- Supporting Information-

Ru(II)-Catalyzed C–H Functionalization on Maleimides with Electrophiles: A Demonstration of Umpolung Strategy

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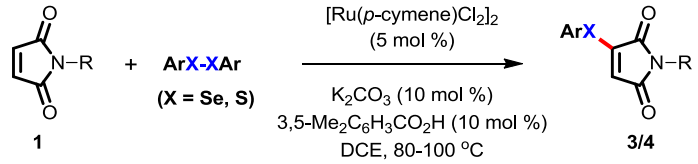
1. General Information

The catalyst $[Ru(p\text{-cymene})Cl_2]_2$ was purchased from Sigma Aldrich company. All reactions were monitored by thin layer chromatography (TLC) on Merck 60 F 254 precoated silica plates and visualized using a UV lamp (366 or 254 nm) or by use of potassium permanganate, 5 g K_2CO_3, / 100 mL water. Products were isolated by column chromatography (Merck silica gel 100-200μm). Yields refer to chromatographically and spectroscopically homogenous materials unless noted otherwise. ^{13}C and ^{1}H NMR spectra were recorded on a Bruker 400 or Bruker 500 MHz spectrometers. Chemical shift values (δ) are reported in ppm and calibrated to the residual solvent peak $CDCl_3$ δ = 7.2600 ppm for ^{1}H, δ = 77.16 for ^{13}C; or calibrated to tetramethylsilane (δ = 0.00). All NMR spectra were recorded at ambient temperature (290 K) unless otherwise noted. ^{1}H NMR spectra are reported as follows: chemical shift (multiplicity, coupling constant, integration). The following abbreviations are used to indicate multiplicities: s, singlet; d, doublet; t, triplet; q, quartet; quint, quintet; sext, sextet; sept, septet; m, multiplet; dd, doublet of doublet; dt, doublet of triplet; dq, doublet of quartet; td, triplet of doublet; tt, triplet of triplet; dq, doublet of quartet; br, broad. Mass spectra were recorded by electron spry ionization (ESI) method on a Q-TOF Micro with lock spray source. The crystal data were collected and integrated using a Bruker Axs kappa apex2 CCD diffractometer, with graphite monochromated Mo-Kα radiation.

2. Typical ruthenium(II)-catalyzed chalcogenation of maleimides:

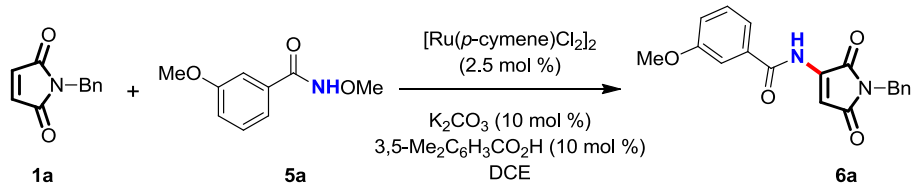


Procedure: To an oven dried reaction tube (10×1.5 cm) equipped with a magnetic stir, corresponding maleimide derivatives **1** (0.1 mmol, 1 equiv), $[Ru(p\text{-cymene})Cl_2]_2$ (5 mol %), mesitylenic acid (10 mol %), K_2CO_3(10 mol %), and diaryldichalcogenide (1.2 equiv) were added. 1,2-Dichloroethane (DCE, 1.0 ml) was added. The reaction tube was capped and the reaction mixture was stirred at 80-100 ^oC for 24 h. After completion (monitored by TLC), the solvent was evaporated under reduced pressure and the resulting residue was purified by silica gel column chromatography with a gradient eluent of hexane and ethyl acetate to provide pure functionalized maleimides **3-4**.

The selenylation reaction of **1a** was also performed in 1.5 mmol scale. To an oven dried Schlenk tube (30 ml) equipped with a magnetic stir, corresponding maleimide derivatives **1** (1.5 mmol, 0.28 g, 1 equiv), $[Ru(p\text{-cymene})Cl_2]_2$ (5 mol %), mesitylenic acid (10 mol %), K_2CO_3(10 mol %), and diaryldichalcogenide (1.2 equiv) were added. 1,2-Dichloroethane (DCE, 15 ml) was added. The Schlenk tube was capped and the reaction mixture was stirred at 80 ^oC for 24 h. After completion, the solvent was evaporated under reduced pressure and the resulting residue was purified by silica gel column chromatography with a gradient eluent of hexane and ethyl acetate to provide pure compound **3a** as yellow oil (0.43 g, 84% yield).

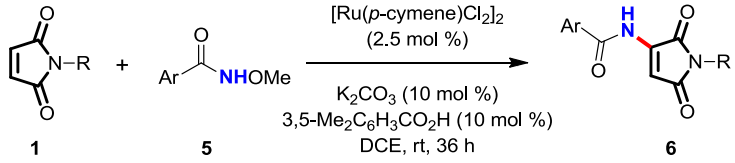
3. Typical ruthenium(II)-catalyzed amidation of maleimides:

a) Optimization of the reaction conditions:



1a **5a** **6a**

entry	**1a** (equiv)	**5a** (equiv)	catalyst (mol %)	temperature (^{o}C)	time (h)	yield (%)
1	1.0	1.2	5.0	60	24	17
2	1.0	1.2	5.0	r.t.	24	30
3	1.0	1.2	2.5	r.t.	24	35
4	2.0	1.0	2.5	r.t.	24	46
5	**2.0**	**1.0**	**2.5**	**r.t.**	**36**	**57**



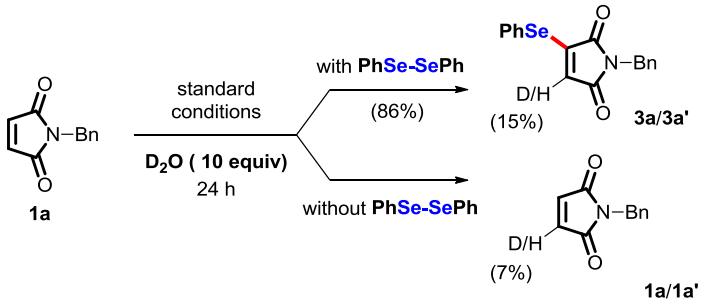
1 **5** **6**

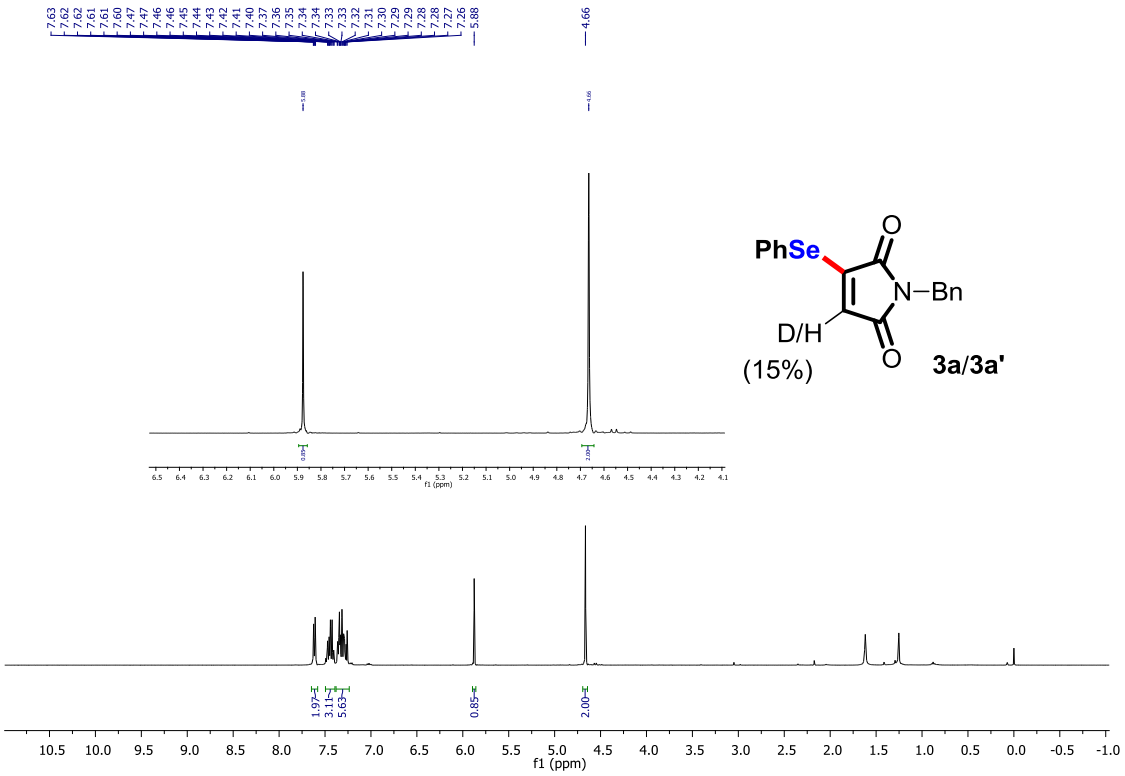
b) General procedure: Corresponding N-methoxybenzamides **5** (0.1 mmol, 1 equiv), maleimide derivatives **1** (2 equiv), [Ru(p-cymene)Cl_2]$_2$ (2.5 mol %), 3,5-dimethylbenzoic acid (10 mol %), and K_2CO_3 (10 mol %) were added to an oven dried reaction tube (10×1.5 cm) and 1,2-dichloroethane (DCE, 0.3 ml) was added. The reaction tube was capped and the reaction mixture was stirred at room temperature for 36 h. After completion (monitored by TLC), the solvent was evaporated under reduced pressure and the resulting residue was purified by silica gel column chromatography with a gradient eluent of hexane and ethyl acetate to provide pure benzamido substituted maleimides **6**.

4. Control experiments:

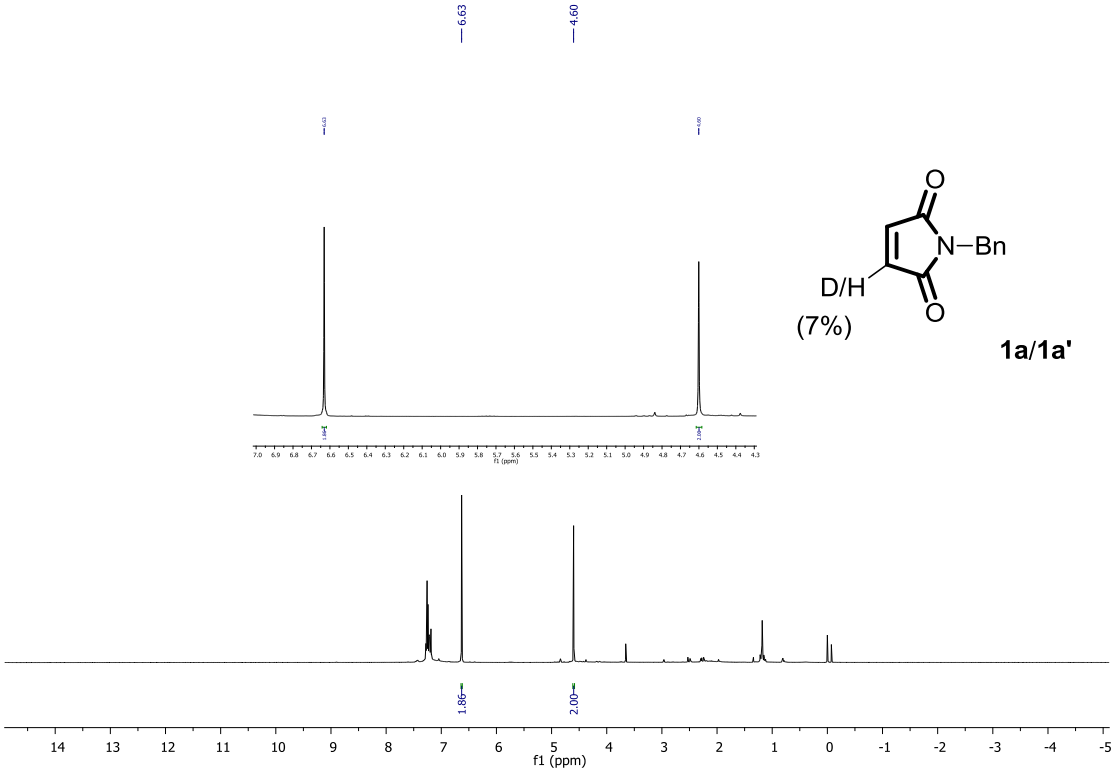
(a) Deuterium exchange reaction:

In order to gain mechanistic insights of the selenylation protocol, we have performed the reaction in the presence of D_2O under the optimal conditions. In the presence of diselenide, 15% deuterium-hydrogen exchange was observed in product (**3a'** *vs* **3a**). In the absence of diselenide, 7% deuterium-hydrogen exchange was observed in maleimide (**1a'** *vs* **1a**). These results favor a reversible metalation process.



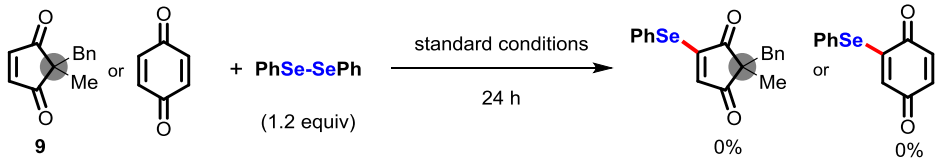


^{1}H NMR spectrum for product (**3a**) of deuterium exchange reaction in the presence of PhSe-SePh.



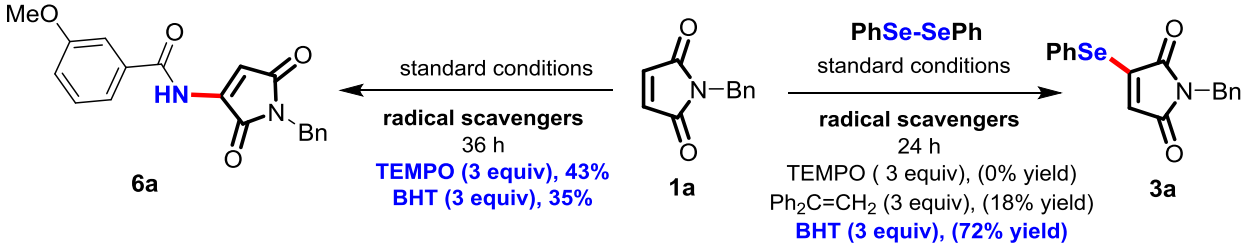
^{1}H NMR spectrum for substrate (**1a**) of deuterium exchange reaction in the absence of PhSe-SePh.

(b) Reaction with 2-benzyl-2-methylcyclopent-4-ene-1,3-dione (9) and *p*-benzoquinone (10):



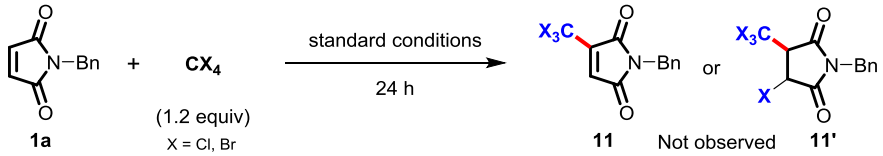
When our synthetic protocol was performed with 2-benzyl-2-methylcyclopent-4-ene-1,3-dione (**9**) and p-benzoquinone (**10**), the reaction did not provide Se-functionalized products. This particular result signifies the pivotal role of the amide linkage in the reaction.

(c) Reactions with radical scavengers:



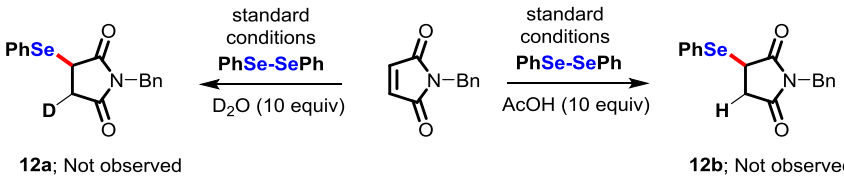
The maleimide functionalization reaction was also performed in presence of radical scavengers under our standard reaction conditions. Radical scavengers such as TEMPO and 1,1-diphenylethylene (3.0 equiv) showed a detrimental effect in the product formation, whereas BHT (3.0 equiv.) did not inhibit the product formation. These observations discard the involvement of a radical species in the reaction mechanism.

(d) Reactions with tetrahalogenomethanes:



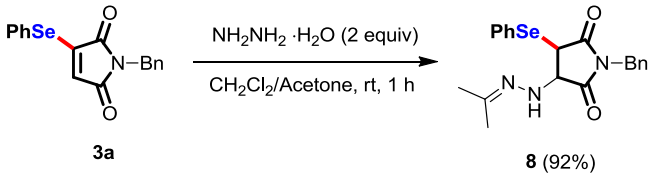
When our synthetic protocol was performed with tetrachloromethane (CCl_4) and tetrabromomethane (CBr_4) as the coupling partners, the reaction compounds **11** and **11′** were not formed. This particular result excludes the possibility of Kharasch type of addition to the olefin bond.

(e) Scrutinization the involvement of migratory insertion:



To probe the mechanistic route of the selenylation protocol, we have performed the reaction in the presence of D_2O and acetic acid under the optimal conditions. Delightfully, the formation of **12a** and **12b** were not observed. These results eliminate the possibility of migratory insertion.

5. Functionalization of selenomaleimide 3a:



Procedure: To an oven dried reaction tube (10×1.5 cm) was added selenomaleimide derivative 3**a** (0.15 mmol, 1 equiv) and hydrazine hydrate (2.0 equiv) in 2.0 ml dichloromethane/acetone mixture (100:1, v/v). The reaction tube was caped and the reaction mixture was stirred at room temperature for 1 h. After completion (monitored by TLC), the solvent was evaporated under reduced pressure. In order to get pure functionalized succinimide, the resulting residue was purified by column chromatography on silica gel with a gradient eluent of hexane and ethyl acetate (57 mg, 92% yield).

6. Crystallographic data analysis:

ORTEP diagram of compound 3e (CCDC number: 1527457)

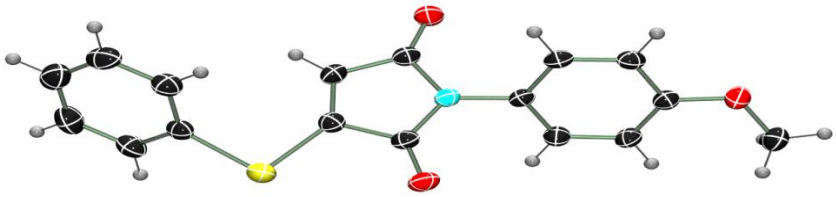
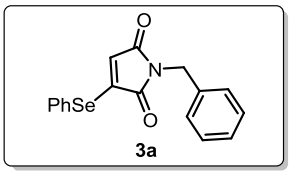


Table S1. Crystal data and structure refinement for imide (Ellipsoid probability 30%).

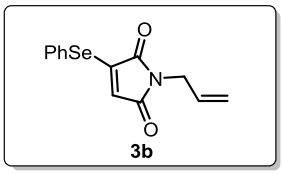
Identification code	imide
Empirical formula	C17 H13 N O3 Se
Formula weight	358.24
Temperature	296(2) K
Wavelength	0.71073 A

Crystal system, space group	Monoclinic, P2(1)/c
Unit cell dimensions	a = 18.8061(9) A alpha = 90 deg.
	b = 5.9523(2) A beta = 90.605(2) deg.
	c = 13.3383(6) A gamma = 90 deg.
Volume	1493.00(11) A^3
Z, Calculated density	4, 1.594 Mg/m^3
Absorption coefficient	2.527 mm^-1
F(000)	720
Crystal size	0.250 x 0.220 x 0.100 mm
Theta range for data collection	2.166 to 24.997 deg.
Limiting indices	-22<=h<=22, -7<=k<=6, -13<=l<=15
Reflections collected / unique	9710 / 2620 [R(int) = 0.0304]
Completeness to theta =	24.997 99.8 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2620 / 0 / 201
Goodness-of-fit on F^2	1.027
Final R indices [I>2sigma(I)]	R1 = 0.0351, wR2 = 0.0658
R indices (all data)	R1 = 0.0550, wR2 = 0.0725
Extinction coefficient	0.0160(7)
Largest diff. peak and hole	0.495 and -0.438 e.A^-3

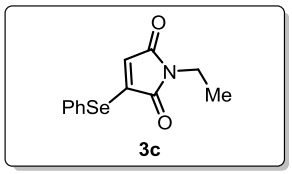
7. Spectroscopic data of synthesized compounds:



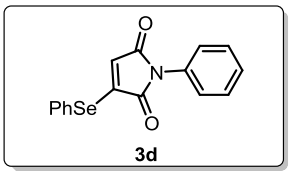
1-benzyl-3-(phenylselanyl)-1H-pyrrole-2,5-dione (3a): Yield 93% (32 mg), yellow liquid; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.54 (dd, *J* = 8.1, 1.4 Hz, 2H), 7.43–7.30 (m, 3H), 7.30–7.15 (m, 5H), 5.80 (s, 1H), 4.58 (s, 2H) ppm; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 169.44 , 168.75, 150.70, 136.34 , 136.00 , 130.40, 130.22 , 128.79, 128.63, 127.96, 124.68, 123.90, 121.27, 41.89 ppm; **HRMS** (ESI/TOF-Q) m/z: 366.0009 [M + Na]+ Calcd. For $C_{17}H_{13}NO_2SeNa$; Found 365.9975.



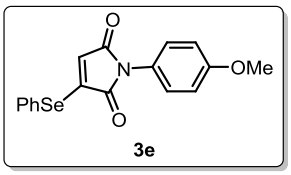
1-allyl-3-(phenylselanyl)-1H-pyrrole-2,5-dione (3b): Yield 94% (27 mg), yellow liquid; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.72 – 7.54 (m, 2H), 7.56 – 7.34 (m, 3H), 5.90 (s, 1H), 5.80 (ddt, *J* = 16.0, 10.5, 5.7 Hz, 1H), 5.29 – 5.09 (m, 2H), 4.12 (dt, *J* = 5.6, 1.2 Hz, 2H) ppm; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 169.33, 168.66, 150.65 (s), 136.01 (s), 131.65 (s), 130.42 (s), 130.23 (s), 127.55 (s), 124.66 (s), 123.92 (s), 117.87 (s), 40.37 (s) ppm; **HRMS** (ESI/TOF-Q) m/z: 315.9853 [M + Na]+ Calcd. For $C_{13}H_{11}NO_2SeNa$; Found 315.9849.



