SUPPORTING INFORMATION

FOR

Synthesis, Antioxidant and Structural Properties of Modified Ebselen Derivatives and Conjugates

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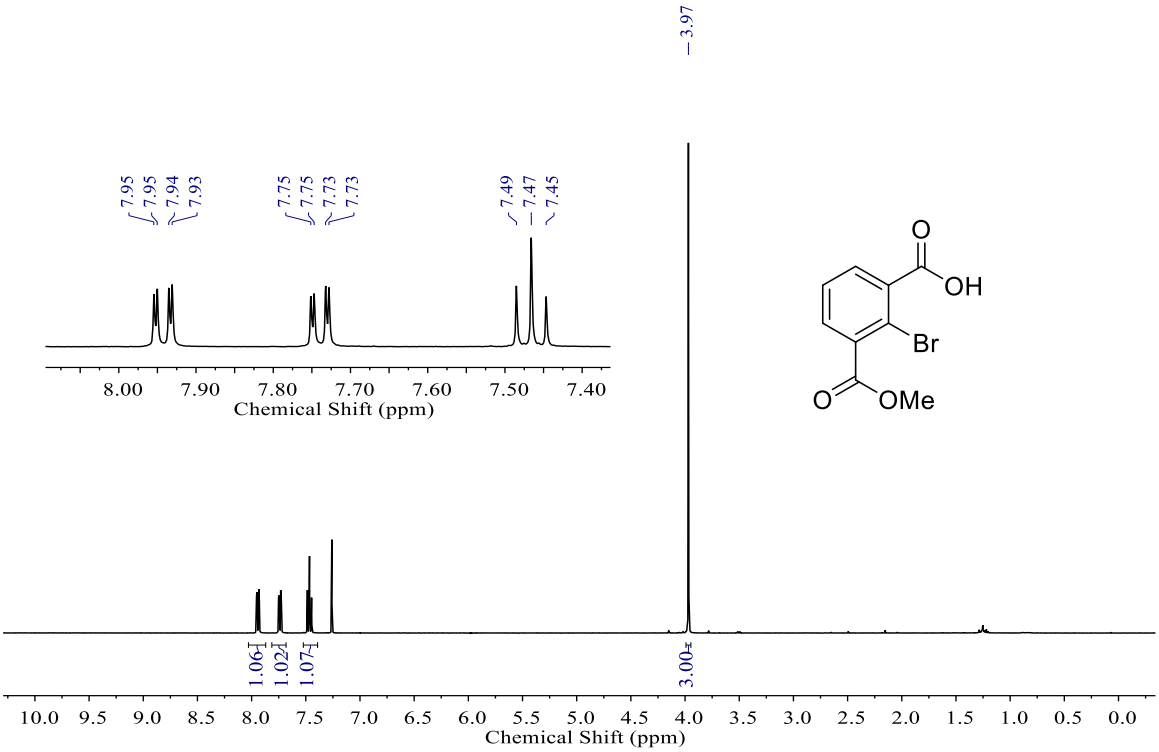
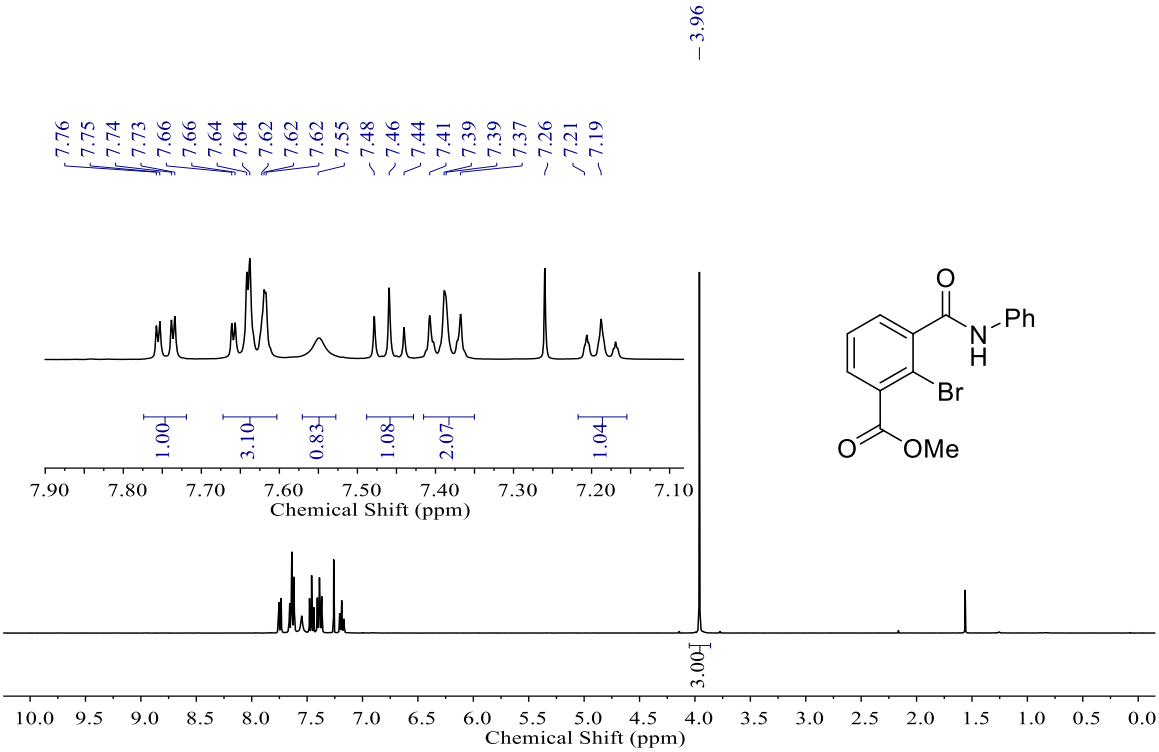


Figure 2. ^{1}H NMR Spectrum of 23 (400 MHz, $CDCl_3$)



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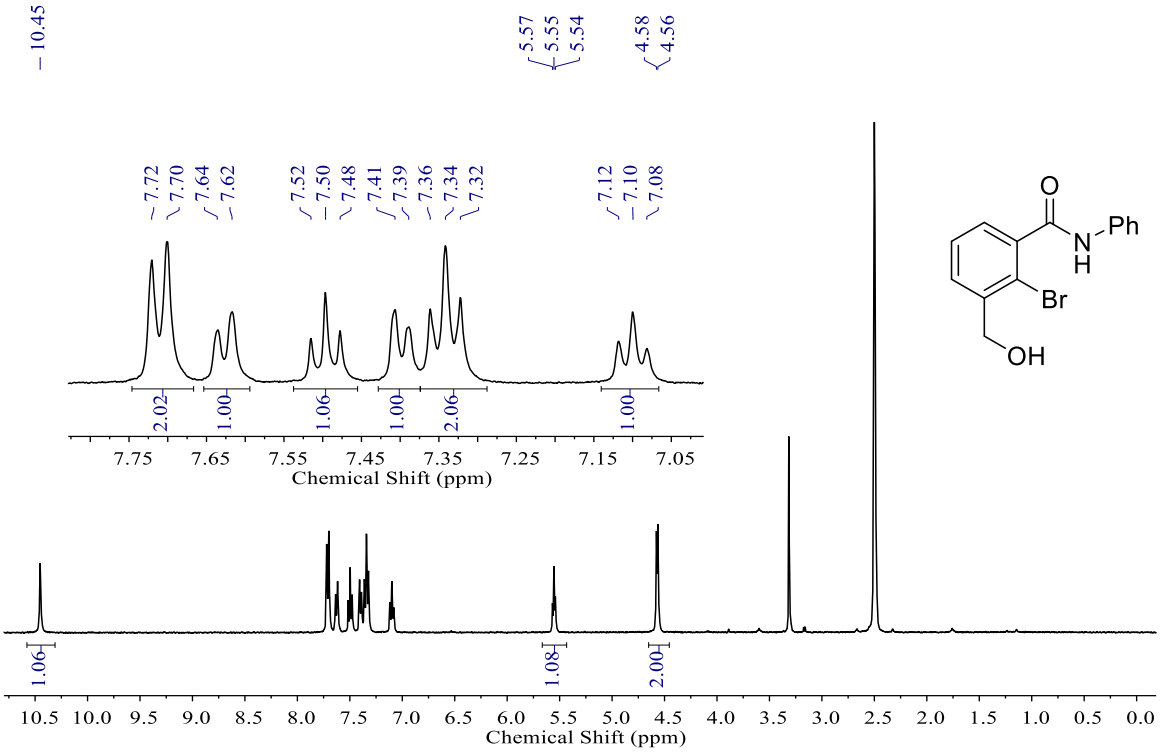
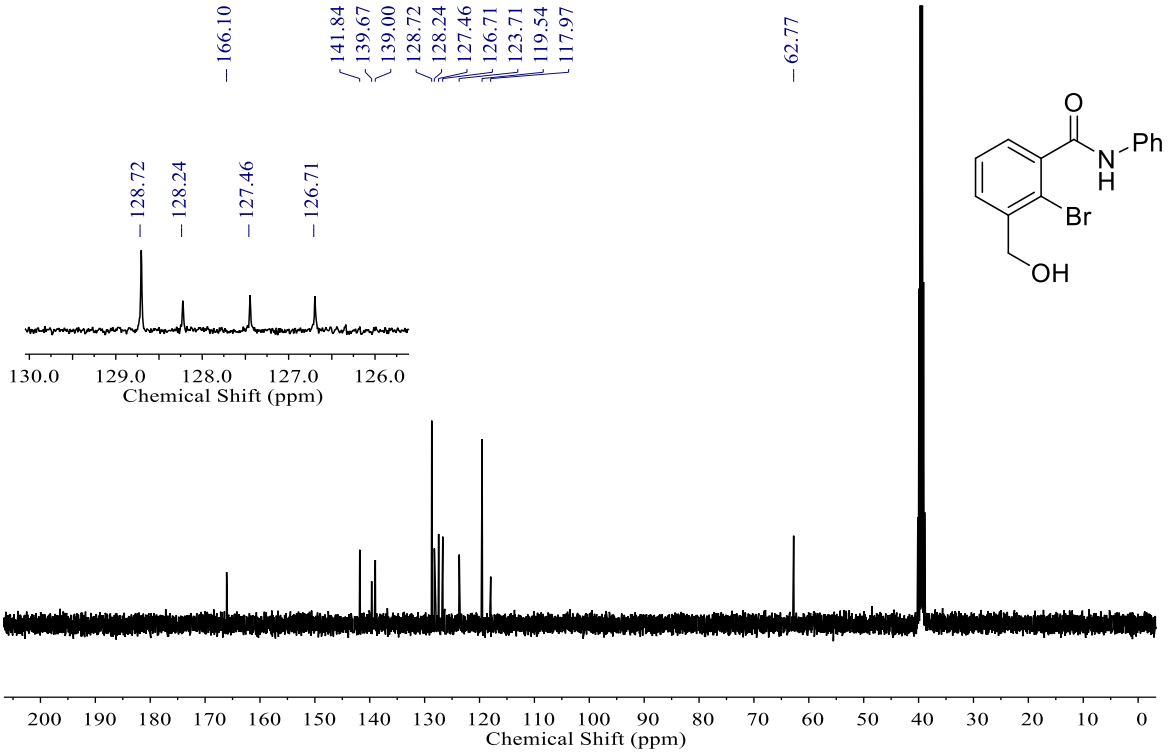


Figure 4. ^{13}C NMR Spectrum of 24 (101 MHz, DMSO-d$_6$)



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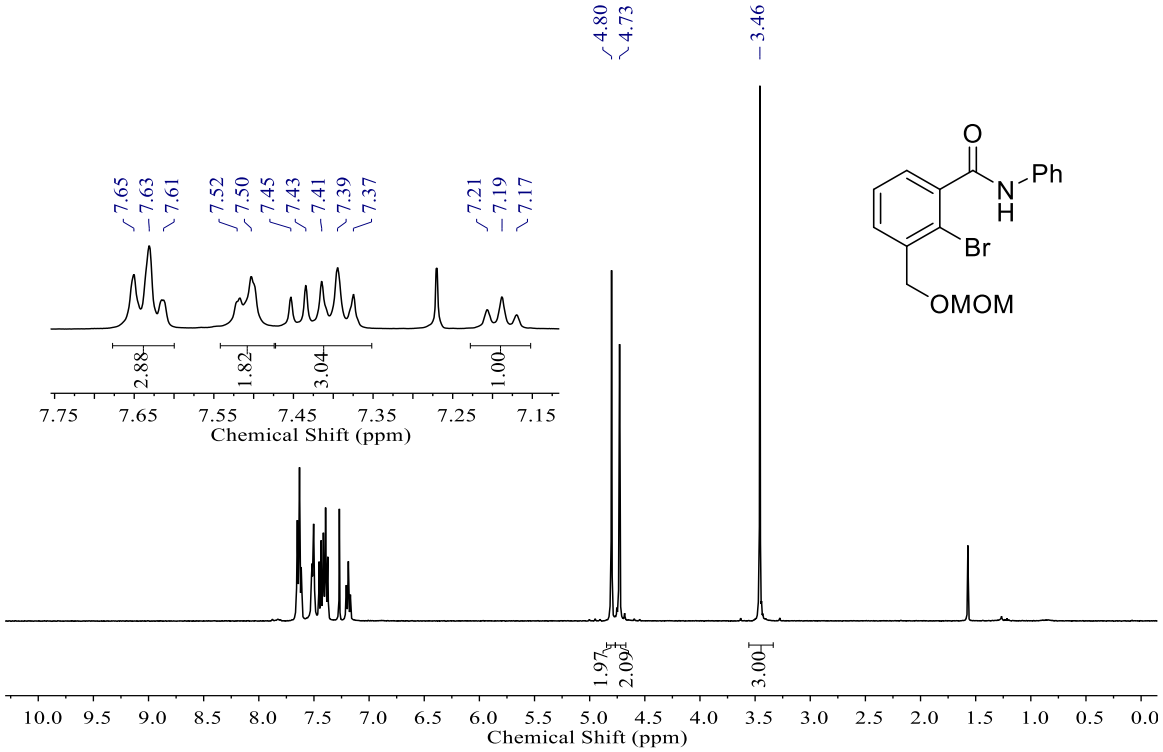

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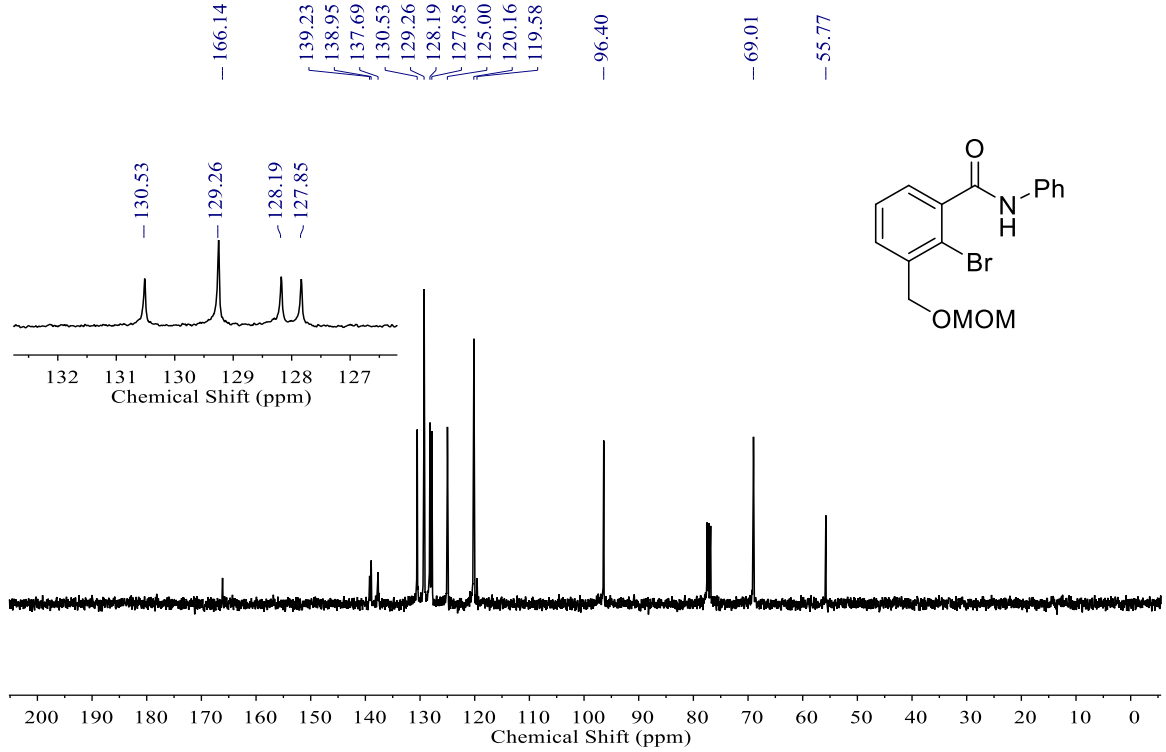


Figure 7. ^{1}H NMR Spectrum of 3 (400 MHz, $CDCl_3$)

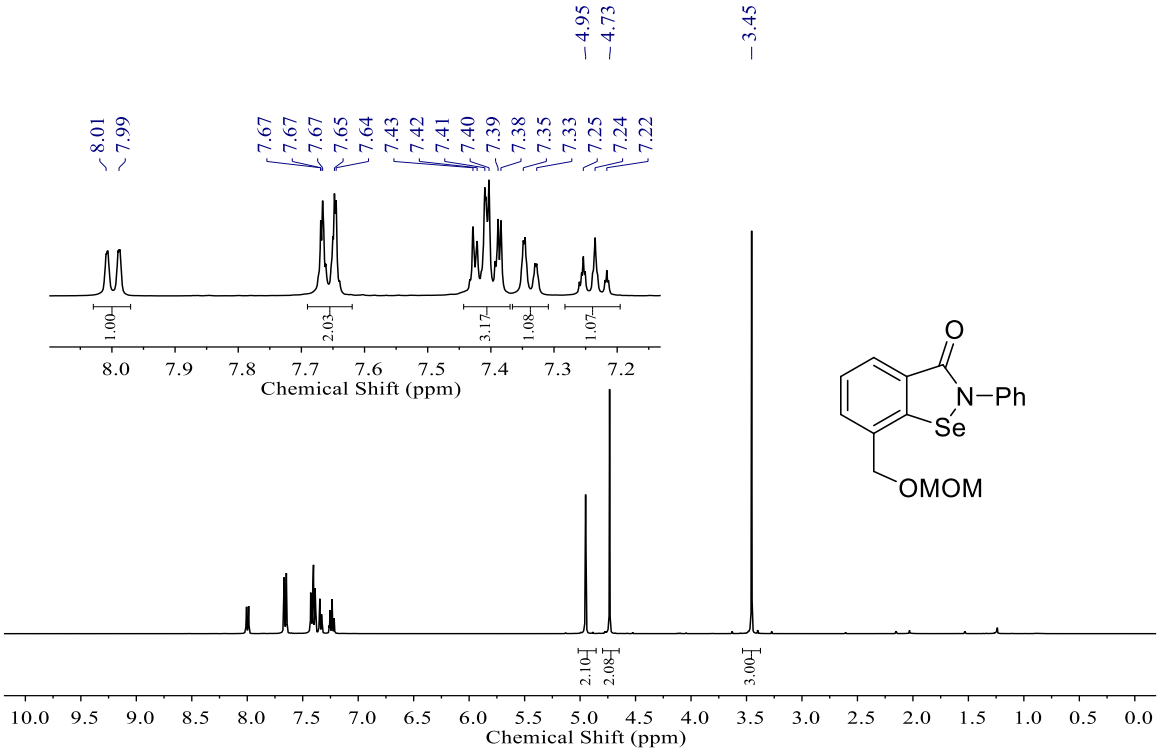


Figure 8. ^{13}C NMR Spectrum of 3 (101 MHz, $CDCl_3$)

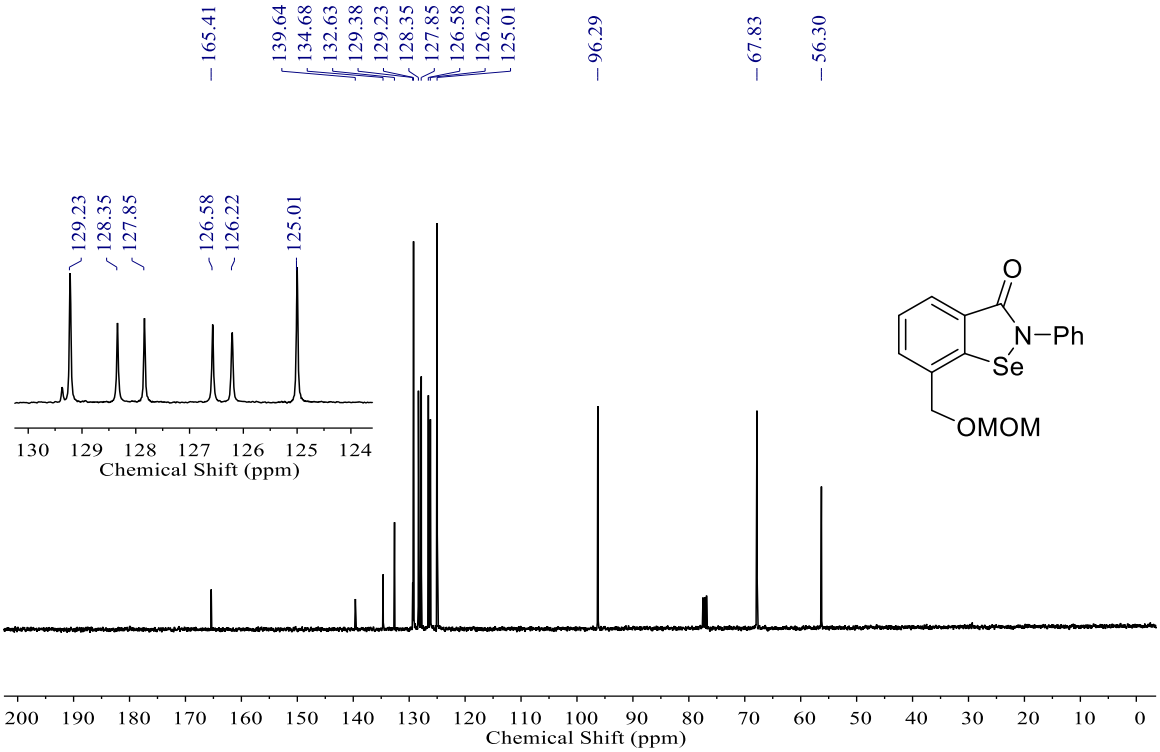


Figure 9. ^{77}Se NMR Spectrum of 3 (76 MHz, $CDCl_3$)

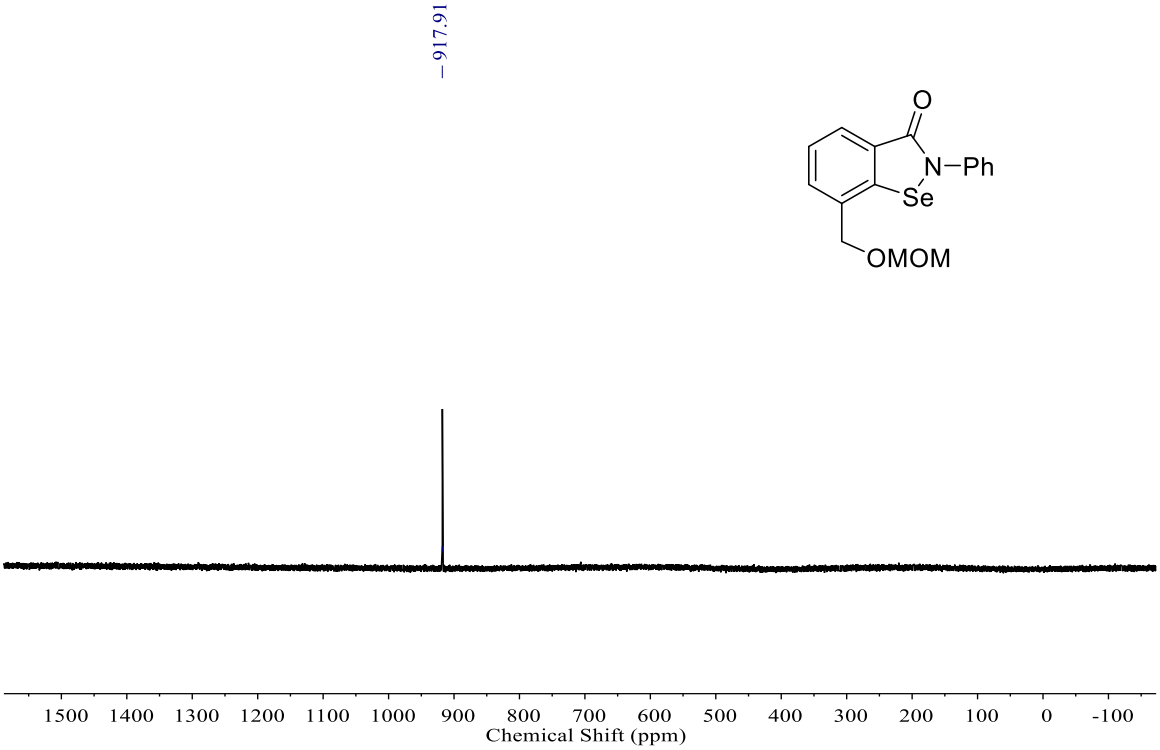


Figure 10. ^{1}H NMR Spectrum of 2 (400 MHz, DMSO-d_6)

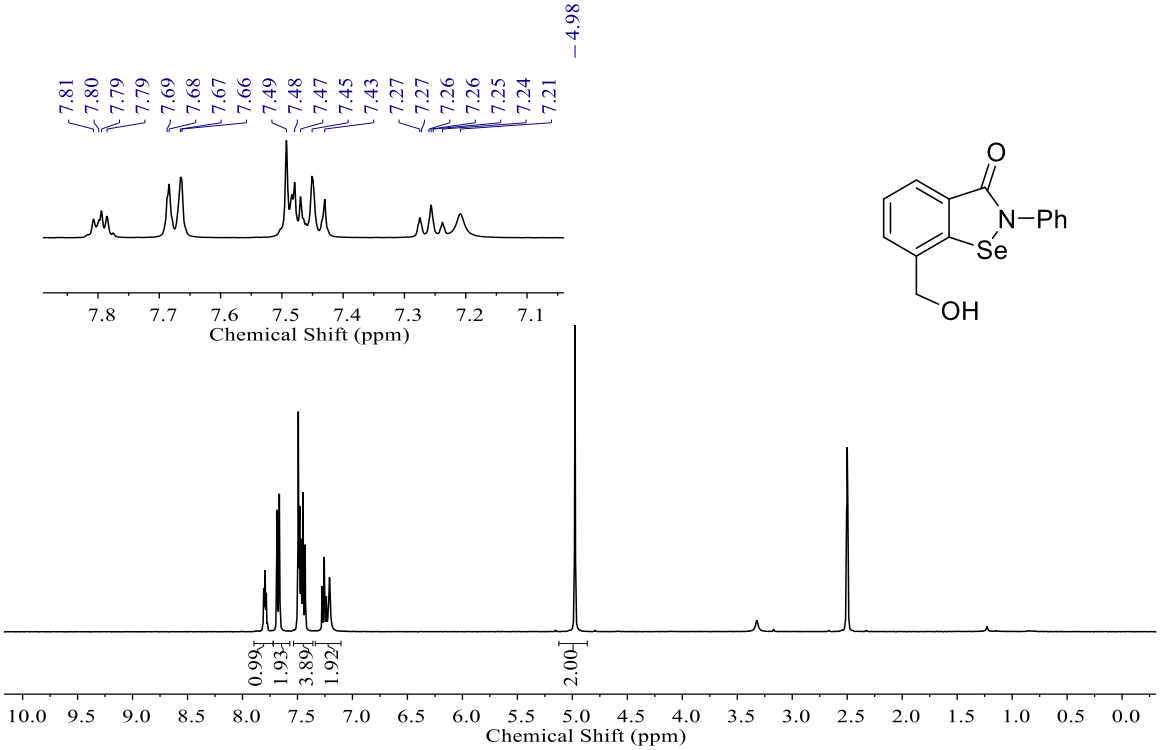


Figure 11. ^{13}C NMR Spectrum of 2 (101 MHz, DMSO-d$_6$)

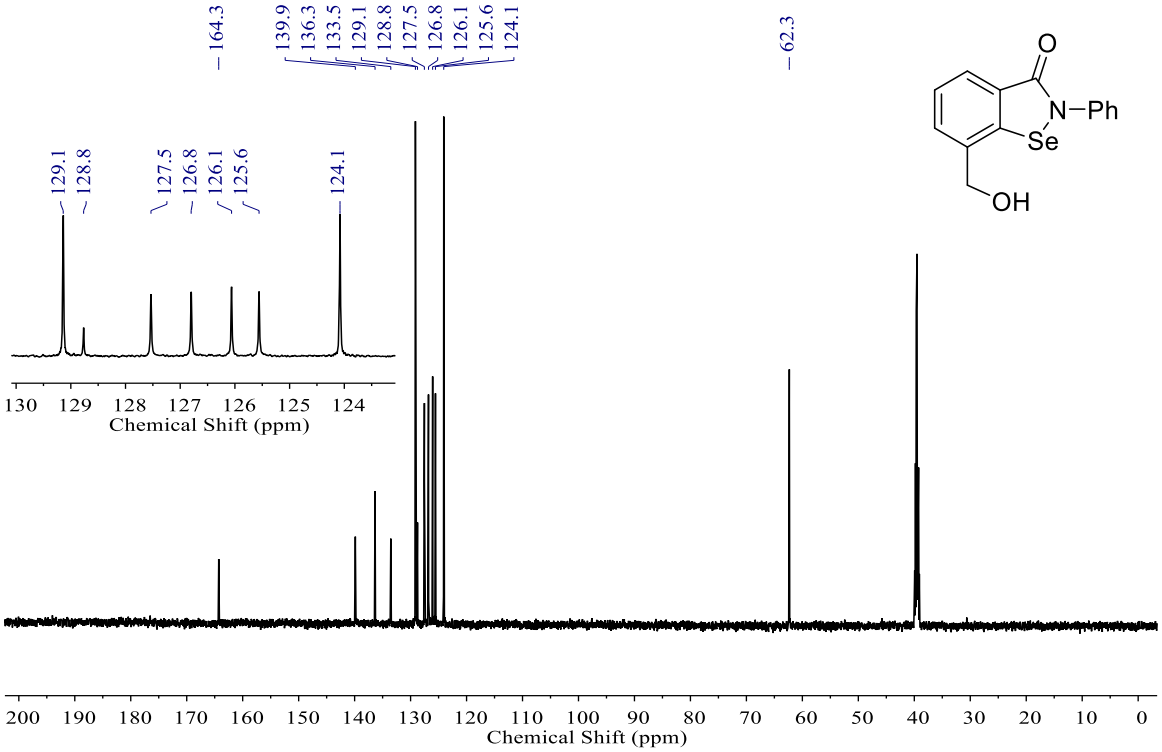


Figure 12. ^{77}Se NMR Spectrum of 2 (76 MHz, DMSO-d$_6$)

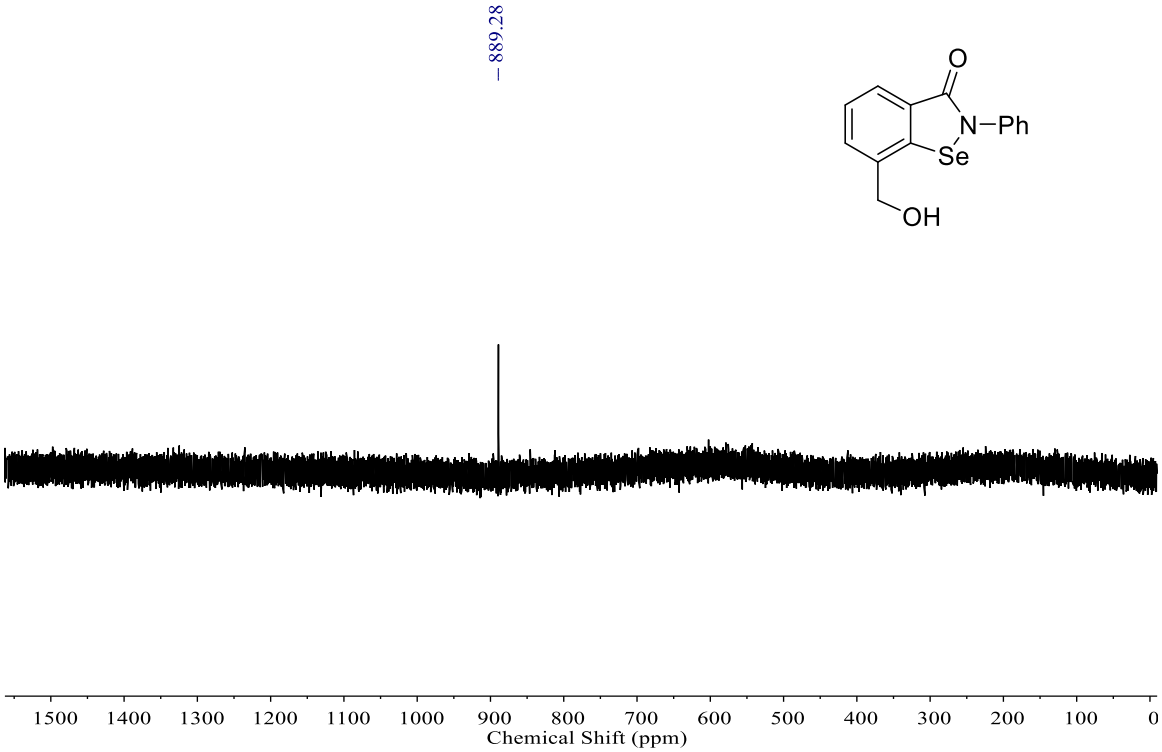


Figure 13. ^{1}H NMR Spectrum of 26 (400 MHz, $CDCl_3$)

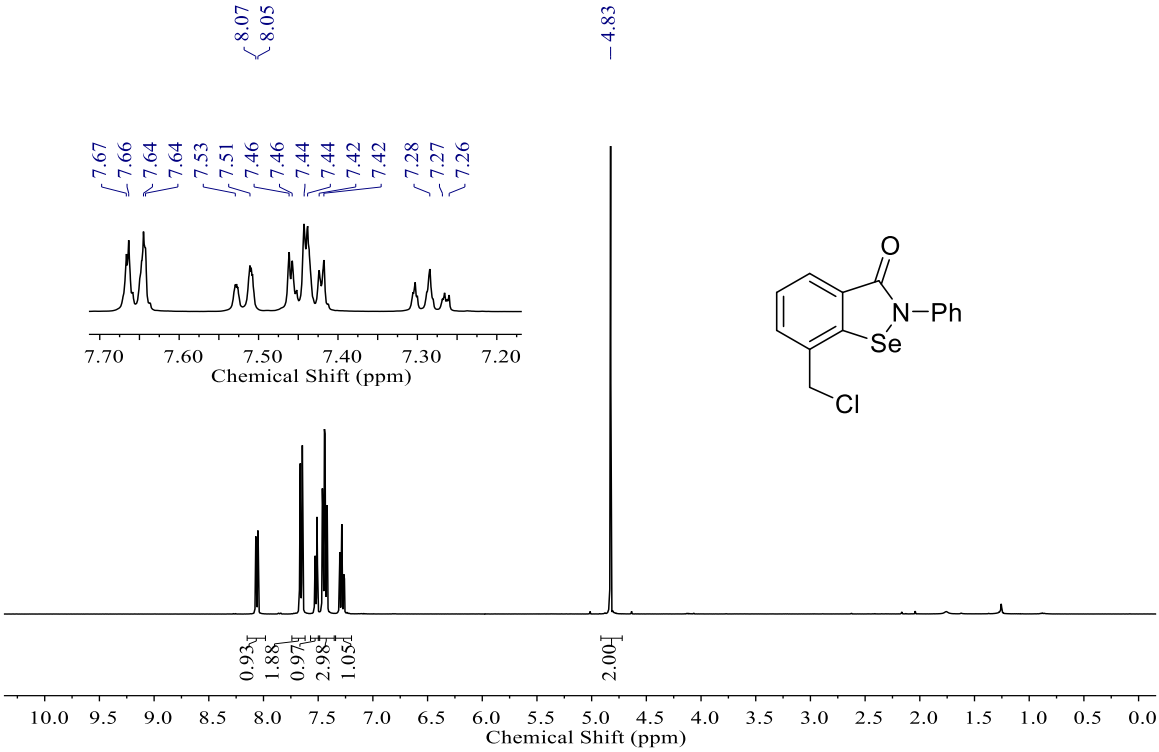
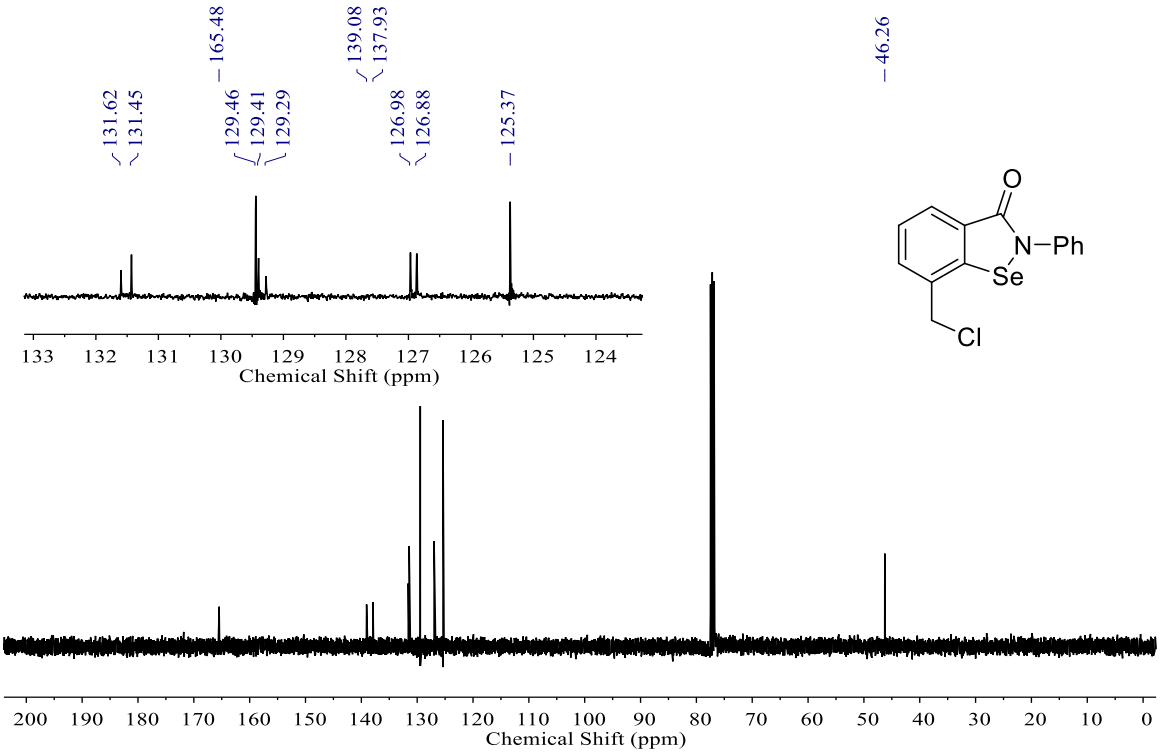


Figure 14. ^{13}C NMR Spectrum of 26 (101 MHz, $CDCl_3$)



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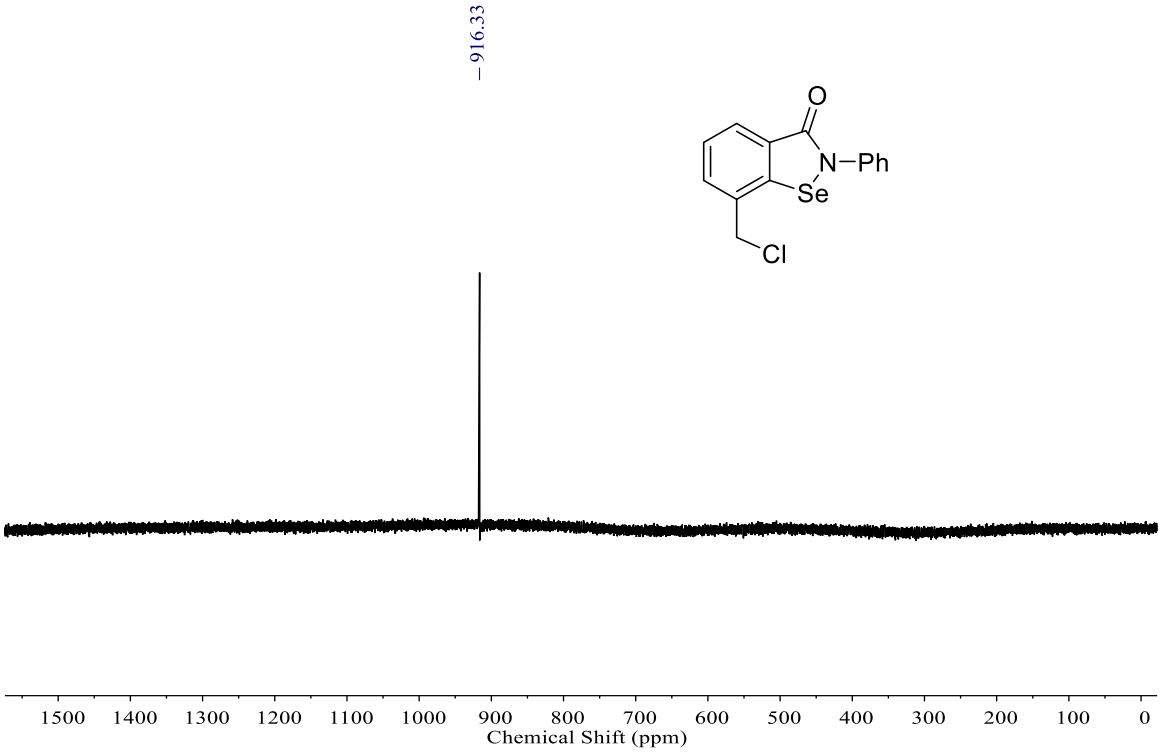


Figure 16. ^{1}H NMR Spectrum of 4 (400 MHz, $CDCl_3$)

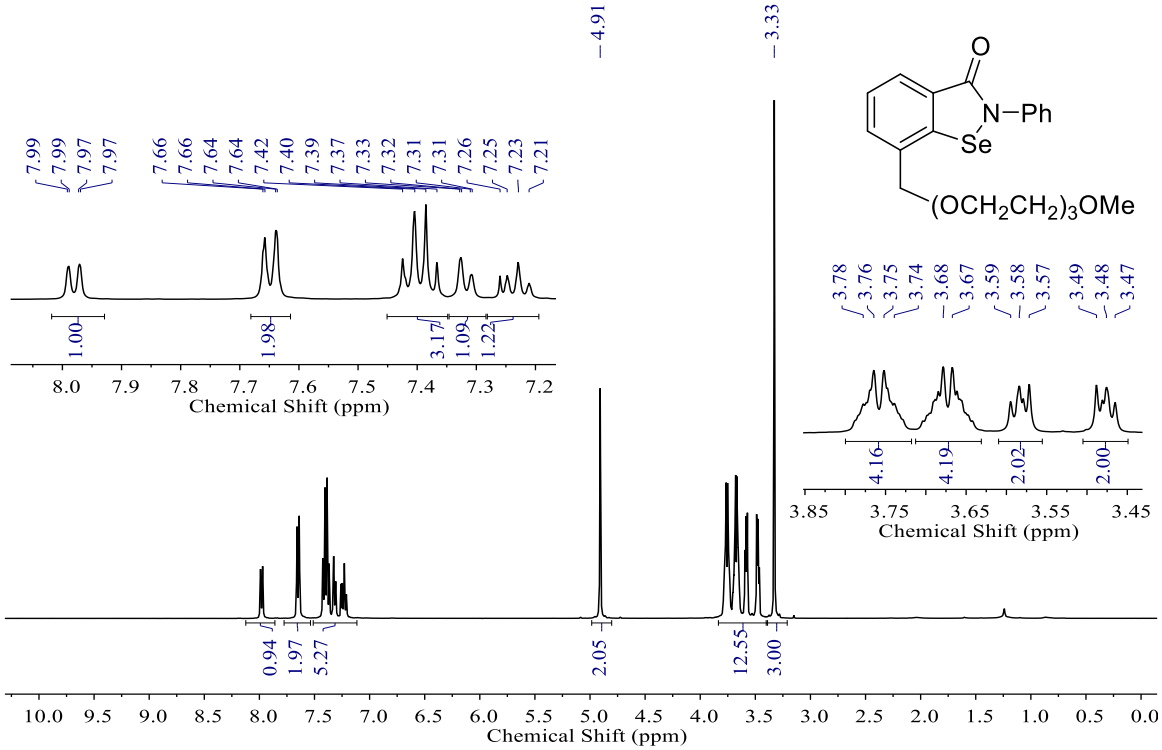


Figure 17. ^{13}C NMR Spectrum of 4 (101 MHz, $CDCl_3$)

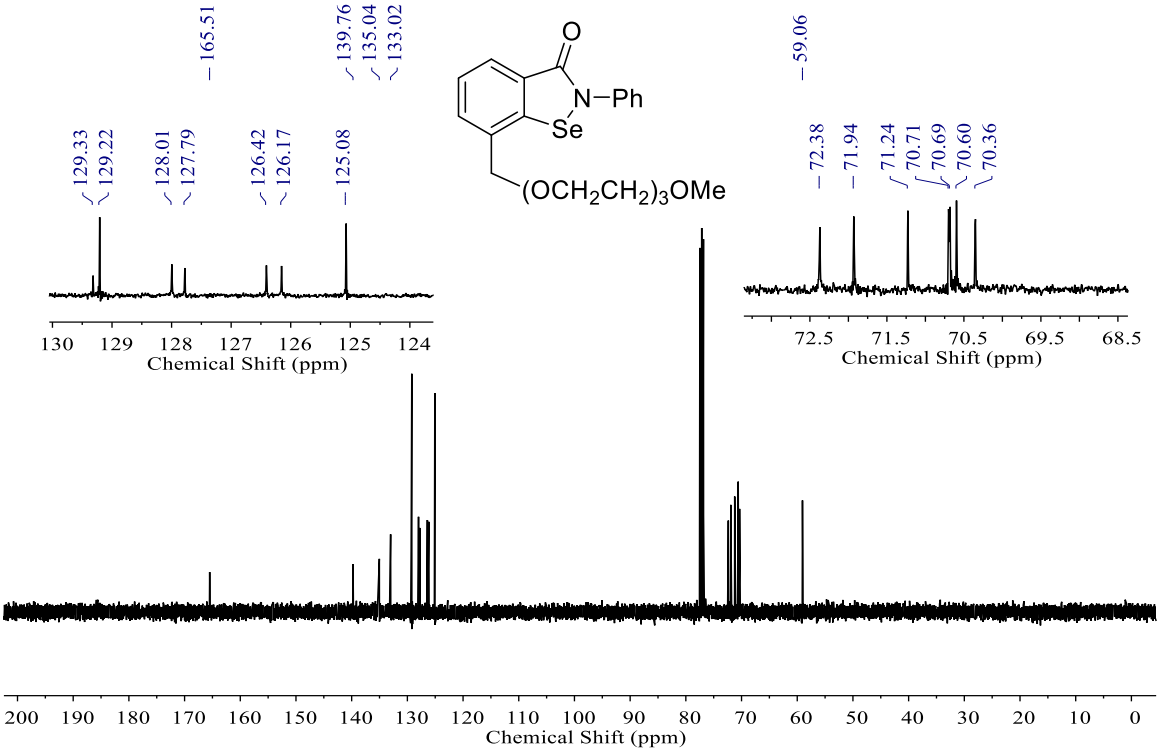


Figure 18. ^{77}Se NMR Spectrum of 4 (76 MHz, $CDCl_3$)

