Supporting Information

for

Catalytic and Highly Regenerable Aminic Organoselenium Antioxidants with Cytoprotective Effects

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---Table of Contents---

Figure S1. ^{1}H NMR spectrum of **5a**

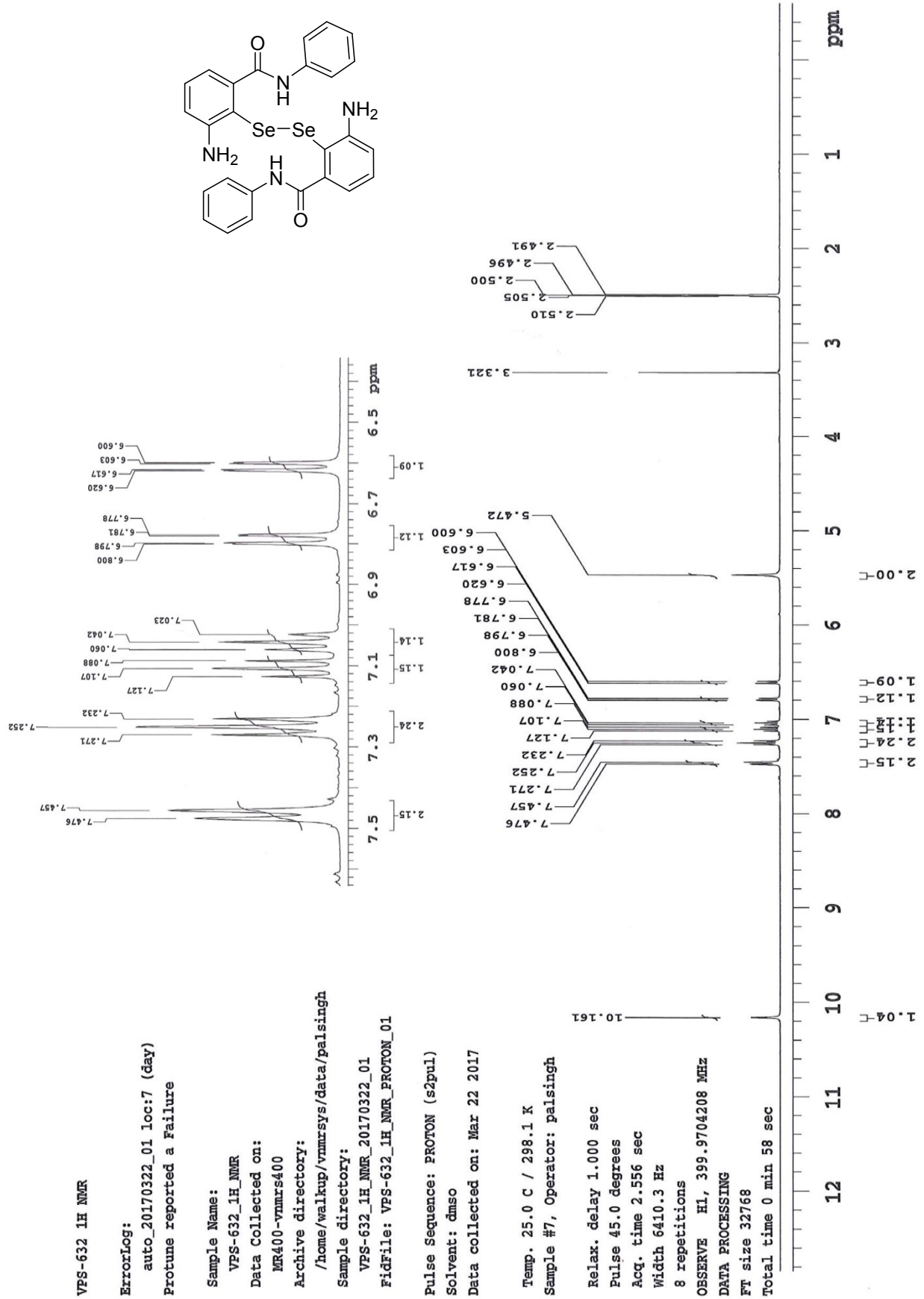


Figure S2. ^{13}C NMR spectrum of **5a**

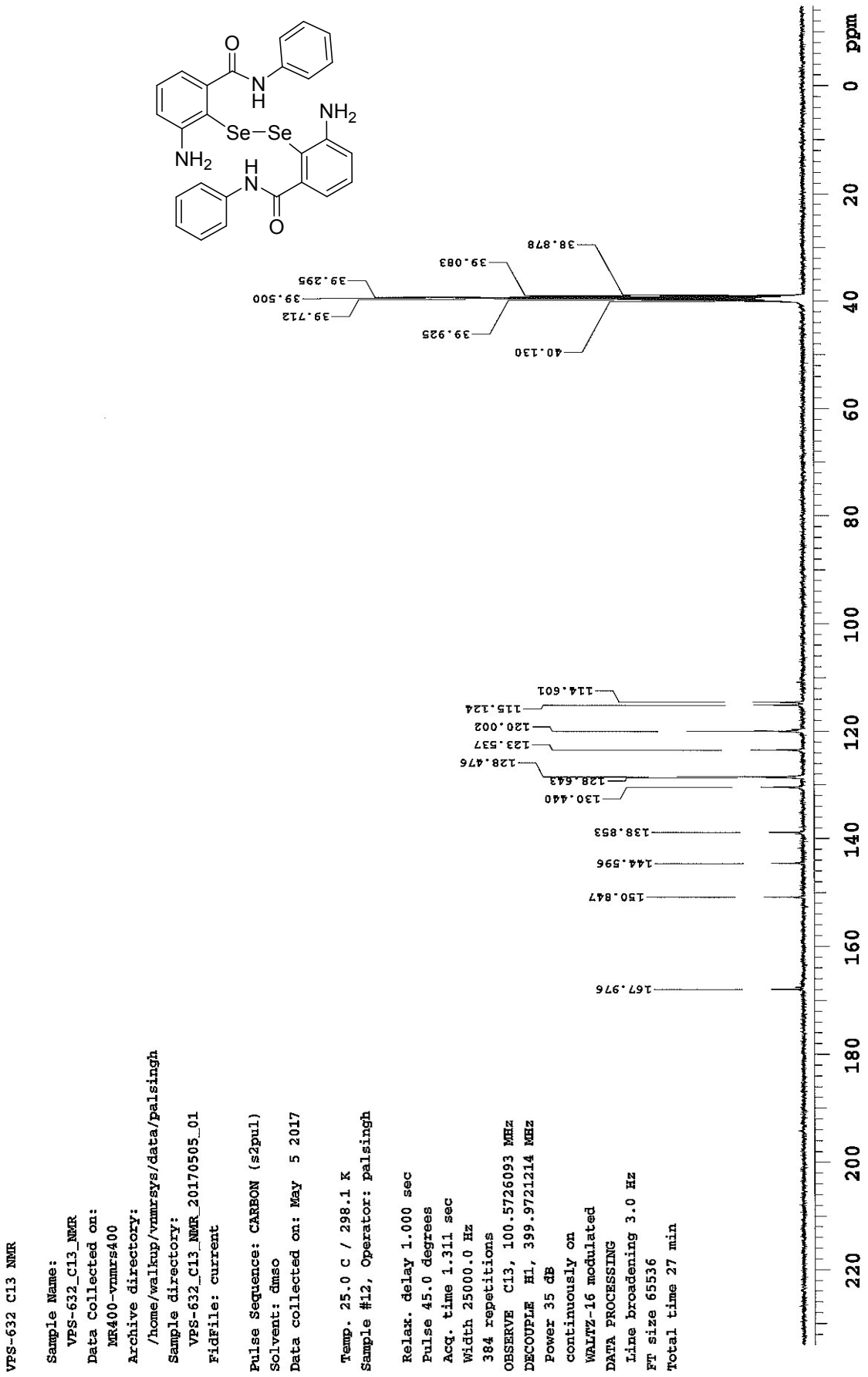


Figure S3.^{77}Se NMR spectrum of **5a**

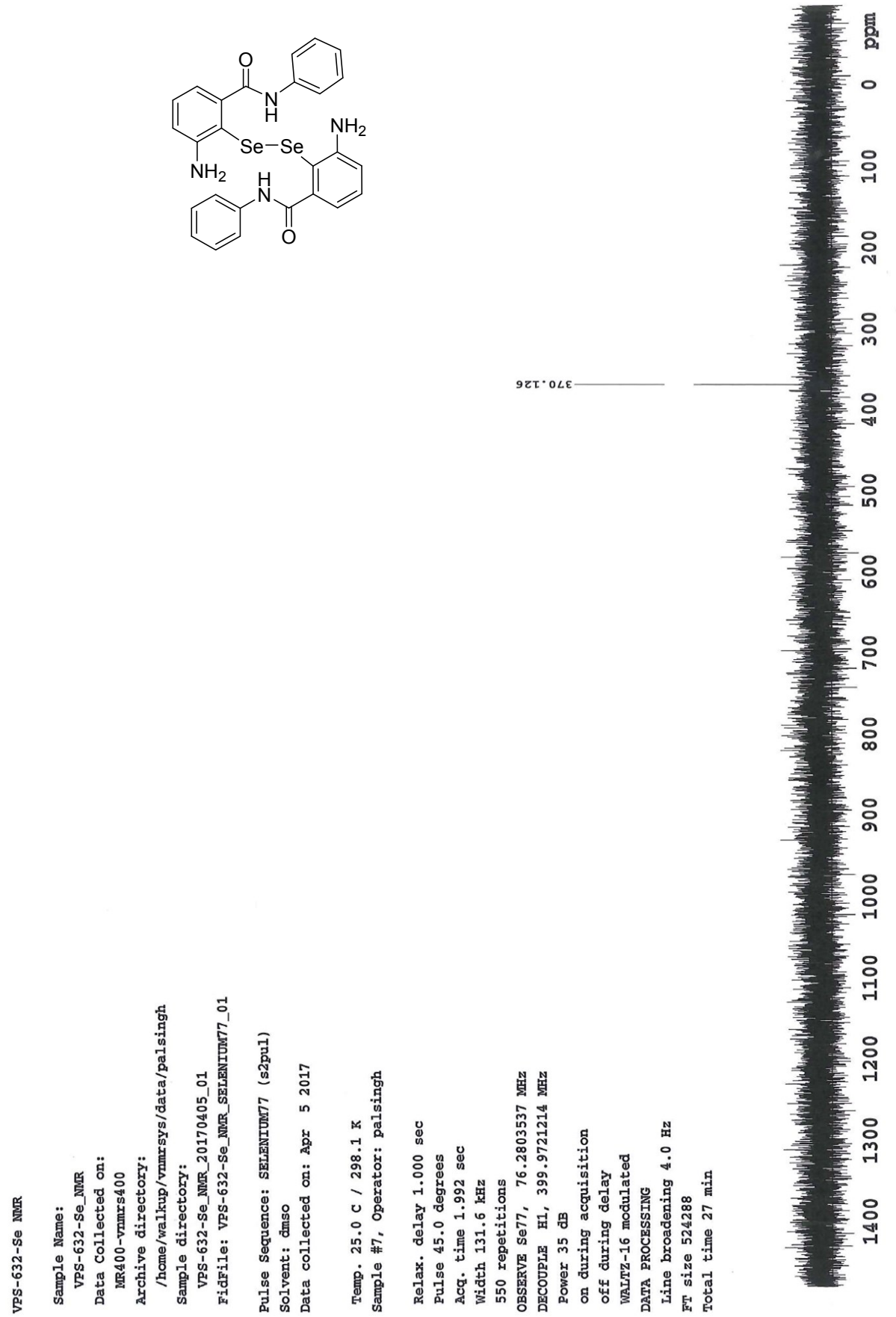


Figure S4. HRMS of **5a**

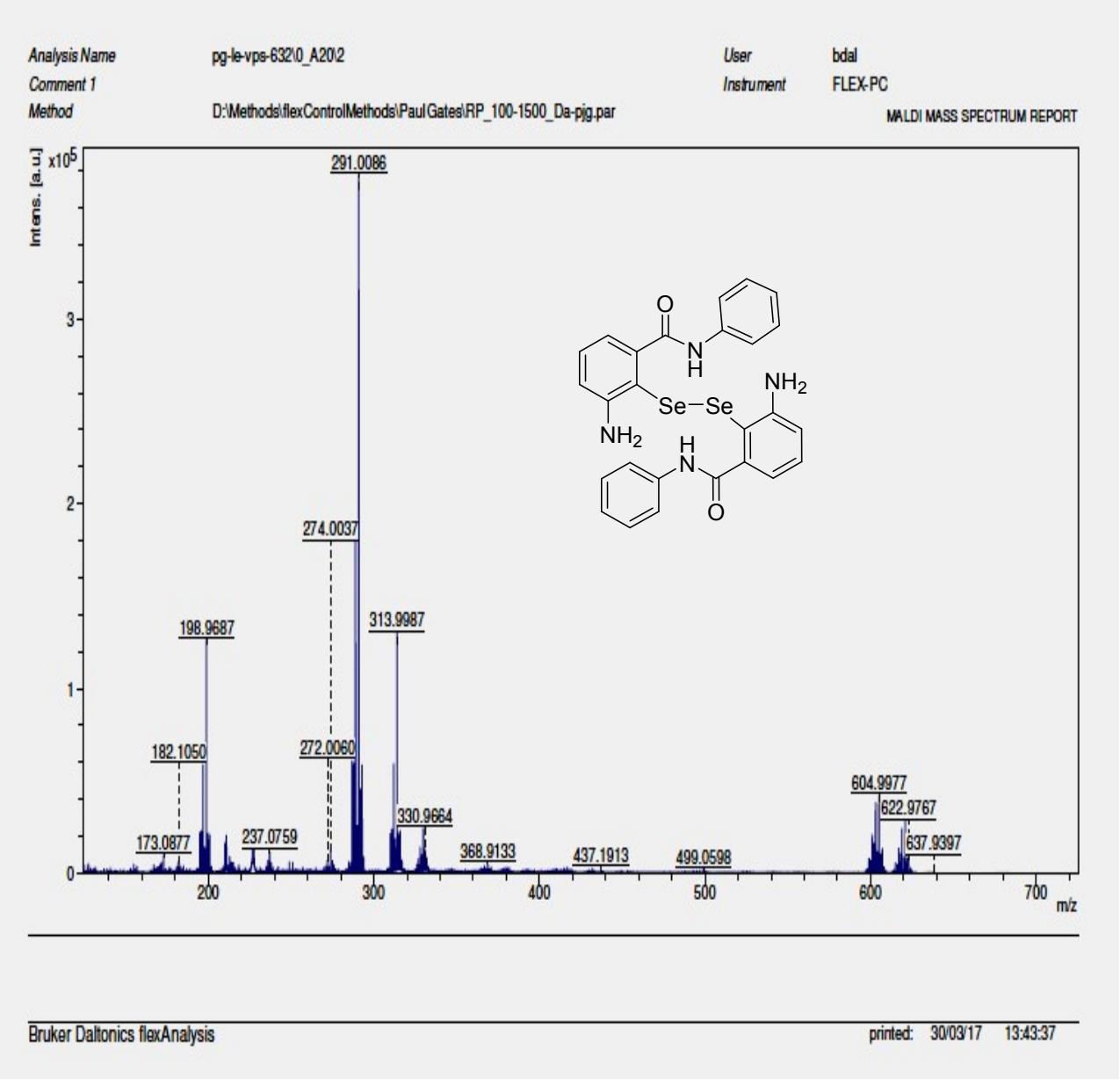
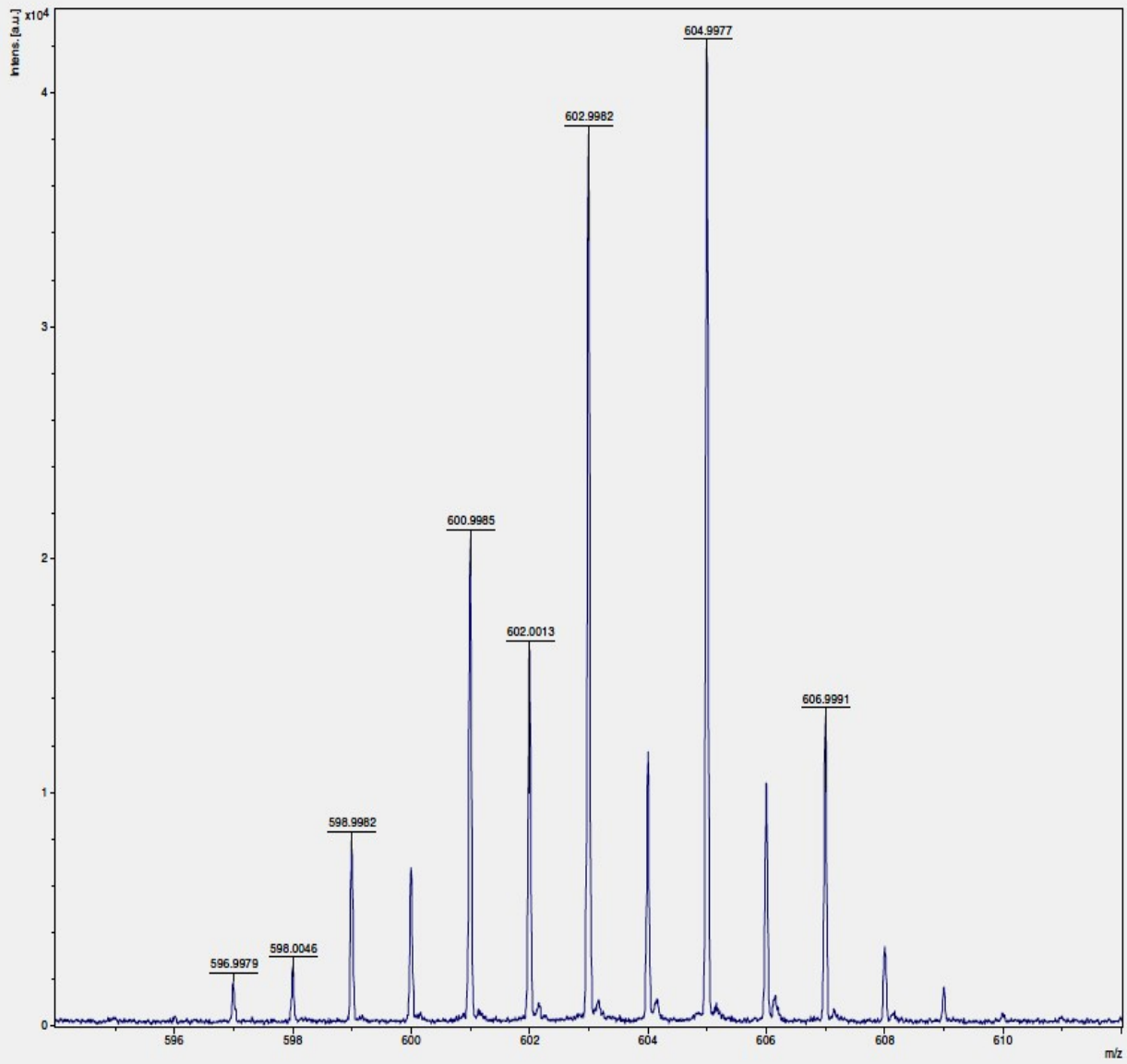


Figure S5. Expansion of the HRMS of **5a**



Formula	Calc m/z	Measured m/z	err [ppm]	ID
$C_{26}H_{22}N_4O_2Se_2$	604.9970	604.9977	1.16	$[M+Na]^+$

Figure S6.[1]H NMR spectrum of **5c**

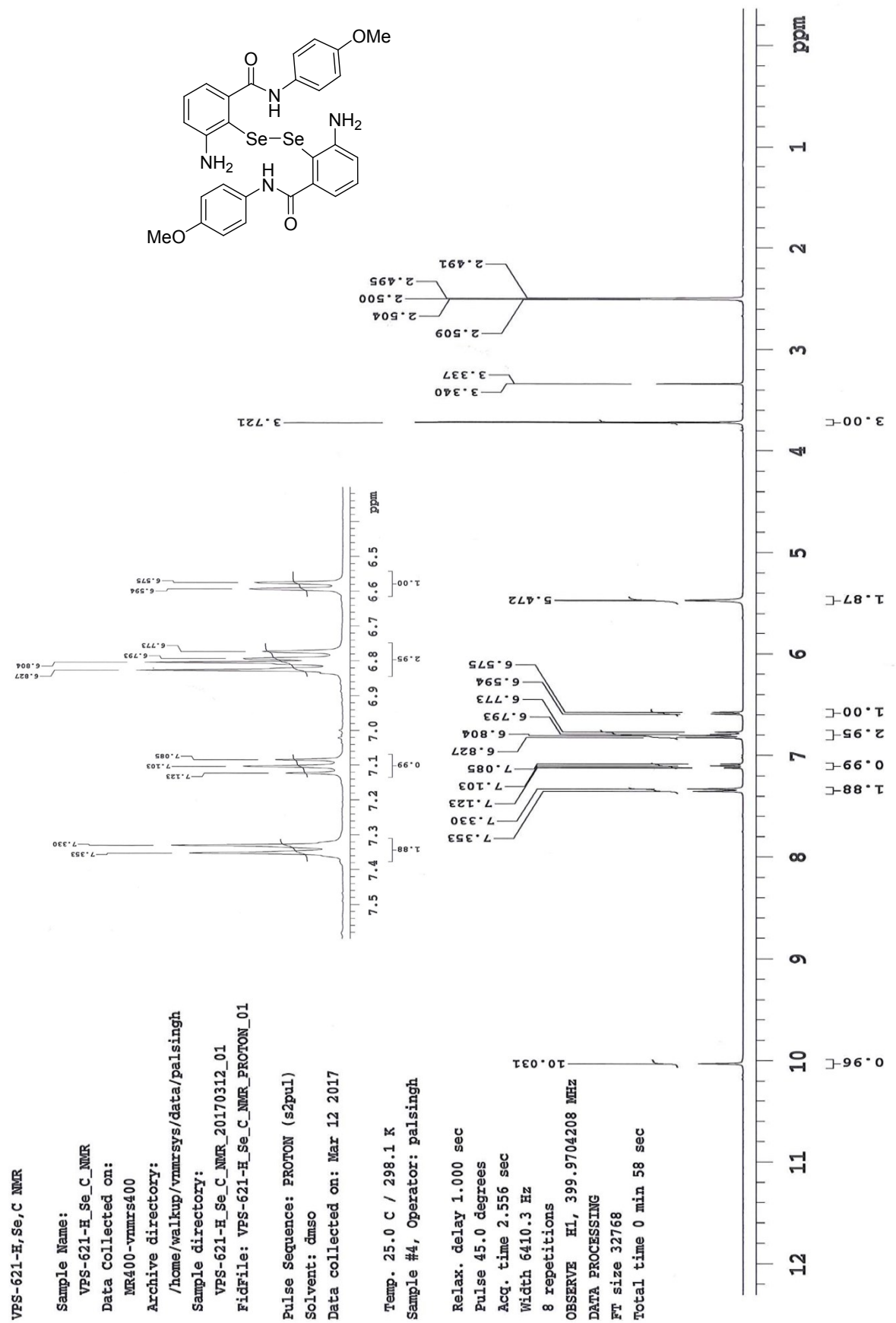


Figure S7. ^{13}C NMR spectrum of **5c**

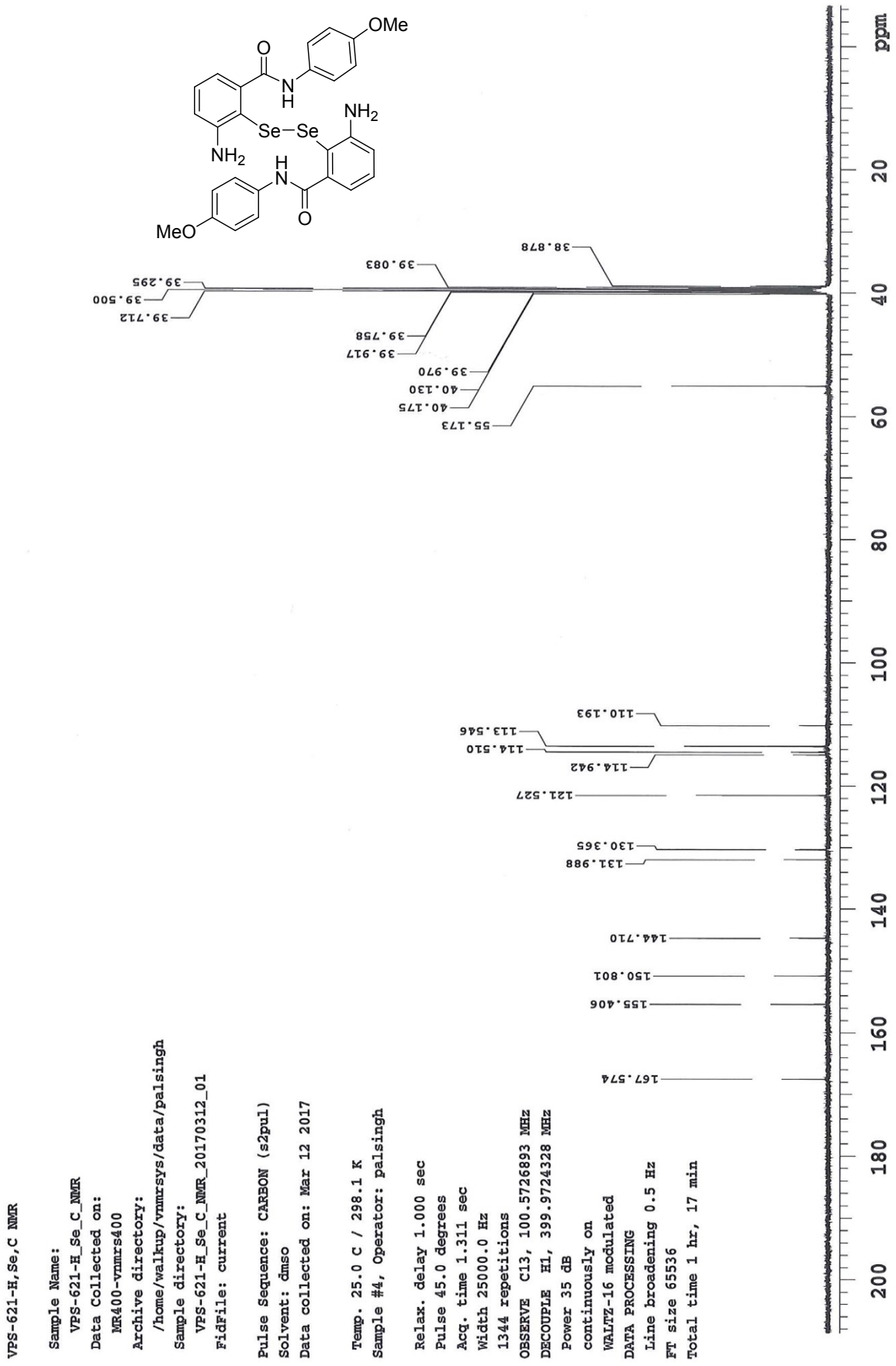


Figure S8. ^{77}Se NMR spectrum of **5c**

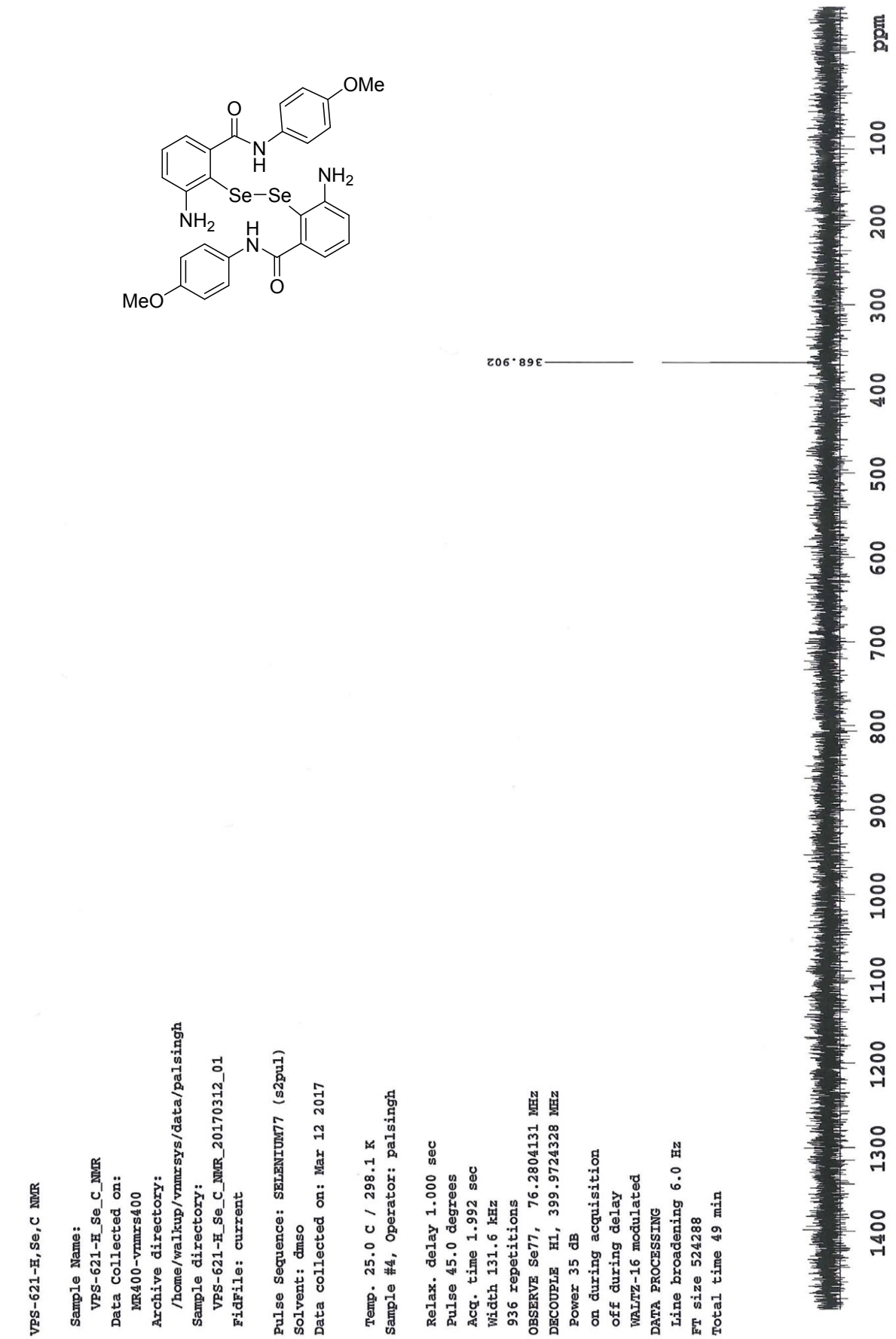


Figure S9. HRMS of **5c**

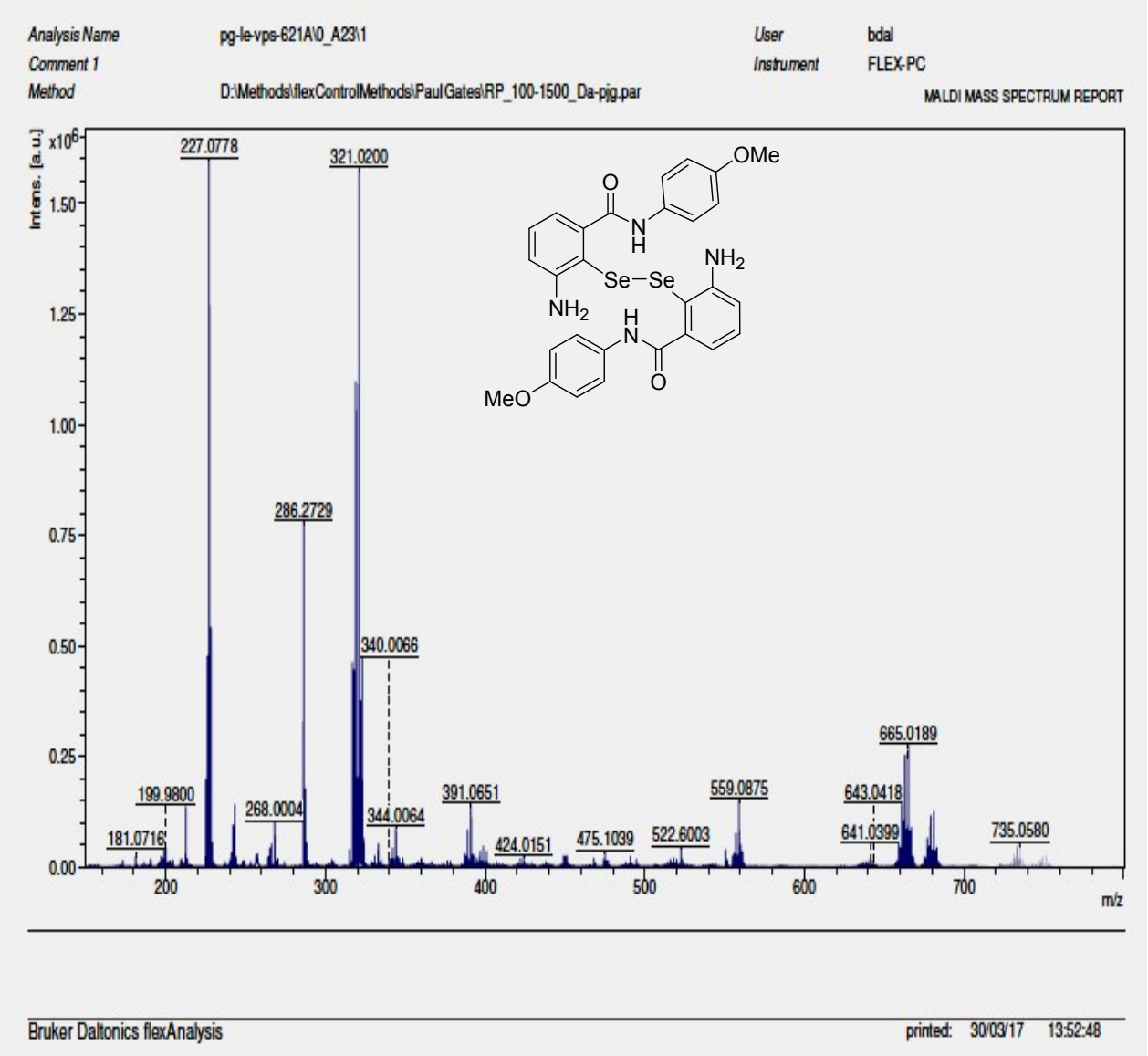
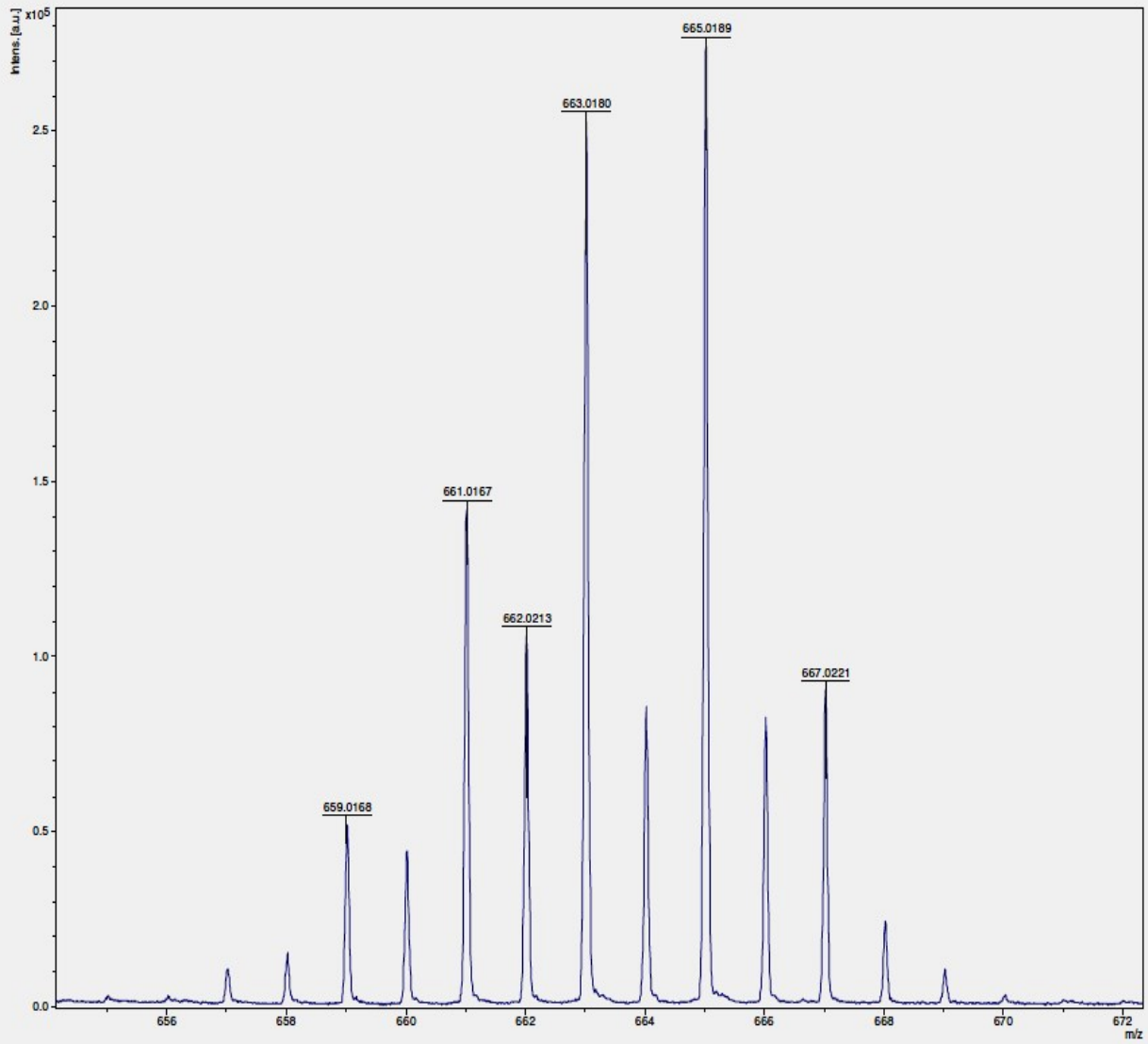


Figure S10. Expansion of the HRMS of **5c**



Formula	Calc m/z	Measured m/z	err [ppm]	ID
$C_{28}H_{26}N_4O_4Se_2$	665.0182	665.0189	1.05	$[M+Na]^+$

Figure S11. ^{1}H NMR spectrum of **6a**

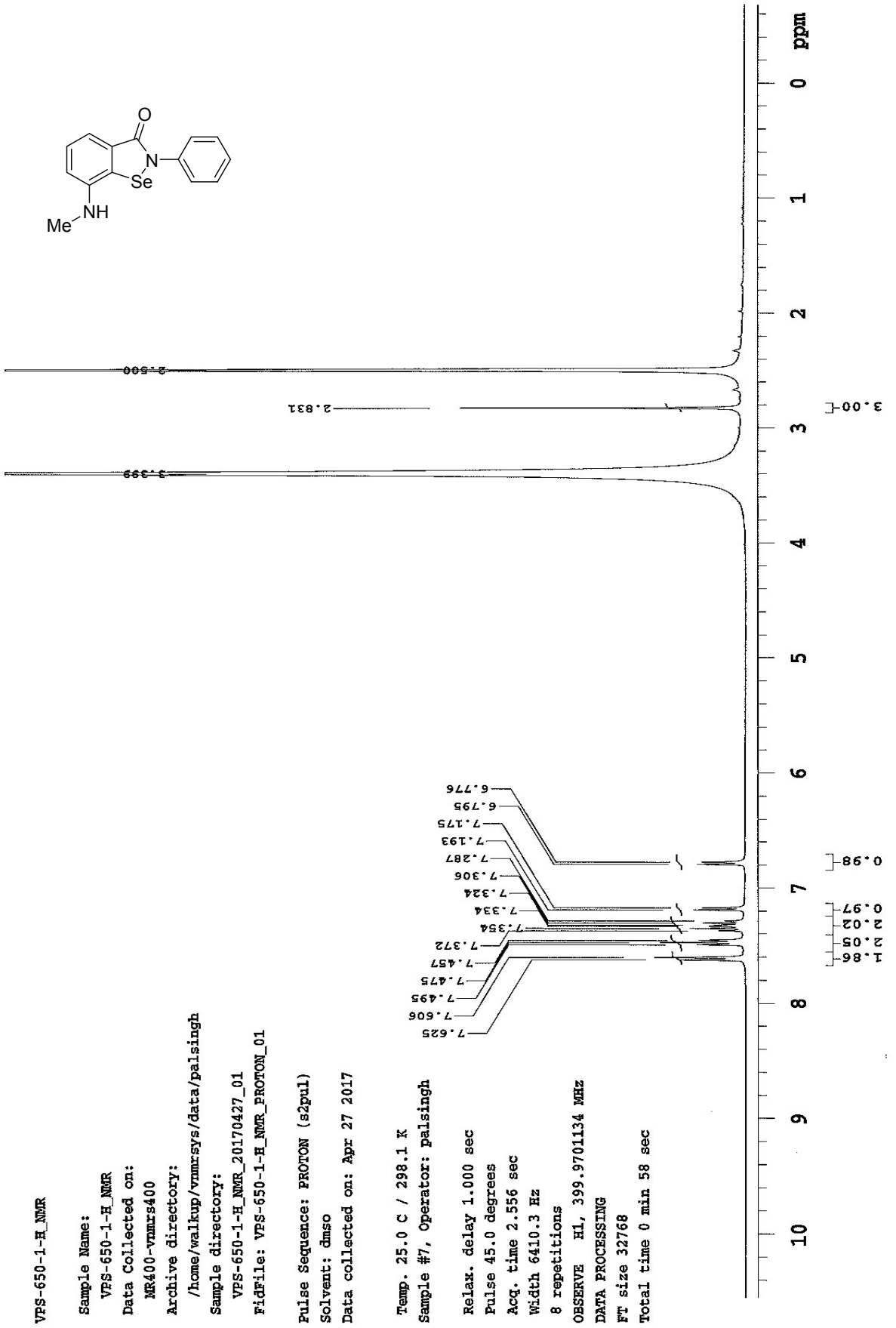


Figure S12. ^{13}C NMR spectrum of **6a**

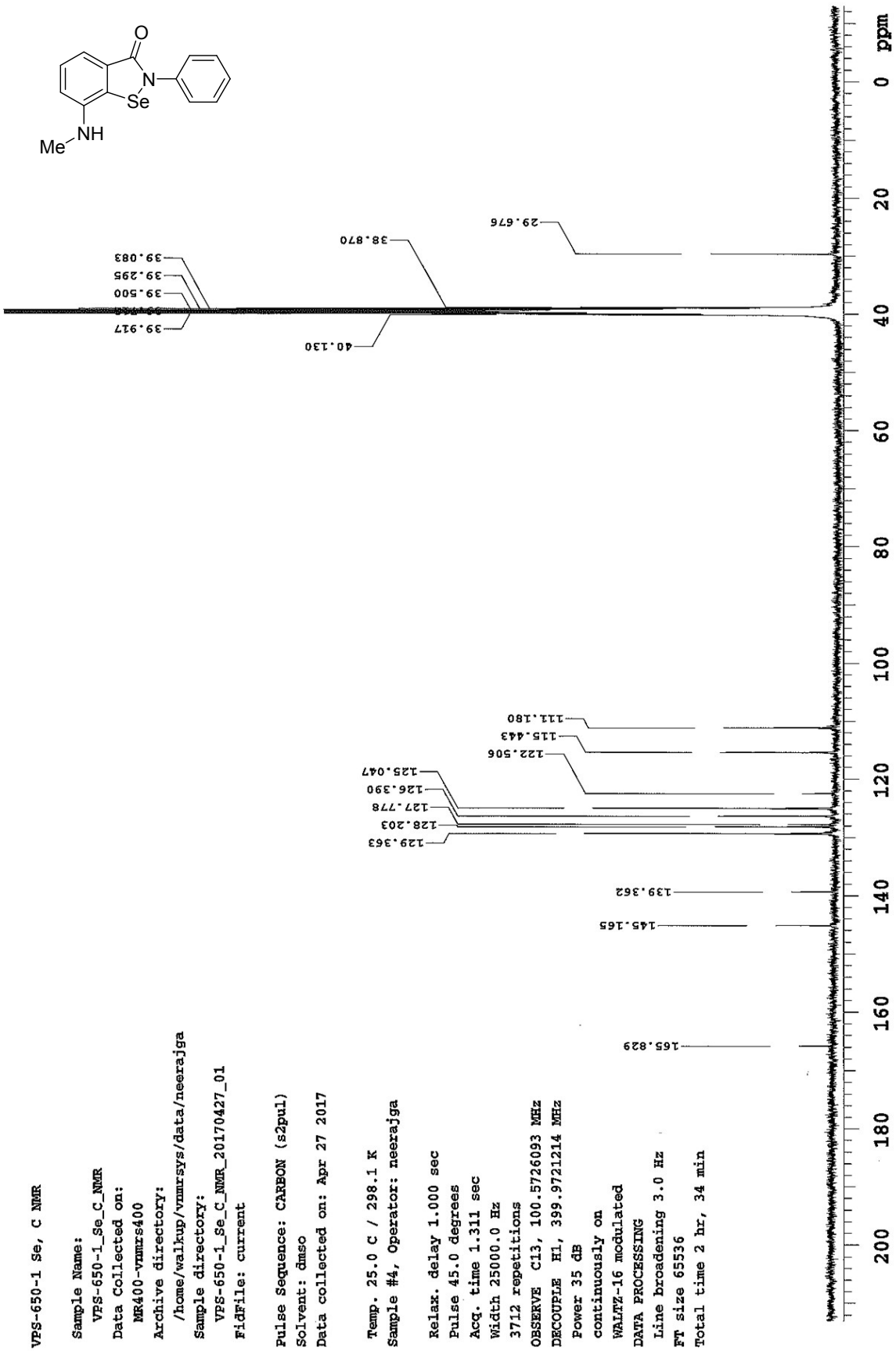


Figure S13. ^{77}Se NMR spectrum of **6a**

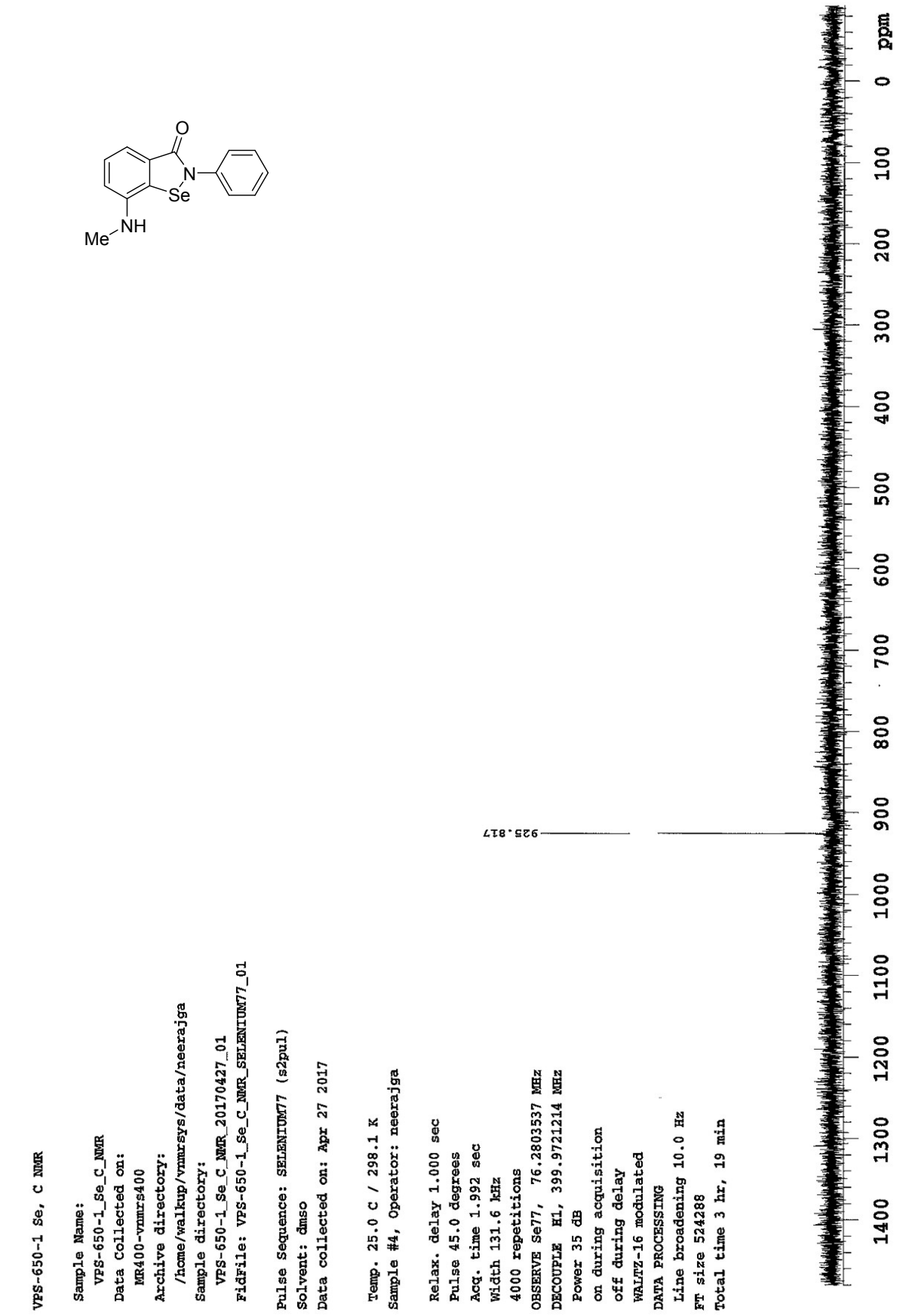


Figure S14. HRMS of **6a**

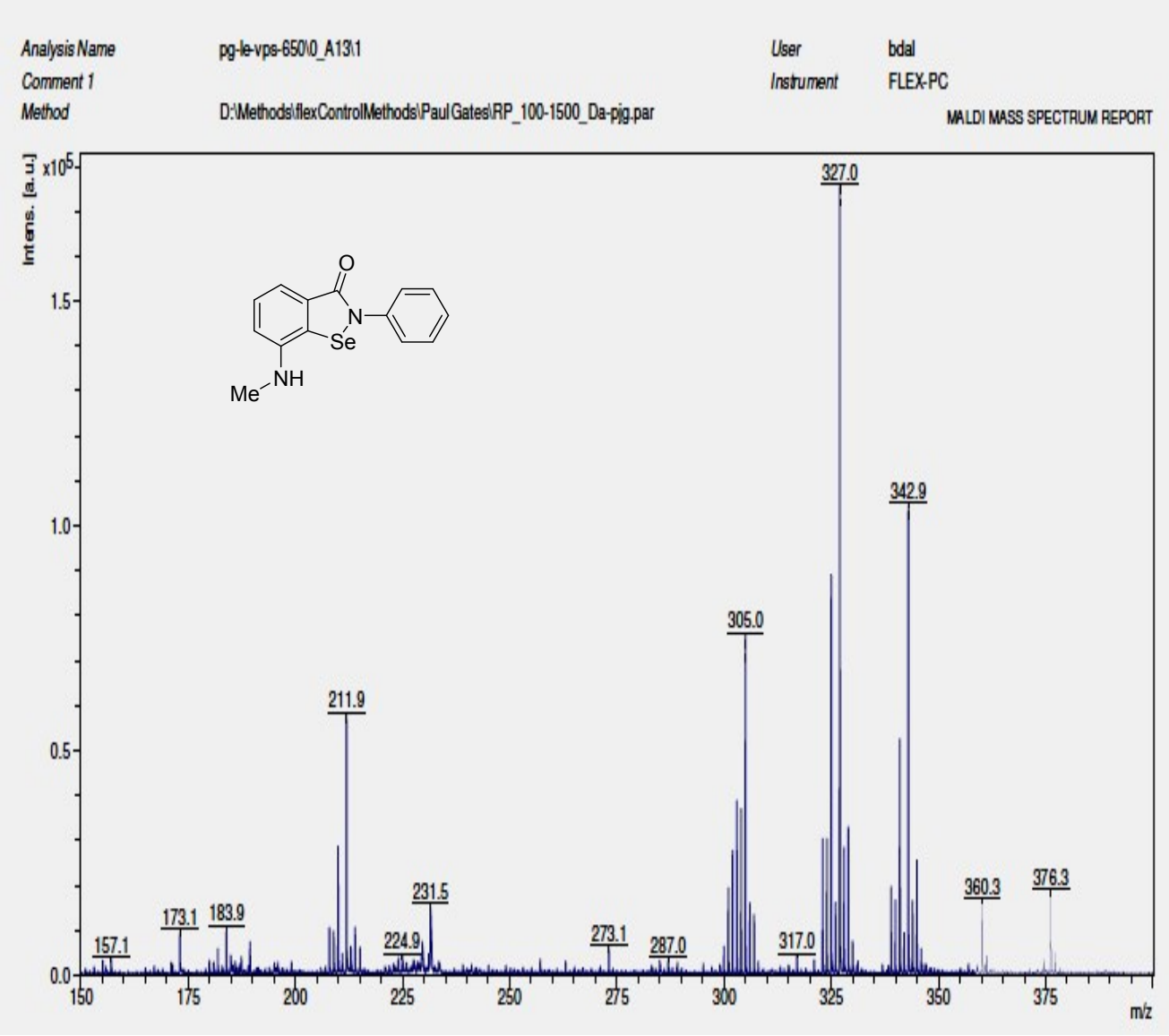
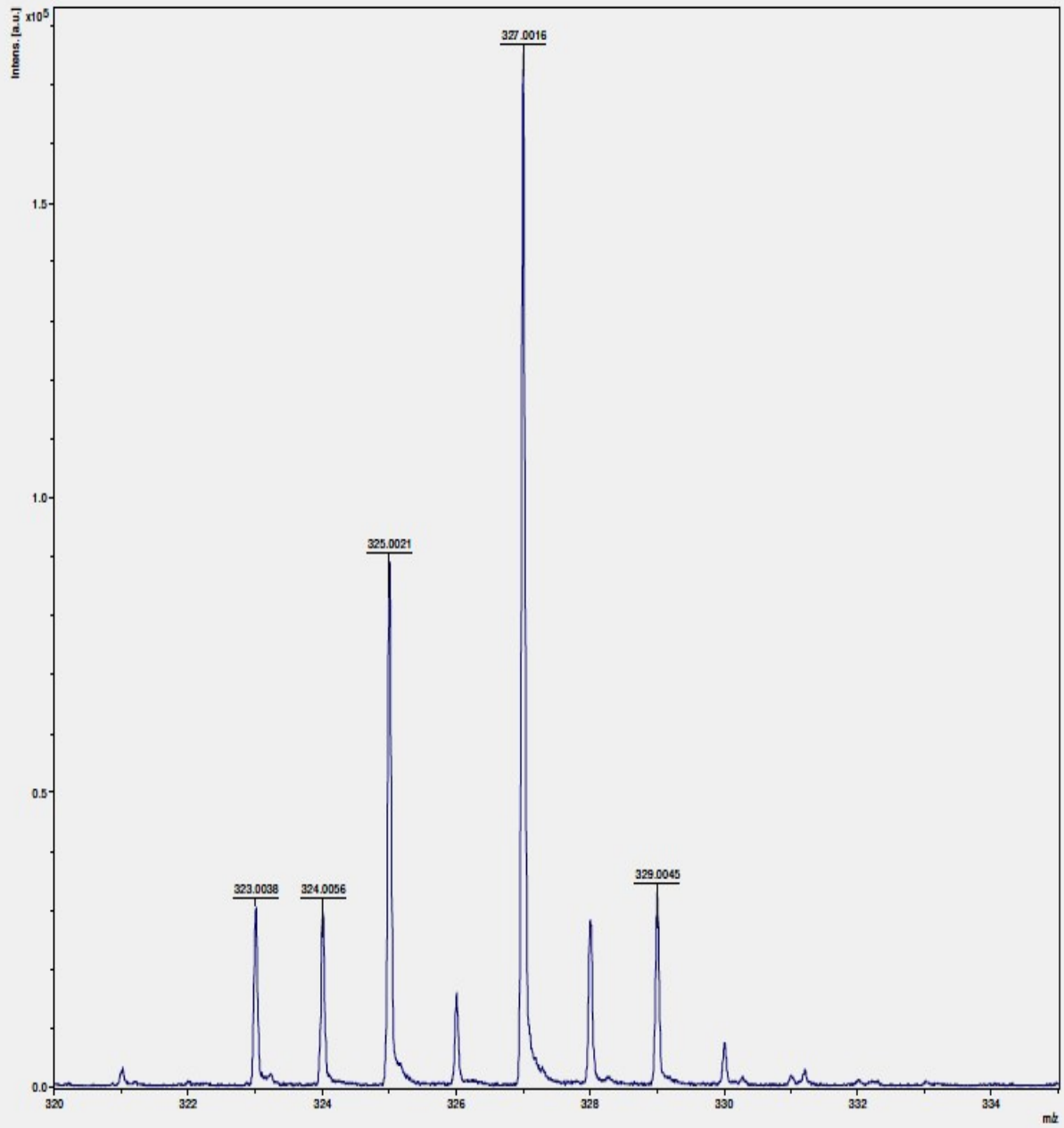


Figure S15. Expansion of the HRMS of **6a**



Formula	Calc m/z	Measured m/z	err [ppm]	ID
$C_{14}H_{12}N_2OSe$	327.0008	327.0016	2.45	$[M+Na]^+$

Figure S16. ^{1}H NMR spectrum of **6b**

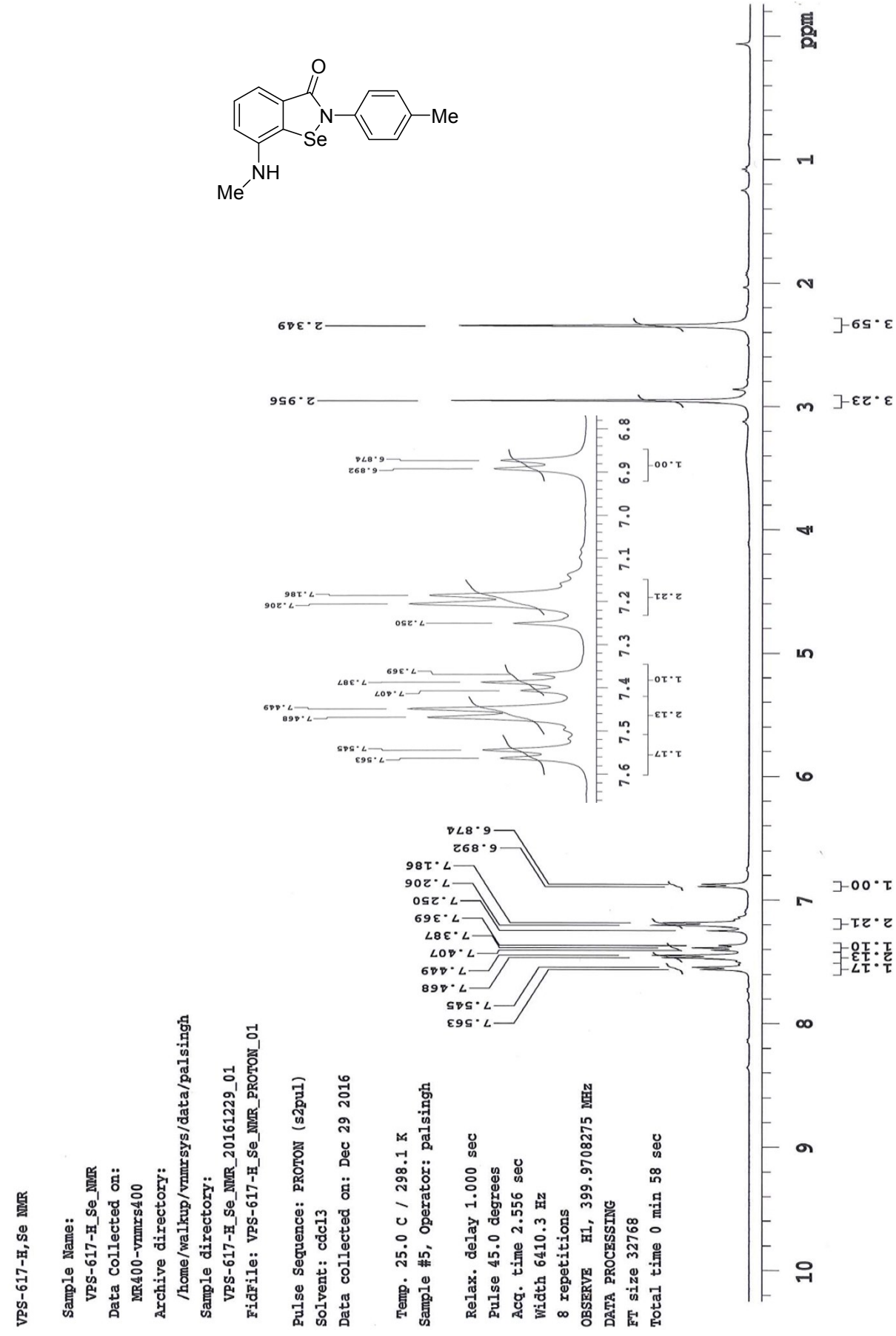


Figure S17. ^{13}C NMR spectrum of **6b**

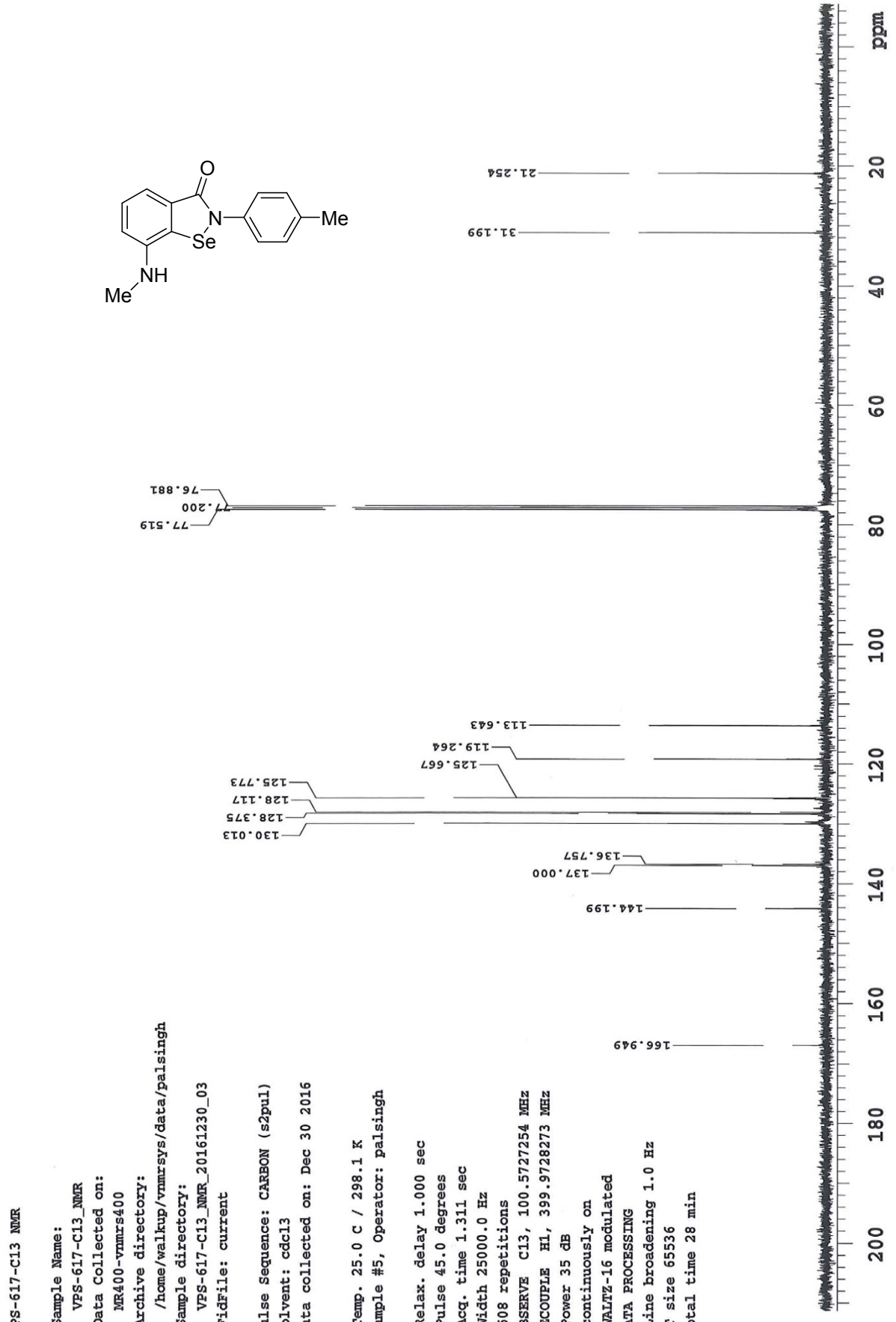


Figure S18. ^{77}Se NMR spectrum of **6b**

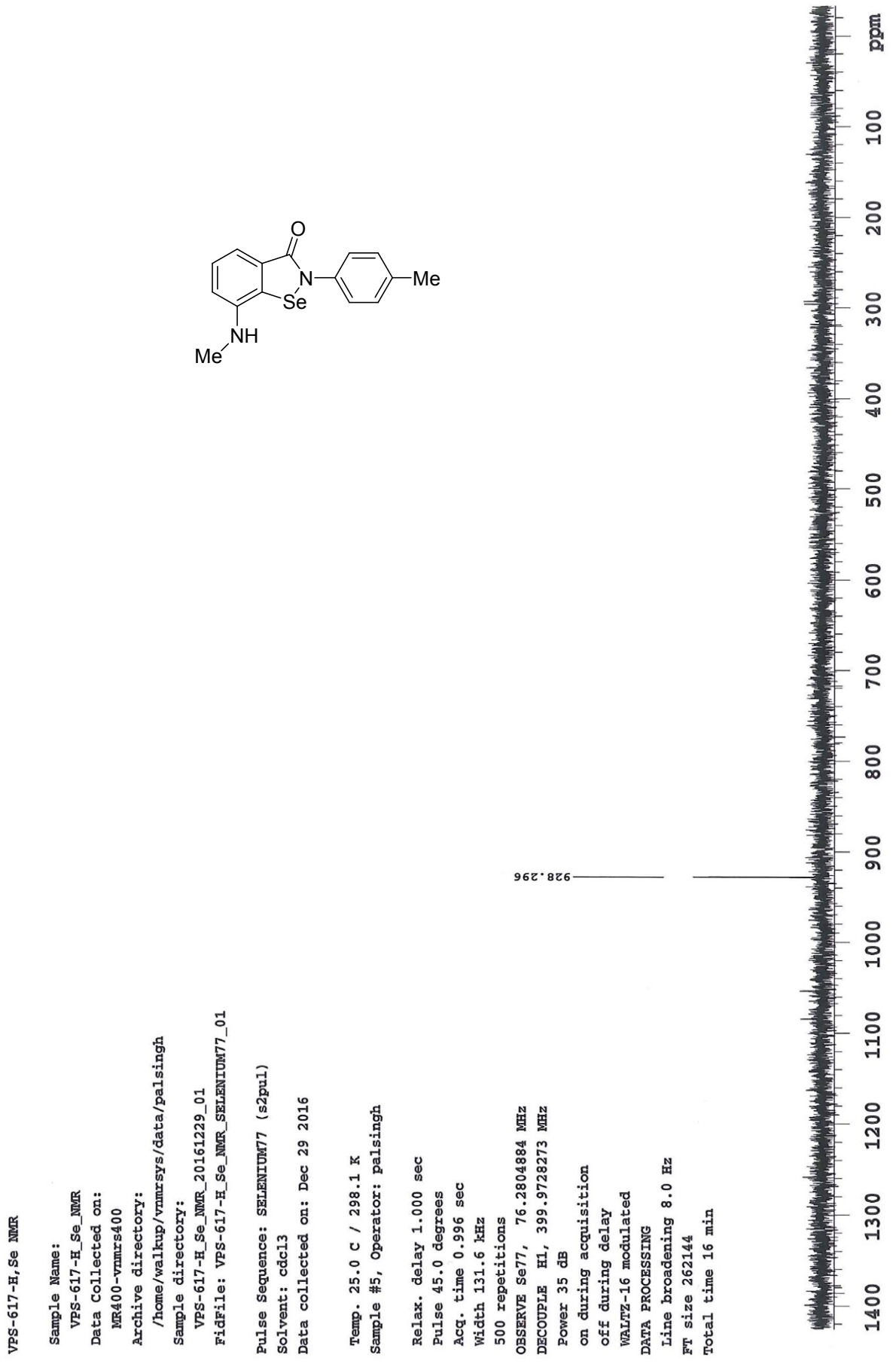


Figure S19. HRMS of 6b

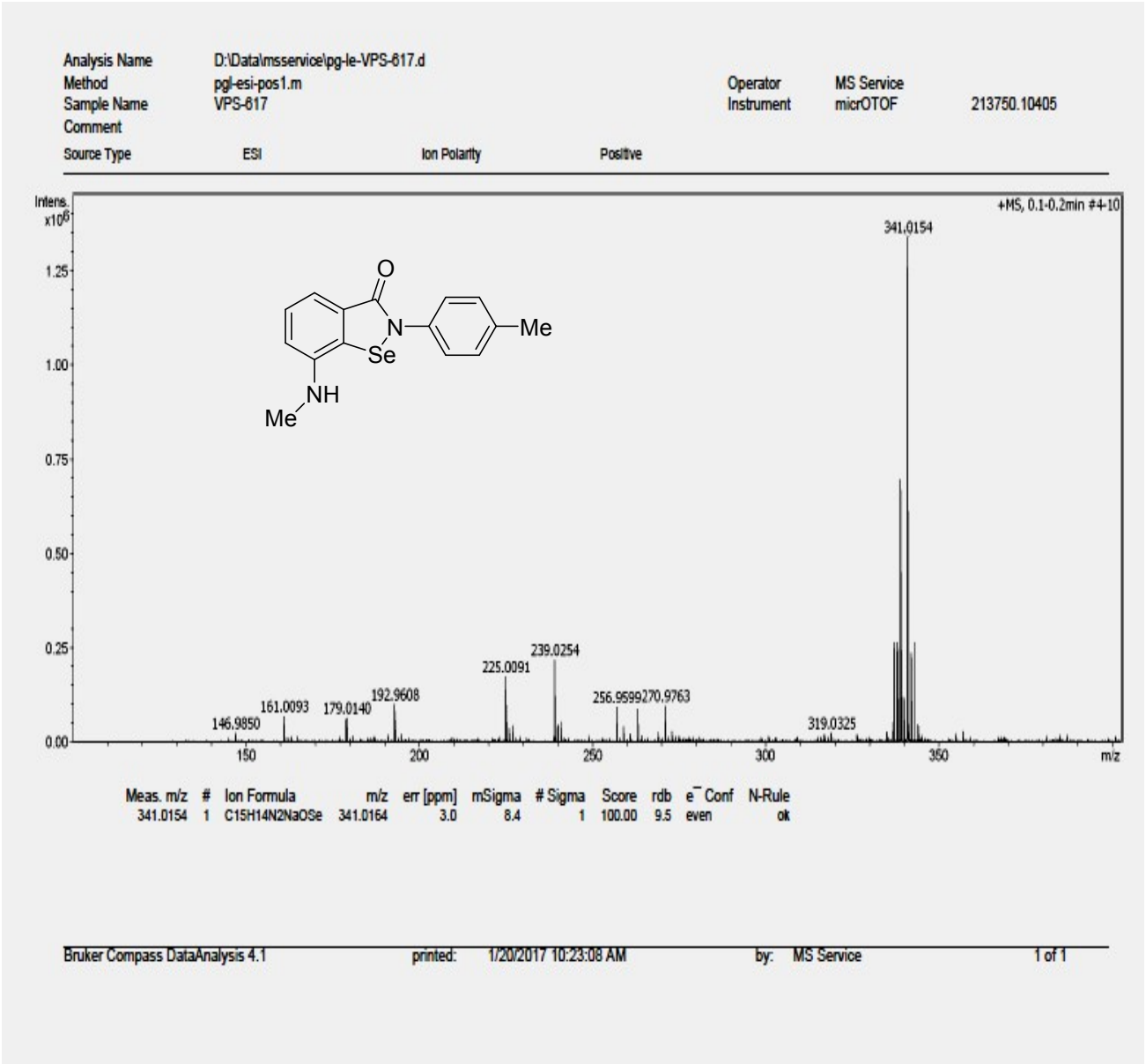


Figure S20. ^{1}H NMR spectrum of **6c**

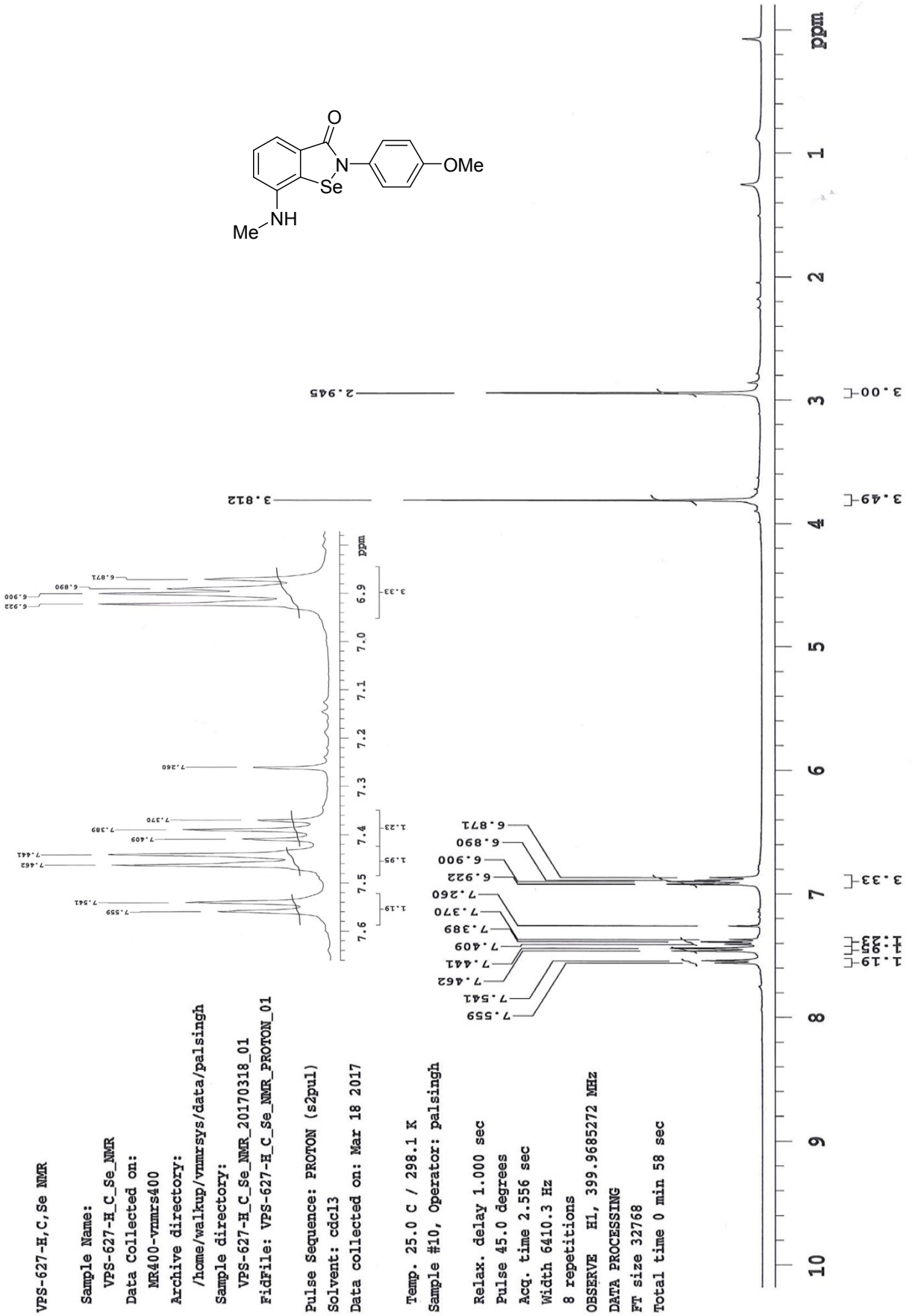


Figure S21. ^{13}C NMR spectrum of **6c**

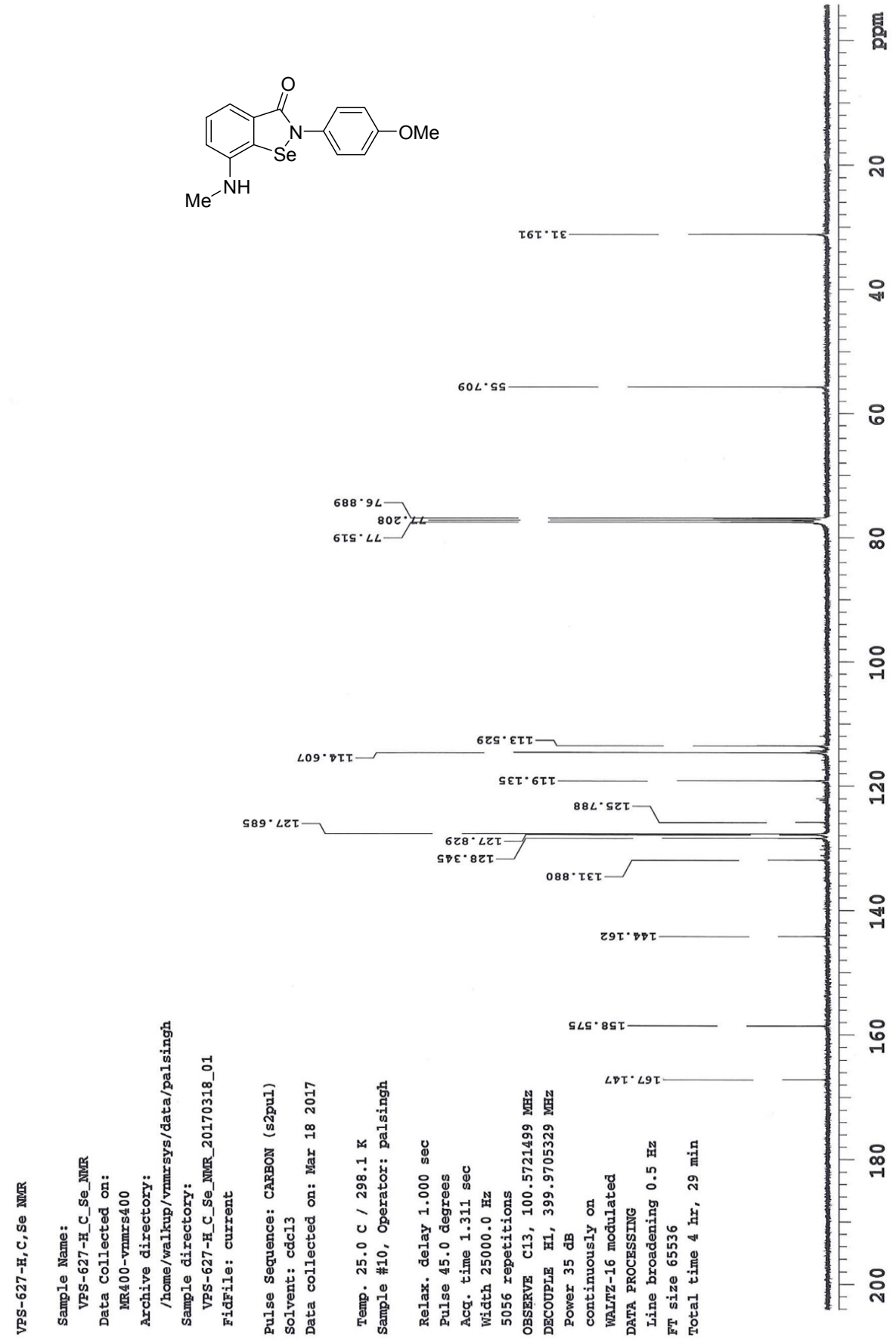


Figure S22. ^{77}Se NMR spectrum of **6c**

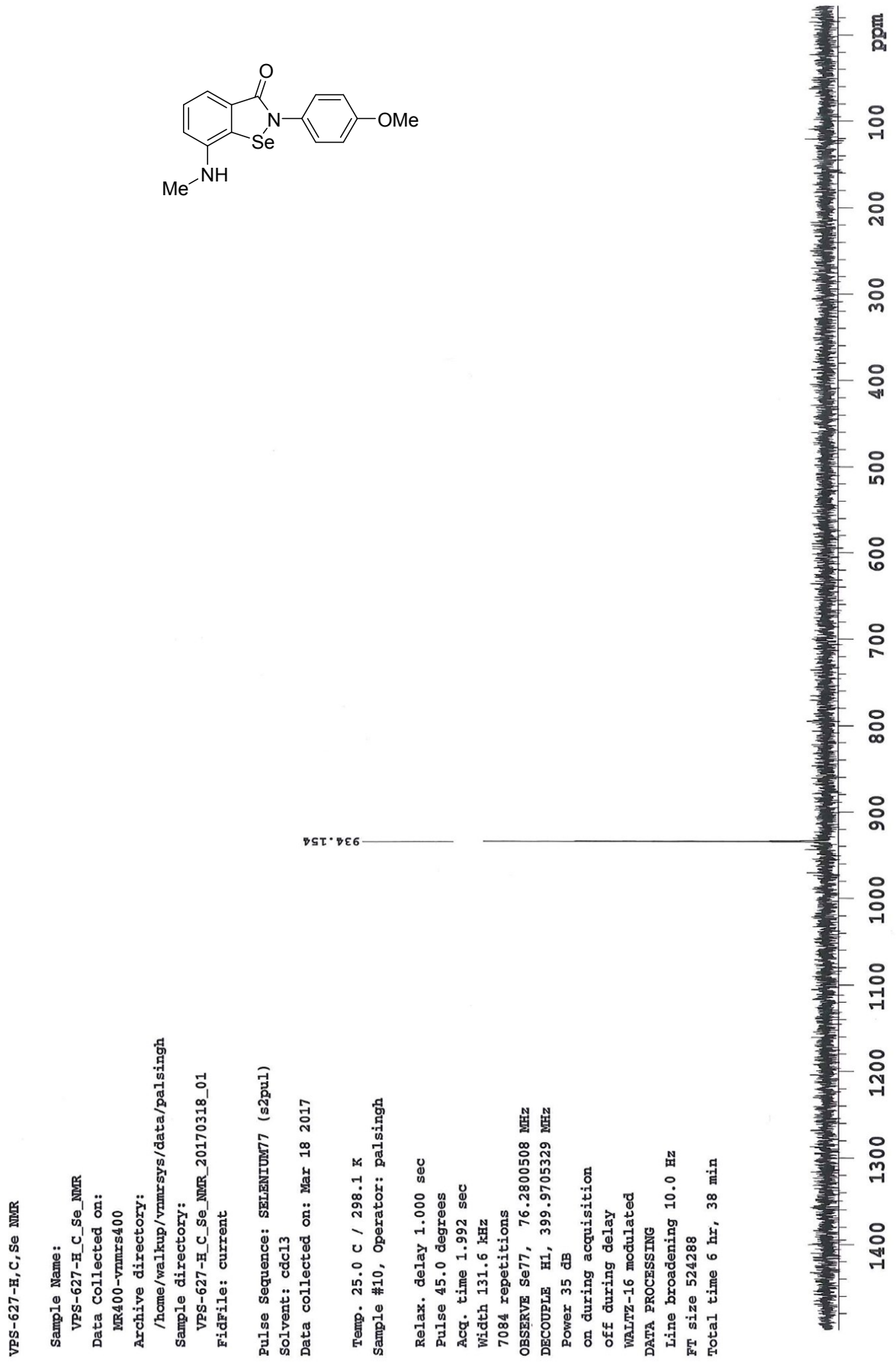
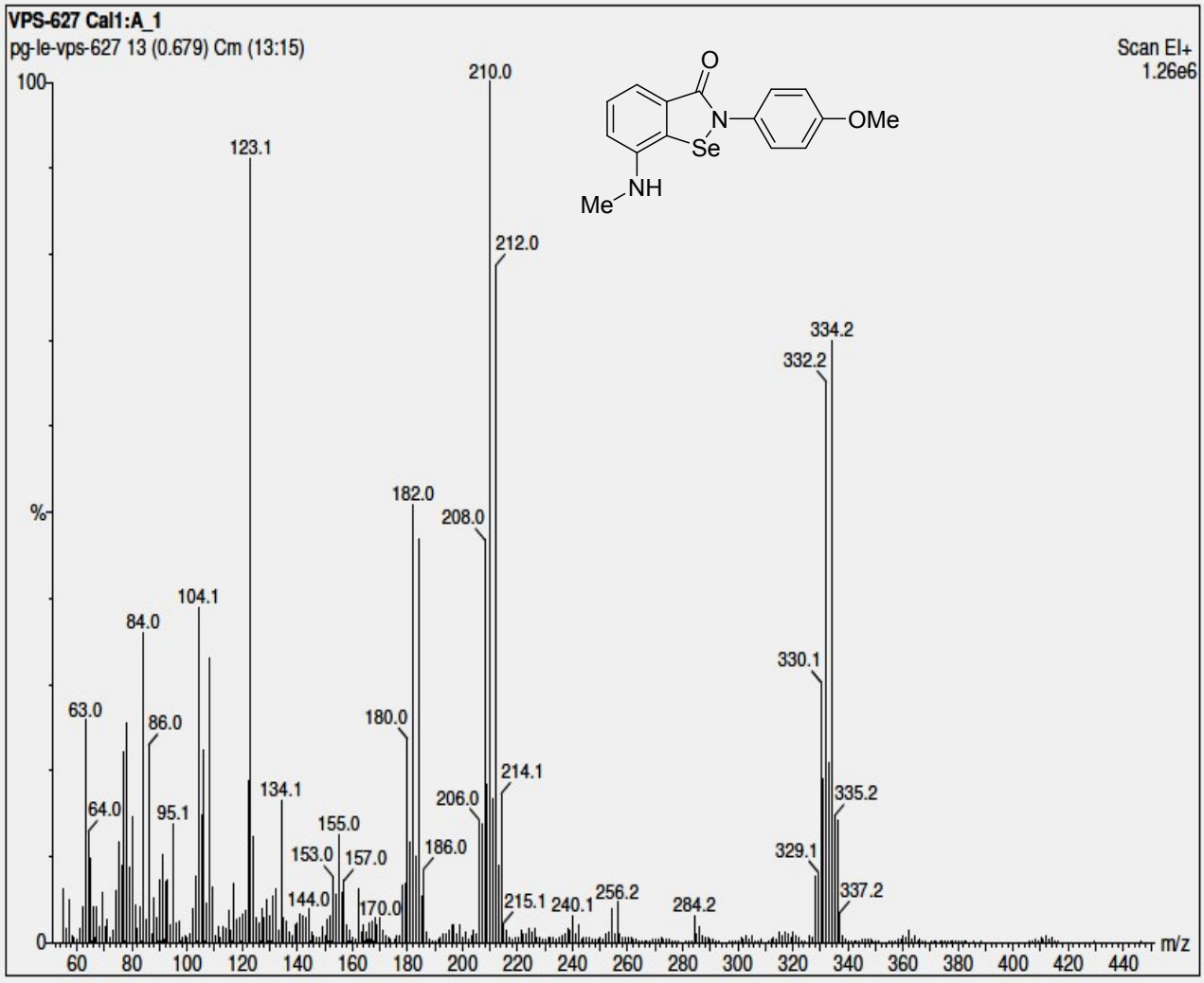


Figure S23. HRMS of **6c**



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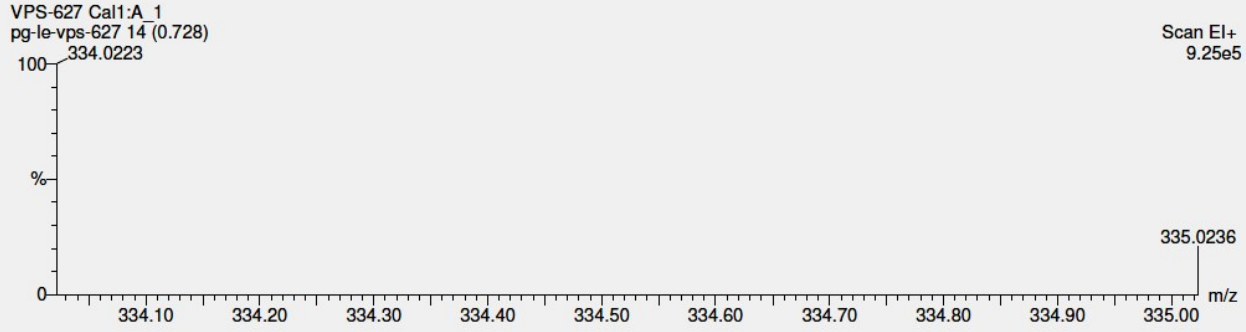
Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions
30 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)



Minimum:	90.00				-1.5		
Maximum:	100.00		200.0	10.0	80.0		
Mass	RA	Calc. Mass	mDa	PPM	DBE	Score	Formula
334.0223	100.00	334.0220	0.3	0.8	11.0	1	C15 H14 N2 O2 Se

Figure S24. ^{1}H NMR spectrum of **6d**

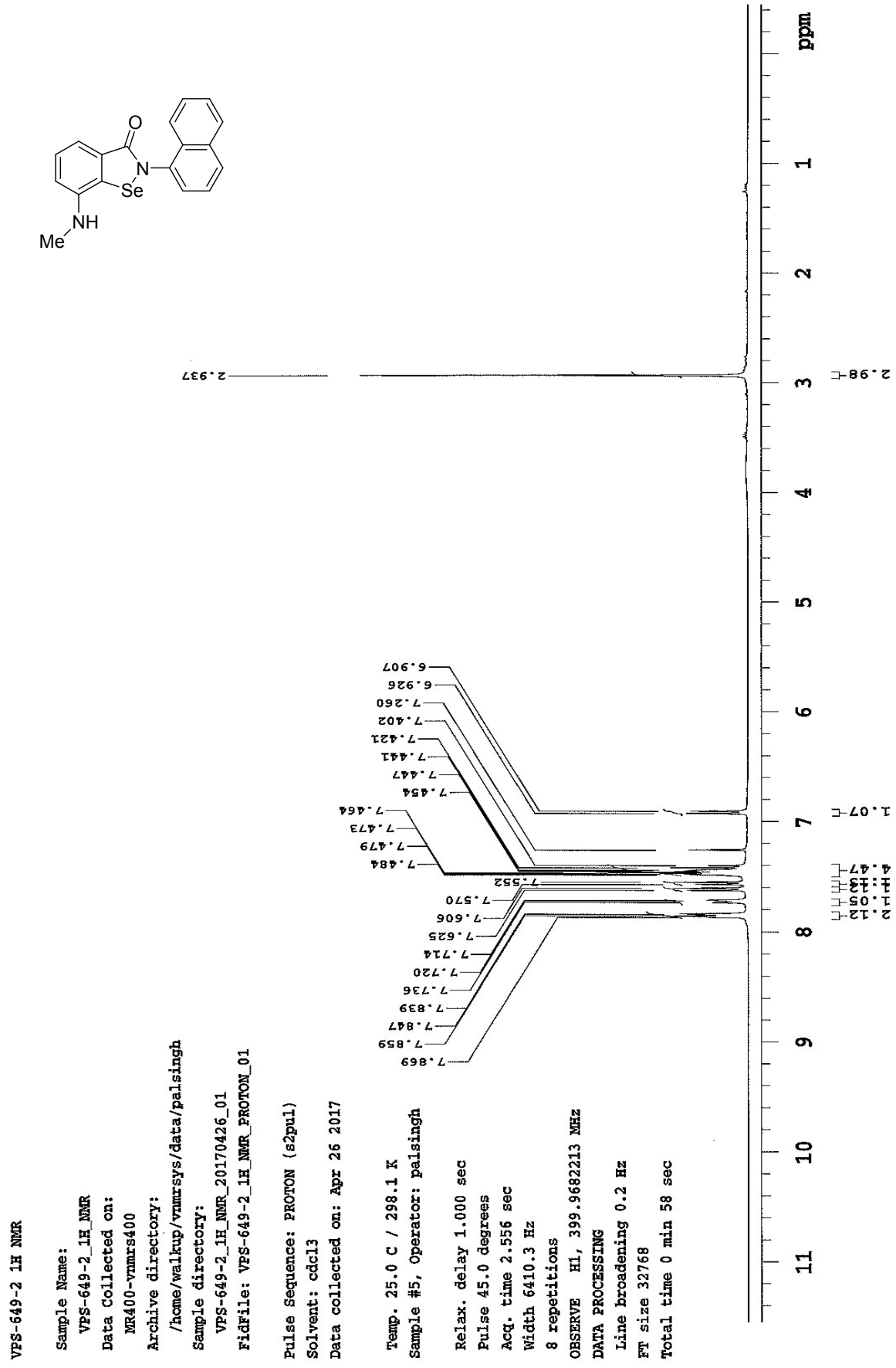


Figure S25. ^{13}C NMR spectrum of **6d**

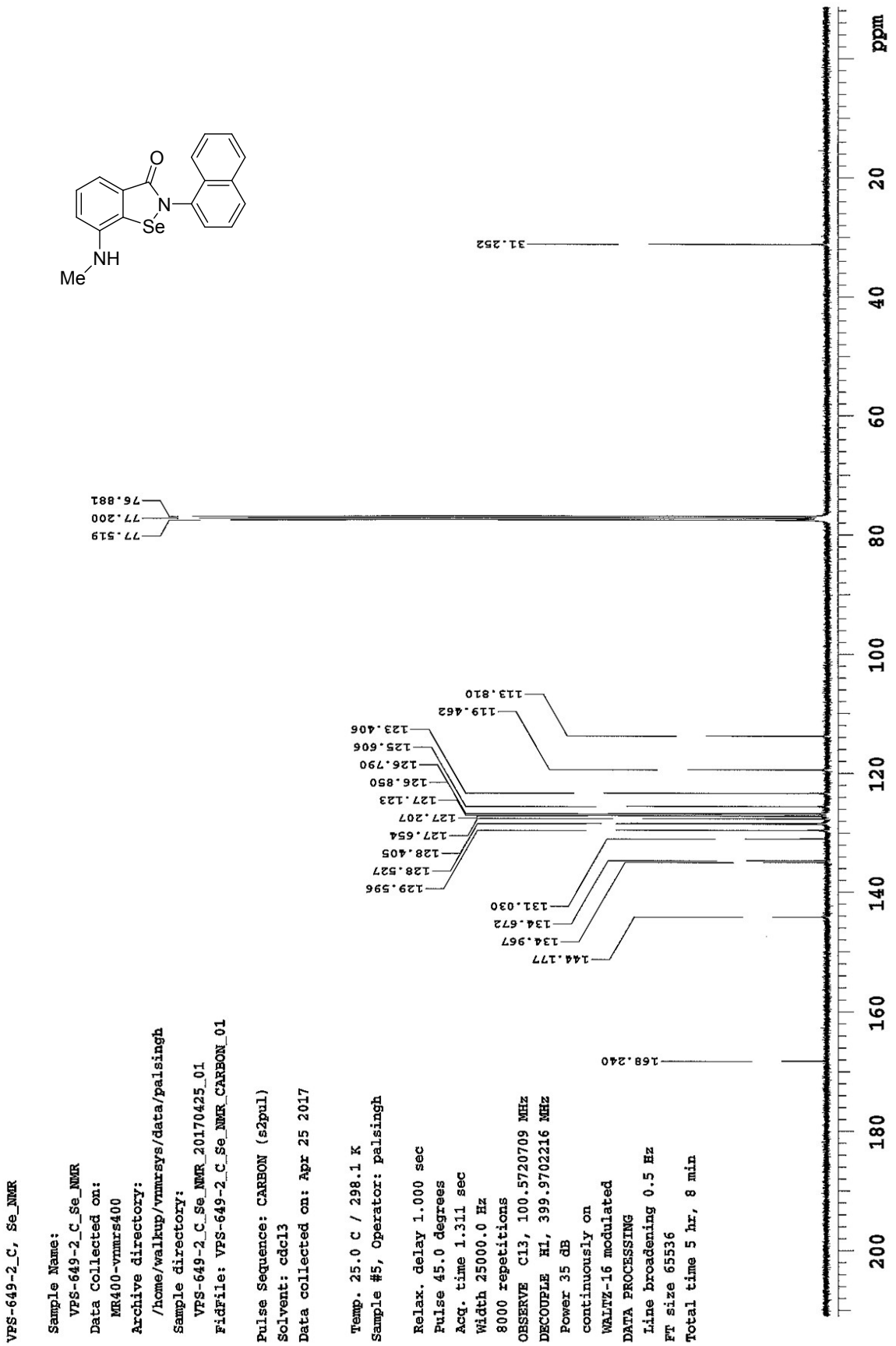


Figure S26. ^{77}Se NMR spectrum of **6d**

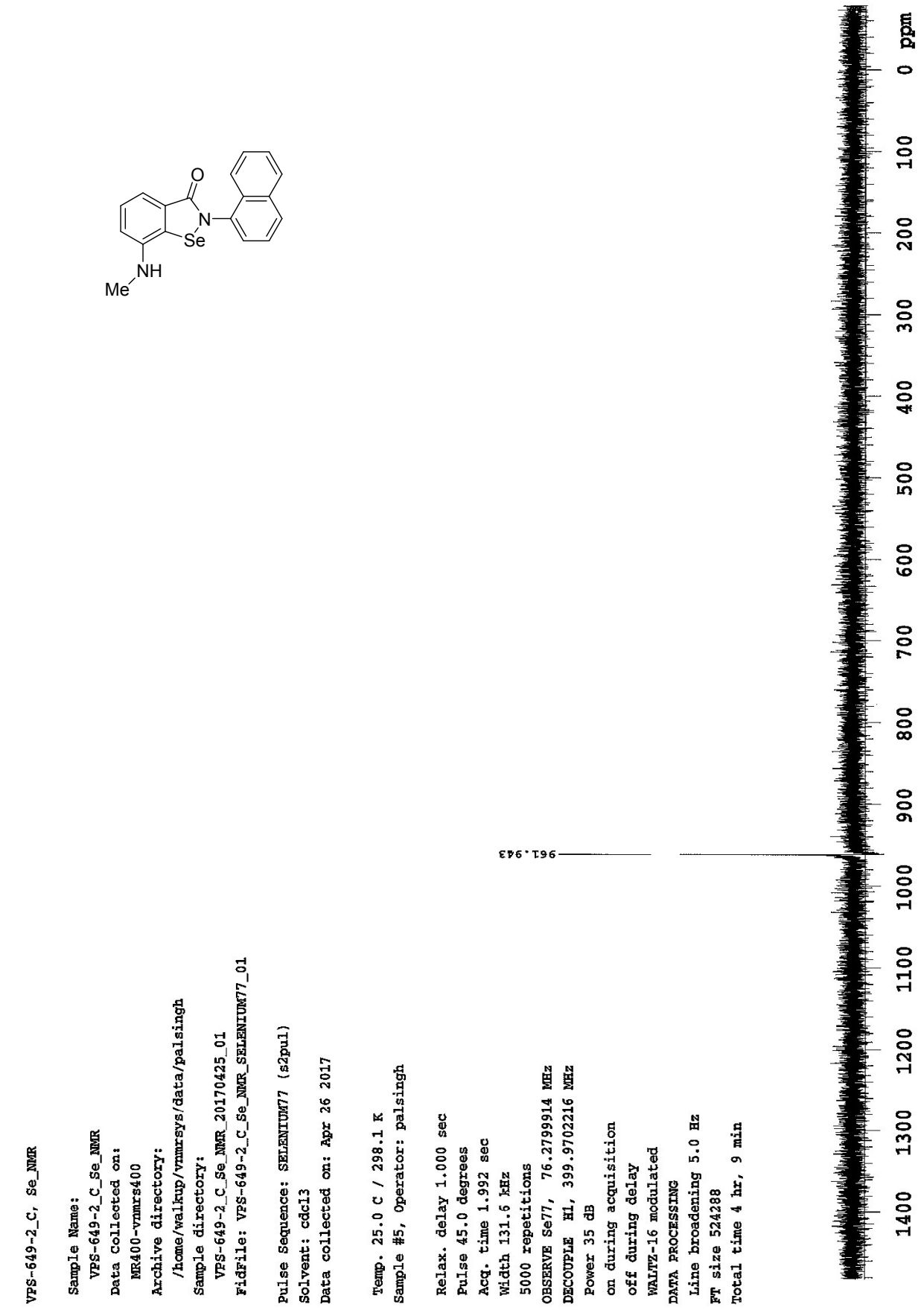


Figure S27. HRMS of **6d**

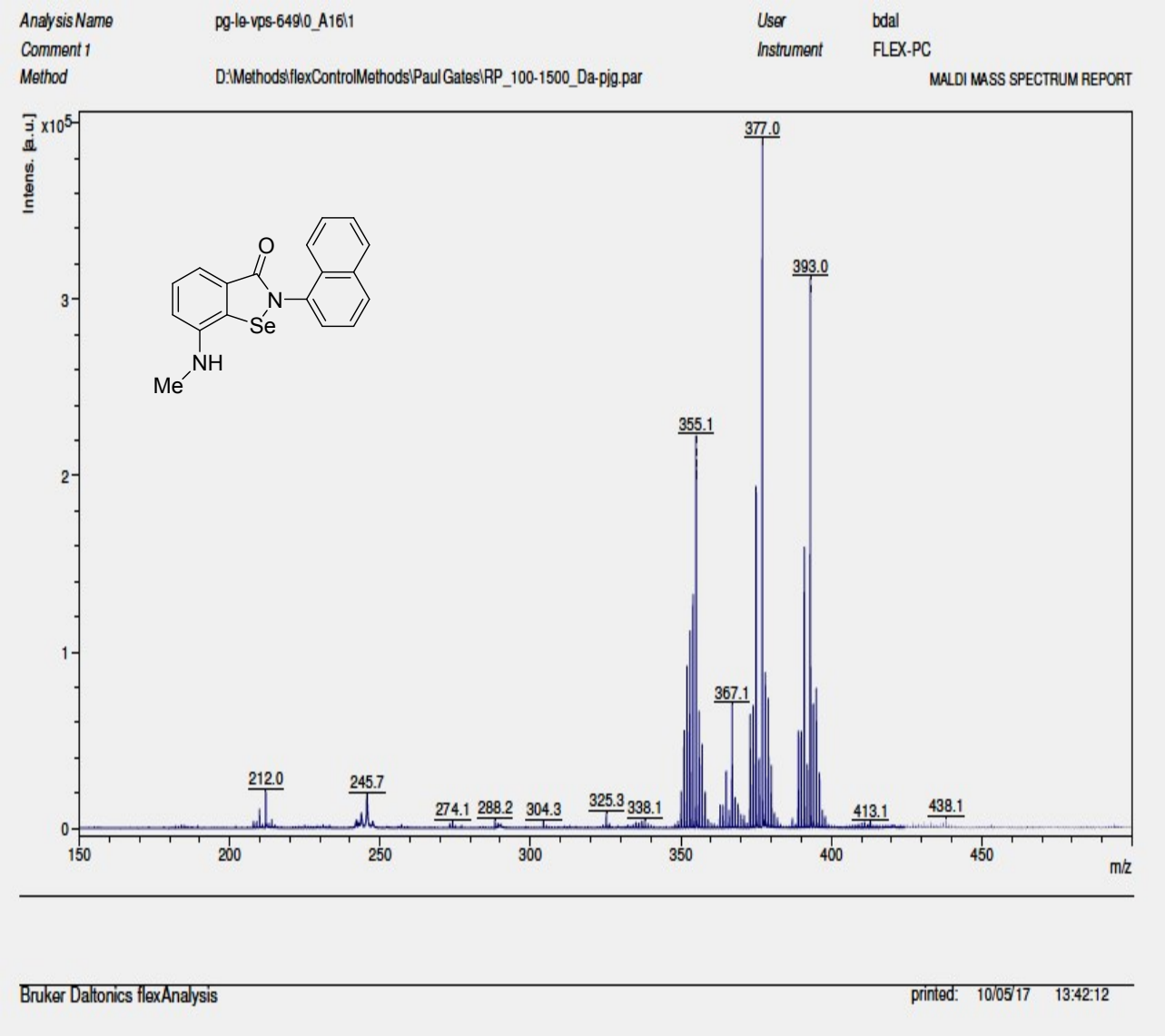
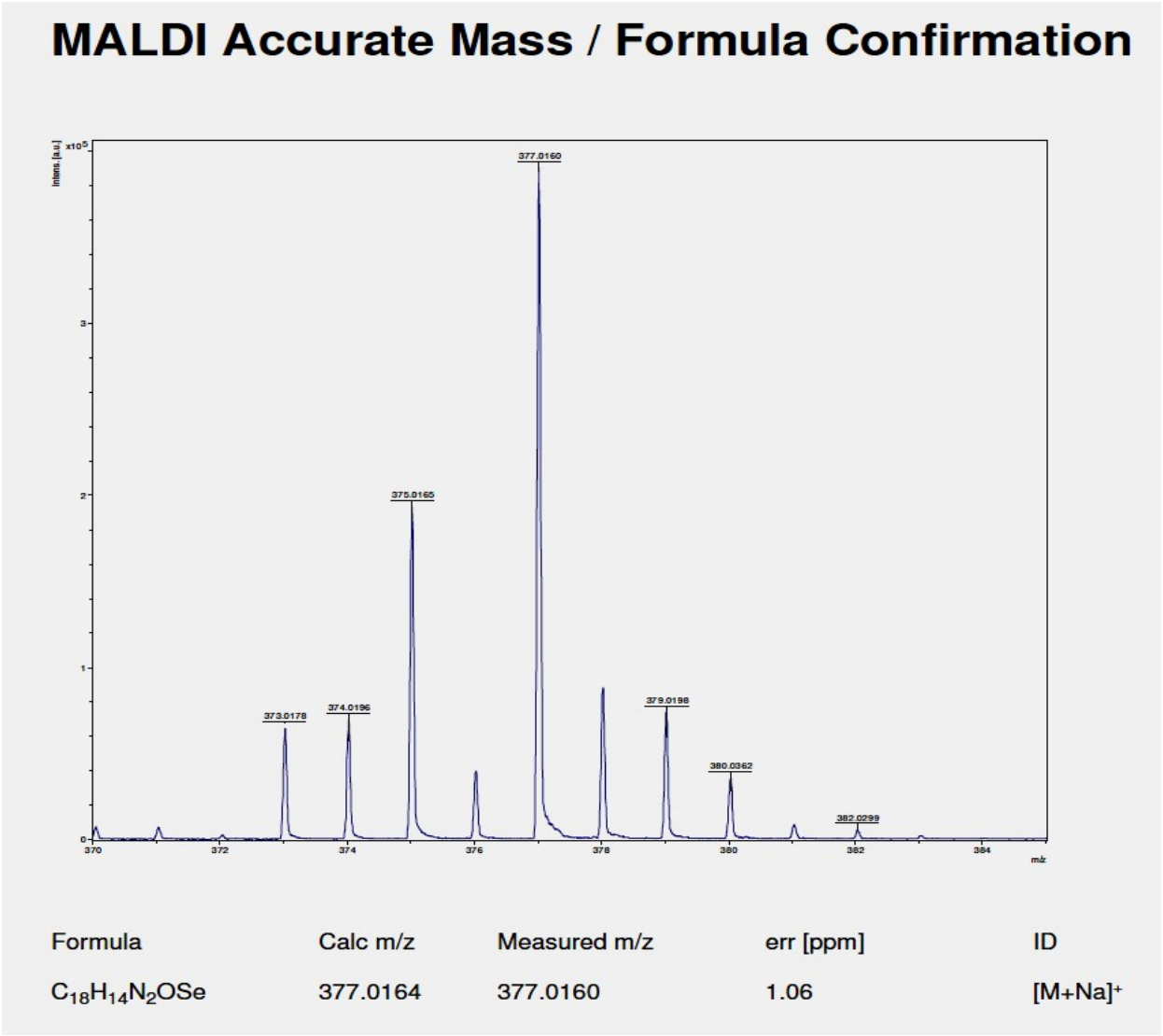


Figure S28. Expansion of the HRMS of **6d**



Mechanistic Studies for the compound 6a using the ^{77}Se NMR spectroscopy

Figure S29. ^{77}Se NMR spectrum of **6a** recorded in DMSO-d_6

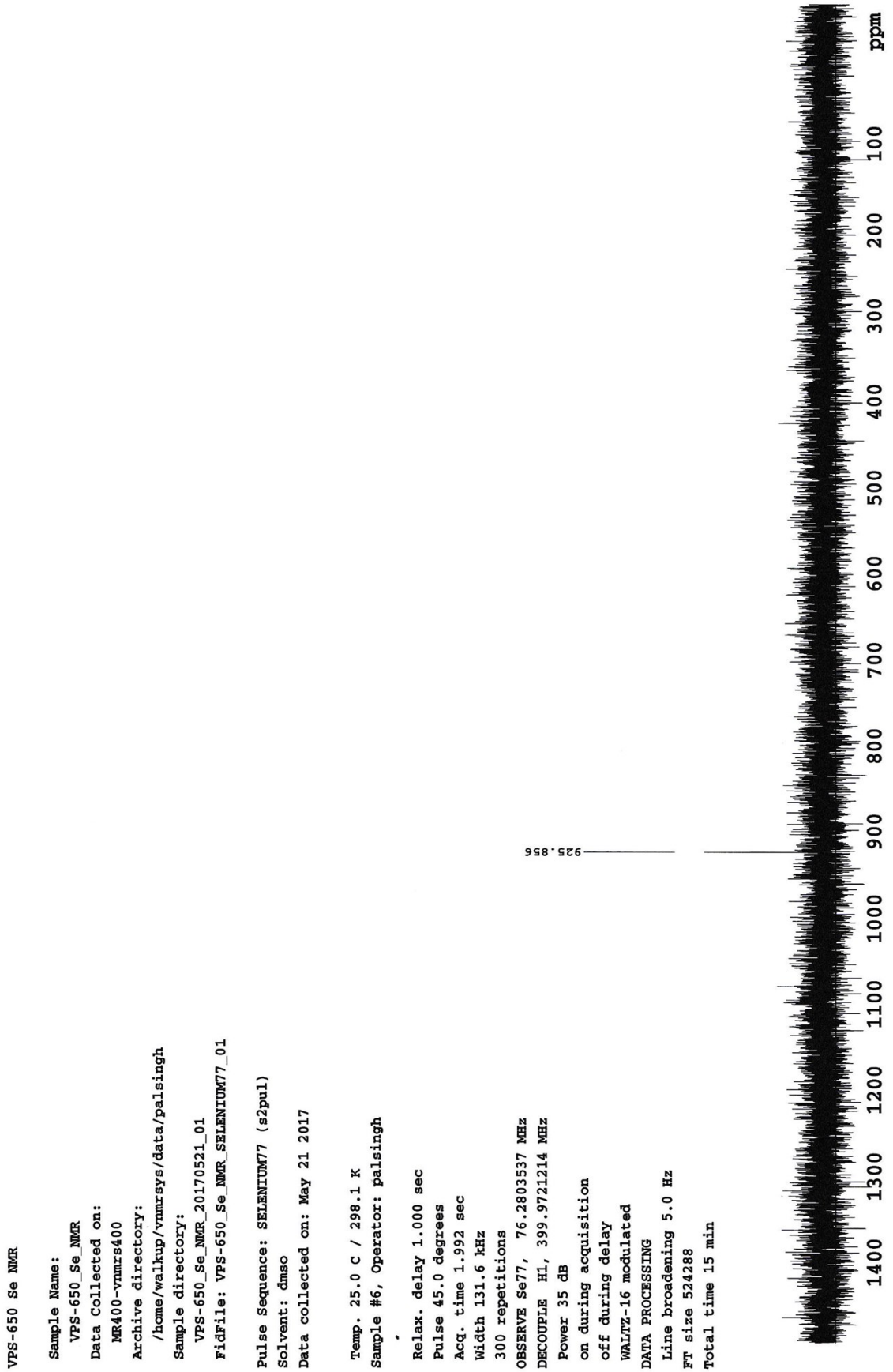


Figure S30. ^{77}Se NMR spectrum of **6a** recorded after the addition of 2 equiv H_2O_2

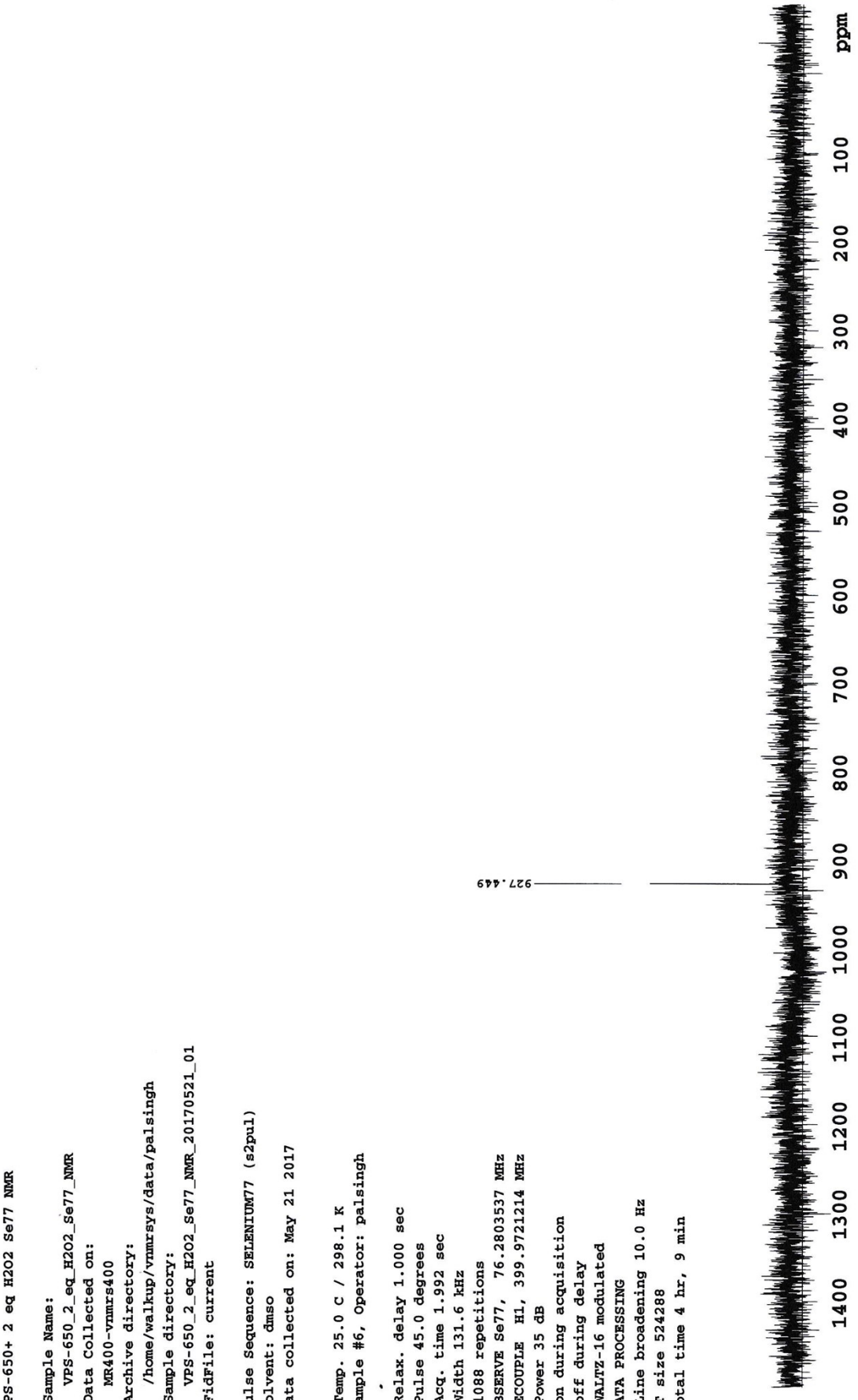


Figure S31. ^{77}Se NMR spectrum of **6a** recorded after the addition of 4 equiv H_2O_2

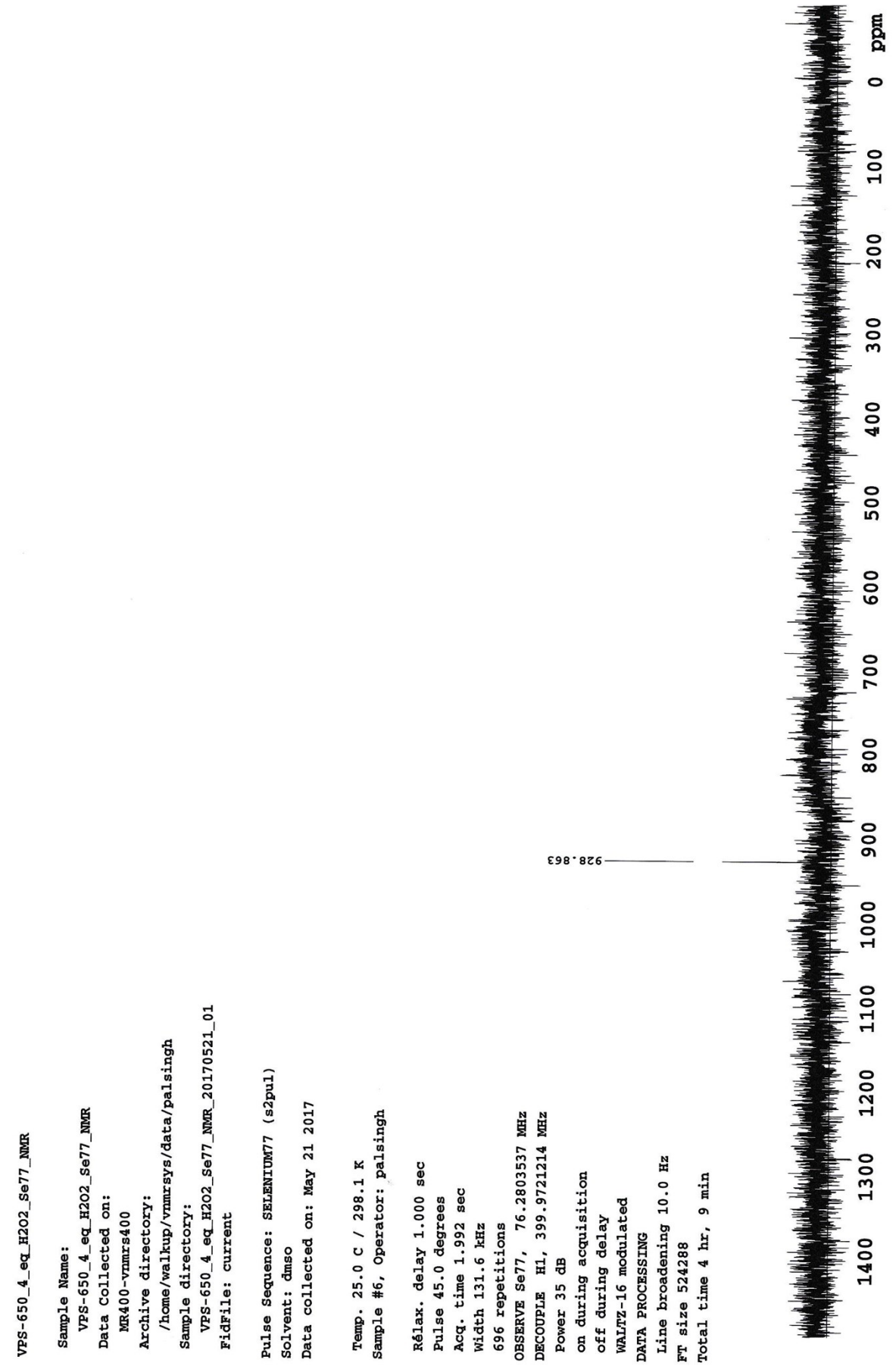


Figure S32. ^{77}Se NMR spectrum of **6a** recorded after the addition of (4 + 3) equiv of H_2O_2 + 3 equiv of PhSH

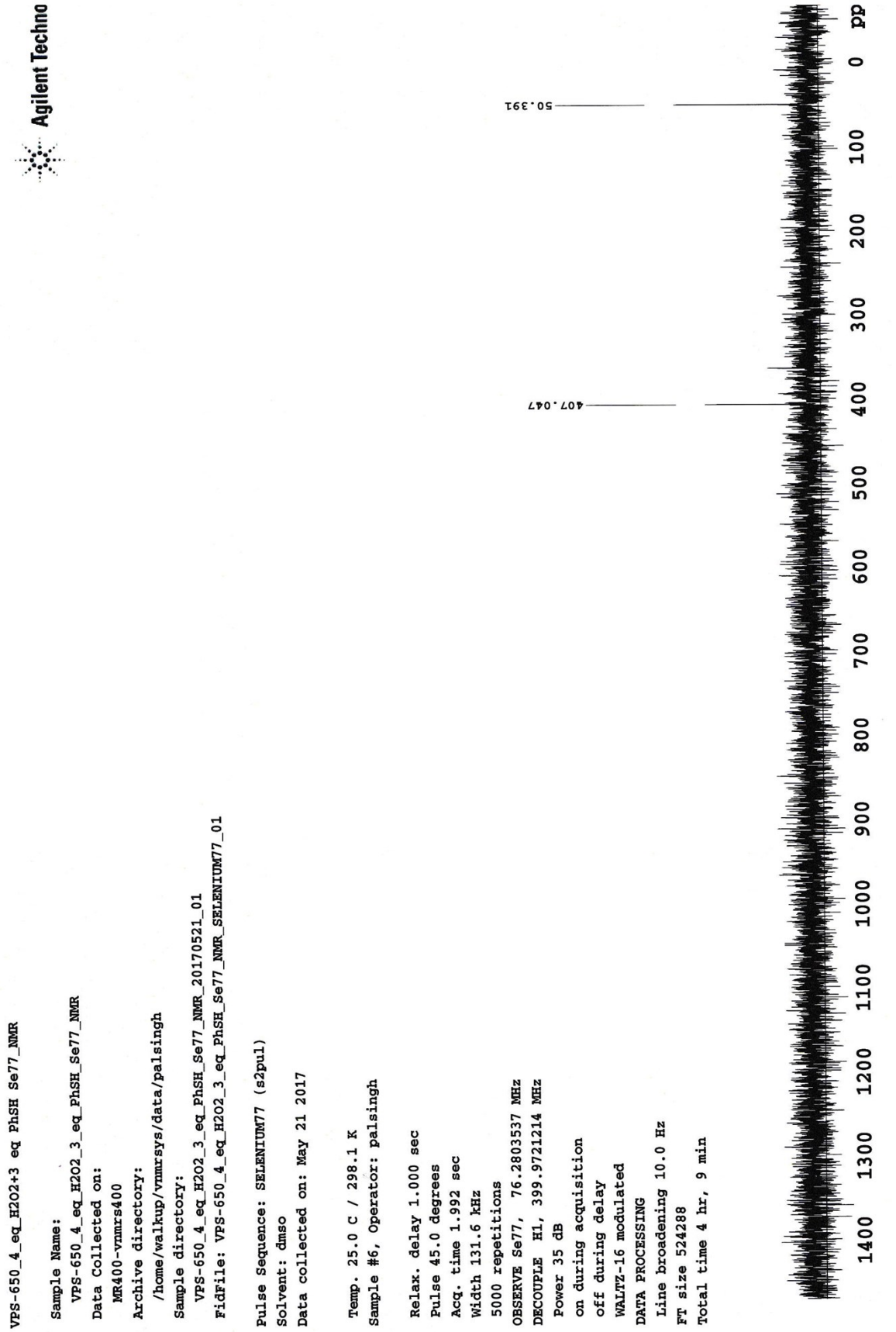


Figure S33. ^{77}Se NMR spectrum of **6a** recorded after the addition of 4 equiv H_2O_2 + (3+3) equiv PhSH

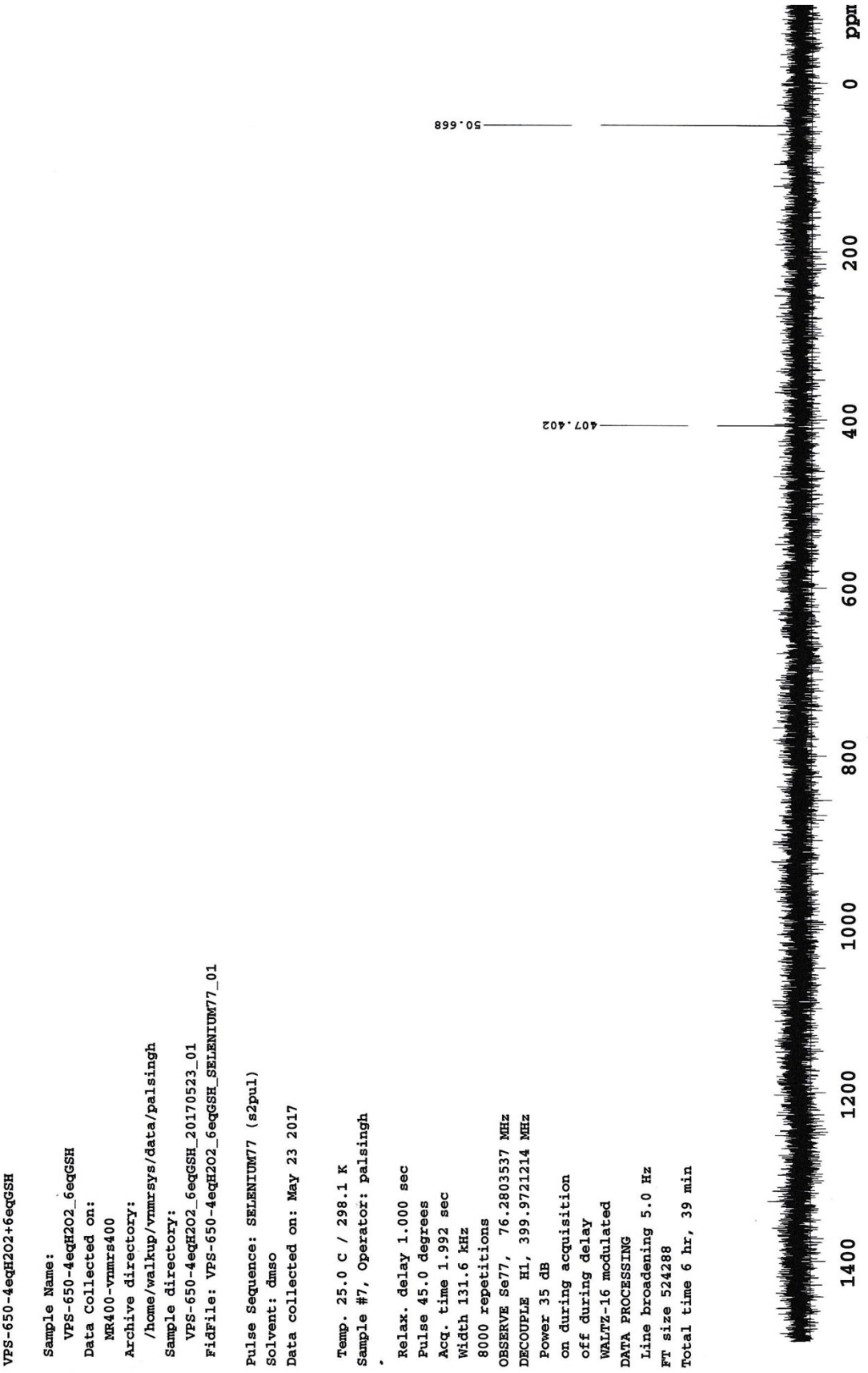
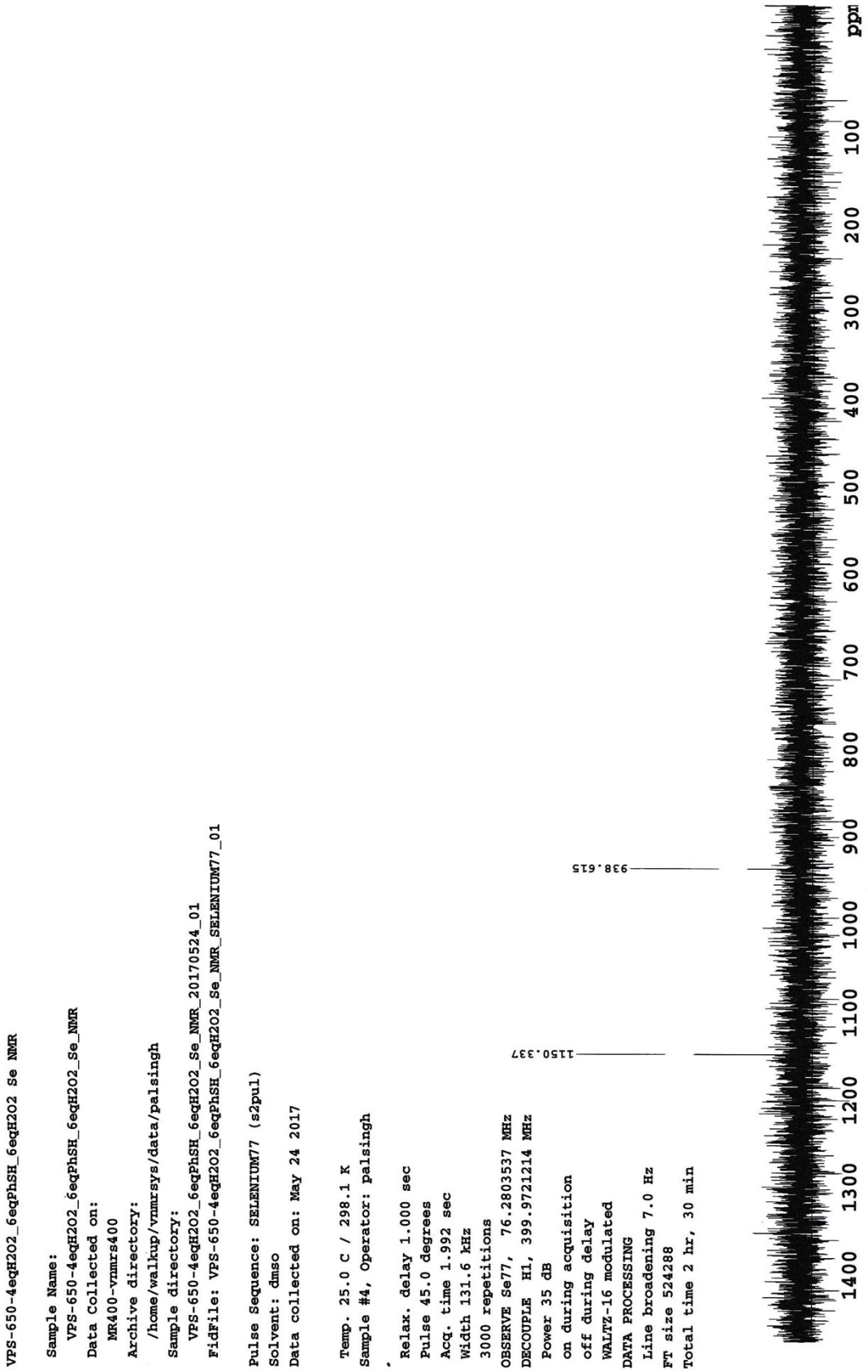
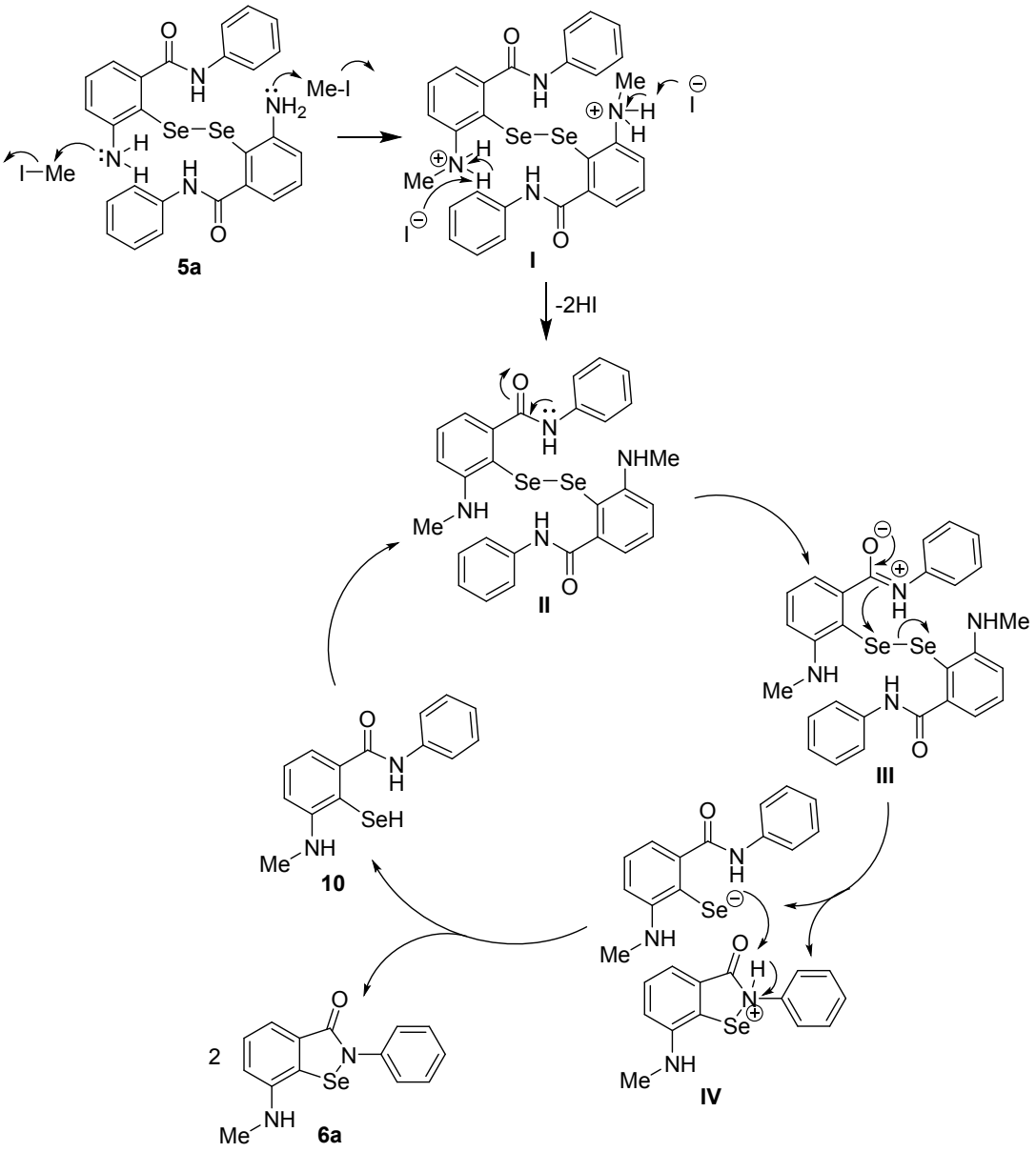


Figure S34. ^{77}Se NMR spectrum of **6a** recorded after the addition of 4 equiv H_2O_2 + 6 equiv PhSH + 6 equiv H_2O_2



Scheme S1. Proposed mechanism for the formation of **6a**



In the reaction, we observed that the primary amine group (-NH_2) in diselenide **5a** acted as nucleophile towards MeI and led to the formation of the methylated intermediate **I** first *via* the S_N2 reaction (Scheme S1). Further, -NHMe group cannot be methylated in **I** with another MeI. Since, the S_N2 reaction does not take place as d-orbitals of the Se atom interact with the nearby lone pair of electrons on the N-atom in -NHMe group. Since diselenides are dimeric molecules, each equivalent should lead to the formation of **6a** (2 equiv). It is therefore indicated that the formation of compound **6a** is observed via the returning of intermediate **10a** to the cycle.

CheckCIF/PLATON report for compound **6c**

Structure factors have been supplied for datablock(s) shelx

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary
Please wait while processing .... Interpreting this report
Structure factor report

Datablock: shelx

Bond precision: C-C = 0.0101 A Wavelength=0.71073

Cell: a=9.0455(5) b=12.1947(6) c=13.2917(7)

alpha=101.367(4) beta=90.571(4) gamma=109.919(5)

Temperature: 100 K

	Calculated	Reported
Volume	1346.68(13)	1346.68(13)
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Hall group	-P 1	-P 1
Moiety formula	C15 H14 N2 O2 Se	C15 H14 N2 O2 Se
Sum formula	C15 H14 N2 O2 Se	C15 H14 N2 O2 Se
Mr	333.24	333.24
Dx,g cm-3	1.644	1.644
Z	4	4
Mu (mm-1)	2.791	2.791
F000	672.0	672.0
F000'	671.88	
h,k,lmax	13,17,19	13,17,19
Nref	8666	7914
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Tmin' 0.417

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Tmax=1.000 AbsCorr = MULTI-SCAN

Data completeness= 0.913 Theta(max)= 31.101

R(reflections)= 0.0888(6632) wR2(reflections)= 0.2492(7914)

S = 1.062 Npar= 365

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level B

PLAT930_ALERT_2_B FCF-based Twin Law (2-1 0)[1 0 0] Est.d BASF
0.22 Check

Alert level C

DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75
The relevant atom site should be identified.
PLAT097_ALERT_2_C Large Reported Max. (Positive) Residual Density
2.59 eA-3
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds .....
0.01012 Ang.
PLAT480_ALERT_4_C Long H...A H-Bond Reported H15E ..SE2 .
3.14 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance .....
6.825 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600
27 Report

Alert level G

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...
40 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms .....
2 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large
34.14 Why ?
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2 Report
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels .....
14 Note
PLAT860_ALERT_3_G Number of Least-Squares Restraints .....
240 Note
PLAT870_ALERT_4_G ALERTS Related to Twinning Effects Suppressed ..
! Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .
Please Do !
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).
1 Note
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29 Note

PLAT941_ALERT_3_G Average HKL Measurement Multiplicity .....
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   1 ALERT level B = A potentially serious problem, consider carefully
   6 ALERT level C = Check. Ensure it is not caused by an omission or
oversight
  13 ALERT level G = General information/check it is not something
unexpected

   2 ALERT type 1 CIF construction/syntax error, inconsistent or missing
data
   5 ALERT type 2 Indicator that the structure model may be wrong or
deficient
   6 ALERT type 3 Indicator that the structure quality may be low
   5 ALERT type 4 Improvement, methodology, query or suggestion
   2 ALERT type 5 Informative message, check
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It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

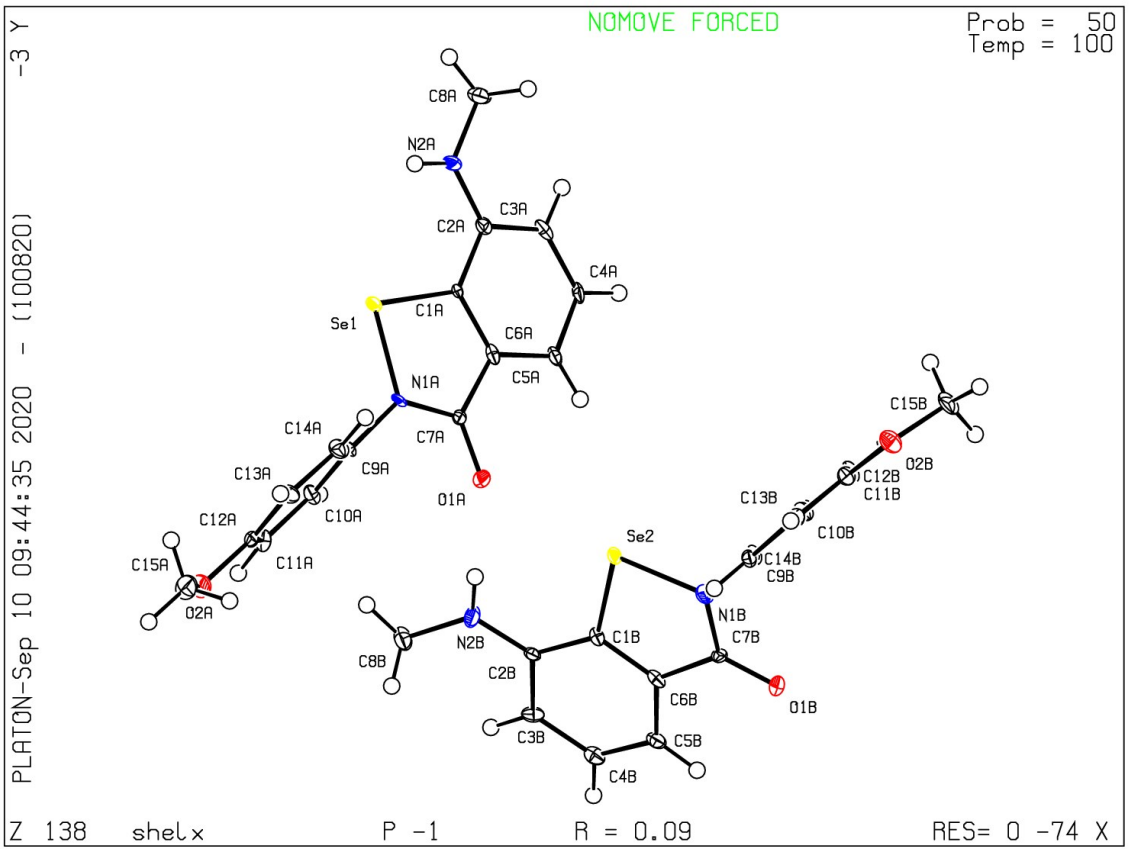
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 10/08/2020; check.def file version of 06/08/2020

Datablock shelx - ellipsoid plot



Crystal data and structure refinement for compound **6c**

Identification code	shelx

Empirical formula	C15 H14 N2 O2 Se	
Formula weight	333.24	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 9.0455(5) Å	α= 101.367(4)°.
	b = 12.1947(6) Å	β= 90.571(4)°.
	c = 13.2917(7) Å	γ = 109.919(5)°.
Volume	1346.68(13) $Å^3$	
Z	4	
Density (calculated)	1.644 Mg/m^3	
Absorption coefficient	2.791 mm^{-1}	
F(000)	672	
Crystal size	0.31 x 0.25 x 0.17 mm^3	
Theta range for data collection	1.818 to 31.101°.	
Index ranges	-12<=h<=13, -17<=k<=17, -19<=l<=19	
Reflections collected	7914	
Independent reflections	7914 [R(int) = 0.1121]	
Completeness to theta = 25.500°	99.4 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.62889	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7914 / 240 / 365	
Goodness-of-fit on F^2	1.062	
Final R indices [I>2sigma(I)]	R1 = 0.0888, wR2 = 0.2418	
R indices (all data)	R1 = 0.1014, wR2 = 0.2492	
Extinction coefficient	n/a	
Largest diff. peak and hole	2.589 and -2.537 $e.Å^{-3}$	

Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for compound **6c**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Se(1)	3864(1)	2720(1)	9460(1)	10(1)
O(1A)	4428(6)	2346(5)	6495(4)	14(1)
O(2A)	11374(6)	5031(5)	8649(4)	18(1)
N(1A)	4857(6)	2881(5)	8237(4)	10(1)
N(2A)	220(7)	1509(6)	9928(5)	15(1)
C(1A)	2018(7)	1817(6)	8593(5)	8(1)
C(2A)	500(8)	1292(6)	8911(5)	11(1)
C(3A)	-671(8)	576(6)	8129(6)	13(1)
C(4A)	-396(8)	441(6)	7103(5)	12(1)
C(5A)	1072(8)	1024(6)	6791(5)	12(1)
C(6A)	2285(8)	1696(6)	7558(5)	11(1)
C(7A)	3922(7)	2321(6)	7353(5)	9(1)
C(8A)	-1342(9)	980(7)	10262(6)	18(1)
C(9A)	6520(7)	3462(6)	8322(5)	8(1)
C(10A)	7486(8)	2796(6)	8035(5)	13(1)
C(11A)	9100(8)	3350(6)	8137(5)	13(1)
C(12A)	9747(8)	4571(6)	8559(5)	10(1)
C(13A)	8803(8)	5236(6)	8848(5)	14(1)
C(14A)	7175(8)	4671(6)	8721(5)	13(1)
C(15A)	12101(9)	6270(7)	9069(6)	21(2)
Se(2)	3528(1)	2666(1)	4502(1)	10(1)
O(1B)	2722(6)	2548(5)	1560(4)	15(1)
O(2B)	-1212(6)	5614(5)	3821(4)	17(1)
N(1B)	2747(7)	2947(5)	3312(5)	13(1)
N(2B)	6115(7)	1443(6)	4903(5)	15(1)
C(1B)	4584(7)	1827(6)	3605(5)	10(1)
C(2B)	5636(7)	1314(6)	3907(5)	9(1)
C(3B)	6201(8)	666(6)	3105(5)	13(1)
C(4B)	5774(8)	596(6)	2067(5)	13(1)
C(5B)	4826(8)	1184(6)	1787(5)	13(1)
C(6B)	4224(7)	1806(6)	2592(5)	11(1)
C(7B)	3169(7)	2447(6)	2400(5)	10(1)
C(8B)	7340(9)	1028(7)	5222(6)	17(1)

C(9B)	1696(8)	3608(6)	3422(5)	12(1)
C(10B)	92(8)	3016(6)	3275(5)	13(1)
C(11B)	-940(8)	3655(6)	3405(6)	14(1)
C(12B)	-327(8)	4899(6)	3701(5)	12(1)
C(13B)	1310(9)	5492(6)	3875(5)	14(1)
C(14B)	2317(8)	4847(6)	3728(5)	12(1)
C(15B)	-2862(9)	5065(7)	3551(6)	19(1)

Bond lengths [Å] and angles [°] for compound **6c**

Se(1)-N(1A)	1.876(6)
Se(1)-C(1A)	1.881(6)
O(1A)-C(7A)	1.235(8)
O(2A)-C(12A)	1.379(8)
O(2A)-C(15A)	1.417(9)
N(1A)-C(7A)	1.354(8)
N(1A)-C(9A)	1.420(8)
N(2A)-C(2A)	1.368(9)
N(2A)-C(8A)	1.454(9)
N(2A)-H(2AA)	0.8800
C(1A)-C(6A)	1.387(9)
C(1A)-C(2A)	1.412(9)
C(2A)-C(3A)	1.399(9)
C(3A)-C(4A)	1.376(10)
C(3A)-H(3AA)	0.9500
C(4A)-C(5A)	1.387(9)
C(4A)-H(4AA)	0.9500
C(5A)-C(6A)	1.396(9)
C(5A)-H(5AA)	0.9500
C(6A)-C(7A)	1.472(9)
C(8A)-H(8AA)	0.9800
C(8A)-H(8AB)	0.9800
C(8A)-H(8AC)	0.9800
C(9A)-C(14A)	1.377(9)
C(9A)-C(10A)	1.392(9)
C(10A)-C(11A)	1.376(9)
C(10A)-H(10A)	0.9500
C(11A)-C(12A)	1.394(9)
C(11A)-H(11A)	0.9500
C(12A)-C(13A)	1.375(9)
C(13A)-C(14A)	1.389(10)
C(13A)-H(13A)	0.9500
C(14A)-H(14A)	0.9500
C(15A)-H(15A)	0.9800
C(15A)-H(15B)	0.9800
C(15A)-H(15C)	0.9800

Se(2)-N(1B)	1.863(6)
Se(2)-C(1B)	1.894(6)
O(1B)-C(7B)	1.226(8)
O(2B)-C(12B)	1.360(8)
O(2B)-C(15B)	1.421(9)
N(1B)-C(7B)	1.365(8)
N(1B)-C(9B)	1.433(8)
N(2B)-C(2B)	1.351(9)
N(2B)-C(8B)	1.457(9)
N(2B)-H(2BA)	0.8800
C(1B)-C(6B)	1.375(9)
C(1B)-C(2B)	1.399(9)
C(2B)-C(3B)	1.406(9)
C(3B)-C(4B)	1.407(10)
C(3B)-H(3BA)	0.9500
C(4B)-C(5B)	1.381(9)
C(4B)-H(4BA)	0.9500
C(5B)-C(6B)	1.411(9)
C(5B)-H(5BA)	0.9500
C(6B)-C(7B)	1.473(9)
C(8B)-H(8BA)	0.9800
C(8B)-H(8BB)	0.9800
C(8B)-H(8BC)	0.9800
C(9B)-C(10B)	1.375(9)
C(9B)-C(14B)	1.392(9)
C(10B)-C(11B)	1.398(9)
C(10B)-H(10B)	0.9500
C(11B)-C(12B)	1.396(9)
C(11B)-H(11B)	0.9500
C(12B)-C(13B)	1.403(10)
C(13B)-C(14B)	1.385(9)
C(13B)-H(13B)	0.9500
C(14B)-H(14B)	0.9500
C(15B)-H(15D)	0.9800
C(15B)-H(15E)	0.9800
C(15B)-H(15F)	0.9800

N(1A)-Se(1)-C(1A)	85.5(3)
C(12A)-O(2A)-C(15A)	117.2(6)
C(7A)-N(1A)-C(9A)	126.2(5)
C(7A)-N(1A)-Se(1)	115.8(4)
C(9A)-N(1A)-Se(1)	117.7(4)
C(2A)-N(2A)-C(8A)	121.1(6)
C(2A)-N(2A)-H(2AA)	119.4
C(8A)-N(2A)-H(2AA)	119.4
C(6A)-C(1A)-C(2A)	121.3(6)
C(6A)-C(1A)-Se(1)	112.5(5)
C(2A)-C(1A)-Se(1)	126.2(5)
N(2A)-C(2A)-C(3A)	123.3(6)
N(2A)-C(2A)-C(1A)	120.7(6)
C(3A)-C(2A)-C(1A)	116.0(6)
C(4A)-C(3A)-C(2A)	122.4(6)
C(4A)-C(3A)-H(3AA)	118.8
C(2A)-C(3A)-H(3AA)	118.8
C(3A)-C(4A)-C(5A)	121.2(6)
C(3A)-C(4A)-H(4AA)	119.4
C(5A)-C(4A)-H(4AA)	119.4
C(4A)-C(5A)-C(6A)	117.5(6)
C(4A)-C(5A)-H(5AA)	121.2
C(6A)-C(5A)-H(5AA)	121.2
C(1A)-C(6A)-C(5A)	121.3(6)
C(1A)-C(6A)-C(7A)	114.6(6)
C(5A)-C(6A)-C(7A)	124.1(6)
O(1A)-C(7A)-N(1A)	122.4(6)
O(1A)-C(7A)-C(6A)	125.9(6)
N(1A)-C(7A)-C(6A)	111.6(5)
N(2A)-C(8A)-H(8AA)	109.5
N(2A)-C(8A)-H(8AB)	109.5
H(8AA)-C(8A)-H(8AB)	109.5
N(2A)-C(8A)-H(8AC)	109.5
H(8AA)-C(8A)-H(8AC)	109.5
H(8AB)-C(8A)-H(8AC)	109.5
C(14A)-C(9A)-C(10A)	120.2(6)
C(14A)-C(9A)-N(1A)	120.1(6)
C(10A)-C(9A)-N(1A)	119.6(6)

C(11A)-C(10A)-C(9A)	119.9(6)
C(11A)-C(10A)-H(10A)	120.1
C(9A)-C(10A)-H(10A)	120.1
C(10A)-C(11A)-C(12A)	119.3(6)
C(10A)-C(11A)-H(11A)	120.3
C(12A)-C(11A)-H(11A)	120.3
C(13A)-C(12A)-O(2A)	124.2(6)
C(13A)-C(12A)-C(11A)	121.2(6)
O(2A)-C(12A)-C(11A)	114.6(6)
C(12A)-C(13A)-C(14A)	118.9(6)
C(12A)-C(13A)-H(13A)	120.5
C(14A)-C(13A)-H(13A)	120.5
C(9A)-C(14A)-C(13A)	120.4(6)
C(9A)-C(14A)-H(14A)	119.8
C(13A)-C(14A)-H(14A)	119.8
O(2A)-C(15A)-H(15A)	109.5
O(2A)-C(15A)-H(15B)	109.5
H(15A)-C(15A)-H(15B)	109.5
O(2A)-C(15A)-H(15C)	109.5
H(15A)-C(15A)-H(15C)	109.5
H(15B)-C(15A)-H(15C)	109.5
N(1B)-Se(2)-C(1B)	85.6(3)
C(12B)-O(2B)-C(15B)	117.6(6)
C(7B)-N(1B)-C(9B)	125.5(6)
C(7B)-N(1B)-Se(2)	116.5(4)
C(9B)-N(1B)-Se(2)	117.9(5)
C(2B)-N(2B)-C(8B)	123.3(6)
C(2B)-N(2B)-H(2BA)	118.4
C(8B)-N(2B)-H(2BA)	118.4
C(6B)-C(1B)-C(2B)	122.9(6)
C(6B)-C(1B)-Se(2)	111.3(5)
C(2B)-C(1B)-Se(2)	125.7(5)
N(2B)-C(2B)-C(1B)	122.8(6)
N(2B)-C(2B)-C(3B)	121.4(6)
C(1B)-C(2B)-C(3B)	115.9(6)
C(2B)-C(3B)-C(4B)	121.1(6)
C(2B)-C(3B)-H(3BA)	119.4
C(4B)-C(3B)-H(3BA)	119.4

C(5B)-C(4B)-C(3B)	122.0(6)
C(5B)-C(4B)-H(4BA)	119.0
C(3B)-C(4B)-H(4BA)	119.0
C(4B)-C(5B)-C(6B)	116.8(6)
C(4B)-C(5B)-H(5BA)	121.6
C(6B)-C(5B)-H(5BA)	121.6
C(1B)-C(6B)-C(5B)	121.1(6)
C(1B)-C(6B)-C(7B)	116.5(6)
C(5B)-C(6B)-C(7B)	122.4(6)
O(1B)-C(7B)-N(1B)	123.3(6)
O(1B)-C(7B)-C(6B)	126.7(6)
N(1B)-C(7B)-C(6B)	110.0(6)
N(2B)-C(8B)-H(8BA)	109.5
N(2B)-C(8B)-H(8BB)	109.5
H(8BA)-C(8B)-H(8BB)	109.5
N(2B)-C(8B)-H(8BC)	109.5
H(8BA)-C(8B)-H(8BC)	109.5
H(8BB)-C(8B)-H(8BC)	109.5
C(10B)-C(9B)-C(14B)	120.7(6)
C(10B)-C(9B)-N(1B)	120.0(6)
C(14B)-C(9B)-N(1B)	119.2(6)
C(9B)-C(10B)-C(11B)	120.2(6)
C(9B)-C(10B)-H(10B)	119.9
C(11B)-C(10B)-H(10B)	119.9
C(12B)-C(11B)-C(10B)	119.4(6)
C(12B)-C(11B)-H(11B)	120.3
C(10B)-C(11B)-H(11B)	120.3
O(2B)-C(12B)-C(11B)	124.6(6)
O(2B)-C(12B)-C(13B)	115.5(6)
C(11B)-C(12B)-C(13B)	119.9(6)
C(14B)-C(13B)-C(12B)	120.0(6)
C(14B)-C(13B)-H(13B)	120.0
C(12B)-C(13B)-H(13B)	120.0
C(13B)-C(14B)-C(9B)	119.7(6)
C(13B)-C(14B)-H(14B)	120.1
C(9B)-C(14B)-H(14B)	120.1
O(2B)-C(15B)-H(15D)	109.5
O(2B)-C(15B)-H(15E)	109.5

H(15D)-C(15B)-H(15E)	109.5
O(2B)-C(15B)-H(15F)	109.5
H(15D)-C(15B)-H(15F)	109.5
H(15E)-C(15B)-H(15F)	109.5

Symmetry transformations used to generate equivalent atoms:

Anisotropic displacement parameters ($Å^2 x\ 10^3$)for compound **6c**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Se(1)	6(1)	15(1)	9(1)	0(1)	1(1)	3(1)
O(1A)	15(2)	21(2)	9(2)	2(2)	1(2)	10(2)
O(2A)	13(2)	17(2)	19(3)	5(2)	-2(2)	0(2)
N(1A)	3(2)	16(2)	10(2)	2(2)	2(2)	2(2)
N(2A)	6(2)	23(3)	12(3)	4(2)	2(2)	1(2)
C(1A)	6(2)	13(3)	8(3)	4(2)	1(2)	6(2)
C(2A)	10(3)	14(3)	12(3)	2(2)	1(2)	7(2)
C(3A)	6(3)	13(3)	22(3)	5(2)	1(2)	4(2)
C(4A)	8(3)	15(3)	12(3)	-1(2)	-5(2)	5(2)
C(5A)	8(3)	16(3)	12(3)	-1(2)	-2(2)	7(2)
C(6A)	8(3)	11(3)	14(3)	0(2)	-3(2)	5(2)
C(7A)	10(3)	12(3)	7(3)	1(2)	1(2)	8(2)
C(8A)	14(3)	23(3)	19(3)	7(3)	8(3)	9(3)
C(9A)	5(2)	13(2)	9(2)	2(2)	0(2)	5(2)
C(10A)	9(3)	14(3)	16(3)	4(2)	0(2)	5(2)
C(11A)	14(3)	12(3)	13(3)	3(2)	-3(2)	5(2)
C(12A)	9(3)	14(3)	10(3)	7(2)	1(2)	4(2)
C(13A)	11(3)	11(3)	17(3)	3(2)	3(2)	2(2)
C(14A)	13(3)	14(3)	15(3)	1(2)	2(2)	7(2)
C(15A)	15(3)	22(4)	19(3)	6(3)	-3(3)	-3(3)
Se(2)	9(1)	13(1)	9(1)	1(1)	0(1)	7(1)
O(1B)	14(2)	22(2)	10(2)	4(2)	-2(2)	8(2)
O(2B)	16(2)	16(2)	23(3)	4(2)	3(2)	10(2)
N(1B)	13(3)	13(2)	15(3)	4(2)	2(2)	8(2)
N(2B)	19(3)	20(3)	9(3)	1(2)	-2(2)	12(2)
C(1B)	8(3)	10(3)	12(3)	1(2)	-1(2)	4(2)
C(2B)	6(2)	12(3)	9(3)	0(2)	2(2)	3(2)
C(3B)	15(3)	12(3)	13(3)	1(2)	6(2)	7(2)
C(4B)	10(3)	12(3)	16(3)	0(2)	2(2)	3(2)
C(5B)	8(3)	16(3)	13(3)	0(2)	2(2)	3(2)
C(6B)	6(3)	11(3)	16(3)	1(2)	1(2)	3(2)
C(7B)	8(2)	12(2)	6(2)	0(2)	1(2)	2(2)
C(8B)	14(3)	20(3)	19(3)	2(3)	-2(3)	9(3)

C(9B)	10(3)	14(3)	15(3)	3(2)	0(2)	8(2)
C(10B)	12(3)	13(3)	15(3)	0(2)	2(2)	7(2)
C(11B)	9(3)	15(3)	20(3)	4(2)	-1(2)	5(2)
C(12B)	14(3)	13(3)	13(3)	3(2)	2(2)	9(2)
C(13B)	19(3)	11(3)	11(3)	0(2)	0(2)	7(2)
C(14B)	9(3)	16(3)	9(3)	0(2)	-1(2)	6(2)
C(15B)	13(3)	24(4)	23(4)	2(3)	2(3)	13(3)

Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for compound **6c**.

	x	y	z	U(eq)
H(2AA)	998	1976	10387	18
H(3AA)	-1694	167	8312	16
H(4AA)	-1226	-61	6600	14
H(5AA)	1245	968	6082	14
H(8AA)	-1307	1215	11013	26
H(8AB)	-1682	108	10055	26
H(8AC)	-2089	1259	9943	26
H(10A)	7032	1960	7769	15
H(11A)	9765	2906	7922	15
H(13A)	9257	6069	9130	16
H(14A)	6509	5121	8912	16
H(15A)	13250	6484	9109	32
H(15B)	11765	6459	9761	32
H(15C)	11789	6723	8627	32
H(2BA)	5664	1795	5383	18
H(3BA)	6882	268	3266	16
H(4BA)	6150	130	1543	16
H(5BA)	4591	1171	1085	15
H(8BA)	7529	1244	5974	26
H(8BB)	8316	1402	4915	26
H(8BC)	7001	159	4992	26
H(10B)	-317	2169	3083	16
H(11B)	-2048	3247	3293	17
H(13B)	1729	6337	4094	16
H(14B)	3427	5248	3836	14
H(15D)	-3336	5682	3582	28
H(15E)	-3339	4559	4035	28
H(15F)	-3050	4574	2851	28

Torsion angles [°] for compound **6c**

C(1A)-Se(1)-N(1A)-C(7A)	-0.9(5)
C(1A)-Se(1)-N(1A)-C(9A)	-174.7(5)
N(1A)-Se(1)-C(1A)-C(6A)	1.5(5)
N(1A)-Se(1)-C(1A)-C(2A)	-178.8(6)
C(8A)-N(2A)-C(2A)-C(3A)	0.9(10)
C(8A)-N(2A)-C(2A)-C(1A)	179.5(6)
C(6A)-C(1A)-C(2A)-N(2A)	-173.9(6)
Se(1)-C(1A)-C(2A)-N(2A)	6.5(9)
C(6A)-C(1A)-C(2A)-C(3A)	4.8(9)
Se(1)-C(1A)-C(2A)-C(3A)	-174.8(5)
N(2A)-C(2A)-C(3A)-C(4A)	175.0(7)
C(1A)-C(2A)-C(3A)-C(4A)	-3.7(10)
C(2A)-C(3A)-C(4A)-C(5A)	-0.5(10)
C(3A)-C(4A)-C(5A)-C(6A)	3.7(10)
C(2A)-C(1A)-C(6A)-C(5A)	-1.8(10)
Se(1)-C(1A)-C(6A)-C(5A)	177.9(5)
C(2A)-C(1A)-C(6A)-C(7A)	178.5(6)
Se(1)-C(1A)-C(6A)-C(7A)	-1.8(7)
C(4A)-C(5A)-C(6A)-C(1A)	-2.6(9)
C(4A)-C(5A)-C(6A)-C(7A)	177.1(6)
C(9A)-N(1A)-C(7A)-O(1A)	-6.2(10)
Se(1)-N(1A)-C(7A)-O(1A)	-179.3(5)
C(9A)-N(1A)-C(7A)-C(6A)	173.3(6)
Se(1)-N(1A)-C(7A)-C(6A)	0.1(7)
C(1A)-C(6A)-C(7A)-O(1A)	-179.5(6)
C(5A)-C(6A)-C(7A)-O(1A)	0.8(10)
C(1A)-C(6A)-C(7A)-N(1A)	1.1(8)
C(5A)-C(6A)-C(7A)-N(1A)	-178.6(6)
C(7A)-N(1A)-C(9A)-C(14A)	117.0(8)
Se(1)-N(1A)-C(9A)-C(14A)	-70.0(7)
C(7A)-N(1A)-C(9A)-C(10A)	-65.4(9)
Se(1)-N(1A)-C(9A)-C(10A)	107.6(6)
C(14A)-C(9A)-C(10A)-C(11A)	-1.0(10)
N(1A)-C(9A)-C(10A)-C(11A)	-178.5(6)
C(9A)-C(10A)-C(11A)-C(12A)	2.1(10)
C(15A)-O(2A)-C(12A)-C(13A)	0.1(10)

C(15A)-O(2A)-C(12A)-C(11A)	179.7(6)
C(10A)-C(11A)-C(12A)-C(13A)	-1.9(10)
C(10A)-C(11A)-C(12A)-O(2A)	178.5(6)
O(2A)-C(12A)-C(13A)-C(14A)	-179.9(6)
C(11A)-C(12A)-C(13A)-C(14A)	0.5(10)
C(10A)-C(9A)-C(14A)-C(13A)	-0.4(10)
N(1A)-C(9A)-C(14A)-C(13A)	177.2(6)
C(12A)-C(13A)-C(14A)-C(9A)	0.6(10)
C(1B)-Se(2)-N(1B)-C(7B)	2.2(5)
C(1B)-Se(2)-N(1B)-C(9B)	179.0(5)
N(1B)-Se(2)-C(1B)-C(6B)	-2.2(5)
N(1B)-Se(2)-C(1B)-C(2B)	176.1(6)
C(8B)-N(2B)-C(2B)-C(1B)	-172.9(7)
C(8B)-N(2B)-C(2B)-C(3B)	5.8(10)
C(6B)-C(1B)-C(2B)-N(2B)	172.9(6)
Se(2)-C(1B)-C(2B)-N(2B)	-5.3(10)
C(6B)-C(1B)-C(2B)-C(3B)	-5.9(10)
Se(2)-C(1B)-C(2B)-C(3B)	176.0(5)
N(2B)-C(2B)-C(3B)-C(4B)	-176.0(6)
C(1B)-C(2B)-C(3B)-C(4B)	2.8(10)
C(2B)-C(3B)-C(4B)-C(5B)	2.0(10)
C(3B)-C(4B)-C(5B)-C(6B)	-3.6(10)
C(2B)-C(1B)-C(6B)-C(5B)	4.4(10)
Se(2)-C(1B)-C(6B)-C(5B)	-177.3(5)
C(2B)-C(1B)-C(6B)-C(7B)	-176.5(6)
Se(2)-C(1B)-C(6B)-C(7B)	1.9(7)
C(4B)-C(5B)-C(6B)-C(1B)	0.6(10)
C(4B)-C(5B)-C(6B)-C(7B)	-178.5(6)
C(9B)-N(1B)-C(7B)-O(1B)	2.5(11)
Se(2)-N(1B)-C(7B)-O(1B)	179.0(5)
C(9B)-N(1B)-C(7B)-C(6B)	-178.1(6)
Se(2)-N(1B)-C(7B)-C(6B)	-1.6(7)
C(1B)-C(6B)-C(7B)-O(1B)	179.1(6)
C(5B)-C(6B)-C(7B)-O(1B)	-1.8(11)
C(1B)-C(6B)-C(7B)-N(1B)	-0.3(8)
C(5B)-C(6B)-C(7B)-N(1B)	178.9(6)
C(7B)-N(1B)-C(9B)-C(10B)	79.2(9)
Se(2)-N(1B)-C(9B)-C(10B)	-97.3(7)

C(7B)-N(1B)-C(9B)-C(14B)	-103.9(8)
Se(2)-N(1B)-C(9B)-C(14B)	79.6(7)
C(14B)-C(9B)-C(10B)-C(11B)	1.7(11)
N(1B)-C(9B)-C(10B)-C(11B)	178.5(6)
C(9B)-C(10B)-C(11B)-C(12B)	-0.9(11)
C(15B)-O(2B)-C(12B)-C(11B)	-5.0(10)
C(15B)-O(2B)-C(12B)-C(13B)	173.7(6)
C(10B)-C(11B)-C(12B)-O(2B)	177.9(7)
C(10B)-C(11B)-C(12B)-C(13B)	-0.7(11)
O(2B)-C(12B)-C(13B)-C(14B)	-177.1(6)
C(11B)-C(12B)-C(13B)-C(14B)	1.6(10)
C(12B)-C(13B)-C(14B)-C(9B)	-0.9(10)
C(10B)-C(9B)-C(14B)-C(13B)	-0.7(10)
N(1B)-C(9B)-C(14B)-C(13B)	-177.5(6)

Symmetry transformations used to generate equivalent atoms:

Hydrogen bonds for compound **6c** [Å and °]

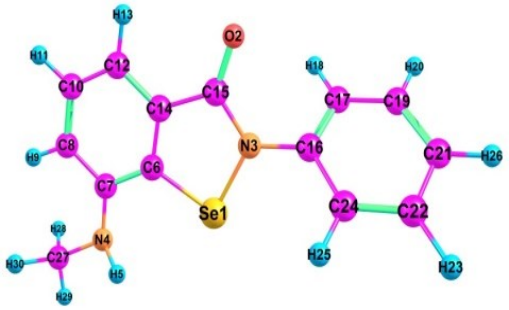
D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(2A)-H(2AA)...Se(1)	0.88	2.82	3.243(6)	111.0
N(2A)-H(2AA)...O(1B)#1	0.88	2.03	2.881(8)	161.7
C(15A)-H(15A)...Se(1)#2	0.98	2.97	3.809(8)	144.3
N(2B)-H(2BA)...O(1A)	0.88	2.01	2.883(8)	171.2
N(2B)-H(2BA)...Se(2)	0.88	2.84	3.263(6)	111.1
C(15B)-H(15D)...Se(2)#3	0.98	2.97	3.614(7)	124.6
C(15B)-H(15E)...Se(2)#4	0.98	3.14	3.981(8)	144.2
C(15B)-H(15F)...O(2A)#5	0.98	2.54	3.230(10)	127.4

Symmetry transformations used to generate equivalent atoms:

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

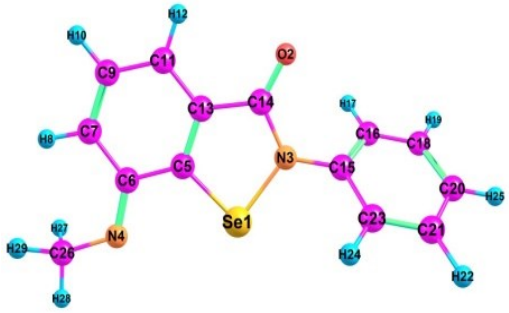
#4 x-1,y,z #5 -x+1,-y+1,-z+1

Table S1. Optimized geometries, Sum of electronic and thermal Enthalpies (a.u.), and Cartesian coordinates for compound **6a** and its radical.



6a

Sum of Electronic and
Thermal Enthalpies = -3126.915038 a.u.



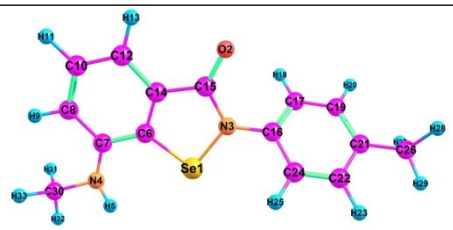
Radical of **6a**

Sum of Electronic and
Thermal Enthalpies = -3126.289315 a.u.

34	-0.179180000	-1.202591000	-0.199051000
8	1.016964000	2.553054000	0.274964000
7	1.009225000	0.257715000	0.046150000
7	-3.386823000	-1.517749000	-0.130772000
1	-2.814357000	-2.174419000	0.384330000
6	-1.572570000	0.082930000	-0.010895000
6	-2.950591000	-0.196752000	-0.016755000
6	-3.811110000	0.905887000	0.056697000
1	-4.883454000	0.750931000	0.046945000
6	-3.314083000	2.212482000	0.156911000
1	-4.017463000	3.036734000	0.211369000
6	-1.950726000	2.461108000	0.205417000
1	-1.547122000	3.462366000	0.300174000
6	-1.075143000	1.373926000	0.121412000
6	0.399231000	1.508534000	0.154733000
6	2.413430000	0.031120000	0.036052000
6	3.264624000	0.867642000	-0.695022000
1	2.854726000	1.707422000	-1.238955000
6	4.635026000	0.624615000	-0.695987000
1	5.288949000	1.282178000	-1.259623000
6	5.168255000	-0.454157000	0.008545000
6	4.318145000	-1.289493000	0.730038000
1	4.720347000	-2.128361000	1.288746000
6	2.947502000	-1.044796000	0.752839000
1	2.291285000	-1.679625000	1.339193000
1	6.237064000	-0.640285000	-0.003159000
6	-4.804185000	-1.837321000	-0.080531000
1	-5.322594000	-1.379704000	-0.926032000
1	-4.919372000	-2.917897000	-0.169918000
1	-5.295257000	-1.509768000	0.846575000

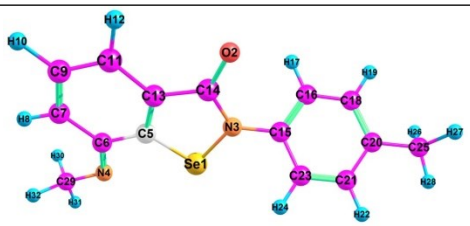
34	-0.219961000	-1.214562000	-0.123183000
8	0.978337000	2.569128000	0.231597000
7	0.978518000	0.264076000	0.032234000
7	-3.272987000	-1.545744000	-0.153430000
6	-1.578850000	0.072801000	-0.000171000
6	-2.970112000	-0.252858000	-0.031136000
6	-3.863197000	0.862012000	0.072978000
1	-4.932689000	0.687881000	0.055438000
6	-3.384448000	2.158845000	0.195704000
1	-4.089253000	2.980127000	0.272759000
6	-2.009414000	2.428946000	0.220715000
1	-1.630475000	3.440327000	0.316583000
6	-1.102836000	1.366184000	0.119748000
6	0.372518000	1.514558000	0.135324000
6	2.383385000	0.041985000	0.019577000
6	3.227729000	0.868404000	-0.730631000
1	2.812299000	1.698018000	-1.286026000
6	4.598563000	0.628148000	-0.738064000
1	5.246872000	1.277623000	-1.317334000
6	5.139194000	-0.437918000	-0.019985000
6	4.296166000	-1.262780000	0.721419000
1	4.703987000	-2.091514000	1.290975000
6	2.925133000	-1.020732000	0.750223000
1	2.276035000	-1.647536000	1.352994000
1	6.208227000	-0.622232000	-0.036556000
6	-4.661439000	-1.941054000	-0.191736000
1	-5.195361000	-1.491391000	-1.040623000
1	-4.722219000	-3.024942000	-0.290601000
1	-5.198517000	-1.651860000	0.722429000

Table S2. Optimized geometries, Sum of electronic and thermal Enthalpies (a.u.), and Cartesian coordinates for compound **6b** and its radical.



6b

Sum of Electronic and
Thermal Enthalpies = -3166.211232 a.u.

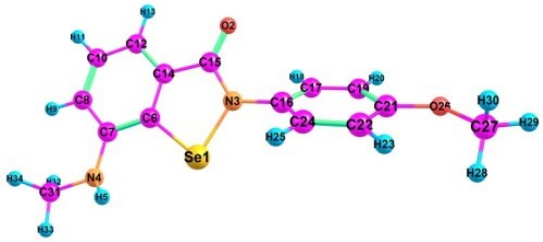


Radical of **6b**

Sum of Electronic and
Thermal Enthalpies = -3165.585511 a.u.

34	-0.492165000	-1.182178000	-0.200384000	34	-0.533430000	-1.196487000	-0.120520000
8	0.600008000	2.603699000	0.278369000	8	0.561542000	2.617034000	0.236828000
7	0.653991000	0.309856000	0.052005000	7	0.622556000	0.313702000	0.041133000
7	-3.691274000	-1.586237000	-0.134315000	7	-3.579280000	-1.610485000	-0.158267000
1	-3.099576000	-2.227686000	0.378239000	6	-1.928202000	0.052309000	-0.000170000
6	-1.921472000	0.063510000	-0.012249000	6	-3.310406000	-0.310366000	-0.034264000
6	-3.291372000	-0.253839000	-0.018299000	6	-4.233290000	0.780340000	0.068451000
6	-4.182152000	0.824346000	0.056902000	1	-5.297721000	0.577661000	0.048793000
1	-5.249814000	0.639838000	0.047212000	6	-3.789840000	2.089472000	0.192123000
6	-3.721348000	2.144091000	0.158211000	1	-4.516550000	2.891601000	0.267785000
1	-4.447171000	2.948618000	0.213561000	6	-2.422481000	2.396219000	0.219843000
6	-2.365328000	2.430080000	0.206846000	1	-2.070839000	3.417375000	0.316360000
1	-1.989426000	3.441986000	0.302672000	6	-1.487450000	1.358365000	0.120971000
6	-1.459860000	1.367708000	0.122011000	6	-0.016359000	1.546520000	0.140579000
6	0.010549000	1.542561000	0.157921000	6	2.033833000	0.132628000	0.028047000
6	2.064617000	0.124602000	0.040081000	6	2.850934000	0.949638000	-0.761456000
6	2.889050000	0.958878000	-0.723400000	1	2.409250000	1.742158000	-1.350663000
1	2.453434000	1.767407000	-1.294855000	6	4.226004000	0.751705000	-0.767721000
6	4.263760000	0.757691000	-0.724444000	1	4.845710000	1.399518000	-1.381683000
1	4.889234000	1.419357000	-1.317443000	6	4.827201000	-0.263490000	-0.012584000
6	4.857318000	-0.277606000	0.009022000	6	3.996229000	-1.075041000	0.762483000
6	4.018848000	-1.106995000	0.756864000	1	4.428835000	-1.868844000	1.364358000
1	4.445318000	-1.917417000	1.340821000	6	2.617247000	-0.877860000	0.794070000
6	2.640334000	-0.906795000	0.783927000	1	1.996001000	-1.504132000	1.426254000
1	2.011934000	-1.547360000	1.394261000	6	6.323251000	-0.458461000	-0.033803000
6	6.353272000	-0.473950000	-0.004082000	1	6.698183000	-0.574629000	-1.055246000
1	6.741959000	-0.528485000	-1.025378000	1	6.842915000	0.400864000	0.402412000
1	6.867756000	0.356436000	0.490716000	1	6.620828000	-1.344240000	0.531417000
1	6.642389000	-1.392717000	0.510723000	6	-4.956960000	-2.041438000	-0.201020000
6	-5.099139000	-1.944525000	-0.080966000	1	-5.500535000	-1.603557000	-1.049941000
1	-5.632099000	-1.499795000	-0.924327000	1	-4.989417000	-3.126305000	-0.302846000
1	-5.185142000	-3.027715000	-0.171870000	1	-5.503546000	-1.768947000	0.712682000
1	-5.596717000	-1.631876000	0.847860000				

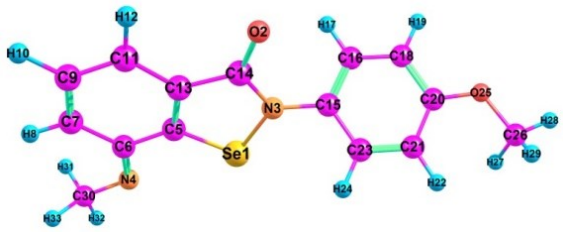
Table S3. Optimized geometries, Sum of electronic and thermal Enthalpies (a.u.), and Cartesian coordinates for compound **6c** and its radical.



6c

Sum of Electronic and Thermal Enthalpies = -3241.434042 a.u.

34	0.776680000	-1.158749000	0.243101000
8	-0.198042000	2.648117000	-0.305728000
7	-0.319610000	0.364795000	-0.042161000
7	3.961775000	-1.673212000	0.135382000
1	3.335539000	-2.309927000	-0.340590000
6	2.245541000	0.031238000	-0.003302000
6	3.604185000	-0.332250000	-0.012887000
6	4.529419000	0.712077000	-0.135601000
1	5.590277000	0.491421000	-0.140696000
6	4.111862000	2.043742000	-0.264562000
1	4.863399000	2.820954000	-0.355908000
6	2.765608000	2.374821000	-0.294798000
1	2.422247000	3.396245000	-0.410260000
6	1.826247000	1.347082000	-0.164779000
6	0.361503000	1.571737000	-0.178440000
6	-1.736775000	0.244970000	0.027360000
6	-2.468351000	0.974210000	0.973894000
1	-1.951888000	1.646638000	1.647435000
6	-3.846343000	0.854852000	1.032820000
1	-4.423889000	1.422559000	1.753648000
6	-4.522506000	-0.009683000	0.161554000
6	-3.797646000	-0.746973000	-0.777949000
1	-4.291621000	-1.418700000	-1.468384000
6	-2.410873000	-0.605991000	-0.844173000
1	-1.851360000	-1.161264000	-1.589761000
8	-5.877092000	-0.060561000	0.308200000
6	-6.625229000	-0.896165000	-0.561718000
1	-6.344024000	-1.948352000	-0.446562000
1	-7.666907000	-0.769322000	-0.272866000
1	-6.500785000	-0.596966000	-1.607679000
6	5.354756000	-2.081698000	0.062055000
1	5.922255000	-1.630045000	0.878840000
1	5.406093000	-3.163943000	0.185110000
1	5.841094000	-1.815183000	-0.886930000

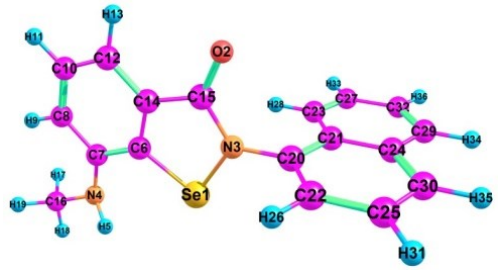


Radical of **6c**

Sum of Electronic and Thermal Enthalpies = -3240.808290 a.u.

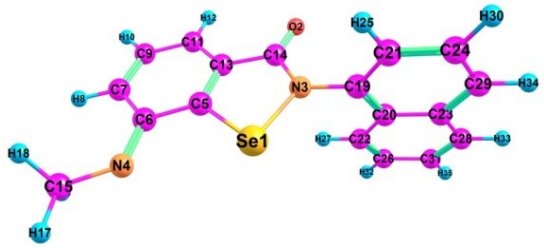
34	0.814316000	-1.173972000	0.167205000
8	-0.152973000	2.664912000	-0.262202000
7	-0.287145000	0.372587000	-0.019973000
7	3.847723000	-1.697615000	0.153109000
6	2.251874000	0.018408000	-0.015467000
6	3.621240000	-0.392666000	-0.000224000
6	4.579768000	0.661228000	-0.150780000
1	5.636520000	0.420751000	-0.148151000
6	4.180907000	1.982006000	-0.299151000
1	4.934021000	2.755081000	-0.410837000
6	2.825018000	2.337083000	-0.306186000
1	2.507671000	3.367560000	-0.421163000
6	1.855881000	1.336780000	-0.161529000
6	0.391777000	1.578033000	-0.156336000
6	-1.704960000	0.255782000	0.042740000
6	-2.438574000	0.992536000	0.981959000
1	-1.923770000	1.669326000	1.652289000
6	-3.816668000	0.873694000	1.039252000
1	-4.395011000	1.446409000	1.755469000
6	-4.491784000	0.002818000	0.173565000
6	-3.765129000	-0.741144000	-0.758943000
1	-4.257486000	-1.418319000	-1.445179000
6	-2.378082000	-0.600973000	-0.824017000
1	-1.819280000	-1.162023000	-1.565905000
8	-5.846566000	-0.047031000	0.318578000
6	-6.592717000	-0.892553000	-0.543572000
1	-6.309695000	-1.942995000	-0.417733000
1	-7.634794000	-0.764614000	-0.256695000
1	-6.468061000	-0.603523000	-1.592364000
6	5.210440000	-2.174873000	0.181067000
1	5.788081000	-1.729283000	1.003043000
1	5.207888000	-3.256426000	0.317767000
1	5.745477000	-1.951698000	-0.752744000

Table S4. Optimized geometries, Sum of electronic and thermal Enthalpies (a.u.), and Cartesian coordinates for compound **6d** and its radical.



6d

Sum of Electronic and
Thermal Enthalpies = -3280.537907 a.u.



Radical of **6d**

Sum of Electronic and
Thermal Enthalpies = -3279.912089 a.u.

34	0.823414000	-1.261035000	-0.035045000	34	0.874330000	-1.272440000	-0.088918000
8	-0.355777000	2.414808000	-0.963883000	8	-0.322480000	2.434542000	-0.922652000
7	-0.330790000	0.152246000	-0.562425000	7	-0.302632000	0.161261000	-0.541345000
7	3.993909000	-1.465458000	0.522827000	7	3.880805000	-1.497304000	0.526270000
1	3.538242000	-2.176177000	-0.034927000	6	2.206559000	0.050135000	-0.042107000
6	2.199059000	0.060621000	-0.042793000	6	3.575848000	-0.226043000	0.264770000
6	3.558208000	-0.171011000	0.237028000	6	4.449114000	0.909363000	0.250273000
6	4.394257000	0.952576000	0.246752000	1	5.500500000	0.771719000	0.474248000
1	5.449321000	0.834187000	0.463550000	6	3.975083000	2.179544000	-0.045347000
6	3.897334000	2.233361000	-0.030681000	1	4.664996000	3.016965000	-0.047701000
1	4.581298000	3.075364000	-0.010763000	6	2.623160000	2.401632000	-0.341395000
6	2.561466000	2.432949000	-0.344662000	1	2.247286000	3.391669000	-0.574705000
1	2.160507000	3.412577000	-0.577382000	6	1.735887000	1.318458000	-0.336774000
6	1.708577000	1.324777000	-0.350946000	6	0.284735000	1.417305000	-0.635746000
6	0.260777000	1.408758000	-0.659798000	6	5.247401000	-1.840483000	0.842925000
6	5.401352000	-1.740760000	0.759025000	1	5.606902000	-1.318772000	1.740980000
1	5.744019000	-1.208246000	1.649044000	1	5.313503000	-2.913001000	1.026549000
1	5.518951000	-2.808080000	0.948807000	1	5.936235000	-1.592446000	0.023214000
1	6.050801000	-1.463124000	-0.083150000	6	-1.686199000	-0.085127000	-0.795084000
6	-1.715370000	-0.096323000	-0.805655000	6	-2.637694000	0.053997000	0.260197000
6	-2.661833000	0.046574000	0.253828000	6	-2.083239000	-0.465288000	-2.057020000
6	-2.118674000	-0.479136000	-2.064810000	6	-2.279736000	0.443523000	1.576125000
6	-2.297602000	0.441953000	1.566282000	6	-4.014836000	-0.209845000	-0.031094000
6	-4.040379000	-0.218093000	-0.030005000	6	-3.442869000	-0.722098000	-2.335644000
6	-3.479811000	-0.734706000	-2.336650000	1	-1.338163000	-0.558976000	-2.839450000
1	-1.376718000	-0.574592000	-2.849892000	6	-3.234877000	0.563175000	2.557428000
6	-3.248248000	0.565103000	2.551563000	1	-1.240487000	0.651503000	1.800423000
1	-1.257626000	0.652284000	1.784738000	6	-4.973724000	-0.074896000	1.007298000
6	-4.994379000	-0.079907000	1.012483000	6	-4.385540000	-0.597788000	-1.344469000
6	-4.417479000	-0.608516000	-1.340820000	1	-3.735956000	-1.015060000	-3.338211000
1	-3.778306000	-1.028328000	-3.337458000	6	-4.595130000	0.302205000	2.272666000
6	-4.609710000	0.301945000	2.274593000	1	-2.944970000	0.864268000	3.558923000
1	-2.953695000	0.871358000	3.550131000	1	-6.017519000	-0.273840000	0.782710000
1	-6.039261000	-0.279524000	0.793514000	1	-5.432324000	-0.794936000	-1.556091000
1	-5.465448000	-0.805329000	-1.547010000	1	-5.338243000	0.403231000	3.057040000
1	-5.349037000	0.405848000	3.062189000				

Table S5. Data for **3** and **6a-6d** obtained by DFT calculations at the B3LYP/6-311+G(d) level in the gas phase. The N-H bond dissociation enthalpies (BDE_{N-H}) of **6a-6d** were calculated.

Calculated BDE_{N-H} (kcal/mol)		r_{Se-N} [Å]	NPA Charges[a]	^{77}Se NMR (ppm)[b]	
			q_{Se}	Exptl.	Calcd.
3		1.897			
6a	78.89	1.898	+0.596	926	936
6b	78.88	1.898	+0.595	928	933
6c	78.90	1.898 (1.876)	+0.588	934	948
6d	78.95	1.899	+0.591	962	975

[a]The NBO analysis was calculated at the B3LYP/6-311+G(d,p) level using the B3LYP/6-311+G(d)-level-optimized geometries. [b] The ^{77}Se NMR values are referenced to Me_2Se ($\delta = 0$). The experimental values are given in parentheses.

Figure S35. Relative cell viability of C6 cells in the presence of 10 - 120 µM of antioxidants ebselen (**3**), **5a-5d** and **6a-6d** as determined by MTT measurements after 24 h at 570 nm.