Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

$MeSeSO_3Na$ Reagent for Oxidative Aminoselenomethylation of Maleimides

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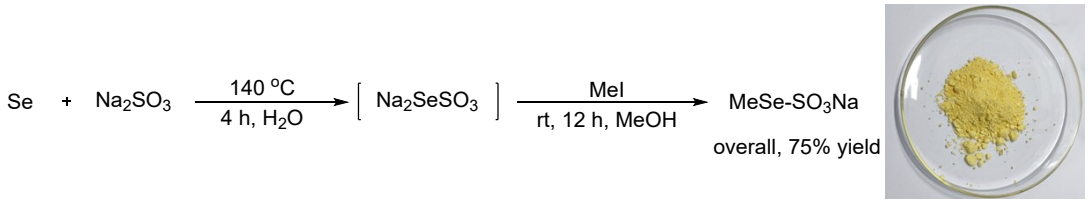
General Information

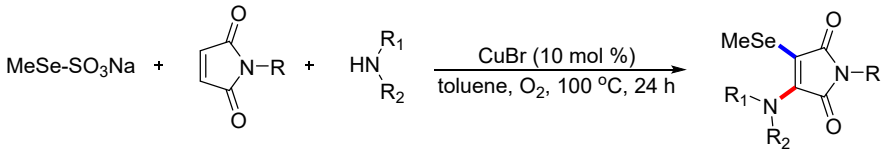
N-substituent Maleimides[1] were prepared according to the reported procedures. ^{1}H and ^{13}C spectra of known compounds were in accordance with those described in the literatures. All other reagents were purchased from TCI, Sigma-Aldrich, Alfa Aesar, Acros, and Meryer and used without further purification. ^{1}H NMR (500 MHz), ^{13}C NMR (125 MHz) and ^{19}F NMR (470 MHz) spectra were recorded in $CDCl_3$ and DMSO-D6 solutions using a Burker AVANCE 500 spectrometer. High-resolution mass spectra were recorded on an ESI-Q-TOF mass spectrometer. Analysis of crude reaction mixture was done on the Varian 4000 GC/MS and 1200 LC. All reactions were conducted using standard Schlenk techniques. Column chromatography was performed using EM silica gel 60 (300−400 m).

Synthesis of MeSe-SO_3Na reagent:



A flask was charged with finely powdered selenium (3.79 g, 48 mmol), sodium thiosulfate (15.178 g, 96 mmol, 2 equiv) and water (50.0 mL). The reaction mixture was stirred and heated to 140 °C for 4 h. The reaction mixture was cooled to rt, and then added the iodomethane (40 mmol) in 120 mL MeOH. The solution was stirred for additional 12 h at room temperature. Then, the mixture was cooled to rt, and concentrated on a rotovap at a bath temperature of 50 °C to remove the MeOH and water. The resultant solid was treated with MeOH (100mL), let it stand at room temperature for 6 hours, and filtered through a frit funnel. The filtrate was concentrated to a solid, trituration with hexanes, filtration, and drying under vacuum to give MeSe-SO_3Na reagent.

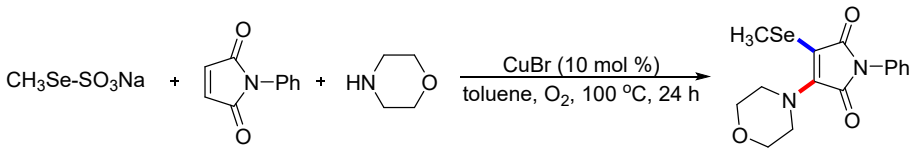
General Procedure of Copper-catalyzed Oxidative Aminoselenomethylation of Maleimides with Alkylamines and $MeSeSO_3Na$ Reagent:



1a **2** **3** **4-5**

A 25 mL Schlenk tube equipped with a stir bar was charged with MeSe-SO_3Na (0.6 mmol), maleimide (0.2 mmol), alkylamines (0.6 mmol), CuBr (0.02 mol) and 2 mL toluene. The tube was fitted with a rubber septum, and then it was evacuated and refilled with dioxygen three times, then the septum was replaced by a Teflon screwcap under oxygen flow. The reaction mixture was stirred at 100 ℃ (aluminium block heating mantle) for 24 h. After cooling down, the reaction mixture was diluted with 10 mL of ethyl ether, filtered through a pad of silica gel, followed by washing the pad of the silica gel with the same solvent (20 mL), concentrated under reduced pressure. The residue was then purified by flash chromatography on silica gel to provide the corresponding product.

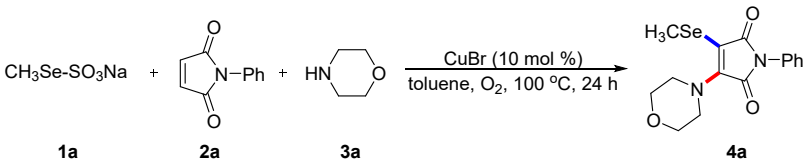
5mmol scale-up reaction:



1a **2a** **3a** **4a**, 66%

A 125 mL Schlenk tube equipped with a stir bar was charged with MeSe-SO_3Na (15.0 mmol), *N*-phenyl maleimide (5.0 mmol), morpholine (15.0 mmol), CuBr (0.5 mol) and 50 mL toluene. The tube was fitted with a rubber septum, and then it was evacuated and refilled with dioxygen three times, then the septum was replaced by a Teflon screwcap under oxygen flow. The reaction mixture was stirred at 100 ℃ (oil bath) for 24 h. After cooling down, the reaction mixture was diluted with 10 mL of ethyl ether, filtered through a pad of silica gel, followed by washing the pad of the silica gel with the same solvent (20 mL), concentrated under reduced pressure. The residue was then purified by flash chromatography on silica gel to provide the corresponding product (66%, isolated yield).

Screening with different reaction conditions



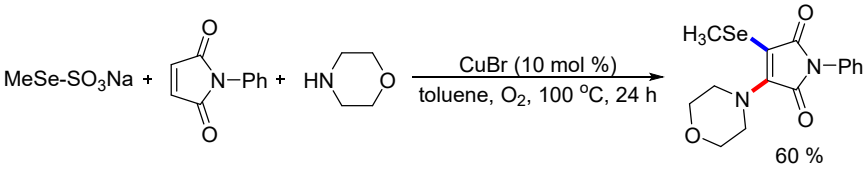
1a 2a 3a 4a

entry	[Cu]	additive	solvent	Yield (%)[b]
1	CuI		toluene	45
2	CuBr		toluene	79
3	CuCl		toluene	30
4	Cu(OAc)2		toluene	0
5	CuF2		toluene	0
6	CuCl2		toluene	0
7	CuBr2		toluene	0
8	Cu(acac)2		toluene	0
9	CuBr	$BF_3.2H_2O$	toluene	23
10	CuBr	TsOH	toluene	47
11	CuBr	$FeCl_3$	toluene	56
12	CuBr	Ag_2CO_3	toluene	0
13	CuBr	1,10-phen	toluene	55
14	CuBr	2,2'-bipyridine	toluene	40
15	CuBr		DCE	61
16	CuBr		CH_3CN	0
17	CuBr		DMSO	0
18	CuBr		benzene	60
19			toluene	0
20[c]	CuBr		toluene	0
21[d]	CuBr		toluene	48

[a]Reaction conditions unless specified otherwise: **1a** (0.6 mmol), **2a** (0.2 mmol), **3a** (0.6 mmol), catalyst (0.02 mmol), additive (0.04 mmol), solvent (2.0 mL), under O_2, 100 °C, 24 h,. [b]Isolated yield. [c]Under N_2. [d]Under air atmosphere.

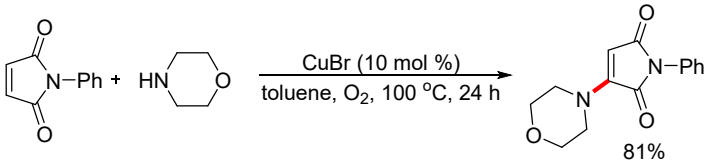
Mechanism investigation:

(a) Radical scavenger

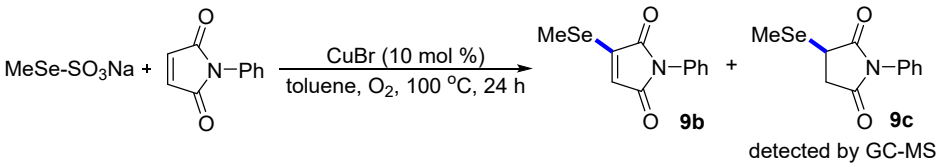


A 25 mL Schlenk tube equipped with a stir bar was charged with MeS-SO_3Na (0.6 mmol), *N*-phenyl maleimide (0.2 mmol), morpholine (0.6 mmol), CuBr (0.02 mol), TEMPO (0.6 mmol) and 2 mL toluene. The tube was fitted with a rubber septum, and then it was evacuated and refilled with dioxygen three times, then the septum was replaced by a Teflon screwcap under oxygen flow. The reaction mixture was stirred at 100 ℃ for 24 h. After cooling down, the reaction mixture was diluted with 10 mL of ethyl ether, filtered through a pad of silica gel, followed by washing the pad of the silica gel with the same solvent (20 mL), concentrated under reduced pressure. The residue was then purified by flash chromatography on silica gel (petroleum ether : EtOAc = 9 : 1) to give **4a** product in 60% yield. This result excludes the involvement of a radical species in the reaction progress.

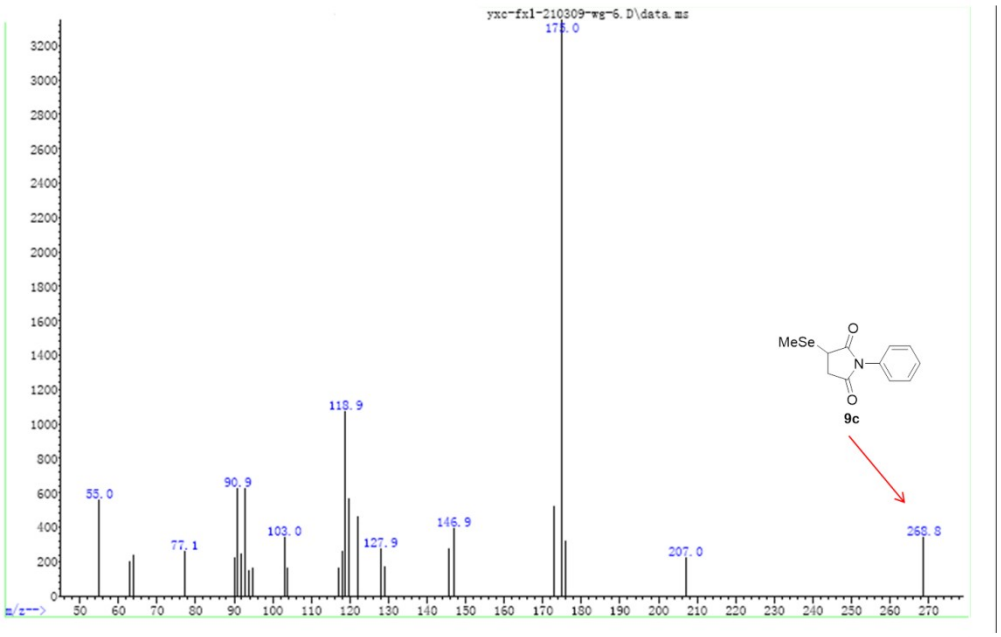
(b) Probing key intermediate

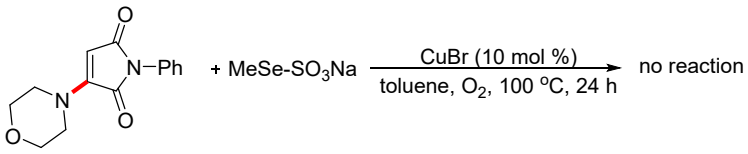


A 25 mL Schlenk tube equipped with a stir bar was charged with *N*-phenyl maleimide (0.2 mmol), morpholine (0.6 mmol), CuBr (0.02 mol) and 2 mL toluene. The tube was fitted with a rubber septum, and then it was evacuated and refilled with dioxygen three times, then the septum was replaced by a Teflon screwcap under oxygen flow. The reaction mixture was stirred at 100 ℃ for 24 h. After cooling down, the reaction mixture was diluted with 10 mL of ethyl ether, filtered through a pad of silica gel, followed by washing the pad of the silica gel with the same solvent (20 mL), concentrated under reduced pressure. The residue was then purified by flash chromatography on silica gel (petroleum ether : EtOAc = 9 : 1) to give product in 81% yield.



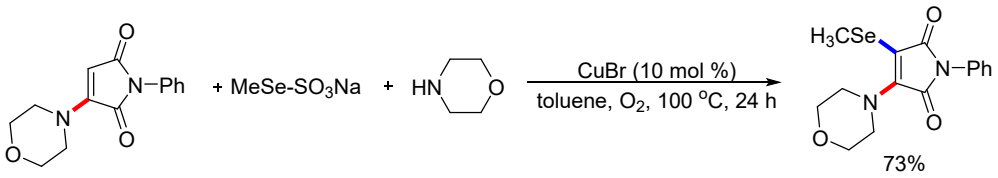
A 25 mL Schlenk tube equipped with a stir bar was charged with *N*-phenyl maleimide (0.2 mmol), MeSe-SO_3Na (0.6 mmol), CuBr (0.02 mol) and 2 mL toluene. The tube was fitted with a rubber septum, and then it was evacuated and refilled with dioxygen three times, then the septum was replaced by a Teflon screwcap under oxygen flow. The reaction mixture was stirred at 100 ℃ for 24 h. After cooling down, the reaction mixture was diluted with 10 mL of ethyl ether, filtered through a pad of silica gel, the oxidative selenomethylation of maleimide was not detected by GC-MS, the Se-Michael addition product was detected by GC-MS.





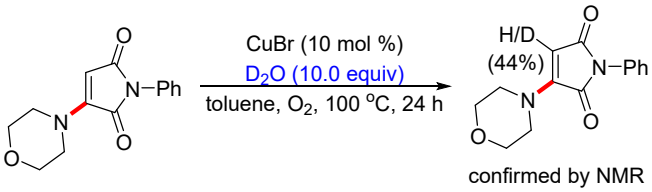
A 25 mL Schlenk tube equipped with a stir bar was charged with 3-morpholino-1-phenyl-1H-pyrrole-2,5-dione (0.2 mmol), MeSe-SO_3Na (0.6 mmol), CuBr (0.02 mol) and 2 mL toluene. The tube was fitted with a rubber septum, and then it was evacuated and refilled with dioxygen three times, then the septum was replaced by a Teflon screwcap under oxygen flow. The reaction

mixture was stirred at 100 ℃ for 24 h. After cooling down, the reaction mixture was diluted with 10 mL of ethyl ether, filtered through a pad of silica gel, the oxidative selenomethylation product was not detected by GC-MS.

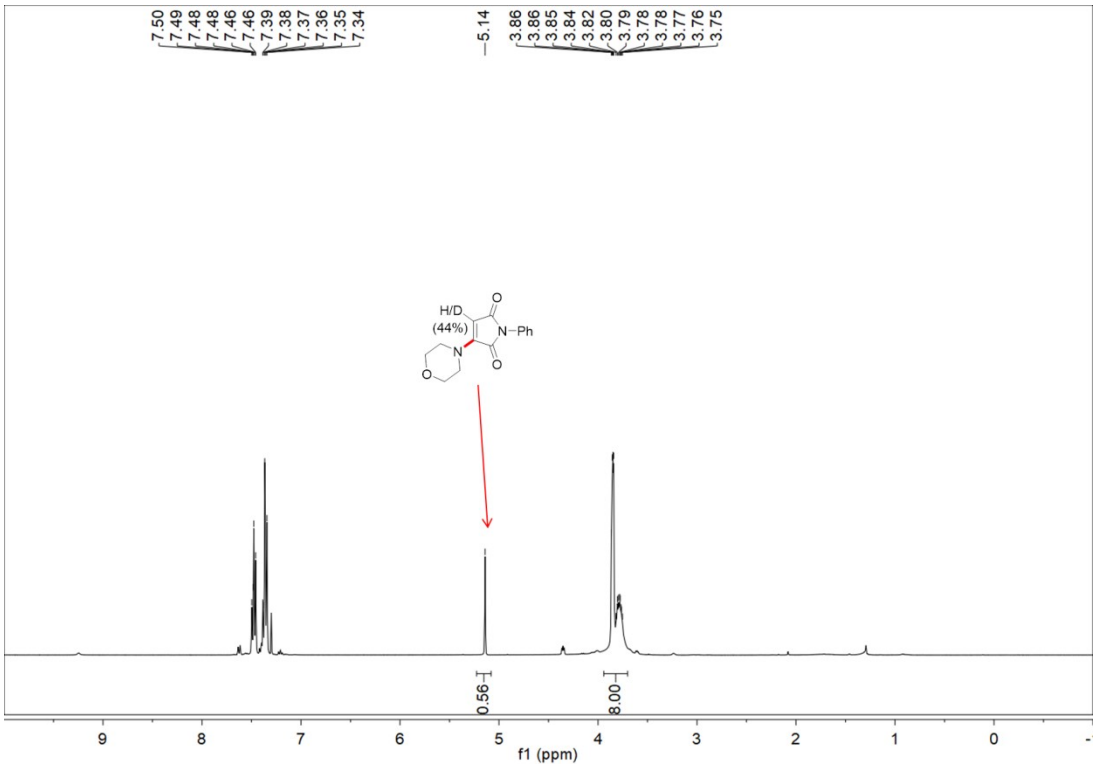


A 25 mL Schlenk tube equipped with a stir bar was charged with 3-morpholino-1-phenyl-1H-pyrrole-2,5-dione (0.2 mmol), MeSe-SO_3Na (0.6 mmol), morpholine (0.6 mmol), CuBr (0.02 mol) and 2 mL toluene. The tube was fitted with a rubber septum, and then it was evacuated and refilled with dioxygen three times, then the septum was replaced by a Teflon screwcap under oxygen flow. The reaction mixture was stirred at 100 ℃ for 24 h. After cooling down, the reaction mixture was diluted with 10 mL of ethyl ether, filtered through a pad of silica gel, the corresponding product was isolated in 73% yield. This result shows that the morpholine not only works as substrate in multi-component reaction, but also function as activator of Se-Bunte salt to furnish the corresponding selenomethylation reactions.

(c) H/D exchange



A 25 mL Schlenk tube equipped with a stir bar was charged with 3-morpholino-1-phenyl-1H-pyrrole-2,5-dione (0.2 mmol), D_2O (2.0 mmol), CuI (0.02 mol), and 1 mL DCE. The tube was fitted with a rubber septum, and then it was evacuated and refilled with dioxygen three times, then the septum was replaced by a Teflon screwcap under oxygen flow. The reaction mixture was stirred at 100 ℃. After stirring for 18 h, the reaction mixture was cooled to room temperature and the reaction was filtered through a pad of Celite and diluted with ethyl acetate (10 mL), deuterium-hydrogen exchange was observed in 3-morpholino-1-phenyl-1H-pyrrole-2,5-dione, which suggest the C-H activation was occurred under the current reaction condition.


7.50
7.49
7.48
7.48
7.46
7.46
7.39
7.38
7.37
7.36
7.35
7.34
5.14
3.86
3.86
3.85
3.84
3.82
3.80
3.79
3.78
3.78
3.77
3.76
3.75
H/D
(44%)
N
N–Ph
O
O
O
0.56
8.00
9
8
7
6
5
4
3
2
1
0
f1 (ppm)

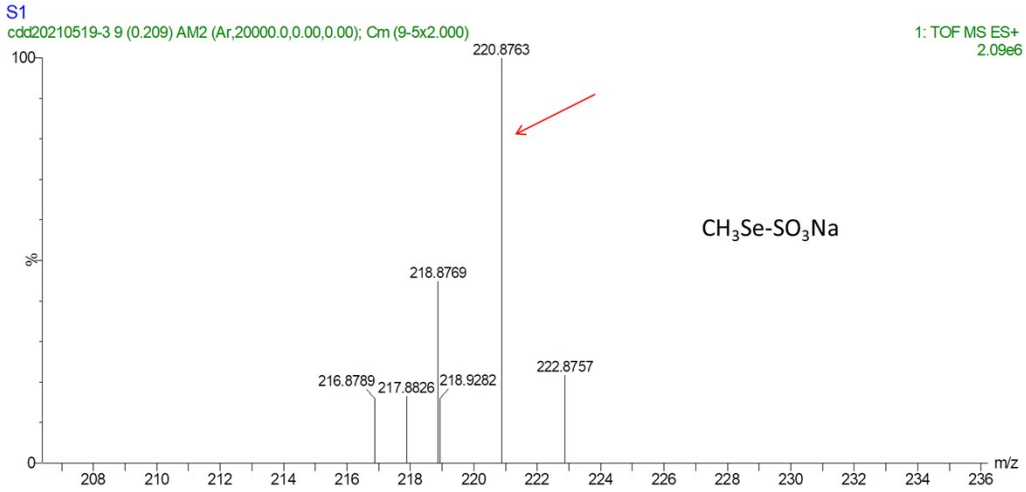
Characterization of Products in Details:

sodium Se-methyl sulfurothioate

$CH_3Se\text{-}SO_3Na$

^{1}H NMR (400 MHz, D_2O): δ 2.77 (s, 3H); **^{13}C NMR** (100MHz, $CDCl_3$): δ 10.8;

HRMS (ESI): calcd for $CH_3O_3Na_2SSe$ $[M + Na]^+$ 220.8764, found 220.8763.

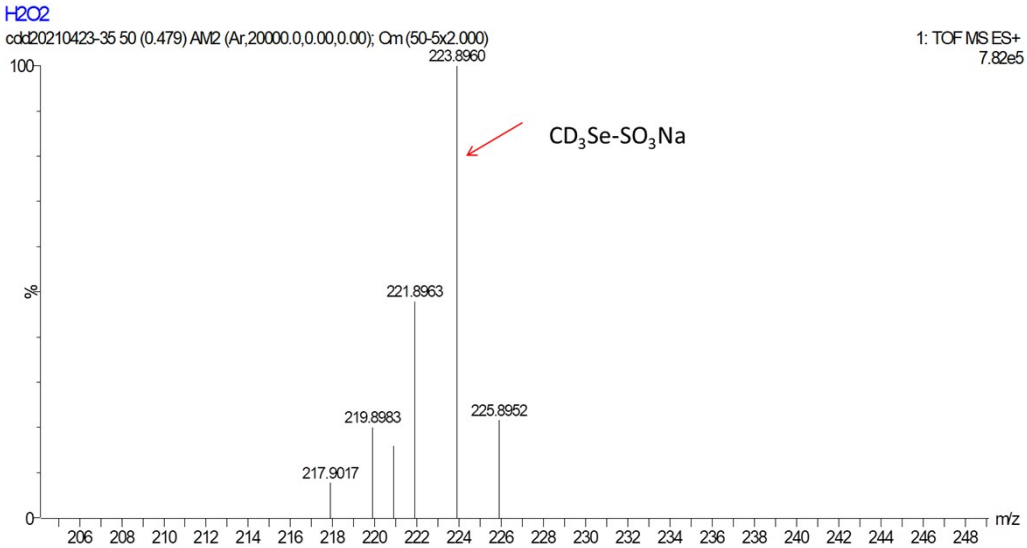


sodium Se-trideuteromethyl sulfurothioate

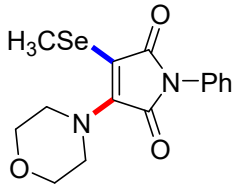
$CD_3Se\text{-}SO_3Na$

^{13}C NMR (100MHz, $CDCl_3$): δ 10.8;

HRMS (ESI): calcd for $CD_3SeSO_3Na_2$ $[M + Na]^+$ 223.8952, found 223.8960.



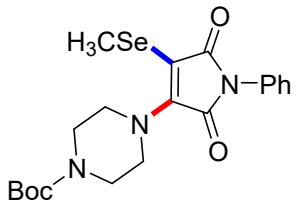
3-(methylselanyl)-4-morpholino-1-phenyl-1H-pyrrole-2,5-dione



4a

Following the general procedure, using (petroleum ether : EtOAc = 9 : 1) as the eluant afforded a yellow solid (55.6 mg, 79% yield), Mp = 106-107 ℃. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.49-7.45 (m, 2H), 7.38-7.35 (m, 3H), 4.20 (t, *J* = 4.72 Hz, 4H), 3.87 (t, *J* = 4.80 Hz, 4H), 2.30 (s, 3H); **^{13}C NMR** (100MHz, $CDCl_3$): δ 169.0, 165.6, 148.4, 131.9, 128.9, 127.7, 126.3, 90.6, 67.1, 48.9, 9.6; **HRMS** (ESI): calcd for $C_{15}H_{17}N_2O_3Se$ $[M + H]^+$ 353.0404, found 353.0410.

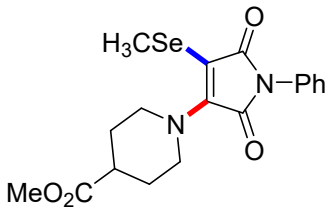
tert-butyl 4-(4-(methylselanyl)-2,5-dioxo-1-phenyl-2,5-dihydro-1H-pyrrol-3-yl)piperazine-1-carboxylate



4b

Following the general procedure, using (petroleum ether : EtOAc = 9 : 1) as the eluant afforded a yellow liquid (65.8 mg, 73% yield). **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.47-7.43 (m, 2H), 7.35-7.33 (m, 3H), 4.11 (t, *J* = 5.2 Hz, 4H), 3.60 (t, *J* = 5.2 Hz, 4H), 2.29 (s, 3H), 1.50 (s, 9H); **^{13}C NMR** (125MHz, $CDCl_3$): δ 168.8, 165.5, 154.5, 148.5, 131.9, 128.9, 127.5, 126.2, 91.3, 80.4, 48.3, 28.4, 26.9, 9.4; **HRMS** (ESI): calcd for $C_{20}H_{25}N_3O_4NaSe$ $[M + Na]^+$ 474.0908, found 474.0912.

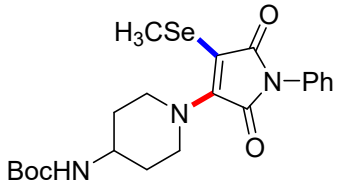
methyl 1-(4-(methylselanyl)-2,5-dioxo-1-phenyl-2,5-dihydro-1H-pyrrol-3-yl)piperidine-4-carboxylate



4c

Following the general procedure, using (petroleum ether : EtOAc = 9 : 1) as the eluant afforded a yellow liquid (53.0 mg, 65% yield). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.47-7.44 (m, 2H), 7.37-7.34 (m, 3H), 4.90-4.84 (m, 2H), 3.74 (s, 3H), 3.41 (ddd, *J* = 13.7, 11.0, 2.9 Hz, 2H), 2.68 (tt, *J* = 10.5, 4.2 Hz, 1H), 2.28 (s, 3H), 2.09 (dt, *J* = 13.8, 3.9 Hz, 2H), 1.93 (dtd, *J* = 14.2, 10.7, 3.8 Hz, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 174.5, 169.1, 165.6, 148.9, 132.0, 128.9, 127.5, 126.3, 89.9, 52.0, 48.2, 40.4, 28.7, 9.6; **HRMS** (ESI): calcd for $C_{18}H_{21}N_2O_4Se$ $[M + H]^+$ 409.0667, found 409.0672.

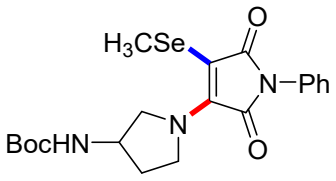
tert-butyl (1-(4-(methylselanyl)-2,5-dioxo-1-phenyl-2,5-dihydro-1H-pyrrol-3-yl)piperidin-4-yl)carbamate



4d

Following the general procedure, using (petroleum ether : EtOAc = 9 : 1) as the eluant afforded a yellow solid (65.1 mg, 70% yield), Mp = 122-123 ℃. **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.46-7.43 (m, 2H), 7.35-7.32 (m, 3H), 4.93 (d, *J* = 13.5 Hz, 2H), 4.53 (d, *J* = 7.9 Hz, 1H), 3.78 (s, 1H), 3.33-3.28 (m, 2H), 2.28 (s, 3H), 2.11 (dd, *J* = 13.4, 3.9 Hz, 2H), 1.55 (dtd, *J* = 13.2, 11.2, 3.9 Hz, 2H), 1.47 (s, 9H); **^{13}C NMR** (125MHz, $CDCl_3$): δ 169.0, 165.5, 155.1, 148.8, 132.0, 128.8, 127.5, 126.2, 90.3, 79.7, 47.8, 47.4, 33.1, 28.4, 9.5; **HRMS** (ESI): calcd for $C_{21}H_{27}N_3O_4NaSe$ $[M + Na]^+$ 488.1064, found 488.1073.

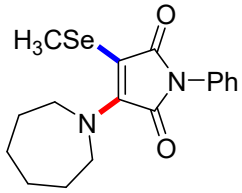
tert-butyl (1-(4-(methylselanyl)-2,5-dioxo-1-phenyl-2,5-dihydro-1H-pyrrol-3-yl)pyrrolidin-3-yl)carbamate



4e

Following the general procedure, using (petroleum ether : EtOAc = 9 : 1) as the eluant afforded a yellow liquid (64.0 mg, 71% yield). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.48-7.44 (m, 2H), 7.38-7.32 (m, 3H), 4.77 (brs, 1H), 4.34 (brs, 1H), 4.26 (dd, *J* = 13.1, 5.8 Hz, 1H), 4.17 (dt, *J* = 8.9, 6.4 Hz, 2H), 4.03 (dd, *J* = 13.1, 4.1 Hz, 1H), 2.6-2.17 (m, 4H), 1.98 (dq, *J* = 12.5, 6.1 Hz, 1H), 1.49 (s, 9H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 169.7, 165.1, 155.3, 147.5, 132.1, 128.9, 127.5, 126.2, 86.2, 80.1, 56.8, 49.7, 31.2, 28.4, 14.3, 10.6; **HRMS** (ESI): calcd for $C_{20}H_{25}N_3O_4NaSe$ $[M + Na]^+$ 474.0908, found 474.0909.

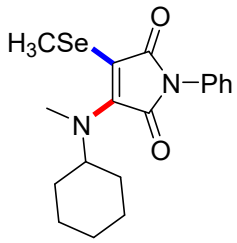
3-(azepan-1-yl)-4-(methylselanyl)-1-phenyl-1H-pyrrole-2,5-dione



4f

Following the general procedure, using (petroleum ether : EtOAc = 9 : 1) as the eluant afforded a yellow solid (56.1 mg, 77% yield), Mp = 70-71 °C. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.49-7.45 (m, 2H), 7.41-7.33 (m, 3H), 4.14 (t, *J* = 6.1 Hz, 4H), 2.28 (s, 3H), 1.92-1.89 (m, 4H), 1.68 (q, *J* = 3.1 Hz, 4H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 165.2, 156.3, 148.4, 132.2, 128.9, 127.4, 126.3, 85.4, 53.0, 28.6, 26.5, 10.3; **HRMS** (ESI): calcd for $C_{17}H_{21}N_2O_2Se$ $[M + H]^+$ 365.0768, found 365.0778.

3-(cyclohexyl(methyl)amino)-4-(methylselanyl)-1-phenyl-1H-pyrrole-2,5-dione

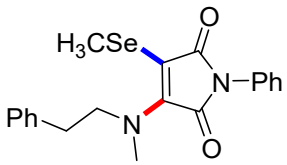


4g

Following the general procedure, using (petroleum ether : EtOAc = 9 : 1) as the eluant afforded a

yellow liquid (55.9 mg, 74% yield). **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.46-7.43 (m, 2H), 7.37-7.31 (m, 3H), 4.79 (tt, *J* = 11.8, 3.5 Hz, 1H), 3.34 (s, 3H), 2.27 (s, 3H), 1.88 (tt, *J* = 11.3, 3.1 Hz, 4H), 1.72 (d, *J* = 13.5 Hz, 1H), 1.60 (qd, *J* = 12.7, 12.1, 3.8 Hz, 3H), 1.45 (qt, *J* = 12.9, 3.7 Hz, 2H), 1.15 (qt, *J* = 13.1, 3.6 Hz, 1H); **^{13}C NMR** (125MHz, $CDCl_3$): δ 169.4, 165.6, 150.0, 132.2, 128.8, 127.3, 126.3, 87.3, 59.5, 33.6, 30.4, 25.4, 25.3, 10.0; **HRMS** (ESI): calcd for $C_{18}H_{23}N_2O_2Se$ $[M + H]^+$ 379.0925, found 379.0926.

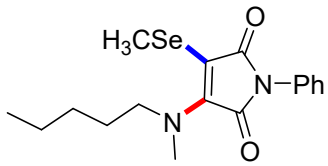
3-(methyl(phenethyl)amino)-4-(methylselanyl)-1-phenyl-1H-pyrrole-2,5-dione



4h

Following the general procedure, using (petroleum ether : EtOAc = 9 : 1) as the eluant afforded a yellow solid (64.0 mg, 80% yield), Mp = 96-97 ℃. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.49-7.46 (m, 2H), 7.38-7.25 (m, 8H), 4.19 (t, *J* = 7.7 Hz, 2H), 3.54 (s, 3H), 3.04 (t, *J* = 7.7 Hz, 2H), 2.27 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 169.3, 165.4, 148.9, 138.0, 132.1, 129.1, 128.9, 128.7, 127.5, 126.8, 126.4, 87.5, 55.6, 41.4, 34.8, 10.3; **HRMS** (ESI): calcd for $C_{20}H_{21}N_2O_2Se$ $[M + H]^+$ 401.0768, found 401.0772.

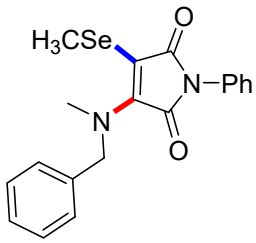
3-(methyl(pentyl)amino)-4-(methylselanyl)-1-phenyl-1H-pyrrole-2,5-dione



4i

Following the general procedure, using (petroleum ether : EtOAc = 9 : 1) as the eluant afforded a yellow liquid (60.0 mg, 82% yield). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.4-7.45 (m, 2H), 7.39-7.33 (m, 3H), 3.93-3.89 (m, 2H), 3.55 (s, 3H), 2.27 (s, 3H), 1.74 (p, *J* = 7.7 Hz, 2H), 1.39 (dq, *J* = 13.0, 7.7, 7.2 Hz, 4H), 0.96 (t, *J* = 6.9 Hz, 3H); **^{13}C NMR** (100MHz, $CDCl_3$): δ 169.5, 165.4, 148.9, 132.2, 128.9, 127.4, 126.4, 86.3, 54.3, 41.0, 28.6, 28.0, 22.5, 14.1, 10.3; **HRMS** (ESI): calcd for $C_{17}H_{23}N_2O_2Se$ $[M + H]^+$ 367.0925, found 367.0928.

