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Supporting Information for the Paper

Oxidative Selenofunctionalization of Allenes: Convenient Access to 2-(Phenylselanyl)-but-2-enals and 4-Oxo-3-(phenylselanyl)pent-2-enoates

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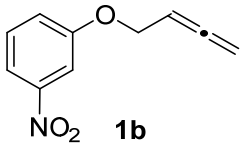
General methods: ^{1}H NMR and ^{13}C NMR spectra were recorded on a Bruker Avance-300 spectrometer. NMR spectra were recorded in $CDCl_3$ or C_6D_6, except otherwise stated. Chemical shifts are given in ppm relative to TMS (^{1}H, 0.00 ppm), or $CDCl_3$ (^{1}H, 7.27 ppm; ^{13}C, 77.0 ppm), or C_6D_6 (^{1}H, 7.16 ppm; ^{13}C, 128.0 ppm). Chemical shifts in ^{77}Se are given in ppm relative to PhSeSePh in $CDCl_3$ (^{77}Se, 0.00 ppm). Low and high resolution mass spectra were taken on an AGILENT 6520 Accurate-Mass QTOF LC/MS spectrometer using the electrospray mode (ES)

unless otherwise stated. IR spectra were recorded on a Bruker Tensor 27 spectrometer. All commercially available compounds were used without further purification.

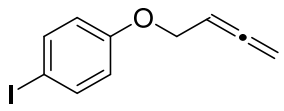
These precursors were readily obtained as described in the literature: 1a and **1g** (Lin, M.-H.; Tsai, W.-S.; Lin, L.-Z.; Hung, S.-F.; Chuang, T.-H.; Su, Y.-J. *J. Org. Chem.* **2011**, *76*, 8518); **1d** (Luo, H.; Ma, S. *Eur. J. Org. Chem.* **2013**, 3041).

General Procedure for the Preparation of Allenes 1b–f and 1h. A well stirred solution of $(CH_2O)_n$ (0.5 mmol), CuI (0.1 mmol), the appropriate alkyne (0.2 mmol), and *N*,*N*-diisopropylethylamine (Hüning's base) (0.36 mmol) in dioxane (1 mL) was refluxed under argon atmosphere. When the reaction was completed as monitored by TLC, it was cooled to RT. Water (5 mL) was added before being extracted with ethyl acetate (3 x 15 mL). The organic phase was washed with water (2 x 5 mL), dried ($MgSO_4$) and concentrated under reduced pressure. Chromatography of the residue eluting with hexanes/ethyl acetate mixtures gave analytically pure compounds **1**. Spectroscopic and analytical data for allenes **1** follow.



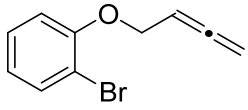
1b

Allene 1b. From 398 mg (2.25 mmol) of the corresponding alkyne, and after chromatography of the residue using hexanes/ethyl acetate (10:1) as eluent gave compound **1b** (260 mg, 60%) as a colorless oil; ^{1}H NMR (300 MHz, $CDCl_3$, 25 ^{o}C): δ = 7.75 (ddd, 1H, *J* = 8.1, 2.1, 0.9 Hz, ArH), 7.69 (t, 1H, *J* = 2.3 Hz, ArH), 7.35 (t, 1H, *J* = 8.2 Hz, ArH), 7.16 (ddd, 1H, *J* = 8.3, 2.5, 0.9 Hz, ArH), 5.30 (q, 1H, *J* = 6.7 Hz, =CH), 4.84 (dt, 2H, *J* = 6.6, 2.5 Hz, CH_2), 4.58 (dt, 2H, *J* = 6.8, 2.5 Hz, =CH_2); ^{13}C NMR (75 MHz, $CDCl_3$, 25 ^{o}C): δ = 209.9 (C=*C*=CH_2), 158.9, 149.3, 130.0 (Ar, CH), 122.2 (Ar, CH), 116.1 (Ar, CH), 109.4 (Ar, CH), 86.3 (=CH), 77.2 (=CH_2), 66.6 (CH_2); IR ($CHCl_3$, cm^{-1}): ν = 3100, 1958, 1529, 1350.



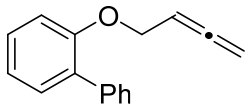
1c

Allene 1c. From 371 mg (1.43 mmol) of the corresponding alkyne, and after chromatography of the residue using hexanes/ethyl acetate (10:1) as eluent gave compound **1c** (228 mg, 59%) as a colorless oil; ^{1}H NMR (300 MHz, $CDCl_3$, 25 ºC): δ = 7.51–7.44 (m, 2H, ArH), 6.65–6.58 (m, 2H, ArH), 5.29 (q, 1H, *J* = 6.7 Hz, =CH), 4.79 (dt, 2H, *J* = 6.6, 2.5 Hz, CH_2), 4.46 (dt, 2H, *J* = 6.8, 2.5 Hz, $=CH_2$); ^{13}C NMR (75 MHz, $CDCl_3$, 25 ºC): δ = 209.6 (C=*C*=CH_2), 158.3, 138.3 (Ar, 2CH), 117.4 (Ar, 2CH), 86.9 (=CH), 83.2, 76.9 ($=CH_2$), 66.0 (CH_2); IR ($CHCl_3$, cm^{-1}): ν = 2984, 1956, 1735, 1483, 1236.



1e

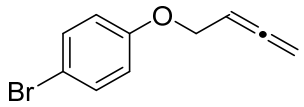
Allene 1e. From 500 mg (2.37 mmol) of the corresponding alkyne, and after chromatography of the residue using hexanes/ethyl acetate (20:1) as eluent gave compound **1e** (324 mg, 61%) as a colorless oil; ^{1}H NMR (300 MHz, $CDCl_3$, 25 ºC): δ = 7.46 (dd, 1H, *J* = 7.9, 1.6 Hz, ArH), 7.17 (m, 1H, ArH), 6.85 (dd, 1H, *J* = 8.3, 1.3 Hz, ArH), 6.77 (td, 1H, *J* = 8.5, 1.4 Hz, ArH), 5.33 (q, 1H, *J* = 7.4 Hz, =CH), 4.80 (dt, 2H, *J* = 6.6, 2.5 Hz, CH_2), 4.58 (dt, 2H, *J* = 6.8, 2.5 Hz, $=CH_2$); ^{13}C NMR (75 MHz, $CDCl_3$, 25 ºC): δ = 209.7 (C=*C*=CH_2), 154.90, 133.6 (Ar, CH), 128.5 (Ar, CH), 122.3 (Ar, CH), 114.1 (Ar, CH), 112.6, 86.9 (=CH), 76.9 ($=CH_2$), 67.2 (CH_2); IR ($CHCl_3$, cm^{-1}): ν = 3065, 1955, 1475, 744.



1f

Allene 1f. From 417 mg (2.37 mmol) of the corresponding alkyne, and after chromatography of the residue using hexanes/ethyl acetate (20:1) as eluent gave compound **1f** (303 mg, 68%) as a colorless oil; ^{1}H NMR (300 MHz, $CDCl_3$, 25 ºC): δ = 7.57 (ddd, 2H, *J* = 4.2, 3.5, 1.8 Hz, ArH), 7.46–7.38 (m, 2H, ArH), 7.38–7.33 (m, 2H, ArH), 7.31 (ddd, 1H, *J* = 7.4, 4.1, 1.8 Hz, ArH), 7.10–7.00 (m, 2H, ArH), 5.34 (q, 1H, *J* = 6.6 Hz, =CH), 4.84 (dt, 2H, *J* = 6.6, 2.7 Hz, CH_2), 4.59 (dt, 2H, *J* = 6.5, 2.7 Hz, $=CH_2$); ^{13}C NMR (75 MHz, $CDCl_3$, 25 ºC): δ = 209.3 (C=*C*=CH_2), 155.4, 138.6, 131.4 (Ar,

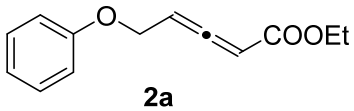
CH), 131.2, 129.7 (Ar, CH), 128.6 (Ar, CH), 128.0 (Ar, CH), 126.9 (Ar, CH), 121.4 (Ar, CH), 113.5 (Ar, CH), 87.45 (=CH), 76.7 (=CH_2), 66.4 (CH_2); IR ($CHCl_3$, cm^{-1}): ν = 3060, 1956, 1479, 1210, 697.



1h

Allene 1h. From 291 mg (1.38 mmol) of the corresponding alkyne, and after chromatography of the residue using hexanes/ethyl acetate (8:1) as eluent gave compound **1h** (210 mg, 68%) as a colorless oil; ^1H NMR (300 MHz, $CDCl_3$, 25 ºC): δ = 7.37(d, 2H, *J* = 8.9 Hz), 6.80 (d, 2H, *J* = 8.9 Hz), 5.37 (q, 1H, *J* = 6.7 Hz), 4.87 (m, 2H), 4.54 (m, 2H); ^{13}C NMR (75 MHz, $CDCl_3$, 25 ºC): δ = 209.4, 157.4, 132.2 (2C), 116.6 (2C), 113.1, 86.7, 76.7, 66.0; IR ($CHCl_3$, cm^{-1}): ν = 3054, 1955, 1481, 1233.

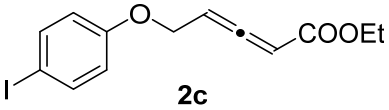
General Procedure for the Preparation of Allenes 2a, 2c, and 2e–h. CuI (0.50 mmol), EDA (1.50 mmol) and Et_3N (1.50 mmol) were added to a solution of the corresponding alkyne (1.00 mmol) in CH_3CN (5.39 mL). The mixture was allowed to react until the reaction was completed (TLC). Once finished, NH_4Cl (30 mL) was added to the solution, and then it extracted three times with AcOEt (3 x 20 mL). The organic phase was washed with water (2 x 5 mL), dried ($MgSO_4$) and concentrated under reduced pressure. Chromatography of the residue eluting with hexanes/ethyl acetate mixtures gave compounds **2** containing a small proportion of the isomeric alkyne (less than 5% as observed in H-NMR). Spectroscopic and analytical data for allenes **2** follow.



2a

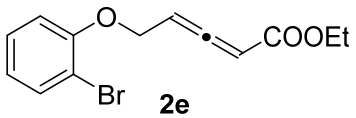
Allene 2a. From 270 mg (2.04 mmol) of the corresponding alkyne, and after chromatography of the residue using hexanes/ethyl acetate (10:1) as eluent gave compound **2a** (188 mg, 40%) as a colorless oil; ^1H NMR (300 MHz, $CDCl_3$, 25 ºC): δ = 7.20 (td, 2H, *J* = 9.0 Hz, *J* = 3.0 Hz, ArH), 6.90 (td, 3H, *J* = 9.0 Hz, *J* = 3.0 Hz, ArH), 5.74 (dt, 1H, *J* = 6.0 Hz, *J* = 3.0 Hz, CH) 5.47 (q, 1H, *J* = 6.0 Hz, CH), 4.24 (dt, 2H, *J* = 6.0 Hz, *J* = 3.0 Hz, OCH_2), 4.06 (qd, 2H, *J* = 6.0 Hz, *J* = 3.0 Hz,

OC*H*$_2$-CH$_3$), 1.02 (t, 3H, *J* = 6.0 Hz, CH$_3$); ^{13}C NMR (75 MHz, CDCl$_3$, 25 ºC): δ = 212.7 (=C=), 166.1 (CO), 159.0 (Ar, C), 130.1 (Ar, 2CH), 121.8 (Ar, CH), 115.6 (Ar, 2CH), 93.1 (=CH), 90.6 (=CH), 64.3 (OCH$_2$), 61.3 (OCH$_2$), 14.6 (CH$_3$); IR (CHCl$_3$, cm^{-1}): ν = 1965, 1717, 1505, 1265, 1029; HRMS (ES): calcd for C$_{13}$H$_{15}$O$_3$ [*M* + H]$^+$: 219.10157; found: 219.10229.



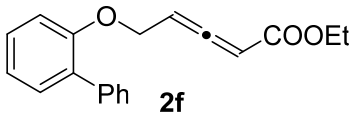
2c

Allene 2c. From 319 mg (1.24 mmol) of the corresponding alkyne, and after chromatography of the residue using hexanes/ethyl acetate (10:1) as eluent gave compound **2c** (178 mg, 42%) as a colorless oil; ^{1}H NMR (300 MHz, CDCl$_3$, 25 ºC): δ = 7.56 (dt, 2H, *J* = 9.0 Hz, *J* = 3.0 Hz ArH), 6.71 (dt, 2H, *J* = 9.0 Hz, *J* = 3.0 Hz, ArH), 5.83 (q, 1H, *J* = 9.0 Hz, CH), 5.75 (dt, 1H, *J* = 9.0 Hz, *J* = 3.0 Hz, CH), 4.67 (dd, 2H, *J* = 6.0 Hz, *J* = 3.0 Hz, OCH$_2$), 4.20 (qd, 2H, *J* = 6.0 Hz, *J* = 3.0 Hz, OC*H*$_2$-CH$_3$), 1.28 (t, 3H, *J* = 6.0 Hz, CH$_3$); ^{13}C NMR (75 MHz, CDCl$_3$, 25 ºC): δ = 212.2 (=C=), 165.1 (CO), 157.8 (Ar, C), 138.3 (Ar, 2CH), 117.4 (Ar, 2CH), 92.3 (=CH), 90.4 (=CH), 83.5 (Ar, C), 64.2 (OCH$_2$), 61.4 (OCH$_2$), 14.2 (CH$_3$); IR (CHCl$_3$, cm^{-1}): ν = 1967, 1712, 1483, 1234, 1173, 1018; HRMS (ES): calcd for C$_{13}$H$_{17}$INO$_3$ [*M* + NH$_4$]$^+$: 362.02476; found: 362.02521.



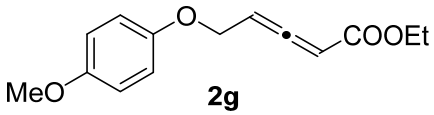
2e

Allene 2e. From 650 mg (2.84 mmol) of the corresponding alkyne, and after chromatography of the residue using hexanes/ethyl acetate (10:1) as eluent gave compound **2e** (320 mg, 38%) as a colorless oil; ^{1}H NMR (300 MHz, CDCl$_3$, 25 ºC): δ = 7.47 (dd, 1H, *J* = 9.0 Hz, *J* = 3.0 Hz, ArH), 7.18 (td, 1H, *J* = 9.0 Hz, *J* = 3.0 Hz, ArH), 6.88 (dd, 1H, *J* = 6.0 Hz, *J* = 3.0 Hz, ArH), 6.79 (td, 1H, *J* = 6.0 Hz, *J* = 3.0 Hz, ArH), 5.81 (q, 1H, *J* = 6.0 Hz, CH), 5.69 (dt, 1H, *J* = 6.0 Hz, *J* = 3.0 Hz, CH), 4.71 (dd, 2H, *J* = 6.0 Hz, *J* = 3.0 Hz, OCH$_2$), 4.12 (qd, 2H, *J* = 6.0 Hz, *J* = 3.0 Hz, OC*H*$_2$-CH$_3$), 1.20 (t, 3H, *J* = 6.0 Hz, CH$_3$); ^{13}C NMR (75 MHz, CDCl$_3$, 25 ºC): δ = 212.3 (=C=), 166.1 (CO), 154.5 (Ar, C), 133.6 (Ar, CH), 128.4 (Ar, CH), 122.6 (Ar, CH), 114.7 (Ar, CH), 112.6 (Ar, C), 92.3 (=CH), 90.4 (=CH), 65.4 (OCH$_2$), 61.2 (OCH$_2$), 14.2 (CH$_3$); IR (CHCl$_3$, cm^{-1}): ν = 1967, 1716, 1477, 1249, 1165, 1030; HRMS (ES): calcd for C$_{13}$H$_{14}$BrO$_3$ [*M* + H]$^+$: 297.01208; found: 297.01314.



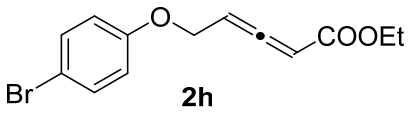
2f

Allene 2f. From 200 mg (0.96 mmol) of the corresponding alkyne, and after chromatography of the residue using hexanes/ethyl acetate (10:1) as eluent gave compound **2f** (94 mg, 42%) as a colorless oil; ^{1}H NMR (300 MHz, $CDCl_3$, 25 ºC): δ = 7.54 (m, 2H, ArH), 7.35 (t, 5H, *J* = 7.4 Hz, ArH), 7.09 (td, 1H, *J* = 9.0 Hz, *J* = 3.0 Hz, ArH), 7.05 (td, 1H, *J* = 9.0 Hz, *J* = 3.0 Hz, ArH) 5.80 (q, 1H, *J* = 6.0 Hz, CH), 5.72 (dt, 1H, *J* = 6.0 Hz, *J* = 3.0 Hz CH), 4.70 (dd, 2H, *J* = 6.0 Hz, *J* = 3.0 Hz, OCH_2), 4.22 (qd, 2H, *J* = 6.0 Hz, *J* = 3.0 Hz, OCH_2-CH_3), 1.30 (t, 3H, *J* = 6.0 Hz, CH_3); ^{13}C NMR (75 MHz, $CDCl_3$, 25 ºC): δ = 212.0 (=C=), 165.3 (CO), 152.5 (Ar, C), 138.3 (Ar, C), 131.4 (Ar, C), 131.1 (Ar, CH), 129.6 (Ar, 2CH), 128.5 (Ar, CH), 127.9 (Ar, 2CH), 127.0 (Ar, CH), 121.7 (Ar, CH), 113.3 (Ar, CH), 92.7 (=CH), 90.3 (=CH), 64.6 (OCH_2), 61.1 (OCH_2), 14.2 (CH_3); IR ($CHCl_3$, cm^{-1}): ν = 1967, 1718, 1505, 1263, 1166, 1026; HRMS (ES): calcd for $C_{19}H_{22}NO_3$ $[M + NH_4]^+$: 312.15942; found: 312.15978.



2g

Allene 2g. From 153 mg (0.94 mmol) of the corresponding alkyne, and after chromatography of the residue using hexanes/ethyl acetate (10:1) as eluent gave compound **2g** (94 mg, 40%) as a colorless oil; ^{1}H NMR (300 MHz, $CDCl_3$, 25 ºC): δ = 6.85 (t, 4H, *J* = 9.0 Hz, ArH), 5.83 (q, 1H, *J* = 6.0 Hz, CH), 5.74 (dt, 1H, *J* = 6.0 Hz, *J* = 3.0 Hz, CH), 4.64 (dd, 2H, *J* = 6.0 Hz, *J* = 3.0 Hz, OCH_2), 4.20 (qd, 2H, *J* = 6.0 Hz, *J* = 3.0 Hz, OCH_2-CH_3), 3.77 (s, 3H, OMe), 1.28 (t, 3H, *J* = 6.0 Hz, CH_3); ^{13}C NMR (75 MHz, $CDCl_3$, 25 ºC): δ = 212.2 (=C=), 166.3 (CO), 154.3 (Ar, C), 151.1 (Ar, C), 116.1 (Ar, 2CH), 114.7 (Ar, 2CH), 92.7 (=CH), 90.0 (=CH), 65.0 (OCH_2), 61.1 (OCH_2), 55.7 (OCH_3), 14.2 (CH_3); IR ($CHCl_3$, cm^{-1}): ν = 1967, 1718, 1508, 1230, 1174, 1037; HRMS (ES): calcd for $C_{14}H_{17}O_4$ $[M + H]^+$: 249.11214; found: 249.11196.

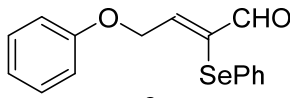


2h

Allene 2h. From 228 mg (1.07 mmol) of the corresponding alkyne, and after chromatography of the residue using hexanes/ethyl acetate (10:1) as eluent gave compound **2h** (117 mg, 36%) as a

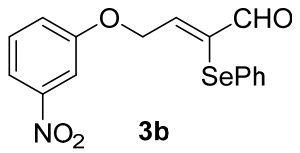
colorless oil; ^{1}H NMR (300 MHz, $CDCl_3$, 25 ºC): δ = 7.38 (dt, 2H, *J* = 9.0 Hz, *J* = 3.0 Hz, ArH), 6.81 (dt, 2H, *J* = 9.0 Hz, *J* = 3.0 Hz, ArH), 5.83 (q, 1H, *J* = 6.0 Hz, CH), 5.75 (dt, 1H, *J* = 6.0 Hz, *J* = 3.0 Hz, CH), 4.65 (dd, 2H, *J* = 6.0 Hz, *J* = 3.0 Hz, OCH_2), 4.20 (qd, 2H, *J* = 6.0 Hz, *J* = 3.0 Hz, OCH_2-CH_3), 1.28 (t, 3H, *J* = 6.0 Hz, CH_3); ^{13}C NMR (75 MHz, $CDCl_3$, 25 ºC): δ = 212.2 (=C=), 165.0 (CO), 157.1 (Ar, C), 132.3 (Ar, 2CH), 116.8 (Ar, 2CH), 113.2 (Ar, C), 92.3 (=CH), 90.4 (=CH), 64.4 (OCH_2), 61.2 (OCH_2), 14.2 (CH_3); IR ($CHCl_3$, cm^{-1}): ν = 1969, 1721, 1510, 1234, 1173, 1026; HRMS (ES): calcd for $C_{13}H_{17}BrNO_3$ $[M + NH_4]^+$: 314.03863; found: 314.03884.

General procedure for the oxidative selenofunctionalization of allenes 1a–h. Synthesis of 2-(phenylselanyl)-but-2-enals 3a–h. $(PhSe)_2$ (0.1 mmol) and $[PyF]^+[OTf]^-$ (0.12 mmol) were successively added to a stirred solution of the appropriate allene **1** (0.1 mmol) in MeCN/THF (1:1, v/v, 2 mL). The reaction was stirred at room temperature until disappearance of the starting material (TLC). The mixture was extracted with ethyl acetate (3 x 10 mL). The organic extract was washed with brine, dried ($MgSO_4$) and concentrated under reduced pressure. Chromatography of the residue using ethyl acetate/hexanes mixtures gave analytically pure compounds **3**. Spectroscopic and analytical data for compounds **3** follows.



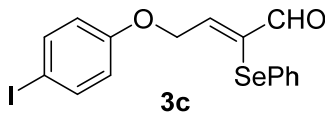
3a

α-Phenylseleno-α,β-unsaturated aldehyde 3a. From 100 mg (0.68 mmol) of allene **1a**, and after chromatography of the residue using hexanes/ethyl acetate (20:1) as eluent gave compound **3a** (158 mg, 73%; containing *ca.* 3% of its *E* diastereomer) as a colorless oil; ^{1}H NMR (300 MHz, $CDCl_3$, 25 ºC): δ = 9.85 (s, 1H), 7.41 (m, 2H), 7.32 (t, 1H, *J* = 5.1 Hz), 7.20 (m, 5H), 6.91 (tt, 1H, *J* = 7.4, 1.0 Hz), 6.75 (dd, 2H, *J* = 7.7, 1.0 Hz), 4.77 (d, 2H, *J* = 5.1 Hz); ^{13}C NMR (75 MHz, $CDCl_3$, 25 ºC): δ = 189.7, 157.8, 154.7, 136.1, 132.9 (2C), 129.7 (2C), 129.5 (2C), 128.0, 127.9, 121.6, 114.5 (2C), 67.1; ^{77}Se-NMR (95 MHz, $CDCl_3$, 25 ºC) δ: 290.1 (s, 1Se, Se); IR ($CHCl_3$, cm^{-1}): ν = 3059, 2916, 2849, 1698 cm^{-1}; HRMS (ES): calcd for $C_{16}H_{18}NO_2Se$ $[M + NH_4]^+$: 336.04979; found: 336.05109.



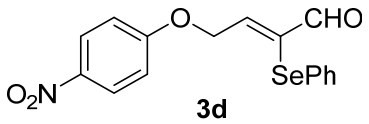
3b

α-Phenylseleno-α,β-unsaturated aldehyde 3b. From 127 mg (0.66 mmol) of allene **1b**, and after chromatography of the residue using hexanes/ethyl acetate (10:1) as eluent gave compound **3b** (102 mg, 42%; containing *ca.* 5% of its *E* diastereomer) as a colorless oil; ^{1}H NMR (300 MHz, $CDCl_3$, 25 ºC): δ = 9.34 (s, 1H, CHO), 7.76 (ddd, 1H, *J* = 8.1, 2.1, 0.9 Hz, ArH), 7.48 (t, 1H, *J* = 2.3 Hz, ArH), 7.45–7.40 (m, 2H, ArH), 7.33 (t, 1H, *J* = 8.2 Hz, =CH), 7.27–7.19 (m, 4H, ArH), 7.06 (ddd, 1H, *J* = 8.3, 2.6, 0.9 Hz, ArH), 4.71 (d, 2H, *J* = 5.1 Hz, CH_2); ^{13}C NMR (75 MHz, $CDCl_3$, 25 ºC): δ = 189.7 (CHO), 158,4, 151.3 (=CH), 137.3, 133.5 (Ar, 2CH), 131.7, 130.4 (Ar, CH), 129.8 (Ar, 2CH), 129.3 (Ar, CH), 128.5, 121.8 (Ar, CH), 116.7 (Ar, CH), 108.9 (Ar, CH), 67.7 (CH_2); ^{77}Se-NMR (95 MHz, $CDCl_3$, 25 ºC) δ: 302.3 (s, 1Se, Se); IR ($CHCl_3$, cm^{-1}): ν = 2926, 1697, 1529, 1351 cm^{-1}; HRMS (ES): calcd for $C_{16}H_{17}N_2O_4Se$ [*M* + NH_4]$^+$: 381.03488; found: 381.03497.



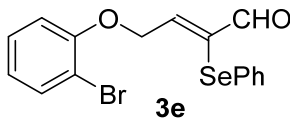
3c

α-Phenylseleno-α,β-unsaturated aldehyde 3c. From 120 mg (0.44 mmol) of allene **1c**, and after chromatography of the residue using hexanes/ethyl acetate (10:1) as eluent gave compound **3c** (91 mg, 47%; containing *ca.* 5% of its *E* diastereomer) as a colorless oil; ^{1}H NMR (300 MHz, $CDCl_3$, 25 ºC): δ = 9.42 (s, 1H, CHO), 7.58–7.51 (m, 2H, ArH), 7.50–7.43 (m, 2H, ArH), 7.33 (dd, 1H, *J* = 8.5, 3.4 Hz, =CH), 7.31–7.26 (m, 3H, ArH), 6.62–6.55 (m, 2H, ArH), 4.78 (d, 2H, *J* = 5.1 Hz, CH_2); ^{13}C NMR (75 MHz, $CDCl_3$, 25 ºC): δ = 189.7 (CHO), 157.8, 153.5 (=CH), 138.6 (Ar, 2CH), 136.6, 133.1 (Ar, 2CH), 129.7 (Ar, 2CH), 128.3 (Ar, CH), 128.2, 117.0 (Ar, 2CH), 83.9, 67.3 (CH_2); ^{77}Se-NMR (95 MHz, $CDCl_3$, 25 ºC) δ: 292.9 (s, 1Se, Se); IR ($CHCl_3$, cm^{-1}): ν = 3061, 2923, 2847, 1694, 1480, 1234 cm^{-1}.



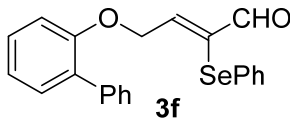
3d

α-Phenylseleno-α,β-unsaturated aldehyde 3d. From 233 mg (1.22 mmol) of allene **1d**, and after chromatography of the residue using hexanes/ethyl acetate (15:1) as eluent gave compound **3d** (154 mg, 32%; containing *ca.* 8% of its *E* diastereomer) as a colorless oil; ^{1}H NMR (300 MHz, $CDCl_3$, 25 ºC): δ = 9.37 (s, 1H, CHO), 8.15–8.06 (m, 2H, ArH), 7.58–7.49 (m, 2H, ArH), 7.46–7.39 (m, 1H, ArH), 7.27–7.22 (m, 2H, ArH), 7.18 (dd, 2H, *J* = 4.8, 2.3 Hz, ArH), 6.83–6.74 (m, 1H, =CH), 4.81 (d, 2H, *J* = 5.2 Hz, CH_2); ^{13}C NMR (75 MHz, $CDCl_3$, 25 ºC): δ = 188.4 (CHO), 161.6, 150.1 (Ar, =CH), 132.0, 130.5 (Ar, 2CH), 128.6, 128.2 (Ar, 2CH), 126.7, 125.0 (Ar, 2CH), 114.6 (Ar, CH), 113.5 (Ar, 2CH), 66.6 (CH_2); ^{77}Se-NMR (95 MHz, $CDCl_3$, 25 ºC) δ: 294.6 (s, 1Se, Se); IR ($CHCl_3$, cm^{-1}): ν = 3061, 2924, 2853, 1697, 1513, 1338, 1257 cm^{-1}.



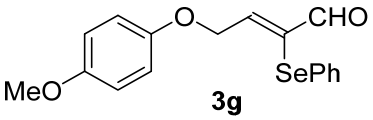
3e

α-Phenylseleno-α,β-unsaturated aldehyde 3e. From 141 mg (0.626 mmol) of allene **1e**, and after chromatography of the residue using hexanes/ethyl acetate (10:1) as eluent gave compound **3e** (98 mg, 42%; containing *ca.* 6% of its *E* diastereomer) as a colorless oil; ^{1}H NMR (300 MHz, C_6D_6, 25 ºC): δ = 8.80 (s, 1H, CHO), 7.41 (dd, 1H, *J* = 7.9, 1.6 Hz, ArH), 7.28–7.22 (m, 2H, ArH), 6.91–6.83 (m, 3H, ArH), 6.80 (dd, 1H, *J* = 7.9, 1.2 Hz, ArH), 6.69 (t, 1H, *J* = 5.1 Hz, =CH), 6.48 (d, 1H, *J* = 1.3 Hz, ArH), 6.28 (dd, 1H, *J* = 8.2, 1.3 Hz, ArH), 4.39 (d, 2H, *J* = 5.1 Hz, CH_2); ^{13}C NMR (75 MHz, C_6D_6, 25 ºC): δ = 188.5 (CHO), 154.8, 152.9 (=CH), 136.5, 134.0 (Ar, CH), 133.2 (Ar, 2CH), 129.5 (Ar, 2CH), 128.9, 128.6 (Ar, CH), 127.9 (Ar, CH), 122.7 (Ar, CH), 113.3 (Ar, CH), 112.6, 68.1 (CH_2); ^{77}Se-NMR (95 MHz, C_6D_6, 25 ºC) δ: 286.7 (s, 1Se, Se); IR (C_6H_6, cm^{-1}): ν = 3036, 2921, 2850, 2717, 1695, 1475, 737 cm^{-1}.



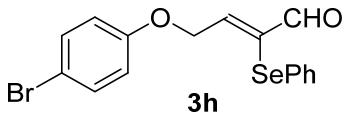
3f

α-Phenylseleno-α,β-unsaturated aldehyde 3f. From 110 mg (0.494 mmol) of allene **1f**, and after chromatography of the residue using hexanes/ethyl acetate (10:1) as eluent gave compound **3f** (69 mg, 37%; containing *ca.* 4% of its *E* diastereomer) as a colorless oil; ^{1}H NMR (300 MHz, C_6D_6, 25 ºC): δ = 8.71 (s, 1H, CHO), 7.56 (dt, 2H, *J* = 2.9, 1.7 Hz, ArH), 7.33–7.20 (m, 5H, ArH), 7.06 (td, 1H, *J* = 7.4, 1.7 Hz, =CH), 6.88 (ddd, 5H, *J* = 7.4, 5.0, 2.6 Hz, ArH), 6.63–6.54 (m, 2H, ArH), 4.46 (d, 2H, *J* = 5.1 Hz, CH_2); ^{13}C NMR (75 MHz, C_6D_6, 25 ºC): δ = 188.6 (CHO), 155.4, 153.7 (=CH), 139.0, 136.2, 133.3 (Ar, 2CH), 132.0, 131.6 (Ar, CH), 130.0 (Ar, 2CH), 129.5 (Ar, 2CH), 129.1, 128.9 (Ar, CH), 128.4 (Ar, 2CH), 127.7 (Ar, CH), 127.4 (Ar, CH), 122.2 (Ar, CH), 113.2 (Ar, CH), 68.0 (CH_2); ^{77}Se-NMR (95 MHz, C_6D_6, 25 ºC) δ: 285.2 (s, 1Se, Se); IR (C_6H_6, cm^{-1}): ν = 3058, 2924, 2849, 2716 1696, 1478 cm^{-1}; HRMS (ES): calcd for $C_{22}H_{18}NaO_2Se$ [*M* + Na]$^+$: 417.03654; found: 417.03610.



3g

α-Phenylseleno-α,β-unsaturated aldehyde 3g. From 100 mg (0.57 mmol) of allene **1g**, and after chromatography of the residue using hexanes/ethyl acetate (10:1) as eluent gave compound **3g** (151 mg, 77%; containing *ca.* 2% of its *E* diastereomer) as a colorless oil; ^{1}H NMR (300 MHz, $CDCl_3$, 25 ºC): δ = 9.30 (s, 1H), 7.39 (m, 2H), 7.31 (t, 1H, *J* = 5.1 Hz), 7.20 (m, 3H), 6.72 (m, 4H), 4.73 (d, 2H, *J* = 5.1 Hz), 3.70 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$, 25 ºC): δ = 189.7, 155.0, 154.4, 151.9, 136.0, 132.9 (2C), 129.5 (2C), 128.4, 127.9, 115.6 (2C), 114.8 (2C), 67.9, 55.7; ^{77}Se-NMR (95 MHz, $CDCl_3$, 25 ºC) δ: 286.6 (s, 1Se, Se); IR ($CHCl_3$, cm^{-1}): ν = 3060, 2926, 2833, 1697 cm^{-1}; HRMS (ES): calcd for $C_{17}H_{16}NaO_3Se$ [*M* + Na]$^+$: 371.01577; found: 371.01756.



3h

α-Phenylseleno-α,β-unsaturated aldehyde 3h. From 130 mg (0.58 mmol) of allene **1h**, and after chromatography of the residue using hexanes/ethyl acetate (20:1) as eluent gave compound **3h** (206 mg, 89%; containing *ca.* 2% of its *E* diastereomer) as a colorless oil; ^{1}H NMR (300 MHz, $CDCl_3$, 25 ºC): δ = 9.34 (s, 1H), 7.40 (m, 2H), 7.25 (m, 6H), 6.62 (d, 2H, *J* = 9.1 Hz), 4.71 (d, 2H, *J* = 5.1 Hz); ^{13}C NMR (75 MHz, $CDCl_3$, 25 ºC): δ = 189.6, 156.9, 153.4, 136.4, 133.0 (2C), 132.5 (2C), 129.6 (2C), 128.2, 128.0, 116.4 (2C), 113.8, 67.4; ^{77}Se-NMR (95 MHz, $CDCl_3$, 25 ºC) δ: 292.6 (s, 1Se, Se); IR ($CHCl_3$, cm^{-1}): ν = 3062, 2920, 2836, 1700 cm^{-1}; HRMS (ES): calcd for $C_{16}H_{13}BrNaO_2Se$ $[M + Na]^+$: 418.91539; found: 418.91558.

General procedure for the chloroselenofunctionalization of allenes 1b,c. Synthesis of chloro-phenylselanes 4b,c. PhSeCl (0.60 mmol) was added to a stirred solution of the appropriate allene **1** (0.40 mmol) in MeCN/water (20:1, v/v, 1.7 mL). After disappearance of the starting material (TLC) the mixture was extracted with ethyl acetate (3 x 20 mL). The organic extract was washed with brine, dried ($MgSO_4$) and concentrated under reduced pressure. Chromatography of the residue using ethyl acetate/hexanes mixtures gave analytically pure compounds **4**. Spectroscopic and analytical data for compounds **4** follows.

Reaction of allene 1b. From 108 mg (0.397 mmol) of allene **1b**, and after chromatography of the residue using hexanes/ethyl acetate (10:1) as eluent, 84 mg (31%) of less polar compound (*Z*)-**4b** and 71 mg (26%) of more polar compound (*E*)-**4b** were obtained.

Chloro-phenylselane (*Z*)-4b. Colorless oil; ^{1}H NMR (300 MHz, $CDCl_3$, 25 ºC): δ = 7.76 (ddd, 1H, *J* = 8.1, 2.1, 0.9 Hz, ArH), 7.65 (t, 1H, *J* = 2.3 Hz, ArH), 7.46 (ddd, 2H, *J* = 3.7, 2.9, 1.8 Hz, ArH), 7.35 (t, 1H, *J* = 8.2 Hz, ArH), 7.25 (dd, 3H, *J* = 4.1, 2.4 Hz, ArH), 7.20–7.14 (m, 1H, ArH), 6.47 (tt, 1H, *J* = 5.8, 1.2 Hz, =CH), 4.79 (dt, 2H, *J* = 5.8, 1.0 Hz, OCH_2), 4.08 (d, 2H, *J* = 1.2 Hz, CH_2–Cl); ^{13}C NMR (75 MHz, $CDCl_3$, 25 ºC): δ = 158.8, 149.3, 133.6 (Ar, 2CH), 133.2, 131.9 (=CH),

130.2 (Ar, CH), 129.8 (Ar, 2CH), 128.4 (Ar, CH), 127.6, 121.9 (Ar, CH), 116.2 (Ar, CH), 109.2 (Ar, CH), 67.5(CH_2), 48.4 (CH_2); ^{77}Se-NMR (95 MHz, $CDCl_3$, 25 ºC) δ: 347.4 (s, 1Se, Se); IR ($CHCl_3$, cm^{-1}): ν = 3074, 2938, 1523, 1477, 1441, 1345 cm^{-1}; HRMS (ES): calcd for $C_{16}H_{18}ClN_2O_3Se$ $[M + NH_4]^+$: 401.01638; found: 401.01738.

Chloro-phenylselane (*E*)-4b. Colorless oil; ^{1}H NMR (300 MHz, $CDCl_3$, 25 ºC): δ = 7.78 (ddd, 1H, *J* = 8.1, 2.1, 0.9 Hz, ArH), 7.64 (t, 1H, *J* = 2.3 Hz, ArH), 7.54–7.48 (m, 2H, ArH), 7.37 (t, 1H, *J* = 8.2 Hz, ArH), 7.30–7.23 (m, 3H, ArH), 7.15 (ddd, 1H, *J* = 8.3, 2.5, 0.8 Hz, ArH), 6.06 (t, 1H, *J* = 6.3 Hz, =CH), 4.66 (d, 2H, *J* = 6.3 Hz, OCH_2), 4.18 (s, 2H, CH_2–Cl); ^{13}C NMR (75 MHz, $CDCl_3$, 25 ºC): δ = 158.7, 149.3, 135.1 (Ar, 2CH), 134.8, 131.5 (=CH), 130.2 (Ar, CH), 129.8 (Ar, 2CH), 128.8 (Ar, CH), 127.8, 121.99 (Ar, CH), 116.4 (Ar, CH), 109.2 (Ar, CH), 65.17 (CH_2), 42.67 (CH_2); ^{77}Se-NMR (95 MHz, $CDCl_3$, 25 ºC) δ: 447.0 (s, 1Se, Se); IR ($CHCl_3$, cm^{-1}): ν = 1618, 1578, 1528, 1350, 1244, 737 cm^{-1}.

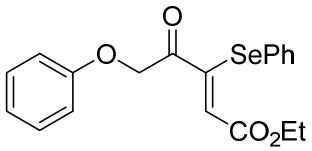
Reaction of allene 1c. From 108 mg (0.395 mmol) of allene **1c**, and after chromatography of the residue using hexanes/ethyl acetate (15:1) as eluent, 87 mg (47%) of less polar compound (*Z*)-**4c** and 76 mg (41%) of more polar compound (*E*)-**4c** were obtained.

Chloro-phenylselane (*Z*)-4c. Colorless oil; ^{1}H NMR (300 MHz, $CDCl_3$, 25 ºC): δ = 7.51–7.44 (m, 2H, ArH), 7.44–7.39 (m, 2H, ArH), 7.28–7.21 (m, 3H, ArH), 6.65–6.59 (m, 2H, ArH), 6.46 (tt, 1H, *J* = 5.7, 1.2 Hz, =CH), 4.69 (d, 2H, *J* = 5.8 Hz, OCH_2), 4.07 (d, 2H, *J* = 1.1 Hz, CH_2–Cl); ^{13}C NMR (75 MHz, $CDCl_3$, 25 ºC): δ = 158.2, 138.4 (Ar, 2CH), 133.4 (Ar, 2CH), 133.3 (=CH), 132.3, 129.8 (Ar, 2CH), 128.3 (Ar, CH), 127.9, 117.3 (Ar, 2CH), 83.4, 67.4 (CH_2), 48.5 (CH_2); ^{77}Se-NMR (95 MHz, $CDCl_3$, 25 ºC) δ: 343.7 (s, 1Se, Se); IR ($CHCl_3$, cm^{-1}): ν = 3058, 2923, 2851, 1873, 1582, 1482 cm^{-1}.

Chloro-phenylselane (*E*)-4c. Colorless oil; ^{1}H NMR (300 MHz, $CDCl_3$, 25 ºC): δ = 7.52–7.47 (m, 4H, ArH), 7.29–7.21 (m, 3H, ArH), 6.63–6.57 (m, 2H, ArH), 6.08 (t, 1H, *J* = 6.3 Hz, =CH), 4.55 (d, 2H, *J* = 6.3 Hz, OCH_2), 4.18–4.13 (m, 2H, CH_2–Cl); ^{13}C NMR (75 MHz, $CDCl_3$, 25 ºC): δ =

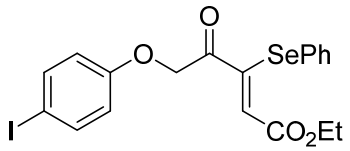
158.1, 138.5 (Ar, 2CH), 134.9 (Ar, 2CH), 133.8, 132.9 (=CH), 129.7 (Ar, 2CH), 128.6 (Ar, CH), 128.0, 117.3 (Ar, 2CH), 83.6, 64.8 (CH_2), 42.8 (CH_2); ^{77}Se-NMR (95 MHz, $CDCl_3$, 25 ºC) δ: 444.9 (s, 1Se, Se); IR ($CHCl_3$, cm^{-1}): ν = 3059, 2924, 2852, 1575, 1483, 1236 cm^{-1}.

General procedure for the oxidative selenofunctionalization of allenes 2a,c and 2e–h. Synthesis of 4-oxo-3-(phenylselanyl)pent-2-enoates 7a,c and 7e–h. $(PhSe)_2$ (0.1 mmol) and $[PyF]^+[OTf]^-$ (0.12 mmol) were successively added to a stirred solution of the appropriate allene **2** (0.1 mmol) in MeCN/THF (1:1, v/v, 2 mL). The reaction was stirred at room temperature until disappearance of the starting material (TLC). The mixture was extracted with ethyl acetate (3 x 10 mL). The organic extract was washed with brine, dried ($MgSO_4$) and concentrated under reduced pressure. Chromatography of the residue using ethyl acetate/hexanes mixtures gave analytically pure compounds **7**. Spectroscopic and analytical data for compounds **7** follows.



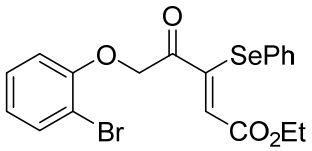
7a

α-Selenoenone 7a. From 35 mg (0.16 mmol) of allene **2a**, and after chromatography of the residue using hexanes/ethyl acetate (10:1) as eluent gave compound **7a** (39 mg, 63%; containing *ca.* 10% of its *E* diastereomer) as a colorless oil; ^{1}H NMR (300 MHz, C_6D_6, 25 ºC): δ = 7.35 (dd, 2H, *J* = 6.0 Hz, *J* = 3.0 Hz, ArH), 7.06 (td, 2H, *J* = 6.0 Hz, *J* = 3.0 Hz, ArH), 6.85 (m, 7H, ArH), 5.85 (s, 1H, CH), 4.66 (s, 2H, OCH_2), 3.74 (q, 2H, *J* = 6.0 Hz, OCH_2-CH_3), 0.76 (t, 3H, *J* = 6.0 Hz, CH_3); ^{13}C NMR (75 MHz, C_6D_6, 25 ºC): δ = 198.5 (CO), 163.4 (CO), 158.3 (Ar, C), 153.8 (Ar, C), 136.6 (Ar, 2CH), 129.6 (Ar, 2CH), 129.4 (Ar, 2CH), 128.0 (Ar, CH), 124.9 (C, Ar), 121.3 (Ar, CH), 118.9 (Ar, 2CH), 115.0 (Ar, CH), 71.7 (OCH_2), 60.6 (OCH_2), 13.5 (CH_3); ^{77}Se-NMR (95 MHz, $CDCl_3$, 25 ºC) δ: 477.6 (s, 1Se, Se); IR (C_6H_6, cm^{-1}): ν = 1700, 1580, 1482, 1311, 1192, 1025 cm^{-1}; HRMS (ES): calcd for $C_{19}H_{19}O_4Se$ $[M + H]^+$: 391.04441; found: 391.04555.



