Synthesis and structural investigation of *N*-acyl selenophosphoramides

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Electronic Supporting Information

X-ray data for: Page

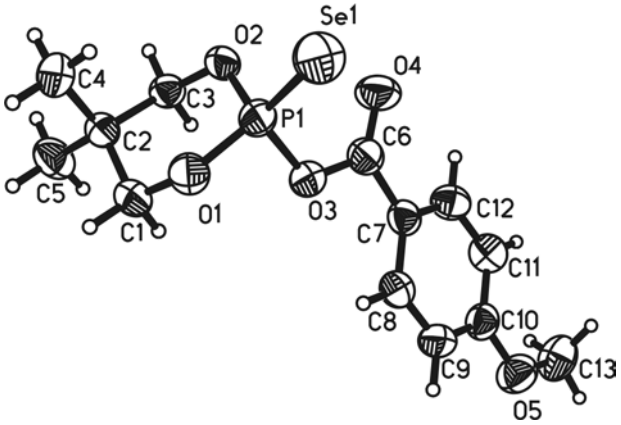
Figures - the ORTEP views for:

^{31}P NMR, ^{1}H NMR, ^{13}C NMR spectra:

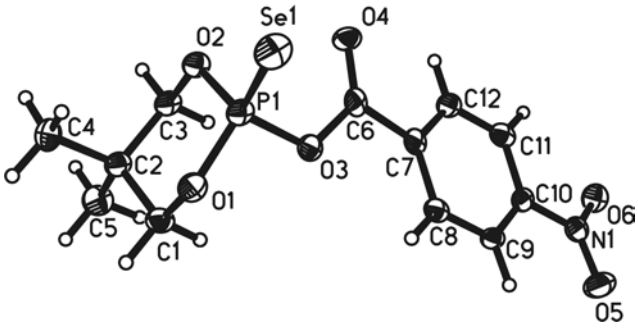
ESI. Table 1. Summary of x-ray structural analyses for **6c**, **6d**, **6e**, **8a**, **8b** and **11a**; units: Å, °.

	6c	**6d**	**6e**	**8a**	**8b**	**11a**
Formula	$C_{12}H_{14}ClO_4PSe$	$C_{13}H_{17}O_5PSe$	$C_{12}H_{14}NO_6PSe$	$C_{12}H_{15}ClNO_3PSe$	$C_{10}H_{20}NO_3PSe$	$C_5H_{12}NO_2PSe$
M, g/mol	367.61	363.2	378.17	366.63	312.2	228.09
Crystal system	Monoclinic	Monoclinic	Monoclinic	Monoclinic	Monoclinic	Monoclinic
a	10.9640(2)	8.6686(3)	16.4014(10)	11.9308(7)	9.9981(2)	7.7108(2)
b	15.2200(3)	14.9809(4)	7.6161(3)	15.4868(9)	27.8966(5)	10.9466(3)
c	8.8822(2)	12.4583(4)	12.2729(6)	8.2832(4)	10.6258(3)	10.9955(3)
α	90	90	90	90	90	90
β	91.581(2)	107.683(4)	103.358(6)	91.617(5)	109.816(3)	103.130(3)
γ	90	90	90	90	90	90
V/ Å^3	1481.63(5)	1541.44(9)	1491.59(13)	1529.88(15)	2788.18(11)	903.83(4)
Space group	$P2_1/c$ (14)	$P2_1/c$ (14)	$P2_1/c$ (14)	$P2_1/c$ (14)	$P2_1/c$ (14)	$P2_1/n$ (14)
Z	4	4	4	4	8	4
Refls: meas./unique	12763/3578	13199/3718	11320/3245	13245/3689	20709/6084	5956/1679
R indices (for obs. refls)						
R_1	0.0289	0.0414	0.0533	0.0431	0.0363	0.0256
wR_2	0.0751	0.0883	0.1438	0.0958	0.0948	0.0648
T, K	120	298	120	295	120	120
μ, mm^{-1}	2.828	2.554	2.65	2.736	2.802	4.279
θ *range*, °	2.29-28.0	2.19-28.0	2.55-27.0	2.16-28.0	2.28-27.0	2.66-25.5

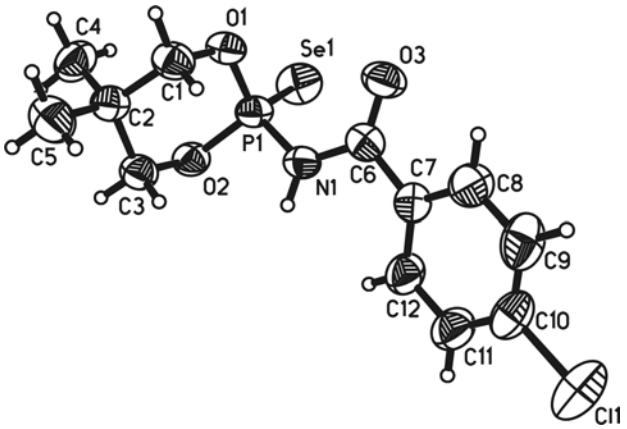
Figures



ESI. Figure 1. The molecular structure of *O*-(*p*-metoxybenzoyl)-2-oxo-2-seleno-5,5-dimethyl-1,3,2-dioxaphosphorinane **6d**. Displacement ellipsoids 50%, C-H hydrogen atoms not labelled. Selected bond lengths (Å) and angles (°): O1-P1 1.5671(19), O2-P1 1.5608(18), C6-C7 1.469(4), O1-P1-O3 99.42(10), O2-P1-O3 106.11(10), P1-O3-C6 122.26(16), Se1-P1-O3-C6 –65.69(19)



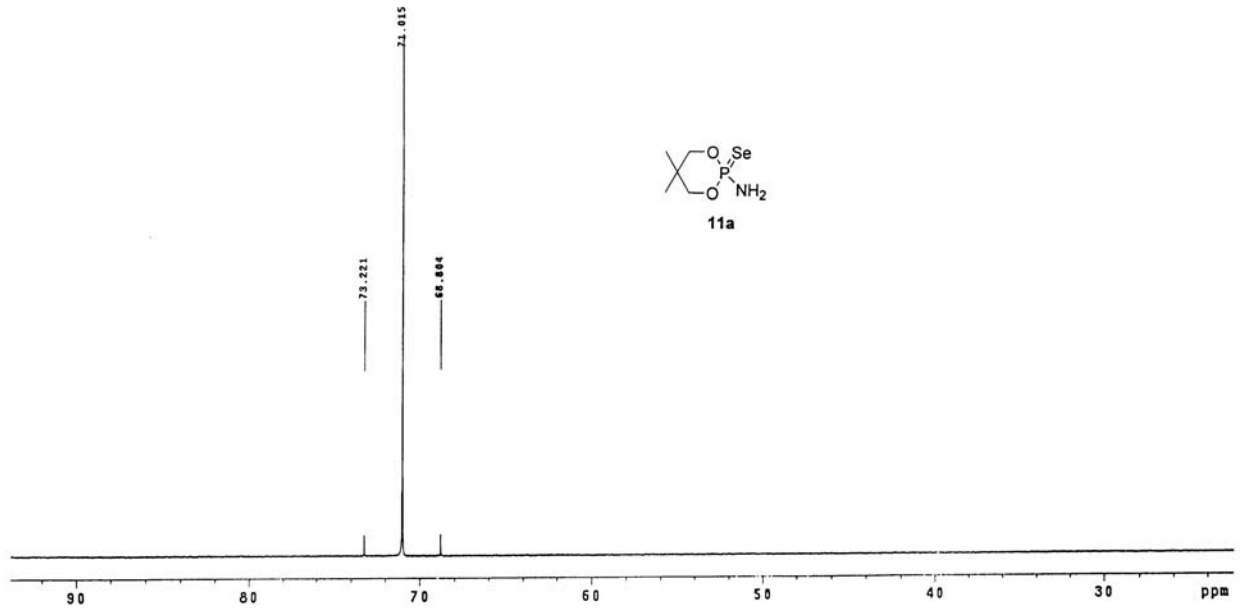
ESI. Figure 2. The molecular structure of *O*-(*p*-nitrobenzoyl)-2-oxo-2-seleno-5,5-dimethyl-1,3,2-dioxaphosphorinane **6e**. Displacement ellipsoids 50%, C-H hydrogen atoms not labelled. Selected bond lengths (Å) and angles (°): O1-P1 1.561(3), O2-P1 1.566(3), C6-C7 1.500(6), O1-P1-O3 98.92(15), O2-P1-O3 104.88(15), P1-O3-C6 119.8(3), Se1-P1-O3-C6 –69.2(3)



