Supporting Information

Visible-Light-Mediated Aerobic Selenation of (hetero)arenes with Diselenides

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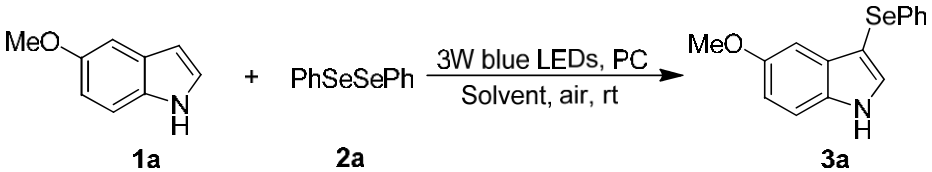
Table of Contents

1. General Considerations

Unless otherwise stated, all reactions were set up in a clear pyrex glass tube and were stirred with a Teflon-coated magnetic stir bar. Analytical grade solvents and commercially available reagents were used to conduct the reactions. Reactions were monitored by thin layer chromatography (TLC), and the products were obtained by column chromatography on silica gel (200-300 mesh) or aluminum oxide neutral (200-300 mesh). NMR spectra were recorded on Bruker AM-400 MHz spectrometer for proton and carbon magnetic resonance spectra (^{1}H NMR and ^{13}C NMR) in the solvent of $CDCl_3$ or $(CD_3)_2SO$ as the internal standard (^{1}H NMR: TMS at 0.00 ppm, $CDCl_3$ at 7.26 ppm, $(CD_3)_2SO$ at 2.50 ppm; ^{13}C NMR: $CDCl_3$ at 77.16 ppm, $(CD_3)_2SO$ at 39.52 ppm). In reporting spectral data the format (δ) chemical shift (multiplicity, *J* values in Hz, integration) was used with the following abbreviations: s = singlet, d = doublet, t = triplet, q = quartet, quint = quintuplet, m = multiplet. Mass spectra were reported in units of m/z, and were obtained with esquire6000, TRACE DSQ and ORBITRAP ELITE. UV-Vis spectra and luminescence spectra were recorded on UV-2600, RF-5301PC respectively. Infrared spectra (IR) were recorded on a Nicolet (NEXUS 670) spectrometer. X-ray crystal structure was recorded on Supernova.

2. Experimental Procedures

2.1. Condition screening for the catalytic system



1a **2a** **3a**

entry	catalyst	2a (equiv)	solvent	Yield[b] (%)
1	Rhodamine B	0.5	CH_3CN	37
2	*fac*-$(Irppy)_3$	0.5	CH_3CN	67

3	Na_2-eosin Y	0.5	CH_3CN	79
4	$Ru(bpy)_3Cl_2$	0.5	CH_3CN	81
5	FIrPic	0.5	CH_3CN	84
6	FIrPic	0.5	DCM	9
7	FIrPic	0.5	DCE	53
8	FIrPic	0.5	DMSO	33
9	FIrPic	0.5	THF	15
10	FIrPic	0.5	DMF	44
11	FIrPic	0.5	acetone	61
12	FIrPic	0.6	CH_3CN	91
13	FIrPic	0.7	CH_3CN	93
14[c]		0.6	CH_3CN	47
15[d]	FIrPic	0.6	CH_3CN	0

[a] Reaction conditions:**1a** (0.2 mmol), solvent (2 mL), **PC** (2 mol %), air. [b] Isolated yield. [c] Reaction was carried out without FIrPic. [d] Reaction was carried out in the dark. The p-rogress of the reaction was monitored by TLC.

2.2. General procedure for the synthesis of starting materials

2.2.1. General procedure for the synthesis of diselenides [1]

To a stirred solution of Se^0 metal (10.0 mmol) and halides (5.0 mmol) in dry DMSO (10.0 mL) was added CuO nanoparticles (10.0 mol %) followed by KOH (2.0 equiv) under nitrogen atmosphere at 90 ºC. The progress of the reaction was monitored by TLC. After the reaction was complete, the reaction mixture was allowed to cool, which was subjected to column chromatographic separation to give pure Diselenides. The identity and purity of the product was confirmed by ^{1}H NMR, ^{13}C NMR and Mass spectra analysis.

2.2.2. General procedure for the synthesis of indole derivatives

***N*-Phenyl-1*H*-indole:** According to a procedure by Glorius *et al.*,[2] indole (490 mg, 4.2 mmol, 1.4 eq), iodobenzene (333 μL, 3.0 mmol, 1.0 eq), copper(I) iodide (115 mg,

0.6 mmol, 20 mol%) and cesium carbonate (1.96 g, 6.0 mmol, 2.0 eq) were stirred for 16 h at 120 °C in DMF (6 mL). After cooling down to room temperature, the reaction mixture was diluted with EtOAc (30 mL) and washed with water (2 x 20 mL). The combined aqueous layer was reextracted with EtOAc (2 x 20 mL). The combined organic layer was dried over Na_2SO_4, filtered and concentrated in vacuo. Purification by silica-gel chromatography (n-pentane) afforded the product as a colorless oil (556 mg, 2.9 mmol, 96%). The identity and purity of the product was confirmed by ^{1}H NMR, ^{13}C NMR and Mass spectra analysis.

***N*-Benzyl-1*H*-indole:** According to a procedure by Glorius *et al*., [2] sodium hydride (60% in mineral oil, 144 mg, 3.6 mmol, 1.2 eq) was added at 0 °C to a solution of indole (352 mg, 3.0 mmol, 1.0 eq) in DMF (3 mL). The reaction mixture was allowed to warm up to room temperature and was stirred for 30 min. At 0 °C, benzyl bromide (400 µL, 3.3 mmol, 1.1 eq) was added. The reaction mixture was allowed to warm up to room temperature and was stirred for 16 h. Water (5 mL) was added and the aqueous layer was extracted with EtOAc (3 x 10 mL). The combined organic layer was washed with brine (20 mL), dried over Na_2SO_4, filtered and concentrated in vacuo. Purification by silica-gel chromatography (2% EtOAc in n-pentane) afforded the product as a colorless oil (341 mg, 1.7 mmol, 55%). The identity and purity of the product was confirmed by ^{1}H NMR, ^{13}C NMR and Mass spectra analysis.

2-Hexyl-1*H*-indole: According to a procedure by Ramón *et al*., [3] to a stirred solution of the corresponding 2-iodoaniline (1 mmol) in toluene (3 mL) under argon atmosphere were added Pd/CuOeFe$_3$O$_4$ (50 mg), NaOH (10 mmol), and the corresponding alkyne (1.5 mmol). The resulting mixture was stirred at 130 °C until the end of reaction. The catalyst was removed by a magnet and the resulting mixture was quenched with water and extracted with EtOAc. The organic phases were dried over $MgSO_4$, followed by evaporation under reduced pressure to remove the solvent. The product was purified by chromatography on silica gel (hexane/ethyl acetate) to give 2-(Oct-1-yn-1-yl)aniline. Then, to a stirred solution of 2-(Oct-1-yn-1-yl)aniline (1 mmol) in toluene (4 mL) was added $ZnBr_2$ (225 mg, 1 mmol). The resulting

mixture was stirred at 130 °C during 24 h. The mixture was quenched with water and extracted with EtOAc. The organic phases were dried over $MgSO_4$, followed by evaporation under reduced pressure to give the pure products.

***N*-methyl-7-azaindoles:** According to a procedure by Das *et al*., [4] a dried round bottom flask equipped with a magnetic stirrer bar was charged 7-azaindole (1g, 8.47 mol) and DMF (5 mL) under nitrogen atmosphere. The reaction mixture was cool down to 0 ^{o}C and NaH (1.2 equiv) was added and stirred for 1 h. After 1 h stirring alkyl methyl iodide (1.1 equiv) was added and continued the stirring for another 1 h. After completion of the reaction it was quenched with ice cold water (50 mL) and was extracted with ethyl acetate (3 x 50 mL). The combined organic layer was dried over Na_2SO_4 the solvent was removed under reduced pressure to give N-methyl-7-azaindoles in quantitative yield. The identity and purity of the product was confirmed by ^{1}H NMR, ^{13}C NMR and Mass spectra analysis.

2.2.3. General procedure for the synthesis of imidazoheterocycles

Imidazo[1,2-a]pyridines: According to a procedure by Kumar *et al*., [5] a clean oven-dried 50 mL round bottom flask was charged with acetophenone (10.0 mmol), 2-amino pyridine (12.0 mmol), CuI (2.0 mmol) and 1,4-dioxane (30.0 mL). The resulting solution was stirred at 100 ºC under ambient air. On completion, the reaction mass was evaporated to dryness. The crude residue was purified by column chromatography to obtain tandem product. The identity and purity of the product was confirmed by ^{1}H NMR, ^{13}C NMR and Mass spectra analysis.

2.3. General procedure for selenylation of aromatics

A 10 mL a clear pyrex glass tube and was stirred with a Teflon-coated magnetic stir bar. Diselenide derivatives (0.12 mmol, 0.6 eq) and FIrPic (2 mol %) were added to the solution of aromatics (0.2 mmol, 1 eq) in MeCN. Under visible-light generated from 3W blue LEDs, the reaction mixture was stirred at 25 °C in the air. The reaction was monitored by TLC, after completion of the reaction, the solvent was removed under reduced pressure by rotary evaporator. Then, the residue was purified by silica

gel column chromatography to give the desired product.

3. X-ray Crystal Structure

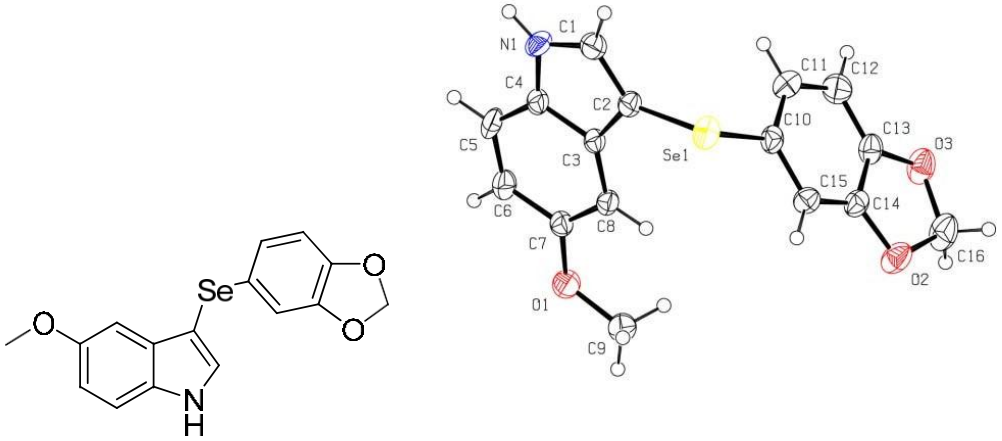


Figure S1. X-ray crystal structure of **3ak**.

4. Mechanism Studies

4.1. Photophysical properties

4.1.1. UV-Vis absorption spectra

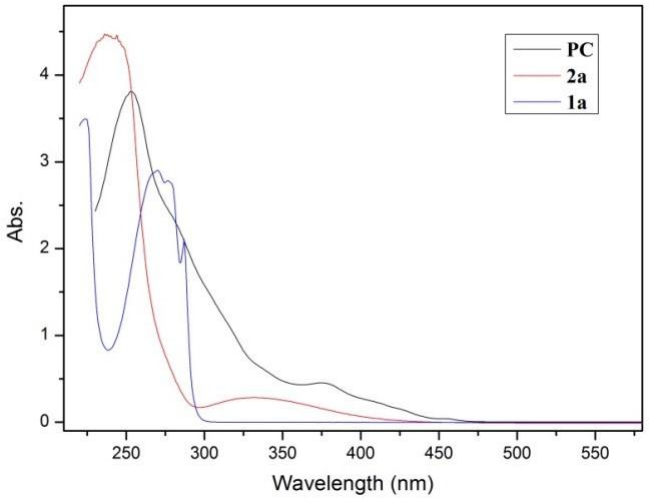


Figure S2. UV-Vis absorption spectra of **1a:** 5-Methoxyindole, **2a:** Diphenyl diselenide and **PC:** FIrPic in MeCN.

4.1.2. Emission Quenching experiments for PC

Emission intensities were recorded using a RF-5301PC Fluorescence Spectrometer. CH_3CN was degassed with a stream of Ar for 30 min. All the solutions were prepared under Ar atmosphere. In a typical experiment, the emission spectrum of a 1×10^{-4} M solution of PC in CH_3CN was collected. Then, appropriate amount of quencher was added to the measured solution and the emission spectrum of the sample was collected. Here I_0 and I represent the intensities of the emission in the absence and presence of the quencher.

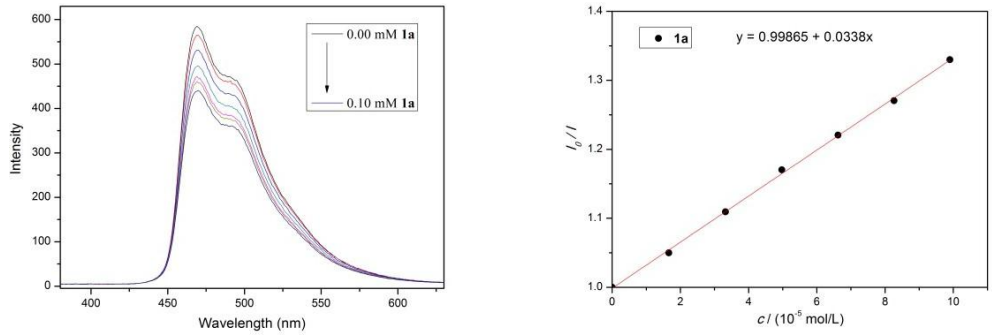


Figure S3. The emission quenching of FIrPic by **1a**

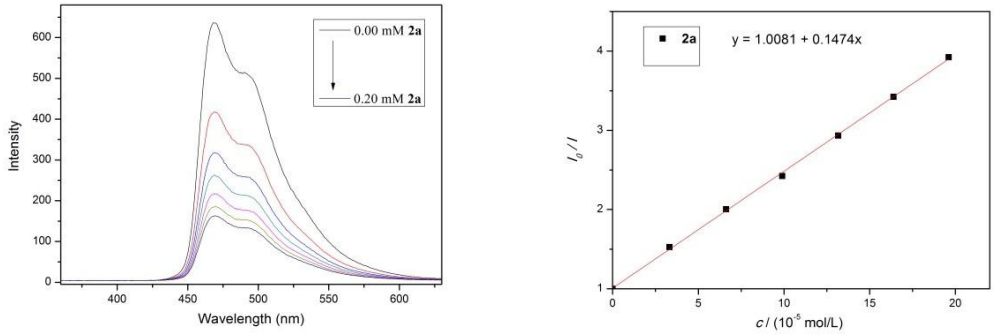
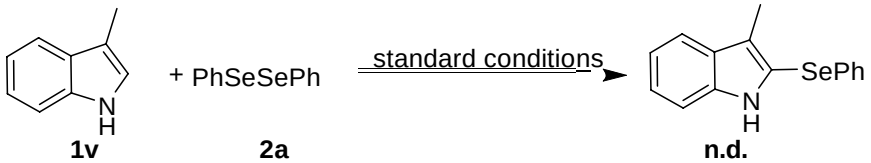


Figure S4. The emission quenching of FIrPic by **2a**

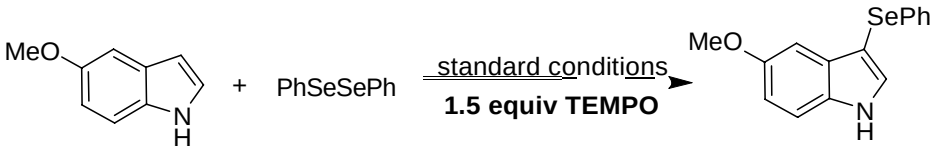
4.2. Control Experiments



1v **2a** **n.d.**

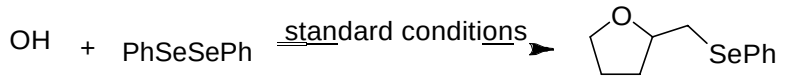
A 10 mL a clear pyrex glass tube and was stirred with a Teflon-coated magnetic stir

bar. Diphenyl diselenide (0.12 mmol, 0.6 eq) and FIrPic (2 mol %) were added to the solution of 3-methylindole (0.2 mmol, 1 eq) in MeCN. The reaction mixture was stirred at 25 °C in the air and irradiated by 3W blue LEDs. The reaction was monitored by TLC, after 36 h, no products were obtained.



1a **2a** **3aa**, 58 %

A 10 mL a clear pyrex glass tube and was stirred with a Teflon-coated magnetic stir bar. Diphenyl diselenide (0.12 mmol, 0.6 eq), FIrPic (2 mol %) and TEMPO (0.3 mmol, 1.5 eq) were added to the solution of 5-methoxyindole, (0.2 mmol, 1 eq) in MeCN. The reaction mixture was stirred at 25 °C in the air and irradiated by 3W blue LEDs. The reaction was monitored by TLC, after completion of the reaction, the solvent was removed under reduced pressure by rotary evaporator. Then, the residue was purified by silica gel column chromatography to give the desired product, (35.3 mg, Yield: 58%).



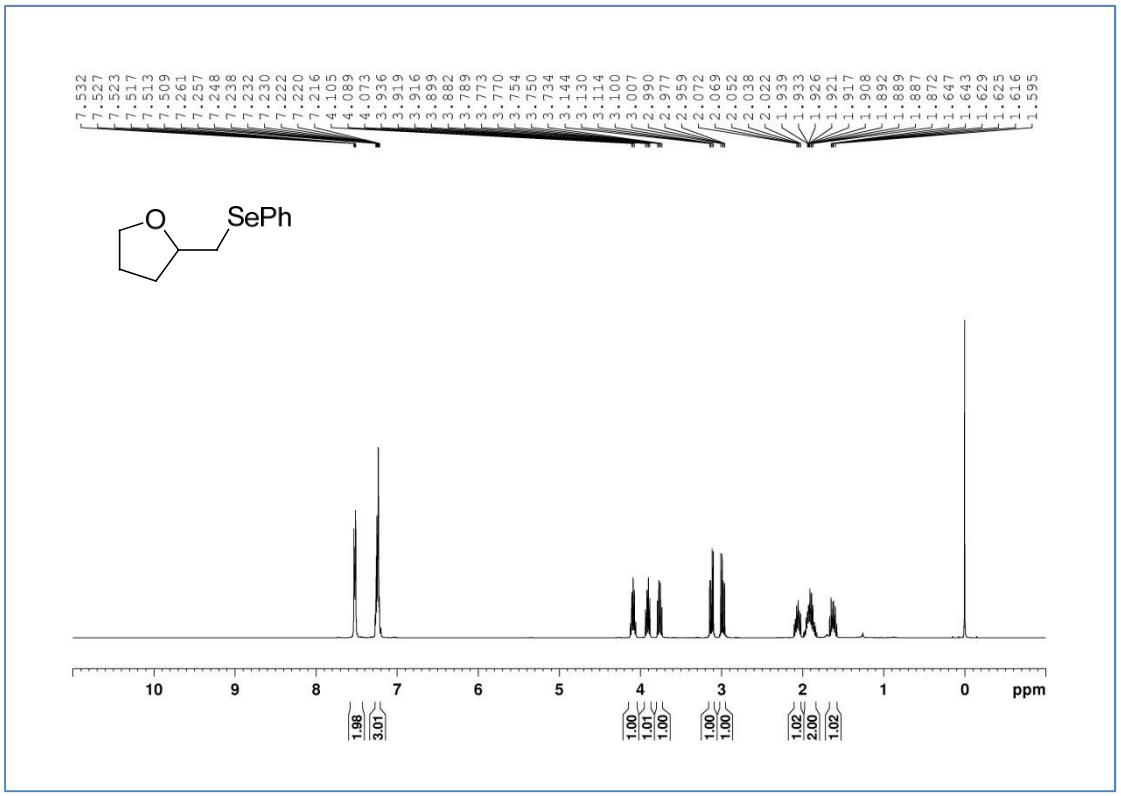
6a **2a** **7aa**, 53 %

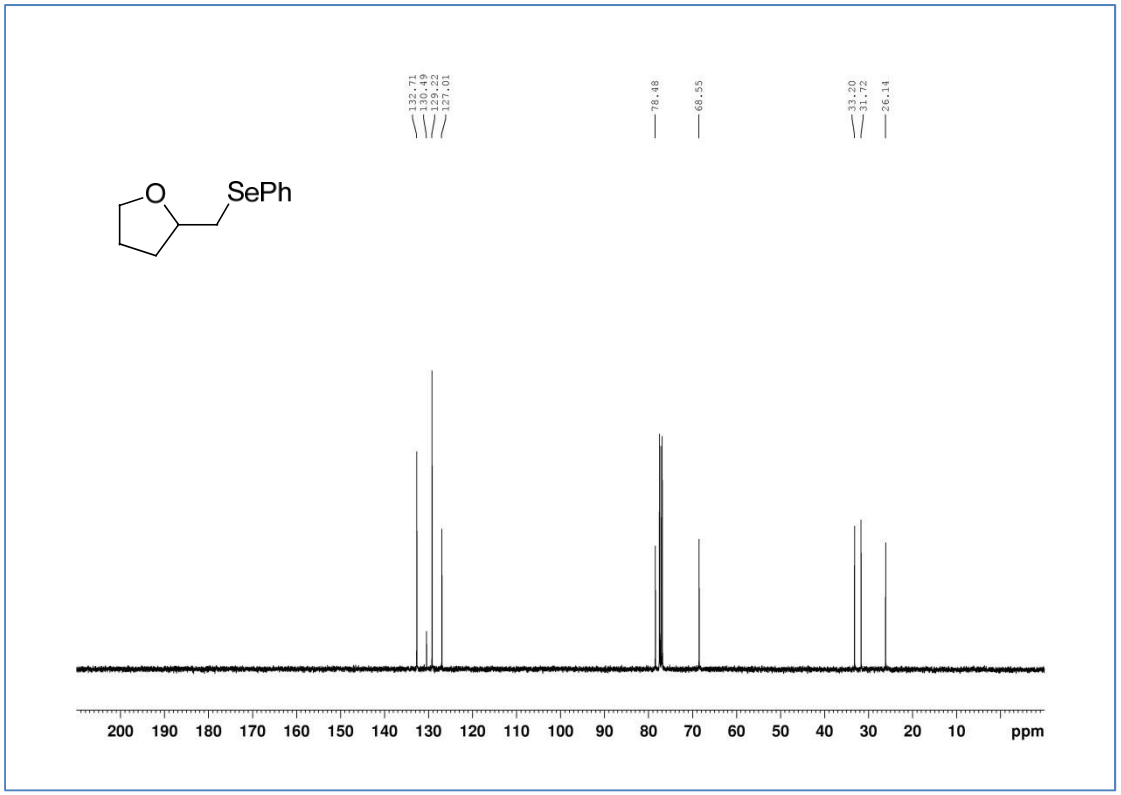
A 10 mL a clear pyrex glass tube and was stirred with a Teflon-coated magnetic stir bar. Diphenyl diselenide (0.12 mmol, 0.6 eq) and FIrPic (2 mol %) were added to the solution of 4-penten-1-ol (0.2 mmol, 1 eq) in MeCN. The reaction mixture was stirred at 25 °C in the air and irradiated by 3W blue LEDs. The reaction was monitored by TLC, after completion of the reaction, the solvent was removed under reduced pressure by rotary evaporator. Then, the residue was purified by silica gel column chromatography to give the desired product, (25.8 mg, Yield: 53 %).

^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.53 – 7.51 (m, 2H), 7.26 – 7.22 (m, 3H), 4.09 (t, J = 6.4 Hz, 1H), 3.94 – 3.88 (m, 1H), 3.79 – 3.73 (m, 1H), 3.14 (dd, J = 12.0 Hz, 1H), 3.01 (dd, J = 12.0 Hz, 1H), 2.07 – 2.02 (m, 1H), 1.94 – 1.87 (m, 2H), 1.65 – 1.60 (m, 1H); **^{13}C NMR ($CDCl_3$, 100 MHz)** δ 132.7, 130.5, 129.2, 127.0, 78.5, 68.6, 33.2,

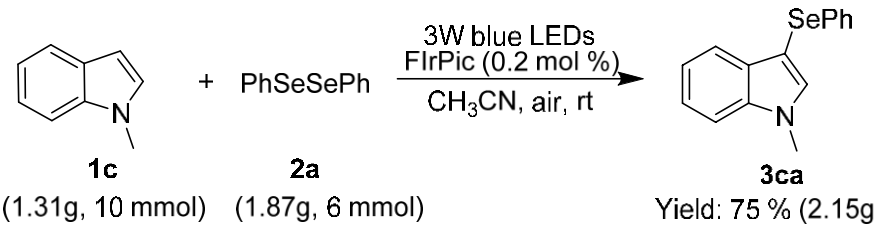
31.7, 26.1; **EI-MS**: m/z $[M+Na]^+$ 265.0.

^{1}H and ^{13}C NMR:





5. Gram-Scale Selenation of 1c



1c (1.31g, 10 mmol) **2a** (1.87g, 6 mmol) **3ca** Yield: 75 % (2.15g)

A 100 mL a clear pyrex glass tube and was stirred with a Teflon-coated magnetic stir bar. Diphenyl diselenide (6.0 mmol, 0.6 eq) and FIrPic (0.2 mol %) were added to the solution of *N*-methylindole (10 mmol, 1 eq) in MeCN. The reaction mixture was stirred at 25 °C in the air and irradiated by 3W blue LEDs. The reaction was monitored by TLC, after 48 h, the solvent was removed under reduced pressure by rotary evaporator. Then, the residue was purified by silica gel column chromatography to give the desired product.

6. Biochemical Studies

Experiment method:

1×10^4 cells were incubated with target compounds (0, 10, 20, 50 μM) for 48 h in triplicate in a 96-well plate for the indicated times at 37 ℃ in a final volume of 100 μl. Cells treated with DMSO alone were used as controls. After 44 h, 10 μl MTT (5 mg/ml) was added to each well and incubated for an additional 4 h at 37 ℃. An extraction buffer (100 μl, 10% SDS, 5% isobutanol, 0.1% HCl) was added, and the cells were incubated overnight at 37 ℃. The absorbance was measured at 570 nm using a microplate reader (Thermo Scientific Multiskan GO, Finland).

Table 1. In vitro cell growth inhibition by the target compounds

compd	IC_{50} (M)	
	HeLa	HepG2
3oa	15.7	>50
3ma	14.5	>50
3ba	42.1	>50
3sa	31.8	30.5
3qa	38.2	37.6
3ra	>50	>50
3ha	>50	>50

2a	>50	>50
3al	6.3	24.4
2l	29.6	41.4
3af	12.2	19.1

[a] IC_{50}: concentration of the compound (mM) producing 50% cell growth inhibition after 48 h of drug exposure, as determined by the MTT assay. Each experiment was carried out in triplicate.

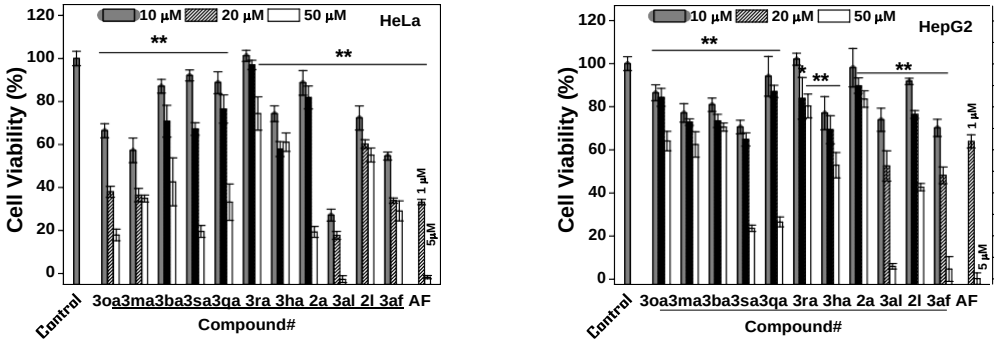
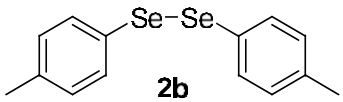


Figure S5. Cytotoxicity Screening of Compounds.

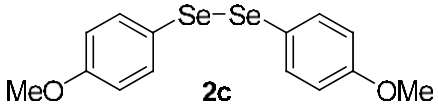
7. Characterization Data

7.1. Characterization data of starting materials



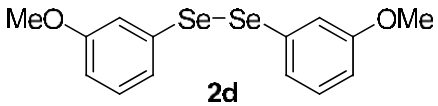
1,2-di-p-tolyldiselane (**2b)**[1]: red liquid.

^{1}H NMR (CDCl$_3$, 400 MHz) δ 7.52 (d, *J* = 8.0 Hz, 4H), 7.10 (d, *J* = 8.0 Hz, 4H), 2.36 (s, 6H); **^{13}C NMR (CDCl$_3$, 100 MHz)** δ 138.2, 133.6, 132.5, 130.1, 21.3. **EI-MS**: m/z (relative intensity, %) 342 (73.83), 340 (70.03), 338 (42.77), 182 (58.11), 171 (100.00), 169 (55.45), 167 (35.82), 91 (71.05).



1, 2-bis(4-methoxyphenyl)diselane (**2c**) [1]: yellow solid.

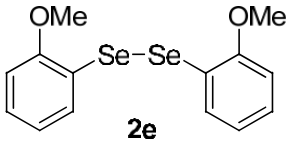
^{1}H NMR (CDCl$_3$, 400 MHz) δ 7.53 (d, *J* = 8.8 Hz, 4H), 6.83 (d, *J* = 8.8 Hz, 4H), 3.82 (s, 6H); **^{13}C NMR (CDCl$_3$, 100 MHz)** δ 160.1, 135.5, 122.0, 114.8, 55.3. **EI-MS**: m/z (relative intensity, %) 374 (26.71), 372 (24.44), 189 (17.71), 187 (100.00), 185 (50.62), 184 (20.92), 183 (20.78), 172 (18.20).



2d

1,2-bis(3-methoxyphenyl)diselane (**2d**)[1]: red liquid.

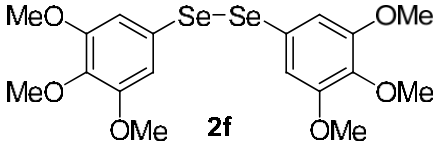
^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.29 – 7.24 (m, 4H), 6.99 (t, *J* = 8.0 Hz, 2H), 6.88 – 6.85 (m, 2H), 3.77 (s, 6H); **^{13}C NMR ($CDCl_3$, 100 MHz)** δ 136.4, 133.2, 133.0, 132.7, 130.5, 118.2, 111.4. **EI-MS**: m/z (relative intensity, %) 374 (45.16), 372 (39.21), 370 (22.75), 294 (50.66), 293 (20.29), 292 (28.65), 214 (100.00), 187 (42.73), 185 (25.79).



2e

1,2-bis(3-methoxyphenyl)diselane (**2e**)[1]: yellow solid. yellow solid.

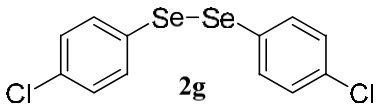
^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.59 (dd, *J* = 8.0 Hz, 2H), 7.25 – 7.21 (m, 2H), 6.91 – 6.87 (m, 2H), 6.85 – 6.83 (dd, *J* = 8.0 Hz, 2H), 3.93 (s, 6H); **^{13}C NMR ($CDCl_3$, 100 MHz)** δ 157.1, 130.8, 128.4, 122.1, 118.9, 110.4, 56.1. **EI-MS**: m/z (relative intensity, %) 374 (100.00), 372 (91.63), 370 (52.75), 207 (28.44), 186 (49.38), 185 (34.01), 159 (52.02), 157 (60.05), 107 (62.45), 78 (39.96), 77 (47.12).



2f

1,2-bis(3,4,5-trimethoxyphenyl)diselane (**2f**)[14]: yellow solid.

^{1}H NMR ($CDCl_3$, 400 MHz) δ 6.85 (s, 4H), 3.83 (s, 6H), 3.81 (s, 12H); **^{13}C NMR ($CDCl_3$, 100 MHz)** δ 153.4, 138.6, 125.5, 110.4, 61.2, 56.4. **EI-MS**: m/z (relative intensity, %) 494 (16.99), 492 (15.62), 249 (17.77), 247 (100.00), 245 (49.25), 244 (19.88), 243 (19.80), 232 (24.01).

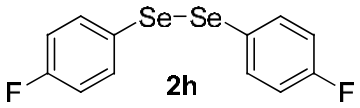


2g

1,2-bis(4-chlorophenyl)diselane (**2g**)[1]: yellow solid.

^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.52 (d, *J* = 8.8 Hz, 4H), 7.25 (d, *J* = 8.4 Hz, 4H); **^{13}C NMR ($CDCl_3$, 100 MHz)** δ 134.5, 133.5, 129.6, 129.0. **EI-MS**: m/z (relative

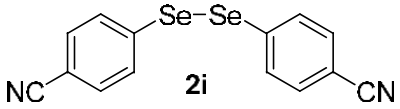
intensity, %) 384 (25.64), 382 (39.87), 380 (29.22), 222 (24.81), 193 (42.70), 191 (100.00), 189 (50.07), 156 (35.46).



2h

1,2-bis(4-fluorophenyl)diselane (**2h**)[6]: red liquid.

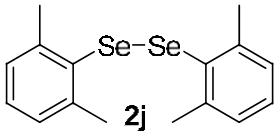
^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.65 – 7.62 (m, 4H), 6.86 – 6.82 (m, 4H); **^{13}C NMR ($CDCl_3$, 100 MHz)** δ 164.4 (d, *J* = 247 Hz), 135.1 (d, *J* = 8 Hz), 125.8 (d, *J* = 4 Hz), 116.7 (d, *J* = 22 Hz). **EI-MS**: m/z (relative intensity, %) 350 (44.89), 348 (38.24), 346 (22.53), 190 (16.49), 177 (16.53), 175 (100.00), 173 (44.53), 172 (17.32), 171 (18.82), 83 (17.75).



2i

4,4'-diselanedibenzonitrile (**2i**)[9]: yellow solid.

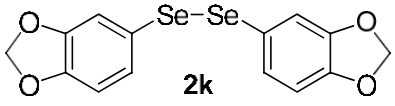
^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.70 (d, *J* = 8.4 Hz, 4H), 7.56 (d, *J* = 8.4 Hz, 4H); **^{13}C NMR ($CDCl_3$, 100 MHz)** δ 136.6, 133.4, 132.9, 130.7, 118.4. **EI-MS**: m/z (relative intensity, %) 364 (10.51), 284 (44.22), 283 (11.70), 282 (24.12), 281 (11.57), 205 (14.31), 204 (100.00), 182 (37.14), 180 (20.61), 44 (24.80).



2j

1,2-bis(2, 6-dimethylphenyl)diselane (**2j**)[7]: yellow solid.

^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.13 – 7.10 (m, 2H), 7.04 (d, *J* = 7.2 Hz, 4H), 2.29 (s, 12H); **^{13}C NMR ($CDCl_3$, 100 MHz)** δ 144.0, 132.2, 129.4, 127.6, 24.4. **EI-MS**: m/z (relative intensity, %) 370 (63.57), 368 (56.04), 366 (34.60), 185 (61.97), 184 (92.65), 183 (50.73), 182 (55.94), 105 (100.00), 91 (32.93).

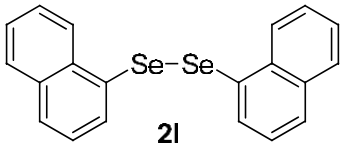


2k

1,2-bis(benzo[*d*][1,3]dioxol-5-yl)diselane (**2k**)[13]: yellow solid.

^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.11 (d, *J* = 1.6 Hz, 2H), 7.08 (dd, *J* = 8.0 Hz, 2H), 6.73 (d, *J* = 8 Hz, 2H), 5.98 (s, 4H); **^{13}C NMR ($CDCl_3$, 100 MHz)** δ 148.5, 148.3,

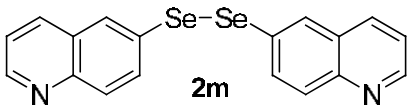
127.7, 123.1, 114.2, 109.0, 101.6. **EI-MS**: m/z (relative intensity, %) 402 (25.82), 400 (23.94), 203 (19.08), 201 (100.00), 199 (46.11), 198 (21.88), 197 (20.72), 44 (19.00).



2l

1,2-di(naphthalen-1-yl)diselane (**2l**)[6]: yellow solid.

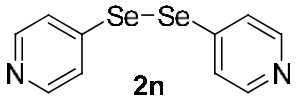
^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.21 (d, *J* = 8.4 Hz, 2H), 7.83 – 7.80 (m, 4H), 7.77 – 7.76 (m, 2H), 7.50 – 7.46 (m, 2H), 7.43 – 7.39 (m, 2H), 7.28 – 7.24 (m, 2H); **^{13}C NMR ($CDCl_3$, 100 MHz)** δ 134.3, 134.2, 134.1, 130.2, 130.0, 128.7, 128.2, 126.9, 126.5, 125.8; **EI-MS**: m/z (relative intensity, %) 414 (25.91), 412 (26.09), 254 (32.60), 253 (22.27), 208 (24.00), 207 (100.00), 205 (51.66), 204 (31.18), 128 (23.39), 115 (79.44), 44 (31.46).



2m

1,2-di(quinolin-6-yl)diselane (**2m**): yellow solid.

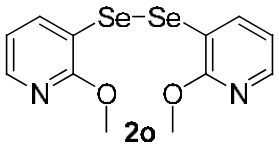
^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.90 (dd, *J* = 4.0 Hz, 2H), 8.04 - 8.00 (m, 6H), 7.95 (dd, *J* = 8.8 Hz, 2H), 7.41 (dd, *J* = 8.2 Hz, 2H); **^{13}C NMR ($CDCl_3$, 100 MHz)** δ 151.0, 147.0, 135.5, 132.1, 130.1, 130.0, 128.2, 128.1, 122.2. **ESI-HRMS:** m/z calculated for $C_{18}H_{12}N_2Se_2$ $[M+H]^+$ 416.9404, found 416.9398.



2n

1,2-di(pyridin-4-yl)diselane (**2n**)[10]: yellow solid.

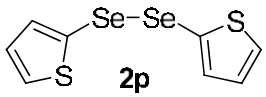
^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.52 (d, *J* = 4.2 Hz, 4H), 7.37 (d, *J* = 4.6 Hz, 4H); **^{13}C NMR ($CDCl_3$, 100 MHz)** δ 150.5, 140.5, 127.3. **EI-MS**: m/z (relative intensity, %) 316 (5.15), 238 (17.37), 237 (15.67), 236 (100.00), 235 (30.52), 234 (48.86), 233 (28.35), 232 (23.85), 78 (23.96), 51 (22.57).



2o

1,2-bis(2-methoxypyridin-3-yl)diselane (**2o**): yellow solid.

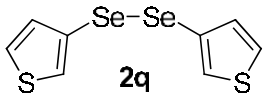
^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.02 (t, *J* = 2.7 Hz, 2H), 7.79 (dd, *J* = 7.6 Hz, 2H), 6.84 – 6.81 (m, 2H); **^{13}C NMR ($CDCl_3$, 100 MHz)** δ 160.8, 145.5, 139.2, 118.6, 113.4, 54.2. **ESI-HRMS:** m/z calculated for $C_{12}H_{12}N_2O_2Se_2$ $[M+H]^+$ 376.9302, found 376.9.



2p

1,2-di(thiophen-2-yl)diselane (**2p**)[11]: yellow solid.

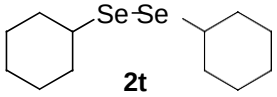
^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.52 (dd, *J* = 5.2 Hz, 2H), 7.26 (dd, *J* = 3.6 Hz, 2H), 7.04 (dd, *J* = 5.2 Hz, 2H); **^{13}C NMR ($CDCl_3$, 100 MHz)** δ 137.2, 133.2, 128.3, 125.8. **EI-MS**: m/z (relative intensity, %) 326 (37.55), 324 (34.26), 322 (19.16), 257 (17.98), 166 (59.17), 165 (24.77), 163 (100.00), 161 (50.40), 119 (18.93).



2q

1,2-di(thiophen-3-yl)diselane (**2q**)[12]: yellow solid.

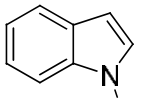
^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.40 (dd, *J* = 2.8 Hz, 2H), 7.36 (dd, *J* = 4.8 Hz, 2H), 7.19 (dd, *J* = 5.0 Hz, 2H); **^{13}C NMR ($CDCl_3$, 100 MHz)** δ 132.6, 129.4, 126.9, 124.4. **EI-MS**: m/z (relative intensity, %) 326 (36.95), 324 (34.20), 322 (18.96), 269 (15.06), 246 (13.54), 166 (100.00), 165 (22.94), 163 (72.19), 161 (32.05).



2t

1,2-dicyclohexyldiselane (**2t**)[8]: red liquid.

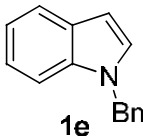
^{1}H NMR ($CDCl_3$, 400 MHz) δ 3.43 – 3.28 (m, 1H), 3.08 – 3.01 (m, 1H), 2.18 – 2.07 (m, 4H), 1.80 – 1.75 (m, 4H), 1.63 – 1.62 (m, 4H), 1.60 – 1.56 (m, 2H), 1.48 – 1.46 (m, 6H); **^{13}C NMR ($CDCl_3$, 100 MHz)** δ 43.7, 34.8, 27.2, 25.9. **EI-MS**: m/z (relative intensity, %) 326 (13.57), 324 (12.80), 246 (8.40), 244 (26.86), 242 (22.99), 240 (15.19), 83 (100.00), 55 (32.41).



1d

1-phenyl-1*H*-indole (**1d**)[2]: yellow liquid.

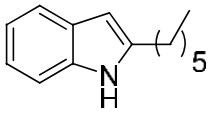
^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.69 (dd, *J* = 7.0 Hz, 2H), 7.56 – 7.54 (m, 2H), 7.47 – 7.46 (m, 4H), 7.32 – 7.28 (m, 2H), 7.22 – 7.13 (m, 2H), 7.67 – 7.66 (m, 1H); **^{13}C NMR ($CDCl_3$, 100 MHz)** δ 140.0, 136.0, 129.8, 129.5, 128.1, 126.6, 124.5, 122.5, 121.3, 120.5, 110.7, 103.8; **EI-MS**: m/z $[M+H]^+$ 193.9.



1e

1-benzyl-1*H*-indole (**1e**)[2]: colorless solid.

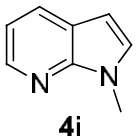
^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.64 (d, *J* = 7.6 Hz, 1H), 7.26 – 7.20 (m, 4H), 7.16 – 7.12 (m, 2H), 7.11 – 7.04 (m, 3H), 6.53 – 6.52 (m, 1H), 5.23 (s, 2H); **^{13}C NMR ($CDCl_3$, 100 MHz)** δ 137.7, 136.5, 128.9, 128.4, 127.7, 126.9, 121.9, 121.2, 119.7, 109.9, 101.9; **EI-MS**: m/z $[M+H]^+$ 208.1.



1j

2-hexyl-1*H*-indole (**1j**)[3]: colorless solid.

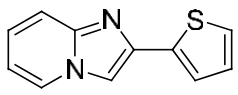
^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.84 (brs, 1H), 7.57 (d, *J* = 7.6 Hz, 1H), 7.32 (d, *J* = 7.6 Hz, 1H), 7.16 – 7.10 (m, 2H), 6.27 (s, 1H), 2.77 (t, *J* = 7.8 Hz, 2H), 1.78 – 1.70 (m, 2H), 1.44 – 1.35 (m, 6H), 0.93 (t, *J* = 6.8 Hz, 3H); **^{13}C NMR ($CDCl_3$, 100 MHz)** δ 140.2, 136.0, 129.1, 121.1, 120.0, 119.8, 110.5, 99.7, 31.9, 29.4, 29.2, 28.5, 22.8, 14.3; **EI-MS**: m/z $[M+H]^+$ 202.2.



4i

1-methyl-1H-pyrrolo[2,3-b]pyridine (**4i**)[4]: colorless liquid.

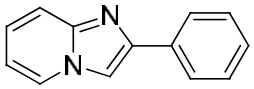
^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.35 (dd, *J* = 4.6 Hz, 1H), 7.92 (dd, *J* = 7.6 Hz, 1H), 7.18 (d, *J* = 3.6 Hz, 1H), 7.07 (dd, *J* = 8.0 Hz, 1H), 6.46 (d, *J* = 3.6 Hz, 1H); 3.90 (s, 3H); **^{13}C NMR ($CDCl_3$, 100 MHz)** δ 148.0, 143.0, 129.2, 128.9, 120.7, 115.7, 99.5, 31.4; **EI-MS**: m/z $[M+H]^+$ 133.1.



4k

2-(thiophen-2-yl)imidazo[1,2-*a*]pyridine (**4k**)[5]: white solid.

^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.06 (d, *J* = 6.8 Hz, 1H), 7.75 (d, *J* = 1.2 Hz, 1H), 7.61 (d, *J* = 9.2 Hz, 1H), 7.48 (d, *J* = 3.6 Hz, 1H), 7.31 (d, *J* = 5.2 Hz, 1H), 7.17 – 7.13 (m, 1H), 7.09 (t, *J* = 4.4 Hz, 1H), 6.76 (t, *J* = 4.4 Hz, 1H); **^{13}C NMR ($CDCl_3$, 100 MHz)** δ 145.6, 141.1, 137.7, 127.9, 125.6, 125.2, 125.0, 123.9, 117.5, 112.7, 107.6; **EI-MS**: m/z $[M+H]^+$ 201.0.

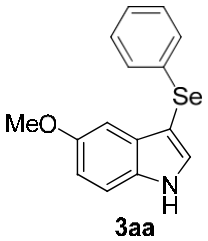


4l

2-phenylimidazo[1,2-*a*]pyridine (**4l**)[5]: colorless solid.

^{1}H NMR ($CDCl_3$, 400 MHz) δ8.10 (d, *J* = 6.8 Hz, 1H), 7.98 – 7.96 (m, 2H), 7.85 (s, 1H), 7.65 (d, *J* = 9.6 Hz, 1H), 7.44 (t, *J* = 7.4 Hz, 2H), 7.33 (t, *J* = 7.4 Hz, 1H), 7.18 – 7.14 (m, 1H), 6.76 (t, *J* = 6.6 Hz, 1H); **^{13}C NMR ($CDCl_3$, 100 MHz)** δ 146.0, 145.9, 134.0, 128.9, 128.2, 126.3, 125.8, 124.8, 117.8, 112.6, 108.3; **EI-MS**: m/z $[M+H]^+$ 195.1.

7.2. Characterization data of products

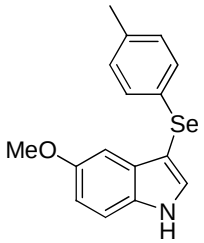


3aa

5-methoxy-3-(phenylselanyl)-1*H*-indole (**3aa**)[15]: colorless liquid, 55.2 mg (Yield: 91 %).

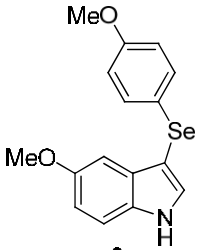
^{1}H NMR (400 MHz, $(CD_3)_2SO$): δ 11.55 (brs, 1H), 7.68 (d, *J* = 2.8 Hz, 1H), 7.40 (d, *J* = 8.4 Hz, 1H), 7.17 – 7.14 (m, 4H), 7.13 – 7.08 (m, 1H), 6.86 (d, *J* = 2.4 Hz, 1H), 6.84 (d, *J* = 2.4 Hz, 1H), 6.82 (d, *J* = 2.4 Hz, 1H); **^{13}C NMR (100 MHz, $(CD_3)_2SO$):** δ 154.2, 133.9, 133.3, 131.6, 130.3, 129.1, 128.0, 125.5, 113.0, 112.2, 100.5, 94.5,

55.2; **IR** ν_{max}: 3409, 1623, 1577, 1477, 1437, 1283, 1208, 1164, 1022, 804, 735; **EI-MS**: m/z (relative intensity, %) 303 (27.71), 301 (14.40), 224 (16.34), 223 (100.00), 208 (28.50), 207 (11.20), 181 (16.14), 180 (15.09).



3ab

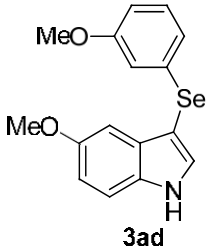
5-methoxy-3-(*p*-tolyllselanyl)-1*H*-indole (**3ab**): yellow liquid, 65.6 mg (Yield: 93 %). **^{1}H NMR (400 MHz, $(CD_3)_2SO$):** δ 11.50 (brs, 1H), 7.65 (d, *J* = 2.8 Hz, 1H), 7.40 (d, *J* = 8.8 Hz, 1H), 7.10 (d, *J* = 8 Hz, 2H), 6.99 (d, *J* = 8 Hz, 2H), 6.88 (d, *J* = 2.4 Hz, 1H), 6.83 – 6.81 (m, 1H) 3.70 (s, 3H), 2.18 (s, 3H); **^{13}C NMR (100 MHz, $(CD_3)_2SO$):** δ 154.2, 134.9, 133.0, 131.6, 130.3, 129.9, 129.7, 128.4, 112.9, 112.1, 100.6, 95.1, 55.3, 20.4; **IR** ν_{max}: 3405, 1624, 1580, 1484, 1453, 1283, 1209, 1165, 1031, 918, 801; **ESI-HRMS:** m/z calculated for $C_{16}H_{15}NOSe$ $[M+H]^+$ 318.0391, found 318.0392.



3ac

5-methoxy-3-((4-methoxyphenyl)selanyl)-1*H*-indole (**3ac**): colorless liquid, 61.8 mg (Yield: 93 %).

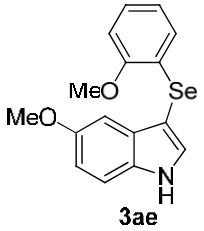
^{1}H NMR (400 MHz, $(CD_3)_2SO$): δ 11.46 (brs, 1H), 7.64 (d, *J* = 2.8 Hz, 1H), 7.38 (d, *J* = 8.8 Hz, 1H), 7.21 – 7.18 (m, 2H), 6.91 (d, *J* = 2.4 Hz, 1H), 6.83 – 6.76 (m, 3H) 3.71 (s, 3H), 3.66 (s, 3H); **^{13}C NMR (100 MHz, $(CD_3)_2SO$):** δ 158.0, 154.2, 132.7, 131.5, 130.7, 130.2, 123.2, 114.9, 112.9, 112.0, 100.7, 96.1, 55.3, 55.1; **IR** ν_{max}: 3404, 1583, 1489, 1455, 1285, 1244, 1209, 1165, 1030, 821, 806; **ESI-HRMS:** m/z calculated for $C_{16}H_{15}NO_2Se$ $[M+Na]^+$ 356.0160, found 356.0157.



3ad

5-methoxy-3-((3-methoxyphenyl)selanyl)-1*H*-indole (**3ad**): colorless liquid, 59.9 mg (Yield: 90 %).

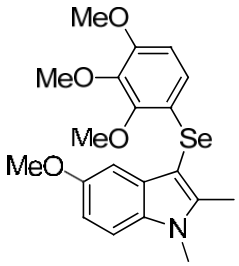
^{1}H NMR (400 MHz, $(CD_3)_2SO$): δ 11.55 (brs, 1H), 7.67 (d, *J* = 2.4 Hz, 1H), 7.41 (d, *J* = 8.8 Hz, 1H), 7.08(t, *J* = 7.8 Hz, 1H), 6.88 (d, *J* = 2.4 Hz, 1H), 6.84 (d, *J* = 2.4 Hz, 1H), 6.82 (d, *J* = 2.8 Hz, 1H), 6.73 – 6.67 (m, 3H), 3.70 (s, 3H), 3.62 (s, 3H); **^{13}C NMR (100 MHz, $(CD_3)_2SO$):** δ 159.7, 154.3, 135.2, 133.4, 131.6, 130.3, 129.9, 120.2, 113.8, 113.0, 112.2, 110.9, 100.6, 94.5, 55.3, 54.9; **IR ν_{max}**: 3404, 1724, 1586, 1477, 1283, 1243, 1166, 1036, 919, 838, 805; **ESI-HRMS:** m/z calculated for $C_{16}H_{15}NO_2Se$ $[M+Na]^+$ 356.0160, found 356.0159.



3ae

5-methoxy-3-((2-methoxyphenyl)selanyl)-1*H*-indole (**3ae**): white solid, 57.9 mg (Yield: 87 %).

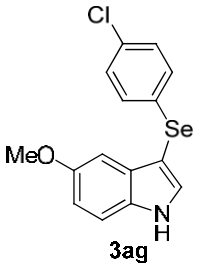
^{1}H NMR (400 MHz, $(CD_3)_2SO$): δ 11.58 (brs, 1H), 7.63 (d, *J* = 2.4 Hz, 1H), 7.43 (d, *J* = 8.8 Hz, 1H), 7.10 – 7.06 (m, 1H), 6.94 (dd, *J* = 8.2 Hz, 1H), 6.85 – 6.81 (m, 2H), 7.68 – 7.64 (m, 1H), 6.50 – 6.47 (m, 1H), 3.88 (s, 3H), 3.68 (s, 3H); **^{13}C NMR (100 MHz, $(CD_3)_2SO$):** δ 155.6, 154.3, 133.8, 131.8, 130.6, 127.0, 126.3, 122.8, 121.3, 113.0, 112.2, 110.5, 100.5, 92.5, 55.7, 55.3; **IR ν_{max}**: 3401, 1726, 1577, 1473, 1238, 1209, 1165, 1032, 919, 805, 750; **ESI-HRMS:** m/z calculated for $C_{16}H_{15}NO_2Se$ $[M+H]^+$ 334.0341, found 334.0340.



3af

5-methoxy-1,2-dimethyl-3-((2,3,4-trimethoxyphenyl)selanyl)-1*H*-indole (**3af**)[14]: white solid, 69.0 mg (Yield: 94 %).

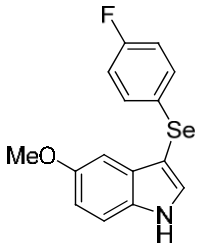
^{1}H NMR (400 MHz, ($CDCl_3$): δ 7.22 (d, *J* = 5.2 Hz, 1H), 7.09 (d, *J* = 2.4 Hz, 1H), 6.88 (dd, *J* = 5.2 Hz, 1H), 6.45 (s, 2H), 3.84 (s, 3H), 3.78 (s, 3H), 3.75 (s, 3H), 3.67 (s, 6H), 2.57 (s, 3H); **^{13}C NMR (100 MHz, ($CDCl_3$):** δ 155.1, 153.7, 143.0, 136.3, 132.5, 131.4, 128.9, 111.9, 110.0, 105.8, 101.6, 95.3, 61.0, 56.2, 56.1, 30.8, 12.3; **IR** ν_{max}: 2935, 1618, 1580, 1494, 1448, 1401, 1302, 1232, 1126, 1006, 906, 732; **EI-MS**: m/z (relative intensity, %) 421 (31.90), 419 (16.10), 342 (21.15), 341 (100.00), 327 (17.36), 326 (86.91), 175 (10.44), 174 (24.05), 131 (10.69).



3ag

3-((4-chlorophenyl)selanyl)-5-methoxy-1*H*-indole (**3ag**)[17]: white solid, 59.8 mg (Yield: 89 %).

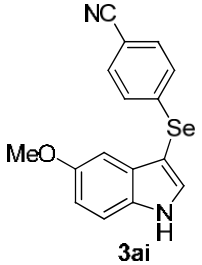
^{1}H NMR (400 MHz, (CD_3)$_2$SO): δ 11.59 (brs, 1H), 7.70 (d, *J* = 2.8 Hz, 1H), 7.42 (d, *J* = 9.2 Hz, 1H), 7.24 – 7.21 (m, 2H), 7.17 – 7.14 (m, 2H), 6.86 – 6.82 (m, 2H), 3.70 (s, 3H); **^{13}C NMR (100 MHz, (CD_3)$_2$SO):** δ 154.4, 133.4, 132.8, 131.6, 130.3, 130.1, 129.6, 128.9, 113.0, 112.3, 100.4, 94.2, 55.3; **IR** ν_{max}: 3336, 1736, 1667, 1474, 1373, 1243, 1167, 1090, 1046, 1010, 809; **EI-MS**: m/z (relative intensity, %) 339 (11.67), 337 (27.55), 335 (12.60), 259 (32.83), 258 (18.24), 257 (100.00), 242 (24.89), 214 (13.98). 207 (12.50), 44 (12.94).



3ah

3-((4-fluorophenyl)selanyl)-5-methoxy-1*H*-indole (**3ah**): yellow liquid, 68.2 mg (Yield: 83 %).

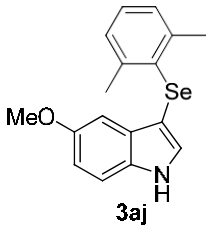
^{1}H NMR (400 MHz, $(CD_3)_2SO$): δ 11.55 (brs, 1H), 7.69 (d, *J* = 2.8 Hz, 1H), 7.24 – 7.20 (m, 2H), 7.06 – 7.01 (m, 2H), 6.89 (d, *J* = 2.4 Hz, 1H), 6.84 (dd, *J* = 8.8 Hz, 1H), 3.71 (s, 3H); **^{13}C NMR (100 MHz, $(CD_3)_2SO$):** δ 162.0 (d, *J* = 241 Hz), 154.3, 133.2, 131.6, 130.3, 130.2, 130.1, 128.6(d, *J* = 2 Hz), 116.2 (d, *J* = 21 Hz), 113.0 (d, *J* = 79 Hz), 100.5, 95.0, 55.3; **IR ν_{max}**: 3404, 1624, 1582, 1485, 1455, 1284, 1224, 1165, 1031, 822, 806; **ESI-HRMS:** m/z calculated for $C_{15}H_{12}NFOSe$ $[M+H]^+$ 322.0141, found 322.0139.



3ai

4-((5-methoxy-1H-indol-3yl)selanyl)benzonitrile (**3ai**): white solid, 50.7 mg (Yield: 78 %).

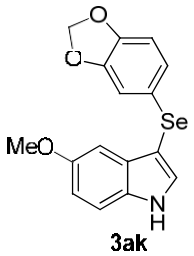
^{1}H NMR (400 MHz, $(CD_3)_2SO$): δ 11.69 (brs, 1H), 7.73 (d, *J* = 2.8 Hz, 1H), 7.59 (d, *J* = 8.4 Hz, 2H), 7.44 (d, *J* = 8.4Hz, 1H) 7.28 – 7.26 (m, 2H), 6.87 (d, *J* = 2.4 Hz, 1H), 6.85 (dd, *J* = 10.2 Hz, 1H), 3.69 (s, 3H); **^{13}C NMR (100 MHz, $(CD_3)_2SO$):** δ 154.5, 142.6, 133.8, 132.4, 131.7, 129.9, 127.9, 118.9, 113.2, 112.4, 107.7, 100.2, 92.9, 55.3; **IR ν_{max}**: 3347, 2226, 1585, 1483, 1285, 1210, 1166, 1032, 919, 820, 806; **ESI-HRMS:** m/z calculated for $C_{16}H_{12}N_2OSe$ $[M+H]^+$ 329.0188, found 329.0185.



3aj

3-((2,6-dimethylphenyl)selanyl)-5-methoxy-1*H*-indole (**3aj**): yellow solid, 54.7 mg (Yield: 83 %).

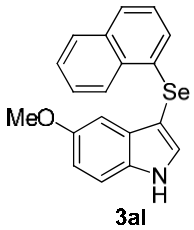
^{1}H NMR (400 MHz, $(CD_3)_2SO$): δ 11.25 (brs, 1H), 7.47 (d, *J* = 2.8 Hz, 1H), 7.30 (d, *J* = 8.4 Hz, 1H), 7.11 – 7.04 (m, 3H), 6.75 – 6.72 (m, 2H), 3.66 (s, 3H), 2.56 (s, 6H); **^{13}C NMR (100 MHz, $(CD_3)_2SO$):** δ 153.7, 141.8, 132.0, 131.2, 130.8, 129.9, 128.0, 127.7, 112.6, 111.6, 100.7, 97.0, 55.0, 24.1; **IR ν_{max}**: 3407, 1625, 1580, 1483, 1456, 1284, 1210, 1164, 1031, 918, 800; **ESI-HRMS:** m/z calculated for $C_{17}H_{17}NOSe$ $[M+H]^+$ 332.0548, found 332.0543.



3ak

3-(benzo[*d*][1,3]dioxol-5-ylselanyl)-5-methoxy-1*H*-indole (**3ak**): yellow solid, 62.3 mg (Yield: 90 %).

^{1}H NMR (400 MHz, $(CD_3)_2SO$): δ 11.5 (brs, 1H), 7.67 (d, *J* = 2.4 Hz, 1H) 7.39 (d, *J* = 8.8 Hz, 1H), 6.91 (d, *J* = 2.4 Hz, 1H), 6.84 (dd, *J* = 8.8 Hz, 1H), 6.76 – 6.75 (m, 3H), 5.93 (s, 2H), 3.72 (s, 3H); **^{13}C NMR (100 MHz, $(CD_3)_2SO$):** δ 154.2, 147.9, 146.0, 133.0, 131.5, 130.2, 125.0, 122.2, 112.9, 112.1, 109.5, 109.0, 101.0, 1006, 95.8, 55.3; **IR ν_{max}**: 3405, 1624, 1580, 1475, 1284, 1232, 1209, 1165, 1036, 934, 804; **ESI-HRMS:** m/z calculated for $C_{16}H_{13}NO_3Se$ $[M+H]^+$ 348.0133, found 348.0132.

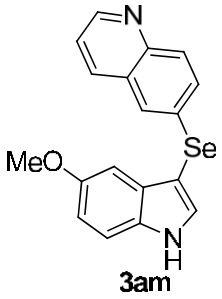


3al

5-methoxy-3-(naphthalen-1-ylselanyl)-1*H*-indole (**3al**): yellow liquid, 60.1 mg (Yield:

85 %).

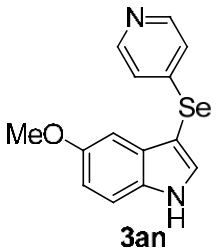
^{1}H NMR (400 MHz, $(CD_3)_2SO$): δ 11.64 (brs, 1H), 8.27 (d, *J* = 8.4 Hz, 1H), 7.92 (d, *J* = 8.0 Hz, 1H), 7.77 (d, *J* = 2.8 Hz, 1H), 7.71 (d, *J* = 8.0 Hz, 1H), 7.63 (t, *J* = 7.2 Hz, 1H), 7.56 (t, *J* = 7.2 Hz, 1H), 7.45 (d, *J* = 8.8 Hz, 1H), 7.22 (t, *J* = 7.8 Hz, 1H), 7.10 (d, *J* = 6.8 Hz, 1H), 6.88 – 6.83 (m, 2H), 3.64 (s, 3H); **^{13}CNMR (100 MHz, $(CD_3)_2SO$):** δ 154.6, 133.8, 132.6, 132.1, 132.0, 130.7, 128.9, 126.9, 126.7, 126.5, 126.4, 125.5, 113.5, 112.6, 100.9, 94.1, 55.6; **IR ν_{max}**: 3406, 1620, 1580, 1483, 1458, 1379, 1284, 1205, 1165, 1029, 794; **ESI-HRMS:** m/z calculated for $C_{19}H_{15}NOSe$ $[M+H]^+$ 354.0392, found 354.0391.



3am

6-((5-methoxy-1H-indole-3-yl)selanyl)quinolone (**3am**): white solid, 44.2 mg (Yield: 65 %).

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.90 (brs, 1H), 8.82 – 8.81 (m, 1H), 7.91 (t, *J* = 8.0 Hz, 2H), 7.61 (d, *J* = 1.6 Hz, 1H), 7.59 (d, *J* = 1.6 Hz, 1H), 7.57 (d, *J* = 1.6 Hz, 1H), 7.54 (d, *J* = 2.4 Hz, 1H), 7.38 (d, *J* = 8.8 Hz, 1H), 7.33 – 7.30 (m, 1H), 7.27 (s, 1H), 7.08 (d, *J* = 2.0 Hz, 1H), 6.95 (dd, *J* = 8.8 Hz, 1H), 3.78 (s, 3H); **^{13}C NMR (100 MHz, $CDCl_3$):** δ 155.5, 149.7, 147.0, 135.3, 133.4, 132.4, 131.7, 130.9, 130.5, 129.7, 129.1, 126.1, 121.6, 113.8, 112.6, 101.6, 97.2, 56.0; **IR ν_{max}**: 3147, 1584, 1487, 1460, 1285, 1201, 1166, 1124, 1032, 829, 797; **ESI-HRMS:** m/z calculated for $C_{18}H_{14}N_2OSe$ $[M+H]^+$ 355.0344, found 355.0337.

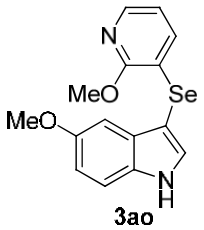


3an

5-methoxy-3-(pyridin-4-ylselanyl)-1*H*-indole (**3an**): colorless liquid, 18.3 mg (Yield:

30 %).

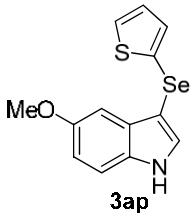
^{1}H NMR (400 MHz, ($CDCl_3$): δ 8.77 (brs, 1H), 8.26 (d, *J* = 4.0 Hz, 2H), 7.49 (d, *J* = 2.4 Hz, 1H), 7.40 (d, *J* = 8.8 Hz, 1H), 7.10 (d, *J* = 6.0 Hz, 2H), 6.97 – 6.94 (m, 2H), 3.81 (s, 3H); **^{13}C NMR (100 MHz, ($CDCl_3$):** δ 155.7, 148.8, 148.2, 132.6, 131.6, 130.5, 123.2, 114.1, 112.8, 101.3, 95.1, 56.0; **IR ν_{max}**: 3141, 1574, 1482, 1460, 1438, 1286, 1202, 1167, 1032, 920, 801; **ESI-HRMS:** m/z calculated for $C_{14}H_{12}N_2OSe$ $[M+H]^+$ 305.0188, found 305.0181.



3ao

5-methoxy-3-((2-methoxypyridin-3-yl)selanyl)-1*H*-indole (**3ao**): colorless liquid, 50.7 mg (Yield: 76 %).

^{1}H NMR (400 MHz, (CD_3)$_2$SO): δ 11.64 (brs, 1H), 7.90 (dd, *J* = 4.8 Hz, 1H), 7.68 (d, *J* = 2.8 Hz, 1H), 7.44 (d, *J* = 8.8 Hz, 1H), 6.85 (dd, *J* = 8.8 Hz, 1H), 6.81 – 6.79 (m, 2H), 6.73 (dd, *J* = 7.2 Hz, 1H), 3.97 (s, 3H), 3.68 (s, 3H); **^{13}C NMR (100 MHz, (CD_3)$_2$SO):** δ 159.5, 154.4, 143.1, 135.8, 133.9, 131.8, 130.2, 118.1, 118.0, 113.1, 112.4, 100.2, 91.6, 55.3, 53.6; **IR ν_{max}**: 3401, 1579, 1460, 1396, 1248, 1210, 1166, 1034, 919, 805, 737; **ESI-HRMS:** m/z calculated for $C_{15}H_{14}N_2O_2Se$ $[M+H]^+$ 335.0293, found 335.0294.