7c

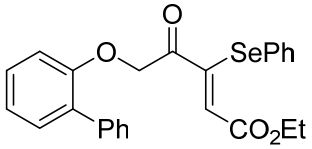
α-Selenoenone 7c. From 74 mg (0.21 mmol) of allene **2c**, and after chromatography of the residue using hexanes/ethyl acetate (8:1) as eluent gave compound **7c** (38 mg, 33%; containing *ca.* 25% of its *E* diastereomer) as a colorless oil; ^{1}H NMR (300 MHz, C_6D_6, 25 ºC): δ = 7.31 (m, 4H, ArH), 6.85 (m, 3H, ArH), 6.38 (dt, 2H, *J* = 9.0 Hz, *J* = 3.0 Hz, ArH), 5.82 (s, 1H, CH), 4.51 (s, 2H, OCH_2), 3.74 (q, 2H, *J* = 6.0 Hz, OCH_2-CH_3), 0.76 (t, 3H, *J* = 6.0 Hz, CH_3); ^{13}C NMR (75 MHz, C_6D_6, 25 ºC): δ = 197.7 (CO), 163.4 (CO), 158.0 (Ar, C), 153.5 (Ar, C), 138.2 (Ar, 2CH), 136.5 (Ar, 2CH), 129.6 (Ar, 3CH), 124.7 (C, Ar), 119.0 (Ar, CH), 117.3 (Ar, 2CH), 83.6 (Ar, C), 71.6 (OCH_2), 60.6 (OCH_2), 13.5 (CH_3); ^{77}Se-NMR (95 MHz, C_6D_6, 25 ºC) δ: 478.9 (s, 1Se, Se); IR (C_6H_6, cm^{-1}): ν = 1742, 1542, 1498, 1420, 1372, 1265, 1210, 1103 cm^{-1}; HRMS (ES): calcd for $C_{19}H_{18}IO_4Se$ $[M+H]^+$: 516.94105; found: 516.94073.



7e

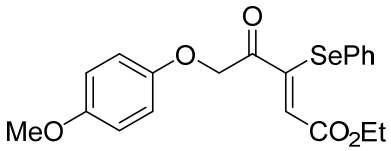
α-Selenoenone 7e. From 96 mg (0.32 mmol) of allene **2e**, and after chromatography of the residue using hexanes/ethyl acetate (8:1) as eluent gave compound **7e** (71 mg, 47%; containing *ca.* 20% of its *E* diastereomer) as a colorless oil; ^{1}H NMR (300 MHz, C_6D_6, 25 ºC): δ = 7.45 (dt, 2H, *J* = 9.0 Hz, *J* = 3.0 Hz, ArH), 7.36 (dt, 2H, *J* = 9.0 Hz, *J* = 3.0 Hz ArH), 6.84 (m, 3H, ArH), 6.45 (td, 1H, *J* = 6.0 Hz, *J* = 3.0 Hz ArH), 6.37 (dt, 1H, *J* = 9.0 Hz, *J* = 3.0 Hz, ArH), 5.92 (s, 1H, CH), 4.51 (s, 2H, OCH_2), 3.77 (q, 2H, *J* = 6.0 Hz, OCH_2-CH_3), 0.77 (t, 3H, *J* = 6.0 Hz, CH_3); ^{13}C NMR (75 MHz, C_6D_6, 25 ºC): δ = 198.4 (CO), 163.7 (CO), 154.5 (Ar, C), 153.4 (Ar, C), 136.7 (Ar, 2CH), 133.3 (Ar, CH), 129.6 (Ar, 2CH), 128.2 (Ar, CH), 128.0 (Ar, CH), 124.8 (Ar, C), 122.2 (Ar, CH), 119.2 (Ar, CH), 113.4 (Ar, CH), 112.0 (Ar, C), 72.2 (OCH_2), 60.6 (OCH_2), 13.6 (CH_3); ^{77}Se-NMR (95 MHz, C_6D_6, 25 ºC) δ: 481.2 (s, 1Se, Se); IR (C_6H_6, cm^{-1}): ν = 1743, 1541, 1496, 1420, 1372,

1261, 1215, 1105 cm^{-1}; HRMS (ES): calcd for $C_{19}H_{18}BrO_4Se$ [M + H]$^+$: 468.95462; found: 468.95336.



7f

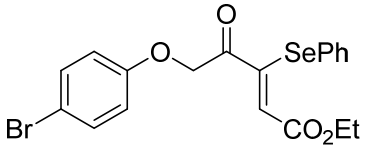
α-Selenoenone 7f. From 349 mg (1.18 mmol) of allene **2f**, and after chromatography of the residue using hexanes/ethyl acetate (7:1) as eluent gave compound **7f** (190 mg, 38%; containing *ca.* 35% of its *E* diastereomer) as a colorless oil; ^{1}H NMR (300 MHz, C_6D_6, 25 ºC): δ = 7.58 (dt, 2H, J = 9.0 Hz, J = 3.0 Hz, ArH), 7.24 (m, 6H, ArH), 7.03 (td, 1H, J = 9.0 Hz, J = 3.0 Hz, ArH), 6.85 (m, 5H, ArH), 6.58 (d, 1H, J = 9.0 Hz, ArH), 5.67 (s, 1H, CH), 4.52 (s, 2H, OCH_2), 3.72 (q, 2H, J = 6 Hz, OCH_2-CH_3), 0.76 (t, 3H, J = 6.0 Hz, CH_3); ^{13}C NMR (75 MHz, C_6D_6, 25 ºC): δ = 198.7 (CO), 163.4 (CO), 154.9 (Ar, C), 153.6 (Ar, C), 138.7 (Ar, C), 136.6 (Ar, 2CH), 131.2 (Ar, C), 131.0 (Ar, CH), 129.8 (Ar, 2CH), 129.5 (Ar, 2CH), 128.0 (Ar, 2CH), 127.8 (Ar, 2CH), 126.8 (Ar, CH), 124.7 (Ar, C), 121.5 (Ar, CH), 118.7 (Ar, CH), 112.6 (Ar, CH), 72.3 (OCH_2), 60.4 (OCH_2), 13.6 (CH_3); ^{77}Se-NMR (95 MHz, C_6D_6, 25 ºC) δ: 477.1 (s, 1Se, Se); IR (C_6H_6, cm^{-1}): ν = 1709, 1593, 1503.69, 1319, 1197, 1031 cm^{-1}; HRMS (ES): calcd for $C_{25}H_{23}O_4Se$ [M + H]$^+$: 467.07577; found: 467.07540.



7g

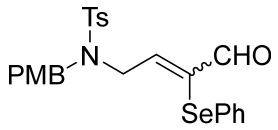
α-Selenoenone 7g. From 47 mg (0.19 mmol) of allene **2g**, and after chromatography of the residue using hexanes/ethyl acetate (10:1) as eluent gave compound **7g** (42 mg, 53%; containing *ca.* 20% of its *E* diastereomer) as a colorless oil; ^{1}H NMR (300 MHz, C_6D_6, 25 ºC): δ = 7.37 (dt, 2H, J = 9.0 Hz, J = 3.0 Hz, ArH), 6.83 (m, 5H, ArH), 6.68 (dt, 2H, J = 9.0 Hz, J = 3.0 Hz, ArH), 5.86 (s, 1H, CH), 4.67 (s, 2H, OCH_2), 3.76 (q, 2H, J = 6.0 Hz, OCH_2-CH_3), 3.28 (s, 3H, OMe), 0.76 (t, 3H, J = 6.0 Hz, CH_3); ^{13}C NMR (75 MHz, C_6D_6, 25 ºC): δ = 198.9 (CO), 163.4 (CO), 154.6 (Ar, C), 154.0

(Ar, C), 152.5 (Ar, C), 136.6 (Ar, 2CH), 129.6 (Ar, 2CH), 128.0 (Ar, CH), 124.9 (Ar, C), 118.8 (Ar, CH), 116.0 (Ar, 2CH), 114.6 (Ar, 2CH), 72.6 (OCH_2), 60.6 (OCH_2), 54.8 (OCH_3), 13.6 (CH_3); ^{77}Se-NMR (95 MHz, C_6D_6, 25 ºC) δ: 477.6 (s, 1Se, Se); IR (C_6H_6, cm^{-1}): ν = 1703, 1591, 1504, 1317, 1192, 1027 cm^{-1}; HRMS (ES): calcd for $C_{20}H_{21}O_5Se$ [*M* + H]$^+$: 421.05499; found: 421.05443.



7h

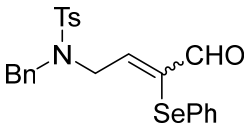
α-Selenoenone 7h. From 59 mg (0.20 mmol) of allene **2h**, and after chromatography of the residue using hexanes/ethyl acetate (10:1) as eluent gave compound **7h** (39 mg, 43%; containing *ca.* 5% of its *E* diastereomer) as a colorless oil; ^{1}H NMR (300 MHz, C_6D_6, 25 ºC): δ = 7.32 (dt, 2H, *J* = 9.0 Hz, *J* = 3.0 Hz, ArH), 7.12 (dt, 2H, *J* = 9.0 Hz, *J* = 3.0 Hz, ArH), 6.82 (m, 3H, ArH), 6.46 (dt, 2H, *J* = 9.0 Hz, *J* = 3.0 Hz, ArH), 5.82 (s, 1H, CH), 4.51 (s, 2H, OCH_2), 3.73 (q, 2H, *J* = 6.0 Hz, O*CH*$_2$-CH_3), 0.76 (t, 3H, *J* = 6.0 Hz, CH_3); ^{13}C NMR (75 MHz, C_6D_6, 25 ºC): δ = 197.8 (CO), 163.4 (CO), 157.3 (Ar, C), 153.6 (Ar, C), 136.6 (Ar, 2CH), 132.2 (Ar, 2CH), 129.6 (Ar, 3CH), 124.7 (Ar, C), 116.7 (Ar, 2CH), 116.7 (Ar, CH), 113.6 (Ar, C), 71.7 (OCH_2), 60.6 (OCH_2), 13.5 (CH_3); ^{77}Se-NMR (95 MHz, C_6D_6, 25 ºC) δ: 478.9 (s, 1Se, Se); IR (C_6H_6, cm^{-1}): ν = 1701, 1582, 1484, 1315, 1193, 1028 cm^{-1}; HRMS (ES): calcd for $C_{19}H_{18}BrO_4Se$ [*M* + H]$^+$: 468.95462; found: 468.95396.



14a

***N*-(4-Methoxybenzyl)-4-methyl-*N*-(4-oxo-3-(phenylselanyl)but-2-en-1-yl)benzenesulfonamide 14a**. From 35 mg (0.11 mmol) of allene **10a**, and after chromatography of the residue using hexanes/ethyl acetate (10:1) as eluent gave compound **14a** (35 mg, 65%; containing *ca.* 10% of its *E* diastereomer) as a yellow oil; ^{1}H NMR (500 MHz, C_6D_6): δ = 8.78 (s, 1H, CHO), 7.64 (d, 2H, *J* = 7.6 Hz, ArH), 7.51 (m, 1H, ArH), 7.26 (m, 2H, ArH), 7.03 (d, 2H, *J* = 7.0 Hz, ArH), 6.88 (m, 2H, ArH), 6.79 (m, 3H, ArH), 6.65 (m, 2H, ArH), 4.02 (s, 2H, CH_2), 3.99 (s, 1H, CHH), 3.98 (s, 1H,

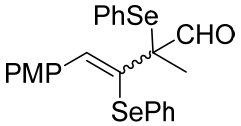
CHH), 3.25 (s, 3H, OCH_3), 1.91 (s, 3H, CH_3); ^{13}C NMR (125 MHz, C_6D_6): δ = 188.6 (CHO), 160.2, 155.4 (Ar, CH), 143.3, 136.8, 135.6, 135.1, 132.6 (Ar, 2CH), 130.5 (Ar, 2CH), 129.9 (Ar, 2CH), 129.6, 129.4 (Ar, 2CH), 129.4 (Ar, CH), 127.8 (Ar, 2CH), 114.4 (Ar, 2CH), 54.8 (OCH_3), 53.1 (CH_2), 49.6 (CH_2), 21.1 (CH_3); ^{77}Se-NMR (95 MHz, C_6D_6) δ: 271.0 (s, 1Se, Se); IR ($CHCl_3$, cm^{-1}): ν = 2925, 2854, 1716, 1164, 742 cm^{-1}; HRMS (ES): calcd for $C_{25}H_{29}N_2O_4SSe$ $[M + NH_4]^+$: 533.1009; found: 533.1001.



14b

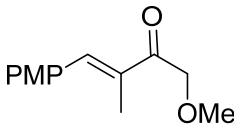
***N*-Benzyl-4-methyl-*N*-(4-oxo-3-(phenylselanyl)but-2-en-1-yl)benzenesulfonamide 14b.** From 45 mg (0.14 mmol) of allene **10b**, and after chromatography of the residue using hexanes/ethyl acetate (11:1) as eluent gave compound **14b** (35 mg, 50%; as a single *Z* diastereomer) as a yellow oil; ^1H NMR (500 MHz, C_6D_6): δ = 8.75 (s, 1H, CHO), 7.62 (d, 2H, *J* = 7.6 Hz, ArH), 7.24 (m, 2H, ArH), 7.10 (m, 2H, ArH), 7.00 (m, 3H, ArH), 6.87 (m, 3H, ArH), 6.77 (d, 2H, *J* = 6.8 Hz, ArH), 6.59 (t, 1H, *J* = 6.6 Hz, ArH), 4.01 (s, 2H, CH_2), 3.96 (s, 1H, CHH), 3.96 (s, 1H, CHH), 1.90 (s, 3H, CH_3); ^{13}C NMR (125 MHz, C_6D_6): δ = 188.5 (CHO), 155.0 (Ar, CH), 143.3, 136.8, 136.1, 135.8, 132.6 (Ar, 2CH), 129.9 (Ar, 2CH), 129.6, 129.4 (Ar, 2CH), 129.0 (Ar, 2CH), 128.9 (Ar, 2CH), 128.3 (Ar, CH), 127.7 (Ar, 2CH), 127.4 (Ar, CH), 53.5 (CH_2), 49.8 (CH_2), 21.1 (CH_3); ^{77}Se-NMR (95 MHz, C_6D_6) δ: 271.3 (s, 1Se, Se); IR ($CHCl_3$, cm^{-1}): ν = 2924, 2854, 1699, 1346, 1162, 740 cm^{-1}; HRMS (ES): calcd for $C_{24}H_{27}N_2O_3SSe$ $[M + NH_4]^+$: 503.0903; found: 503.0890.

Reaction of allene 12. From 50 mg (0.25 mmol) of allene **12**, and after chromatography of the residue using hexanes/ethyl acetate (14:1) as eluent gave compound **15** (24 mg, 20%; containing *ca.* 9% of its *E* diastereomer) and compound **16** (14 mg, 25%; single *Z* diastereomer).



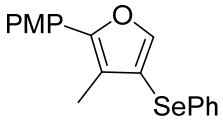
15

4-(4-Methoxyphenyl)-2-methyl-2,3-bis(phenylselanyl)but-3-enal 15. Yellow oil (containing *ca.* 9% of its *E* diastereomer); ^{1}H NMR (500 MHz, C_6D_6): δ = 9.82 (s, 1H, CHO), 7.51 (m, 2H, ArH), 7.27 (s, 1H, CH), 7.25 (d, 2H, *J* = 7.3 Hz, ArH), 7.08 (m, 2H, ArH), 6.93 (m, 3H, ArH), 6.83 (m, 3H, ArH), 6.77 (m, 2H, ArH), 3.26 (s, 3H, OCH_3), 1.91 (s, 3H, CH_3); ^{13}C NMR (125 MHz, C_6D_6): δ = 194.9 (CHO), 159.8, 134.0 (Ar, 2CH), 133.7, 132.9, 132.0 (Ar, 2CH), 131.9, 131.0 (CH), 130.3, 130.2 (Ar, 2CH), 129.7 (Ar, 2CH), 129.5 (Ar, 2CH), 128.0 (Ar, CH), 127.4 (Ar, CH), 115.0 (Ar, 2CH), 62.6, 54.7 (OCH_3), 18.0 (CH_3); ^{77}Se-NMR (95 MHz, C_6D_6) δ: 468.9 (s, 1Se, Se), 420.4 (s, 1Se, Se); IR ($CHCl_3$, cm^{-1}): ν = 3019, 1510, 1255, 747 cm^{-1}; HRMS (ES): calcd for $C_{24}H_{22}NaO_2Se_2$ [*M* + Na]$^+$: 524.9847; found: 524.9850.



16

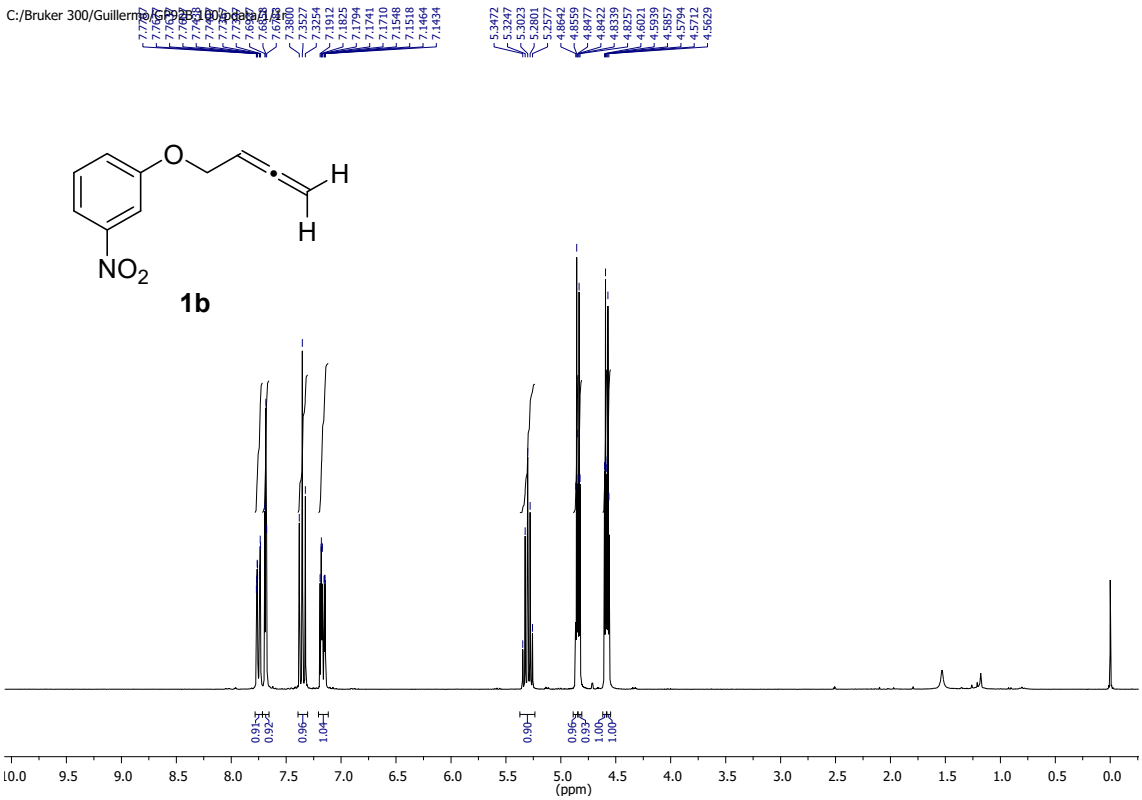
(*E*)-1-Methoxy-4-(4-methoxyphenyl)-3-methylbut-3-en-2-one 16. Yellow oil (single *Z* diastereomer); ^{1}H NMR (500 MHz, C_6D_6): δ = 7.33 (s, 1H, CH), 7.15 (m, 2H, ArH), 6.71 (m, 2H, ArH), 4.17 (s, 2H, CH_2), 3.27 (s, 3H, OCH_3), 3.23 (s, 3H, OCH_3), 2.07 (d, *J* = 2.1 Hz, 3H, CH_3); ^{13}C NMR (125 MHz, C_6D_6): δ = 197.5, 160.4, 138.9 (Ar, CH), 133.9, 131.9 (Ar, 2CH), 128.7, 114.2 (Ar, 2CH), 75.1 (CH_2), 58.8 (OCH_3), 54.8 (OCH_3), 13.2 (CH_3); IR ($CHCl_3$, cm^{-1}): ν = 2925, 2853, 1679, 1605, 1259, 1182; HRMS (ES): calcd for $C_{13}H_{16}NaO_3$ [*M* + Na]$^+$: 243.0992; found: 243.0991.



17

2-(4-Methoxyphenyl)-3-methyl-4-(phenylselanyl)furan 17. From 20 mg (0.11 mmol) of allenone **13**, and after chromatography of the residue using hexanes/ethyl acetate (9:1) as eluent gave compound **17** (23 mg, 63%) as a yellow oil; ^{1}H NMR (300 MHz, C_6D_6): δ = 7.50 (m, 2H, ArH),

7.27 (d, 2H, *J* = 7.3 Hz, ArH), 7.16 (s, 1H, H_{Ar}), 6.91 (m, 3H, ArH), 6.63 (d, 2H, *J* = 6.6 Hz, ArH), 3.21 (s, 3H, OCH_3), 1.61 (s, 3H, CH_3); ^{13}C NMR (75 MHz, C_6D_6): δ = 169.9, 160.8, 133.4 (Ar, 2CH), 129.5 (Ar, 2CH), 129.0, 128.5, 128.3 (Ar, CH), 128.0, 127.9 (Ar, CH), 127.5 (Ar, 2CH), 119.3, 114.3 (Ar, 2CH), 54.8 (OCH_3), 13.0 (CH_3); ^{77}Se-NMR (95 MHz, C_6D_6) δ: 262.2 (s, 1Se, Se); IR ($CHCl_3$, cm^{-1}): ν = 3387, 2924, 2854, 1761, 1255 cm^{-1}; HRMS (ES): calcd for $C_{18}H_{17}O_2Se$ [*M* + H]$^+$: 343.0400; found: 343.0422.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1b
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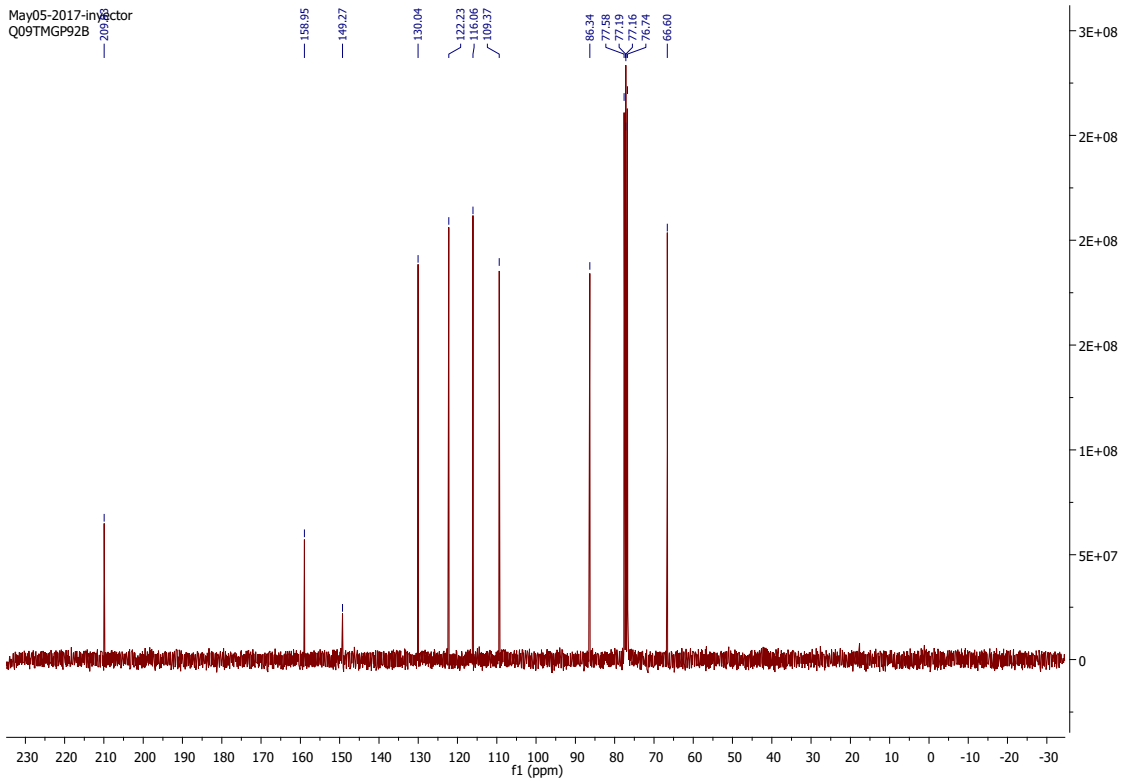
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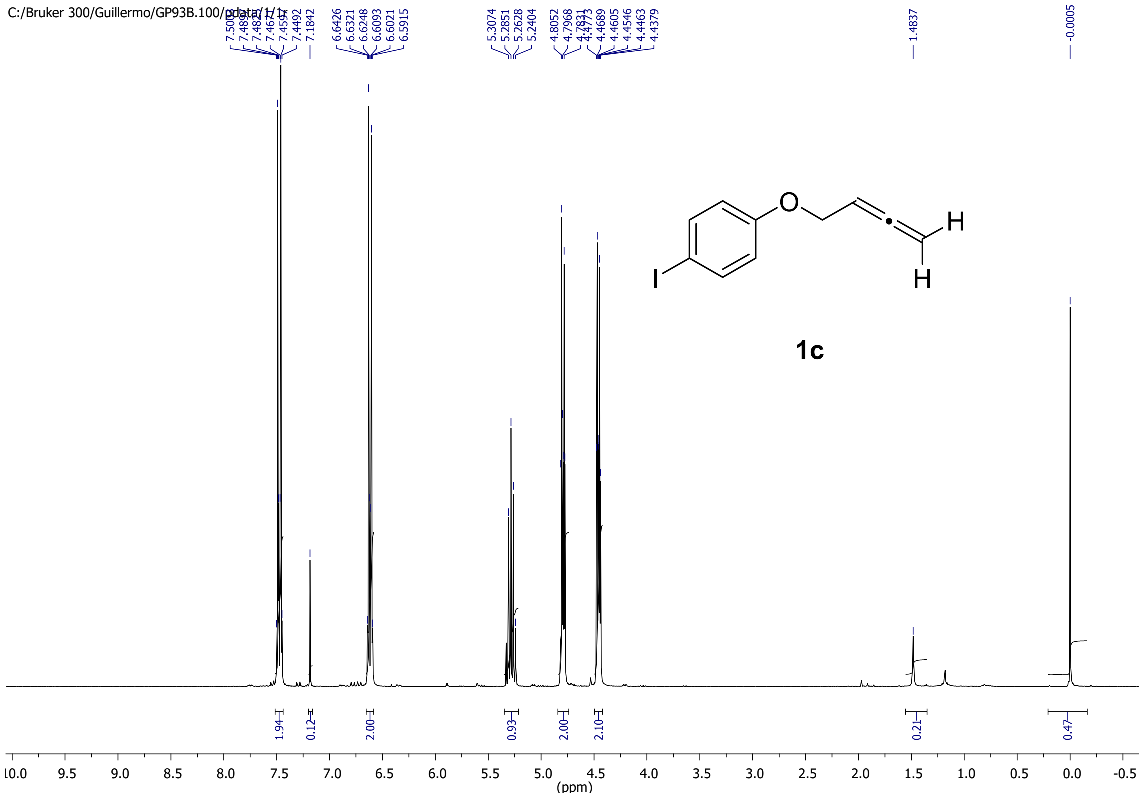
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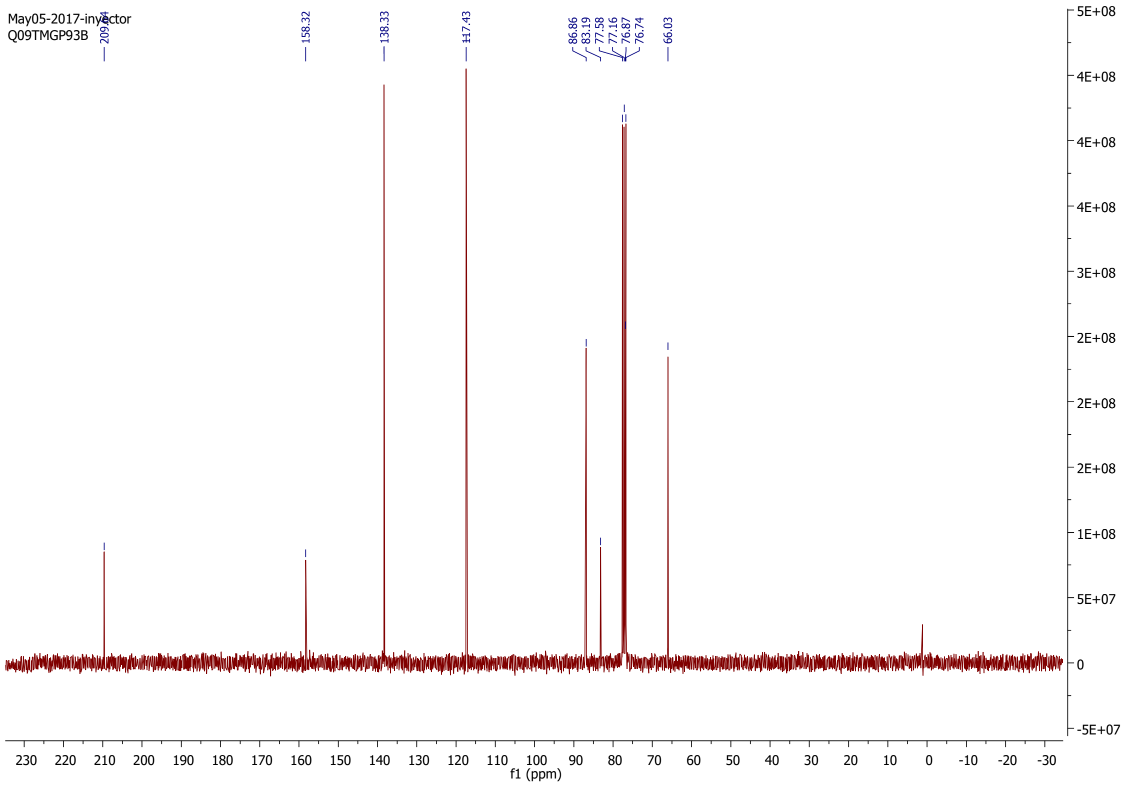
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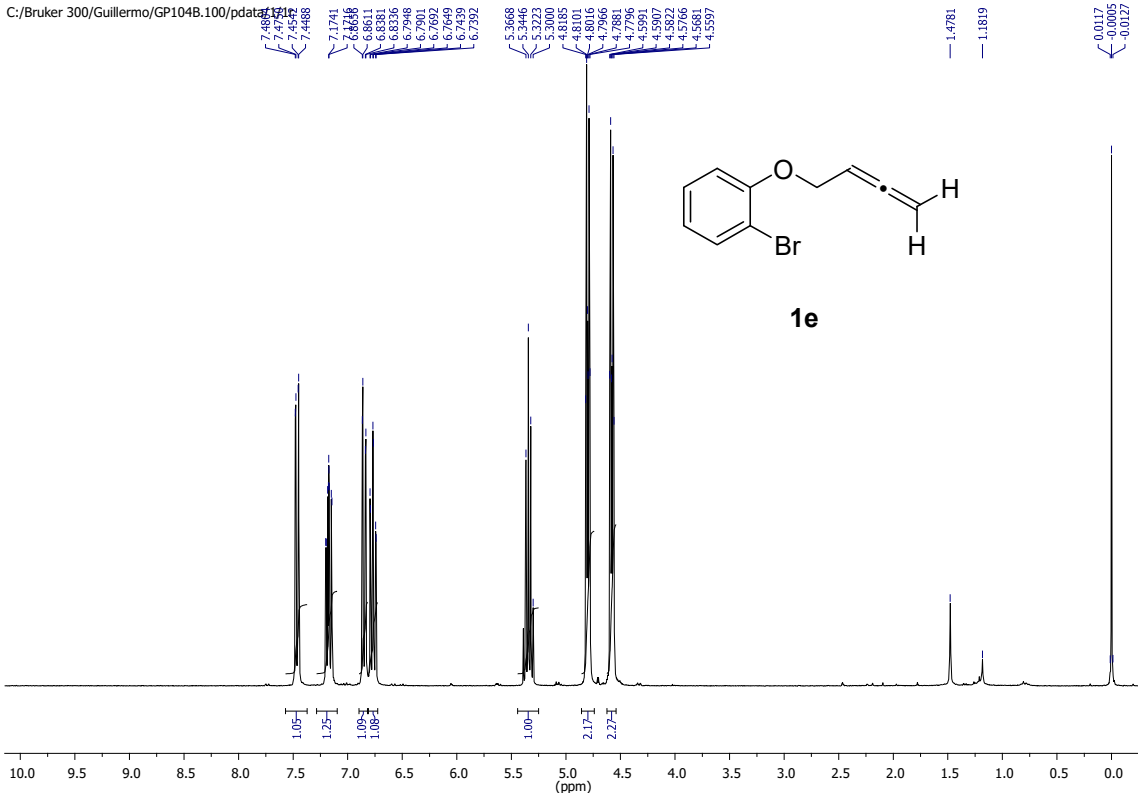
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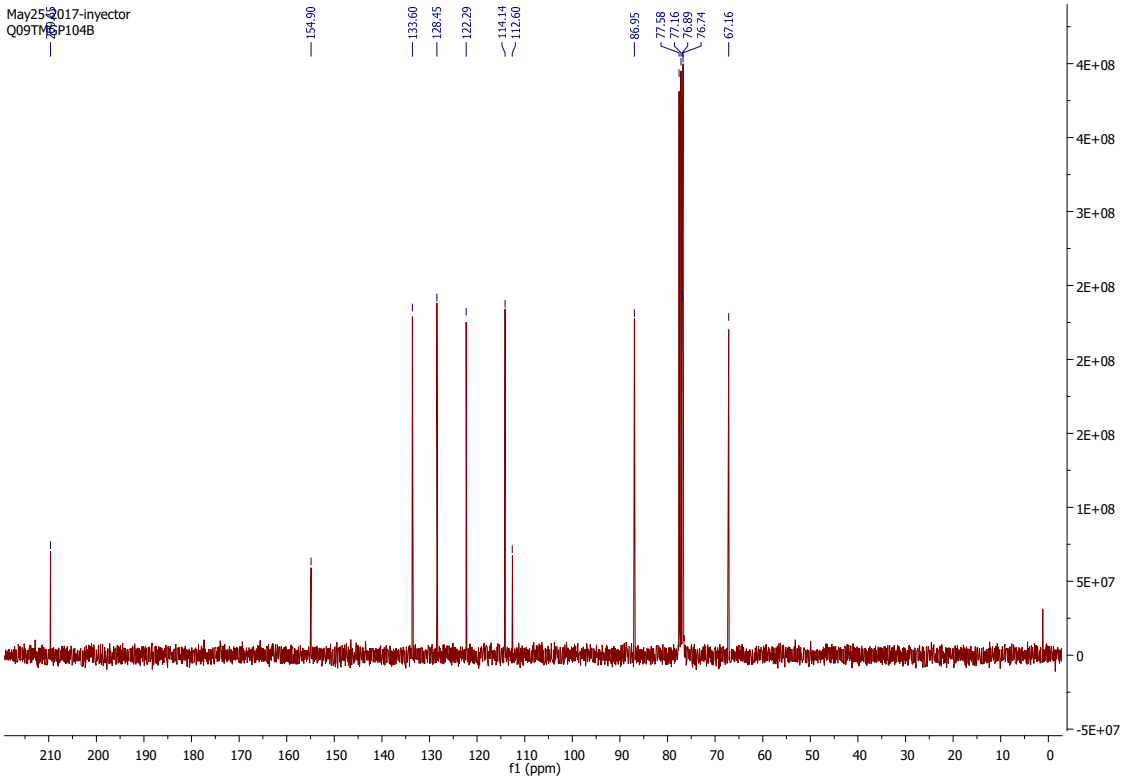
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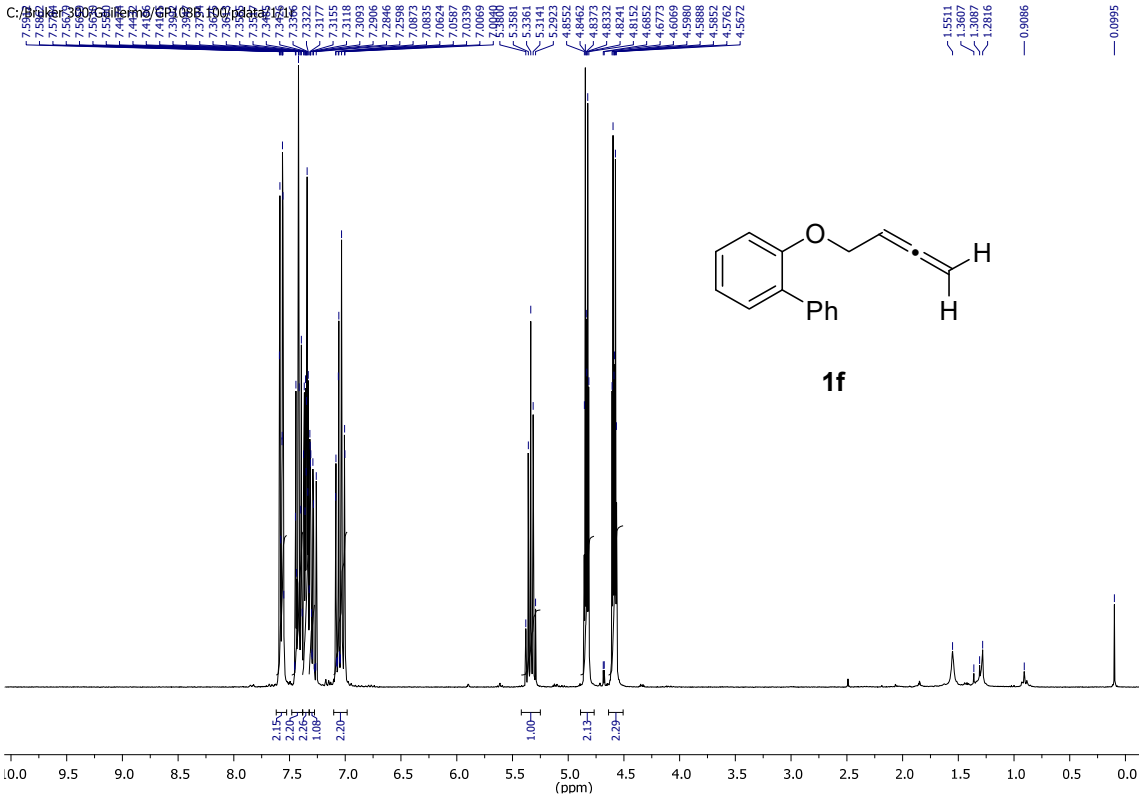
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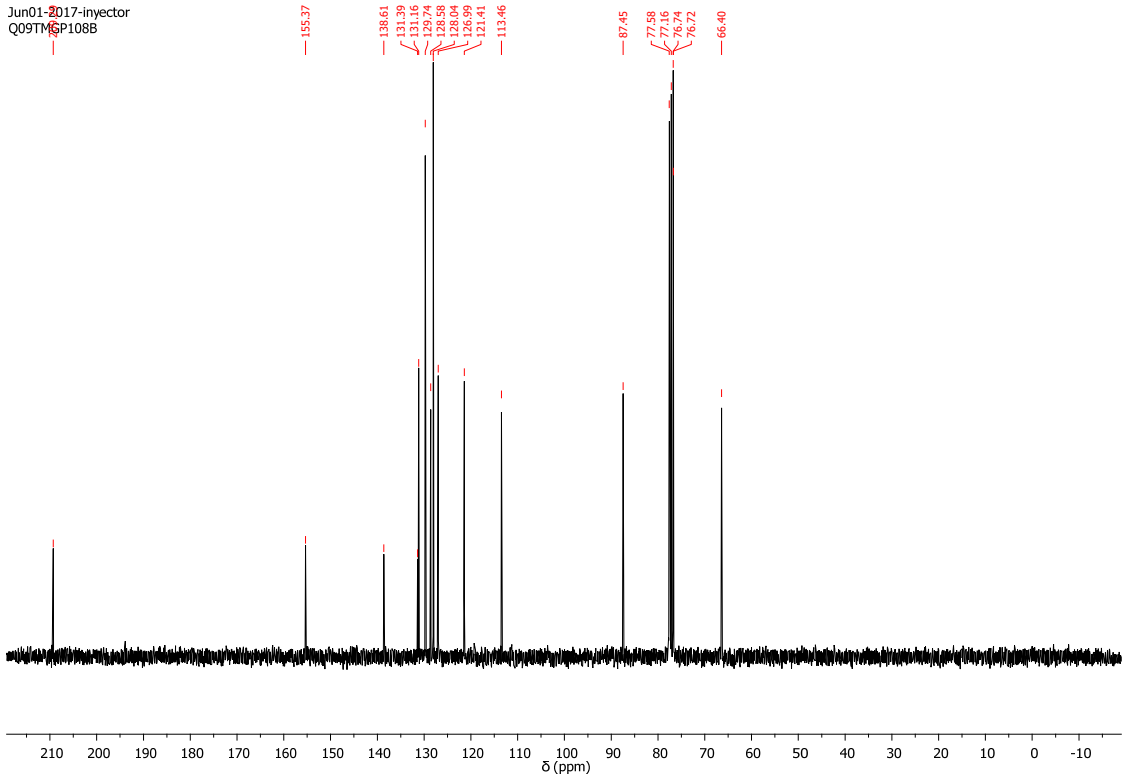
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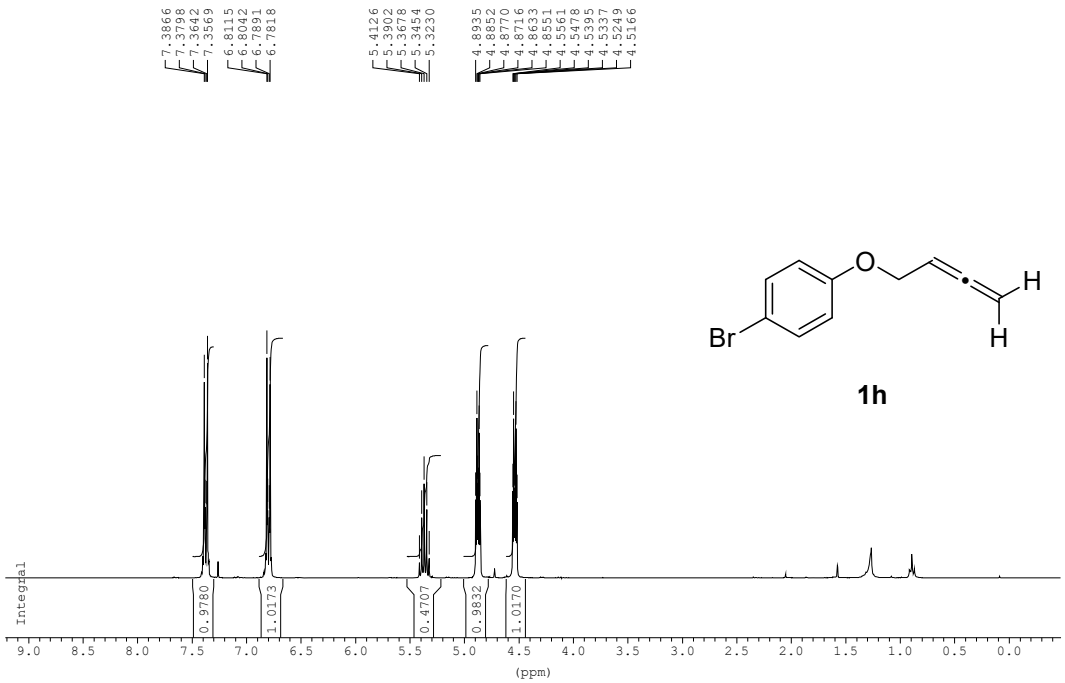