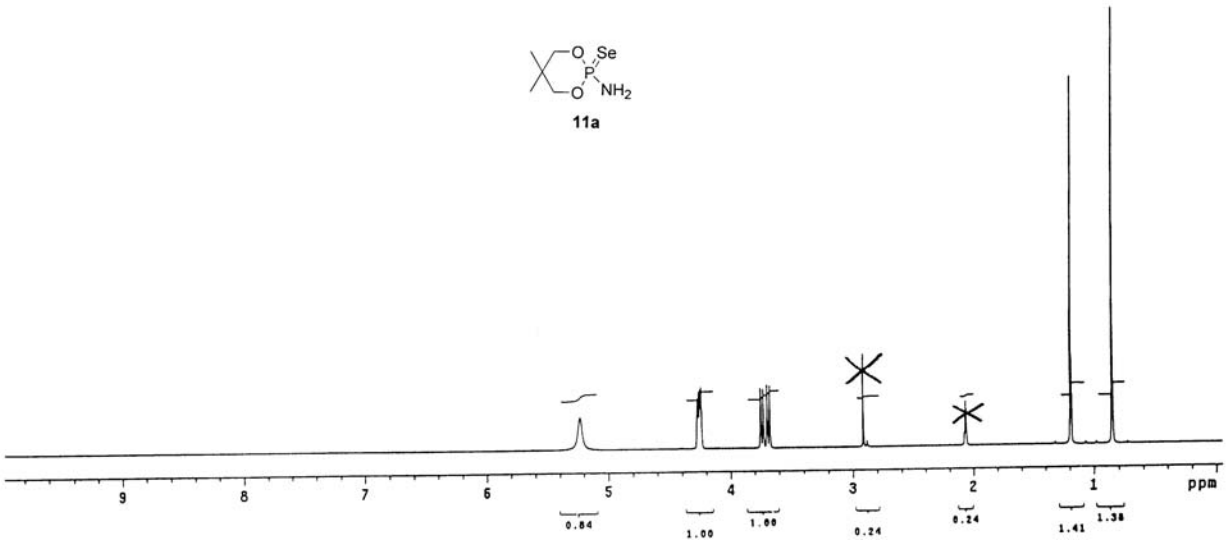
ESI. Figure 3. The molecular structure of *N*-(*p*-chlorobenzoyl)-2-amino-2-seleno-5,5-dimethyl-1,3,2-dioxaphosphorinane **8a**. Displacement ellipsoids 50%, hydrogen atoms not labelled. Selected bond lengths (Å) and angles (°): O1-P1 1.567(2), O2-P1 1.587(2), C6-C7 1.500(5), O1-P1-N1 106.92(14), O2-P1-N1 100.60(14), P1-N1-C6 125.1(3), P1-N1-H1 116(3), C6-N1-H1 116(3), Se1-P1-N1-C6 63.4(3).

2-amino-2-seleno-5,5-dimethyl-1,3,2-dioxaphosphorinane **11a**

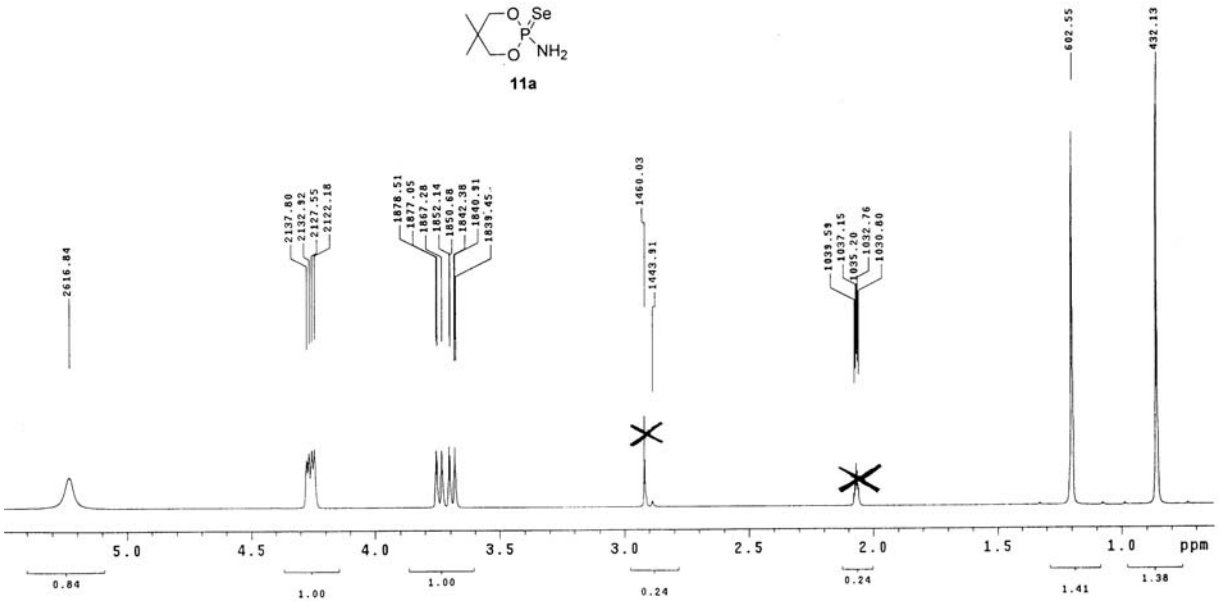
^{31}P NMR (acetone-d_6):