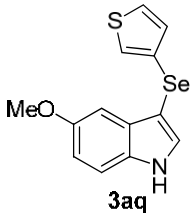


3ap

5-methoxy-3-(thiophen-2-ylselanyl)-1*H*-indole (**3ap**): colorless liquid, 40.8 mg (Yield: 66 %).

^{1}H NMR (400 MHz, (CD_3)$_2$SO): δ 11.43 (brs, 1H), 7.65 (d, *J* = 2.8 Hz, 1H), 7.47 (dd, *J* = 5.2 Hz, 1H), 7.35 (d, *J* = 8.8 Hz, 1H), 7.23 (dd, *J* = 3.6 Hz, 1H), 7.06 (d, *J* = 2.4 Hz, 1H), 6.94 (dd, *J* = 5.2 Hz, 1H), 6.82 (dd, *J* = 8.8 Hz, 1H), 3.77 (s, 3H); **^{13}C NMR (100 MHz, (CD_3)$_2$SO):** δ 154.2, 132.3, 132.0, 131.2, 129.7, 128.0, 127.5, 112.8,

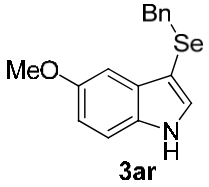
112.1, 100.7, 97.8, 55.3; **IR** ν_{max}: 3406, 1624, 1580, 1483, 1284, 1210, 1165, 1029, 918, 803, 703; **ESI-HRMS:** m/z calculated for $C_{13}H_{11}NOSSe$ $[M+H]^+$ 309.9799, found 309.9796.



3aq

5-methoxy-3-(thiophen-3-ylselanyl)-1*H*-indole (**3aq**): white solid, 46.3 mg (Yield: 75 %).

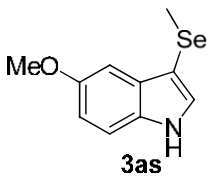
^{1}H NMR (400 MHz, $(CD_3)_2SO$): δ 11.43 (brs, 1H), 7.64 (d, *J* = 2.8 Hz, 1H), 7.47 (dd, *J* = 5.2 Hz, 1H), 7.37 (d, *J* = 8.8 Hz, 1H), 7.22 (dd, *J* = 2.8 Hz, 1H), 6.95 (d, *J* = 2.8 Hz, 1H), 6.93 (dd, *J* = 4.8 Hz, 1H), 6.82 (dd, *J* = 8.8 Hz, 1H), 3.73 (s, 3H); **^{13}C NMR (100 MHz, $(CD_3)_2SO$):** δ 154.1, 132.3, 131.4, 130.0, 129.8, 127.0, 126.2, 122.9, 112.8, 112.0, 100.6, 95.9, 55.3; **IR** ν_{max}: 3404, 1624, 1580, 1483, 1454, 1284, 1209, 1165, 1029, 805, 765; **ESI-HRMS:** m/z calculated for $C_{13}H_{11}NOSSe$ $[M+H]^+$ 309.9799, found 309.9794.



3ar

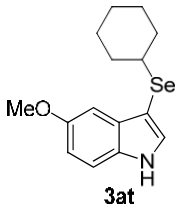
3-(benzylselanyl)-5-methoxy-1*H*-indole (**3ar**): yellow liquid, 25.4 mg (Yield: 41 %).

^{1}H NMR (400 MHz, $(CD_3)_2SO$): δ 11.22 (brs, 1H), 7.31 (d, *J* = 8.8Hz, 1H), 7.25 (d, *J* = 2.4 Hz, 1H), 7.20 – 7.12 (m, 3H), 7.07 – 7.05 (m, 2H), 6.84 (d, *J* = 2.4 Hz, 1H), 6.77 (dd, *J* = 8.8 Hz, 1H), 3.86 (s, 2H), 3.72 (s, 3H); **^{13}CNMR (100 MHz, $(CD_3)_2SO$):** δ153.9,140.0, 132.0, 131.2, 130.5, 128.1, 126.3, 112.5, 111.9, 100.5, 96.2, 55.2, 31.8; **IR** ν_{max}: 3409, 1624, 1580, 1482, 1453, 1283, 1209, 1164, 1030, 803, 697; **ESI-HRMS:** m/z calculated for $C_{16}H_{15}NOSe$ $[M+H]^+$ 318.0392, found 318.0389.



3as

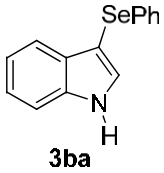
5-methoxy-3-(methylselanyl)-1*H*-indole (**3as**): yellow liquid, 36.8 mg (Yield: 77 %). **^{1}H NMR (400 MHz, $(CD_3)_2SO$):** δ 11.20 (brs, 1H), 7.44 (d, *J* = 2.4 Hz, 1H), 7.33 (d, *J* = 8.8 Hz, 1H), 7.00 (d, *J* = 2.4 Hz, 1H), 6.80 (dd, *J* = 8.8 Hz, 1H), 3.79 (s, 3H), 2.12(s, 3H); **^{13}CNMR (100 MHz, $(CD_3)_2SO$):** δ153.9, 131.3, 130.7, 130.0, 112.6, 111.9, 100.6, 97.1, 55.3, 8.9; **IR ν_{max}**: 3403, 1624, 1579, 1482, 1453, 1283, 1209, 1164, 1030, 917, 803; **ESI-HRMS:** m/z calculated for $C_{10}H_{11}NOSe$ $[M+H]^+$ 242.0079, found 242.0077.



3at

3-(cyclohexylselanyl)-5-methoxy-1*H*-indole (**3at**): yellow solid, 43.2 mg (Yield: 70 %).

^{1}H NMR (400 MHz, $(CD_3)_2SO$): δ 11.26 (brs, 1H), 7.41 (d, *J* = 2.4 Hz, 1H), 7.32 (d, *J* = 8.8 Hz, 1H), 7.01 (d, *J* = 8.4 Hz, 1H), 6.79 (dd, *J* = 8.6 Hz, 1H), 3.77 (s, 3H), 2.96 – 2.89 (m, 1H), 1.90 – 1.86 (m, 2H), 1.66 – 1.61 (m, 2H), 1.50 – 1.46 (m, 2H), 1.40 – 1.36 (m,3H); **^{13}CNMR (100 MHz, $(CD_3)_2SO$):** δ 153.9, 132.6, 131.4, 131.3, 112.5, 111.6, 101.1, 94.9, 55.3, 42.0, 33.9, 26.2, 25.2; **IR ν_{max}**: 3412, 1624, 1582, 1480, 1285, 1225, 1151, 1029, 799, 757, 725; **ESI-HRMS:** m/z calculated for $C_{15}H_{19}NOSe$ $[M+H]^+$ 310.0705, found 310.0701.

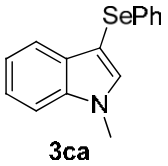


3ba

3-(phenylselanyl)-1H-indole (**3ba**)[15]: white solid, 50.0 mg (Yield: 91 %).

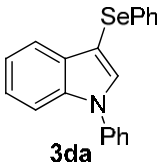
^{1}H NMR (400 MHz, $(CD_3)_2SO$): δ 11.71 (brs, 1H), 7.75(d, *J* = 2.4 Hz, 1H), 7.51 (d, *J* = 8.0 Hz, 1H), 7.4 (d, *J* = 7.6 Hz, 1H), 7.20 – 7.15 (m, 5 H), 7.14 – 7.05 (m, 2H); **^{13}CNMR (100 MHz, $(CD_3)_2SO$)**: δ 136.7, 133.8, 132.8, 129.5, 129.1, 128.1, 125.6, 122.0, 120.1, 119.0, 112.1, 95.0; **IR ν_{max}**: 3411, 1575, 1475, 1452, 1404, 1236, 1095, 1020, 745, 733, 514; **EI-MS**: m/z (relative intensity, %) 273 (21.11), 271 (11.38), 194

(15.56), 193 (100.00), 192 (10.97), 165 (10.14).



3ca

1-methyl-3-(phenylselanyl)-1*H*-indole (**3ca**)[15]: white solid, 53.8 mg (Yield: 94 %). **^{1}H NMR (400 MHz, $(CD_3)_2SO$):** δ 7.33 (s, 1H), 7.54 (d, *J* = 8.4 Hz, 1H), 7.45 (d, *J* = 7.6 Hz, 1H), 7.26 – 7.22 (m, 1H), 7.20 – 7.10 (m, 6H), 3.86 (s, 3H); **^{13}CNMR (100 MHz, $(CD_3)_2SO$):** δ 137.2, 136.6, 133.7, 129.9, 129.1, 128.1, 125.6, 122.1, 120.2, 119.3, 110.4, 93.9, 32.7; **IR ν_{max}**: 3053, 1576, 1507, 1476, 1458, 1332, 1239, 1154, 1021, 736, 690; **EI-MS**: m/z (relative intensity, %) 287 (23.60), 285 (12.01), 208 (18.38), 207 (100.00), 206 (18.30), 165 (7.07), 130 (7.94).



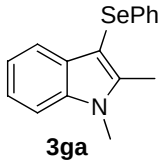
3da

1-phenyl-3-(phenylselanyl)-1*H*-indole (**3da**)[15]: yellow liquid, 61.1 mg (Yield: 88 %). **^{1}H NMR (400 MHz, $(CD_3)_2SO$):** δ 8.06 (s, 1H), 7.67 (d, *J* = 7.6 Hz, 2H), 7.61 – 7.58 (m, 3H), 7.53(d, *J* = 7.6 Hz, 1H), 7.44 (t, *J* = 7.4 Hz, 1H), 7.31 – 7.25 (m, 3H), 7.21 – 7.15 (m, 3H), 7.14 (d, *J* = 7.2Hz, 1H); **^{13}CNMR (100 MHz, $(CD_3)_2SO$):** δ 138.2, 136.0, 134.9, 132.7, 130.6, 129.8, 129.2, 128.7, 127.0, 125.9, 124.1, 123.3, 121.3, 119.9, 110.9, 98.1; **IR ν_{max}**: 3053, 1736, 1596, 1508, 1476, 1453, 1363, 1223, 1021, 736, 694; **EI-MS**: m/z (relative intensity, %) 349 (20.42), 270 (23.46), 269 (100.00), 268 (14.68), 267 (9.19), 165 (23.79), 149 (10.12).

3ea

1- benzyl-3-(phenylselanyl)-1*H*-indole (**3ea**)[18]: yellow liquid, 64.6 mg (Yield: 90 %). **^{1}H NMR (400 MHz, $(CD_3)_2SO$):** δ 7.96 (s, 1H), 7.56 (d, *J* = 8.4 Hz, 1H), 7.45 (d, *J* = 7.6 Hz, 1H), 7.42 – 7.31 (m, 2H), 7.28 – 7.25 (m, 3H), 7.25 – 7.20 (m, 5H), 7.18 –7.08 (m, 2H), 5.51 (s, 2H); **^{13}CNMR (100 MHz, $(CD_3)_2SO$):** δ 137.7, 136.6, 136.1,

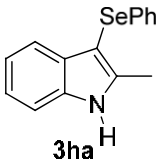
133.5, 130.2, 129.1, 128.6, 128.1, 127.5, 127.1, 125.7, 122.3, 120.4, 119.4, 110.9, 94.8, 49.4; **IR** ν_{max}: 3055, 1735, 1577, 1503, 1476, 1455, 1249, 1160, 1022, 732, 691; **EI-MS**: m/z (relative intensity, %) 363 (17.83), 284 (13.02), 283 (65.53), 208 (15.47), 207 (95.54), 206 (20.35), 192 (28.93), 165 (14.15), 91 (100.00).



3ga

1,2-dimethyl-3-(phenylselanyl)-1*H*-indole (**3ga**): colorless liquid, 49.6 mg (Yield: 83 %).

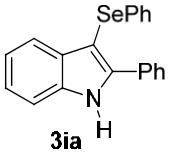
^{1}H NMR (400 MHz, $(CD_3)_2SO$): δ 7.50 (d, *J* = 8.4 Hz, 1H), 7.39 (d, *J* = 7.6 Hz, 1H), 7.19 – 7.04 (m, 7H), 3.78 (s, 3H), 2.53 (s, 3H); **^{13}CNMR (100 MHz, $(CD_3)_2SO$):** δ 143.1, 137.1, 133.7, 129.8, 129.1, 127.9, 125.5, 121.4, 120.1, 118.6, 109.8, 93.5, 30.4, 11.6; **IR** ν_{max}: 3419, 1575, 1518, 1473, 1437, 1392, 1235, 1021, 745, 731, 688; **ESI-HRMS:** m/z calculated for $C_{16}H_{15}NSe$ $[M+H]^+$ 302.0442, found 302.0438.



3ha

2- dimethyl-3-(phenylselanyl)-1*H*-indole (**3ha**)[15]: white solid, 54.4 mg (Yield: 95 %).

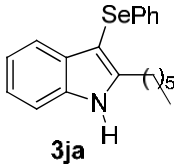
^{1}H NMR (400 MHz, $(CD_3)_2SO$): δ 11.58 (brs, 1H), 7.32 (d, *J* = 8.0 Hz, 1H), 7.27 (d, *J* = 8.0 Hz, 1H), 7.10 – 7.04 (m, 2H), 7.03 – 7.00 (m, 4H), 6,96 – 6.92 (m, 1H), 2.52 (s, 3H); **^{13}CNMR (100 MHz, $(CD_3)_2SO$):** δ 141.7, 136.0, 133.7, 130.6, 129.1, 127.8, 125.4, 121.3, 119.8, 118.4, 111.1, 93.5, 12.7; **IR** ν_{max}: 3397, 1576, 1541, 1475, 1454, 1401, 1289, 1059, 1021, 736, 690; **EI-MS**: m/z (relative intensity, %) 287 (28.68), 285 (14.79), 208 (16.36), 207 (100.00), 206 (32.08), 130 (29.53).



3ia

2-phenyl-3-(phenylselanyl)-1*H*-indole (**3ia**)[15]: colorless liquid, 58.6 mg (Yield: 84 %).

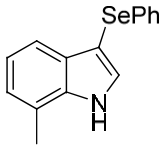
^{1}H NMR (400 MHz, $(CD_3)_2SO$): δ 12.10 (brs, 1H), 7.85 (d, *J* = 1.2 Hz, 2H), 7.83 – 7.46 (m, 4H), 7.41 – 7.38 (m, 1H), 7.24 – 7.20 (m, 1H), 7.18 – 7.10 (m, 6H); **^{13}CNMR (100 MHz, $(CD_3)_2SO$):** δ 142.2, 136.6, 133.8, 131.8, 131.4, 129.2, 128.6, 128.4, 127.6, 125.5, 122.6, 120.4, 119.6, 111.9, 93.2; **IR** ν_{max}: 3404, 3056, 1576, 1476, 1454, 1398, 1295, 1224, 1022, 736, 692; **EI-MS**: m/z (relative intensity, %) 349 (10.43), 270 (13.06), 269 (50.46), 268 (11.69), 194 (14.59), 193 (100.00), 192 (17.72), 165 (27.87), 44 (9.79).



3ja

2-hexyl-3-(phenylselanyl)-1*H*-indole (**3ja**): yellow liquid, 64.8 mg (Yield: 91 %).

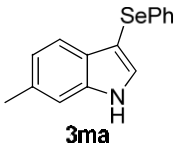
^{1}H NMR (400 MHz, $(CD_3)_2SO$): δ 11.58 (brs, 1H), 7.40 (d, *J* = 8.0 Hz, 1H), 7.34 (d, *J* = 7.6 Hz, 1H), 7.15 – 7.16 (m, 6H), 7.05 – 7.00 (m, 1H), 2.87 (t, *J* = 7.6 Hz, 2H), 1.67 – 1.60 (m, 2H), 1.24 – 1.15 (m, 6H), 0.78 (t, *J* = 7.0 Hz, 3H); **^{13}CNMR (100 MHz, $(CD_3)_2SO$):** δ 145.9, 136.1, 133.9, 130.5, 129.0, 127.7, 125.3, 121.3, 119.8, 118.5, 111.3, 93.3, 30.9, 29.1, 28.2, 26.7, 21.9, 13.8; **IR** ν_{max}: 3399, 2926, 2855, 1577, 1454, 1410, 1289, 1228, 1022, 735, 690; **ESI-HRMS:** m/z calculated for $C_{20}H_{23}NSe$ $[M+H]^+$ 358.1068, found 358.1066.



3la

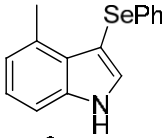
7-methyl-3-(phenylselanyl)-1*H*-indole (**3la**)[16]: colorless liquid, 51.9 mg (Yield: 90 %).

^{1}H NMR (400 MHz, $(CD_3)_2SO$): δ 11.69 (brs, 1H), 7.73 (d, *J* = 6.8 Hz, 1H), 7.25 (t, *J* = 4.6 Hz, 1H), 7.16 – 7.11 (m, 4H), 7.10 – 7.08 (m, 1H), 7.08 – 6.97 (m, 2H), 2.52 (s, 3H); **^{13}CNMR (100 MHz, $(CD_3)_2SO$):** δ 136.1, 133.8, 132.4, 129.3, 129.0, 128.0, 125.5, 122.5, 121.4, 120.2, 116.6, 95.4, 16.6; **IR** ν_{max}: 3412, 1721, 1577, 1476, 1438, 1250, 1115, 1046, 781, 735, 690; **EI-MS**: m/z (relative intensity, %) 287 (25.25), 285 (13.50), 208 (17.70), 207 (100.00), 206 (31.28), 130 (8.84).



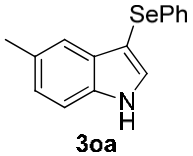
3ma

6-methyl-3-(phenylselanyl)-1*H*-indole (**3ma**)[16]: white solid, 49.8 mg (Yield: 87 %). **^{1}H NMR (400 MHz, $(CD_3)_2SO$):** δ 11.53 (brs, 1H), 7.64 (s, 1H), 7.28 (s, 2H), 7.15 –7.08 (m, 5H), 6.91 (d, *J* = 8.4 Hz, 1H), 2.40 (s, 3H); **^{13}CNMR (100 MHz, $(CD_3)_2SO$):** δ 137.0, 133.8, 132.1, 131.2, 129.0, 128.0, 127.4, 125.5, 121.8, 118.7, 111.8, 94.8, 21.3; **IR ν_{max}**: 3398, 1575, 1474, 1450, 1382, 1149, 1095, 1021, 805, 733, 521; **EI-MS**: m/z (relative intensity, %) 287 (26.10), 285 (13.07), 223 (8.19), 208 (19.81), 207 (100.00), 206 (40.05), 130 (9.10).



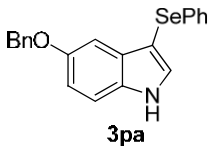
3na

4-methyl-3-(phenylselanyl)-1*H*-indole (**3na**)[16]: yellow solid, 53.4 mg (Yield: 93 %). **^{1}H NMR (400 MHz, $(CD_3)_2SO$):** δ 11.66 (brs, 1H), 7.66 (d, *J* = 2.4 Hz, 1H), 7.35 (d, *J* = 8.0 Hz, 1H), 7.20 – 7.08 (m, 5H), 7.06 – 7.02 (t, *J* = 7,8 Hz, 1H), 6.78 (d, *J* = 6.8 Hz, 1H), 2.58 (s, 3H); **^{13}CNMR (100 MHz, $(CD_3)_2SO$):** δ 137.1, 136.2, 133.8, 130.2, 129.1, 127.5, 126.8, 125.3, 122.0, 121.5, 110.2, 93.8, 18.4; **IR ν_{max}**: 3407, 1575, 1474, 1437, 1391, 1112, 1069, 1019, 773, 734, 689; **EI-MS**: m/z (relative intensity, %) 287 (37.01), 285 (18.64), 284 (7.69), 208 (18.83), 207 (100.00), 206 (40.77), 130 (26.23).



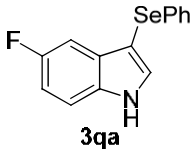
3oa

5-methyl-3-(phenylselanyl)-1*H*-indole (**3oa**)[15]: white solid, 50.3 mg (Yield: 88 %). **^{1}H NMR (400 MHz, $(CD_3)_2SO$):** δ 11.57 (brs, 1H), 7.68 (d, *J* = 2.4 Hz, 1H), 7.39 (d, *J* = 8.4 Hz, 1H), 7.20 – 7.01 (m, 6H), 6.99 (d, *J* = 1.2 Hz, 1H), 2.34 (s, 3H); **^{13}CNMR (100 MHz, $(CD_3)_2SO$):** δ 135.0, 134.0, 132.9, 129.8, 129.1, 128.7, 127.9, 125.5, 123.6, 118.5, 111.8, 94.2, 21.2; **IR ν_{max}**: 3403, 1576, 1474, 1436, 1236, 1159, 1093, 1022, 804, 734, 594; **EI-MS**: m/z (relative intensity, %) 287 (24.41), 285 (13.27), 208 (18.94), 207 (100.00), 206 (38.51), 130 (8.19).



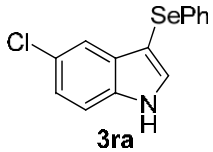
3pa

5-(benzyloxy)-3-(phenylselanyl)-1*H*-indole (**3pa**): white solid, 69.6 mg (Yield: 90 %). **^{1}H NMR (400 MHz, $(CD_3)_2SO$):** δ 11.55 (brs, 1H), 7.68 (d, *J* = 2.8 Hz, 1H), 7.43 – 7.34 (m, 3H), 7.32 – 7.28 (m, 2H), 7.27 (d, *J* = 5.2 Hz, 1H), 7.17 – 7.09 (m, 5H), 6.99 (d, *J* = 2,4 Hz, 1H), 6.92 (dd, *J* = 4.8 Hz, 1H), 5.03 (s, 2H); **^{13}CNMR (100 MHz, $(CD_3)_2SO$):** δ 153.2, 137.5, 133.8, 133.4, 131.7, 130.3, 129.1, 128.3, 128.2, 127.6, 125.6, 112.9, 112.8, 102.2, 94.7, 69.7; **IR ν_{max}**: 3412, 1723, 1620, 1578, 1477, 1453, 1279, 1172, 1021, 762, 692; **ESI-HRMS:** m/z calculated for $C_{21}H_{17}NOSe$ $[M+H]^+$ 380.0548, found 380.0546.



3qa

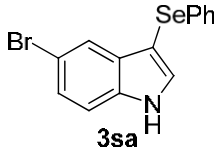
5-fluoro-3-(phenylselanyl)-1*H*-indole (**3qa**)[16]: white solid, 50.8 mg (Yield: 87 %). **^{1}H NMR (400 MHz, $(CD_3)_2SO$):** δ 11.81 (brs, 1H), 7.83 (d, *J* = 2.4 Hz, 1H), 7.52 (dd, *J* = 8.8 Hz, 1H), 7.17 – 7.00 (m, 7H); **^{13}CNMR (100 MHz, $(CD_3)_2SO$):** δ 158.8 (d, *J* = 232 Hz), 134.8, 133.4, 133.3, 130.3 (d, *J* = 10 Hz), 129.1, 128.2, 125.7, 113.5 (d, J = 10 Hz), 110.4 (d, *J* = 26 Hz), 103.7 (d, *J* = 23 Hz), 95.1 (d, *J* = 5 Hz); **IR ν_{max}**: 3415, 1581, 1484, 1451, 1151, 1092, 1019, 928, 858, 807, 734; **EI-MS**: m/z (relative intensity, %) 291 (19.98), 289 (11.05), 212 (17.19), 211 (100.00), 210 (10.98), 183 (10.38), 44 (8.29).



3ra

5-chloro-3-(phenylselanyl)-1*H*-indole (**3ra**)[15]: white solid, 51.4 mg (Yield: 84 %). **^{1}H NMR (400 MHz, $(CD_3)_2SO$):** δ 11.90 (brs, 1H), 7.84 (d, *J* = 2.4 Hz, 1H), 7.53 (d, *J* = 8.8 Hz, 1H), 7.36 (d, *J* = 2.0 Hz, 1H), 7.20 – 7.10 (m, 6H); **^{13}CNMR (100 MHz, $(CD_3)_2SO$):** δ 135.2, 134.6, 133.3, 130.9, 129.2, 128.2, 128.1, 125.8, 124.9, 122.1, 118.0, 113.9, 94.8; **IR ν_{max}**: 3333, 1574, 1474, 1439, 1097, 1020, 891, 806, 730, 589, 521; **EI-MS**: m/z (relative intensity, %) 309 (9.17), 307 (21.12), 229 (31.73), 228

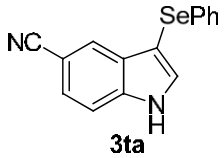
(17.93), 227 (100.00), 192 (13.22), 165 (9.36), 135 (5.58).



3sa

5-bromo-3-(phenylselanyl)-1*H*-indole (**3sa**)[15]: white solid, 60.2 mg (Yield: 86 %).

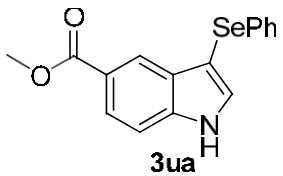
^{1}H NMR (400 MHz, $(CD_3)_2SO$): δ 11.90 (brs, 1H), 7.82 (d, *J* = 2.4 Hz, 1H), 7.51 (d, *J* = 2.0 Hz, 1H), 7.49 (d, *J* = 8.4 Hz, 1H), 7.31 (dd, *J* = 8.4 Hz, 1H), 7.21 – 7.11 (m, 5H) ; **^{13}CNMR (100 MHz, $(CD_3)_2SO$):** δ 135.4, 134.5, 133.2, 131.5, 129.2, 128.2, 125.8, 124.7, 121.1, 114.3, 112.8, 94.7; **IR ν_{max}**: 3418, 1572, 1474, 1454, 1400, 1093, 881, 808, 736, 688, 583; **EI-MS**: m/z (relative intensity, %) 353 (30.12), 351 (35.13), 273 (94.72), 272 (44.83), 271 (100.00), 192 (30.62), 165 (24.19), 44 (56.77).



3ta

3-(phenylselanyl)-1*H*-indole-5-carbonitrile (**3ta**)[16]: white solid, 42.1 mg (Yield: 71 %).

^{1}H NMR (400 MHz, $(CD_3)_2SO$): δ 12.24 (brs, 1H), 7.98 (s, 1H), 7.83 (s, 1H), 7.68 (d, *J* = 8.4 Hz, 1H), 7.54 (dd, *J* = 8.4 Hz, 1H), 7.19 – 7.12 (m, 5H); **^{13}CNMR (100 MHz, $(CD_3)_2SO$):** δ 138.6, 135.5, 132.8, 129.5, 129.2, 128.6, 126.0, 124.8, 124.3, 120.2, 113.6, 102.3, 96.5; **IR ν_{max}**: 3393, 2221, 1610, 1576, 1463, 1409, 1336, 1092, 829, 730, 685; **EI-MS**: m/z (relative intensity, %) 298 (18.74), 296 (10.15), 295 (4.28), 219 (18.06), 218 (100.00), 217 (9.41), 190 (11.13).

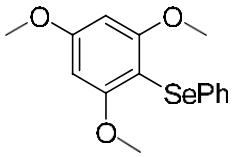


3ua

Methyl3-(phenylselanyl)-1H-indole-5-carboxylate (**3ua**)[15]: white solid, 42.0 mg (Yield: 64 %).

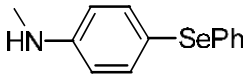
^{1}H NMR (400 MHz, $(CD_3)_2SO$): δ 12.09 (brs, 1H), 8.11 (s, 1H), 7.91 (d, *J* = 2.0 Hz, 1H), 7.83 (dd, *J* = 8.4 Hz, 1H), 7.60 (d, *J* = 8.4 Hz, 1H), 7.20 – 7.10 (m, 5H), 3.81 (s, 3H); **^{13}CNMR (100 MHz, $(CD_3)_2SO$):** δ 166.9, 139.4, 134.9, 133.3, 132.1, 129.2,

128.0, 125.8, 123.0, 121.6, 121.4, 112.3, 96.6, 51.8; **IR** ν_{max}: 3303, 1689, 1615, 1579, 1476, 1348, 1290, 1237,1197, 1105, 738; **EI-MS**: m/z (relative intensity, %) 331 (29.03), 329 (14.36), 269 (18.36), 252 (16.81), 251 (100.00), 220 (44.36), 192 (14.00), 165 (16.56), 44 (32.09).



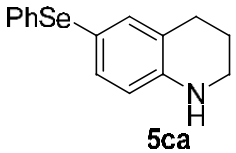
5aa

Phenyl(2,4,6-trimethoxyphenyl)selane (**5aa**): white solid, 58.2 mg (Yield: 90 %). **^{1}H NMR (400 MHz, $(CD_3)_2SO$):** δ 7.18 – 7.14 (m, 2H), 7.10 – 7.03 (m, 3H), 6.34 (s, 2H), 3.84 (s, 3H), 3.72 (s, 6H); **^{13}CNMR (100 MHz, $(CD_3)_2SO$):** δ 162.9, 161.5, 133.7, 128.9, 127.8, 125.1, 95.5, 91.4, 56.1, 55.4; **IR** ν_{max}: 1578, 1467, 1452, 1409, 1336, 1228, 1204, 1162, 1123, 814, 735; **EI-MS**: m/z $[M+H]^+$ 324.9. **ESI-HRMS:** m/z calculated for $C_{15}H_{16}O_3Se$ $[M+H]^+$ 325.0337, found 325.0339.



5ba

N-methyl-4-(phenylselanyl)aniline (**5ba**)[19]: colorless liquid, 36.2 mg, (Yield: 90 %). **^{1}H NMR (400 MHz, $CDCl_3$):** δ 7.48 (d, *J* = 8.4 Hz, 2H), 7.31 – 7.29 (m, 2H), 7.23 – 7.14 (m, 2H), 6.60 (d, *J* = 8.8 Hz, 1H), 4.01 (brs, 1H), 2.87 (s, 3H); **^{13}CNMR (100 MHz, $CDCl_3$):** δ 149.6, 137.5, 134.7, 130.0, 129.2, 126.1, 114.9, 113.6, 30.7; **IR** ν_{max}: 3421, 1596, 1504, 1476, 1437, 1320, 1262, 1182, 1021, 816, 735; **EI-MS**: m/z (relative intensity, %) 263 (38.88), 261 (19.47), 260 (8.53), 259 (8.72), 184 (17.61), 183 (100.00), 182 (38.93).

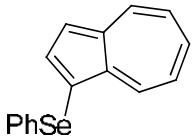


5ca

6-(phenylselanyl)-1,2,3,4-tetrahydroquinoline (**5ca**)[20]: white solid, 32.5 mg (Yield: 54 %).

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.29 – 7.27 (m, 2H), 7.22 – 7.14 (m, 4H), 7.13 – 7.11 (m, 1H), 6.42 (d, *J* = 5.6 Hz, 1H), 3.91 (brs, 1H), 3.31 (s, 2H), 2.73 (s, 2H), 1.95 – 1.89 (m, 2H); **^{13}CNMR (100 MHz, $CDCl_3$):** δ 145.3, 137.5, 135.1, 134.9, 129.9,

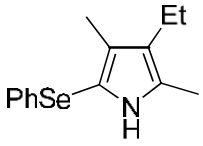
129.2, 126.0, 122.6, 115.1, 114.1, 42.0, 27.0, 21.9; **IR** ν_{max}: 3414, 2927, 1595, 1501, 1475, 1437, 1299, 1021, 810, 735, 690; **EI-MS**: m/z (relative intensity, %) 289 (35.67), 287 (18.61), 285 (10.40), 210 (18.65), 209 (100.00), 208 (41.02), 205 (7.64), 130 (23.03).



5da

Azulen-1-yl(phenyl)selane (**5da**): colorless liquid, 28.9 mg, (Yield: 51 %).

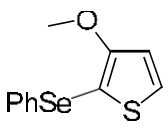
^{1}H NMR (400 MHz, $(CD_3)_2SO$): δ 8.60 – 8.55 (m, 2H), 8.10 (d, *J* = 4.0 Hz, 1H), 7.84 (t, *J* = 10.0 Hz, 1 H), 7.57 (d, *J* = 4.0 Hz, 1H), 7.47 – 7.40 (m, 2H), 7.17 – 7.12 (m, 3H), 7.11 – 7.05 (m, 2H); **^{13}CNMR (100 MHz, $(CD_3)_2SO$):** δ 144.2, 141.6, 141.1, 139.2, 137.6, 136.8, 134.2, 129.2, 128.4, 125.8, 125.2, 124.8, 118.4, 110.9; **IR** ν_{max}: 1575, 1473, 1435, 1390, 1291, 1064, 1019, 861, 776, 733, 689; **ESI-HRMS:** m/z calculated for $C_{16}H_{12}Se$ $[M+H]^+$ 285.0177, found 285.0174.



5ea

3-ethyl-2,4-dimethyl-5-(phenylselanyl)-1H-pyrrole (**5ea**): yellow liquid, 43.0 mg, (Yield: 77 %).

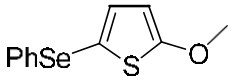
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.73 (brs, 1H), 7.23 – 7.19 (m, 2H), 7.16 – 7.12 (m, 3H), 2.50 (q, *J* = 7.6 Hz, 2H), 2.23 (s, 3H), 2.13 (s, 3H), 1.13 (t, *J* = 7.6 Hz, 3H); **^{13}CNMR (100 MHz, $CDCl_3$):** δ 135.0, 129.3, 128.2, 127.6, 126.9, 125.8, 122.4, 105.7, 18.4, 15.7, 11.5, 11.0; **IR** ν_{max}: 3422, 2960, 2925, 2859, 1578, 1475, 1438, 1292, 1021, 735, 690; **ESI-HRMS:** m/z calculated for $C_{14}H_{17}NSe$ $[M+H]^+$ 280.0599, found 280.0593.



5fa

3-methoxy-2-(phenylselanyl)thiophene (**5fa**): yellow liquid, 43.3 mg, (Yield: 80 %).

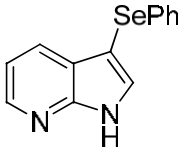
^{1}H NMR (400 MHz, ($CDCl_3$): δ 7.46 (d, *J* = 5.6 Hz, 1H), 7.32 – 7.29 (m, 2H), 7.25 – 7.16 (m, 3H), 6.93 (d, *J* = 5.6 Hz, 1H), 3.92 (s, 3H); **^{13}CNMR (100 MHz, ($CDCl_3$):** δ 161.0, 133.7, 130.4, 129.4, 129.3, 126.5, 116.4, 99.5, 59.3; **IR ν_{max}**: 1577, 1533, 1475, 1438, 1376, 1249, 1067, 1021, 834, 734, 689; **ESI-HRMS:** m/z calculated for $C_{11}H_{10}NOSSe$ $[M+H]^+$ 270.9690, found 270.9687.



5ga

2-methoxy-5-(phenylselanyl)thiophene (**5ga**): colorless liquid, 36.0 mg, (Yield: 67 %).

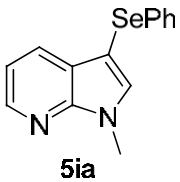
^{1}H NMR (400 MHz, ($CDCl_3$): δ 7.33 – 7.30 (m, 2H), 7.24 – 7.15 (m, 3H), 7.05 (d, *J* = 4.0 Hz, 1H), 6.17 (d, *J* = 4.0 Hz, 1H), 3.89 (s, 3H); **^{13}CNMR (100 MHz, ($CDCl_3$):** δ 171.4, 136.6, 134.4, 129.4, 129.3, 126.6, 107.9, 105.5, 60.4; **IR ν_{max}**: 1577, 1540, 1476, 1465, 1419, 1237, 1202, 1062, 997, 735, 689; **ESI-HRMS:** m/z calculated for $C_{11}H_{10}NOSSe$ $[M+H]^+$ 270.9690, found 270.9688.



5ha

3-(phenylselanyl)-1*H*-pyrrolo[2,3-*b*]pyridine (**5ha**): white solid, 36.1 mg (Yield: 66 %).

^{1}H NMR (400 MHz, $(CD_3)_2SO$): δ 12.24 (brs, 1H), 8.29 (dd, *J* = 4.4 Hz, 1H), 7.88 (s, 1H), 7.79 (dd, *J* = 7.8 Hz, 1H), 7.18 – 7.11 (m, 6H); **^{13}CNMR (100 MHz, $(CD_3)_2SO$):** δ 146.9, 141.6, 131.5, 131.2, 127.2, 126.4, 125.3, 123.9, 119.9, 114.6, 92.0; **IR ν_{max}**: 2923, 1740, 1580, 1475, 1409, 1280, 1242, 794, 770, 734, 689; **ESI-HRMS:** m/z calculated for $C_{13}H_{10}N_2Se$ $[M+H]^+$ 275.0082, found 275.0083.



5ia

1-methyl-3-(phenylselanyl)-1*H*-pyrrolo[2,3-*b*]pyridine (**5ia**): yellow liquid, 44.5 mg,

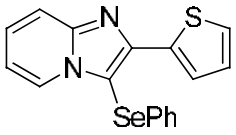
(Yield: 78 %).

^{1}H NMR (400 MHz, $(CD_3)_2SO$): δ 8.34 (dd, *J* = 4.8 Hz, 1H), 7.94 (s, 1H), 7.80 (dd, *J* = 7.8 Hz, 1H), 7.21 – 7.12 (m, 6H), 3.89 (s, 1H); **^{13}CNMR (100 MHz, $(CD_3)_2SO$):** δ 147.9, 143.4, 136.9, 133.1, 129.2, 128.4, 127.6, 125.9, 122.2, 116.6, 92.9, 31.1; **IR** ν_{max}: 1577, 1566, 1511, 1476, 1436, 1403, 1297, 1134, 1021, 771, 735; **ESI-HRMS:** m/z calculated for $C_{14}H_{12}N_2Se$ $[M+H]^+$ 289.0238, found 289.0231.

5ja

3-(phenylselanyl)imidazole[1,2-*a*]pyridine (**5ja**)[21]: colorless liquid, 21.3 mg, (Yield: 39 %).

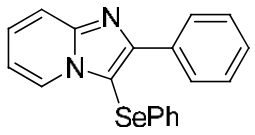
^{1}H NMR (400 MHz, $(CDCl_3)$): δ 8.29 (d, *J* = 6.8 Hz, 1H), 7.98 (s, 1H), 7.71 (d, *J* = 9.2 Hz, 1H), 7.31 – 7.28 (m, 1H), 7.23 – 7.13 (m, 5H), 6.88 – 6.85 (m, 1H); **^{13}CNMR (100 MHz, $(CDCl_3)$):** δ 148.4, 143.1, 130.7, 129.7, 129.2, 127.0, 126.0, 125.4, 118.1, 113.3, 106.7; **IR** ν_{max}: 1632, 1577, 1499, 1476, 1438, 1337, 1289, 1149, 757, 736, 690; **EI-MS**: m/z (relative intensity, %) 274 (23.73), 272 (12.20), 195 (16.46), 194 (100.00), 193 (13.45), 105 (8.72), 78 (23.72).



5ka

3-(phenylselanyl)-2-(thiophen-2-yl)imidazo[1,2-*a*]pyridine (**5ka**)[21]: colorless liquid, 32.8 mg, (Yield: 46 %).

^{1}H NMR (400 MHz, $(CD_3)_2SO$): δ 8.47 – 8.46 (m, 1H), 7.92 (dd, *J* = 3.8 Hz, 1H), 7.72 (d, *J* = 8.0 Hz, 1H), 7.69 – 7.60 (m, 1H), 7.46 – 7.42 (m, 1H), 7.26 – 7.21 (m, 3H), 7.20 – 7.14 (m, 3H), 7.07 – 7.03 (m, 1H); **^{13}CNMR (100 MHz, $(CD_3)_2SO$):** δ 146.9, 145.7, 136.5, 130.4, 129.8, 128.4, 127.8, 127.4, 127.3, 126.9, 126.1, 125.6, 116.7, 113.7, 101.7; **IR** ν_{max}: 1574, 1474, 1435, 1341, 1210, 1021, 852, 760, 735, 708; **EI-MS**: m/z $[M+H]^+$ 357.0.



5la

2-phenyl-3-(phenylselanyl)imidazo[1,2-*a*]pyridine (**5la**)[21]: yellow liquid, 24.8 mg, (Yield: 35 %).

^{1}H NMR (400 MHz, $(CD_3)_2SO$): δ 8.46 (d, *J* = 6.8 Hz, 1H), 8.14 – 8.12 (m, 2H), 7.76 (d, *J* = 8.8 Hz, 1H), 7.48 – 7.43 (m, 3H), 7.40 – 7.37 (m, 1H), 7.25 – 7.16 (m, 3H), 7.09 – 7.02 (m, 3H); **^{13}CNMR (100 MHz, $(CD_3)_2SO$):** δ 150.4, 147.1, 133.7, 130.8, 129.9, 128.4, 128.3, 128.2, 127.9, 127.1, 126.8, 125.7, 117.1, 113.6, 102.4; **IR** ν_{max}: 1677, 1576, 1476, 1464, 1432, 1342, 1304, 1230, 755, 736, 695; **EI-MS**: m/z $[M+H]^+$ 351.0.

8. References

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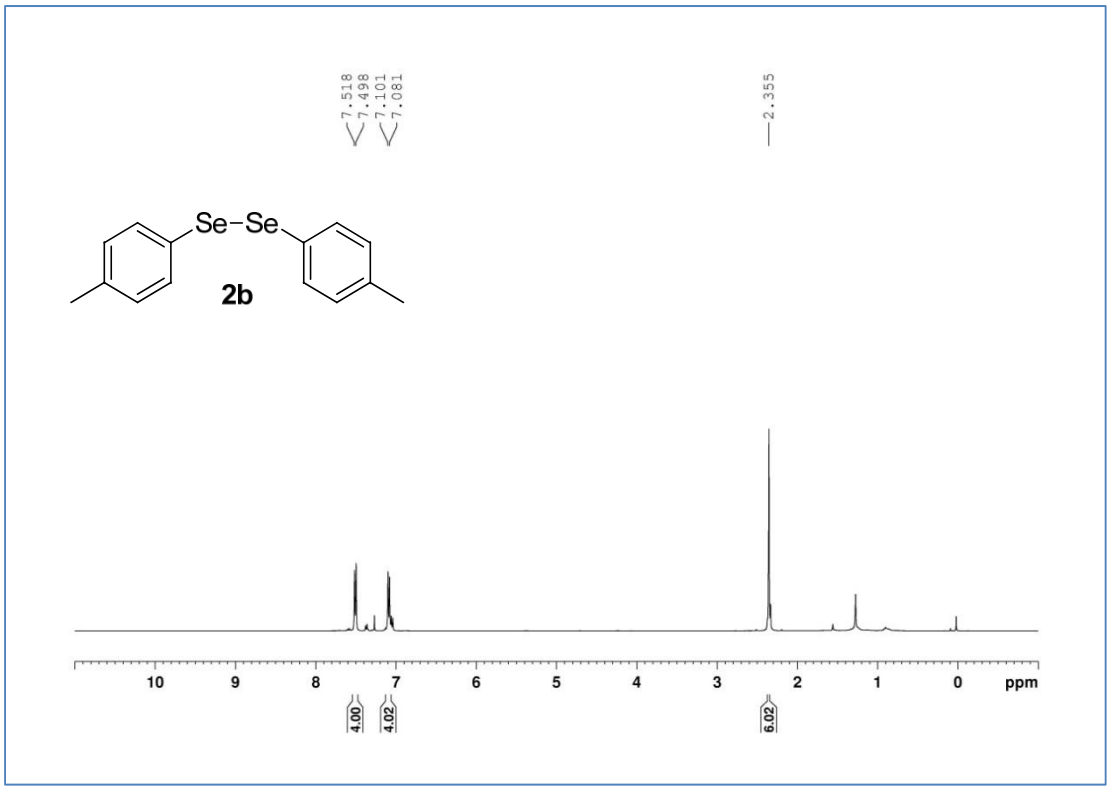
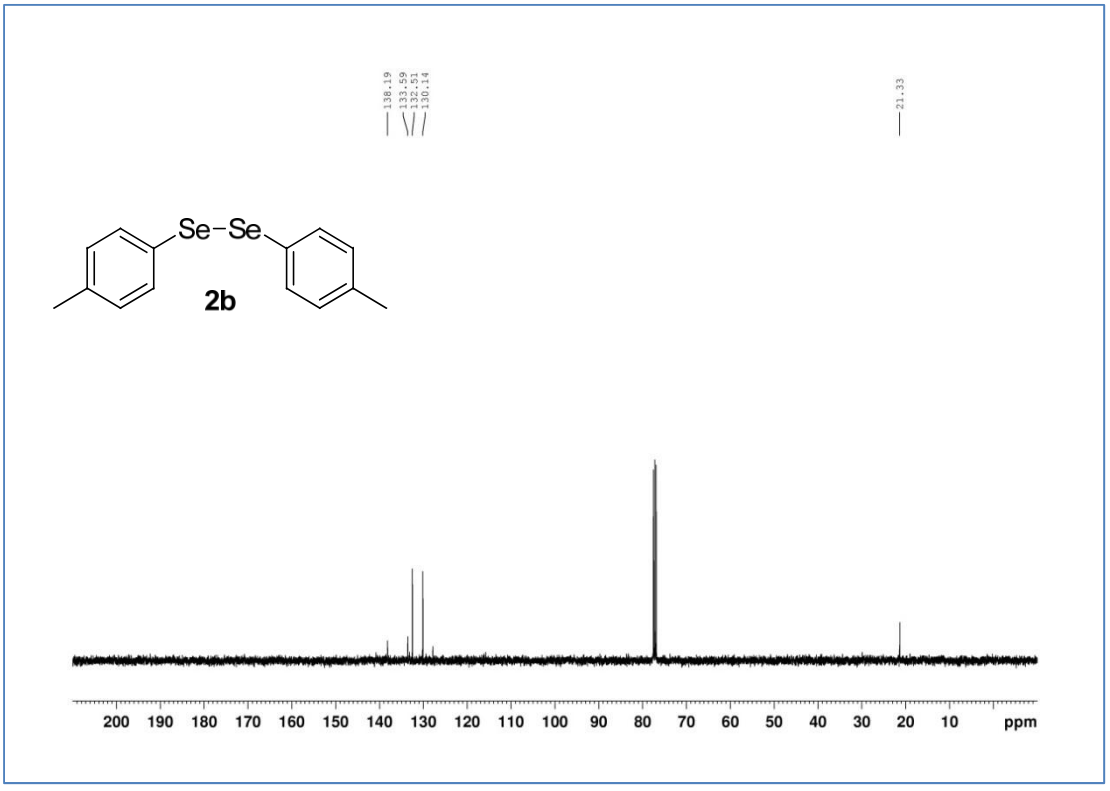
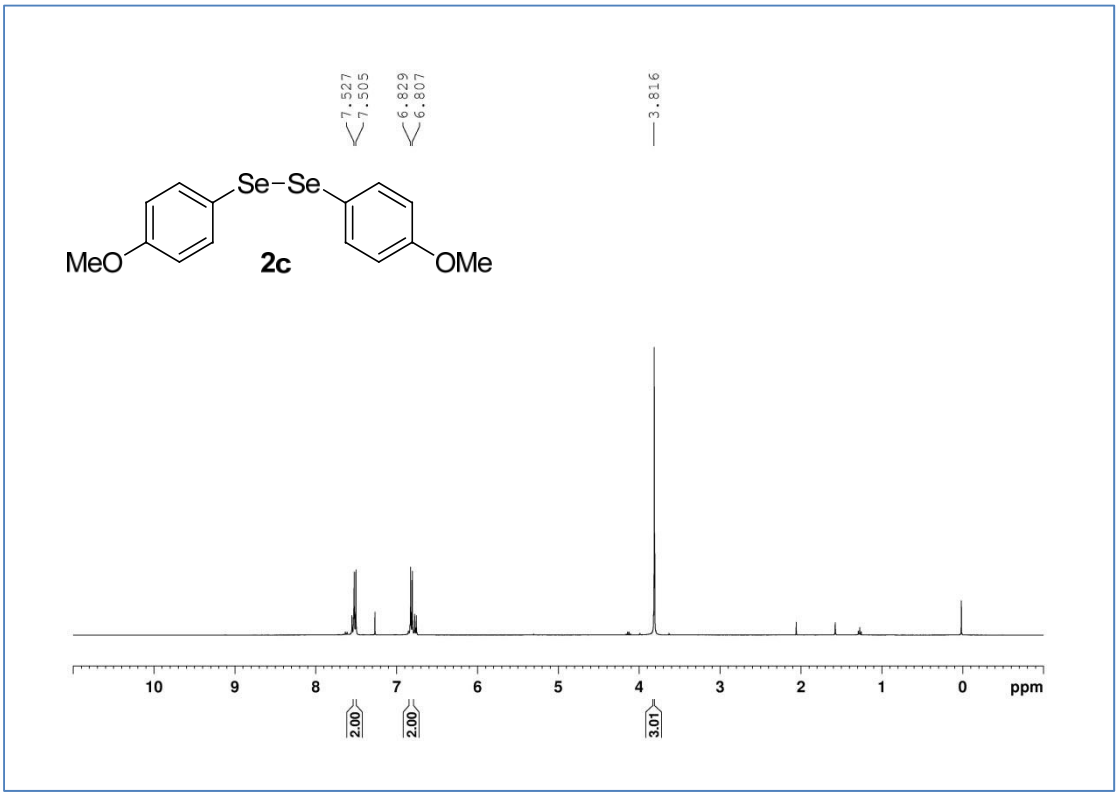
9. NMR Spectra

9.1 NMR spectra of starting materials



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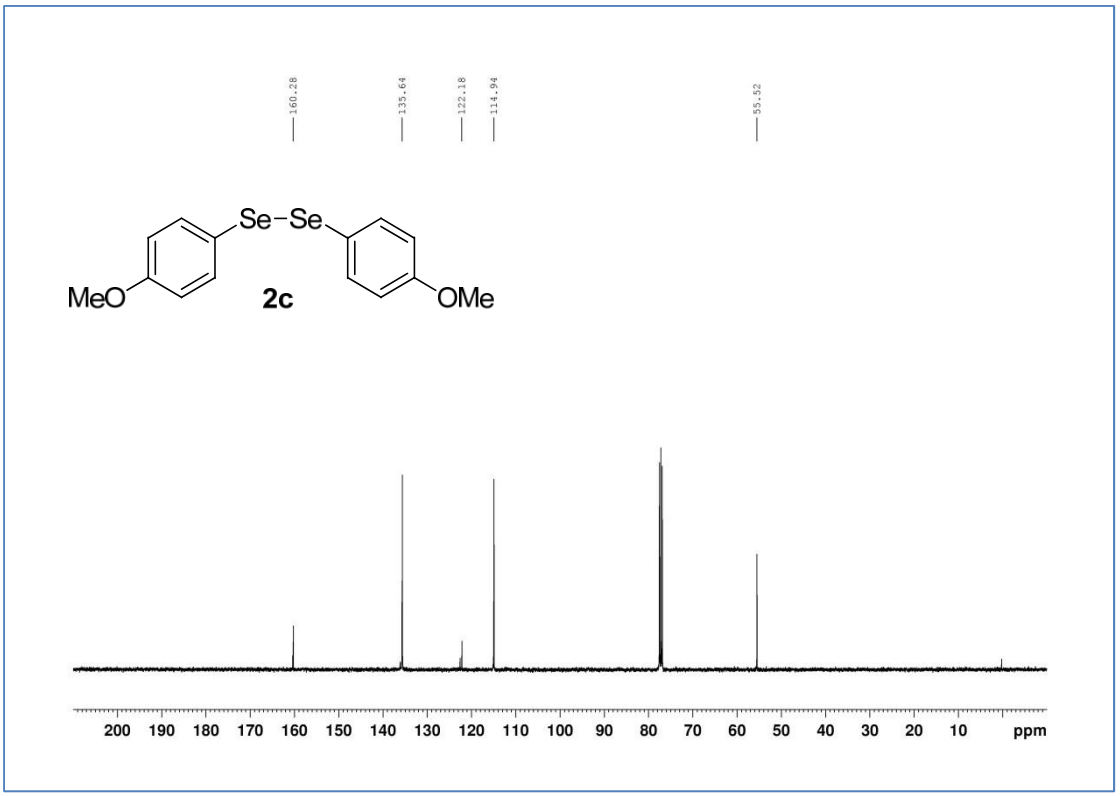
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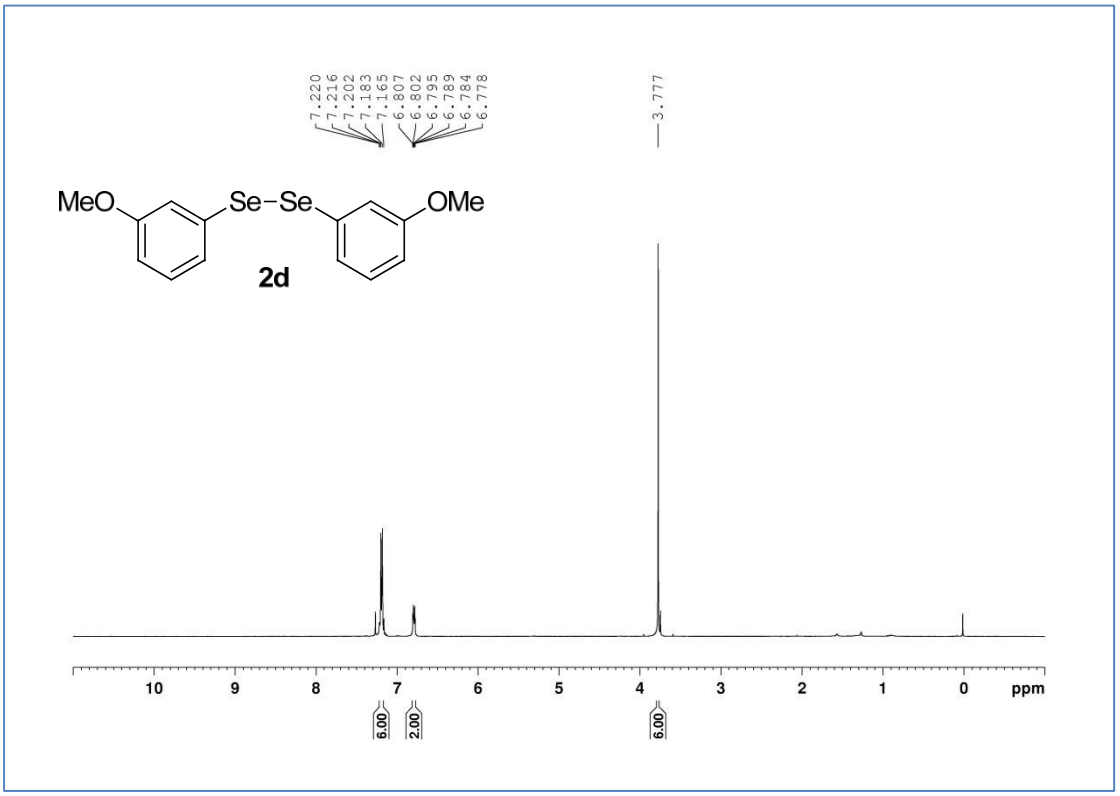
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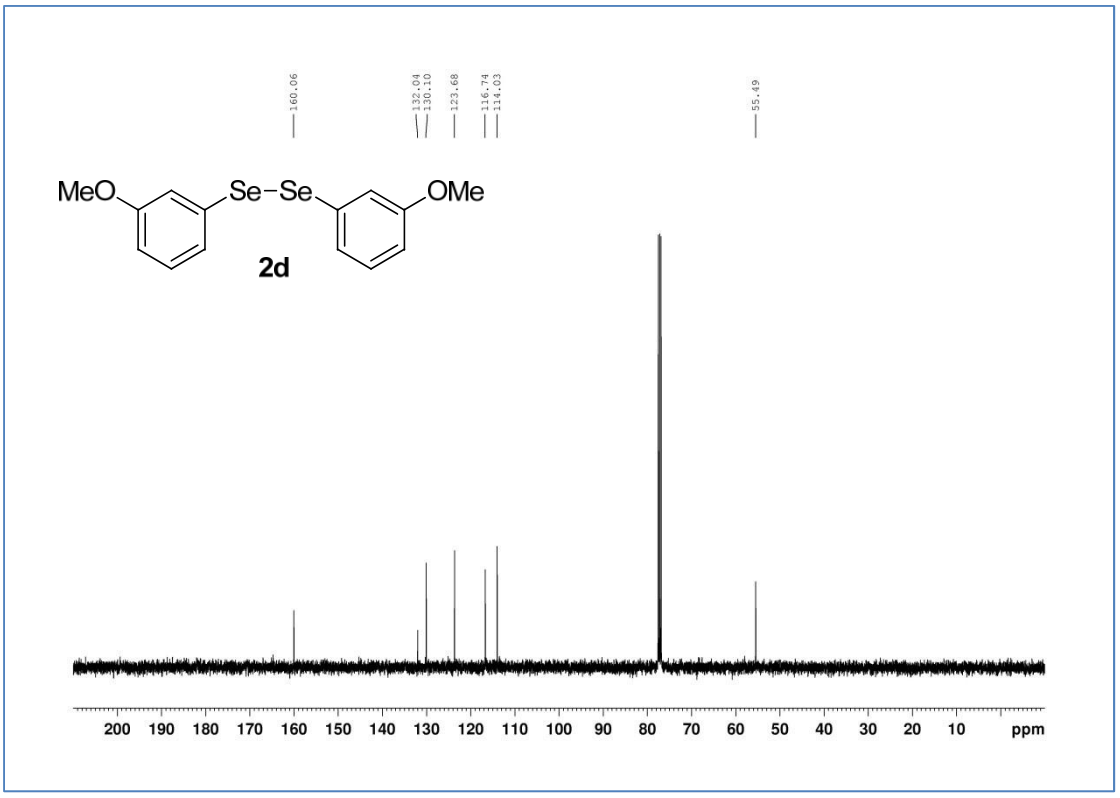
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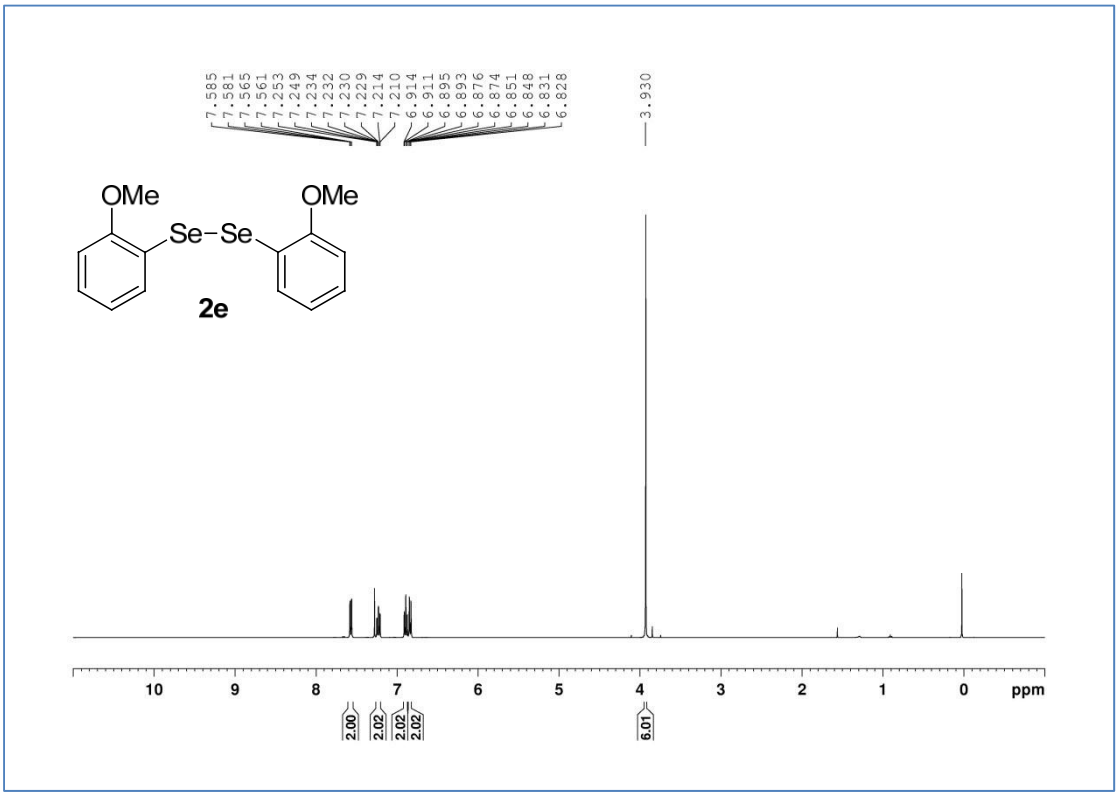
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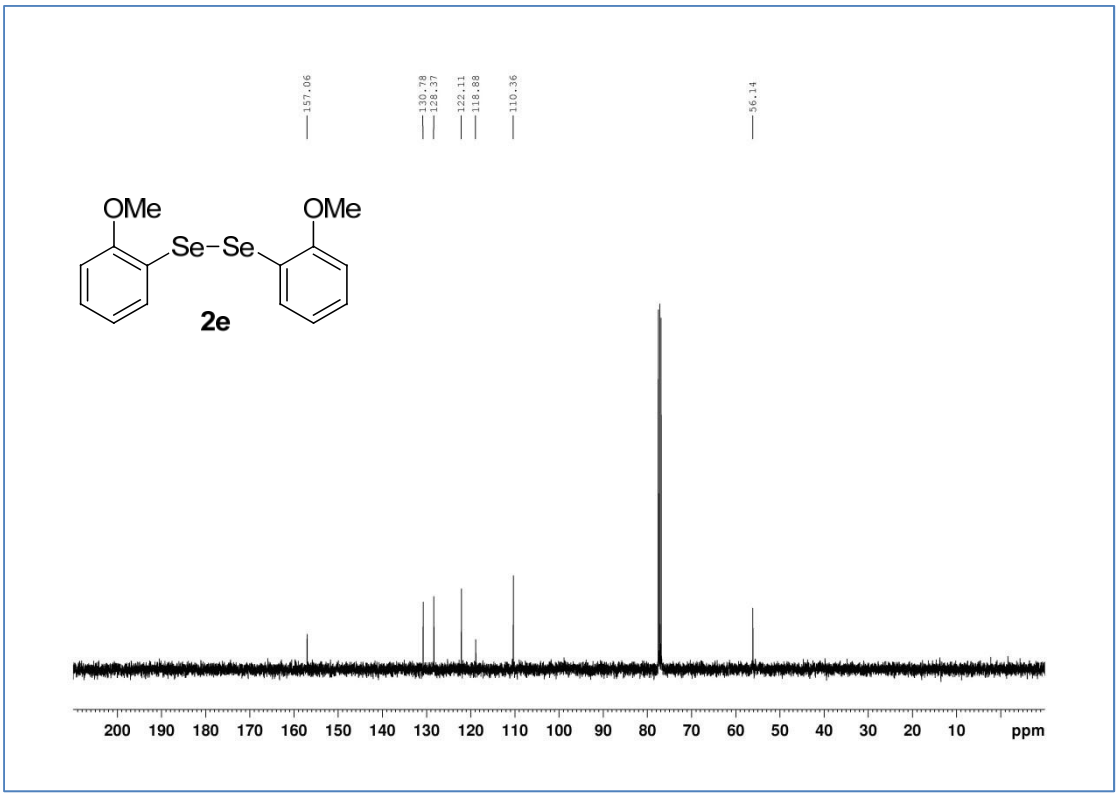
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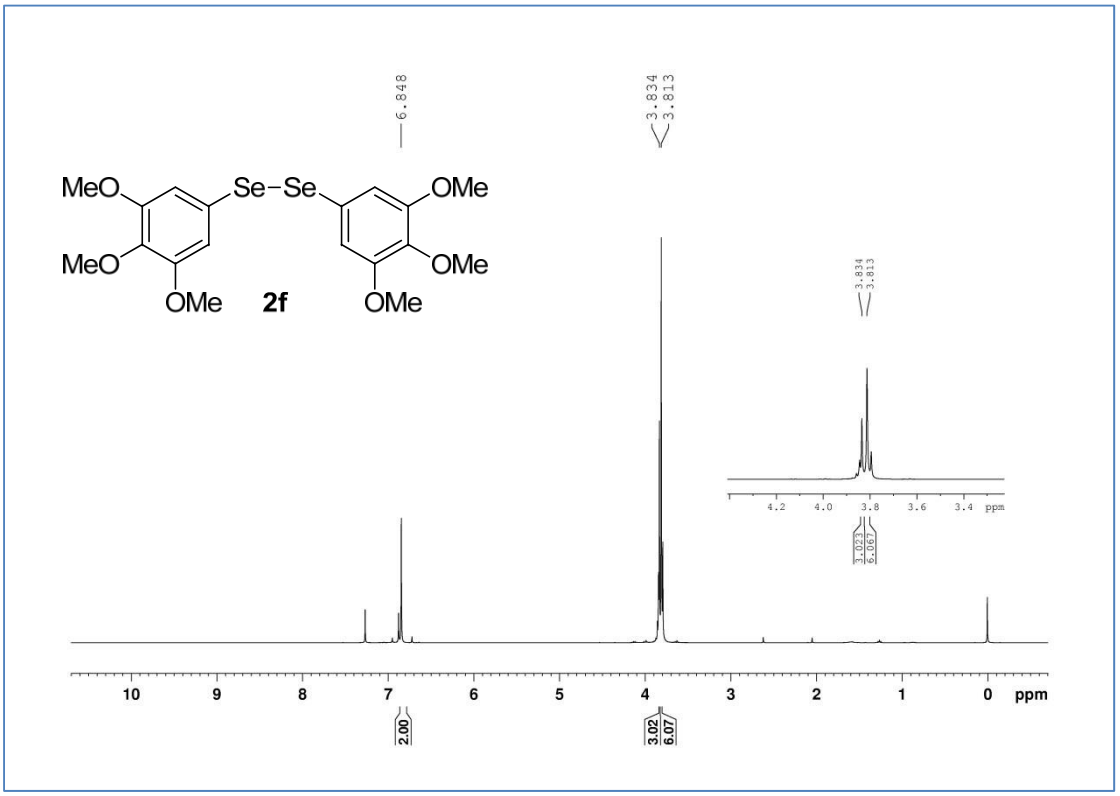
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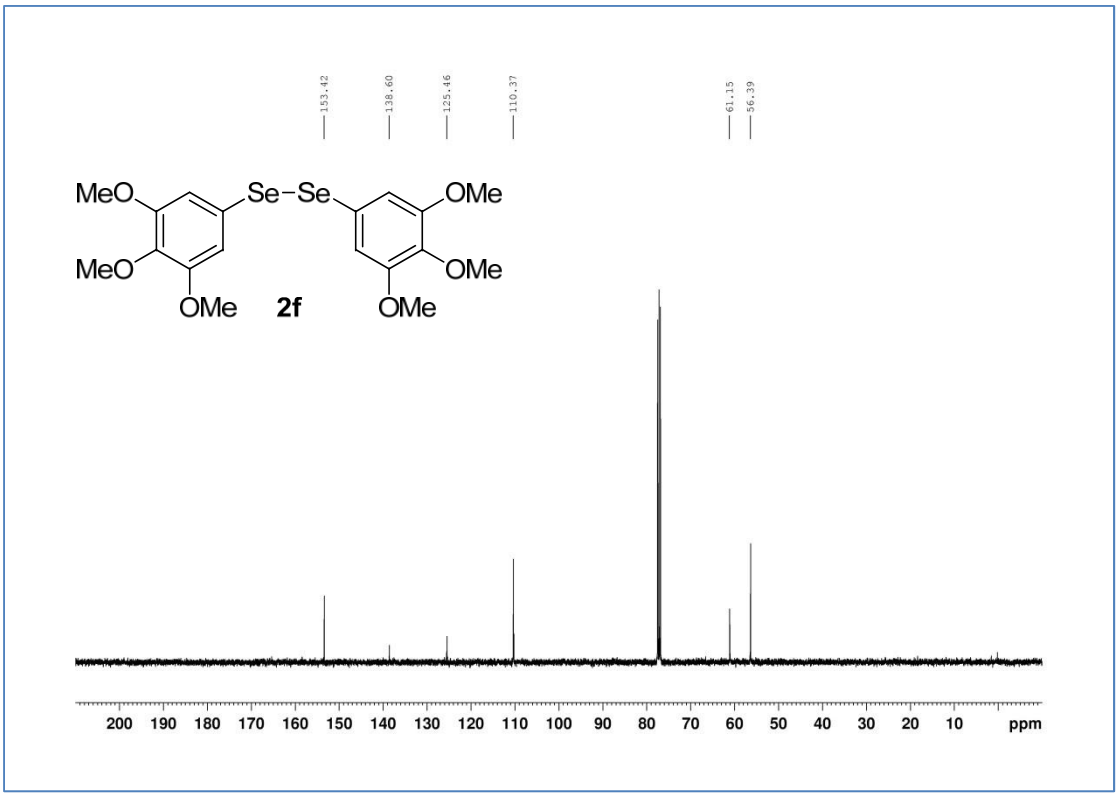
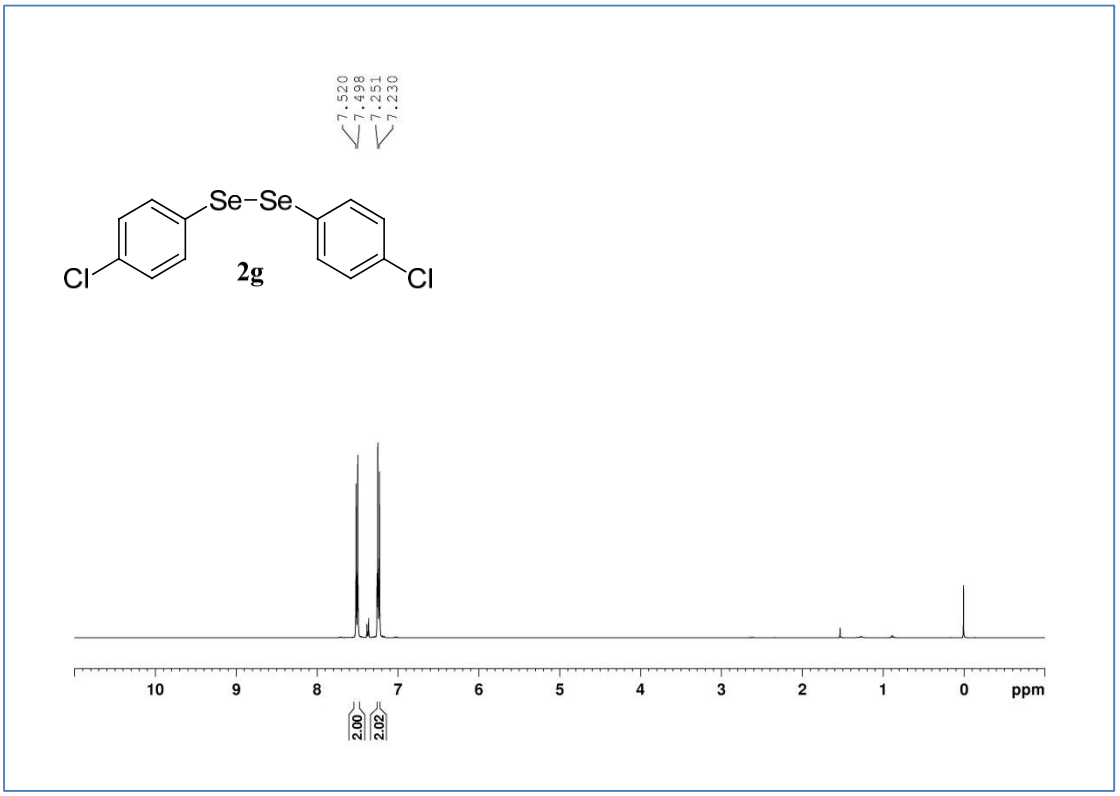
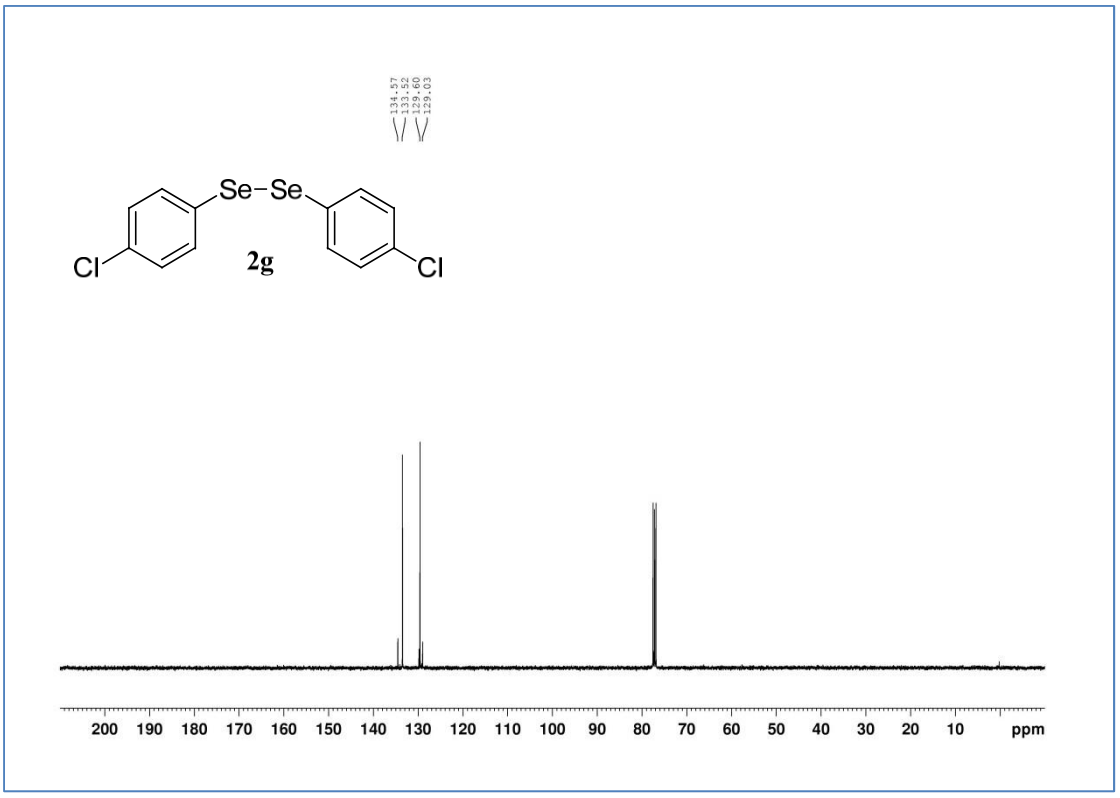
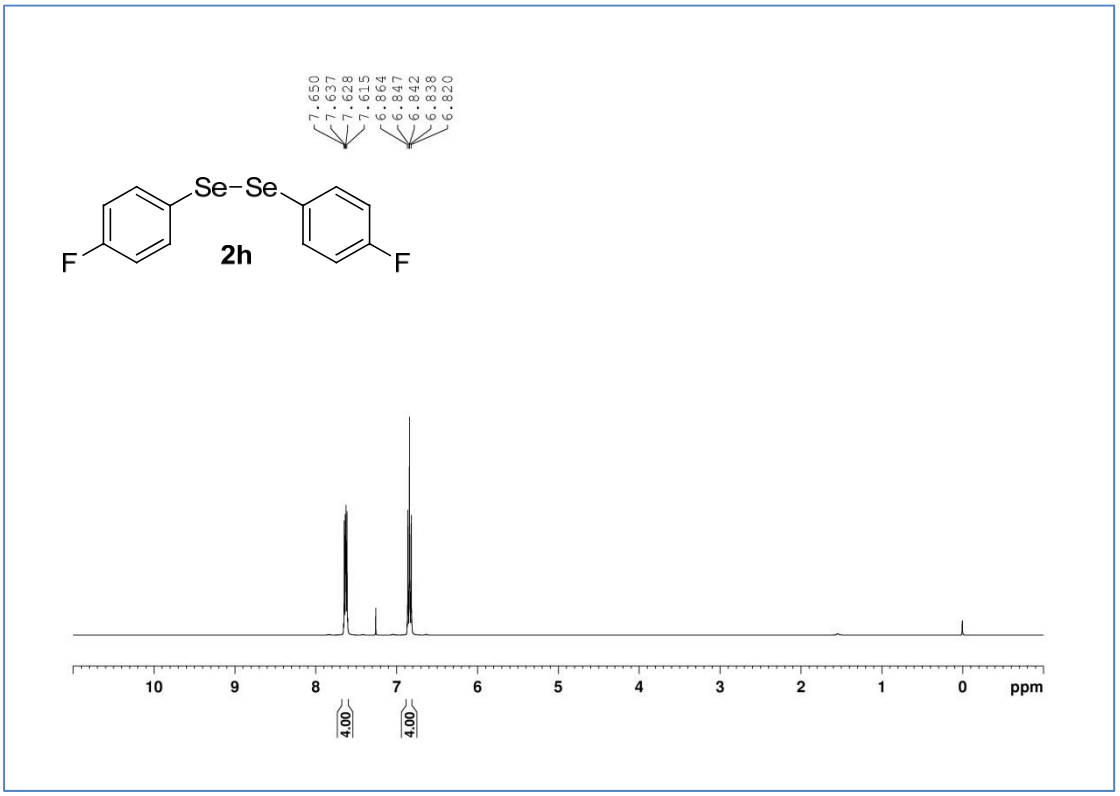
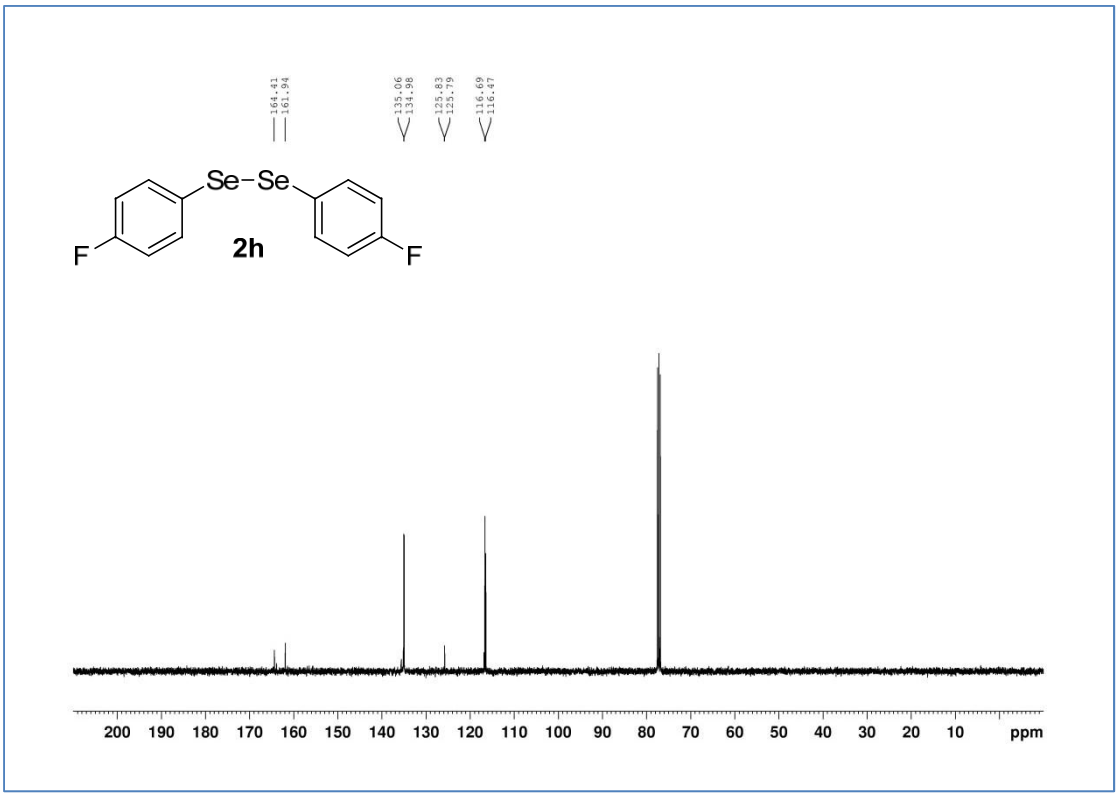
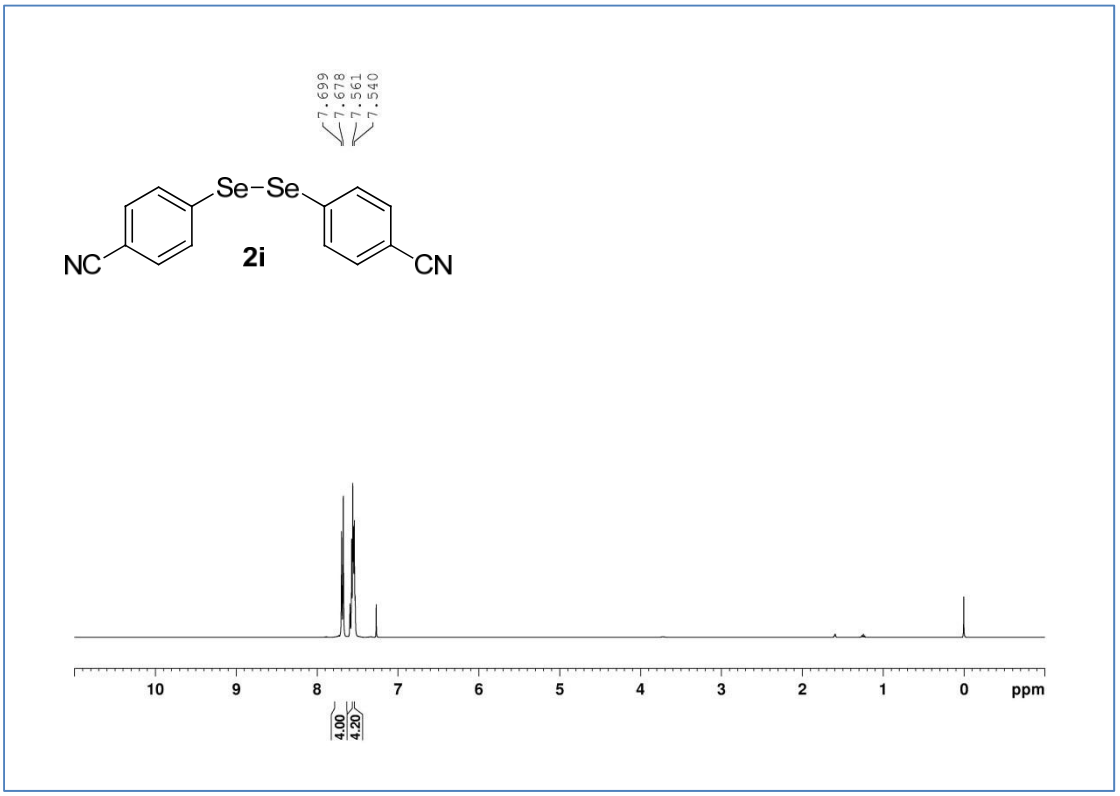