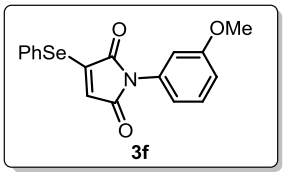
1-ethyl-3-(phenylselanyl)-1H-pyrrole-2,5-dione (3c): Yield 77% (22 mg), yellow liquid; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.62 (d, *J* = 6.9 Hz, 2H), 7.44 (m, 3H), 5.85 (s, 1H), 3.55 (q, *J* = 7.2 Hz, 2H), 1.17 (t, *J* = 7.2 Hz, 3H) ppm; 13C NMR (101 MHz, CDCl3) δ 169.65, 168.92, 150.43, 135.97, 130.35, 130.18, 124.65, 123.98, 33.24, 14.05 ppm.



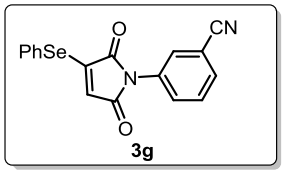
1-phenyl-3-(phenylselanyl)-1H-pyrrole-2,5-dione (3d): Yield 75% (25 mg), yellow solid; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.72 – 7.65 (m, 2H), 7.53 – 7.41 (m, 5H), 7.38 – 7.31 (m, 3H), 6.02 (s, 1H) ppm; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 168.56, 167.90, 151.27, 136.07, 131.50, 130.51, 130.36, 129.23, 127.96, 126.03, 124.61, 123.79 ppm; **HRMS** (ESI/TOF-Q) m/z: 351.9853 [M + Na]+ Calcd. For $C_{16}H_{11}NO_2SeNa$; Found 351.9861.



1-(4-methoxyphenyl)-3-(phenylselanyl)-1H-pyrrole-2,5-dione (3e): Yield 87% (31 mg), yellow solid; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.68 (dd, *J* = 7.9, 1.5 Hz, 2H), 7.57 – 7.41 (m, 3H), 7.23 (d, *J* = 9.0 Hz, 2H), 6.96 (d, *J* = 9.0 Hz, 2H), 6.00 (s, 1H), 3.82 (s, 3H) ppm; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 168.88, 168.14, 159.21, 151.10, 136.08, 130.49, 130.33, 127.55, 124.60, 124.16, 123.89, 114.57, 55.62; **HRMS** (ESI/TOF-Q) m/z: 381.9958 [M + Na]+ Calcd. For $C_{17}H_{13}NO_3SeNa$; Found 381.9966.

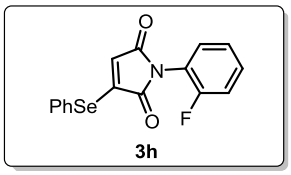


1-(3-methoxyphenyl)-3-(phenylselanyl)-1H-pyrrole-2,5-dione (3f): Yield 66% (24 mg), yellow solid; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.71 – 7.63 (m, 2H), 7.57 – 7.39 (m, 3H), 7.39 – 7.29 (m, 1H), 6.99 – 6.83 (m, 3H), 6.01 (s, 1H), 3.81 (s, 3H) ppm; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 168.48, 167.85, 160.15, 151.29, 136.09, 132.53, 130.53, 130.38, 129.91, 124.67, 123.83, 118.30, 113.95, 111.80, 55.55 ppm; **HRMS** (ESI/TOF-Q) m/z: 381.9958 [M + Na]+ Calcd. For $C_{17}H_{13}NO_3SeNa$; Found 381.9945.



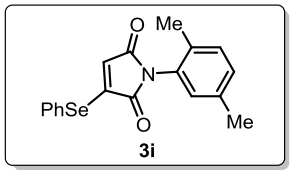
3-(2,5-dioxo-3-(phenylselanyl)-2,5-dihydro-1H-pyrrol-1-yl)benzonitrile (3g): Yield 86% (30 mg), yellow solid; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.68 (d, *J* = 6.8 Hz, 3H), 7.59 (s, 3H), 7.55 – 7.43 (m, 3H), 6.05 (s, 1H) ppm; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 167.92, 167.52, 151.74, 136.08, 132.22, 129.78, 128.92, 124.66, 124.50,

124.46, 123.64, 122.72, 122.68 ppm; **HRMS** (ESI/TOF-Q) m/z: 376.9805 [M + Na]+ Calcd. For $C_{17}H_{10}N_2O_2SeNa$; Found 376.9791.



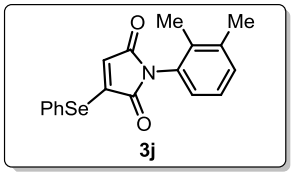
3h

1-(2-fluorophenyl)-3-(phenylselanyl)-1H-pyrrole-2,5-dione (3h): Yield 89% (31 mg), yellow solid; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.61 (m, 2H), 7.45 – 7.29 (m, 4H), 7.22 – 7.11 (m, 3H), 5.98 (s, 1H) ppm; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 167.69, 167.13, 157.89 (d, J = 252.6 Hz), 151.58, 136.09, 130.75 (d, J = 7.7 Hz), 130.53, 130.41, 129.81, 125.10, 124.73 (d, J = 3.8 Hz), 123.80, 119.12 (d, J = 13.3 Hz), 116.85 (d, J = 19.7 Hz) ppm; **HRMS** (ESI/TOF-Q) m/z: 369.9758 [M + Na]+ Calcd. For $C_{16}H_{10}NO_2FSeNa$; Found 369.9732.



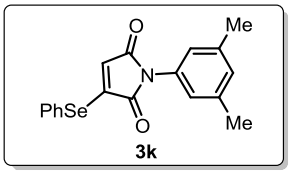
3i

1-(2,5-dimethylphenyl)-3-(phenylselanyl)-1H-pyrrole-2,5-dione (3i): Yield 86% (31 mg), yellow solid; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.74 – 7.65 (m, 2H), 7.58 – 7.39 (m, 3H), 7.16 (m, 2H), 6.89 (m, 1H), 6.03 (s, 1H), 2.33 (s, 3H), 2.13 (s, 3H) ppm; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 168.84, 167.97, 151.13, 136.80, 136.09, 134.49, 133.42, 131.04, 130.50, 130.39, 130.34, 130.04, 129.22, 20.89, 17.64 ppm.



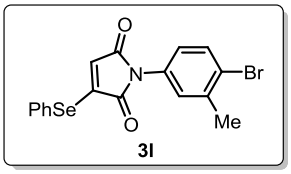
3j

1-(2,3-dimethylphenyl)-3-(phenylselanyl)-1H-pyrrole-2,5-dione (3j): Yield 81% (29 mg), yellow solid; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.73 – 7.67 (m, 2H), 7.54 – 7.42 (m, 3H), 7.24 – 7.14 (m, 2H), 6.97 (d, J = 7.5 Hz, 1H), 6.04 (s, 1H), 2.32 (s, 3H), 2.06 (s, 3H) ppm; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 168.94, 168.06, 151.13, 138.53, 136.08, 135.28, 131.01, 130.49, 130.33, 130.22, 126.34, 124.84, 123.93, 20.51, 14.74 ppm; **HRMS** (ESI/TOF-Q) m/z: 358.0346 [M + H]+ Calcd. For $C_{18}H_{16}NO_2Se$; Found 358.0327.



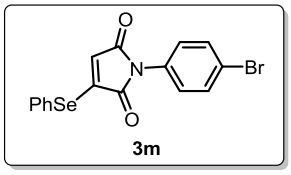
3k

1-(3,5-dimethylphenyl)-3-(phenylselanyl)-1H-pyrrole-2,5-dione (3k): Yield 72% (26 mg), yellow solid; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.68 (dd, *J* = 8.0, 1.6 Hz, 2H), 7.53 – 7.42 (m, 3H), 6.99 (s, 1H), 6.93 (s, 2H), 6.01 (s, 1H), 2.34 (s, 6H) ppm; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 168.78, 168.07, 151.12, 139.01, 136.08, 131.21, 130.49, 130.32, 129.96, 124.65, 124.03, 123.92, 21.39 ppm; **HRMS** (ESI/TOF-Q) m/z: 380.0166 [M + Na]+ Calcd. For $C_{18}H_{15}NO_2SeNa$; Found 380.0184.



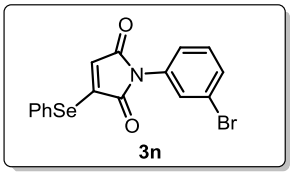
3l

1-(4-bromo-3-methylphenyl)-3-(phenylselanyl)-1H-pyrrole-2,5-dione (3l): Yield 68% (29 mg), yellow solid; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.59 (d, *J* = 6.7 Hz, 2H), 7.52 (d, *J* = 8.5 Hz, 1H), 7.45 – 7.32 (m, 3H), 7.17 (d, *J* = 7.3 Hz, 1H), 6.98 (d, *J* = 8.4 Hz, 1H), 5.93 (s, 1H), 2.34 (s, 3H) ppm; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 168.23, 167.67, 151.45, 139.13, 136.06, 133.03, 130.55, 130.41, 128.08, 124.80, 124.66, 124.23, 123.77, 23.20 ppm.



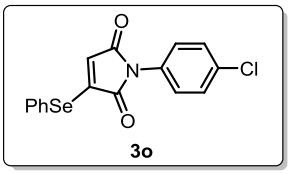
3m

1-(4-bromophenyl)-3-(phenylselanyl)-1H-pyrrole-2,5-dione (3m): Yield 78% (32 mg), yellow solid; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.71 – 7.64 (m, 2H), 7.60 – 7.55 (m, 2H), 7.53 – 7.43 (m, 3H), 7.29 – 7.24 (m, 2H), 6.02 (s, 1H) ppm; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 168.09, 167.57, 151.57, 136.07, 132.38, 130.67, 130.57, 130.45, 127.31, 124.66, 123.72, 121.56 ppm.



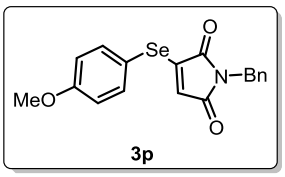
3n

1-(3-bromophenyl)-3-(phenylselanyl)-1H-pyrrole-2,5-dione (3n): Yield 88% (36 mg), yellow solid; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.71 – 7.63 (m, 2H), 7.56 (s, 1H), 7.54 – 7.41 (m, 4H), 7.36 – 7.29 (m, 2H), 6.02 (s, 1H) ppm; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 167.97 (s), 167.46 (s), 151.58 (s), 136.07 (s), 132.81 (s), 130.93 (s), 130.58 (s), 130.46 (s), 130.40 (s), 128.84 (s), 124.66 (s), 124.40 (s), 123.71 (s), 122.53 (s) ppm.



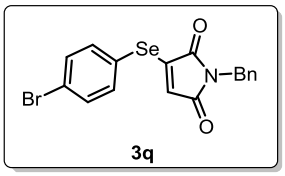
3o

1-(4-chlorophenyl)-3-(phenylselanyl)-1H-pyrrole-2,5-dione (3o): Yield 60% (22 mg), yellow solid; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.71 – 7.63 (m, 2H), 7.47 (m, 5H), 7.32 (m, 2H), 6.02 (s, 1H) ppm; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 168.18, 167.64, 151.54, 136.08, 133.60, 130.58, 130.45, 130.13, 129.41, 127.06, 124.66, 123.73 ppm; **HRMS** (ESI/TOF-Q) m/z: 385.9463 [M + Na]+ Calcd. For $C_{16}H_{10}NO_2ClSeNa$; Found 385.9478.



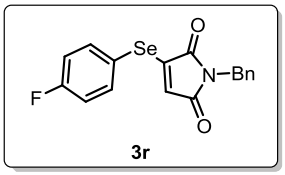
3p

1-benzyl-3-((4-methoxyphenyl)selanyl)-1H-pyrrole-2,5-dione (3p): Yield 54% (20 mg), yellow solid; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.51 – 7.39 (m, 2H), 7.36 – 7.12 (m, 5H), 6.86 (d, *J* = 8.9 Hz, 2H), 5.77 (s, 1H), 4.58 (s, 2H), 3.77 (s, 3H) ppm; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 169.46, 168.82, 161.27, 151.66, 137.58, 136.42, 128.80, 128.65, 127.96, 124.64, 116.10, 113.90, 55.56, 41.87 ppm.



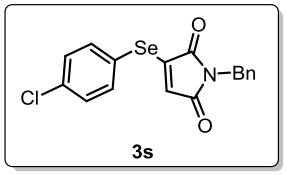
3q

1-benzyl-3-((4-bromophenyl)selanyl)-1H-pyrrole-2,5-dione (3q): Yield 57% (24 mg), yellow solid; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.58 – 7.53 (m, 2H), 7.50 – 7.45 (m, 2H), 7.37 – 7.23 (m, 5H), 5.90 (s, 1H), 4.66 (s, 2H) ppm; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 169.15, 168.54, 149.87, 137.54, 136.25, 133.68, 128.83, 128.68, 128.03, 125.16, 124.94, 122.61, 41.97 ppm.



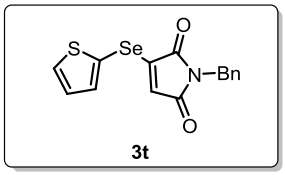
3r

1-benzyl-3-((4-fluorophenyl)selanyl)-1H-pyrrole-2,5-dione (3r): Yield 51% (18 mg), yellow solid; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.53 (m, 2H), 7.31 – 7.16 (m, 5H), 7.06 (s, 2H), 5.78 (s, 1H), 4.59 (s, 2H) ppm; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 169.24 (s), 168.62 (s), 164.04 (d, *J* = 251.7 Hz), 150.56 (s), 138.24 (d, *J* = 8.4 Hz), 136.30 (s), 128.83 (s), 128.68 (s), 128.03 (s), 124.83 (s), 118.58 (d, *J* = 3.3 Hz), 117.87 (d, *J* = 21.9 Hz), 41.96 (s) ppm; **HRMS** (ESI/TOF-Q) m/z: 383.9915 [M + Na]+ Calcd. For $C_{17}H_{12}FNO_2SeNa$; Found 383.9931.



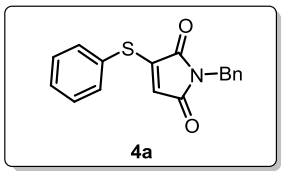
3s

1-benzyl-3-((4-chlorophenyl)selanyl)-1H-pyrrole-2,5-dione (3s): Yield 87% (33 mg), yellow solid; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.57 – 7.51 (m, 2H), 7.44 – 7.37 (m, 2H), 7.36 – 7.23 (m, 5H), 5.89 (s, 1H), 4.66 (s, 2H) ppm; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 169.15, 168.54, 149.99, 136.91, 136.25, 130.71, 128.81, 128.66, 128.01, 124.90, 121.92, 41.95 ppm.



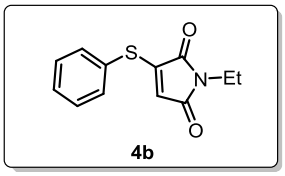
3t

1-benzyl-3-(thiophen-2-ylselanyl)-1H-pyrrole-2,5-dione (3t): Yield 44% (15 mg), yellow solid; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.60 (d, *J* = 5.1 Hz, 1H), 7.30 (m, 6H), 7.13 (m, 1H), 5.96 (s, 1H), 4.66 (s, 2H) ppm; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 169.16, 168.40, 150.62, 138.25, 136.25, 133.88, 129.09, 128.84, 128.65, 128.04, 125.90, 41.93 ppm; **HRMS** (ESI/TOF-Q) m/z: 349.9754 [M + H]+ Calcd. For $C_{15}H_{12}NO_2SSe$; Found 349.9753.



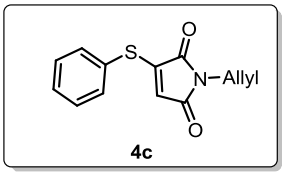
4a

1-benzyl-3-(phenylthio)-1H-pyrrole-2,5-dione (4a): Yield 33% (10 mg), colorless liquid; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.54 (d, *J* = 7.5 Hz, 2H), 7.48 (s, 3H), 7.35 (t, *J* = 6.7 Hz, 2H), 7.32 – 7.25 (m, 3H), 5.64 (s, 1H), 4.66 (s, 2H) ppm; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 169.19, 167.72, 152.79, 143.94, 134.51, 130.61, 130.37, 128.82, 128.69, 128.01, 127.43, 119.02, 41.89 ppm.



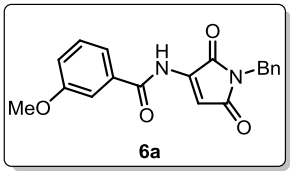
4b

1-ethyl-3-(phenylthio)-1H-pyrrole-2,5-dione (4b): Yield 30% (7 mg), colorless liquid; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.63 – 7.52 (m, 2H), 7.50 – 7.40 (m, 3H), 5.63 (s, 1H), 3.57 (q, *J* = 7.2 Hz, 2H), 1.20 (t, *J* = 7.2 Hz, 3H) ppm; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 169.55, 167.92, 152.60, 134.50, 130.56, 130.34, 127.56, 119.00, 33.26, 14.06 ppm.



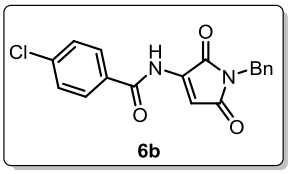
4c

1-allyl-3-(phenylthio)-1H-pyrrole-2,5-dione (4c): Yield 35% (9 mg), colorless liquid; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.62 – 7.53 (m, 2H), 7.52 – 7.40 (m, 3H), 5.89 – 5.72 (m, 1H), 5.66 (s, 1H), 5.19 (ddd, *J* = 11.7, 9.4, 1.1 Hz, 2H), 4.12 (dt, *J* = 5.7, 1.4 Hz, 2H) ppm; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 169.17, 167.61, 152.75, 134.51, 131.64, 130.62, 130.38, 127.46, 118.99, 117.95, 40.36 ppm.



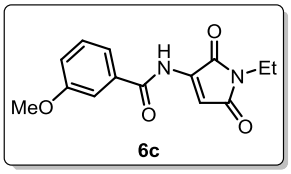
6a

N-(1-benzyl-2,5-dioxo-2,5-dihydro-1H-pyrrol-3-yl)-3-methoxybenzamide (6a): Yield 57% (19 mg), white solid; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.48 (s, 1H), 7.37 – 7.32 (m, 2H), 7.29 – 7.17 (m, 5H), 7.07 (dt, *J* = 7.3, 2.2 Hz, 1H), 6.62 (s, 1H), 4.63 (s, 2H), 3.79 (s, 3H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.74, 167.95, 165.41, 160.32, 138.50, 136.14, 133.49, 130.27, 128.86, 128.46, 128.07, 119.77, 119.22, 112.84, 105.03, 55.69, 41.65 ppm; **HRMS** (ESI/TOF-Q) m/z: 337.1188 [M + H]+ Calcd. For $C_{19}H_{17}N_2O_4$; Found 337.1164.



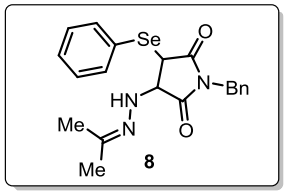
6b

N-(1-benzyl-2,5-dioxo-2,5-dihydro-1H-pyrrol-3-yl)-4-chlorobenzamide (6b): Yield 54% (18 mg), white solid; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.51 (s, 1H), 7.87 – 7.79 (m, 2H), 7.55 – 7.49 (m, 2H), 7.37 – 7.31 (m, 5H), 6.71 (s, 1H), 4.72 (s, 2H) ppm; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 171.58, 167.93, 164.45, 140.14, 138.35, 136.10, 130.49, 129.66, 129.00, 128.90, 128.49, 128.13, 105.36, 41.73 ppm; **HRMS** (ESI/TOF-Q) m/z: 379.0252 [M + K]+ Calcd. For $C_{18}H_{13}N_2O_3ClK$; Found 379.0253.



6c

N-(1-ethyl-2,5-dioxo-2,5-dihydro-1H-pyrrol-3-yl)-3-methoxybenzamide (6c): Yield 56% (15 mg), white solid; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.57 (s, 1H), 7.51 – 7.32 (m, 3H), 7.27 (s, 1H), 7.16 (dt, *J* = 7.0, 2.5 Hz, 1H), 3.88 (s, 3H), 3.61 (q, *J* = 7.2 Hz, 2H), 1.22 (t, *J* = 7.2 Hz, 3H) ppm; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 172.06, 168.12, 165.46, 160.32, 138.40, 133.55, 130.28, 119.73, 119.23, 112.88, 104.97, 55.71, 33.07, 14.11 ppm.



8

1-benzyl-3-(phenylthio)-4-(2-(propan-2-ylidene)hydrazinyl)pyrrolidine-2,5-dione (8): Yield 92% (57 mg), white solid; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.55 (dd, *J* = 8.1, 1.2 Hz, 2H), 7.34 – 7.21 (m, 6H), 7.20 – 7.15 (m, 2H), 5.14 (s, 1H), 4.60 (q, *J* = 14.4 Hz, 2H), 4.35 (d, *J* = 4.4 Hz, 1H), 3.94 (d, *J* = 4.4 Hz, 1H), 1.79 (s, 3H), 1.72 (s, 3H) ppm; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 176.25, 174.87, 151.45, 136.21, 135.40, 129.53, 129.30, 128.62, 128.27, 127.78, 125.71, 65.02, 42.79, 41.50, 25.24, 16.03 ppm; **HRMS** (ESI/TOF-Q) m/z: 438.0697 [M + Na]+ Calcd. For $C_{20}H_{21}N_3O_2SeNa$; Found 438.0647.

