Supporting Information

Enantioselective Synthesis of Allylic Boronates bearing a Stereodefined (*E*)-Alkenyl Chloride by Cu-Catalyzed Borylation of Allylic *gem*-Dichlorides

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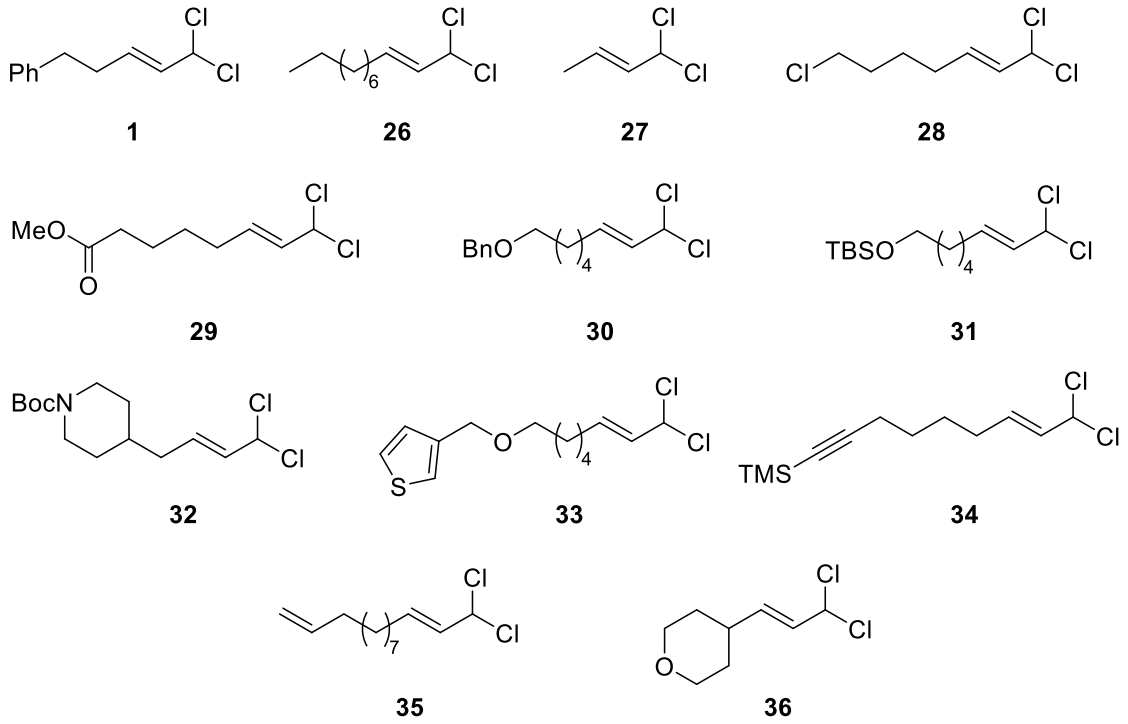
1. General methods.

- All reactions were performed under argon atmosphere using oven dried glassware and using standard Schlenk techniques. Solvents were dried using an MBraun SPS 800 system. All chemicals were purchased from Acros Organics Ltd., Aldrich Chemical Co. Ltd., Alfa Aesar, Apollo, Strem Chemicals Inc., Fluorochem Ltd., TCI Europe N.V., BLD Pharmatec or Eurisotop chemical companies and used without further purification, unless otherwise noted.
- In order to preclude side hydroboration reactions, B_2pin_2 was dried over Na_2SO_4 prior to being used.
- Analytical thin layer chromatography was carried out on silica-coated aluminium plates (silica gel 60 F254 Merck) and components were visualized by UV light and $KMnO_4$ staining. Flash column chromatography was performed in Büchi Pure C-815 flash using Büchi flash pure eco flex cartridges or on silica gel 60 (Merck, 230-400 mesh) without previous deactivation, unless otherwise stated.
- GC-MS analyses were performed in an Agilent instrument GC-6890N equipped with Chemical Ionization (CI) MS-5973 detector.
- High Resolution Mass spectrometry was carried out on a Bruker microTOF spectrometer using ESI or APCI.
- ^{1}H, ^{13}C, ^{11}B and 2D NMR experiments were carried out using a Varian Inova 500MHz or a Varian Mercury 300MHz NMR spectrometer. Chemical shift values are reported in ppm with the solvent resonance as the internal standard ($CHCl_3$: δ 7.26 for ^{1}H, δ 77.16 for ^{13}C). Coupling constants (*J*) are given in Hertz (Hz). Multiplicities are reported as follows: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet or as a combination of them.
- Because of quadrupolar relaxation, in all cases the carbon directly attached to the boron atom was not detected by ^{13}C NMR technique.
- Melting point were determined using a Buchi-M565 apparatus.
- Specific rotation was determined in a Jasco P-2000 Polarimeter.
- Enantiomeric ratios were determined by Supercritical Fluid Chromatography (SFC) analysis in a Jasco Series 4000 instrument or by High Performance Liquid Chromatography (uHPLC) analysis using a WATERS ACQUITY Arc System, consisting of a quaternary pump, column oven and autosampler coupled with a 2998 PDA detector.

2. List of starting materials, boron sources and chiral ligands

Ligands **L1-L4** and **L11-L21** and diboron compounds **37**, **39-42** were purchased from commercial sources. Dichloride **27**,[1] diboron compound **38**[2] and ligands **L5**,[3] **L22**,[4] **L23**,[5] **L24**,[6] **L25**,[7] **L6**,[8] **L28**,[9] **L29**,[10] **L8**,[11] **L9**,[12] **L10**[13] were prepared according to literature procedures.

- **Allylic *gem*-dichlorides:**



Note: allylic *gem*-dichlorides were synthesized from the corresponding aldehyde.

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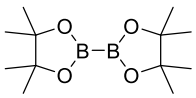
- **Boronic esters**



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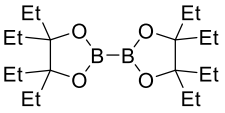

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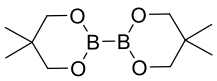

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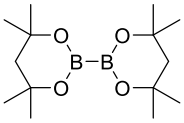

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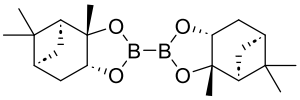

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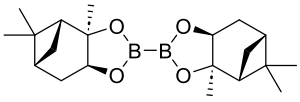

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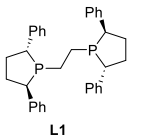

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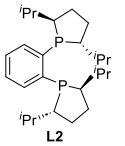

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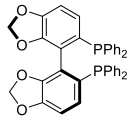

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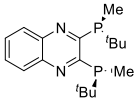

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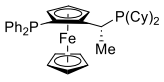

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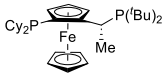

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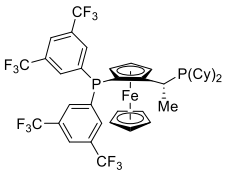

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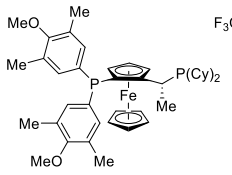

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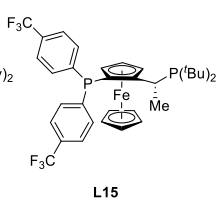

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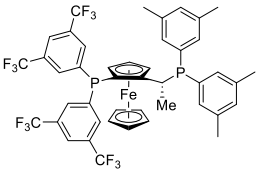

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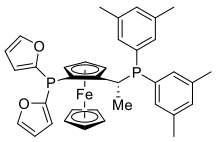