153.42
138.60
125.46
110.37
61.15
56.39
MeO
MeO
OMe
Se–Se
OMe
OMe
OMe
2f
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

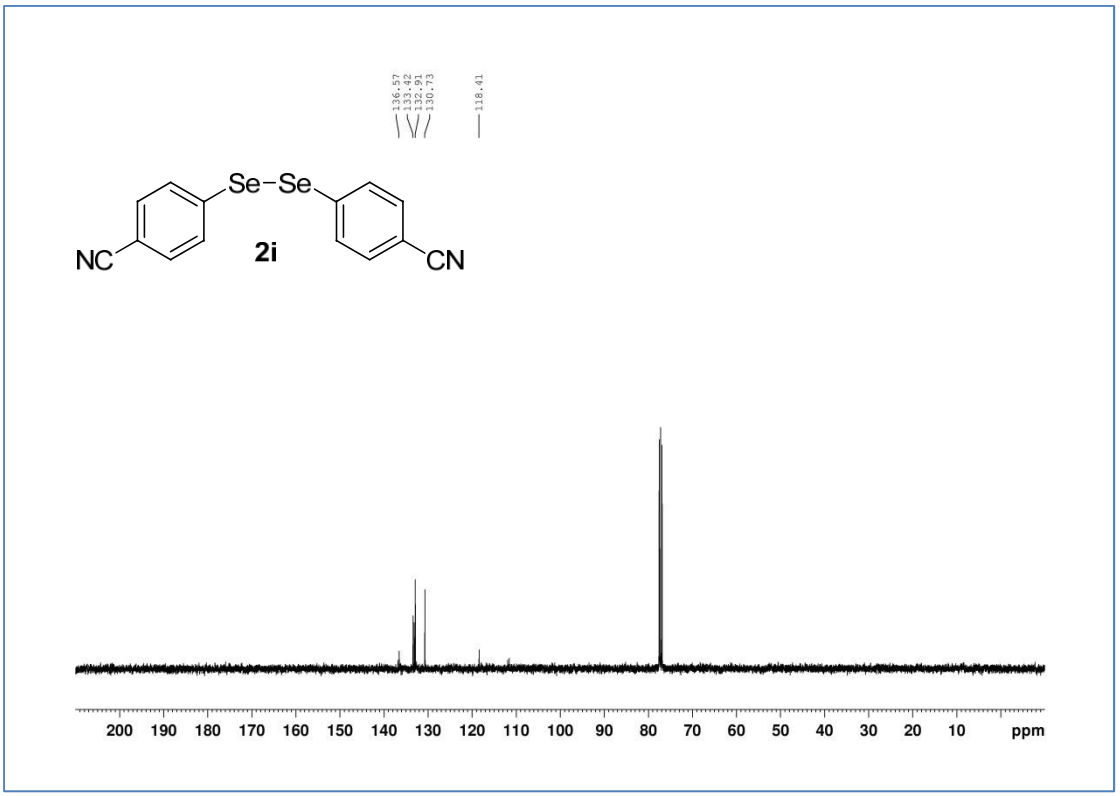

7.520
7.498
7.251
7.230
Se–Se
Cl
Cl
2g
10
9
8
7
6
5
4
3
2
1
0
ppm
2.00
2.02

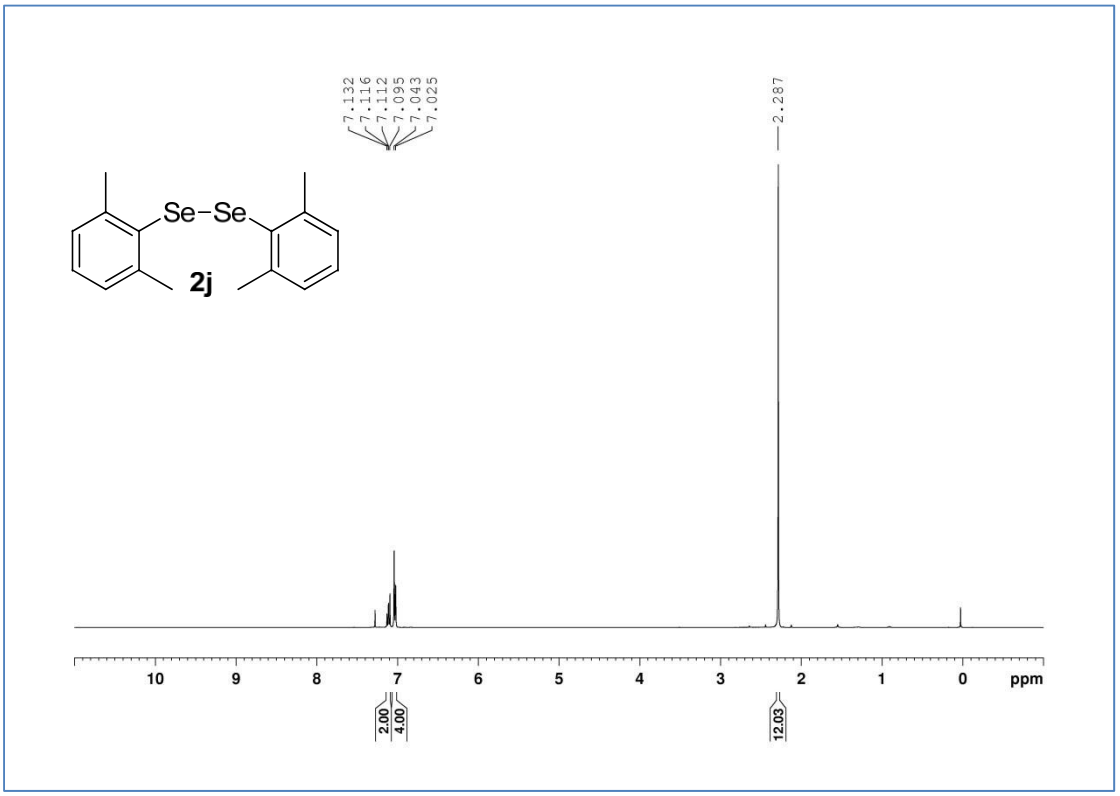

134.57
133.52
129.60
129.03
Se–Se
Cl
Cl
2g
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

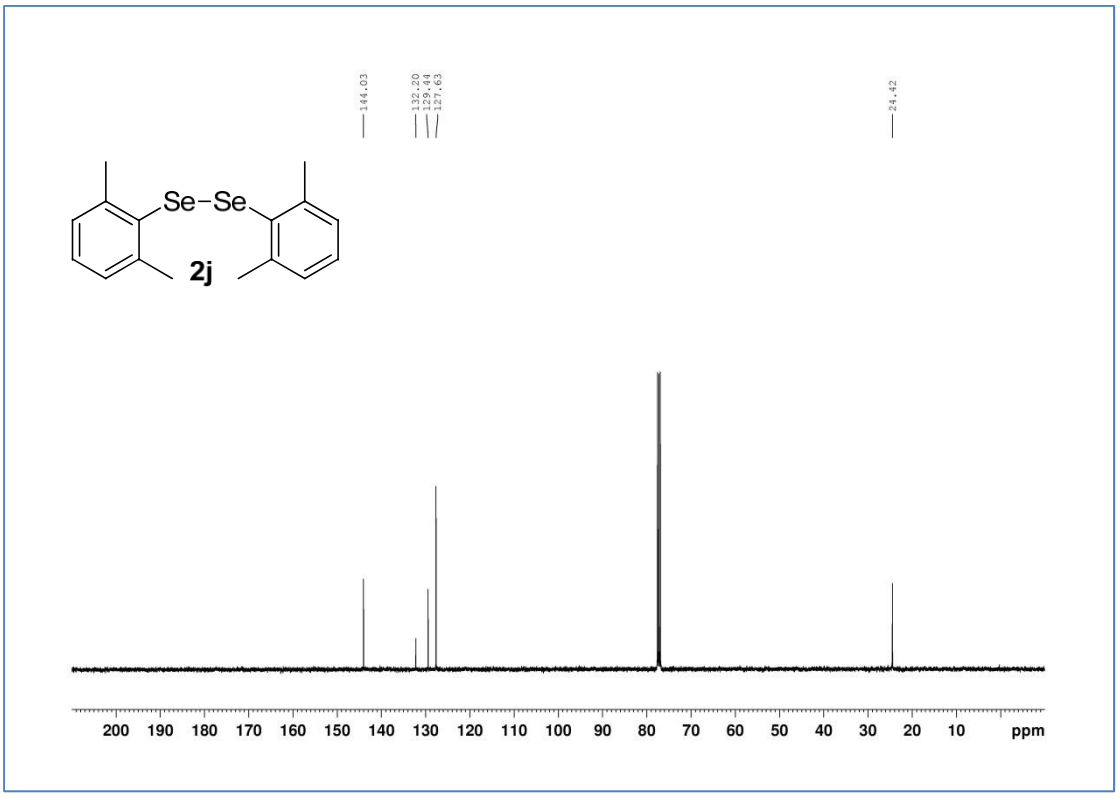

7.650
7.637
7.628
7.615
6.864
6.847
6.842
6.838
6.820
Se–Se
F
F
2h
10
9
8
7
6
5
4
3
2
1
0
ppm
4.00
4.00

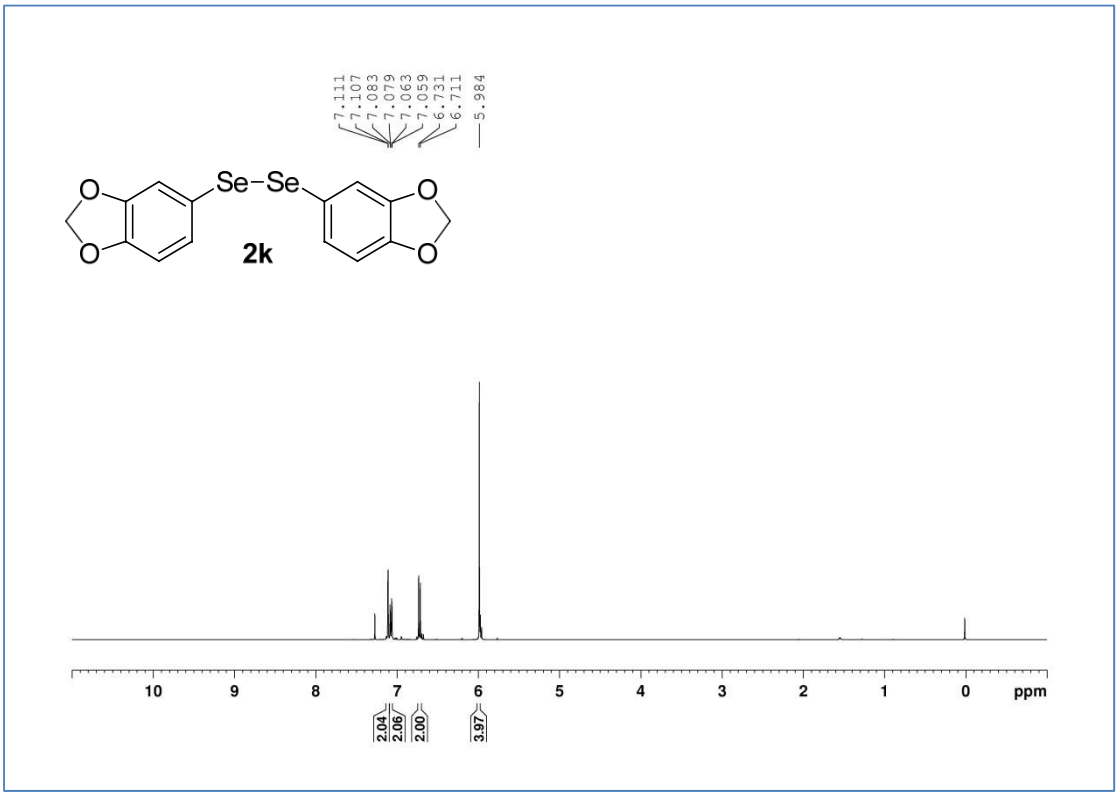

164.41
161.94
135.06
134.98
125.83
125.79
116.69
116.47
Se–Se
F
F
2h
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

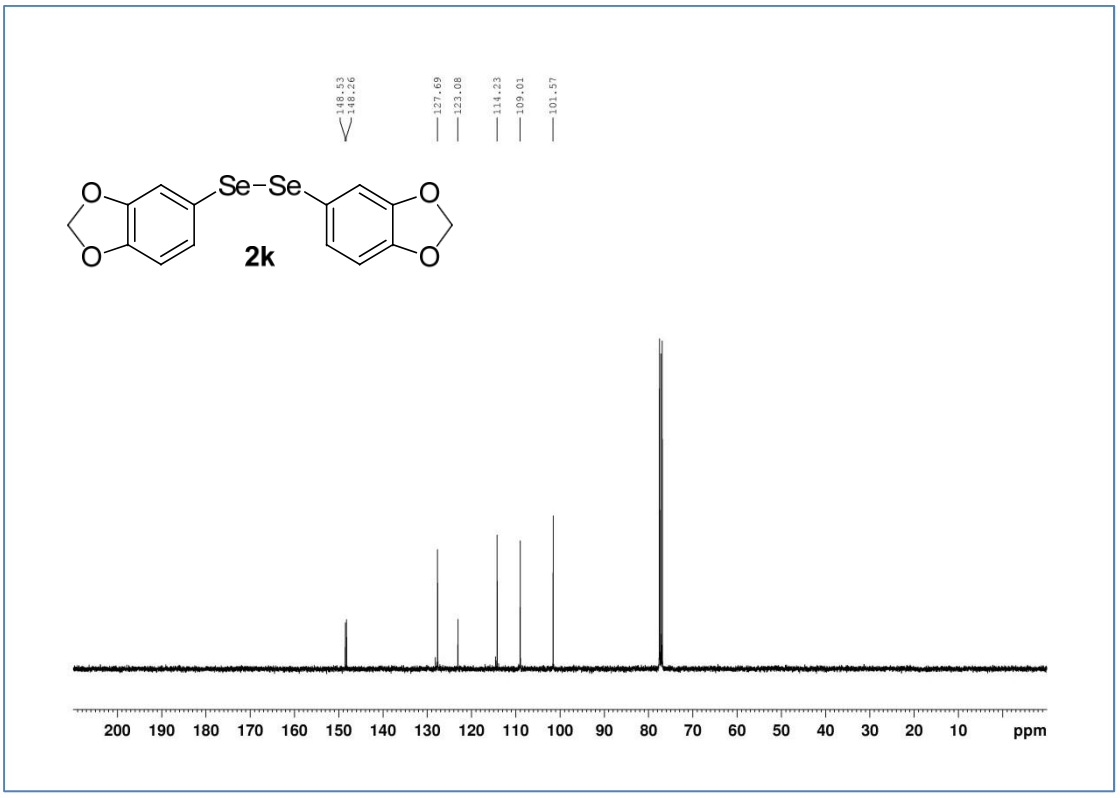

7.699
7.678
7.561
7.540
Se–Se
NC
CN
2i
10
9
8
7
6
5
4
3
2
1
0
ppm
4.00
4.20

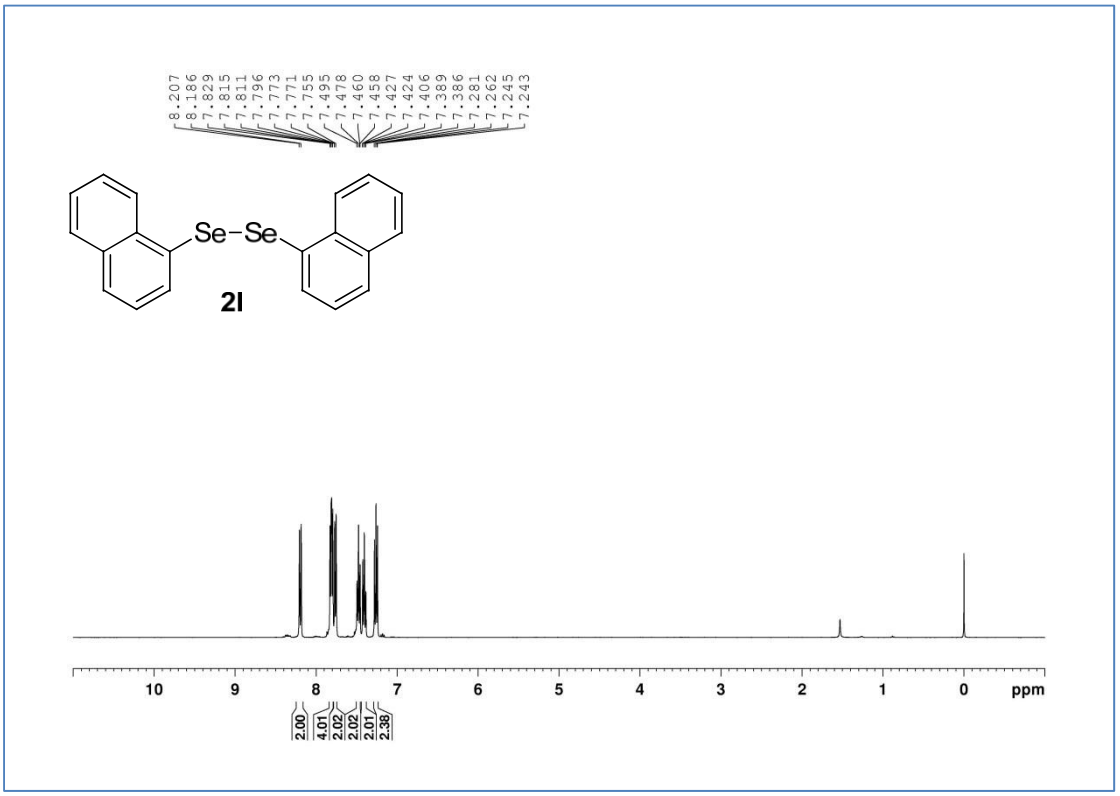

136.57
133.42
132.91
130.73
118.41
Se–Se
NC
CN
2i
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

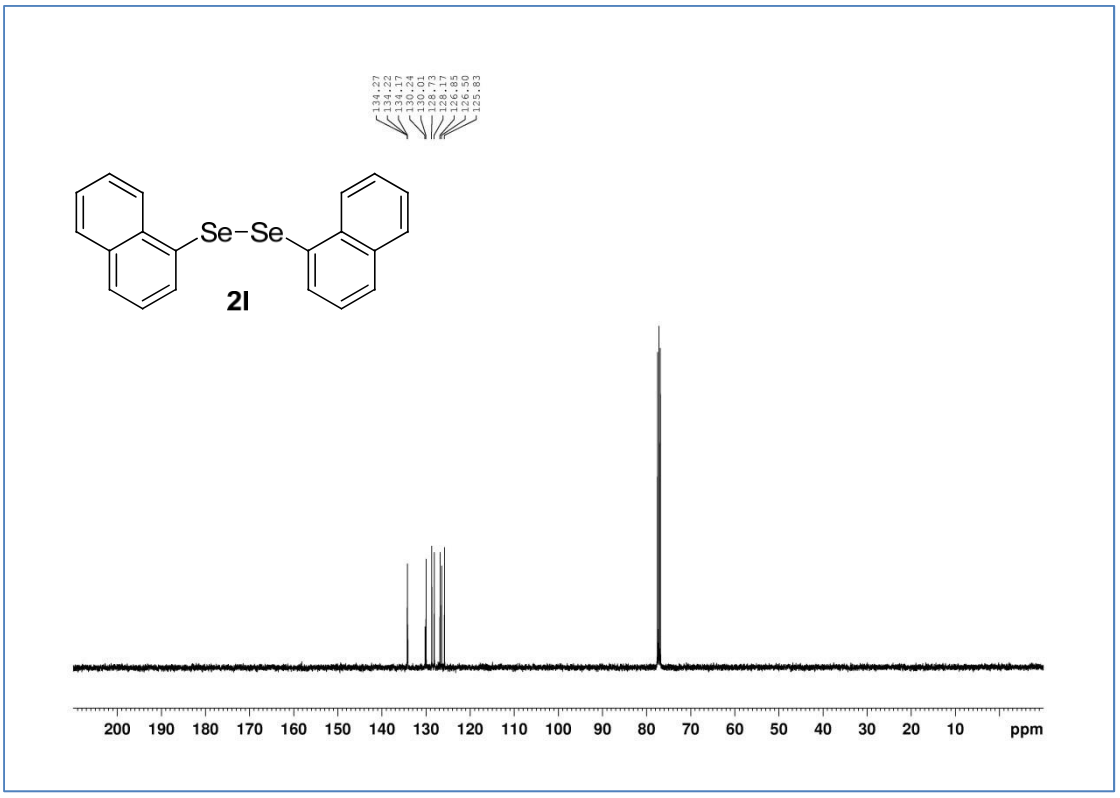

7.132
7.116
7.112
7.095
7.043
7.025
2.287
Se–Se
2j
10
9
8
7
6
5
4
3
2
1
0
ppm
2.00
4.00
12.03

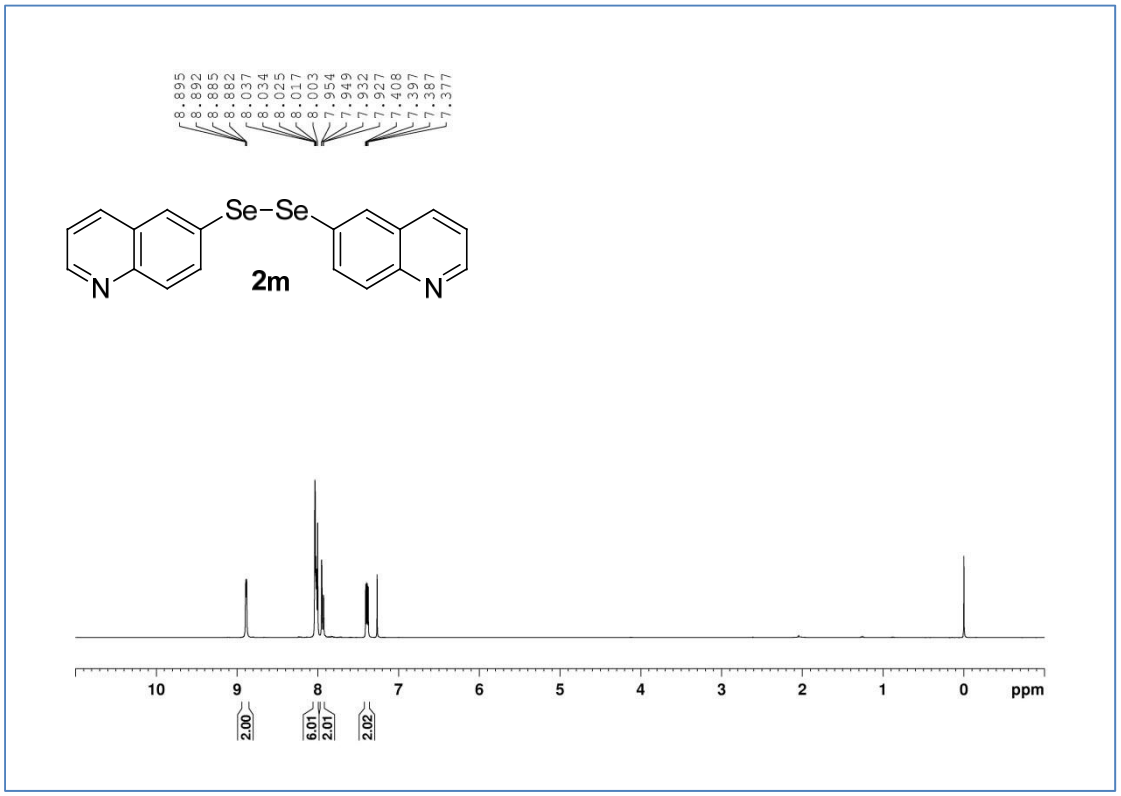

144.03
132.20
129.44
127.63
24.42
Se–Se
2j
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

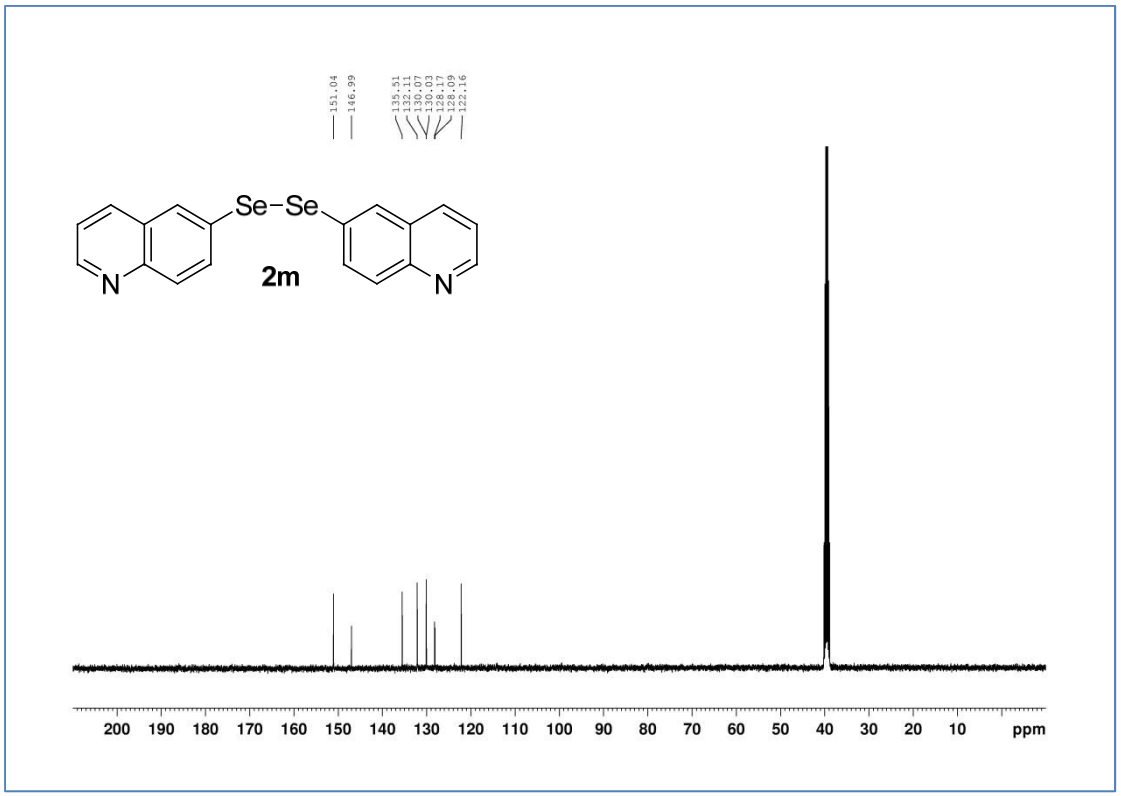

7.111
7.107
7.083
7.079
7.063
7.059
6.731
6.711
5.984
Se–Se
O
O
O
O
2k
10
9
8
7
6
5
4
3
2
1
0
ppm
2.04
2.06
2.00
3.97

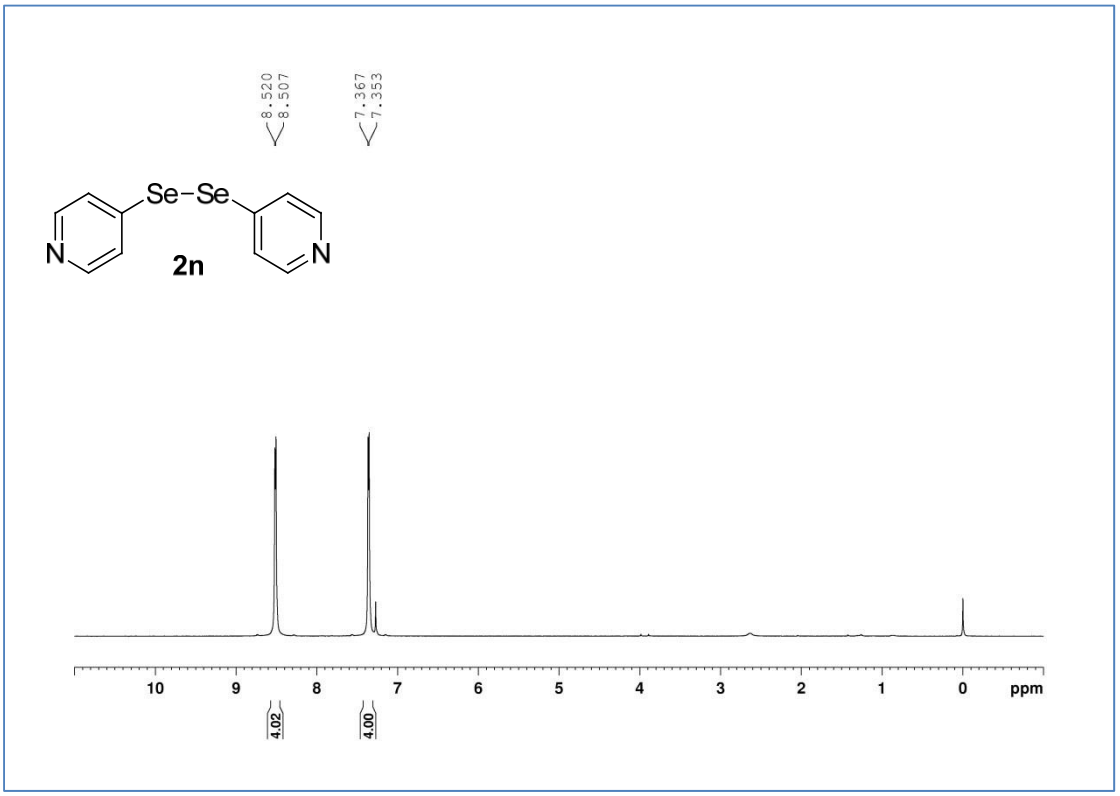

148.53
148.26
127.69
123.08
114.23
109.01
101.57
Se–Se
O
O
O
O
2k
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

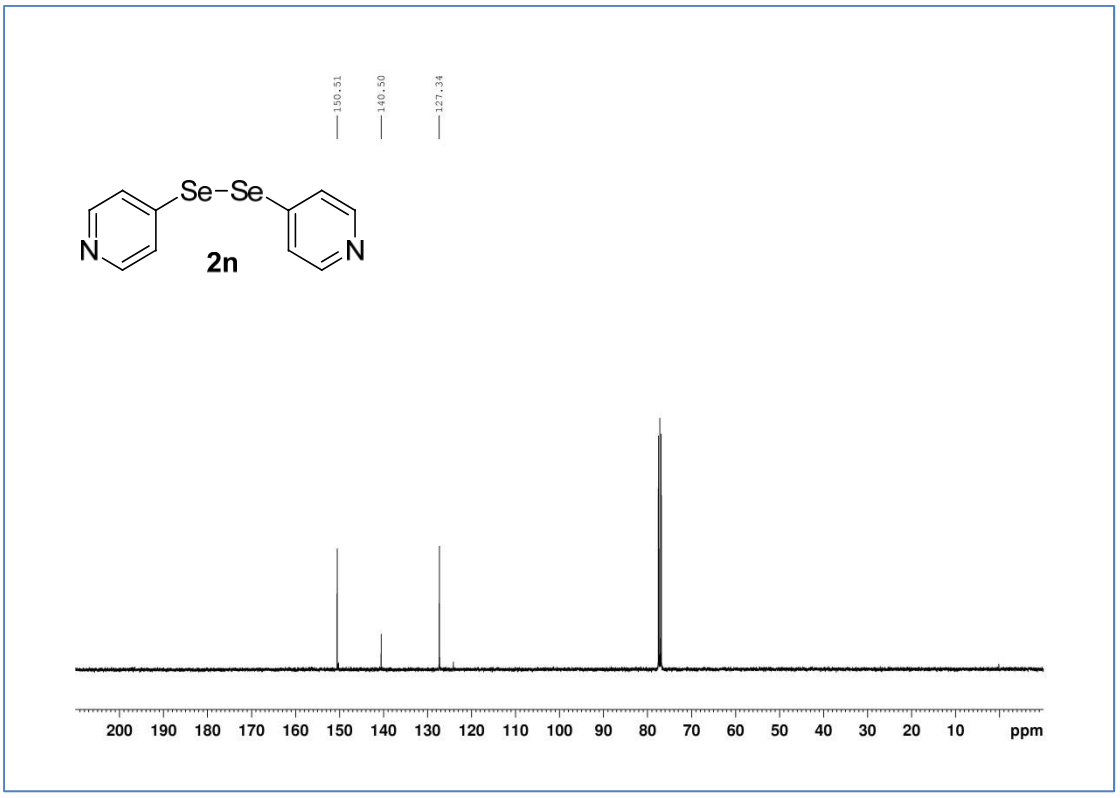

8.207
8.186
7.829
7.815
7.811
7.796
7.773
7.771
7.755
7.495
7.478
7.460
7.458
7.427
7.424
7.406
7.389
7.386
7.281
7.262
7.245
7.243
Se–Se
2l
10
9
8
7
6
5
4
3
2
1
0
ppm
2.00
4.01
2.02
2.02
2.01
2.38

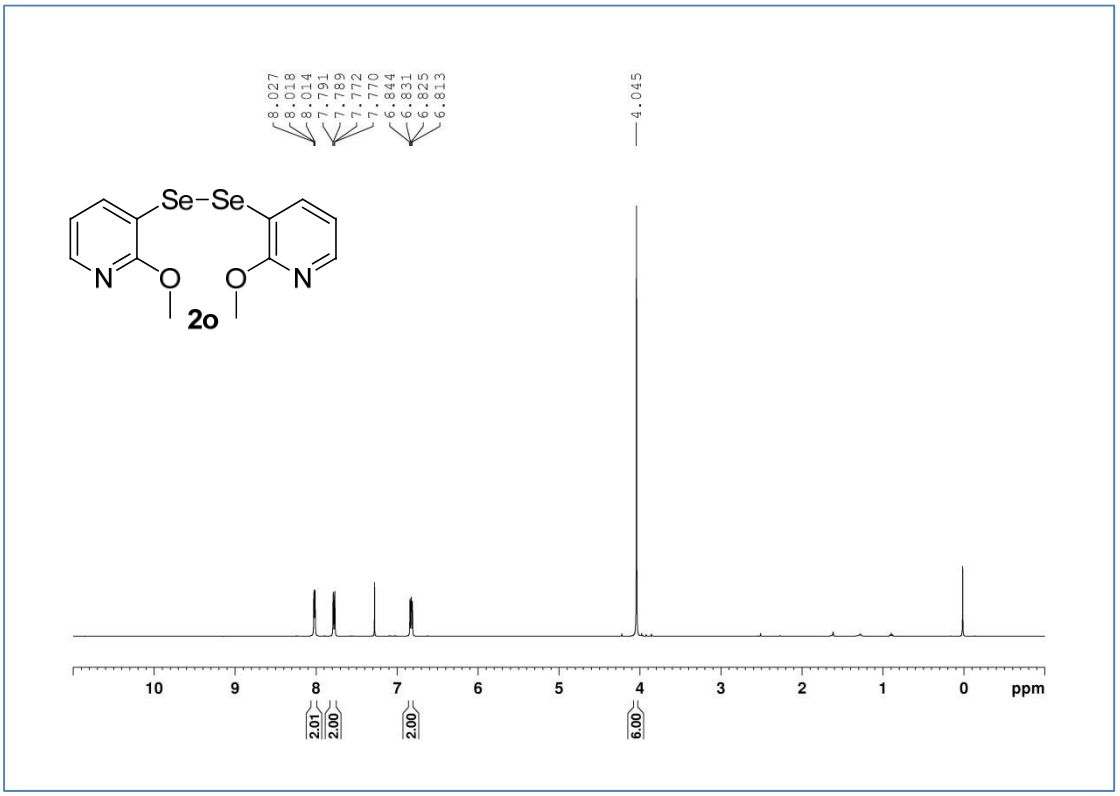

134.27
134.22
134.17
130.24
130.01
128.73
128.17
126.85
126.50
125.83
Se–Se
2l
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

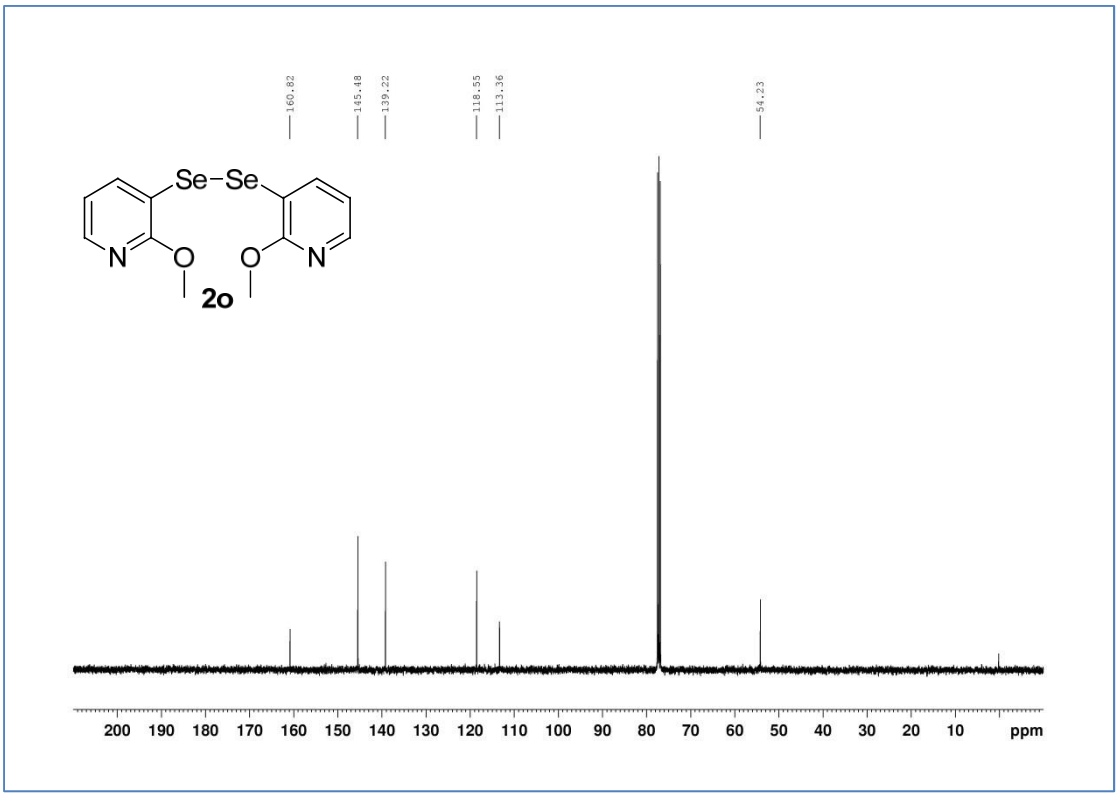

8.895
8.892
8.885
8.882
8.037
8.034
8.025
8.017
8.003
7.954
7.949
7.932
7.927
7.408
7.397
7.387
7.377
Se–Se
N
N
2m
10
9
8
7
6
5
4
3
2
1
0
ppm
2.00
6.01
2.01
2.02

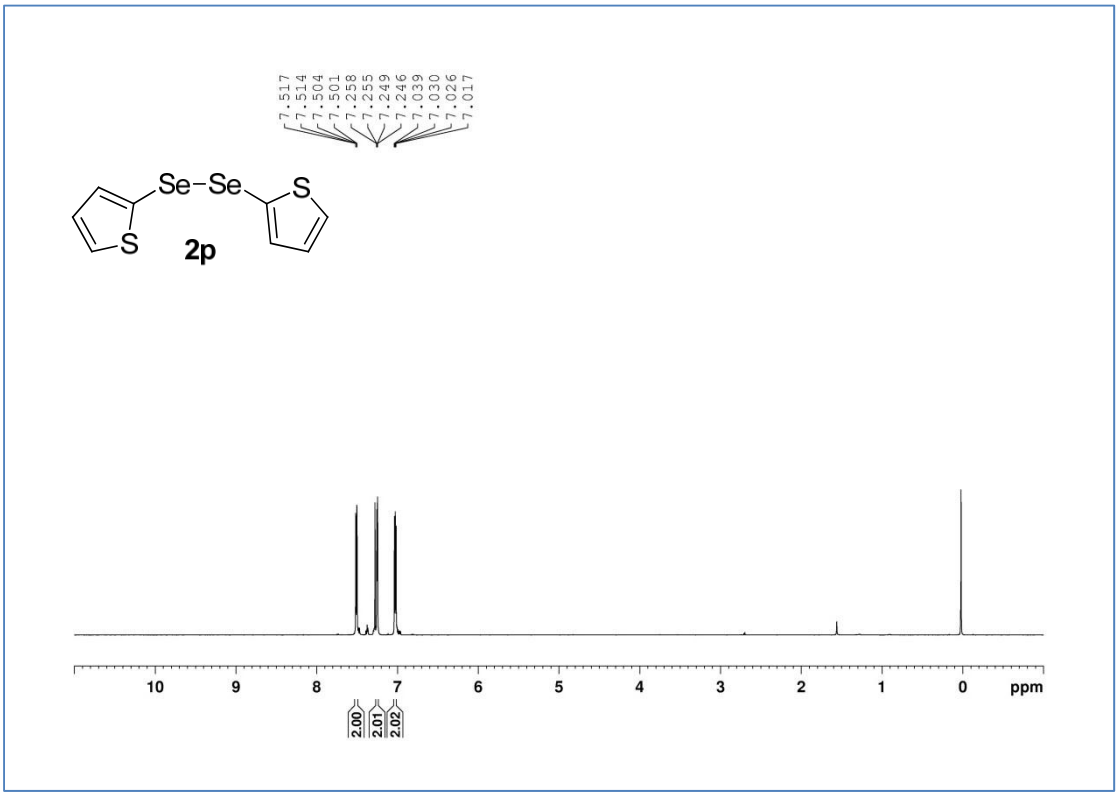

151.04
146.99
139.51
132.11
130.07
130.03
128.17
128.09
122.16
Se–Se
N
N
2m
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

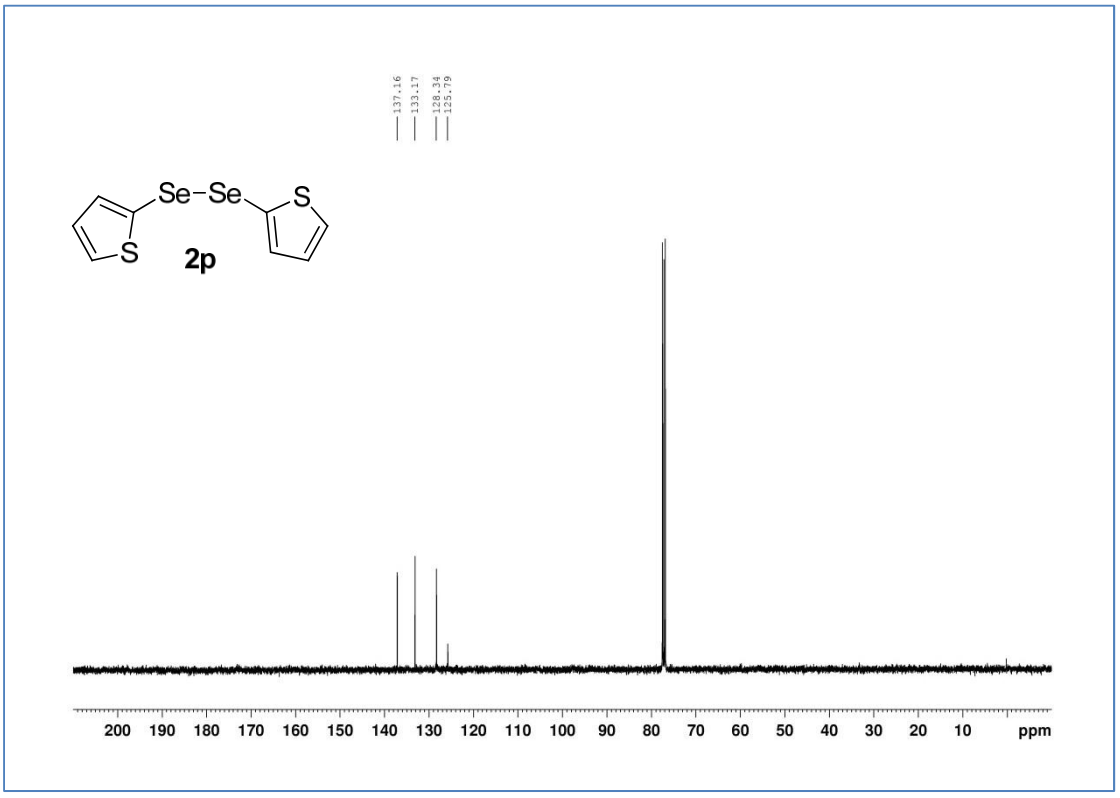

8.520
8.507
7.367
7.353
Se–Se
N
N
2n
10
9
8
7
6
5
4
3
2
1
0
ppm
4.02
4.00

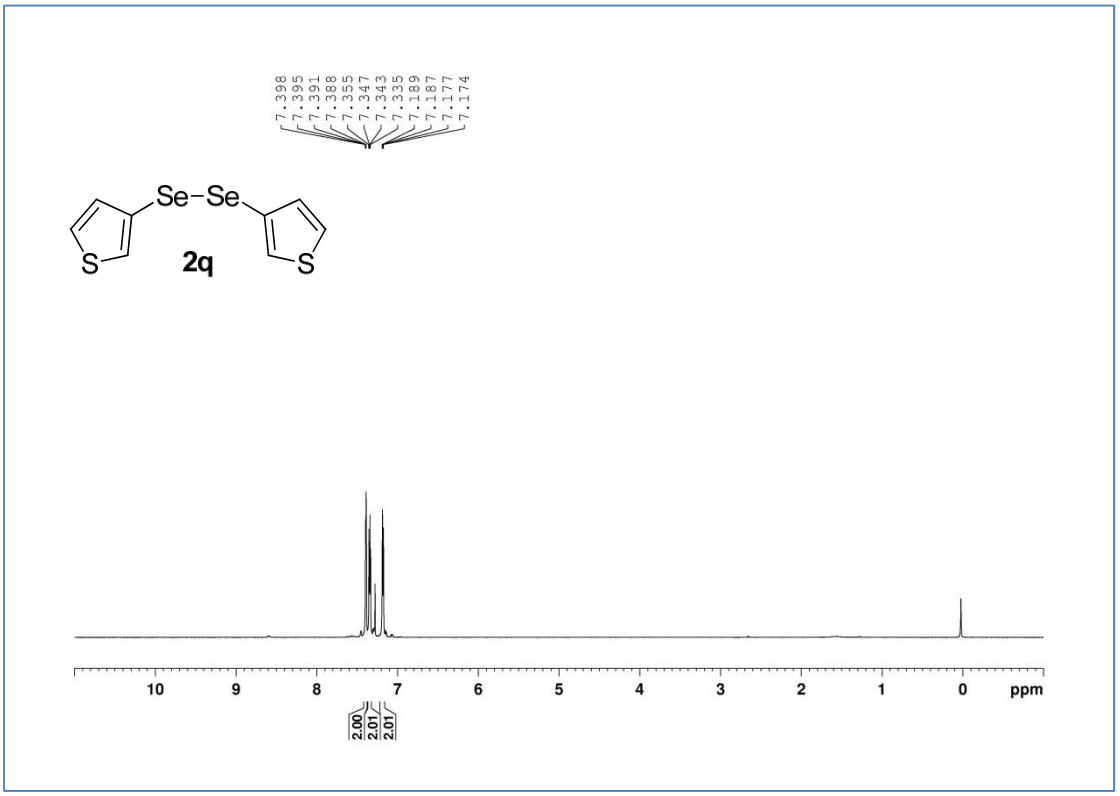

150.51
140.50
127.34
Se–Se
N
N
2n
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

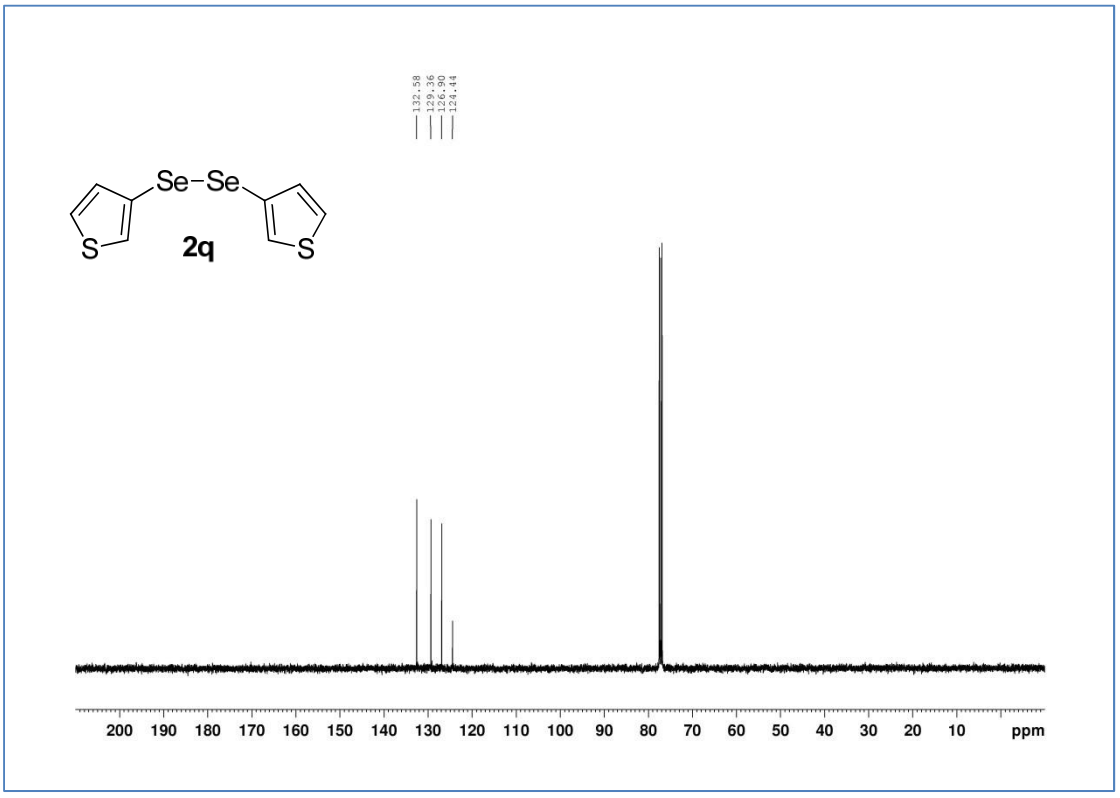

8.027
8.018
8.014
7.791
7.789
7.772
7.770
6.844
6.831
6.825
6.813
4.045
Se–Se
N
O
O
N
2o
10
9
8
7
6
5
4
3
2
1
0
ppm
2.01
2.00
2.00
6.00