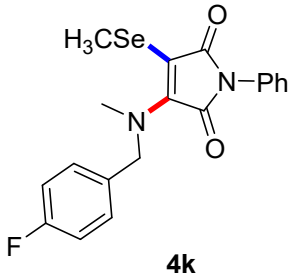
3-(benzyl(methyl)amino)-4-(methylselanyl)-1-phenyl-1H-pyrrole-2,5-dione



4j

Following the general procedure, using (petroleum ether : EtOAc = 9 : 1) as the eluant afforded a yellow liquid (54.0 mg, 70% yield). **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.48-7.45 (m, 2H), 7.42-7.39 (m, 4H), 7.36-7.32 (m, 2H), 7.31-7.28 (m, 2H), 5.23 (s, 2H), 3.47 (s, 3H), 2.21 (s, 3H); **^{13}C NMR** (125MHz, $CDCl_3$): δ 169.2, 165.5, 149.4, 136.7, 134.2, 132.1, 128.9, 128.8, 127.8, 127.4, 126.3, 88.7, 56.8, 40.5, 10.3; **HRMS** (ESI): calcd for $C_{19}H_{19}N_2O_2Se$ $[M + H]^+$ 387.0612, found 387.0606.

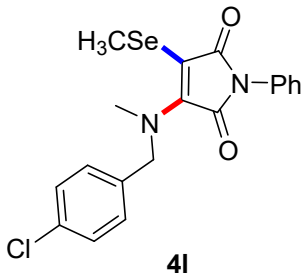
3-((4-fluorobenzyl)(methyl)amino)-4-(methylselanyl)-1-phenyl-1H-pyrrole-2,5-dione



4k

Following the general procedure, using (petroleum ether : EtOAc = 9 : 1) as the eluant afforded a yellow liquid (46.8 mg, 58% yield). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.47 (t, *J* = 7.7 Hz, 2H), 7.42-7.34 (m, 3H), 7.29 (dd, *J* = 8.4, 5.3 Hz, 2H), 7.10 (td, *J* = 8.8, 2.4 Hz, 2H), 5.17 (s, 2H), 3.45 (s, 3H), 2.23 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 169.2, 165.6, 162.4 (d, *J* = 246.3 Hz), 149.3, 132.4 (d, *J* = 3.2 Hz), 132.1, 129.3 (d, *J* = 8.2 Hz), 128.9, 127.6, 126.3, 115.8 (d, *J* = 21.6 Hz), 89.0, 56.1, 40.4, 10.3; **^{19}F NMR** (375 MHz, $CDCl_3$): δ -114.4 (s, 1F); **HRMS** (ESI): calcd for $C_{19}H_{17}N_2O_2NaSeF$ $[M + Na]^+$ 427.0337, found 427.0340.

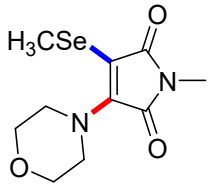
3-((4-chlorobenzyl)(methyl)amino)-4-(methylselanyl)-1-phenyl-1H-pyrrole-2,5-dione



4l

Following the general procedure, using (petroleum ether : EtOAc = 9 : 1) as the eluant afforded a yellow liquid (55.4 mg, 66% yield). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.50-7.46 (m, 2H), 7.41-7.34 (m, 5H), 7.25 (d, *J* = 8.3 Hz, 2H), 5.18 (s, 2H), 3.47 (s, 3H), 2.24 (s, 3H); **^{13}C NMR** (125MHz, $CDCl_3$): δ 169.1, 165.5, 149.1, 135.2, 133.7, 132.0, 129.0, 128.9, 128.8, 127.5, 126.2, 89.4, 56.2, 40.4, 10.2; **HRMS** (ESI): calcd for $C_{19}H_{17}N_2O_2NaClSe$ $[M + Na]^+$ 443.0041, found 443.0042.

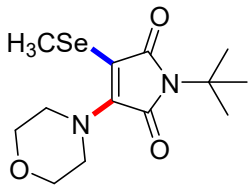
1-methyl-3-(methylselanyl)-4-morpholino-1H-pyrrole-2,5-dione



5a

Following the general procedure, using (petroleum ether : EtOAc = 9 : 1) as the eluant afforded a yellow liquid (43.5 mg, 75% yield). **^{1}H NMR** (500 MHz, $CDCl_3$): δ 4.15 (t, *J* = 4.7 Hz, 4H), 3.81 (t, *J* = 4.7 Hz, 4H), 3.00 (s, 3H), 2.19 (s, 3H); **^{13}C NMR** (125MHz, $CDCl_3$): δ 170.3, 166.9, 148.8, 89.6, 67.0, 48.6, 24.2, 9.7; **HRMS** (ESI): calcd for $C_{10}H_{14}N_2O_3NaSe$ $[M + Na]^+$ 313.0067, found 313.0072.

1-(tert-butyl)-3-(methylselanyl)-4-morpholino-1H-pyrrole-2,5-dione

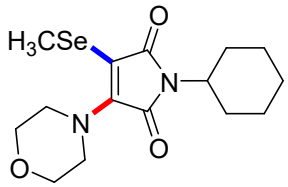


5b

Following the general procedure, using (petroleum ether : EtOAc = 9 : 1) as the eluant afforded a yellow liquid (47.8 mg, 72% yield). **^{1}H NMR** (500 MHz, $CDCl_3$): δ 4.03 (t, *J* = 4.5 Hz, 4H), 3.80 (t, *J* = 4.8 Hz, 4H), 2.19 (s, 3H), 1.58 (s, 9H); **^{13}C NMR** (125MHz, $CDCl_3$): δ 171.2, 167.4, 148.4,

92.0, 67.0, 57.8, 48.7, 29.1, 9.3; **HRMS** (ESI): calcd for $C_{13}H_{20}N_2O_3NaSe$ $[M + Na]^+$ 355.0537, found 355.0540.

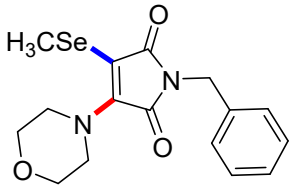
1-cyclohexyl-3-(methylselanyl)-4-morpholino-1H-pyrrole-2,5-dione



5c

Following the general procedure, using (petroleum ether : EtOAc = 9 : 1) as the eluant afforded a yellow solid (53.0 mg, 74% yield), Mp = 63-64 °C. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 4.12 (t, *J* = 4.7 Hz, 4H), 3.94 (tt, *J* = 12.6, 4.0 Hz, 1H), 3.82 (t, *J* = 4.7 Hz, 4H), 2.21 (s, 3H), 2.06 (qd, *J* = 12.5, 3.5 Hz, 2H), 1.85-1.81 (m, 2H), 1.68-1.64 (m, 3H), 1.37-1.19 (m, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 170.2, 166.6, 148.5, 89.9, 67.1, 51.1, 48.6, 29.9, 26.1, 25.2, 9.5; **HRMS** (ESI): calcd for $C_{15}H_{22}N_2O_3NaSe$ $[M + Na]^+$ 381.0693, found 381.0692.

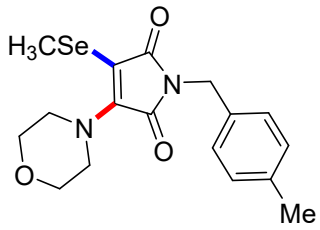
1-benzyl-3-(methylselanyl)-4-morpholino-1H-pyrrole-2,5-dione



5d

Following the general procedure, using (petroleum ether : EtOAc = 9 : 1) as the eluant afforded a yellow solid (55.6 mg, 76% yield), Mp = 97-98 °C. **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.30-7.28 (m, 2H), 7.25-7.22 (m, 2H), 7.20-7.17 (m, 1H), 4.57 (s, 2H), 4.04 (t, *J* = 4.5 Hz, 4H), 3.71 (t, *J* = 4.6 Hz, 4H), 2.11 (s, 3H); **^{13}C NMR** (125MHz, $CDCl_3$): δ 169.9, 166.4, 148.6, 136.6, 128.6, 128.6, 127.7, 89.5, 67.0, 48.5, 41.9, 9.6; **HRMS** (ESI): calcd for $C_{16}H_{18}N_2O_3NaSe$ $[M + Na]^+$ 389.0380, found 389.0382.

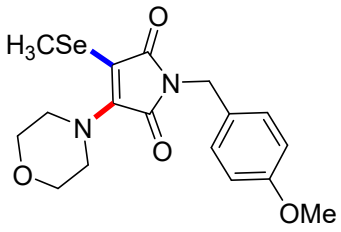
1-(4-methylbenzyl)-3-(methylselanyl)-4-morpholino-1H-pyrrole-2,5-dione



5e

Following the general procedure, using (petroleum ether : EtOAc = 9 : 1) as the eluant afforded a yellow solid (59.3 mg, 78% yield), Mp = 85-86 °C. **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.29 (d, *J* = 8.0 Hz, 2H), 7.14 (d, *J* = 7.8 Hz, 2H), 4.63 (s, 2H), 4.13 (t, *J* = 4.5 Hz, 4H), 3.80 (t, *J* = 4.6 Hz, 4H), 2.34 (s, 3H), 2.20 (s, 3H); **^{13}C NMR** (125MHz, $CDCl_3$): δ 169.9, 166.4, 148.7, 137.4, 133.7, 129.2, 128.7, 89.7, 67.0, 48.5, 41.6, 21.1, 9.6; **HRMS** (ESI): calcd for $C_{17}H_{20}N_2O_3NaSe$ $[M + Na]^+$ 403.0537, found 403.0537.

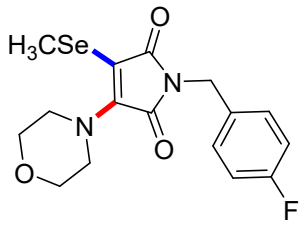
1-(4-methoxybenzyl)-3-(methylselanyl)-4-morpholino-1H-pyrrole-2,5-dione



5f

Following the general procedure, using (petroleum ether : EtOAc = 9 : 1) as the eluant afforded a yellow liquid (63.4 mg, 80% yield). **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.33 (d, *J* = 8.6 Hz, 2H), 6.85 (d, *J* = 8.6 Hz, 2H), 4.60 (s, 2H), 4.14-4.12 (m, 4H), 3.80-3.78 (m, 7H), 2.20 (s, 3H); **^{13}C NMR** (125MHz, $CDCl_3$): δ 169.9, 166.4, 159.2, 148.7, 130.1, 128.9, 113.9, 89.7, 67.0, 55.2, 48.5, 41.3, 9.6; **HRMS** (ESI): calcd for $C_{17}H_{20}N_2O_4NaSe$ $[M + Na]^+$ 419.0486, found 419.0487.

1-(4-fluorobenzyl)-3-(methylselanyl)-4-morpholino-1H-pyrrole-2,5-dione

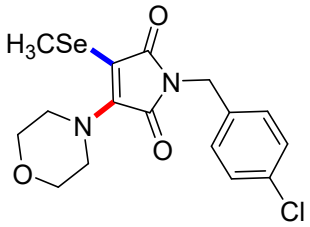


5g

Following the general procedure, using (petroleum ether : EtOAc = 9 : 1) as the eluant afforded a

yellow solid (53.0 mg, 69% yield), Mp = 115-116 ℃. **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.37-7.35 (m, 2H), 7.02-6.98 (m, 2H), 4.62 (s, 2H), 4.14 (t, *J* = 4.7 Hz, 4H), 3.80 (t, *J* = 4.7 Hz, 4H), 2.20 (s, 3H); **^{13}C NMR** (125MHz, $CDCl_3$): δ 169.8, 166.3, 162.3 (d, *J* = 246.2 Hz), 148.6, 132.4 (d, *J* = 3.2 Hz), 130.5 (d, *J* = 8.2 Hz), 115.4 (d, *J* = 21.4 Hz), 89.5, 67.0, 48.5, 41.1, 9.6; **^{19}F NMR** (375 MHz, $CDCl_3$): δ -114.5 (s, 1F); **HRMS** (ESI): calcd for $C_{16}H_{17}N_2O_3NaSeF$ $[M + Na]^+$ 407.0286, found 407.0288.

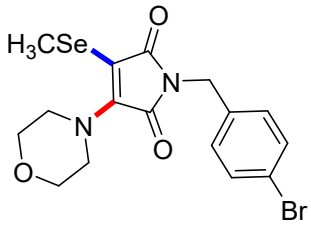
1-(4-chlorobenzyl)-3-(methylselanyl)-4-morpholino-1H-pyrrole-2,5-dione



5h

Following the general procedure, using (petroleum ether : EtOAc = 9 : 1) as the eluant afforded a yellow solid (56.8 mg, 71% yield), Mp = 95-96 ℃. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.35-7.29 (m, 4H), 4.64 (s, 2H), 4.15 (t, *J* = 4.7 Hz, 4H), 3.82 (t, *J* = 4.7 Hz, 4H), 2.22 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 169.9, 166.4, 148.7, 135.1, 133.7, 130.2, 128.8, 89.5, 67.0, 48.6, 41.2, 9.8; **HRMS** (ESI): calcd for $C_{16}H_{17}N_2O_3NaClSe$ $[M + Na]^+$ 422.9991, found 422.9988.

1-(4-bromobenzyl)-3-(methylselanyl)-4-morpholino-1H-pyrrole-2,5-dione

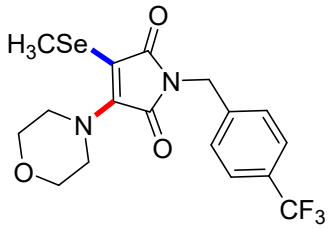


5i

Following the general procedure, using (petroleum ether : EtOAc = 9 : 1) as the eluant afforded a yellow solid (64.8 mg, 73% yield), Mp = 80-81 ℃. **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.43 (d, *J* = 8.3 Hz, 2H), 7.25 (d, *J* = 8.4 Hz, 2H), 4.60 (s, 2H), 4.13 (t, *J* = 4.7 Hz, 4H), 3.79 (t, *J* = 4.7 Hz, 4H), 2.19 (s, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$): δ 169.7, 166.3, 148.6, 135.5, 131.7, 130.4, 121.8, 89.6, 67.0, 48.6, 41.2, 9.6; **HRMS** (ESI): calcd for $C_{16}H_{17}N_2O_3NaSeBr$ $[M + Na]^+$ 466.9485,

found 466.9483.

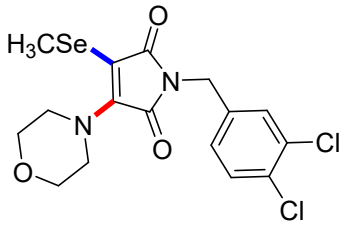
3-(methylselanyl)-4-morpholino-1-(4-(trifluoromethyl)benzyl)-1H-pyrrole-2,5-dione



5j

Following the general procedure, using (petroleum ether : EtOAc = 9 : 1) as the eluant afforded a yellow solid (52.9 mg, 61% yield), Mp = 88-89 °C. **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.58 (d, *J* = 8.0 Hz, 2H), 7.48 (d, *J* = 8.0 Hz, 2H), 4.71 (s, 2H), 4.15 (t, *J* = 4.7 Hz, 4H), 3.81 (t, *J* = 4.7 Hz, 4H), 2.21 (s, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$): δ 169.6, 166.3, 148.6, 140.4, 130.0 (q, *J* = 32.4 Hz), 128.9, 125.6 (q, *J* = 3.7 Hz), 124.0 (q, *J* = 270.5 Hz), 89.6, 67.0, 48.6, 41.4, 9.6; **^{19}F NMR** (375 MHz, $CDCl_3$): δ -62.5 (s, 3F); **HRMS** (ESI): calcd for $C_{17}H_{17}N_2O_3F_3NaSe$ $[M + Na]^+$ 457.0254, found 457.0255.

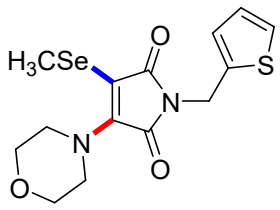
1-(3,4-dichlorobenzyl)-3-(methylselanyl)-4-morpholino-1H-pyrrole-2,5-dione



5k

Following the general procedure, using (petroleum ether : EtOAc = 9 : 1) as the eluant afforded a yellow liquid (55.5 mg, 64% yield). **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.46 (d, *J* = 2.1 Hz, 1H), 7.39 (d, *J* = 8.2 Hz, 1H), 7.22 (dd, *J* = 8.2, 2.1 Hz, 1H), 4.60 (s, 2H), 4.15 (t, *J* = 4.7 Hz, 4H), 3.81 (t, *J* = 4.7 Hz, 4H), 2.21 (s, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$): δ 169.6, 166.2, 148.6, 136.6, 132.6, 131.9, 130.6, 130.6, 128.1, 89.5, 67.0, 48.6, 40.8, 9.7; **HRMS** (ESI): calcd for $C_{16}H_{16}N_2O_3NaCl_2Se$ $[M + H]^+$ 456.9601, found 456.9605.

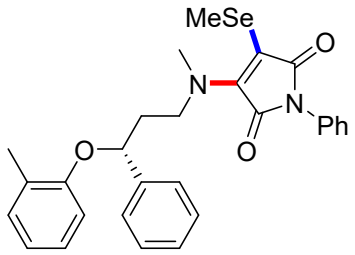
3-(methylselanyl)-4-morpholino-1-(thiophen-2-ylmethyl)-1H-pyrrole-2,5-dione



5l

Following the general procedure, using (petroleum ether : EtOAc = 9 : 1) as the eluant afforded a yellow solid (52.1 mg, 70% yield), Mp = 96-97 ℃. **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.22 (dd, *J* = 5.1, 1.3 Hz, 1H), 7.08 (dd, *J* = 3.5, 1.2 Hz, 1H), 6.94 (dd, *J* = 5.1, 3.5 Hz, 1H), 4.84 (s, 2H), 4.14 (t, *J* = 4.7 Hz, 4H), 3.80 (t, *J* = 4.7 Hz, 4H), 2.21 (s, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$): δ 169.3, 166.0, 148.6, 138.4, 127.5, 126.8, 125.7, 89.7, 67.0, 48.6, 35.9, 9.6; **HRMS** (ESI): calcd for $C_{14}H_{16}N_2O_3NaSSe$ $[M + Na]^+$ 394.9945, found 394.9948.

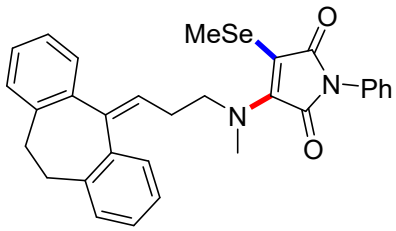
(R)-3-(methyl(3-phenyl-3-(o-tolyloxy)propyl)amino)-4-(methylselanyl)-1-phenyl-1H-pyrrole-2,5-dione



6a

Following the general procedure, using (petroleum ether : EtOAc = 9 : 1) as the eluant afforded a yellow liquid (63.4 mg, 61% yield). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.46 (t, *J* = 7.7 Hz, 2H), 7.39-7.35 (m, 5H), 7.32-7.16 (m, 3H), 7.17 (d, *J* = 7.3 Hz, 1H), 7.00 (td, *J* = 7.8, 1.8 Hz, 1H), 6.83 (t, *J* = 7.4 Hz, 1H), 6.63 (d, *J* = 8.2 Hz, 1H), 5.32 (dd, *J* = 8.9, 3.7 Hz, 1H), 4.06 (qdd, *J* = 14.2, 9.3, 5.8 Hz, 2H), 3.47 (s, 3H), 2.45 (ddt, *J* = 12.9, 8.8, 4.5 Hz, 1H), 2.39 (s, 3H), 2.31 (tdd, *J* = 10.1, 6.0, 3.1 Hz, 1H), 1.47 (s, 1H), 1.35-1.30 (m, 1H), 0.93-0.90 (m, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 165.6, 164.3, 155.5, 141.5, 141.1, 131.5, 130.9, 129.0, 128.9, 127.9, 127.8, 126.9, 126.7, 126.4, 125.7, 120.6, 112.5, 93.2, 51.0, 40.1, 37.6, 27.0, 22.7, 16.6; **HRMS** (ESI): calcd for $C_{28}H_{28}N_2O_3NaSe$ $[M + Na]^+$ 543.1163, found 543.1170.

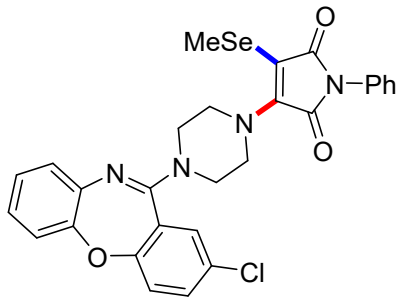
3-((3-(10,11-dihydro-5H-dibenzo[a,d][7]annulen-5-ylidene)propyl)(methyl)amino)-4-(methylselanyl)-1-phenyl-1H-pyrrole-2,5-dione



6b

Following the general procedure, using (petroleum ether : EtOAc = 9 : 1) as the eluant afforded a yellow liquid (69.7 mg, 66% yield). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.47 (dd, *J* = 8.8, 6.8 Hz, 2H), 7.38-7.30 (m, 4H), 7.26-7.16 (m, 6H), 7.09 (dd, *J* = 6.9, 2.1 Hz, 1H), 5.93 (t, *J* = 7.5 Hz, 1H), 4.03 (q, *J* = 7.8 Hz, 2H), 3.45-3.33 (m, 5H), 3.00 (t, *J* = 14.6 Hz, 1H), 2.82 (d, *J* = 13.9 Hz, 1H), 2.65-2.56 (m, 2H), 2.17 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 169.3, 165.4, 148.6, 145.7, 140.8, 139.7, 139.5, 137.2, 132.1, 130.2, 128.9, 128.5, 128.3, 128.2, 127.8, 127.5, 127.4, 126.6, 126.4, 126.2, 125.9, 86.9, 53.7, 41.2, 33.8, 32.1, 28.7, 10.2; **HRMS** (ESI): calcd for $C_{30}H_{28}N_2O_2NaSe$ $[M + Na]^+$ 551.1214, found 551.1222.

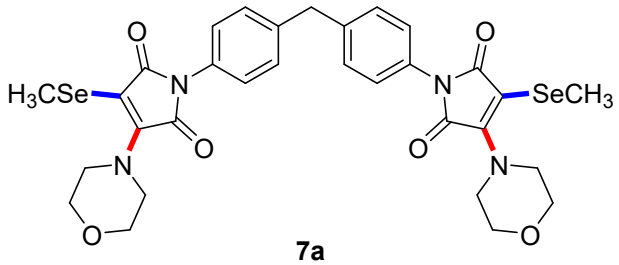
3-(4-(2-chlorodibenzo[b,f][1,4]oxazepin-11-yl)piperazin-1-yl)-4-(methylselanyl)-1-phenyl-1H-pyrrole-2,5-dione



6c

Following the general procedure, using (petroleum ether : EtOAc = 9 : 1) as the eluant afforded a yellow liquid (65.9 mg, 57% yield). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.50-7.46 (m, 3H), 7.40-7.35 (m, 4H), 7.30-7.26 (m, 2H), 7.19-7.14 (m, 2H), 7.11-7.07 (m, 1H), 4.32 (brs, 4H), 3.79 (brs, 4H), 2.32 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 170.0, 165.6, 159.5, 158.6, 151.9, 148.6, 133.0, 131.9, 130.6, 129.0, 128.9, 127.7, 127.2, 126.3, 126.0, 125.2, 124.7, 123.0, 120.3, 91.3, 48.2, 47.9, 9.6; **HRMS** (ESI): calcd for $C_{28}H_{24}N_4O_3ClSe$ $[M + Na]^+$ 579.0702, found 579.0703.

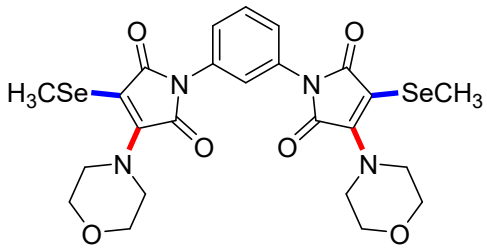
1,1'-(methylenebis(4,1-phenylene))bis(3-(methylselanyl)-4-morpholino-1H-pyrrole-2,5-dione)



7a

Following the general procedure, using (petroleum ether : EtOAc = 9 : 1) as the eluant afforded a yellow liquid (97.4 mg, 68% yield). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.24 (brs, 8H), 4.16 (t, *J* = 4.7 Hz, 8H), 4.01 (s, 2H), 3.83 (t, *J* = 4.7 Hz, 8H), 2.25 (s, 6H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 169.0, 165.6, 148.4, 140.1, 130.0, 129.6, 126.3, 90.6, 67.1, 48.9, 41.1, 9.6; **HRMS** (ESI): calcd for $C_{31}H_{32}N_4O_6NaSe_2$ $[M + Na]^+$ 739.0564, found 739.0565.

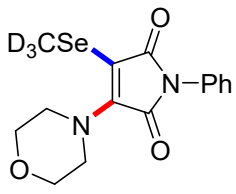
1,1'-(1,3-phenylene)bis(3-(methylselanyl)-4-morpholino-1H-pyrrole-2,5-dione)



7b

Following the general procedure, using (petroleum ether : EtOAc = 9 : 1) as the eluant afforded a yellow solid (81.4 mg, 65% yield), Mp = 84-85 °C. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.55-7.49 (m, 2H), 7.39 (dd, *J* = 8.1, 2.0 Hz, 2H), 4.20 (t, *J* = 4.7 Hz, 8H), 3.87 (t, *J* = 4.7 Hz, 8H), 2.29 (s, 6H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ 168.6, 165.2, 148.3, 132.3, 129.1, 124.6, 123.1, 90.8, 67.1, 48.9, 9.6; **HRMS** (ESI): calcd for $C_{24}H_{26}N_4O_6NaSe_2$ $[M + Na]^+$ 649.0080, found 649.0087.

3-((methyl-d3)selanyl)-4-morpholino-1-phenyl-1H-pyrrole-2,5-dione

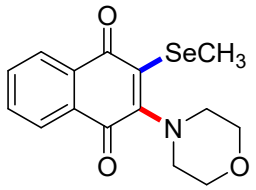


8a

Following the general procedure, using (petroleum ether : EtOAc = 9 : 1) as the eluant afforded a

yellow solid (54.7 mg, 77% yield), Mp = 107-108 ℃. **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.49-7.45 (m, 2H), 7.38-7.34 (m, 3H), 4.20 (t, *J* = 4.72 Hz, 4H), 3.87 (t, *J* = 4.80 Hz, 4H); **^{13}C NMR** (100MHz, $CDCl_3$): δ 169.0, 165.6, 148.4, 131.9, 128.9, 127.7, 126.3, 90.6, 67.1, 48.9; **HRMS** (ESI): calcd for $C_{15}H_{13}D_3N_2O_3NaSe$ $[M + Na]^+$ 378.0412, found 378.0415.

2-(methylselanyl)-3-morpholinonaphthalene-1,4-dione



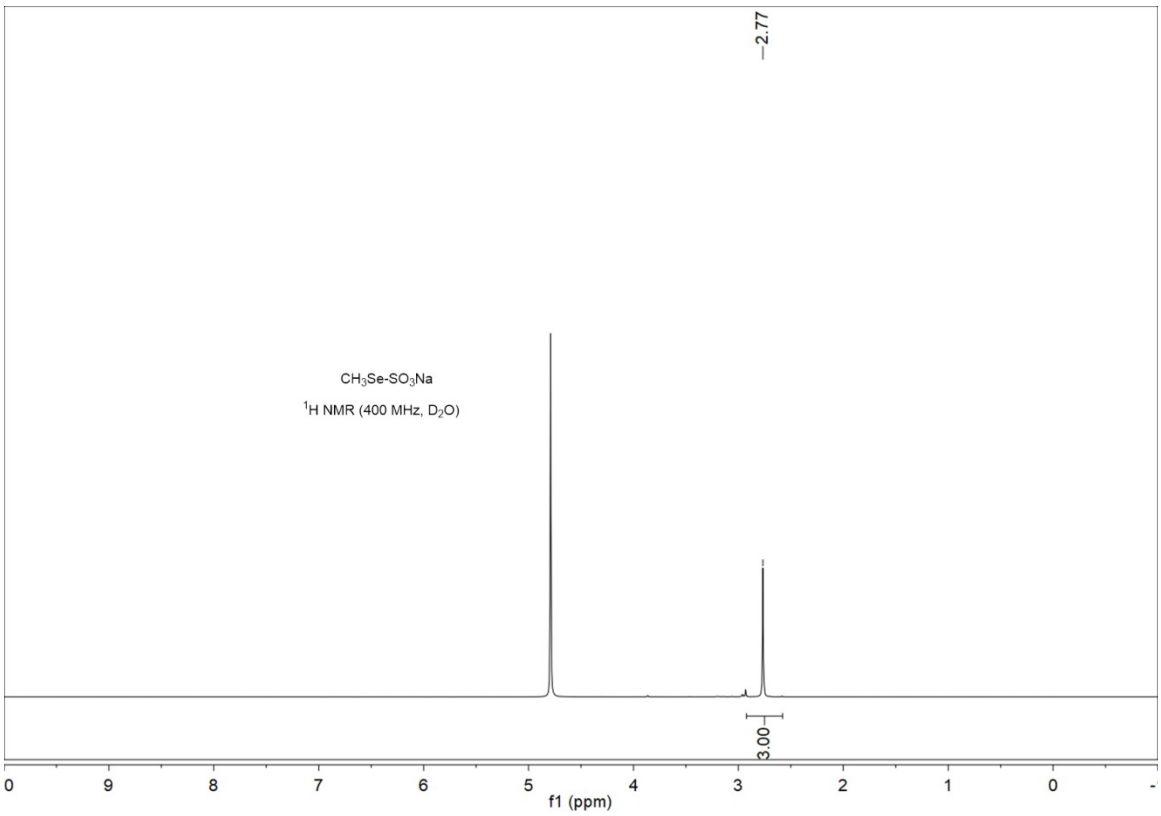
8b

Following the general procedure, using (petroleum ether : EtOAc = 9 : 1) as the eluant afforded a purple liquid (45.8 mg, 68% yield). **^{1}H NMR** (500 MHz, $CDCl_3$): δ 8.08-8.06 (m, 1H), 8.02-8.00 (m, 1H), 7.72-7.65 (m, 2H), 3.89 (t, *J* = 4.5 Hz, 4H), 3.59 (t, *J* = 4.5 Hz, 4H), 2.47 (s, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$): δ 182.1, 181.7, 152.6, 133.7, 133.0, 132.1, 128.6, 126.6, 126.3, 67.6, 52.3, 18.5； **HRMS** (ESI): calcd for $C_{15}H_{15}NO_3NaSe$ $[M + Na]^+$ 360.0115, found 360.0119.

References:

(1) (a) Ding, G.; Li, C.; Shen, Y.; Lu, B.; Zhang, Z.; Xie, X. *Adv. Synth. Catal.* **2016**, *358*, 1241-1250. (b) Matuszak, N.; Muccioli, G. G.; Labar, G.; Lambert, D. M. *J. Med Chem*. **2009**, *52*, 7410-7420.

