

Understanding the mechanism of transition metal-free *anti* addition to alkynes: the selenoboration case

Diego García-López,^a Marc G. Civit,^a Christopher M. Vogels,^b Josep M. Ricart,^a Stephen A. Westcott,^b Elena Fernández^{a*} and Jorge J. Carbó^{a*}

[a] *Department Química Física i Inorgànica University Rovira i Virgili
C/Marcel·lí Domingo s/n, Tarragona, Spain*

[b] *Department of Chemistry and Biochemistry, Mount Allison University,
Sackville, New Brunswick E4L 1G8, Canada*

E-mail: j.carbo@urv.cat ; mariaelena.fernandez@urv.cat

Table of Contents

1. General information.....	
2. Experimental procedures and spectral data.....	
I.- General Procedure A: Synthesis of alkynoates and alkynamides.....	
Spectral data of alkynoates and alkynamidess.....	
II.- General Procedure B: β -selenation of alkynoates and alkynamides.....	
Spectral data of β -selenated products.....	
III.- General Procedure C: Insertion of pinB-SeR into alkynoates and alkynamides	
Spectral data of inserted products	
IV.- General Procedure D: One pot α -selenation of alkynoates	
Spectral data of α -selenated products	
3. ¹ H, ¹³ C, ¹¹ B and ²⁹ Si spectra.....	
4. X-ray Diffraction data for (Z)-3-phenyl-3-(phenylselanyl)acrylate (Z-8)	
5. Kinetic Studies	
6. Additional Figures of the computational study.....	
7. Cartesian coordinates and electronic energy of the computed structures.....	

1. General Information

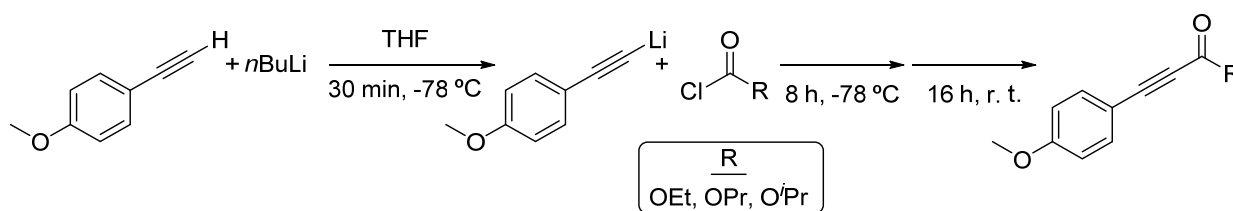
Solvents and reagents: Solvents and reagents were obtained from commercial suppliers and dried and/or purified (if needed) by standard procedures, as specified in "Purification of Laboratory Chemicals".¹ Tetrahydrofuran was dried by distillation from sodium benzophenone ketyl. Phenylselenium pinacolborane (PhSe-Bpin) was synthesized in the laboratory of Prof. Stephen A. Westcott at Mount Allison University, Sackville, NB (Canada).² Tricyclohexylphosphine was purchased from Sigma-Aldrich Inc. All reactions were conducted in oven and flame-dried glassware under an inert atmosphere of argon, using Schlenk-type techniques. *Flash chromatography* was performed on standard silica gel (Merck Kieselgel 60 F254 400-630 mesh). *Thin layer chromatography* was performed on Merck Kieselgel 60 F254 which was developed using standard visualizing agents: UV fluorescence (254 and 366 nm) or potassium permanganate/Δ. *NMR spectra* were recorded at a Varian Goku 400 or a Varian Mercury 400 spectrometer. ¹H NMR and ¹³C{¹H} NMR chemical shifts (δ) are reported in ppm with the solvent resonance as the internal standard (CHCl₃: 7.26 ppm (¹H)) and (CDCl₃: 77.16 ppm (¹³C)). ¹¹B{¹H} NMR chemical shifts (δ) are reported in ppm relative to (CH₃)₂O···BF₃. Data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, hept = heptuplet, br = broad, m = multiplet), coupling constants (Hz) and integration. *High resolution mass spectra (HRMS)* were recorded using a 6210 Time of Flight (TOF) mass spectrometer from Agilent Technologies (Waldbronn, Germany) with an ESI interface and it was performed at the Servei de Recursos Científics i Tècnics (Universitat Rovira I Virgili, Tarragona). GC-MS analyses were performed on a HP6890 gas chromatograph and an Agilent Technologies 5973 Mass selective detector (Waldbronn, Germany) equipped with an achiral capillary column HP-5 (30m, 0.25mm i. d., 0.25μm thickness) using He as the carrier gas. Substrates **1** and **2** were commercially available.

¹ D. D. Perrin, W. L. F. Armarego, *Purification of Laboratory Chemicals*, Pergamon Press, 1988, 3rd Ed.

² a) S. A. Westcott, J. D. Webb, D. I. McIsaac and C. M. Vogels, WO Pat., 2006/089402 A1, 2006;

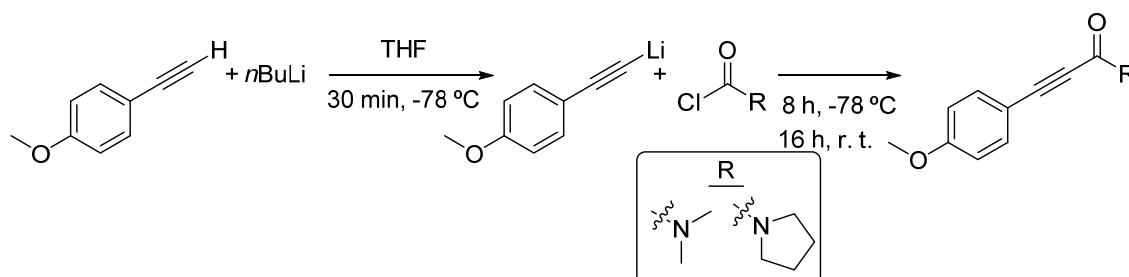
2. Experimental Procedures and Spectral data

I.- General Procedure A: Synthesis of alkynoates



An oven-dried Schlenk equipped with a magnetic stir bar was charged with 2 mmol of the appropriate alkyne and dissolved in 3 mL of THF. At $-78\text{ }^\circ\text{C}$, 1.05 eq. of $n\text{BuLi}$ (1.6M) were added dropwise. After stirring for 30 min, 1 eq. of the chloroformate or carbamoyl chloride was added drop wise. After 8 h stirring the reaction was allowed to rise to room temperature and let it react overnight. The reaction was quenched with 2mL of saturated $\text{Na}_2\text{S}_2\text{O}_4$ and extracted 3 times with 5mL of DCM. All the organic layers were collected and dry over MgSO_4 and evaporated to dryness. The crude residue was analysed by ^1H NMR. Then the products were purified by silica gel flash chromatography.

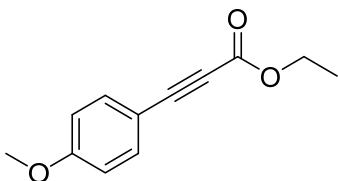
General Procedure A: Synthesis of alkynamides



An oven-dried Schlenk equipped with a magnetic stir bar was charged with 2 mmol of the appropriate alkyne and dissolved in 3 mL of THF. At $-78\text{ }^\circ\text{C}$, 1.05 eq. of $n\text{BuLi}$ (1.6M) were added dropwise. After stirring for 30 min, 1 eq. of carbamoyl chloride was added drop wise. After 8 h stirring the reaction was allowed to rise to room temperature and let it react overnight. The reaction was quenched with 2mL of saturated $\text{Na}_2\text{S}_2\text{O}_4$ and extracted 3 times with 5mL of DCM. All the organic layers were collected and dry over MgSO_4 and evaporated to dryness. The crude residue was analysed by ^1H NMR. Then the products were purified by silica gel flash chromatography.

Spectral data of Alkynoates

Ethyl 3-(4-methoxyphenyl)propiolate



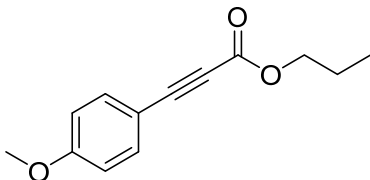
Flash column chromatography yielded **3** (367.6 mg, 90 %) as a colourless oil.

$^1\text{H NMR}$ (CDCl_3 , 400 MHz) δ 7.53 – 7.49 (m, 2H), 6.87 – 6.84 (m, 2H), 4.26 (q, J = 7.1 Hz, 2H), 3.80 (s, 3H), 1.32 (t, J = 7.1 Hz, 3H). ^{13}C $\{^1\text{H}\}$ NMR (CDCl_3 , 100 MHz) δ 161.5, 154.4, 135.0, 114.3, 111.4, 86.9, 80.2, 62.0, 55.4, 14.2.

HRMS (ESI) for $\text{C}_{12}\text{H}_{13}\text{O}_3$ $[\text{M}+\text{H}]^+$: calculated: 205.0865, found: 205.0862.

Characterization data matches literature³

Propyl 3-(4-methoxyphenyl)propiolate

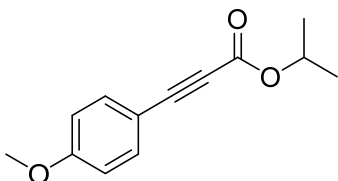


Flash column chromatography yielded **4** (388.5 mg, 89 %) as a yellowish oil.

$^1\text{H NMR}$ (CDCl_3 , 400 MHz) δ 7.55 – 7.51 (m, 2H), 6.89 – 6.85 (m, 2H), 4.17 (t, J = 6.8 Hz, 2H), 3.82 (s, 3H), 1.77 – 1.68 (m, 2H), 0.98 (t, J = 7.4 Hz, 3H). ^{13}C $\{^1\text{H}\}$ NMR (CDCl_3 , 100 MHz) δ 161.5, 154.6, 135.0, 114.3, 111.4, 87.0, 80.2, 67.6, 55.5, 22.0, 10.5.

HRMS (ESI) for $\text{C}_{13}\text{H}_{15}\text{O}_3$ $[\text{M}+\text{H}]^+$: calculated: 219.1021, found: 219.1018.

Isopropyl 3-(4-methoxyphenyl)propiolate



Flash column chromatography yielded **5** (379.8 mg, 87 %) as a white solid.

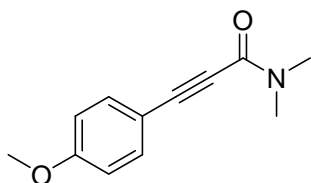
$^1\text{H NMR}$ (CDCl_3 , 400 MHz) δ 7.56 – 7.52 (m, 2H), 6.89 – 6.86 (m, 2H), 5.15 (hept, J = 6.3 Hz, 1H), 3.83 (s, 3H), 1.33 (d, J = 6.3 Hz, 6H). ^{13}C $\{^1\text{H}\}$ NMR (CDCl_3 , 100 MHz) δ 161.5, 154.1, 135.0, 114.4, 111.6, 86.6, 80.6, 69.9, 55.5, 21.9.

HRMS (ESI) for $\text{C}_{13}\text{H}_{15}\text{O}_3$ $[\text{M}+\text{H}]^+$: calculated: 219.1021, found: 219.1017.

³ P. R. Andrews, R. I. Brinkworth, A. C. Partridge, J. A. Reiss, *Aus. J. Chem.* 1988, **41**, 1717.

Spectral data of Alkynamides

3-(4-methoxyphenyl)-N,N-dimethylpropiolamide

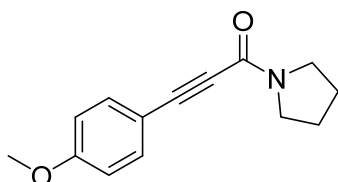


Flash column chromatography yielded **6** (281.1 mg, 92 %) as a colourless oil.

$^1\text{H NMR}$ (CDCl_3 , 400 MHz) δ 7.54 – 7.43 (m, 2H), 6.93 – 6.80 (m, 2H), 3.83 (s, 3H), 3.28 (s, 3H), 3.02 (s, 3H). ^{13}C $\{^1\text{H}\}$ NMR (CDCl_3 , 100 MHz) δ 161.0, 155.1, 134.2, 114.3, 112.6, 90.8, 81.0, 77.2, 55.5, 38.6, 34.3.

HRMS (ESI) for $\text{C}_{12}\text{H}_{14}\text{NO}_2$ $[\text{M}+\text{H}]^+$: calculated: 204.1025, found: 204.1023.

3-(4-methoxyphenyl)-1-(pyrrolidin-1-yl)prop-2-yn-1-one

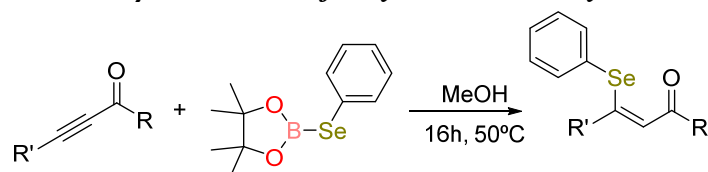


Flash column chromatography yielded **7** (330.3 mg, 96 %) as a colourless oil.

$^1\text{H NMR}$ (CDCl_3 , 400 MHz) δ 7.52 – 7.45 (m, 2H), 6.90 – 6.84 (m, 2H), 3.83 (s, 3H), 3.76 – 3.68 (m, 2H), 3.56 – 3.49 (m, 2H), 2.02 – 1.90 (m, 4H). ^{13}C $\{^1\text{H}\}$ NMR (CDCl_3 , 100 MHz) δ 161.0, 152.7, 134.3, 114.3, 112.7, 89.3, 82.1, 77.2, 55.5, 48.3, 45.5, 25.6, 24.9.

HRMS (ESI) for $\text{C}_{14}\text{H}_{15}\text{NNaO}_2$ $[\text{M}+\text{Na}]^+$: calculated: 252.1000, found: 252.1001.

II.- General Procedure B: β -selenation of alkynoates and alkynamides

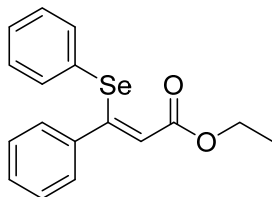


R'	R
Ph	OEt
Hex	OMe
<i>p</i> -MeOPh	OEt, OPr, O <i>i</i> Pr

In the glove-box, an oven-dried resealable vial equipped with a magnetic stir bar was charged with 0.2 mmol of the alkynoate or ynamide compound. Then, the vial was charged with 1.1 eq. of pinB-SePh solved in 0.15mL of dry MeOH. After 16 h at 50°C the reaction was evaporated to dryness. The crude residue was analysed by GC-MS and $^1\text{H NMR}$ using naphthalene as an internal standard. Then the products were purified by silica gel flash chromatography.

Spectral data of β -selenated products

Ethyl (Z)-3-phenyl-3-(phenylselanyl)acrylate

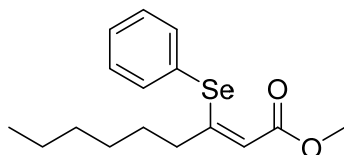


Flash column chromatography yielded **Z-8** (49.0 mg, 74 %) as a yellowish solid.

$^1\text{H NMR}$ (CDCl_3 , 400 MHz) δ 7.25 – 7.20 (m, 2H), 7.11 – 6.96 (m, 8H), 6.32 (s, 1H), 4.30 (q, $J = 7.1$ Hz, 2H), 1.35 (t, $J = 7.1$ Hz, 3H). ^{13}C $\{^1\text{H}\}$ NMR (CDCl_3 , 100 MHz) δ 166.9, 161.4, 139.2, 136.4, 129.3, 128.7, 128.5, 128.1, 128.0, 127.6, 117.1, 60.7, 14.5.

HRMS (ESI) for $\text{C}_{17}\text{H}_{17}\text{O}_2\text{Se}$ $[\text{M}+\text{H}]^+$: calculated: 333.0394, found: 333.0391.

Methyl (Z)-3-(phenylselanyl)non-2-enoate

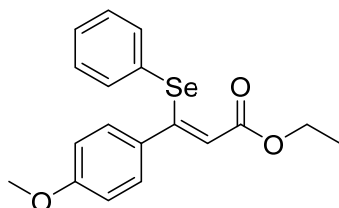


Flash column chromatography yielded **Z-9** (51.4 mg, 79 %) as a yellowish oil.

$^1\text{H NMR}$ (CDCl_3 , 400 MHz) δ 7.69 – 7.65 (m, 2H), 7.43 – 7.38 (m, 1H), 7.36 – 7.32 (m, 2H), 6.16 (s, 1H), 3.76 (s, 3H), 2.17 – 2.13 (m, 2H), 1.34 – 1.26 (m, 2H), 1.17 – 1.10 (m, 2H), 1.05 – 0.97 (m, 4H), 0.79 (t, $J = 7.3$ Hz, 3H). ^{13}C $\{^1\text{H}\}$ NMR (CDCl_3 , 100 MHz) δ 167.7, 164.4, 137.7, 129.3, 129.2, 127.6, 113.2, 51.5, 37.9, 31.4, 29.8, 28.5, 22.5, 14.1.

HRMS (ESI) for $\text{C}_{16}\text{H}_{23}\text{O}_2\text{Se}$ $[\text{M}+\text{H}]^+$: calculated: 327.0863, found: 327.0855.

Ethyl (Z)-3-(4-methoxyphenyl)-3-(phenylselanyl)acrylate

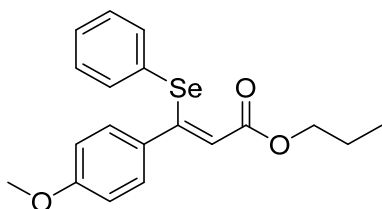


Flash column chromatography yielded **Z-10** (52.0 mg, 72 %) as a yellowish oil.

$^1\text{H NMR}$ (CDCl_3 , 400 MHz) δ 7.24 – 7.21 (m, 2H), 7.11 – 7.07 (m, 1H), 7.04 – 6.95 (m, 4H), 6.58 – 6.54 (m, 2H), 6.30 (s, 1H), 4.28 (q, $J = 7.1$ Hz, 2H), 3.68 (s, 3H), 1.34 (t, $J = 7.1$ Hz, 3H). ^{13}C $\{^1\text{H}\}$ NMR (CDCl_3 , 100 MHz) δ 166.9, 161.0, 159.6, 136.1, 131.8, 130.2, 129.7, 128.5, 127.9, 116.7, 113.0, 60.6, 55.3, 14.5.

HRMS (ESI) for $\text{C}_{18}\text{H}_{19}\text{O}_3\text{Se}$ $[\text{M}+\text{H}]^+$: calculated: 363.0499, found: 363.0495.

Propyl (Z)-3-(4-methoxyphenyl)-3-(phenylselanyl)acrylate

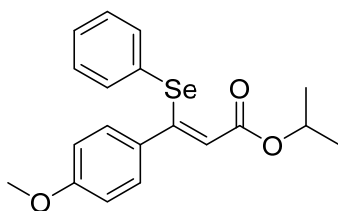


Flash column chromatography yielded **Z-11** (54.0 mg, 72 %) as a yellowish oil.

$^1\text{H NMR}$ (CDCl_3 , 400 MHz) δ 7.24 – 7.22 (m, 2H), 7.11 – 7.07 (m, 1H), 7.03 – 6.95 (m, 4H), 6.57 – 6.54 (m, 2H), 6.31 (s, 1H), 4.19 (t, $J = 6.7$ Hz, 2H), 3.68 (s, 3H), 1.78 – 1.69 (m, 2H), 0.99 (t, $J = 7.4$ Hz, 3H). ^{13}C $\{^1\text{H}\}$ NMR (CDCl_3 , 100 MHz) δ 167.0, 160.9, 159.5, 136.1, 131.7, 130.2, 129.7, 128.5, 127.8, 116.7, 113.0, 66.2, 55.3, 22.2, 10.6.

HRMS (ESI) for $\text{C}_{19}\text{H}_{21}\text{O}_3\text{Se}$ $[\text{M}+\text{H}]^+$: calculated: 377.0656, found: 377.0651.

Isopropyl (Z)-3-(4-methoxyphenyl)-3-(phenylselanyl)acrylate

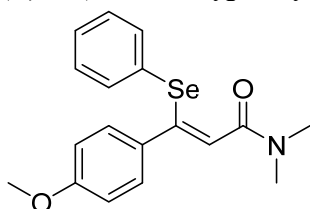


Flash column chromatography yielded **Z-12** (51.8 mg, 69 %) as a yellowish oil.

$^1\text{H NMR}$ (CDCl_3 , 400 MHz) δ 7.23 – 7.21 (m, 2H), 7.11 – 7.07 (m, 1H), 7.03 – 6.95 (m, 4H), 6.57 – 6.53 (m, 2H), 6.27 (s, 1H), 5.17 (hept, $J = 6.2$ Hz, 1H), 3.67 (s, 3H), 1.32 (d, $J = 6.3$ Hz, 6H). ^{13}C $\{^1\text{H}\}$ NMR (CDCl_3 , 100 MHz) δ 166.5, 160.6, 159.5, 136.1, 131.8, 130.2, 129.7, 128.5, 127.8, 117.2, 113.0, 67.9, 55.3, 22.2.

HRMS (ESI) for $\text{C}_{19}\text{H}_{21}\text{O}_3\text{Se}$ $[\text{M}+\text{H}]^+$: calculated: 377.0656, found: 377.0648.

(Z)-3-(4-methoxyphenyl)-N,N-dimethyl-3-(phenylselanyl)acrylamide

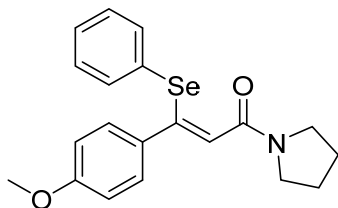


Flash column chromatography yielded **Z-13** (54.8 mg, 76 %) as a colourless oil.

$^1\text{H NMR}$ (CDCl_3 , 400 MHz) δ 7.26 – 7.20 (m, 2H), 7.09 – 6.95 (m, 5H), 6.60 (s, 1H), 6.58 – 6.54 (m, 2H), 3.68 (s, 3H), 3.08 (brs, 6H). ^{13}C $\{^1\text{H}\}$ NMR (CDCl_3 , 100 MHz) δ 167.1, 159.3, 156.1, 135.9, 132.6, 130.8, 130.2, 128.3, 127.4, 117.1, 113.0, 55.3, 24.9.

HRMS (ESI) for $\text{C}_{18}\text{H}_{20}\text{NO}_2\text{Se}$ $[\text{M}+\text{H}]^+$: calculated: 362.0659, found: 362.0651.

(Z)-3-(4-methoxyphenyl)-3-(phenylselanyl)-1-(pyrrolidin-1-yl)prop-2-en-1-one



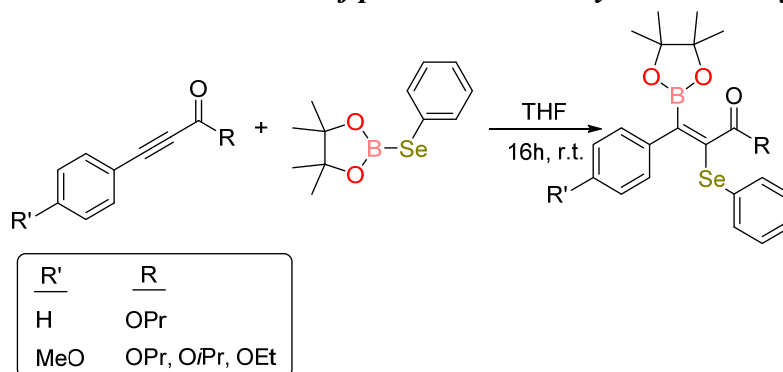
Flash column chromatography yielded **Z-14** (49.2 mg, 69 %) as a colourless oil.

$^1\text{H NMR}$ (CDCl_3 , 400 MHz) δ 7.25 – 7.20 (m, 2H), 7.08 – 7.03 (m, 1H), 7.01 – 6.93 (m, 4H), 6.58 – 6.52 (m, 2H), 6.45 (s, 1H), 3.67 (s, 3H), 3.55 (brs, 4H), 1.93 (brs, 4H).

$^{13}\text{C } \{^1\text{H}\}$ NMR (CDCl_3 , 100 MHz) δ 165.3, 159.2, 156.9, 136.2, 132.6, 130.9, 130.2, 128.3, 127.5, 117.6, 112.9, 77.2, 55.3, 46.4 (brs), 25.7 (brs).

HRMS (ESI) for $\text{C}_{20}\text{H}_{22}\text{NO}_2\text{Se}$ $[\text{M}+\text{H}]^+$: calculated: 388.0816, found: 388.0811.

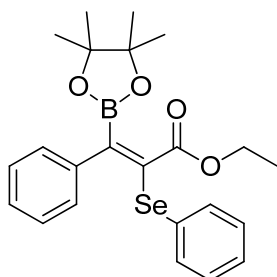
III.- General Procedure C: Insertion of pinB-SeR into alkynoates or alkynamides



In the glove-box, an oven-dried resealable vial equipped with a magnetic stir bar was charged with 0.2 mmol of the alkynoate or ynamide compound. Then, 15mol% of tricyclohexylphosphine in 0.15ml of dry THF was added. After stirring in the glove-box for 5 min the vial was charged with 1.1 eq. of pinB-SePh. After 16 h at room temperature the reaction was evaporated to dryness. The crude residue was analysed by GC-MS and $^1\text{H NMR}$ using naphthalene as an internal standard. Then the products were purified by silica gel flash chromatography.

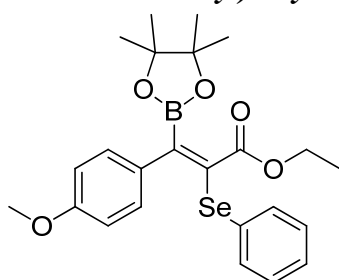
Spectral data of inserted products

(Z)-3-phenyl-2-(phenylselanyl)-3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)acrylate. No isolated product **15**.



$^1\text{H NMR}$ of main signals (CDCl_3 , 400 MHz) δ 3.97 (q, $J = 7.1$ Hz, 2H), 1.26 (s, 12H), 0.94 (t, $J = 7.2$ Hz, 3H).

Ethyl (Z)-3-(4-methoxyphenyl)-2-(phenylselanyl)-3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)acrylate



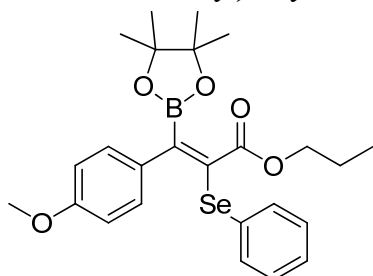
Flash column chromatography yielded **16** (4.9 mg, 5 %) as a yellowish oil.

$^1\text{H NMR}$ (CDCl_3 , 400 MHz) δ 7.29 – 7.35 (m, 3H), 7.19 – 7.16 (m, 3H), 6.92 – 6.88 (m, 2H), 4.01 (q, $J = 7.2$ Hz, 2H), 3.82 (s, 3H), 1.29 (s, 12H), 0.94 (t, $J = 7.1$ Hz, 3H).

^{13}C $\{^1\text{H}\}$ NMR (CDCl_3 , 100 MHz) δ 169.4, 159.8, 134.5, 132.9, 131.6, 131.0, 129.9, 129.0, 127.2, 113.5, 83.9, 62.8, 55.4, 25.0, 13.7. $^{11}\text{B NMR}$ (128.3 MHz, CDCl_3) δ 28.3.

HRMS (ESI) for $\text{C}_{24}\text{H}_{30}\text{BO}_5\text{Se}$ $[\text{M}+\text{H}]^+$: calculated: 489.1352, found: 489.1358.

Propyl (Z)-3-(4-methoxyphenyl)-2-(phenylselanyl)-3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)acrylate



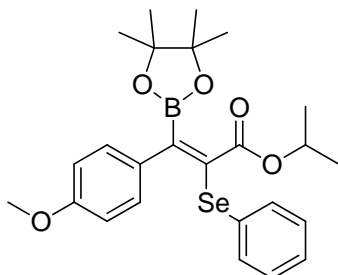
Flash column chromatography yielded **17** (23.1 mg, 23 %) as a yellowish oil.

$^1\text{H NMR}$ (CDCl_3 , 400 MHz) δ 7.40 – 7.33 (m, 3H), 7.17 – 7.14 (m, 3H), 6.91 – 6.88 (m, 2H), 3.93 (t, $J = 6.7$ Hz, 2H), 3.82 (s, 3H), 1.41 – 1.32 (m, 2H), 1.29 (s, 12H), 0.70 (t, $J = 7.4$ Hz, 3H). ^{13}C $\{^1\text{H}\}$ NMR (CDCl_3 , 100 MHz) δ 169.9, 159.8, 134.3, 132.3,

131.5, 131.2, 129.9, 129.0, 128.3 (bs), 127.0, 113.4, 83.8, 68.6, 55.3, 25.0, 21.6, 10.3.
 ^{11}B NMR (128.3 MHz, CDCl_3) δ 27.9.

HRMS (ESI) for $\text{C}_{50}\text{H}_{62}\text{B}_2\text{NaO}_{10}\text{Se}_2$ [$2\text{M}+\text{Na}$] $^+$: calculated: 1027.2757, found: 1027.2789.

Isopropyl (Z)-3-(4-methoxyphenyl)-2-(phenylselanyl)-3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)acrylate

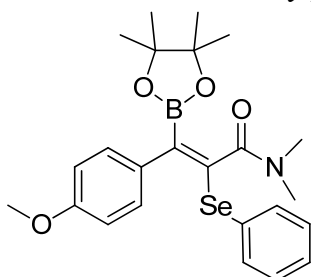


Flash column chromatography yielded **18** (31.1 mg, 31 %) as a yellowish oil.

^1H NMR (CDCl_3 , 400 MHz) δ 7.41 – 7.36 (m, 3H), 7.18 – 7.15 (m, 3H), 6.92 – 6.89 (m, 2H), 4.85 (hept, J = 6.3 Hz, 1H), 3.82 (s, 3H), 1.29 (s, 12H), 0.95 (d, J = 6.3 Hz, 6H). ^{13}C { ^1H } NMR (CDCl_3 , 100 MHz) δ 169.6, 159.9, 132.6, 131.5, 131.4, 130.0, 129.0, 128.3, 127.1, 113.4, 83.6, 71.3, 55.3, 25.0, 21.3. ^{11}B NMR (128.3 MHz, CDCl_3) δ 27.8.

HRMS (ESI) for $\text{C}_{25}\text{H}_{31}\text{BNaO}_5\text{Se}$ [$\text{M}+\text{Na}$] $^+$: calculated: 525.1327, found: 525.1332.

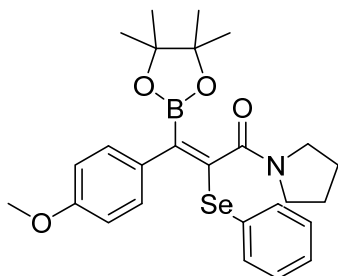
(Z)-3-(4-methoxyphenyl)-N,N-dimethyl-2-(phenylselanyl)-3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)acrylamide



No Isolated Product **23**

^1H NMR (CDCl_3 , 400 MHz) δ 7.25 – 7.21 (m, 2H), 7.19 – 7.13 (m, 2H), 7.09 – 6.98 (m, 3H), 6.63 – 6.57 (m, 2H), 3.69 (s, 3H), 3.09 (brs, 6H), 1.06 (s, 13H). ^{11}B NMR (128.3 MHz, CDCl_3) δ 27.3.

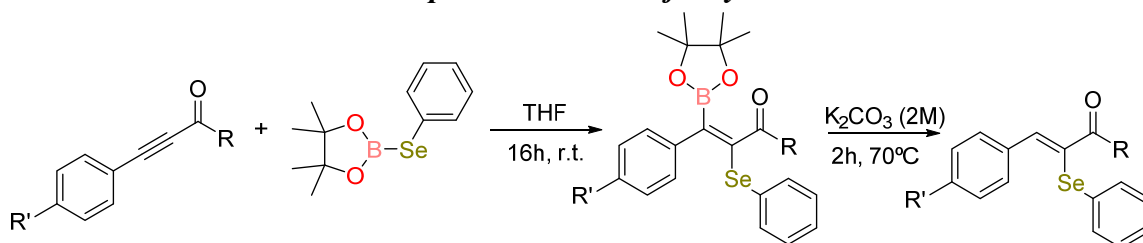
(Z)-3-(4-methoxyphenyl)-N,N-dimethyl-2-(phenylselanyl)-3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)acrylamide



No Isolated Product **24**

¹H NMR (CDCl₃, 400 MHz) δ 7.24 – 7.19 (m, 2H), 7.14 – 7.09 (m, 2H), 7.08 – 6.95 (m, 3H), 6.60 – 6.54 (m, 2H), 3.68 (s, 3H), 3.56 (brs, 4H), 1.92 (brs, 4H), 1.04 (s, 12H).

IV.- General Procedure D: One pot α-selenation of alkynoates

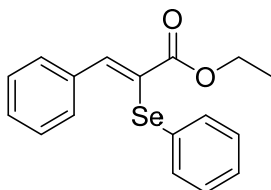


R'	R
H	OPr
MeO	OPr, O I Pr, OEt

In the glove-box, an oven-dried resealable vial equipped with a magnetic stir bar was charged with 0.2 mmol of the alkynoate or ynamide compound. Then, 15mol% of tricyclohexylphosphine in 0.15ml of dry THF was added. After stirring in the glove-box for 5 min the vial was charged with 1.1 eq. of pinB-SePh. After 16 h at room temperature the reaction was evaporated to dryness. The crude residue was solved in 2 mL of THF and 0.2 mL of K₂CO₃ (2M) water solution was added dropwise. The reaction was heated to reflux for 2h. Then the reaction was extracted with DCM and filtered through a pad of Celite and MgSO₄. The solvent was removed and the residue was analysed by GC-MS and ¹H NMR using naphthalene as an internal standard. Then the products were purified by silica gel flash chromatography.

Spectral data of α-selenated products

Ethyl (Z)-3-phenyl-2-(phenylselanyl)acrylate

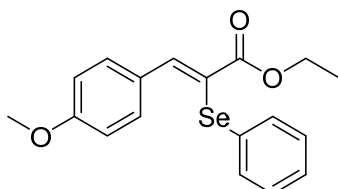


Flash column chromatography yielded **19** (14.6 mg, 22 %) as a yellowish oil.

¹H NMR (CDCl₃, 400 MHz) δ 8.15 (s, 1H), 7.66 – 7.64 (m, 2H), 7.42 – 7.37 (m, 5H), 7.22 – 7.19 (m, 3H), 4.07 (q, J = 7.1 Hz, 2H), 1.04 (t, J = 7.1 Hz, 3H). **¹³C {¹H} NMR** (CDCl₃, 100 MHz) δ 166.8, 145.0, 138.4, 135.3, 134.4, 131.9, 130.4, 129.2, 128.3, 127.2, 124.5, 62.0, 13.9.

HRMS (ESI) for C₁₇H₁₇O₂Se [M+H]⁺: calculated: 333.0394, found: 333.0392.

Ethyl (Z)-3-(4-methoxyphenyl)-2-(phenylselanyl)acrylate

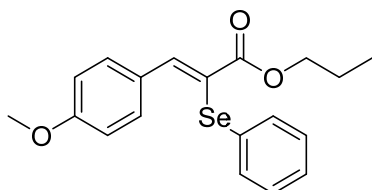


Flash column chromatography yielded **20** (15.2 mg, 21 %) as a yellowish oil.

¹H NMR (CDCl₃, 400 MHz) δ 8.17 (s, 1H), 7.75 – 7.72 (m, 2H), 7.40 – 7.37 (m, 2H), 7.22 – 7.18 (m, 3H), 6.93 – 6.90 (m, 2H), 4.08 (q, J = 7.1 Hz, 2H), 3.83 (s, 3H), 1.06 (t, J = 7.1 Hz, 3H). **¹³C {¹H} NMR** (CDCl₃, 100 MHz) δ 167.0, 161.0, 145.8, 132.7, 131.3, 129.8, 129.2, 127.7, 127.0, 113.8, 70.7, 61.9, 55.5, 14.0.

HRMS (ESI) for C₁₈H₁₉O₃Se [M+H]⁺: calculated: 363.0499, found: 363.0507

Propyl (Z)-3-(4-methoxyphenyl)-2-(phenylselanyl)acrylate

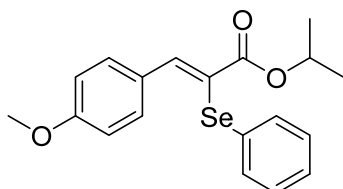


Flash column chromatography yielded **21** (9.7 mg, 13 %) as a yellowish oil.

¹H NMR (CDCl₃, 400 MHz) δ 8.20 (s, 1H), 7.77 – 7.73 (m, 2H), 7.39 – 7.36 (m, 2H), 7.22 – 7.18 (m, 3H), 6.93 – 6.89 (m, 2H), 4.00 (t, J = 6.7 Hz, 2H), 3.83 (s, 3H), 1.53 – 1.44 (m, 2H), 0.81 (t, J = 7.4 Hz, 3H). **¹³C {¹H} NMR** (CDCl₃, 100 MHz) δ 167.1, 161.0, 146.2, 136.0, 132.7, 131.0, 129.2, 127.7, 126.8, 120.4, 113.8, 67.6, 55.5, 21.9, 10.5.

HRMS (ESI) for C₁₉H₂₁O₃Se [M+H]⁺: calculated: 377.0656, found: 377.0651.

Isopropyl (Z)-3-(4-methoxyphenyl)-2-(phenylselanyl)acrylate



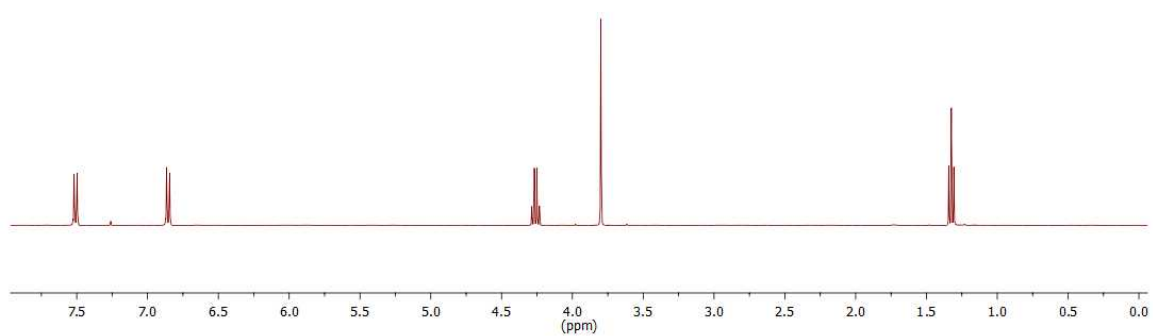
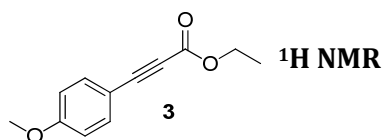
Flash column chromatography yielded **22** (23.3 mg, 31 %) as a yellowish oil.

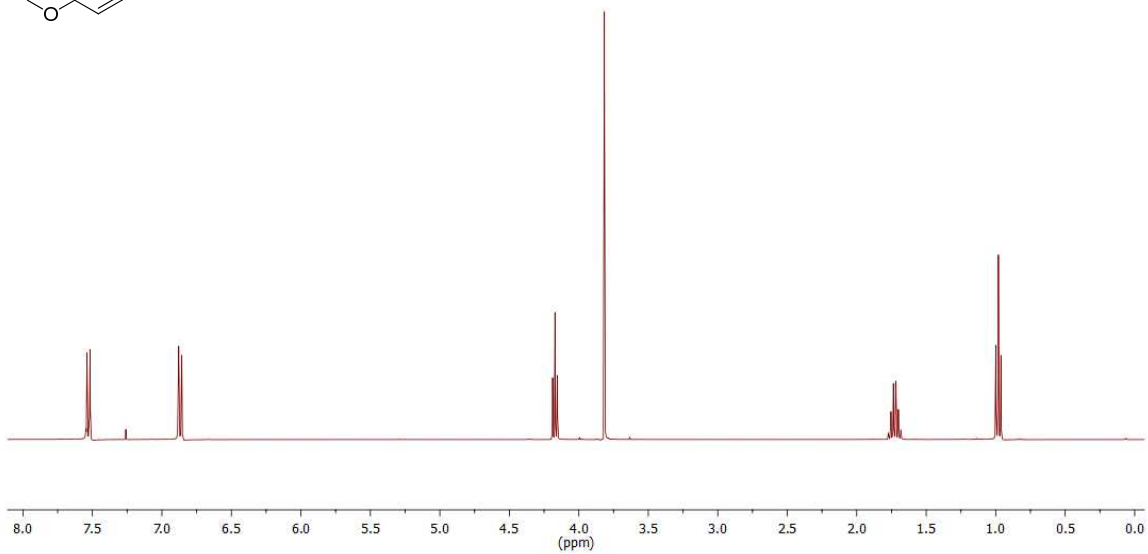
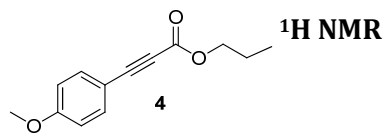
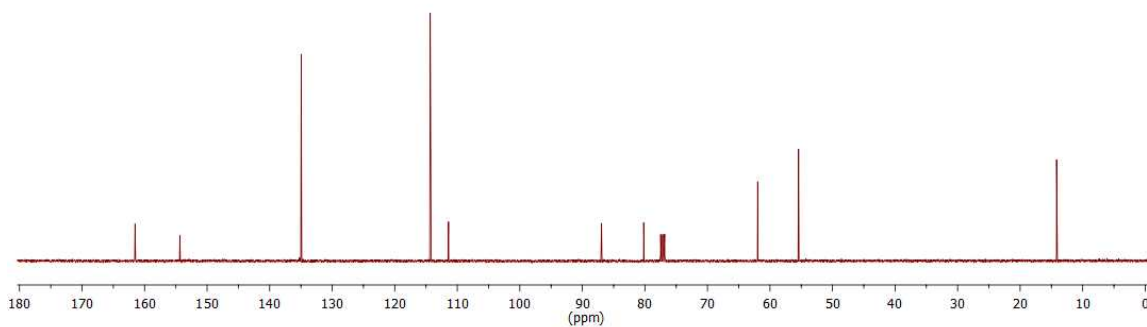
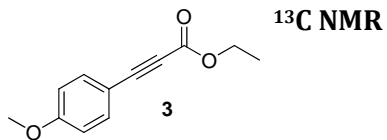
¹H NMR (CDCl₃, 400 MHz) δ 8.15 (s, 1H), 7.73 – 7.70 (m, 2H), 7.40 – 7.37 (m, 2H), 7.23 – 7.17 (m, 3H), 6.94 – 6.90 (m, 2H), 4.91 (hept, J = 6.2 Hz, 1H), 3.84 (s, 3H), 1.04

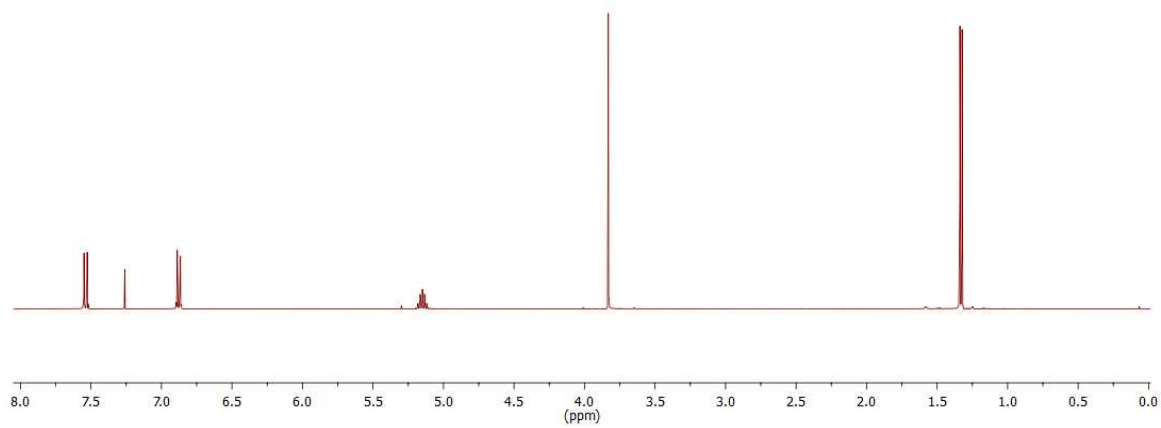
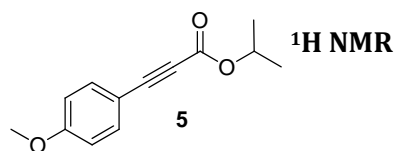
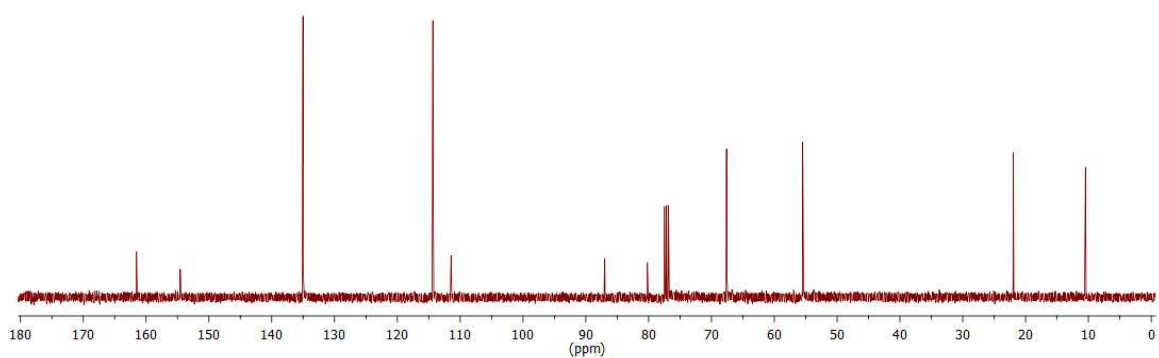
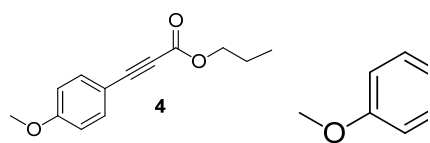
(d, $J = 6.3$ Hz, 6H). ^{13}C $\{^1\text{H}\}$ NMR (CDCl_3 , 100 MHz) δ 166.5, 160.9, 145.3, 132.6, 131.4, 130.2, 129.2, 127.8, 126.9, 121.4, 113.8, 69.5, 55.5, 21.5.

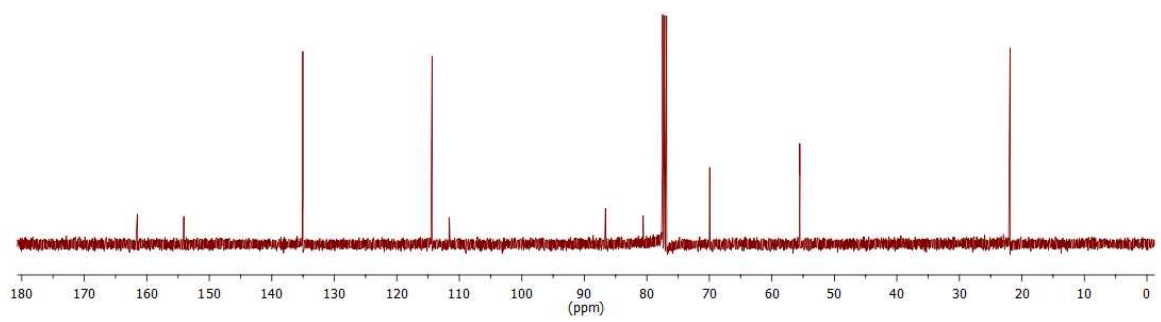
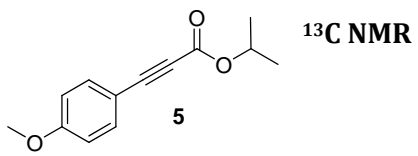
HRMS (ESI) for $\text{C}_{19}\text{H}_{21}\text{O}_3\text{Se}$ $[\text{M}+\text{H}]^+$: calculated: 377.0656, found: 377.0651

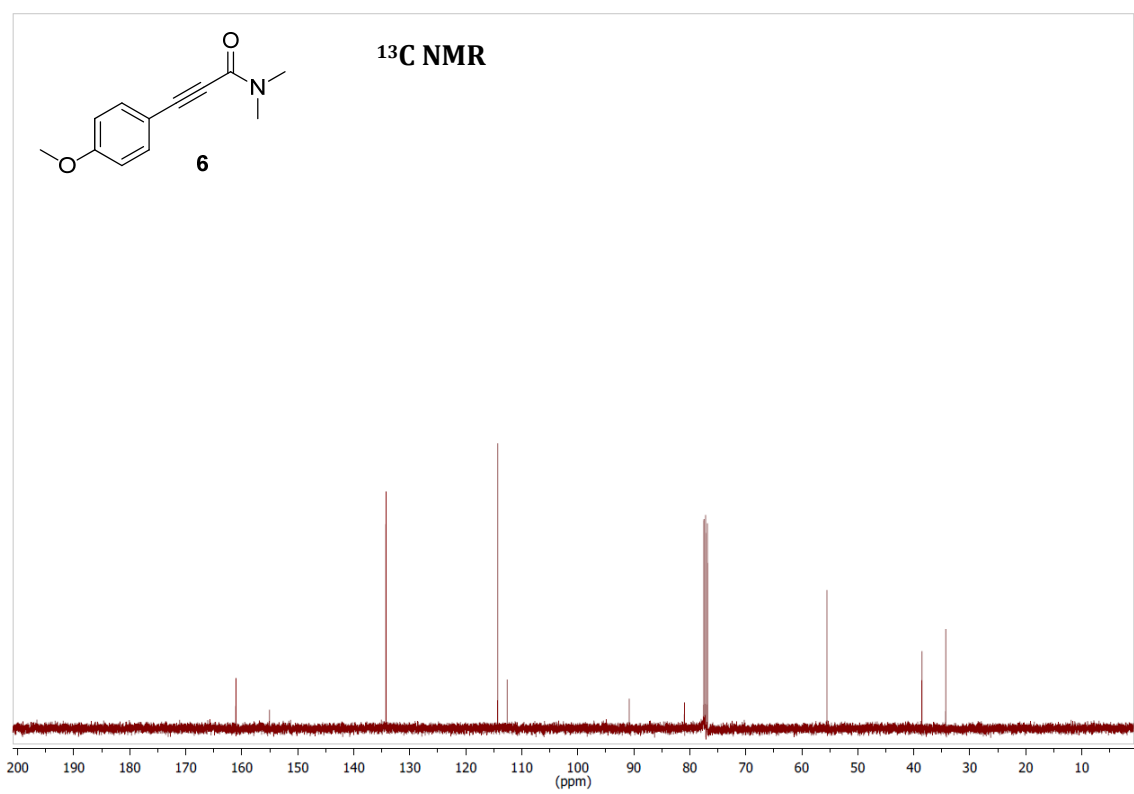
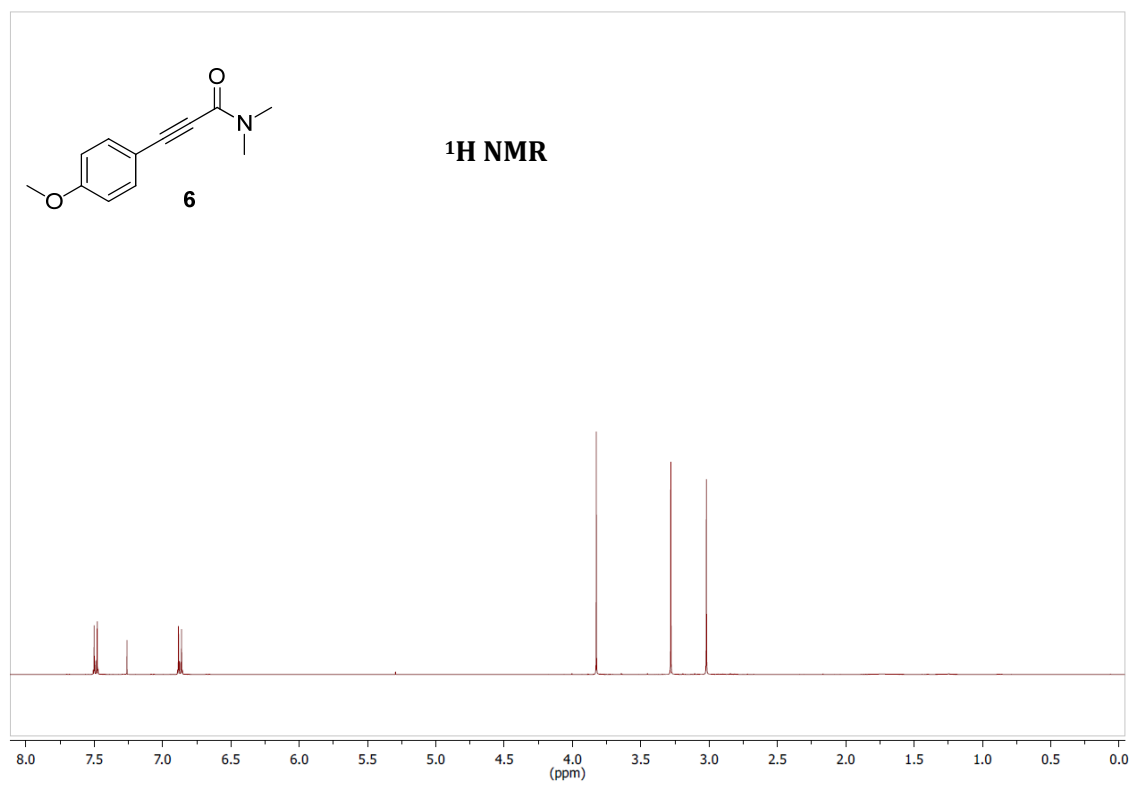
3. ^1H , ^{13}C and ^{11}B spectra

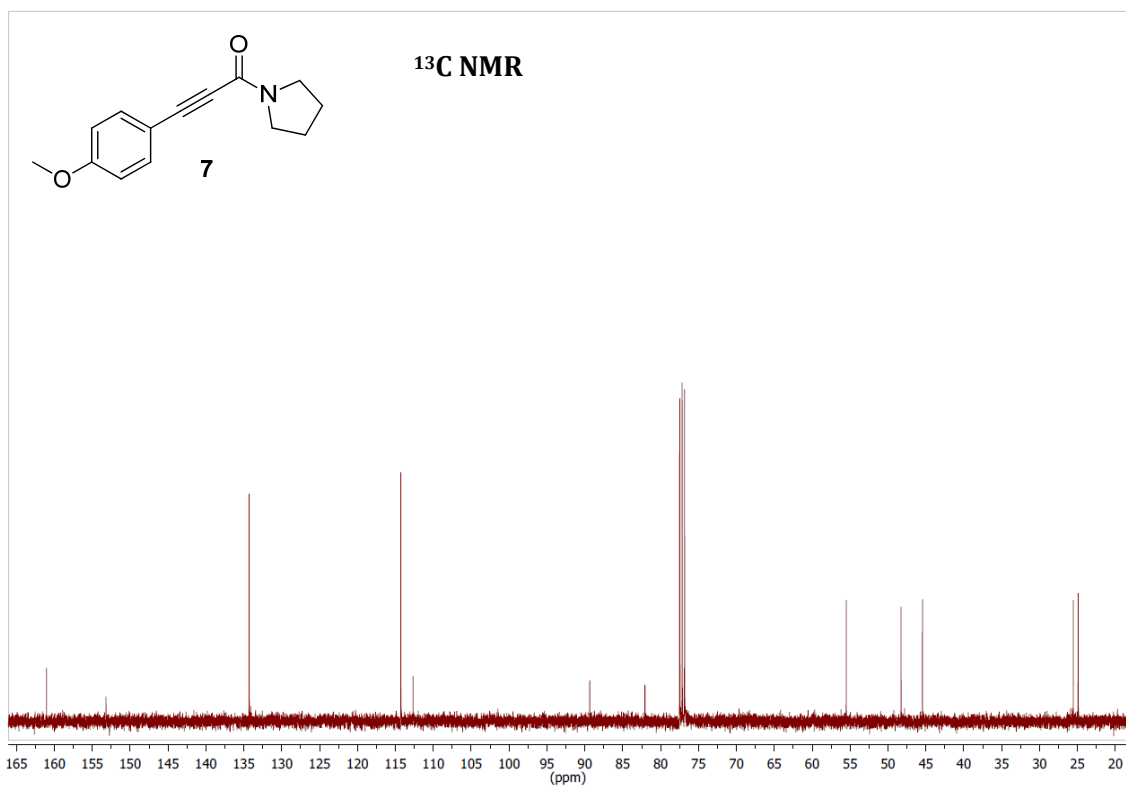
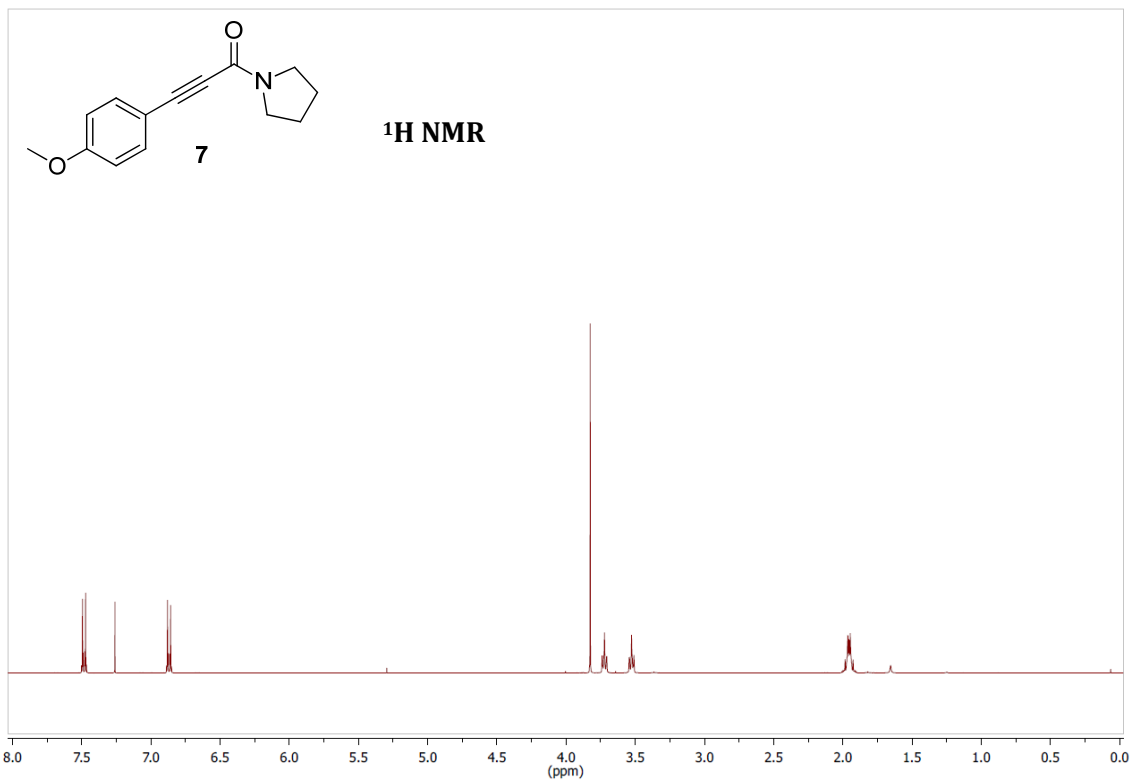


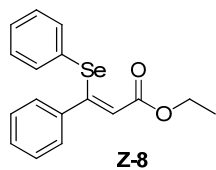




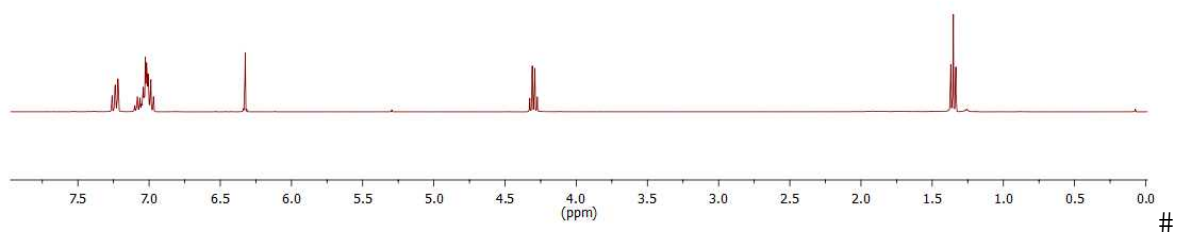




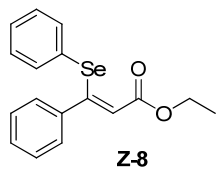




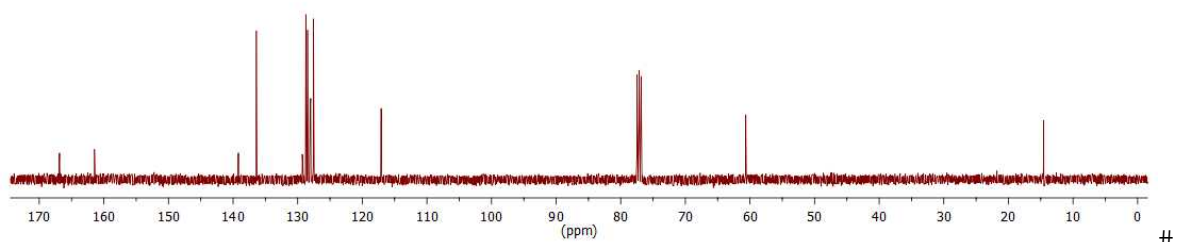
¹H NMR



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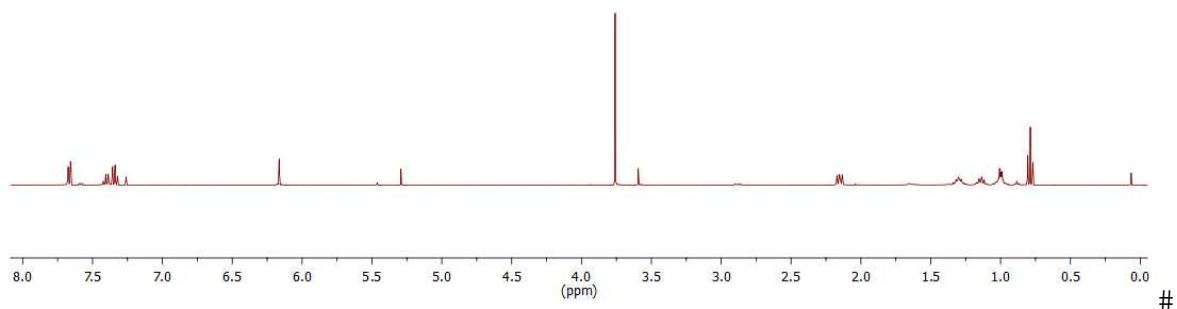
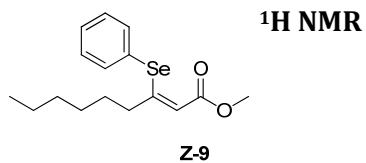


¹³C NMR

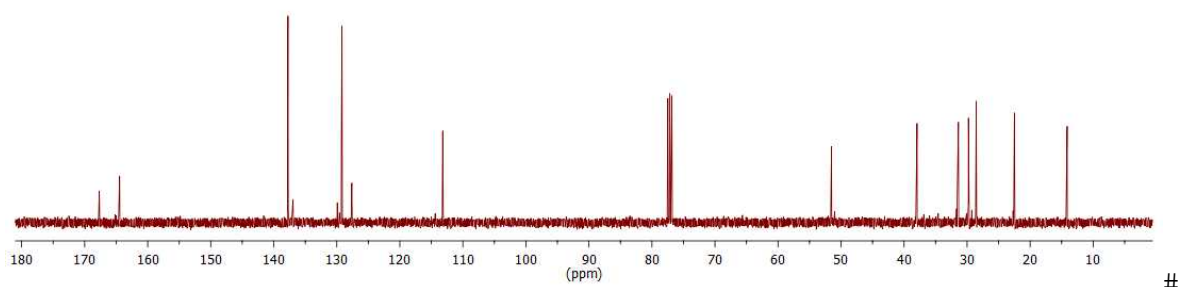
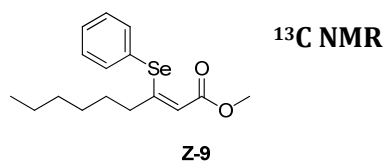


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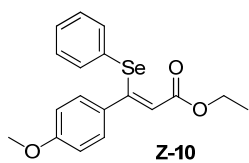
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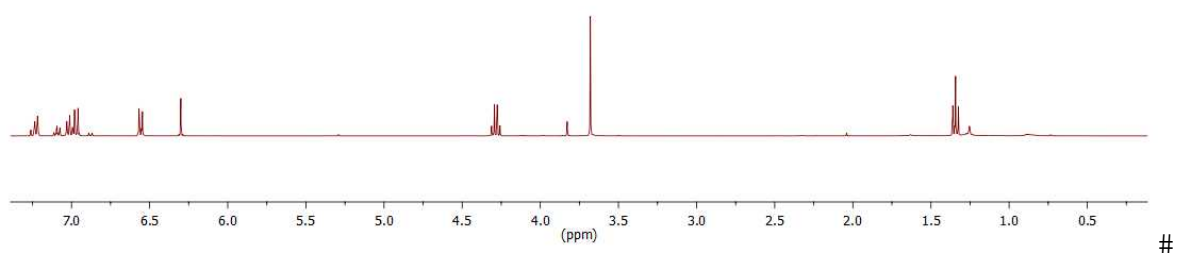
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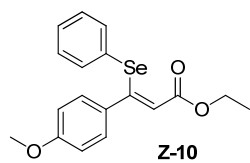
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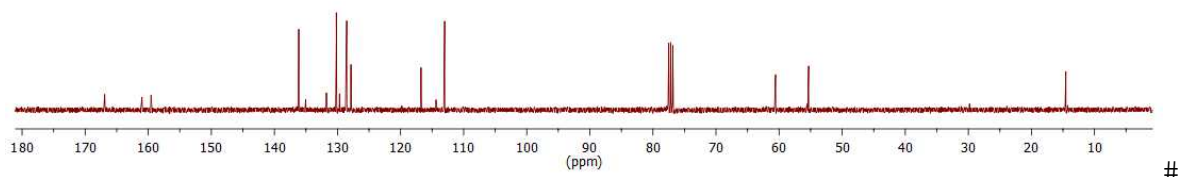
¹H NMR



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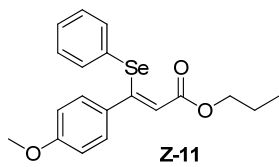
¹³C NMR



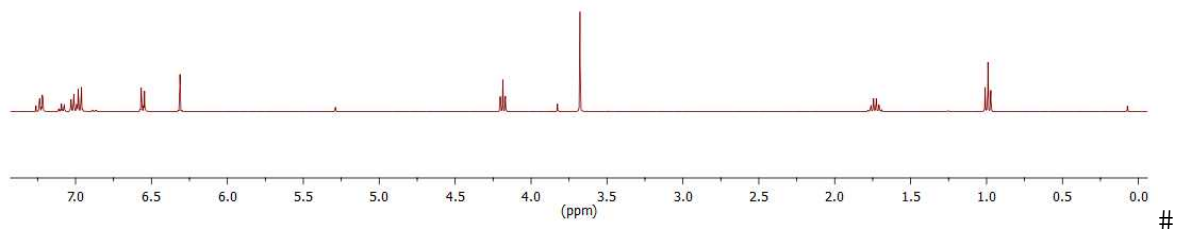
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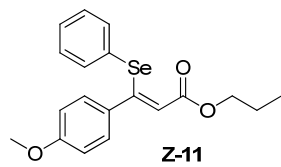
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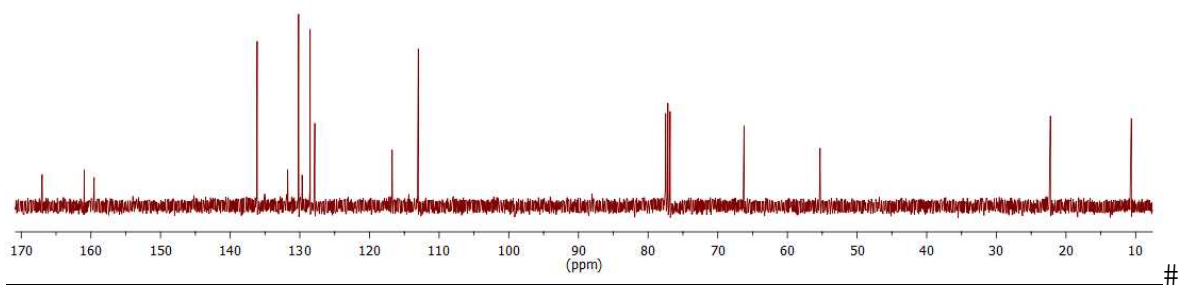
¹H NMR

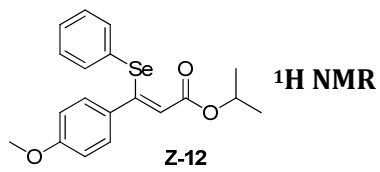


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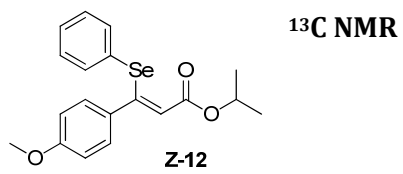
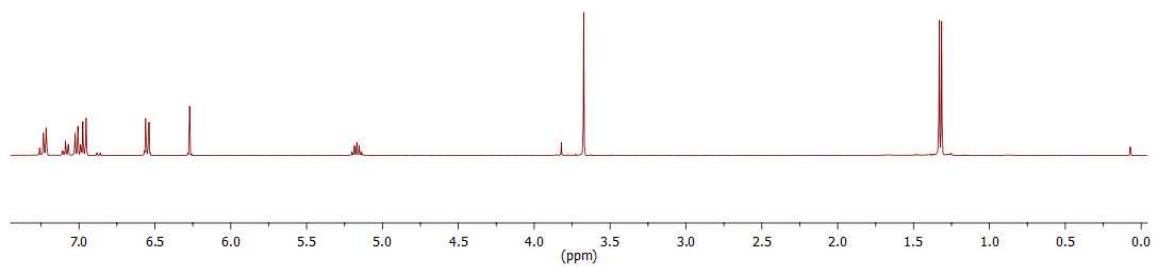


¹³C NMR

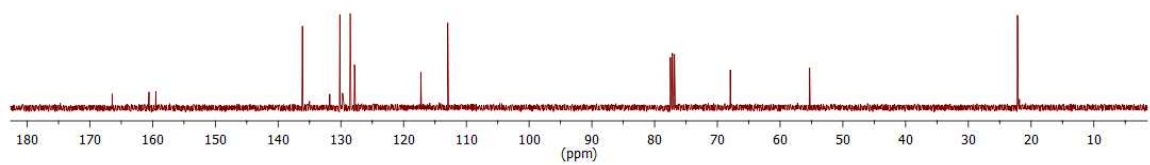


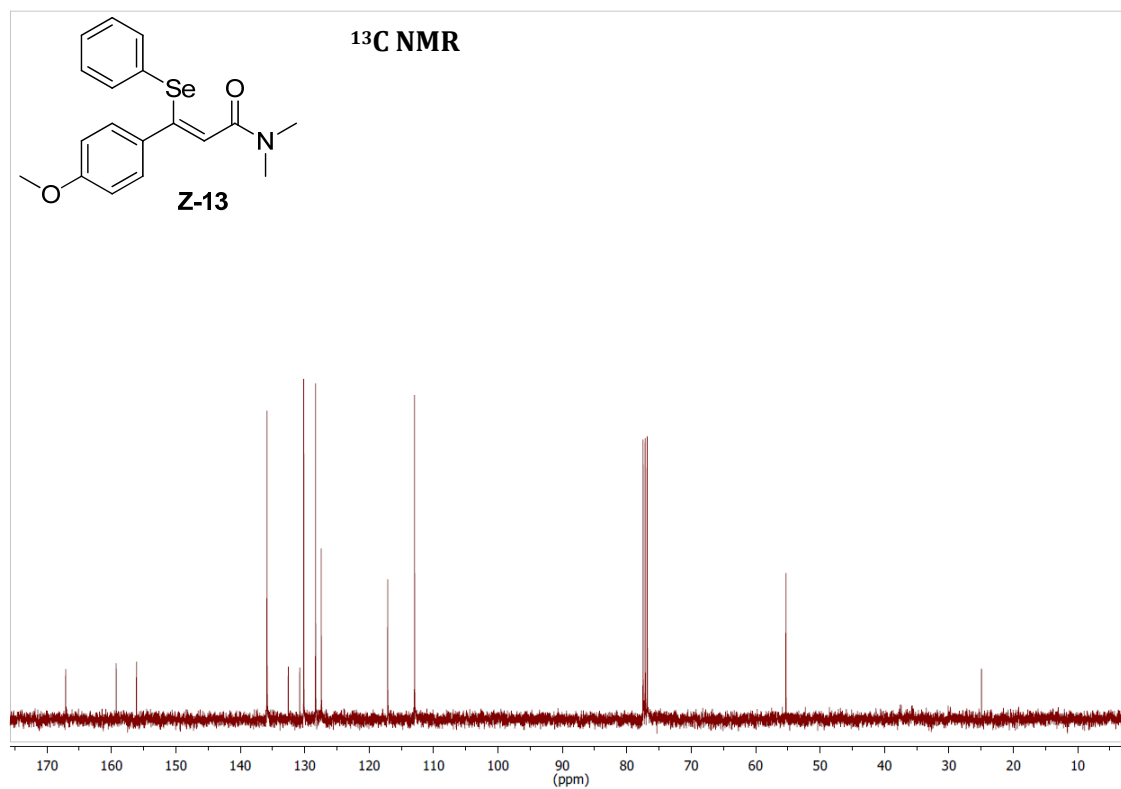
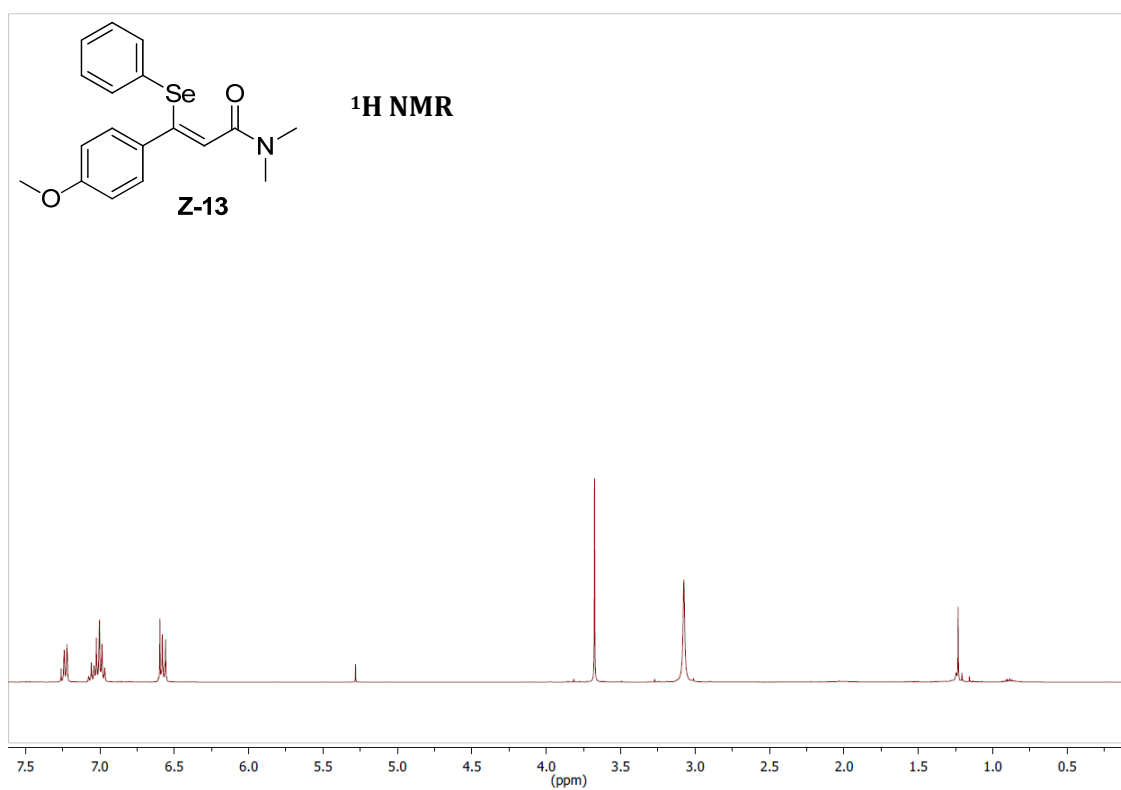


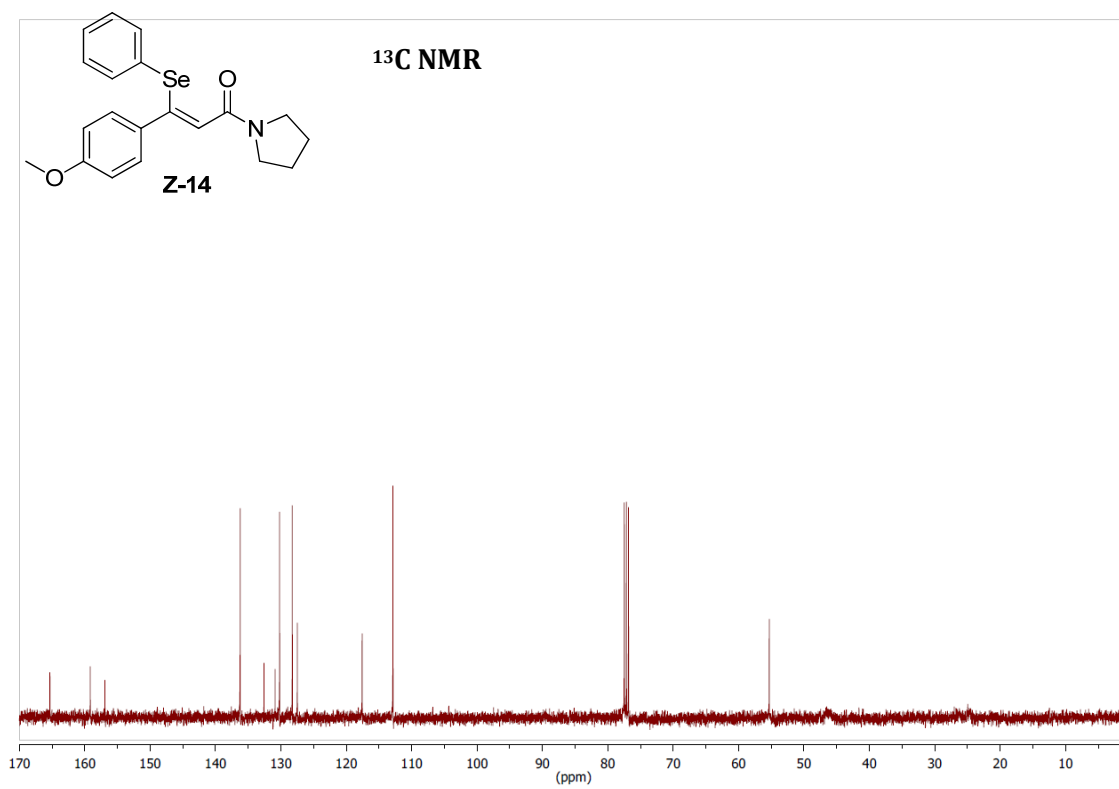
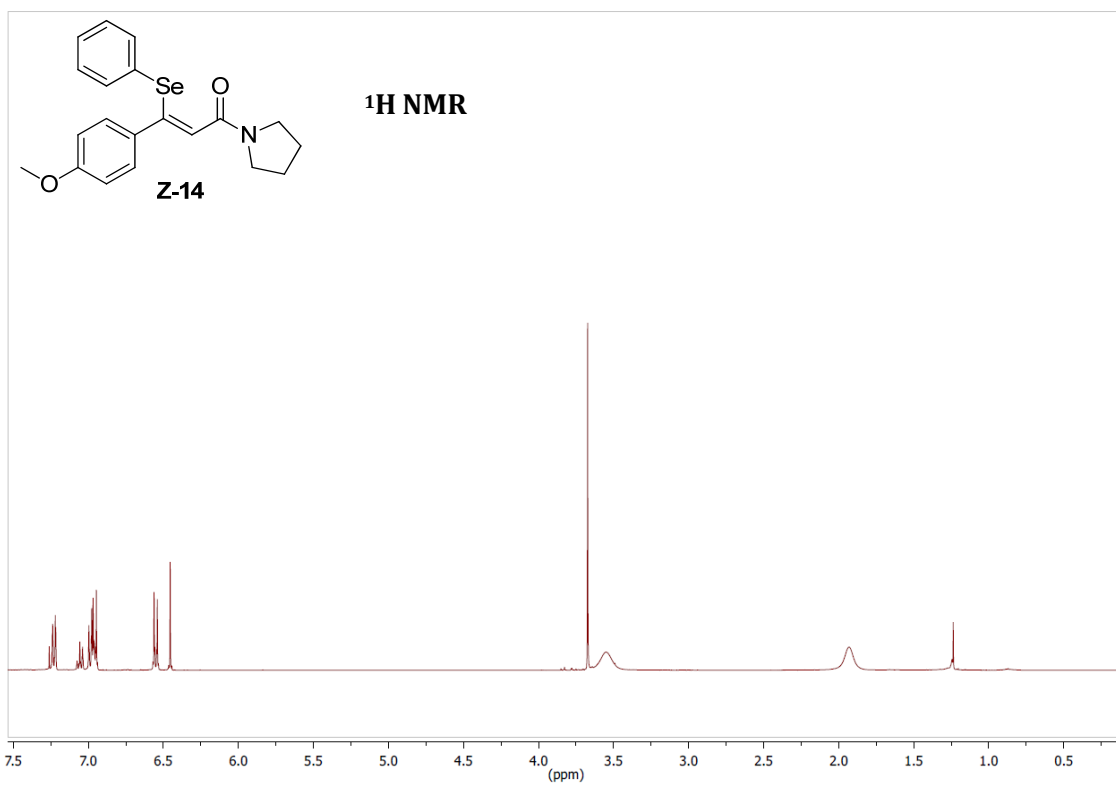
¹H NMR

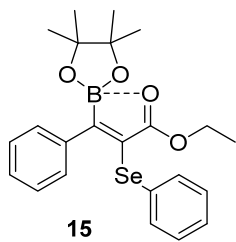


¹³C NMR

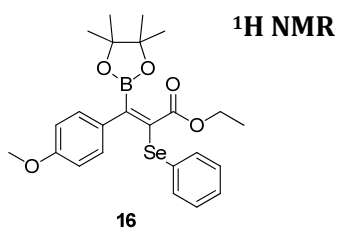
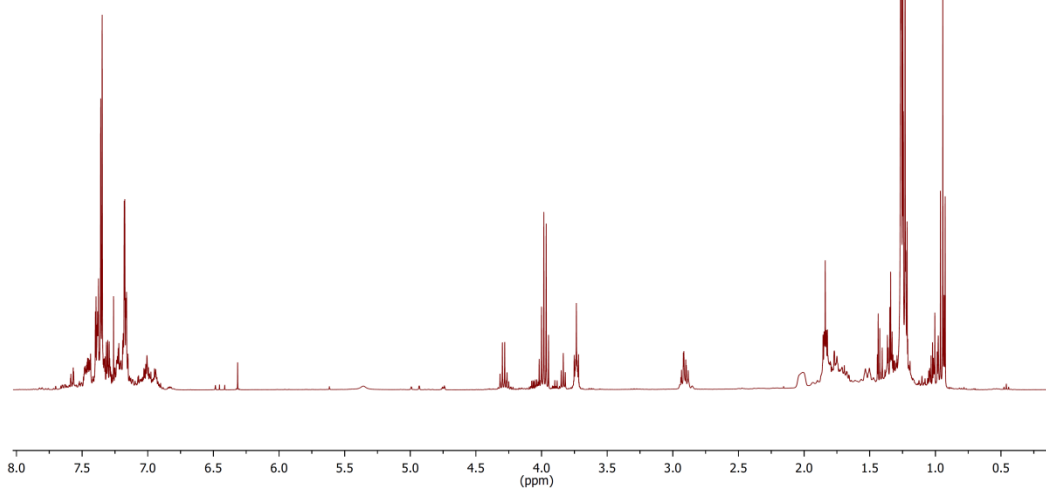




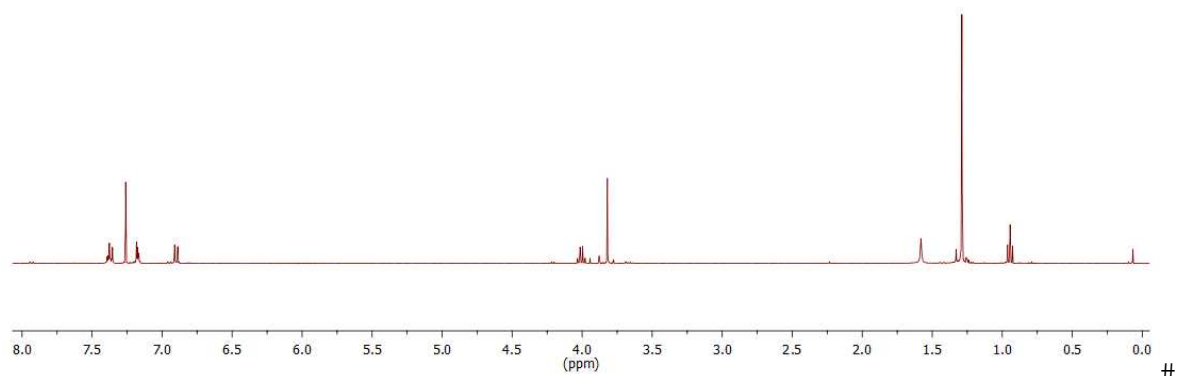




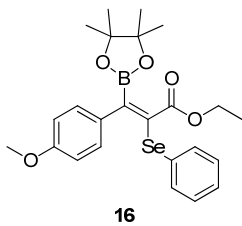
¹H NMR of the crude



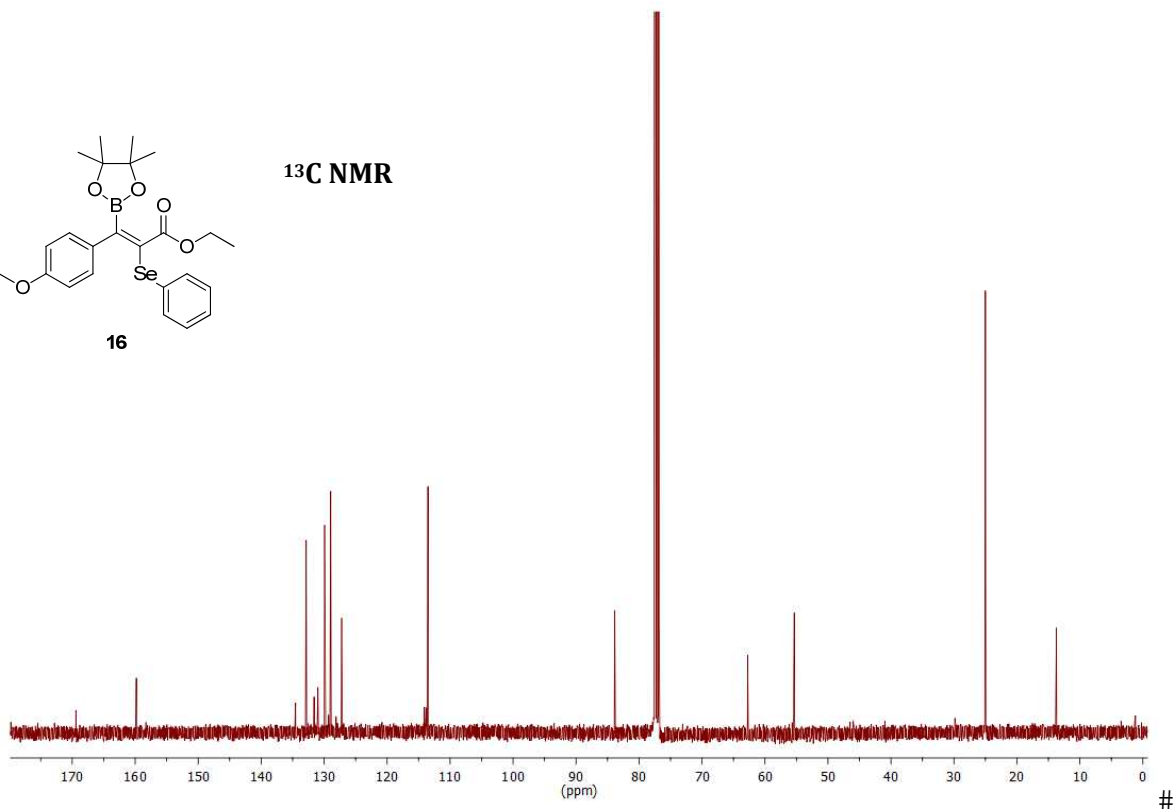
¹H NMR



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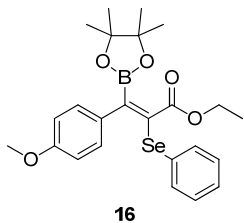


¹³C NMR

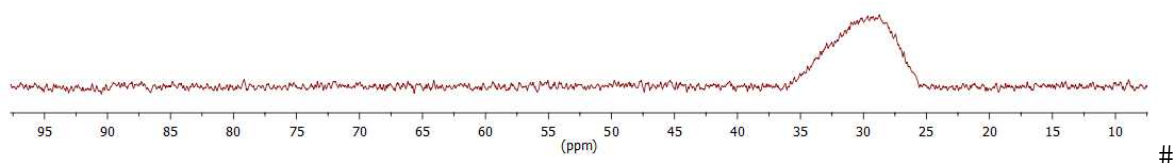


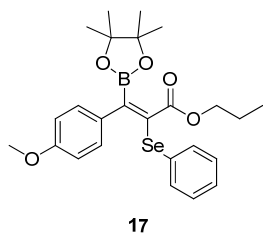
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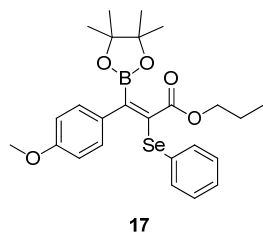
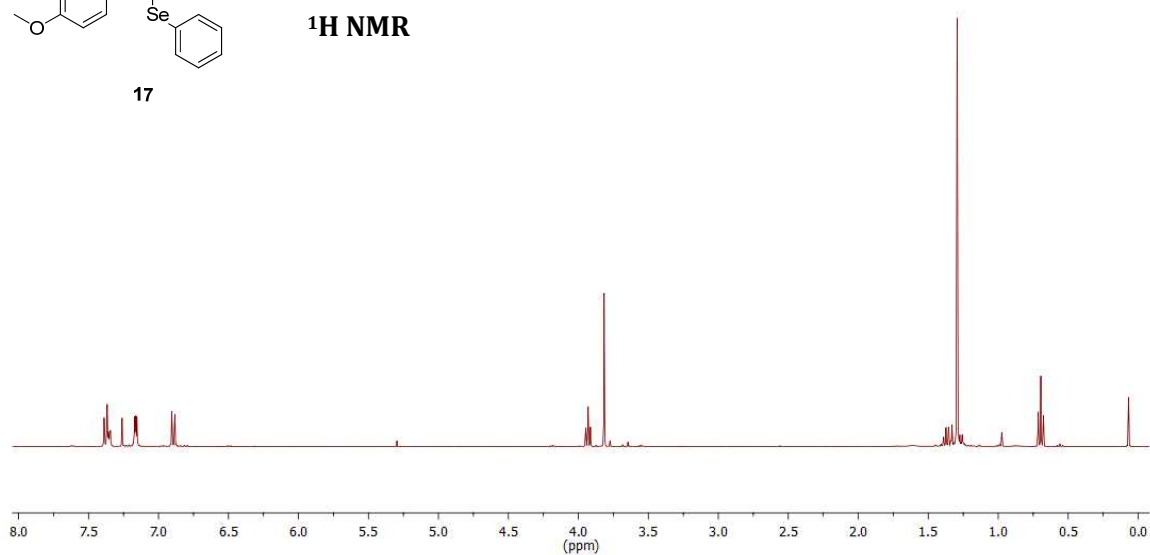


¹¹B NMR

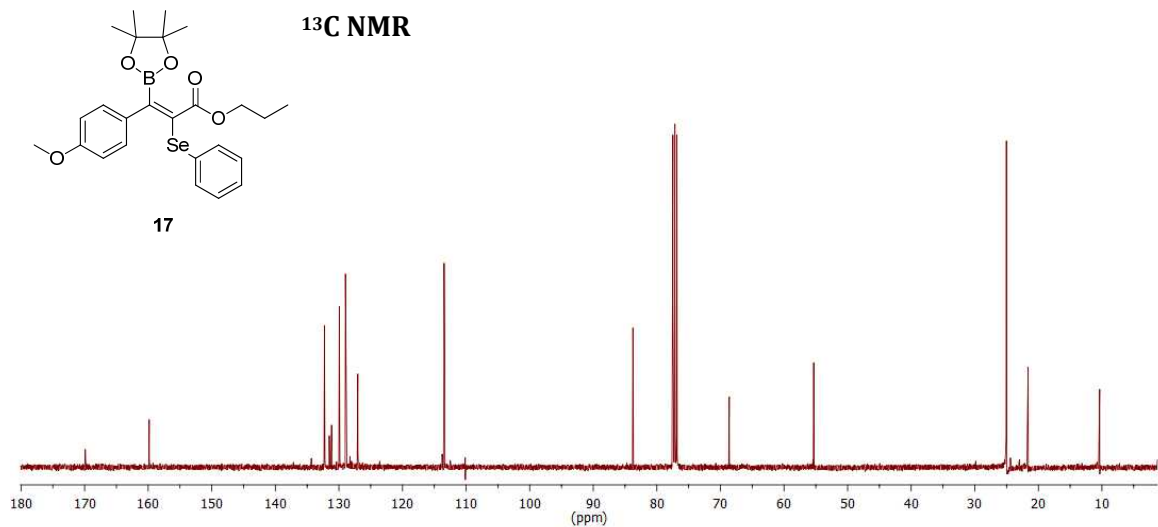


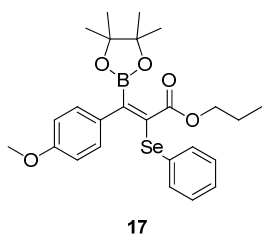


¹H NMR

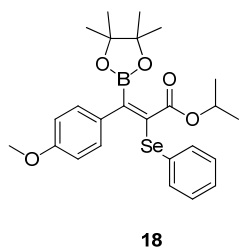
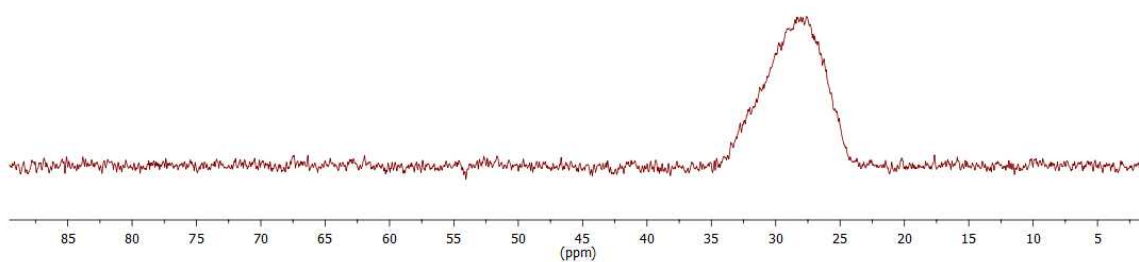


¹³C NMR

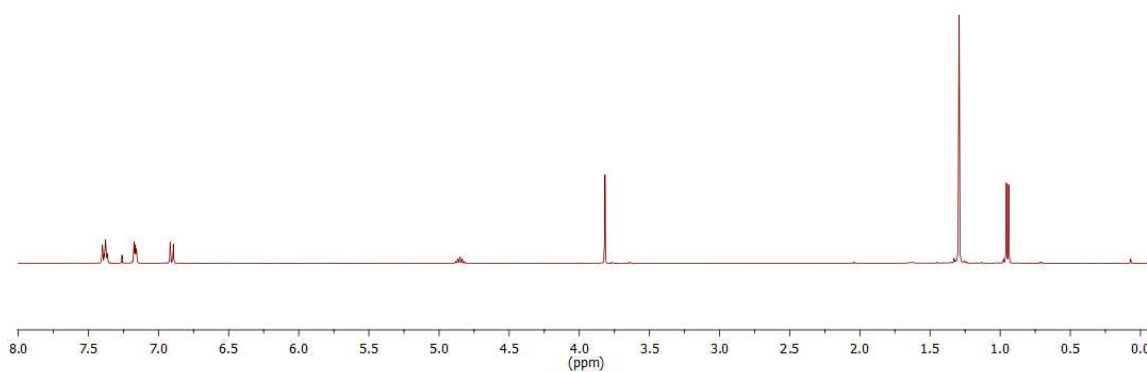


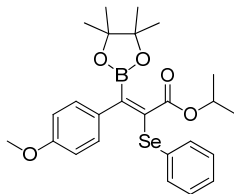


¹¹B NMR



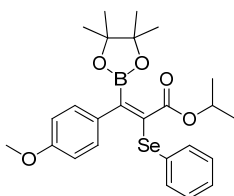
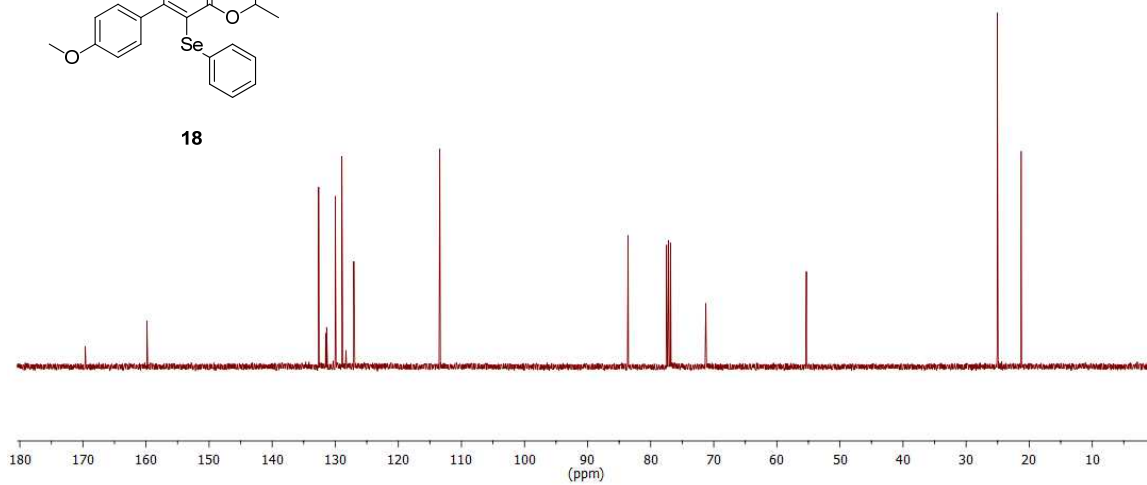
¹H NMR





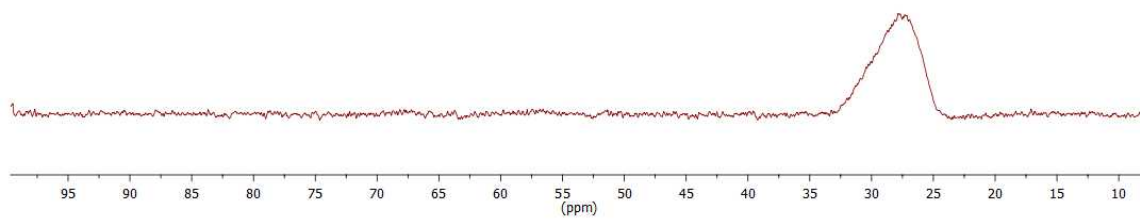
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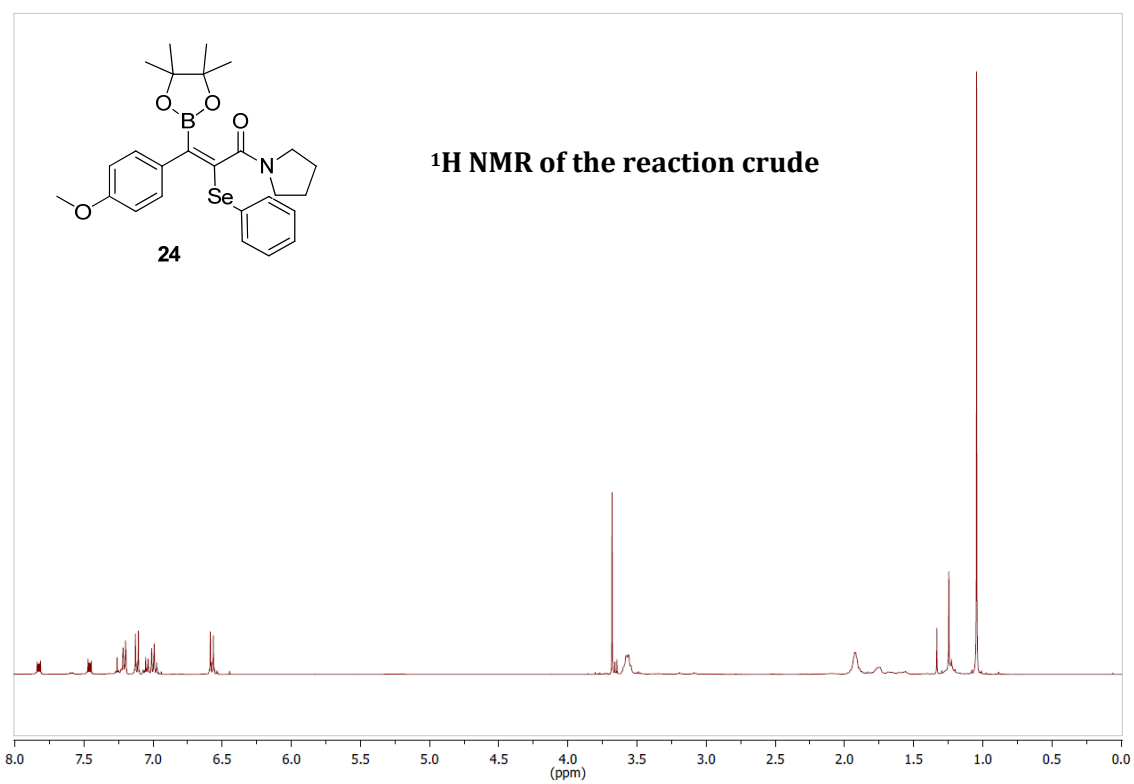
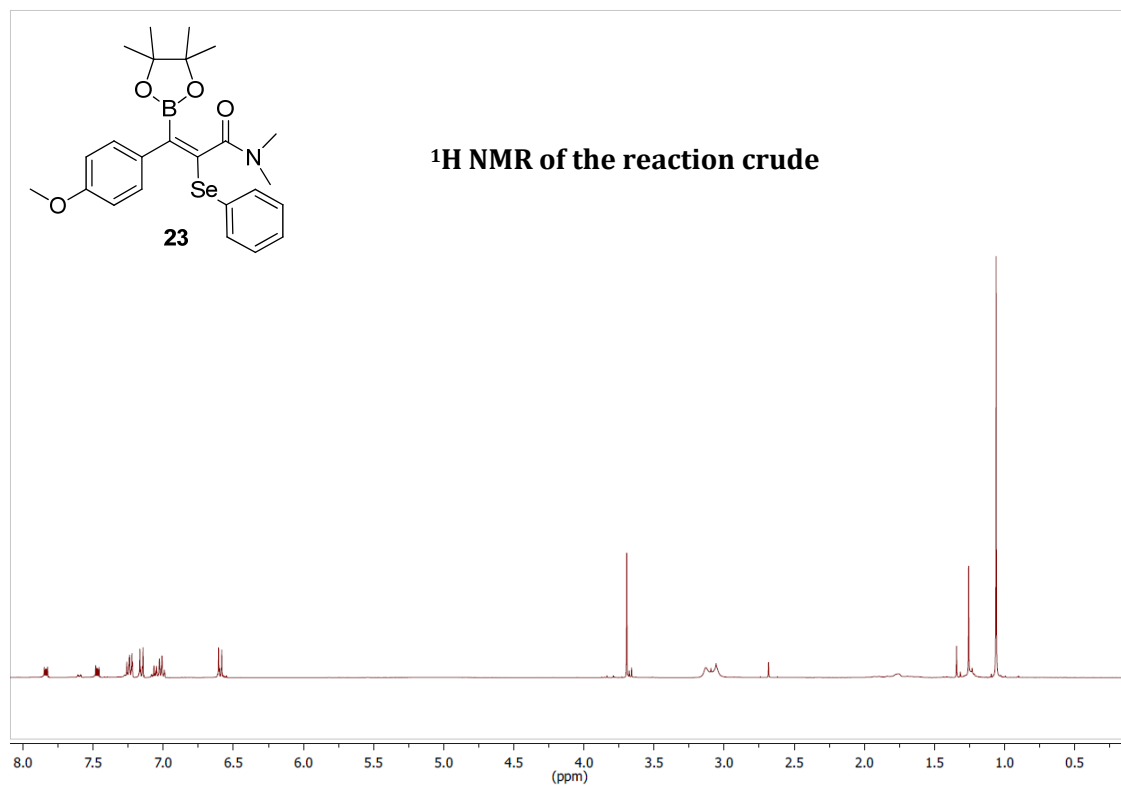
¹³C NMR

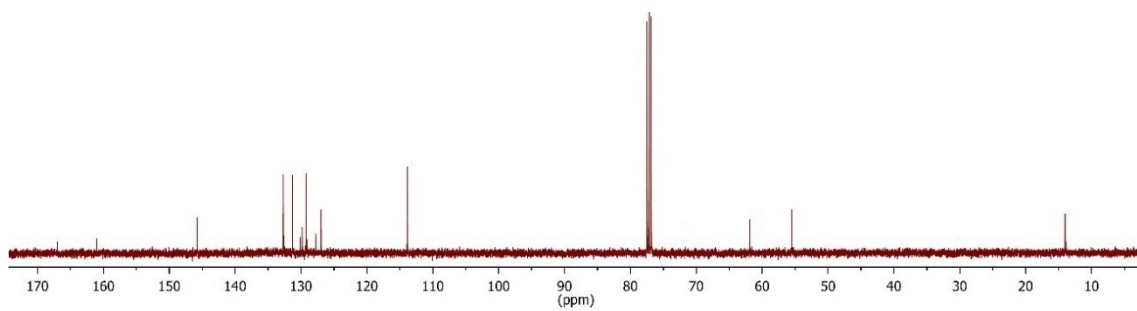
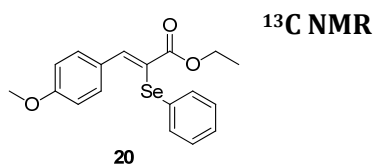
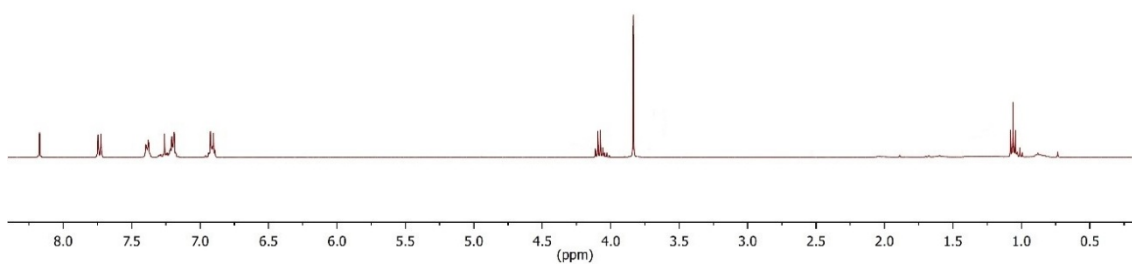
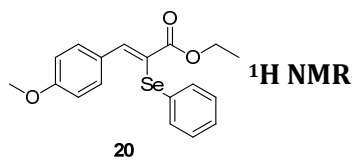


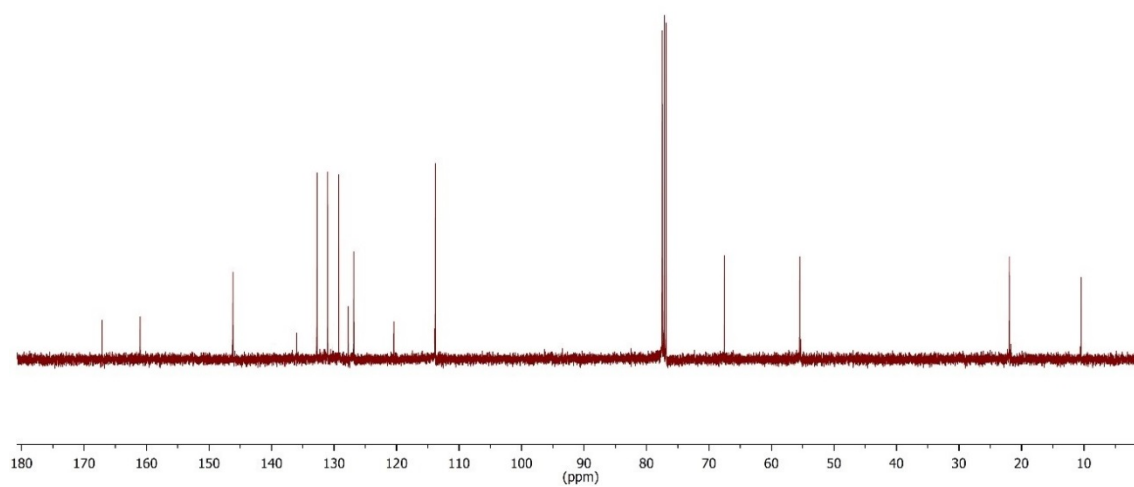
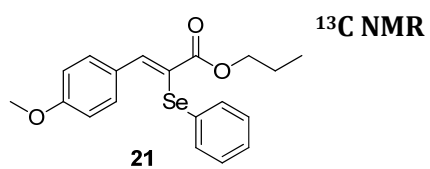
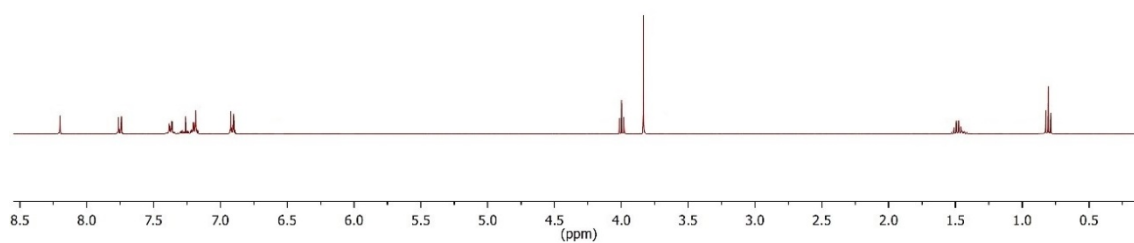
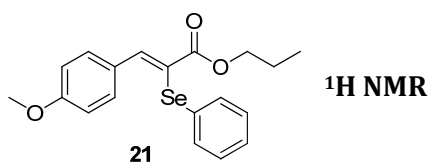
18

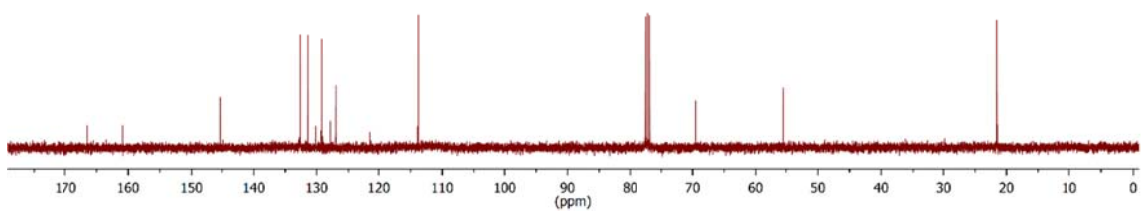
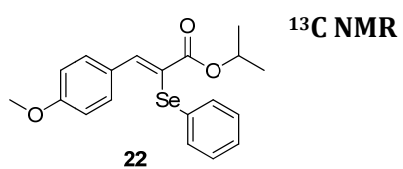
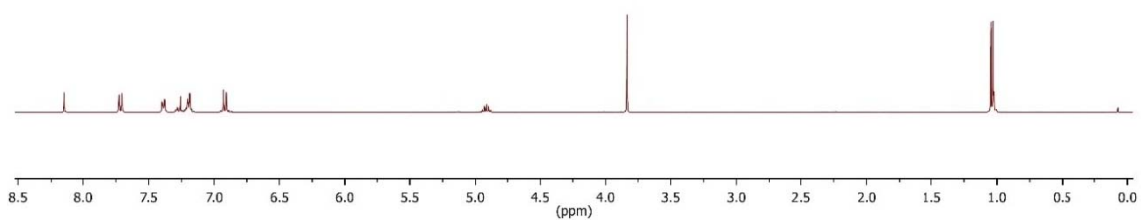
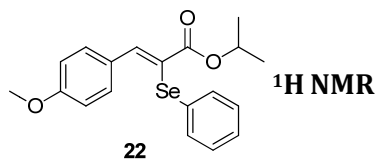
¹¹B NMR











4. X-ray Diffraction data for (Z)-3-phenyl-3-(phenylselanyl)acrylate (Z-8)

Table 1. Crystal data and structure refinement for mo_MGC007f1_0m.

Identification code	mo_MGC007f1_0m
Empirical formula	C17 H16 O2 Se
Formula weight	331.26
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P1
Unit cell dimensions	a = 6.7562(4)Å a= 107.8301(18)°. b = 7.5182(5)Å b = 98.9760(17)°. c = 8.7692(5)Å g = 113.0598(18)°.
Volume	370.28(4) Å ³
Z	1
Density (calculated)	1.486 Mg/m ³
Absorption coefficient	2.533 mm ⁻¹
F(000)	168
Crystal size	0.20 x 0.10 x 0.10 mm ³
Theta range for data collection	2.571 to 28.312°.
Index ranges	-8<=h<=8,-8<=k<=9,-11<=l<=11
Reflections collected	4368
Independent reflections	2430[R(int) = 0.0147]
Completeness to theta =28.312°	96.6%
Absorption correction	Multi-scan
Max. and min. transmission	0.786 and 0.652
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	2430/ 3/ 182
Goodness-of-fit on F ²	1.303
Final R indices [I>2sigma(I)]	R1 = 0.0187, wR2 = 0.0573
R indices (all data)	R1 = 0.0198, wR2 = 0.0729
Flack parameter	x = -0.022(8)
Largest diff. peak and hole	0.446 and -0.409 e.Å ⁻³

Table 2. Bond lengths [\AA] and angles [$^\circ$] for mo_MGC007f1_0m.

Bond lengths-----	
C1-C2	1.342(6)
C1-C6	1.483(5)
C1-Se1	1.910(4)
C2-C3	1.469(5)
C3-O1	1.226(5)
C3-O2	1.341(5)
C4-O2	1.451(4)
C4-C5	1.505(6)
C6-C7	1.398(6)
C6-C11	1.400(5)
C7-C8	1.399(5)
C8-C9	1.378(6)
C9-C10	1.391(6)
C10-C11	1.390(5)
C12-C13	1.394(6)
C12-C17	1.395(6)
C12-Se1	1.927(4)
C13-C14	1.389(6)
C14-C15	1.388(6)
C15-C16	1.388(7)
C16-C17	1.390(6)
Angles-----	
C2-C1-C6	120.0(3)
C2-C1-Se1	122.1(3)
C6-C1-Se1	118.0(3)
C1-C2-C3	122.8(4)
O1-C3-O2	123.3(3)
O1-C3-C2	124.7(4)
O2-C3-C2	112.0(3)
O2-C4-C5	107.5(3)
C7-C6-C11	119.5(3)
C7-C6-C1	119.8(4)
C11-C6-C1	120.7(4)
C6-C7-C8	119.6(4)

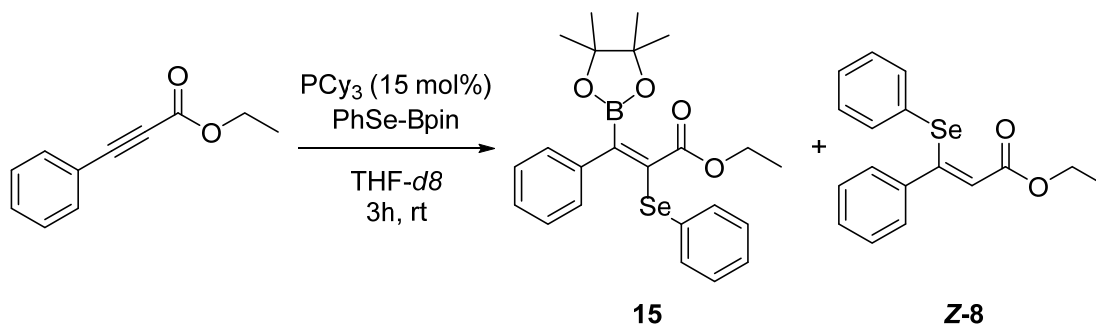
C9-C8-C7	120.3(4)
C8-C9-C10	120.7(4)
C11-C10-C9	119.5(4)
C10-C11-C6	120.5(4)
C13-C12-C17	120.0(4)
C13-C12-Se1	121.6(3)
C17-C12-Se1	118.3(3)
C14-C13-C12	119.9(4)
C15-C14-C13	119.7(4)
C14-C15-C16	120.7(4)
C15-C16-C17	119.7(4)
C16-C17-C12	120.0(4)
C3-O2-C4	116.1(3)
C1-Se1-C12	99.41(16)

Table 3. Torsion angles [°] for mo_MGC007f1_0m.

C6-C1-C2-C3	179.5(4)
Se1-C1-C2-C3	-0.5(6)
C1-C2-C3-O1	4.8(7)
C1-C2-C3-O2	-173.7(4)
C2-C1-C6-C7	-64.9(6)
Se1-C1-C6-C7	115.1(4)
C2-C1-C6-C11	114.9(5)
Se1-C1-C6-C11	-65.1(5)
C11-C6-C7-C8	0.2(6)
C1-C6-C7-C8	-180.0(4)
C6-C7-C8-C9	-0.1(7)
C7-C8-C9-C10	-0.4(7)
C8-C9-C10-C11	0.9(7)
C9-C10-C11-C6	-0.9(6)
C7-C6-C11-C10	0.3(6)
C1-C6-C11-C10	-179.5(4)
C17-C12-C13-C14	-3.0(6)
Se1-C12-C13-C14	-179.8(3)
C12-C13-C14-C15	2.8(6)
C13-C14-C15-C16	-0.6(6)
C14-C15-C16-C17	-1.3(7)
C15-C16-C17-C12	1.1(7)
C13-C12-C17-C16	1.1(6)
Se1-C12-C17-C16	178.0(3)
O1-C3-O2-C4	-0.6(6)
C2-C3-O2-C4	178.0(3)
C5-C4-O2-C3	-178.6(4)

5. Kinetic Studies

Experimental Kinetic study of the *anti*-3,4-selenoboration of ethyl phenylpropiolate (**1**) with PhSe-Bpin.



Inside the glovebox, Stock solutions of Naphthalene (0.0483 M) and Tricyclohexylphosphine (0.09 M) were prepared in THF-*d*₈. Then 10 μ L of Ethyl phenylpropiolate (**1**) (0.061 mmol) were transferred into an oven-dried NMR tube and dissolved in 0.4 mL of the Naphthalene Stock solution (0.0193 mmol), followed by the addition of 0.1 mL of the Tricyclohexylphosphine Stock solution (0.009 mmol, 15 mol%). After that, 18.9 mg of PhSe-Bpin (0.067 mmol, 1.1 eq.) were weighted in a mass vial and dissolved in 0.1 mL of THF-*d*₈. Before starting to acquire the ¹H-NMR spectra the 0.1 mL of PhSe-Bpin solution were added to the NMR tube through a septum cap. The formation of products was followed by NMR spectroscopy.

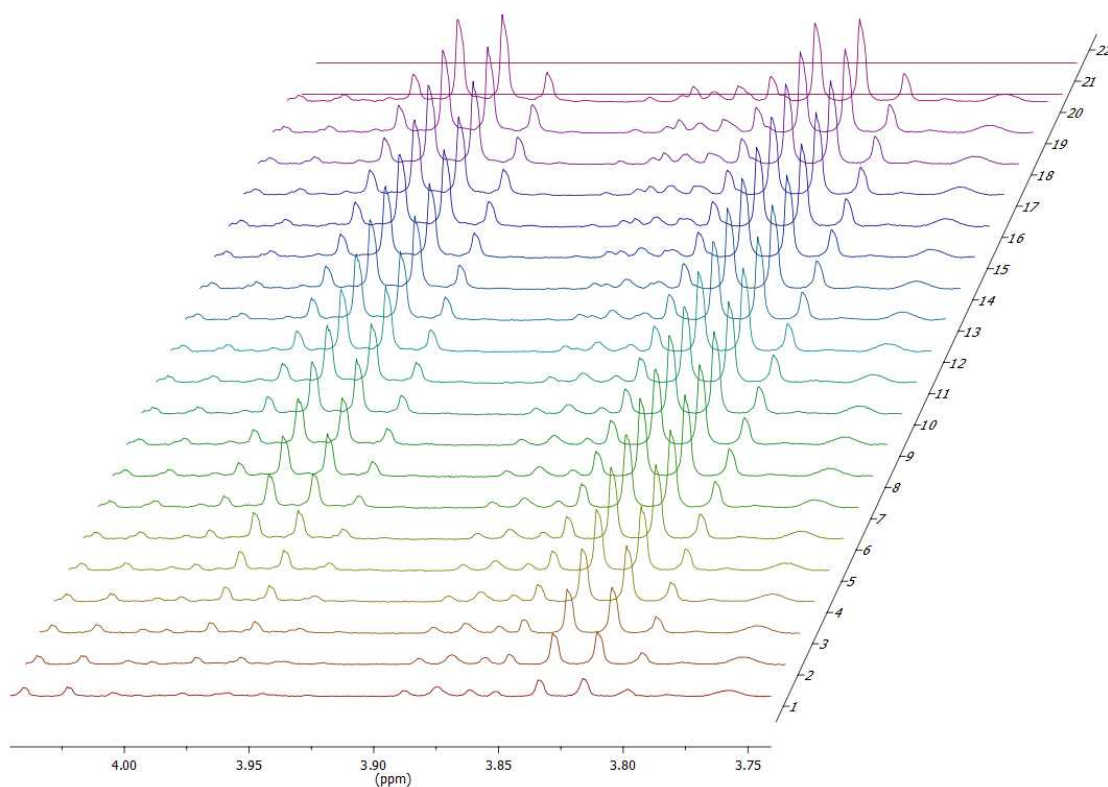


Figure S1 Progress of the reaction between **1** and pinB-SePh in THF- d_8 followed by $^1\text{H-NMR}$

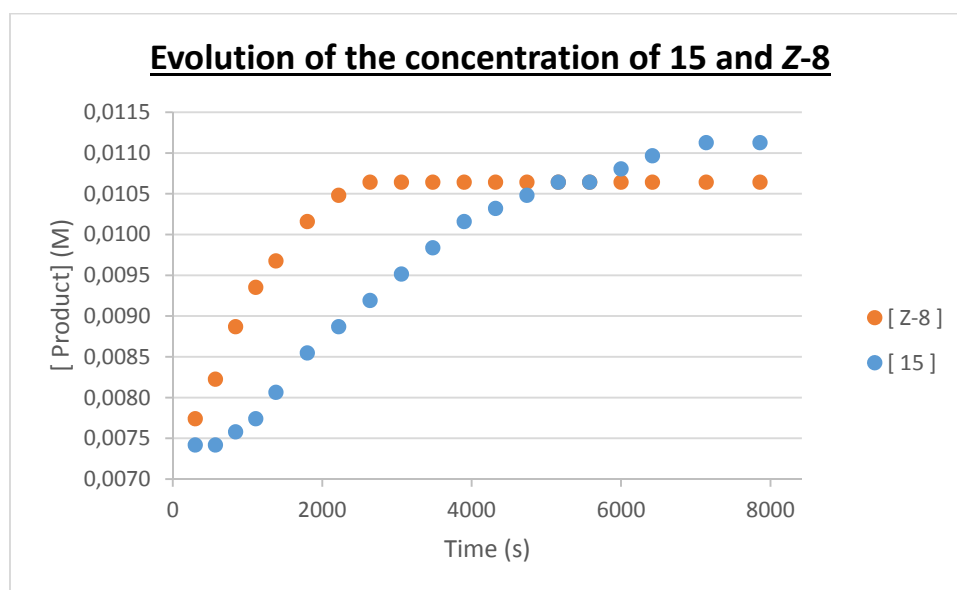


Figure S2 Kinetic profile for the reaction between **1** and pinB-SePh in THF- d_8

Figure S2 shows that under NMR experimental conditions the formation of β -selenated **Z-8** product is competitive with the formation of α -selenated product **15**. In this conditions we used larger amount of THF- d_8 solvent, which in addition contains a percentage of water. The water impurity provides the source of protons similar to methanol solvent that allows the reaction to proceed yielding **Z-8** product. According to the Karl Fischer Titration of commercial source (205 ppm = 0.021%), which corresponds to an approximate concentration of 0.0113 M. Interestingly, the amount of formed **Z-8** product is roughly the same as water impurity, which as a limiting reactant (see Figure S2). In fact, it is well known that the water present in the solvents is the responsible for the Cu-borylation/protonation of α,β -unsaturated carbonyl compounds.⁴

Kinetic simulations of the *anti*-3,4-selenoboration of ethyl phenylpropiolate (1**) with PhSe-Bpin, using PMe_3 as model phosphine.**

The kinetic simulation was carried out with the Acuchem software.⁵ All rate constants were calculated using Eyring approximation and transition state theory using the Gibbs free-energy values on Scheme 4 and Figure 3 of the main text. The default ΔG values provided by Gaussian

⁴ (a) Miyaura *et al.*, *Chem. Lett.* 2000, 982; (b) Hosomi *et al.*, *Tetrahedron Lett.* 2000, **41**, 6821

⁵ W. Braun, J. T. Herron, D. K. Kahaner, *Int. J. Chem. Kinet.* **1988**, *20*, 51

overestimate the entropic cost for bimolecular processes and in this case it results in the overestimation of key free-energy barriers and in low conversions. In order to reduce this error and to obtain a better fit in kinetic simulations, we corrected ΔG values by changing the reference state from an ideal gas standard state of 1 atm to 1 mol·L⁻¹ at 298.15 K. As a result the simulations estimate larger yields, which are closer to experimental results. Another factor that may influence the ΔG values, and consequently kinetic simulations, is the use of model PMe₃ phosphine. As discussed in the main text, the replacement of PMe₃ by PCy₃ reduces the free-energy barrier of its addition to alkyne by ~ 3 kcal·mol⁻¹. To account for this phosphine effect we applied a constant correction to all the barriers involving the phosphine obtaining a good fit with experimental yields. The simulation was carried out concentration conditions for experimental NMR kinetic study (Figure S3).

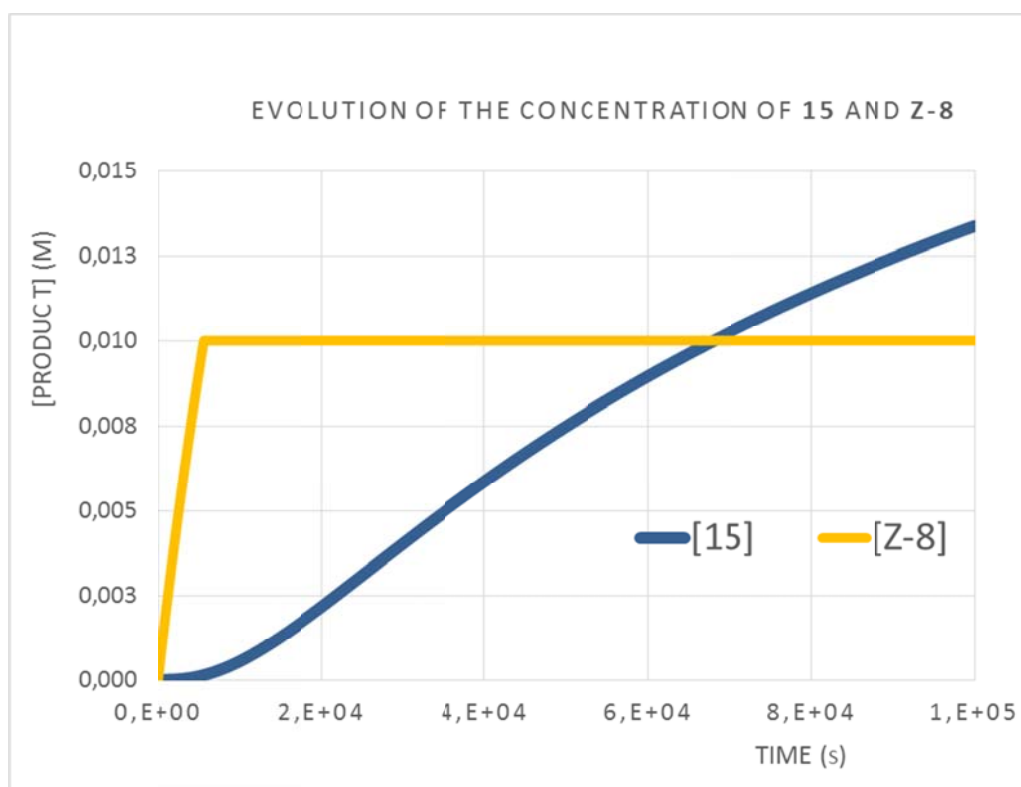


Figure S3. Simulated, kinetic profile of **15** and **Z-8** for the reaction between **1** and pinB-SePh catalysed by PMe₃, using the concentration and temperature conditions of experiment in NMR kinetic study described in previous section.

Additionally, we repeated the simulation in “dry THF” (no water in the simulation) introducing both the equations of β - and α -selonoboration reactions (blue line in Figure S4) and introducing exclusively the equations of α -selonoboration reactions (green line in Figure S4).

Under these conditions the β -selenated reaction (Scheme 4) is still competitive, accumulating intermediate **B** which cannot evolve to products in the absence of a proton source. As a consequence of this off-cycle reaction, the profile of α -selenated product **15** shows a sigmoidal profile analogous to that observed in the experiments (blue line in Figure S4). Interestingly, when the β -selenated reaction is removed from the kinetic model, the rate of formation of **15** increases significantly and the shape of the curve is not sigmoidal anymore (green line in Figure S4).

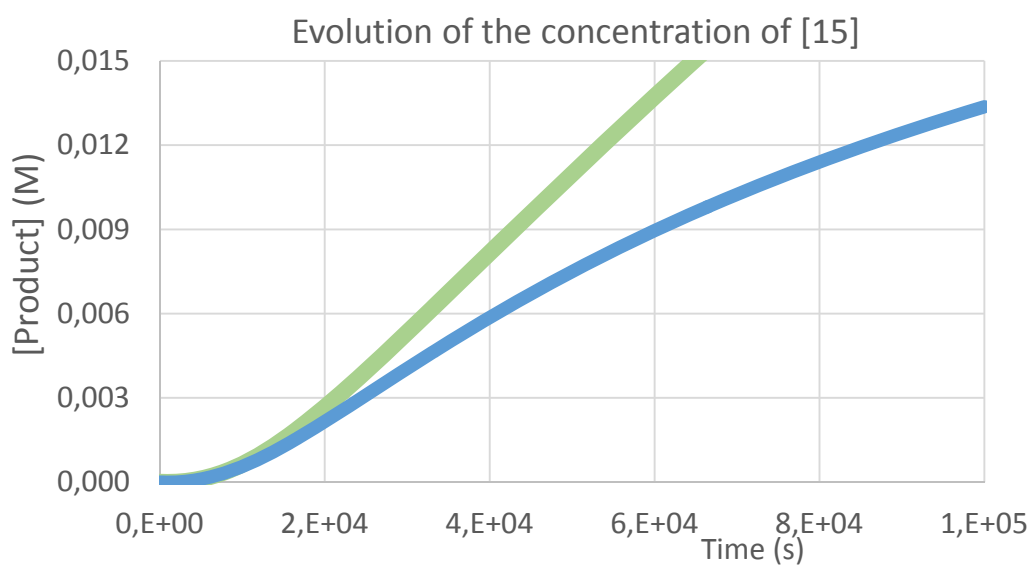


Figure S4. Simulated, kinetic profile of **15** and **Z-8** for the reaction between **1** and pinB-SePh catalysed by PMe_3 , using the concentration and temperature conditions of experiment in NMR kinetic study described in previous section but excluding the presence of water (blue line) and supposing that β -selenation reaction is not operative (green line).

6. Additional Figures of the computational study

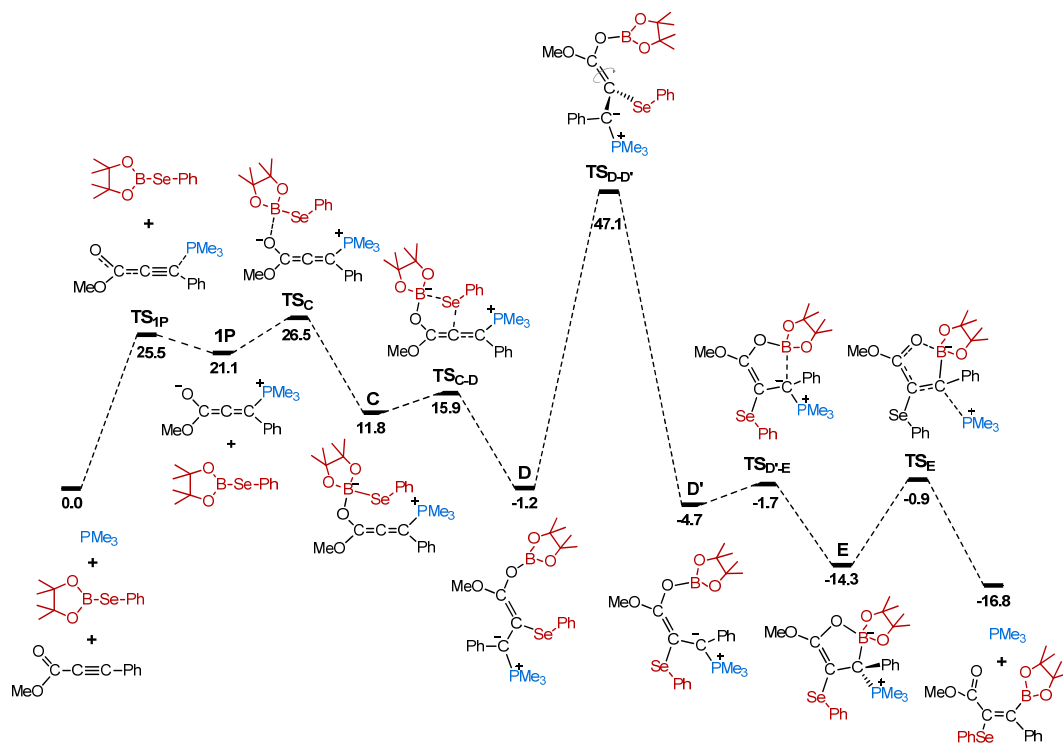


Figure S5. Computed free-energy profile ($\text{kcal}\cdot\text{mol}^{-1}$) for *anti*-3,4-addition of PhSe-Bpin to α,β -acetylenic ester adapted from the proposal for analogous *anti*-selective carboboration, silaboration and diboration.

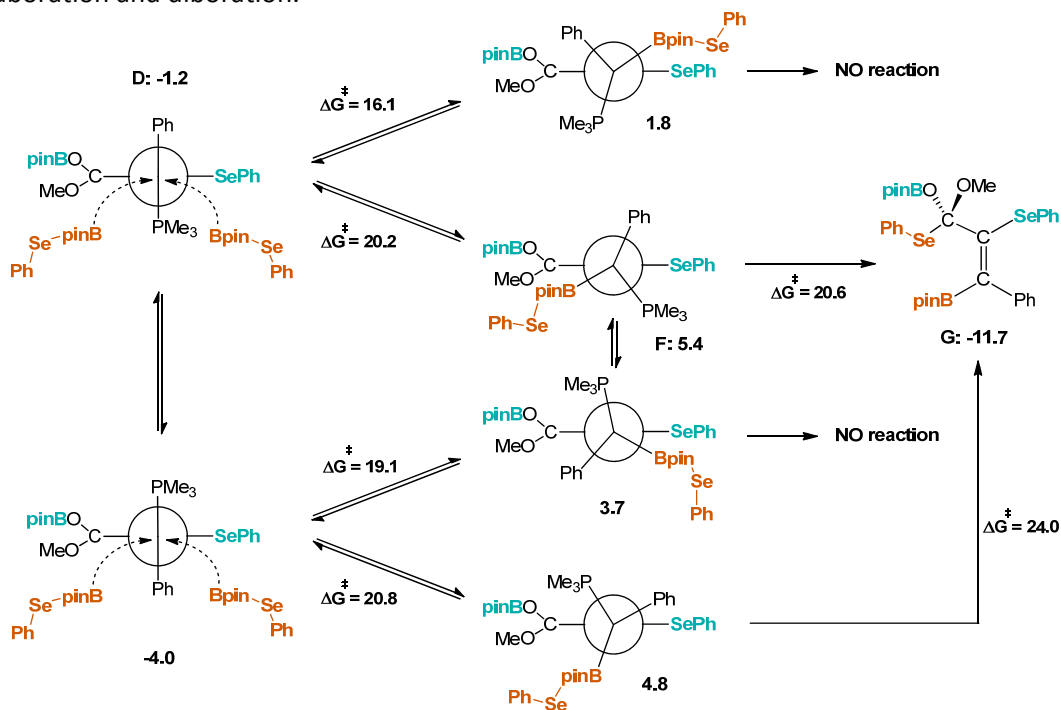


Figure S6. Schematic representation of the possible paths of the stereoselectivity determining step yielding *anti* isomer. Relative free-energies and barriers in $\text{kcal}\cdot\text{mol}^{-1}$.

7. Cartesian coordinates in Å and the electronic energies for the computed structures

TS_{1P}: $E = -997.212131$ a.u.

C	-2.196761	-1.261651	0.276522
O	-2.798472	-1.196316	1.329756
O	-2.830128	-1.518849	-0.898631
C	-4.232965	-1.739126	-0.777895
H	-4.729643	-0.858859	-0.366530
H	-4.586163	-1.941190	-1.786036
H	-4.433335	-2.588971	-0.124662
C	-0.795236	-1.113278	0.107752
C	0.238551	-0.401306	0.003056
C	1.694894	-0.580442	-0.049031
C	2.212211	-1.810831	0.377664
C	2.577988	0.390679	-0.518503
C	3.576523	-2.051810	0.338498
H	1.520967	-2.562902	0.737663
C	3.946251	0.144452	-0.562412
H	2.196279	1.342145	-0.869113
C	4.451535	-1.074893	-0.131151
H	3.960803	-3.006354	0.678043
H	4.616362	0.908734	-0.937693
H	5.517524	-1.265203	-0.160920
P	-0.343439	1.690017	0.052109
C	-1.168066	1.756622	1.679795
H	-1.786003	0.867222	1.815107
H	-0.407097	1.770407	2.461993
H	-1.785284	2.654073	1.761455
C	-1.705432	1.798736	-1.160205
H	-1.294460	2.076651	-2.132072
H	-2.190565	0.827043	-1.256954
H	-2.439117	2.546766	-0.852854
C	0.436845	3.361567	-0.069893
H	1.240880	3.438923	0.663575
H	0.859215	3.501772	-1.066205
H	-0.298014	4.148498	0.119373

1P: $E = -997.221779$ a.u.

C	2.005466	-1.116683	-0.990502
O	2.557188	-0.504495	-1.896172
O	2.734942	-1.827532	-0.081275
C	4.136460	-1.838490	-0.316671
H	4.563434	-0.836739	-0.217919
H	4.558586	-2.499204	0.437328
H	4.359166	-2.208642	-1.317737
C	0.598500	-1.253152	-0.792948
C	-0.222743	-0.301961	-0.342395
C	-1.703667	-0.448405	-0.253185
C	-2.236189	-1.653416	0.212764
C	-2.586678	0.555897	-0.658177
C	-3.609603	-1.838944	0.287030
H	-1.546254	-2.438535	0.498506
C	-3.963715	0.372918	-0.582689
H	-2.201414	1.478776	-1.082721
C	-4.480068	-0.824222	-0.102398

H	-4.004838	-2.779944	0.651587
H	-4.631420	1.159274	-0.914890
H	-5.551770	-0.970276	-0.042113
P	0.484595	1.299433	0.117895
C	0.790096	2.330500	-1.342238
H	1.407352	1.728347	-2.014338
H	-0.151347	2.570656	-1.836660
H	1.310043	3.249750	-1.065467
C	2.105483	1.096798	0.910461
H	2.091737	0.218541	1.555399
H	2.861246	0.956737	0.137373
H	2.331697	1.994010	1.488297
C	-0.507034	2.266796	1.298890
H	-1.487119	2.496672	0.885443
H	-0.645563	1.670474	2.202329
H	0.015648	3.192109	1.547715

TS_C: $E = -4041.629217$ a.u.

C	0.334436	1.297885	1.659562
O	1.366010	0.766805	1.190420
O	0.455181	2.174329	2.697977
C	1.760528	2.288965	3.256298
H	2.457386	2.726205	2.538775
H	1.652272	2.940831	4.120287
H	2.136988	1.312351	3.563589
C	-0.961289	0.985642	1.294753
C	-1.832473	1.263871	0.344291
C	-3.074695	0.495754	0.078102
C	-3.757205	-0.081179	1.152074
C	-3.525197	0.245063	-1.219340
C	-4.876786	-0.868986	0.931602
H	-3.375006	0.082530	2.152962
C	-4.649964	-0.543457	-1.439917
H	-2.960610	0.614559	-2.068442
C	-5.333544	-1.096535	-0.364427
H	-5.391329	-1.316606	1.773858
H	-4.978961	-0.739889	-2.453745
H	-6.208452	-1.712840	-0.534110
P	-1.391036	2.732908	-0.624870
C	0.234585	2.622125	-1.409054
H	0.970223	2.224700	-0.706413
H	0.184699	1.940409	-2.257188
H	0.528871	3.619475	-1.743646
C	-1.312584	4.109892	0.552504
H	-2.309423	4.277695	0.962893
H	-0.641164	3.835807	1.367970
H	-0.959156	5.015241	0.055968
C	-2.564774	3.285775	-1.904863
H	-2.462429	2.678356	-2.803181
H	-3.584340	3.194005	-1.528212
H	-2.356102	4.328559	-2.151966
Se	0.220082	-0.956537	-1.397439
B	1.896355	-0.471074	-0.400734
O	2.613584	-1.373466	0.355261
O	2.706214	0.403192	-1.105340
C	3.987914	-1.255585	-0.062034
C	4.053141	0.205290	-0.620668

C	4.889032	-1.519118	1.132292
H	4.773700	-2.557502	1.447556
H	5.937222	-1.353233	0.867582
H	4.626892	-0.875559	1.971159
C	4.213851	-2.309204	-1.145264
H	5.254326	-2.330757	-1.477621
H	3.953300	-3.285703	-0.734544
H	3.566610	-2.121713	-2.004723
C	4.328898	1.240727	0.467012
H	5.370166	1.195970	0.795469
H	4.135195	2.234595	0.056272
H	3.666036	1.084531	1.316744
C	5.012488	0.396421	-1.784372
H	4.996506	1.441819	-2.098861
H	6.033478	0.143851	-1.485016
H	4.728863	-0.222211	-2.634859
C	-0.759111	-2.015658	-0.134020
C	-0.404280	-2.104915	1.210496
C	-1.894953	-2.680750	-0.598356
C	-1.188130	-2.860374	2.077228
H	0.477883	-1.595291	1.576961
C	-2.672150	-3.429258	0.275629
H	-2.173647	-2.607299	-1.643633
C	-2.321946	-3.521122	1.619153
H	-0.907109	-2.924907	3.122107
H	-3.556686	-3.934098	-0.095503
H	-2.927910	-4.104368	2.302515

C: $E = -4041.651954$ a.u.

C	-0.219324	0.264511	1.868765
O	-1.109624	0.988820	1.246652
O	-0.246028	0.327332	3.216773
C	-0.824838	1.515146	3.762955
H	-1.883656	1.583666	3.516326
H	-0.688821	1.429656	4.838315
H	-0.307588	2.399426	3.385059
C	0.712189	-0.492114	1.294341
C	1.433249	-1.384455	0.667373
C	2.809372	-1.147481	0.157707
C	3.691269	-0.393682	0.934695
C	3.222093	-1.589477	-1.100418
C	4.958480	-0.087242	0.461231
H	3.354863	-0.030312	1.898790
C	4.491558	-1.278931	-1.576331
H	2.537115	-2.130770	-1.743158
C	5.363125	-0.528095	-0.795986
H	5.629037	0.507193	1.070210
H	4.791284	-1.608518	-2.563801
H	6.350401	-0.282422	-1.168001
P	0.579924	-2.937192	0.308559
C	-0.218095	-2.967321	-1.312699
H	-0.959698	-2.162852	-1.305307
H	0.499332	-2.795843	-2.113065
H	-0.705028	-3.936436	-1.445195
C	-0.730396	-3.154119	1.524745
H	-0.323661	-3.054689	2.531130
H	-1.457854	-2.361489	1.336091

H	-1.191510	-4.134204	1.390632
C	1.723486	-4.340541	0.428228
H	2.528698	-4.223963	-0.297355
H	2.155889	-4.358397	1.429631
H	1.191111	-5.274007	0.240021
Se	-0.159894	0.832777	-1.605120
B	-1.669396	0.634320	-0.096780
O	-2.809714	1.461842	-0.301578
O	-2.119323	-0.752465	-0.162101
C	-3.874119	0.645495	-0.769949
C	-3.551635	-0.724108	-0.094639
C	-5.194334	1.267377	-0.338600
H	-5.342726	2.204036	-0.879099
H	-6.033847	0.602925	-0.564038
H	-5.188715	1.489658	0.728186
C	-3.810801	0.560549	-2.297238
H	-4.682137	0.043528	-2.708336
H	-3.779518	1.575789	-2.695412
H	-2.903618	0.049047	-2.625073
C	-3.971450	-0.742342	1.377235
H	-5.058088	-0.772687	1.486553
H	-3.557797	-1.630509	1.862172
H	-3.586226	0.142382	1.887762
C	-4.098349	-1.945384	-0.817559
H	-3.821511	-2.852515	-0.272022
H	-5.189565	-1.906965	-0.875612
H	-3.696064	-2.013660	-1.828766
C	0.968839	2.147753	-0.782131
C	0.417057	3.203934	-0.049644
C	2.355958	2.066459	-0.915020
C	1.244231	4.141349	0.557372
H	-0.660143	3.285265	0.037126
C	3.177846	3.017609	-0.317658
H	2.795012	1.251097	-1.480296
C	2.628219	4.053684	0.428242
H	0.802834	4.954722	1.122845
H	4.253437	2.937057	-0.432213
H	3.269017	4.790969	0.897413

TS_{C-D}: $E = -4041.647466$ a.u.

C	-0.114537	-0.075218	1.765083
O	-1.303528	0.390121	1.458395
O	0.107095	-0.271487	3.084828
C	-0.555766	0.654680	3.949344
H	-1.636765	0.530644	3.895659
H	-0.193950	0.427875	4.949311
H	-0.292780	1.680009	3.678634
C	0.878763	-0.348642	0.908009
C	1.856959	-1.198821	0.547014
C	3.113928	-0.749853	-0.077130
C	3.448656	0.608948	0.018343
C	3.966709	-1.585955	-0.807527
C	4.599055	1.101619	-0.577030
H	2.785515	1.269144	0.566055
C	5.121384	-1.089798	-1.402694
H	3.736278	-2.636865	-0.937556
C	5.446385	0.255660	-1.288753

H	4.834213	2.156183	-0.486342
H	5.763430	-1.758544	-1.963875
H	6.344236	0.642786	-1.754606
P	1.280730	-2.877780	0.419636
C	0.643122	-3.236531	-1.239639
H	-0.219120	-2.578120	-1.384680
H	1.406969	-3.008760	-1.984409
H	0.337170	-4.281422	-1.320632
C	-0.097964	-3.139295	1.553688
H	0.177159	-2.803274	2.553959
H	-0.944778	-2.554294	1.188245
H	-0.349685	-4.201520	1.558540
C	2.547587	-4.128106	0.830889
H	3.051986	-4.486066	-0.065524
H	3.282950	-3.682942	1.501780
H	2.068816	-4.973467	1.326312
Se	-0.127779	0.933006	-1.152968
B	-1.764592	0.204866	0.067219
O	-3.009800	0.844814	-0.113199
O	-1.891041	-1.178345	-0.347684
C	-3.832517	-0.009623	-0.906309
C	-3.293914	-1.425633	-0.523095
C	-5.286496	0.235350	-0.531426
H	-5.578215	1.234998	-0.858650
H	-5.942877	-0.491222	-1.019150
H	-5.426320	0.176951	0.547587
C	-3.611736	0.313523	-2.384912
H	-4.308139	-0.237848	-3.022018
H	-3.772515	1.383122	-2.530066
H	-2.589146	0.085623	-2.689077
C	-3.863456	-1.910887	0.811449
H	-4.925225	-2.155783	0.733444
H	-3.328641	-2.812315	1.121165
H	-3.729545	-1.146391	1.579766
C	-3.473942	-2.489251	-1.594364
H	-3.075664	-3.442431	-1.235822
H	-4.532856	-2.630901	-1.827483
H	-2.946048	-2.215923	-2.508111
C	0.171265	2.672406	-0.405127
C	-0.774596	3.291401	0.415830
C	1.363214	3.339233	-0.701130
C	-0.511553	4.550511	0.947325
H	-1.716522	2.798660	0.623200
C	1.612977	4.600047	-0.172335
H	2.092558	2.864127	-1.348008
C	0.679568	5.208715	0.660884
H	-1.252374	5.022949	1.582506
H	2.540380	5.107490	-0.413067
H	0.875641	6.189995	1.076150

D: $E = -4041.674424$ a.u.

C	-0.586262	-0.699909	1.472387
O	-1.697716	-0.026506	1.880018
O	-0.415437	-1.823583	2.211718
C	0.716605	-1.834626	3.084208
H	0.721581	-0.934687	3.703996
H	0.597782	-2.711449	3.718286

H	1.643879	-1.898826	2.513719
C	0.221747	-0.335774	0.464969
C	1.387485	-1.127891	0.053673
C	2.750755	-0.743719	0.387542
C	2.993404	0.223628	1.388053
C	3.892837	-1.277596	-0.247676
C	4.275876	0.632652	1.711513
H	2.145877	0.677649	1.889308
C	5.178200	-0.876364	0.094827
H	3.786797	-1.997856	-1.052082
C	5.388709	0.085527	1.074861
H	4.408070	1.395536	2.471306
H	6.023518	-1.314035	-0.425497
H	6.390284	0.406366	1.332004
P	1.037566	-2.464295	-0.959370
C	1.460918	-2.315997	-2.740705
H	0.875094	-1.488316	-3.145560
H	2.518958	-2.084747	-2.863609
H	1.223403	-3.234104	-3.282567
C	-0.741308	-2.796873	-0.971865
H	-1.066400	-3.025564	0.043877
H	-1.281452	-1.913209	-1.314993
H	-0.938170	-3.643696	-1.631944
C	1.821929	-4.024169	-0.423078
H	2.876160	-3.858994	-0.203562
H	1.322672	-4.339588	0.494447
H	1.720957	-4.799402	-1.184836
Se	-0.333067	1.206010	-0.626103
B	-2.791003	0.117033	1.083731
O	-3.888174	0.828552	1.470175
O	-2.911799	-0.458052	-0.158335
C	-4.714045	0.974521	0.293103
C	-4.282514	-0.257637	-0.573411
C	-6.173154	0.973691	0.713309
H	-6.376649	1.864529	1.309399
H	-6.823459	0.991178	-0.165357
H	-6.412717	0.097987	1.315210
C	-4.339812	2.307059	-0.349757
H	-4.962703	2.518145	-1.221530
H	-4.485203	3.098928	0.386361
H	-3.289905	2.312917	-0.651384
C	-5.042961	-1.530352	-0.212960
H	-6.080872	-1.483342	-0.548846
H	-4.556099	-2.378058	-0.698372
H	-5.030022	-1.698652	0.866005
C	-4.306558	-0.020718	-2.073042
H	-4.006774	-0.934216	-2.590558
H	-5.314391	0.244628	-2.403042
H	-3.617566	0.774862	-2.354991
C	1.368972	2.108323	-0.662575
C	1.612960	3.163260	0.214322
C	2.368053	1.677738	-1.531711
C	2.864340	3.768849	0.236519
H	0.829753	3.490339	0.887732
C	3.624391	2.271615	-1.491021
H	2.170695	0.852433	-2.205496
C	3.873523	3.314810	-0.606338

H	3.054957	4.585070	0.923558
H	4.412341	1.908719	-2.140128
H	4.855860	3.770808	-0.570970

TS_{D-D'}: $E = -4041.598105$ a.u.

C	-0.592267	-1.436517	-1.415701
O	0.421624	-1.152200	-2.202465
O	-1.267467	-2.469906	-1.853222
C	-0.814477	-3.196028	-3.011479
H	0.187432	-3.583673	-2.833439
H	-1.525799	-4.007517	-3.135415
H	-0.811701	-2.542367	-3.882223
C	-0.935612	-0.691009	-0.255198
C	-2.040493	0.283750	-0.394362
C	-1.809998	1.735832	-0.414965
C	-0.697641	2.269854	-1.097287
C	-2.647133	2.676085	0.221697
C	-0.456387	3.633773	-1.152611
H	-0.028078	1.595283	-1.615225
C	-2.411175	4.044764	0.155522
H	-3.484558	2.338616	0.822032
C	-1.313087	4.542138	-0.533872
H	0.402406	3.996426	-1.707807
H	-3.082906	4.723722	0.669735
H	-1.124890	5.607365	-0.584653
P	-3.647537	-0.272067	-0.081319
C	-4.244134	-0.266605	1.662402
H	-3.564332	-0.897986	2.237582
H	-4.205798	0.739935	2.077628
H	-5.264081	-0.651911	1.733985
C	-3.889608	-2.014458	-0.532749
H	-3.745307	-2.141947	-1.603736
H	-3.169824	-2.638082	-0.003357
H	-4.903937	-2.305760	-0.253969
C	-4.955383	0.606500	-1.008988
H	-4.859055	0.337909	-2.061503
H	-5.943322	0.319203	-0.644054
H	-4.829864	1.683874	-0.916147
Se	-0.609297	-1.769626	1.300567
B	1.559961	-0.509185	-1.666299
O	2.122044	0.550298	-2.291102
O	2.286034	-1.060317	-0.669616
C	3.273224	0.921196	-1.477784
C	3.585715	-0.413833	-0.713078
C	4.379966	1.399698	-2.399763
H	4.067284	2.323414	-2.888869
H	5.286375	1.604932	-1.824342
H	4.608431	0.663487	-3.169423
C	2.816519	2.040469	-0.552280
H	3.637666	2.387962	0.078268
H	2.459292	2.874870	-1.157362
H	1.997052	1.708148	0.087201
C	4.503167	-1.347079	-1.497655
H	5.523684	-0.960676	-1.533296
H	4.513763	-2.319395	-1.003311
H	4.144538	-1.484129	-2.520529
C	4.084098	-0.231468	0.707014

H	4.261149	-1.210145	1.156402
H	5.023460	0.328675	0.711566
H	3.349977	0.290670	1.318494
C	0.689554	-0.707962	2.260202
C	0.686339	0.681421	2.147416
C	1.559513	-1.328758	3.155134
C	1.549338	1.441407	2.931012
H	0.005269	1.159503	1.450507
C	2.419165	-0.562734	3.937507
H	1.566281	-2.410250	3.238408
C	2.415562	0.824729	3.830936
H	1.535436	2.522264	2.840903
H	3.095634	-1.052852	4.628702
H	3.081176	1.420673	4.444056

D': $E = -4041.682009$ a.u.

C	-0.866377	-0.036734	-1.438096
O	0.249443	-0.570011	-2.038916
O	-2.012921	-0.404929	-2.031323
C	-2.245193	-1.814093	-2.039681
H	-2.278425	-2.192581	-1.013277
H	-3.212111	-1.958913	-2.515638
H	-1.466977	-2.328033	-2.607314
C	-0.771865	0.865593	-0.452024
C	0.497440	1.468434	-0.031115
C	1.012837	1.286265	1.317069
C	0.502406	0.246610	2.123736
C	2.043735	2.066718	1.883396
C	0.986585	0.013951	3.401532
H	-0.251448	-0.406885	1.703264
C	2.539102	1.814186	3.155752
H	2.475743	2.893182	1.330290
C	2.015763	0.787597	3.934068
H	0.565521	-0.798666	3.984828
H	3.336123	2.437630	3.545961
H	2.394935	0.598948	4.930497
P	1.222804	2.567174	-1.139128
C	1.172595	4.353756	-0.717404
H	0.126289	4.664522	-0.728134
H	1.568607	4.528047	0.281906
H	1.737373	4.942871	-1.443268
C	0.389559	2.503064	-2.746217
H	0.522183	1.516869	-3.189898
H	-0.675429	2.695185	-2.609444
H	0.822925	3.267405	-3.393401
C	2.978567	2.214092	-1.481604
H	3.543650	2.201376	-0.549287
H	3.031223	1.219761	-1.930882
H	3.400424	2.961732	-2.155953
Se	-2.385763	1.590501	0.361160
B	1.195774	-1.203547	-1.273849
O	2.504376	-1.260538	-1.670283
O	0.918092	-1.939993	-0.157442
C	3.221723	-1.941470	-0.610023
C	2.083579	-2.761692	0.087060
C	4.322572	-2.784177	-1.229884
H	5.067803	-2.129014	-1.684223

H	4.817335	-3.386377	-0.463333
H	3.931453	-3.445115	-2.002440
C	3.810323	-0.870069	0.301746
H	4.407752	-1.316076	1.099622
H	4.458341	-0.222219	-0.292336
H	3.023855	-0.260815	0.754303
C	1.821341	-4.102541	-0.594950
H	2.633081	-4.809439	-0.411697
H	0.895936	-4.520233	-0.195521
H	1.703631	-3.975935	-1.673874
C	2.261213	-2.947490	1.582672
H	1.414133	-3.511813	1.978016
H	3.175243	-3.511872	1.787561
H	2.305684	-1.989972	2.099338
C	-3.486481	0.011831	0.499788
C	-4.543684	-0.193689	-0.384714
C	-3.224822	-0.925438	1.497347
C	-5.329109	-1.336214	-0.275428
H	-4.728140	0.531387	-1.167820
C	-4.002984	-2.075805	1.593316
H	-2.418800	-0.746634	2.199083
C	-5.055001	-2.282861	0.707567
H	-6.151272	-1.491171	-0.964672
H	-3.792333	-2.803722	2.368053
H	-5.664159	-3.175524	0.786681

$TD_{D,E}: E = -4041.677367 \text{ a.u.}$

C	-0.330836	0.904208	-1.840888
O	0.955723	0.677348	-2.170205
O	-1.134913	1.102411	-2.892751
C	-0.741315	0.500694	-4.123998
H	-0.600296	-0.575836	-3.999469
H	-1.561170	0.692148	-4.812029
H	0.179558	0.944368	-4.501253
C	-0.713094	1.008384	-0.552163
C	0.334148	0.949405	0.497103
C	0.202012	-0.043655	1.571130
C	-0.549857	-1.212745	1.340619
C	0.805836	0.069358	2.838321
C	-0.695610	-2.189050	2.312933
H	-1.002659	-1.357423	0.369088
C	0.676448	-0.921944	3.805595
H	1.397459	0.942793	3.092300
C	-0.081010	-2.059728	3.556722
H	-1.293038	-3.066271	2.088958
H	1.164478	-0.792320	4.765331
H	-0.192878	-2.825515	4.314316
P	0.968279	2.530719	0.856202
C	0.142164	3.472911	2.192772
H	0.611757	4.447617	2.339753
H	-0.904700	3.601180	1.911384
H	0.174674	2.902816	3.121346
C	0.822910	3.594604	-0.604980
H	1.318762	3.110606	-1.447650
H	-0.227069	3.751733	-0.851125
H	1.300329	4.552791	-0.393633
C	2.744915	2.593721	1.249756

H	2.979927	2.018263	2.143360
H	3.281649	2.163245	0.402647
H	3.043161	3.633085	1.400849
Se	-2.554828	1.460600	-0.150990
B	1.727917	-0.097515	-1.286787
O	3.067466	0.177815	-1.139923
O	1.393949	-1.388615	-0.976021
C	3.670882	-0.960541	-0.484831
C	2.610504	-2.108391	-0.709181
C	5.024950	-1.216096	-1.130231
H	5.678893	-0.363000	-0.940671
H	5.490778	-2.107542	-0.702149
H	4.937127	-1.345429	-2.207949
C	3.862517	-0.609855	0.986676
H	4.317720	-1.439454	1.531202
H	4.526739	0.253625	1.061752
H	2.908066	-0.369619	1.456612
C	2.892564	-2.947631	-1.954082
H	3.791605	-3.556461	-1.837547
H	2.041198	-3.608669	-2.123064
H	3.008077	-2.310956	-2.833816
C	2.391205	-3.008581	0.497015
H	1.609496	-3.732890	0.260332
H	3.307058	-3.554401	0.741054
H	2.063300	-2.441111	1.368735
C	-3.364414	-0.289418	-0.158872
C	-3.248790	-1.109887	-1.279579
C	-4.059117	-0.734040	0.962706
C	-3.805422	-2.383686	-1.263258
H	-2.718183	-0.747352	-2.152048
C	-4.633582	-2.001277	0.963690
H	-4.121534	-0.102774	1.840786
C	-4.501072	-2.831578	-0.143889
H	-3.703737	-3.024482	-2.131502
H	-5.167775	-2.346075	1.841338
H	-4.937807	-3.823052	-0.136003

E: $E = -4041.699920$ a.u.

C	-0.221848	-1.843487	-1.160123
O	-1.469099	-1.457722	-1.263428
O	0.216488	-2.759961	-2.020410
C	-0.677173	-3.128087	-3.070154
H	-0.947937	-2.258432	-3.669757
H	-0.130238	-3.849245	-3.672068
H	-1.584011	-3.579794	-2.667048
C	0.530563	-1.303931	-0.156221
C	-0.323847	-0.326230	0.631958
C	0.380923	0.969062	0.989521
C	0.812432	1.785635	-0.066821
C	0.684550	1.384259	2.287708
C	1.505412	2.960979	0.170985
H	0.598091	1.482380	-1.081400
C	1.379768	2.569336	2.530622
H	0.397708	0.792622	3.148918
C	1.793478	3.363317	1.473658
H	1.834948	3.560724	-0.669418
H	1.598914	2.859105	3.551783

H	2.339088	4.281216	1.657572
P	-0.967838	-1.264359	2.055391
C	0.333650	-1.981392	3.110806
H	0.828760	-2.779678	2.558367
H	1.086051	-1.242697	3.379207
H	-0.128854	-2.395113	4.009151
C	-1.900107	-2.710184	1.487499
H	-2.753032	-2.375679	0.899362
H	-1.250253	-3.342035	0.881901
H	-2.231219	-3.264660	2.368109
C	-2.116673	-0.354429	3.135137
H	-1.810561	0.685378	3.236331
H	-3.093221	-0.384318	2.654923
H	-2.154485	-0.830596	4.116369
Se	2.330375	-1.765970	0.202997
B	-1.659891	-0.171743	-0.428473
O	-2.966590	-0.179051	0.204175
O	-1.607512	0.978769	-1.272445
C	-3.629424	1.040222	-0.148274
C	-2.945614	1.404731	-1.501478
C	-5.125596	0.782727	-0.239362
H	-5.520865	0.549485	0.752295
H	-5.648821	1.666808	-0.614695
H	-5.335438	-0.059656	-0.897769
C	-3.334956	2.088583	0.927529
H	-3.831204	3.036914	0.709611
H	-3.704903	1.731951	1.891207
H	-2.257489	2.264840	1.003859
C	-3.527395	0.605885	-2.671203
H	-4.524327	0.959779	-2.946200
H	-2.864048	0.725527	-3.530006
H	-3.577550	-0.456318	-2.424280
C	-2.933885	2.889829	-1.831436
H	-2.472269	3.038636	-2.809653
H	-3.950259	3.292973	-1.866881
H	-2.352261	3.443664	-1.094463
C	3.230534	-0.226263	-0.545707
C	4.066951	0.541417	0.257180
C	3.032161	0.114900	-1.881482
C	4.704651	1.657425	-0.277582
H	4.193482	0.285917	1.302703
C	3.657690	1.239006	-2.405629
H	2.374461	-0.491889	-2.494250
C	4.497310	2.010973	-1.605415
H	5.346417	2.261898	0.352840
H	3.495874	1.509576	-3.442688
H	4.986087	2.885828	-2.017770

TS_E: $E = -4041.674127$ a.u.

C	-0.377087	-1.561155	-1.591987
O	-1.517621	-1.003409	-1.629635
O	-0.060342	-2.465468	-2.488204
C	-1.037708	-2.734205	-3.501818
H	-1.264652	-1.824276	-4.056182
H	-0.582265	-3.478374	-4.148131
H	-1.950441	-3.120396	-3.048524
C	0.514233	-1.183629	-0.555072

C	-0.125803	-0.239138	0.247986
C	0.663982	0.675315	1.120908
C	0.856511	1.988768	0.675279
C	1.314529	0.263960	2.285835
C	1.670164	2.862450	1.388560
H	0.373933	2.306986	-0.240194
C	2.111396	1.145470	3.006406
H	1.216562	-0.760152	2.619396
C	2.292642	2.449849	2.560690
H	1.816531	3.871584	1.021301
H	2.599392	0.807106	3.913289
H	2.919470	3.135788	3.118278
P	-1.363253	-1.672475	1.913576
C	-0.327287	-2.808468	2.937398
H	0.543284	-3.123322	2.356400
H	0.023278	-2.290135	3.831553
H	-0.892757	-3.693189	3.240995
C	-2.165403	-2.893608	0.799910
H	-2.922233	-2.383571	0.204748
H	-1.412828	-3.324547	0.133946
H	-2.618667	-3.701873	1.378606
C	-2.734839	-1.265827	3.069233
H	-2.380858	-0.562924	3.825128
H	-3.522785	-0.789942	2.485453
H	-3.122101	-2.162463	3.560127
Se	2.296933	-1.845313	-0.407862
B	-1.525915	0.186911	-0.521427
O	-2.774907	0.114133	0.175203
O	-1.462167	1.441045	-1.193034
C	-3.392204	1.403086	0.099216
C	-2.786691	1.978078	-1.219012
C	-4.903078	1.229871	0.080542
H	-5.240369	0.841872	1.044608
H	-5.400521	2.188502	-0.091850
H	-5.206424	0.527990	-0.695749
C	-2.963323	2.205747	1.328829
H	-3.449508	3.183655	1.365042
H	-3.241482	1.649378	2.226630
H	-1.879570	2.346585	1.337718
C	-3.501928	1.447147	-2.462789
H	-4.491707	1.894903	-2.581319
H	-2.898378	1.694763	-3.338100
H	-3.604334	0.361415	-2.412823
C	-2.696640	3.495303	-1.267045
H	-2.278331	3.804467	-2.227031
H	-3.686791	3.947851	-1.161882
H	-2.049146	3.871276	-0.474604
C	3.179128	-0.153680	-0.722097
C	4.113388	0.312662	0.195650
C	2.861044	0.603349	-1.847517
C	4.733486	1.541169	-0.015749
H	4.330657	-0.264746	1.086373
C	3.472492	1.834388	-2.044540
H	2.124365	0.236369	-2.552987
C	4.411853	2.304915	-1.130564
H	5.451880	1.908496	0.707807
H	3.216089	2.426503	-2.915174

H 4.886527 3.266343 -1.286217

TS_{D-F}: $E = -7086.061572$ a.u.

C -1.031434 -0.699185 0.519940
O -2.176506 -0.902818 1.234732
O -0.161268 -1.716570 0.605801
C -0.729393 -3.013980 0.802530
H -1.535145 -3.191273 0.083209
H 0.078003 -3.721501 0.633752
H -1.108445 -3.120817 1.819120
C -0.766322 0.424001 -0.175084
C 0.415836 0.639162 -1.057830
C 0.906440 2.031093 -1.078914
C 0.911176 2.748441 0.132008
C 1.309703 2.738734 -2.226556
C 1.206621 4.103062 0.180016
H 0.653244 2.223468 1.044275
C 1.625206 4.091599 -2.175270
H 1.359580 2.249550 -3.192832
C 1.557011 4.794240 -0.977297
H 1.158319 4.618927 1.133476
H 1.916107 4.601534 -3.087018
H 1.782719 5.852964 -0.944410
P 0.128959 -0.115295 -2.614569
C -1.118499 0.728813 -3.662469
H -0.874763 1.786848 -3.760179
H -1.175137 0.262741 -4.648588
H -2.086606 0.639346 -3.164269
C -0.564718 -1.779944 -2.454303
H 0.105907 -2.392300 -1.853001
H -1.550784 -1.716409 -1.991080
H -0.657344 -2.200113 -3.458345
C 1.640183 -0.267267 -3.630463
H 1.494469 0.216423 -4.597488
H 2.481194 0.191679 -3.108737
H 1.857385 -1.324806 -3.786465
Se -2.221483 1.742608 -0.228926
B -3.371475 -1.076187 0.589923
O -4.553680 -1.122193 1.260531
O -3.478854 -1.350186 -0.753480
C -5.593430 -1.184304 0.256751
C -4.836954 -1.802178 -0.969896
C -6.735561 -2.032623 0.787502
H -7.197499 -1.523663 1.634691
H -7.496038 -2.174730 0.015060
H -6.385200 -3.007443 1.124488
C -6.057601 0.247244 0.006927
H -6.888629 0.277776 -0.701002
H -6.387375 0.673754 0.955278
H -5.237355 0.860211 -0.371917
C -4.801556 -3.327523 -0.937212
H -5.784032 -3.755261 -1.146300
H -4.099565 -3.678790 -1.696024
H -4.463872 -3.687218 0.037632
C -5.307359 -1.302711 -2.324136
H -4.727404 -1.786866 -3.112522
H -6.362081 -1.545764 -2.476697

H	-5.176693	-0.224494	-2.410863
C	-1.983354	2.722792	1.411402
C	-1.740300	2.073574	2.620056
C	-2.072421	4.112756	1.368171
C	-1.565982	2.823655	3.778426
H	-1.687177	0.992543	2.653544
C	-1.921863	4.852578	2.536090
H	-2.227386	4.612649	0.419118
C	-1.660284	4.211353	3.742362
H	-1.366570	2.317473	4.715751
H	-1.989481	5.933607	2.497211
H	-1.530004	4.789437	4.649294
Se	2.758062	-2.260991	-0.872137
B	2.787320	-0.308176	-0.350000
O	3.594247	0.430808	-1.190741
O	2.817134	0.137813	0.946453
C	4.530135	1.170403	-0.367580
C	4.093286	0.802905	1.116247
C	5.925819	0.678275	-0.741568
H	6.117940	0.937174	-1.784189
H	6.688143	1.158764	-0.123250
H	6.010398	-0.403160	-0.639440
C	4.412616	2.646862	-0.707983
H	5.159938	3.227815	-0.161251
H	4.590117	2.774202	-1.777748
H	3.425625	3.036469	-0.481429
C	5.009736	-0.218724	1.792405
H	6.015388	0.178650	1.943624
H	4.586730	-0.472375	2.766214
H	5.073356	-1.139244	1.208441
C	3.896577	1.999025	2.033477
H	3.530696	1.646084	2.999482
H	4.846549	2.515700	2.193286
H	3.173420	2.702297	1.625495
C	2.537885	-3.245159	0.763165
C	2.247257	-2.670454	2.000990
C	2.663012	-4.633269	0.659994
C	2.072558	-3.488516	3.113209
H	2.138882	-1.599130	2.085222
C	2.481015	-5.440222	1.776930
H	2.898007	-5.082697	-0.298685
C	2.180212	-4.871287	3.010155
H	1.841394	-3.033774	4.069885
H	2.576783	-6.515510	1.680182
H	2.036902	-5.498647	3.881544

F: $E = -7086.086564$ a.u.

C	0.982677	-0.340082	-1.238647
O	1.951932	-1.154109	-1.729915
O	-0.015753	-0.144555	-2.078243
C	-0.438741	-1.218805	-2.918328
H	-0.681419	-2.095009	-2.312786
H	-1.336364	-0.846322	-3.405570
H	0.331737	-1.451498	-3.654190
C	1.047602	0.334813	-0.072707
C	-0.142744	1.080916	0.523072
C	-0.078501	2.573813	0.213579

C	0.447612	2.986653	-1.014136
C	-0.608156	3.557513	1.054488
C	0.495535	4.330013	-1.361973
H	0.810677	2.244162	-1.711534
C	-0.559678	4.904711	0.711841
H	-1.094271	3.277507	1.981820
C	0.003628	5.299959	-0.495721
H	0.920524	4.615480	-2.317343
H	-0.973716	5.642887	1.389359
H	0.044489	6.348999	-0.763569
P	0.002893	0.789898	2.380811
C	1.065517	2.054622	3.185078
H	0.467724	2.620740	3.900989
H	1.887807	1.557856	3.697810
H	1.466339	2.735932	2.439067
C	0.713025	-0.853795	2.758077
H	1.007125	-1.385647	1.852334
H	1.578400	-0.726177	3.409359
H	-0.057089	-1.440974	3.257818
C	-1.509469	0.809547	3.391308
H	-2.011667	1.771679	3.339403
H	-2.186148	0.039031	3.026073
H	-1.180326	0.596163	4.412584
Se	2.820050	0.490176	0.704403
B	2.410232	-2.229161	-1.008311
O	3.339915	-3.077056	-1.526185
O	1.951441	-2.586478	0.228075
C	3.691274	-3.991660	-0.458445
C	2.419373	-3.937682	0.453740
C	3.984722	-5.354599	-1.057606
H	4.884854	-5.295452	-1.671651
H	4.154887	-6.089885	-0.266675
H	3.162729	-5.695114	-1.685972
C	4.929455	-3.419182	0.223821
H	5.295156	-4.085857	1.007688
H	5.713138	-3.293655	-0.524775
H	4.714348	-2.440509	0.659686
C	1.307364	-4.869927	-0.015117
H	1.553199	-5.914895	0.186325
H	0.388109	-4.607619	0.511220
H	1.126961	-4.751536	-1.086275
C	2.683730	-4.115433	1.937775
H	1.737273	-4.060893	2.479692
H	3.135023	-5.091981	2.132115
H	3.346542	-3.337155	2.316726
C	3.415488	2.064892	-0.249100
C	3.582099	2.002786	-1.631576
C	3.662772	3.250498	0.434532
C	3.963828	3.141753	-2.329382
H	3.396428	1.070516	-2.154067
C	4.054776	4.386011	-0.269271
H	3.541534	3.292162	1.510622
C	4.197102	4.335099	-1.650316
H	4.085355	3.096226	-3.405386
H	4.235508	5.312198	0.263078
H	4.492520	5.221847	-2.198511
Se	-1.617861	-1.628411	0.535766

B	-1.761166	0.598835	0.101903
O	-2.617641	1.309155	1.001768
O	-2.291136	0.777378	-1.203126
C	-3.820925	1.694333	0.340044
C	-3.403965	1.678923	-1.173238
C	-4.910940	0.680313	0.689525
H	-5.005259	0.637649	1.777535
H	-5.877097	0.971511	0.269497
H	-4.661235	-0.317911	0.334050
C	-4.235292	3.066491	0.860599
H	-5.124318	3.425861	0.334926
H	-4.479431	2.988242	1.923219
H	-3.436577	3.798085	0.739755
C	-4.490677	1.160281	-2.108848
H	-5.354027	1.832070	-2.098825
H	-4.097846	1.128486	-3.128249
H	-4.822407	0.161370	-1.833449
C	-2.933933	3.040391	-1.691081
H	-2.464550	2.889625	-2.665636
H	-3.773524	3.730647	-1.808982
H	-2.197655	3.496893	-1.032769
C	-3.286697	-2.340929	-0.076360
C	-3.701308	-2.151913	-1.396384
C	-4.092998	-3.093579	0.782301
C	-4.902592	-2.693449	-1.842921
H	-3.093231	-1.543064	-2.053148
C	-5.288297	-3.641036	0.329774
H	-3.779790	-3.238070	1.809531
C	-5.700877	-3.441564	-0.984122
H	-5.215874	-2.525666	-2.867783
H	-5.903123	-4.221181	1.008870
H	-6.635393	-3.863478	-1.334512

TS_{F-G}: $E = -7086.048128$ a.u.

C	-0.670568	0.405142	-1.302980
O	-1.650151	1.262028	-1.499613
O	0.228834	0.385639	-2.238739
C	0.378453	1.546453	-3.072303
H	0.639504	2.400862	-2.445665
H	1.195804	1.304039	-3.743329
H	-0.541963	1.727316	-3.624906
C	-0.681339	-0.626688	-0.352941
C	0.499407	-1.235732	0.089935
C	0.477680	-2.698606	0.347953
C	-0.156380	-3.490350	-0.619538
C	1.196266	-3.345096	1.361546
C	-0.080848	-4.877999	-0.574107
H	-0.679214	-3.005790	-1.435490
C	1.252600	-4.730108	1.418244
H	1.736187	-2.751804	2.085196
C	0.617024	-5.504470	0.450241
H	-0.567296	-5.464378	-1.345267
H	1.808940	-5.208897	2.215817
H	0.674008	-6.585660	0.492348
P	0.392722	-0.498246	2.800184
C	-0.403044	-1.741501	3.912531
H	-0.462641	-1.368902	4.938766

H	-1.408605	-1.956492	3.545992
H	0.163358	-2.673697	3.903155
C	-0.619797	0.984252	3.209792
H	-0.225253	1.849481	2.675830
H	-1.641987	0.820071	2.865914
H	-0.619760	1.171383	4.287741
C	1.958024	-0.149547	3.697608
H	2.590378	-1.038076	3.673580
H	2.483563	0.644559	3.165146
H	1.761671	0.145540	4.731914
Se	-2.377184	-1.063399	0.459340
B	-2.435116	1.918483	-0.554303
O	-3.654775	2.367133	-0.952533
O	-2.052127	2.298654	0.686209
C	-4.262075	2.967272	0.221613
C	-3.008948	3.313389	1.098503
C	-5.081215	4.168900	-0.212880
H	-5.926308	3.832516	-0.815478
H	-5.470853	4.697541	0.660876
H	-4.487422	4.860440	-0.809021
C	-5.154290	1.901507	0.848678
H	-5.698170	2.296853	1.708827
H	-5.876490	1.567326	0.101773
H	-4.564799	1.038234	1.164590
C	-2.383207	4.658603	0.744229
H	-3.008007	5.488761	1.079655
H	-1.409725	4.726266	1.231904
H	-2.228955	4.747524	-0.333422
C	-3.241171	3.210056	2.594291
H	-2.316975	3.444792	3.124820
H	-4.008208	3.925800	2.902052
H	-3.558606	2.209178	2.884069
C	-3.363128	-1.875073	-0.994832
C	-4.027617	-1.080486	-1.928612
C	-3.456535	-3.264591	-1.060406
C	-4.756198	-1.685225	-2.948669
H	-3.987320	0.000278	-1.857181
C	-4.195523	-3.859636	-2.077318
H	-2.946169	-3.871341	-0.321698
C	-4.839226	-3.071120	-3.025465
H	-5.266922	-1.068519	-3.678584
H	-4.267924	-4.939668	-2.126930
H	-5.411636	-3.536533	-3.818932
Se	1.621292	1.636884	0.346972
B	2.025794	-0.569913	-0.053958
O	2.884366	-1.084297	0.961110
O	2.671594	-0.755898	-1.310670
C	4.182051	-1.292687	0.406006
C	3.870251	-1.516646	-1.111532
C	5.028071	-0.046167	0.670046
H	5.012045	0.157372	1.743121
H	6.065008	-0.192396	0.356733
H	4.625417	0.827005	0.156004
C	4.812896	-2.494404	1.098727
H	5.774866	-2.744841	0.642520
H	4.988119	-2.252545	2.149843
H	4.160785	-3.367093	1.048011

C	4.953725	-1.005323	-2.053222
H	5.886331	-1.553837	-1.892114
H	4.638328	-1.166887	-3.086894
H	5.143694	0.057780	-1.911232
C	3.556886	-2.975832	-1.452018
H	3.150859	-3.009921	-2.465024
H	4.453797	-3.599285	-1.413044
H	2.810574	-3.392754	-0.774202
C	2.935280	2.610353	-0.654562
C	3.407521	2.170616	-1.895787
C	3.424532	3.815422	-0.138968
C	4.348155	2.919742	-2.596695
H	3.058874	1.221773	-2.283282
C	4.354205	4.564915	-0.850042
H	3.075683	4.156770	0.828755
C	4.822940	4.121756	-2.083273
H	4.712458	2.555681	-3.551630
H	4.720697	5.496135	-0.432774
H	5.553240	4.703333	-2.632971

G: $E = -6625.035674$ a.u.

C	-0.661167	-0.986972	0.039226
O	-1.900042	-1.003173	-0.602882
O	-0.604867	-1.991481	0.962150
C	-1.261441	-3.212466	0.625196
H	-1.047372	-3.499775	-0.406622
H	-0.856900	-3.958563	1.306443
H	-2.338760	-3.106124	0.766101
C	-0.418198	0.322265	0.779787
C	0.715298	1.020265	0.789031
C	0.884645	2.262719	1.605127
C	1.067872	2.186490	2.987238
C	0.962745	3.504208	0.971691
C	1.304821	3.337790	3.726759
H	1.019087	1.217432	3.470900
C	1.190561	4.657121	1.716333
H	0.855550	3.551732	-0.106209
C	1.363561	4.576179	3.093603
H	1.444036	3.269621	4.799220
H	1.239785	5.618357	1.218347
H	1.547091	5.473639	3.672246
Se	-1.976296	1.049233	1.690541
B	-2.244785	-0.017766	-1.480496
O	-3.497710	0.066504	-2.017158
O	-1.378312	0.942912	-1.923310
C	-3.550011	1.336619	-2.712153
C	-2.038253	1.611897	-3.021913
C	-4.430724	1.187916	-3.939563
H	-5.459122	1.000580	-3.626633
H	-4.413226	2.105416	-4.533743
H	-4.104874	0.355891	-4.562477
C	-4.144230	2.349274	-1.737848
H	-4.264763	3.328622	-2.205591
H	-5.125103	1.991746	-1.419305
H	-3.513478	2.451187	-0.851704
C	-1.560124	0.931253	-4.301035
H	-1.967732	1.418820	-5.189049

H	-0.470899	0.985634	-4.336205
H	-1.848418	-0.122361	-4.312114
C	-1.638395	3.076202	-3.007064
H	-0.571720	3.158450	-3.222846
H	-2.191046	3.632632	-3.768759
H	-1.825965	3.524023	-2.031723
C	-2.938530	-0.550911	2.177766
C	-4.086457	-0.909810	1.476035
C	-2.519217	-1.306427	3.270620
C	-4.818777	-2.024595	1.875623
H	-4.387454	-0.337967	0.605776
C	-3.244198	-2.428318	3.654072
H	-1.620754	-1.021604	3.804170
C	-4.398266	-2.784744	2.961241
H	-5.711542	-2.302794	1.328348
H	-2.911759	-3.020196	4.498651
H	-4.966838	-3.655076	3.266849
Se	0.763771	-1.271372	-1.426638
B	2.094307	0.733603	0.079714
O	2.586318	1.518610	-0.933037
O	3.084601	0.044311	0.743162
C	3.979876	1.174101	-1.102358
C	4.346663	0.591775	0.301259
C	4.076207	0.133169	-2.214639
H	3.568834	0.520355	-3.100096
H	5.118675	-0.073721	-2.467240
H	3.595126	-0.802293	-1.924499
C	4.740561	2.432154	-1.485985
H	5.816589	2.239130	-1.506944
H	4.429581	2.752988	-2.481848
H	4.537627	3.241646	-0.785424
C	5.385033	-0.516510	0.285162
H	6.325346	-0.155855	-0.140745
H	5.576196	-0.846945	1.307808
H	5.037255	-1.374380	-0.290107
C	4.721998	1.676818	1.308792
H	4.762254	1.228410	2.302850
H	5.695555	2.116555	1.081120
H	3.967707	2.468595	1.326020
C	1.601113	-2.873633	-0.776052
C	2.163102	-2.944143	0.499341
C	1.674353	-3.972365	-1.633591
C	2.776733	-4.122290	0.912264
H	2.124951	-2.085397	1.155049
C	2.308488	-5.138443	-1.218742
H	1.225305	-3.915150	-2.618385
C	2.854386	-5.217680	0.057628
H	3.205452	-4.177998	1.906074
H	2.363948	-5.987288	-1.889953
H	3.339930	-6.129334	0.384930

TS_G: $E = -6625.000863$ a.u.

C	-0.625288	0.197492	0.751037
O	-1.880631	0.085268	0.428064
O	-0.308871	-0.024713	1.992939
C	-1.345126	-0.452053	2.908826
H	-1.912715	-1.280386	2.493337

H	-0.812047	-0.755328	3.804453
H	-1.993857	0.402810	3.105233
C	0.292787	1.180543	0.087465
C	1.553364	0.959623	-0.283886
C	2.446672	2.052988	-0.773903
C	2.896906	3.045175	0.099346
C	2.904549	2.045073	-2.092494
C	3.773801	4.026705	-0.343984
H	2.551549	3.040957	1.126642
C	3.769344	3.038291	-2.538183
H	2.581843	1.254079	-2.758834
C	4.206792	4.029240	-1.666161
H	4.116093	4.792329	0.342001
H	4.107622	3.032629	-3.567497
H	4.886110	4.798344	-2.013768
Se	-0.573963	2.908607	-0.083666
B	-2.080625	-0.516355	-0.919591
O	-3.287871	-1.198674	-1.082116
O	-1.810953	0.313928	-2.011361
C	-3.928526	-0.626741	-2.238453
C	-2.713795	-0.080152	-3.056775
C	-4.737698	-1.702995	-2.940964
H	-5.564847	-2.013907	-2.299879
H	-5.153612	-1.320841	-3.877395
H	-4.123555	-2.576681	-3.156836
C	-4.839973	0.494869	-1.741871
H	-5.423280	0.932810	-2.555183
H	-5.524715	0.082379	-0.999043
H	-4.247013	1.280757	-1.267643
C	-2.040695	-1.164760	-3.896741
H	-2.649643	-1.429294	-4.764359
H	-1.078872	-0.784638	-4.246247
H	-1.856978	-2.063269	-3.304898
C	-3.021072	1.137068	-3.913429
H	-2.121360	1.433567	-4.455687
H	-3.803258	0.908012	-4.642716
H	-3.339815	1.977978	-3.298425
C	-1.359189	2.946976	1.678929
C	-2.745805	2.931804	1.813159
C	-0.548876	3.003230	2.813004
C	-3.320026	2.992630	3.080330
H	-3.367933	2.858543	0.929812
C	-1.126635	3.042661	4.076358
H	0.528858	3.004471	2.702263
C	-2.512887	3.045303	4.211318
H	-4.398750	2.985999	3.180849
H	-0.494107	3.080807	4.955264
H	-2.961446	3.085988	5.196695
Se	-0.262419	-1.899071	-0.717851
B	2.357028	-0.398917	-0.184556
O	3.028141	-0.909304	-1.258044
O	2.755592	-0.944994	1.009669
C	3.863168	-1.990968	-0.778880
C	3.997876	-1.644332	0.739491
C	3.129928	-3.304526	-1.027299
H	2.848093	-3.354694	-2.080163
H	3.772728	-4.156153	-0.792267

H	2.216709	-3.374848	-0.435011
C	5.170187	-1.959970	-1.554001
H	5.878439	-2.682311	-1.139231
H	4.977456	-2.227317	-2.594285
H	5.619024	-0.967421	-1.532788
C	4.113448	-2.843889	1.663208
H	5.026831	-3.402427	1.441883
H	4.164333	-2.499652	2.697850
H	3.262376	-3.516459	1.562486
C	5.116725	-0.642829	1.018883
H	5.025853	-0.297616	2.049940
H	6.101650	-1.094450	0.884086
H	5.032892	0.225539	0.359691
C	-0.767233	-2.934450	0.812596
C	0.151338	-3.099005	1.852601
C	-2.050387	-3.473998	0.924889
C	-0.213170	-3.803695	2.995543
H	1.127575	-2.631517	1.780335
C	-2.407337	-4.169133	2.075971
H	-2.766576	-3.317264	0.126915
C	-1.492937	-4.337267	3.112673
H	0.502683	-3.924719	3.800991
H	-3.406965	-4.579040	2.163229
H	-1.777015	-4.881135	4.005682

TS_{1P}(PC₃): E = -1583.178416

C	-2.428029	-2.073723	-0.705198
O	-2.893678	-2.554598	0.307780
O	-3.189709	-1.360268	-1.579760
C	-4.557493	-1.227478	-1.204805
H	-4.651251	-0.637696	-0.289554
H	-5.043759	-0.717843	-2.033675
H	-5.009587	-2.205176	-1.037723
C	-1.078010	-2.170362	-1.135546
C	0.064653	-1.661185	-1.100886
C	1.451212	-1.856566	-1.520736
C	2.156550	-2.973223	-1.070637
C	2.094016	-0.922472	-2.337760
C	3.494578	-3.138595	-1.414185
H	1.646883	-3.695815	-0.444486
C	3.426135	-1.094710	-2.686258
H	1.539644	-0.058605	-2.689887
C	4.133641	-2.198986	-2.215497
H	4.038872	-4.002964	-1.052729
H	3.915528	-0.368303	-3.324313
H	5.176685	-2.327673	-2.478307
P	0.141996	0.315727	0.117012
C	-0.388363	-0.097792	1.863325
C	-1.229957	1.287833	-0.672821
C	1.675498	1.363827	0.308048
C	-1.882746	0.105412	2.161464
C	0.017254	-1.547241	2.200070
H	0.180128	0.576477	2.515986

C	-1.467872	2.728556	-0.196888
C	-1.123798	1.270504	-2.207905
H	-2.115502	0.690707	-0.416823
C	1.608037	2.616977	1.198049
C	2.818673	0.453321	0.804165
H	1.913854	1.675229	-0.719251
C	-2.192712	-0.232830	3.623797
H	-2.473347	-0.559440	1.523408
H	-2.190240	1.131741	1.949831
C	-0.287424	-1.874028	3.663645
H	-0.553855	-2.225536	1.558460
H	1.076880	-1.710121	1.977868
C	-2.773547	3.269766	-0.787525
H	-0.644116	3.356625	-0.554105
H	-1.476515	2.800754	0.893129
C	-2.399673	1.841561	-2.835362
H	-0.256387	1.869263	-2.519089
H	-0.974757	0.250242	-2.564388
C	2.948120	3.364599	1.187505
H	1.380717	2.317654	2.227652
H	0.814883	3.290861	0.881049
C	4.158396	1.192932	0.790781
H	2.593578	0.140485	1.832502
H	2.888285	-0.453753	0.200160
C	-1.773114	-1.664071	3.960494
H	-3.261267	-0.096117	3.809903
H	-1.661197	0.467992	4.279822
H	0.000910	-2.906558	3.876696
H	0.312962	-1.231200	4.319944
C	-2.722097	3.243854	-2.316454
H	-2.953699	4.286749	-0.428999
H	-3.609432	2.652279	-0.436149
H	-2.304127	1.851556	-3.924147
H	-3.223543	1.160104	-2.594746
C	4.098843	2.464603	1.637403
H	2.880768	4.247360	1.829002
H	3.146495	3.725238	0.171040
H	4.949304	0.529656	1.150105
H	4.407375	1.451870	-0.245542
H	-1.990596	-1.887688	5.008154
H	-2.357950	-2.358191	3.346618
H	-3.668463	3.595040	-2.735736
H	-1.946587	3.941702	-2.655164
H	5.047380	3.005079	1.584632
H	3.947583	2.188137	2.687828