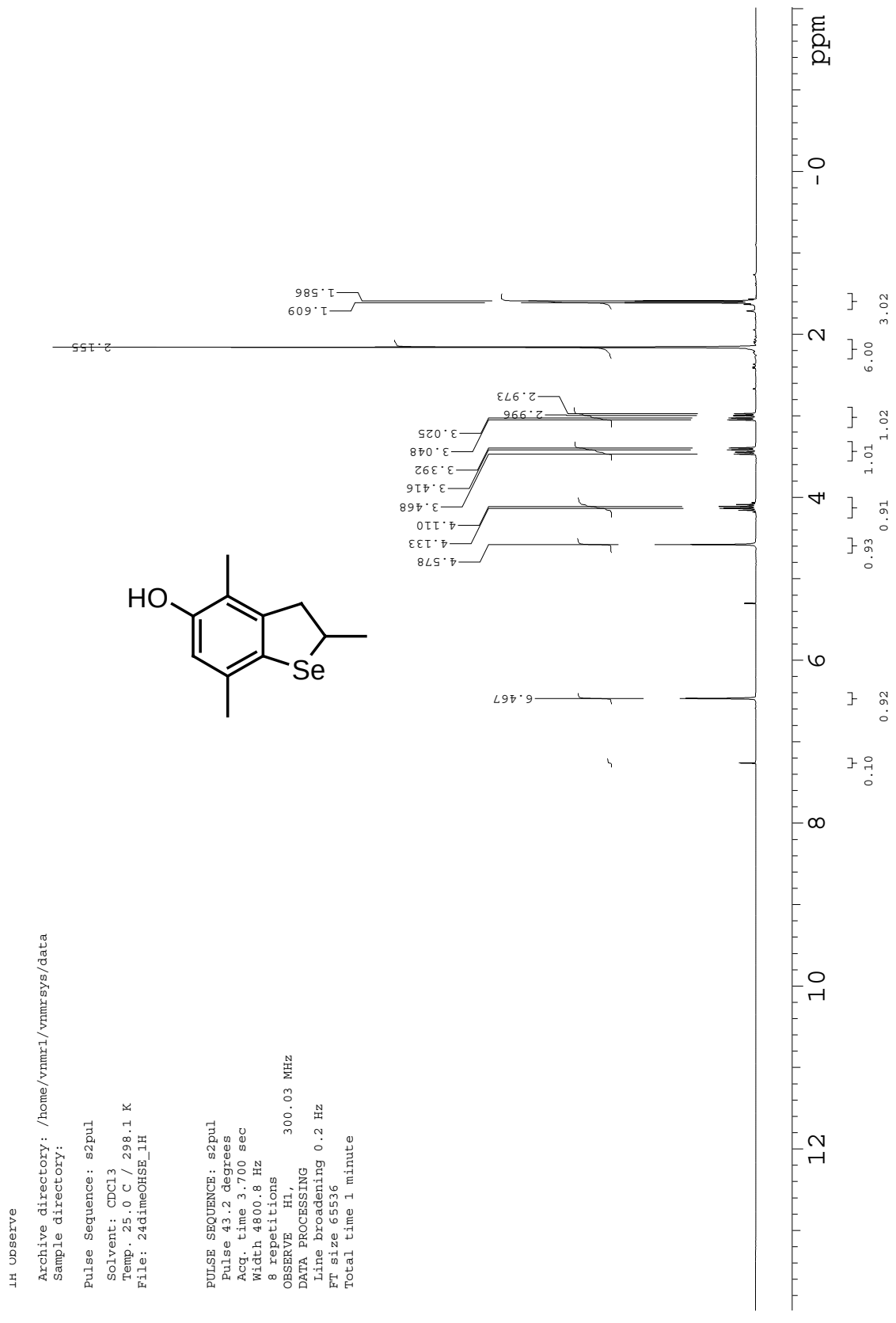
^{13}C NMR spectrum of **5e**.



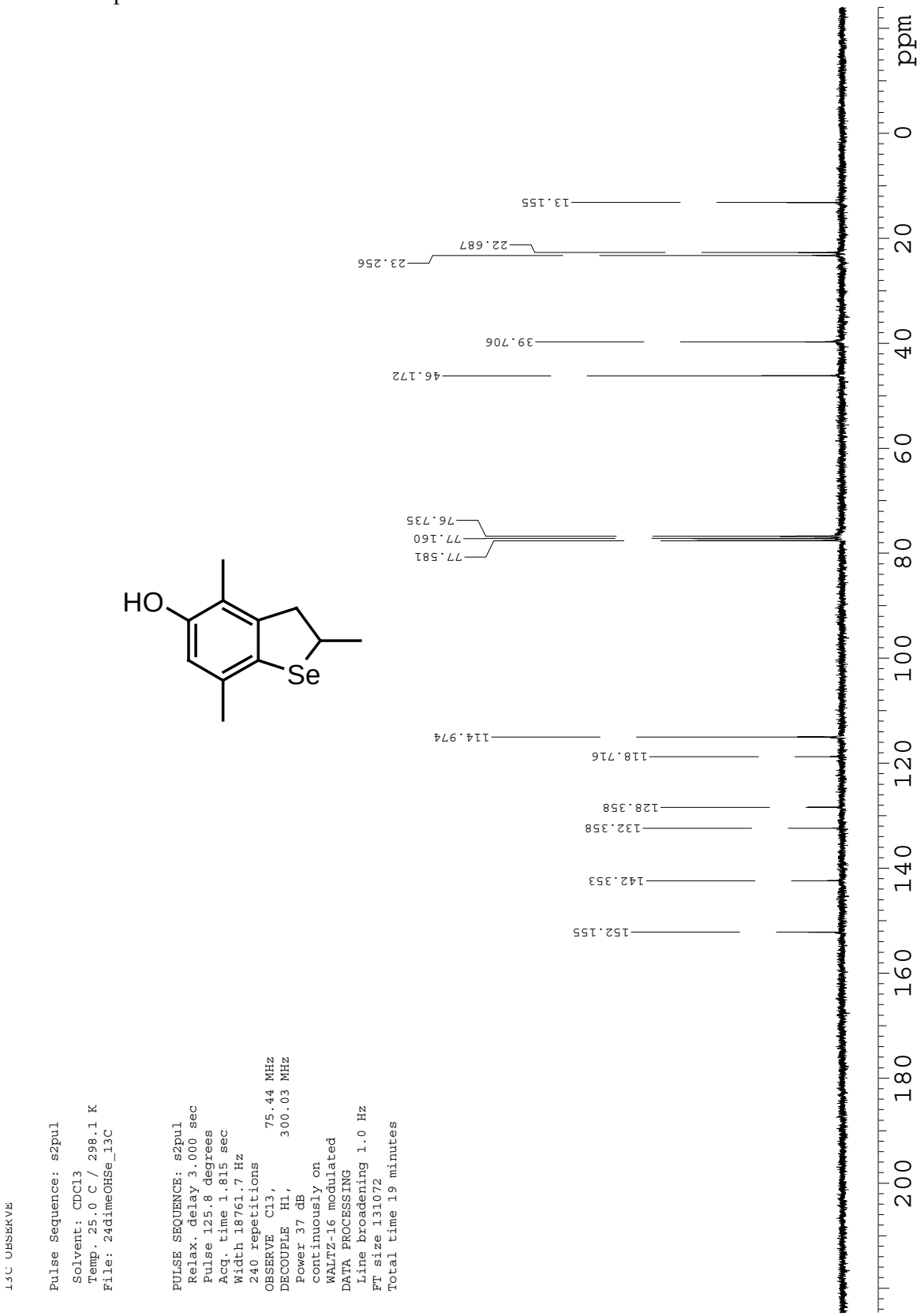
^{77}Se NMR spectrum of **5e**.



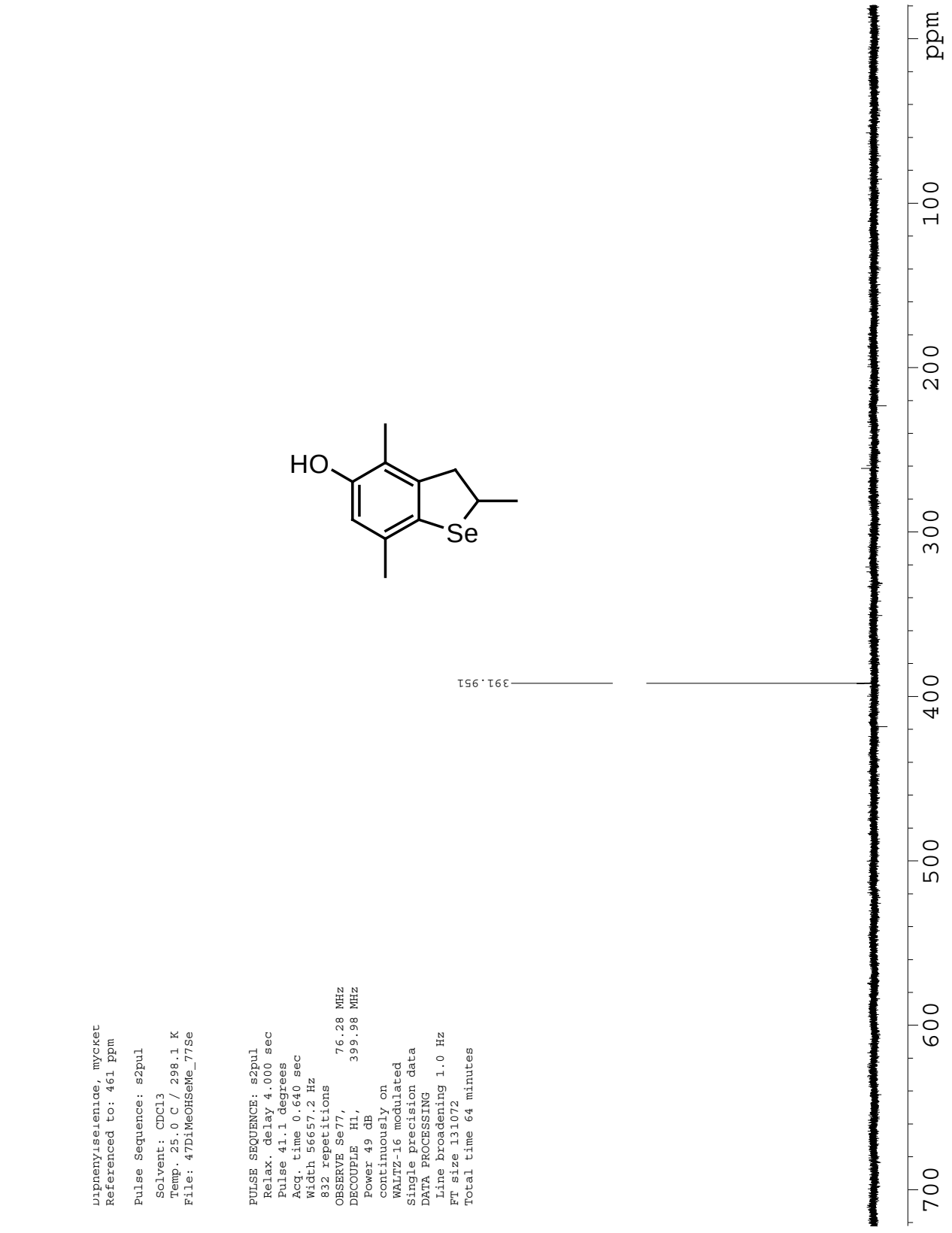
^{1}H NMR spectrum of **5f**.