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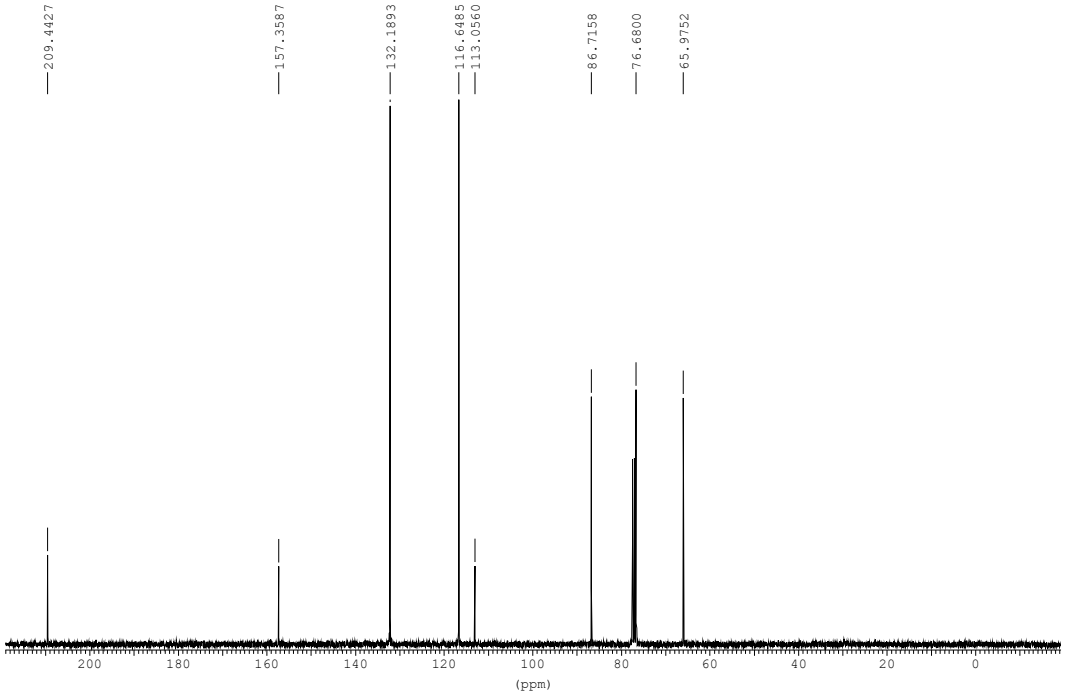

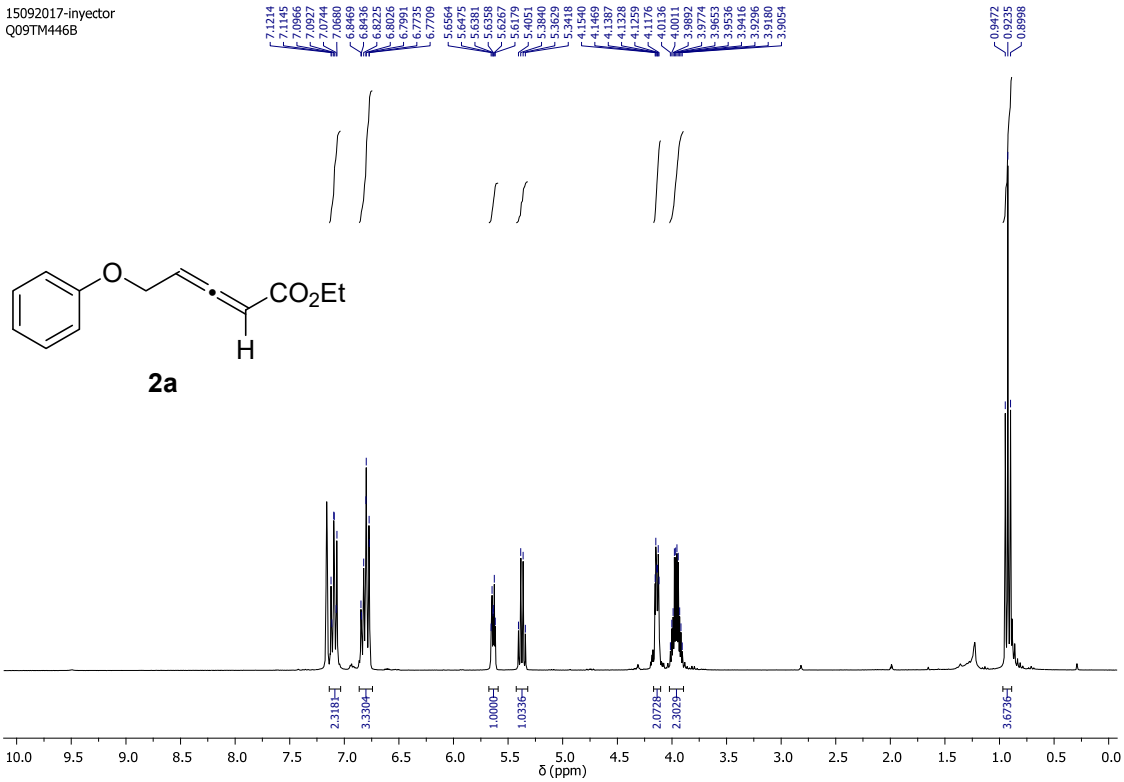
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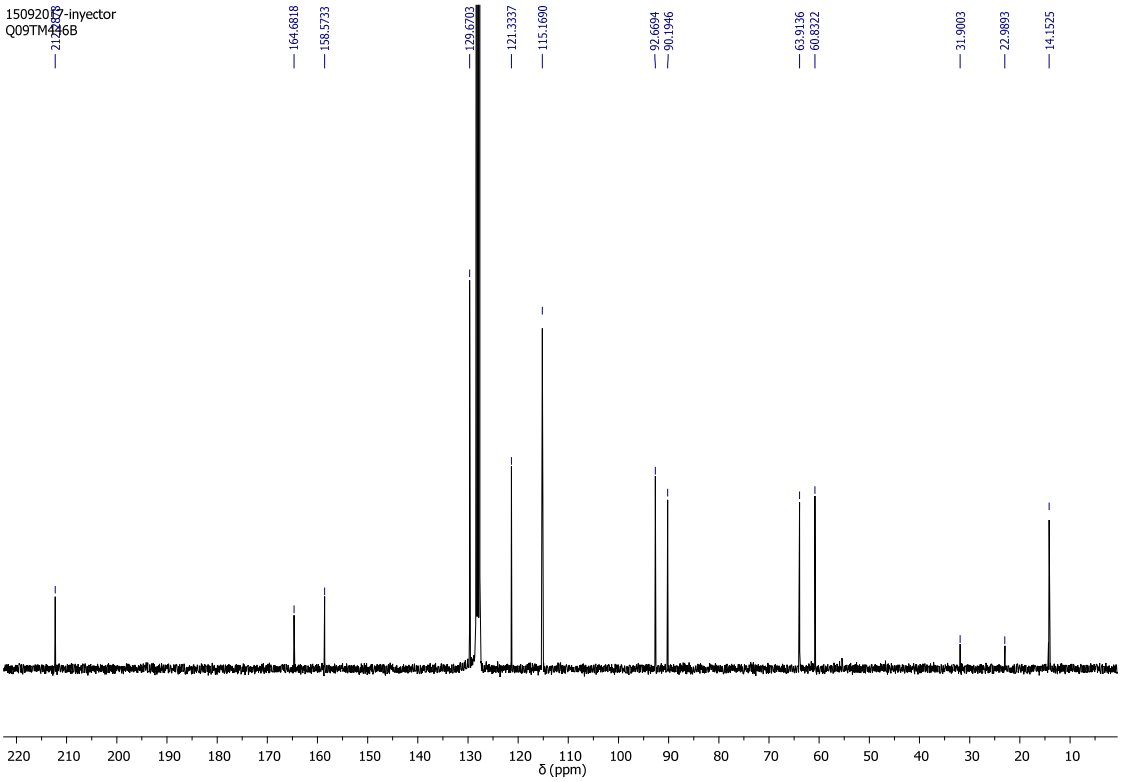
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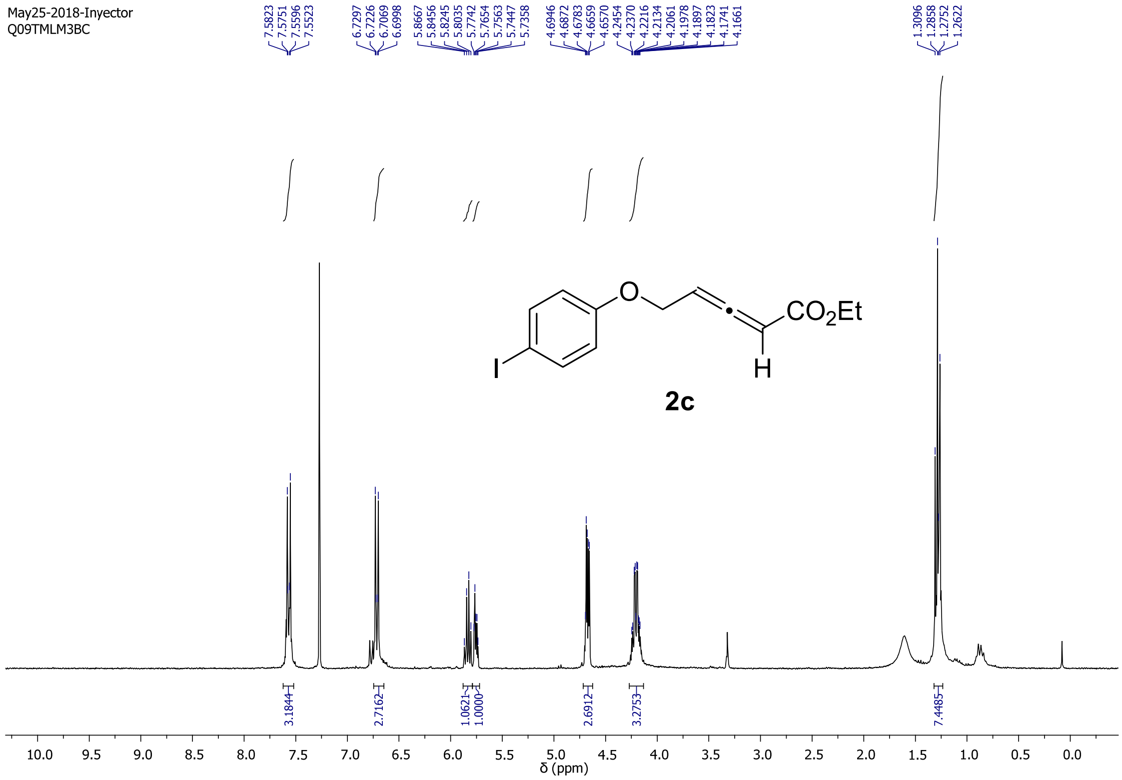
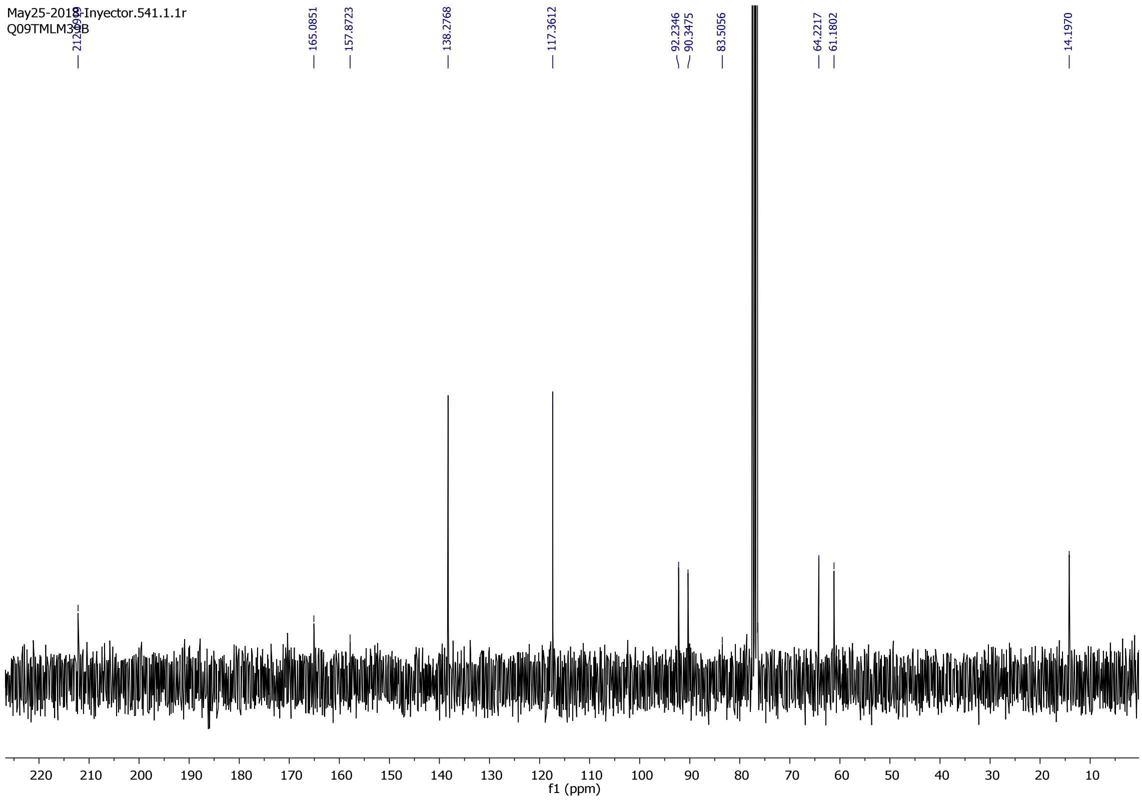
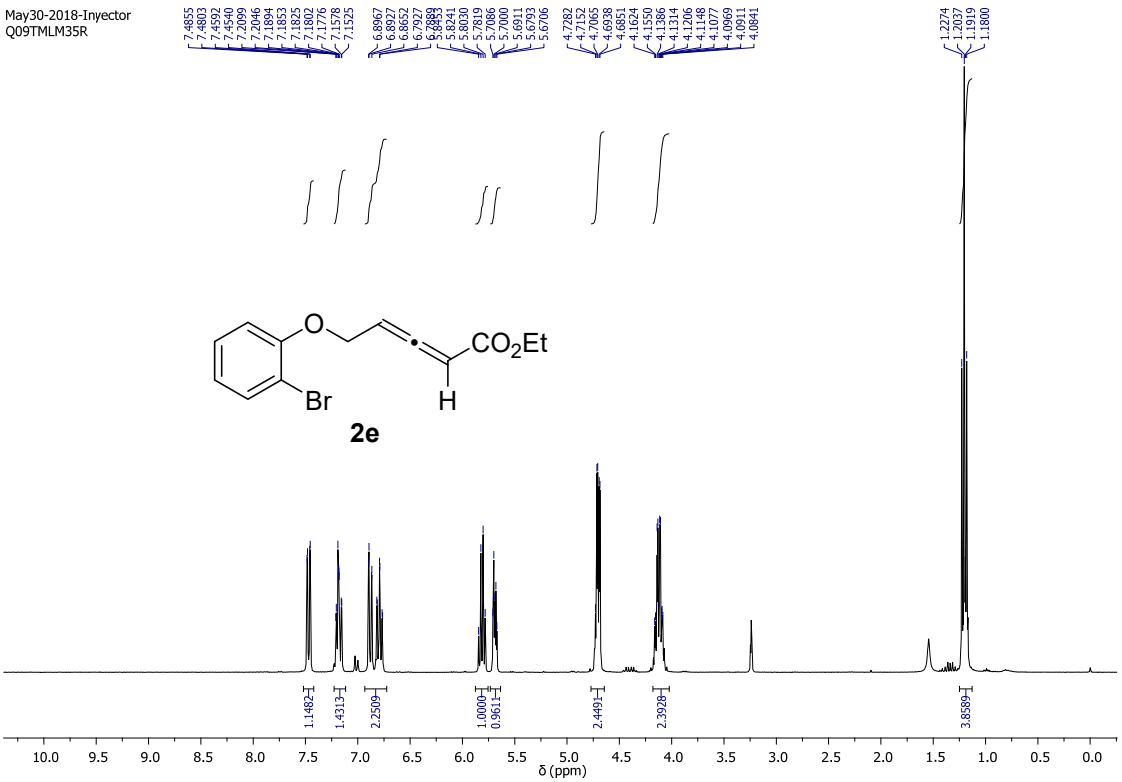
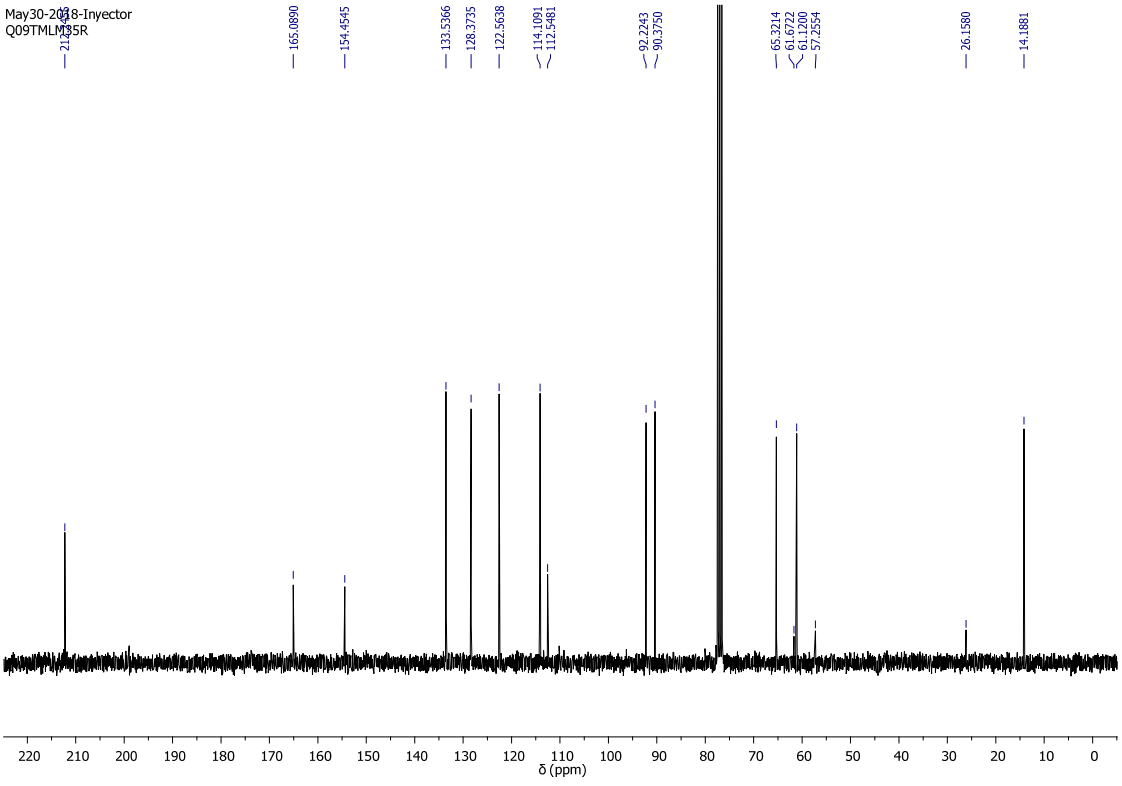
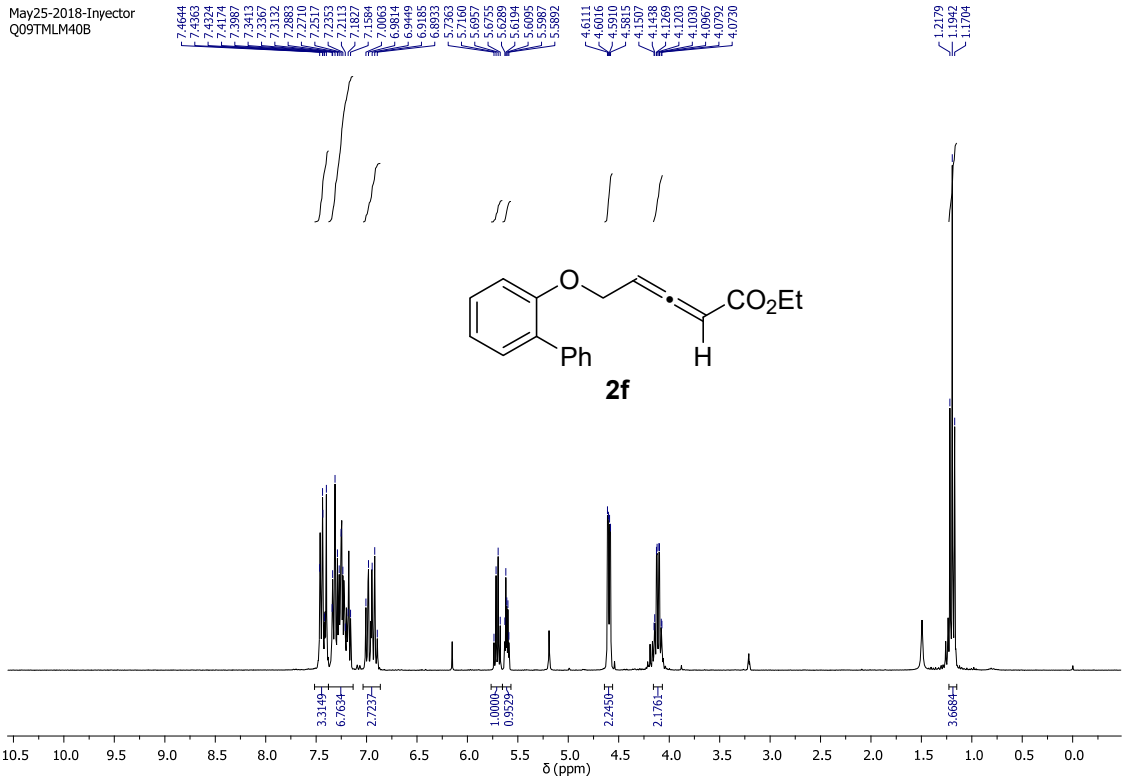
14.1525
δ (ppm)

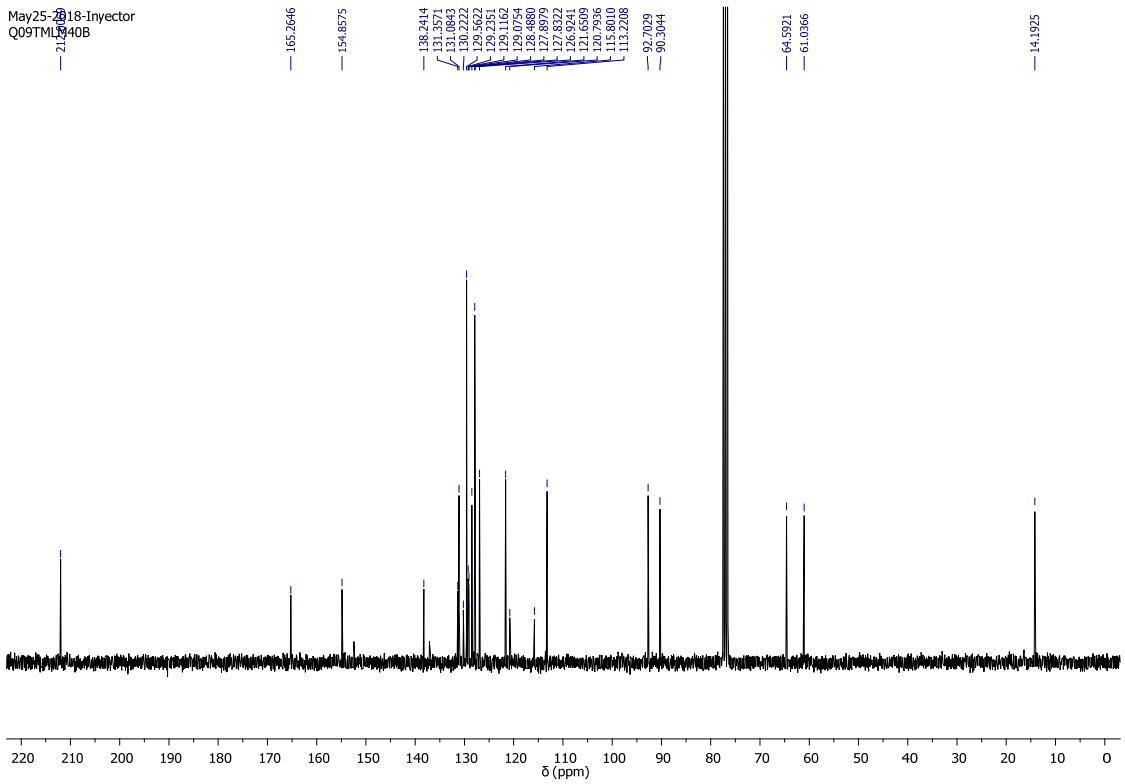

May25-2018-Inyector
Q09TMLM3BC
7.5823 7.5751 7.5596 7.5523
6.7297 6.7226 6.7069 6.6998
5.8667 5.8456 5.8245 5.8035 5.7742 5.7654 5.7563 5.7447 5.7358
4.6946 4.6872 4.6783 4.6659 4.6570 4.2454 4.2370 4.2216 4.2134 4.2061 4.1978 4.1897 4.1823 4.1741 4.1661
1.3096 1.2858 1.2752 1.2622
O
CO_2Et
I
H
2c
3.1844
2.7162
1.0621
1.0000
2.6912
3.2753
7.4485
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
δ (ppm)

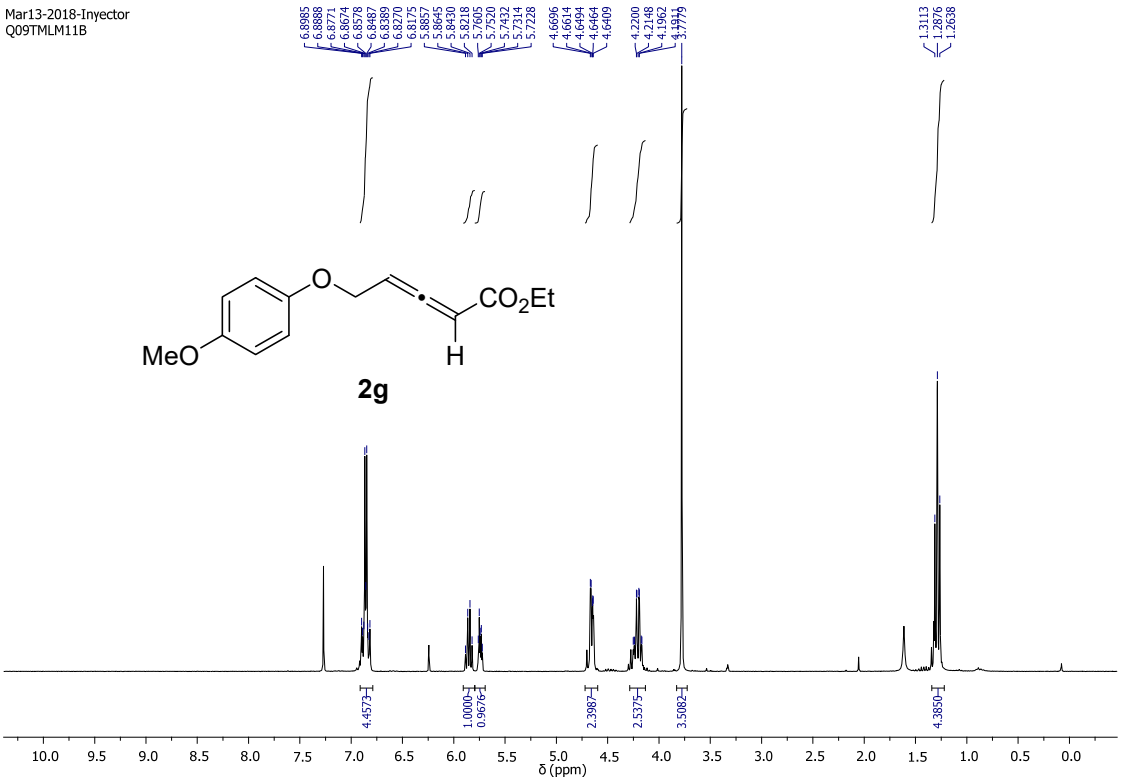

May25-2018-Inyector.541.1.1r
Q09TMLM39B
165.0851
157.8723
138.2768
117.3612
92.2346
90.3475
83.5056
64.2217
61.1802
14.1970
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

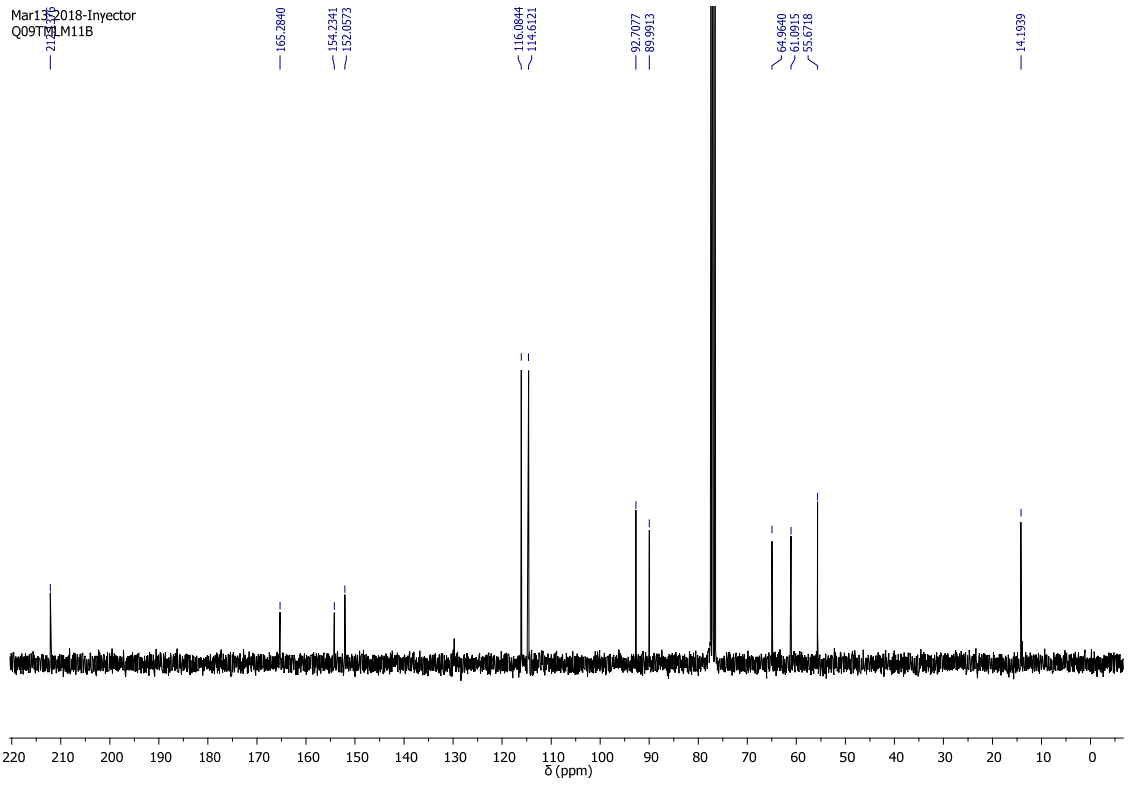

May30-2018-Inyector
Q09TMLM35R
O
CO2Et
Br
H
2e
δ (ppm)

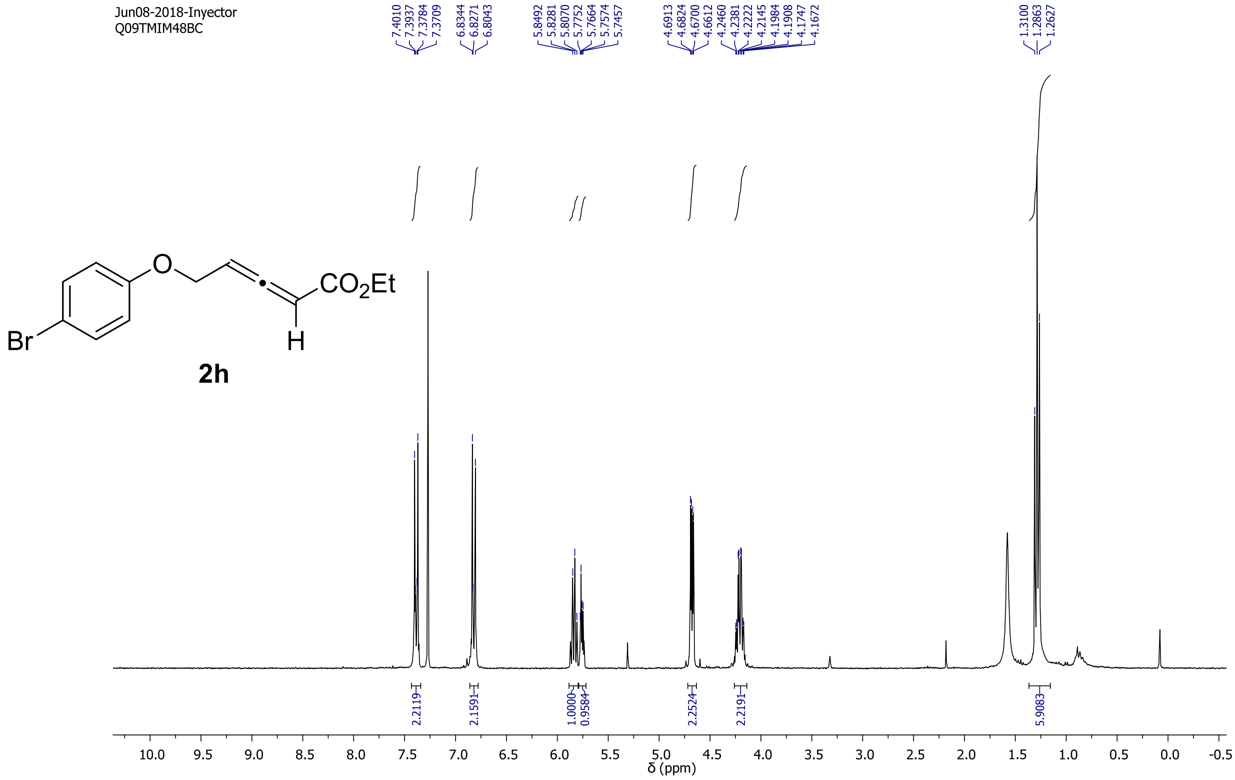

May30-2018-Inyector
Q09TMLM35R
δ (ppm)


May25-2018-Inyector
Q09TMLM40B
O
CO2Et
Ph
H
2f
δ (ppm)

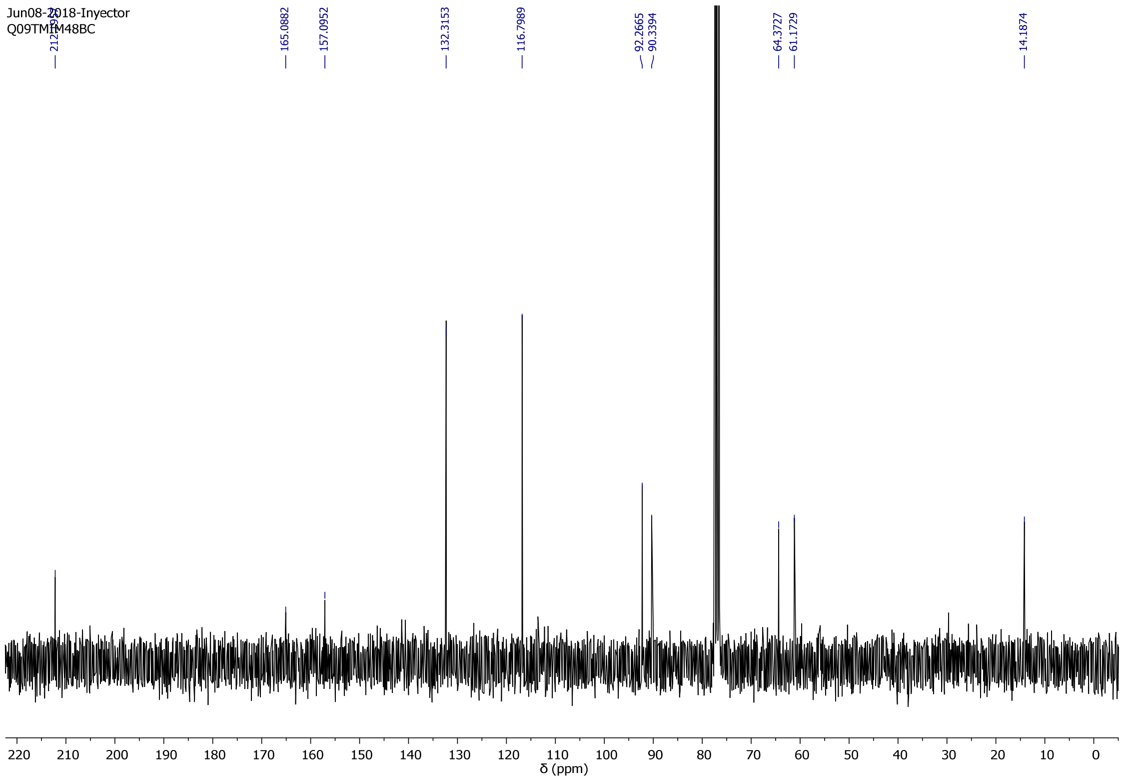

May25-2018-Inyector
Q09TMLM40B
δ (ppm)

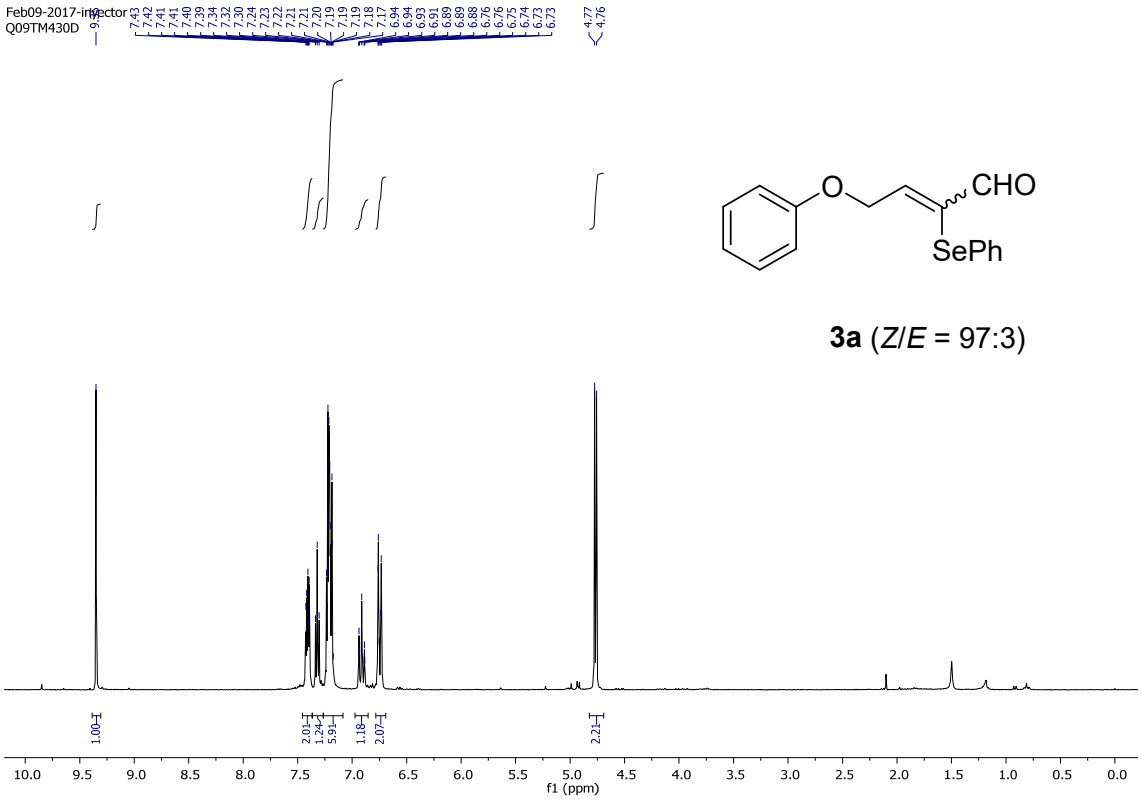

Mar13-2018-Inyector
Q09TMLM11B
MeO
O
CO2Et
H
2g
δ (ppm)


Mar13-2018-Inyector
Q09TMLM11B
δ (ppm)

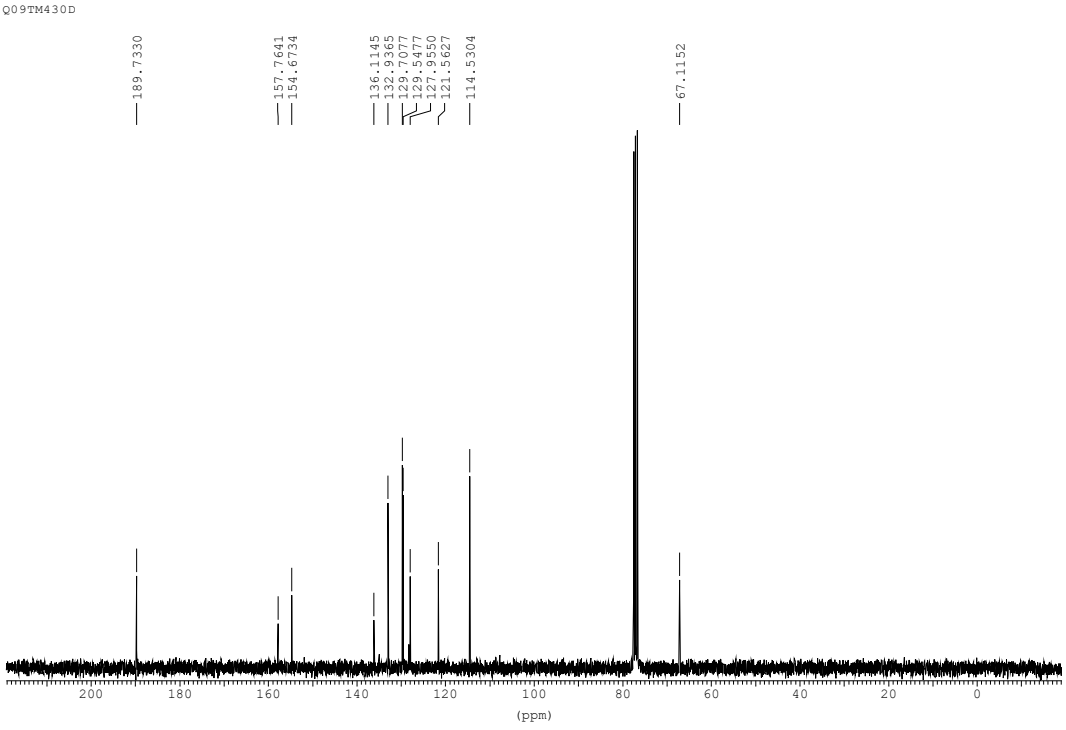

Jun08-2018-Inyector
Q09TMIM48BC
7.4010
7.3937
7.3784
7.3709
6.8344
6.8271
6.8043
5.8492
5.8281
5.8070
5.7752
5.7664
5.7574
5.7457
4.6913
4.6824
4.6700
4.6612
4.2460
4.2381
4.2222
4.2145
4.1984
4.1908
4.1747
4.1672
1.3100
1.2863
1.2627
2.2119
2.1591
1.0000
0.9584
2.2524
2.2191
5.9083
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
δ (ppm)
O
CO2Et
H
Br