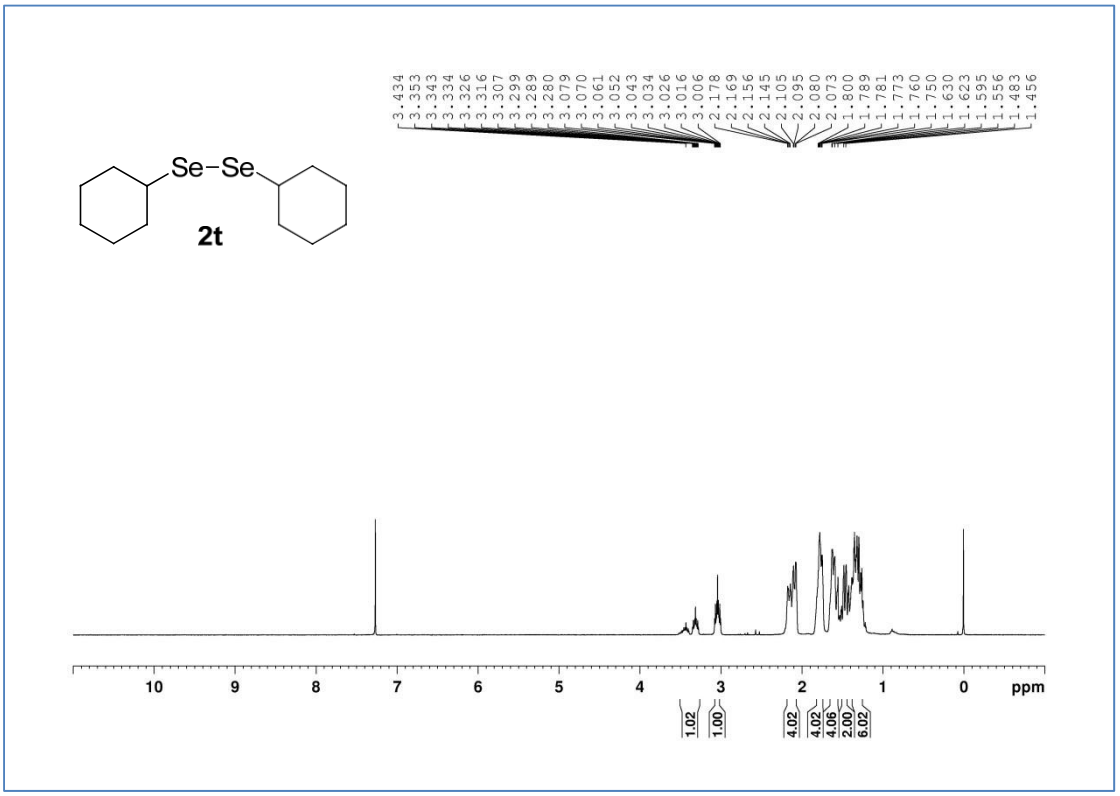

160.82
145.48
139.22
118.55
113.36
54.23
Se–Se
N
O
O
N
2o
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

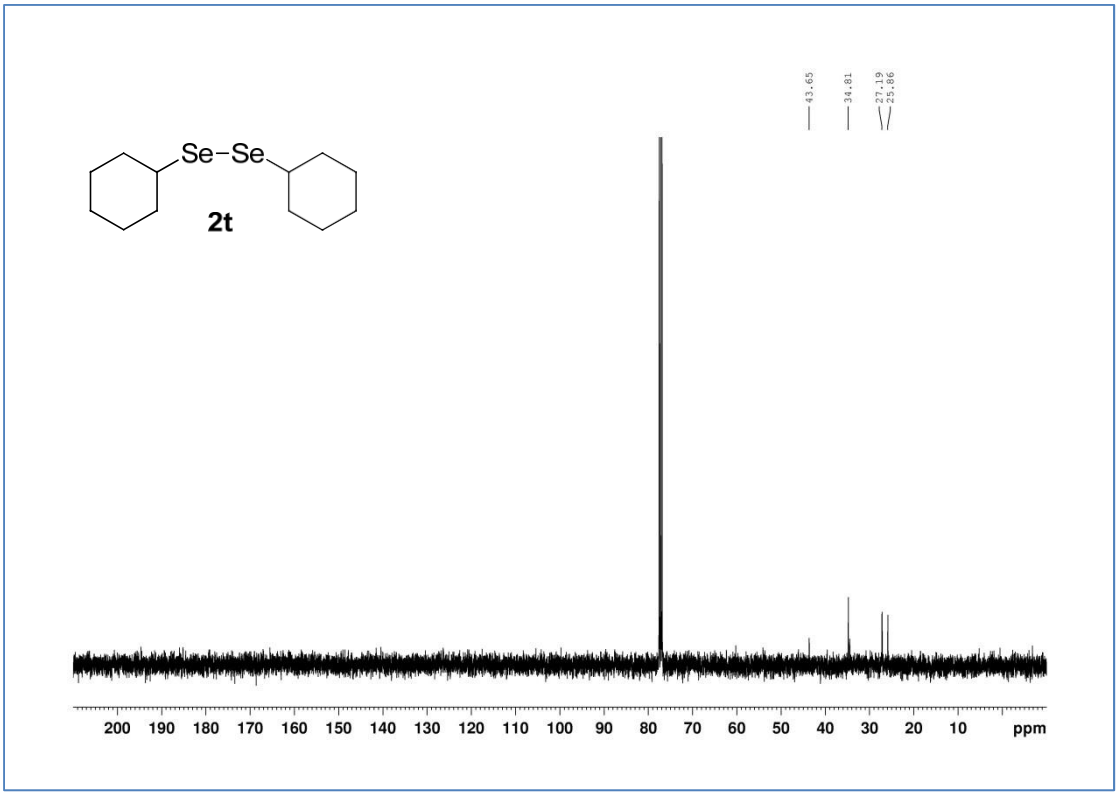

7.517
7.514
7.504
7.501
7.258
7.255
7.249
7.246
7.039
7.030
7.026
7.017
Se–Se
S
S
2p
10
9
8
7
6
5
4
3
2
1
0
ppm
2.00
2.01
2.02

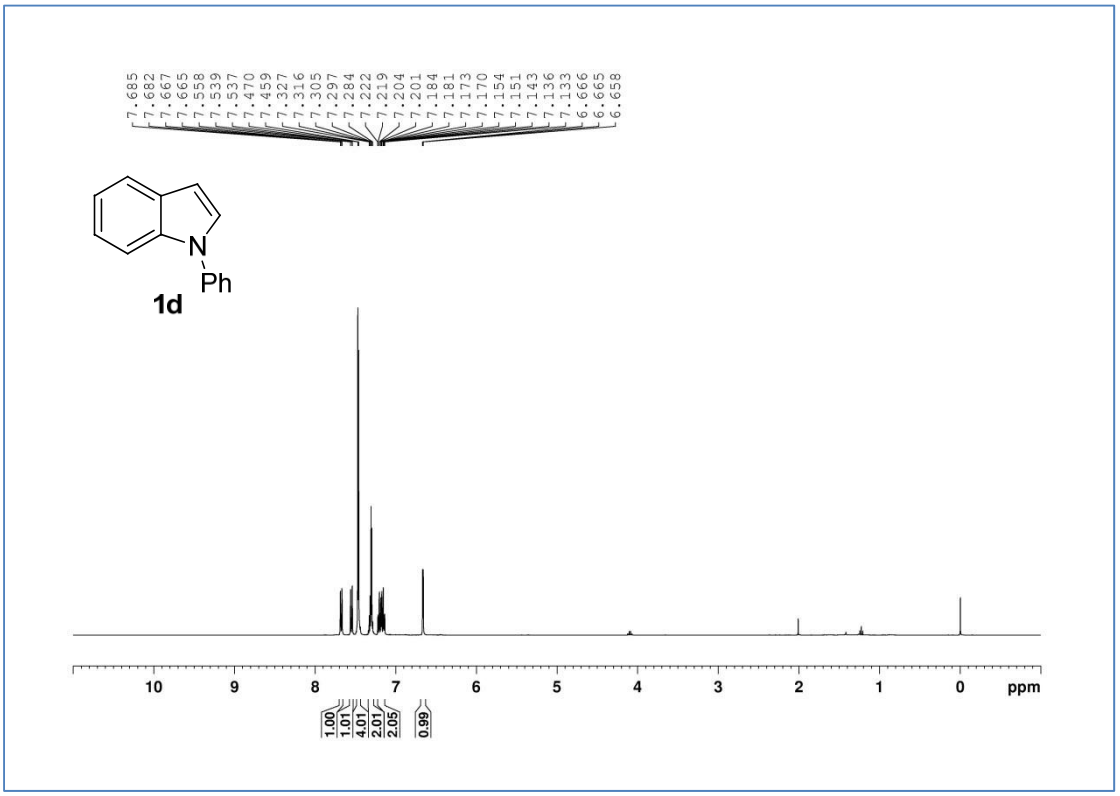

137.16
133.17
128.34
125.79
Se–Se
S
S
2p
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

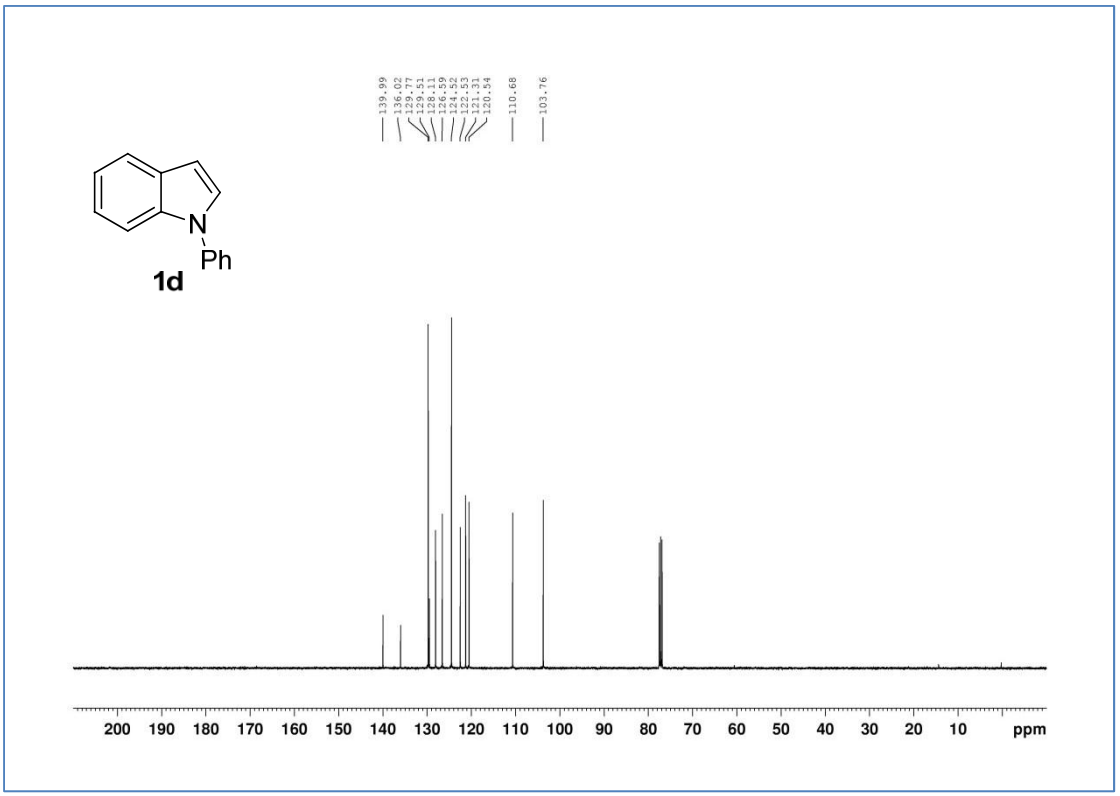

7.398
7.395
7.391
7.388
7.355
7.347
7.343
7.335
7.189
7.187
7.177
7.174
Se–Se
S
S
2q
10
9
8
7
6
5
4
3
2
1
0
ppm
2.00
2.01
2.01

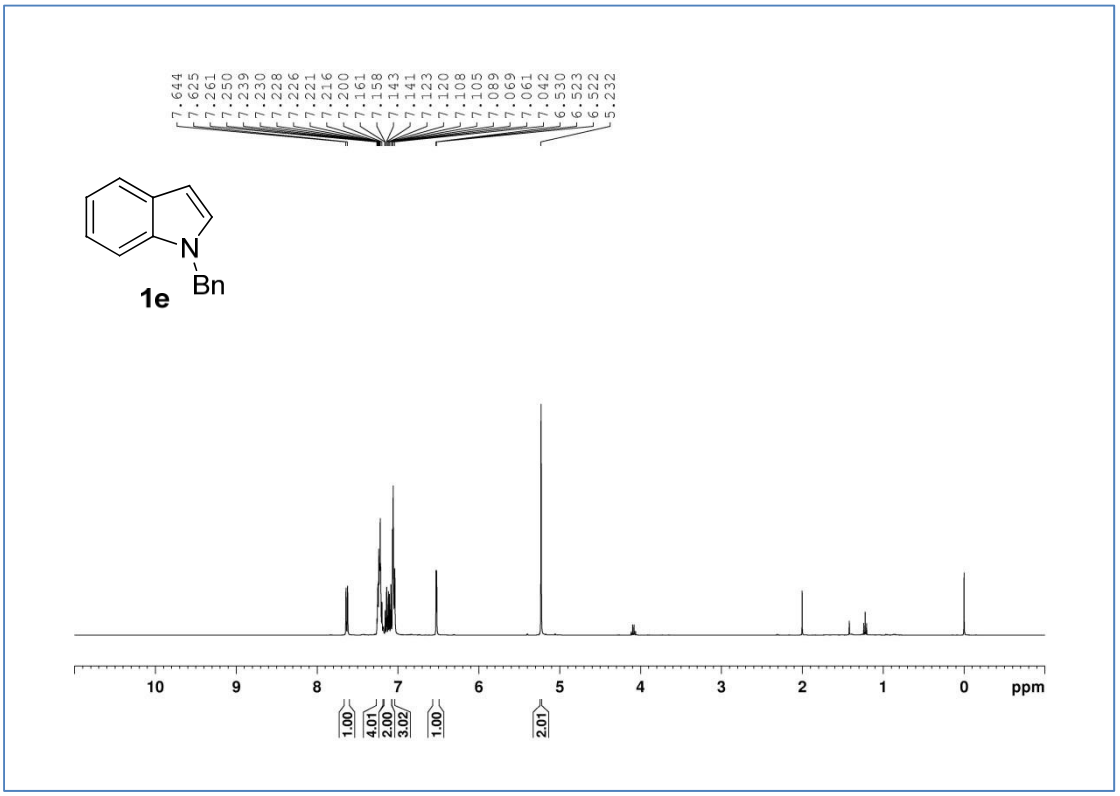

132.58
129.36
126.90
124.44
Se–Se
S
S
2q
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

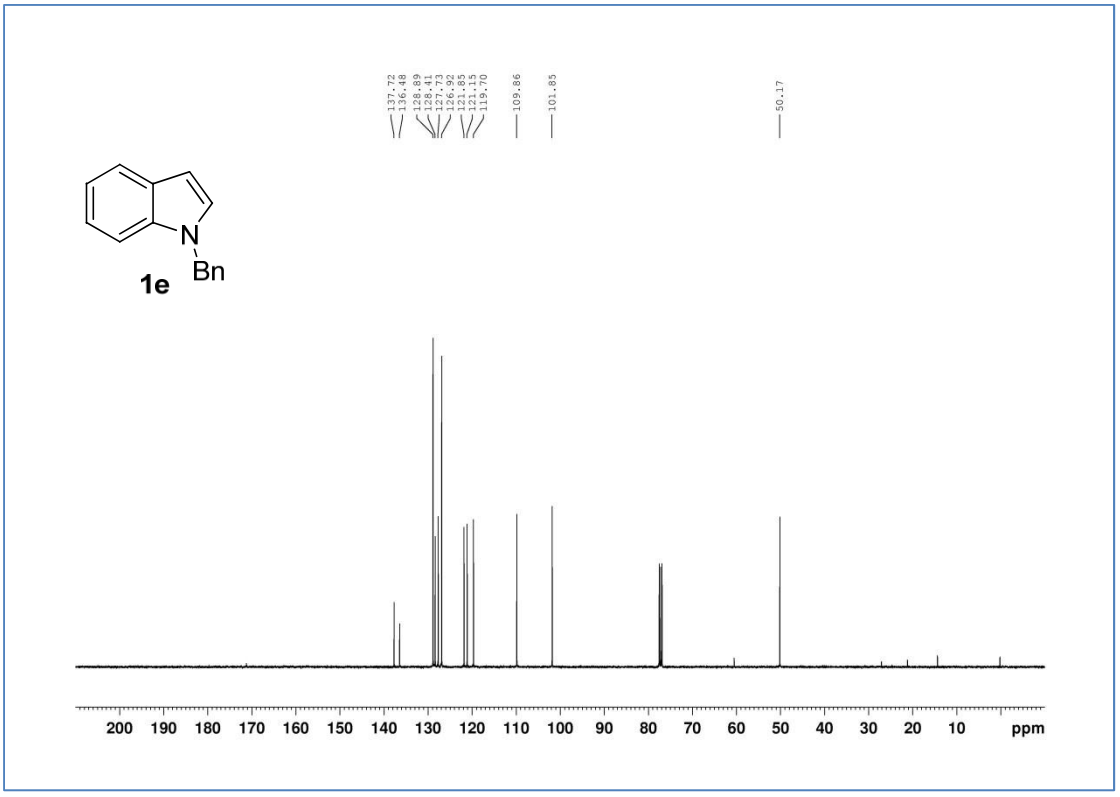

Se–Se
2t
3.434
3.353
3.343
3.334
3.326
3.316
3.307
3.299
3.289
3.280
3.079
3.070
3.061
3.052
3.043
3.034
3.026
3.016
3.006
2.178
2.169
2.156
2.145
2.105
2.095
2.080
2.073
1.800
1.789
1.781
1.773
1.760
1.750
1.630
1.623
1.595
1.556
1.483
1.456
10 9 8 7 6 5 4 3 2 1 0 ppm
1.02
1.00
4.02
4.02
4.06
2.00
6.02

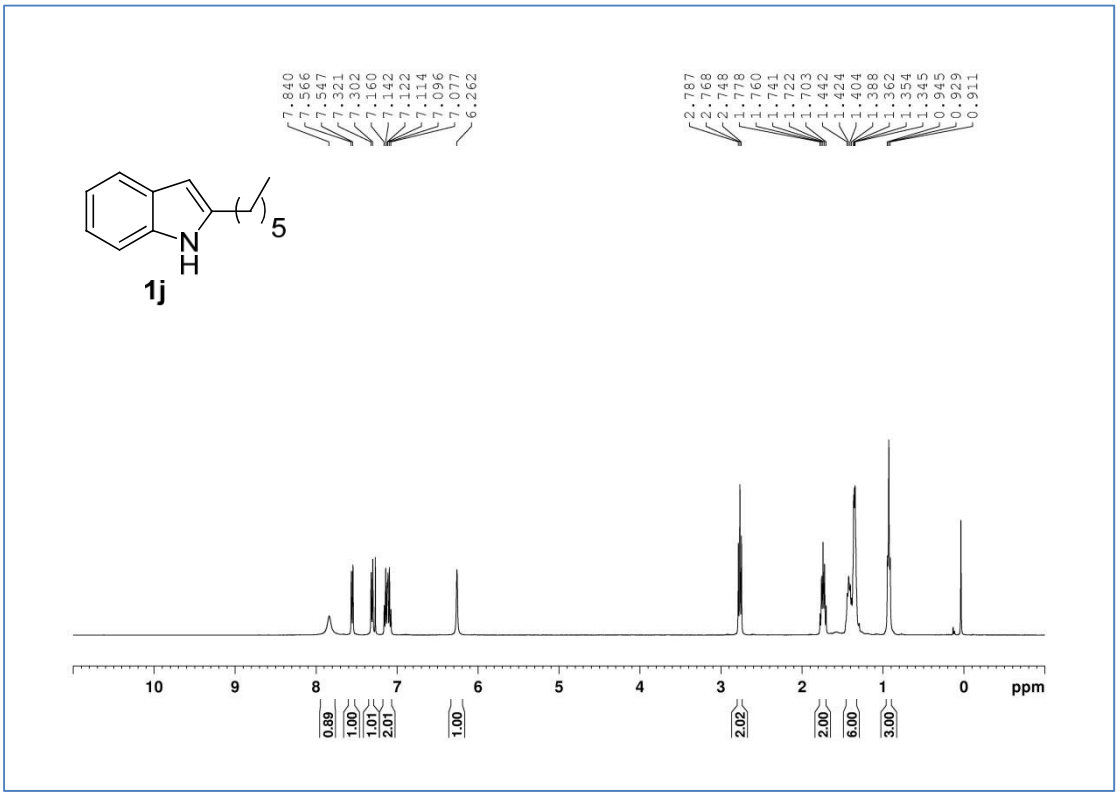

Se–Se
2t
43.65
34.81
27.19
25.86
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


7.685
7.682
7.667
7.665
7.558
7.539
7.537
7.470
7.459
7.327
7.316
7.305
7.297
7.284
7.222
7.219
7.204
7.201
7.184
7.181
7.173
7.170
7.154
7.151
7.143
7.136
7.133
6.666
6.665
6.658
N
Ph
1d
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.01
4.01
2.01
2.05
0.99


139.99
136.02
129.77
129.51
128.11
126.59
124.52
122.53
121.31
120.54
110.68
103.76
N
Ph
1d
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


7.644
7.625
7.261
7.250
7.239
7.230
7.228
7.226
7.221
7.216
7.200
7.161
7.158
7.143
7.141
7.123
7.120
7.108
7.105
7.089
7.069
7.061
7.042
6.530
6.523
6.522
5.232
N
Bn
1e
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
4.01
2.00
3.02
1.00
2.01


137.72
136.48
128.89
128.41
127.73
126.92
121.85
121.15
119.70
109.86
101.85
50.17
N
Bn
1e
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


7.840
7.566
7.547
7.321
7.302
7.160
7.142
7.122
7.114
7.096
7.077
6.262
2.787
2.768
2.748
1.778
1.760
1.741
1.722
1.703
1.442
1.424
1.404
1.388
1.362
1.354
1.345
0.945
0.929
0.911
5
N
H
1j
10
9
8
7
6
5
4
3
2
1
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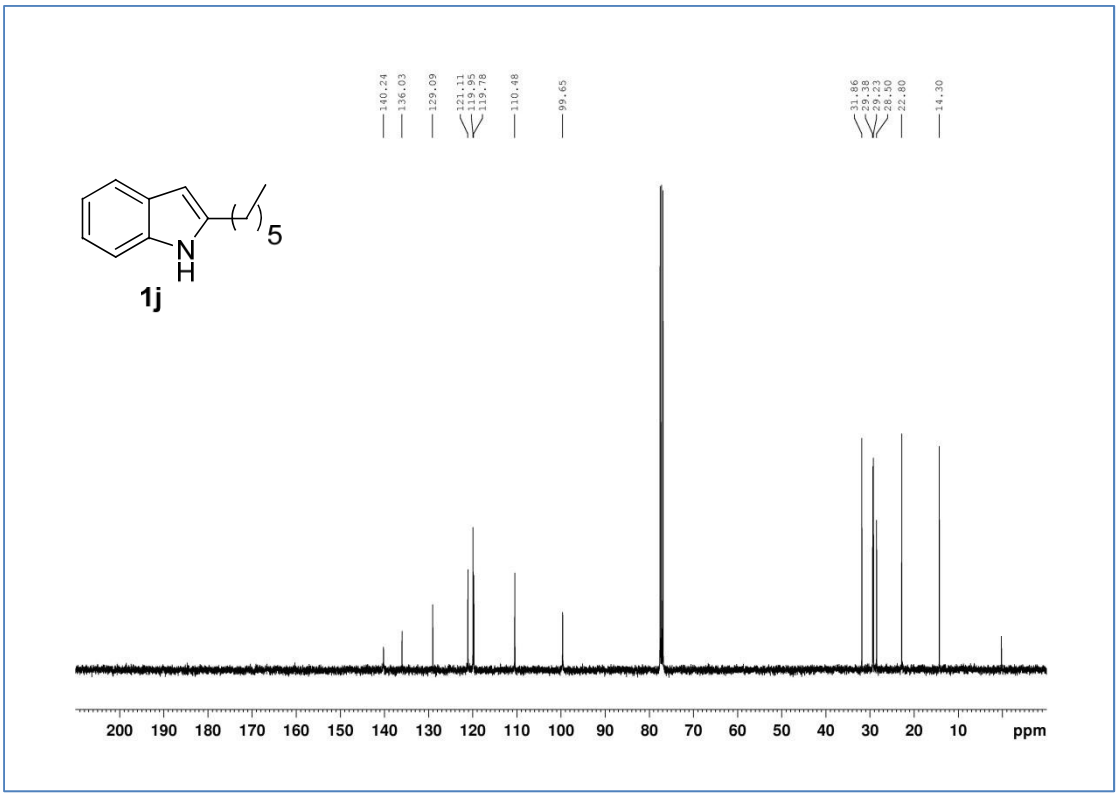
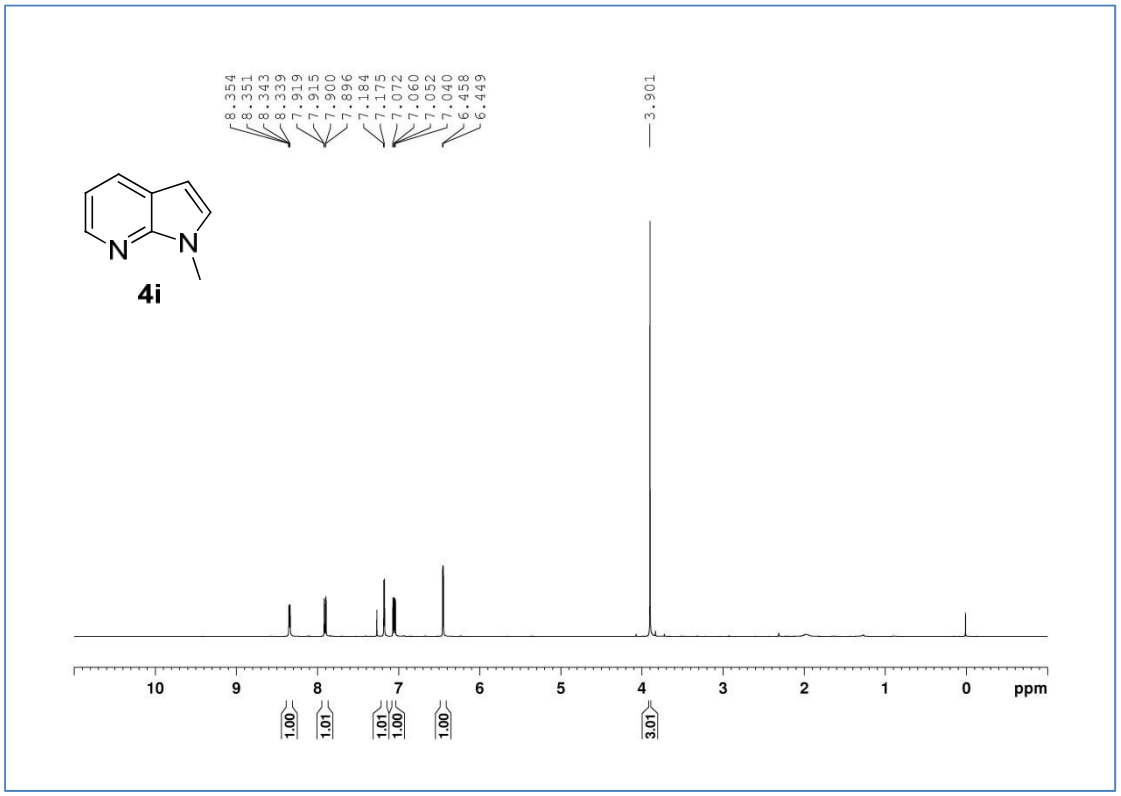
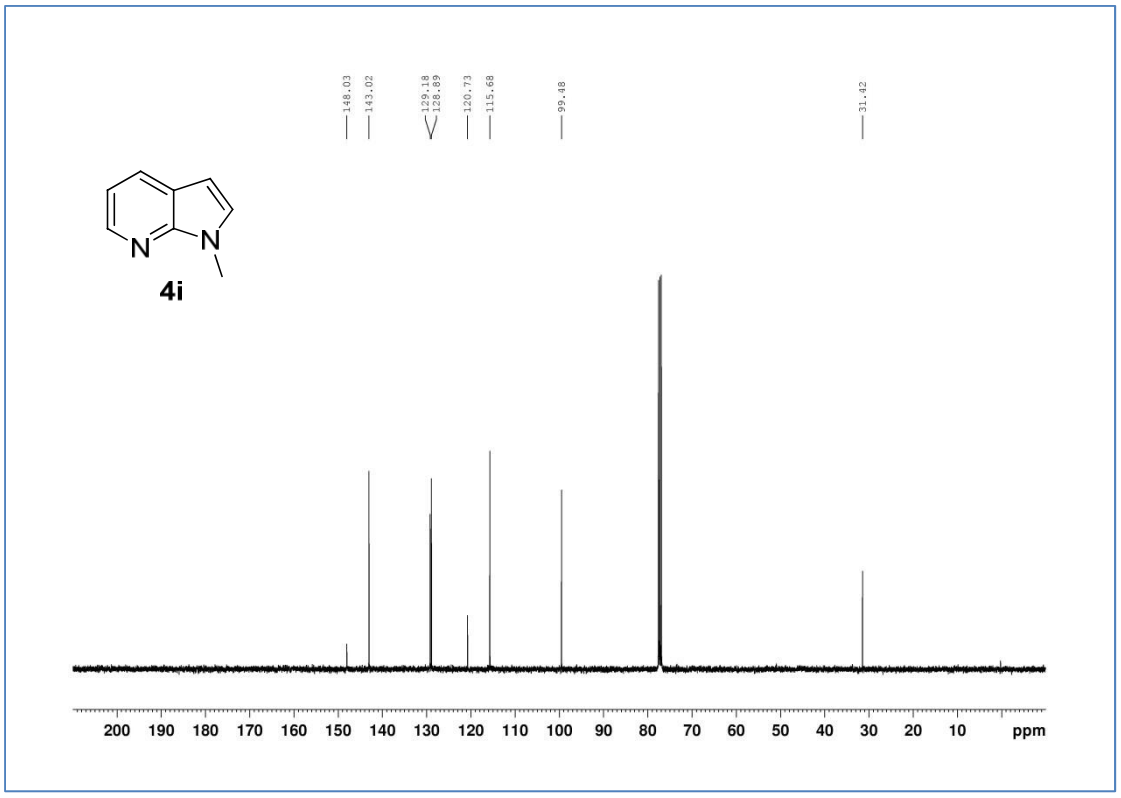
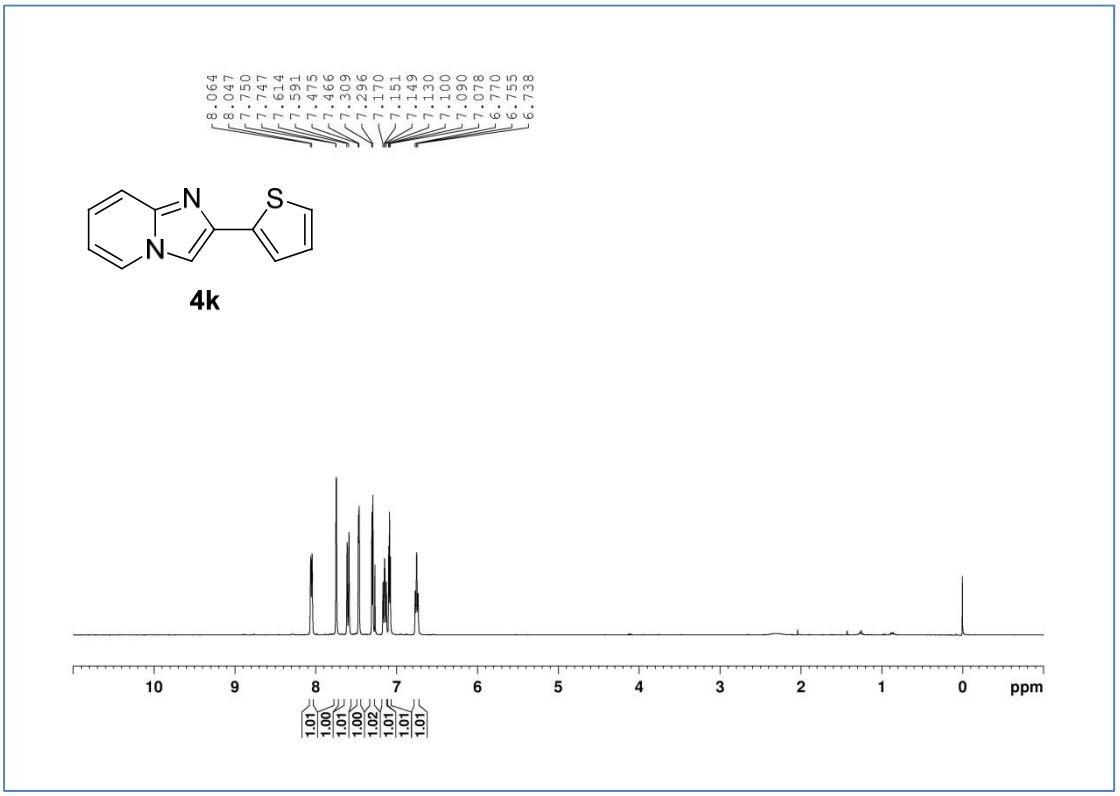
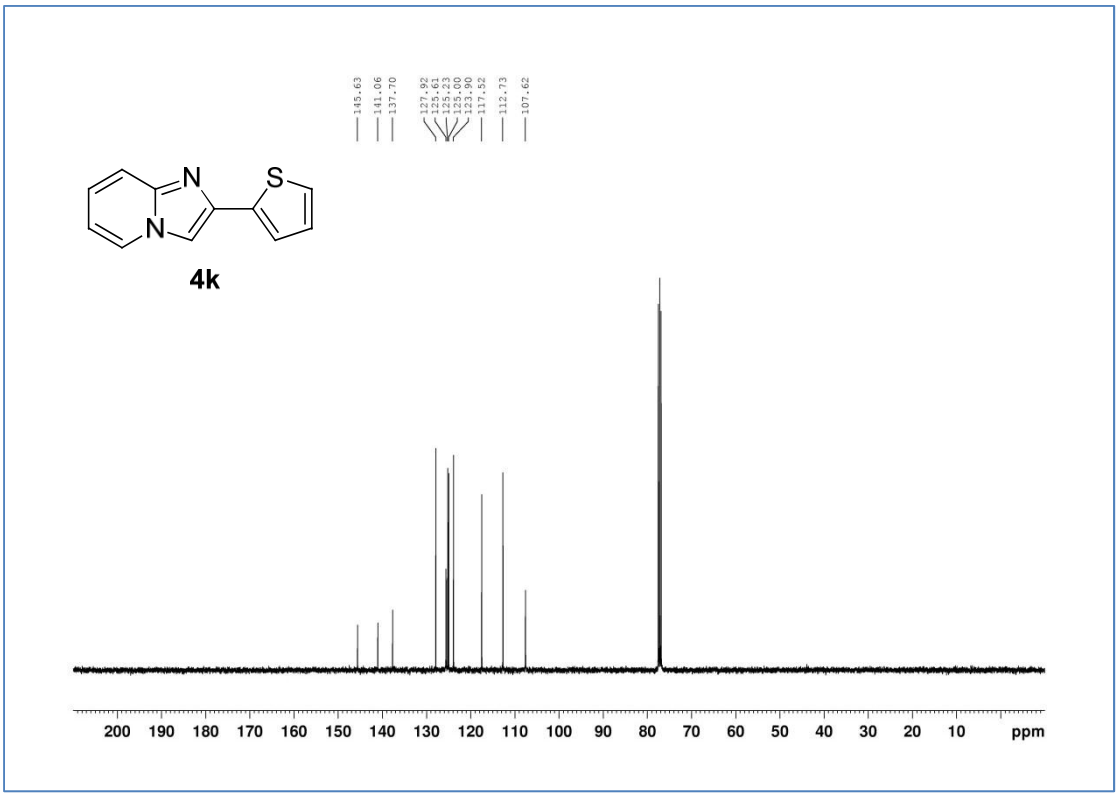
ppm
0.89
1.00
1.01
2.01
1.00
2.02
2.00
6.00
3.00

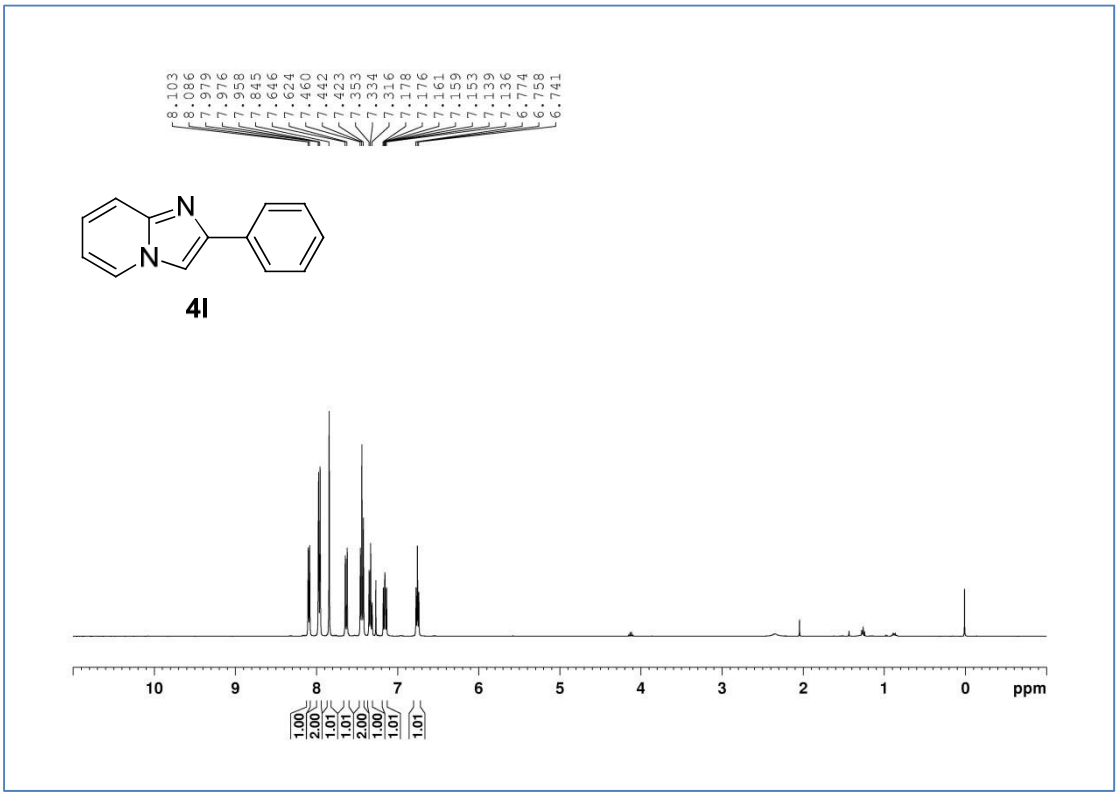

140.24
136.03
129.09
121.11
119.95
119.78
110.48
99.65
31.86
29.38
29.23
28.50
22.80
14.30
5
N
H
1j
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

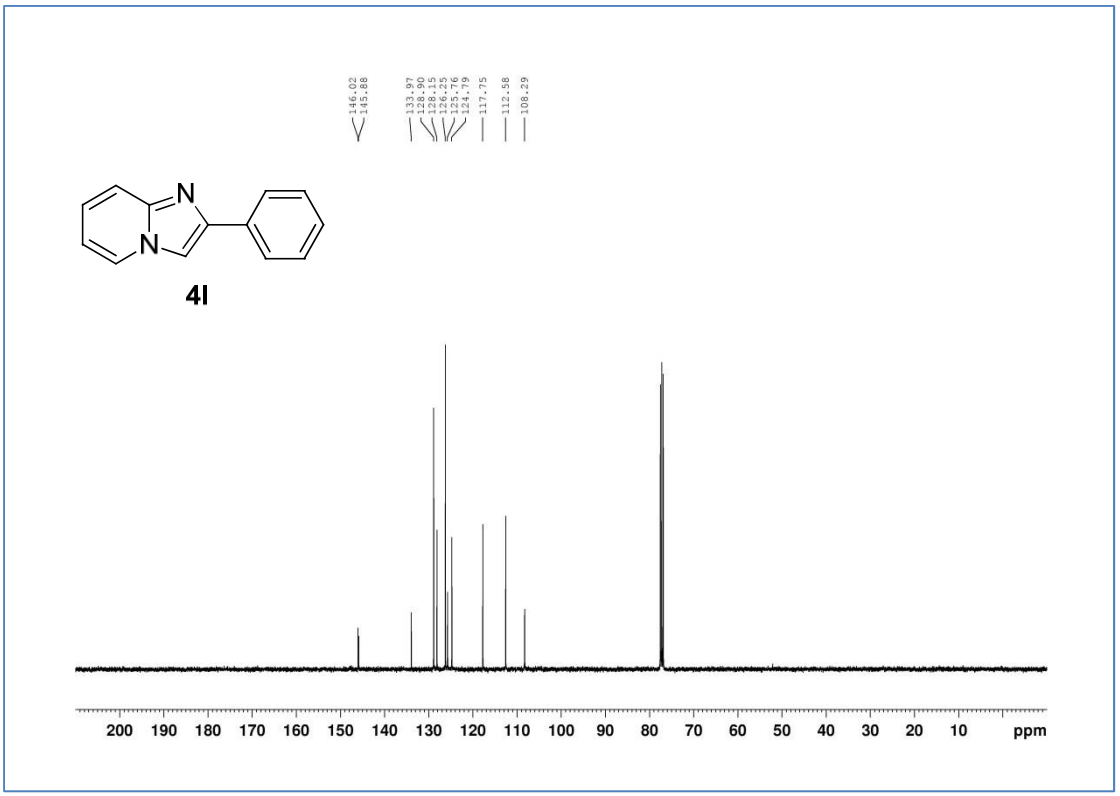

8.354
8.351
8.343
8.339
7.919
7.915
7.900
7.896
7.184
7.175
7.072
7.060
7.052
7.040
6.458
6.449
3.901
4i
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.01
1.01
1.00
1.00
3.01


148.03
143.02
129.18
128.89
120.73
115.68
99.48
31.42
4i
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

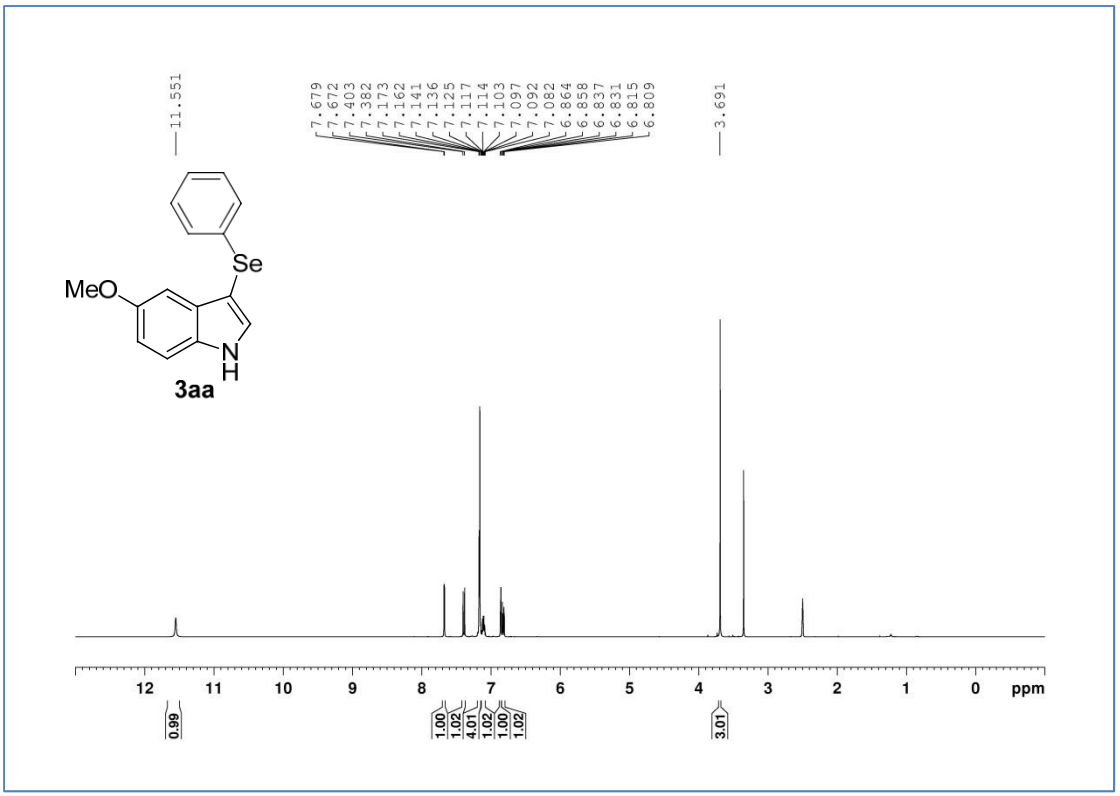

8.064
8.047
7.750
7.747
7.614
7.591
7.475
7.466
7.309
7.296
7.170
7.151
7.149
7.130
7.100
7.090
7.078
6.770
6.755
6.738
N
S
N
4k
10
9
8
7
6
5
4
3
2
1
0
ppm
1.01
1.00
1.01
1.00
1.02
1.01
1.01
1.01

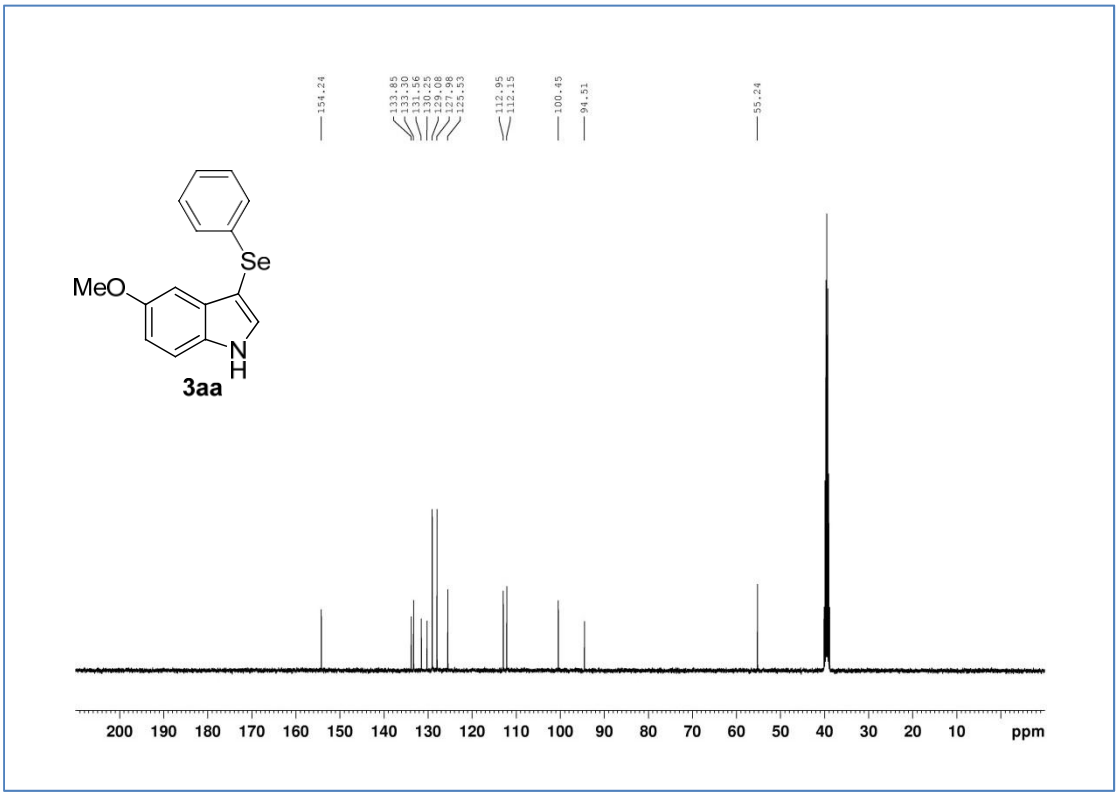

145.63
141.06
137.70
127.92
125.61
125.23
125.00
123.90
117.52
112.73
107.62
N
S
N
4k
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

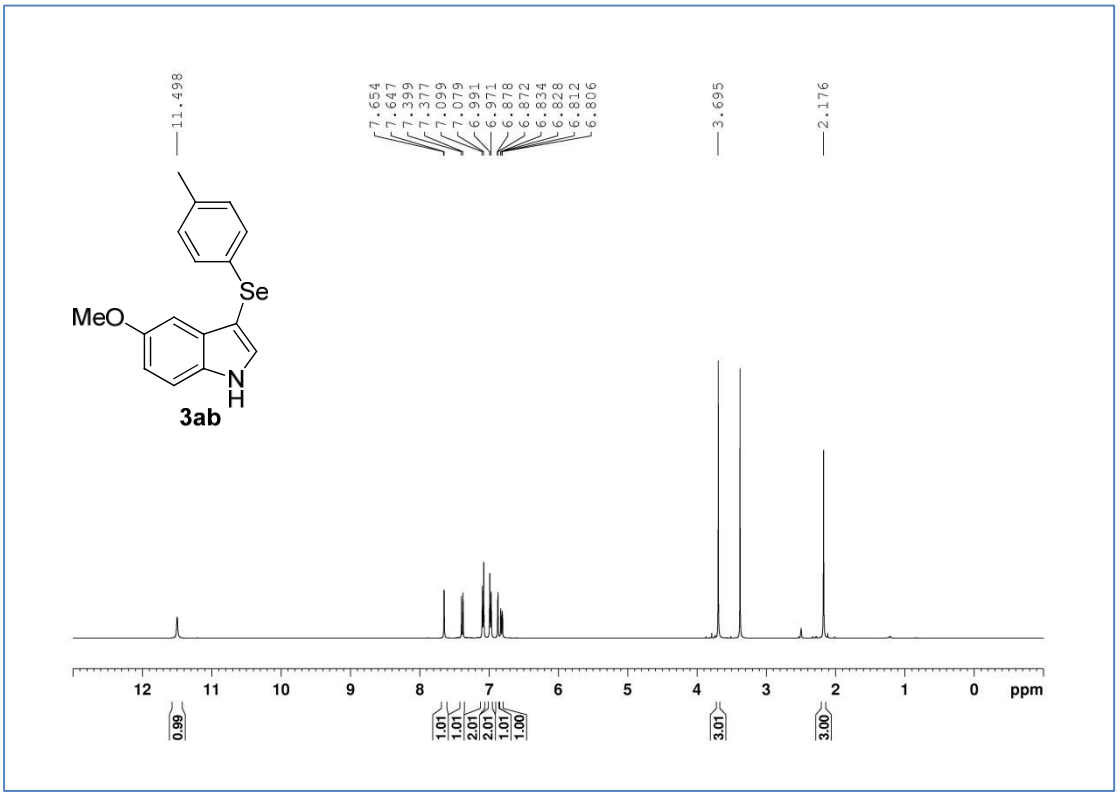

8.103
8.086
7.979
7.976
7.958
7.845
7.646
7.624
7.460
7.442
7.423
7.353
7.334
7.316
7.178
7.176
7.161
7.159
7.153
7.139
7.136
6.774
6.758
6.741
N
N
4l
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
2.00
1.01
1.01
2.00
1.00
1.01
1.01


146.02
145.88
133.97
128.90
128.15
126.25
125.76
124.79
117.75
112.58
108.29
N
N
4l
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

9.2 NMR spectra of products



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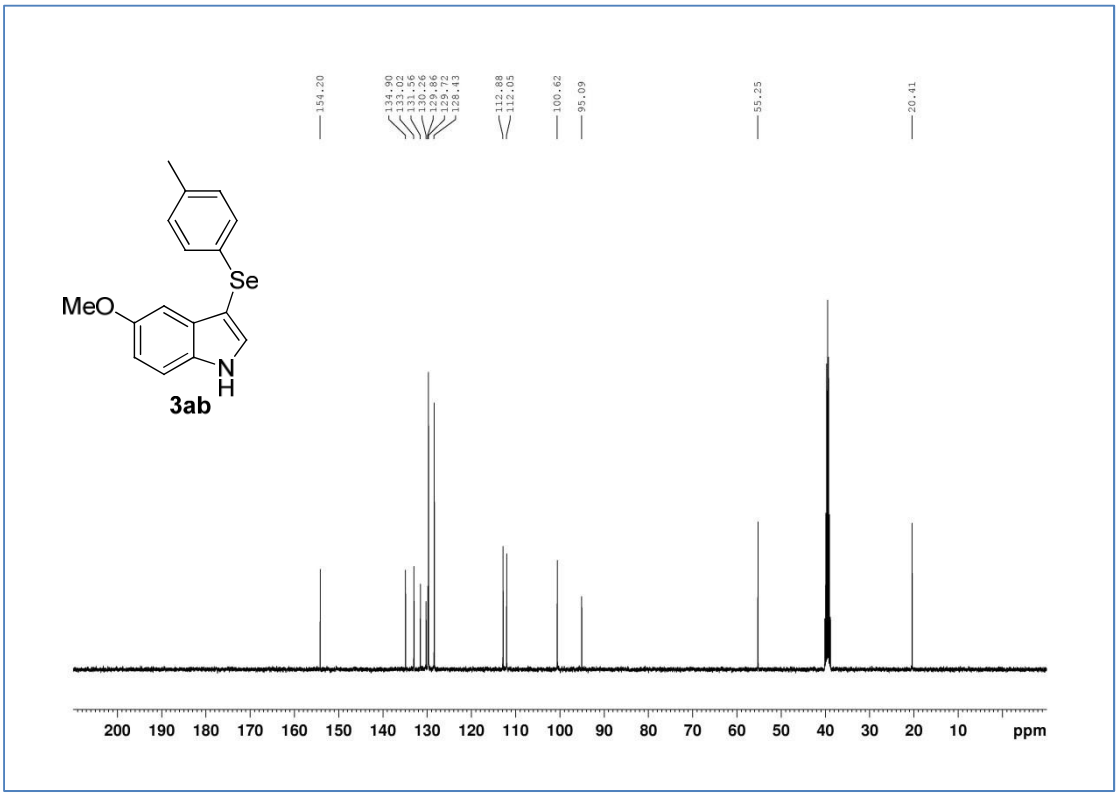
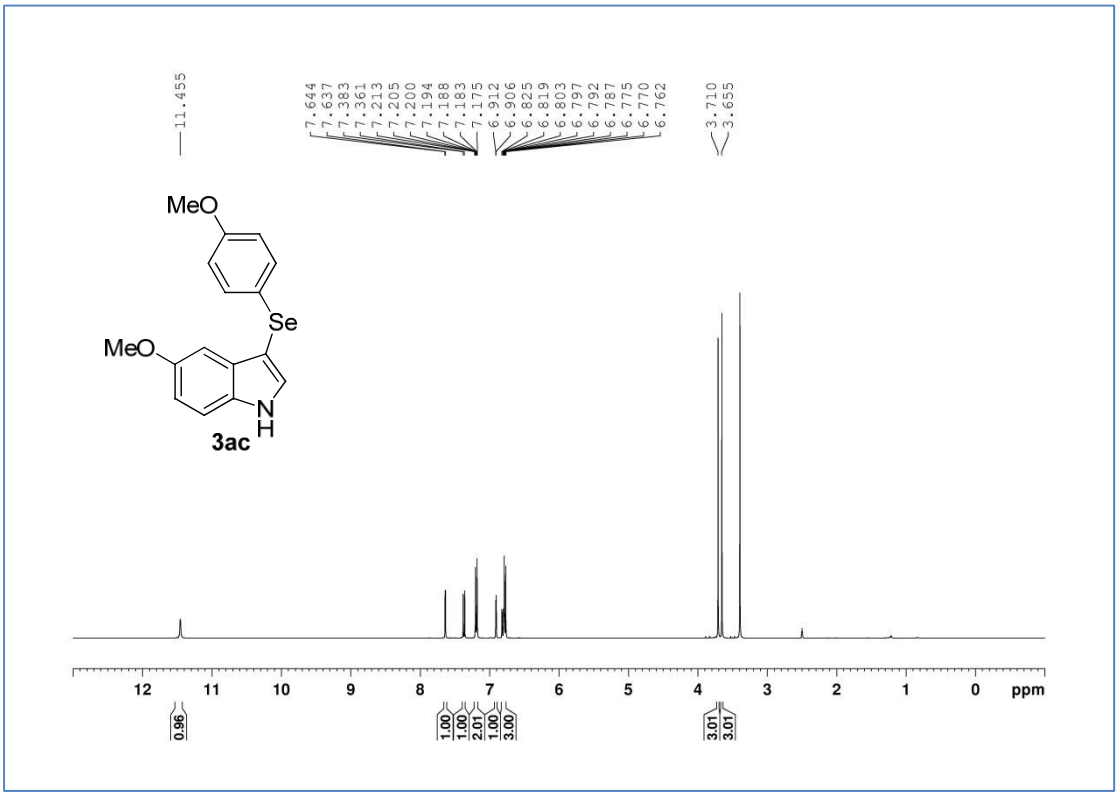
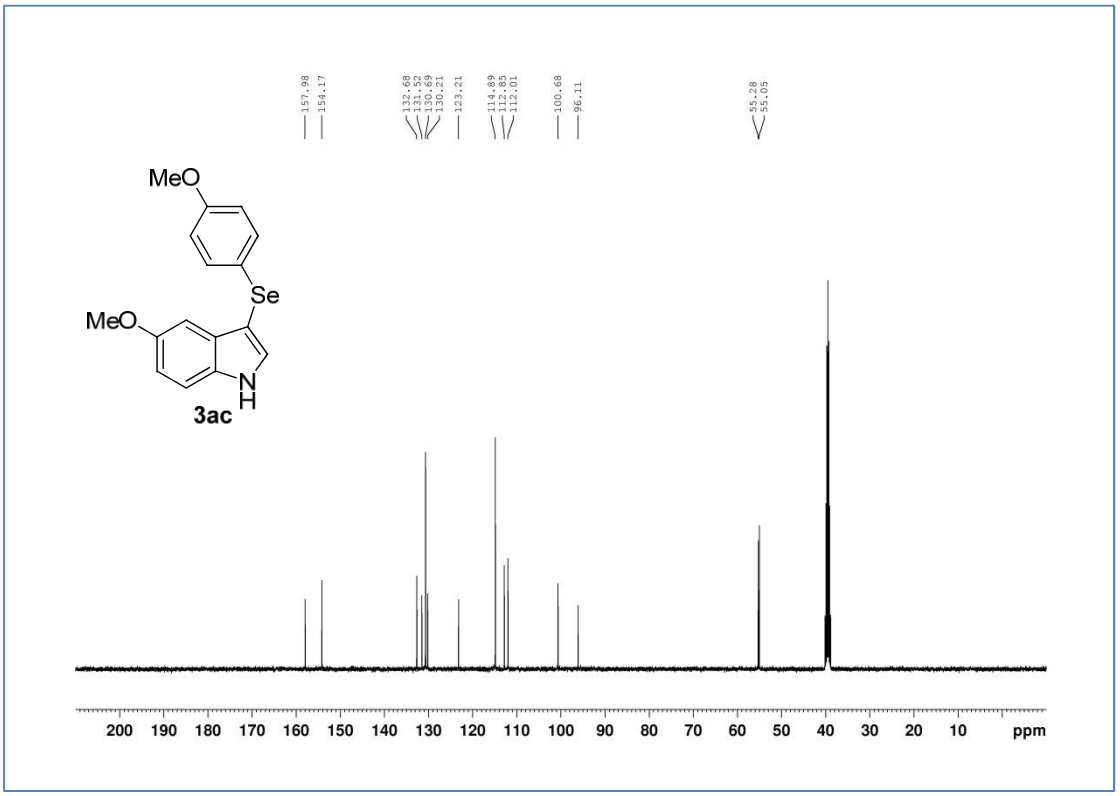
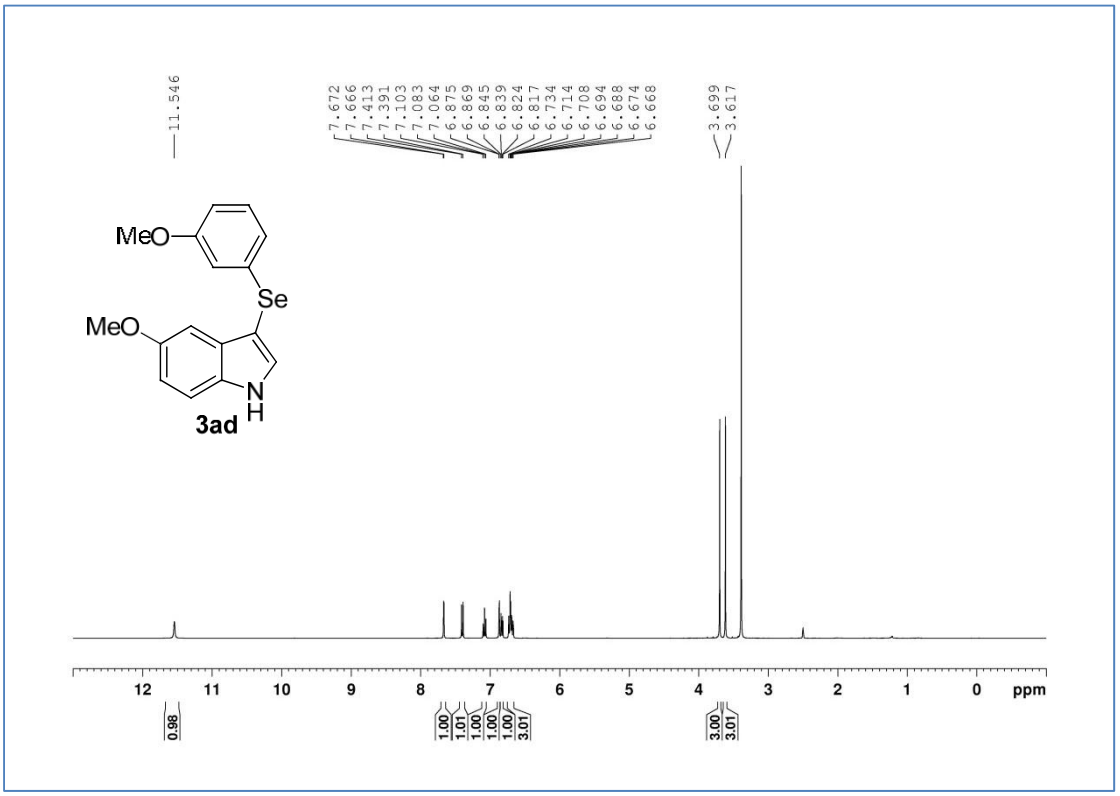
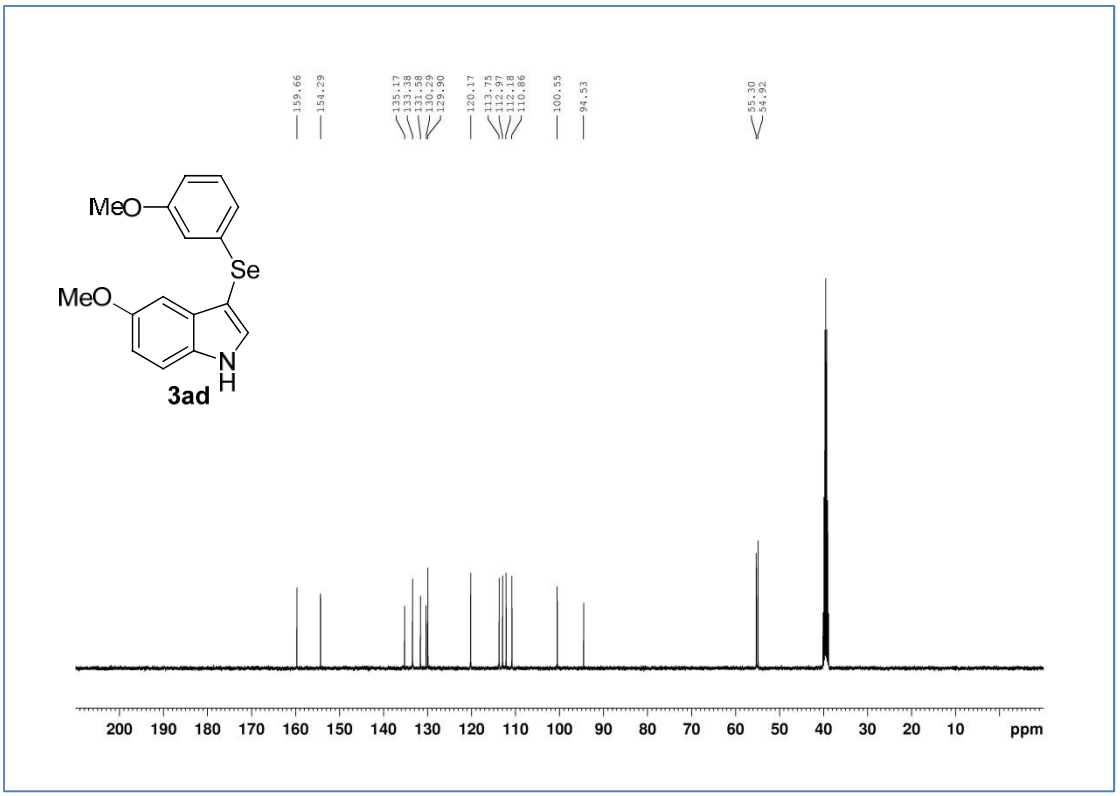
7.654
7.647
7.399
7.377
7.099
7.079
6.991
6.971
6.878
6.872
6.834
6.828
6.812
6.806
3.695
2.176
Se
MeO
N
H
3ab
12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
0.99
1.01
1.01
2.01
2.01
1.01
1.00
3.01
3.00