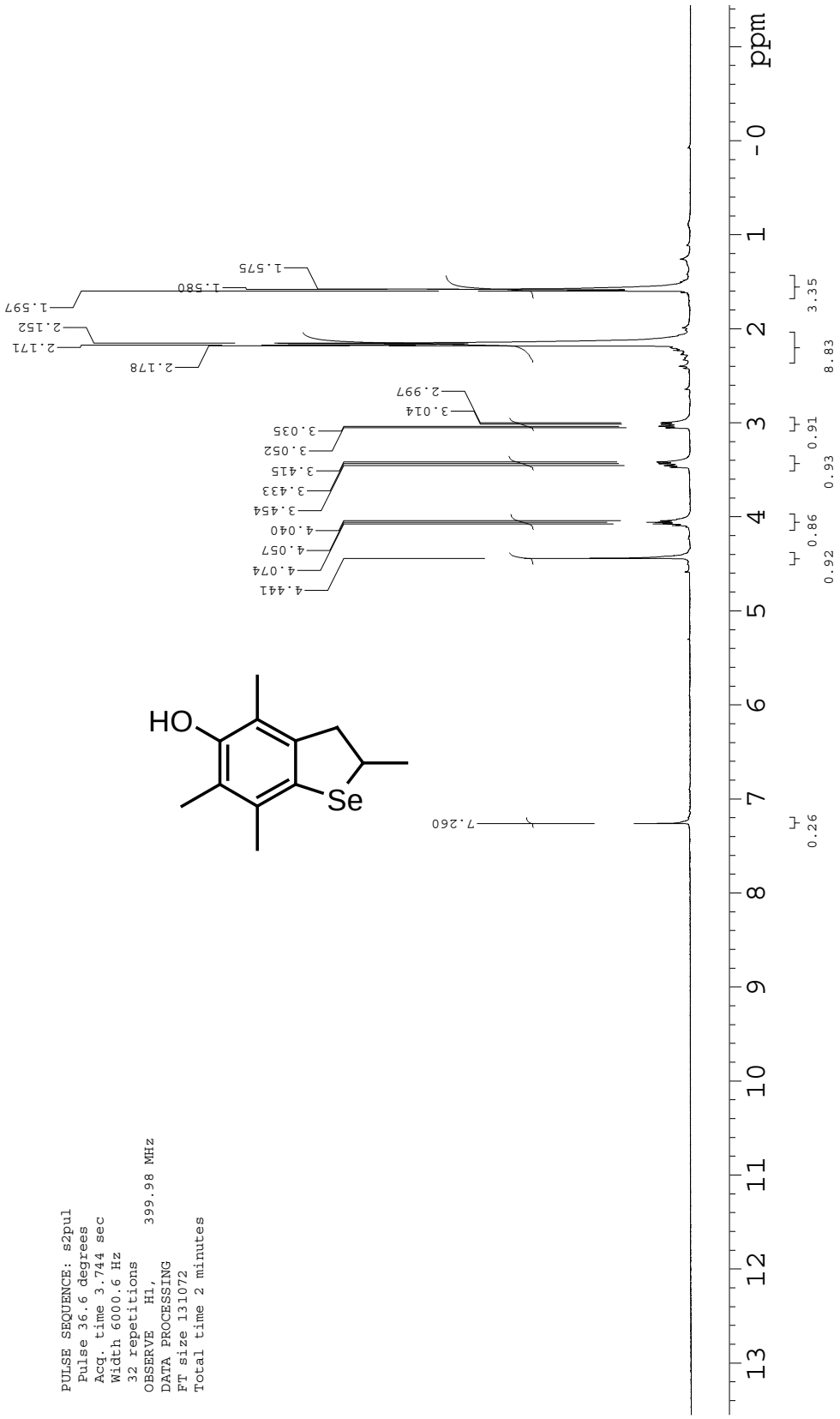
^{13}C NMR spectrum of **5f**.



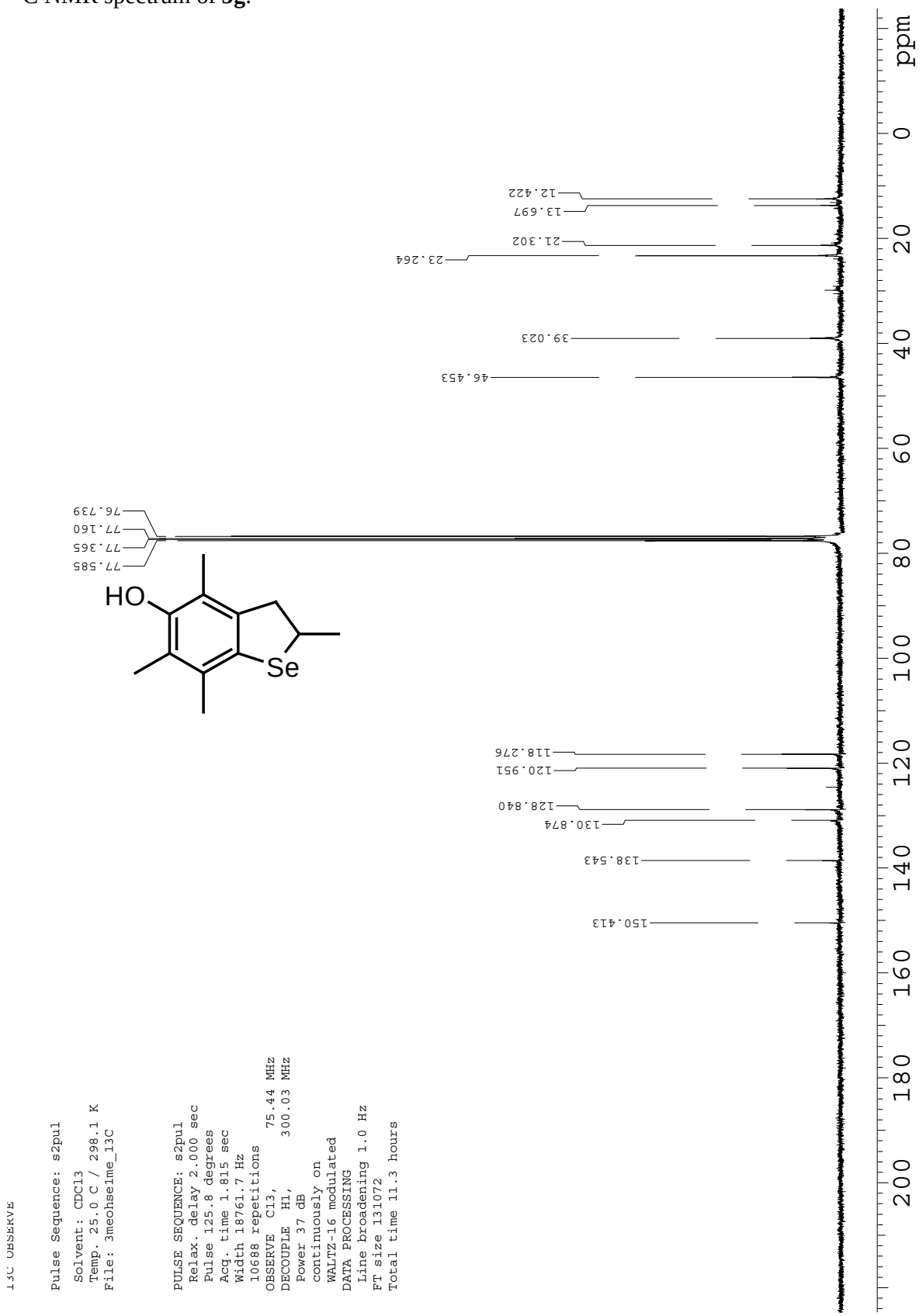
^{77}Se NMR spectrum of **5f**.



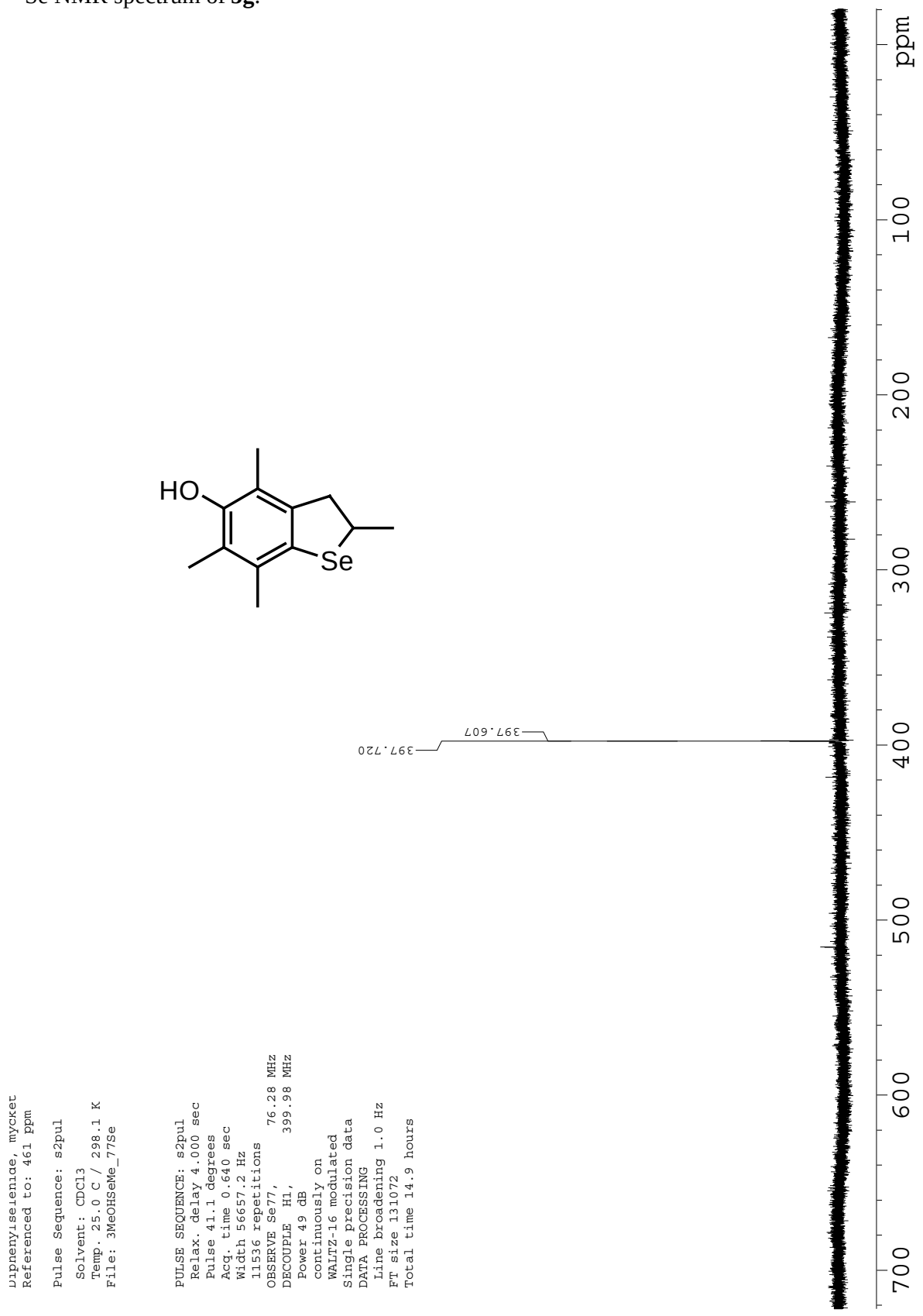
^{1}H NMR spectrum of **5g**.



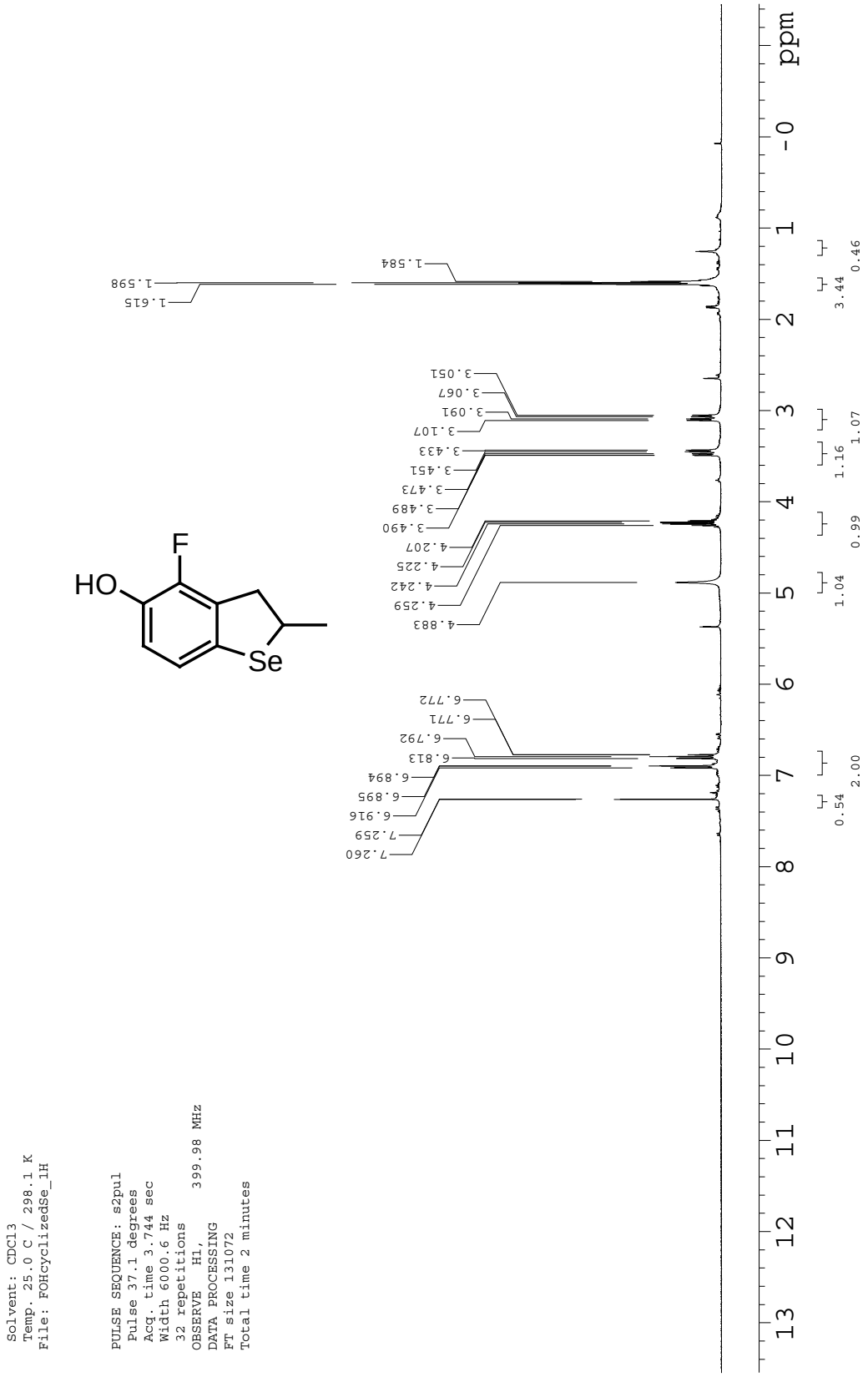
^{13}C NMR spectrum of **5g**.