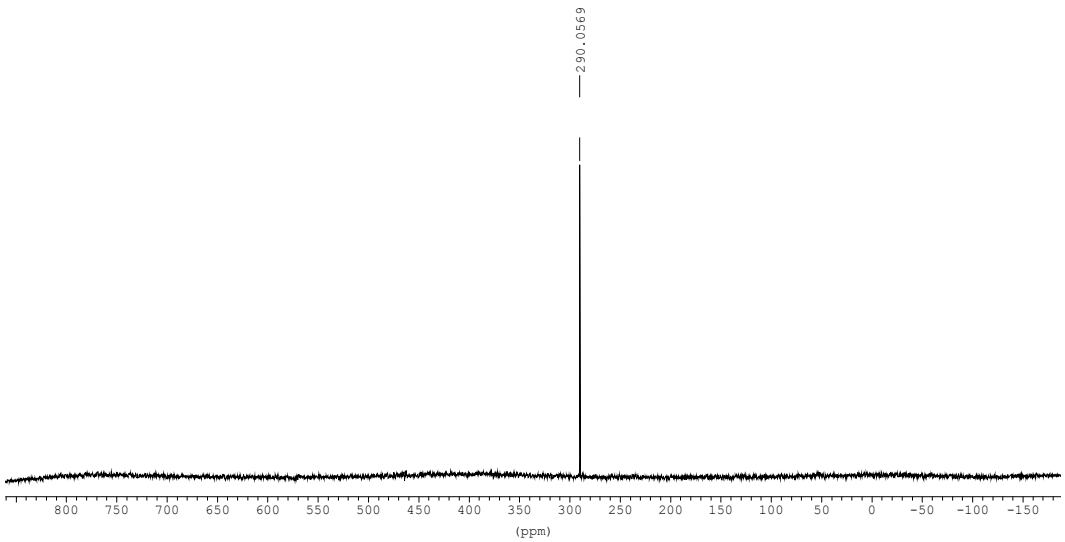
2h

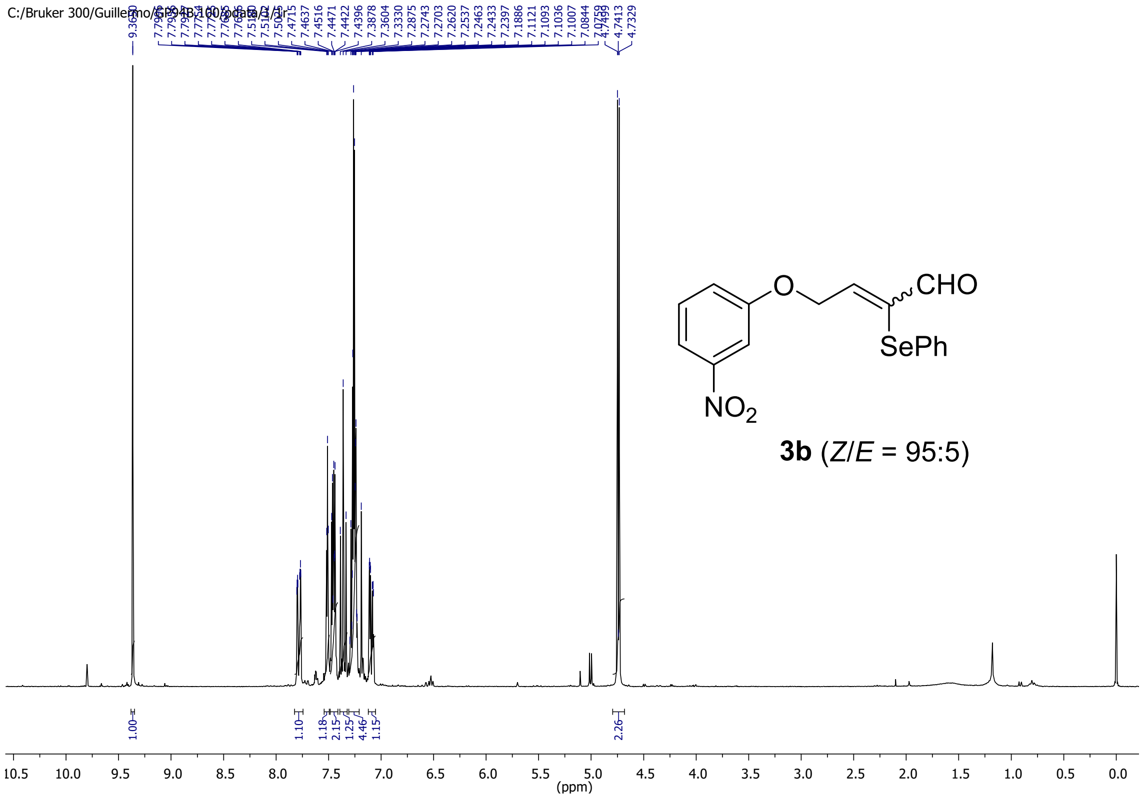

Jun08-2018-Inyector
Q09TMIM48BC
165.0882
157.0952
132.3153
116.7989
92.2665
90.3394
64.3727
61.1729
14.1874
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
δ (ppm)

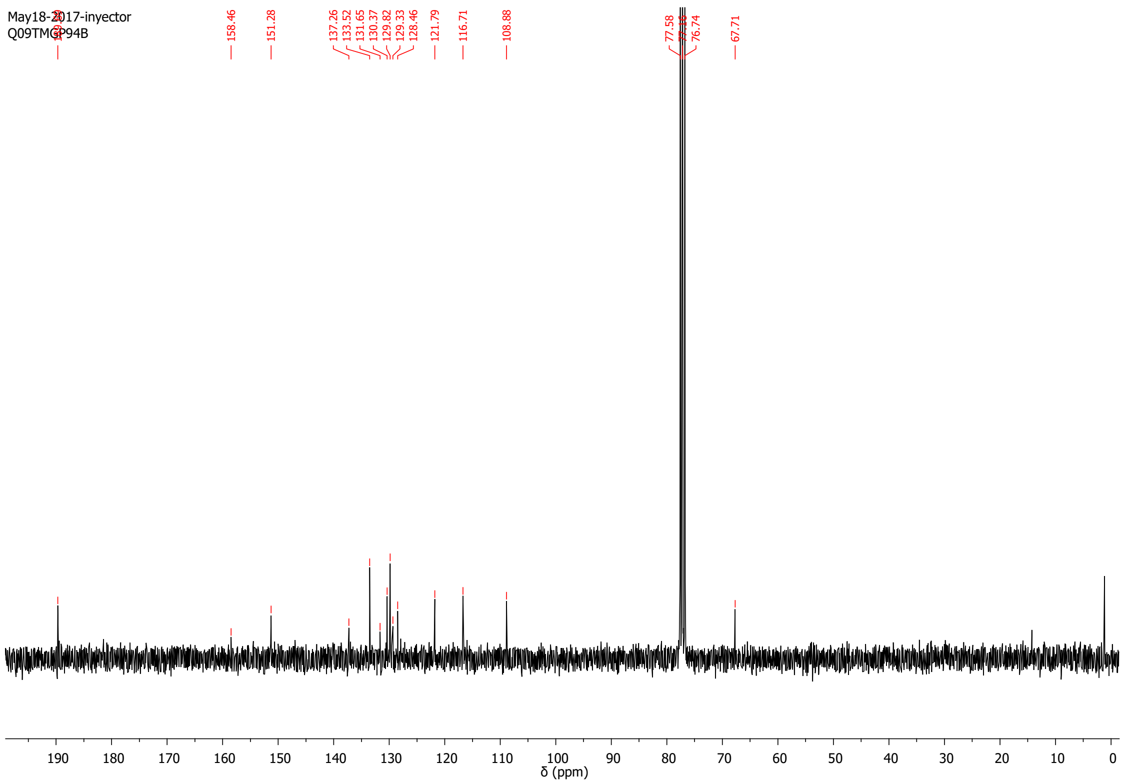

Feb09-2017-injector
Q09TM430D
9.41
7.43
7.42
7.41
7.41
7.40
7.39
7.34
7.32
7.30
7.24
7.23
7.22
7.21
7.21
7.20
7.19
7.19
7.19
7.18
7.17
6.94
6.94
6.93
6.91
6.89
6.89
6.88
6.76
6.76
6.75
6.74
6.73
6.73
4.77
4.76
O
CHO
SePh
1.00
2.01
1.24
5.91
1.18
2.07
2.21
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

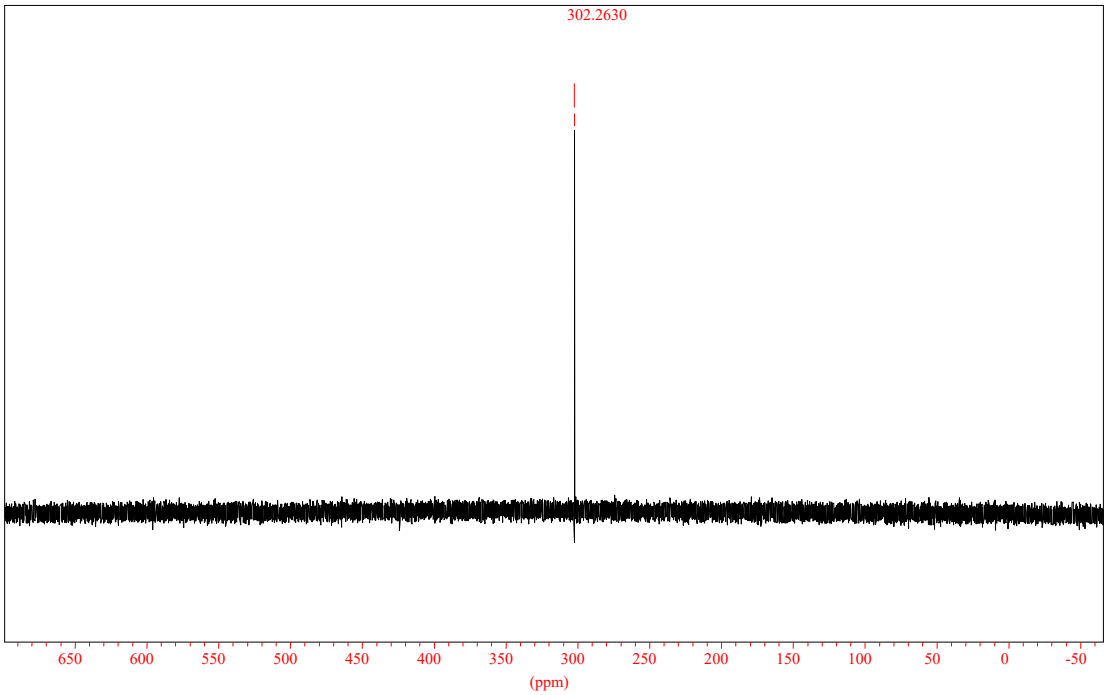
3a (*Z*/*E* = 97:3)

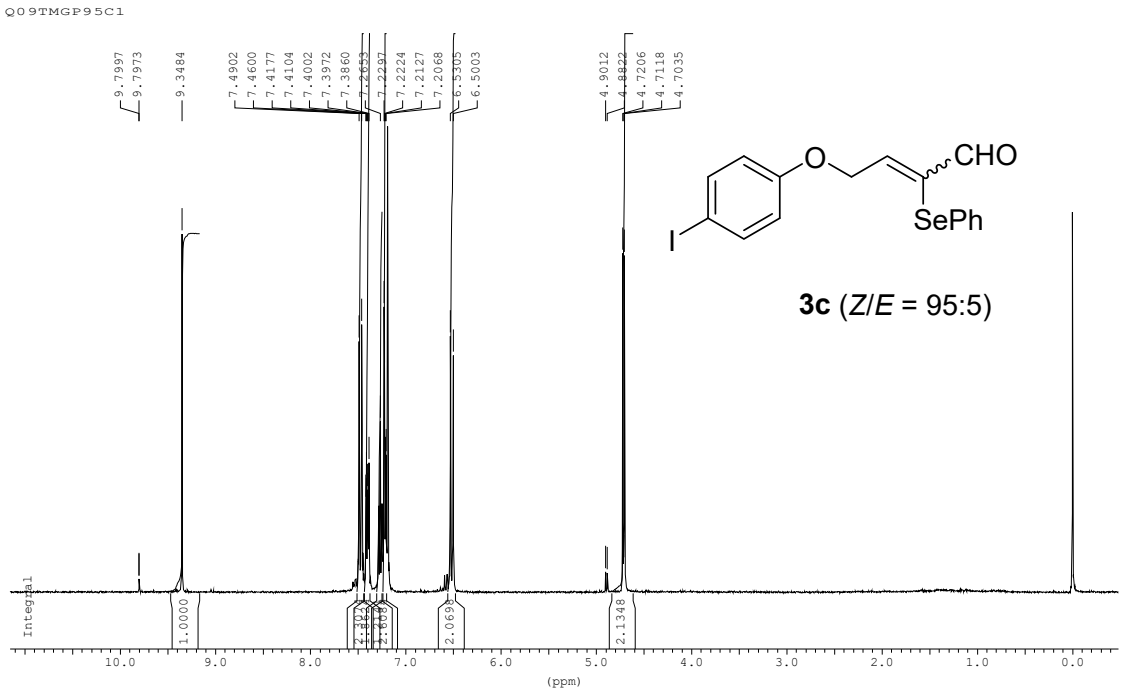

Q09TM430D
189.7330
157.7641
154.6734
136.1145
132.9365
129.7077
129.5477
127.9550
121.5627
114.5304
67.1152
200
180
160
140
120
100
80
60
40
20
0
(ppm)


290.0569
800
750
700
650
600
550
500
450
400
350
300
250
200
150
100
50
0
-50
-100
-150
(ppm)

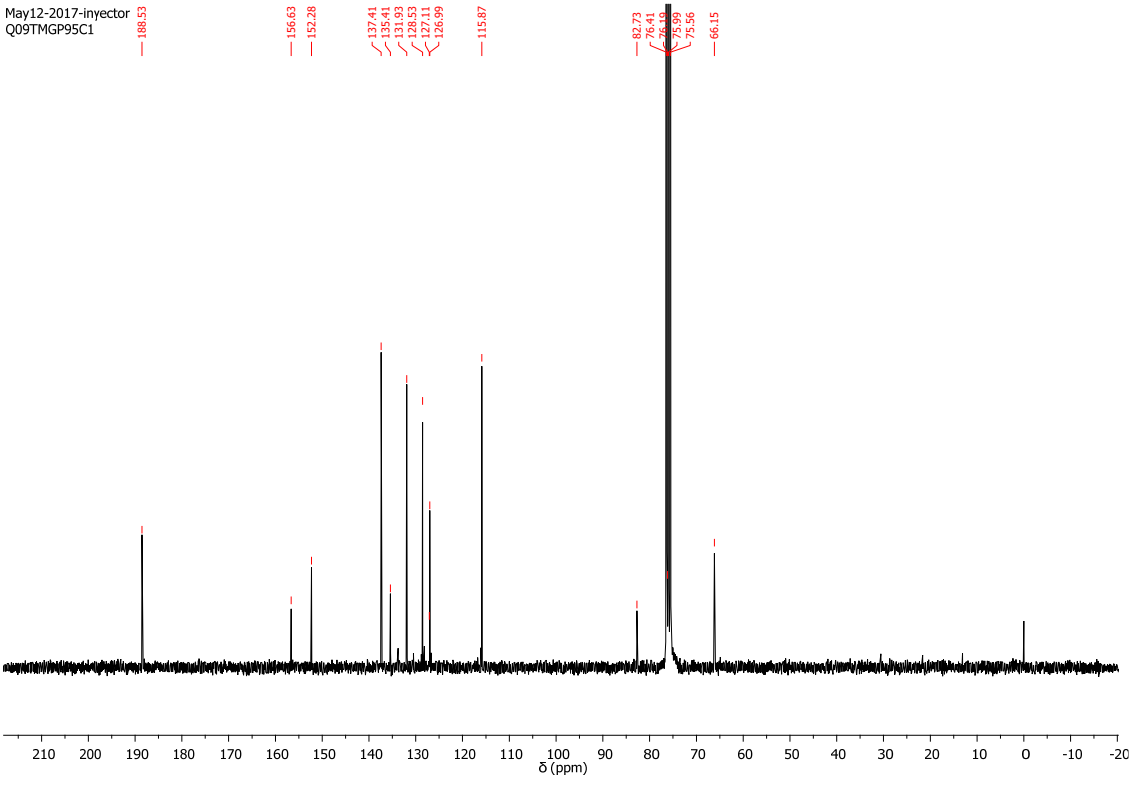

9.3620
4.7413
4.7329
O
CHO
SePh
NO2
3b (Z/E = 95:5)
1.00
1.10
1.18
2.15
1.29
4.46
1.15
2.26
(ppm)

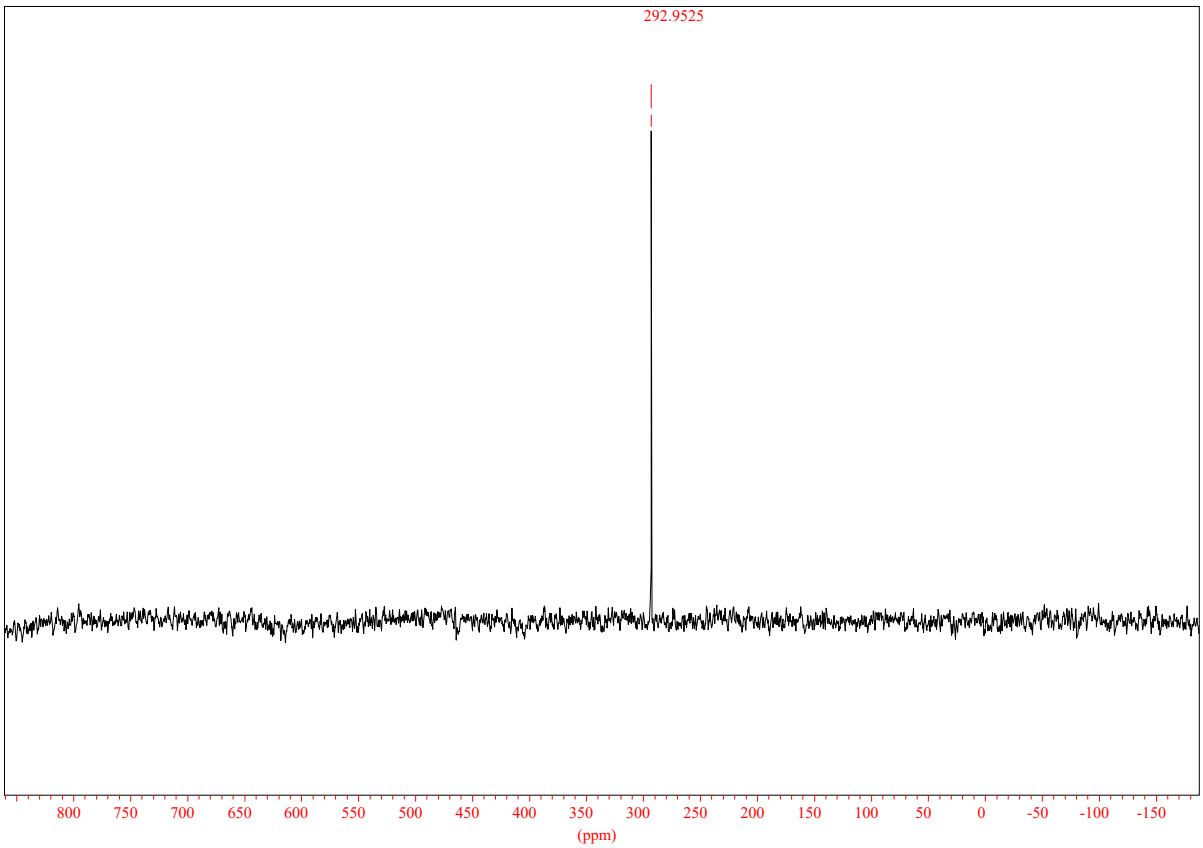

May18-2017-inyector
158.46
151.28
137.26
133.52
131.65
130.37
129.82
129.33
128.46
121.79
116.71
108.88
77.58
76.74
67.71
δ (ppm)

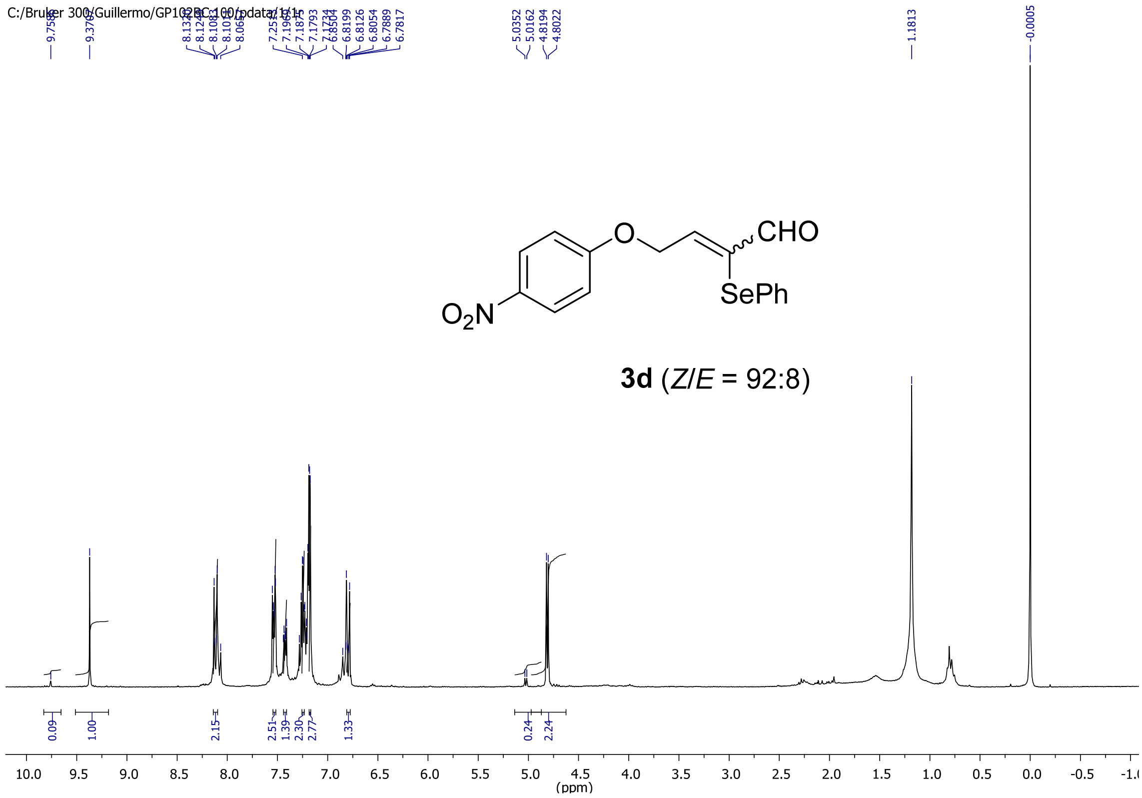

302.2630
650
600
550
500
450
400
350
300
250
200
150
100
50
0
-50
(ppm)


Q09TMGP95C1
9.7997
9.7973
9.3484
7.4902
7.4600
7.4177
7.4104
7.4002
7.3972
7.3860
7.2653
7.2297
7.2224
7.2127
7.2068
6.5305
6.5003
4.9012
4.8822
4.7206
4.7118
4.7035
Integral
1.0000
2.0691
2.1348
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
(ppm)
O
CHO
SePh
I

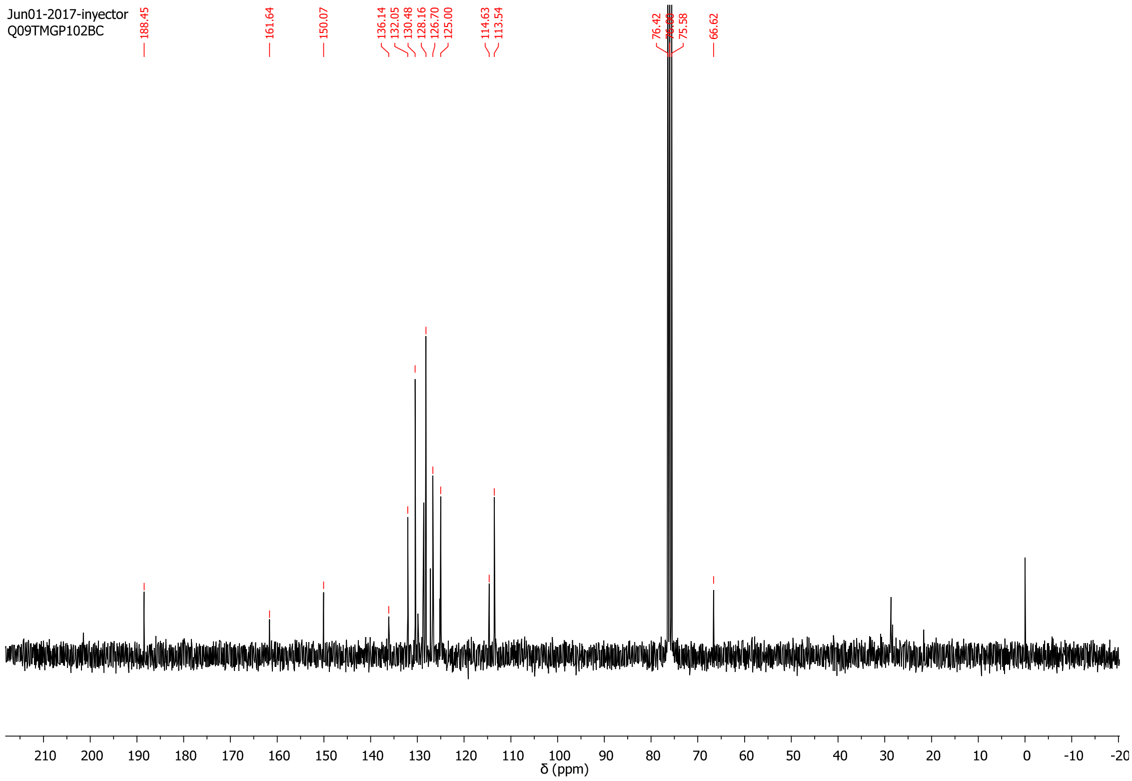
3c (*Z*/*E* = 95:5)

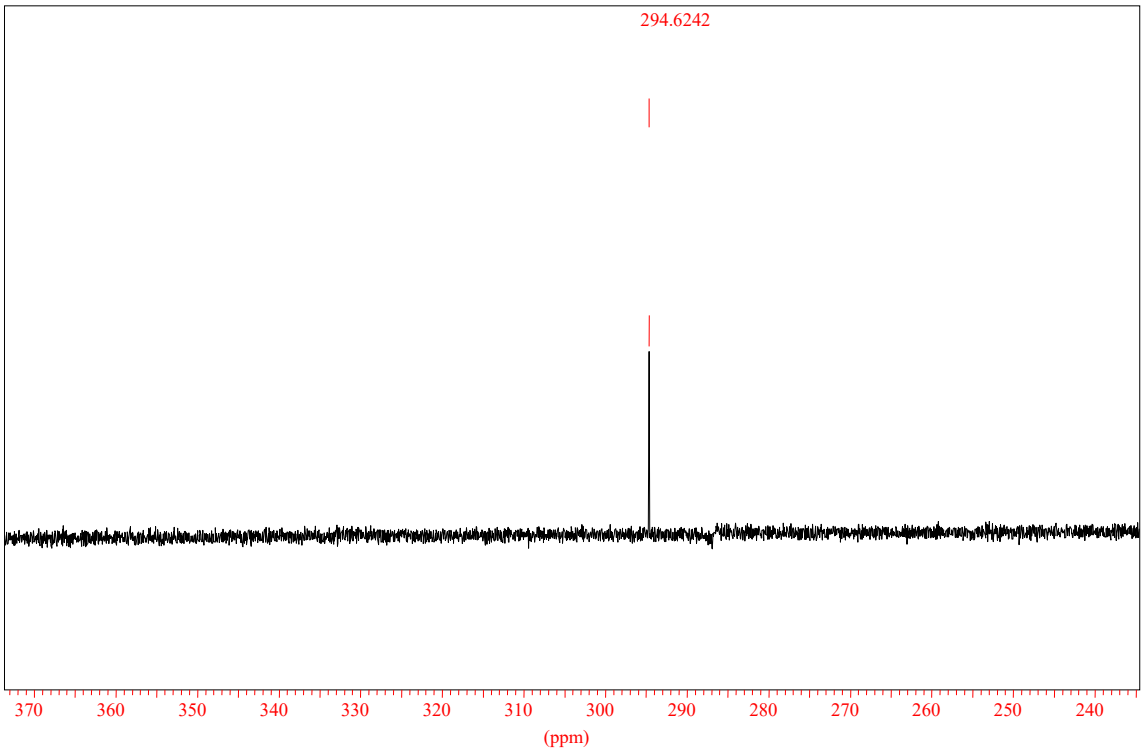

May12-2017-inyector
Q09TMGP95C1
188.53
156.63
152.28
137.41
135.41
131.93
128.53
127.11
126.99
115.87
82.73
76.41
76.19
75.99
75.56
66.15
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
-20
δ (ppm)

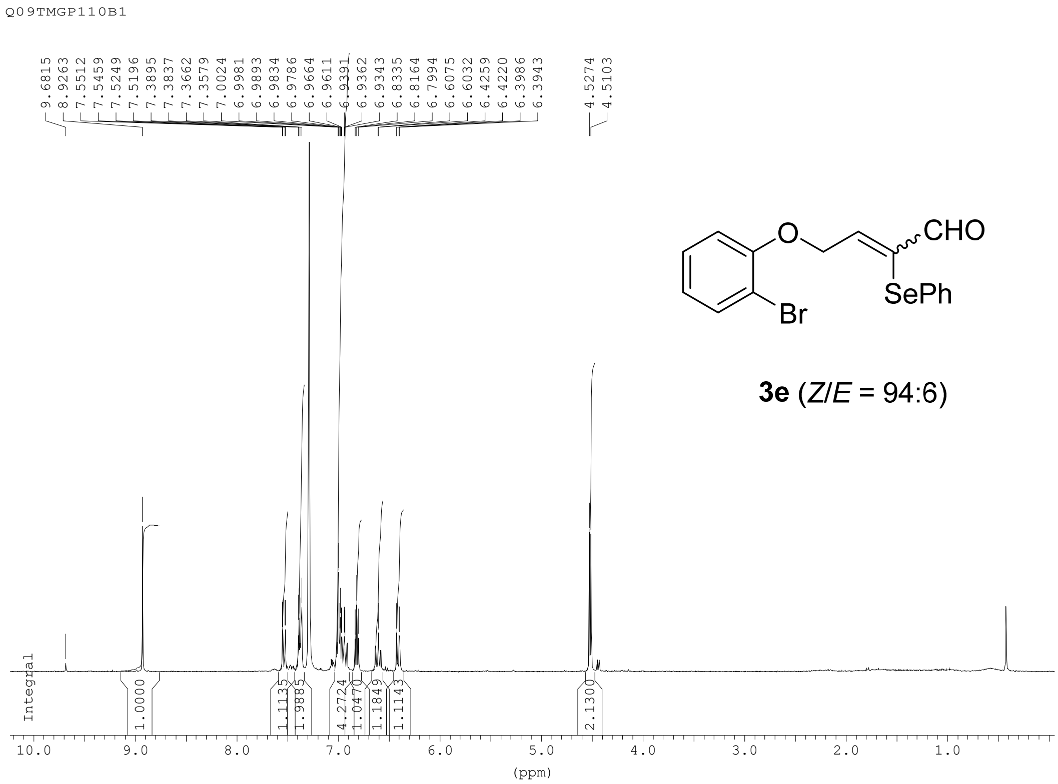

292.9525
800
750
700
650
600
550
500
450
400
350
300
250
200
150
100
50
0
-50
-100
-150
(ppm)

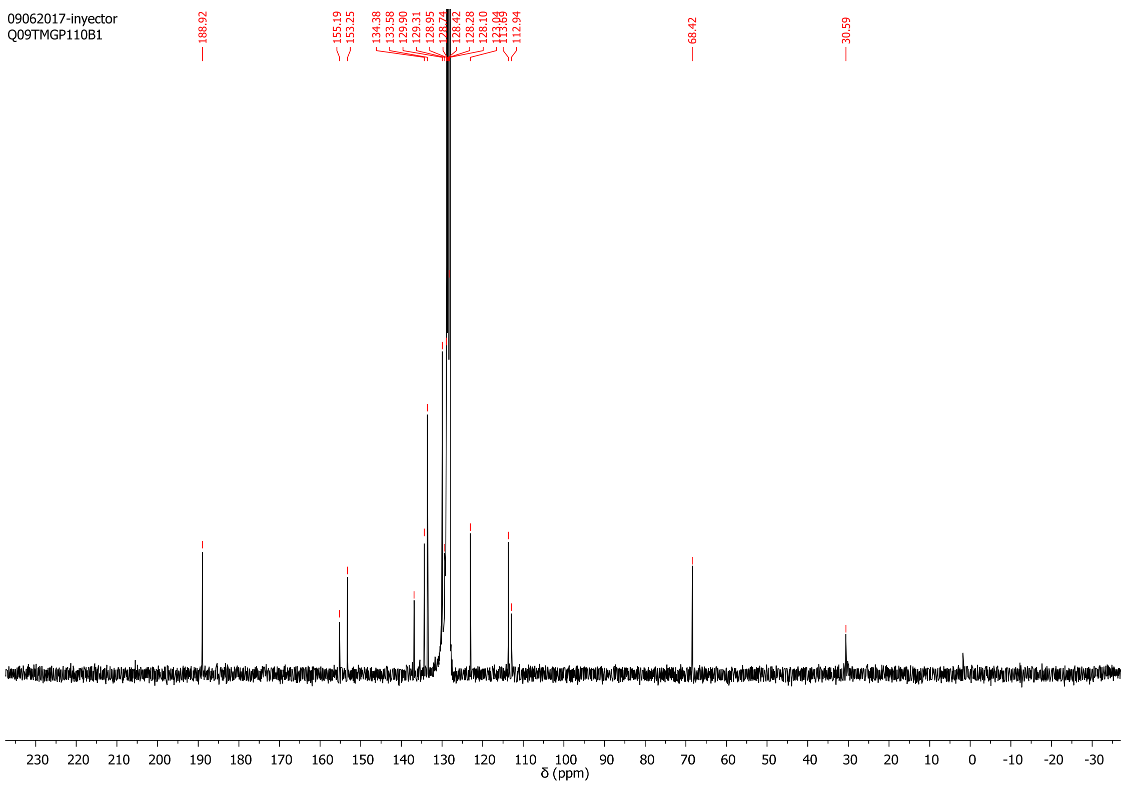

C:/Bruker 300/Guillermo/GP102BC.100/pdata/1/1r
CHO
SePh
O_2N
O
(ppm)

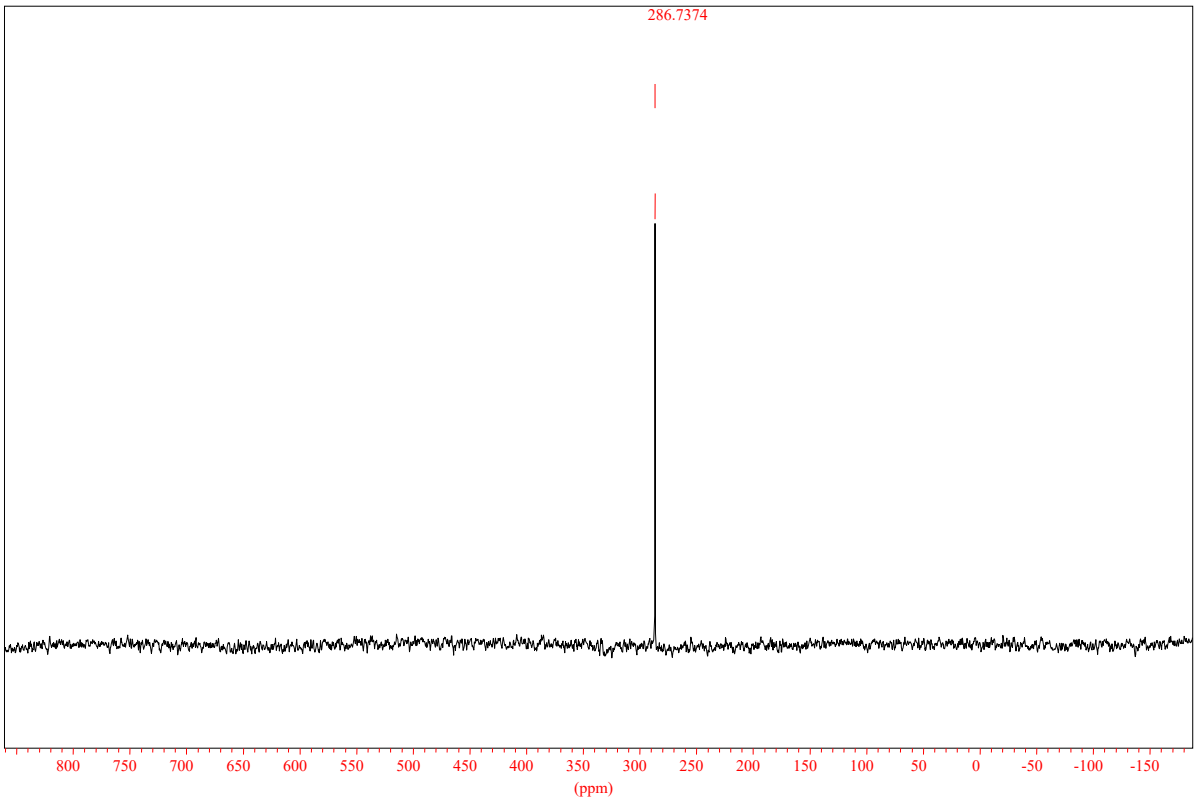
3d (*Z*/*E* = 92:8)

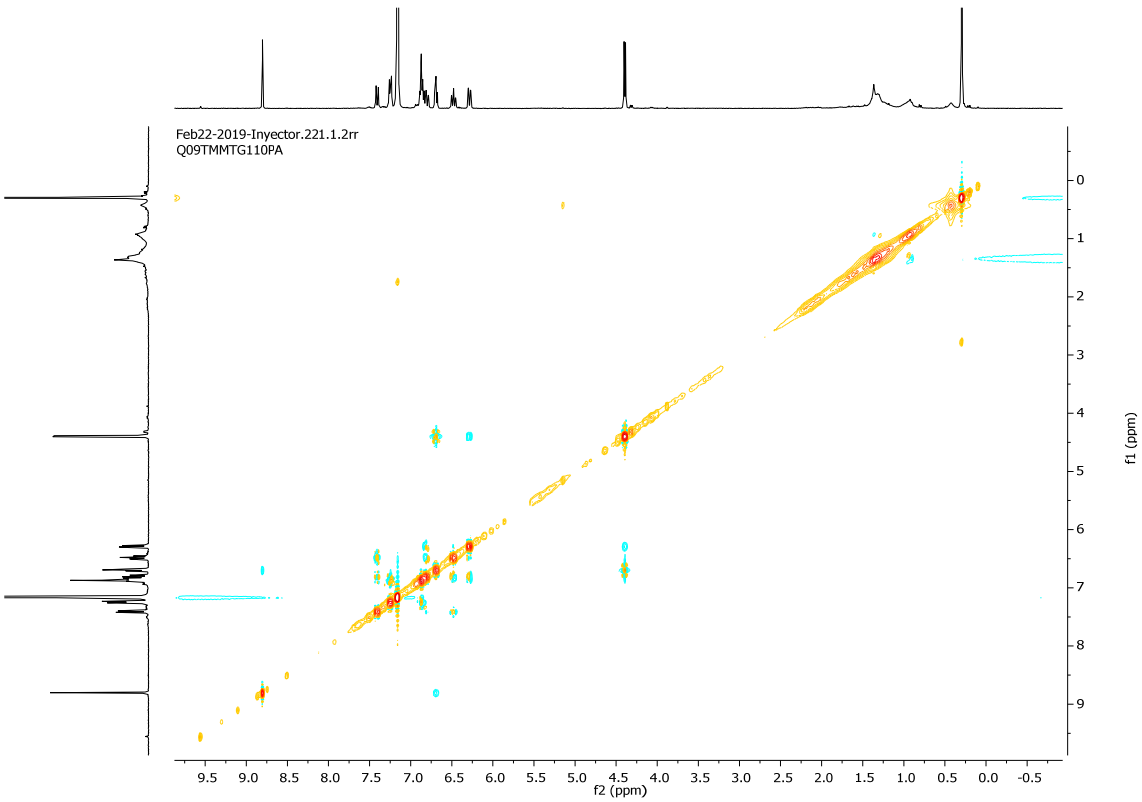

Jun01-2017-inyector
Q09TMGP102BC
188.45
161.64
150.07
136.14
132.05
130.48
128.16
126.70
125.00
114.63
113.54
76.42
75.58
66.62
δ (ppm)

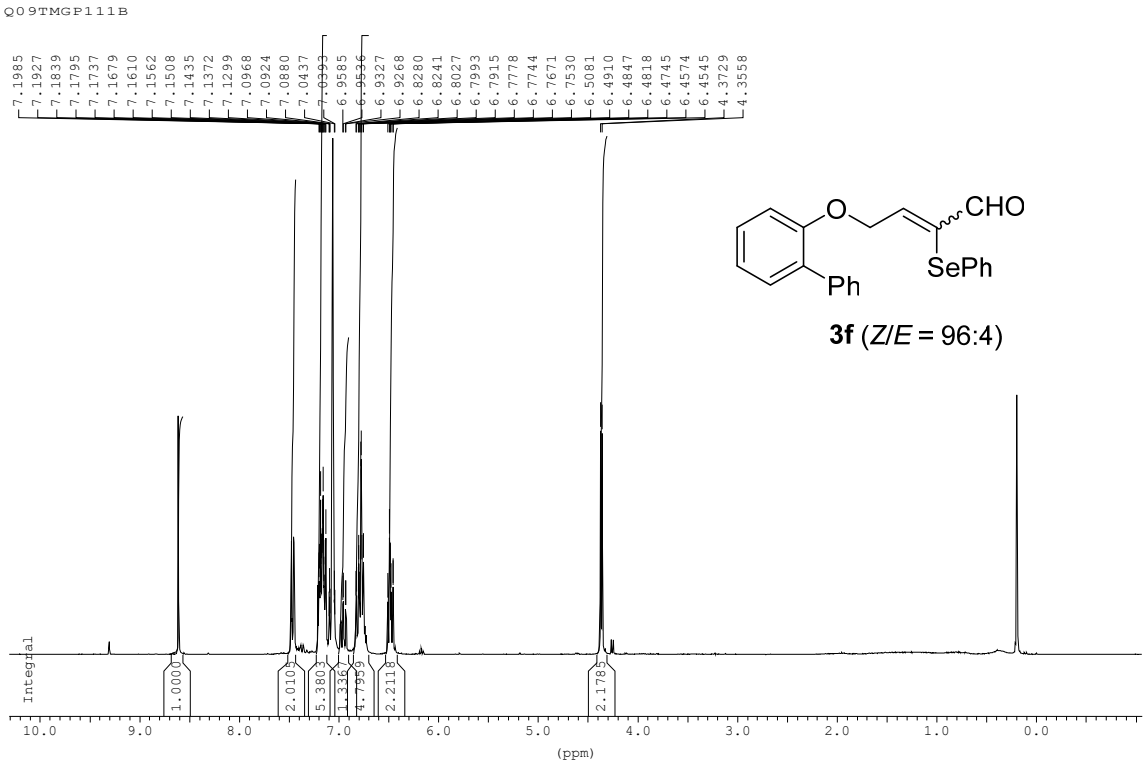

294.6242
370
360
350
340
330
320
310
300
290
280
270
260
250
240
(ppm)

