

# Supporting Information

## Copper(I) Catalyzed Synthesis of Selanyl methylene 4-chromanol and aurone Derivatives

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Osnabrück, Germany

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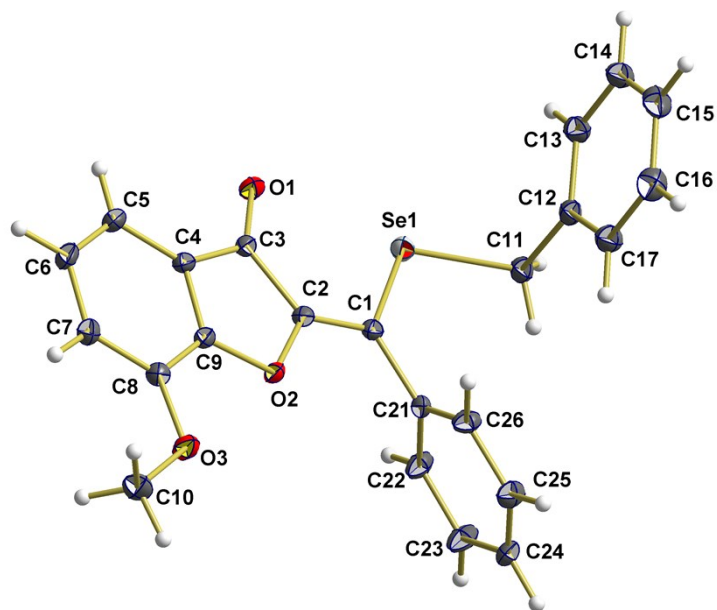
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## Crystallographic Experimental Section

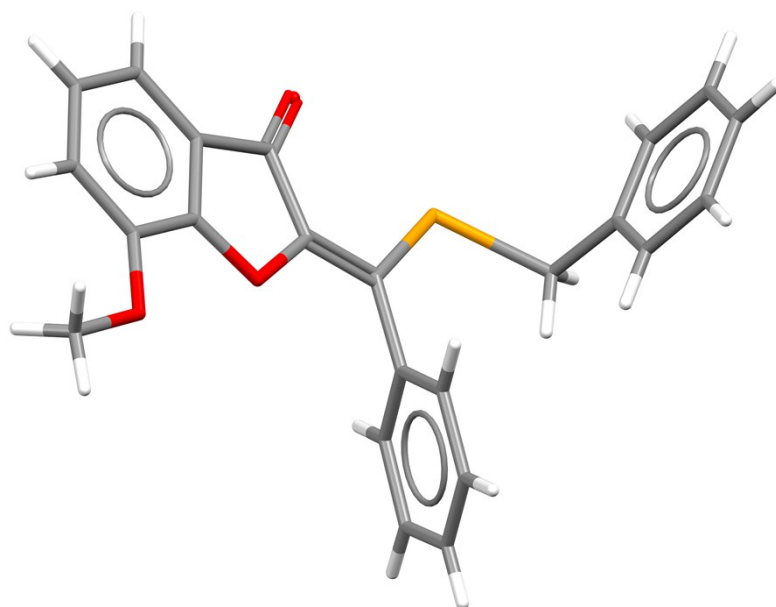
### Sample Preparation for Crystal Growth:

5 mg of **5e** compound was kept in a round bottom (50 mL) flask, soluble in 1:1 (v/v) dry DCM and Hexane 20 mL and the leave the flask in a dark place for 4-5 days at 25 °C. After those 4-5 days, we found needle shape crystal on the wall of the flask. Dry the flask with the help of high vacuum for half an hour and took out the crystal from flask.

ORTEP diagram of **5e**; CCDC 1963733



**Figure S1:** Ball-and-stick model of the solid state structure of **5e**



**Figure S2:** Stick-model of the solid state structure of **5e**

**Table S1.** Crystal data and structure refinement for **5e**.

Empirical formula	C <sub>23</sub> H <sub>18</sub> O <sub>3</sub> Se
Formula weight	421.33
Temperature	150(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P2(1)
Unit cell dimensions	a = 12.2311(4) Å b = 5.5378(2) Å β = 95.773(2)° c = 13.6984(4) Å
Volume	923.13(5) Å <sup>3</sup>
Z, Calculated density	2, 1.516 g/cm <sup>3</sup>
Absorption coefficient	2.055 mm <sup>-1</sup>
F(000)	428
Crystal size	0.486 x 0.132 x 0.064 mm
Theta range for data collection	2.989 to 27.999 deg.
Limiting indices	-16 ≤ h ≤ 16, -7 ≤ k ≤ 7, -18 ≤ l ≤ 18
Reflections collected / unique	87218 / 4465 [R(int) = 0.0504]
Completeness to theta = 25.242	99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.746 and 0.581
Refinement method	Full-matrix least-squares on F <sup>2</sup>
Data / restraints / parameters	4465 / 1 / 249
Goodness-of-fit on F <sup>2</sup>	1.033
Final R indices [I > 2σ(I)]	R1 = 0.0211, wR2 = 0.0487
Final R indices [all data]	R1 = 0.0238, wR2 = 0.0498
Absolute structure parameter	-0.008(3)
Extinction coefficient	n/a
Largest diff. peak and hole	0.242 and -0.210 eÅ <sup>-3</sup>

**Table S2.** Atomic coordinates (x 104) and equivalent isotropic displacement parameters ( $\text{\AA}^2$  x 103) for **5e**.  $U(\text{eq})$  is defined as one third of the trace of the orthogonalized  $U_{ij}$  tensor.

	x	y	z	$U(\text{eq})$
Se(1)	3120(1)	10382(1)	8064(1)	24(1)
C(1)	2529(2)	7977(4)	7164(2)	18(1)
C(2)	1735(2)	6561(4)	7457(2)	18(1)
C(3)	1248(2)	6582(5)	8404(2)	20(1)
O(1)	1480(2)	8007(4)	9076(1)	26(1)
C(4)	460(2)	4598(4)	8324(2)	20(1)
C(5)	-254(2)	3668(5)	8962(2)	24(1)
C(6)	-919(2)	1766(5)	8630(2)	27(1)
C(7)	-878(2)	785(5)	7688(2)	25(1)
C(8)	-166(2)	1710(5)	7050(2)	21(1)
O(3)	-41(2)	915(3)	6127(1)	28(1)
C(9)	494(2)	3639(5)	7393(2)	20(1)
O(2)	1228(1)	4780(3)	6843(1)	20(1)
C(10)	-737(2)	-1007(5)	5752(2)	30(1)
C(11)	4564(2)	10952(4)	7577(2)	24(1)
C(12)	5452(2)	9541(4)	8145(2)	22(1)
C(13)	5814(2)	10208(7)	9108(2)	28(1)
C(14)	6616(2)	8878(6)	9656(2)	33(1)
C(15)	7072(2)	6867(6)	9252(2)	36(1)
C(16)	6735(3)	6212(5)	8291(2)	35(1)
C(17)	5931(2)	7543(5)	7745(2)	29(1)
C(21)	2885(2)	7824(5)	6158(2)	18(1)
C(22)	2583(2)	9629(5)	5481(2)	26(1)
C(23)	2882(2)	9459(5)	4530(2)	31(1)
C(24)	3488(2)	7521(5)	4253(2)	25(1)
C(25)	3807(2)	5749(5)	4929(2)	27(1)
C(26)	3494(2)	5885(4)	5878(2)	24(1)

**Table S3.** Bond lengths [ $\text{\AA}$ ] and angles [ $^\circ$ ] for **5e**.

Se(1)-C(1)	1.907(2)
Se(1)-C(11)	1.976(2)
C(1)-C(2)	1.340(3)
C(1)-C(21)	1.488(3)
C(2)-O(2)	1.400(3)
C(2)-C(3)	1.481(3)
C(3)-O(1)	1.225(3)
C(3)-C(4)	1.458(3)
C(4)-C(9)	1.386(3)
C(4)-C(5)	1.395(3)

C(5)-C(6)	1.380(4)
C(6)-C(7)	1.406(4)
C(7)-C(8)	1.391(4)
C(8)-O(3)	1.363(3)
C(8)-C(9)	1.392(3)
O(3)-C(10)	1.425(3)
C(9)-O(2)	1.381(3)
C(11)-C(12)	1.492(3)
C(12)-C(17)	1.390(4)
C(12)-C(13)	1.398(3)
C(13)-C(14)	1.385(4)
C(14)-C(15)	1.386(5)
C(15)-C(16)	1.388(4)
C(16)-C(17)	1.386(4)
C(21)-C(26)	1.383(3)
C(21)-C(22)	1.388(3)
C(22)-C(23)	1.391(4)
C(23)-C(24)	1.380(4)
C(24)-C(25)	1.379(4)
C(25)-C(26)	1.393(3)
C(1)-Se(1)-C(11)	100.8(1)
C(2)-C(1)-C(21)	122.1(2)
C(2)-C(1)-Se(1)	117.0(2)
C(21)-C(1)-Se(1)	120.7(2)
C(1)-C(2)-O(2)	121.6(2)
C(1)-C(2)-C(3)	128.7(2)
O(2)-C(2)-C(3)	109.7(2)
O(1)-C(3)-C(4)	130.0(2)
O(1)-C(3)-C(2)	125.5(2)
C(4)-C(3)-C(2)	104.5(2)
C(9)-C(4)-C(5)	120.9(2)
C(9)-C(4)-C(3)	106.1(2)
C(5)-C(4)-C(3)	133.0(2)
C(6)-C(5)-C(4)	117.4(2)
C(5)-C(6)-C(7)	121.6(2)
C(8)-C(7)-C(6)	121.0(2)
O(3)-C(8)-C(7)	126.8(2)
O(3)-C(8)-C(9)	116.5(2)
C(7)-C(8)-C(9)	116.7(2)
C(8)-O(3)-C(10)	117.2(2)
O(2)-C(9)-C(4)	114.0(2)
O(2)-C(9)-C(8)	123.6(2)
C(4)-C(9)-C(8)	122.3(2)
C(9)-O(2)-C(2)	105.6(2)
C(12)-C(11)-Se(1)	111.7(2)
C(17)-C(12)-C(13)	118.5(3)
C(17)-C(12)-C(11)	121.6(2)
C(13)-C(12)-C(11)	119.9(2)
C(14)-C(13)-C(12)	120.7(3)
C(13)-C(14)-C(15)	120.2(3)

C(14)-C(15)-C(16)	119.7(3)
C(17)-C(16)-C(15)	120.0(3)
C(16)-C(17)-C(12)	121.0(3)
C(26)-C(21)-C(22)	119.2(2)
C(26)-C(21)-C(1)	121.1(2)
C(22)-C(21)-C(1)	119.7(2)
C(21)-C(22)-C(23)	120.0(2)
C(24)-C(23)-C(22)	120.6(2)
C(25)-C(24)-C(23)	119.5(2)
C(24)-C(25)-C(26)	120.2(2)
C(21)-C(26)-C(25)	120.5(2)

**Table S4.** Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for **5e**. The anisotropic displacement factor exponent takes the form:  $-2\pi^2[h^2a^*2U_{11} + \dots + 2hka^*b^*U_{12}]$

	U11	U22	U33	U23	U13	U12
Se(1)	21(1)	29(1)	23(1)	-7(1)	3(1)	-3(1)
C(1)	18(1)	21(1)	15(1)	1(1)	1(1)	2(1)
C(2)	18(1)	22(1)	15(1)	-1(1)	1(1)	1(1)
C(3)	17(1)	26(1)	15(1)	1(1)	3(1)	3(1)
O(1)	25(1)	34(1)	19(1)	-6(1)	5(1)	-3(1)
C(4)	19(1)	26(1)	15(1)	2(1)	2(1)	1(1)
C(5)	23(1)	33(1)	17(1)	1(1)	6(1)	0(1)
C(6)	23(1)	33(1)	25(1)	5(1)	9(1)	-3(1)
C(7)	21(1)	29(2)	25(1)	2(1)	3(1)	-4(1)
C(8)	20(1)	25(1)	19(1)	0(1)	2(1)	0(1)
O(3)	30(1)	33(1)	21(1)	-7(1)	7(1)	-10(1)
C(9)	17(1)	25(1)	17(1)	3(1)	4(1)	1(1)
O(2)	20(1)	25(1)	15(1)	-1(1)	6(1)	-5(1)
C(10)	32(2)	28(1)	28(1)	-7(1)	1(1)	-6(1)
C(11)	21(1)	25(2)	25(1)	6(1)	2(1)	-5(1)
C(12)	20(1)	23(1)	24(1)	6(1)	2(1)	-5(1)
C(13)	27(1)	29(1)	26(1)	2(1)	0(1)	-6(2)
C(14)	28(1)	43(2)	26(1)	8(1)	-3(1)	-6(1)
C(15)	27(2)	41(2)	40(2)	18(1)	-1(1)	2(1)
C(16)	35(2)	31(2)	40(2)	7(1)	7(1)	8(1)
C(17)	29(1)	30(1)	28(1)	2(1)	1(1)	-2(1)
C(21)	15(1)	21(1)	17(1)	0(1)	2(1)	-2(1)
C(22)	30(1)	27(1)	24(1)	5(1)	10(1)	9(1)
C(23)	39(2)	31(1)	25(1)	11(1)	10(1)	10(1)
C(24)	23(1)	35(2)	20(1)	0(1)	8(1)	1(1)
C(25)	29(1)	26(2)	25(1)	-3(1)	5(1)	9(1)
C(26)	29(1)	24(2)	20(1)	3(1)	2(1)	5(1)

**Table S5.** Hydrogen coordinates (x 104) and isotropic displacement parameters ( $\text{\AA}^2 \times 103$ ) for **5e**.

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	x	y	z	U(eq)
H(5)	-281	4320	9601	26(5)
H(6)	-1417	1105	9048	26(5)
H(7)	-1344	-532	7483	26(5)
H(10A)	-601	-2435	6169	46(6)
H(10B)	-579	-1391	5082	46(6)
H(10C)	-1507	-515	5748	46(6)
H(11A)	4526	10489	6876	37(3)
H(11B)	4742	12694	7627	37(3)
H(13)	5506	11586	9390	37(3)
H(14)	6854	9346	10310	37(3)
H(15)	7614	5941	9631	37(3)
H(16)	7055	4852	8007	37(3)
H(17)	5703	7083	7087	37(3)
H(22)	2173	10981	5667	37(4)
H(23)	2665	10689	4067	37(4)
H(24)	3685	7409	3601	37(4)
H(25)	4241	4431	4748	37(4)
H(26)	3701	4637	6336	37(4)

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**Table S6.** Torsion angles [ $^\circ$ ] for **5e**.

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C(21)-C(1)-C(2)-O(2)	2.8(4)
Se(1)-C(1)-C(2)-O(2)	178.4(2)
C(21)-C(1)-C(2)-C(3)	-176.3(2)
Se(1)-C(1)-C(2)-C(3)	-0.6(4)
C(1)-C(2)-C(3)-O(1)	2.7(4)
O(2)-C(2)-C(3)-O(1)	-176.4(2)
C(1)-C(2)-C(3)-C(4)	-177.8(2)
O(2)-C(2)-C(3)-C(4)	3.1(3)
O(1)-C(3)-C(4)-C(9)	177.5(3)
C(2)-C(3)-C(4)-C(9)	-1.9(3)
O(1)-C(3)-C(4)-C(5)	-1.0(5)
C(2)-C(3)-C(4)-C(5)	179.6(3)
C(9)-C(4)-C(5)-C(6)	0.1(4)
C(3)-C(4)-C(5)-C(6)	178.4(3)
C(4)-C(5)-C(6)-C(7)	0.4(4)
C(5)-C(6)-C(7)-C(8)	-0.4(4)
C(6)-C(7)-C(8)-O(3)	179.5(2)
C(6)-C(7)-C(8)-C(9)	-0.1(4)

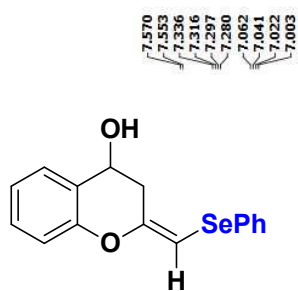


C(7)-C(8)-O(3)-C(10)	2.5(4)
C(9)-C(8)-O(3)-C(10)	-178.0(2)
C(5)-C(4)-C(9)-O(2)	178.9(2)
C(3)-C(4)-C(9)-O(2)	0.2(3)
C(5)-C(4)-C(9)-C(8)	-0.6(4)
C(3)-C(4)-C(9)-C(8)	-179.3(2)
O(3)-C(8)-C(9)-O(2)	1.6(4)
C(7)-C(8)-C(9)-O(2)	-178.8(2)
O(3)-C(8)-C(9)-C(4)	-179.0(2)
C(7)-C(8)-C(9)-C(4)	0.5(4)
C(4)-C(9)-O(2)-C(2)	1.8(3)
C(8)-C(9)-O(2)-C(2)	-178.8(2)
C(1)-C(2)-O(2)-C(9)	177.9(2)
C(3)-C(2)-O(2)-C(9)	-3.0(2)
Se(1)-C(11)-C(12)-C(17)	107.6(2)
Se(1)-C(11)-C(12)-C(13)	-71.8(3)
C(17)-C(12)-C(13)-C(14)	-1.2(4)
C(11)-C(12)-C(13)-C(14)	178.2(2)
C(12)-C(13)-C(14)-C(15)	0.2(4)
C(13)-C(14)-C(15)-C(16)	1.0(5)
C(14)-C(15)-C(16)-C(17)	-1.1(5)
C(15)-C(16)-C(17)-C(12)	0.1(5)
C(13)-C(12)-C(17)-C(16)	1.1(4)
C(11)-C(12)-C(17)-C(16)	-178.3(3)
C(2)-C(1)-C(21)-C(26)	-72.3(3)
Se(1)-C(1)-C(21)-C(26)	112.2(2)
C(2)-C(1)-C(21)-C(22)	106.3(3)
Se(1)-C(1)-C(21)-C(22)	-69.2(3)
C(26)-C(21)-C(22)-C(23)	0.8(4)
C(1)-C(21)-C(22)-C(23)	-177.9(3)
C(21)-C(22)-C(23)-C(24)	-0.8(5)
C(22)-C(23)-C(24)-C(25)	-0.4(5)
C(23)-C(24)-C(25)-C(26)	1.6(4)
C(22)-C(21)-C(26)-C(25)	0.3(4)
C(1)-C(21)-C(26)-C(25)	179.0(2)
C(24)-C(25)-C(26)-C(21)	-1.6(4)

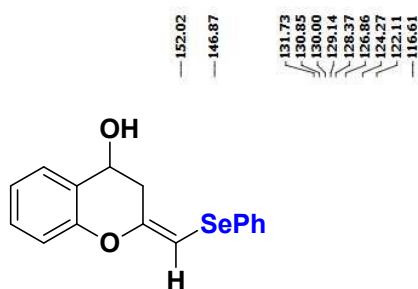
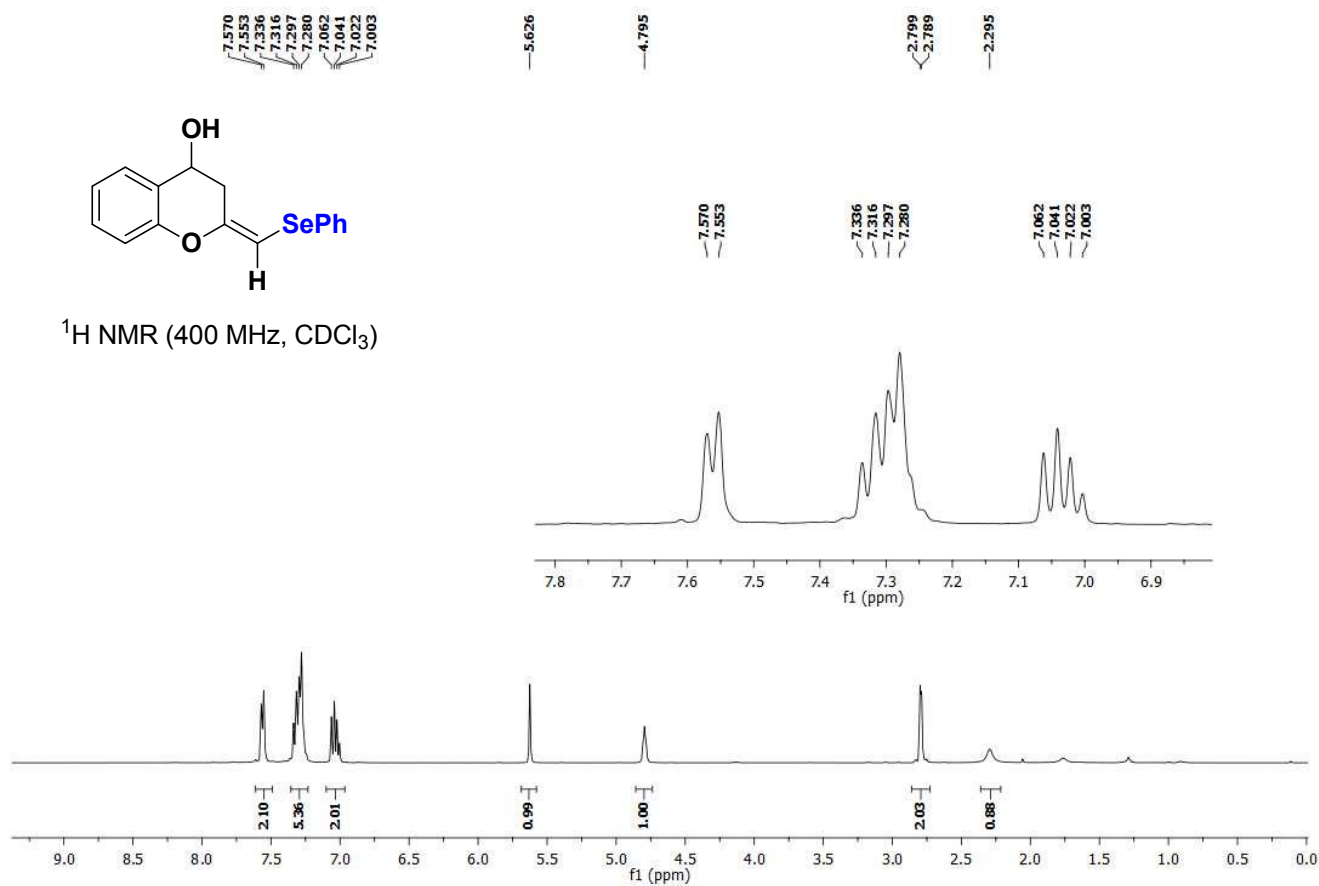
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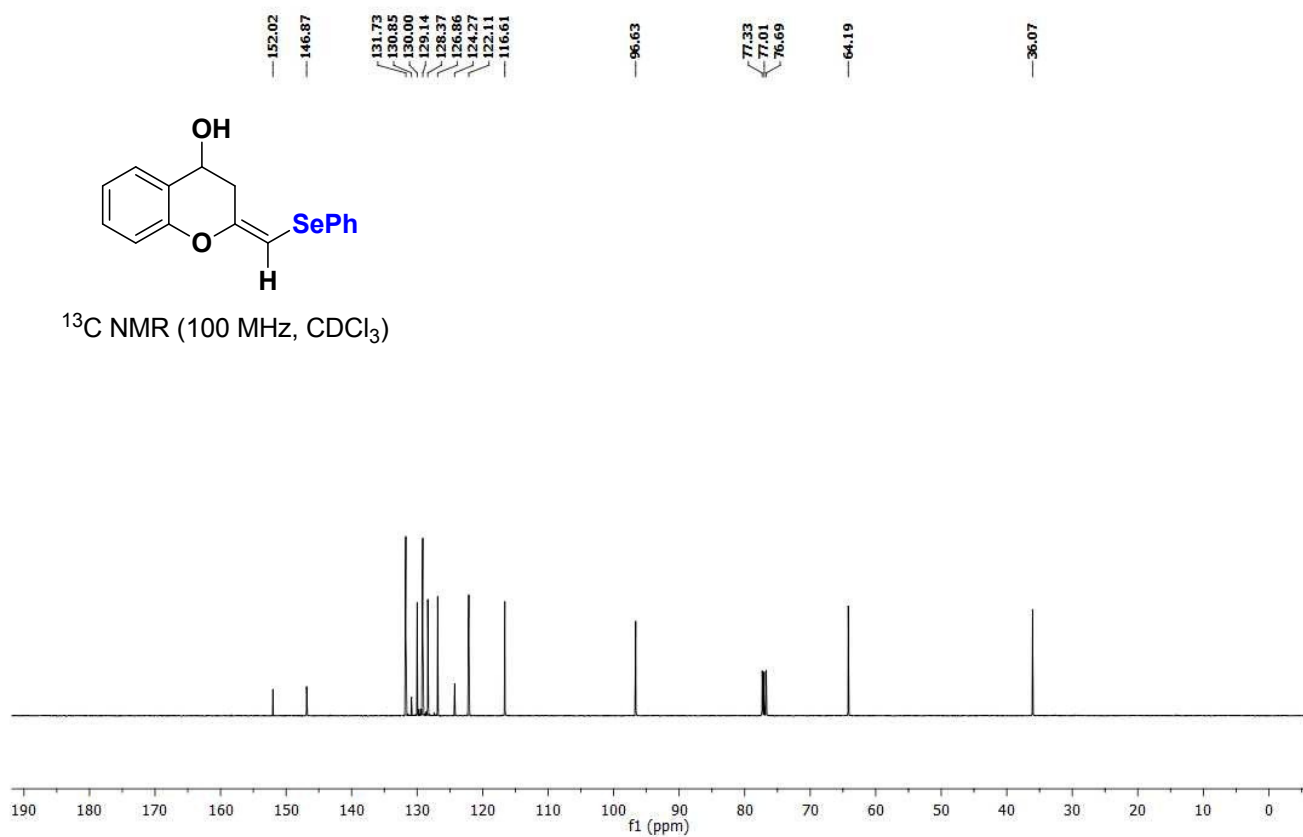
## (E)-2-((phenylselanyl)methylene)chroman-4-ol (4a)