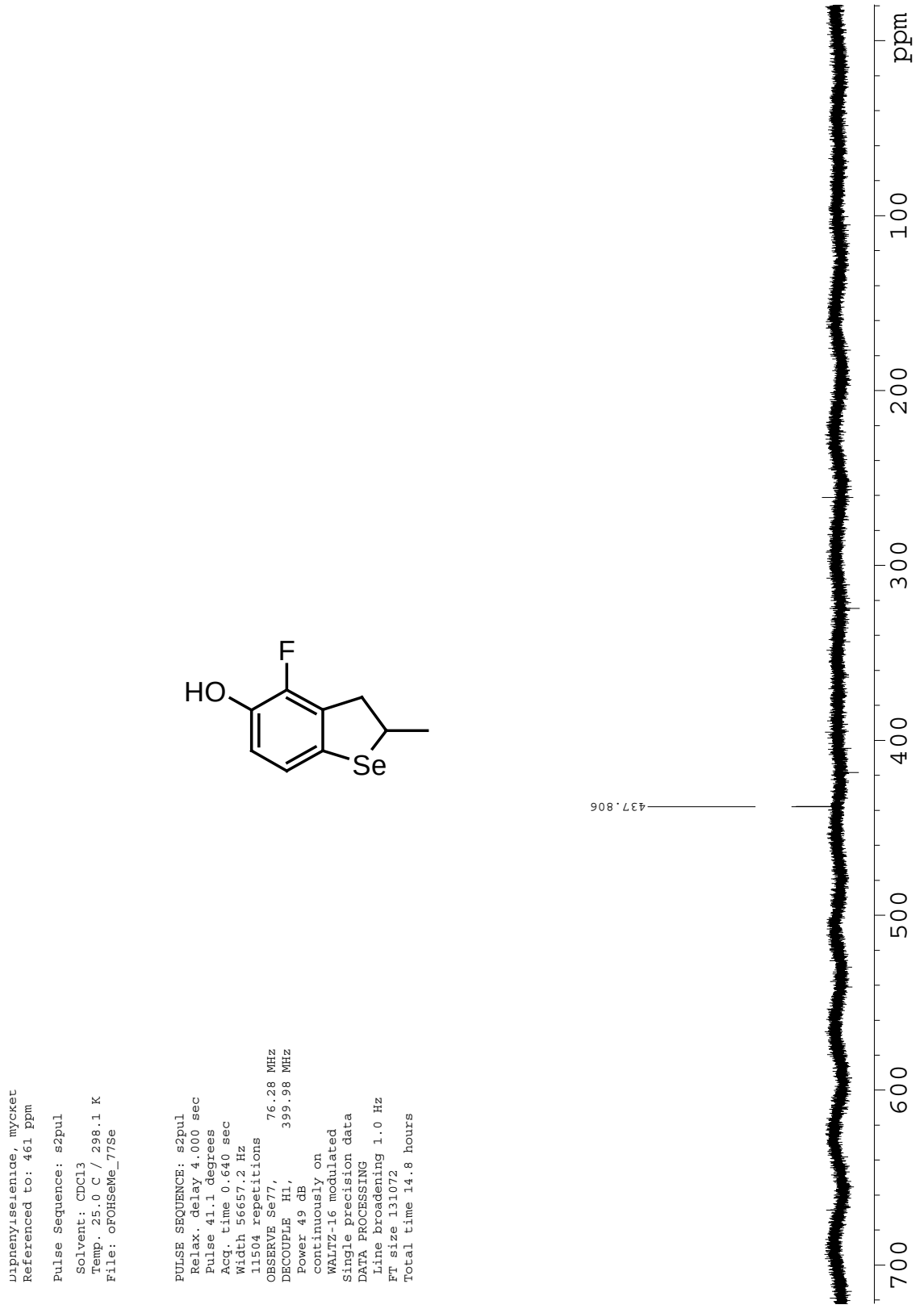
^{77}Se NMR spectrum of **5g**.



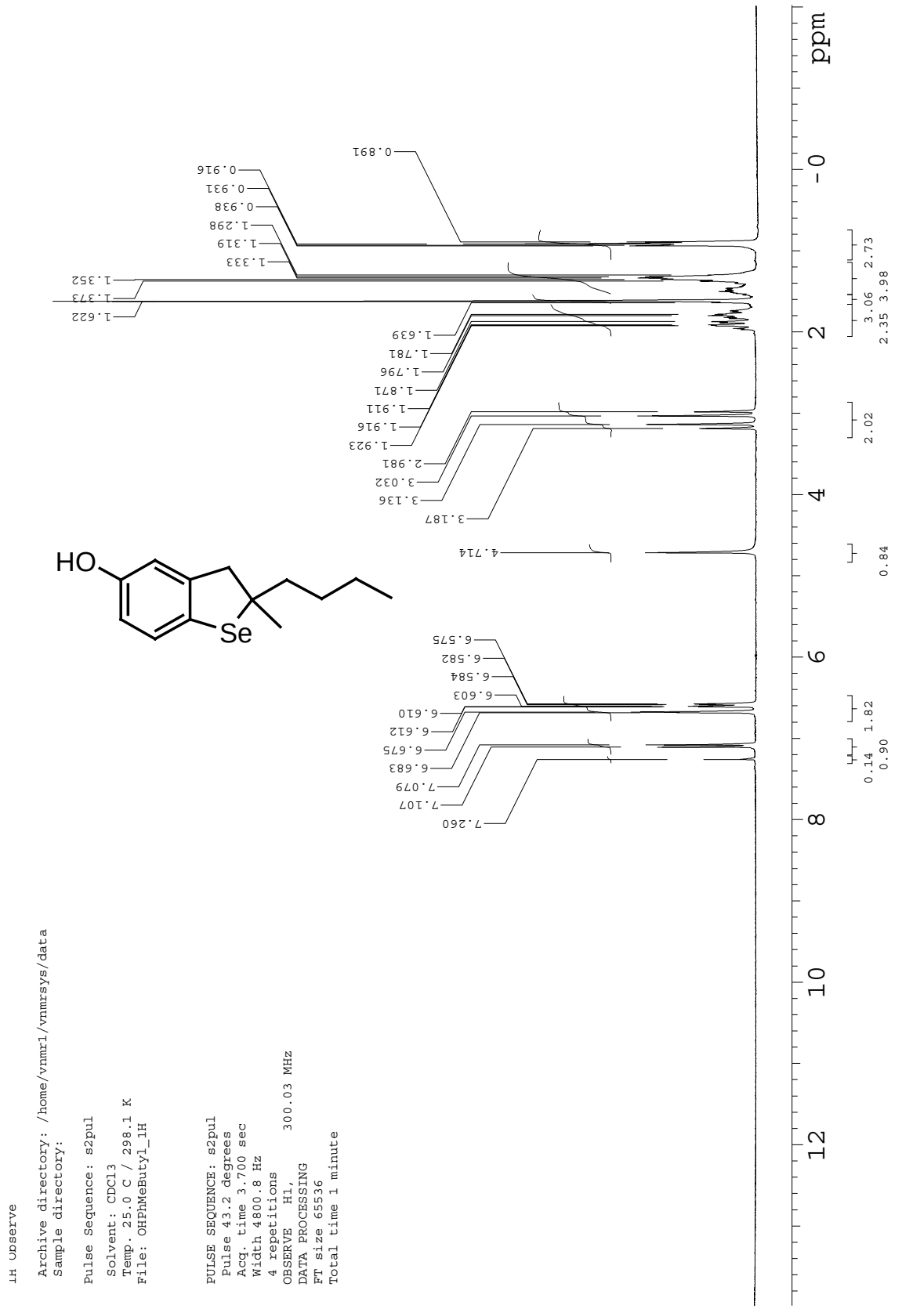
^{1}H NMR spectrum of **6**.



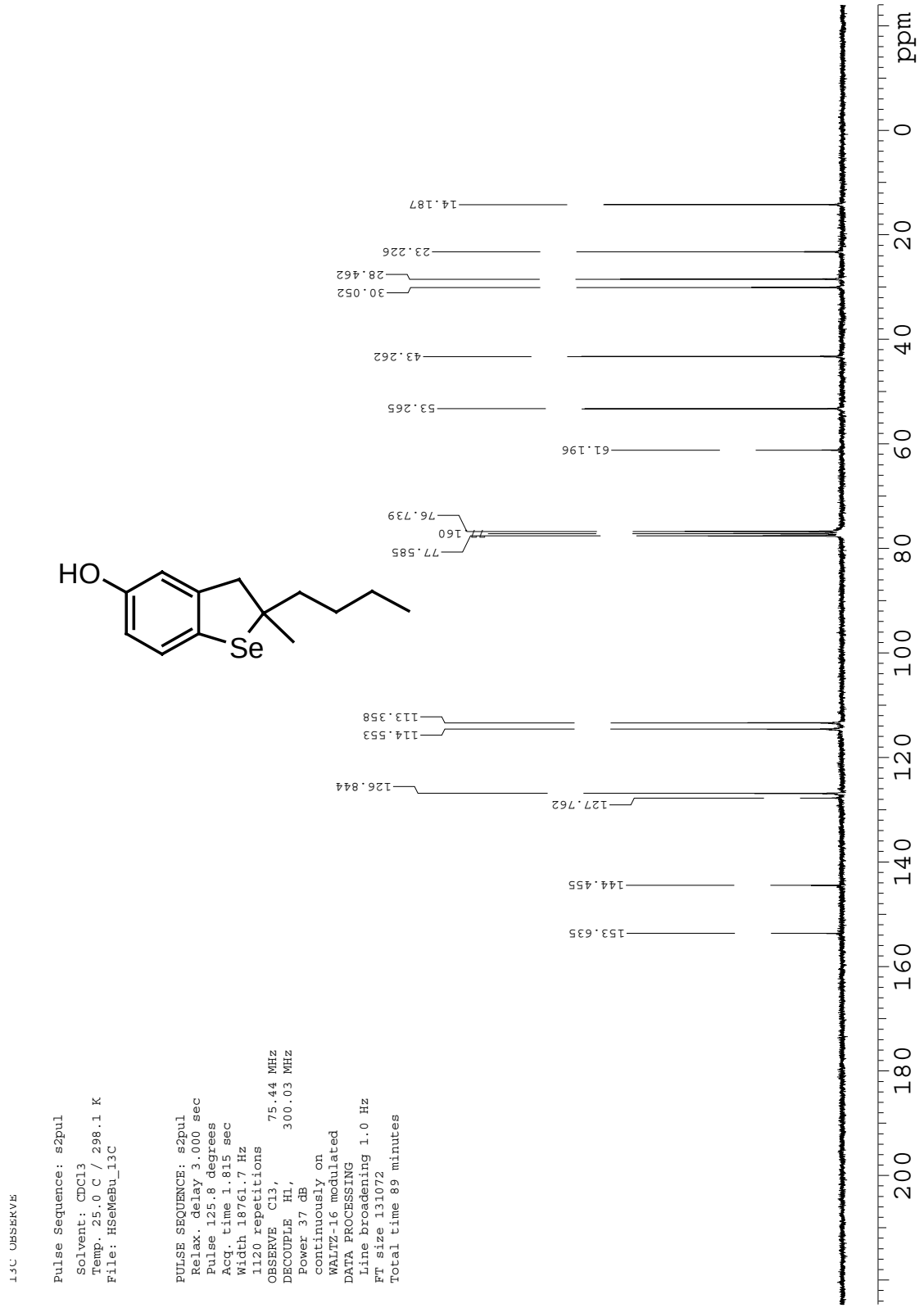
^{7}Se NMR spectrum of **6**.



