Supporting Information

Iodosobenzene-mediated three-component selenofunctionalization of olefins

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1. Mechanistic studies

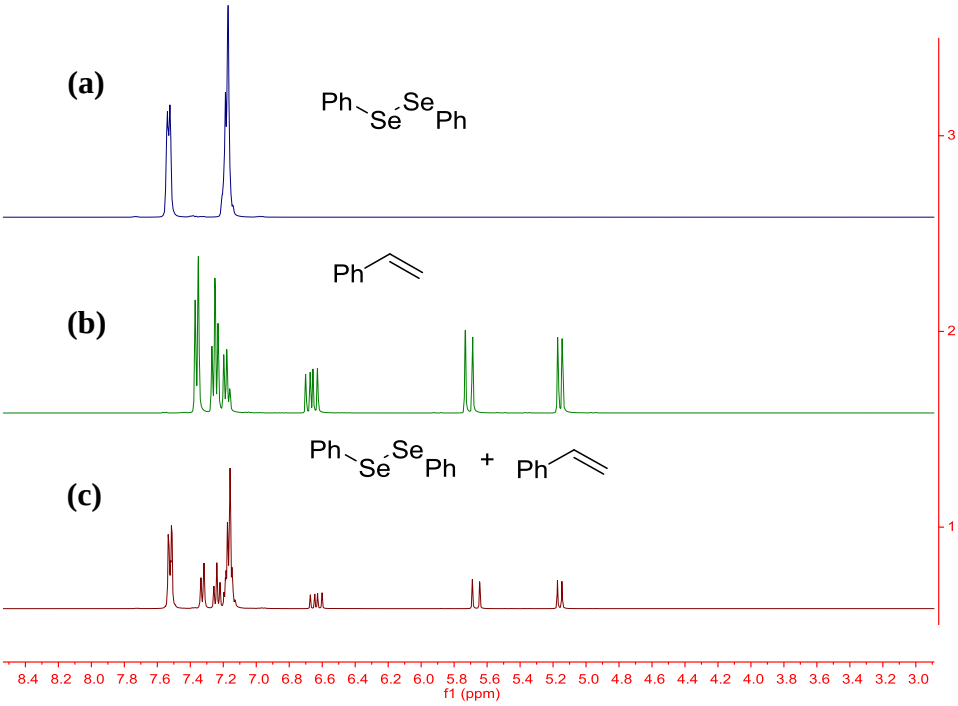


Figure S1. ^{1}H NMR spectra. (a) ^{1}H NMR spectrum of Ph_2Se_2. (b) ^{1}H NMR spectrum of styrene. (c) ^{1}H NMR spectrum of the mixture of styrene and Ph_2Se_2 (1:1).

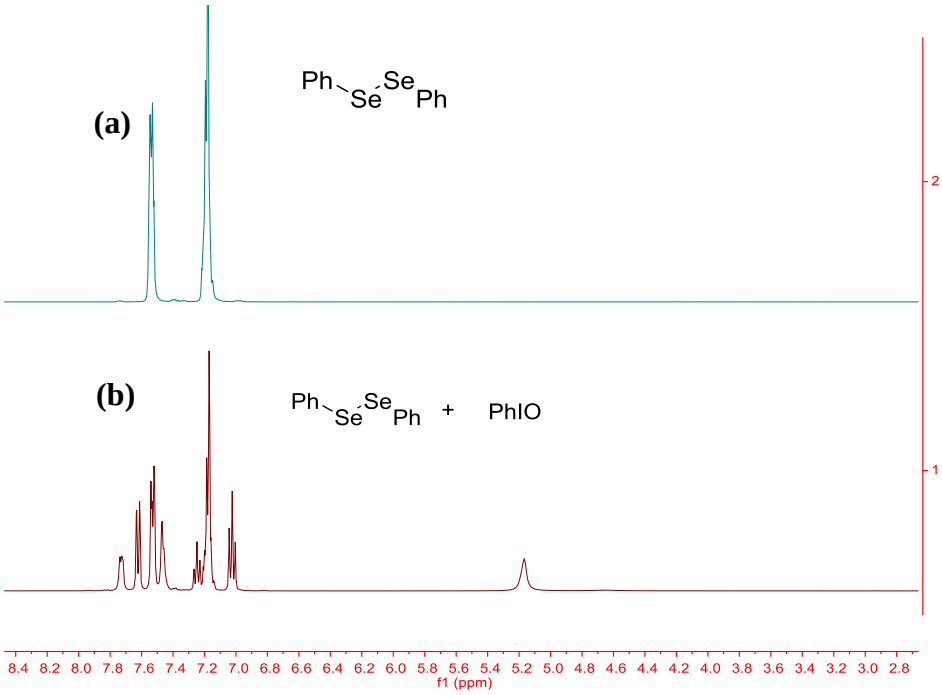


Figure S2. ^{1}H NMR spectra. (a) ^{1}H NMR spectrum of Ph_2Se_2. (b) ^{1}H NMR spectrum of the mixture of Ph_2Se_2 and PhIO (1:1).

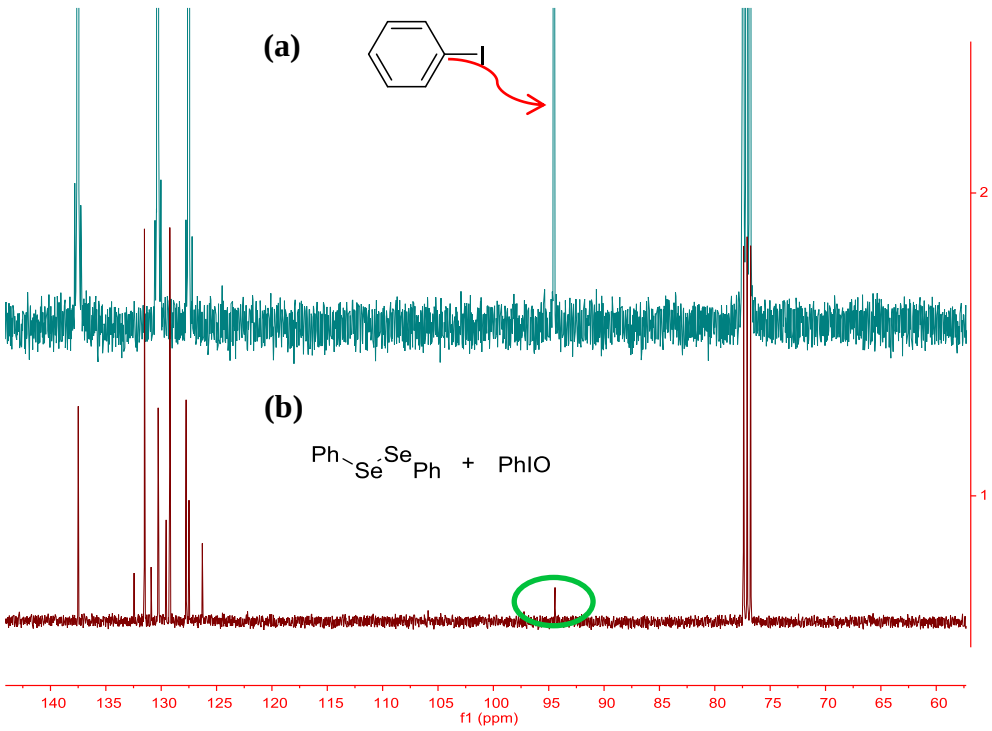


Figure S3. $^{13}C\{^{1}H\}$ NMR spectrum. (a) $^{13}C\{^{1}H\}$ NMR spectrum of PhI. (b) $^{13}C\{^{1}H\}$ NMR spectrum of the mixture of Ph_2Se_2 and PhIO (1:1)

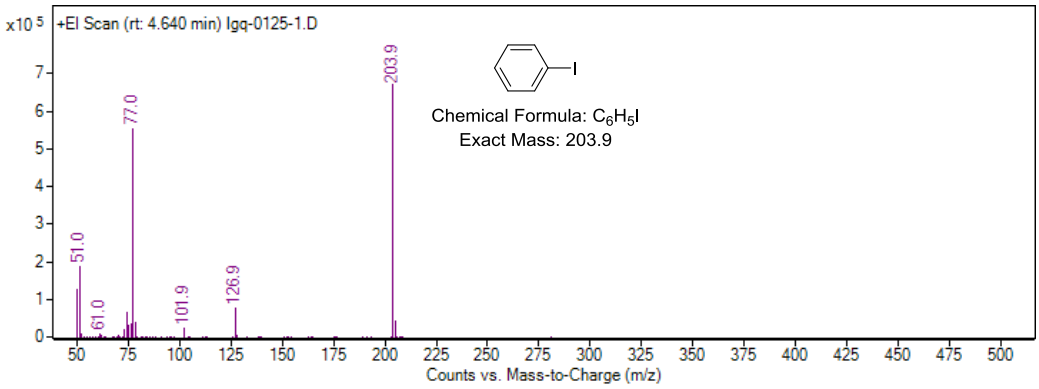


Figure S4. GC-MS spectra of iodobenzene generated from the reaction of Ph_2Se_2 and PhIO

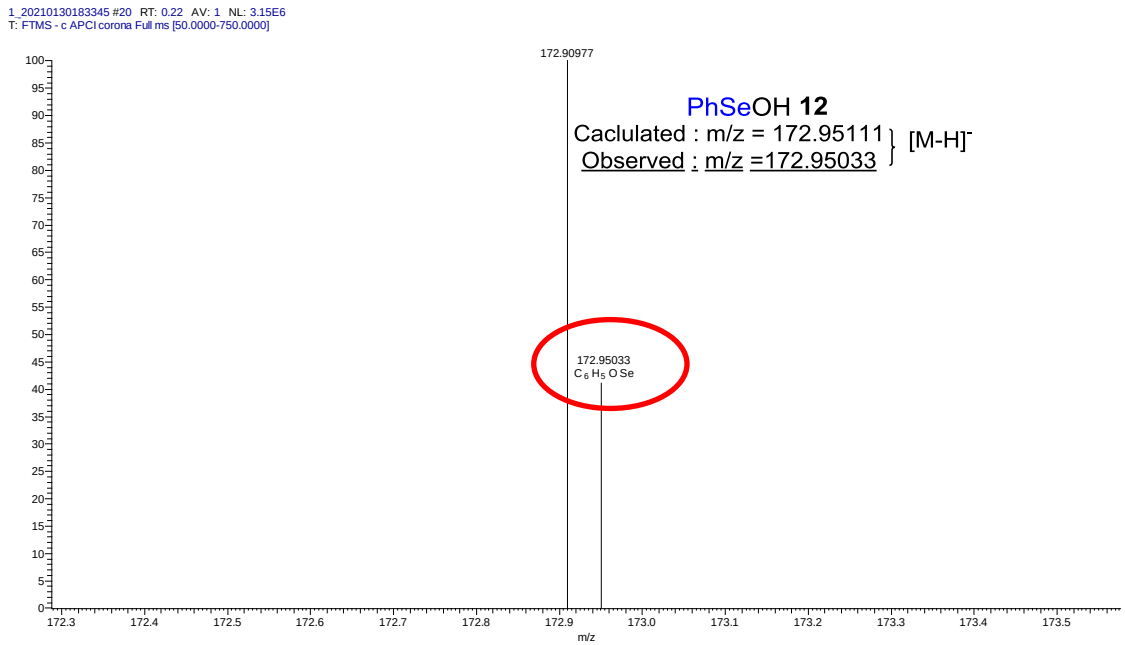


Figure S5. HRMS spectra of **12**

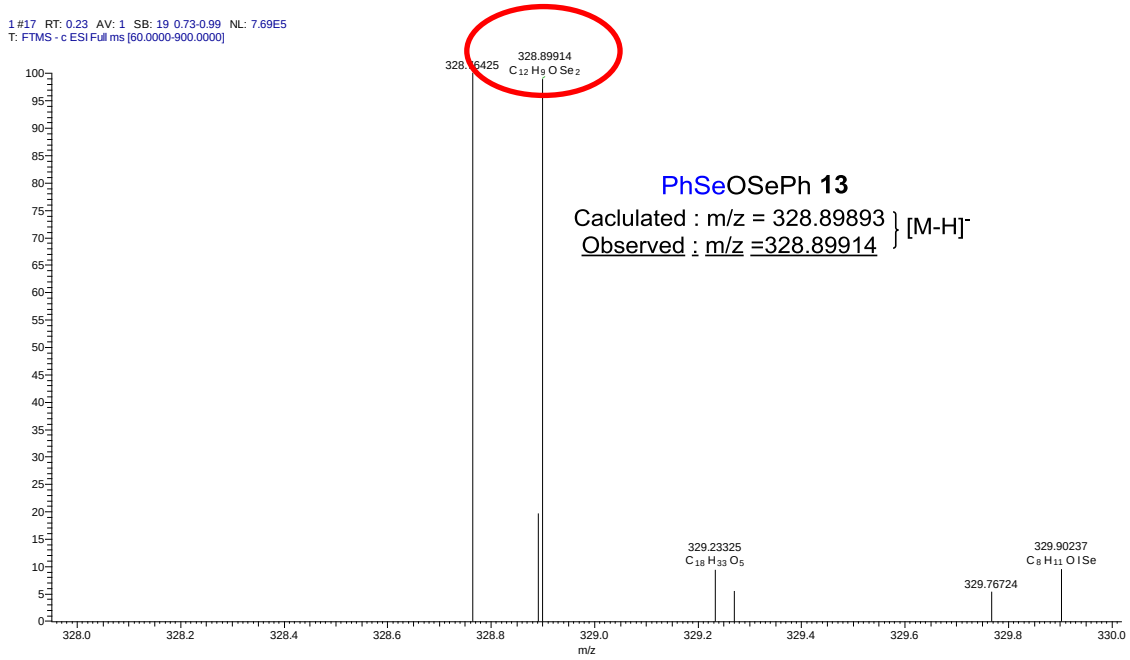
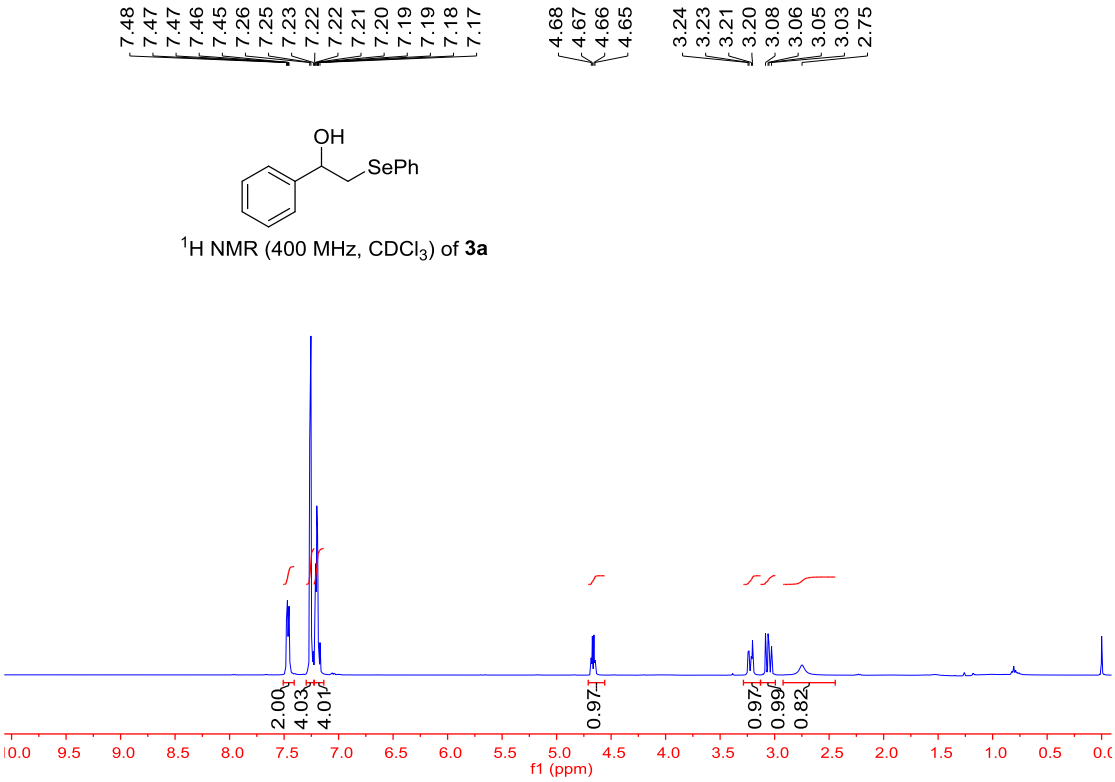
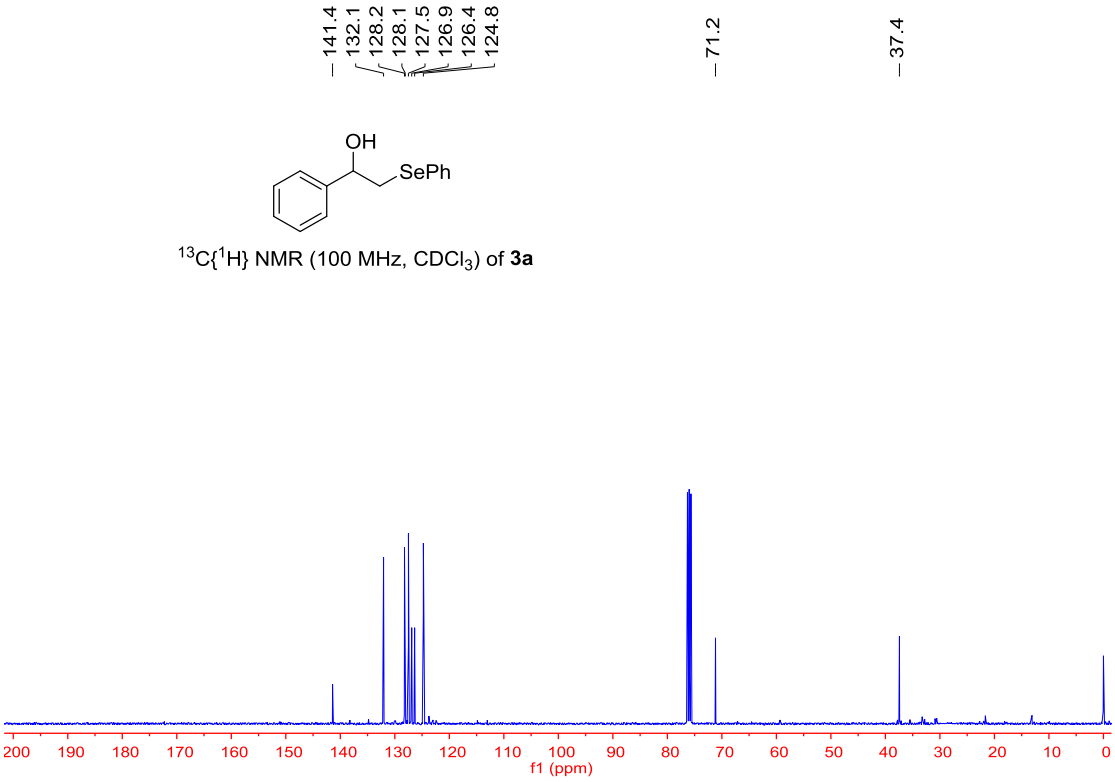


Figure S6. HRMS spectra of **13**

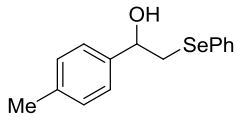
2. Copies of NMR spectra



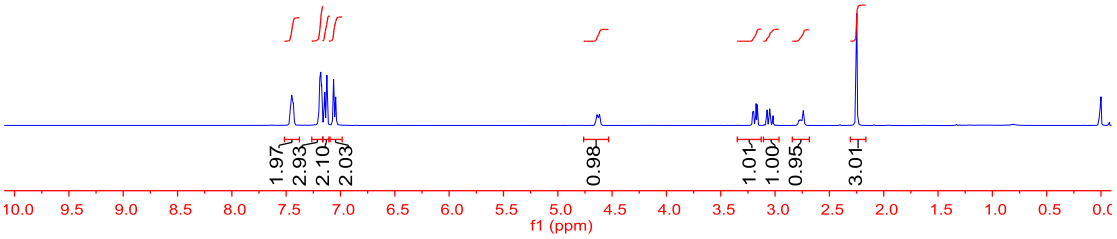
^{1}H NMR (400 MHz, $CDCl_3$) of **3a**

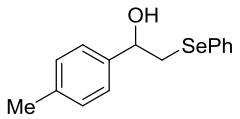


^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) of **3a**

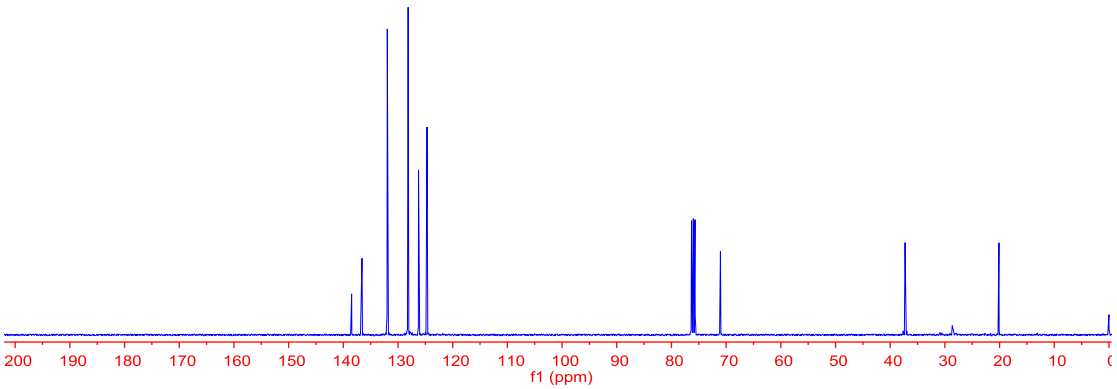


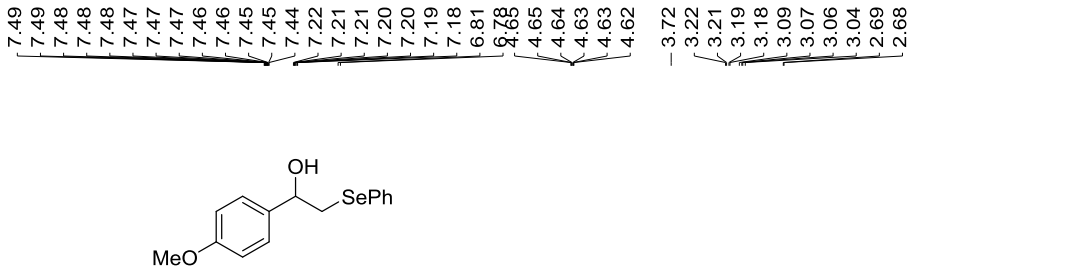
^{1}H NMR (400 MHz, $CDCl_3$) of **3b**



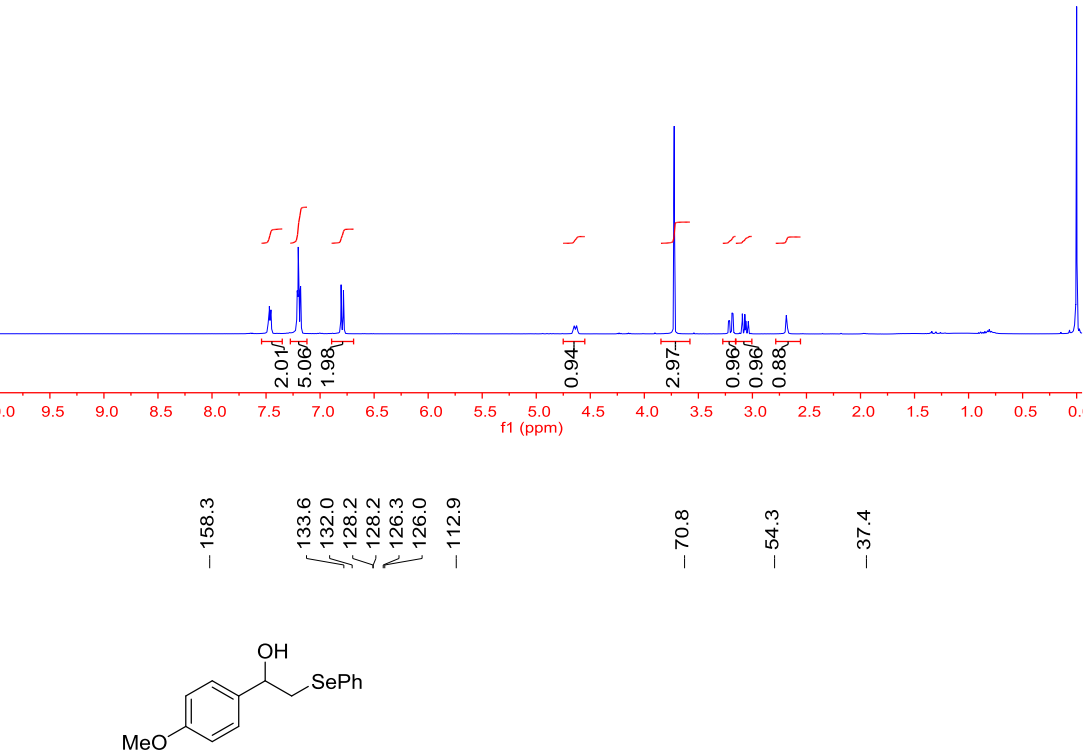


^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) of **3b**

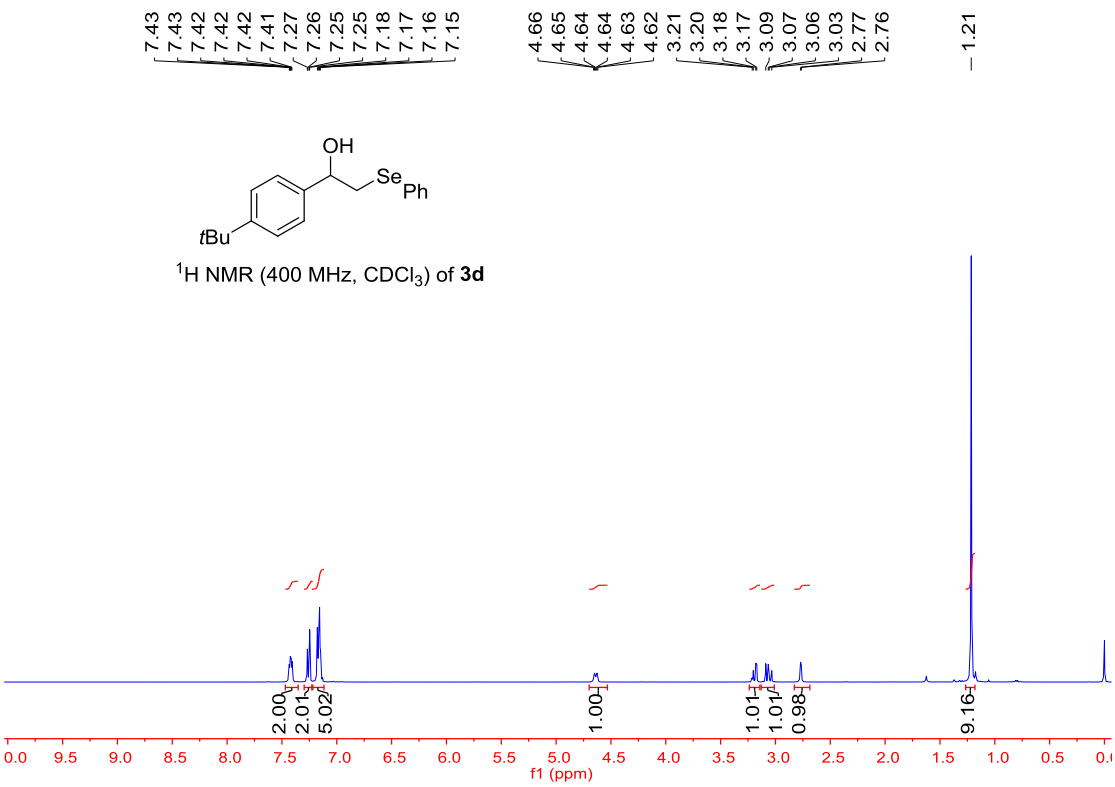




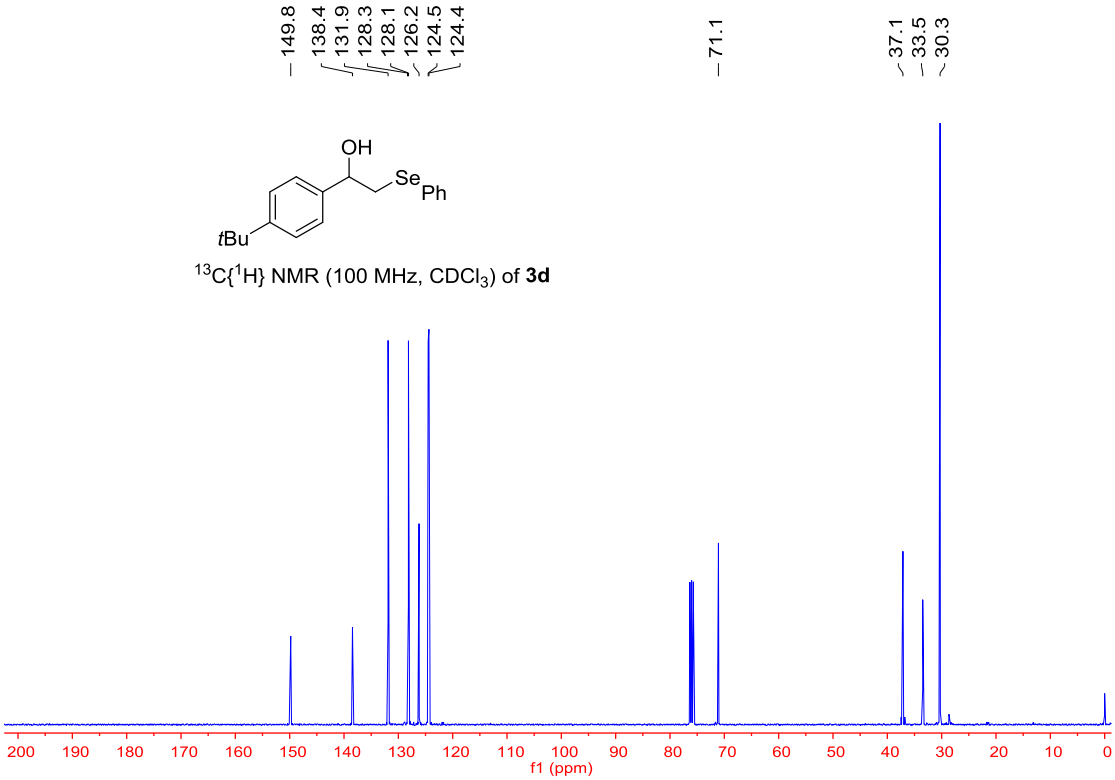
^{1}H NMR (400 MHz, $CDCl_3$) of **3c**



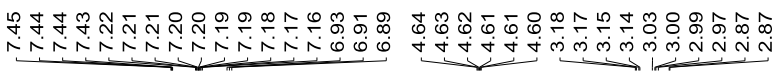
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) of **3c**

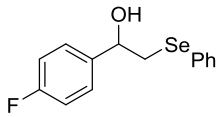


^{1}H NMR (400 MHz, $CDCl_3$) of **3d**

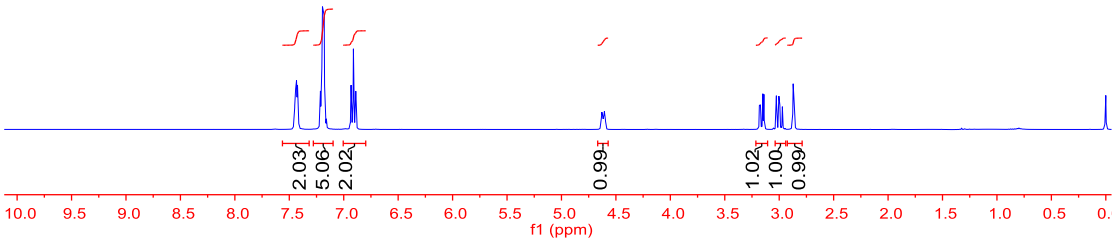


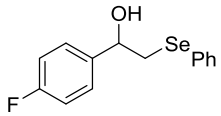
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) of **3d**