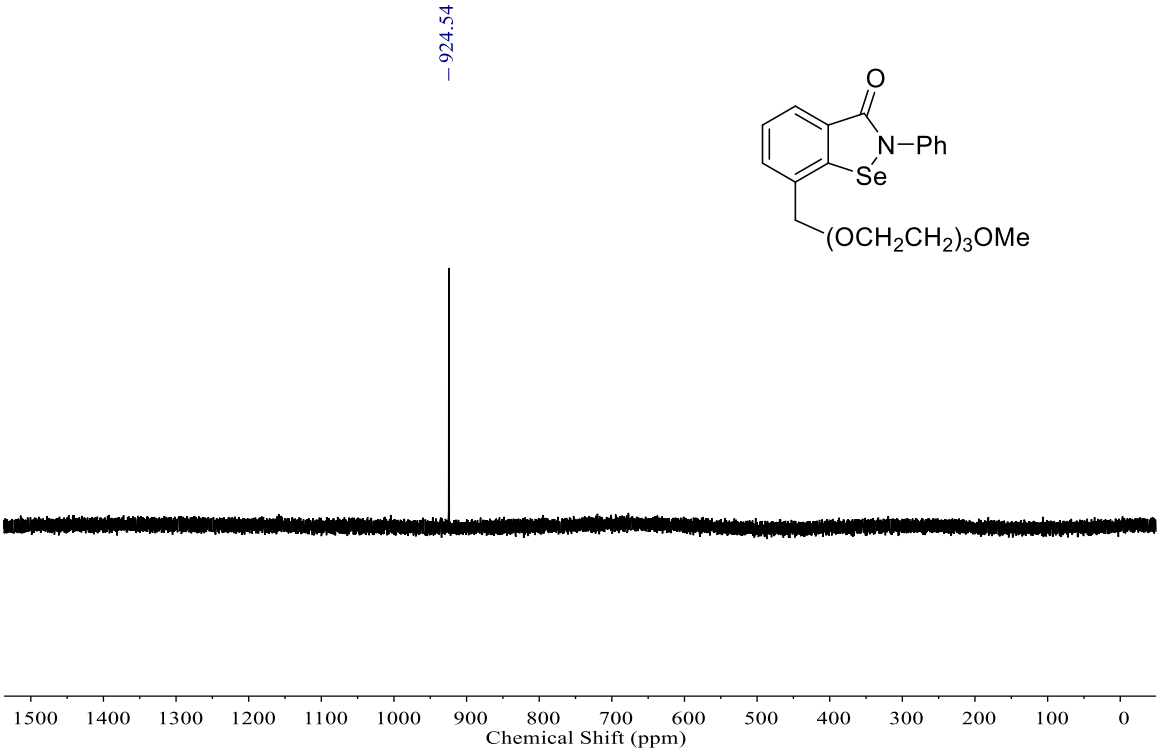


Figure 19. ^{1}H NMR Spectrum of 9 (400 MHz, $CDCl_3$)

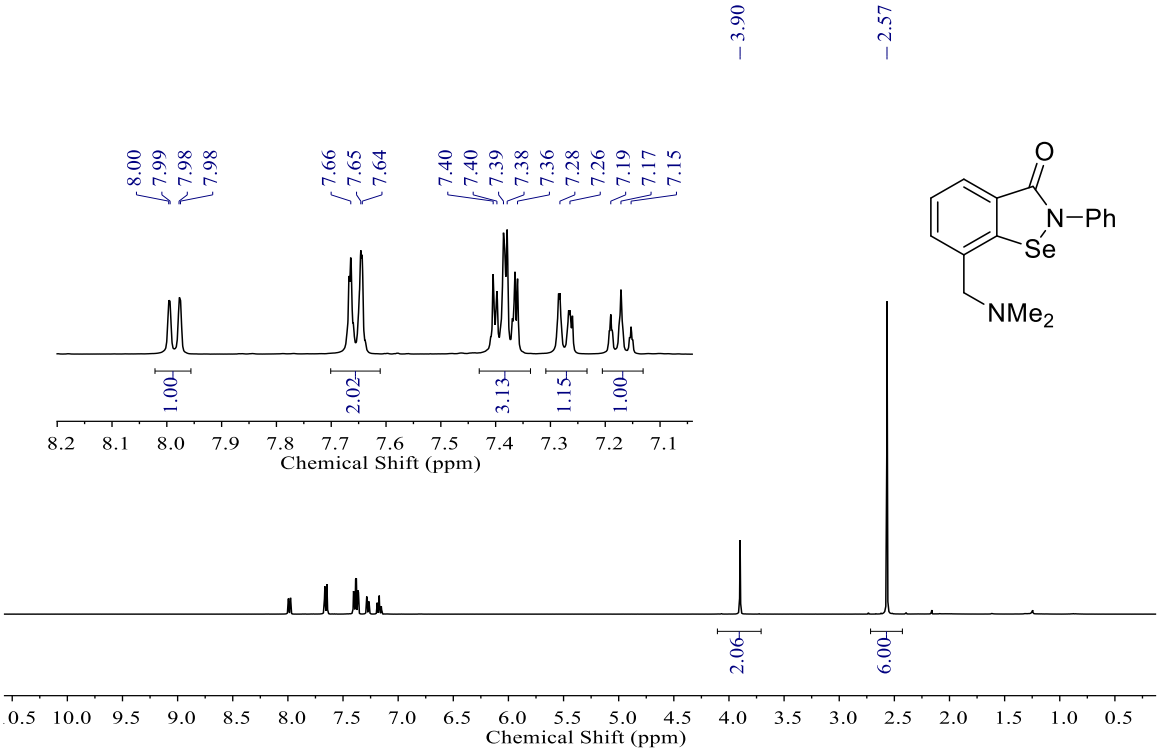


Figure 20. ^{13}C NMR Spectrum of 9 (101 MHz, $CDCl_3$)

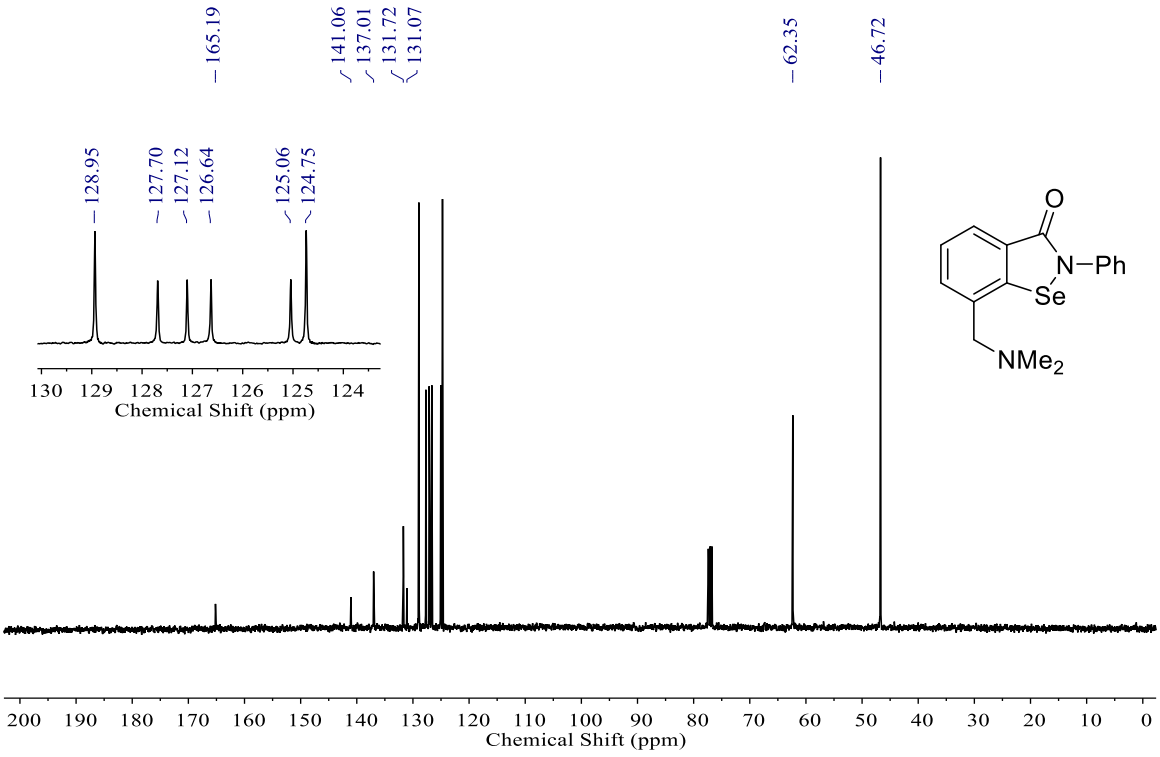


Figure 21. ^{77}Se NMR Spectrum of 9 (76 MHz, $CDCl_3$)

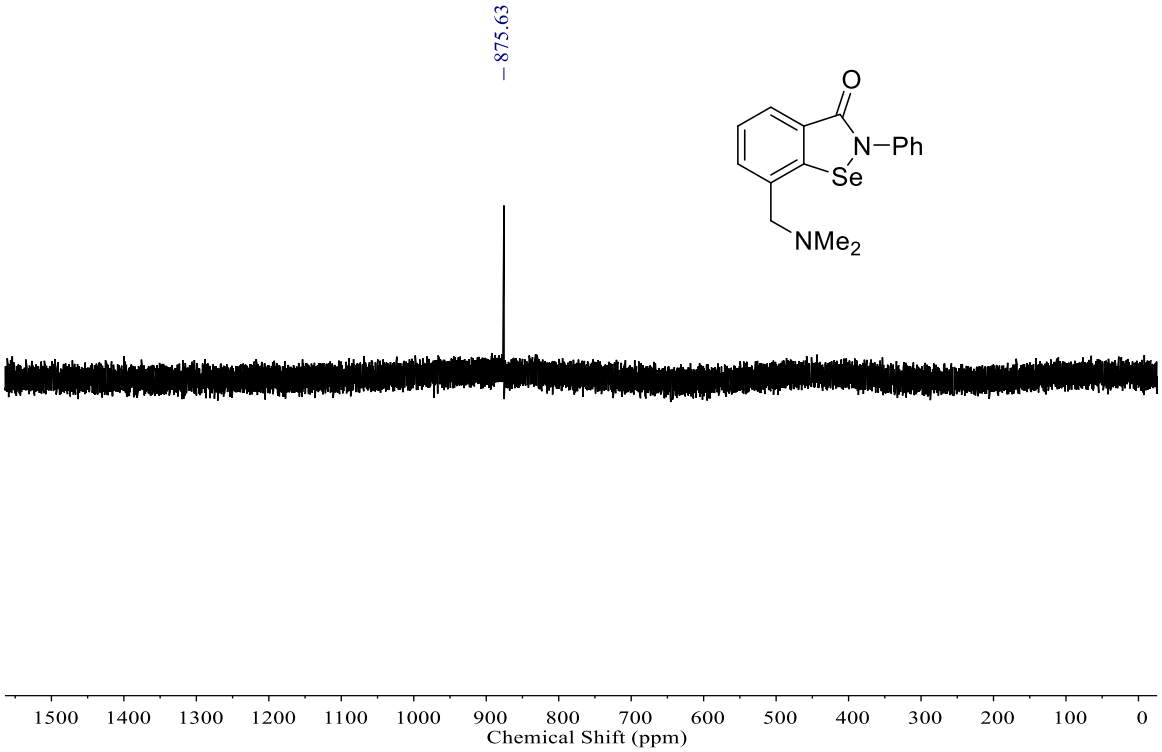


Figure 22. ^{1}H NMR Spectrum of 10 (400 MHz, $CDCl_3$)

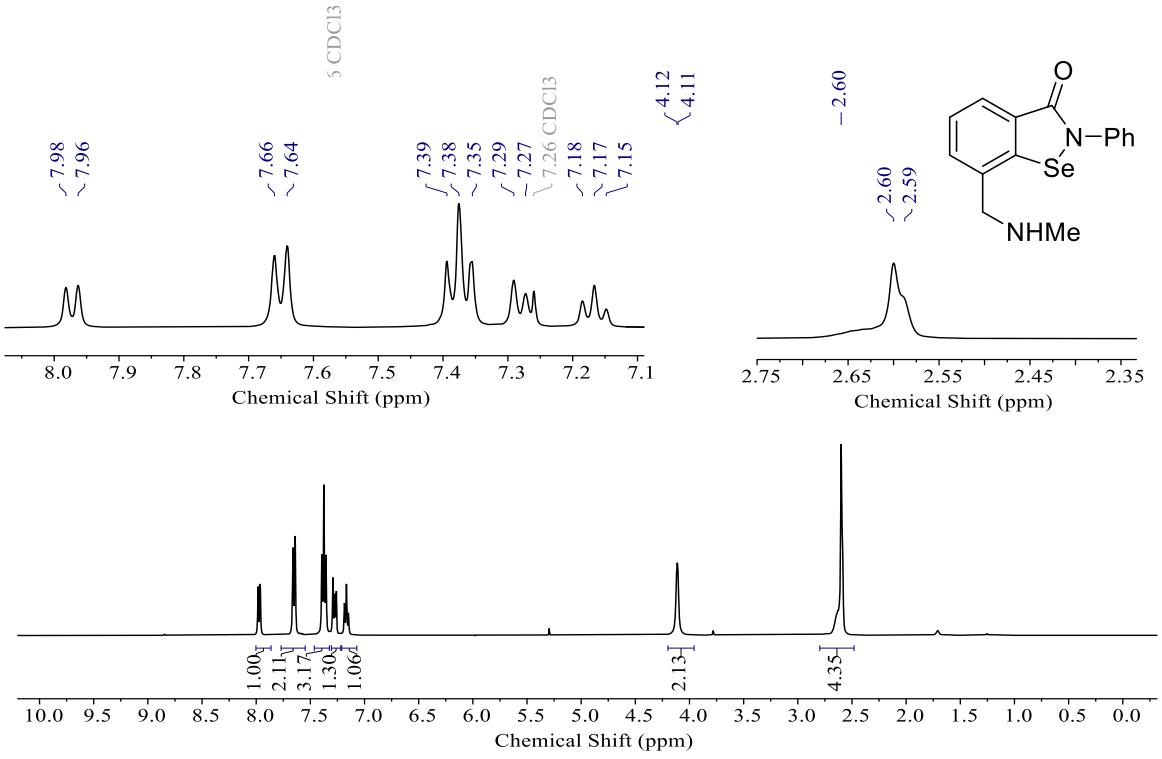


Figure 23. ^{13}C NMR Spectrum of 10 (101 MHz, $CDCl_3$)

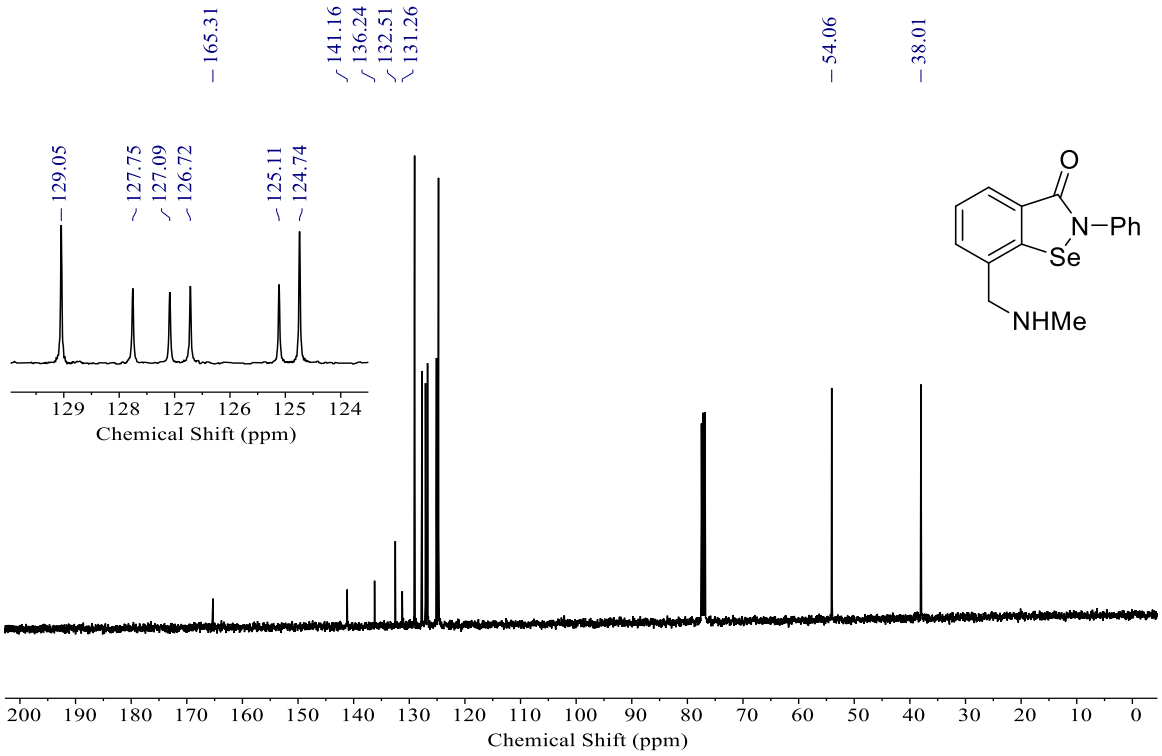


Figure 24. ^{77}Se NMR Spectrum of 10 (76 MHz, $CDCl_3$)

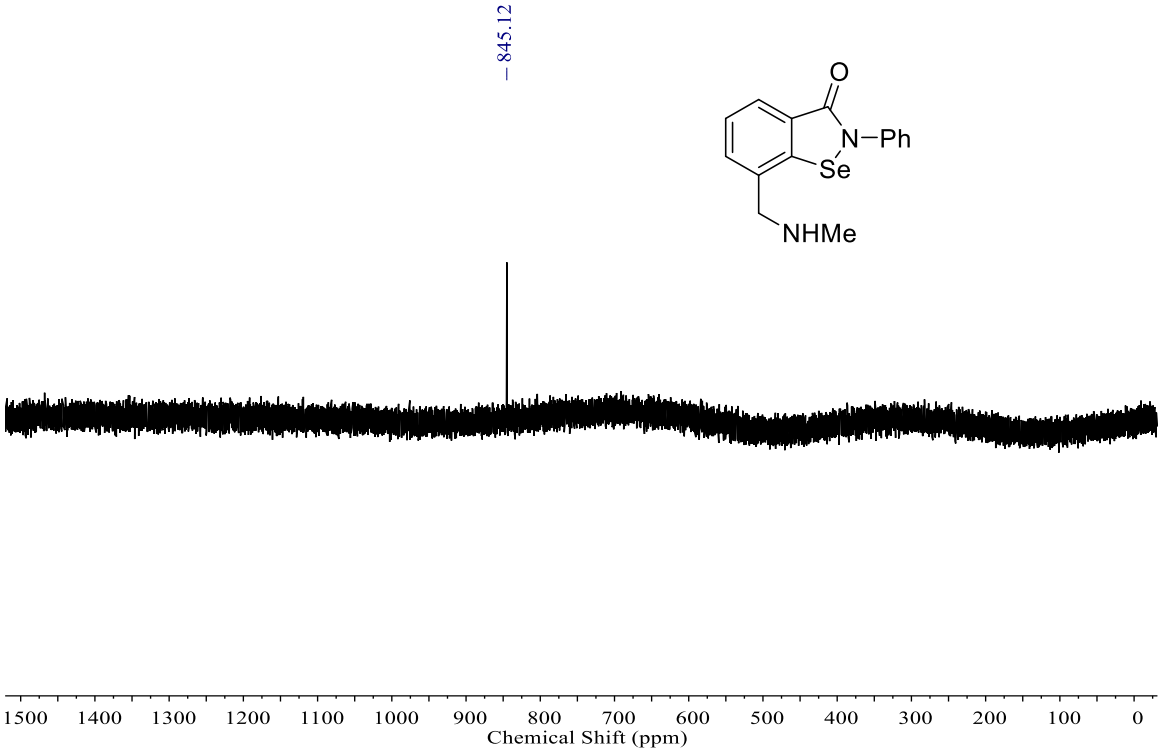


Figure 25. ^{1}H NMR Spectrum of 11 (400 MHz, $CDCl_3$)

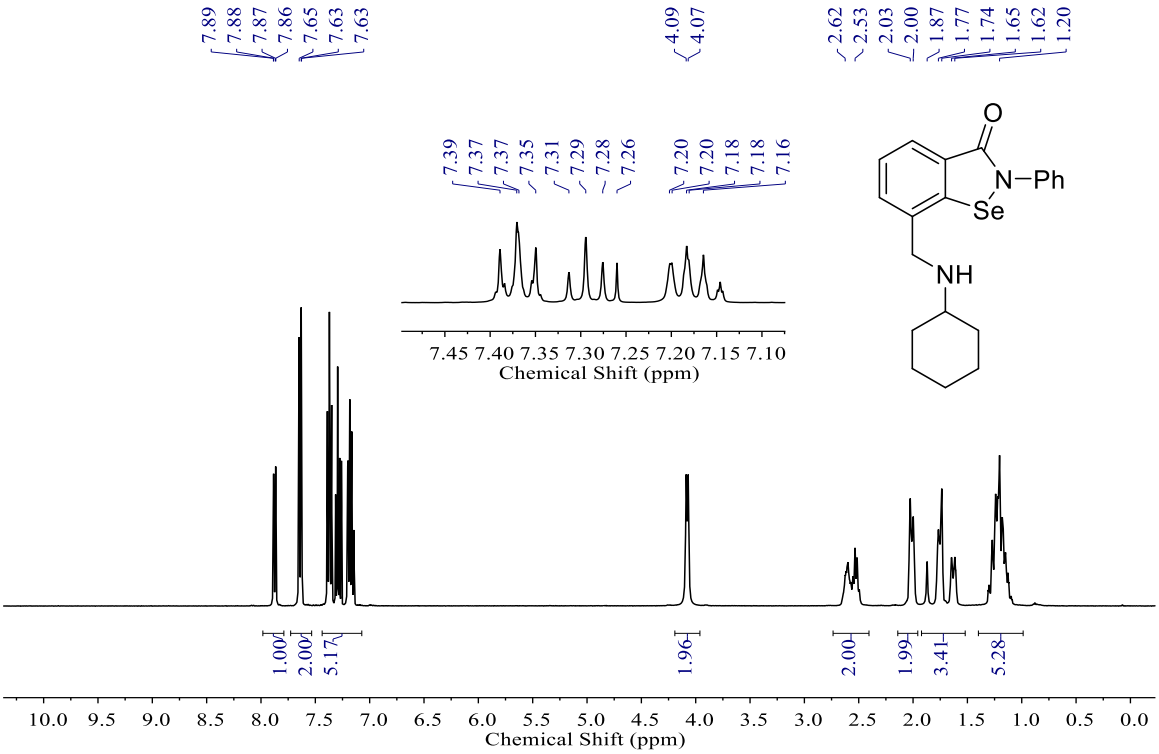


Figure 26. ^{13}C NMR Spectrum of 11 (101 MHz, $CDCl_3$)

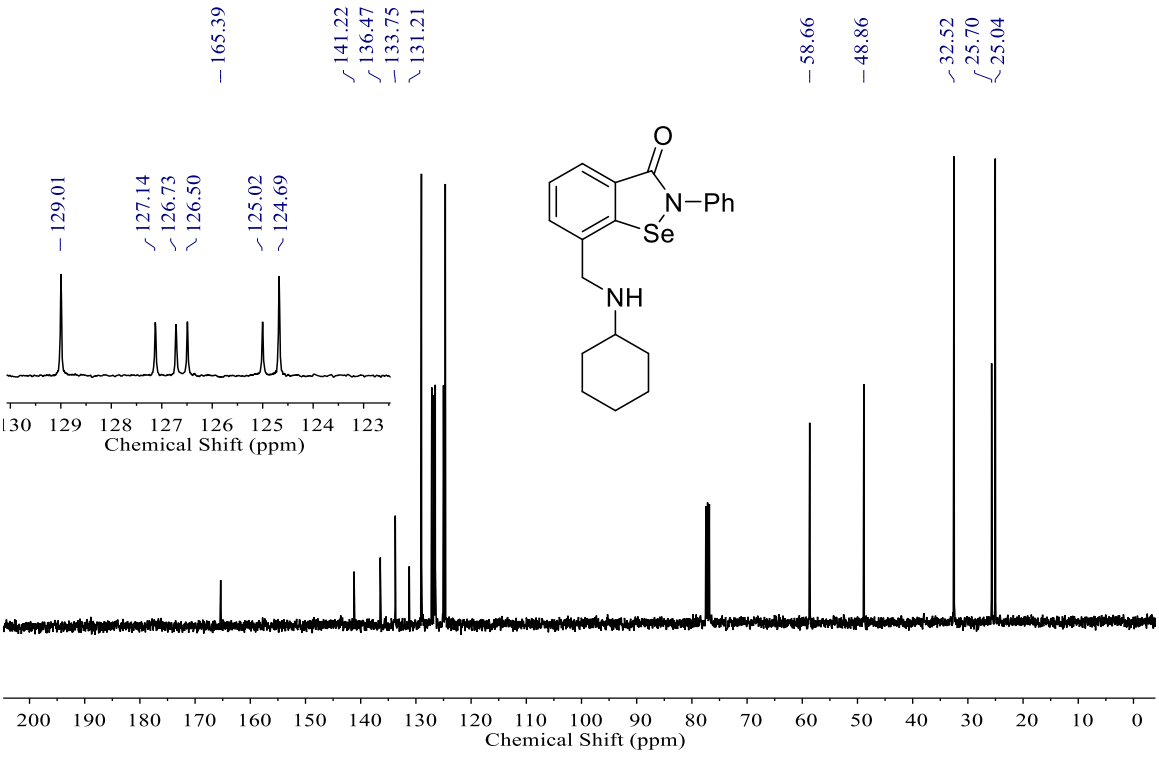
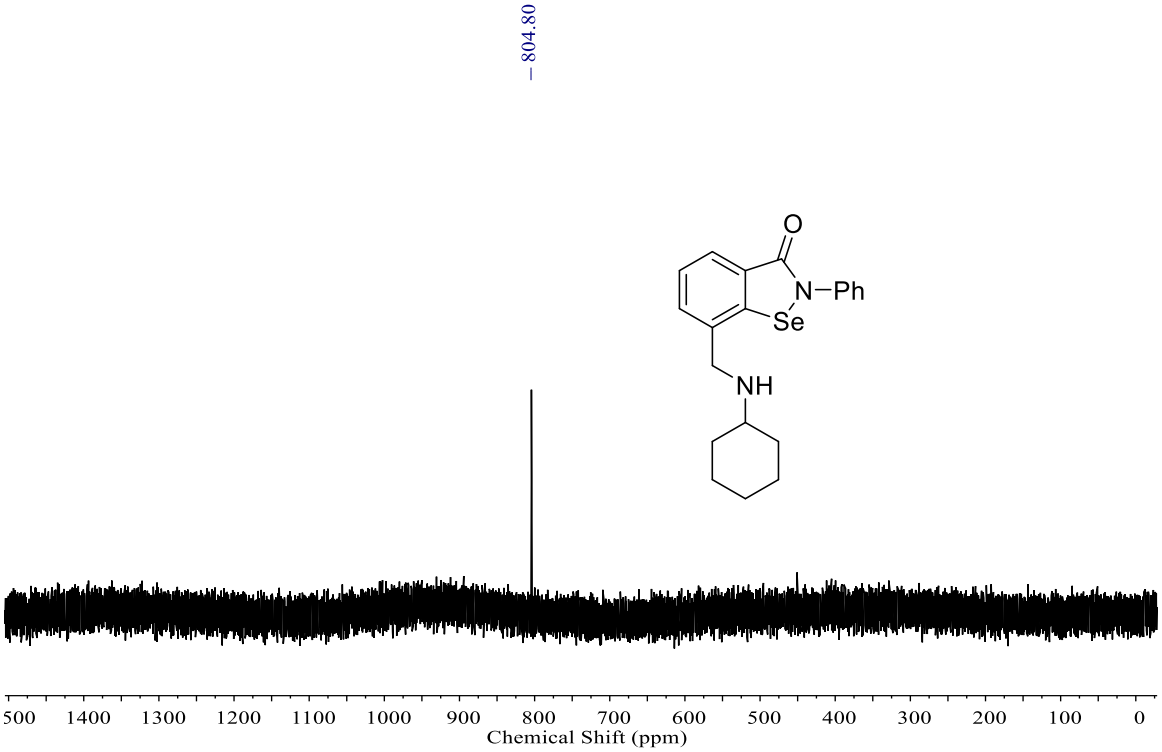


Figure 27. ^{77}Se NMR Spectrum of 11 (76 MHz, $CDCl_3$)



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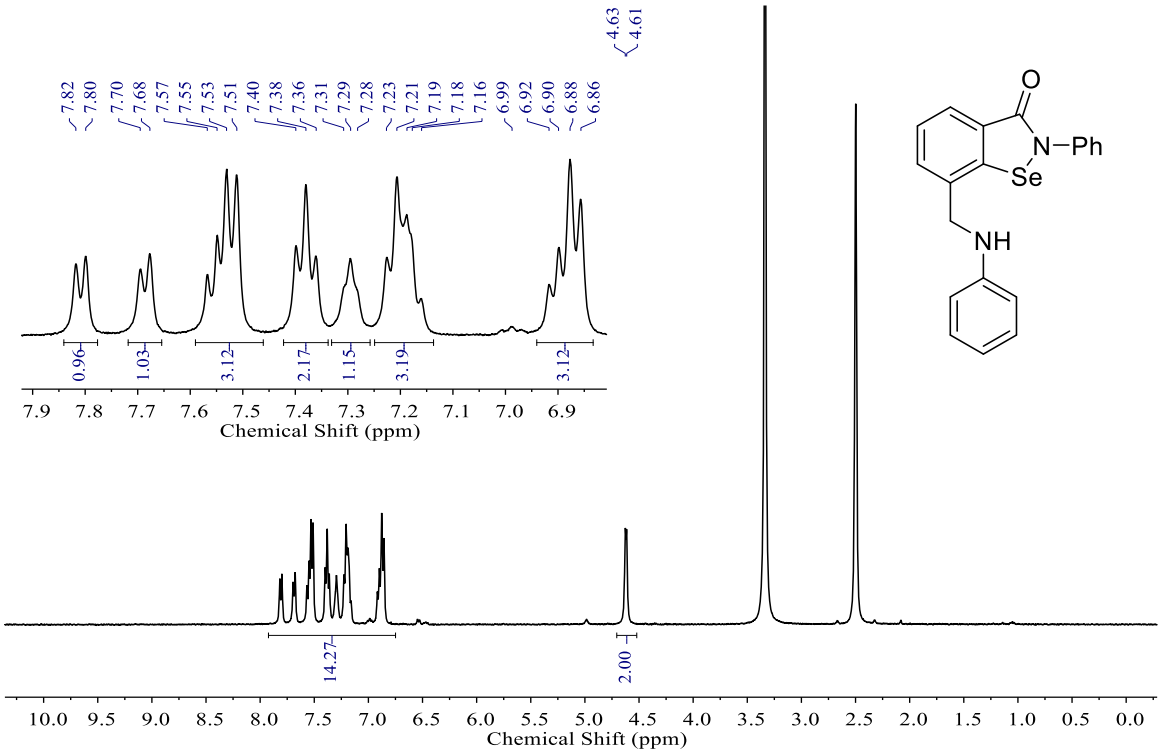


Figure 29. ^{13}C NMR Spectrum of 12 (101 MHz, DMSO-d_6)

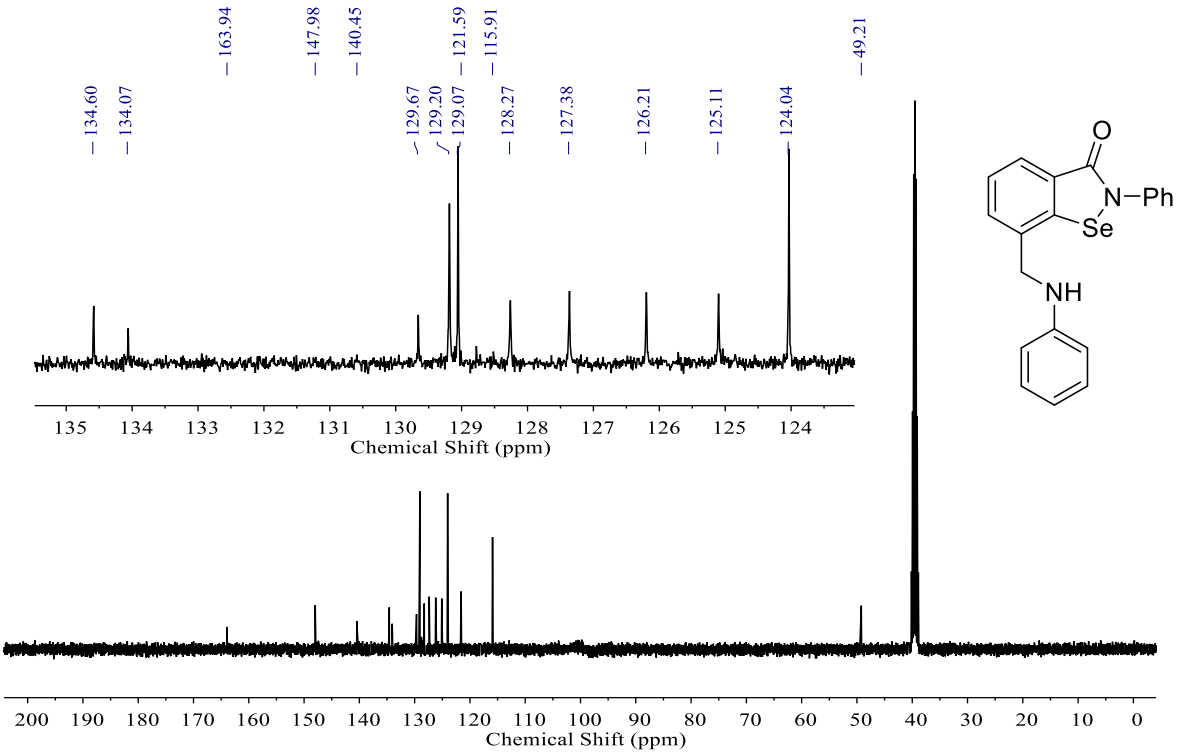


Figure 30. ^{77}Se NMR Spectrum of 12 (76 MHz, DMSO-d_6)

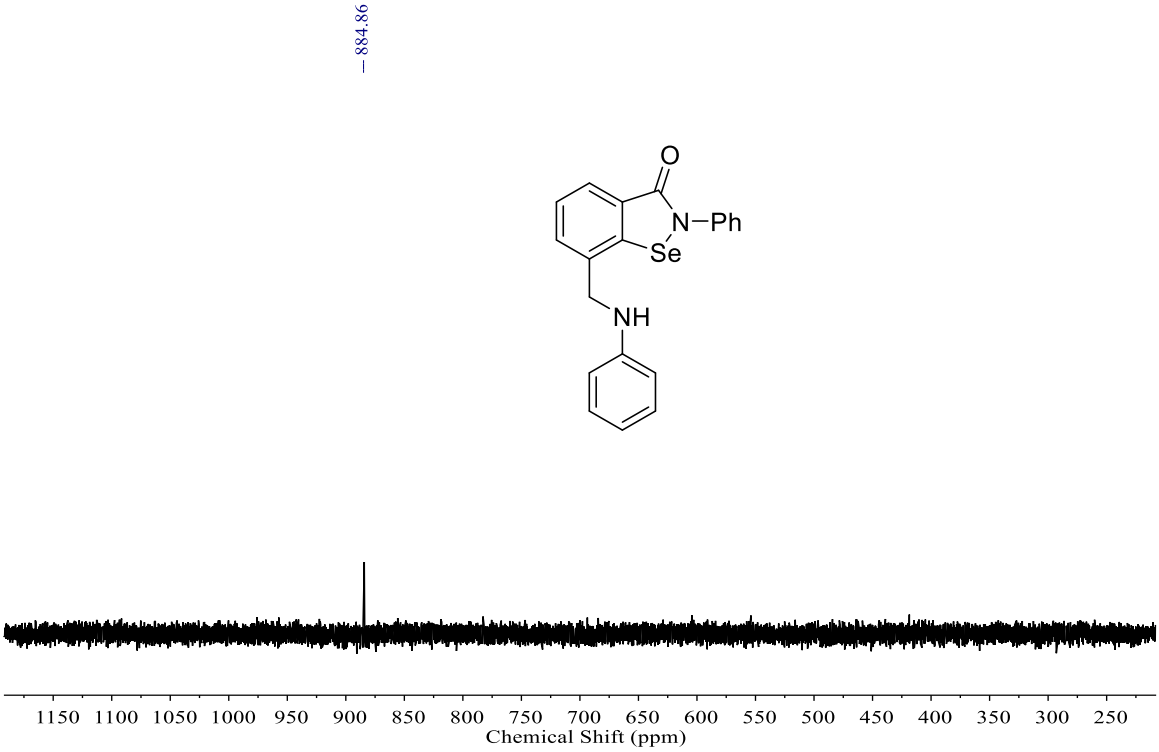


Figure 31. ^{1}H NMR Spectrum of 13 (400 MHz, DMSO-d$_6$)

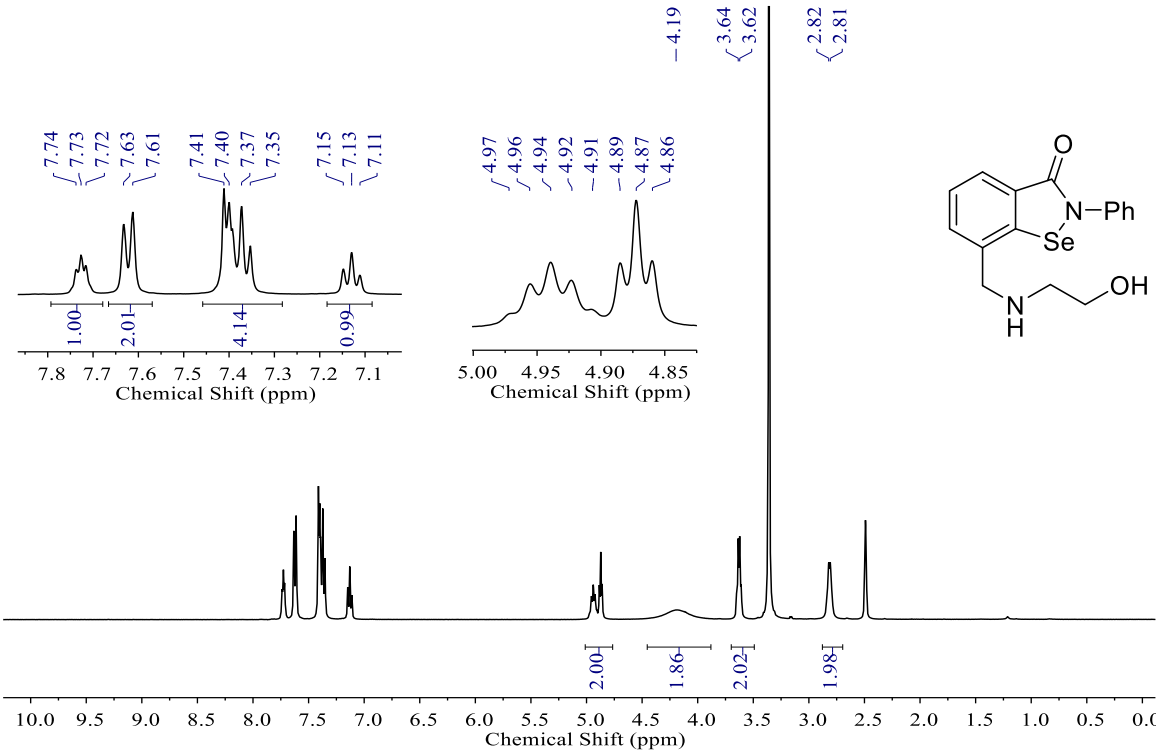


Figure 32. ^{13}C NMR Spectrum of 13 (101 MHz, DMSO-d$_6$)

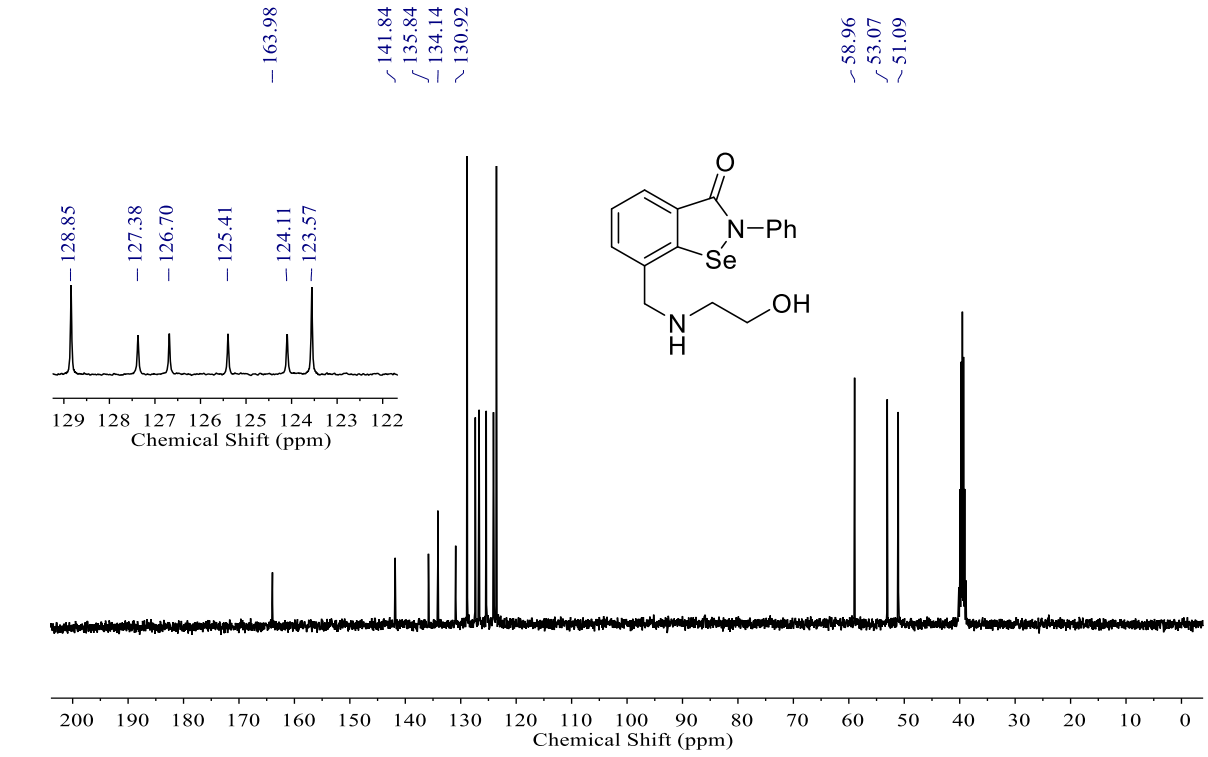


Figure 33. ^{77}Se NMR Spectrum of 13 (76 MHz, $CDCl_3$)

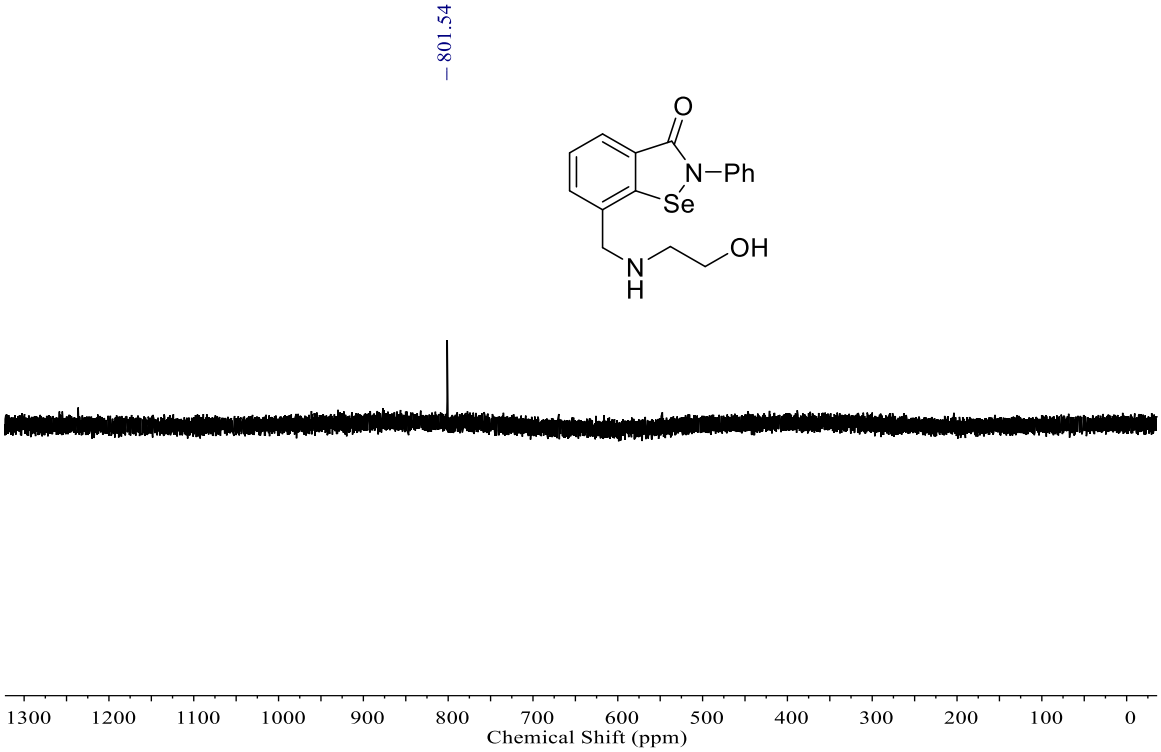


Figure 34. ^{1}H NMR Spectrum of 14 (400 MHz, $CDCl_3$)

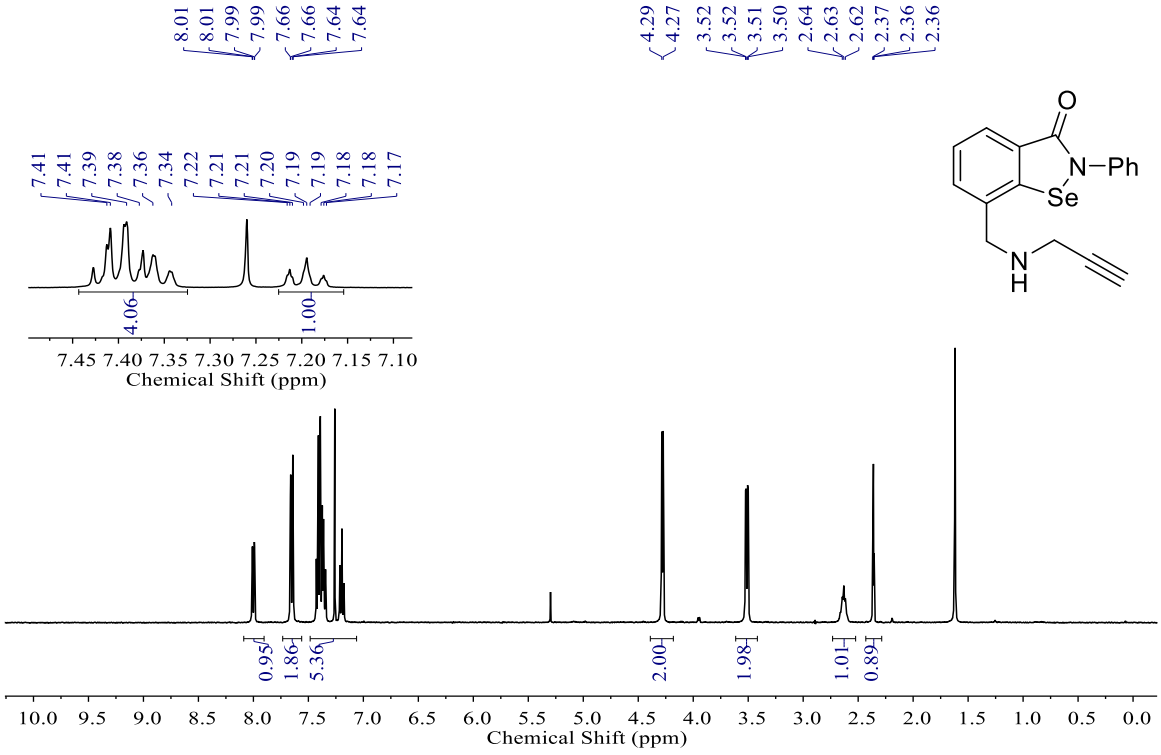


Figure 35. ^{13}C NMR Spectrum of 14 (101 MHz, DMSO-d$_6$)