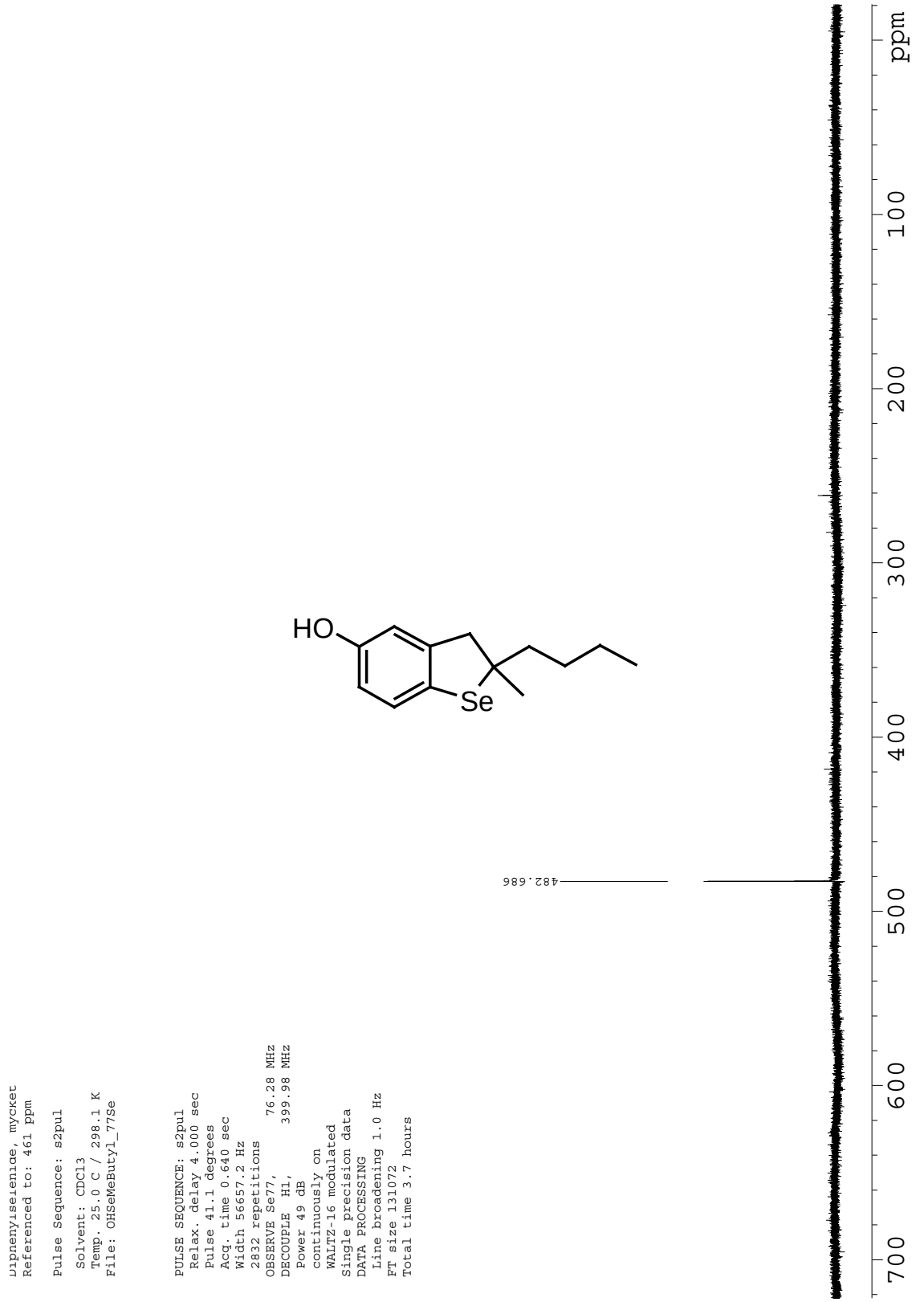
^{1}H NMR spectrum of **7**.



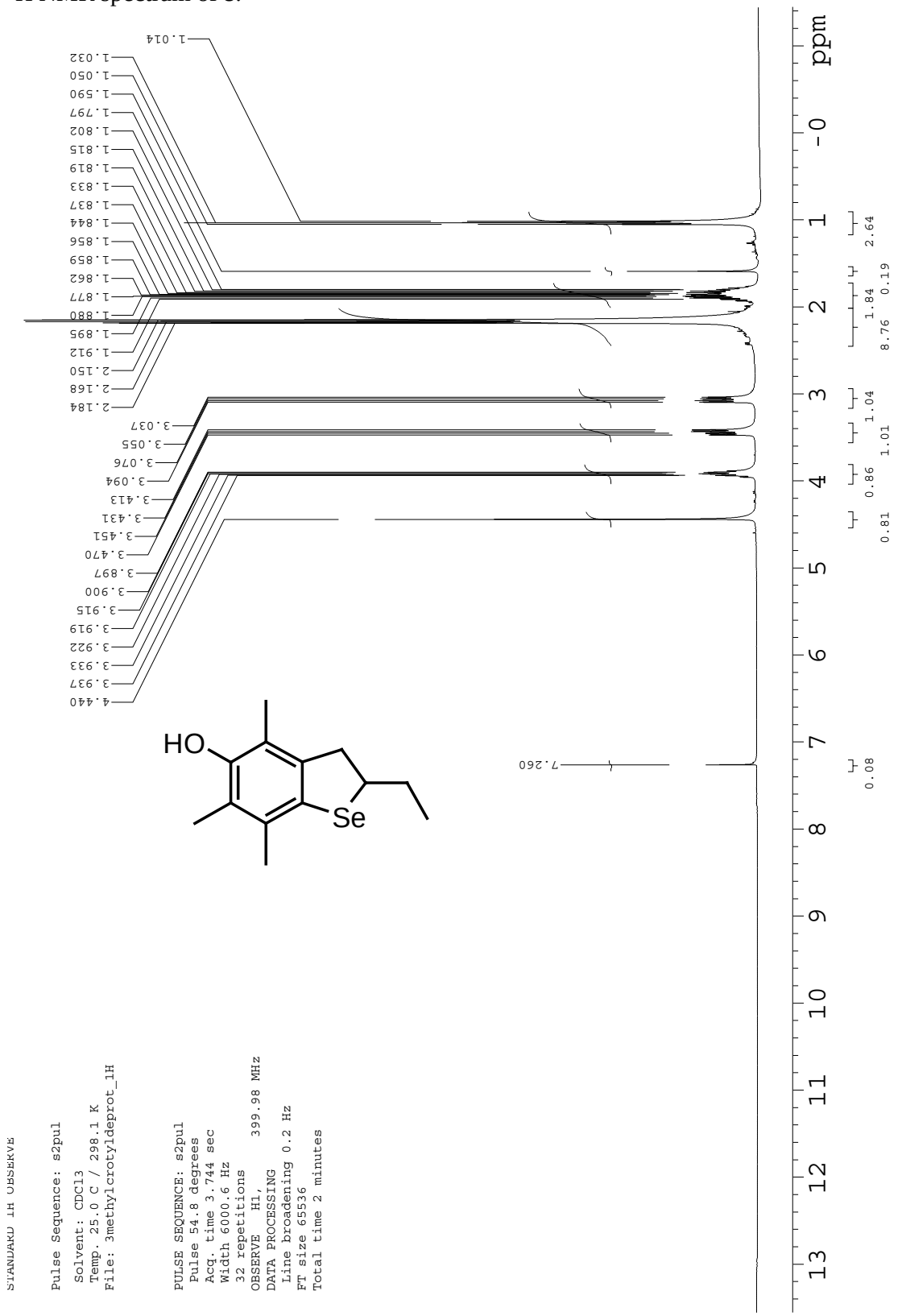
^{13}C NMR spectrum of **7**.



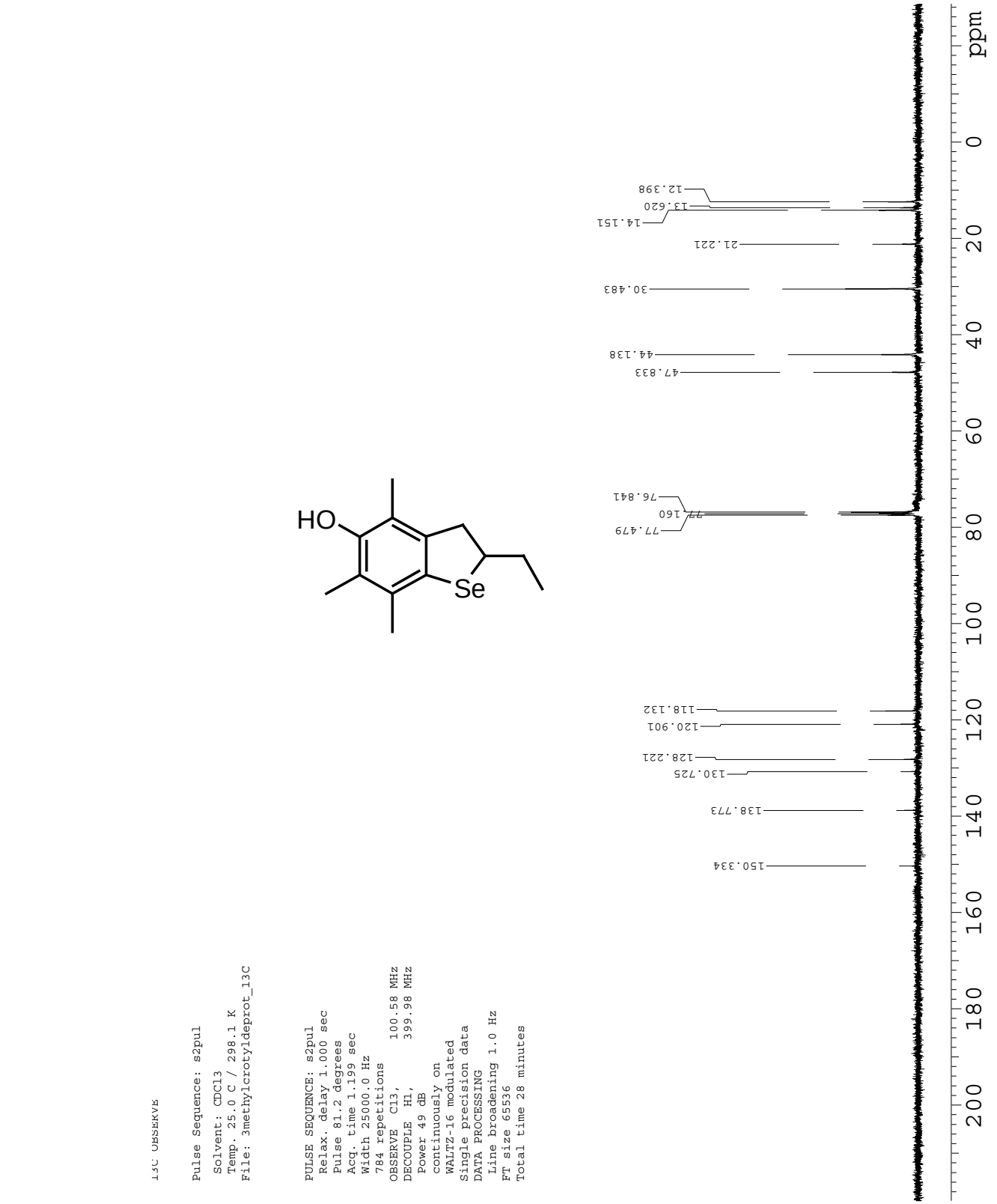
^{77}Se NMR spectrum of **7**.



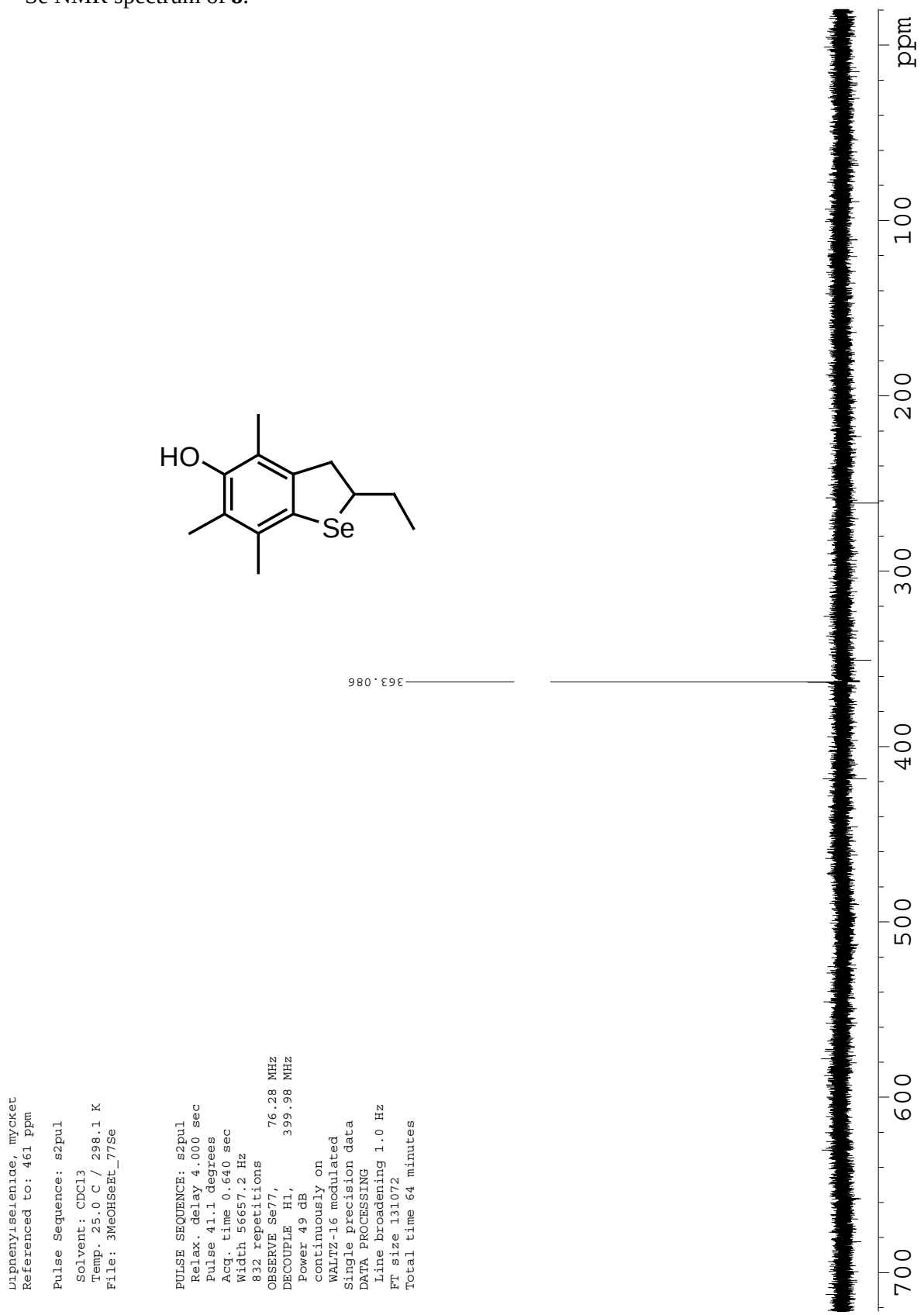
^{1}H NMR spectrum of **8**.