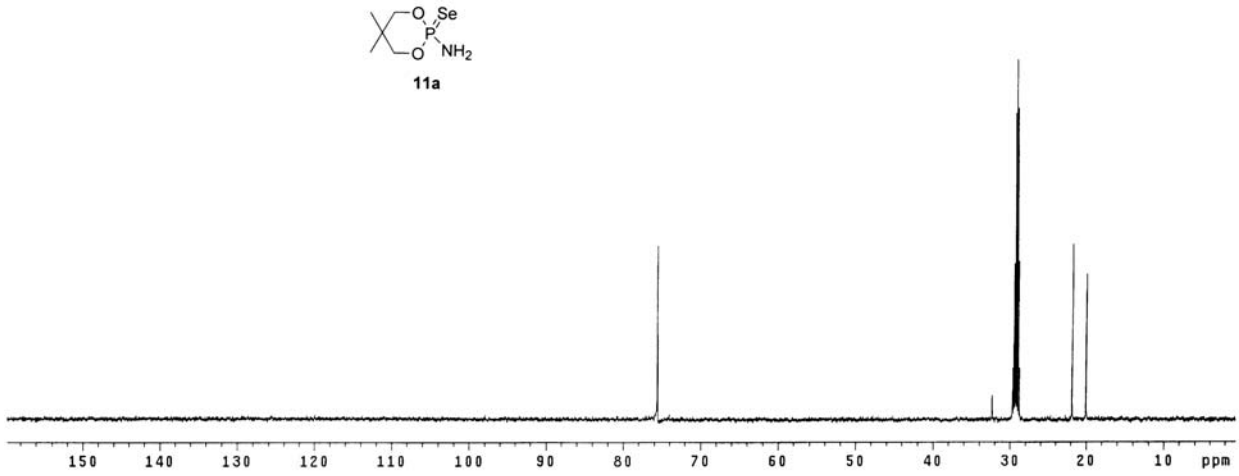
^{1}H NMR (acetone-d_6):



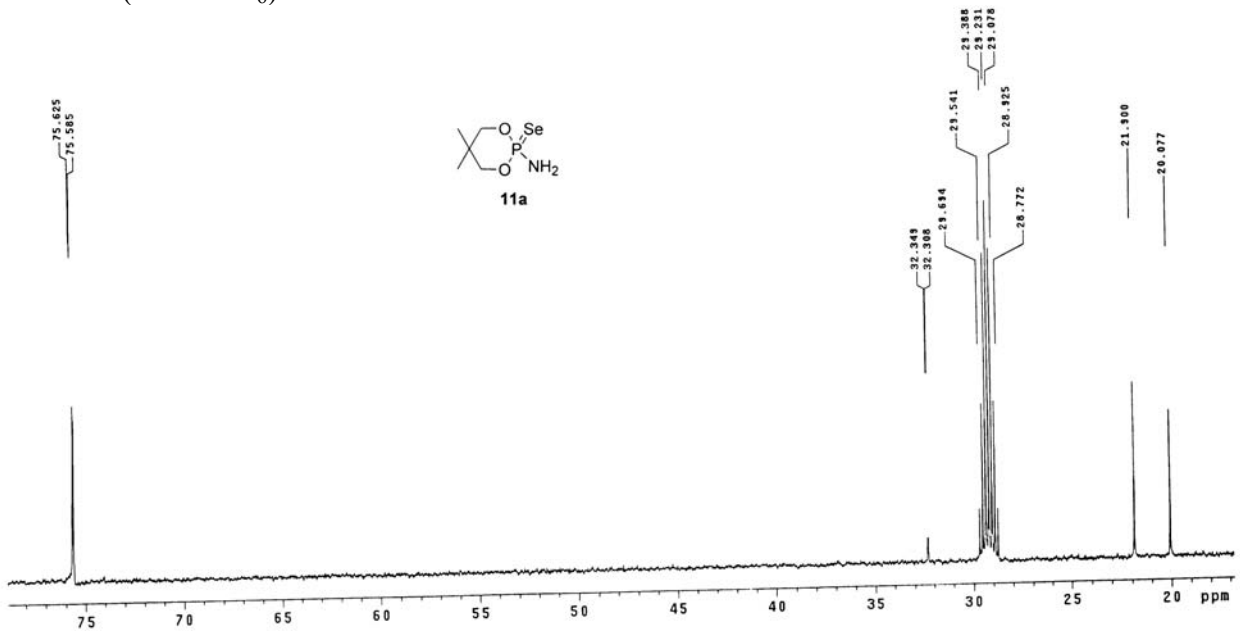
^{1}H NMR (acetone-d_6):



^{13}C NMR (acetone-d_6):

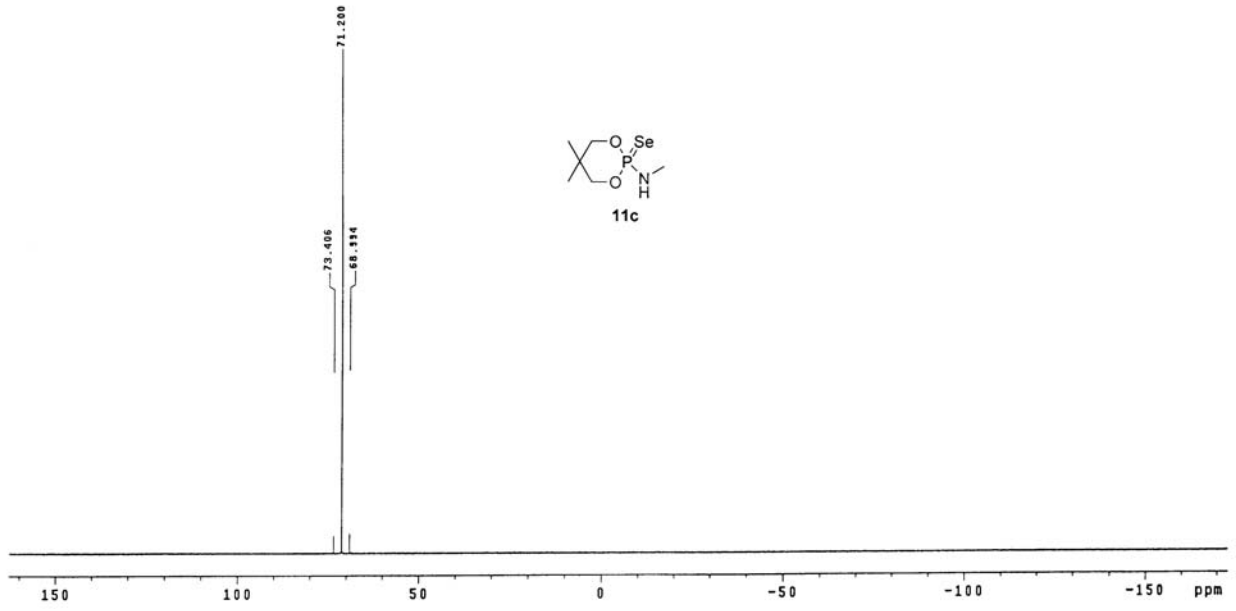


^{13}C NMR (acetone-d_6):