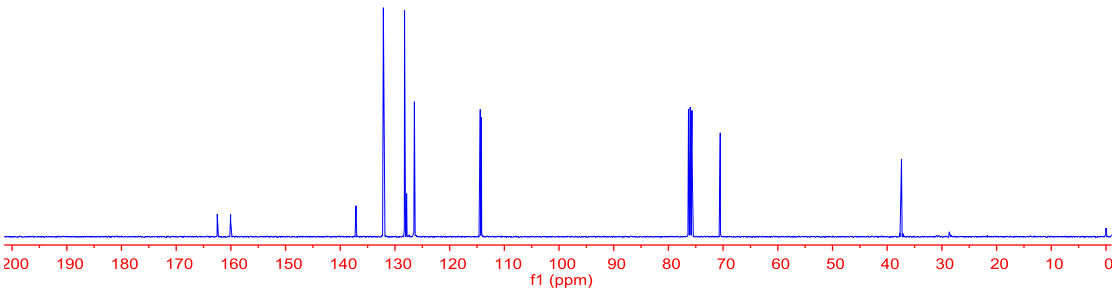


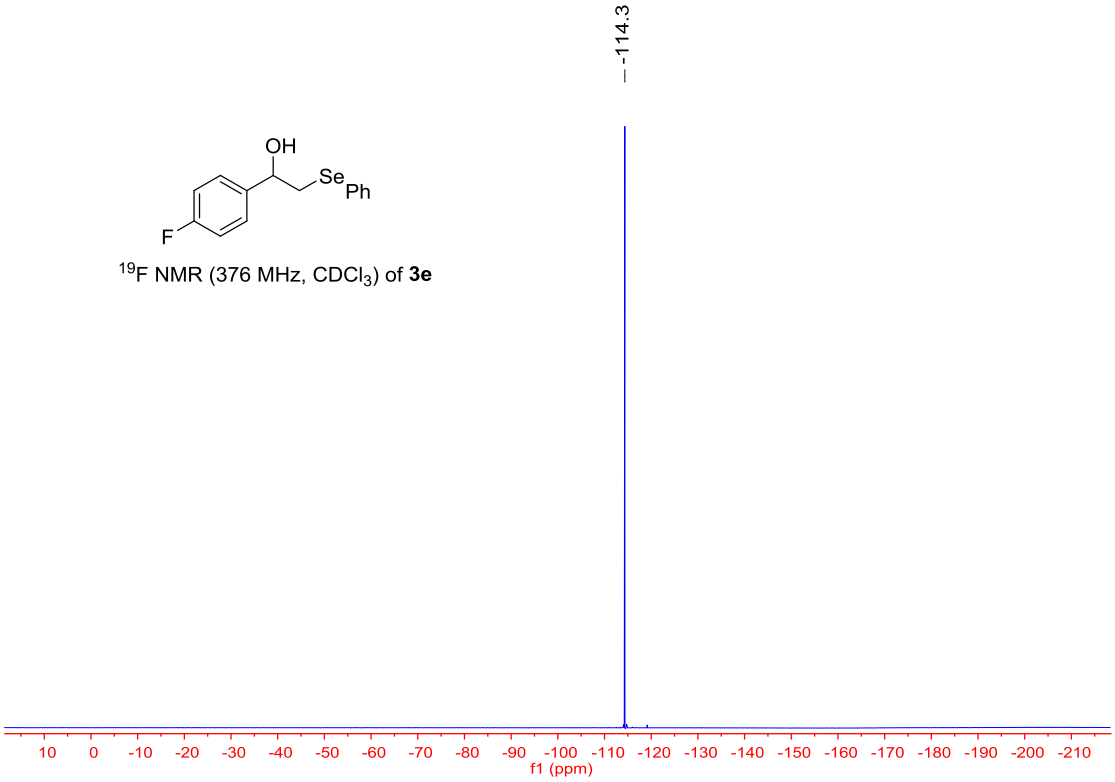
^{1}H NMR (400 MHz, $CDCl_3$) of **3e**



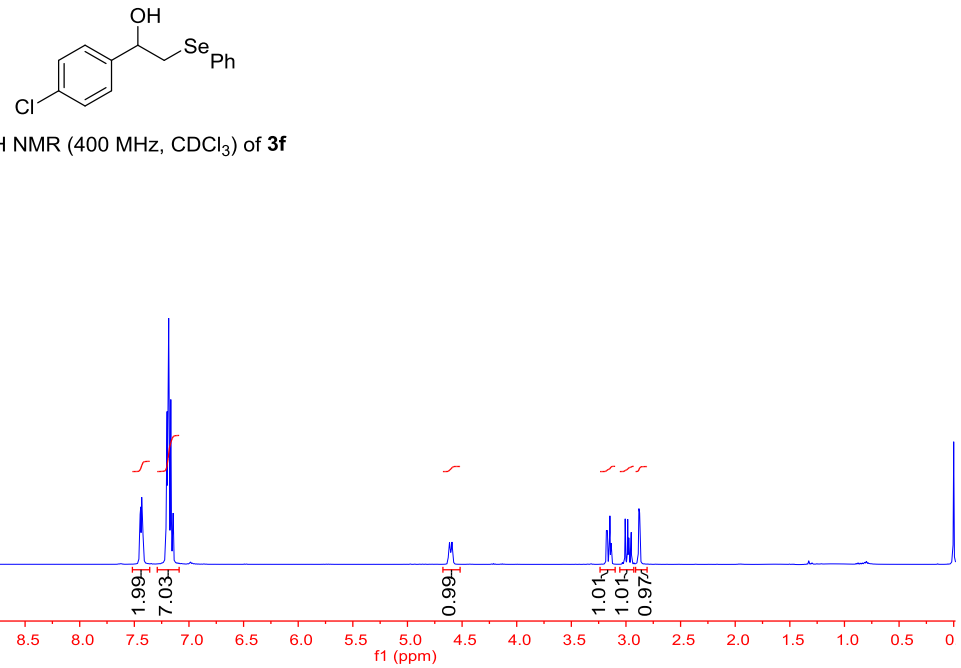


^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) of **3e**

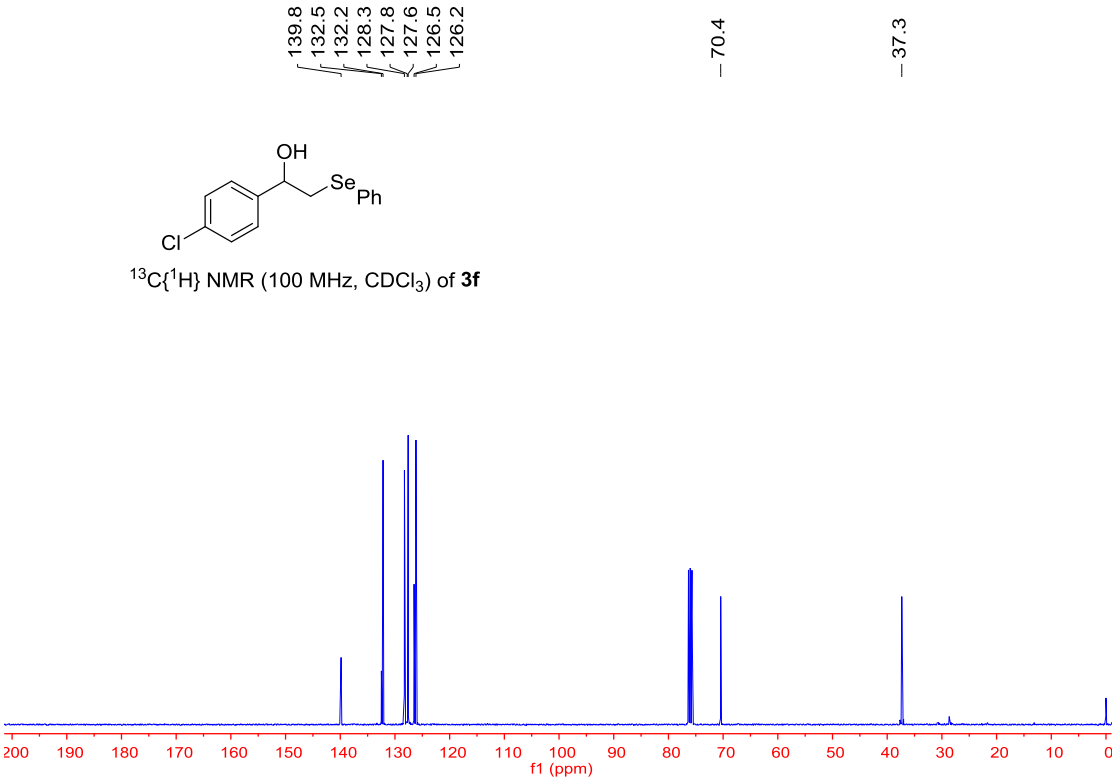




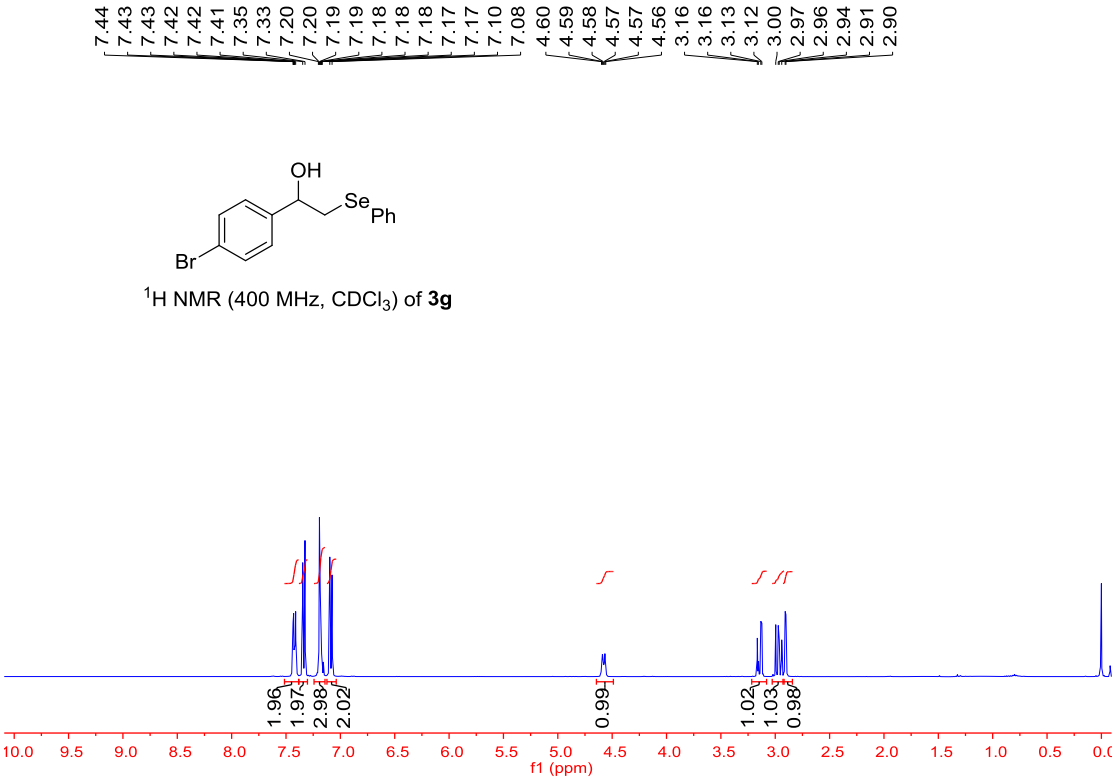
^{19}F NMR (376 MHz, $CDCl_3$) of **3e**



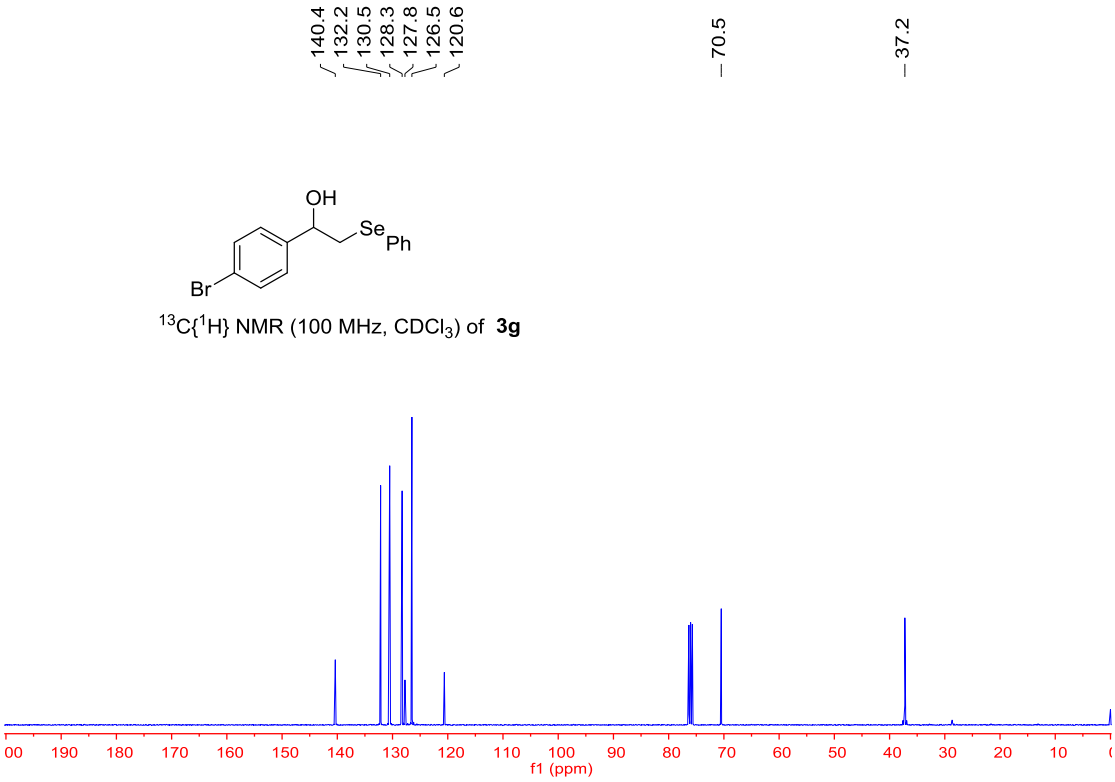
^{1}H NMR (400 MHz, $CDCl_3$) of **3f**



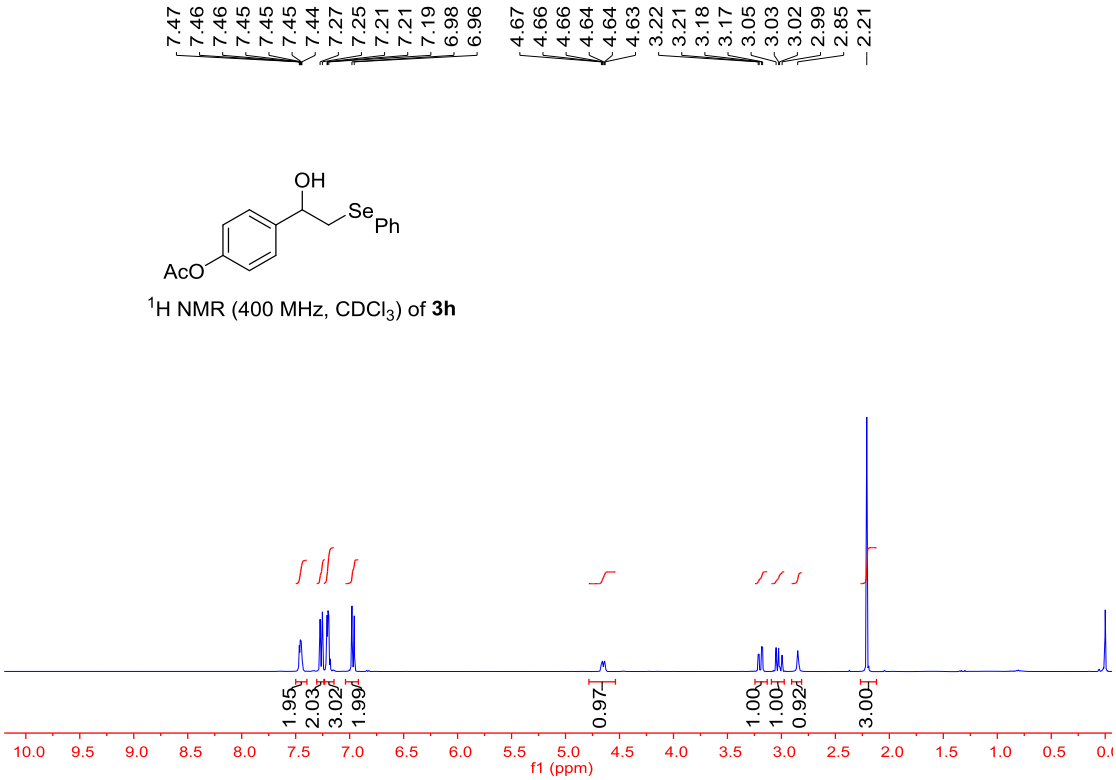
$^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) of **3f**



^1H NMR (400 MHz, $CDCl_3$) of **3g**

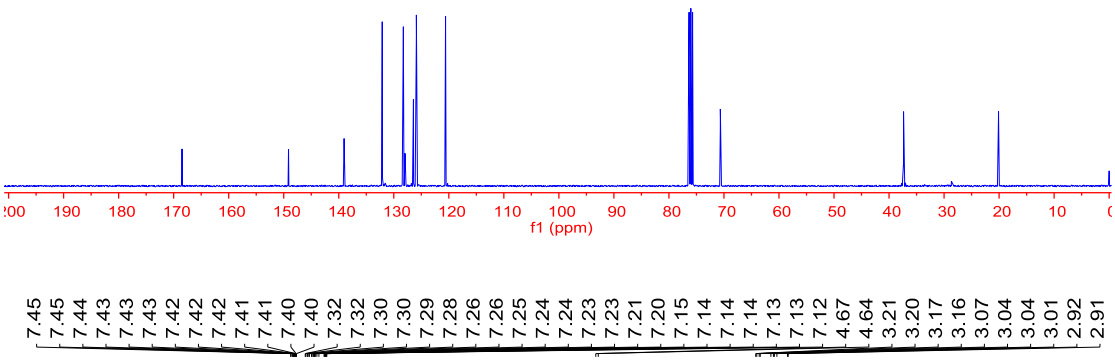


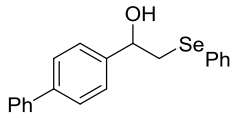
$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) of **3g**



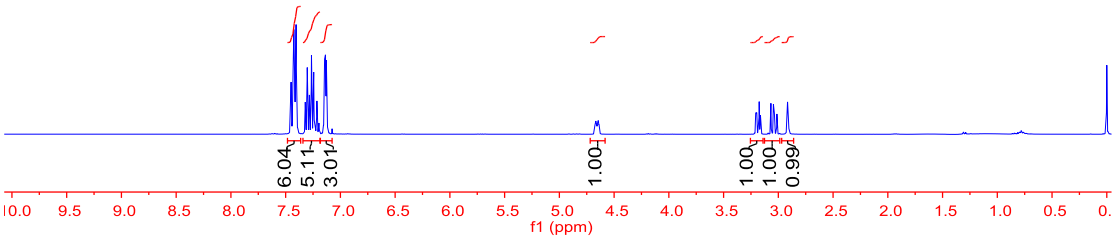
^{1}H NMR (400 MHz, $CDCl_3$) of **3h**

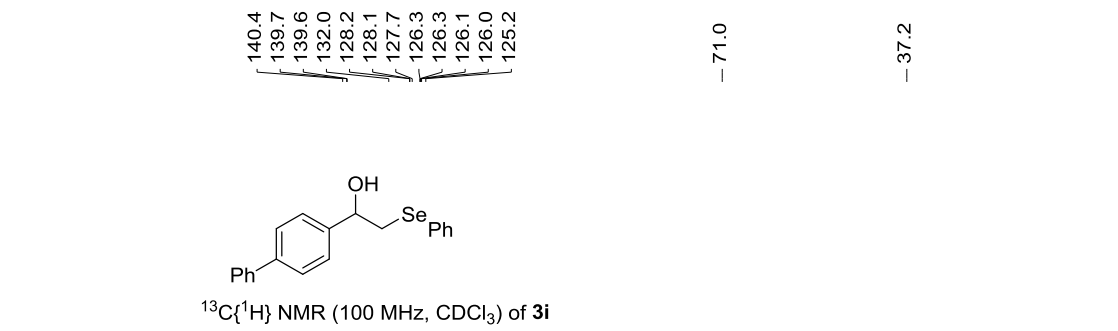
$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) of **3h**



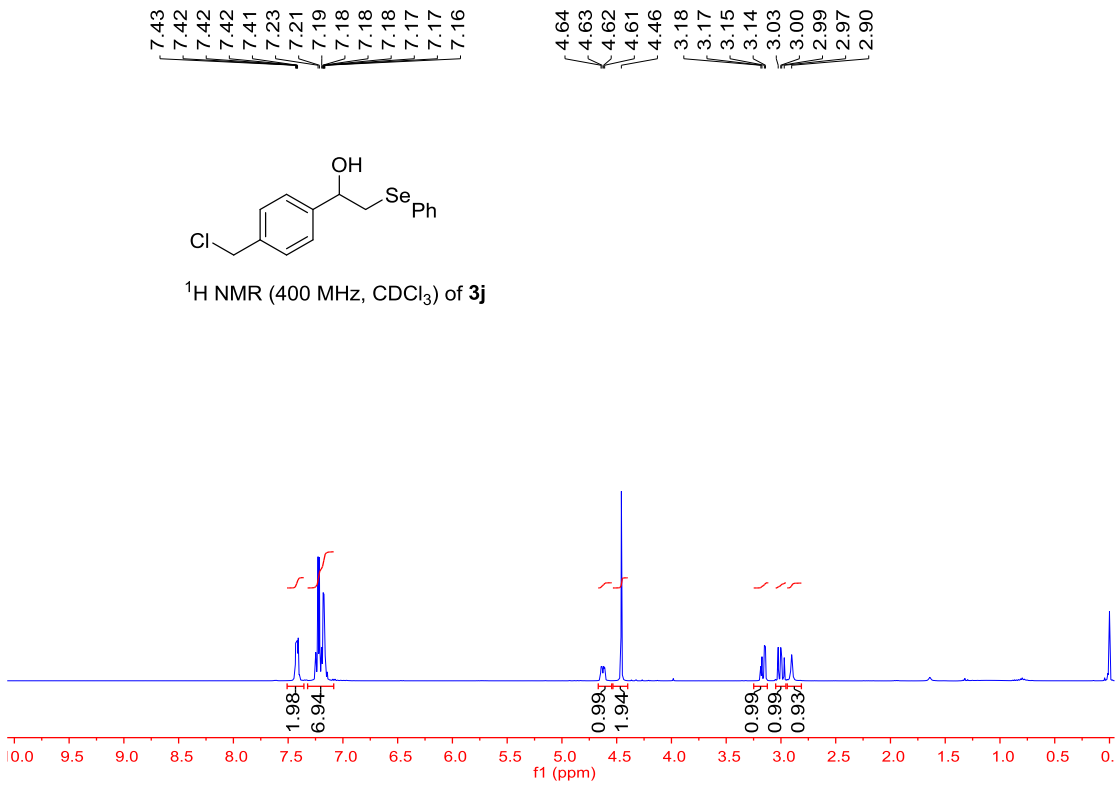


^{1}H NMR (400 MHz, $CDCl_3$) of **3i**





$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) of **3i**



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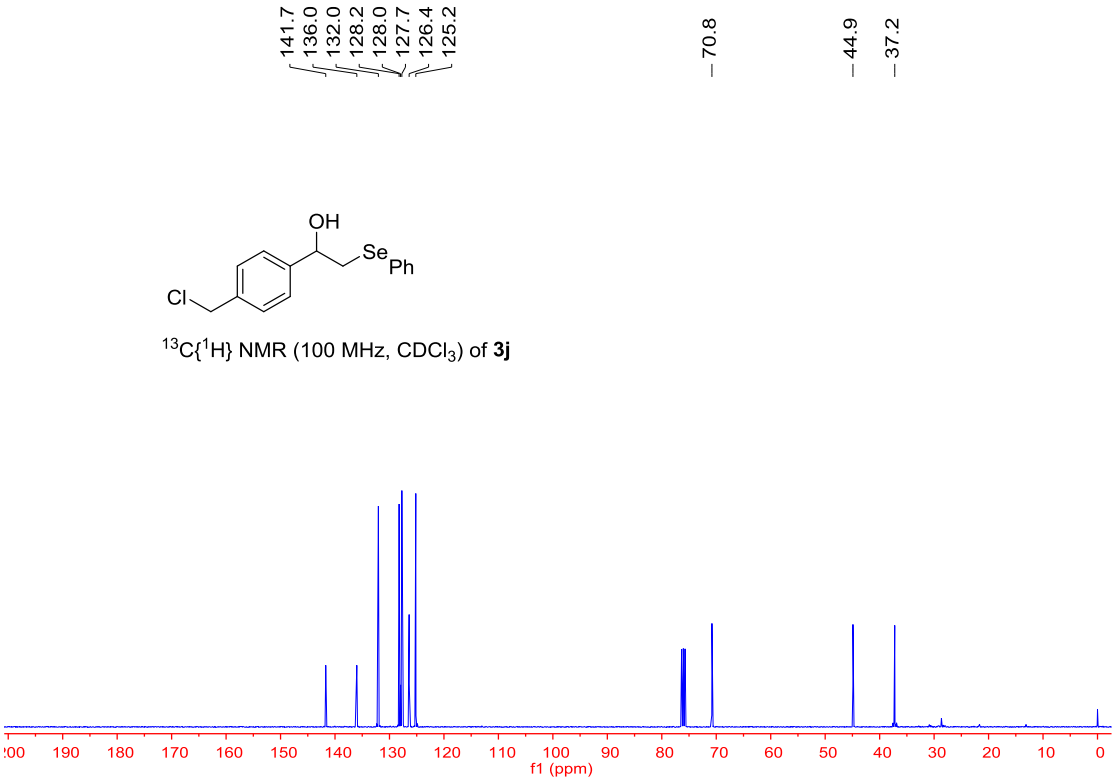

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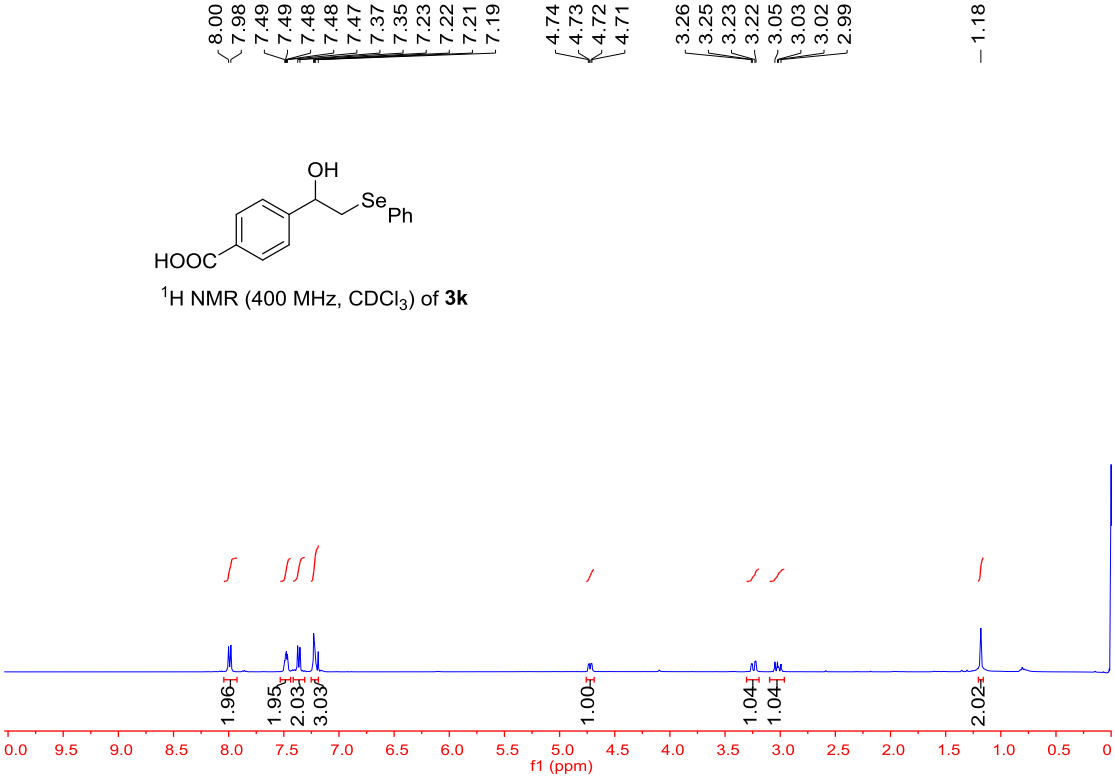

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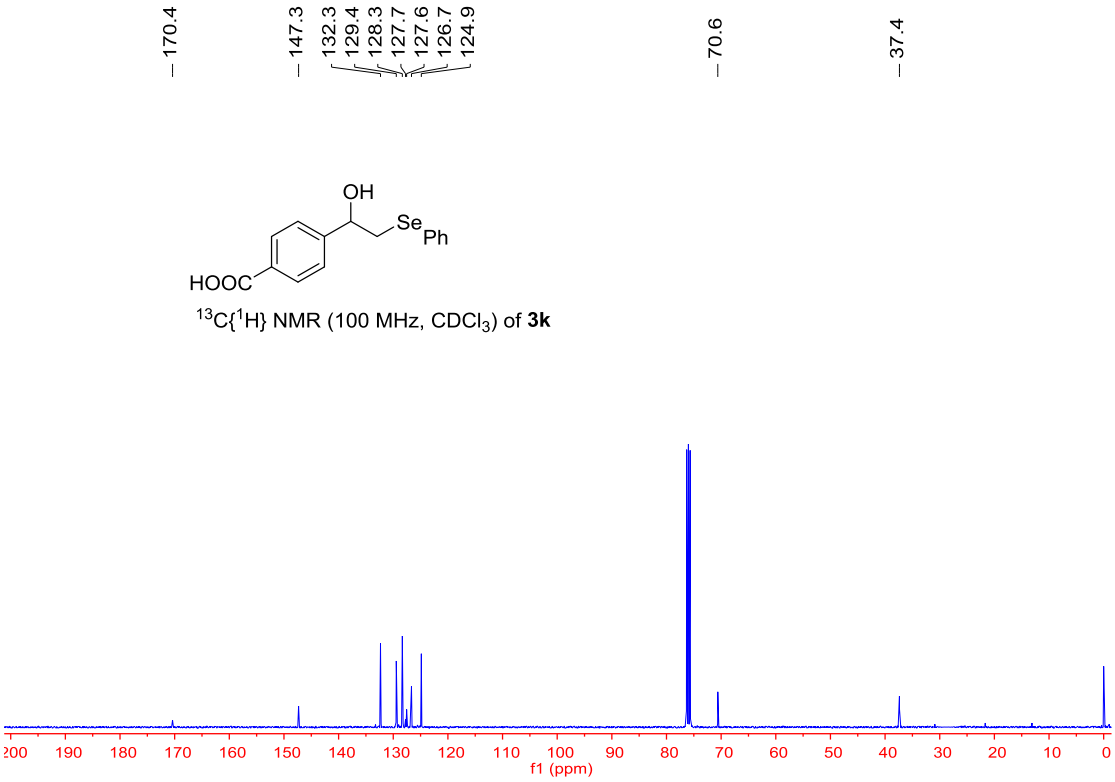
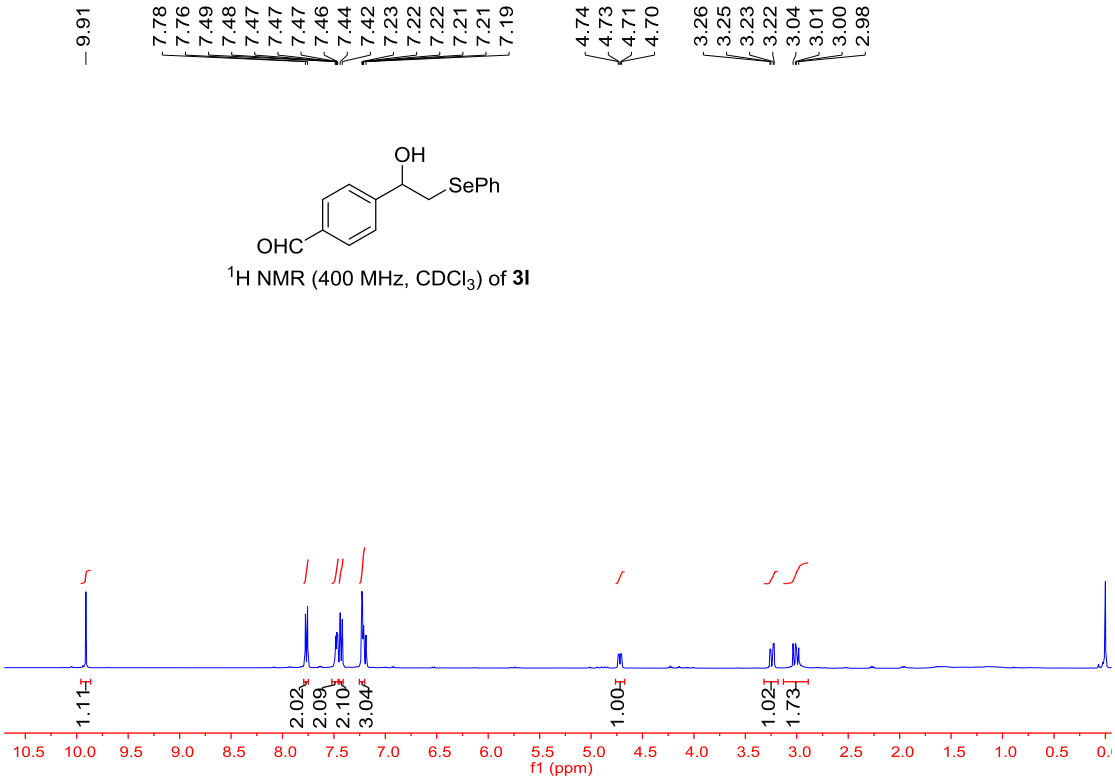
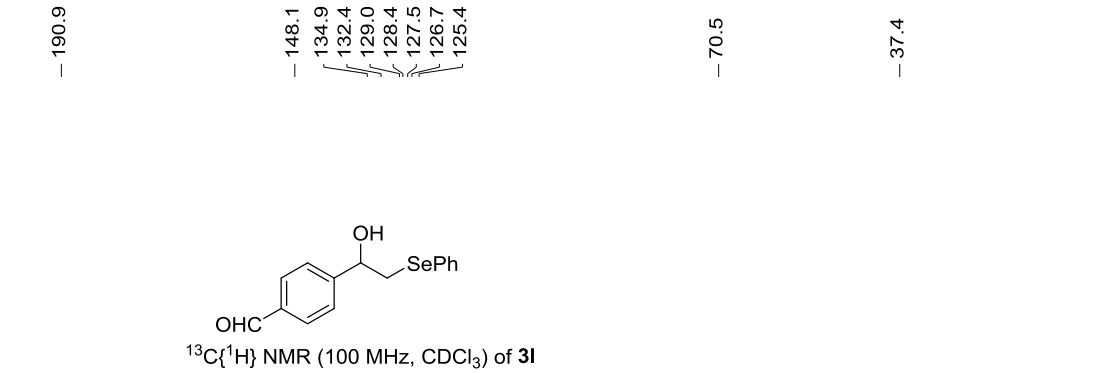


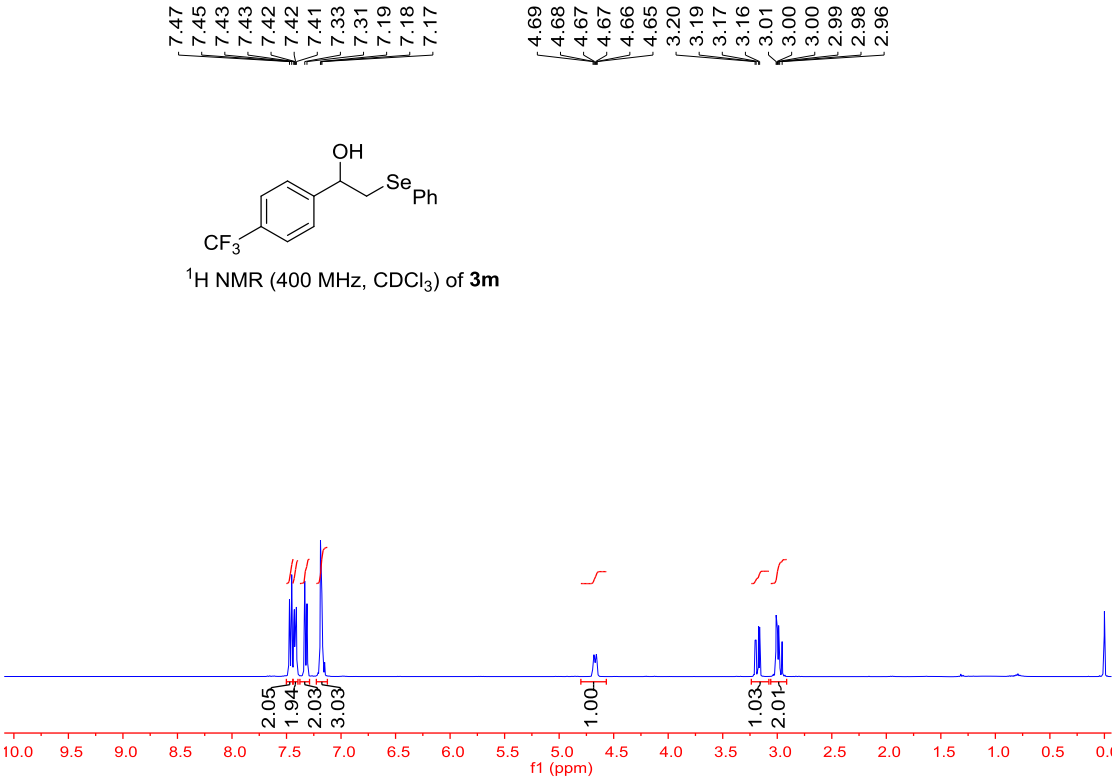
$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) of **3k**



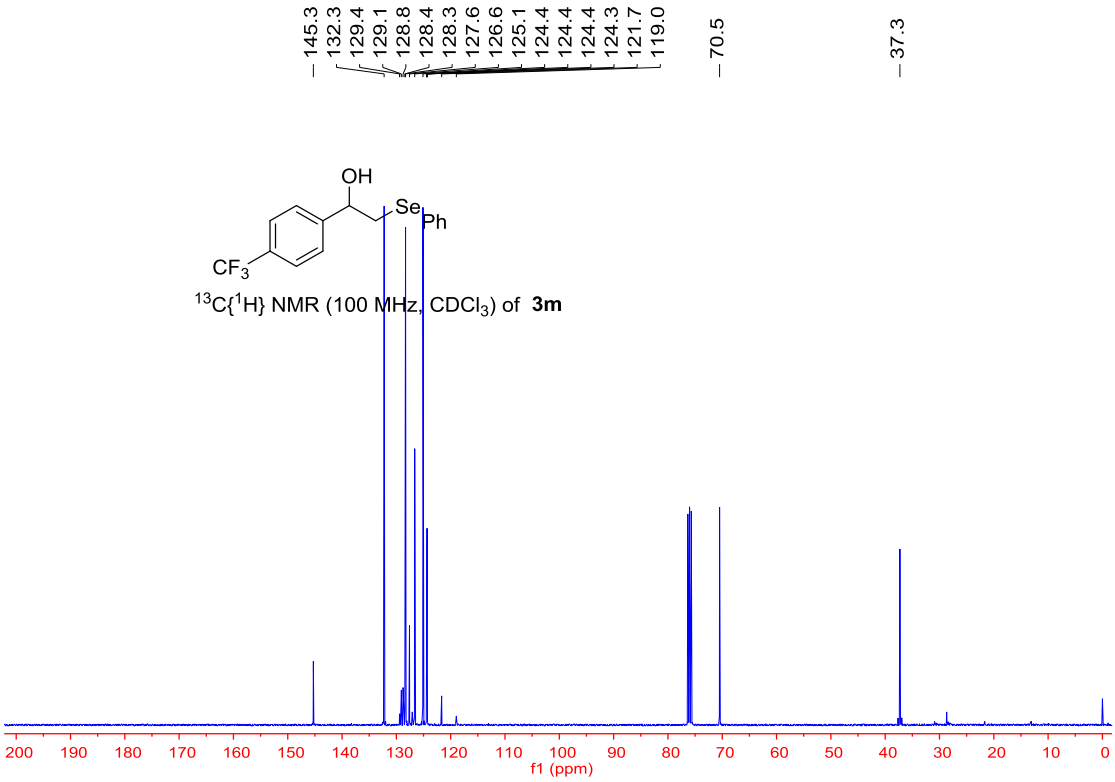
^{1}H NMR (400 MHz, $CDCl_3$) of **3l**



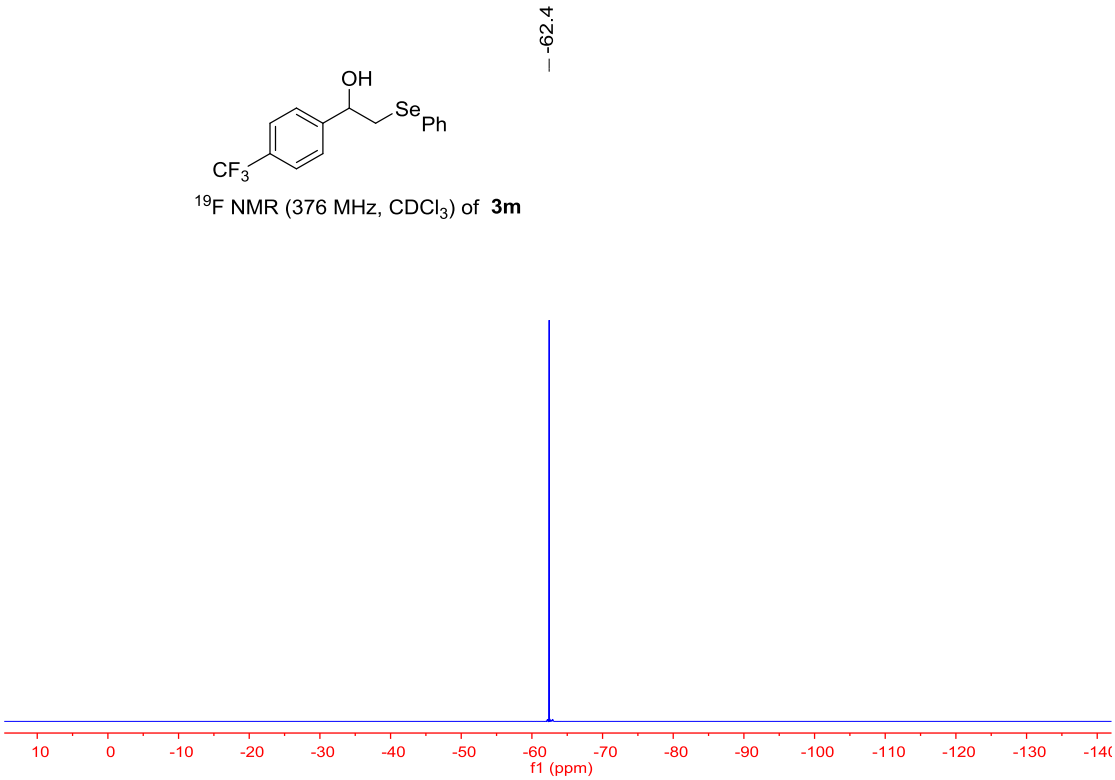
$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) of **3l**