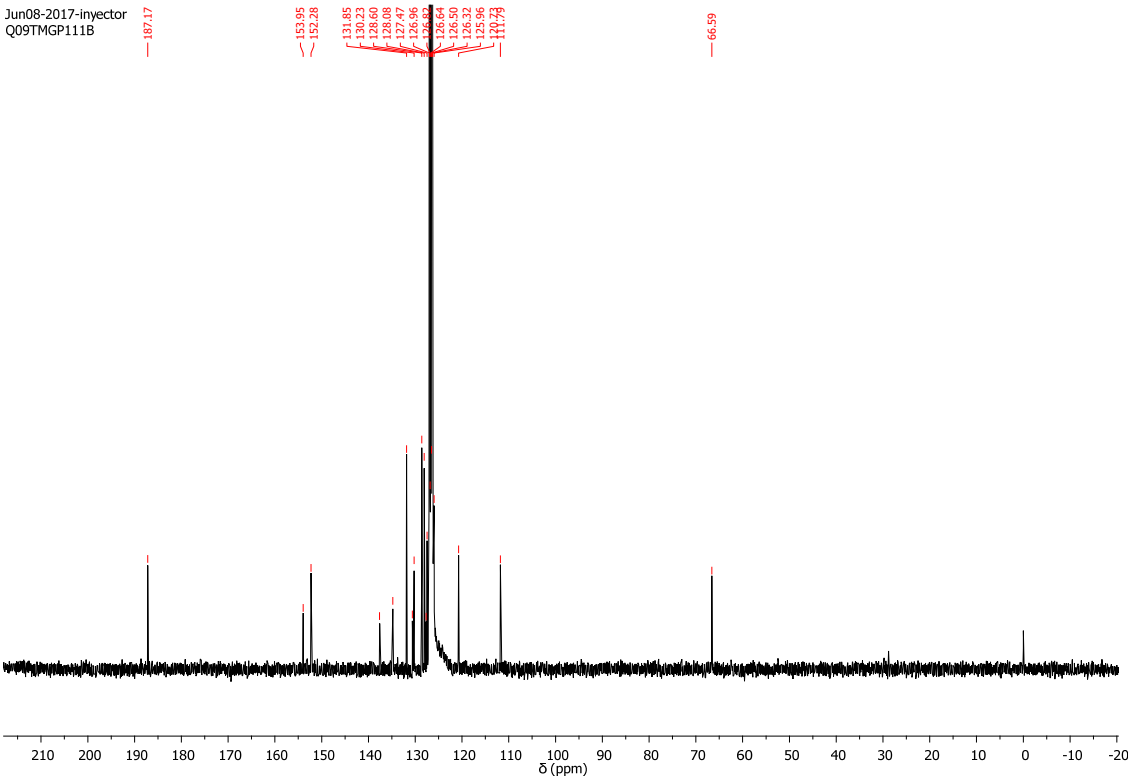

Q09TMGP110B1
9.6815
8.9263
7.5512
7.5459
7.5249
7.5196
7.3895
7.3837
7.3662
7.3579
7.0024
6.9981
6.9893
6.9834
6.9786
6.9664
6.9611
6.9391
6.9362
6.9343
6.8335
6.8164
6.7994
6.6075
6.6032
6.4259
6.4220
6.3986
6.3943
4.5274
4.5103
CHO
O
SePh
Br
3e (Z/E = 94:6)
Integral
1.0000
1.1135
1.9885
4.2724
1.0470
1.1849
1.1143
2.1300
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
(ppm)

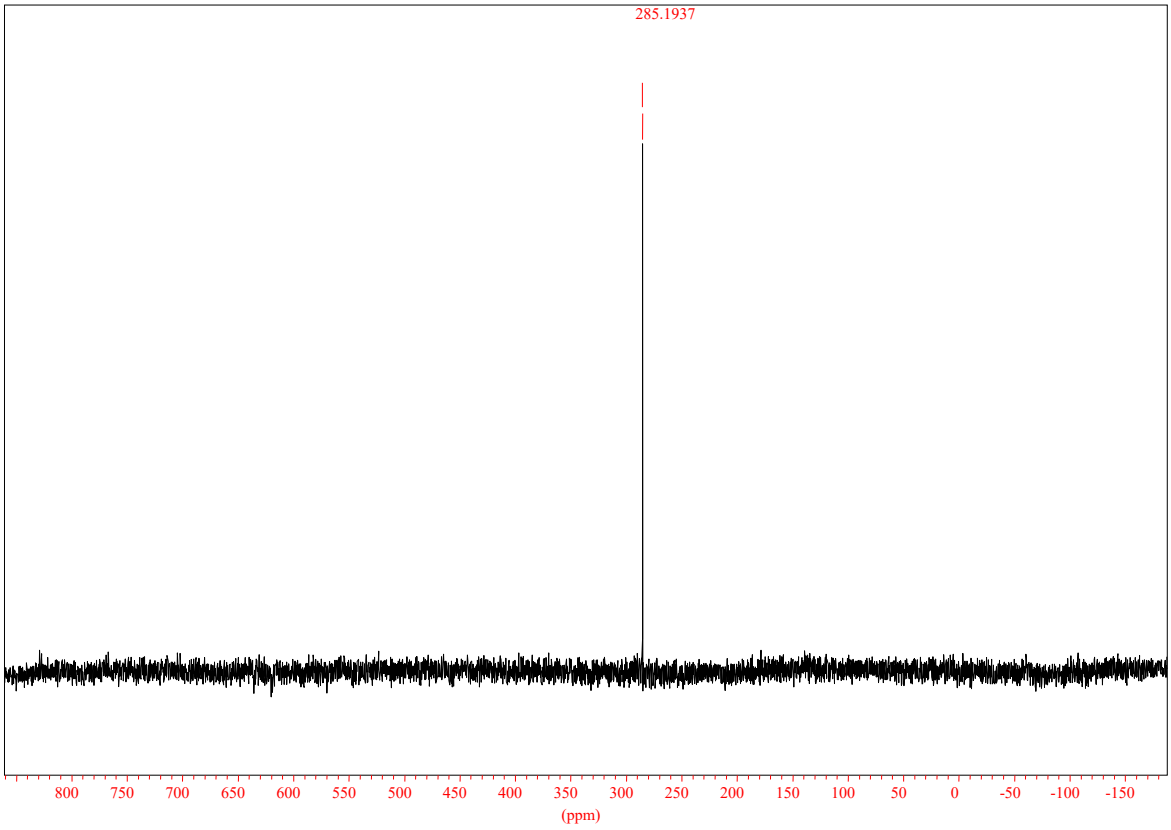

09062017-inyector
Q09TMGP110B1
188.92
155.19
153.25
134.38
133.58
129.90
129.31
128.95
128.74
128.42
128.28
128.10
123.04
113.69
112.94
68.42
30.59
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
δ (ppm)

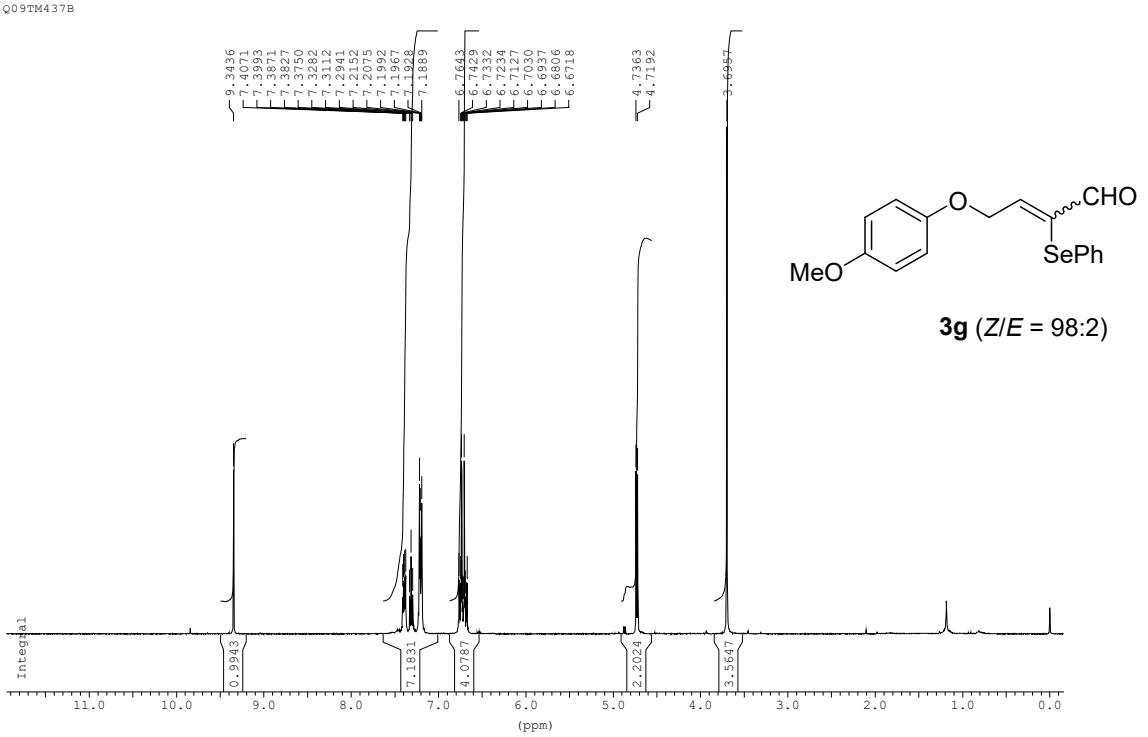

286.7374
800 750 700 650 600 550 500 450 400 350 300 250 200 150 100 50 0 -50 -100 -150
(ppm)


Feb22-2019-Inyector.221.1.2rr
Q09TMMTG110PA
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
f2 (ppm)
0 1 2 3 4 5 6 7 8 9
f1 (ppm)

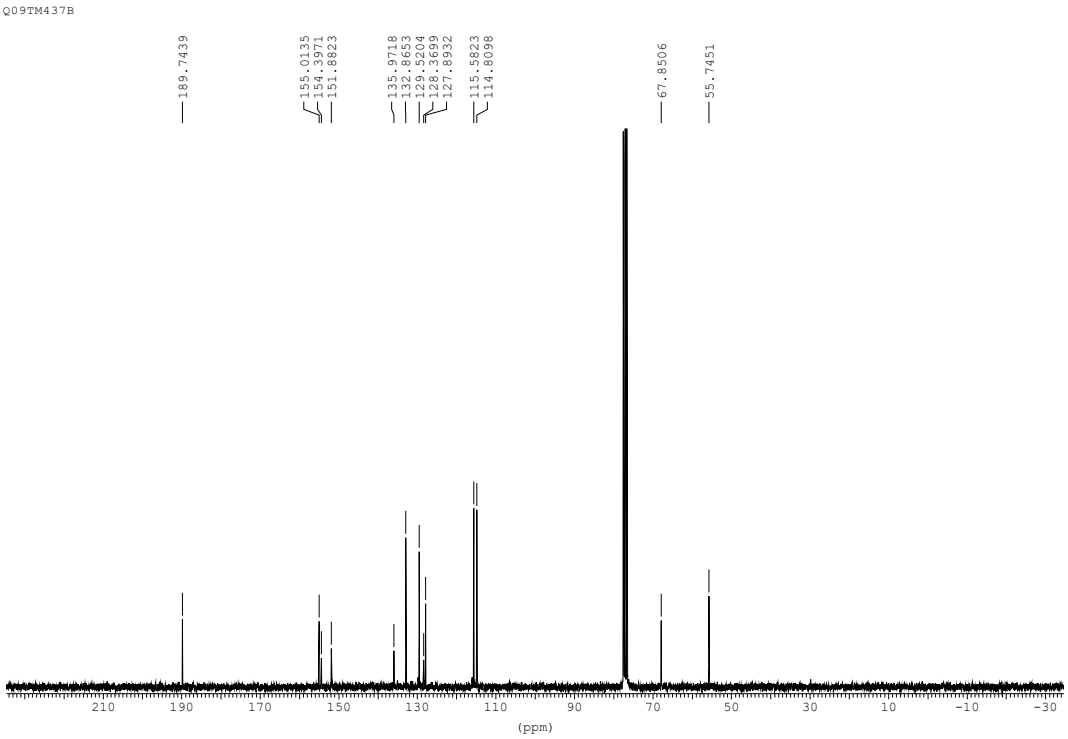

Q09TMGP111B
7.1985
7.1927
7.1839
7.1795
7.1737
7.1679
7.1610
7.1562
7.1508
7.1435
7.1372
7.1299
7.0968
7.0924
7.0880
7.0437
7.0393
6.9585
6.9536
6.9327
6.9268
6.8280
6.8241
6.8027
6.7993
6.7915
6.7778
6.7744
6.7671
6.7530
6.5081
6.4910
6.4847
6.4818
6.4745
6.4574
6.4545
4.3729
4.3558
Integral
1.0000
2.0103
5.3803
1.3363
4.7959
2.2118
2.1785
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
(ppm)
O
CHO
SePh
Ph
3f (Z/E = 96:4)

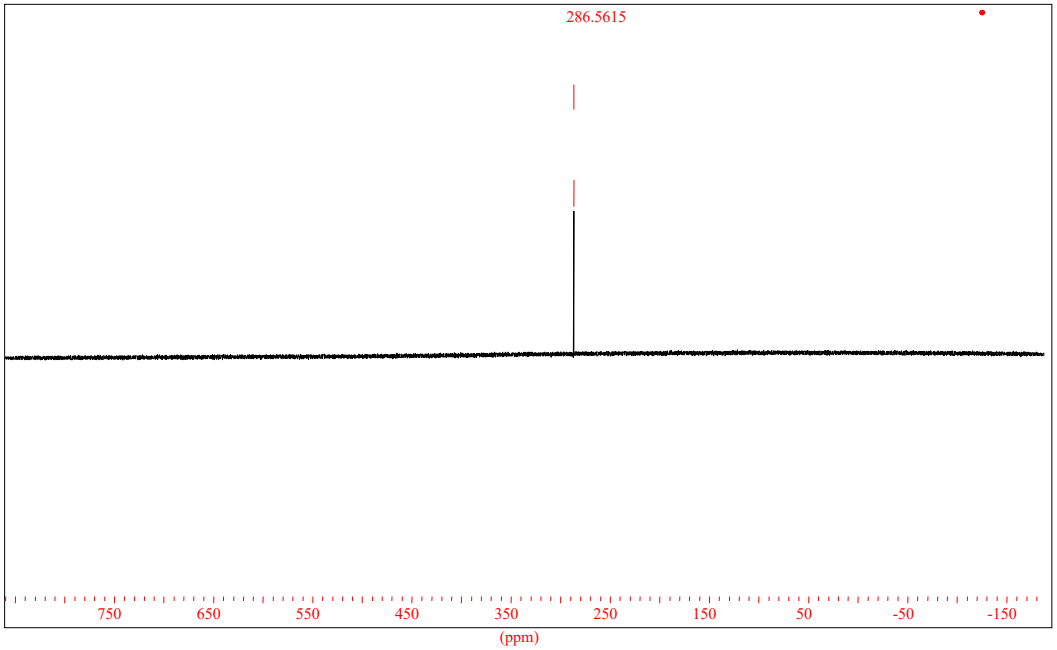

Jun08-2017-inyector
Q09TMGP111B
187.17
153.95
152.28
131.85
130.23
128.60
128.08
127.47
126.96
126.64
126.50
126.32
125.96
120.73
111.79
66.59
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
-20
δ (ppm)


285.1937
800
750
700
650
600
550
500
450
400
350
300
250
200
150
100
50
0
-50
-100
-150
(ppm)

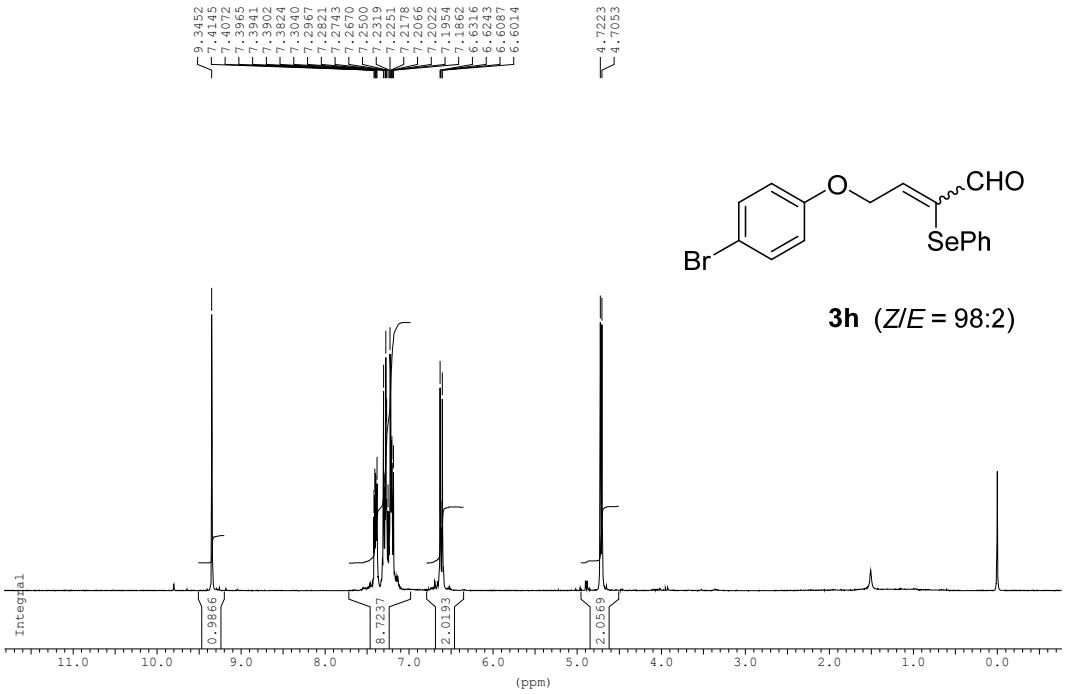

Q09TM437B
9.3436
7.4071
7.3993
7.3871
7.3827
7.3750
7.3282
7.3112
7.2941
7.2152
7.2075
7.1992
7.1967
7.1928
7.1889
6.7643
6.7429
6.7332
6.7234
6.7127
6.7030
6.6937
6.6806
6.6718
4.7363
4.7192
3.6957
Integral
0.9943
7.1831
4.0787
2.2024
3.5647
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
(ppm)
O
CHO
SePh
MeO

3g (*Z*/*E* = 98:2)


Q09TM437B
189.7439
155.0135
154.3971
151.8823
135.9718
132.8653
129.5204
128.3699
127.8932
115.5823
114.8098
67.8506
55.7451
210
190
170
150
130
110
90
70
50
30
10
-10
-30
(ppm)

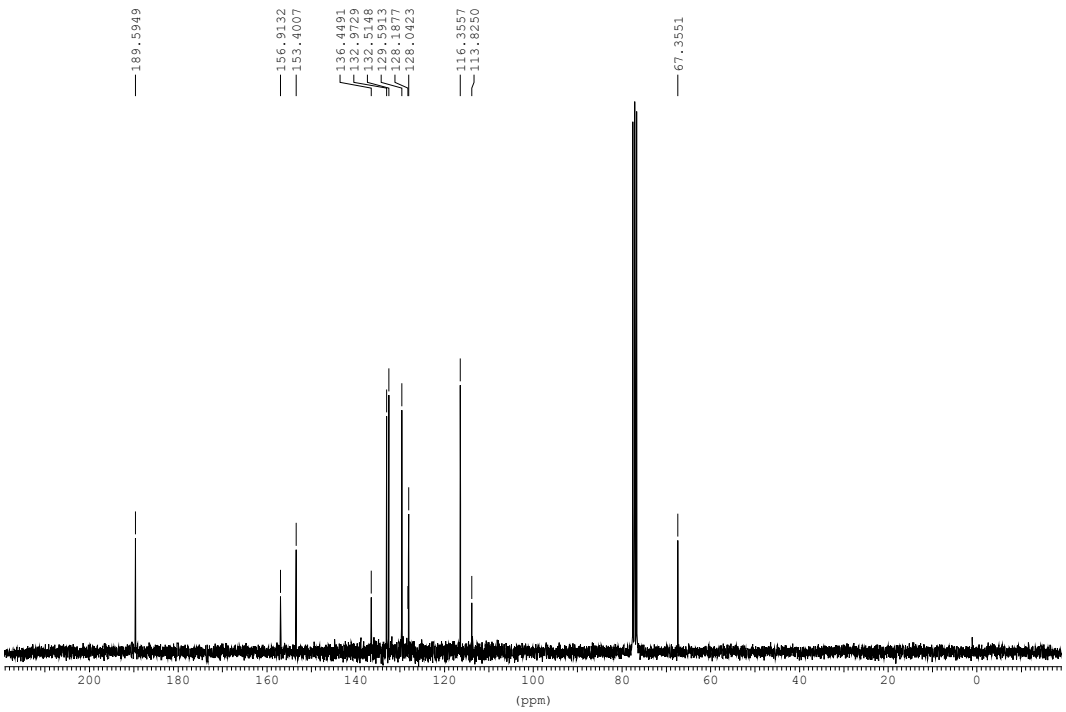

286.5615
750
650
550
450
350
250
150
50
-50
-150
(ppm)

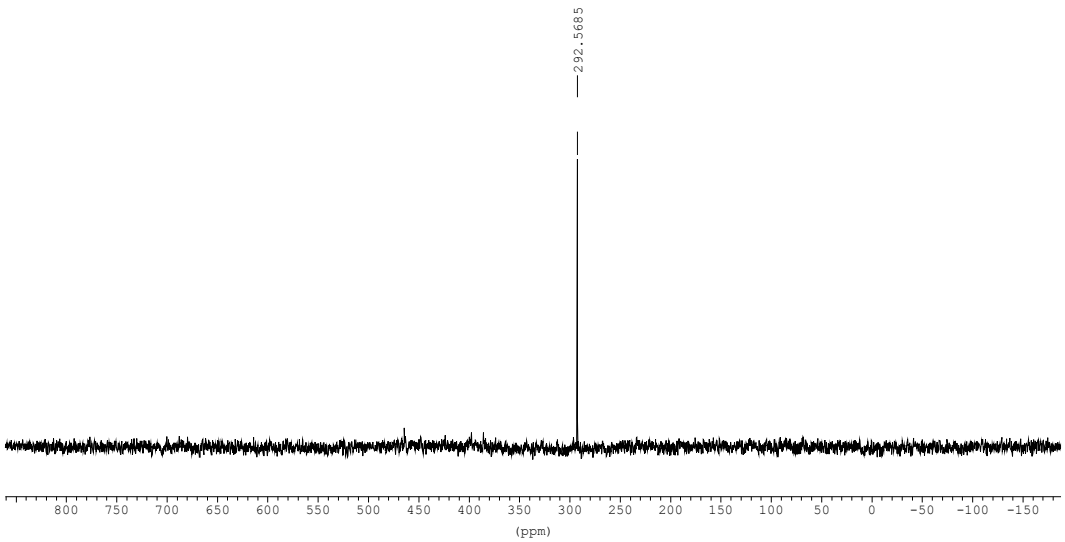
Q09TM441C



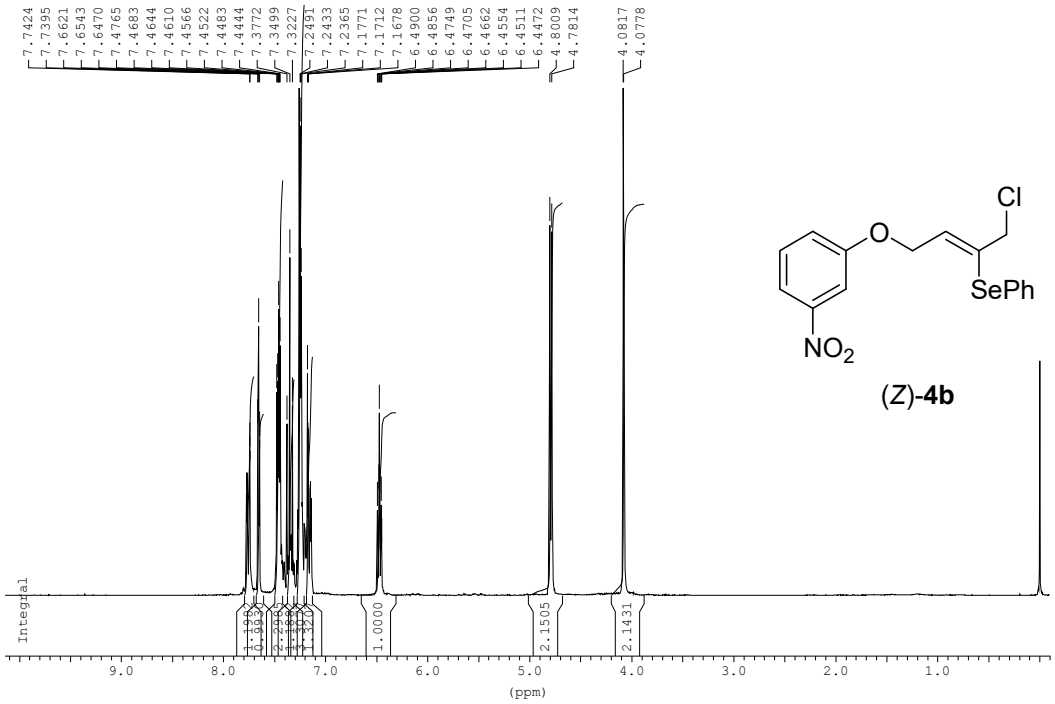
3h (*Z*/*E* = 98:2)

Q09TM441C



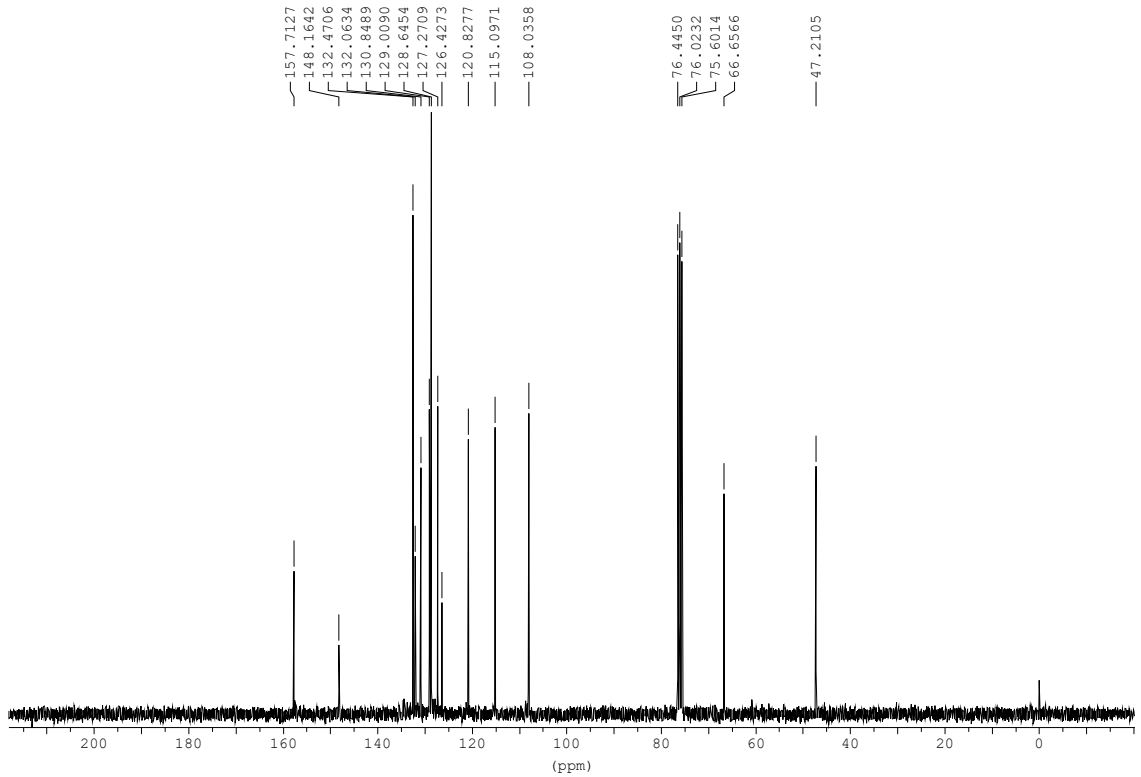

292.5685
800 750 700 650 600 550 500 450 400 350 300 250 200 150 100 50 0 -50 -100 -150
(ppm)

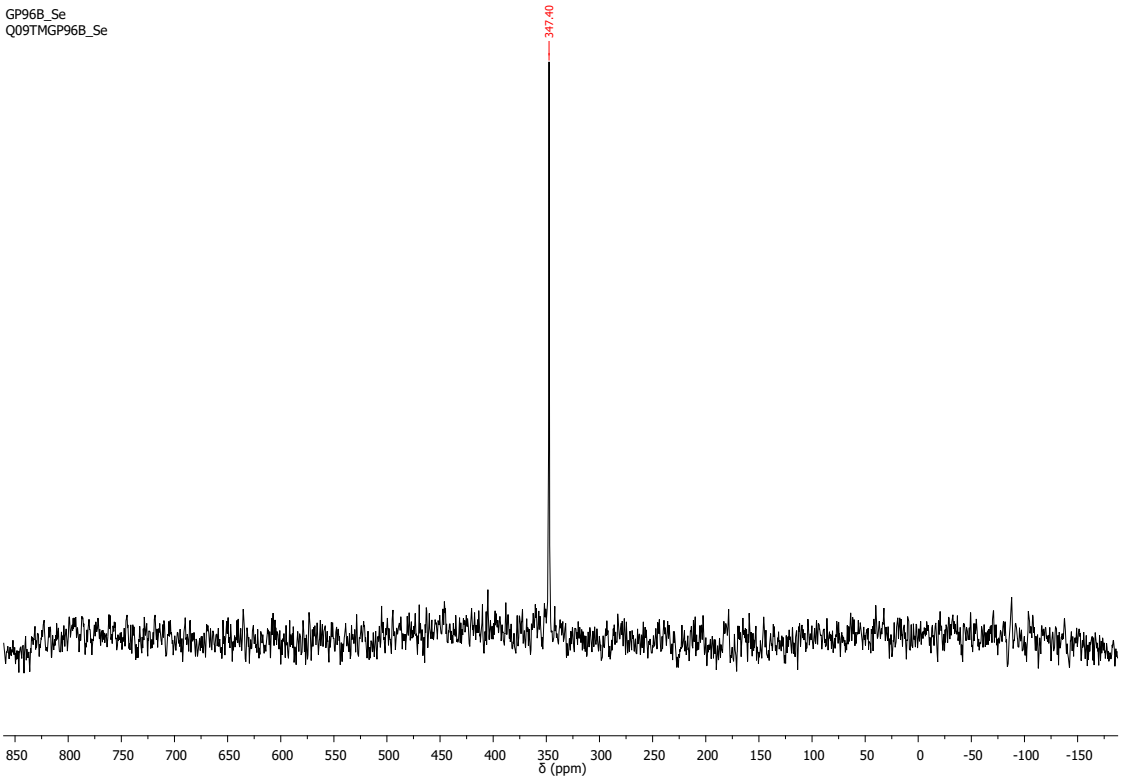
Q09TMGP96B

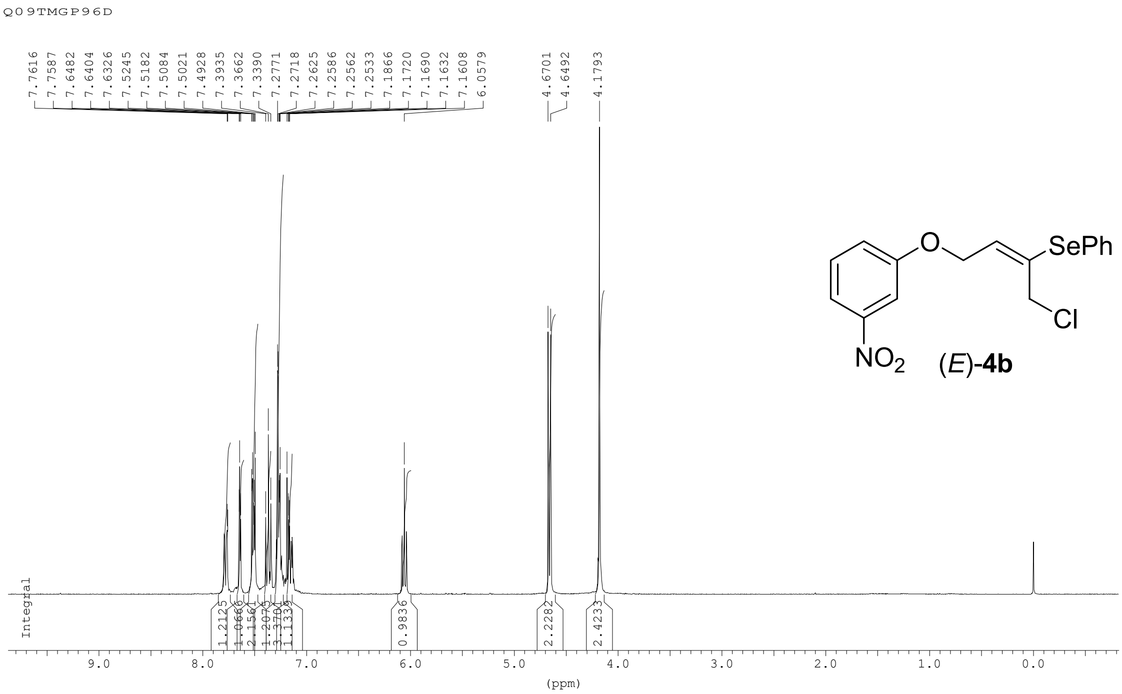


(*Z*)-**4b**

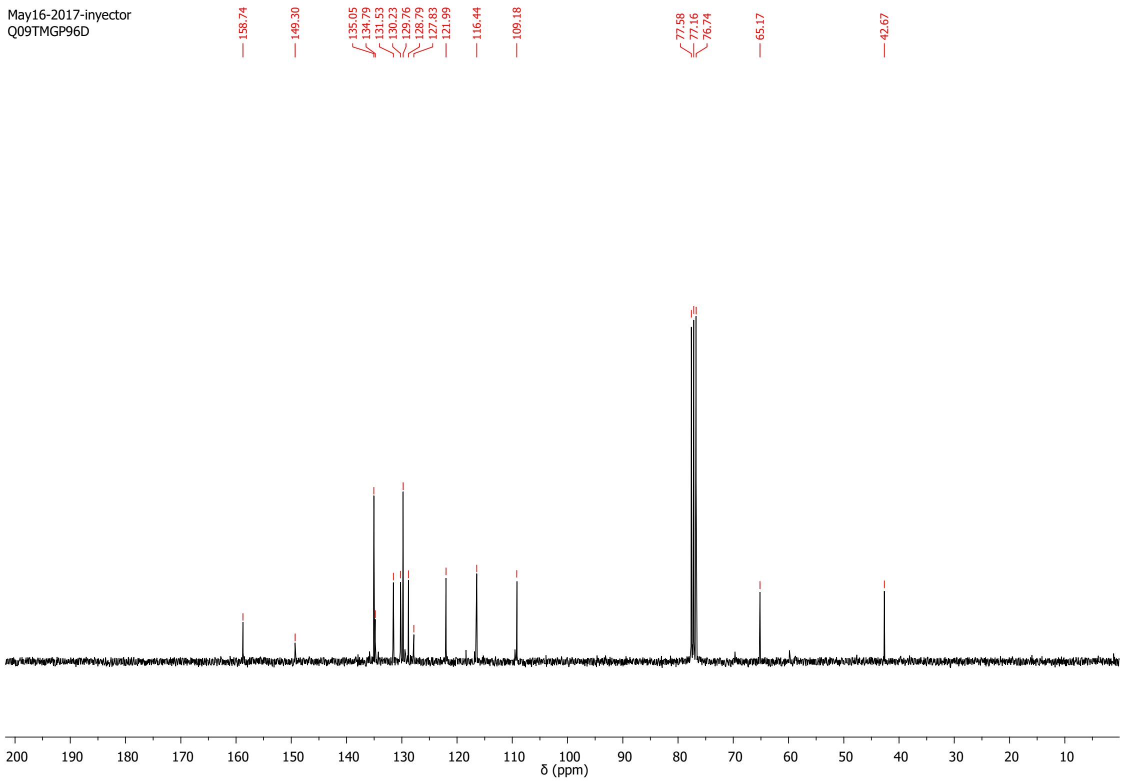
Q09TMGP96B

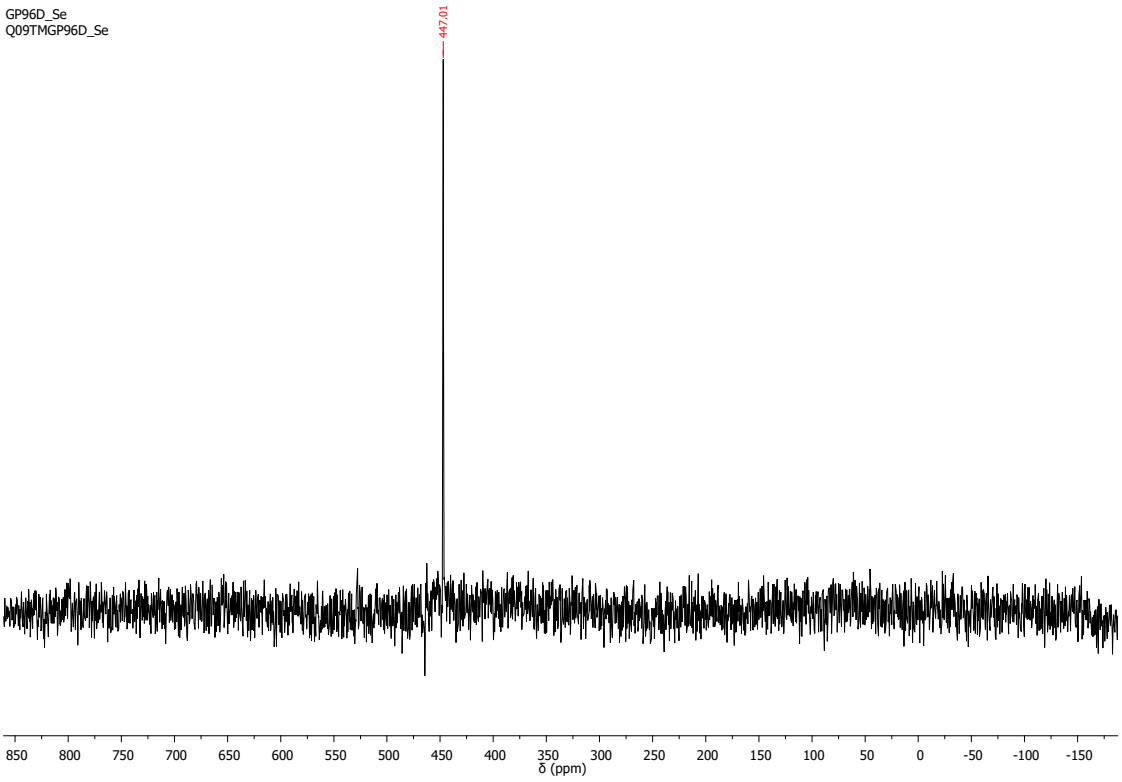


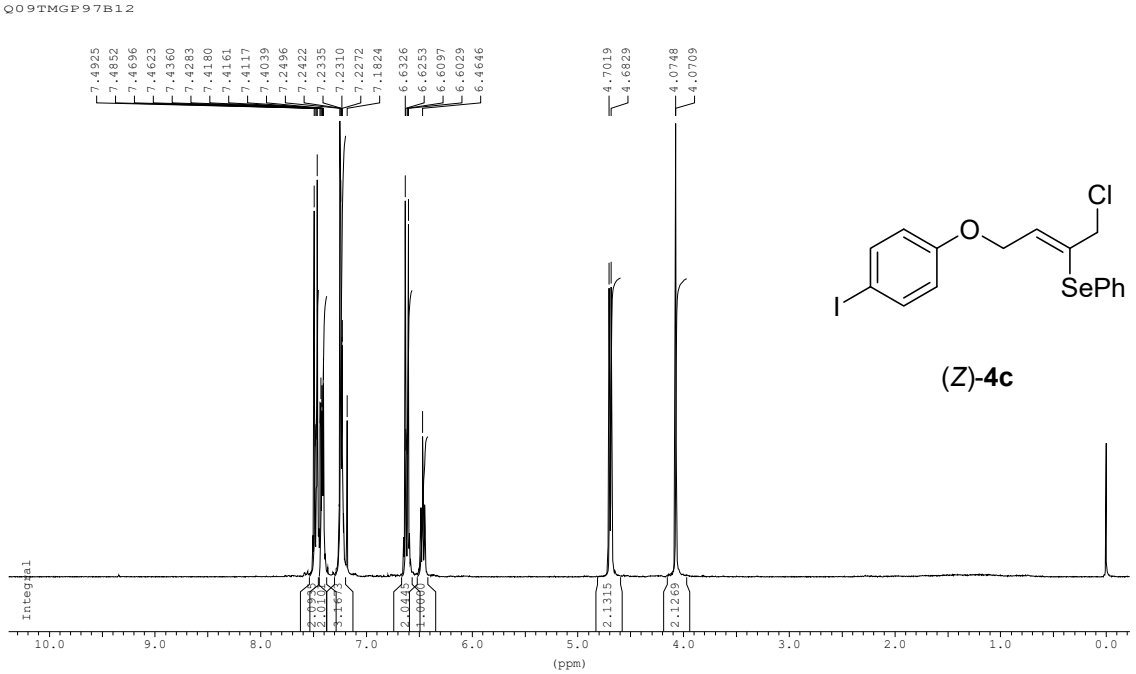

GP96B_Se
Q09TMGP96B_Se
347.40
850 800 750 700 650 600 550 500 450 400 350 300 250 200 150 100 50 0 -50 -100 -150
δ (ppm)


Q09TMGP96D
7.7616
7.7587
7.6482
7.6404
7.6326
7.5245
7.5182
7.5084
7.5021
7.4928
7.3935
7.3662
7.3390
7.2771
7.2718
7.2625
7.2586
7.2562
7.2533
7.1866
7.1720
7.1690
7.1632
7.1608
6.0579
4.6701
4.6492
4.1793
Integral
1.2125
1.0666
2.1561
1.2076
3.3701
1.1338
0.9836
2.2282
2.4233
(ppm)
O
SePh
Cl
NO_2