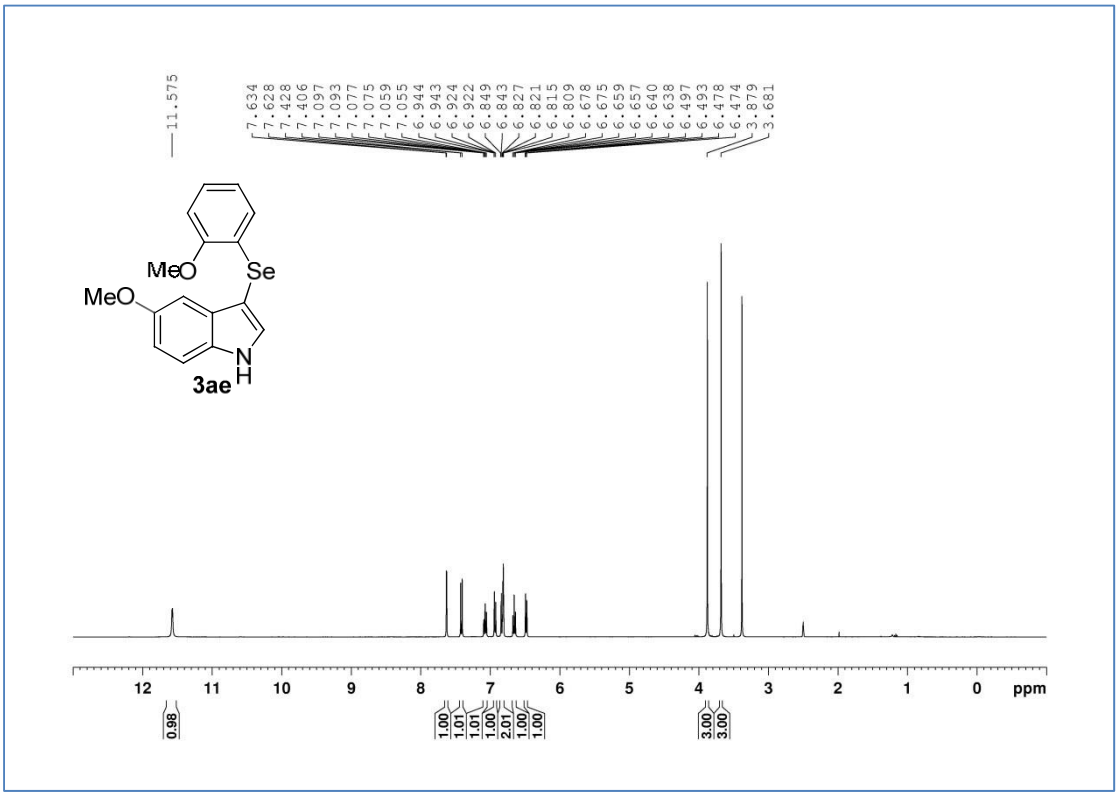

154.20
134.90
133.02
131.56
130.26
129.86
129.72
128.43
112.88
112.05
100.62
95.09
55.25
20.41
Se
MeO
N
H
3ab
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


11.455
7.644
7.637
7.383
7.361
7.213
7.205
7.200
7.194
7.188
7.183
7.175
6.912
6.906
6.825
6.819
6.803
6.797
6.792
6.787
6.775
6.770
6.762
3.710
3.655
MeO
Se
MeO
N
H
3ac
12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
0.96
1.00
1.00
2.01
1.00
3.00
3.01
3.01


157.98
154.17
132.68
131.52
130.69
130.21
123.21
114.89
112.85
112.01
100.68
96.11
55.28
55.05
MeO
Se
MeO
N
H
3ac
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


11.546
7.672
7.666
7.413
7.391
7.103
7.083
7.064
6.875
6.869
6.845
6.839
6.824
6.817
6.734
6.714
6.708
6.694
6.688
6.674
6.668
3.699
3.617
MeO
Se
MeO
N
H
3ad
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
0.98
1.00
1.01
1.00
1.00
1.00
3.01
3.00
3.01


159.66
154.29
135.17
133.38
131.58
130.29
129.90
120.17
113.75
112.97
112.18
110.86
100.55
94.53
55.30
54.92
MeO
Se
MeO
N
H
3ad
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm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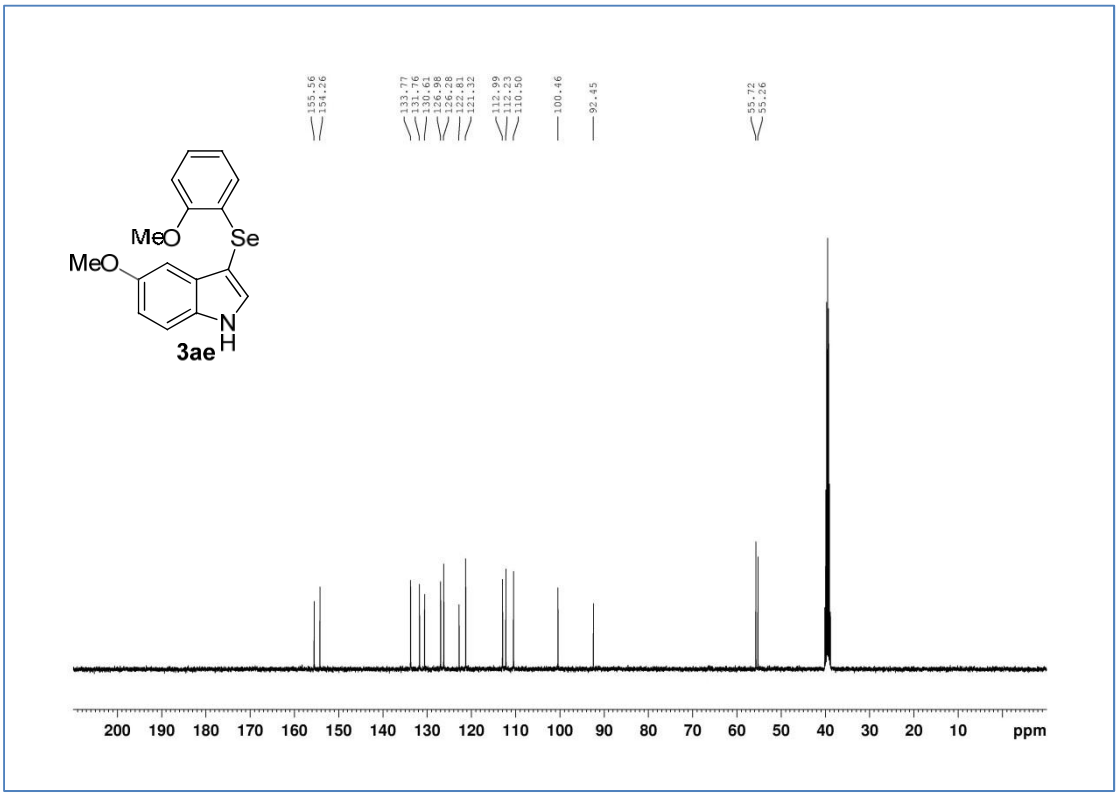
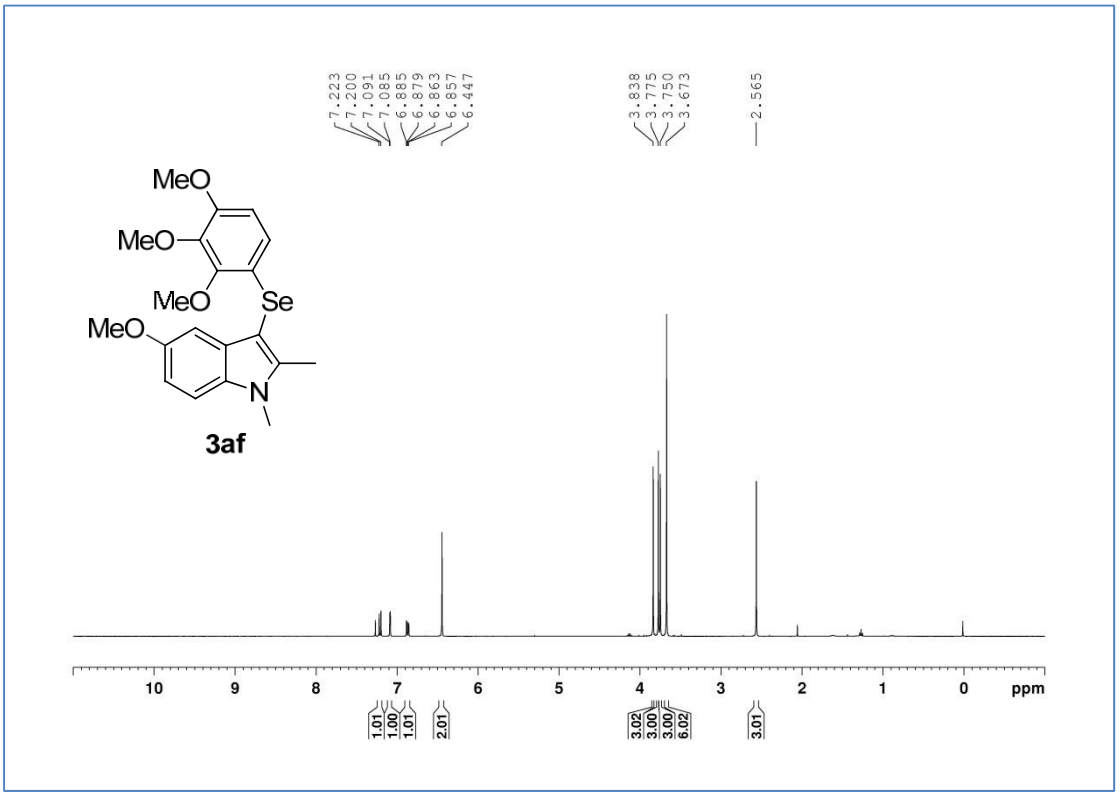
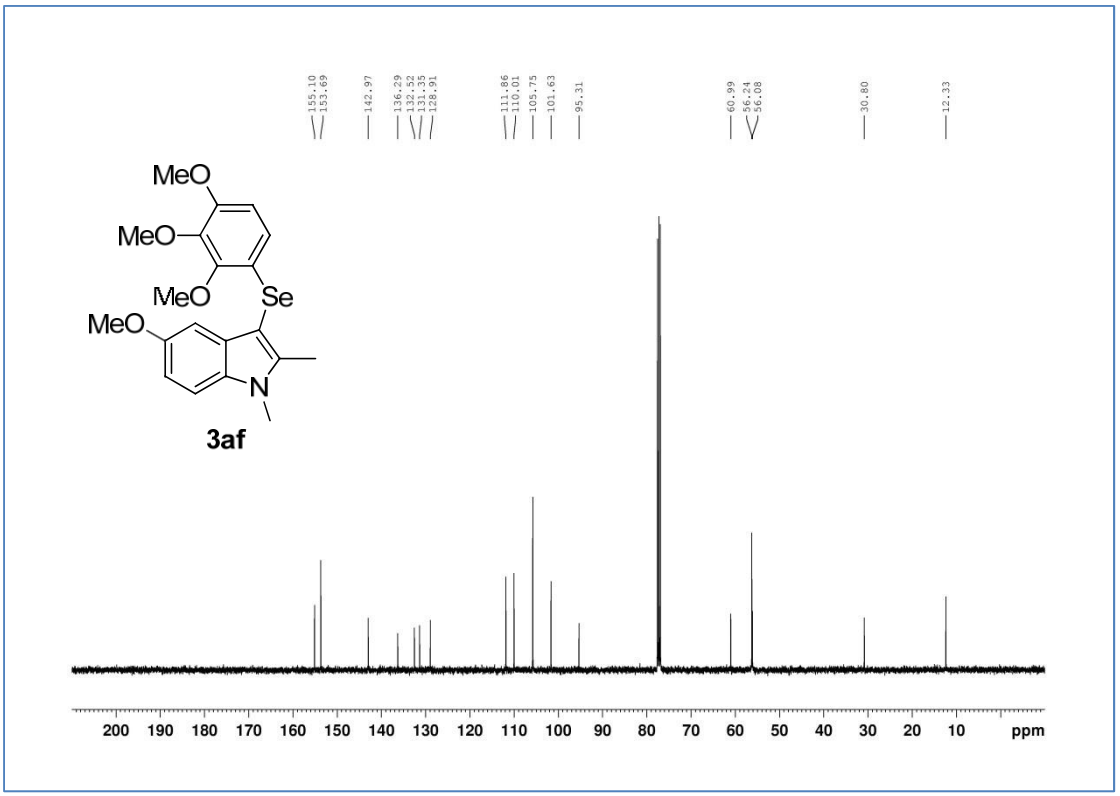
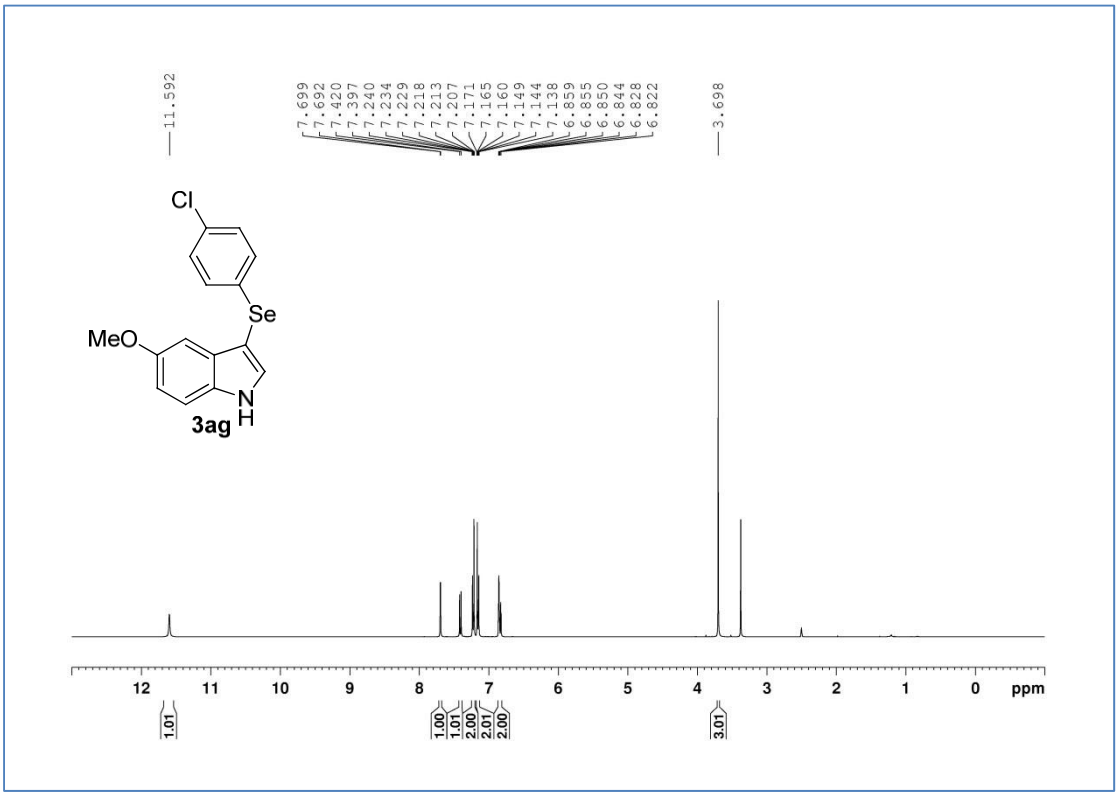
7.634
7.628
7.428
7.406
7.097
7.093
7.077
7.075
7.059
7.055
6.944
6.943
6.924
6.922
6.849
6.843
6.827
6.821
6.815
6.809
6.678
6.675
6.659
6.657
6.640
6.638
6.497
6.493
6.478
6.474
3.879
3.681
MeO
Se
MeO
N
H
3ae
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
0.98
1.00
1.01
1.01
1.00
2.01
1.00
1.00
3.00
3.00


155.56
134.26
133.77
131.76
130.61
126.98
126.28
122.81
121.32
112.99
112.23
110.50
100.46
92.45
55.72
55.26
MeO
Se
MeO
N
H
3ae
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


7.223
7.200
7.091
7.085
6.885
6.879
6.863
6.857
6.447
3.838
3.775
3.750
3.673
2.565
MeO
MeO
MeO
MeO
Se
N
3af
10
9
8
7
6
5
4
3
2
1
0
ppm
1.01
1.00
1.01
2.01
3.02
3.00
3.00
6.02
3.01


155.10
153.69
142.97
136.29
132.52
131.35
128.91
111.86
110.01
105.75
101.63
95.31
60.99
56.24
56.08
30.80
12.33
MeO
MeO
MeO
MeO
Se
N
3af
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm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7.692
7.420
7.397
7.240
7.234
7.229
7.218
7.213
7.207
7.171
7.165
7.160
7.149
7.144
7.138
6.859
6.855
6.850
6.844
6.828
6.822
3.698
Cl
Se
MeO
N
H
3ag
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
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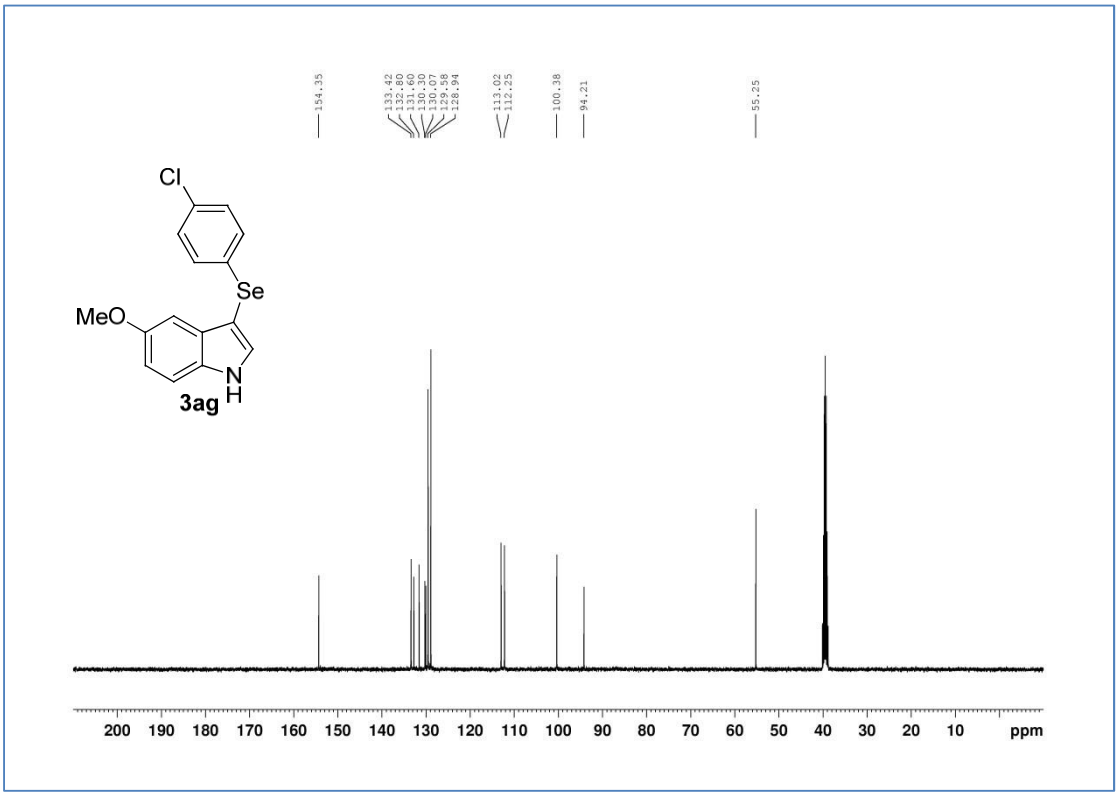
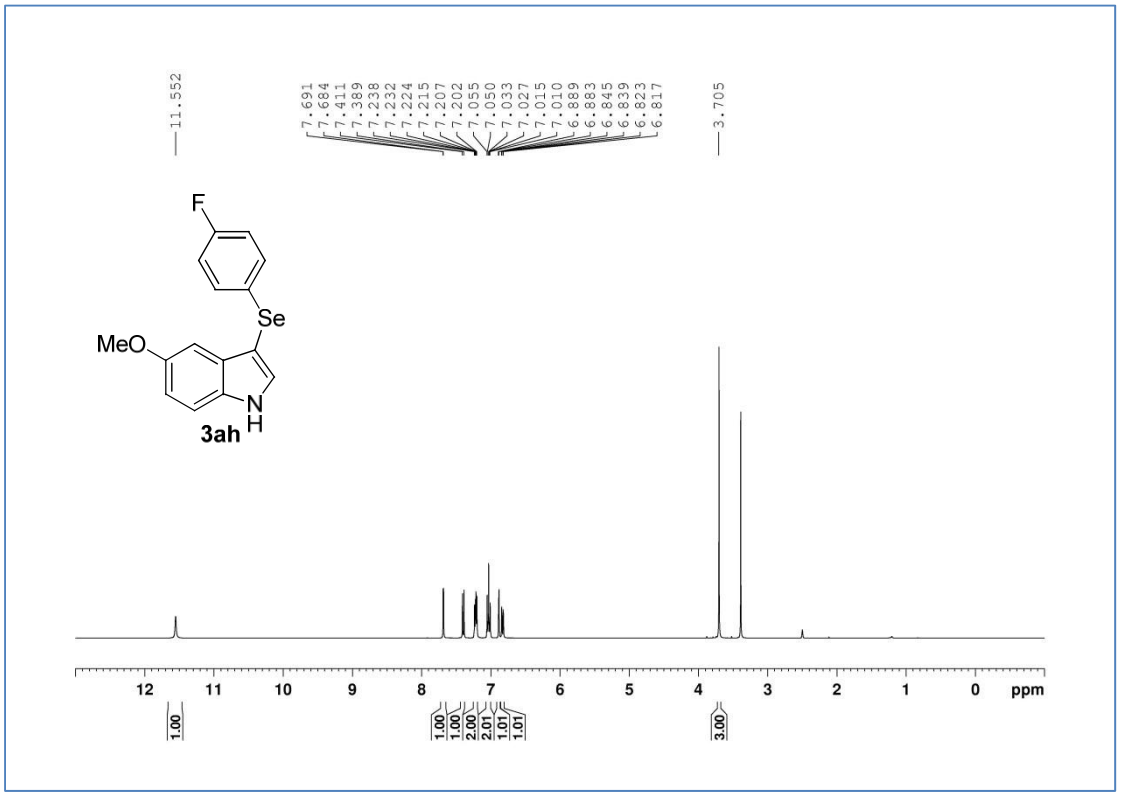
1.00
1.01
2.00
2.01
2.00
3.01


154.35
133.42
132.80
131.60
130.30
130.07
129.58
128.94
113.02
112.25
100.38
94.21
55.25
Cl
Se
MeO
N
H
3ag
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm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7.684
7.411
7.389
7.238
7.232
7.224
7.215
7.207
7.202
7.055
7.050
7.033
7.027
7.015
7.010
6.889
6.883
6.845
6.839
6.823
6.817
3.705
F
Se
MeO
N
H
3ah
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
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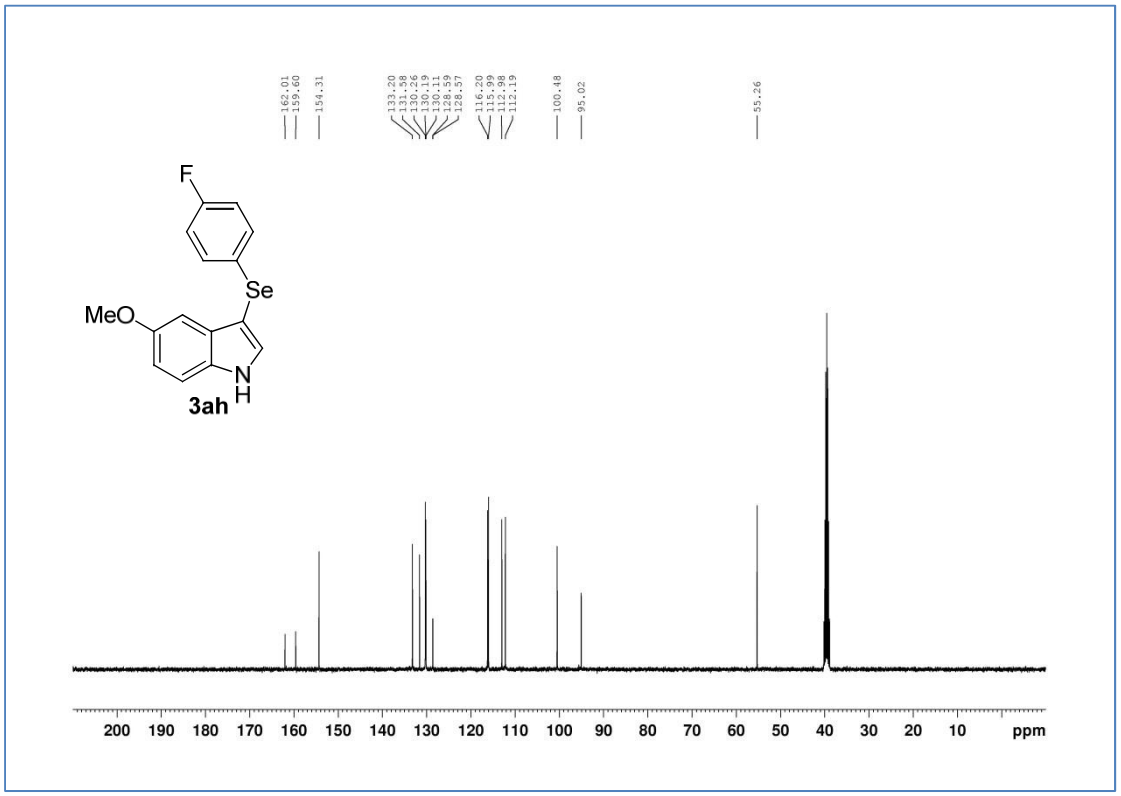
1.00
1.00
2.00
2.01
1.01
1.01
3.00


162.01
159.60
154.31
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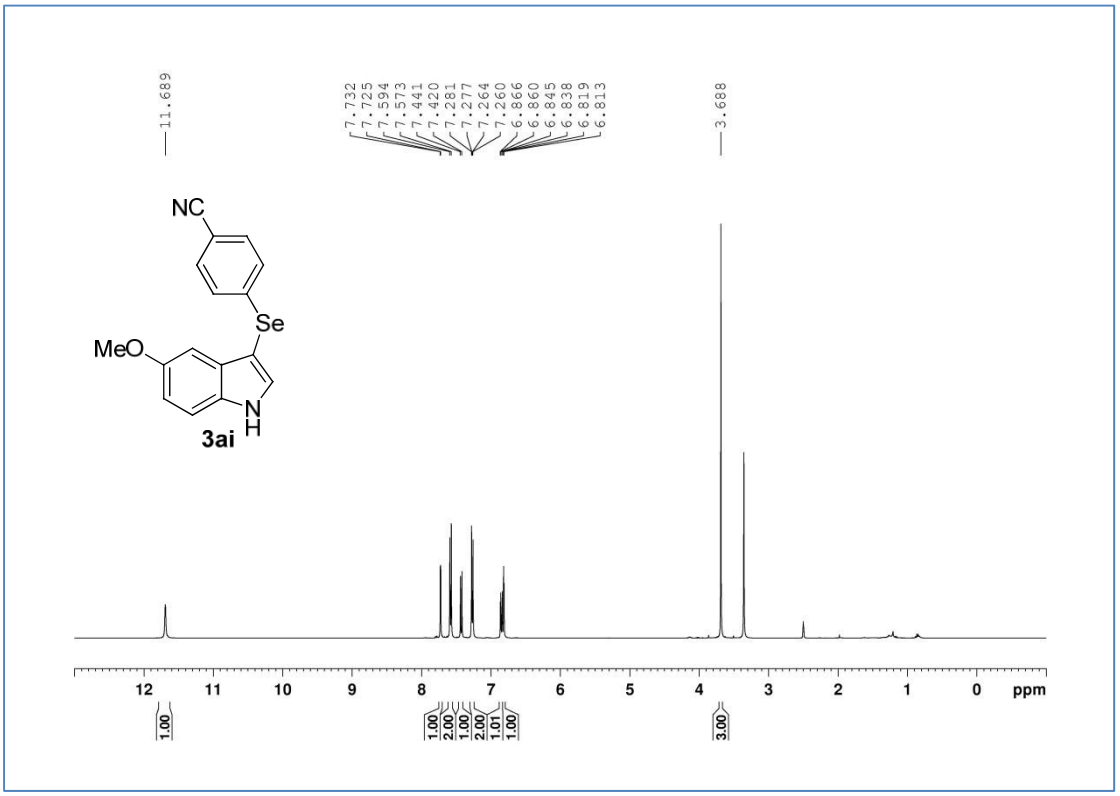
131.58
130.26
130.19
130.11
128.59
128.57
116.20
115.99
112.98
112.19
100.48
95.02
55.26
F
Se
MeO
N
H
3ah
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm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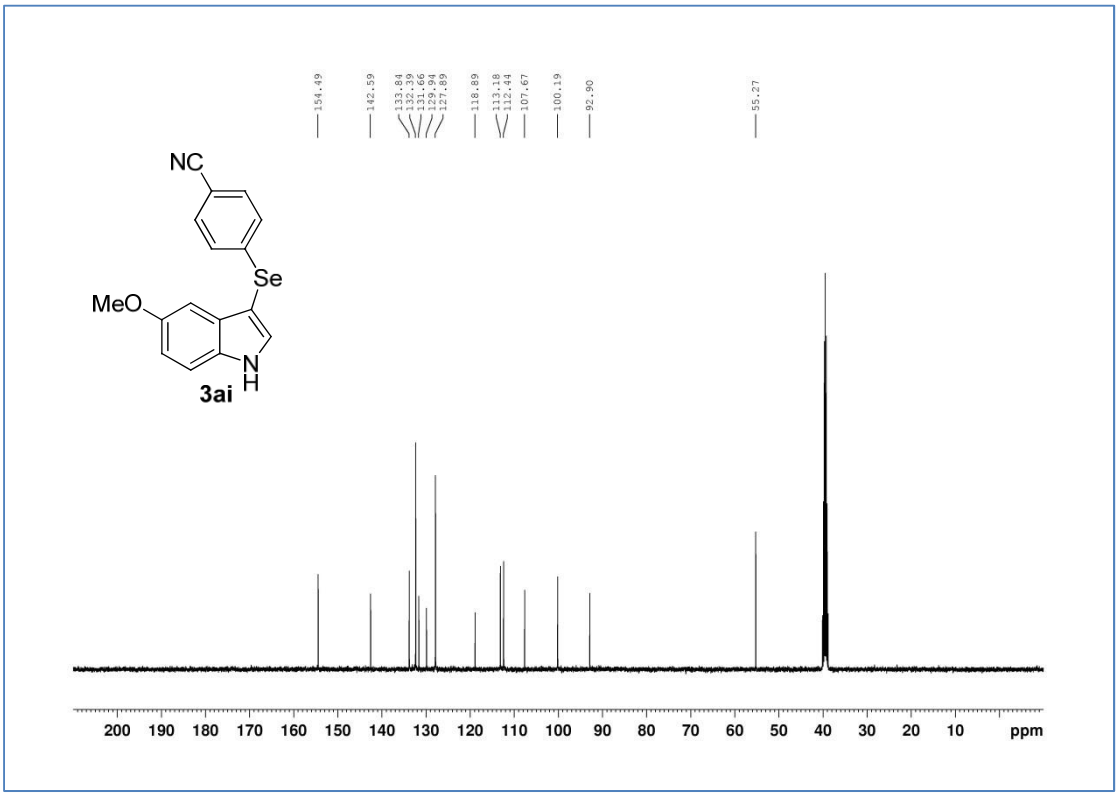
7.573
7.441
7.420
7.281
7.277
7.264
7.260
6.866
6.860
6.845
6.838
6.819
6.813
3.688
NC
Se
MeO
N
H
3ai
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.00
2.00
1.00
2.00
1.01
1.00
3.00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132.39
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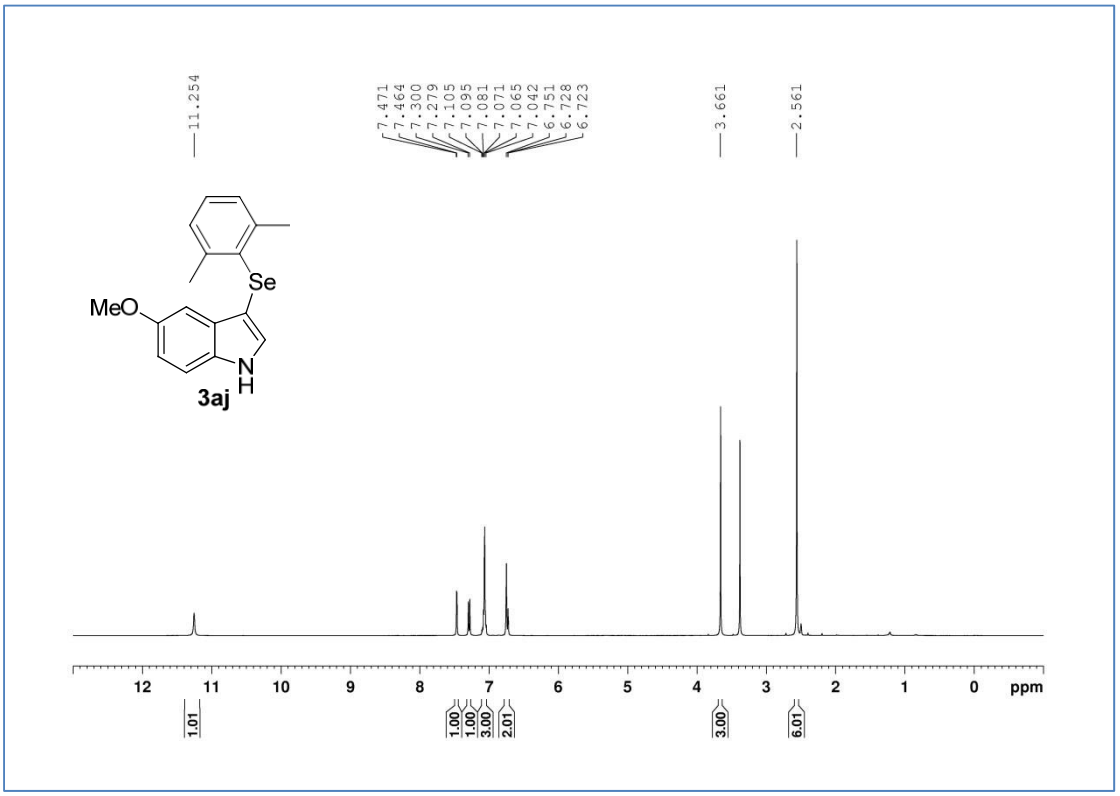
129.84
127.89
118.89
113.18
112.44
107.67
100.19
92.90
55.27
NC
Se
MeO
N
H
3ai
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm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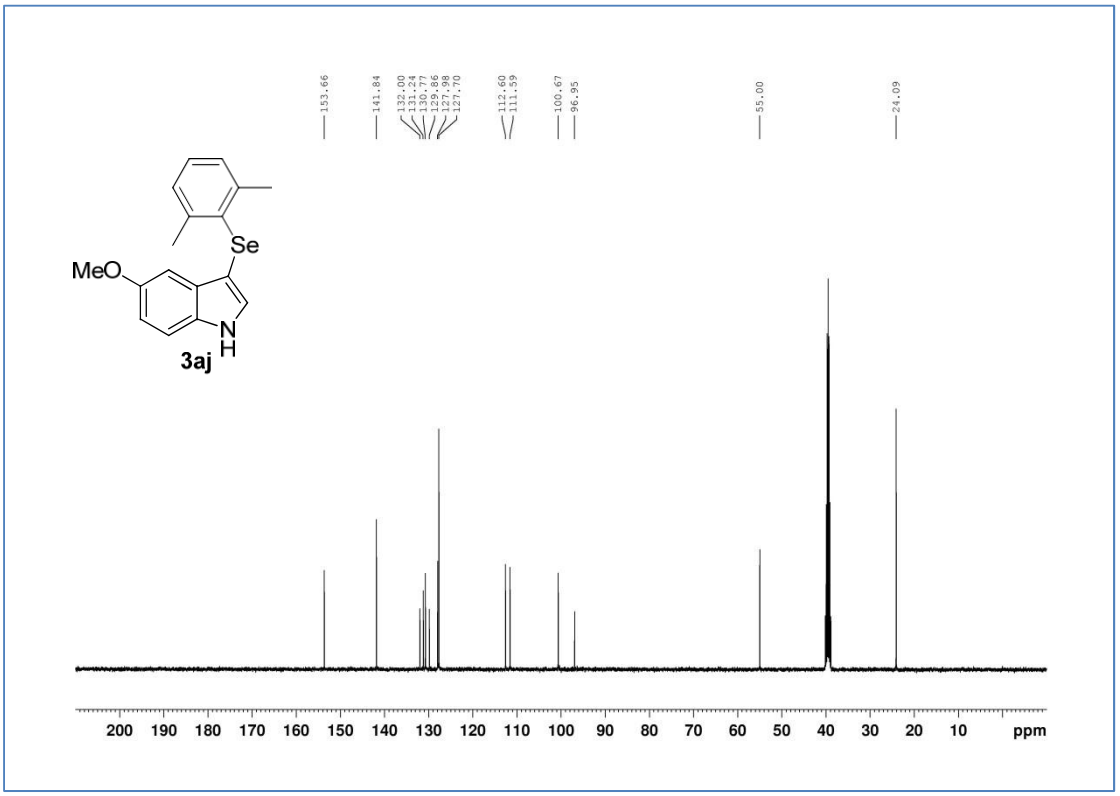
7.081
7.071
7.065
7.042
6.751
6.728
6.723
3.661
2.561
Se
MeO
N
H
3aj
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.01
1.00
1.00
3.00
2.01
3.00
6.01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130.77
129.86
127.98
121.70
112.60
111.59
100.67
96.95
55.00
24.09
Se
MeO
N
H
3aj
200
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150
140
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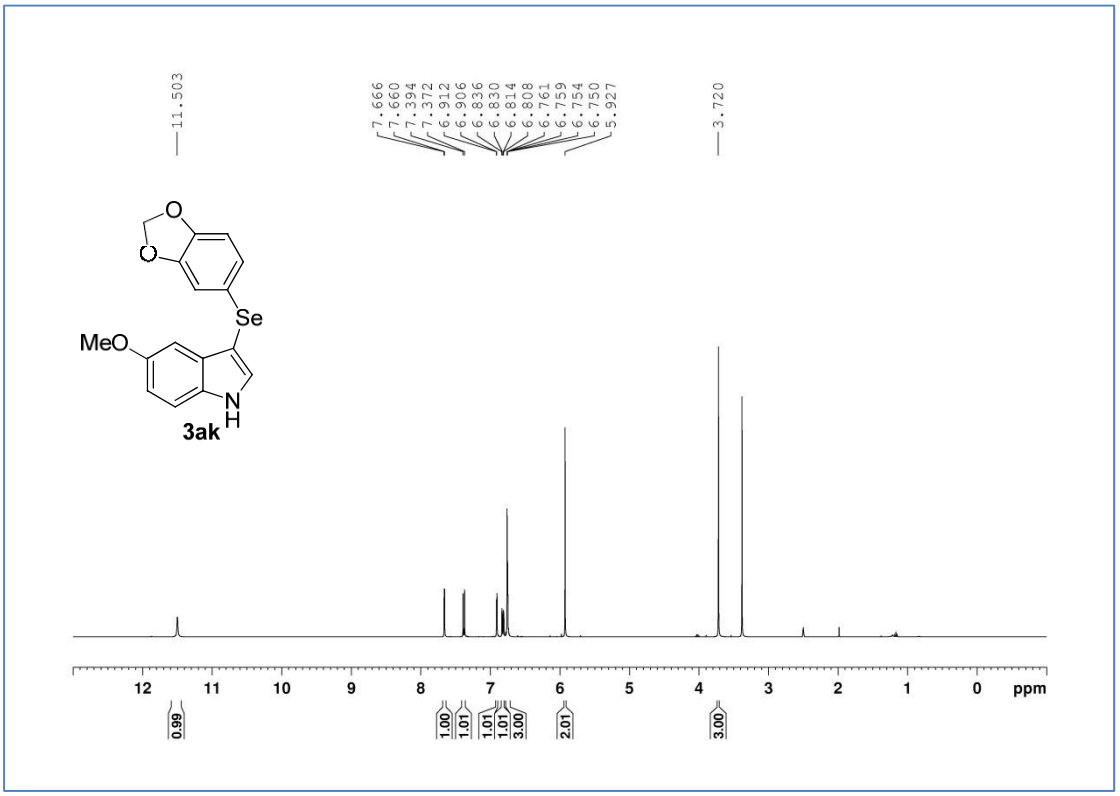
120
110
100
90
80
70
60
50
40
30
20
10
ppm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7.660
7.394
7.372
6.912
6.906
6.836
6.830
6.814
6.808
6.761
6.759
6.754
6.750
5.927
3.720
O
O
Se
MeO
N
H
3ak
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
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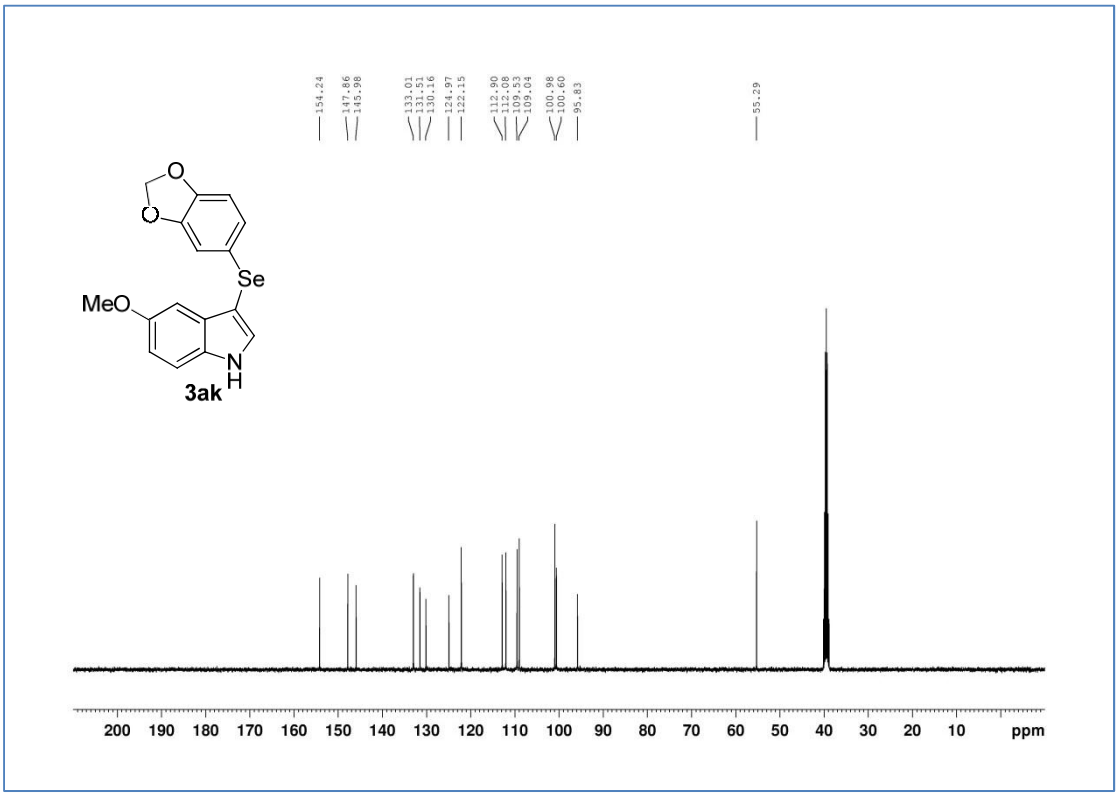
1.01
1.01
1.01
3.00
2.01
3.00