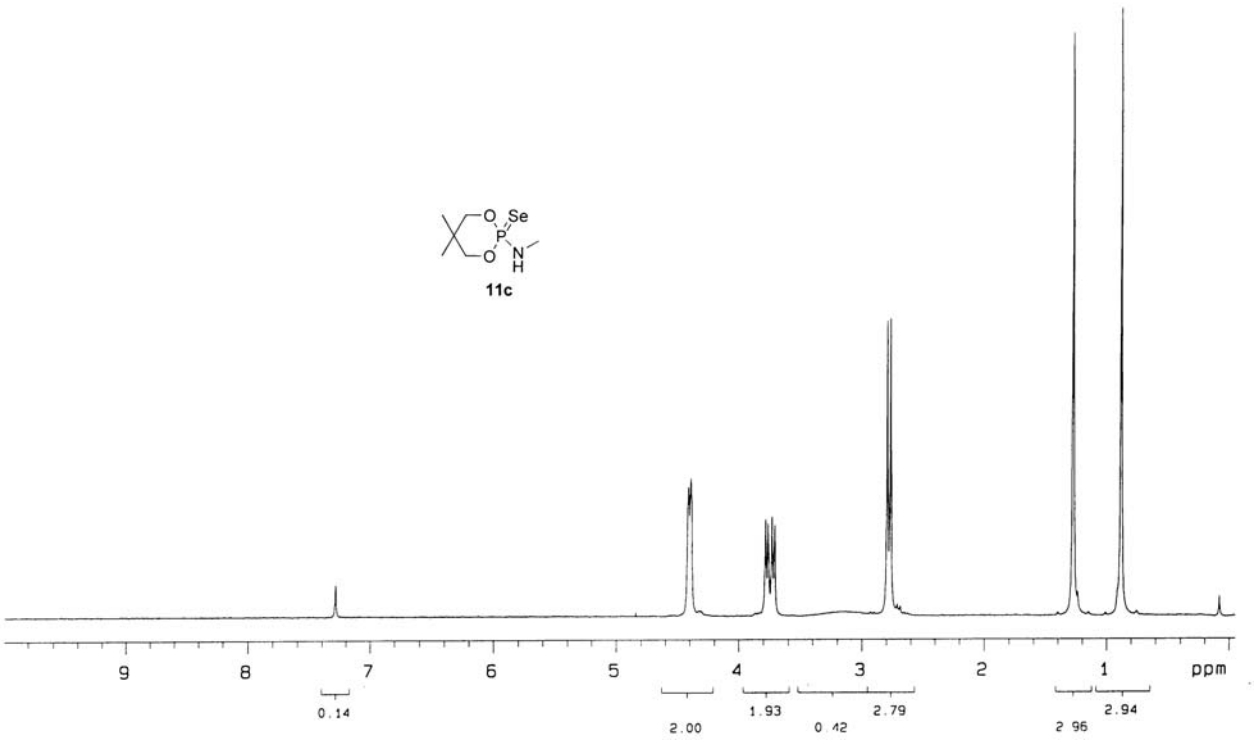


2-metyloamino-2-seleno-5,5-dimethyl-1,3,2-dioxaphosphorinane **11c**

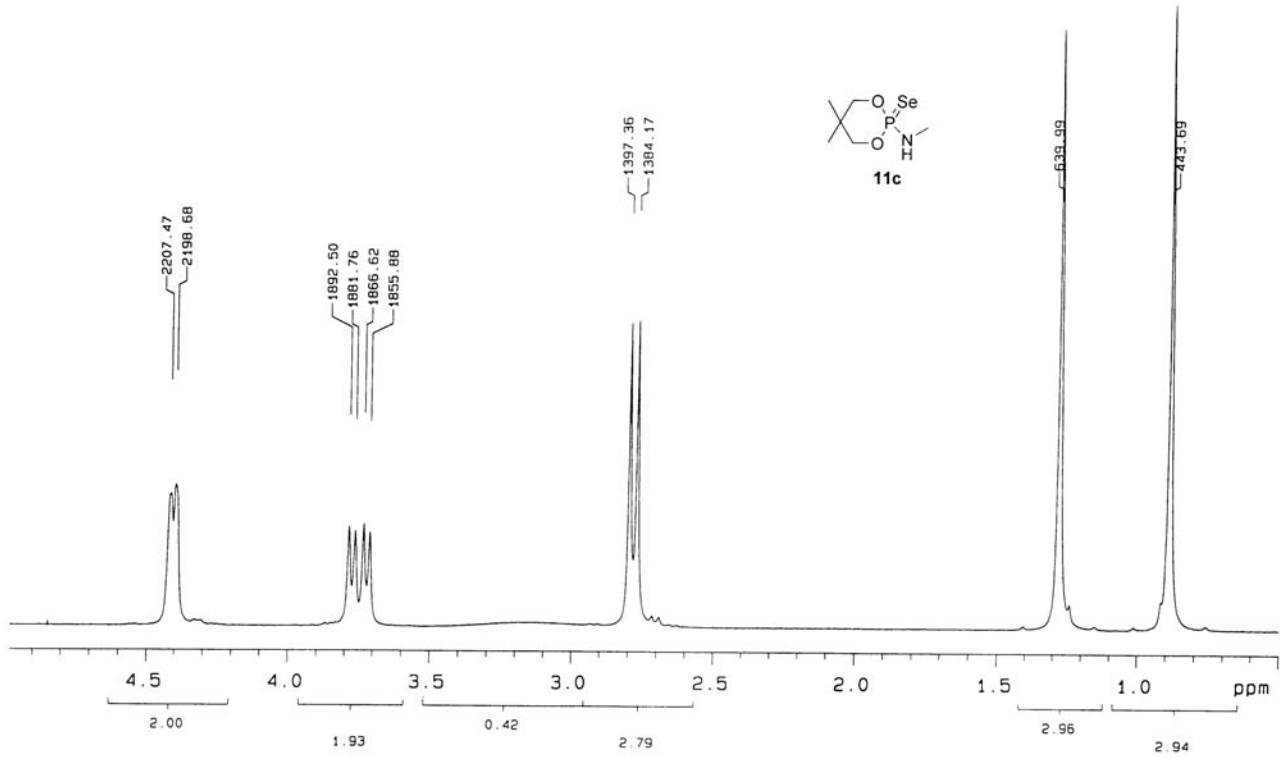
^{31}P NMR ($CDCl_3$):



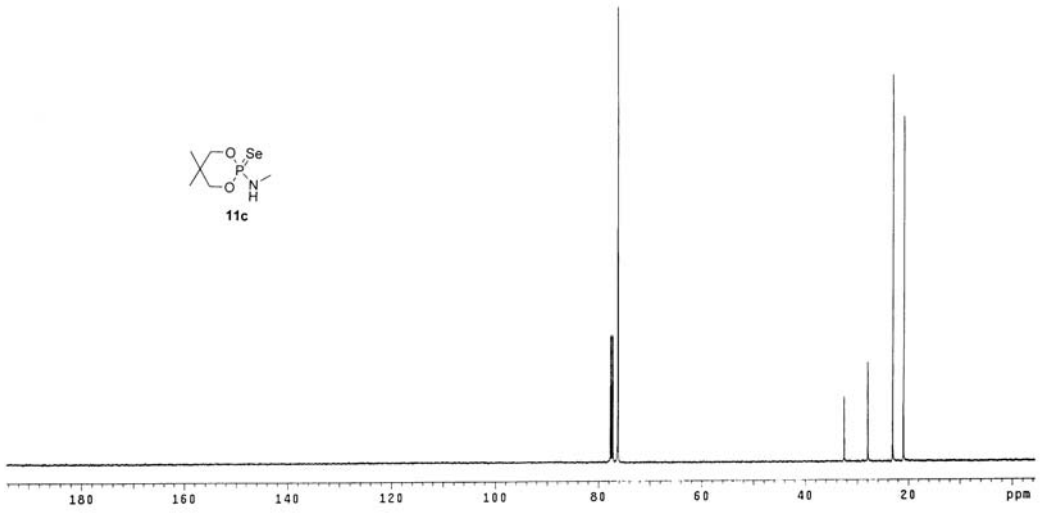
^{1}H NMR ($CDCl_3$):