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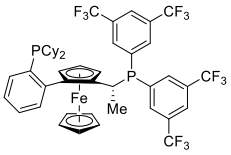

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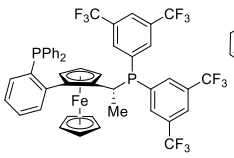

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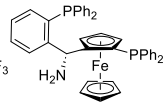

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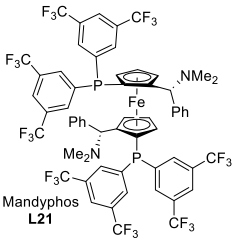

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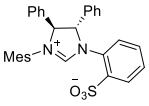

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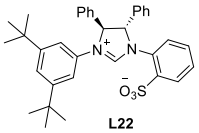

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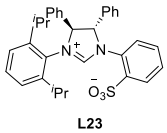

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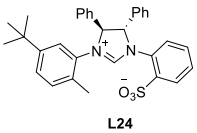

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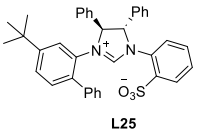

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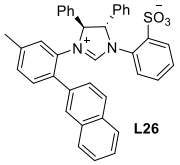

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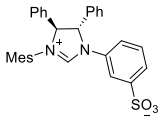

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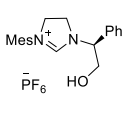

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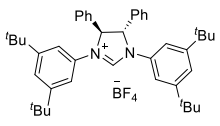

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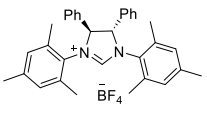

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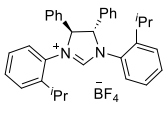

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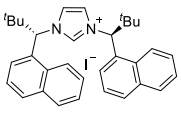

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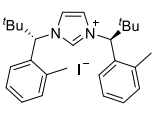

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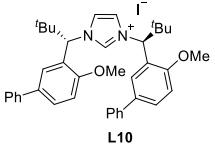

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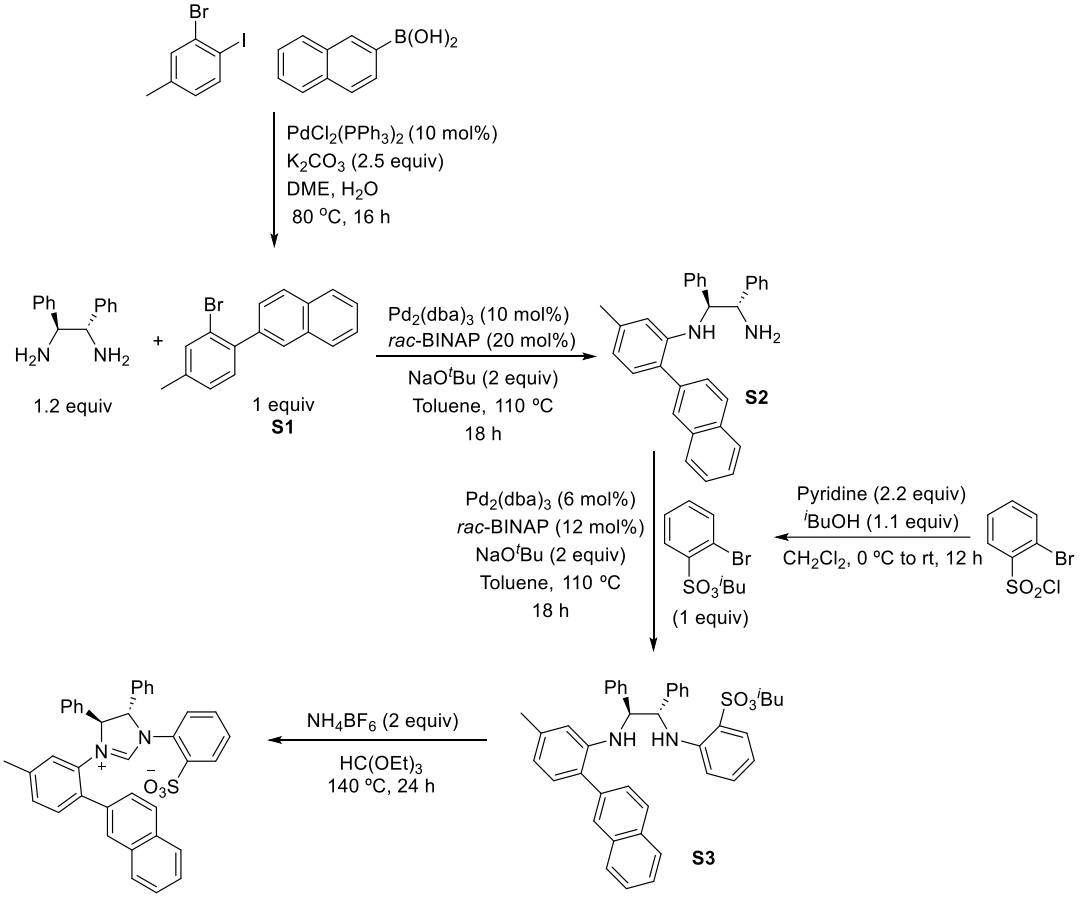
3. Synthesis and characterization of chiral ligands.

3.1. Synthesis of chiral ligand L26.



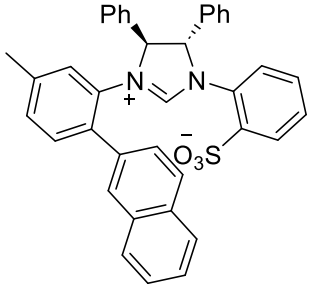
First step: A flame-dried round-bottom flask equipped with reflux condenser was charged with naphthalen-2-ylboronic acid (1 equiv, 10 mmol), $PdCl_2(PPh_3)_2$ (10 mol%, 1 mmol) and K_2CO_3 (2.5 equiv, 25 mmol) under a dry argon atmosphere. A solution of the 2-bromo-1-iodo-4-methylbenzene (1 equiv, 10 mmol) in DME [0.3 M] was added and then H_2O [0.5 M]. The resulting mixture was stirred at 80 °C for 22 h. After that time, the mixture was allowed to cool to room temperature and filtered through a celite pad. The resulting brown oil was purified by silica gel column chromatography (Hexane) to afford the corresponding bromobenzene derivative as a white solid **S1** in 74% yield.

Second step: A flame-dried round-bottom flask equipped with reflux condenser was charged with (-)-(*S*,*S*)-1,2-Diphenylethylenediamine (1.2 equiv, 8.9 mmol), $Pd_2(dba)_3$ (10 mol%, 0.74 mmol), *rac*-BINAP (20 mol%, 1.5 mmol) and NaO^{t}Bu (1.5 equiv, 18.6 mmol) under a dry argon atmosphere. A solution of the bromobenzene derivative **S1** (1 equiv, 7.4 mmol) in toluene [0.1 M] was added through a syringe. The resulting mixture was stirred at 110 °C for 18 h. After that time, the mixture was allowed to cool to room temperature and filtered through a celite pad, the resulting brown oil was purified by silica gel column chromatography (Hexane:AcOEt, 95:5 to 90:10) to afford the corresponding diamine **S2** as a yellow oil in 96% yield.