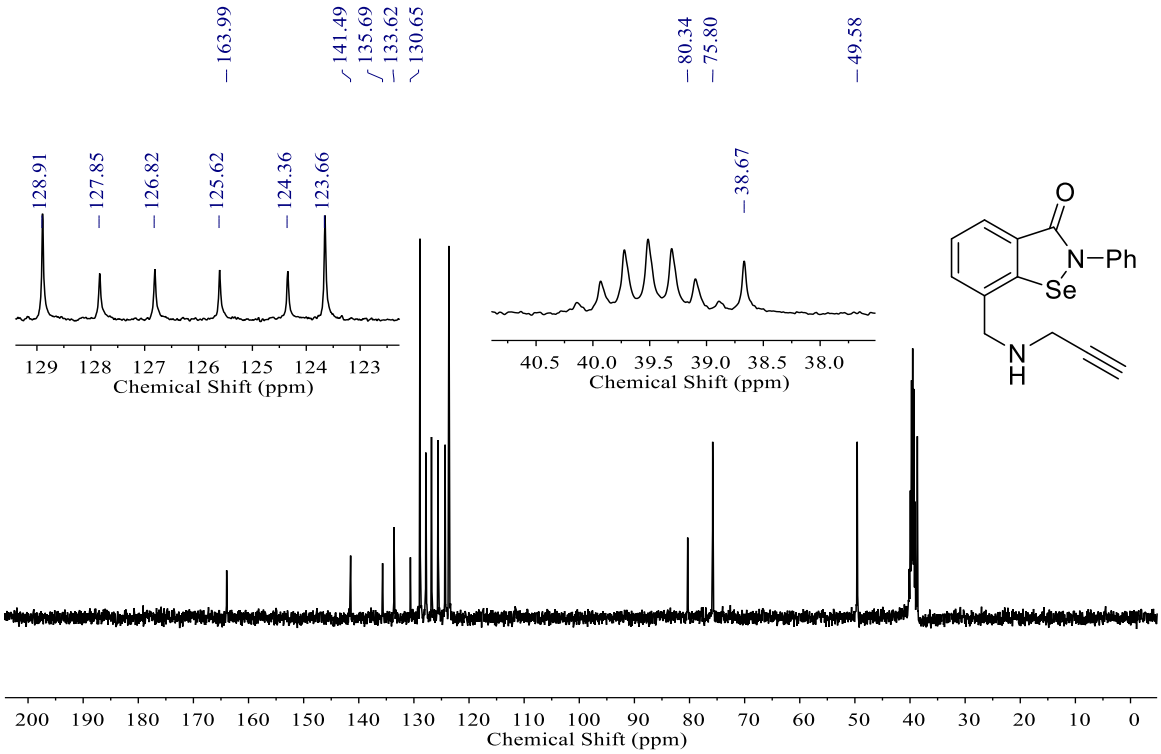


Figure 36. ^{77}Se NMR Spectrum of 14 (76 MHz, DMSO-d$_6$)

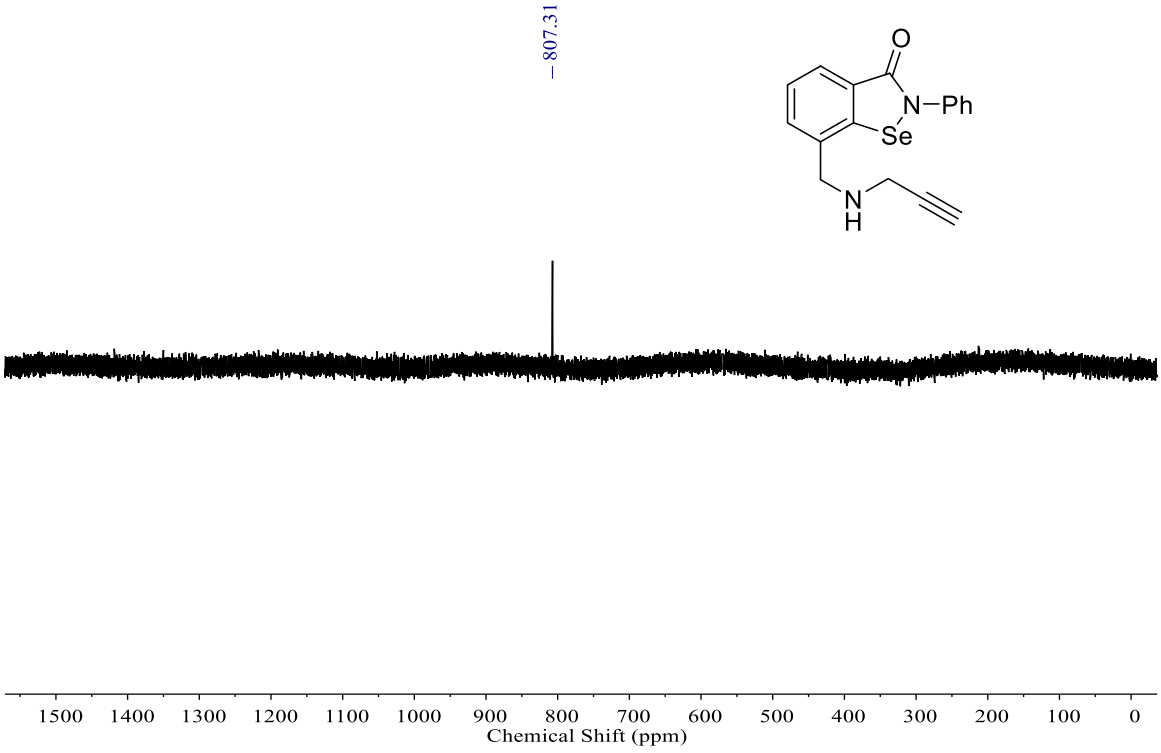


Figure 37. ^{1}H NMR Spectrum of 15 (400 MHz, $CDCl_3$)

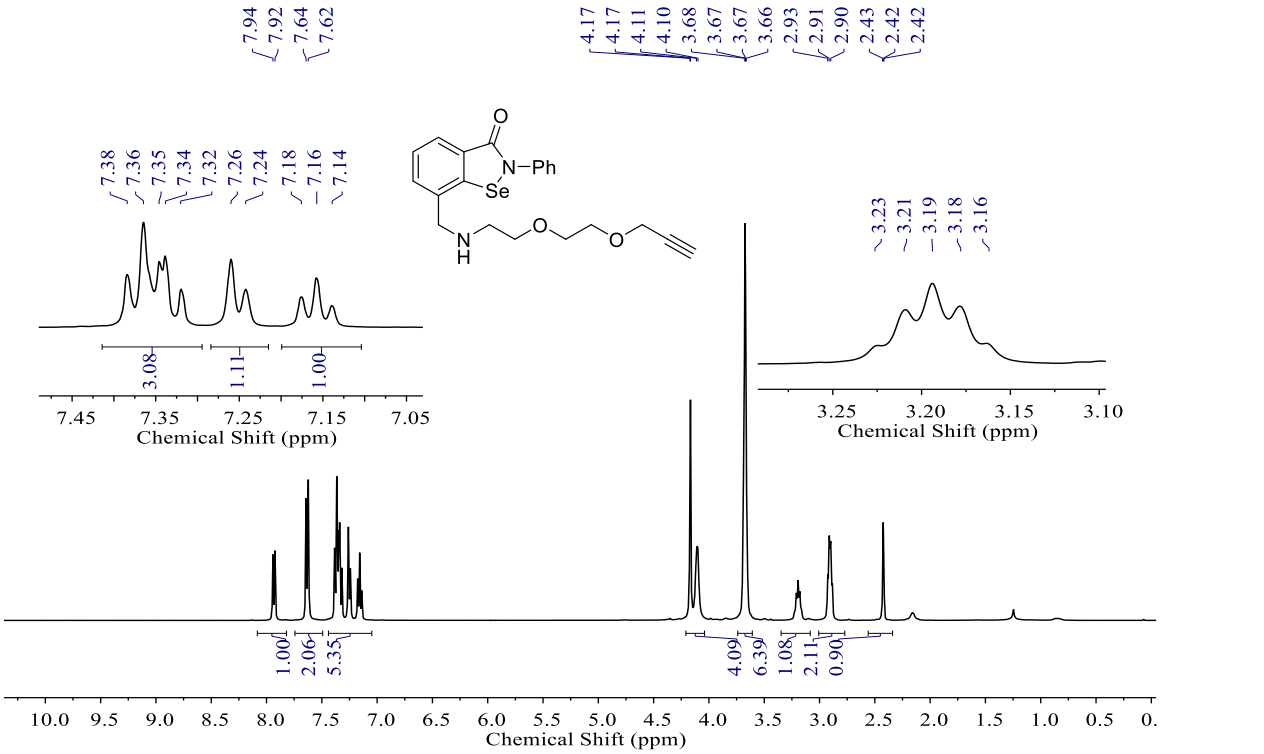


Figure 38. ^{13}C NMR Spectrum of 15 (101 MHz, $CDCl_3$)

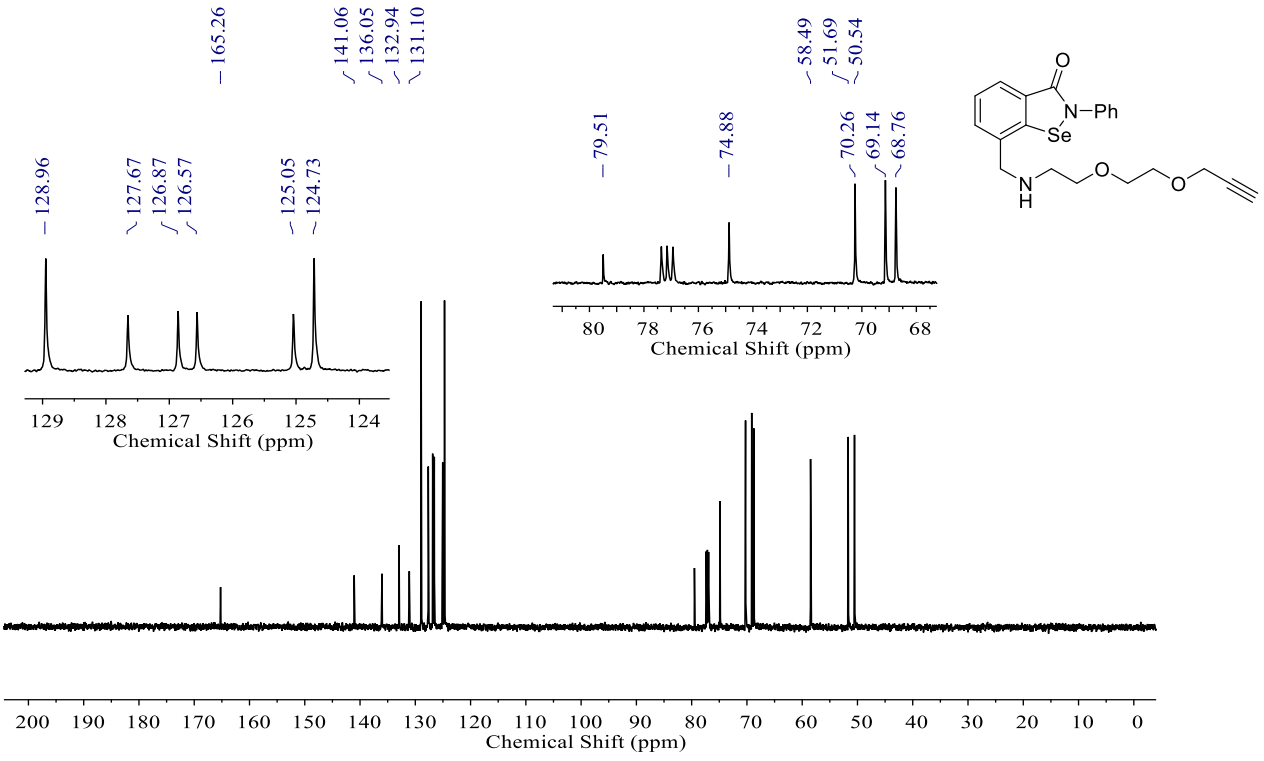


Figure 39. ^{77}Se NMR Spectrum of 15 (76 MHz, $CDCl_3$)

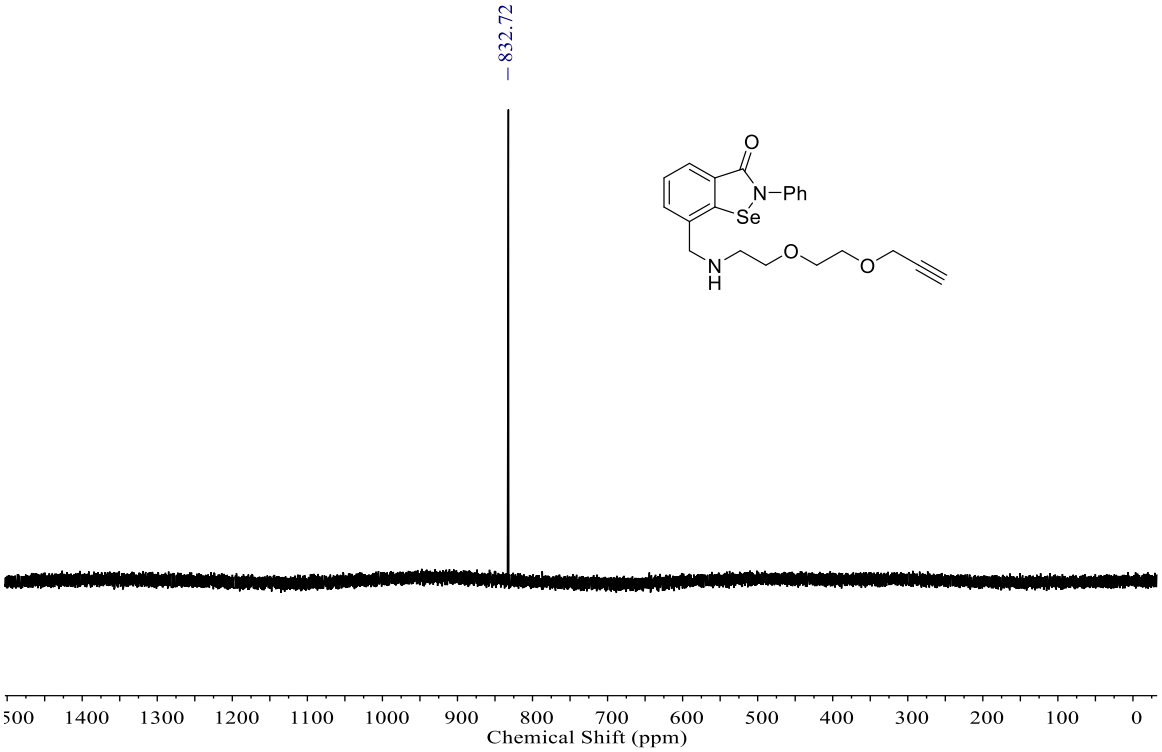


Figure 40. ^{1}H NMR Spectrum of 5 (400 MHz, DMSO-d_6)

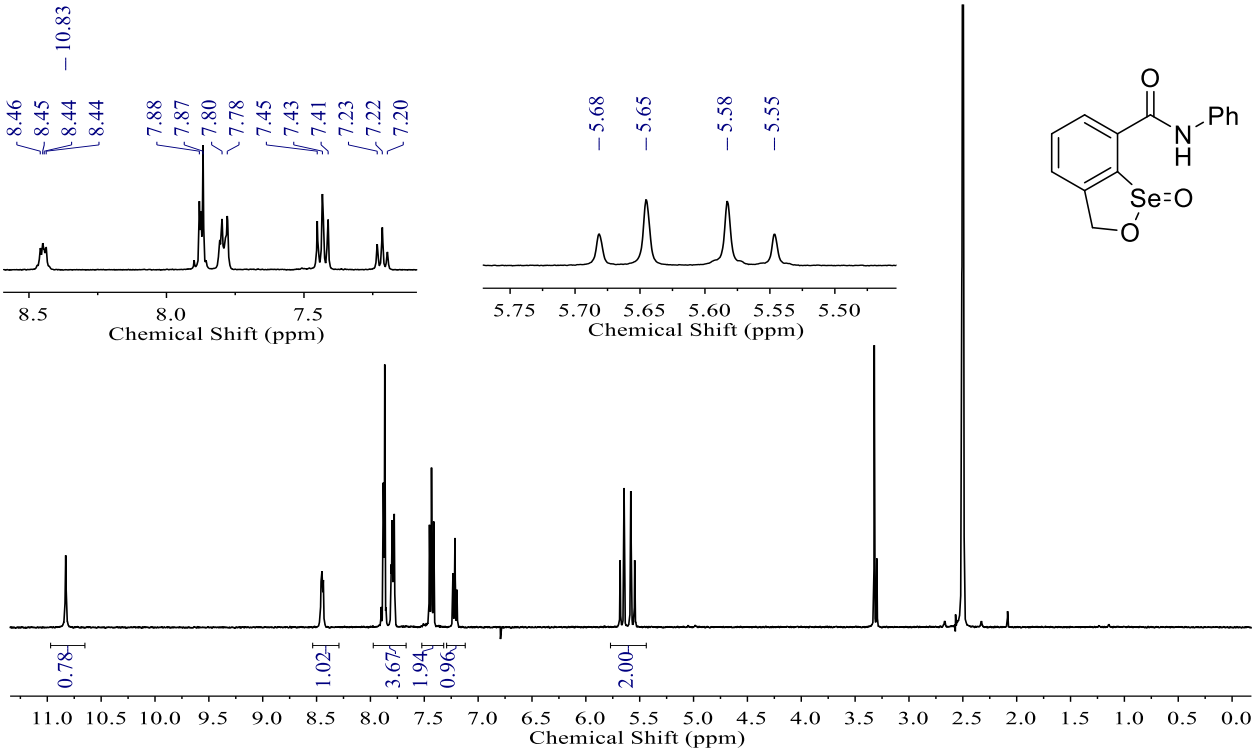


Figure 41. ^{13}C NMR Spectrum of 5 (101 MHz, DMSO-d_6)

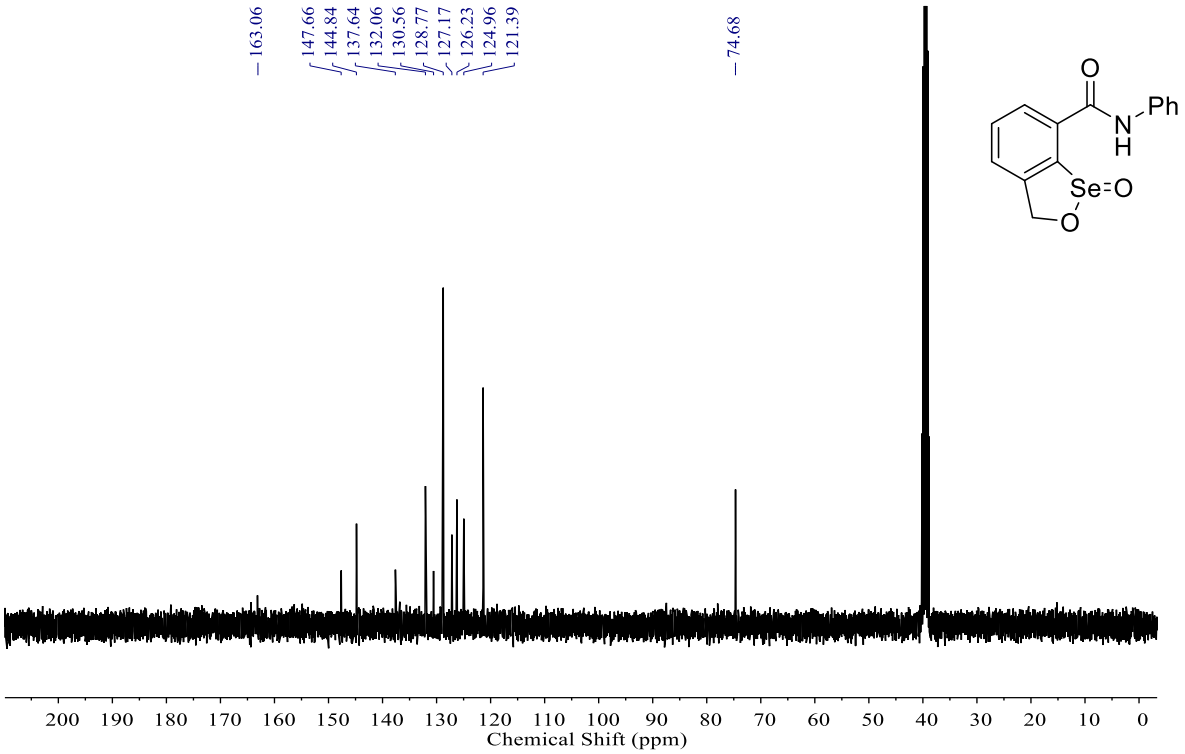


Figure 42. ^{77}Se NMR Spectrum of 5 (76 MHz, DMSO-d_6)

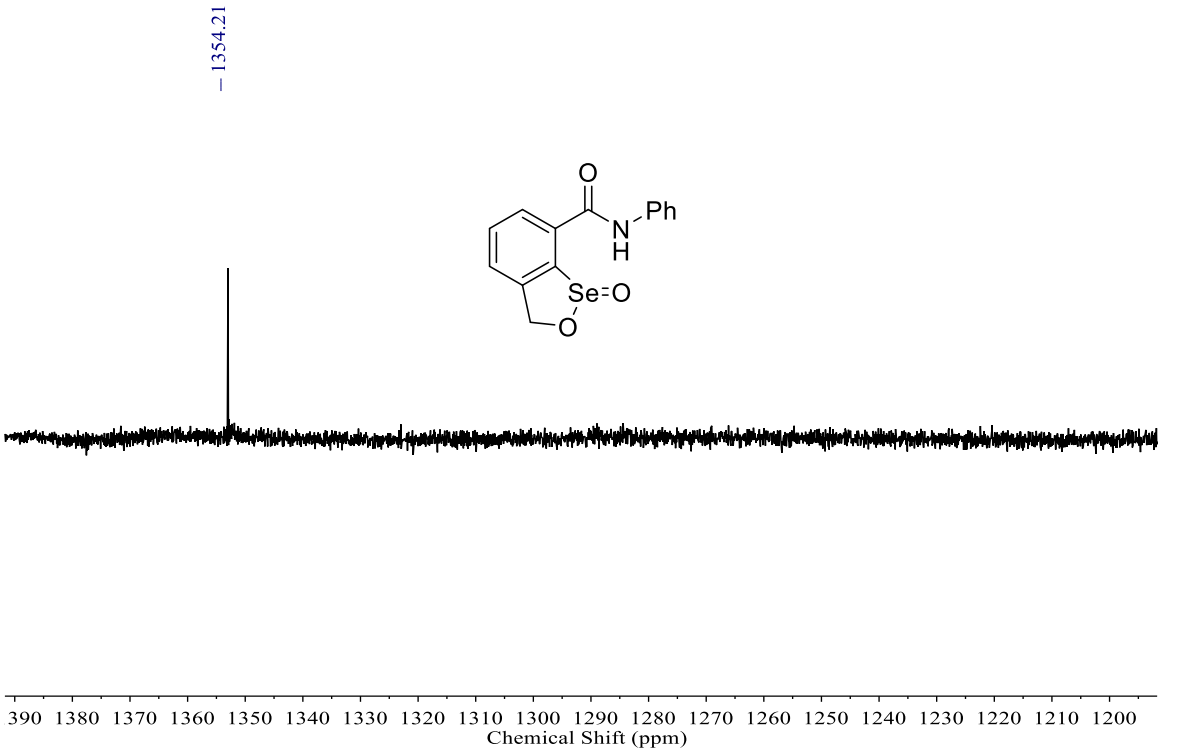


Figure 43. ^{1}H NMR Spectrum of 6 (400 MHz, CD_3OD)

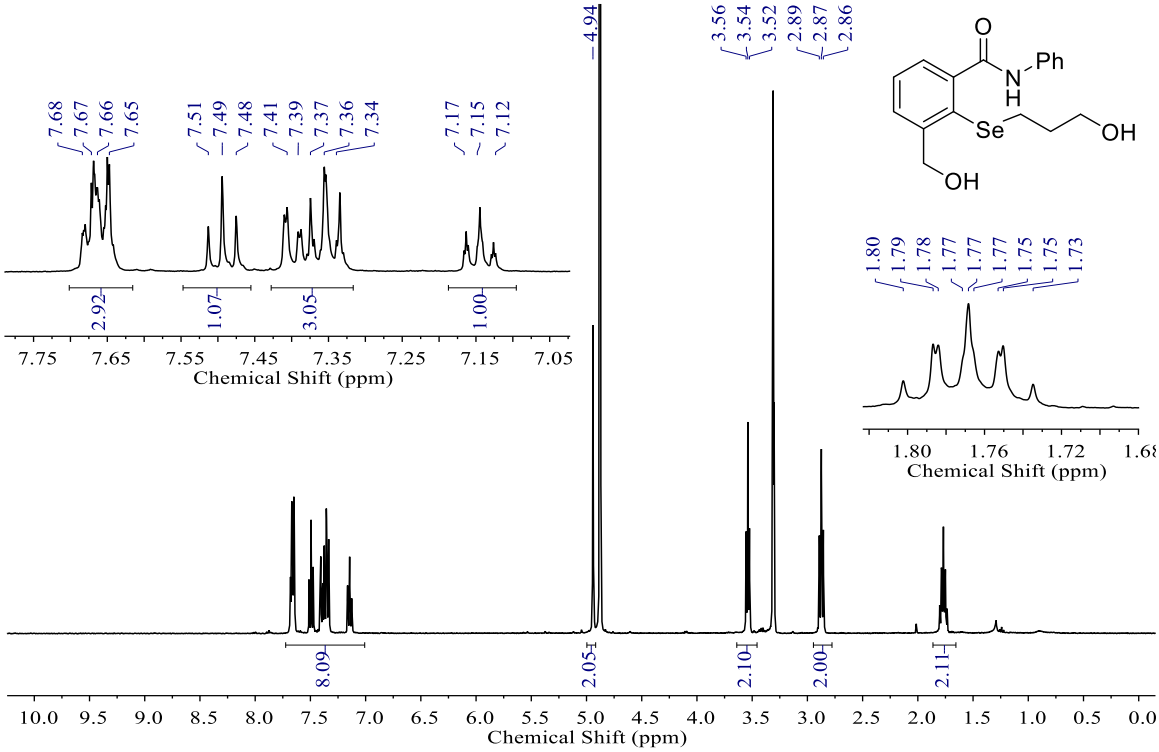


Figure 44. ^{13}C NMR Spectrum of 6 (101 MHz, CD_3OD)

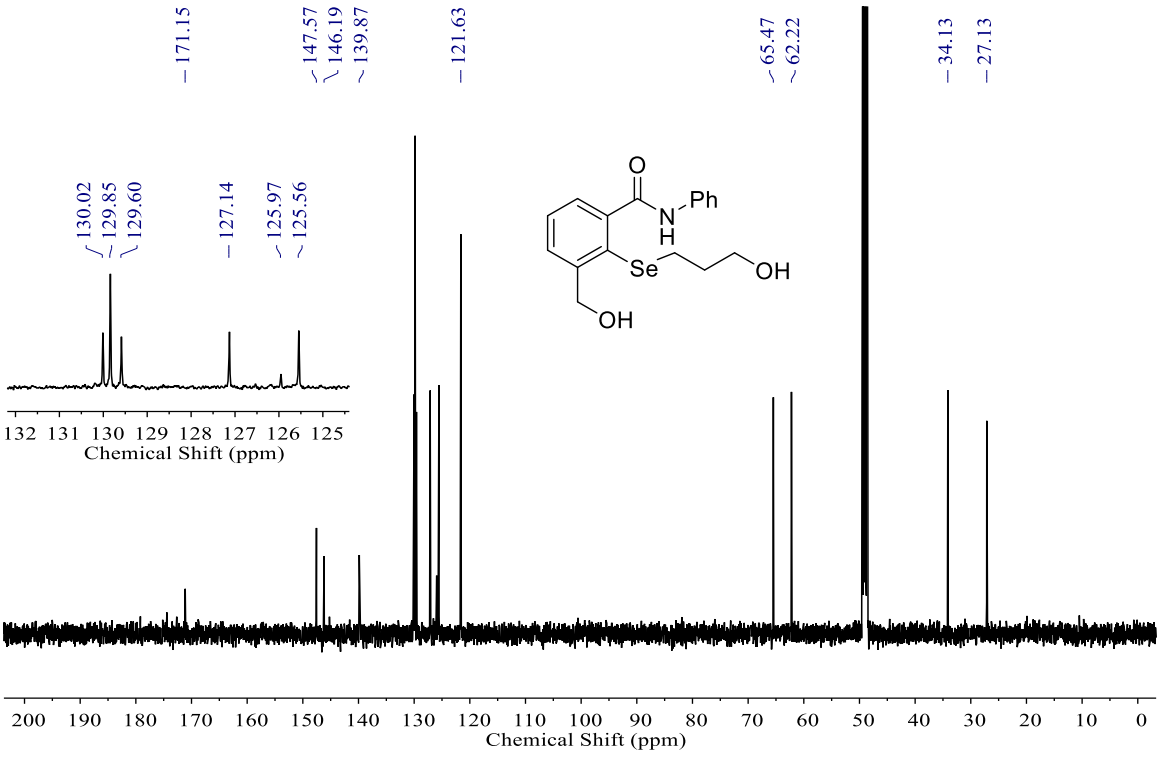


Figure 45. ^{77}Se NMR Spectrum of 6 (76 MHz, CD_3OD)

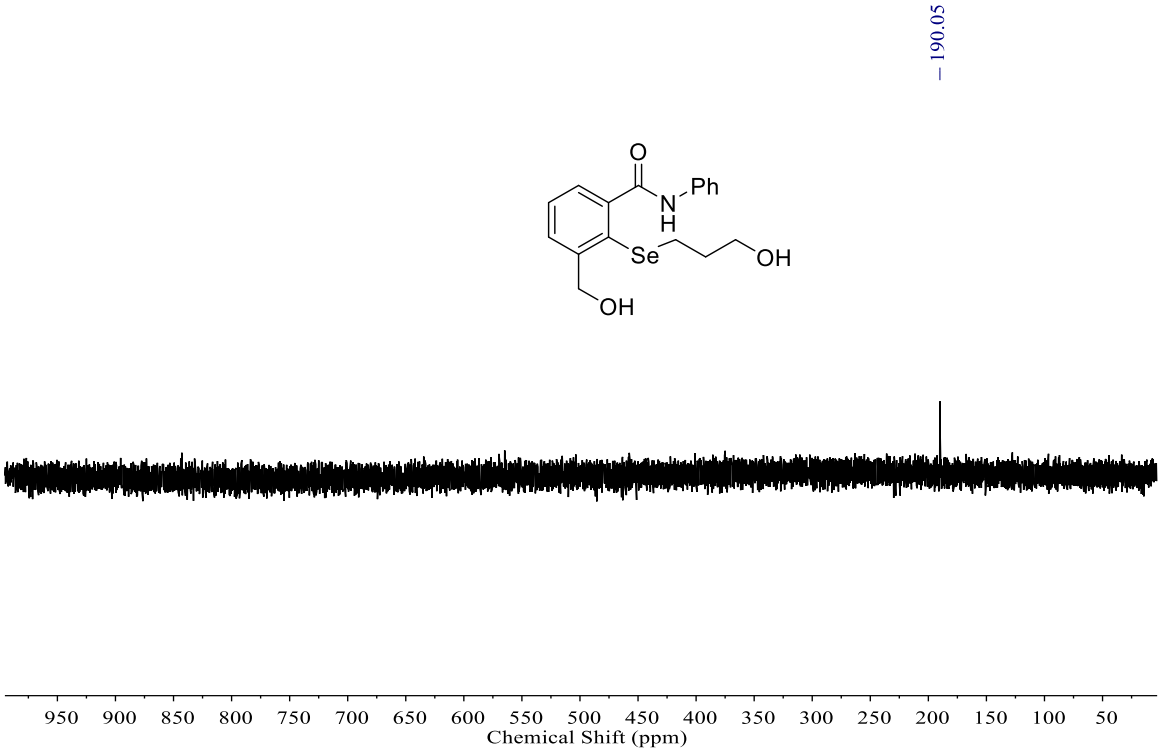


Figure 46. ^{1}H NMR Spectrum of 39 (400 MHz, $CDCl_3$)

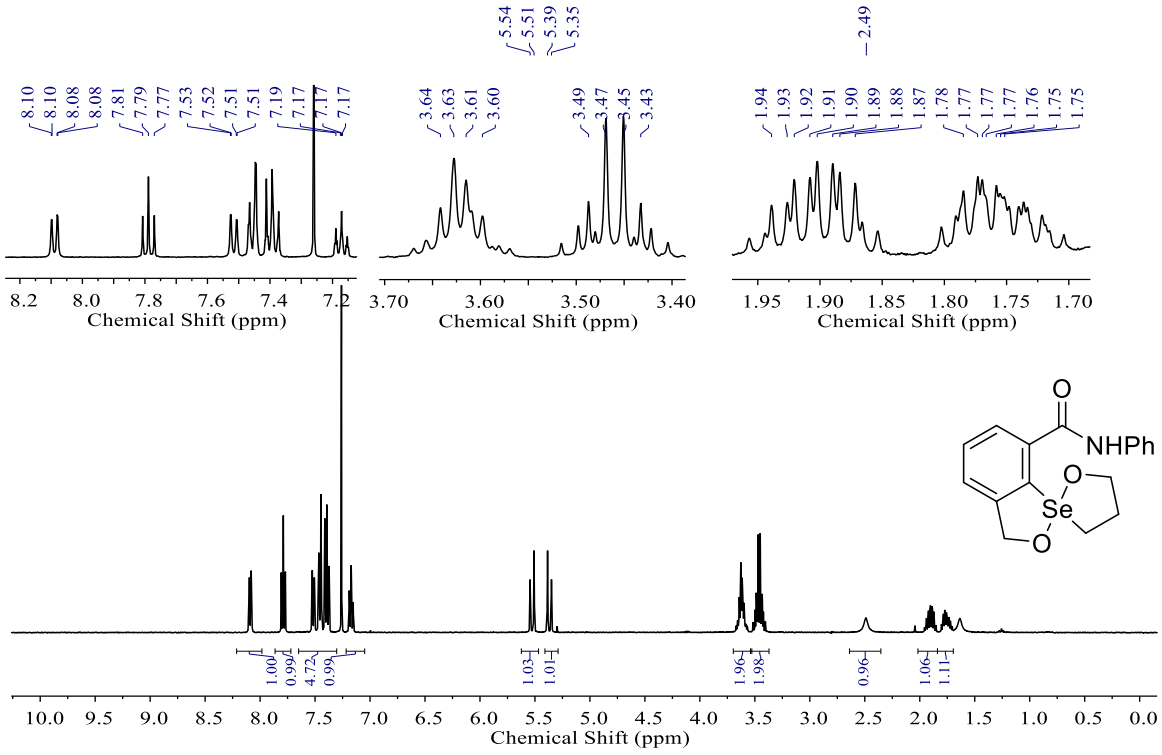


Figure 47. ^{13}C NMR Spectrum of 39 (101 MHz, $CDCl_3$)

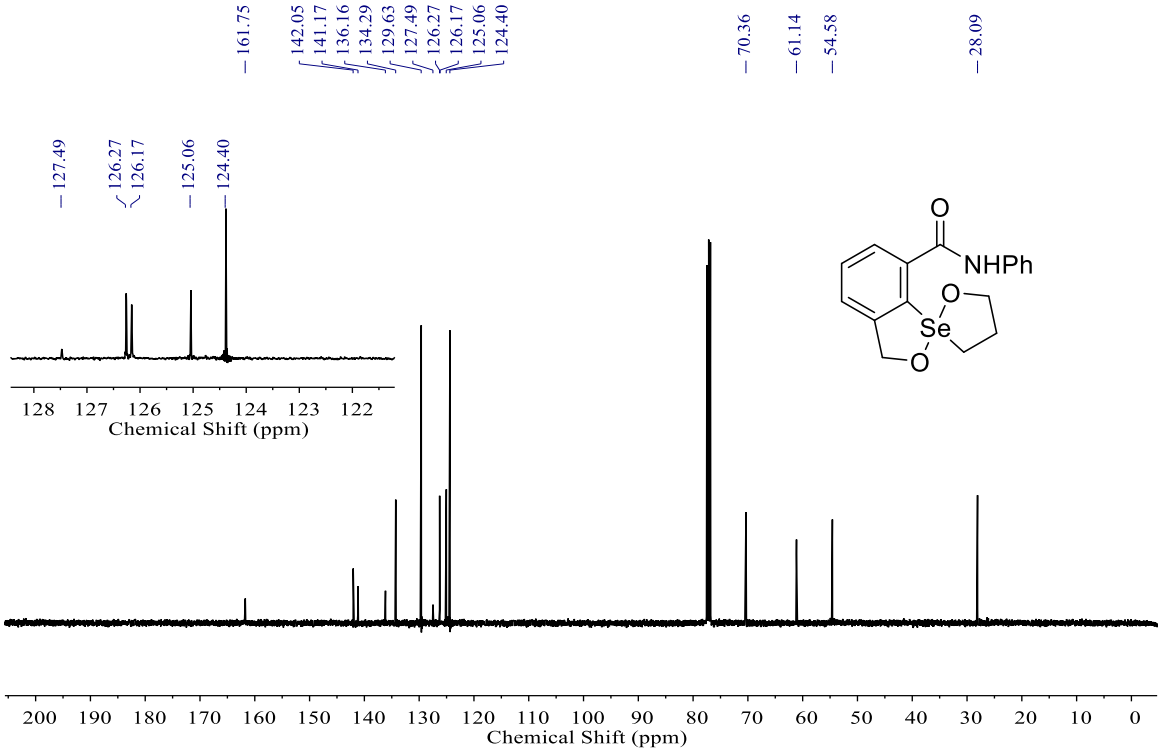


Figure 48. ^{77}Se C NMR Spectrum of 39 ($CDCl_3$, 76 MHz)

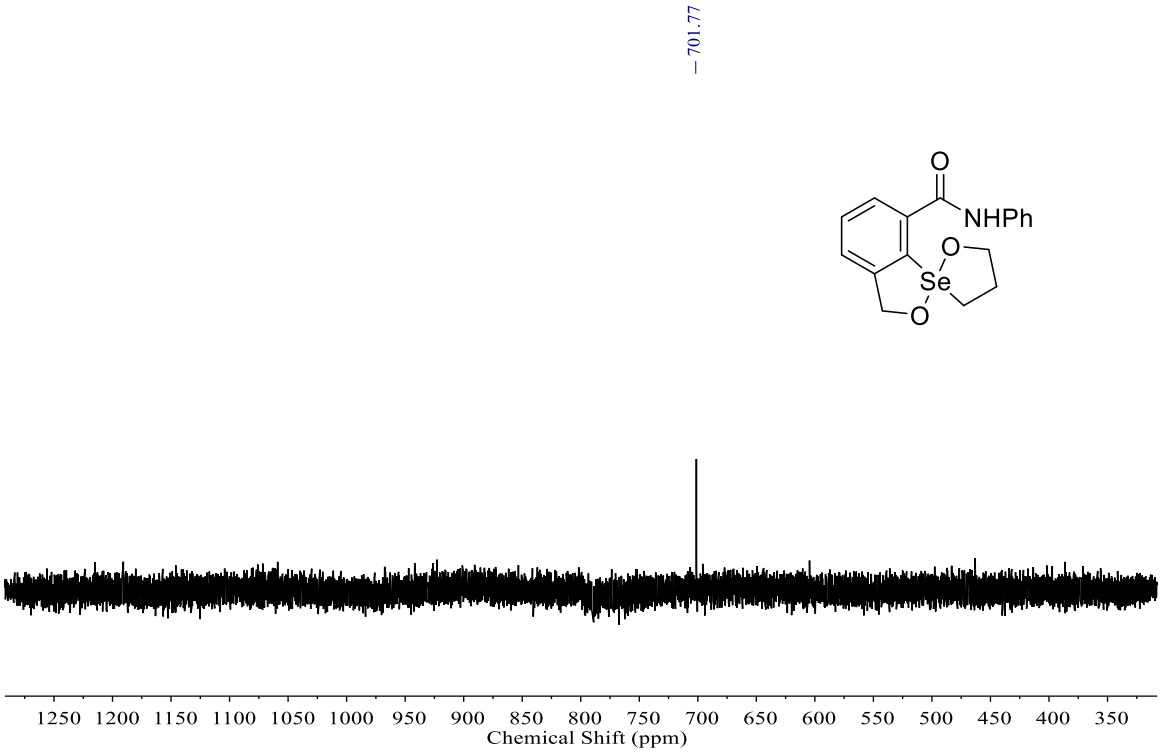


Figure 49. ^{1}H NMR Spectrum of 27 (400 MHz, DMSO-d$_6$)

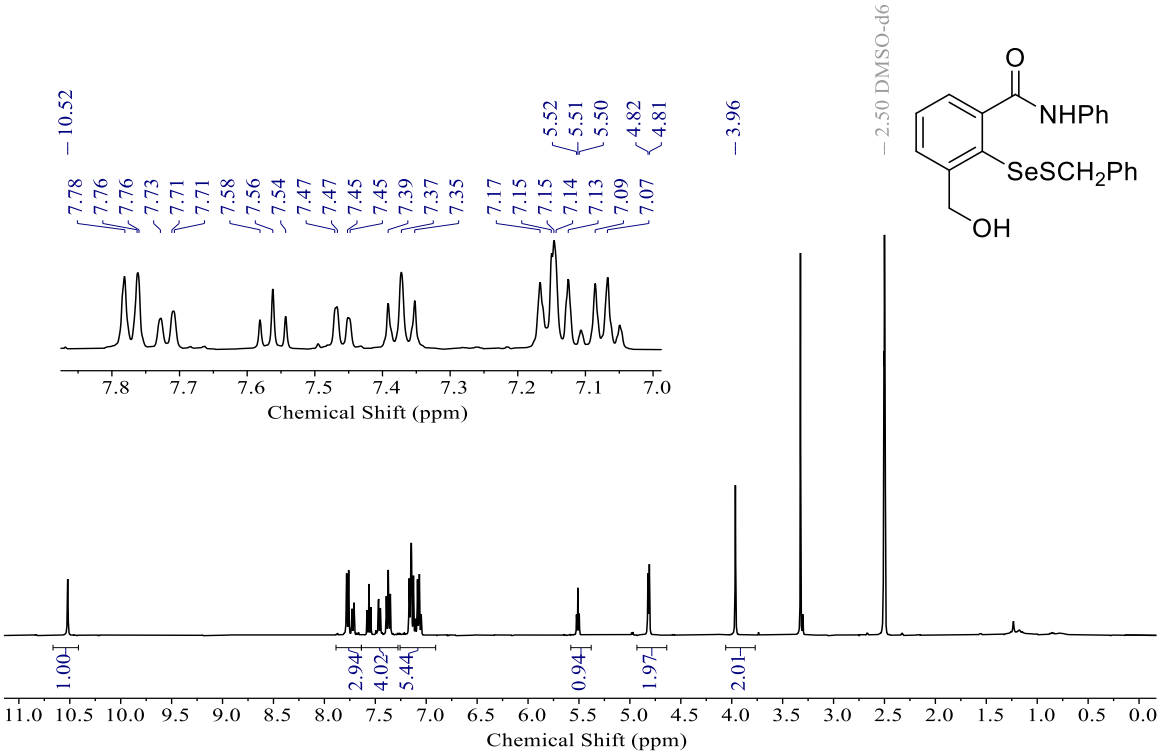


Figure 50. ^{13}C NMR Spectrum of 27 (101 MHz, DMSO-d$_6$)

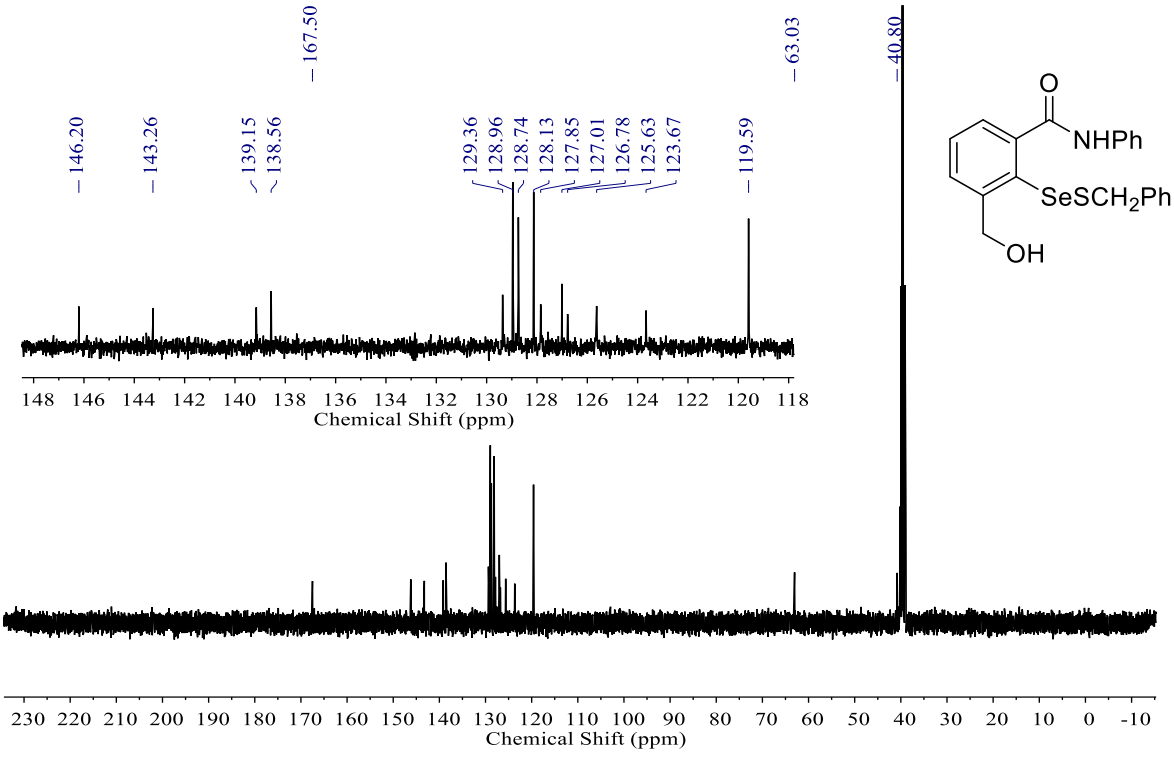


Figure 51. ^{77}Se NMR Spectrum of 27 (76 MHz, CD_3CN)