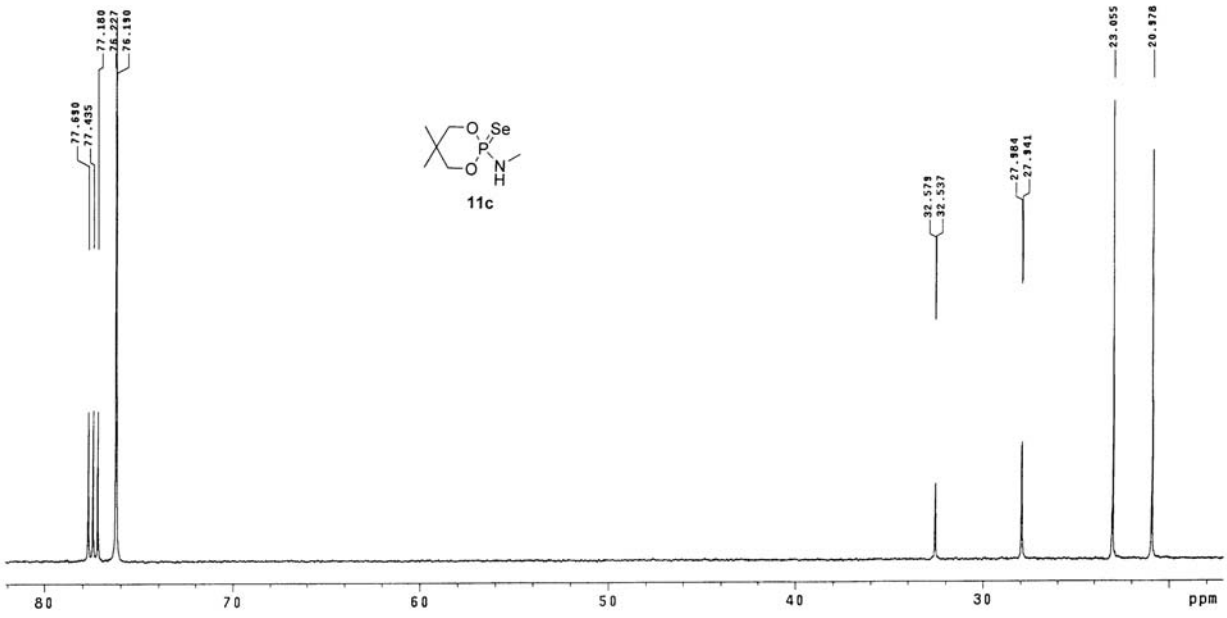
^{1}H NMR ($CDCl_3$):



^{13}C NMR ($CDCl_3$):

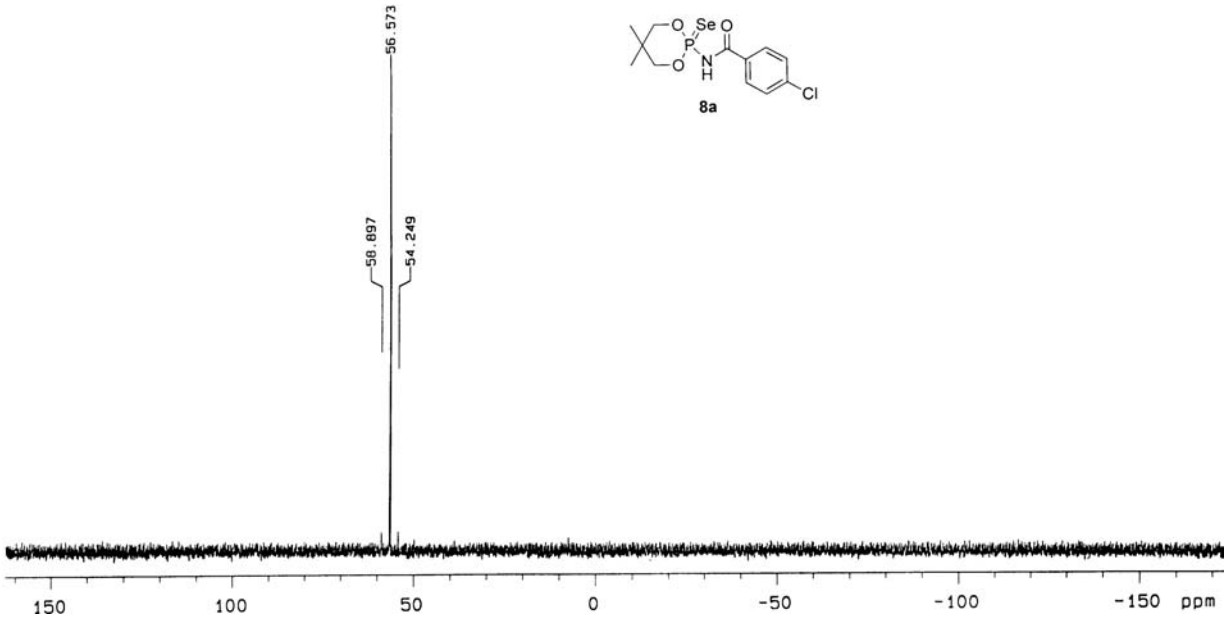


^{13}C NMR ($CDCl_3$):

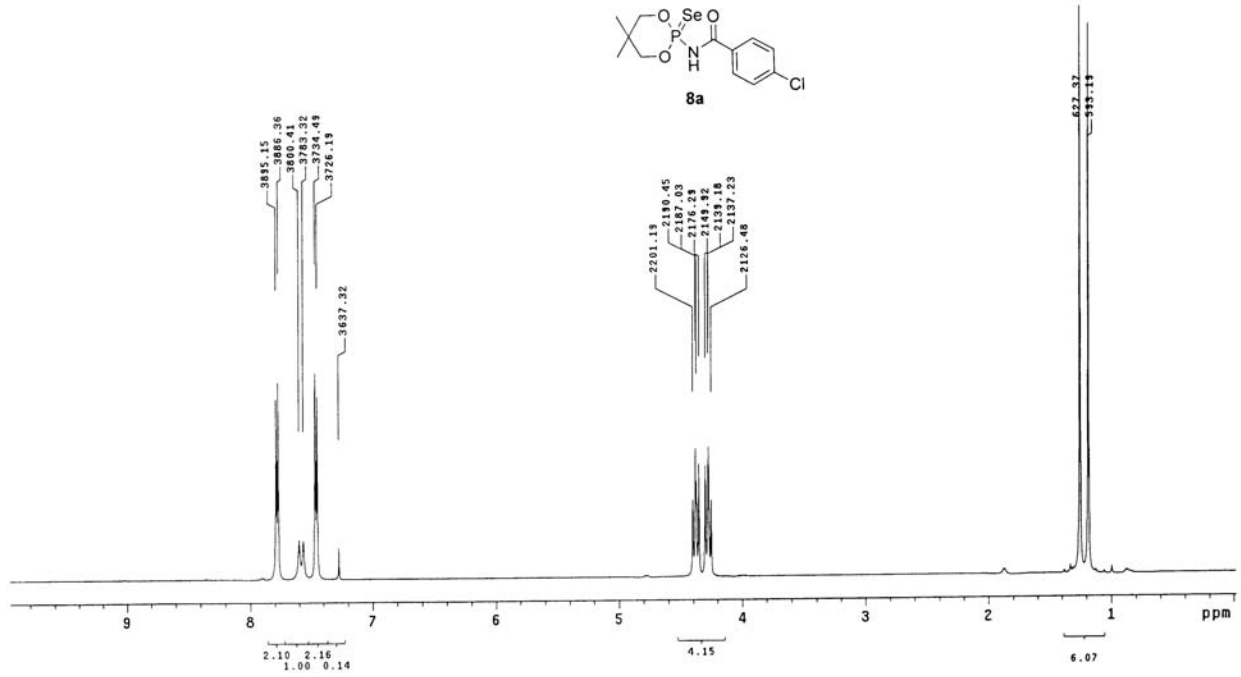


N-(*p*-chlorobenzoyl)-2-amino-2-seleno-5,5-dimethyl-1,3,2-dioxaphosphorinane **8a**