Third step: $Pd_2(dba)_3$ (6 mol%, 0.42 mmol), *rac*-BINAP (18 mol%, 1.3 mmol), and NaO^{t}Bu (2 equiv, 14.2 mmol) were weighed into an oven-dried 100 mL round bottom flask inside a glove box. The flask was removed from the glove box and fitted with a reflux condenser. A solution of the corresponding diamine **S2** (1 equiv, 7.1 mmol) in toluene [0.1 M] and a solution of the isobutyl-2-bromobenzenesulfonate (1 equiv, 7.1 mmol) in toluene [0.1 M] were sequentially added to the mixture which was stirred at 110 °C during 21 h. After that time, the mixture was cooled down to room temperature and filtered through a celite pad, the solvents were removed and the residue was purified by silica gel column chromatography (Hexane:AcOEt, 95:5) to afford the corresponding diamine **S3** as a yellow oil in 53% yield.

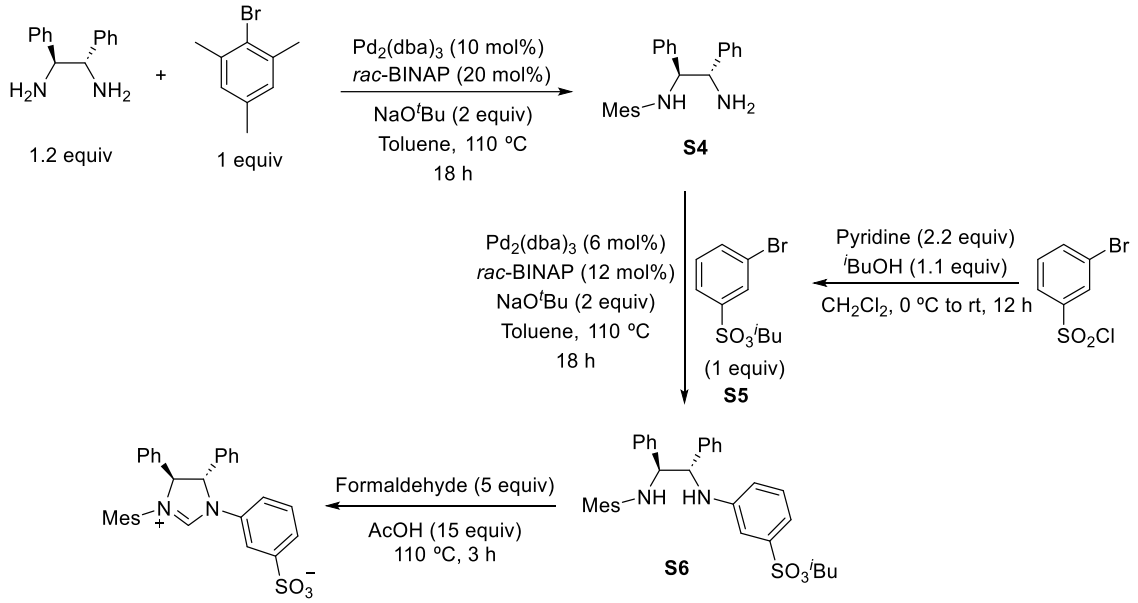
Fourth step: The corresponding diamine **S3** (1 equiv, 3.8 mmol) and NH_4BF_6 (2 equiv, 7.6 mmol) was placed into a 25 mL round bottom flask. The flask was fitted with a reflux condenser. $HC(OEt)_3$ [0.05 M] was added through a syringe and stirred at 140 °C during 22 h. Then, the mixture was cooled to room temperature and the solvent was removed under reduced pressure and the resulting crude was purified by silica gel flash chromatography (AcOEt:MeOH, 100:0 to 90:10) to afford the corresponding imidazolium salt **L26** as a white solid in 31% yield.

2-((4*S*,5*S*)-3-(5-Methyl-2-(naphthalen-2-yl)phenyl)-4,5-diphenyl-4,5-dihydro-1H-imidazol-3-ium-1-yl)benzenesulfonate (L26)



^{1}H NMR (300 MHz, $CDCl_3$) δ 9.16 (s, 1H), 8.25 (d, *J* = 7.9 Hz, 1H), 8.10 (t, *J* = 8.0 Hz, 2H), 8.05 – 7.99 (m, 1H), 7.92 (s, 1H), 7.77 – 7.64 (m, 3H), 7.49 (d, *J* = 8.4 Hz, 1H), 7.37 – 7.29 (m, 3H), 7.29 – 7.21 (m, 6H), 7.18 (t, *J* = 7.4 Hz, 1H), 7.07 – 7.00 (m, 1H), 6.95 (t, *J* = 7.8 Hz, 2H), 6.78 (d, *J* = 8.1 Hz, 2H), 6.37 (d, *J* = 6.9 Hz, 1H), 5.86 (d, *J* = 10.8 Hz, 1H), 4.68 (d, *J* = 10.7 Hz, 1H), 2.36 (s, 3H) ppm. **^{13}C NMR** (75 MHz, $CDCl_3$) δ 158.7, 143.6, 140.1, 135.5, 134.9, 134.7, 133.6, 133.3, 133.0, 132.2, 131.1, 131.0, 130.9, 130.0, 129.9, 129.9, 129.7, 129.6, 129.3, 129.2, 129.1, 128.8, 128.3, 128.3, 128.2, 127.5, 127.2, 126.9, 77.0, 75.2, 21.1 ppm. **HRMS (APCI)** Calc. for $C_{38}H_{31}N_2O_3S$ [M+H$^+$] 595.2050, found 595.2052. **Specific rotation:** $[\alpha]_D^{21}$ -94.9 (*c* = 0.99, $CHCl_3$). **Mp (°C):** 236.5-241.2.

3.2. Synthesis of chiral ligand L27.



First step: A flame-dried round-bottom flask equipped with reflux condenser was charged with (-)-(*S*,*S*) -1,2-Diphenylethylenediamine (1.2 equiv, 6.0 mmol), $Pd_2(dba)_3$ (10 mol%, 0.50 mmol), *rac*-BINAP (20 mol%, 1.0 mmol) and NaO^{t}Bu (1.5 equiv, 7.5 mmol) under a dry argon atmosphere. A solution of the mesityl bromide (1 equiv, 5.0 mmol) in toluene [0.1 M] was added through a syringe. The resulting mixture was stirred at 110 ºC during 18 h. After that time, the mixture was allowed to cool to room temperature and filtered through a celite pad, the resulting brown oil was purified by silica gel column chromatography (Hexane:AcOEt, 95:5 to 80:20) to afford the corresponding diamine **S4** as a yellow oil in 73% yield.

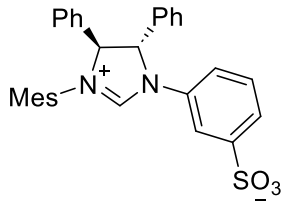
Second step: (Prior to use in this reaction, commercially available 3-bromobenzenesulfonyl chloride was dissolved in toluene and washed with a 1.0 M aq solution of KOH. The organic layer was dried with Na_2SO_4, filtered and concentrated in vacuo to afford A as a clear oil). In two separate syringes, pyridine (2.2 equiv, 31.3 mmol) and a solution of 3-bromobenzenesulfonyl chloride (1 equiv, 31.3 mmol) in CH_2Cl_2 (15 mL) were added dropwise at the same time over 20 min to a solution of 2-methylpropanol (1.1 equiv, 17.2 mmol) dissolved in CH_2Cl_2 (10 mL) at 0 ºC under an argon atmosphere. The solution was allowed to stir at rt. After 20 h, the reaction was quenched upon addition of a 0.1 M aq solution of HCl (20 mL) and allowed to stir for five minutes. The CH_2Cl_2 layer was separated and washed with a 0.1 M aq solution of HCl (20 mL), water (2 × 15 mL) and brine (15 mL). The organic layer was dried over Na_2SO_4, filtered and concentrated in vacuo to afford **S5** as clear oil and was used without further purification.