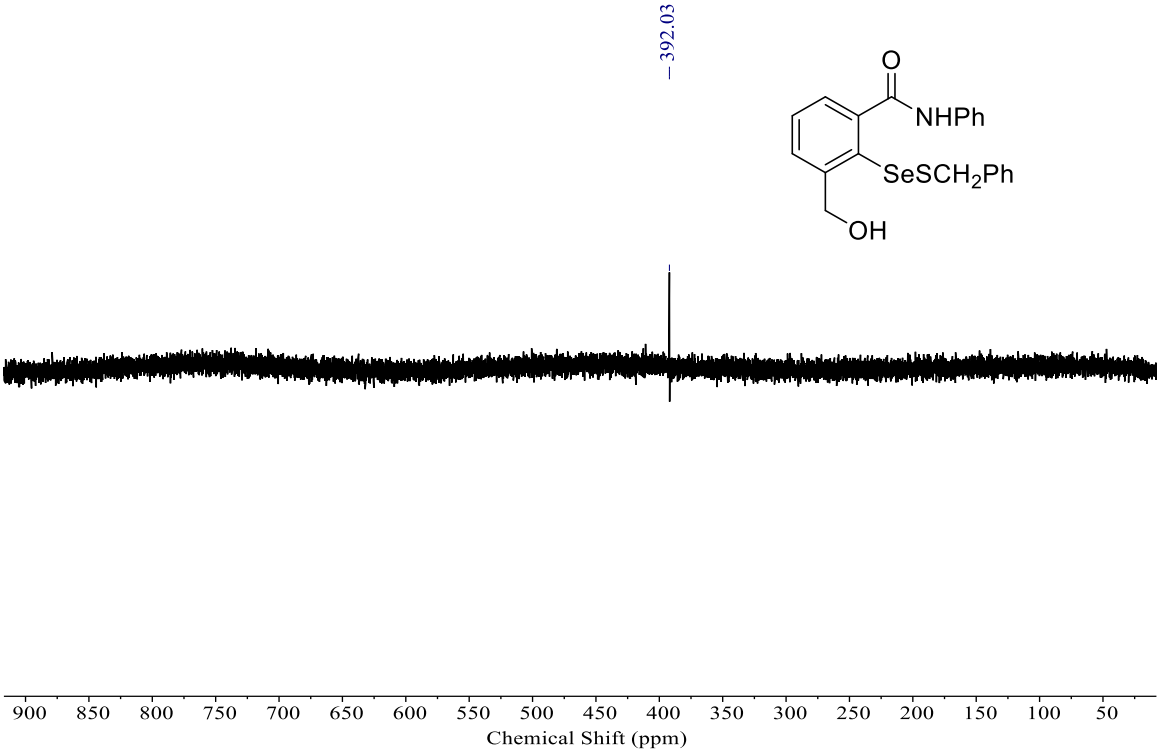


Figure 52. ^{1}H NMR Spectrum of 28 (400 MHz, DMSO-d_6)

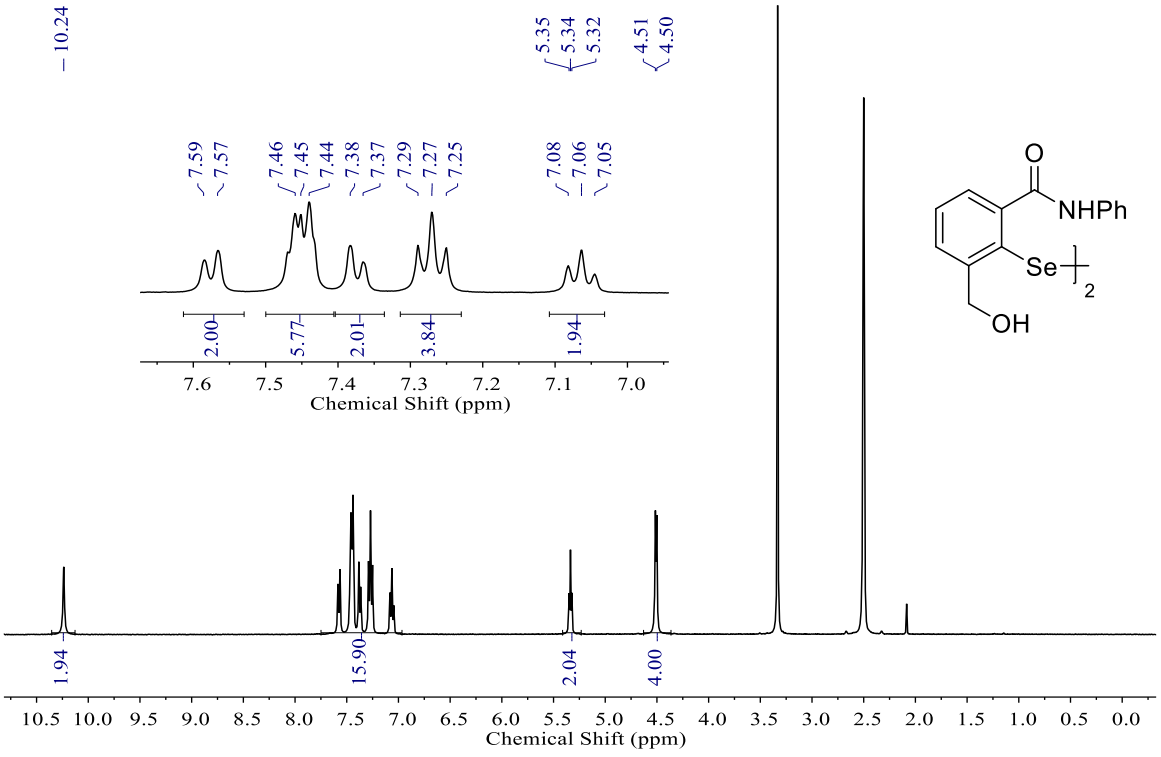


Figure 53. ^{13}C NMR Spectrum of 28 (101 MHz, DMSO-d$_6$)

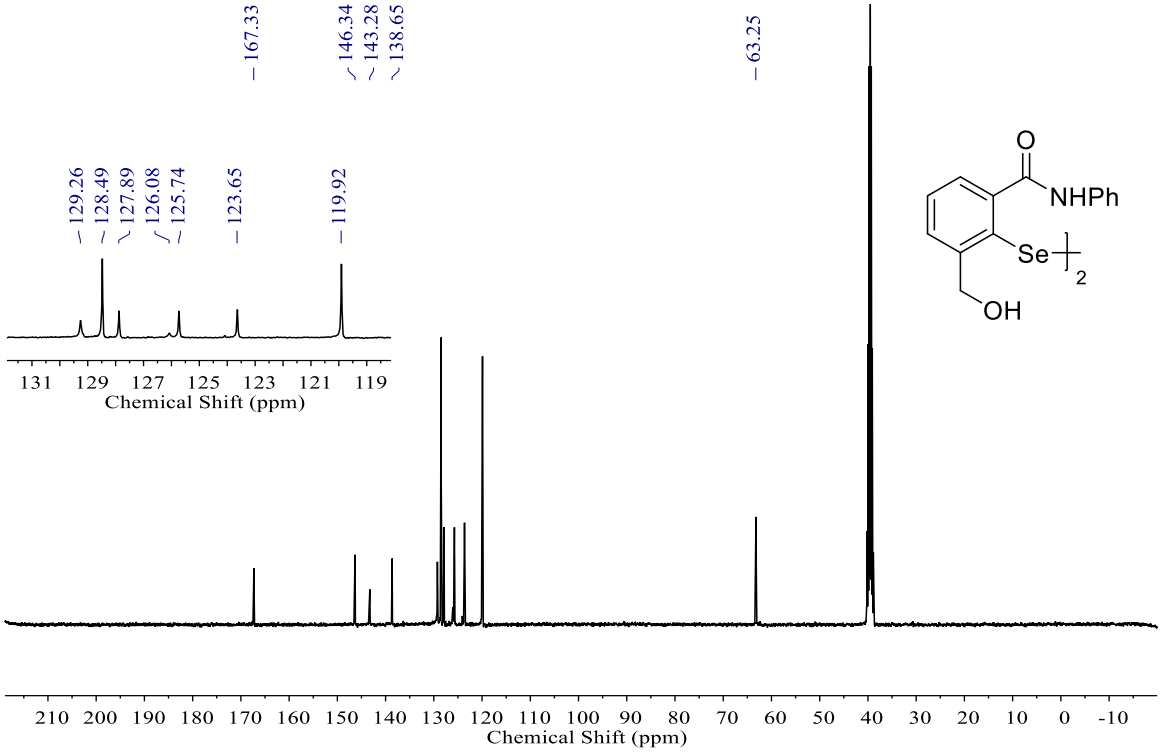


Figure 54. ^{77}Se NMR Spectrum of 28 (76 MHz, DMSO-d$_6$)

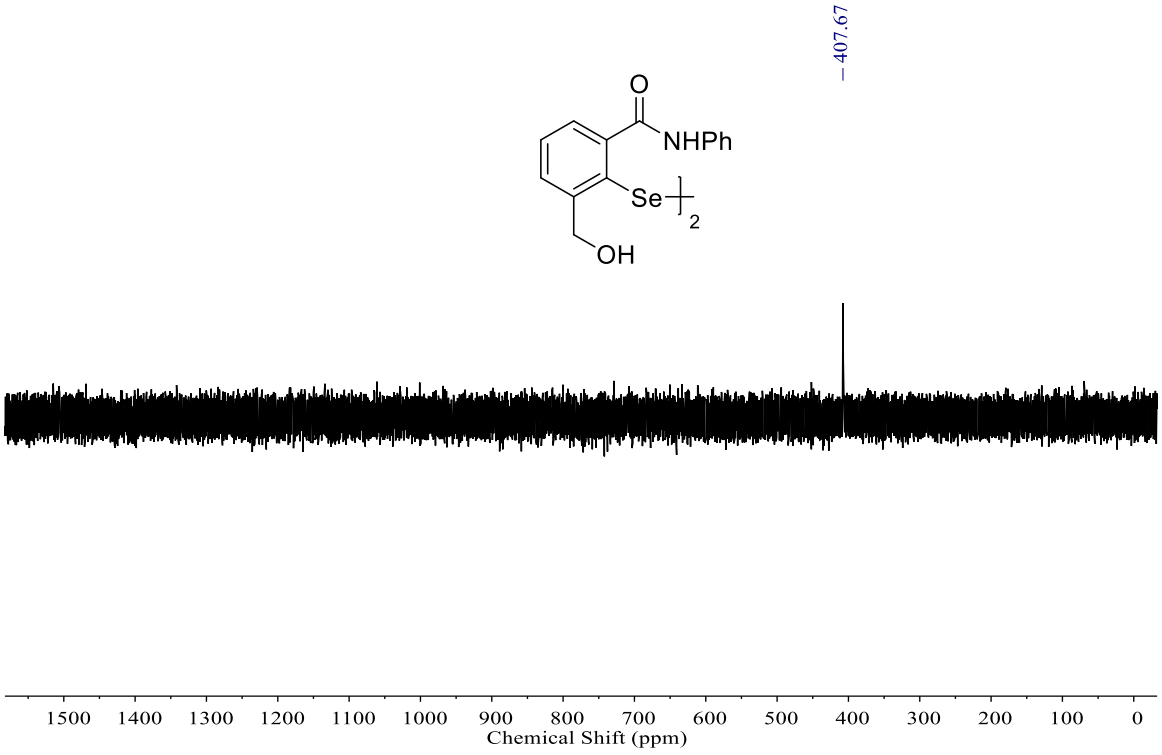


Figure 55. ^{1}H NMR Spectrum of 7 (400 MHz, DMSO-d$_6$)

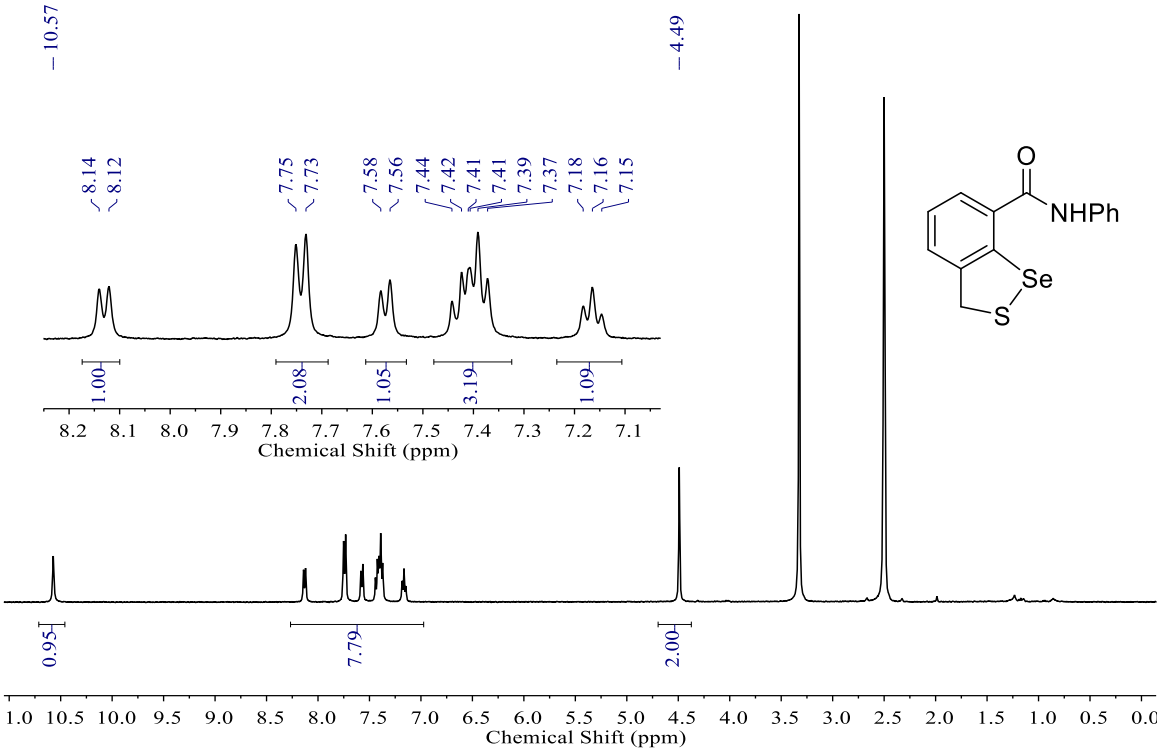


Figure 56. ^{13}C NMR Spectrum of 7 (101 MHz, DMSO-d$_6$)

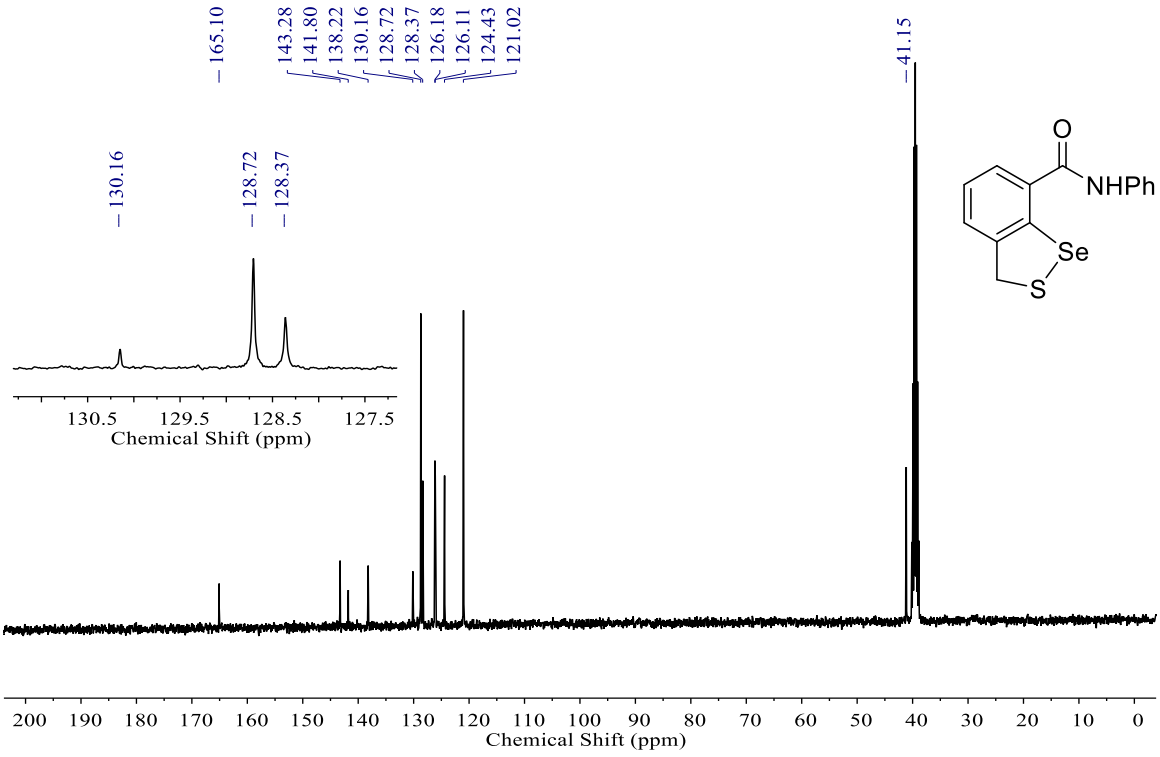


Figure 57. ^{77}Se NMR Spectrum of 7 (76 MHz, DMSO-d$_6$)

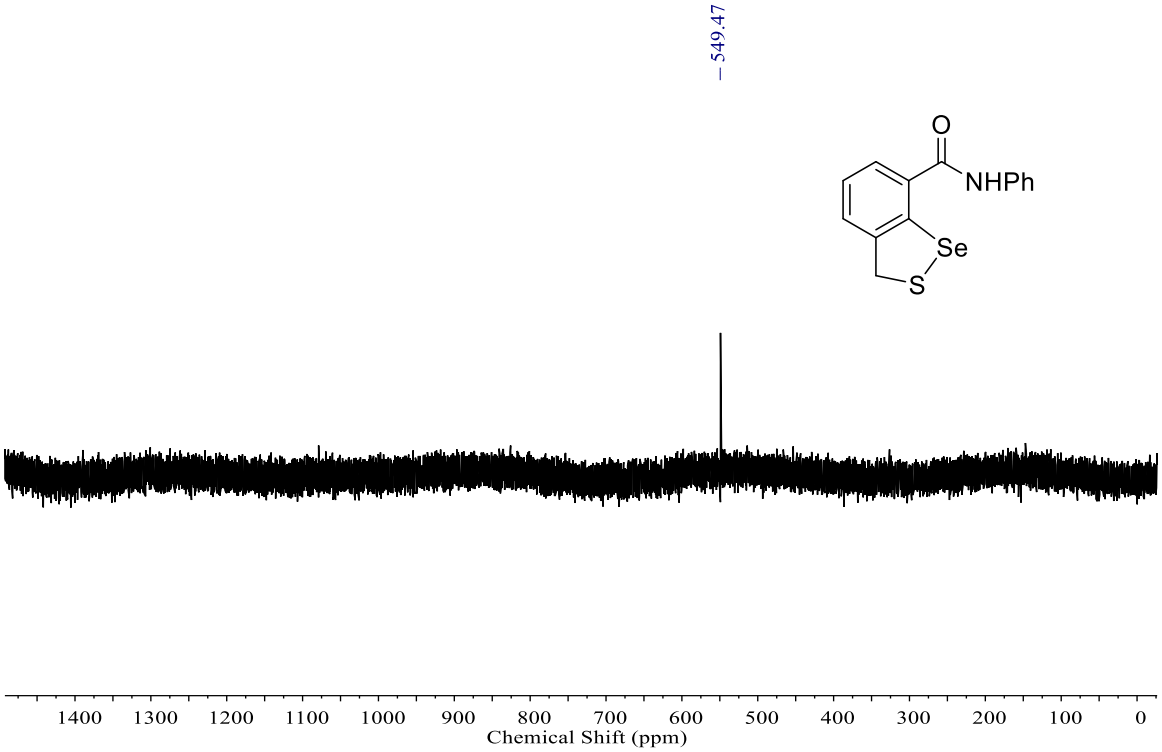


Figure 58. ^{1}H NMR Spectrum of 16 (400 MHz, CDCl$_3$)

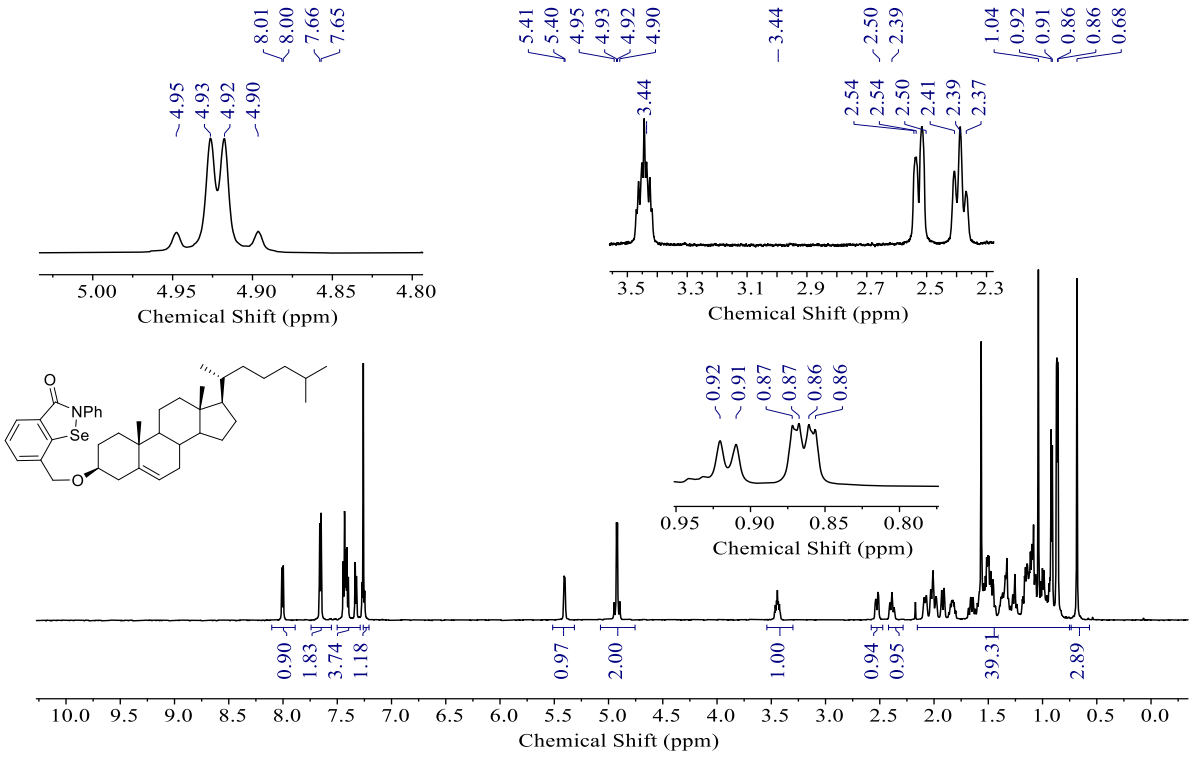


Figure 59. ^{13}C NMR Spectrum of 16 (101 MHz, $CDCl_3$)

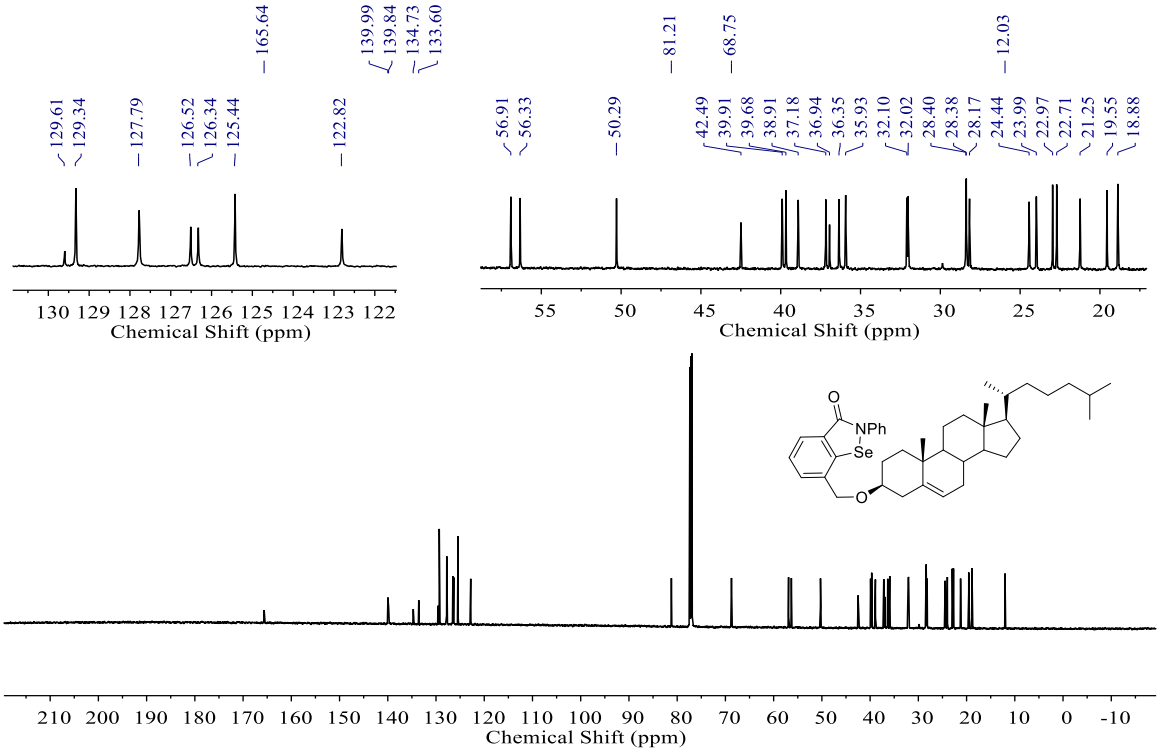


Figure 60. ^{77}Se NMR Spectrum of 16 (76 MHz, $CDCl_3$)

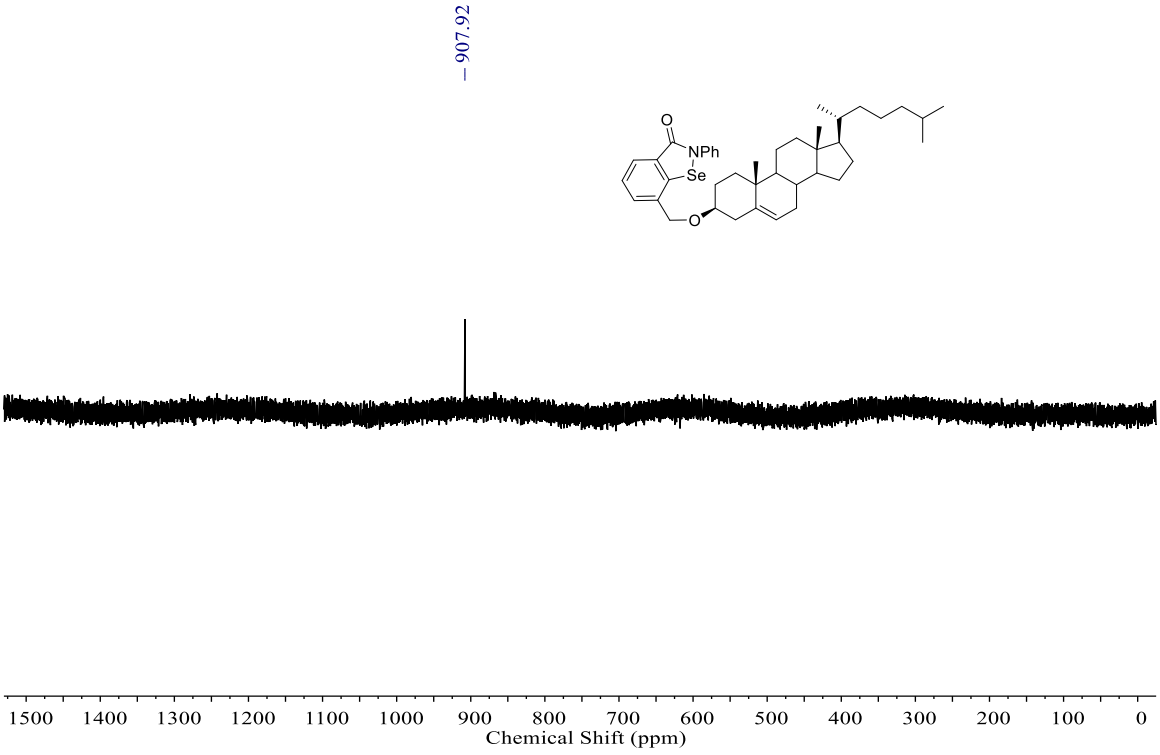


Figure 61. ^{1}H NMR Spectrum of 30 (400 MHz, $CDCl_3$)

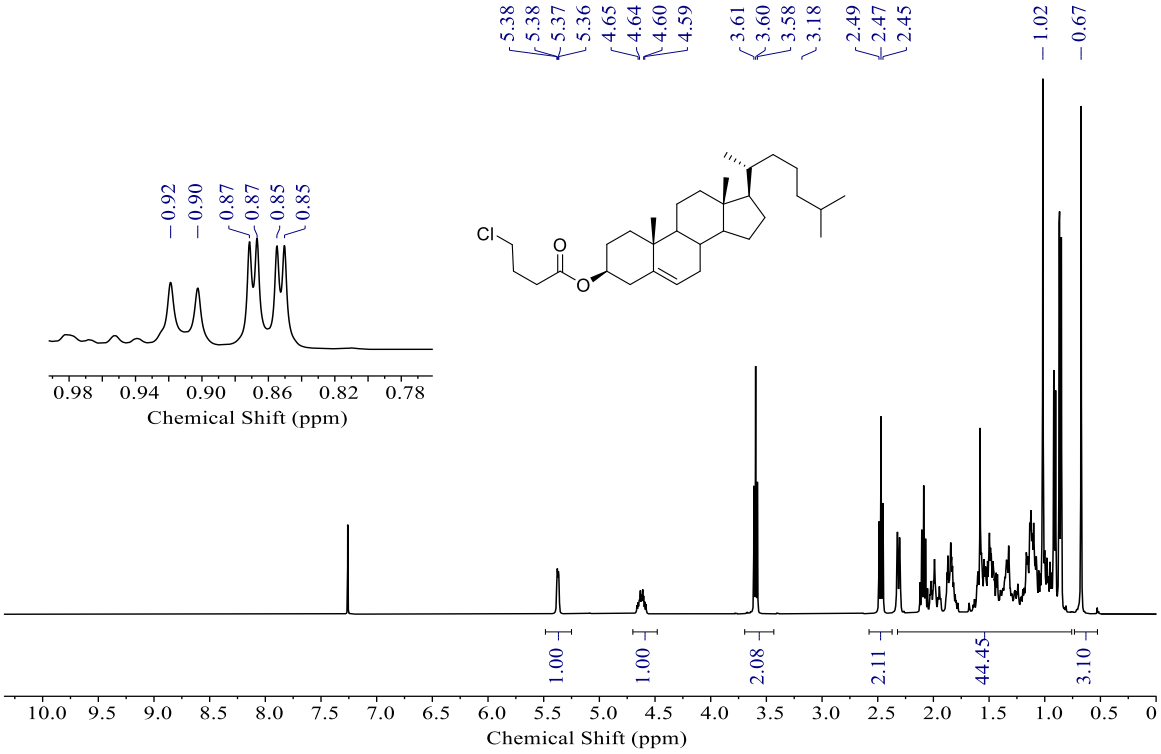


Figure 62. ^{13}C NMR Spectrum of 30 (101 MHz, $CDCl_3$)

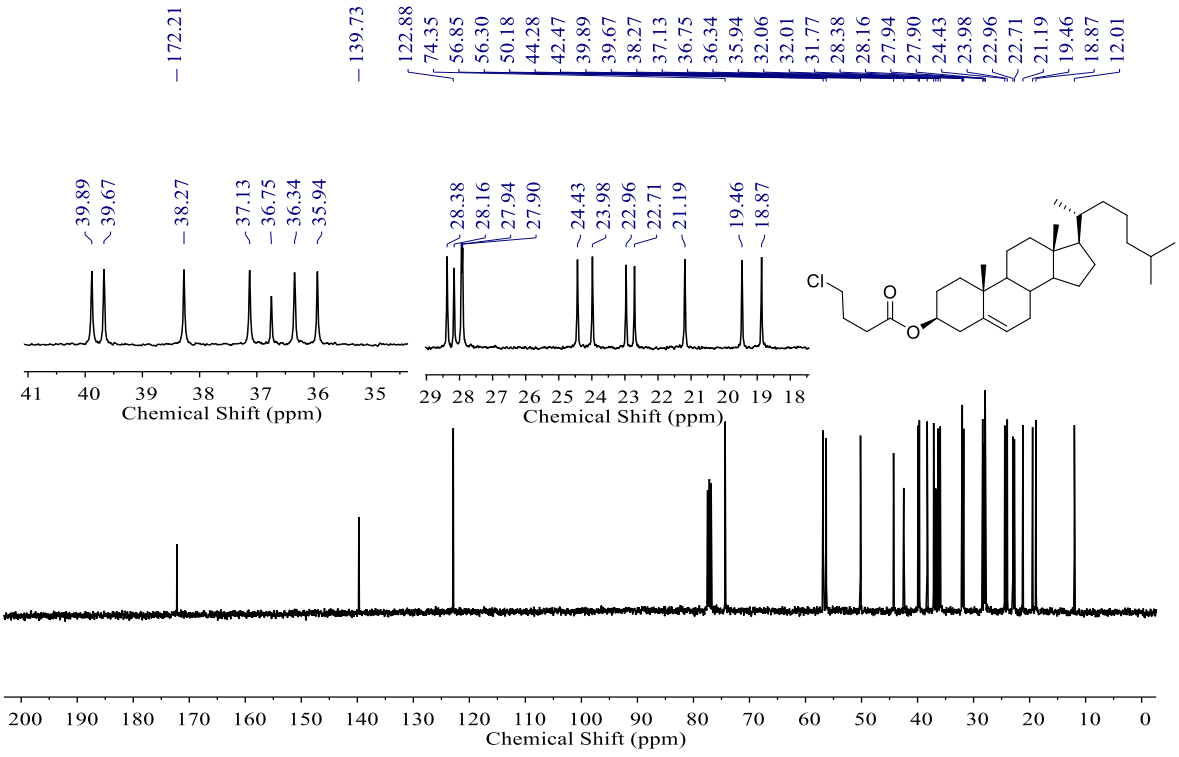


Figure 63. ^{1}H NMR Spectrum of 32 (400 MHz, $CDCl_3$)

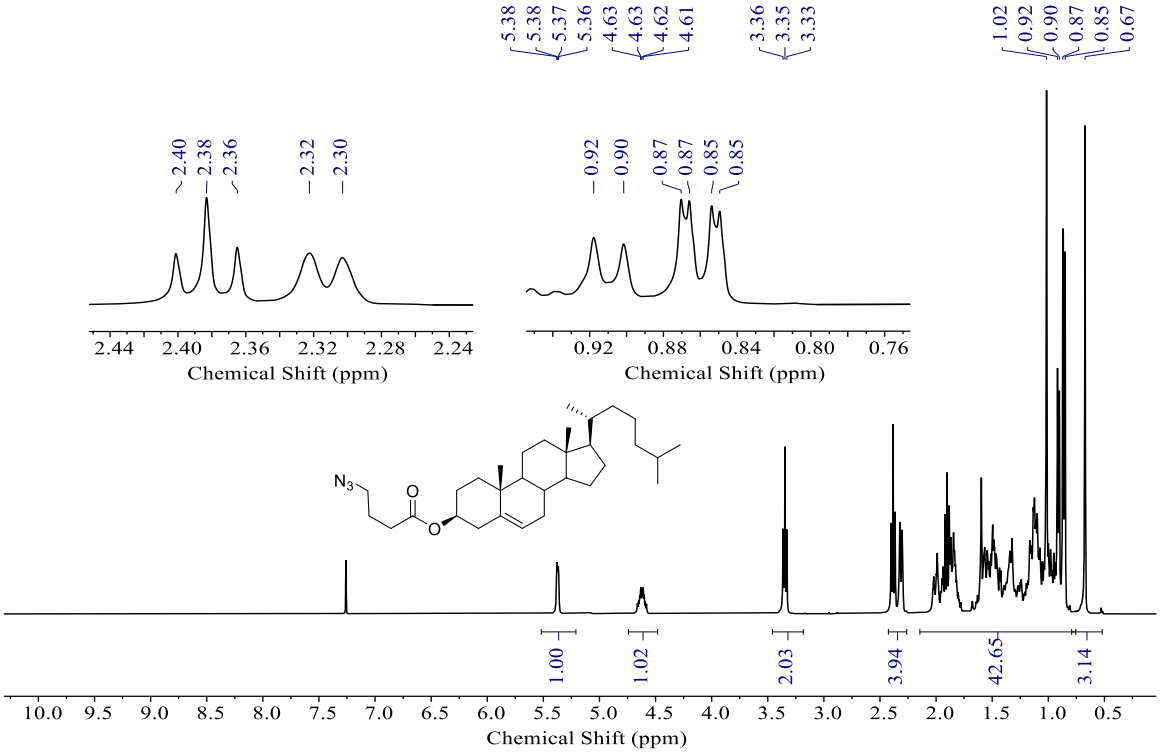


Figure 64. ^{13}C NMR Spectrum of 32 (101 MHz, $CDCl_3$)

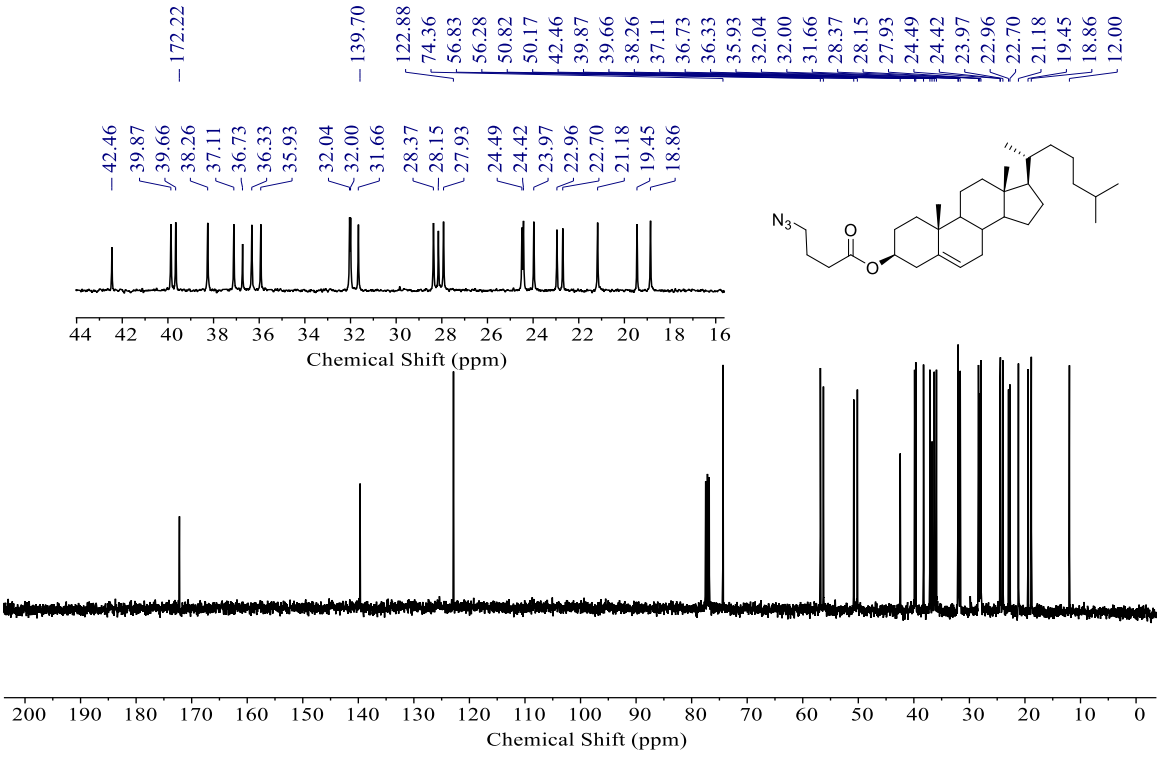


Figure 65. ^{1}H NMR Spectrum of 31 (400 MHz, $CDCl_3$)

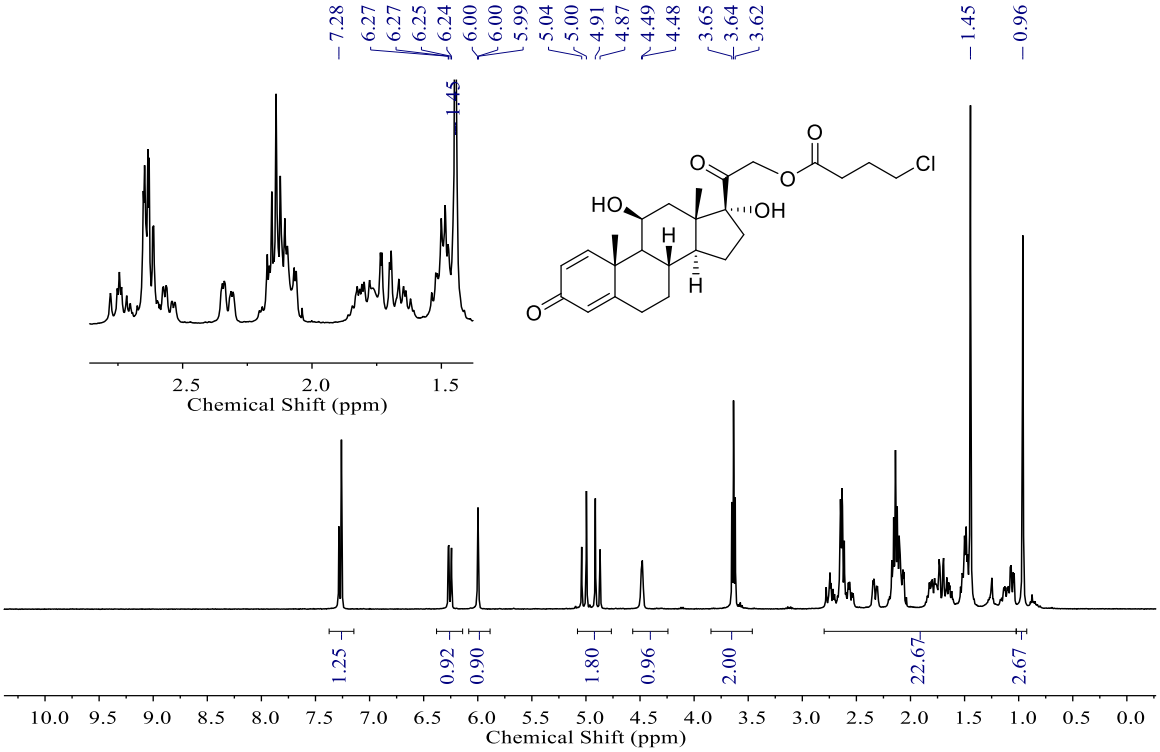


Figure 66. ^{13}C NMR Spectrum of 31 (101 MHz, $CDCl_3$)

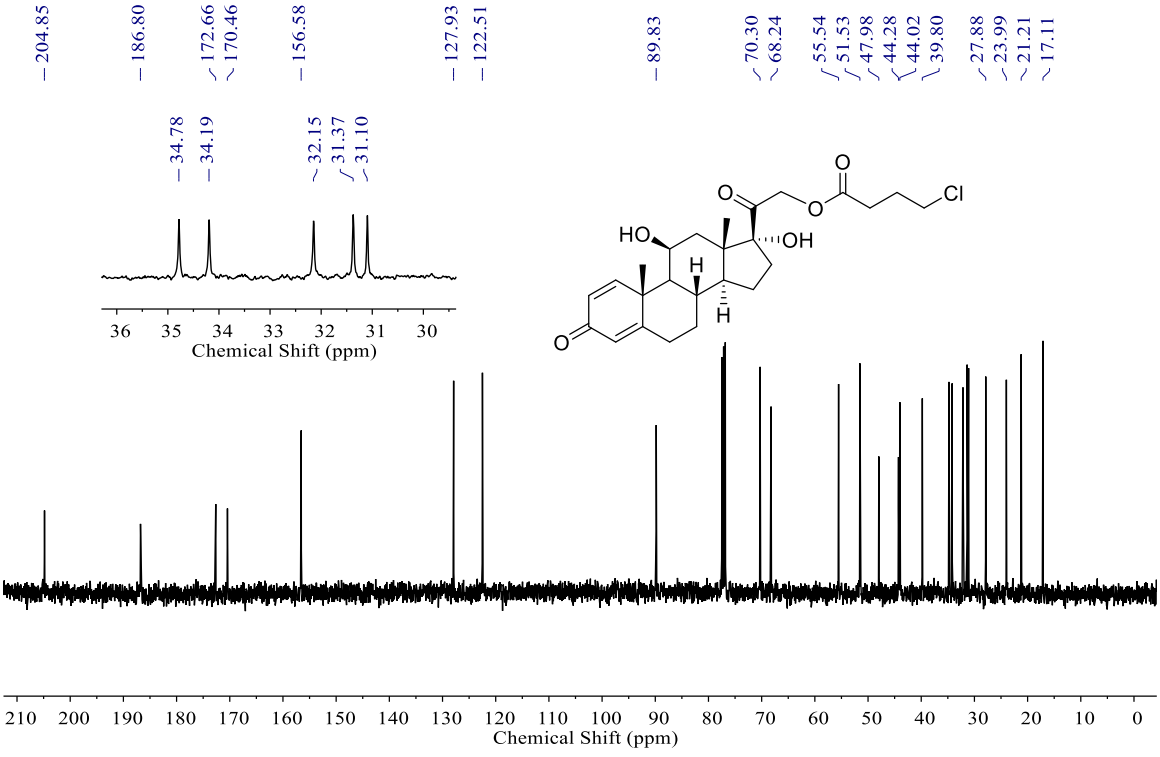


Figure 67. ^{1}H NMR Spectrum of 33 (400 MHz, $CDCl_3$)