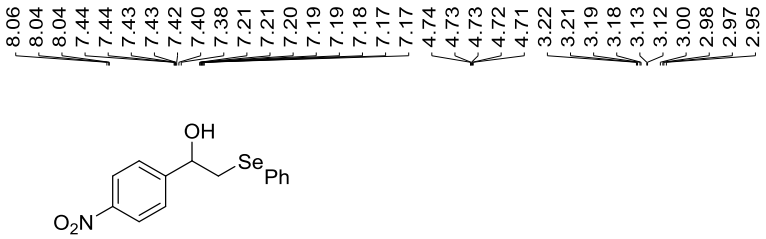
^{1}H NMR (400 MHz, $CDCl_3$) of **3m**



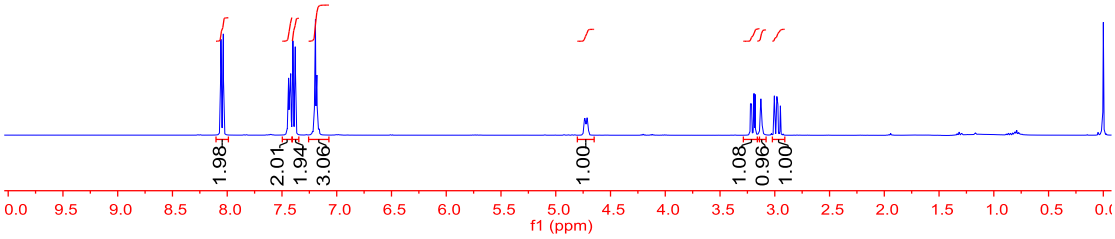
$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) of **3m**

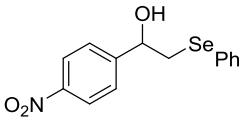


^{19}F NMR (376 MHz, $CDCl_3$) of **3m**

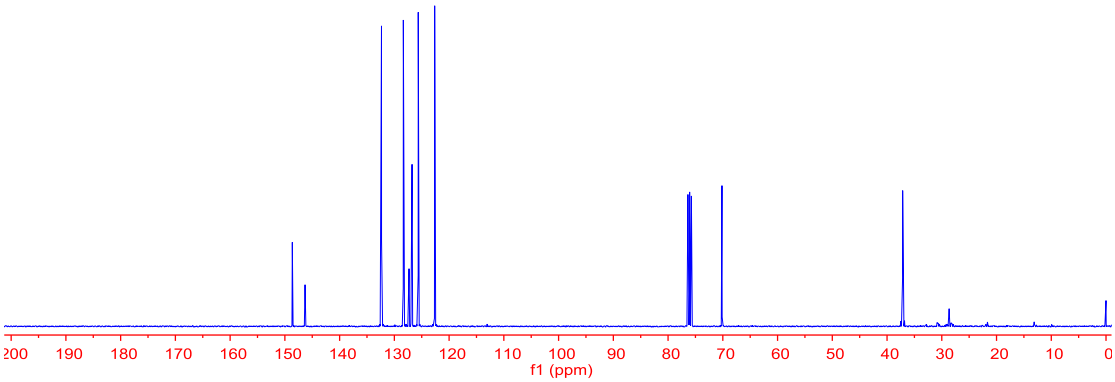


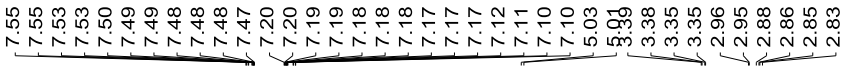
^{1}H NMR (400 MHz, $CDCl_3$) of **3n**

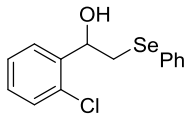




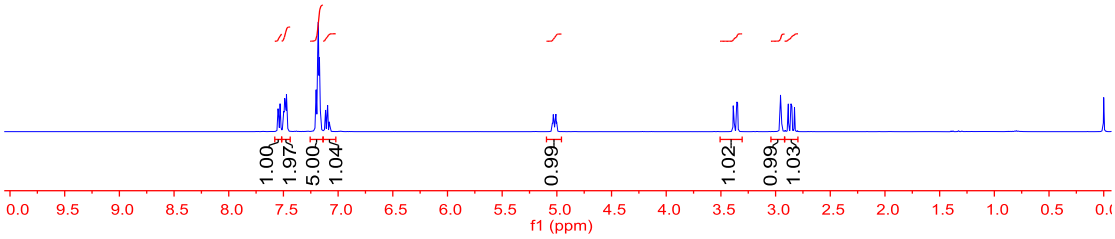
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) of **3n**

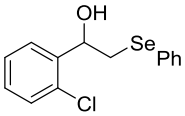




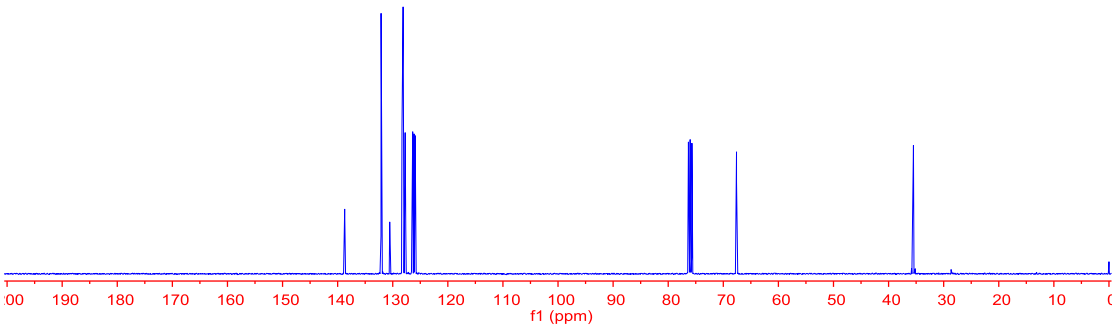


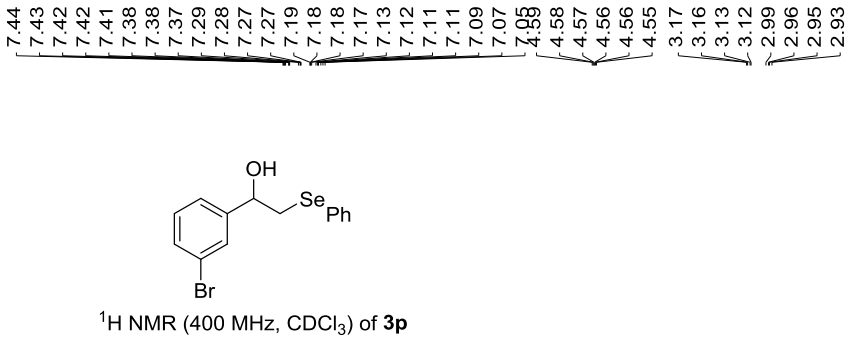
^{1}H NMR (400 MHz, $CDCl_3$) of **3o**



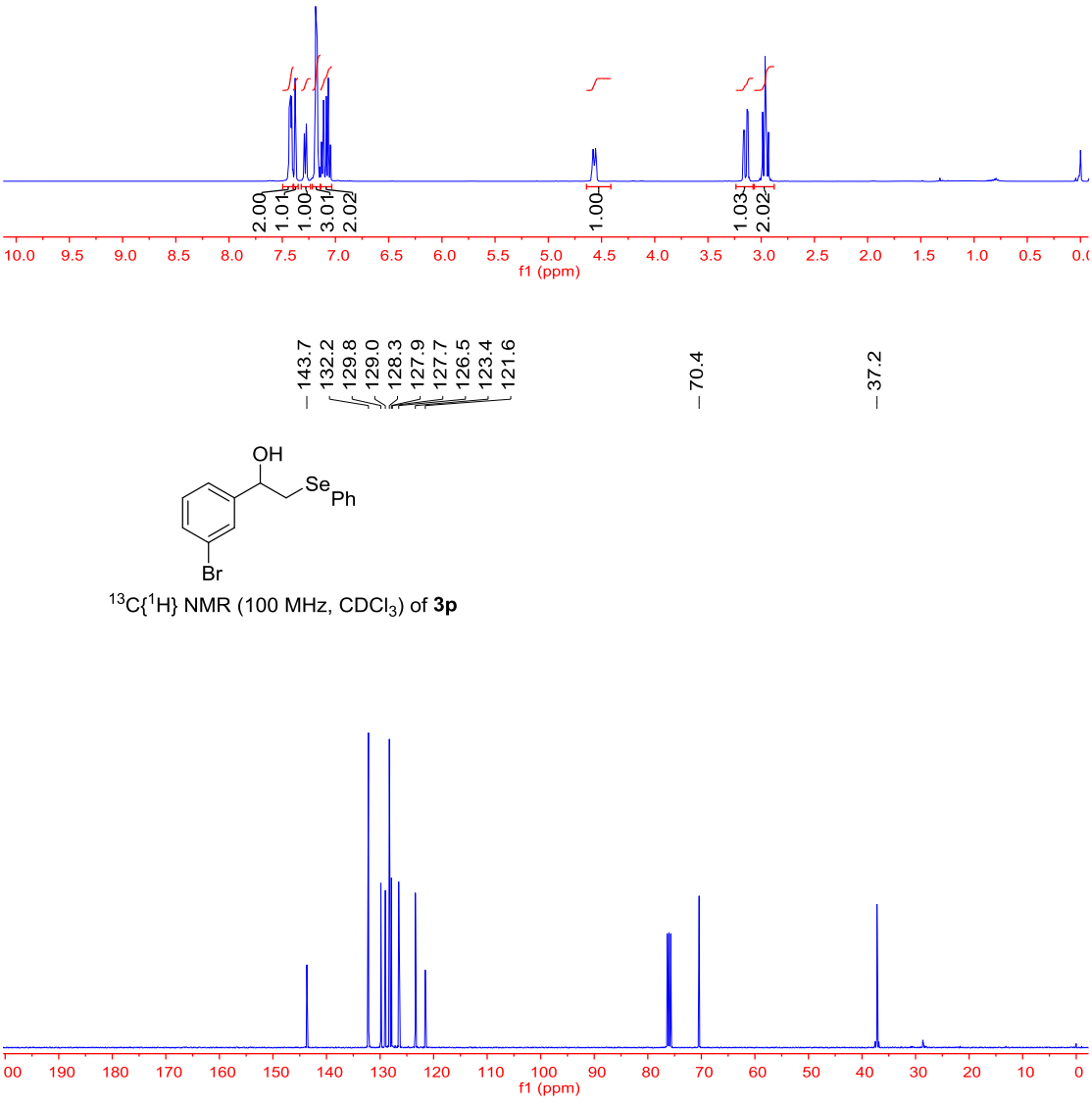


^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) of **3o**

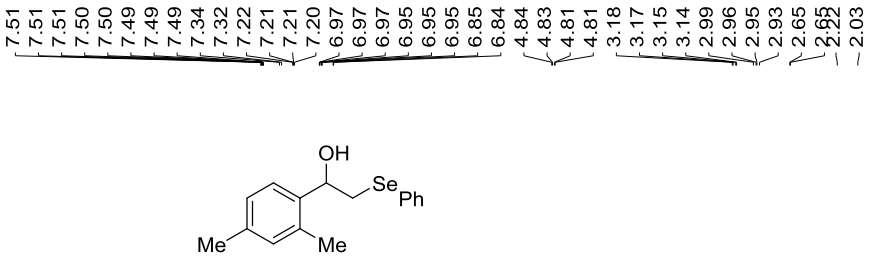




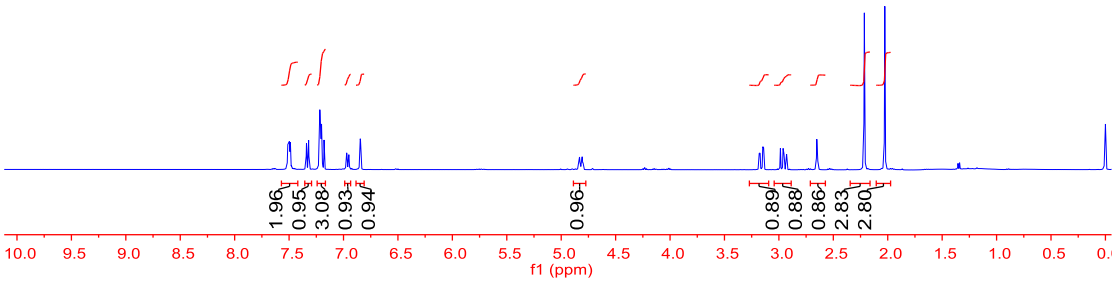
^{1}H NMR (400 MHz, $CDCl_3$) of **3p**

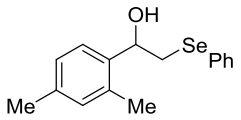


^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) of **3p**

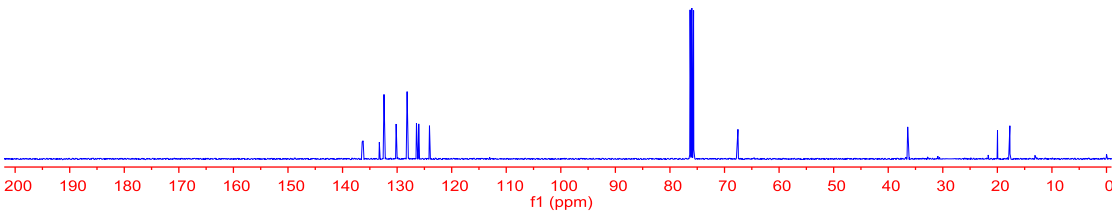


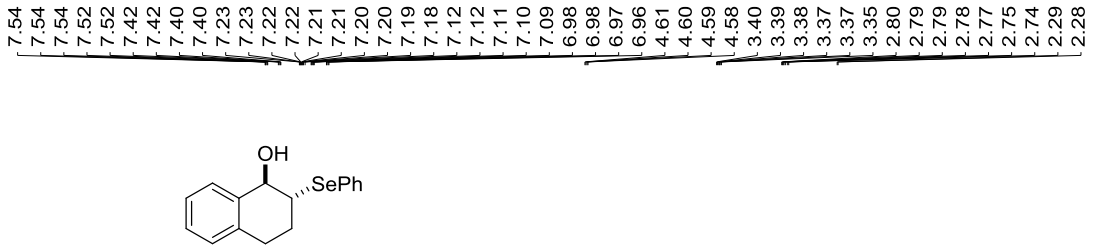
^{1}H NMR (400 MHz, $CDCl_3$) of **3q**



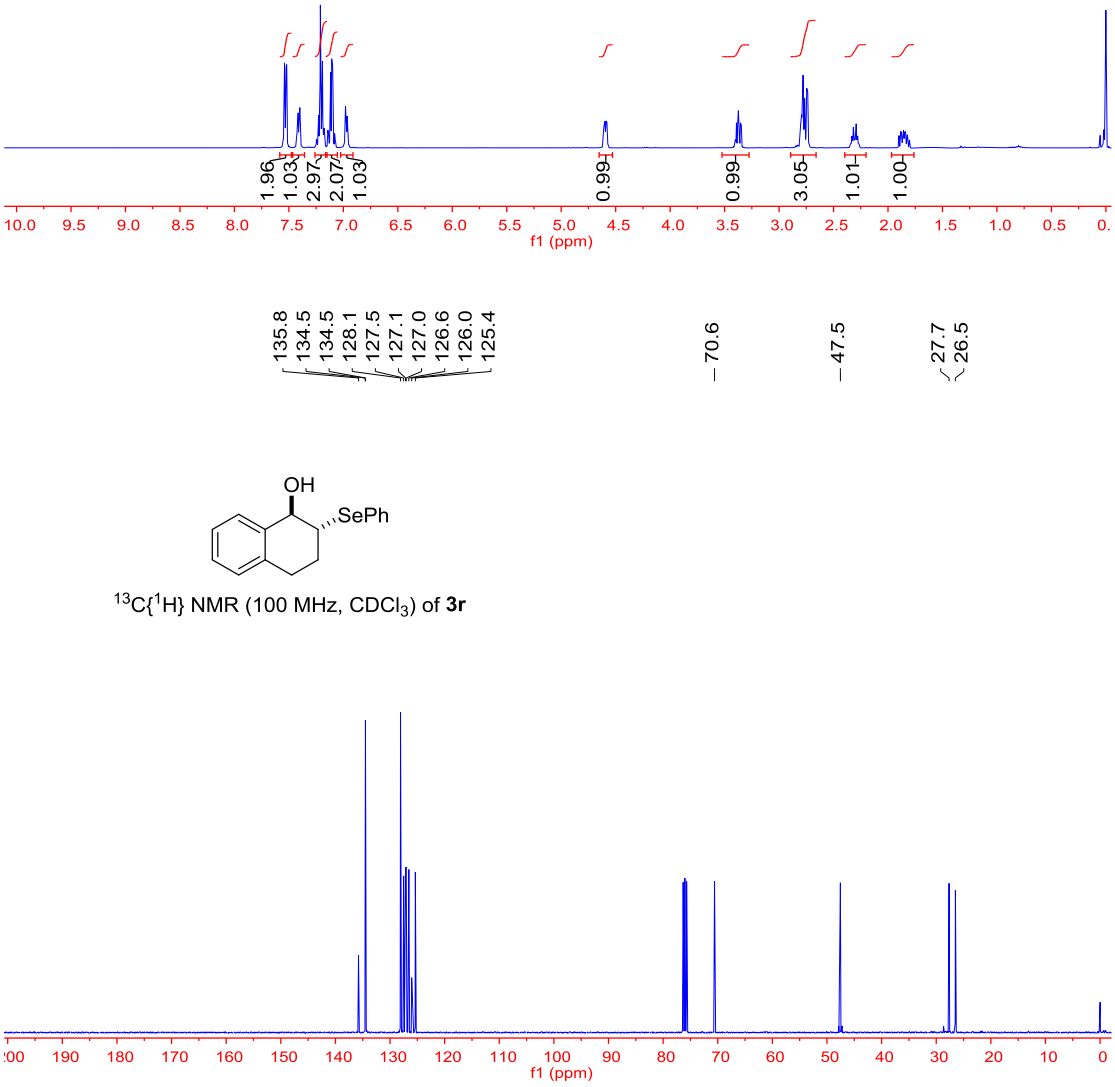


^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) of **3q**

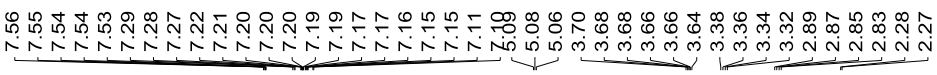


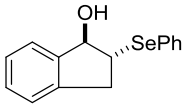


^{1}H NMR (400 MHz, $CDCl_3$) of **3r**

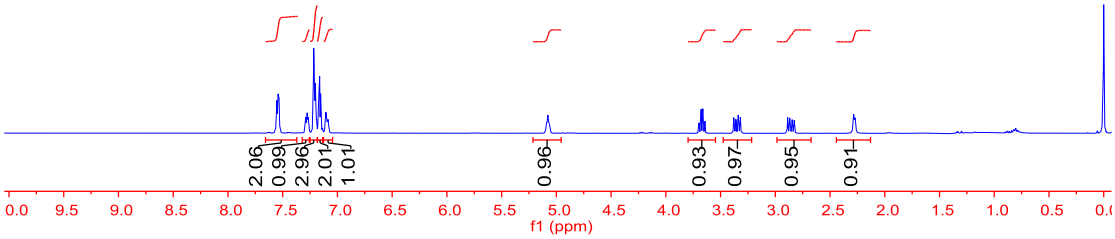


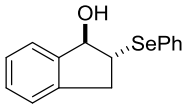
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) of **3r**



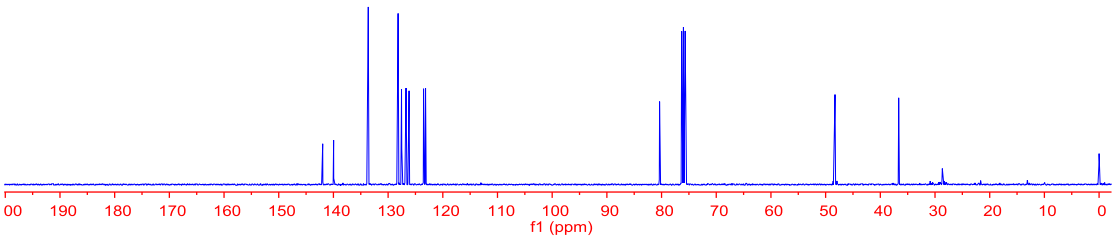


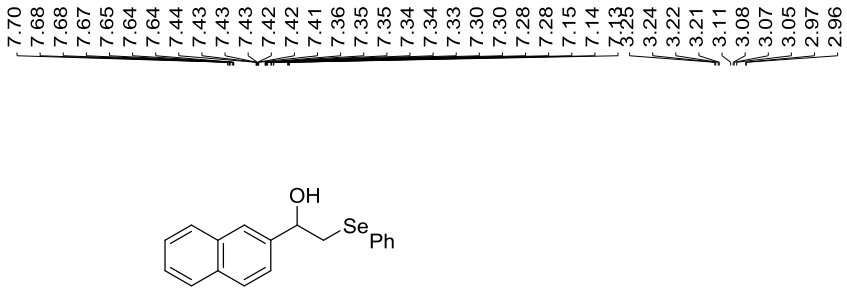
^{1}H NMR (400 MHz, $CDCl_3$) of **3s**



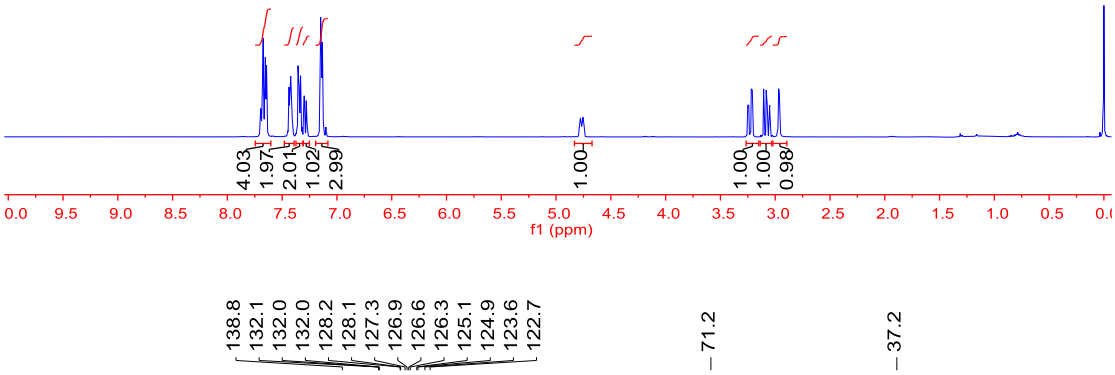


^{13}C{^{1}H}NMR (100 MHz, $CDCl_3$) of **3s**

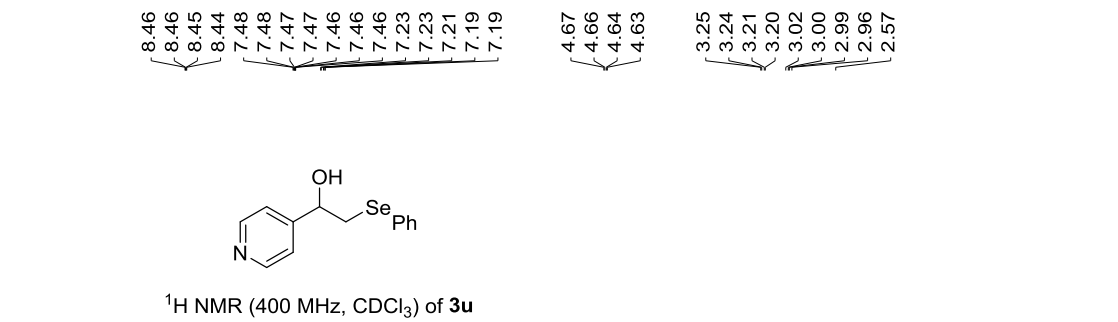




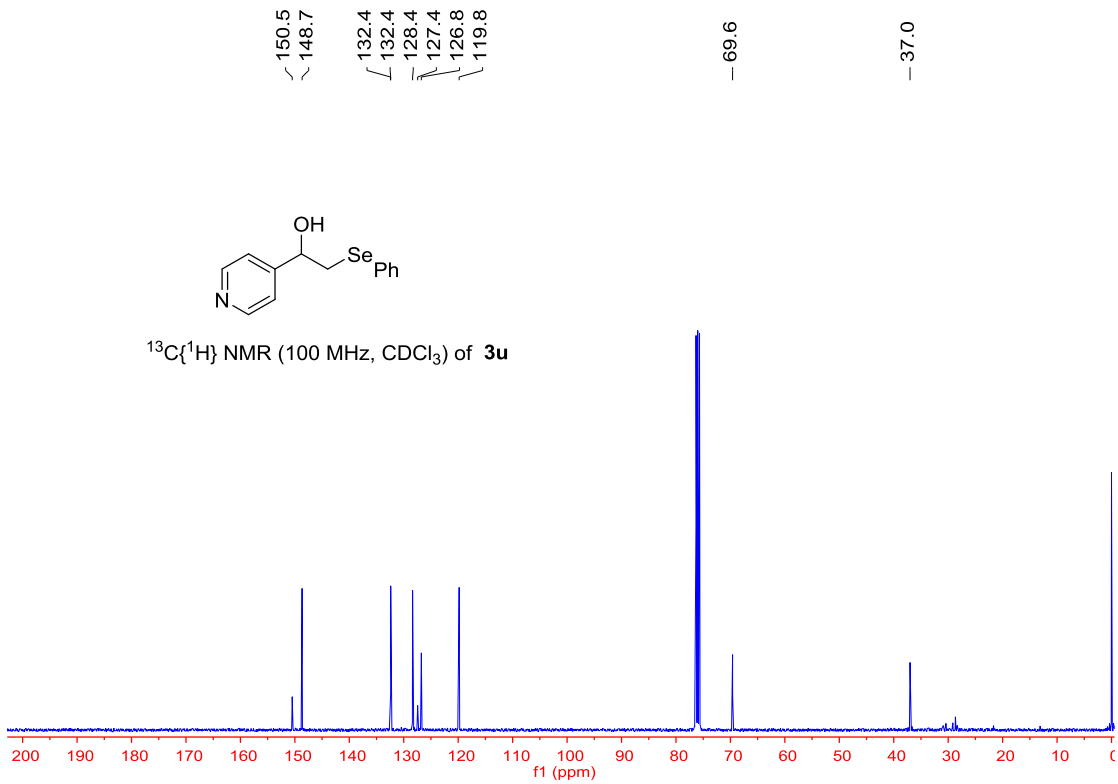
^{1}H NMR (400 MHz, $CDCl_3$) of **3t**



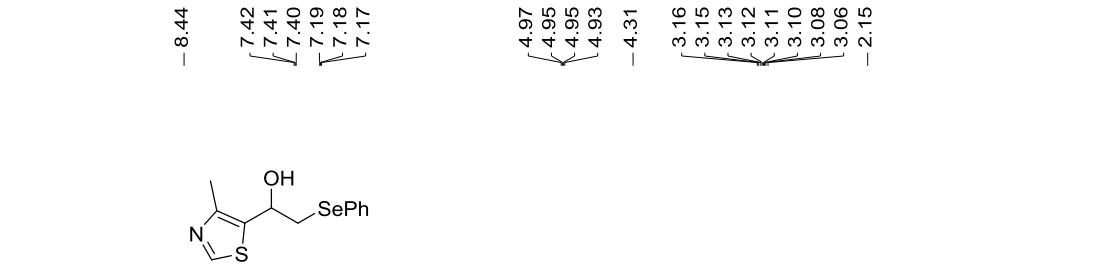
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) of **3s**



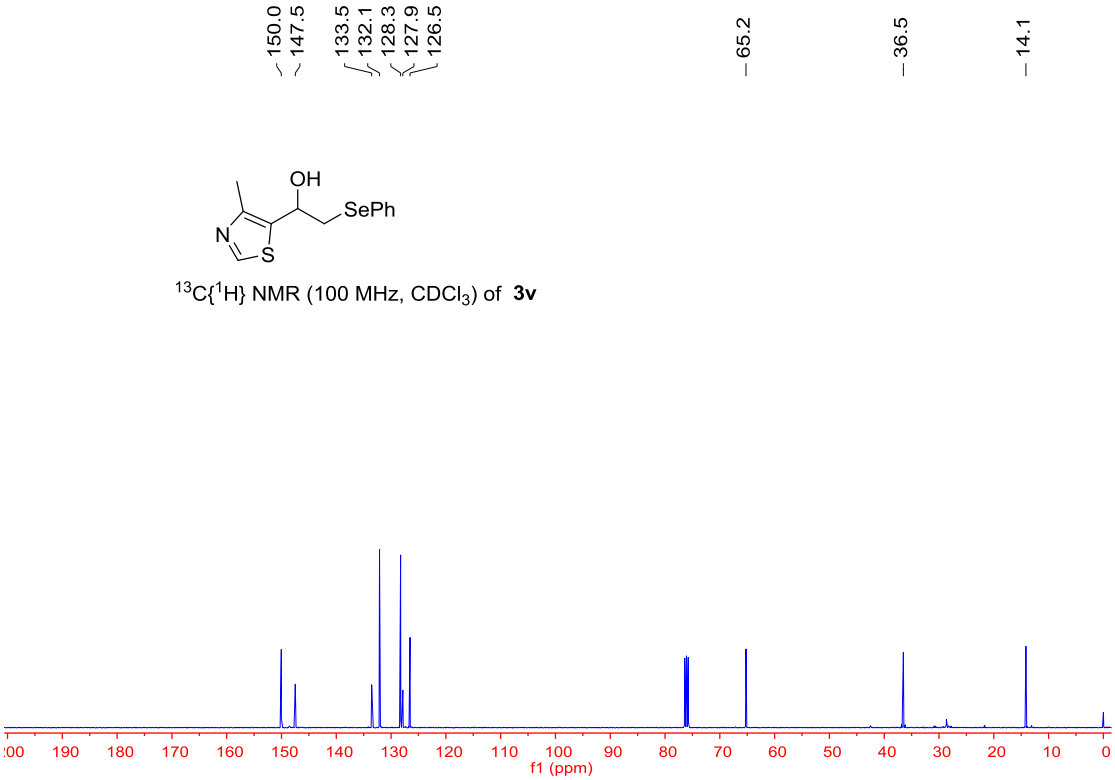
^{1}H NMR (400 MHz, $CDCl_3$) of **3u**



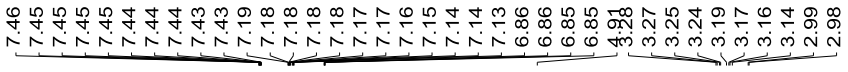
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) of **3u**

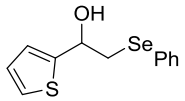


^{1}H NMR (400 MHz, $CDCl_3$) of **3v**

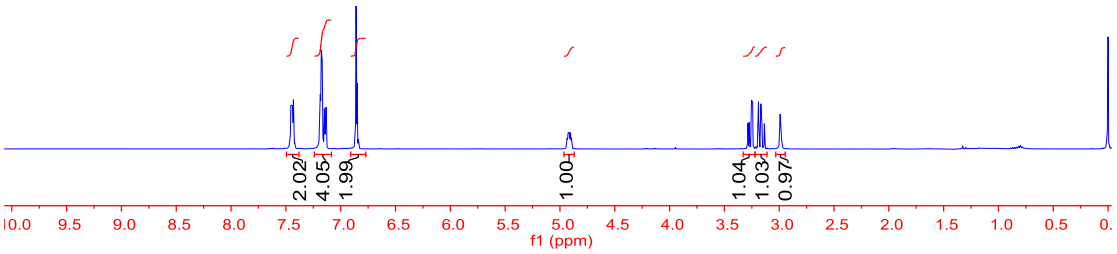


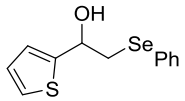
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) of **3v**



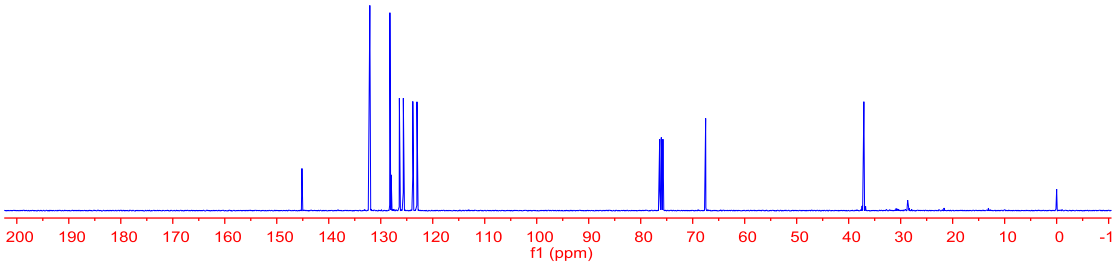


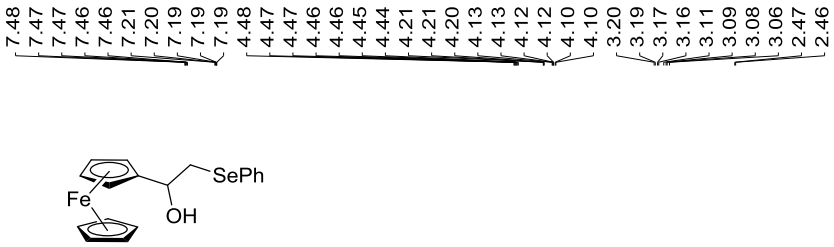
^{1}H NMR (400 MHz, $CDCl_3$) of **3w**



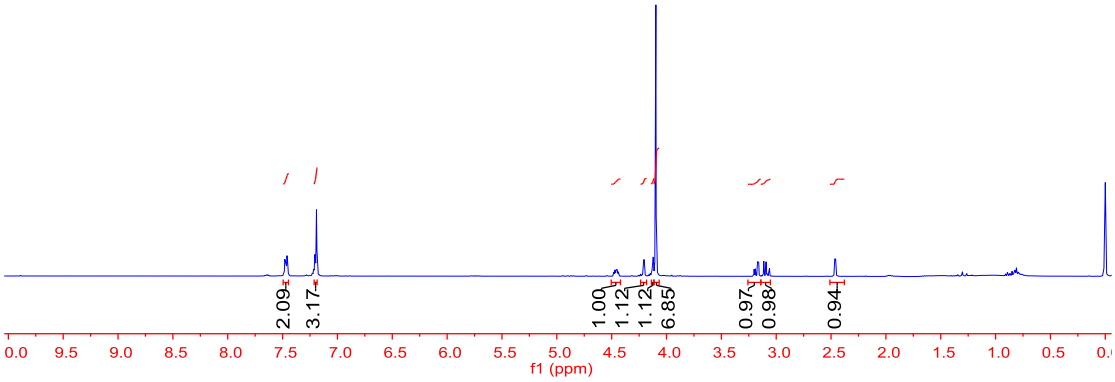


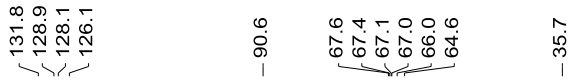
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) of **3w**