Third step: $Pd_2(dba)_3$ (6 mol%, 0.20 mmol), *rac*-BINAP (18 mol%, 0.22 mmol), and NaO^{t}Bu (2 equiv, 7.3 mmol) were weighed into an oven-dried 100 mL round bottom flask inside a glove box. The flask was removed from the glove box and fitted with a reflux condenser. A solution of the corresponding diamine **S4** (1 equiv, 3.63 mmol) in toluene [0.1 M] and a solution of the isobutyl-3-bromobenzenesulfonate **S5** (1 equiv, 3.63 mmol) in toluene [0.1 M] were sequentially added to the mixture which was stirred at 110

ºC during 18 h. After that time, the mixture was cooled down to room temperature and filtered through a celite pad, the solvents were removed and the residue was purified by silica gel column chromatography (Hexane:AcOEt, 95:5 to 90:10) to afford the corresponding diamine **S6** as a yellow oil in 42% yield.

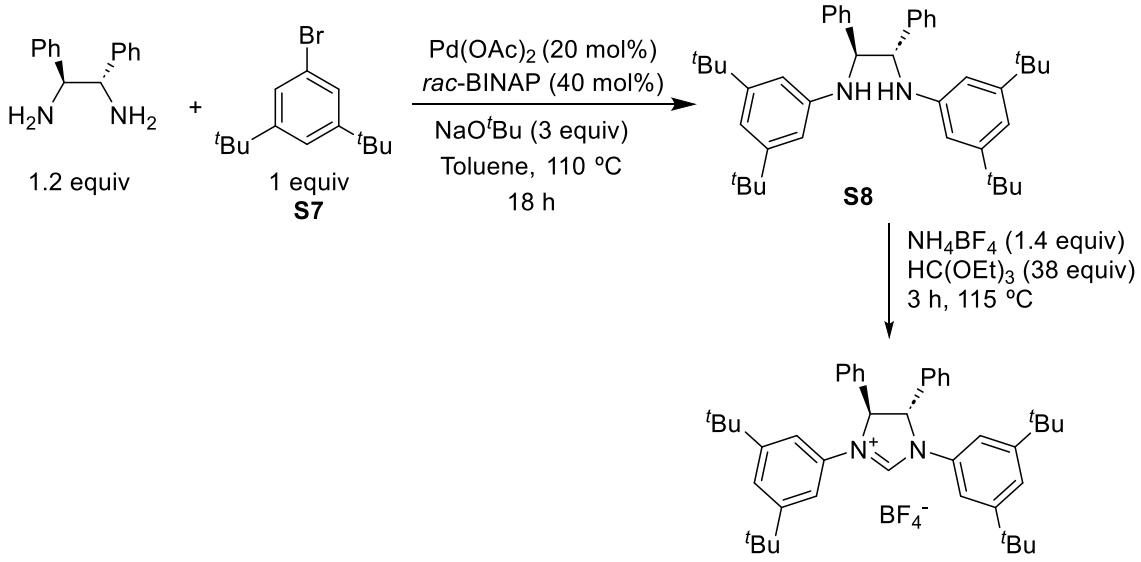
Fourth step: The corresponding diamine **S6** (1 equiv, 1.51 mmol) was placed into a 25 mL round bottom flask. The flask was fitted with a reflux condenser. Acetic acid (15 equiv, 22.7 mmol), followed by formaldehyde (5 equiv, 7.6 mmol) were added through a syringe and stirred at 110 ºC during 3 h. Then, the mixture was cooled to room temperature and neutralized by the slow addition of a saturated $NaHCO_3$ aq. solution until gas evolution ceased. The mixture was extracted with CH_2Cl_2 (2x10 mL) and the resulting organic phase washed with brine, dried over anhydrous Na_2SO_4 and filtered. The solvent was removed under reduced pressure, and the resulting crude was purified by silica gel flash chromatography (AcOEt:MeOH, 100:0 to 80:20) to afford the corresponding imidazolium salt **L27** as a yellow pale solid in 23% yield.

3-((4*S*,5*S*)-3-Mesityl-4,5-diphenyl-4,5-dihydro-1H-imidazol-3-ium-1-yl)benzenesulfonate (L27)



^{1}H NMR (300 MHz, $CDCl_3$) δ 9.45 (s, 1H), 7.79 (s, 1H), 7.46 – 7.30 (m, 11H), 6.93 (d, *J* = 6.2 Hz, 3H), 6.73 (s, 1H), 6.28 (d, *J* = 9.0 Hz, 1H), 5.14 (d, *J* = 9.0 Hz, 1H), 2.39 (s, 3H), 2.22 (s, 3H), 1.91 (s, 3H) ppm. **^{13}C NMR** (75 MHz, $CDCl_3$) δ 157.6, 140.2, 137.2, 135.7, 134.7, 134.3, 132.7, 130.7, 130.2, 130.0, 129.7, 129.5, 129.5, 129.3, 126.8, 125.3, 121.1, 118.1, 76.9, 71.3, 21.0, 18.7, 18.4 ppm. **HRMS (ESI)** Calc. for $C_{30}H_{27}N_2O_3S$ [M-H$^+$] 495.1748, found 495.1750. **Specific rotation:** $[\alpha]_D^{22}$ -254.5 (*c* = 0.55, $CHCl_3$). **Mp (°C):** 247.6-253.0.

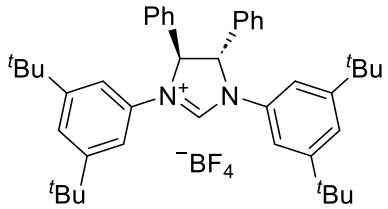
3.3. Synthesis of chiral ligand L7.



First step: A flame-dried round-bottom flask equipped with reflux condenser was charged with (-)-(*S*,*S*)-1,2-Diphenylethylenediamine (1 equiv, 2 mmol), $Pd(OAc)_2$ (20 mol%, 0.4 mmol), *rac*-BINAP (40 mol%, 0.8 mmol) and NaO^tBu (3 equiv, 6 mmol) under a dry argon atmosphere. A solution of the bromobenzene **S7** (2.1 equiv, 4.2 mmol) in toluene [0.08 M] was added through a syringe. The resulting mixture was stirred at 110 ºC during 18 h. After that time, the mixture was allowed to cool to room temperature, loaded directly on top of a column containing silica gel and purified by silica gel column chromatography (Hexane:AcOEt, 100:0 to 90:10) to afford the corresponding diamine **S8** in 73% yield.

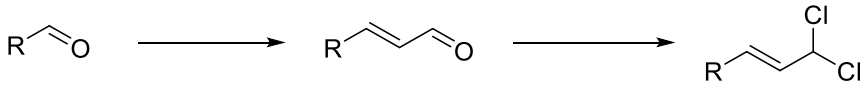
Second step: The corresponding diamine **S8** (1 equiv, 1.46 mmol) and the ammonium tetrafluoroborate (1.4 equiv, 2.04 mmol) were weighed into a 25 mL round bottom flask. The flask was fitted with a reflux condenser. Triethyl orthoformate (38 equiv, 55,46 mmol) was added through a syringe and stirred at 115 ºC during 3 h. After that time, the mixture was allowed to cool to room temperature, loaded directly on top of a column containing silica gel and purified by silica gel column chromatography (Hexane:AcOEt, 95:5 to 0:100) to afford the corresponding imidazolium salt **L7** as a white solid in 67% yield.