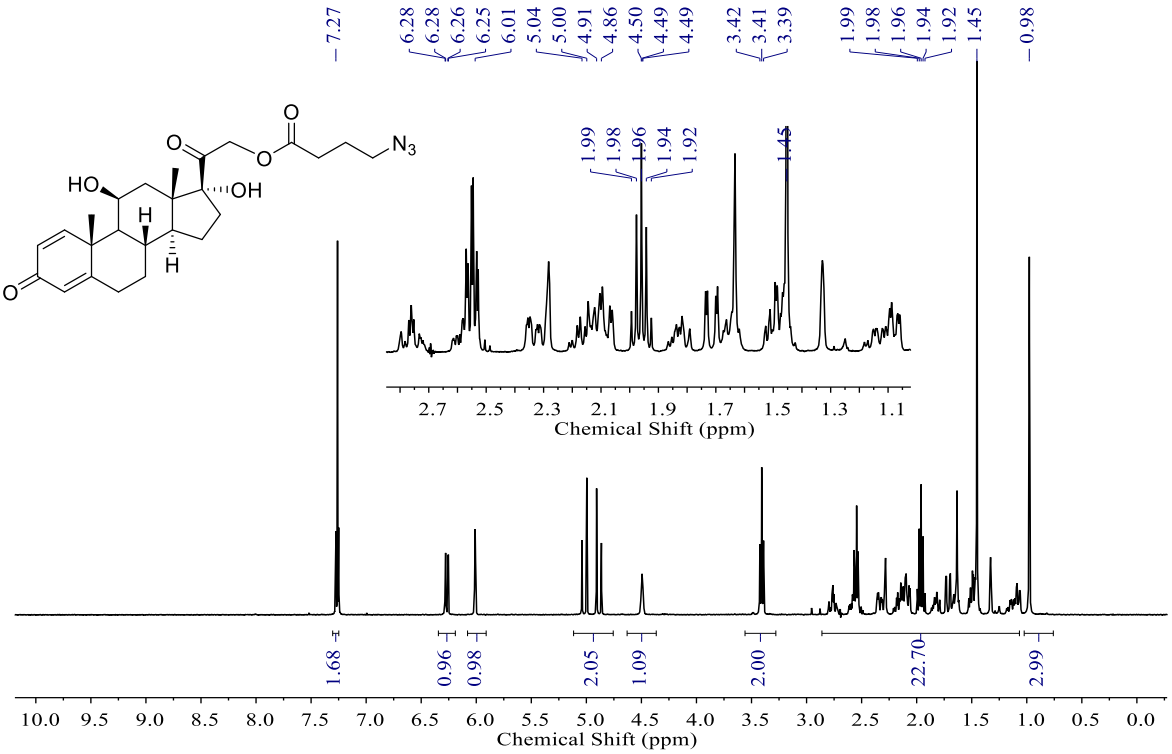


Figure 68. ^{13}C NMR Spectrum of 33 (101 MHz, DMSO-d_6)

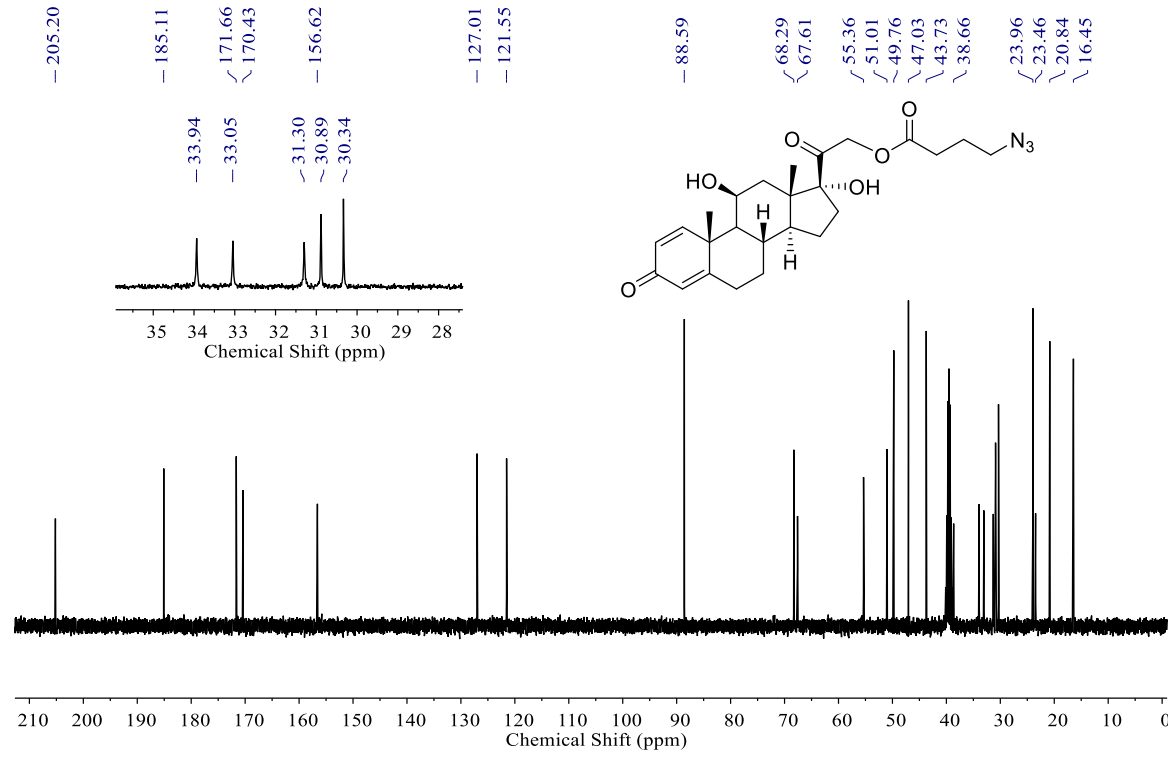


Figure 69. ^{1}H NMR Spectrum of 17 (600 MHz, $CDCl_3$)

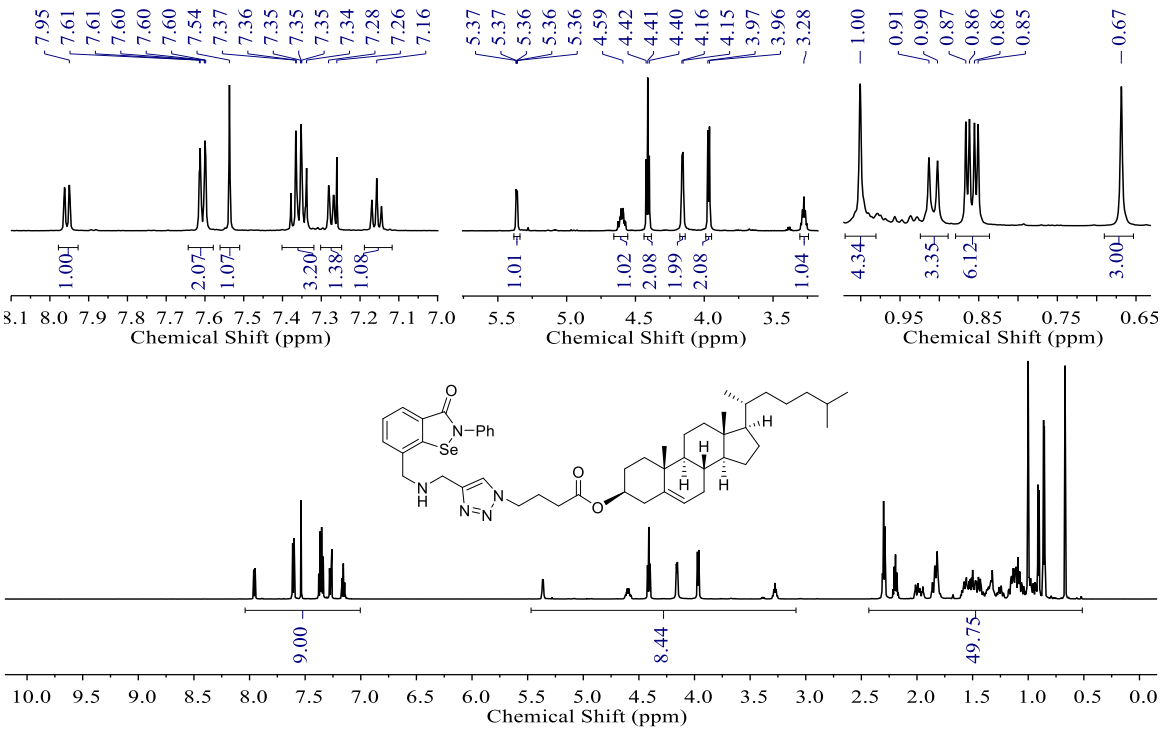


Figure 70. ^{13}C NMR Spectrum of 17 (151 MHz, $CDCl_3$)

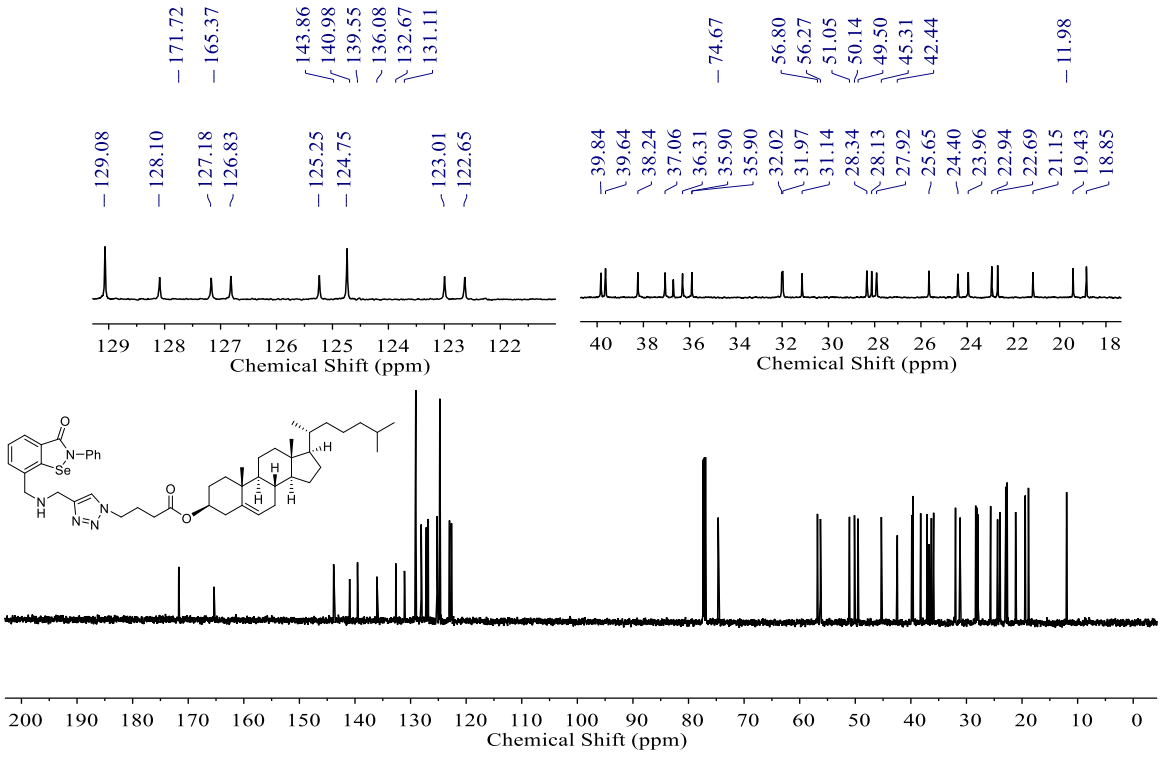


Figure 71. ^{77}Se NMR Spectrum of 17 (114 MHz, $CDCl_3$)

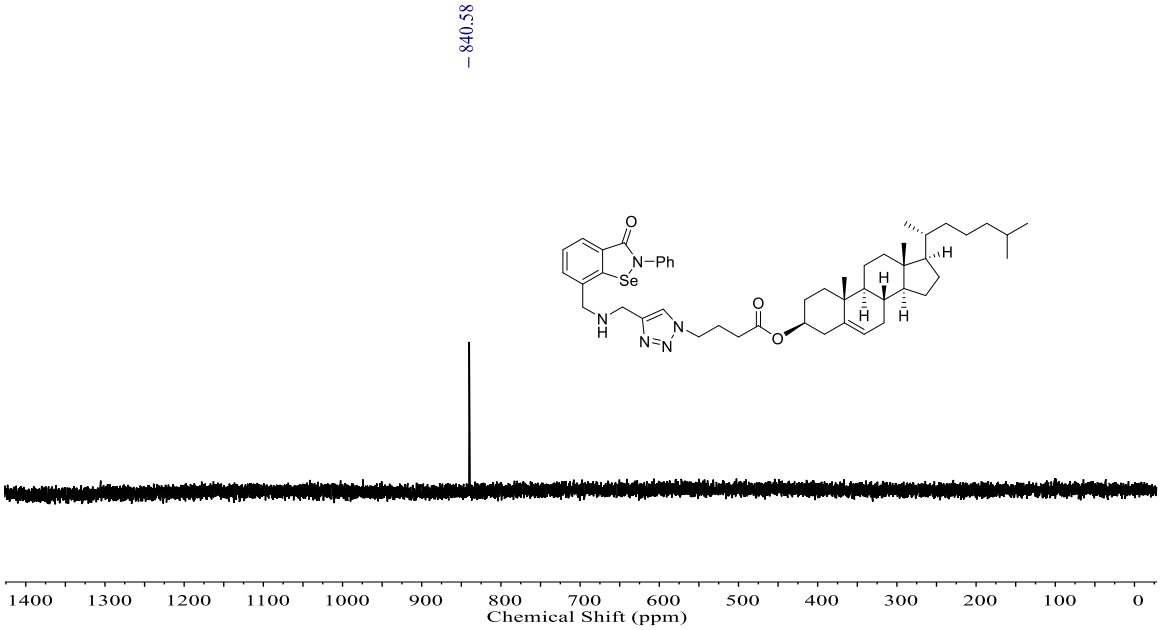


Figure 72. ^{1}H NMR Spectrum of 18 (400 MHz, $CDCl_3$)

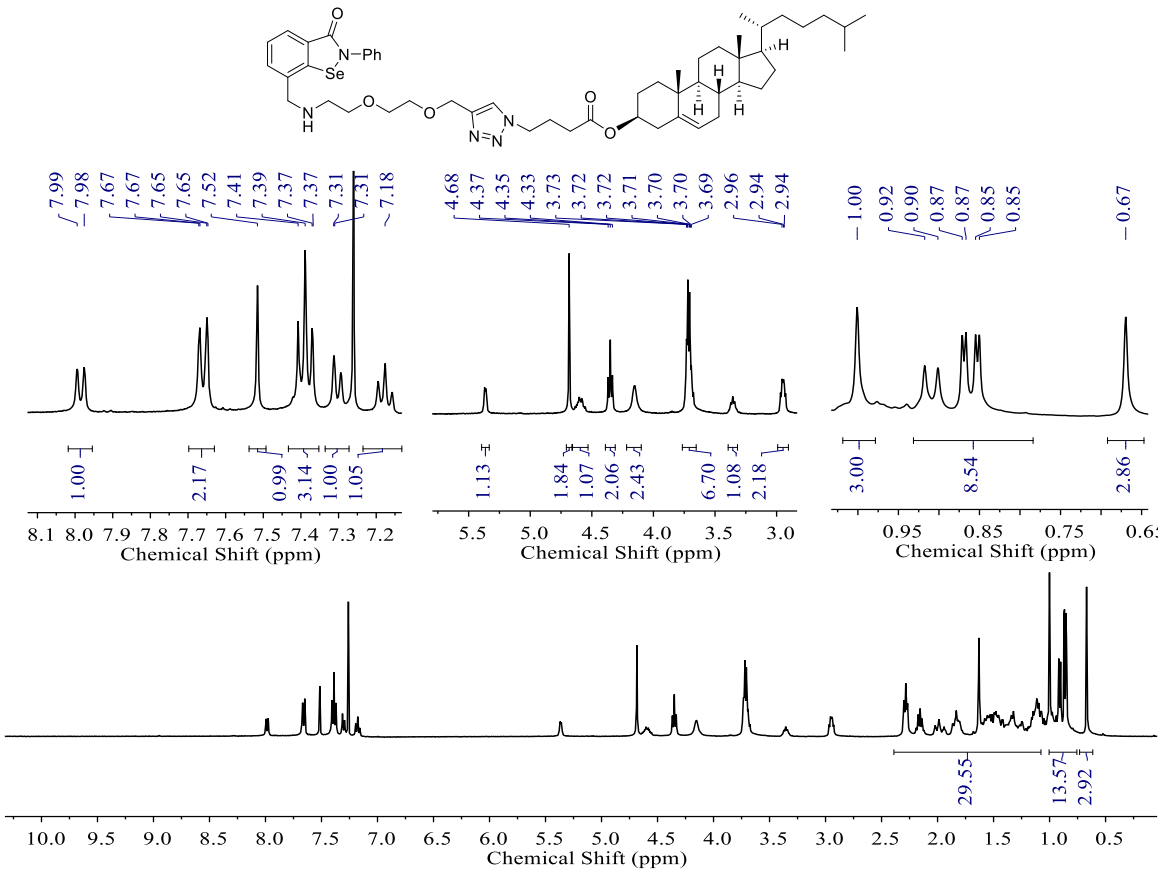


Figure 73. ^{13}C NMR Spectrum of 18 (101 MHz, $CDCl_3$)

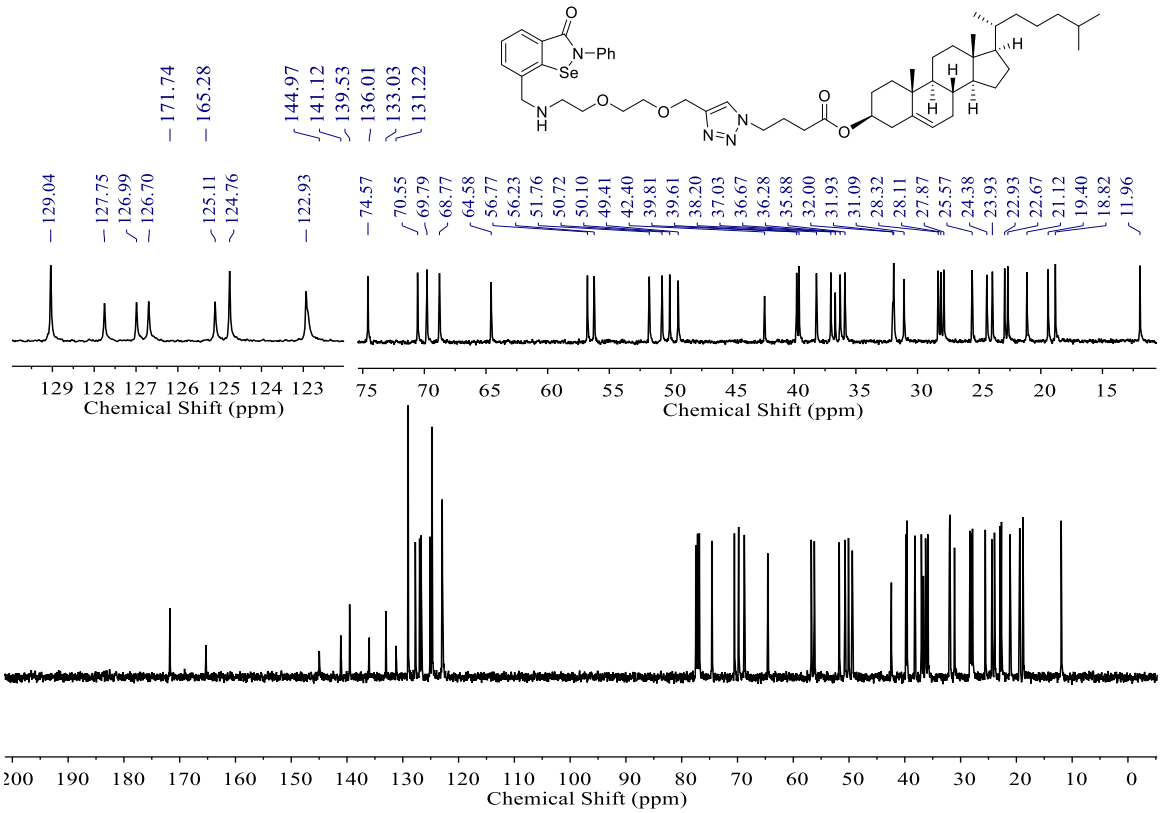


Figure 74. ^{77}Se NMR Spectrum of 18 (76 MHz, $CDCl_3$)

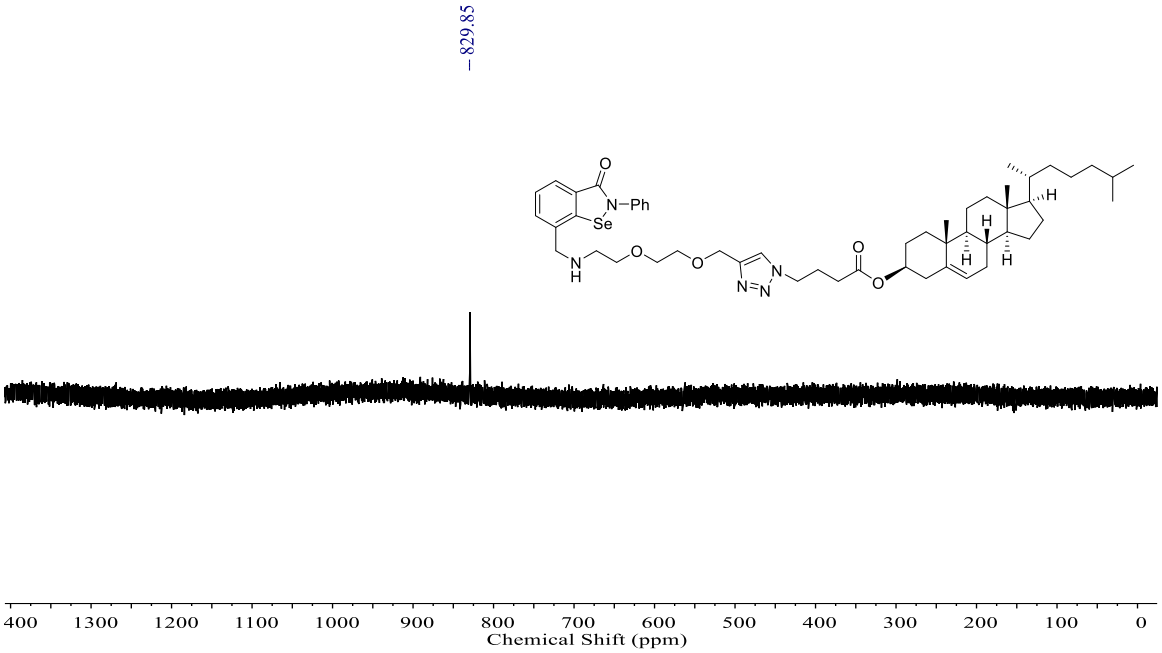


Figure 75. ^{1}H NMR Spectrum of 19 (600 MHz, $CDCl_3$)

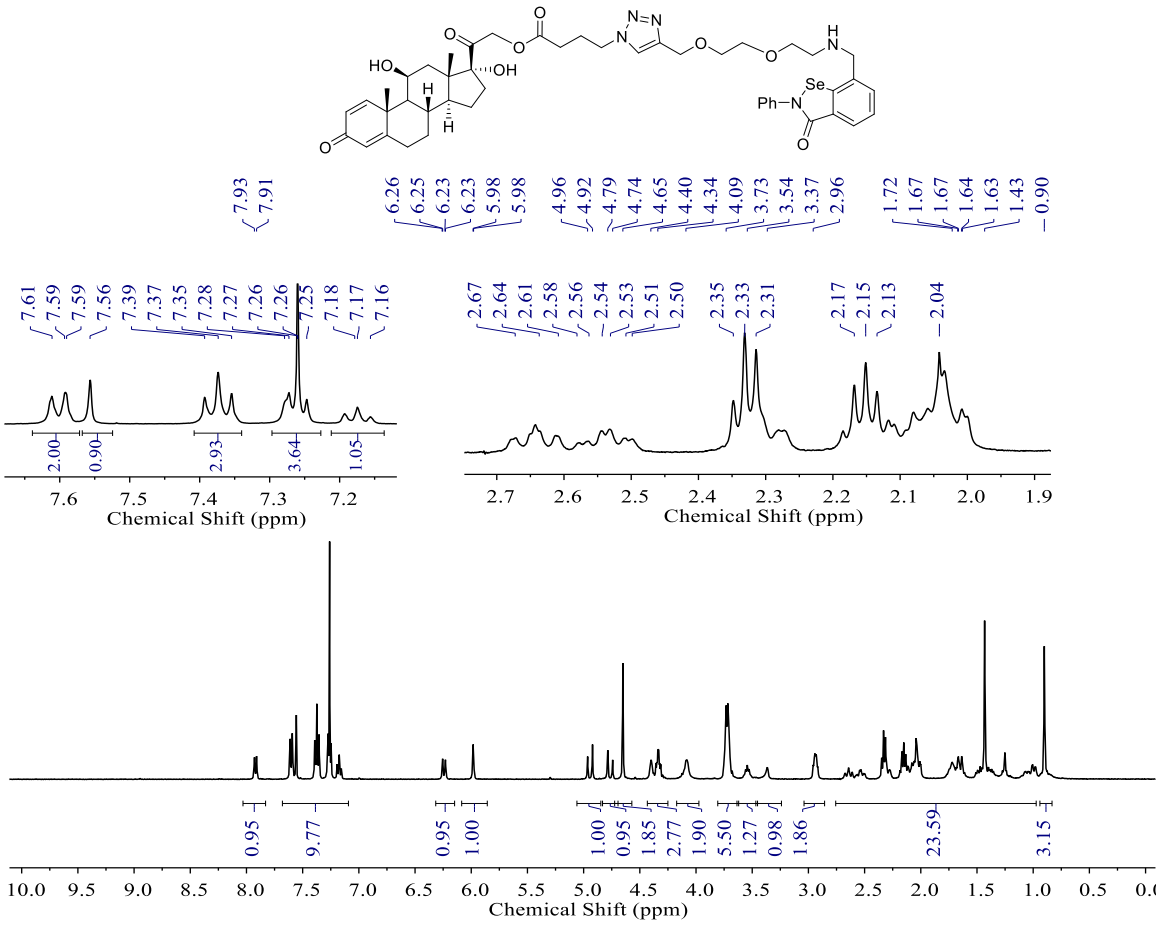


Figure 76. ^{13}C NMR Spectrum of 19 (101 MHz, $CDCl_3$)

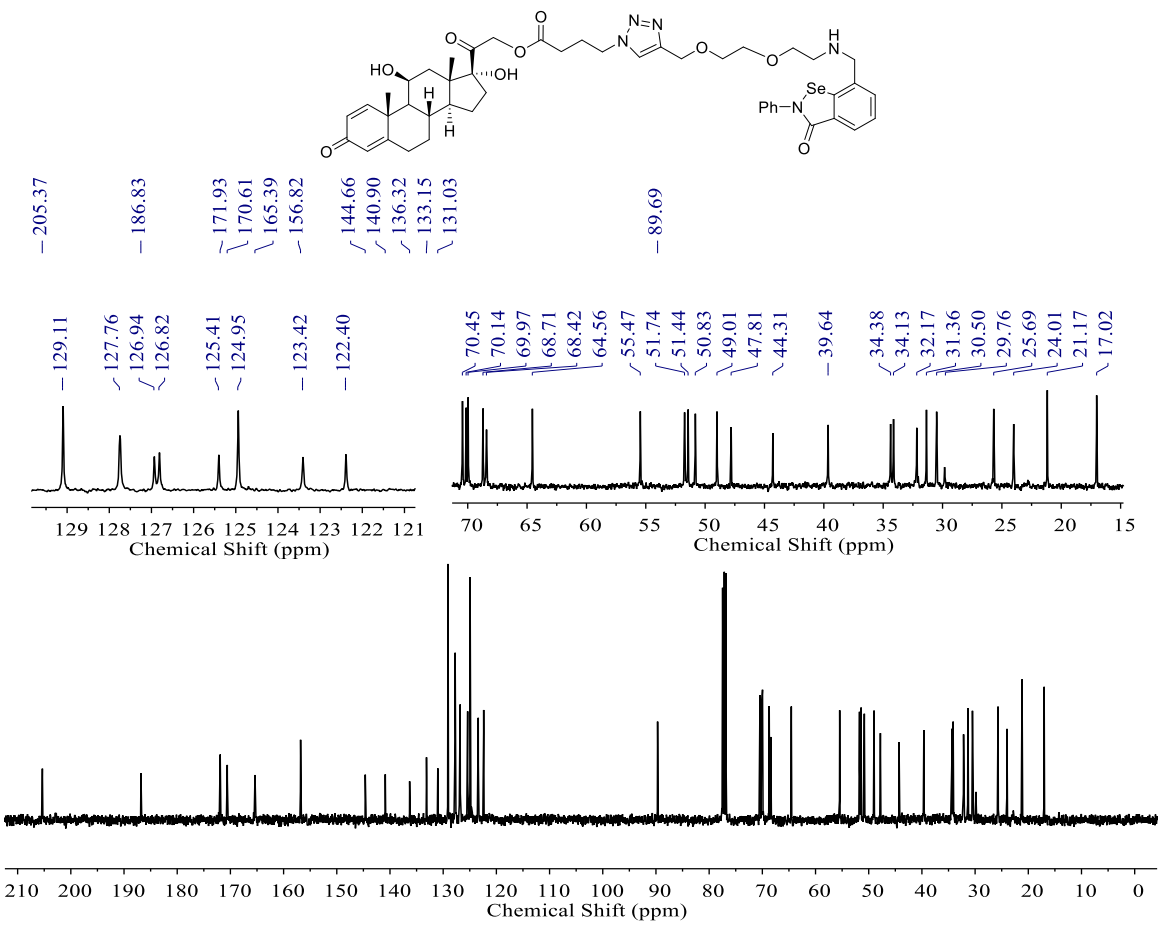


Figure 77. ^{77}Se NMR Spectrum of 19 (76 MHz, $CDCl_3$)

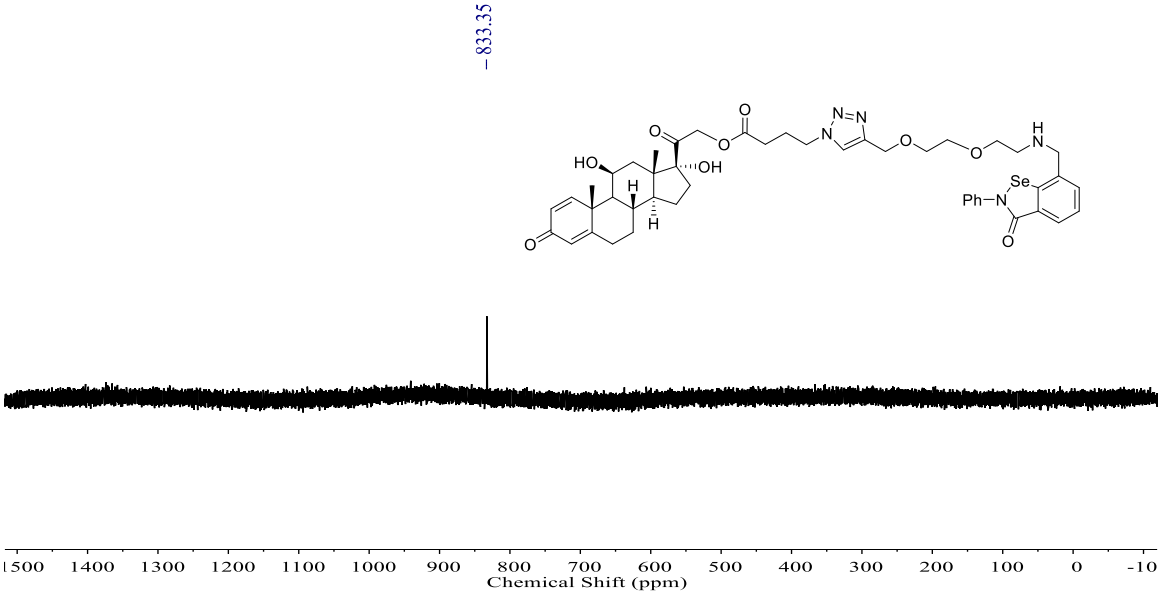


Figure 78. ^{1}H NMR Spectrum of 20 (400 MHz, $CDCl_3$)

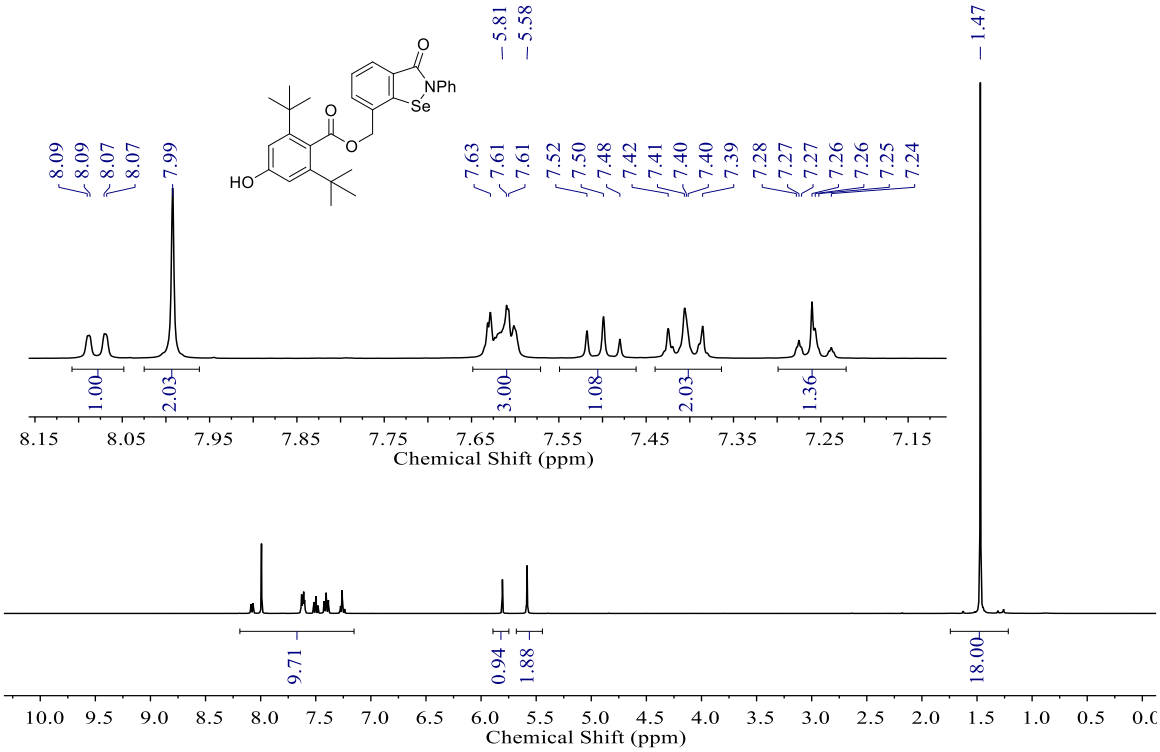


Figure 79. ^{13}C NMR Spectrum of 20 (101 MHz, $CDCl_3$)

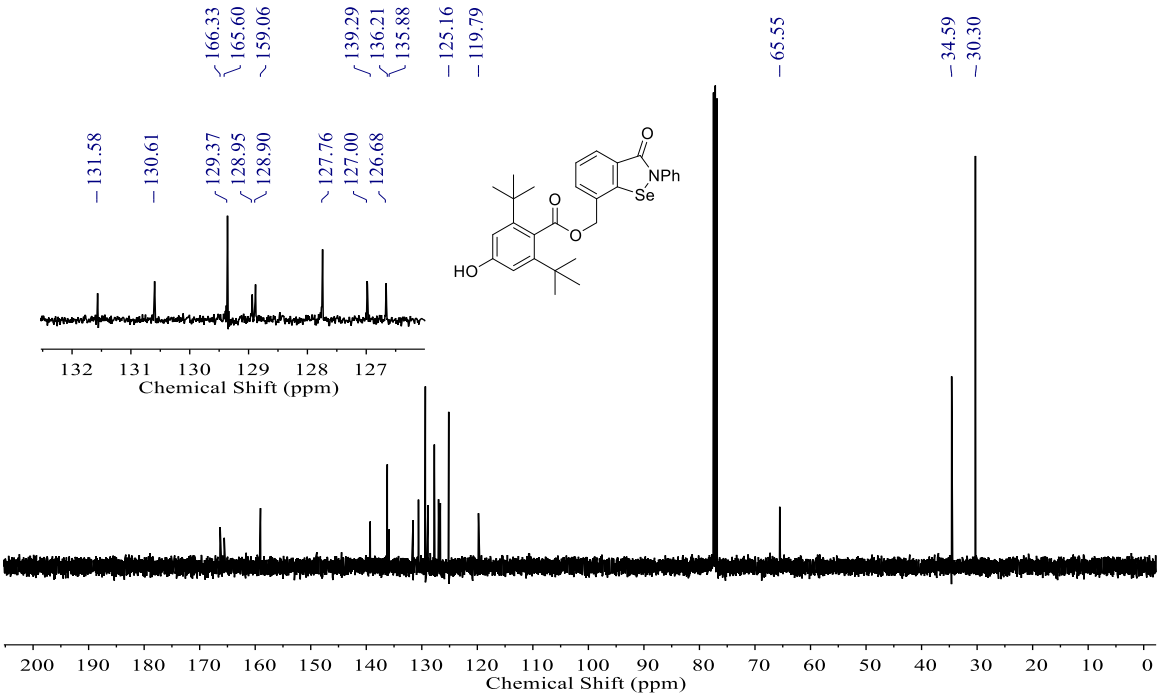


Figure 80. ^{77}Se NMR Spectrum of 20 (76 MHz, $CDCl_3$)

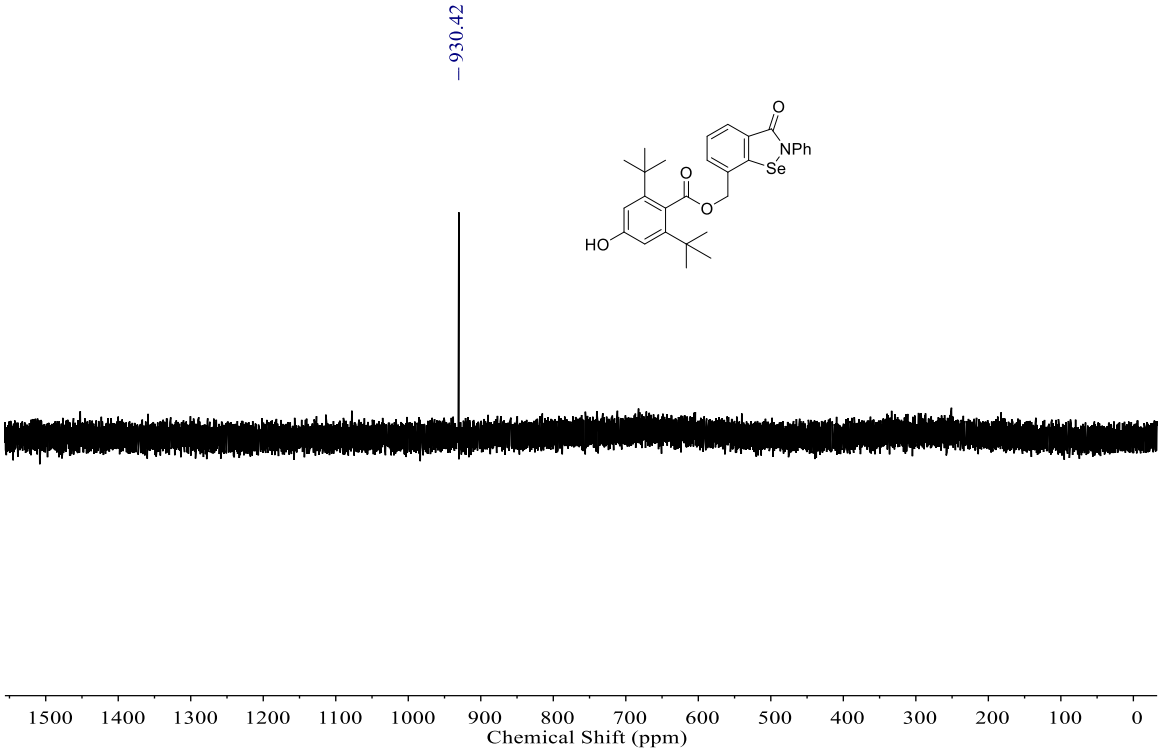


Figure 81. ^{1}H NMR Spectrum of 8 (400 MHz, DMSO-d_6)

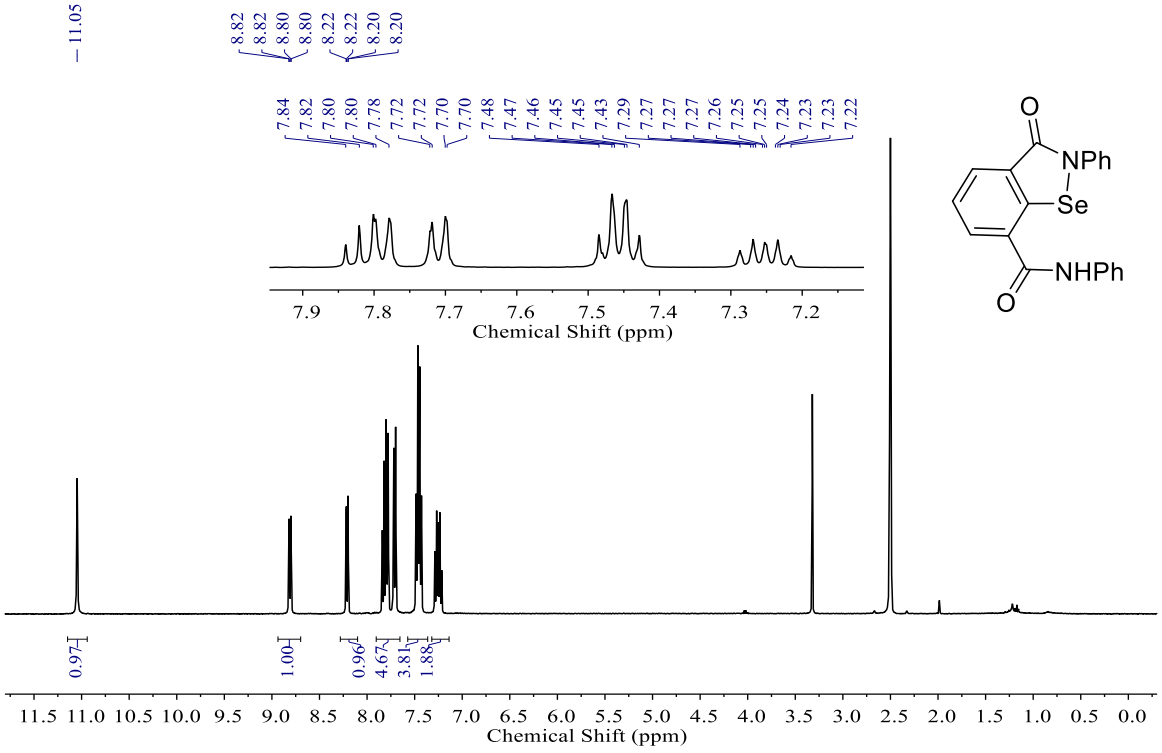


Figure 82. ^{13}C NMR Spectrum of 8 (101 MHz, DMSO-d$_6$)

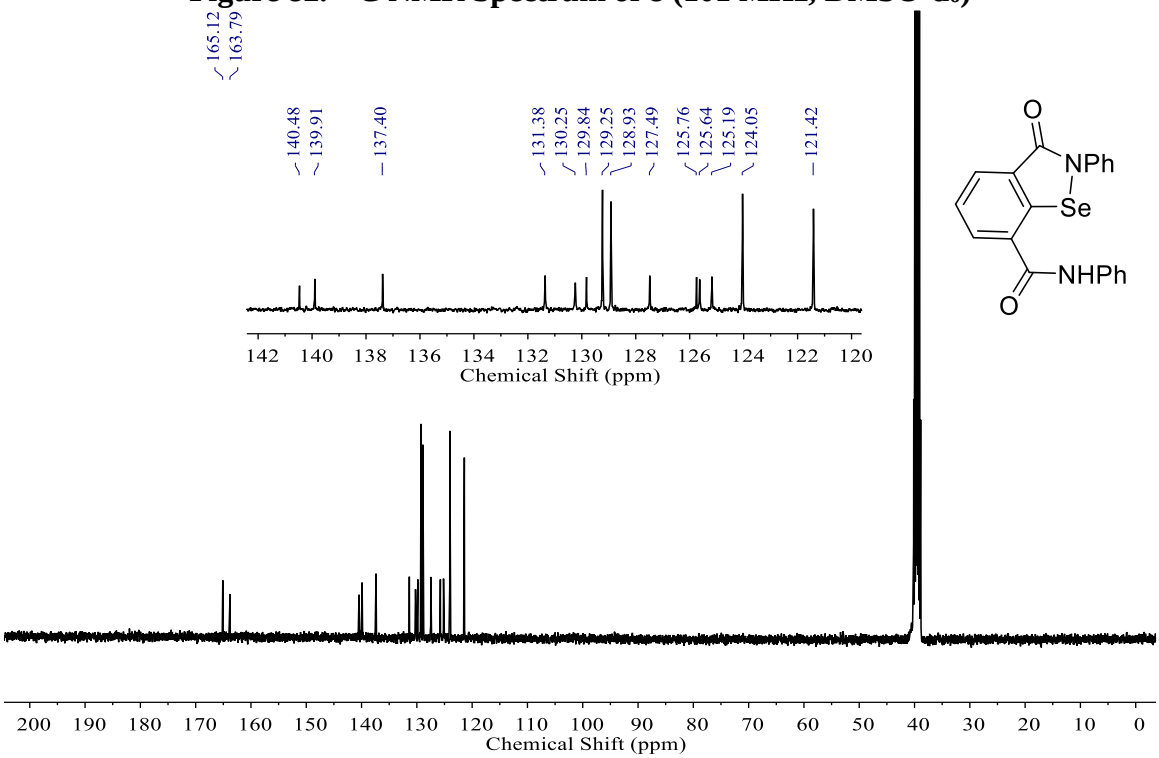


Figure 83. ^{77}Se NMR Spectrum of 8 (76 MHz, DMSO-d$_6$)

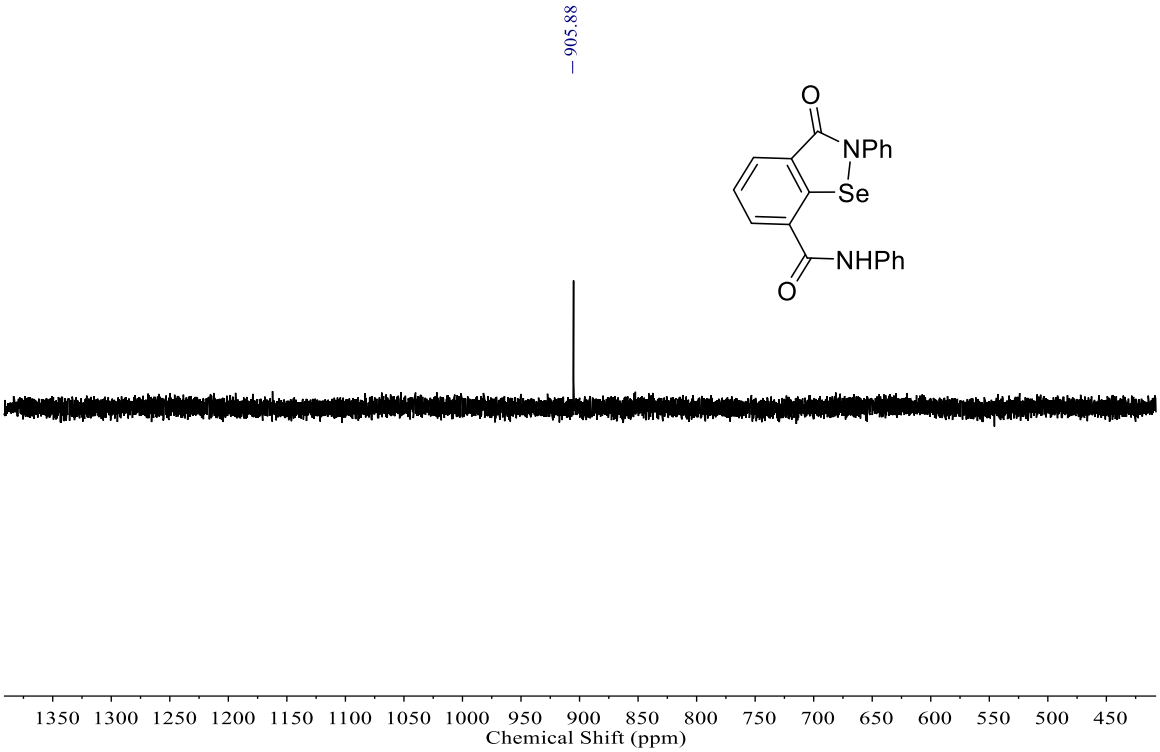


Figure 84. ^{1}H NMR Spectrum of 42a (400 MHz, DMSO-d$_6$)