^{1}H, ^{13}C and ^{19}F NMR spectra of product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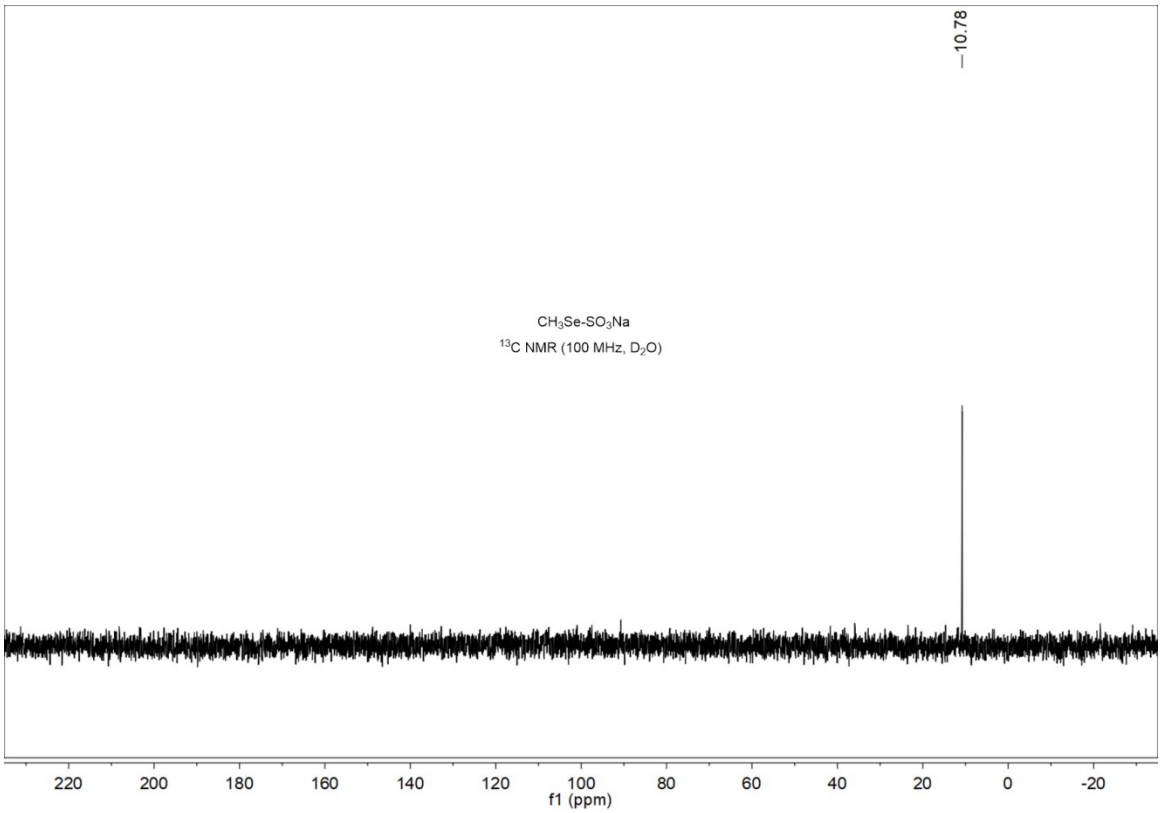
9
8
7
6
5
4
3
2
1
0
f1 (ppm)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160
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120
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80
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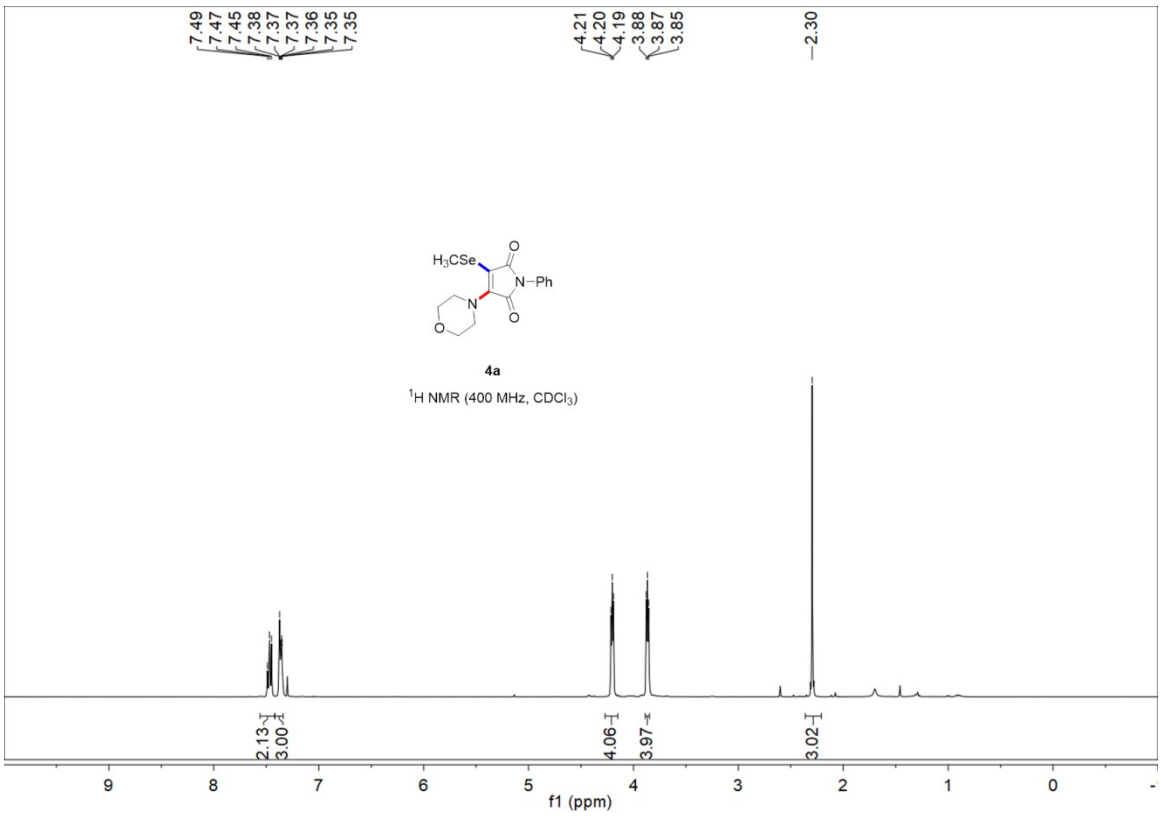
40
20
0
-20
f1 (ppm)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7.37
7.37
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7.35
7.35
4.21
4.20
4.19
3.88
3.87
3.85
2.30
H3CSe
N–Ph
O
O
N
O
4a
1H NMR (400 MHz, CDCl3)
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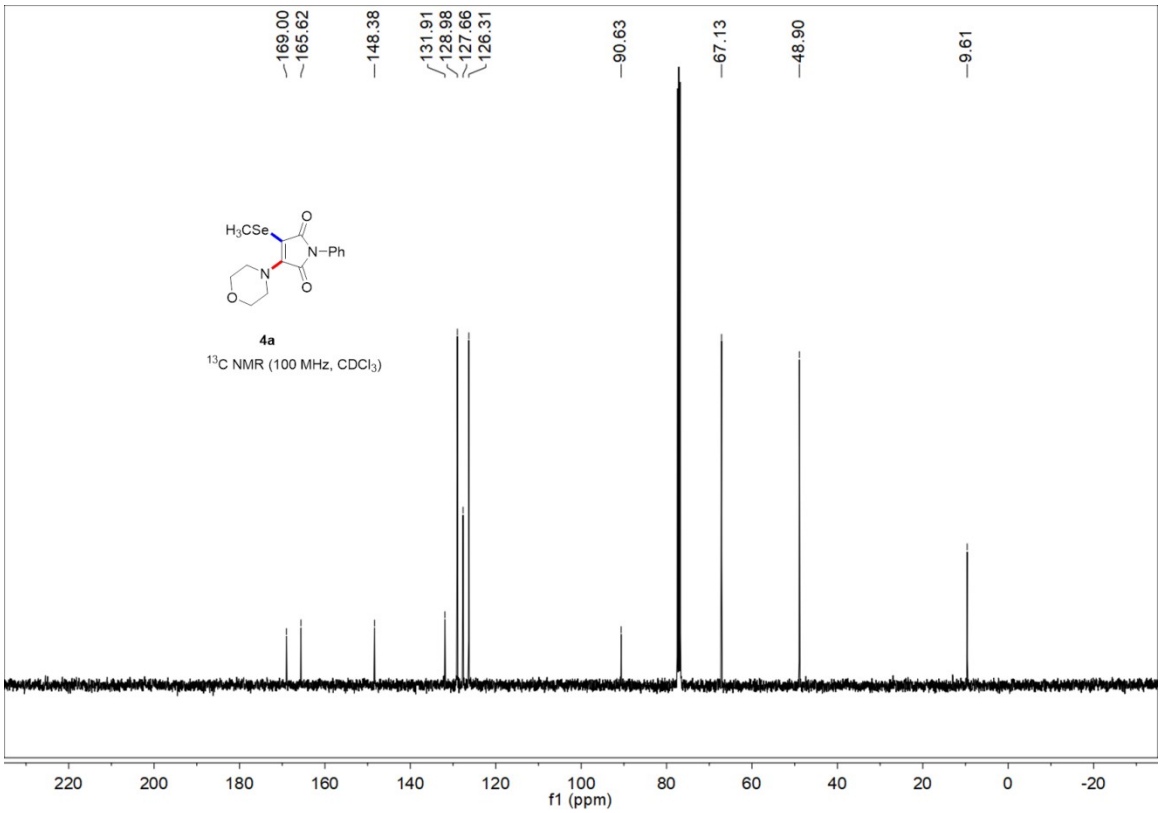
3.97
3.02
9
8
7
6
5
4
3
2
1
0
f1 (ppm)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48.90
9.61
H3CSe
N–Ph
O
O
N
O
4a
13C NMR (100 MHz, CDCl3)
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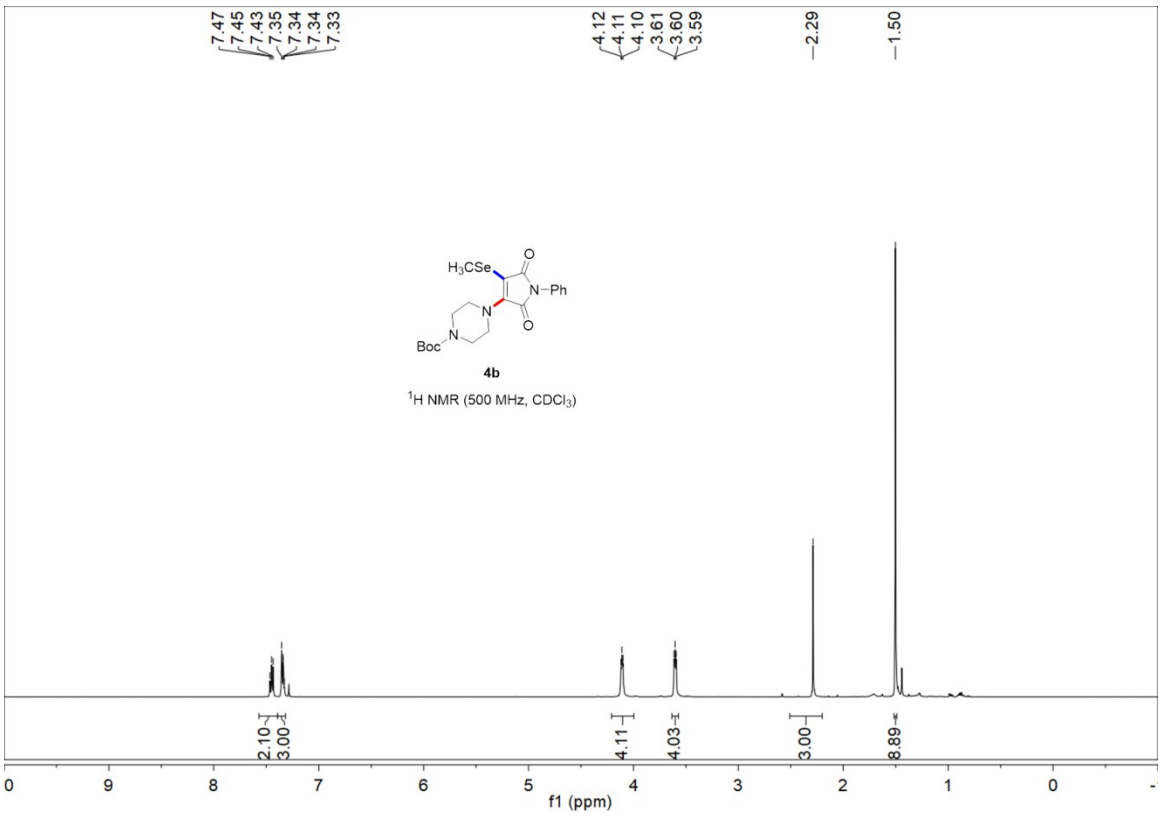
200
180
160
140
120
100
80
60
40
20
0
-20
f1 (ppm)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3.60
3.59
2.29
1.50
H3CSe
O
N–Ph
N
O
N
Boc
4b
1H NMR (500 MHz, CDCl3)
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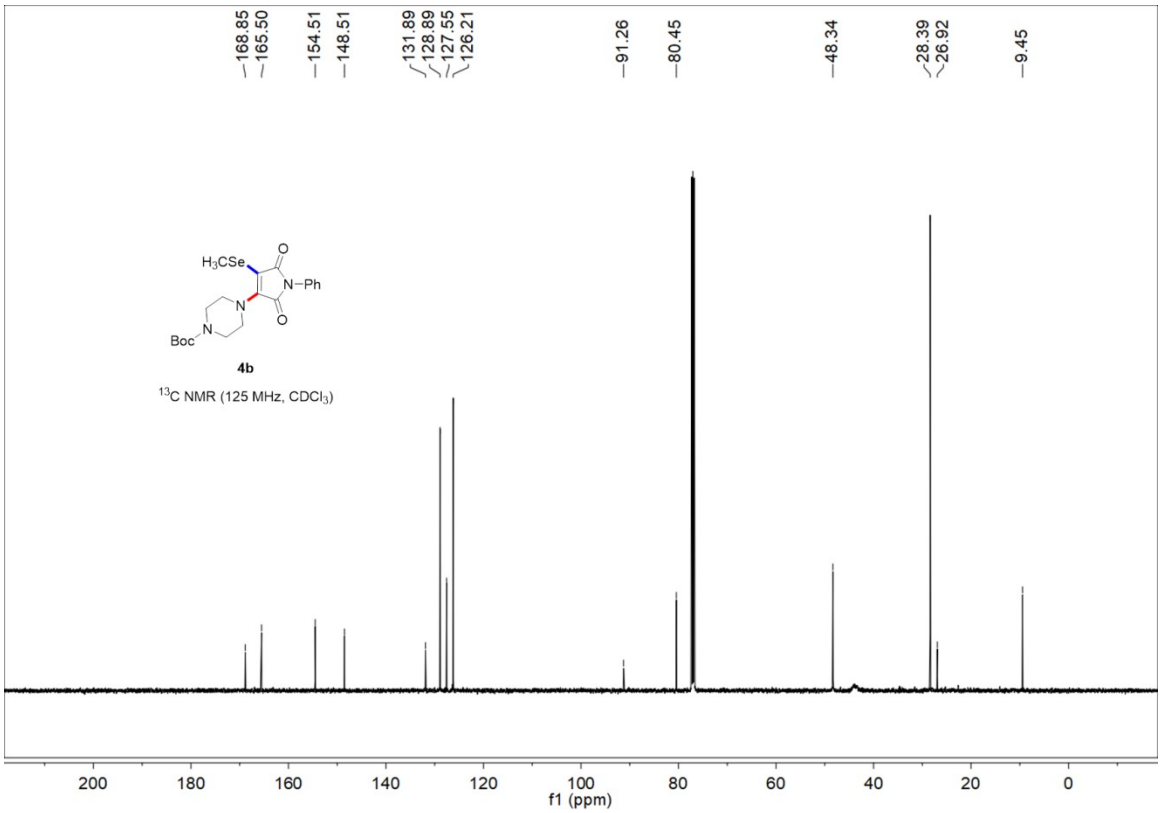
3.00
4.11
4.03
3.00
8.89
f1 (ppm)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126.21
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48.34
28.39
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9.45
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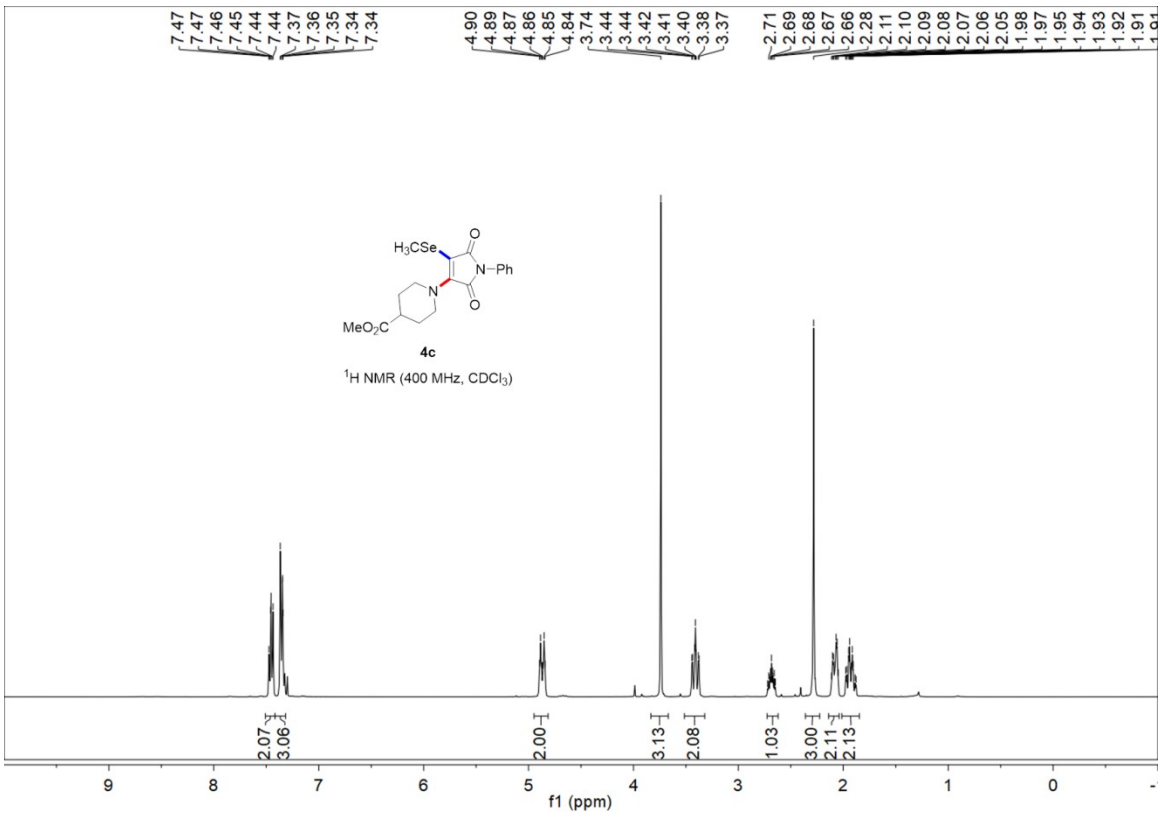
O
N–Ph
N
O
N
Boc
4b
13C NMR (125 MHz, CDCl3)
f1 (ppm)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2.06
2.05
1.98
1.97
1.95
1.94
1.93
1.92
1.91
H3CSe
O
N–Ph
N
O
MeO2C
4c
1H NMR (400 MHz, CDCl3)
2.07
3.06
2.00
3.13
2.08
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2.11
2.13
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5
4
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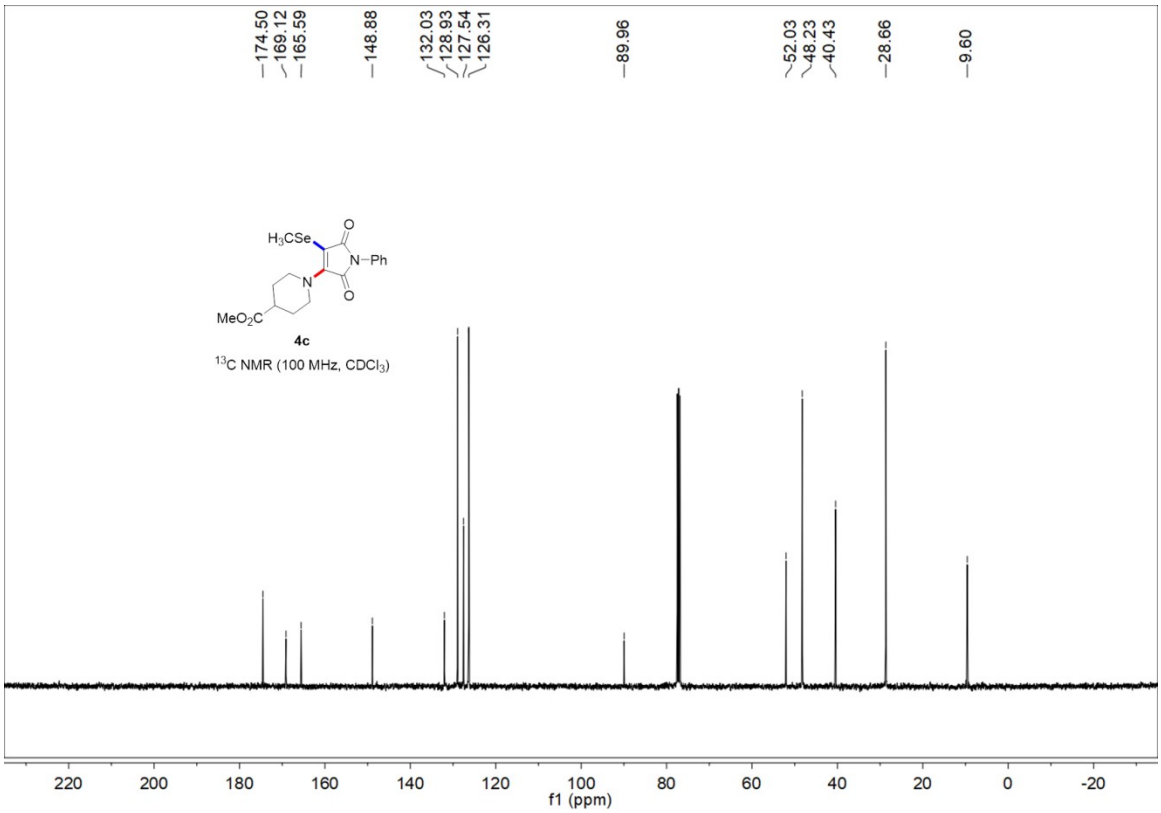
f1 (ppm)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52.03
48.23
40.43
28.66
9.60
H3CSe
O
N–Ph
N
O
MeO2C
4c
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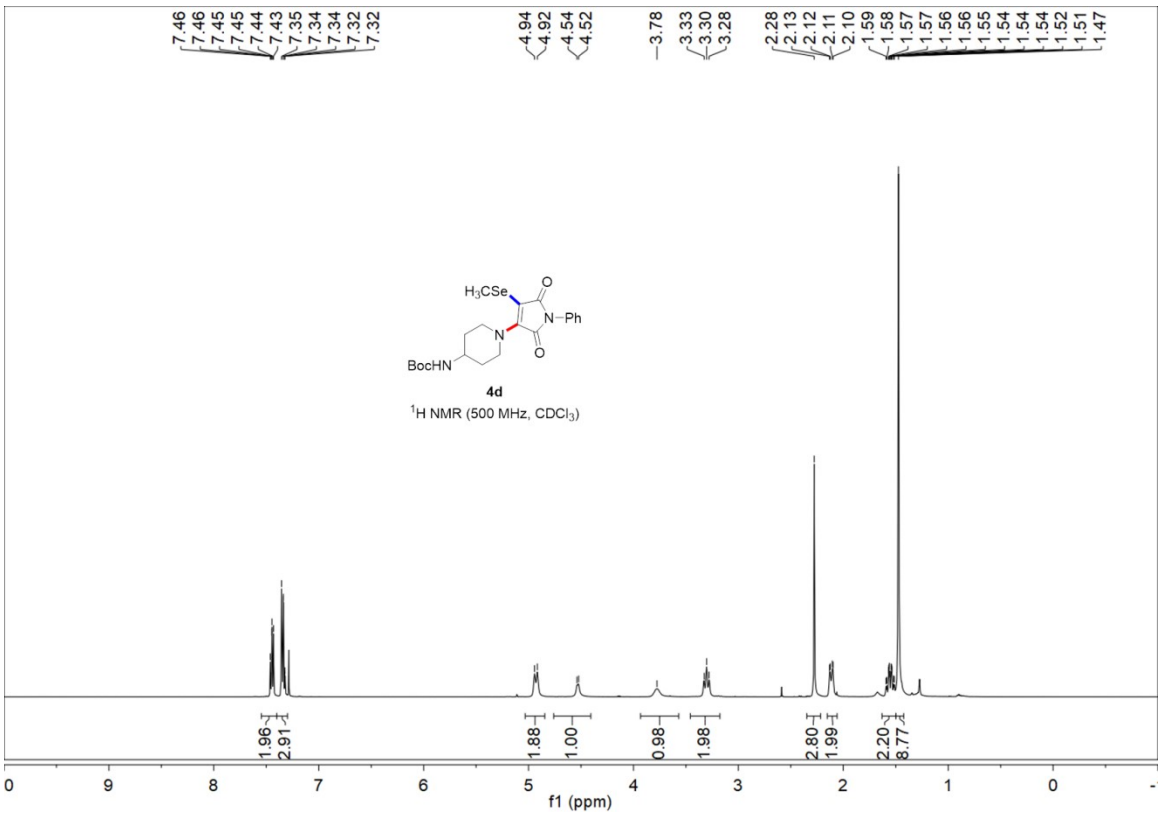
f1 (ppm)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O
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N
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4d
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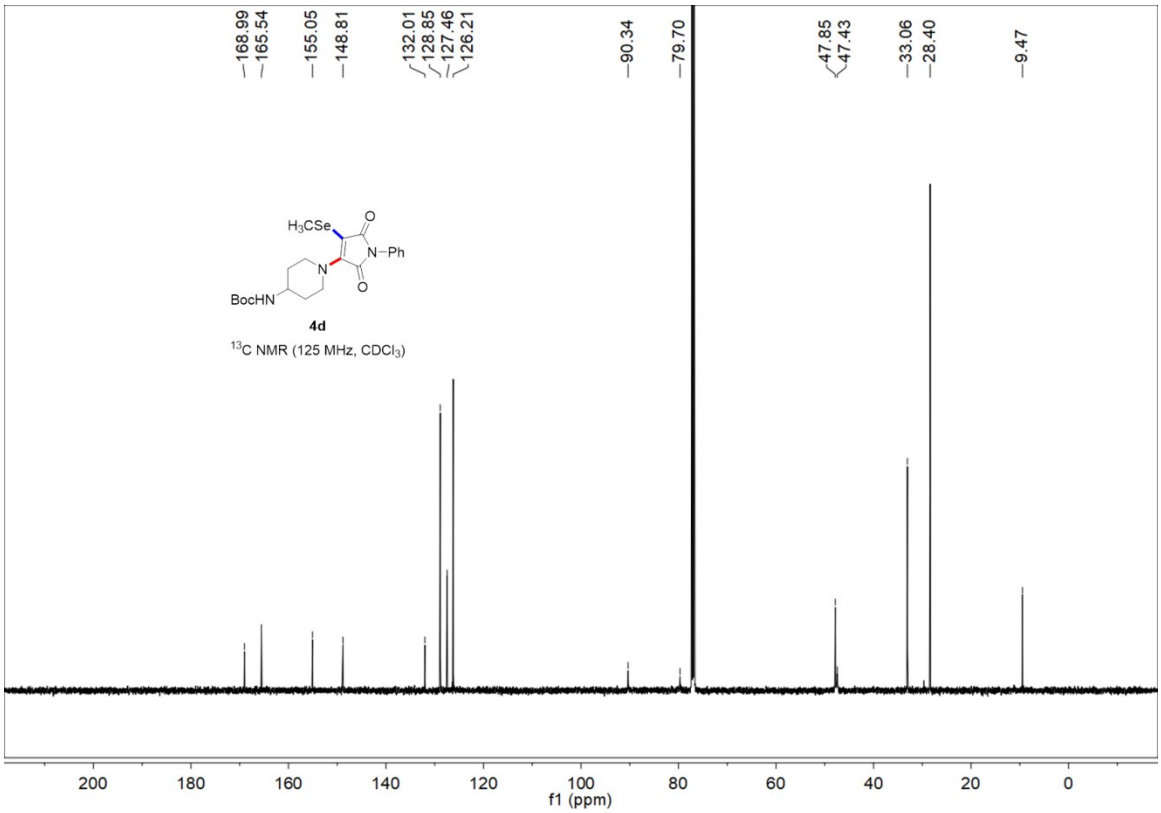
8.77
f1 (ppm)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N
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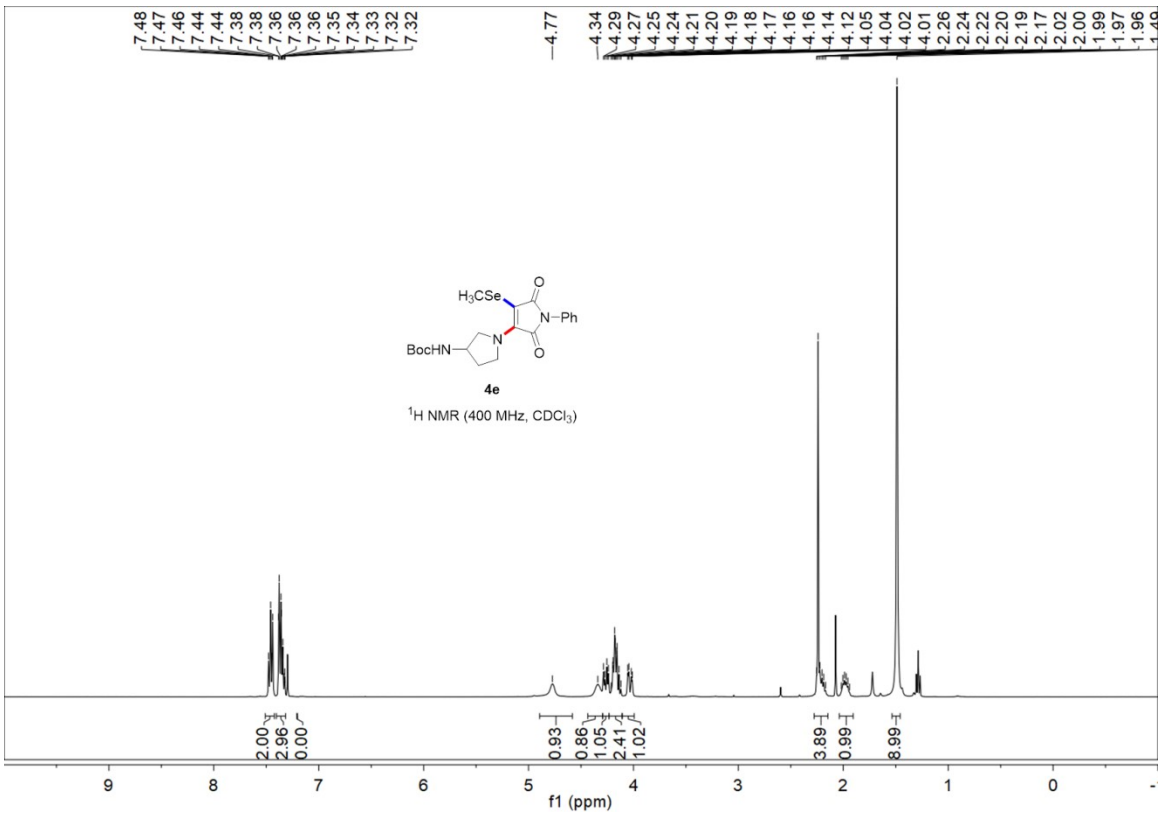
4d
13C NMR (125 MHz, CDCl3)
f1 (ppm)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7.32
7.32
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4.34
4.29
4.27
4.25
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4.20
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4.18
4.17
4.16
4.16
4.14
4.12
4.05
4.04
4.02
4.01
2.26
2.24
2.22
2.20
2.19
2.17
2.02
2.00
1.99
1.97
1.96
H3CSe
O
N–Ph
BocHN
N
O
4e
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0.86
1.05
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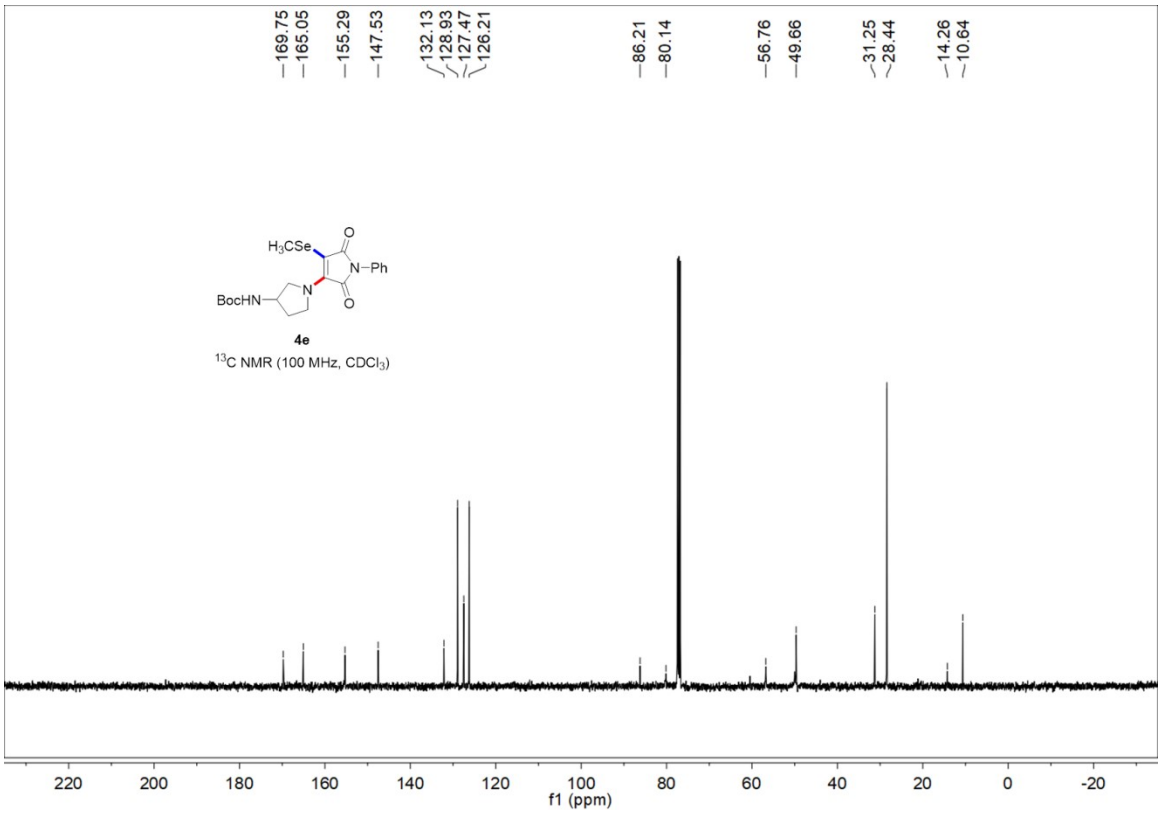
f1 (ppm)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14.26
10.64
H3CSe
O
N–Ph
BocHN
N
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4e
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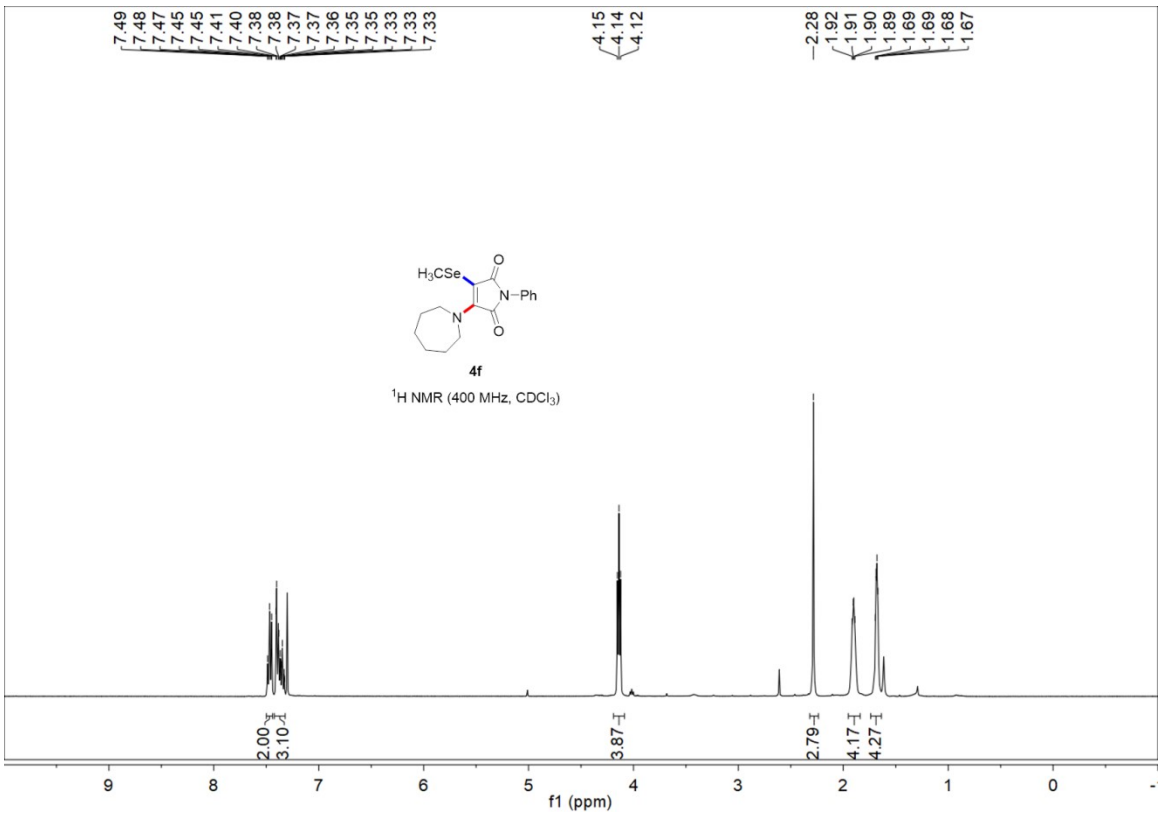
f1 (ppm)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O
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4.17
4.27
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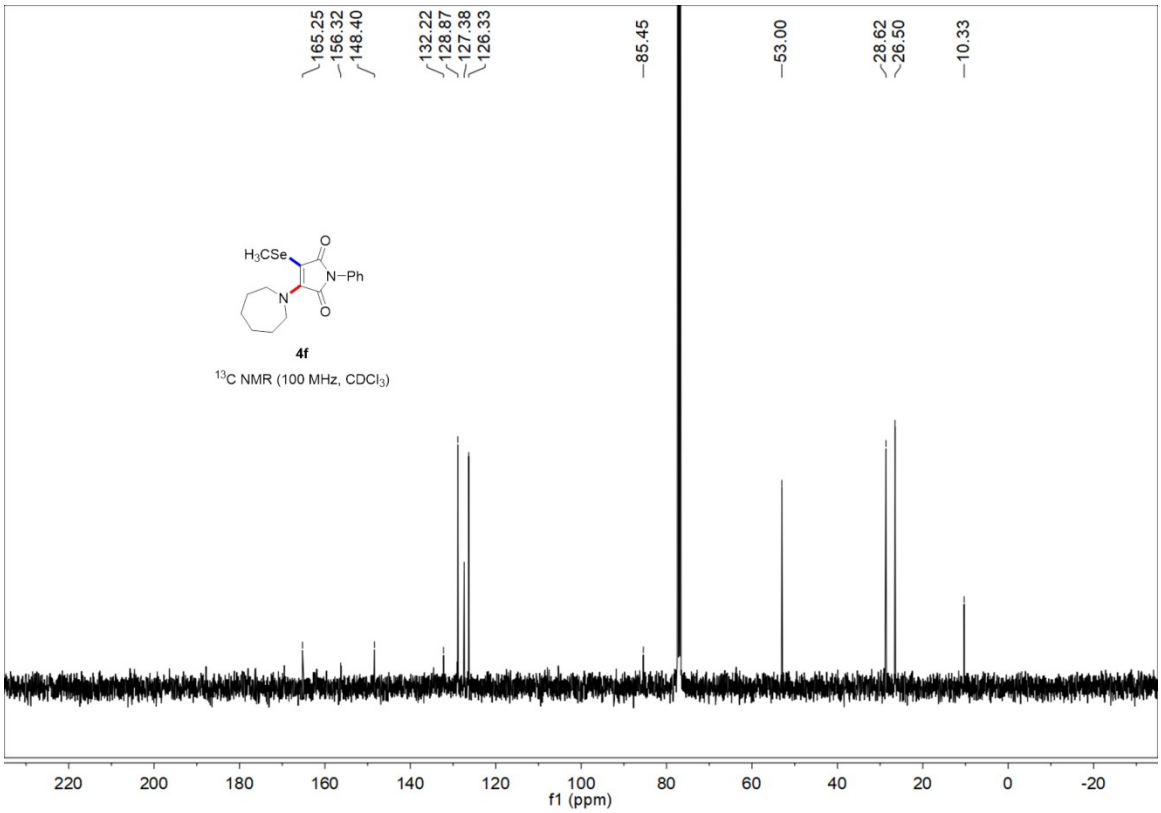
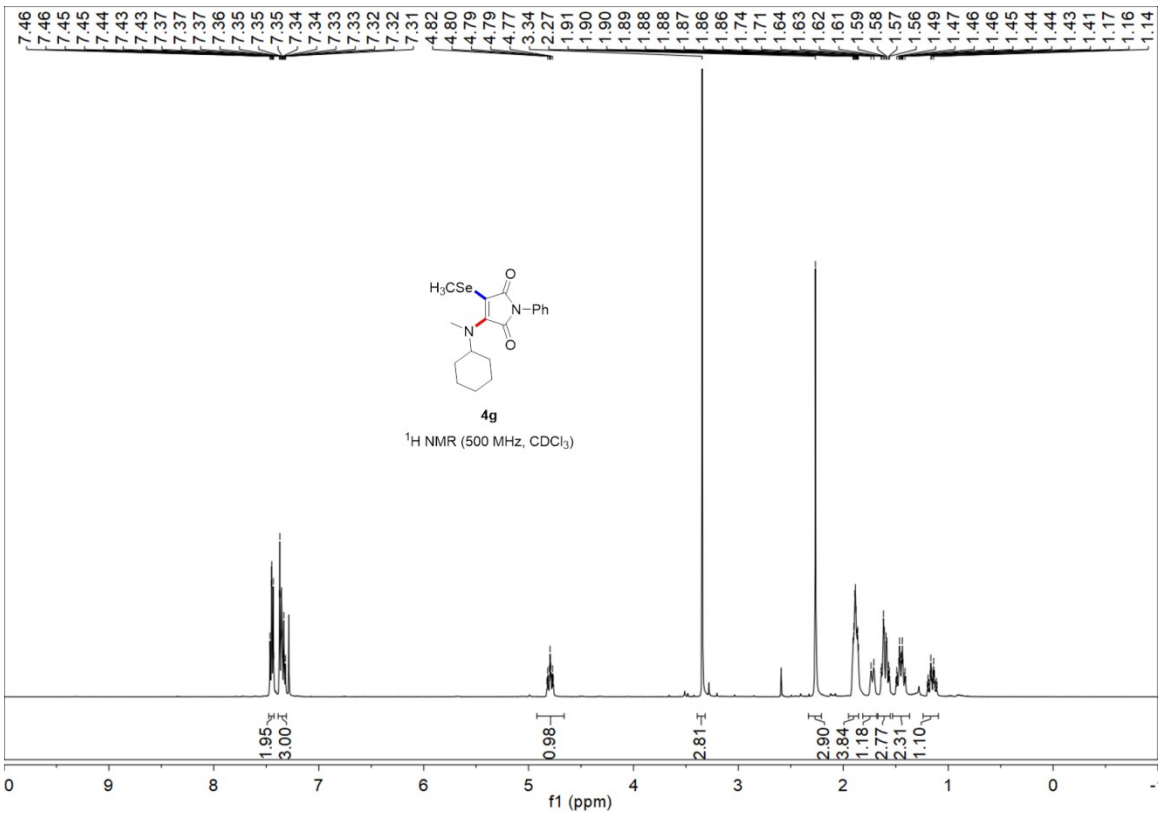
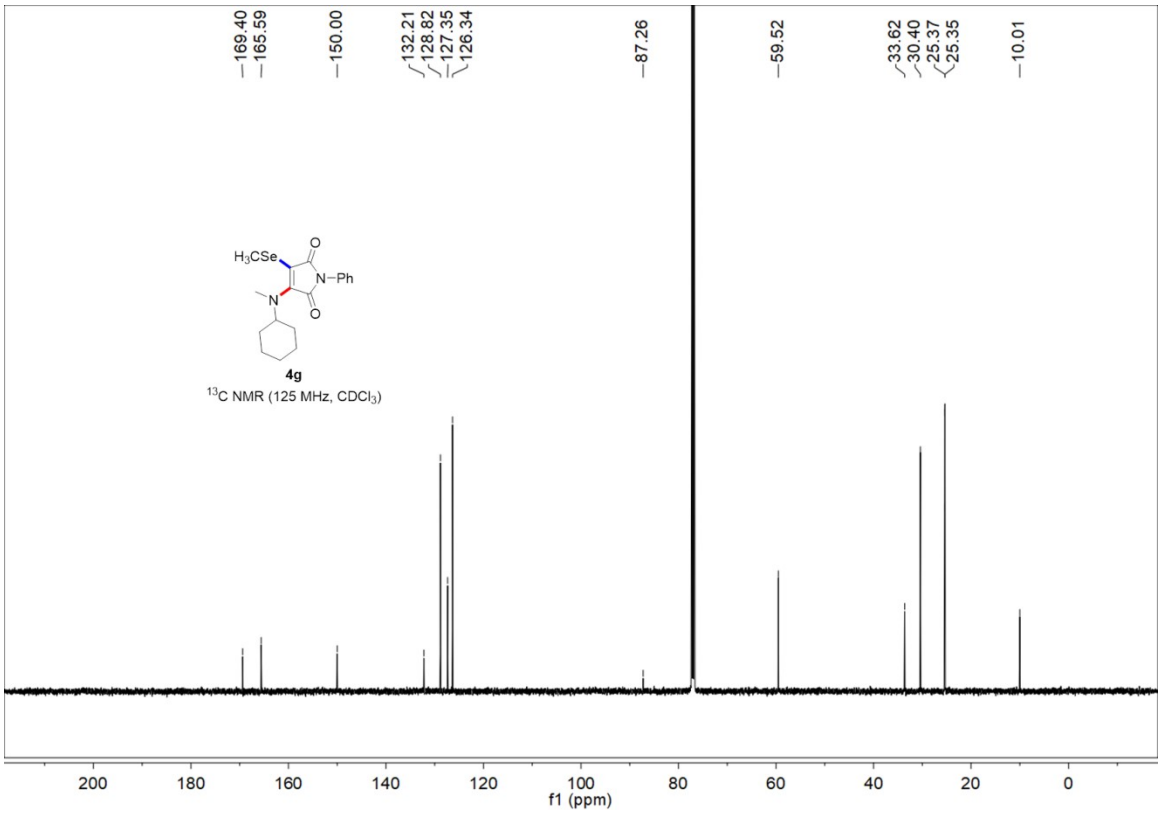
7
6
5
4
3
2
1
0
f1 (ppm)