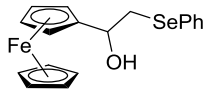




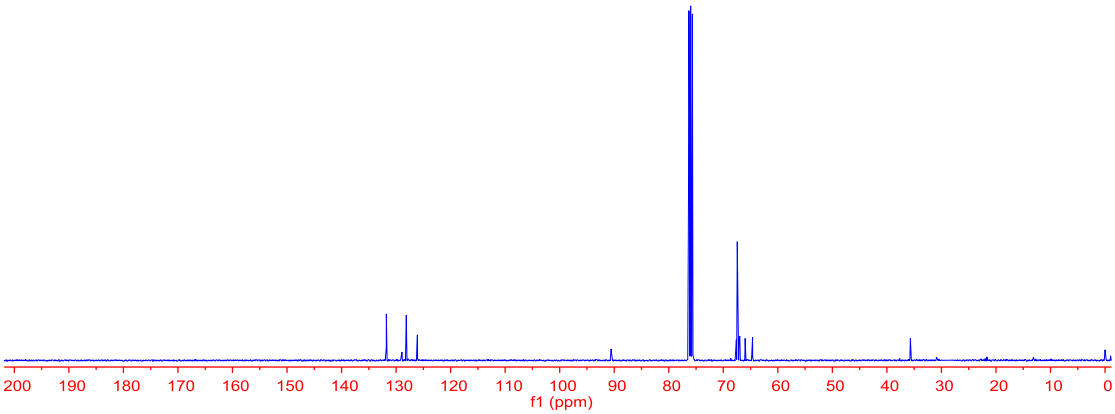
^{1}H NMR (400 MHz, $CDCl_3$) of **3x**

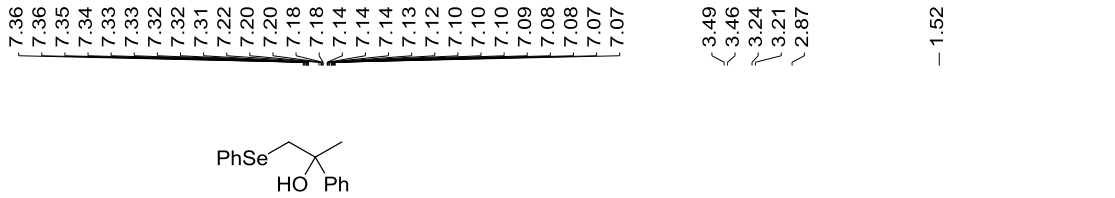




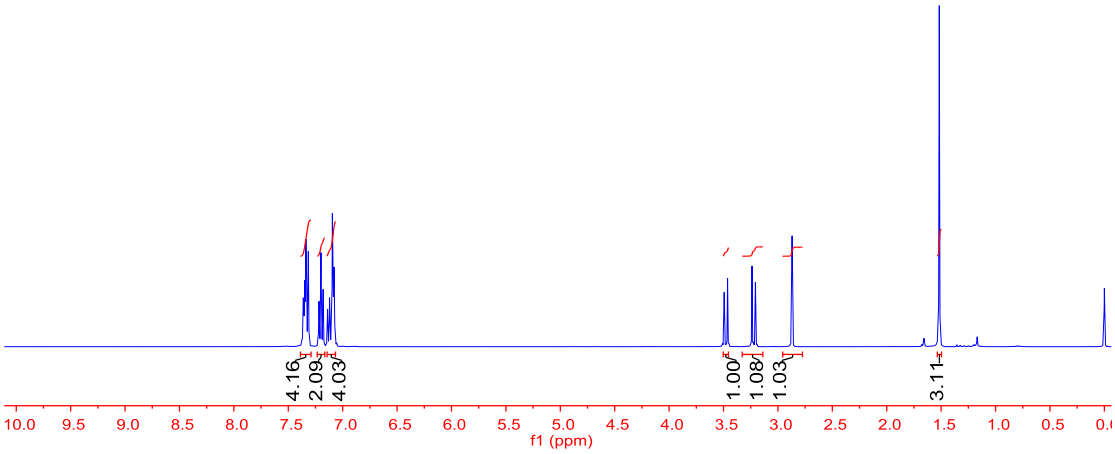


^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) of **3x**

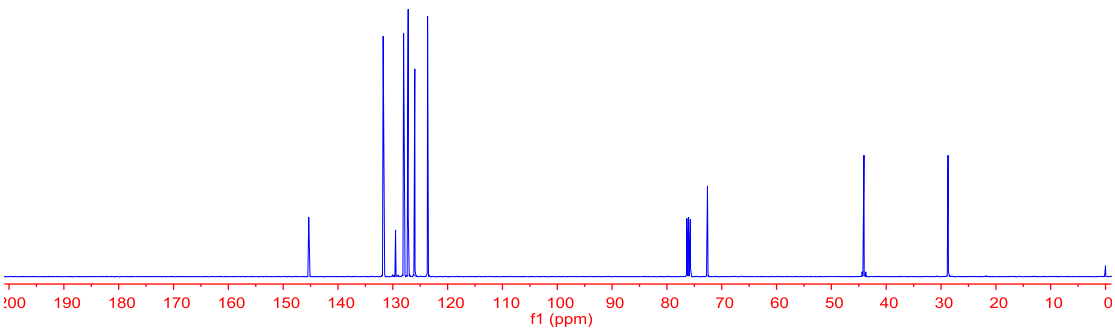


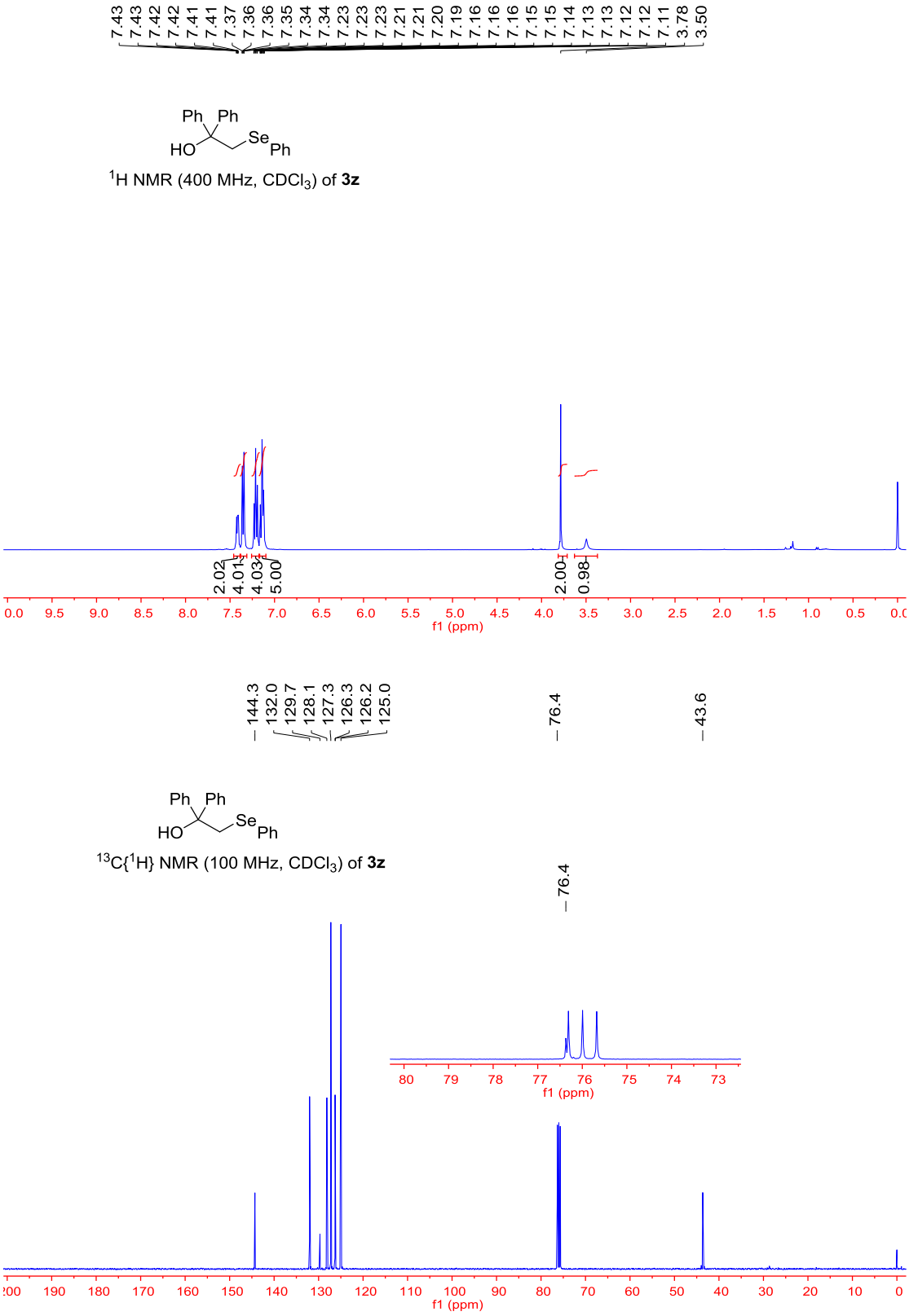


^{1}H NMR (400 MHz, $CDCl_3$) of **3y**



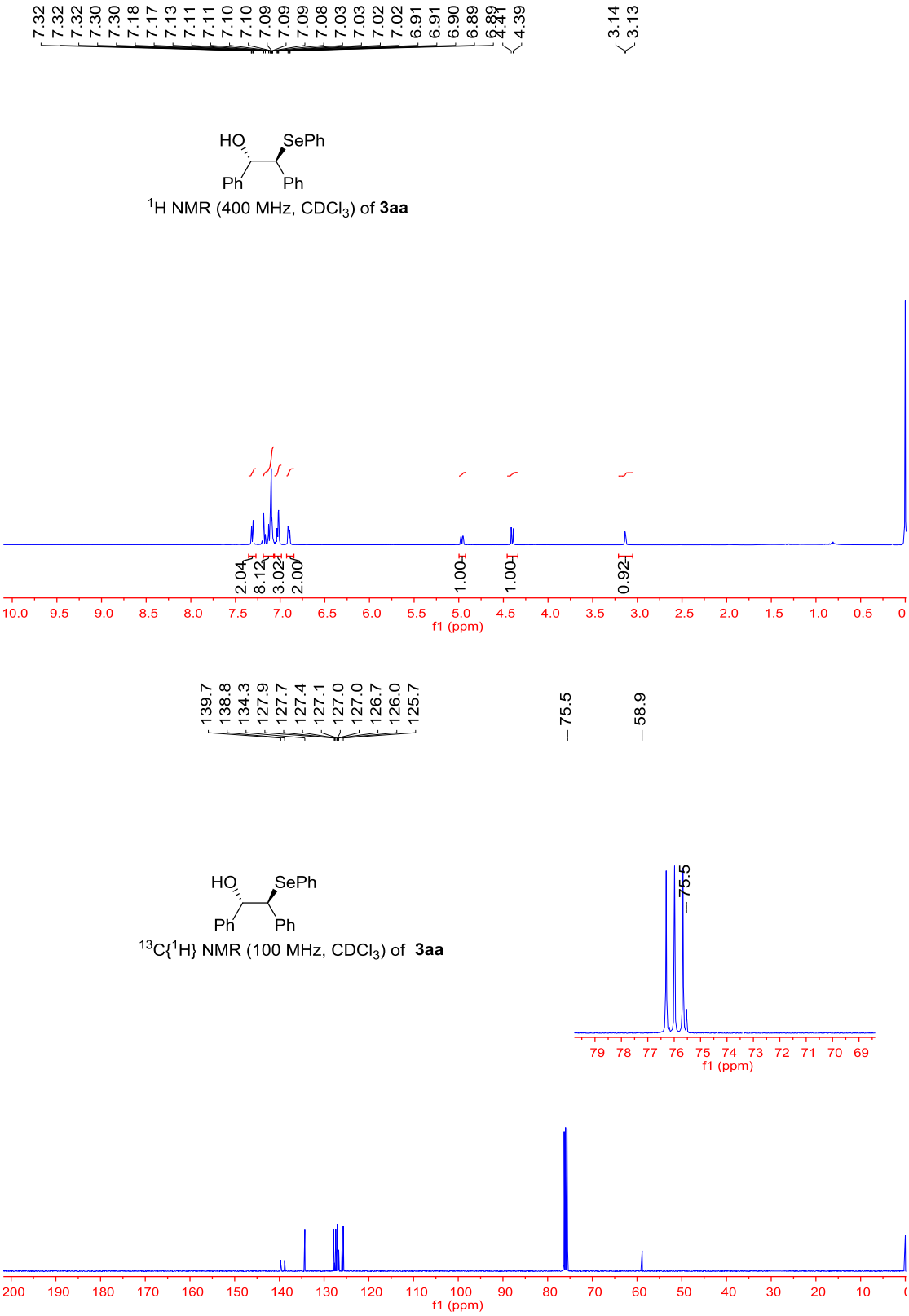
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) of **3y**

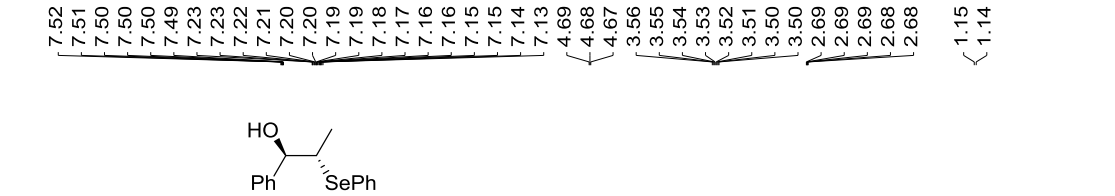




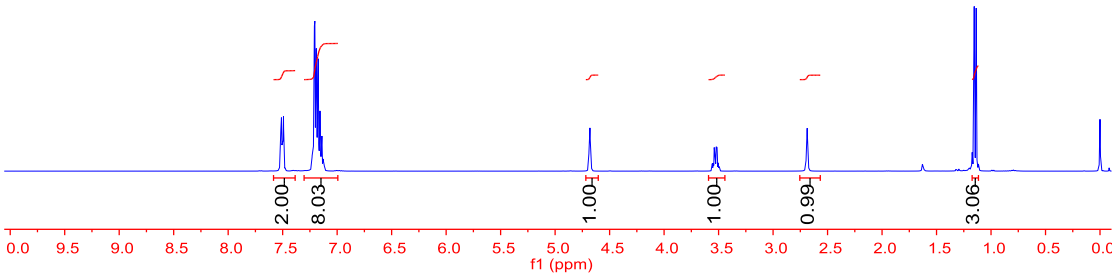
^{1}H NMR (400 MHz, $CDCl_3$) of **3z**

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) of **3z**

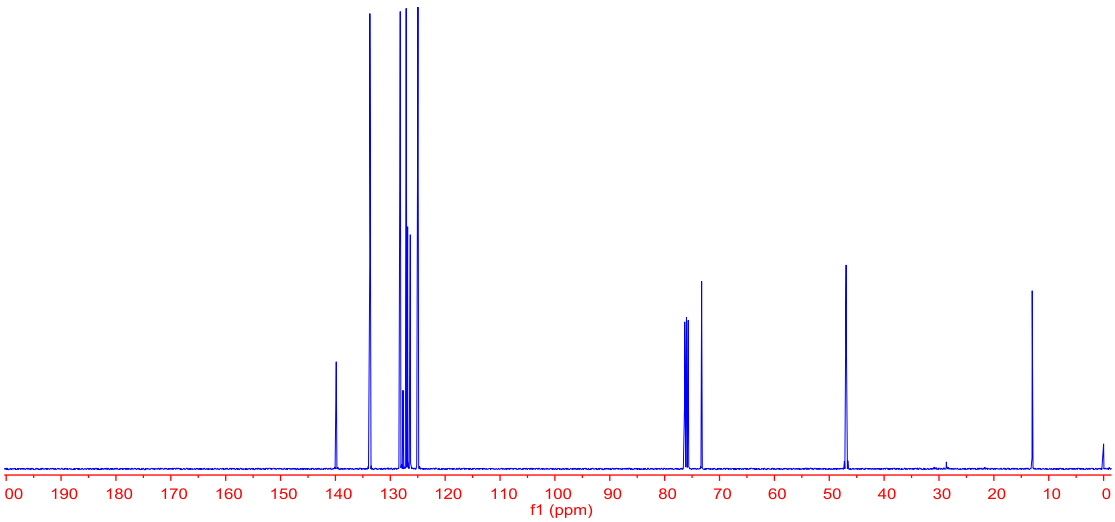

7.32 7.32 7.32 7.30 7.30 7.18 7.17 7.13 7.11 7.11 7.10 7.10 7.09 7.09 7.09 7.08 7.03 7.03 7.02 7.02 6.91 6.91 6.90 6.89 6.89 4.41 4.39
3.14 3.13
HO
SePh
Ph
Ph
^{1}H NMR (400 MHz, $CDCl_3$) of **3aa**
2.04 8.12 3.02 2.00 1.00 1.00 0.92
f1 (ppm)
139.7 138.8 134.3 127.9 127.7 127.4 127.1 127.0 127.0 126.7 126.0 125.7
75.5
58.9
HO
SePh
Ph
Ph
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) of **3aa**
75.5
f1 (ppm)
f1 (ppm)

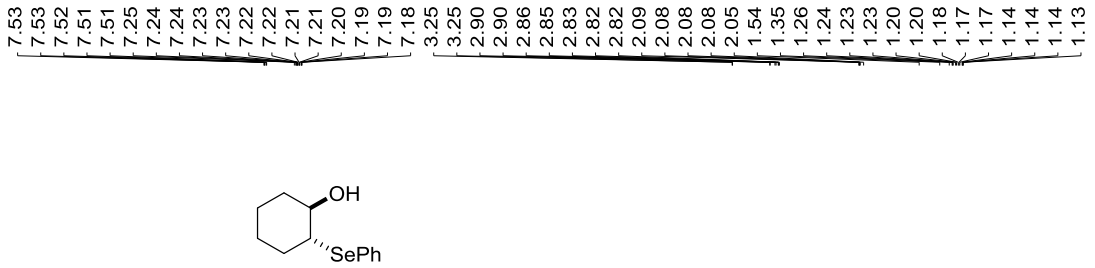


^{1}H NMR (400 MHz, $CDCl_3$) of **3ab**

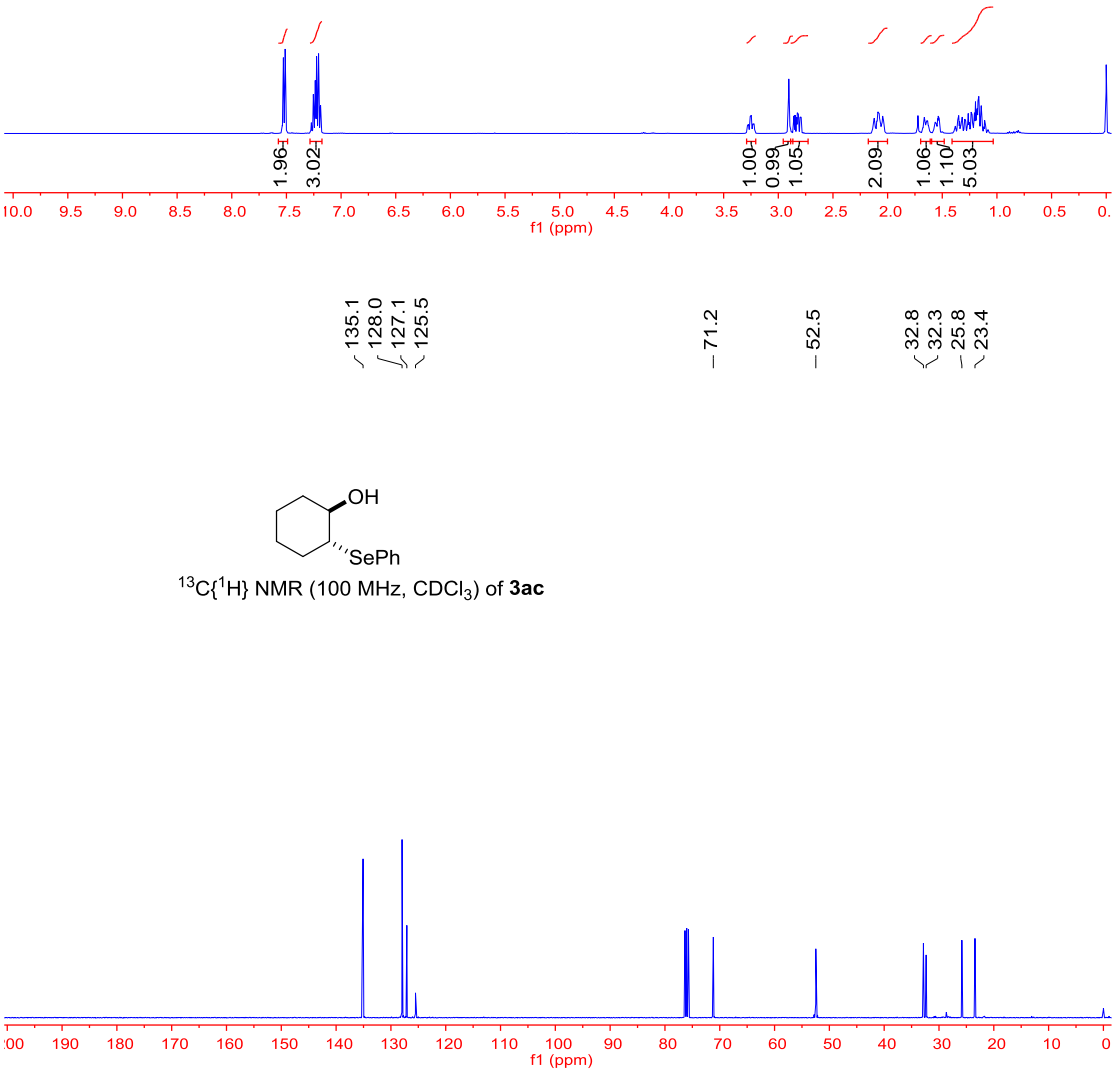


^{13}C{^{1}H} (100 MHz, $CDCl_3$) of **3ab**

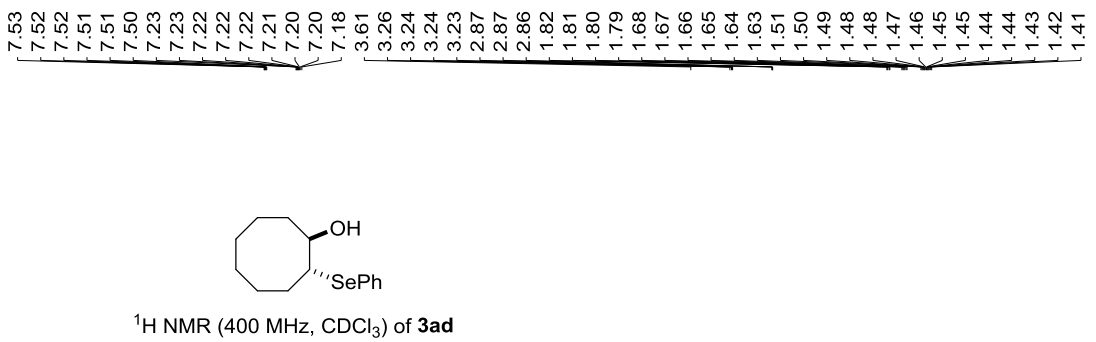




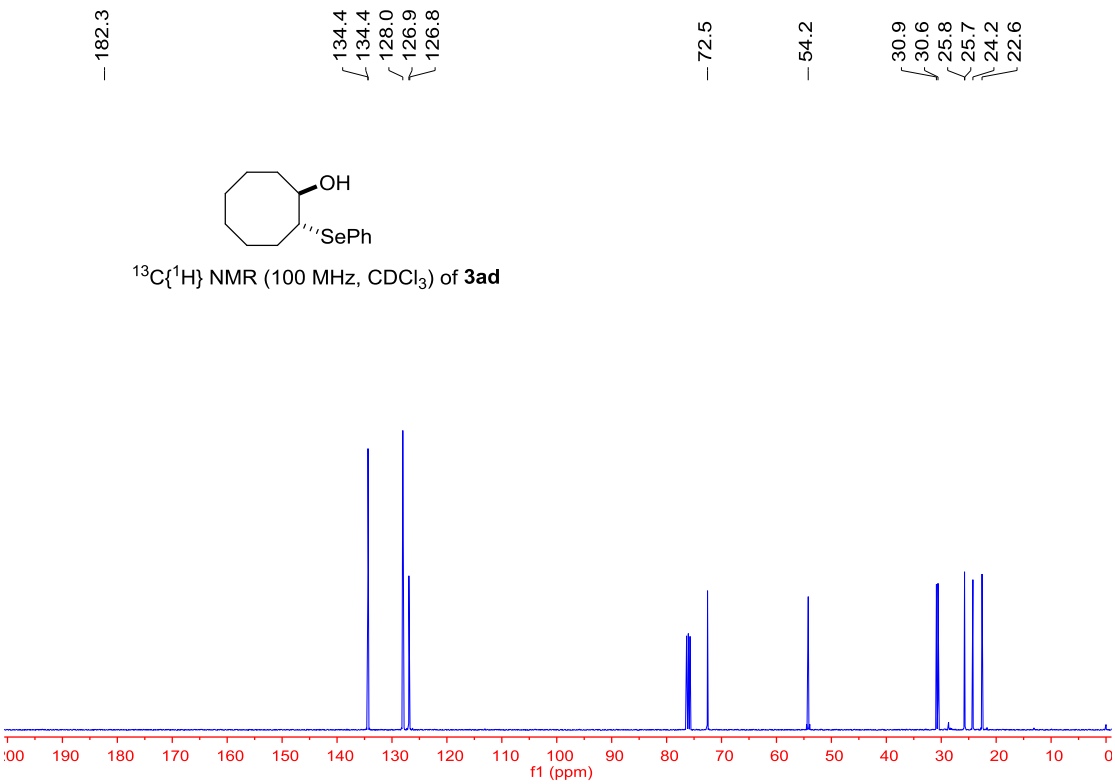
^{1}H NMR (400 MHz, $CDCl_3$) of **3ac**



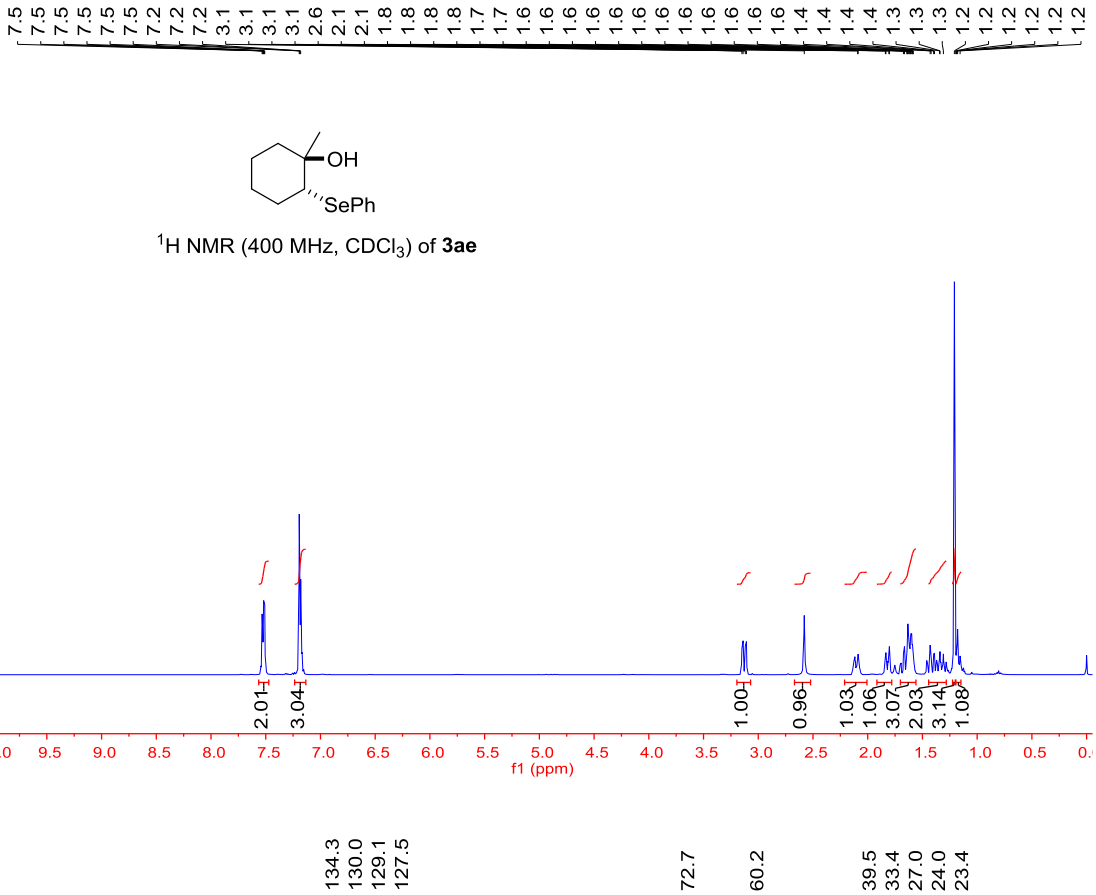
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) of **3ac**



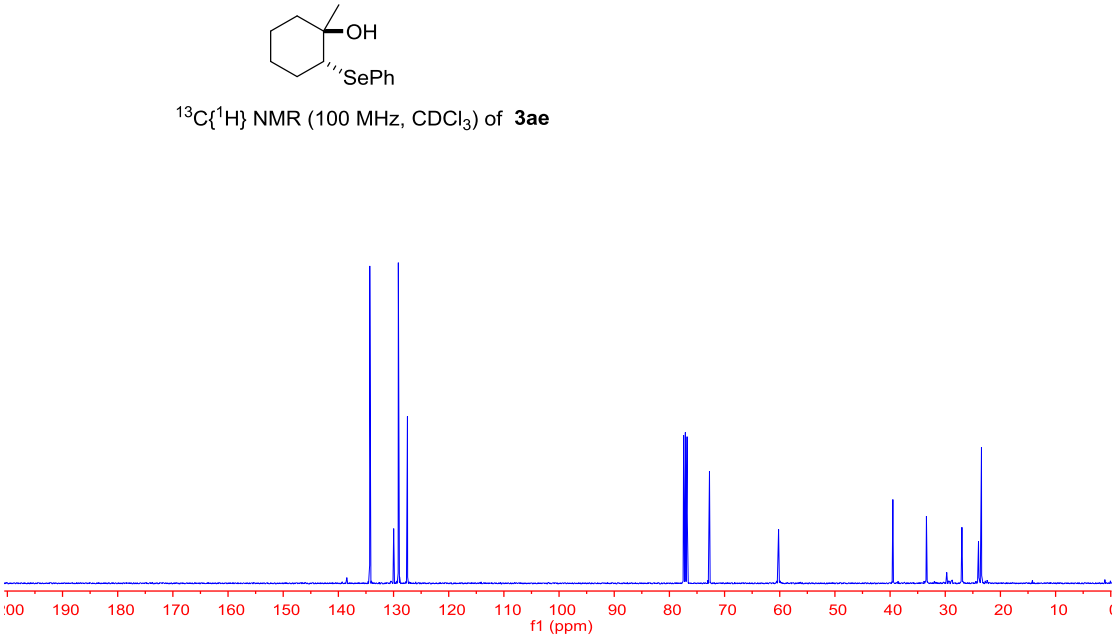
^{1}H NMR (400 MHz, $CDCl_3$) of **3ad**



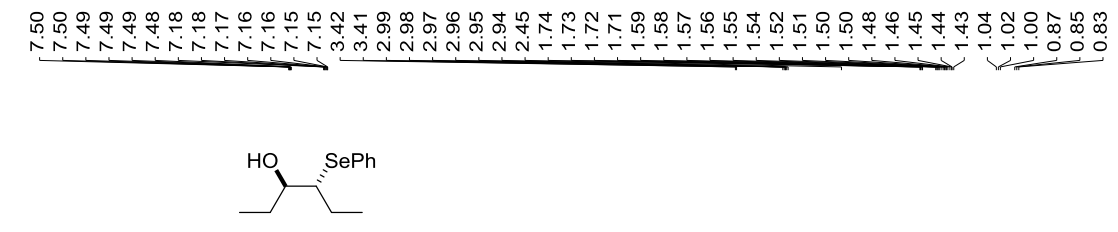
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) of **3ad**



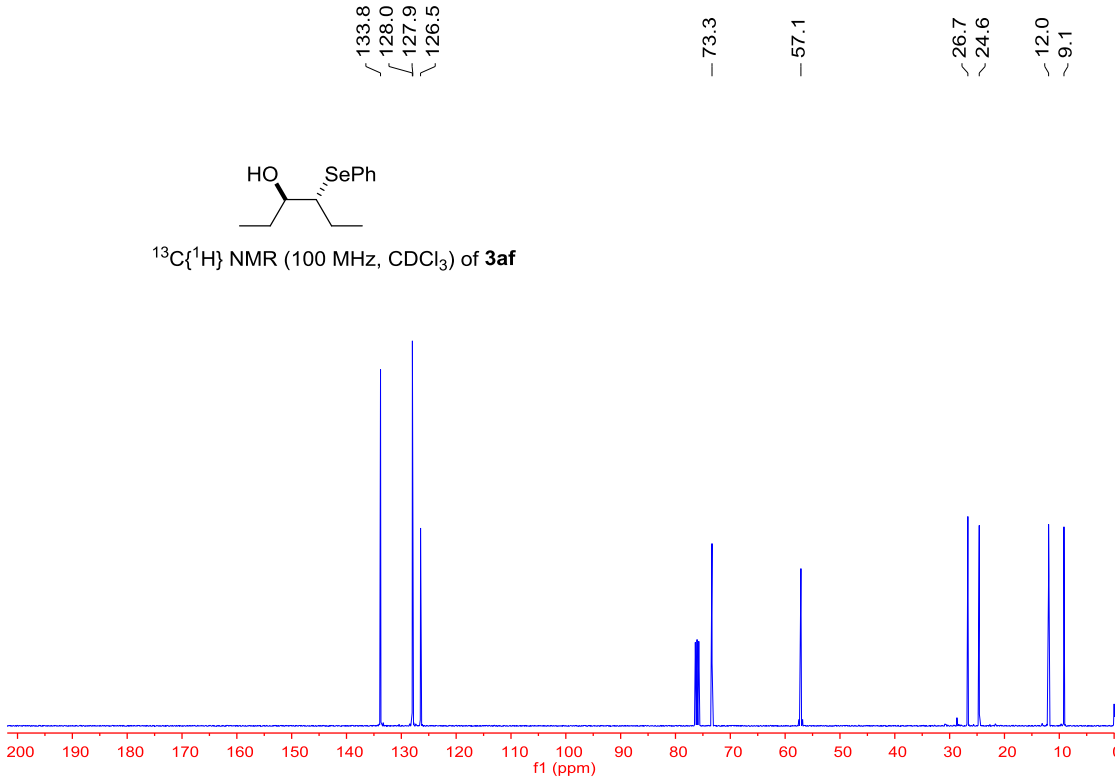
^{1}H NMR (400 MHz, $CDCl_3$) of **3ae**



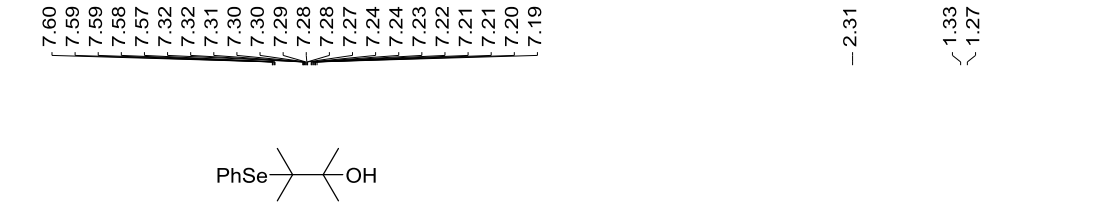
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) of **3ae**



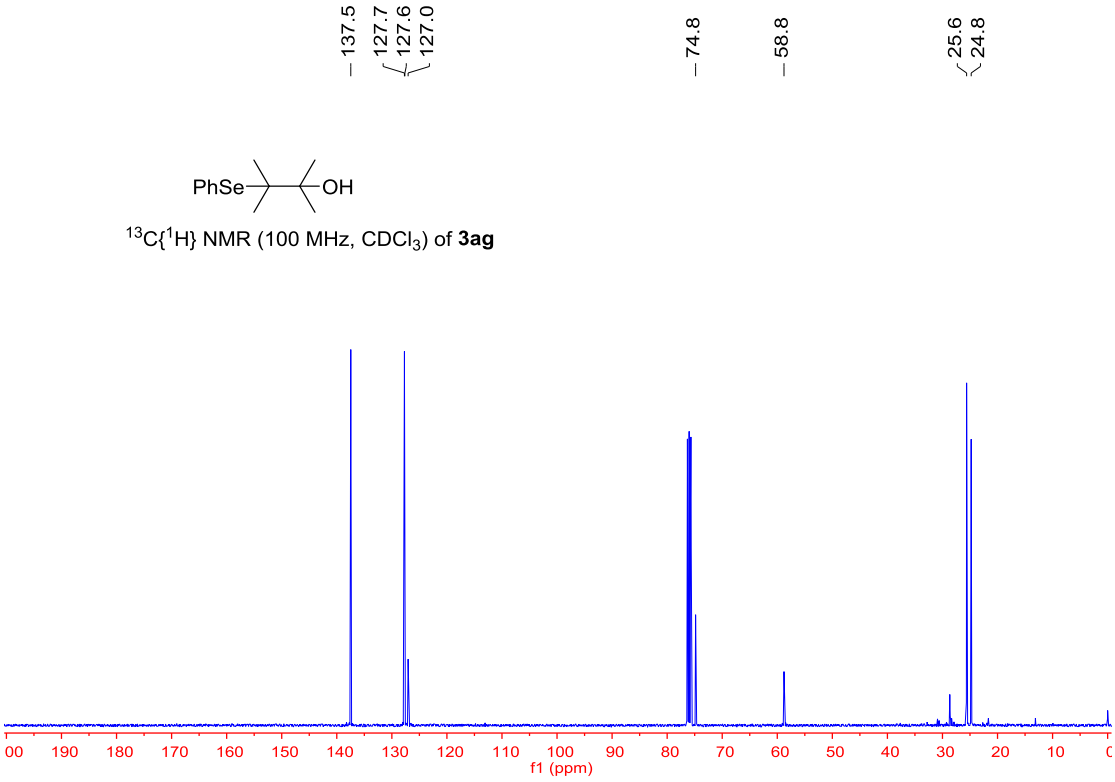
^{1}H NMR (400 MHz, $CDCl_3$) of **3af**