(4*S*,5*S*)-1,3-Bis(3,5-di-*tert*-butylphenyl)-4,5-diphenyl-4,5-dihydro-1*H*-imidazol-3-ium tetrafluoroborate (L7)



^{1}H NMR (500 MHz, $CDCl_3$) δ 9.37 (s, 1H), 7.47 – 7.38 (m, 10H), 7.31 (t, *J* = 1.7 Hz, 2H), 7.16 (d, *J* = 1.6 Hz, 4H), 1.22 (s, 36H) ppm. **^{13}C NMR** (126 MHz, $CDCl_3$) δ 153.5, 153.2, 135.0, 134.1, 130.2, 130.1, 127.5, 122.9, 116.2, 75.4, 35.3, 31.2 ppm. **HRMS (APCI)** Calc. for $C_{43}H_{55}N_2^+$ [M-BF_4^-] 599.4360, found 599.4363. **Specific rotation:** $[\alpha]_D^{19}$ -180.0 (*c* = 0.60, $CHCl_3$). **Mp (°C):** 264.9-266.6.

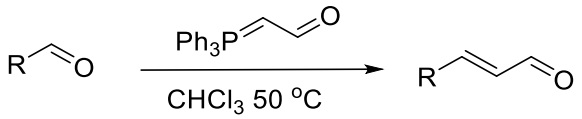
4. General methods for the synthesis of starting materials.



- **General procedure A. Dess-Martin oxidation.**

To a solution of aliphatic alcohol (1 equiv) in CH_2Cl_2 [0.125 M]. Dess-Martin periodinane (1.2 equiv) was added under argon atmosphere. The reaction mixture was stirred at room temperature for 5 h. The reaction mixture was quenched with aqueous $NaHCO_3$ and $Na_2S_2O_3$. Then the mixture was extracted with CH_2Cl_2. The combined organic layers were dried over Na_2SO_4. After the removal of the solvent, the residue was purified by flash chromatography on silica gel using the indicated mixture of solvents as eluent to give the aldehyde.

- **General procedure B. Synthesis of α,β-unsaturated aldehydes via Wittig reactions in chloroform.**

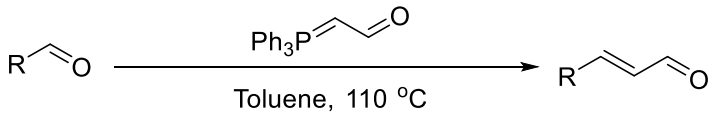


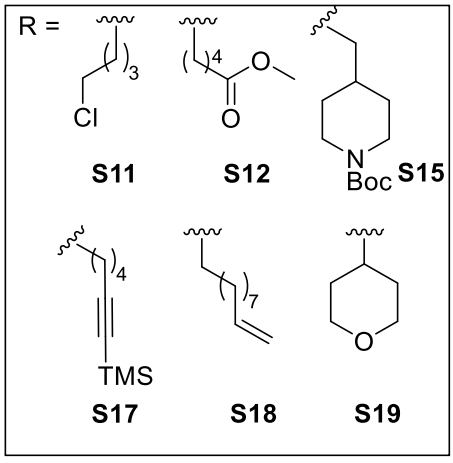
R = -CH_2Ph, **S9**
-$(CH_2)_7CH_3$, **S10**

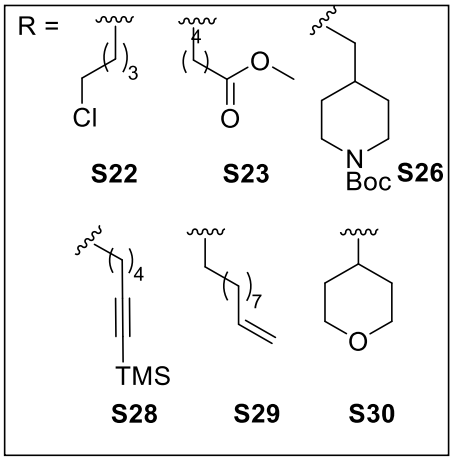
R = -CH_2Ph, **S20**
-$(CH_2)_7CH_3$, **S21**

A solution of (triphenylphosphoranylidene)-acetaldehyde (1.1 equiv) and the aldehyde (1 equiv) in $CHCl_3$ [0.3 M] was heated at 50 °C for the indicated time. Then the solution was concentrated under reduced pressure. Purification by flash column chromatography using the indicated mixture of solvents as eluent afforded the final aldehyde.

- **General procedure C. Synthesis of α,β-unsaturated aldehydes via Wittig reactions in toluene.**

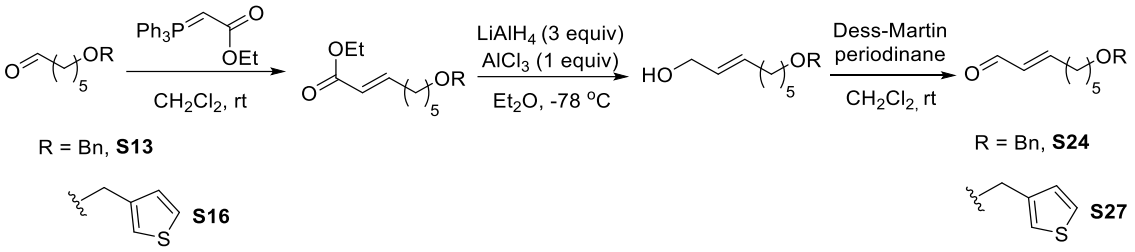






A solution of (triphenylphosphoranylidene)-acetaldehyde (1.2 equiv.) and the aldehyde (1 equiv) in Toluene [0.2 M] was heated at 110 °C for the indicated time Then the solution was concentrated under reduced pressure. Purification by flash column chromatography using the indicated mixture of solvents as eluent afforded the product.

- **General procedure D. Synthesis of α,β-unsaturated aldehydes when R is Bn or CH_2-3-thiophene**



R = Bn, **S13**

S16

R = Bn, **S24**

S27

A 100 mL single necked round bottomed flask was charged with [(ethoxycarbonyl)methylene]triphenylphosphorane (1 equiv) and the resulting solution was cooled to 0 ºC. A solution of the aldehyde (1 equiv) CH_2Cl_2 [0.5 M] was added dropwise and the mixture was stirred overnight at rt. Then the solvent was removed by rotary evaporation. The crude was purified by flash column chromatography (Hexane:AcOEt).

$LiAlH_4$ (3 equiv.), $AlCl_3$ (1 equiv) and α,β-unsaturated ester (1 equiv) was diluted in Et_2O [0.1 M] and stirred under argon atmosphere at -78 ºC for 2 h. After this time, the reaction was quenched by the addition of ice at -78 ºC and a solution of L(+)-Tartaric acid potassium sodium salt (Rochelle's salt). The mixture was stirred for 2 h. The layers were separated and the aqueous layer extracted two times with Et_2O. The combined organic layers were dried with Na_2SO_4 and the solvent was removed in vacuo.

The last step is a Dess-Martin oxidation following general procedure A.