NMR Spectra of Synthesized Compounds


7.55
7.54
7.53
7.52
7.39
7.38
7.37
7.36
7.34
7.29
7.28
7.28
7.27
7.26
7.25
7.25
7.25
7.23
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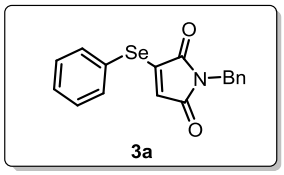
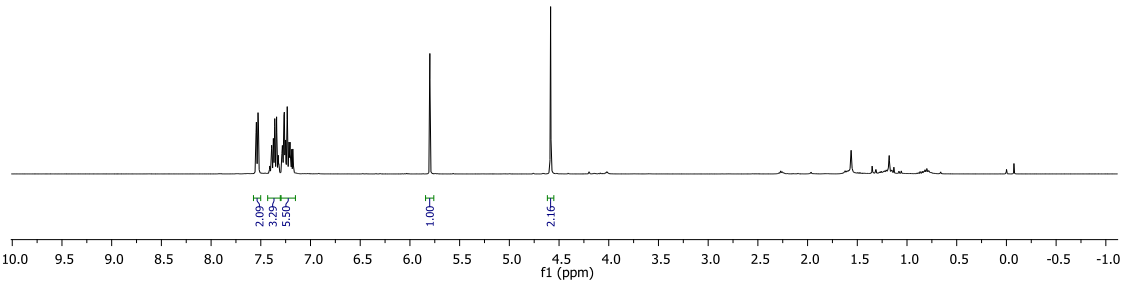
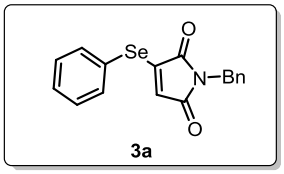
7.20
7.19
7.18
7.17
5.80
4.58


Se
O
N–Bn
O

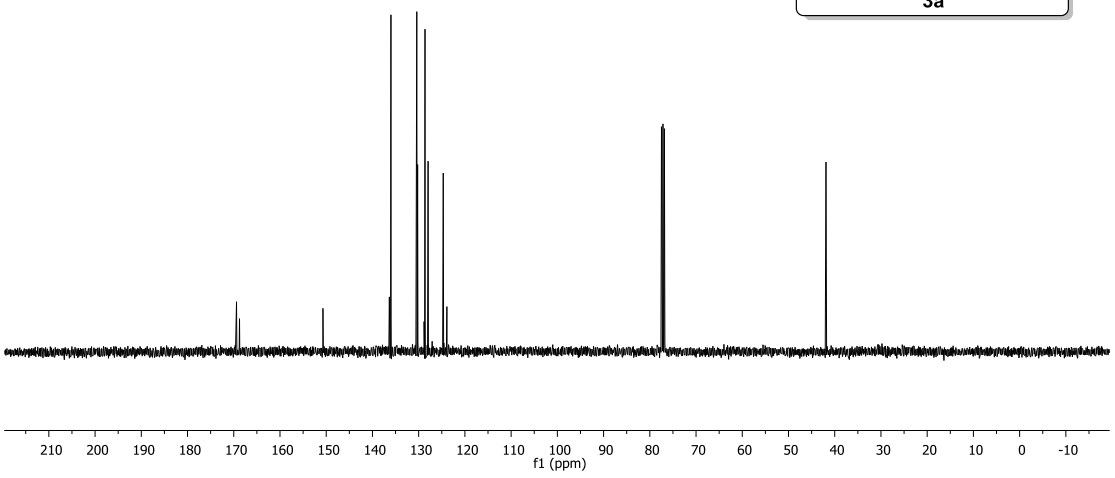
3a


2.09
3.29
5.50
1.00
2.16
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)


169.44
168.75
150.70
136.34
136.00
130.40
130.22
128.79
128.63
127.96
124.68
123.90
121.27
77.48
77.16
76.84
41.89


Se
O
N–Bn
O

3a


210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.65
7.65
7.63
7.63
7.62
7.48
7.48
7.47
7.47
7.46
7.45
7.44
7.44
7.42
7.42
7.41
7.27
5.90
5.83
5.81
5.79
5.78
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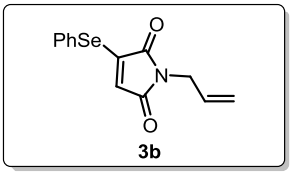
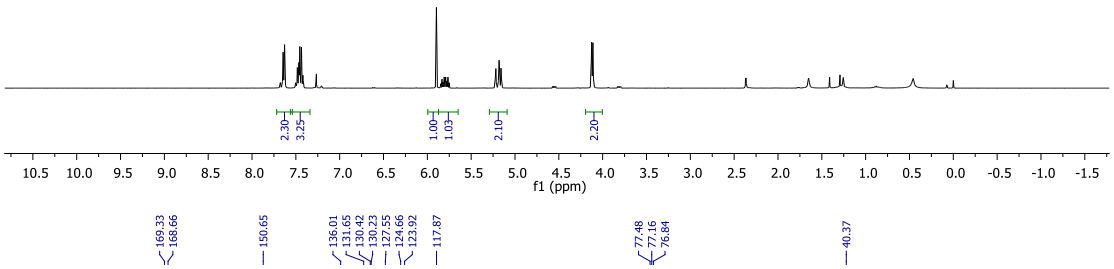
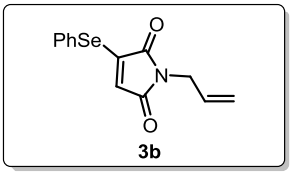
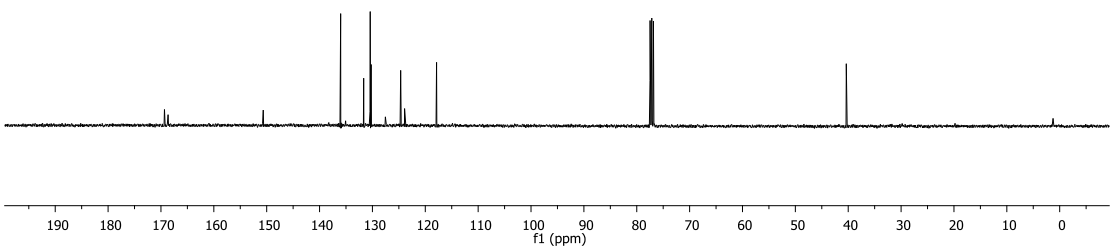
5.18
4.13
4.12
4.11
4.11
4.11

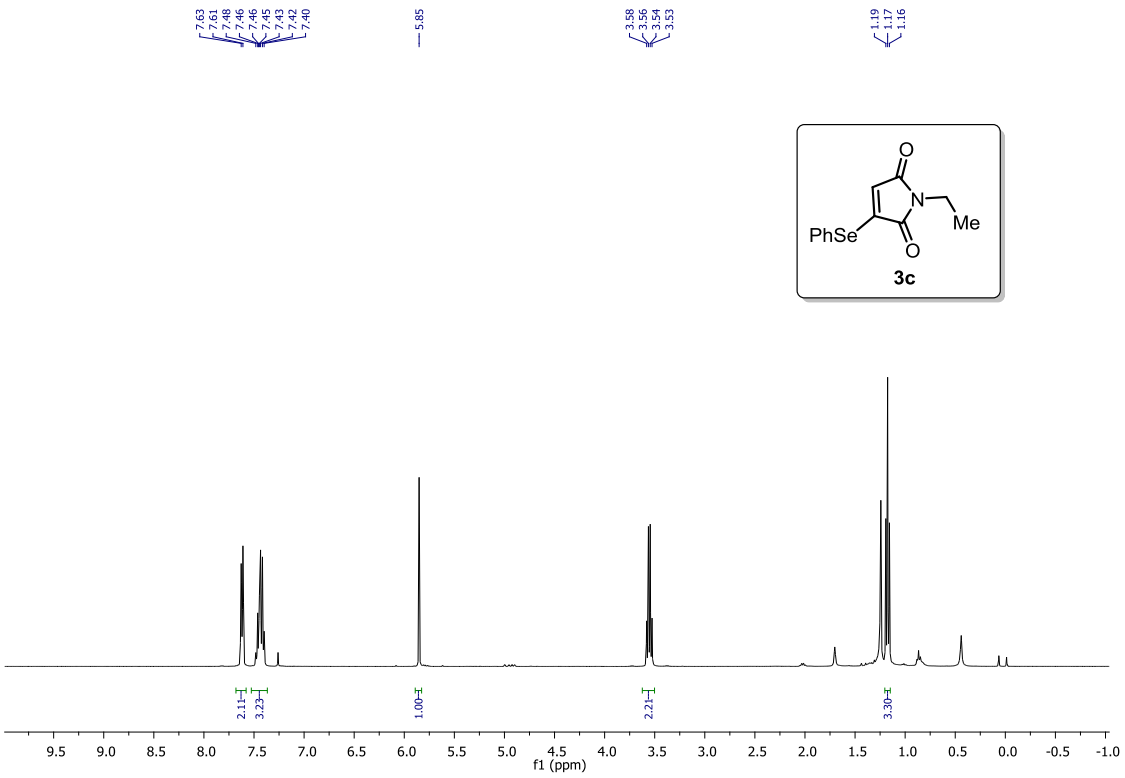

PhSe
O
N
O
3b

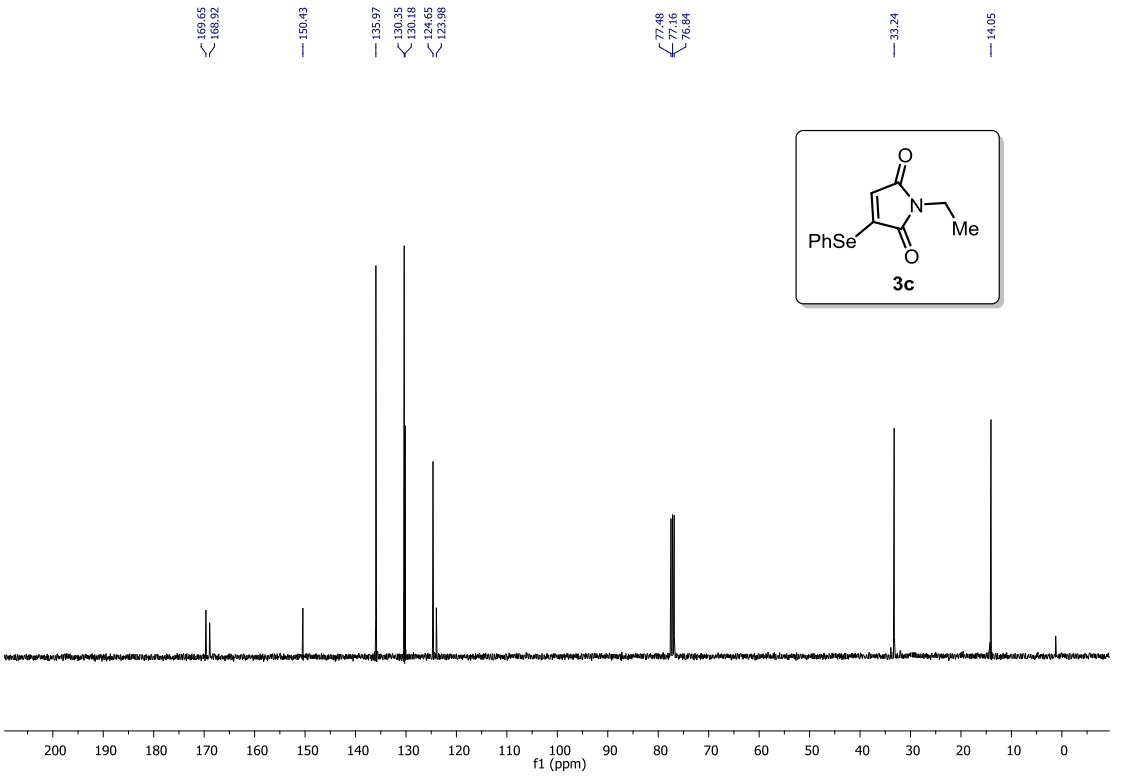

2.30
3.25
1.00
1.03
2.10
2.20
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5
f1 (ppm)

169.33
168.66
150.65
136.01
131.65
130.42
130.23
127.55
124.66
123.92
117.87
77.48
77.16
76.84
40.37

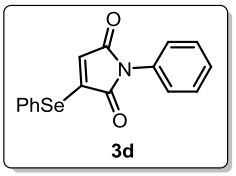

PhSe
O
N
O
3b


190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

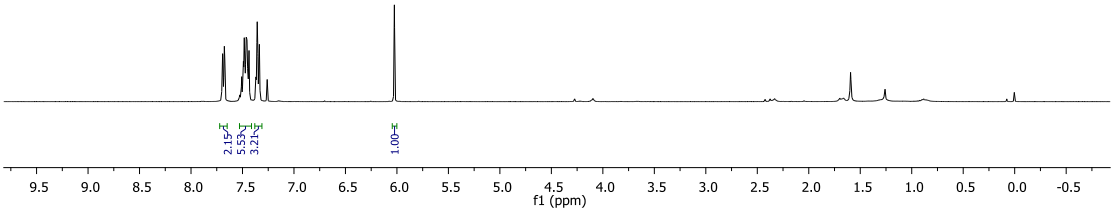

7.63
7.61
7.48
7.46
7.46
7.45
7.43
7.42
7.40
5.85
3.58
3.56
3.54
3.53
1.19
1.17
1.16
PhSe
N
Me
O
O
3c
2.11
3.23
1.00
2.21
3.30
f1 (ppm)


169.65
168.92
150.43
135.97
130.35
130.18
124.65
123.98
77.48
77.16
76.84
33.24
14.05
PhSe
N
Me
O
O
3c
f1 (ppm)

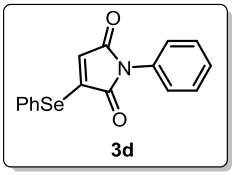

7.69
7.68
7.67
7.51
7.49
7.48
7.46
7.46
7.45
7.44
7.36
7.35
7.34
6.02


O
N
PhSe
O

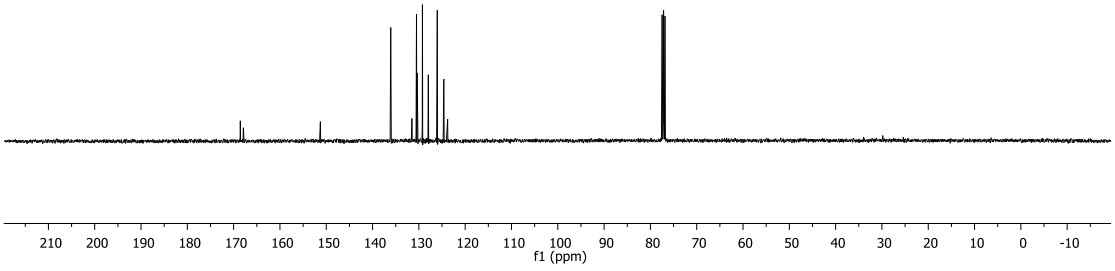
3d

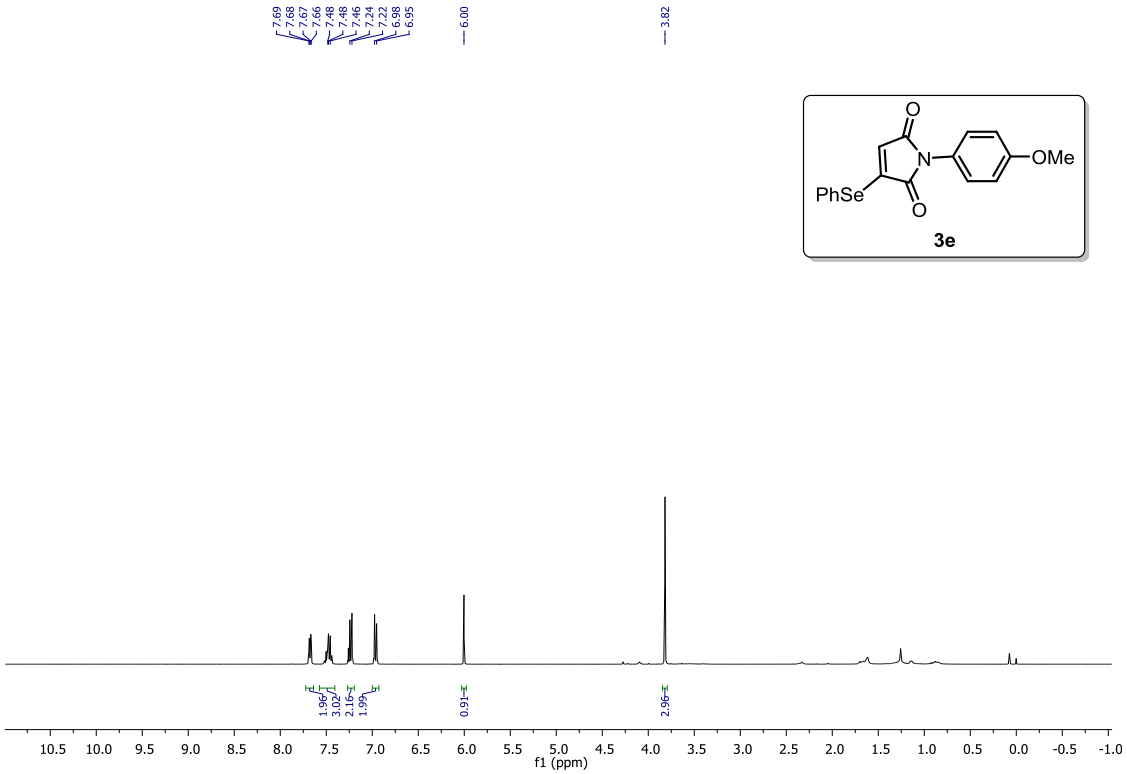

2.15
5.53
3.21
1.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

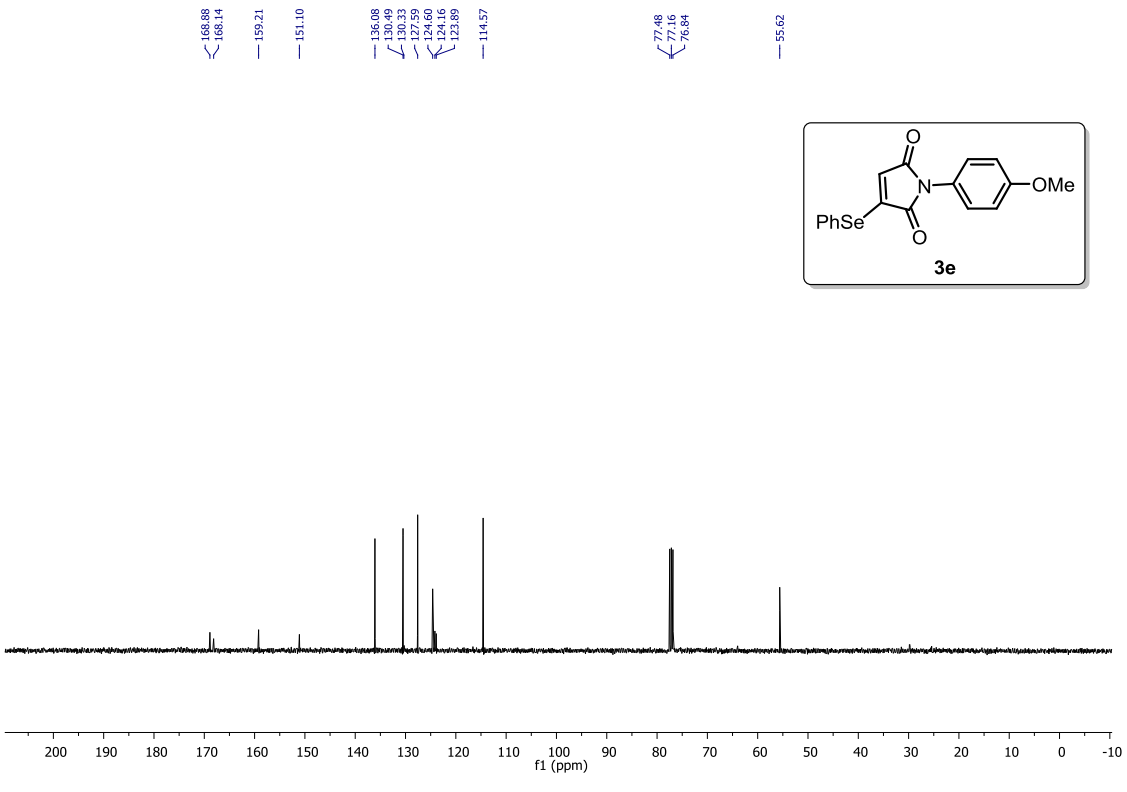

168.56
167.90
151.27
136.07
131.50
130.51
130.36
129.23
127.96
126.03
124.61
123.79
77.48
77.16
76.84


O
N
PhSe
O

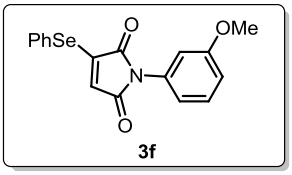
3d

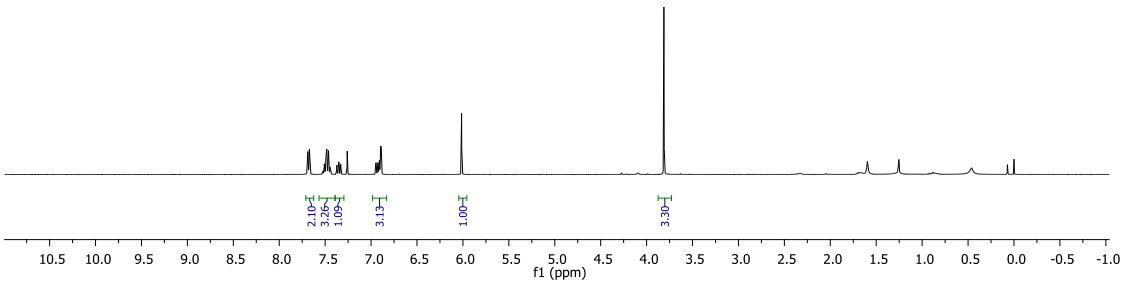

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

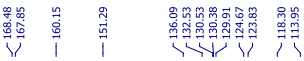

7.69
7.68
7.67
7.66
7.48
7.46
7.24
7.22
6.98
6.95
6.00
3.82
PhSe
OMe
3e
1.96
3.02
2.16
1.99
0.91
2.96
f1 (ppm)

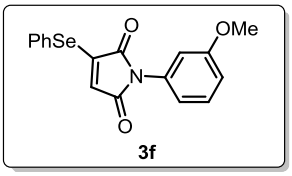

168.88
168.14
159.21
151.10
136.08
130.49
130.33
127.59
124.60
124.16
123.89
114.57
77.48
77.16
76.84
55.62
PhSe
OMe
3e
f1 (ppm)

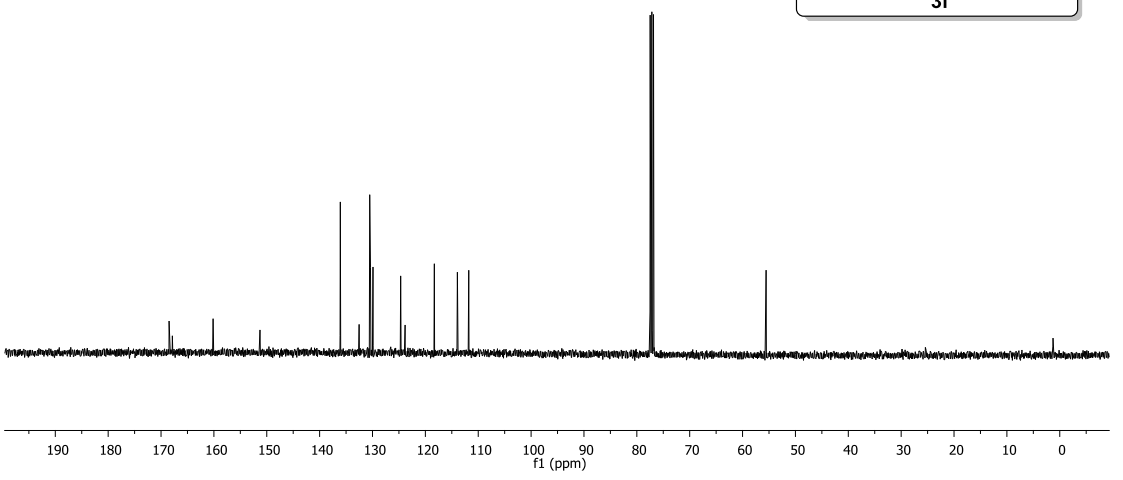

7.69
7.69
7.68
7.68
7.67
7.67
7.51
7.49
7.49
7.48
7.48
7.47
7.46
7.45
7.37
7.35
7.33
7.26
6.93
6.91
6.91
6.90
6.90
6.89
6.89
6.89
3.81