165.25
156.32
148.40
132.22
128.87
127.38
126.33
85.45
53.00
28.62
26.50
10.33
H3CSe
O
N–Ph
N
O
4f
13C NMR (100 MHz, CDCl3)
220
200
180
160
140
120
100
80
60
40
20
0
-20
f1 (ppm)


7.46 7.46 7.45 7.45 7.44 7.43 7.43 7.37 7.37 7.37 7.36 7.35 7.35 7.35 7.34 7.34 7.33 7.33 7.32 7.32 7.31 4.82 4.80 4.79 4.79 4.77 3.34 2.27 1.91 1.90 1.90 1.89 1.88 1.88 1.87 1.86 1.86 1.74 1.71 1.64 1.63 1.62 1.61 1.59 1.58 1.57 1.56 1.49 1.47 1.46 1.46 1.45 1.44 1.44 1.43 1.41 1.17 1.16 1.14
H3CSe
N–Ph
O
O
N
4g
1H NMR (500 MHz, CDCl3)
1.95
3.00
0.98
2.81
2.90
3.84
1.18
2.77
2.31
1.10
f1 (ppm)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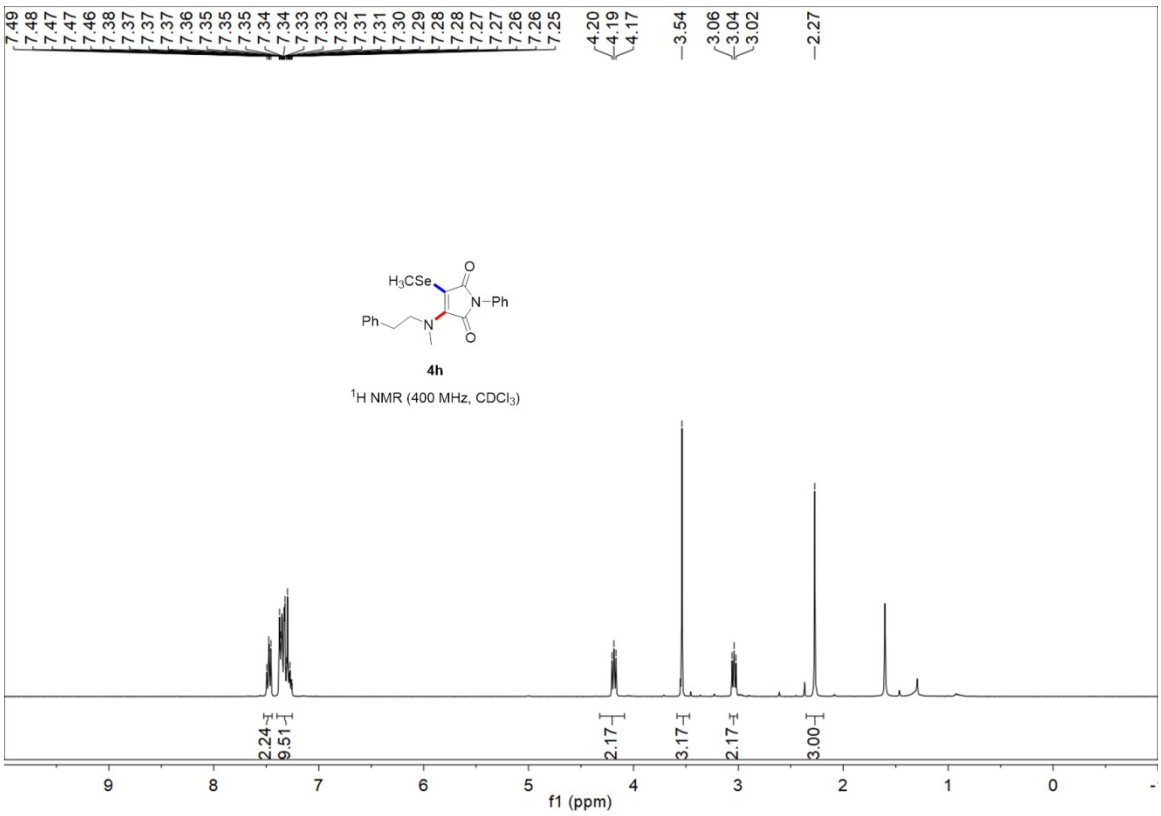
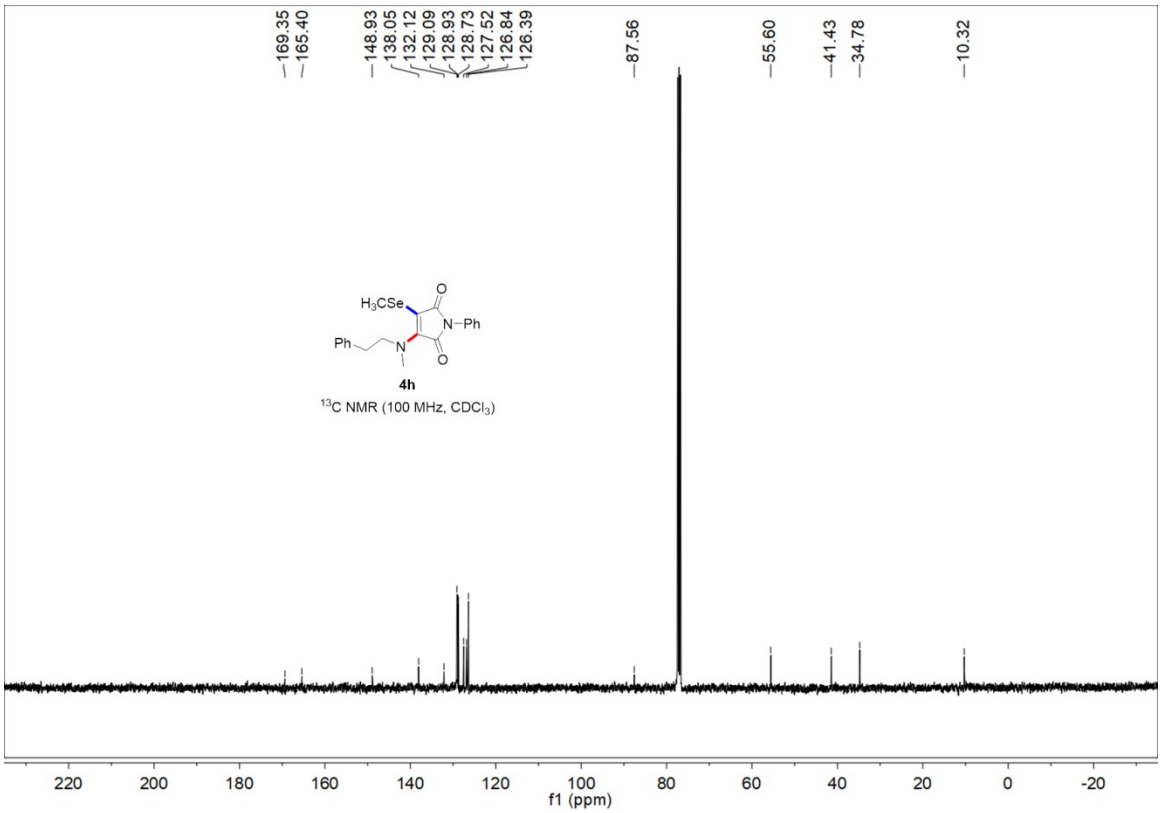
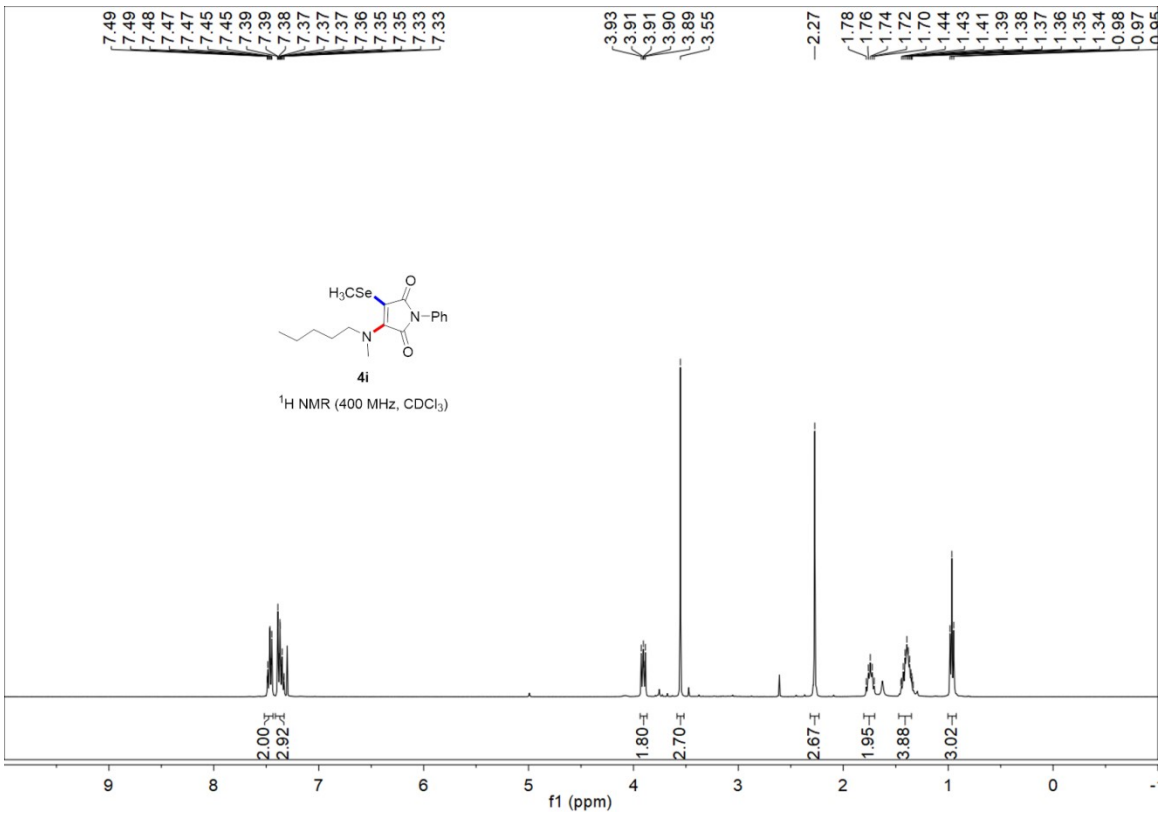
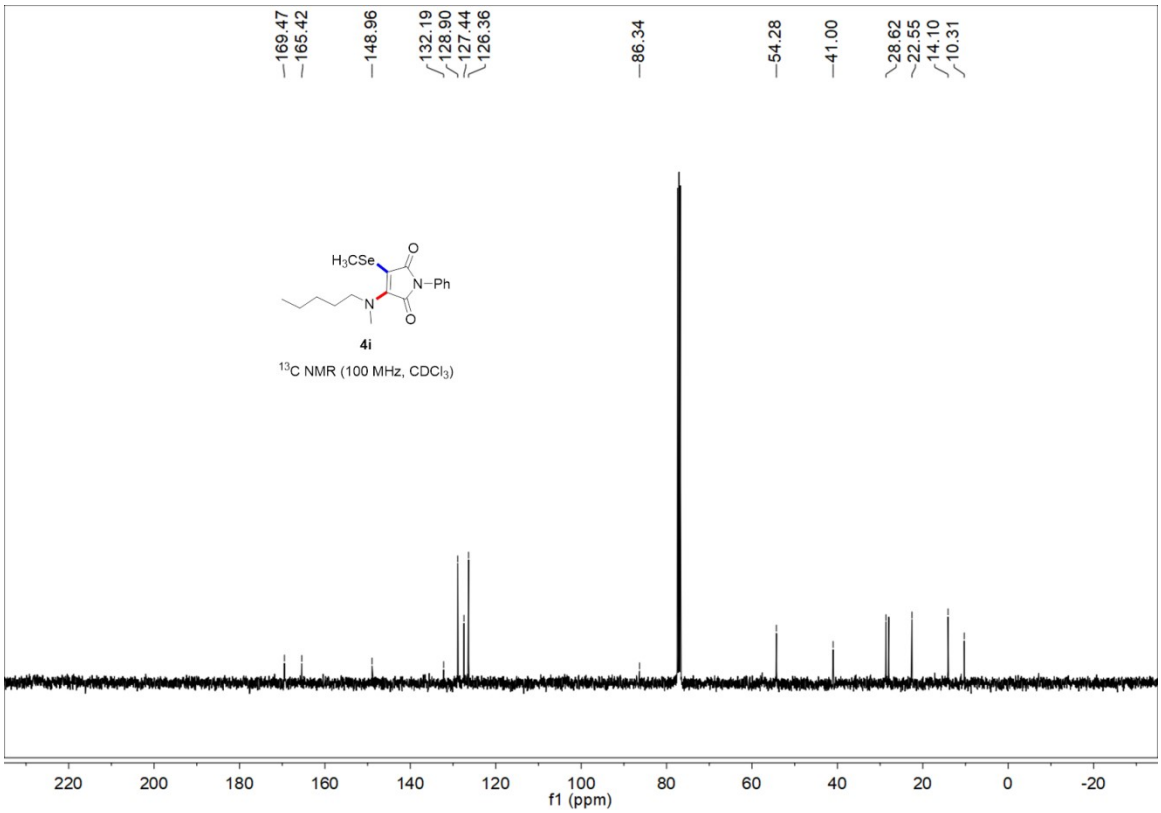
165.59
150.00
132.21
128.82
127.35
126.34
87.26
59.52
33.62
30.40
25.37
25.35
10.01
H3CSe
N–Ph
O
O
N
4g
13C NMR (125 MHz, CDCl3)
f1 (ppm)


7.49 7.48 7.47 7.47 7.46 7.38 7.37 7.37 7.37 7.36 7.35 7.35 7.35 7.34 7.34 7.33 7.33 7.32 7.31 7.31 7.30 7.29 7.28 7.28 7.27 7.27 7.26 7.26 7.25
4.20 4.19 4.17
3.54
3.06 3.04 3.02
2.27
H3CSe
O
N–Ph
Ph
N
O
4h
1H NMR (400 MHz, CDCl3)
2.24 9.51 2.17 3.17 2.17 3.00
9 8 7 6 5 4 3 2 1 0
f1 (ppm)


169.35 165.40
148.93 138.05 132.12 129.09 128.93 128.73 127.52 126.84 126.39
87.56
55.60
41.43
34.78
10.32
H3CSe
O
N–Ph
Ph
N
O
4h
13C NMR (100 MHz, CDCl3)
220 200 180 160 140 120 100 80 60 40 20 0 -20
f1 (ppm)


7.49
7.49
7.48
7.47
7.47
7.45
7.45
7.39
7.39
7.38
7.37
7.37
7.37
7.36
7.35
7.35
7.33
7.33
3.93
3.91
3.91
3.90
3.89
3.55
2.27
1.78
1.76
1.74
1.72
1.70
1.44
1.43
1.41
1.39
1.38
1.37
1.36
1.35
1.34
0.98
0.97
H3CSe
N–Ph
4i
1H NMR (400 MHz, CDCl3)
2.00
2.92
1.80
2.70
2.67
1.95
3.88
3.02
f1 (ppm)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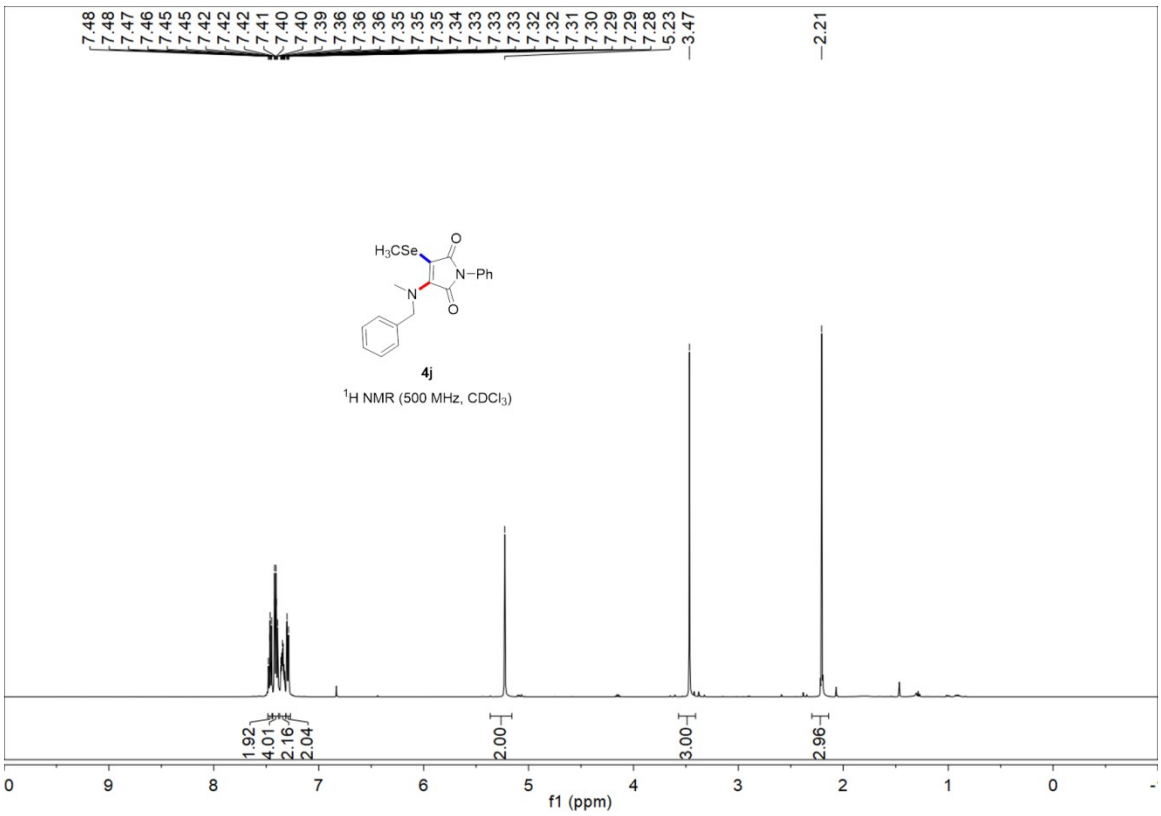
165.42
148.96
132.19
128.90
127.44
126.36
86.34
54.28
41.00
28.62
22.55
14.10
10.31
H3CSe
N–Ph
4i
13C NMR (100 MHz, CDCl3)
f1 (ppm)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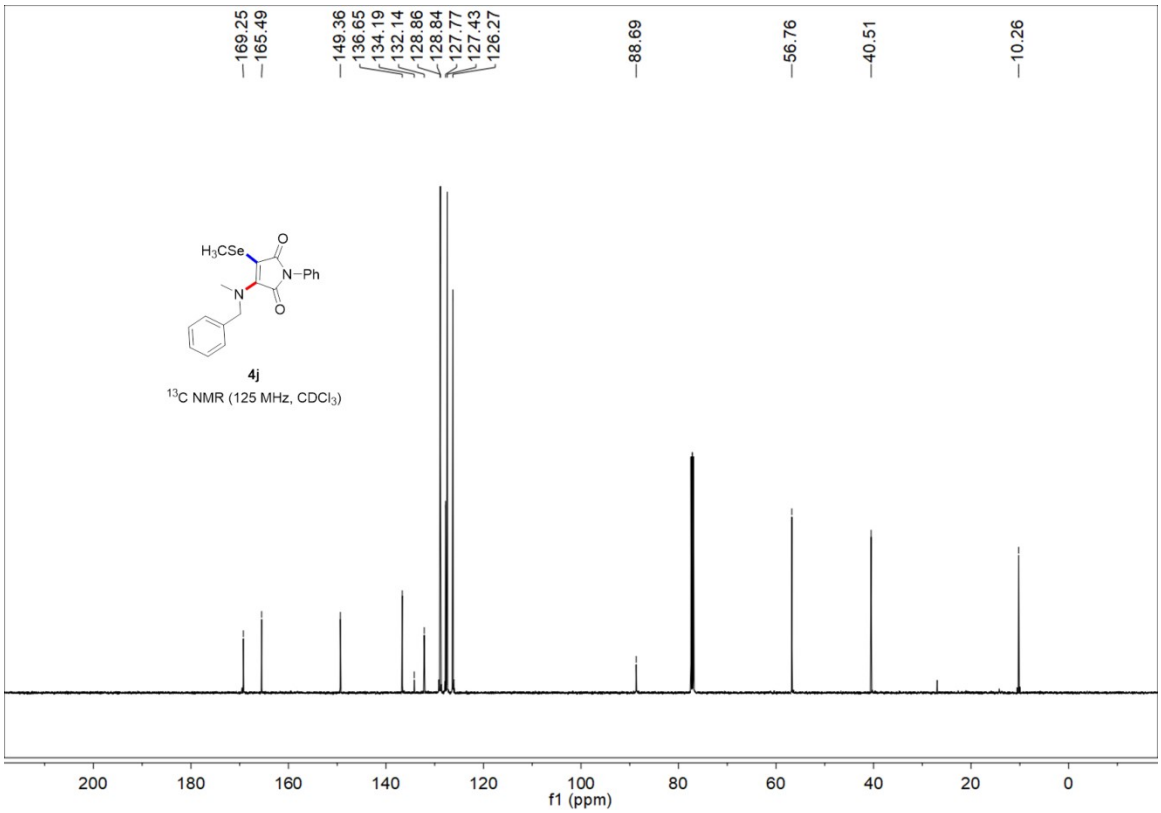
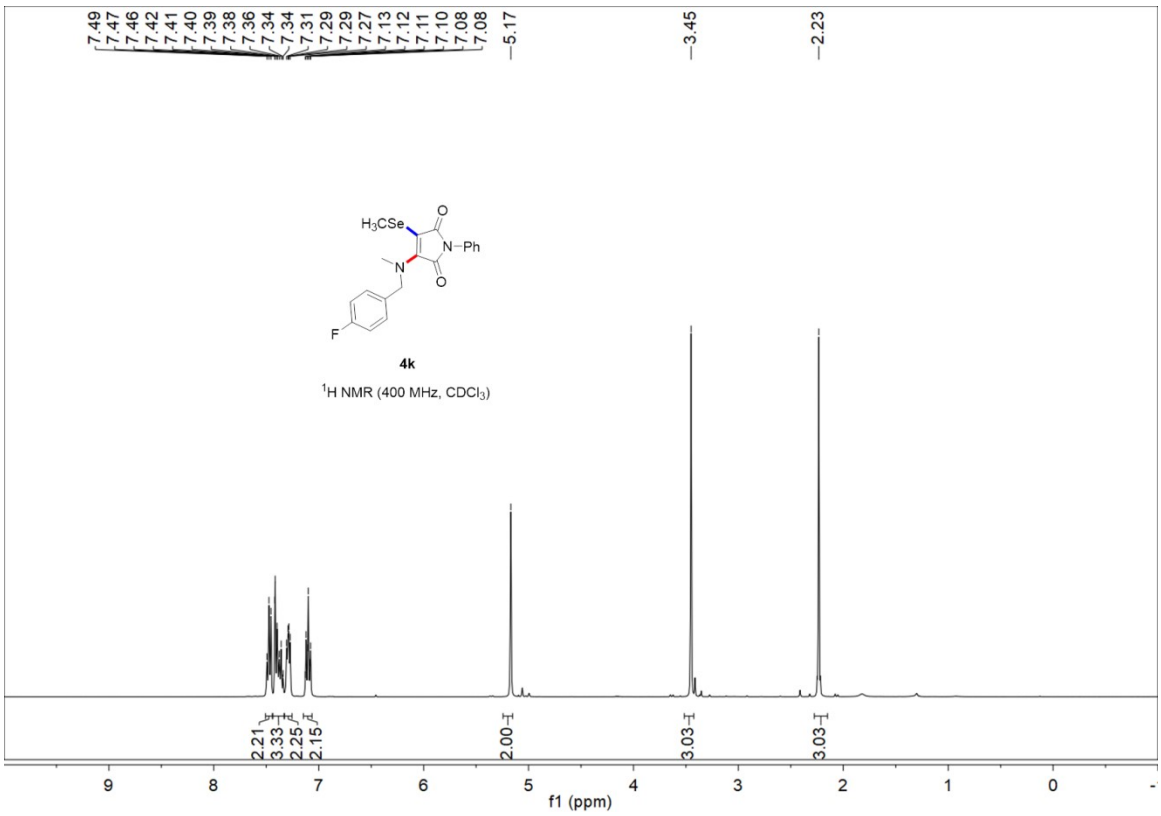
7.48
7.47
7.46
7.45
7.45
7.42
7.42
7.42
7.41
7.40
7.40
7.39
7.36
7.36
7.36
7.35
7.35
7.35
7.34
7.33
7.33
7.33
7.32
7.32
7.31
7.30
7.29
7.29
7.28
5.23
3.47
2.21
H3CSe
N
N–Ph
O
O
4j
1H NMR (500 MHz, CDCl3)
1.92
4.01
2.16
2.04
2.00
3.00
2.96
0
9
8
7
6
5
4
3
2
1
0
f1 (ppm)