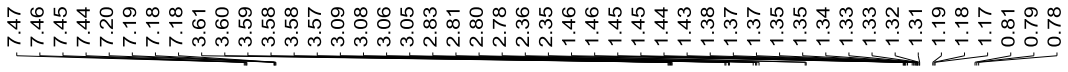
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) of **3af**

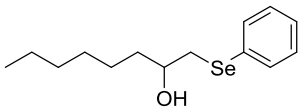


^{1}H NMR (400 MHz, $CDCl_3$) of **3ag**

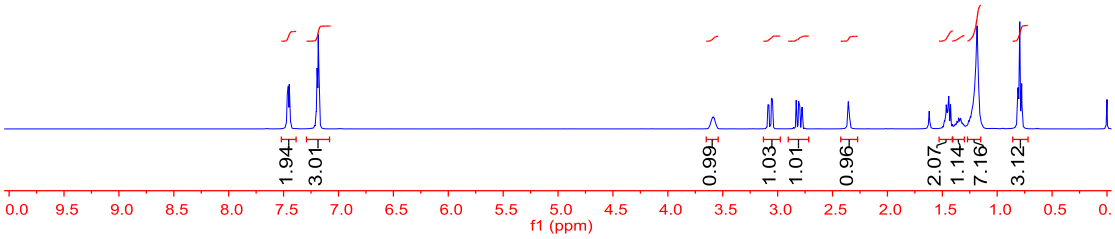


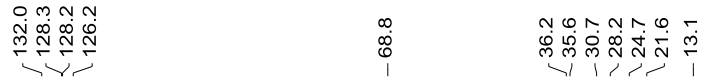
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) of **3ag**

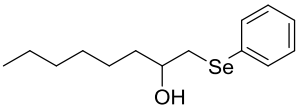




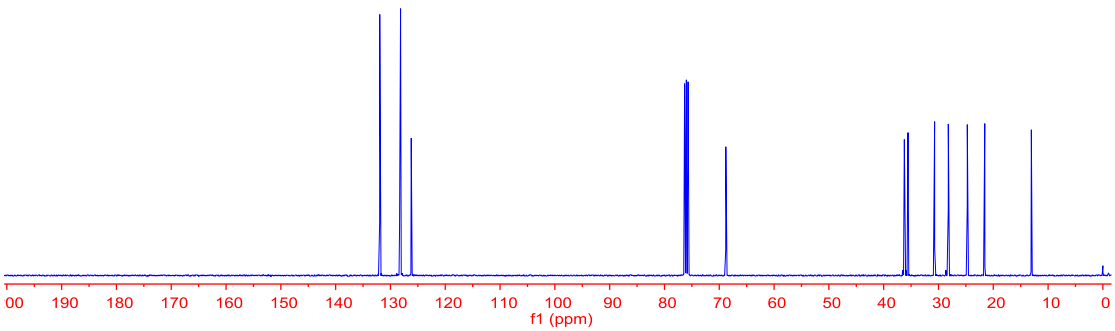
^{1}H NMR (400 MHz, $CDCl_3$) of **3ah**

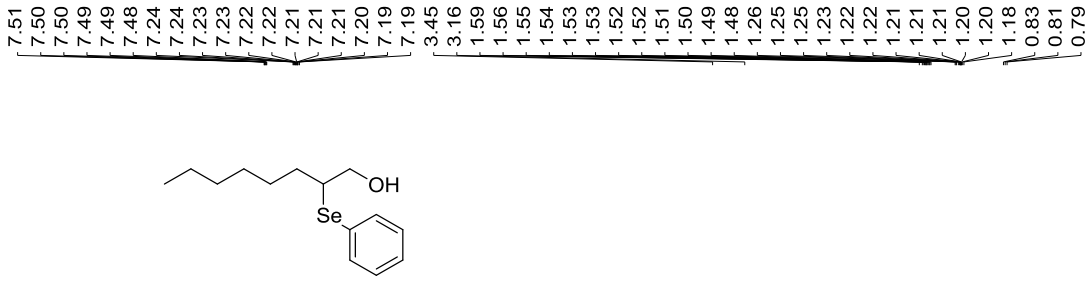




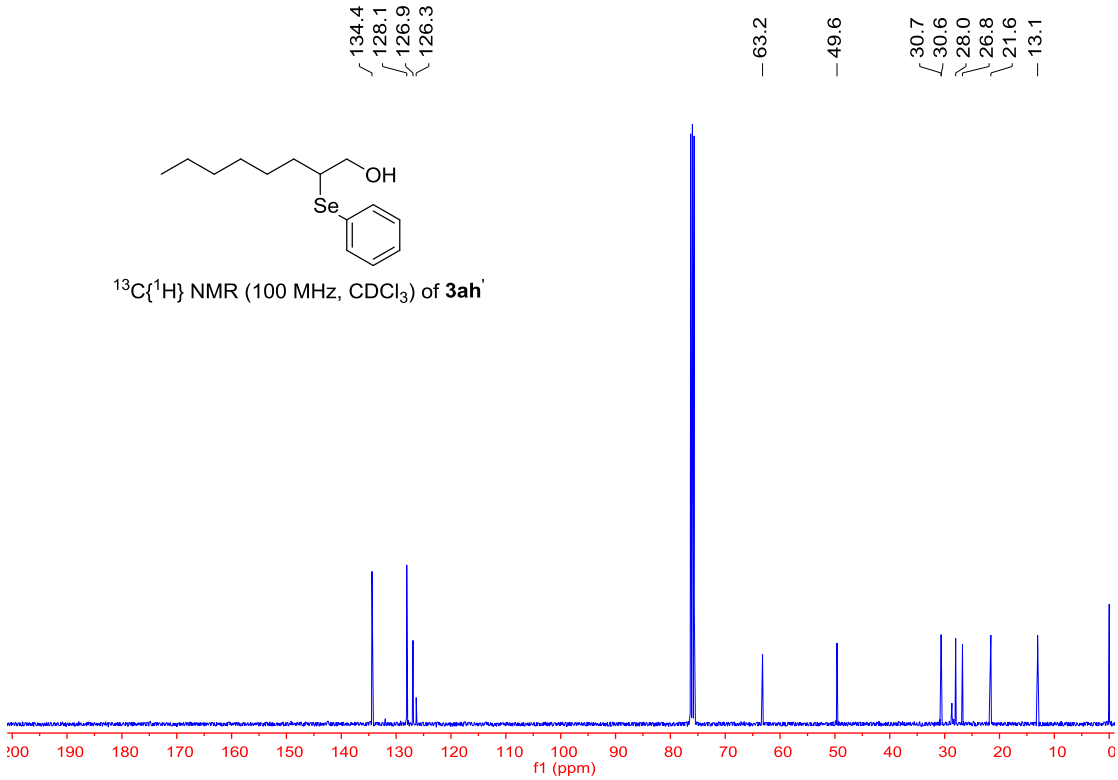


^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) of **3ah**

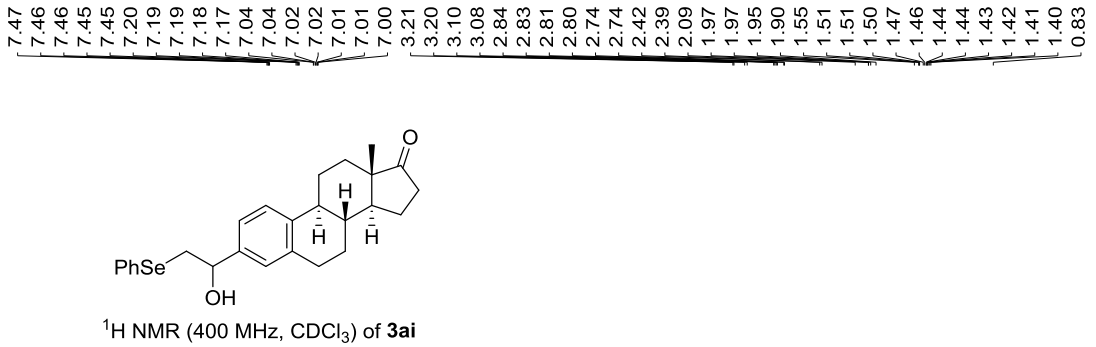




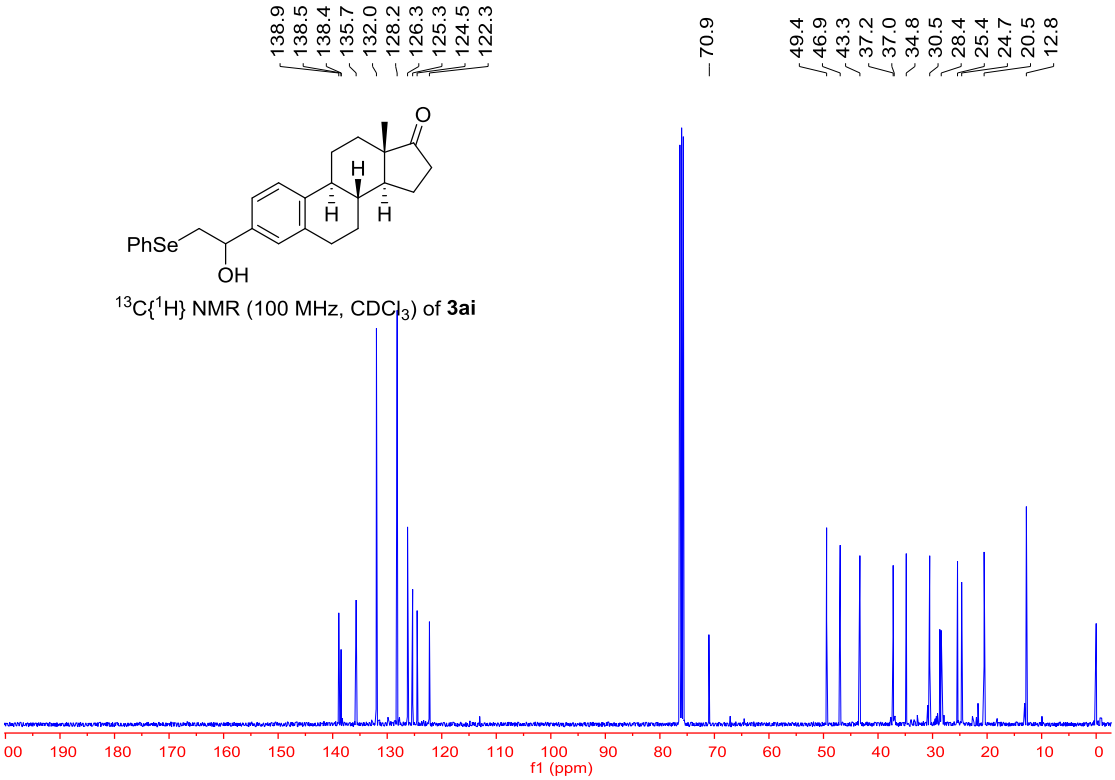
^{1}H NMR (400 MHz, $CDCl_3$) of **3ah'**



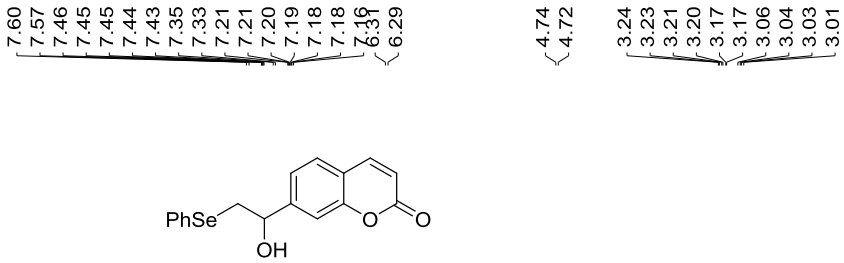
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) of **3ah'**



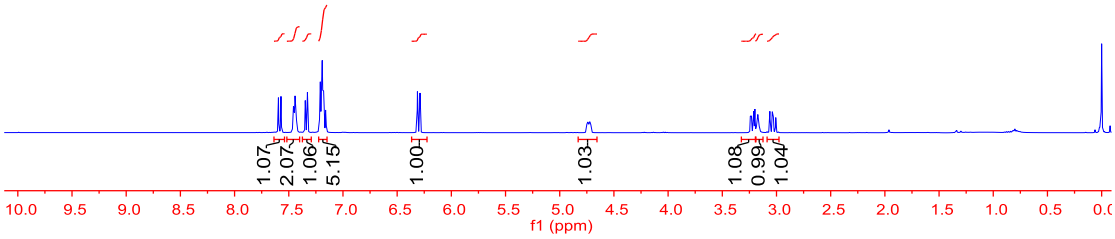
^{1}H NMR (400 MHz, $CDCl_3$) of **3ai**



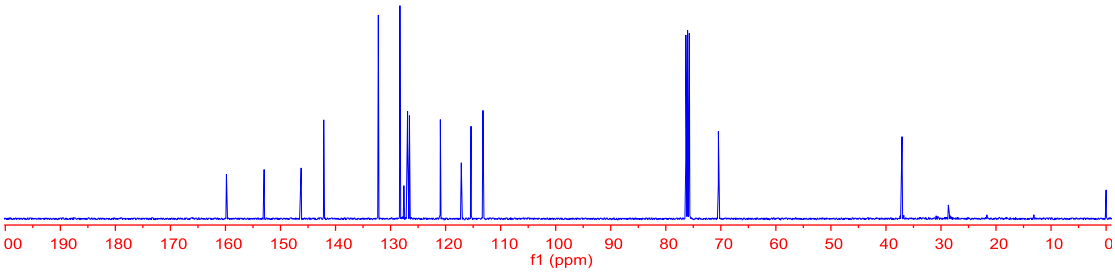
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) of **3ai**

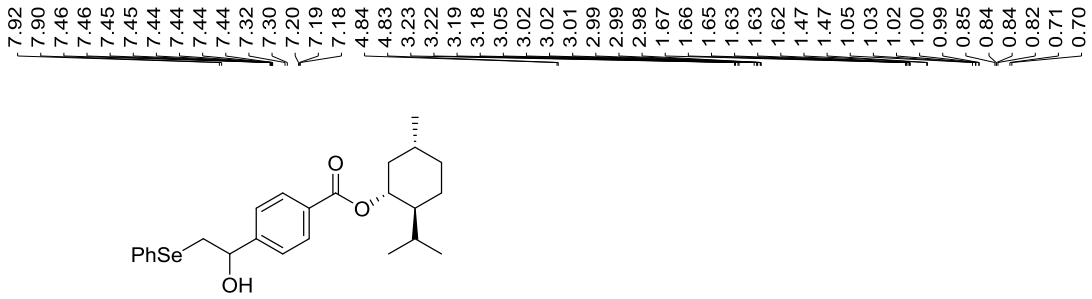


^{1}H NMR (400 MHz, $CDCl_3$) of **3aj**

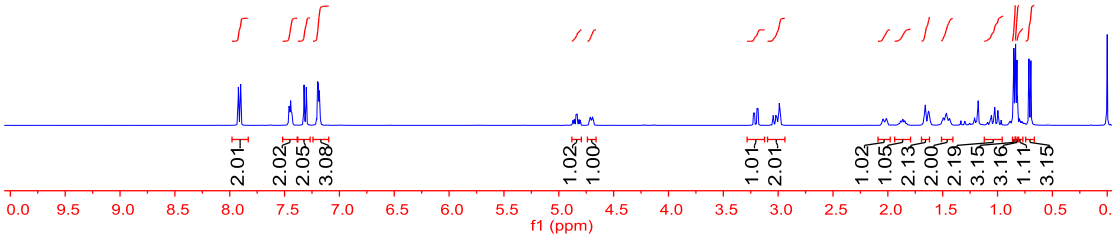


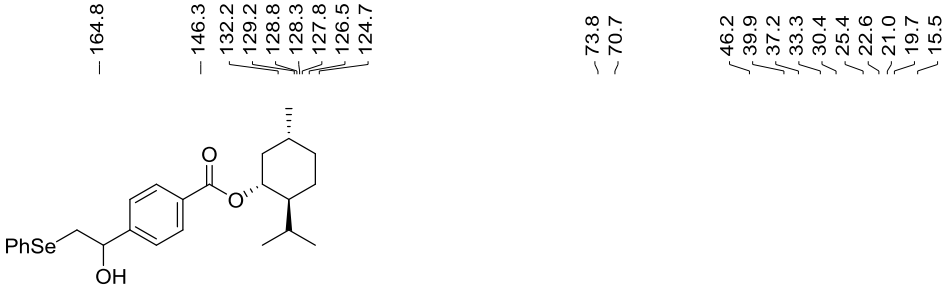
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) of **3aj**



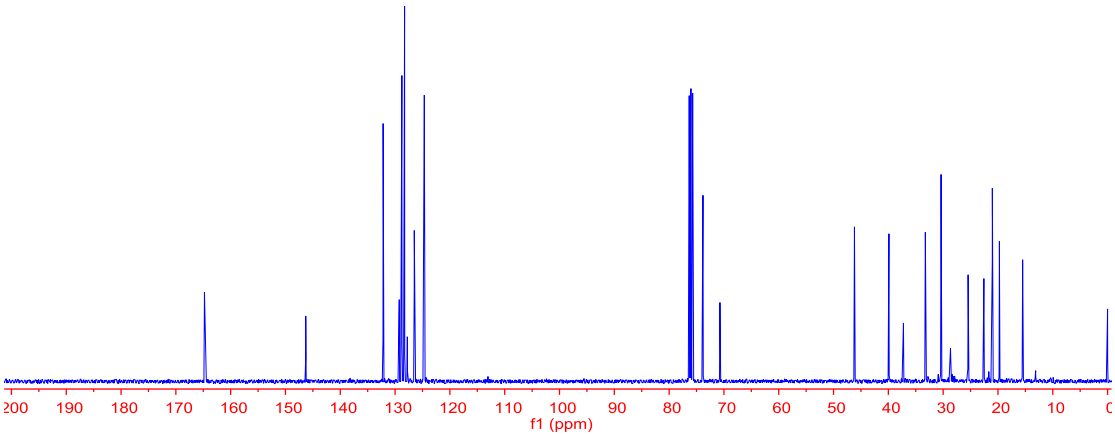


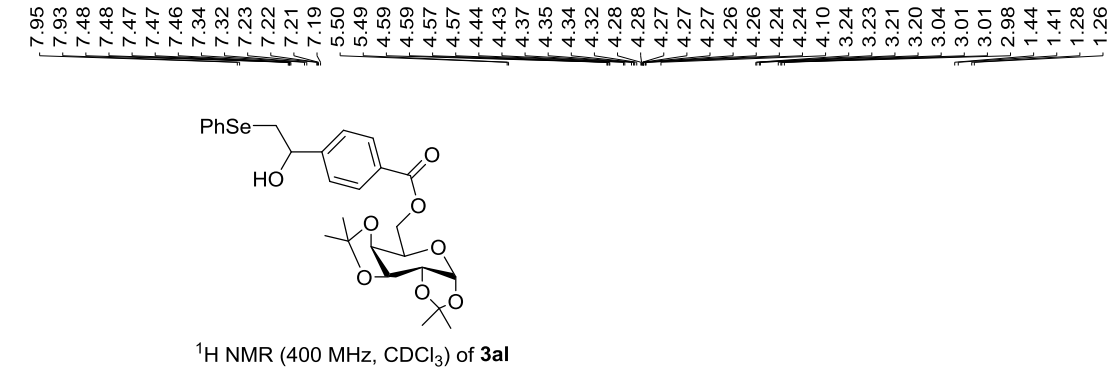
^{1}H NMR (400 MHz, $CDCl_3$) of **3ak**



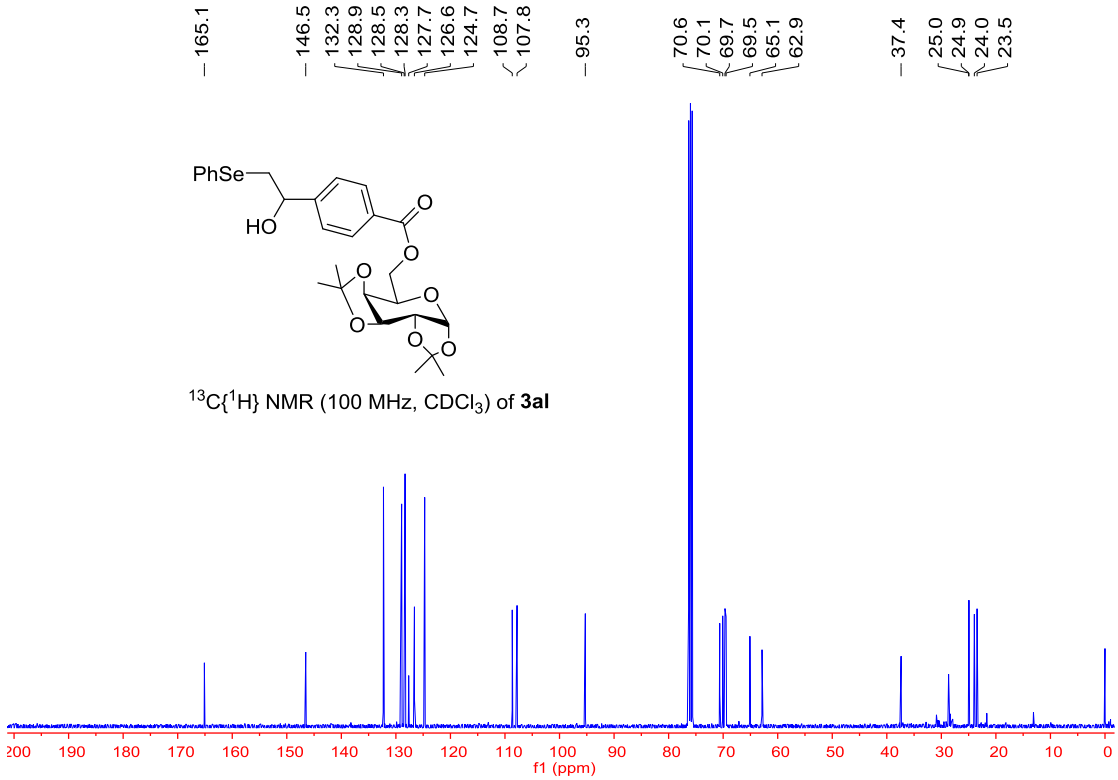


^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) of **3ak**

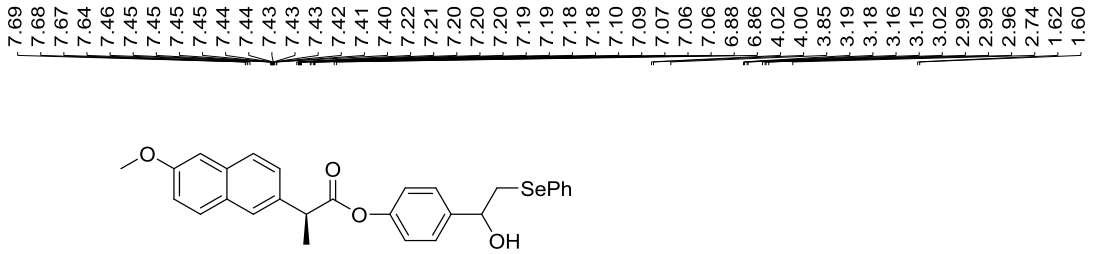




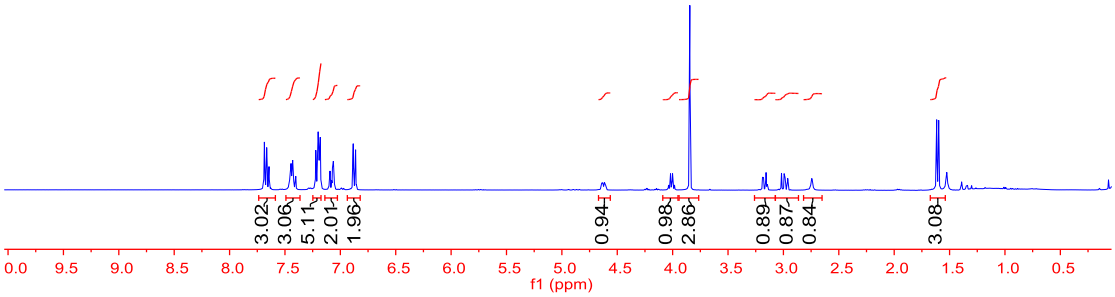
^{1}H NMR (400 MHz, $CDCl_3$) of **3al**

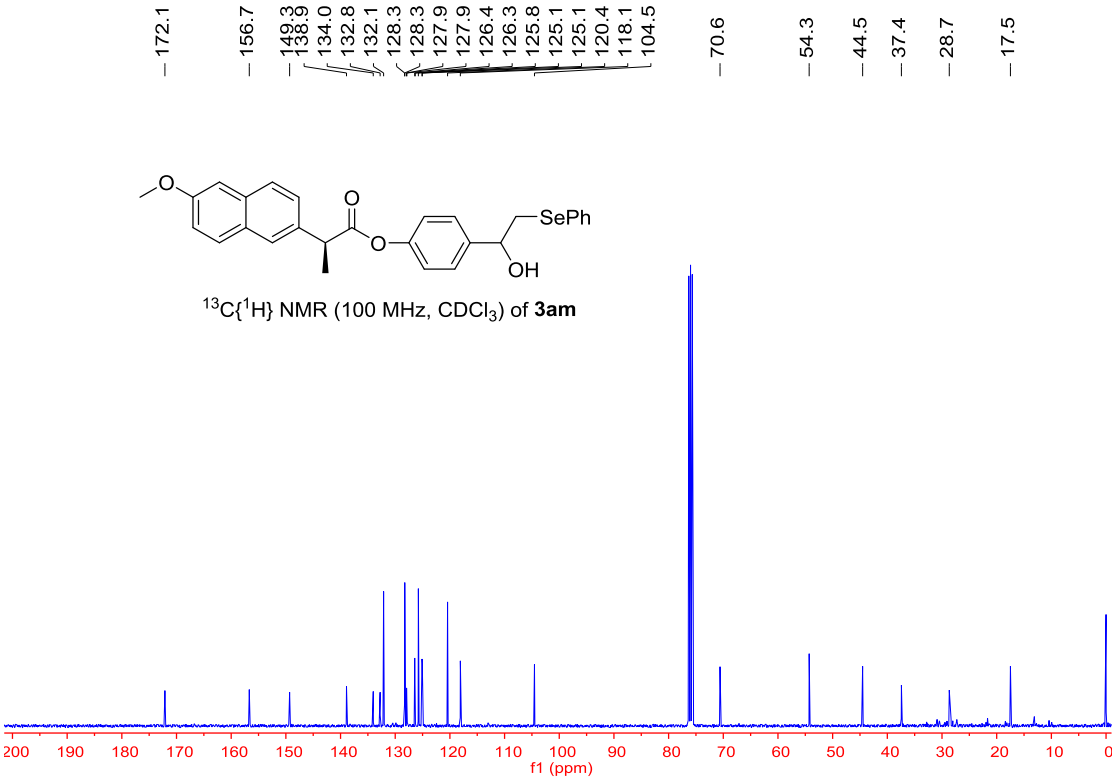


^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) of **3al**

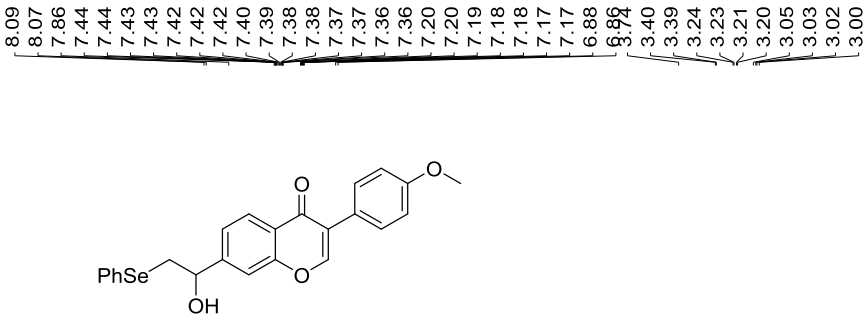


^{1}H NMR (400 MHz, $CDCl_3$) of **3am**

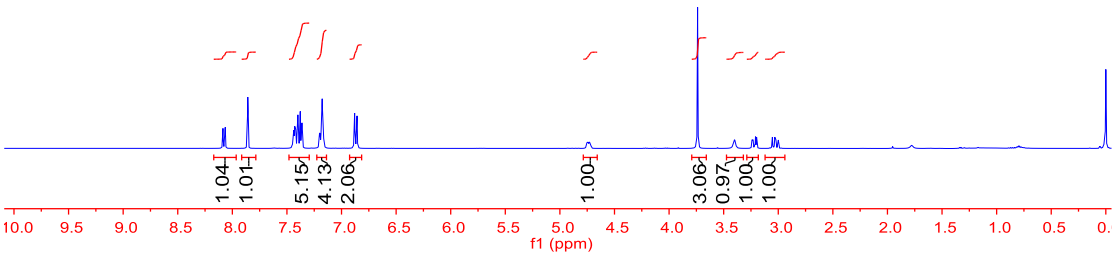


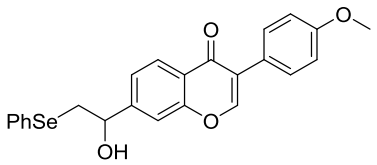


^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) of **3am**

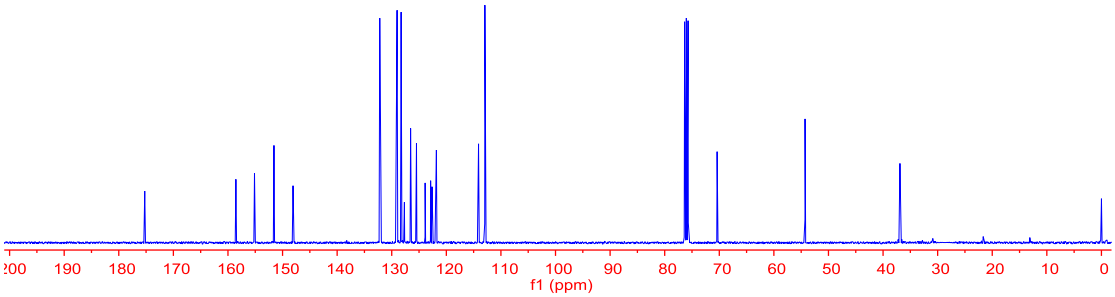


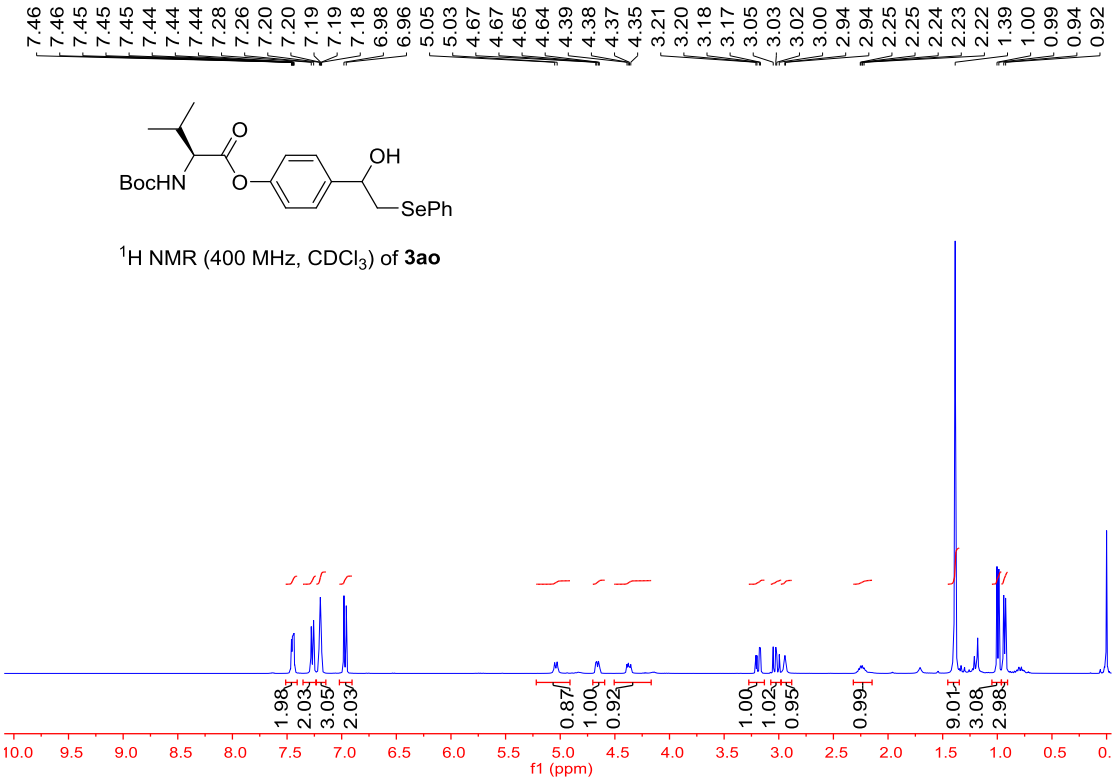
^{1}H NMR (400 MHz, $CDCl_3$) of **3an**



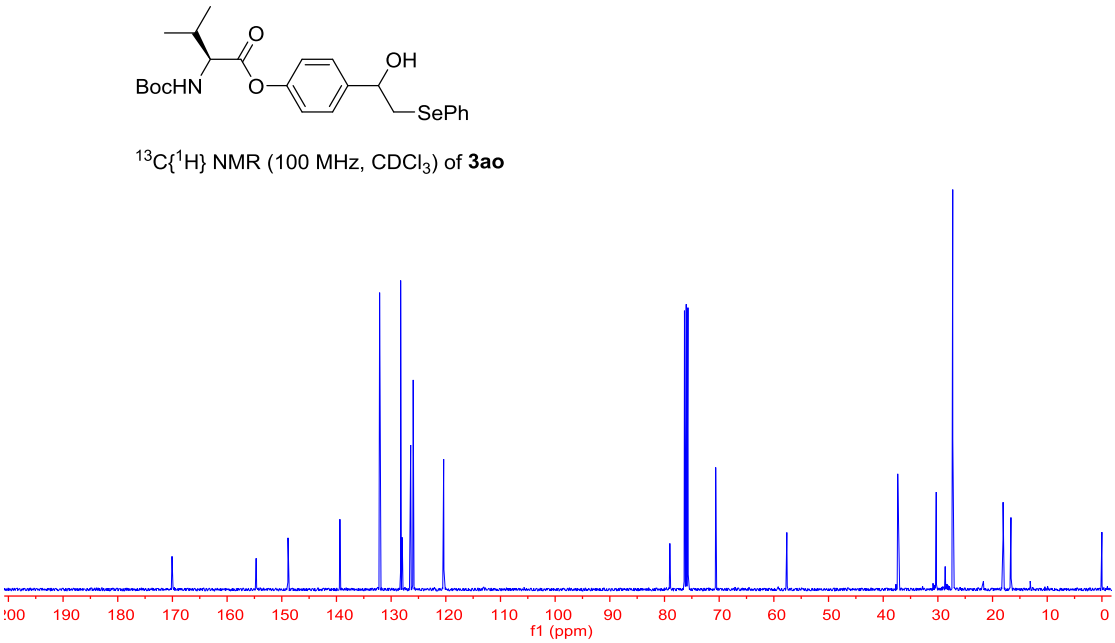


^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) of **3an**

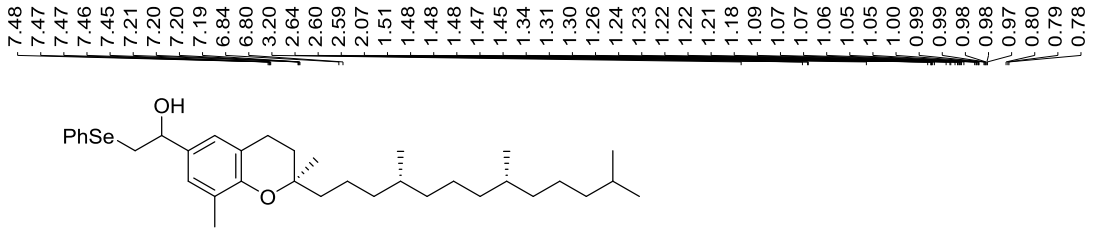




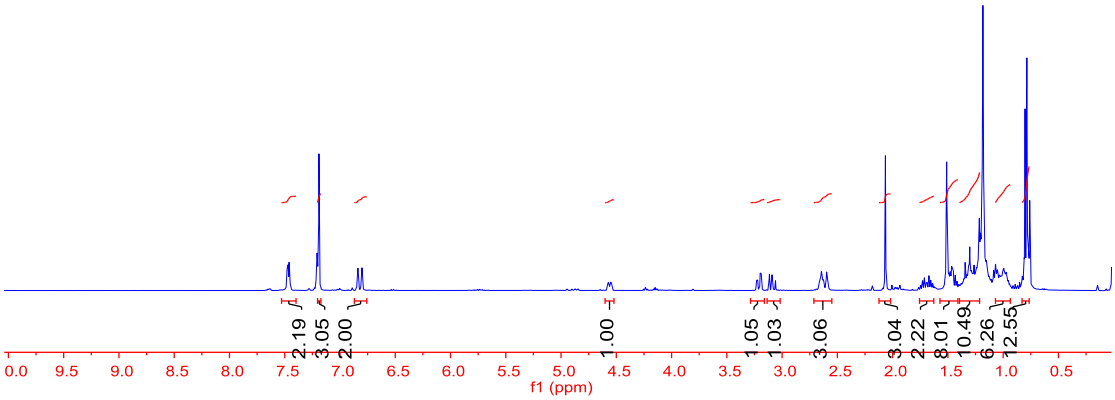
^{1}H NMR (400 MHz, $CDCl_3$) of **3ao**

