Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supplementary Information

Iodine-Mediated Regioselective 5-*endo* dig Electrophilic Cyclization Reaction of Selenoenynes: Synthesis of Selenophene Derivatives

Renan P. Pistoia,[1] Juliano A. Roehrs,[1] Davi F. Back[2] and Gilson Zeni[1,*]

[1]Laboratório de Síntese, Reatividade, Avaliação Farmacológica e Toxicológica de Organocalcogênios, CCNE, UFSM, Santa Maria, Rio Grande do Sul, Brazil 97105-900.

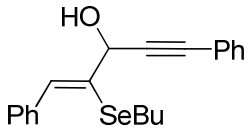
[2]Laboratório de Materiais Inorgânicos, CCNE, UFSM, Santa Maria, Rio Grande do Sul, Brazil 97105-900.

Table of Contents

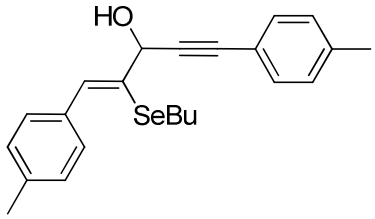
Materials and Methods

Proton nuclear magnetic resonance spectra (^{1}H NMR) were obtained on a NMR spectrometer at 400 MHz. Spectra were recorded in $CD.Cl_3$ solutions. Chemical shifts are reported in ppm, referenced to the solvent peak of $CDCl_3$ or tetramethylsilane (TMS) as the external reference. Data are reported as follows: chemical shift (δ), multiplicity, coupling constant *(J)* in Hertz and integrated intensity. Carbon-13 nuclear magnetic resonance spectra (^{13}C NMR) were obtained on a 400 NMR spectrometer at 100 MHz. Spectra were recorded in $CDCl_3$ solutions. Chemical shifts are reported in ppm, referenced to the solvent peak of $CDCl_3$. Abbreviations to denote the multiplicity of a particular signal are s (singlet), d (doublet), t (triplet), quart (quartet), quint (quintet), sex (sextet), dd (double doublet) and m (multiplet). High resolution mass spectra were recorded on a mass spectrometer using electrospray ionization (ESI). Column chromatography was performed using Silica Gel (230-400 mesh) following the methods described by Still.[1] Thin layer chromatography (TLC) was performed using Gel GF254, 0.25 mm thickness. For visualization, TLC plates were either placed under ultraviolet light, or stained with iodine vapor, or acidic vanillin. Most reactions were monitored by TLC for disappearance of starting material. The following solvents were dried and purified by distillation from the reagents indicated: tetrahydrofuran from sodium with a benzophenone ketyl indicator. All other solvents were ACS or HPLC grade unless otherwise noted. Air- and moisture-sensitive reactions were conducted in flame-dried or oven dried glassware equipped with tightly fitted rubber septa and under a positive atmosphere of dry nitrogen or argon. Reagents and solvents were handled using standard syringe techniques.

General Procedure for the Preparation of the (Z)-selenoenynes 1. $NaBH_4$ (0.19g; 5 mmol) was added to a solution of 1,5-diphenylpenta-1,4-diyn-3-ol (0.370g; 1.0 mmol) and appropriate dibutyl diselenide (2.5 mmol) in ethanol (15 mL) under a argon atmosphere, at room temperature. The reaction mixture was stirred at room temperature for 12 hours. The mixture was diluted with ethyl acetate (10 mL) and washed with a saturated solution of NH_4Cl (3 x 10 mL). The organic phase was separated, dried over $MgSO_4$, and concentrated under vacuum. The residue was purified by flash chromatography and eluted with hexane/ ethyl acetate.

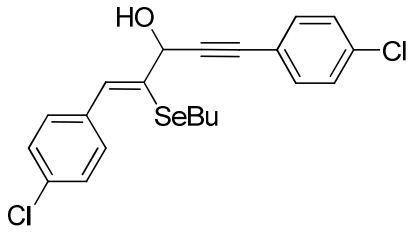


(Z)-2-(butylselanyl)-1,5-diphenylpent-1-en-4-yn-3-ol (1a). Isolated by column chromatography (hexane and ethyl acetate 9:1 as eluent) as a yellow oil. Yield: 0.274 g (74%); ^{1}H NMR (CDCl3, 400 MHz): δ 7.71-7.66 (m, 2H), 7.53-7.47 (m, 2H), 7.42-7.29 (m, 7H), 5.30 (dd, J = 7.7 Hz, 0.9 Hz, 1H), 2.86 (d, J = 7.7 Hz, 1H), 2.78-2.71 (m, 2H), 1.65-1.56 (m, 2H), 1.31 (qui, J =7.3 Hz, 2H), 0.83 (t, J = 7.3 Hz, 3H). ^{13}C NMR (CDCl3, 100 MHz): δ 136.45, 134.23, 133.00, 131.76, 129.30, 128.60, 128.29, 128.08, 127.8, 122.4, 88.1, 86.6, 68.7, 32.3, 27.0, 22.8, 13.3. MS (EI, 70 eV; m/z (relativeintensity)): 371 (8), 370 (37), 233 (71), 215 (81), 132 (85), 102 (100), 91 (44). HRMS (ESI-TOF) m/z calcd for $C_{21}H_{23}OSe$ (M + H+): 371.0914, found: 371.0921.



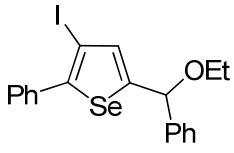
(Z)-2-(butylselanyl)-1,5-dip-tolylpent-1-en-4-yn-3-ol (2a). Isolated by column chromatography (hexane and ethyl acetate 90:10 as eluent) as a yellow oil. Yield: 0.272 g (68%); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.60 (d, J = 8.3 Hz, 2H), 7.41-7.37 (m, 2H), 7.31 (s, 1H), 7.21-7.13 (m, 4H), 5.27 (dd, J = 7.7Hz, 0.8 Hz, 1H), 2.84 (d, J = 7.7 Hz, 1H), 2.79-2.74 (m, 2H), 2.39 (s, 3H), 2.38 (s, 3H), 1.66-1.57 (m, 2H), 1.32 (qui, J = 7.4 Hz, 2H), 0.84 (t, J = 7.4 Hz, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 38.7, 137.7, 134.2, 133.5, 132.0, 131.6, 129.2, 129.0, 128.7, 119.4, 87.5, 86.7, 68.8, 32.3, 27.0, 22.8, 21.4, 21.2, 13.4. MS (EI, 70 eV; m/z (relativeintensity)): 399 (4), 398(11), 261 (32), 218 (32), 146

(45), 115 (100), 91 (25). HRMS (ESI-TOF) m/z calcd for$C_{23}H_{27}OSe$ (M + H+): 399.1227, found: 399.1235.



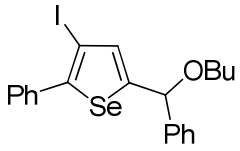
(Z)-2-(butylselanyl)-1,5-bis(4-chlorophenyl)pent-1-en-4-yn-3-ol (1c). Isolated by column chromatography (hexane and ethyl acetate 90:10 as eluent) as a yellow oil. Yield: 0.249 g (56%); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.63 (d, J = 8.4 Hz, 2H), 7.42-7.26 (m, 7H), 5.26 (s, 1H), 2.80 (s, 1H), 2.74 (t, J = 7.3 Hz, 2H), 1.62-1.58 (m, 2H), 1.37-1.26 (m, 2H), 0.84 (t, J = 7.3 Hz, 3H).^{13}C NMR ($CDCl_3$, 100 MHz): δ 134.8, 134.7, 133.7, 133.6, 133.0, 132.9, 130.5, 128.6, 128.3, 120.8, 88.9, 85.5, 68.6, 32.2, 27.2, 22.7, 13.3. MS (EI, 70 eV; m/z (relativeintensity)): 439 (6),438 (32), 268 (17), 205 (58), 135 (76), 102 (90), 91 (39). HRMS (ESI-TOF) m/z calcd for$C_{21}H_{21}Cl_2OSe$ (M + H+): 439.0135, found: 439.0143.

General Procedure for the 3-iodoselenophene 2. To a solution of (Z)-selenoenyne **1** (0.25 mmol) in CH_2Cl_2 (3 mL) were added I_2 (1.5 equiv) and EtOH (3 equiv). The reaction mixture was stirred for time indicated in Table 2. The mixture was diluted with ethyl acetate (10 mL) and washed with a saturated solution of $Na_2S_2O_3$ (10 mL). The organic phase was separated, dried over $MgSO_4$, and concentrated under vacuum. The residue was purified by flash chromatography and eluted with hexane/dichloromethane.

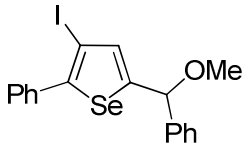


5-(ethoxy(phenyl)methyl)-3-iodo-2-phenylselenophene (2a). Isolated by column chromatography (hexane and dichloromethane 75:25 as eluent) as a yellow oil. Yield: 0.093 g (80%); ^{1}H NMR ($CDCl_3$, 400 MHz): *δ* 7.56-7.28 (m, 10H), 6.98 (s, 1H), 5.48 (s, 1H), 3.62-3.51 (m, 2H), 1.25 (t, *J* = 6.9 Hz, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): *δ* 155.5, 146.8, 141.3, 136.7, 135.7, 129.3, 128.6, 128.3, 128.2, 128.2, 126.8, 80.8, 78.5, 64.8, 15.3. MS (EI, 70 eV; *m/z* (relativeintensity)): 468 (4),467 (6), 422 (17), 253 (58), 212 (38), 102 (26), 77

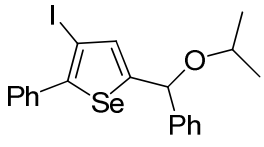
(39). HRMS (ESI-TOF) m/z calcd for $C_{19}H_{18}IOSe$ (M + H^+): 468.9568, found: 468.9675.



5-(butoxy(phenyl)methyl)-3-iodo-2-phenylselenophene (2b). Isolated by column chromatography (hexane and dichloromethane 75:25 as eluent) as a yellow solid. Yield: 0.089 g (72%); mp 44.6-47.2°C. ^{1}H NMR ($CDCl_3$, 400 MHz): *δ* 7.61 (dd, *J*= 8.1 Hz, *J*= 1.6 Hz, 2H), 7.51-7.37 (m, 8H), 7.05 (s, 1H), 5.55 (s, 1H), 3.65-3.54 (m, 2H), 1.71 (qui, *J* = 6.9 Hz, 2H), 1.52 (sex, *J* = 6.9 Hz, 2H), 1.01 (t, *J* = 6.9 Hz, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): *δ*155.6, 146.6, 141.2, 136.6, 135.4, 129.1, 128.5, 128.2, 128.0, 126.8, 88.9, 78.4, 69.0, 31.8, 19.3, 13.8, 13.7. MS (EI, 70 eV; *m/z* (relativeintensity)): 496 (11), 495 (13), 423 (32), 235 (37), 215 (44), 105 (92), 57 (38). HRMS (ESI-TOF) m/z calcd for $C_{21}H_{22}IOSe$(M + H^+): 496.9881, found: 496.9888.

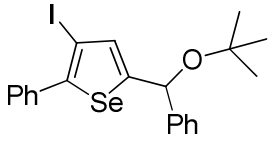


3-iodo-5-(methoxy(phenyl)methyl)-2-phenylselenophene (2c). Isolated by column chromatography (hexane and dichloromethane 75:25 as eluent) as a yellow oil. Yield: 0.089 g (78%); mp 83.1-85.7°C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.47-7.41 (m, 2H), 7.35-7.29 (m, 8H), 6.98 (d, *J*= 1.1 Hz, 1H), 5.36 (s, 1H), 3.39 (s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): *δ* 154.8, 146.9, 140.7, 136.6, 135.9, 129.2, 128.7, 128.4, 128.3, 128.2, 126.8, 82.7, 78.4, 57.0. MS (EI, 70 eV; *m/z* (relative intensity)): 455 (4), 454 (24), 422 (17), 247 (100), 215 (38), 115 (36), 77 (49). HRMS (ESI-TOF) m/z calcd for $C_{18}H_{16}IOSe$ (M + H^+): 454.9411, found: 454.9416. 423 (32), 235 (37), 215 (44), 105 (92), 57 (38). HRMS (ESI-TOF) m/z calcd for $C_{21}H_{22}IOSe$ (M + H^+): 496.9881, found: 496.9888.

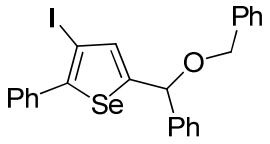


3-iodo-5-(isopropoxy(phenyl)methyl)-2-phenylselenophene (2d). Isolated by column chromatography (hexane and dichloromethane 75:25 as eluent) as a white solid. Yield: 0.087 g (72%); mp 87.7-89.6°C. ^{1}H NMR ($CDCl_3$, 400 MHz): *δ* 7.51-7.28 (m, 10H), 6.95 (s, 1H),

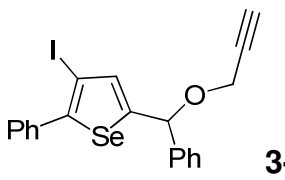
5.59 (s, 1H), 3.75 (sep, *J* = 6.1 Hz, 1H), 1.25 (d, *J*= 6.1 Hz, 3H), 1.18 (d, *J* =6.1 Hz, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): *δ* 156.3, 146.6, 141.8, 136.7, 135.3, 129.2, 128.5, 128.2, 128.1, 128.0, 126.8, 78.4, 78.0, 69.8, 22.4, 22.0. MS (EI, 70 eV; *m/z* (relativeintensity)): 482 (3), 481 (12), 422 (12), 233(48), 215 (27), 107 (17), 105 (100). HRMS (ESI-TOF) m/z calcd for $C_{20}H_{20}IOSe$ (M + H^+): 482.9724, found: 482.9730.



5-(tert-butoxy(phenyl)methyl)-3-iodo-2-phenylselenophene (2e). Isolated by column chromatography (hexane and dichloromethane 75:25 as eluent) as a yellow solid. Yield: 0.034 g (28%); mp 85.5-87.8°C. ^{1}H NMR ($CDCl_3$, 400 MHz): *δ* 7.57-7.29 (m, 10H), 6.85 (d, *J*= 1.3 Hz 1H), 5.75 (s, 1H), 1.29 (t, *J* = 6.9 Hz, 9H). ^{13}C NMR ($CDCl_3$, 100 MHz): *δ*158.8, 146.1, 143.9, 136.8, 134.3, 129.2, 128.4, 128.2, 128.0, 127.6, 126.6, 78.6, 75.8, 73.6, 28.6. MS (EI, 70 eV; *m/z* (relativeintensity)): 496(3), 495 (15), 422 (16), 233 (40), 215 (24),105(100), 57 (55). HRMS (ESI-TOF) m/z calcd for $C_{21}H_{22}IOSe$ (M + H^+): 496.9881, found: 496.9885.

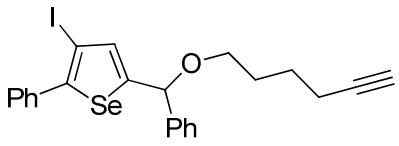


5-(benzyloxy(phenyl)methyl)-3-iodo-2-phenylselenophene (2f). Isolated by column chromatography (hexane and dichloromethane 75:25 as eluent) as a white solid. Yield: 0.115 g (87%); mp 76.5-76.9°C. ^{1}H NMR ($CDCl_3$, 400 MHz): *δ* 7.61-7.55 (m, 4H), 7.51-7.36 (m, 11) 7.08 (d, *J*= 1.1 Hz 1H), 5.66 (s, 1H), 4.69 (m, 2H). ^{13}C NMR ($CDCl_3$, 100 MHz): *δ* 155.1, 147.1, 140.8, 137.8, 136.7, 136.0 129.3, 128.7, 128.7, 128.5, 128.4, 128.2, 127.8, 127.8, 127.1, 79.9, 78.5, 70.7. MS (EI, 70 eV; *m/z* (relativeintensity)): 530 (8), 438 (15), 422 (18), 217 (37), 215 (34), 105 (100), 91 (73). HRMS (ESI-TOF) m/z calcd for $C_{24}H_{20}IOSe$ (M + H^+): 530.9724, found: 530.9728.

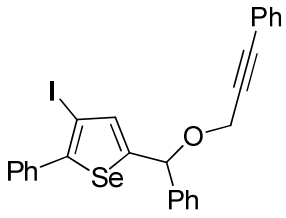


3-iodo-2-phenyl-5-(phenyl(prop-2-ynyloxy)methyl)selenophene (2g). Isolated by column chromatography

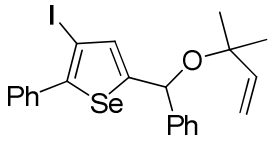
(hexane and dichloromethane 75:25 as eluent) as a yellow oil. Yield: 0.078 g (66%); ^{1}H NMR ($CDCl_3$, 400 MHz): *δ* 7.50-7.41 (m, 6H), 7.38-7.31 (m, 4), 7.04 (s, 1H), 5.50 (s, 1H), 4.69 (m, 2H), 2.44 (t, *J*= 2.3, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz): *δ* 153.7, 147.3, 139.8, 136.5, 136.4, 129.1, 128.6, 128.4, 128.2, 128.2, 127.1, 79.1, 78.8, 78.4, 75.1, 55.8. MS (EI, 70 eV; *m/z* (relativeintensity)): 478(3), 477 (35), 371 (7), 215 (18), 165 (12), 126 (12), 105 (100). HRMS (ESI-TOF) m/z calcd for $C_{20}H_{16}IOSe$ (M + H^+): 478.9411, found: 478.9416.



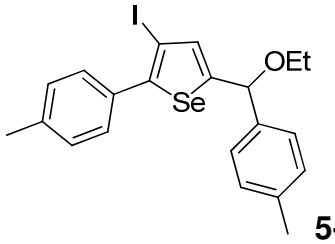
5-((hex-5-ynyloxy)(phenyl)methyl)-3-iodo-2-phenylselenophene (2h). Isolated by column chromatography (hexane and dichloromethane 75:25 as eluent) as a yellowoil. Yield: 0.091 g (70%); ^{1}H NMR ($CDCl_3$, 400 MHz): *δ* 7.53-7.48 (m, 2H), 7.42-7.30 (m, 8H), 6.95 (d, *J* = 1.2 Hz, 1H), 5.46 (s, 1H), 3.60-3.45 (m, 2H), 2.21 (td, *J* = 6.9, 2.7 Hz, 2H), 1.93 (t, *J* = 2.7 Hz, 1H), 1.79 - 1.60 (m, 4H). ^{13}C NMR ($CDCl_3$,100 MHz): *δ* 155.4, 146.7, 141.0, 136.6, 135.5, 129.2, 128.6, 128.2, 128.1, 128.1, 126.8, 84.2, 81.0, 78.4, 68.6, 68.4, 28.7, 25.1, 18.1. MS (EI, 70 eV; *m/z* (relative intensity)): 520 (3), 519 (4), 422 (36), 313 (41), 215 (100), 115 (38), 105 (95). HRMS (ESI-TOF) m/z calcd for $C_{23}H_{22}IOSe$ (M + H^+): 520.9881, found: 520.9892.



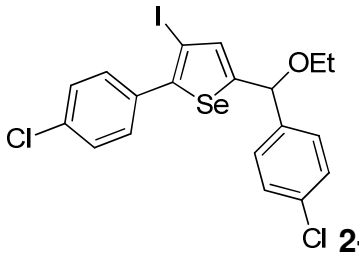
3-iodo-2-phenyl-5-(phenyl(3-phenylprop-2-ynyloxy)methyl)selenophene (2i). Isolated by column chromatography (hexane and dichloromethane 75:25 as eluent) as a black oil. Yield: 0.070 g (51%); ^{1}H NMR ($CDCl_3$, 400 MHz): *δ* 7.53-7.42 (m, 6H), 7.40-7.28 (m, 9H), 7.05 (s, 1H), 5.58 (s, 1H), 4.69 (m, 2H). ^{13}C NMR ($CDCl_3$, 100 MHz): *δ* 154.1, 147.4, 140.2, 136.6, 131.8, 129.3, 128.7, 128.5, 128.5, 128.3, 128.3, 128.2, 127.6, 127.2, 122.6, 87.1, 84.6, 79.1, 78.5, 56.8. MS (EI, 70 eV; *m/z* (relativeintensity)): 554 (2), 553 (4),438 (15), 217 (25), 115 (10), 105 (100), 77 (14). HRMS (ESI-TOF) m/z calcd for $C_{26}H_{20}IOSe$ (M + H^+): 554.9724, found: 554.9731.



3-iodo-5-((2-methylbut-3-en-2-yloxy)(phenyl)methyl)-2-phenylselenophene (2j). Isolated by column chromatography (hexane and dichloromethane 75:25 as eluent) as a yellow oil. Yield: 0.086 g (68%); ^{1}H NMR ($CDCl_3$, 400 MHz): *δ* 6.57-6.53 (m, 2H), 6.52-6.47 (m, 2H), 6.43-6.31 (m, 8H), 5.86 (d, *J* = 1.3 Hz, 1H), 5.08 (s, 1H), 1.50 (s, 1H), 0.64 (s, 3H), 0.37 (s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): *δ* 157.2, 146.8, 142.8, 135.3, 129.3, 129.2, 128.4, 128.3, 128.3, 128.1, 127.8, 126.9, 78.6, 76.2, 73.2, 72.4, 30.3, 29.7. MS (EI, 70 eV; *m/z* (relativeintensity)): 508 (3), 507 (14), 422 (36), 311 (41), 215 (52), 115 (87), 105 (95). HRMS (ESI-TOF) m/z calcd for $C_{22}H_{22}IOSe$ ($M + H^+$): 508.9881, found: 508.9889.

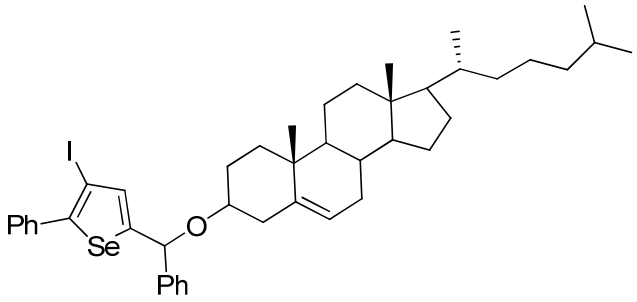


5-(ethoxy(p-tolyl)methyl)-3-iodo-2-p-tolylselenophene (2k). Isolated by column chromatography (hexane and dichloromethane 75:25 as eluent) as a yellowoil. Yield: 0.081 g (65%); ^{1}H NMR ($CDCl_3$, 400 MHz): *δ* 7.39 (d, *J*= 8.1 Hz, 2H), 7.30 (d, *J* = 8.1 Hz, 2H), 7.16 (d, *J* = 8.4 Hz, 4H), 6.95 (d, *J*= 1.1 Hz, 1H), 5.44 (s, 1H), 3.63-3.47 (m, 2H), 2.35 (s, 3H), 2.34 (s, 3H), 1.24 (t, *J* = 7.0 Hz, 3H). ^{13}C NMR (CDCl3, 100 MHz): *δ* 155.3, 146.8, 138.3, 138.0, 137.8, 135.4, 133.8, 129.2, 129.0, 129.0, 126.7, 80.6, 78.1, 64.6, 21.2, 21.1, 15.2. MS (EI, 70 eV; *m/z* (relativeintensity)): 496 (25),495 (5), 417 (22), 313 (37), 233 (24),128 (28), 107 (55). HRMS (ESI-TOF) m/z calcd for $C_{21}H_{22}IOSe$ ($M + H^+$): 496.9881, found: 496.9890.

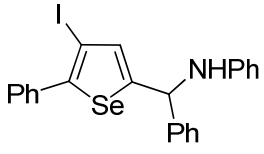


2-(4-chlorophenyl)-5-((4-chlorophenyl)(ethoxy)methyl)-3-iodoselenophene (2l). Isolated by column chromatography (hexane and dichloromethane 75:25 as eluent) as a yellowoil.

Yield: 0.075 g (56%); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.47-7.27 (m, 8H), 6.96 (d, J = 1.1 Hz, 1H), 5.45 (d, J = 1.1 Hz, 1H), 3.65-3.46 (m, 2H), 1.26 (t, J = 7.0 Hz, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 155.4, 145.5, 139.7, 135.8, 135.0, 134.3, 134.0, 130.4, 128.8, 128.6, 128.1, 80.0, 78.9, 64.9, 15.1. MS (EI, 70 eV; *m/z* (relative intensity)): 536 (6), 535 (23), 491 (25), 329 (100), 301 (40), 202 (27), 113 (53). HRMS (ESI-TOF) m/z calcd for $C_{19}H_{16}Cl_2IOSe$ (M + H^+): 536.8788, found: 536.8795.

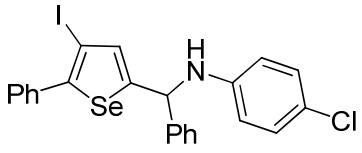


5-(((10R,13R)-10,13-dimethyl-17-((R)-6-methylheptan-2-yl)-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-3-yloxy)(phenyl)methyl)-3-iodo-2-phenylselenophene (2m). Isolated by column chromatography (hexane and dichloromethane 75:25 as eluent) as a yellow oil. Yield: 0.111 g (55%); ^{1}H NMR ($CDCl_3$, 400 MHz): 7.63-7.35 (m, 10H), 7.04 (d, J = 3.5 Hz, 1H), 5.76 (s, 1H), 5.40 (m, 1H), 3.53-3.41 (m, 1H), 2.59-2.37 (m, 1H), 2.15-1.86 (m, 4H), 1.76-1.32 (m, 13H), 1.28-0.94 (m, 22H), 0.77 (s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 156.4, 146.7, 141.9, 140.7, 136.8, 135.4, 129.3, 128.6, 128.3, 128.1, 128.1, 126.9, 121.9, 78.5, 78.0, 77.6, 56.8, 56.3, 50.2, 42.4, 39.9, 39.6, 39.2, 37.2, 36.9, 36.3, 35.8, 34.7, 34.5, 32.0, 28.9, 28.5, 28.3, 28.0, 27.0, 25.4, 24.3, 23.9, 22.9, 22.6, 21.1, 19.4, 18.8, 11.9. HRMS (ESI-TOF) m/z calcd for $C_{44}H_{58}IOSe$ (M + H^+): 809.2698, found: 809.2703.

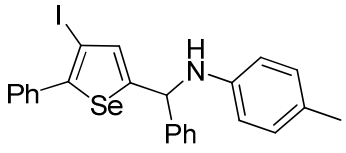


N-((4-iodo-5-phenylselenophen-2-yl)(phenyl)methyl)aniline (2n). Isolated by column chromatography (hexane and dichloromethane 75:25 as eluent) as a black oil. Yield: 0.062 g (48%); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.51 (d, J = 6.3 Hz, 2H), 7.45 (d, J = 7.4 Hz, 2H),

7.40-7.31 (m, 6H), 7.16 (t, *J* = 7.9 Hz, 2H), 7.09 (s, 1H), 6.75 (t, *J* = 7.4 Hz, 1H), 6.65 (d, *J* = 7.8 Hz, 2H), 5.70 (s, 1H), 4.39 (s, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz): *δ* 156.5, 146.6, 142.0, 136.5, 135.9, 129.2, 129.2, 129.0, 129.0, 128.3, 128.3, 128.2, 128.1, 127.0, 118.6, 113.9, 78.8, 60.5. MS (EI, 70 eV; *m/z* (relative intensity)): 515 (6), 422 (100), 420 (51), 295 (23), 207 (61), 115 (26), 77 (59). HRMS (ESI-TOF) m/z calcd for $C_{23}H_{19}INSe$ (M + H^+): 515.9727, found: 515.9735.

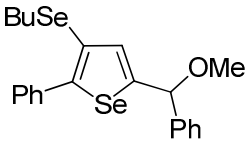


4-chloro-N-((4-iodo-5-phenylselenophen-2-yl)(phenyl)methyl)aniline (2o). Isolated by column chromatography (hexane and dichloromethane 75:25 as eluent) as a gren oil. Yield: 0.109 g (80%); mp 62.1-65.2 °C. ^{1}H NMR ($CDCl_3$, 400 MHz): *δ* 7.58-7.53 (m, 2H), 7.49-7.35 (m, 8H), 7.16-7.12 (m, 3H), 6.64-6.58 (m, 2H), 5.70 (d, *J* = 4.5 Hz, 1H), 4.42 (d, *J* = 4.5 Hz, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz): *δ* 155.8, 146.8, 145.1, 141.6, 136.4, 136.2, 129.2, 129.1, 128.3, 128.3, 128.3, 127.0, 123.4, 115.1, 78.8, 60.6. MS (EI, 70 eV; *m/z* (relativeintensity)): 549 (14), 546 (32), 340 (42), 281 (25), 207(100), 151(18), 111 (44). HRMS (ESI-TOF) m/z calcd for $C_{23}H_{18}ClINSe$ (M + H^+): 549.9338, found: 549.9346.

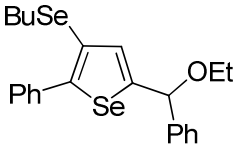


N-((4-iodo-5-phenylselenophen-2-yl)(phenyl)methyl)-4-methylaniline (2p). Isolated by column chromatography (hexane and dichloromethane 75:25 as eluent) as a yellow solid. Yield: 0.101 g (77%); mp 62.1-65.2°C. ^{1}H NMR ($CDCl_3$, 400 MHz): *δ* 7.52-7.47 (m, 2H), 7.44-7.40 (m, 2H), 7.37-7.27 (m, 6H), 7.07 (d, *J* = 1.1 Hz, 1H), 6.95 (d, *J* = 8.1 Hz, 2H), 6.56 (d, *J* = 8.4 Hz, 2H), 5.65 (s, 1H), 4.25 (s, 1H), 2.21 (s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): *δ* 156.8, 146.5, 144.3, 142.2, 136.6, 135.8, 129.7, 129.2, 128.9, 128.3, 128.1, 128.0, 127.9, 127.0, 114.1, 78.7, 60.8, 20.3. MS (EI, 70 eV; *m/z* (relativeintensity)): 529 (5), 420 (56), 337 (43), 295 (23), 208 (45), 111 (33), 77 (60). HRMS (ESI-TOF) m/z calcd for $C_{24}H_{21}INSe$ (M + H^+): 529.9884, found: 529.9890.

General Procedure for the 3- chalcogenyl-Selenophenes 4. To a Schlenck tube, under ambient atmosphere, containing CH_2Cl_2 (3 mL) were added (n-BuSe)$_2$ (1.5 equiv) and NBS (1.5 equiv), and the reaction mixture was stirred for 30 min at room temperature. After this time, the appropriate (Z)-selenoenyne**1** (0.25 mmol) and EtOH (3 equiv) was added and the reaction mixture was stirred for a determined time. Afterward, the mixture was diluted with ethyl acetate (15 mL) and washed with a saturated solution of $Na_2S_2O_3$ (15 mL). The organic phase was separated, dried over $MgSO_4$, and concentrated under vacuum. The residue was purified by flash chromatography and eluted with hexane/ dichloromethane.

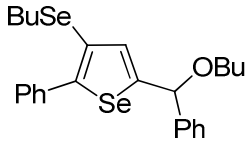


3-(butylselanyl)-5-(methoxy(phenyl)methyl)-2-phenylselenophene (4a). Isolated by column chromatography (hexane and dichloromethane 75:25 as eluent) as a yellow oil. Yield: 0.074 g (64 %); ^{1}H NMR ($CDCl_3$, 400 MHz): *δ* 7.59-7.32 (m, 10H), 7.08 (d, *J* = 1.1 Hz, 1H), 5.45 (s, 1H), 3.48 (s, 3H), 2.72 (t, *J* = 7.3 Hz, 2H), 1.55 (qui, *J* = 7.3 Hz, 2H), 1.32 (sex, *J* = 7.3 Hz, 2H), 0.86 (t, *J* = 7.3 Hz, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): *δ* 152.3, 147.9, 141.2, 136.5, 133.2, 129.4, 128.6, 128.2, 128.1, 127.7, 126.9, 120.7, 83.1, 57.0, 32.2, 28.3, 22.7, 13.4. MS (EI, 70 eV; *m/z* (relative intensity)): 465 (2), 418 (47), 373 (55), 215 (18), 202 (15),115 (21), 105 (100). HRMS (ESI-TOF) m/z calcd for $C_{22}H_{25}OSe_2$ (M + H^+): 465.0236, found: 465.0240.

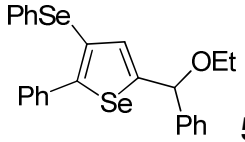


3-(butylselanyl)-5-(ethoxy(phenyl)methyl)-2-phenylselenophene (4b). Isolated by column chromatography (hexane and dichloromethane 75:25 as eluent) as a yellow oil. Yield: 0.099 g (83%); ^{1}H NMR ($CDCl_3$, 400 MHz): *δ* 7.50-7.26 (m, 10H), 7.00 (d, *J* = 1.0 Hz, 1H), 5.49 (s, 1H) 3.68-3.46 (m, 2H), 2.66 (t, *J* = 7.4 Hz, 2H), 1.49 (qui, *J* = 7.8 Hz, 2H), 1.30-1.19 (m, 5H), 0.78 (t, *J* = 7.3 Hz, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): *δ* 152.9, 147.6, 141.6, 136.5, 132.8, 129.2, 128.4, 128.0, 127.88, 127.5, 126.7, 120.6, 81.1, 64.6, 32.1, 28.2, 22.6, 15.2, 13.3. MS (EI, 70 eV; *m/z* (relative intensity)): 479

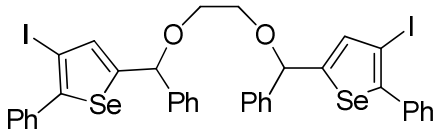
(12), 478(44), 433 (23), 261 (100), 215 (27), 135 (15), 105 (28). HRMS (ESI-TOF) m/z calcd for $C_{23}H_{27}OSe_2$ (M + H^+): 479.0392, found: 479.0403.



5-(butoxy(phenyl)methyl)-3-(butylselanyl)-2-phenylselenophene (4c). Isolated by column chromatography (hexane and dichloromethane 75:25 as eluent) as a yellow oil. Yield: 0.091g (72%); ^{1}H NMR ($CDCl_3$, 400 MHz): *δ* 7.53-7.23 (m, 10H), 6.97 (d, *J* = 1.1 Hz, 1H), 5.47 (s, 1H), 3.58-3.42 (m, 2H), 2.64 (t, *J* = 7.5 Hz, 2H), 1.67-1.59 (m, 2H), 1.53-1.38 (m, 4H), 1.25 (sex, *J* = 7.3 Hz, 2H), 0.91 (t, *J* = 7.4 Hz, 3H), 0.78 (t, *J* = 7.3 Hz, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): *δ* 153.1, 147.5, 141.6, 136.5, 132.7, 129.2, 128.4, 128.0, 127.8, 127.5, 126.8, 120.6, 81.3, 69.0, 32.1, 31.8, 28.2, 22.6, 19.3, 13.8, 13.3. MS (EI, 70 eV; *m/z* (relative intensity)): 507 (2), 506 (20), 433 (16), 289 (32), 222 (100), 202 (15), 105 (35). HRMS (ESI-TOF) m/z calcd for $C_{25}H_{31}OSe_2$ (M + H^+): 507.0705, found: 507.0705.



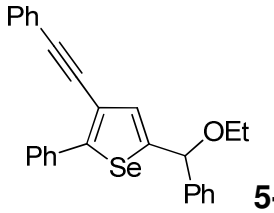
5-(ethoxy(phenyl)methyl)-2-phenyl-3-(phenylselanyl)selenophene (4d). Isolated by column chromatography (hexane and dichloromethane 75:25 as eluent) as a yellow oil. Yield: 0.067 g (54%); ^{1}H NMR ($CDCl_3$, 400 MHz): *δ* 7.47-7.13 (m, 15H), 6.92 (d, *J* = 1.1 Hz, 1H), 5.45 (s, 1H), 3.63-3.47 (m, 2H), 1.24 (t, *J* = 7.0 Hz, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): *δ* 153.6, 150.4, 141.6, 136.1, 133.9, 132.8, 130.7, 129.2, 129.0, 128.4, 128.1, 127.9, 126.7, 126.4, 120.1, 81.0, 64.6, 15.2. MS (EI, 70 eV; *m/z* (relative intensity)): 499 (5), 498 (20), 453 (20), 261 (100), 233 (63), 233 (63), 216 (32), 105 (41). HRMS (ESI-TOF) m/z calcd for $C_{25}H_{23}OSe_2$ (M + H^+): 499.0079, found: 499.0085.



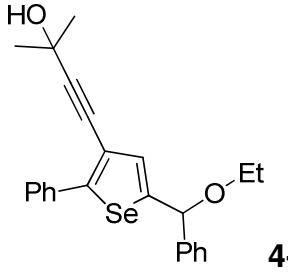
1,2-bis((4-iodo-5-phenylselenophen-2-yl)(phenyl)methoxy)ethane (5). Isolated by column chromatography (hexane and dichloromethane 75:25 as eluent) as a yellow oil. Yield: 0.061 g (27%); ^{1}H NMR ($CDCl_3$, 400 MHz): *δ* 7.55-7.34 (m, 20H), 7.03 (m, 2H), 5.65 (s, 2H), 3.85-

3.72 (m, 4H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 155.0, 146.9, 140.8, 136.6, 135.8, 129.2, 128.7, 128.3, 128.3, 128.1, 126.9, 81.4, 81.3, 78.4, 68.6, 68.5. HRMS (ESI-TOF) m/z calcd for $C_{36}H_{29}I_2O_2Se_2$ ($M + H^+$): 906.8587, found: 906.8595.

General Procedure for the Sonogashira Coupling Reaction 6. The 3-iodoselenophene (0.25 mmol) was added to a Schlenk tube containing $PdCl_2(PPh_3)_2$ (0.0088 g, 5 mol %) and Et_3N (5 mL). To the resulting solution was added CuI (0.0010 g, 2 mol %). The reaction mixture was stirred for 15 min at room temperature, and a solution of the terminal alkyne (1.5 mmol) in Et_3N (1 mL) was added dropwise. The reaction mixture was stirred under reflux temperature for 12 h. Subsequently, the mixture was diluted with ethyl acetate (15 mL) and washed with brine (3 × 15 mL). The organic phase was separated, dried ($MgSO_4$), and concentrated under vacuum. The residue was purified by flash chromatography (silica gel, hexane/ethyl acetate).



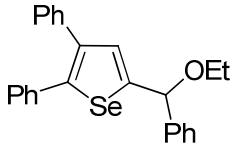
5-(ethoxy(phenyl)methyl)-2-phenyl-3-(phenylethynyl)selenophene (6a). Isolated by column chromatography (hexane and dichloromethane 75:25 as eluent) as a yellow oil. Yield: 0.068 g (62%); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.84-7.77 (m, 2H), 7.49-7.23 (m, 13H), 7.08 (d, J = 1.1 Hz, 1H), 5.49 (s, 1H), 3.68-3.52 (m, 2H), 1.27 (t, J = 7.0 Hz, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 152.6, 152.0, 141.4, 135.9, 131.4, 131.0, 128.6, 128.5, 128.3, 128.1, 128.1, 128.0, 126.9, 123.4, 118.9, 89.9, 87.1, 81.0, 64.8, 15.3. MS (EI, 70 eV; *m/z* (relative intensity)): 443 (28), 442 (100), 397 (98), 315 (62), 304 (27), 239 (26), 156 (22), 77 (50). HRMS (ESI-TOF) m/z calcd for $C_{27}H_{23}OSe$ ($M + H^+$): 443.0914, found: 443.0921.



4-(5-(ethoxy(phenyl)methyl)-2-phenylselenophen-3-yl)-2-methylbut-3-yn-2-ol (6b). Isolated by column chromatography (hexane and

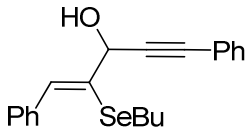
ethyl acetate 90:10 as eluent) as a yellow oil. Yield: 0.051 g (48%); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.78-7.75 (m, 2H), 7.48-7.29 (m, 8H), 7.00 (d, J = 1.1 Hz, 1H), 5.50 (s, 1H), 3.68-3.55 (m, 2H), 1.57 (s, 6H), 1.30 (t, J = 7.0 Hz, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 152.6, 151.9, 141.4, 135.8, 130.8, 128.5, 128.3, 128.0, 128.0, 127.9, 126.8, 118.3, 94.2, 81.0, 79.7, 65.6, 64.7, 31.2, 15.2. MS (EI, 70 eV; *m/z* (relativeintensity)): 425 (8), 424 (30), 406 (44), 361 (51), 319 (29), 239 (36), 152 (26), 105 (100). HRMS (ESI-TOF) m/z calcd for $C_{24}H_{25}O_2Se$ ($M + H^+$): 425.1020, found: 425.1027.

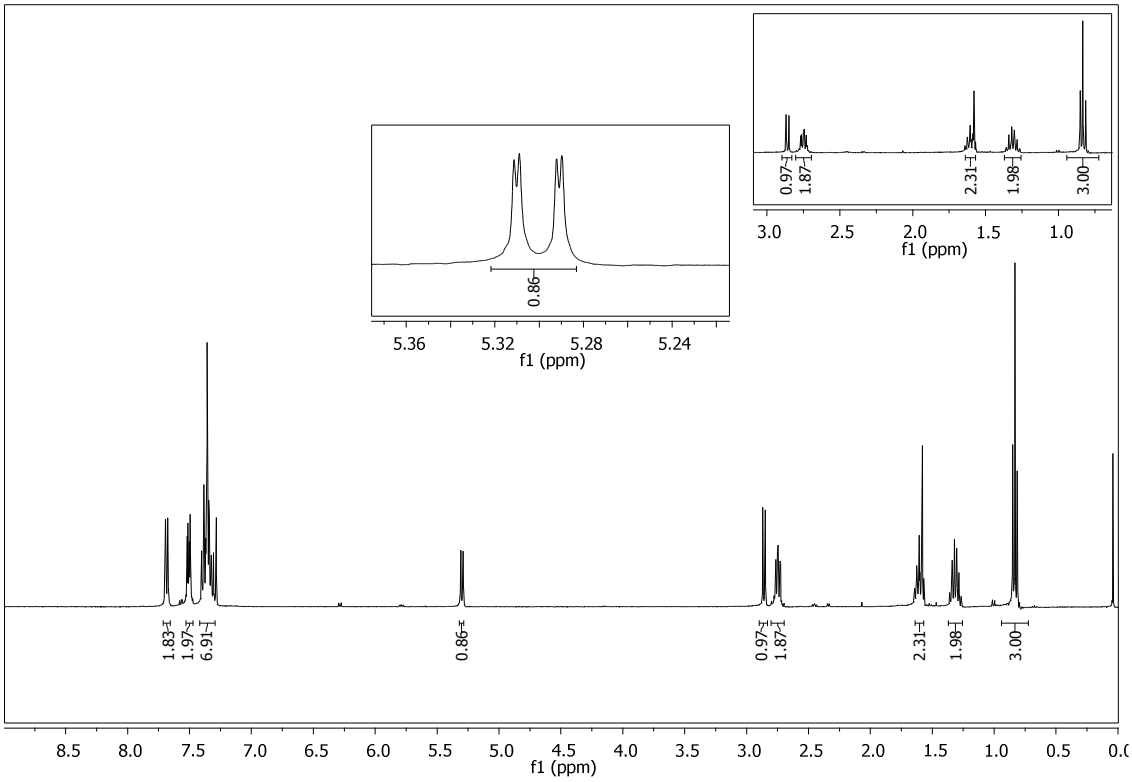
General Procedure for the Suzuki Coupling Reaction. A solution of 3-iodoselenophene (0.25 mmol) in DMF/H_2O (5:1, 5 mL) was added to a mixture of $Pd(PPh_3)_4$ (2 mol %) and K_2CO_3 (2 equiv). After that, the boronic acid (1.5 equiv) in DMF (0.5 mL) was added dropwise, and the reaction mixture was stirred under reflux temperature for 12 h. The organic phase was separated, dried with $MgSO_4$, and concentrated under vacuum. The residue was purified by flash chromatography (hexane/ethyl acetate).

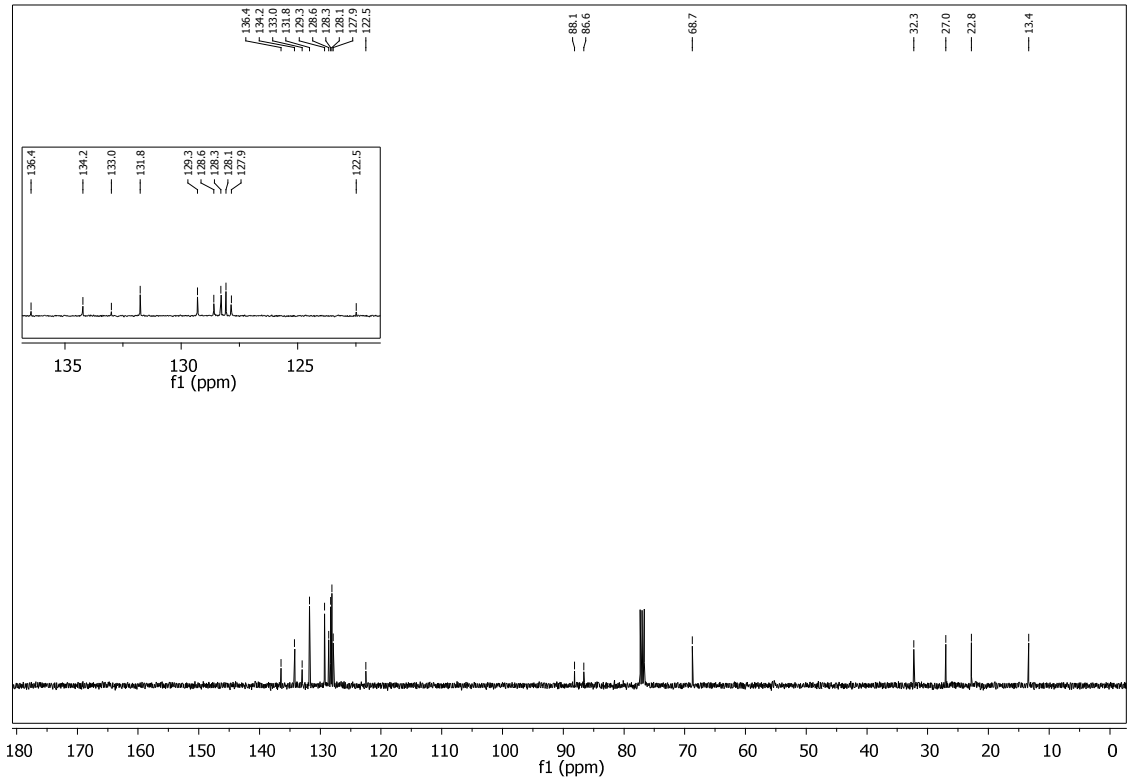


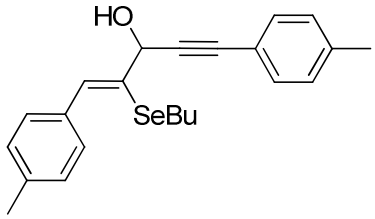
5-(ethoxy(phenyl)methyl)-2,3-diphenylselenophene (7). Isolated by column chromatography (hexane and ethyl acetate 99:1 as eluent) as a blackoil. Yield: 0.066 g (63%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.51-7.13 (m, 15H), 7.08 (d, J = 1.0 Hz, 1H), 5.54 (s, 1H), 3.71-3.50 (m, 2H), 1.28 (t, J = 7.0 Hz, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 152.6, 144.6, 141.9, 139.1, 137.8, 136.5, 130.8, 129.2, 129.2, 128.5, 128.3, 128.2, 127.9, 127.1, 126.8, 126.6, 81.4, 64.7, 15.3. MS (EI, 70 eV; *m/z* (relative intensity)): 419 (13), 418 (52), 416 (28), 373 (60), 215 (18), 115 (20), 105 (100). HRMS (ESI-TOF) m/z calcd for $C_{25}H_{23}OSe$ ($M + H^+$): 419.0914, found: 419.0923.

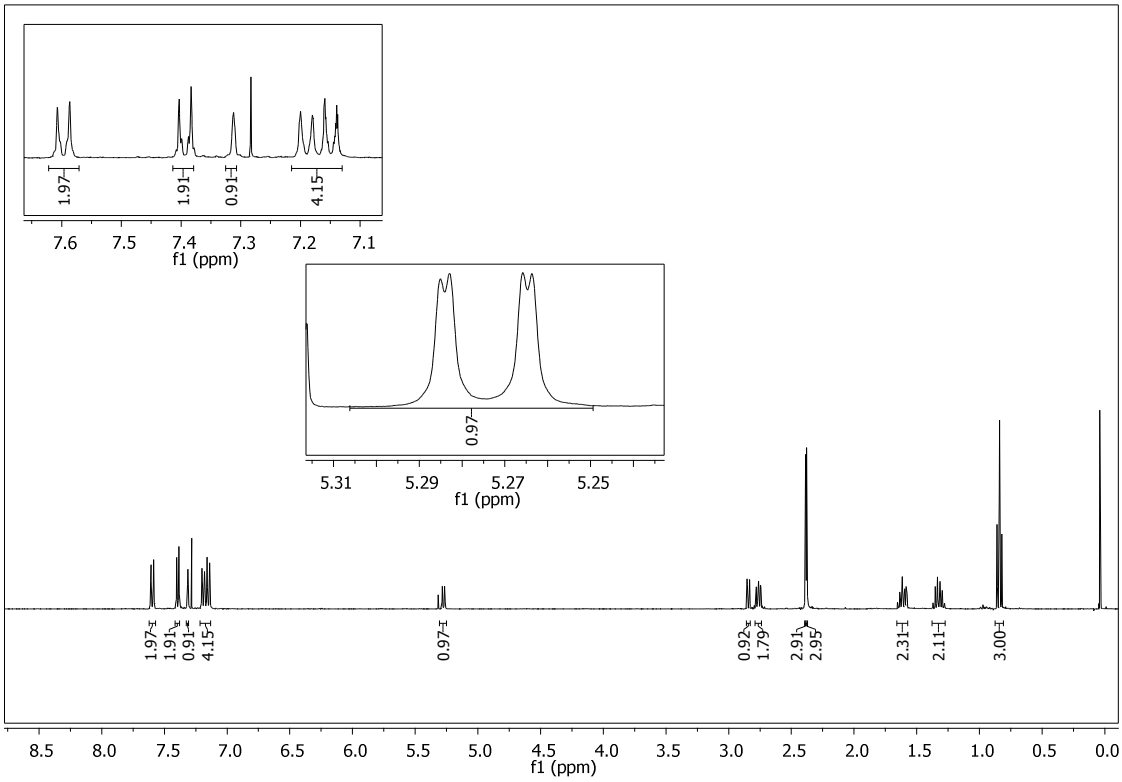
NMR Spectra

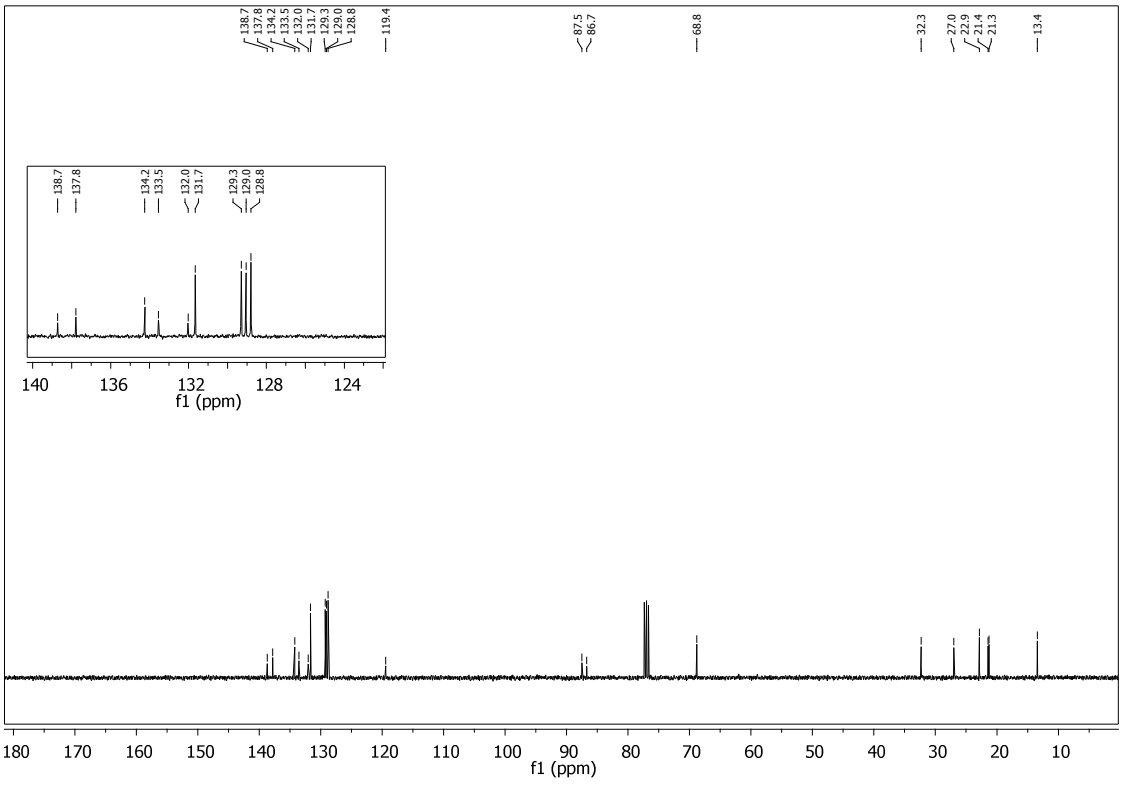

HO
Ph
Ph
SeBu

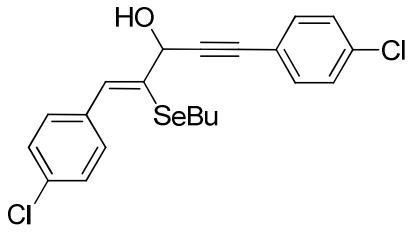

0.86
0.97
1.87
2.31
1.98
3.00
f1 (ppm)
1.83
1.97
6.91
0.86
0.97
1.87
2.31
1.98
3.00
f1 (ppm)

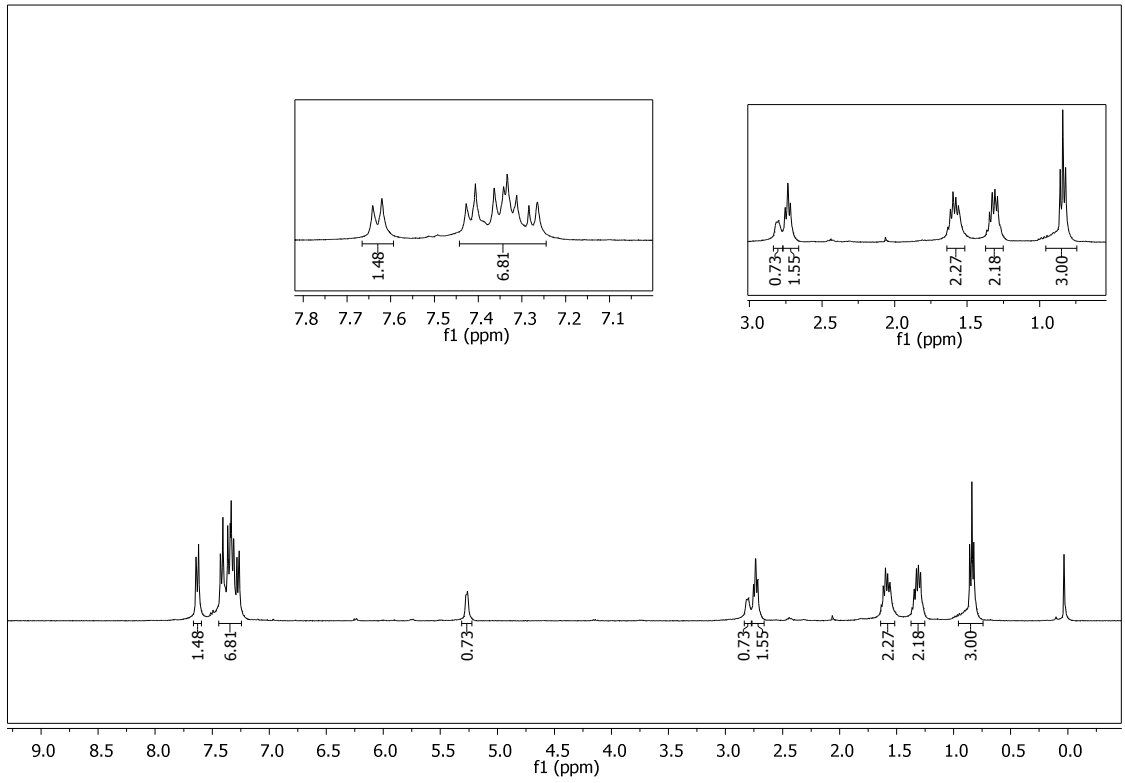

136.4
134.2
133.0
131.8
129.3
128.6
128.3
128.1
127.9
122.5
88.1
86.6
68.7
32.3
27.0
22.8
13.4
f1 (ppm)
f1 (ppm)

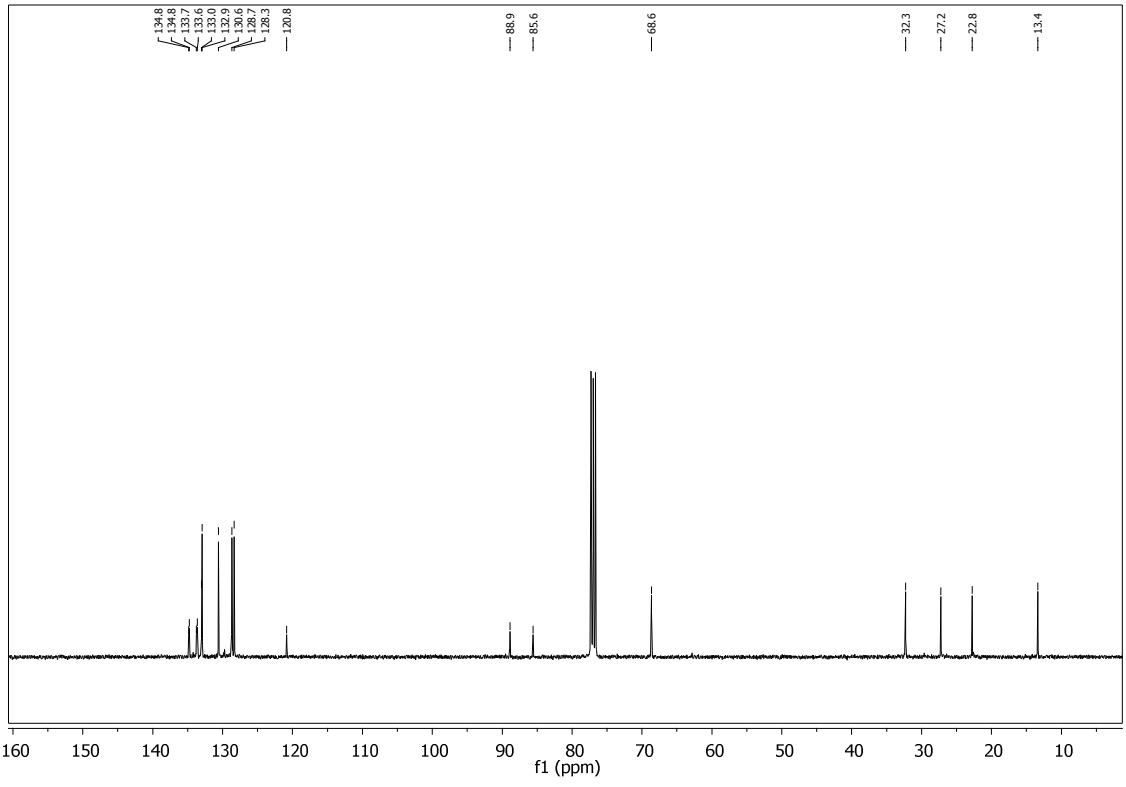

HO
SeBu

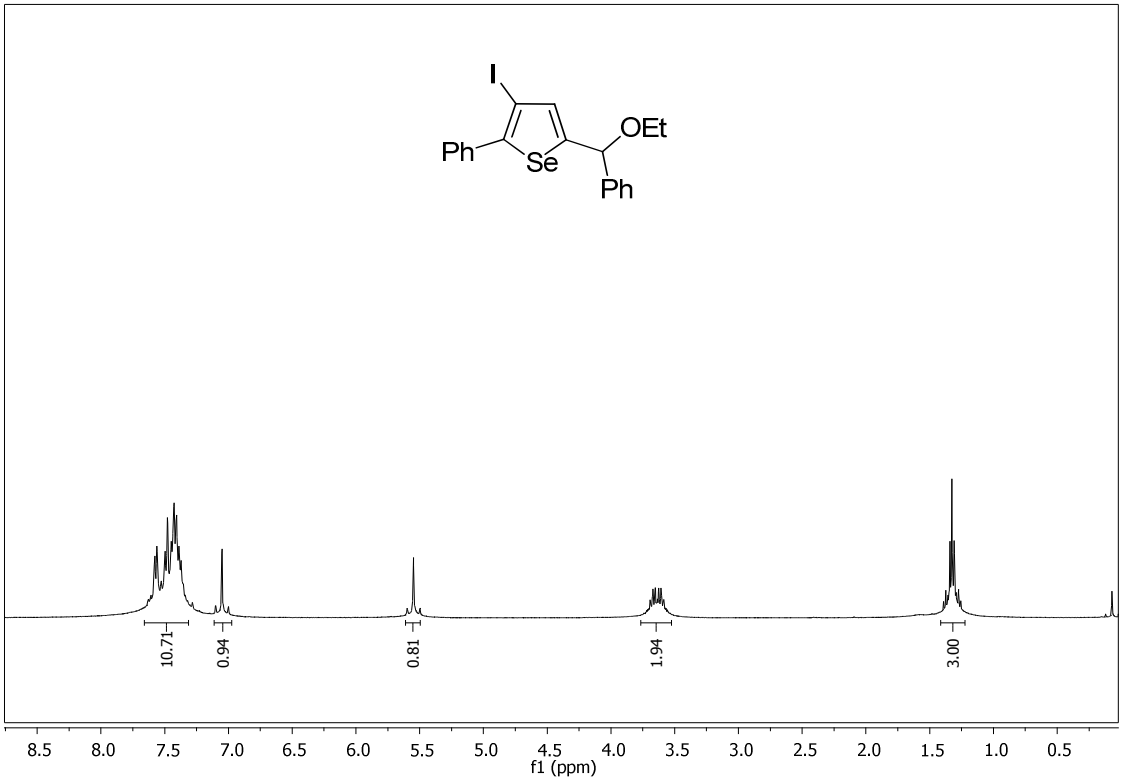

1.97
1.91
0.91
4.15
7.6
7.5
7.4
7.3
7.2
7.1
f1 (ppm)
0.97
5.31
5.29
5.27
5.25
f1 (ppm)
1.97
1.91
0.91
4.15
0.97
0.92
1.79
2.91
2.95
2.31
2.11
3.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

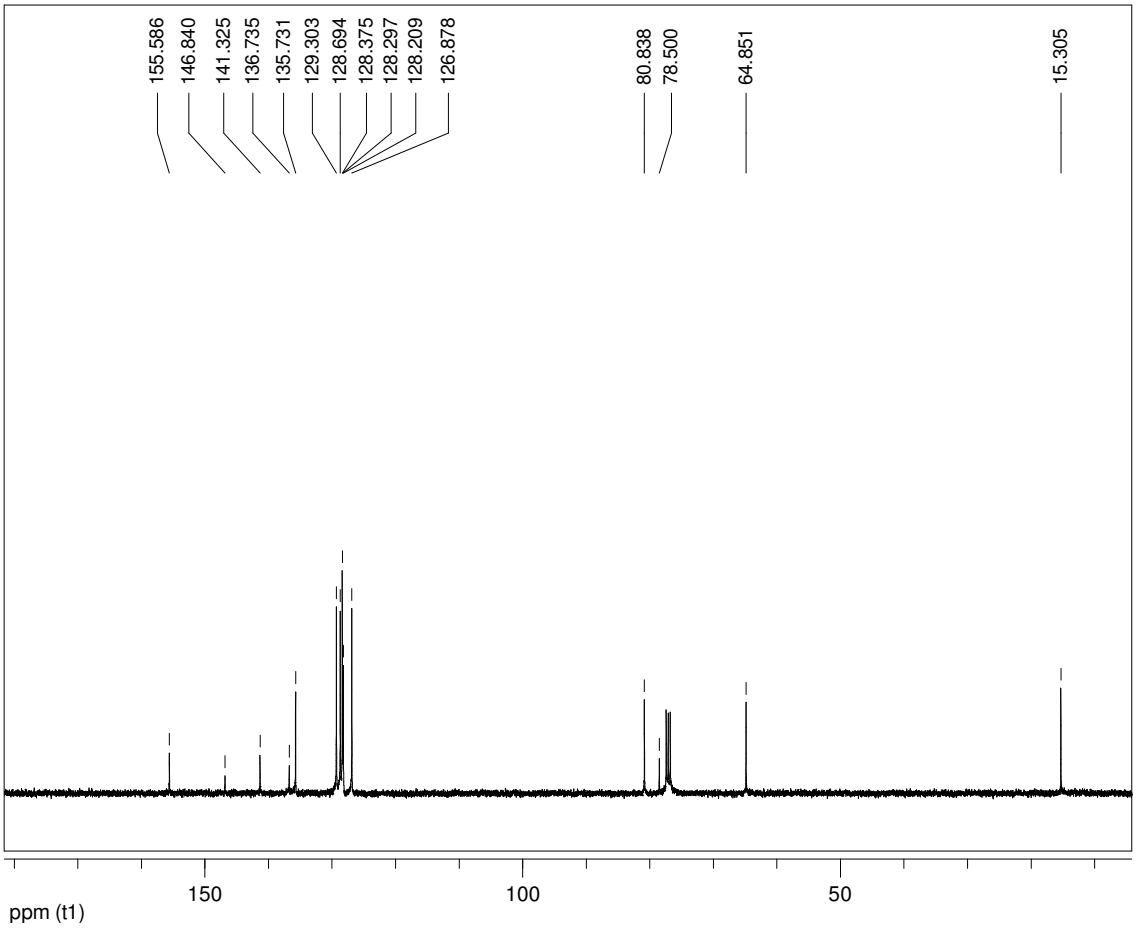

138.7
137.8
134.2
133.5
132.0
131.7
129.3
129.0
128.8
119.4
87.5
86.7
68.8
32.3
27.0
22.9
21.4
21.3
13.4
140
136
132
128
124
f1 (ppm)
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

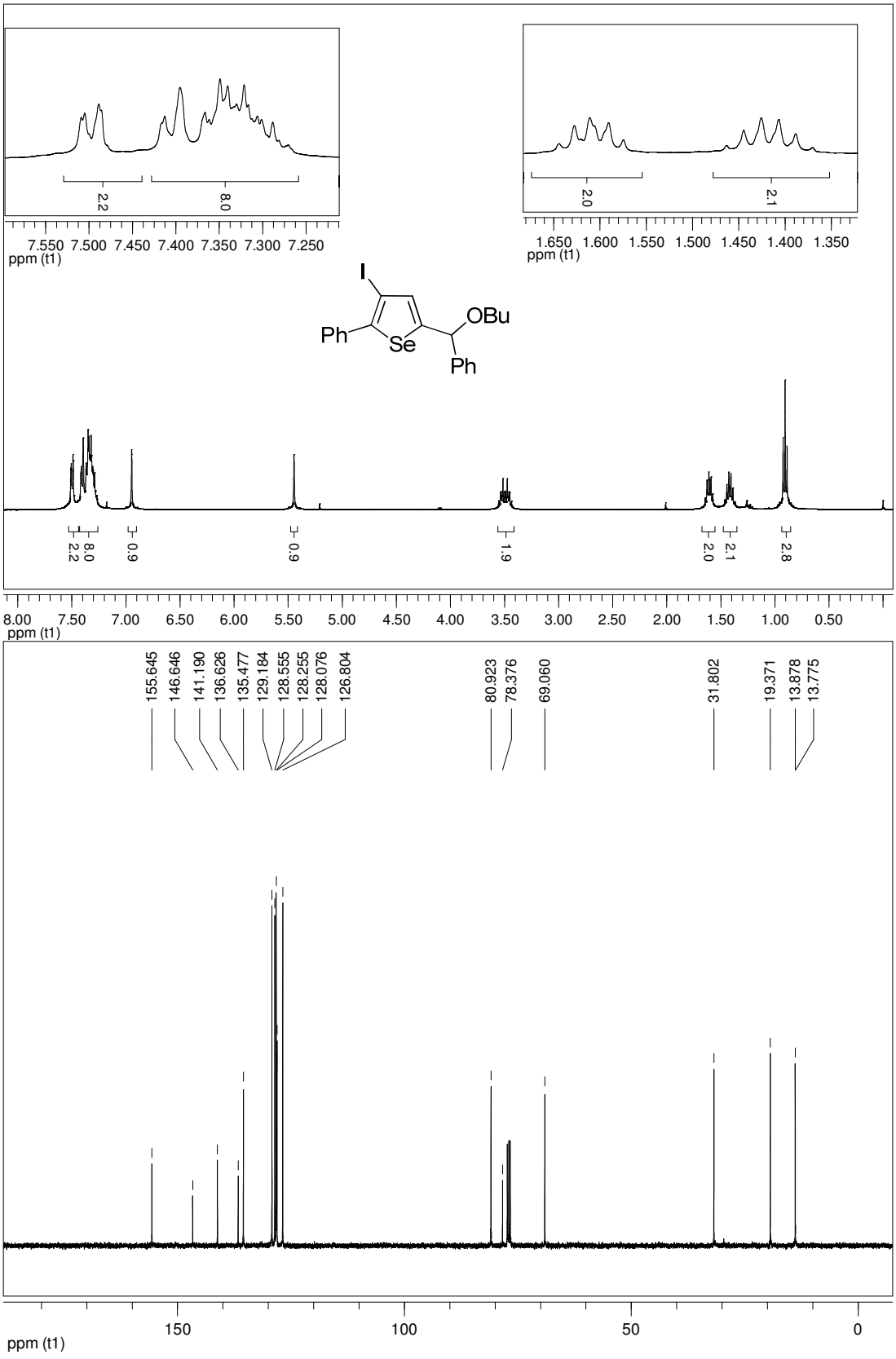

HO
Cl
SeBu
Cl


1.48
6.81
0.73
1.55
2.27
2.18
3.00
f1 (ppm)

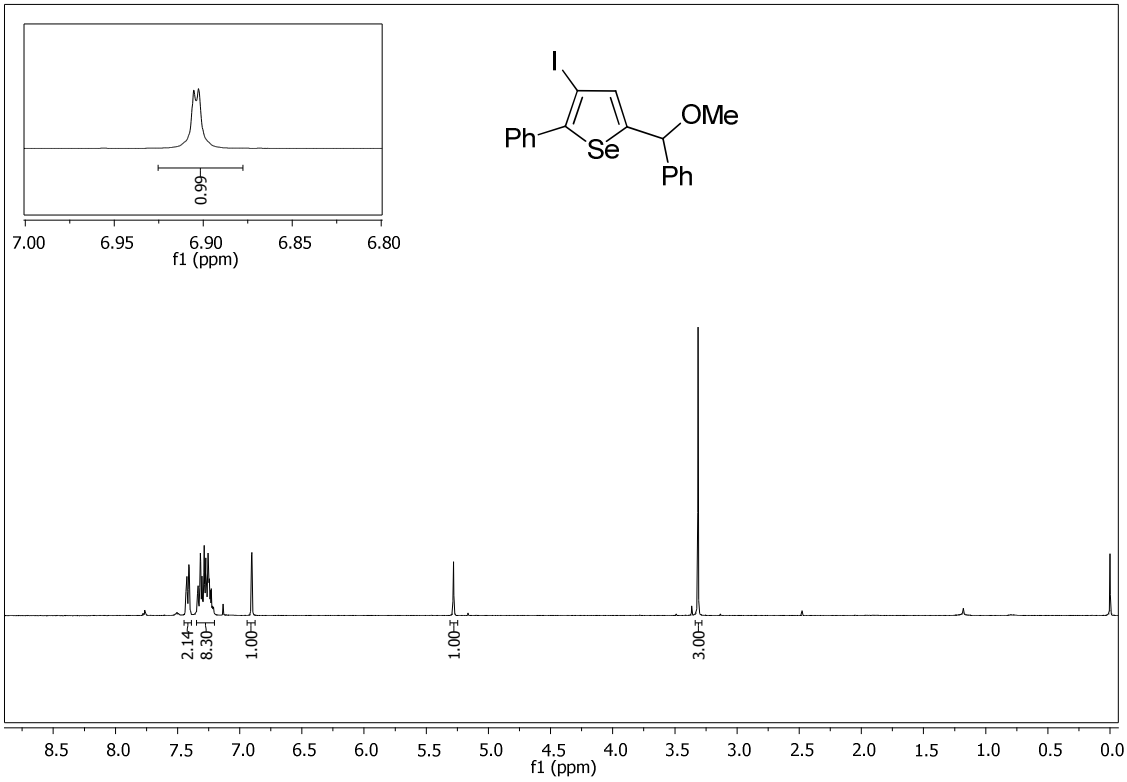

134.8
134.8
133.7
133.6
133.0
132.9
130.6
128.7
128.3
120.8
88.9
85.6
68.6
32.3
27.2
22.8
13.4
f1 (ppm)

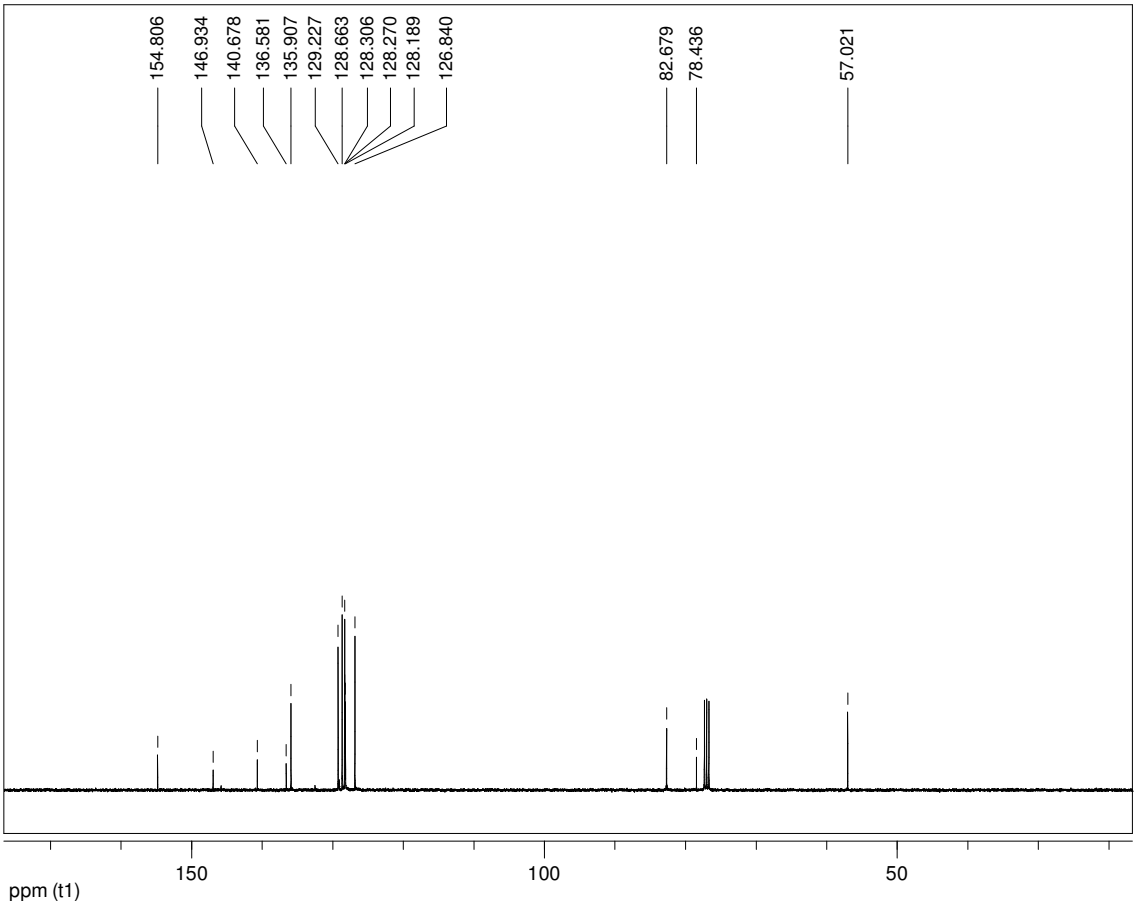

I
Ph
Se
OEt
Ph
10.71
0.94
0.81
1.94
3.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

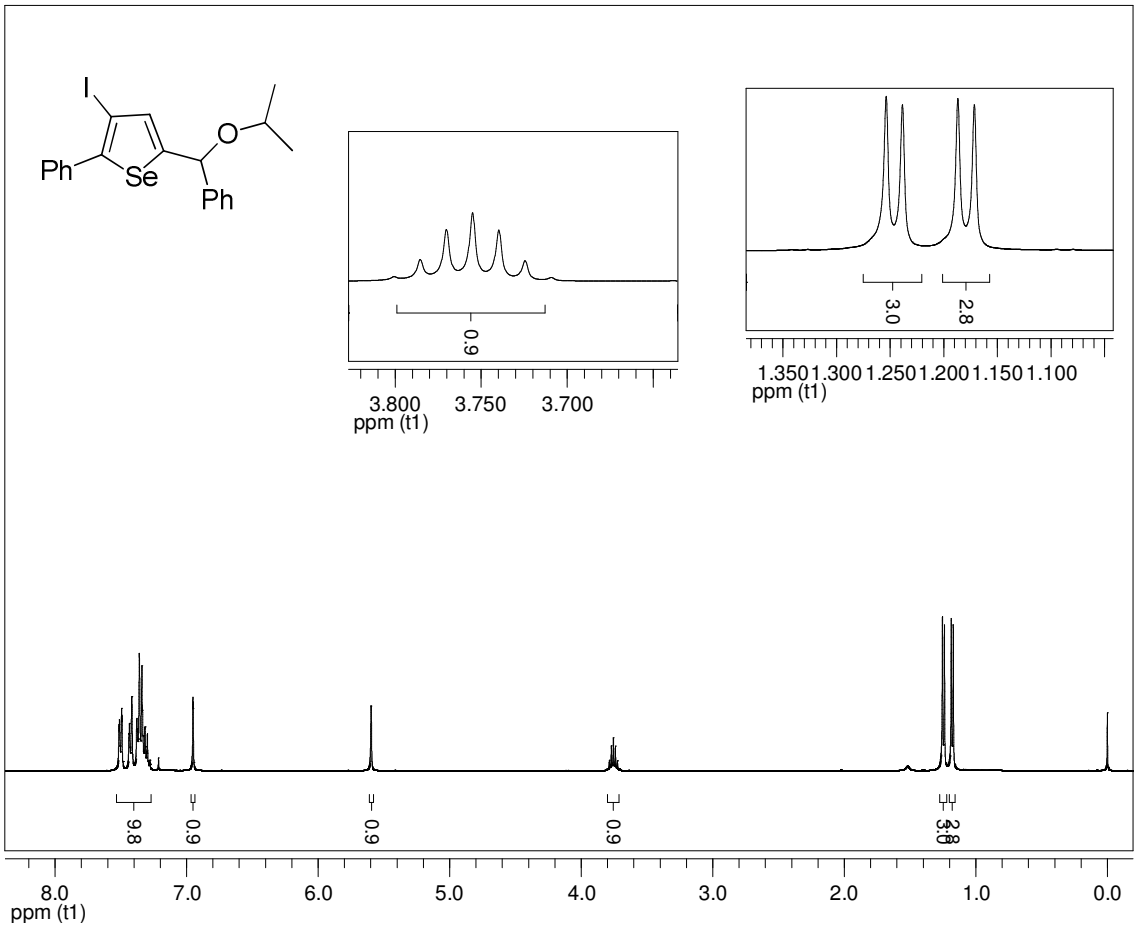

155.586
146.840
141.325
136.735
135.731
129.303
128.694
128.375
128.297
128.209
126.878
80.838
78.500
64.851
15.305
150
100
50
ppm (t1)

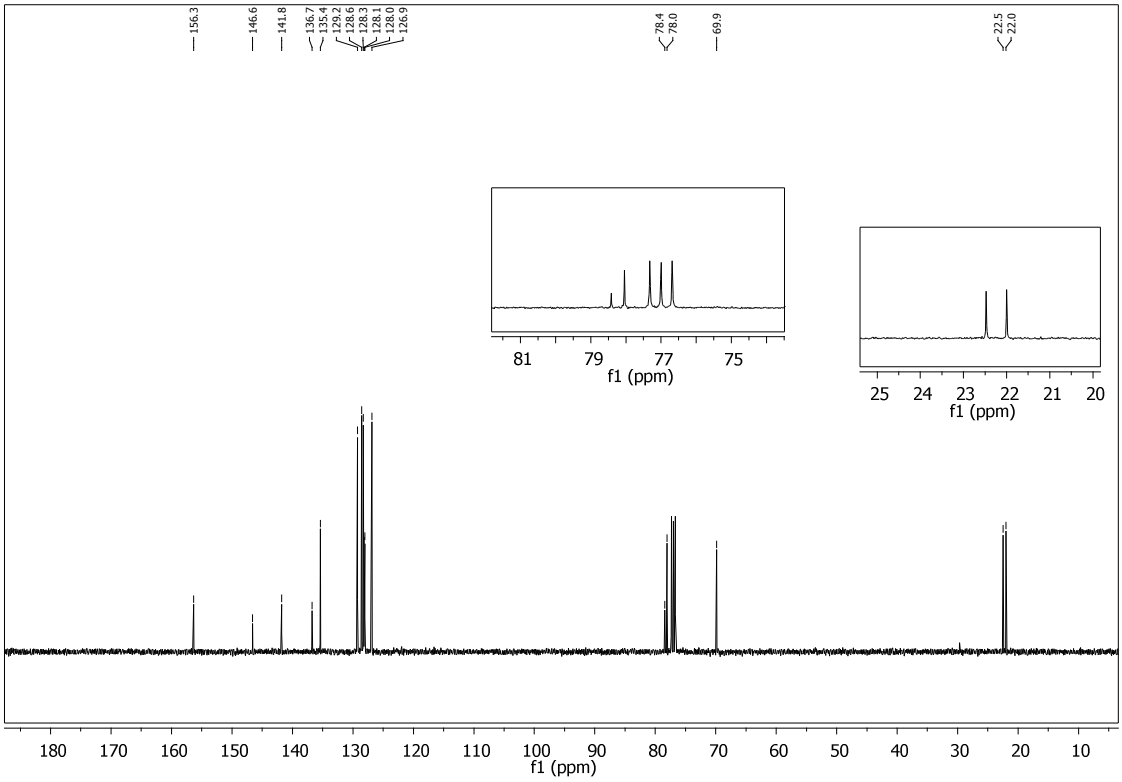

2.2
8.0
7.550 7.500 7.450 7.400 7.350 7.300 7.250
ppm (t1)
2.0
2.1
1.650 1.600 1.550 1.500 1.450 1.400 1.350
ppm (t1)
I
Ph
Se
OBu
Ph
2.2
8.0
0.9
0.9
1.9
2.0
2.1
2.8
8.00 7.50 7.00 6.50 6.00 5.50 5.00 4.50 4.00 3.50 3.00 2.50 2.00 1.50 1.00 0.50
ppm (t1)

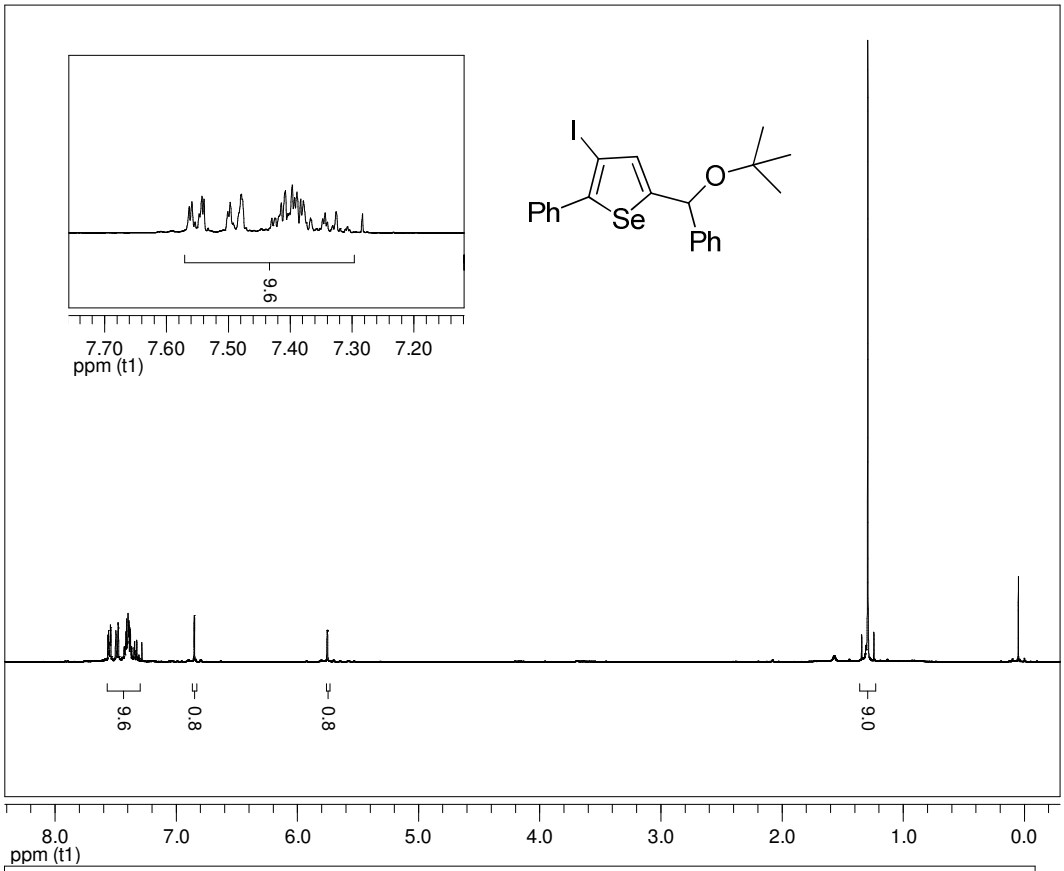
155.645
146.646
141.190
136.626
135.477
129.184
128.555
128.255
128.076
126.804
80.923
78.376
69.060
31.802
19.371
13.878
13.775
150
100
50
0
ppm (t1)

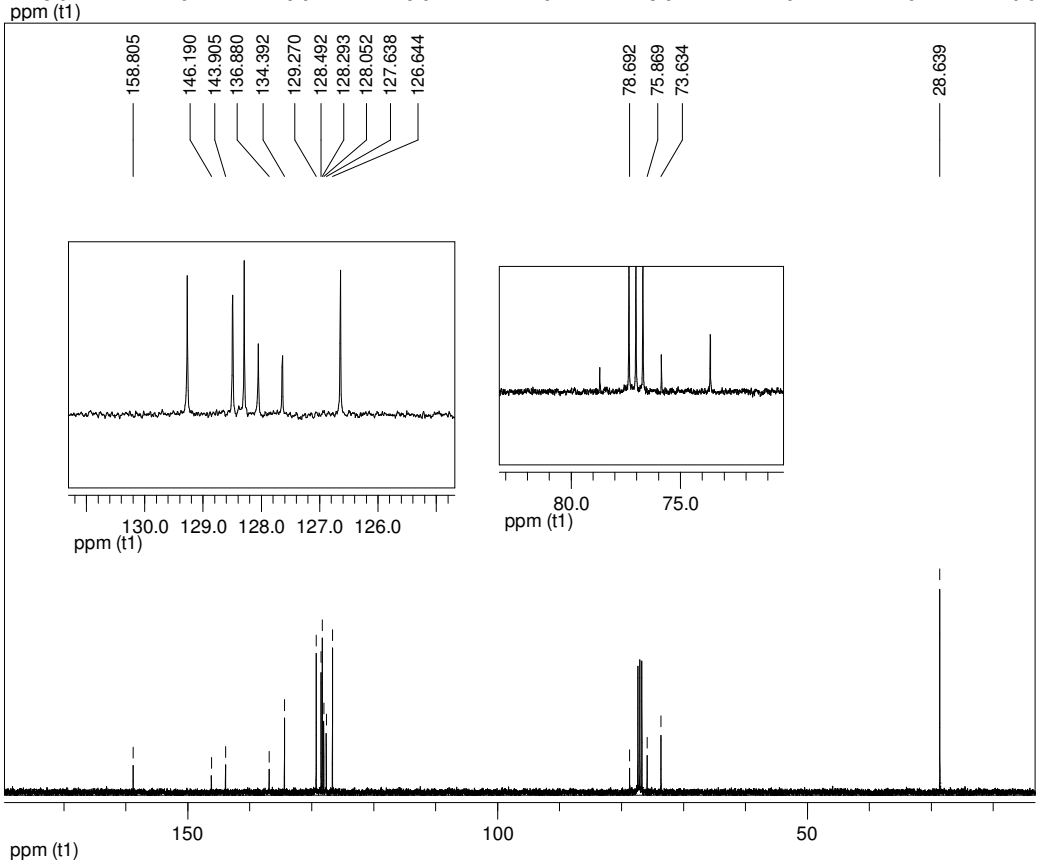

I
OMe
Ph
Se
Ph
0.99
7.00
6.95
6.90
6.85
6.80
f1 (ppm)
2.14
8.30
1.00
1.00
3.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

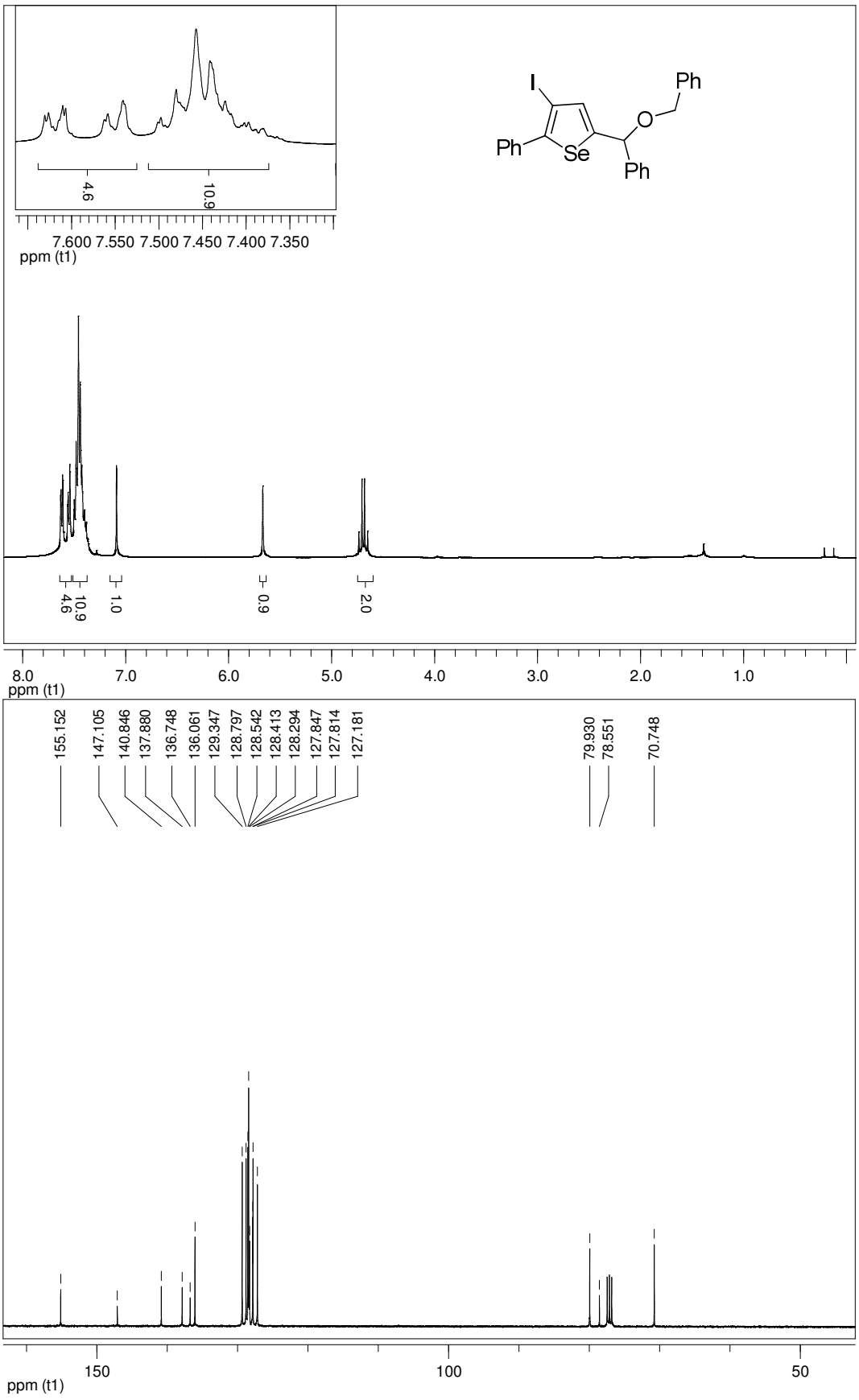

154.806
146.934
140.678
136.581
135.907
129.227
128.663
128.306
128.270
128.189
126.840
82.679
78.436
57.021
150
100
50
ppm (t1)

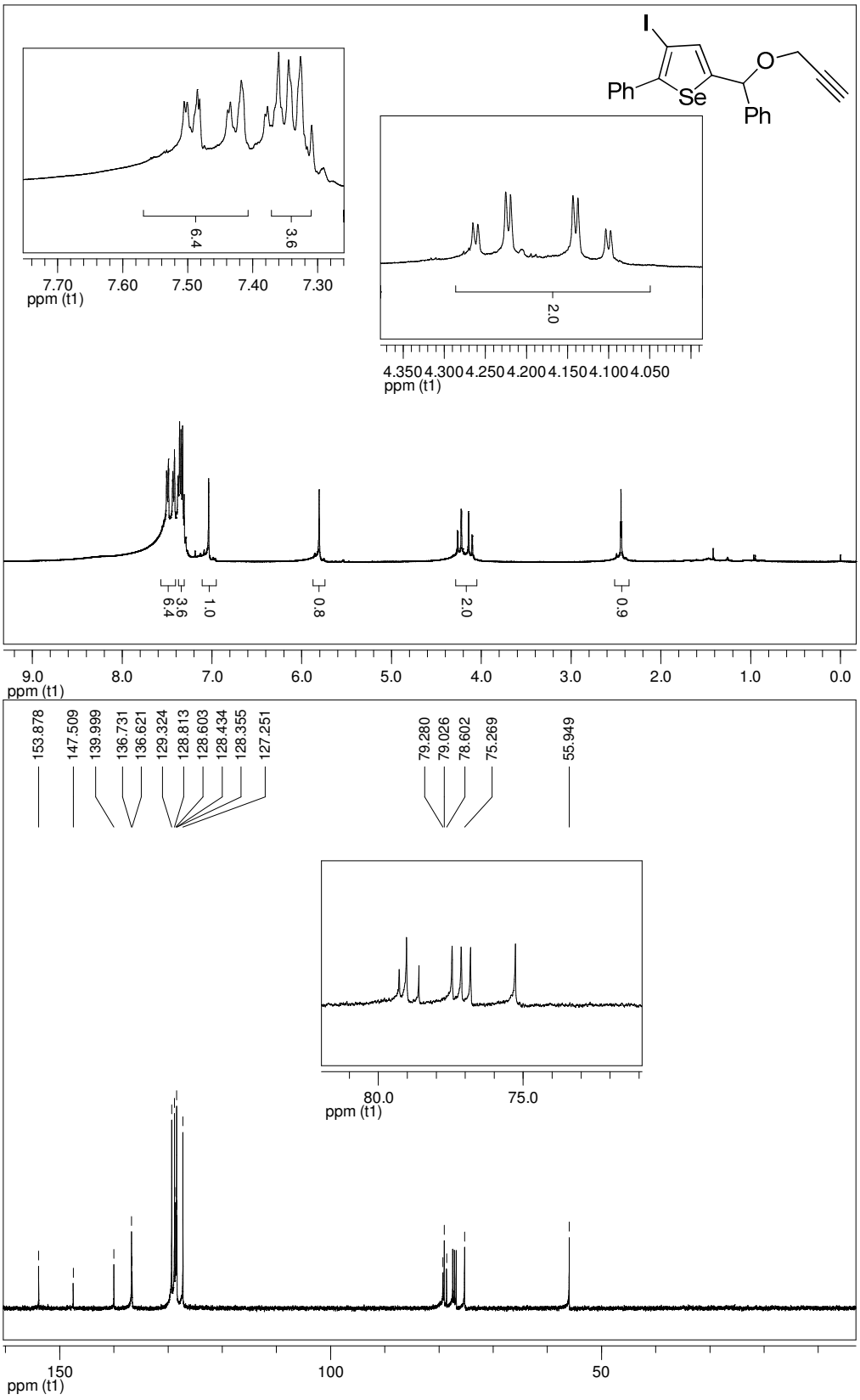

I
Ph
Se
O
Ph
0.9
3.800
3.750
3.700
ppm (t1)
3.0
2.8
1.350
1.300
1.250
1.200
1.150
1.100
ppm (t1)
2.8
0.9
0.9
0.9
3.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)

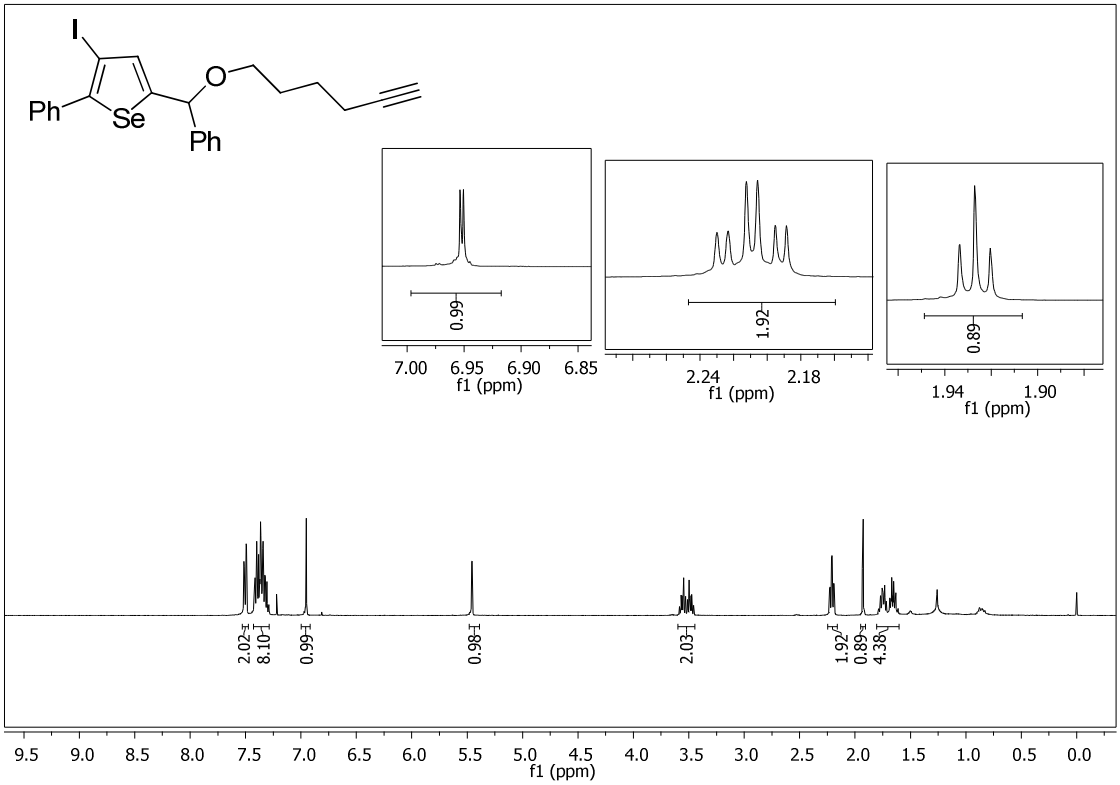

156.3
146.6
141.8
136.7
135.4
129.2
128.6
128.3
128.1
128.0
126.9
78.4
78.0
69.9
22.5
22.0
81
79
77
75
f1 (ppm)
25
24
23
22
21
20
f1 (ppm)
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

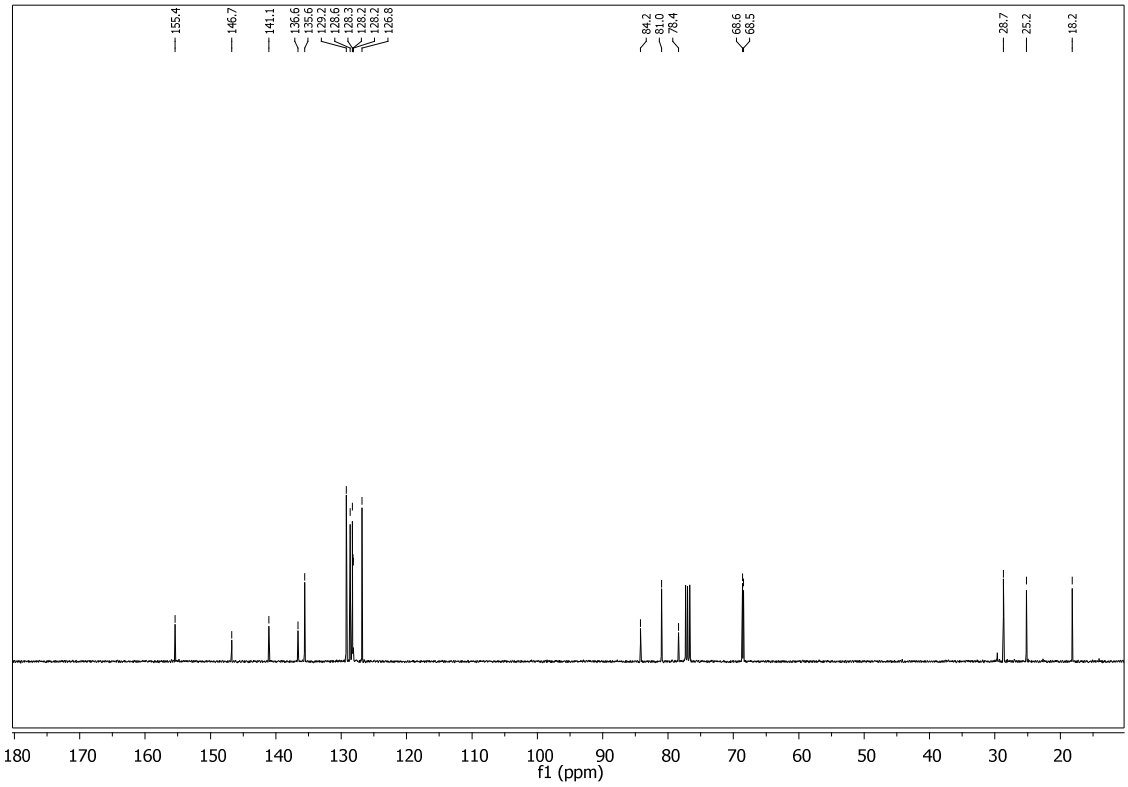

I
Ph
Se
O
Ph
9.6
7.70 7.60 7.50 7.40 7.30 7.20
ppm (t1)
9.6
0.8
0.8
9.0
8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0
ppm (t1)

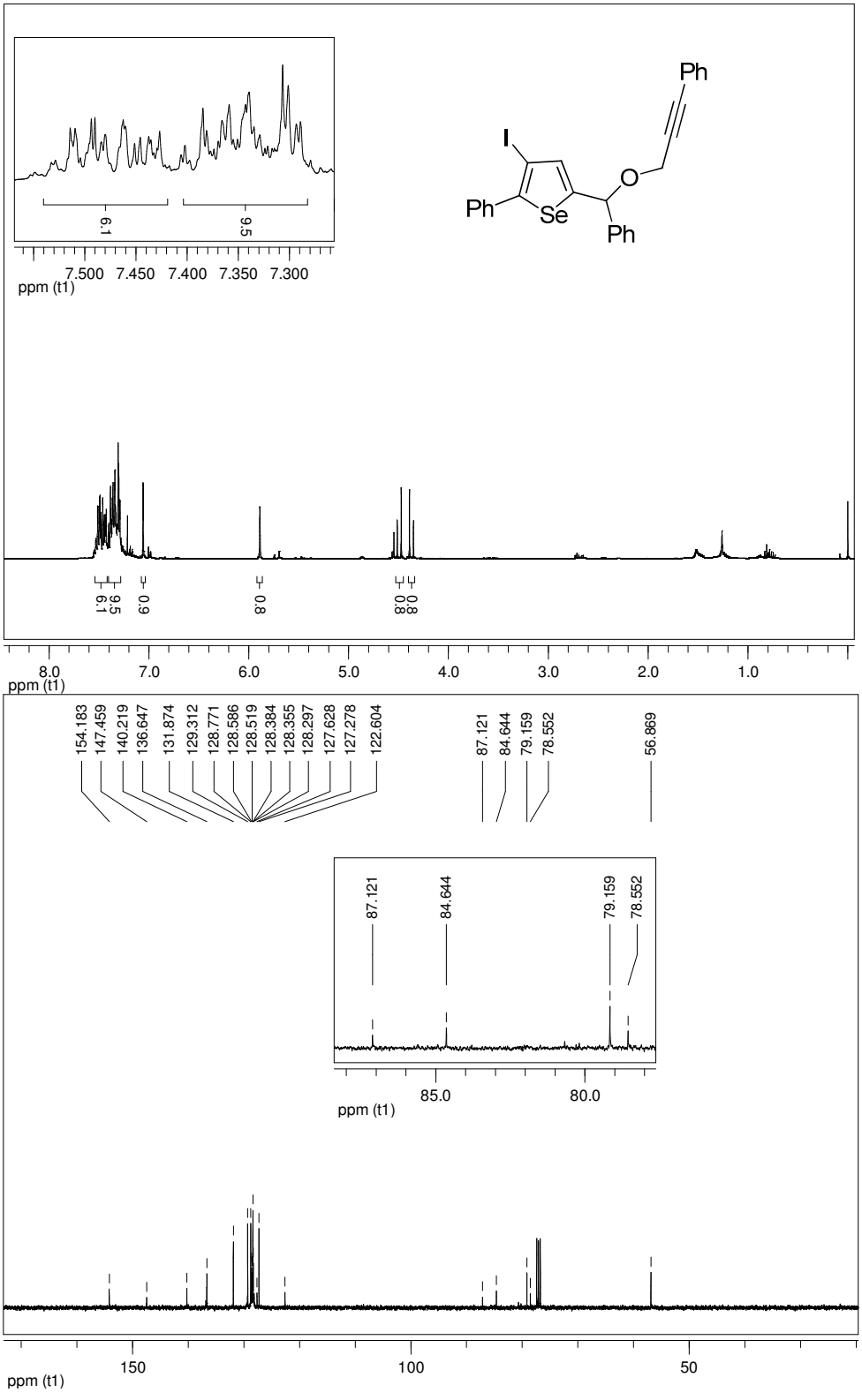

158.805
146.190
143.905
136.880
134.392
129.270
128.492
128.293
128.052
127.638
126.644
78.692
75.869
73.634
28.639
130.0 129.0 128.0 127.0 126.0
ppm (t1)
80.0 75.0
ppm (t1)
150 100 50
ppm (t1)

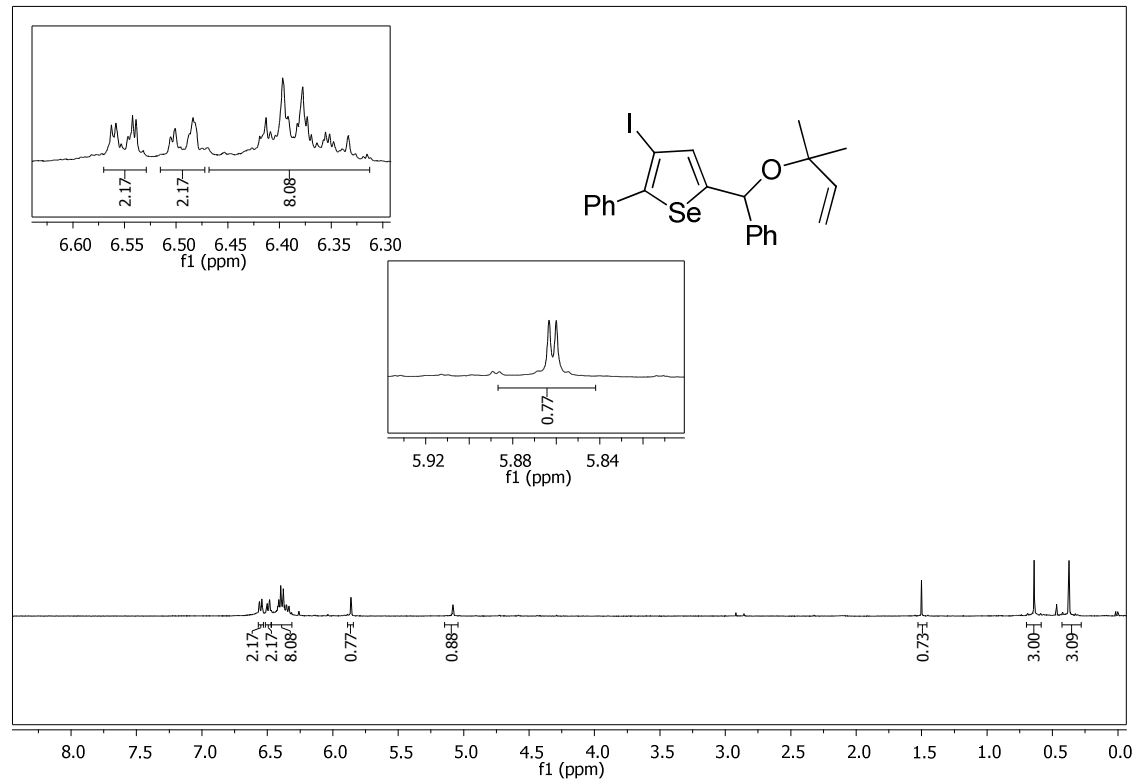

I
Ph
O
Ph
Se
Ph
4.6
10.9
7.600 7.550 7.500 7.450 7.400 7.350
ppm (t1)
4.6
10.9
1.0
6.0
2.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm (t1)
155.152
147.105
140.846
137.880
136.748
136.061
129.347
128.797
128.542
128.413
128.294
127.847
127.814
127.181
79.930
78.551
70.748
150
100
50
ppm (t1)

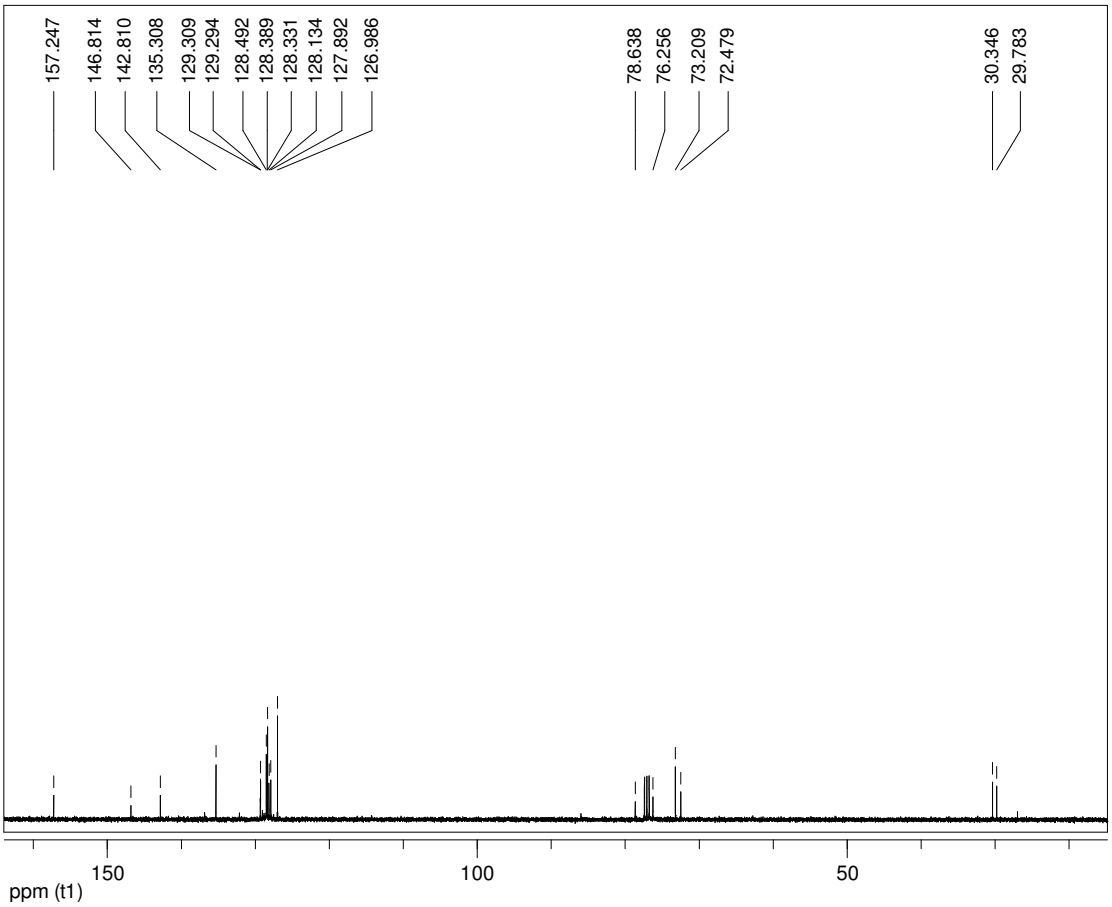

I
Ph
Se
O
Ph
6.4
3.6
7.70
7.60
7.50
7.40
7.30
ppm (t1)
2.0
4.350
4.300
4.250
4.200
4.150
4.100
4.050
ppm (t1)
6.4
3.6
1.0
0.8
2.0
0.9
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)
153.878
147.509
139.999
136.731
136.621
129.324
128.813
128.603
128.434
128.355
127.251
79.280
79.026
78.602
75.269
55.949
80.0
75.0
ppm (t1)
150
100
50
ppm (t1)

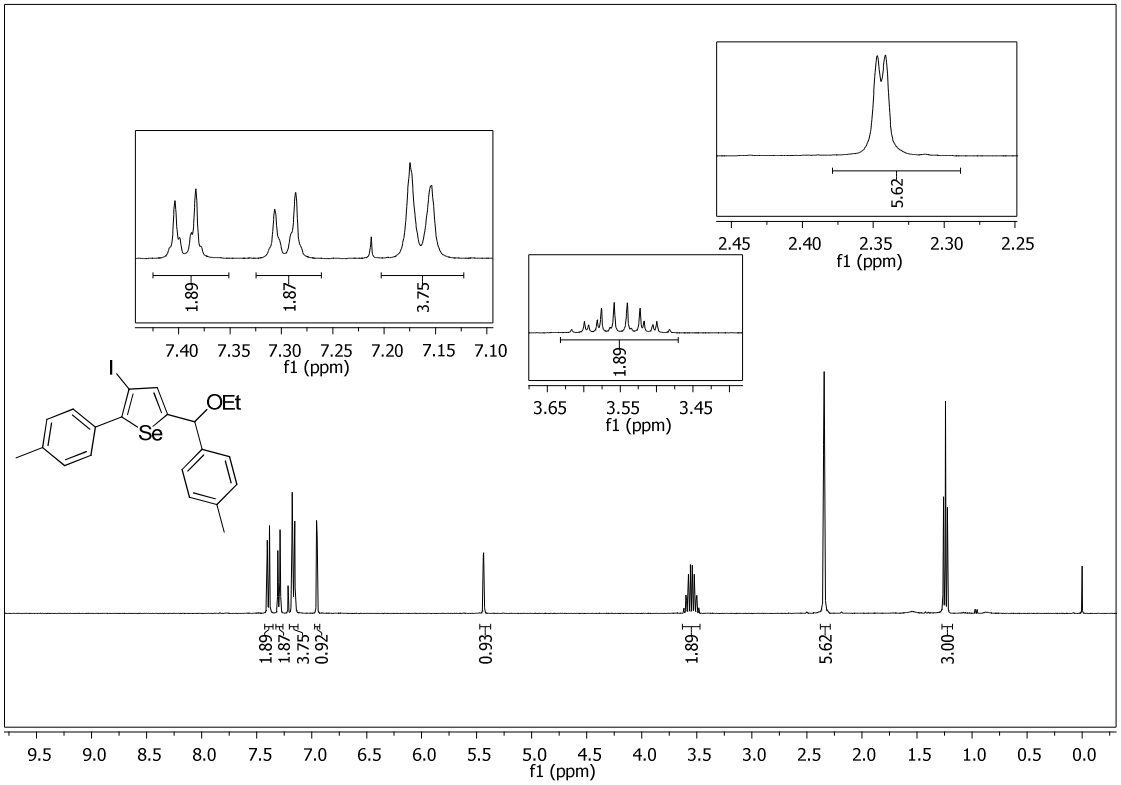

I
Ph
Se
O
Ph
0.99
1.92
0.89
7.00 6.95 6.90 6.85
f1 (ppm)
2.24 2.18
f1 (ppm)
1.94 1.90
f1 (ppm)
2.02
8.10
0.99
0.98
2.03
1.92
0.89
4.38
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

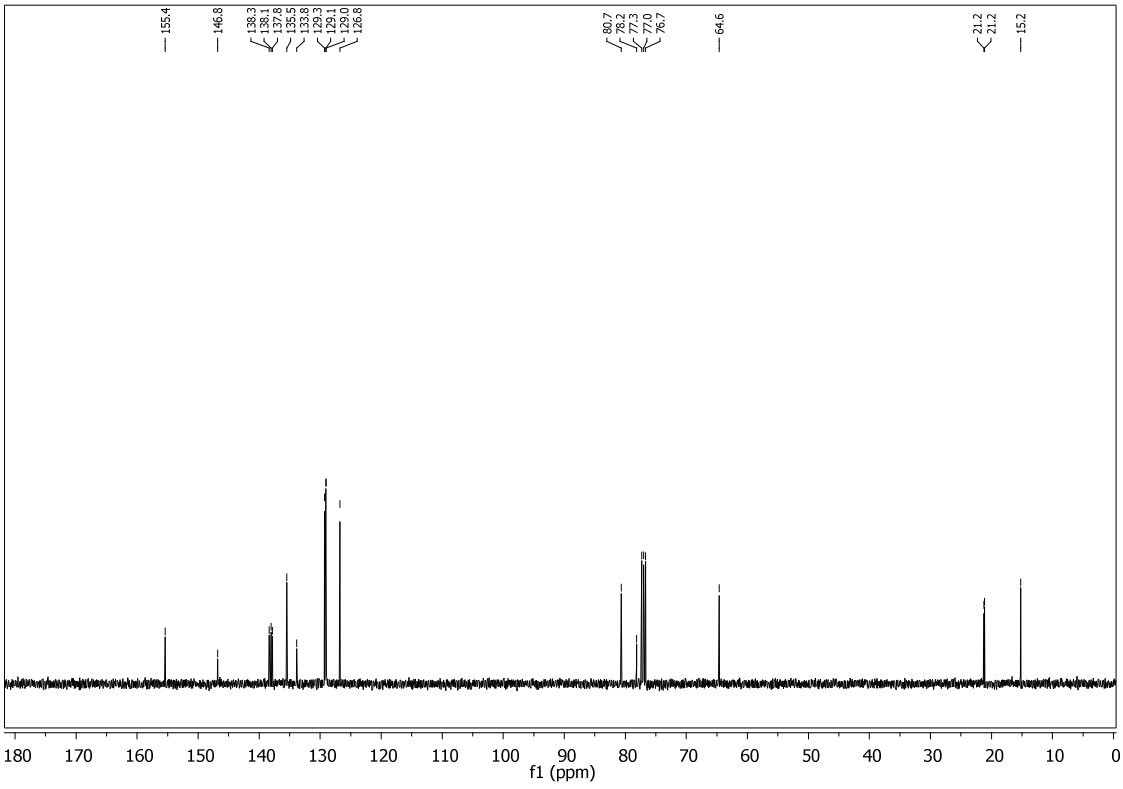

155.4
146.7
141.1
136.6
135.6
129.2
128.6
128.3
128.2
128.2
126.8
84.2
81.0
78.4
68.6
68.5
28.7
25.2
18.2
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20
f1 (ppm)

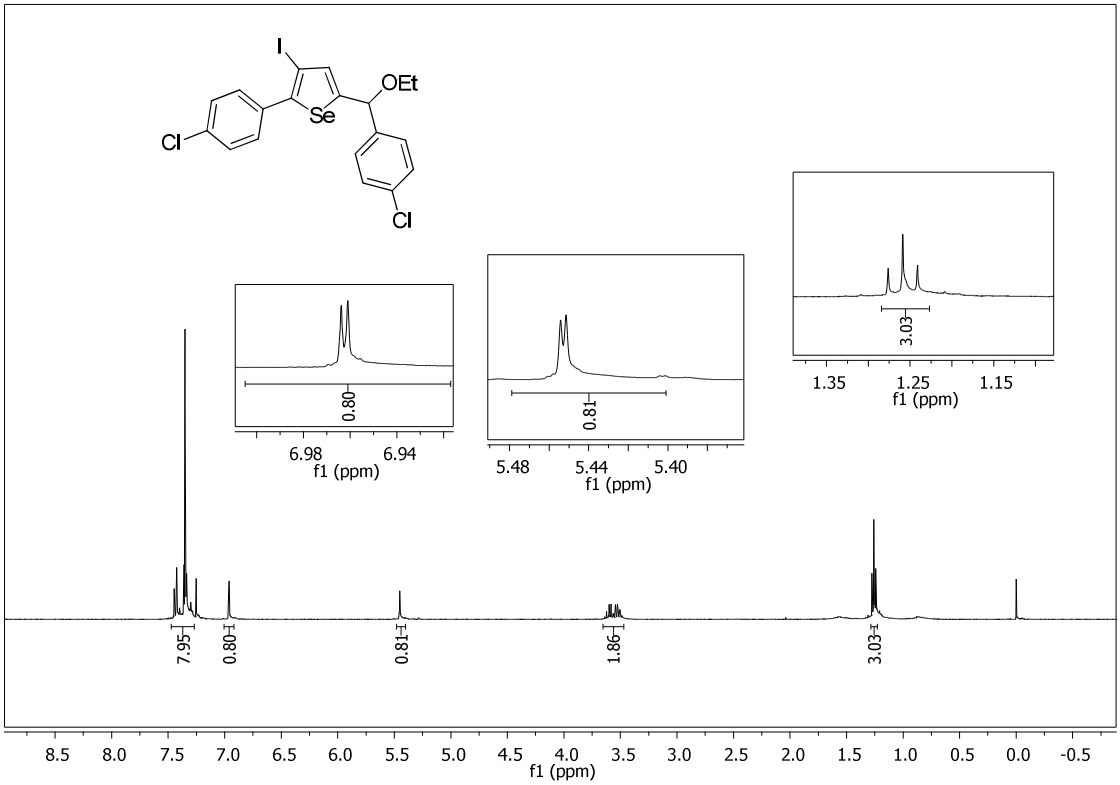

Ph
I
O
Ph
Se
Ph
6.1
9.5
7.500 7.450 7.400 7.350 7.300
ppm (t1)
6.1
9.5
6.0
0.9
0.8
0.8
0.8
8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0
ppm (t1)
154.183
147.459
140.219
136.647
131.874
129.312
128.771
128.586
128.519
128.384
128.355
128.297
127.628
127.278
122.604
87.121
84.644
79.159
78.552
56.869
87.121
84.644
79.159
78.552
85.0
80.0
ppm (t1)
150
100
50
ppm (t1)

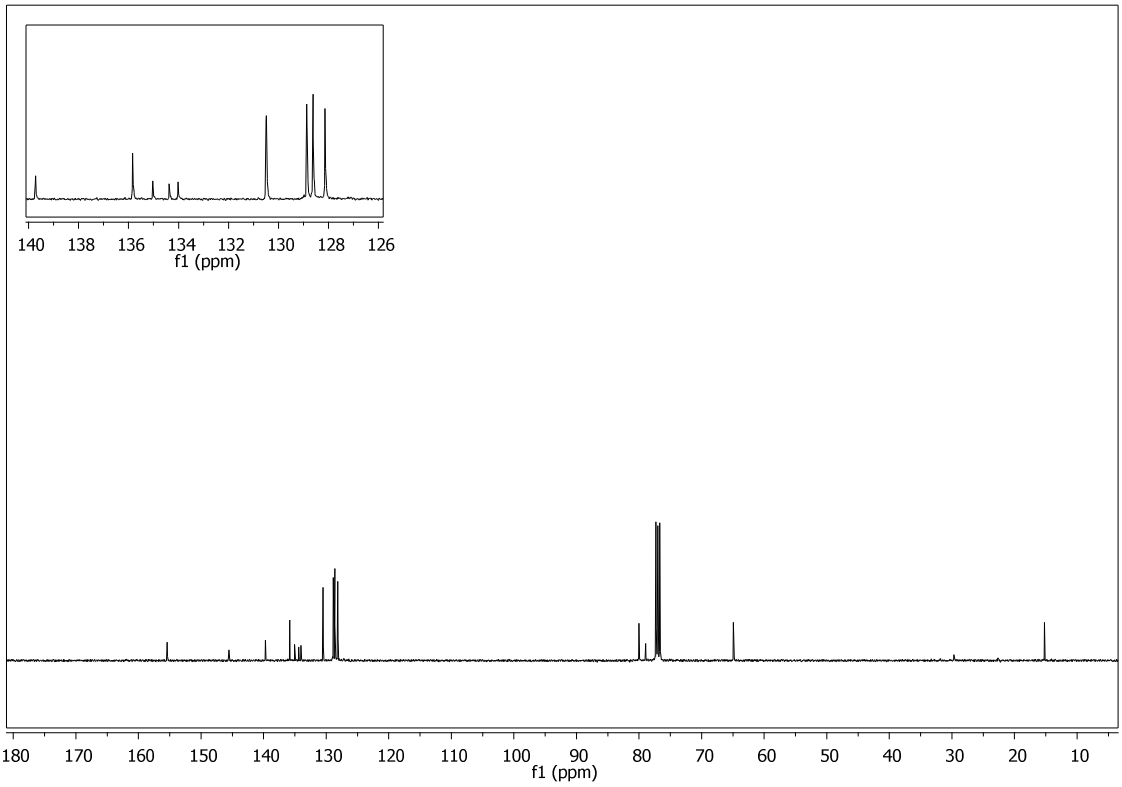

I
Ph
Se
O
Ph
2.17
2.17
8.08
6.60 6.55 6.50 6.45 6.40 6.35 6.30
f1 (ppm)
0.77
5.92 5.88 5.84
f1 (ppm)
2.17
2.17
8.08
0.77
0.88
0.73
3.00
3.09
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

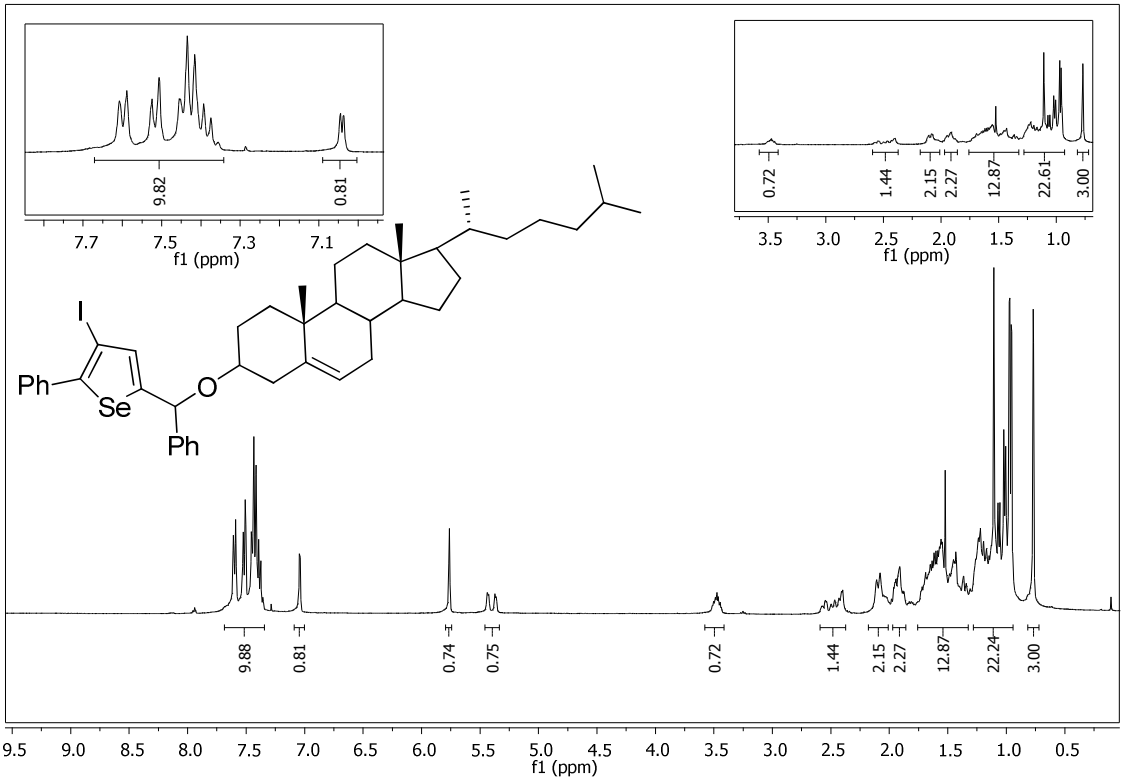

157.247
146.814
142.810
135.308
129.309
129.294
128.492
128.389
128.331
128.134
127.892
126.986
78.638
76.256
73.209
72.479
30.346
29.783
150
100
50
ppm (t1)

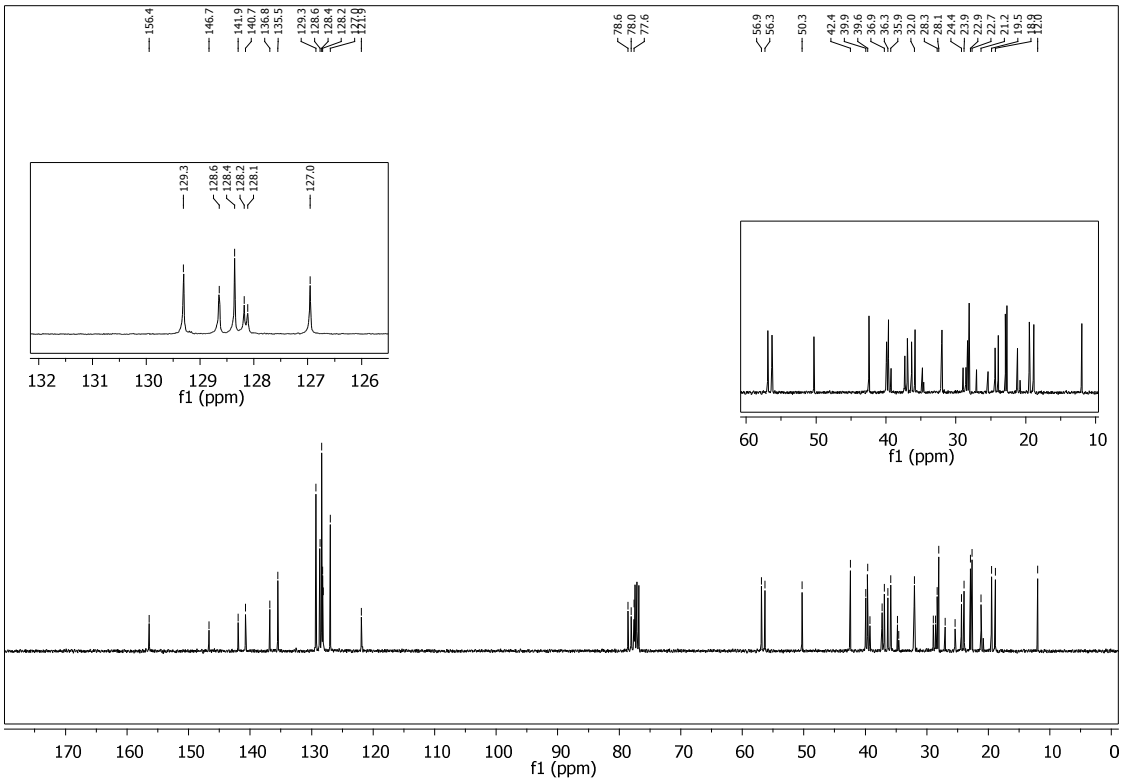

I
OEt
Se
1.89
1.87
3.75
0.92
0.93
1.89
5.62
3.00
f1 (ppm)

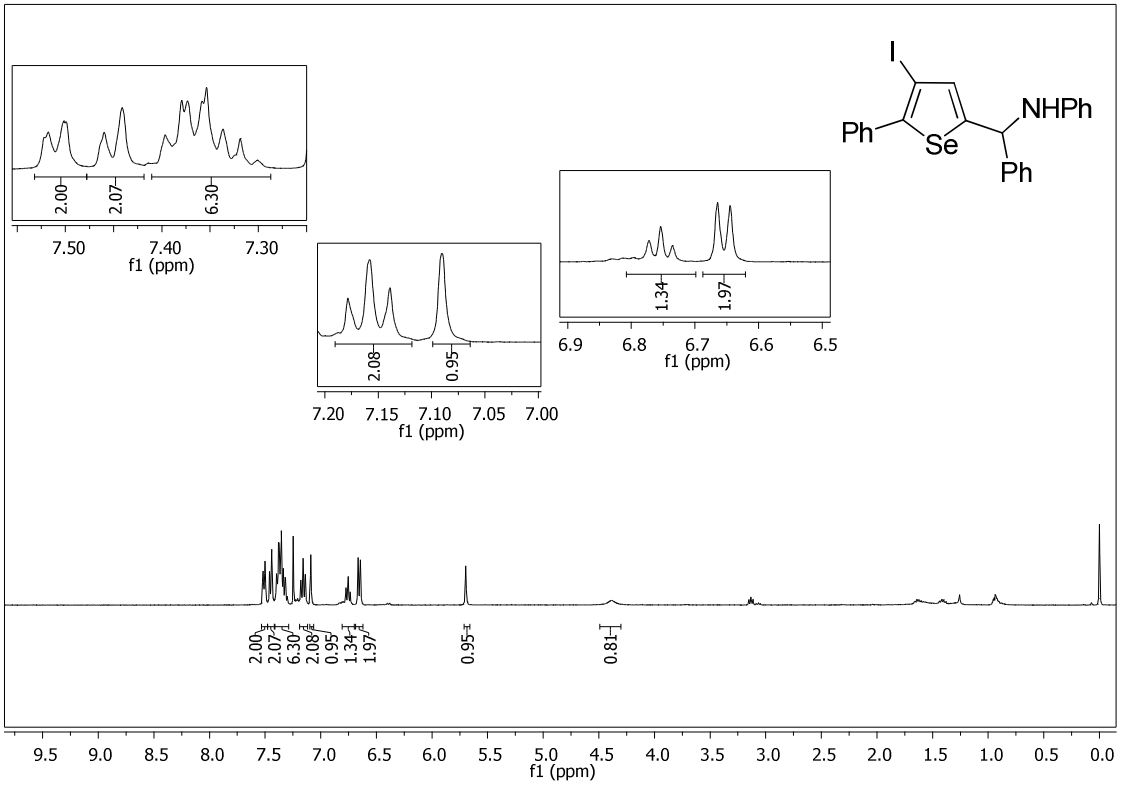

155.4
146.8
138.3
138.1
137.8
135.5
133.8
129.3
129.1
129.0
126.8
80.7
78.2
77.3
77.0
76.7
64.6
21.2
21.2
15.2
f1 (ppm)

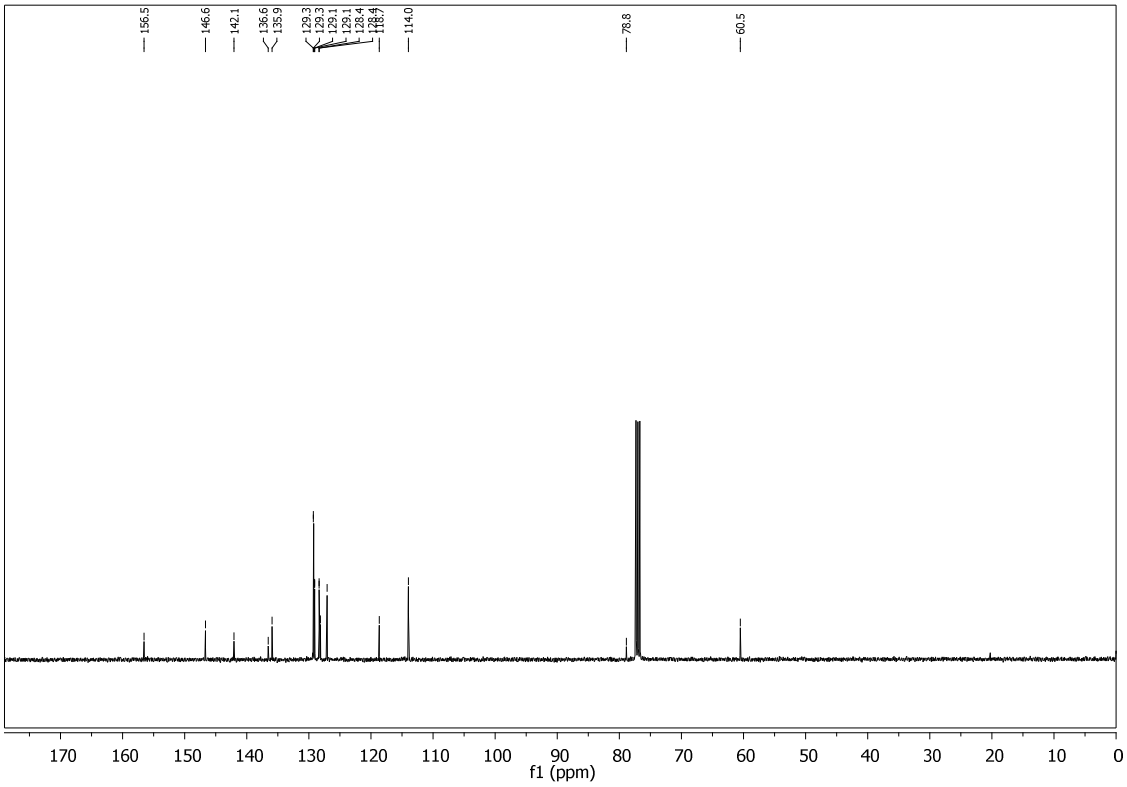

I
OEt
Se
Cl
Cl
0.80
6.98
6.94
f1 (ppm)
0.81
5.48
5.44
5.40
f1 (ppm)
3.03
1.35
1.25
1.15
f1 (ppm)
7.95
0.80
0.81
1.86
3.03
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

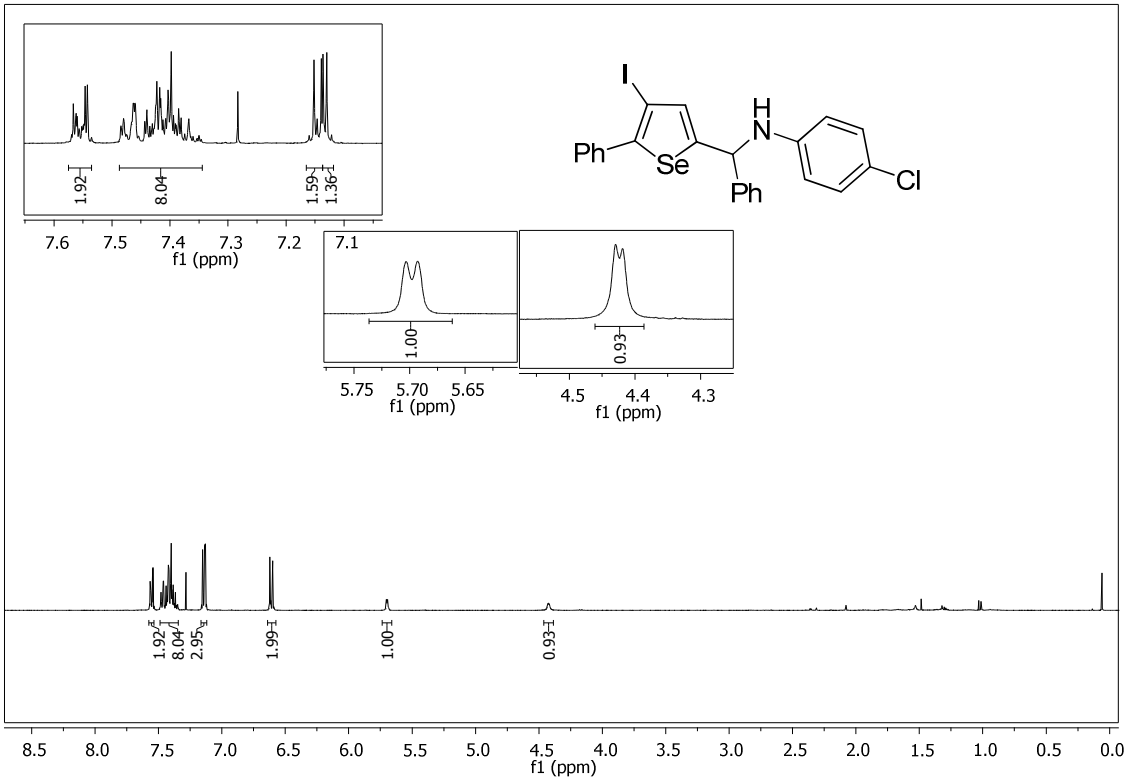

140 138 136 134 132 130 128 126
f1 (ppm)
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

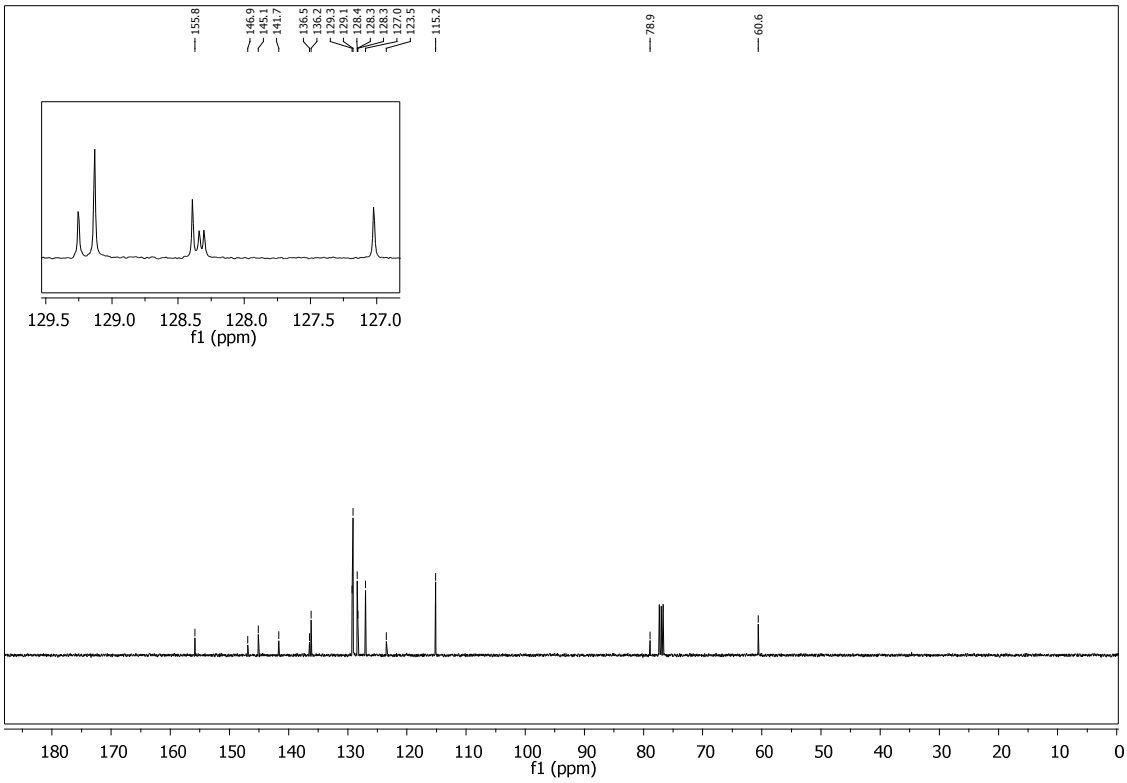

I
Ph
Se
O
Ph
9.82
0.81
7.7
7.5
7.3
7.1
f1 (ppm)
0.72
1.44
2.15
2.27
12.87
22.61
3.00
3.5
3.0
2.5
2.0
1.5
1.0
f1 (ppm)
9.88
0.81
0.74
0.75
0.72
1.44
2.15
2.27
12.87
22.24
3.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

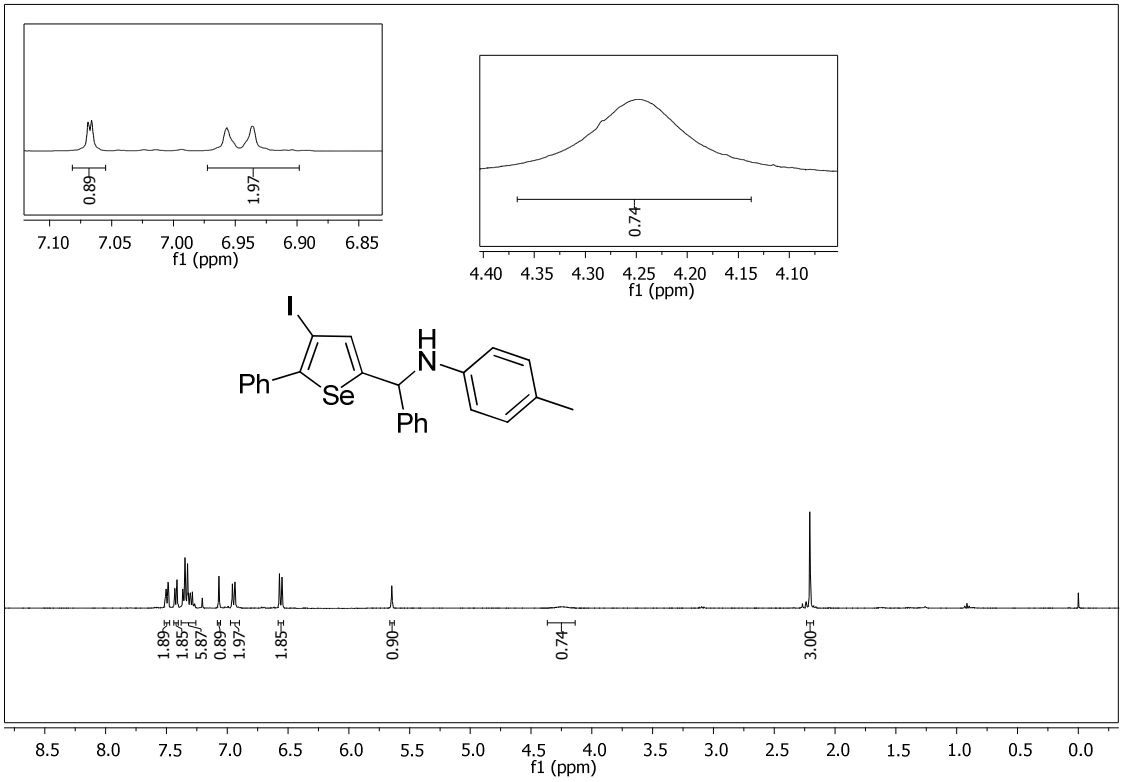

156.4
146.7
141.9
140.7
136.8
135.5
129.3
128.6
128.4
128.2
128.1
127.0
78.6
78.0
77.6
56.9
56.3
50.3
42.4
39.9
39.6
36.9
36.3
35.9
32.0
28.3
28.1
24.4
23.9
22.9
22.7
21.2
19.5
18.8
18.0
132
131
130
129
128
127
126
f1 (ppm)
60
50
40
30
20
10
f1 (ppm)
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

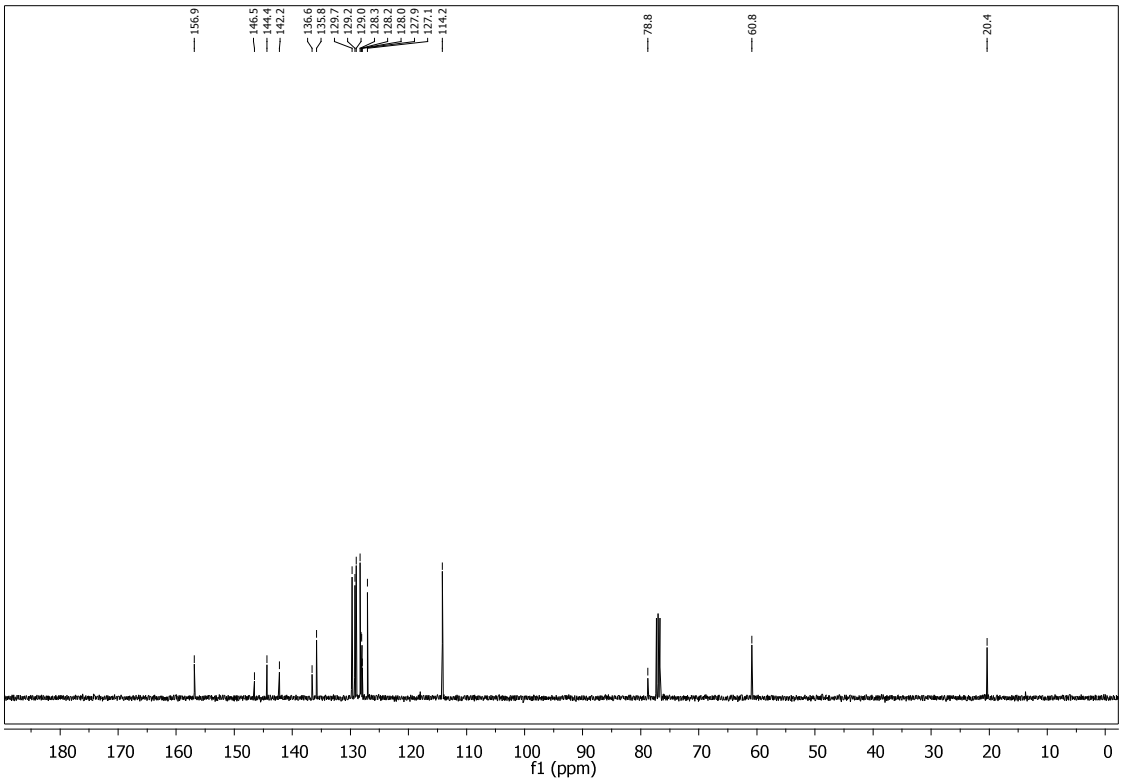

I
NHPh
Ph
Se
Ph
2.00
2.07
6.30
7.50
7.40
7.30
f1 (ppm)
2.08
0.95
7.20
7.15
7.10
7.05
7.00
f1 (ppm)
1.34
1.97
6.9
6.8
6.7
6.6
6.5
f1 (ppm)
2.00
2.07
6.30
2.08
0.95
1.34
1.97
0.95
0.81
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

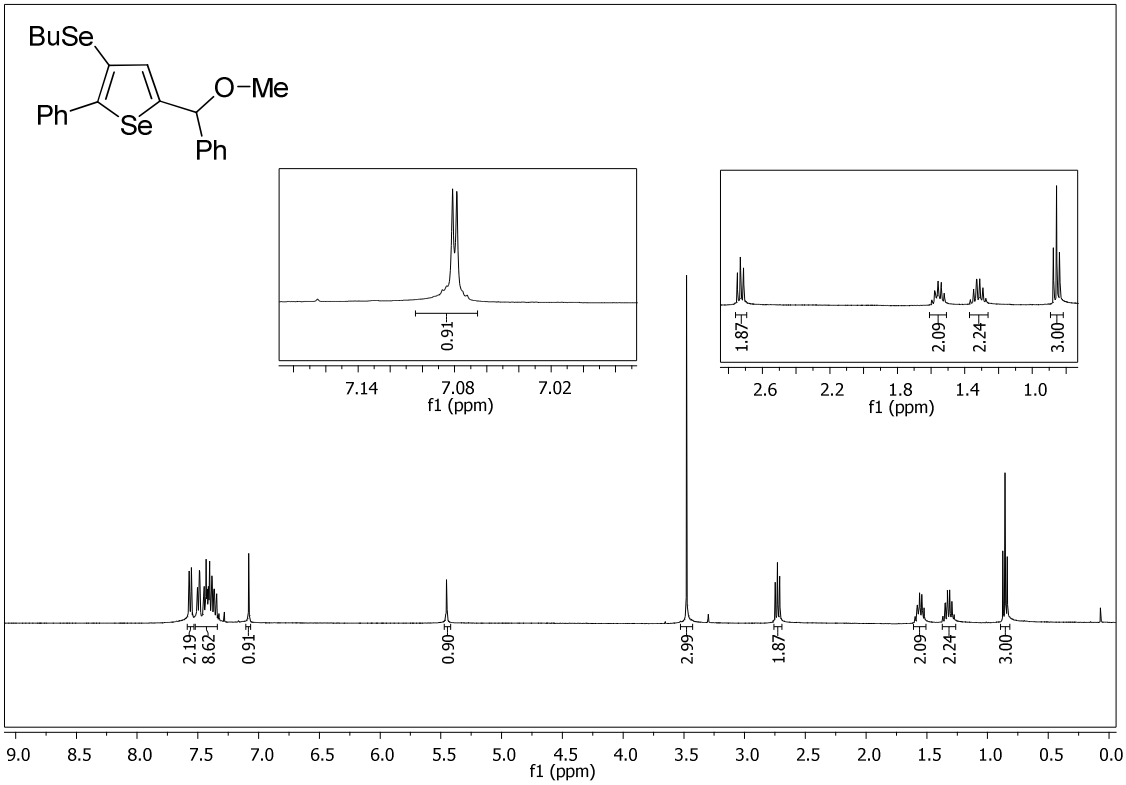

156.5
146.6
142.1
136.6
135.9
129.3
129.3
129.1
129.1
128.4
118.7
114.0
78.8
60.5
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

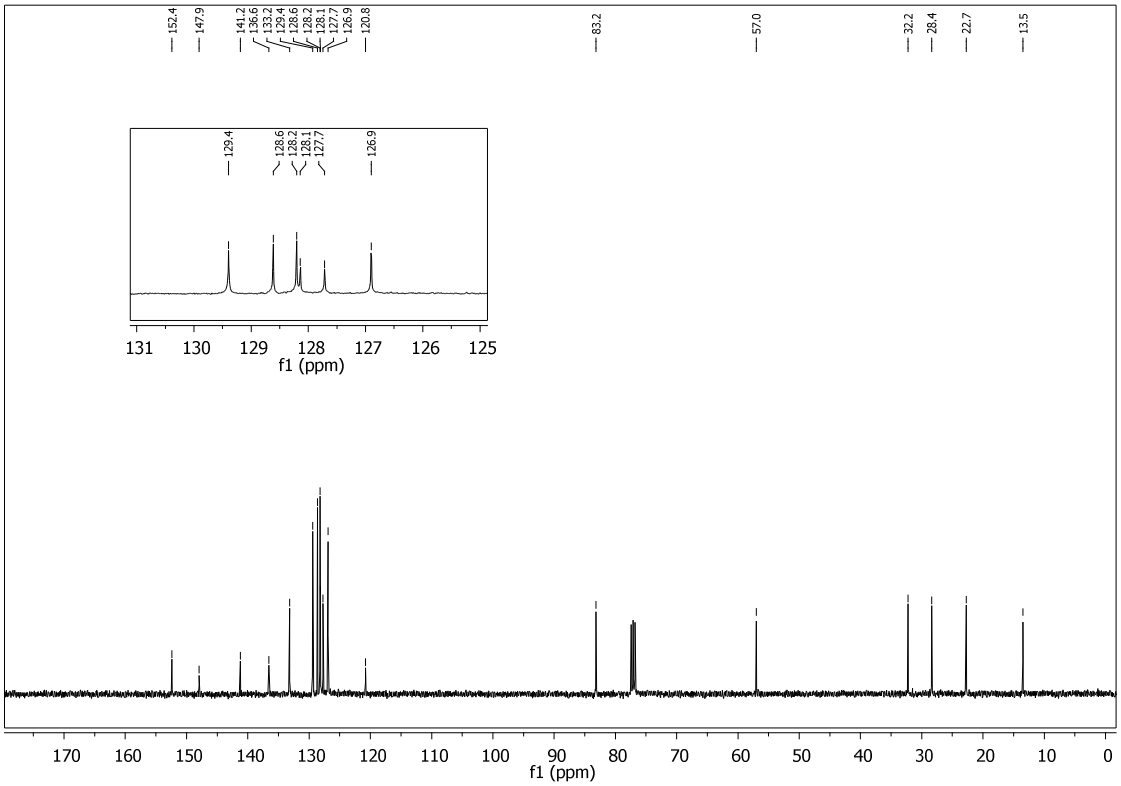

I
H
N
Ph
Se
Ph
Cl
1.92
8.04
1.59
1.36
7.6 7.5 7.4 7.3 7.2
f1 (ppm)
7.1
1.00
0.93
5.75 5.70 5.65
4.5 4.4 4.3
f1 (ppm)
1.92
8.04
2.95
1.99
1.00
0.93
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

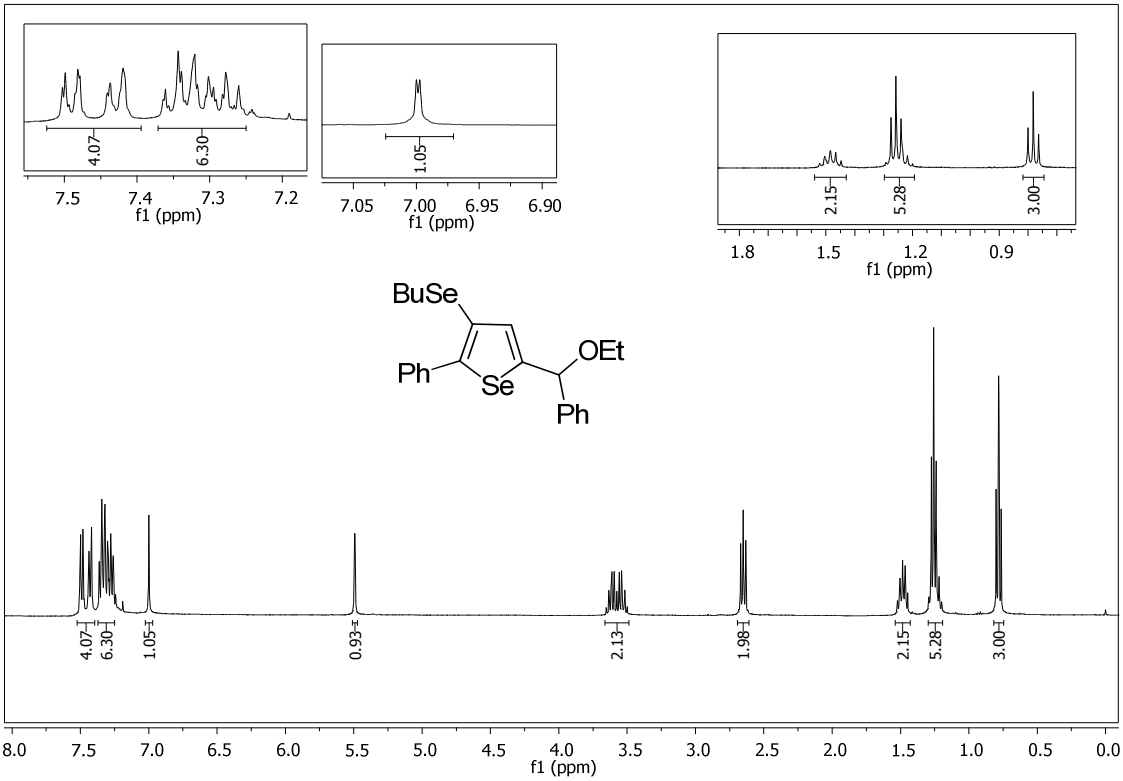

155.8
146.9
145.1
141.7
136.5
136.2
129.3
129.1
128.4
128.3
128.3
127.0
125.5
115.2
78.9
60.6
129.5 129.0 128.5 128.0 127.5 127.0
f1 (ppm)
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

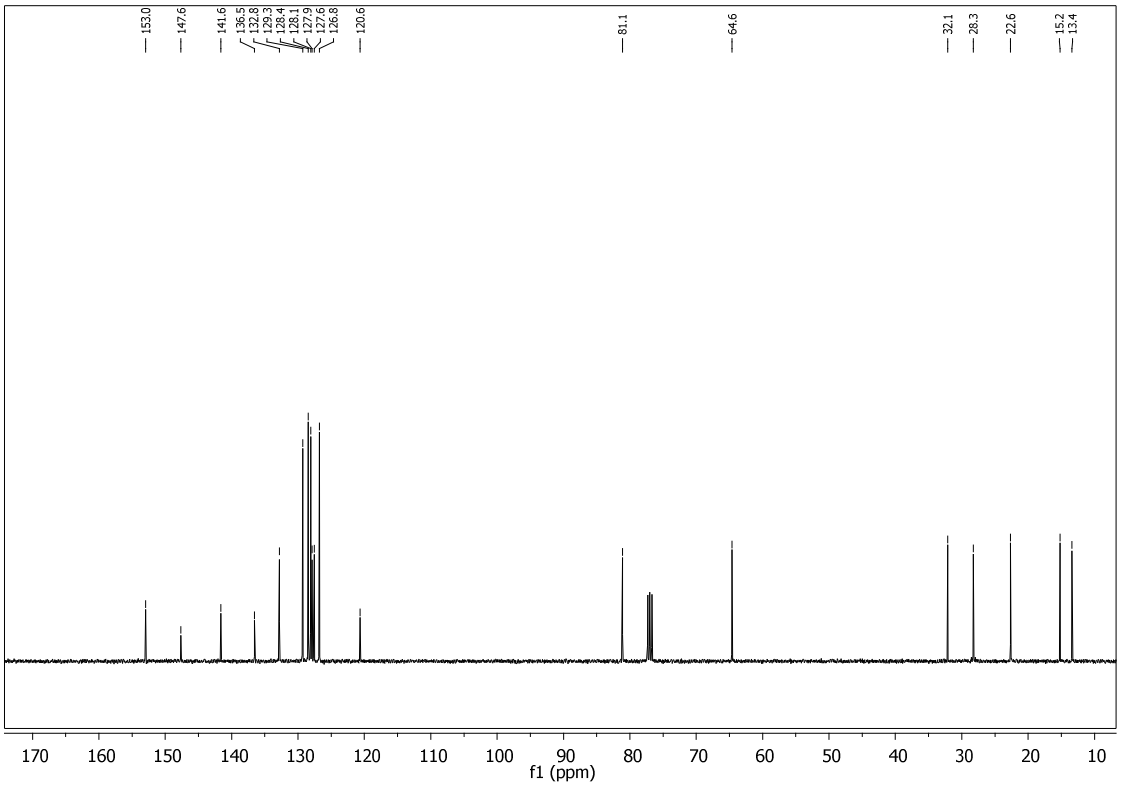

0.89
1.97
7.10 7.05 7.00 6.95 6.90 6.85
f1 (ppm)
0.74
4.40 4.35 4.30 4.25 4.20 4.15 4.10
f1 (ppm)
I
H
N
Ph
Se
Ph
1.89
1.85
5.87
0.89
1.97
1.85
0.90
0.74
3.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

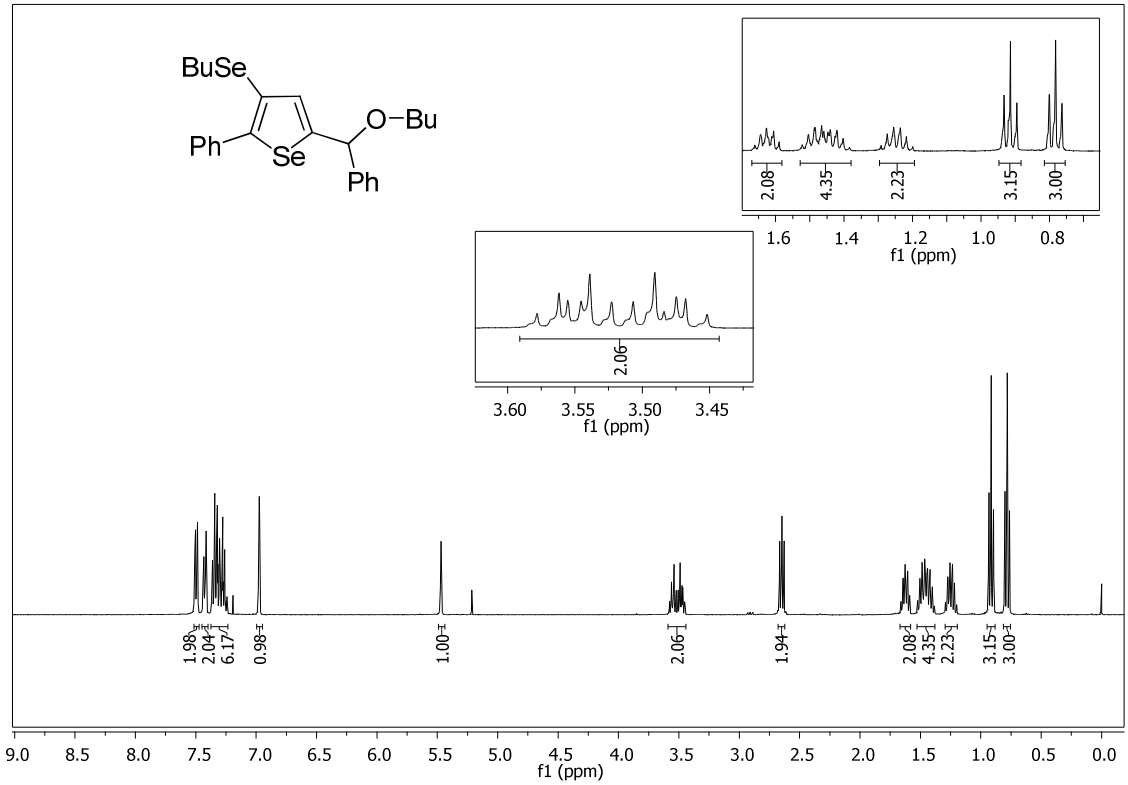

156.9
146.5
144.4
142.2
136.6
135.8
129.7
129.2
129.0
128.3
128.2
128.0
127.9
127.1
114.2
78.8
60.8
20.4
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

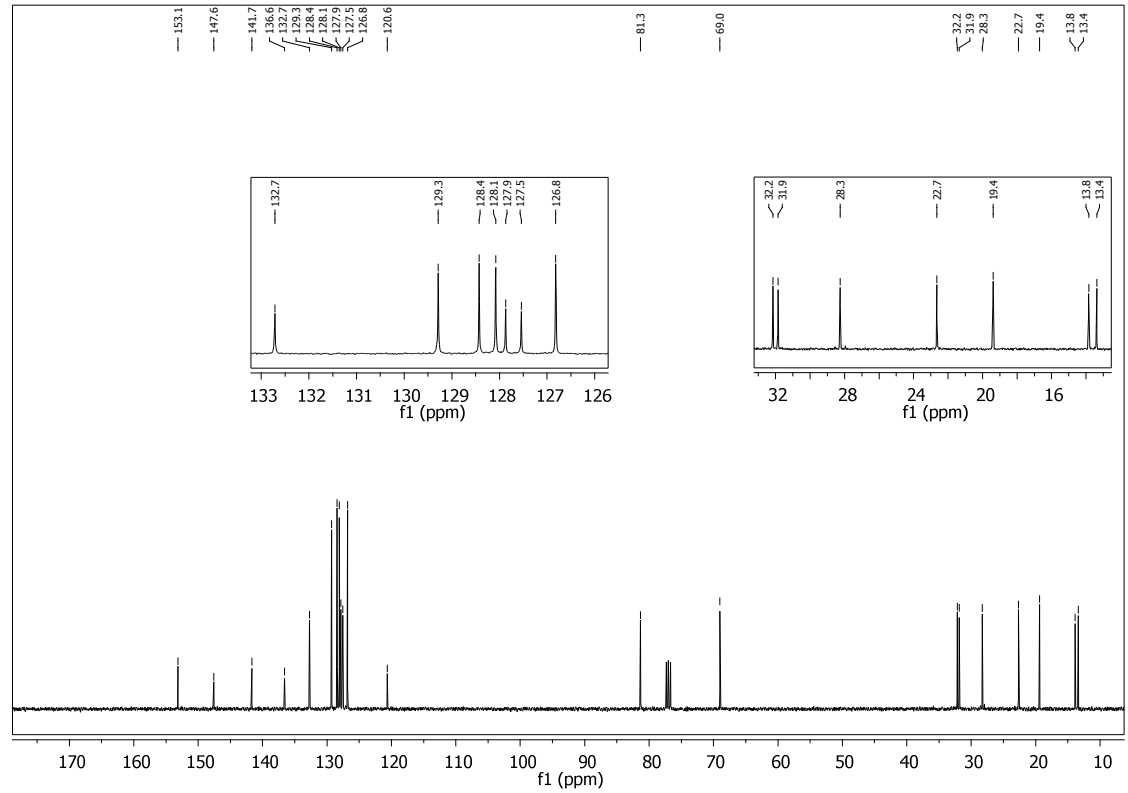

BuSe
Ph
Se
O–Me
Ph
0.91
7.14
7.08
7.02
f1 (ppm)
1.87
2.09
2.24
3.00
2.6
2.2
1.8
1.4
1.0
f1 (ppm)
2.19
8.62
0.91
0.90
2.99
1.87
2.09
2.24
3.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

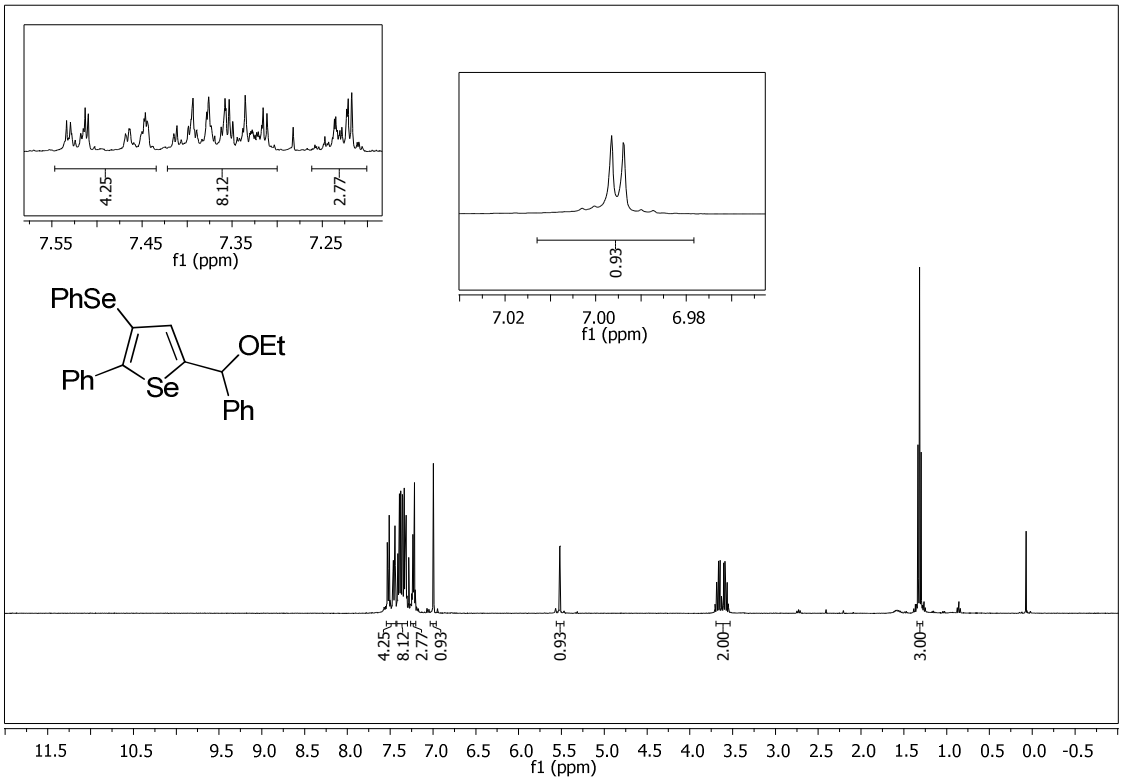

152.4
147.9
141.2
136.6
133.2
129.4
128.6
128.2
128.1
127.7
126.9
120.8
83.2
57.0
32.2
28.4
22.7
13.5
129.4
128.6
128.2
128.1
127.7
126.9
131
130
129
128
127
126
125
f1 (ppm)
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

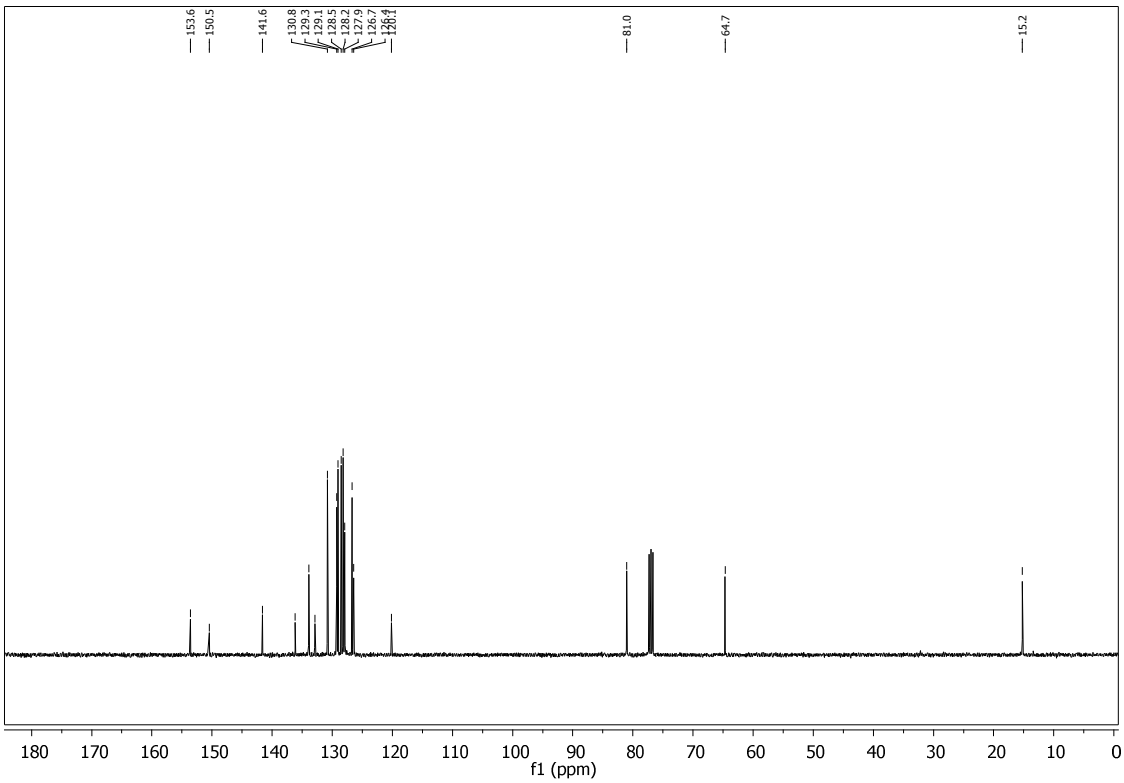

4.07
6.30
1.05
2.15
5.28
3.00
f1 (ppm)
BuSe
Ph
Se
OEt
Ph
0.93
2.13
1.98

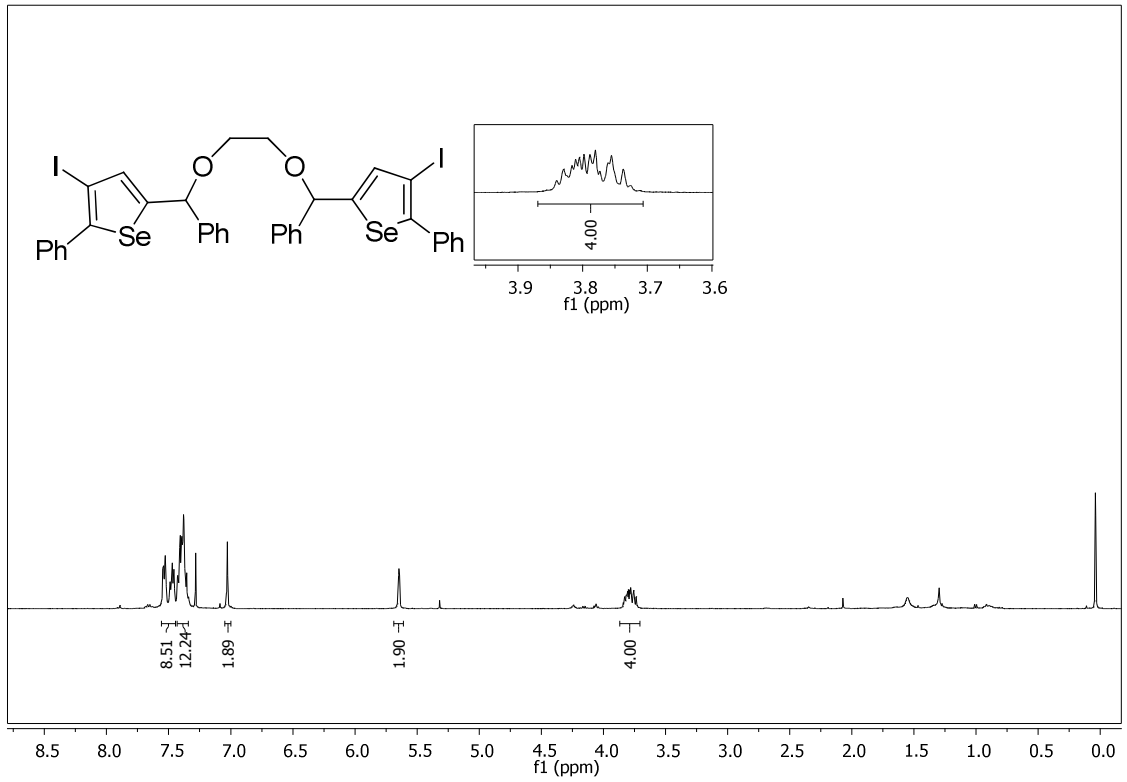

153.0
147.6
141.6
136.5
132.8
129.3
128.4
128.1
127.9
127.6
126.8
120.6
81.1
64.6
32.1
28.3
22.6
15.2
13.4
f1 (ppm)

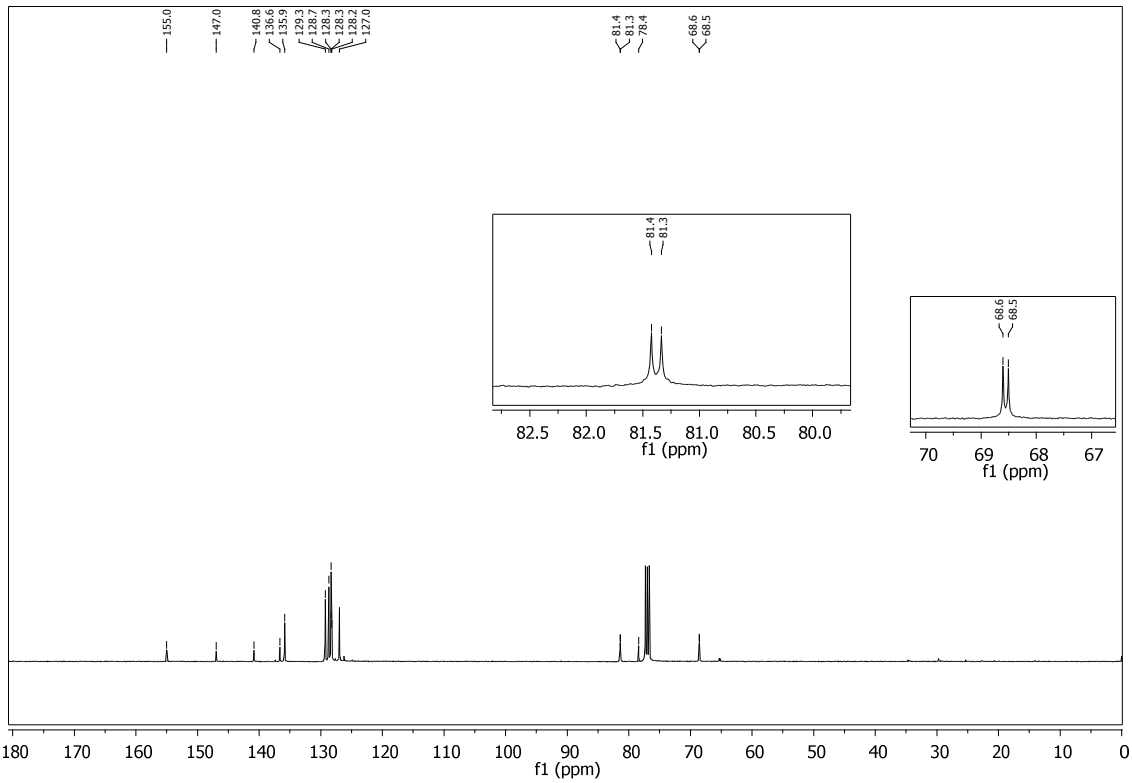

BuSe
Ph
Se
O–Bu
Ph
2.08
4.35
2.23
3.15
3.00
1.6
1.4
1.2
1.0
0.8
f1 (ppm)
2.06
3.60
3.55
3.50
3.45
f1 (ppm)
1.98
2.04
6.17
0.98
1.00
2.06
1.94
2.08
4.35
2.23
3.15
3.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

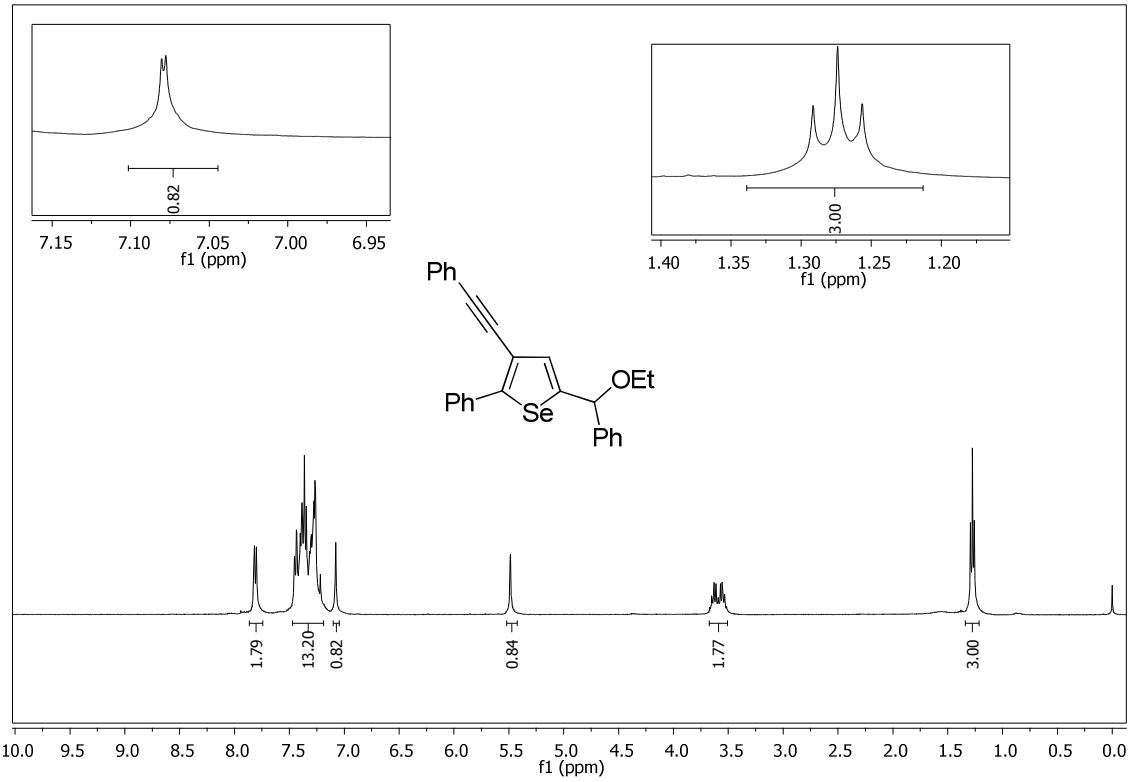

153.1
147.6
141.7
136.6
132.7
129.3
128.4
128.1
127.9
127.5
126.8
120.6
81.3
69.0
32.2
31.9
28.3
22.7
19.4
13.8
13.4
132.7
129.3
128.4
128.1
127.9
127.5
126.8
133
132
131
130
129
128
127
126
f1 (ppm)
32.2
31.9
28.3
22.7
19.4
13.8
13.4
32
28
24
20
16
f1 (ppm)
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

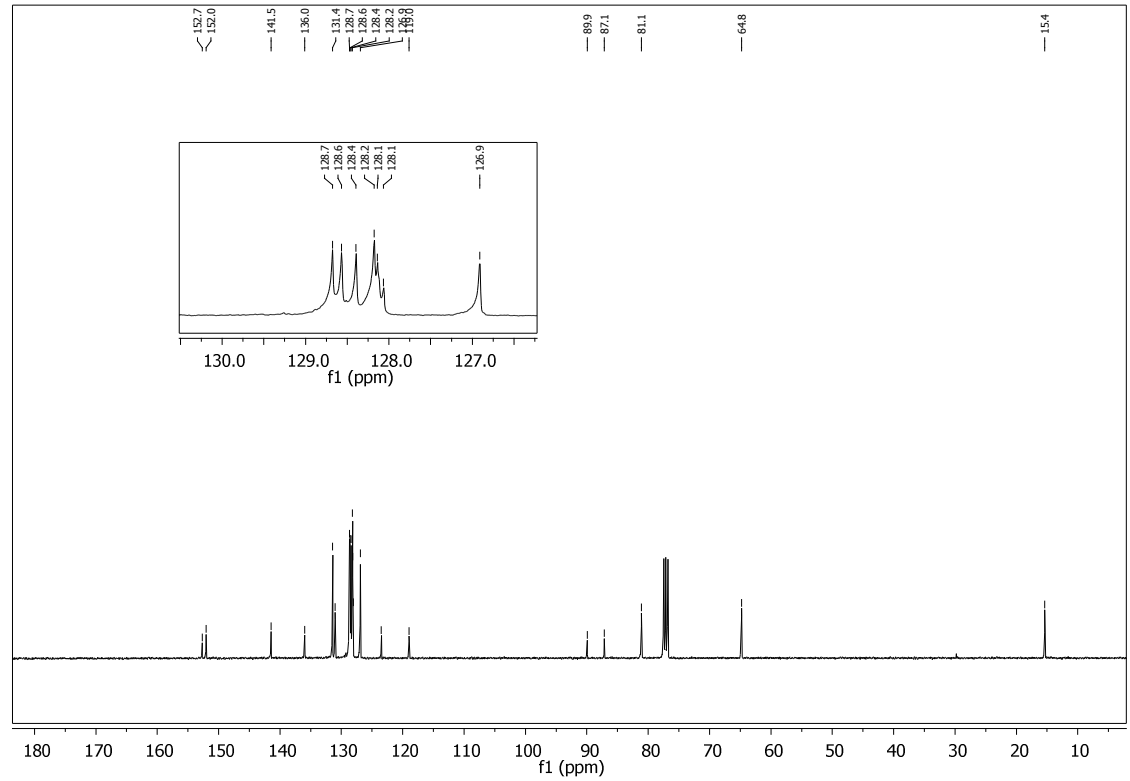

4.25
8.12
2.77
7.55
7.45
7.35
7.25
f1 (ppm)
0.93
7.02
7.00
6.98
f1 (ppm)
PhSe
OEt
Ph
Se
Ph
4.25
8.12
2.77
0.93
0.93
2.00
3.00
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

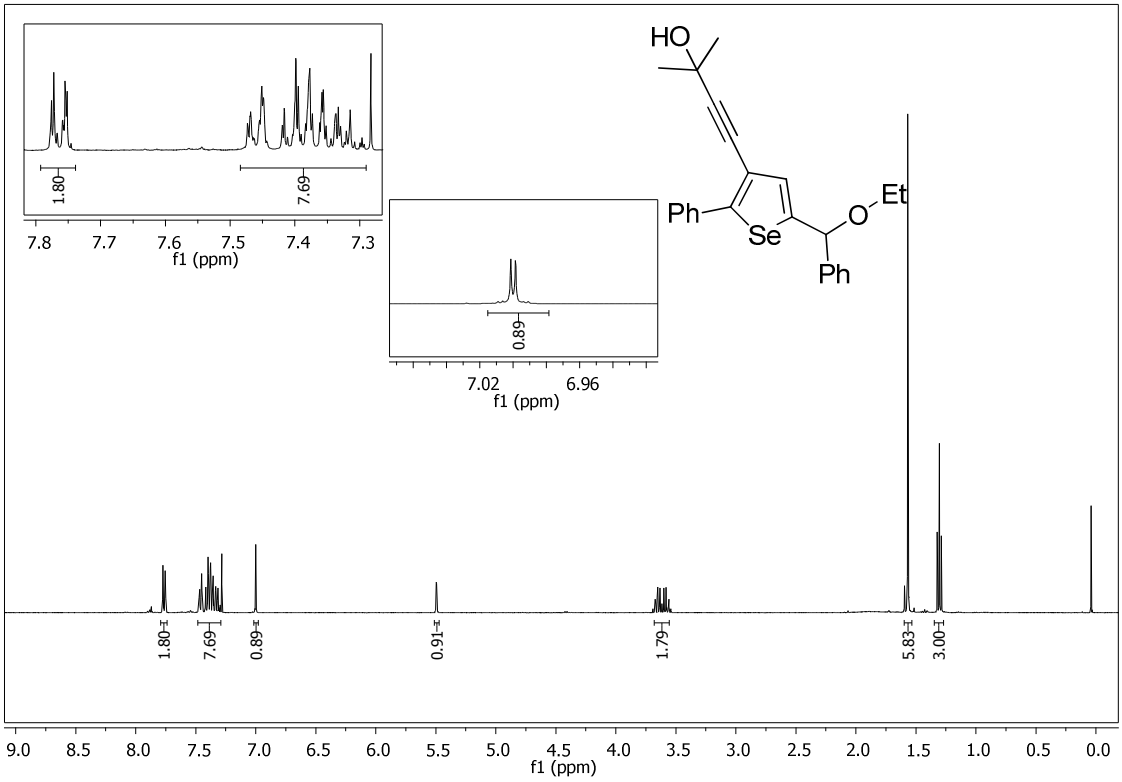

153.6
150.5
141.6
130.8
129.3
129.1
128.5
128.2
127.9
126.7
81.0
64.7
15.2
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

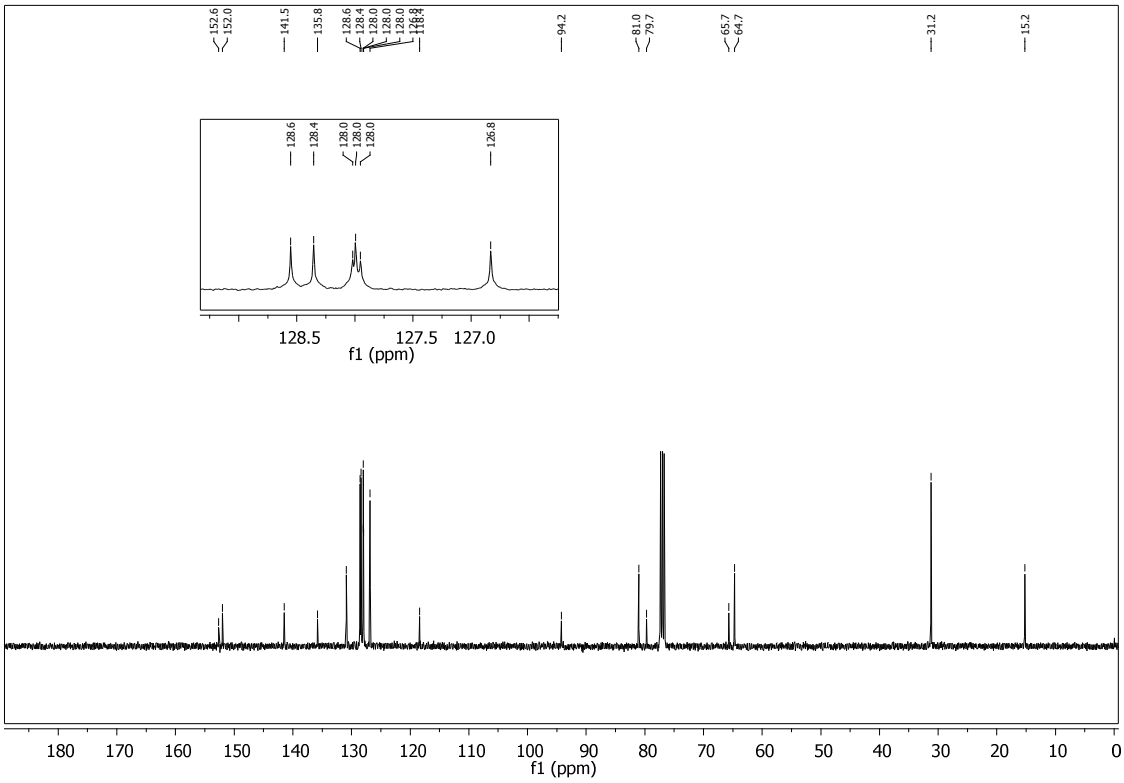

I
O
O
I
Ph
Se
Ph
Ph
Se
Ph
4.00
3.9
3.8
3.7
3.6
f1 (ppm)
8.51
12.24
1.89
1.90
4.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

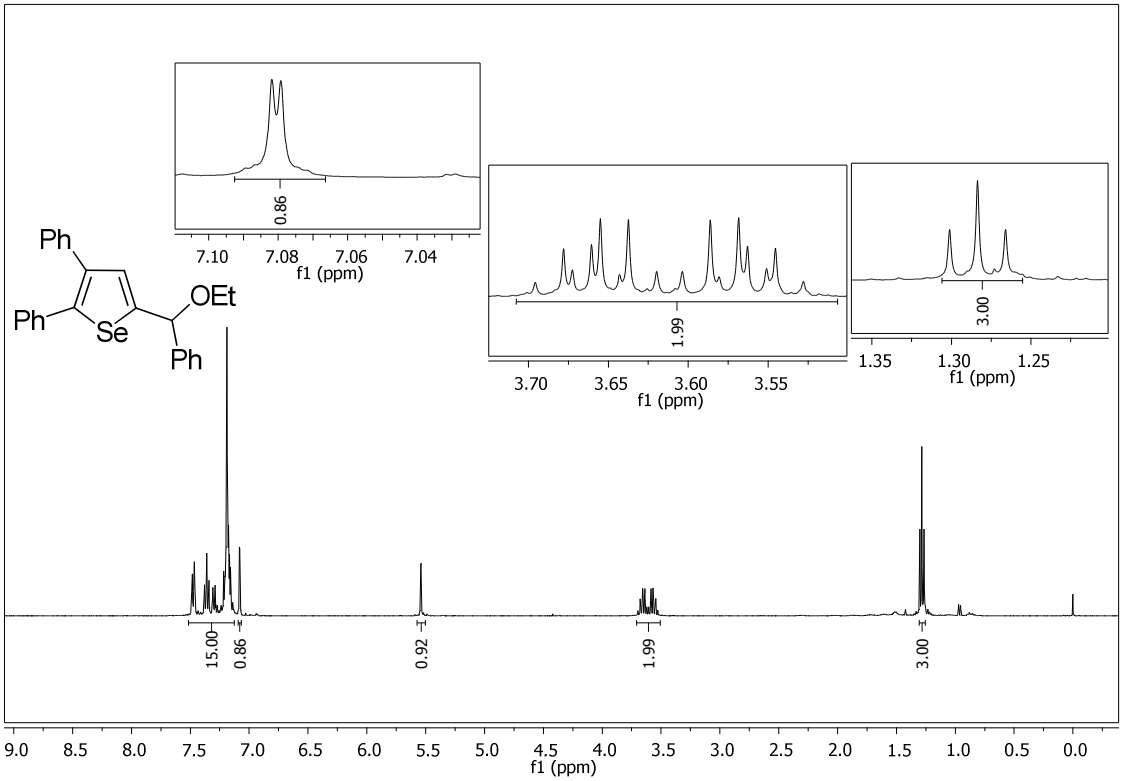

155.0
147.0
140.8
136.6
135.9
129.3
128.7
128.3
128.3
128.2
127.0
81.4
81.3
78.4
68.6
68.5
81.4
81.3
82.5
82.0
81.5
81.0
80.5
80.0
f1 (ppm)
68.6
68.5
70
69
68
67
f1 (ppm)
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

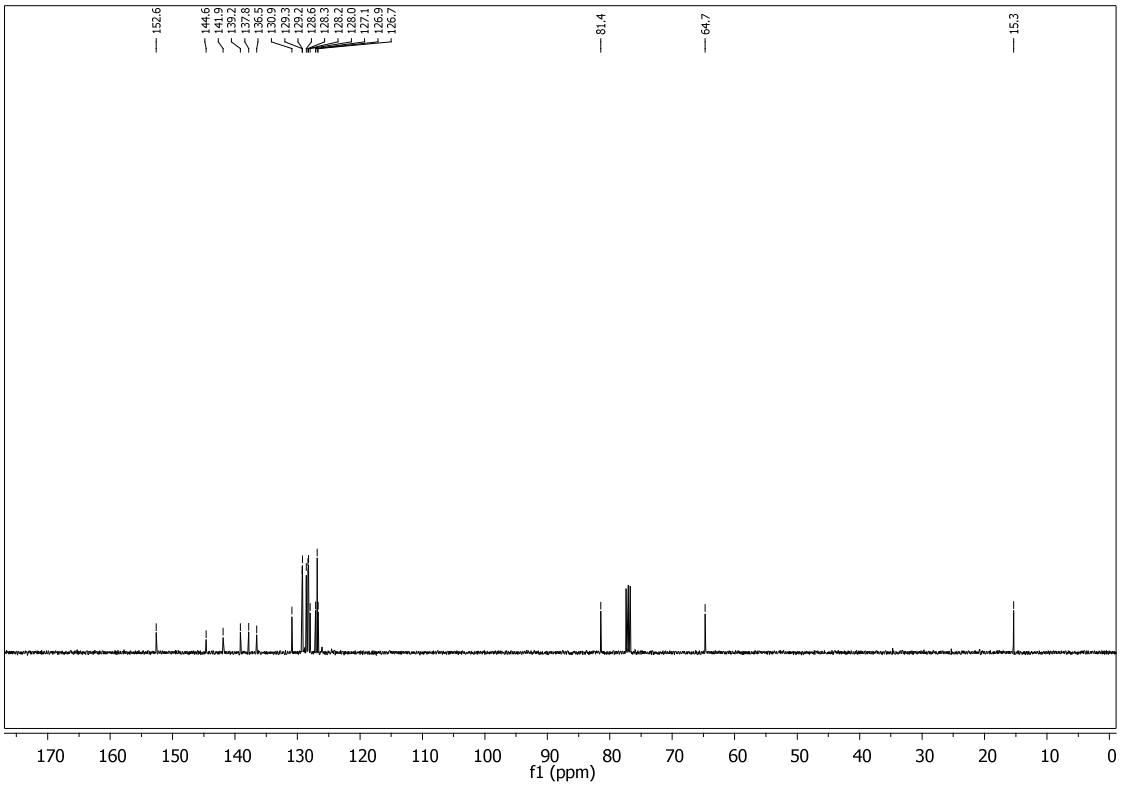

0.82
7.15
7.10
7.05
7.00
6.95
f1 (ppm)
3.00
1.40
1.35
1.30
1.25
1.20
f1 (ppm)
Ph
Ph
Se
OEt
Ph
1.79
13.20
0.82
0.84
1.77
3.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


152.7
152.0
141.5
136.0
131.4
128.7
128.6
128.4
128.2
128.1
126.9
89.9
87.1
81.1
64.8
15.4
128.7
128.6
128.4
128.2
128.1
126.9
130.0
129.0
128.0
127.0
f1 (ppm)
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


HO
Et
O
Ph
Se
Ph
1.80
7.69
0.89
f1 (ppm)
1.80
7.69
0.89
0.91
1.79
5.83
3.00
f1 (ppm)


152.6
152.0
141.5
135.8
128.6
128.4
128.0
128.0
128.0
128.0
94.2
81.0
79.7
65.7
64.7
31.2
15.2
128.6
128.4
128.0
128.0
128.0
126.8
f1 (ppm)
f1 (ppm)


Ph
Ph
Se
OEt
Ph
0.86
7.10
7.08
7.06
7.04
f1 (ppm)
1.99
3.70
3.65
3.60
3.55
f1 (ppm)
3.00
1.35
1.30
1.25
f1 (ppm)
15.00
0.86
0.92
1.99
3.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


152.6
144.6
141.9
139.2
137.8
136.5
130.9
129.3
129.2
128.6
128.3
128.2
128.0
127.1
126.9
126.7
81.4
64.7
15.3
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)