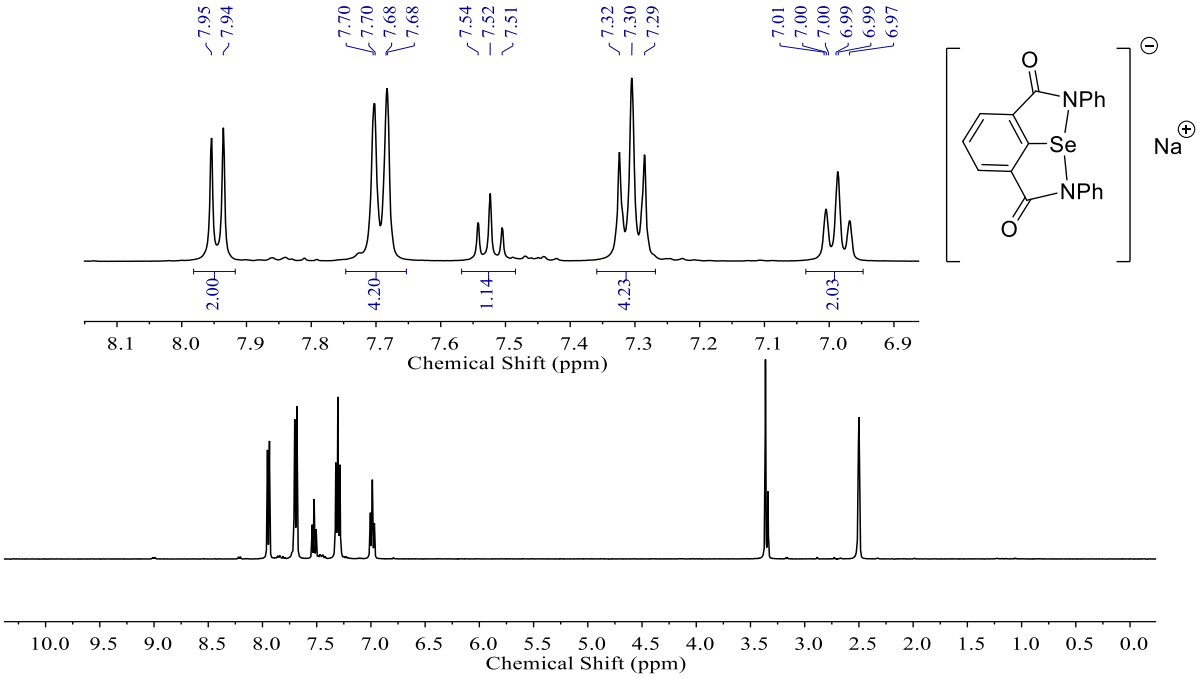


Figure 85. ^{13}C NMR Spectrum of 42a (101MHz, DMSO-d$_6$)

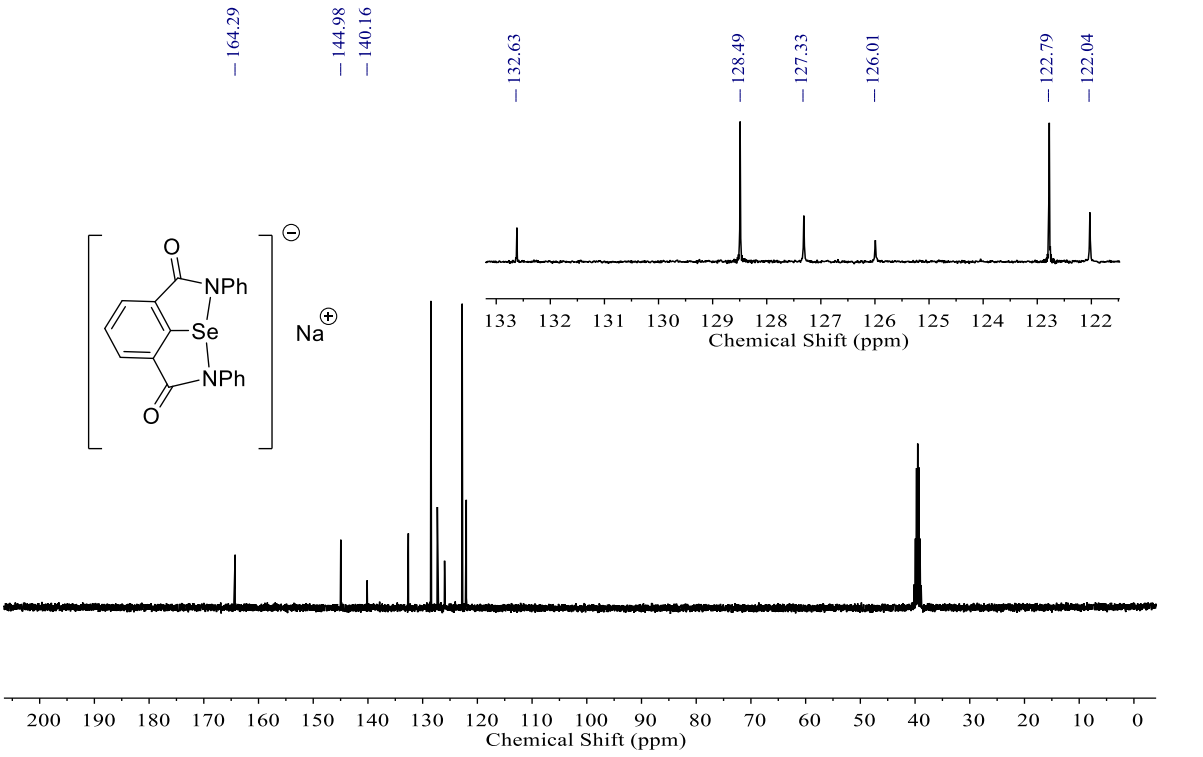


Figure 86. ^{77}Se NMR Spectrum of 42a (76 MHz, DMSO-d$_6$)

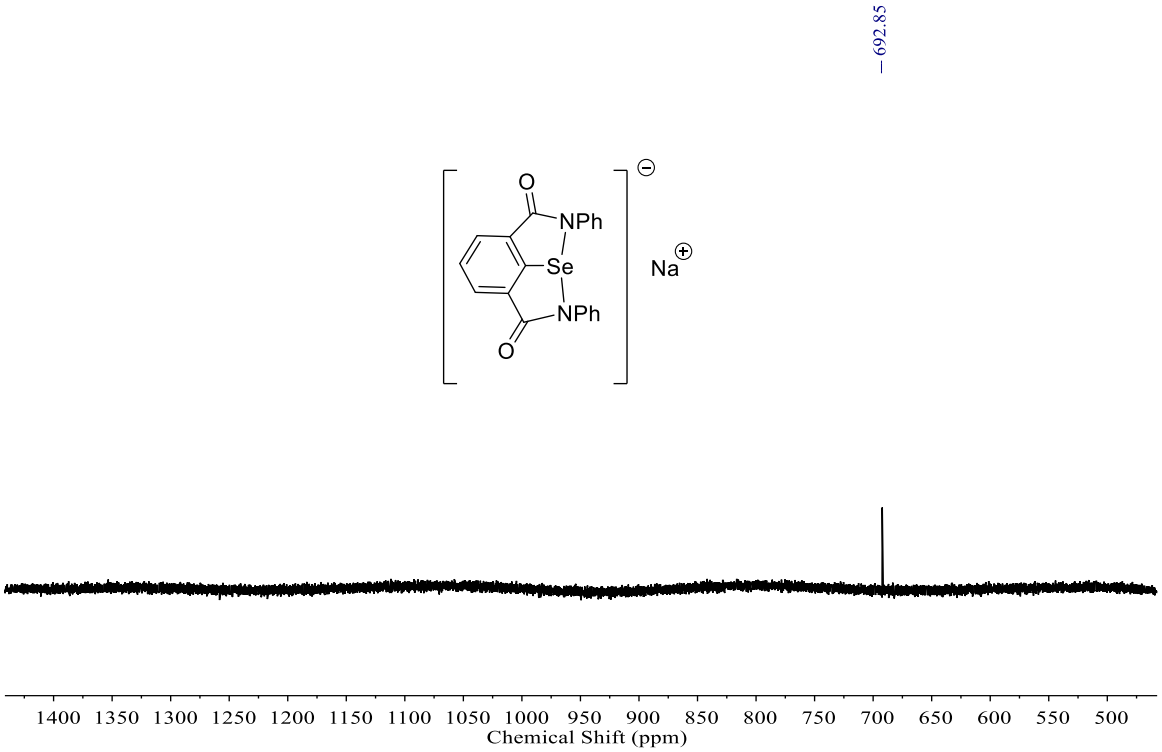


Figure 87. ^{1}H NMR Spectrum of 42b (400 MHz, CD$_3$OD)

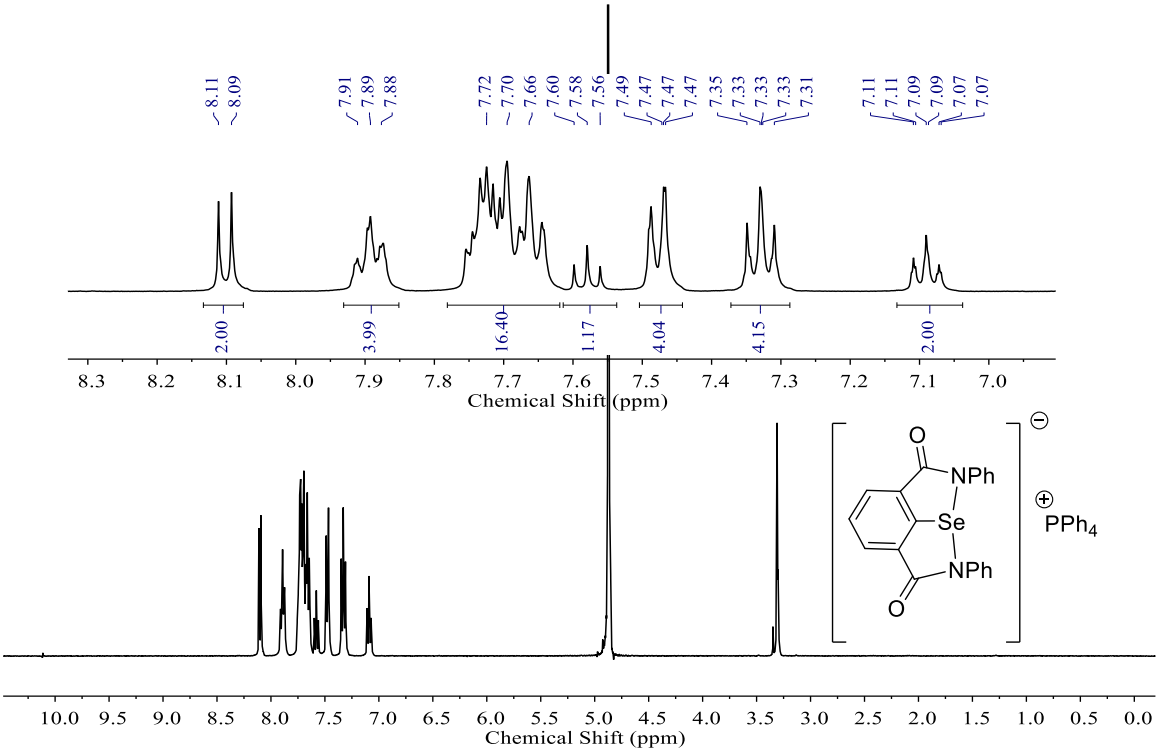


Figure 88. ^{13}C NMR Spectrum of 42b (101 MHz, CD_3OD)

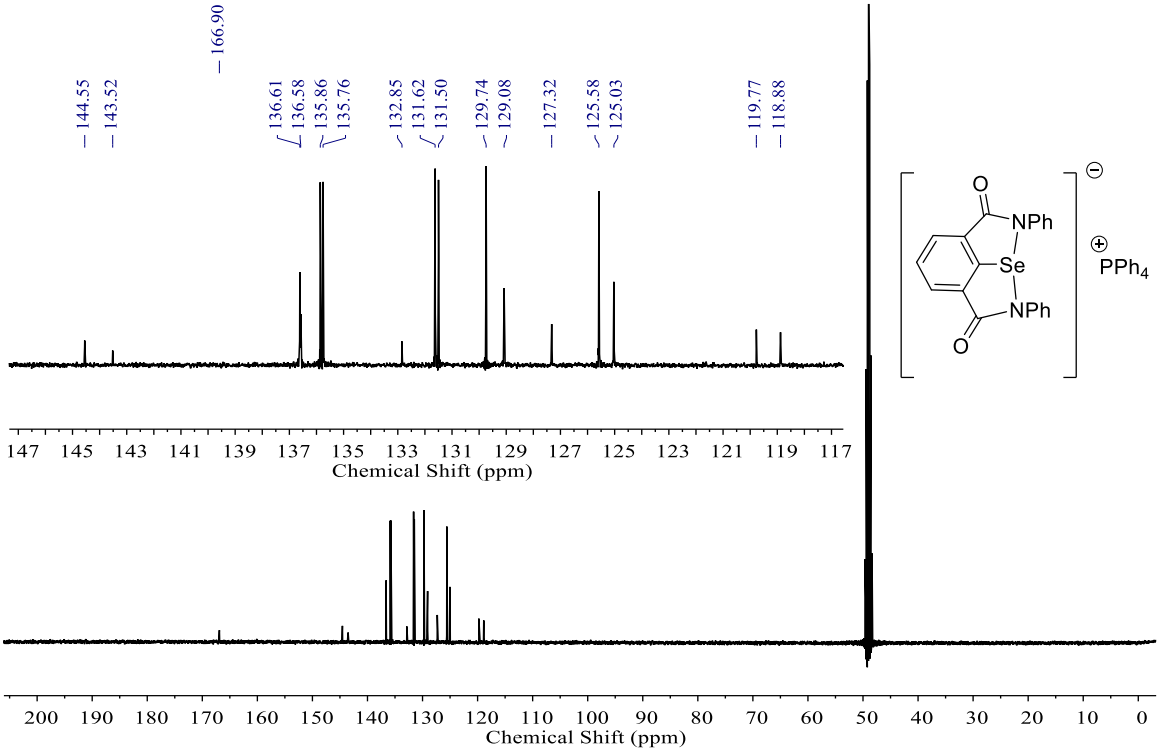


Figure 89. ^{77}Se NMR Spectrum of 42b (76 MHz, CD_3OD)

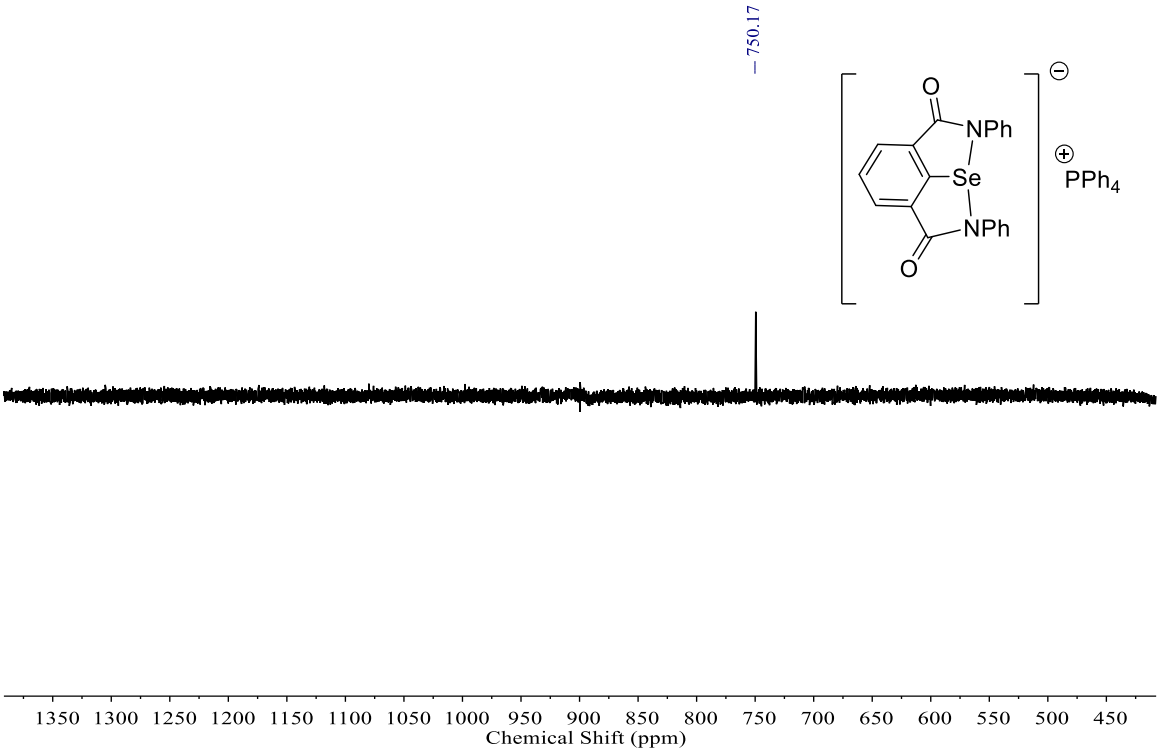


Figure 90. ^{1}H NMR Spectrum of 43 (400 MHz, DMSO-d$_6$)

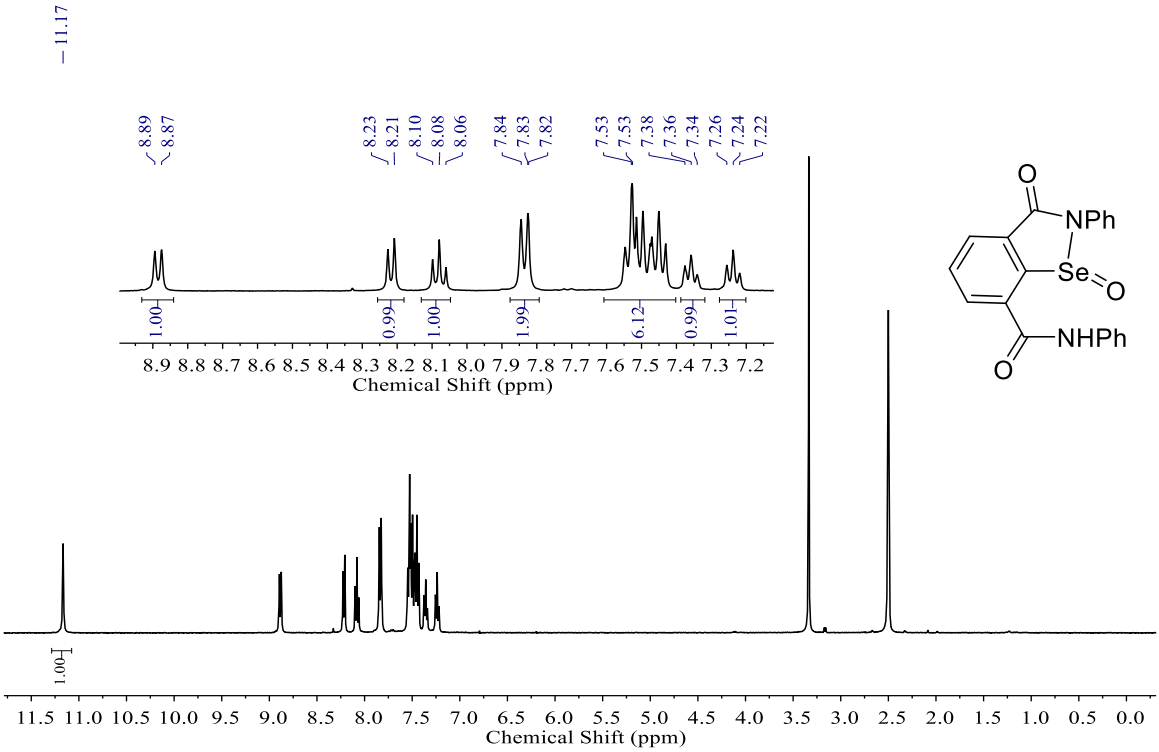


Figure 91. ^{13}C NMR Spectrum of 43 (101 MHz, DMSO-d$_6$)

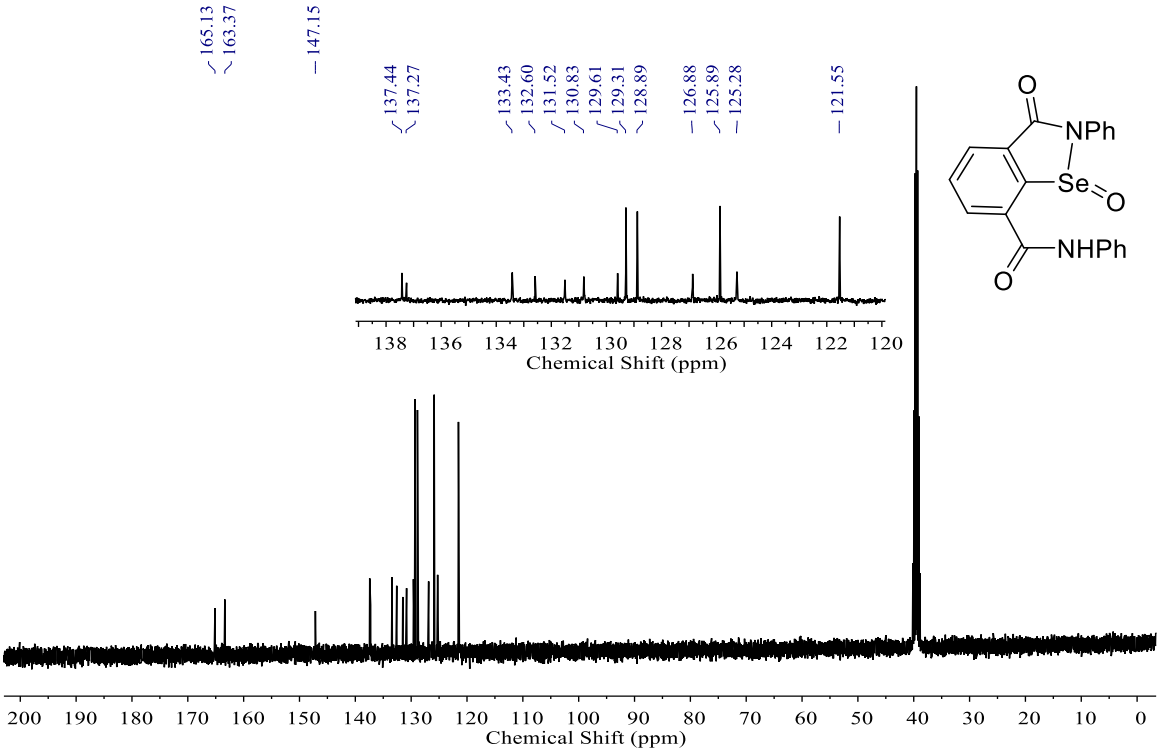


Figure 92. ^{77}Se NMR Spectrum of 43 (76 MHz, DMSO-d$_6$)

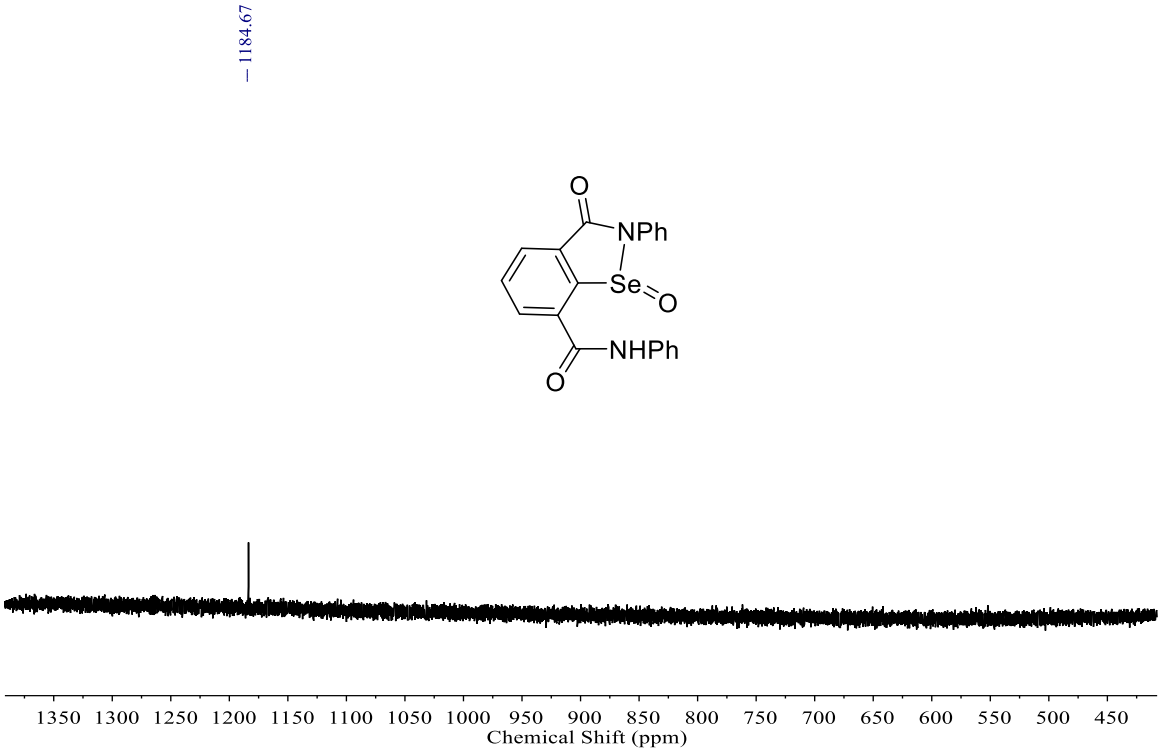


Figure 93. ^{1}H NMR Spectrum of 44 (DMSO-d$_6$, 400 MHz)

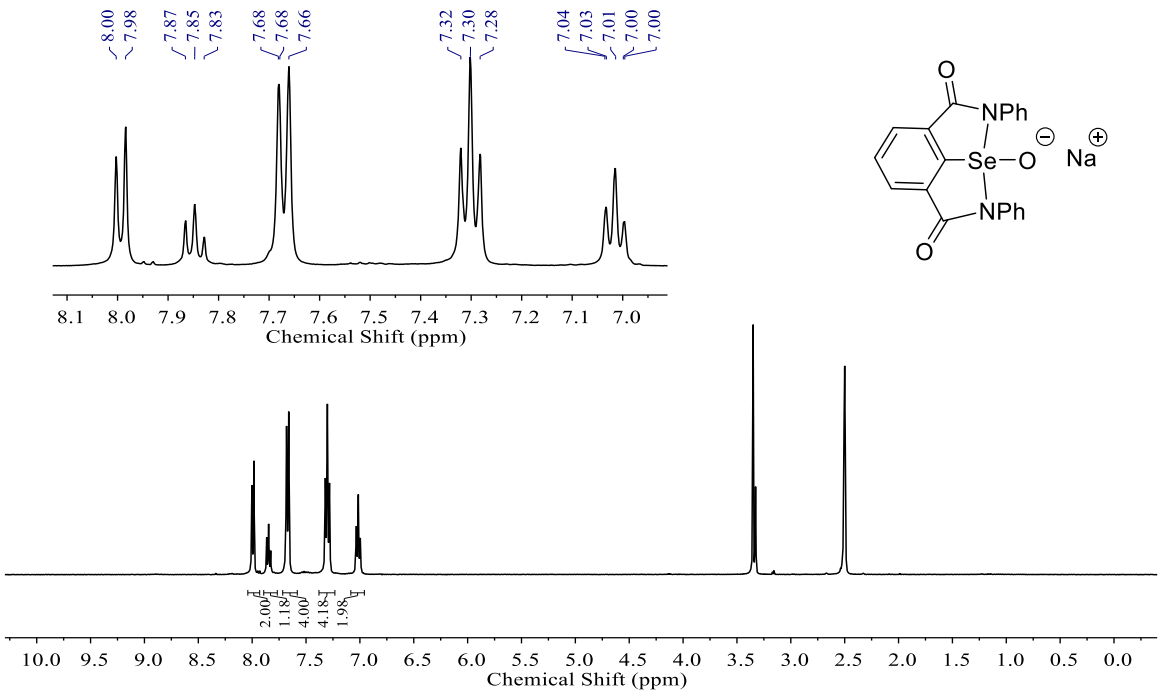


Figure 94. ^{13}C NMR Spectrum of 44 (101 MHz, DMSO-d$_6$)

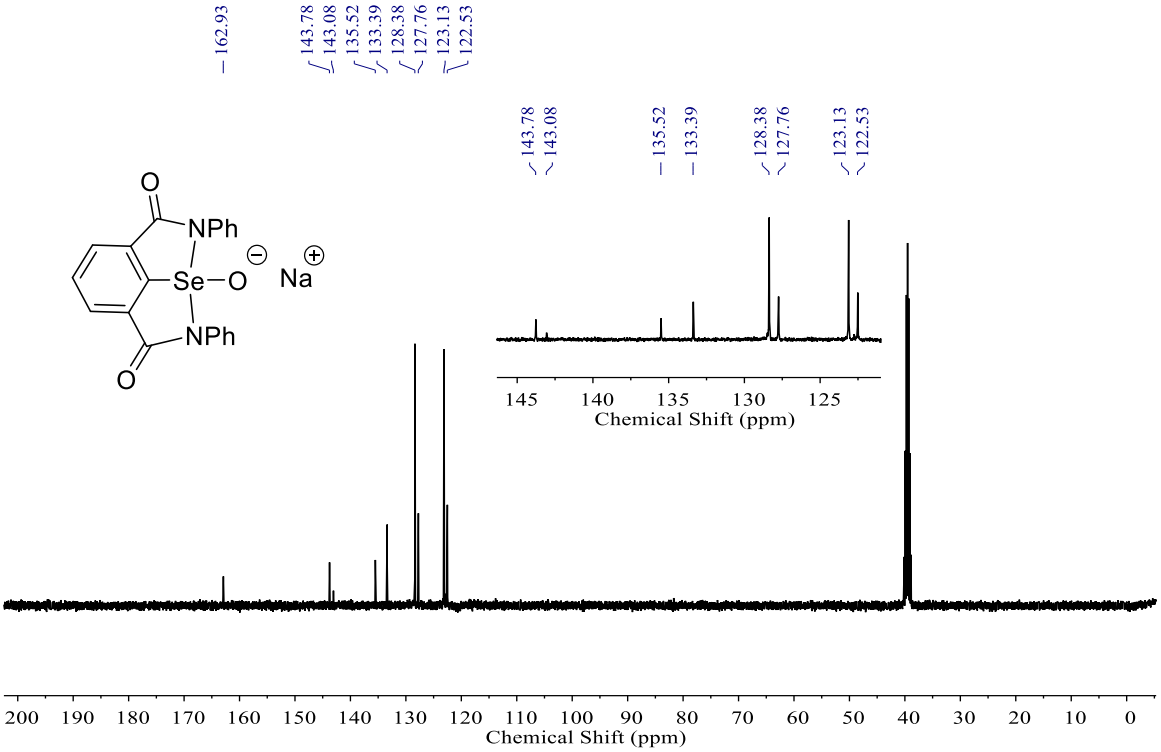
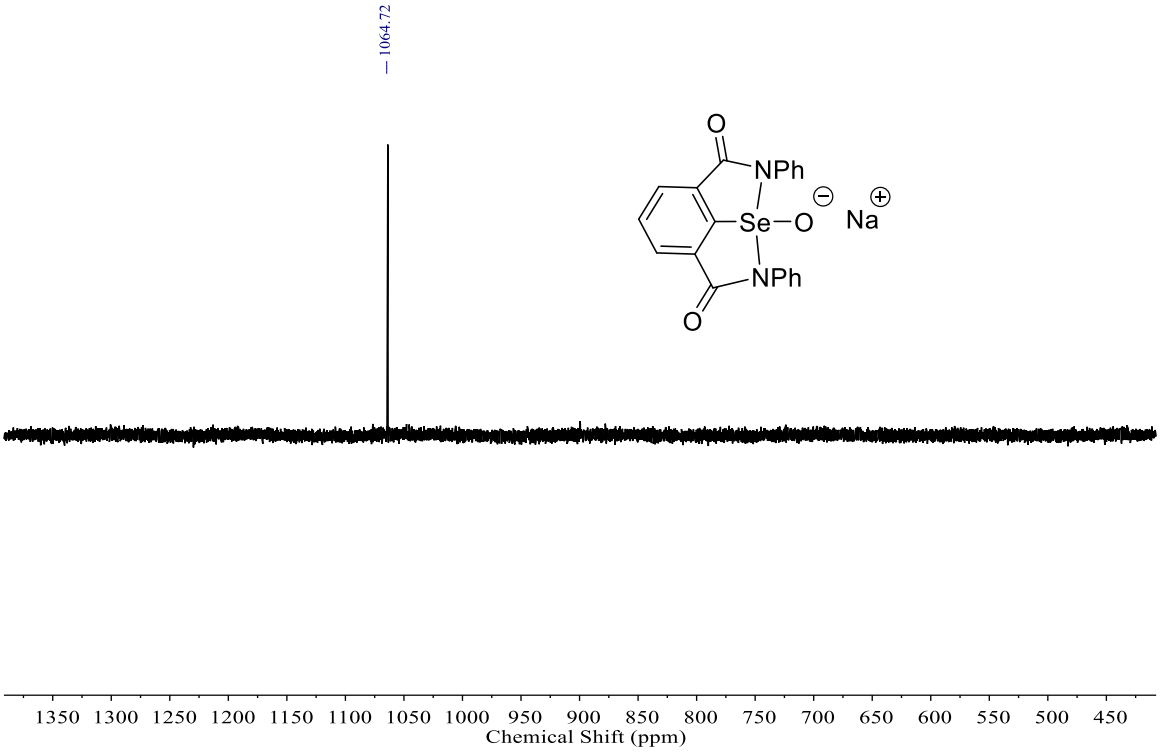


Figure 95. ^{77}Se NMR Spectrum of 44 (76 MHz, DMSO-d$_6$)



Kinetic Plots

Figure 96. Kinetic Plot of Ebselen (1)