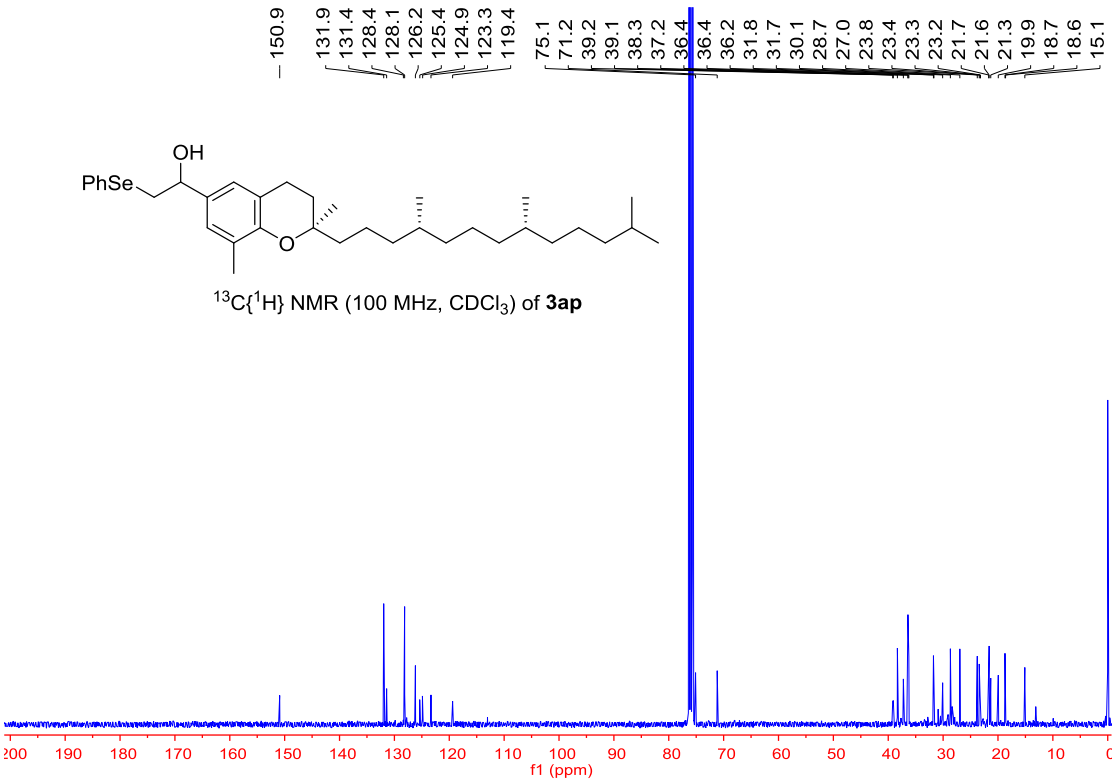


^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) of **3ao**

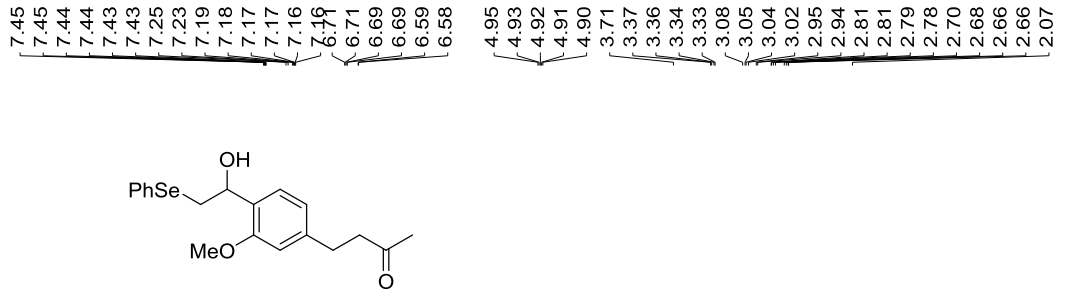


^{1}H NMR (400 MHz, $CDCl_3$) of **3ap**

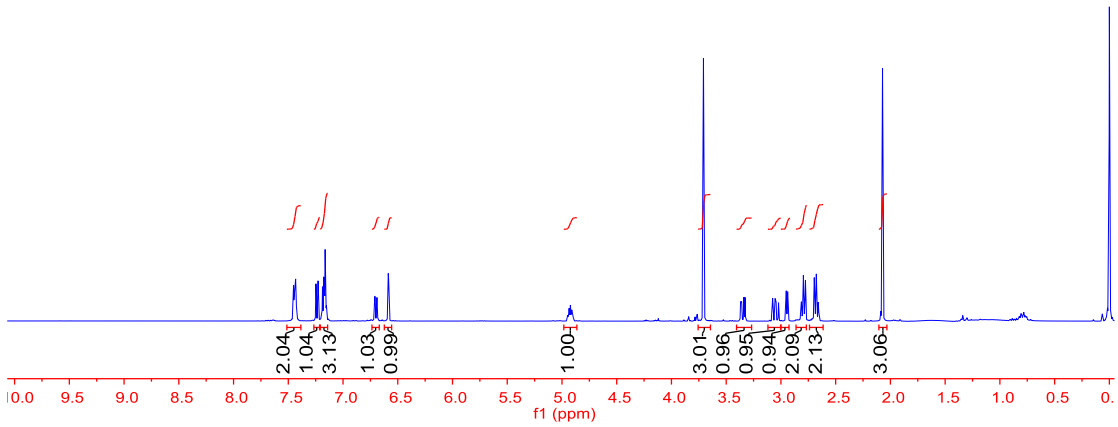


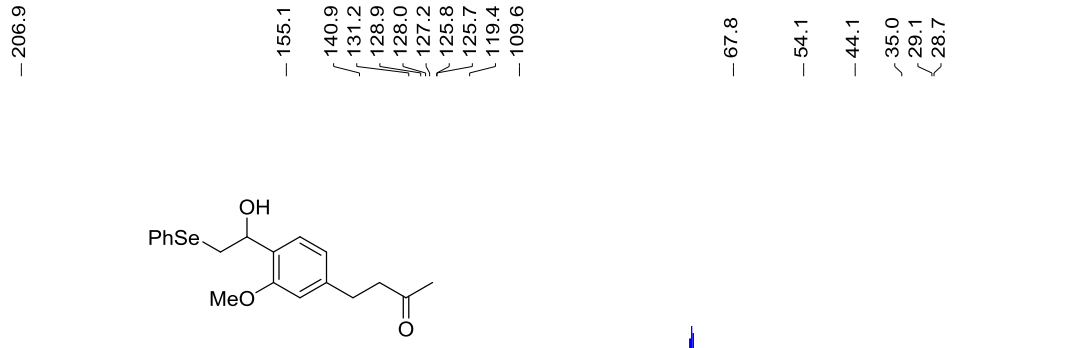


^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) of **3ap**



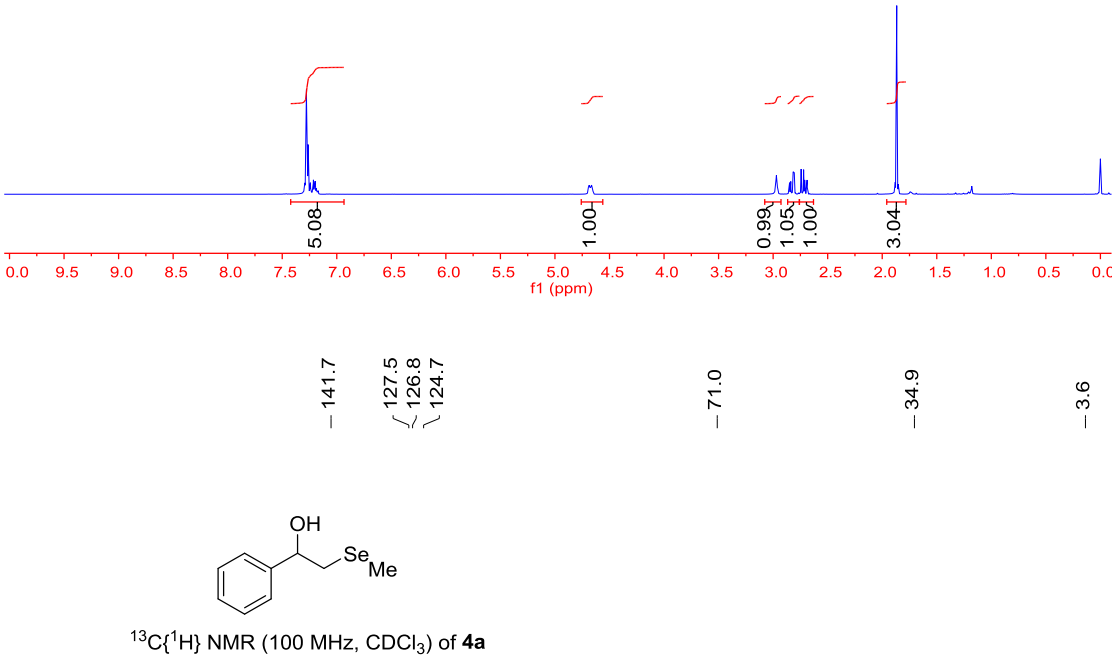
^{1}H NMR (400 MHz, $CDCl_3$) of **3aq**



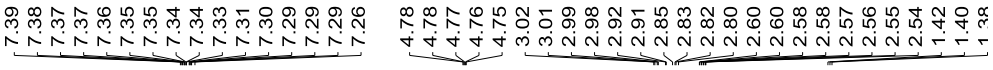


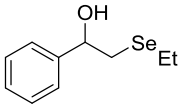
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) of **3aq**

^{1}H NMR (400 MHz, $CDCl_3$) of **4a**

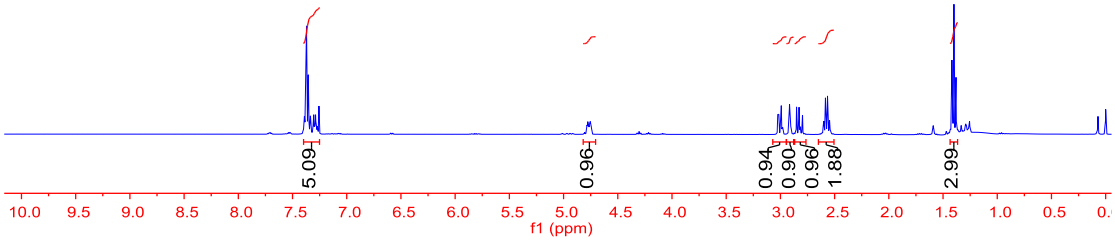


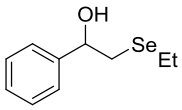
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) of **4a**



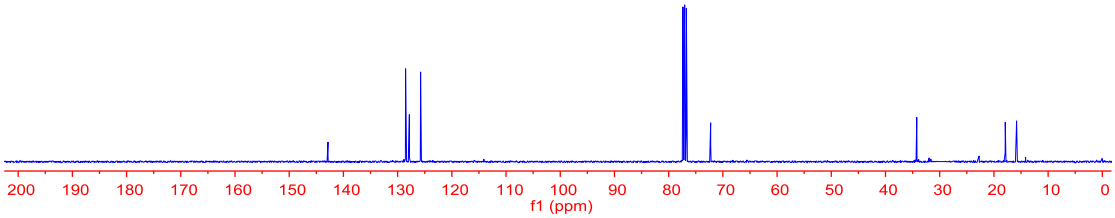


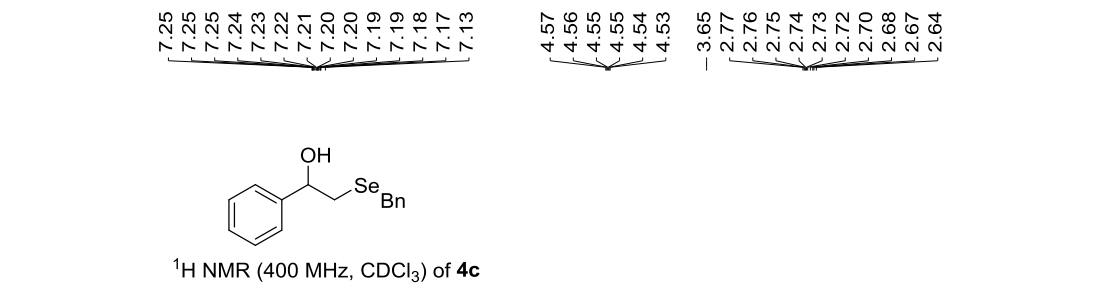
^{1}H NMR (400 MHz, $CDCl_3$) of **4b**



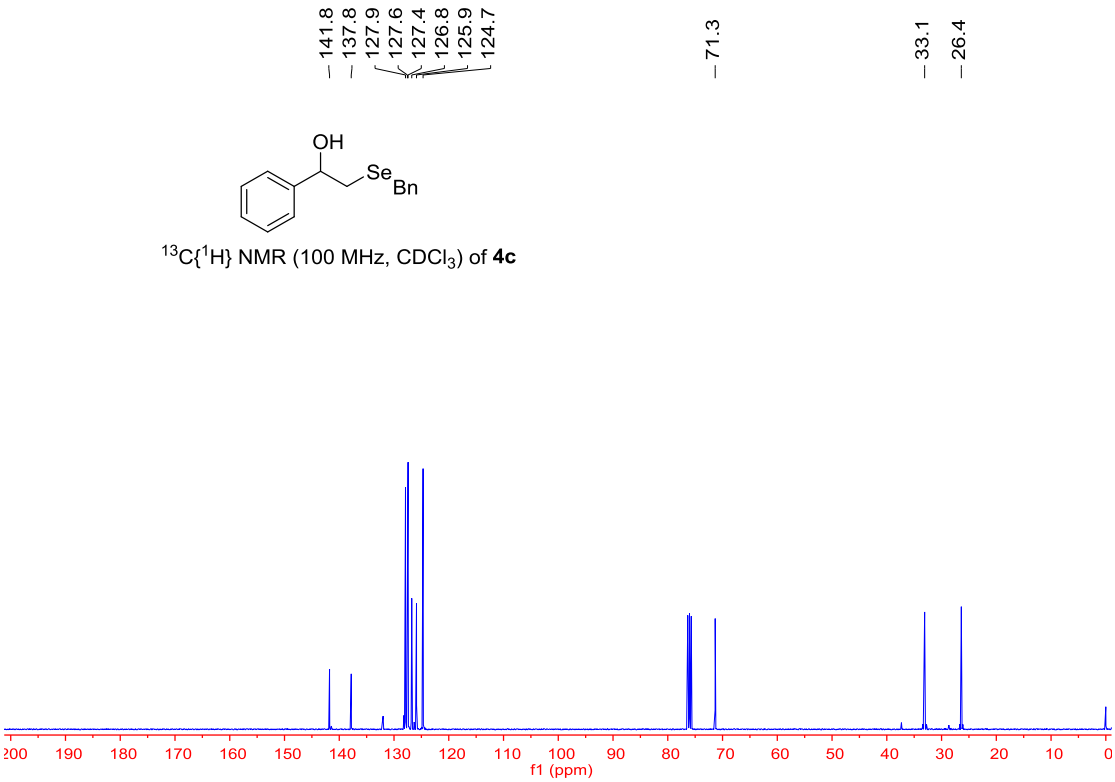


^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) of **4b**

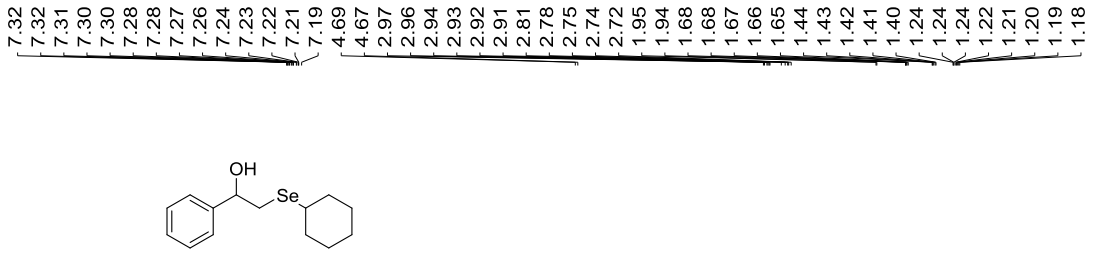




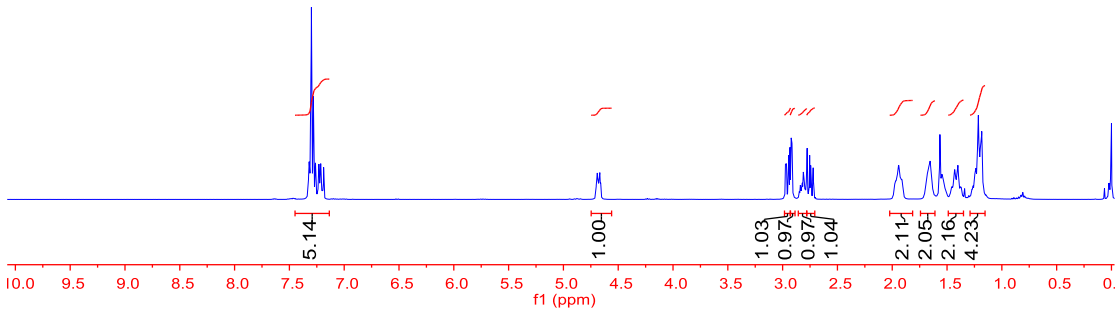
^{1}H NMR (400 MHz, $CDCl_3$) of **4c**

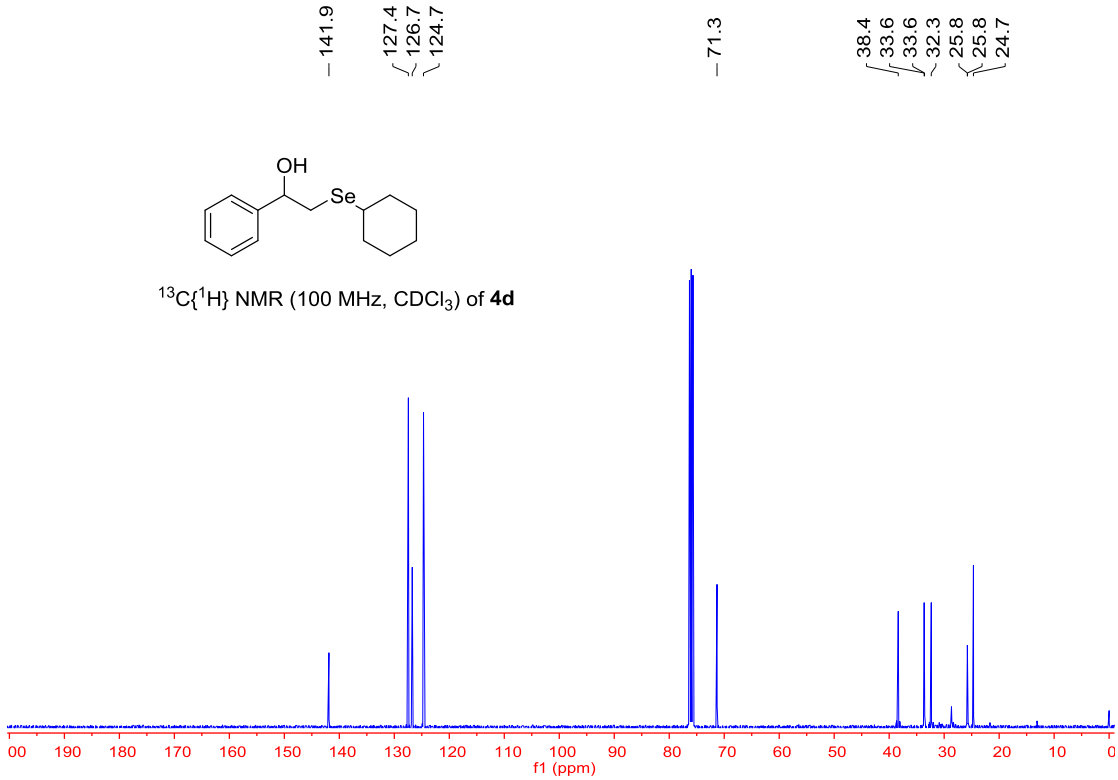


^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) of **4c**

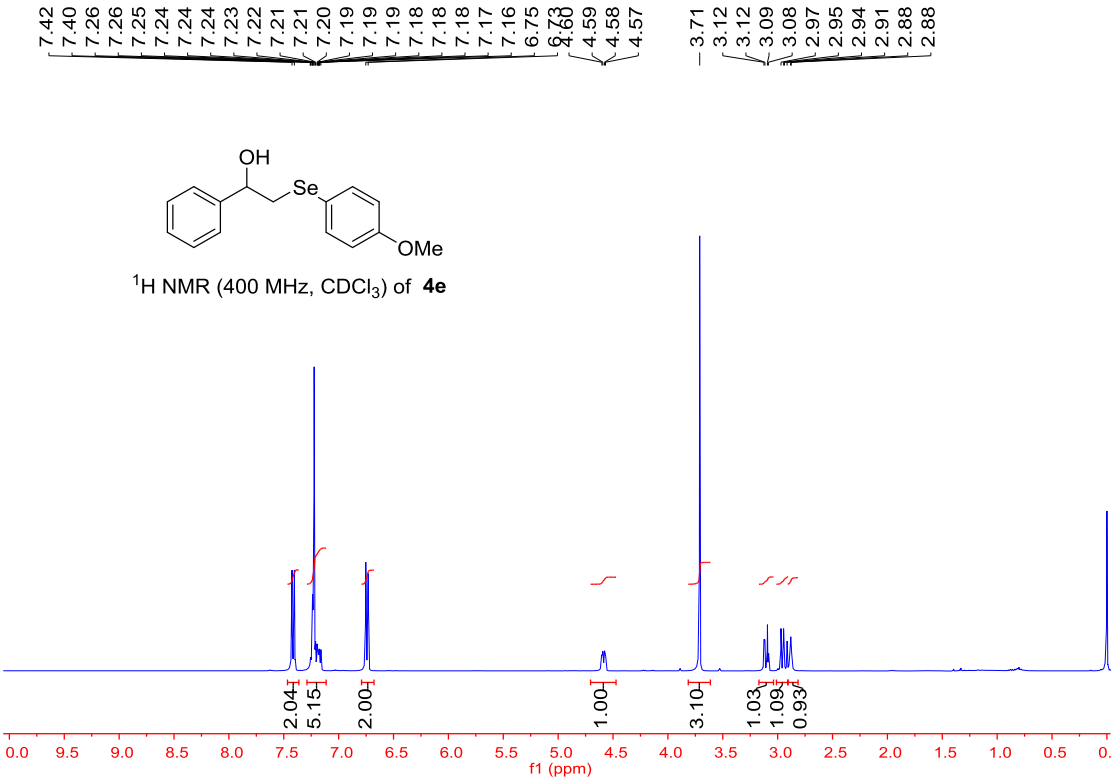


^{1}H NMR (400 MHz, $CDCl_3$) of **4d**

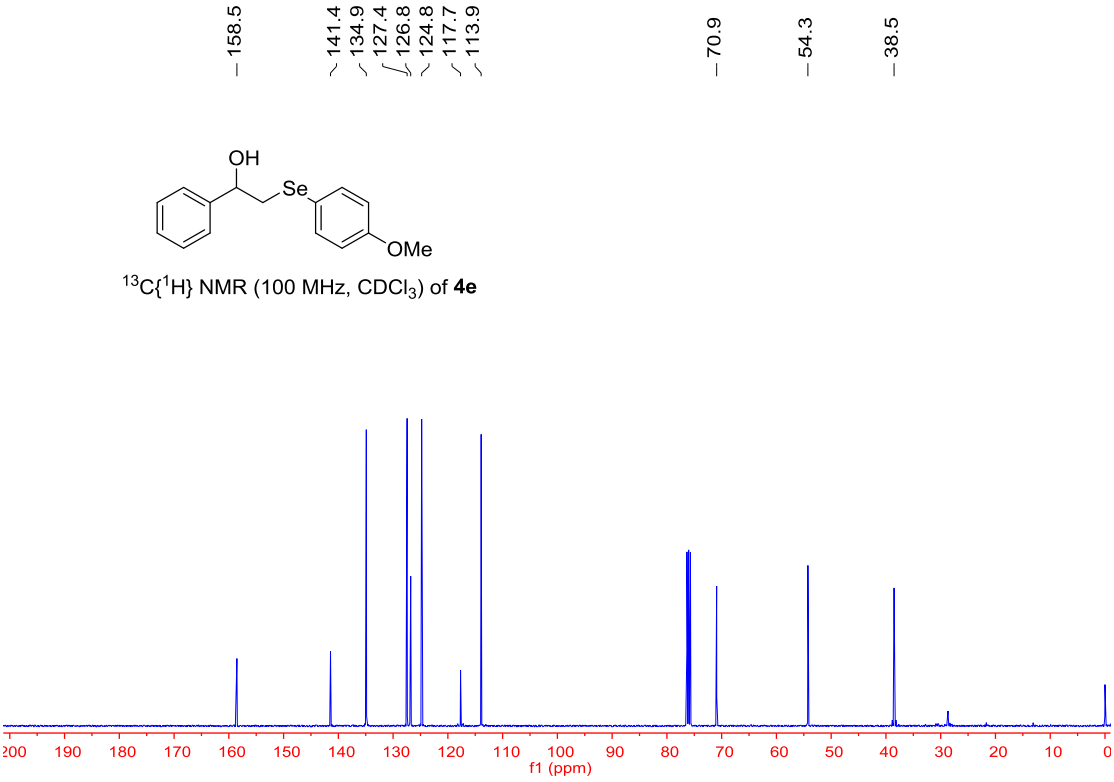




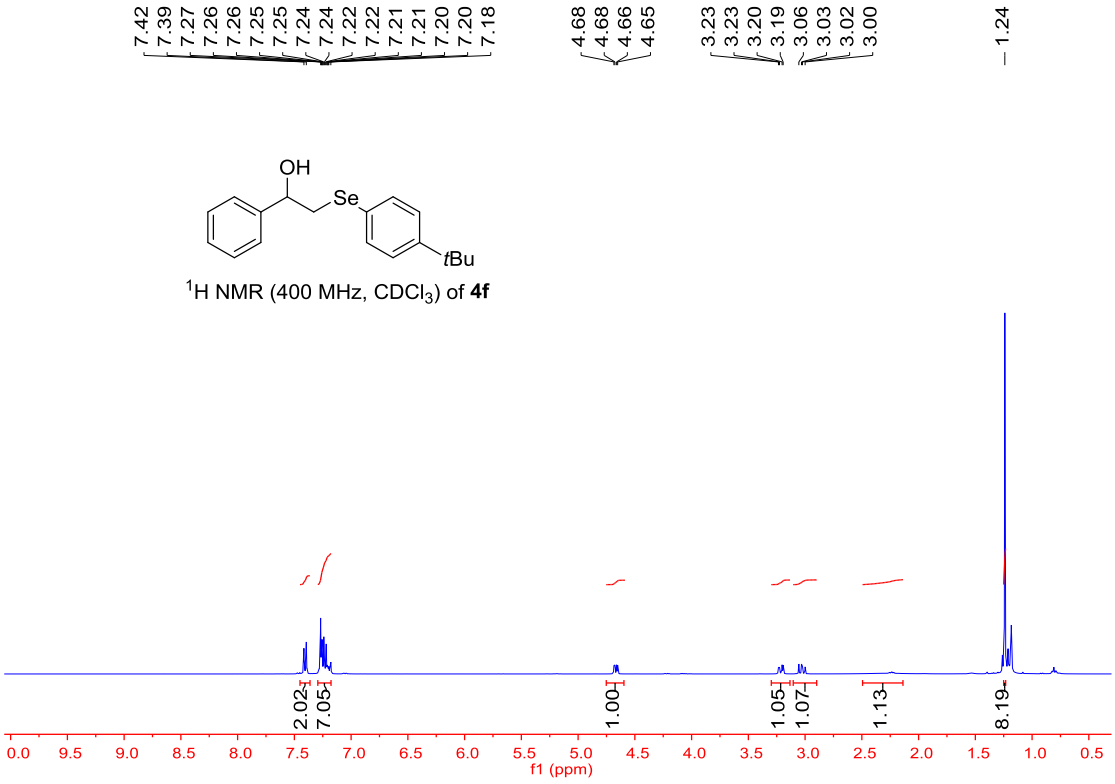
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) of **4d**



^{1}H NMR (400 MHz, $CDCl_3$) of **4e**



^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) of **4e**



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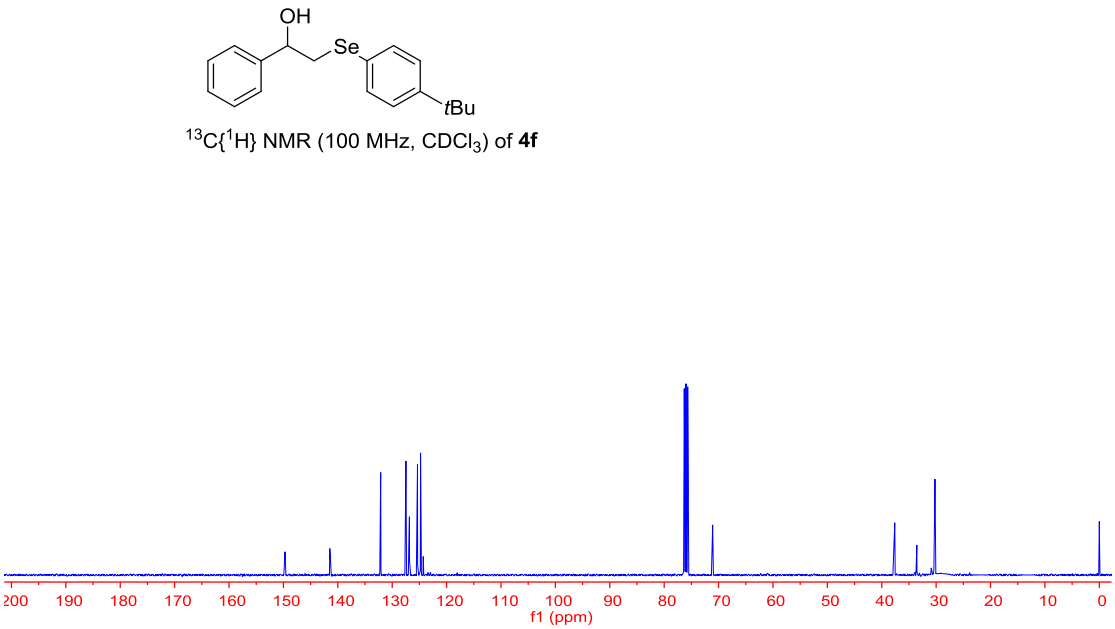
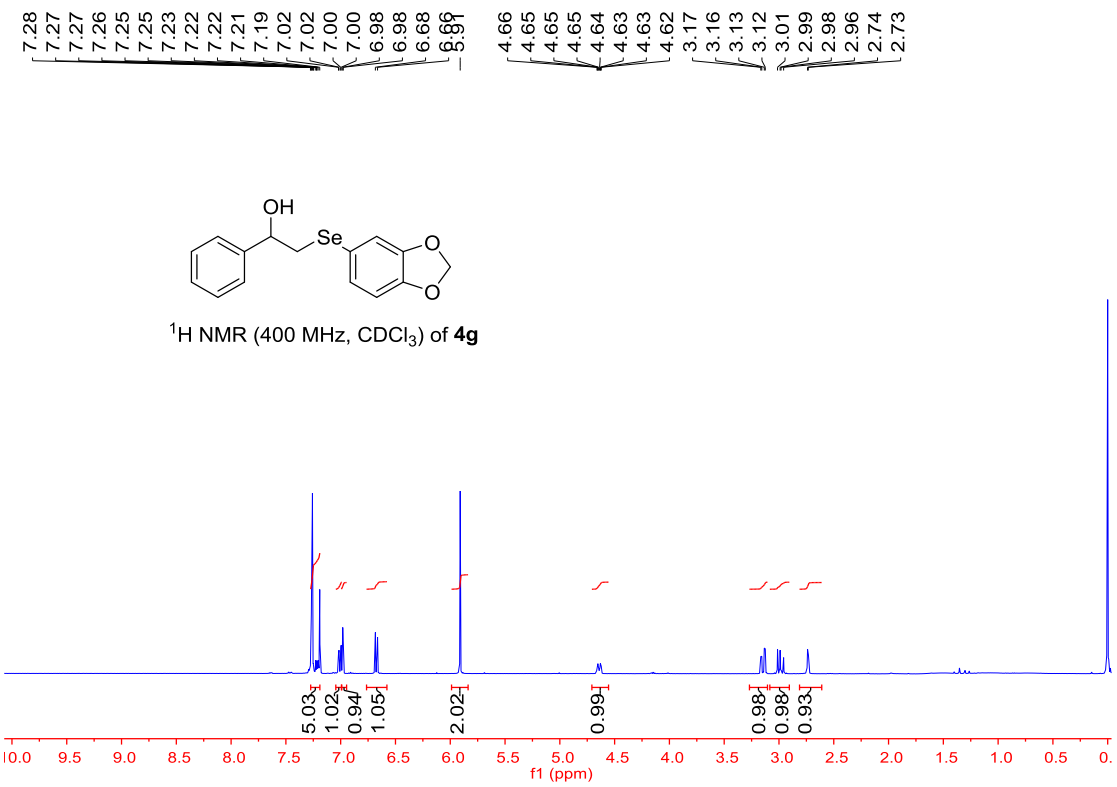
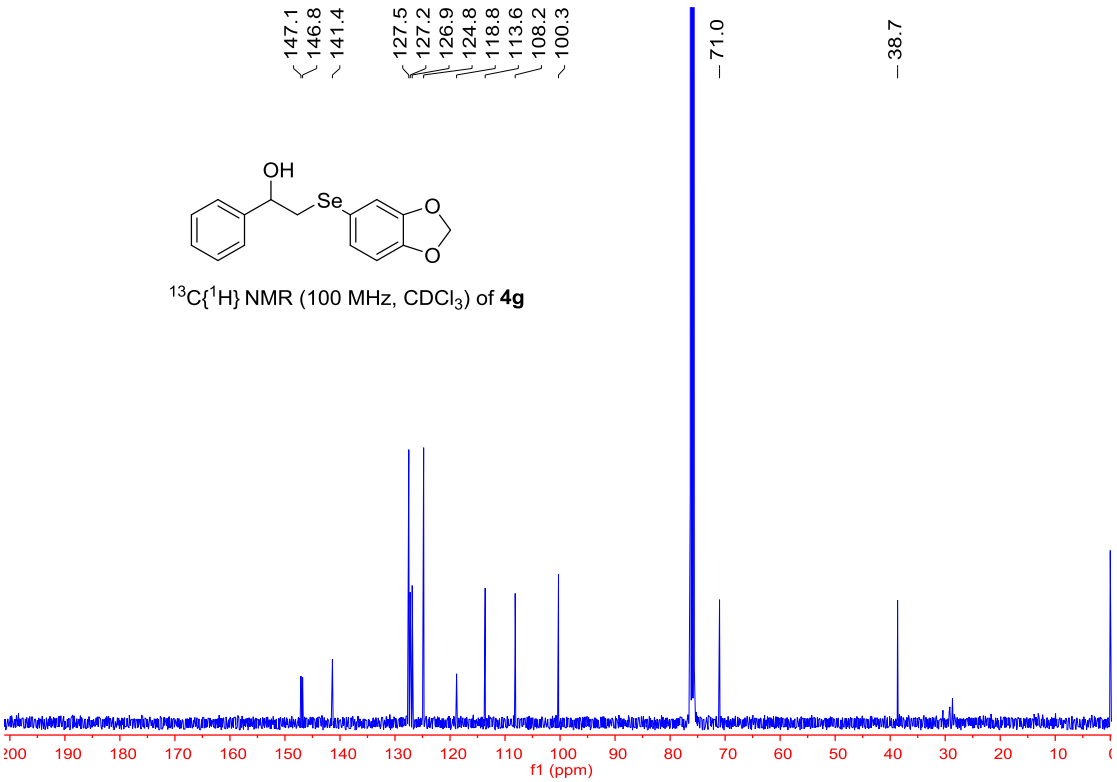
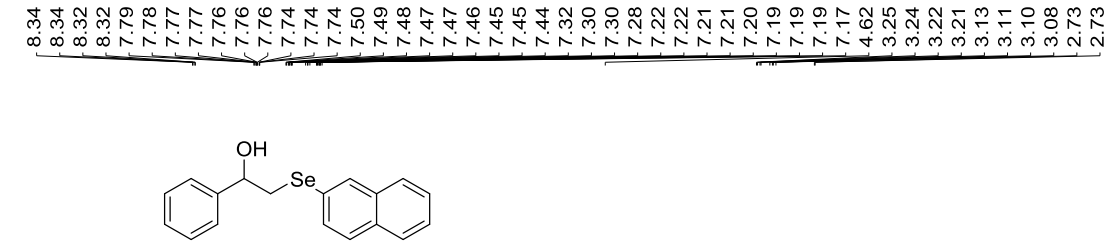