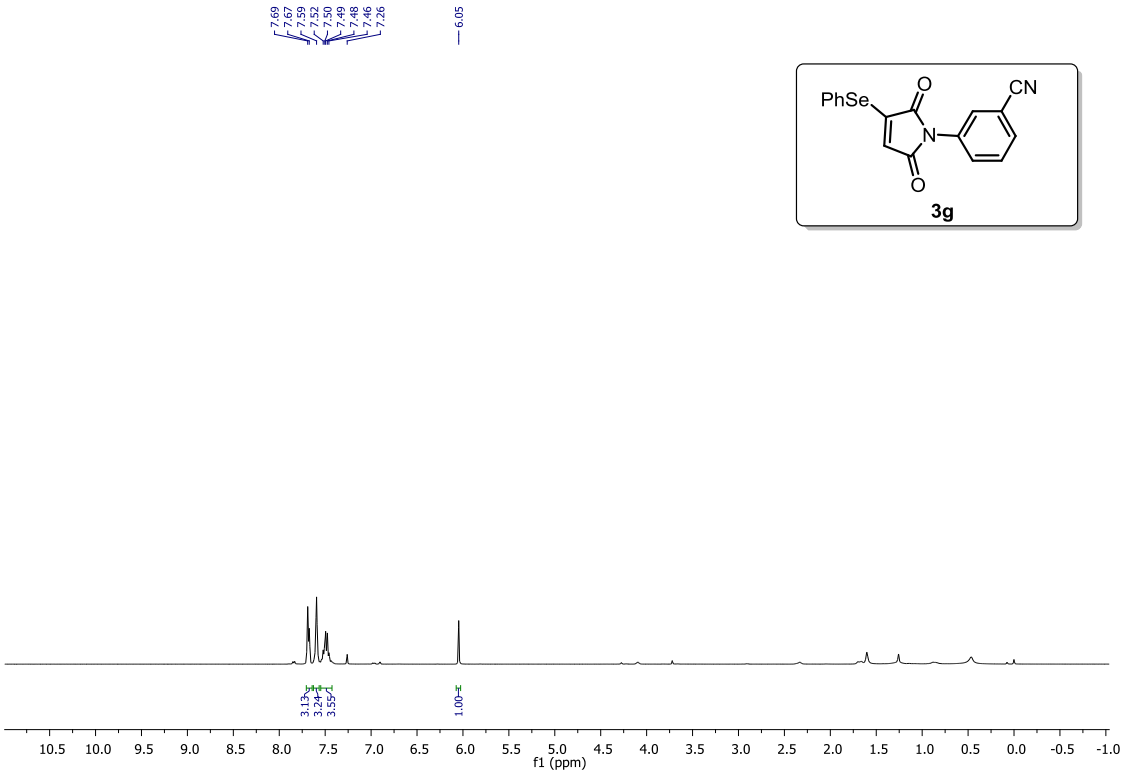

PhSe
O
OMe
N
O
3f

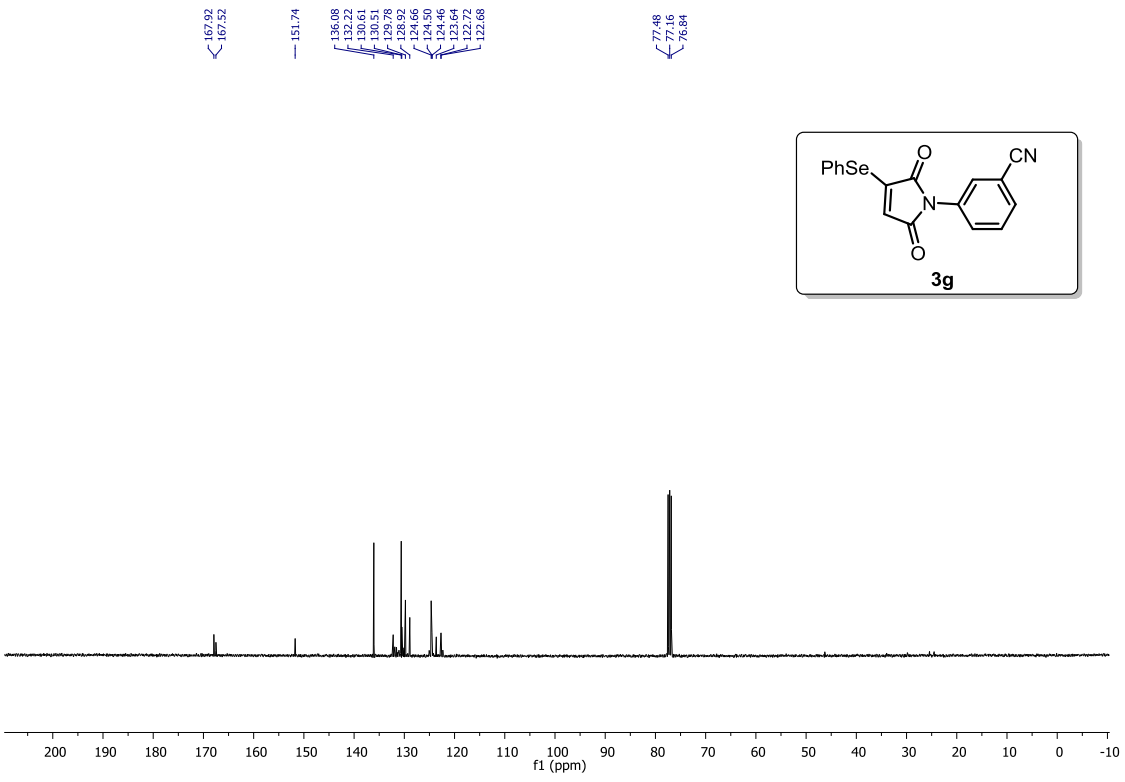

2.10
3.26
1.09
3.13
1.00
3.30
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)


168.48
167.85
160.15
151.29
136.09
132.53
130.53
130.38
129.91
124.67
123.83
118.30
113.95
111.80
77.48
77.16
76.84
55.55


PhSe
O
OMe
N
O
3f


190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.69
7.67
7.59
7.52
7.50
7.49
7.48
7.46
7.26
6.05
PhSe
O
CN
N
O
3g
3.15
3.24
3.55
1.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)


167.92
167.52
151.74
136.08
132.22
130.61
130.51
129.78
128.92
124.66
124.50
124.46
123.64
122.72
122.68
77.48
77.16
76.84
PhSe
O
CN
N
O
3g
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.62
7.62
7.60
7.60
7.43
7.43
7.42
7.42
7.41
7.41
7.40
7.39
7.39
7.39
7.37
7.37
7.33
7.33
7.33
7.32
7.31
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7.18
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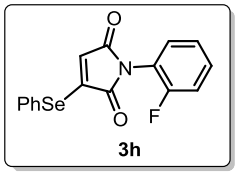
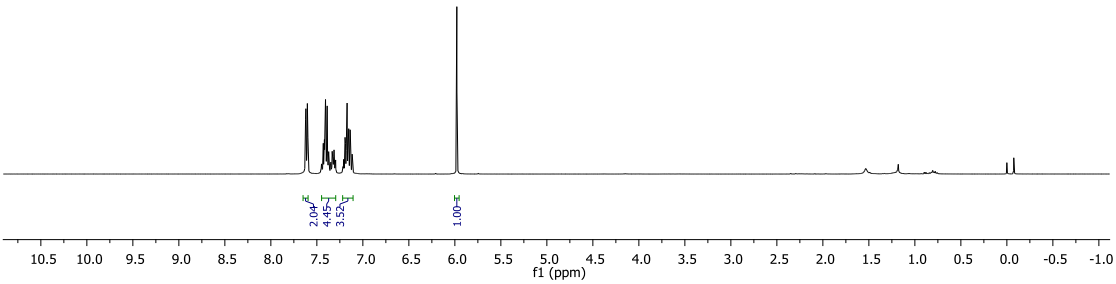
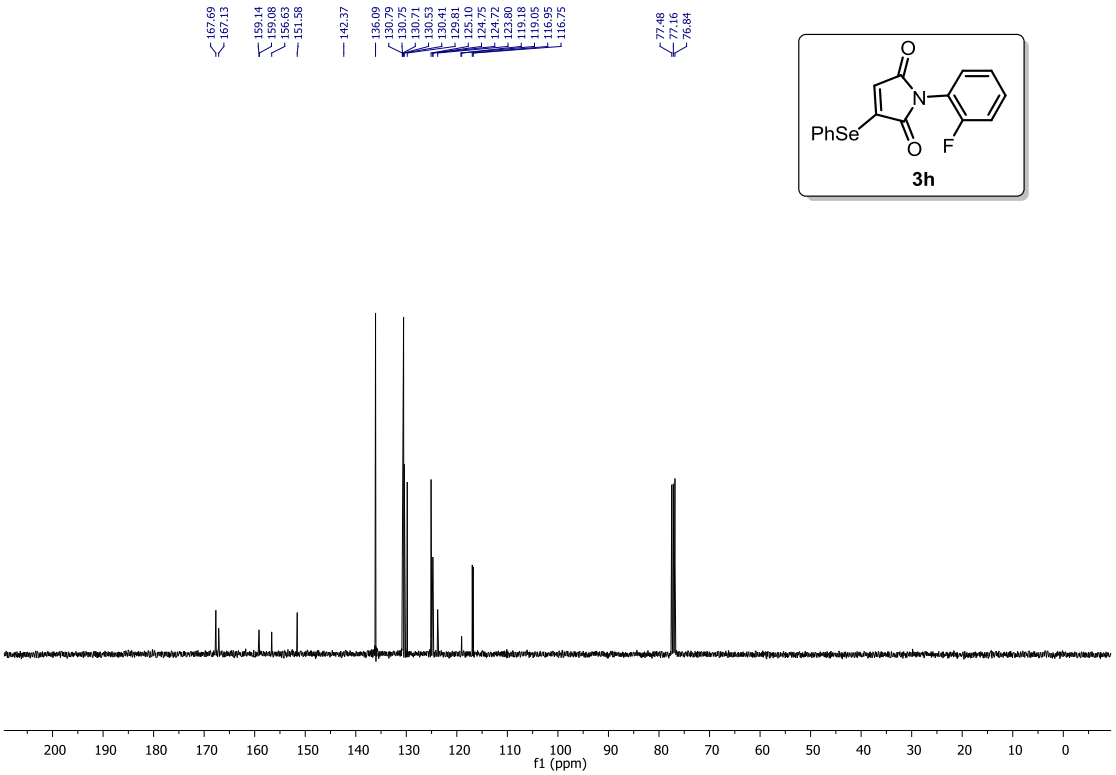
7.16
7.16
7.15
7.14
7.14
5.98


O
N
PhSe
O
F

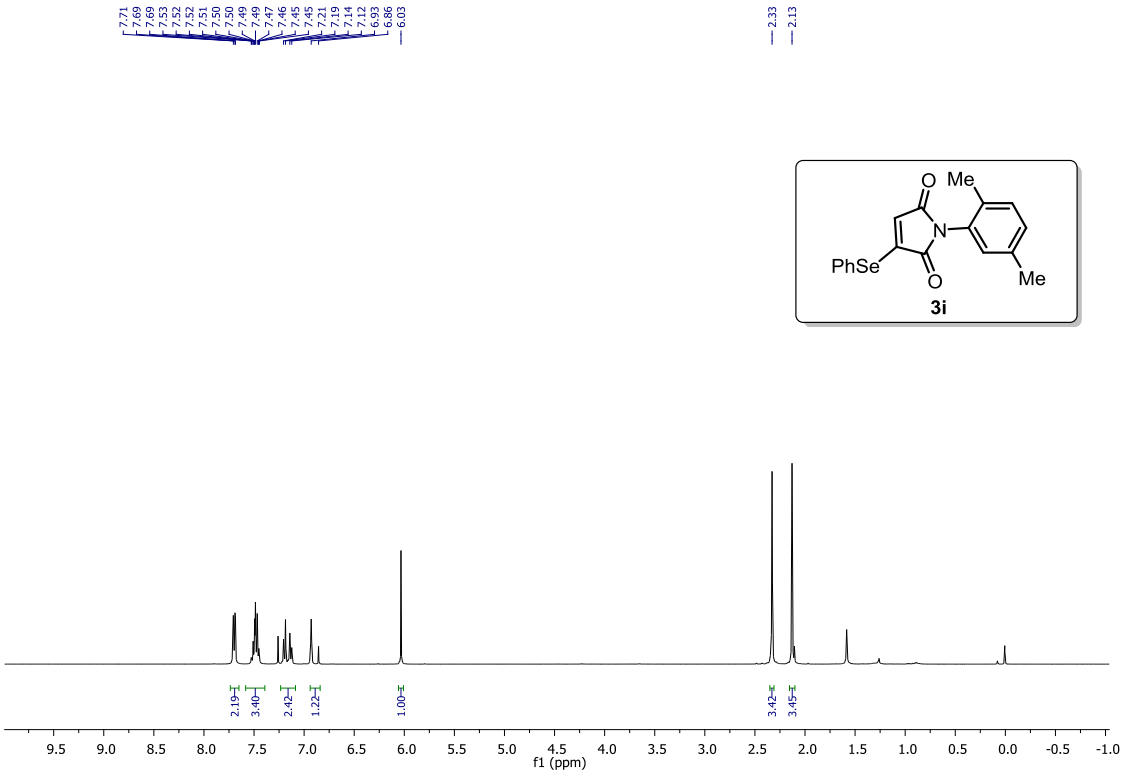
3h

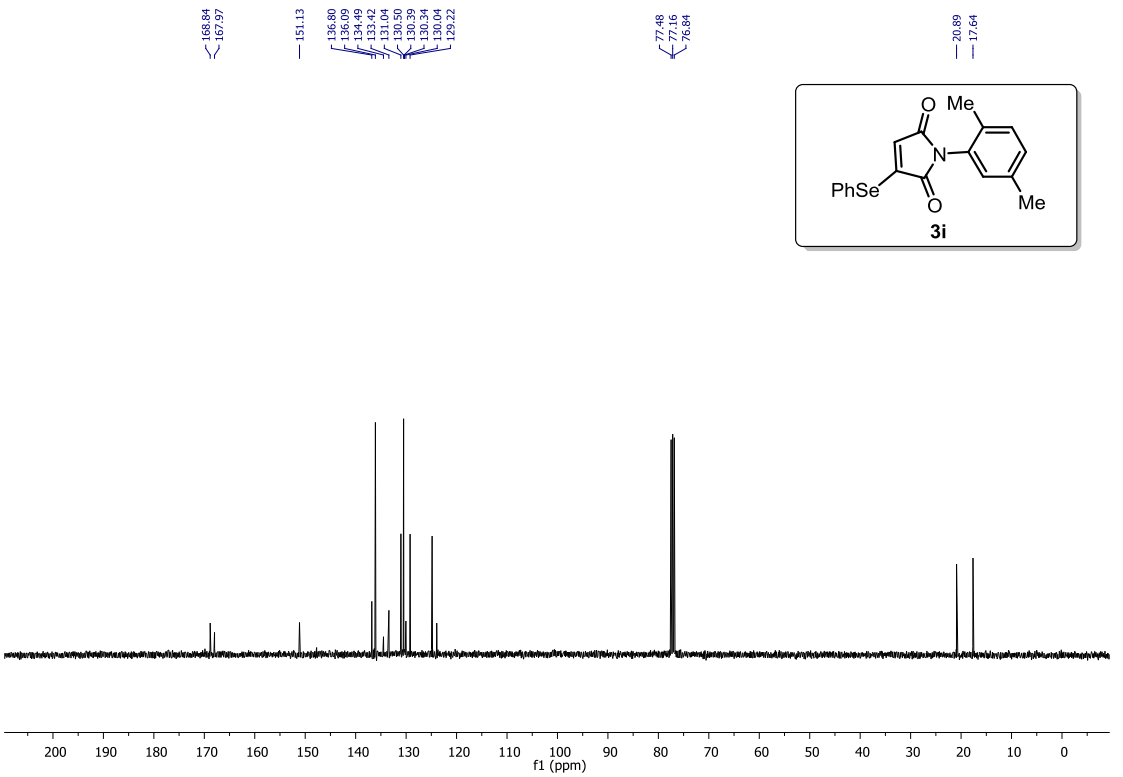

2.04
4.45
3.52
1.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

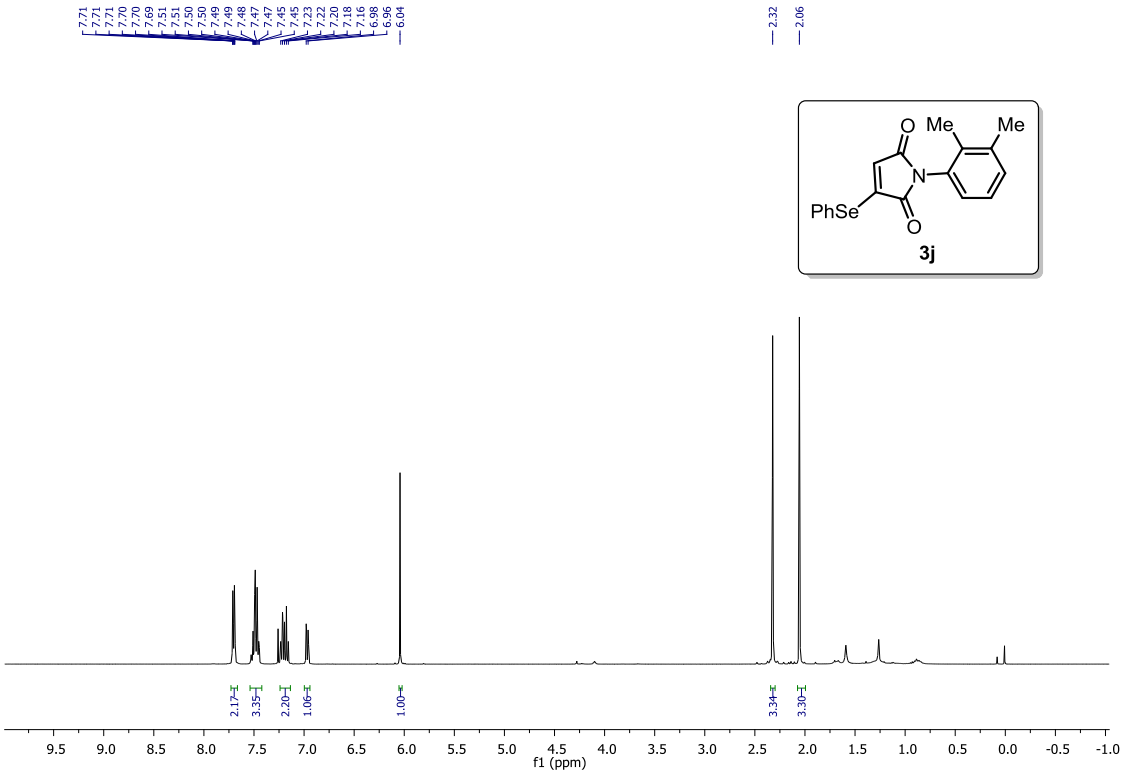

167.69
167.13
159.14
159.08
156.63
151.58
142.37
136.09
130.79
130.75
130.71
130.53
130.41
129.81
125.10
124.75
124.72
123.80
119.18
119.05
116.95
116.75
77.48
77.16
76.84
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

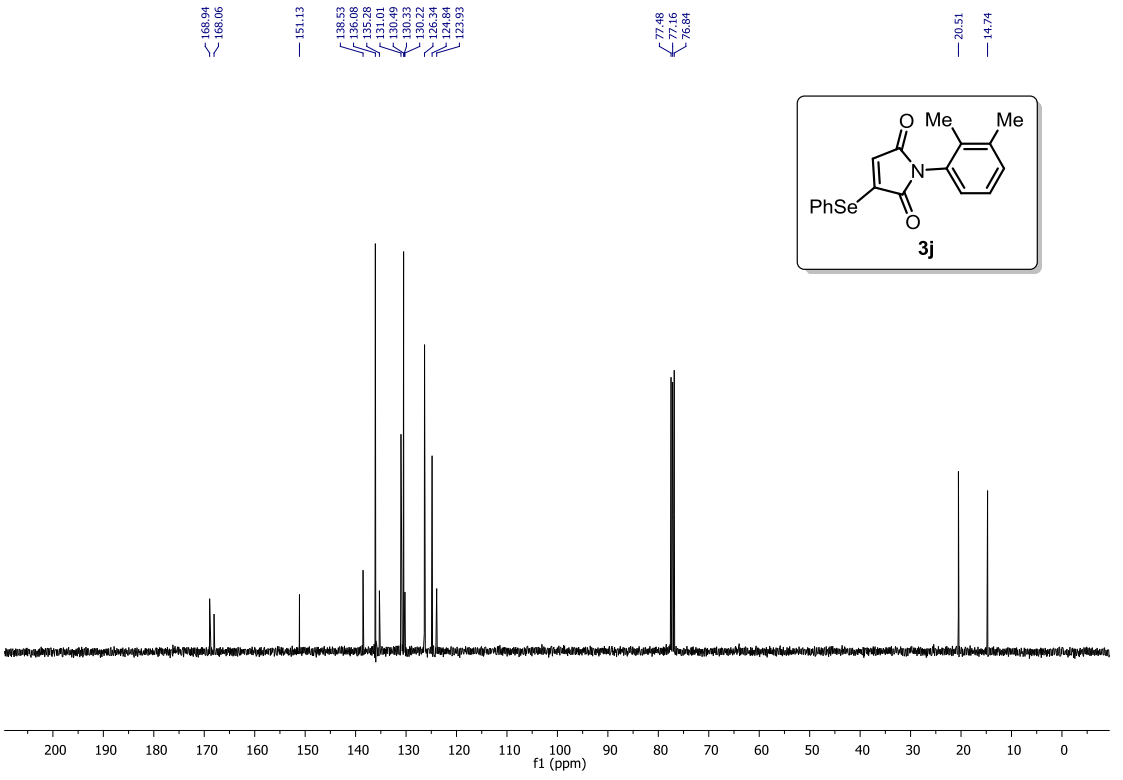
O
N
PhSe
O
F

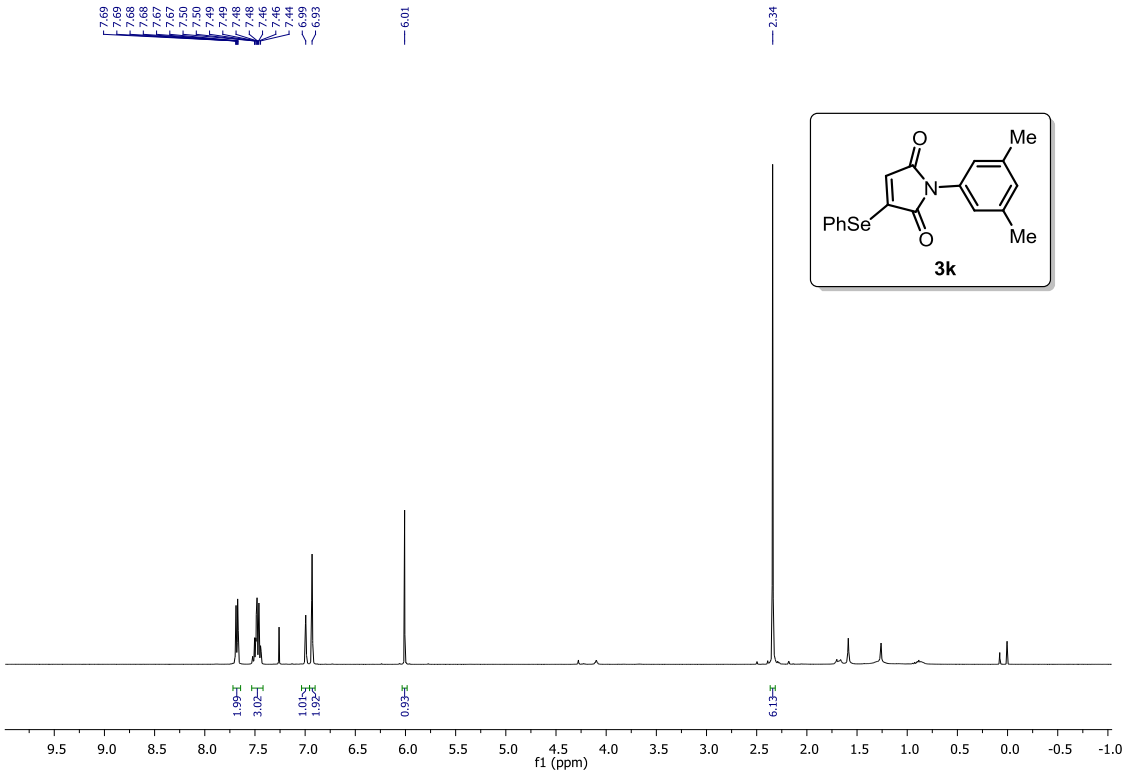
3h

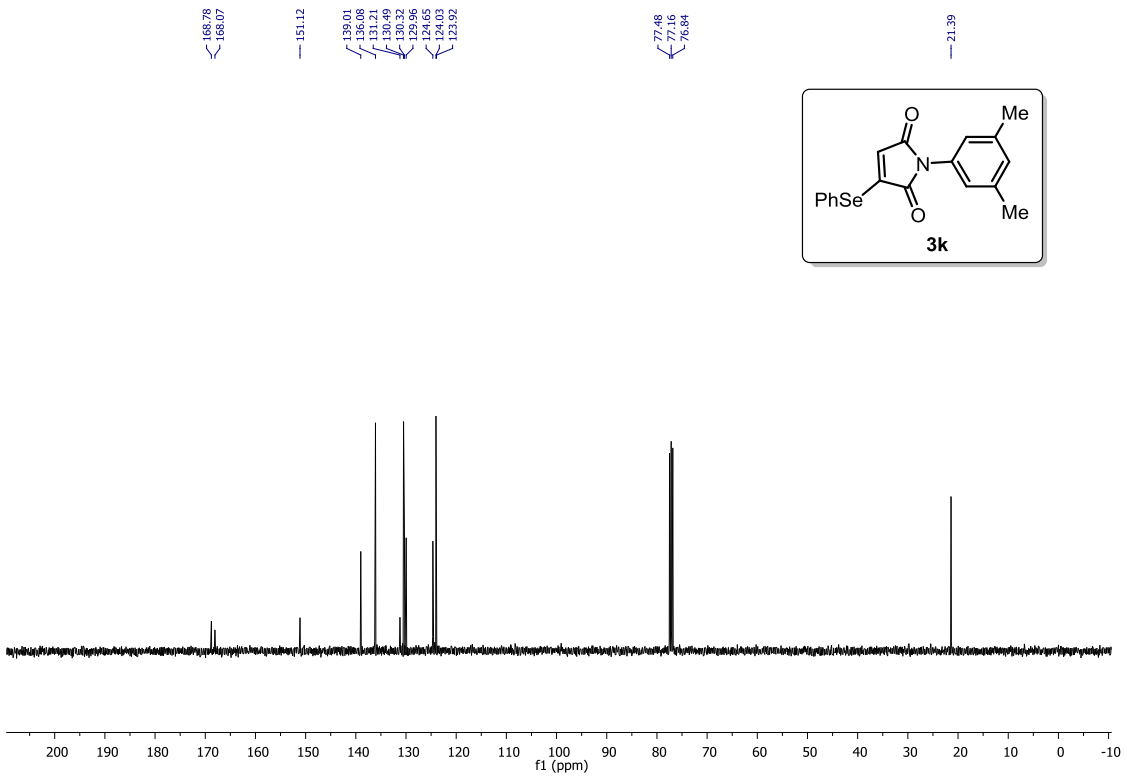

7.71
7.69
7.69
7.53
7.52
7.52
7.51
7.50
7.50
7.49
7.47
7.46
7.45
7.45
7.21
7.19
7.14
7.12
6.93
6.86
6.03
2.33
2.13
O
Me
N
PhSe
O
Me
3i
2.19
3.40
2.42
1.22
1.00
3.42
3.45
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

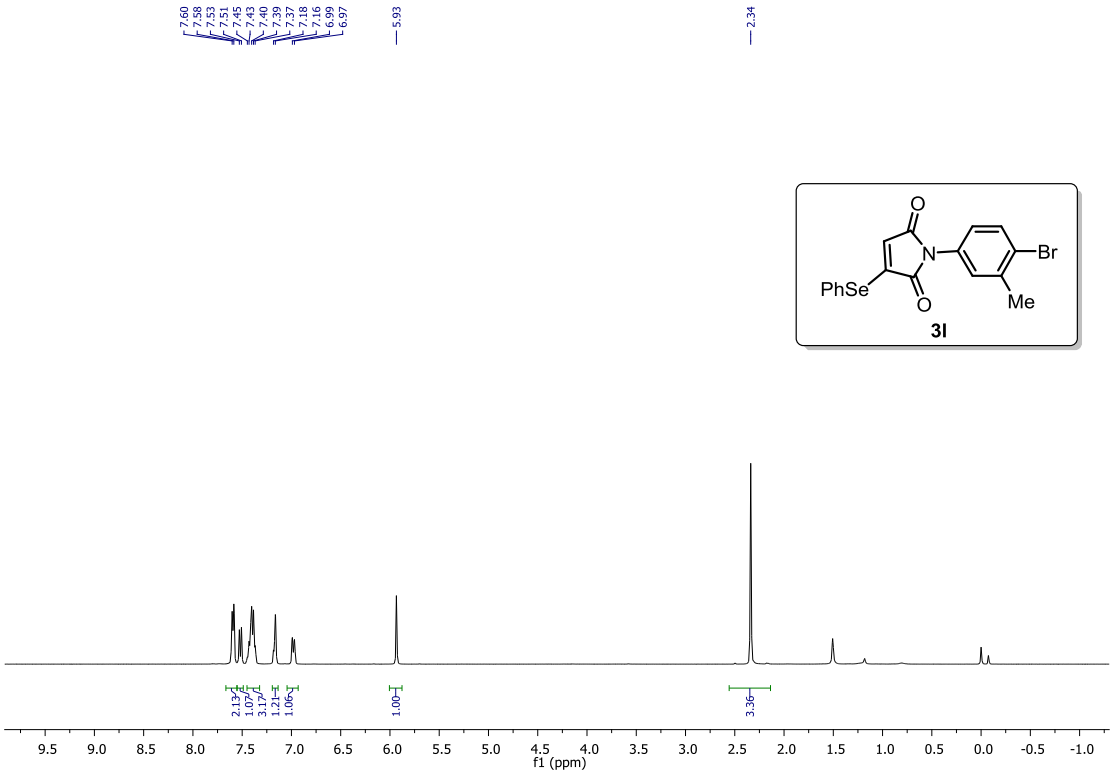

168.84
167.97
151.13
136.80
136.09
134.49
133.42
131.04
130.50
130.39
130.34
130.04
129.22
77.48
77.16
76.84
20.89
17.64
O
Me
N
PhSe
O
Me
3i
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

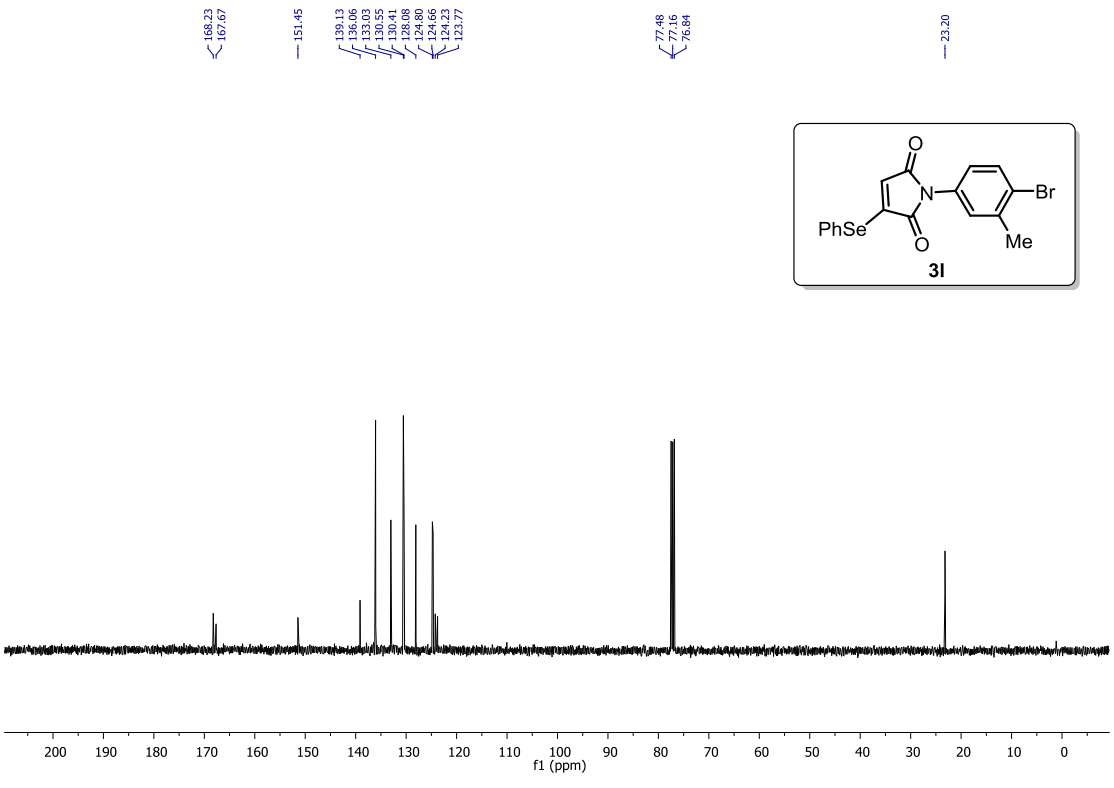

7.71
7.71
7.71
7.70
7.70
7.69
7.51
7.51
7.50
7.49
7.49
7.48
7.47
7.47
7.45
7.45
7.23
7.22
7.20
7.18
7.16
6.98
6.96
6.04
2.32
2.06
O
Me
Me
N
PhSe
O
3j
2.17
3.35
2.20
1.06
1.00
3.34
3.30
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

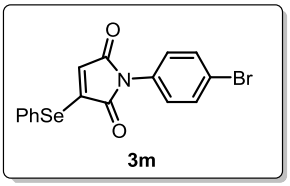

168.94
168.06
151.13
138.53
136.08
135.28
131.01
130.49
130.33
130.22
126.34
124.84
123.93
77.48
77.16
76.84
20.51
14.74
O
Me
Me
N
PhSe
O
3j
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.69
7.69
7.68
7.68
7.67
7.67
7.50
7.50
7.49
7.49
7.48
7.48
7.46
7.46
7.44
6.99
6.93
6.01
2.34
O
N
O
PhSe
Me
Me
3k
1.99
3.02
1.01
1.92
0.93
6.13
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

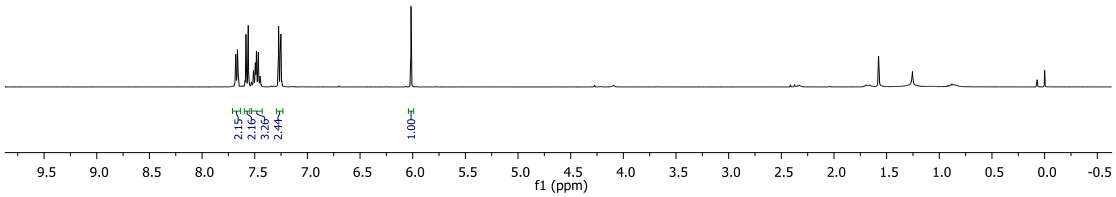

168.78
168.07
151.12
139.01
136.08
131.21
130.49
130.32
129.96
124.65
124.03
123.92
77.48
77.16
76.84
21.39
O
N
O
PhSe
Me
Me
3k
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

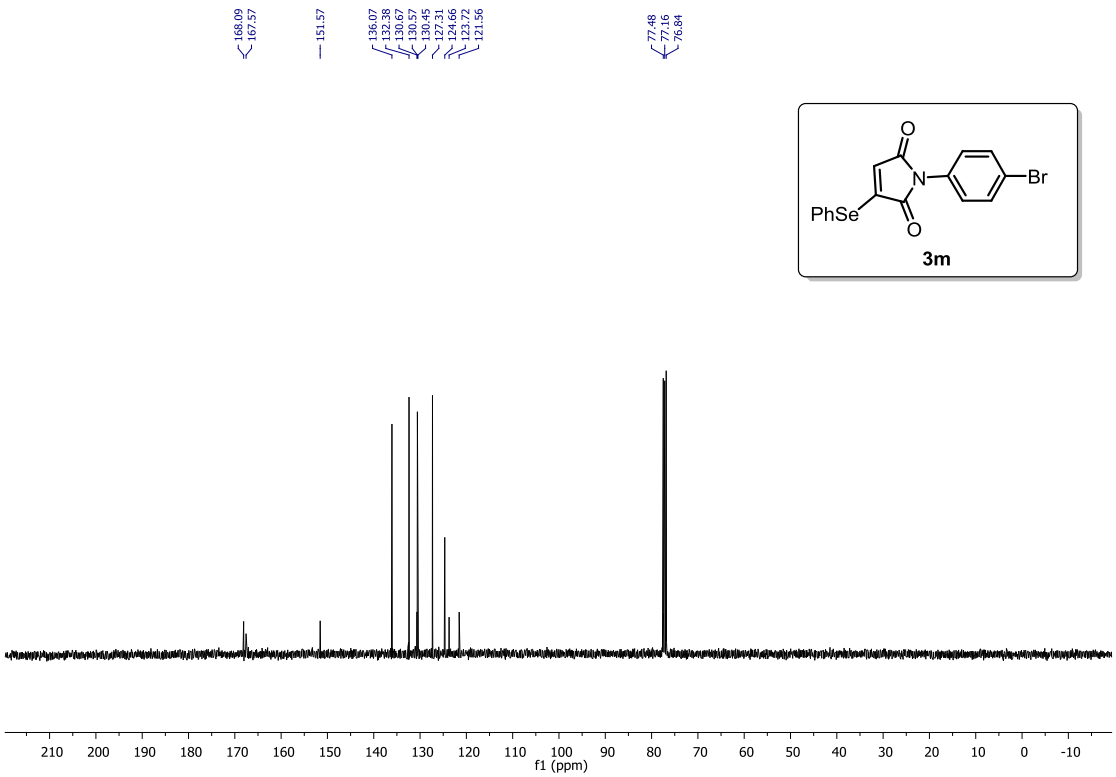

7.60
7.58
7.53
7.51
7.45
7.43
7.40
7.39
7.37
7.18
7.16
6.99
6.97
5.93
2.34
O
N
Br
PhSe
O
Me
3l
2.13
1.07
3.17
1.21
1.06
1.00
3.36
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)


168.23
167.67
151.45
139.13
136.06
133.03
130.55
130.41
128.08
124.80
124.66
124.23
123.77
77.48
77.16
76.84
23.20
O
N
Br
PhSe
O
Me
3l
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


O
N
Br
PhSe
O

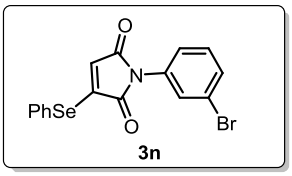
3m


2.15
2.16
3.26
2.44
1.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

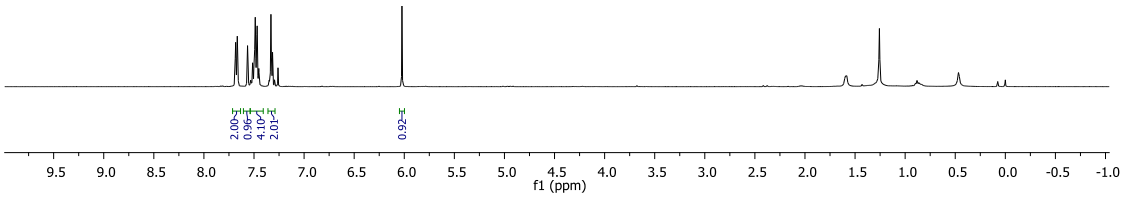

168.09
167.57
151.57
136.07
132.38
130.67
130.57
130.45
127.31
124.66
123.72
121.56
77.48
77.16
76.84
O
N
Br
PhSe
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

3m

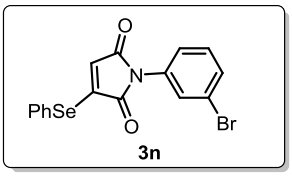

7.68
7.67
7.66
7.56
7.51
7.50
7.50
7.49
7.49
7.47
7.45
7.33
7.32
7.32
6.02


O
N
PhSe
O
Br

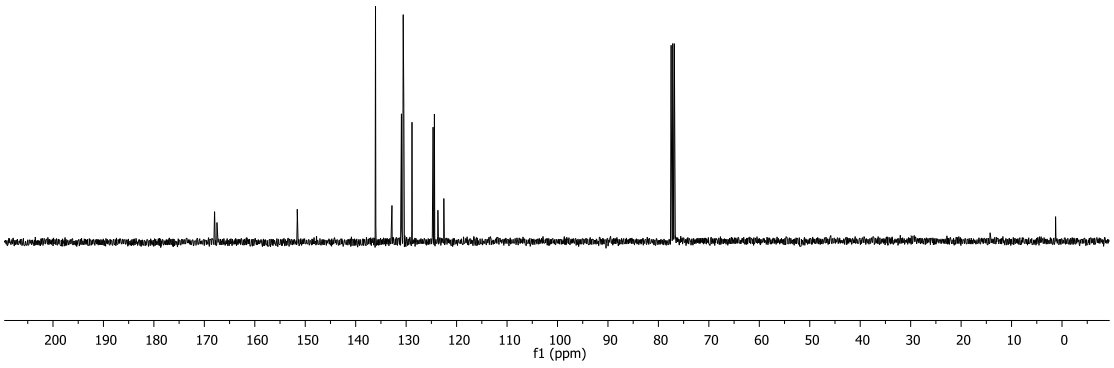
3n


2.00
0.96
4.10
2.01
0.92
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)


167.97
167.46
151.58
136.07
132.81
130.93
130.58
130.46
130.40
128.84
124.66
124.40
123.71
122.53
77.48
77.16
76.84