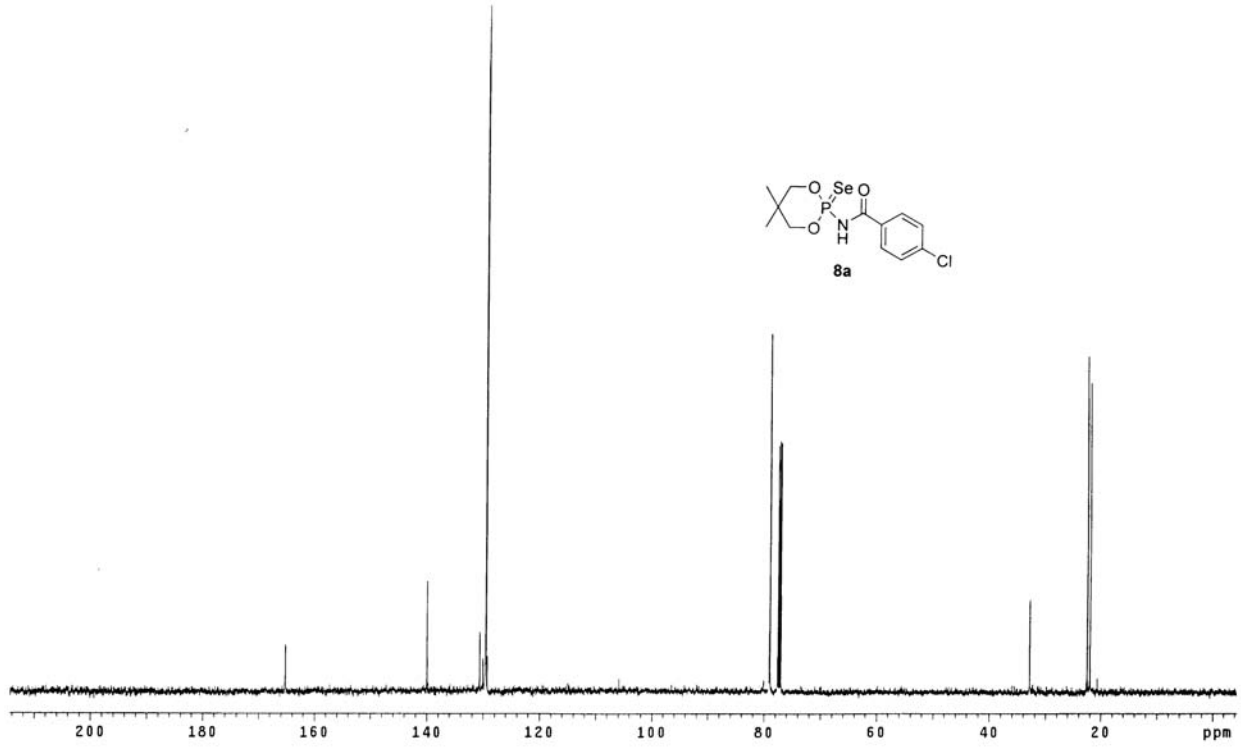
^{31}P NMR ($CDCl_3$):



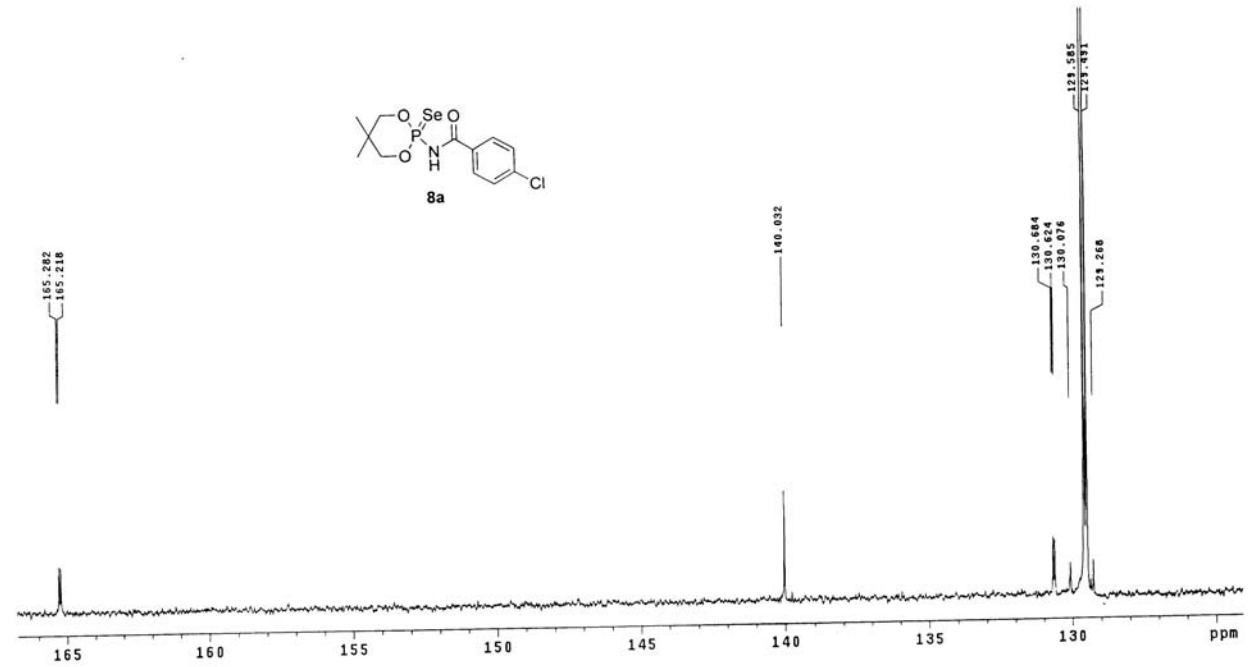
^{1}H NMR ($CDCl_3$):



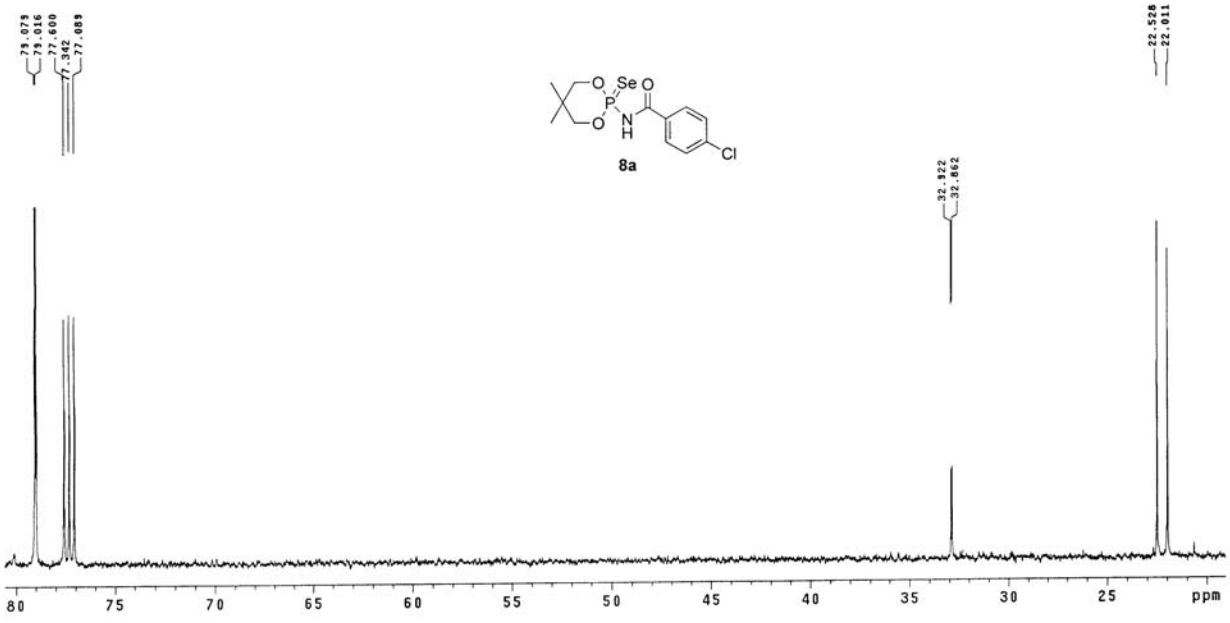
^{13}C NMR ($CDCl_3$):