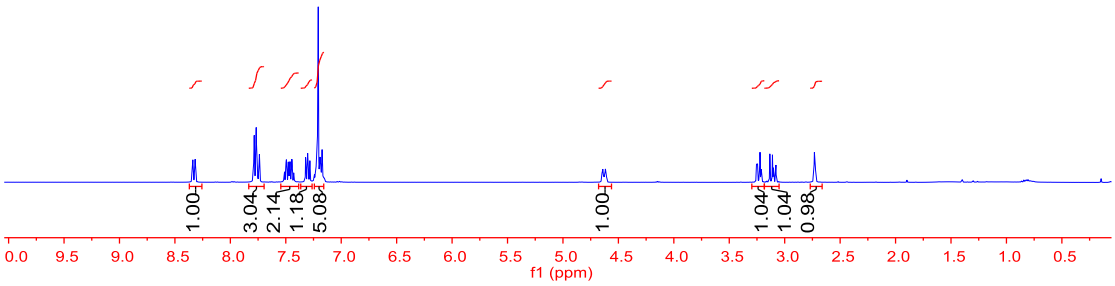
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) of **4f**

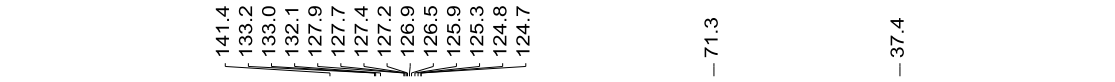

7.28
7.27
7.27
7.26
7.25
7.25
7.23
7.22
7.22
7.21
7.19
7.02
7.02
7.00
7.00
6.98
6.98
6.68
6.66
5.91
4.66
4.65
4.65
4.65
4.64
4.63
4.63
4.62
3.17
3.16
3.13
3.12
3.01
2.99
2.98
2.96
2.74
2.73
OH
Se
O
O
^{1}H NMR (400 MHz, $CDCl_3$) of **4g**
5.03
1.02
0.94
1.05
2.02
0.99
0.98
0.98
0.93
f1 (ppm)


147.1
146.8
141.4
127.5
127.2
126.9
124.8
118.8
113.6
108.2
100.3
71.0
38.7
OH
Se
O
O
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) of **4g**
f1 (ppm)

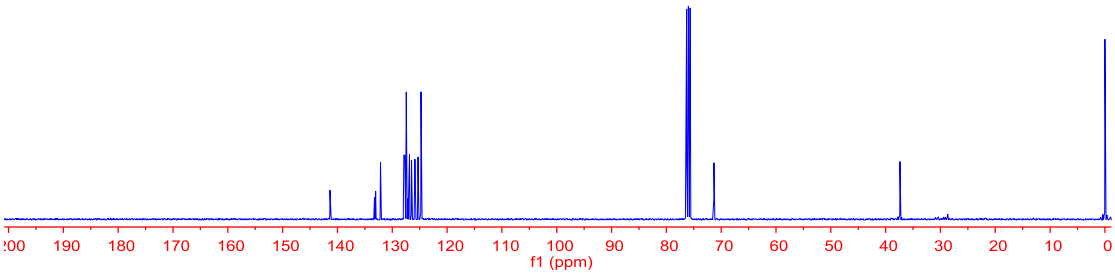


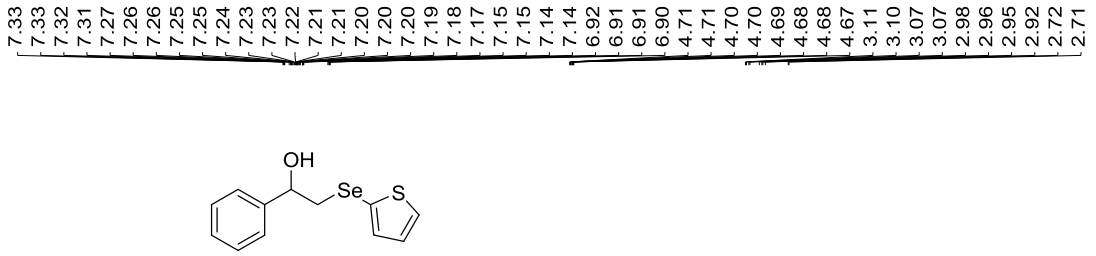
^{1}H NMR (400 MHz, $CDCl_3$) of **4h**



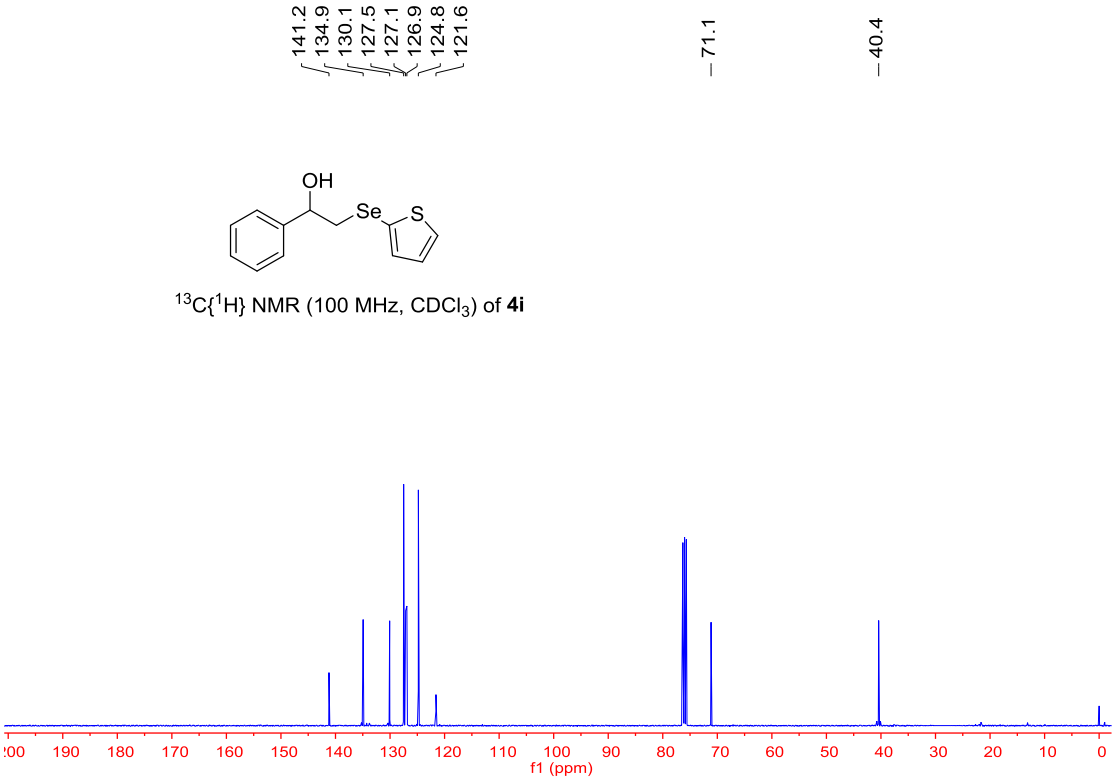


^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) of **4h**

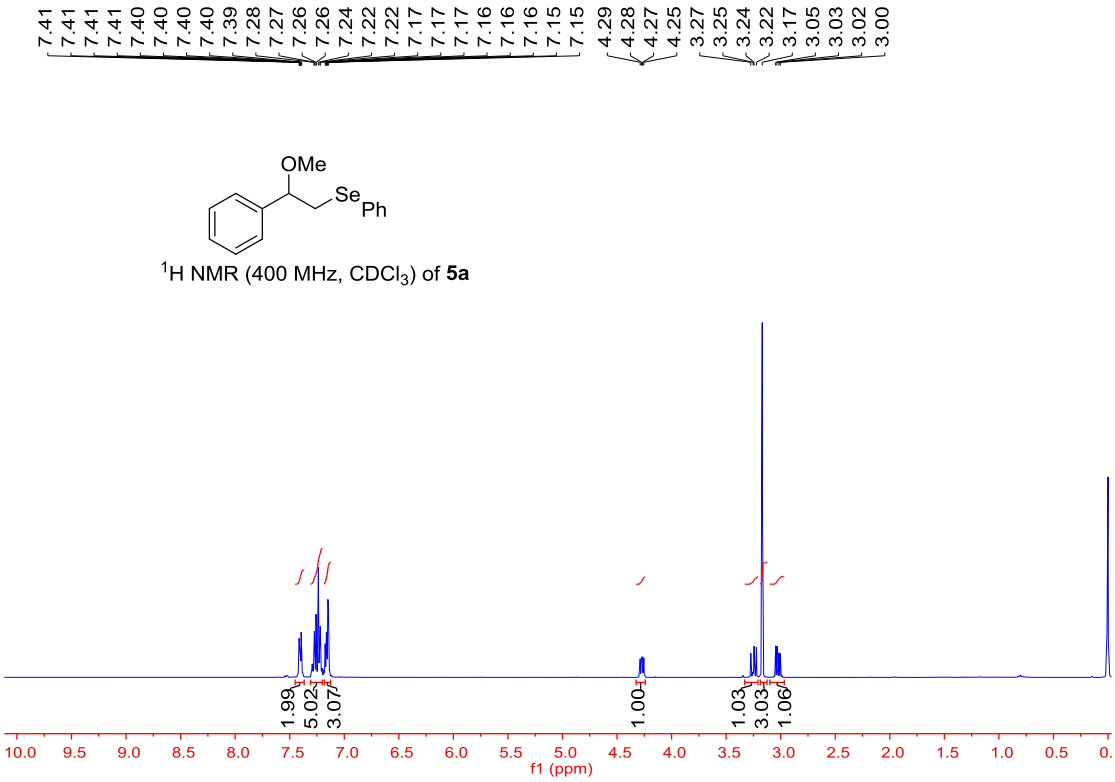




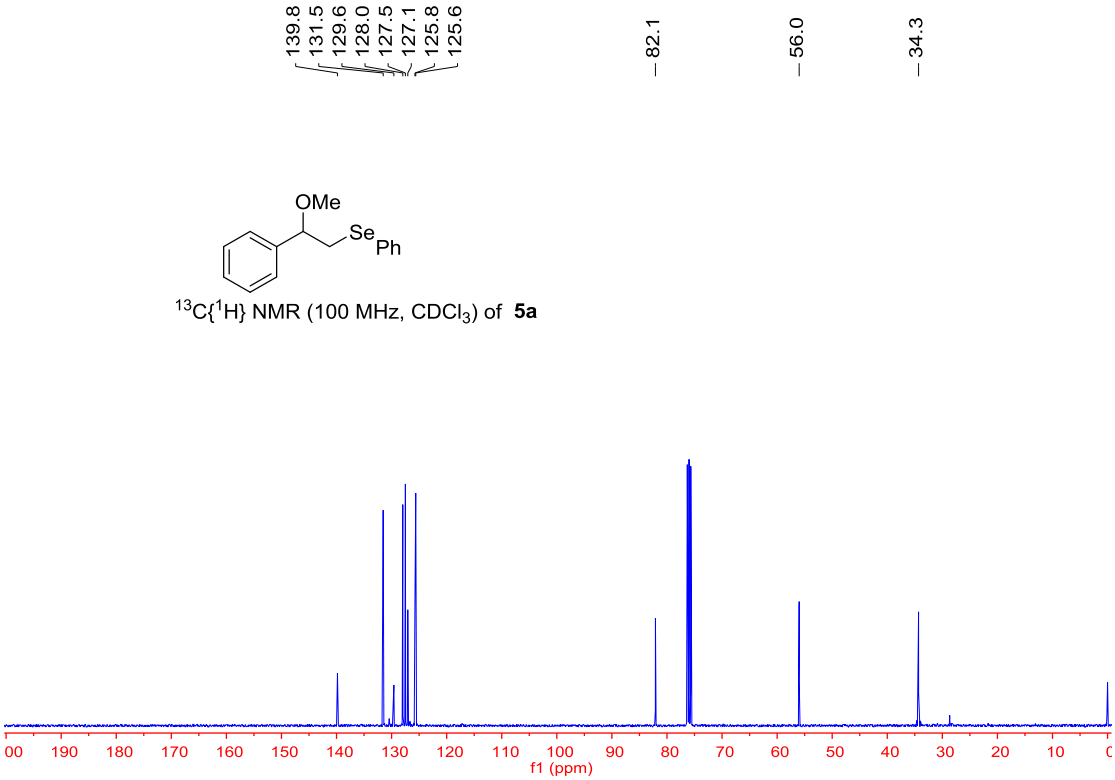
^{1}H NMR (400 MHz, $CDCl_3$) of **4i**



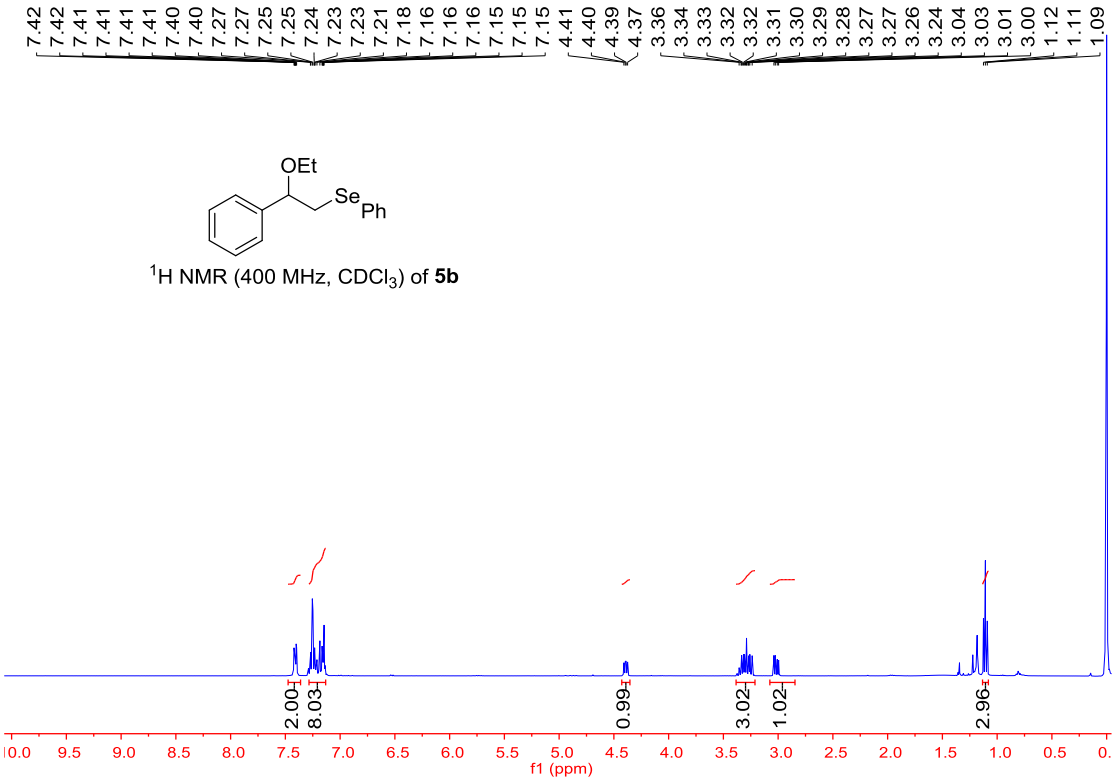
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) of **4i**



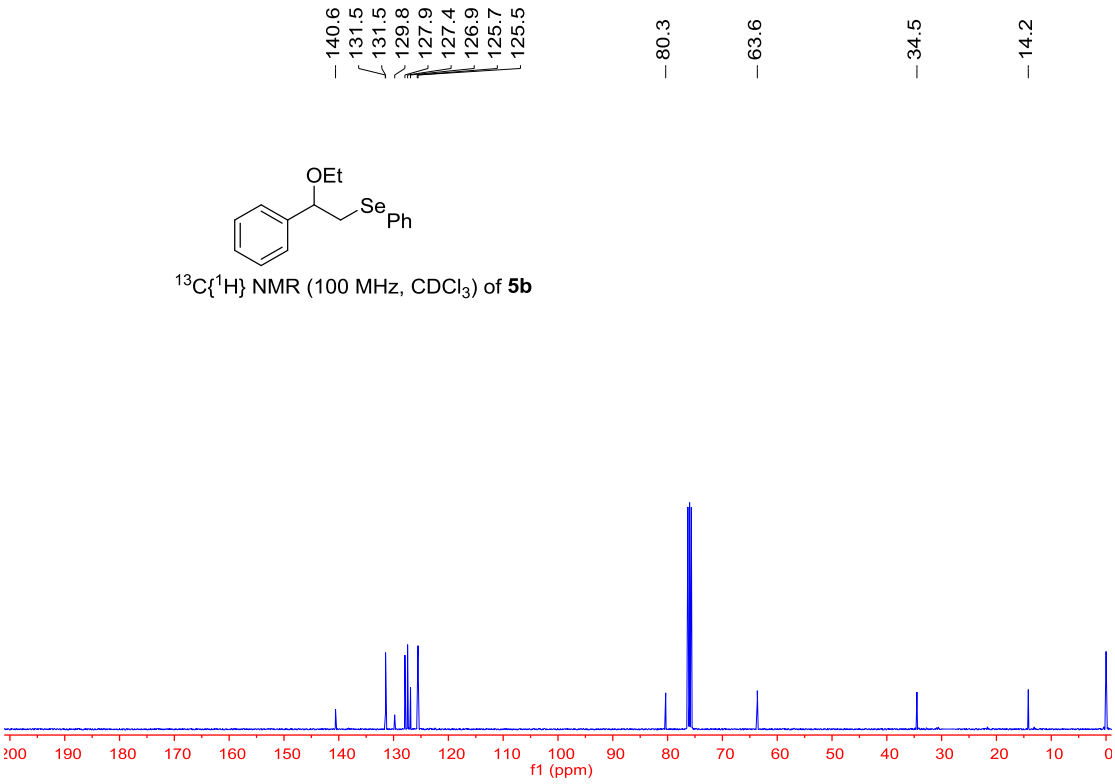
^{1}H NMR (400 MHz, $CDCl_3$) of **5a**



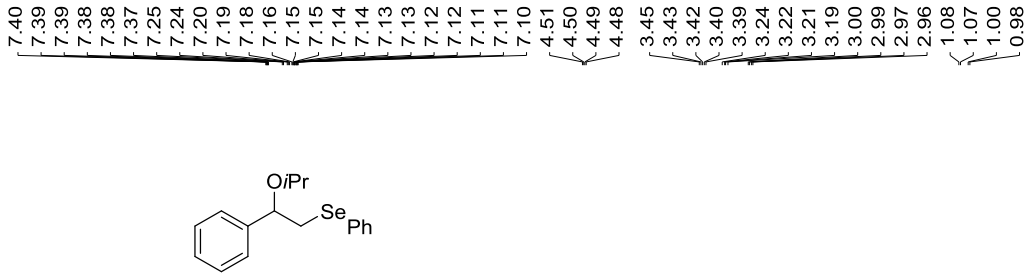
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) of **5a**



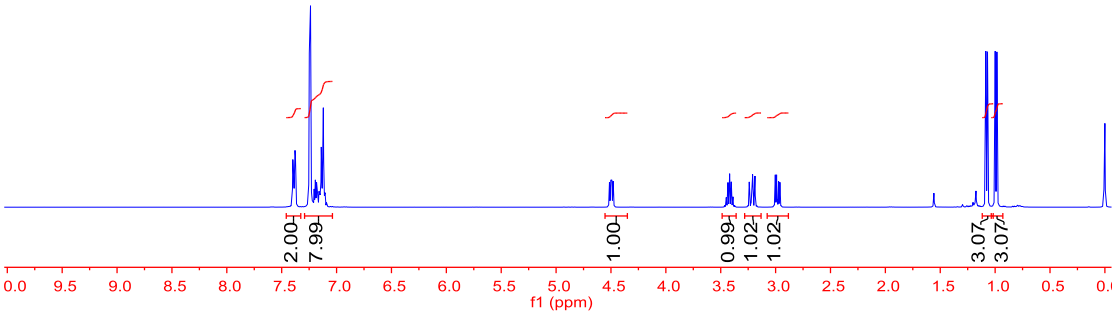
^{1}H NMR (400 MHz, $CDCl_3$) of **5b**



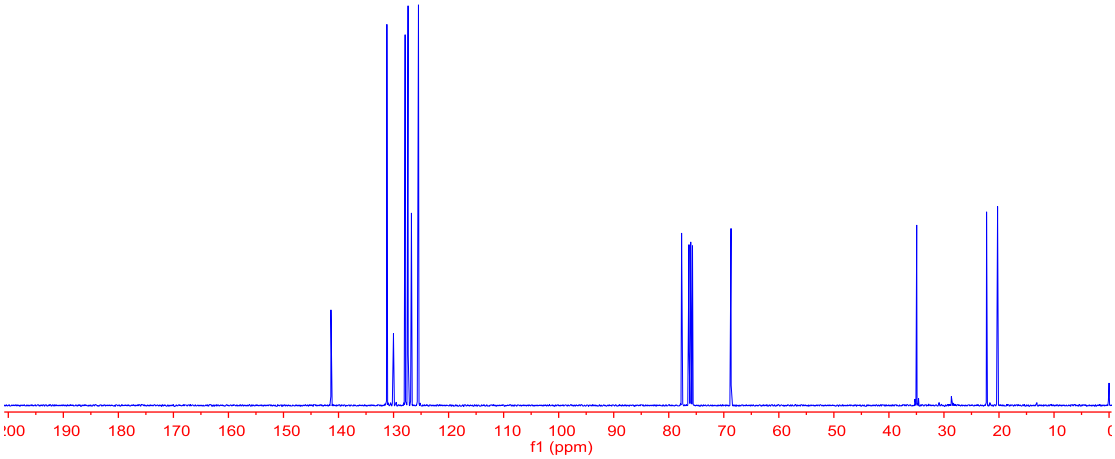
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) of **5b**

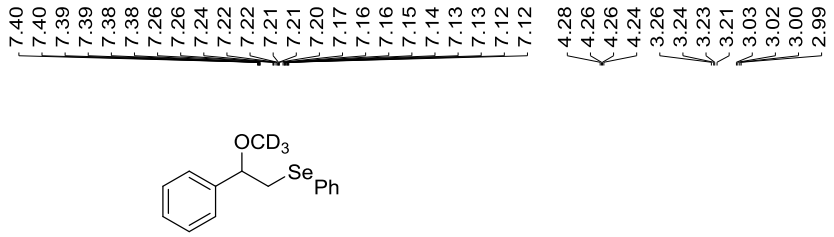


^{1}H NMR (400 MHz, $CDCl_3$) of **5c**

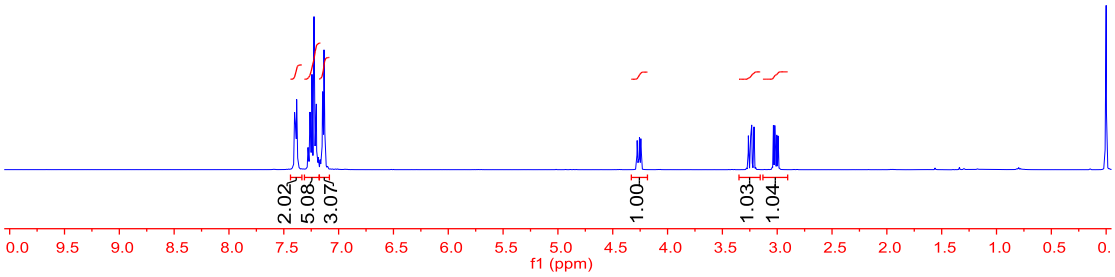


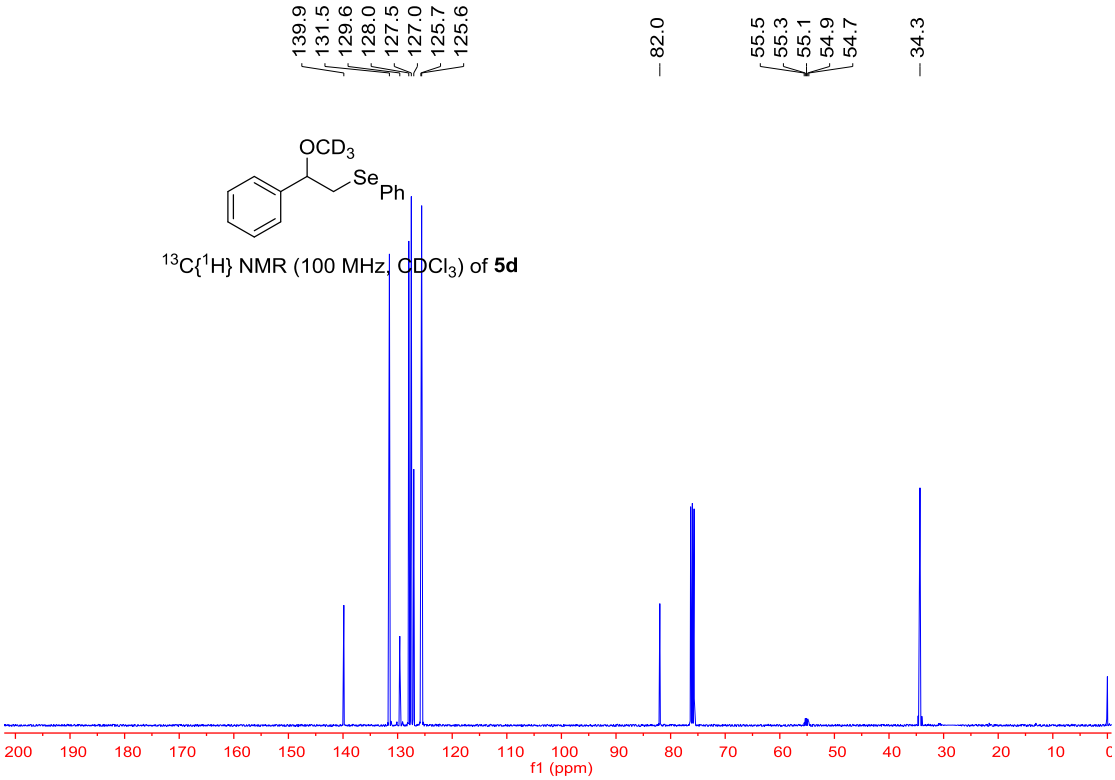
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) of **5c**



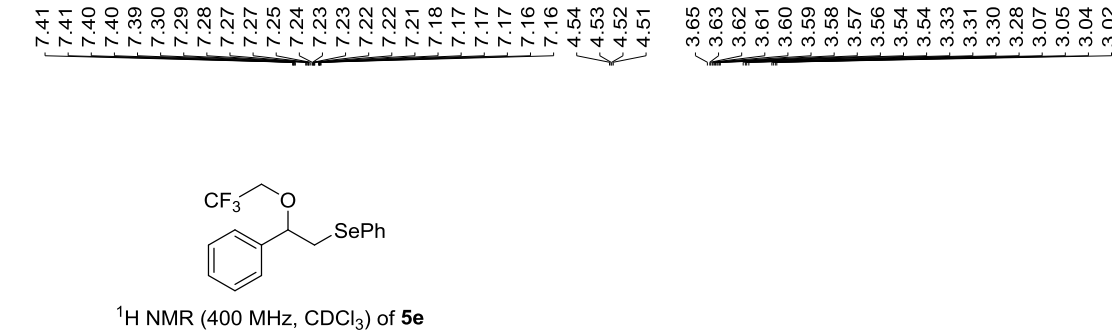


^{1}H NMR (400 MHz, $CDCl_3$) of **5d**

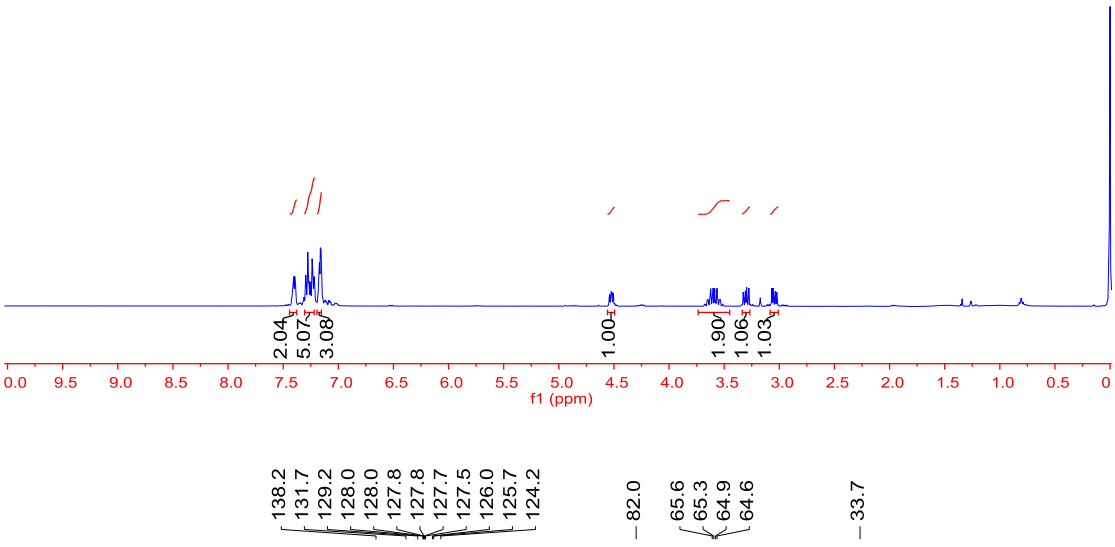


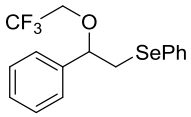


^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) of **5d**

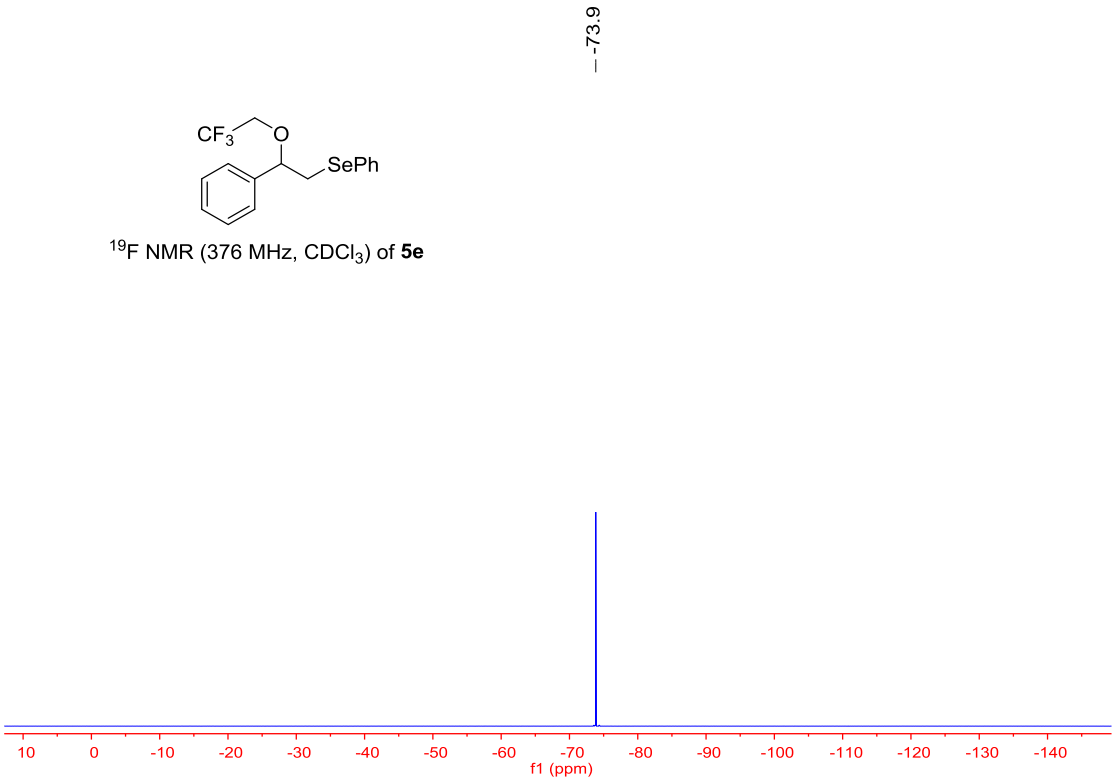


^{1}H NMR (400 MHz, $CDCl_3$) of **5e**

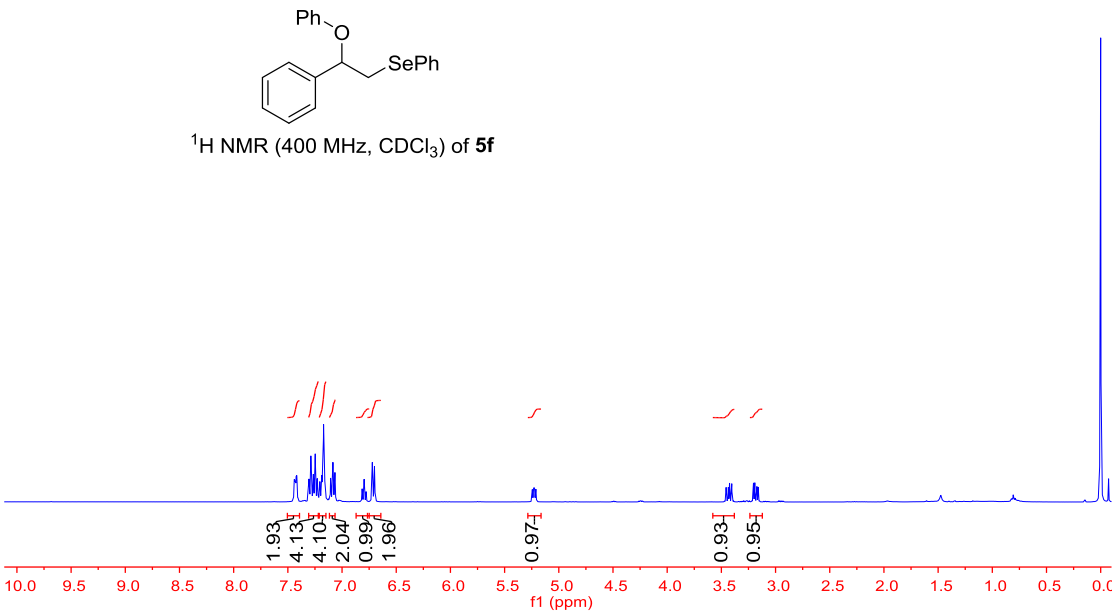




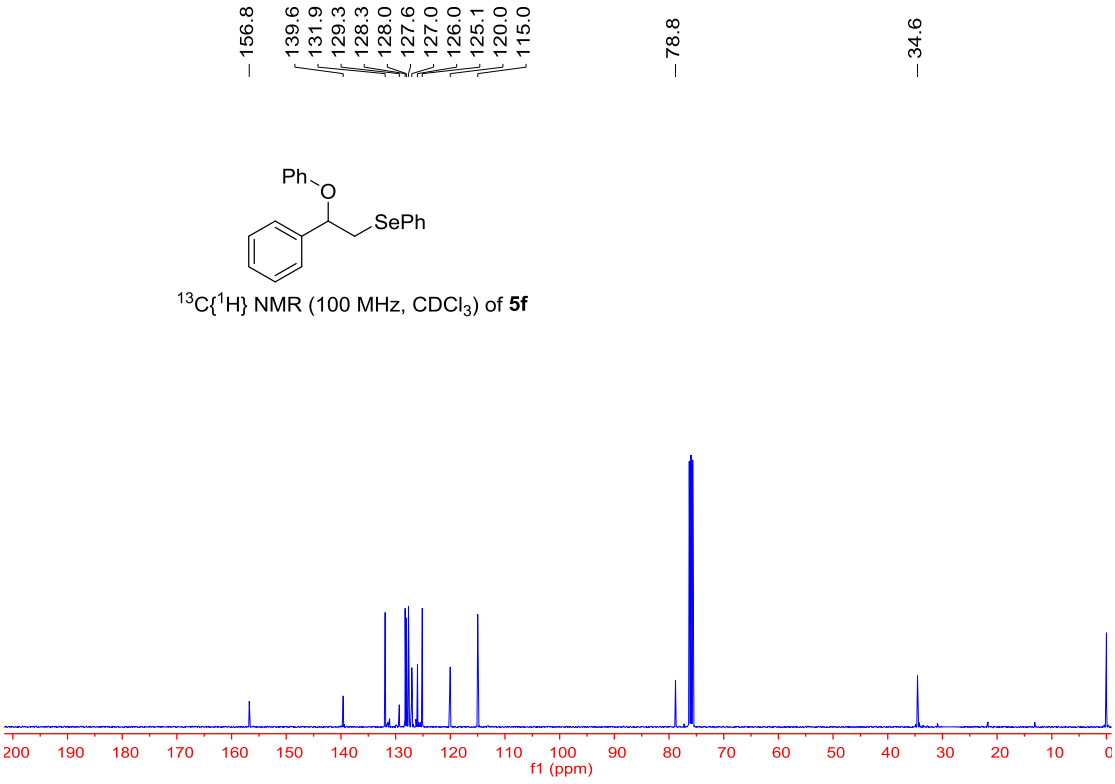
^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) of **5e**