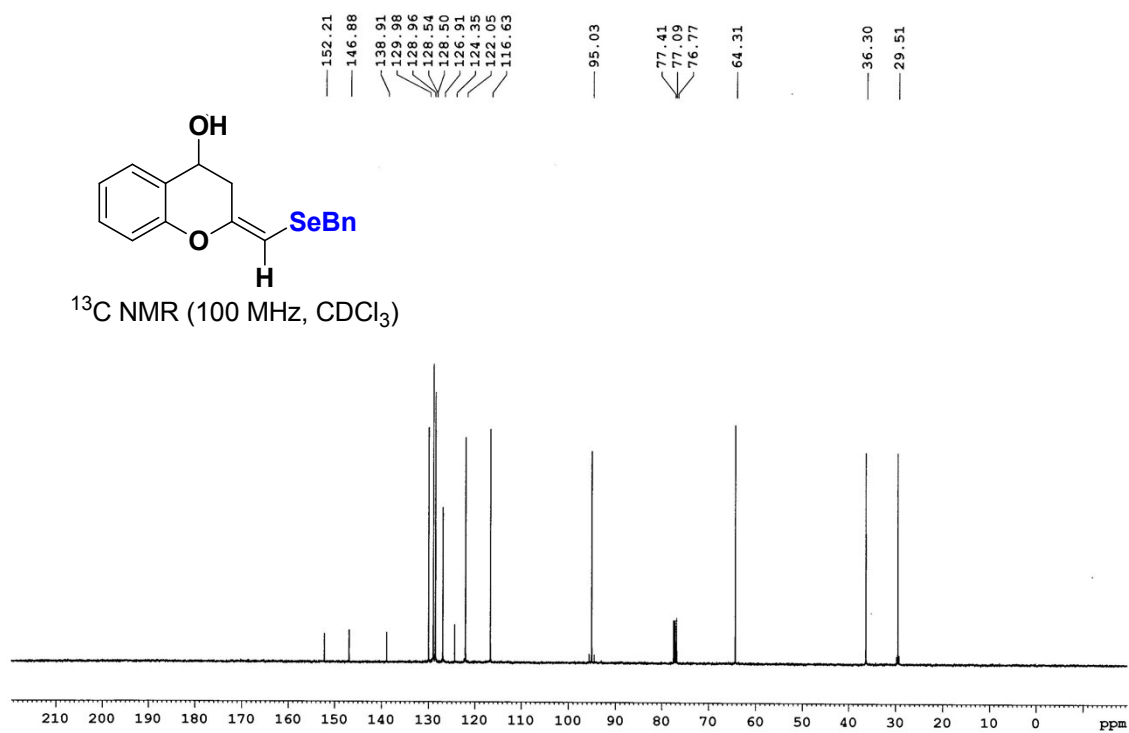
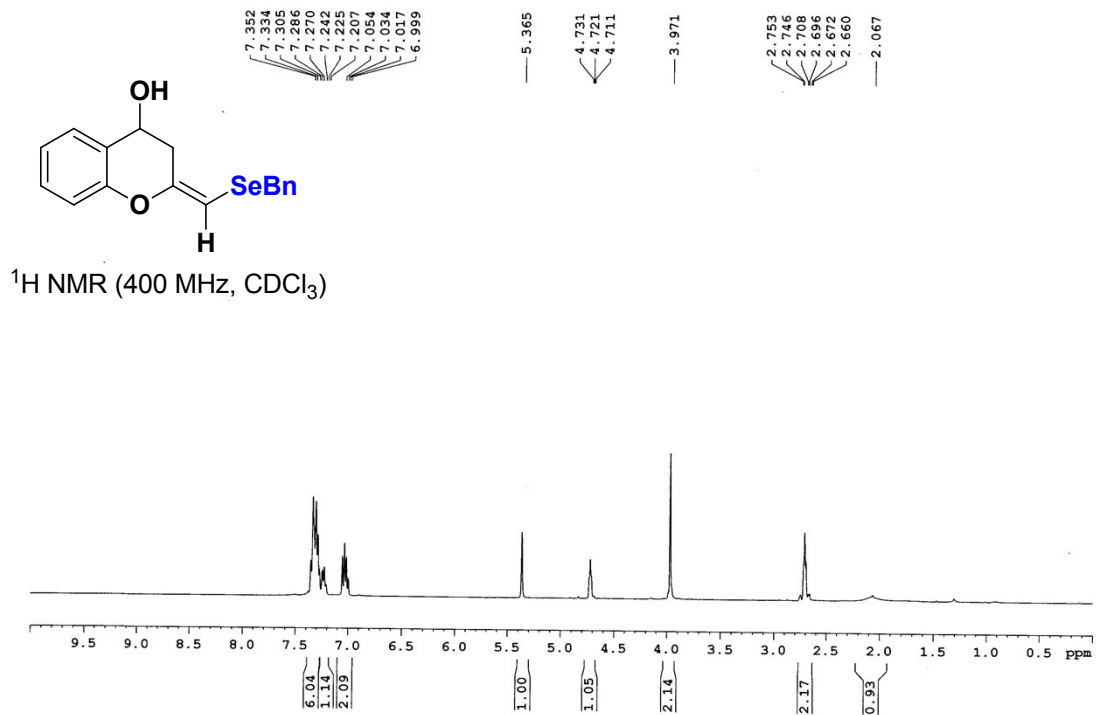
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )



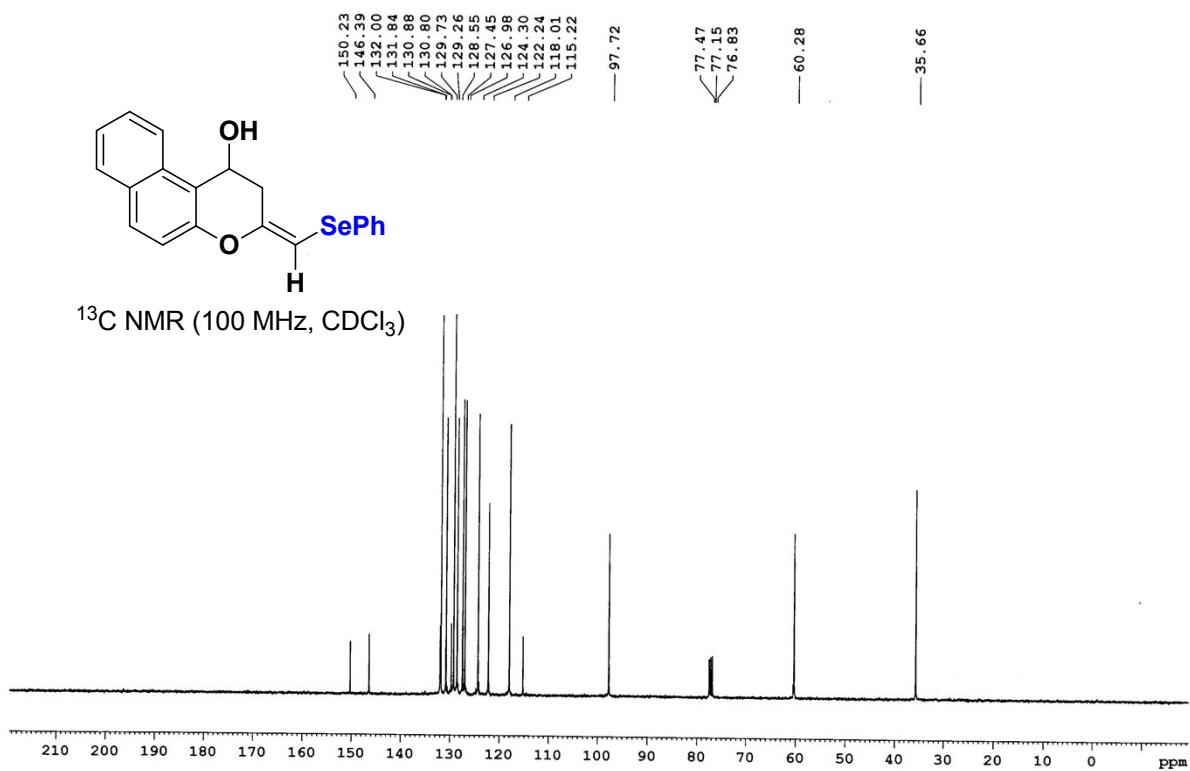
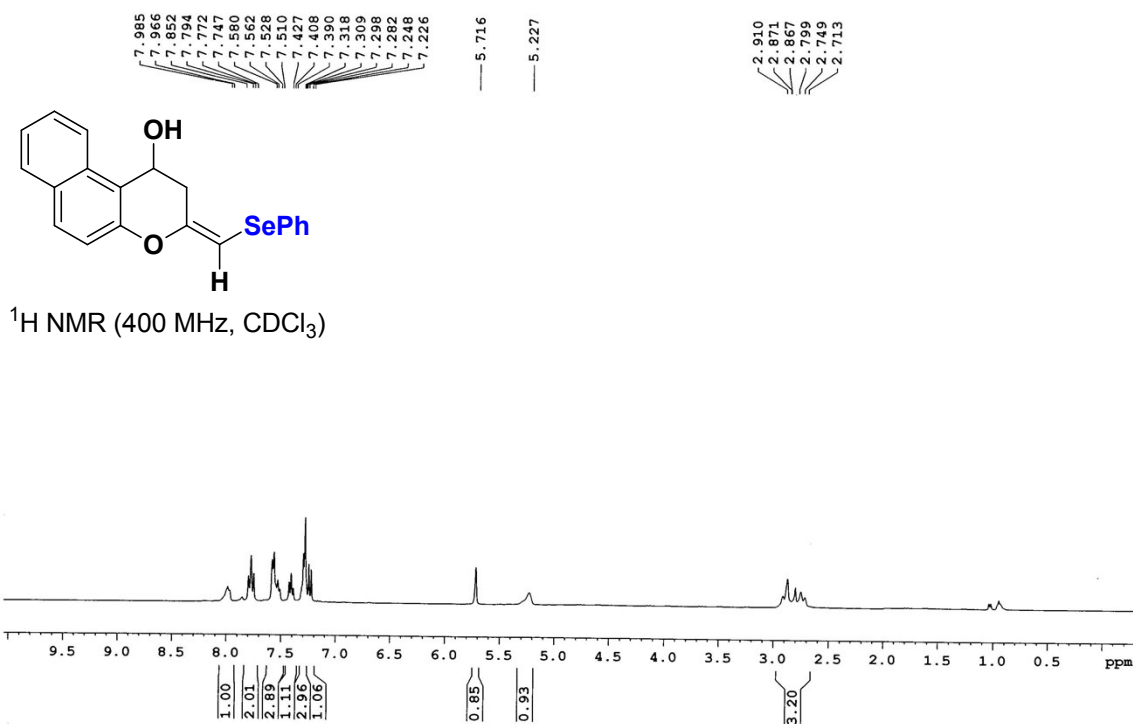
$^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )



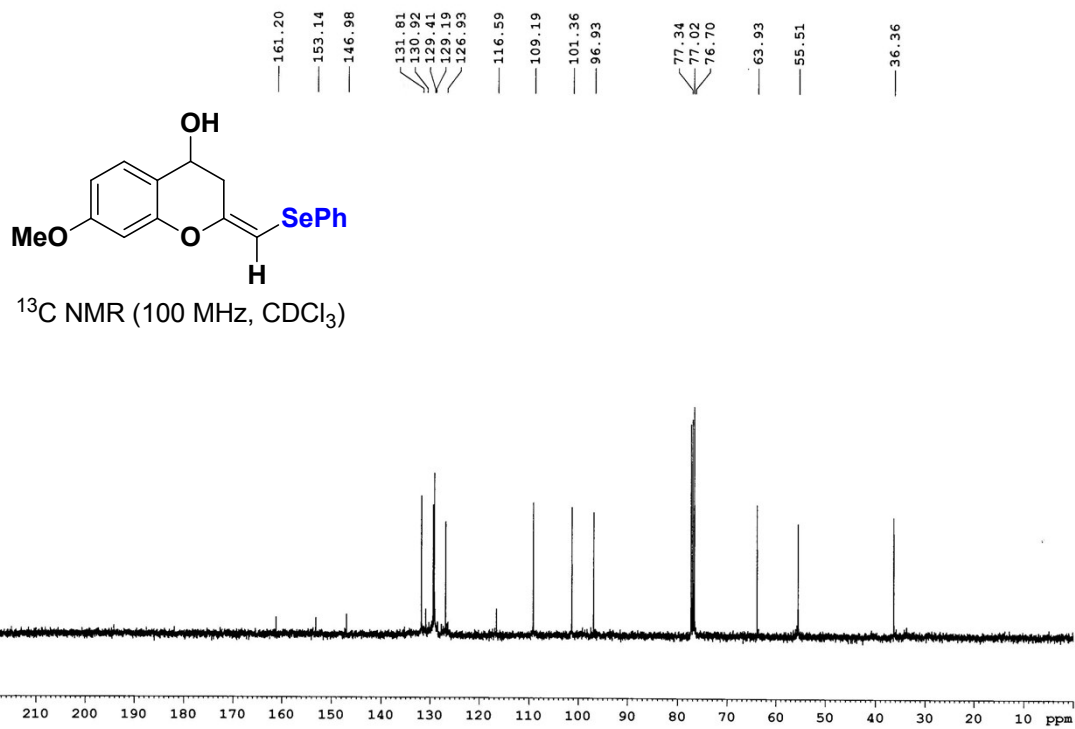
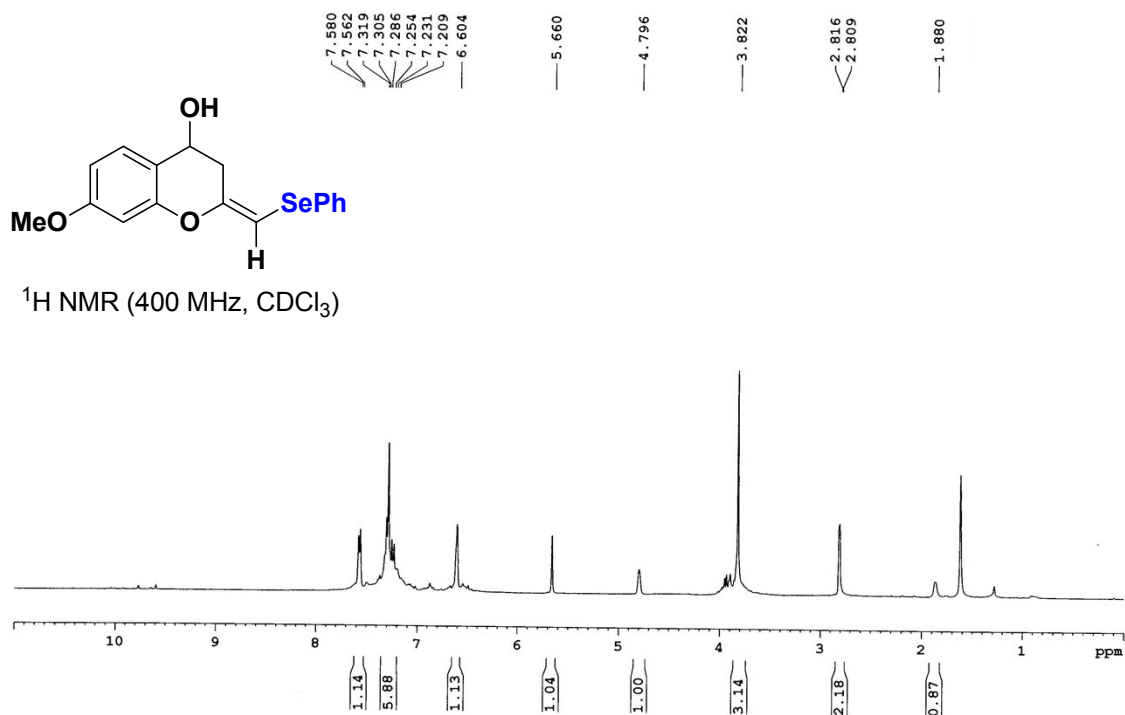
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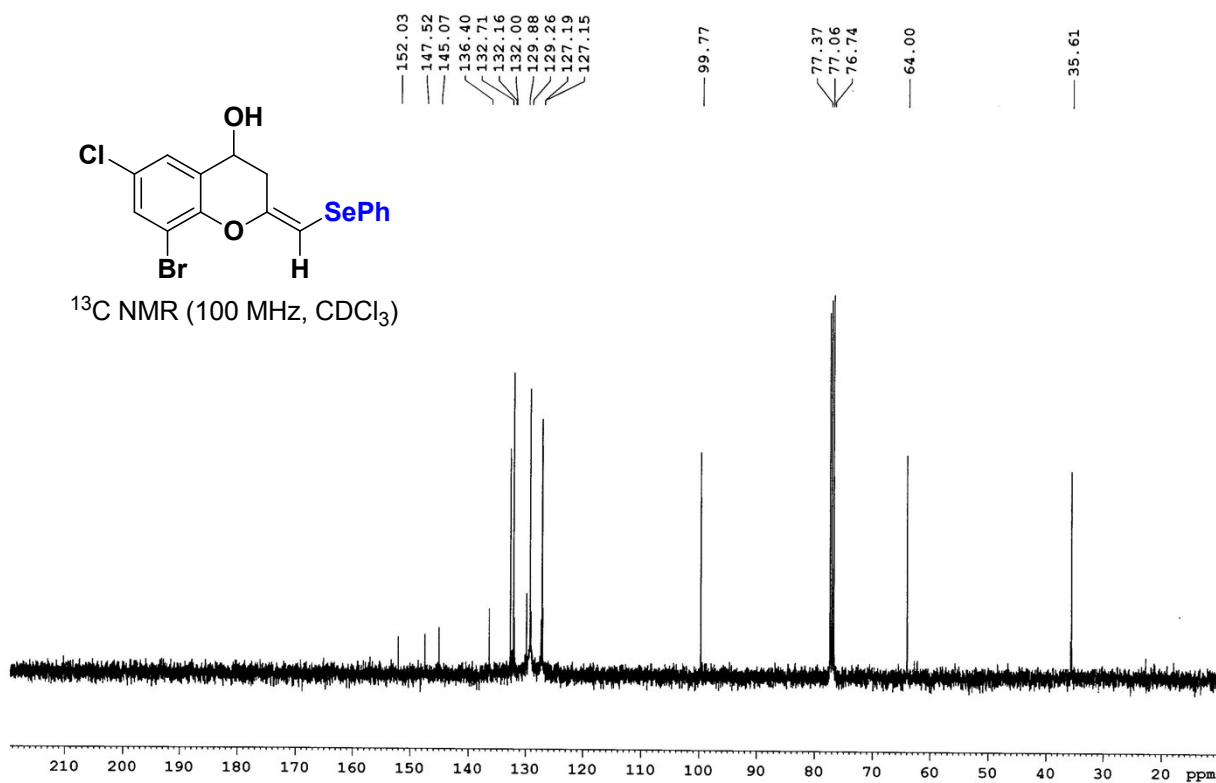
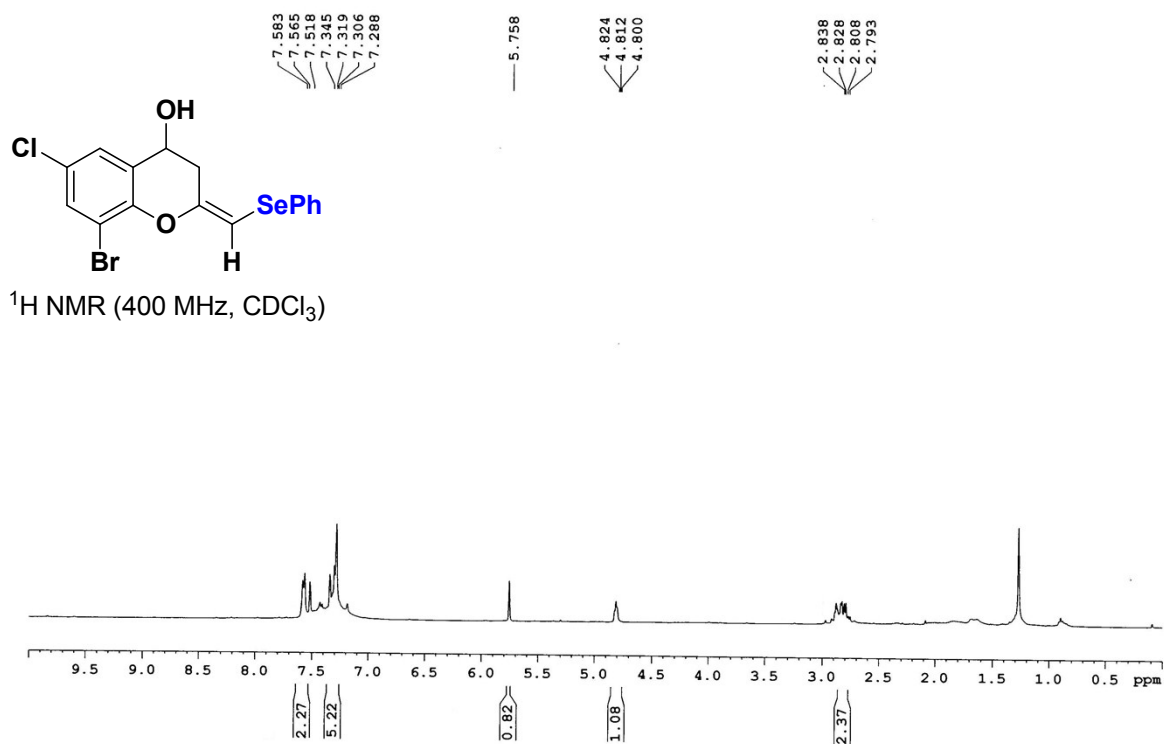
*(E)*-3-((phenylselanyl)methylene)-2,3-dihydro-1H-benzo[*f*]chromen-1-ol (**4c**)



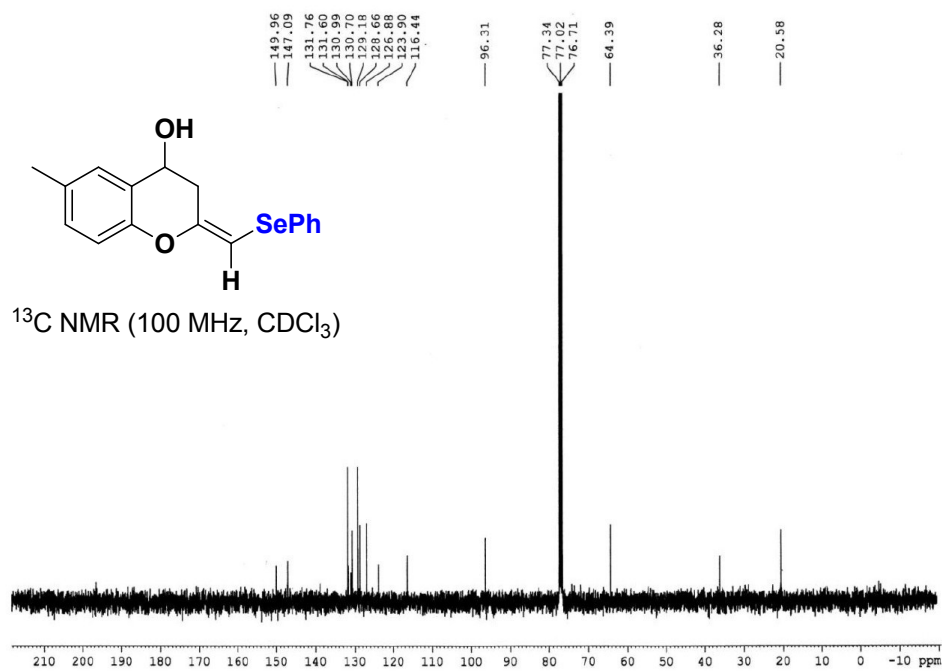
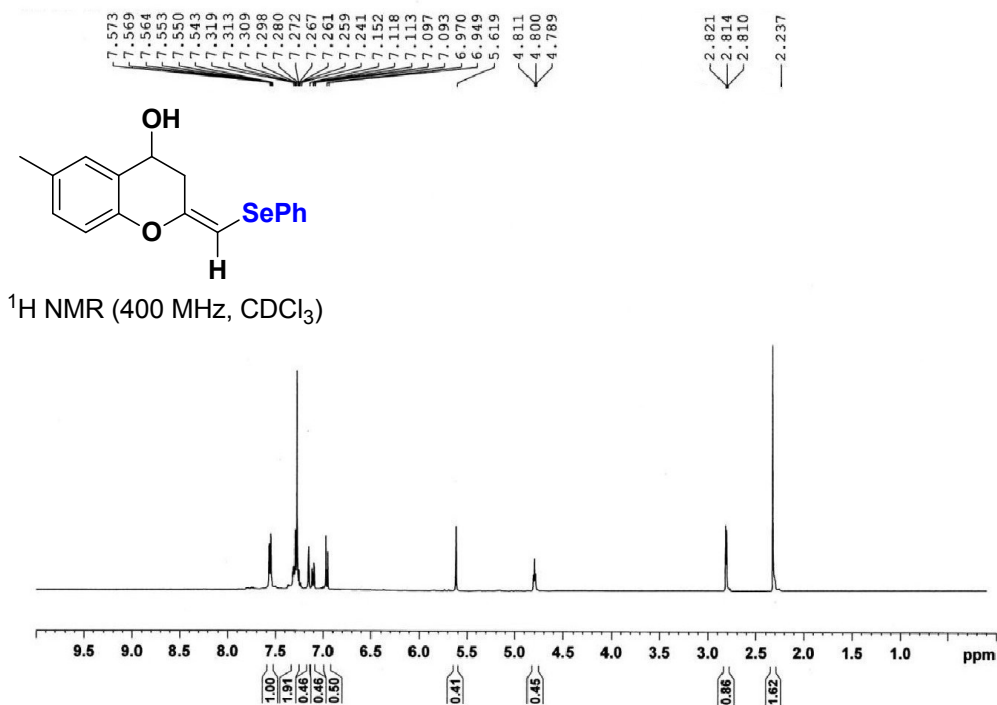
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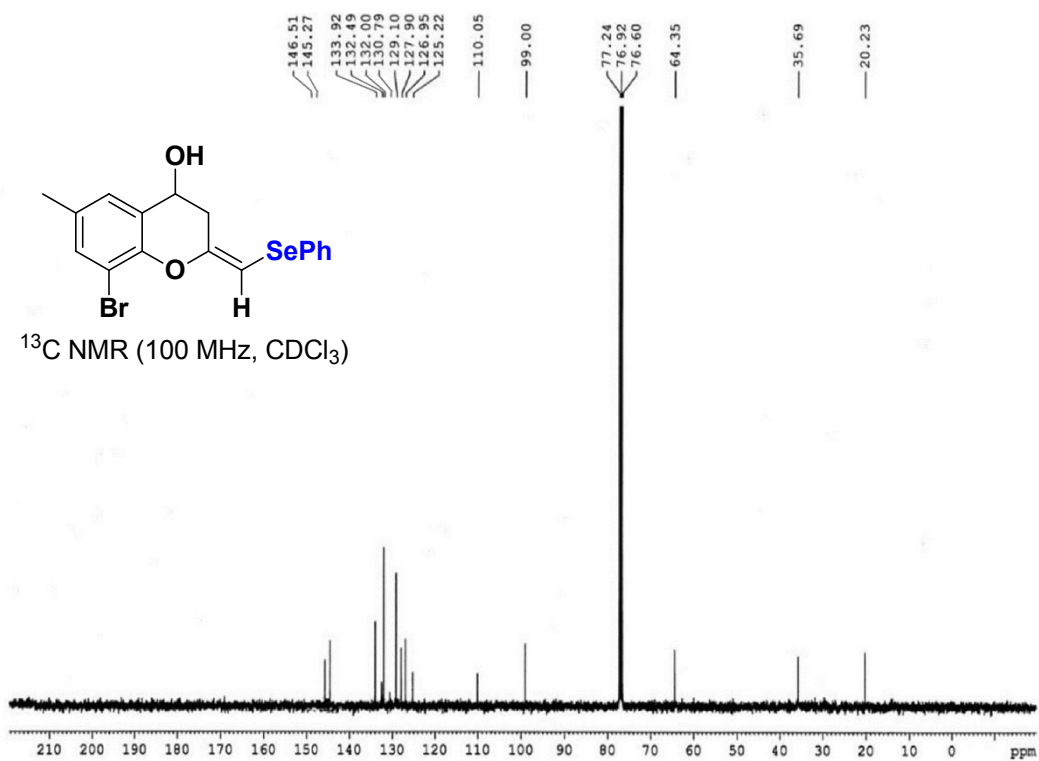
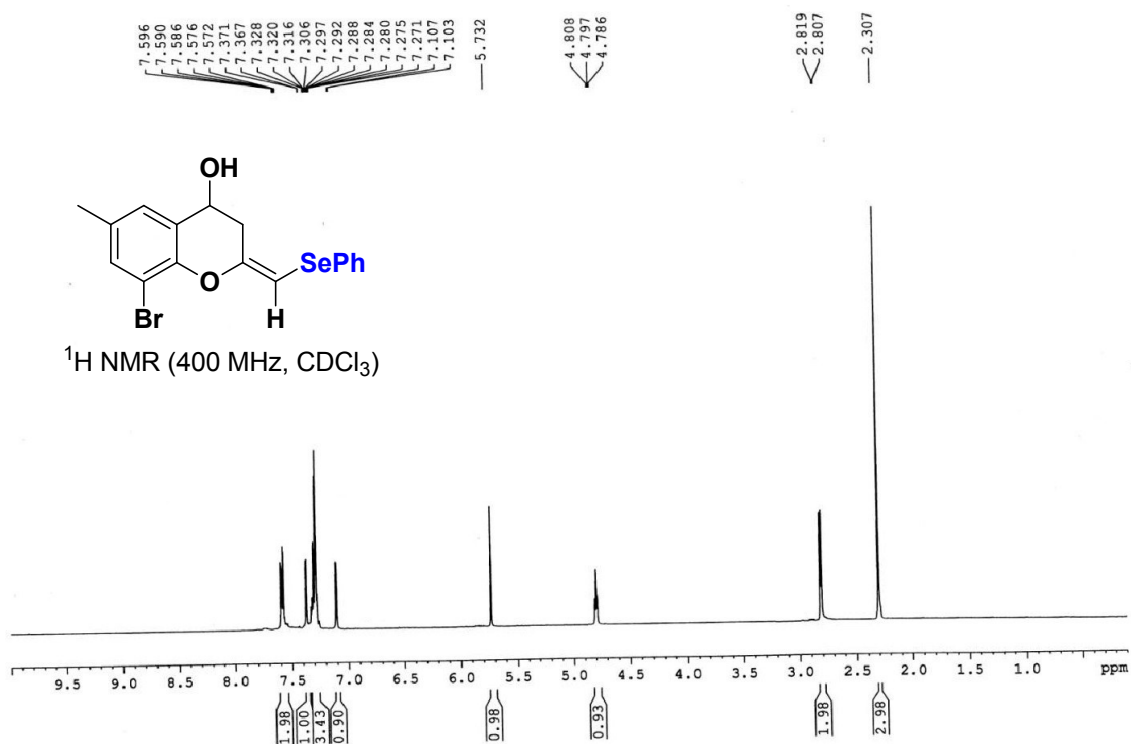
**(E)-8-bromo-6-chloro-2-((phenylselanyl)methylene)chroman-4-ol (4e)**



**(E)-6-methyl-2-((phenylselanyl)methylene)chroman-4-ol (4f)**

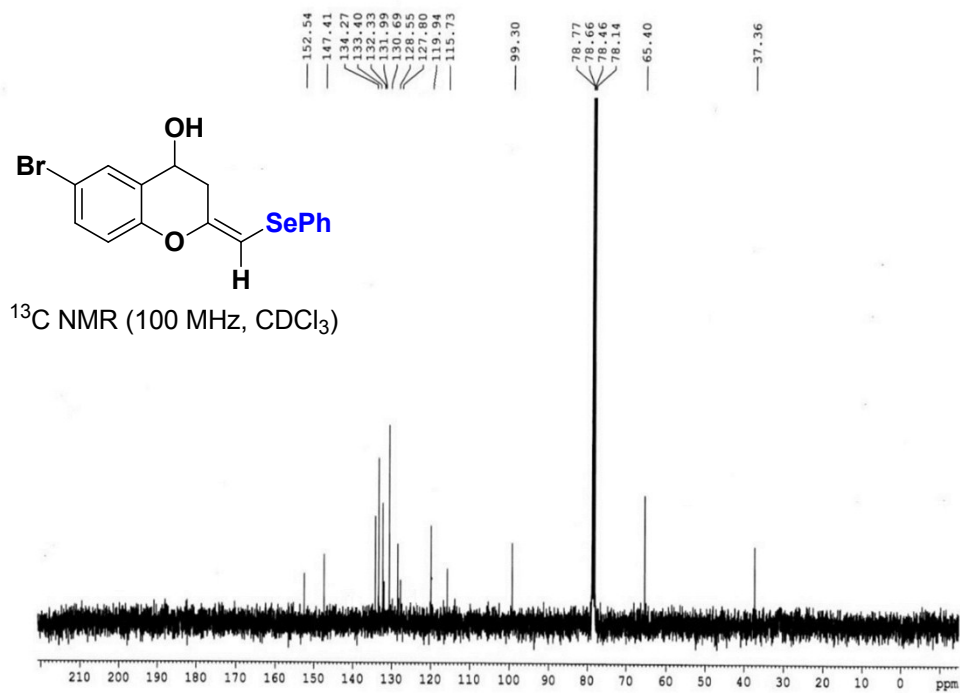
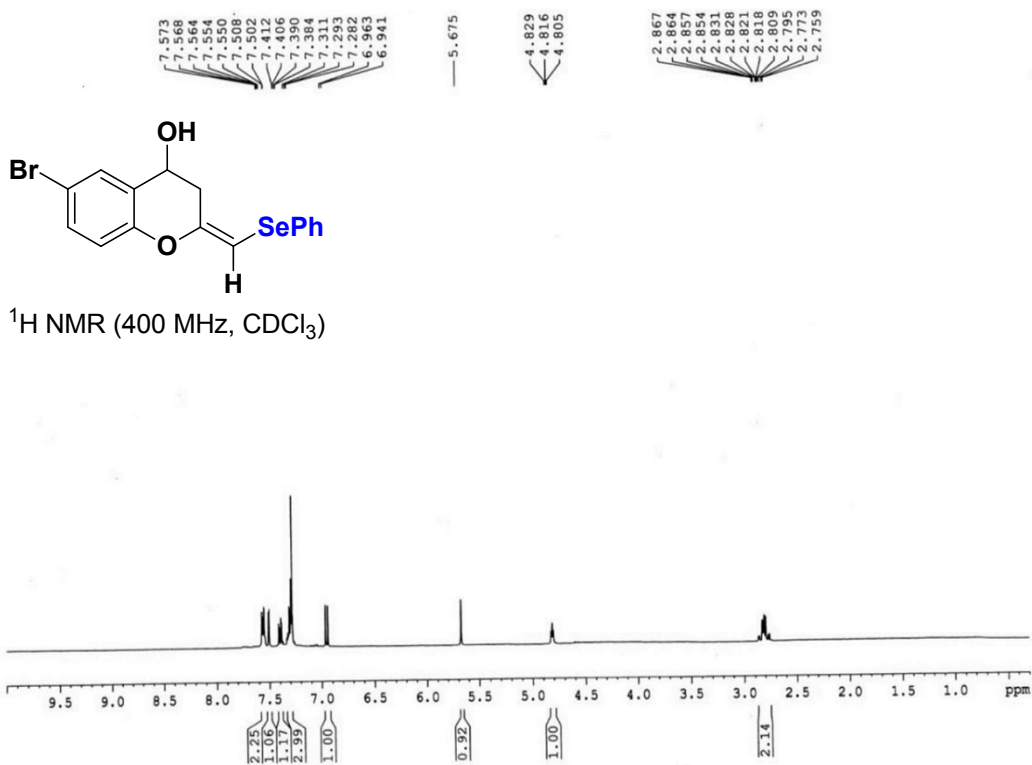


**(E)-8-bromo-6-methyl-2-((phenylselanyl)methylene)chroman-4-ol (4g)**

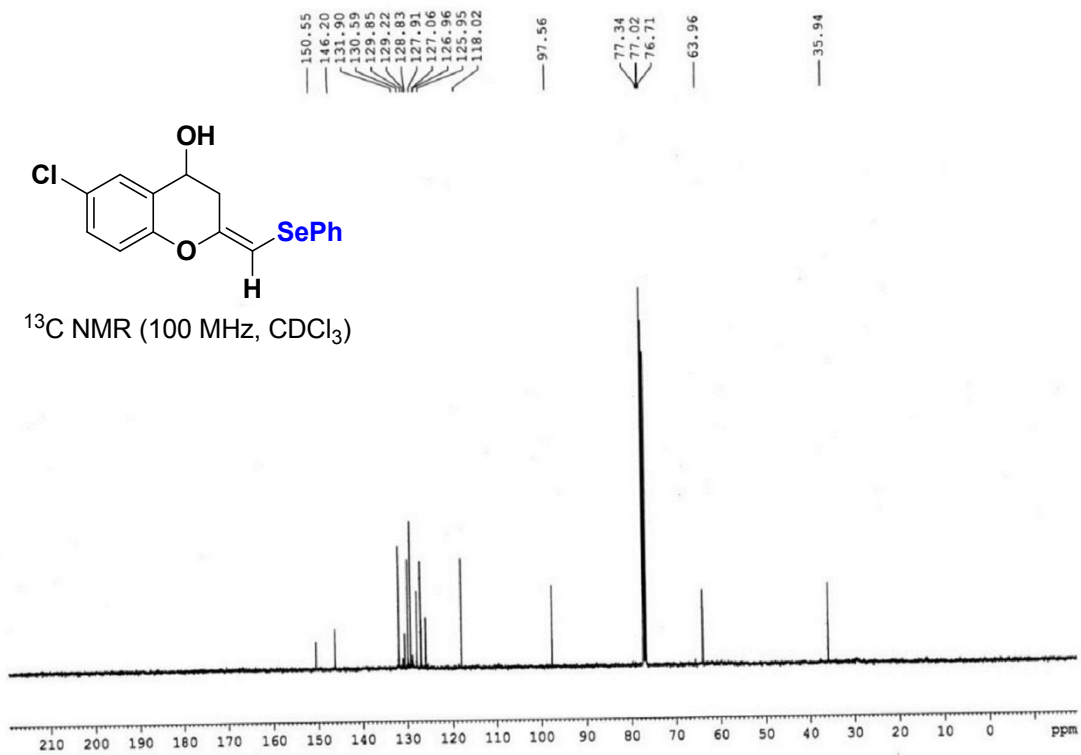
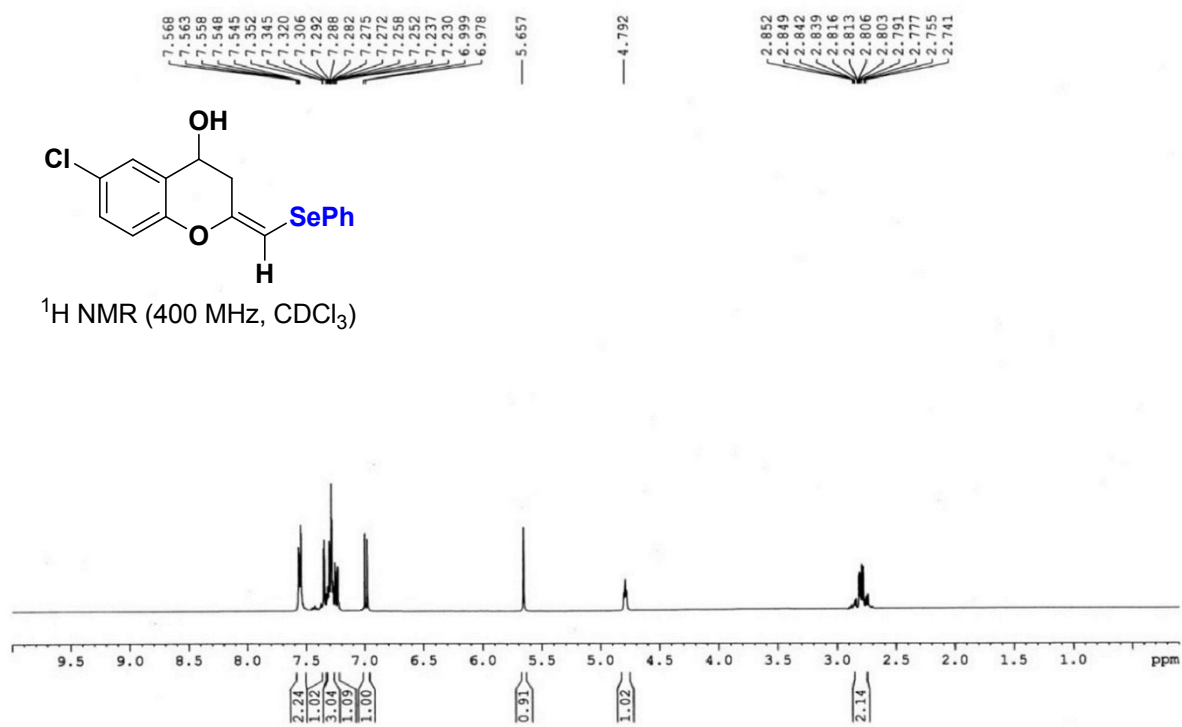




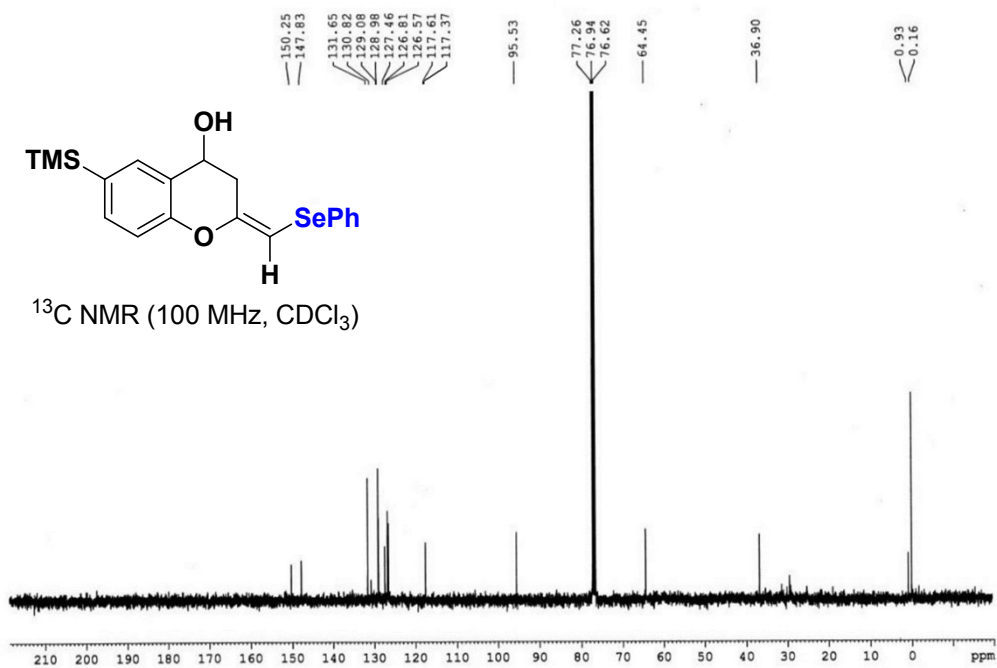
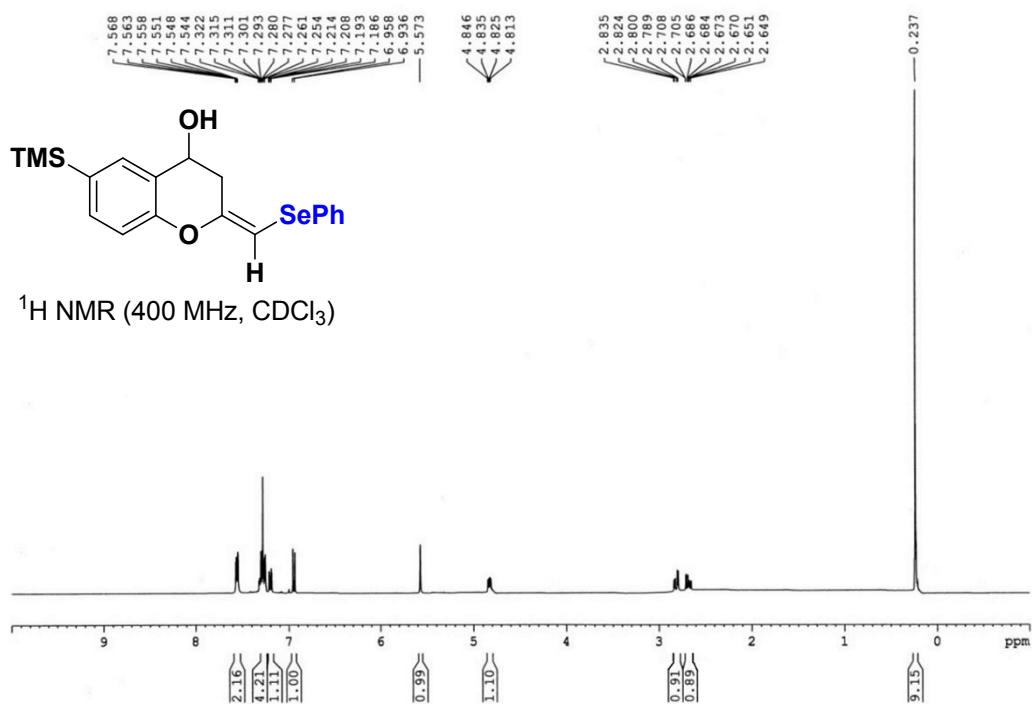
**(E)-6-bromo-2-((phenylselanyl)methylene)chroman-4-ol (4h)**



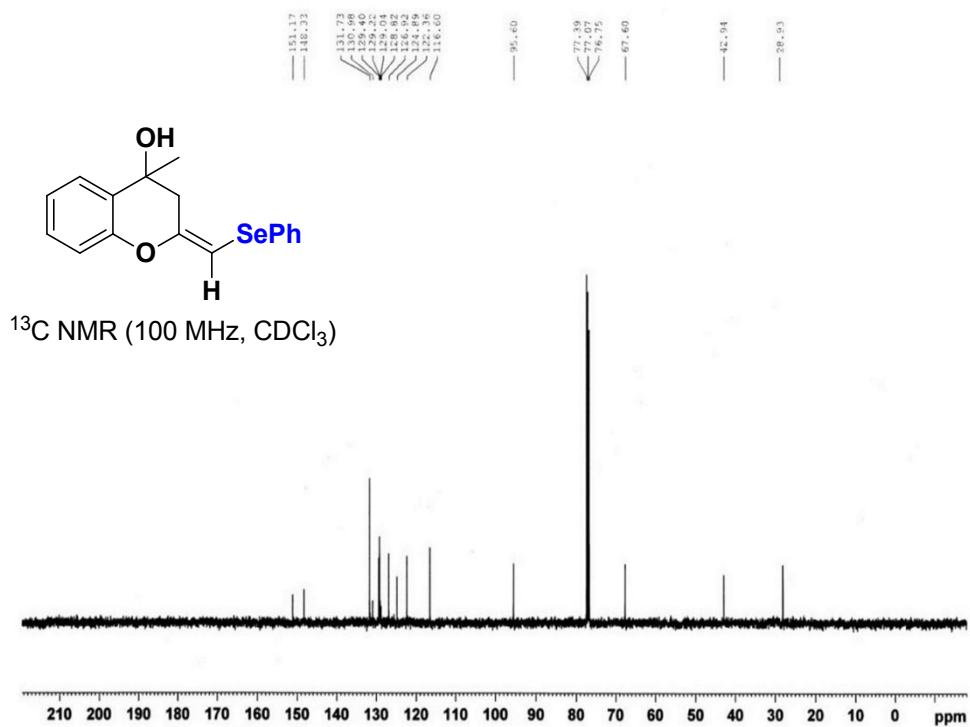
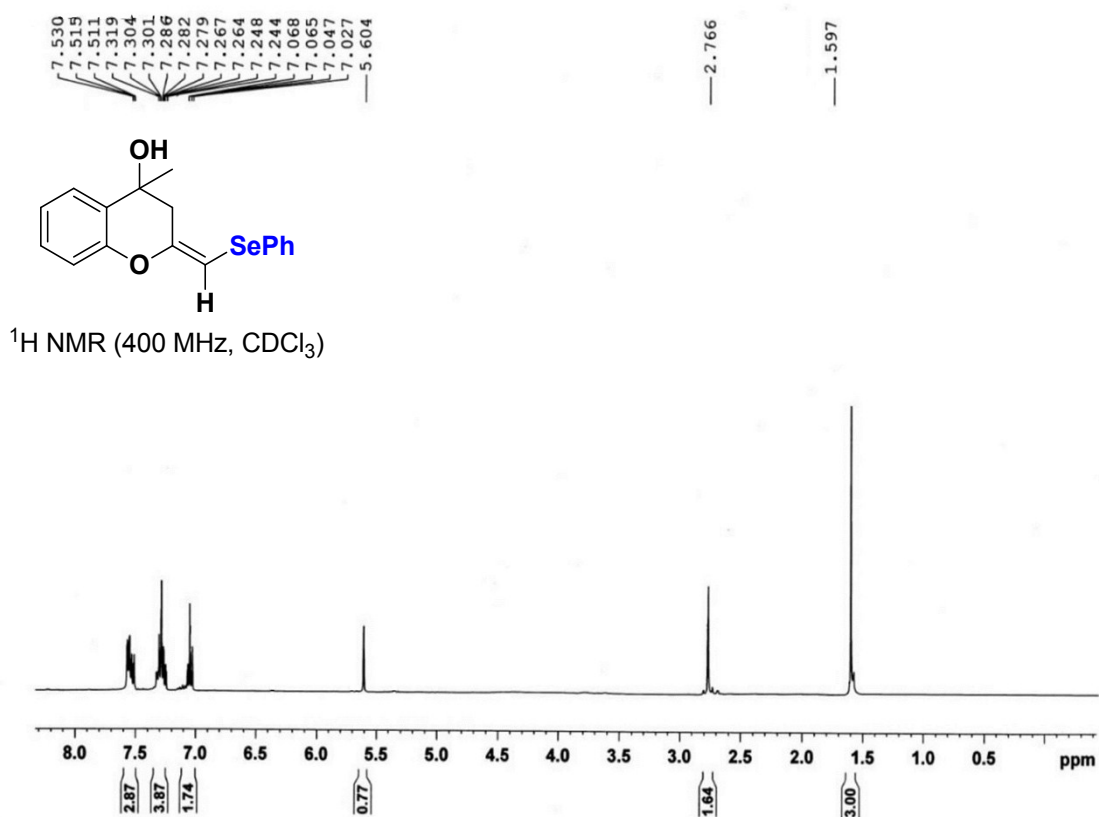
**(E)-6-chloro-2-((phenylselanyl)methylene)chroman-4-ol (4i)**



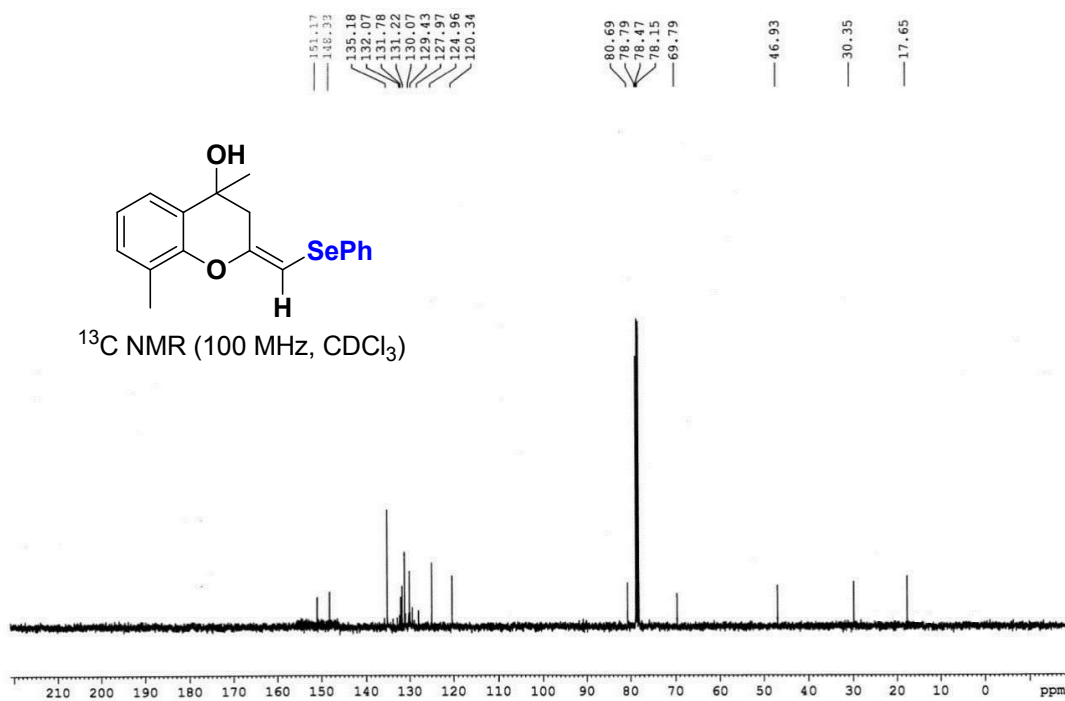
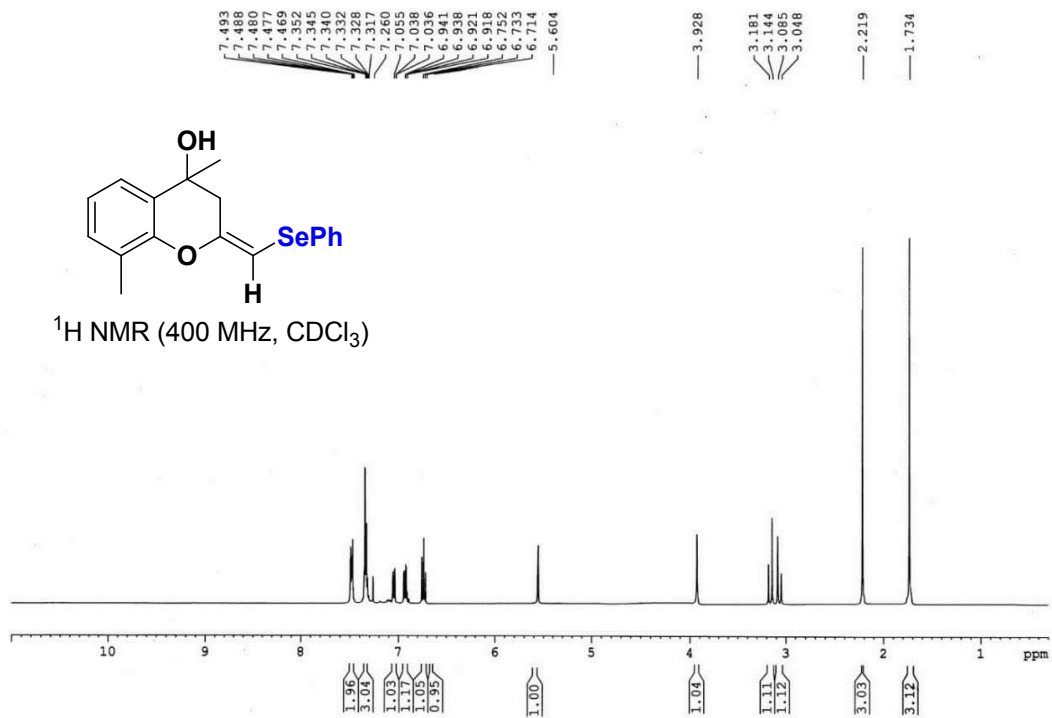
**(E)-2-((phenylselanyl)methylene)-6-(trimethylsilyl)chroman-4-ol (4j)**



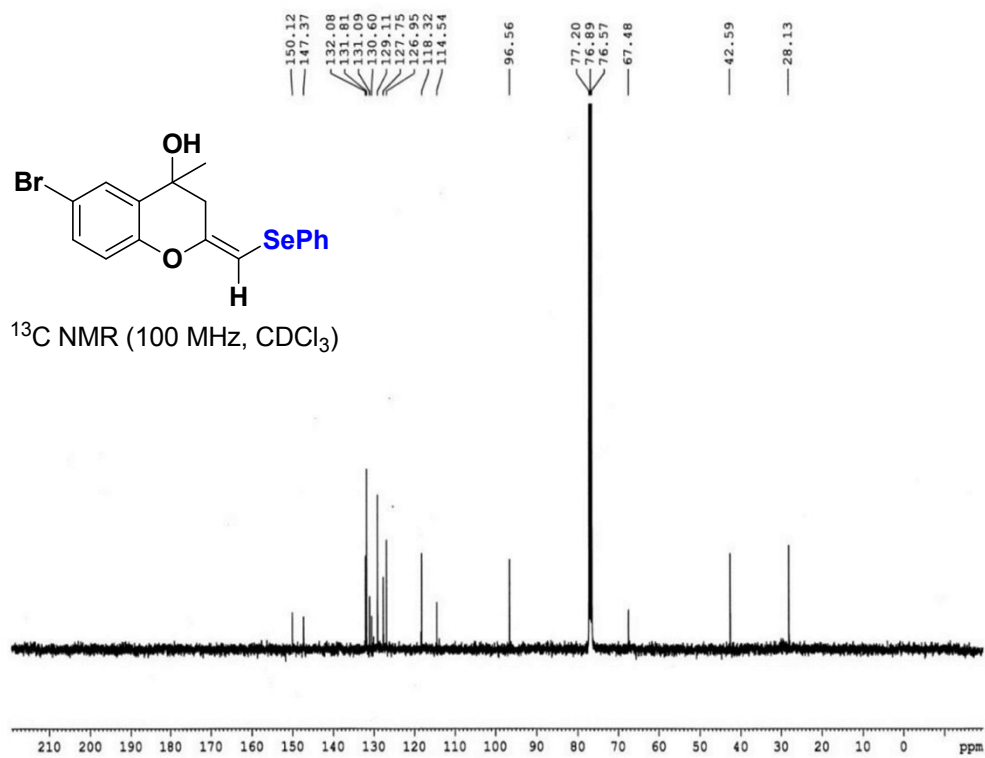
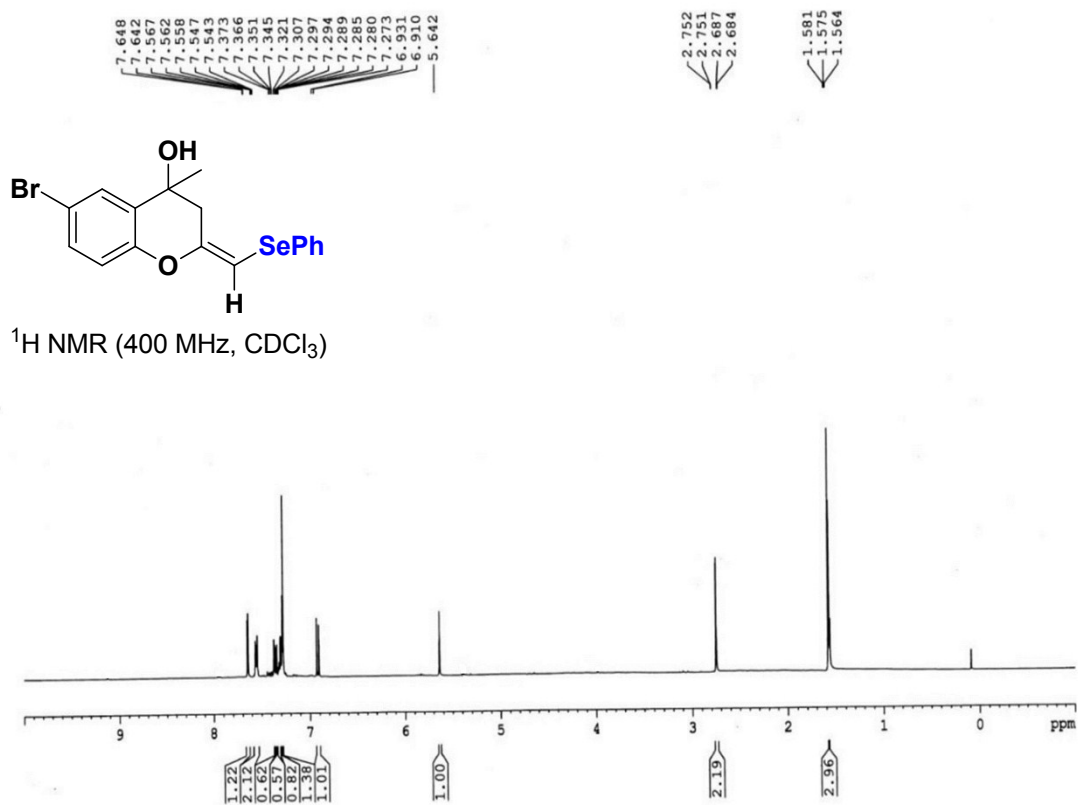
**(E)-4-methyl-2-((phenylselanyl)methylene)chroman-4-ol (4k)**



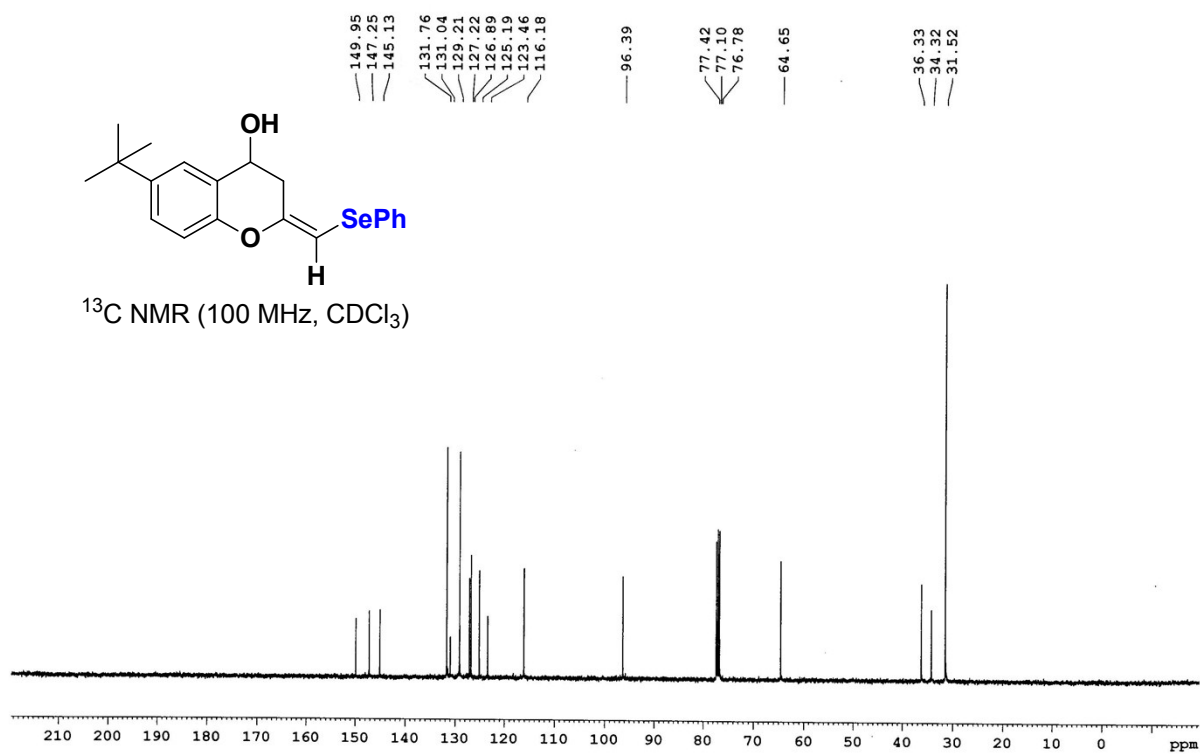
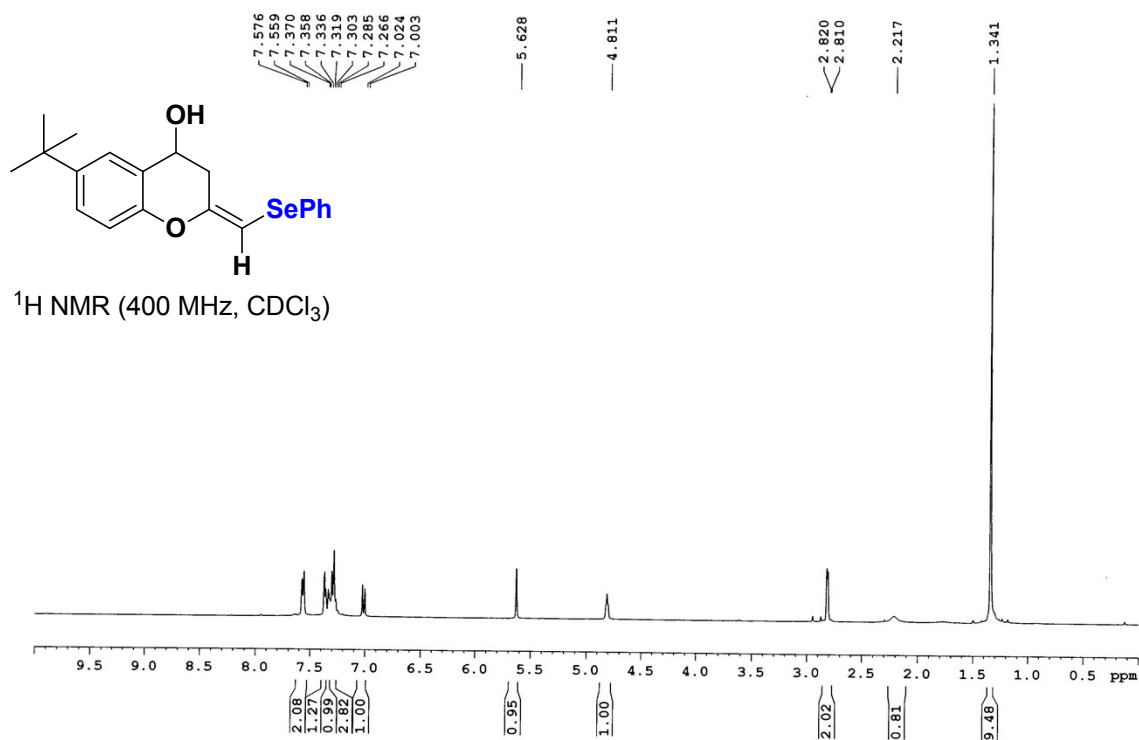
**(E)-4,8-dimethyl-2-((phenylselanyl)methylene)chroman-4-ol (4l)**



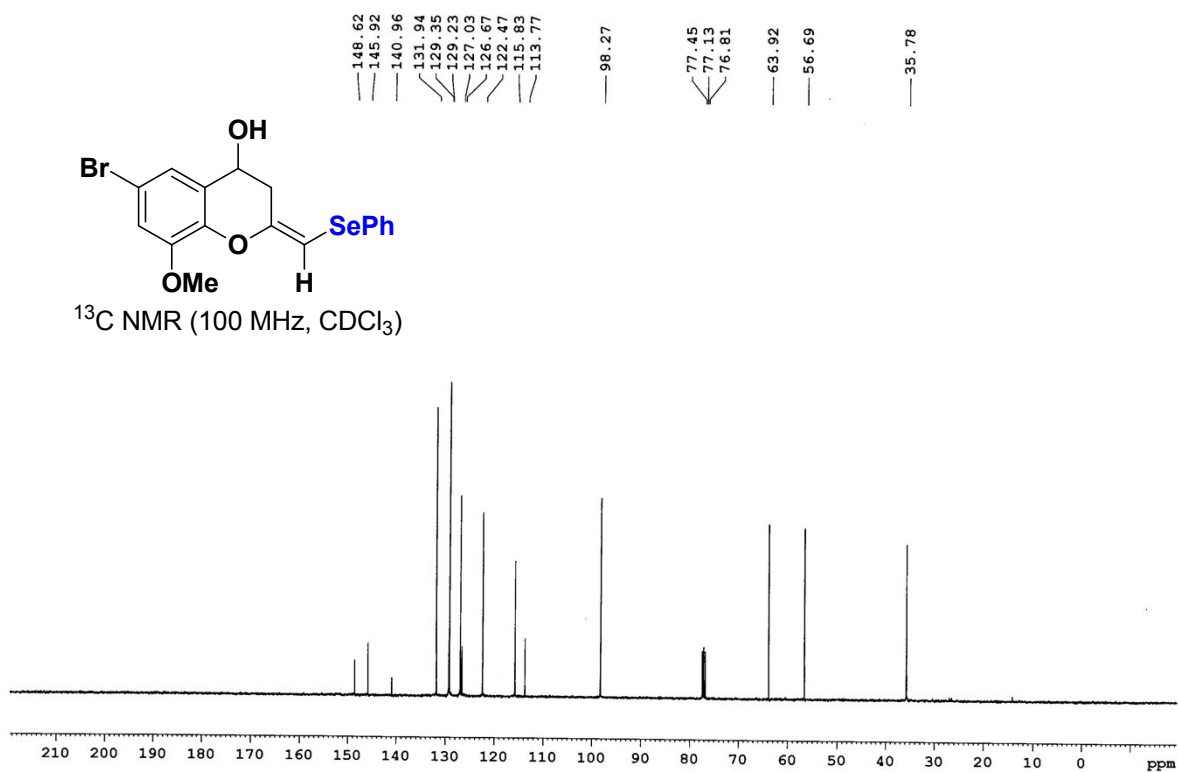
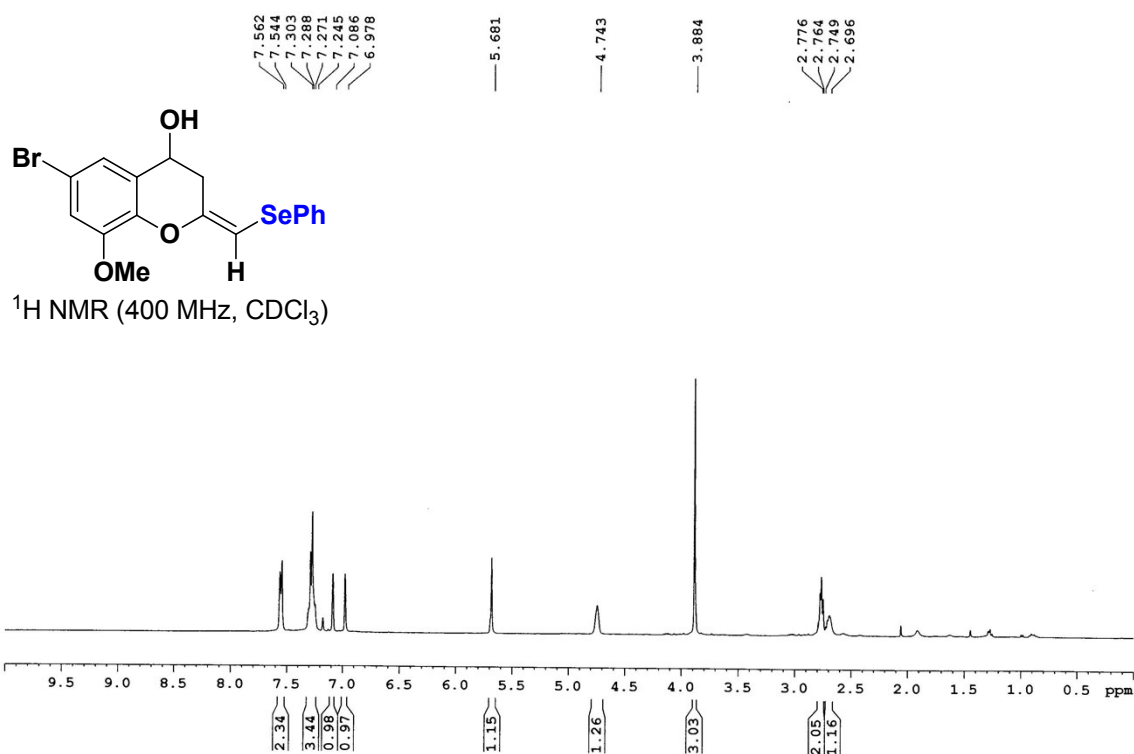
**(E)-6-bromo-4-methyl-2-((phenylselanyl)methylene)chroman-4-ol (4m)**



**(E)-6-(tert-butyl)-2-((phenylselanyl)methylene)chroman-4-ol (4n)**

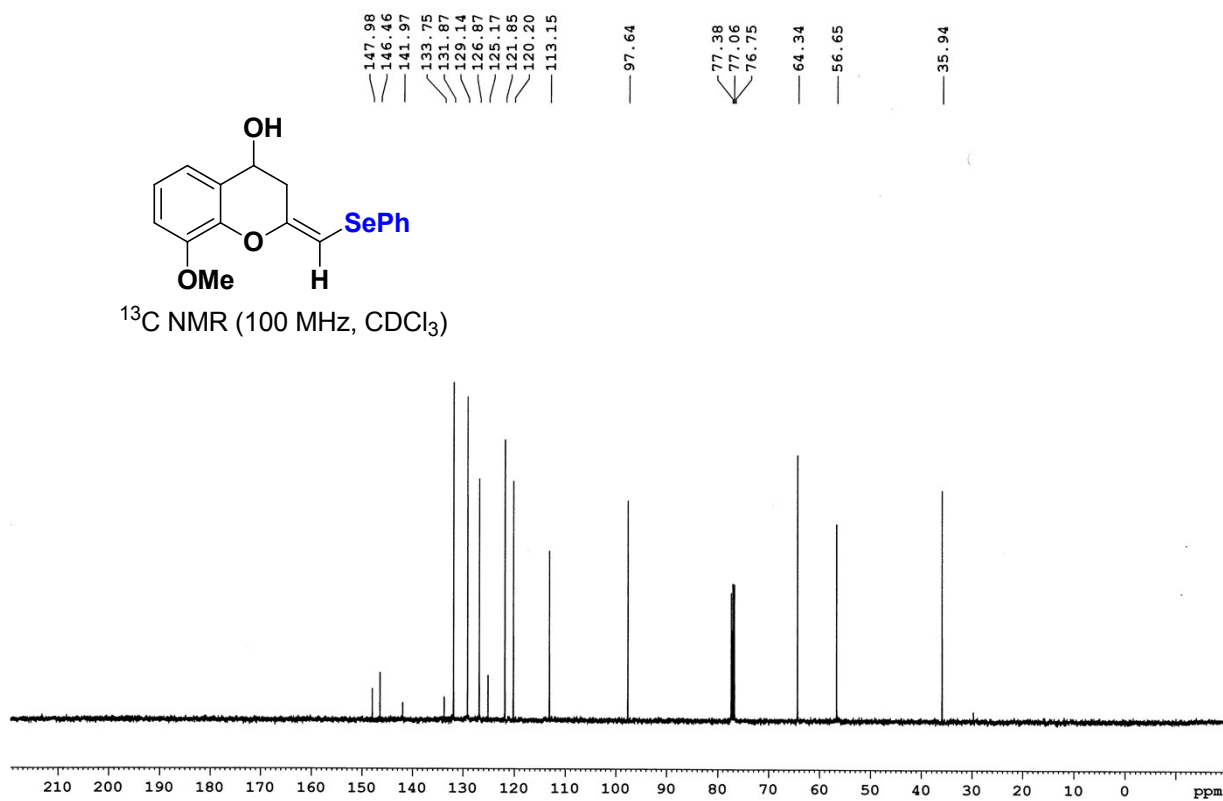
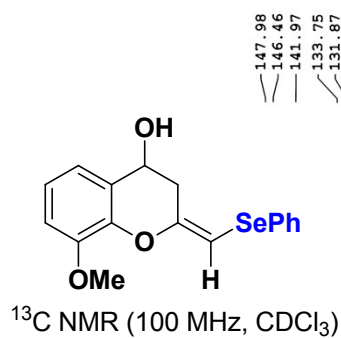
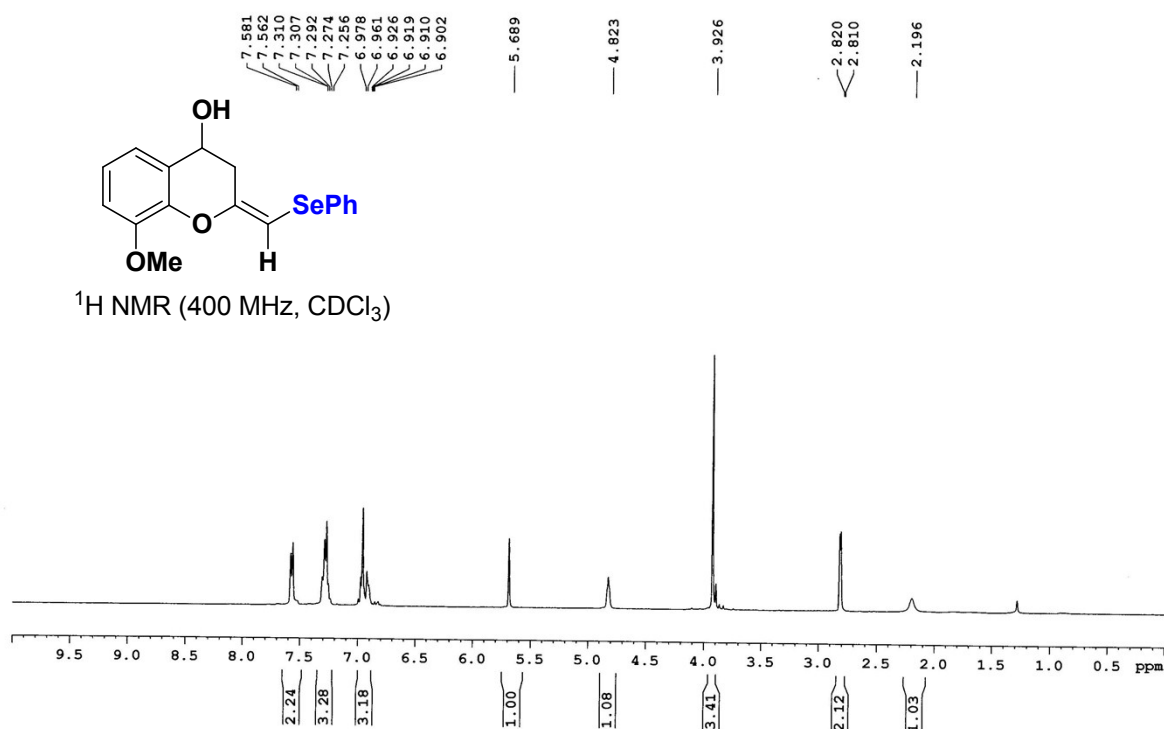
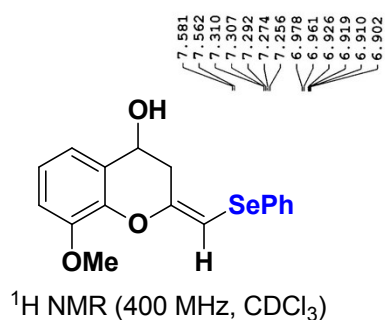


**(E)-6-bromo-8-methoxy-2-((phenylselanyl)methylene)chroman-4-ol (4o)**

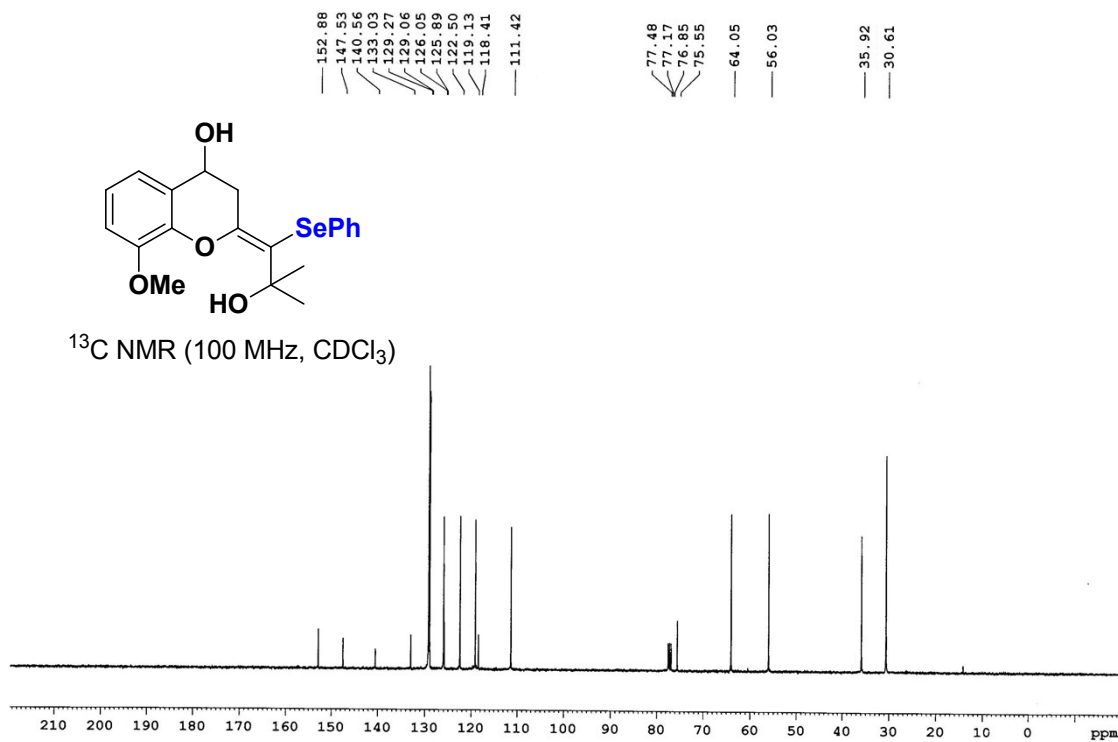
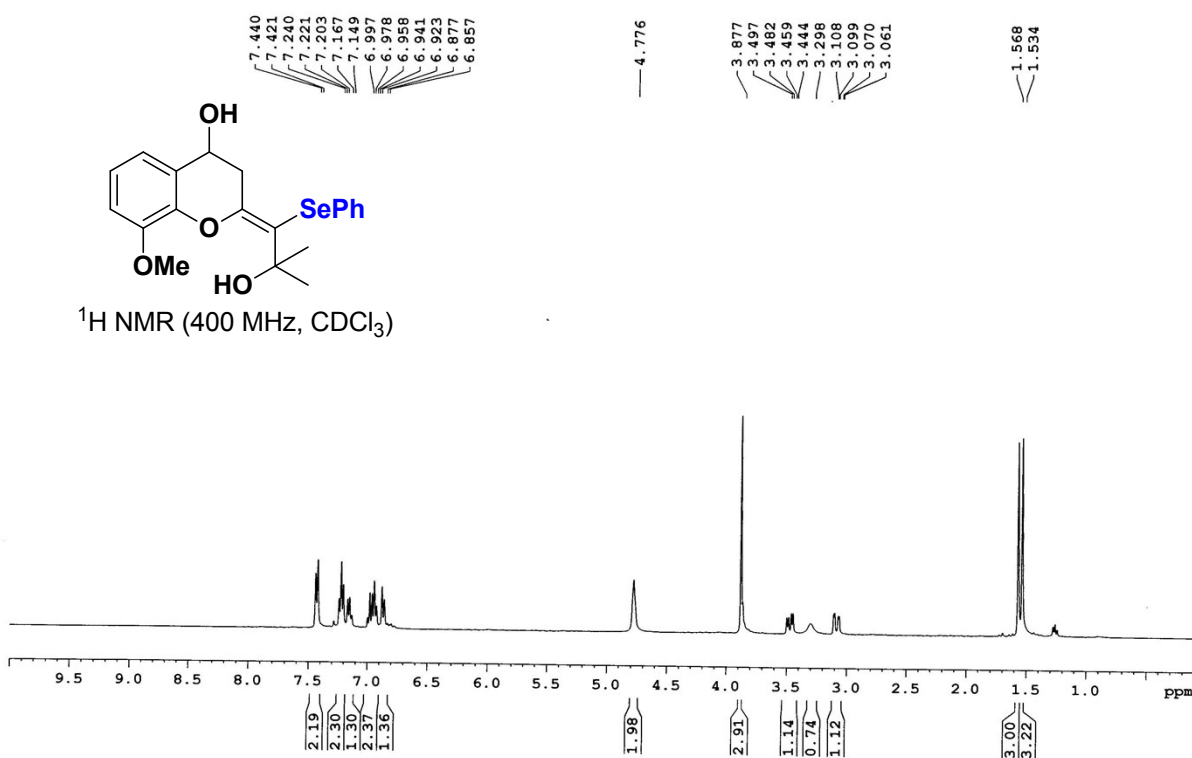




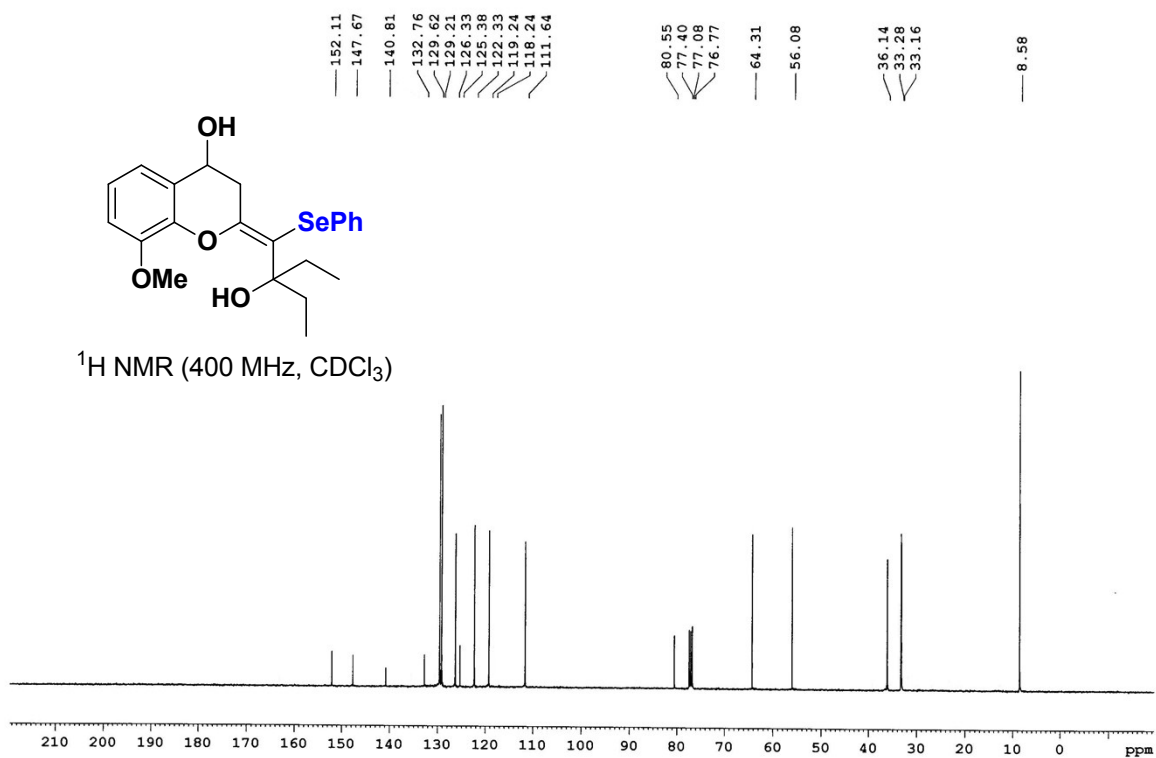
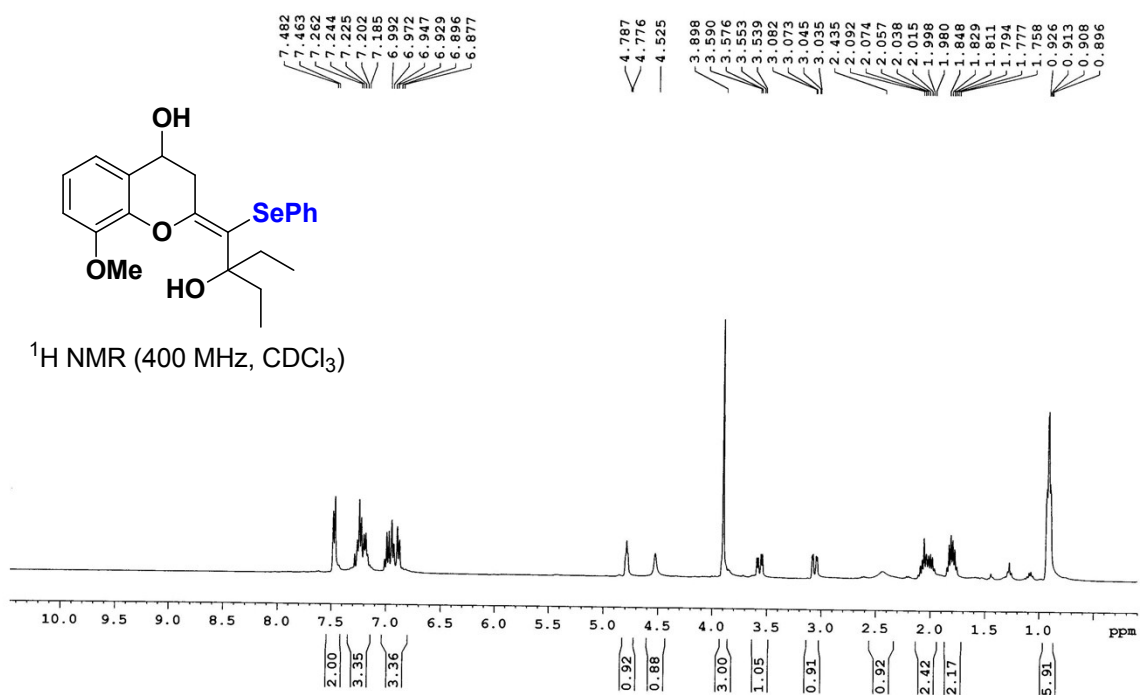
**(E)-8-methoxy-2-((phenylselanyl)methylene)chroman-4-ol (4p)**



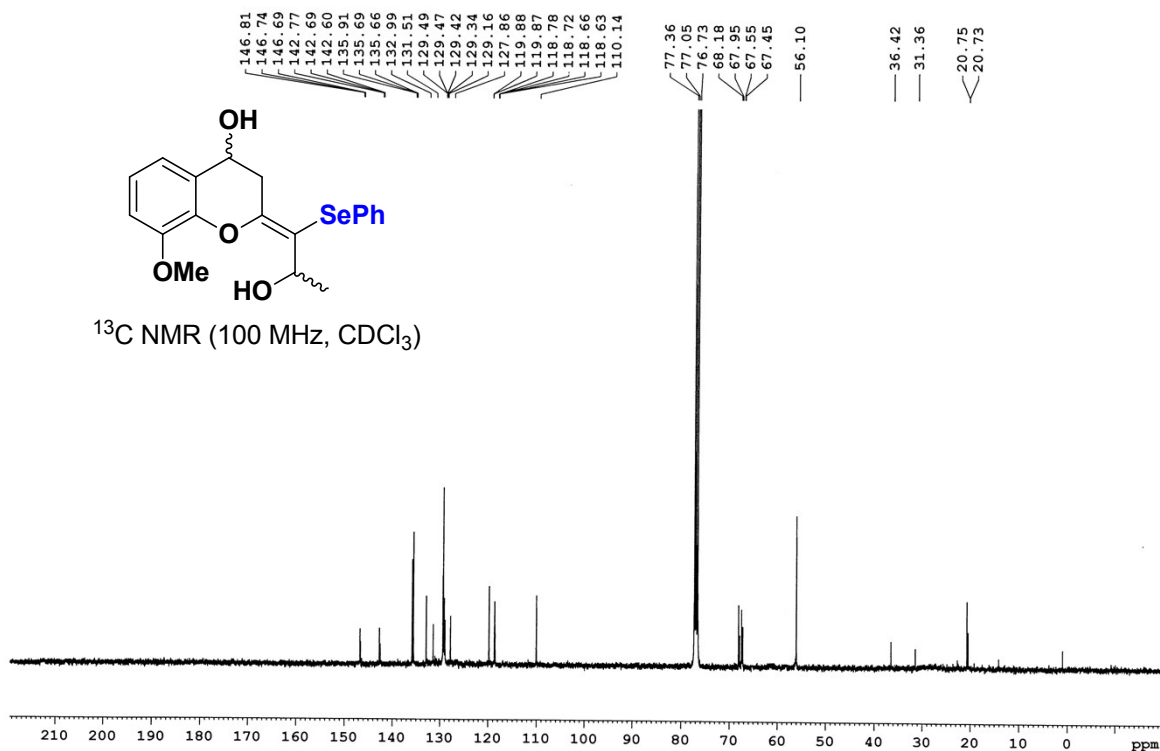
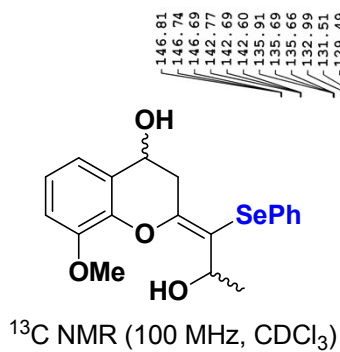
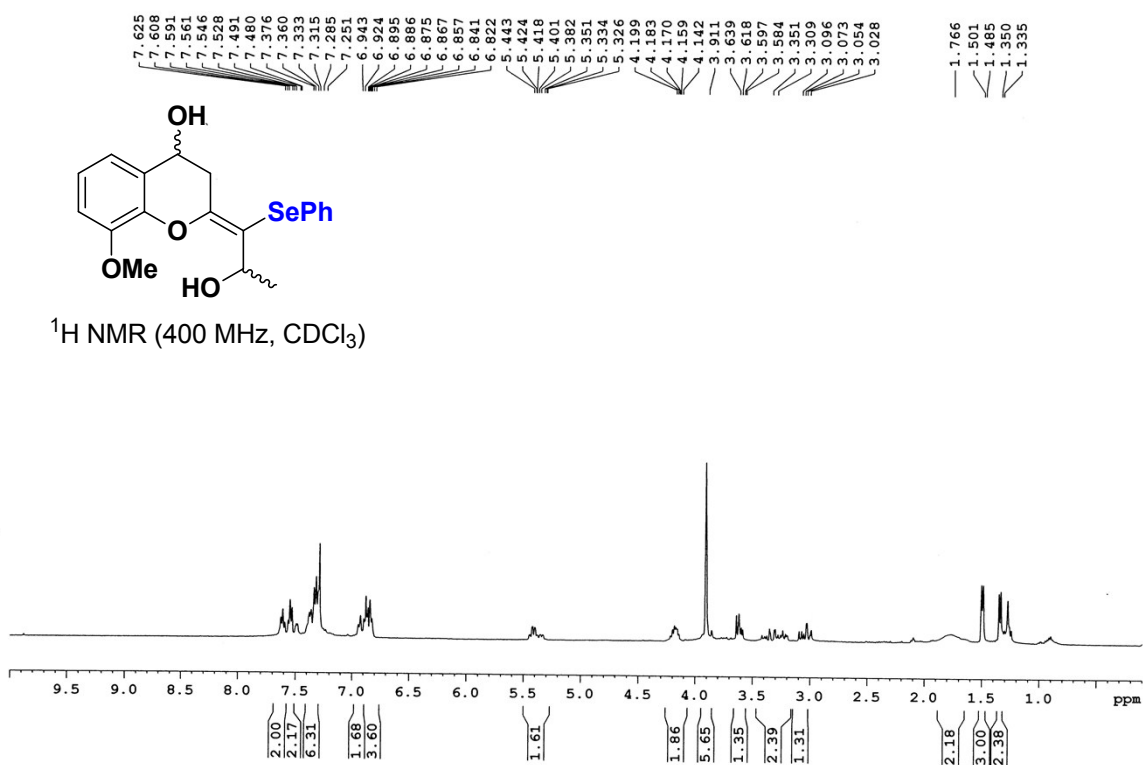
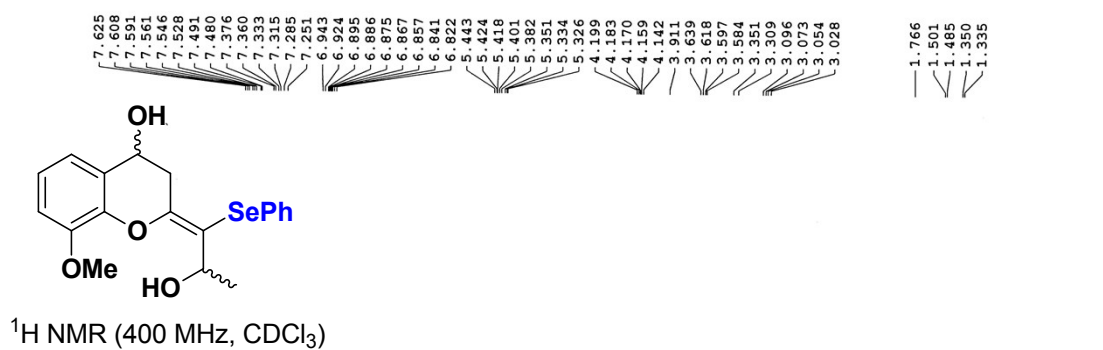
**(E)-2-(2-hydroxy-2-methyl-1-(phenylselanyl)propylidene)-8-methoxychroman-4-ol (4q)**

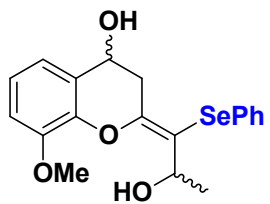


**(E)-2-(2-ethyl-2-hydroxy-1-(phenylselanyl)butylidene)-8-methoxychroman-4-ol (4r)**



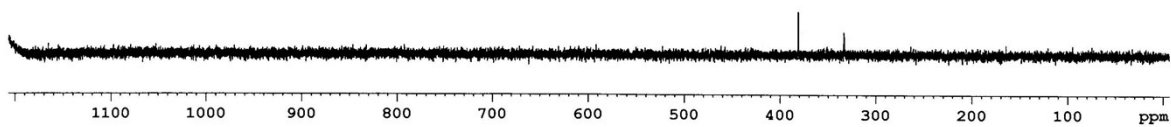
**(E)-2-(2-hydroxy-1-(phenylselanyl)propylidene)-8-methoxychroman-4-ol (4s)**



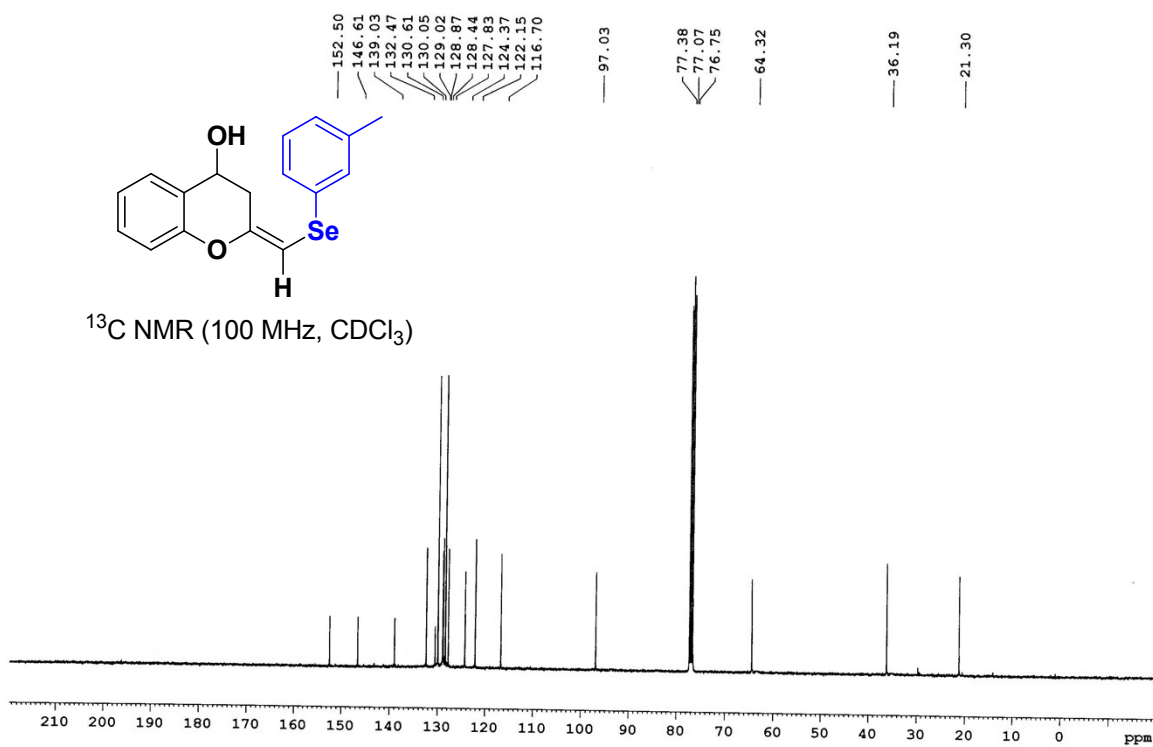
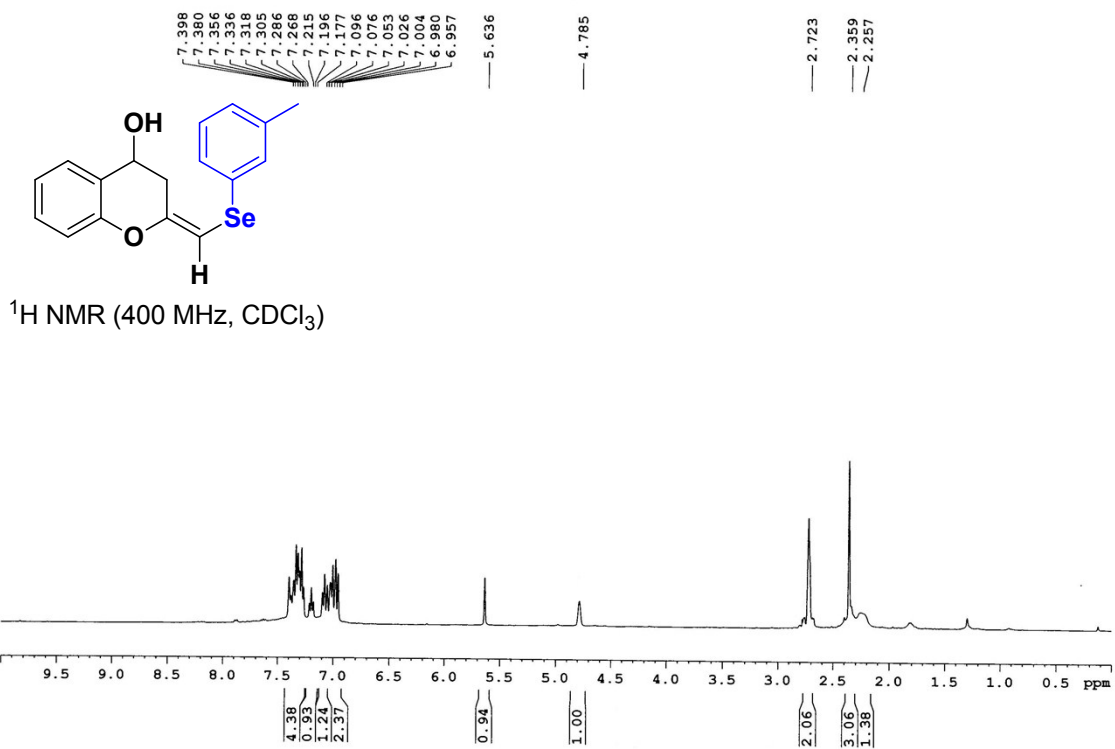


$^{77}\text{Se}$  NMR (76 MHz,  $\text{CDCl}_3$ )

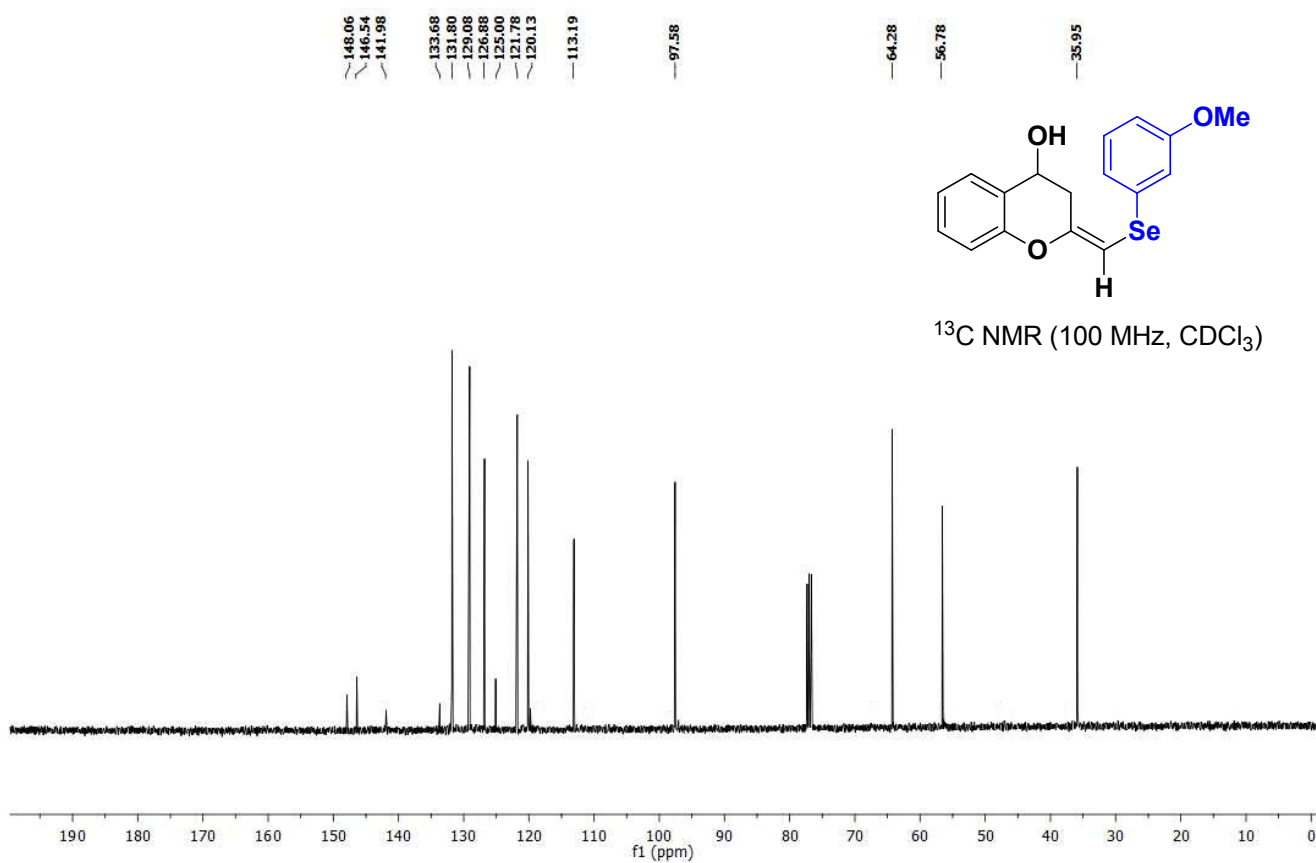
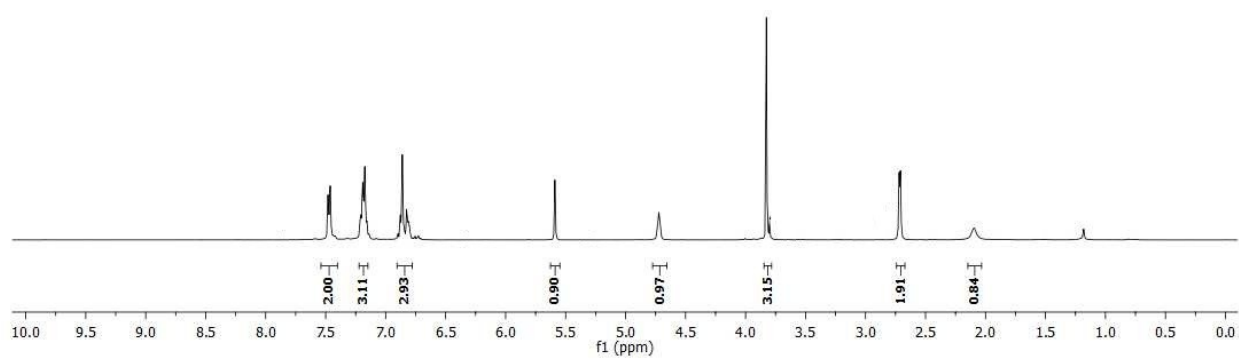
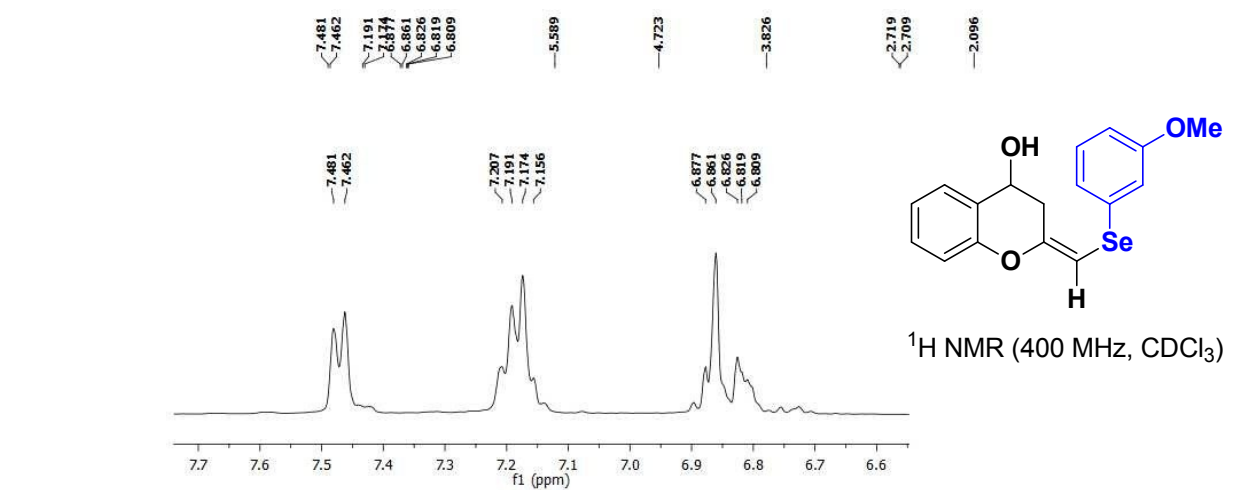
381.35  
381.14  
333.14  
332.92



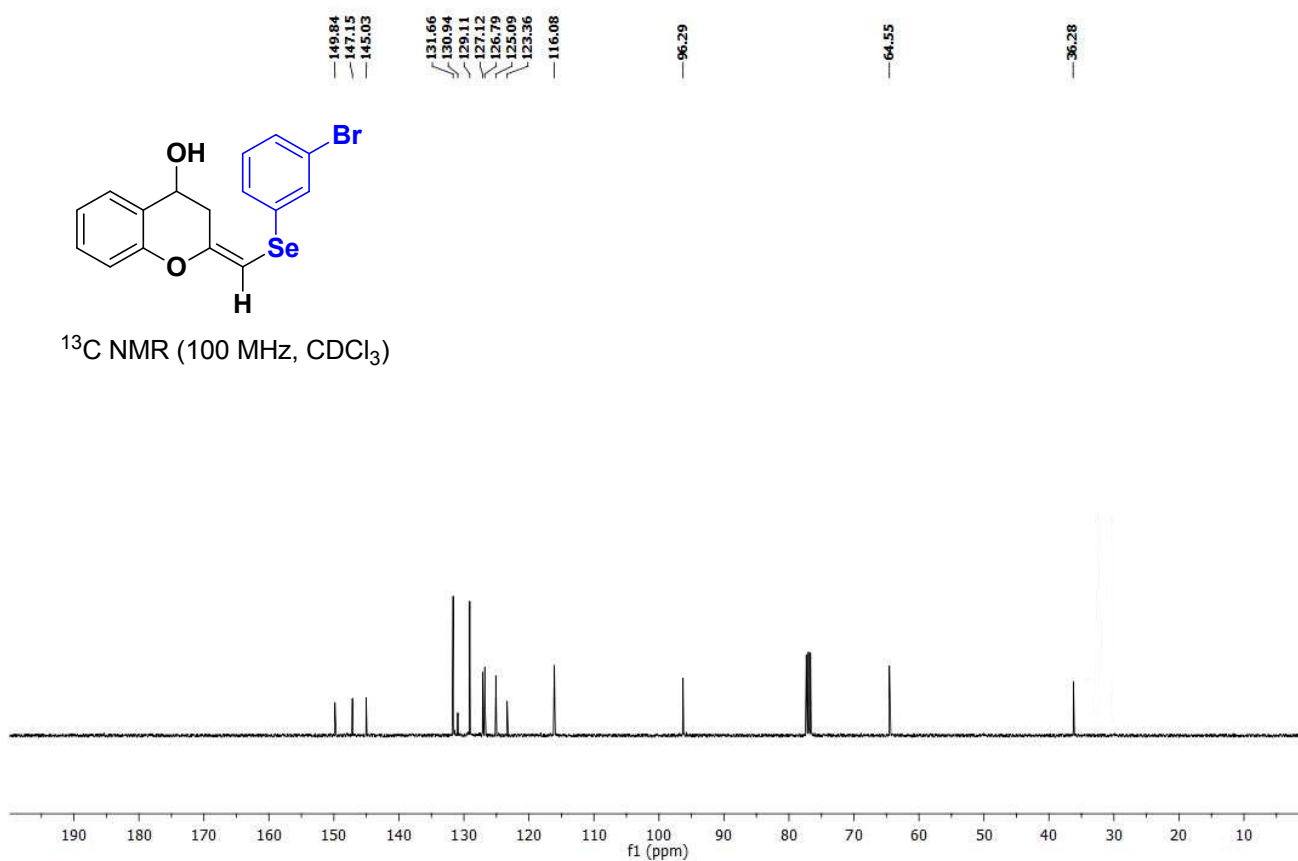
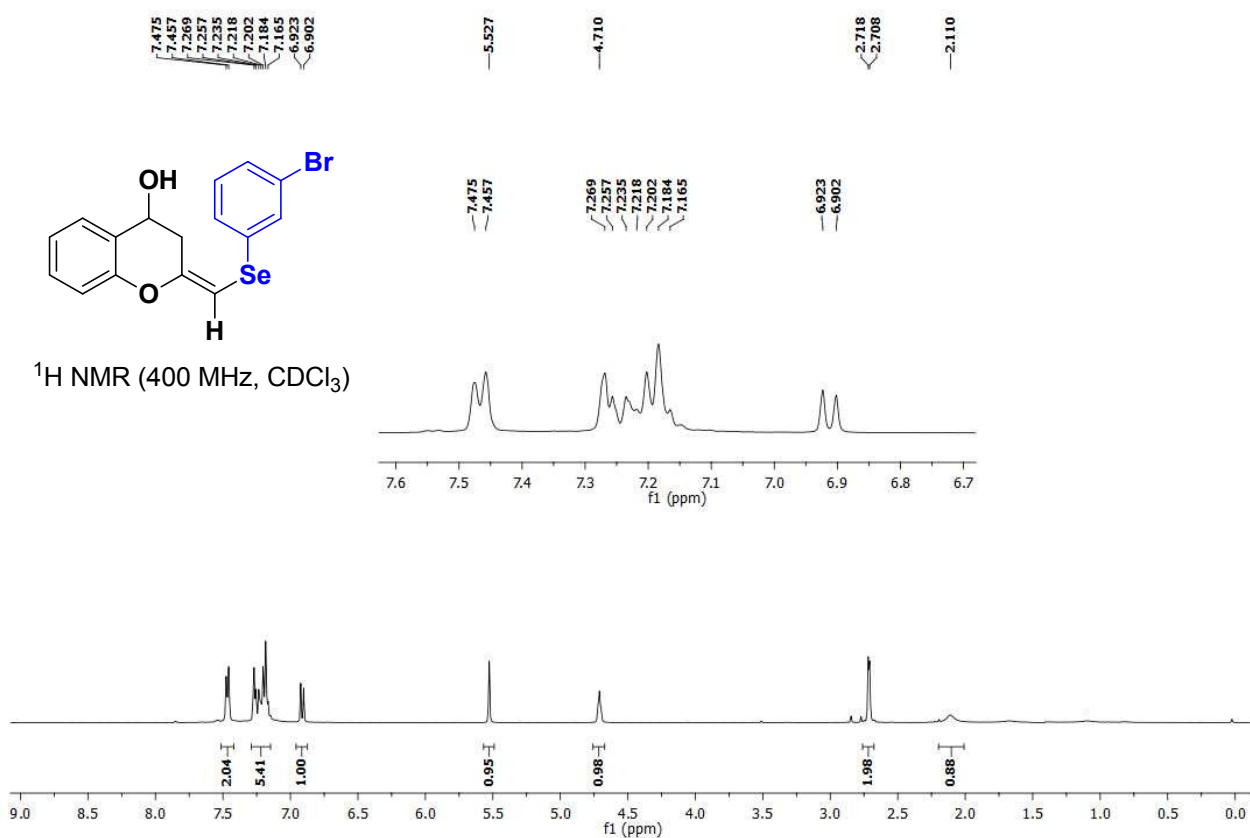
**(E)-2-((m-tolylselanyl)methylene)chroman-4-ol (4t)**



**(E)-2-(((3-methoxyphenyl)selenyl)methylene)chroman-4-ol (4u)**

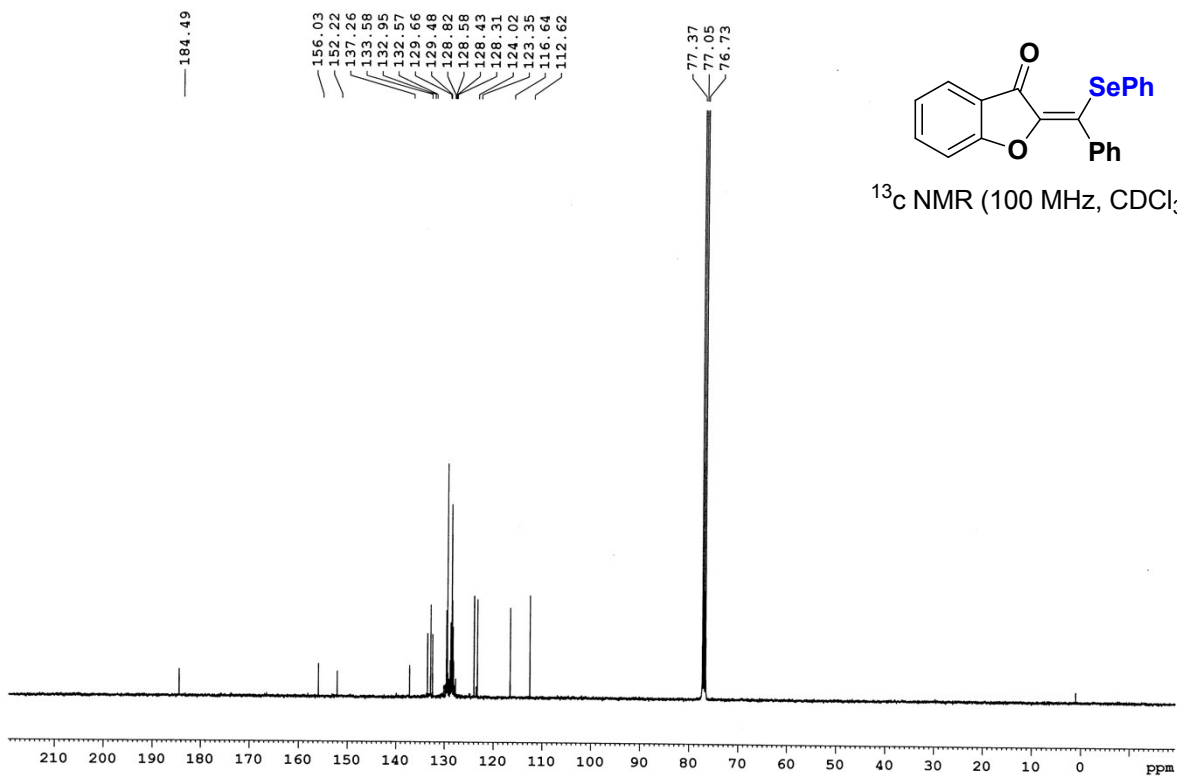
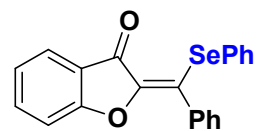
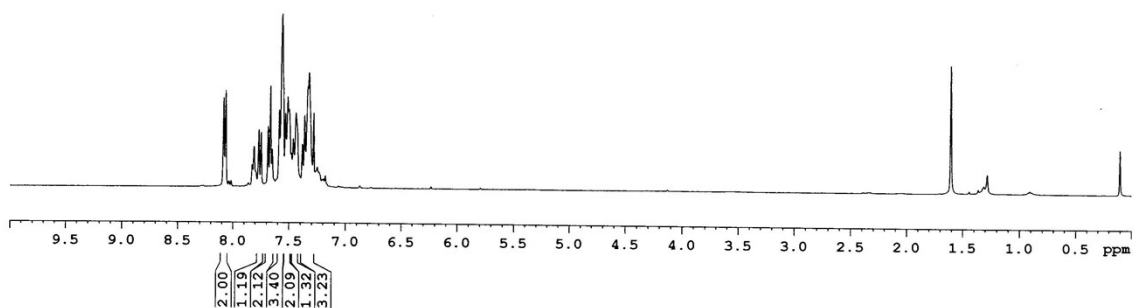
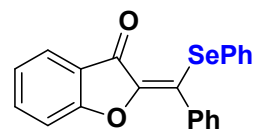
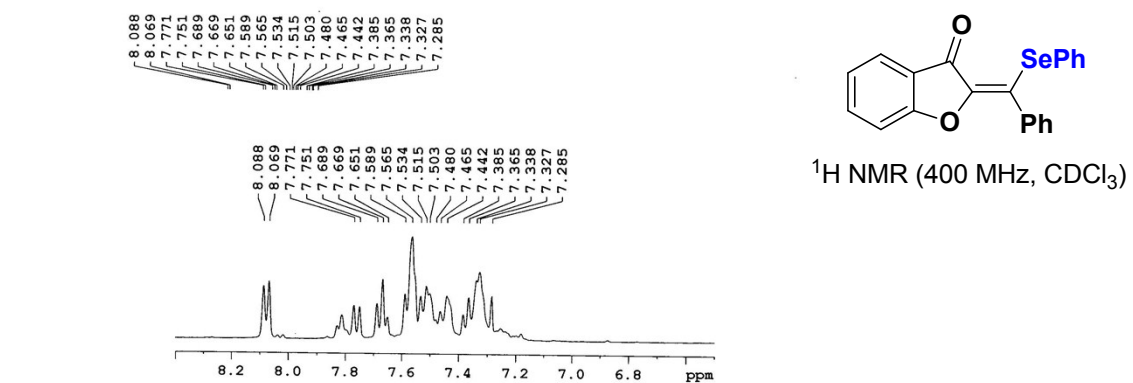


**(E)-2-(((3-bromophenyl)selenyl)methylene)chroman-4-ol (4v)**

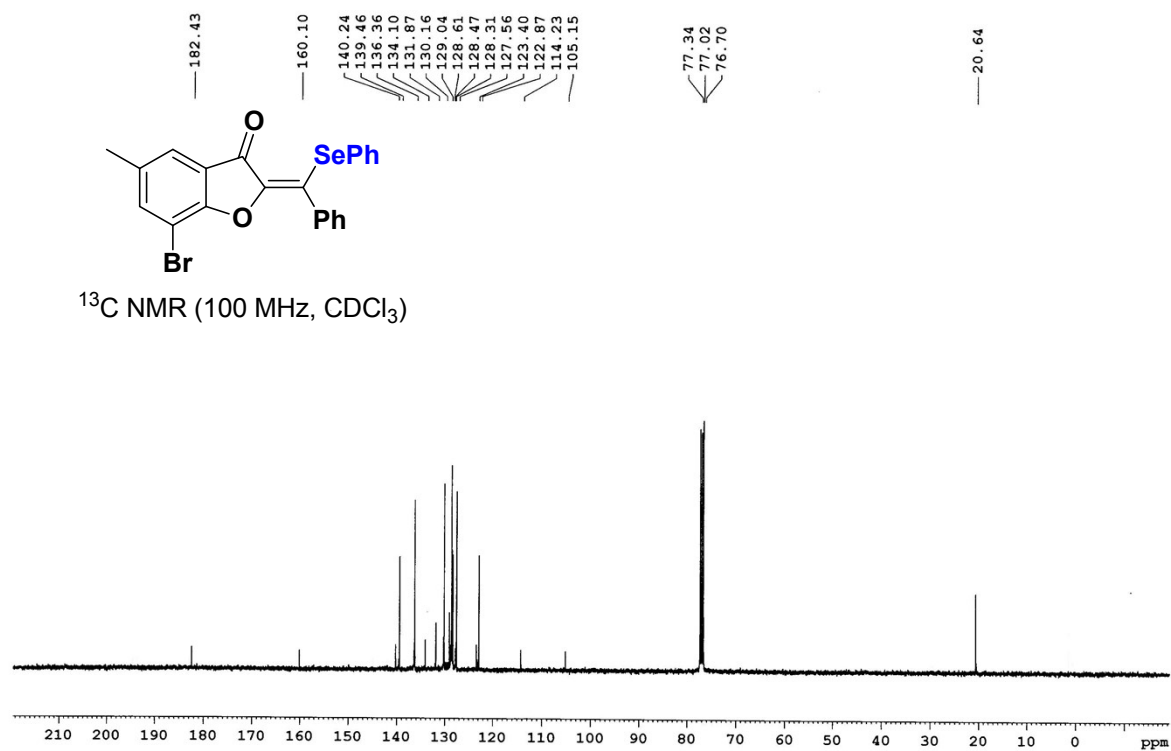
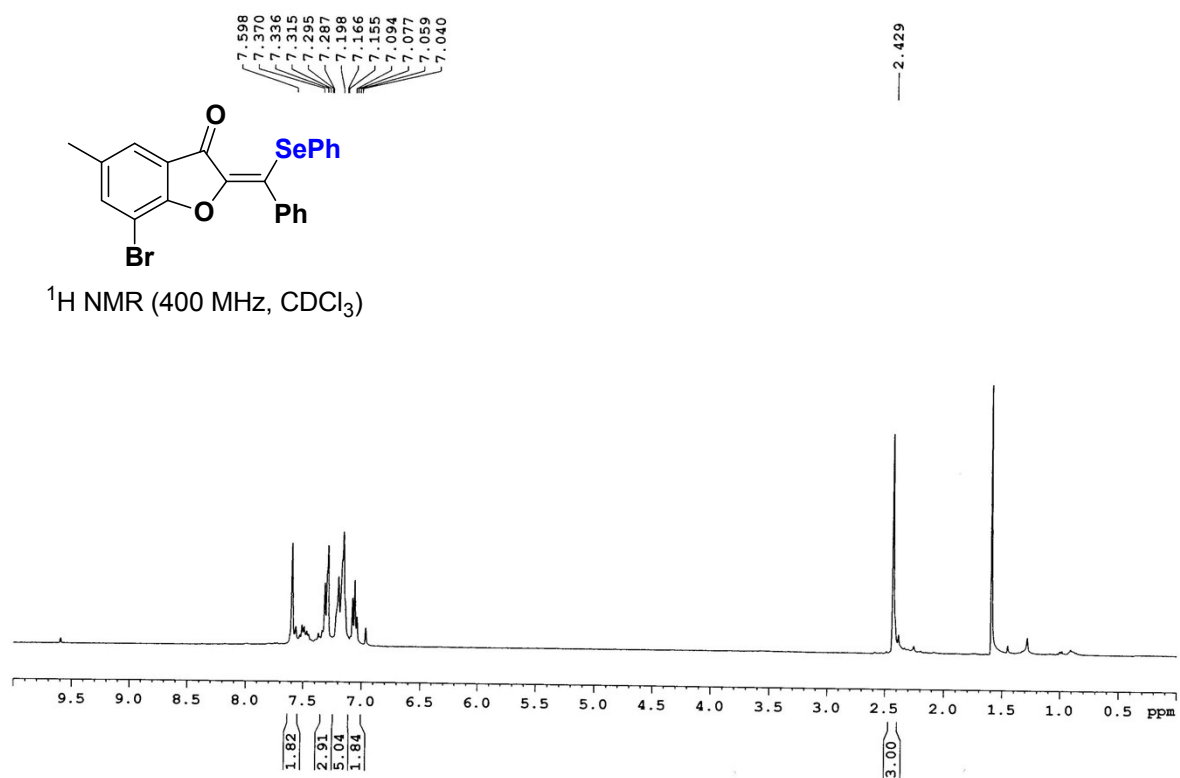




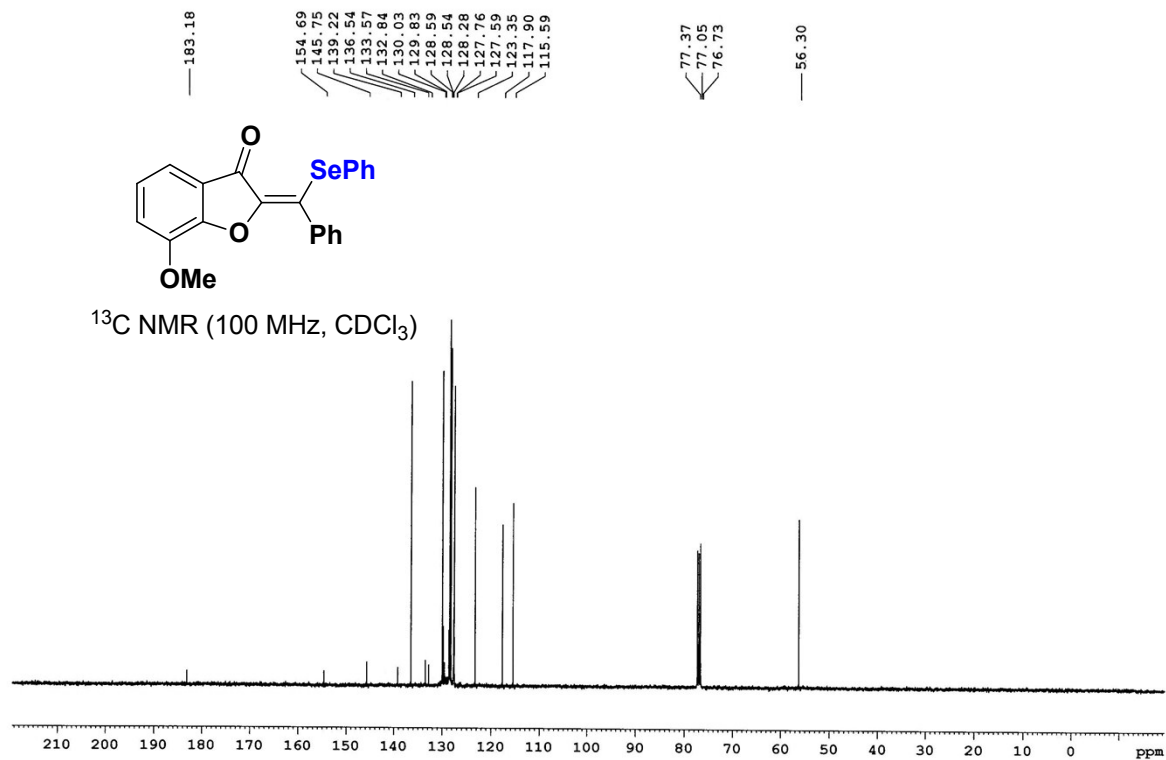
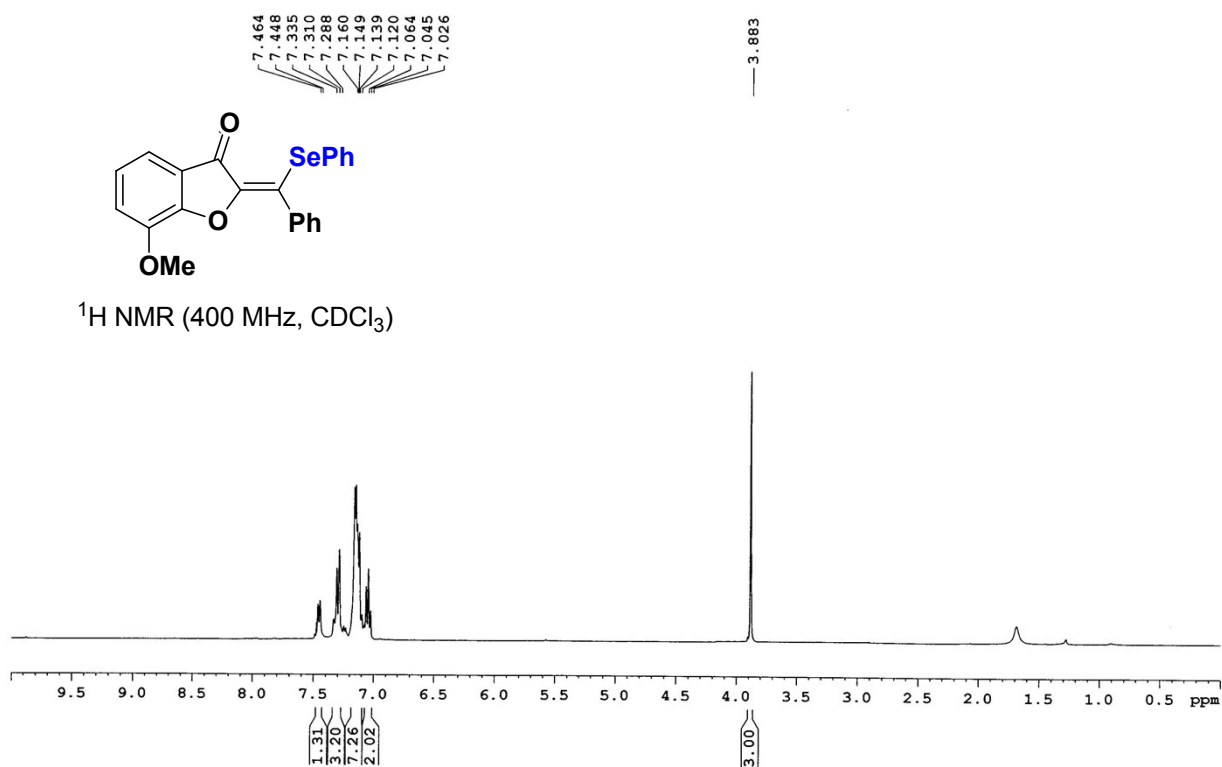
**(E)-2-(phenyl(phenylselanyl)methylene)benzofuran-3(2H)-one (5a)**



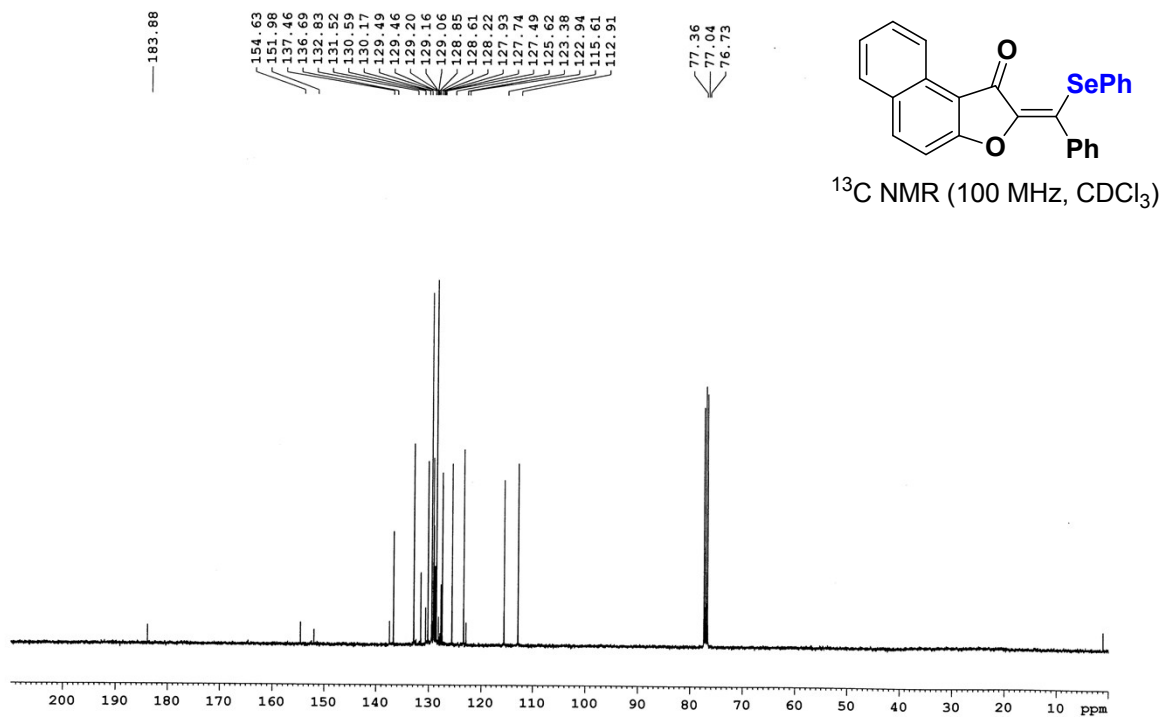
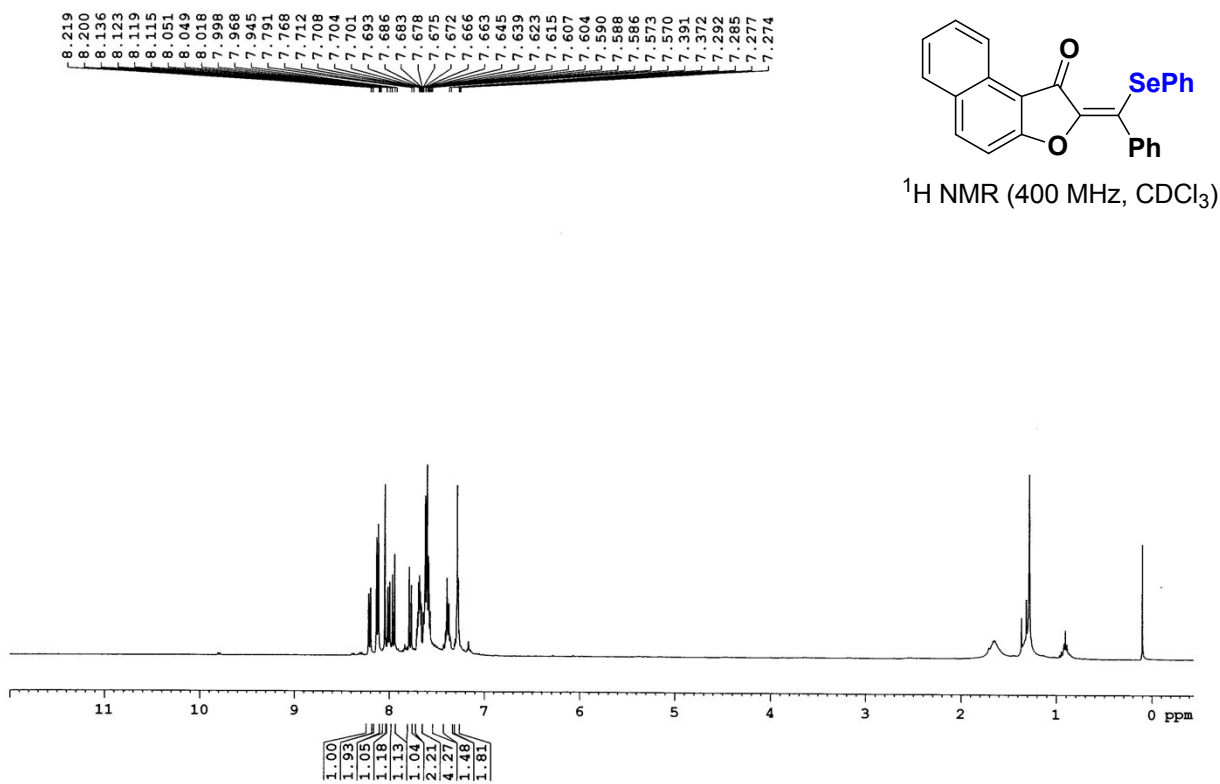
**(E)-7-bromo-5-methyl-2-(phenyl(phenylselanyl)methylene)benzofuran-3(2H)-one (5b)**



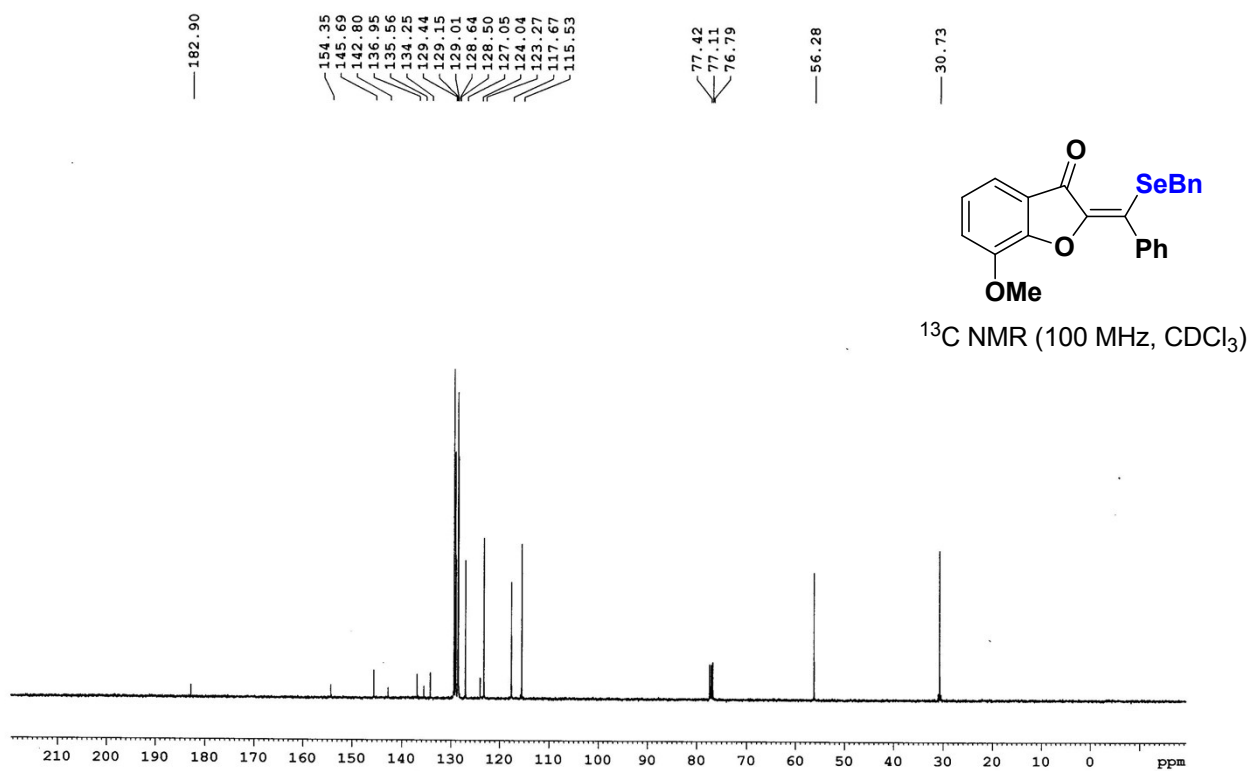
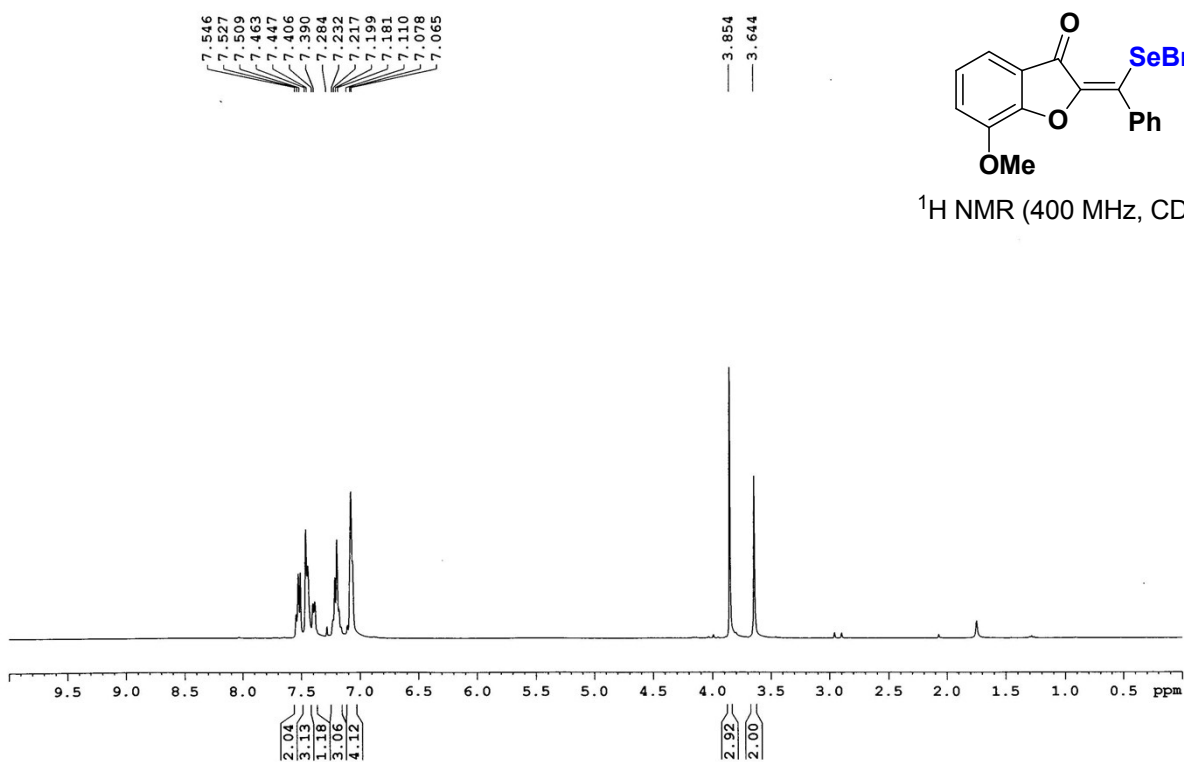
**(E)-7-methoxy-2-(phenyl(phenylselanyl)methylene)benzofuran-3(2H)-one (5c)**

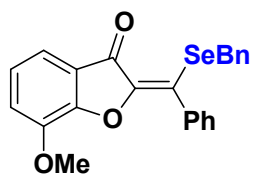


**(E)-2-(phenyl(phenylselanyl)methylene)naphtho[2,1-b]furan-1(2H)-one (5d)**



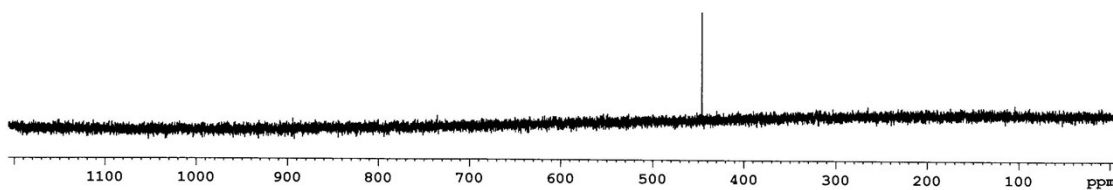
**(E)-2-((benzylselanyl)(phenyl)methylene)-7-methoxybenzofuran-3(2H)-one (5e)**



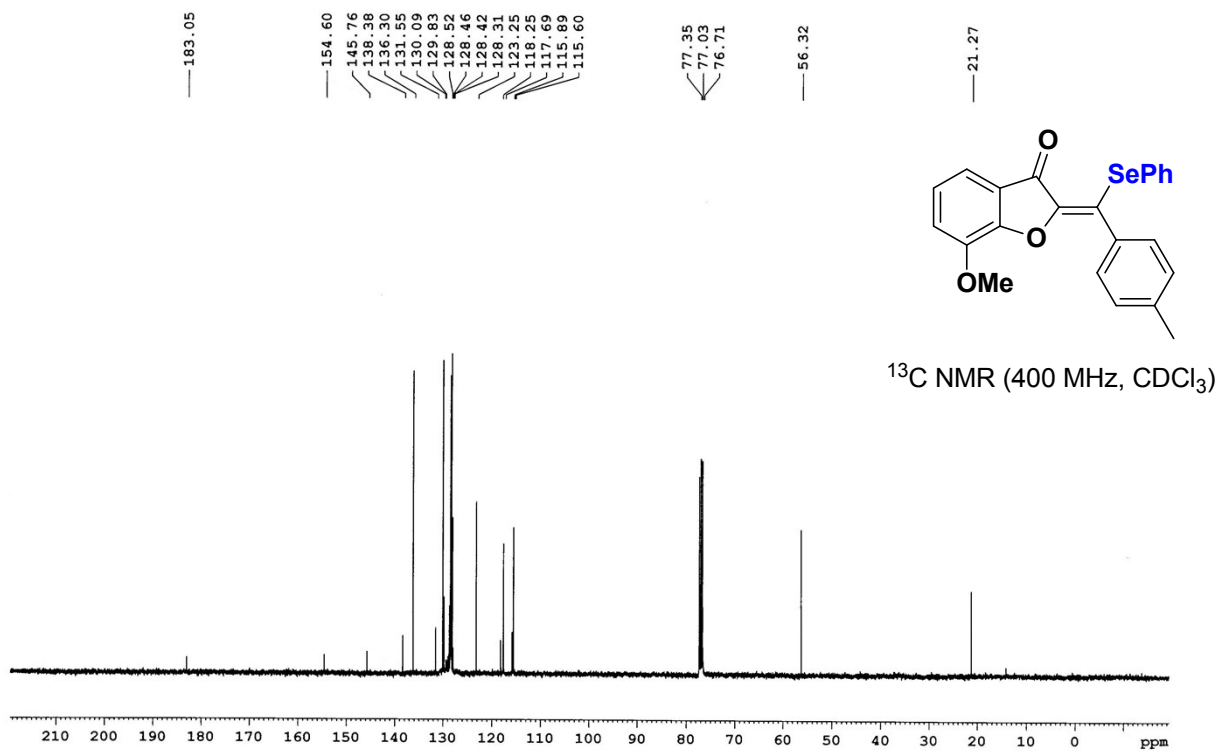
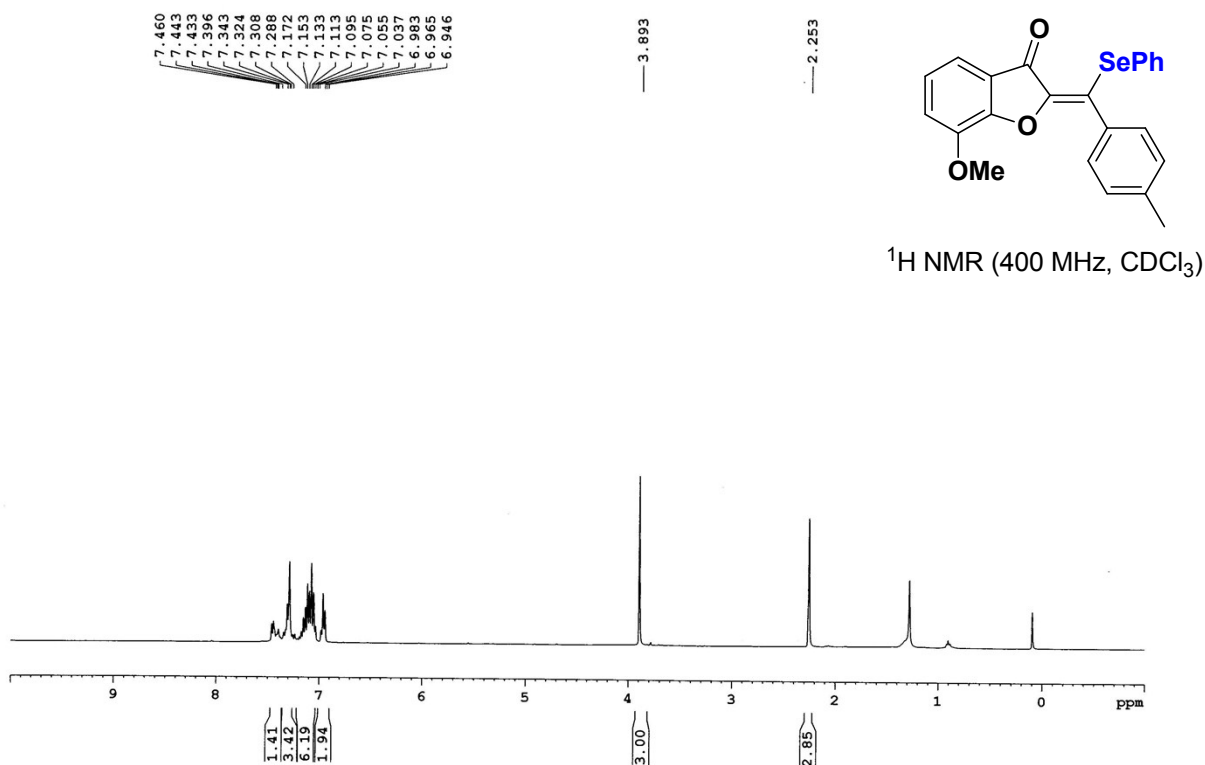


$^{77}\text{Se}$  NMR (76 MHz,  $\text{CDCl}_3$ )

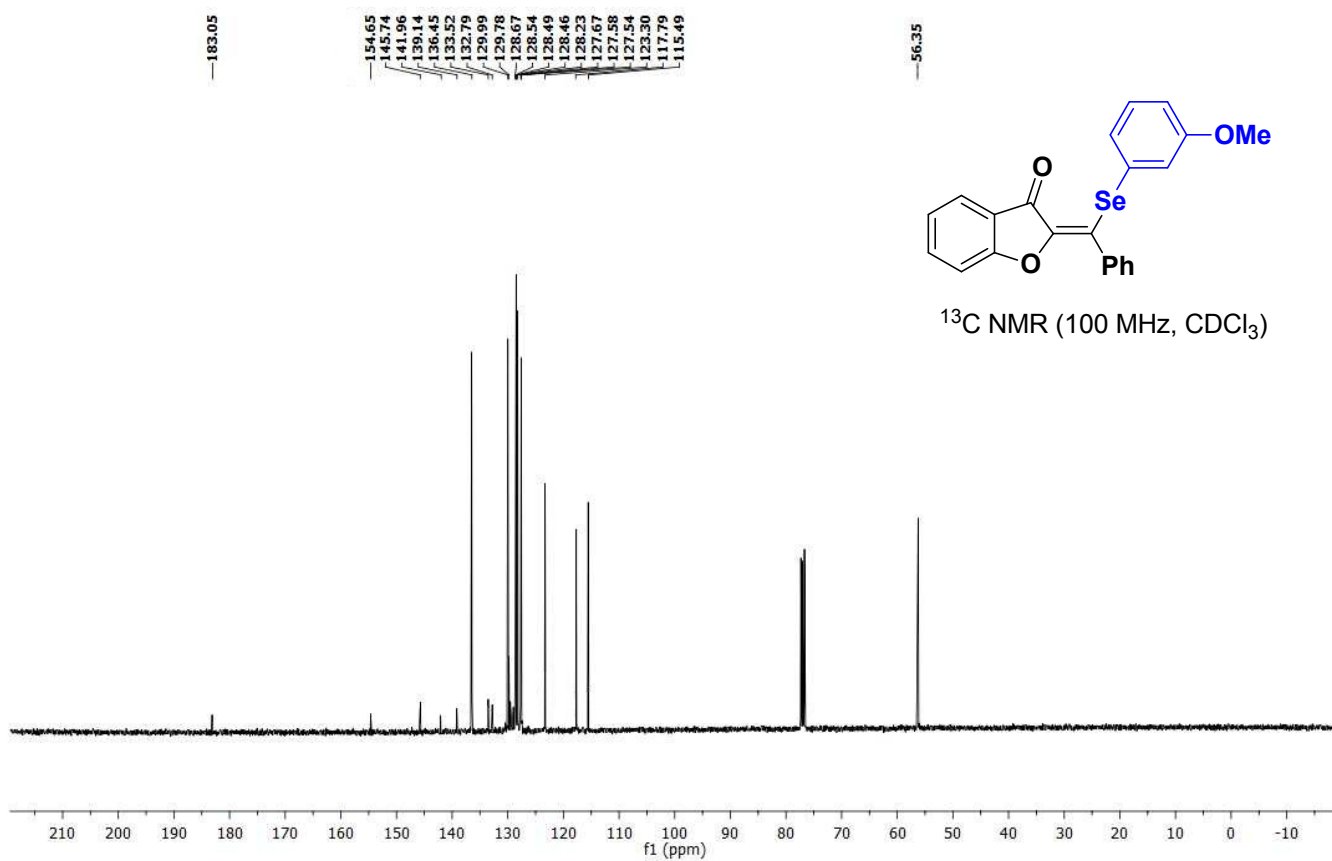
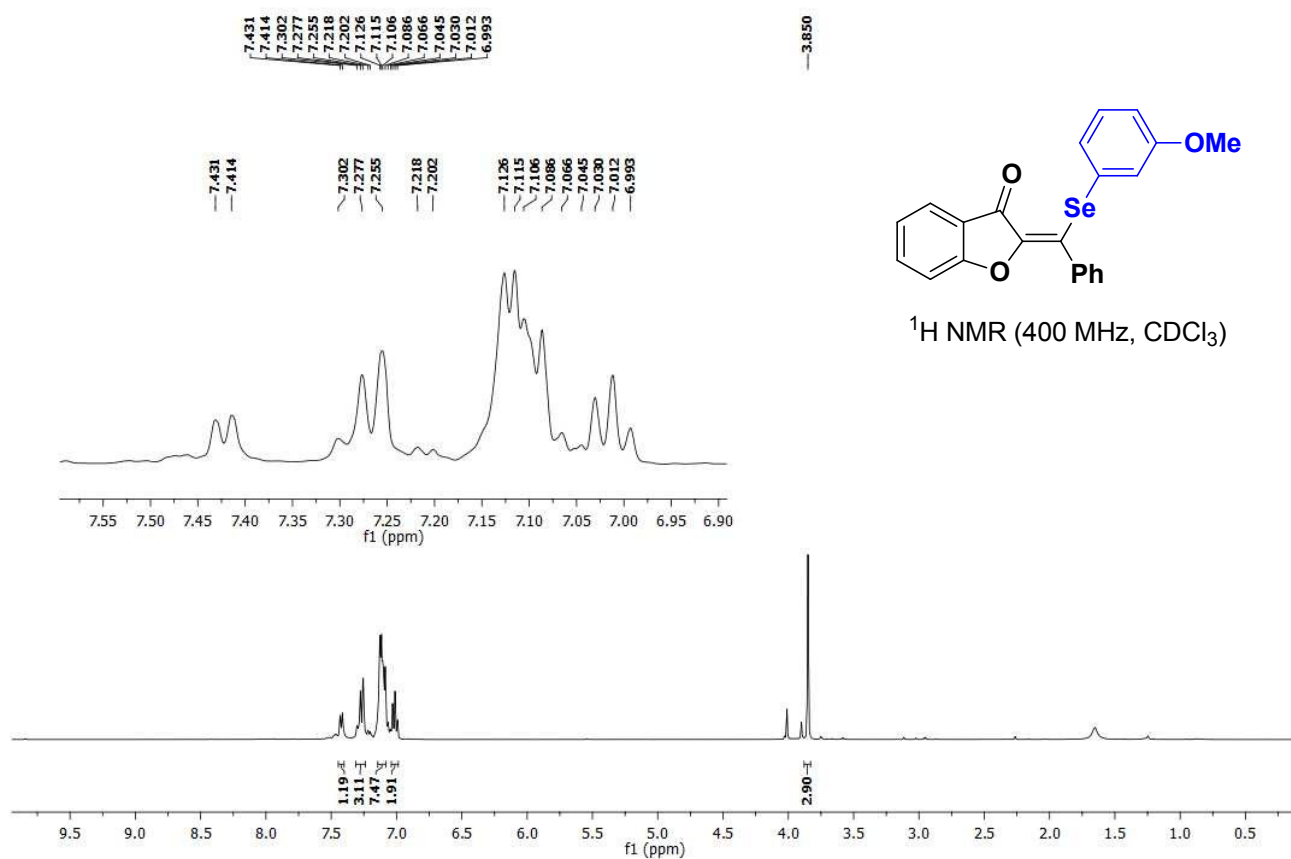
446.37  
446.24  
446.10



**(E)-7-methoxy-2-((phenylselanyl)(p-tolyl)methylene)benzofuran-3(2H)-one (5f)**



**(E)-2-(((3-methoxyphenyl)selenyl)(phenyl)methylene)benzofuran-3(2H)-one (5g)**





**(E)-2-(((4-bromophenyl)selenanyl)(phenyl)methylene)-7-methoxybenzofuran-3(2H)-one**  
**(5h)**