- **General procedure E. Synthesis of *gem*-dichlorides using oxalyl chloride**

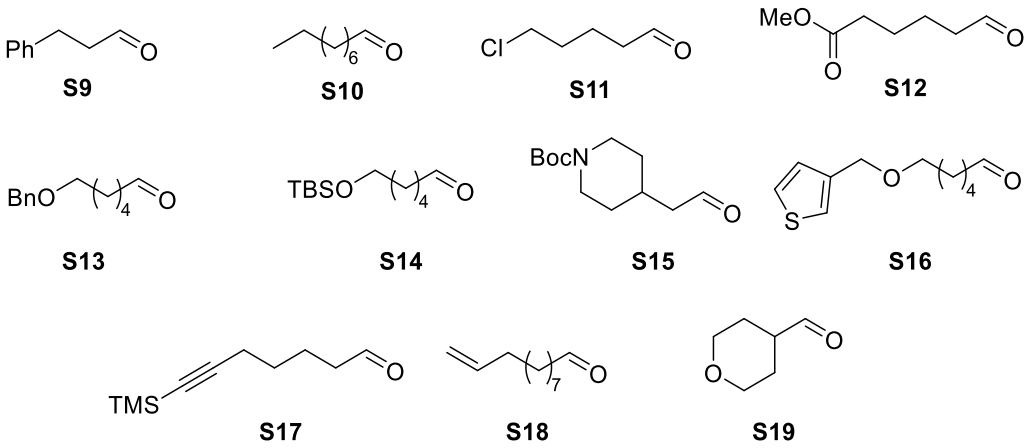
In a Schlenk tube under argon atmosphere equipped with a magnetic stirring bar, the corresponding α-β-unsaturated aldehyde (1 equiv) and triphenylphosphine oxide (0.075 equiv) were added and dissolved in CH_2Cl_2 [1 M]. In a separate vial, oxalyl chloride (1.3 equiv) was dissolved in the same volume of previous solvent and the resulting solution was added over 2 h via syringe pump to the other mixture which was previously heated at 40-50 ºC. The resulting mixture was stirred at that temperature overnight. Then, the mixture was diluted with Et_2O and washed with a saturated $NaCl_{(aq)}$ solution (3x20 mL). Combined organic phases were dried over anhydrous Na_2SO_4, filtered and solvent was removed under reduced pressure. Crude product was purified through flash column chromatography using the indicated mixture of solvents as eluent.

- **General procedure F. Synthesis of *gem*-dichlorides using thionyl chloride**

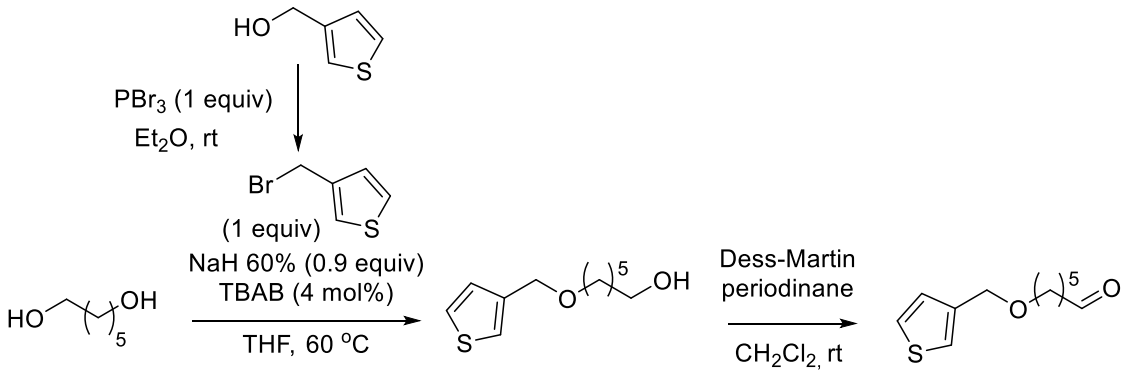
To a solution of $SOCl_2$ (9 equiv) and DMF (25 mol%), α-β-unsaturated aldehyde (1 equiv) was added dropwise at -5 ºC. After the indicated time, the reaction was carefully quenched by pouring it on ice and the mixture was extracted with Et_2O when it was still cold. The organic phase was dried over Na_2SO_4 and the solvent evaporated under reduced pressure. Crude product was purified through flash column chromatography using the indicated mixture of solvents as eluent.

5. List, synthesis and characterization of aldehydes.

S9, **S10**, **S11**, **S15**, **S18** and **S19** and were purchased from commercial sources. **S12**,[14] **S13**[15] and **S14**[16] were prepared according to literature procedures.



- **Synthesis of 6-(Thiophen-3-ylmethoxy)hexanal** (**S16**).



Thiophen-3-ylmethanol was synthetized via a modified literature protocol:[17] PBr_3 (1.1 equiv, 33 mmol) was added to thiophen-3-ylmethanol (1 equiv, 30 mmol) in Et_2O [0.5 M] at rt. The reaction mixture was stirred for 16 h and then quenched with methanol and water. After extraction with Et_2O, the combined organic layers were dried with Na_2SO_4 and the solvent was removed under reduced pressure, leading to crude compound.

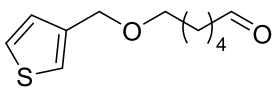
A suspension of NaH (60% in mineral oil, 0.9 equiv) and 1,6-hexanediol (1 equiv) in dry THF [1.1 M] was stirred for 1 h at 0 °C. Subsequently, a solution of 3-(bromomethyl)thiophene (1 equiv) and TBAB (4 mol%) in THF [1.1 M] was added. The reaction was then stirred for 24 h at 60 °C. After completion of the reaction, it was quenched with a saturated solution of ammonium chloride and the product was extracted with Et_2O (2x20mL). The combined organic layers were then washed with water, brine, and dried over anhydrous Na_2SO_4. Solvent was removed under reduced pressure. After

[14] Jeon, J.; Ryu, H.; Lee, C.; Cho, D.; Baik, M.-H.; Hong, S. *J. Am. Chem. Soc.* **2019**, *141*, 10048-10059
[15] Koyanagi, T.; Leriche, G.; Onofrei, D.; Holland, G. P.; Mayer, M.; Yang, J. *Angew. Chem. Int. Ed.* **2016**, *55*, 1890-1893
[16] Harrison, A. N.; Reichau, S.; Parker, E. J. *Bioorg. Med. Chem. Lett.* **2012**, *22*, 907-911
[17] Liu, D.; Ke, M.; Ru, T.; Ning, Y.; Chen, F.-E. *Chem. Commun.* **2022**, *58*, 1041-1044

column chromatography purification using Hexane:AcOEt (90:10 to 70:30) as eluent the product was obtained as a yellow oil in 57% yield.

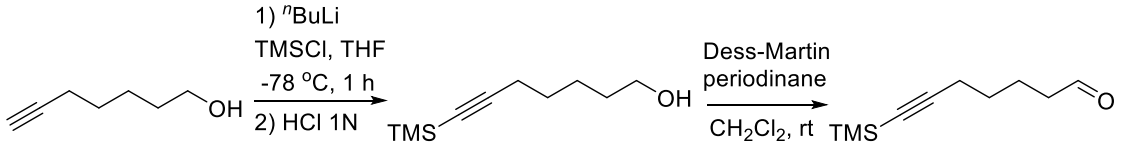
Finally, aldehyde **S16** was synthesized according to general procedure A after quenching with NaOH 1M (2x100 mL). Yellow pale oil is obtained in 84% yield after filtration through a pad of silica and subsequent solvent evaporation.