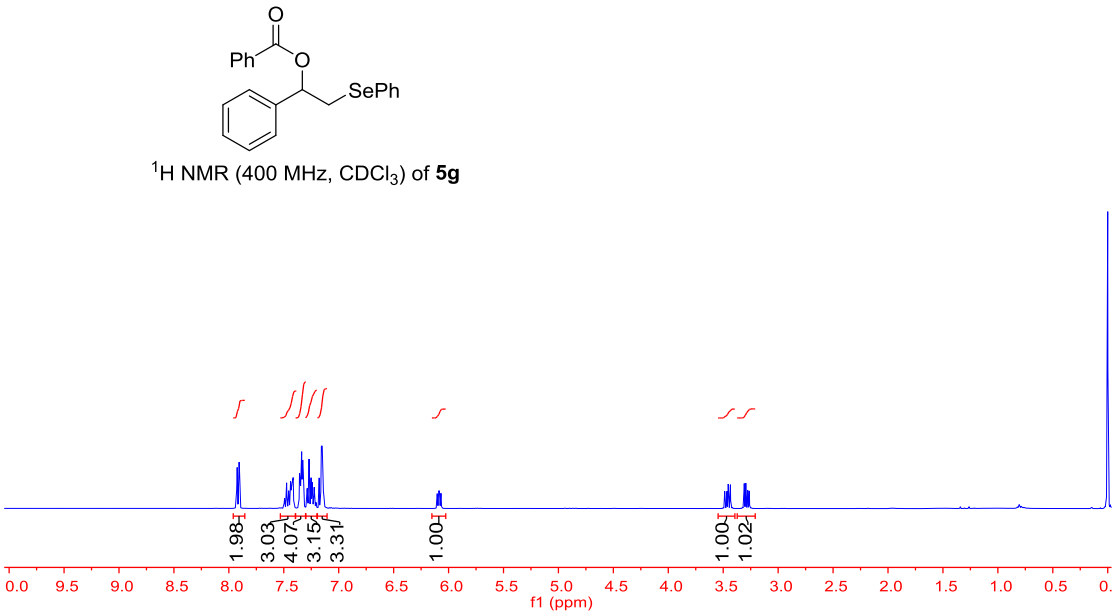
^{19}F NMR (376 MHz, $CDCl_3$) of **5e**



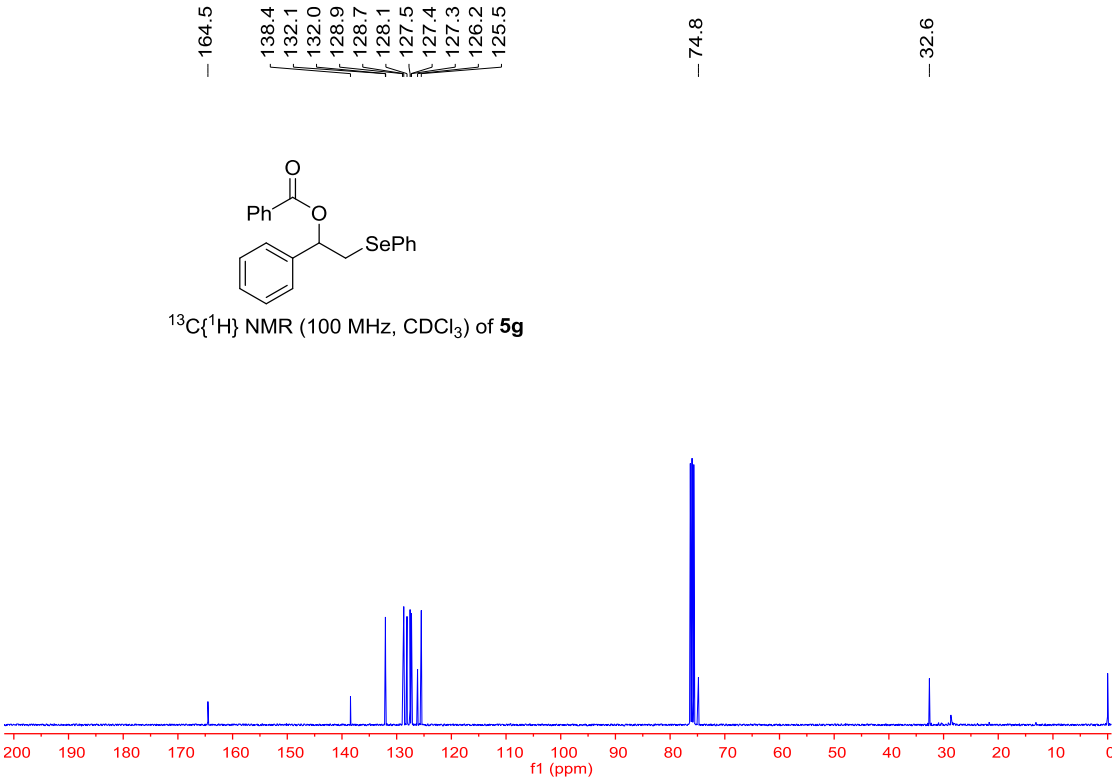
^{1}H NMR (400 MHz, $CDCl_3$) of **5f**



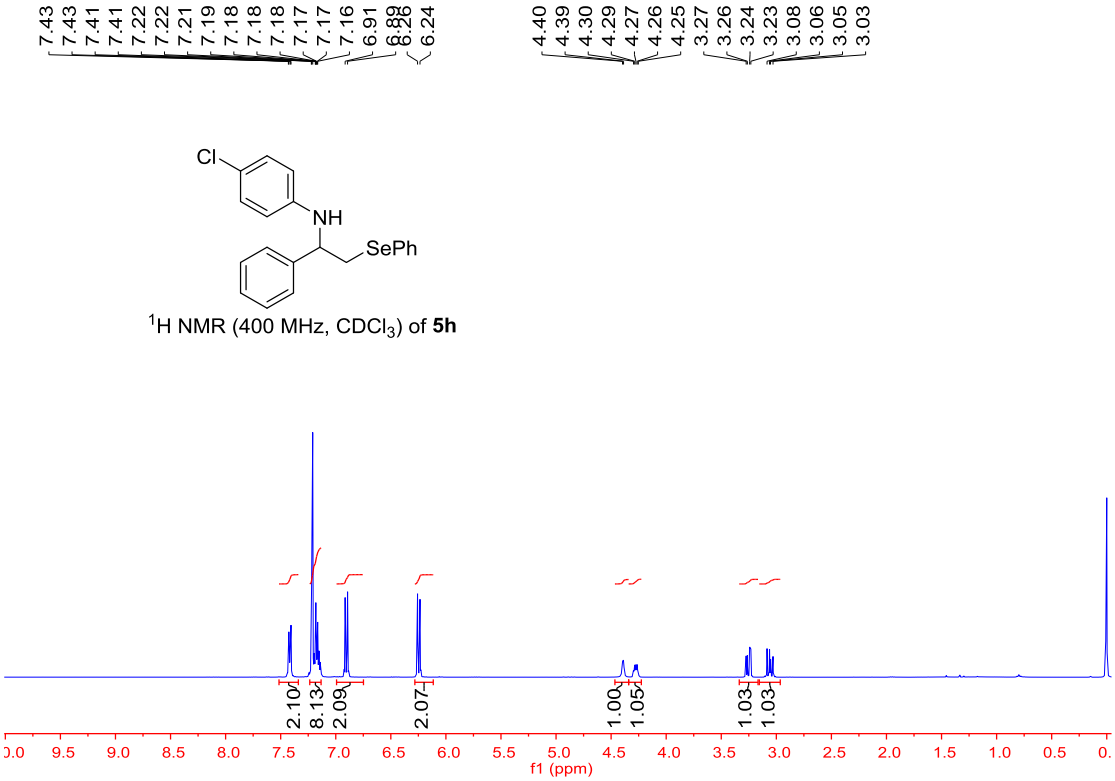
$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) of **5f**



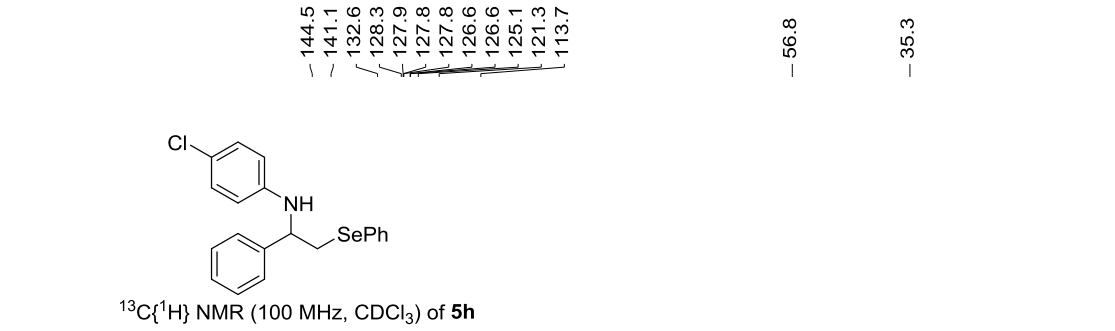
^{1}H NMR (400 MHz, $CDCl_3$) of **5g**



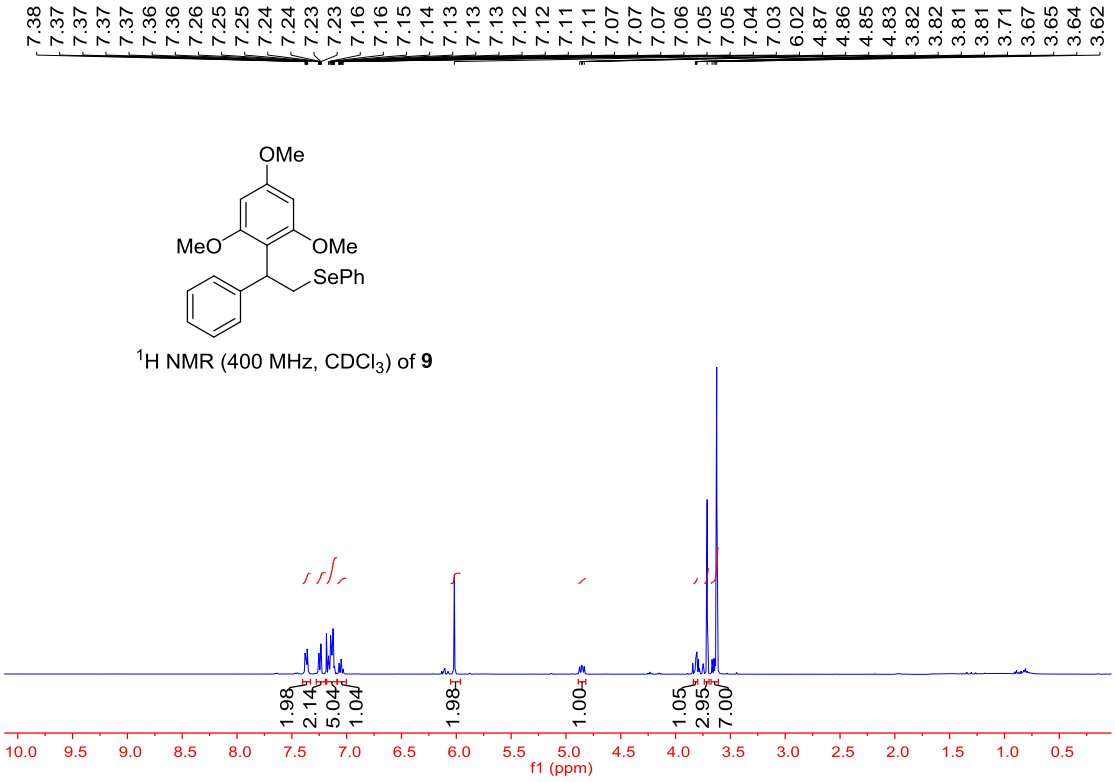
$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) of **5g**



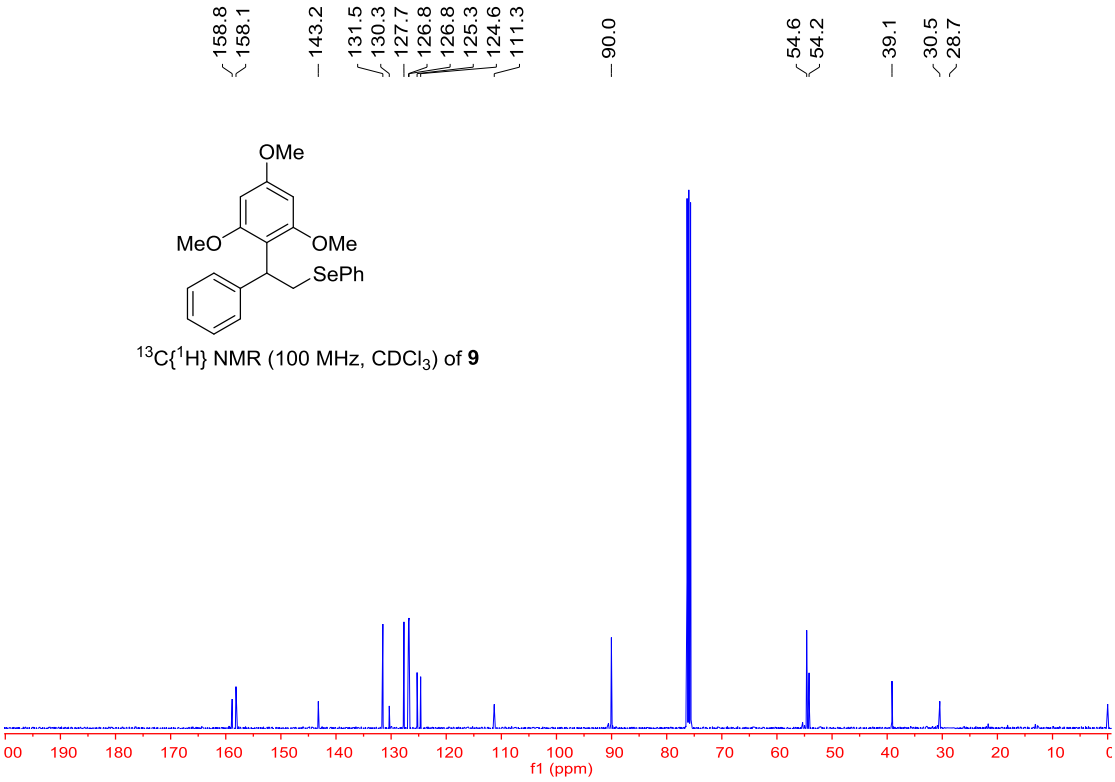
^{1}H NMR (400 MHz, $CDCl_3$) of **5h**



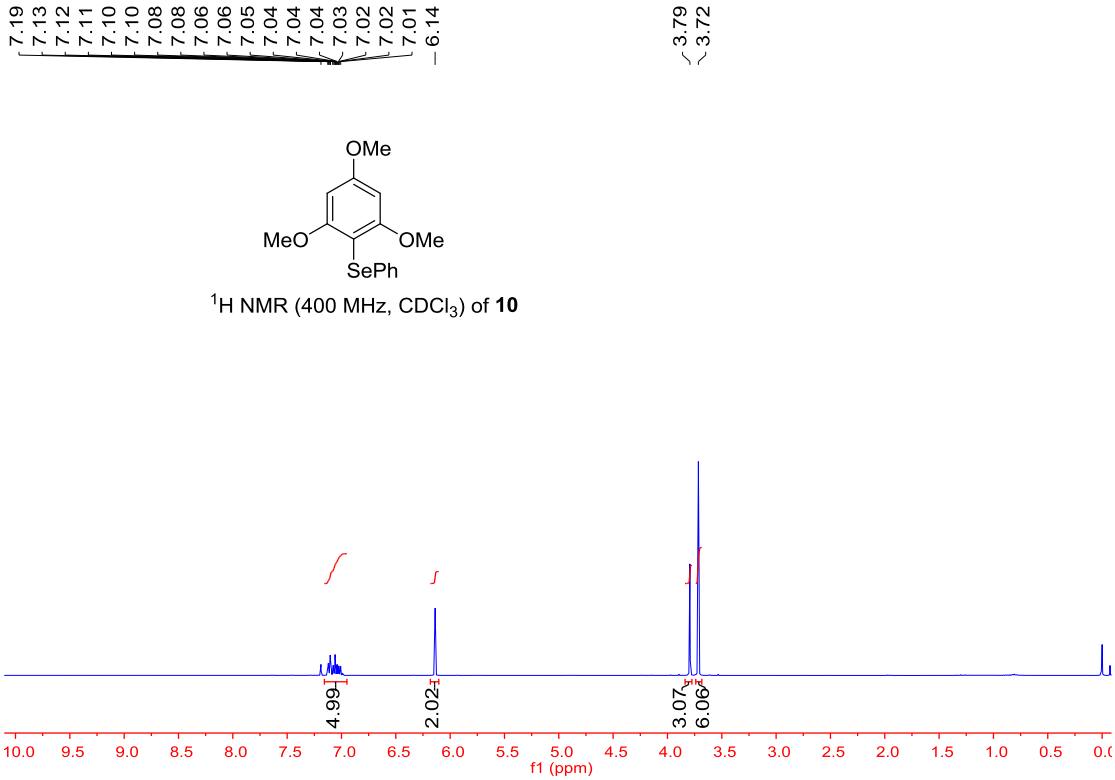
$^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) of **5h**



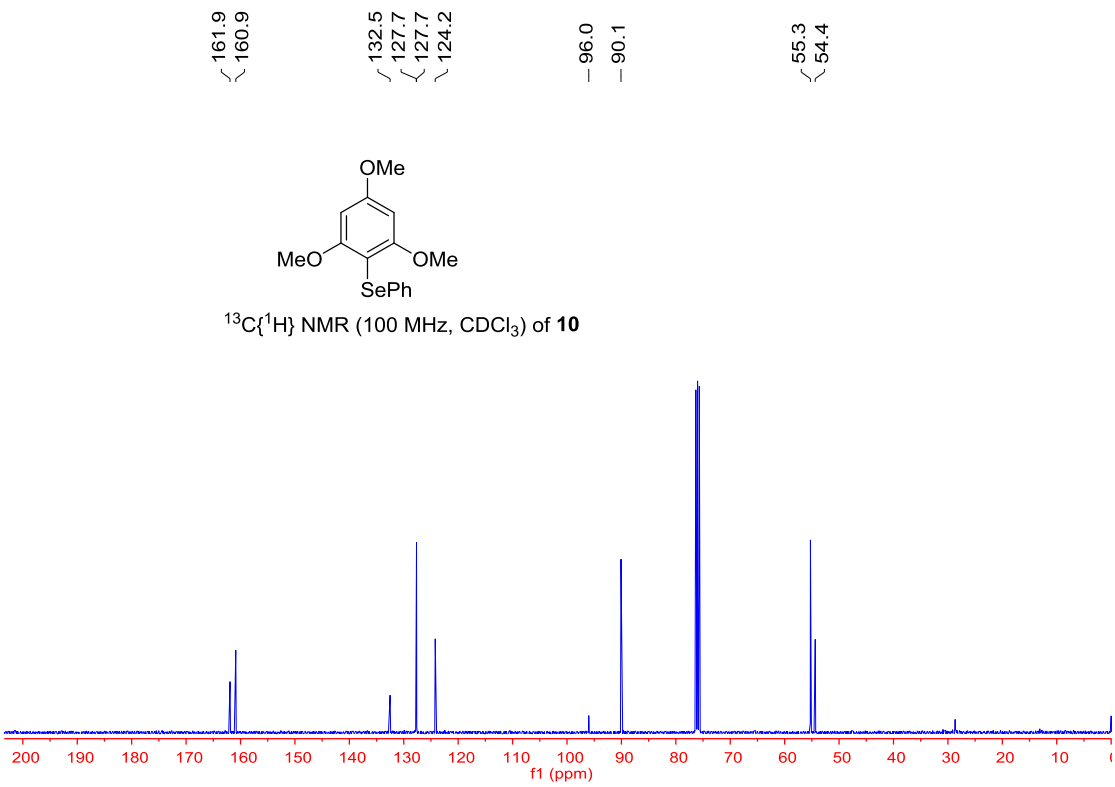
^1H NMR (400 MHz, $CDCl_3$) of **9**



$^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) of **9**



^{1}H NMR (400 MHz, $CDCl_3$) of **10**



3. ORTEP drawing of 3s

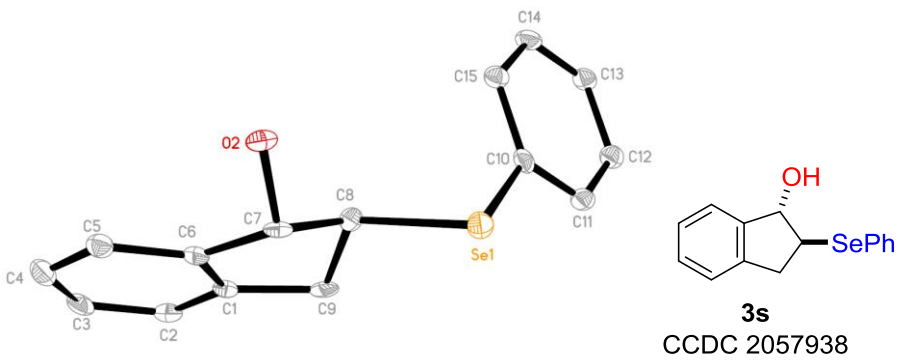


Figure S7. ORTEP drawing of **3s** with the thermal ellipsoids at 30% probability. Hydrogen atoms were omitted for clarity.

The crystal of compound **3s** were obtained by slowly evaporating a mixture of ethyl acetate and *n*-hexane solution (1:5) at ambient temperature. The data were collected at 100 K on a Rigaku Oxford Diffraction Supernova Dual Source, Cu at Zero equipped with an AtlasS2 CCD using Cu Kα radiation. Crystallographic data for the structure reported in this paper have been deposited at the Cambridge Crystallographic Data Center and allocated with the deposition numbers: CCDC 2057938 for compounds **3s**.

Table S1 Crystal data and structure refinement for **3s**.

Empirical formula	$C_{15}H_{14}OSe$

Formula weight	289.22
Temperature/K	100.00(10)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	4.9852(4)
b/Å	27.816(2)
c/Å	18.1283(12)
a/ °	90
ß/ °	96.822(8)
γ/°	90
Volume/$Å^3$	2496.1(3)
Z	8
ρ_{calc}g/cm^3	1.539
μ/mm^{-1}	3.898
F(000)	1168.0
Crystal size/mm^3	0.14 × 0.12 × 0.1
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	5.848 to 147.398
Index ranges	$-4 \leq h \leq 6$, $-23 \leq k \leq 34$, $-20 \leq l \leq 22$
Reflections collected	9797
Independent reflections	4869 [R_{int} = 0.1174, R_{sigma} = 0.0923]
Data/restraints/parameters	4869/0/309
Goodness-of-fit on F^2	1.098
Final R indexes [I>=2σ (I)]	R_1 = 0.0960, wR_2 = 0.2182
Final R indexes [all data]	R_1 = 0.1037, wR_2 = 0.2226
Largest diff. peak/hole / e $Å^{-3}$	1.77/-1.38

Table S2 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **3s**. Ueq is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	**x**	**y**	**z**	**U(eq)**
Se1	10277.2(18)	6947.9(3)	1934.4(5)	25.9(2)
O2	7524(12)	5785(2)	1784(3)	24.0(12)
C1	4251(16)	6472(3)	301(4)	20.8(16)
C2	2083(18)	6486(3)	-252(4)	27.0(18)
C3	906(18)	6053(3)	-496(4)	28.4(19)
C4	1880(20)	5616(3)	-206(5)	30.6(19)
C5	4045(17)	5605(3)	343(4)	24.8(17)
C6	5264(16)	6037(3)	595(4)	20.6(16)
C7	7583(16)	6115(3)	1186(4)	19.9(16)
C8	7074(16)	6638(3)	1411(4)	21.8(16)
C9	5880(17)	6880(3)	685(4)	24.0(17)

C10	8453(17)	7420(3)	2465(4)	24.0(17)
C11	9013(17)	7903(3)	2384(5)	24.9(17)
C12	7809(18)	8247(3)	2788(5)	27.2(18)
C13	5993(17)	8109(3)	3270(4)	25.5(17)
C14	5427(18)	7625(3)	3345(4)	27.2(18)
C15	6629(17)	7282(3)	2954(4)	23.6(16)
Se2	6205.1(18)	5878.3(3)	4047.4(5)	28.0(3)
O1	2748(12)	5603(2)	2310(3)	26.3(13)
C16	1238(16)	4877(3)	2869(4)	20.8(16)
C17	-161(17)	4659(3)	2251(4)	22.9(16)
C18	-2104(18)	4309(3)	2357(5)	26.7(18)
C19	-2530(18)	4177(3)	3068(5)	28.2(18)
C20	-1142(17)	4392(3)	3689(4)	24.3(17)
C21	752(16)	4749(3)	3585(4)	20.9(16)
C22	2450(18)	5058(3)	4146(4)	25.0(17)
C23	3082(16)	5488(3)	3653(4)	20.8(16)
C24	3311(16)	5270(3)	2893(4)	19.6(15)
C25	4339(17)	6346(3)	4582(4)	23.2(16)
C26	2145(17)	6603(3)	4218(4)	23.8(17)
C27	842(18)	6936(3)	4615(5)	26.8(18)
C28	1736(18)	7027(3)	5359(5)	25.6(17)
C29	3978(18)	6785(3)	5713(4)	25.3(17)
C30	5250(18)	6439(3)	5318(5)	26.5(17)

Table S3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for 3s. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	**U11**	**U22**	**U33**	**U23**	**U13**	**U12**
Se1	21.1(5)	29.7(5)	27.8(5)	-5.3(3)	6.7(3)	0.2(3)
O2	23(3)	30(3)	21(3)	8(2)	7(2)	0(2)
C1	21(4)	26(4)	16(4)	0(3)	9(3)	2(3)
C2	31(5)	31(4)	20(4)	5(3)	10(3)	2(4)
C3	31(5)	41(5)	12(4)	0(3)	-1(3)	0(4)
C4	42(5)	29(4)	21(4)	-6(3)	5(4)	0(4)
C5	28(4)	25(4)	23(4)	-1(3)	8(3)	2(3)
C6	23(4)	25(4)	15(4)	-1(3)	8(3)	1(3)
C7	19(4)	27(4)	16(4)	5(3)	10(3)	4(3)
C8	15(4)	28(4)	23(4)	-1(3)	3(3)	-2(3)
C9	24(4)	29(4)	23(4)	2(3)	17(3)	3(3)
C10	22(4)	31(4)	17(4)	-3(3)	-4(3)	-1(3)
C11	19(4)	34(5)	23(4)	-1(3)	5(3)	0(3)
C12	29(5)	27(4)	25(4)	1(3)	2(3)	0(3)
C13	22(4)	33(4)	23(4)	-6(3)	7(3)	2(3)
C14	30(5)	34(5)	19(4)	-1(3)	10(3)	1(4)

C15	23(4)	27(4)	21(4)	3(3)	2(3)	2(3)
Se2	21.4(5)	32.4(5)	31.6(5)	-8.2(4)	9.0(4)	-3.3(3)
O1	25(3)	34(3)	23(3)	11(2)	13(2)	3(2)
C16	21(4)	24(4)	19(4)	0(3)	6(3)	2(3)
C17	28(4)	28(4)	14(3)	-1(3)	8(3)	-1(3)
C18	27(4)	28(4)	26(4)	-7(3)	4(3)	5(3)
C19	25(4)	26(4)	33(5)	2(3)	5(4)	-2(3)
C20	24(4)	30(4)	20(4)	4(3)	7(3)	-1(3)
C21	17(4)	29(4)	17(4)	2(3)	6(3)	4(3)
C22	30(5)	36(5)	10(3)	0(3)	9(3)	-3(4)
C23	15(4)	25(4)	24(4)	-3(3)	8(3)	-3(3)
C24	18(4)	27(4)	14(4)	1(3)	2(3)	1(3)
C25	26(4)	24(4)	21(4)	-1(3)	8(3)	-6(3)
C26	24(4)	29(4)	19(4)	-1(3)	5(3)	-4(3)
C27	31(5)	25(4)	26(4)	2(3)	8(4)	-2(3)
C28	27(5)	28(4)	25(4)	-4(3)	15(3)	-4(3)
C29	31(5)	28(4)	16(4)	-1(3)	1(3)	-5(3)
C30	28(5)	27(4)	24(4)	4(3)	4(3)	-4(3)

Table S4 Bond Lengths for **3s**.

Atom	**Atom**	**Length/Å**
Se1	C8	1.959(8)
Se1	C10	1.920(8)
O2	C7	1.422(9)
C1	C2	1.385(12)
C1	C6	1.392(11)
C1	C9	1.517(11)
C2	C3	1.388(12)
C3	C4	1.388(12)
C4	C5	1.379(12)
C5	C6	1.398(11)
C6	C7	1.497(11)
C7	C8	1.539(11)
C8	C9	1.534(11)
C10	C11	1.382(12)
C10	C15	1.398(11)
C11	C12	1.386(12)
C12	C13	1.385(12)
C13	C14	1.385(12)
C14	C15	1.369(12)

Atom	**Atom**	**Length/Å**
Se2	C23	1.963(8)
Se2	C25	1.926(8)
O1	C24	1.407(9)
C16	C17	1.387(11)
C16	C21	1.394(10)
C16	C24	1.503(11)
C17	C18	1.404(12)
C18	C19	1.380(12)
C19	C20	1.387(12)
C20	C21	1.398(11)
C21	C22	1.512(11)
C22	C23	1.548(11)
C23	C24	1.522(10)
C25	C26	1.404(12)
C25	C30	1.381(11)
C26	C27	1.383(12)
C27	C28	1.392(12)
C28	C29	1.394(12)
C29	C30	1.397(12)

Table S5 Bond Angles for **3S**.

Atom	Atom	Atom	Angle/°
C10	Se1	C8	97.9(3)
C2	C1	C6	121.2(8)
C2	C1	C9	129.8(8)
C6	C1	C9	109.0(7)
C1	C2	C3	118.1(8)
C4	C3	C2	121.5(8)
C5	C4	C3	120.1(8)
C4	C5	C6	119.3(8)
C1	C6	C5	119.9(8)
C1	C6	C7	111.2(7)
C5	C6	C7	128.9(7)
O2	C7	C6	111.6(6)
O2	C7	C8	112.9(6)
C6	C7	C8	100.9(6)
C7	C8	Se1	113.2(5)
C9	C8	Se1	115.7(6)
C9	C8	C7	104.4(6)
C1	C9	C8	101.3(6)
C11	C10	Se1	119.8(6)
C11	C10	C15	119.4(8)
C15	C10	Se1	120.8(6)
C10	C11	C12	120.6(8)
C13	C12	C11	119.9(8)
C14	C13	C12	119.1(8)
C15	C14	C13	121.4(8)
C14	C15	C10	119.5(8)

Atom	Atom	Atom	Angle/°
C25	Se2	C23	98.5(3)
C17	C16	C21	121.0(7)
C17	C16	C24	128.2(7)
C21	C16	C24	110.8(7)
C16	C17	C18	118.8(7)
C19	C18	C17	119.8(8)
C18	C19	C20	121.8(8)
C19	C20	C21	118.4(7)
C16	C21	C20	120.1(7)
C16	C21	C22	109.7(7)
C20	C21	C22	130.2(7)
C21	C22	C23	100.7(6)
C22	C23	Se2	115.1(5)
C24	C23	Se2	114.1(5)
C24	C23	C22	105.0(6)
O1	C24	C16	112.5(6)
O1	C24	C23	112.9(6)
C16	C24	C23	100.9(6)
C26	C25	Se2	120.2(6)
C30	C25	Se2	119.3(7)
C30	C25	C26	120.4(8)
C27	C26	C25	119.0(8)
C26	C27	C28	120.7(8)
C27	C28	C29	120.3(8)
C28	C29	C30	119.0(7)
C25	C30	C29	120.5(8)

Table S6 Torsion Angles for **3s**.

A	B	C	D	Angle/°
Se1	C8	C9	C1	159.7(5)
Se1	C10	C11	C12	-177.1(6)
Se1	C10	C15	C14	177.8(6)
O2	C7	C8	Se1	79.9(7)
O2	C7	C8	C9	-153.5(6)
C1	C2	C3	C4	-0.9(13)
C1	C6	C7	O2	141.6(7)
C1	C6	C7	C8	21.4(8)
C2	C1	C6	C5	-1.5(12)
C2	C1	C6	C7	-179.5(7)
C2	C1	C9	C8	157.8(8)
C2	C3	C4	C5	0.7(13)
C3	C4	C5	C6	-0.9(13)

A	B	C	D	Angle/°
Se2	C23	C24	O1	-78.3(7)
Se2	C23	C24	C16	161.4(5)
Se2	C25	C26	C27	180.0(6)
Se2	C25	C30	C29	178.3(6)
C16	C17	C18	C19	-1.8(12)
C16	C21	C22	C23	20.4(9)
C17	C16	C21	C20	0.9(12)
C17	C16	C21	C22	-177.3(8)
C17	C16	C24	O1	35.2(11)
C17	C16	C24	C23	155.8(8)
C17	C18	C19	C20	1.9(13)
C18	C19	C20	C21	-0.5(13)
C19	C20	C21	C16	-0.9(12)

C4	C5	C6	C1	1.3(12)
C4	C5	C6	C7	178.9(8)
C5	C6	C7	O2	-36.2(11)
C5	C6	C7	C8	-156.4(8)
C6	C1	C2	C3	1.3(12)
C6	C1	C9	C8	-22.0(8)
C6	C7	C8	Se1	-160.9(5)
C6	C7	C8	C9	-34.3(7)
C7	C8	C9	C1	34.6(7)
C9	C1	C2	C3	-178.5(8)
C9	C1	C6	C5	178.3(7)
C9	C1	C6	C7	0.3(9)
C10	C11	C12	C13	-1.0(13)
C11	C10	C15	C14	0.0(12)
C11	C12	C13	C14	0.5(13)
C12	C13	C14	C15	0.3(13)
C13	C14	C15	C10	-0.5(13)
C15	C10	C11	C12	0.8(12)

C19	C20	C21	C22	176.9(8)
C20	C21	C22	C23	-157.5(8)
C21	C16	C17	C18	0.5(12)
C21	C16	C24	O1	-142.9(7)
C21	C16	C24	C23	-22.3(8)
C21	C22	C23	Se2	-160.3(5)
C21	C22	C23	C24	-34.0(8)
C22	C23	C24	O1	154.7(7)
C22	C23	C24	C16	34.4(8)
C24	C16	C17	C18	-177.5(8)
C24	C16	C21	C20	179.2(7)
C24	C16	C21	C22	1.0(9)
C25	C26	C27	C28	2.0(12)
C26	C25	C30	C29	0.9(12)
C26	C27	C28	C29	0.5(13)
C27	C28	C29	C30	-2.3(12)
C28	C29	C30	C25	1.5(12)
C30	C25	C26	C27	-2.7(12)

Table S7 Hydrogen Atom Coordinates (Å$\times10^4$) and Isotropic Displacement Parameters (Å$^2\times10^3$) for **3s**.

Atom	**x**	**y**	**z**	**U(eq)**
H2	9070.09	5732.6	1974.96	36
H2A	1433.63	6776.51	-453.51	32
H3	-567.63	6055.63	-862.43	34
H4	1070.85	5330.8	-382.3	37
H5	4687.96	5313.45	543.26	30
H7	9301.34	6090.23	976.75	24
H8	5671	6633.69	1746.24	26
H9A	4737.29	7150.38	778.46	29
H9B	7285.77	6988.3	396.81	29
H11	10209.1	7996.75	2054.61	30
H12	8218.39	8570.69	2735.35	33
H13	5166.12	8338.45	3540.87	31
H14	4203.08	7532.01	3666.79	33
H15	6234.17	6958.21	3014.3	28
H1	4130.63	5657.99	2121.2	39
H17	180.45	4744.47	1774.78	28
H18	-3100.65	4165.29	1949.23	32
H19	-3783.36	3937.52	3131.51	34
H20	-1462.8	4301.5	4164.86	29
H22A	4083.85	4892.84	4352.71	30
H22B	1444.22	5157.68	4546.33	30

H23	1495.3	5698.35	3602.45	25
H24	5114.56	5132.4	2880.74	24
H26	1577.88	6549.82	3716.89	29
H27	-647.05	7101.1	4383.41	32
H28	832.12	7250.23	5621.39	31
H29	4617.88	6853.52	6204.8	30
H30	6720.79	6269.76	5551.45	32