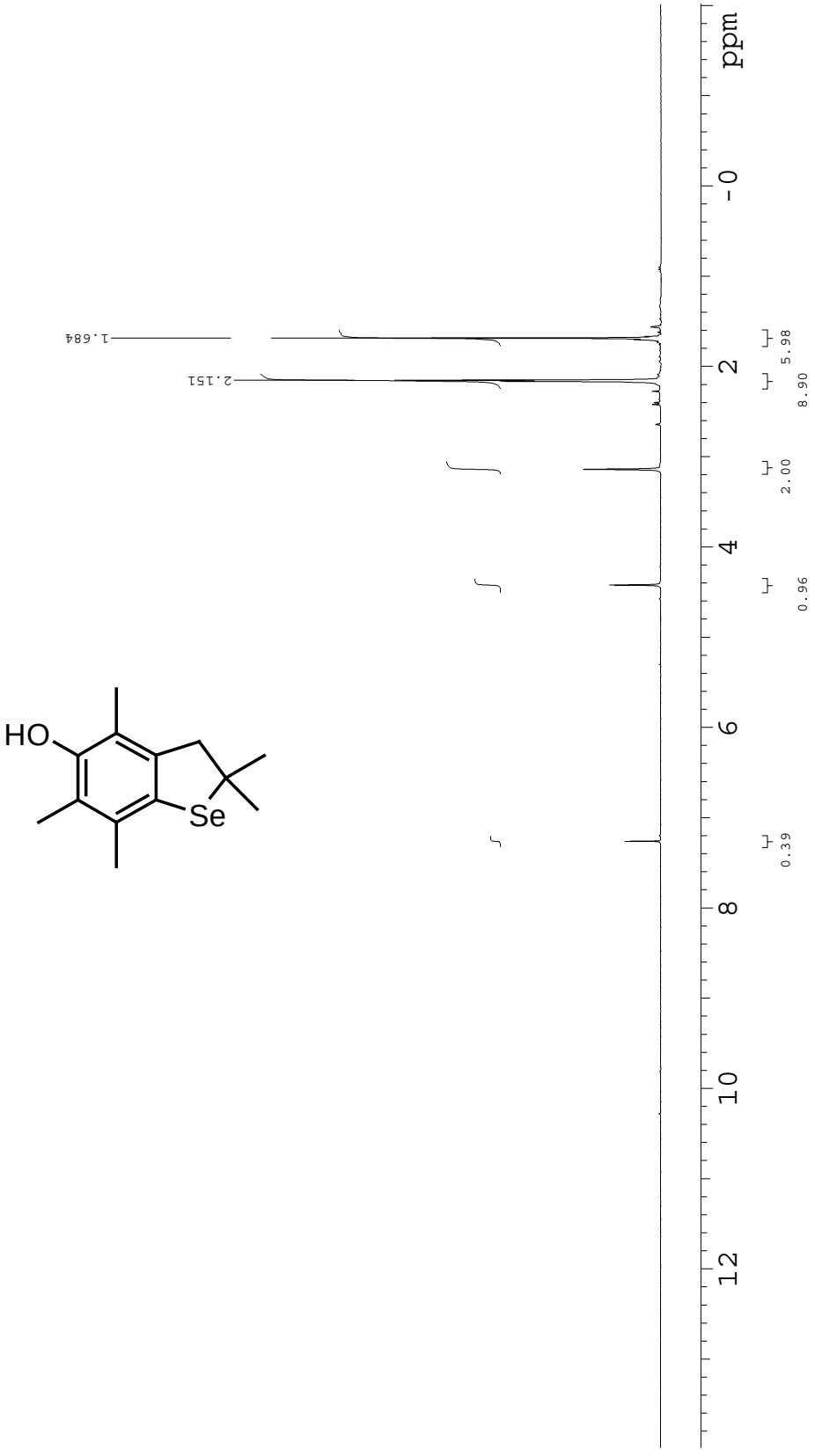
^{13}C NMR spectrum of **8**.



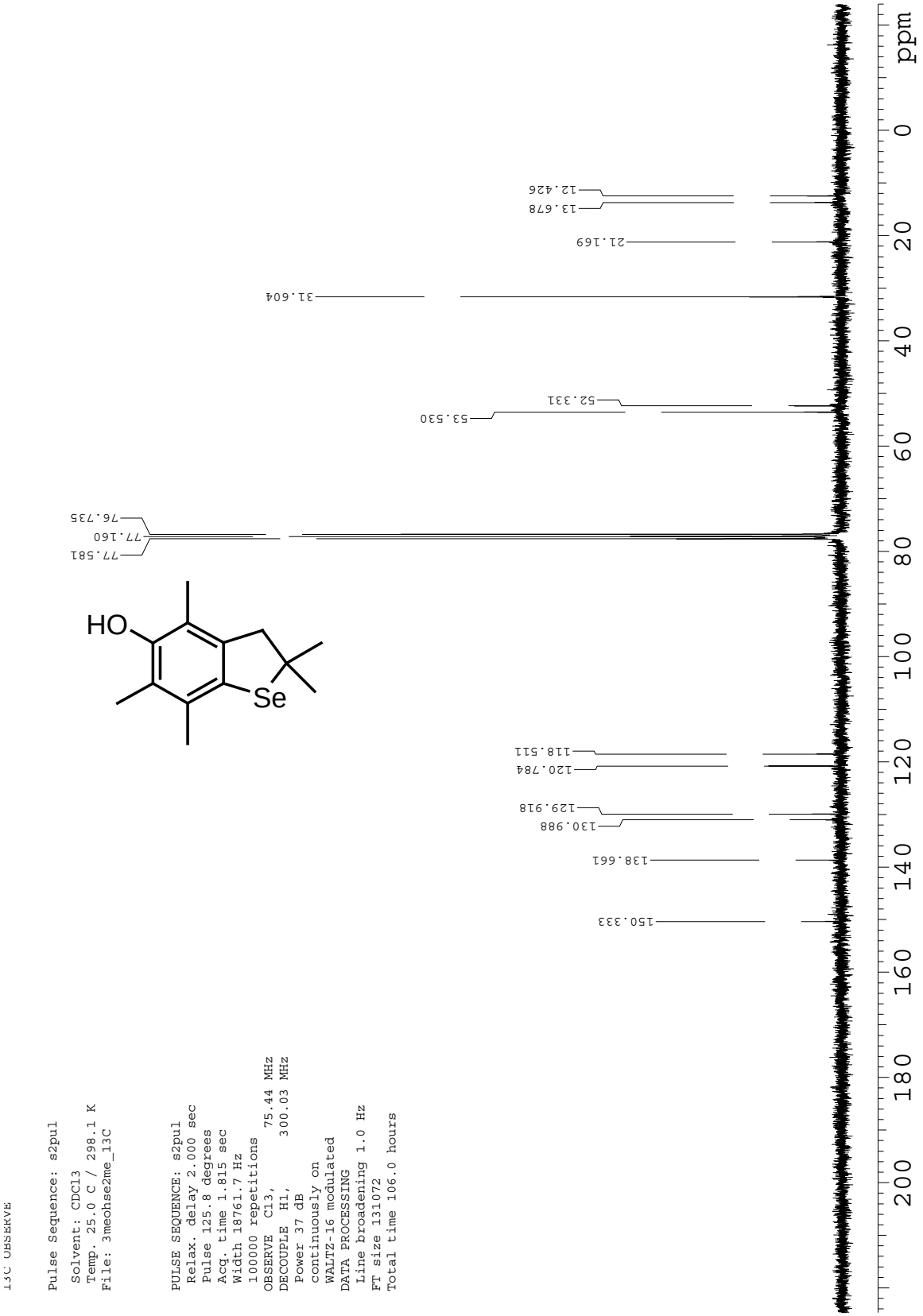
^{77}Se NMR spectrum of **8**.



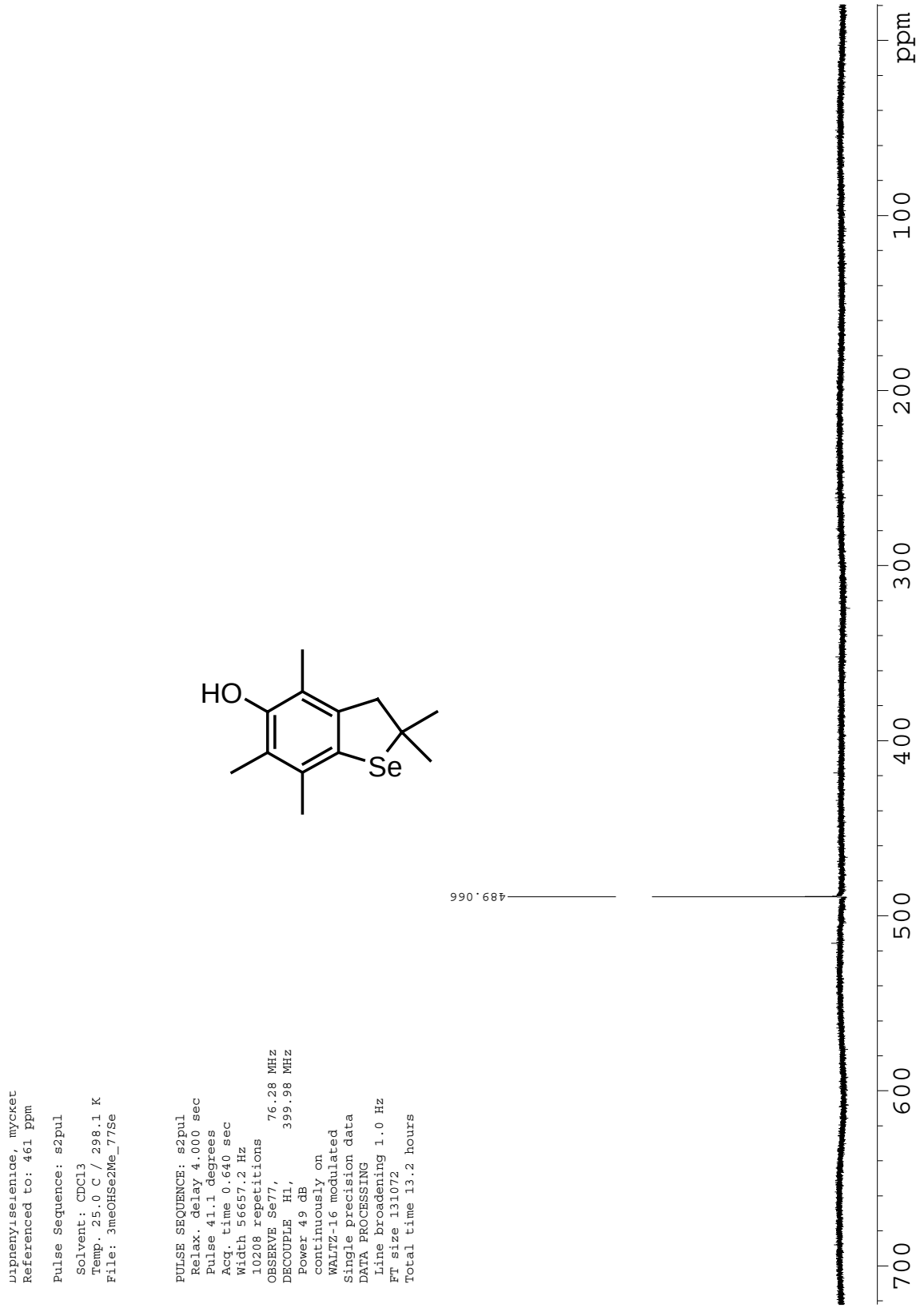
^{1}H NMR spectrum of **9**.



^{13}C NMR spectrum of **9**.



^{77}Se NMR spectrum of **9**.