169.25
165.49
149.36
136.65
134.19
132.14
128.86
128.84
127.77
127.43
126.27
88.69
56.76
40.51
10.26
H3CSe
N
N–Ph
O
O
4j
13C NMR (125 MHz, CDCl3)
200
180
160
140
120
100
80
60
40
20
0
f1 (ppm)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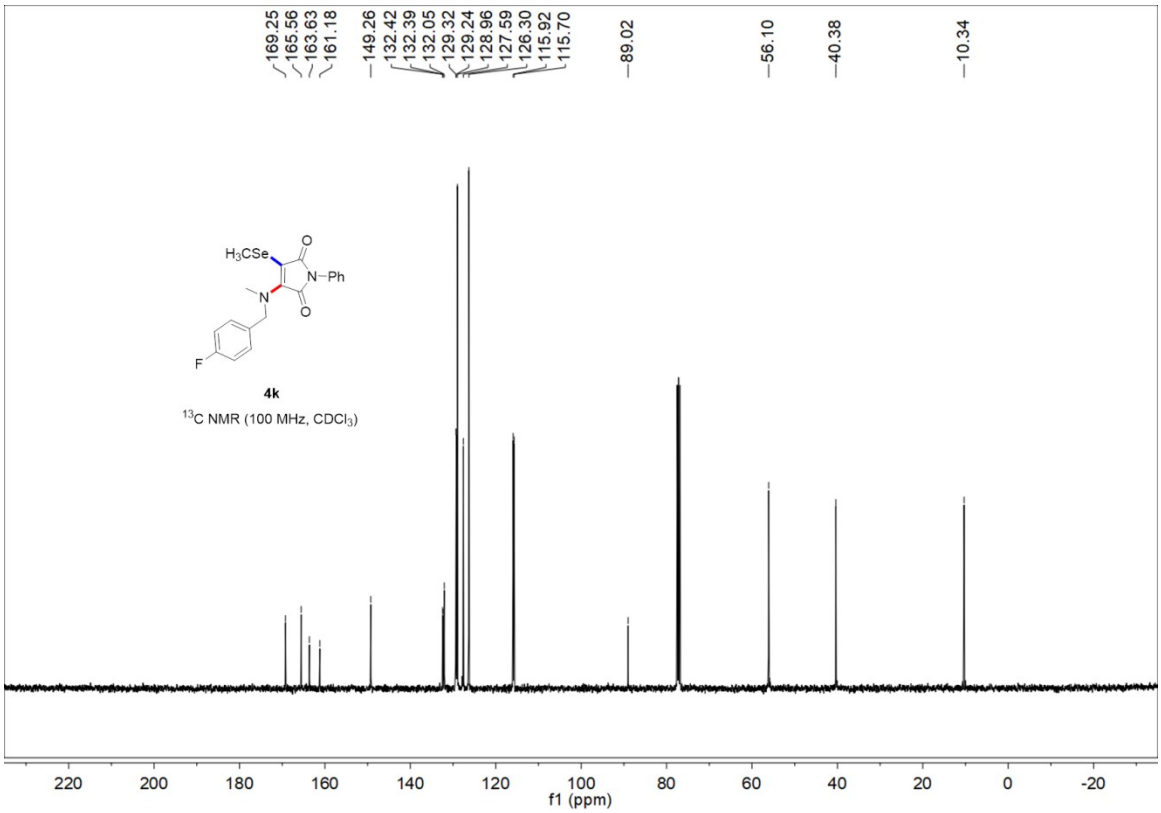
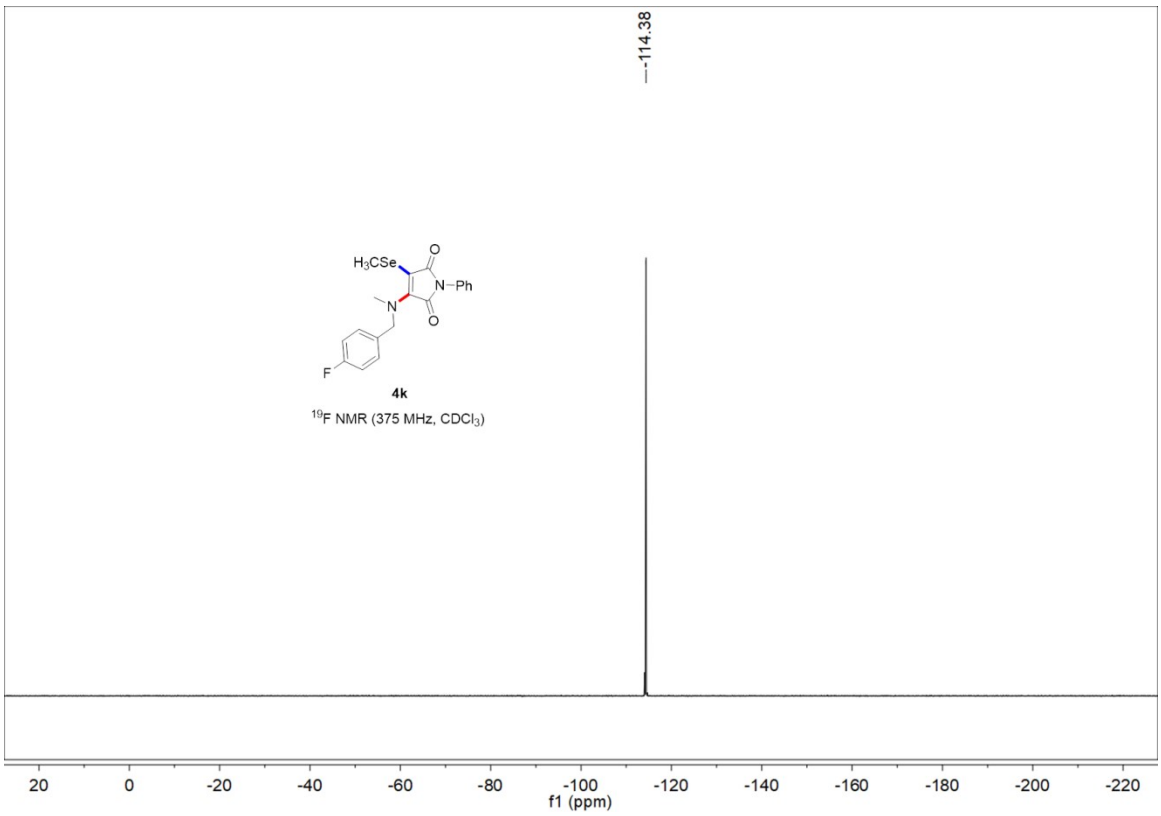
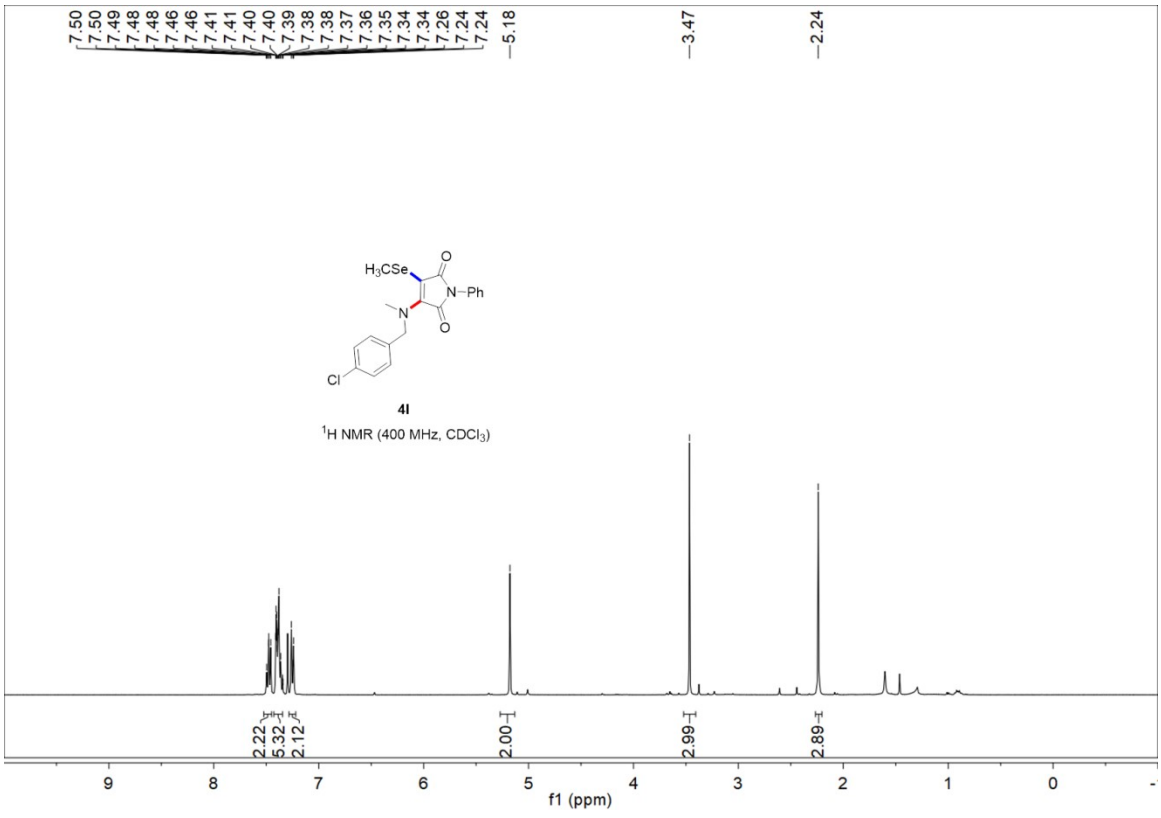
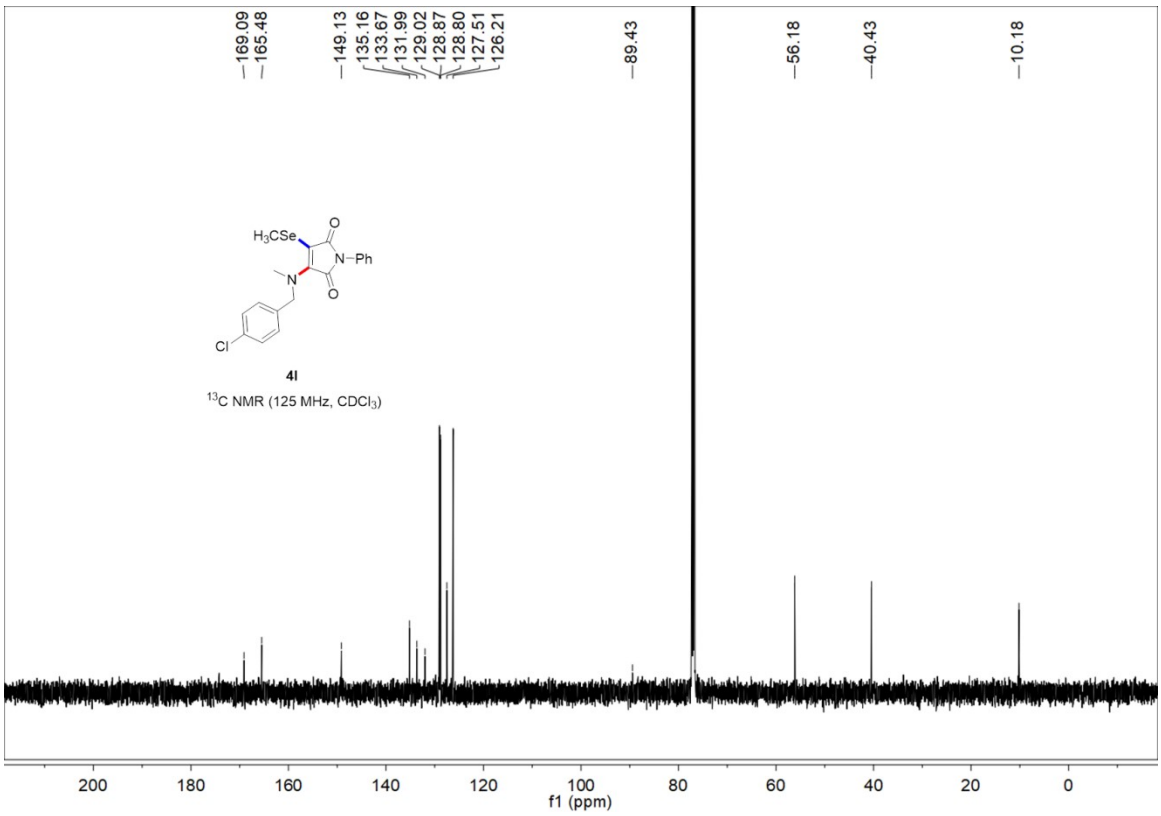
7.47
7.46
7.42
7.41
7.40
7.39
7.38
7.36
7.34
7.34
7.31
7.29
7.29
7.27
7.13
7.12
7.11
7.10
7.08
7.08
5.17
3.45
2.23
H3CSe
O
N–Ph
N
O
F
4k
1H NMR (400 MHz, CDCl3)
2.21
3.33
2.25
2.15
2.00
3.03
3.03
9
8
7
6
5
4
3
2
1
0
f1 (ppm)


169.25
165.56
163.63
161.18
149.26
132.42
132.39
132.05
129.32
129.24
128.96
127.59
126.30
115.92
115.70
89.02
56.10
40.38
10.34
H3CSe
O
N–Ph
N
O
F
4k
13C NMR (100 MHz, CDCl3)
220
200
180
160
140
120
100
80
60
40
20
0
-20
f1 (ppm)

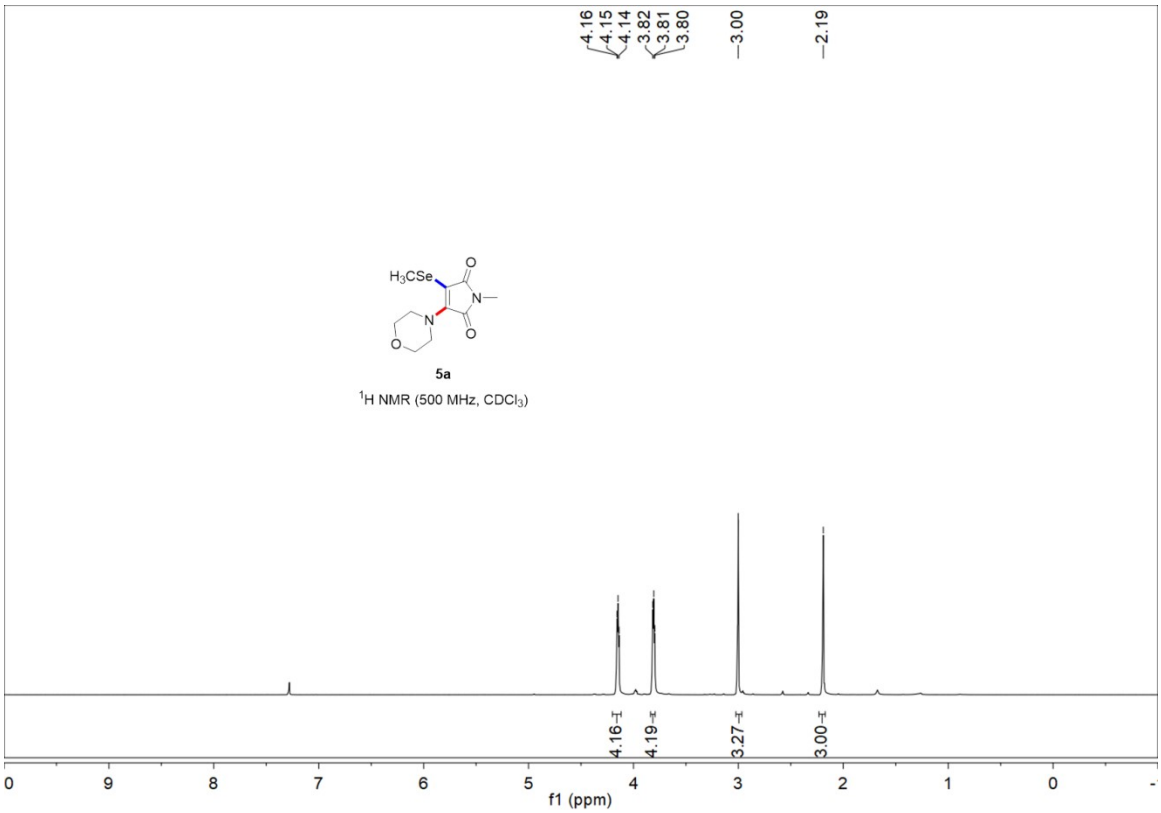

-114.38
H3CSe
O
N–Ph
N
O
F
4k
19F NMR (375 MHz, CDCl3)
20
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
-220
f1 (ppm)


7.50
7.50
7.49
7.48
7.48
7.46
7.46
7.41
7.41
7.40
7.40
7.39
7.38
7.38
7.37
7.36
7.35
7.34
7.34
7.26
7.24
7.24
5.18
3.47
2.24
H3CSe
O
N–Ph
N
O
Cl
4l
1H NMR (400 MHz, CDCl3)
2.22
5.32
2.12
2.00
2.99
2.89
9
8
7
6
5
4
3
2
1
0
f1 (ppm)



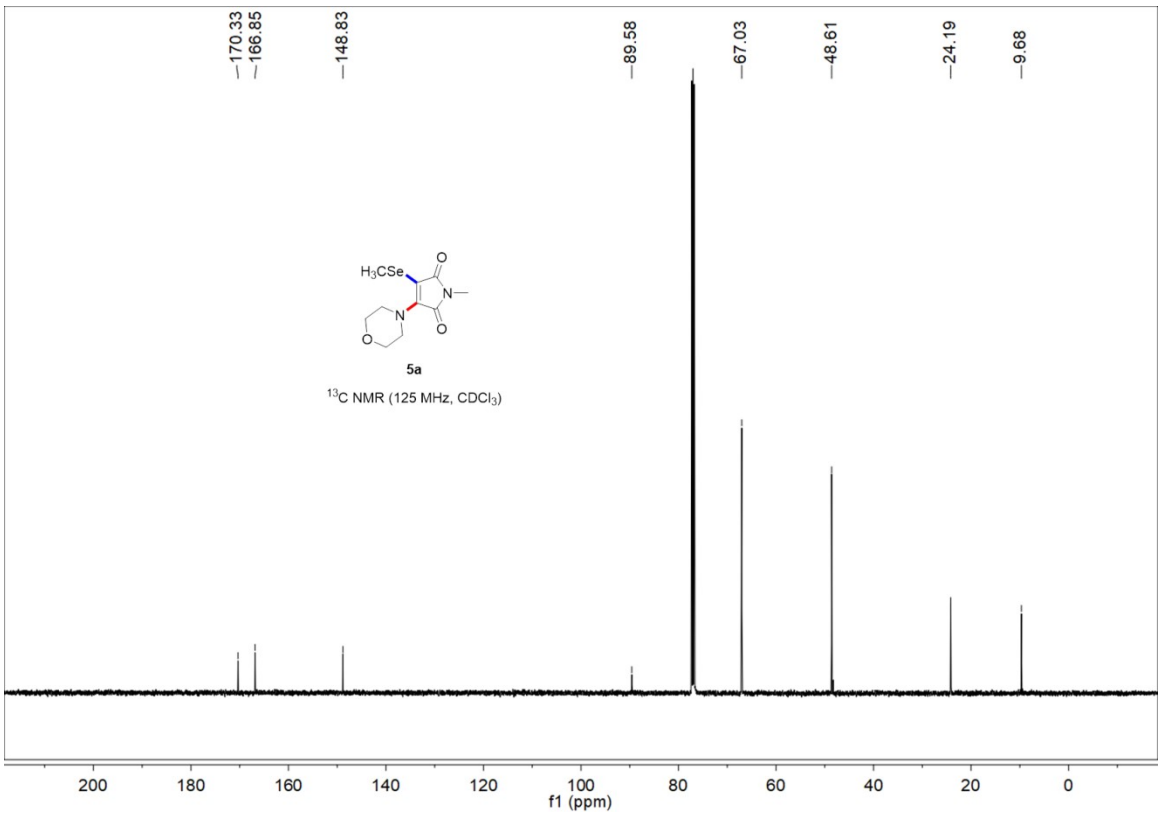
4l

^{13}C NMR (125 MHz, $CDCl_3$)



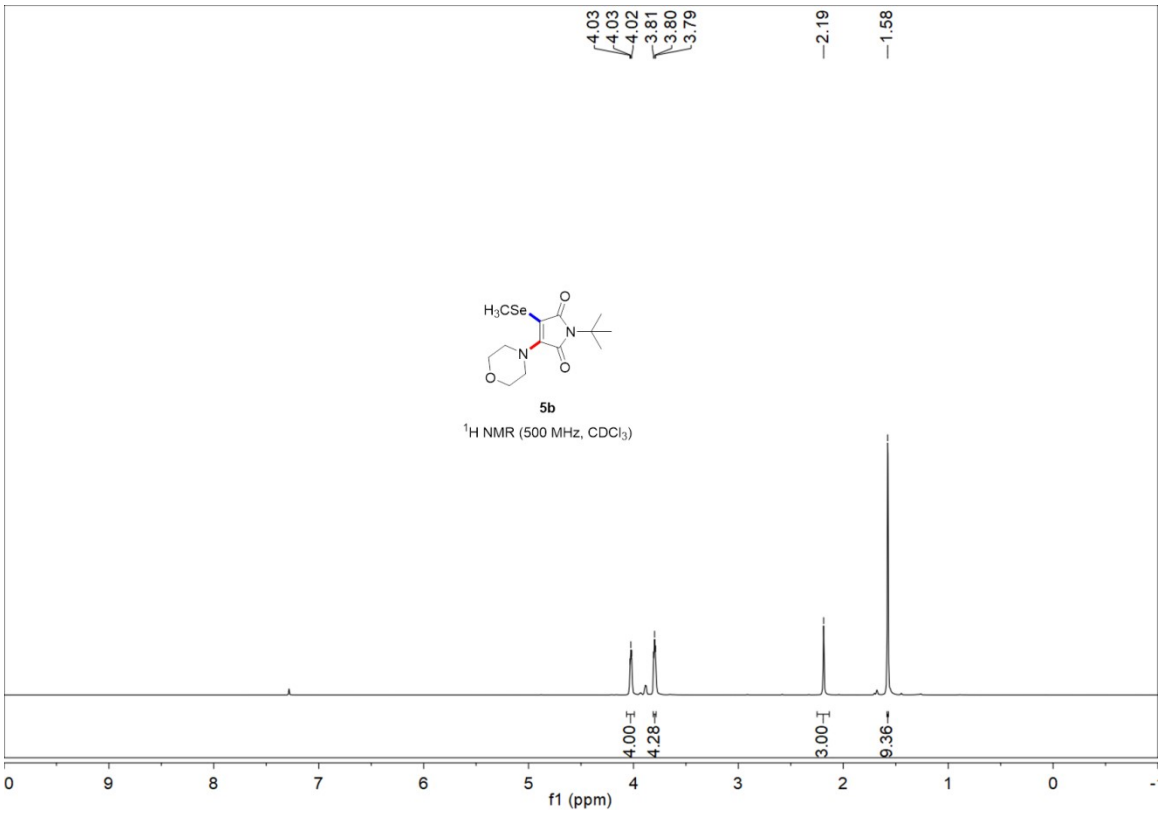
5a

^{1}H NMR (500 MHz, $CDCl_3$)



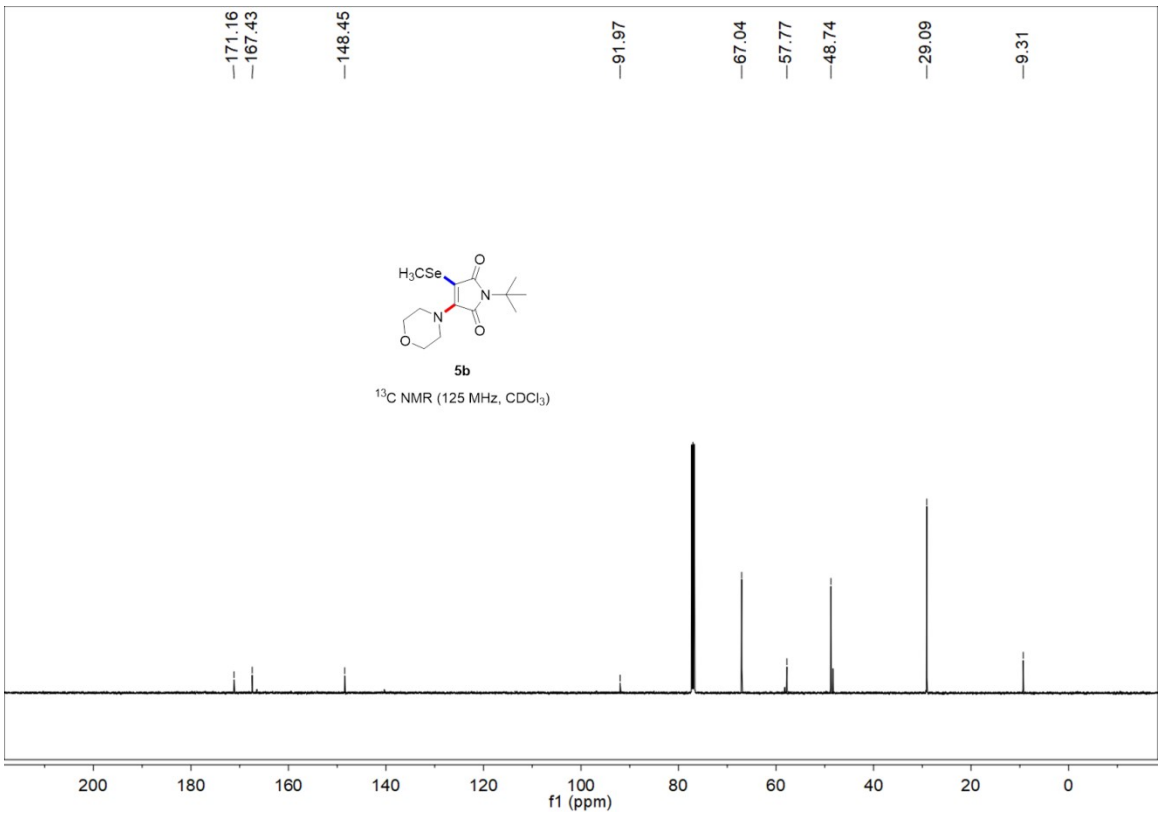
5a

^{13}C NMR (125 MHz, $CDCl_3$)



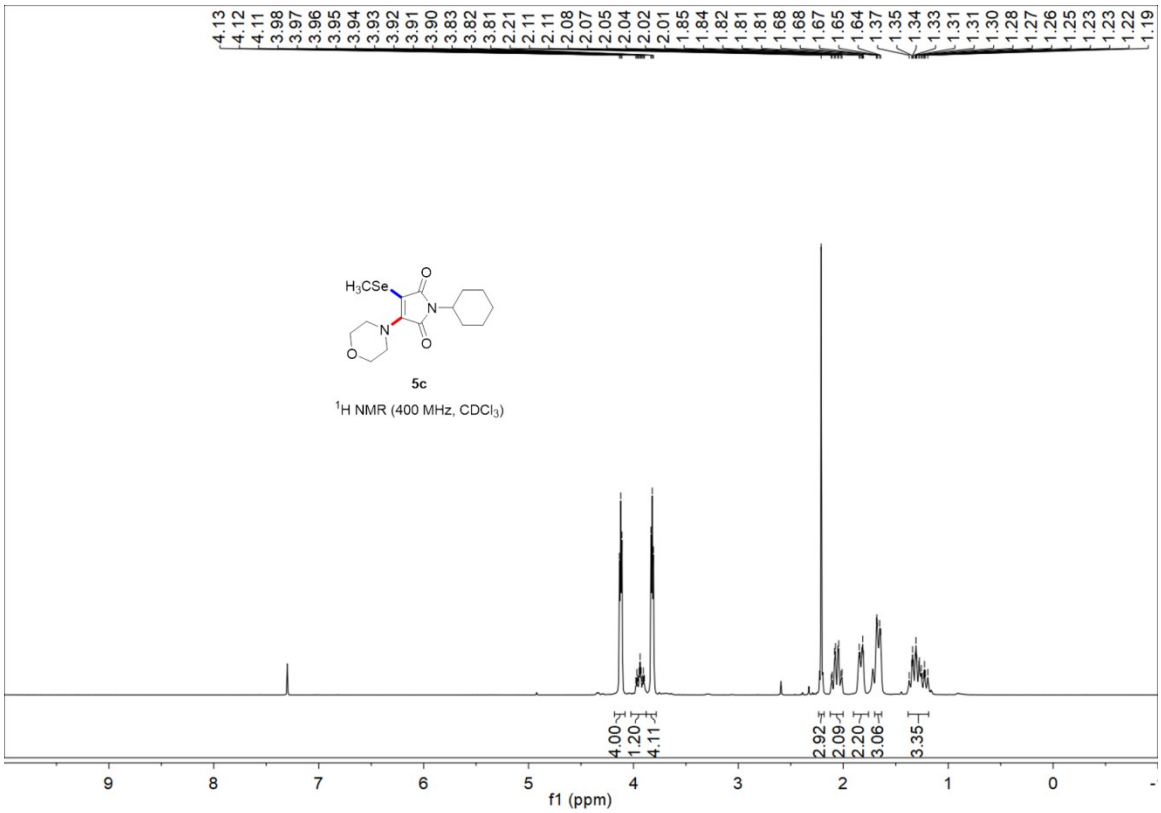
5b

^{1}H NMR (500 MHz, $CDCl_3$)



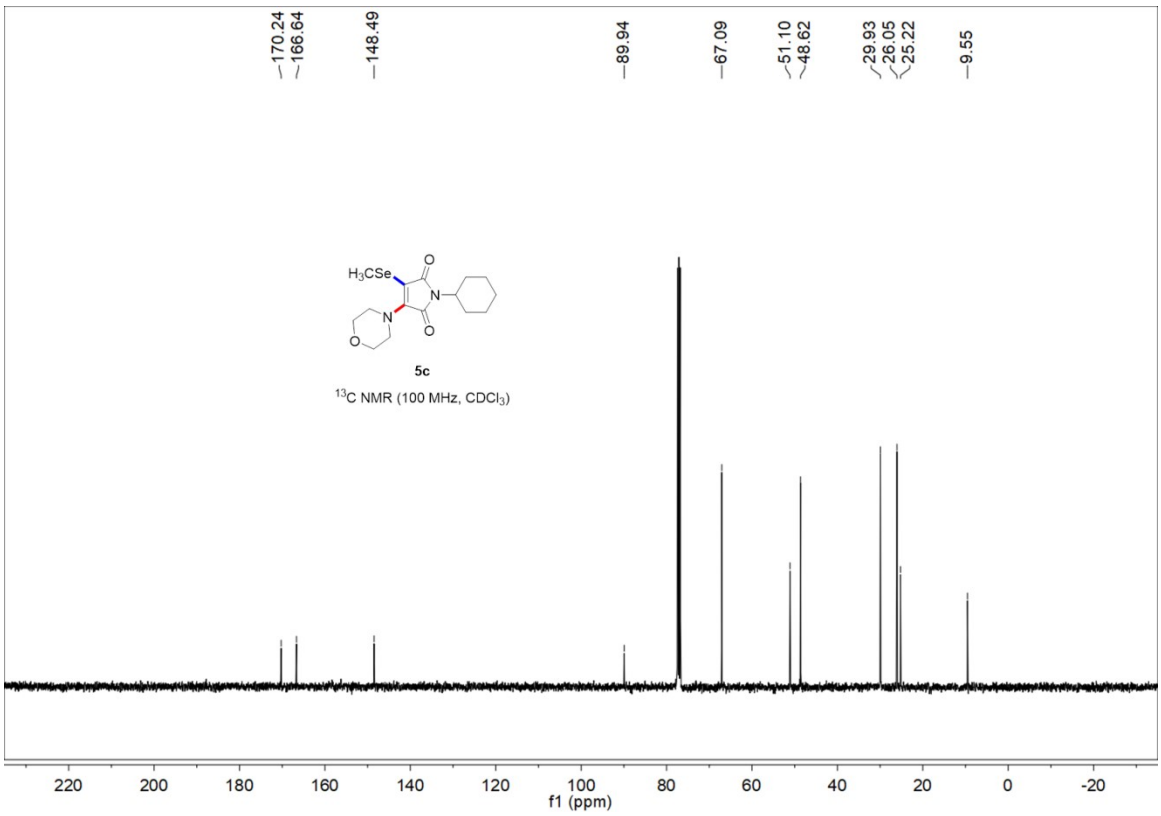
5b

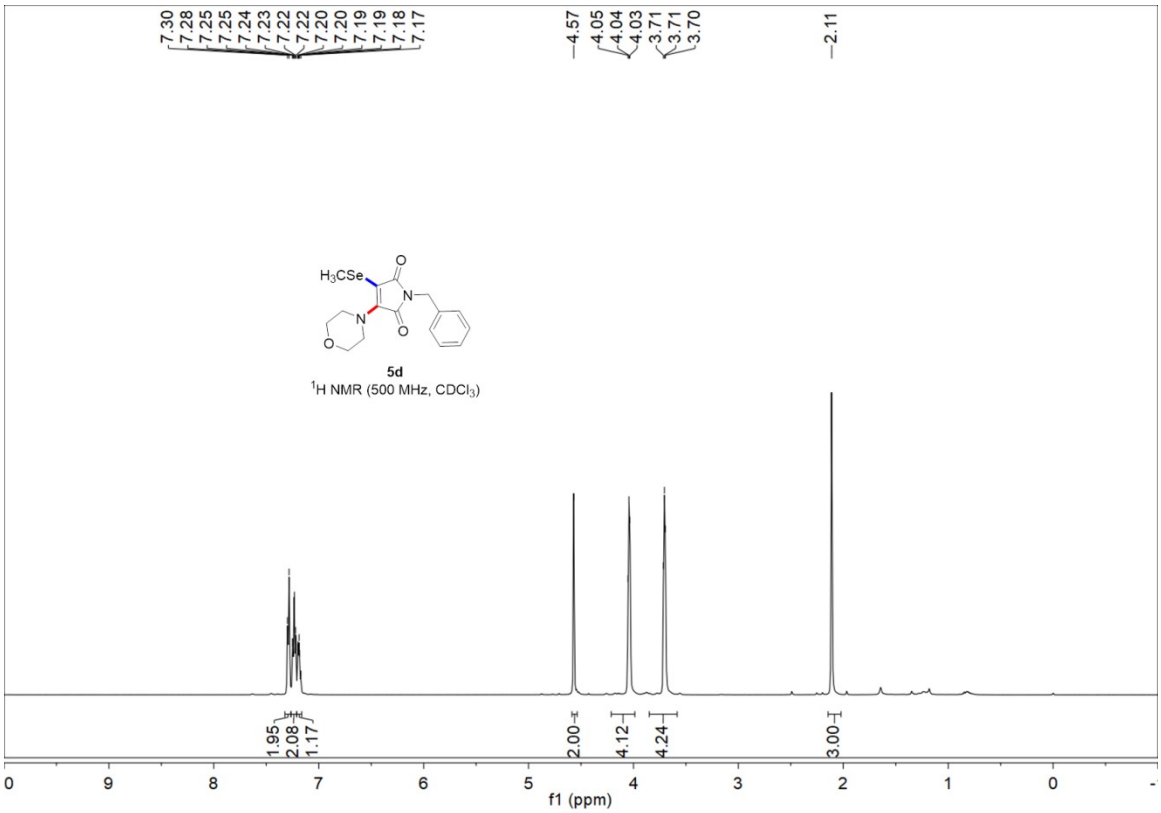
^{13}C NMR (125 MHz, $CDCl_3$)