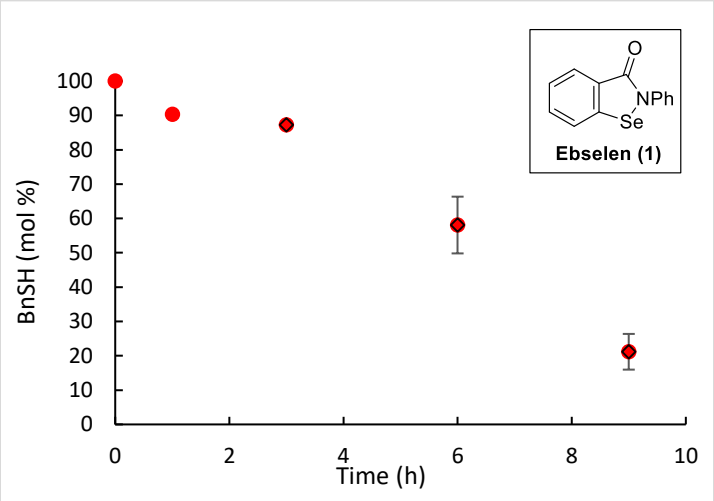


Figure 97. Kinetic Plot of Compound 2

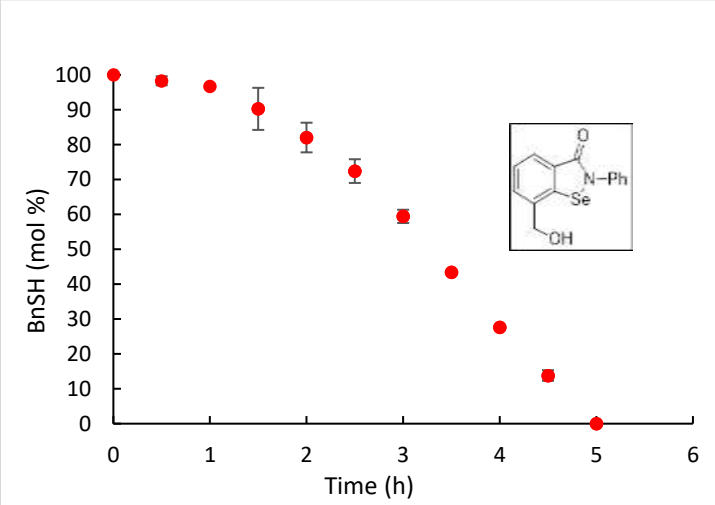


Figure 98. Kinetic Plot of Compound 2 with 2% DIPEA

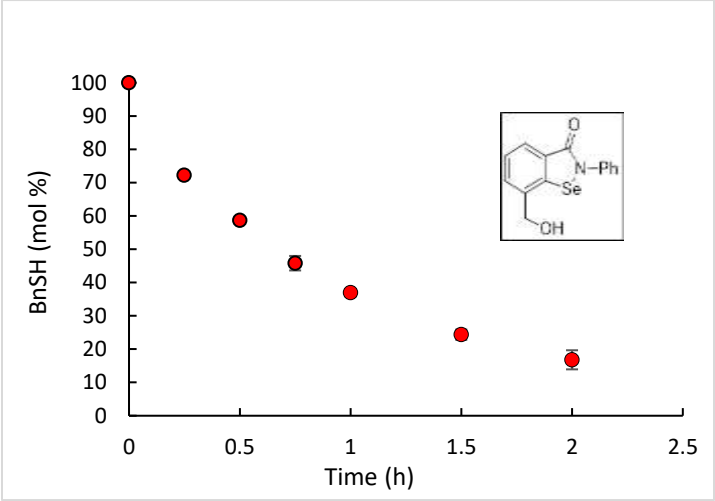


Figure 99. Kinetic Plot of Compound 3

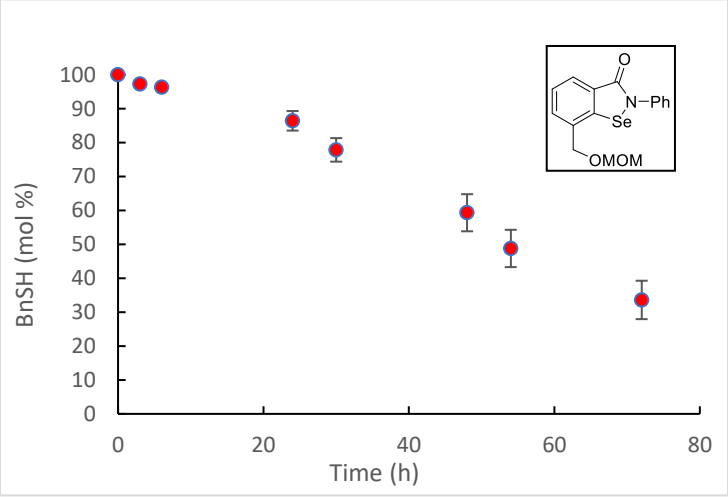


Figure 100. Kinetic Plot of Compound 4

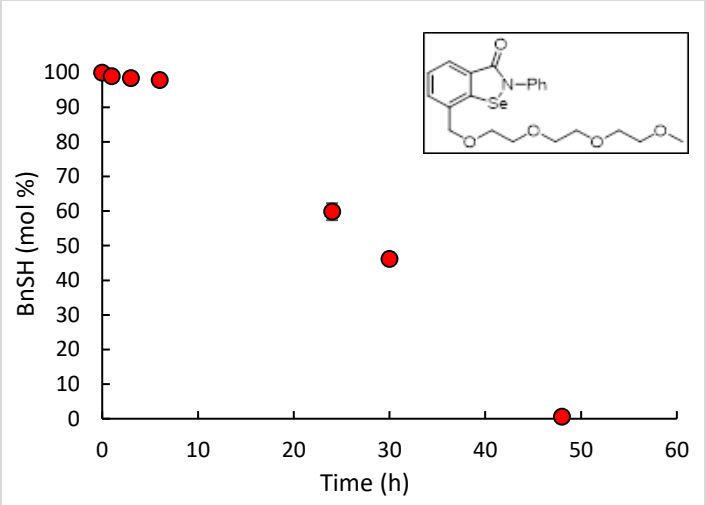


Figure 101. Kinetic Plot of Compund 5

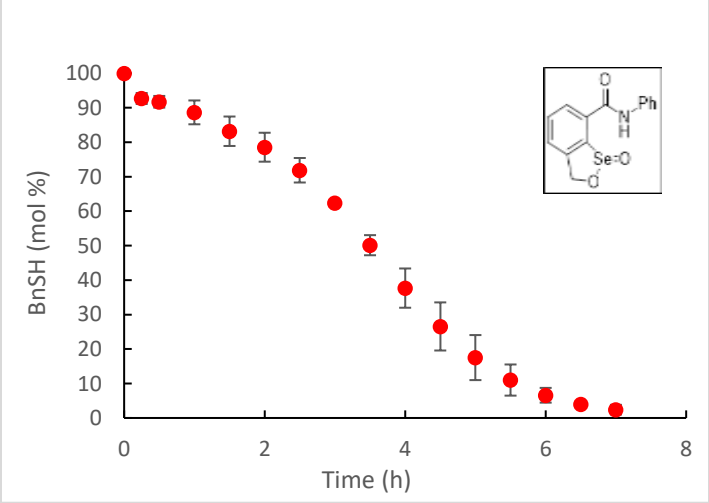


Figure 102. Kinetic Plot of Compound 6

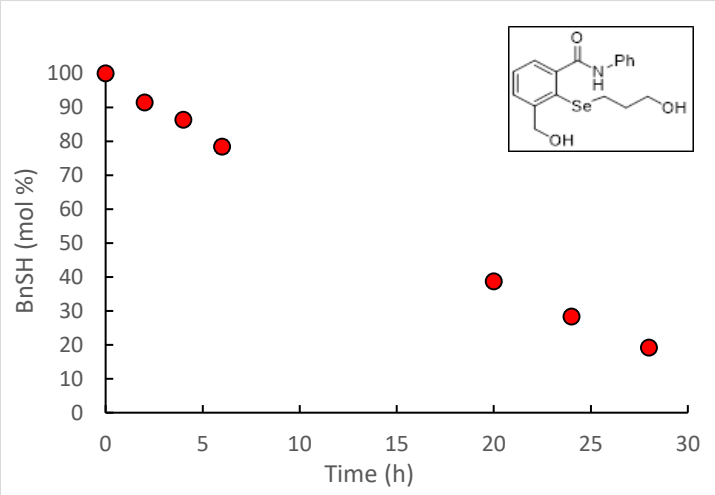


Figure 103. Kinetic Plot of Compound 7

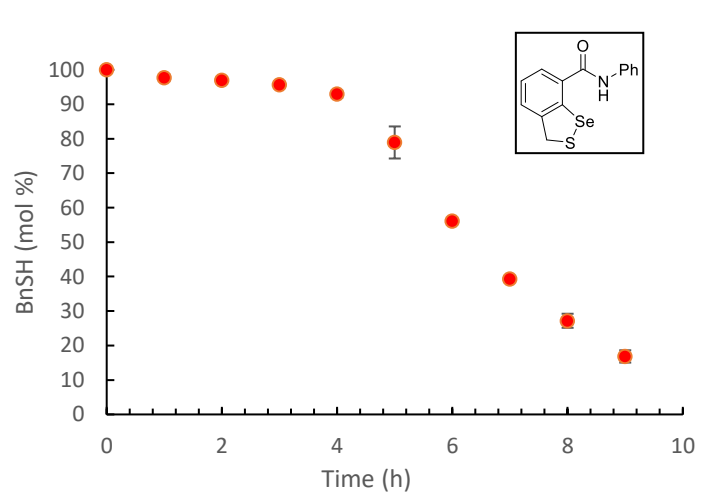


Figure 104. Kinetic Plot of Compound 9

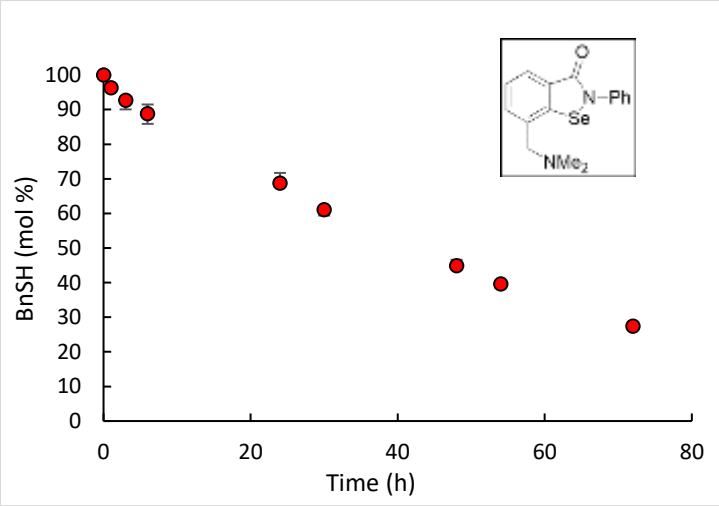


Figure 105. Kinetic Plot of Compound 10

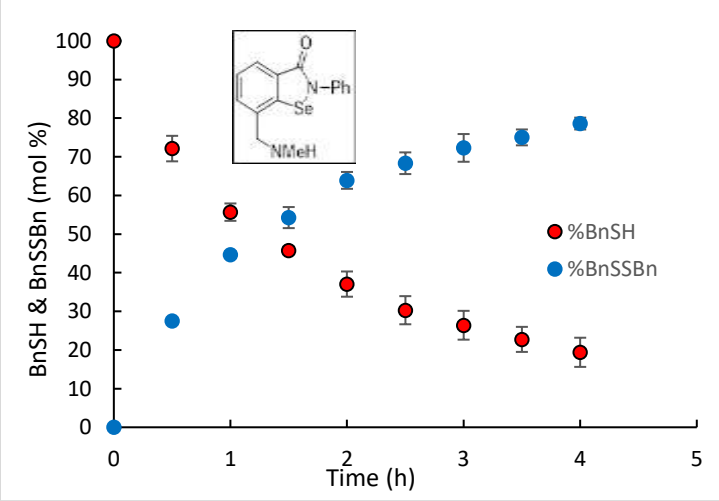


Figure 106. Kinetic Plot of Compound 11

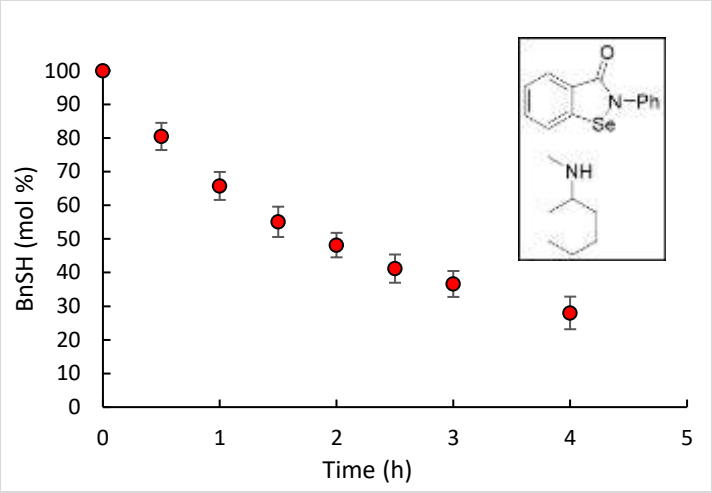


Figure 107. Kinetic Plot of Compound 12

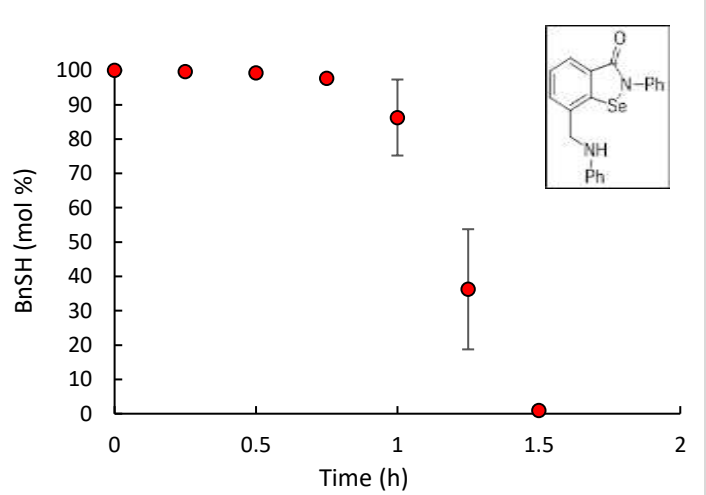


Figure 108. Kinetic Plot of Compound 13

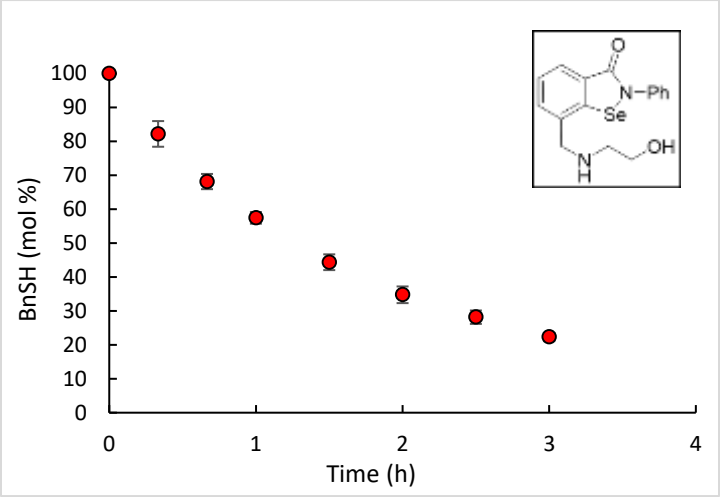


Figure 109. Kinetic Plot of Compound 14

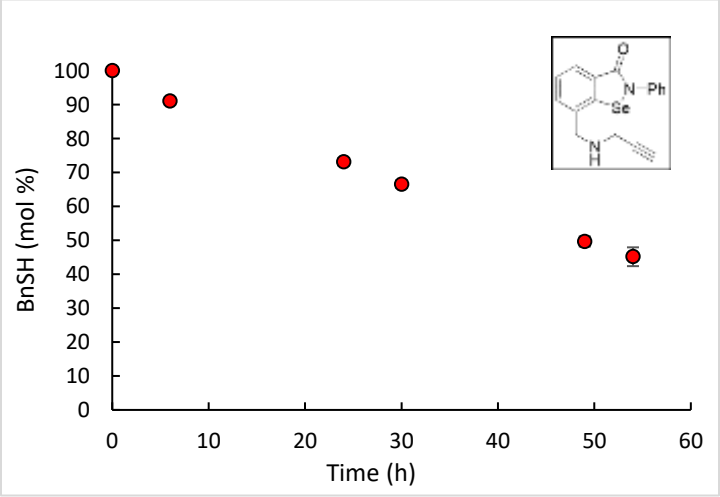


Figure 110. Kinetic Plot of Compound 15

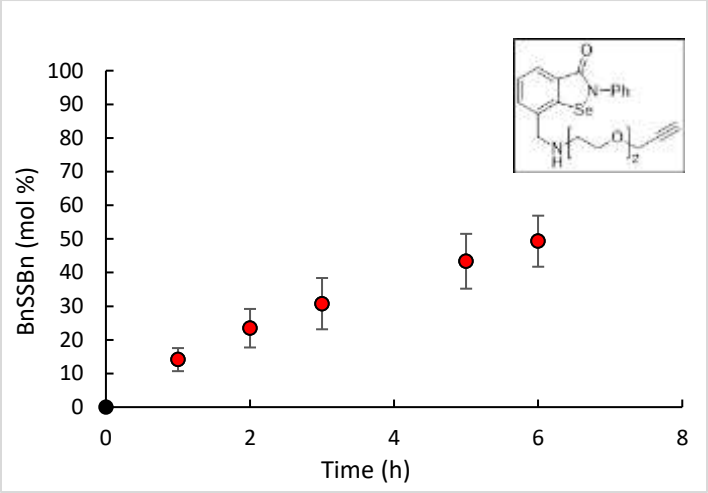


Figure 111. Kinetic Plot of Compound 16

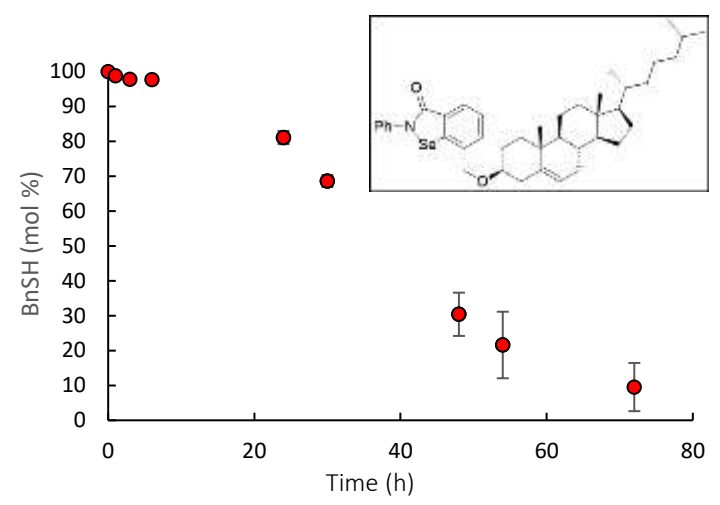


Figure 112. Kinetic Plot of Compound 17

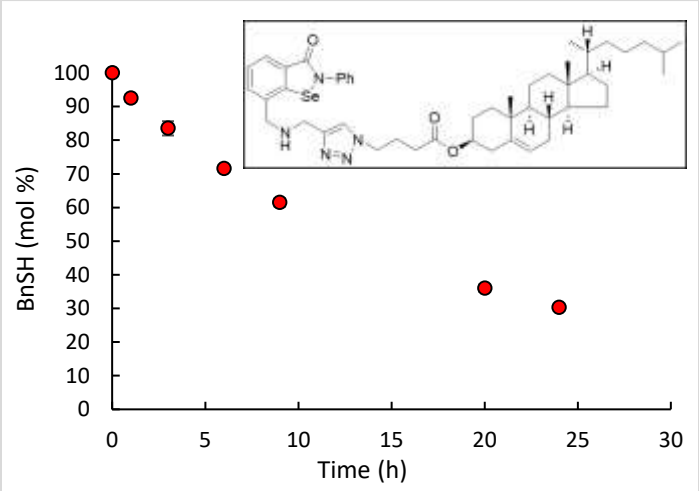


Figure 113. Kinetic Plot of Compound 18

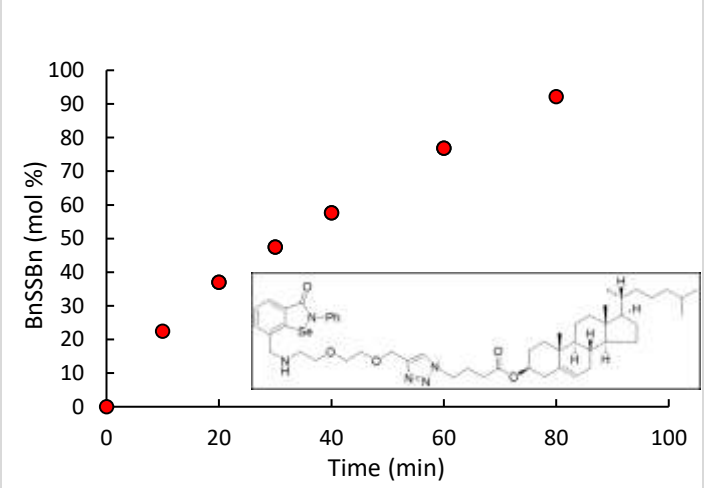


Figure 114. Kinetic Plot of Compound 19

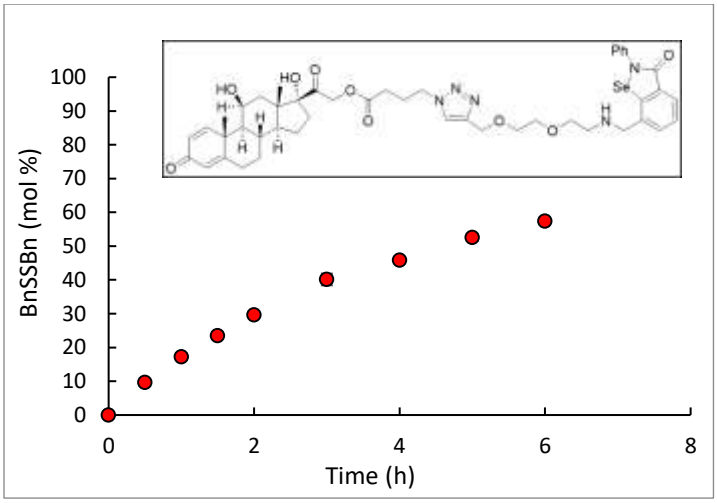


Figure 115. Kinetic Plot of Compound 20

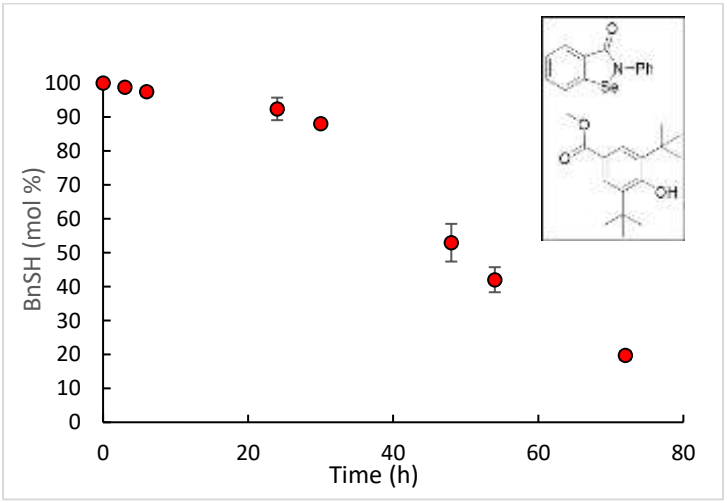


Figure 116. Kinetic Plot of Compound 27

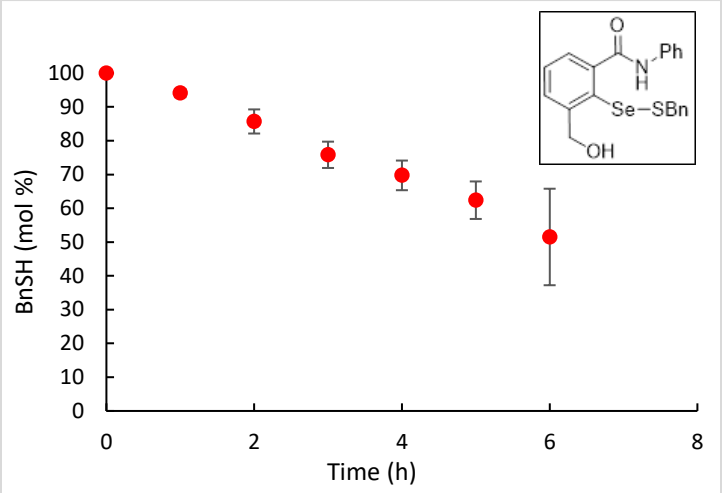


Figure 117. Kinetic Plot of Compound 27 with 2 mol % of DIPEA

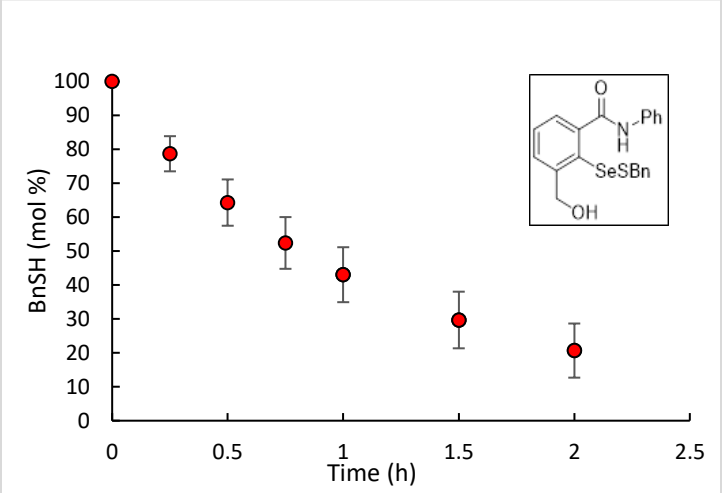


Figure 118. Kinetic Plot of Compound 8

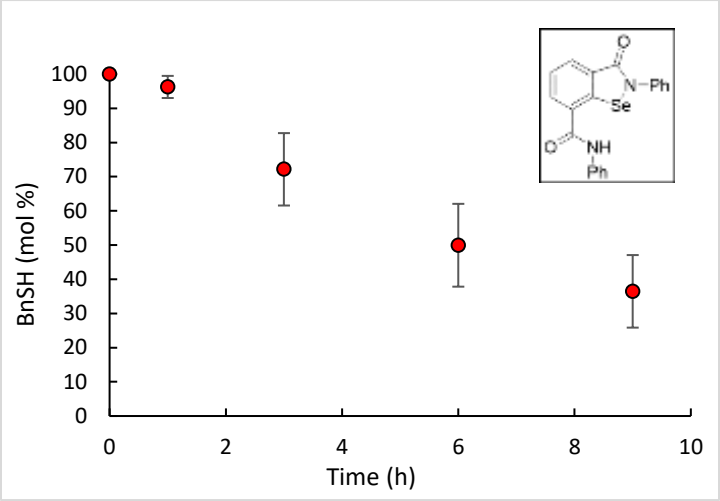


Figure 119. Kinetic Plot of Compound 42a

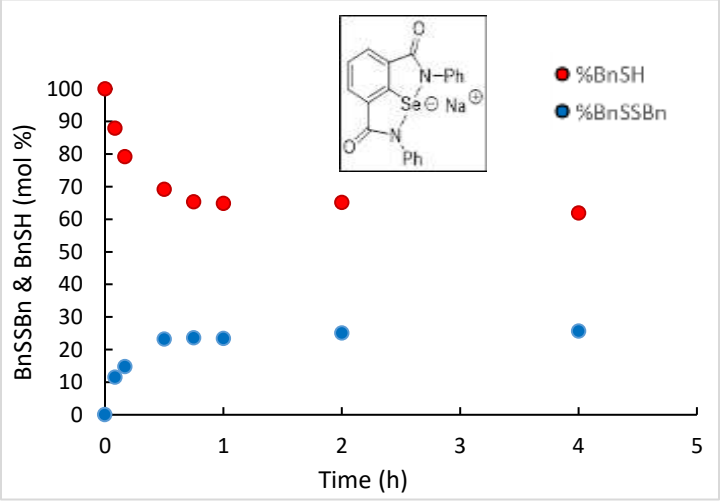


Figure 120. Kinetic Plot of Compound 42b

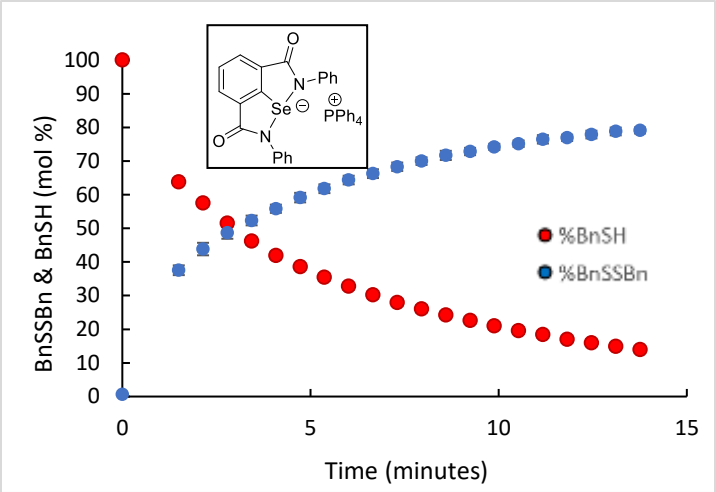
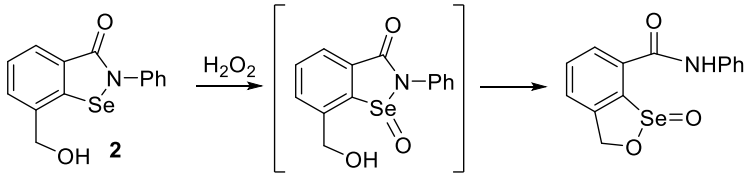


Figure 121. Control experiment – oxidation of 2 in the absence of BnSH



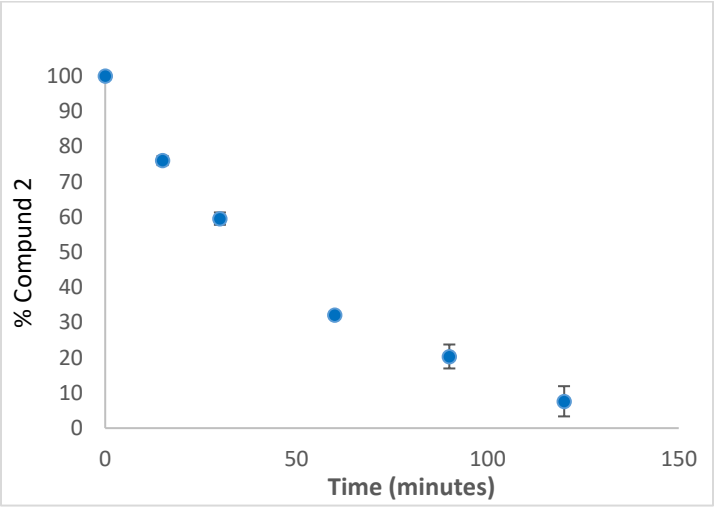
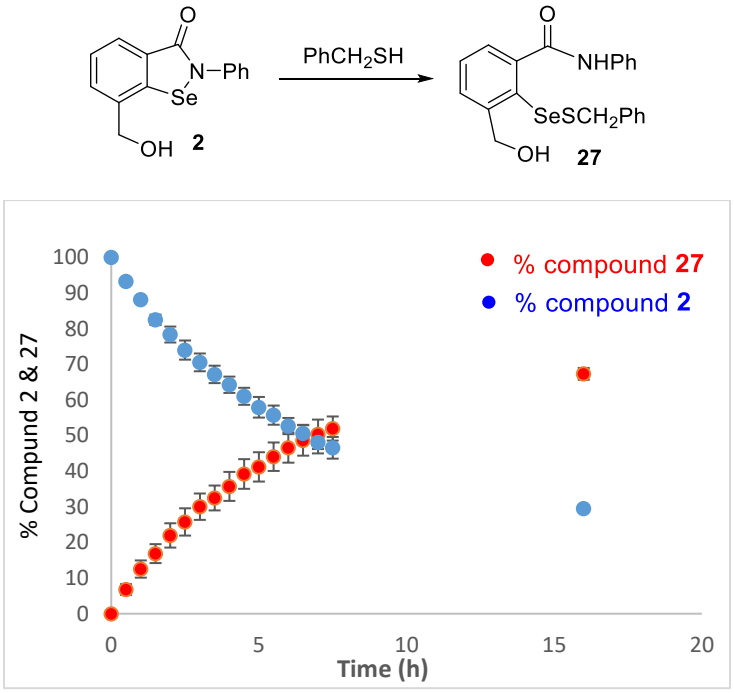


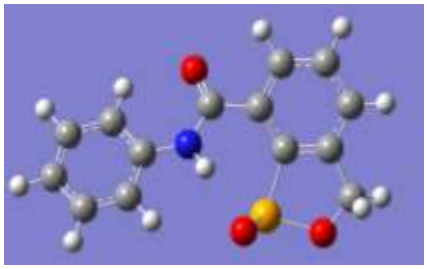
Figure 122. Control experiment – thiolysis of 2 in the absence of H_2O_2



Computational Studies

All computations were performed with Gaussian 09, [1] employing the DFT (B3LYP) platform and a split basis set with 6-311G(d,p) for C, H, N, O, S and cc-pVTZ for Se. The energies and Z-matrices from geometry optimizations are provided, including key structural data and images of optimized structures.

Table 1. Structure 5:

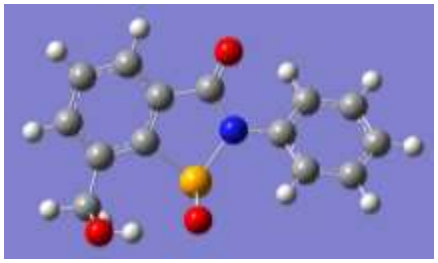


```
E(RB3LYP) =  -3222.34345227 A.U.
No imaginary frequencies were observed.

Symbolic Z-matrix:
 Charge =  0 Multiplicity = 1
 C                    -1.85073  -0.00608   0.13041
 C                    -1.14606   1.19022   0.2447
 C                    -1.82241   2.35351   0.03333
 C                    -3.20011   2.32332  -0.29318
 C                    -3.86675   1.08973  -0.43365
 C                    -3.13264  -0.07919  -0.23875
 C                     0.35095   1.19756   0.60598
 H                    -1.31302   3.29081   0.11633
 H                    -3.73522   3.23881  -0.43617
 H                    -4.90543   1.05134  -0.68776
 O                     0.96846   2.28936   0.70709
 C                     2.47065   0.0813    0.45358
 C                     3.19045  -1.02182  -0.02489
 C                     3.09705   1.32944   0.57058
 C                     4.53665  -0.87681  -0.38634
 H                     2.71218  -1.97481  -0.11422
 C                     4.44324   1.47446   0.20913
 H                     2.54746   2.1717    0.9359
 C                     5.16304   0.37134  -0.26933
 H                     5.08623  -1.71907  -0.75166
 H                     4.92151   2.42745   0.29847
 H                     6.19089   0.48206  -0.54531
 C                    -3.6733   -1.5553   -0.44421
 H                    -3.48406  -1.84482  -1.45676
 H                    -4.72421  -1.60756  -0.24994
 O                    -2.95554  -2.45566   0.46303
 N                     1.05856  -0.07081   0.83273
```

H	0.64003	-0.78982	0.27787
Se	-1.26906	-1.77854	0.42875
O	-0.30281	-2.33464	-0.73336

Table 2. Structure 37

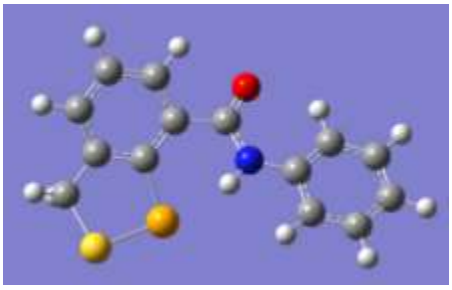


E(RB3LYP) = -3222.33443633 A.U.
No imaginary frequencies were observed

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	-1.4118	0.14866	-0.09058
C	-1.11814	1.55451	0.07558
C	-2.14138	2.47789	0.15078
C	-3.4659	2.0179	0.06227
C	-3.74822	0.6663	-0.09735
C	-2.71887	-0.28663	-0.1757
C	0.33256	1.6841	0.13047
H	-1.93438	3.54974	0.27684
H	-4.28996	2.74457	0.12095
H	-4.79405	0.33112	-0.16395
O	1.03957	2.93416	-0.08537
C	1.96961	0.1737	0.00607
C	2.4062	-1.14466	-0.13005
C	2.89837	1.20475	0.14711
C	3.77115	-1.43123	-0.12432
H	1.67397	-1.9575	-0.2415
C	4.26372	0.91804	0.15183
H	2.5546	2.24388	0.25441
C	4.70008	-0.39983	0.01628
H	4.1155	-2.47002	-0.23193
H	4.99572	1.73105	0.26283
H	5.77618	-0.62592	0.02033
Se	-0.1344	-0.55218	-0.13392
O	0.04476	-2.34094	0.20834
C	-3.05455	-1.77917	-0.35248
H	-2.56314	-2.15426	-1.22583
H	-4.11261	-1.89643	-0.46048
O	-2.60895	-2.50711	0.79488
H	-1.64548	-2.63649	-0.02237
N	0.89335	0.3994	0.00159

Table 3. Structure 7

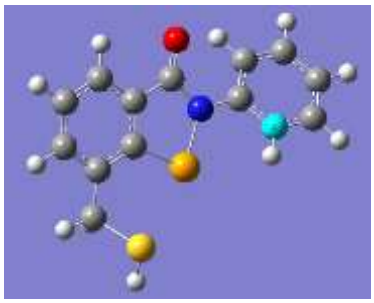


E(RB3LYP) = -3470.12866952 A.U.
No imaginary frequencies were observed.

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	-1.48777	0.28014	0.2208
C	-1.35544	1.61921	0.74962
C	-2.34784	2.55507	0.53841
C	-3.48145	2.17382	-0.19872
C	-3.60873	0.88641	-0.70703
C	-2.6082	-0.07817	-0.50129
C	-0.07969	1.67671	1.4521
H	-2.26187	3.57681	0.93371
H	-4.27914	2.91117	-0.37356
H	-4.50644	0.61232	-1.28109
O	0.97042	2.63038	1.14079
C	0.90848	0.24503	2.84872
C	0.98735	-1.00769	3.45839
C	1.85024	1.22838	3.15145
C	2.00744	-1.27604	4.37089
H	0.24501	-1.78303	3.21951
C	2.87115	0.95946	4.06351
H	1.78835	2.21576	2.67114
C	2.94967	-0.29256	4.67329
H	2.07006	-2.26326	4.85122
H	3.61359	1.73477	4.30186
H	3.7541	-0.50448	5.3924
C	-2.77005	-1.49875	-1.07345
H	-2.8597	-1.44626	-2.13839
H	-3.64908	-1.95043	-0.66335
N	0.10406	0.4564	2.12933
H	-0.04948	-0.42891	2.56827
S	-1.526	-2.14765	-0.6295
Se	-0.38974	-0.59003	0.51082

Table 4. Structure 41



E(RB3LYP) = -3470. 10626653 A.U.
No imaginary frequencies were observed

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	-1.48777	0.28014	0.2208
C	-1.35544	1.61921	0.74962
C	-2.34784	2.55507	0.53841
C	-3.48145	2.17382	-0.19872
C	-3.60873	0.88641	-0.70703

C	-2.6082	-0.07817	-0.50129
C	-0.07969	1.67671	1.4521
H	-2.26187	3.57681	0.93371
H	-4.27914	2.91117	-0.37356
H	-4.50644	0.61232	-1.28109
O	0.97042	2.63038	1.14079
C	0.90848	0.24503	2.84872
C	0.98735	-1.00769	3.45839
C	1.85024	1.22838	3.15145
C	2.00744	-1.27604	4.37089
H	0.24501	-1.78303	3.21951
C	2.87115	0.95946	4.06351
H	1.78835	2.21576	2.67114
C	2.94967	-0.29256	4.67329
H	2.07006	-2.26326	4.85122
H	3.61359	1.73477	4.30186
H	3.7541	-0.50448	5.3924
C	-2.77005	-1.49875	-1.07345
H	-2.8597	-1.44626	-2.13839
H	-3.64908	-1.95043	-0.66335
N	0.10406	0.4564	2.12933
S	-1.526	-2.14765	-0.6295
Se	-0.38974	-0.59003	0.51082
H	-0.49703	-1.47851	-1.0873

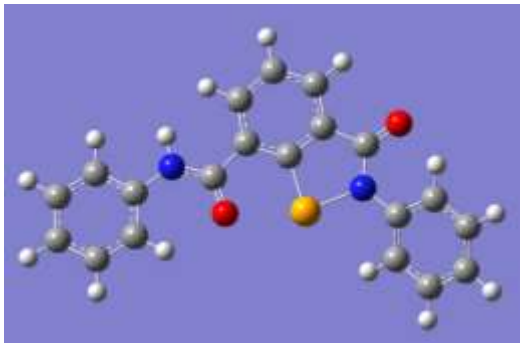


Table 5. Structure 8a

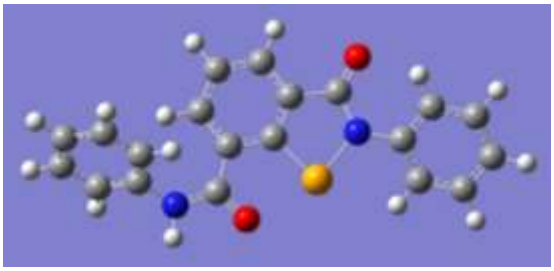
E(RB3LYP) = -3432.43377268 A.U.
No imaginary frequencies were observed

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	-2.35116	0.57965	-0.00207
C	-1.19937	1.60157	-0.02755
C	-1.45691	2.98503	-0.0605
C	0.12928	1.18616	-0.02635
C	-0.38262	3.90765	-0.09408
H	-2.46618	3.34034	-0.06334
C	1.1798	2.07714	0.02051
C	0.9511	3.45106	-0.05397
H	-0.58422	4.95714	-0.14732
H	1.76769	4.14221	-0.07404
O	-2.09835	-0.65283	0.02378
N	-3.74592	1.04388	-0.00794
H	-3.91796	1.57197	-0.83952

C	-4.64849	-0.11573	0.03163
C	-5.0856	-0.70451	-1.1626
C	-5.07183	-0.63245	1.26358
C	-5.94605	-1.81	-1.12488
H	-4.76237	-0.30998	-2.10323
C	-5.93228	-1.73794	1.30131
H	-4.73808	-0.1829	2.17541
C	-6.36939	-2.32672	0.10707
H	-6.2798	-2.25955	-2.0367
H	-6.2555	-2.13247	2.24193
H	-7.02637	-3.17079	0.13587
C	2.56672	1.38126	0.16384
O	3.60658	1.92045	-0.29609
N	2.48989	-0.07009	0.50888
C	3.75018	-0.78667	0.26582
C	4.69928	-0.9024	1.29039
C	4.00257	-1.35408	-0.99048
C	5.90075	-1.58554	1.05867
H	4.50658	-0.46917	2.2496
C	5.20404	-2.03722	-1.2222
H	3.27791	-1.26571	-1.77276
C	6.15314	-2.15295	-0.19762
H	6.62541	-1.6739	1.84095
H	5.39675	-2.47045	-2.1814
H	7.07049	-2.67454	-0.37455
Se	0.81038	-0.60293	-0.10654

Table 6. Structure 8b



E(RB3LYP) = -3432.43377268 A.U.
No imaginary frequencies were observed

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	-4.08331	2.60568	-0.52784
C	-3.43268	2.55697	-1.9228
C	-2.34296	1.70582	-2.18628
C	-3.89882	3.3588	-2.96091
C	-1.75265	1.68424	-3.47372
H	-1.95776	1.07617	-1.41164
C	-3.38184	3.28703	-4.23653
C	-2.2756	2.48322	-4.51154
H	-0.9069	1.05603	-3.66067
H	-1.83806	2.46854	-5.48788
O	-5.05452	3.37653	-0.31313
N	-3.56984	1.75171	0.55289
H	-4.10857	1.90287	1.38169
C	-3.67156	0.34084	0.15288
C	-3.24071	-0.66766	1.02535

C	-4.19938	0.00432	-1.10095
C	-3.33768	-2.01268	0.64401
H	-2.83771	-0.41071	1.98268
C	-4.29635	-1.34071	-1.4823
H	-4.52834	0.77433	-1.76711
C	-3.8655	-2.34921	-0.60982
H	-3.00872	-2.78269	1.31016
H	-4.69935	-1.59765	-2.43962
H	-3.93954	-3.37616	-0.90099
C	-4.15771	4.16738	-5.26189
O	-3.57392	4.64678	-6.26834
N	-5.46277	4.68899	-4.75583
C	-5.9882	5.80182	-5.55984
C	-6.07682	5.67901	-6.95303
C	-6.40049	6.98554	-4.93314
C	-6.57773	6.7399	-7.71952
H	-5.76202	4.77521	-7.43153
C	-6.9014	8.04644	-5.69963
H	-6.33283	7.07931	-3.8694
C	-6.99003	7.92362	-7.09282
H	-6.64539	6.64613	-8.78325
H	-7.2162	8.95023	-5.22112
H	-7.37248	8.73364	-7.67805
Se	-5.26838	4.69734	-2.8996

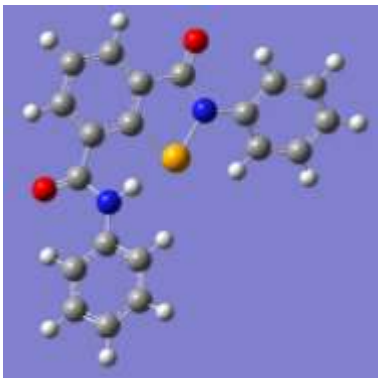


Table 7. Structure 8c

E(RB3LYP) = -3432.42216700 A.U.
No imaginary frequencies were observed

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	-2.35116	0.57965	-0.00207
C	-1.19937	1.60157	-0.02755
C	-0.65665	2.11367	1.16601
C	-0.66716	2.05374	-1.23178
C	0.39561	3.06079	1.11972
H	-1.04184	1.78919	2.11007
C	0.40797	2.91449	-1.28518
C	0.93491	3.4677	-0.11821
H	0.78543	3.46773	2.0293
H	1.7331	4.17902	-0.16088
O	-2.81735	0.18433	1.09792
N	-2.90601	0.06596	-1.26269

H	-2.18733	-0.40196	-1.77704
C	-3.99369	-0.87873	-0.97039
C	-3.71328	-2.24244	-0.81048
C	-5.31101	-0.41561	-0.85166
C	-4.75019	-3.14304	-0.53183
H	-2.70747	-2.59604	-0.90114
C	-6.34793	-1.31621	-0.573
H	-5.52511	0.62562	-0.97375
C	-6.06752	-2.67992	-0.41309
H	-4.53609	-4.18427	-0.40973
H	-7.35373	-0.96261	-0.48234
H	-6.85923	-3.36755	-0.20033
C	0.92177	3.16296	-2.73522
O	1.48075	4.24796	-3.04161
N	0.36026	2.22391	-3.75221
C	0.5409	2.69582	-5.13264
C	1.68044	2.32182	-5.85754
C	-0.42643	3.51971	-5.72374
C	1.85265	2.7717	-7.17355
H	2.41902	1.69276	-5.40622
C	-0.25422	3.9696	-7.03974
H	-1.2965	3.80527	-5.17026
C	0.88532	3.59559	-7.76465
H	2.72272	2.48614	-7.72703
H	-0.9928	4.59865	-7.49106
H	1.0168	3.93909	-8.76945
Se	-1.25403	1.65139	-3.01078

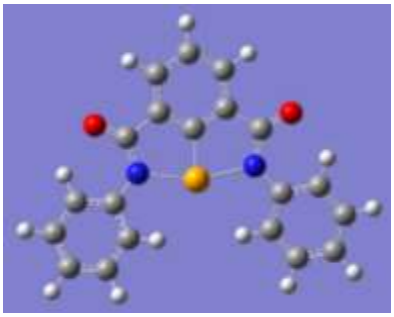


Table 8. Structure 45a

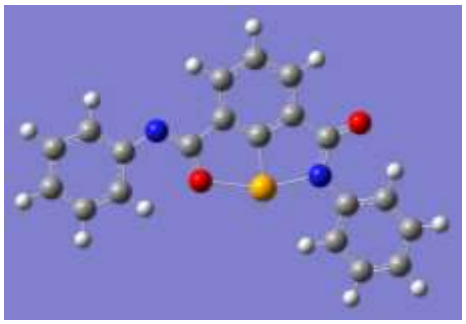
E(RB3LYP) = -3431.90874973 A.U.
No imaginary frequencies were observed

Symbolic Z-matrix:
Charge = -1 Multiplicity = 1

C	-0.70768	3.83737	-0.64558
C	0.12101	2.59319	-0.27561
C	-0.45834	1.31035	-0.27012
C	1.46474	2.70258	0.07126
C	0.31935	0.18047	0.08342
H	-1.48904	1.18885	-0.53049
C	2.24837	1.60106	0.33997
C	1.68763	0.32503	0.39295
H	-0.13324	-0.78865	0.11307
H	2.28259	-0.52448	0.65612

O	-1.92286	3.71646	-0.94939
N	0.25358	5.05436	-0.52543
C	-0.74313	6.06827	-0.89886
C	-2.04308	5.67783	-1.24759
C	-0.39338	7.4253	-0.90614
C	-2.99327	6.64442	-1.6036
H	-2.31012	4.6417	-1.24204
C	-1.34358	8.3919	-1.26214
H	0.59916	7.72341	-0.63987
C	-2.64352	8.00146	-1.61088
H	-3.98581	6.34631	-1.86987
H	-1.07654	9.42802	-1.26769
H	-3.36902	8.73947	-1.8827
C	3.75002	1.95639	0.5571
O	4.47733	1.24656	1.29921
N	4.11255	3.34958	0.15839
C	5.40128	3.78948	0.71207
C	5.49076	5.01049	1.39402
C	6.54038	2.98785	0.55797
C	6.71935	5.42986	1.92187
H	4.62103	5.62255	1.51169
C	7.76897	3.40722	1.08582
H	6.47206	2.05558	0.03728
C	7.85845	4.62823	1.76777
H	6.78767	6.36213	2.44256
H	8.6387	2.79516	0.96816
H	8.7965	4.94843	2.1708
Se	2.17562	4.4081	0.15847

Table 9. Structure 45b



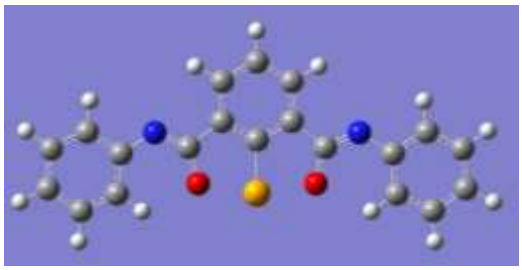
E(RB3LYP) = -3431.90237267 A.U.
No imaginary frequencies were observed

Symbolic Z-matrix:
Charge = -1 Multiplicity = 1

C	-2.11989	0.39877	0.00329
C	-1.15486	1.5379	-0.02187
C	-1.46396	2.89868	-0.0371
C	0.19017	1.18341	-0.02733
C	-0.44145	3.8542	-0.0549
H	-2.50917	3.1839	-0.03369
C	1.22265	2.11222	-0.04201
C	0.90056	3.46986	-0.0561
H	-0.69709	4.90878	-0.0661
H	1.70454	4.19718	-0.0671

O	-1.54773	-0.76344	0.02666
N	-3.39433	0.69525	-0.00065
C	-4.40935	-0.25119	0.02081
C	-4.27124	-1.66027	0.05693
C	-5.7271	0.26177	0.00496
C	-5.39371	-2.48419	0.07562
H	-3.27736	-2.0811	0.06913
C	-6.83889	-0.5683	0.02342
H	-5.83574	1.34043	-0.02253
C	-6.6839	-1.95592	0.05918
H	-5.25416	-3.56159	0.10334
H	-7.83407	-0.13252	0.01005
H	-7.55016	-2.60961	0.07384
C	2.60169	1.56088	-0.03339
O	3.60603	2.2751	-0.03007
N	2.56757	0.18151	-0.03547
C	3.69778	-0.64578	-0.01607
C	3.54903	-2.01438	-0.31784
C	4.99142	-0.1854	0.31088
C	4.63292	-2.8833	-0.28286
H	2.57501	-2.3948	-0.5983
C	6.06663	-1.06762	0.33748
H	5.12981	0.86262	0.5228
C	5.90521	-2.42086	0.04642
H	4.47744	-3.93071	-0.52169
H	7.04948	-0.6832	0.59335
H	6.75148	-3.09896	0.0718
Se	0.67849	-0.61982	-0.00447

Table 10. Structure 45c



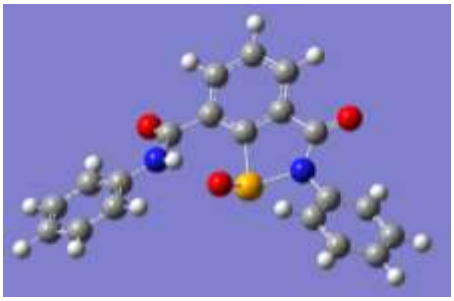
E(RB3LYP) = -3431.89124391 A.U.
No imaginary frequencies were observed

Symbolic Z-matrix:
Charge = -1 Multiplicity = 1

C	-0.79649	2.23985	2.58305
C	0.06813	1.80096	1.38664
C	0.38586	2.70063	0.35175
C	0.55386	0.4999	1.29072
C	1.17402	2.27328	-0.74489
H	0.02869	3.70845	0.392
C	1.38583	0.09753	0.26819
C	1.68002	0.95766	-0.78971
H	1.38907	2.95338	-1.54246
H	2.28015	0.62915	-1.6124

O	-1.0666	1.41983	3.49857
N	-1.14201	3.7379	2.3464
C	-1.92315	3.90679	3.58017
C	-2.12925	2.81483	4.43403
C	-2.46174	5.15976	3.90251
C	-2.87394	2.97585	5.61022
H	-1.71802	1.85816	4.18792
C	-3.20644	5.32078	5.0787
H	-2.30438	5.9935	3.25057
C	-3.41254	4.22882	5.93256
H	-3.03131	2.14211	6.26216
H	-3.61766	6.27745	5.32481
H	-3.98113	4.35176	6.83061
C	1.92052	-1.35489	0.44966
O	1.59658	-2.03766	1.45587
N	2.96835	-1.99203	-0.3282
C	3.68719	-3.1946	0.11676
C	5.07623	-3.15378	0.29793
C	2.98345	-4.38187	0.35979
C	5.76153	-4.30023	0.72213
H	5.61356	-2.24727	0.11237
C	3.66875	-5.52831	0.78399
H	1.92289	-4.41303	0.22146
C	5.05779	-5.48749	0.96516
H	6.82209	-4.26906	0.86045
H	3.13143	-6.43482	0.96954
H	5.58103	-6.36283	1.28904
Se	-0.2172	-0.49948	2.73206

Table 11. Structure 43a



E(RB3LYP) = -3507.62990002 A.U.
No imaginary frequencies were observed

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	-3.79946	1.8203	3.0231
C	-2.81552	1.29215	1.96268
C	-1.91636	2.15761	1.31164
C	-2.79242	-0.05491	1.61227
C	-1.02681	1.65272	0.33172
H	-1.90696	3.19948	1.5552
C	-1.87774	-0.56804	0.71801
C	-1.00597	0.27538	0.0294
H	-0.36491	2.31972	-0.18003
H	-0.33341	-0.11404	-0.70606

O	-3.7002	3.00363	3.43959
N	-4.61464	0.70998	3.5365
H	-4.1966	-0.15966	3.27392
C	-4.69034	0.79451	5.00212
C	-5.22234	-0.25594	5.76202
C	-4.51394	2.0586	5.58081
C	-5.57794	-0.0423	7.10061
H	-5.35702	-1.2211	5.32017
C	-4.86955	2.27224	6.9194
H	-4.10775	2.86065	5.00061
C	-5.40154	1.22179	7.6793
H	-5.98413	-0.84435	7.68081
H	-4.73486	3.2374	7.36125
H	-5.67305	1.3849	8.70134
C	-1.94577	-2.12005	0.59553
O	-1.6191	-2.69488	-0.47519
N	-2.7663	-2.78157	1.65405
C	-3.13518	-4.16382	1.31607
C	-4.47085	-4.57651	1.41403
C	-2.15117	-5.06886	0.89591
C	-4.82251	-5.89425	1.09182
H	-5.22216	-3.88549	1.73483
C	-2.50283	-6.38661	0.5737
H	-1.13136	-4.75376	0.82112
C	-3.8385	-6.7993	0.67165
H	-5.84232	-6.20935	1.16661
H	-1.75151	-7.07763	0.2529
H	-4.107	-7.80542	0.42564
O	-5.05274	-1.48938	2.75937
Se	-3.95341	-1.455	2.21477

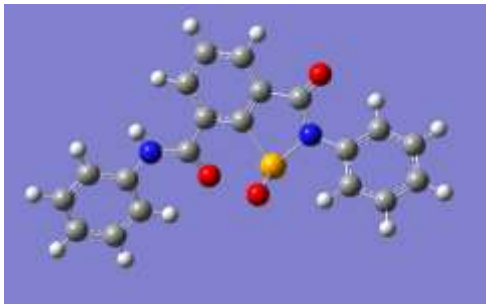


Table 12. Structure 43b

E(RB3LYP) = -3507.62808731 A.U.
No imaginary frequencies were observed

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	-2.1703	0.99804	-0.12208
C	-1.07785	1.83326	-0.81529
C	-1.39079	3.04247	-1.46433
C	0.24906	1.41246	-0.82631
C	-0.37223	3.79	-2.10477
H	-2.40059	3.39607	-1.47663
C	1.25825	2.17168	-1.37837
C	0.96749	3.35144	-2.0633
H	-0.62027	4.69407	-2.62055
H	1.74299	3.91335	-2.54055

O	-1.86901	-0.08187	0.4494
N	-3.56506	1.46227	-0.12795
H	-3.62552	2.32989	-0.6215
C	-4.41202	0.46085	-0.79181
C	-4.62865	0.53212	-2.17453
C	-5.00283	-0.56512	-0.04196
C	-5.43608	-0.42257	-2.8074
H	-4.17755	1.31546	-2.74705
C	-5.81026	-1.51981	-0.67484
H	-4.83743	-0.61953	1.01377
C	-6.02689	-1.44854	-2.05756
H	-5.60148	-0.36816	-3.86314
H	-6.26136	-2.30316	-0.10232
H	-6.64339	-2.17747	-2.54077
C	2.6762	1.5702	-1.14176
O	3.60763	1.77908	-1.96174
N	2.71175	0.46483	-0.13763
C	3.94392	-0.334	-0.20485
C	5.04813	0.01332	0.58511
C	4.01439	-1.44286	-1.05888
C	6.2228	-0.74823	0.52103
H	4.99432	0.85997	1.23718
C	5.18907	-2.20441	-1.12296
H	3.17131	-1.70804	-1.66203
C	6.29327	-1.8571	-0.333
H	7.06589	-0.48304	1.12418
H	5.24287	-3.05105	-1.77503
H	7.19016	-2.43856	-0.38193
O	0.39423	-1.57407	0.23879
Se	0.97749	-0.22484	-0.14823

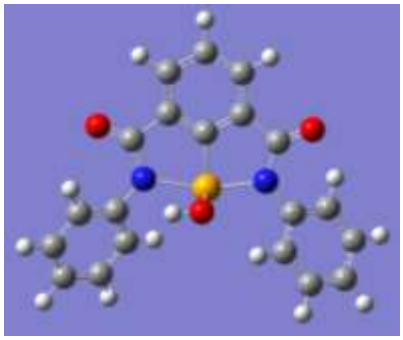


Table 13. Structure 43c

E(RB3LYP) = -3507.60963872 A.U.
No imaginary frequencies were observed

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	2.44019	1.51807	-0.03197
C	1.23376	2.41182	-0.04001
C	1.22522	3.80543	-0.02265
C	0.01416	1.7705	-0.07933
C	-0.0046	4.47496	-0.03936
H	2.16325	4.34637	0.00309
C	-1.21684	2.38875	-0.09044
C	-1.22201	3.78437	-0.07047

H	-0.01317	5.55839	-0.02458
H	-2.16996	4.30783	-0.07464
O	3.58095	1.94373	-0.00707
N	2.04319	0.1927	0.05965
C	2.94245	-0.90332	0.03963
C	4.09995	-0.88174	-0.75252
C	2.64813	-2.04766	0.79207
C	4.93699	-1.99101	-0.78521
H	4.344	0.00754	-1.31496
C	3.48611	-3.15867	0.73729
H	1.78061	-2.05037	1.44079
C	4.63397	-3.13634	-0.04932
H	5.83276	-1.96022	-1.395
H	3.24392	-4.03746	1.32364
H	5.29042	-3.9975	-0.08435
C	-2.43002	1.49639	-0.10552
O	-3.56664	1.9504	-0.10429
N	-2.04304	0.17781	-0.16934
C	-2.95622	-0.90546	-0.19735
C	-2.5556	-2.12703	-0.76792
C	-4.24647	-0.81204	0.35265
C	-3.40892	-3.22535	-0.76803
H	-1.58037	-2.2114	-1.23122
C	-5.09335	-1.91619	0.33675
H	-4.57584	0.1345	0.75151
C	-4.68325	-3.12807	-0.21402
H	-3.07926	-4.15659	-1.21424
H	-6.08759	-1.82304	0.75894
H	-5.35049	-3.9816	-0.22181
O	-0.05111	-0.46159	1.69204
Se	0.0713	-0.11894	-0.05612
H	-0.99079	-0.6509	1.84765

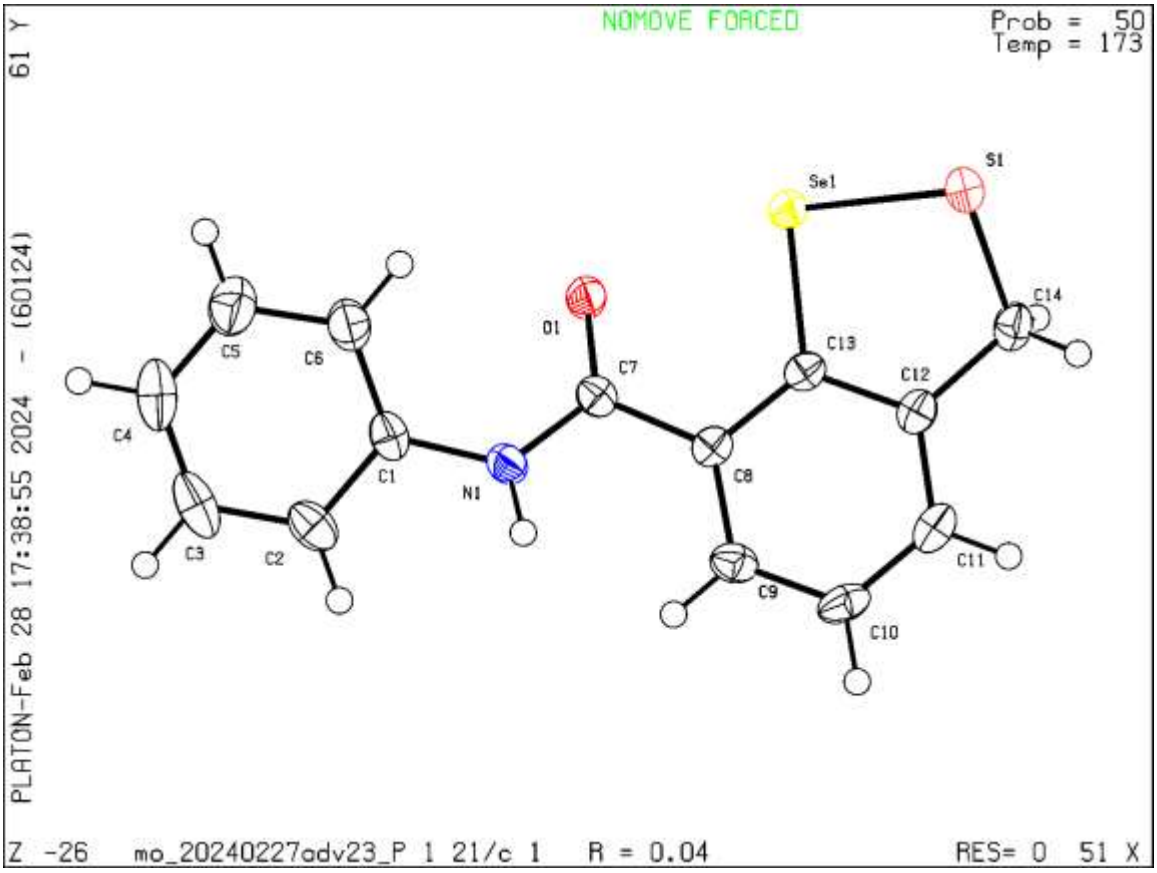
Reference for Gaussian 09, Revision A.02:

M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

X-Ray Structures

X-Ray Structure 1. Compound 7.