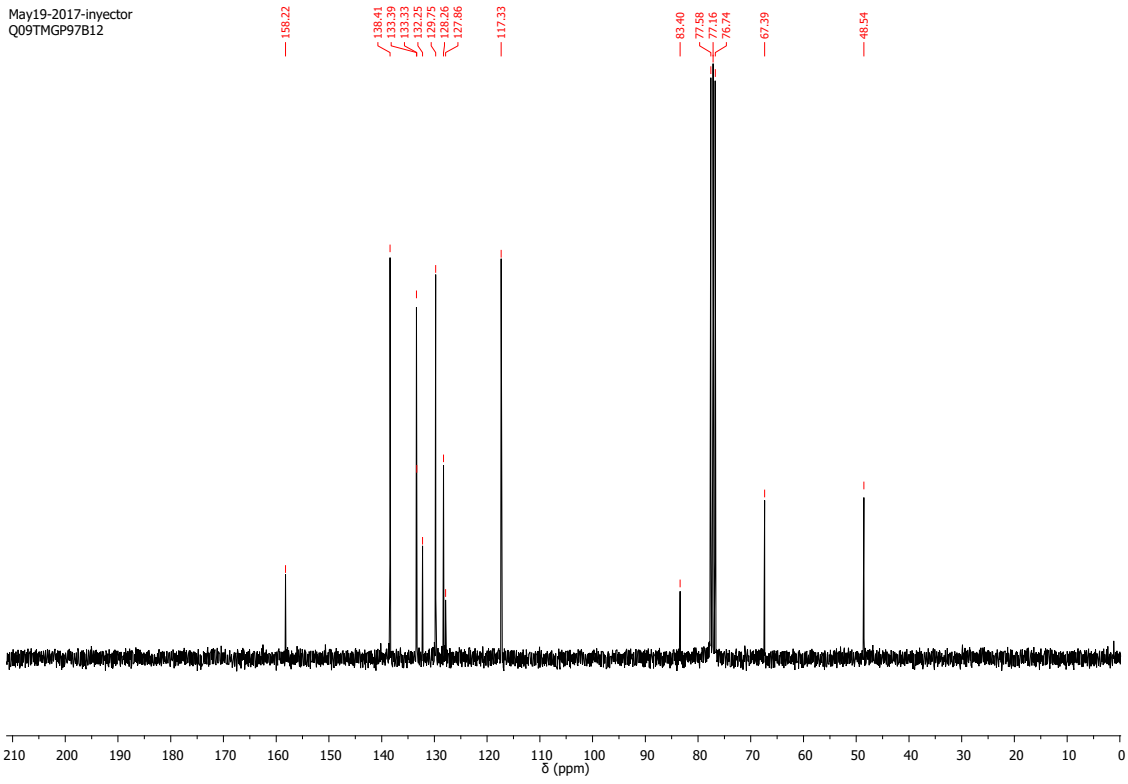
(*E*)-**4b**

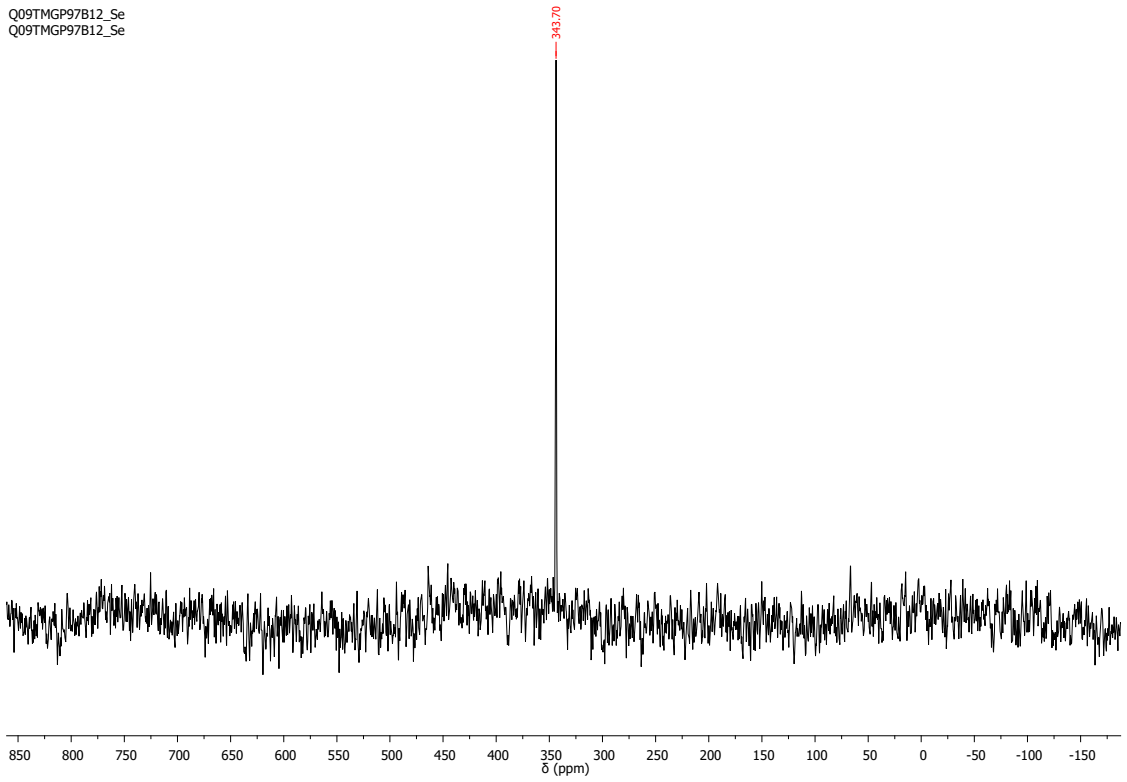

May16-2017-inyector
Q09TMGP96D
158.74
149.30
135.05
134.79
131.53
130.23
129.76
128.79
127.83
121.99
116.44
109.18
77.58
77.16
76.74
65.17
42.67
δ (ppm)

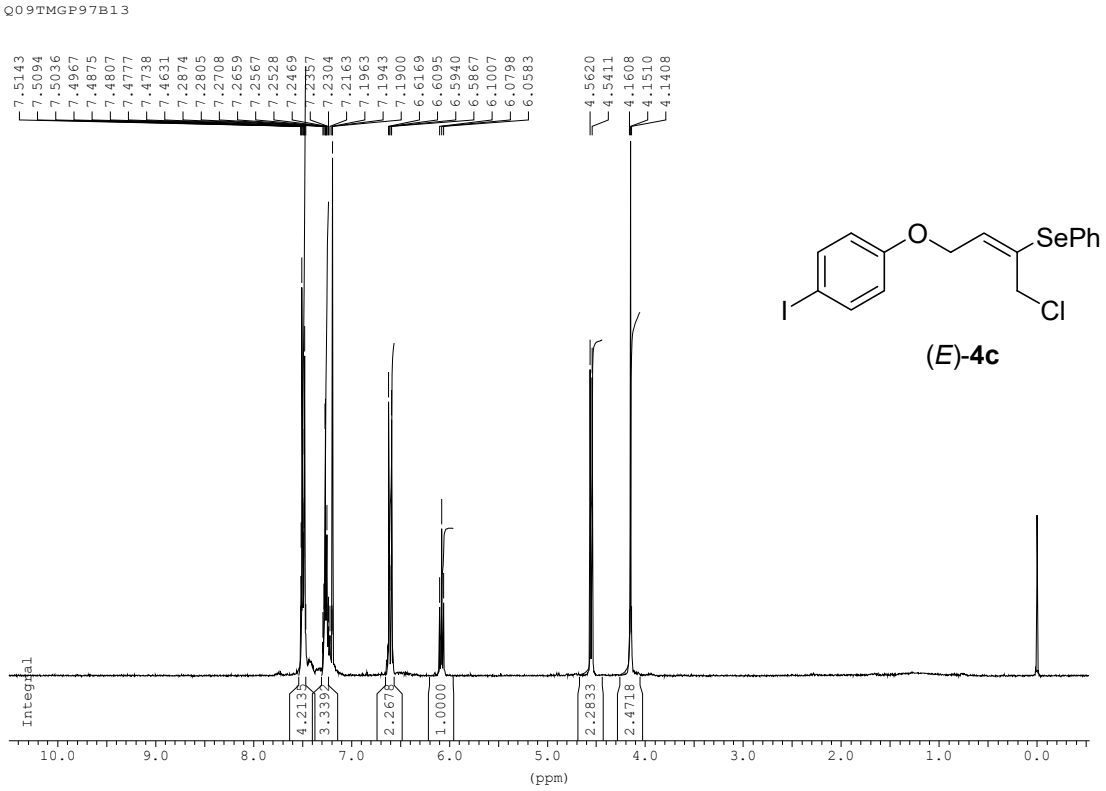

GP96D_Se
Q09TMGP96D_Se
447.01
850 800 750 700 650 600 550 500 450 400 350 300 250 200 150 100 50 0 -50 -100 -150
δ (ppm)

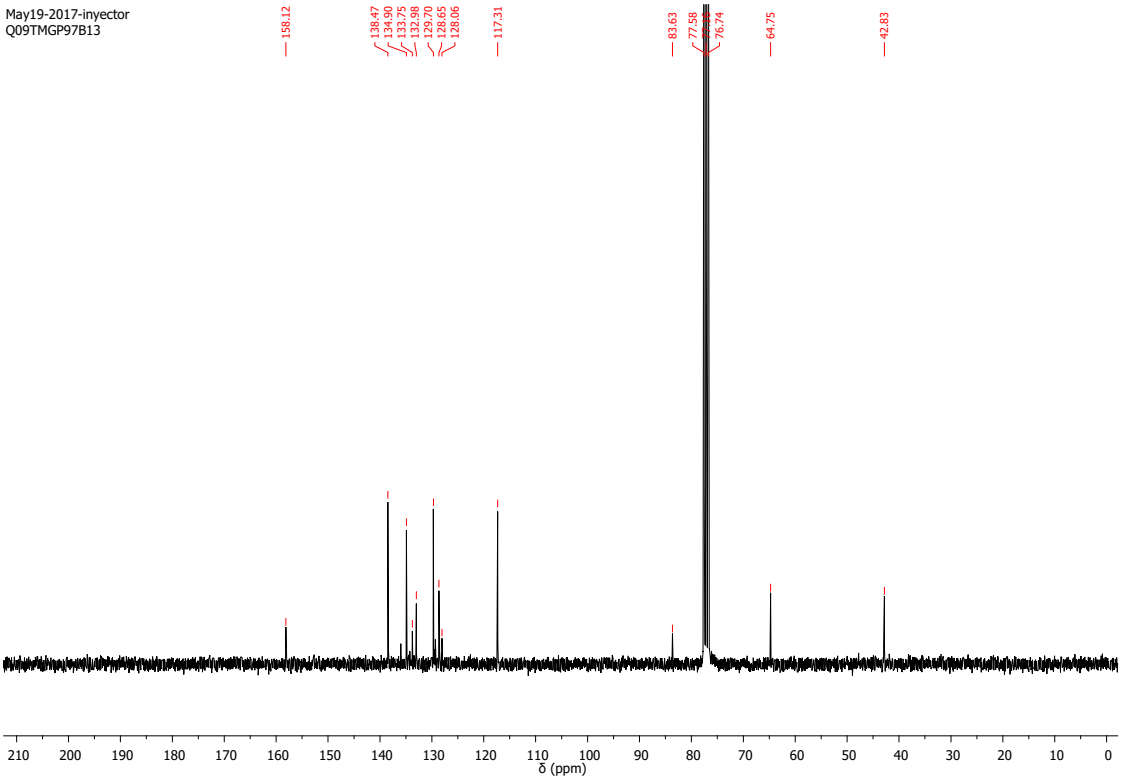

Q09TMGP97B12
7.4925
7.4852
7.4696
7.4623
7.4360
7.4283
7.4180
7.4161
7.4117
7.4039
7.2496
7.2422
7.2335
7.2310
7.2272
7.1824
6.6326
6.6253
6.6097
6.6029
6.4646
4.7019
4.6829
4.0748
4.0709
Integral
2.0000
2.0107
3.1687
2.0443
1.0000
2.1315
2.1269
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
(ppm)
Cl
O
SePh
I

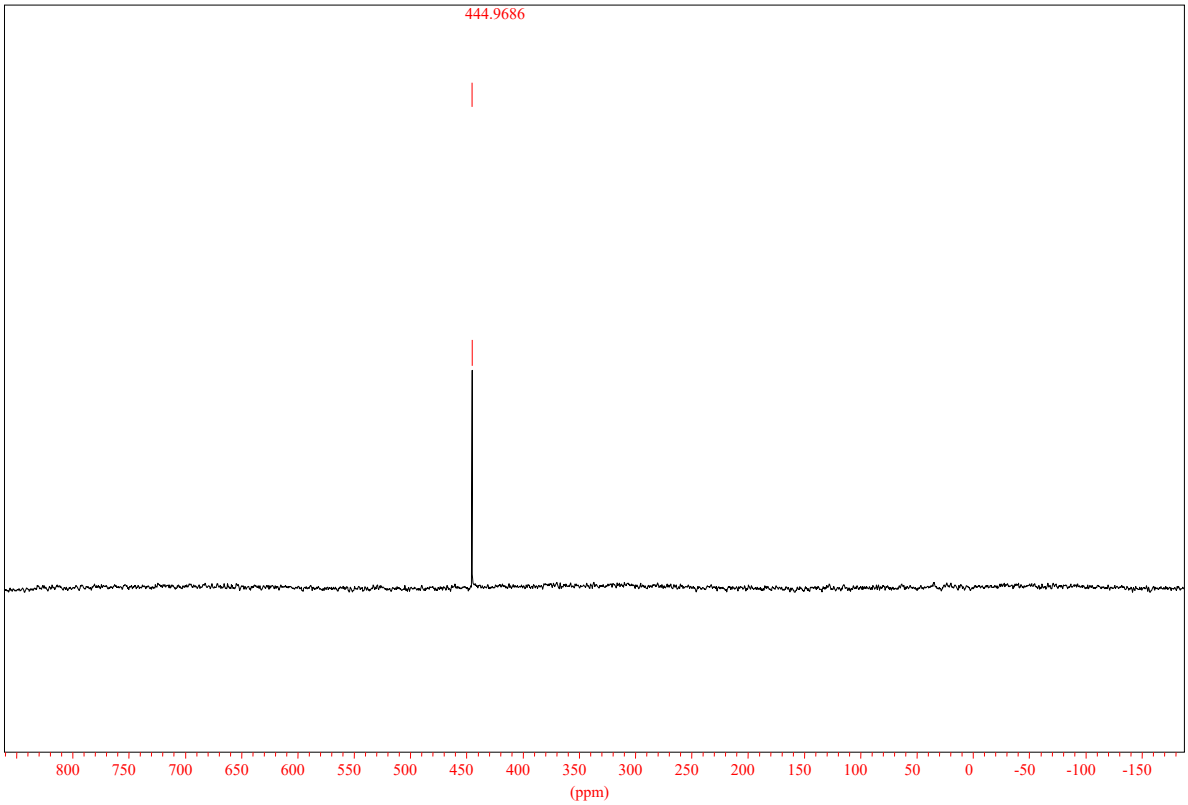
(*Z*)-4c

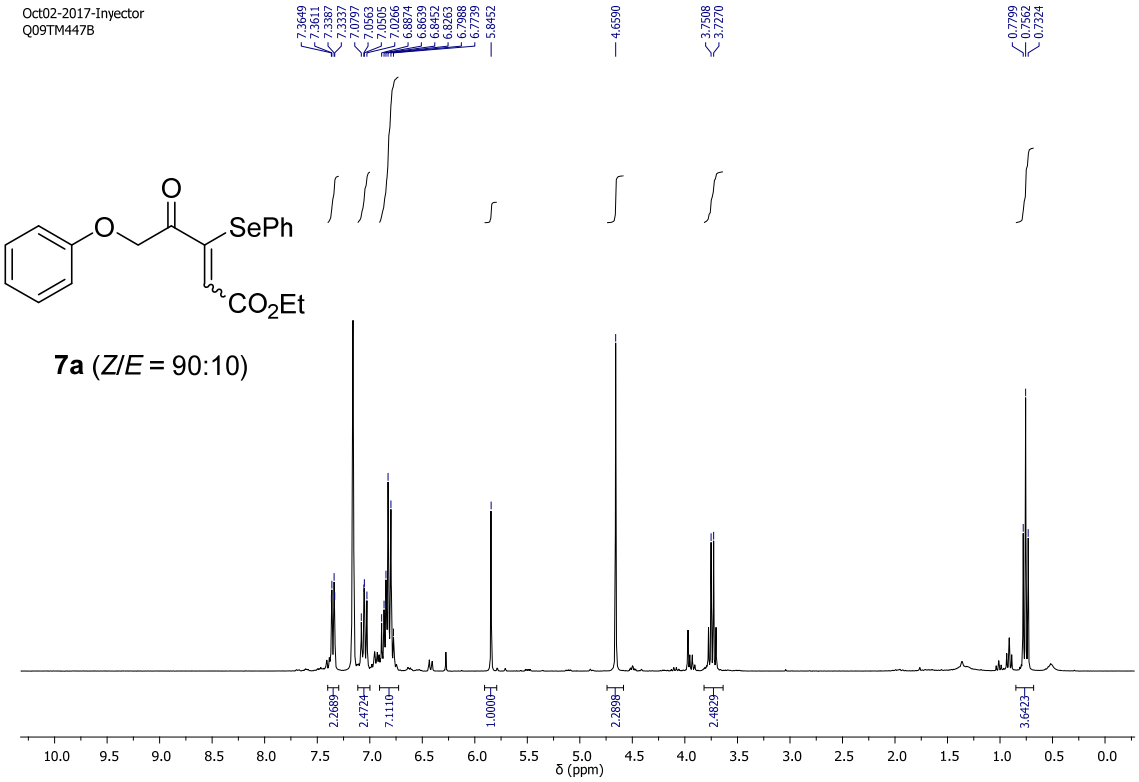

May19-2017-inyector
Q09TMGP97B12
158.22
138.41
133.39
133.33
132.25
129.75
128.26
127.86
117.33
83.40
77.58
77.16
76.74
67.39
48.54
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
δ (ppm)

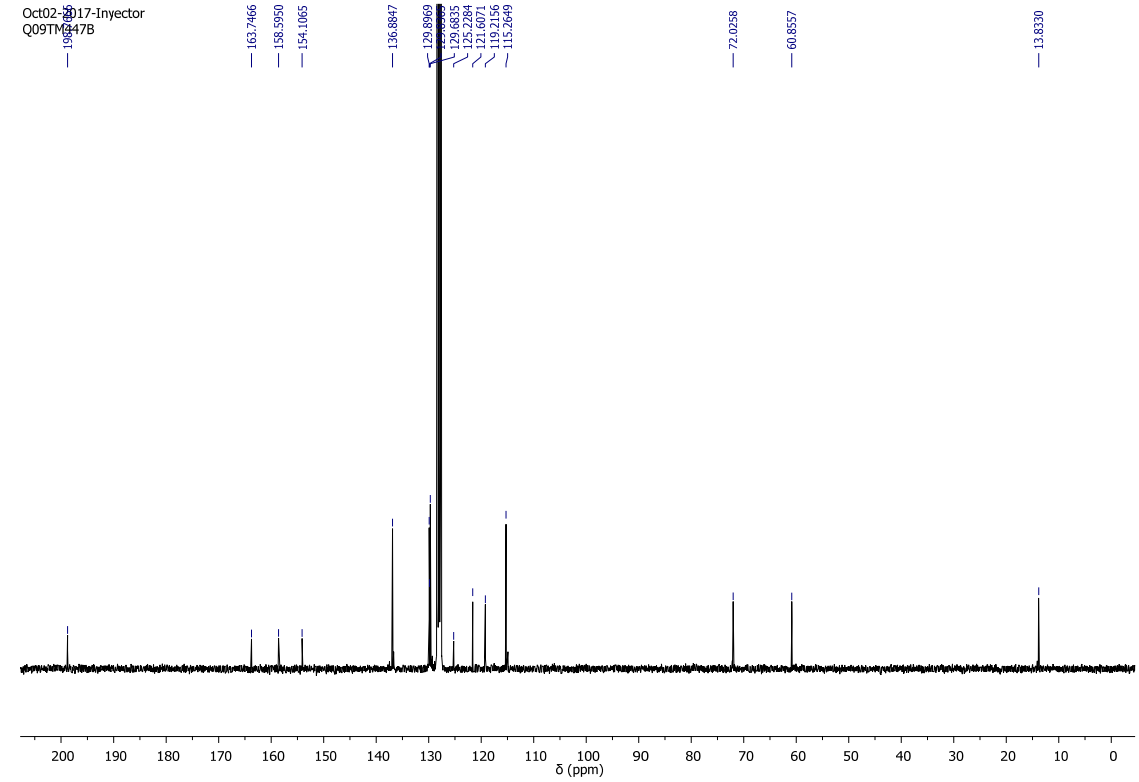

Q09TMGP97B12_Se
Q09TMGP97B12_Se
343.70
850 800 750 700 650 600 550 500 450 400 350 300 250 200 150 100 50 0 -50 -100 -150
δ (ppm)

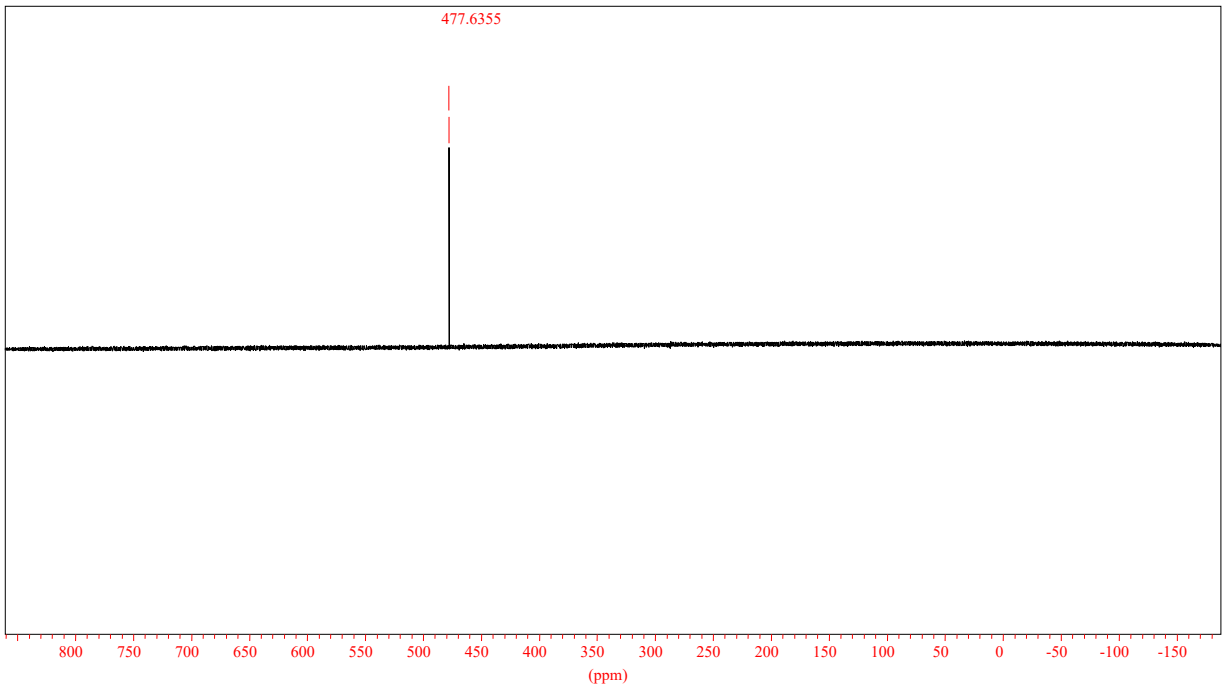

Q09TMGP97B13
7.5143
7.5094
7.5036
7.4967
7.4875
7.4807
7.4777
7.4738
7.4631
7.2874
7.2805
7.2708
7.2659
7.2567
7.2528
7.2469
7.2357
7.2304
7.2163
7.1963
7.1943
7.1900
6.6169
6.6095
6.5940
6.5867
6.1007
6.0798
6.0583
4.5620
4.5411
4.1608
4.1510
4.1408
Integral
4.2132
3.3392
2.2678
1.0000
2.2833
2.4718
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
(ppm)
O
SePh
I
Cl
(E)-4c

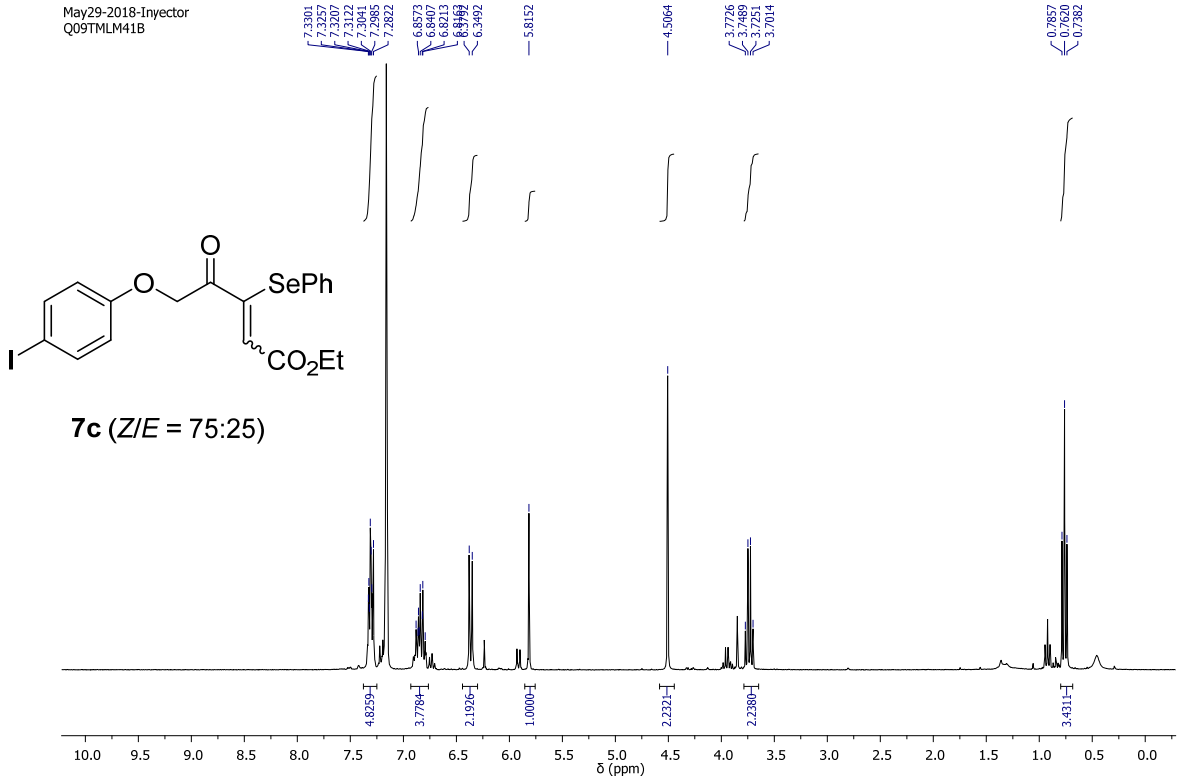

May19-2017-inyector
Q09TMGP97B13
158.12
138.47
134.90
133.35
132.98
129.70
128.65
128.06
117.31
83.63
77.58
77.16
76.74
64.75
42.83
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
δ (ppm)

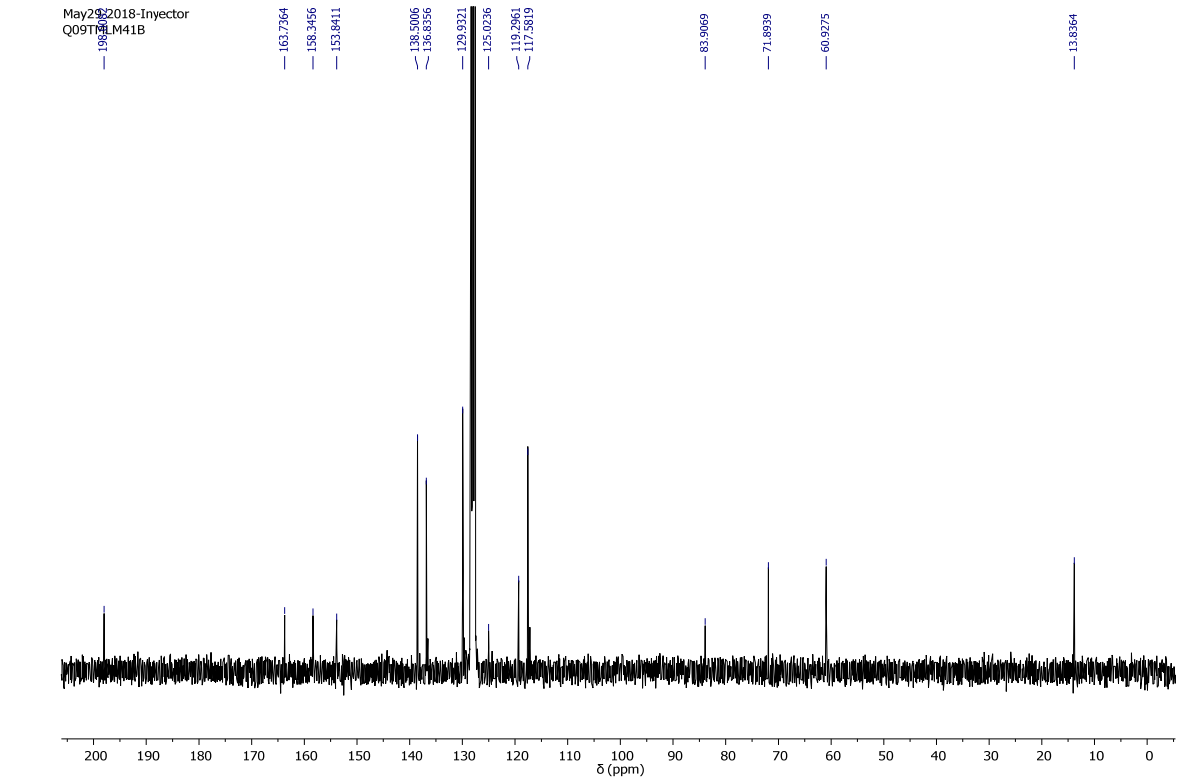

444.9686
800
750
700
650
600
550
500
450
400
350
300
250
200
150
100
50
0
-50
-100
-150
(ppm)

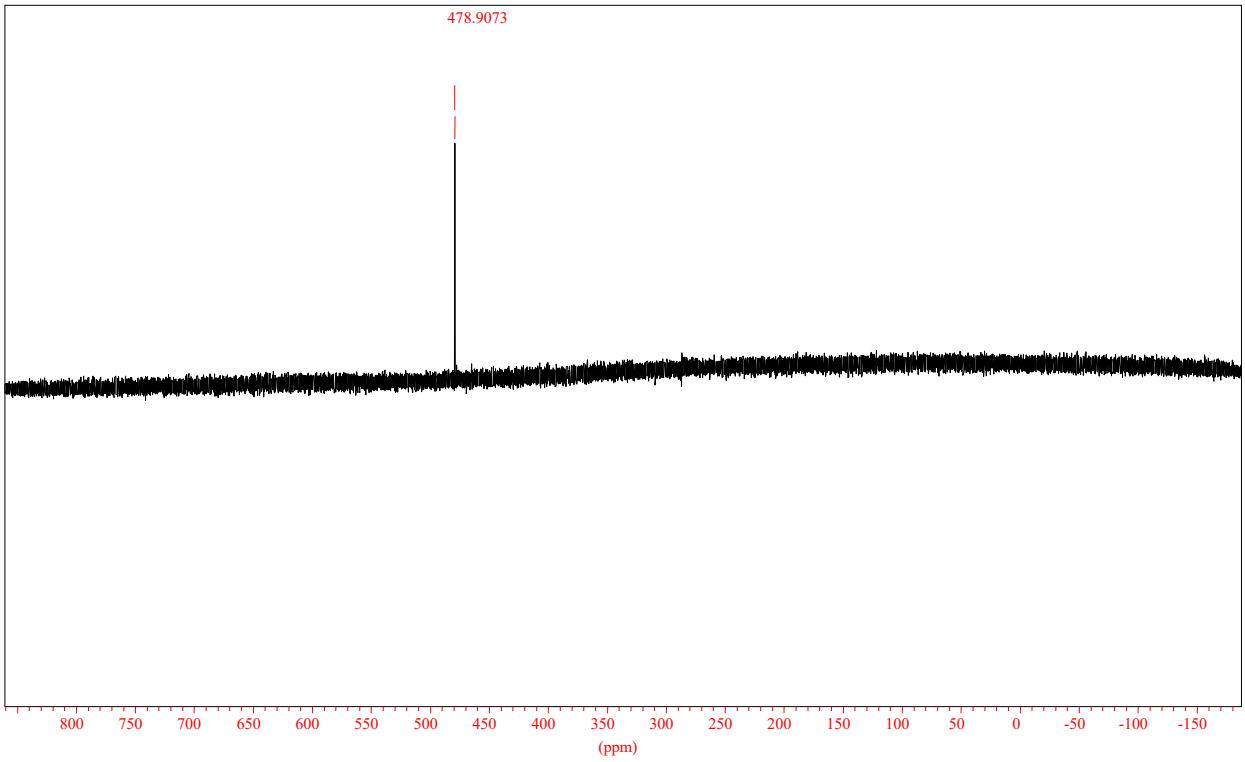

Oct02-2017-Inyector
Q09TM447B
O
O
SePh
CO2Et
7a (Z/E = 90:10)
δ (ppm)

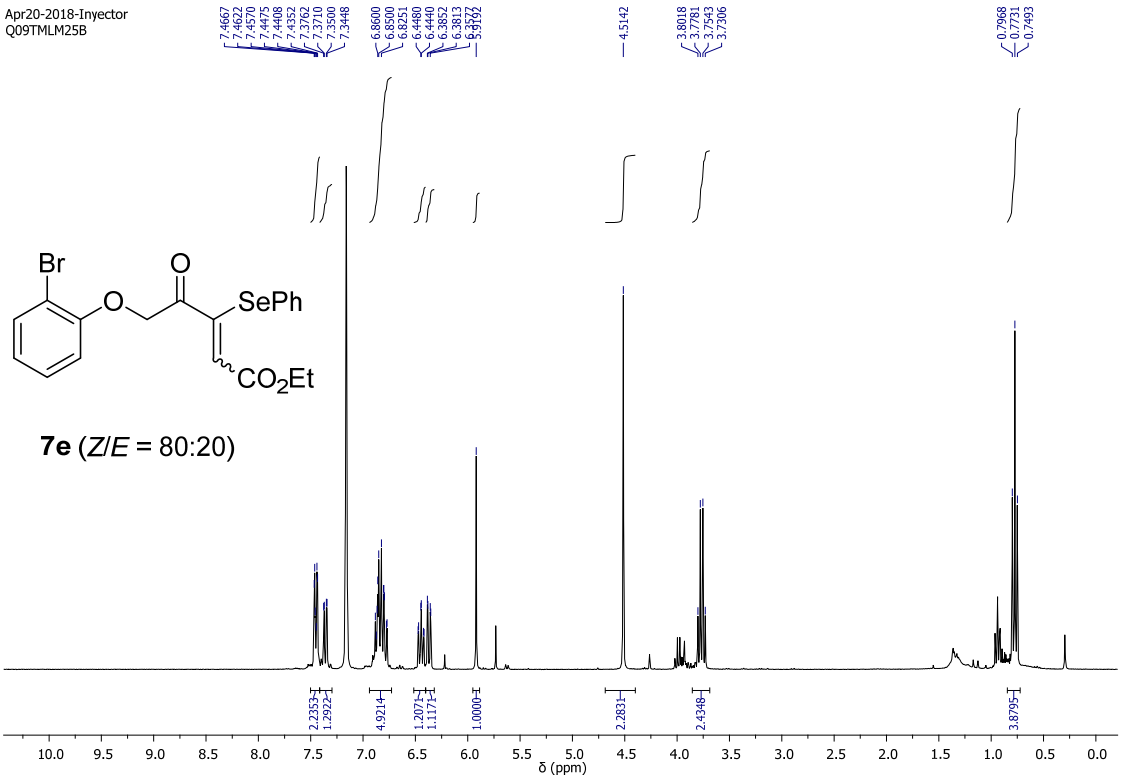

Oct02-2017-Inyector
Q09TM447B
δ (ppm)

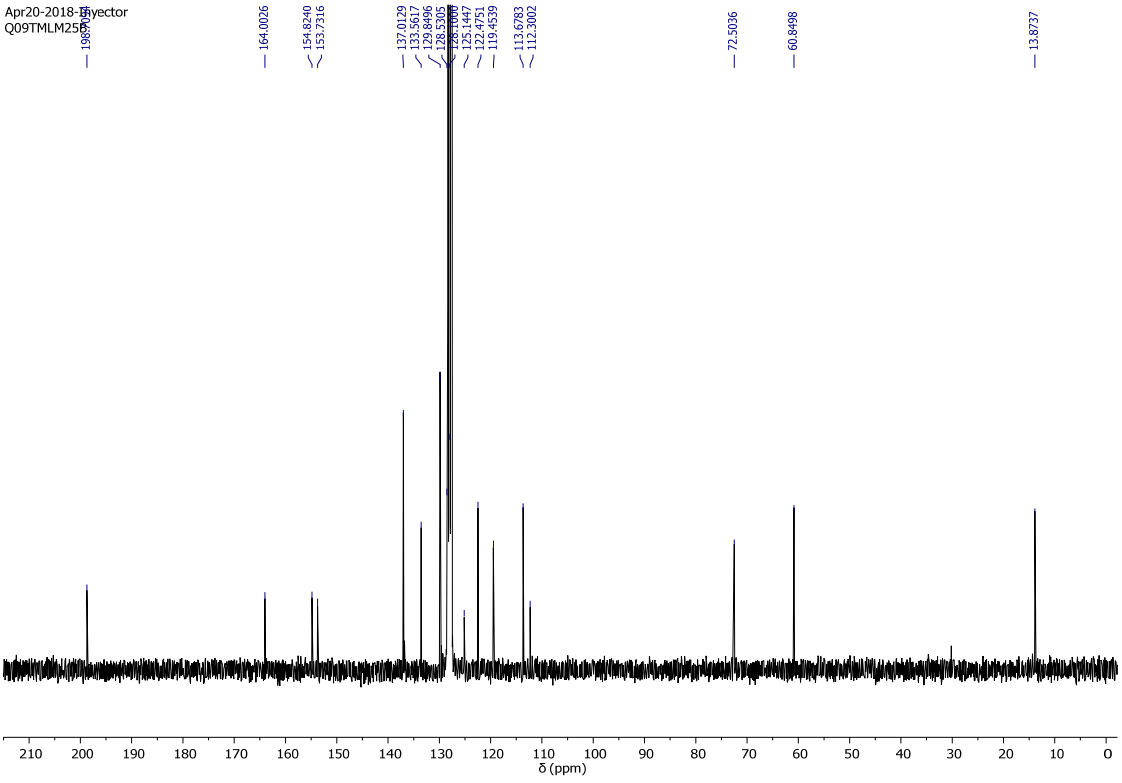

477.6355
800
750
700
650
600
550
500
450
400
350
300
250
200
150
100
50
0
-50
-100
-150
(ppm)

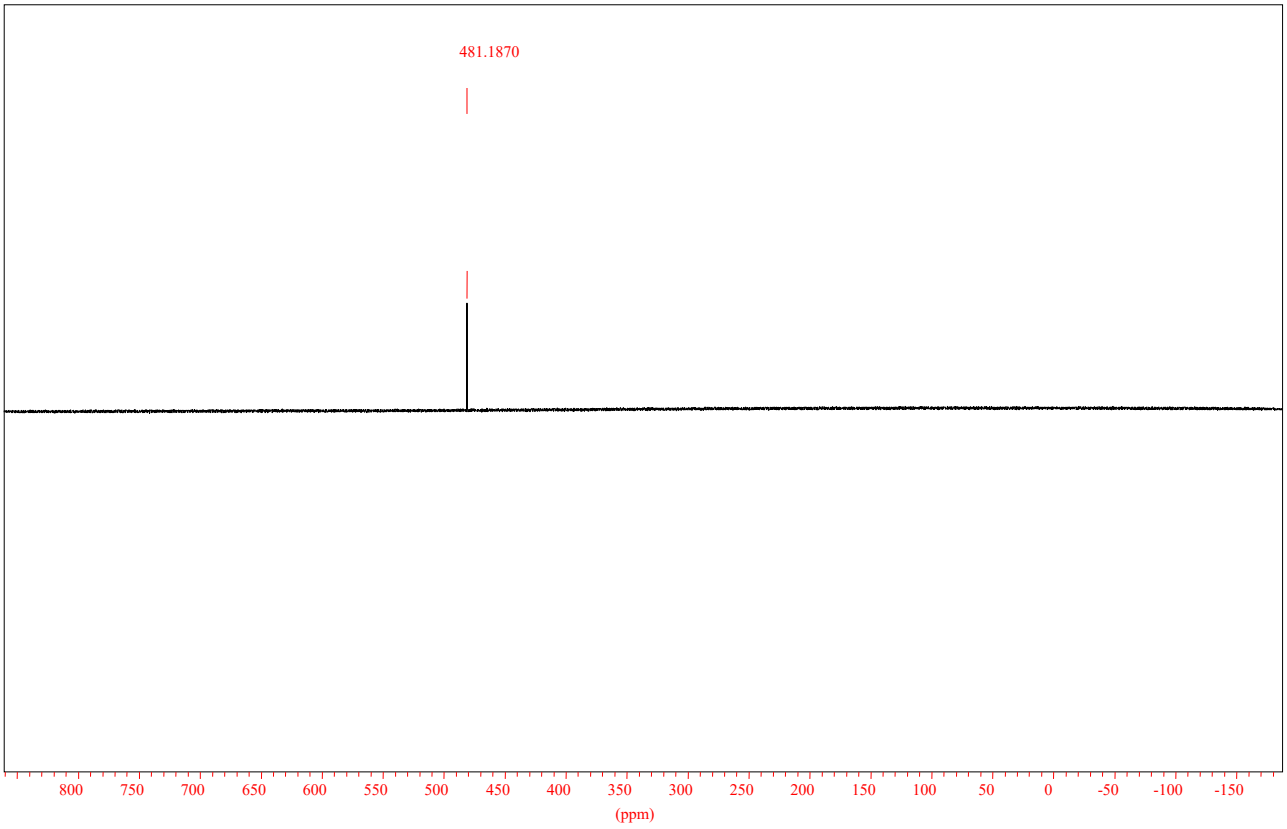

May29-2018-Inyector
Q09TMLM41B
7.3301
7.3257
7.3207
7.3122
7.3041
7.2985
7.2822
6.8573
6.8407
6.8213
6.3492
5.8152
4.5064
3.7726
3.7489
3.7251
3.7014
0.7857
0.7620
0.7382
O
O
SePh
I
CO2Et
7c (Z/E = 75:25)
4.8259
3.7784
2.1926
1.0000
2.2321
2.2380
3.4311
δ (ppm)

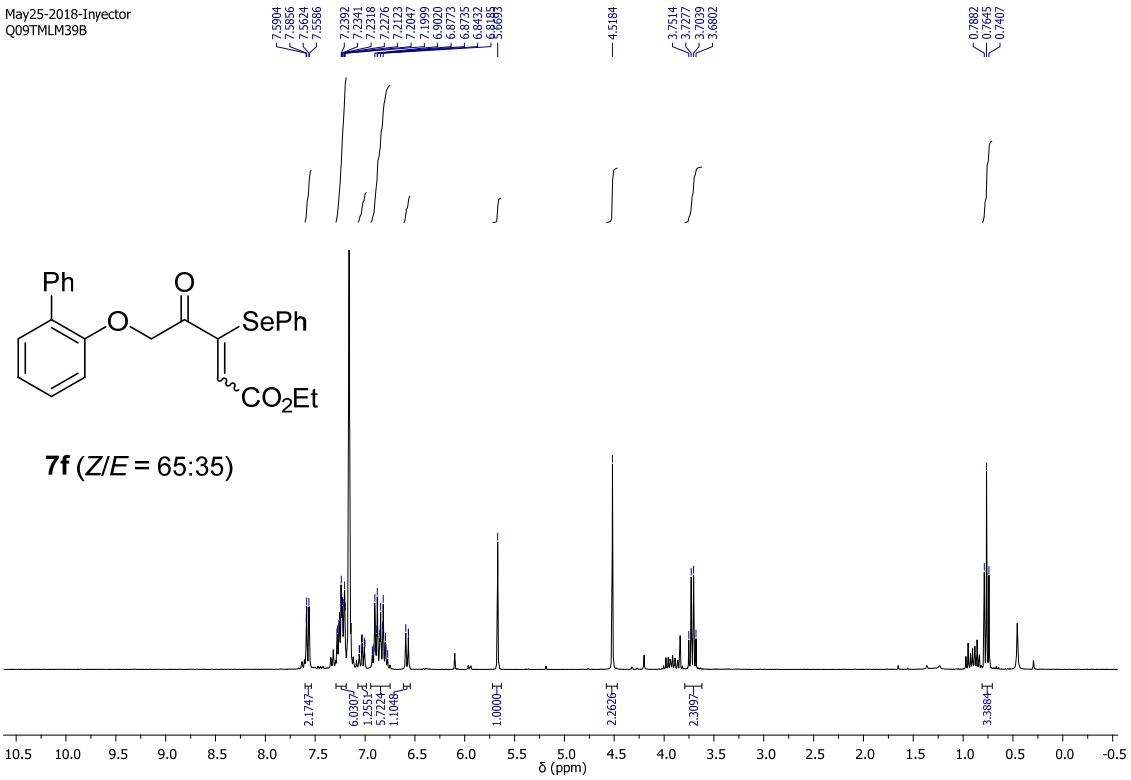

May29-2018-Inyector
Q09TMLM41B
163.7364
158.3456
153.8411
138.5006
136.8356
129.9321
125.0236
119.2961
117.5819
83.9069
71.8939
60.9275
13.8364
δ (ppm)