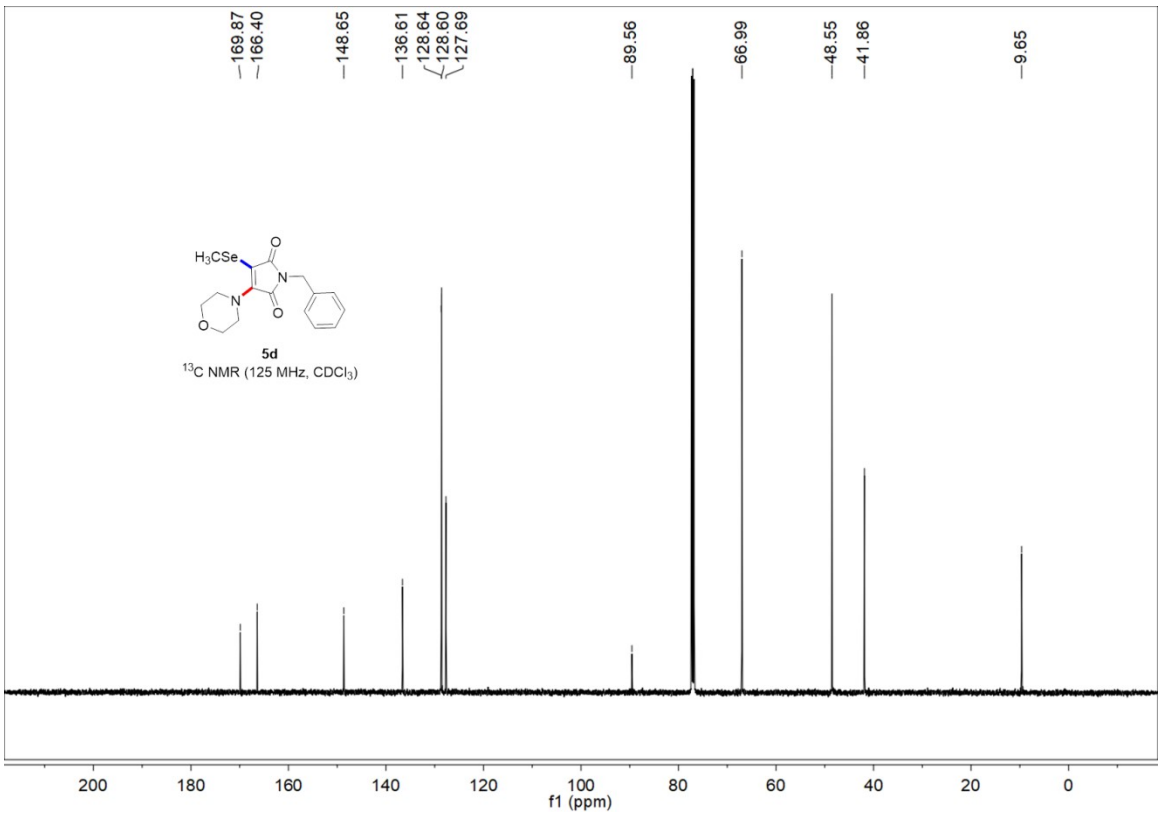


5c

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

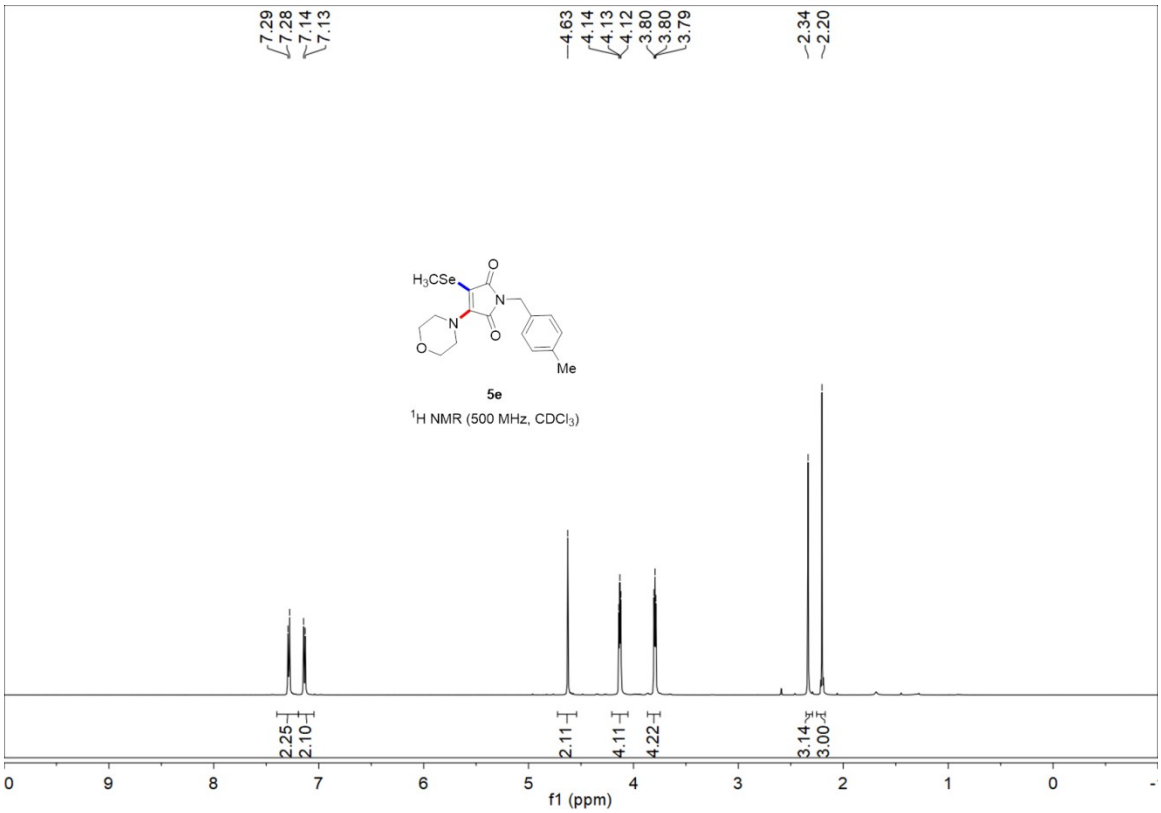

170.24
166.64
148.49
89.94
67.09
51.10
48.62
29.93
26.05
25.22
9.55
H3CSe
O
N
O
N
O
5c
13C NMR (100 MHz, CDCl3)
220
200
180
160
140
120
100
80
60
40
20
0
-20
f1 (ppm)


7.30
7.28
7.25
7.25
7.24
7.23
7.22
7.22
7.20
7.20
7.19
7.19
7.18
7.17
4.57
4.05
4.04
4.03
3.71
3.71
3.70
2.11
H3CSe
O
N
O
N
O
5d
1H NMR (500 MHz, CDCl3)
1.95
2.08
1.17
2.00
4.12
4.24
3.00
0
9
8
7
6
5
4
3
2
1
0
f1 (ppm)



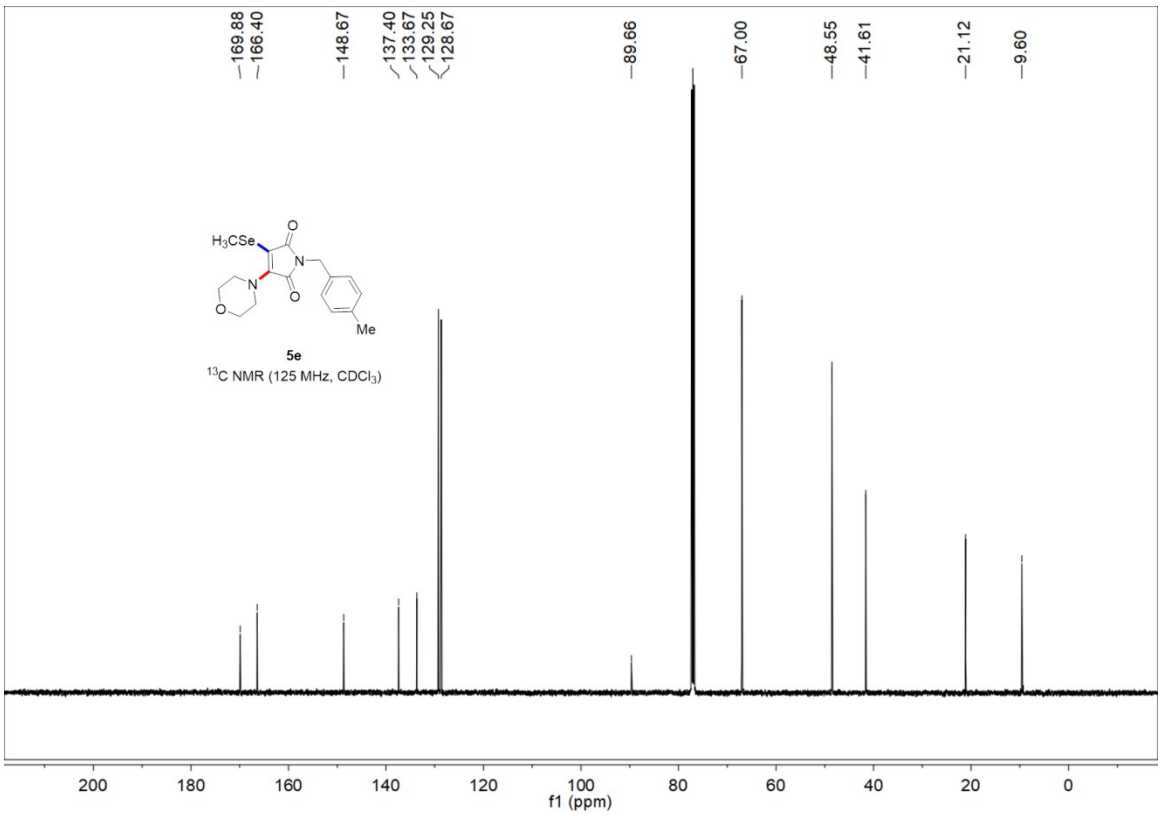
5d

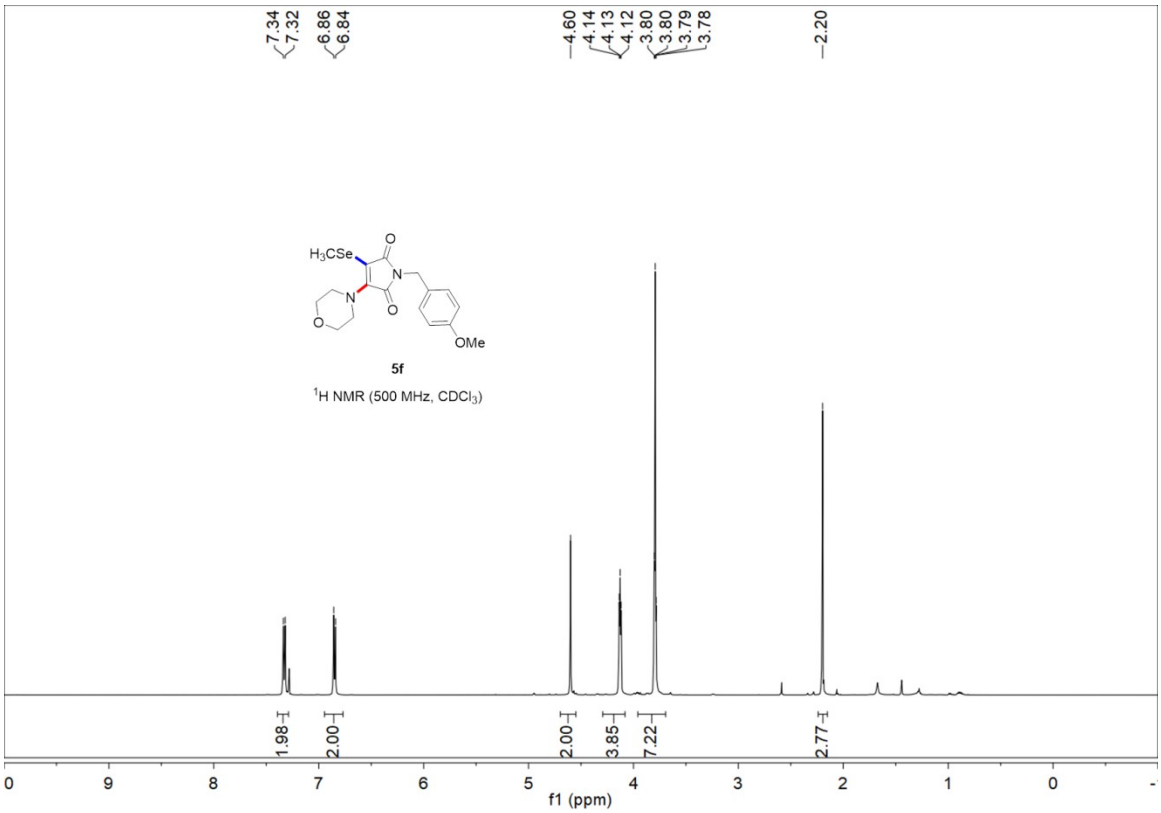
^{13}C NMR (125 MHz, $CDCl_3$)

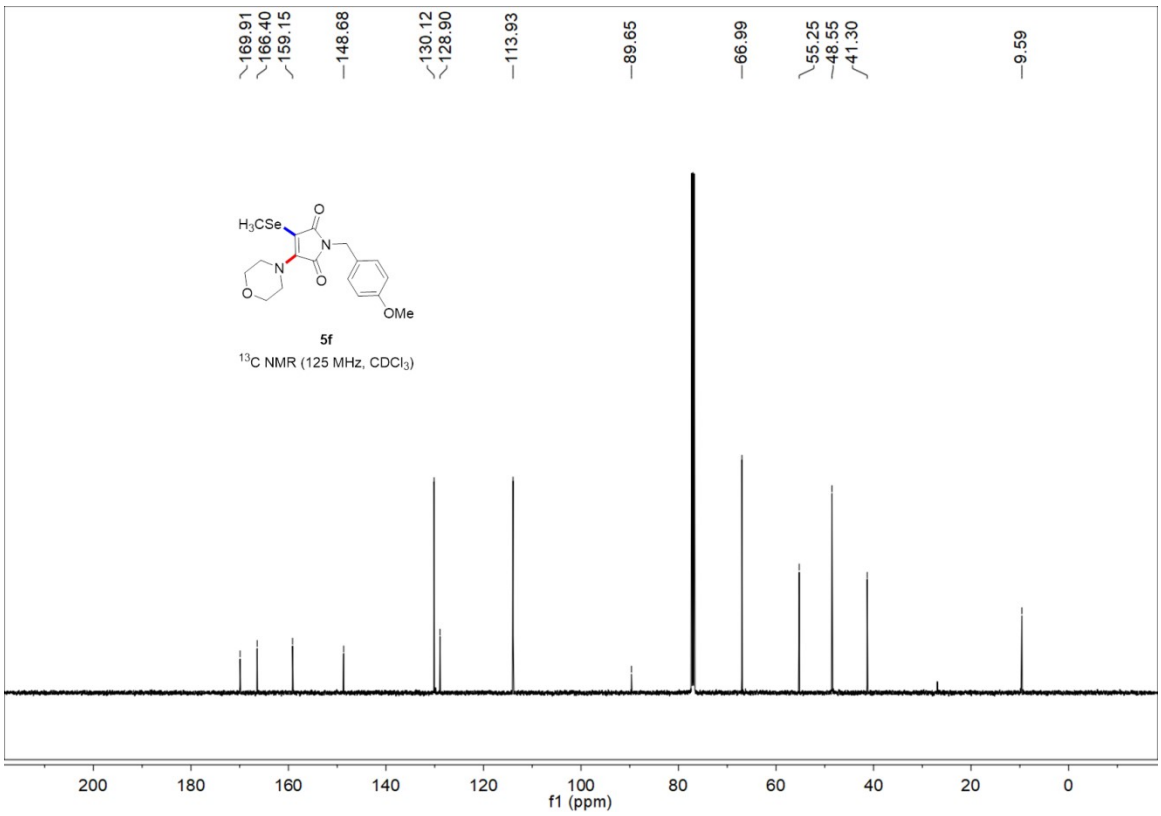


5e

^{1}H NMR (500 MHz, $CDCl_3$)

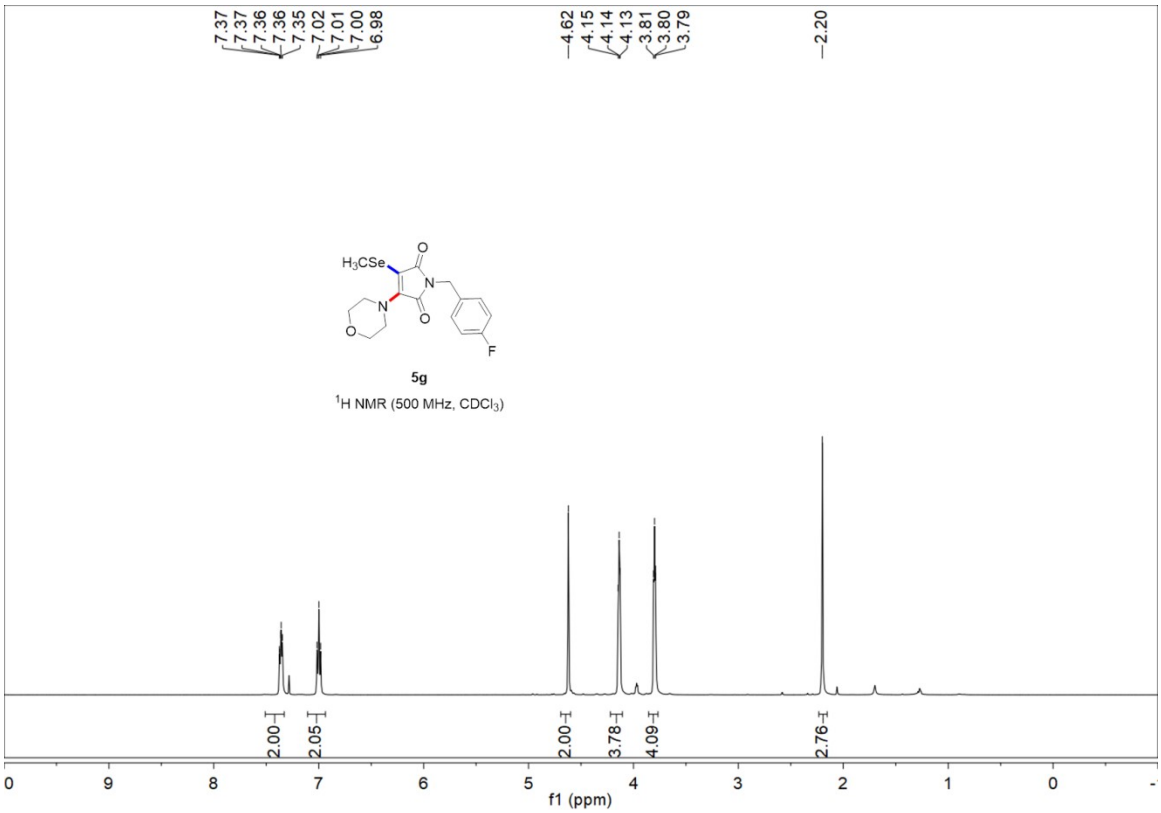

169.88
166.40
148.67
137.40
133.67
129.25
128.67
89.66
67.00
48.55
41.61
21.12
9.60
H3CSe
O
N
O
N
O
Me
5e
13C NMR (125 MHz, CDCl3)
200
180
160
140
120
100
80
60
40
20
0
f1 (ppm)


7.34
7.32
6.86
6.84
4.60
4.14
4.13
4.12
3.80
3.80
3.79
3.78
2.20
H3CSe
O
N
O
N
O
OMe
5f
1H NMR (500 MHz, CDCl3)
1.98
2.00
2.00
3.85
7.22
2.77
0
9
8
7
6
5
4
3
2
1
0
f1 (ppm)



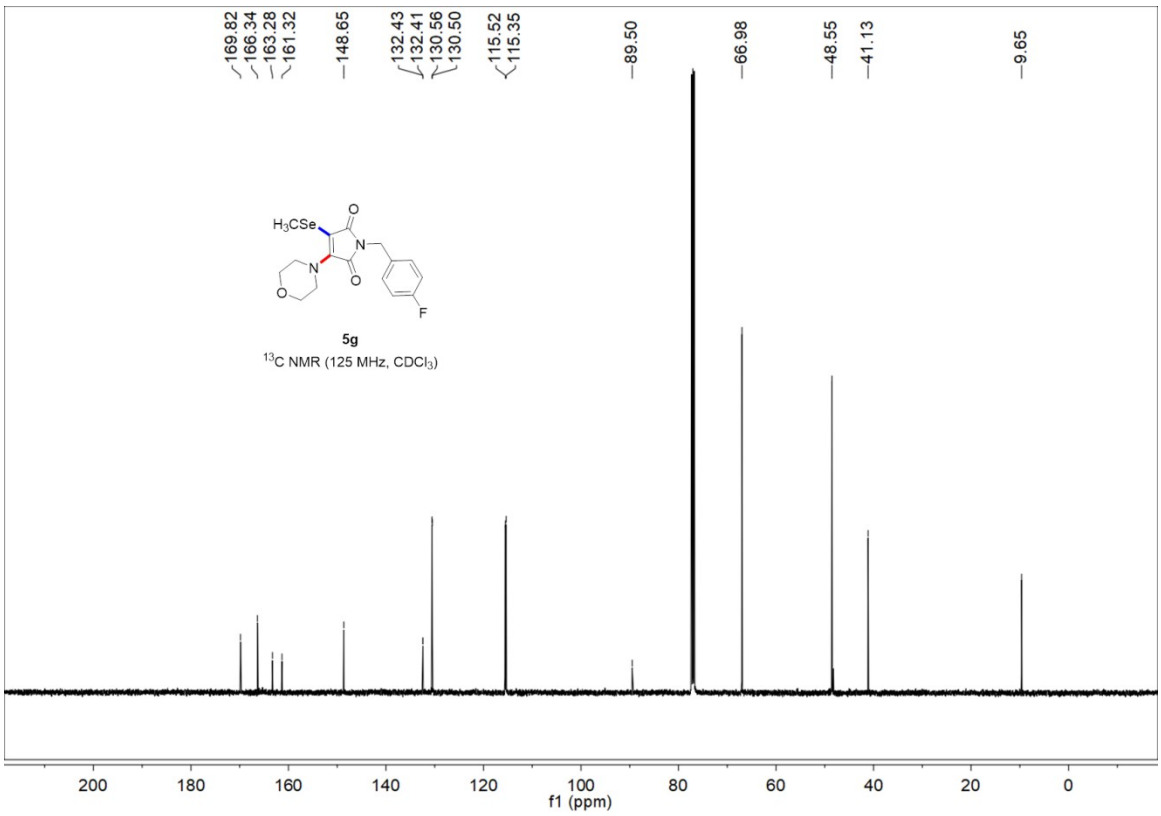
5f

^{13}C NMR (125 MHz, $CDCl_3$)



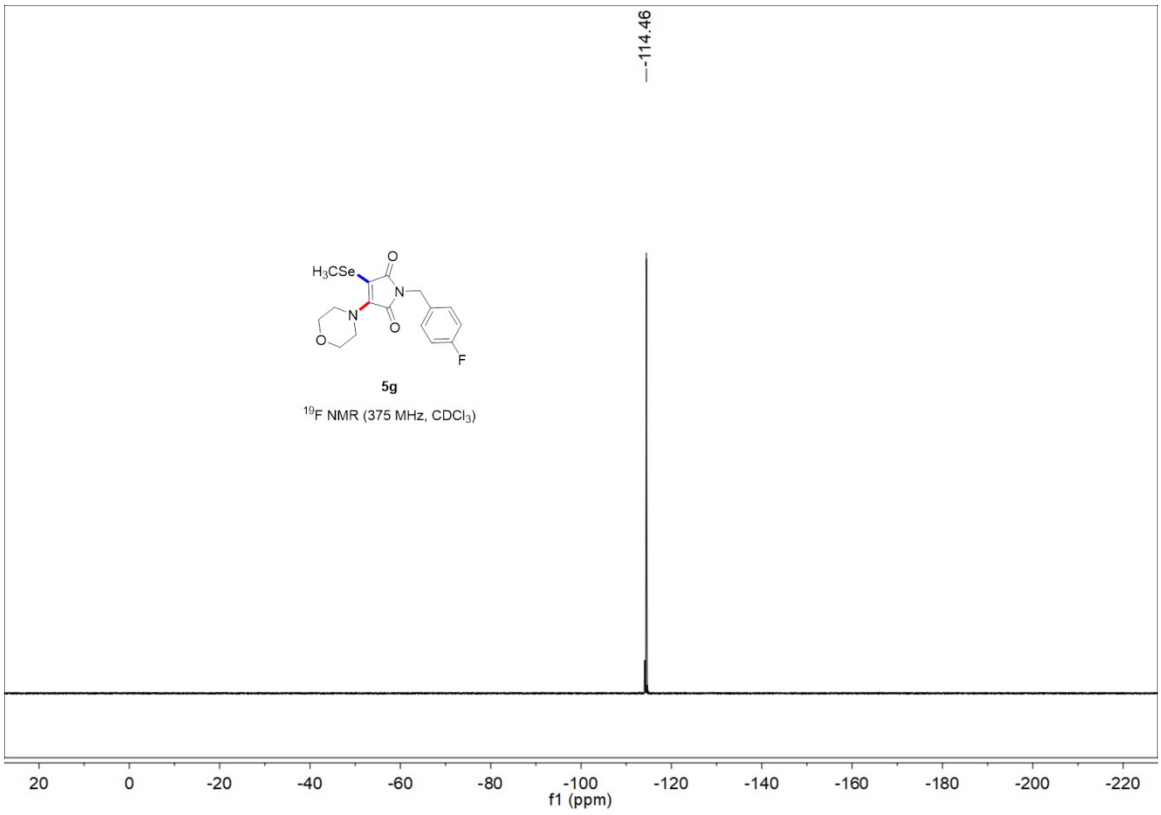
5g

^{1}H NMR (500 MHz, $CDCl_3$)



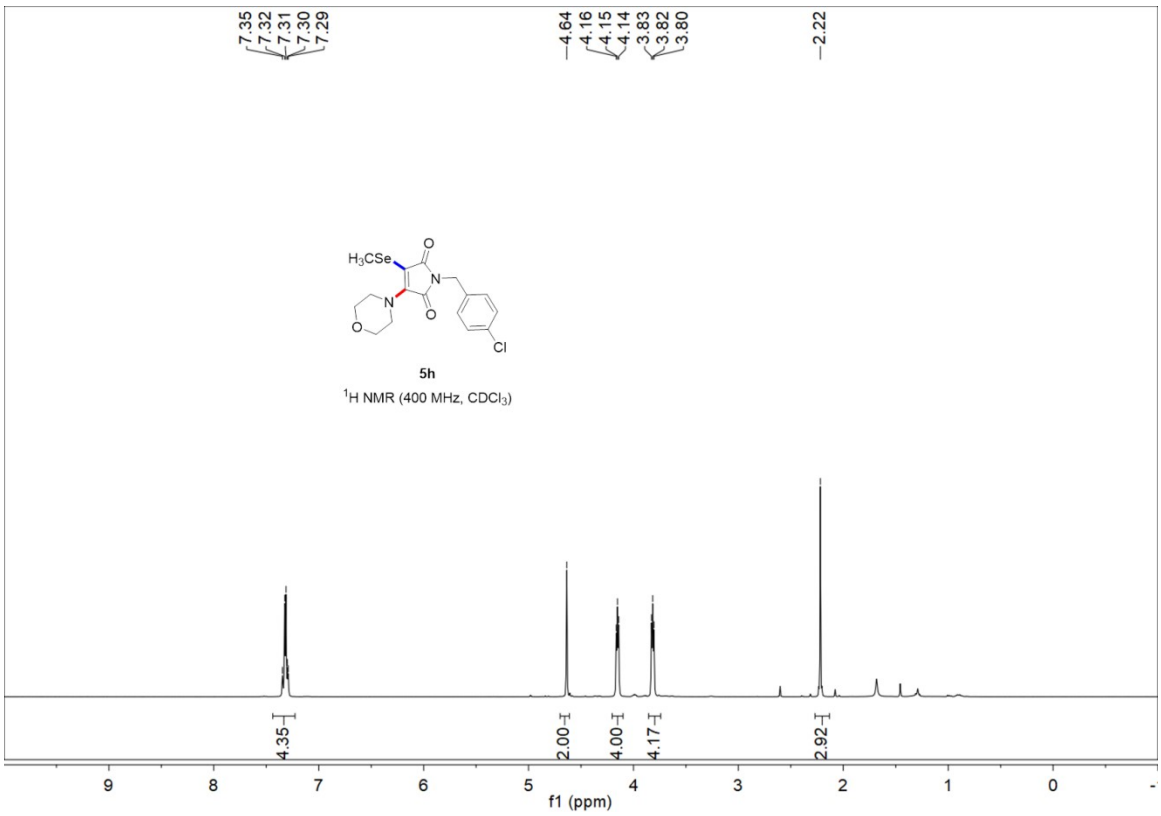
5g

^{13}C NMR (125 MHz, $CDCl_3$)



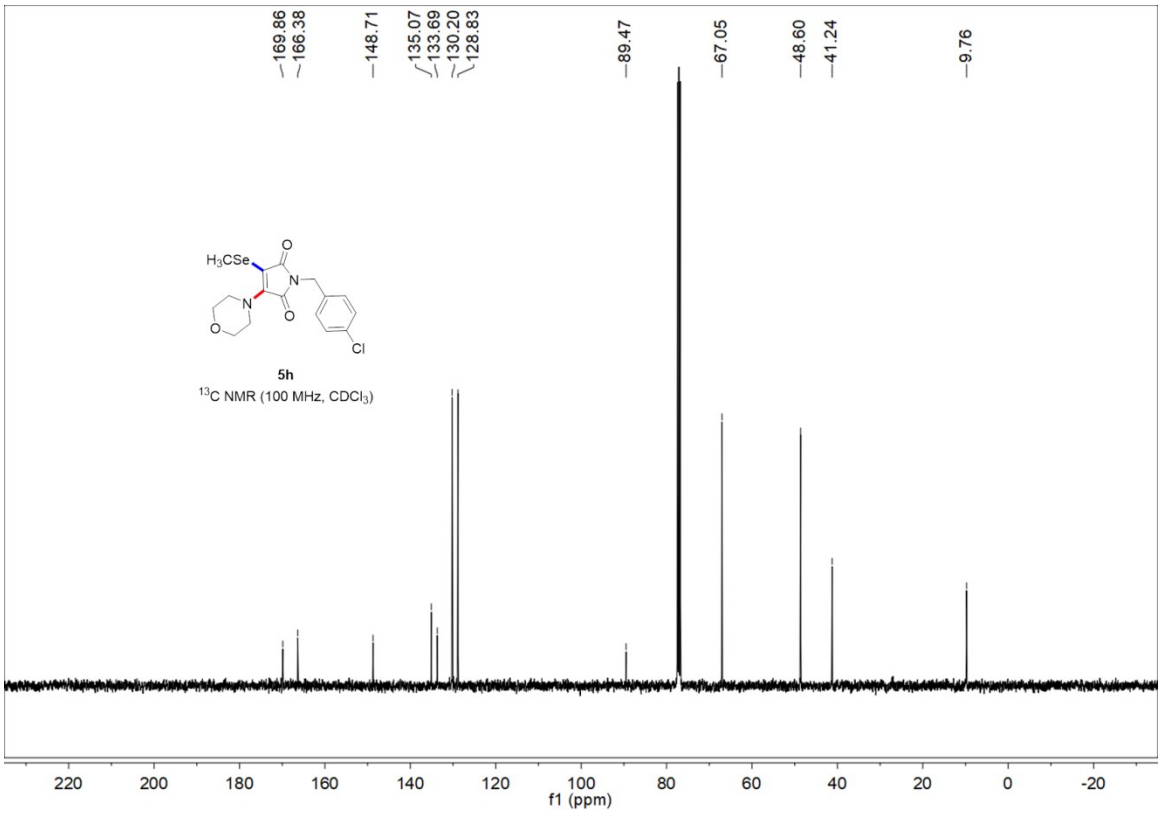
5g

^{19}F NMR (375 MHz, $CDCl_3$)



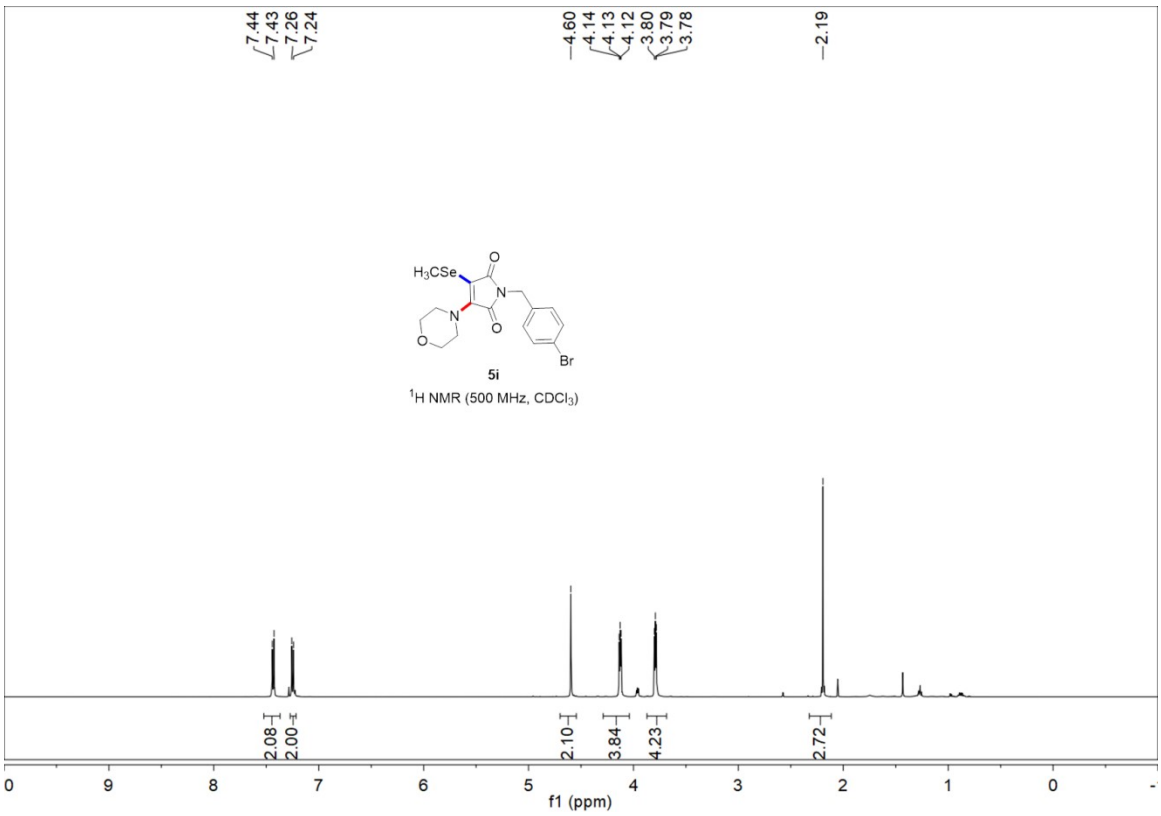
5h

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



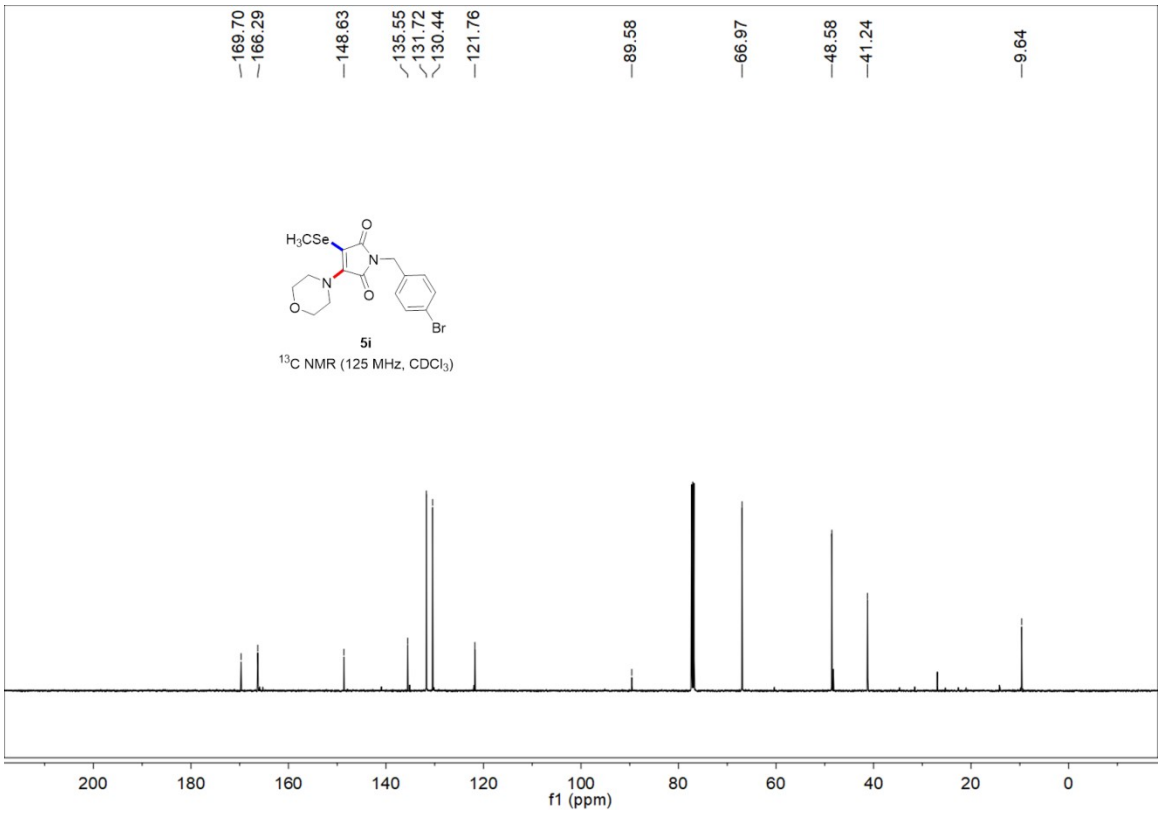
5h

^{13}C NMR (100 MHz, $CDCl_3$)