154.24
147.86
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133.01
131.51
130.16
124.97
122.15
112.90
112.08
109.53
109.04
100.98
100.60
95.83
55.29
O
O
Se
MeO
N
H
3ak
200
190
180
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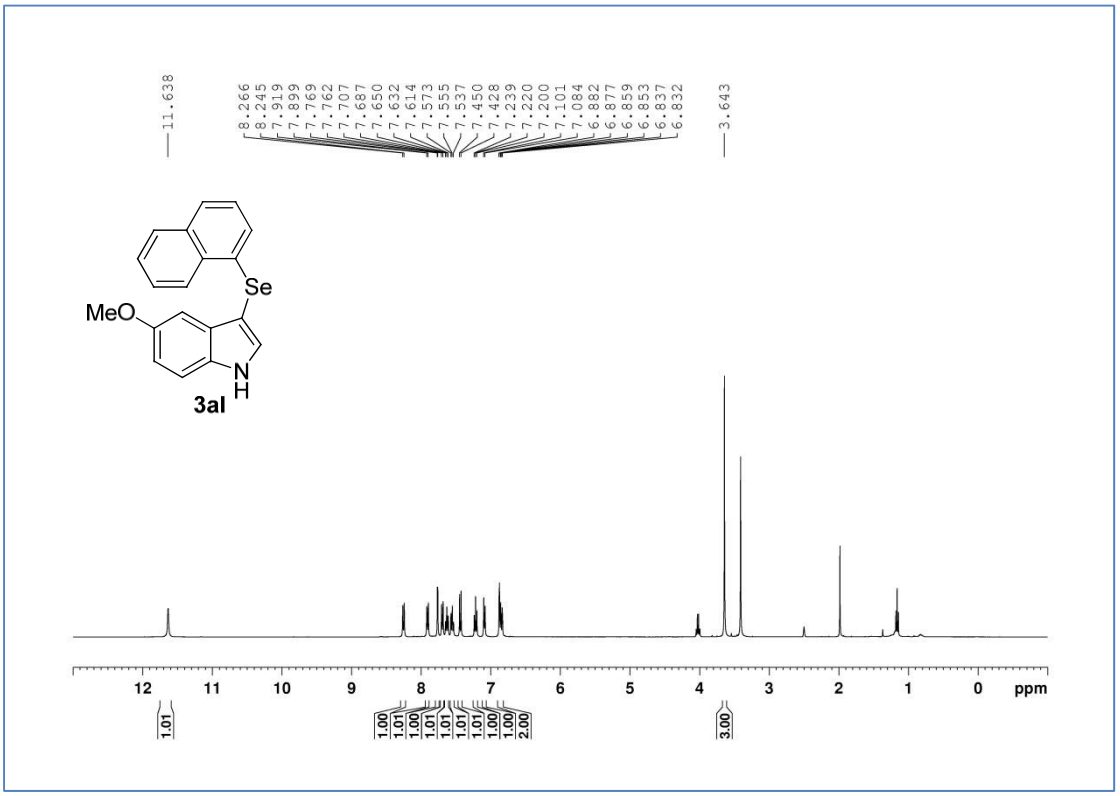
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm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8.245
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7.769
7.762
7.707
7.687
7.650
7.632
7.614
7.573
7.555
7.537
7.450
7.428
7.239
7.220
7.200
7.101
7.084
6.882
6.877
6.859
6.853
6.837
6.832
3.643
Se
MeO
N
H
3al
12
11
10
9
8
7
6
5
4
3
2
1
0
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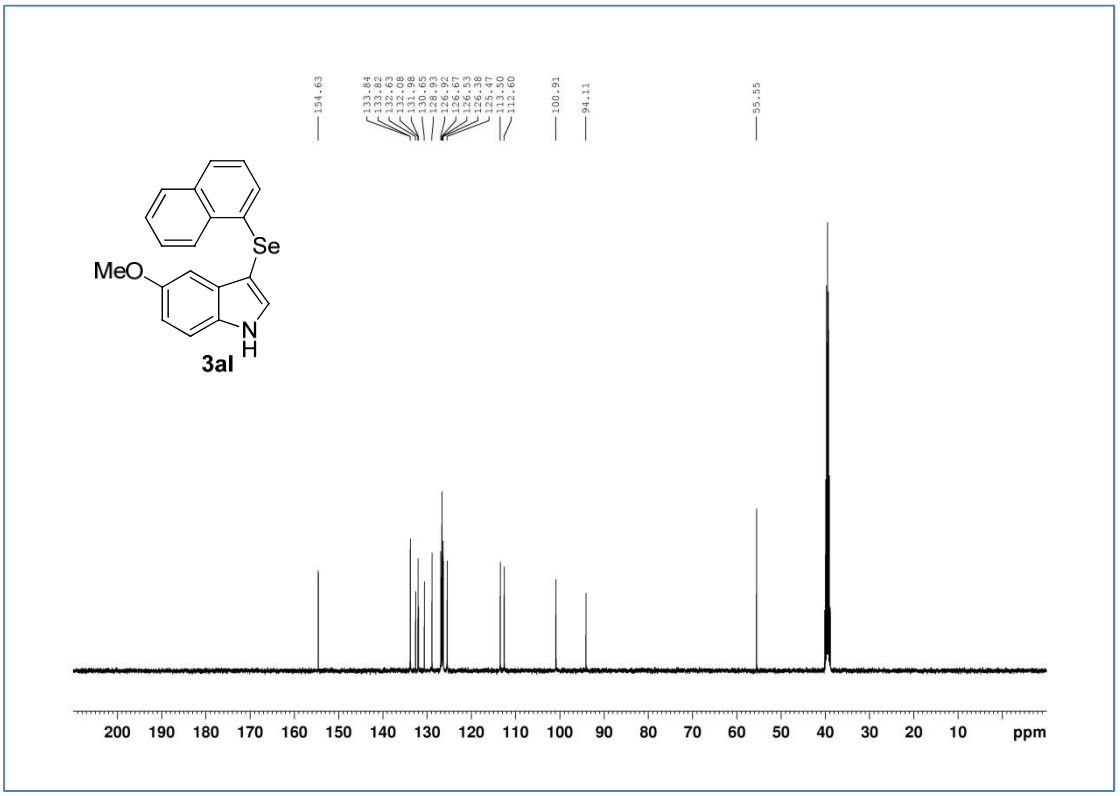
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125.47
113.50
112.60
100.91
94.11
55.55
Se
MeO
N
H
3al
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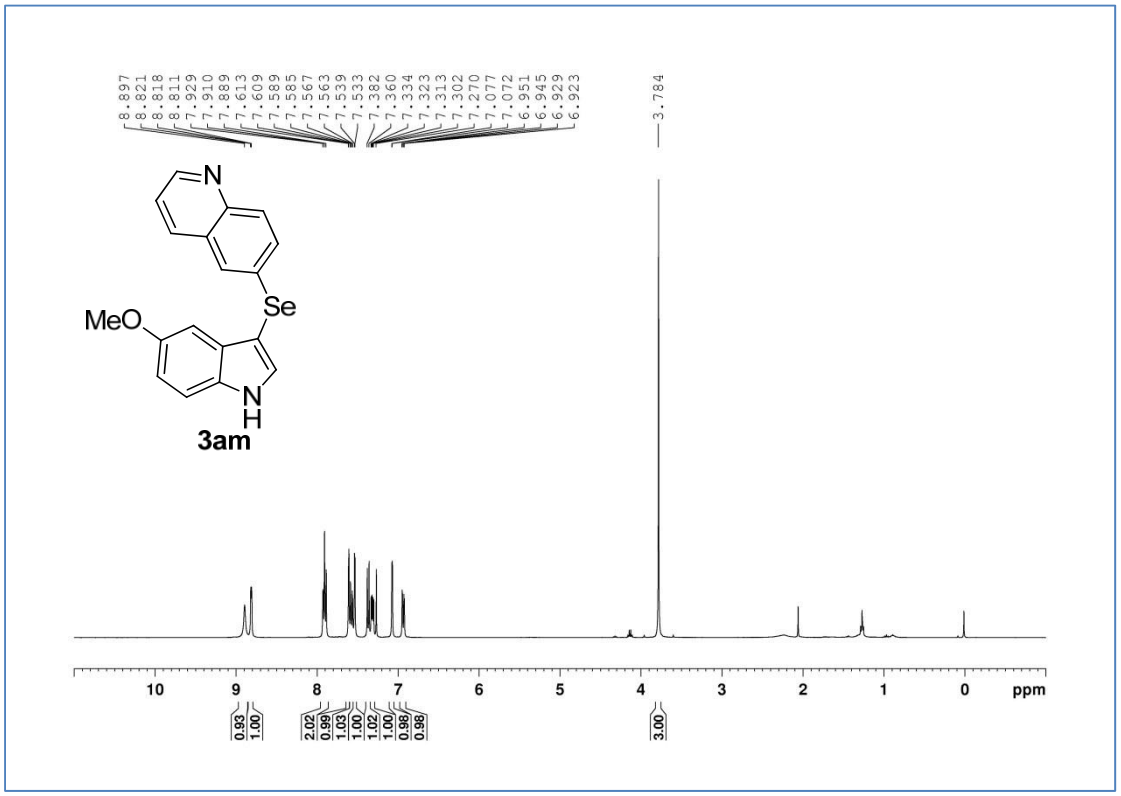
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7.567
7.563
7.539
7.533
7.382
7.360
7.334
7.323
7.313
7.302
7.270
7.077
7.072
6.951
6.945
6.929
6.923
3.784
N
Se
MeO
N
H
3am
10
9
8
7
6
5
4
3
2
1
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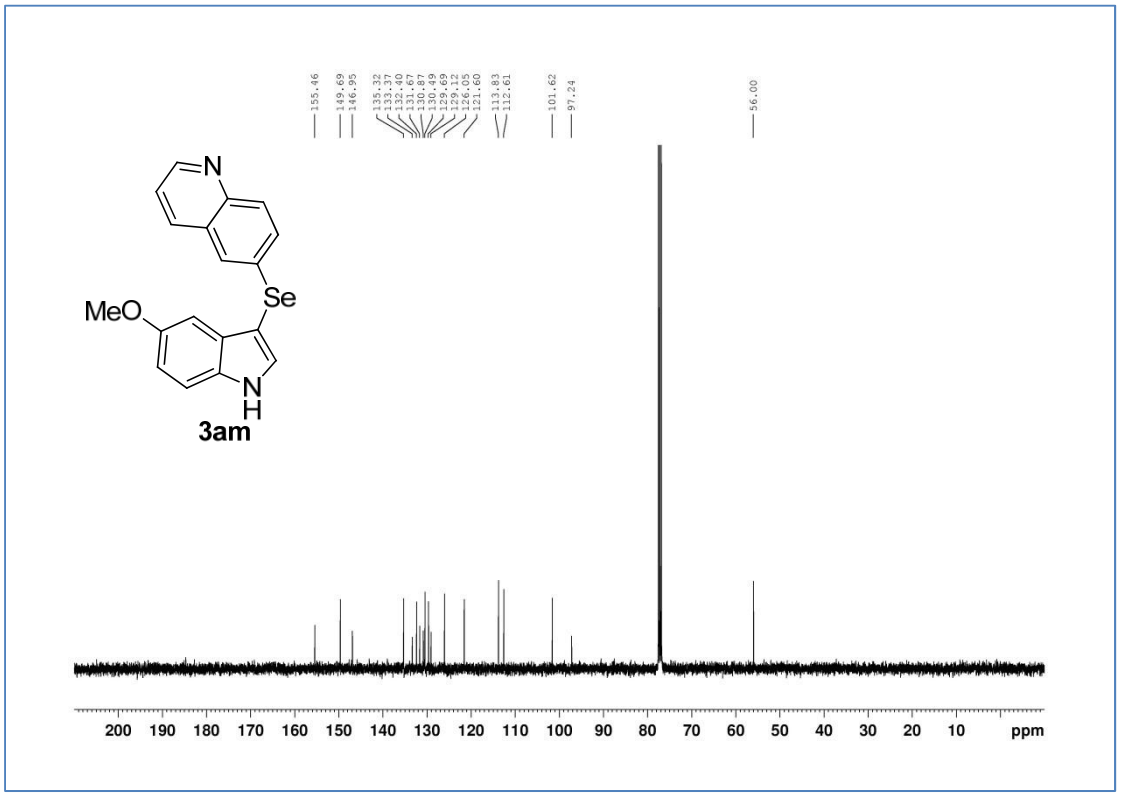
3.00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131.67
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129.12
126.05
121.60
113.83
112.61
101.62
97.24
56.00
N
Se
MeO
N
H
3am
200
190
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150
140
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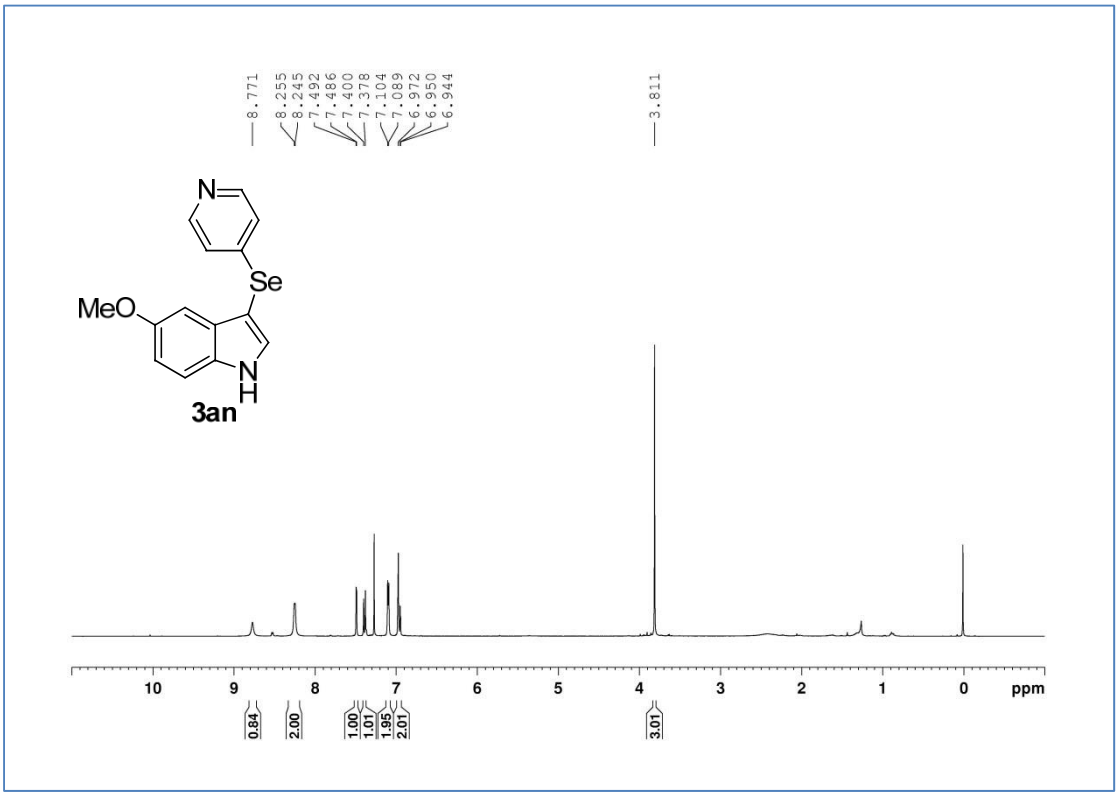
ppm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6.950
6.944
3.811
N
Se
MeO
N
H
3an
10
9
8
7
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1.00
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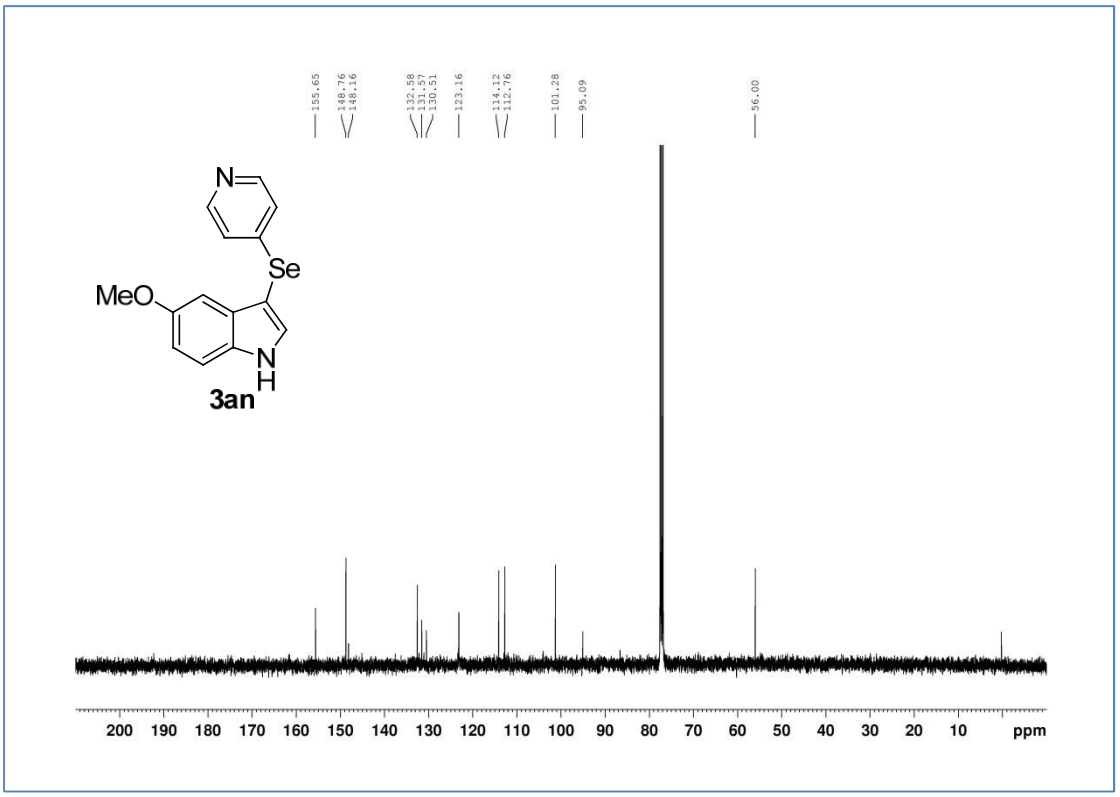
2.01
3.01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130.51
123.16
114.12
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101.28
95.09
56.00
N
Se
MeO
N
H
3an
200
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150
140
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120
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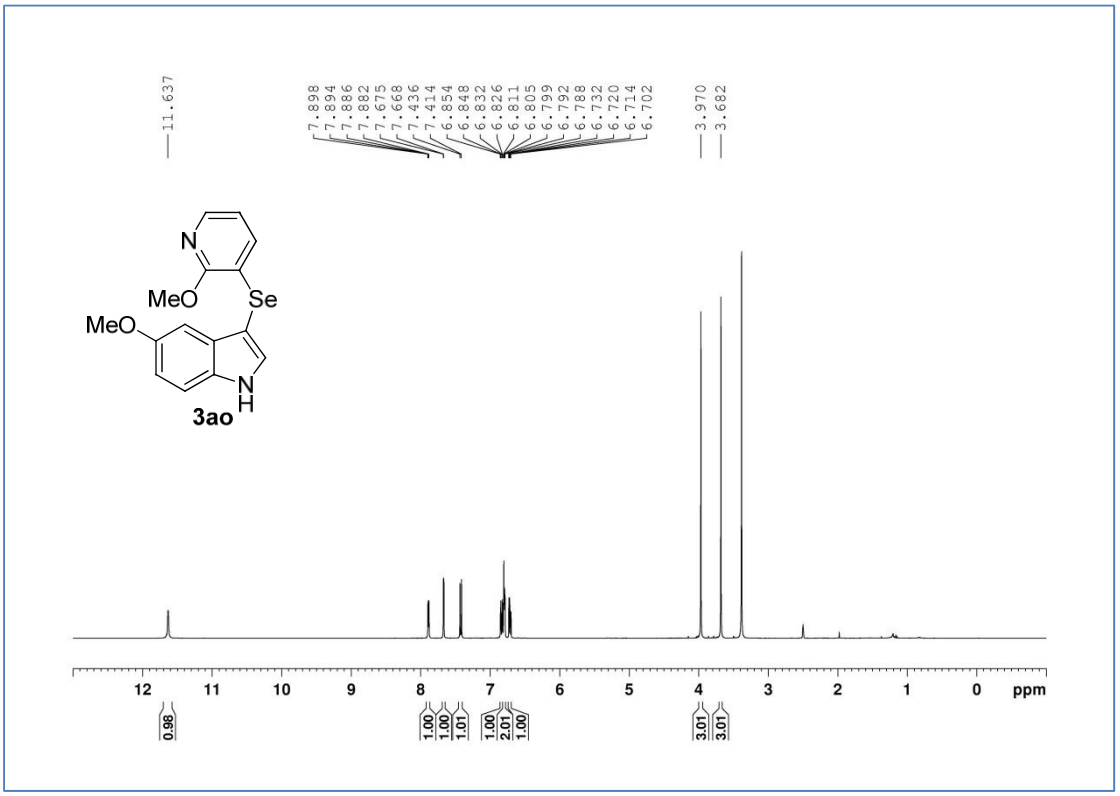
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6.826
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6.805
6.799
6.792
6.788
6.732
6.720
6.714
6.702
3.970
3.682
N
MeO
Se
MeO
N
H
3ao
12
11
10
9
8
7
6
5
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ppm
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1.00
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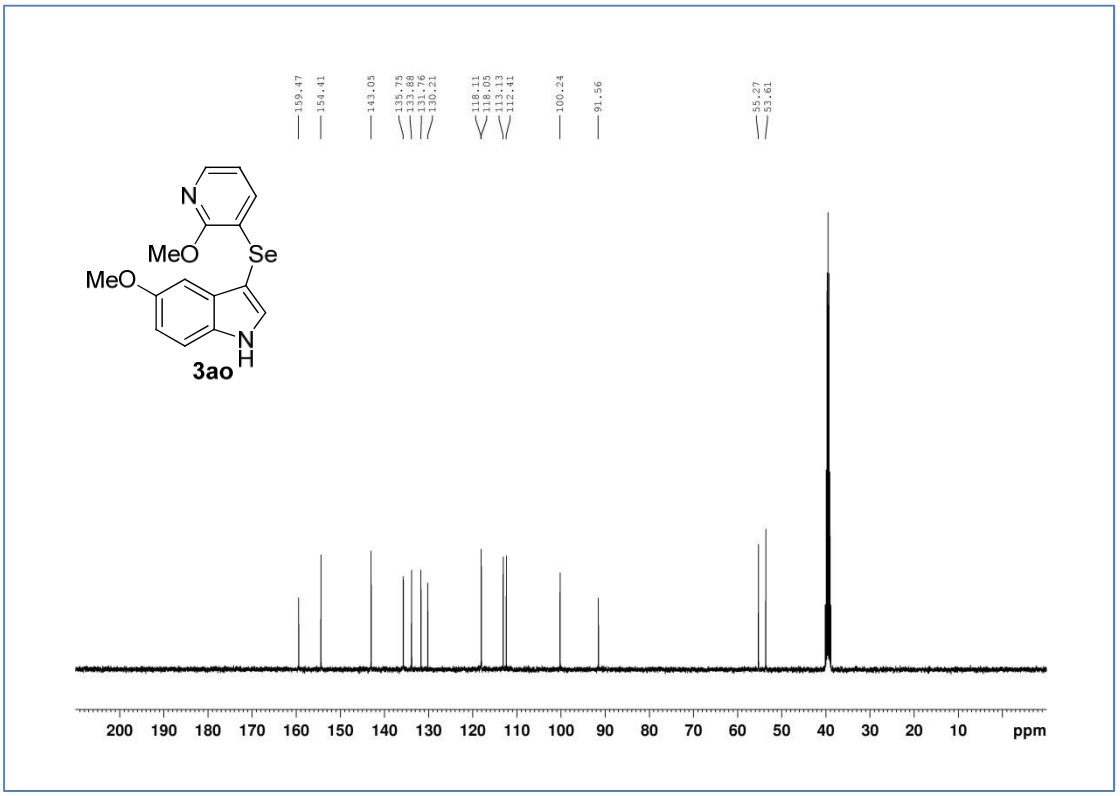
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131.76
130.21
118.11
118.05
113.13
112.41
100.24
91.56
55.27
53.61
N
MeO
Se
MeO
N
H
3ao
200
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150
140
130
120
110
100
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80
70
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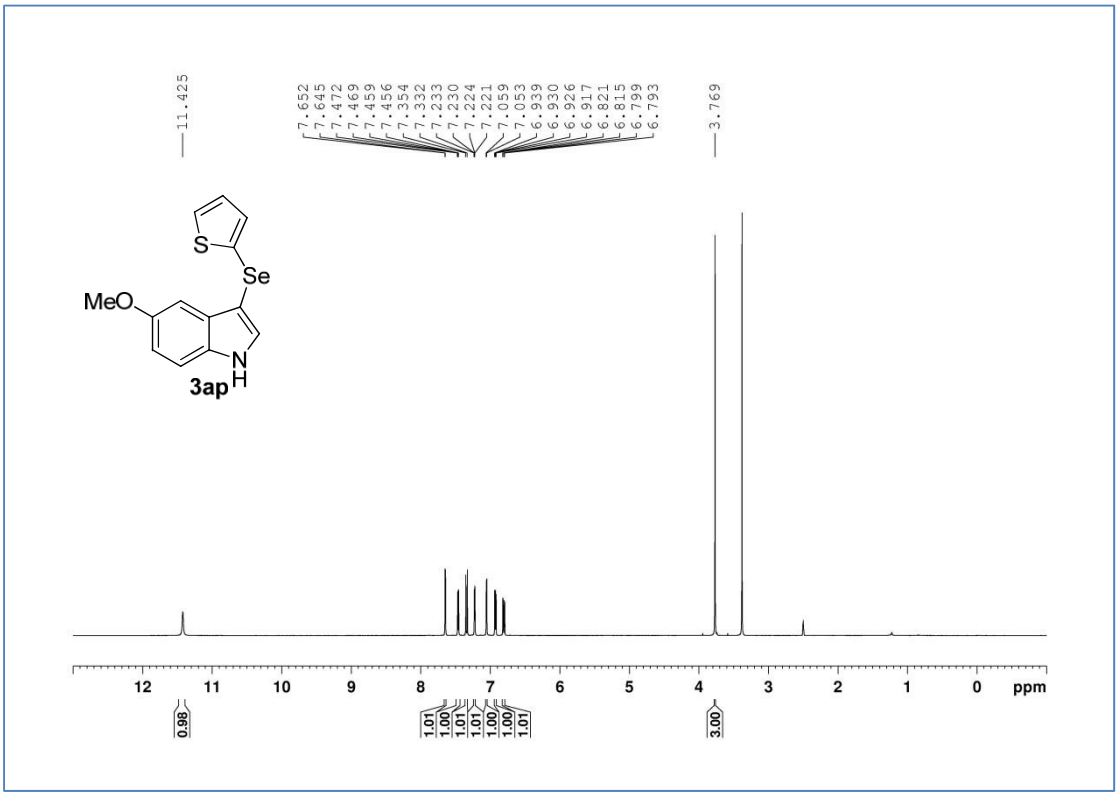
30
20
10
ppm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7.469
7.459
7.456
7.354
7.332
7.233
7.230
7.224
7.221
7.059
7.053
6.939
6.930
6.926
6.917
6.821
6.815
6.799
6.793
3.769
S
Se
MeO
N
H
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12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
0.99
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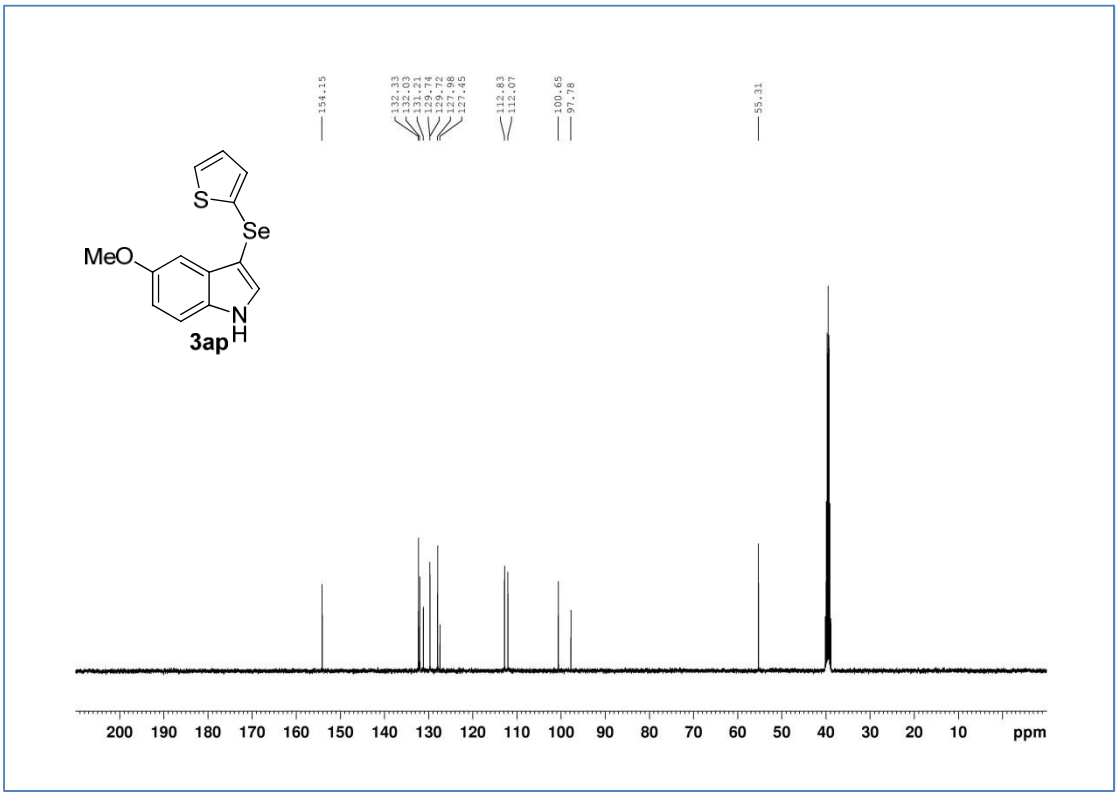
3.00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132.03
131.21
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127.98
127.45
112.83
112.07
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55.31
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Se
MeO
N
H
3ap
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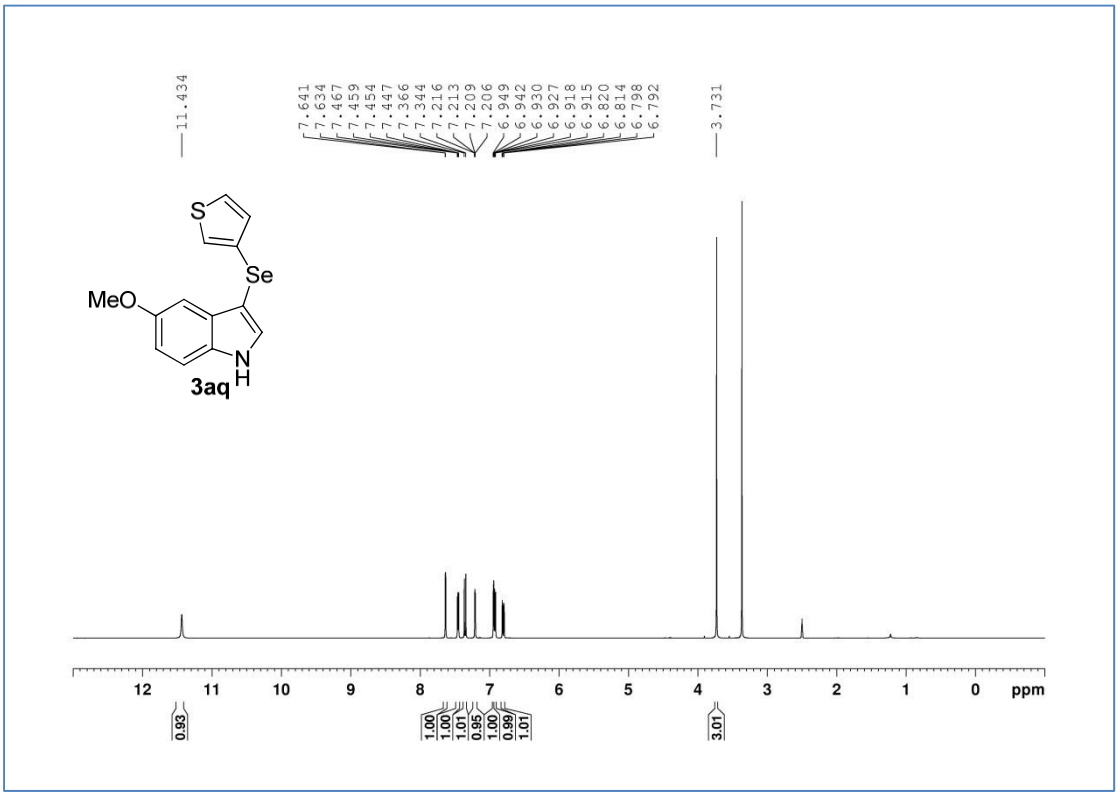
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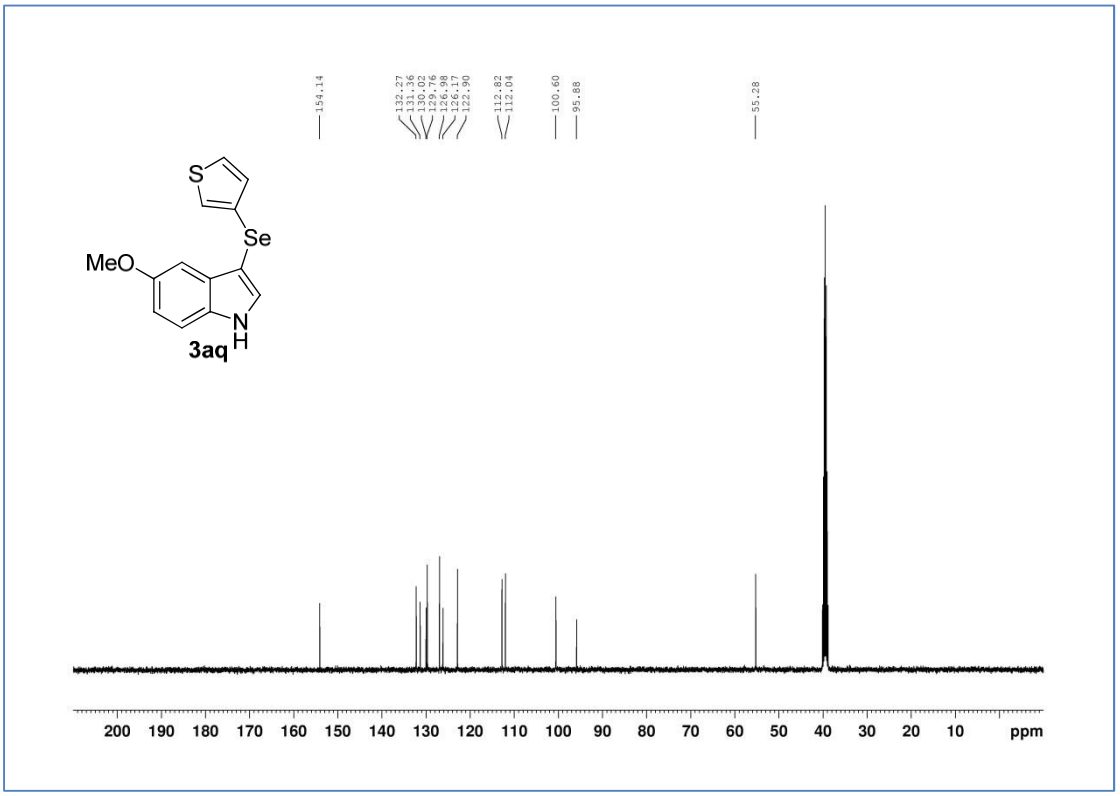
7.454
7.447
7.366
7.344
7.216
7.213
7.209
7.206
6.949
6.942
6.930
6.927
6.918
6.915
6.820
6.814
6.798
6.792
3.731
S
Se
MeO
N
H
3aq
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
0.93
1.00
1.00
1.01
0.95
1.00
0.99
1.01
3.01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126.98
126.17
122.90
112.82
112.04
100.60
95.88
55.28
S
Se
MeO
N
H
3aq
200
190
180
170
160
150
140
130
120
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100
90
80
70
60
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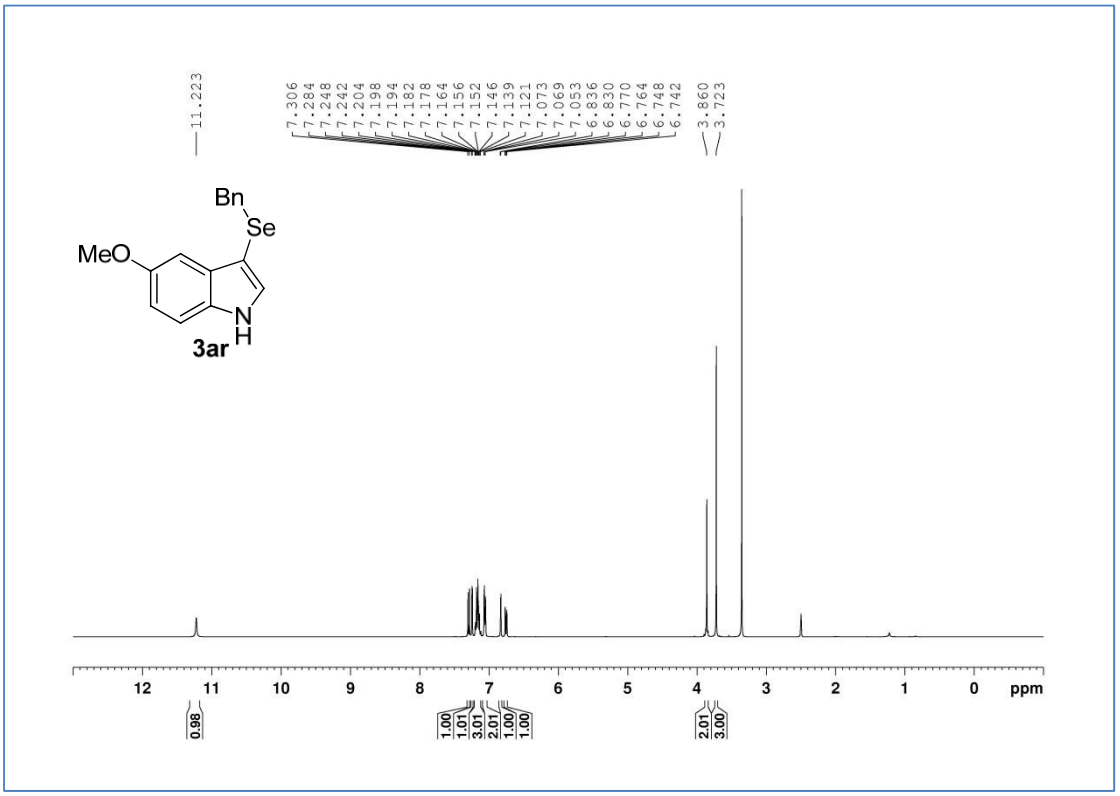
40
30
20
10
ppm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7.156
7.152
7.146
7.139
7.121
7.073
7.069
7.053
6.836
6.830
6.770
6.764
6.748
6.742
3.860
3.723
Bn
Se
MeO
N
H
3ar
12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
0.98
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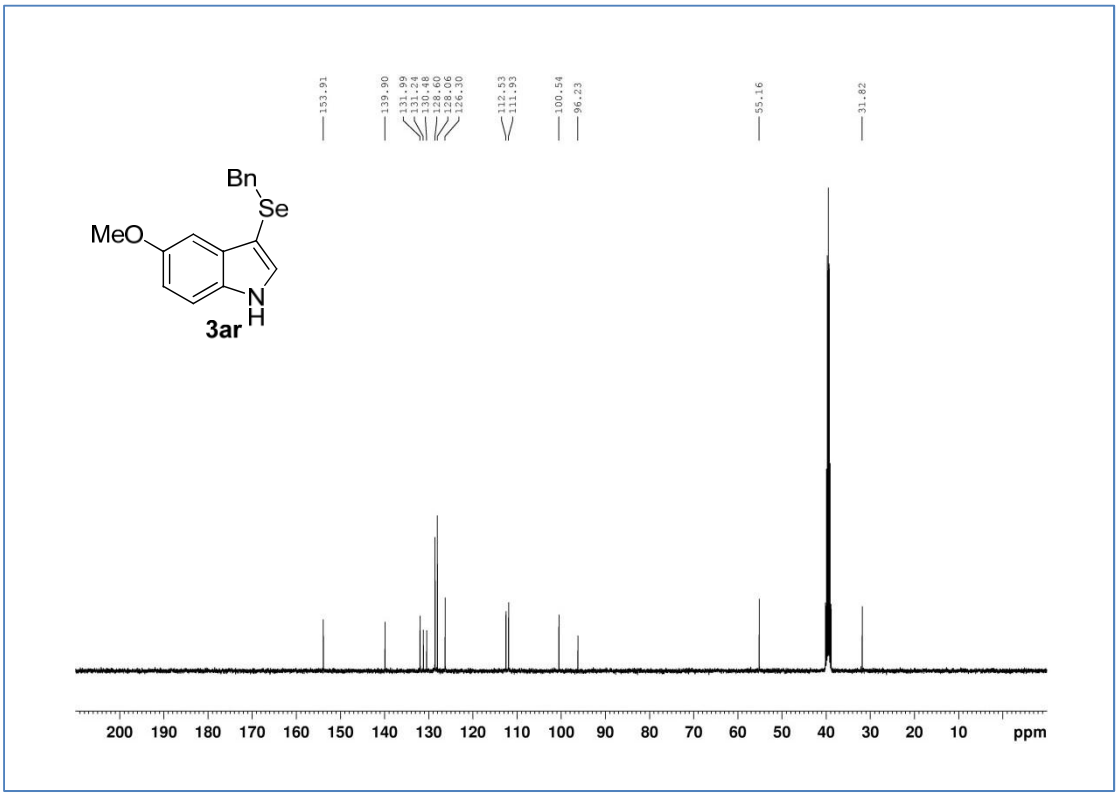
2.01 3.00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131.24
130.48
128.60
128.06
126.50
112.53
111.93
100.54
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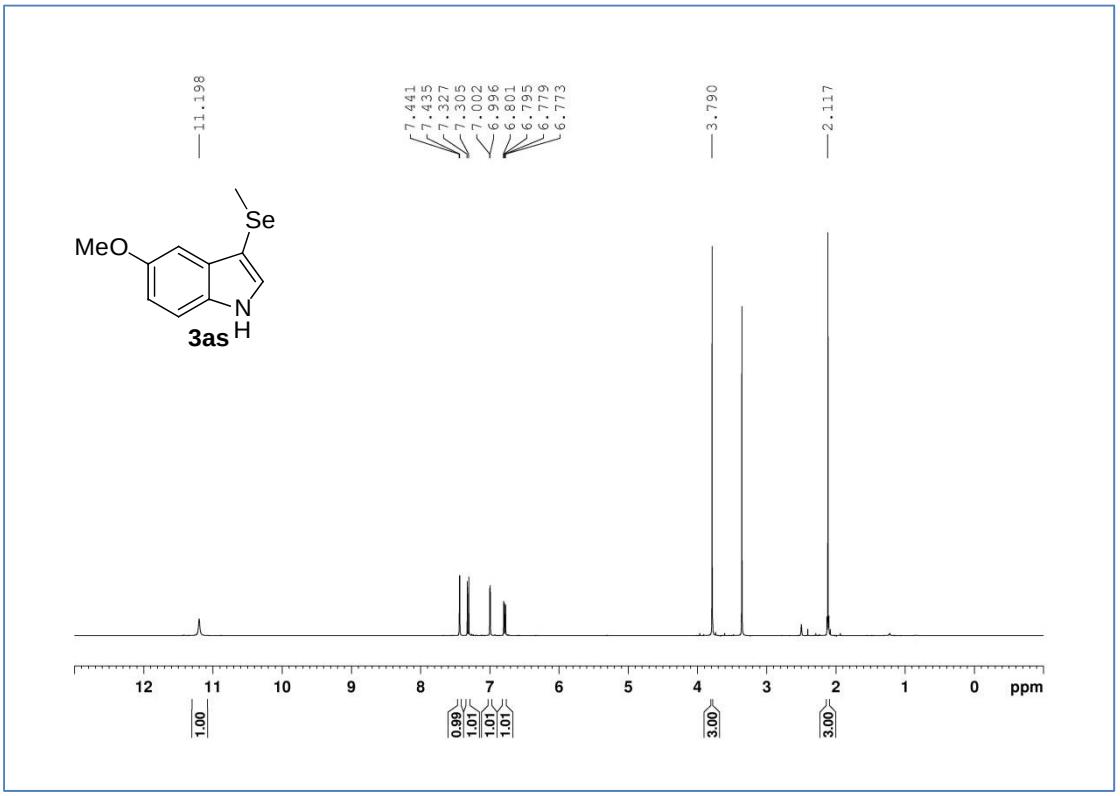
31.82
Bn
Se
MeO
N
H
3ar
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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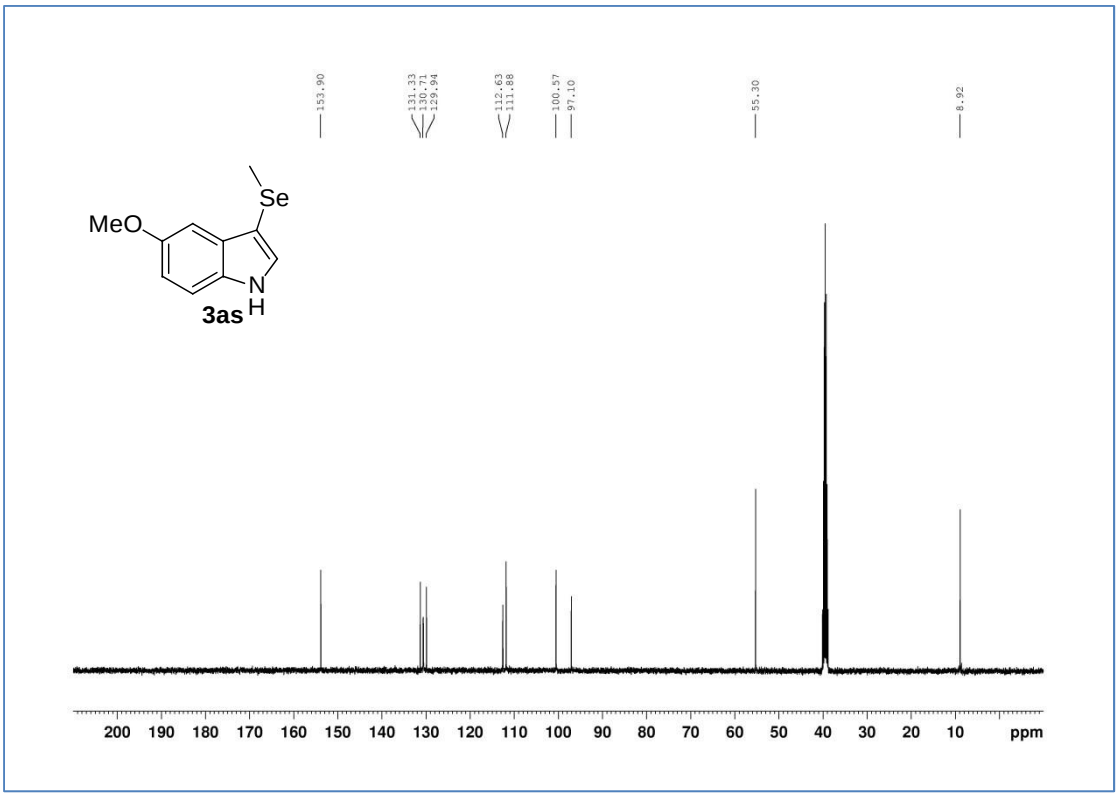
6.779
6.773
3.790
2.117
MeO
Se
N
H
3as
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
0.99
1.01
1.01
1.01
3.00
3.00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100.57
97.10
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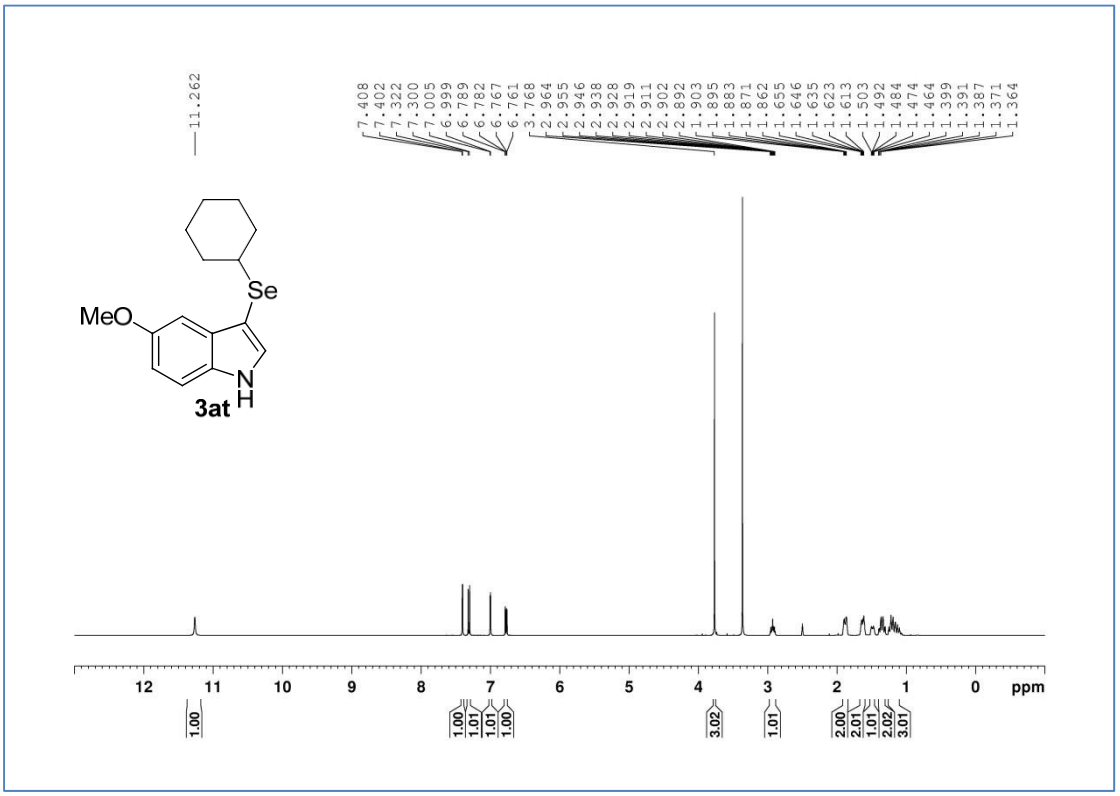
8.92
MeO
Se
N
H
3as
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm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2.955
2.946
2.938
2.928
2.919
2.911
2.902
2.892
1.903
1.895
1.883
1.871
1.862
1.655
1.646
1.635
1.623
1.613
1.503
1.492
1.484
1.474
1.464
1.399
1.391
1.387
1.371
1.364
Se
MeO
N
H
3at
12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
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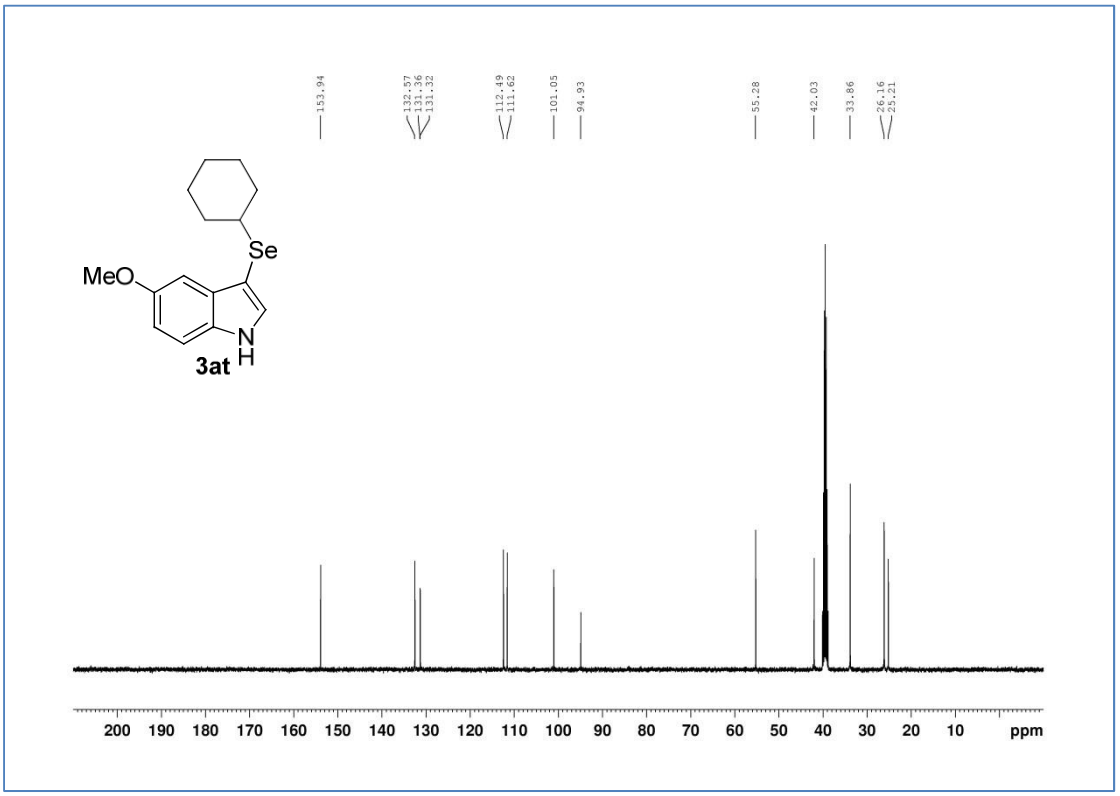
1.00
1.01
1.01
1.00
3.02
1.01
2.00
2.01
1.01
2.02
3.01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H