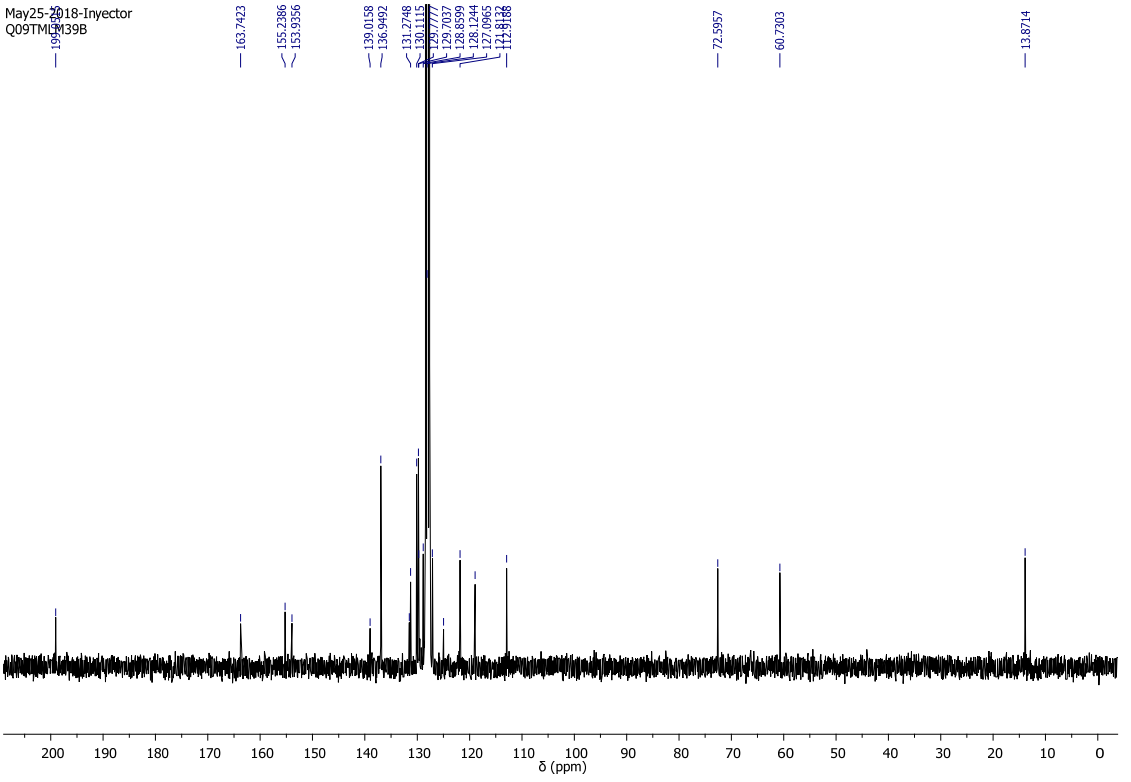

478.9073
800
750
700
650
600
550
500
450
400
350
300
250
200
150
100
50
0
-50
-100
-150
(ppm)

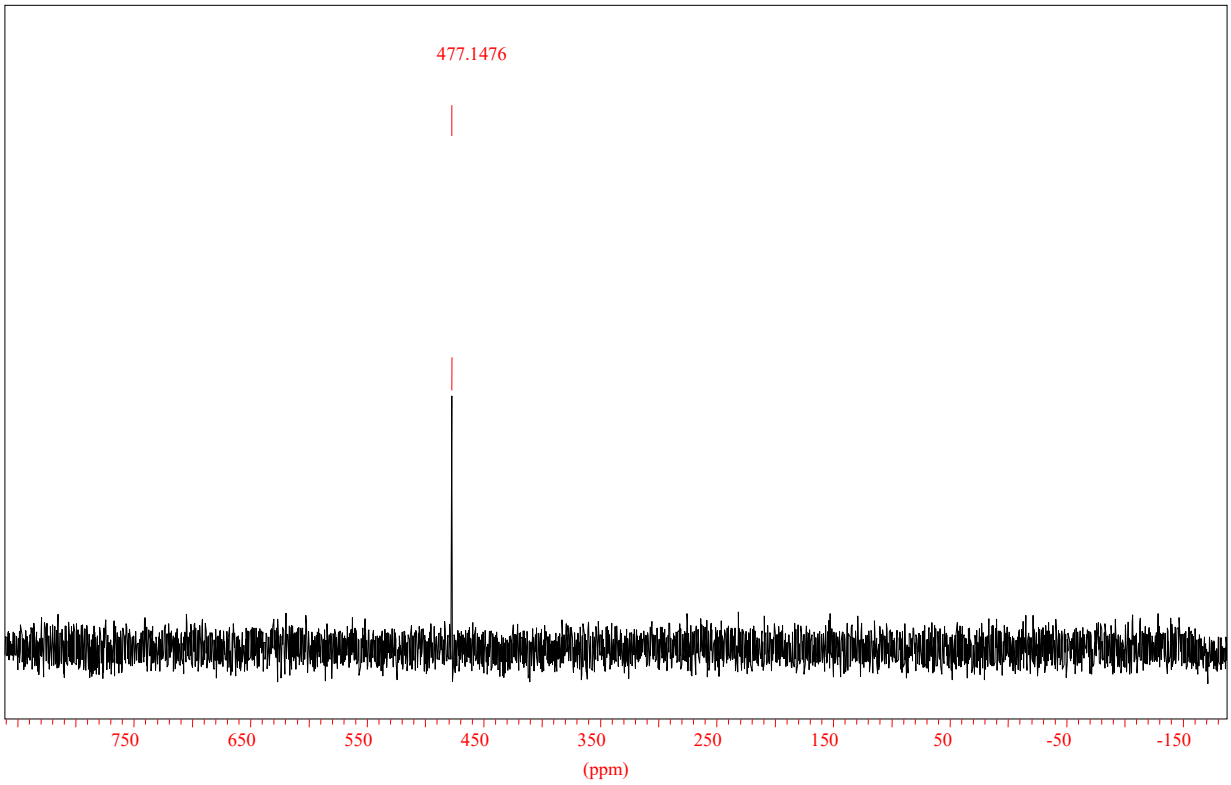

Apr20-2018-Inyector
Q09TMLM25B
Br
O
O
SePh
CO2Et
7e (Z/E = 80:20)
δ (ppm)

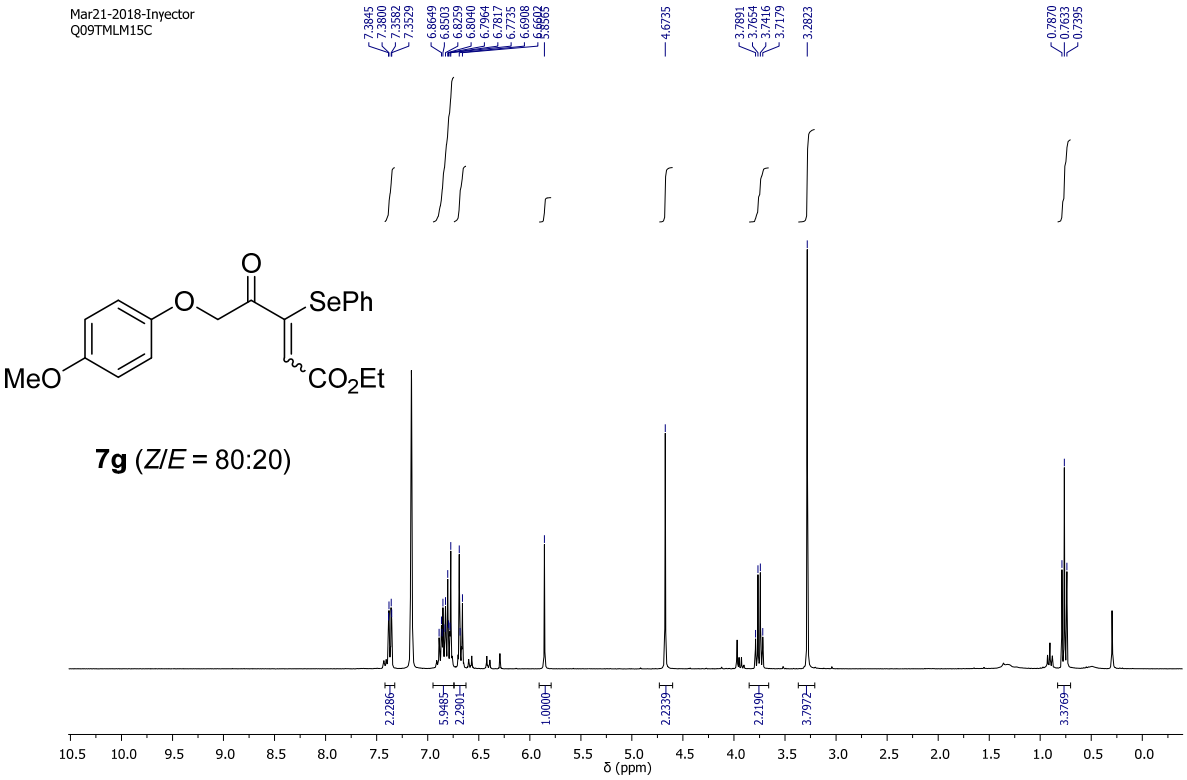

Apr20-2018-Inyector
Q09TMLM25B
δ (ppm)

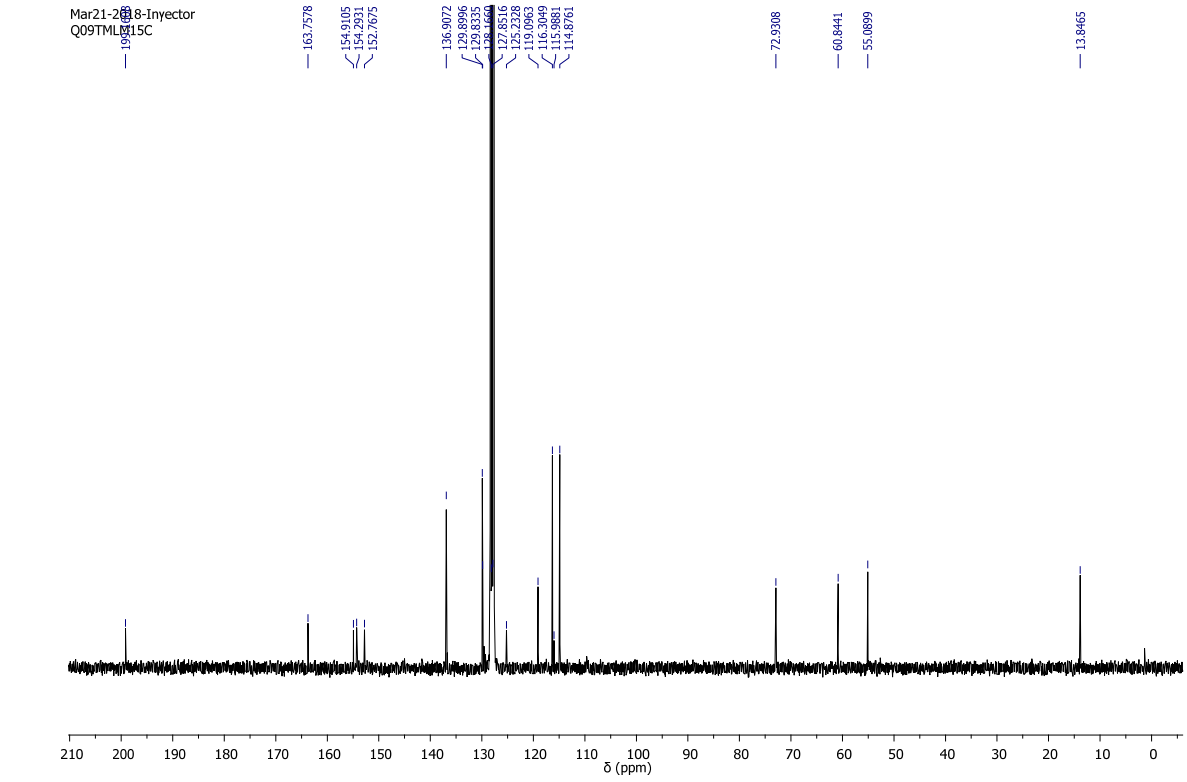

481.1870
800
750
700
650
600
550
500
450
400
350
300
250
200
150
100
50
0
-50
-100
-150
(ppm)

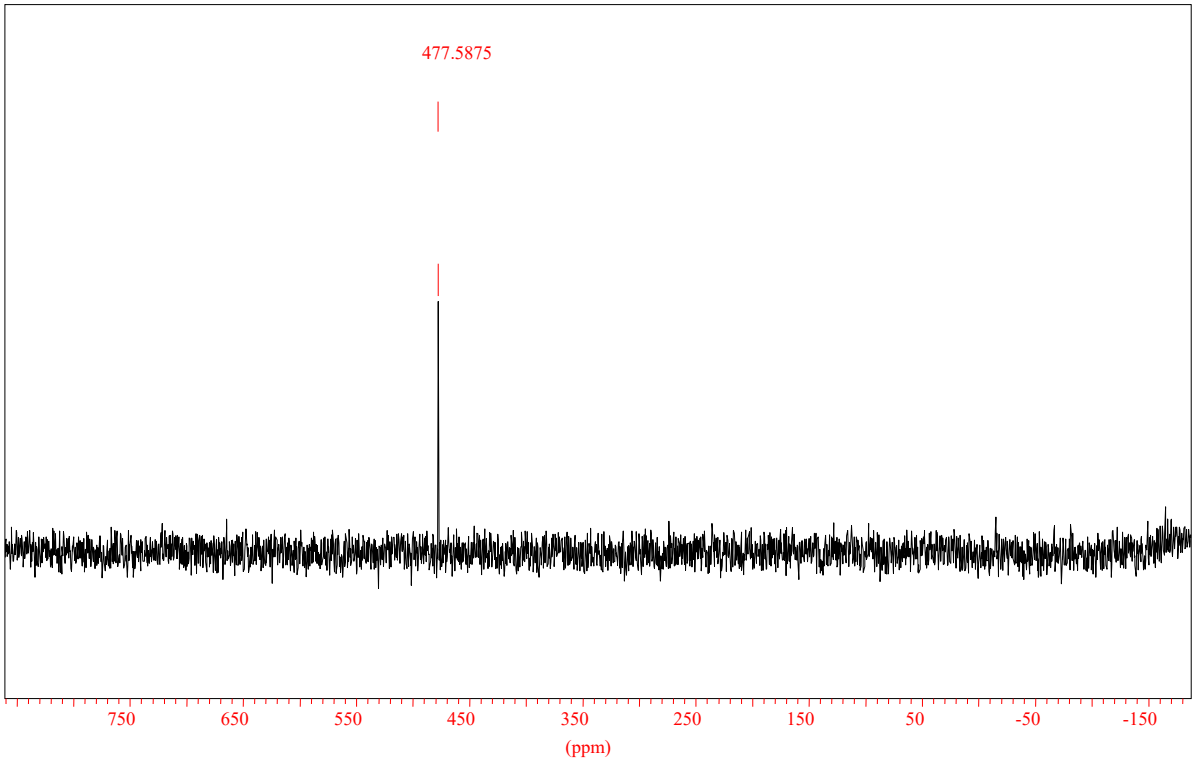

May25-2018-Inyector
Q09TMLM39B
Ph
O
O
SePh
CO2Et
7f (Z/E = 65:35)
δ (ppm)

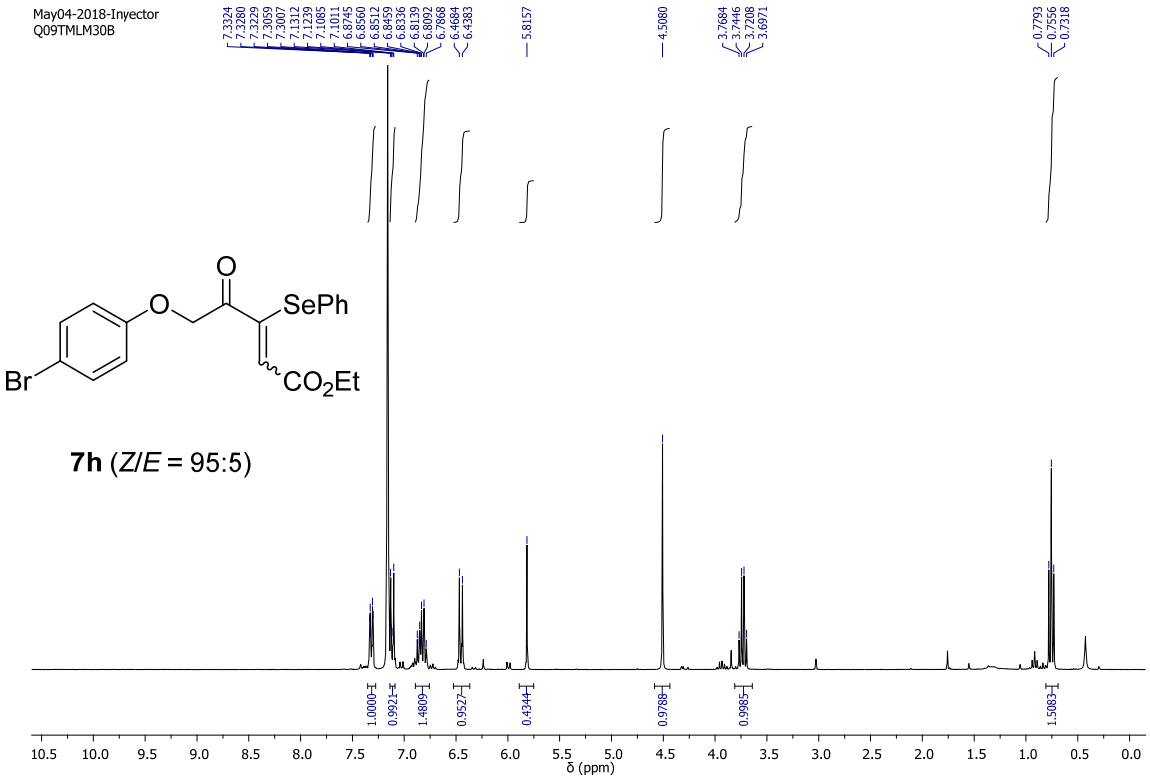

May25-2018-Inyector
Q09TMLM39B
δ (ppm)

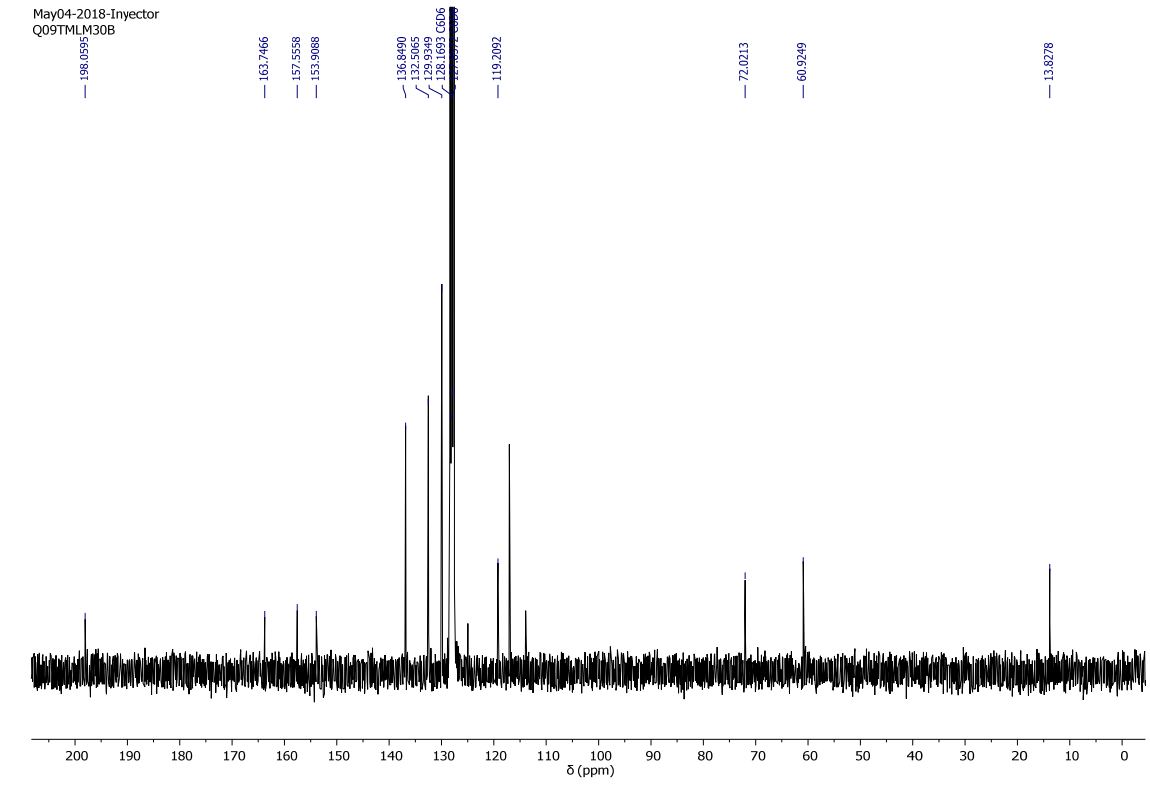

477.1476
750
650
550
450
350
250
150
50
-50
-150
(ppm)

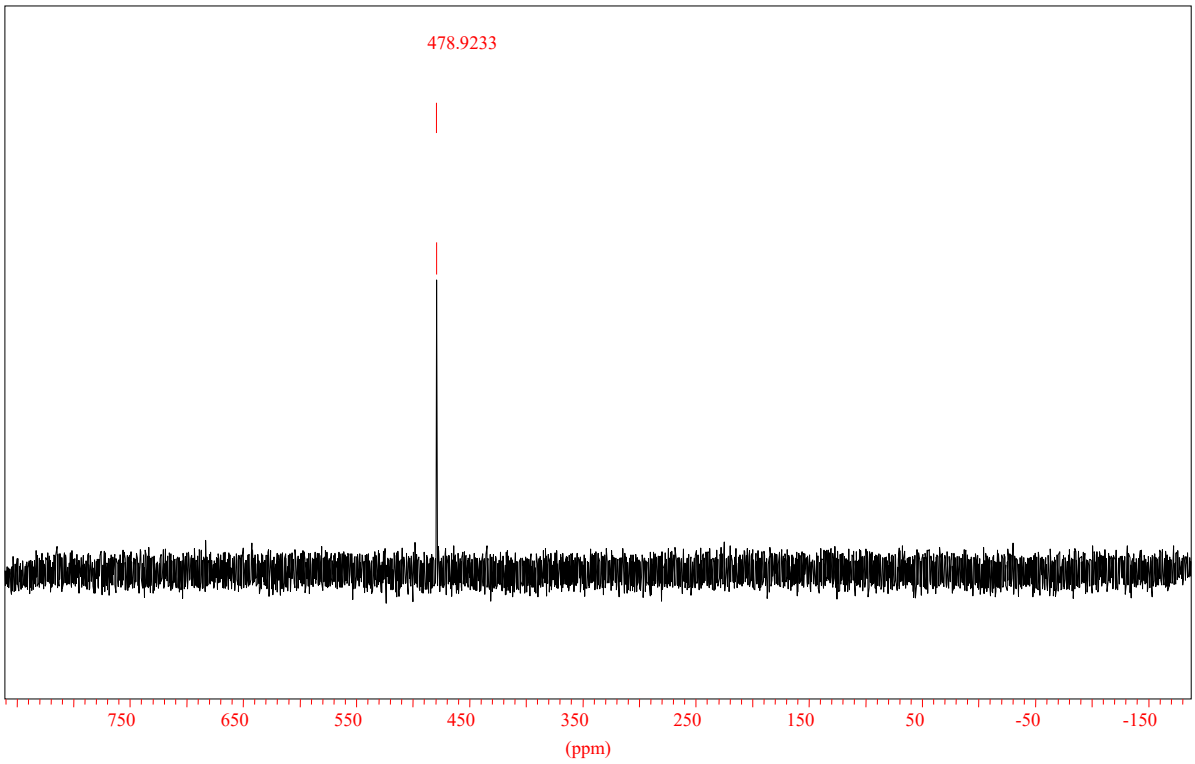

Mar21-2018-Inyector
Q09TMLM15C
MeO
O
O
SePh
CO2Et
7g (Z/E = 80:20)
δ (ppm)

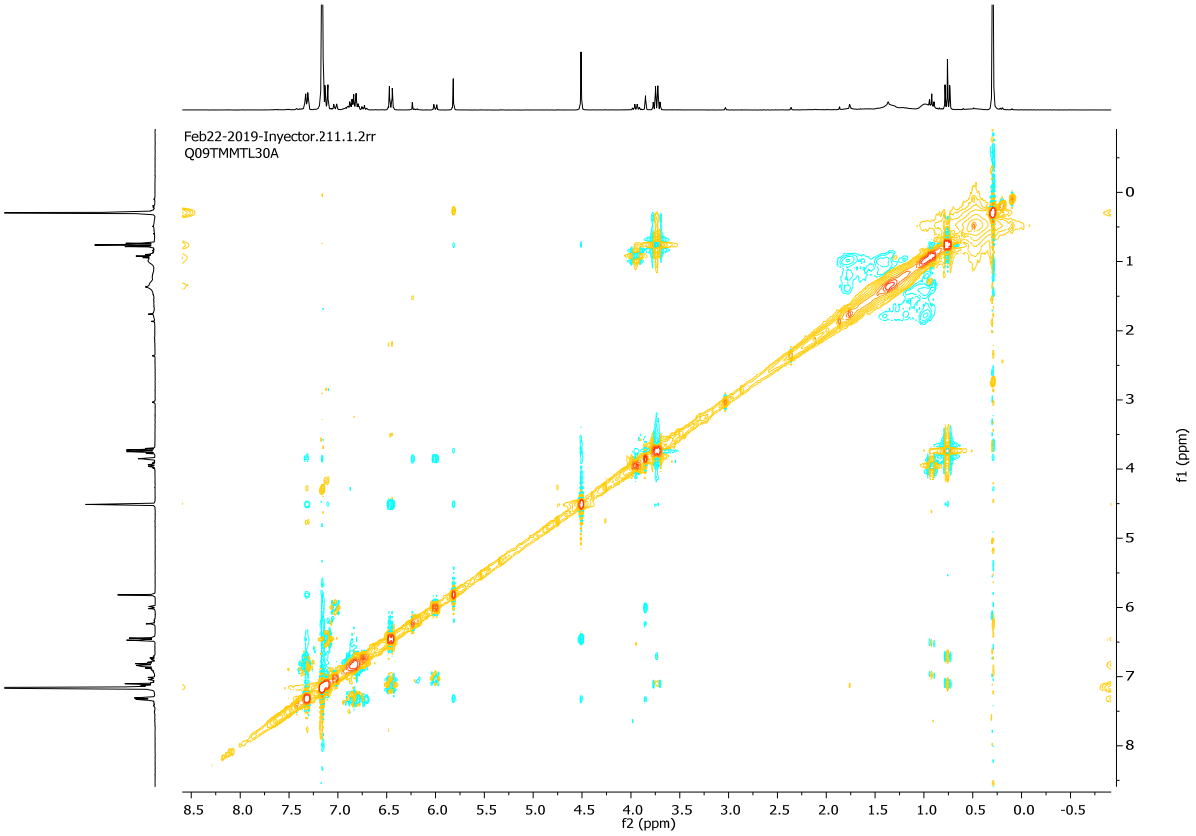

Mar21-2018-Inyector
Q09TMLM15C
δ (ppm)

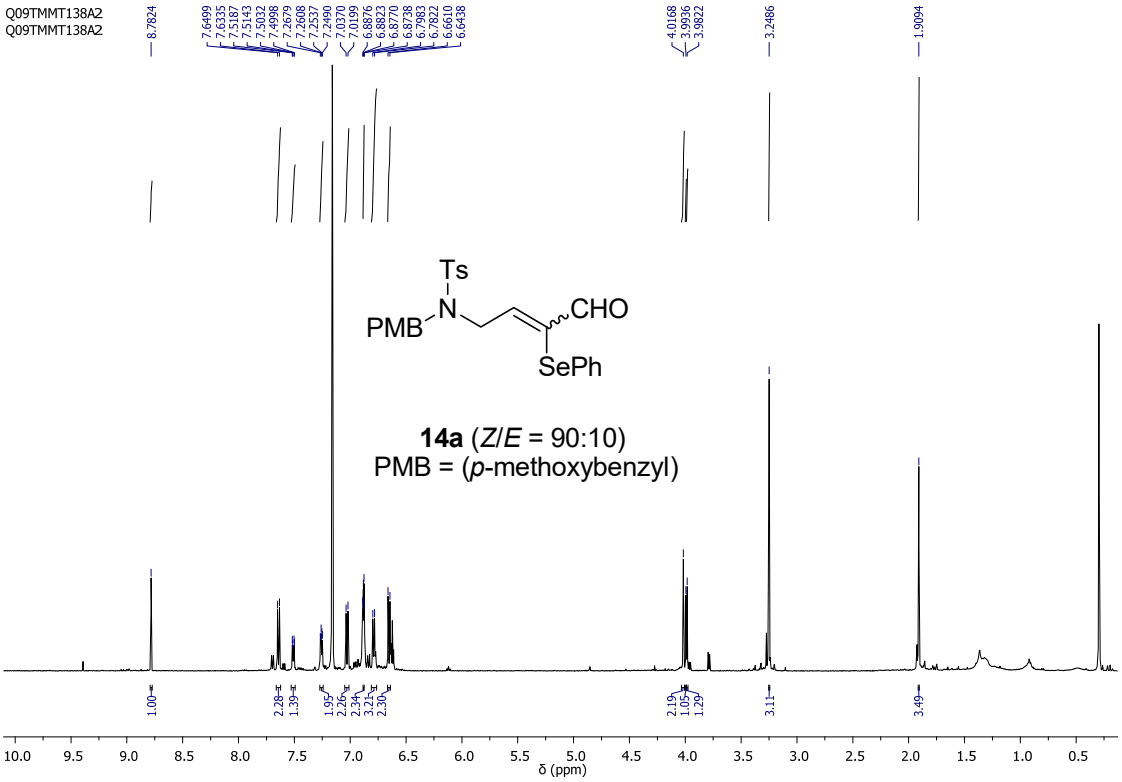

477.5875
750
650
550
450
350
250
150
50
-50
-150
(ppm)

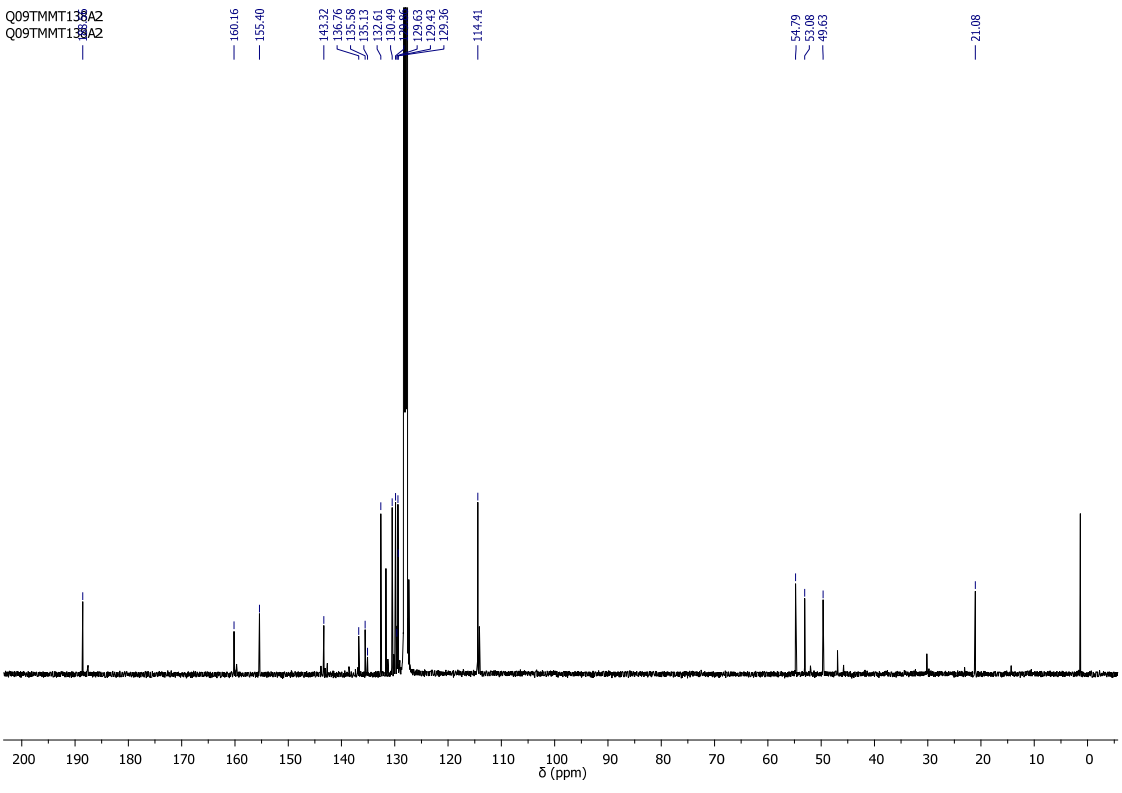

May04-2018-Inyector
Q09TMLM30B
7.3324
7.3280
7.3229
7.3059
7.3007
7.1312
7.1239
7.1085
7.1011
6.8745
6.8560
6.8512
6.8459
6.8336
6.8139
6.8092
6.7868
6.4684
6.4383
5.8157
4.5080
3.7684
3.7446
3.7208
3.6971
0.7793
0.7556
0.7318
O
O
SePh
Br
CO2Et
7h (Z/E = 95:5)
1.0000
0.9921
1.4809
0.9527
0.4344
0.9788
0.9985
1.5083
δ (ppm)

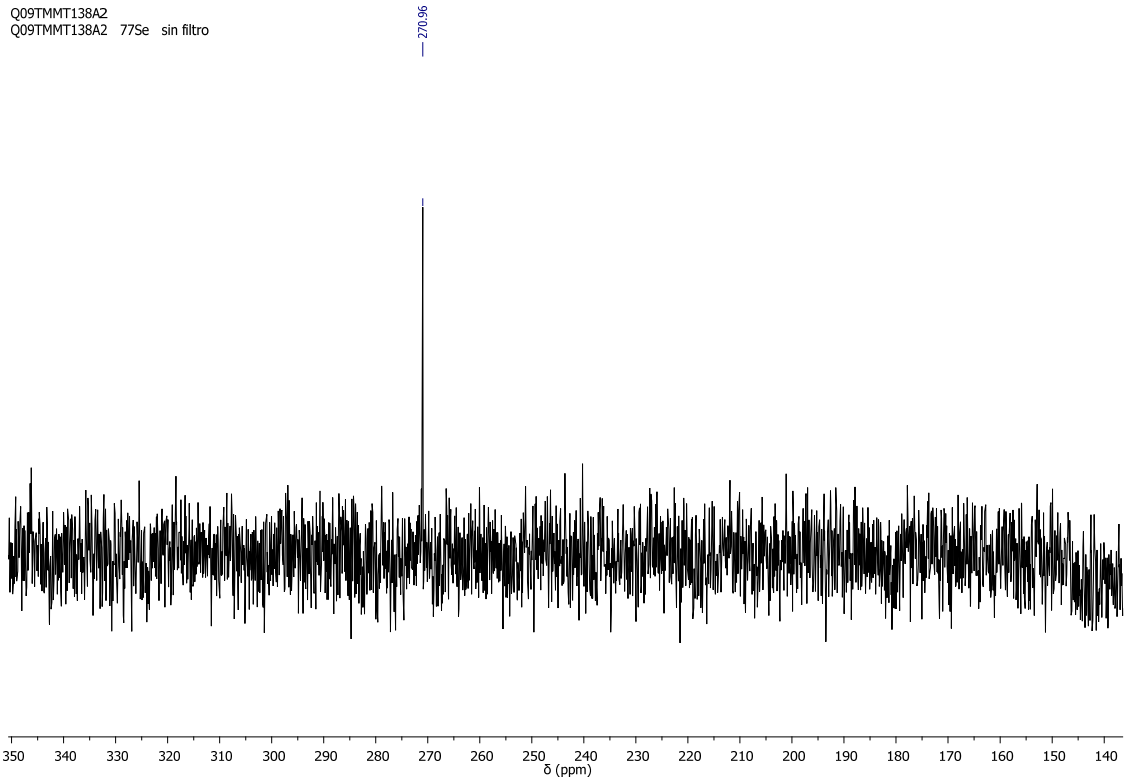

May04-2018-Inyector
Q09TMLM30B
198.0595
163.7466
157.5558
153.9088
136.8490
132.5065
129.9349
128.1693
C6D6
119.2092
72.0213
60.9249
13.8278
δ (ppm)

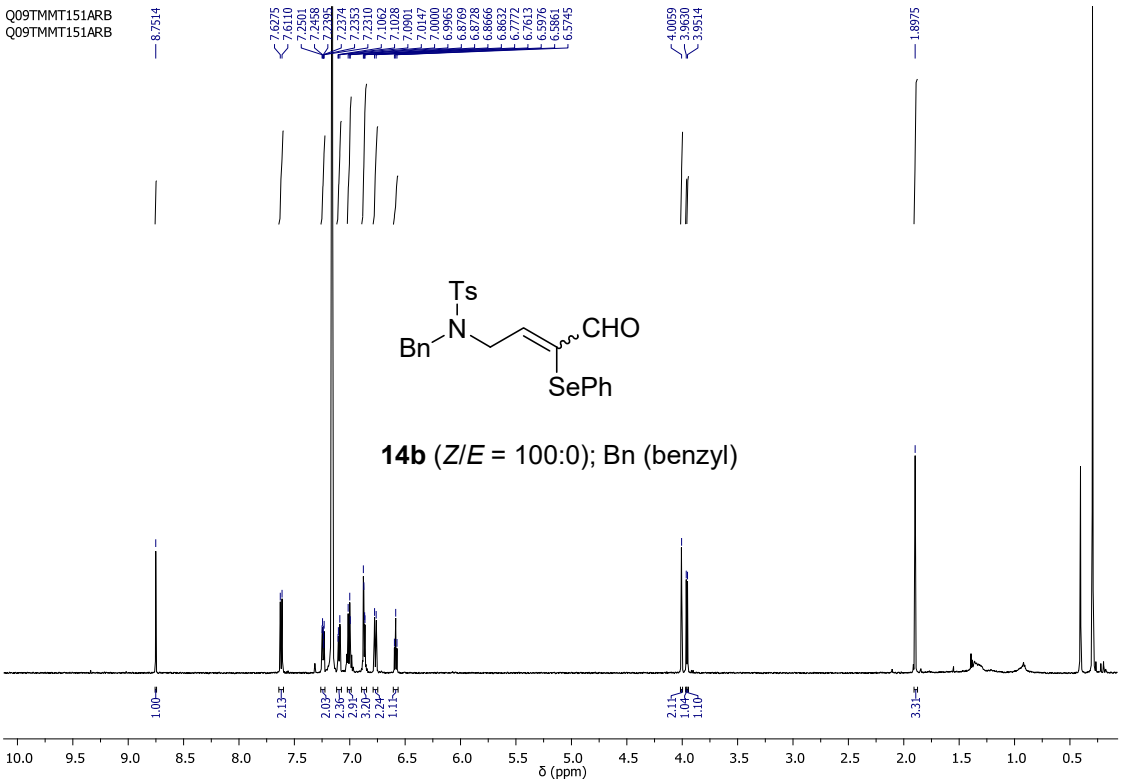

478.9233
750
650
550
450
350
250
150
50
-50
-150
(ppm)


Feb22-2019-Inyector.211.1.2rr
Q09TMMTL30A
f2 (ppm)
f1 (ppm)

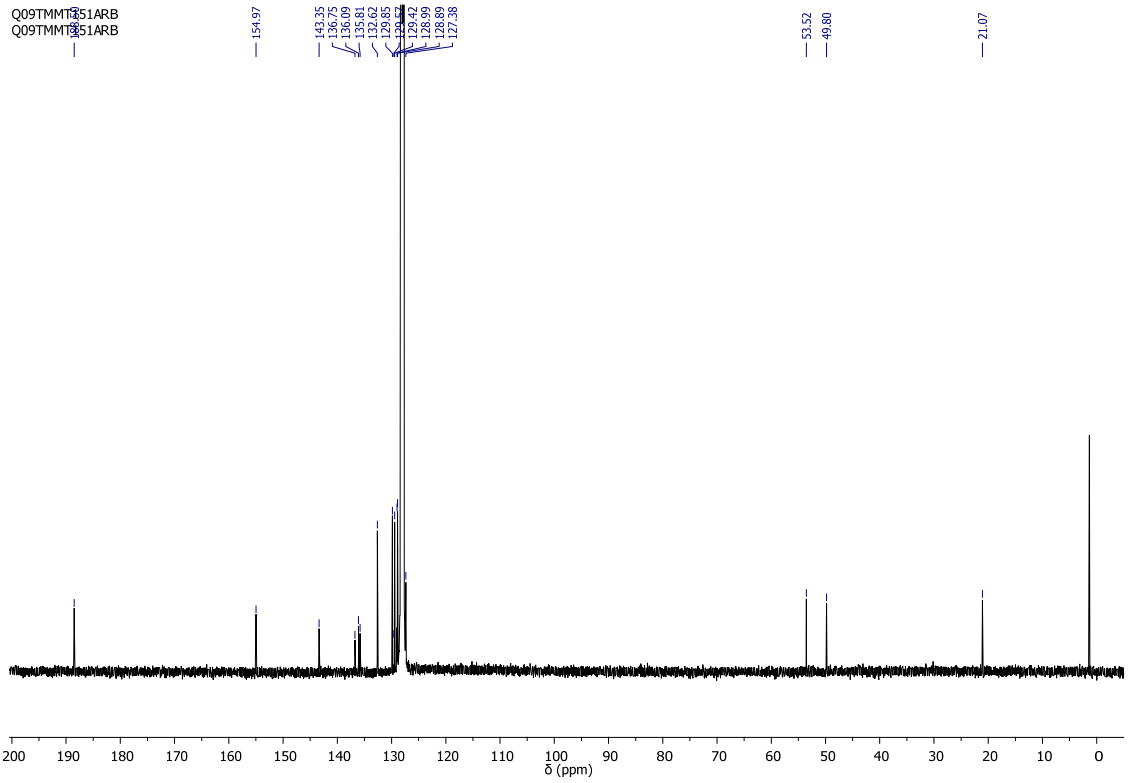

Q09TMMT138A2
Q09TMMT138A2
8.7824
7.6499
7.6335
7.5197
7.5143
7.5032
7.4998
7.2679
7.2608
7.2537
7.2490
7.0370
7.0199
6.8876
6.8823
6.8770
6.8738
6.7983
6.7822
6.6610
6.6438
4.0168
3.9936
3.9822
3.2486
1.9094
Ts
N
PMB
CHO
SePh
14a (Z/E = 90:10)
PMB = (p-methoxybenzyl)
1.00
2.28
1.39
1.95
2.26
2.34
3.21
2.30
2.19
1.05
1.29
3.11
3.49
δ (ppm)