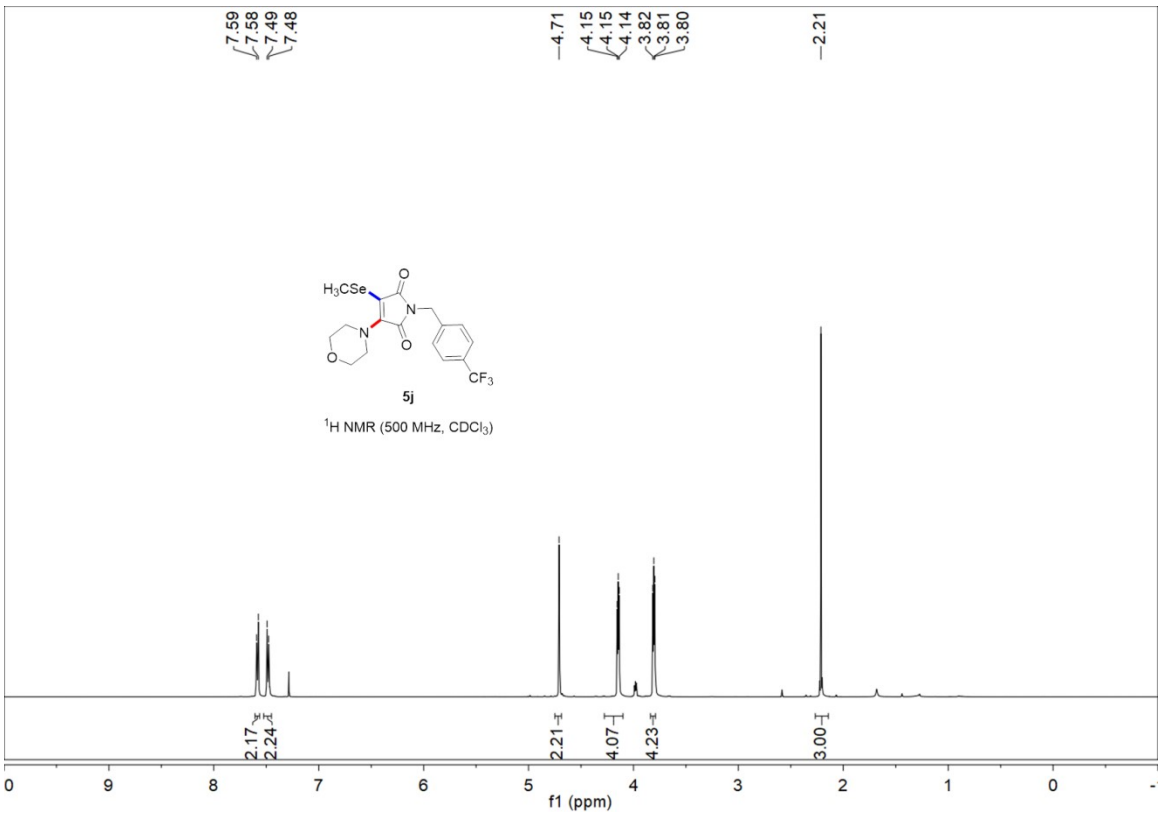
5i

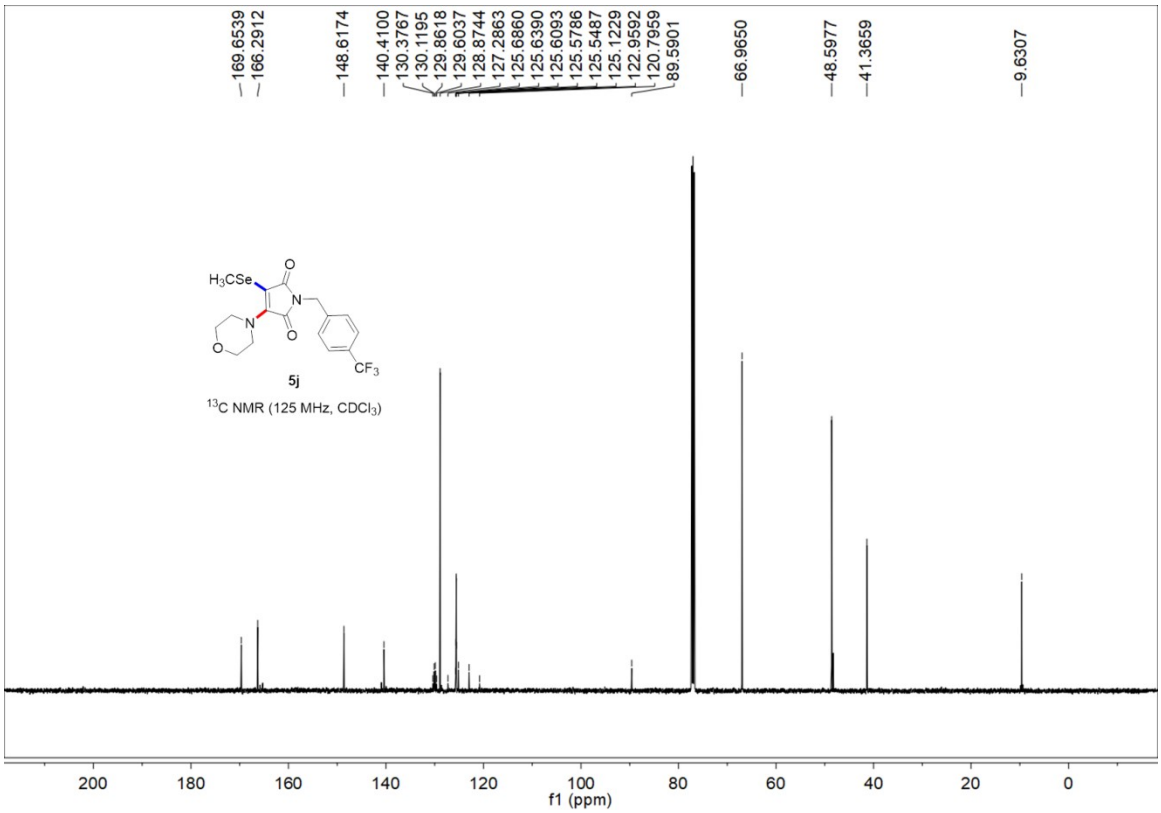
^{1}H NMR (500 MHz, $CDCl_3$)

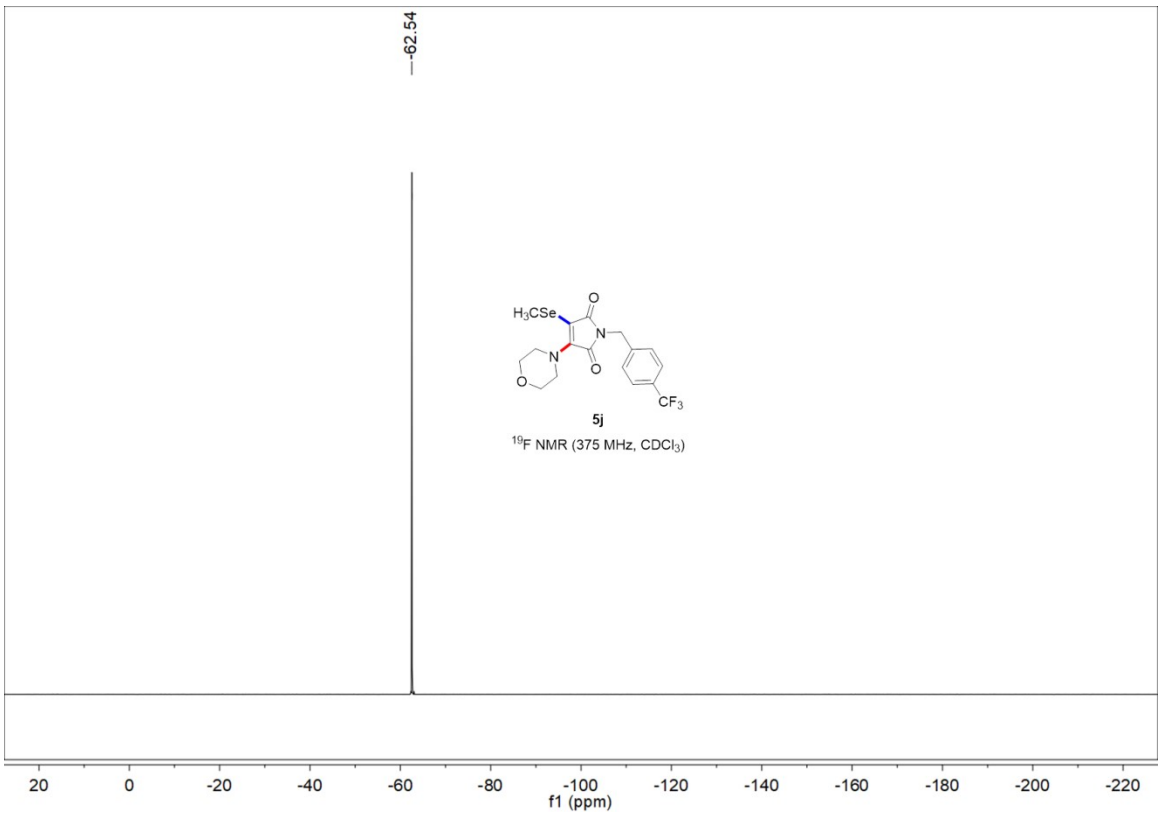


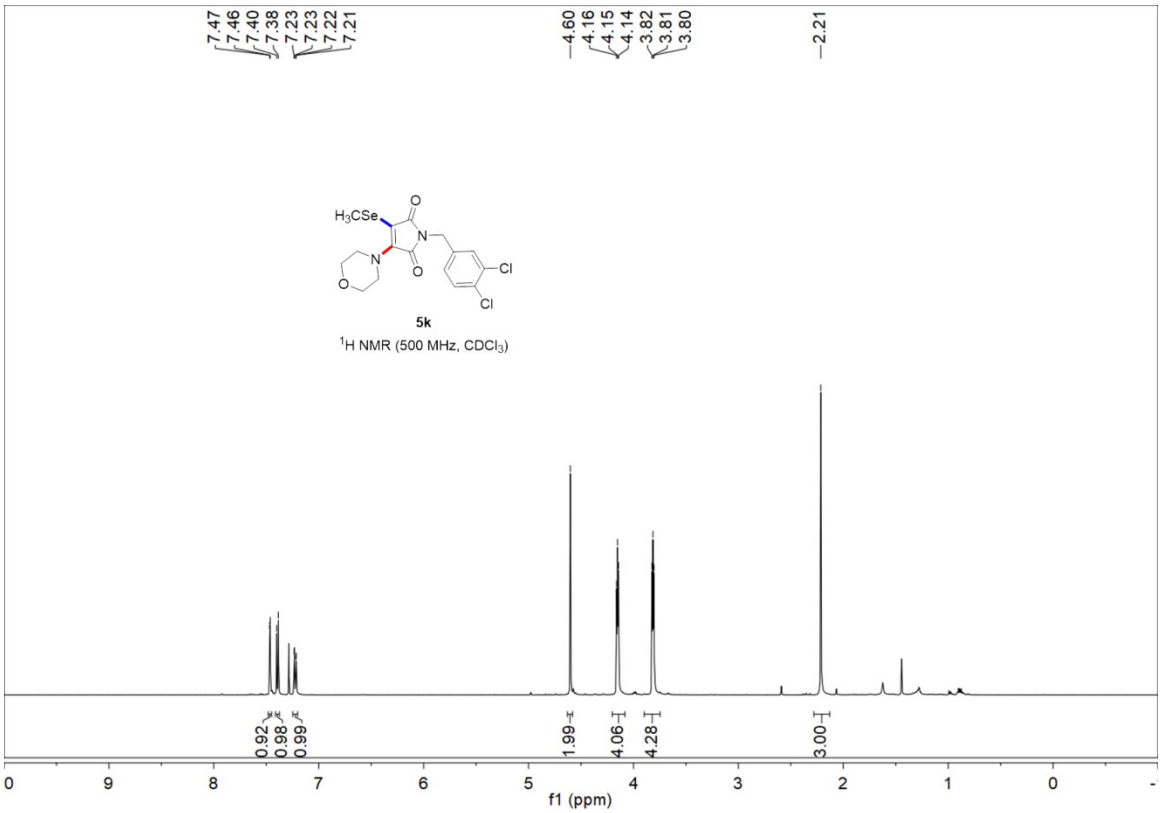
5i

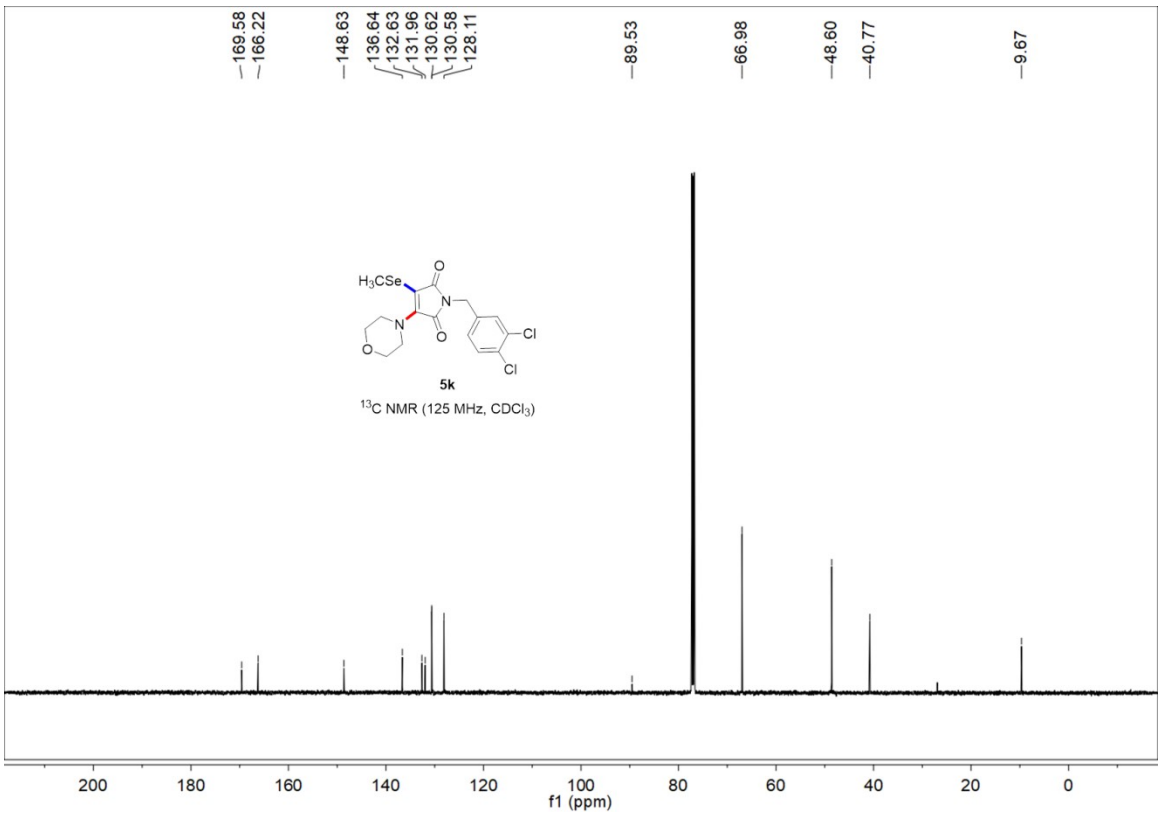
^{13}C NMR (125 MHz, $CDCl_3$)


7.59
7.58
7.49
7.48
4.71
4.15
4.15
4.14
3.82
3.81
3.80
2.21
H3CSe
O
N
O
N
O
CF3
5j
1H NMR (500 MHz, CDCl3)
2.17
2.24
2.21
4.07
4.23
3.00
f1 (ppm)


169.6539
166.2912
148.6174
140.4100
130.3767
130.1195
129.8618
129.6037
128.8744
127.2863
125.6860
125.6390
125.6093
125.5786
125.5487
125.1229
122.9592
120.7959
89.5901
66.9650
48.5977
41.3659
9.6307
H3CSe
O
N
O
N
O
CF3
5j
13C NMR (125 MHz, CDCl3)
f1 (ppm)

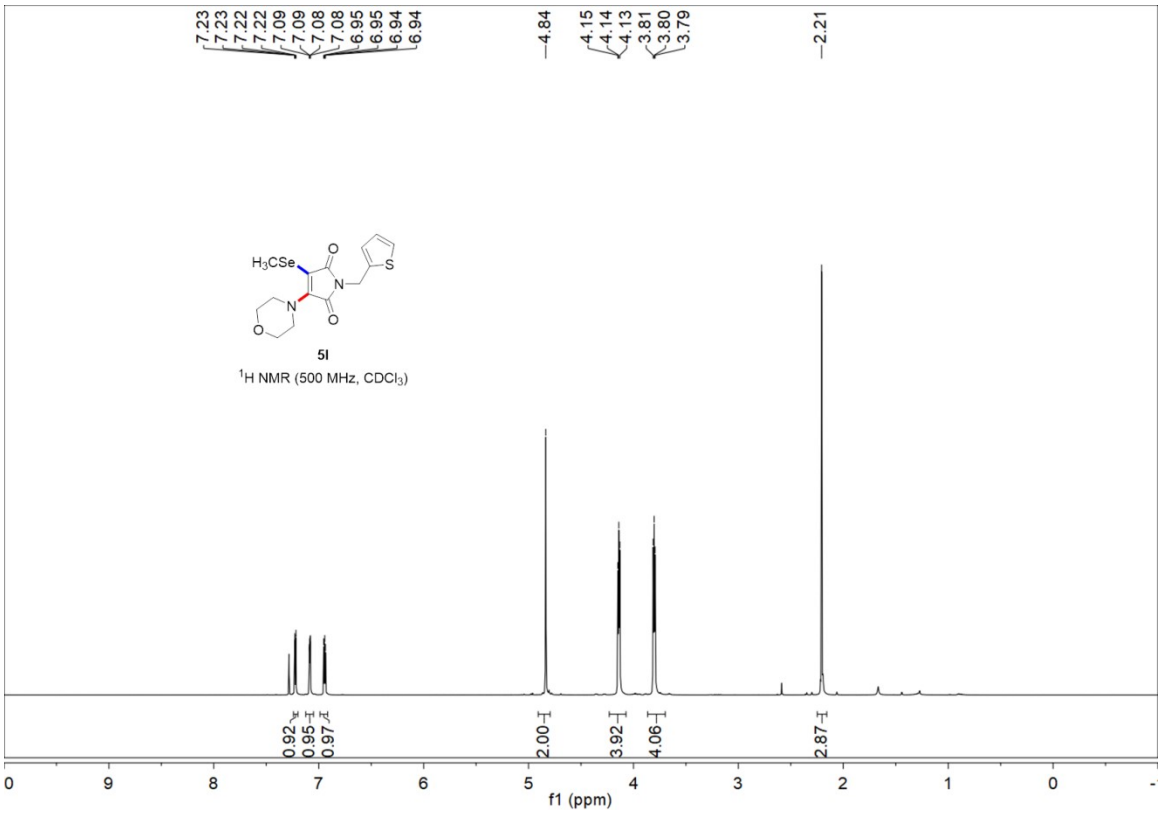

-62.54
H3CSe
O
N
O
N
O
CF3
5j
19F NMR (375 MHz, CDCl3)
20
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
-220
f1 (ppm)


7.47
7.46
7.40
7.38
7.23
7.23
7.22
7.21
4.60
4.16
4.15
4.14
3.82
3.81
3.80
2.21
H3CSe
O
N
O
N
O
Cl
Cl
5k
1H NMR (500 MHz, CDCl3)
0.92
0.98
0.99
1.99
4.06
4.28
3.00
0
9
8
7
6
5
4
3
2
1
0
f1 (ppm)



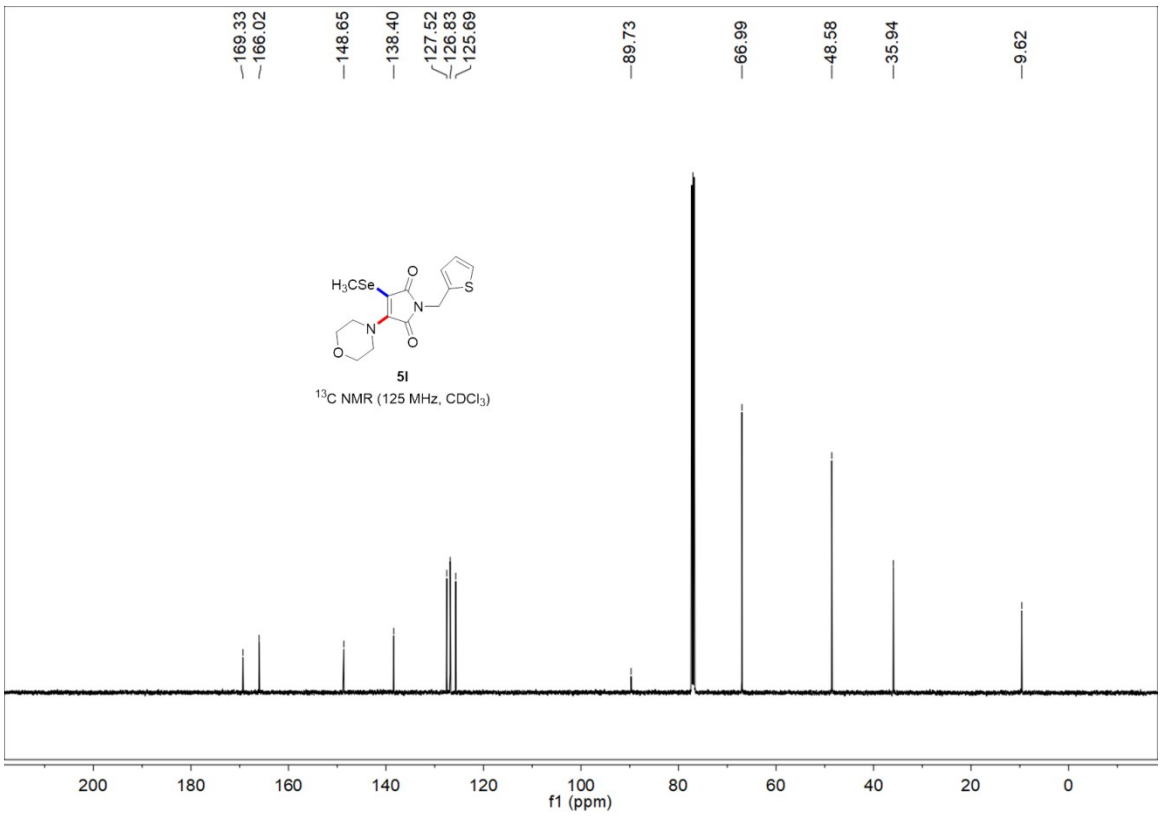
5k

^{13}C NMR (125 MHz, $CDCl_3$)



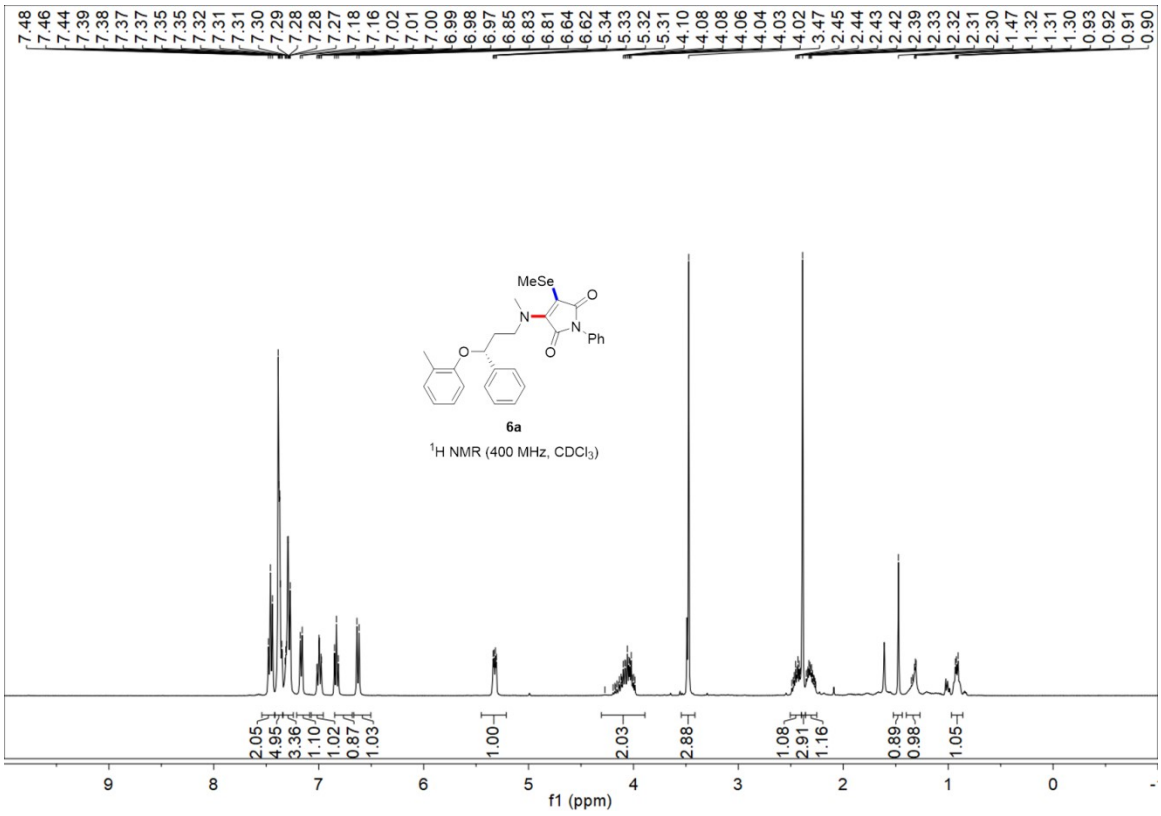
5l

^{1}H NMR (500 MHz, $CDCl_3$)



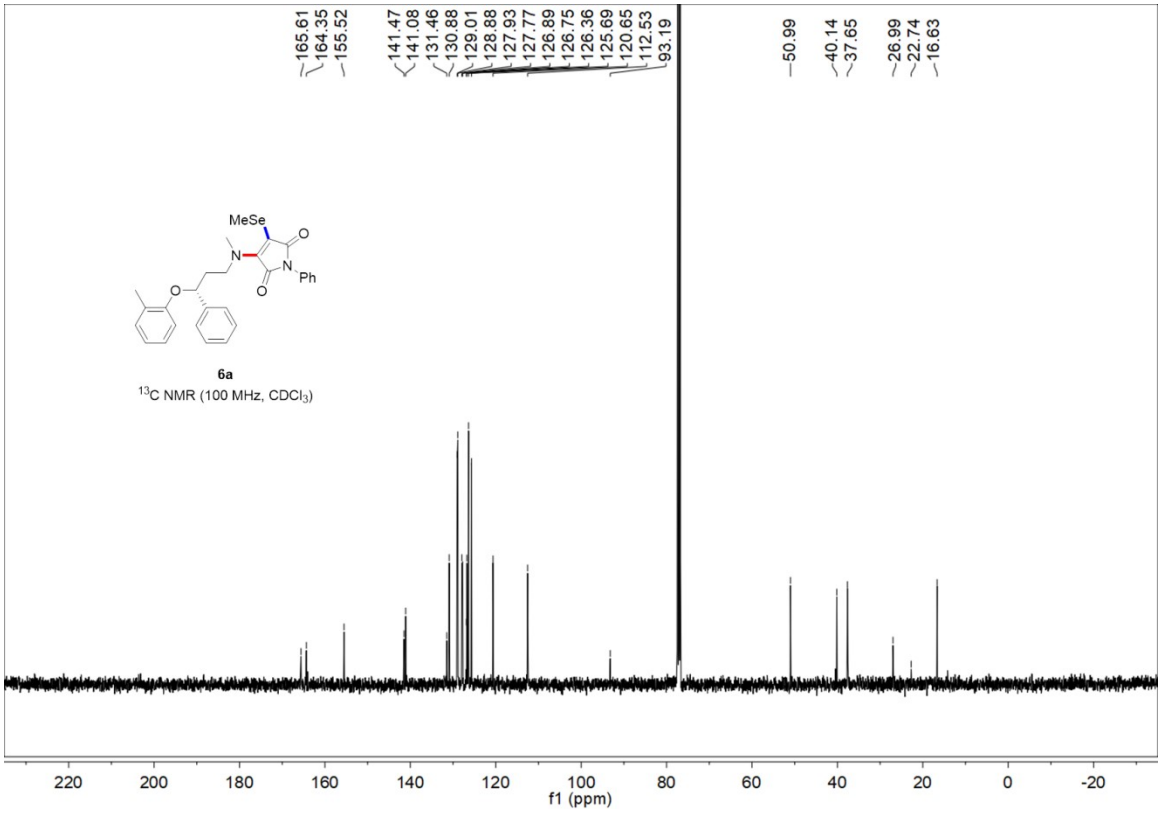
5l

^{13}C NMR (125 MHz, $CDCl_3$)