6-(Thiophen-3-ylmethoxy)hexanal (S16)



^{1}H NMR (300 MHz, $CDCl_3$) δ 9.76 (t, *J* = 1.8 Hz, 1H), 7.29 (dd, *J* = 4.9, 2.9 Hz, 1H), 7.21 – 7.18 (m, 1H), 7.07 (d, *J* = 5.0 Hz, 1H), 4.50 (s, 2H), 3.46 (t, *J* = 6.4 Hz, 2H), 2.44 (t, *J* = 7.3 Hz, 2H), 1.64 (h, *J* = 6.8 Hz, 4H), 1.41 (tt, *J* = 9.1, 5.6 Hz, 2H) ppm. **^{13}C NMR** (75 MHz, $CDCl_3$) δ 202.4, 139.6, 127.1, 125.7, 122.4, 69.8, 68.0, 43.6, 29.3, 25.7, 21.7 ppm. **HRMS (APCI)** Calc. for $C_{11}H_{17}O_2S$ [M+H$^+$]: 213.0944 found 213.0943.

- **Synthesis of 7-(trimethylsilyl)hept-6-ynal (S17)**

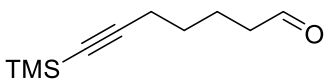


hept-6-yn-1-ol 7-(trimethylsilyl)hept-6-yn-1-ol **S17**

To a solution of hept-6-yn-1-ol (1 equiv, 10 mmol) in dry THF [0.18 M] under argon at –78 °C, *n*BuLi (2.5 M in Hexane, 2.3 equiv, 23 mmol) was added. After stirring for 1 h at –78 °C, a solution of chlorotrimethylsilane (2.3 equiv, 23 mmol) in dry THF [0.7 M] was added over the mixture. The was warmed to up to rt and stirred for an additional 15 h before it was quenched with 1 N HCl solution. The layers were separated and the aqueous layer extracted three times with Et_2O (3x30 mL). The combined organic layers were dried over Na_2SO_4 and the solvent was removed in vacuo. The crude product was purified by flash column chromatography (90:10 to 80:20 Hexane:EtOAc) to yield 7-(trimethylsilyl)hept-6-yn-1-ol in 98% of yield as a pale-yellow oil.

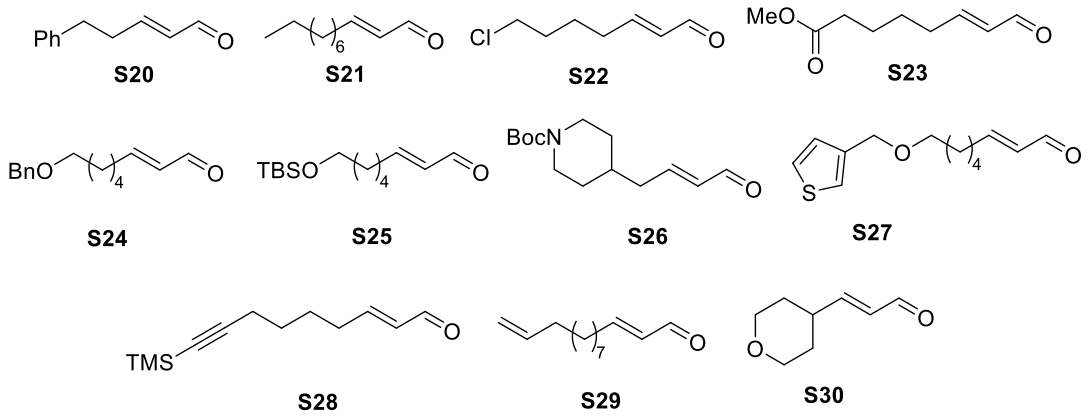
S17 was synthesized from yield 7-(trimethylsilyl)hept-6-yn-1-ol (1 equiv, 9.82 mmol) according to general procedure A (reaction time = 5 h), quenching with $Na_2S_2O_3$ (50 mL) and $NaHCO_3$ (50 mL). Yellow pale oil is obtained in 84% yield after flash column chromatography on silica gel (pentane:CH_2Cl_2 90:10).

7-(Trimethylsilyl)hept-6-ynal (S17)

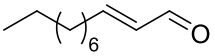


^{1}H NMR (300 MHz, $CDCl_3$) δ 9.76 (d, *J* = 1.7 Hz, 1H), 2.45 (t, *J* = 7.2 Hz, 2H), 2.24 (t, *J* = 7.0 Hz, 2H), 1.74 (p, *J* = 7.1 Hz, 2H), 1.63 – 1.48 (m, 2H), 0.13 (s, 9H) ppm. **^{13}C NMR** (75 MHz, $CDCl_3$) δ 202.3, 106.7, 85.2, 43.5, 28.1, 21.3, 19.7 ppm. **HRMS (APCI)** Calc. for $C_{10}H_{19}OSi$ [M+H$^+$]: 183.1200 found 183.1203.

6. Synthesis and characterization of allylic α,β-unsaturated aldehydes

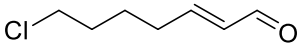


(*E*)-Undec-2-enal (S21)



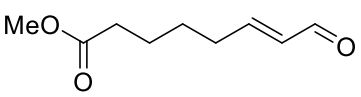
Synthesized from **S10** according to general procedure B for 48 h. Yellow oil is obtained in 50% yield after flash column chromatography on silica gel (Hexane:Et_2O 90:10). **^{1}H NMR** (300 MHz, $CDCl_3$) δ 9.49 (d, *J* = 7.9 Hz, 1H), 6.84 (dt, *J* = 15.6, 6.8 Hz, 1H), 6.11 (dd, *J* = 15.6, 7.9 Hz, 1H), 2.32 (q, *J* = 7.0 Hz, 2H), 1.49 (q, *J* = 7.4 Hz, 2H), 1.37 – 1.21 (m, 14H), 0.87 (t, *J* = 6.8 Hz, 3H) ppm. **^{13}C NMR** (75 MHz, $CDCl_3$) δ 194.1, 159.0, 133.1, 32.8, 31.9, 29.4, 29.2, 28.0, 22.7, 14.1 ppm. **HRMS (APCI)** Calc. for $C_{11}H_{20}O$ [M+H^+]: 169.1587 found 169.1579.

(*E*)-7-Chlorohept-2-enal (S22)



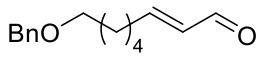
Synthesized from **S11** according to general procedure C for 7 h. Yellow oil is obtained in 51% yield after flash column chromatography on silica gel (Hexane:AcOEt 95:5). **^{1}H NMR** (300 MHz, $CDCl_3$) δ 9.51 (d, *J* = 7.8 Hz, 1H), 6.83 (dt, *J* = 15.6, 6.7 Hz, 1H), 6.13 (dd, *J* = 15.6, 7.9 Hz, 1H), 3.55 (t, *J* = 6.4 Hz, 2H), 2.38 (q, *J* = 7.3 Hz, 2H), 1.88 – 1.77 (m, 2H), 1.75 – 1.62 (m, 2H) ppm. **^{13}C NMR** (75 MHz, $CDCl_3$) δ 193.9, 157.6, 133.4, 44.5, 31.9, 25.1 ppm. **HRMS (APCI)** Calc. for $C_7H_{12}ClO$ [M+H^+]: 147.0571 found 147.0577.