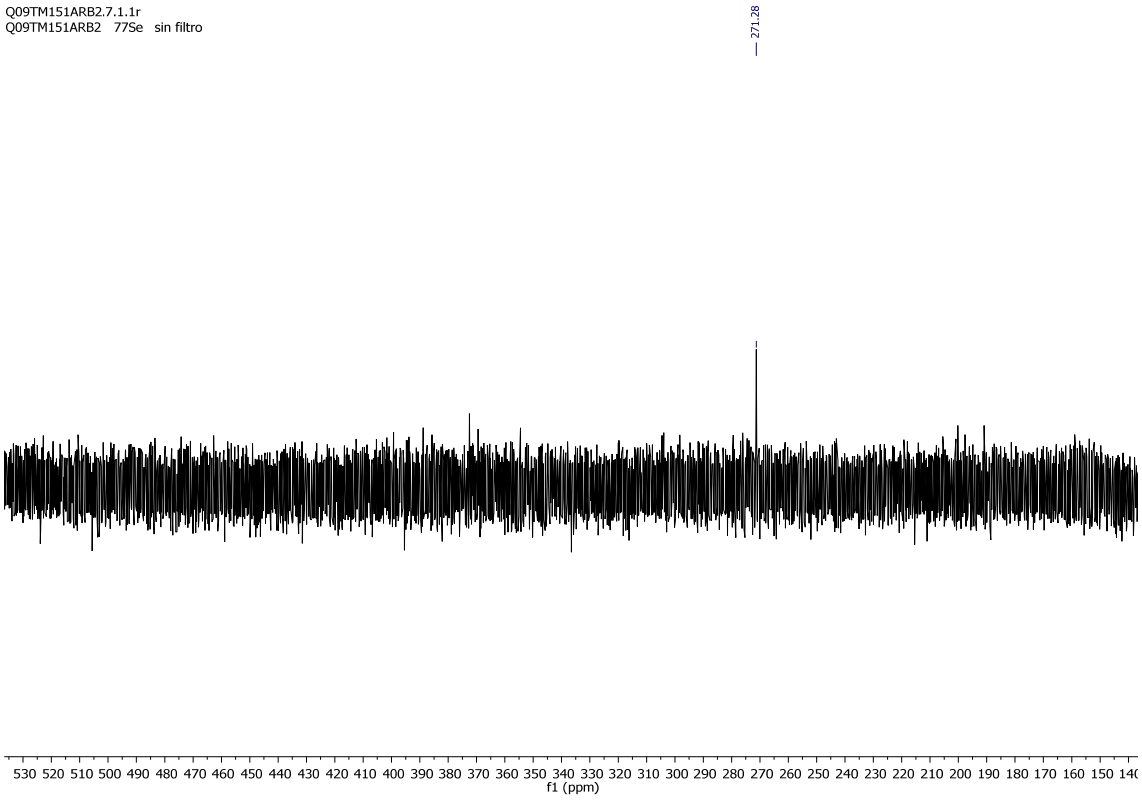

Q09TMMT138A2
Q09TMMT138A2
160.16
155.40
143.32
136.76
135.58
135.13
132.61
130.49
129.63
129.43
129.36
114.41
54.79
53.08
49.63
21.08
δ (ppm)

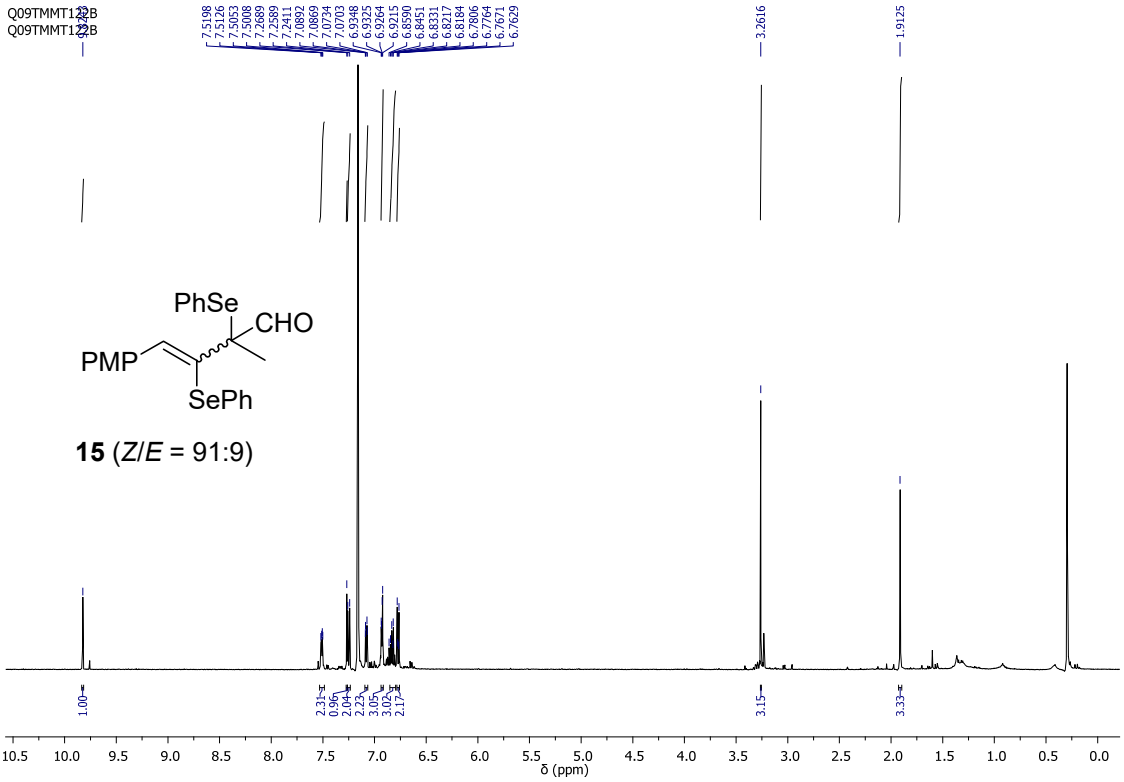

Q09TMMT138A2
Q09TMMT138A2 77Se sin filtro
270.96
350 340 330 320 310 300 290 280 270 260 250 240 230 220 210 200 190 180 170 160 150 140
δ (ppm)

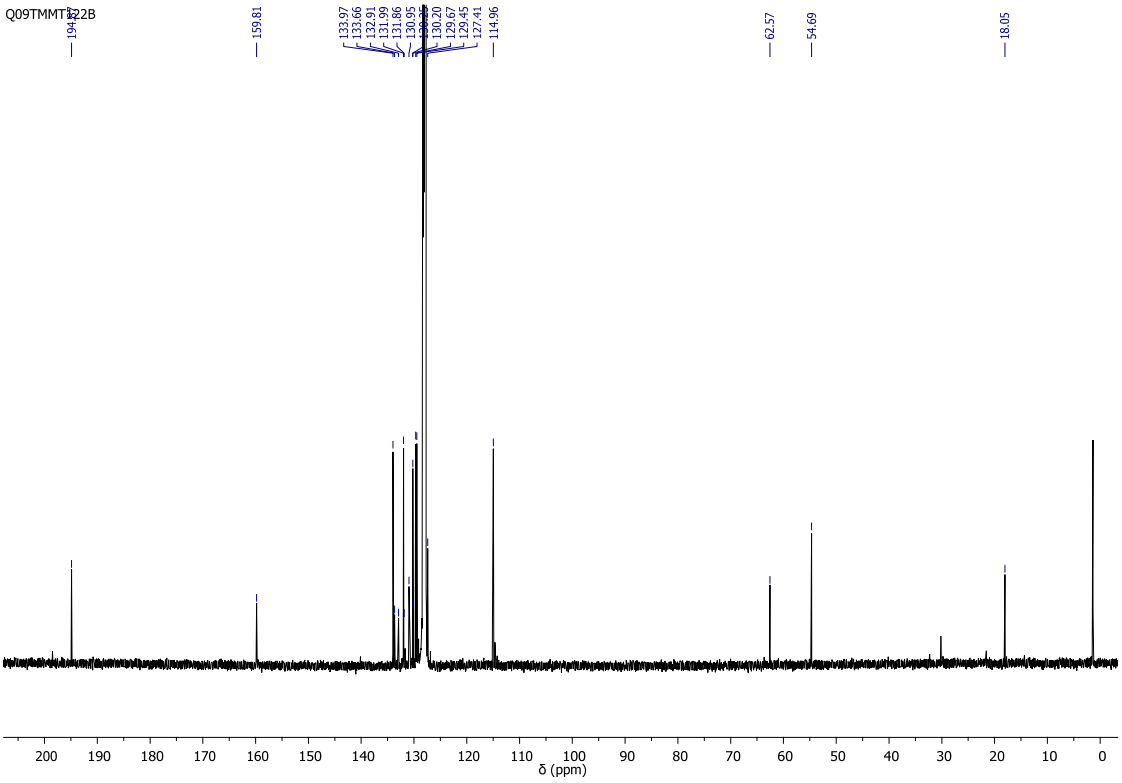


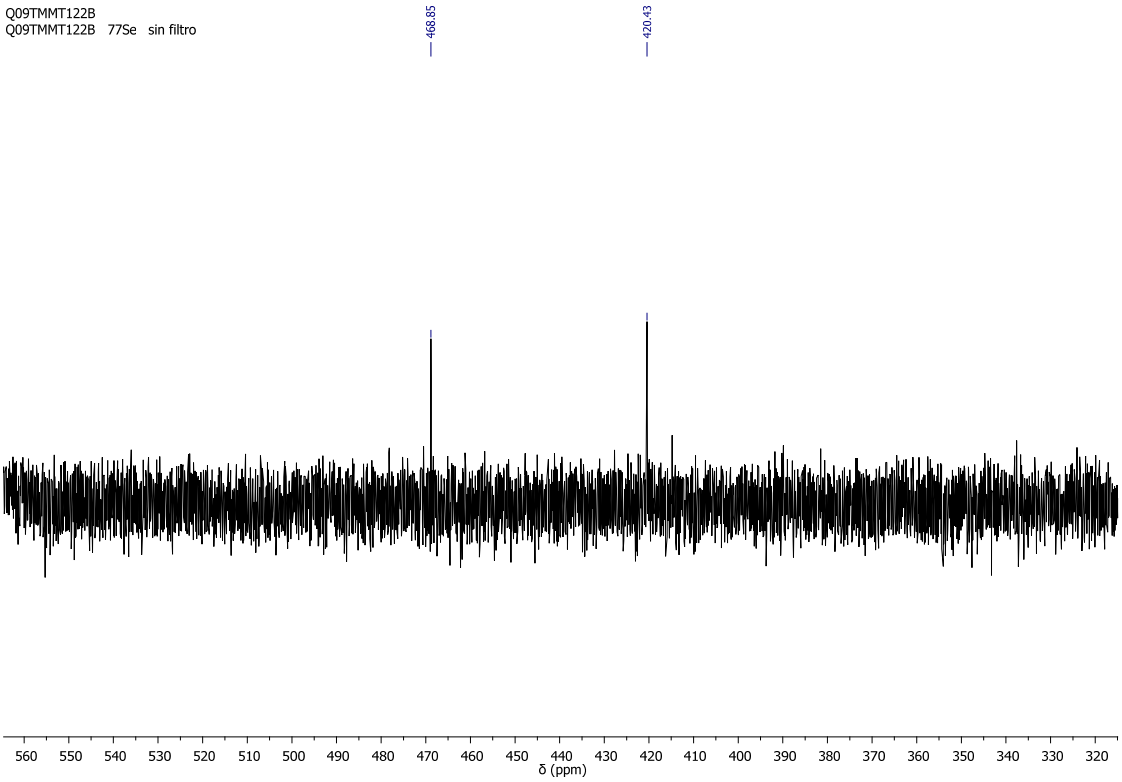
14b (*Z*/*E* = 100:0); Bn (benzyl)

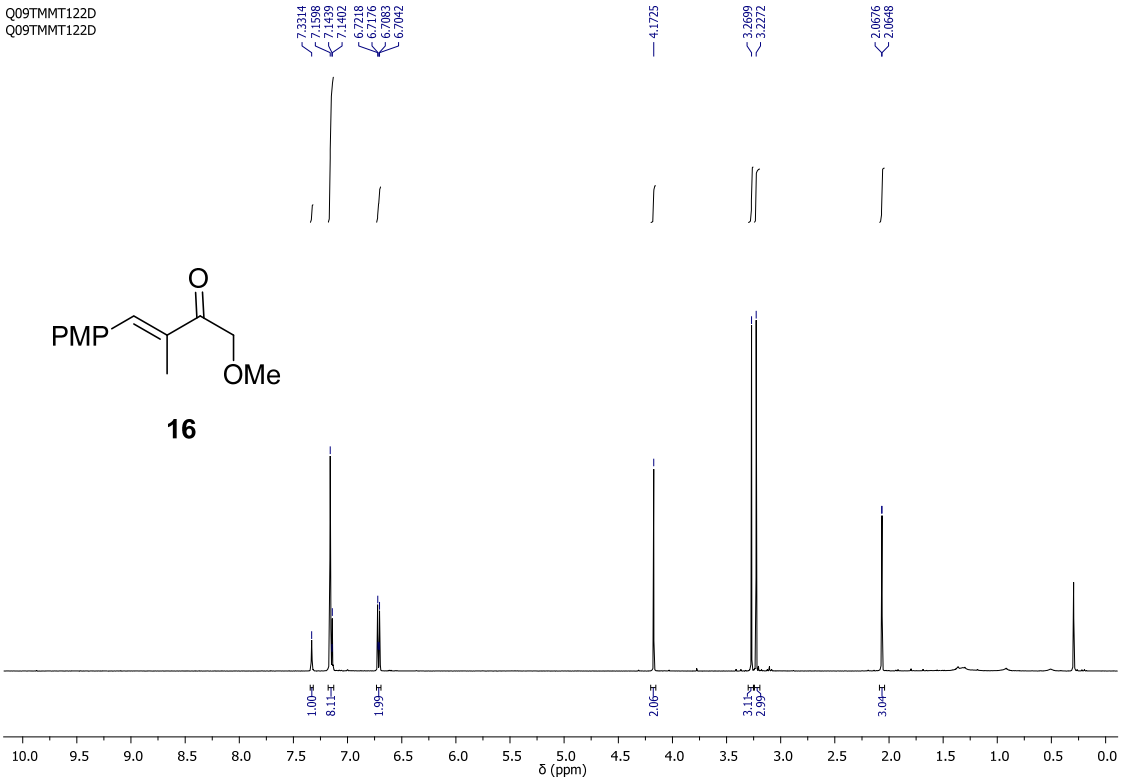


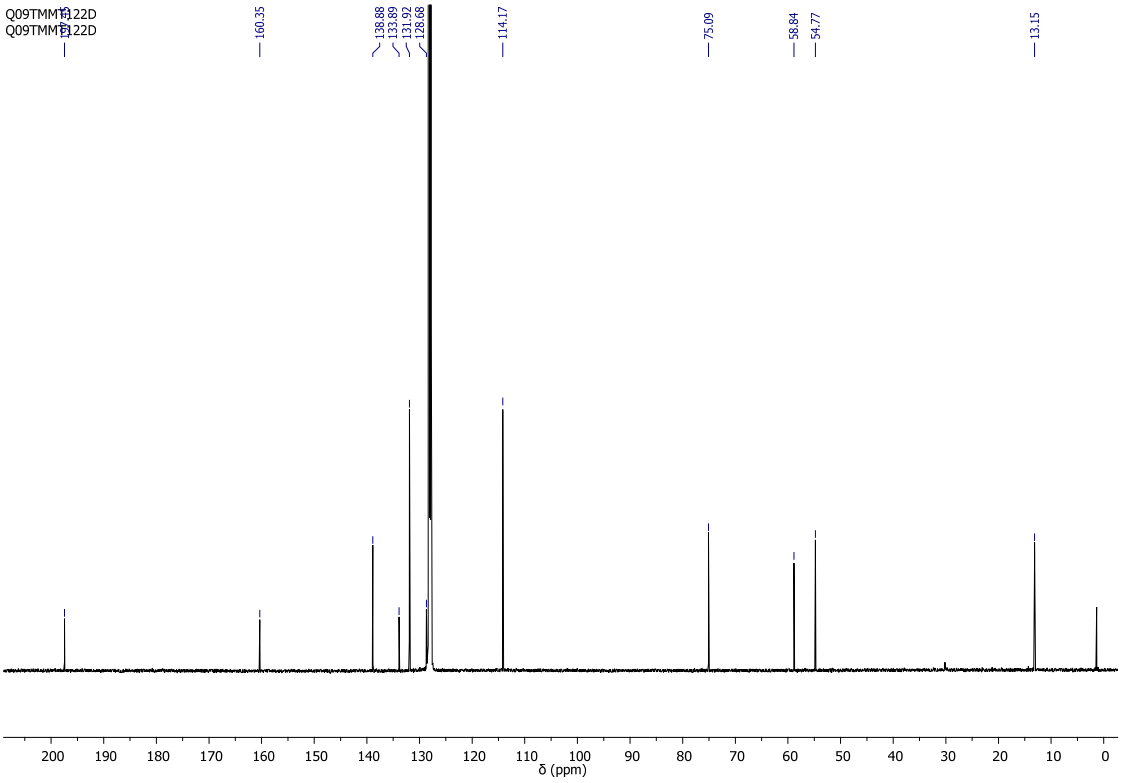

Q09TM151ARB2.7.1.1r
Q09TM151ARB2 77Se sin filtro
271.28
530 520 510 500 490 480 470 460 450 440 430 420 410 400 390 380 370 360 350 340 330 320 310 300 290 280 270 260 250 240 230 220 210 200 190 180 170 160 150 140
f1 (ppm)

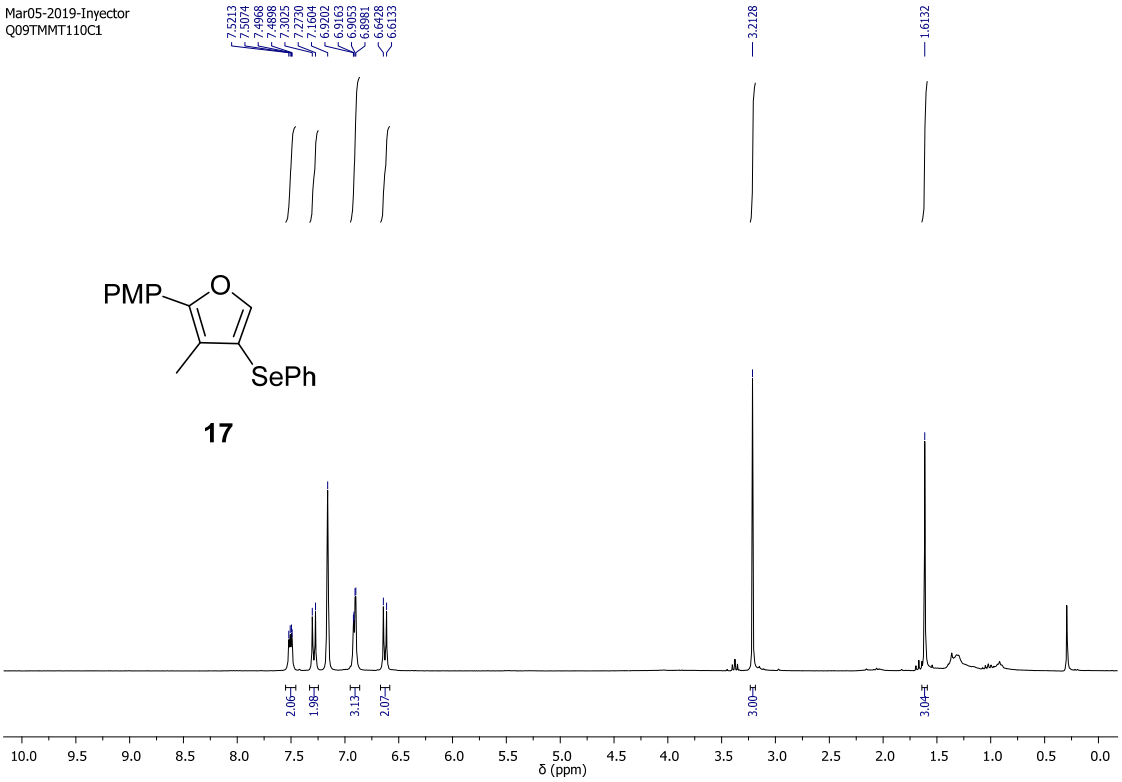

Q09TMMT122B
Q09TMMT122B
PhSe
CHO
PMP
SePh
15 (Z/E = 91:9)
δ (ppm)

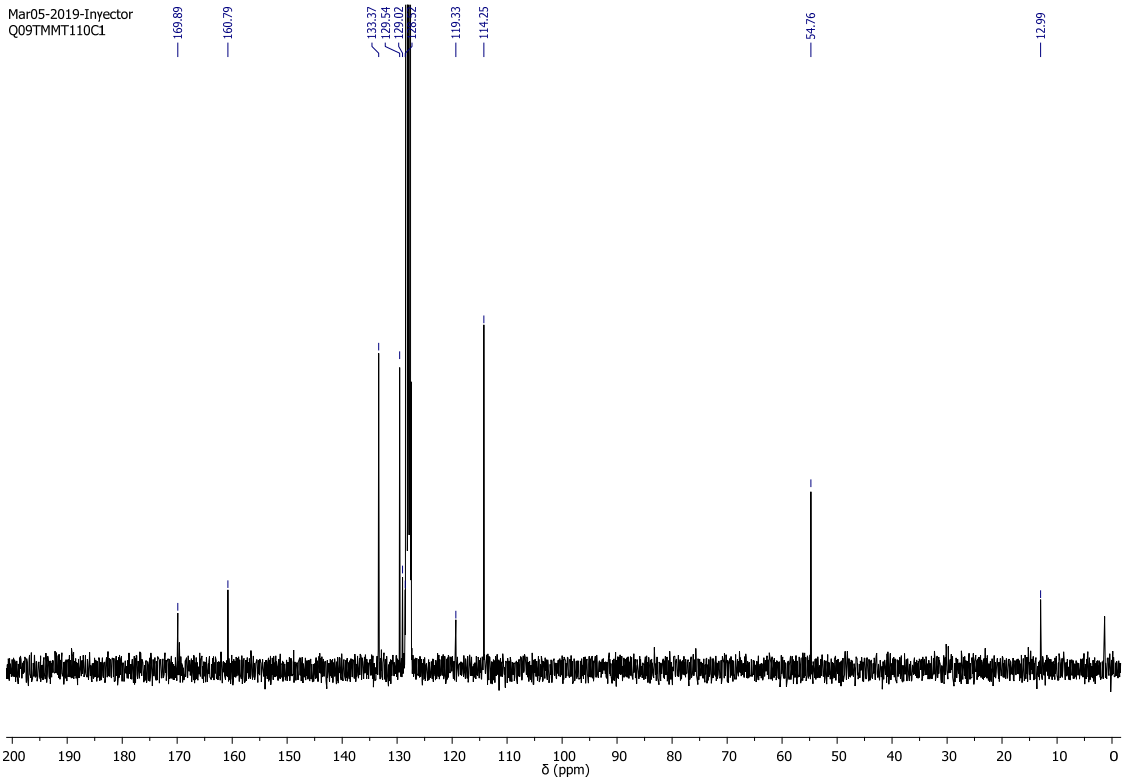

Q09TMMT122B
δ (ppm)

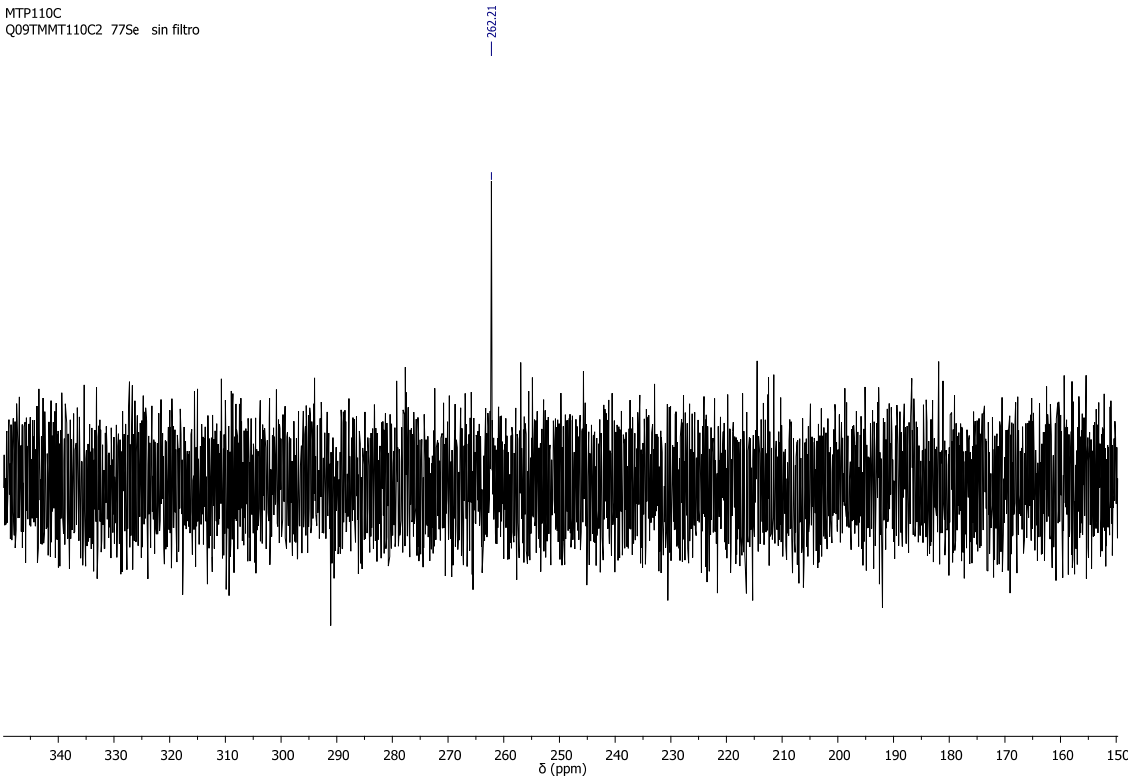

Q09TMMT122B
Q09TMMT122B 77Se sin filtro
468.85
420.43
560 550 540 530 520 510 500 490 480 470 460 450 440 430 420 410 400 390 380 370 360 350 340 330 320
δ (ppm)


Q09TMMT122D
Q09TMMT122D
7.3314
7.1598
7.1439
7.1402
6.7218
6.7176
6.7083
6.7042
4.1725
3.2699
3.2272
2.0676
2.0648
PMP
O
OMe
16
1.00
8.11
1.99
2.06
3.11
2.99
3.04
δ (ppm)


Q09TMMT122D
Q09TMMT122D
160.35
138.88
133.89
131.92
128.68
114.17
75.09
58.84
54.77
13.15
δ (ppm)


Mar05-2019-Inyector
Q09TMMT110C1
7.5213
7.5074
7.4968
7.4898
7.3025
7.2730
7.1604
6.9202
6.9163
6.9053
6.8981
6.6428
6.6133
3.2128
1.6132
PMP
O
SePh
17
2.06
1.98
3.13
2.07
3.00
3.04
δ (ppm)


Mar05-2019-Inyector
Q09TMMT110C1
169.89
160.79
133.37
129.54
129.02
128.32
119.33
114.25
54.76
12.99
δ (ppm)

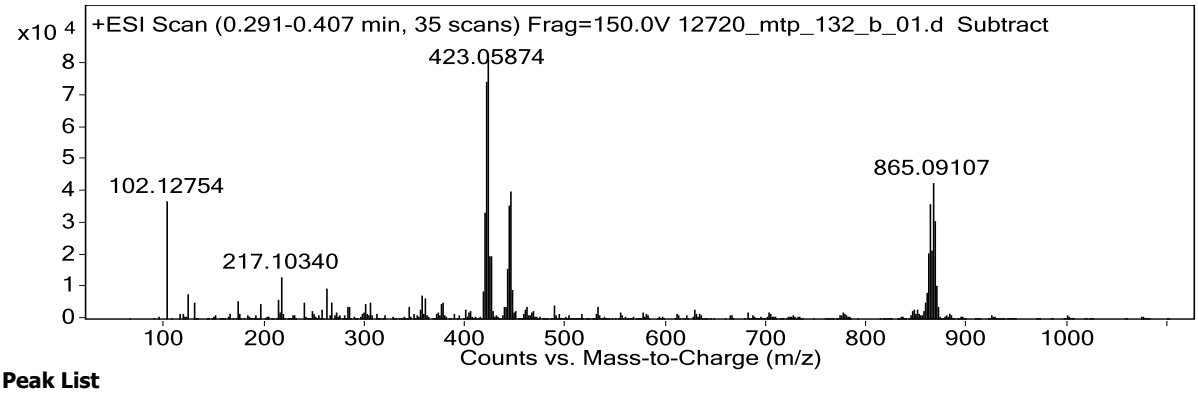

MTP110C
Q09TMMT110C2 77Se sin filtro
262.21
340
330
320
310
300
290
280
270
260
250
240
230
220
210
200
190
180
170
160
δ (ppm)

Qualitative Analysis Report

Data Filename	12720_mtp_132_b_01.d	**Sample Name**	mtp_132_b
Sample Type	Sample	**Position**	Vial 2
Instrument Name	Instrument 1	**User Name**	
Acq Method	ESI_ACN_75_pos.m	**IRM Calibration Status**	Success
DA Method	Defecto_modificado_CS.m	**Comment**	

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
150	0	Esi



Peak List

m/z	z	Abund
102.12754		37012
419.05788		33330
421.05735	1	74521
423.05874	1	81370
443.03899	1	35547
445.04012	1	39910
863.09084	1	36107
864.09365	1	21559
865.09107	1	42861
867.09170	1	30615

--- End Of Report ---

Qualitative Compound Report

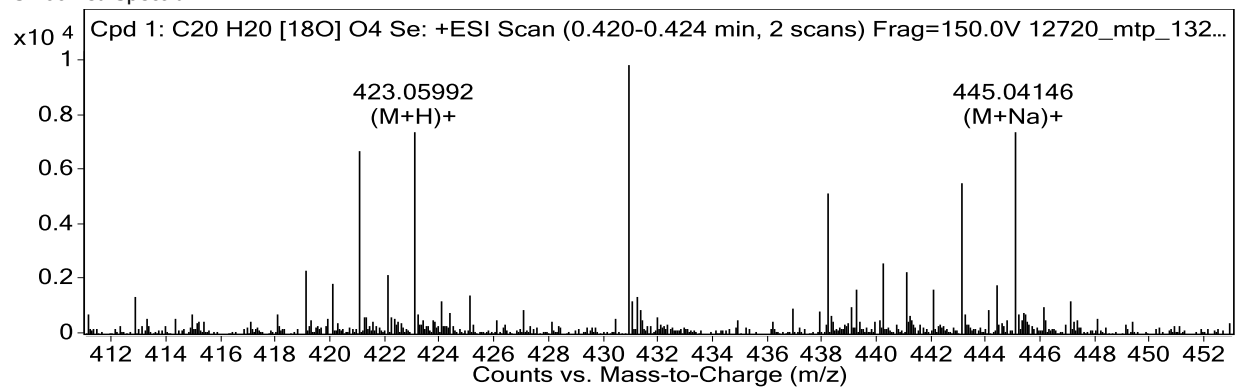
Data File	12720_mtp_132_b_01.d	**Sample Name**	mtp_132_b
Sample Type	Sample	**Position**	Vial 2
Instrument Name	Instrument 1	**User Name**	
Acq Method	ESI_ACN_75_pos.m	**IRM Calibration Status**	Success
DA Method	Defecto_modificado_CS.m	**Comment**	

Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: C20 H20 [18O] O4 Se	0.424	416.05729	7406	C20 H20 [18O] O4 Se	416.0578	-1.21

Compound Label	RT	Algorithm	Mass
Cpd 1: C20 H20 [18O] O4 Se	0.424	Find By Formula	416.05729

MS Zoomed Spectrum

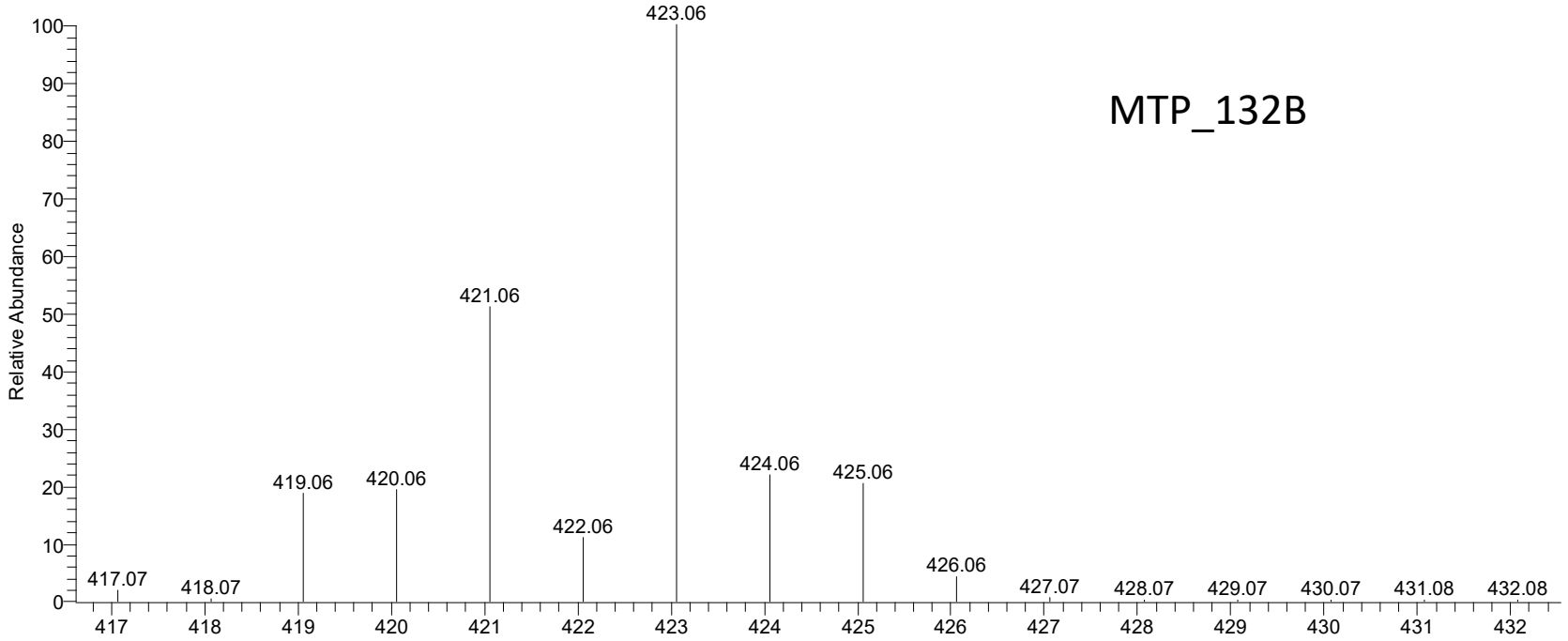


MS Spectrum Peak List

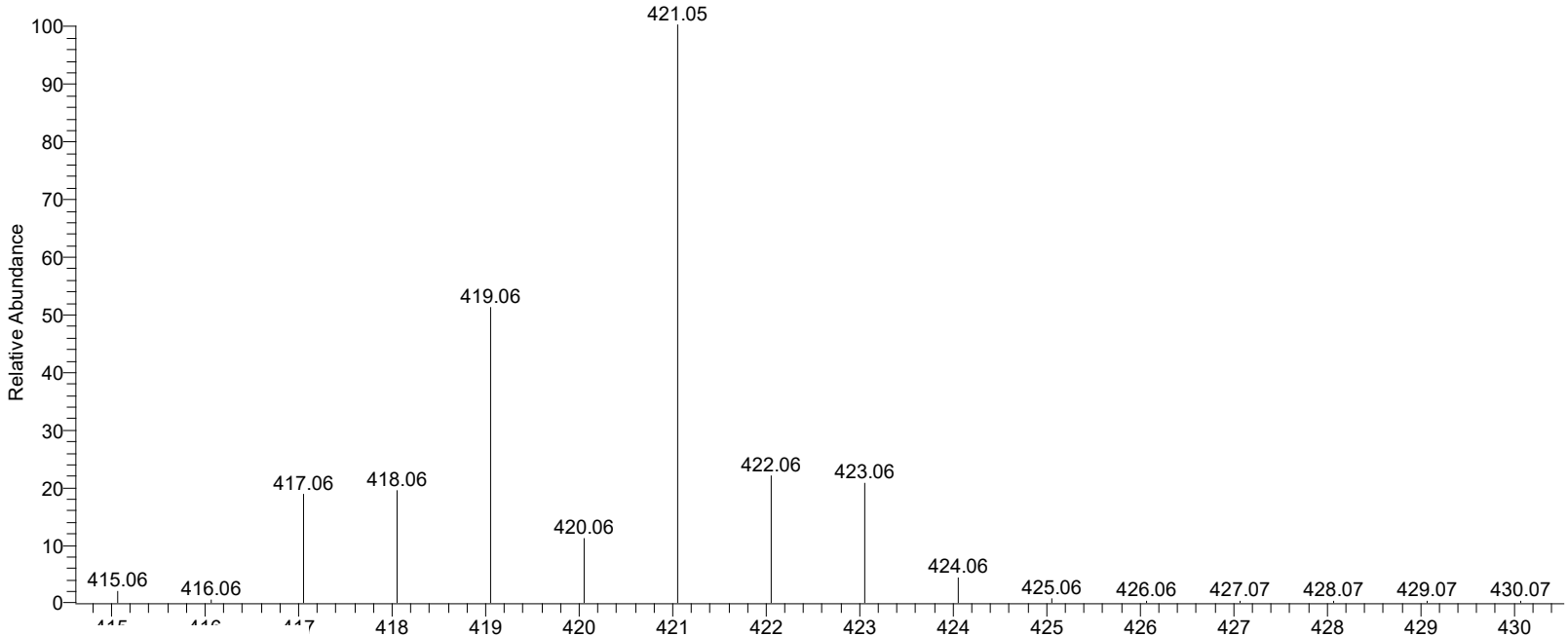
m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
100.07505				2493		
102.12814				66565		
102.18457				8030		
102.25875				3055		
102.27492				2991		
103.13217				5185		
421.0575	421.06039	-6.86	1	6724	C20 H21 O4 [18O] Se	(M+H)+
423.05992	423.05923	1.64	1	7424	C20 H21 O4 [18O] Se	(M+H)+
443.04154	443.04233	-1.79	1	5540	C20 H20 Na O4 [18O] Se	(M+Na)+
445.04146	445.04117	0.65	1	7406	C20 H20 Na O4 [18O] Se	(M+Na)+

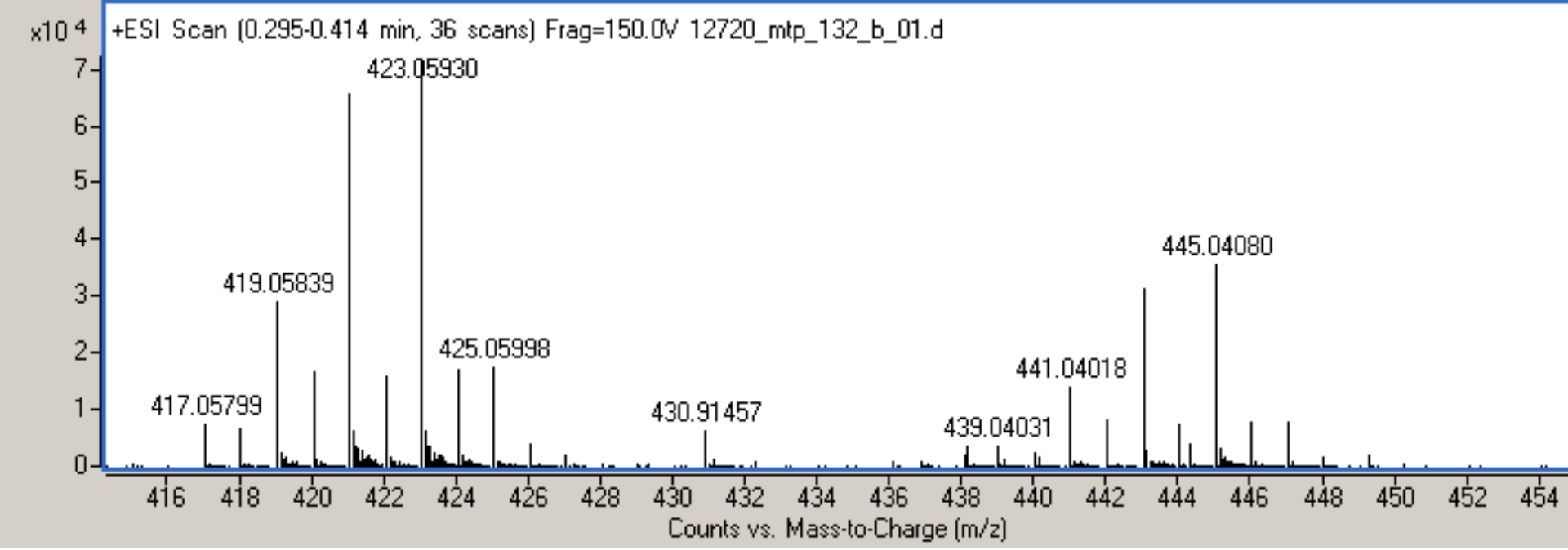
--- End Of Report ---

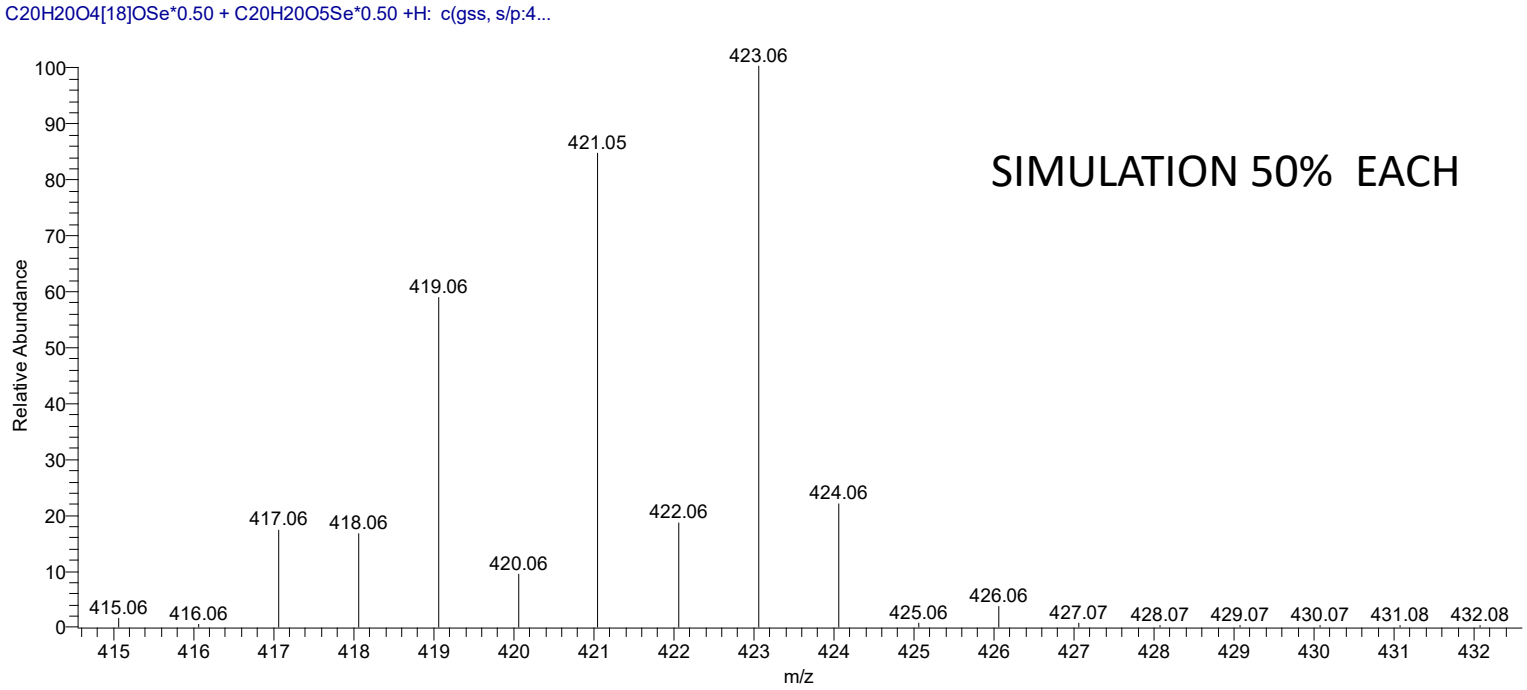
C20H20O4[18]OSe +H: C20 H21 O4 [18]O1 Se1 c(gss, s/p...



C20H20O5Se +H: C20 H21 O5 Se1 c(gss, s/p:40)(Val) Ch...







SIMULATION 50% EACH