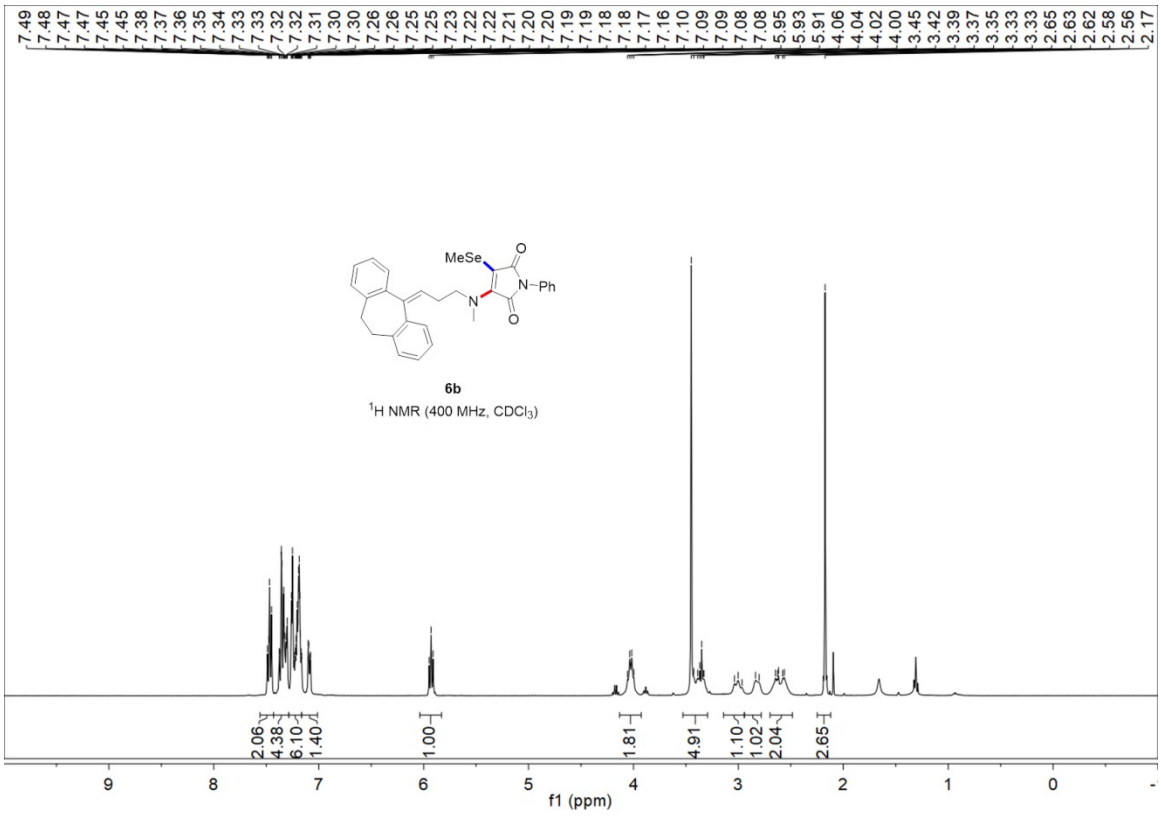
6a

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



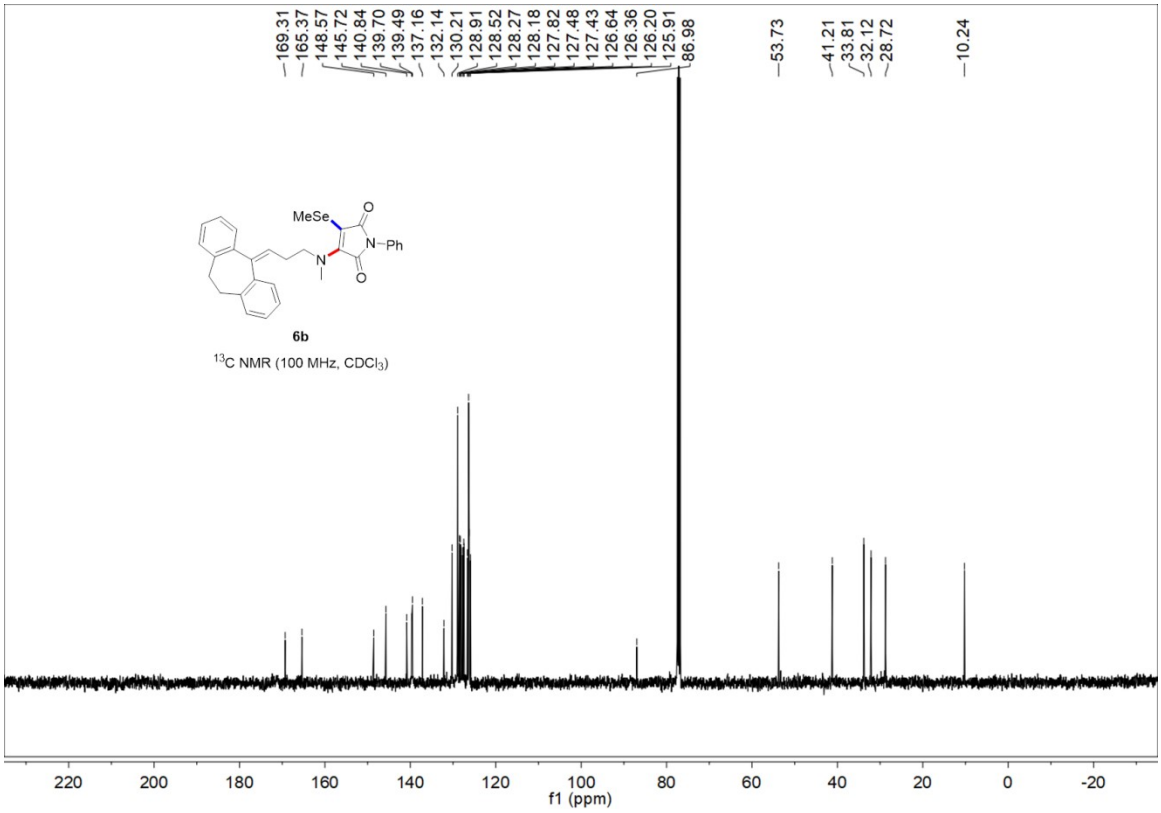
6a

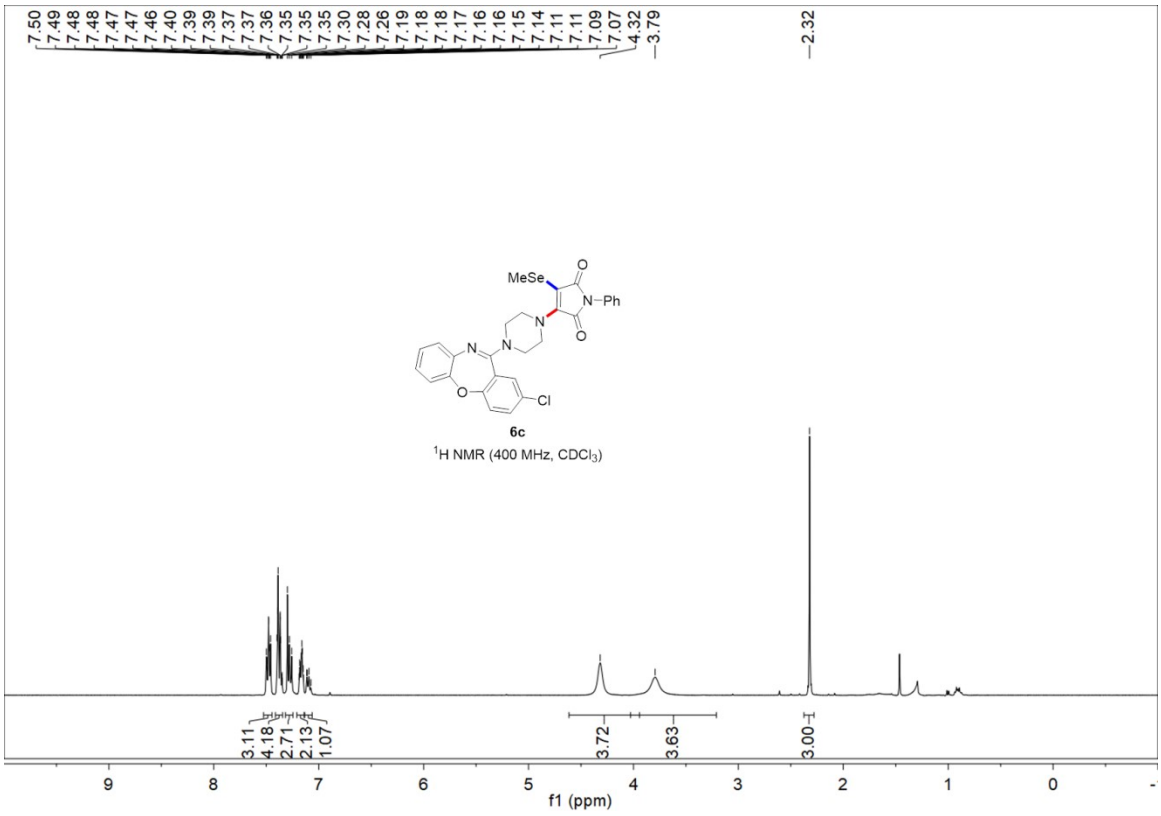
^{13}C NMR (100 MHz, $CDCl_3$)

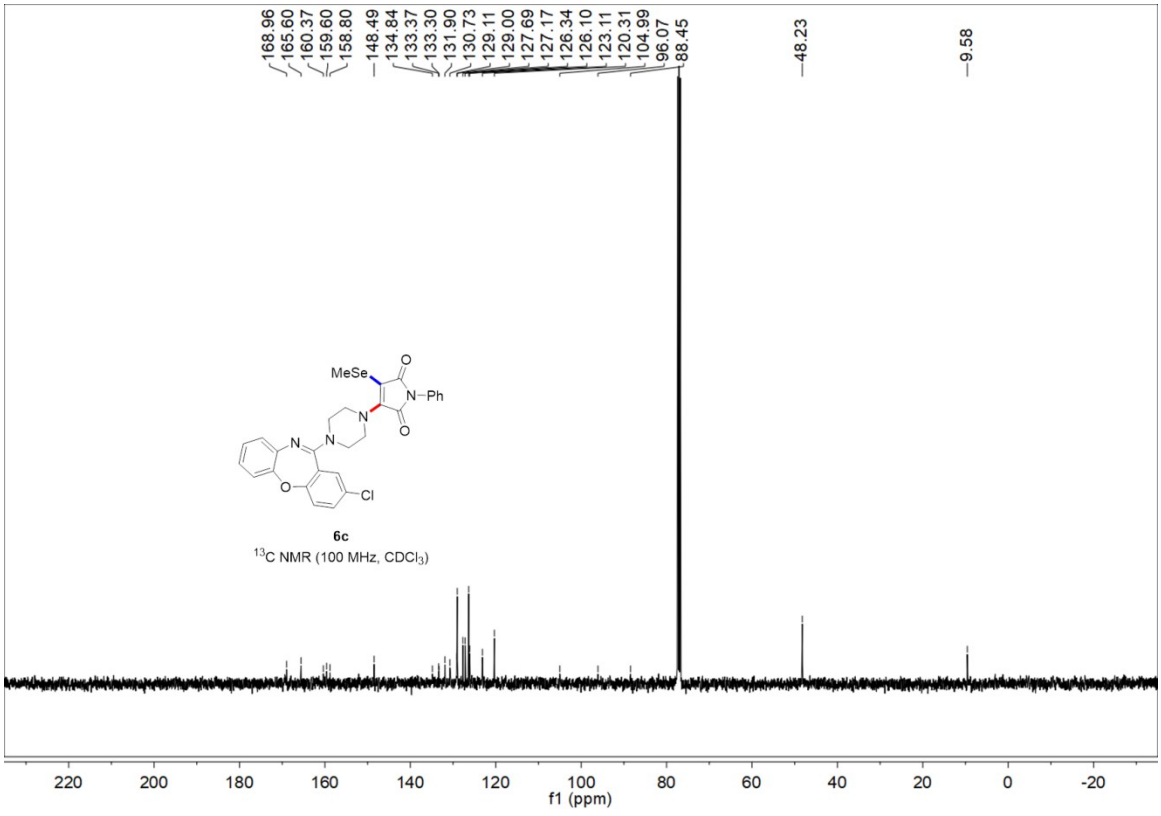


6b

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

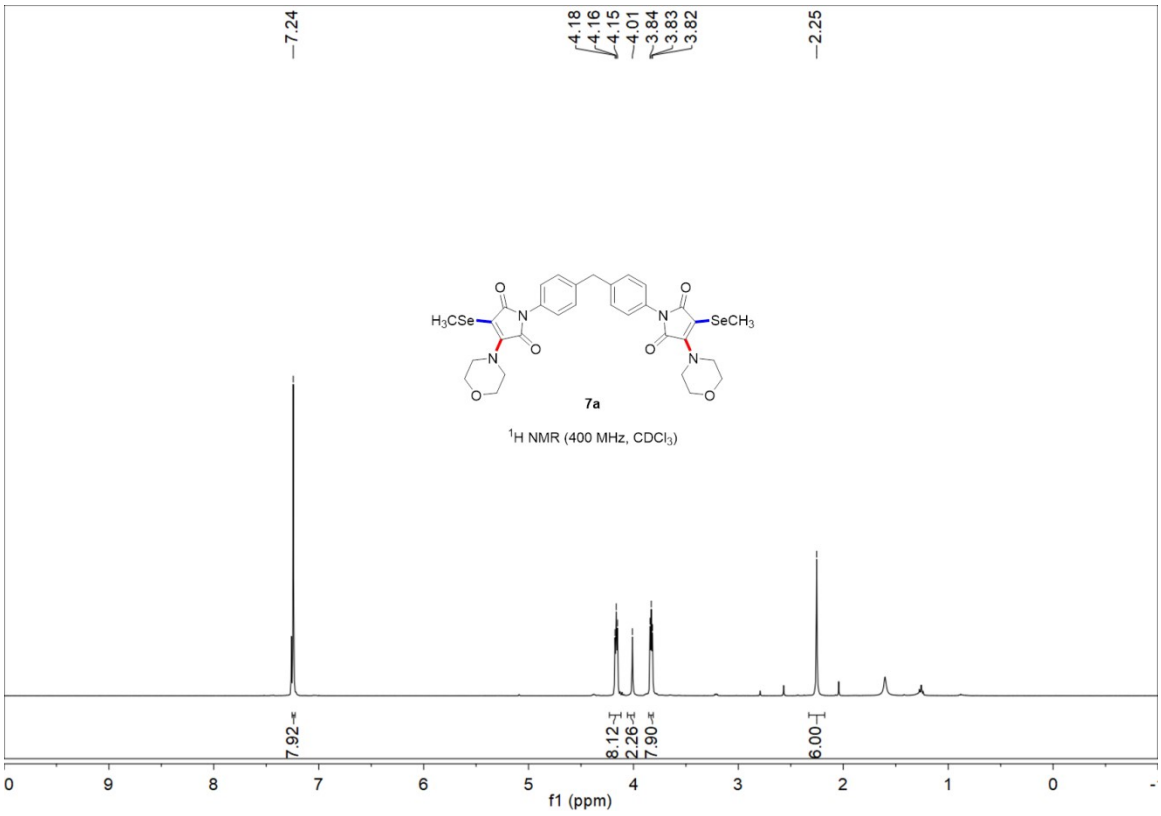

169.31
165.37
148.57
145.72
140.84
139.70
139.49
137.16
132.14
130.21
128.91
128.52
128.27
128.18
127.82
127.48
127.43
126.64
126.36
126.20
125.91
86.98
53.73
41.21
33.81
32.12
28.72
10.24
MeSe
N–Ph
N
O
O
O
6b
13C NMR (100 MHz, CDCl3)
220
200
180
160
140
120
100
80
60
40
20
0
-20
f1 (ppm)


7.50
7.49
7.48
7.48
7.47
7.47
7.46
7.40
7.39
7.39
7.37
7.37
7.36
7.35
7.35
7.35
7.30
7.28
7.26
7.19
7.18
7.18
7.17
7.16
7.16
7.15
7.14
7.11
7.11
7.09
7.07
4.32
3.79
2.32
MeSe
N–Ph
N
N
N
O
O
O
Cl
6c
1H NMR (400 MHz, CDCl3)
3.11
4.18
2.71
2.13
1.07
3.72
3.63
3.00
9
8
7
6
5
4
3
2
1
0
f1 (ppm)



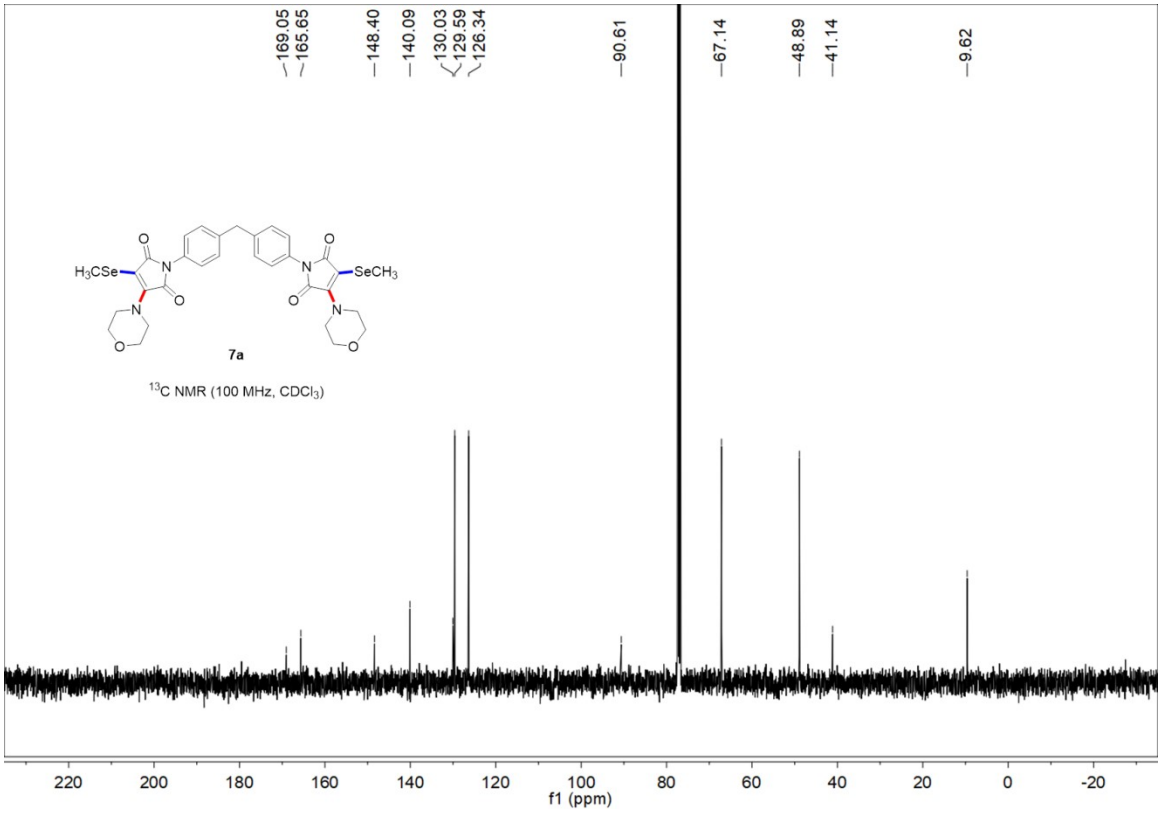
6c

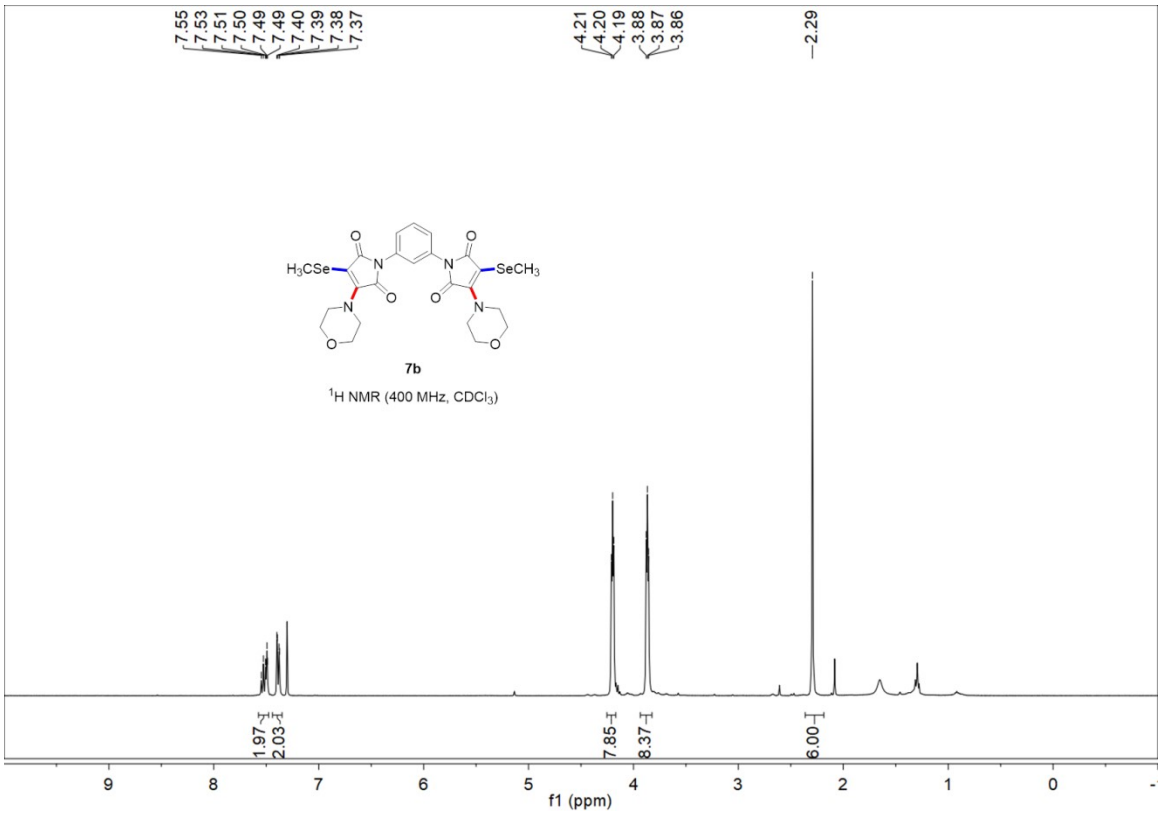
^{13}C NMR (100 MHz, $CDCl_3$)

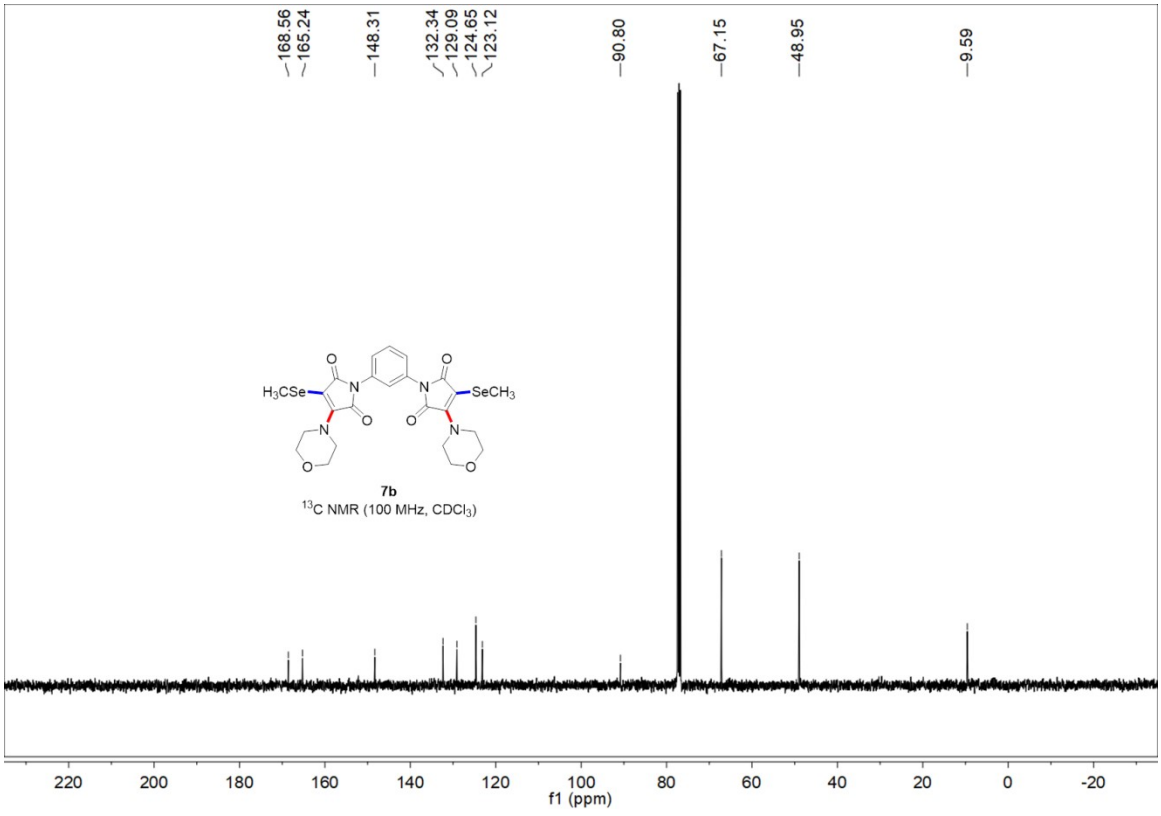


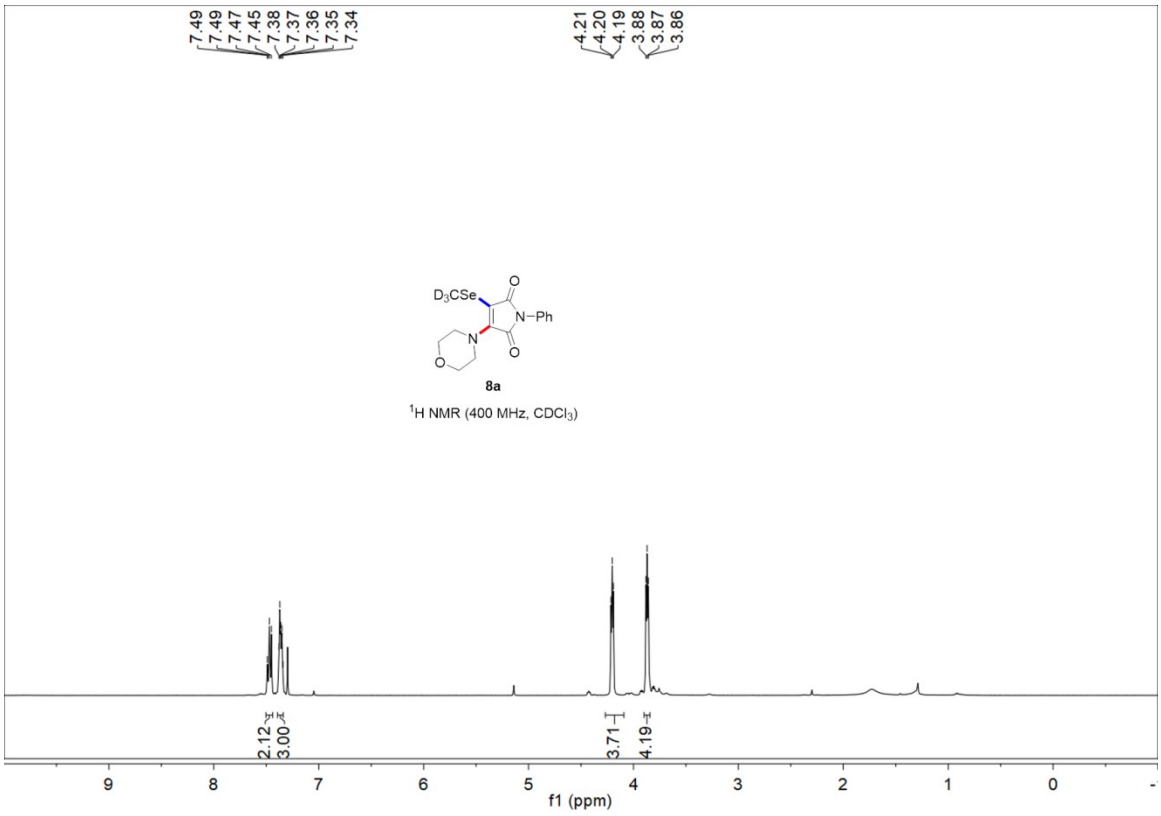
7a

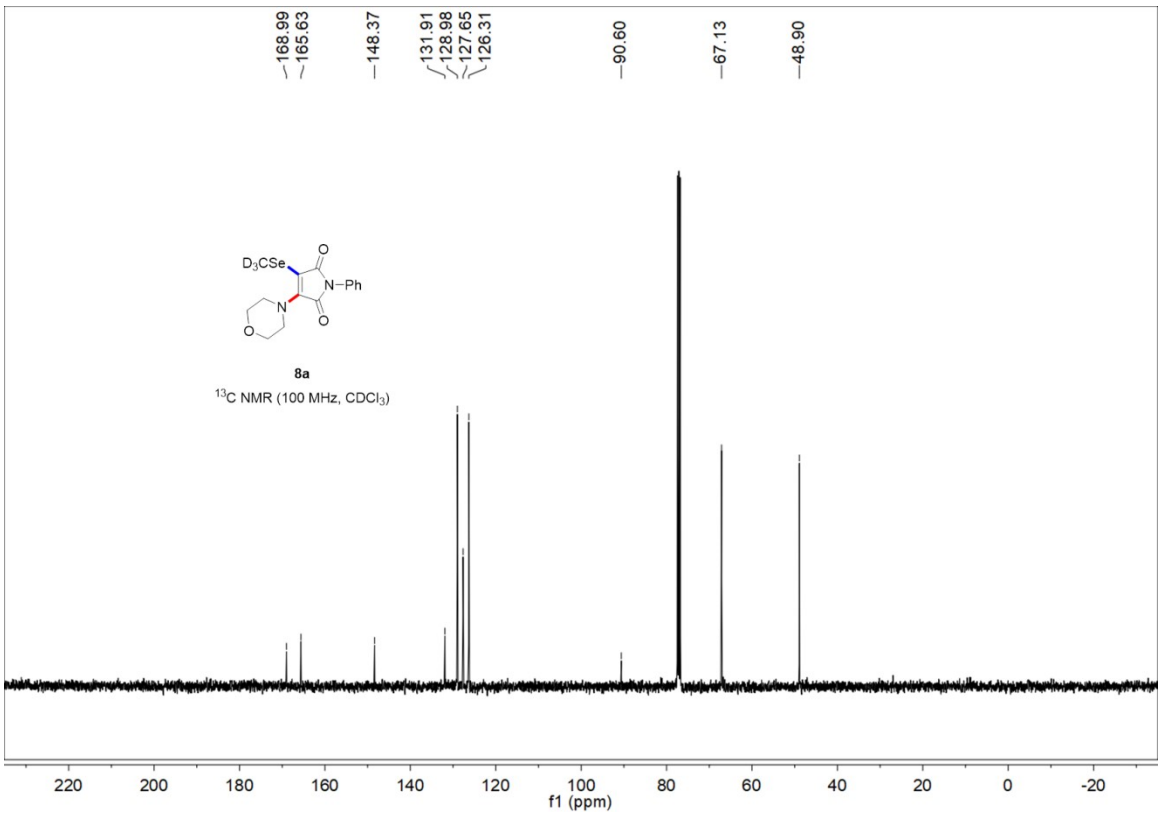
^{1}H NMR (400 MHz, $CDCl_3$)

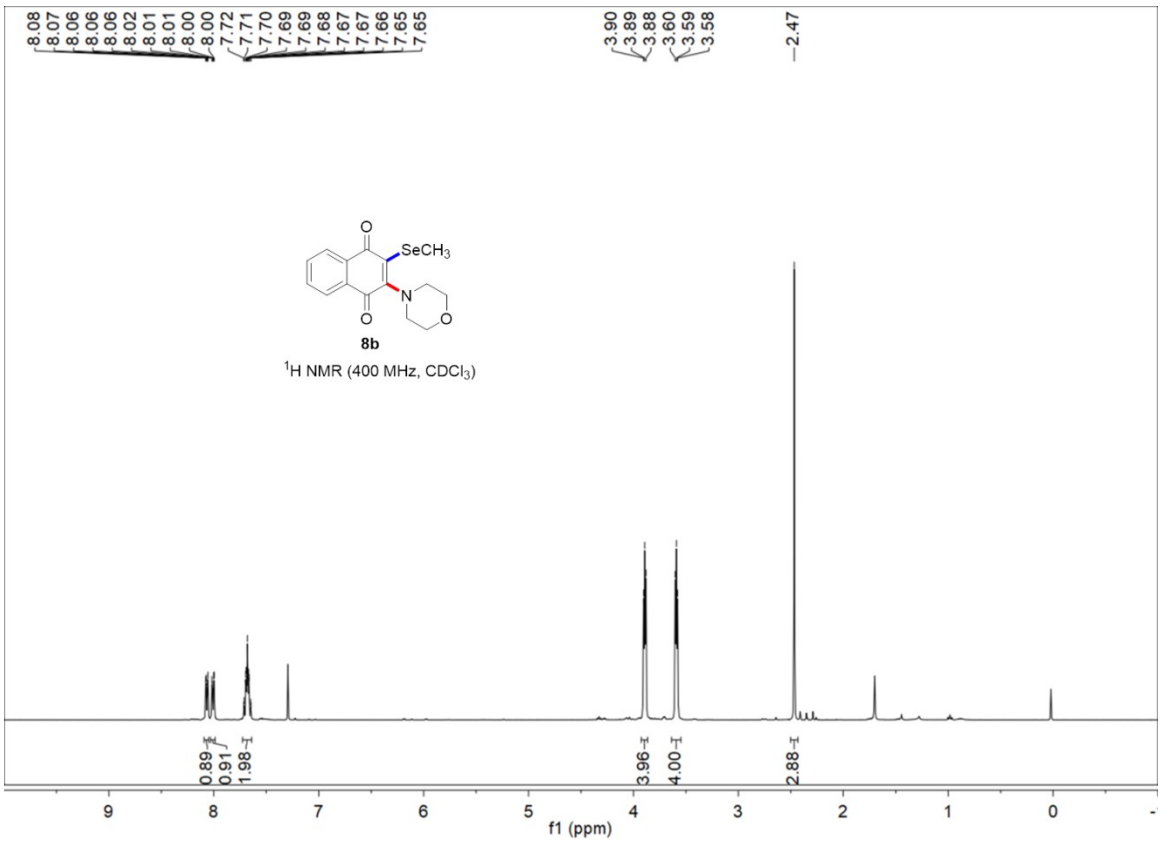

169.05
165.65
148.40
140.09
130.03
129.59
126.34
90.61
67.14
48.89
41.14
9.62
H3CSe
SeCH3
7a
13C NMR (100 MHz, CDCl3)
f1 (ppm)

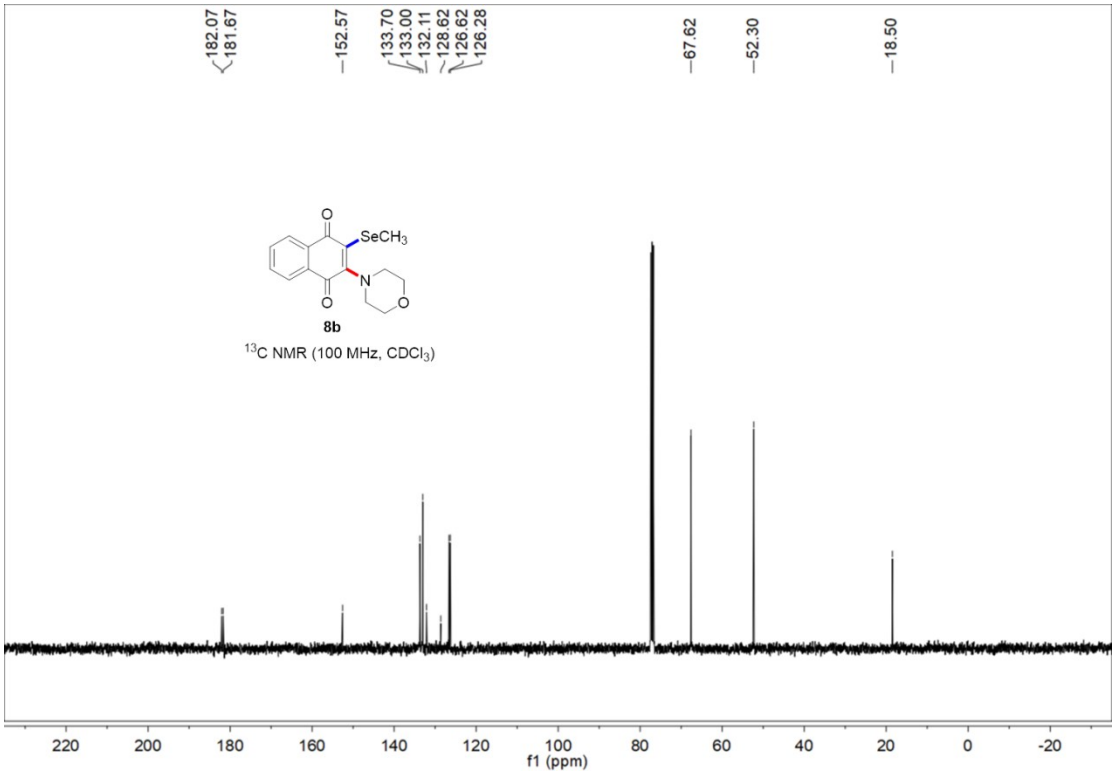

7.55
7.53
7.51
7.50
7.49
7.49
7.40
7.39
7.38
7.37
4.21
4.20
4.19
3.88
3.87
3.86
2.29
H3CSe
SeCH3
7b
1H NMR (400 MHz, CDCl3)
1.97
2.03
7.85
8.37
6.00
f1 (ppm)


168.56
165.24
148.31
132.34
129.09
124.65
123.12
90.80
67.15
48.95
9.59
H3CSe
SeCH3
7b
13C NMR (100 MHz, CDCl3)
220
200
180
160
140
120
100
80
60
40
20
0
-20
f1 (ppm)


7.49
7.49
7.47
7.45
7.38
7.37
7.36
7.35
7.34
4.21
4.20
4.19
3.88
3.87
3.86
D3CSe
N–Ph
8a
1H NMR (400 MHz, CDCl3)
2.12
3.00
3.71
4.19
9
8
7
6
5
4
3
2
1
0
f1 (ppm)


168.99
165.63
148.37
131.91
128.98
127.65
126.31
90.60
67.13
48.90
D3CSe
N–Ph
8a
13C NMR (100 MHz, CDCl3)
f1 (ppm)


8.08
8.07
8.06
8.06
8.06
8.02
8.01
8.01
8.00
8.00
7.72
7.71
7.70
7.69
7.69
7.68
7.67
7.67
7.66
7.65
7.65
3.90
3.89
3.88
3.60
3.59
3.58
2.47
SeCH3
8b
1H NMR (400 MHz, CDCl3)
0.89
0.91
1.98
3.96
4.00
2.88
f1 (ppm)


182.07
181.67
152.57
133.70
133.00
132.11
128.62
126.62
126.28
67.62
52.30
18.50
SeCH3
N
O
O
O
8b
13C NMR (100 MHz, CDCl3)
220
200
180
160
140
120
100
80
60
40
20
0
-20
f1 (ppm)