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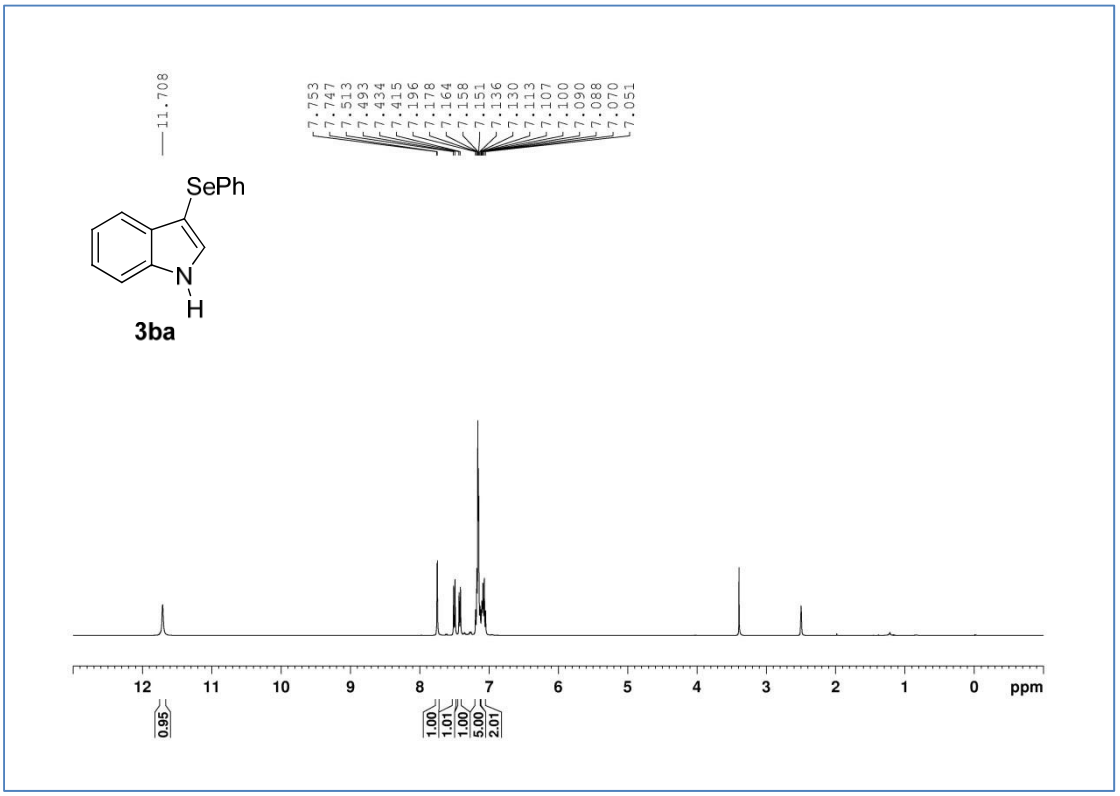
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7.136
7.130
7.113
7.107
7.100
7.090
7.088
7.070
7.051
SePh
N
H
3ba
12
11
10
9
8
7
6
5
4
3
2
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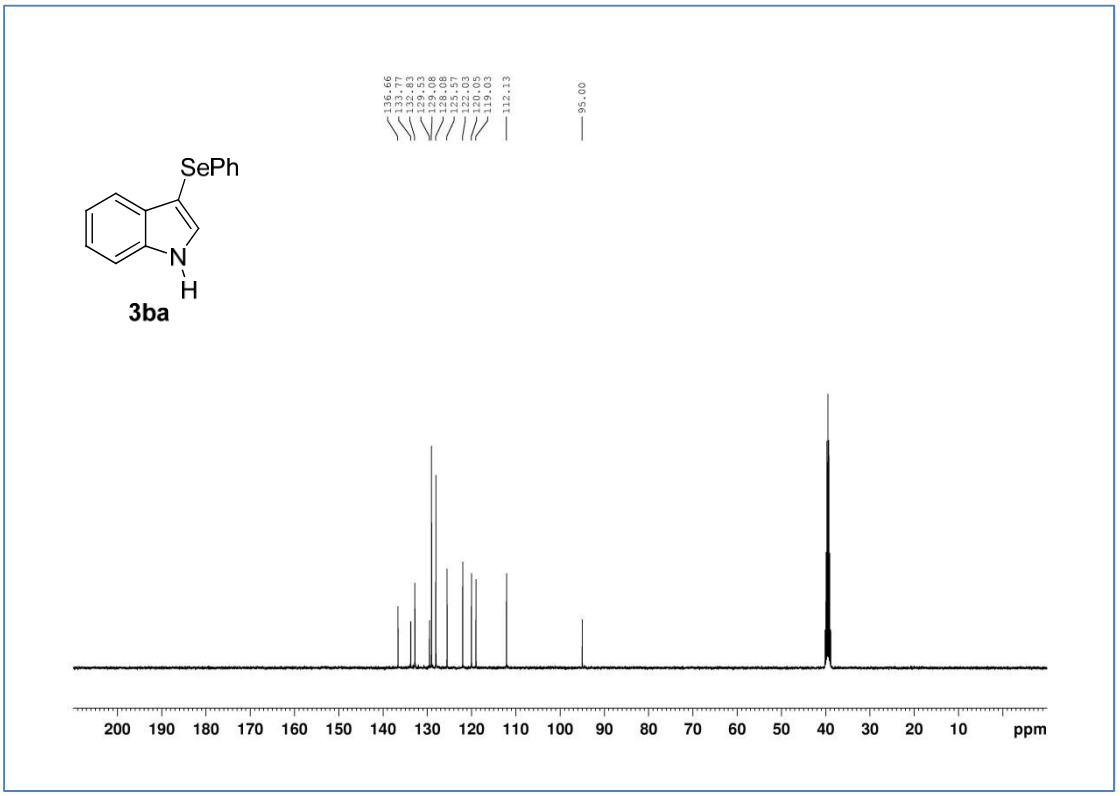
1.00
5.00
2.01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128.08
125.57
122.03
120.05
119.03
112.13
95.00
SePh
N
H
3ba
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180
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150
140
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100
90
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70
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30
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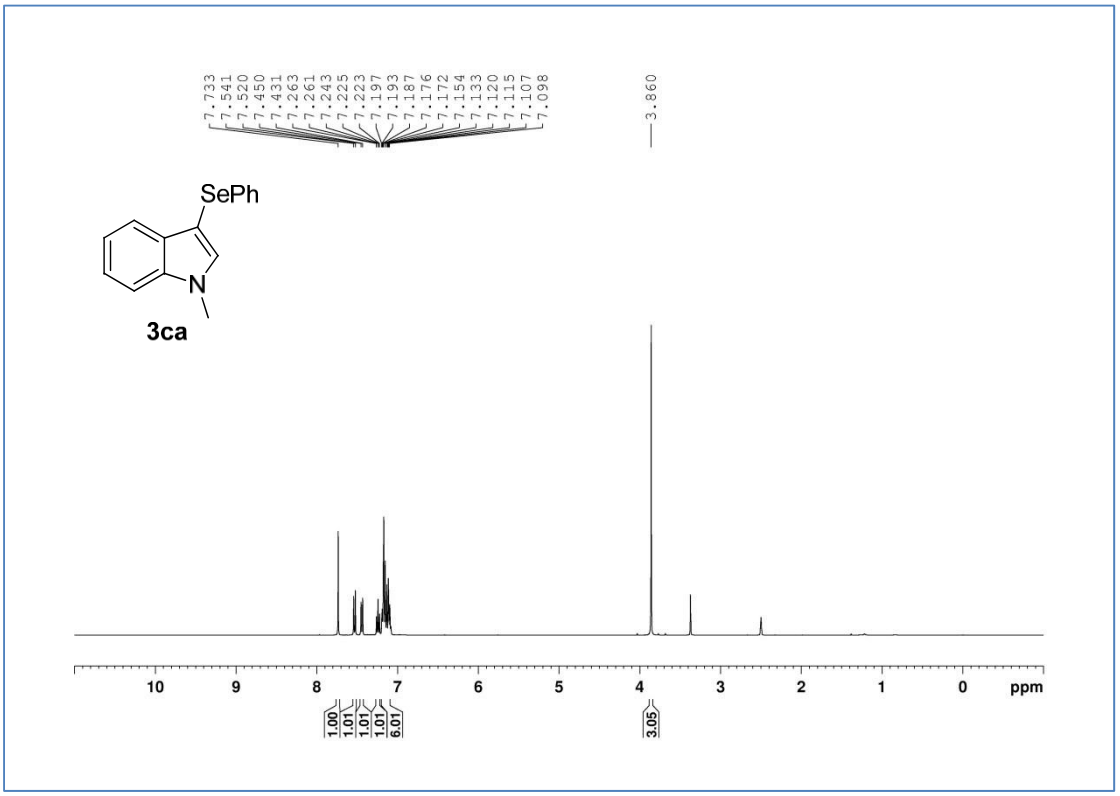
10
ppm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7.187
7.176
7.172
7.154
7.133
7.120
7.115
7.107
7.098
3.860
SePh
N
3ca
10
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4
3
2
1
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ppm
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1.01
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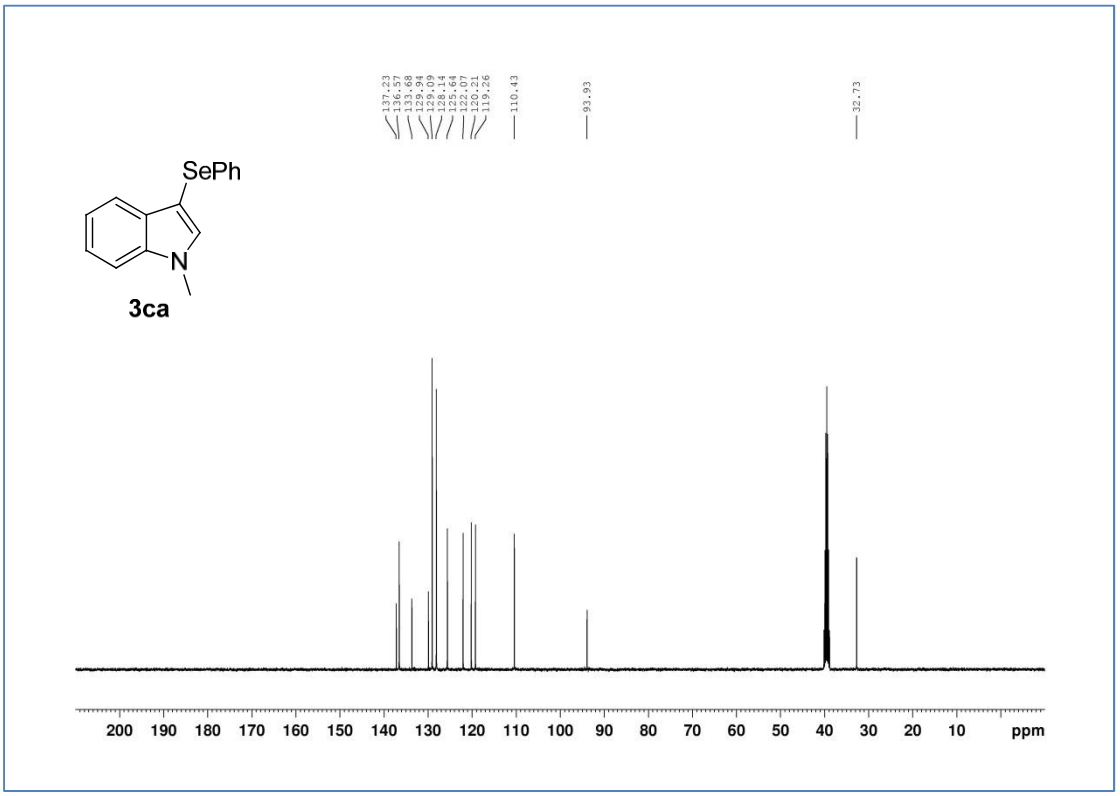
1.01
6.01
3.05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128.14
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93.93
32.73
SePh
N
3ca
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150
140
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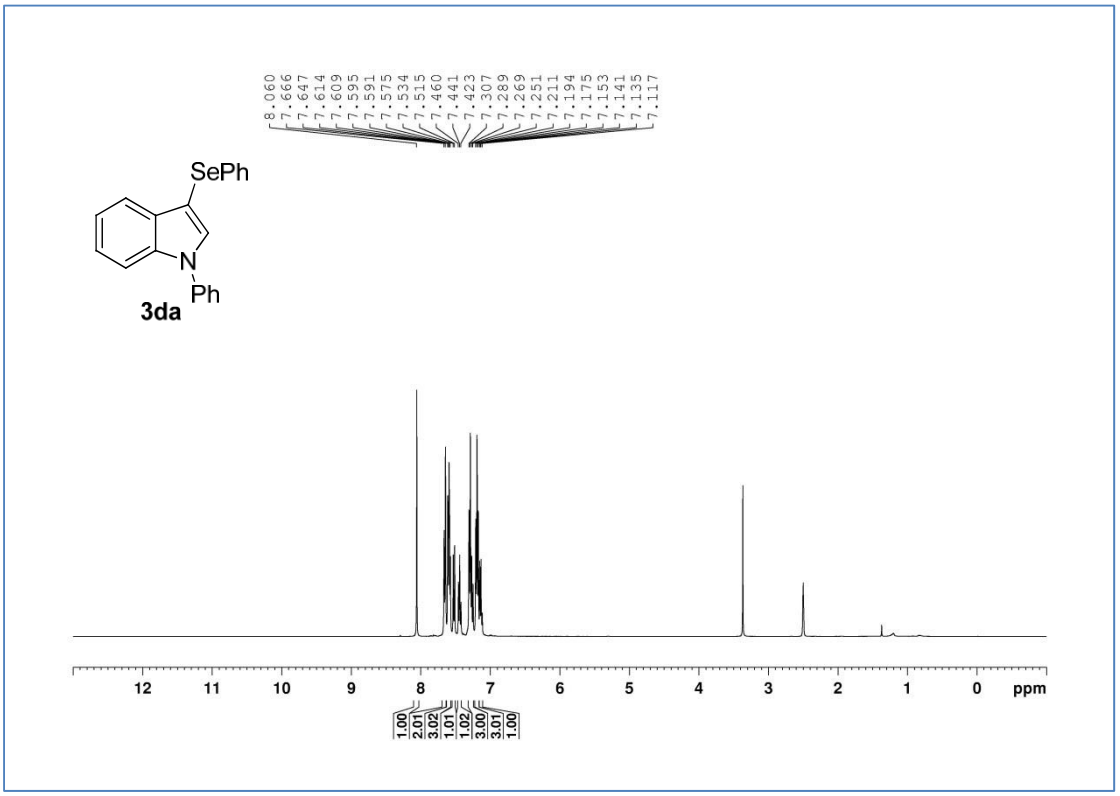
80
70
60
50
40
30
20
10
ppm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7.515
7.460
7.441
7.423
7.307
7.289
7.269
7.251
7.211
7.194
7.175
7.153
7.141
7.135
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N
Ph
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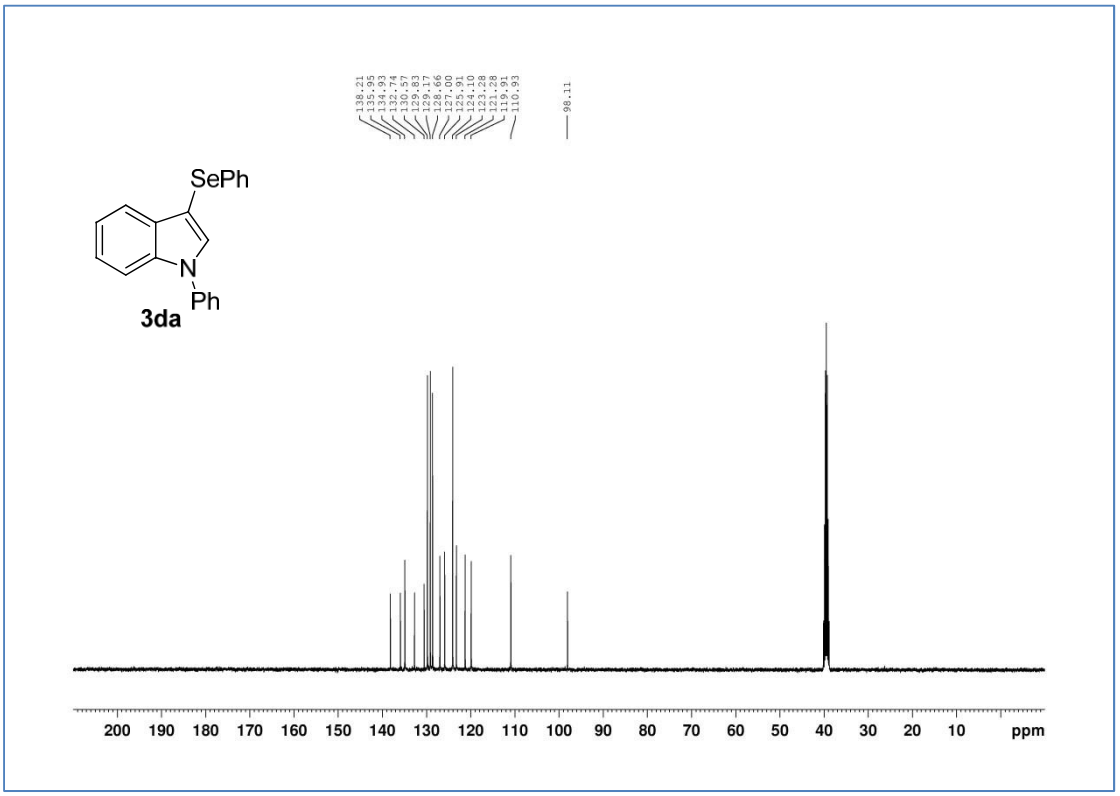
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129.83
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128.66
127.00
124.91
124.10
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110.93
98.11
SePh
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Ph
3da
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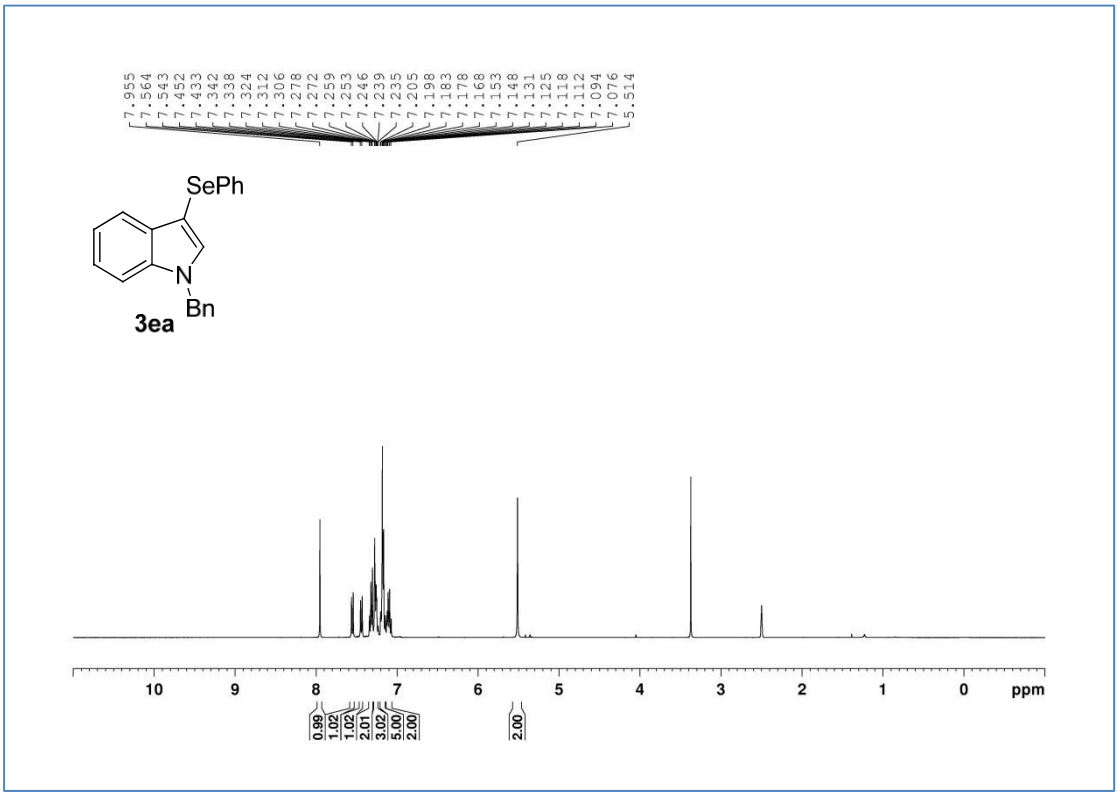
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7.259
7.253
7.246
7.239
7.235
7.205
7.198
7.183
7.178
7.168
7.153
7.148
7.131
7.125
7.118
7.112
7.094
7.076
5.514
SePh
N
Bn
3ea
10
9
8
7
6
5
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1
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ppm
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1.02
2.01
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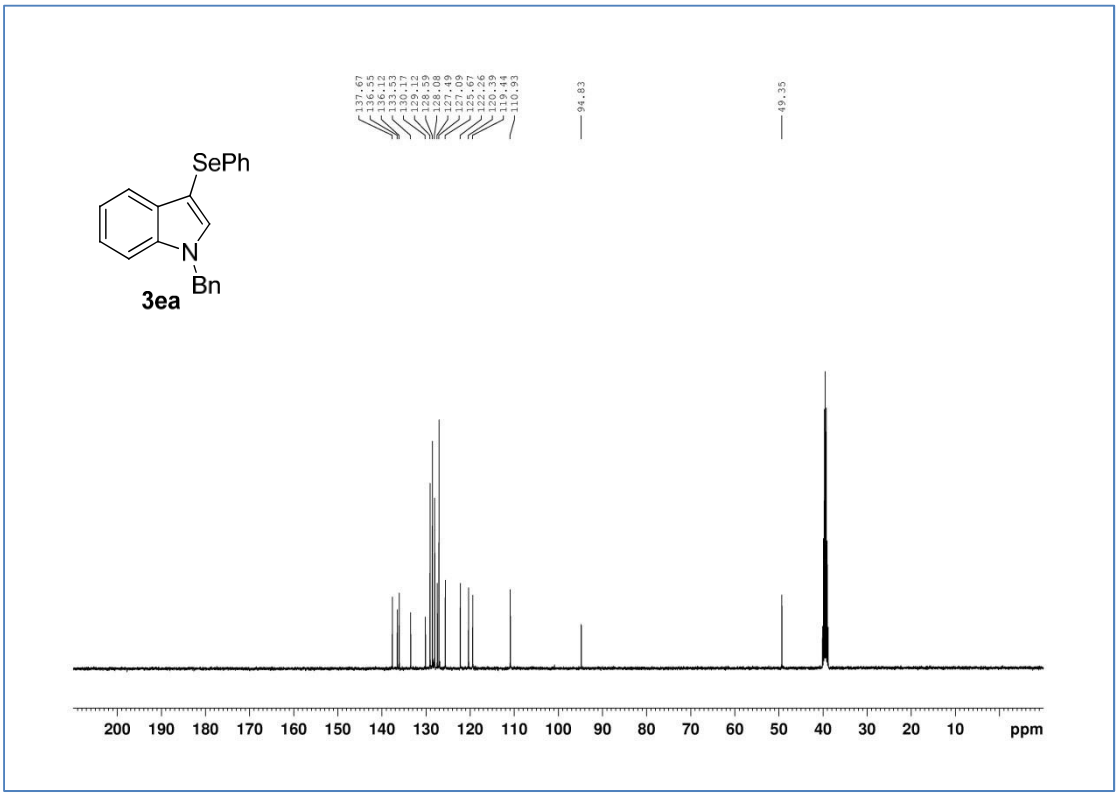
2.00
2.00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128.08
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127.09
125.67
122.26
120.39
119.44
110.93
94.83
49.35
SePh
N
Bn
3ea
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150
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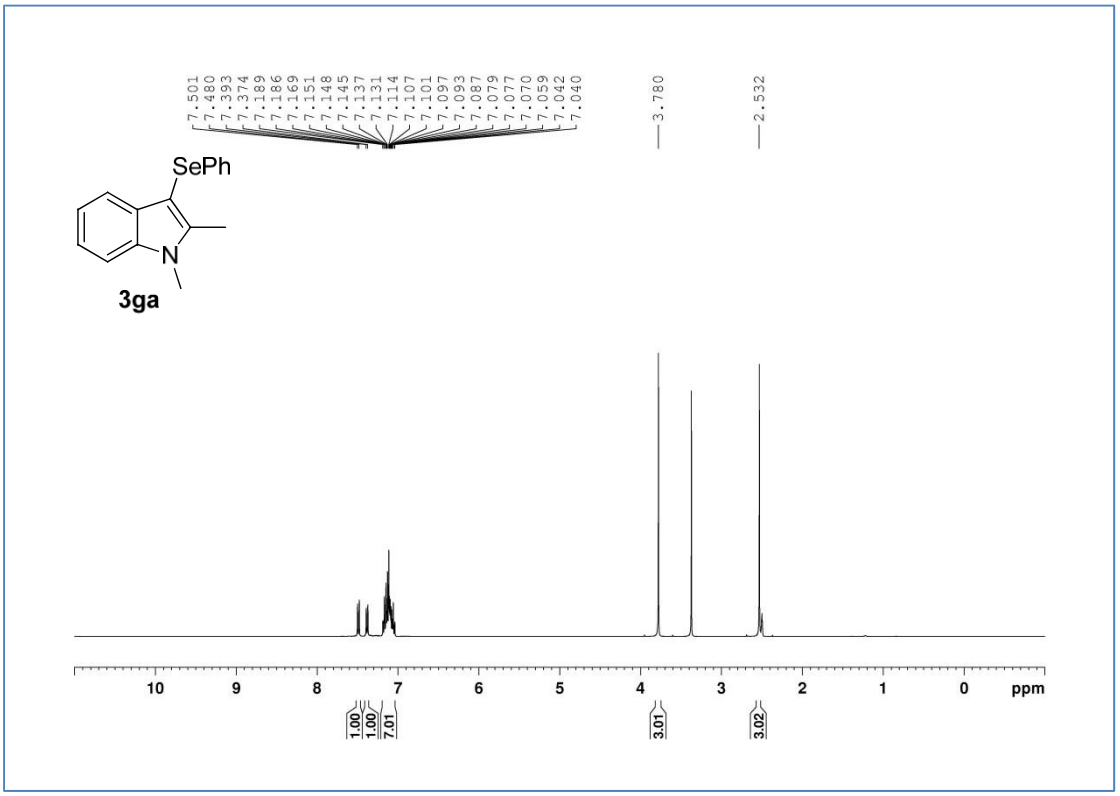
10
ppm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7.101
7.097
7.093
7.087
7.079
7.077
7.070
7.059
7.042
7.040
3.780
2.532
SePh
N
3ga
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.00
7.01
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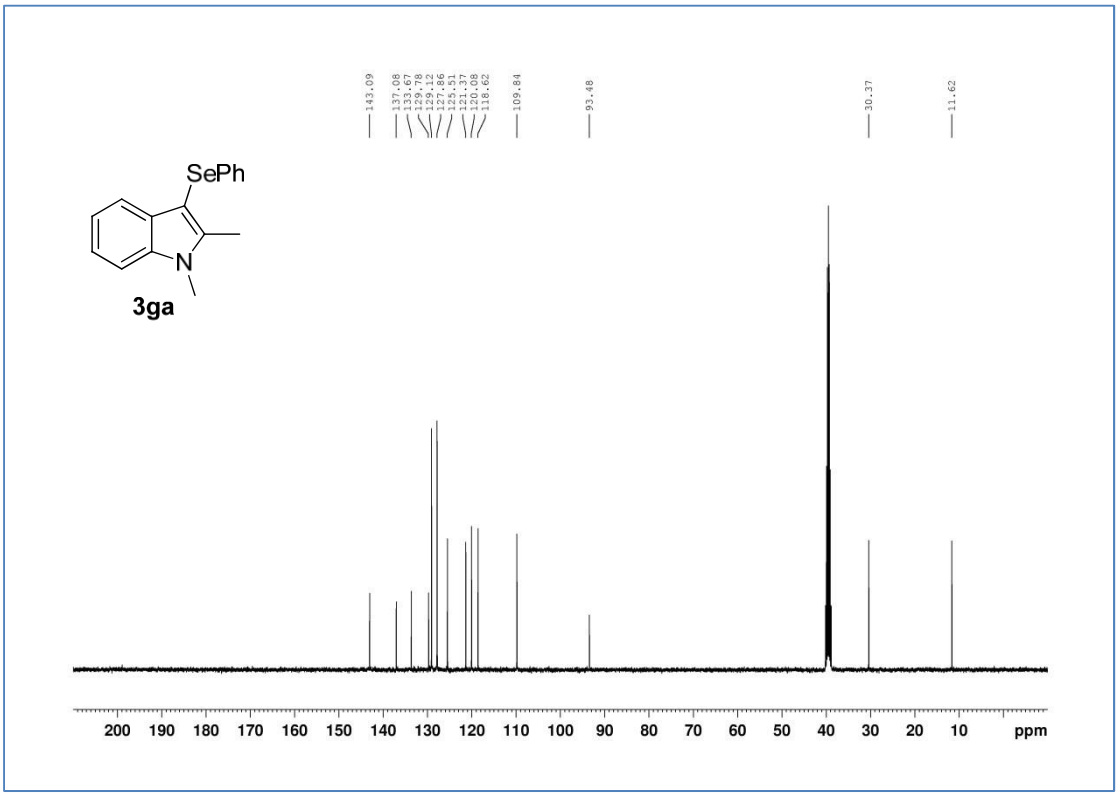
3.02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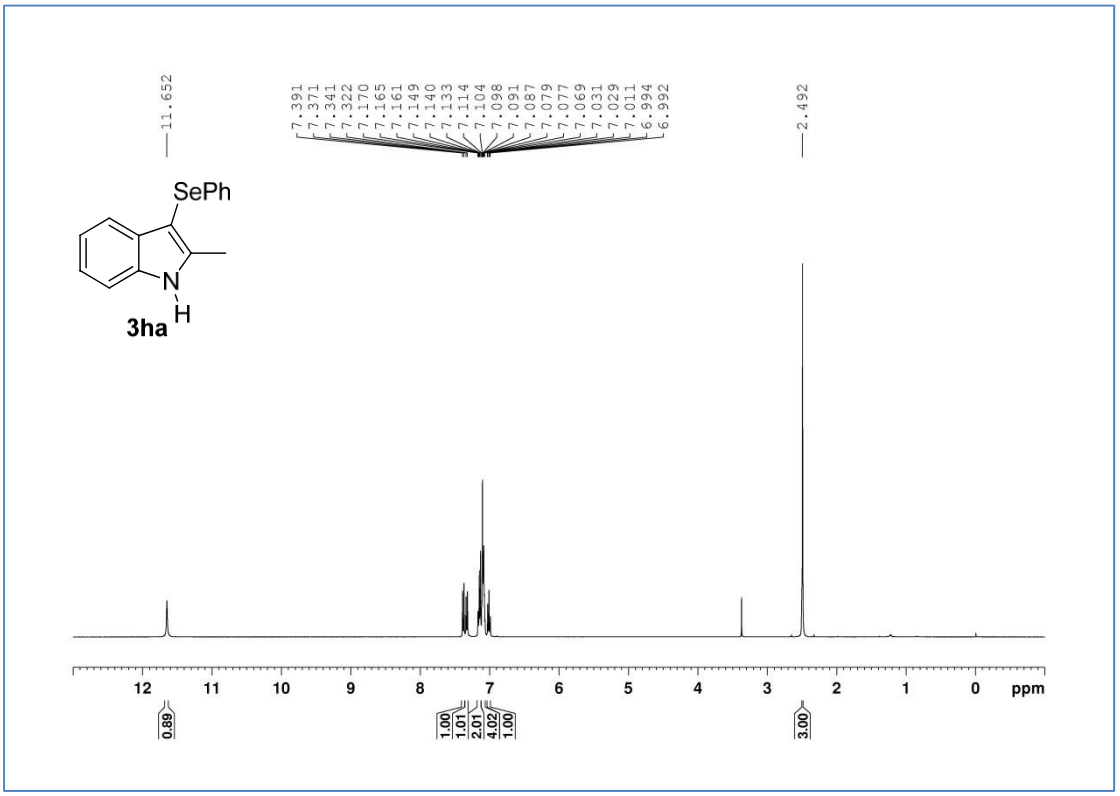
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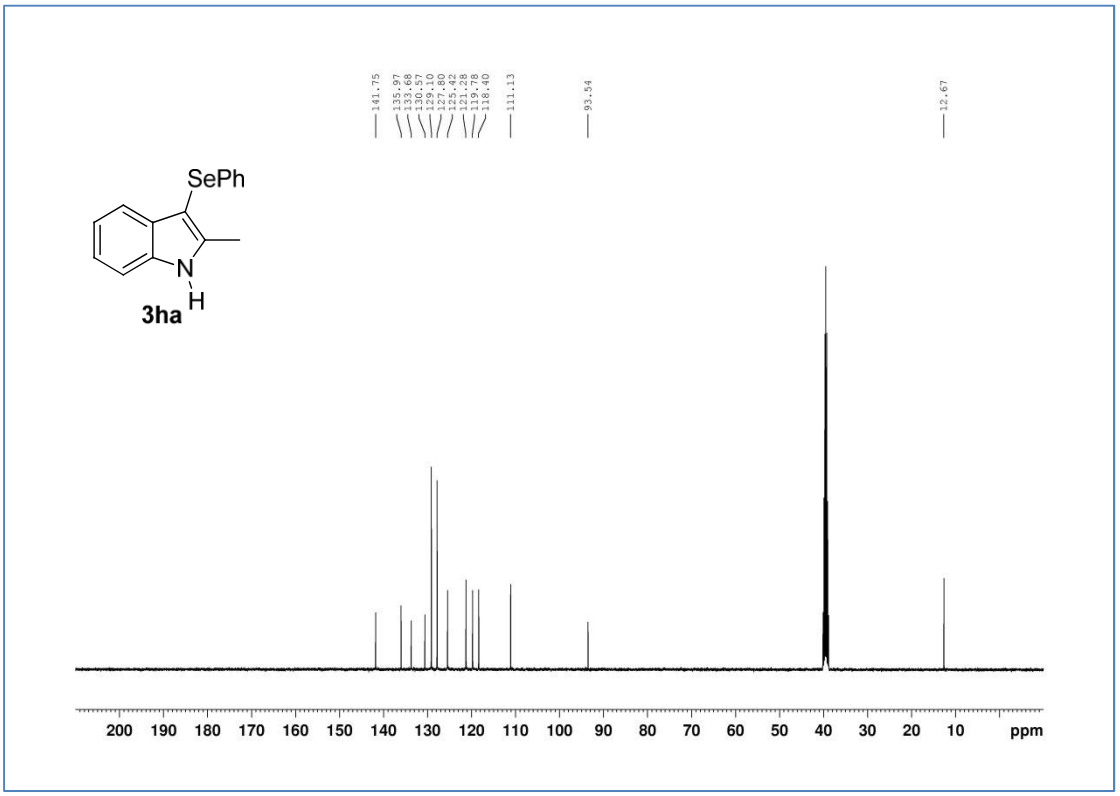
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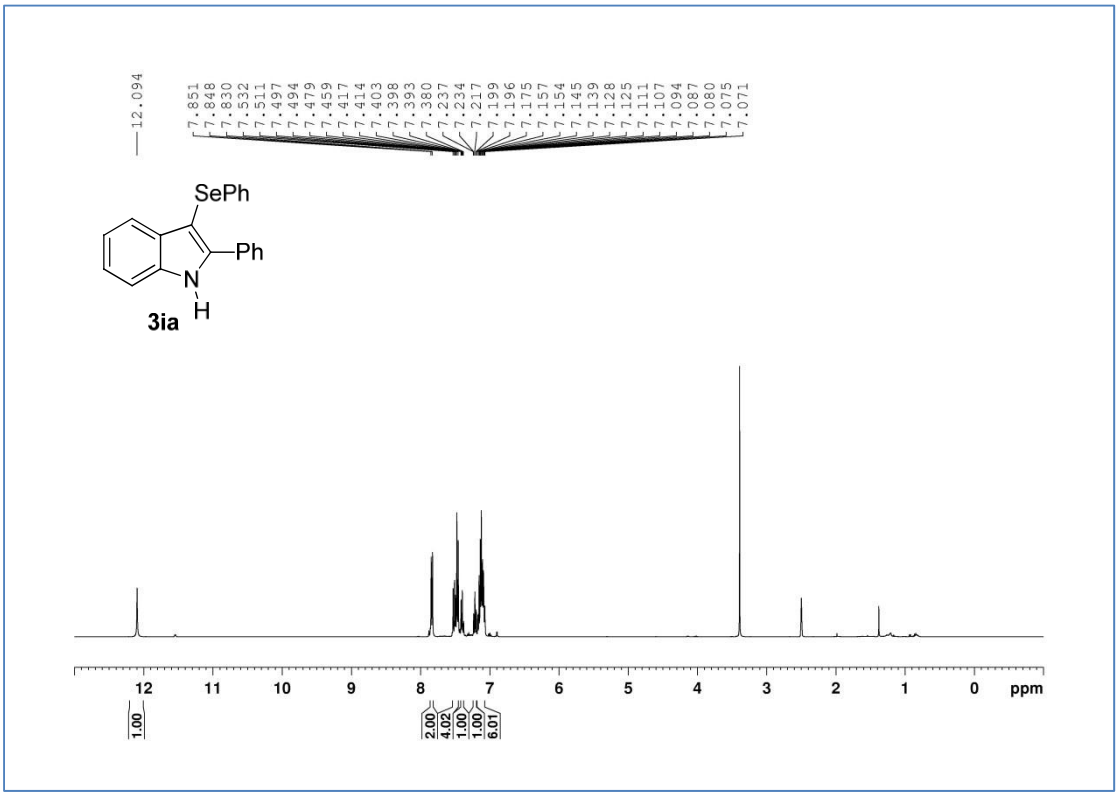
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Ph
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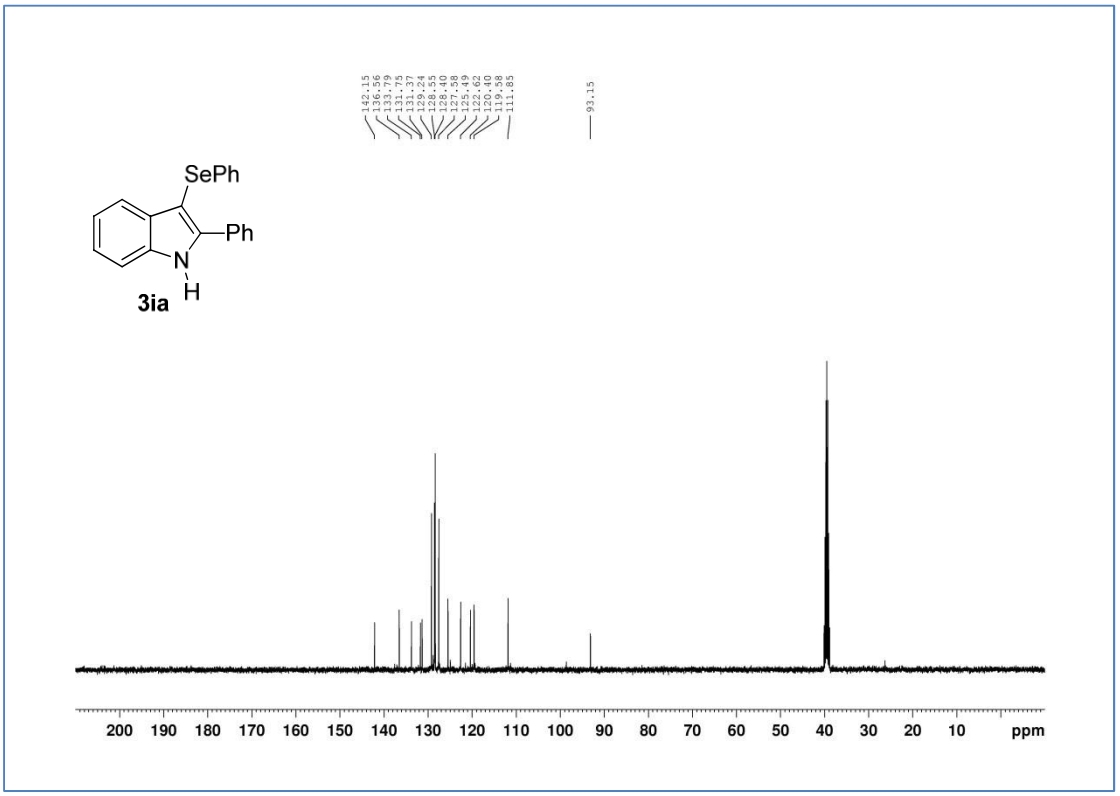
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Ph
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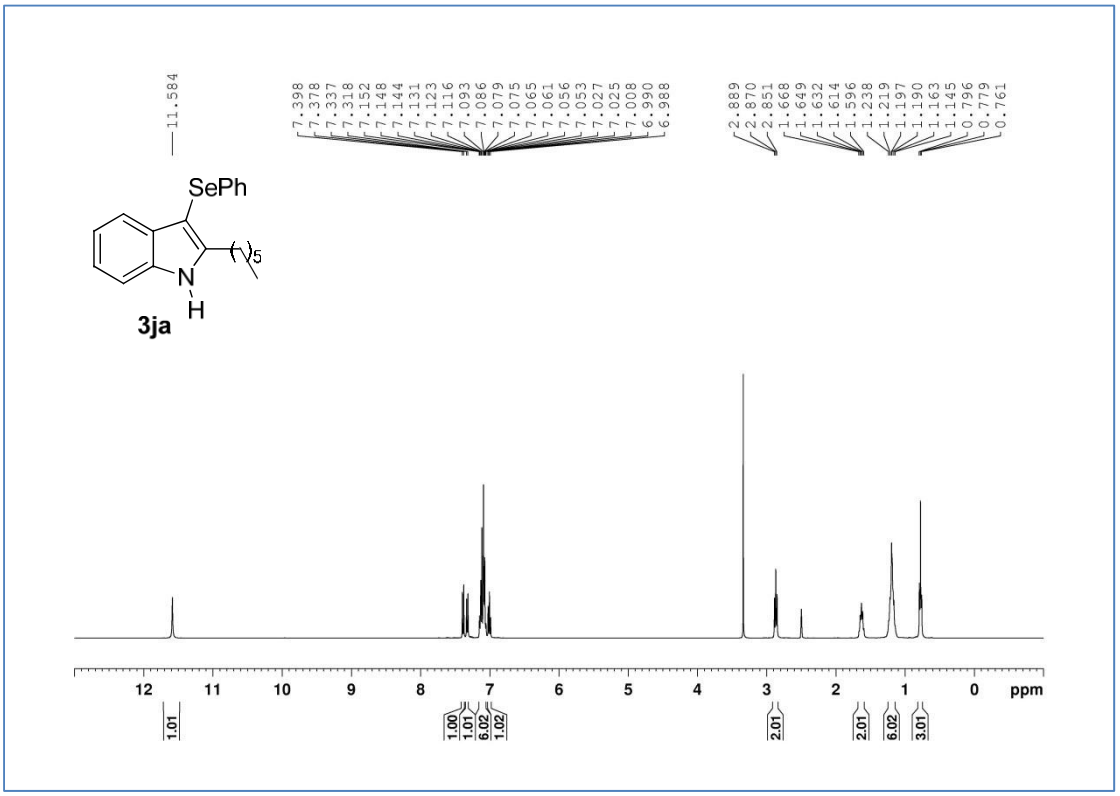
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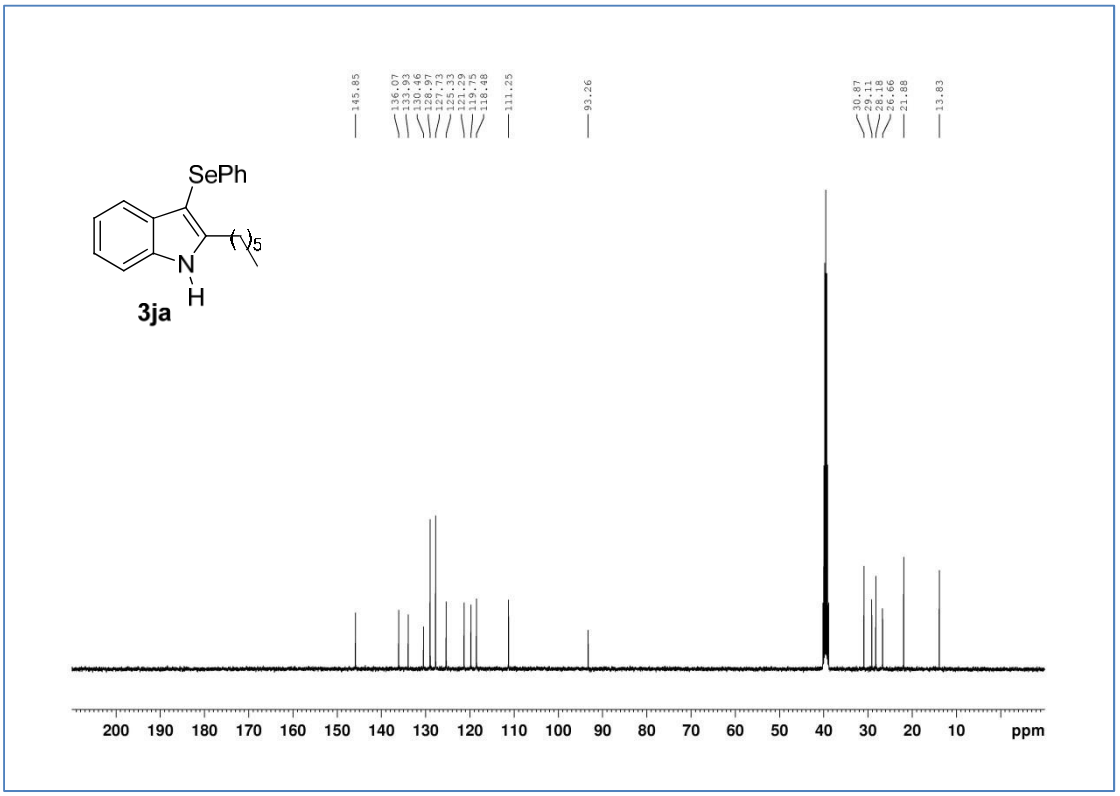
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26.66
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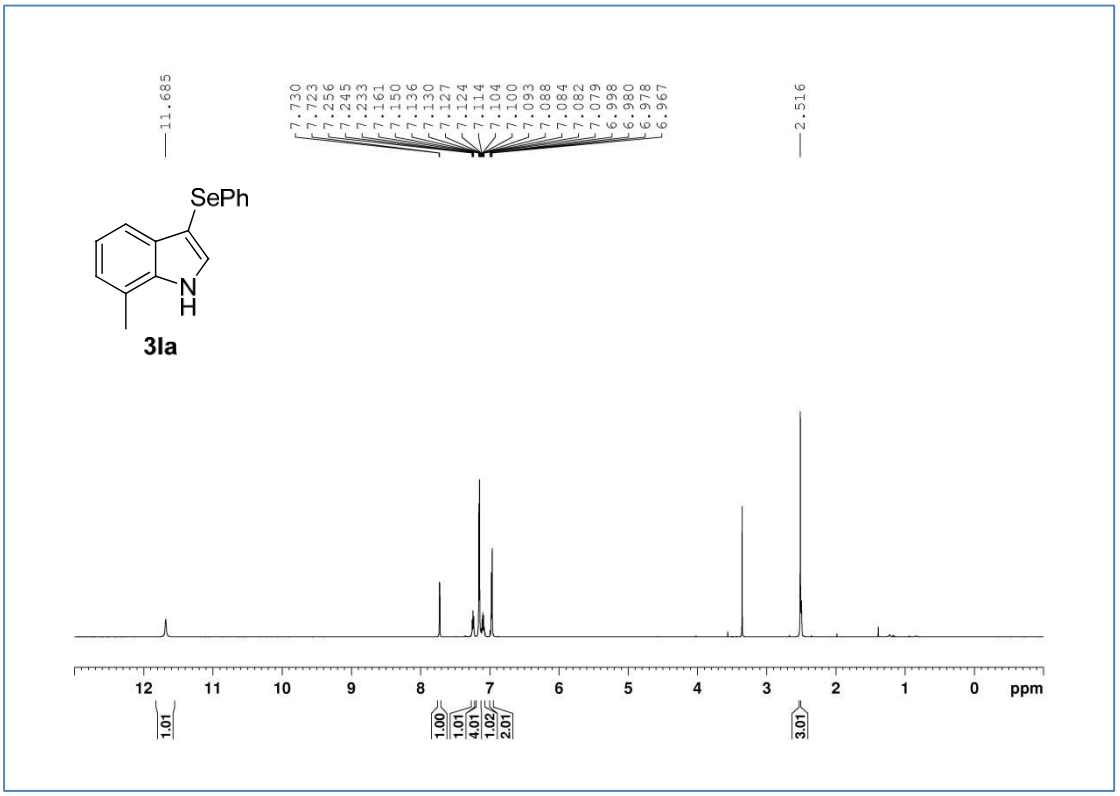
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N
H
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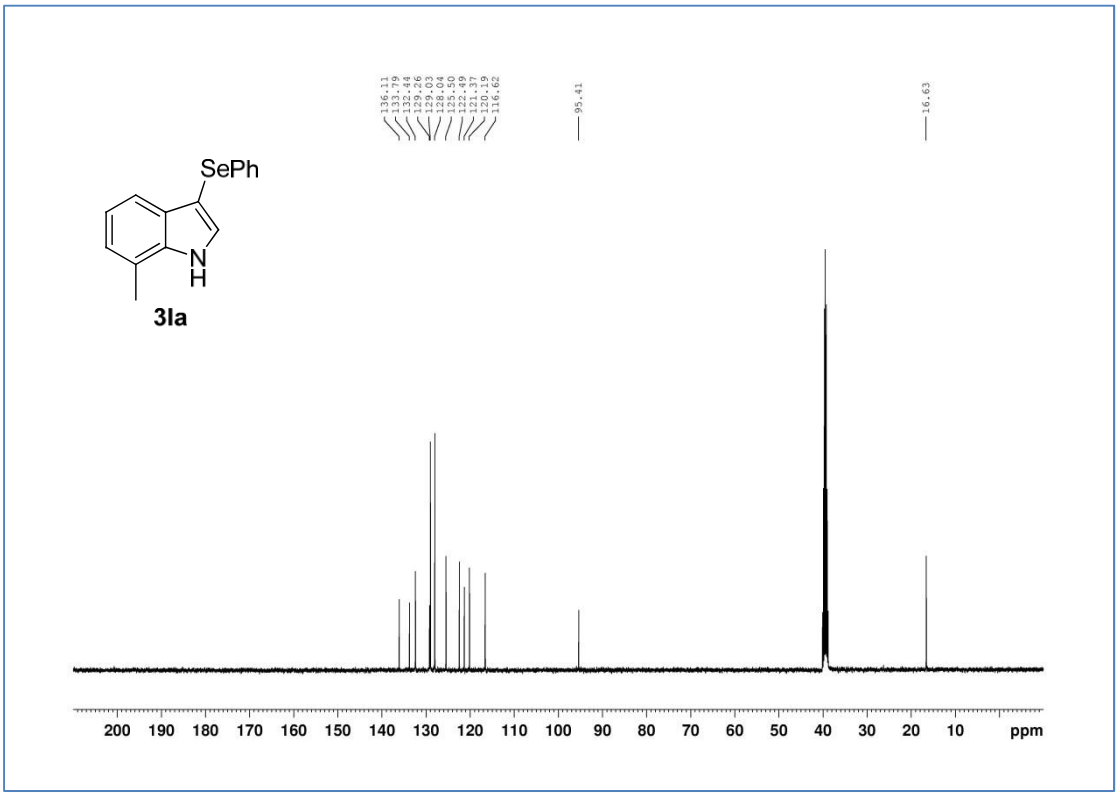
3.01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H
3Ia
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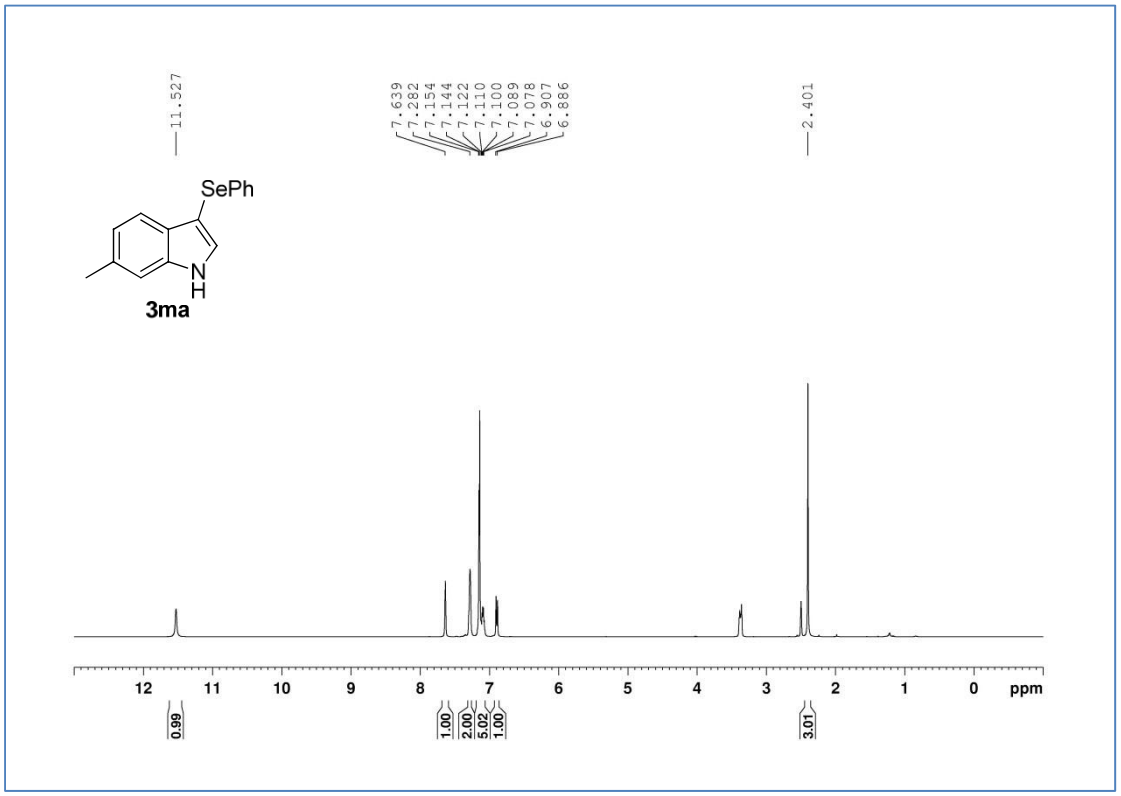
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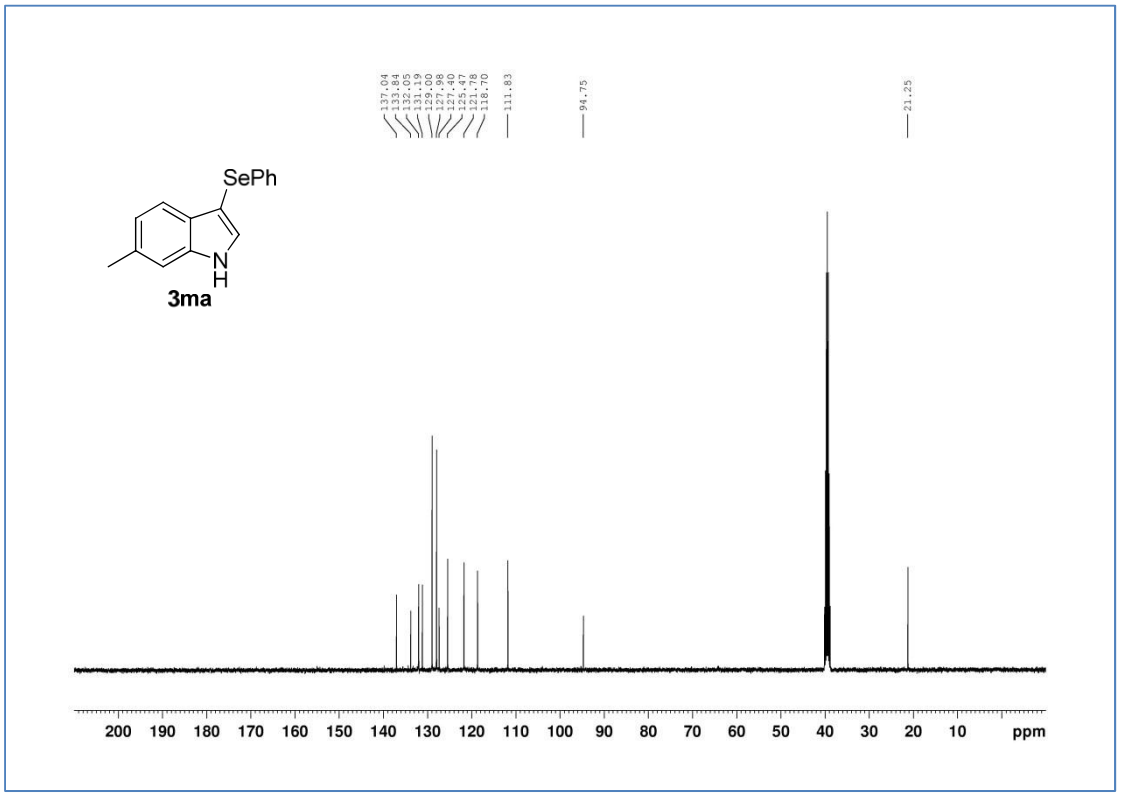
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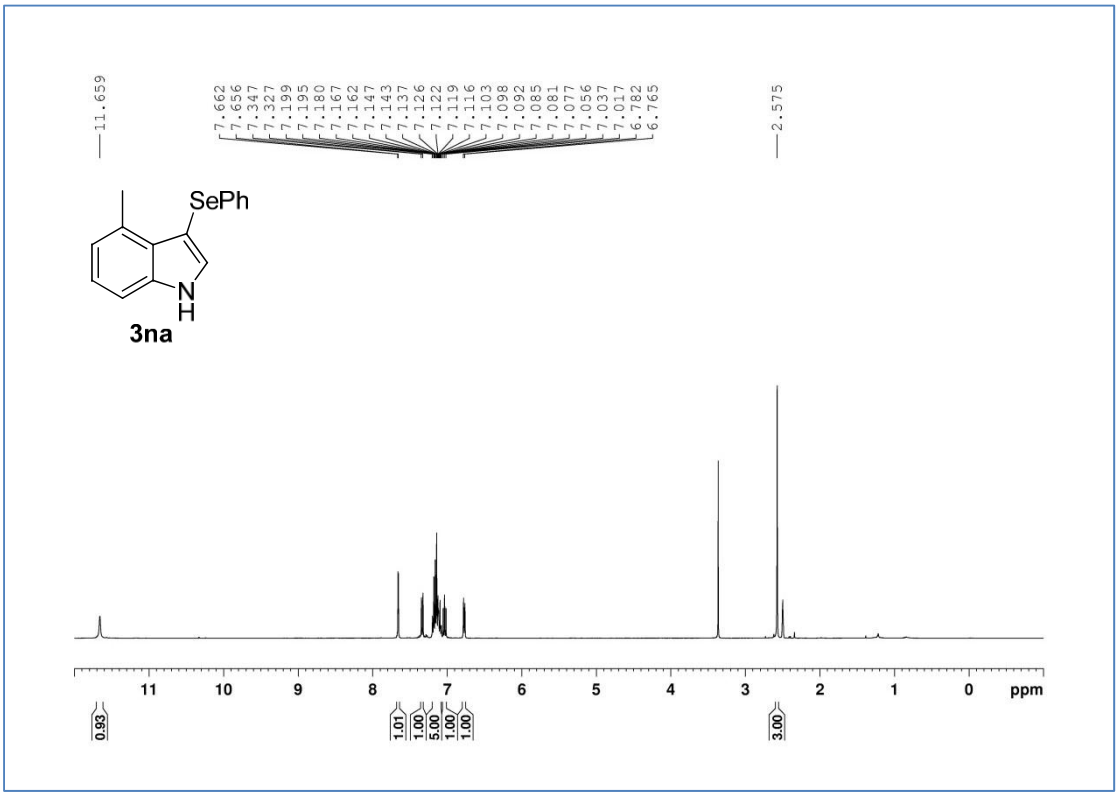
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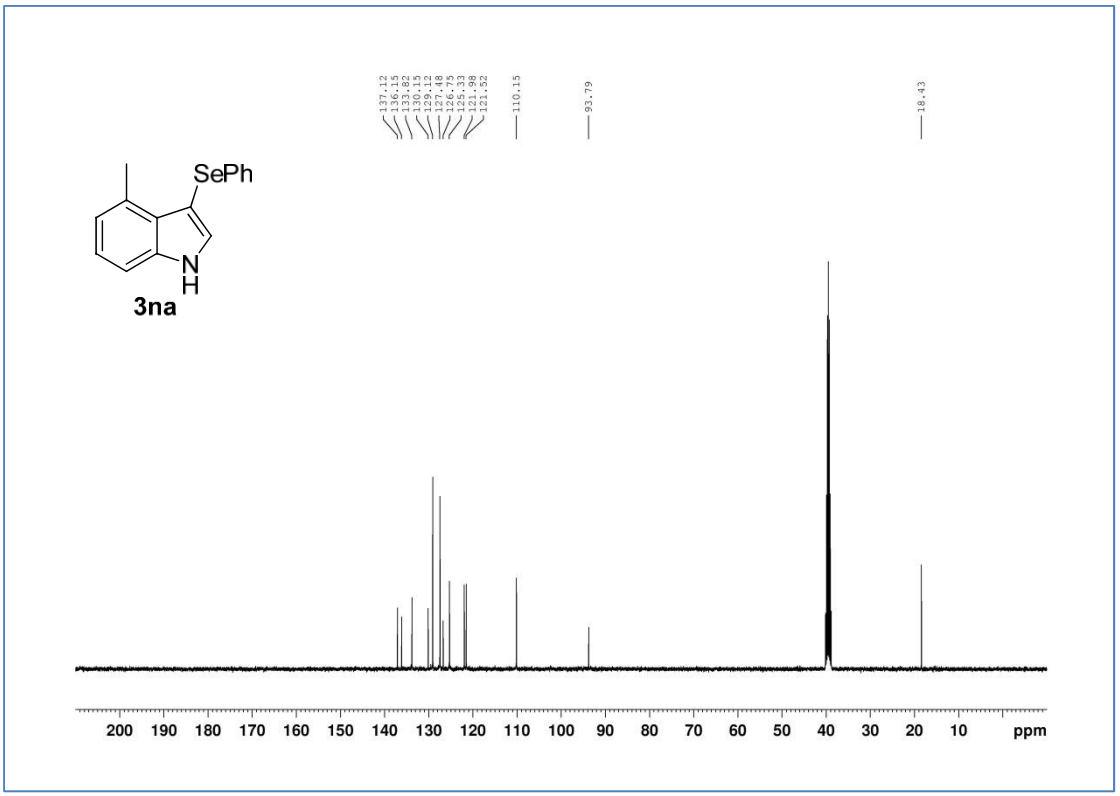
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H
3na
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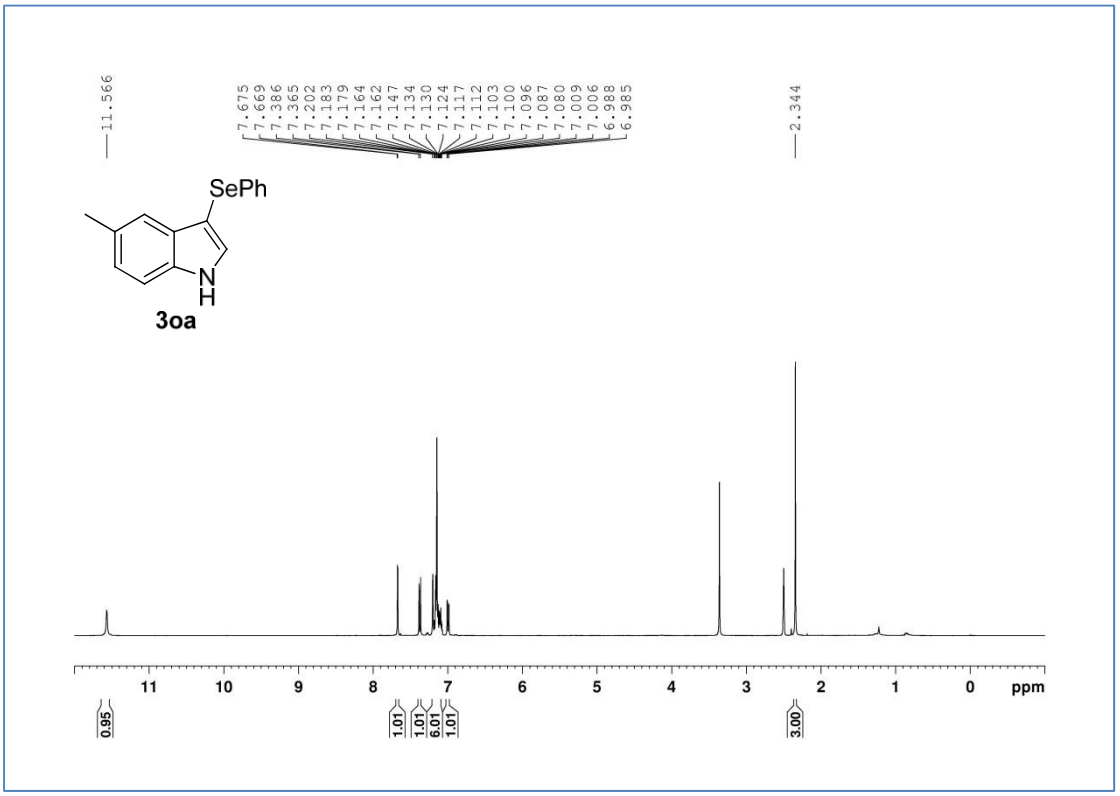
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7.117
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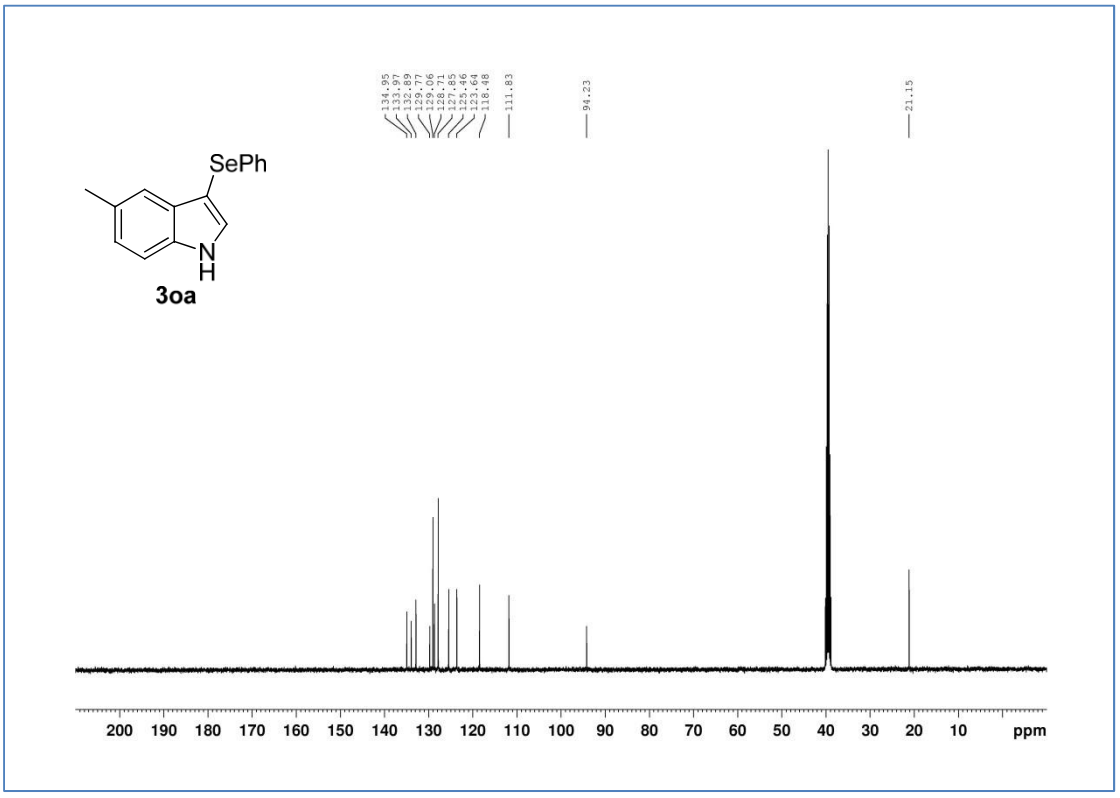
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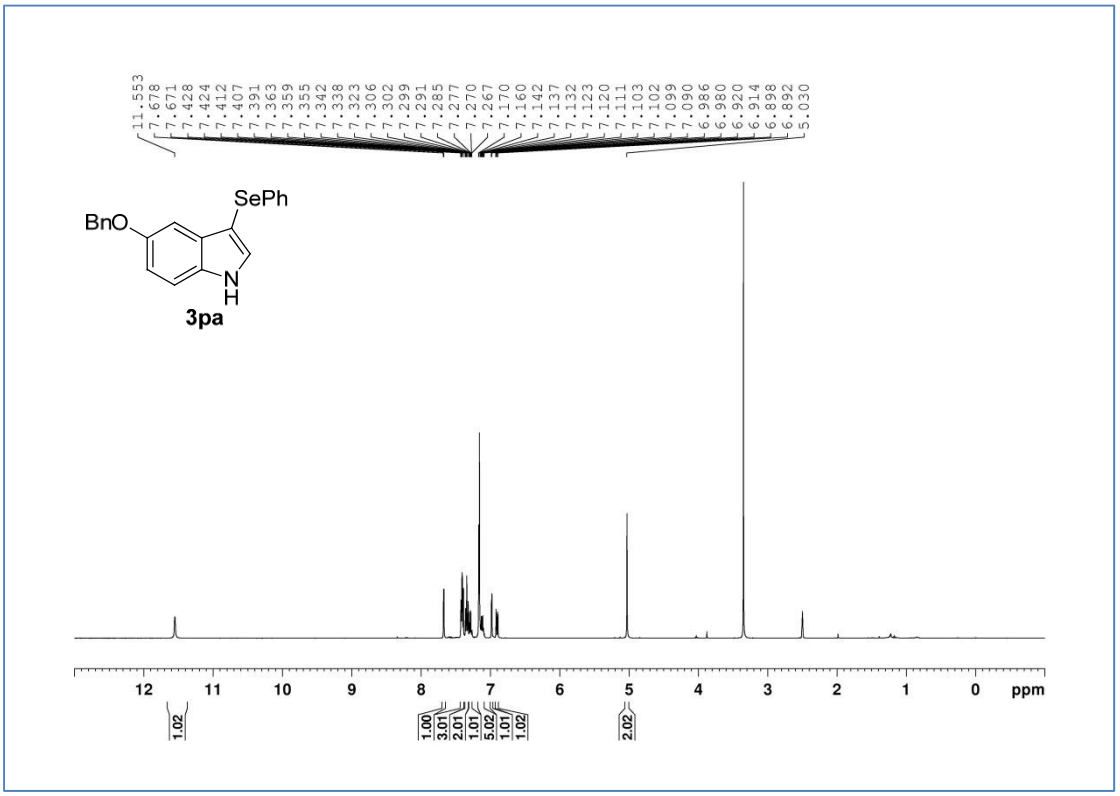
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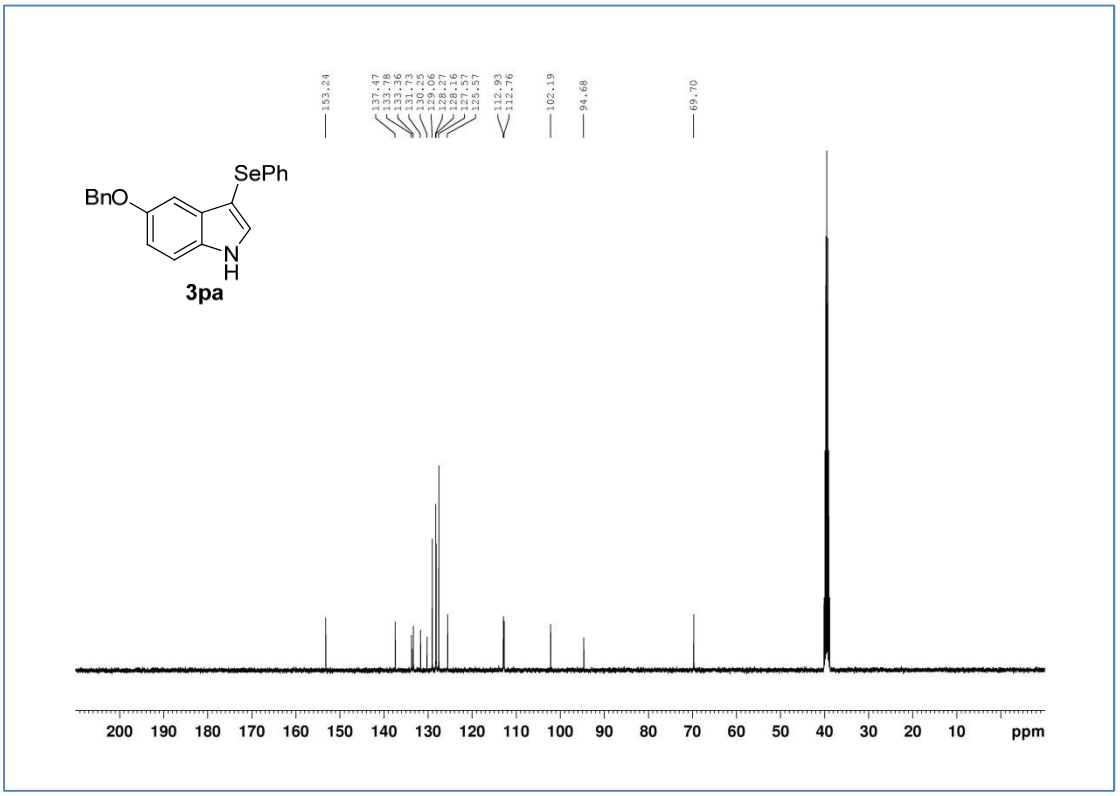
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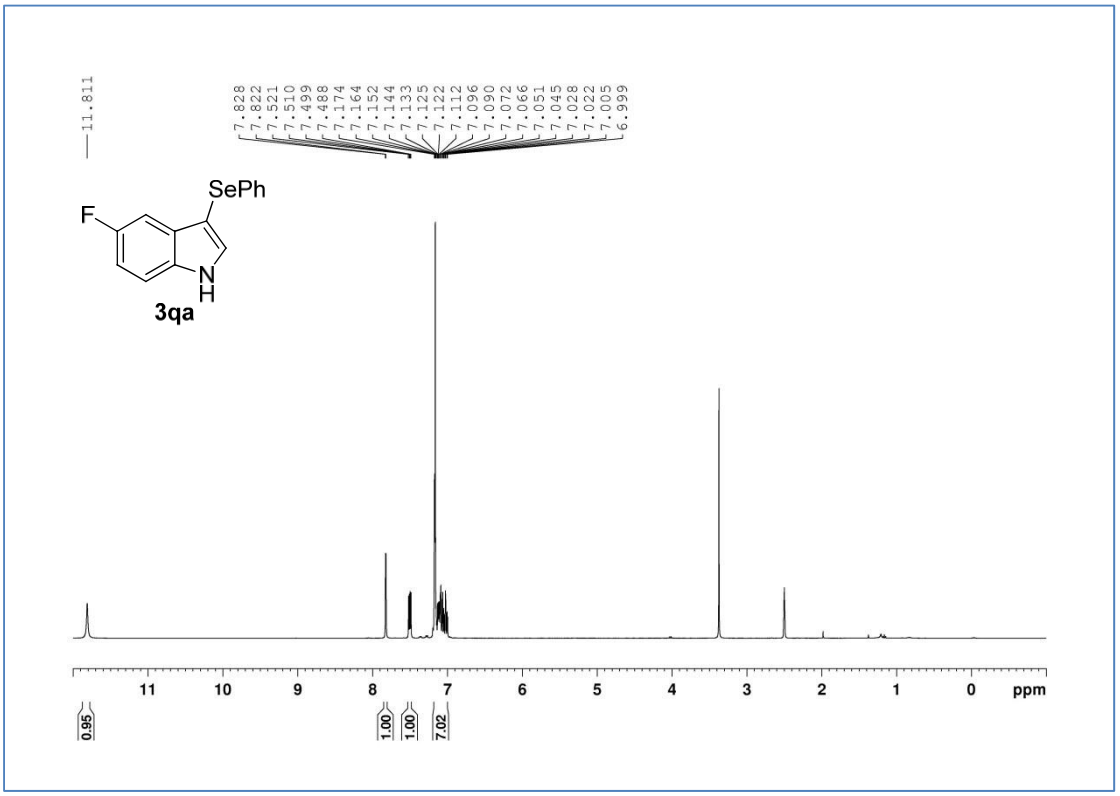
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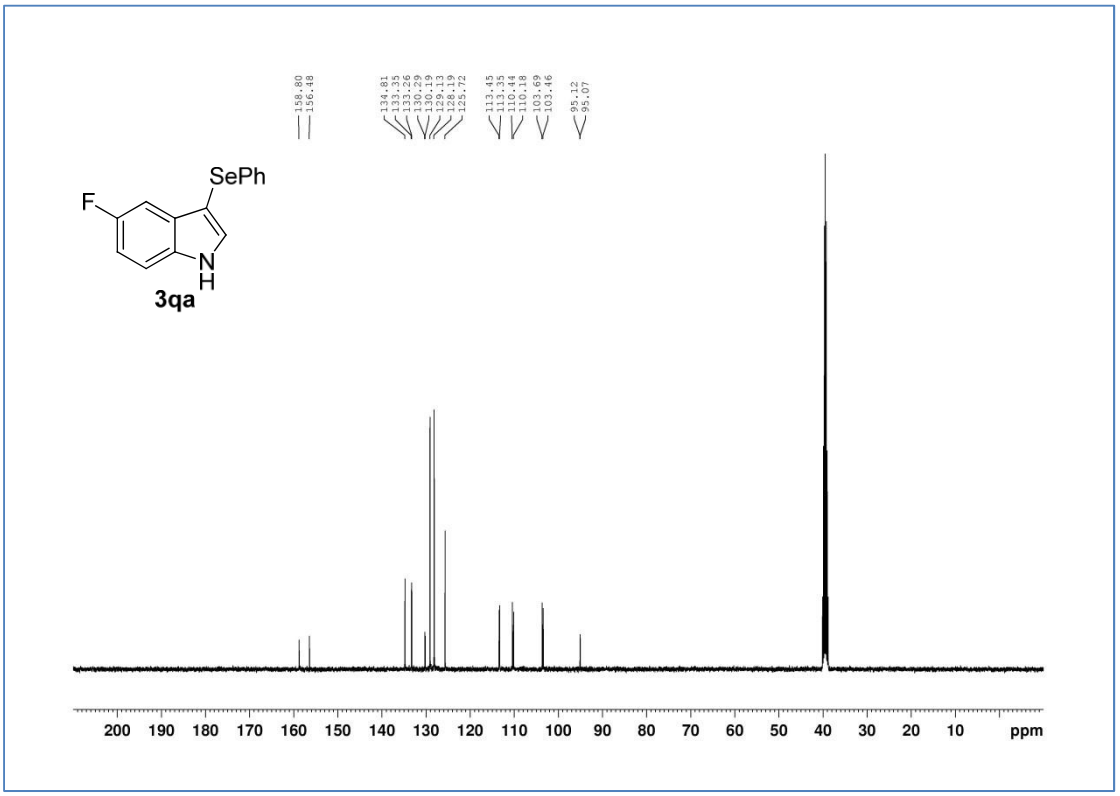
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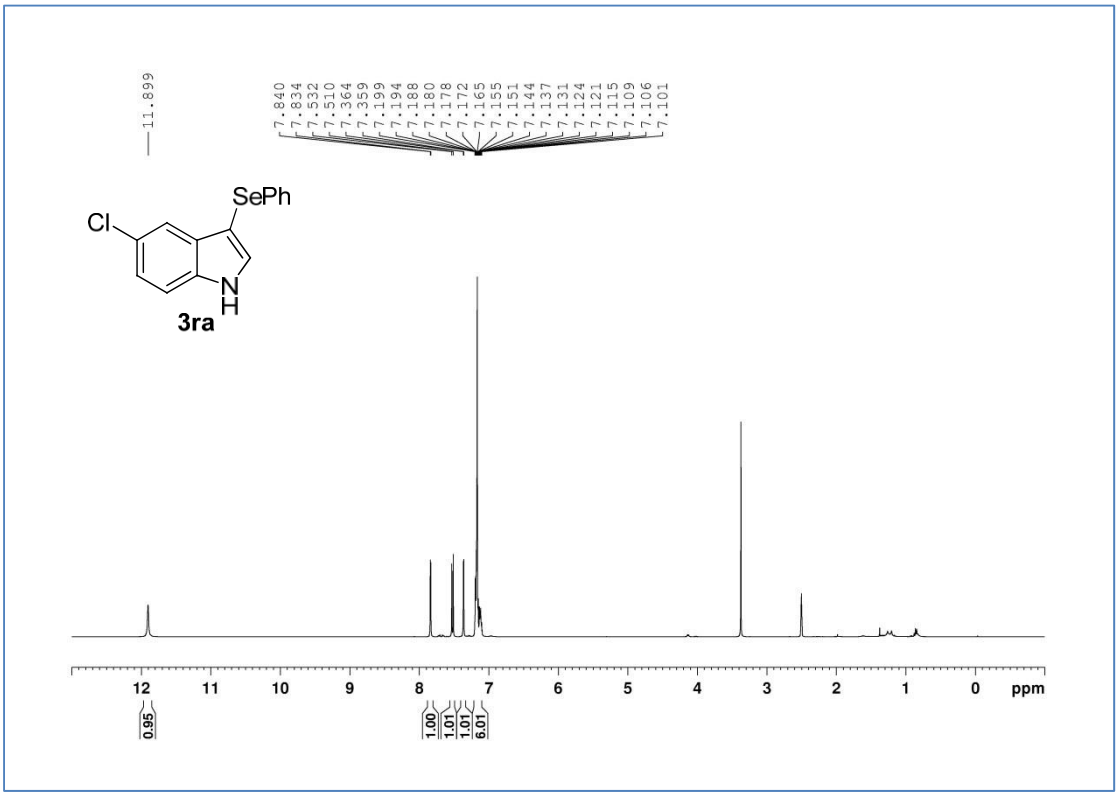
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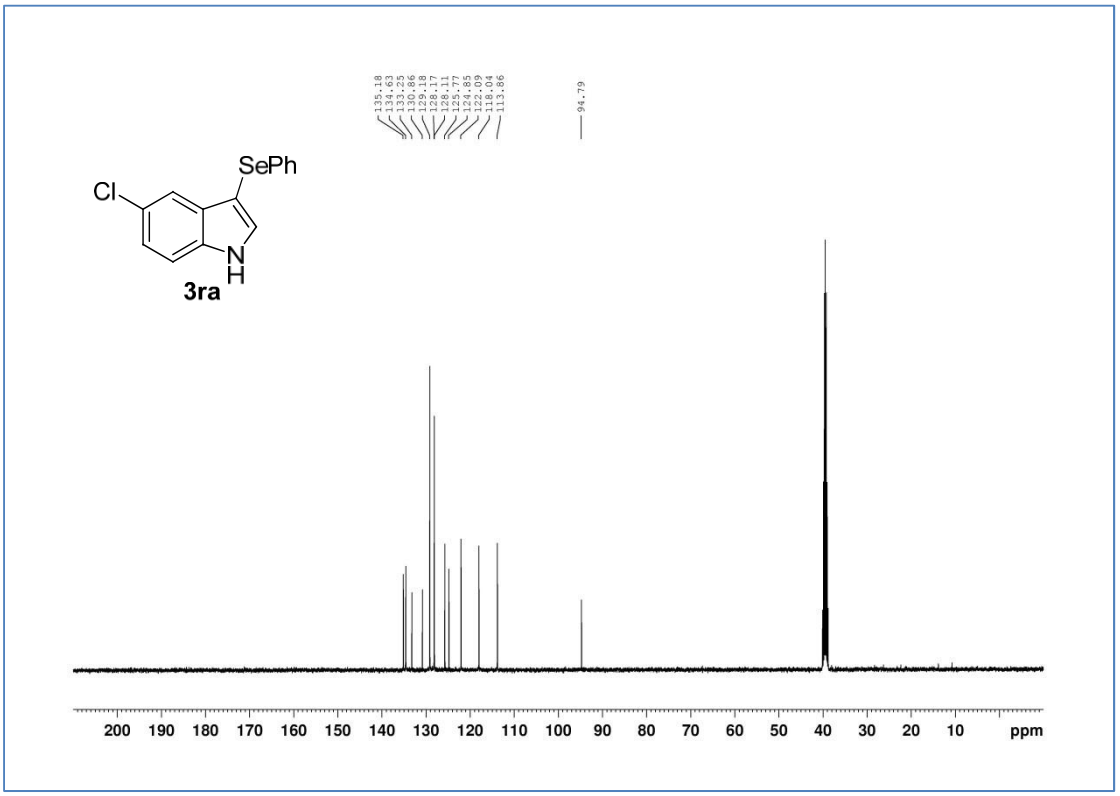
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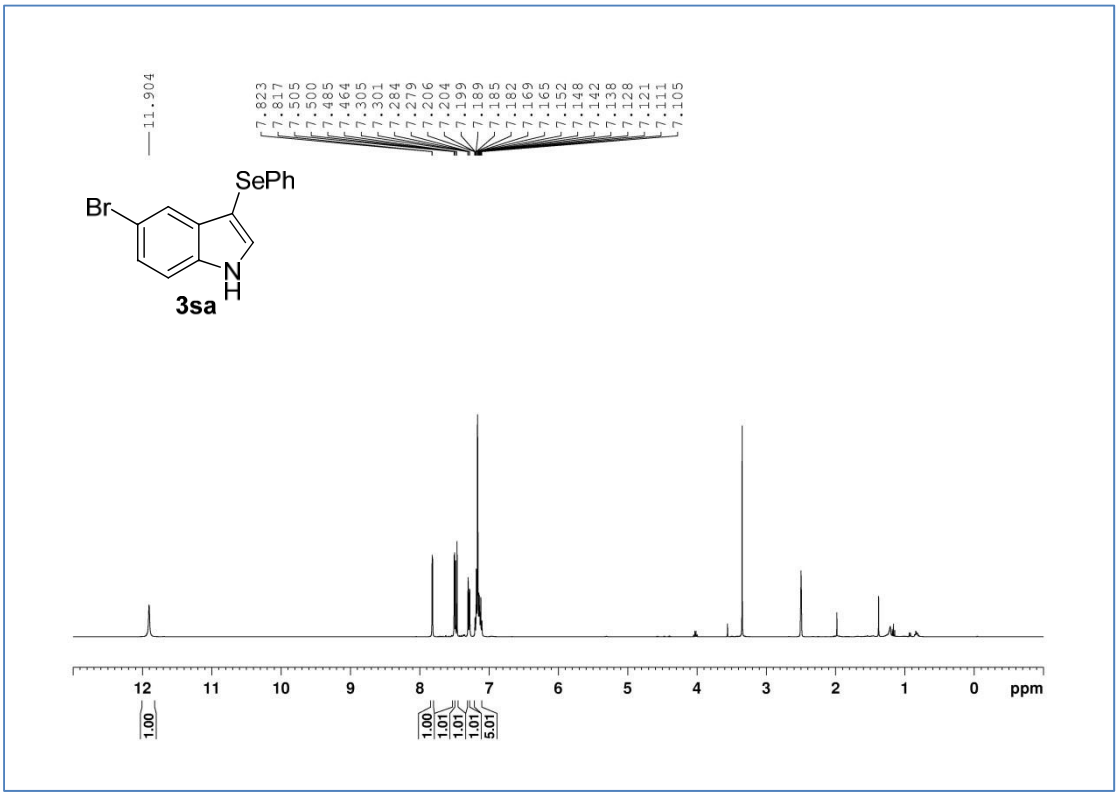
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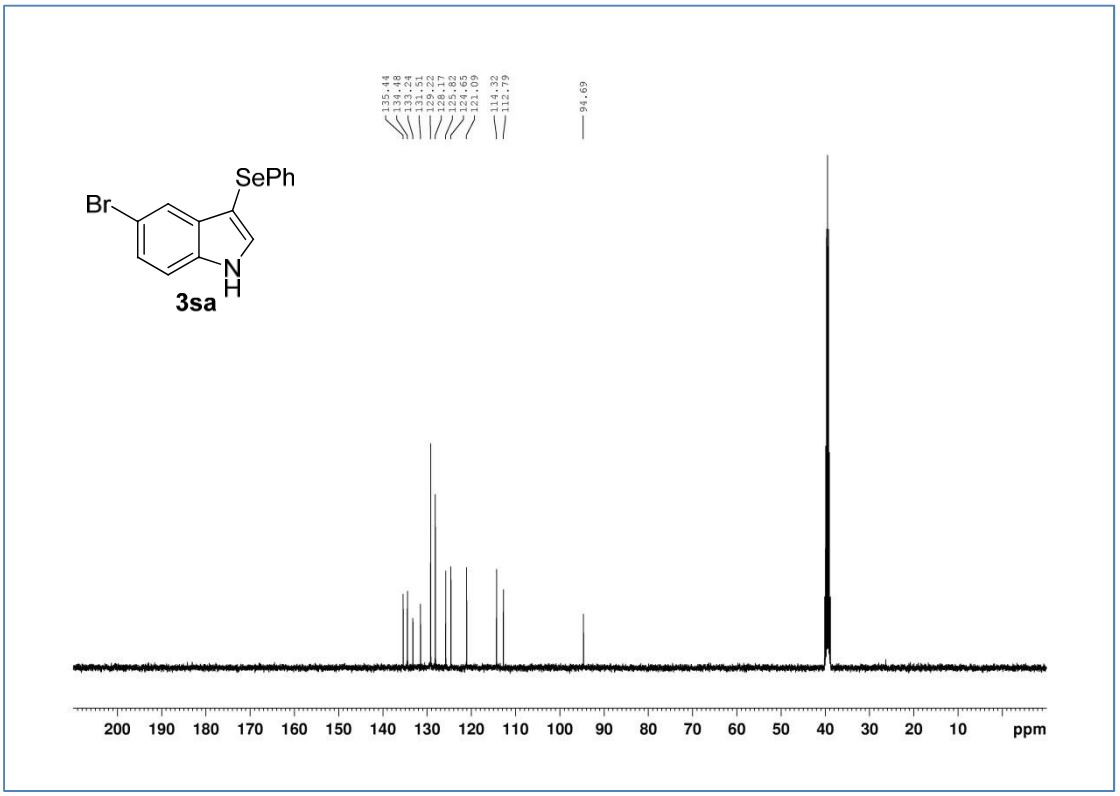
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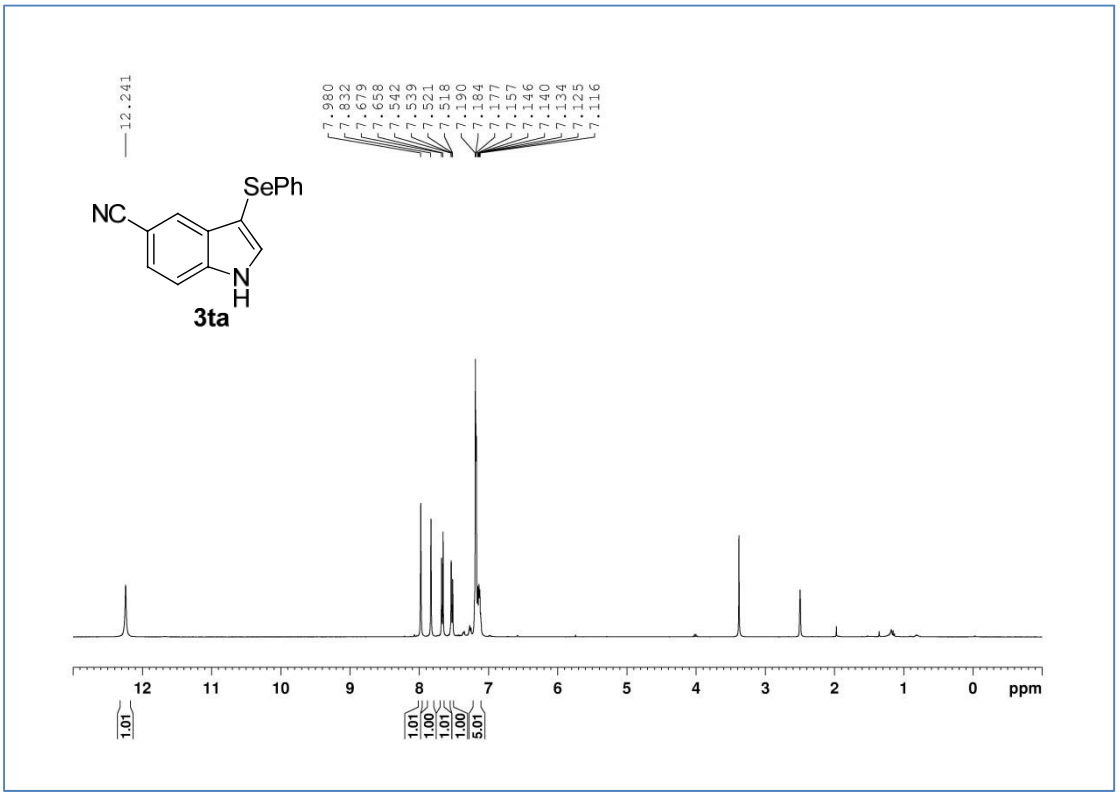
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7.116
SePh