^{13}C NMR ($CDCl_3$):

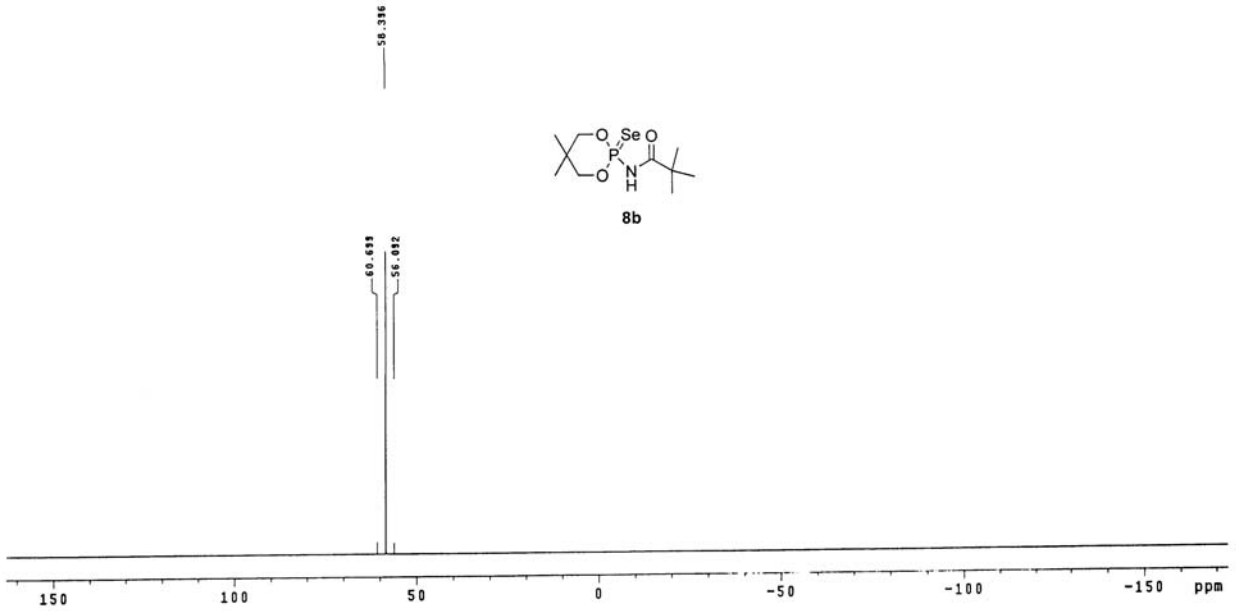


^{13}C NMR ($CDCl_3$):