O
N
PhSe
O
Br

3n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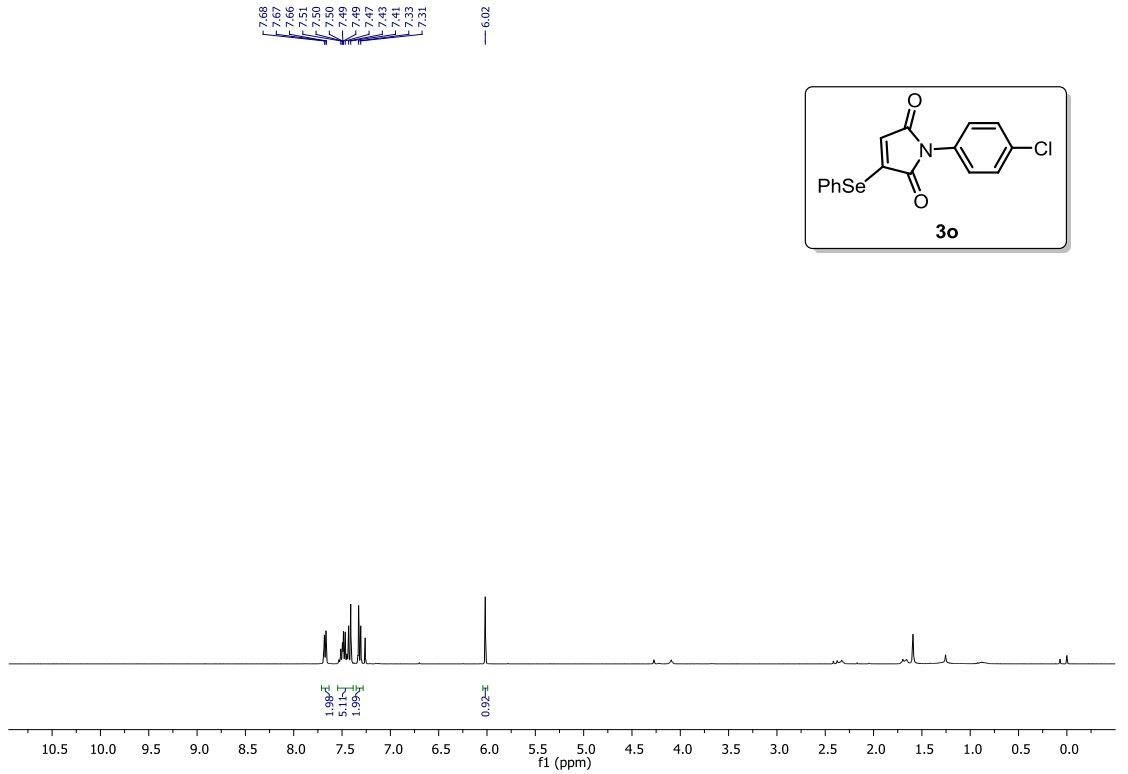
f1 (ppm)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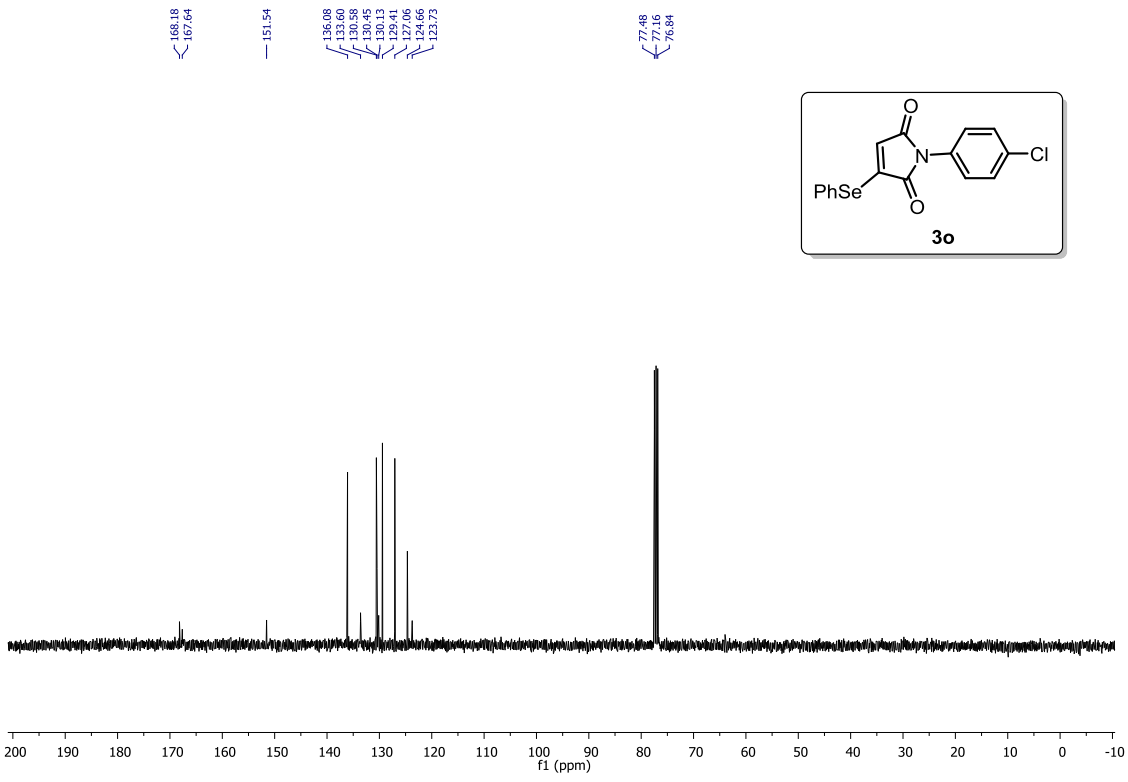
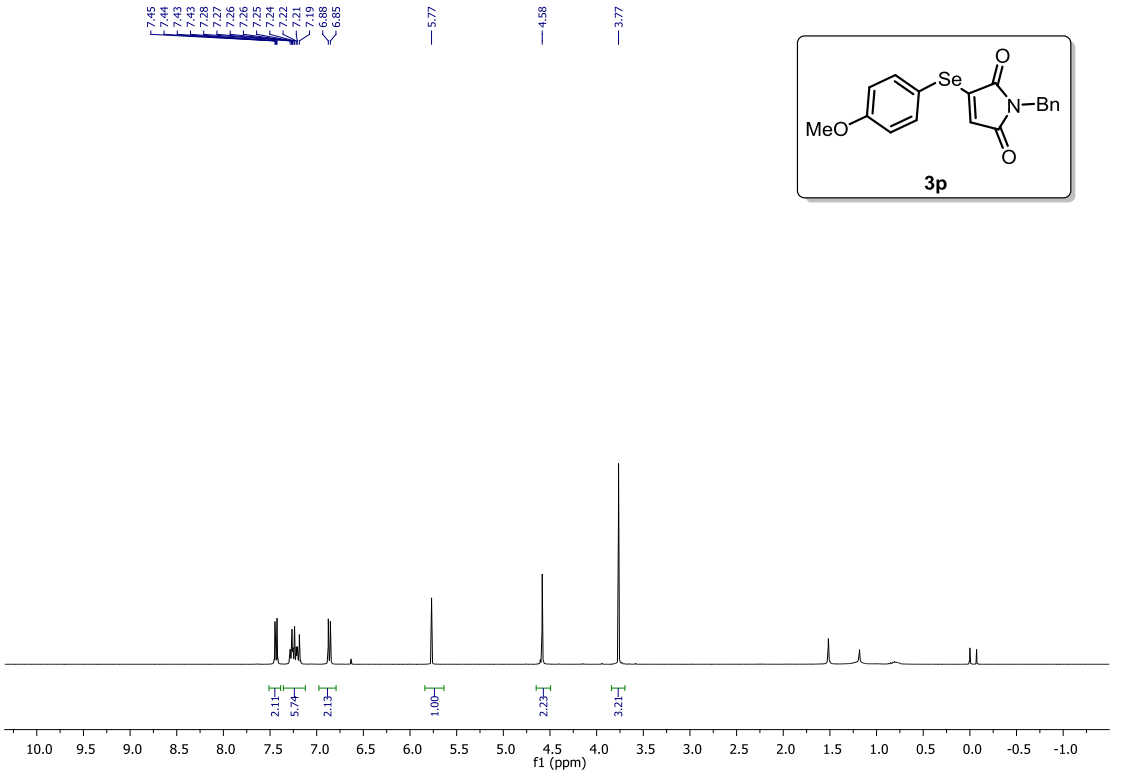
7.67
7.66
7.51
7.50
7.50
7.49
7.49
7.47
7.43
7.41
7.33
7.31
6.02
O
N
Cl
PhSe
O
3o
1.98
5.11
1.99
0.92
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


168.18
167.64
151.54
136.08
133.60
130.58
130.45
130.13
129.41
127.06
124.66
123.73
77.48
77.16
76.84
O
N
Cl
PhSe
O
3o
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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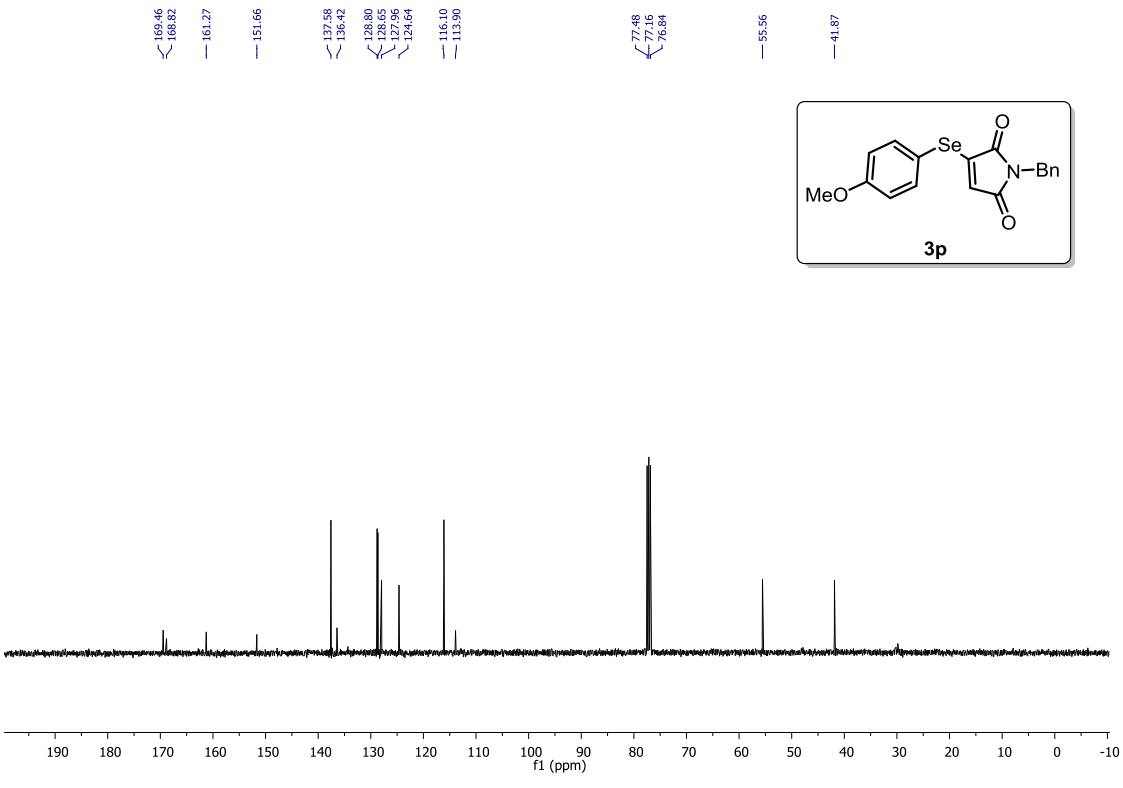
7.44
7.43
7.43
7.28
7.27
7.26
7.25
7.24
7.22
7.21
7.19
6.88
6.85
5.77
4.58
3.77
Se
O
N–Bn
O
MeO
3p
2.11
5.74
2.13
1.00
2.23
3.21
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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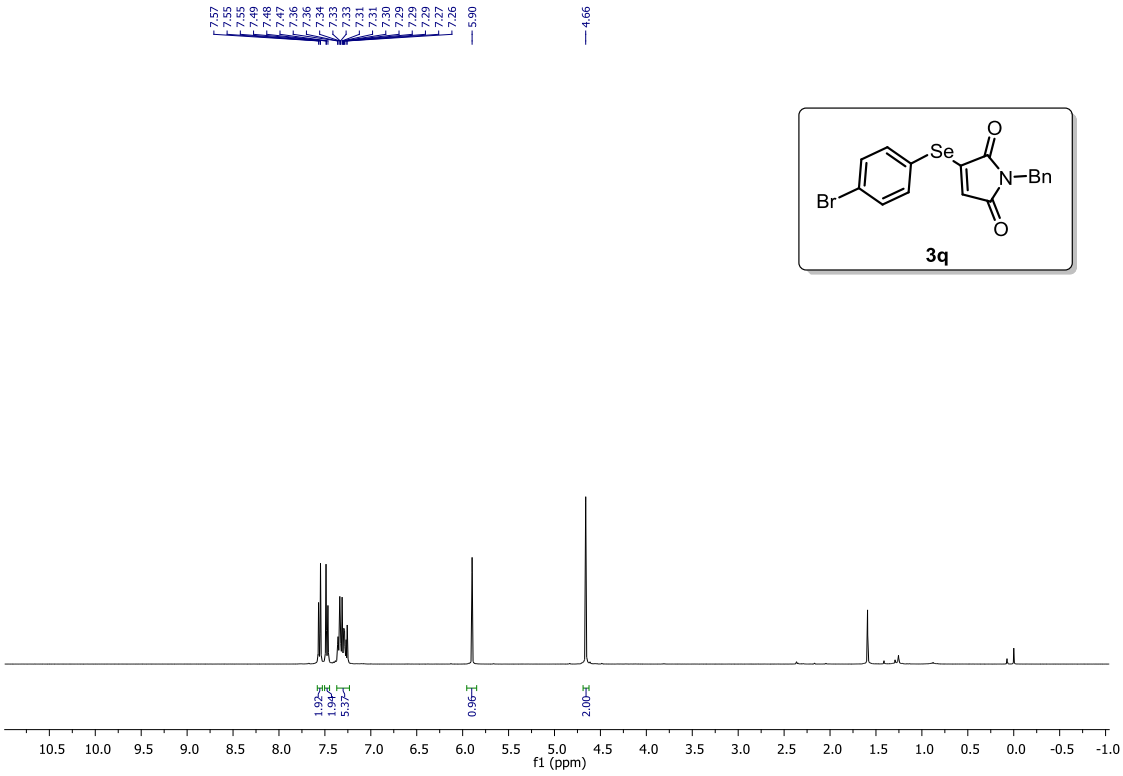
168.82
161.27
151.66
137.58
136.42
128.80
128.65
127.96
124.64
116.10
113.90
77.48
77.16
76.84
55.56
41.87
Se
O
N–Bn
O
MeO
3p
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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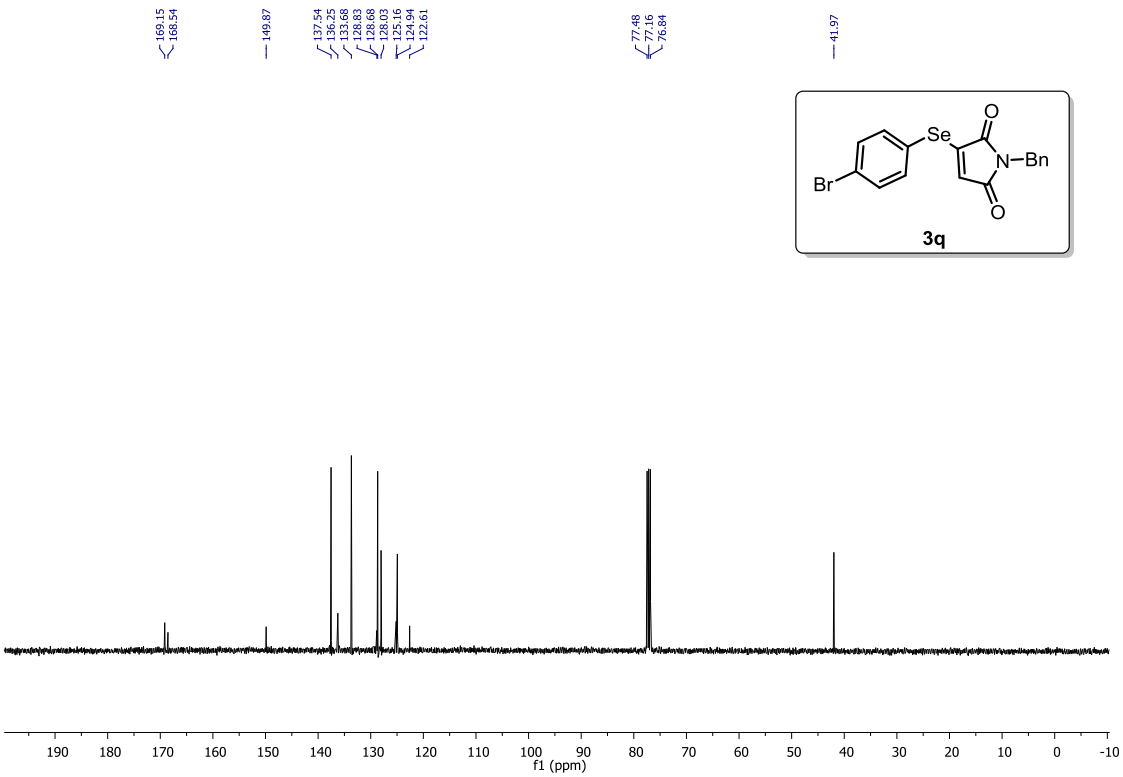
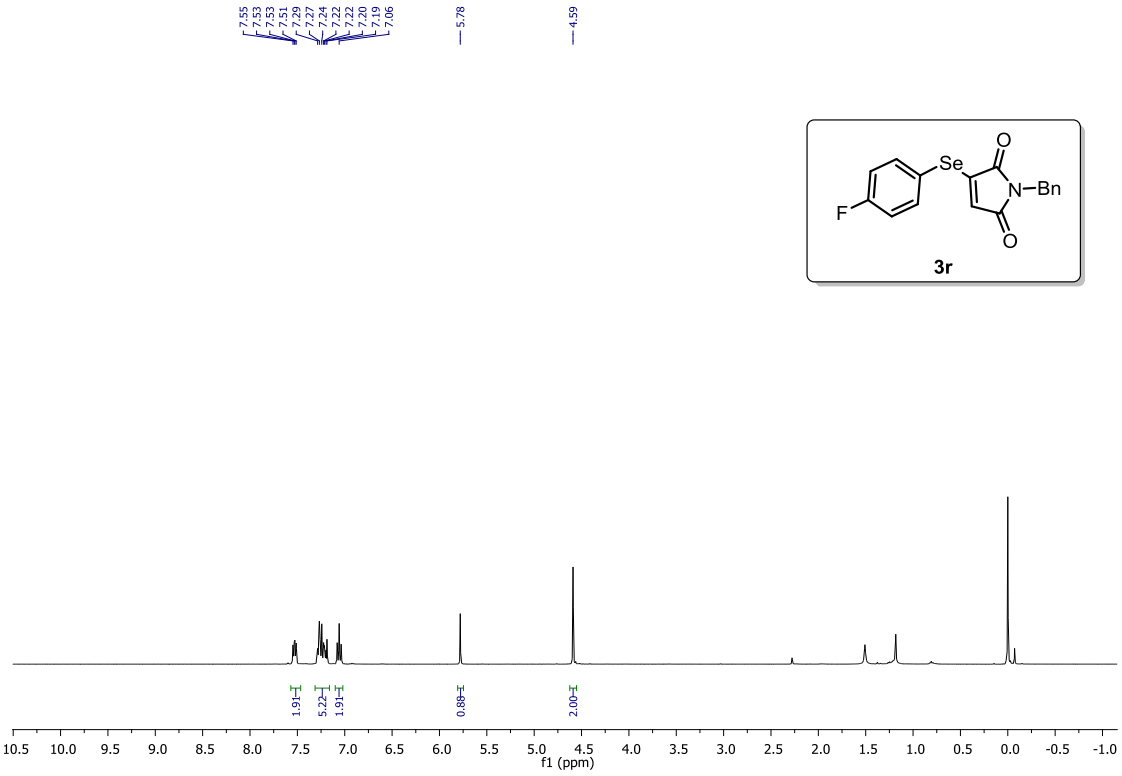
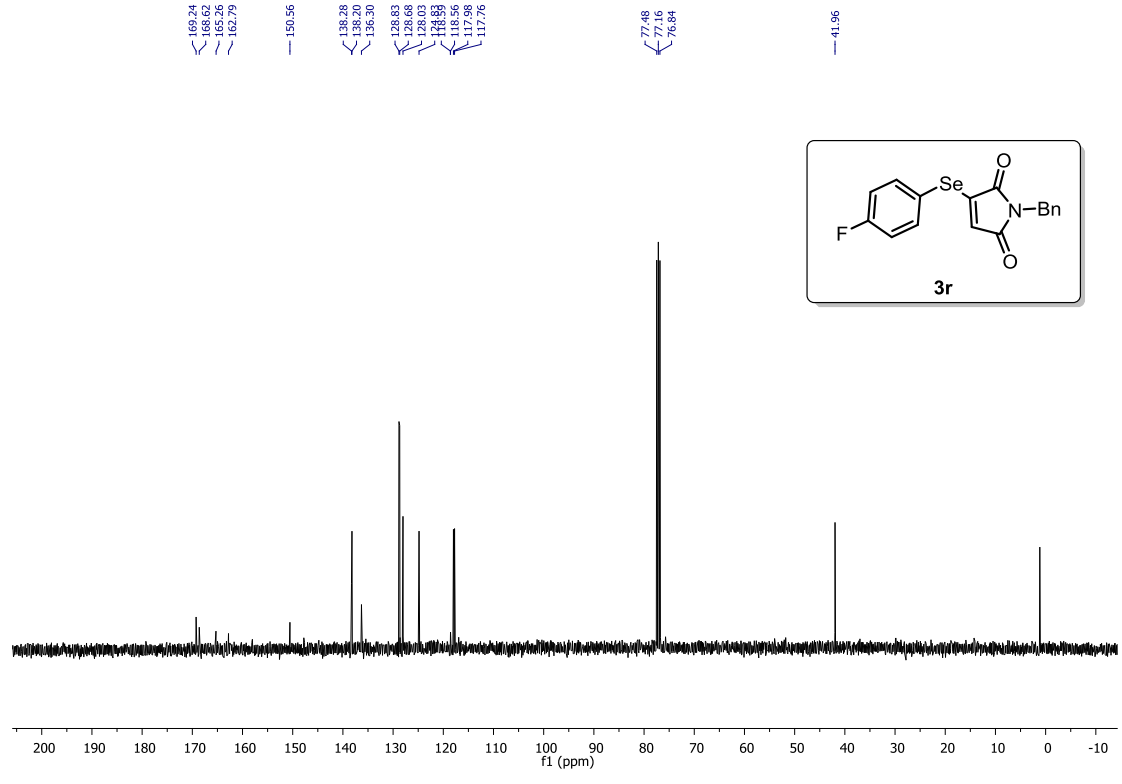
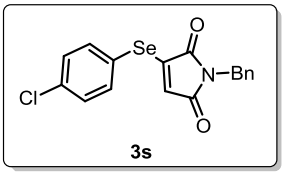
7.55
7.55
7.49
7.48
7.47
7.36
7.36
7.34
7.33
7.33
7.31
7.31
7.30
7.29
7.29
7.27
7.26
5.90
4.66
Se
O
N–Bn
Br
O
3q
1.92
1.94
5.37
0.96
2.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

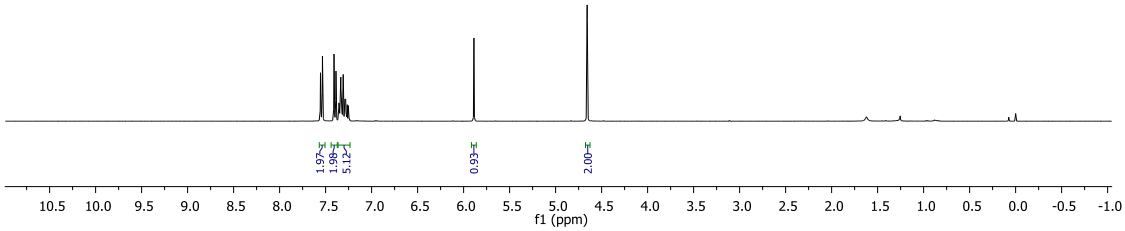

169.15
168.54
149.87
137.54
136.25
133.68
128.83
128.68
128.03
125.16
124.94
122.61
77.48
77.16
76.84
41.97
Se
O
N–Bn
Br
O
3q
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.55
7.53
7.53
7.51
7.29
7.27
7.24
7.22
7.22
7.20
7.19
7.06
5.78
4.59
Se
O
N–Bn
F
O
3r
1.91
5.22
1.91
0.88
2.00
f1 (ppm)

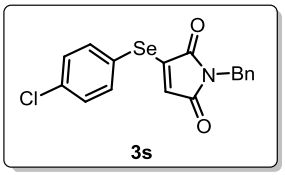

169.24
168.62
165.26
162.79
150.56
138.28
138.20
136.30
128.83
128.68
128.03
118.56
117.98
117.76
77.48
77.16
76.84
41.96
Se
O
N–Bn
F
O
3r
f1 (ppm)

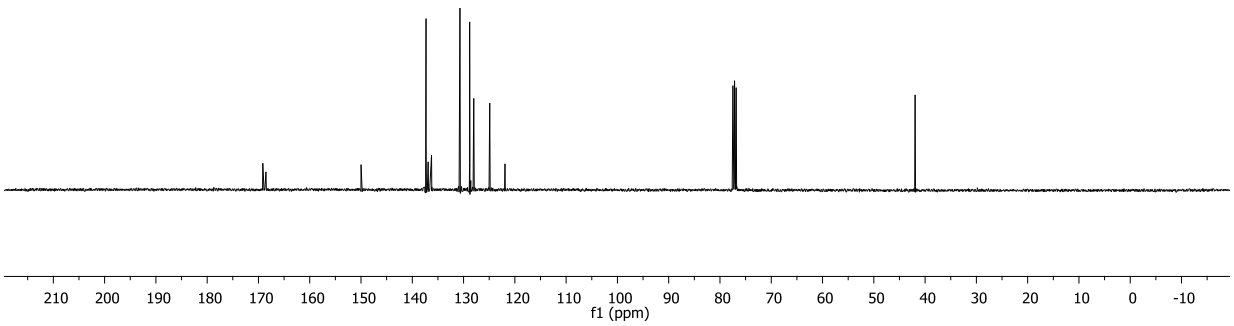

7.56
7.53
7.41
7.41
7.40
7.39
7.39
7.36
7.35
7.34
7.33
7.33
7.31
7.30
7.29
7.29
7.28
7.28
7.27
7.25
5.89
4.66

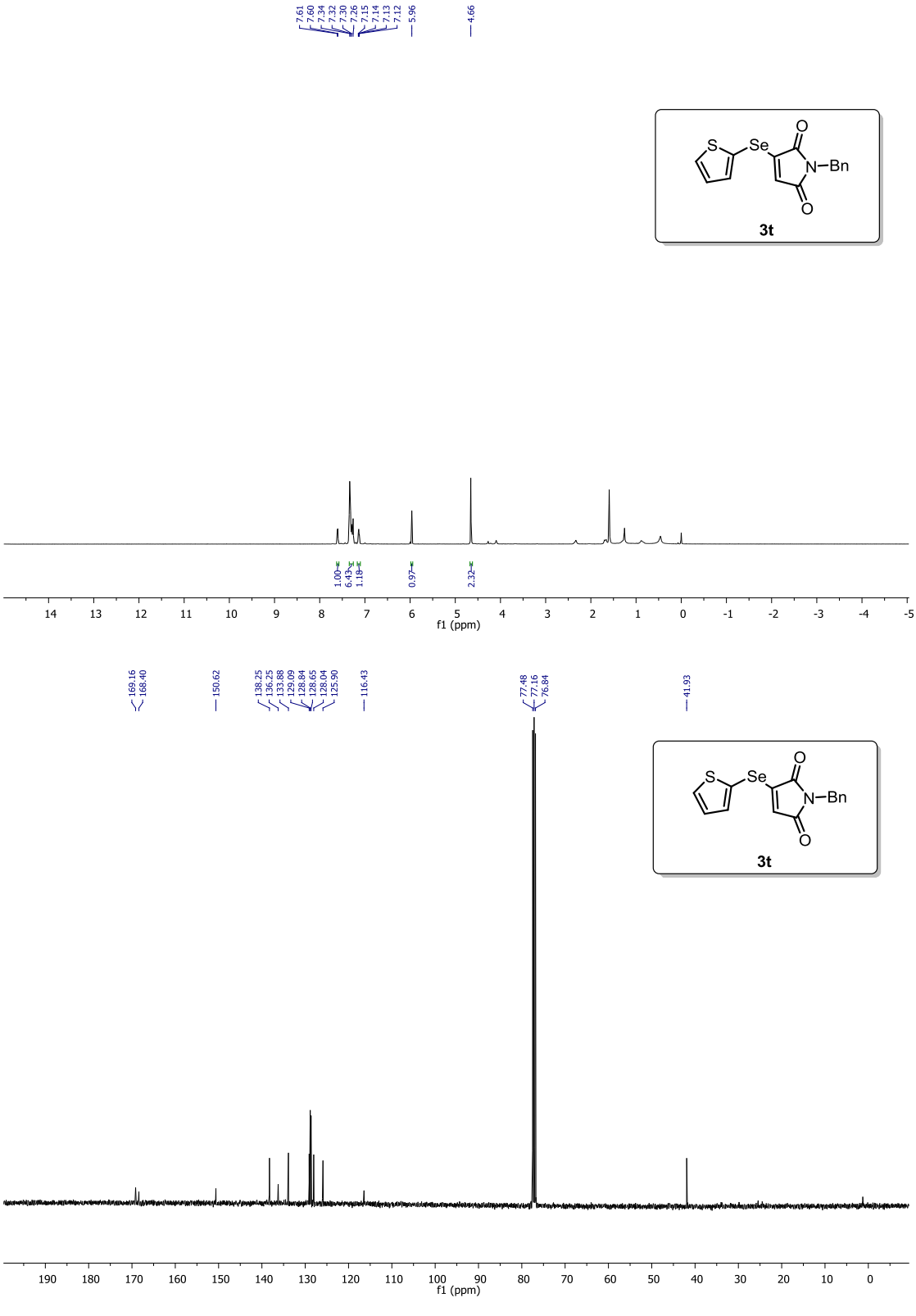

Se
O
N–Bn
Cl
O
3s

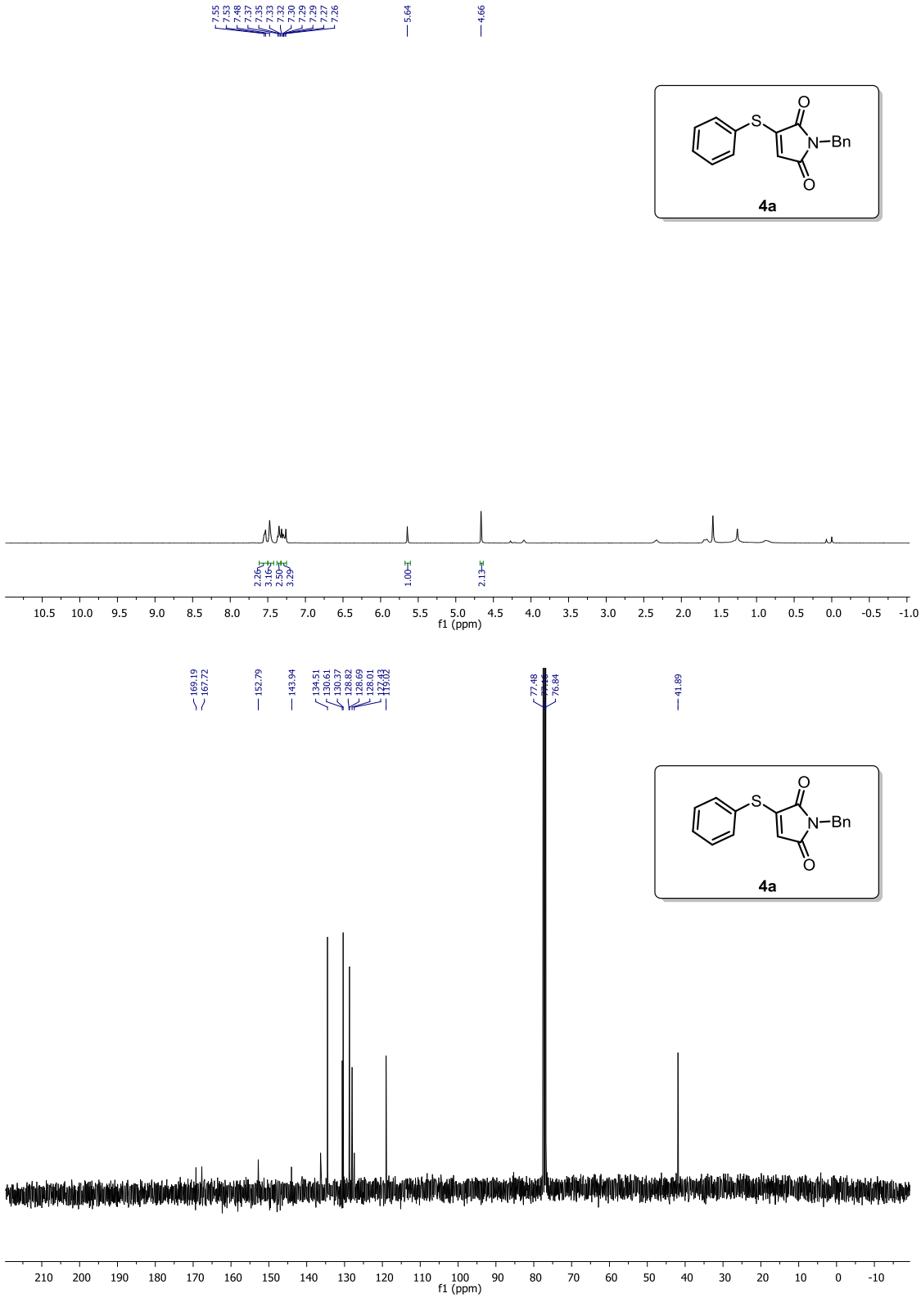

1.97
1.96
5.12
0.93
2.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)


169.15
168.54
149.99
137.32
136.91
136.25
130.71
128.81
128.66
128.01
124.90
121.92
77.48
77.16
76.84
41.95


Se
O
N–Bn
Cl
O
3s


210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.61
7.60
7.34
7.32
7.30
7.26
7.15
7.14
7.13
7.12
5.96
4.66
S
Se
O
N–Bn
O
3t
1.00
6.43
1.18
0.97
2.32
f1 (ppm)
169.16
168.40
150.62
138.25
136.25
133.88
129.09
128.84
128.65
128.04
125.90
116.43
77.48
77.16
76.84
41.93
S
Se
O
N–Bn
O
3t
f1 (ppm)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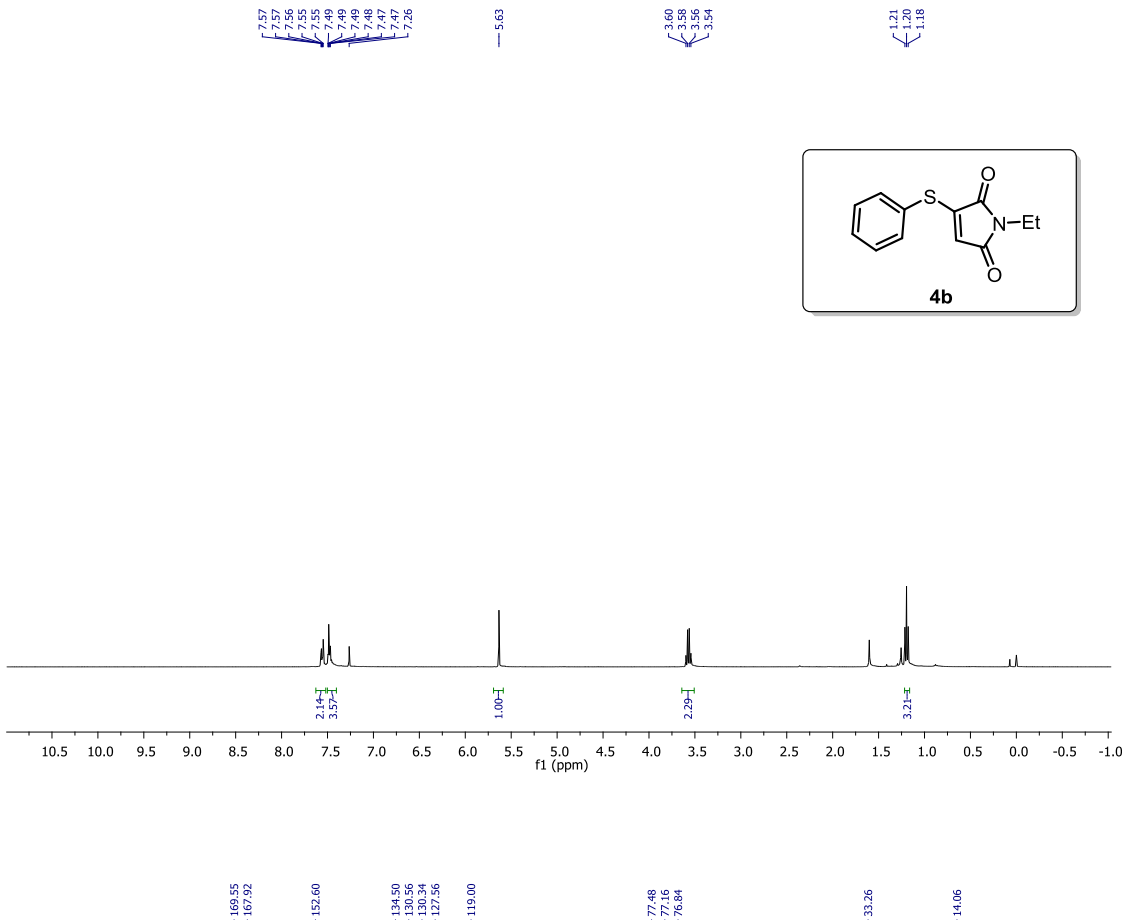
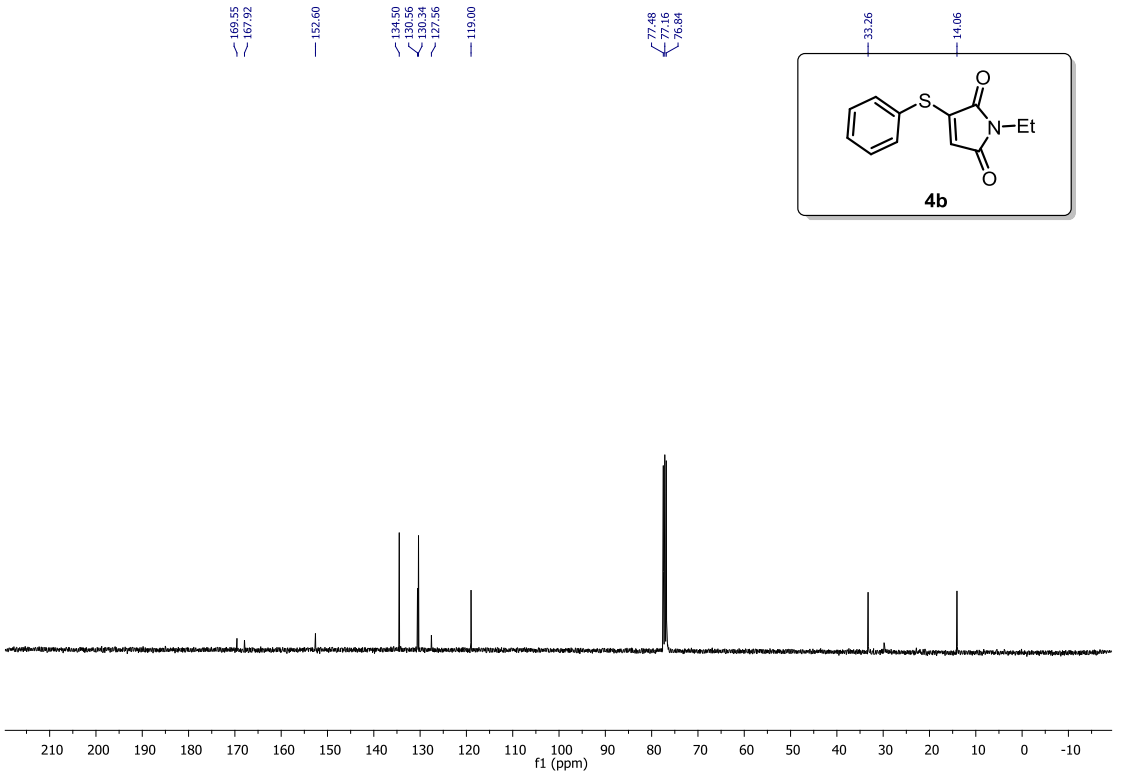
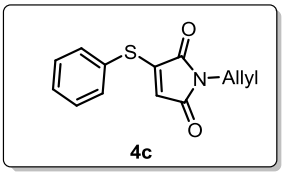
7.53
7.48
7.37
7.35
7.33
7.32
7.30
7.29
7.29
7.27
7.26
5.64
4.66
S
O
N–Bn
O
4a
2.26
3.16
2.50
3.29
1.00
2.13
f1 (ppm)
169.19
167.72
152.79
143.94
134.51
130.61
130.37
128.82
128.69
128.01
77.48
76.84
41.89
4a
f1 (ppm)

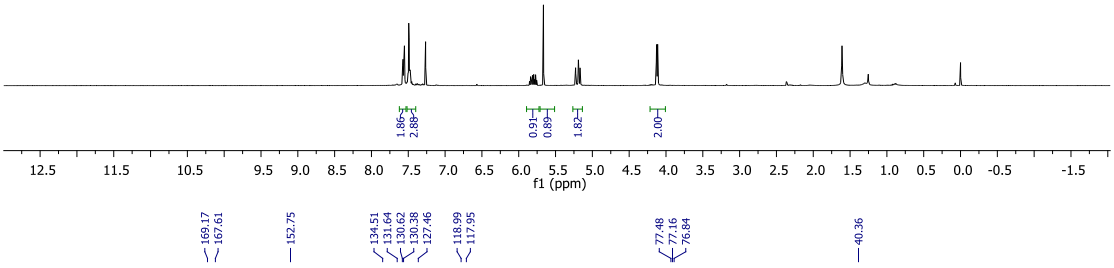

7.57
7.57
7.56
7.55
7.55
7.49
7.49
7.48
7.47
7.47
7.26
5.63
3.60
3.58
3.56
3.54
1.21
1.20
1.18
S
O
N–Et
O
4b
2.14
3.57
1.00
2.29
3.21
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)


169.55
167.92
152.60
134.50
130.56
130.34
127.56
119.00
77.48
77.16
76.84
33.26
14.06
S
O
N–Et
O
4b
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

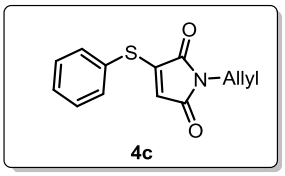

7.58
7.57
7.56
7.56
7.55
7.49
7.49
7.48
7.48
7.48
7.48
7.26
5.84
5.81
5.81
5.80
5.77
5.66
5.19
5.19
5.19
5.18
4.13
4.12
4.12
4.11
4.11


O
S
N–Allyl
O

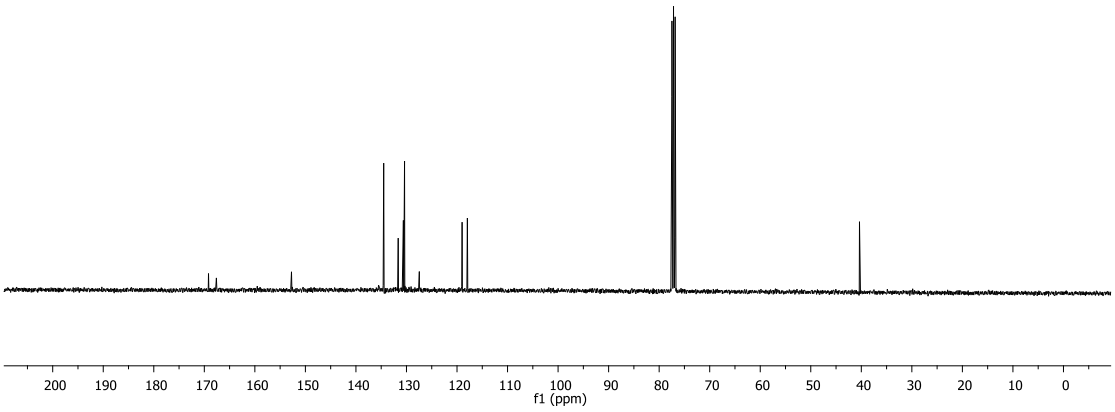
4c


1.86
2.88
0.91
0.89
1.82
2.00
12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.5
f1 (ppm)

169.17
167.61
152.75
134.51
131.64
130.62
130.38
127.46
118.99
117.95
77.48
77.16
76.84
40.36


O
S
N–Allyl
O

4c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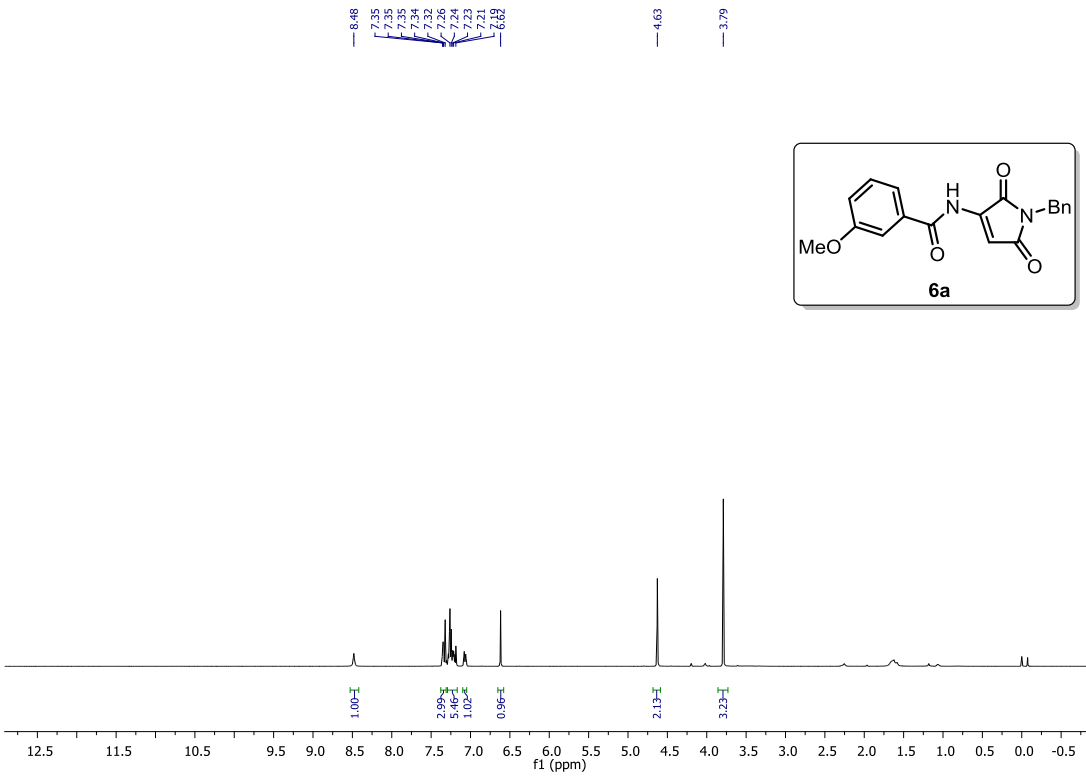
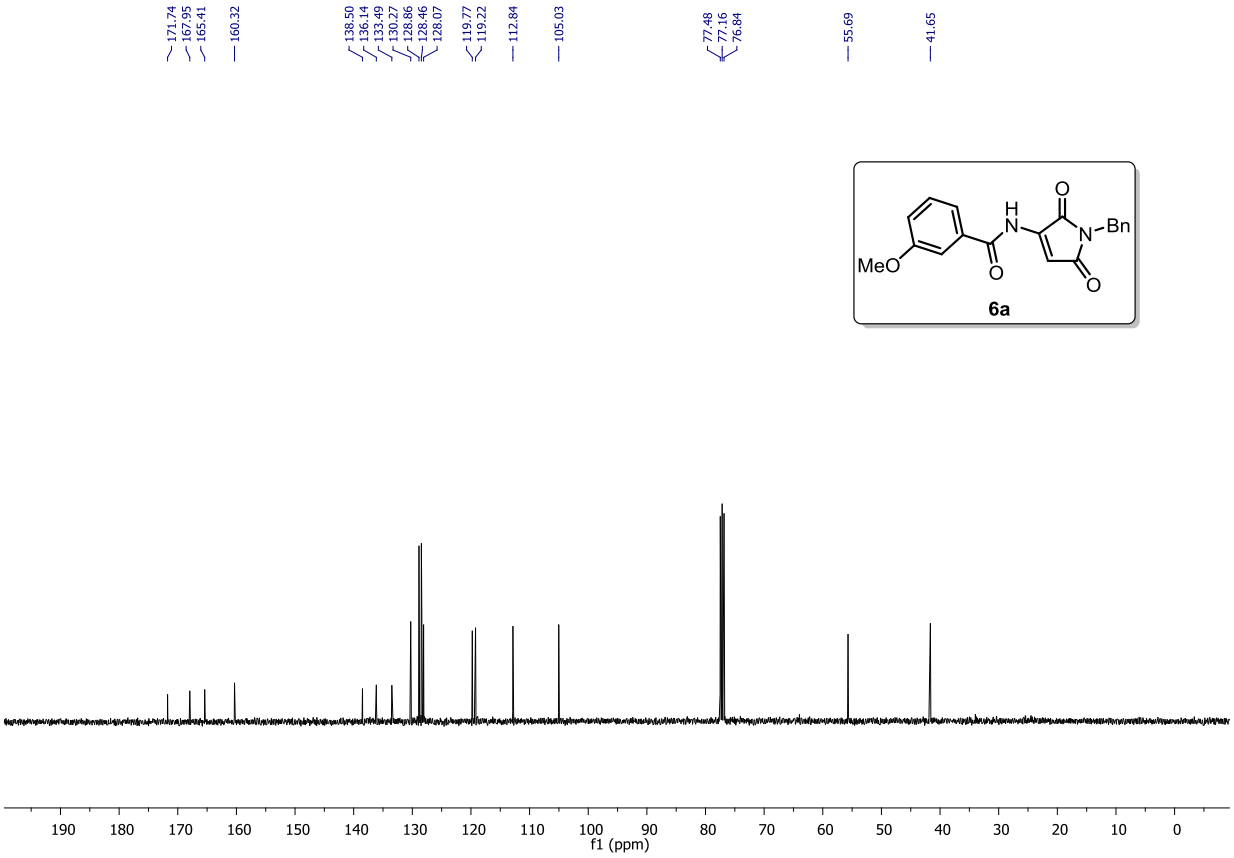
f1 (ppm)


8.48
7.35
7.35
7.35
7.34
7.32
7.26
7.24
7.23
7.21
7.19
6.62
4.63
3.79
MeO
N
H
O
Bn
6a
1.00
2.99
5.46
1.02
0.96
2.13
3.23
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)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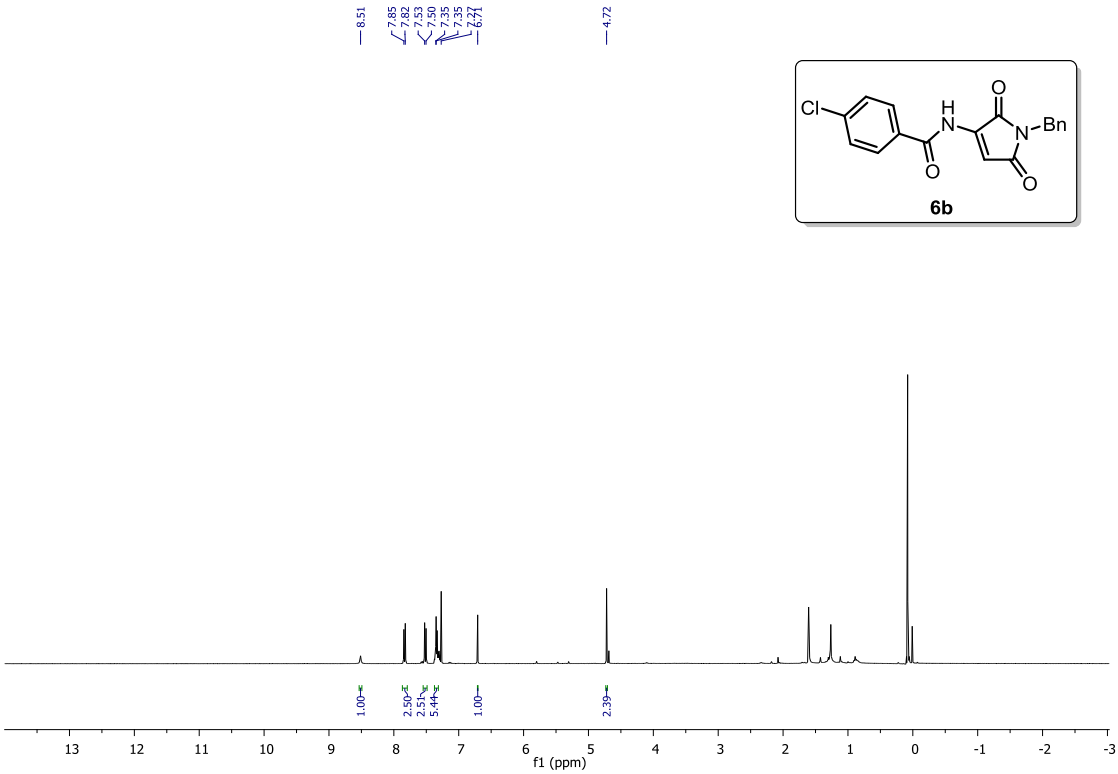
138.50
136.14
133.49
130.27
128.86
128.46
128.07
119.77
119.22
112.84
105.03
77.48
77.16
76.84
55.69
41.65
MeO
N
H
O
Bn
6a
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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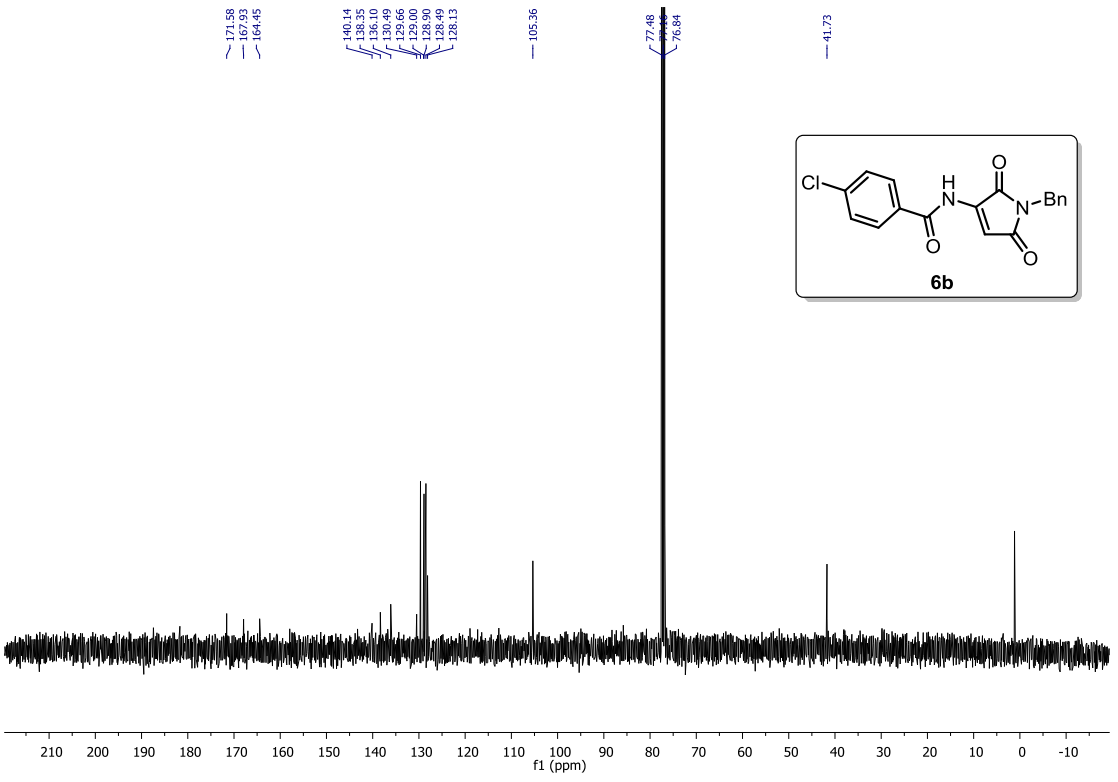
7.85
7.82
7.53
7.50
7.35
7.35
6.71
4.72
Cl
H
N
O
O
N
Bn
O
6b
1.00
2.50
2.51
5.44
1.00
2.39
f1 (ppm)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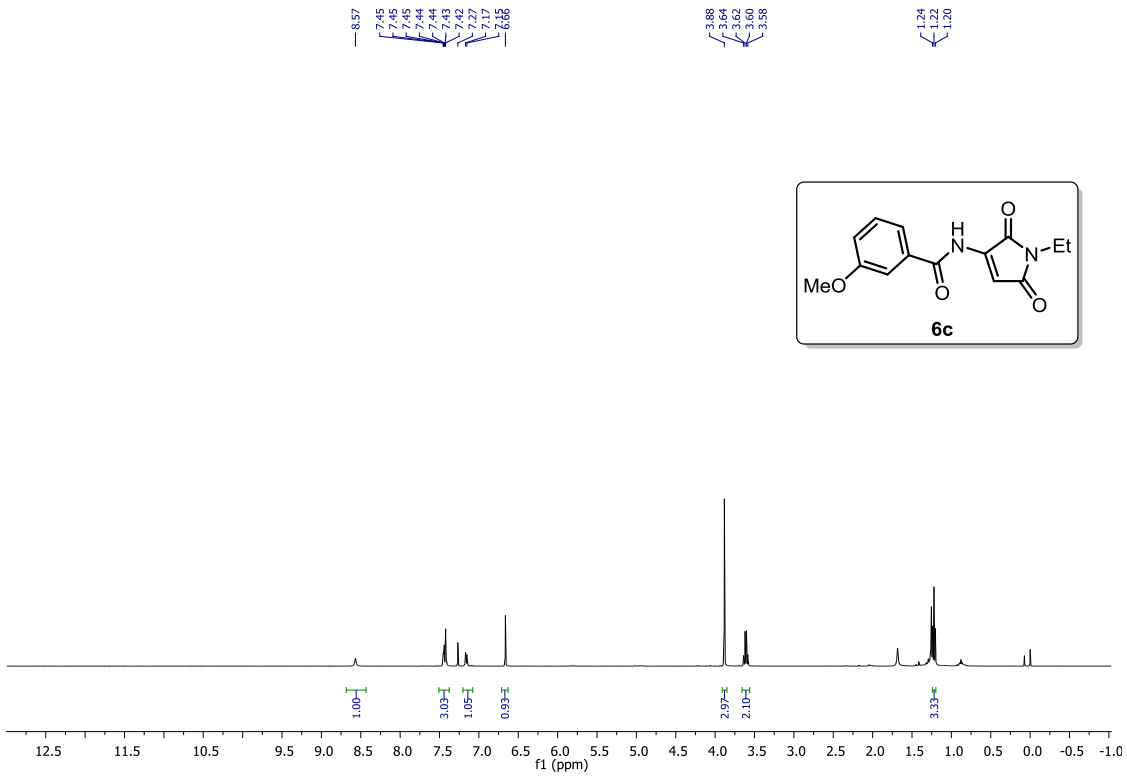
136.10
130.49
129.66
129.00
128.60
128.49
128.13
105.36
77.48
77.16
76.84
41.73
Cl
H
N
O
O
N
Bn
O
6b
f1 (ppm)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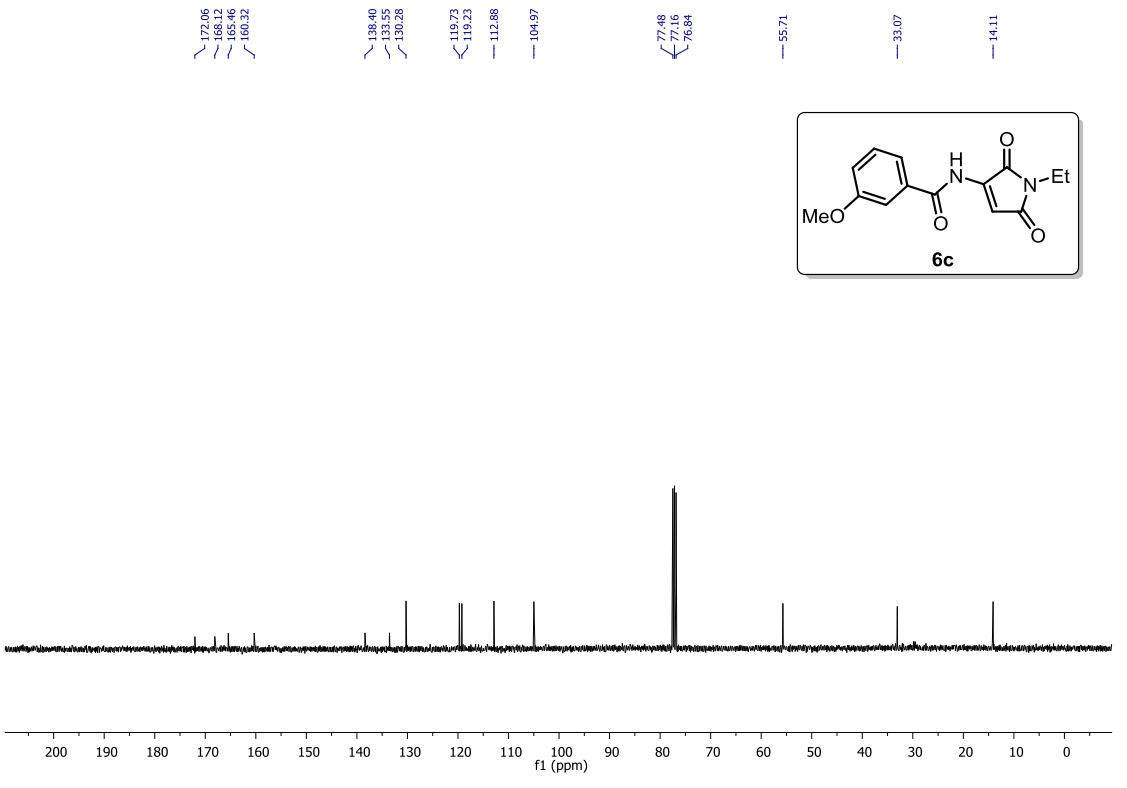
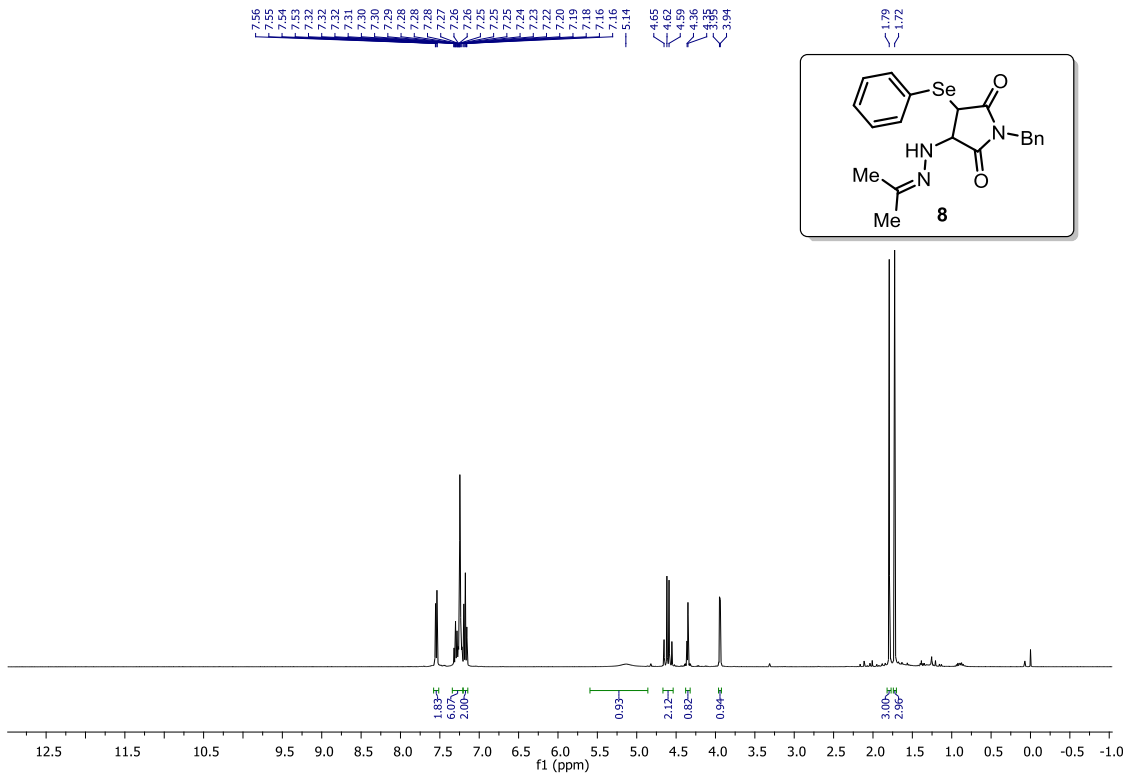
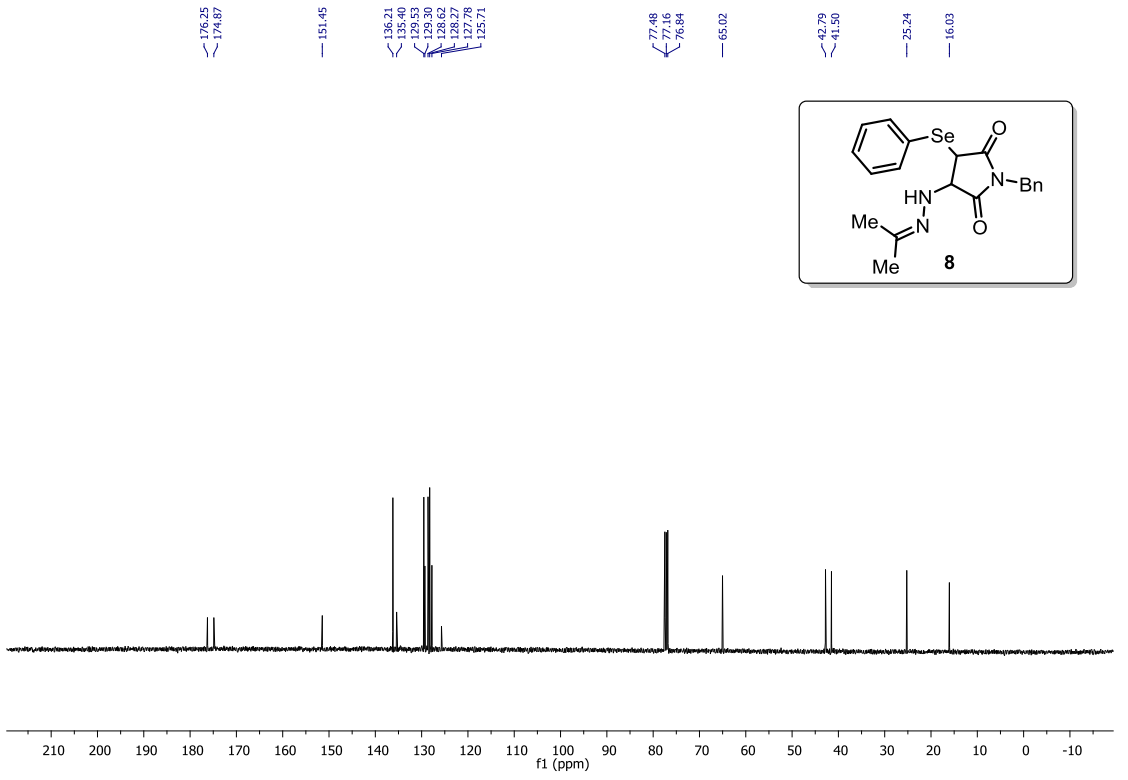
7.45
7.45
7.44
7.44
7.43
7.42
7.27
7.17
6.65
6.65
3.88
3.64
3.62
3.60
3.58
1.24
1.22
1.20
MeO
H
N
O
O
N
Et
O
O
6c
1.00
3.03
1.05
0.93
2.97
2.10
3.33
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)


172.06
168.12
165.46
160.32
138.40
133.55
130.28
119.73
119.23
112.88
104.97
77.48
77.16
76.84
55.71
33.07
14.11
MeO
H
N
O
O
N
Et
O
O
6c
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.56 7.55 7.54 7.53 7.32 7.32 7.32 7.31 7.30 7.30 7.29 7.28 7.28 7.28 7.27 7.26 7.26 7.25 7.25 7.25 7.24 7.23 7.22 7.20 7.19 7.18 7.16 7.16 5.14
4.65 4.62 4.59 4.36 3.95 3.94
1.79 1.72
Se
O
N
Bn
HN
N
O
Me
Me
8
1.83 6.07 2.00 0.93 2.12 0.82 0.94 3.00 2.96
12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)


176.25 174.87 151.45 136.21 135.40 129.53 129.30 128.62 128.27 127.78 125.71
77.48 77.16 76.84 65.02 42.79 41.50 25.24 16.03
Se
O
N
Bn
HN
N
O
Me
Me
8
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)