ORTEP Diagram



Experimental.

Single crystals of $C_{14}H_{11}NOSSe$ [selenenyl sulfide **7**] were grown from chloroform-hexane by slow evaporation. A suitable crystal was selected and run on a Bruker APEX-II CCD diffractometer. The crystal was kept at 296.15 K during data collection. Using Olex2 [1], the structure was solved with the olex2.solve [2] structure solution program using Charge Flipping and refined with the SHELXL [3] refinement package using Least Squares minimisation.

1. Dolomanov, O.V., Bourhis, L.J., Gildea, R.J, Howard, J.A.K. & Puschmann, H. (2009), J. Appl. Cryst. 42, 339-341.
2. Bourhis, L.J., Dolomanov, O.V., Gildea, R.J., Howard, J.A.K., Puschmann, H. (2015). Acta Cryst. A71, 59-75.
3. Sheldrick, G.M. (2015). Acta Cryst. C71, 3-8.

Crystal structure determination of selenenyl sulfide **7**

Crystal Data for $C_{14}H_{11}NOSSe$ (M =320.26 g/mol): monoclinic, space group $P2_1/c$ (no. 14), a = 7.6587(6) Å, b = 12.8138(10) Å, c = 13.2244(10) Å, β = 101.1960(10)°, V = 1273.10(17) Å^3, Z = 4, T = 296.15 K, μ(MoKα) = 3.099 mm^{-1}, *Dcalc* = 1.671 g/cm^3, 10086 reflections measured (4.468° ≤ 2Θ ≤ 56.918°), 3196 unique (R_{int} = 0.0456, R_{sigma} = 0.0519) which were used in all calculations. The final R_1 was 0.0368 (I > 2σ(I)) and wR_2 was 0.0819 (all data).

Table 1 Crystal data and structure refinement for selenenyl sulfide **7**.

Empirical formula	$C_{14}H_{11}NOSSe$
Formula weight	320.26
Temperature/K	296.15
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	7.6587(6)
b/Å	12.8138(10)
c/Å	13.2244(10)
α/°	90
β/°	101.1960(10)
γ/°	90
Volume/Å^3	1273.10(17)
Z	4
ρ_{calc}g/cm^3	1.671
μ/mm^{-1}	3.099
F(000)	640.0
Crystal size/mm^3	0.313 × 0.158 × 0.084
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.468 to 56.918
Index ranges	-9 ≤ h ≤ 10, -15 ≤ k ≤ 17, -17 ≤ l ≤ 17
Reflections collected	10086
Independent reflections	3196 [R_{int} = 0.0456, R_{sigma} = 0.0519]
Data/restraints/parameters	3196/0/163
Goodness-of-fit on F^2	1.030
Final R indexes [I>=2σ (I)]	R_1 = 0.0368, wR_2 = 0.0756
Final R indexes [all data]	R_1 = 0.0559, wR_2 = 0.0819
Largest diff. peak/hole / e Å^{-3}	0.88/-0.41

Table 2 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for compound **7**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	***x***	***y***	***z***	**U(eq)**
Se1	3928.2(4)	7414.4(2)	5034.3(2)	26.38(10)
S1	5759.5(11)	7888.2(6)	3983.8(5)	31.51(18)
O1	2149(3)	6209.9(13)	6075.5(14)	28.9(4)
N1	1928(3)	4443.8(16)	6130.0(16)	25.5(5)
C1	1536(4)	4296(2)	7126(2)	26.2(6)
C2	670(4)	3378(2)	7293(2)	31.9(7)
C3	306(4)	3170(3)	8259(3)	39.3(8)
C4	795(4)	3869(3)	9049(2)	44.4(8)
C5	1672(4)	4771(3)	8887(2)	44.7(8)
C6	2053(4)	4998(2)	7930(2)	35.8(7)
C7	2238(3)	5350(2)	5672.7(19)	22.6(6)
C8	2676(3)	5277.5(19)	4630.0(18)	21.0(5)
C9	2349(4)	4406(2)	3995(2)	27.3(6)
C10	2745(4)	4407(2)	3023(2)	30.9(7)
C11	3486(4)	5284(2)	2666(2)	29.9(6)
C12	3846(3)	6166(2)	3271.3(19)	23.1(6)
C13	3441(3)	6156.2(19)	4258.1(19)	20.8(5)
C14	4528(4)	7165(2)	2891(2)	28.4(6)

Table 3. Bond Lengths for selenenyl sulfide **7**.

Atom	**Atom**	**Length/Å**	**Atom**	**Atom**	**Length/Å**
Se1	S1	2.2411(8)	C4	C5	1.375(4)
Se1	C13	1.909(2)	C5	C6	1.384(4)
S1	C14	1.818(3)	C7	C8	1.484(3)
O1	C7	1.231(3)	C8	C9	1.391(3)
N1	C1	1.419(3)	C8	C13	1.402(3)
N1	C7	1.351(3)	C9	C10	1.376(4)
C1	C2	1.389(4)	C10	C11	1.383(4)
C1	C6	1.390(4)	C11	C12	1.381(4)
C2	C3	1.386(4)	C12	C13	1.398(3)
C3	C4	1.371(5)	C12	C14	1.504(4)

Table 4. Bond Angles for selenenyl sulfide **7**.

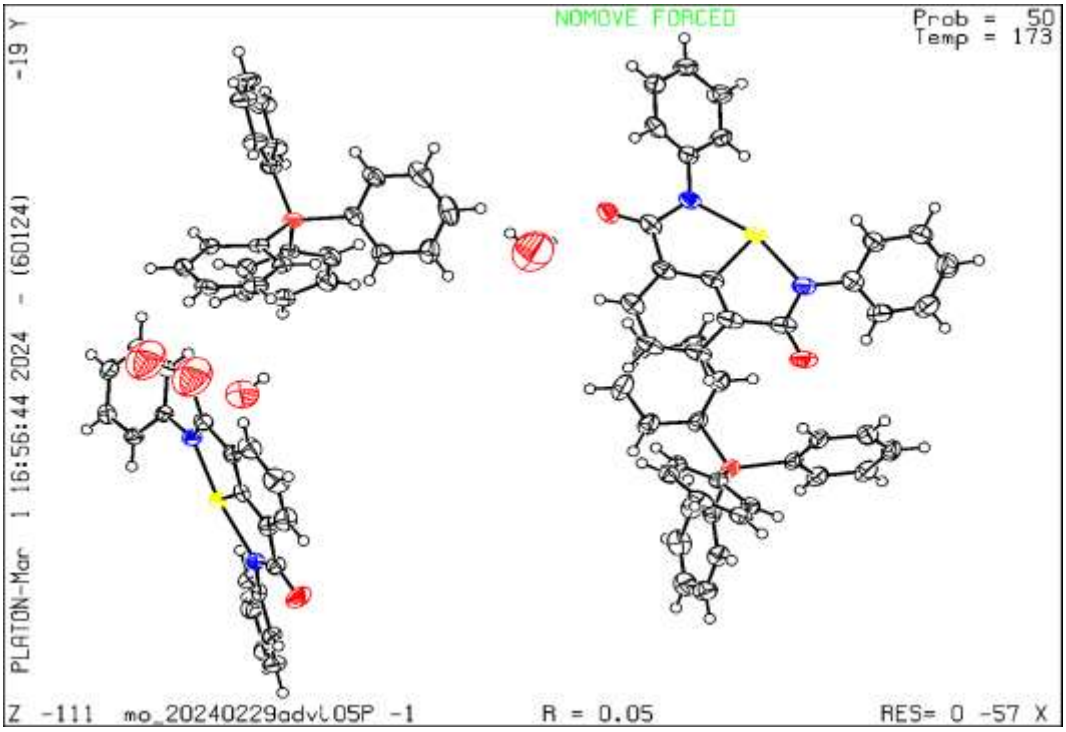
Atom	**Atom**	**Atom**	**Angle/°**	**Atom**	**Atom**	**Atom**	**Angle/°**
C13	Se1	S1	88.62(8)	C9	C8	C7	124.4(2)
C14	S1	Se1	93.65(9)	C9	C8	C13	118.1(2)
C7	N1	C1	128.1(2)	C13	C8	C7	117.5(2)
C2	C1	N1	117.0(3)	C10	C9	C8	121.1(3)
C2	C1	C6	120.0(3)	C9	C10	C11	119.9(3)
C6	C1	N1	122.9(2)	C12	C11	C10	121.1(2)
C3	C2	C1	119.8(3)	C11	C12	C13	118.5(2)
C4	C3	C2	120.2(3)	C11	C12	C14	123.1(2)
C3	C4	C5	120.0(3)	C13	C12	C14	118.3(2)
C4	C5	C6	121.0(3)	C8	C13	Se1	122.76(19)
C5	C6	C1	119.0(3)	C12	C13	Se1	116.00(19)
O1	C7	N1	123.1(2)	C12	C13	C8	121.2(2)
O1	C7	C8	119.9(2)	C12	C14	S1	109.18(18)
N1	C7	C8	116.9(2)				

Table 5.Torsion Angles for selenenyl sulfide **7**.

A	**B**	**C**	**D**	**Angle/°**	**A**	**B**	**C**	**D**	**Angle/°**
Se1	S1	C14	C12	-36.48(19)	C7	C8	C9	C10	178.1(2)
O1	C7	C8	C9	-161.8(3)	C7	C8	C13	Se1	0.1(3)
O1	C7	C8	C13	17.0(4)	C7	C8	C13	C12	-178.0(2)
N1	C1	C2	C3	177.7(2)	C8	C9	C10	C11	0.2(4)
N1	C1	C6	C5	-177.6(3)	C9	C8	C13	Se1	178.93(18)
N1	C7	C8	C9	17.3(4)	C9	C8	C13	C12	0.8(4)
N1	C7	C8	C13	-163.9(2)	C9	C10	C11	C12	0.2(4)
C1	N1	C7	O1	-2.9(4)	C10	C11	C12	C13	-0.1(4)
C1	N1	C7	C8	178.1(2)	C10	C11	C12	C14	-175.5(3)
C1	C2	C3	C4	0.1(4)	C11	C12	C13	Se1	-178.65(19)
C2	C1	C6	C5	-0.8(4)	C11	C12	C13	C8	-0.4(4)
C2	C3	C4	C5	-1.0(5)	C11	C12	C14	S1	-154.2(2)
C3	C4	C5	C6	0.9(5)	C13	C8	C9	C10	-0.7(4)
C4	C5	C6	C1	0.0(5)	C13	C12	C14	S1	30.4(3)
C6	C1	C2	C3	0.7(4)	C14	C12	C13	Se1	-3.0(3)
C7	N1	C1	C2	157.9(3)	C14	C12	C13	C8	175.2(2)
C7	N1	C1	C6	-25.2(4)					

X-Ray Structure 2. Salt 42b.

ORTEP Diagram of salt **42b** (unit cell containing 2 molecules of **42b** along with water)**.**



ORTEP Diagram of **42b** (single molecule)

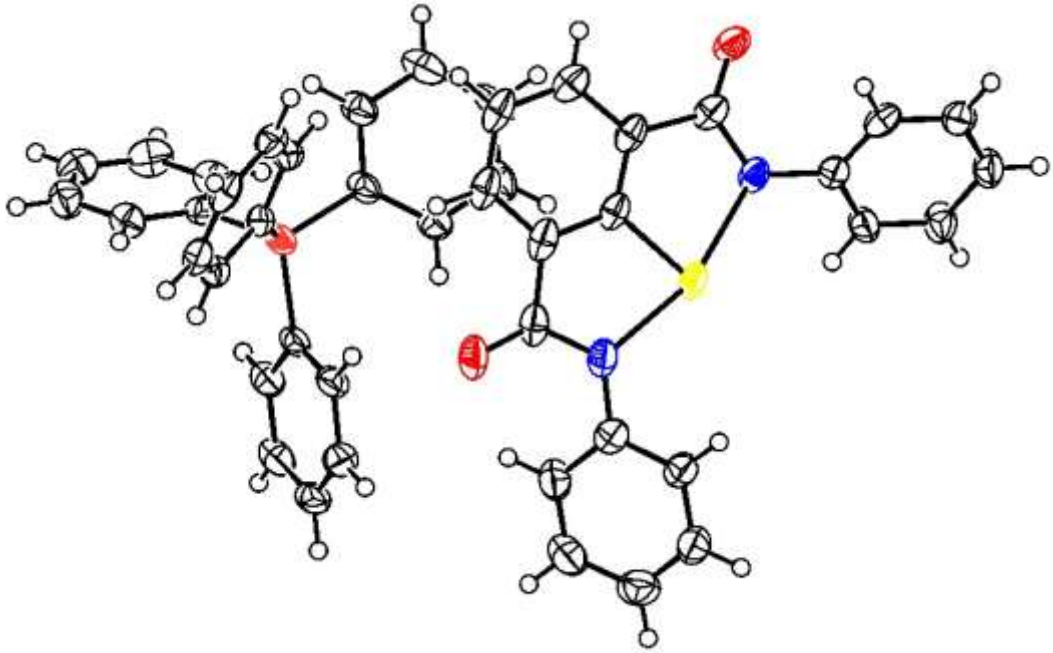


Table 1 Crystal data and structure refinement for salt **40**.

Empirical formula	$C_{176}H_{137.21}N_8O_{11}P_4Se_4$
Formula weight	2979.86
Temperature/K	296.15
Crystal system	triclinic
Space group	P-1
a/Å	13.1170(5)
b/Å	16.3872(7)
c/Å	16.8435(7)
α/°	90.4720(10)
β/°	90.4550(10)
γ/°	103.3810(10)
Volume/Å^3	3521.9(2)
Z	1
ρ_{calc}g/cm^3	1.405
μ/mm^{-1}	1.156
F(000)	1533.0
Crystal size/mm^3	0.348 × 0.319 × 0.143
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	2.554 to 50.054
Index ranges	$-15 \leq h \leq 15$, $-19 \leq k \leq 19$, $-19 \leq l \leq 20$
Reflections collected	27309
Independent reflections	12196 [R_{int} = 0.0477, R_{sigma} = 0.0714]
Data/restraints/parameters	12196/12/935
Goodness-of-fit on F^2	1.043
Final R indexes [I>=2σ (I)]	R_1 = 0.0457, wR_2 = 0.1013
Final R indexes [all data]	R_1 = 0.0738, wR_2 = 0.1138
Largest diff. peak/hole / e Å^{-3}	0.60/-0.71

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for salt **40**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	***x***	***y***	***z***	**U(eq)**
Se1	2198.8(3)	6964.9(2)	-1966.7(2)	27.86(11)
Se2	2212.5(3)	2014.9(3)	6969.6(2)	34.24(12)
P1	7480.5(7)	5894.2(6)	956.1(6)	28.6(2)
P2	-2272.7(7)	1061.4(6)	4082.9(6)	30.7(2)

Table 2 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for salt **40**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	***x***	***y***	***z***	**U(eq)**
O1	-880.3(19)	6968.0(19)	-1260.2(17)	49.8(8)
O2	4656.8(19)	8446.2(16)	-666.0(15)	40.5(7)
O3	4208(2)	3531.6(18)	5359.1(15)	43.1(7)
O4	-997(2)	1791.0(18)	6728.3(16)	46.8(7)
O5	4034(4)	4917(4)	4508(5)	142.6(19)
O6	4549(11)	9915(10)	306(9)	137(6)
O7	3420(20)	10569(19)	1479(18)	99(10)
N1	492(2)	6637.2(18)	-1965.5(17)	27.7(7)
N2	3747(2)	7522.2(18)	-1621.5(17)	28.6(7)
N3	3643(2)	2652(2)	6421.0(17)	34.1(8)
N4	604(2)	1608(2)	7201.0(18)	37.8(8)
C1	-98(3)	6042(2)	-2504(2)	29.7(8)
C2	424(3)	5514(2)	-2900(2)	37.1(10)
C3	-95(3)	4909(3)	-3425(2)	45.7(11)
C4	-1149(3)	4822(3)	-3584(3)	49.1(11)
C5	-1670(3)	5347(3)	-3207(3)	47.2(11)
C6	-1165(3)	5955(2)	-2668(2)	37.7(10)
C7	1931(3)	7591(2)	-1100(2)	27.4(8)
C8	900(3)	7567(2)	-896(2)	32.8(9)
C9	65(3)	7023(2)	-1393(2)	33.8(9)
C10	3835(3)	8037(2)	-979(2)	30.8(9)
C11	2785(3)	8066(2)	-683(2)	30.7(9)
C12	4630(3)	7372(2)	-2032(2)	27.1(8)
C13	4557(3)	7233(2)	-2850(2)	29.1(8)
C14	5396(3)	7074(2)	-3267(2)	32.8(9)
C15	6324(3)	7054(2)	-2875(2)	36.4(9)
C16	6401(3)	7188(3)	-2065(2)	41.1(10)
C17	5564(3)	7338(2)	-1642(2)	35.1(9)
C18	731(3)	8035(3)	-242(2)	44.0(10)
C19	2594(3)	8542(2)	-32(2)	43.3(10)
C20	1569(3)	8518(3)	186(3)	49.3(11)
C21	4645(3)	2586(2)	6706(2)	31.2(9)
C22	4766(3)	1818(3)	6975(2)	39.1(10)
C23	5731(3)	1717(3)	7229(3)	44.5(11)

Table 2 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for salt **40**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	***x***	***y***	***z***	**U(eq)**
C24	6594(3)	2388(3)	7232(2)	41.6(10)
C25	6467(3)	3158(3)	6995(2)	38.3(10)
C26	5502(3)	3267(2)	6742(2)	35.6(9)
C27	1683(3)	2586(2)	6171(2)	31.9(9)
C28	2384(3)	3078(2)	5653(2)	36.5(10)
C29	3511(3)	3120(3)	5791(2)	35.4(9)
C30	-35(3)	1929(3)	6712(2)	38.4(10)
C31	613(3)	2506(3)	6132(2)	38.9(10)
C32	237(3)	969(3)	7747(2)	35.7(9)
C33	825(3)	942(3)	8429(2)	37.6(10)
C34	534(3)	287(3)	8950(2)	46.1(11)
C35	-338(3)	-336(3)	8811(3)	53.4(12)
C36	-953(3)	-306(3)	8137(3)	57.3(13)
C37	-655(3)	337(3)	7610(3)	49.6(11)
C38	1960(3)	3485(3)	5057(2)	41.2(10)
C39	220(3)	2937(3)	5541(2)	41.1(10)
C40	884(3)	3418(3)	5008(2)	46.4(11)
C41	7156(2)	6879(2)	728(2)	27.3(8)
C42	6397(3)	7153(2)	1164(2)	30.7(9)
C43	6131(3)	7891(2)	961(2)	36.3(10)
C44	6614(3)	8351(2)	331(2)	36.6(10)
C45	7374(3)	8088(2)	-92(2)	34.9(9)
C46	7655(3)	7358(2)	106(2)	31.8(9)
C47	6883(3)	5507(2)	1870(2)	29.7(8)
C48	7482(3)	5531(2)	2556(2)	39.1(10)
C49	7006(4)	5228(3)	3253(3)	50.7(12)
C50	5956(4)	4905(3)	3279(3)	50.7(12)
C51	5332(3)	4895(3)	2601(3)	45.2(11)
C52	5796(3)	5186(2)	1898(2)	36.2(9)
C53	8869(3)	6052(2)	1071(2)	31.5(9)
C54	9358(3)	5409(3)	894(2)	40.1(10)
C55	10414(3)	5516(3)	1078(2)	47.1(11)
C56	10966(3)	6248(3)	1425(3)	50.0(12)
C57	10479(3)	6886(3)	1605(2)	47.6(11)

Table 2 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for salt **40**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	***x***	***y***	***z***	**U(eq)**
C58	9432(3)	6792(3)	1426(2)	40.4(10)
C59	7017(3)	5123(2)	187(2)	28.2(8)
C60	7150(3)	5351(2)	-609(2)	35.7(9)
C61	6807(3)	4750(3)	-1192(2)	40.2(10)
C62	6336(3)	3936(2)	-1000(2)	35.9(9)
C63	6218(3)	3712(2)	-213(2)	40.4(10)
C64	6569(3)	4297(2)	380(2)	38.4(10)
C65	-890(3)	1219(2)	3956(2)	34.4(9)
C66	-260(3)	996(2)	4544(2)	37.8(10)
C67	816(3)	1187(3)	4461(3)	49.4(12)
C68	1255(3)	1602(3)	3806(3)	53.5(13)
C69	647(3)	1832(3)	3219(3)	50.9(12)
C70	-427(3)	1640(2)	3286(3)	40.7(10)
C71	-2573(3)	2037(2)	4365(2)	28.7(8)
C72	-3521(3)	2028(2)	4740(2)	33.1(9)
C73	-3771(3)	2776(3)	4942(2)	36.0(10)
C74	-3082(3)	3528(3)	4789(2)	38.1(10)
C75	-2136(3)	3541(2)	4417(2)	35.0(9)
C76	-1888(3)	2798(2)	4200(2)	30.2(9)
C77	-2924(3)	684(2)	3169(2)	31.8(9)
C78	-3932(3)	801(2)	3024(2)	36.0(9)
C79	-4454(3)	508(2)	2331(2)	42.6(10)
C80	-3986(3)	103(3)	1773(3)	45.4(11)
C81	-3000(3)	-25(3)	1909(3)	48.4(11)
C82	-2463(3)	264(2)	2602(2)	41.5(10)
C83	-2739(3)	321(2)	4862(2)	31.5(9)
C84	-3192(3)	-509(2)	4668(3)	37.9(10)
C85	-3569(3)	-1069(3)	5263(3)	42.7(11)
C86	-3500(3)	-798(3)	6052(3)	42.1(11)
C87	-3040(3)	22(3)	6236(2)	40.8(10)
C88	-2649(3)	590(2)	5653(2)	37.4(10)

Table 3. Bond Lengths for salt **40**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Se1	N1	2.178(3)	C31	C39	1.389(5)
Se1	N2	2.100(3)	C32	C33	1.385(5)
Se1	C7	1.860(3)	C32	C37	1.388(5)
Se2	N3	2.145(3)	C33	C34	1.379(6)
Se2	N4	2.100(3)	C34	C35	1.362(6)
Se2	C27	1.863(3)	C35	C36	1.395(6)
P1	C41	1.805(3)	C36	C37	1.371(6)
P1	C47	1.786(4)	C38	C40	1.392(5)
P1	C53	1.788(3)	C39	C40	1.375(6)
P1	C59	1.802(4)	C41	C42	1.395(5)
P2	C65	1.786(3)	C41	C46	1.389(5)
P2	C71	1.795(4)	C42	C43	1.380(5)
P2	C77	1.789(4)	C43	C44	1.378(5)
P2	C83	1.807(4)	C44	C45	1.375(5)
O1	C9	1.244(4)	C45	C46	1.374(5)
O2	C10	1.241(4)	C47	C48	1.388(5)
O3	C29	1.245(5)	C47	C52	1.403(5)
O4	C30	1.230(4)	C48	C49	1.376(6)
O6	$O6^{1}$	1.55(3)	C49	C50	1.357(6)
N1	C1	1.414(4)	C50	C51	1.397(6)
N1	C9	1.344(4)	C51	C52	1.373(5)
N2	C10	1.355(4)	C53	C54	1.386(5)
N2	C12	1.423(4)	C53	C58	1.393(5)
N3	C21	1.423(4)	C54	C55	1.387(5)
N3	C29	1.349(5)	C55	C56	1.372(6)
N4	C30	1.364(4)	C56	C57	1.378(6)
N4	C32	1.401(5)	C57	C58	1.377(5)
C1	C2	1.391(5)	C59	C60	1.397(5)
C1	C6	1.398(5)	C59	C64	1.388(5)
C2	C3	1.376(5)	C60	C61	1.382(5)
C3	C4	1.380(5)	C61	C62	1.376(5)
C4	C5	1.371(6)	C62	C63	1.379(5)
C5	C6	1.388(5)	C63	C64	1.379(5)
C7	C8	1.389(5)	C65	C66	1.390(5)
C7	C11	1.389(5)	C65	C70	1.396(5)
C8	C9	1.489(5)	C66	C67	1.382(5)

Table 3. Bond Lengths for salt **40**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C8	C18	1.386(5)	C67	C68	1.361(6)
C10	C11	1.478(5)	C68	C69	1.374(6)
C11	C19	1.399(5)	C69	C70	1.376(5)
C12	C13	1.394(5)	C71	C72	1.396(5)
C12	C17	1.398(5)	C71	C76	1.390(5)
C13	C14	1.383(5)	C72	C73	1.380(5)
C14	C15	1.387(5)	C73	C74	1.378(5)
C15	C16	1.379(5)	C74	C75	1.390(5)
C16	C17	1.382(5)	C75	C76	1.378(5)
C18	C20	1.390(6)	C77	C78	1.400(5)
C19	C20	1.388(6)	C77	C82	1.393(5)
C21	C22	1.384(5)	C78	C79	1.374(5)
C21	C26	1.389(5)	C79	C80	1.374(5)
C22	C23	1.379(5)	C80	C81	1.374(5)
C23	C24	1.383(5)	C81	C82	1.380(6)
C24	C25	1.374(5)	C83	C84	1.387(5)
C25	C26	1.383(5)	C83	C88	1.396(5)
C27	C28	1.392(5)	C84	C85	1.379(5)
C27	C31	1.381(5)	C85	C86	1.393(6)
C28	C29	1.480(5)	C86	C87	1.372(6)
C28	C38	1.391(5)	C87	C88	1.376(5)
C30	C31	1.492(6)			

[1]1-X,2-Y,-Z

Table 4. Bond Angles for salt **40**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N2	Se1	N1	159.97(11)	O4	C30	N4	127.3(4)
C7	Se1	N1	79.20(13)	O4	C30	C31	123.2(3)
C7	Se1	N2	80.76(13)	N4	C30	C31	109.5(3)
N4	Se2	N3	160.42(12)	C27	C31	C30	116.9(3)
C27	Se2	N3	79.75(14)	C27	C31	C39	117.9(4)
C27	Se2	N4	80.67(15)	C39	C31	C30	125.1(3)
C47	P1	C41	109.37(16)	C33	C32	N4	118.4(4)
C47	P1	C53	108.29(17)	C33	C32	C37	118.8(4)

Table 4. Bond Angles for salt **40**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C47	P1	C59	108.58(17)	C37	C32	N4	122.7(4)
C53	P1	C41	109.62(16)	C34	C33	C32	120.2(4)
C53	P1	C59	109.82(16)	C35	C34	C33	120.8(4)
C59	P1	C41	111.11(16)	C34	C35	C36	119.7(4)
C65	P2	C71	109.27(17)	C37	C36	C35	119.6(4)
C65	P2	C77	109.09(18)	C36	C37	C32	120.9(4)
C65	P2	C83	111.46(16)	C28	C38	C40	120.7(4)
C71	P2	C83	107.34(17)	C40	C39	C31	120.5(4)
C77	P2	C71	110.08(16)	C39	C40	C38	120.5(4)
C77	P2	C83	109.58(18)	C42	C41	P1	120.4(3)
C1	N1	Se1	122.1(2)	C46	C41	P1	119.7(3)
C9	N1	Se1	114.1(2)	C46	C41	C42	119.9(3)
C9	N1	C1	123.8(3)	C43	C42	C41	119.5(4)
C10	N2	Se1	114.6(2)	C44	C43	C42	119.9(4)
C10	N2	C12	122.9(3)	C45	C44	C43	120.6(4)
C12	N2	Se1	122.6(2)	C46	C45	C44	120.3(4)
C21	N3	Se2	122.4(2)	C45	C46	C41	119.7(3)
C29	N3	Se2	114.4(2)	C48	C47	P1	120.6(3)
C29	N3	C21	123.2(3)	C48	C47	C52	119.6(4)
C30	N4	Se2	114.9(3)	C52	C47	P1	119.8(3)
C30	N4	C32	123.6(3)	C49	C48	C47	119.7(4)
C32	N4	Se2	120.9(2)	C50	C49	C48	120.8(4)
C2	C1	N1	117.4(3)	C49	C50	C51	120.5(4)
C2	C1	C6	118.2(3)	C52	C51	C50	119.4(4)
C6	C1	N1	124.4(3)	C51	C52	C47	120.0(4)
C3	C2	C1	121.2(4)	C54	C53	P1	120.3(3)
C2	C3	C4	120.6(4)	C54	C53	C58	120.3(3)
C5	C4	C3	118.8(4)	C58	C53	P1	119.0(3)
C4	C5	C6	121.6(4)	C53	C54	C55	118.9(4)
C5	C6	C1	119.6(4)	C56	C55	C54	120.6(4)
C8	C7	Se1	119.4(3)	C55	C56	C57	120.6(4)
C11	C7	Se1	117.7(3)	C58	C57	C56	119.7(4)
C11	C7	C8	123.0(3)	C57	C58	C53	119.9(4)
C7	C8	C9	116.9(3)	C60	C59	P1	119.7(3)
C18	C8	C7	117.8(4)	C64	C59	P1	120.5(3)
C18	C8	C9	125.3(3)	C64	C59	C60	119.7(3)

Table 4. Bond Angles for salt **40**.

Atom	**Atom**	**Atom**	**Angle/°**	**Atom**	**Atom**	**Atom**	**Angle/°**
O1	C9	N1	128.2(4)	C61	C60	C59	119.1(4)
O1	C9	C8	121.5(3)	C62	C61	C60	121.1(4)
N1	C9	C8	110.3(3)	C61	C62	C63	119.6(4)
O2	C10	N2	127.0(3)	C64	C63	C62	120.4(4)
O2	C10	C11	122.7(3)	C63	C64	C59	120.0(4)
N2	C10	C11	110.3(3)	C66	C65	P2	121.0(3)
C7	C11	C10	116.7(3)	C66	C65	C70	119.5(3)
C7	C11	C19	118.2(3)	C70	C65	P2	119.2(3)
C19	C11	C10	125.1(3)	C67	C66	C65	119.9(4)
C13	C12	N2	119.0(3)	C68	C67	C66	119.8(4)
C13	C12	C17	118.7(3)	C67	C68	C69	121.2(4)
C17	C12	N2	122.3(3)	C68	C69	C70	119.9(4)
C14	C13	C12	120.5(3)	C69	C70	C65	119.6(4)
C13	C14	C15	120.4(4)	C72	C71	P2	119.2(3)
C16	C15	C14	119.4(3)	C76	C71	P2	121.0(3)
C15	C16	C17	120.7(3)	C76	C71	C72	119.8(3)
C16	C17	C12	120.3(4)	C73	C72	C71	119.7(4)
C8	C18	C20	120.7(4)	C74	C73	C72	120.3(4)
C20	C19	C11	119.7(4)	C73	C74	C75	120.3(4)
C19	C20	C18	120.7(4)	C76	C75	C74	119.8(4)
C22	C21	N3	118.8(3)	C75	C76	C71	120.1(3)
C22	C21	C26	118.6(3)	C78	C77	P2	119.1(3)
C26	C21	N3	122.6(3)	C82	C77	P2	121.9(3)
C23	C22	C21	120.8(4)	C82	C77	C78	119.0(4)
C22	C23	C24	120.5(4)	C79	C78	C77	120.2(4)
C25	C24	C23	118.8(4)	C80	C79	C78	120.2(4)
C24	C25	C26	121.2(4)	C79	C80	C81	120.4(4)
C25	C26	C21	120.0(4)	C80	C81	C82	120.4(4)
C28	C27	Se2	118.6(3)	C81	C82	C77	119.9(4)
C31	C27	Se2	118.0(3)	C84	C83	P2	119.7(3)
C31	C27	C28	123.4(3)	C84	C83	C88	120.6(4)
C27	C28	C29	116.8(3)	C88	C83	P2	119.7(3)
C38	C28	C27	117.0(3)	C85	C84	C83	119.6(4)
C38	C28	C29	126.2(4)	C84	C85	C86	120.0(4)
O3	C29	N3	127.1(3)	C87	C86	C85	119.8(4)
O3	C29	C28	122.5(3)	C86	C87	C88	121.2(4)

Table 4. Bond Angles for salt **40**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N3	C29	C28	110.4(3)	C87	C88	C83	118.8(4)

Table 5 Torsion Angles for salt **40**.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
Se1	N1	C1	C2	16.1(4)	C29	N3	C21	C26	39.8(5)
Se1	N1	C1	C6	-163.5(3)	C29	C28	C38	C40	-177.7(4)
Se1	N1	C9	O1	178.6(3)	C30	N4	C32	C33	-151.3(3)
Se1	N1	C9	C8	-1.2(4)	C30	N4	C32	C37	32.6(6)
Se1	N2	C10	O2	-179.0(3)	C30	C31	C39	C40	-176.4(4)
Se1	N2	C10	C11	0.2(4)	C31	C27	C28	C29	178.0(3)
Se1	N2	C12	C13	33.1(4)	C31	C27	C28	C38	-1.7(6)
Se1	N2	C12	C17	-145.3(3)	C31	C39	C40	C38	-0.6(6)
Se1	C7	C8	C9	0.5(4)	C32	N4	C30	O4	8.7(6)
Se1	C7	C8	C18	179.4(3)	C32	N4	C30	C31	-171.9(3)
Se1	C7	C11	C10	0.9(4)	C32	C33	C34	C35	-0.9(6)
Se1	C7	C11	C19	179.7(3)	C33	C32	C37	C36	-0.1(6)
Se2	N3	C21	C22	38.8(4)	C33	C34	C35	C36	-0.8(6)
Se2	N3	C21	C26	-139.7(3)	C34	C35	C36	C37	2.0(7)
Se2	N3	C29	O3	-178.0(3)	C35	C36	C37	C32	-1.5(7)
Se2	N3	C29	C28	1.0(4)	C37	C32	C33	C34	1.3(6)
Se2	N4	C30	O4	-179.7(3)	C38	C28	C29	O3	-1.2(6)
Se2	N4	C30	C31	-0.4(4)	C38	C28	C29	N3	179.7(4)
Se2	N4	C32	C33	37.6(4)	C41	P1	C47	C48	-106.9(3)
Se2	N4	C32	C37	-138.5(3)	C41	P1	C47	C52	72.3(3)
Se2	C27	C28	C29	-1.2(5)	C41	P1	C53	C54	-150.8(3)
Se2	C27	C28	C38	179.1(3)	C41	P1	C53	C58	36.5(4)
Se2	C27	C31	C30	-3.0(5)	C41	P1	C59	C60	43.6(3)
Se2	C27	C31	C39	179.5(3)	C41	P1	C59	C64	-139.2(3)
P1	C41	C42	C43	-177.5(3)	C41	C42	C43	C44	0.1(5)
P1	C41	C46	C45	177.0(3)	C42	C41	C46	C45	-2.0(5)
P1	C47	C48	C49	-179.8(3)	C42	C43	C44	C45	-1.1(5)
P1	C47	C52	C51	-179.4(3)	C43	C44	C45	C46	0.5(5)
P1	C53	C54	C55	-172.4(3)	C44	C45	C46	C41	1.0(5)
P1	C53	C58	C57	172.5(3)	C46	C41	C42	C43	1.4(5)

Table 5 Torsion Angles for salt **40**.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
P1	C59	C60	C61	178.9(3)	C47	P1	C41	C42	-10.3(3)
P1	C59	C64	C63	-179.8(3)	C47	P1	C41	C46	170.7(3)
P2	C65	C66	C67	-174.6(3)	C47	P1	C53	C54	90.0(3)
P2	C65	C70	C69	174.0(3)	C47	P1	C53	C58	-82.7(3)
P2	C71	C72	C73	-178.5(3)	C47	P1	C59	C60	163.9(3)
P2	C71	C76	C75	179.6(3)	C47	P1	C59	C64	-18.9(3)
P2	C77	C78	C79	-179.2(3)	C47	C48	C49	C50	-0.1(6)
P2	C77	C82	C81	179.2(3)	C48	C47	C52	C51	-0.3(5)
P2	C83	C84	C85	-178.5(3)	C48	C49	C50	C51	-1.6(6)
P2	C83	C88	C87	177.9(3)	C49	C50	C51	C52	2.3(6)
O2	C10	C11	C7	178.6(3)	C50	C51	C52	C47	-1.4(6)
O2	C10	C11	C19	-0.1(6)	C52	C47	C48	C49	1.0(5)
O4	C30	C31	C27	-178.5(4)	C53	P1	C41	C42	-128.9(3)
O4	C30	C31	C39	-1.2(6)	C53	P1	C41	C46	52.1(3)
N1	Se1	C7	C8	-0.9(3)	C53	P1	C47	C48	12.5(3)
N1	Se1	C7	C11	179.0(3)	C53	P1	C47	C52	-168.3(3)
N1	C1	C2	C3	179.0(4)	C53	P1	C59	C60	-77.9(3)
N1	C1	C6	C5	-179.8(3)	C53	P1	C59	C64	99.4(3)
N2	Se1	C7	C8	179.5(3)	C53	C54	C55	C56	-0.4(6)
N2	Se1	C7	C11	-0.6(3)	C54	C53	C58	C57	-0.2(6)
N2	C10	C11	C7	-0.7(4)	C54	C55	C56	C57	0.8(7)
N2	C10	C11	C19	-179.4(3)	C55	C56	C57	C58	-0.8(7)
N2	C12	C13	C14	-179.2(3)	C56	C57	C58	C53	0.5(6)
N2	C12	C17	C16	179.9(3)	C58	C53	C54	C55	0.2(6)
N3	Se2	C27	C28	1.3(3)	C59	P1	C41	C42	109.5(3)
N3	Se2	C27	C31	-177.9(3)	C59	P1	C41	C46	-69.4(3)
N3	C21	C22	C23	177.6(3)	C59	P1	C47	C48	131.7(3)
N3	C21	C26	C25	-177.4(3)	C59	P1	C47	C52	-49.1(3)
N4	Se2	C27	C28	-178.7(3)	C59	P1	C53	C54	-28.5(4)
N4	Se2	C27	C31	2.1(3)	C59	P1	C53	C58	158.9(3)
N4	C30	C31	C27	2.1(5)	C59	C60	C61	C62	0.2(5)
N4	C30	C31	C39	179.4(4)	C60	C59	C64	C63	-2.6(5)
N4	C32	C33	C34	-174.9(3)	C60	C61	C62	C63	-1.0(6)
N4	C32	C37	C36	176.0(4)	C61	C62	C63	C64	0.0(6)
C1	N1	C9	O1	-4.0(6)	C62	C63	C64	C59	1.8(6)
C1	N1	C9	C8	176.2(3)	C64	C59	C60	C61	1.6(5)

Table 5 Torsion Angles for salt **40**.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
C1	C2	C3	C4	1.3(6)	C65	P2	C71	C72	-159.5(3)
C2	C1	C6	C5	0.6(5)	C65	P2	C71	C76	21.9(3)
C2	C3	C4	C5	-0.4(6)	C65	P2	C77	C78	-156.9(3)
C3	C4	C5	C6	-0.4(7)	C65	P2	C77	C82	24.2(4)
C4	C5	C6	C1	0.3(6)	C65	P2	C83	C84	-98.7(3)
C6	C1	C2	C3	-1.4(6)	C65	P2	C83	C88	82.0(3)
C7	C8	C9	O1	-179.3(3)	C65	C66	C67	C68	0.7(6)
C7	C8	C9	N1	0.6(5)	C66	C65	C70	C69	-0.3(6)
C7	C8	C18	C20	0.7(6)	C66	C67	C68	C69	-0.3(7)
C7	C11	C19	C20	1.1(6)	C67	C68	C69	C70	-0.4(7)
C8	C7	C11	C10	-179.1(3)	C68	C69	C70	C65	0.7(6)
C8	C7	C11	C19	-0.3(5)	C70	C65	C66	C67	-0.4(6)
C8	C18	C20	C19	0.0(6)	C71	P2	C65	C66	100.4(3)
C9	N1	C1	C2	-161.1(3)	C71	P2	C65	C70	-73.8(4)
C9	N1	C1	C6	19.3(5)	C71	P2	C77	C78	-37.0(4)
C9	C8	C18	C20	179.5(4)	C71	P2	C77	C82	144.1(3)
C10	N2	C12	C13	-146.7(3)	C71	P2	C83	C84	141.7(3)
C10	N2	C12	C17	34.9(5)	C71	P2	C83	C88	-37.6(3)
C10	C11	C19	C20	179.8(4)	C71	C72	C73	C74	-1.2(5)
C11	C7	C8	C9	-179.4(3)	C72	C71	C76	C75	1.0(5)
C11	C7	C8	C18	-0.6(5)	C72	C73	C74	C75	1.1(5)
C11	C19	C20	C18	-0.9(6)	C73	C74	C75	C76	0.1(5)
C12	N2	C10	O2	0.8(6)	C74	C75	C76	C71	-1.1(5)
C12	N2	C10	C11	-179.9(3)	C76	C71	C72	C73	0.1(5)
C12	C13	C14	C15	-0.2(5)	C77	P2	C65	C66	-139.2(3)
C13	C12	C17	C16	1.5(5)	C77	P2	C65	C70	46.6(4)
C13	C14	C15	C16	0.4(6)	C77	P2	C71	C72	80.7(3)
C14	C15	C16	C17	0.3(6)	C77	P2	C71	C76	-97.8(3)
C15	C16	C17	C12	-1.3(6)	C77	P2	C83	C84	22.2(3)
C17	C12	C13	C14	-0.8(5)	C77	P2	C83	C88	-157.2(3)
C18	C8	C9	O1	2.0(6)	C77	C78	C79	C80	-0.5(6)
C18	C8	C9	N1	-178.2(3)	C78	C77	C82	C81	0.3(6)
C21	N3	C29	O3	2.4(6)	C78	C79	C80	C81	1.1(6)
C21	N3	C29	C28	-178.6(3)	C79	C80	C81	C82	-1.1(6)
C21	C22	C23	C24	1.0(6)	C80	C81	C82	C77	0.3(6)
C22	C21	C26	C25	4.0(5)	C82	C77	C78	C79	-0.3(6)

Table 5 Torsion Angles for salt **40**.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
C22	C23	C24	C25	1.5(6)	C83	P2	C65	C66	-18.0(4)
C23	C24	C25	C26	-1.2(6)	C83	P2	C65	C70	167.7(3)
C24	C25	C26	C21	-1.6(6)	C83	P2	C71	C72	-38.5(3)
C26	C21	C22	C23	-3.8(6)	C83	P2	C71	C76	142.9(3)
C27	C28	C29	O3	179.1(4)	C83	P2	C77	C78	80.8(3)
C27	C28	C29	N3	0.0(5)	C83	P2	C77	C82	-98.0(3)
C27	C28	C38	C40	2.0(6)	C83	C84	C85	C86	0.4(5)
C27	C31	C39	C40	0.9(6)	C84	C83	C88	C87	-1.4(5)
C28	C27	C31	C30	177.8(3)	C84	C85	C86	C87	-1.1(5)
C28	C27	C31	C39	0.3(6)	C85	C86	C87	C88	0.5(5)
C28	C38	C40	C39	-0.9(6)	C86	C87	C88	C83	0.8(5)
C29	N3	C21	C22	-141.6(4)	C88	C83	C84	C85	0.9(5)