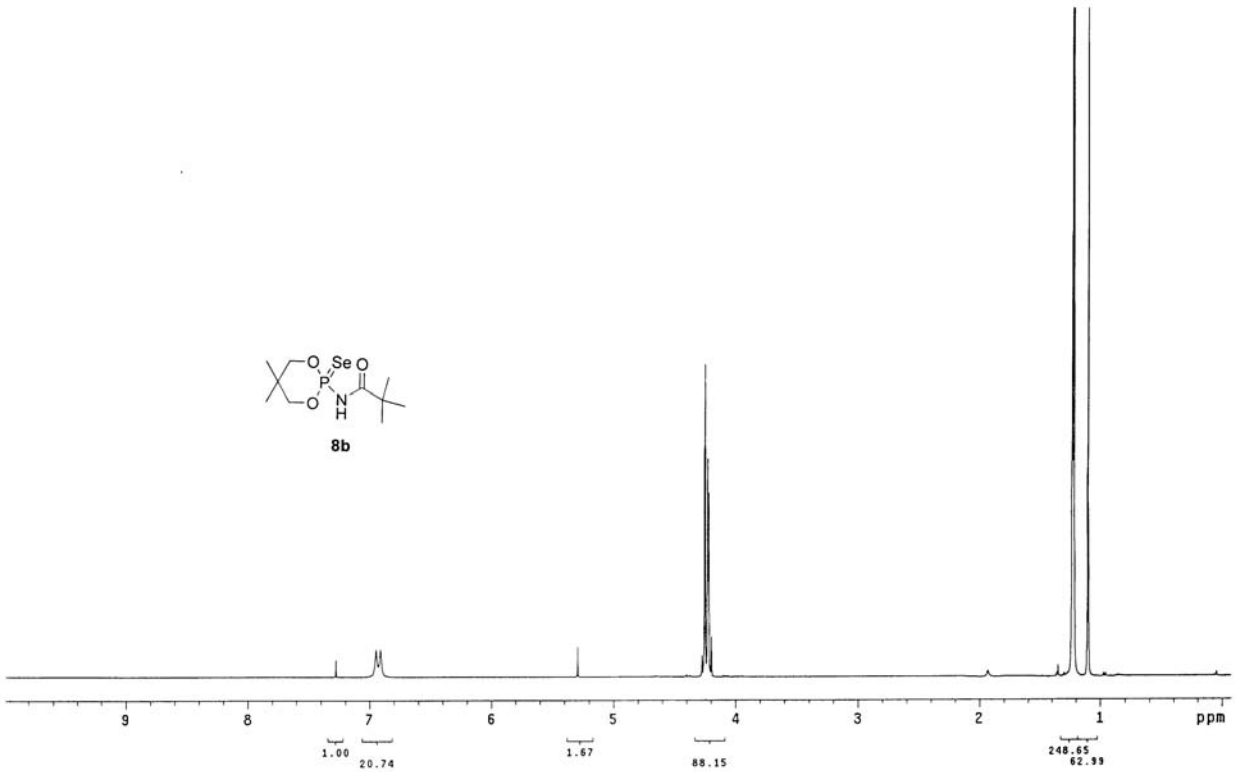


N-pivaloyl-2-amino-2-seleno-5,5-dimethyl-1,3,2-dioxaphosphorinane **8b**

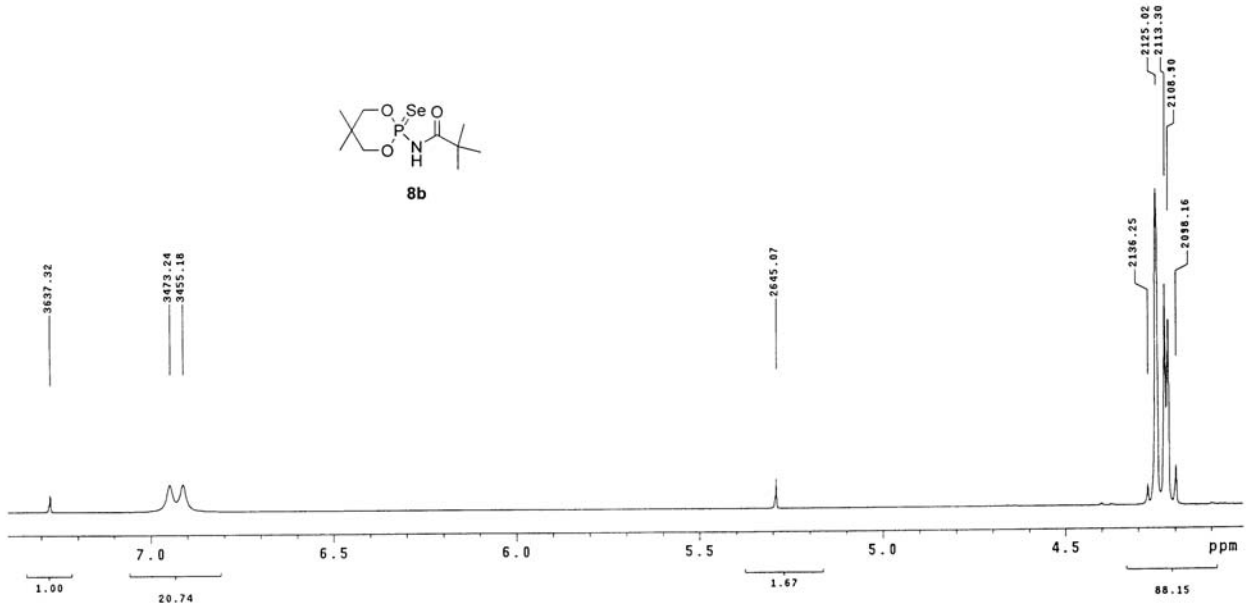
^{31}P NMR ($CDCl_3$):



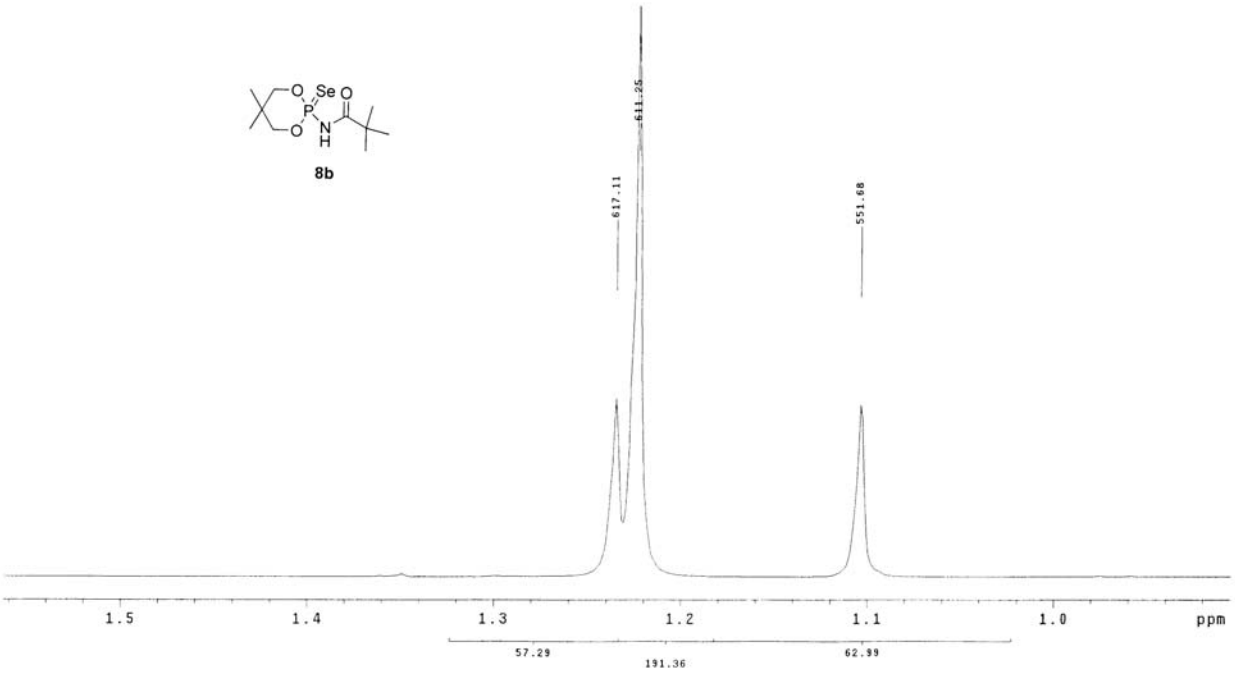
^{1}H NMR ($CDCl_3$):



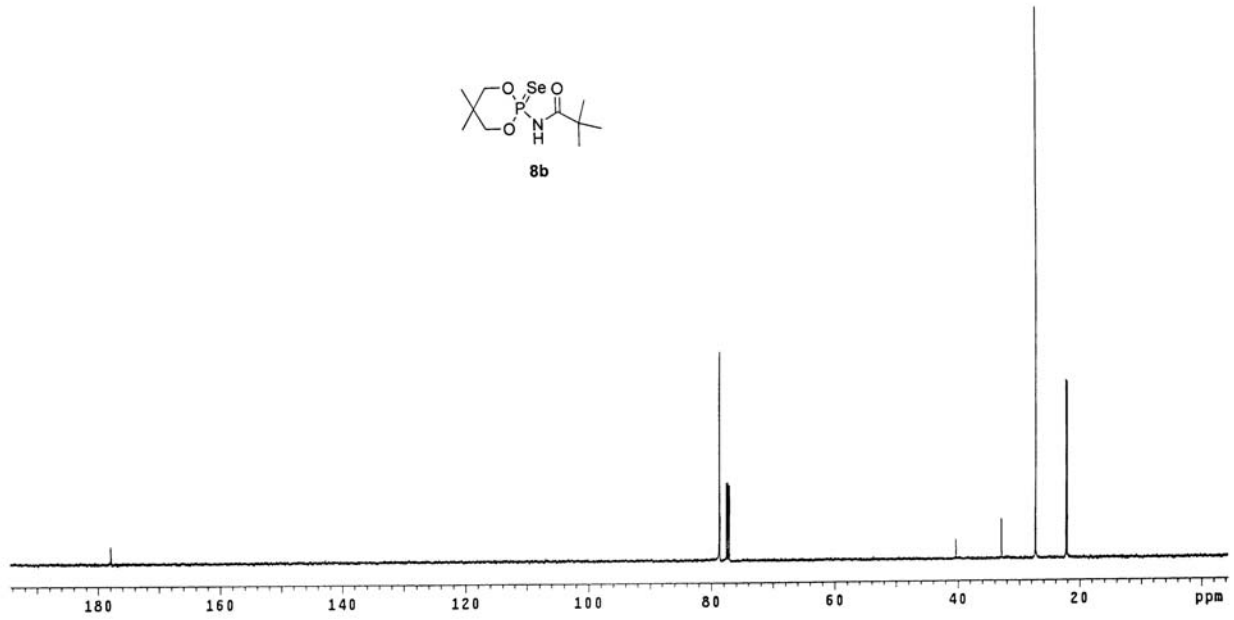
^{1}H NMR ($CDCl_3$):



^{1}H NMR ($CDCl_3$):



^{13}C NMR ($CDCl_3$):



^{13}C NMR ($CDCl_3$):