5a Antioxidant

E(RB+HF-LYP) = -433.362181139 (LANL2DZ)
E(ROB+HF-LYP) = -433.500455572 (LANL2DZdp)

Zero-point correction = 0.168945
Thermal correction to Enthalpy = 0.180114

Standard orientation:

1	6	0	-1.895649	1.222685	-0.038158
2	6	0	-0.567262	0.777985	-0.055365
3	6	0	-0.289248	-0.611285	-0.021106
4	6	0	-2.942219	0.281135	0.006767
5	6	0	-2.669842	-1.099204	0.032982
6	6	0	-1.331611	-1.546260	0.022648
7	34	0	1.629226	-1.000401	-0.040898
8	6	0	0.648988	1.683013	-0.170626
9	8	0	-4.248449	0.795789	0.025031
10	1	0	-2.141892	2.280519	-0.060135
11	1	0	-3.483133	-1.822776	0.070793
12	1	0	-1.126107	-2.612932	0.055263
13	1	0	0.486597	2.651036	0.322589
14	1	0	0.846463	1.885463	-1.235743
15	1	0	-4.921467	0.085884	0.056725
16	6	0	1.882498	0.972590	0.437015
17	6	0	3.229473	1.516678	-0.052032
18	1	0	1.828170	1.002273	1.531459
19	1	0	4.073522	0.986927	0.406600
20	1	0	3.322526	2.580228	0.211612
21	1	0	3.318464	1.426671	-1.141643

5a Phenoxyl radical

E(ROB+HF-LYP) = -432.861571247 (LANL2DZdp)
Thermal correction to Enthalpy = 0.167379

Standard orientation:

1	6	0	-2.712187	-1.082028	0.001361
2	6	0	-1.396002	-1.532023	-0.016273
3	6	0	-0.336734	-0.589606	-0.028644
4	6	0	-0.597248	0.820160	-0.039831
5	6	0	-1.905378	1.273561	-0.015718
6	6	0	-3.021616	0.339981	0.010339
7	34	0	1.543458	-1.013590	-0.020882
8	6	0	1.869795	0.959581	0.426438
9	6	0	3.217568	1.455645	-0.108465
10	6	0	0.638890	1.699548	-0.148985
11	8	0	-4.249842	0.759639	0.035895
12	1	0	-2.144502	2.334393	-0.022783
13	1	0	-3.550131	-1.773879	0.019754
14	1	0	-1.183455	-2.598004	-0.009045
15	1	0	0.500642	2.657967	0.368020
16	1	0	0.825395	1.923714	-1.210845
17	1	0	1.851708	0.991126	1.521540
18	1	0	4.059296	0.904916	0.328578
19	1	0	3.348731	2.516926	0.145845
20	1	0	3.270947	1.358878	-1.199568

5a Radical cation

E(UB+HF-LYP) = -433.102850843 (LANL2DZ)
Zero-point correction = 0.169722

Standard orientation:

1	6	0	-1.865592	1.252732	0.024918
2	6	0	-0.547891	0.819898	0.009328
3	6	0	-0.273077	-0.593420	-0.026111
4	6	0	-2.915665	0.294105	-0.005329
5	6	0	-2.645873	-1.108542	-0.062026
6	6	0	-1.327659	-1.548699	-0.074198
7	34	0	1.567398	-1.013691	0.016963
8	6	0	0.665449	1.725490	-0.048080
9	8	0	-4.179476	0.800973	0.016093
10	1	0	-2.128806	2.305305	0.052643
11	1	0	-3.463840	-1.824382	-0.088458
12	1	0	-1.114128	-2.612767	-0.108797
13	1	0	0.529557	2.619266	0.572680
14	1	0	0.798892	2.072365	-1.083476
15	1	0	-4.906417	0.141057	-0.009401
16	6	0	1.945480	0.976364	0.400245
17	6	0	3.243592	1.449082	-0.262612
18	1	0	2.036690	0.987045	1.492770
19	1	0	4.118128	0.896668	0.097817
20	1	0	3.402277	2.506786	-0.013858
21	1	0	3.199348	1.364325	-1.354225

5b Antioxidant

E(RB+HF-LYP) = -472.673726932 (LANL2DZ)
E(ROB+HF-LYP) = -472.822424648 (LANL2DZdp)

Zero-point correction = 0.196606
Thermal correction to Enthalpy = 0.209550

Standard orientation:

1	6	0	1.382966	1.522790	-0.302287
2	6	0	0.108161	0.943185	-0.344195
3	6	0	-0.025904	-0.447204	-0.129236
4	6	0	2.508372	0.715835	-0.057408
5	6	0	2.392347	-0.679203	0.150985
6	6	0	1.098950	-1.247256	0.114898
7	6	0	-1.180724	1.682583	-0.667924
8	34	0	-1.887447	-1.047958	-0.212121
9	8	0	3.749842	1.376617	-0.030307
10	6	0	3.620632	-1.532974	0.414708
11	1	0	1.529131	2.588011	-0.457825
12	1	0	0.991475	-2.315917	0.285839
13	1	0	-1.304746	1.717449	-1.761238
14	1	0	-1.158241	2.719810	-0.306682
15	1	0	4.491630	0.764515	0.148018
16	1	0	4.329348	-1.509266	-0.427431
17	1	0	3.337487	-2.579625	0.564668
18	1	0	4.161209	-1.214027	1.319284
19	6	0	-2.384720	0.928163	-0.043692
20	6	0	-2.648154	1.307035	1.423313
21	1	0	-3.289210	1.061680	-0.645542
22	1	0	-3.463496	0.711571	1.849557
23	1	0	-2.927603	2.369393	1.493553
24	1	0	-1.754068	1.146337	2.037398

5b Phenoxyl radical

E(ROB+HF-LYP) = -472.187159526 (LANL2DZdp)
Thermal correction to Enthalpy = 0.196978

Standard orientation:

1	6	0	1.168796	-1.226769	0.096664
2	6	0	0.021636	-0.429827	-0.134580
3	6	0	0.121737	0.983756	-0.337384
4	6	0	1.366695	1.584234	-0.283848
5	6	0	2.570011	0.804946	-0.038741
6	6	0	2.437314	-0.646124	0.146951
7	6	0	-1.189783	1.680127	-0.667654
8	6	0	-2.378160	0.884996	-0.066972
9	6	0	-2.693918	1.254513	1.391901
10	34	0	-1.795395	-1.073616	-0.202306
11	8	0	3.733268	1.375742	0.012533
12	6	0	3.685723	-1.454427	0.399737
13	1	0	1.494562	2.654211	-0.429984
14	1	0	1.065993	-2.298774	0.247976
15	1	0	-1.300154	1.723350	-1.761368
16	1	0	-1.204292	2.712747	-0.295656
17	1	0	4.399861	-1.331221	-0.424353

18	1	0	3.457710	-2.519527	0.516972
19	1	0	4.201407	-1.099074	1.300942
20	1	0	-3.272120	0.972984	-0.691588
21	1	0	-3.488327	0.622633	1.804958
22	1	0	-3.029786	2.300580	1.445303
23	1	0	-1.807861	1.146568	2.028486

5b Radical cation

E(UB+HF-LYP) = -472.418658116 (LANL2DZ)
Zero-point correction = 0.197476

Standard orientation:

1	6	0	1.344755	1.575187	-0.236900
2	6	0	0.090813	0.986899	-0.295172
3	6	0	-0.012964	-0.437767	-0.123045
4	6	0	2.488868	0.762291	-0.019748
5	6	0	2.406394	-0.669290	0.136935
6	6	0	1.139156	-1.246273	0.079974
7	6	0	-1.205128	1.709768	-0.602725
8	34	0	-1.789110	-1.077554	-0.188250
9	8	0	3.677507	1.428700	0.026030
10	6	0	3.660020	-1.486772	0.360944
11	1	0	1.489822	2.643860	-0.358418
12	1	0	1.039497	-2.321022	0.202036
13	1	0	-1.264050	1.872486	-1.688523
14	1	0	-1.234532	2.698429	-0.129907
15	1	0	4.473117	0.872376	0.172692
16	1	0	4.363865	-1.395249	-0.479186
17	1	0	3.421255	-2.548739	0.460337
18	1	0	4.184146	-1.189738	1.281058
19	6	0	-2.429135	0.877457	-0.136582
20	6	0	-2.923648	1.212770	1.282790
21	1	0	-3.251012	0.924406	-0.855733
22	1	0	-3.732074	0.548148	1.605660
23	1	0	-3.320260	2.236819	1.282784
24	1	0	-2.114865	1.159858	2.020630

5c Antioxidant

E(RB+HF-LYP) = -472.675549965 (LANL2DZ)
E(ROB+HF-LYP) = -472.823914686 (LANL2DZdp)

Zero-point correction = 0.196794
Thermal correction to Enthalpy = 0.209679

Standard orientation:

1	6	0	-1.738532	-1.469868	-0.240892
2	6	0	-0.420930	-0.999646	-0.319534
3	6	0	-0.148165	0.373873	-0.125136
4	6	0	-2.773044	-0.555263	0.023939
5	6	0	-2.500604	0.813347	0.206002
6	6	0	-1.175677	1.300887	0.134823
7	6	0	0.782682	-1.861707	-0.667662
8	6	0	2.072037	-1.224269	-0.087062
9	34	0	1.762076	0.789165	-0.247906
10	6	0	2.346176	-1.624250	1.372516
11	6	0	-0.880594	2.774448	0.330765
12	8	0	-4.074223	-1.079384	0.095062
13	1	0	-1.981259	-2.519098	-0.380787
14	1	0	-3.313740	1.509701	0.410452
15	1	0	0.870224	-1.917794	-1.763642
16	1	0	0.668803	-2.888695	-0.294964
17	1	0	2.939718	-1.444136	-0.716994
18	1	0	1.490799	-1.381331	2.014198
19	1	0	3.226318	-1.106671	1.770724
20	1	0	2.528001	-2.707864	1.437816
21	1	0	-4.738035	-0.385823	0.285454
22	1	0	-1.781519	3.332342	0.608815
23	1	0	-0.477202	3.224135	-0.587826
24	1	0	-0.129001	2.923373	1.118511

5c Phenoxyl radical

E(ROB+HF-LYP) = -472.185210061 (LANL2DZdp)
Thermal correction to Enthalpy = 0.197001

Standard orientation:

1	6	0	-1.262508	1.273207	0.125730
2	6	0	-0.199997	0.354858	-0.125426
3	6	0	-0.431580	-1.045001	-0.312790
4	6	0	-1.718611	-1.546957	-0.222432
5	6	0	-2.837103	-0.659713	0.048970
6	6	0	-2.554158	0.757351	0.209290
7	6	0	0.802929	-1.858167	-0.673000
8	6	0	2.075472	-1.173241	-0.113119
9	6	0	2.404137	-1.570537	1.335641
10	34	0	1.668216	0.828460	-0.233046
11	8	0	-4.050047	-1.115062	0.141072
12	6	0	-0.987733	2.753507	0.300092
13	1	0	-1.936310	-2.603595	-0.356799
14	1	0	-3.403335	1.406772	0.407930
15	1	0	0.876529	-1.916535	-1.769167
16	1	0	0.733043	-2.886093	-0.294509
17	1	0	2.937574	-1.339790	-0.765779
18	1	0	1.550786	-1.388888	1.999640
19	1	0	3.262293	-1.009845	1.723233
20	1	0	2.650592	-2.641595	1.379432
21	1	0	-1.909802	3.303984	0.511902
22	1	0	-0.538834	3.184575	-0.605958
23	1	0	-0.286617	2.932032	1.127331

5c Radical cation

E(UB+HF-LYP) = -472.419275074 (LANL2DZ)
Zero-point correction = 0.197595

Standard orientation:

1	6	0	-1.684052	-1.539658	-0.189792
2	6	0	-0.392749	-1.047869	-0.277520
3	6	0	-0.159175	0.363524	-0.113663
4	6	0	-2.749884	-0.629019	0.051082
5	6	0	-2.521834	0.771205	0.193072
6	6	0	-1.231124	1.293633	0.112186
7	6	0	0.828280	-1.881727	-0.613452
8	6	0	2.130163	-1.165394	-0.171090
9	34	0	1.667113	0.836753	-0.215020
10	6	0	2.618553	-1.541618	1.240029
11	6	0	-0.975585	2.775958	0.265097
12	8	0	-3.991780	-1.183438	0.129607
13	1	0	-1.916073	-2.593294	-0.305048
14	1	0	-3.361962	1.438764	0.371548
15	1	0	0.849413	-2.043504	-1.700735
16	1	0	0.778245	-2.871312	-0.144554
17	1	0	2.931353	-1.285531	-0.904925
18	1	0	1.831038	-1.416378	1.992059
19	1	0	3.488811	-0.951412	1.546611
20	1	0	2.922647	-2.596829	1.235961
21	1	0	-4.730083	-0.556631	0.292474
22	1	0	-1.907032	3.327380	0.418205
23	1	0	-0.487387	3.190914	-0.626971
24	1	0	-0.322134	2.981511	1.123521

5d Antioxidant

E(RB+HF-LYP) = -511.984400953 (LANL2DZ)
E(ROB+HF-LYP) = -512.143195989 (LANL2DZdp)

Zero-point correction = 0.224477
Thermal correction to Enthalpy = 0.239196

Standard orientation:

1	6	0	1.420907	1.211316	-0.175295

2	6	0	0.089955	0.749827	-0.247833
3	6	0	-0.193894	-0.627254	-0.123039
4	6	0	2.439554	0.252618	0.029410
5	6	0	2.171746	-1.131143	0.155384
6	6	0	0.830627	-1.561445	0.077026
7	6	0	-1.114847	1.637826	-0.525995
8	6	0	-2.404298	0.966124	0.015759
9	34	0	-2.102983	-1.031332	-0.275490
10	6	0	-2.670389	1.271739	1.499712
11	8	0	3.759778	0.746398	0.103772
12	6	0	1.760959	2.683119	-0.319637
13	6	0	3.299967	-2.124567	0.374801
14	1	0	0.607794	-2.620669	0.179471
15	1	0	-1.208315	1.781040	-1.614324
16	1	0	-1.003111	2.634376	-0.078579
17	1	0	-3.273452	1.231848	-0.594341
18	1	0	-1.815352	0.977309	2.119926
19	1	0	-3.554032	0.736643	1.865734
20	1	0	-2.842018	2.350298	1.637755
21	1	0	1.338643	3.098933	-1.244314
22	1	0	2.842620	2.828544	-0.337906
23	1	0	1.353327	3.268582	0.516989
24	1	0	4.412251	0.028521	0.225203
25	1	0	3.853230	-1.926560	1.305957
26	1	0	4.023861	-2.120732	-0.455133
27	1	0	2.906030	-3.143002	0.448291

5d Phenoxyl radical

E(ROB+HF-LYP) = -511.509461435 (LANL2DZdp)

Thermal correction to Enthalpy = 0.225634

Standard orientation:

1	6	0	0.896753	-1.554840	0.063951
2	6	0	-0.144371	-0.618572	-0.125074
3	6	0	0.113446	0.781406	-0.240660
4	6	0	1.418079	1.259718	-0.159470
5	6	0	2.519261	0.309611	0.049474
6	6	0	2.220650	-1.123727	0.154244
7	6	0	1.751789	2.729301	-0.293926
8	6	0	-1.112306	1.637249	-0.528341
9	6	0	-2.395710	0.932068	-0.018119
10	6	0	-2.723234	1.242714	1.452413
11	34	0	-2.018158	-1.061191	-0.263105
12	8	0	3.743660	0.732187	0.135688
13	6	0	3.359858	-2.096181	0.364105
14	1	0	0.671599	-2.615635	0.150018
15	1	0	-1.188575	1.793015	-1.615536
16	1	0	-1.031772	2.629957	-0.067286
17	1	0	-3.253491	1.154597	-0.659887
18	1	0	-1.874794	1.005451	2.105217
19	1	0	-3.590629	0.671181	1.801803
20	1	0	-2.954216	2.312477	1.563920
21	1	0	1.269157	3.323665	0.495127
22	1	0	1.411166	3.131285	-1.258526
23	1	0	2.832460	2.869850	-0.220014
24	1	0	4.309581	-1.558214	0.408693
25	1	0	3.409668	-2.827893	-0.454001
26	1	0	3.232659	-2.659212	1.298957

5d Radical cation

E(UB+HF-LYP) = -511.733266382 (LANL2DZ)

Thermal correction to Enthalpy = 0.239897

Standard orientation:

1	6	0	1.388436	1.264971	-0.137368
2	6	0	0.079781	0.784195	-0.213063
3	6	0	-0.173878	-0.624162	-0.113279
4	6	0	2.429746	0.299080	0.048312
5	6	0	2.195113	-1.120814	0.141444
6	6	0	0.880050	-1.564640	0.054343
7	6	0	-1.136770	1.652081	-0.473997
8	6	0	-2.450718	0.914448	-0.102004
9	34	0	-2.001839	-1.083626	-0.235110
10	6	0	-2.972997	1.226063	1.313359
11	8	0	3.696799	0.804997	0.128083
12	6	0	1.714916	2.738328	-0.250512
13	6	0	3.355539	-2.074697	0.329847
14	1	0	0.666177	-2.627026	0.123848
15	1	0	-1.153804	1.922462	-1.540298
16	1	0	-1.084698	2.592641	0.086853
17	1	0	-3.233415	1.078953	-0.847246
18	1	0	-2.206096	1.055175	2.077684
19	1	0	-3.854992	0.628621	1.568049
20	1	0	-3.268606	2.282897	1.354611
21	1	0	1.202027	3.191070	-1.107423
22	1	0	2.787429	2.898732	-0.366900
23	1	0	1.392914	3.280422	0.649497
24	1	0	4.408652	0.140159	0.248392
25	1	0	3.901283	-1.879943	1.264739
26	1	0	4.071254	-2.021345	-0.503735
27	1	0	3.004688	-3.108631	0.378514

5e Antioxidant

E(RB+HF-LYP) = -511.982827731 (LANL2DZ)
E(ROB+HF-LYP) = -512.141679416 (LANL2DZdp)

Zero-point correction = 0.224674
Thermal correction to Enthalpy = 0.239309

Standard orientation:

1	6	0	-1.219866	-1.794966	-0.264991
2	6	0	0.013659	-1.140163	-0.327557
3	6	0	0.064597	0.262720	-0.160564
4	6	0	-2.384163	-1.039471	-0.051712
5	6	0	-2.353874	0.366332	0.100825
6	6	0	-1.095941	1.033026	0.052946
7	6	0	1.339711	-1.821964	-0.624144
8	6	0	2.500049	-0.990857	-0.019043
9	34	0	1.906095	0.946437	-0.259975
10	6	0	2.771413	-1.306896	1.461333
11	8	0	-3.585723	-1.769878	-0.001864
12	6	0	-3.665183	1.109415	0.311664
13	6	0	-1.008289	2.541352	0.224234
14	1	0	-1.305079	-2.871481	-0.379815
15	1	0	1.470976	-1.881438	-1.715629
16	1	0	1.365336	-2.848660	-0.234224
17	1	0	3.414599	-1.098674	-0.610918
18	1	0	1.865623	-1.170914	2.064166
19	1	0	3.552806	-0.657374	1.872056
20	1	0	3.102931	-2.350997	1.569227
21	1	0	-4.362220	-1.199695	0.165351
22	1	0	-4.379541	0.909311	-0.502284
23	1	0	-3.521108	2.190933	0.339592
24	1	0	-4.148309	0.826753	1.260282
25	1	0	-1.523382	2.878488	1.132951
26	1	0	-1.459308	3.071797	-0.626332
27	1	0	0.032553	2.870964	0.301694

5e Phenoxyl radical

E(ROB+HF-LYP) = -511.507289932 (LANL2DZdp)

Thermal correction to Enthalpy = 0.226696

Standard orientation:

1	6	0	1.168963	-0.992553	0.042029
2	6	0	-0.018928	-0.235950	-0.159326

3	6	0	-0.013430	1.185670	-0.320357
4	6	0	1.186172	1.865320	-0.248039
5	6	0	2.431394	1.151824	-0.029726
6	6	0	2.397434	-0.311545	0.107364
7	6	0	-1.364992	1.810086	-0.630109
8	6	0	-2.502232	0.928764	-0.054490
9	6	0	-2.842745	1.240165	1.412471
10	34	0	-1.801479	-0.983867	-0.238474
11	8	0	3.552495	1.803955	0.036363
12	6	0	3.716796	-1.021687	0.322175
13	6	0	1.074722	-2.501998	0.175570
14	1	0	1.247320	2.944868	-0.359464
15	1	0	-1.478734	1.877422	-1.722344
16	1	0	-1.439779	2.829433	-0.229922
17	1	0	-3.399053	0.977404	-0.679373
18	1	0	-1.951927	1.171958	2.048006
19	1	0	-3.595849	0.548710	1.807263
20	1	0	-3.244063	2.261201	1.492268
21	1	0	4.527865	-0.290025	0.308113
22	1	0	3.905163	-1.769434	-0.460035
23	1	0	3.741712	-1.545450	1.288147
24	1	0	2.019422	-2.948420	0.493094
25	1	0	0.793996	-2.964327	-0.782171
26	1	0	0.305325	-2.782068	0.908260

Radical cation

E(UB+HF-LYP) = -511.731398118 (LANL2DZ)

Zero-point correction = 0.225630

Standard orientation:

1	6	0	-1.162188	-1.843690	-0.218158
2	6	0	0.045146	-1.175379	-0.290294
3	6	0	0.057588	0.258719	-0.149640
4	6	0	-2.350493	-1.092761	-0.018512
5	6	0	-2.363662	0.339833	0.100526
6	6	0	-1.140265	1.028251	0.030807
7	6	0	1.380326	-1.829044	-0.584388
8	6	0	2.551152	-0.927821	-0.116870
9	34	0	1.808370	0.981820	-0.217258
10	6	0	3.040257	-1.211462	1.315533
11	8	0	-3.493835	-1.834579	0.046171
12	6	0	-3.697860	1.032129	0.302539
13	6	0	-1.088982	2.539639	0.148563
14	1	0	-1.241119	-2.921424	-0.314475
15	1	0	1.455261	-1.994494	-1.668797
16	1	0	1.458828	-2.811889	-0.105238
17	1	0	3.385574	-0.944470	-0.822845
18	1	0	2.217575	-1.189061	2.039519
19	1	0	3.805997	-0.497991	1.638386
20	1	0	3.491178	-2.212423	1.341067
21	1	0	-4.323579	-1.327684	0.180002
22	1	0	-4.189913	0.699122	1.228518
23	1	0	-4.382887	0.842421	-0.537240
24	1	0	-3.592320	2.114296	0.378559
25	1	0	-1.678420	3.017693	-0.643462
26	1	0	-0.070887	2.931711	0.073227
27	1	0	-1.495308	2.878453	1.109567

5f Antioxidant

E(RB+HF-LYP) = -511.985980306 (LANL2DZ)
E(ROB+HF-LYP) = -512.144622470 (LANL2DZdp)

Zero-point correction = 0.224719
Thermal correction to Enthalpy = 0.239334

Standard orientation:

1	6	0	-1.842950	-0.938806	-0.141923
2	6	0	-0.450933	-0.733231	-0.241732
3	6	0	0.104484	0.559157	-0.110350
4	6	0	-2.643670	0.200019	0.099582
5	6	0	-2.088987	1.486614	0.226509
6	6	0	-0.697275	1.692064	0.121256
7	6	0	0.548352	-1.837156	-0.557939
8	6	0	1.956378	-1.447938	-0.038106
9	34	0	2.055158	0.574626	-0.287410
10	6	0	2.187475	-1.830760	1.433756
11	6	0	-2.467312	-2.313792	-0.291244
12	6	0	-0.100789	3.079030	0.251327
13	8	0	-4.033662	-0.008370	0.206692
14	1	0	-2.739316	2.341563	0.412194
15	1	0	0.588849	-1.974931	-1.650217
16	1	0	0.247635	-2.799396	-0.123291
17	1	0	2.742186	-1.868254	-0.673683
18	1	0	1.419528	-1.387155	2.078720
19	1	0	3.166396	-1.487659	1.787588
20	1	0	2.146372	-2.924531	1.550267
21	1	0	-2.163638	-2.981220	0.528040
22	1	0	-2.159899	-2.790870	-1.231483
23	1	0	-3.556768	-2.242396	-0.281014
24	1	0	-0.862489	3.821233	0.514731
25	1	0	0.369058	3.400616	-0.689289
26	1	0	0.679782	3.101338	1.024522
27	1	0	-4.512398	0.830138	0.364489

5f Phenoxyl radical

E(ROB+HF-LYP) = -511.509019029 (LANL2DZdp)
Thermal correction to Enthalpy = 0.226599

Standard orientation:

1	6	0	-0.744179	1.711323	0.116215
2	6	0	0.063101	0.556090	-0.108257
3	6	0	-0.491215	-0.753206	-0.234383
4	6	0	-1.865965	-0.958939	-0.125977
5	6	0	-2.728048	0.200890	0.125432
6	6	0	-2.115222	1.513541	0.232173
7	6	0	-2.504594	-2.322206	-0.268938
8	6	0	0.516782	-1.845721	-0.564604
9	6	0	1.931218	-1.445575	-0.074181
10	6	0	2.213585	-1.853462	1.381914
11	34	0	1.987446	0.586732	-0.270420
12	8	0	-4.014217	0.067035	0.245321
13	6	0	-0.126093	3.090510	0.226758
14	1	0	-2.787615	2.348393	0.413707
15	1	0	0.535375	-1.989544	-1.655975
16	1	0	0.232516	-2.807368	-0.119186
17	1	0	2.708101	-1.831024	-0.741205
18	1	0	1.448503	-1.454799	2.058733
19	1	0	3.190295	-1.489983	1.721133
20	1	0	2.210955	-2.950094	1.467902
21	1	0	-2.153320	-3.014614	0.509666
22	1	0	-2.268309	-2.778064	-1.240562
23	1	0	-3.589706	-2.228262	-0.181738
24	1	0	-0.887556	3.848046	0.437865
25	1	0	0.382090	3.375518	-0.705456
26	1	0	0.623043	3.127152	1.029920

5f Radical cation

E(UB+HF-LYP) = -511.733879761 (LANL2DZ)
Zero-point correction = 0.225364

Standard orientation:

1	6	0	-1.810508	-1.009774	-0.109559
2	6	0	-0.439277	-0.773856	-0.208104
3	6	0	0.086434	0.557619	-0.097396
4	6	0	-2.643286	0.137171	0.112434
5	6	0	-2.124397	1.460432	0.209849
6	6	0	-0.758100	1.703807	0.103022
7	6	0	0.581413	-1.855986	-0.509220
8	6	0	2.017467	-1.400190	-0.143385