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H
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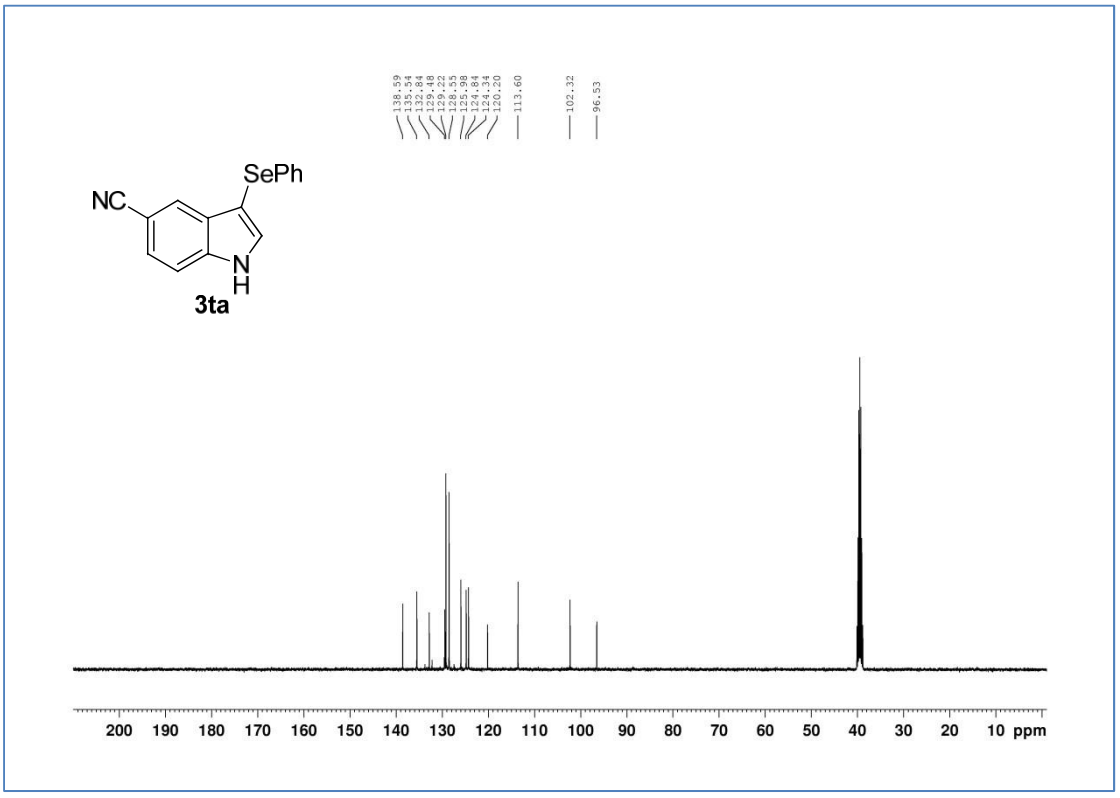
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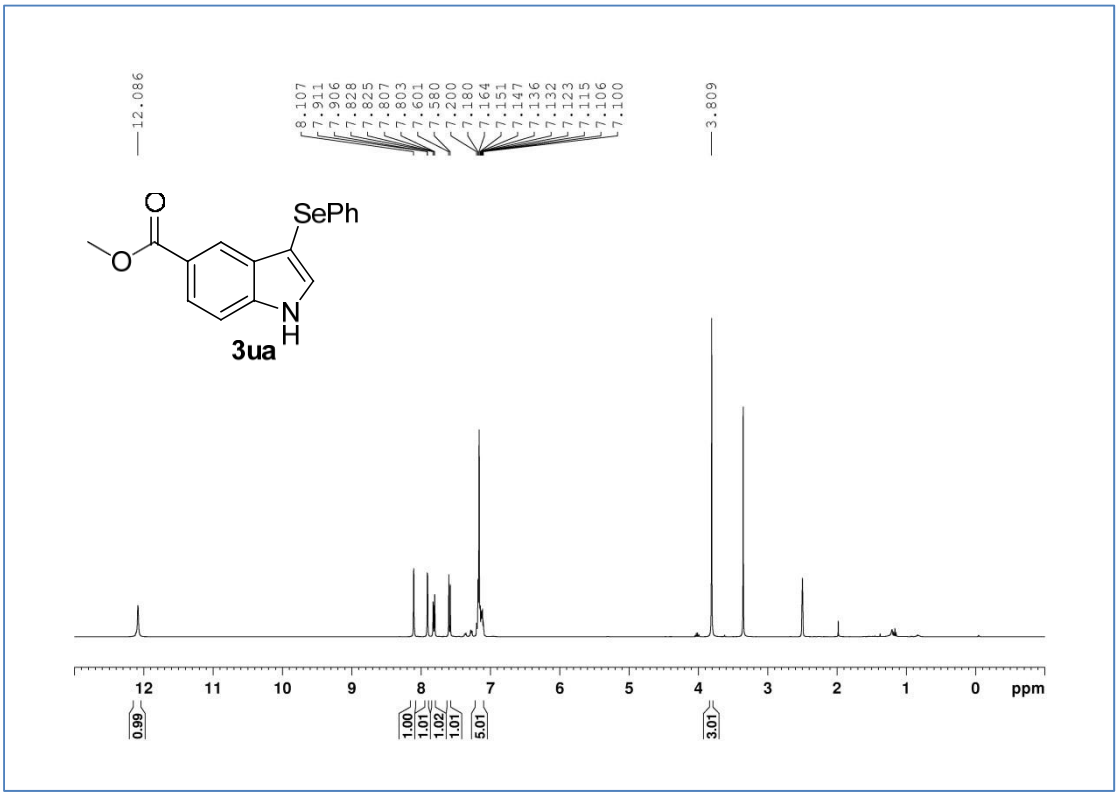
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7.115
7.106
7.100
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O
N
H
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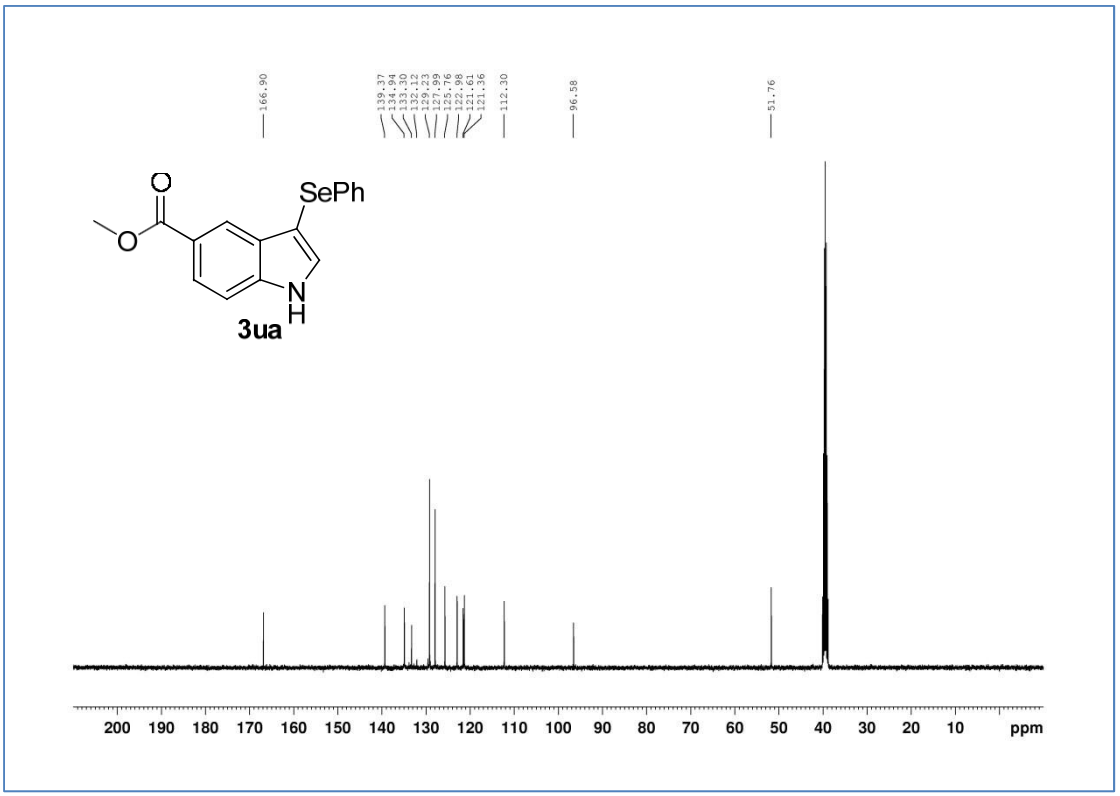
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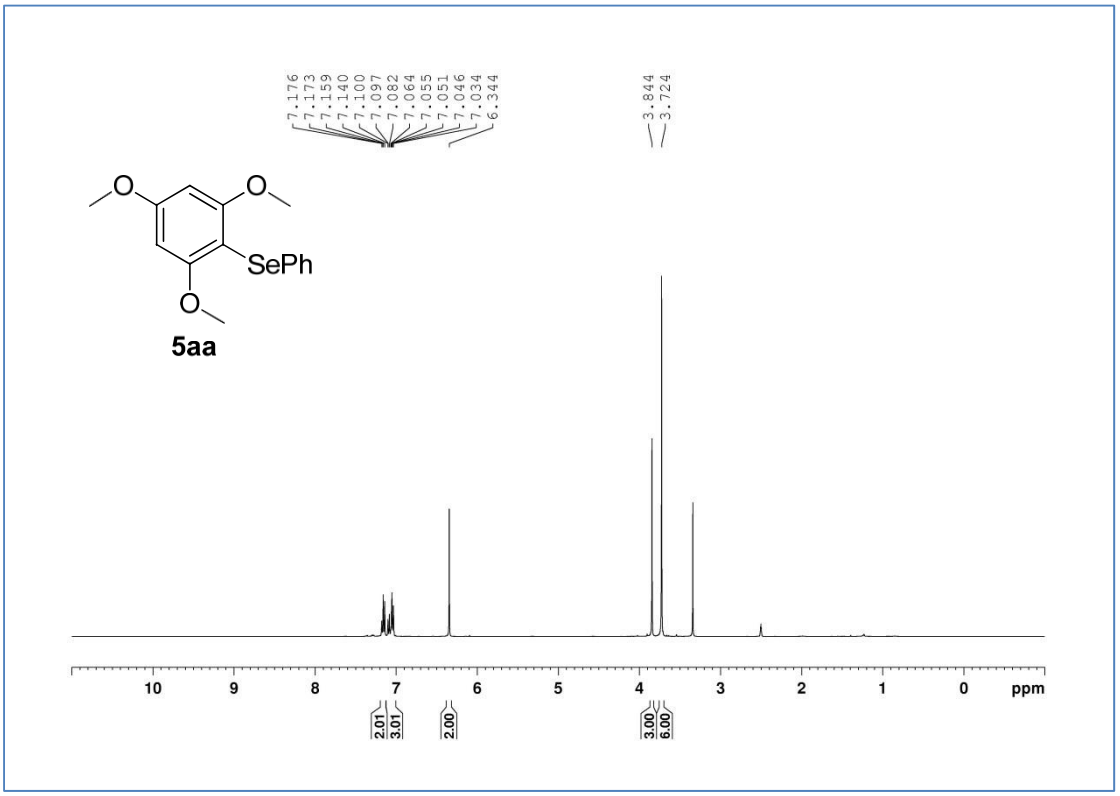
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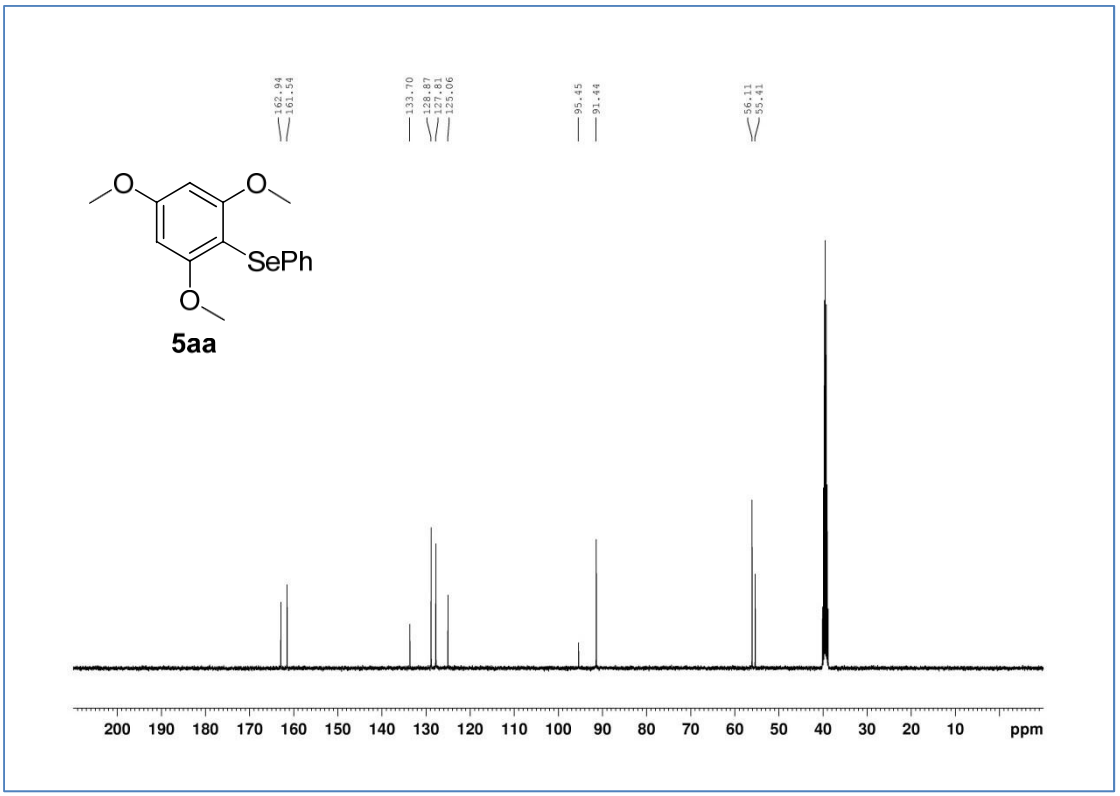
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5aa
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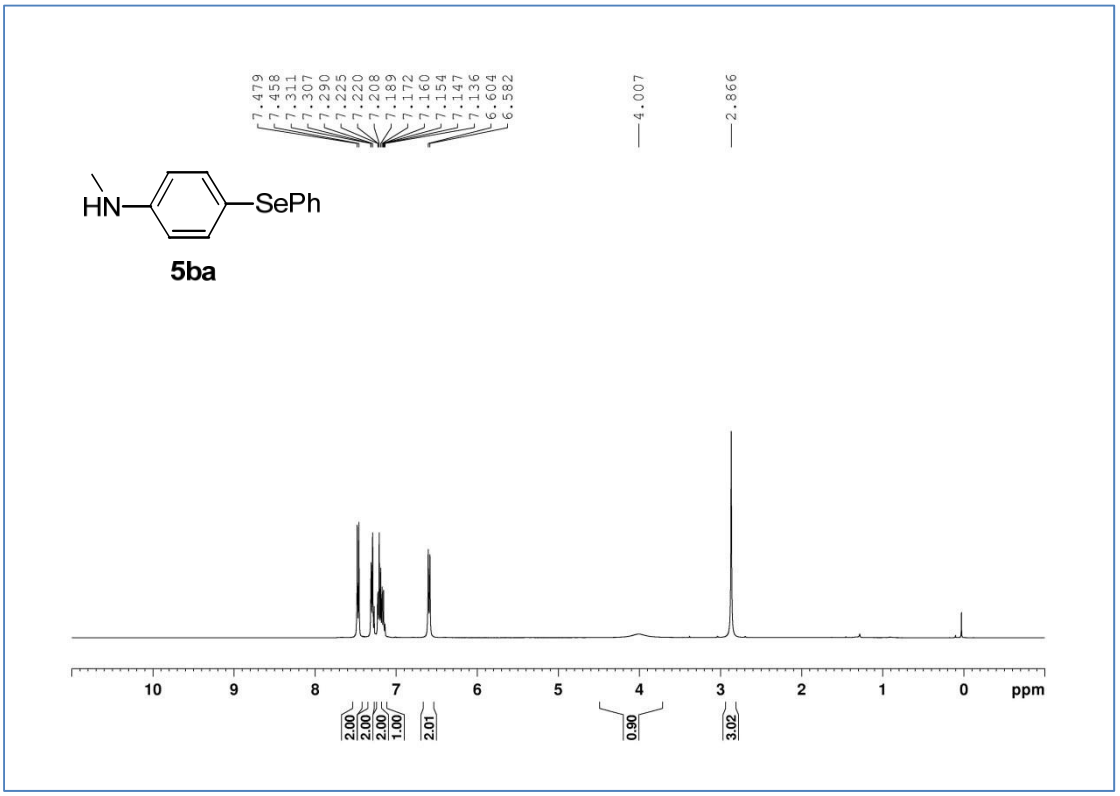
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HN
SePh
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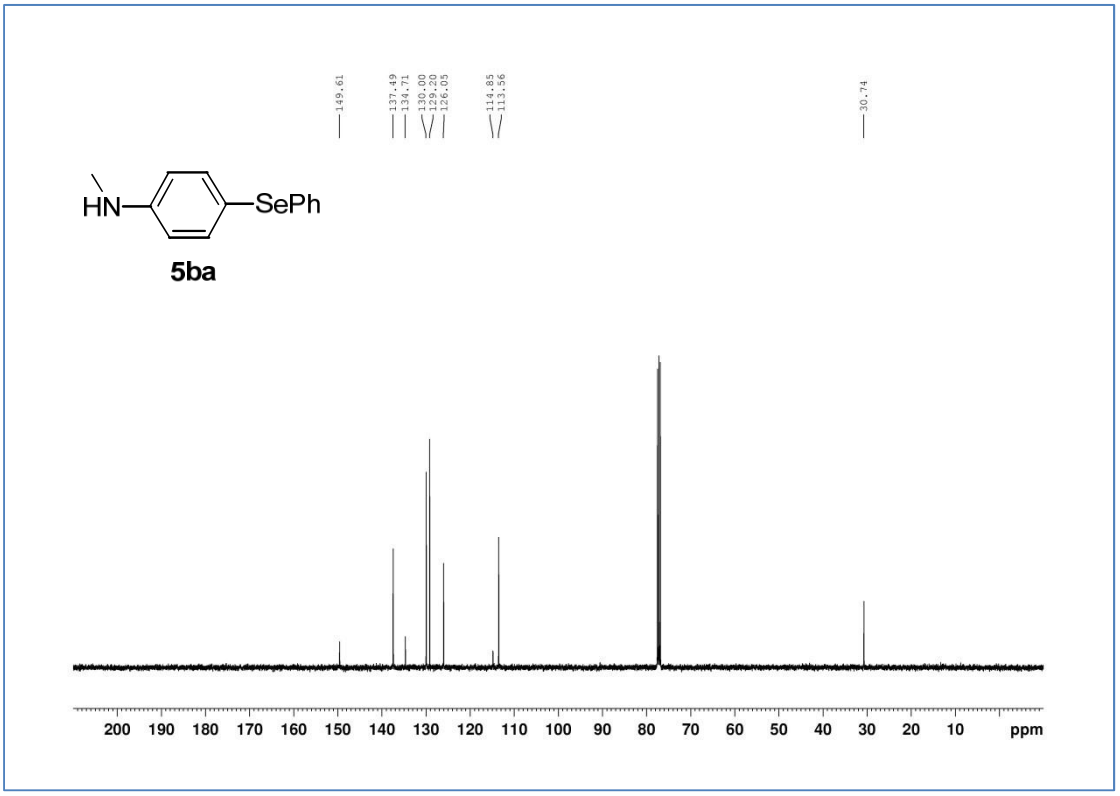
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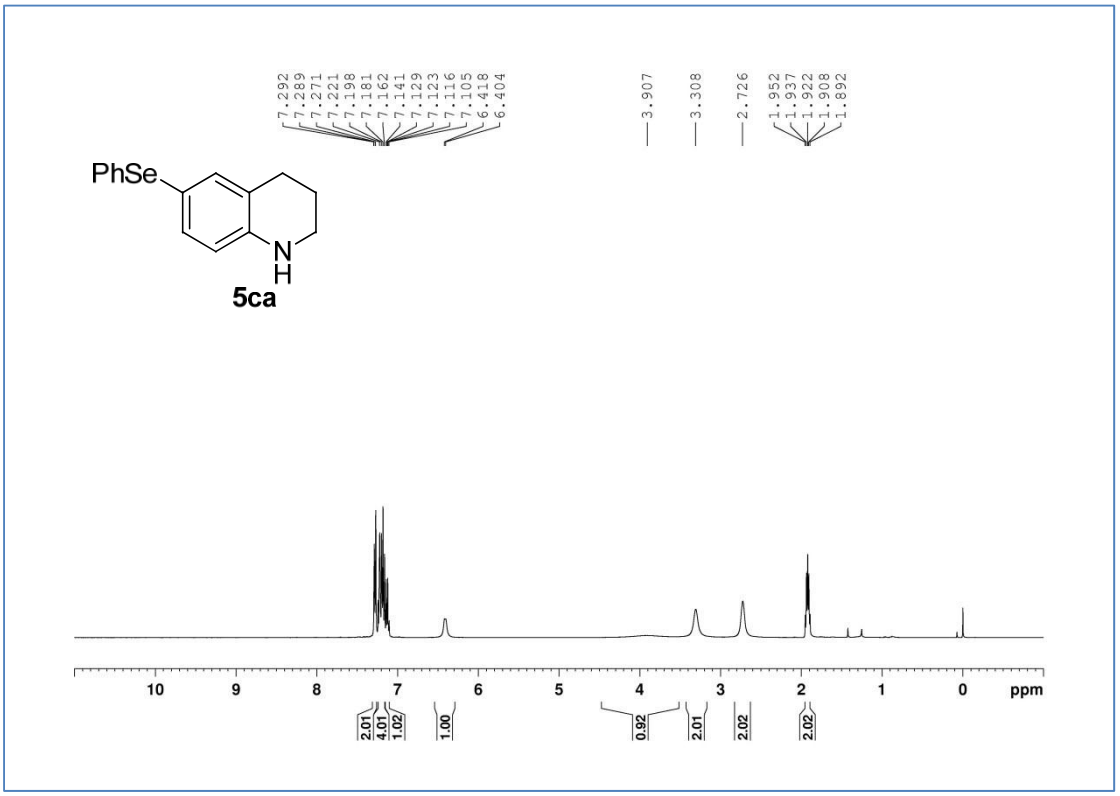
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6.404
3.907
3.308
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1.937
1.922
1.908
1.892
PhSe
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H
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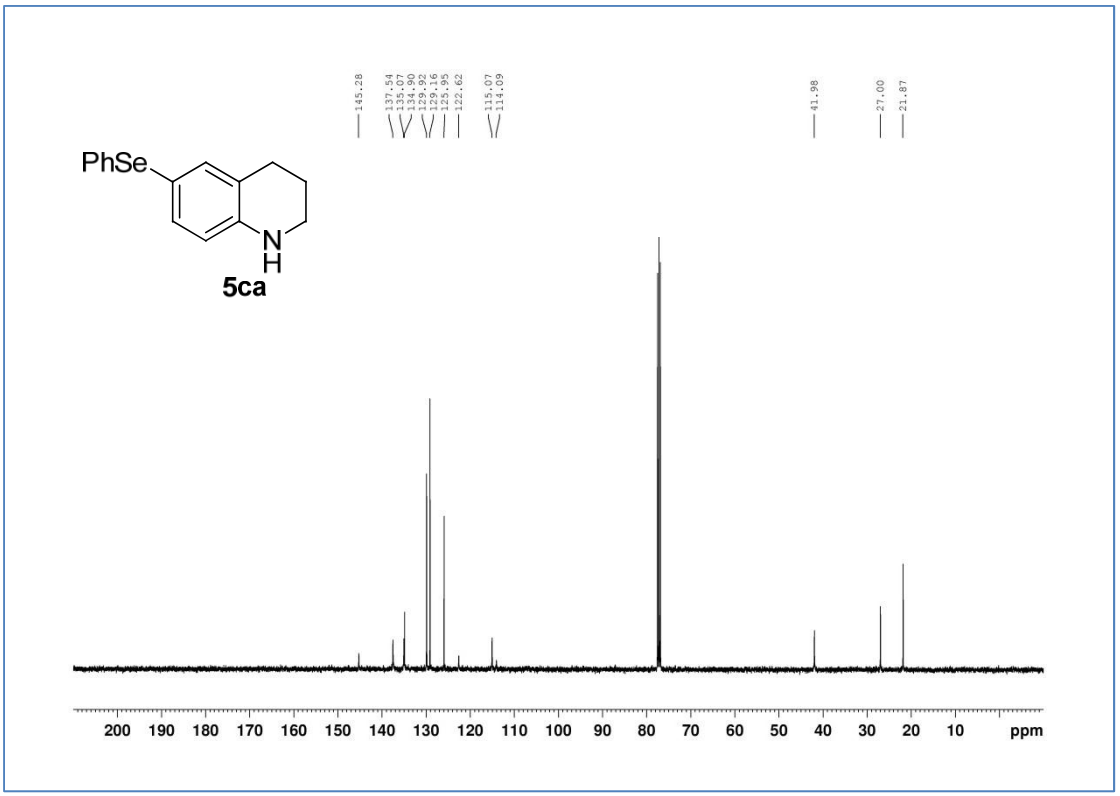
2.02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H
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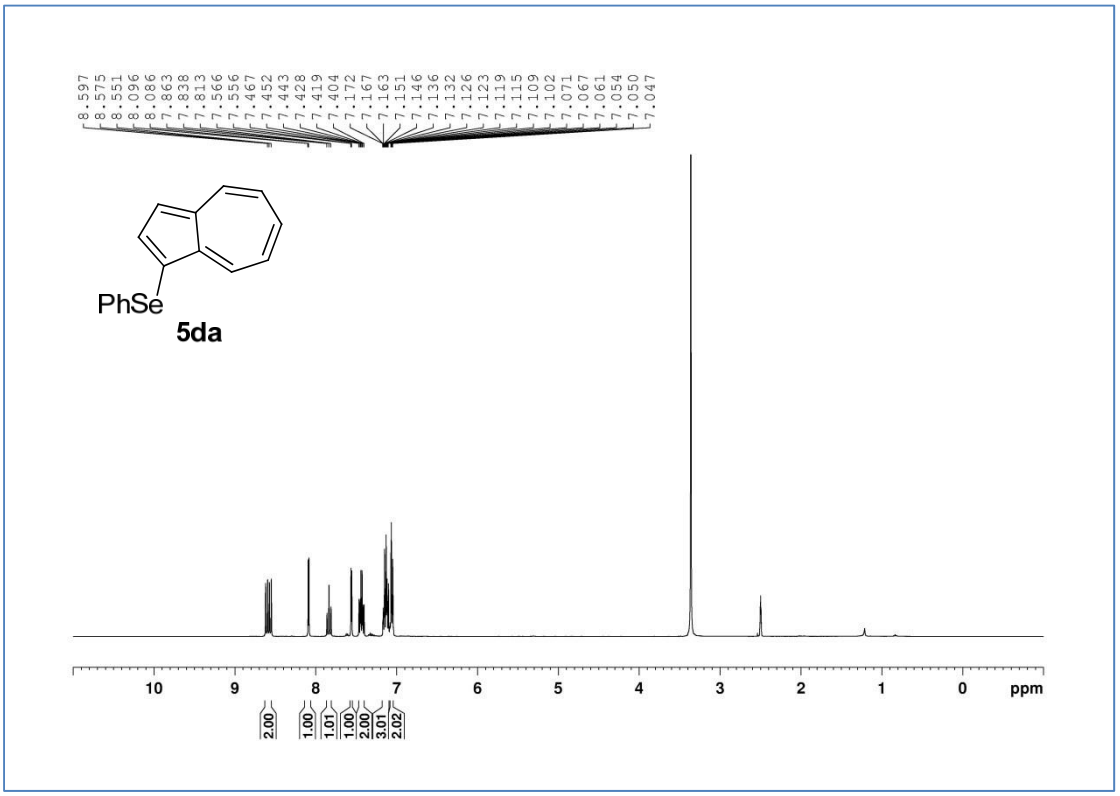
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7.443
7.428
7.419
7.404
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7.151
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7.136
7.132
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7.119
7.115
7.109
7.102
7.071
7.067
7.061
7.054
7.050
7.047
PhSe
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9
8
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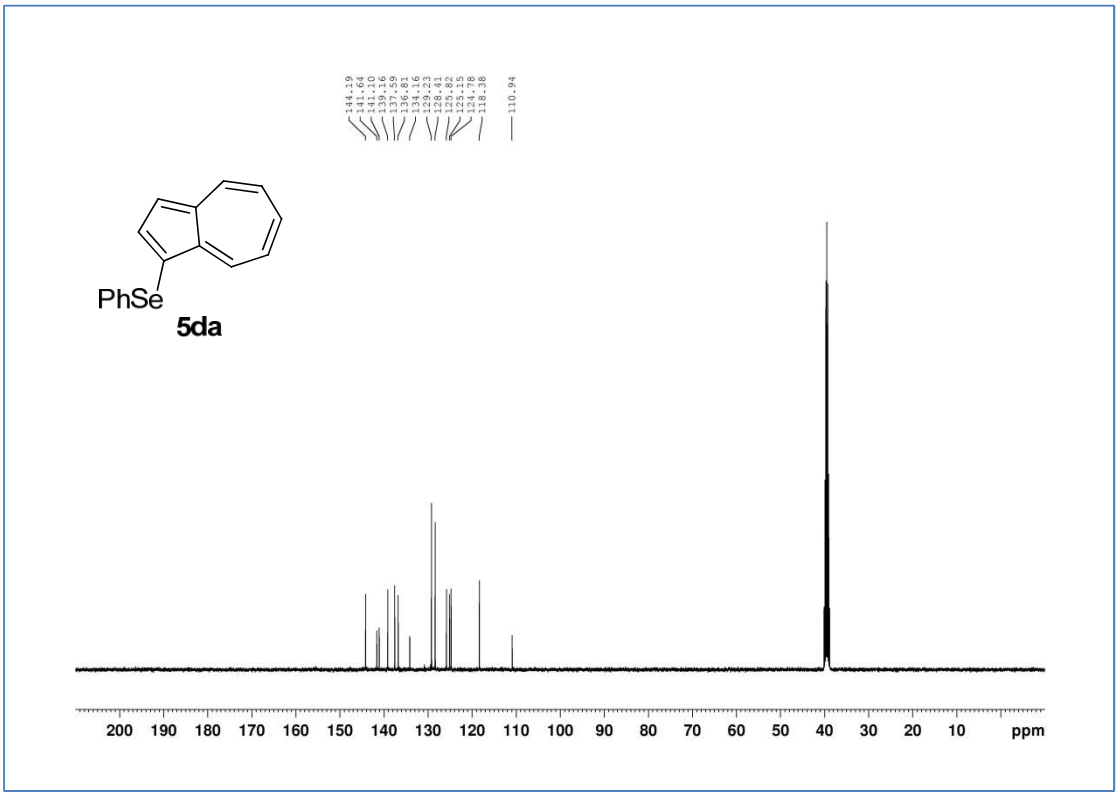
2.02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PhSe
5da
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150
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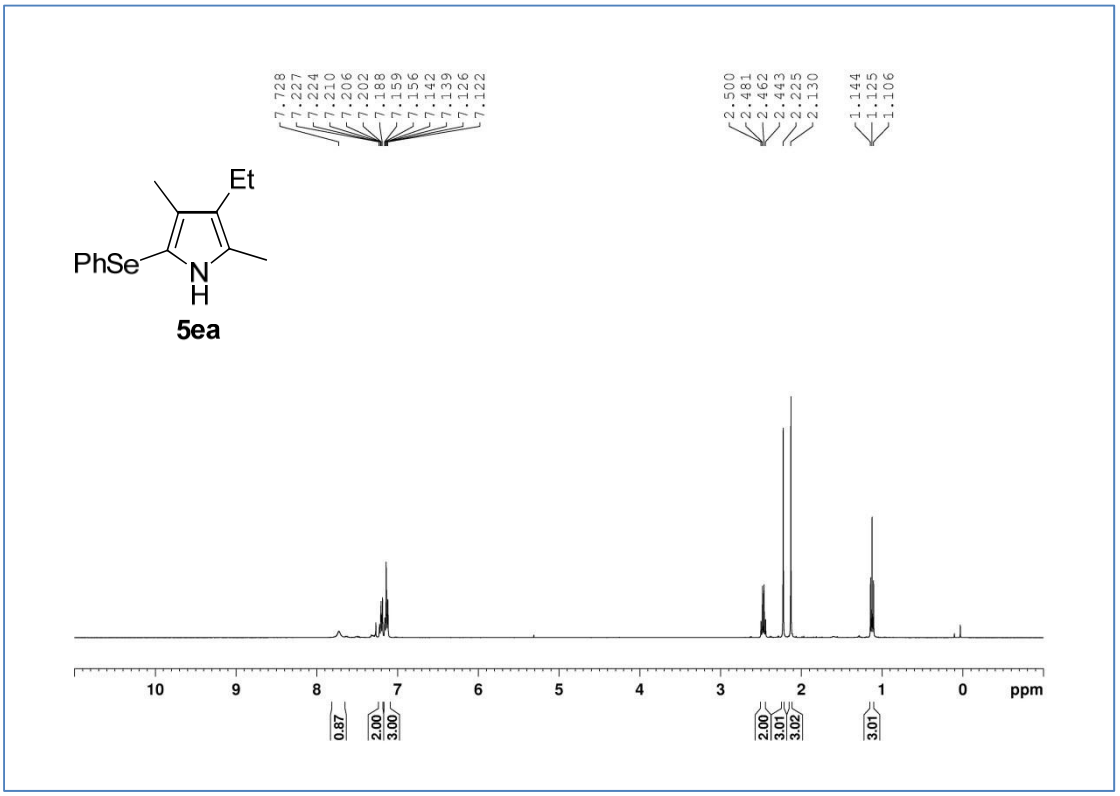
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2.130
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1.125
1.106
Et
PhSe
N
H
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8
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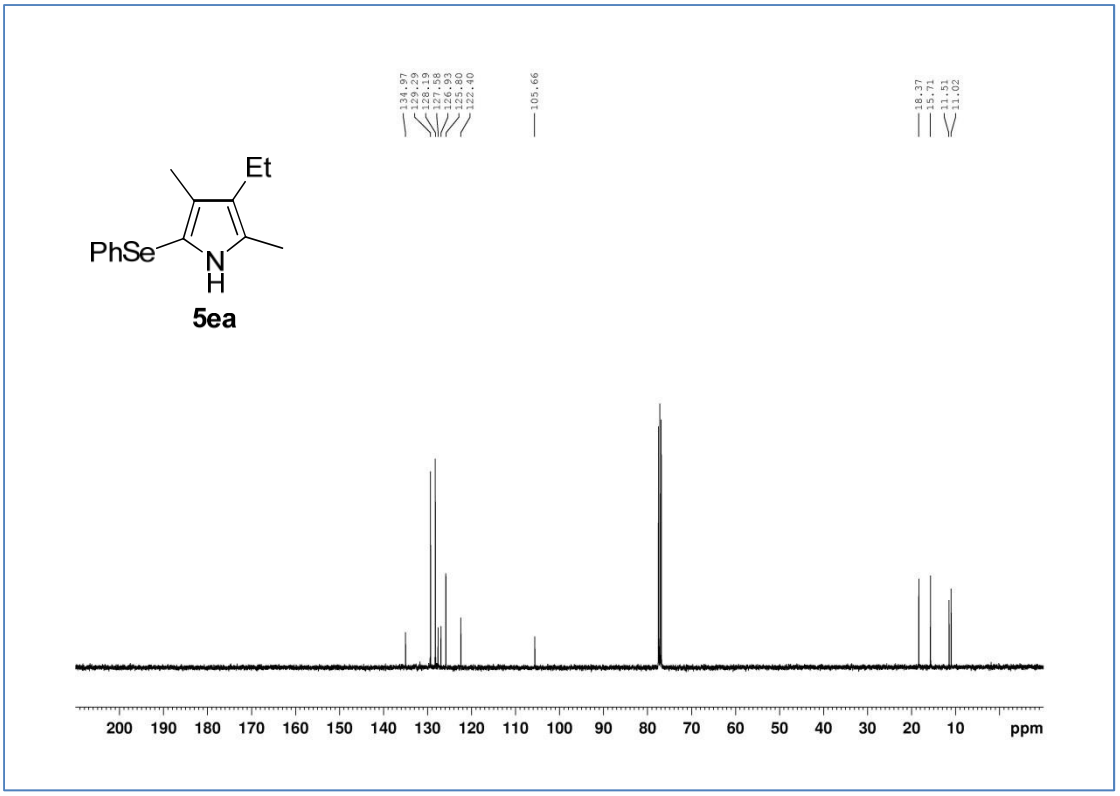
3.01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11.51
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PhSe
N
H
5ea
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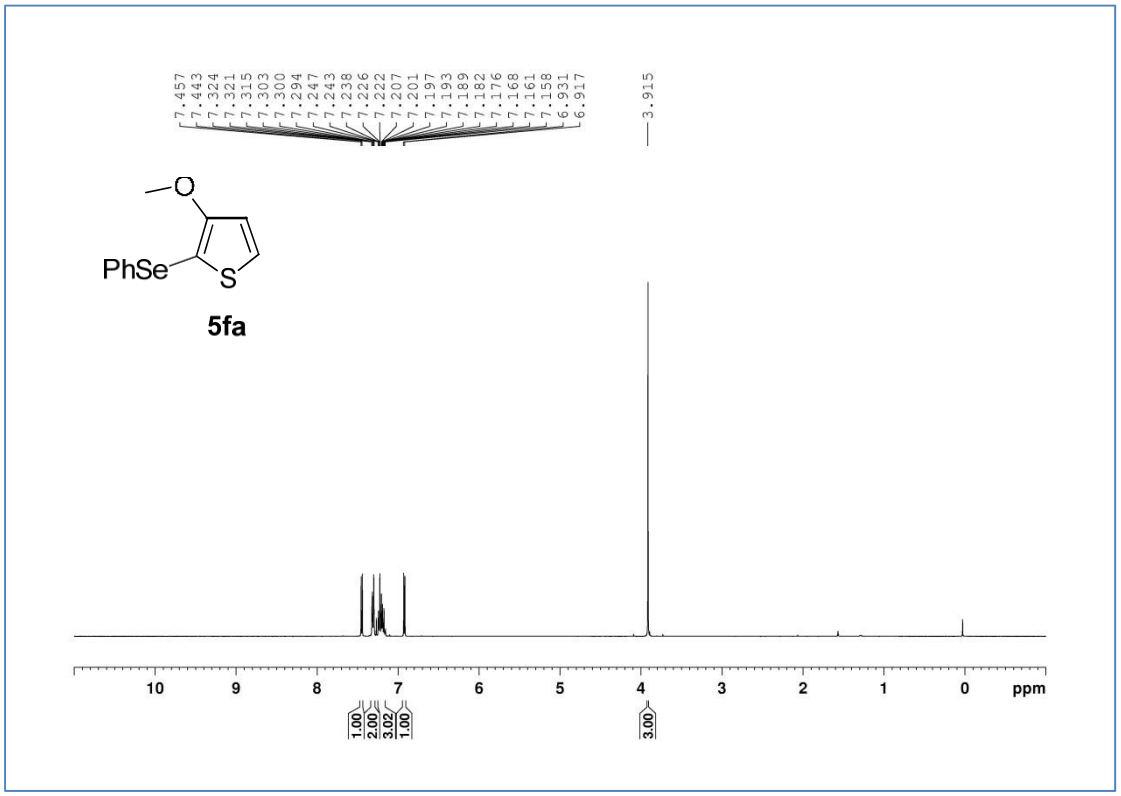
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7.207
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7.197
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7.189
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7.158
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6.917
3.915
O
PhSe
S
5fa
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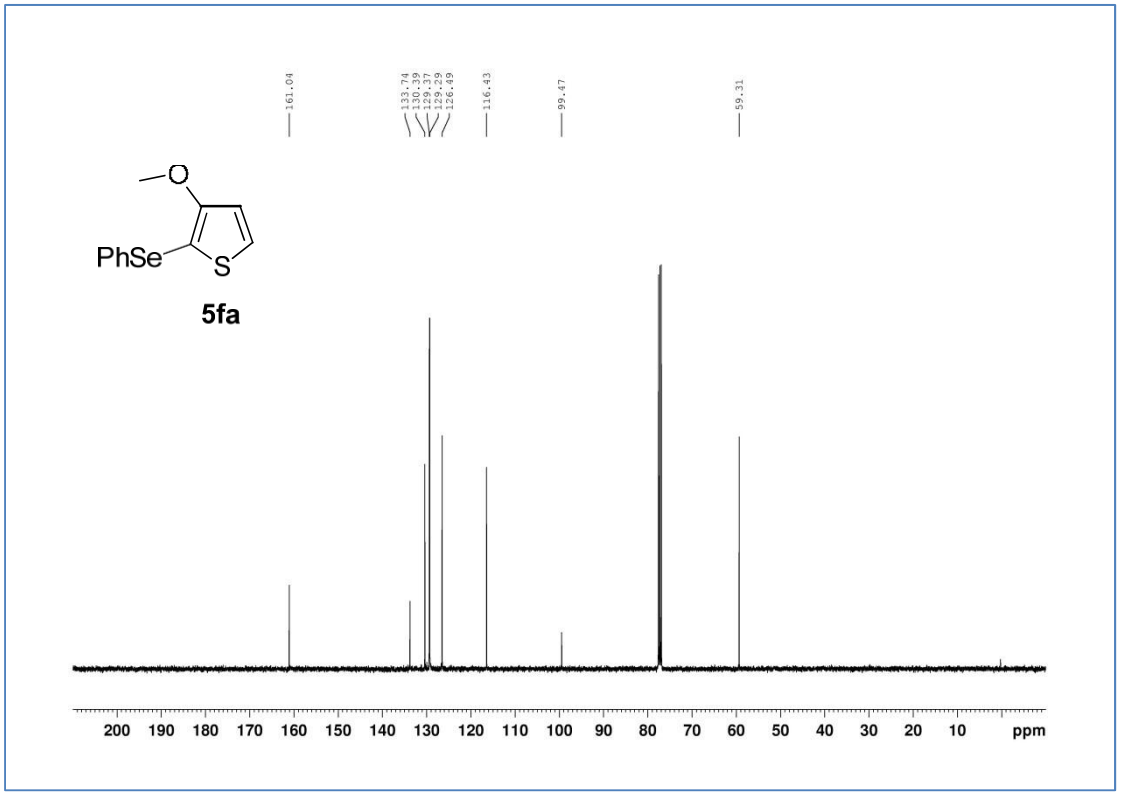
1.00
3.00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PhSe
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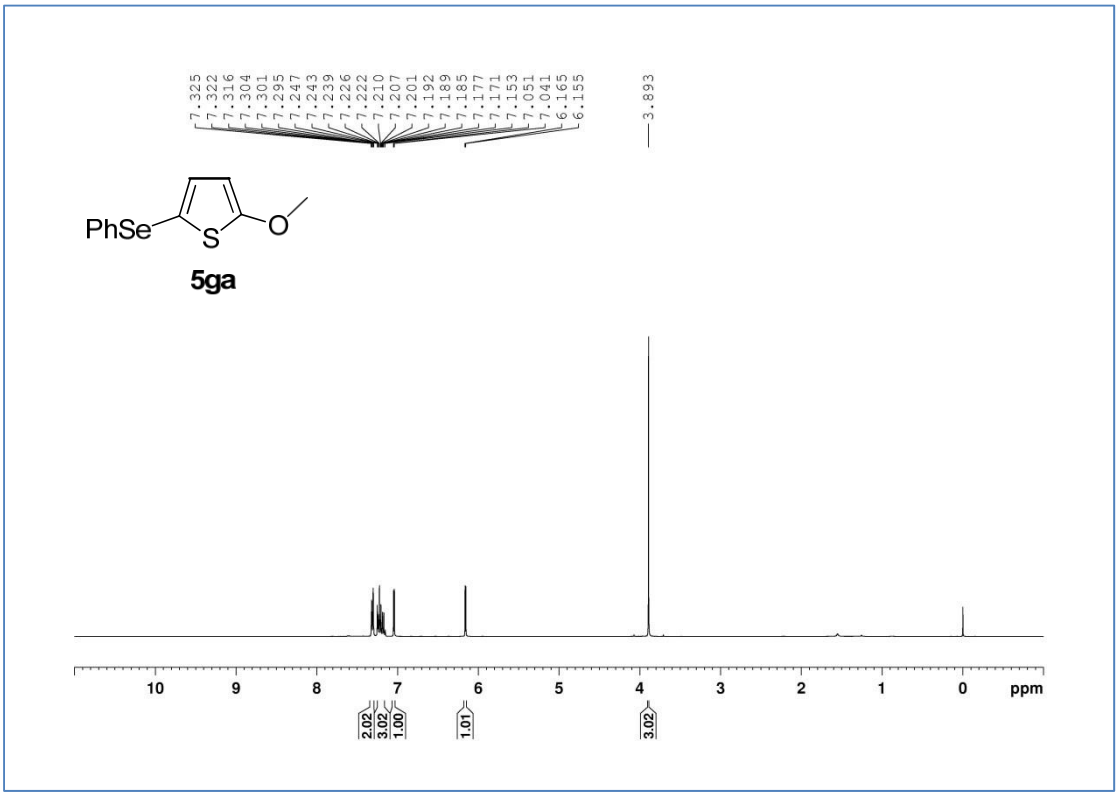
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7.189
7.185
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7.171
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7.051
7.041
6.165
6.155
3.893
PhSe
S
O
5ga
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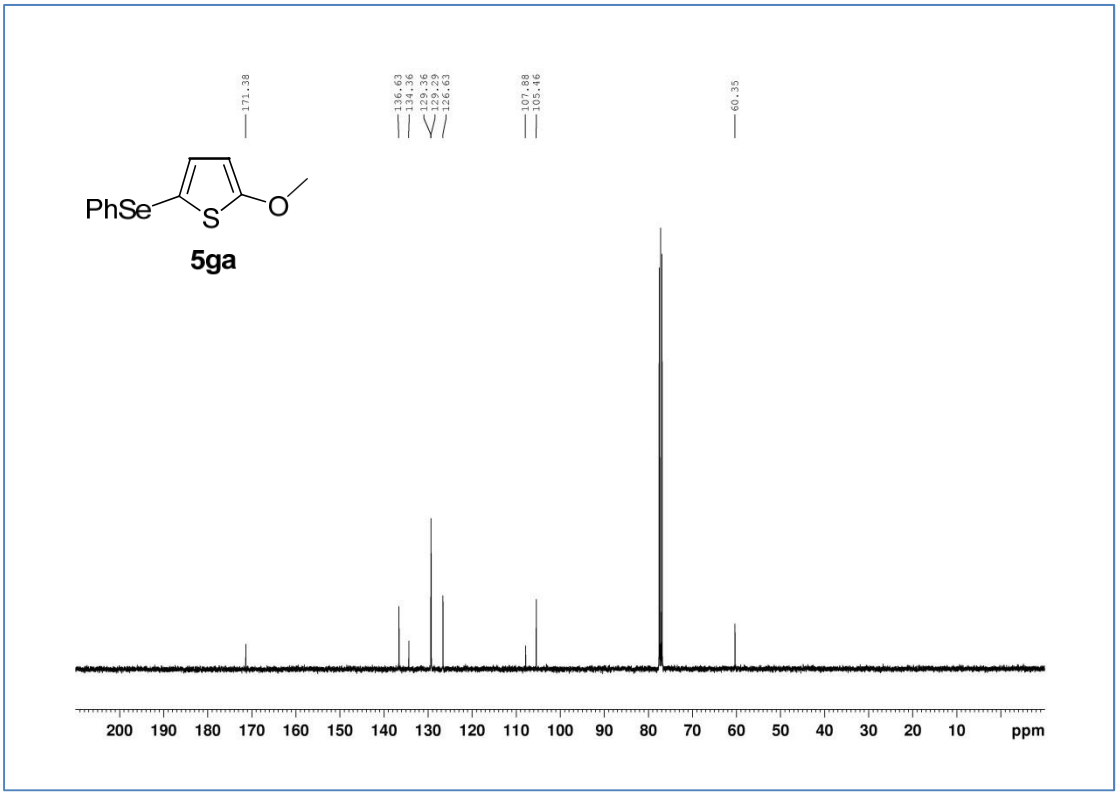
3.02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PhSe
S
O
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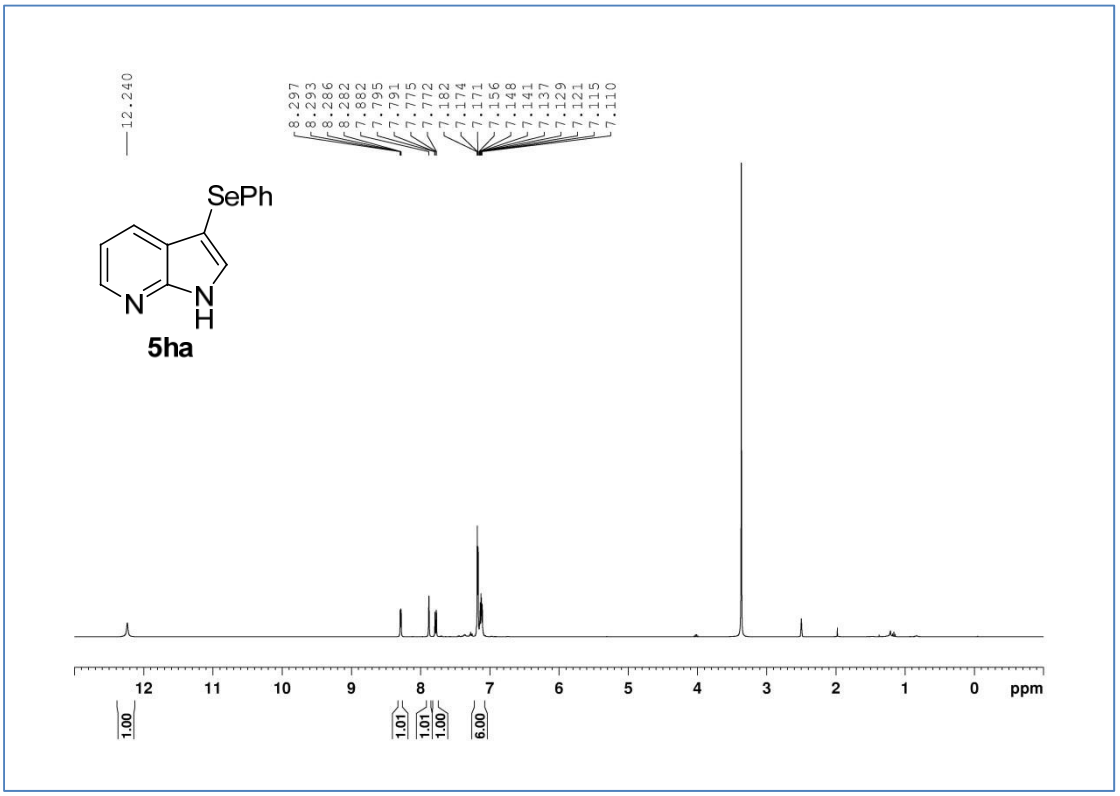
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7.171
7.156
7.148
7.141
7.137
7.129
7.121
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7.110
SePh
N
N
H
5ha
12
11
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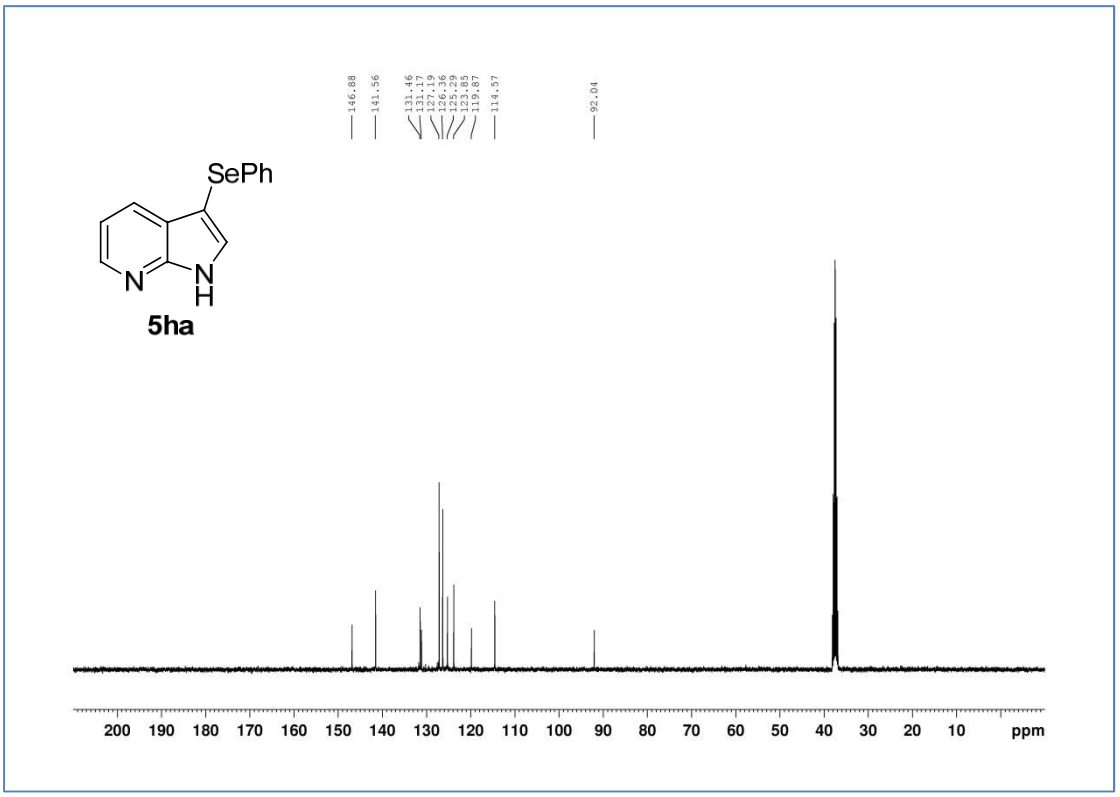
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N
H
5ha
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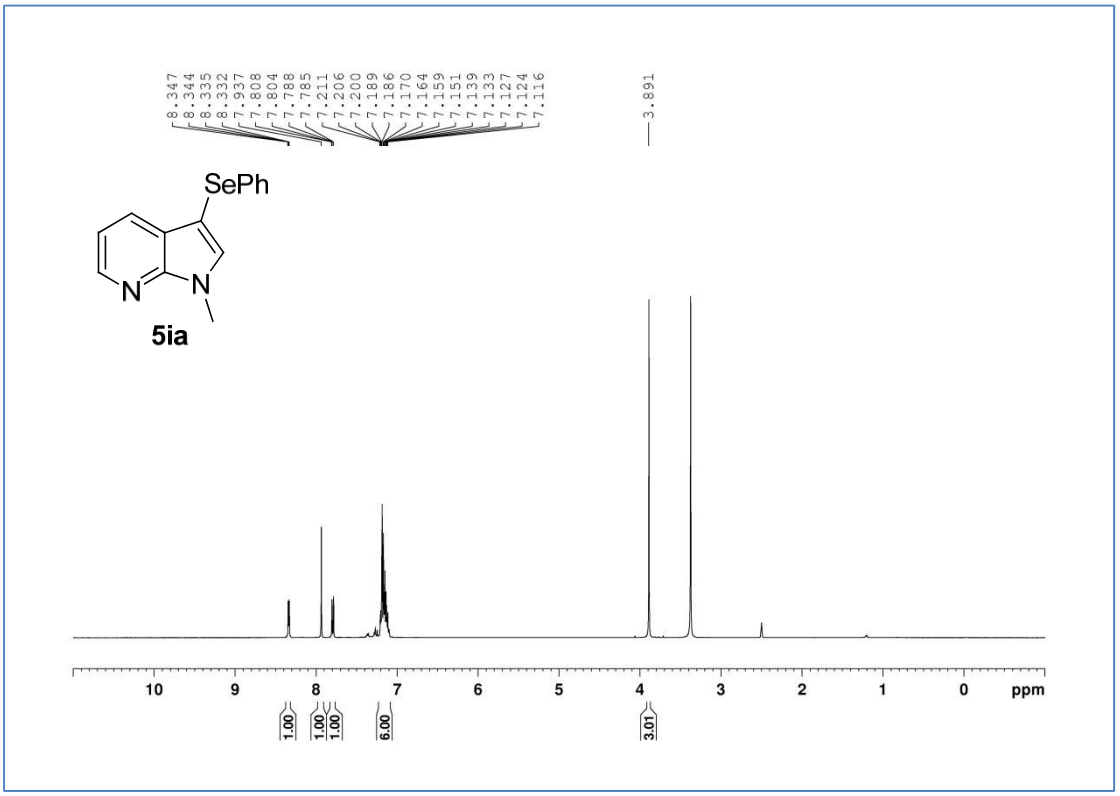
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7.116
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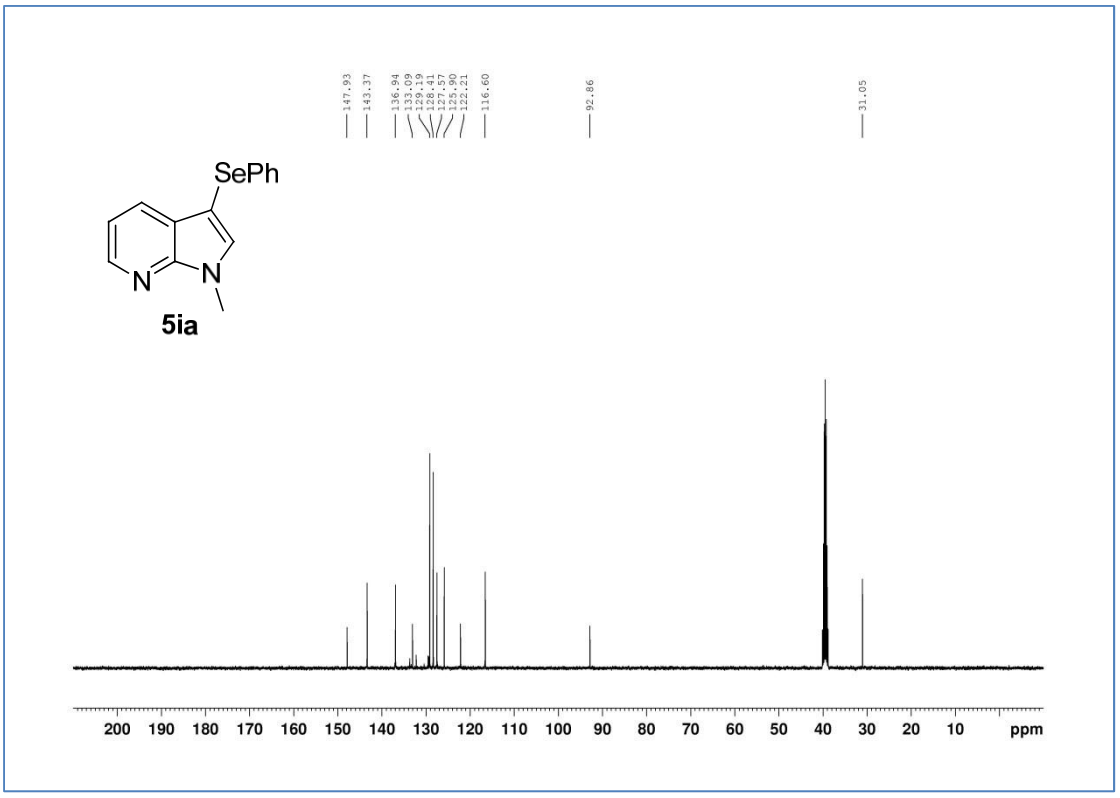
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N
5ia
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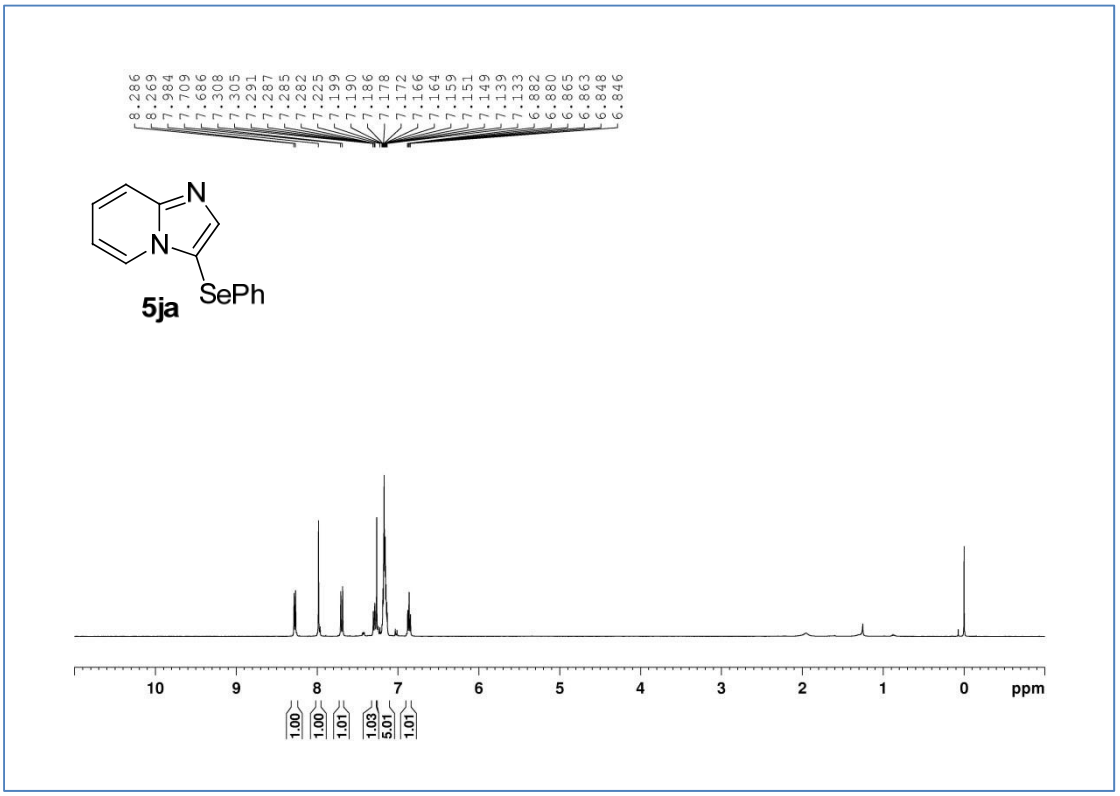
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7.186
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7.159
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7.139
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6.848
6.846
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N
SePh
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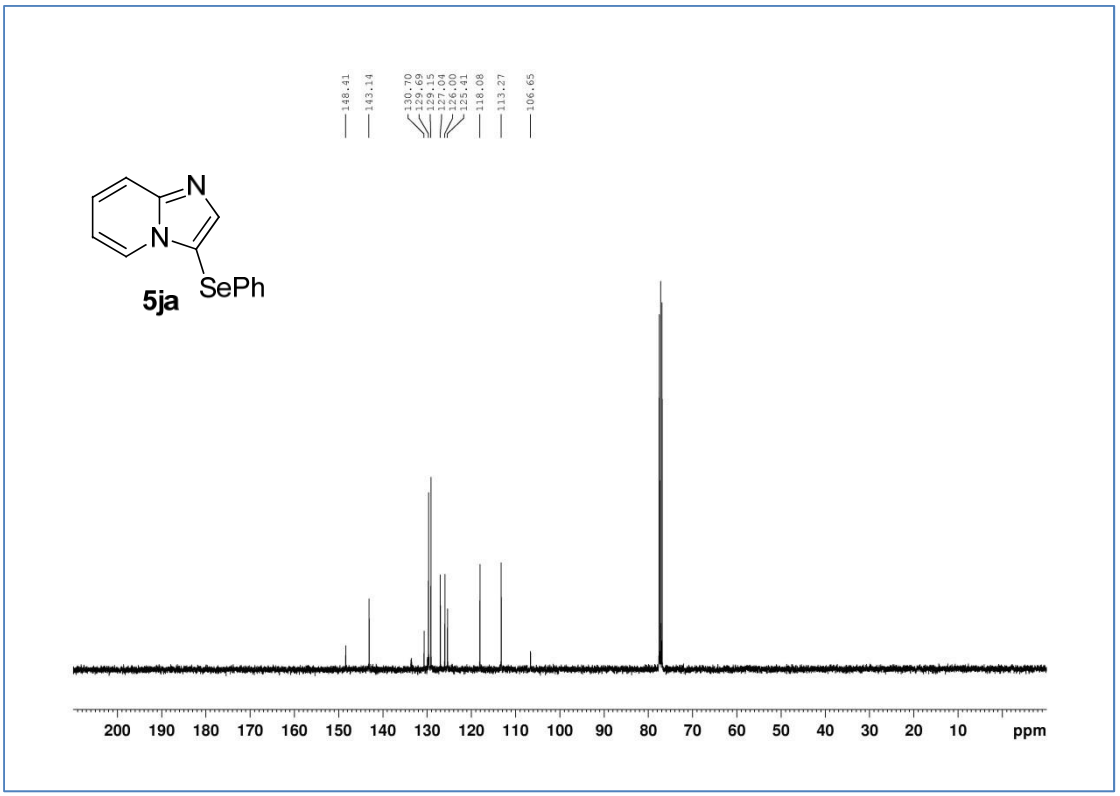
1.01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SePh
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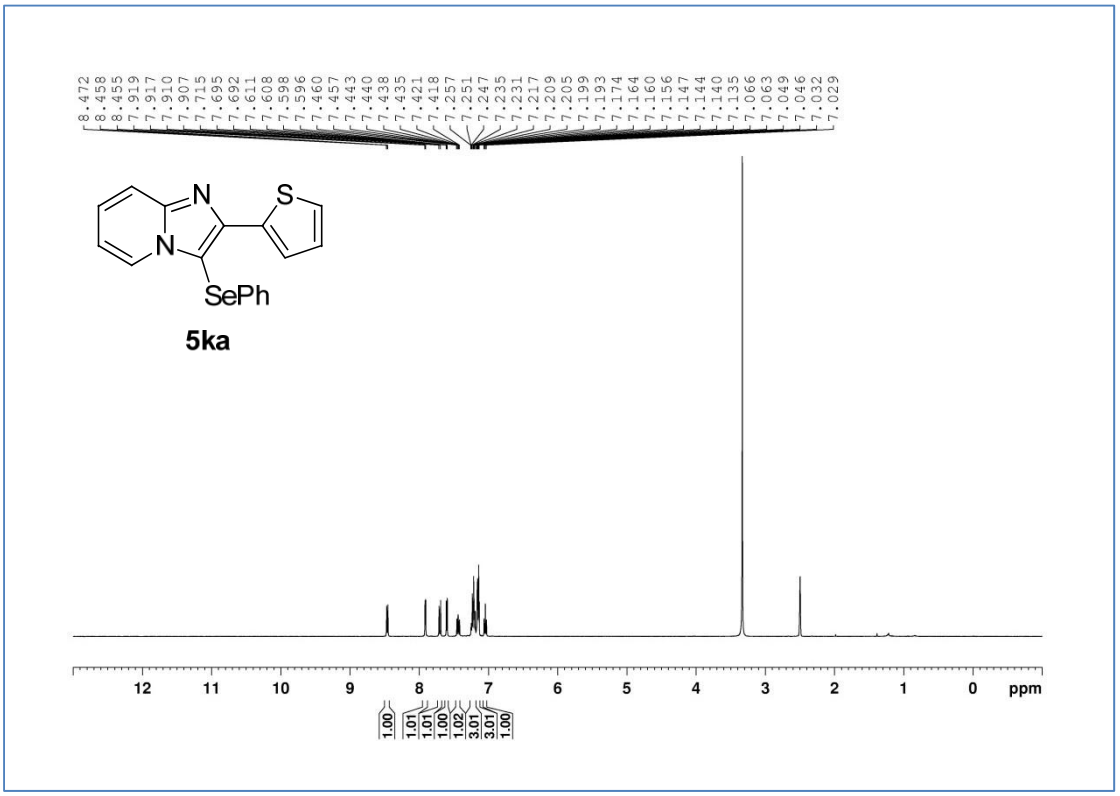
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7.247
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7.160
7.156
7.147
7.144
7.140
7.135
7.066
7.063
7.049
7.046
7.032
7.029
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S
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SePh
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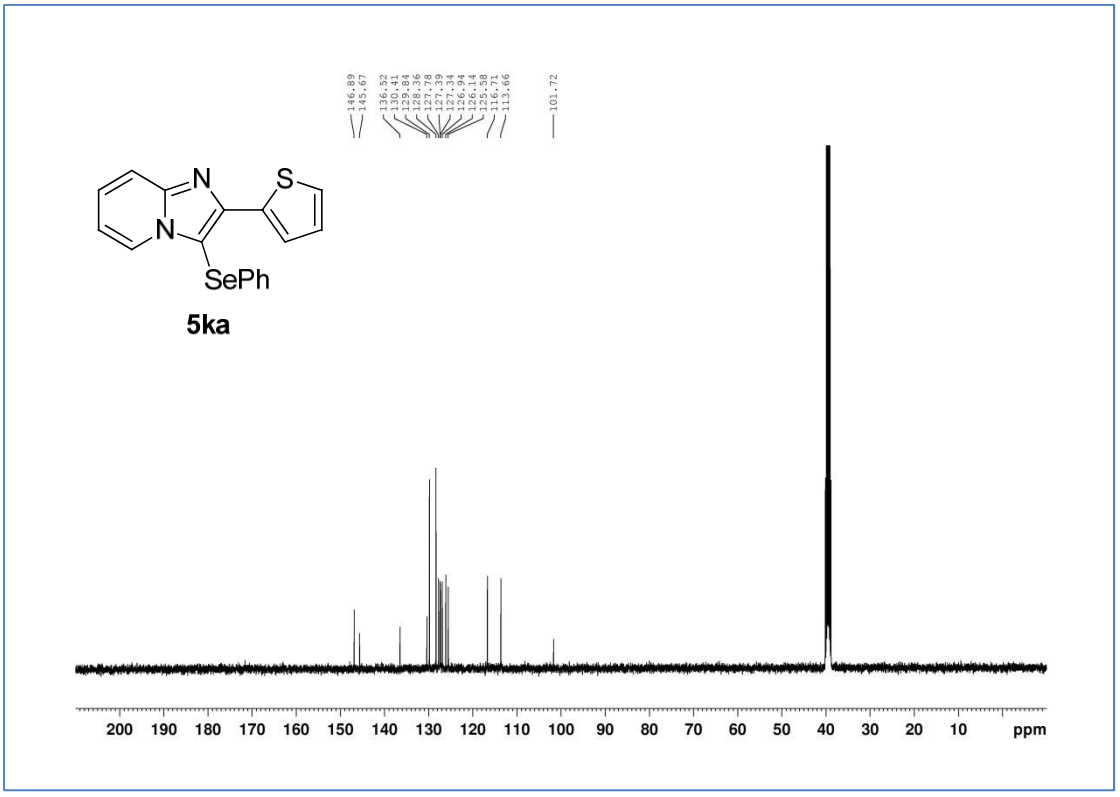
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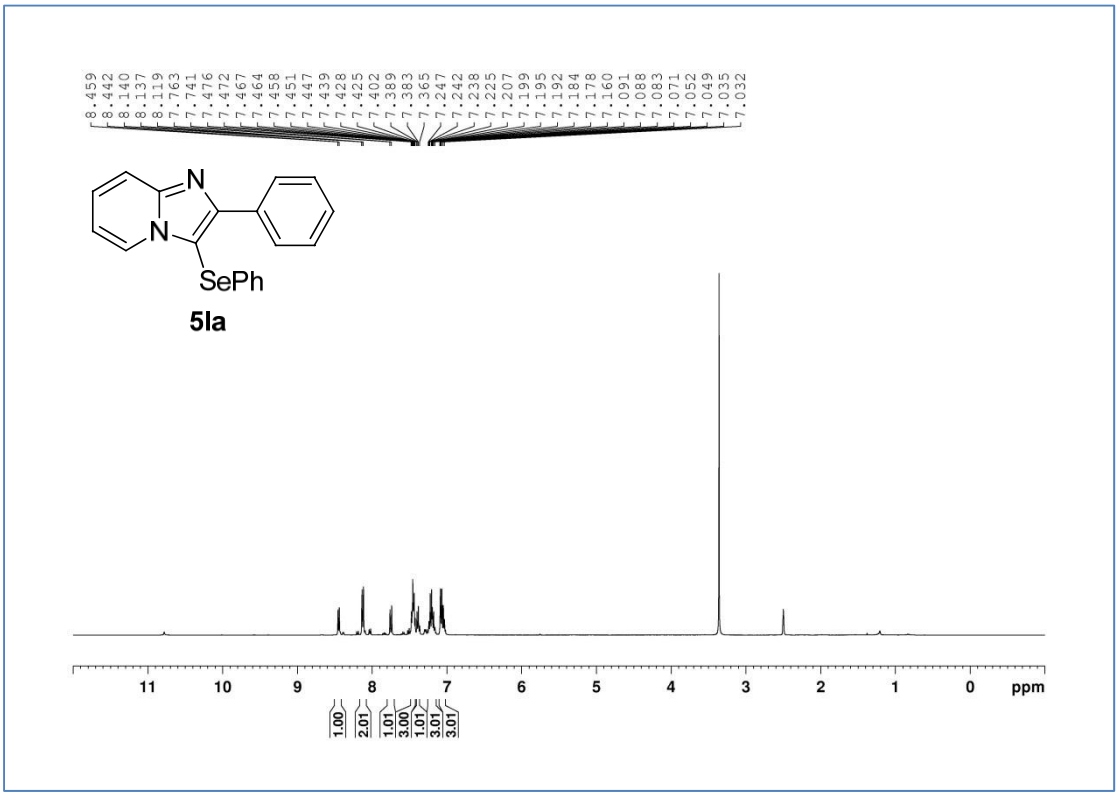
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7.184
7.178
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7.088
7.083
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7.052
7.049
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SePh
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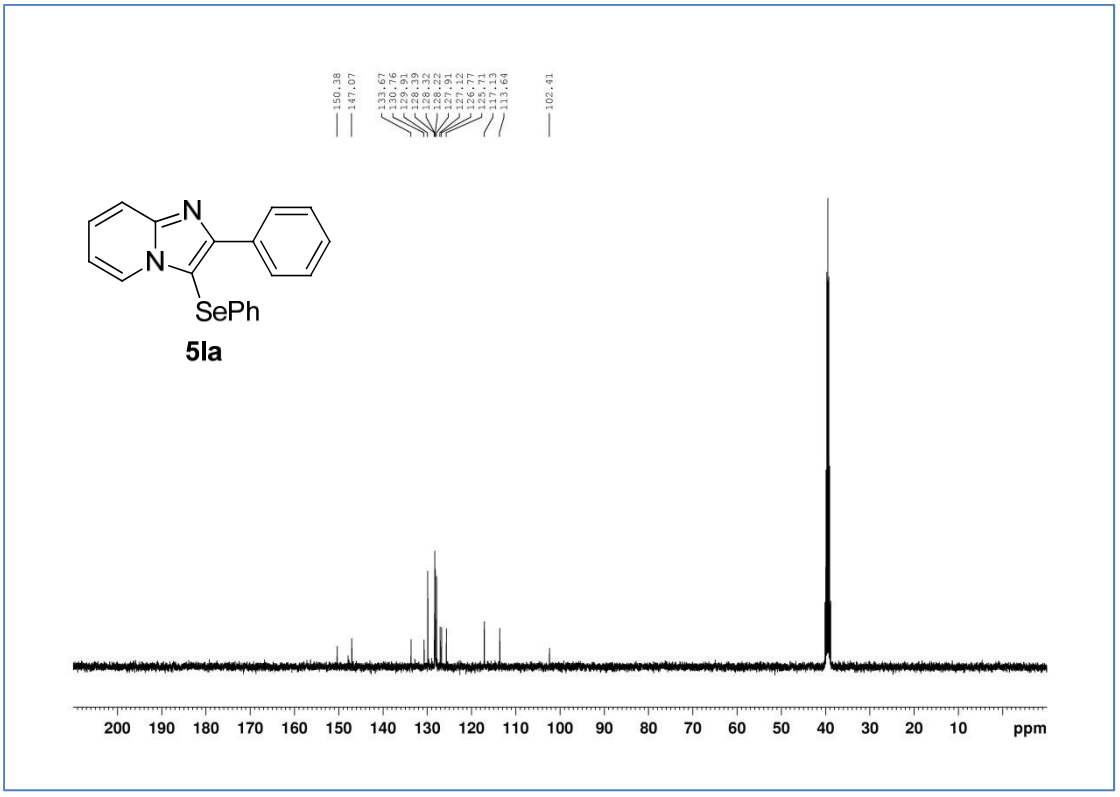
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113.64
102.41
N
N
SePh
5la
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm