Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Copper(I)/Succinic Acid Cooperatively Catalyzed One-pot Synthesis of Organoselenium-propargylamines via A^3-Coupling

Isadora M. de Oliveira,[a] Daniel C. Pimenta,[b] Julio Zukerman-Schpector,[c] Hélio A. Stefani,[d] Flávia Manarin[e]

[a]Departamento de Química Fundamental, Instituto de Química, Universidade de São Paulo, São Paulo, SP – Brasil. [b]Instituto Butantã, São Paulo, SP – Brasil. [c]Departamento de Química, Universidade Federal de São Carlos, São Carlos, SP – Brasil. [d]Departamento de Farmácia, Faculdade de Ciências Farmacêuticas, Universidade de São Paulo, São Paulo, SP – Brasil. [e]Centro de Engenharias e Ciências Exatas- CECE, Universidade Estadual do Oeste do Paraná, Toledo, PR - Brasil

Corresponding Authors: hstefani@usp.br and fgmanarin@gmail.com

Contents

I. General Information.

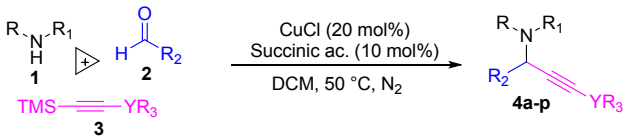
Materials and methods

All reactions were carried out under a nitrogen atmosphere; all compounds were characterized by ^{1}H NMR, ^{13}C NMR, ESI-MS. Copies of the ^{1}H, ^{13}C spectra can be found at the end of the Supporting Information. Nuclear Magnetic Resonance spectra were obtained using a Bruker DPX 300 (^{1}H at 300 MHz and ^{13}C at 75 MHz) instrument in $CDCl_3$ and acetone-*d6* solvent. All ^{1}H NMR experiments are reported in δ units, parts per million (ppm), and were measured relative to the signals for TMS (0.00 ppm). All 77Se NMR experiments are reported in δ units, parts per million (ppm), and were measured relative to the signals for diphenyl disselenide (463 ppm). Data are reported as follows: chemical shift (δ), multiplicity, coupling constant (J) in Hertz and integrated intensity. Abbreviations to denote the multiplicity of a particular signal are: s (singlet), d (doublet), t (triplet), q (quartet), quint (quintet), sex (sextet) and m (multiplet). All ^{13}C NMR spectra are reported in ppm relative to deuterated-chloroform (77.23 ppm), unless otherwise stated, and all were obtained with ^{1}H decoupling. High-resolution mass spectra (HRMS) were recorded on a Shimadzu LCMS-IT-TOF ESI-TOF mass spectrometer. Reactions were monitored with the same mass spectrometer. Column chromatography was performed using silica gel (230−400 mesh). Thin Layer Chromatography (TLC) was performed using silica gel UV254, 0.20 mm thickness. FTIR data were obtained using an Agilent Technologies Cary 630. Melting points were obtained using a Buchi B-545 melting point apparatus.

Unless stated otherwise, commercial reagents were used without further purifcation. All reagents were weighed and handled in air at room temperature.

II. Experimental Details and Characterization Data

Synthesis of selenium-containing propargylamines.



Into a sealed tube, 10 mL, under nitrogen flow and mounted heating apparatus (silicone bath) was added the secondary amine (1.1 eq.), the solvent dichloromethane (3 mL), the aldehyde (1 eq.) CuCl catalysts (20 mol%), succinic acid (10 mol%) and acetylenic selenide (1.2 eq.). The solution was stirred at 50 ° C until the total consumption of the starting material (TLC). The solvent was evaporated under reduced pressure and the product was purified on a column chromatography eluting with hexane and ethyl acetate (95:5).

*1-(1-(4-methoxyphenyl)-3-(phenylselanyl)prop-2-yn-1-yl)piperidine (**4a**)*. Orange oil, 165 mg, 85%. IR υ_{max} cm^{-1}: 2834, 2706, 1631, 1527, 1460, 2021, 1393, 1205, 1121, 711, 666. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.55 (d, *J* = 7.7 Hz, 2H), 7.48 (d, *J* = 8.5 Hz, 2H), 7.37 – 7.17 (m, 3H), 6.86 (d, *J* = 8.5 Hz, 2H), 4.74 (s, 1H), 3.79 (s, 3H), 2.50 (q, *J* = 5.1 Hz, 4H), 1.56 (q, *J* = 5.6 Hz, 4H), 1.42 (q, *J* = 5.6 Hz, 2H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.1, 130.5, 129.6 (3C), 129.5 (2C), 129.2, 129.0, 127.0, 113.5 (2C), 101.0, 65.6, 62.8, 55.3 (2C), 50.7, 26.2 (2C), 24.5 ppm. ^{77}Se NMR (57 MHz, $CDCl_3$) δ 658.0. HRMS (ESI) *m/z,* calcd for $C_{21}H_{23}NOSe$ $(M+H)^+$: 386.1029, found: 386.1045.

*1-(1-(4-methoxyphenyl)-3-(phenylselanyl)prop-2-yn-1-yl)pyrrolidine (**4b**)*. Red oil, 149 mg, 80%. IR υ_{max} cm^{-1}: 2857, 2834, 2021, 1557, 1460, 1393, 1205, 1134, 711, 666. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.57 – 7.49 (m, 2H), 7.46 (d, *J* = 8.3 Hz, 2H), 7.36 – 7.16 (m, 3H), 6.85 (d, *J* = 8.4 Hz, 2H), 4.84 (s, 1H), 3.76 (s, 3H), 2.63 (s, 4H), 1.75 (s, 4H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.1, 131.5, 129.4 (2C), 129.3 (2C), 128.9 (3C), 126.9, 113.6 (2C), 101.6, 65.0, 59.4, 55.2, 50.3, 50.2, 23.5 ppm. HRMS (ESI) *m/z* calcd for $C_{20}H_{21}NOSe$ $(M+H)^+$: 372.0878, found: 372,0889 .

*4-(1-(4-methoxyphenyl)-3-(phenylselanyl)prop-2-yn-1-yl)morpholine (**4c**)*. Yellow oil, 77 mg, 50%. IR υ_{max} cm^{-1}: 2957, 2822, 2741, 2021, 1557, 1460, 1393, 1205, 1080, 961, 711, 666. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.55 (d, *J* = 6.8 Hz, 2H), 7.48 (d, *J* = 8.3 Hz, 2H), 7.39 – 7.18 (m, 3H), 6.87 (d, *J* = 8.5 Hz, 2H), 4.72 (s, 1H), 3.80 (s, 3H), 3.70 (q, *J* = 4.6 Hz, 4H), 2.57 (q, *J* = 5.1 Hz, 4H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.2, 129.6 (3C), 129.5 (2C), 129.1 (2C), 128.8, 127.0, 113.6 (2C), 99.9, 67.1 (2C), 66.7, 62.4, 55.2, 49.8 (2C) ppm. HRMS (ESI) *m/z* calcd for $C_{20}H_{21}NO_2Se$ $(M+H)^+$: 388.0828, found: 388.0847.

*1-(1-phenyl-3-(phenylselanyl)prop-2-yn-1-yl)piperidine (**4d**)*. Red oil, 108 mg, 61%. IR υ_{max} cm^{-1}: 2957, 2834, 2756, 2712, 2021, 1527, 1430, 1293, 989, 709, 680. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.65 (t, *J* = 8.0 Hz, 4H), 7.44 – 7.28 (m, 6H), 4.88 (s, 1H), 2.61 (t, *J* = 5.4

Hz, 4H), 1.66 (st, *J* = 5.0 Hz, 4H), 1.51 (q, *J* = 5.6 Hz, 2H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 138.4, 129.5 (2C), 129.1 (2C), 129.0, 128.4 (2C), 128.1 (2C), 127.5, 126.9, 100.7, 65.9, 63.4, 50.7 (2C), 26.2 (2C), 24.4 ppm. HRMS (ESI) *m/z,* calcd for $C_{20}H_{21}NSe$ $(M+H)^+$: 356.0929, found: 356.0948

*1-(1-(4-bromophenyl)-3-(phenylselanyl)prop-2-yn-1-yl)piperidine (**4e**)*. Yellow oil, 108 mg, 50%. IR υ_{max} cm^{-1}: 2956, 2833, 2756, 2713, 2021, 1527, 1430, 1035, 955, 709, 666. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7,46 (d, *J* = 7.4 Hz, 2H), 7.37 (s, 4H), 7.29 – 7.11 (m, 3H), 4.65 (s, 1H), 2.41 (t, *J* = 5.3 Hz, 4H), 1.48 (q, *J* = 5.8 Hz, 5H), 1.34 (d, *J* = 5.7 Hz, 3H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 136.5, 130.1 (2C), 129.0 (2C), 128.4 (3C), 128.0 (2C), 126.0, 120.4, 98.7, 65.6, 61.7, 49.6 (2C), 25.1 (2C), 23.3 ppm. HRMS (ESI) *m/z,* calcd for $C_{20}H_{20}BrNSe$ $(M+H)^+$: 434.0024, found: 434.0042.

*1-(1-(2,6-dichlorophenyl)-3-(phenylselanyl)prop-2-yn-1-yl)piperidine (**4f**)*. Red oil, 163 mg, 77%. IR υ_{max} cm^{-1}: 957, 2834, 2758, 2659, 2021, 1654, 1510, 1389, 1056, 745, 709, 666. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.51 (d, *J* = 8.5 Hz, 2H), 7.26 (t, *J* = 8.4 Hz, 5H), 7.10 (t, *J* = 8.0 Hz, 1H), 5.26 (s, 1H), 2.87 – 2.71 (m, 2H), 2.39 (dt, *J* = 10.8, 5.2 Hz, 2H), 1.55 (t, *J* = 5.8 Hz, 4H), 1.41 (d, *J* = 5.6 Hz, 2H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 136.2 (2C), 134.2, 129.7, 129.4 (2C), 129.2 (2C), 129.0 (2C), 126.9 (2C), 100.2, 65.5, 59.3, 52.0 (2C), 26.1 (2C), 24.4 ppm. HRMS (ESI) *m/z*, calcd for $C_{20}H_{19}Cl_2NSe$ $(M+H)^+$: 424.0148, found: 424.0152.

*1-(1-(2-chlorophenyl)-3-(phenylselanyl)prop-2-yn-1-yl)piperidine (**4g**)*. Yellow oil, 152 mg, 78%. IR υ_{max} cm^{-1}: 2959, 2834, 2758, 2704, 2021, 1527, 1428, 1393, 955, 709, 666. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7,67 (dd, *J* = 6,8 2,6 Hz, 1H); 7,53 (d, *J* = 7,2 Hz, 2H); 7,36 (d, *J* = 6,8 Hz, 1H); 7,32 – 7,17 (m, 5H); 5,09 (s, 1H); 2,70 – 2,49 (m, 4H); 1,53 (q, *J* = 6,1 Hz, 4H); 1,40 (q, *J* = 5,7 Hz, 2H) ppm, ^{13}C NMR (75 MHz; $CDCl_3$) δ 136.2, 134.6, 130.5, 129.8, 129.5 (2C), 129.0 (2C), 129.0, 128.8, 127.0, 126.2, 100.2, 66.1, 60.3, 50.8 (2C), 26.1 (2C), 24.4 ppm. HRMS (ESI) *m/z*, calcd for $C_{20}H_{20}ClNSe$ $(M+H)^+$: 390.0535; found: 390.0558.

*1-(1-(2,6-dimethoxyphenyl)-3-(phenylselanyl)prop-2-yn-1-yl)piperidine (**4h**)*. Yellow solid, 166 mg, 80%. Mp: 87-90 °C. IR υ_{max} cm^{-1}: 2829, 2704, 2021, 1527, 1425, 1387, 1207, 1054, 951, 711, 667. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.55 (d, *J* = 8.6 Hz, 2H), 7.21 (dd, *J* = 15.3, 6.2 Hz, 4H), 6.54 (d, *J* = 8.4 Hz, 2H), 5.36 (s, 1H), 3.76 (s, 6H), 2.80 – 2.49 (m, 4H), 1.57 (q, *J* = 5.5 Hz, 4H), 1.36 (t, *J* = 5.8 Hz, 2H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 158.9 (2C), 130.0, 129.2 (2C), 129.2, 128.6 (2C), 126.5, 114.8, 104.9 (2C),

103.9, 60.7, 56.1 (2C), 52.7, 51.5 (2C), 26.2 (2C), 24.3 ppm. HRMS (ESI) *m/z* calcd for $C_{22}H_{25}NO_2Se$ (M+H)+: 416.1135, found: 416.1150.

*1-(1-(2,6-dimethylphenyl)-3-(phenylselanyl)prop-2-yn-1-yl)piperidine (**4i**)*. Red oil, 102 mg, 53%. IR υ_{max} cm^{-1}: 2958, 2834, 2021, 1527, 1428, 1393, 989, 707, 665. ^1H NMR (300 MHz, $CDCl_3$) δ 7.54 – 7.50 (m, 3H), 7.30 – 7.23 (m, 5H), 4.66 (s, 1H), 2.51 (s, 6H), 2.40 – 2.17 (m, 2H), 1.51 (q, *J* = 5.2, 4.7 Hz, 4H), 1.41 (d, *J* = 6.2 Hz, 2H), 0.23 (s, 2H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 137.6, 133.0, 129.7, 129.5 (2C), 129.3, 129.0, 128.8 (2C), 128.7, 127.2 (2C), 126.7, 102.7, 84.7, 58.9, 52.3 (2C), 26.3, 24.7, 21.1 (2C) ppm. HRMS (ESI) *m/z*, calcd for $C_{22}H_{25}NSe$ $(M+H)^+$: 384.1232, found: 384.1246.

*1-(1-(furan-2-yl)-3-(phenylselanyl)prop-2-yn-1-yl)piperidine (**4j**)*. Red oil, 69 mg, 40%. IR υ_{max} cm^{-1}: 2957, 2834, 2758, 2712, 1527, 1430, 1393, 959, 709, 666. ^1H NMR (300 MHz, $CDCl_3$) δ 7.55 (d, *J* = 7.2 Hz, 2H), 7.40 (s, 1H), 7.27 (dq, *J* = 13.9, 7.0 Hz, 3H), 6.41 (d, *J* = 3.3 Hz, 1H), 6.33 (d, *J* = 2.5 Hz, 1H), 4.87 (s, 1H), 2.55 (t, *J* = 5.5 Hz, 4H), 1.61 (dq, *J* = 11.4, 6.2, 5.8 Hz, 4H), 1.43 (q, *J* = 5.8 Hz, 2H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 151.3, 142.5, 129.4 (2C), 129.0 (2C), 128.7, 127.0, 110.0 (2C), 109.2, 98.2, 57.5, 50.5 (2C), 25.9 (2C), 24.2 ppm. HRMS (ESI) *m/z*, calcd for $C_{18}H_{19}NOSe$ (M+H)+: 346.0719, found: 346.0749.

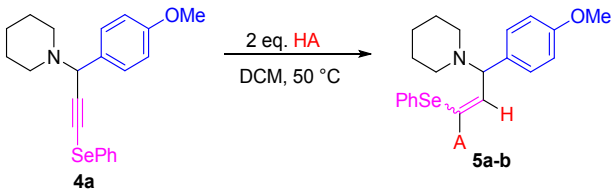
*1-(3-(phenylselanyl)-1-(p-tolyl)prop-2-yn-1-yl)piperidine (**4k**)*. Yellow oil, 79 mg, 43%. IR υ_{max} cm^{-1}: 2857, 2834, 2758, 2708, 2021, 1527, 1430, 1393, 966, 709, 666. ^1H NMR (300 MHz, $CDCl_3$) δ 7.62 – 7.51 (m, 2H), 7.46 (d, *J* = 8.0 Hz, 2H), 7.38 – 7.20 (m, 3H), 7.14 (d, *J* = 7.8 Hz, 2H), 4.76 (s, 1H), 2.53 (d, *J* = 5.3 Hz, 4H), 2.34 (s, 3H), 1.56 (q, *J* = 5.6 Hz, 4H), 1.42 (q, *J* = 5.4 Hz, 2H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 137.1, 135.3 (2C), 129.4 (2C), 128.9 (2C), 128.7 (2C), 128.3 (2C), 126.9, 100.9, 65.6, 63.1, 50.7 (2C), 26.2 (2C), 24.4, 21.1 ppm. HRMS (ESI) *m/z*, calcd for $C_{21}H_{23}NSe$ (M+H)+: 370.1076, found: 370.1080.

*1-(4-methyl-1-(phenylselanyl)pent-1-yn-3-yl)piperidine (**4l**)*. Yellow oil, 24 mg, 15%. IR υ_{max} cm^{-1}: 2833, 2760, 2710, 2021, 1631, 1557, 1460, 1205, 1132, 1004, 750, 666. ^1H NMR (300 MHz, $CDCl_3$) δ 7.54 (d, *J* = 7.4 Hz, 2H), 7.26 (dq, *J* = 14.9, 7.1 Hz, 3H), 3.00 (d, *J* = 9.9 Hz, 1H), 2.59 (td, *J* = 6.9, 3.6 Hz, 2H), 2.44 – 2.34 (m, 2H), 1.57 (q, *J* = 6.3 Hz, 5H), 1.43 (q, *J* = 5.6 Hz, 2H), 1.07 (d, *J* = 6.6 Hz, 3H), 0.98 (d, *J* = 6.5 Hz, 3H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 129.3 (2C), 128.6 (2C), 126.6, 102.7, 66.7, 50.7 (2C), 30.5, 26.2 (2C), 24.6, 20.7, 19.8 (2C) ppm. HRMS (ESI) *m/z*, calcd for $C_{17}H_{23}NSe$ $(M+H)^+$: 322.1076, found: 322.1090.

*1-(3-(butylselanyl)-1-(4-methoxyphenyl)prop-2-yn-1-yl)piperidine (**4o**)*. Orange oil, 173 mg, 95%. IR υ_{max} cm^{-1}: 2833, 2760, 2710, 2021, 1631, 1557, 1460, 1205, 1132, 1004, 750, 666. ^1H NMR (300 MHz, $CDCl_3$) δ 7.45 (d, *J* = 6.4 Hz, 2H), 6.85 (d, *J* = 9.0 Hz, 2H), 4.63 (s, 1H), 3.78 (d, *J* = 2.3 Hz, 3H), 2.81 (t, *J* = 7.3 Hz, 2H), 2.52 – 2.34 (m, 4H), 1.84 (t, *J* = 7.3 Hz, 2H), 1.54 (q, *J* = 10.6, 8.2 Hz, 5H), 1.44 (dd, *J* = 13.9, 7.0 Hz, 3H), 0.94 (t, *J* = 7.3 Hz, 3H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 158.9, 130.8, 129.5 (2C), 113.3 (2C), 96.7, 66.6, 62.6, 55.2 (2C), 50.5, 32.3, 29.0, 26.2 (2C), 24.5, 22.5, 13.5 ppm. HRMS (ESI) *m/z*, calcd for $C_{19}H_{27}NOSe$ $(M+H)^+$: 366.1348, found: 366.1377.

*1-(1-(4-methoxyphenyl)-3-(phenyltellanyl)prop-2-yn-1-yl)piperidine (**4p**)*. Orange oil, 126 mg, 58%. IR υ_{max} cm^{-1}: 2833, 2756, 2710, 2021, 1523, 1460, 1389, 1205, 1132, 948, 706, 668. ^1H NMR (300 MHz, $CDCl_3$) δ 7.79 – 7.64 (m, 2H), 7.46 (d, *J* = 8.7 Hz, 2H), 7.24 (d, *J* = 5.3 Hz, 3H), 6.85 (d, *J* = 8.5 Hz, 2H), 4.82 (s, 1H), 3.78 (s, 3H), 2.49 (t, *J* = 5.3 Hz, 4H), 1.55 (q, *J* = 5.6 Hz, 4H), 1.41 (q, *J* = 5.6 Hz, 2H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.0, 135.0 (2C), 130.6 (2C), 129.6, 129.6 (2C), 127.7, 113.4 (2C), 113.2, 112.5, 63.1, 55.2, 50.6 (2C), 43.2, 26.2 (2C), 24.5 ppm. HRMS (ESI) *m/z*, calcd for $C_{21}H_{23}NOTe$ $(M+H)^+$: 436.0922, found: 434.0947.

Synthesis of hydrohalogenation



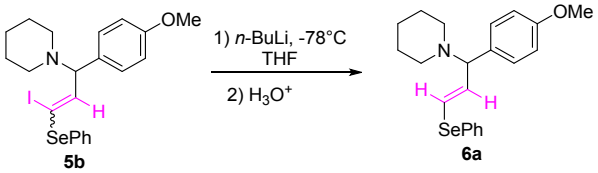
In a sealed tube, 10 mL, and mounted heating apparatus (silicone bath) was added selenium-propargylamine (1eq.), Dichloromethane solvent (3 mL) and the respective acid (2 eq.). The solution was stirred at 50 °C until the total consumption of the starting material (TLC). The solvent was evaporated under reduced pressure and the product was purified on a column chromatography eluting with hexane and ethyl acetate (90:10).

*1-(3-bromo-1-(4-methoxyphenyl)-3-(phenylselanyl)allyl)piperidine (**5a**)*. Oil red, 433 mg, 93%. IR υ_{max} cm^{-1}: 2956, 2834, 2699, 1557, 1460, 1393, 1203, 1002, 804, 713, 668. ^1H NMR (300 MHz, $CDCl_3$) δ 7.50 – 7.40 (m, 2H), 7.34 – 7.21 (m, 5H), 6.85 (d, *J* = 8.6 Hz, 2H), 6.62 (d, *J* = 8.9 Hz, 1H), 4.15 (d, *J* = 8.9 Hz, 1H), 3.77 (s, 3H), 2.50 – 2.29 (m,

4H), 1.53 (t, *J* = 5.6 Hz, 4H), 1.42 (d, *J* = 5.7 Hz, 2H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 158.9, 142.8, 133.0 (2C), 132.3, 131.9, 129.3 (2C), 129.0 (2C), 128.0, 113.9 (2C), 108.2, 72.3, 55.2, 52.1 (2C), 26.1 (2C), 24.6 ppm. ^{77}Se NMR (57 MHz, $CDCl_3$) δ 578.28, 462.78. HRMS (ESI) *m/z*, calcd for $C_{21}H_{24}BrNOSe$ $(M+H)^+$: 466.0285, found: 466.0291.

*1-(3-iodo-1-(4-methoxyphenyl)-3-(phenylselanyl)allyl)piperidine (**5b**)*. Oil red, 478 mg, 93%. IR υ_{max} cm^{-1}: 2834, 2756, 2699, 2658, 1631, 1547, 1460, 1393, 1203, 1002, 804, 713. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.51 – 7.42 (m, 2H), 7.31 (dd, *J* = 8.0, 3.7 Hz, 5H), 6.88 (d, *J* = 8.7 Hz, 2H), 6.50 (d, *J* = 8.7 Hz, 1H), 3.96 (d, *J* = 8.7 Hz, 1H), 3.81 (s, 3H), 2.42 (tt, *J* = 11.3, 6.1 Hz, 4H), 1.55 (p, *J* = 5.4 Hz, 4H), 1.45 (q, *J* = 5.7 Hz, 2H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 158.9, 146.9, 133.4 (2C), 131.9, 131.7, 129.4 (2C), 129.1 (2C), 128.2, 113.9 (2C), 80.0, 77.0, 55.2, 52.2 (2C), 26.1 (2C), 24.6 ppm. ^{77}Se NMR (57 MHz, $CDCl_3$) δ 625.24, 462.68. HRMS (ESI) *m/z*, calcd for $C_{21}H_{24}INOSe$ $(M+H)^+$: 514.0158, found: 514.0177.

Synthesis of selenide-vinyl

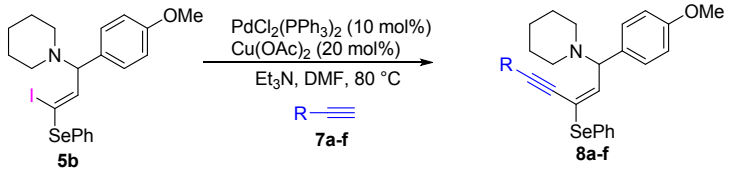


A solution of seleno-vinyl iodide (1 eq.) in THF was added to a 10 mL pre-flushed flask under nitrogen flow. The solution was cooled to -78 ° C for the dropwise addition of n-butyllithium. The solution was held at that temperature for one hour. Then a saturated solution of NH_4Cl was added to the mixture, then allowed to reach room temperature, maintaining stirring for about 1 hour at that same temperature. The reaction mixture was diluted with ethyl acetate, the organic phase was collected and dried with magnesium sulfate, filtered and the solvent removed in vacuo. The reaction residue was subjected directly to column chromatography using flash silica and hexane/ethyl acetate (90/10) as the elution solvent.

*(E)-1-(1-(4-methoxyphenyl)-3-(phenylselanyl)allyl)piperidine (**6a**)*. Solid yellow, 58 mg, 50%. Mp: 63-66 °C. IR υ_{max} cm^{-1}: 2831, 1555, 1527, 1460, 1393, 1203, 1000, 715, 670. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.45 – 7.37 (m, 2H), 7.27 – 7.18 (m, 5H), 6.85 (d, *J* = 8.4 Hz, 2H), 6.56 (d, *J* = 15.3 Hz, 1H), 6.14 (dd, *J* = 15.3, 8.6 Hz, 1H), 3.78 (s, 3H), 3.75 (d, *J* = 8.3 Hz, 1H), 2.43 (dd, J = 10.9, 5.3 Hz, 2H), 2.36 – 2.24 (m, 2H), 1.58 – 1.51 (m, 4H),

1.45 – 1.37 (m, 2H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 158.7, 139.4, 133.5 (2C), 131.9 (2C), 130.7, 129.4(2C), 129.2 (2C), 129.0 (2C), 126.9, 118.7, 113.8 (2C), 113.4, 74.3, 55.2, 52.3 (2C), 26.1 (2C), 24.6 ppm. ^{77}Se NMR (57 MHz, CDCl3) δ 370.64 ppm. HRMS (ESI) m/z, calcd for $C_{21}H_{25}NOSe$ $(M+H)^+$: 388,1180, found: 388.1198.

Synthesis of Derivatives of Sonogashira Reaction



In a pre-flushed 10 mL tube, under nitrogen flow and mounted heating apparatus (silicone bath) was added the selenium-vinyl iodide (1 eq.), The solvent DMF (3 mL), the palladium (10 mol%), acetylene (2 eq.), The copper catalyst (20 mol%) and the base (2 eq.). The solution was stirred at 80 ° C until the total consumption of the starting material (TLC) (24 hours). To the mixture was added saturated NH_4Cl solution and then extracted with ethyl acetate three times. The organic phase was dried with $MgSO_4$, the solvent was evaporated under reduced pressure. The product was purified on a column chromatography eluting with hexane/ethyl acetate.

(E)-7-(4-methoxyphenyl)-2-methyl-5-(phenylselanyl)-7-(piperidin-1-yl)hept-5-en-3-yn-2-ol ***(8a)***. Oil red, 65 mg, 57%. IR υ_{max} cm^{-1}: 3257, 2834, 2047, 1557, 1460, 1393, 1203, 1132, 1002, 806, 715, 666. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.47 – 7.38 (m, 2H), 7.19 (d, J = 8.9 Hz, 5H), 6.77 (d, J = 8.5 Hz, 2H), 6.27 (d, J = 9.4 Hz, 1H), 4.14 (d, J = 9.5 Hz, 1H), 3.71 (s, 3H), 2.40 – 2.23 (m, 4H), 1.54 – 1.46 (m, 4H), 1.44 (s, 3H), 1.36 (d, J = 6.0 Hz, 2H), 1.31 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 158.8, 135.7, 134.5 (2C), 129.4, 129.0 (2C), 128.9 (2C), 127.9, 113.9 (2C), 102.5, 84.1, 78.8, 71.3, 66.3, 65.4, 55.2, 52.3, 52.1, 31.0 (2C), 25.8 (2C), 24.48 ppm. ^{77}Se NMR (57 MHz, CDCl3) δ 498.5. HRMS (ESI) m/z, calcd for $C_{26}H_{31}NO_2Se$ $(M-C_5H_{10}N)$: 385.0710, found: 385.0728.

(E)-6-(4-methoxyphenyl)-4-(phenylselanyl)-6-(piperidin-1-yl)hex-4-en-2-yn-1-ol ***(8b)***. Oil brown, 50 mg, 47%. IR υ_{max} cm^{-1}: 3254, 2831, 2760, 2002, 1510, 1460, 1393, 1205, 1138, 989, 713, 668. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.44 – 7.38 (m, 2H), 7.21 (dd, J = 5.8, 2.4 Hz, 5H), 6.81 – 6.77 (m, 2H), 6.36 (d, J = 9.9 Hz, 1H), 4.25 (d, J = 4.1 Hz, 3H), 3.73 (s, 3H), 2.45 – 2.33 (m, 4H), 1.57 – 1.50 (m, 4H), 1.38 (s, 2H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.2, 135.1, 134.3 (2C), 131.5, 129.4 (2C), 129.1, 129.1 (3C), 128.8,

128.0, 114.1 (2C), 71.2, 55.2 (2C), 52.1, 51.3, 29.6, 25.1 (2C), 24.00 ppm. HRMS (ESI) m/z, calcd for $C_{24}H_{27}NO_2Se$ (M-$C_5H_{10}N$): 357.0397, found: 357.0413.

(E)-7-(4-methoxyphenyl)-5-(phenylselanyl)-7-(piperidin-1-yl)hept-5-en-3-yn-1-ol ***(8c)***. Oil red, 51 mg, 46%. IR υ_{max} cm^{-1}: 3255, 2833, 2758, 2045, 1555, 1460, 1393, 1203, 1203, 1000, 715, 668. ^1H NMR (300 MHz, $CDCl_3$) δ 7.40 (d, J = 3.7 Hz, 2H), 7.20 (d, J = 7.0 Hz, 5H), 6.79 (s, 2H), 6.29 (d, J = 9.5 Hz, 1H), 4.21 (d, J = 9.6 Hz, 1H), 3.72 (s, 3H), 3.47 (t, J = 6.2 Hz, 2H), 2.46 (t, J = 6.2 Hz, 2H), 2.41 – 2.28 (m, 4H), 1.50 (t, J = 5.7 Hz, 4H), 1.37 (d, J = 5.6 Hz, 2H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 158.9, 135.0, 134.0 (2C), 129.6, 129.1 (3C), 129.0, 128.8, 127.8 (2C), 114.0 (2C), 95.6, 79.2, 71.3, 60.8, 55.2, 52.2 (2C), 25.6 (2C), 24.3, 24.1 ppm. HRMS (ESI) m/z, calcd for $C_{25}H_{29}NO_2Se$ (M-$C_5H_{10}N$): 371.0553, found: 371.0562.

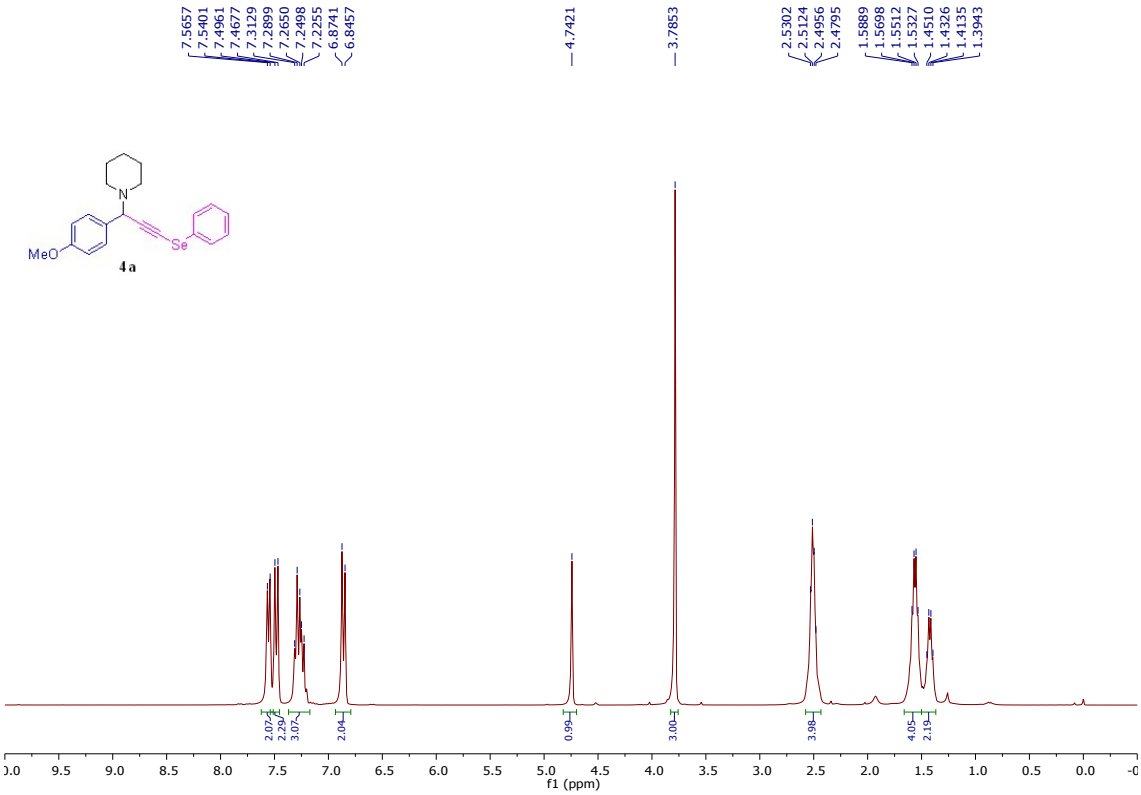
(E)-1-(1-(4-methoxyphenyl)-3-(phenylselanyl)non-2-en-4-yn-1-yl)piperidine ***(8d)***. Oil red, 56 mg, 49%. IR υ_{max} cm^{-1}: 2833, 2760, 2045, 1553, 1460, 1393, 1203, 1134, 991, 713, 668. ^1H NMR (300 MHz, Chloroform-d) δ 7.53 – 7.46 (m, 2H), 7.32 – 7.26 (m, 5H), 6.88 (d, J = 8.7 Hz, 2H), 6.29 (d, J = 9.5 Hz, 1H), 4.31 (s, 1H), 3.83 (s, 3H), 2.45 (d, J = 16.8 Hz, 4H), 2.33 (t, J = 6.7 Hz, 2H), 1.62 – 1.55 (m, 4H), 1.46 (d, J = 4.2 Hz, 2H), 1.41 – 1.34 (m, 2H), 1.31 (d, J = 4.7 Hz, 2H), 0.90 (s, 3H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 158.8, 133.9 (2C), 129.8, 129.0 (2C), 128.9 (2C), 127.5 (2C), 114.5, 113.9 (2C), 71.3, 55.2 (2C), 52.4, 30.5 (2C), 29.6, 25.7, 24.4, 21.8, 19.3, 13.5 ppm. HRMS (ESI) m/z, calcd for $C_{27}H_{33}NOSe$ (M-$C_5H_{10}N$): 383.0397, found: 383.0407.

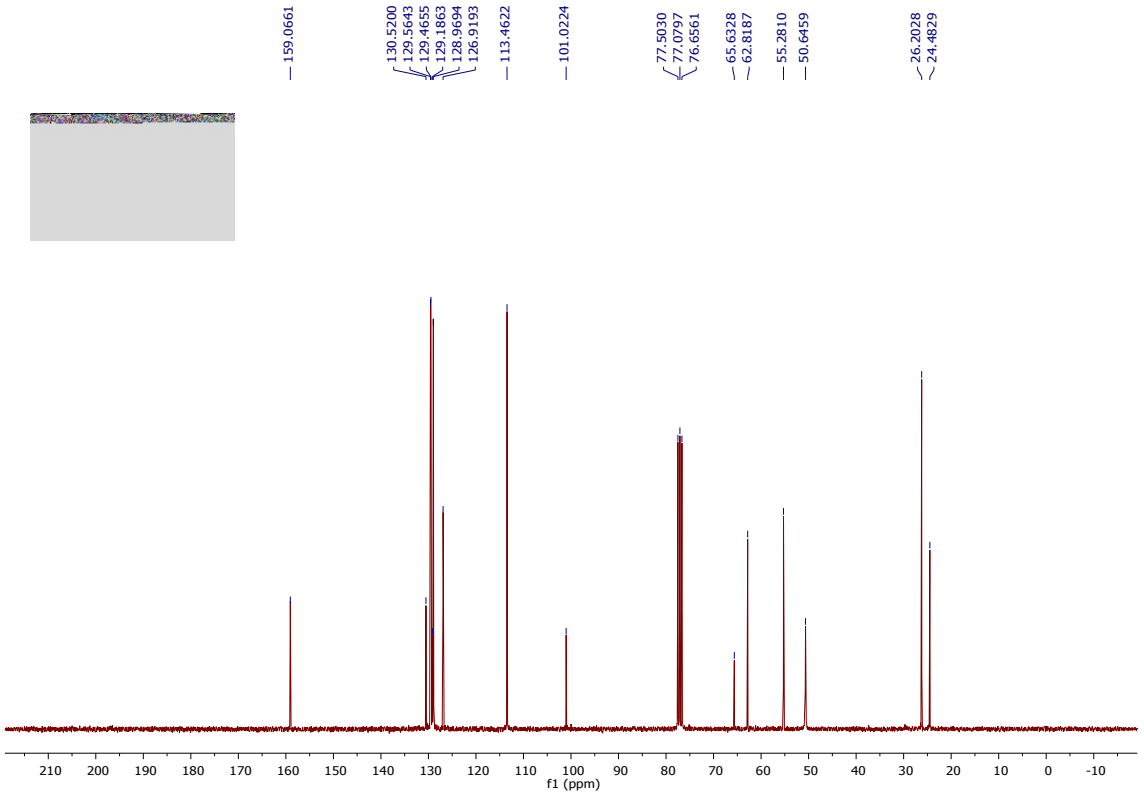
(E)-1-(1-(4-methoxyphenyl)-5-(naphthalen-1-yl)-3-(phenylselanyl)pent-2-en-4-yn-1-yl)piperidine ***(8e)***. Oil brown, 89 mg, 66%. IR υ_{max} cm^{-1}: 2834, 2741, 2032, 1460, 1393, 1203, 739, 670. ^1H NMR (300 MHz, $CDCl_3$) δ 7.62 (t, J = 5.8 Hz, 6H), 7.50 – 7.47 (m, 2H), 7.40 – 7.35 (m, 6H), 6.96 – 6.90 (m, 2H), 6.51 (d, J = 9.5 Hz, 1H), 4.45 (d, J = 11.0 Hz, 1H), 3.85 (s, 3H), 2.60 – 2.47 (m, 4H), 1.65 (t, J = 6.1 Hz, 4H), 1.55 – 1.48 (m, 2H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.0, 141.3, 140.2, 135.4, 134.3, 132.9, 132.0, 131.9, 131.7, 129.5, 129.1, 128.9, 128.9, 128.8, 128.6, 127.8, 127.7, 127.1, 127.0, 127.0, 126.9, 126.9, 126.7, 121.7, 114.0, 89.0, 86.9, 71.7, 55.2, 52.5, 52.2, 25.9, 24.5 ppm. HRMS (ESI) m/z, calcd for $C_{33}H_{31}NOSe$ (M-$C_5H_{10}N$): 453.0761, found: 453.0772.

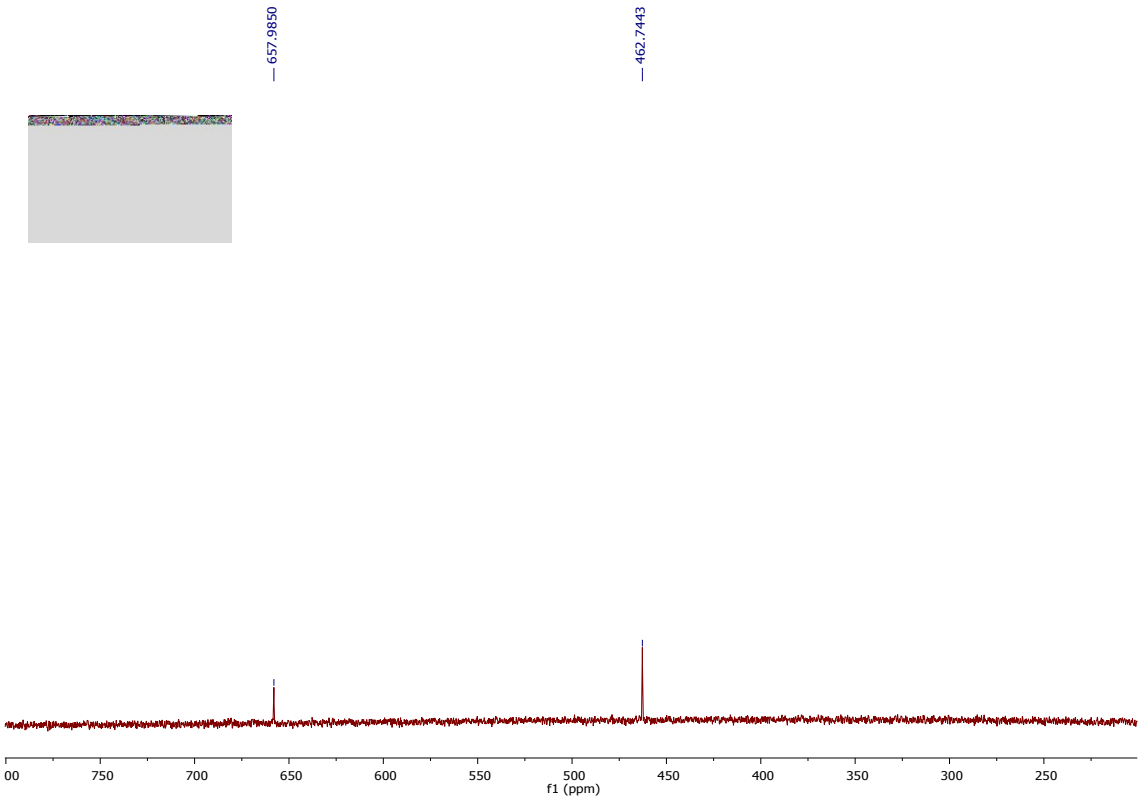
(E)-1-(1-(4-methoxyphenyl)-3-(phenylselanyl)-5-(p-tolyl)pent-2-en-4-yn-1-yl)piperidine ***(8f)***. Oil brown, 71 mg, 57%. IR υ_{max} cm^{-1}: 2834, 2741, 2037, 1551, 1460, 1393, 1205, 1136, 989, 715, 670. ^1H NMR (300 MHz, $CDCl_3$) δ 7.59 (s, 2H), 7.39 – 7.32 (m, 5H), 7.20 (d, *J* = 8.1 Hz, 2H), 7.13 (d, *J* = 8.5 Hz, 2H), 6.91 (d, *J* = 8.8 Hz, 2H), 6.46 (d, *J* = 9.5 Hz, 1H), 4.42 (d, *J* = 9.9 Hz, 1H), 3.83 (d, *J* = 2.6 Hz, 3H), 2.63 – 2.44 (m, 4H), 2.38

(s, 3H), 1.64 (t, J = 6.1 Hz, 4H), 1.49 (d, J = 6.4 Hz, 2H) ppm. ^{13}C NMR (75 MHz, Acetone) δ 160.1, 140.0, 135.0 (2C), 132.7 (2C), 132.6 (2C), 132.1, 130.2, 130.1, 130.09, 129.9 (2C), 129.8, 129.5, 129.3, 128.9, 120.4, 114.9 (2C), 86.2, 72.3, 55.5, 53.0 (2C), 26.7 (2C), 25.2, 21.4 ppm. HRMS (ESI) m/z, calcd for $C_{30}H_{31}NOSe$ (M-$C_5H_{10}N$): 417.0761, found: 417.0783.

III. Copies of ^{1}H NMR, ^{13}C NMR and ^{77}Se NMR spectra of all compounds



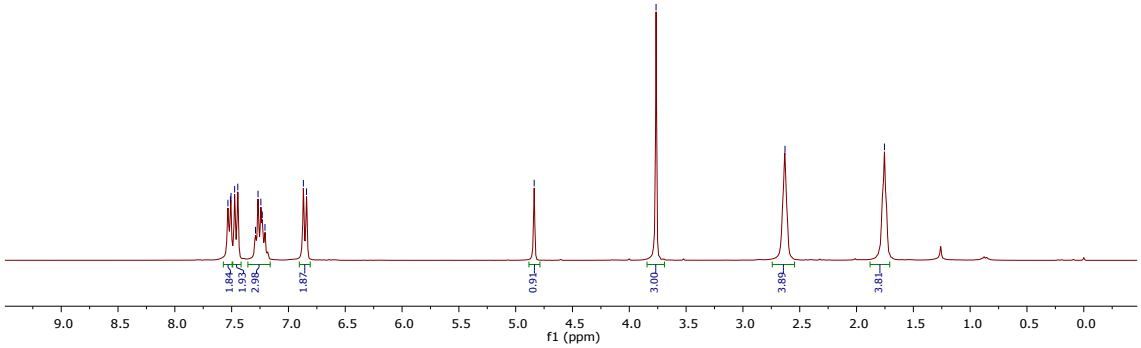

159.0661
130.5200
129.5643
129.4655
129.1863
128.9694
126.9193
113.4622
101.0224
77.5030
77.0797
76.6561
65.6328
62.8187
55.2810
50.6459
26.2028
24.4829
f1 (ppm)


657.9850
462.7443
f1 (ppm)

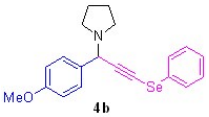

7.5326
7.5105
7.5056
7.4734
7.4459
7.2900
7.2677
7.2429
7.2304
7.2066
6.8686
6.8408
4.8374
3.7645
2.6298
1.7545

N
MeO
Se

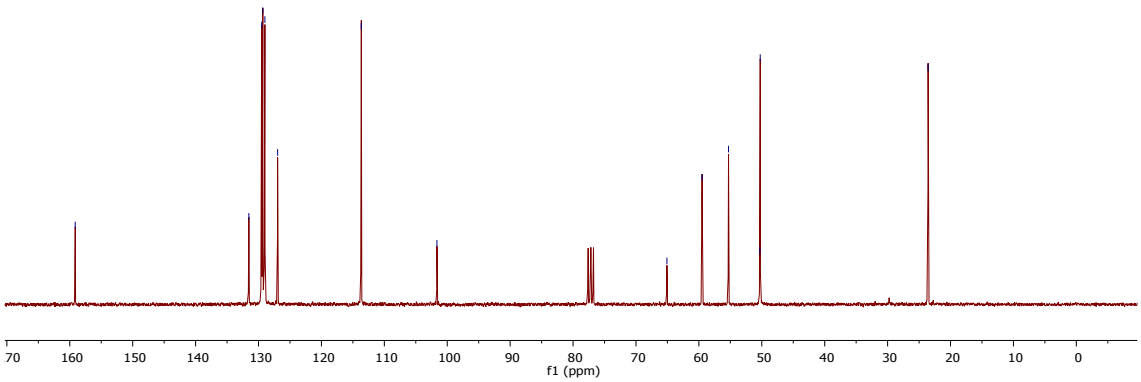
4b

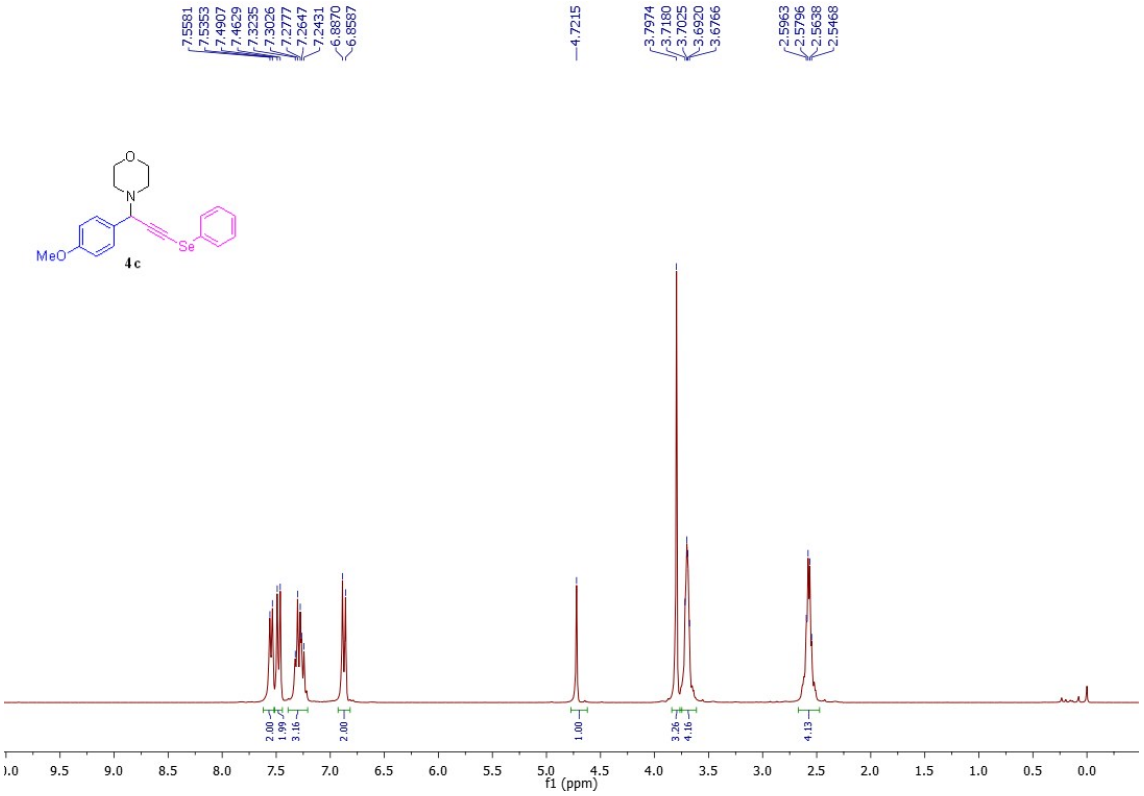

1.84
1.93
2.98
1.87
0.91
3.00
3.89
3.81
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

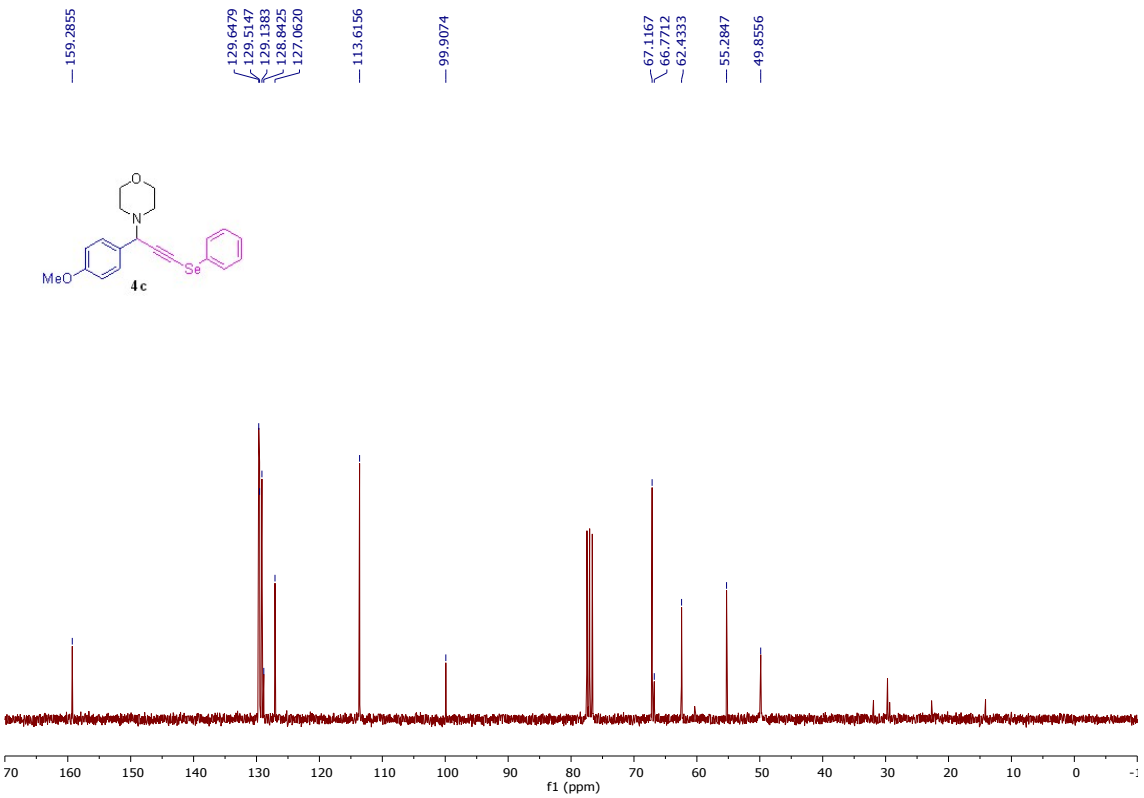

159.1355
131.5366
129.4943
129.3184
128.9856
126.9639
113.6619
101.6372
65.0793
59.4898
55.2883
50.3103
50.2492
23.5663

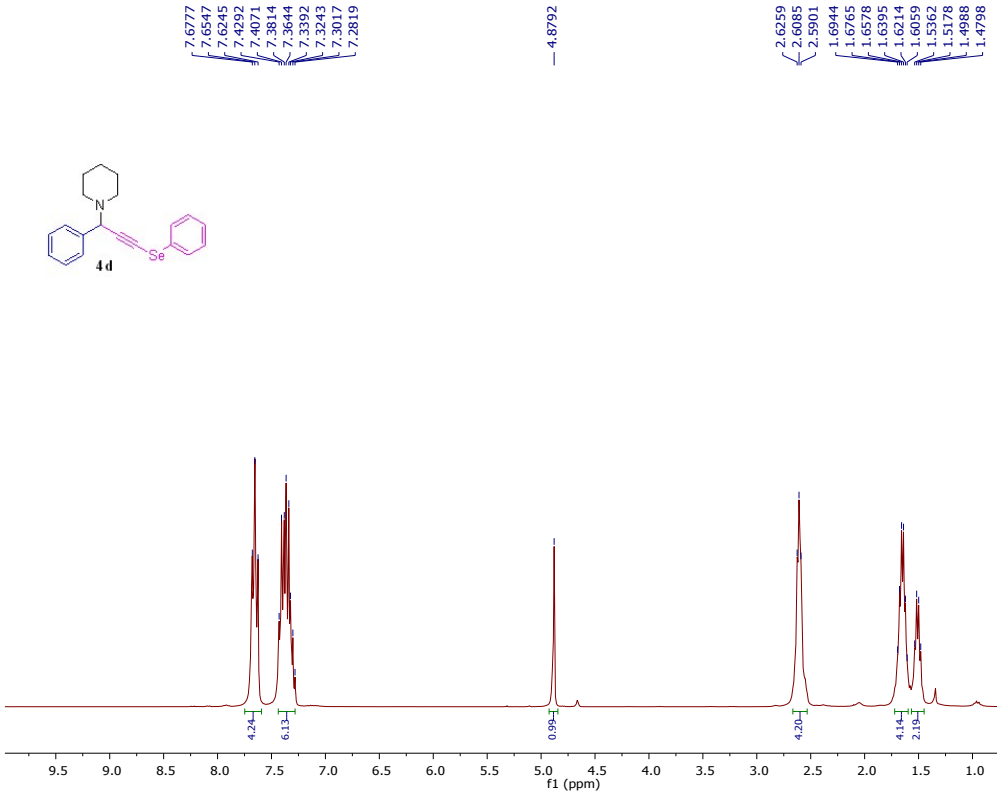

N
MeO
Se

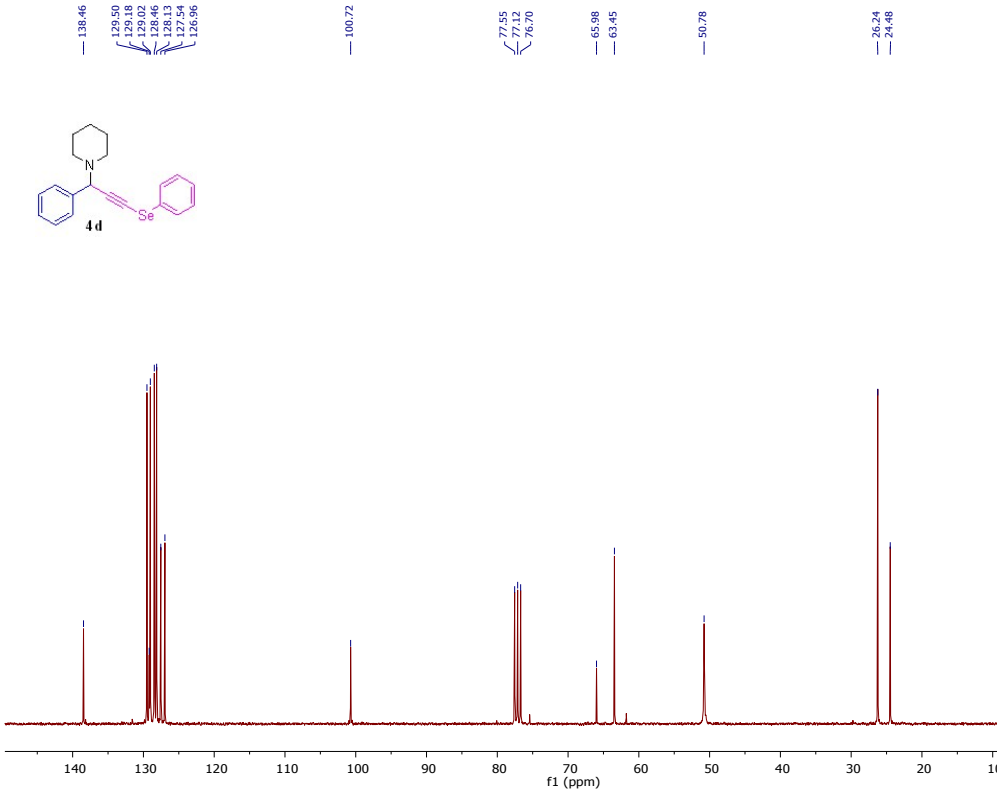
4b

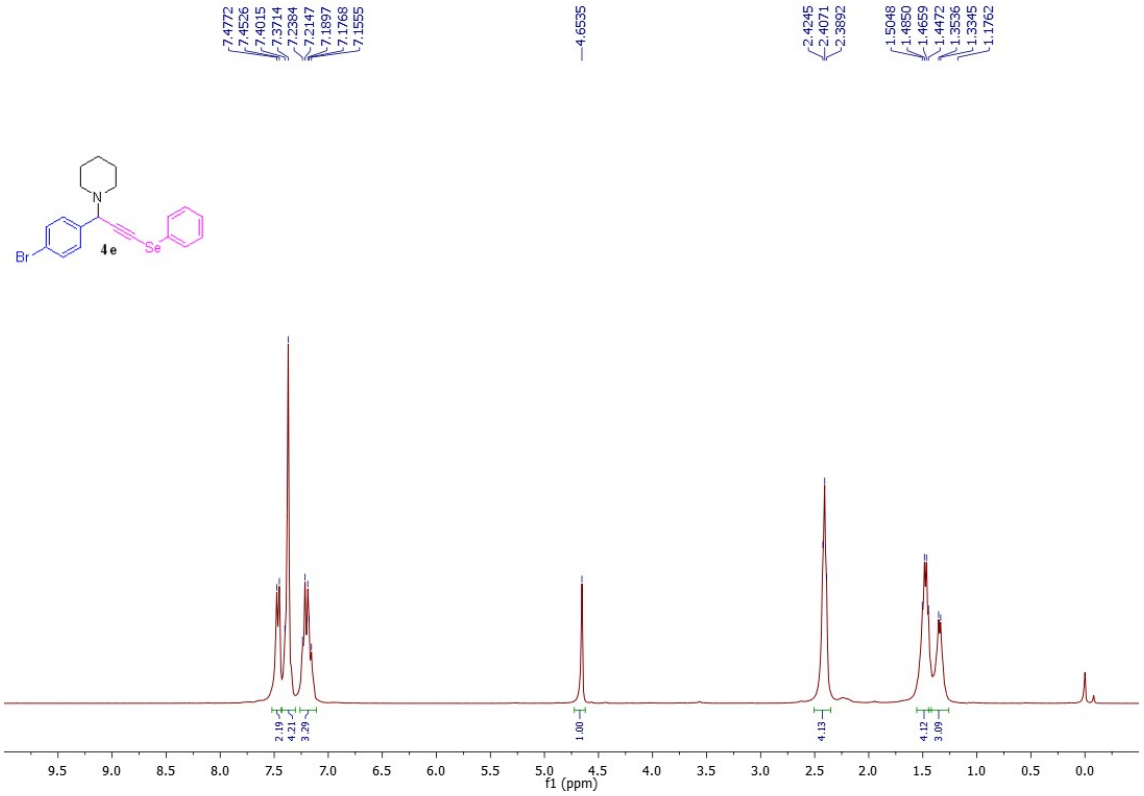

70
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

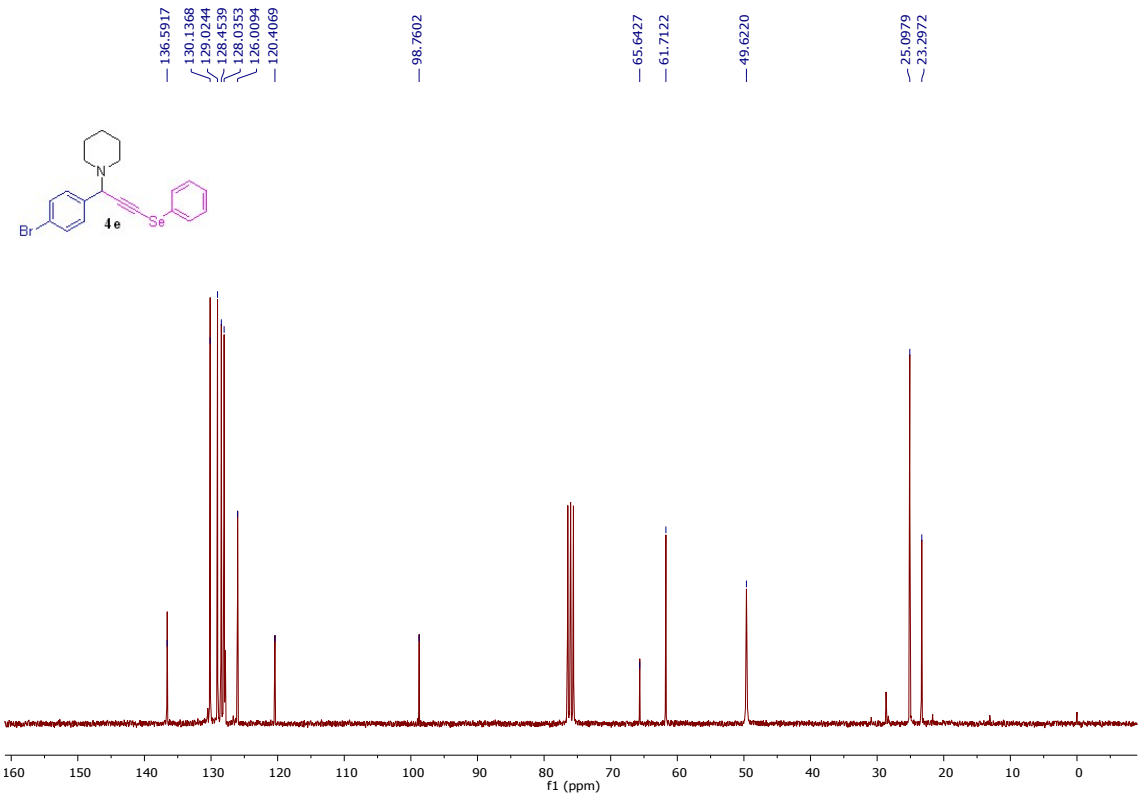

7.5581
7.5353
7.4907
7.4629
7.3235
7.3026
7.2777
7.2647
7.2431
6.8870
6.8587
4.7215
3.7974
3.7180
3.7025
3.6920
3.6766
2.5963
2.5796
2.5638
2.5468
MeO
Se
4c
f1 (ppm)

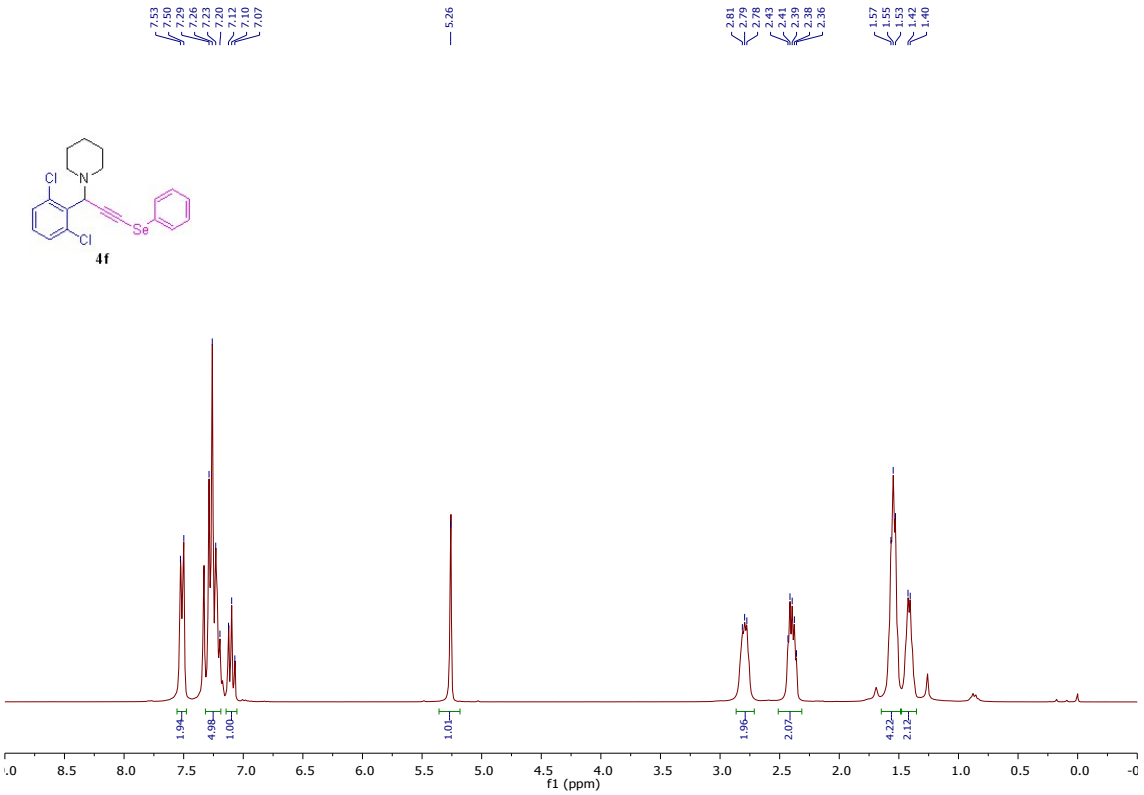

159.2855
129.6479
129.5147
129.1383
128.8425
127.0620
113.6156
99.9074
67.1167
66.7712
62.4333
55.2847
49.8556
MeO
Se
4c
f1 (ppm)

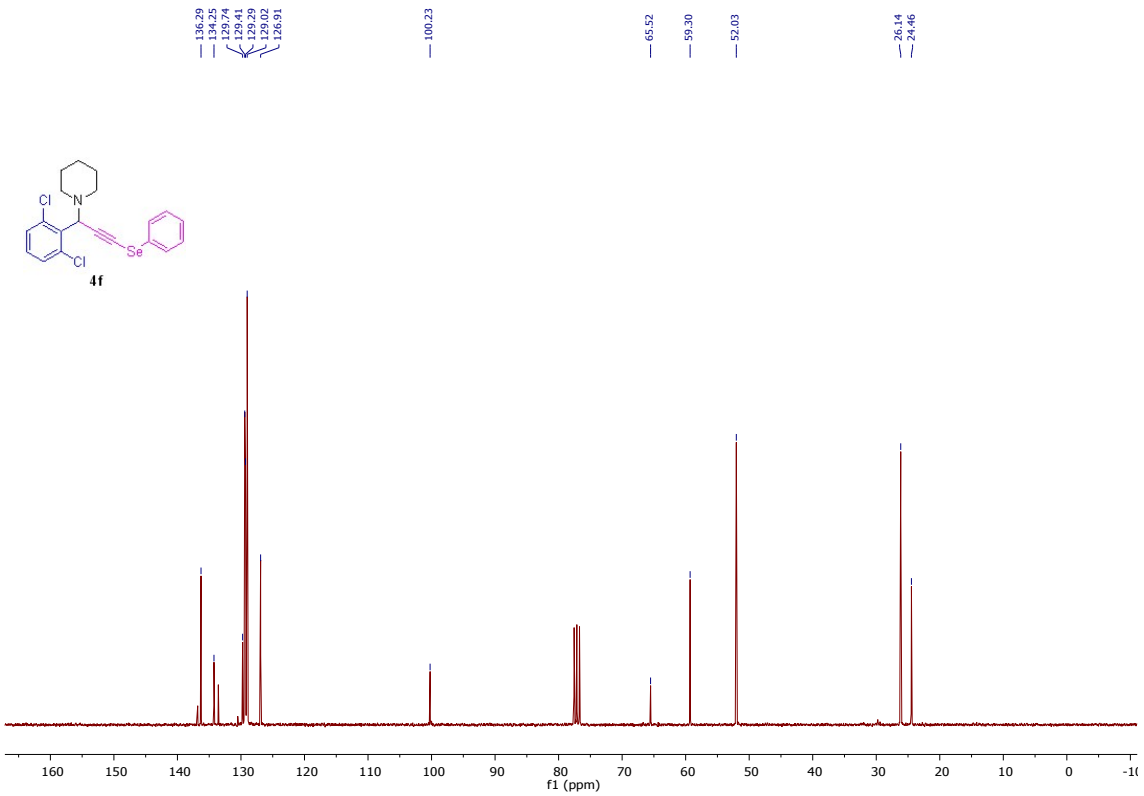

7.6777
7.6547
7.6245
7.4292
7.4071
7.3814
7.3644
7.3392
7.3243
7.3017
7.2819
4.8792
2.6259
2.6085
2.5901
1.6944
1.6765
1.6578
1.6395
1.6214
1.6059
1.5362
1.5178
1.4988
1.4798
4d
4.24
6.13
0.99
4.20
4.14
2.19
f1 (ppm)


138.46
129.50
129.18
129.02
128.46
128.13
127.54
126.96
100.72
77.55
77.12
76.70
65.98
63.45
50.78
26.24
24.48
4d
f1 (ppm)

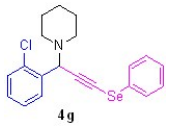

7.4772
7.4526
7.4015
7.3714
7.2384
7.2147
7.1897
7.1768
7.1555
4.6535
2.4245
2.4071
2.3892
1.5048
1.4850
1.4659
1.4472
1.3536
1.3345
1.1762
N
Br
Se
4e
2.19
4.21
3.29
1.00
4.13
4.12
3.09
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


136.5917
130.1368
129.0244
128.4539
128.0353
126.0094
120.4069
98.7602
65.6427
61.7122
49.6220
25.0979
23.2972
N
Br
Se
4e
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

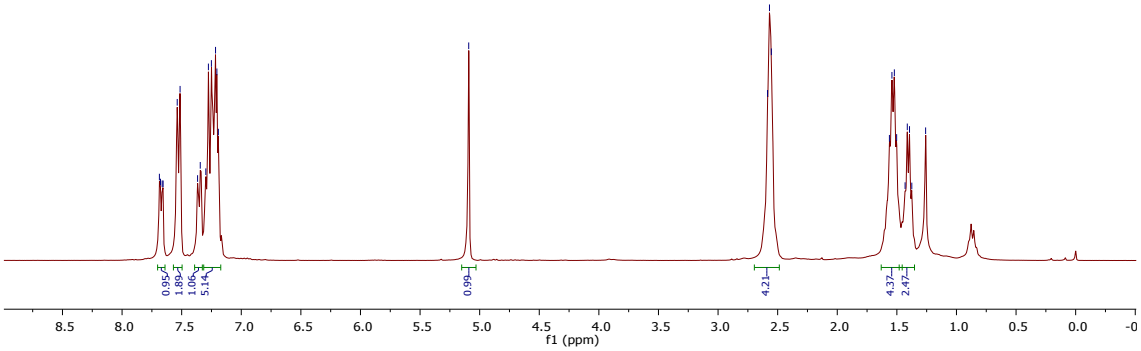

7.53
7.50
7.29
7.26
7.23
7.20
7.12
7.10
7.07
5.26
2.81
2.79
2.78
2.43
2.41
2.39
2.38
2.36
1.57
1.55
1.53
1.42
1.40
Cl
N
Cl
Se
4f
1.94
4.98
1.00
1.01
1.96
2.07
4.22
2.12
f1 (ppm)


136.29
134.25
132.74
129.41
129.29
129.02
126.91
100.23
65.52
59.30
52.03
26.14
24.46
Cl
N
Cl
Se
4f
f1 (ppm)

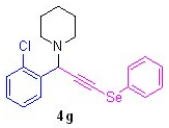

7.69
7.68
7.66
7.66
7.54
7.51
7.37
7.34
7.30
7.28
7.25
7.22
7.20
7.19
5.09
2.59
2.57
2.55
1.56
1.54
1.52
1.50
1.43
1.41
1.39
1.37
1.26


Cl
N
Se

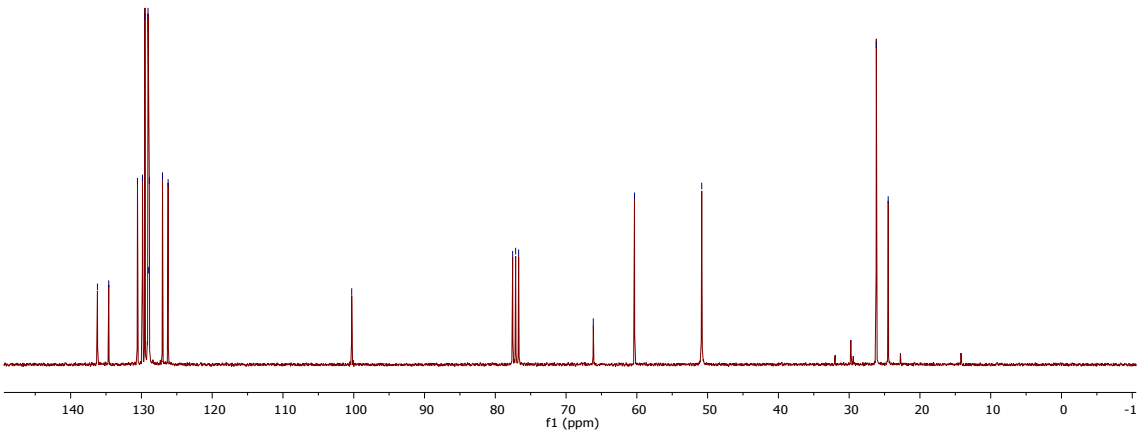
4g


0.95
1.89
1.06
5.14
0.99
4.21
4.37
2.47
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
f1 (ppm)

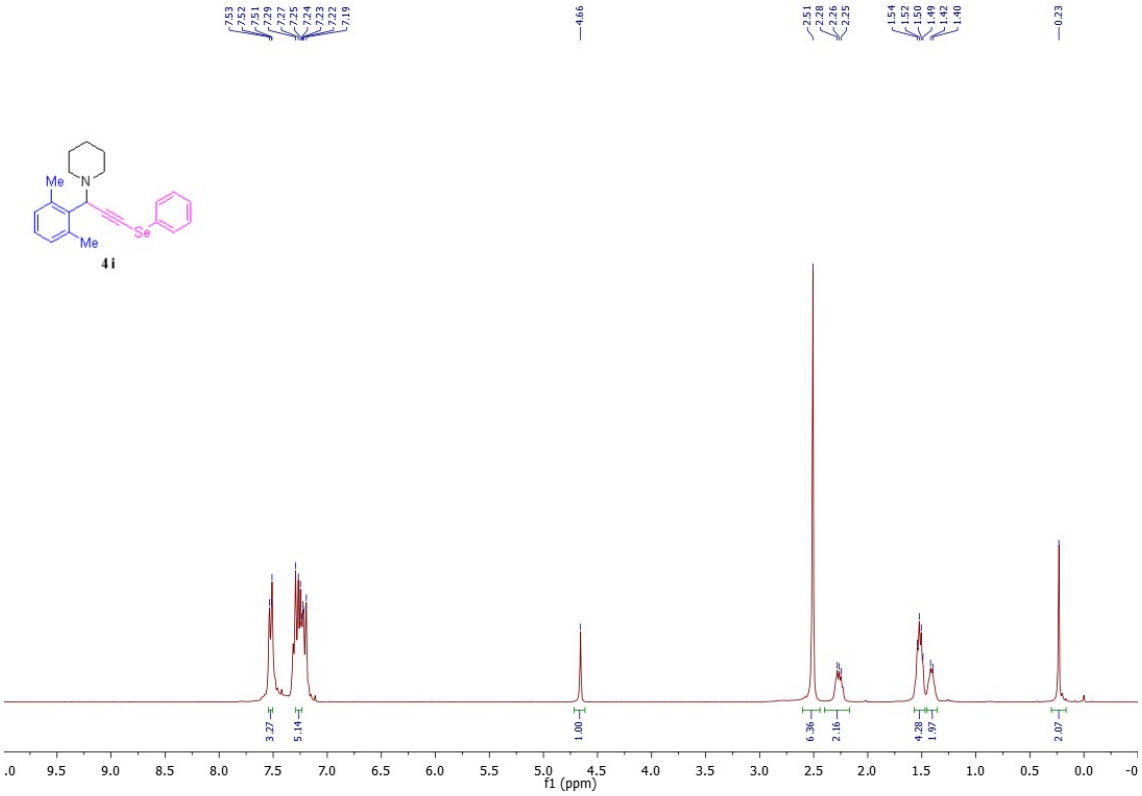

136.21
134.62
130.56
129.85
129.51
129.07
129.03
128.89
127.02
126.23
100.29
77.55
77.12
76.70
66.15
60.33
50.83
26.17
24.48

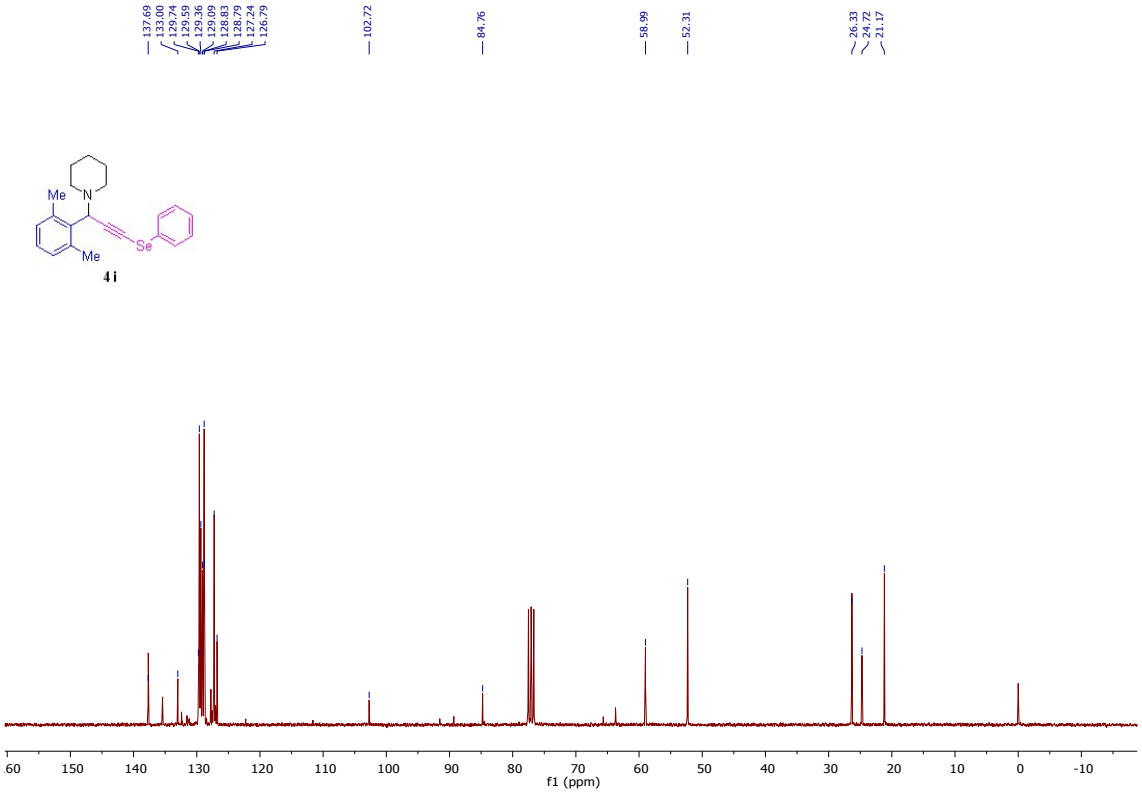

Cl
N
Se

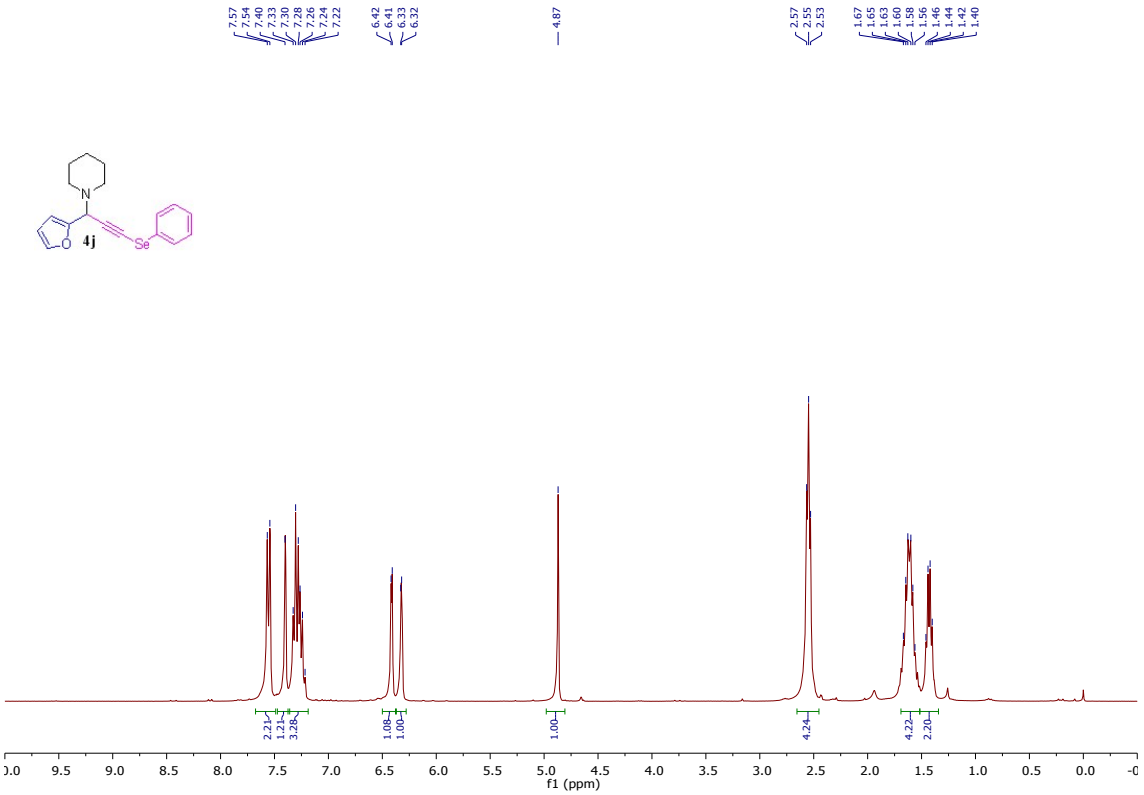
4g

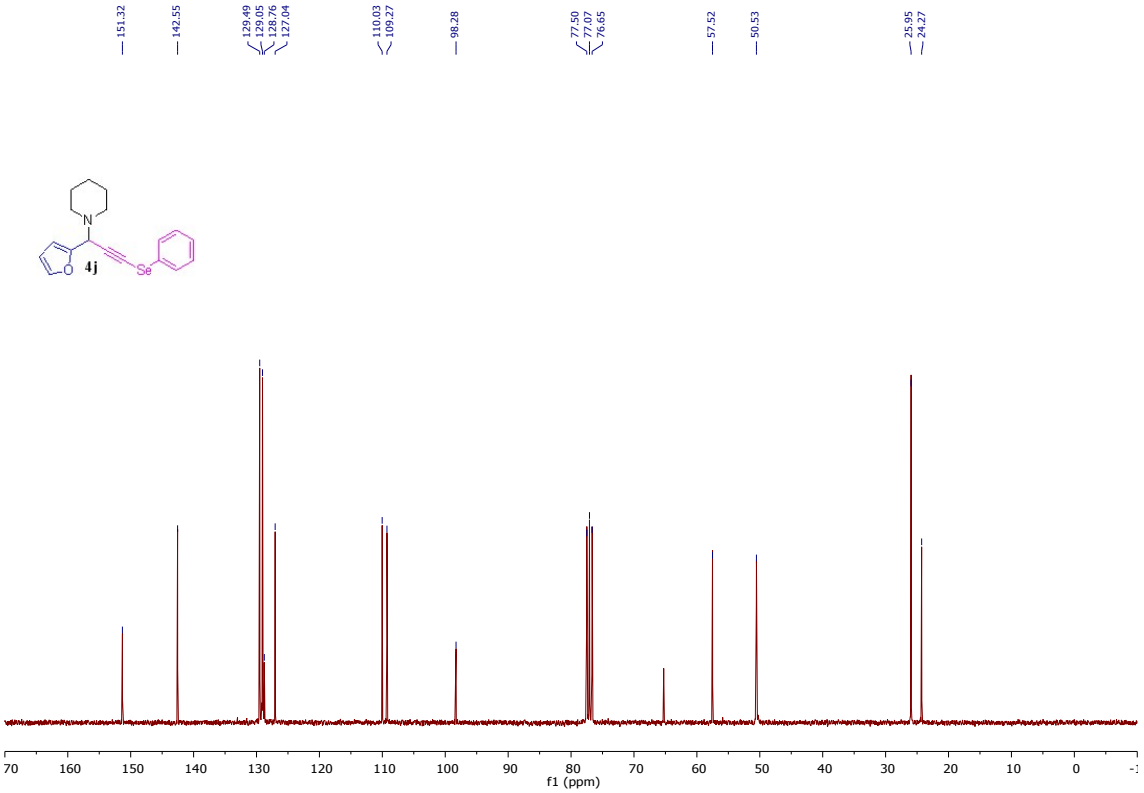

140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1
f1 (ppm)

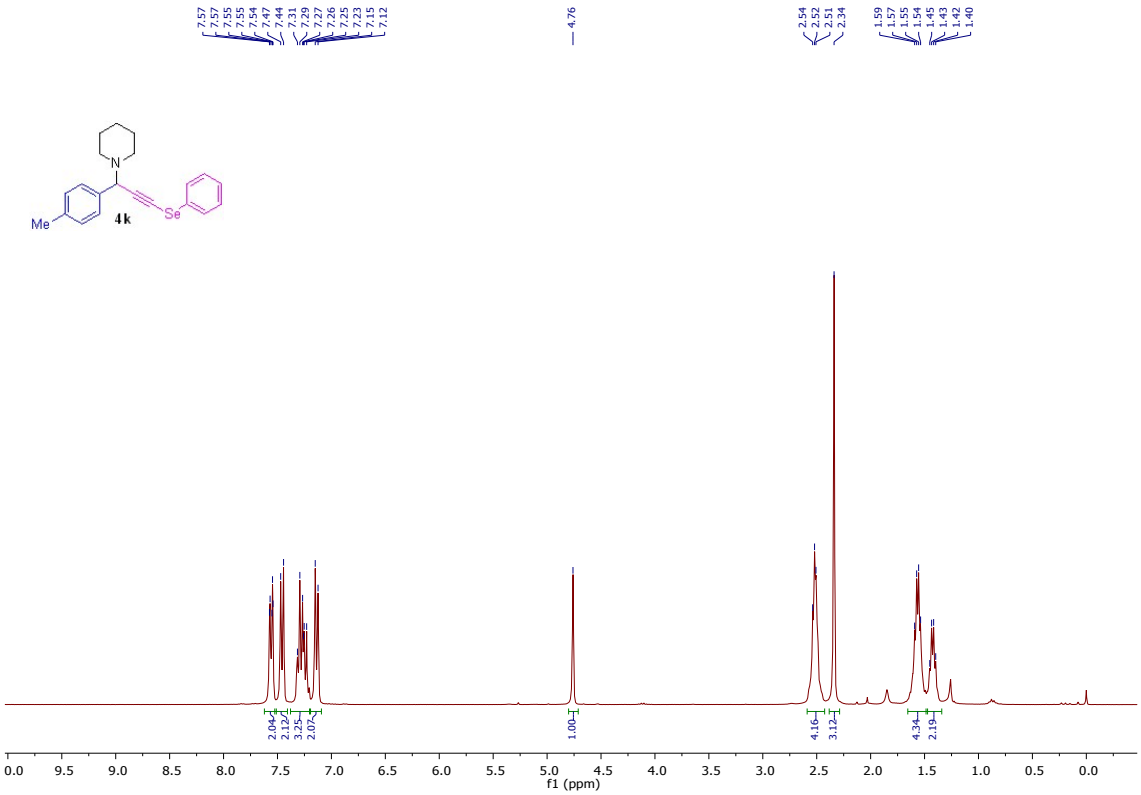

7.56
7.53
7.27
7.25
7.22
7.19
7.17
6.56
6.53
5.36
3.76
2.69
2.68
2.67
2.65
2.60
2.58
2.56
2.55
1.60
1.59
1.57
1.55
1.53
1.40
1.38
1.36
1.34
OMe
N
Se
OMe
4 h
1.95
4.20
2.07
1.00
6.17
4.39
4.27
2.15
f1 (ppm)
158.93
130.02
129.27
129.20
128.63
126.54
114.81
104.96
103.94
77.66
77.23
76.81
60.79
56.11
52.77
51.50
26.26
24.39
OMe
N
Se
OMe
4 h
f1 (ppm)

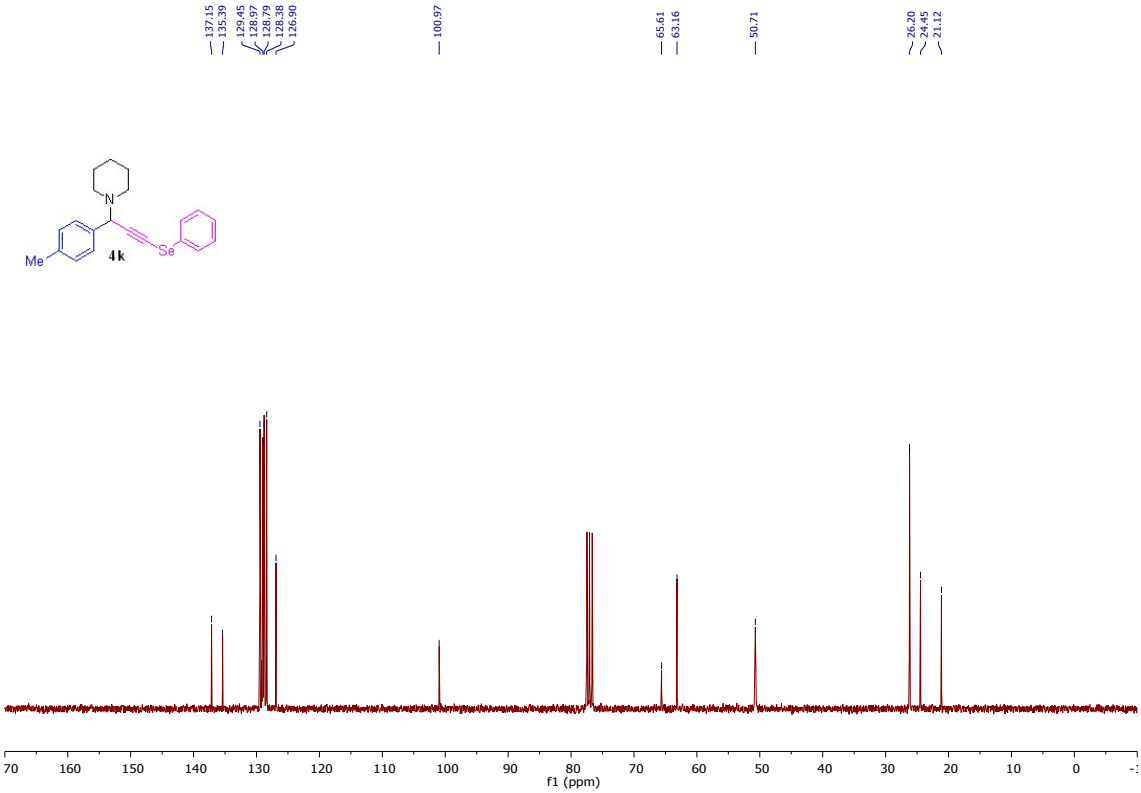

7.53
7.52
7.51
7.29
7.27
7.25
7.24
7.23
7.22
7.19
4.66
2.51
2.28
2.26
2.25
1.54
1.52
1.50
1.49
1.42
1.40
0.23
Me
N
Se
Me
4i
3.27
5.14
1.00
6.36
2.16
4.28
1.97
2.07
f1 (ppm)

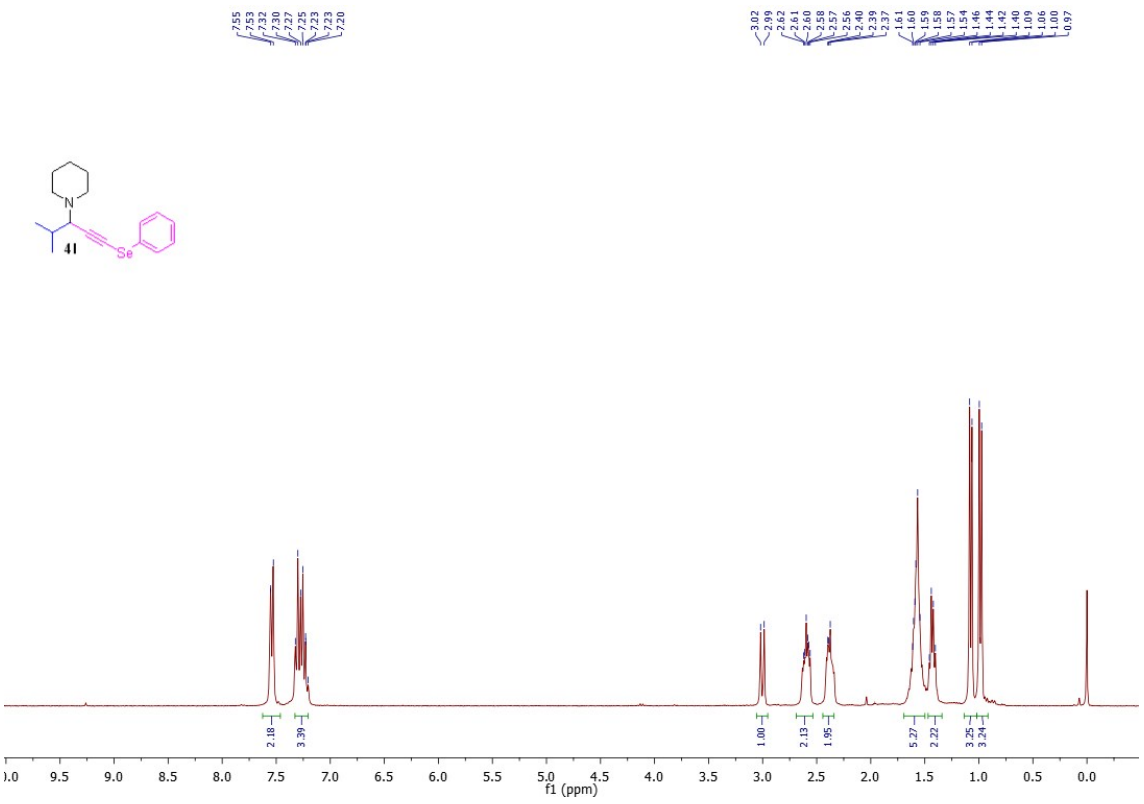

137.69
133.00
129.74
129.59
129.36
129.09
128.83
128.79
127.24
126.79
102.72
84.76
58.99
52.31
26.33
24.72
21.17
Me
N
Se
Me
4i
f1 (ppm)

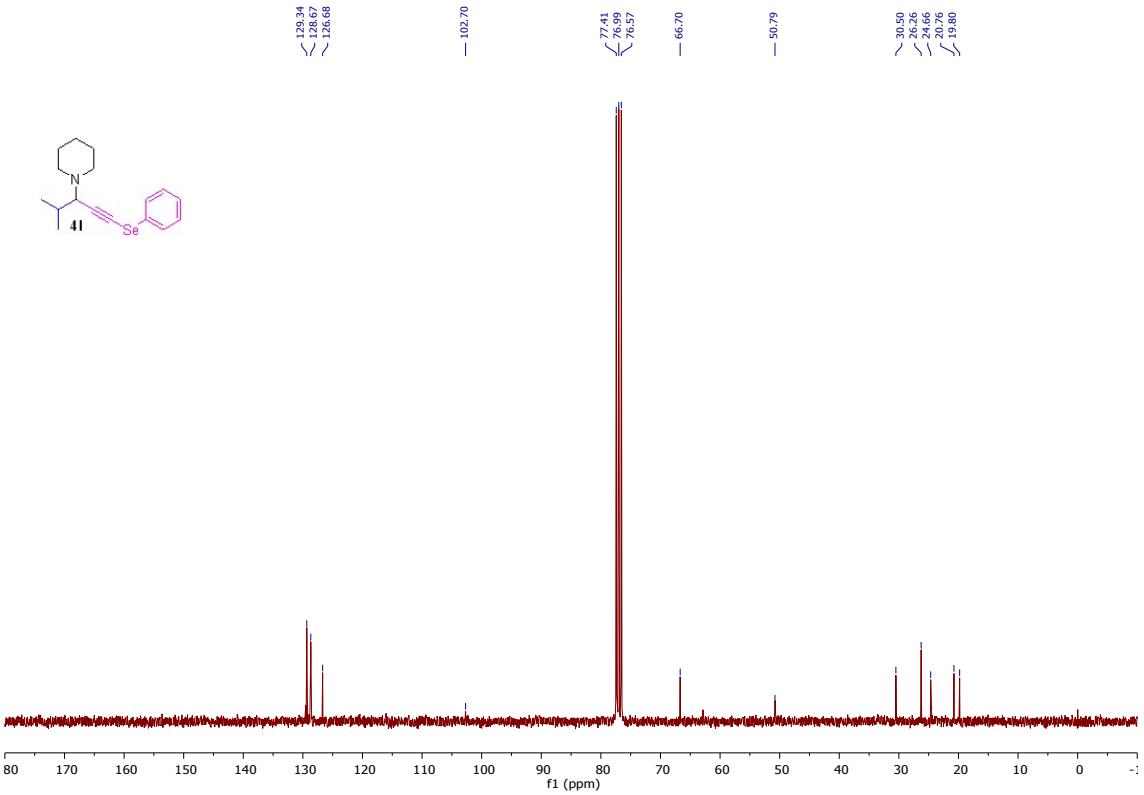

7.57
7.54
7.40
7.33
7.30
7.28
7.26
7.24
7.22
6.42
6.41
6.33
6.32
4.87
2.57
2.55
2.53
1.67
1.65
1.63
1.60
1.58
1.56
1.46
1.44
1.42
1.40
4j
Se
2.21
1.21
3.28
1.08
1.00
1.00
4.24
4.22
2.20
f1 (ppm)

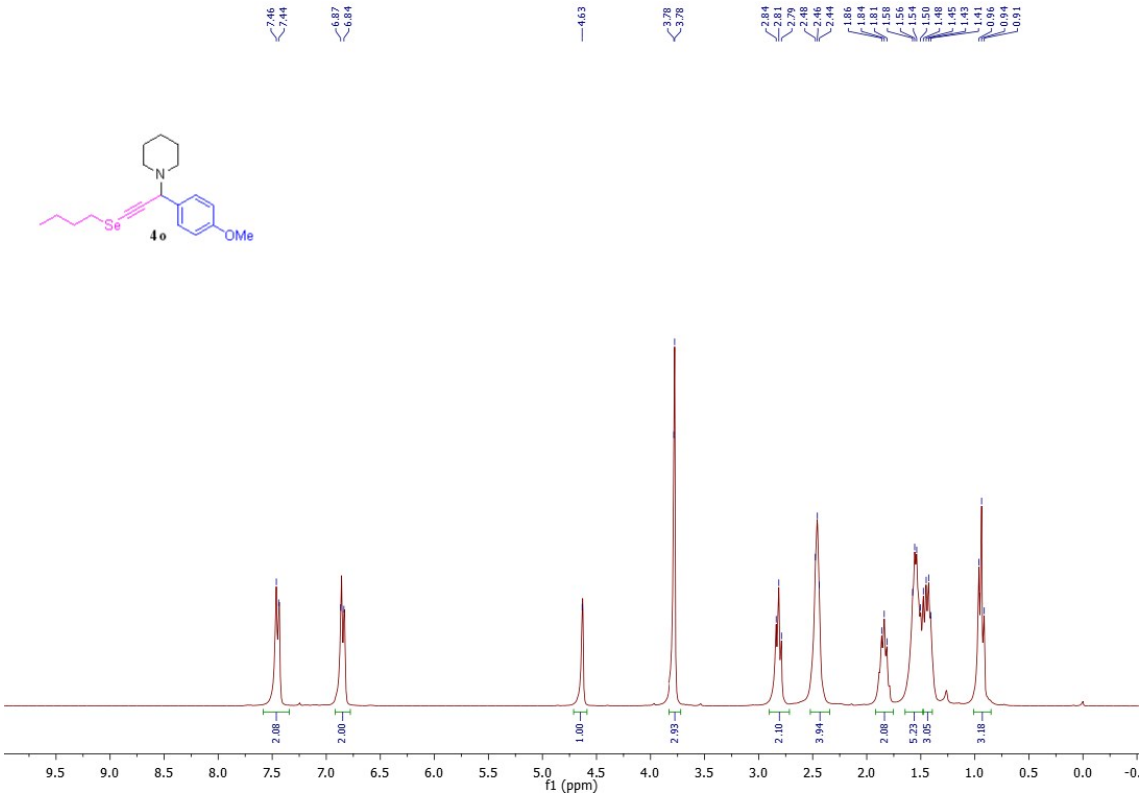

151.32
142.55
129.49
129.05
128.76
127.04
110.03
109.27
98.28
77.50
77.07
76.65
57.52
50.53
25.95
24.27
4j
Se
f1 (ppm)

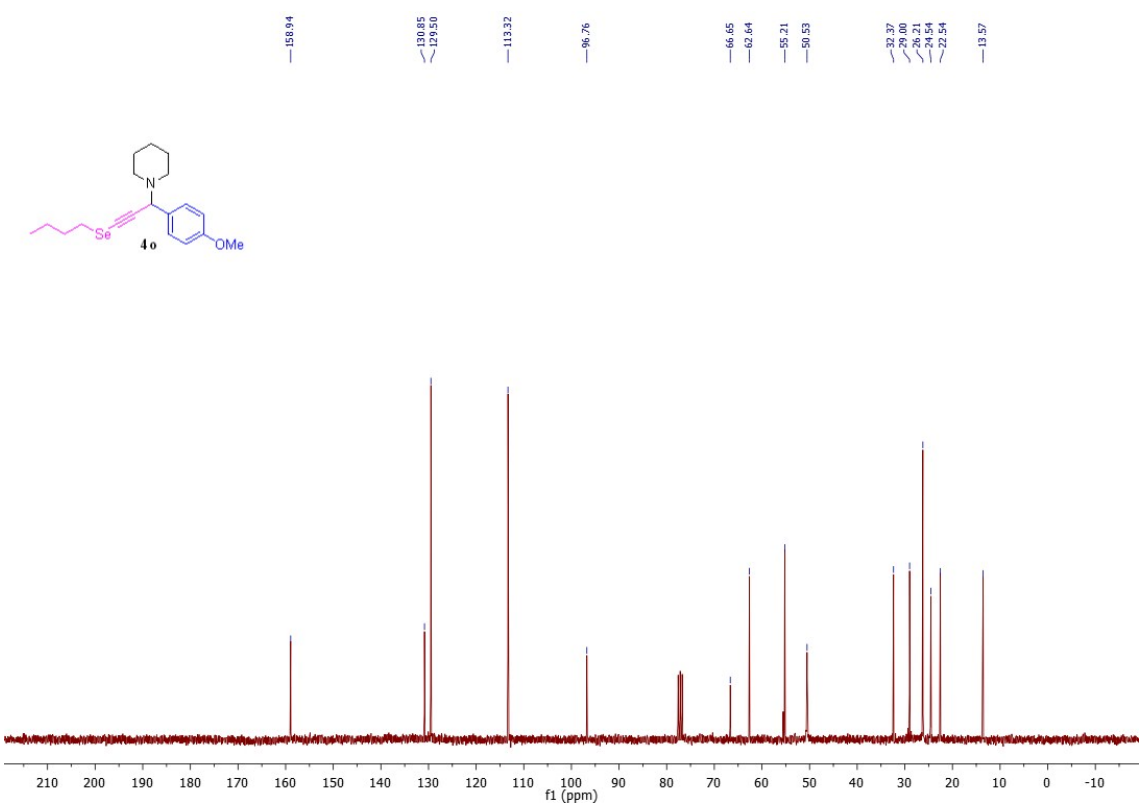

7.57
7.57
7.55
7.55
7.54
7.47
7.44
7.31
7.29
7.27
7.26
7.25
7.23
7.15
7.12
4.76
2.54
2.52
2.51
2.34
1.59
1.57
1.55
1.54
1.45
1.43
1.42
1.40
Me
4k
Se
2.04
2.12
3.25
2.07
1.00
4.16
3.12
4.34
2.19
f1 (ppm)

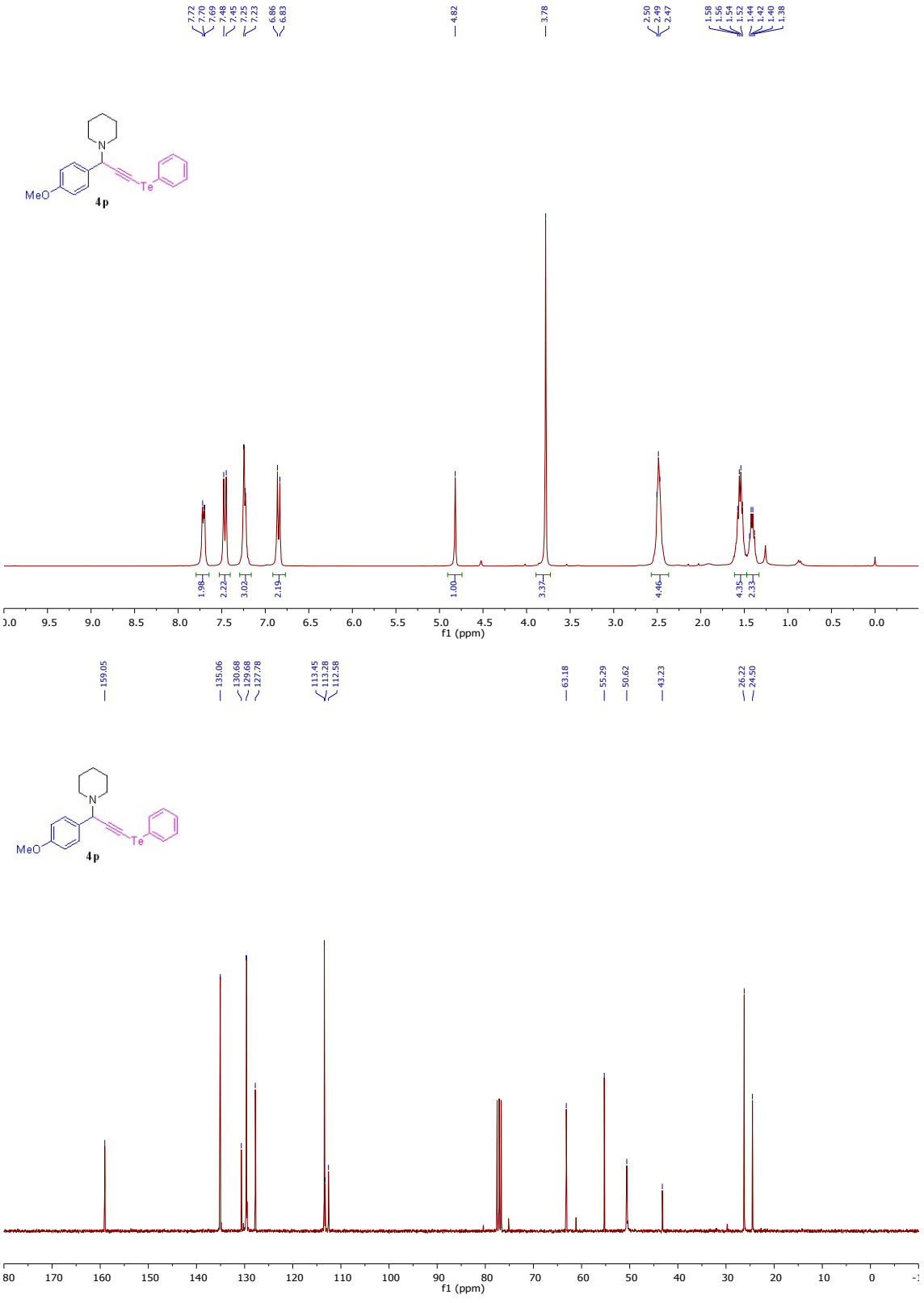

137.15
135.39
129.45
128.97
128.79
128.38
126.90
100.97
65.61
63.16
50.71
26.20
24.45
21.12
Me
4k
Se
f1 (ppm)

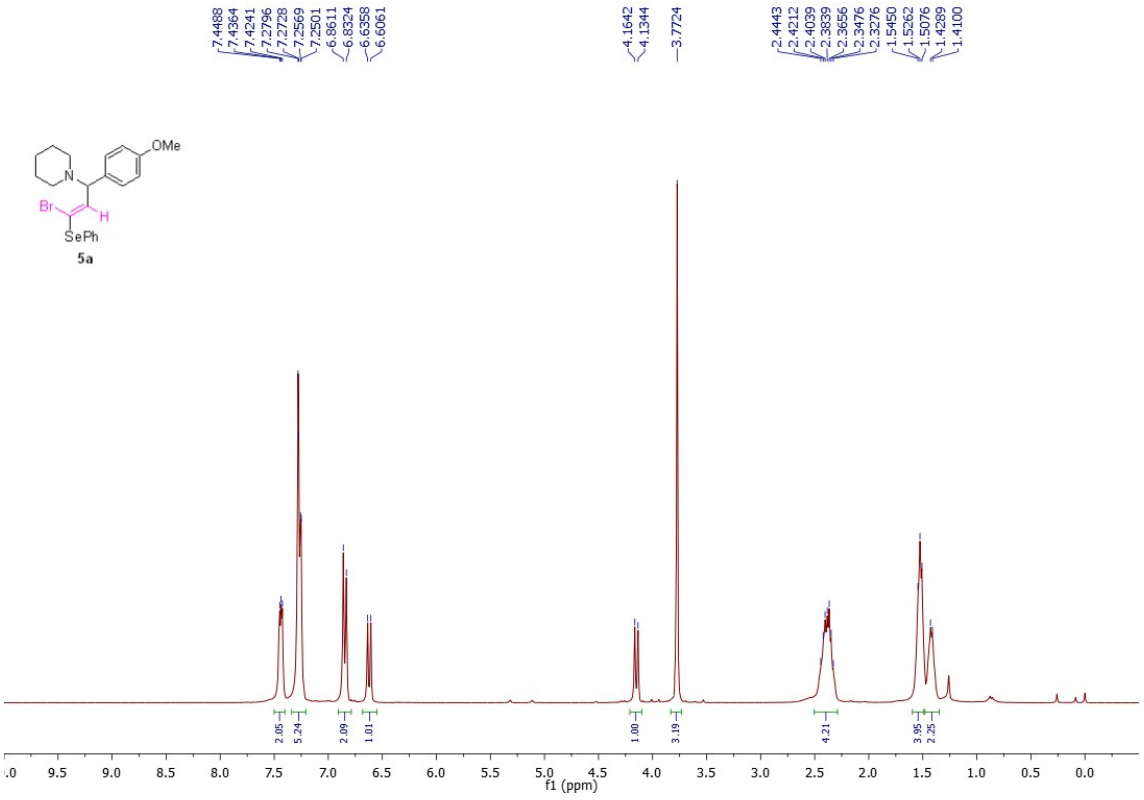

41
f1 (ppm)

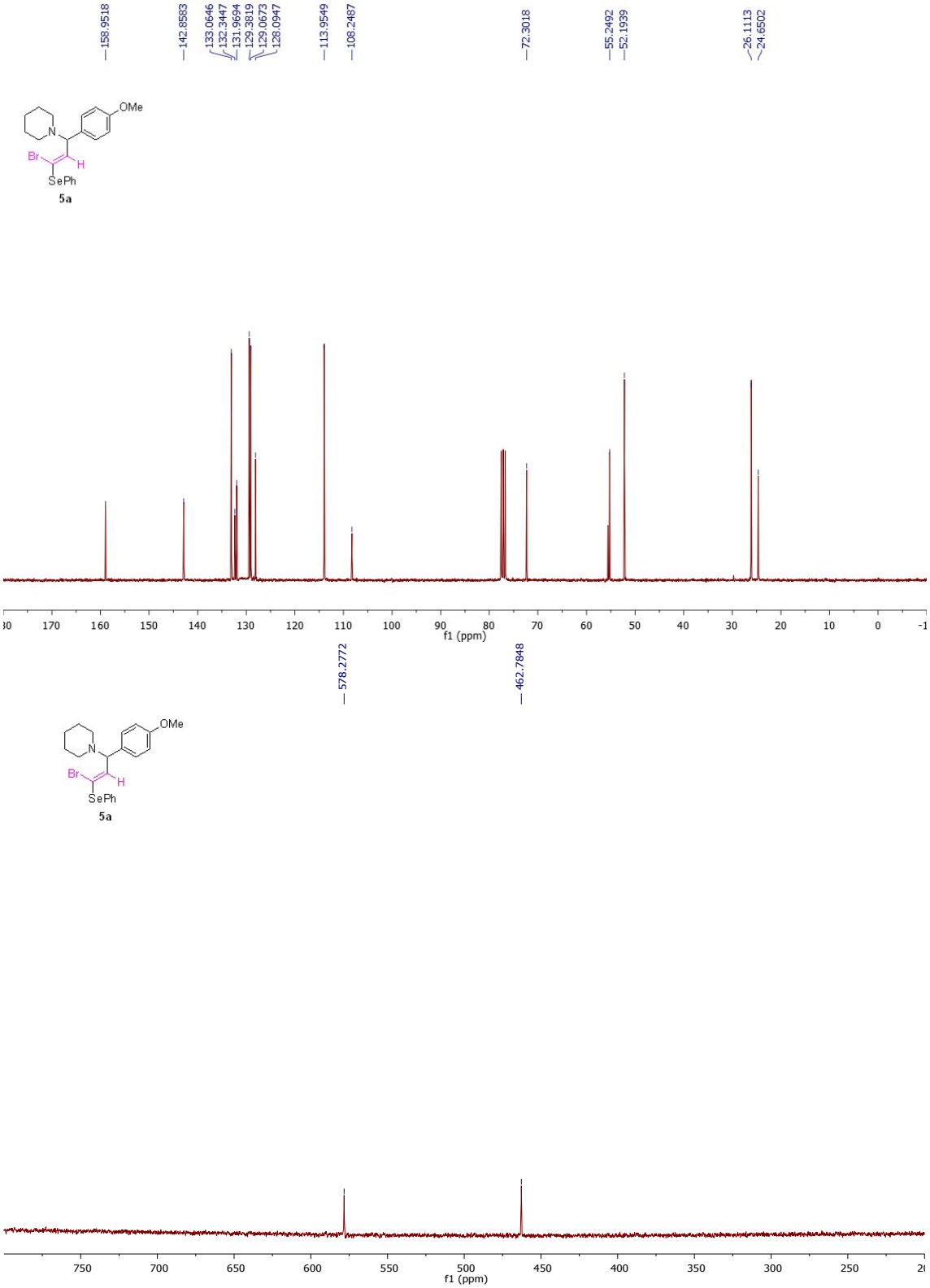

41
f1 (ppm)

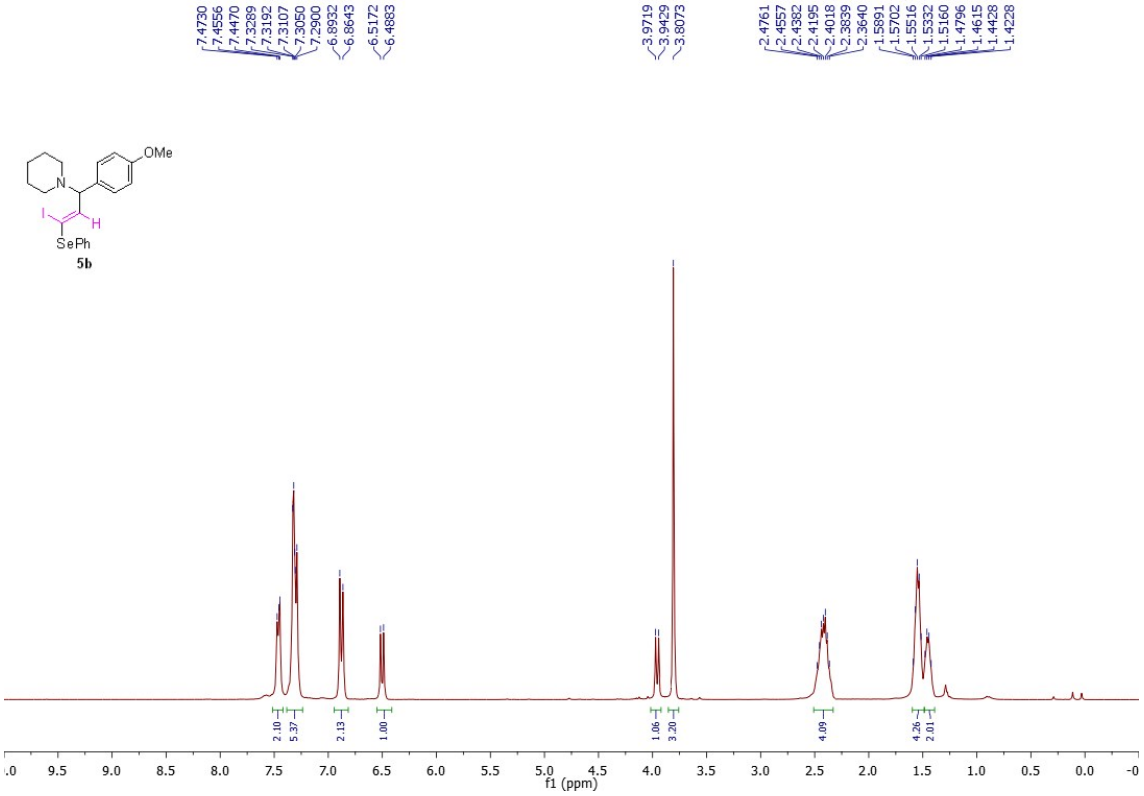

7.46
7.44
6.87
6.84
4.63
3.78
3.78
2.84
2.81
2.79
2.48
2.46
2.44
1.86
1.84
1.81
1.58
1.56
1.54
1.55
1.48
1.45
1.43
1.41
0.96
0.94
0.91
N
Se
OMe
4o
2.08
2.00
1.00
2.93
2.10
3.94
2.08
5.23
3.05
3.18
f1 (ppm)

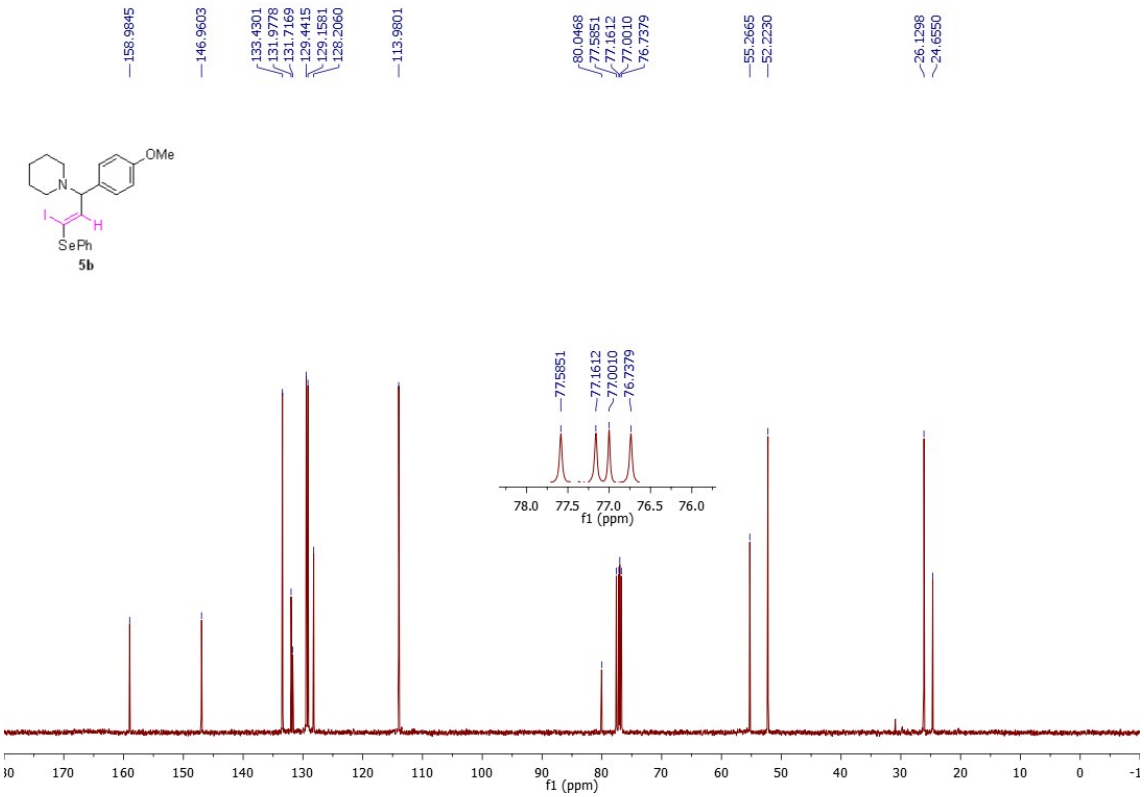

158.94
130.85
129.50
113.32
96.76
66.65
62.64
55.21
50.53
32.37
29.00
26.21
24.54
22.54
13.57
N
Se
OMe
4o
f1 (ppm)

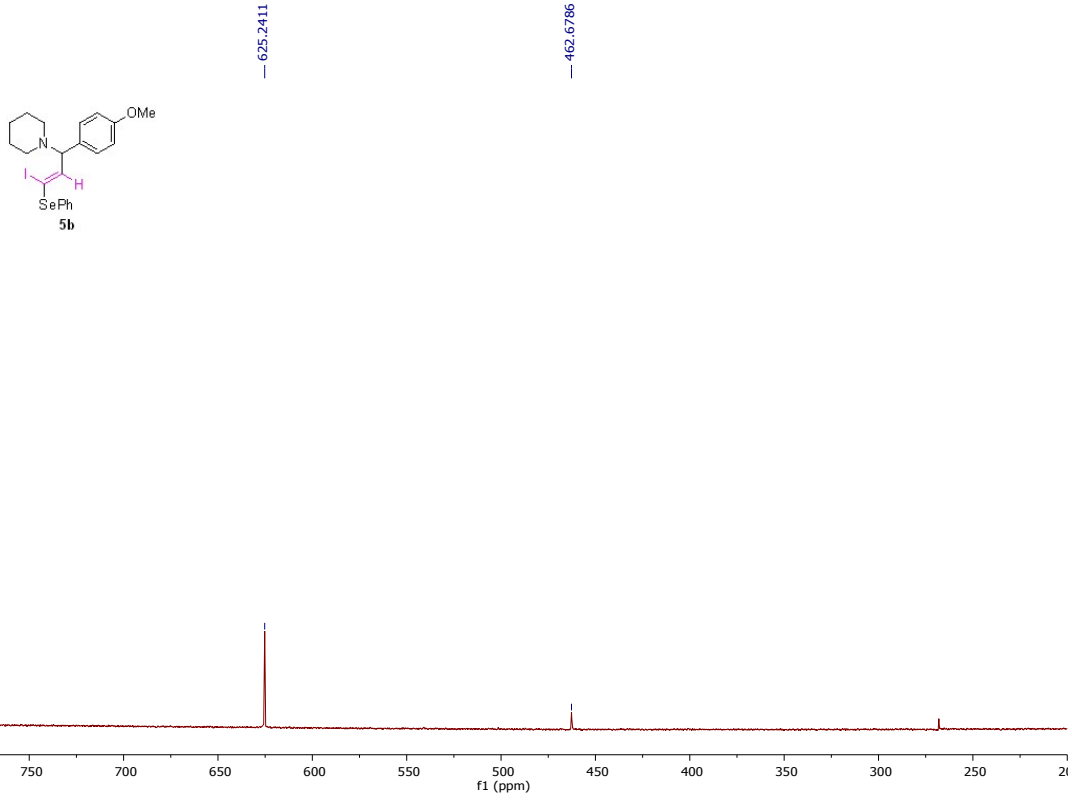

7.72
7.70
7.69
7.48
7.45
7.25
7.23
6.86
6.83
4.82
3.78
2.50
2.49
2.47
1.58
1.56
1.54
1.52
1.44
1.42
1.40
1.38
MeO
Te
4p
1.98
2.22
3.02
2.19
1.00
3.37
4.46
4.35
2.33
f1 (ppm)
159.05
135.06
130.68
129.68
127.78
113.45
113.28
112.58
63.18
55.29
50.62
43.23
26.22
24.50
MeO
Te
4p
f1 (ppm)

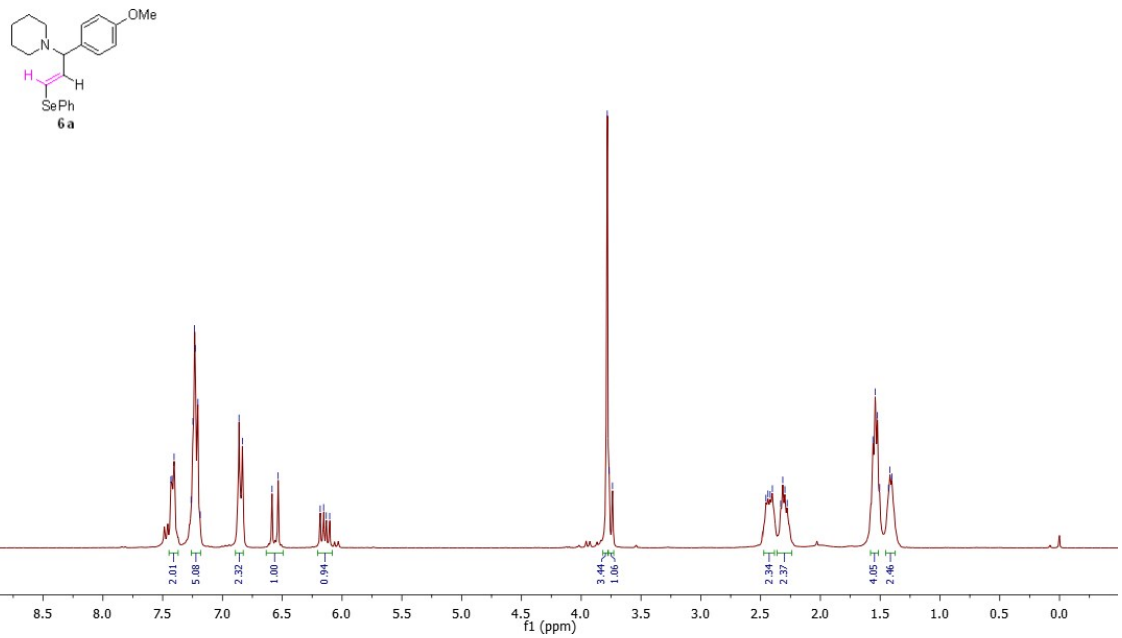

7.4488
7.4364
7.4241
7.2796
7.2728
7.2569
7.2501
6.8611
6.8324
6.6358
6.6061
4.1642
4.1344
3.7724
2.4443
2.4212
2.4039
2.3839
2.3656
2.3476
2.3276
1.5450
1.5262
1.5076
1.4289
1.4100
OMe
N
Br
H
SePh
5a
2.05
5.24
2.09
1.01
1.00
3.19
4.21
3.95
2.25
f1 (ppm)

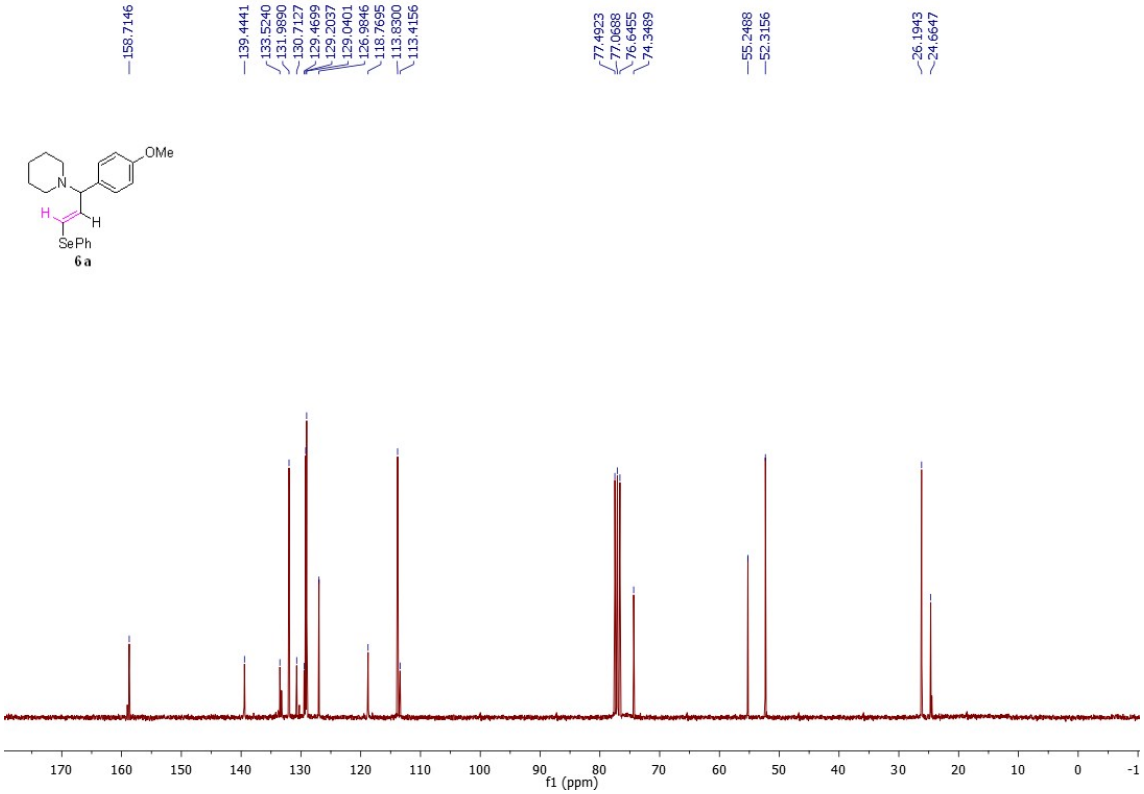

158.9518
142.8583
133.0646
132.3447
131.9694
129.3819
129.0673
128.0947
113.9549
108.2487
72.3018
55.2492
52.1939
26.1113
24.6502
OMe
Br
H
SePh
5a
f1 (ppm)
578.2772
462.7848
OMe
Br
H
SePh
5a
f1 (ppm)

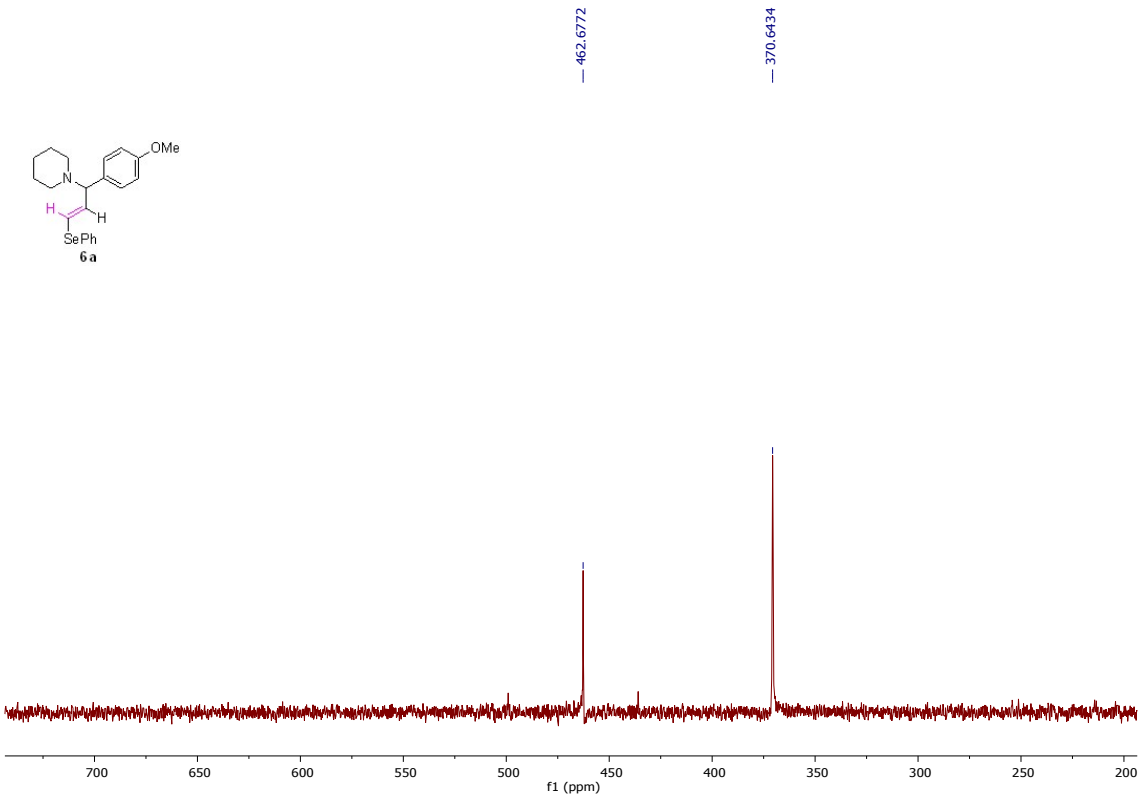

7.4730
7.4556
7.4470
7.3289
7.3192
7.3107
7.3050
7.2900
6.8932
6.8643
6.5172
6.4883
3.9719
3.9429
3.8073
2.4761
2.4557
2.4382
2.4195
2.4018
2.3839
2.3640
1.5891
1.5702
1.5516
1.5332
1.5160
1.4796
1.4615
1.4428
1.4228
OMe
I
H
SePh
5b
2.10
5.37
2.13
1.00
1.06
3.20
4.09
4.26
2.01
f1 (ppm)

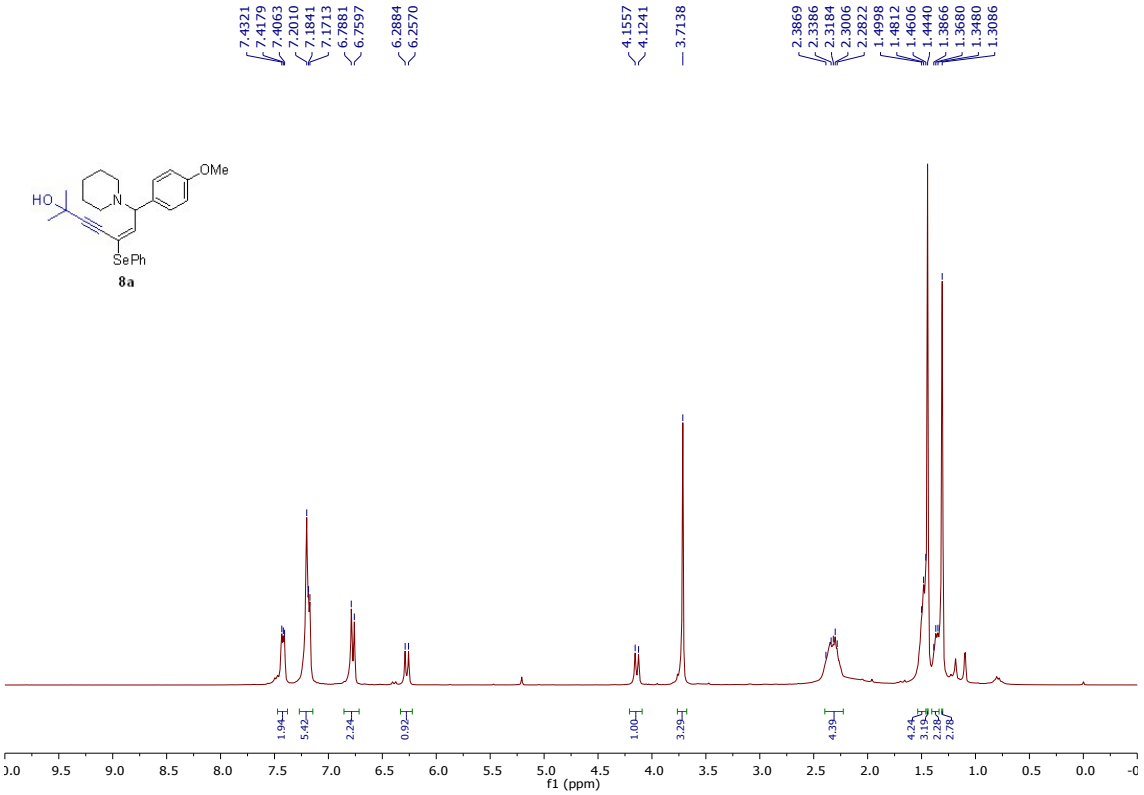

158.9845
146.9603
133.4301
131.9778
131.7169
129.4415
129.1581
128.2060
113.9801
80.0468
77.5851
77.1612
77.0010
76.7379
55.2665
52.2230
26.1298
24.6550
OMe
I
H
SePh
5b
77.5851
77.1612
77.0010
76.7379
f1 (ppm)

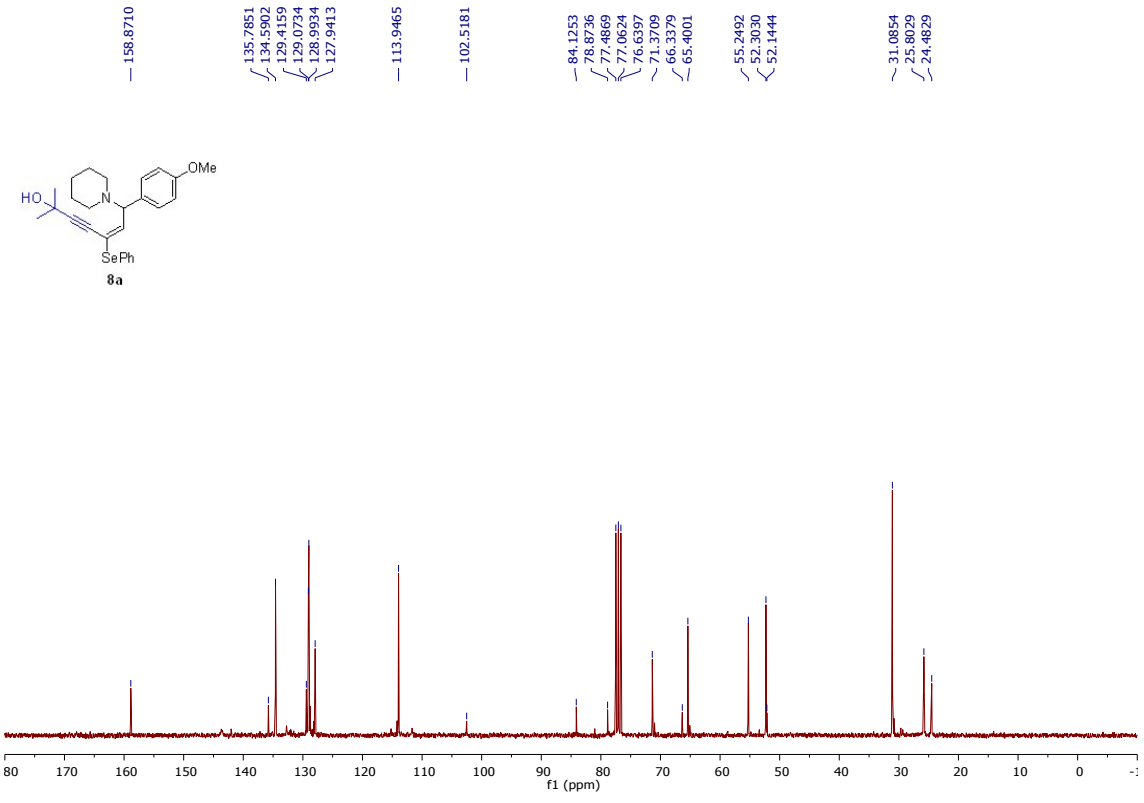

625.2411
462.6786
OMe
I
H
SePh
5b
f1 (ppm)
7.4314
7.4213
7.4050
7.2625
7.2469
7.2333
7.2277
7.2054
7.1860
6.8614
6.8333
6.5855
6.5347
6.1829
6.1541
6.1320
6.1034
3.7822
3.7658
3.7382
2.4554
2.4384
2.4199
2.4013
2.3319
2.3143
2.2962
2.2773
1.5609
1.5416
1.5224
1.5038
1.4305
1.4186
1.4012

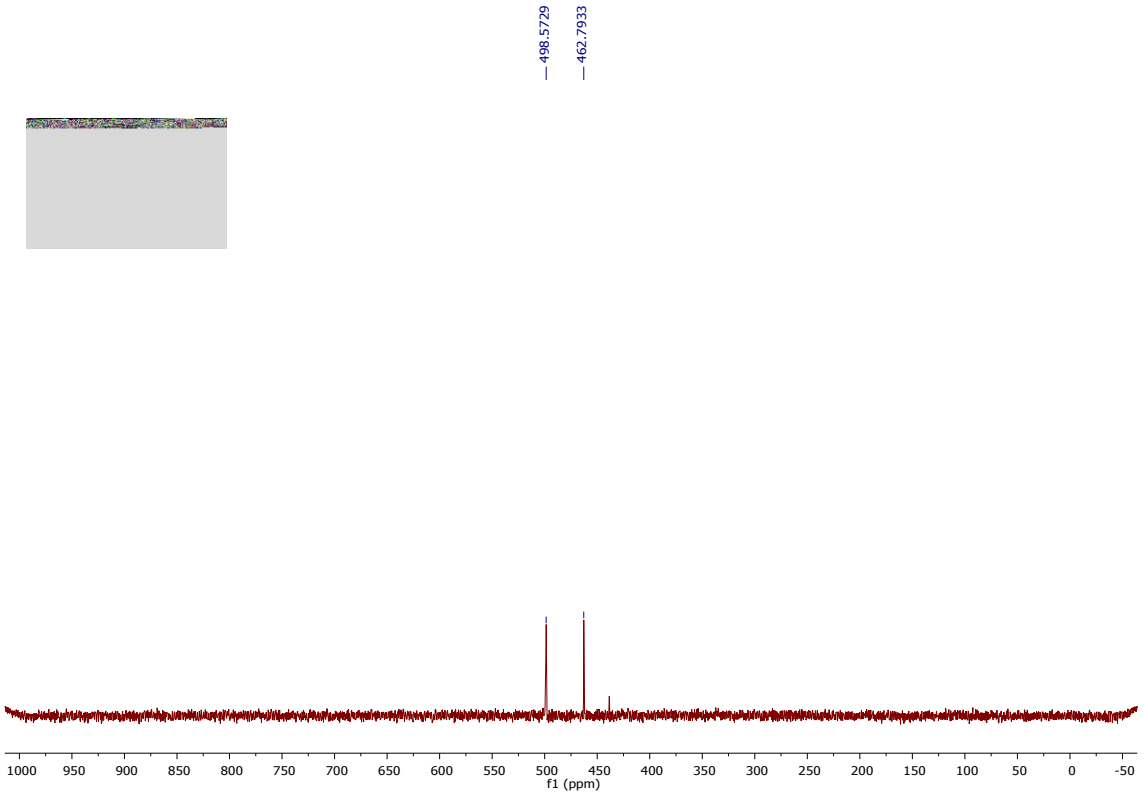

OMe
H
H
SePh
6a
2.01
5.08
2.32
1.00
0.94
3.44
1.06
2.34
2.37
4.05
2.46
f1 (ppm)

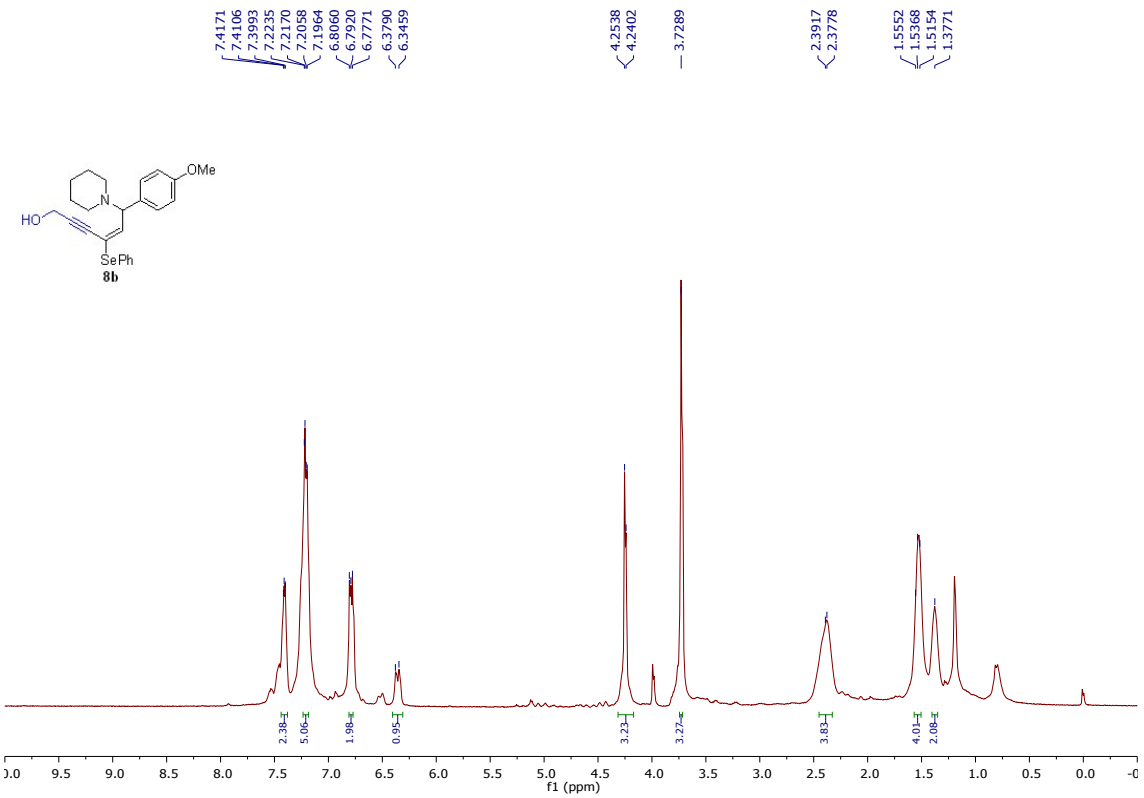

158.7146
139.4441
133.5240
131.9890
130.7127
129.4699
129.2037
129.0401
126.9846
118.7695
113.8300
113.4156
77.4923
77.0688
76.6455
74.3489
55.2488
52.3156
26.1943
24.6647
OMe
N
H
H
SePh
6a
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1
f1 (ppm)

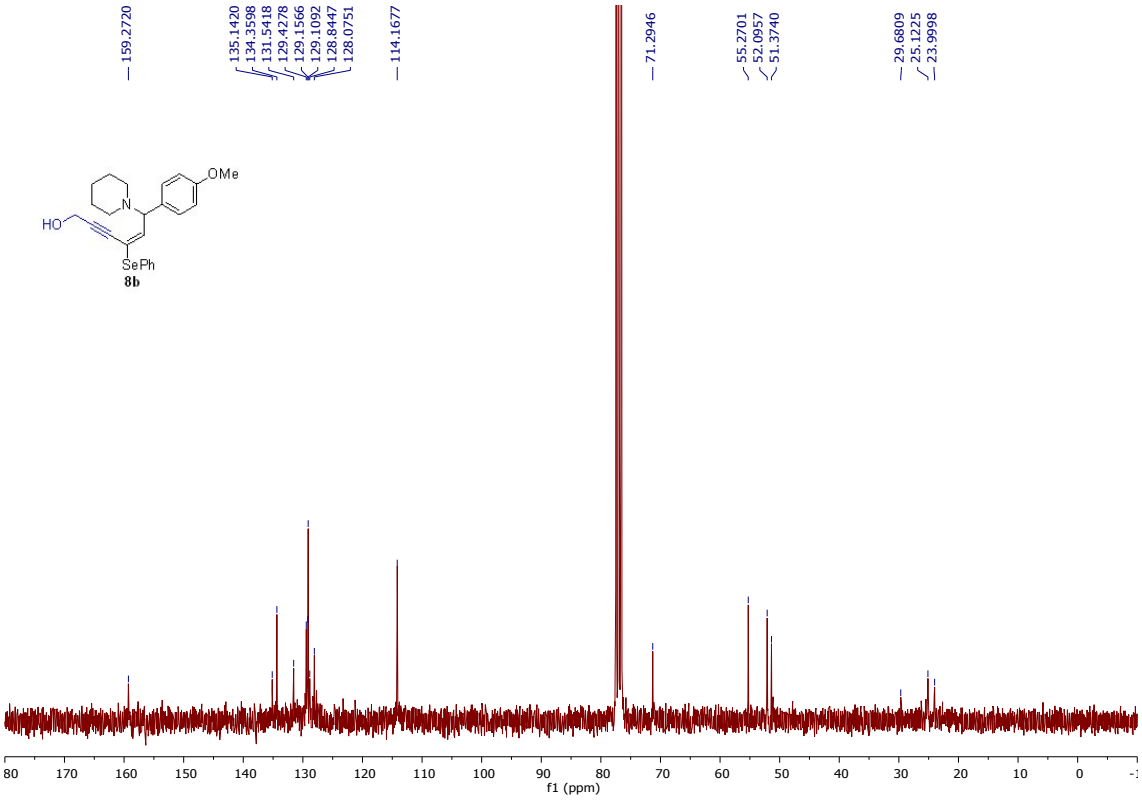

462.6772
370.6434
OMe
N
H
H
SePh
6a
700
650
600
550
500
450
400
350
300
250
200
f1 (ppm)

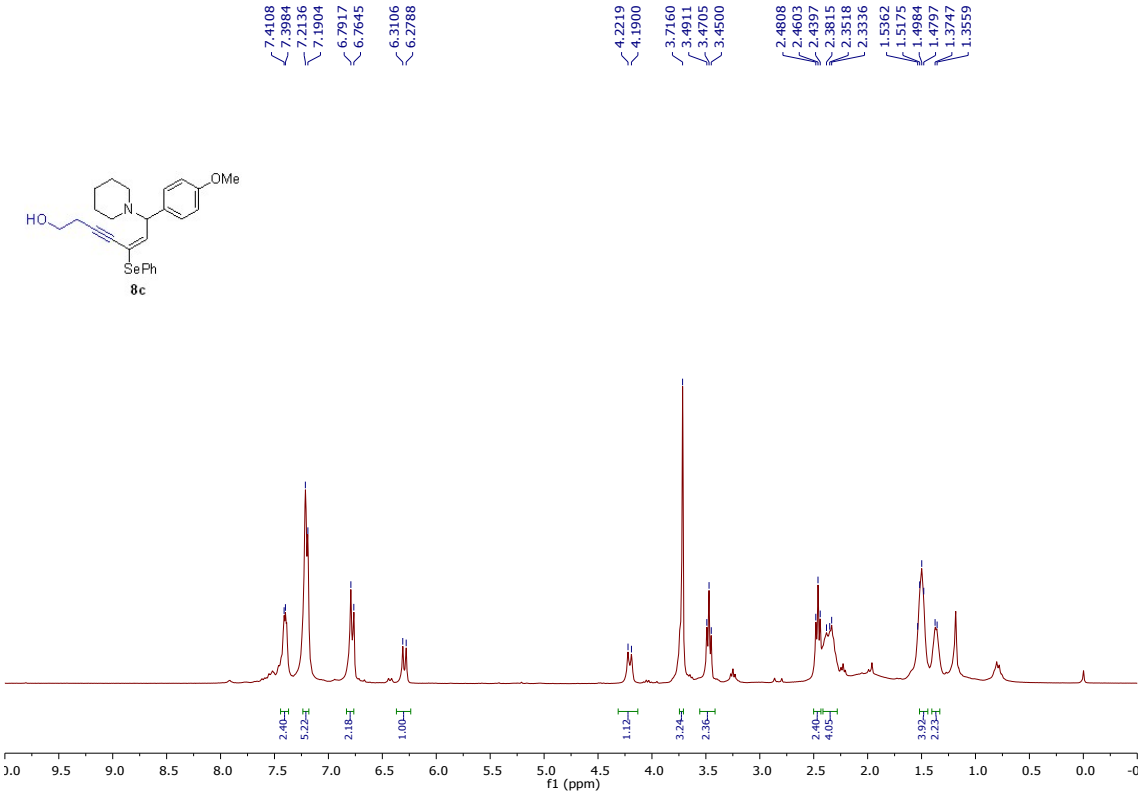

7.4321
7.4179
7.4063
7.2010
7.1841
7.1713
6.7881
6.7597
6.2884
6.2570
4.1557
4.1241
3.7138
2.3869
2.3386
2.3184
2.3006
2.2822
1.4998
1.4812
1.4606
1.4440
1.3866
1.3680
1.3480
1.3086
OMe
HO
N
SePh
8a
1.94
5.42
2.24
0.92
1.00
3.29
4.39
4.24
3.19
2.28
2.78
f1 (ppm)

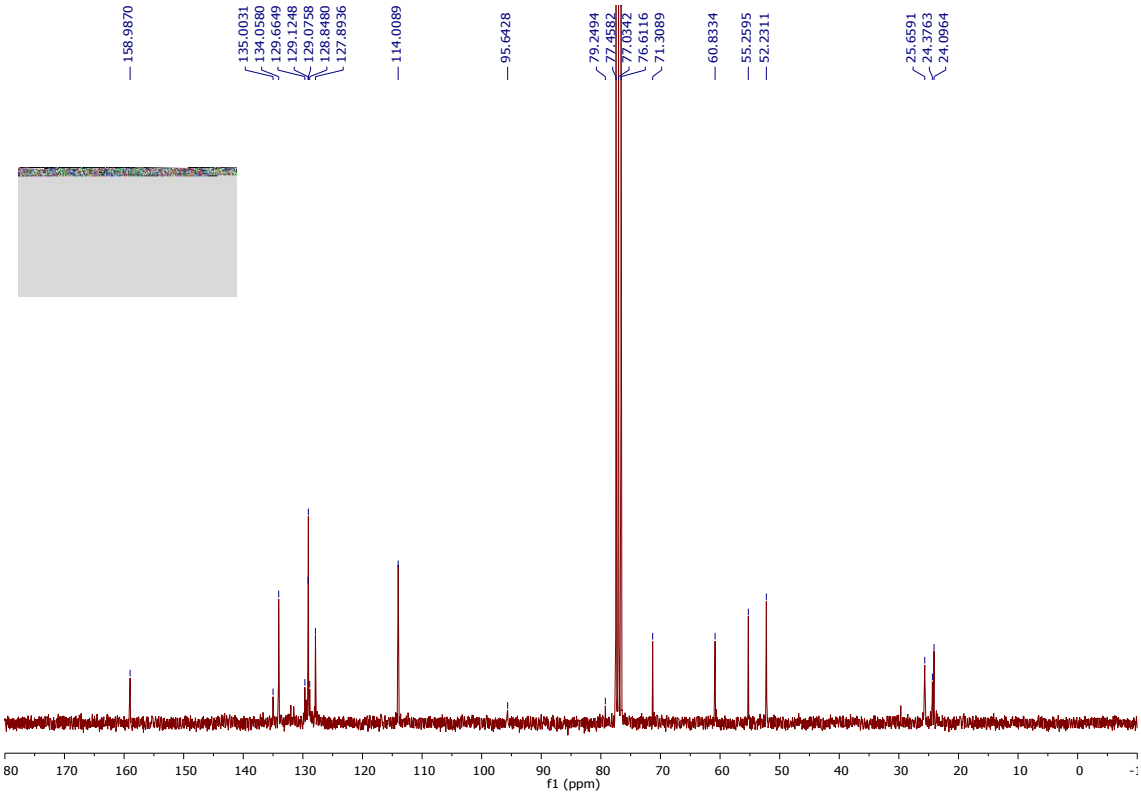

158.8710
135.7851
134.5902
129.4159
129.0734
128.9934
127.9413
113.9465
102.5181
84.1253
78.8736
77.4869
77.0624
76.6397
71.3709
66.3379
65.4001
55.2492
52.3030
52.1444
31.0854
25.8029
24.4829
OMe
HO
N
SePh
8a
f1 (ppm)


498.5729
462.7933
f1 (ppm)

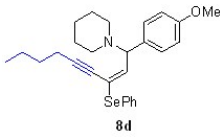

7.4171
7.4106
7.3993
7.2235
7.2170
7.2058
7.1964
6.8060
6.7920
6.7771
6.3790
6.3459
4.2538
4.2402
3.7289
2.3917
2.3778
1.5552
1.5368
1.5154
1.3771
OMe
HO
SePh
8b
2.38
5.06
1.98
0.95
3.23
3.27
3.83
4.01
2.08
f1 (ppm)


159.2720
135.1420
134.3598
131.5418
129.4278
129.1566
129.1092
128.8447
128.0751
114.1677
71.2946
55.2701
52.0957
51.3740
29.6809
25.1225
23.9998
OMe
HO
SePh
8b
f1 (ppm)

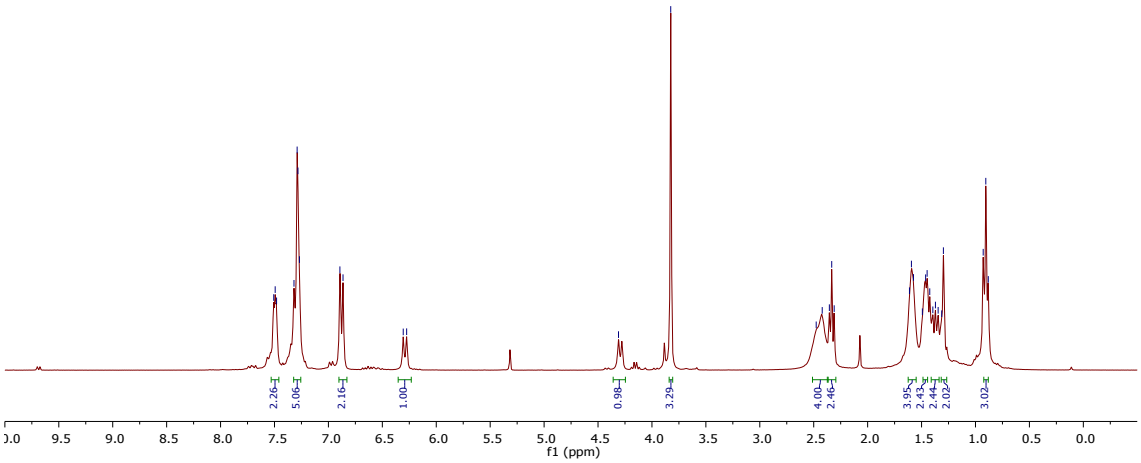

7.4108
7.3984
7.2136
7.1904
6.7917
6.7645
6.3106
6.2788
4.2219
4.1900
3.7160
3.4911
3.4705
3.4500
2.4808
2.4603
2.4397
2.3815
2.3518
2.3336
1.5362
1.5175
1.4984
1.4797
1.3747
1.3559
OMe
HO
SePh
8c
2.40
5.22
2.18
1.00
1.12
3.24
2.36
2.40
4.05
3.92
2.23
f1 (ppm)

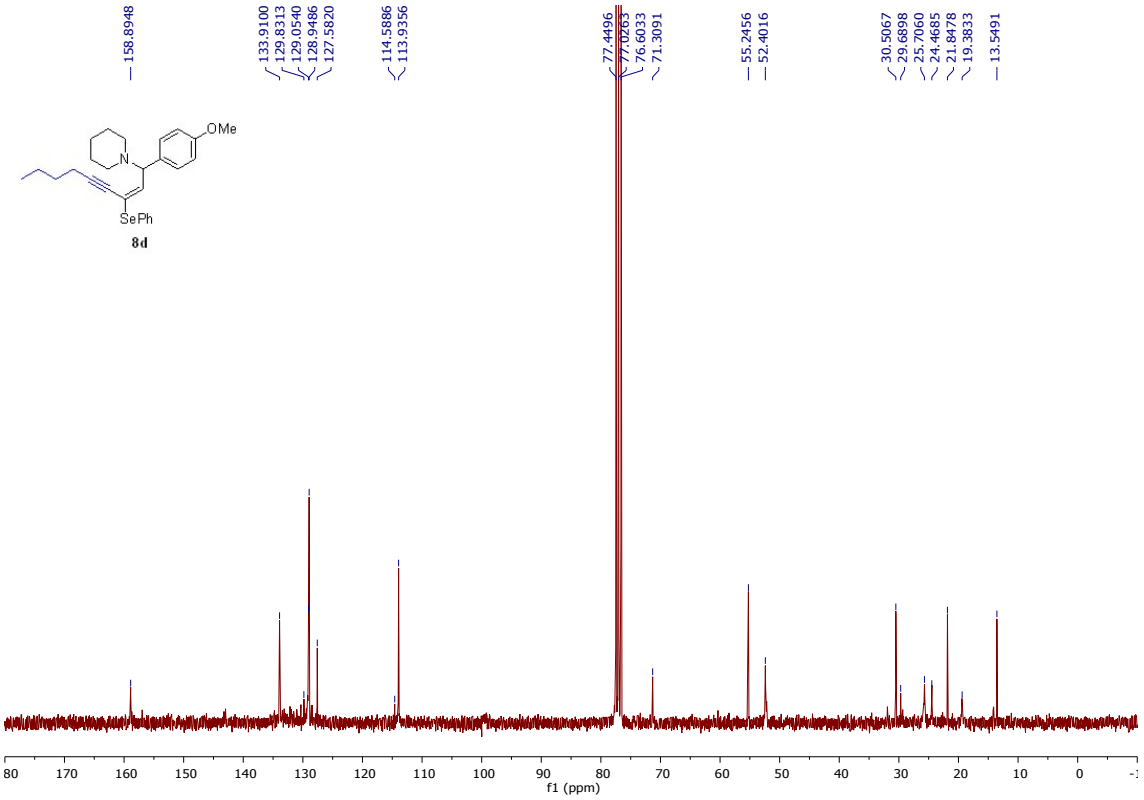

158.9870
135.0031
134.0580
129.6649
129.1248
129.0758
128.8480
127.8936
114.0089
95.6428
79.2494
77.4582
77.0342
76.6116
71.3089
60.8334
55.2595
52.2311
25.6591
24.3763
24.0964
f1 (ppm)


7.5069
7.4936
7.4807
7.3193
7.2900
7.2827
7.2684
6.8934
6.8646
6.3062
6.2745
4.3101
3.8259
2.4770
2.4212
2.3550
2.3331
2.3102
1.6122
1.5940
1.5748
1.4925
1.4624
1.4485
1.4241
1.3954
1.3714
1.3463
1.3132
1.2975
0.9285
0.9044
0.8812

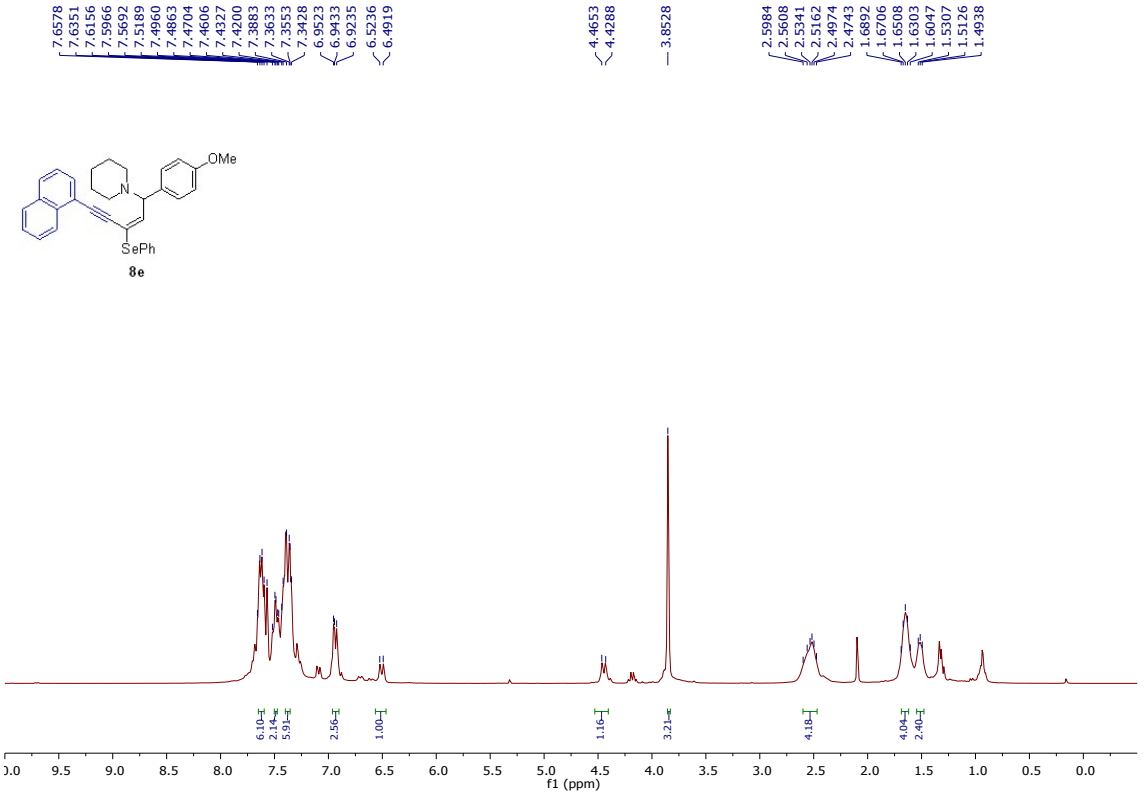

OMe
N
SePh

8d

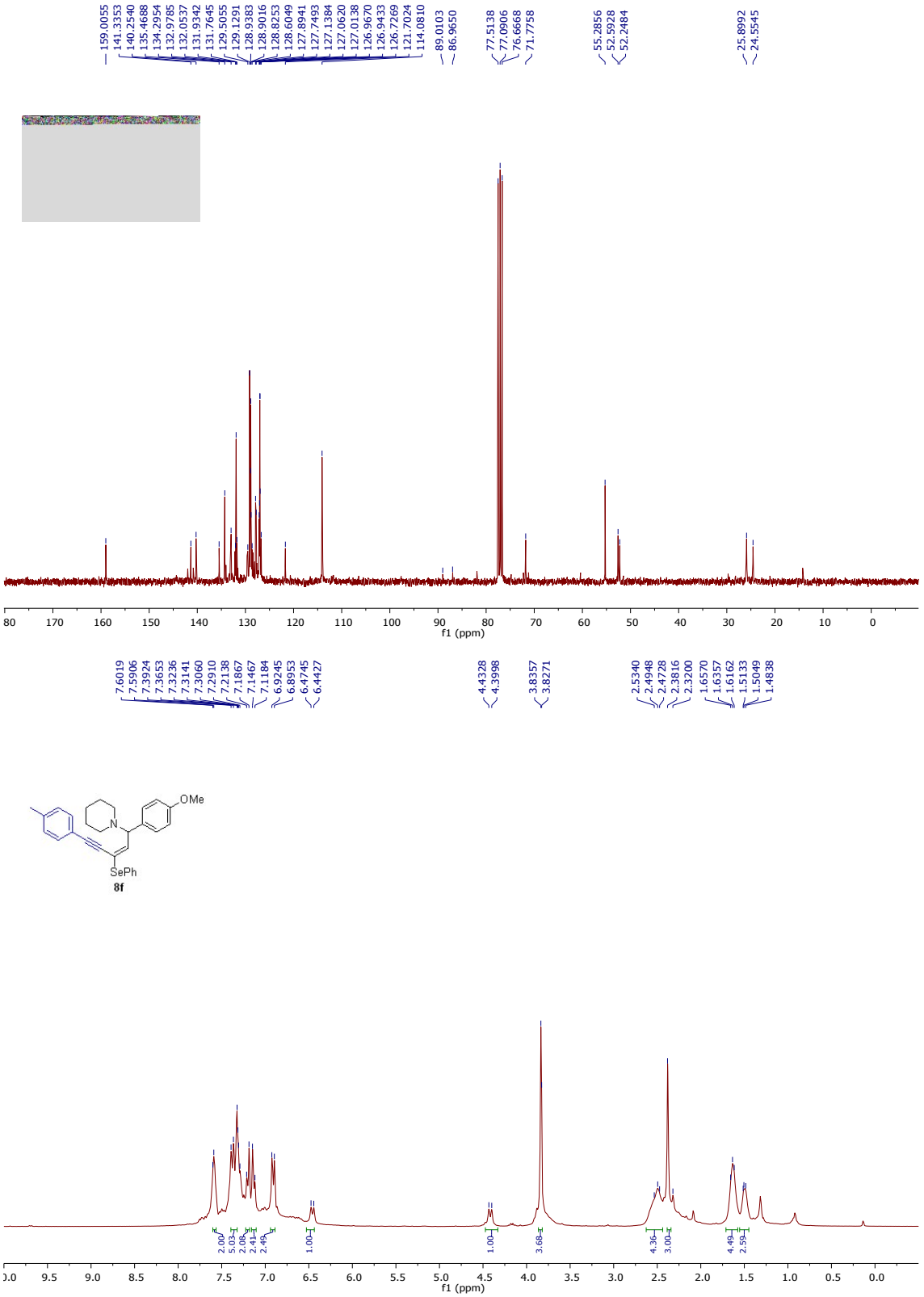

2.26
5.06
2.16
1.00
0.98
3.29
4.00
2.46
3.95
2.43
2.44
2.02
3.02
f1 (ppm)

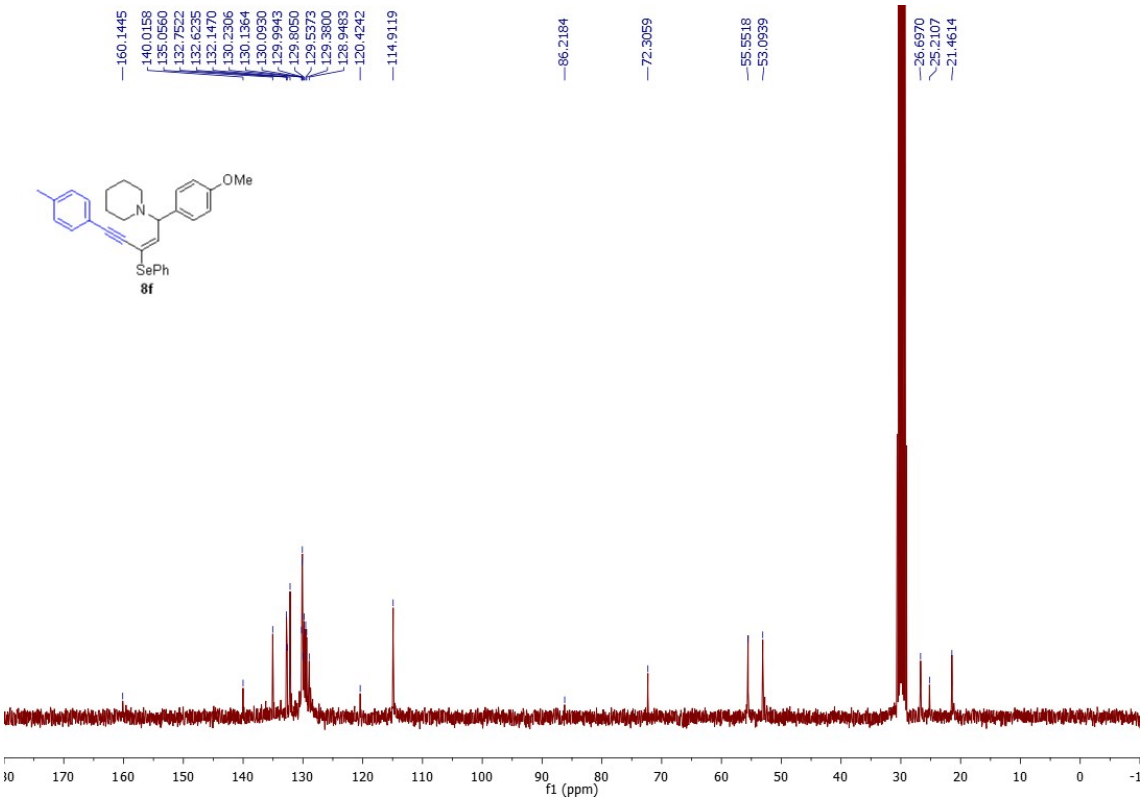

158.8948
133.9100
129.8313
129.0540
128.9486
127.5820
114.5886
113.9356
77.4496
77.0263
76.6033
71.3091
55.2456
52.4016
30.5067
29.6898
25.7060
24.4685
21.8478
19.3833
13.5491
OMe
N
SePh
f1 (ppm)

8d


7.6578
7.6351
7.6156
7.5966
7.5692
7.5189
7.4960
7.4863
7.4704
7.4606
7.4327
7.4200
7.3883
7.3633
7.3553
7.3428
6.9523
6.9433
6.9235
6.5236
6.4919
4.4653
4.4288
3.8528
2.5984
2.5608
2.5341
2.5162
2.4974
2.4743
1.6892
1.6706
1.6508
1.6303
1.6047
1.5307
1.5126
1.4938
OMe
N
SePh
6.10
2.14
5.91
2.56
1.00
1.16
3.21
4.18
4.04
2.40
f1 (ppm)

8e


159.0055
141.3353
140.2540
135.4688
134.2954
132.9785
132.0537
131.9342
131.7645
129.5055
129.1291
128.9383
128.9016
128.8253
128.6049
127.8941
127.7493
127.1384
127.0620
127.0138
126.9670
126.9433
126.7269
121.7024
114.0810
89.0103
86.9650
77.5138
77.0906
76.6668
71.7758
55.2856
52.5928
52.2484
25.8992
24.5545
f1 (ppm)
7.6019
7.5906
7.3924
7.3653
7.3236
7.3141
7.3060
7.2910
7.2138
7.1867
7.1467
7.1184
6.9245
6.8953
6.4745
6.4427
4.4328
4.3998
3.8357
3.8271
2.5340
2.4948
2.4728
2.3816
2.3200
1.6570
1.6357
1.6162
1.5133
1.5049
1.4838
OMe
N
SePh
8f
2.00
5.03
2.08
2.41
2.49
1.00
1.00
3.68
4.36
3.00
4.49
2.59
f1 (ppm)


160.1445
140.0158
135.0560
132.7522
132.6235
132.1470
130.2306
130.1364
130.0930
129.9943
129.8050
129.5373
129.3800
128.9483
120.4242
114.9119
86.2184
72.3059
55.5518
53.0939
26.6970
25.2107
21.4614
OMe
N
SePh
8f
f1 (ppm)