Electronic Supplementary Material (ESI) for New Journal of Chemistry.
This journal is © The Royal Society of Chemistry and the Centre National de la Recherche Scientifique 2022

Supporting Information

for

Synthesis and Antioxidant Activities of *N*-Thiophenyl Ebselenamines: The $^{77}Se\{^{1}H\}$ NMR Mechanistic Study†

Manish Kumar and Vijay P. Singh*

Department of Chemistry & Centre of Advanced Studies in Chemistry, Panjab University, Sector-14, Chandigarh – 160 014, India

*E-mail: vijay@pu.ac.in

---Table of Contents---

Figure S1. The ^{1}H NMR spectrum of compound **8** in $CDCl_3$

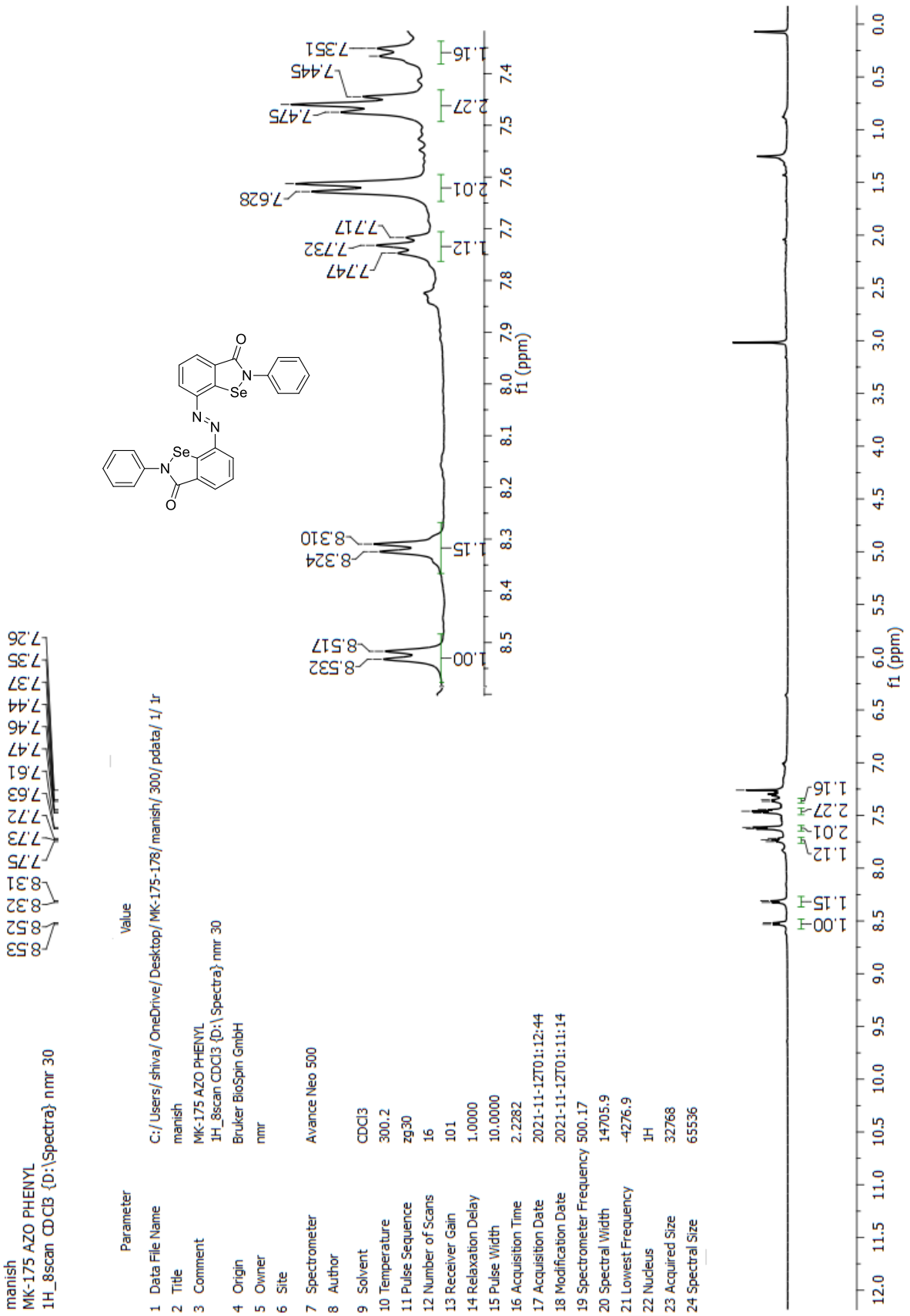


Figure S2. The ^{13}C NMR spectrum of compound **8** in $CDCl_3$

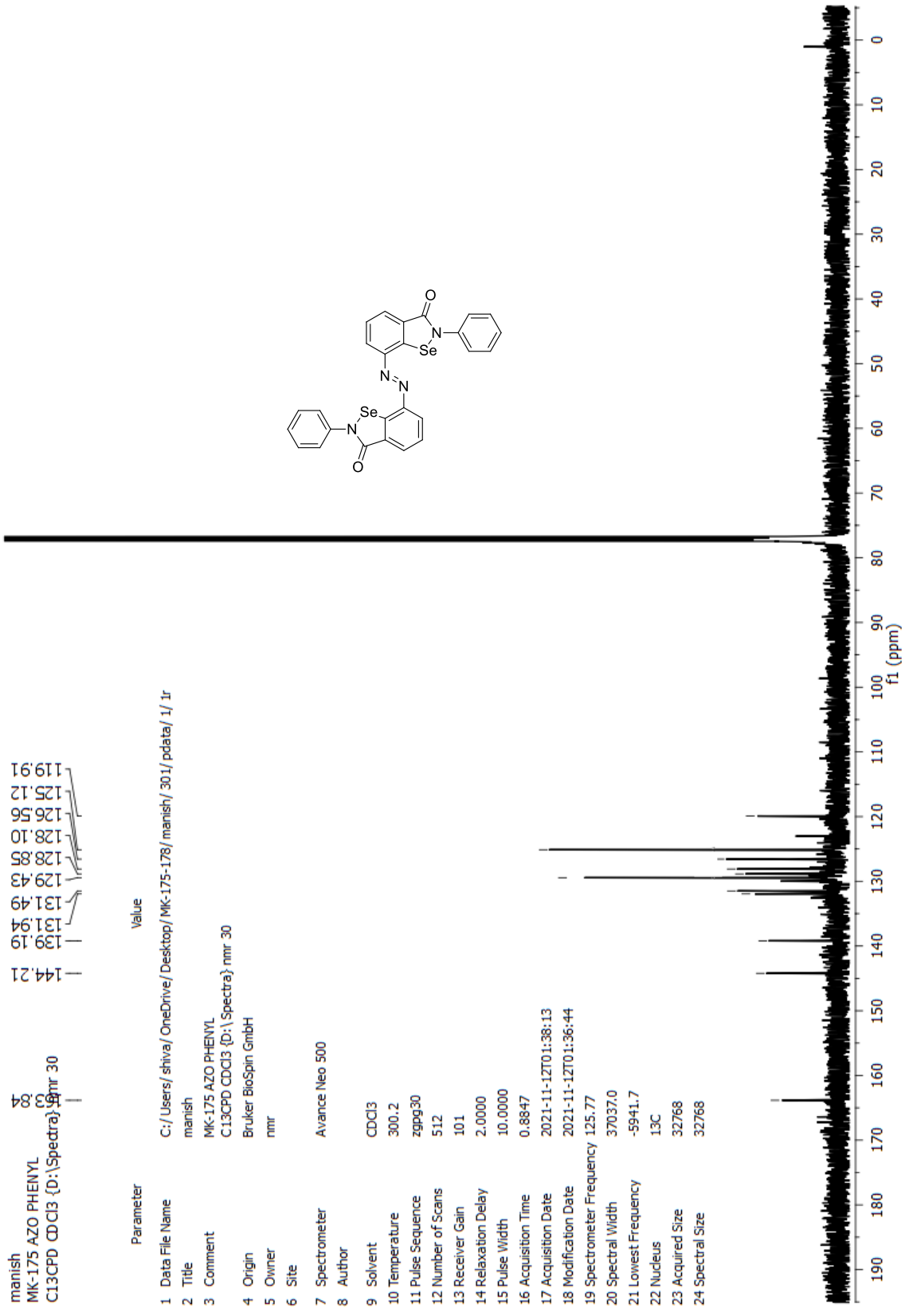


Figure S3. The $^{77}Se\{^{1}H\}$ NMR spectrum of compound **8** in $CDCl_3$

Figure S4. The ^{1}H NMR spectrum of diselenide **9** in $CDCl_3$

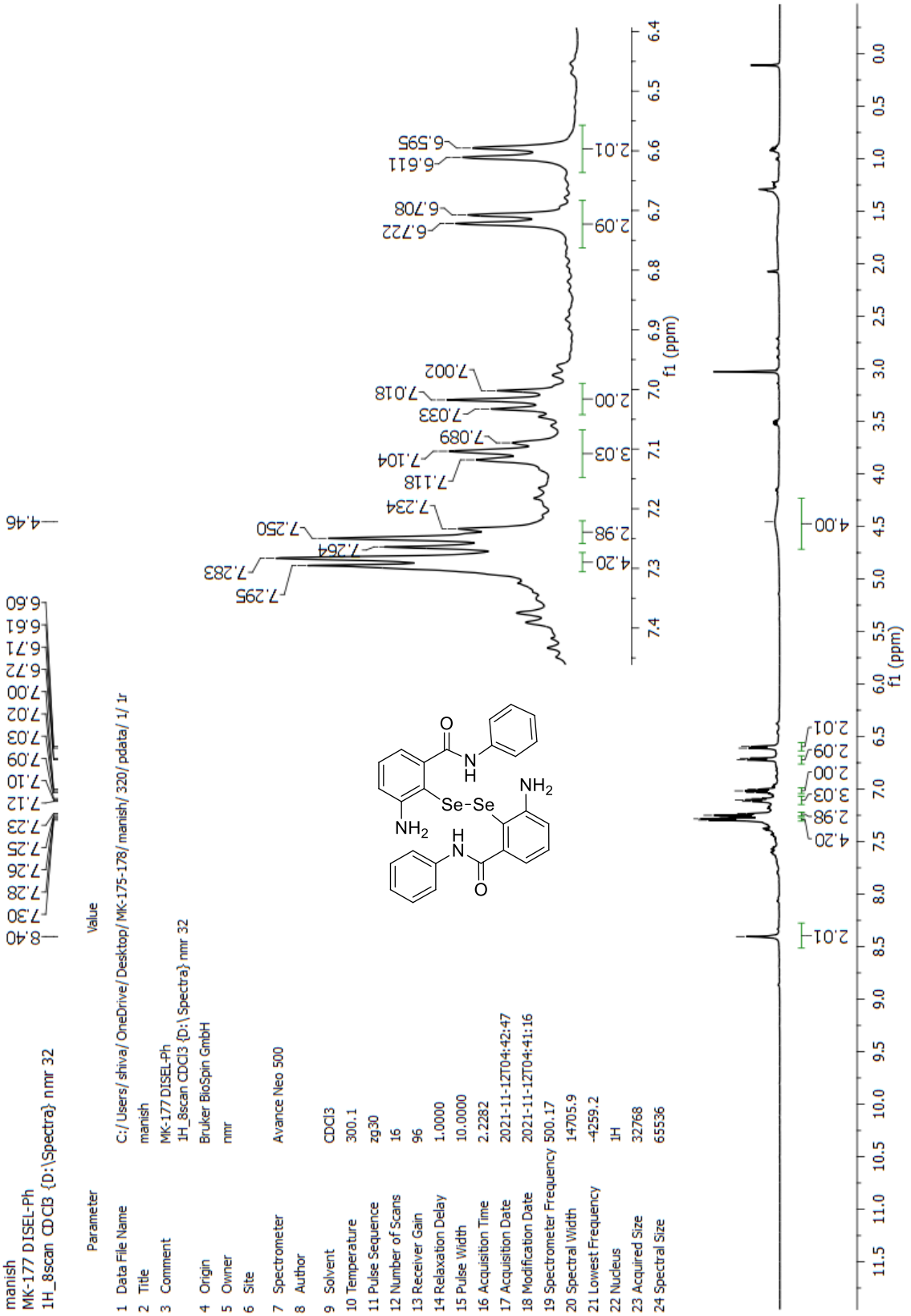


Figure S5. The ^{13}C NMR spectrum of diselenide **9** in $CDCl_3$

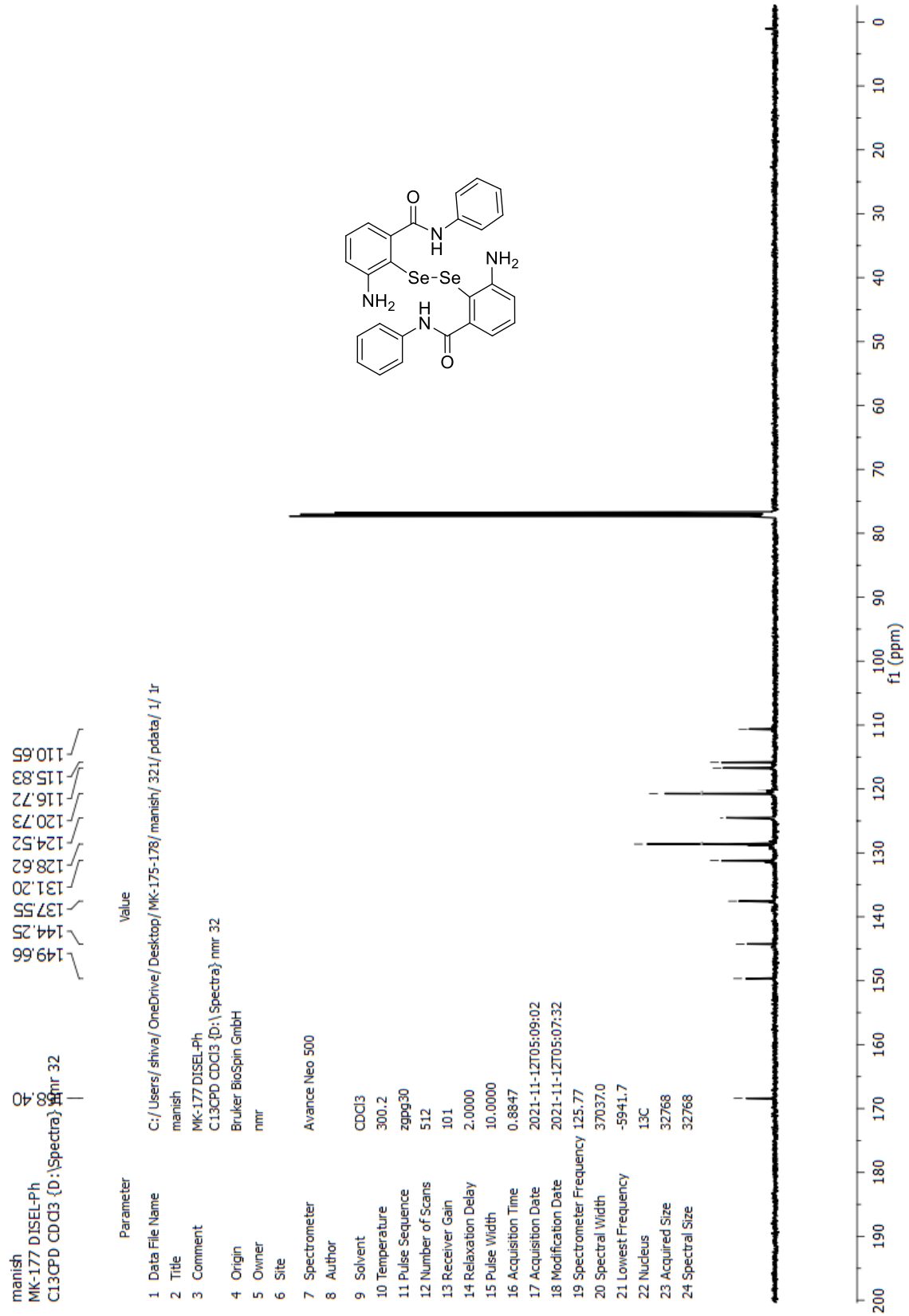


Figure S6. The $^{77}Se\{^{1}H\}$ NMR spectrum of diselenide **9** in $CDCl_3$

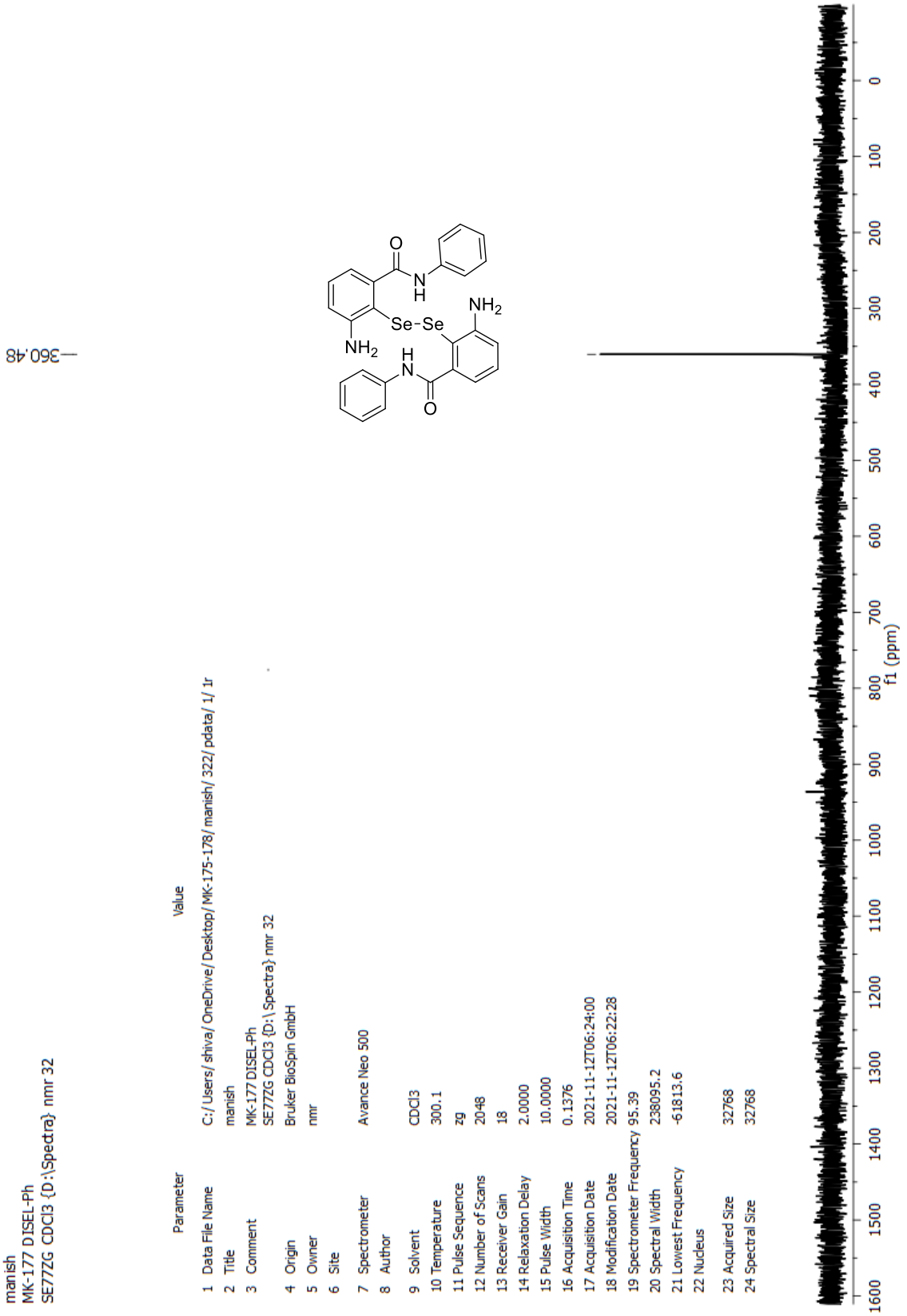


Figure S7. The ^{1}H NMR spectrum of diselenide **15** in $CDCl_3$

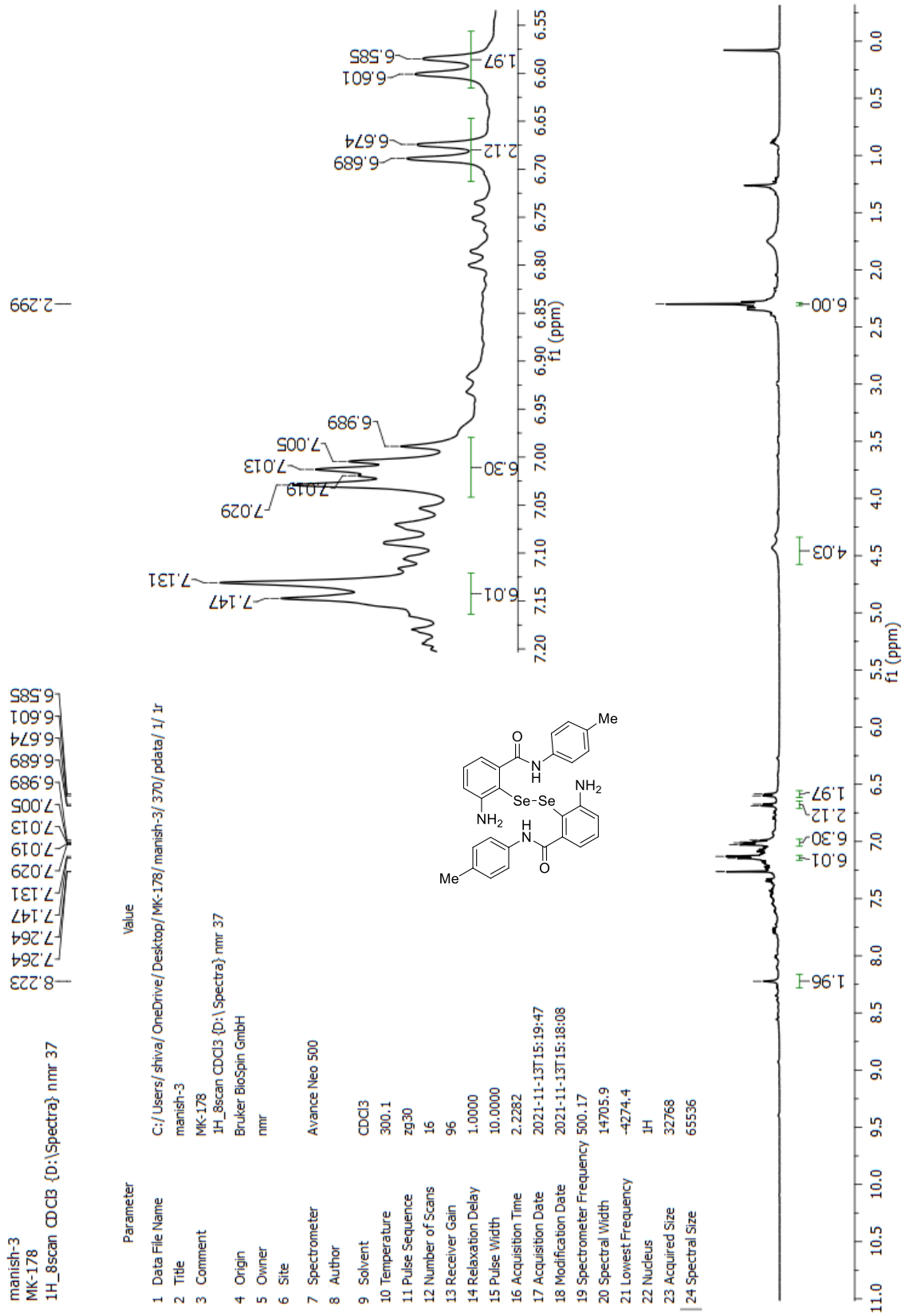


Figure S8. The ^{13}C NMR spectrum of diselenide **15** in $CDCl_3$

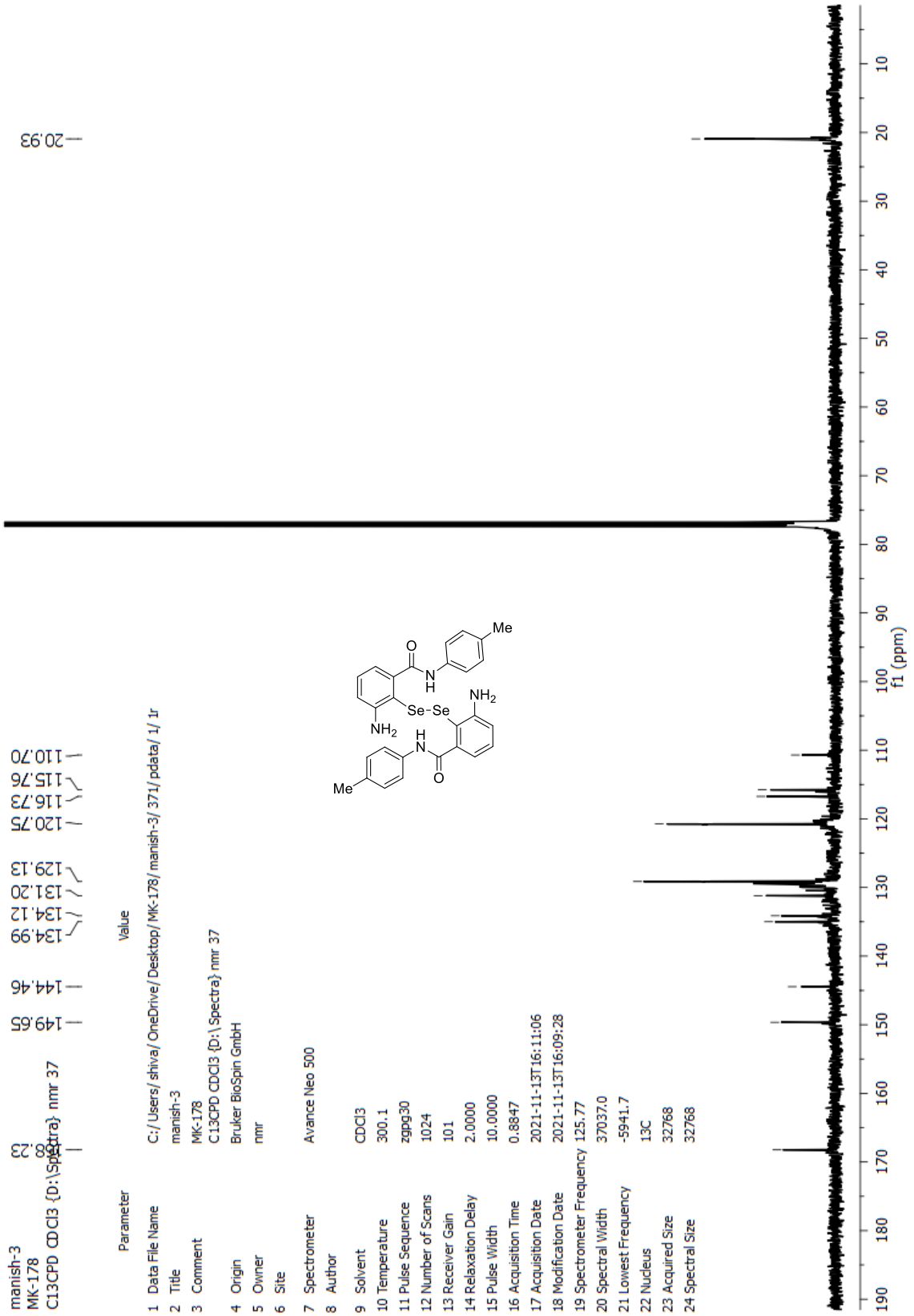


Figure S9. The $^{77}Se\{^{1}H\}$ NMR spectrum of diselenide **15** in $CDCl_3$

Figure S10. The $^{77}Se\{^{1}H\}$ NMR spectrum of compound **7a** in DMSO-d_6

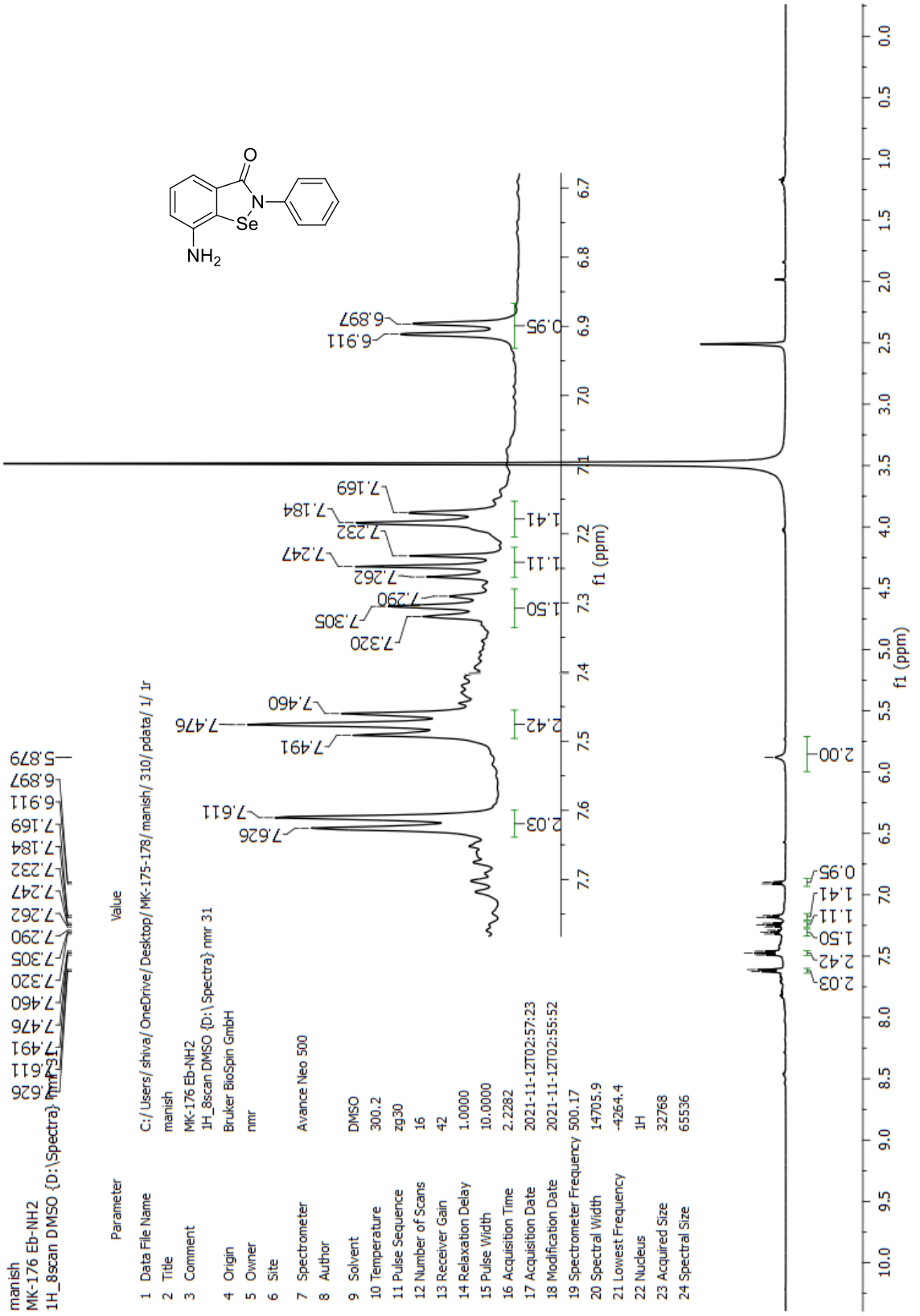
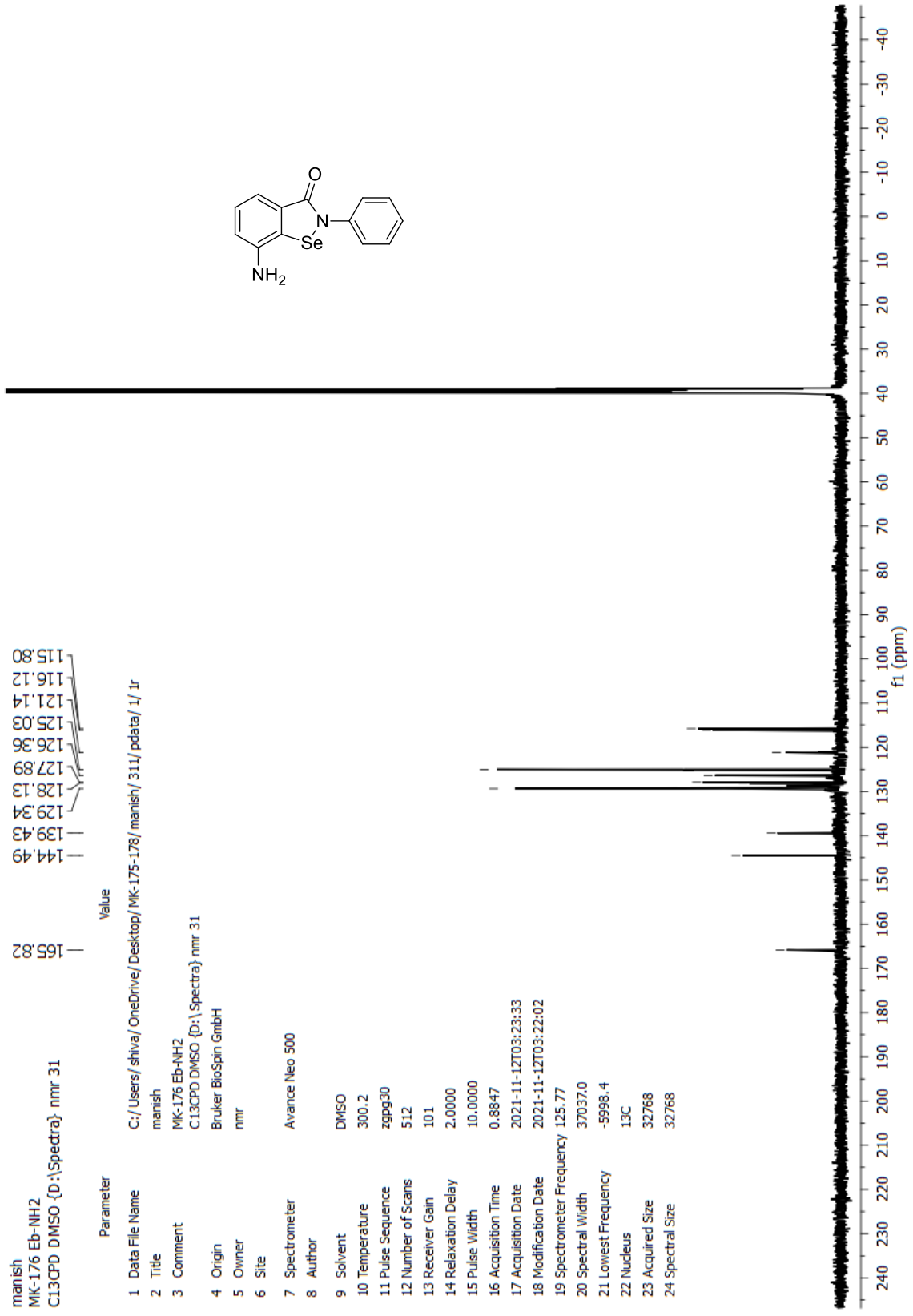


Figure S11. The ^{13}C NMR spectrum of compound **7a** in DMSO-d_6



Parameter	Value
1 Data File Name	C:/Users/shiva/OneDrive/Desktop/MK-175-178/manish/311/pdata/1/1r
2 Title	manish
3 Comment	MK-176 Eb-NH2 C13CPD DMSO {D:\Spectra} nmr 31
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Spectrometer	Avance Neo 500
8 Author	
9 Solvent	DMSO
10 Temperature	300.2
11 Pulse Sequence	zgpg30
12 Number of Scans	512
13 Receiver Gain	101
14 Relaxation Delay	2.0000
15 Pulse Width	10.0000
16 Acquisition Time	0.8847
17 Acquisition Date	2021-11-12T03:23:33
18 Modification Date	2021-11-12T03:22:02
19 Spectrometer Frequency	125.77
20 Spectral Width	37037.0
21 Lowest Frequency	-5998.4
22 Nucleus	13C
23 Acquired Size	32768
24 Spectral Size	32768

Figure S12. The $^{77}Se\{^{1}H\}$ NMR spectrum of compound **7a** in DMSO-d_6

Mechanistic study of 8 with PhSH and H_2O_2

Figure S13. The $^{77}Se\{^{1}H\}$ NMR spectrum of compound **8** in $CDCl_3$

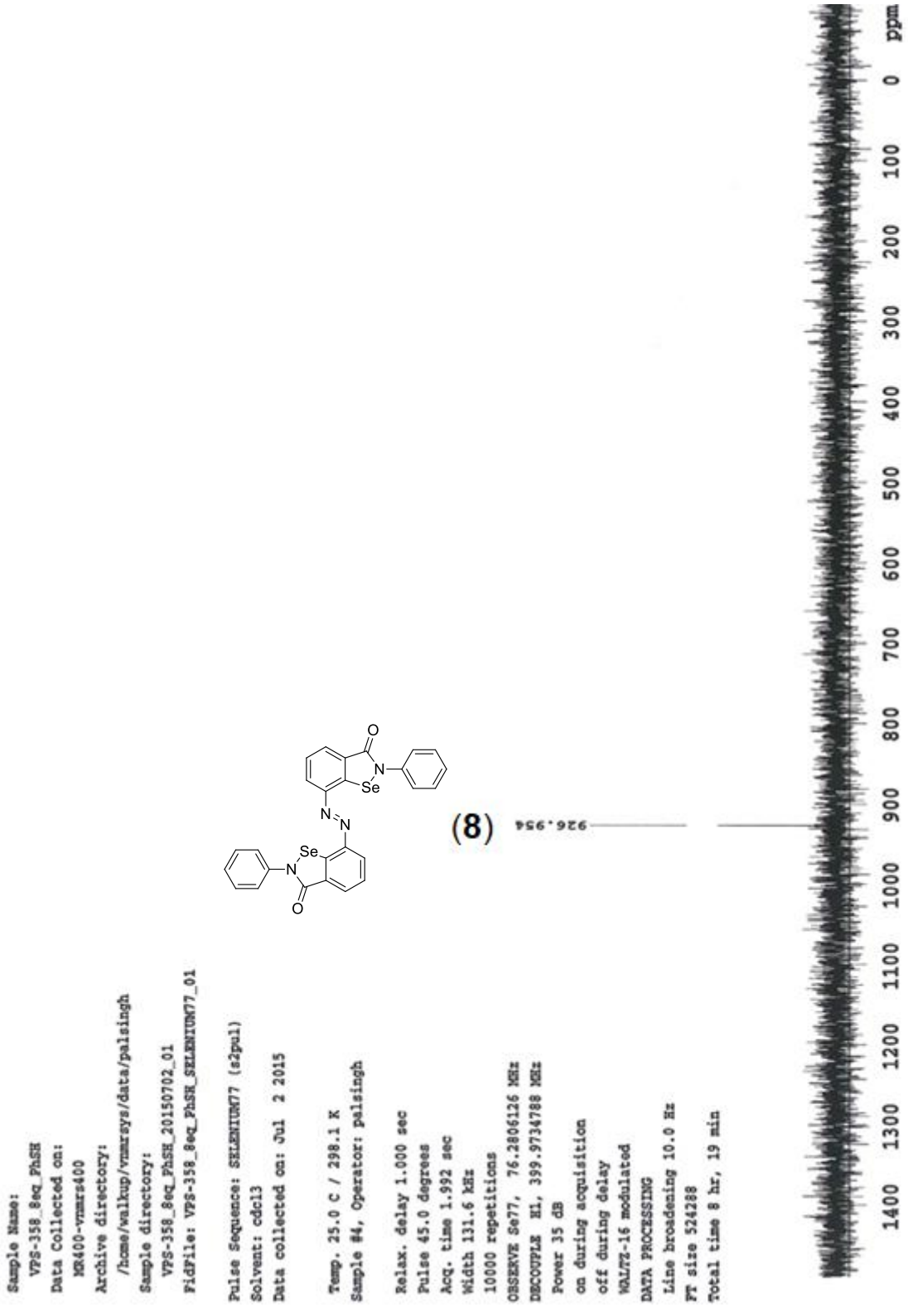


Figure S14. The $^{77}Se\{^{1}H\}$ NMR spectrum of **8** with PhSH (8 equiv)

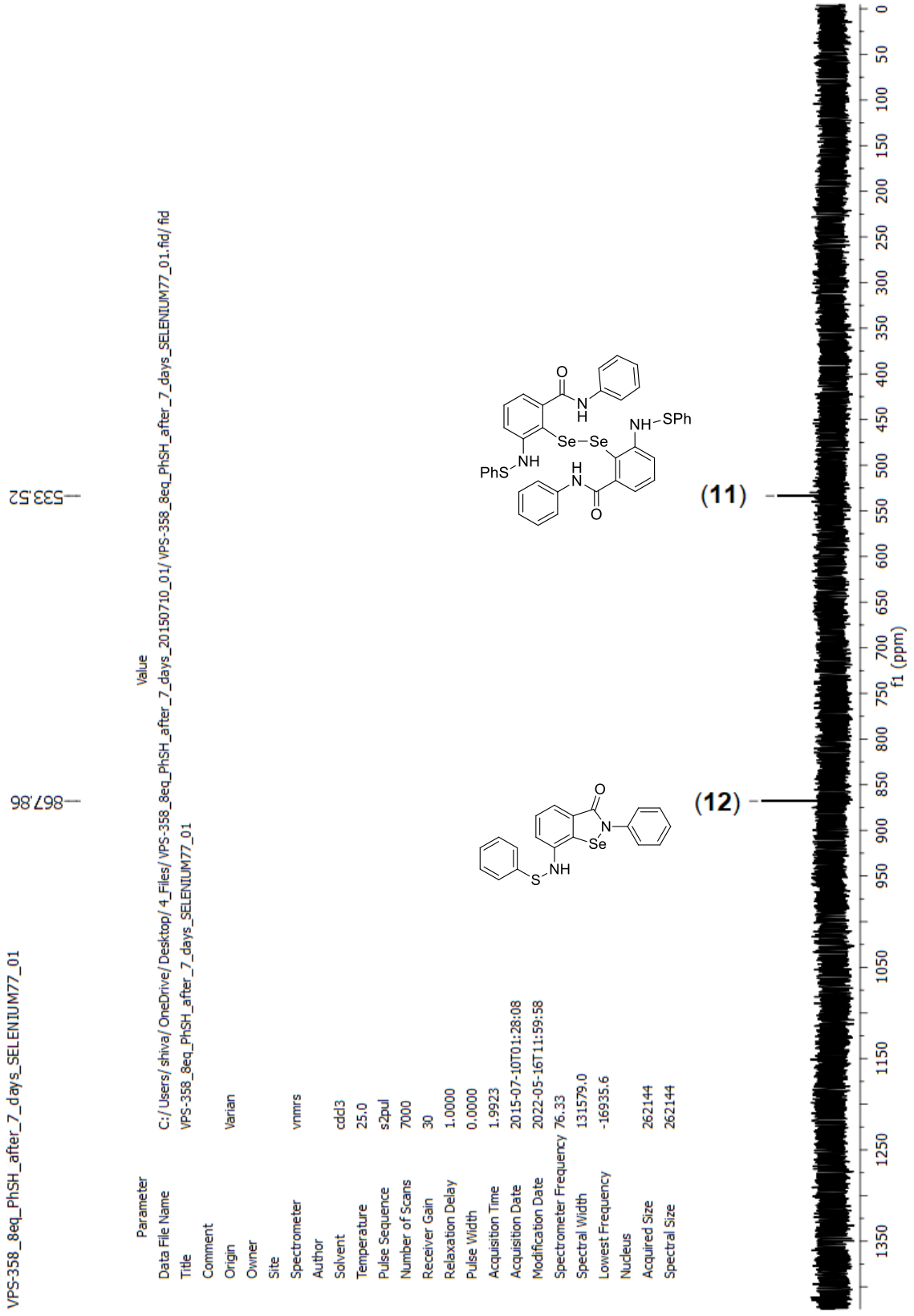


Figure S15. The $^{77}Se\{^{1}H\}$ NMR spectrum of **8** with PhSH (8 + 8 equiv)

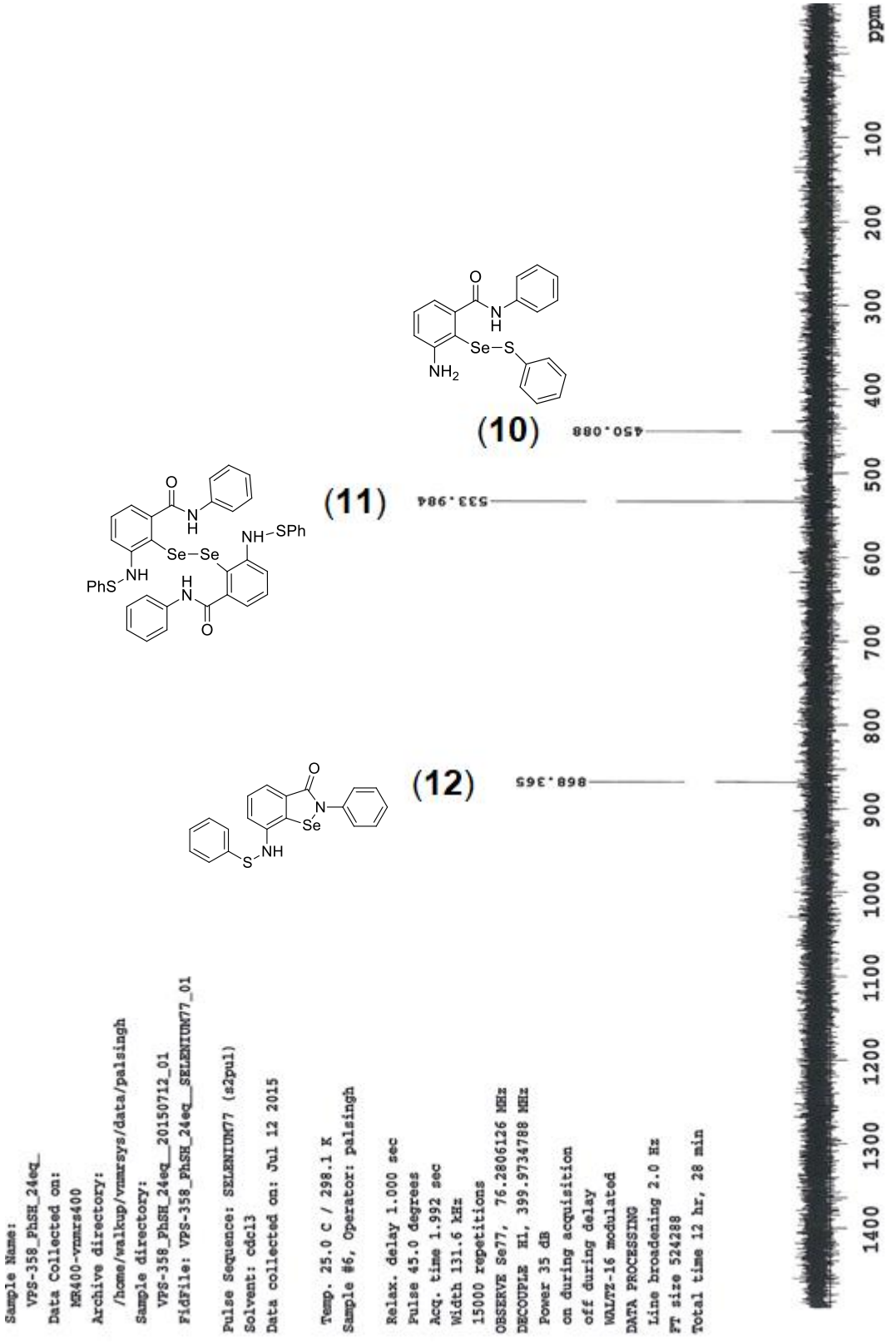


Figure S16. The $^{77}Se\{^{1}H\}$ NMR spectrum of **8** with PhSH (24 equiv)

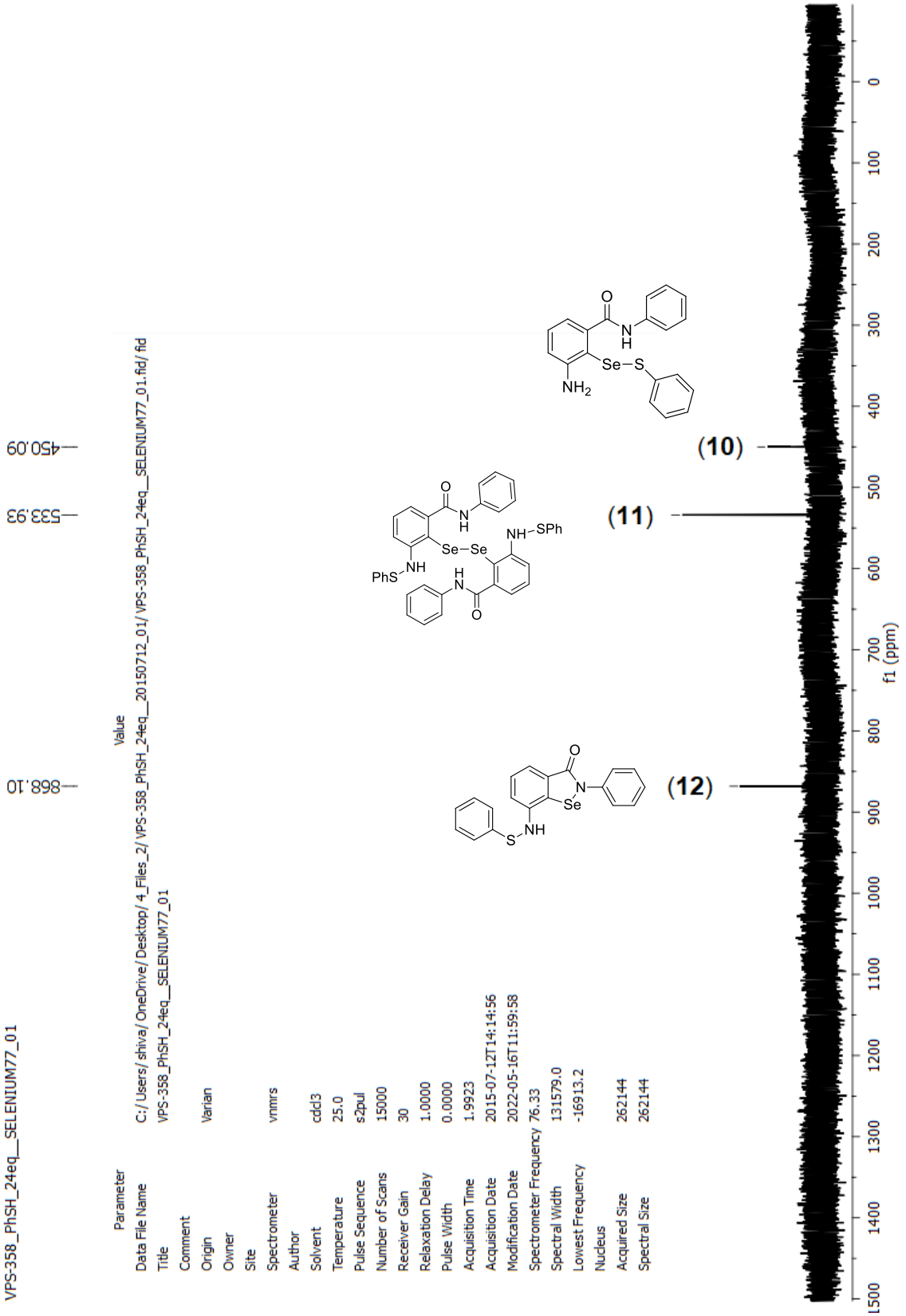


Figure S17. The $^{77}Se\{^{1}H\}$ NMR spectrum of **8** with PhSH (24 equiv) and H_2O_2 (6 equiv)

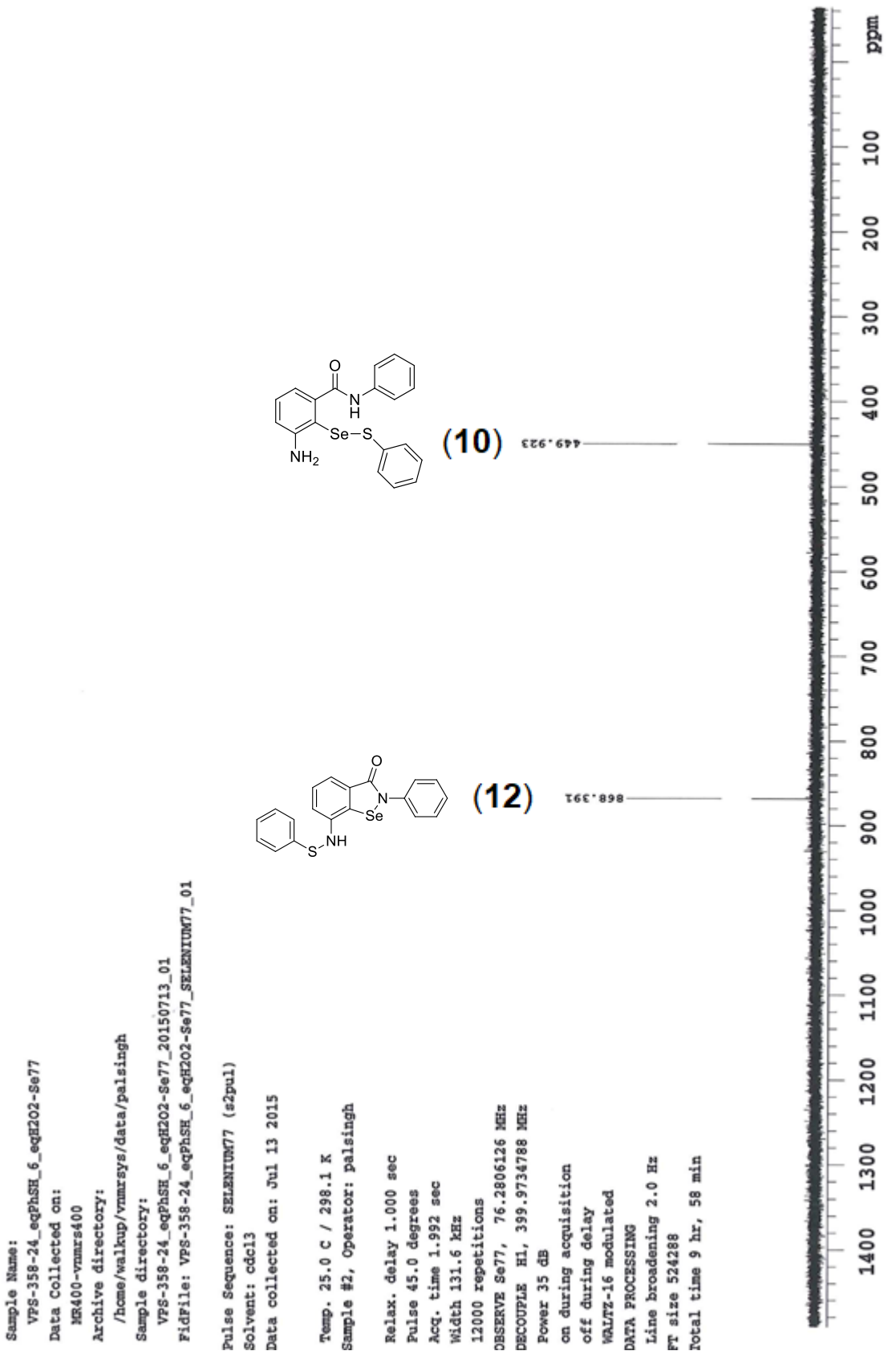
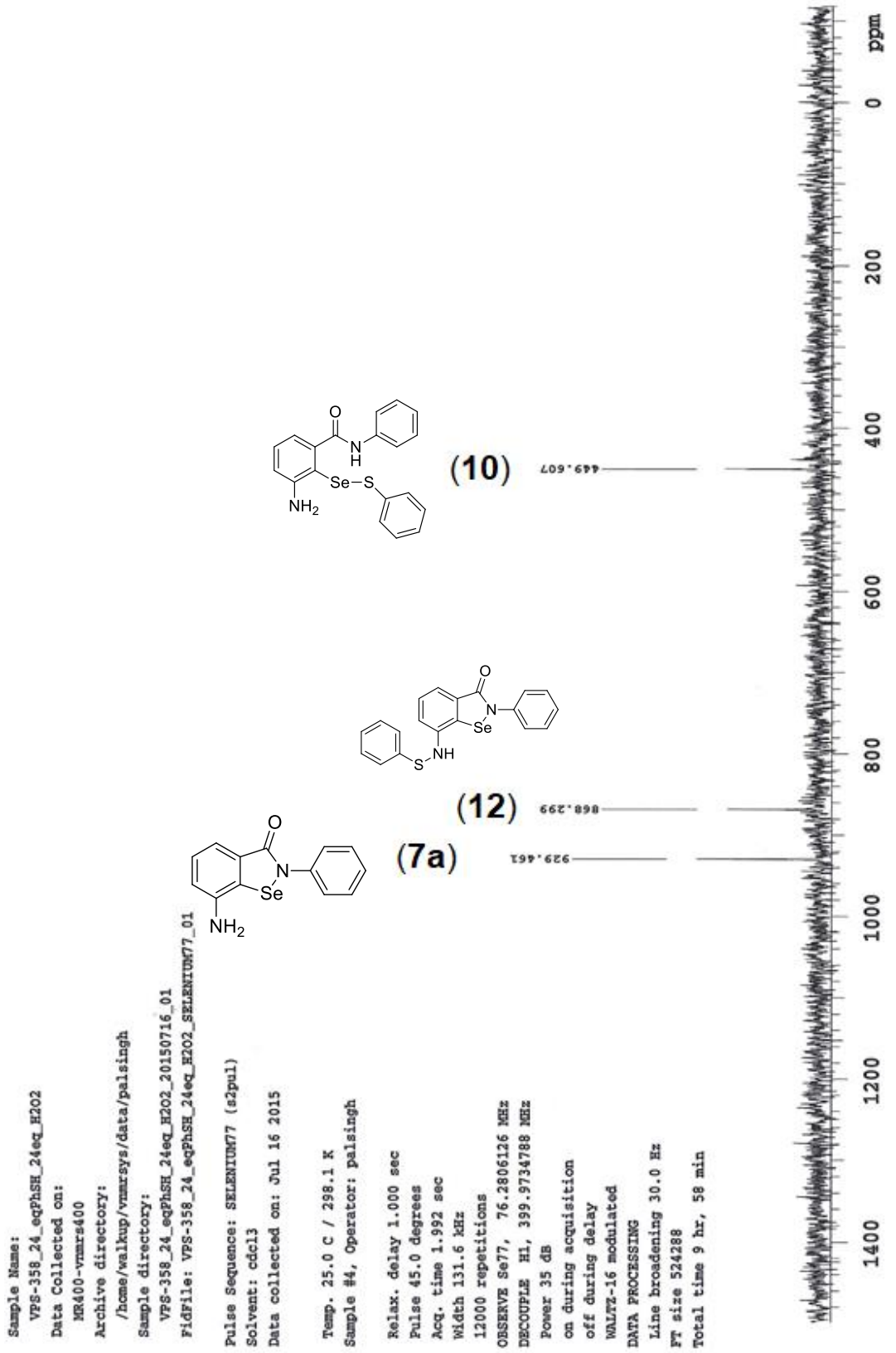


Figure S18. $^{77}Se\{^{1}H\}$ NMR spectrum of **8** with PhSH (24 equiv) and H_2O_2 (24 equiv)



Repeated mechanistic experiment of 8 with PhSH and H_2O_2

Figure S19. The $^{77}Se\{^{1}H\}$ NMR spectrum of **8** with PhSH (8 equiv) in $CDCl_3$)

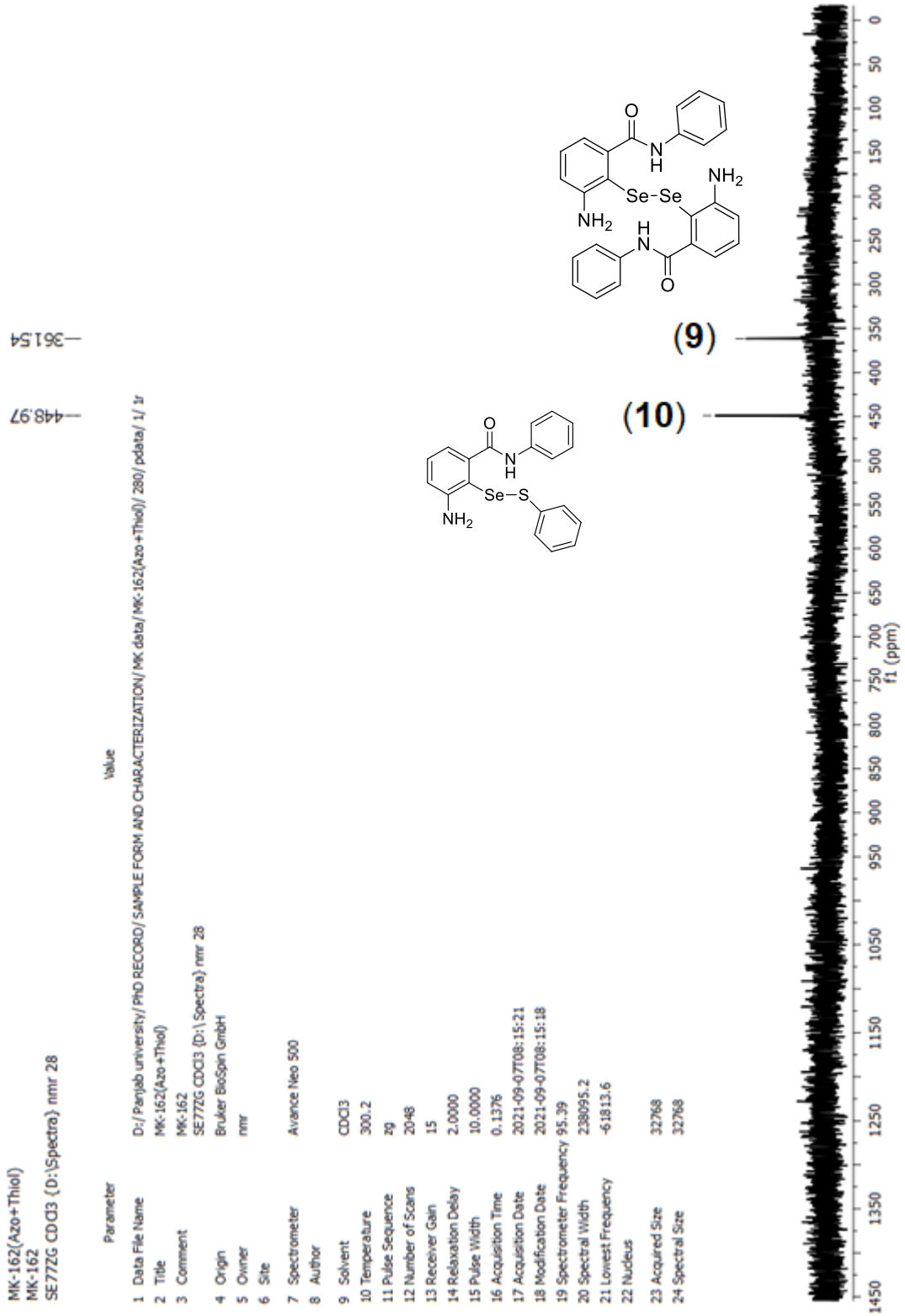


Figure S20.The $^{77}Se\{^{1}H\}$ NMR of **8** and PhSH (8+8 equiv) in $CDCl_3$

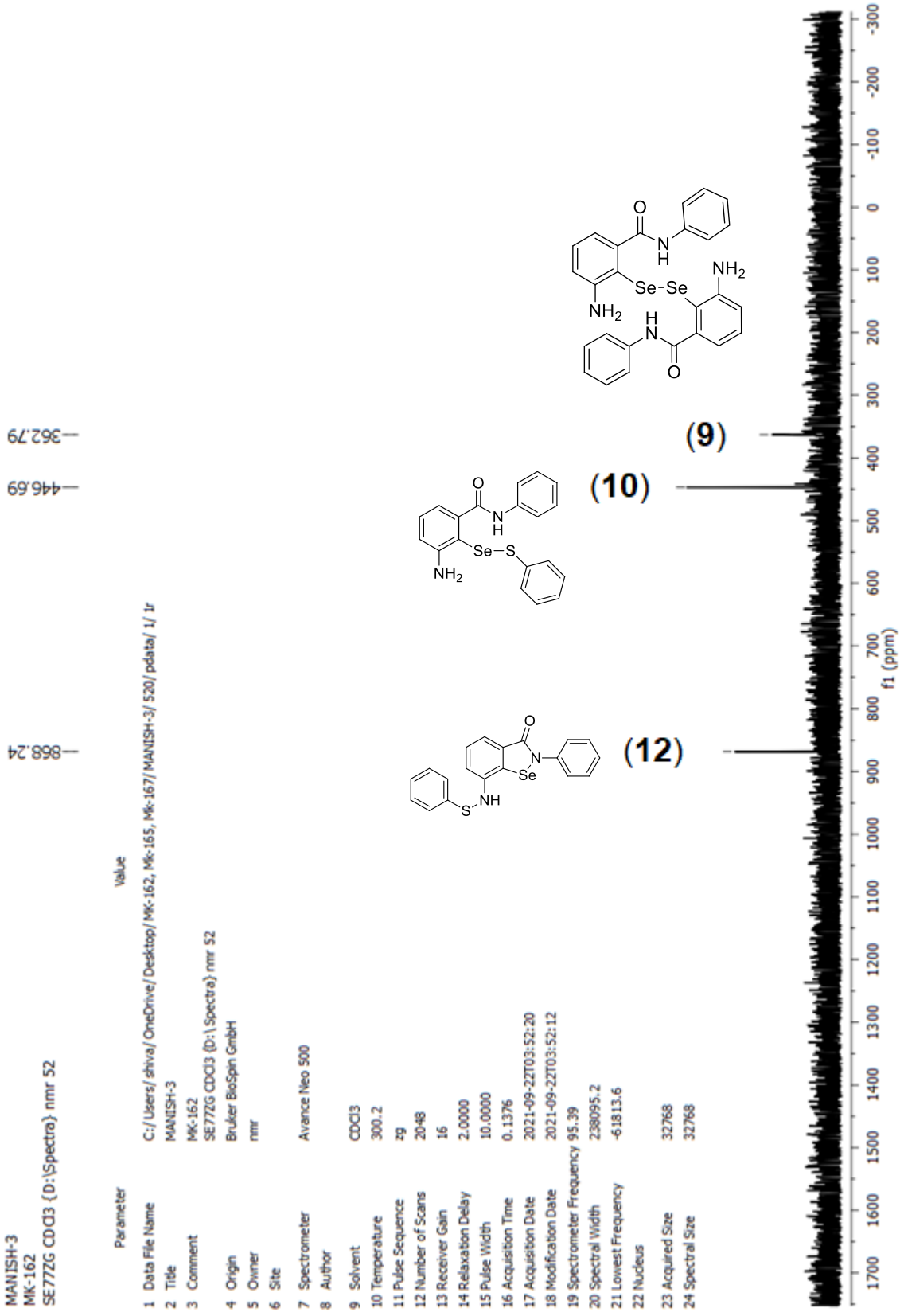


Figure S21. The $^{77}Se\{^{1}H\}$ NMR of **8** with PhSH (16 equiv) + H_2O_2 (4 equiv) in $CDCl_3$

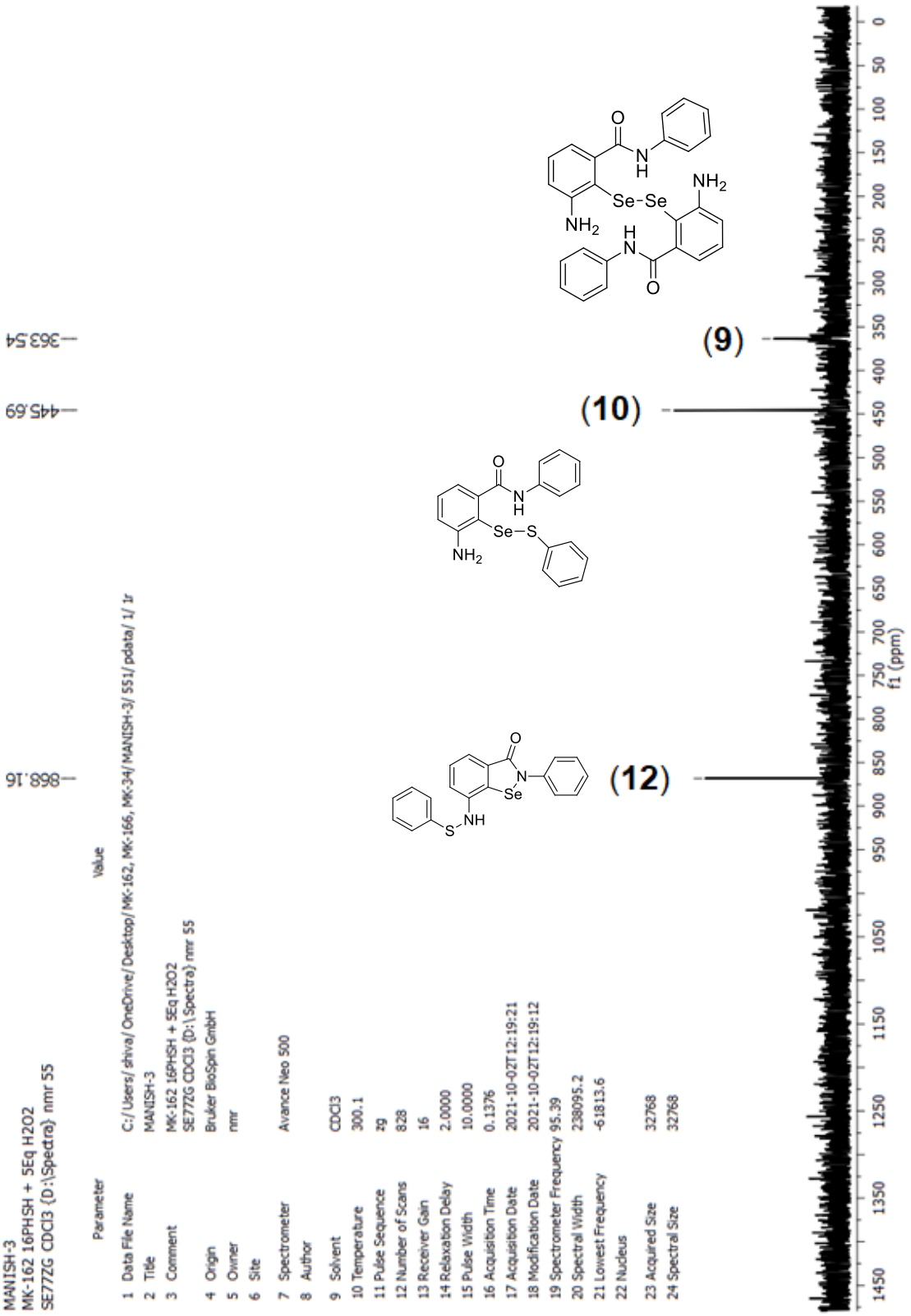


Figure S22. The $^{77}Se\{^{1}H\}$ NMR of **8** with PhSH (16 equiv) + H_2O_2 (6 equiv) in $CDCl_3$)

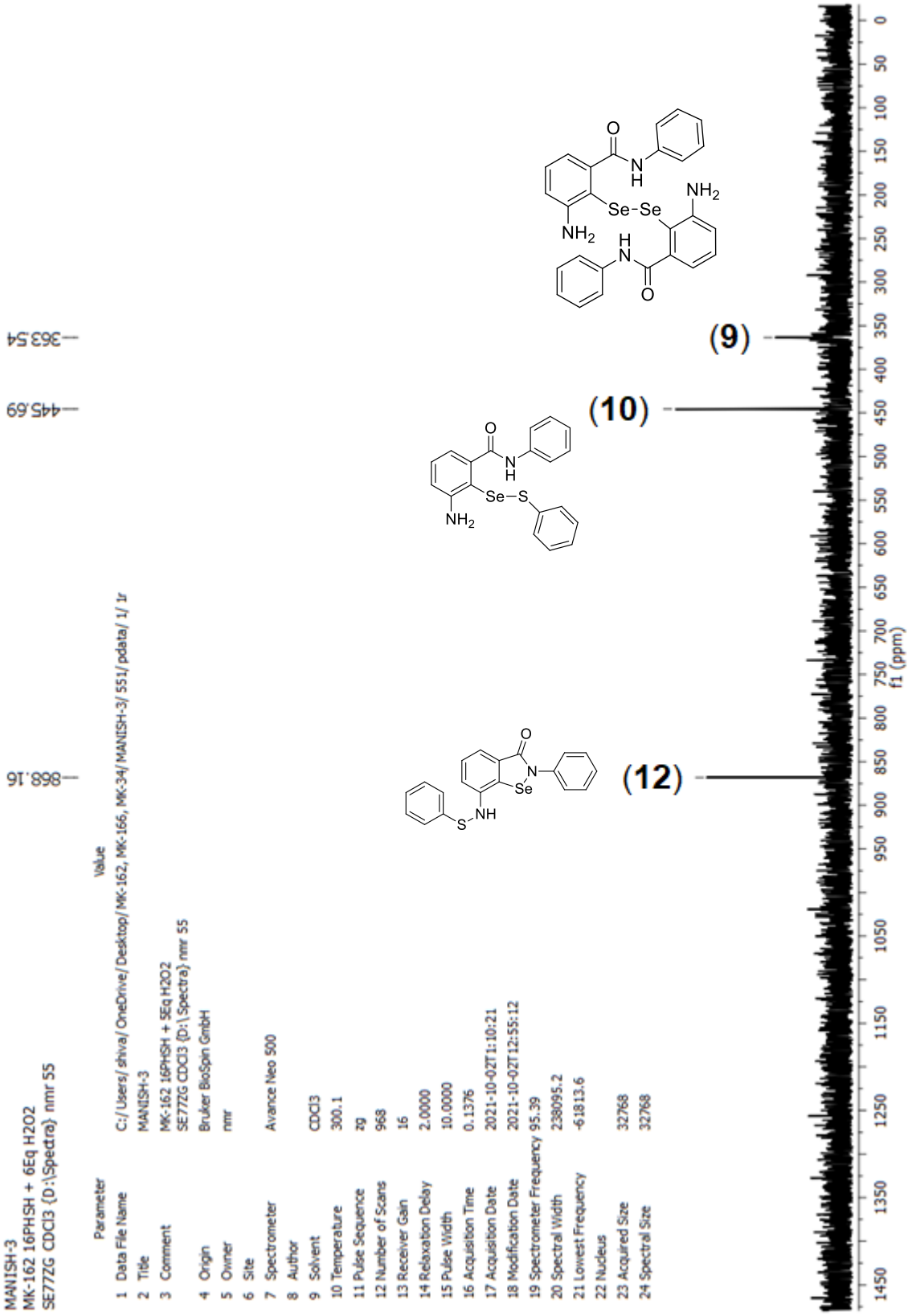
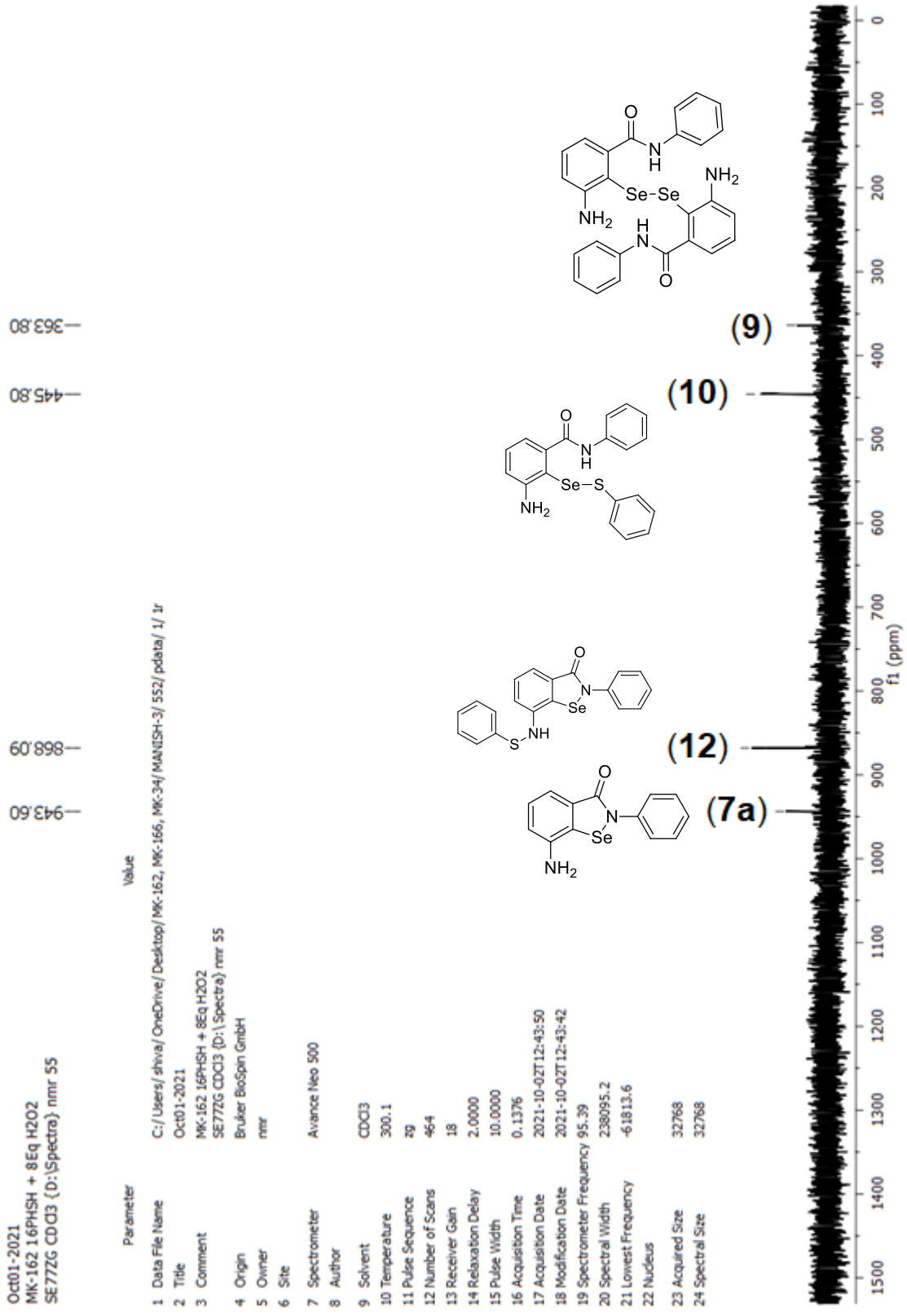


Figure S23. The $^{77}Se\{^{1}H\}$ NMR of **8** with PhSH (16 equiv) + H_2O_2 (8 equiv) in $CDCl_3$



Mechanistic Studies of Diselenide 9 with PhSH and H_2O_2

Figure S24. The $^{77}Se\{^{1}H\}$ NMR spectrum of diselenide **9**

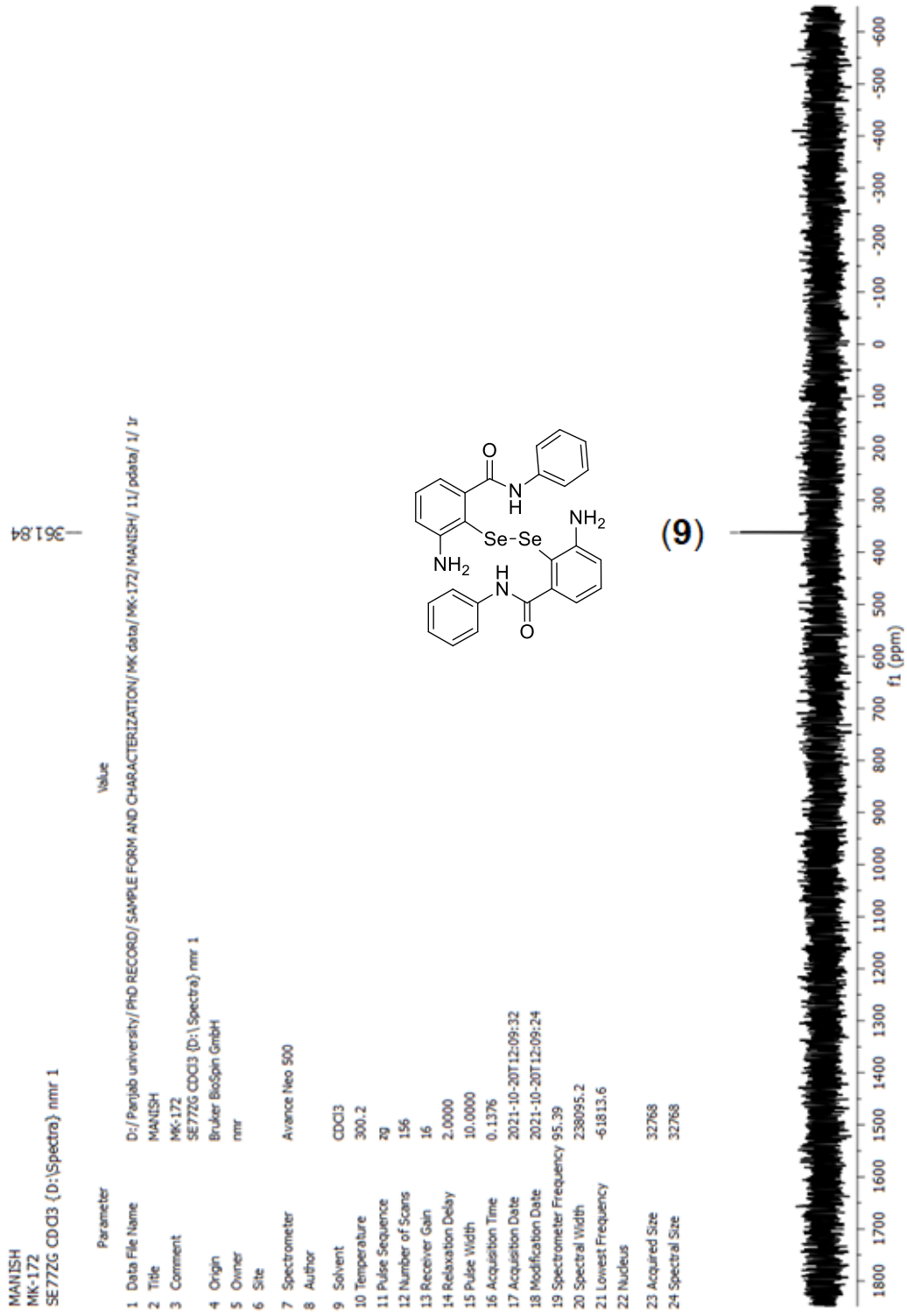


Figure S25. The $^{77}Se\{^{1}H\}$ NMR spectrum of diselenide **9** + PhSH (1 equiv)

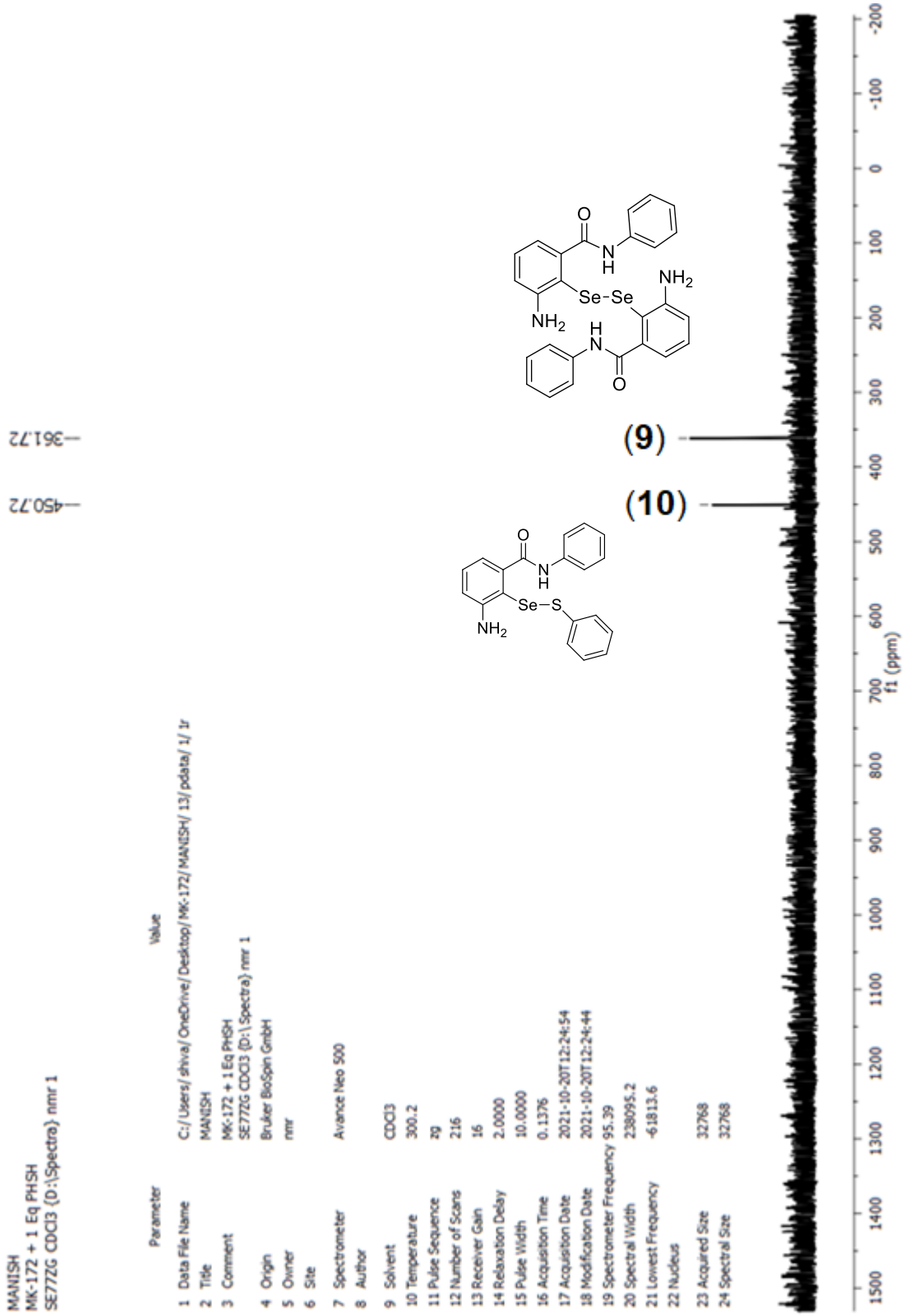


Figure S26. The $^{77}Se\{^{1}H\}$ NMR spectrum of diselenide **9** + PhSH (2 equiv)

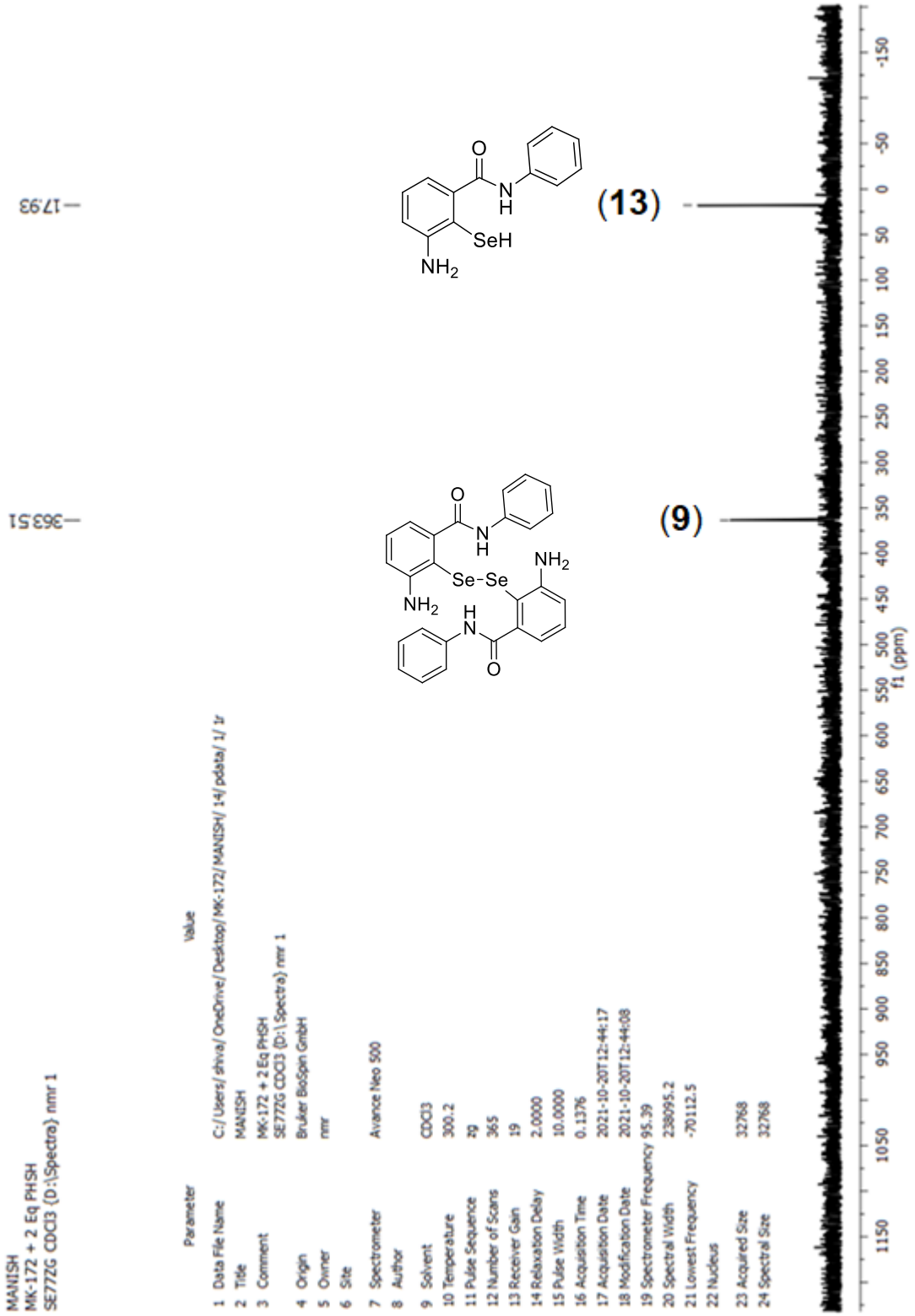


Figure S27. The $^{77}Se\{^{1}H\}$ NMR spectrum of diselenide **9** + PhSH (4 equiv)

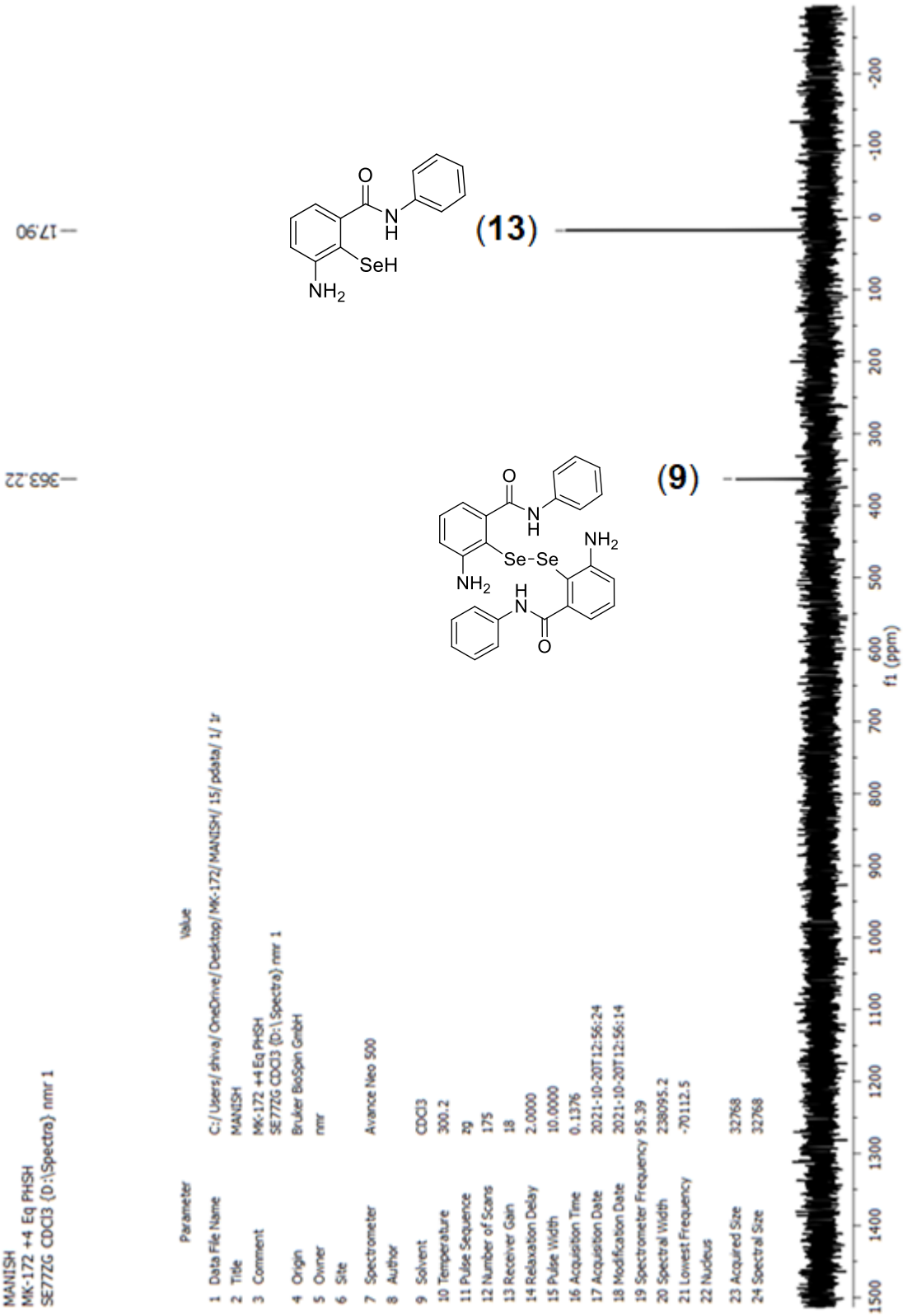


Figure S28. The $^{77}Se\{^{1}H\}$ NMR spectrum of diselenide **9** + PhSH (4 equiv) + H_2O_2 (2 equiv)

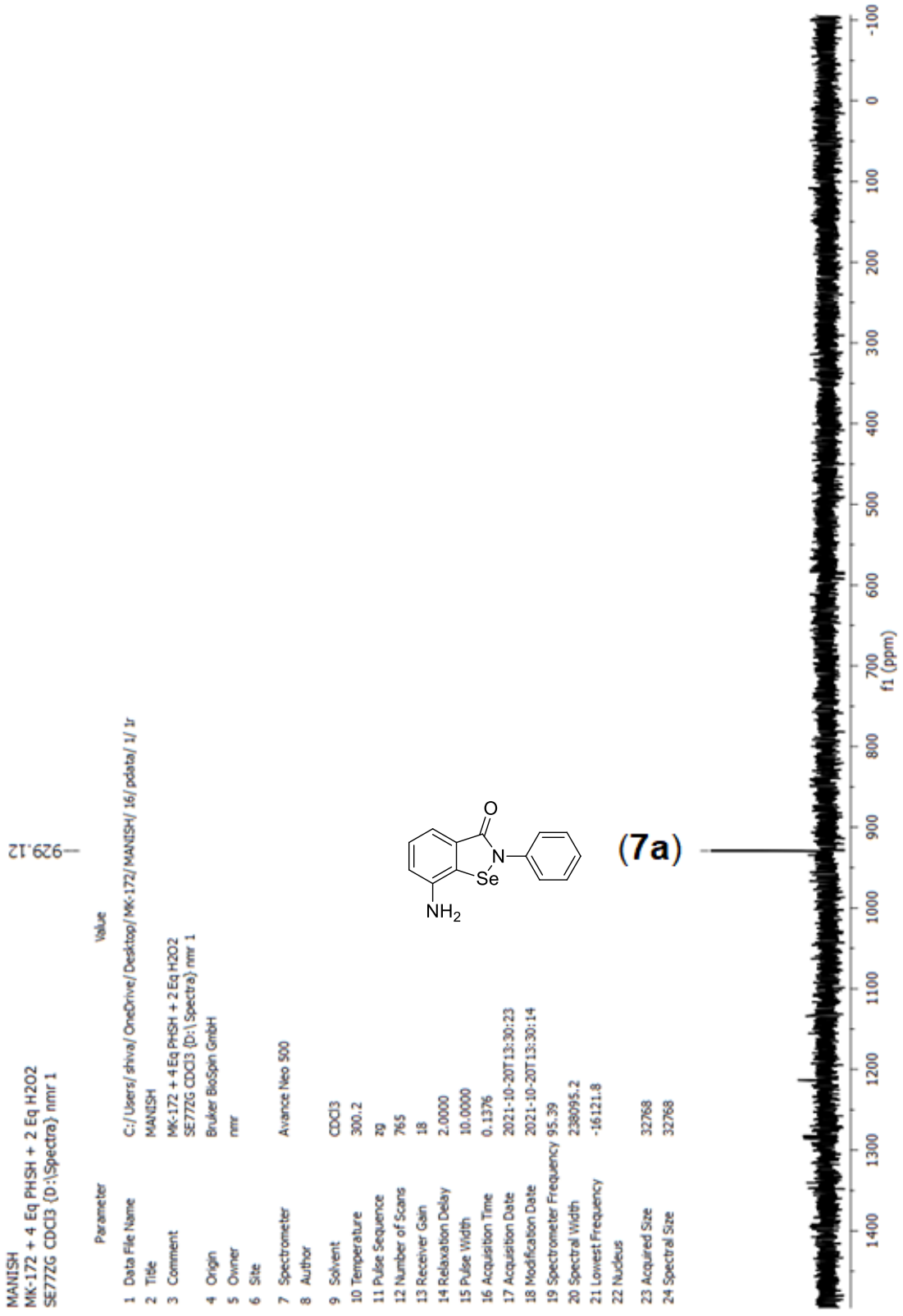


Figure S29. The $^{77}Se\{^{1}H\}$ NMR spectrum of diselenide **9** + PhSH (4 equiv) + H_2O_2 (2 equiv) recorded after 30 min

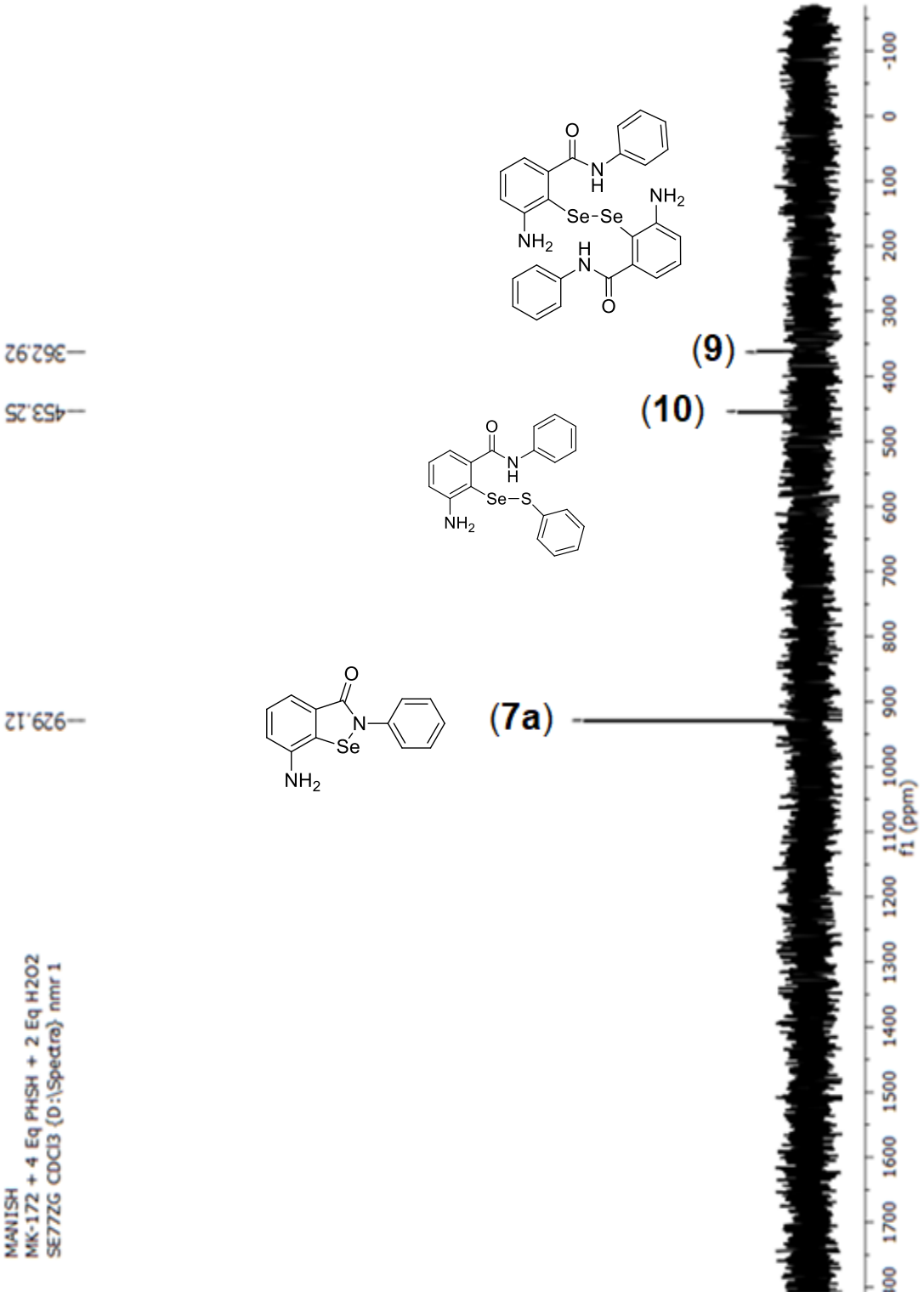
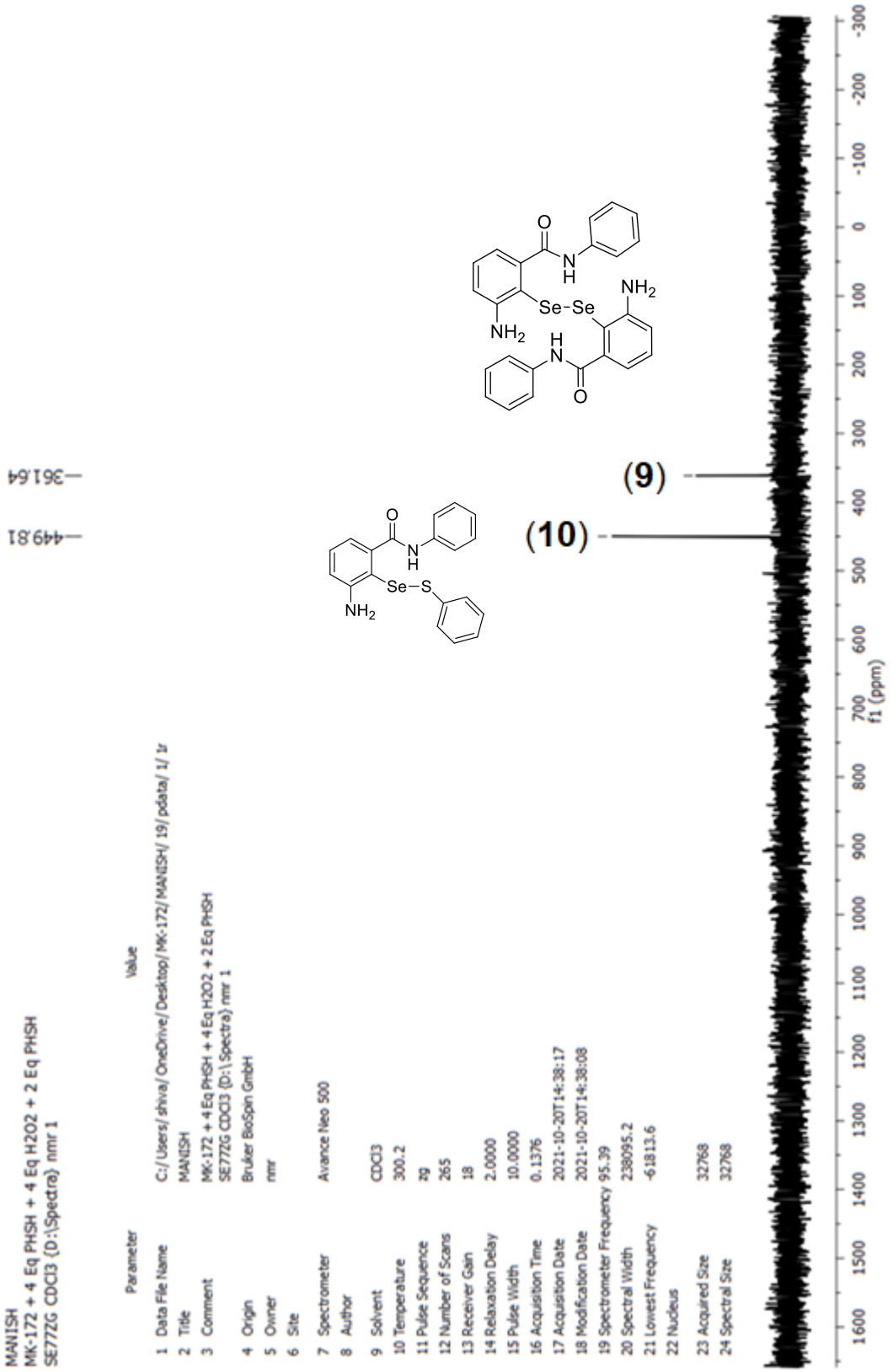


Figure S30. The $^{77}Se\{^{1}H\}$ NMR of diselenide **9** + PhSH (4 equiv) + H_2O_2 (2 equiv) + PhSH (2 equiv)



Mechanistic Studies of Diselenide 9 with PhSSPh and H_2O_2 in $CDCl_3$

Figure S31. The $^{77}Se\{^1H\}$ NMR spectrum of diselenide **9** + PhSSPh (3 equiv)

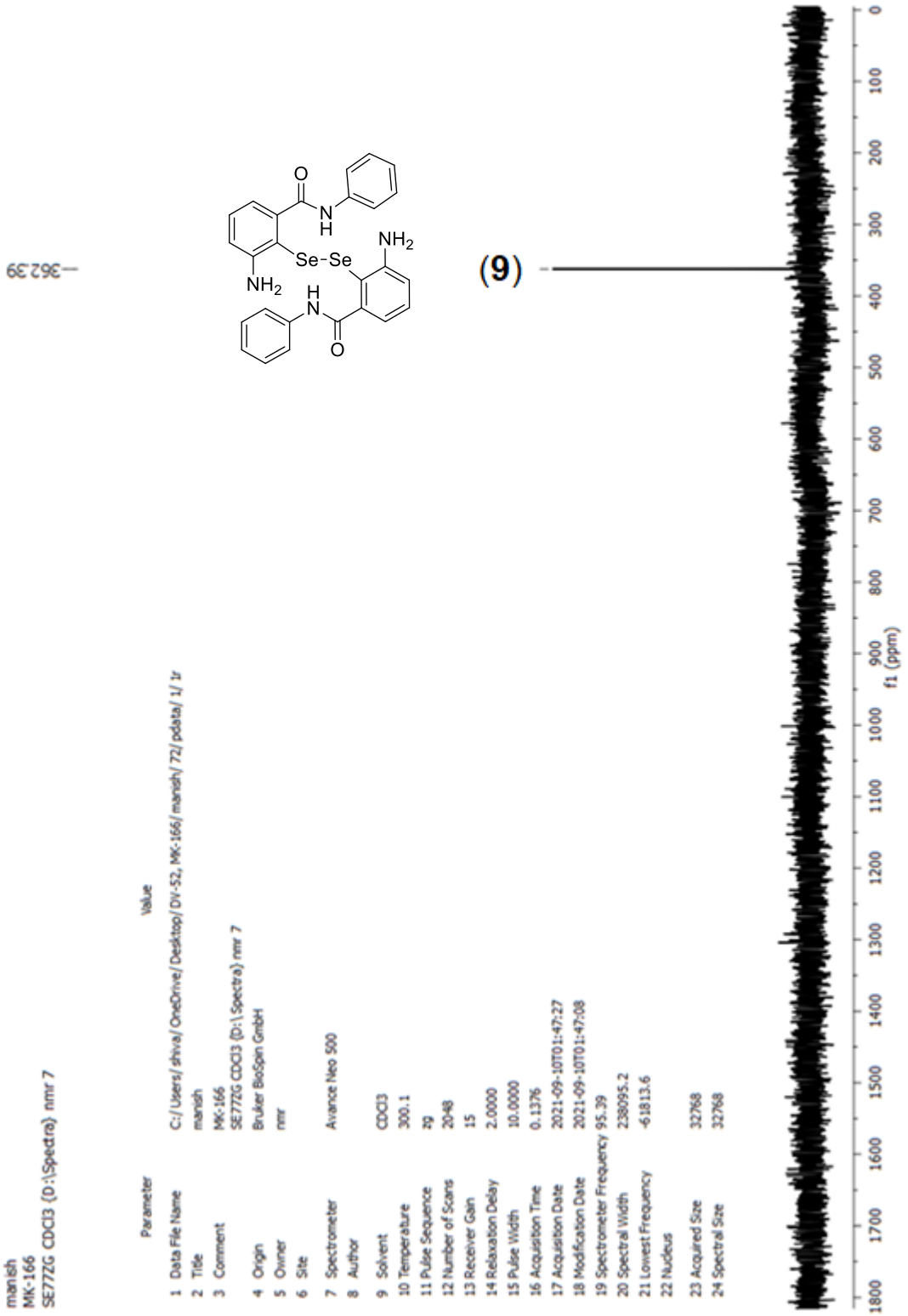


Figure S32. The $^{77}Se\{^{1}H\}$ NMR spectrum of diselenide **9** + PhSSPh (3 equiv) + H_2O_2 (1 equiv)

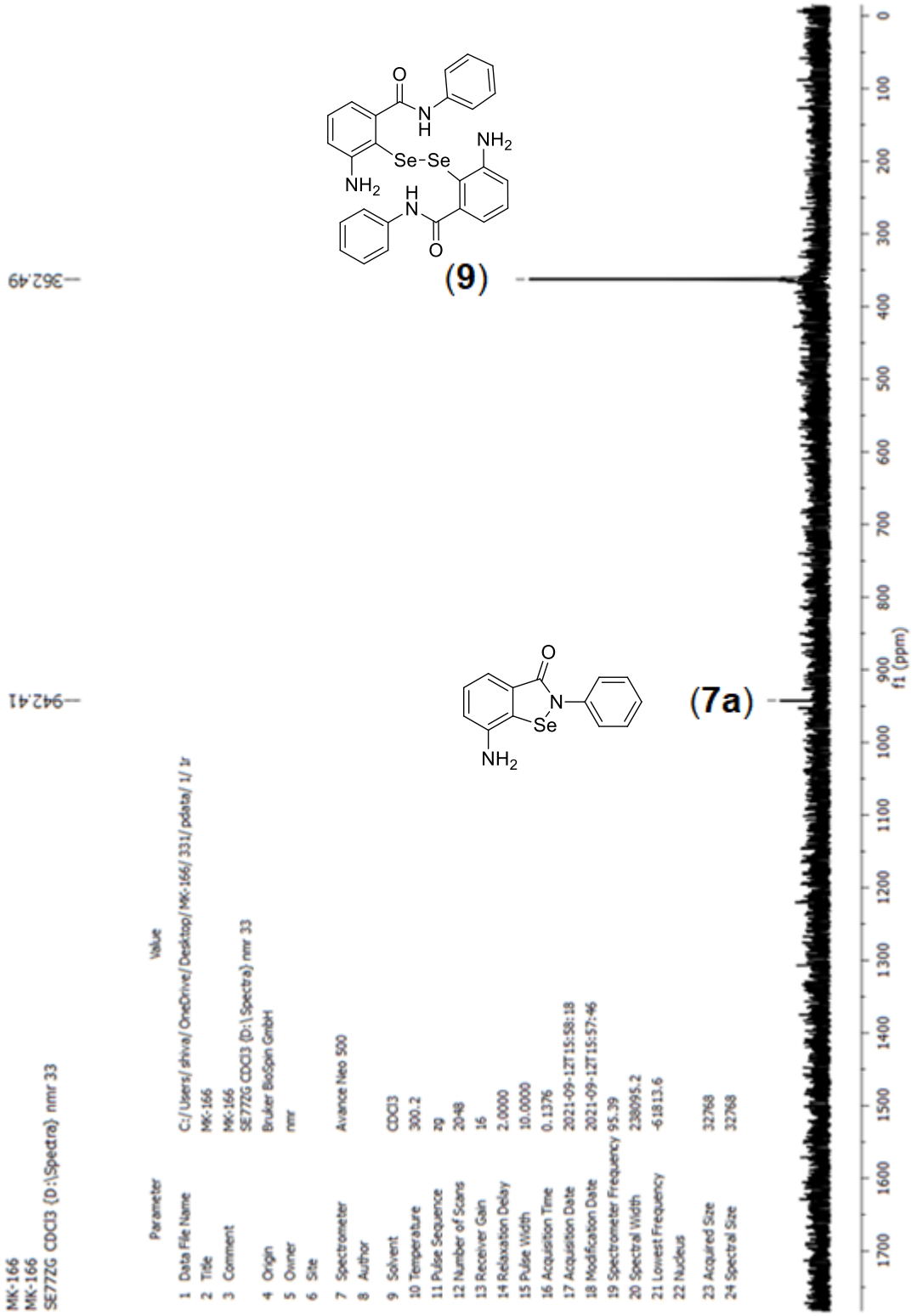


Figure S33. The $^{77}Se\{^{1}H\}$ NMR of diselenide + PhSSPh + 1 equiv H_2O_2 (recorded 2 days later)

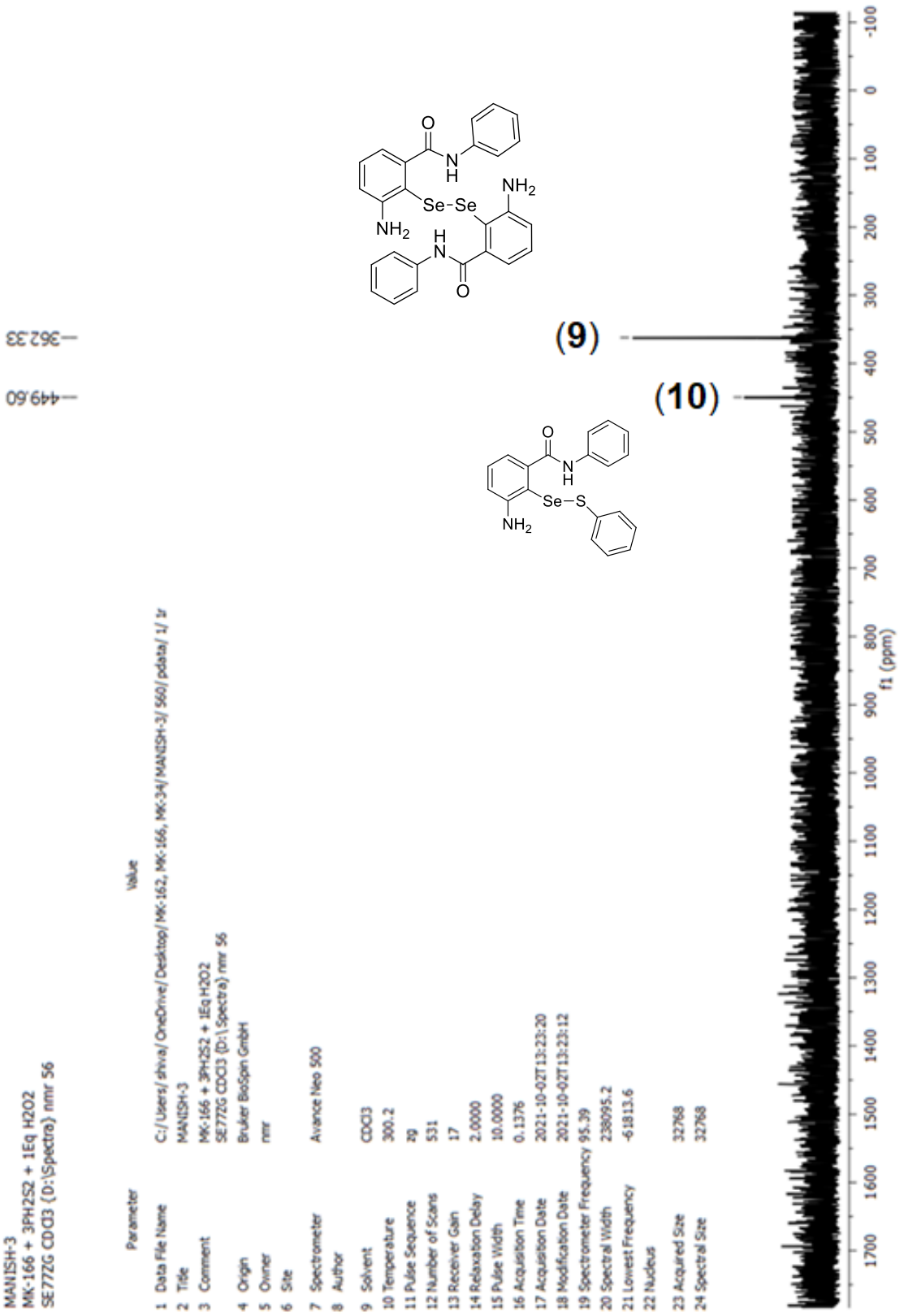


Figure S34. The $^{77}Se\{^{1}H\}$ NMR of diselenide **9** + PhSSPh + 3 equiv H_2O_2

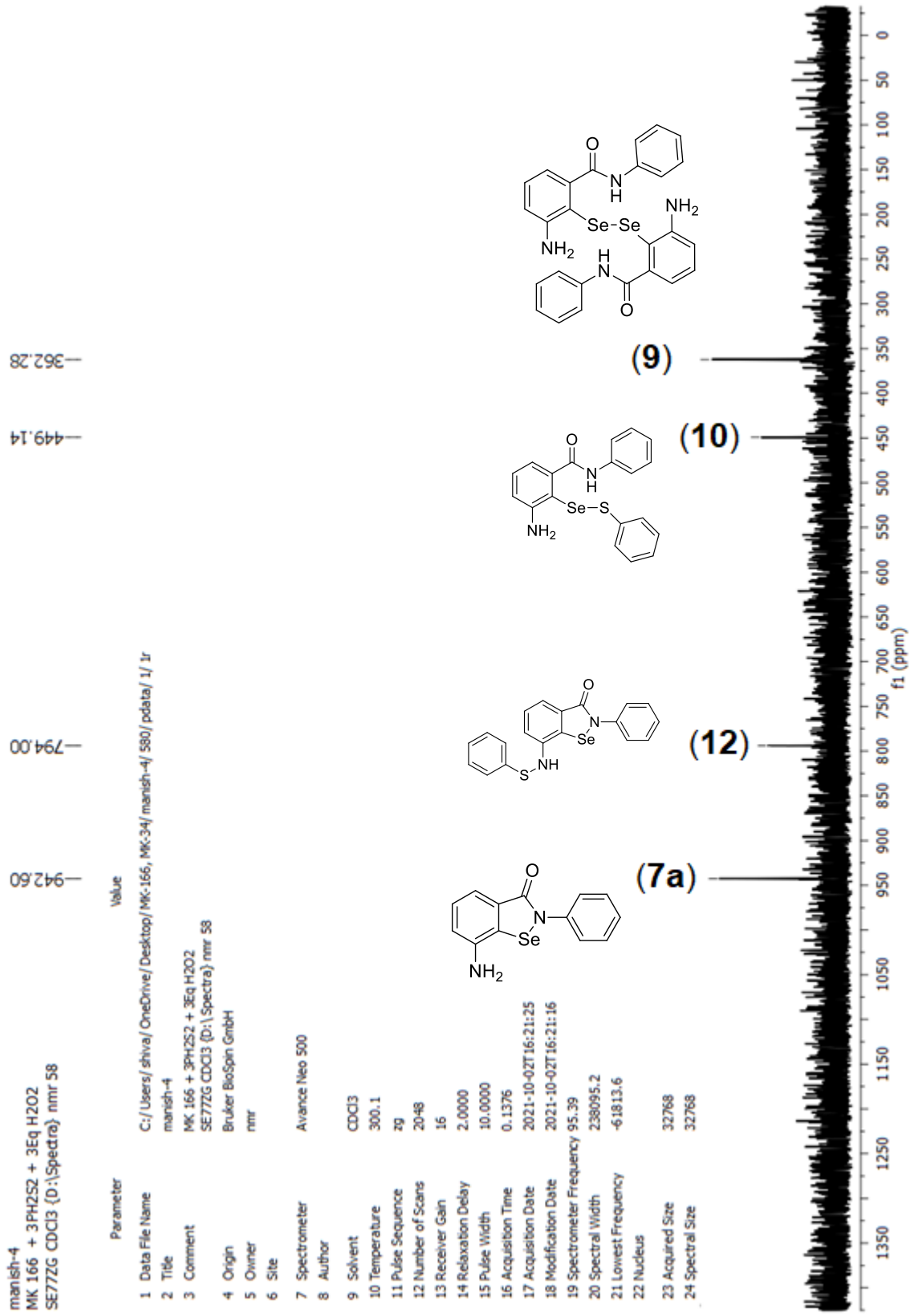


Figure S35. The $^{77}Se\{^{1}H\}$ NMR spectrum of diselenide **15** + H_2O_2 + PhSH

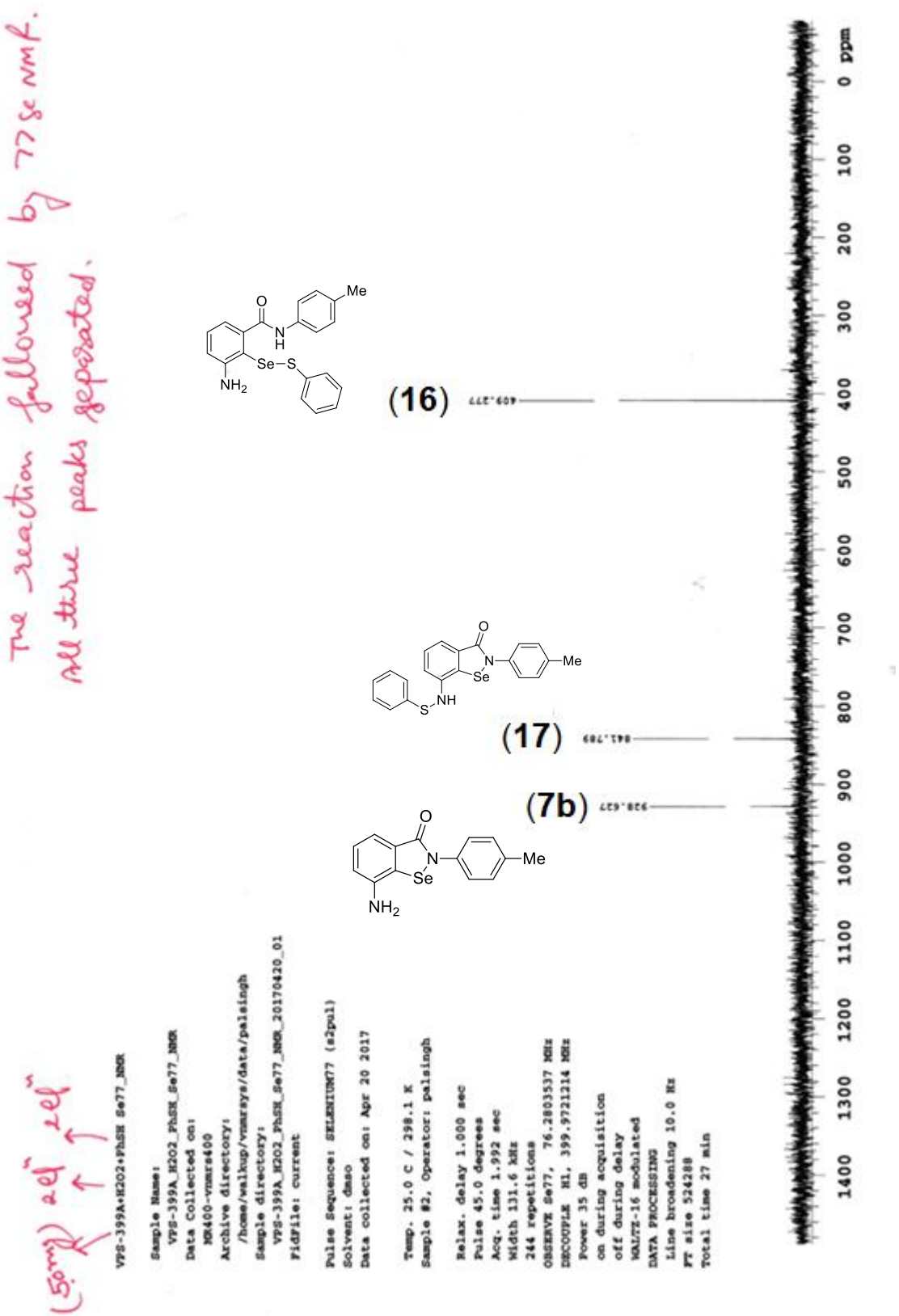
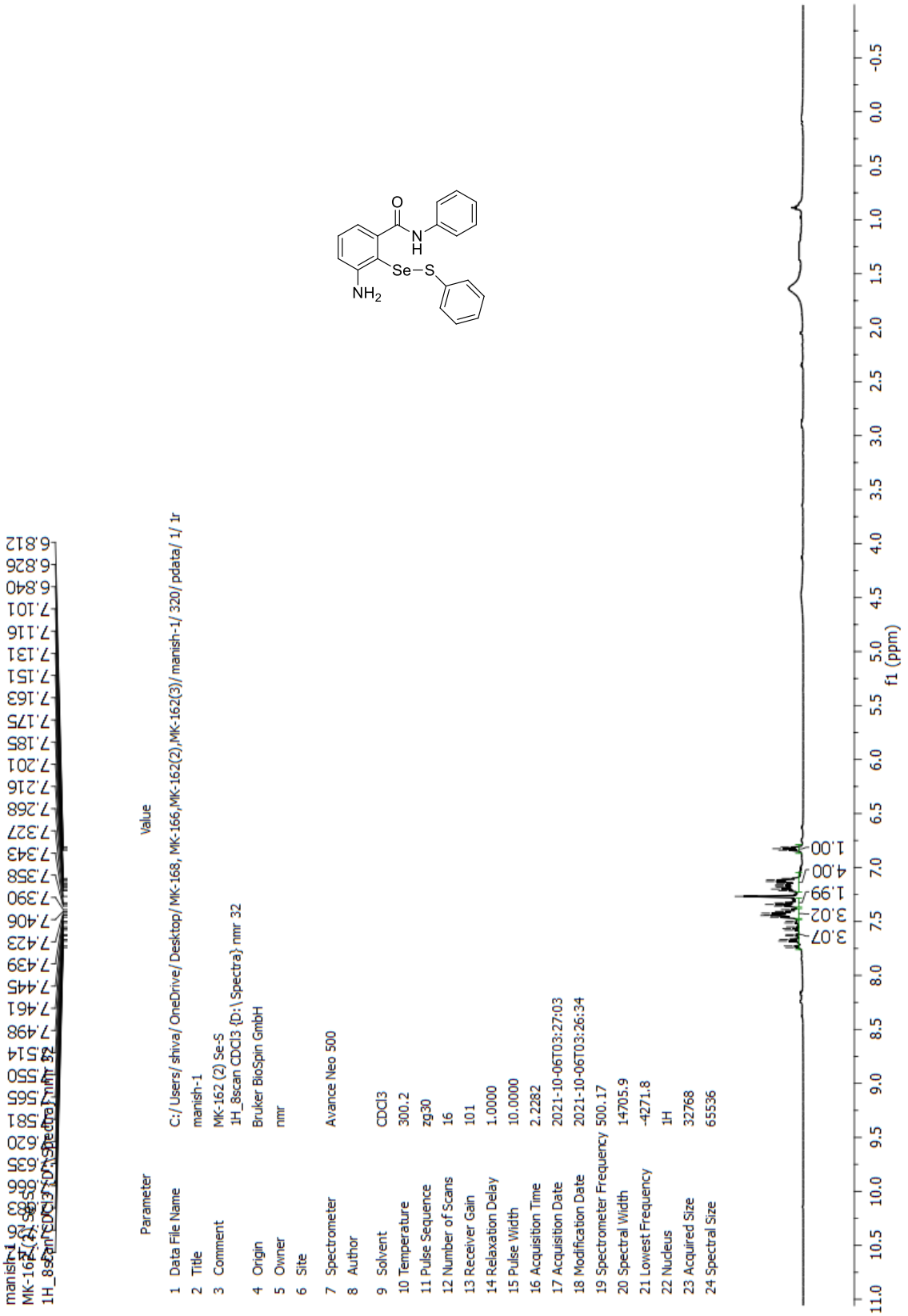


Figure S36. The ^{1}H NMR spectrum of **10** in $CDCl_3$



Parameter	Value
1 Data File Name	C:/Users/shiva/OneDrive/Desktop/MK-168, MK-166,MK-162(2),MK-162(3)/manish-1/320/pdata/1/1r
2 Title	manish-1
3 Comment	MK-162 (2) Se-S 1H_8scan CDCl3 {D:\Spectra} nmr 32
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Spectrometer	Avance Neo 500
8 Author	
9 Solvent	CDCl3
10 Temperature	300.2
11 Pulse Sequence	zg30
12 Number of Scans	16
13 Receiver Gain	101
14 Relaxation Delay	1.0000
15 Pulse Width	10.0000
16 Acquisition Time	2.2282
17 Acquisition Date	2021-10-06T03:27:03
18 Modification Date	2021-10-06T03:26:34
19 Spectrometer Frequency	500.17
20 Spectral Width	14705.9
21 Lowest Frequency	-4271.8
22 Nucleus	1H
23 Acquired Size	32768
24 Spectral Size	65536

Figure S37. The ^{1}H NMR Expansion spectrum of **10** in $CDCl_3$

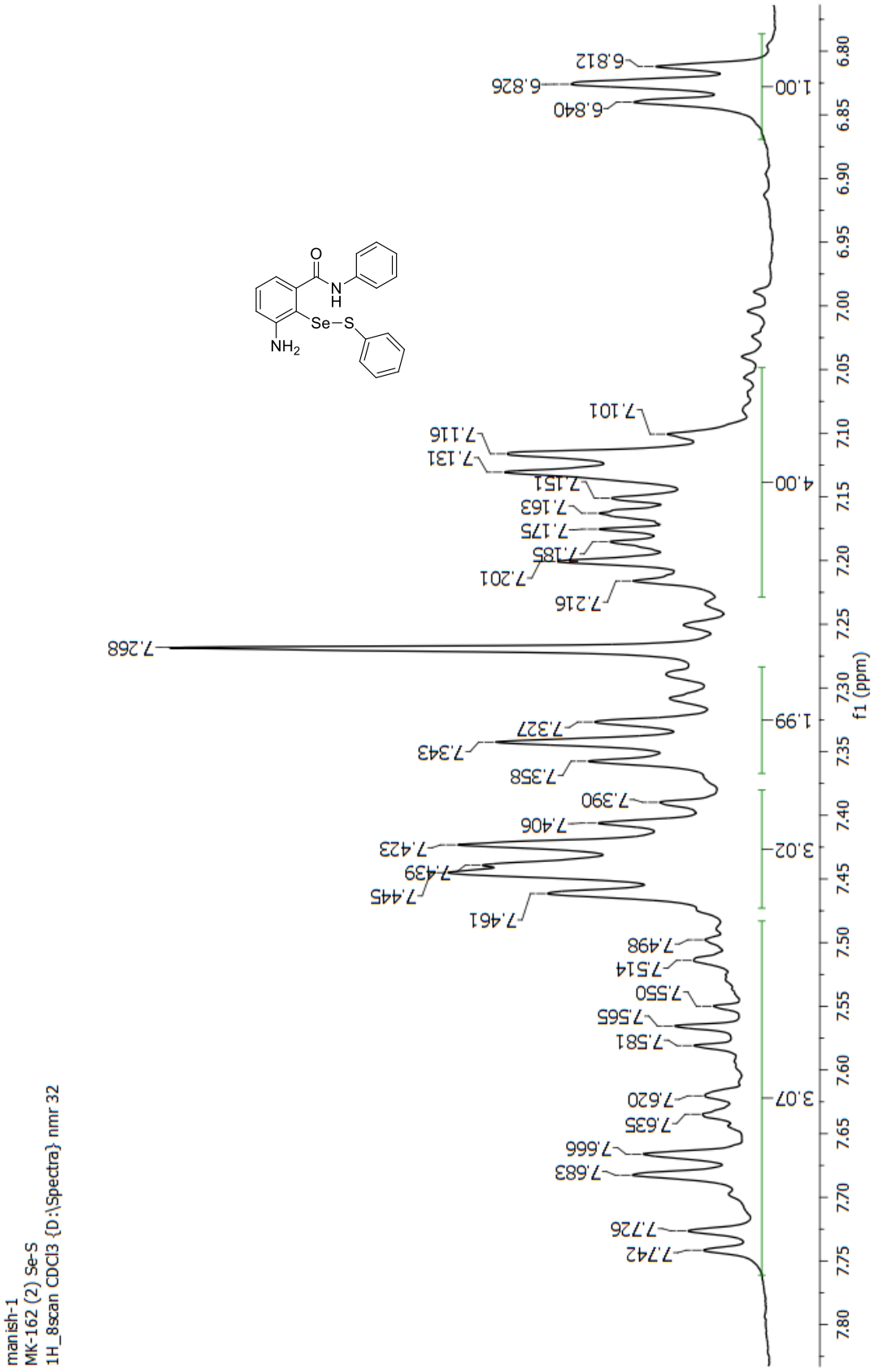


Figure S38. The ^{13}C NMR spectrum of **10** in $CDCl_3$

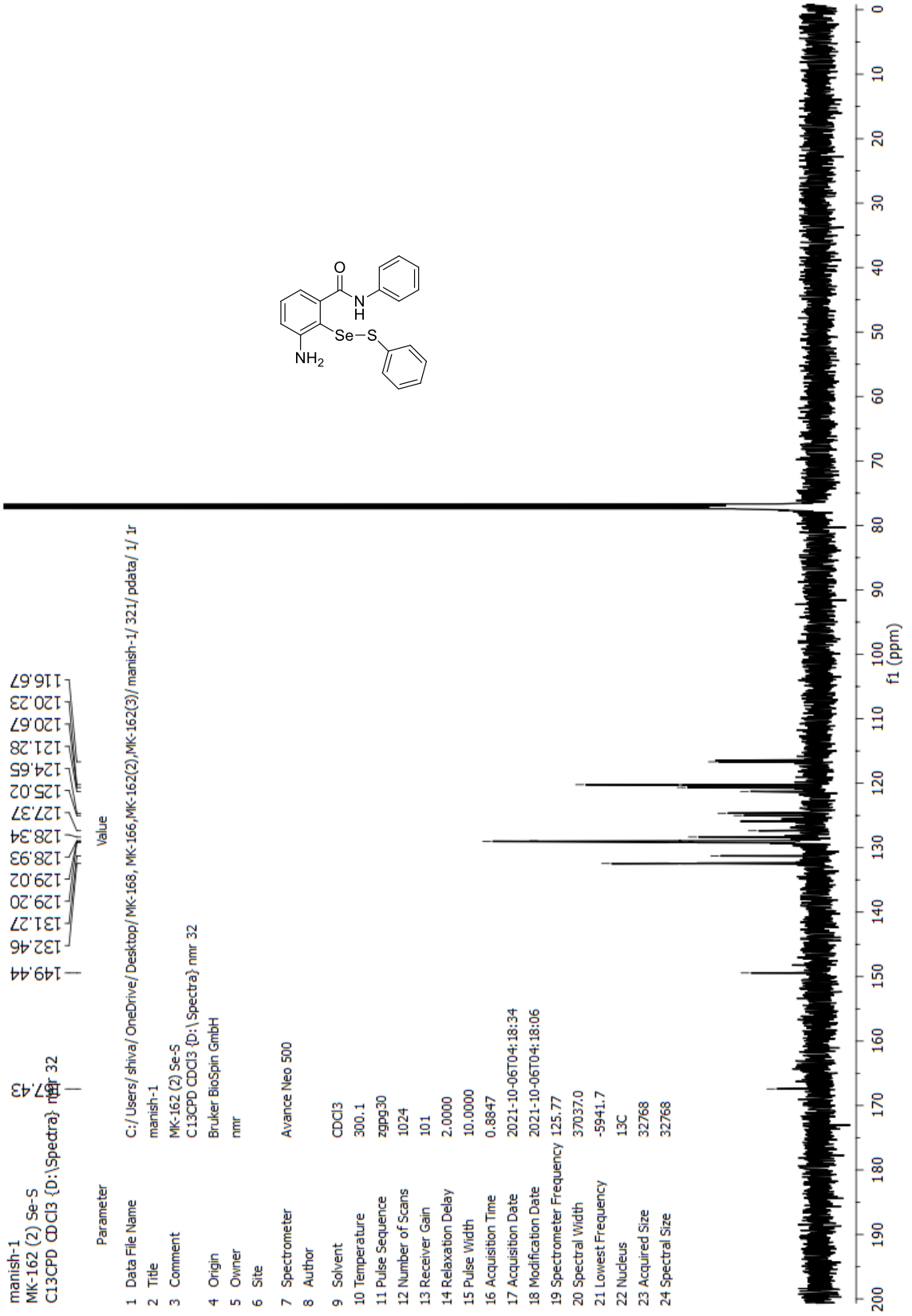


Figure S39. The ^{13}C NMR expansion spectrum of **10** in $CDCl_3$

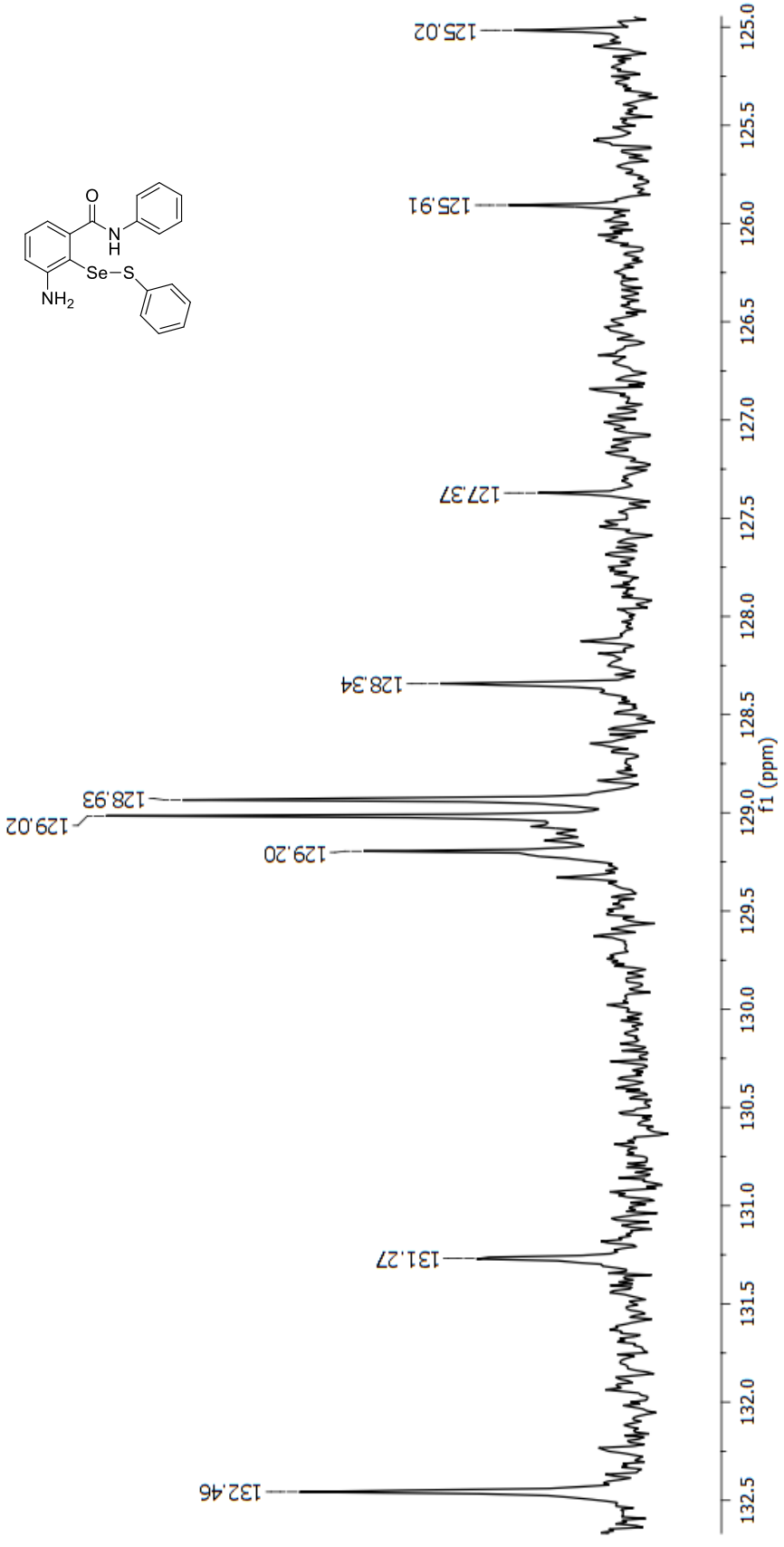


Figure S40. The $^{77}Se\{^{1}H\}$ NMR spectrum of **10** in $CDCl_3$

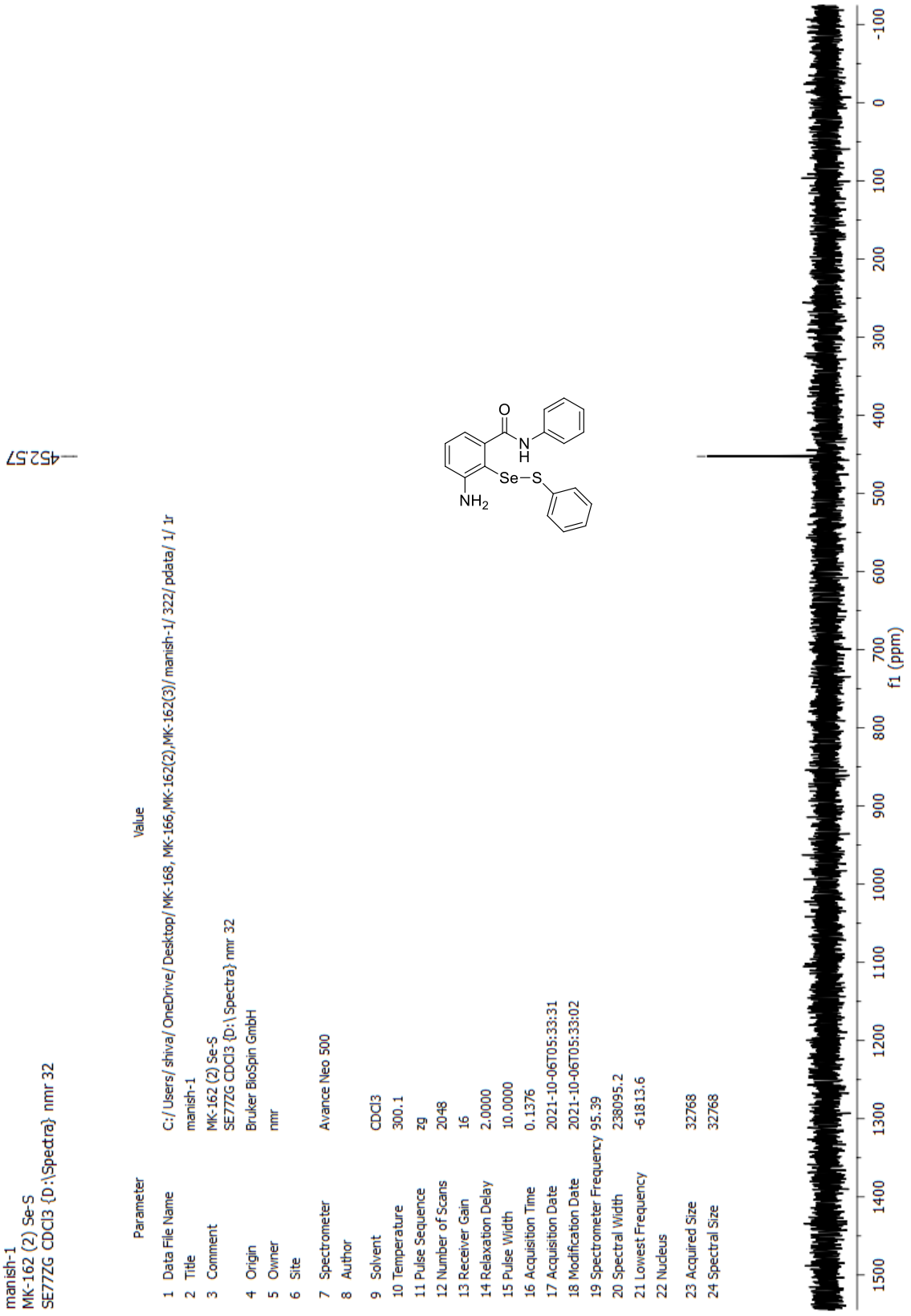


Figure S41. The $^{77}Se\{^{1}H\}$ NMR spectrum of **10** in DMSO-d_6

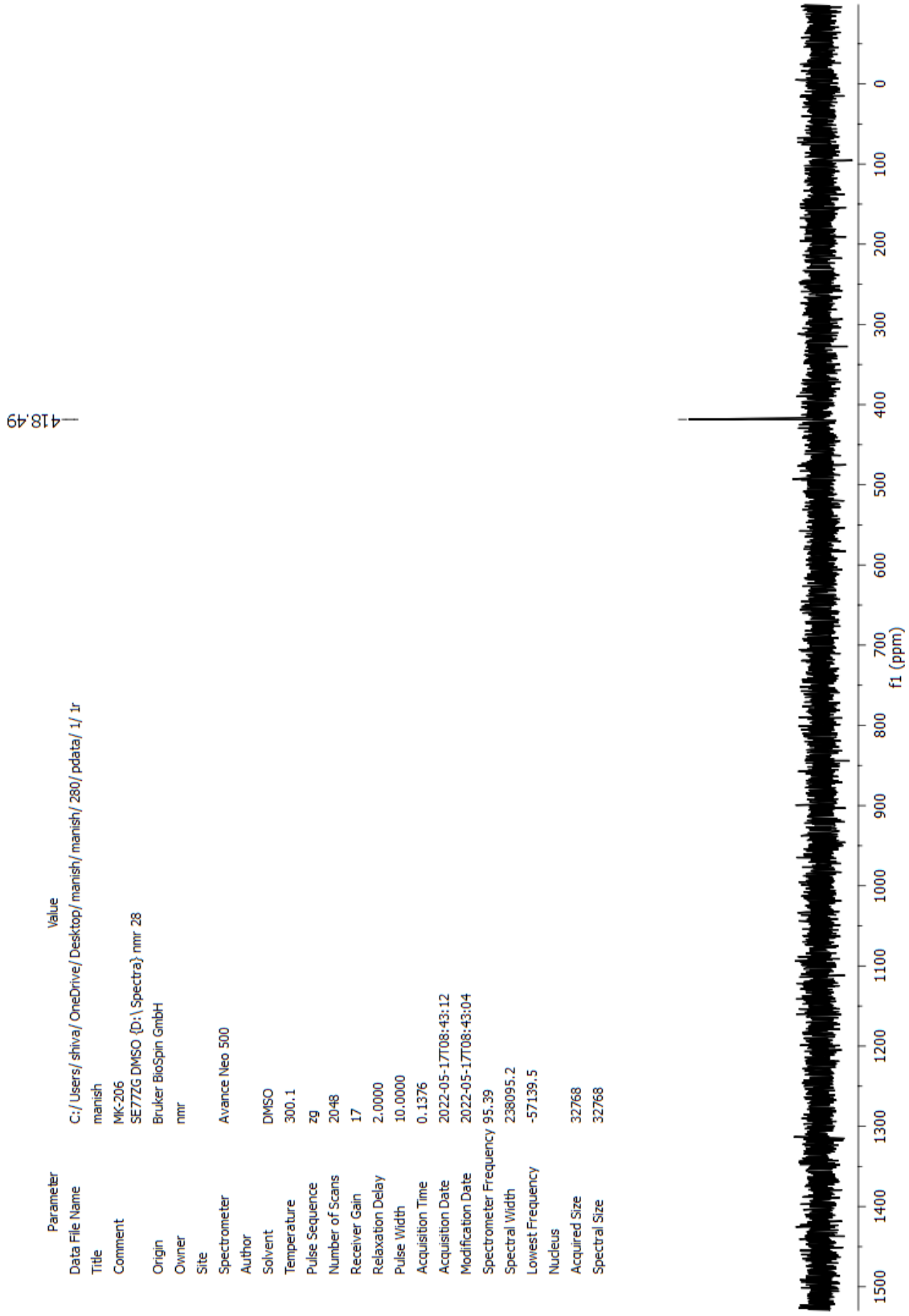
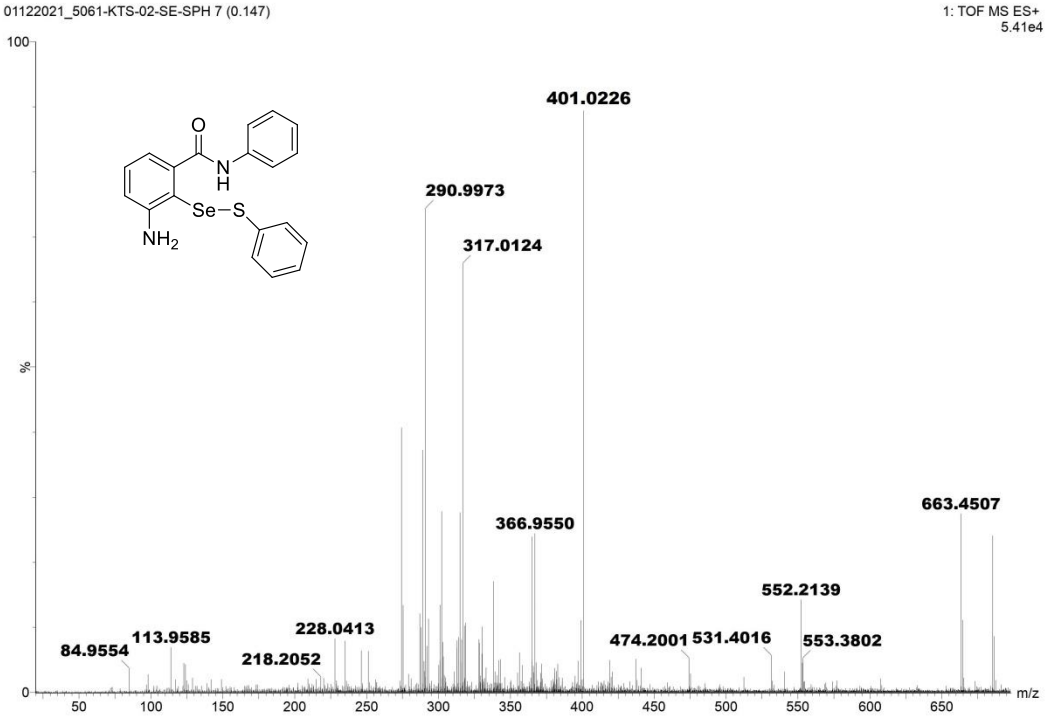


Figure S42. The HRMS of **10**



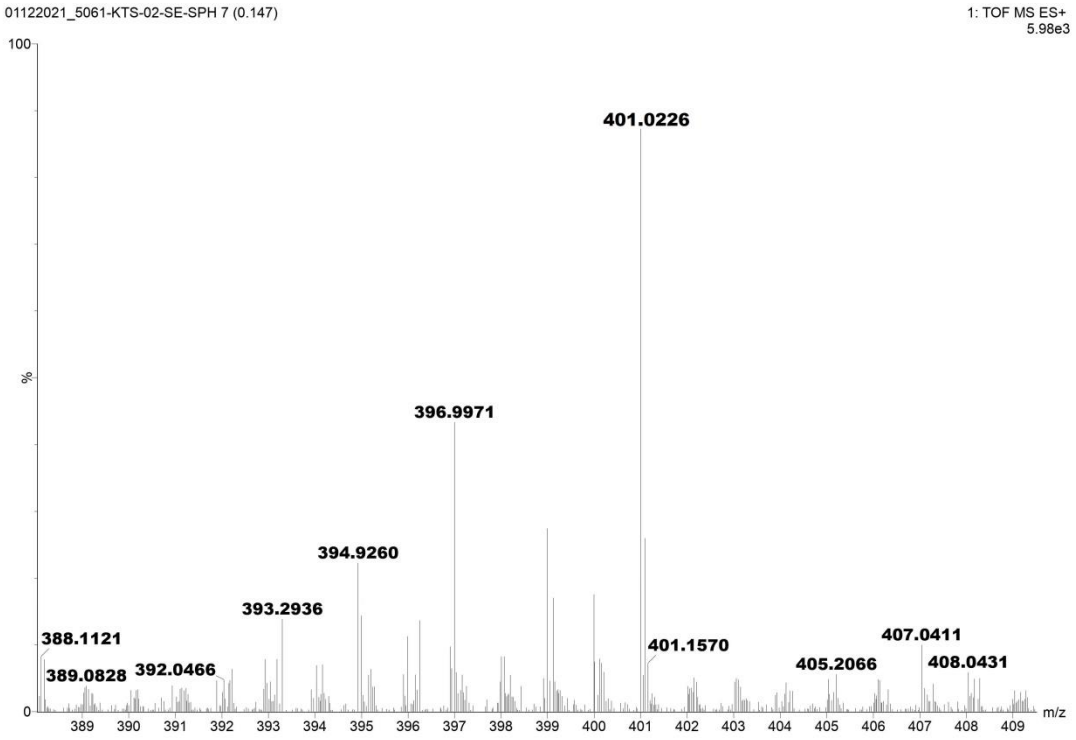


Figure S43. The ^{1}H NMR spectrum of **12**

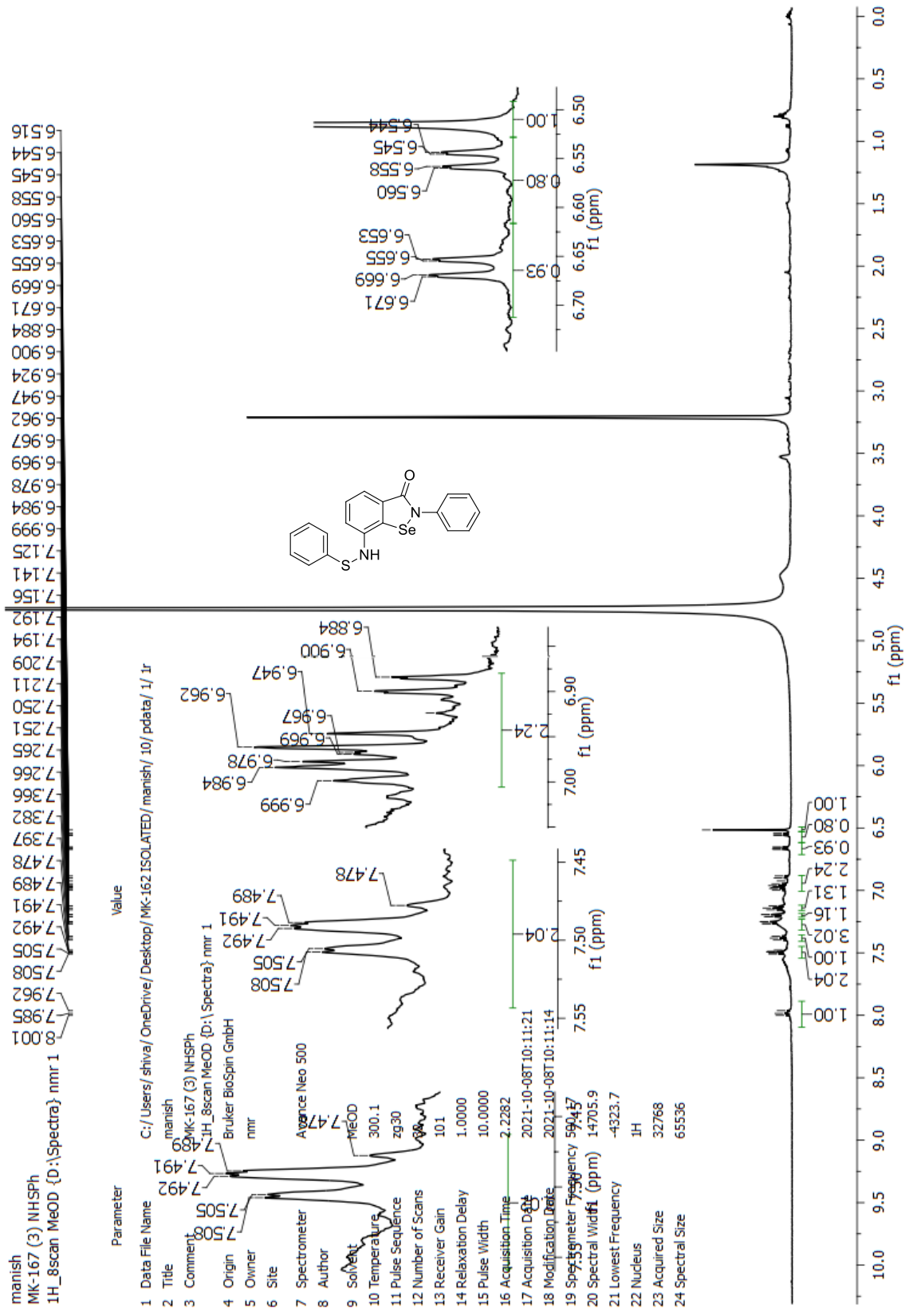


Figure S44. The ^{13}C NMR spectrum of **12**

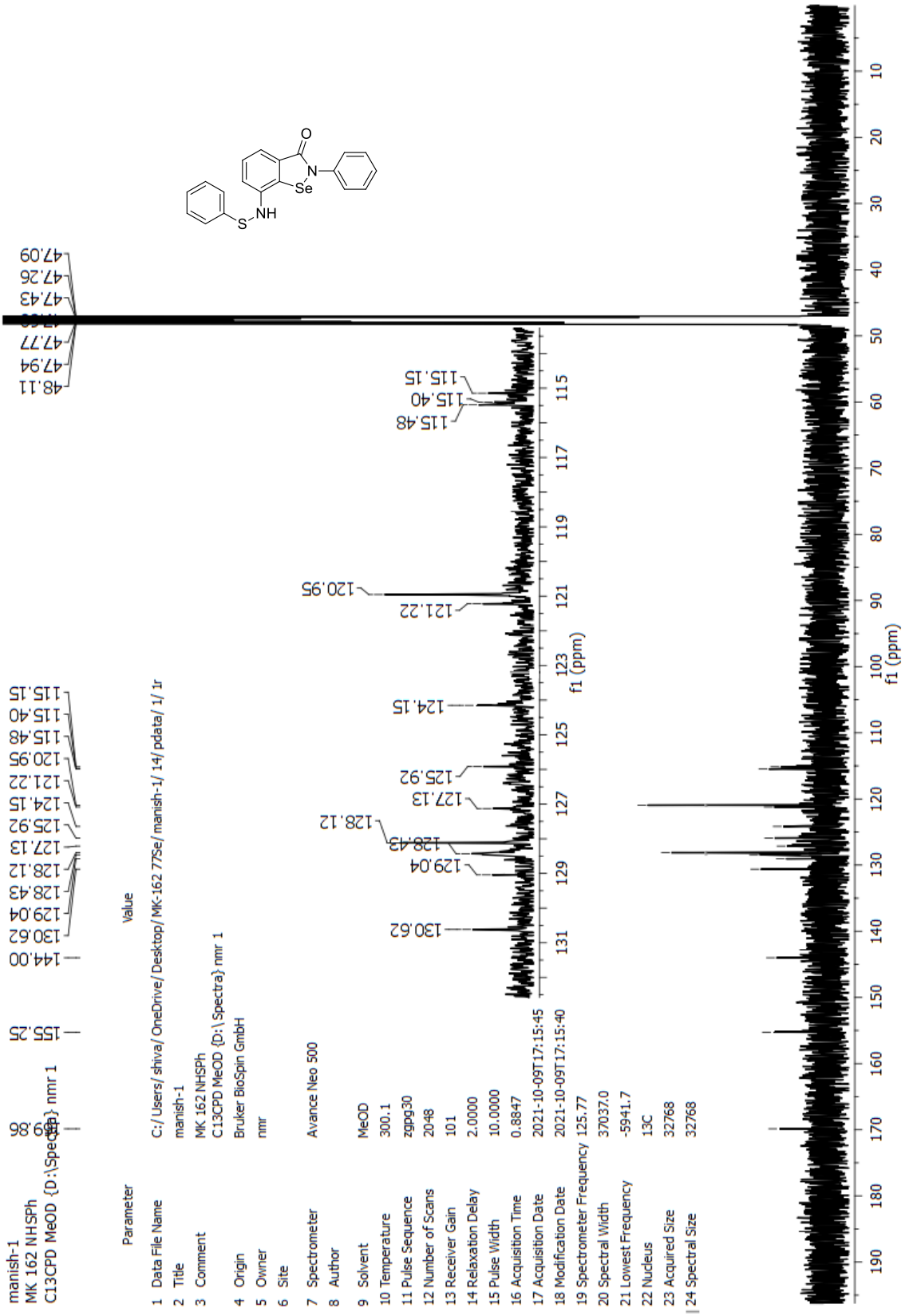


Figure S45. The $^{77}Se\{^{1}H\}$ NMR spectrum of **12**

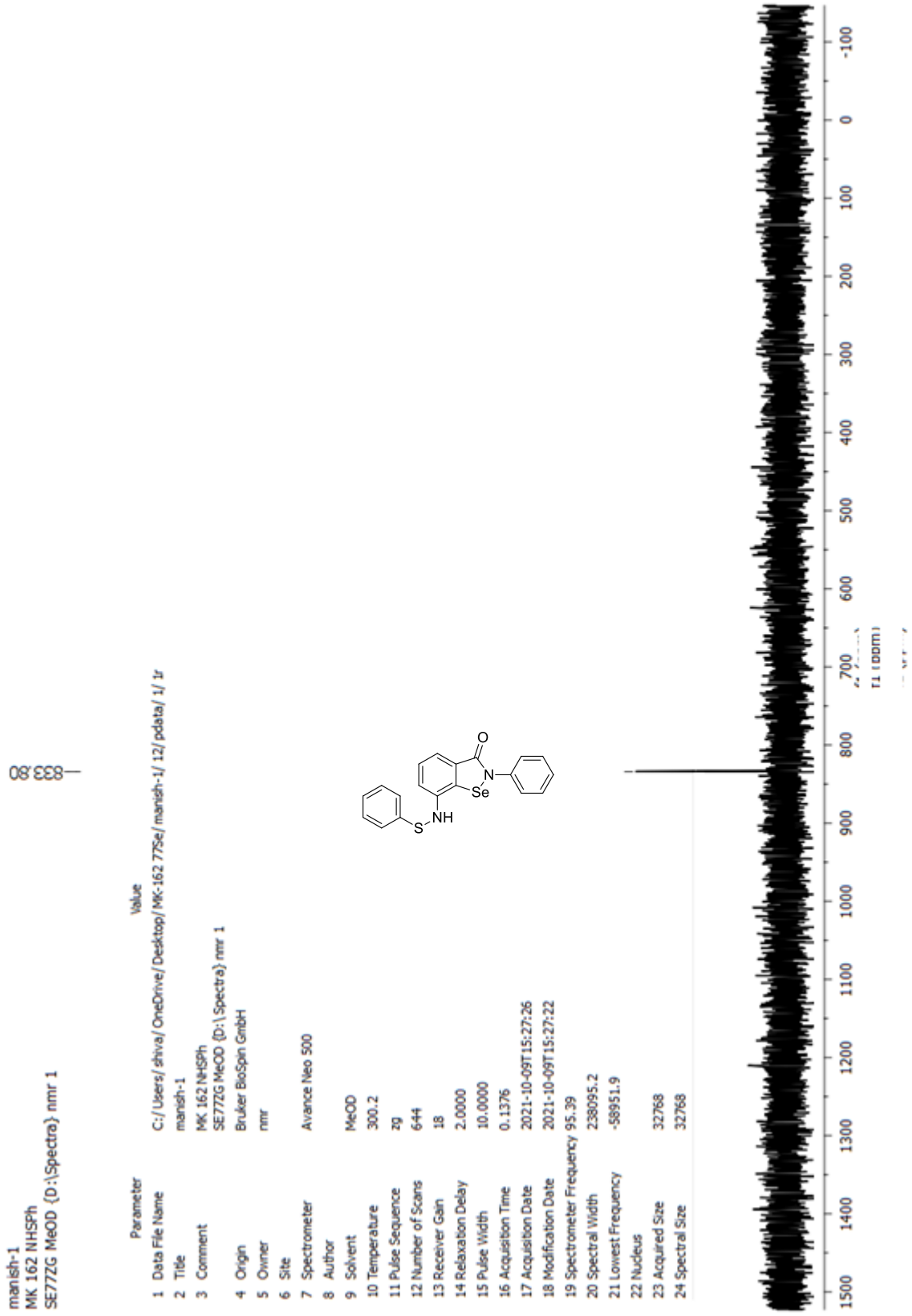


Figure S46. The HRMS of **12**

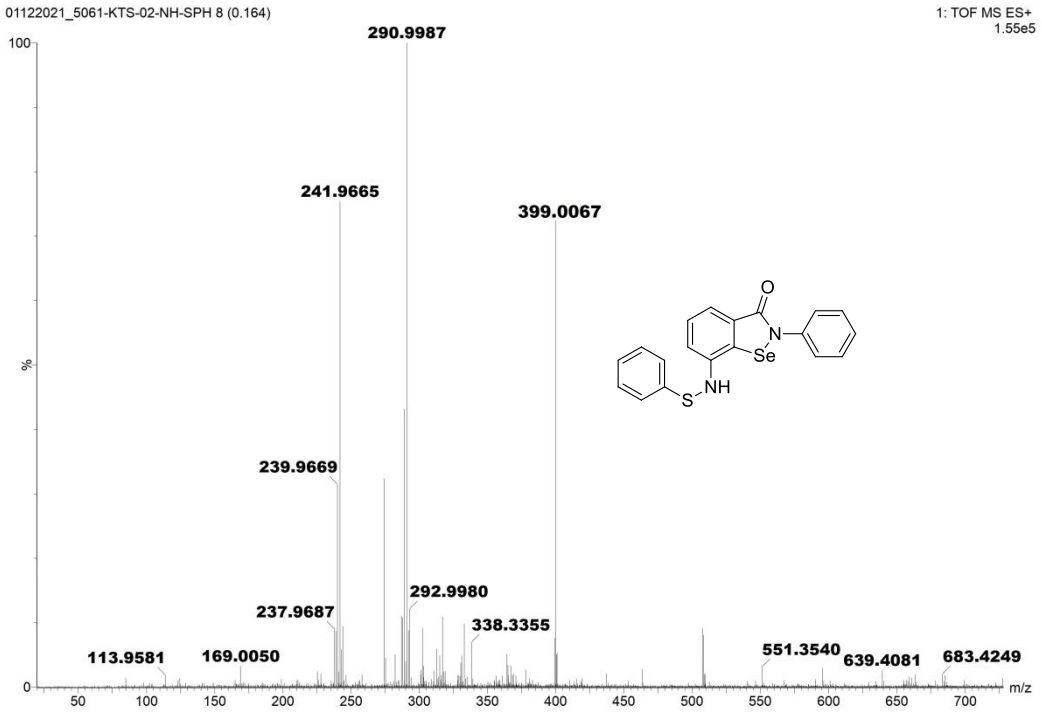


Figure S47. The ^{1}H NMR spectrum of **16** in $CDCl_3$

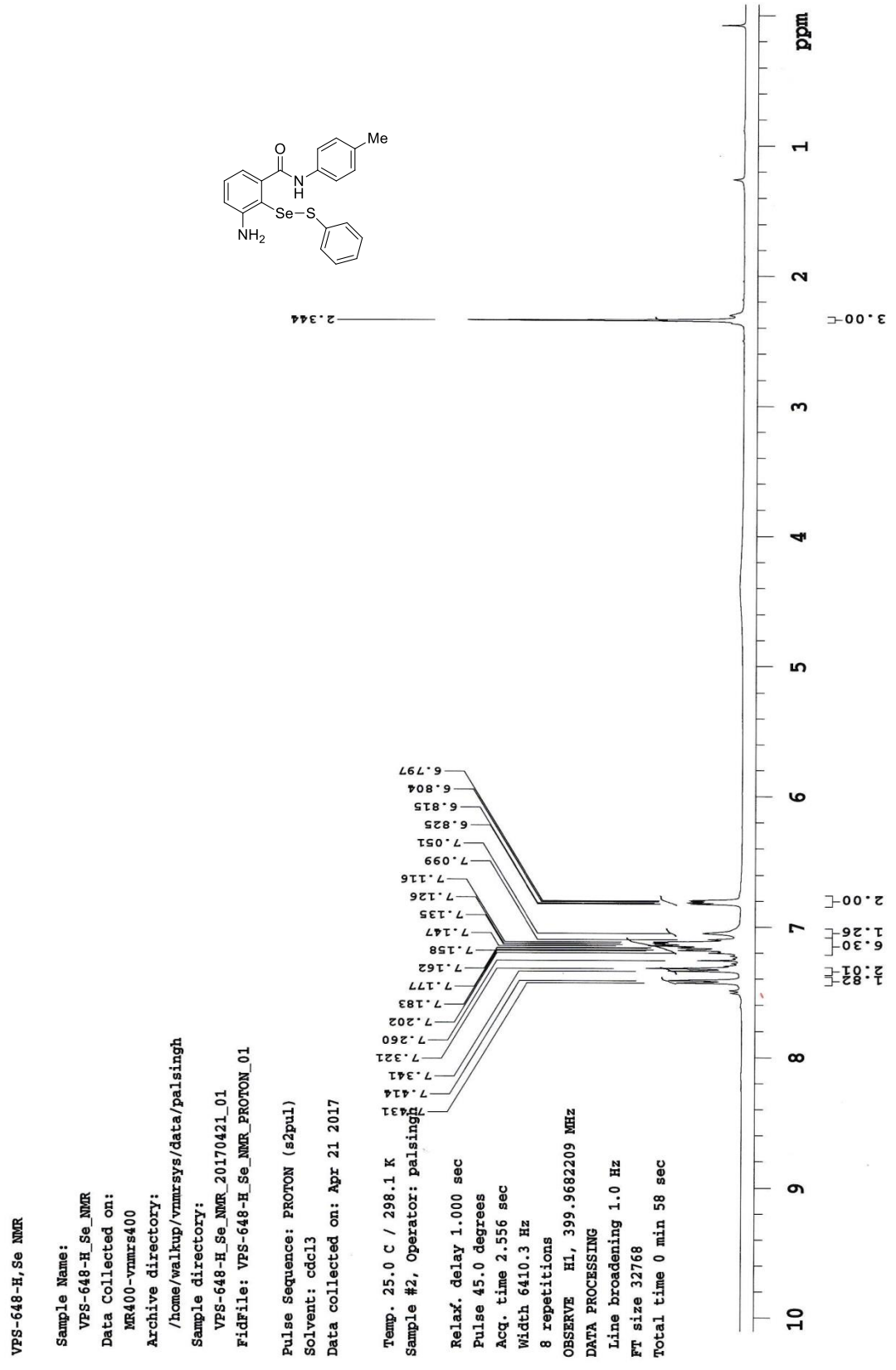


Figure S48. The Expanded version of the ^{1}H NMR spectrum of **16** in $CDCl_3$

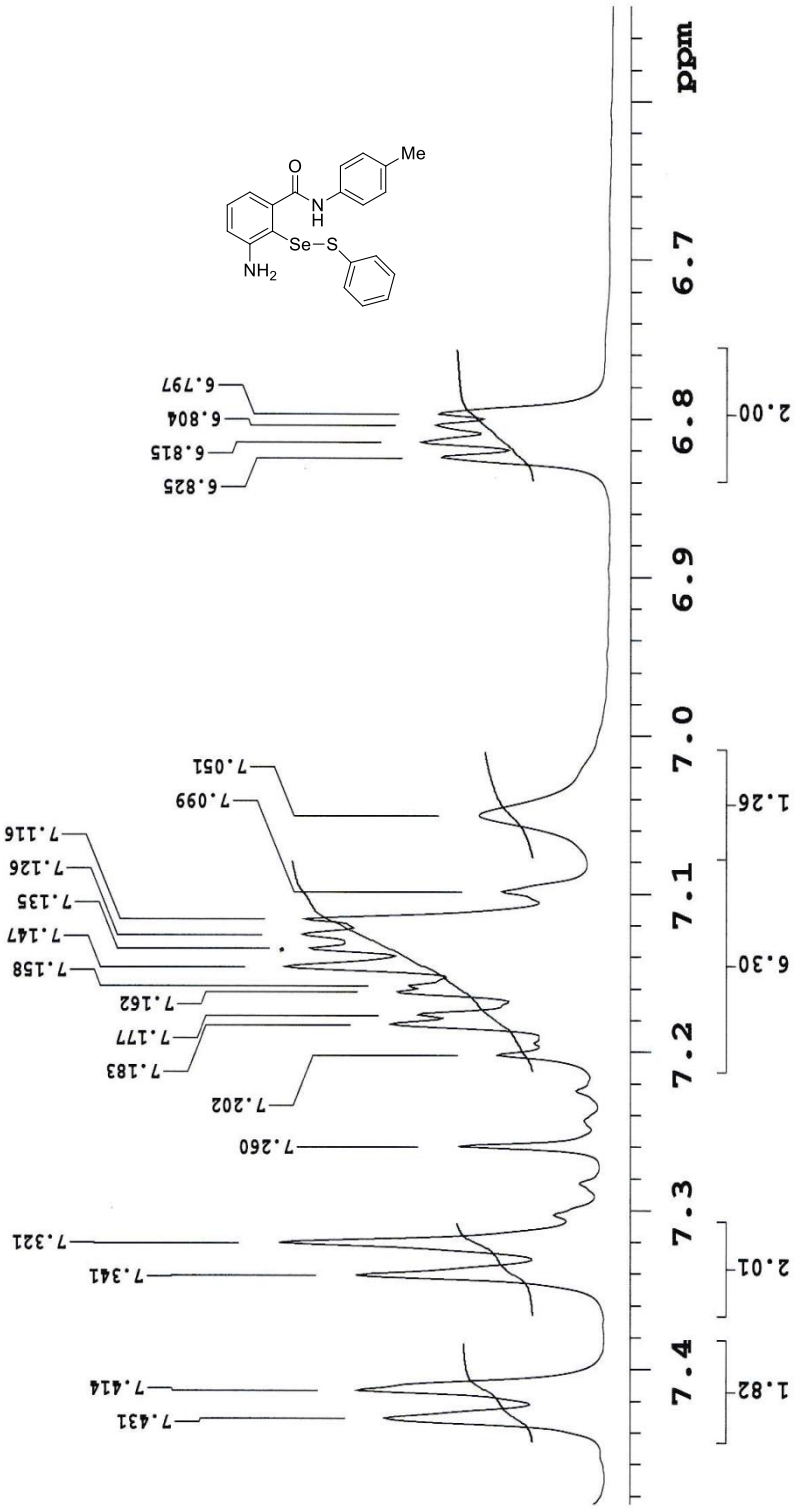


Figure S49. The ^{13}C NMR spectrum of **16** in $CDCl_3$

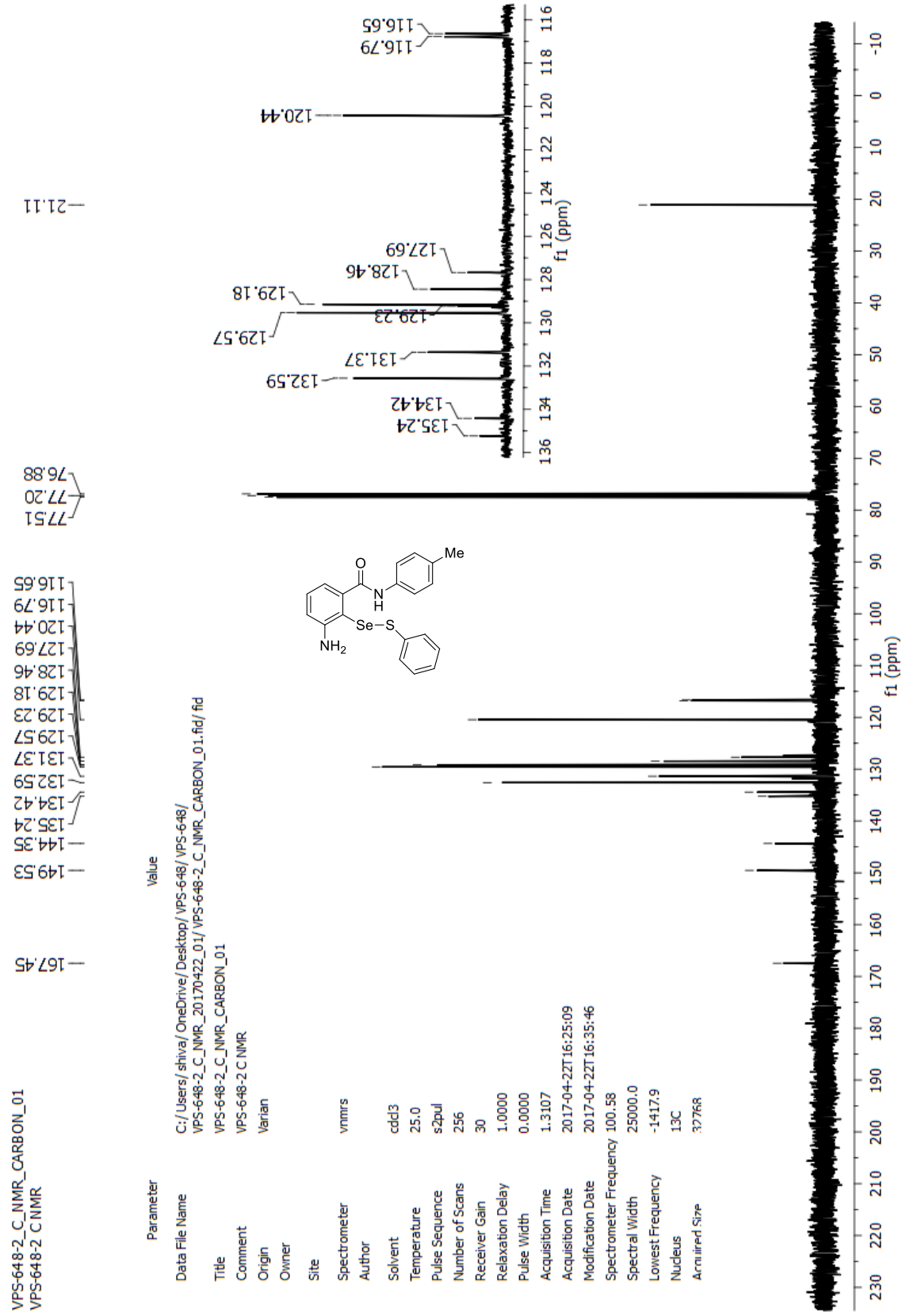


Figure S50. The $^{77}Se\{^{1}H\}$ NMR spectrum of **16** in $CDCl_3$

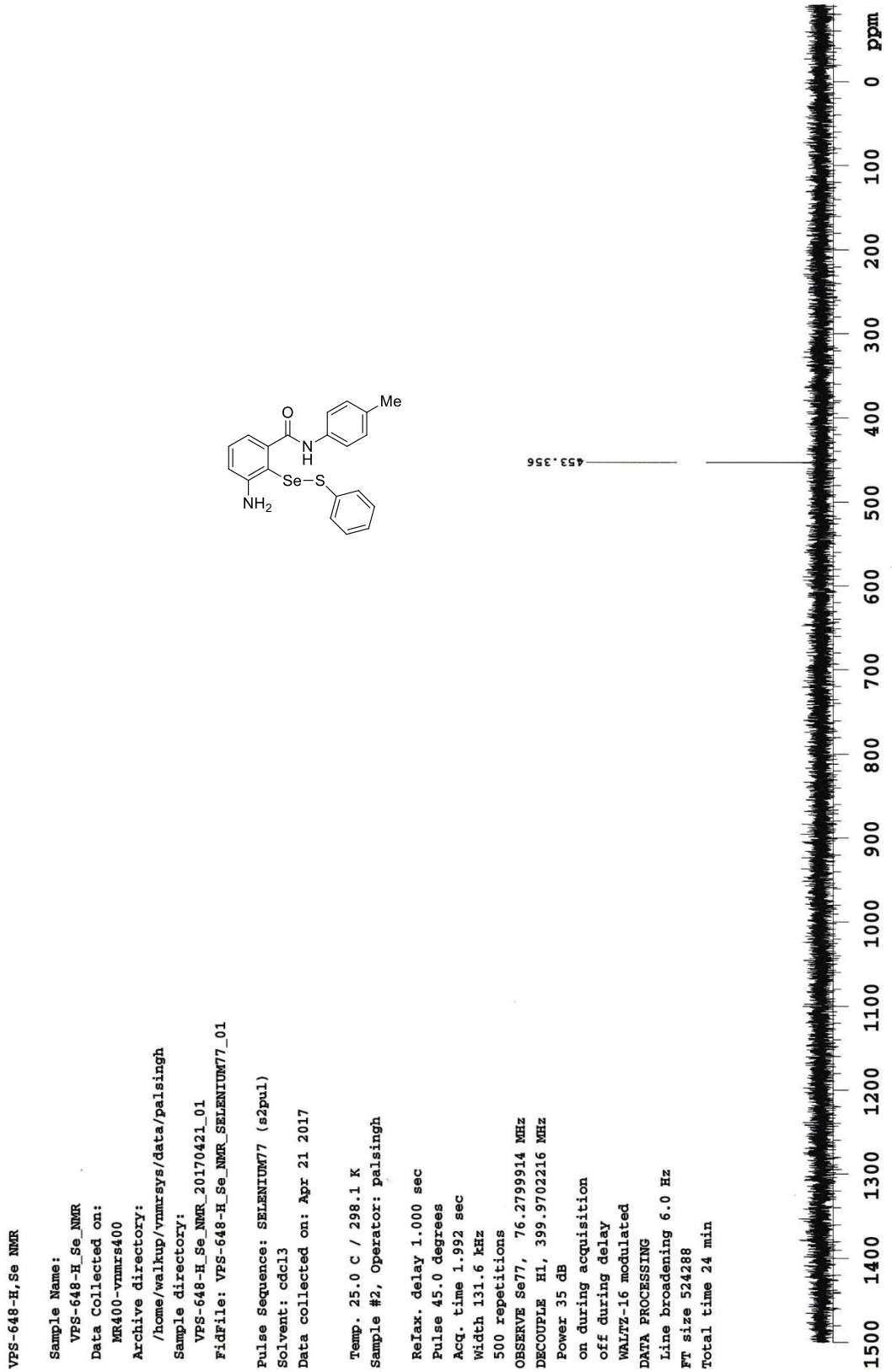
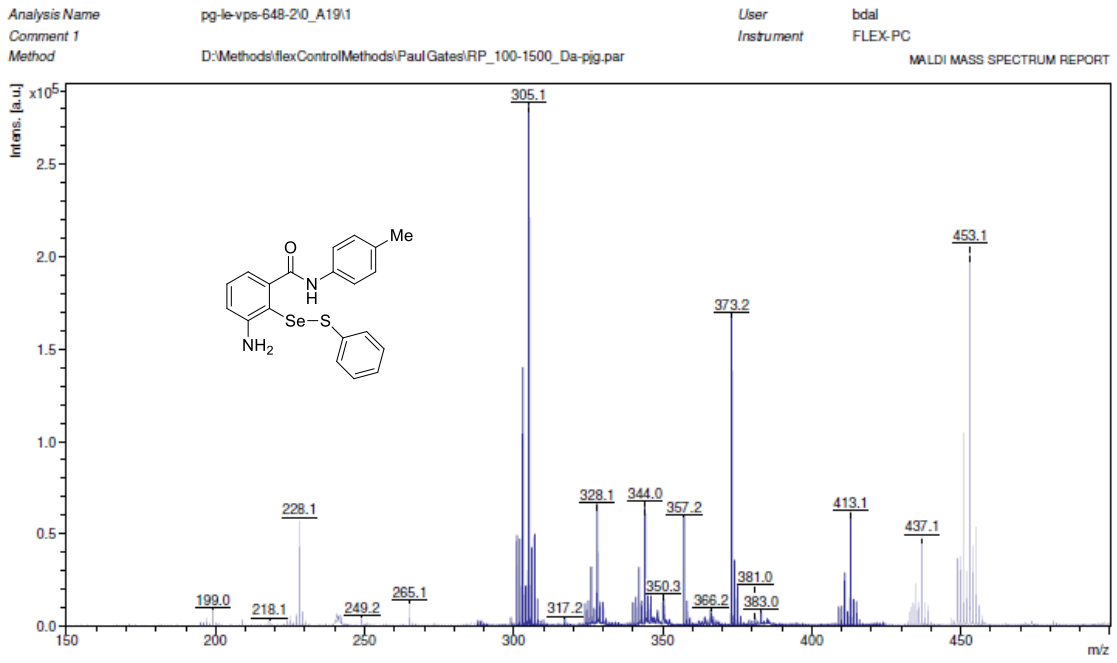
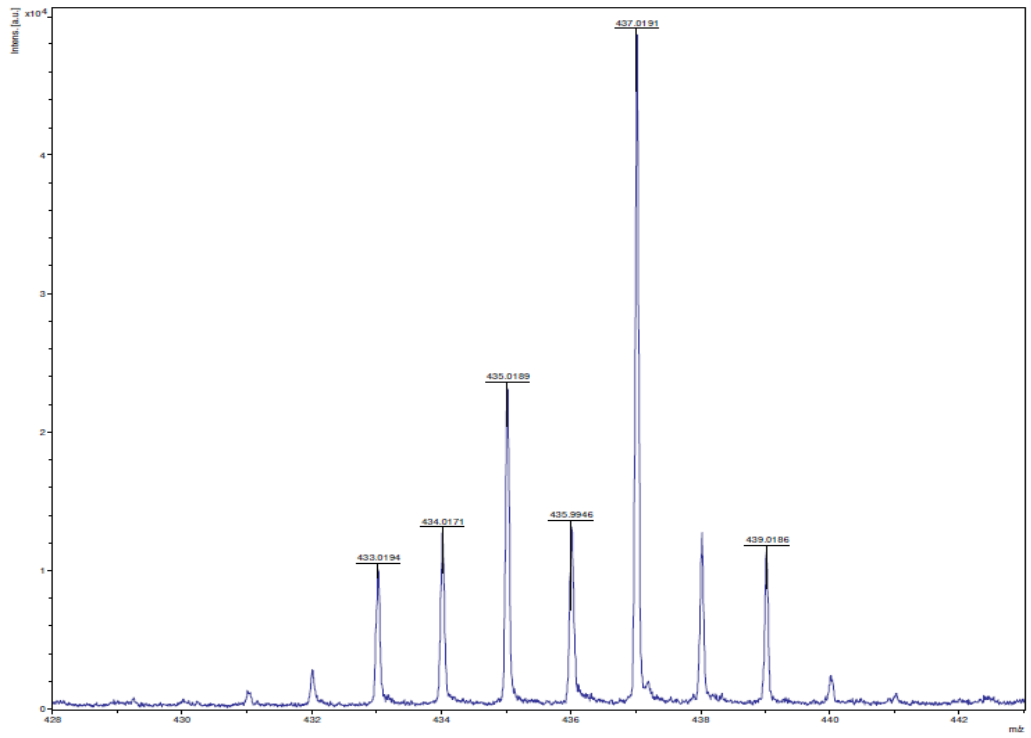


Figure S51. The HRMS of **16**





Formula	Calc m/z	Measured m/z	err [ppm]	ID
$C_{20}H_{18}N_2OSeS$	437.0198	437.0191	1.60	$[M+Na]^+$

Figure S52. The ^{1}H NMR spectrum of **17** in $CDCl_3$

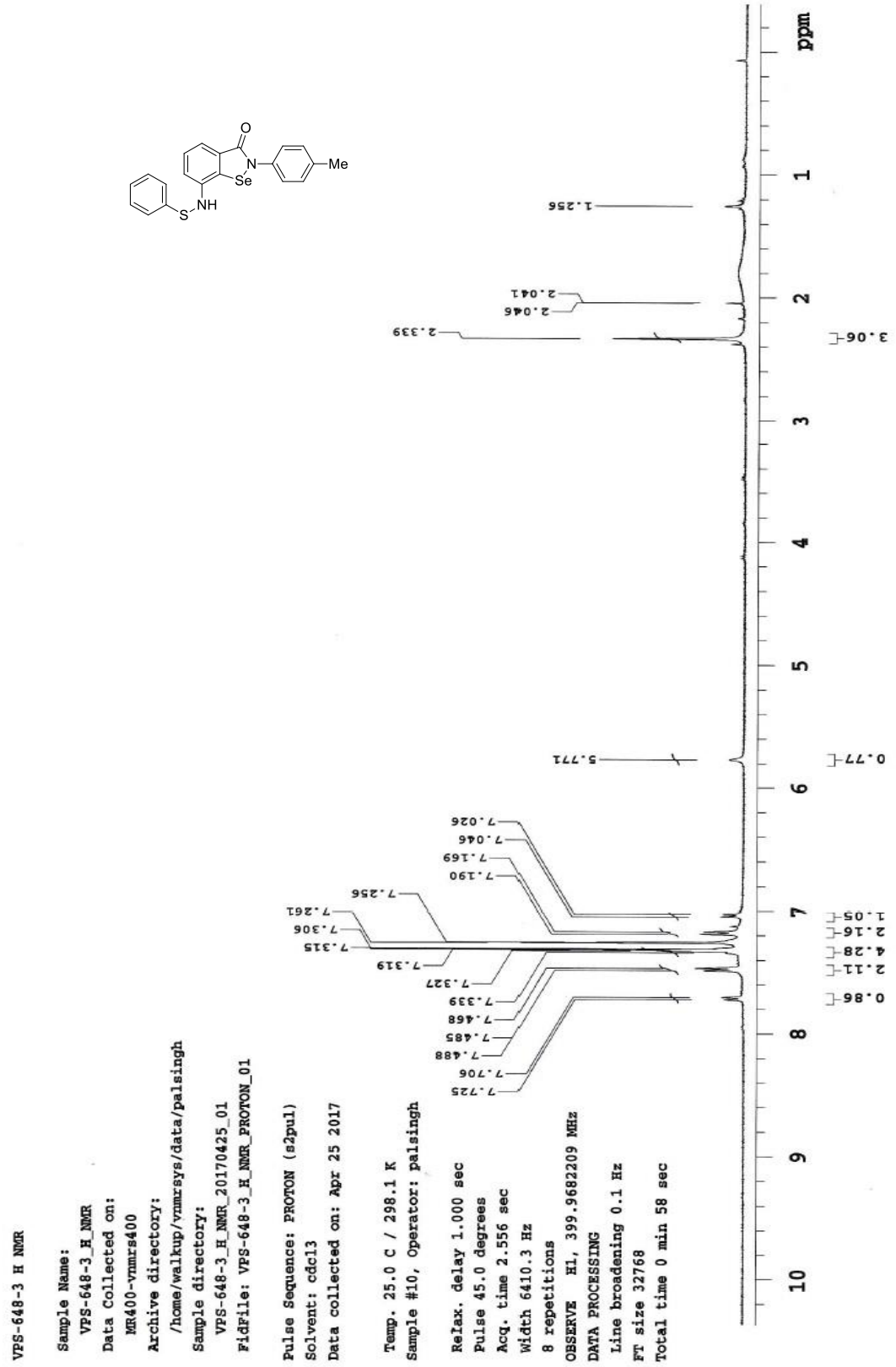


Figure S53. The Expanded version of the ^{1}H NMR spectrum of **17** in $CDCl_3$

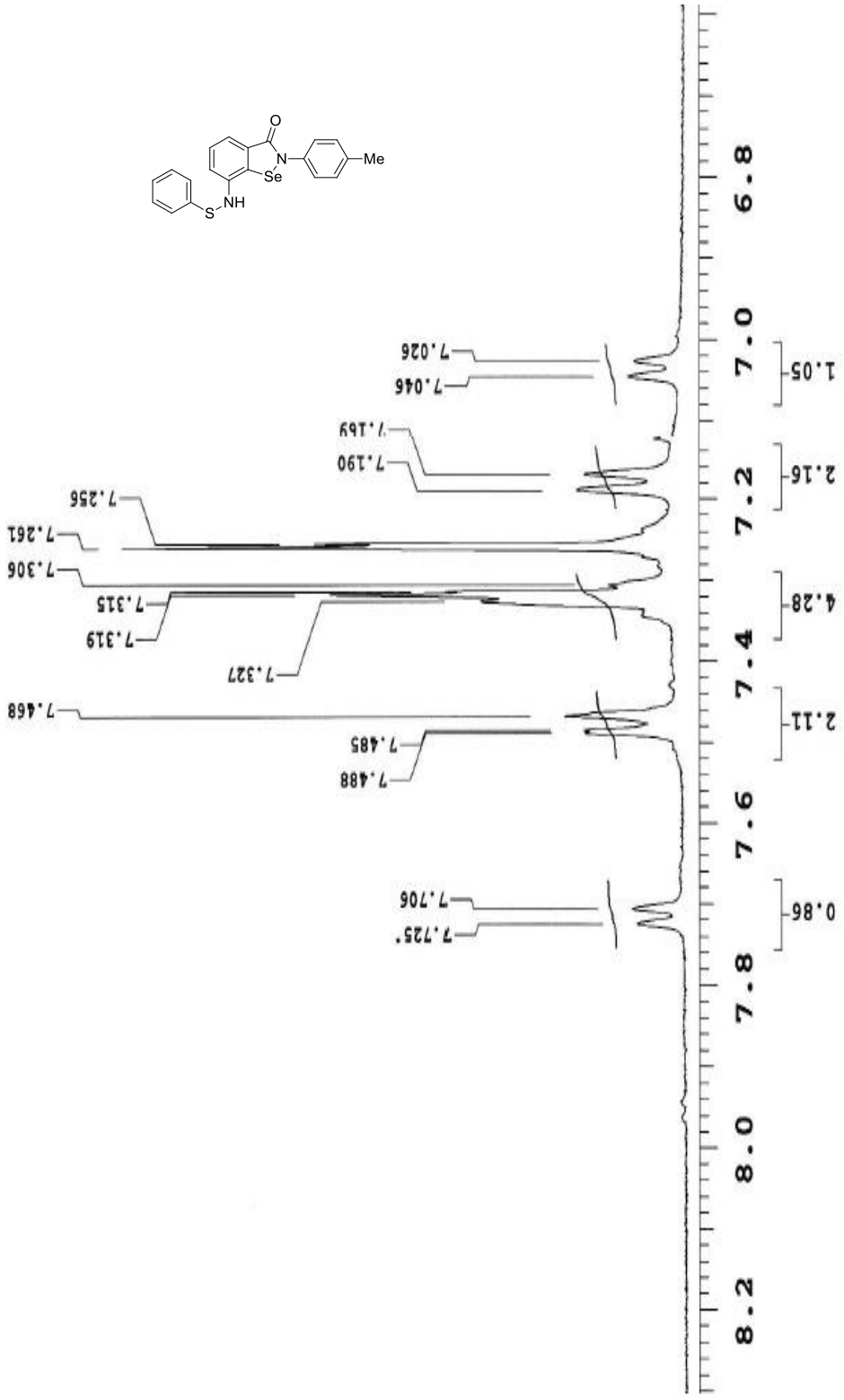


Figure S54. The ^{13}C NMR spectrum of **17** in $CDCl_3$

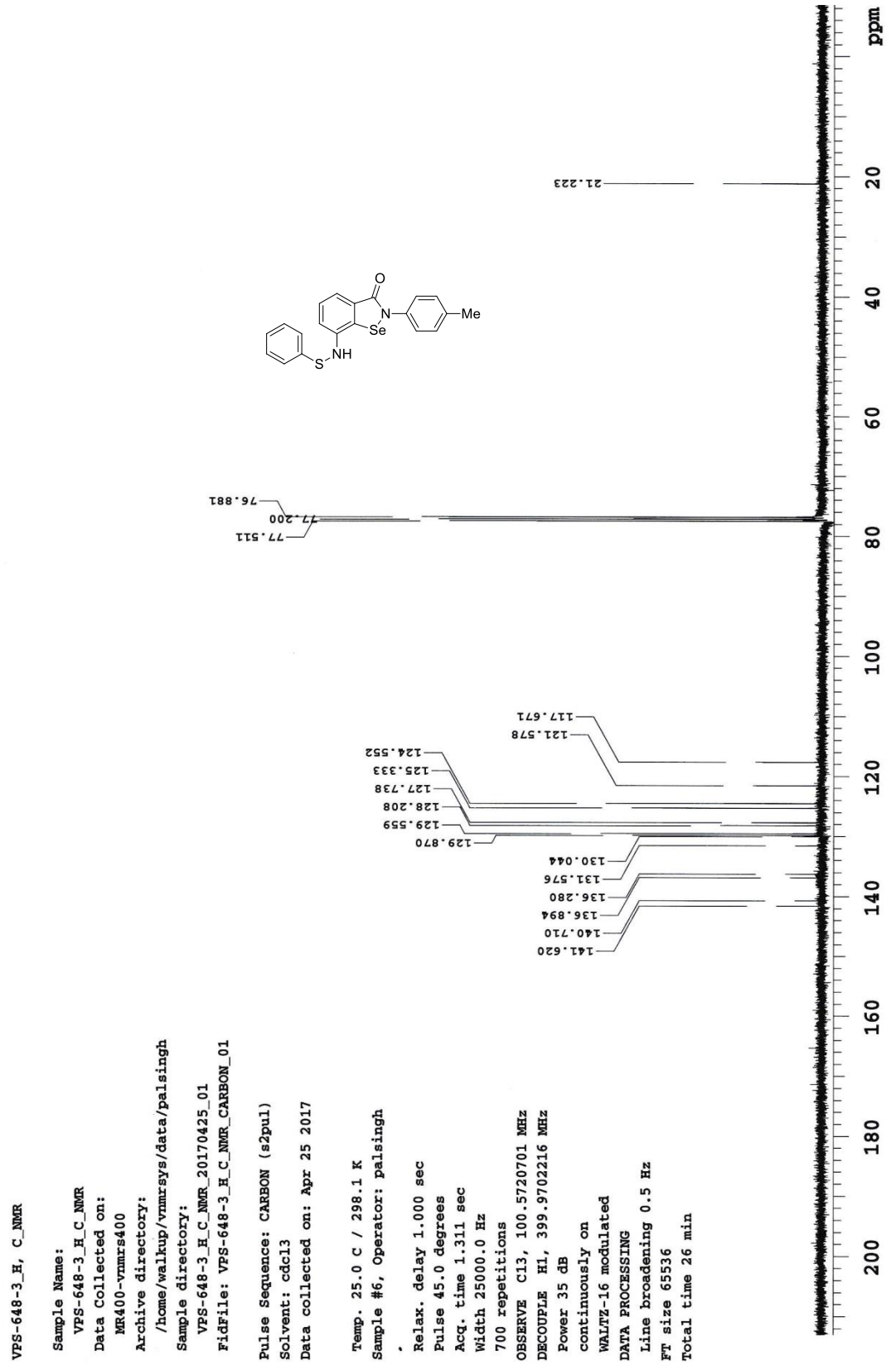


Figure S55. The $^{77}Se\{^{1}H\}$ NMR spectrum of **17** in $CDCl_3$

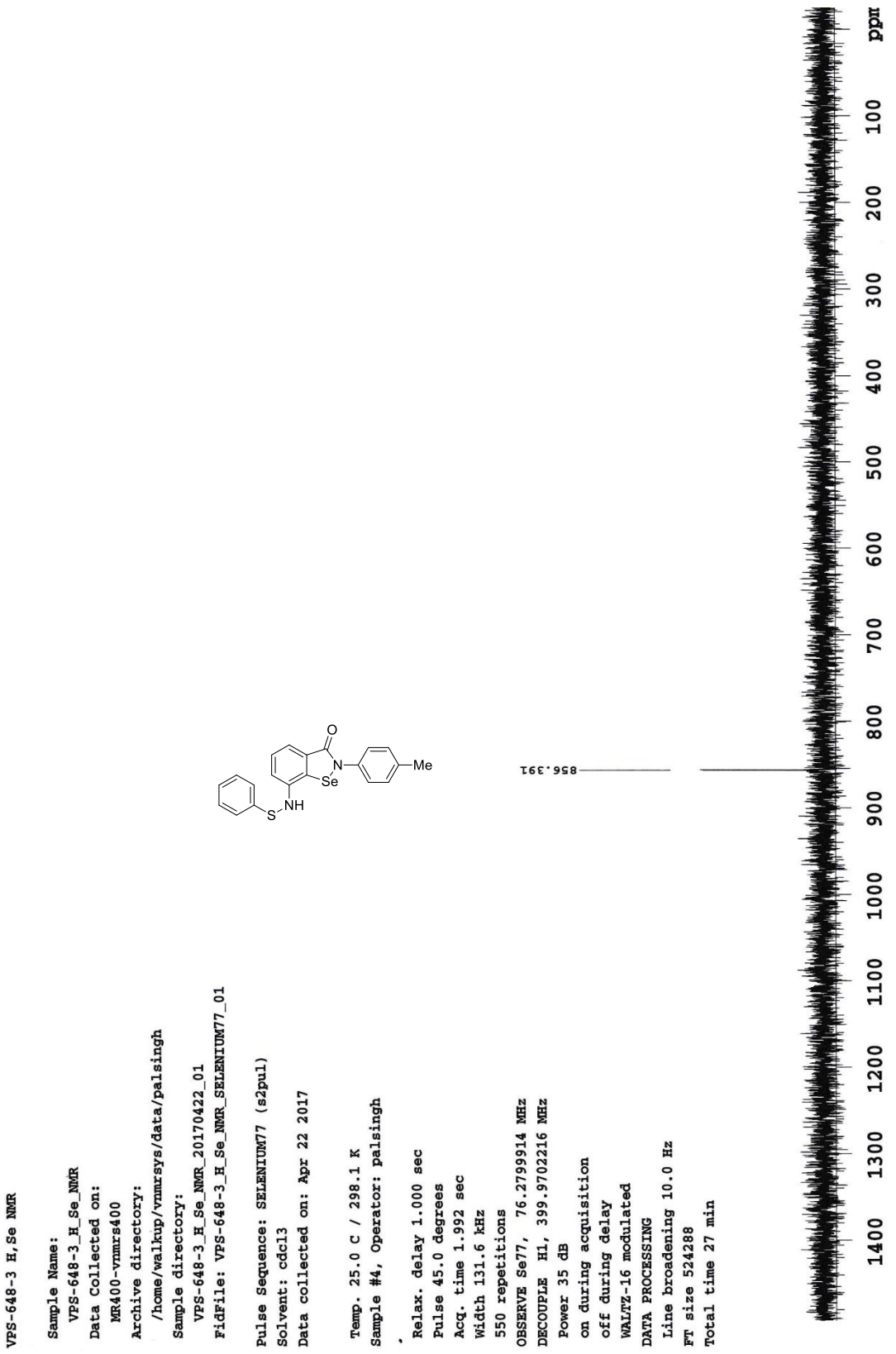
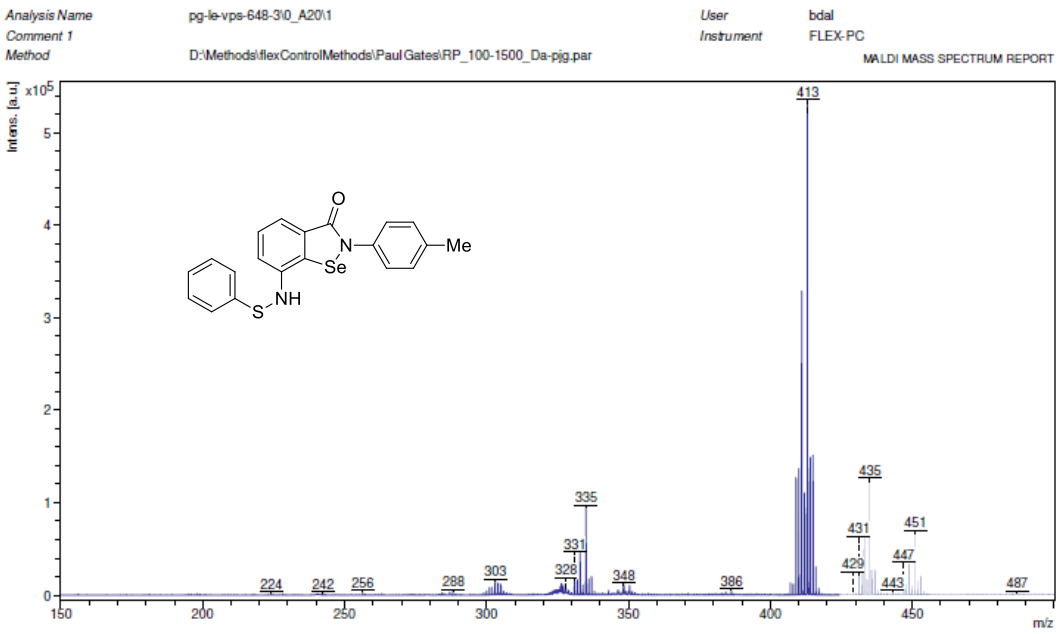
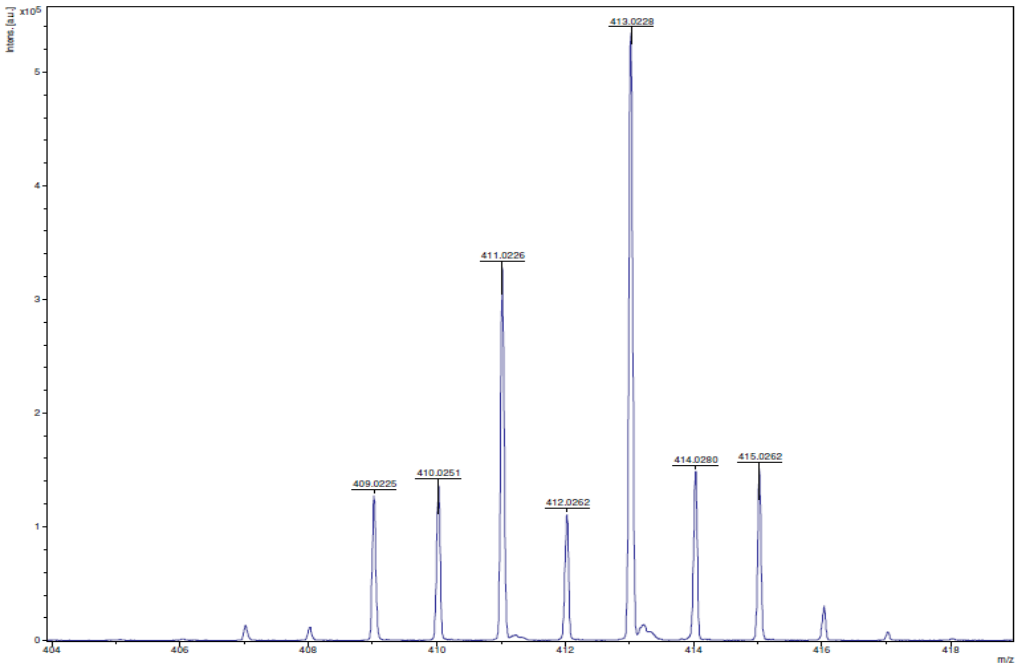


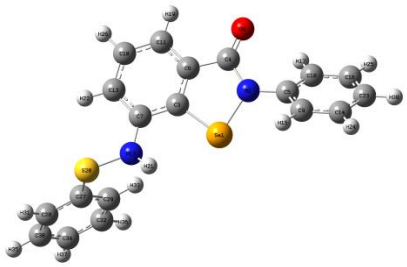
Figure S56. The HRMS of **17**





Formula	Calc m/z	Measured m/z	err [ppm]	ID
$C_{20}H_{16}N_2OSeS$	413.0222	413.0228	1.45	$[M+H]^+$

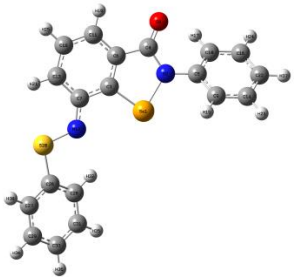
Table S1. Optimized geometries, Sum of electronic and thermal Enthalpies (a.u.), and Cartesian coordinates for compound **12** and its radical.



12

Sum of Electronic and Thermal Enthalpies = -3716.837267a.u.

34	-0.000000165	0.000000393	-0.000000160
7	-0.000000728	-0.000001308	0.000000731
6	0.000000090	0.000000655	0.000001328
6	-0.000000933	-0.000000014	0.000000332
6	0.000002446	0.000004819	0.000002910
6	0.000000497	0.000000506	0.000000183
6	0.000000491	-0.000001864	0.000002336
8	0.000000355	-0.000000111	0.000000600
6	-0.000004831	-0.000000732	-0.000001883
6	0.000002610	-0.000000429	-0.000002764
6	0.000000883	-0.000000108	0.000000713
7	0.000003015	0.000003050	-0.000005021
6	0.000000262	0.000000138	-0.000000505
6	0.000004877	0.000002207	-0.000001455
1	-0.000000529	0.000000751	-0.000000534
6	-0.000001466	-0.000000843	-0.000001976
1	-0.000001185	0.000000105	0.000001167
6	0.000000460	-0.000000108	0.000001295
1	0.000000674	-0.000000166	0.000001411
16	-0.000004473	-0.000001996	0.000002198
1	0.000000214	0.000000712	0.000000303
1	0.000000396	-0.000000290	0.000000900
6	-0.000000096	0.000003289	0.000002675
1	-0.000000568	0.000001365	-0.000001434
1	0.000000416	0.000001123	0.000000805
1	0.000000694	-0.000000317	0.000001260
6	0.000000843	-0.000000126	0.000000895
6	-0.000000136	-0.000000847	-0.000000285
6	-0.000000105	-0.000001337	-0.000001067
6	-0.000000283	-0.000001378	-0.000000762
1	-0.000000064	-0.000000104	0.000000056
6	-0.000000388	-0.000001149	-0.000000420
1	-0.000000222	-0.000000380	-0.000000154
6	-0.000000486	-0.000001381	-0.000000626
1	-0.000000243	-0.000001338	-0.000000426
1	-0.000000329	-0.000001436	-0.000000721
1	-0.000000382	-0.000001783	-0.000000809
1	-0.000001608	0.000000431	-0.000001097

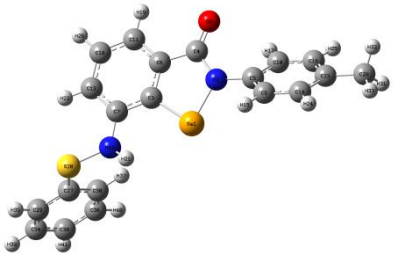


12 Radical

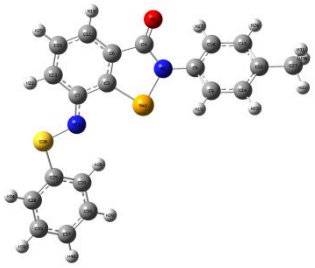
Sum of Electronic and Thermal Enthalpies = -3716.225659a.u.

34	0.000000529	-0.000000336	0.000001825
7	-0.000002985	0.000005242	-0.000008597
6	0.000002506	-0.000003307	-0.000001019
6	0.000004554	-0.000002320	0.000003349
6	-0.000001050	0.000002396	0.000007459
6	-0.000000685	0.000002392	-0.000002622
6	0.000001356	-0.000001948	-0.000000385
8	-0.000001507	0.000002422	-0.000000750
6	-0.000000800	-0.000000568	0.000001369
6	0.000000751	0.000002619	0.000000372
6	0.000001805	0.000000183	-0.000001241
7	0.000008291	0.000005965	-0.000001184
6	0.000003259	0.000002254	-0.000002385
6	0.000000195	0.000001600	0.000002308
1	-0.000001095	0.000000467	0.000001844
6	-0.000000085	0.000001357	0.000001287
1	0.000000379	0.000002640	0.000000610
6	-0.000000046	-0.000002066	-0.000002815
1	0.000000249	-0.000000571	-0.000001853
16	-0.000007632	-0.000005713	-0.000001132
1	0.000000918	-0.000003089	-0.000002659
6	-0.000001576	0.000003003	0.000003586
1	-0.000001729	0.000001139	0.000003204
1	0.000000189	0.000003587	0.000002262
1	0.000002126	-0.000001091	-0.000003040
6	-0.000004018	-0.000002692	0.000000211
6	0.000004079	-0.000005127	-0.000001069
6	0.000000602	0.000001528	-0.000001579
6	-0.000001860	0.000002088	-0.000001580
1	-0.000000759	-0.000002368	-0.000001724
6	0.000001872	-0.000002953	0.000000766
1	-0.000000114	-0.000000221	0.000000223
6	-0.000003879	-0.000004121	0.000000765
1	-0.000000808	-0.000003511	-0.000000859
1	-0.000001414	-0.000000353	0.000000759
1	-0.000000582	-0.000001331	0.000000951
1	-0.000001038	0.000002804	0.000003341

Table S2. Optimized geometries, Sum of electronic and thermal Enthalpies (a.u.), and Cartesian coordinates for compound **17** and its radical.



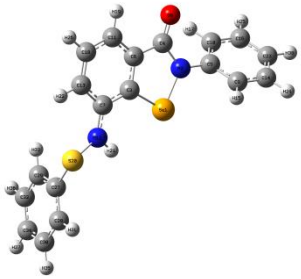
17
Sum of Electronic and Thermal Enthalpies = -3756.133564 a.u.



17 Radical
Sum of Electronic and Thermal Enthalpies = -3755.521805 a.u.

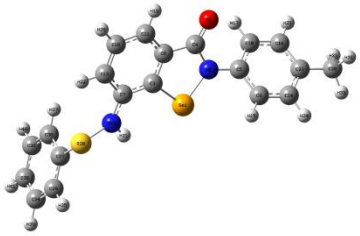
34	-0.000000619	-0.000000042	0.000000840	34	-0.000000713	0.000000410	-0.000000257
7	-0.000000551	-0.000000299	0.000001236	7	0.000000455	-0.000000770	0.000003637
6	0.000000954	0.000000283	-0.000002386	6	0.000001112	-0.000000730	-0.000000335
6	-0.000001842	0.000002311	-0.000000567	6	-0.000000482	0.000002116	-0.000000228
6	-0.000000289	-0.000000477	-0.000000365	6	-0.000000243	0.000000012	-0.000000202
6	-0.000001979	0.000001722	0.000001001	6	0.000000076	0.000000694	-0.000000074
6	-0.000001568	-0.000000709	0.000002605	6	-0.000001347	-0.000001012	-0.000000312
8	-0.000000771	0.000001966	-0.000000074	8	0.000000372	-0.000000701	0.000001109
6	-0.000002764	0.000000256	0.000000940	6	-0.000001121	-0.000000195	0.000000027
6	0.000000157	0.000001376	0.000001372	6	0.000001136	0.000000852	-0.000000046
6	0.000000626	0.000001973	-0.000000283	6	0.000000004	0.000000140	0.000000705
7	0.000002438	0.000003119	0.000001407	7	0.000005178	0.000001943	-0.000000483
6	-0.000000729	0.000001493	-0.000000146	6	0.000000255	0.000001205	-0.000000188
6	-0.000000246	0.000001014	0.000002191	6	0.000000695	0.000000613	0.000000289
1	-0.000001385	-0.000000641	0.000001997	1	-0.000000443	0.000000310	0.000000553
6	-0.000002684	0.000000542	0.000000571	6	-0.000000579	-0.000000620	0.000000599
1	-0.000000523	0.000001058	-0.000000395	1	0.000000401	0.000000105	0.000001317
6	-0.000000897	0.000002175	-0.000002050	6	0.000000110	-0.000000653	0.000000073
1	-0.000000990	0.000002800	-0.000000829	1	-0.000000192	-0.000000187	0.000000643
16	-0.000001058	0.000001068	-0.000004160	16	-0.000003571	-0.000001240	-0.000001769
1	-0.000000521	-0.000002264	0.000000236	1	0.000000182	-0.000000801	-0.000000199
1	0.000000025	0.000001143	-0.000000893	6	0.000000459	-0.000000126	0.000002257
6	-0.000000300	-0.000002006	0.000000539	1	-0.000000633	0.000000399	0.000001094
1	-0.000001878	-0.000001102	0.000002266	1	0.000000515	0.000000081	0.000001741
1	-0.000000498	0.000000648	0.000000170	1	0.000000236	-0.000000109	0.000000269
1	-0.000000469	0.000002903	-0.000000965	6	-0.000001953	-0.000001883	0.000000893
6	0.000004770	-0.000005021	0.000008126	6	0.000000067	-0.000000556	0.000001208
6	-0.000001606	-0.000000537	0.000001862	6	0.000000908	-0.000000241	-0.000002133
6	-0.000001258	0.000005036	-0.000009207	6	0.000000296	0.000000300	-0.000002041
6	0.000000755	-0.000005203	-0.000001072	1	-0.000000175	0.000000915	0.000001358
1	-0.000000381	-0.000000586	0.000000593	1	-0.000000918	0.000000902	0.000001431
1	-0.000001840	0.000000910	0.000001519	1	-0.000000166	0.000001003	0.000001230
1	-0.000001738	-0.000001260	0.000002386	6	-0.000000320	0.000000779	-0.000002290
6	0.000001326	-0.000010417	0.000001036	1	-0.000000042	-0.000000092	-0.000001223
1	0.000001150	-0.000002062	0.000000739	6	0.000001048	-0.000000828	-0.000001434
6	0.000000323	0.000001281	-0.000006847	1	0.000000348	0.000000121	-0.000000701
1	0.000001478	-0.000000136	-0.000000950	6	-0.000000907	-0.000000903	-0.000001229
6	0.000006821	0.000003022	0.000003140	1	-0.000000203	-0.000000512	-0.000002047
1	0.000002825	-0.000000938	-0.000001492	1	0.000000116	-0.000000379	-0.000001348
1	0.000002980	-0.000001953	-0.000001174	1	0.000000038	-0.000000364	-0.000001896
1	0.000002755	-0.000002446	-0.000002921				

Table S3. Optimized geometries, Sum of electronic and thermal Enthalpies (a.u.), and Cartesian coordinates for compound **12** and **17** Radical Cation.



12 Radical Cation
Sum of Electronic and Thermal Enthalpies = -3716.601313a.u.

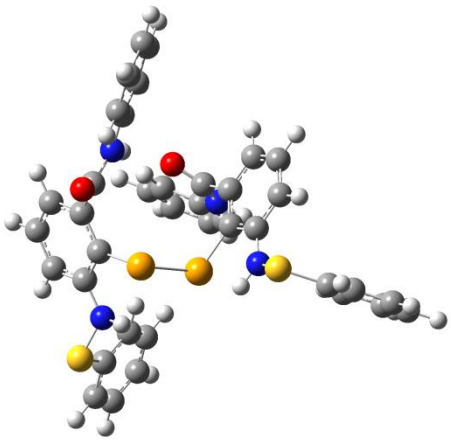
34	0.000000036	0.000002127	-0.000000598
7	0.000014722	0.000024288	0.000014718
6	-0.000013661	-0.000005681	0.000002362
6	-0.000006289	-0.000030501	-0.000011875
6	-0.000017612	-0.000013163	-0.000008666
6	0.000010346	0.000010711	0.000000094
6	0.000027151	-0.000017824	-0.000002478
8	-0.000003299	0.000007420	0.000004314
6	0.000005842	0.000002461	0.000000189
6	0.000003055	0.000003006	0.000001097
6	-0.000011075	-0.000005262	0.000003286
7	-0.000034429	0.000010233	0.000015168
6	-0.000007195	0.000007092	-0.000000731
6	-0.000002210	-0.000000338	-0.000000378
1	0.000000133	0.000000703	-0.000000594
6	0.000001442	-0.000001015	0.000000073
1	0.000000849	-0.000001153	-0.000000992
6	0.000010047	-0.000001708	0.000000203
1	0.000000409	0.000000304	0.000001319
16	0.000019907	0.000006213	-0.000007669
1	0.000002085	0.000000151	-0.000006420
1	-0.000000786	0.000001921	0.000001088
6	0.000001479	0.000000067	-0.000003127
1	0.000000355	-0.000000339	-0.000001056
1	-0.000000988	-0.000001838	-0.000001656
1	-0.000000798	0.000000316	0.000001181
6	0.000001229	-0.000001617	0.000008996
6	-0.000004121	0.000003729	-0.000004980
6	-0.000002892	-0.000001191	-0.000002030
6	0.000002466	-0.000003145	0.000003891
1	0.000001088	0.000000904	0.000000631
6	0.000000820	0.000002004	0.000000516
1	0.000000665	0.000000866	-0.000000227
6	0.000000027	-0.000000440	-0.000004371
1	0.000001112	0.000002050	-0.000001116
1	0.000000258	-0.000001133	0.000000215
1	-0.000000239	0.000000324	0.000000752
1	0.000000071	-0.000000542	-0.000001128



17 Radical Cation
Sum of Electronic and Thermal Enthalpies = -3755.902322 a.u.

34	0.000001899	-0.000000961	-0.000000360
7	-0.000003518	0.000000901	-0.000003565
6	0.000002013	-0.000000393	0.000001462
6	0.000001081	-0.000001824	0.000002126
6	-0.000005077	0.000011517	0.000027264
6	-0.000001521	0.000000018	0.000001583
6	-0.000003502	-0.000002654	0.000001533
8	-0.000001794	-0.000001188	0.000001206
6	-0.000024832	-0.000013041	-0.000018587
6	0.000025090	0.000009712	-0.000017450
6	-0.000002328	-0.000000856	0.000001549
7	-0.000003023	0.000002770	0.000001791
6	0.000000023	0.000004492	0.000002282
6	0.000022541	0.000006172	-0.000024502
1	0.000001979	-0.000000606	0.000000177
6	-0.000020771	-0.000015057	-0.000023467
1	-0.000000732	-0.000003391	0.000001469
6	0.000000776	-0.000000254	0.000002017
1	-0.000001468	-0.000000623	0.000002664
16	0.000003032	0.000002985	0.000000441
1	0.000000243	0.000000753	-0.000000001
1	-0.000001062	0.000000865	0.000001712
6	-0.000010917	0.000007201	0.000063227
1	0.000002974	-0.000006512	-0.000000488
1	0.000004828	-0.000007683	-0.000000269
1	-0.000001838	0.000000408	0.000003012
6	-0.000000262	0.000001117	0.000000161
6	0.000025579	-0.000042431	0.000023967
6	0.000003366	-0.000000099	0.000000863
6	-0.000000868	0.000002979	-0.000001836
1	-0.000002666	0.000009174	-0.000017353
1	-0.000009100	0.000013783	-0.000016265
1	-0.000002880	0.000011611	-0.000015374
6	0.000000176	0.000002915	-0.000002599
1	0.000000049	0.000003405	0.000000030
6	0.000001810	-0.000001348	0.000000973
1	-0.000000505	-0.000000084	0.000001121
6	-0.000000676	0.000002402	0.000001282
1	0.000001084	0.000002373	-0.000000409
1	-0.000000261	0.000000345	-0.000000179
1	0.000001054	0.000001105	-0.000001208

Table S4. Optimized geometries and Cartesian coordinates for compound **11**.



11

Se	-0.07021287	0.26466912	-2.22437912	C	-2.17764388	1.83297067	3.36190186
Se	-0.30488869	-1.15689016	-0.28154456	H	-1.41397595	0.55858950	1.80626739
O	-0.06477773	3.62480610	-2.73960113	C	0.00744992	0.89110137	2.20107370
N	2.77396609	-1.03377844	-2.27519394	C	1.92636085	-0.12043996	3.47515671
H	1.85404802	-1.37454281	-2.52652374	C	2.23717521	-1.21014896	4.30373313
N	0.14278766	3.87072396	-0.45931003	H	1.48865514	-1.97245028	4.50290261
H	0.61993534	3.46249073	0.34235363	C	3.49659286	-1.31898036	4.87718937
C	1.64774304	1.10120426	-1.92280179	H	3.72227307	-2.16543807	5.51788559
C	2.83919531	0.34190071	-2.03178916	C	4.45224403	-0.33871529	4.62574168
C	4.06950342	0.98641326	-1.83997218	C	4.15227775	0.74205982	3.80473062
H	4.98453189	0.41270351	-1.92173999	H	4.89917434	1.50330190	3.60556011
C	4.11748859	2.34334197	-1.55867424	C	2.89278587	0.86238189	3.22205538
H	5.08112998	2.82232852	-1.41763960	H	2.65780789	1.70091647	2.58476841
C	2.94874032	3.09524822	-1.46223204	C	-5.70892127	-2.89084118	-0.52799529
H	2.99340081	4.15999298	-1.26150058	C	-7.02274509	-3.18935860	-0.90384837
C	1.71417747	2.47623995	-1.64995009	C	-5.07963056	-3.63590213	0.46776357
C	0.48261796	3.35981986	-1.68108063	C	-7.69891661	-4.23595677	-0.28313621
C	-0.83354909	4.84380909	-0.16112845	H	-7.51765679	-2.60858943	-1.67731949
C	-1.75690147	5.32710576	-1.10049209	C	-5.76811409	-4.67922613	1.08633849
H	-1.74420076	4.94780075	-2.11086711	H	-4.06112730	-3.40214927	0.75496090
C	-2.67852080	6.29797842	-0.71614324	C	-7.07579193	-4.98486637	0.71546107
H	-3.38871183	6.66826189	-1.44887604	H	-8.71760710	-4.46370898	-0.58036673
C	-2.69070419	6.78785897	0.58530038	H	-5.27450146	-5.25583680	1.86242898
C	-1.77653747	6.31219773	1.52196659	H	-7.60580046	-5.79841647	1.19919631
H	-1.77362663	6.69527010	2.53788886	S	-4.91250486	-1.53111974	-1.39819773
C	-0.85090310	5.34642523	1.15101188	C	4.69732265	-2.80716865	-1.45142096
H	-0.12822693	4.98125919	1.87378508	C	4.29342819	-2.50542270	-0.15157217
O	0.51624739	1.97314624	1.93177684	C	5.66373298	-3.79302730	-1.67678400
N	-3.39949776	-1.40450534	-0.64359118	C	4.86064246	-3.19164027	0.92199697
H	-2.61802237	-1.81952015	-1.13343357	H	3.54122827	-1.74468699	0.01845156
N	0.62448471	-0.08772428	2.92710120	C	6.22385604	-4.47097024	-0.59756404
H	0.06463358	-0.91020021	3.10036892	H	5.97522025	-4.03513188	-2.68910276
C	-1.71996589	-0.28898592	0.72786059	C	5.82533238	-4.17374720	0.70598909
C	-3.07848659	-0.53989562	0.40066395	H	4.54786556	-2.94572481	1.93169610
C	-4.08289362	0.07699754	1.16164989	H	6.97113221	-5.23712301	-0.77858442
H	-5.12069007	-0.10775500	0.91315441	H	6.26390777	-4.70385616	1.54491447
C	-3.75812940	0.92197485	2.21063372	S	4.06147315	-1.95809941	-2.90245196
H	-4.55270327	1.39487099	2.77779908	H	-3.42012783	7.55417409	0.87503167
C	-2.42823839	1.16846333	2.54296209	H	5.44727027	-0.41972875	5.07849002

Table S5. Data for **12** and **17** 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 **12** and **17** were calculated.

AOs	Calculated BDE_{N-H} (Kcal/mol)	Energy of 1-e oxidation (Kcal/mol)	r_{Se-N} [Å]	NPA Charges[a]		$^{77}Se\{^{1}H\}$ NMR (ppm)[b]	
				*q*Se	*q*S	Exptl.	Calcd.
12	70.03	148.81	1.897	+0.590	+0.466	833	936
17	70.12	145.85	1.896	+0.587	+0.466	856	925
10				+0.213	+0.063	452	455, 421[c],403[d]
16				+0.216	+0.063	453	440,404[c],386[d]
11						534	548

[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 $^{77}Se\{^{1}H\}$ NMR values are referenced to Me_2Se ($\delta = 0$). The experimental values are given in parentheses.[c]The $^{77}Se\{^{1}H\}$ NMR value calculated in chloroform solvent. [d]The $^{77}Se\{^{1}H\}$ NMR value calculated in DMSO solvent.

Formula used for Bond Dissociation Energy:-

BDE_{N-H} = [Energy (Molecule Radical) + Energy (H)] - [Energy (Molecule)]

Formula used for calculation of 1-electron oxidation**:-**

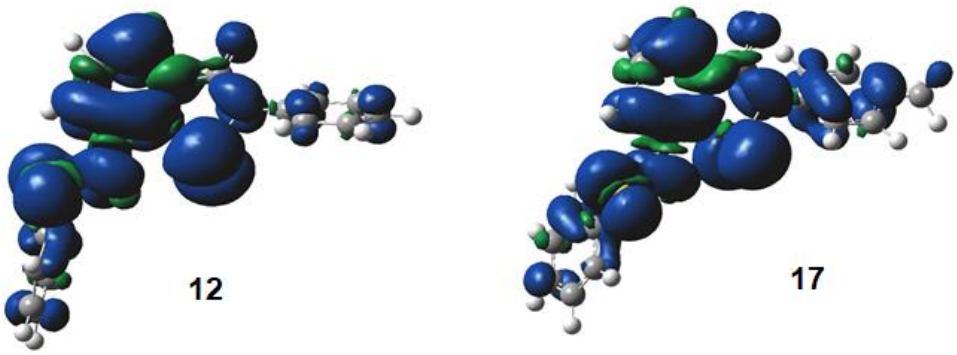
[Energy (Molecule Radical Cation) + Energy (electron)] - [Energy (Molecule)]

Table S6. The calculated $^{77}Se\{^{1}H\}$ NMR value of isolated compounds with isotropic and anisotropic values (ppm)

Compound 12 SCF GIAO Magnetic shielding tensor (ppm): 1 Se Isotropic = 691.1663 Anisotropy = 1312.2695	**Compound 17** SCF GIAO Magnetic shielding tensor (ppm): 1 Se Isotropic = 693.7769 Anisotropy = 1313.9572
Compound 10 SCF GIAO Magnetic shielding tensor (ppm): 1 Se Isotropic = 1166.2349 Anisotropy = 1053.4431	**Compound 16** SCF GIAO Magnetic shielding tensor (ppm): 1 Se Isotropic = 1181.7122 Anisotropy = 1053.3671
Compound 11 SCF GIAO Magnetic shielding tensor (ppm): 1 Se Isotropic = 1073.8904 Anisotropy = 1228.5857	

The $^{77}Se\{^{1}H\}$ NMR calculations were performed at B3LYP/6-311+G (d,p) level on B3LYP/6–311+G(d)-level-optimized geometries by using the gauge-including atomic orbital (GIAO) method (referenced with respect to the peak of Me_2Se).

Figure S57. Spin density maps of the radical cations of **12** and **17** formed upon 1-electron oxidation calculated at the UB3LYP/6-311+G(d) level in gas phase.



Scheme S1: Proposed mechanism for **12** from diselenide **9**