9	34	0	1.968446	0.646883	-0.242713
10	6	0	2.481435	-1.830764	1.260877
11	6	0	-2.413279	-2.391669	-0.234189
12	6	0	-0.196411	3.103751	0.199296
13	8	0	-3.982308	-0.109100	0.218668
14	1	0	-2.806728	2.292202	0.371674
15	1	0	0.531404	-2.095510	-1.581812
16	1	0	0.352036	-2.782628	0.029773
17	1	0	2.745499	-1.702788	-0.900626
18	1	0	1.768827	-1.527376	2.036628
19	1	0	3.464837	-1.420066	1.513782
20	1	0	2.566354	-2.925417	1.283212
21	1	0	-2.034353	-2.909233	-1.123723
22	1	0	-3.500858	-2.342807	-0.301723
23	1	0	-2.160780	-3.010271	0.638256
24	1	0	-0.988352	3.840342	0.359447
25	1	0	0.335576	3.384324	-0.719887
26	1	0	0.514888	3.193544	1.031067
27	1	0	-4.545990	0.681219	0.365089

5g Antioxidant

E(RB+HF-LYP) = -551.293115887 (LANL2DZ)
E(ROB+HF-LYP) = -551.462211330 (LANL2DZdp)

Zero-point correction = 0.252283
Thermal correction to Enthalpy = 0.268831

Standard orientation:

1	6	0	1.331357	1.466209	-0.165098
2	6	0	0.026118	0.945936	-0.245722
3	6	0	-0.198915	-0.444682	-0.141417
4	6	0	2.382256	0.542426	0.023125
5	6	0	2.175891	-0.853579	0.123035
6	6	0	0.851461	-1.364178	0.042785
7	6	0	-1.209824	1.794050	-0.509488
8	6	0	-2.472703	1.072670	0.025845
9	34	0	-2.104322	-0.903229	-0.301221
10	6	0	-2.743294	1.344816	1.515496
11	8	0	3.680856	1.089541	0.105964
12	6	0	1.611187	2.952716	-0.284907
13	6	0	3.383779	-1.760937	0.309810
14	6	0	0.578128	-2.856106	0.148719
15	1	0	-1.311342	1.946994	-1.595872
16	1	0	-1.130204	2.788628	-0.051171
17	1	0	-3.353165	1.317953	-0.576717
18	1	0	-1.875661	1.070305	2.127333
19	1	0	-3.606227	0.773283	1.875956
20	1	0	-2.951813	2.414292	1.672198
21	1	0	4.362752	0.400083	0.227228
22	1	0	1.177305	3.365749	-1.205567
23	1	0	2.686177	3.141456	-0.295426
24	1	0	1.176672	3.509372	0.557931
25	1	0	3.899061	-1.568118	1.264194
26	1	0	4.118781	-1.633455	-0.501008
27	1	0	3.103743	-2.815705	0.310095
28	1	0	0.966888	-3.402734	-0.722174
29	1	0	-0.495777	-3.058390	0.209947
30	1	0	1.040272	-3.292296	1.043772

5g Phenoxyl radical

E(ROB+HF-LYP) = -550.830669399 (LANL2DZdp)

Thermal correction to Enthalpy = 0.256296

Standard orientation:

1	6	0	0.925449	-1.344565	0.034356
2	6	0	-0.149094	-0.428037	-0.139544
3	6	0	0.039506	0.982738	-0.239111
4	6	0	1.316506	1.525099	-0.151378
5	6	0	2.453670	0.620864	0.045167
6	6	0	2.226233	-0.828681	0.130203
7	6	0	1.580818	3.010147	-0.265710
8	6	0	-1.222438	1.787441	-0.516442
9	6	0	-2.473927	1.021625	-0.018370
10	6	0	-2.821877	1.305446	1.453127
11	34	0	-2.008012	-0.947968	-0.277062
12	8	0	3.657012	1.100192	0.137543
13	6	0	3.440498	-1.712760	0.323199
14	6	0	0.636400	-2.833177	0.104074
15	1	0	-1.304090	1.954263	-1.601686
16	1	0	-1.184176	2.776607	-0.042783
17	1	0	-3.338497	1.210653	-0.661832
18	1	0	-1.965204	1.104473	2.107453
19	1	0	-3.661968	0.690169	1.795064
20	1	0	-3.104533	2.361943	1.571854
21	1	0	1.080123	3.569993	0.537414
22	1	0	1.212410	3.411772	-1.220210
23	1	0	2.654644	3.198317	-0.199129
24	1	0	4.340128	-1.094372	0.350069
25	1	0	3.541810	-2.443107	-0.491157
26	1	0	3.381944	-2.278592	1.263657
27	1	0	0.338376	-3.223029	-0.880462
28	1	0	-0.189765	-3.040048	0.797945
29	1	0	1.504645	-3.406501	0.436148

5g Radical cation

E(UB+HF-LYP) = -551.045540248 (LANL2DZ)

Zero-point correction = 0.253261

Standard orientation:

1	6	0	1.284702	1.518604	-0.138758
2	6	0	0.001458	0.986639	-0.217227
3	6	0	-0.189961	-0.437545	-0.131847
4	6	0	2.357735	0.585533	0.045101
5	6	0	2.190575	-0.837069	0.122228
6	6	0	0.894821	-1.365342	0.024729
7	6	0	-1.254126	1.805231	-0.467736
8	6	0	-2.530788	1.016065	-0.081271
9	34	0	-2.009492	-0.952320	-0.256487
10	6	0	-3.033834	1.287302	1.349265
11	8	0	3.596642	1.157049	0.135984
12	6	0	1.604812	2.992011	-0.244988
13	6	0	3.425462	-1.699224	0.305374
14	6	0	0.651432	-2.860738	0.088627
15	1	0	-1.294003	2.072505	-1.533725
16	1	0	-1.239459	2.745218	0.094714
17	1	0	-3.334207	1.164322	-0.807628
18	1	0	-2.243798	1.134834	2.093740
19	1	0	-3.886161	0.652158	1.613780
20	1	0	-3.368414	2.331271	1.413766
21	1	0	4.341573	0.530066	0.257222
22	1	0	0.743705	3.577549	-0.573587
23	1	0	2.426341	3.159067	-0.949922
24	1	0	1.944734	3.387908	0.721145
25	1	0	3.954074	-1.459263	1.240192
26	1	0	4.132379	-1.578930	-0.529296
27	1	0	3.180349	-2.760206	0.352579
28	1	0	1.185610	-3.383244	-0.714504
29	1	0	-0.406722	-3.119233	-0.007389
30	1	0	0.999856	-3.280346	1.040631

6 Antioxidant

E(RB+HF-LYP) = -532.599991864 (LANL2DZ)
E(ROB+HF-LYP) = -532.751710235 (LANL2DZdp)

Zero-point correction = 0.160560
Thermal correction to Enthalpy = 0.172664

Standard orientation:

1	6	0	1.810638	0.700685	-0.163108
2	6	0	0.433560	0.514108	-0.259994
3	6	0	-0.087181	-0.783815	-0.046744
4	6	0	2.692016	-0.356900	0.133986
5	6	0	2.153971	-1.641769	0.333916
6	6	0	0.762964	-1.858954	0.247000
7	6	0	-0.568137	1.588077	-0.639537
8	6	0	-1.964584	1.202558	-0.083103
9	34	0	-2.032665	-0.837429	-0.220832
10	6	0	-2.191048	1.663312	1.366268
11	9	0	2.337723	1.980675	-0.375050
12	8	0	4.053907	-0.061541	0.211654
13	1	0	2.817475	-2.473431	0.565438
14	1	0	0.367385	-2.856430	0.414364
15	1	0	-0.614140	1.654605	-1.736767
16	1	0	-0.267835	2.574587	-0.266328
17	1	0	-2.167990	2.762155	1.418829
18	1	0	-1.411434	1.272443	2.030993
19	1	0	-3.161502	1.324927	1.746588
20	1	0	-2.761712	1.572031	-0.735518
21	1	0	4.586394	-0.855851	0.420802

6 Phenoxyl radical

E(ROB+HF-LYP) = -532.114727784 (LANL2DZdp)

Thermal correction to Enthalpy = 0.160056

Standard orientation:

1	6	0	0.816343	-1.875144	0.227020
2	6	0	-0.041162	-0.778631	-0.053241
3	6	0	0.475153	0.537462	-0.251159
4	6	0	1.838004	0.725874	-0.144826
5	6	0	2.779594	-0.346628	0.154469
6	6	0	2.186596	-1.664444	0.327599
7	9	0	2.356026	2.003392	-0.344458
8	6	0	-0.537126	1.600839	-0.633286
9	6	0	-1.940582	1.192643	-0.113225
10	6	0	-2.225137	1.663656	1.322549
11	34	0	-1.957828	-0.854035	-0.211006
12	8	0	4.051020	-0.144530	0.255608
13	1	0	2.871914	-2.477988	0.548614
14	1	0	0.405393	-2.870241	0.371980
15	1	0	-0.559065	1.688417	-1.729091
16	1	0	-0.259290	2.583679	-0.235272
17	1	0	-2.244223	2.762686	1.353375
18	1	0	-1.450037	1.316255	2.015833
19	1	0	-3.193284	1.298562	1.683471
20	1	0	-2.727729	1.527755	-0.794847

6 Radical cation

E(UB+HF-LYP) = -532.330548201 (LANL2DZ)

Zero-point correction = 0.161231

Standard orientation:

1	6	0	1.794663	0.757245	-0.126344
2	6	0	0.431500	0.556838	-0.227562
3	6	0	-0.067026	-0.774869	-0.053879
4	6	0	2.693762	-0.319450	0.139041
5	6	0	2.177590	-1.640425	0.293815
6	6	0	0.809199	-1.870592	0.196381
7	6	0	-0.580399	1.624671	-0.578598
8	6	0	-2.009554	1.171065	-0.176078
9	34	0	-1.946569	-0.889672	-0.189258
10	6	0	-2.460726	1.649730	1.216451
11	9	0	2.316359	2.023665	-0.293402
12	8	0	4.007485	0.000724	0.220730
13	1	0	2.858659	-2.464168	0.491709
14	1	0	0.420923	-2.876720	0.319428
15	1	0	-0.536254	1.808523	-1.661273
16	1	0	-0.344783	2.575791	-0.087977
17	1	0	-2.548752	2.744091	1.194668
18	1	0	-1.738847	1.382153	1.996539
19	1	0	-3.440663	1.247648	1.494702
20	1	0	-2.749218	1.432828	-0.937166
21	1	0	4.621126	-0.745362	0.399568

4a Methoxy analogue

E(RB+HF-LYP) = -472.657659009 (LANL2DZ)

Zero-point correction = 0.197695
Thermal correction to Enthalpy = 0.210217

Standard orientation:

1	6	0	1.459919	1.158512	-0.364386
2	6	0	0.123082	0.747401	-0.383107
3	6	0	-0.201728	-0.597095	-0.074652
4	6	0	2.477785	0.231401	-0.047964
5	6	0	2.155761	-1.107537	0.250069
6	6	0	0.804232	-1.517881	0.239283
7	8	0	3.778665	0.749175	-0.056673
8	6	0	-1.055002	1.626891	-0.774223
9	34	0	-2.126960	-0.942673	-0.142010
10	6	0	-2.350016	1.089685	-0.109367
11	6	0	-2.556458	1.599001	1.326886
12	1	0	1.742635	2.182638	-0.592303
13	1	0	2.926956	-1.829977	0.497518
14	1	0	0.561800	-2.549147	0.482992
15	1	0	-1.172173	1.594292	-1.868306
16	1	0	-0.892688	2.675909	-0.491869
17	1	0	-3.228561	1.304549	-0.725921
18	1	0	-1.692623	1.357551	1.957571
19	1	0	-3.445836	1.151965	1.785366
20	1	0	-2.686074	2.692096	1.324121
21	6	0	4.884206	-0.143195	0.256810
22	1	0	5.782253	0.474291	0.188754
23	1	0	4.948431	-0.969048	-0.465925
24	1	0	4.792522	-0.550758	1.273647

4a Radical cation

E(UB+HF-LYP) = -472.403817176 (LANL2DZ)

Zero-point correction = 0.198210

Standard orientation:

1	6	0	1.438997	1.202215	-0.303043
2	6	0	0.117264	0.792270	-0.340262
3	6	0	-0.195572	-0.588989	-0.085838
4	6	0	2.469704	0.252344	-0.024474
5	6	0	2.158177	-1.125493	0.208930
6	6	0	0.831400	-1.539316	0.175956
7	8	0	3.723976	0.762091	-0.008760
8	6	0	-1.064347	1.670270	-0.706810
9	34	0	-2.045683	-0.969046	-0.124748
10	6	0	-2.389463	1.060082	-0.178586
11	6	0	-2.797828	1.542369	1.225262
12	1	0	1.730044	2.231640	-0.487517
13	1	0	2.942912	-1.844427	0.416410
14	1	0	0.588280	-2.581622	0.360526
15	1	0	-1.109642	1.753228	-1.802100
16	1	0	-0.948183	2.686543	-0.312481
17	1	0	-3.209351	1.189823	-0.889664
18	1	0	-1.991135	1.406570	1.954798
19	1	0	-3.690288	1.026158	1.594738
20	1	0	-3.034984	2.613392	1.172946
21	6	0	4.911923	-0.077987	0.255674
22	1	0	5.751715	0.613066	0.198660
23	1	0	5.003555	-0.853146	-0.512738
24	1	0	4.846945	-0.516969	1.257071