Methyl (*E*)-8-oxooct-6-enoate (S23)



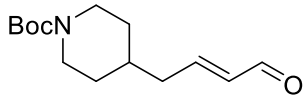
Synthesized from **S12** according to general procedure C for 24 h. Yellow oil is obtained in 51% yield after flash column chromatography on silica gel (Hexane:AcOEt 85:15). **^{1}H NMR** (300 MHz, $CDCl_3$) δ 9.45 (d, *J* = 7.8 Hz, 1H), 6.79 (dt, *J* = 15.6, 6.7 Hz, 1H), 6.07 (dd, *J* = 15.6, 7.9 Hz, 1H), 3.62 (s, 3H), 2.31 (q, *J* = 8.2 Hz, 4H), 1.70 – 1.58 (m, 2H), 1.51 (p, *J* = 7.0 Hz, 2H) ppm. **^{13}C NMR** (75 MHz, $CDCl_3$) δ 193.9, 173.7, 157.9, 133.2, 51.5, 33.7, 32.3, 27.3, 24.4 ppm. **HRMS (APCI)** Calc. for $C_9H_{15}O_3$ [M+H^+]: 171.1016, found 171.1012.

(*E*)-8-(Benzyloxy)oct-2-enal (S24)



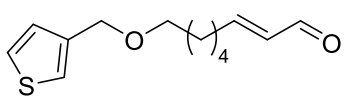
Synthesized from **S13** according to general procedure D. Yellow oil is obtained in 38% overall yield. **^{1}H NMR** (300 MHz, $CDCl_3$) δ 9.49 (d, *J* = 7.9 Hz, 1H), 7.40 – 7.21 (m, 5H), 6.82 (dt, *J* = 15.5, 6.8 Hz, 1H), 6.10 (dd, *J* = 15.6, 7.9 Hz, 1H), 4.49 (s, 2H), 3.47 (t, *J* = 6.4 Hz, 2H), 2.33 (q, *J* = 7.0 Hz, 2H), 1.64 (p, *J* = 6.6 Hz, 2H), 1.56 – 1.36 (m, 4H) ppm. **^{13}C NMR** (75 MHz, $CDCl_3$) δ 194.1, 158.7, 138.6, 133.1, 128.4, 127.6, 127.6, 72.9, 70.1, 32.7, 29.5, 27.7, 25.8 ppm. **HRMS (APCI)** Calc. for $C_{15}H_{21}O_2$ [M+H$^+$]: 233.1536, found 233.1534.

***Tert*-butyl (*E*)-4-(4-oxobut-2-en-1-yl)piperidine-1-carboxylate (S26)**



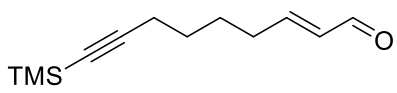
Synthesized from **S15** according to general procedure C for 6 h. Yellow oil is obtained in 48% yield after flash column chromatography on silica gel (Hexane:AcOEt 90:10). **^{1}H NMR** (300 MHz, $CDCl_3$) δ 9.51 (d, *J* = 7.9 Hz, 1H), 6.80 (dt, *J* = 15.3, 7.3 Hz, 1H), 6.12 (dd, *J* = 15.4, 8.0 Hz, 1H), 4.09 (d, *J* = 12.4 Hz, 2H), 2.75 – 2.64 (m, 2H), 2.33 – 2.25 (m, 2H), 1.67 (d, *J* = 10.6 Hz, 3H), 1.45 (s, 9H), 1.26 – 1.07 (m, 2H) ppm. **^{13}C NMR** (75 MHz, $CDCl_3$) δ 193.8, 156.0, 154.9, 134.6, 79.6, 43.9, 39.7, 35.7, 32.1, 28.6 ppm. **HRMS (APCI)** Calc. for $C_{14}H_{24}NO_3$ [M+H$^+$]: 254.1751, found 254.1741.

(*E*)-8-(Thiophen-3-ylmethoxy)oct-2-enal (S27)



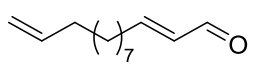
Synthesized from **S16** according to general procedure D. Yellow oil is obtained in 86% overall yield. **^{1}H NMR** (300 MHz, $CDCl_3$) δ 9.52 (d, *J* = 7.9 Hz, 1H), 7.33 – 7.27 (m, 1H), 7.21 (s, 1H), 7.08 (d, *J* = 5.0 Hz, 1H), 6.85 (dt, *J* = 15.7, 6.8 Hz, 1H), 6.13 (dd, *J* = 15.6, 7.9 Hz, 1H), 4.52 (s, 2H), 3.48 (t, *J* = 6.4 Hz, 2H), 2.36 (q, *J* = 7.2 Hz, 2H), 1.64 (p, *J* = 6.8 Hz, 2H), 1.59 – 1.39 (m, 4H) ppm. **^{13}C NMR** (75 MHz, $CDCl_3$) δ 194.1, 158.7, 139.8, 133.2, 127.4, 126.0, 122.7, 70.1, 68.3, 32.7, 29.6, 27.8, 25.9 ppm. **HRMS (APCI)** Calc. for $C_{13}H_{19}O_2S$ [M+H$^+$]: 239.1100, found 239.1096.

(*E*)-9-(Trimethylsilyl)non-2-en-8-ynal (S28)



Synthesized from **S17** according to general procedure C for 13 h. Yellow oil is obtained in 42% yield after flash column chromatography on silica gel (Pentane:Et_2O 95:5). **^{1}H NMR** (300 MHz, $CDCl_3$) δ 9.51 (d, *J* = 7.9 Hz, 1H), 6.91 – 6.75 (m, 1H), 6.13 (dd, *J* = 15.6, 7.9 Hz, 1H), 2.41 – 2.32 (m, 2H), 2.25 (t, *J* = 6.3 Hz, 2H), 1.69 – 1.50 (m, 4H), 0.13 (s, 9H) ppm. **^{13}C NMR** (75 MHz, $CDCl_3$) δ 194.1, 158.2, 133.3, 106.8, 85.2, 32.3, 28.1, 27.0, 19.7, 0.3 ppm. **HRMS (APCI)** Calc. for $C_{12}H_{21}OSi$ [M+H$^+$]: 209.1356, found 209.1358.

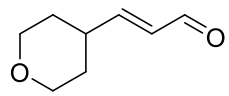
(*E*)-Trideca-2,12-dienal (S29)



Synthesized from **S18** according to general procedure C for 9 h. Yellow oil is obtained in 54% yield after flash column chromatography on silica gel (Hexane:AcOEt 98:2). **^{1}H NMR** (300 MHz, $CDCl_3$) δ 9.50

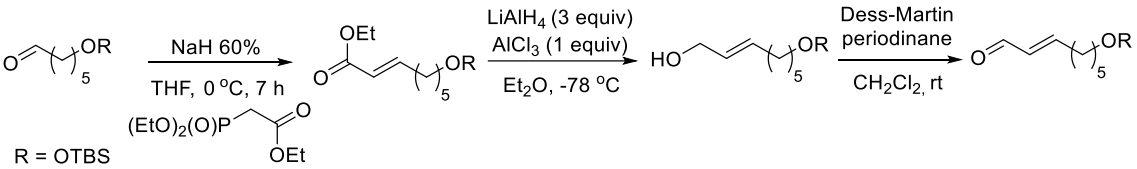
(d, *J* = 7.9 Hz, 1H), 6.84 (dt, *J* = 15.6, 6.8 Hz, 1H), 6.11 (dd, *J* = 15.6, 7.8 Hz, 1H), 5.81 (ddt, *J* = 16.9, 10.1, 6.7 Hz, 1H), 5.03 – 4.89 (m, 2H), 2.33 (q, *J* = 7.4 Hz, 2H), 2.04 (q, *J* = 6.8 Hz, 2H), 1.49 (q, *J* = 7.4 Hz, 2H), 1.42 – 1.23 (m, 10H) ppm. **^{13}C NMR** (75 MHz, $CDCl_3$) δ 194.2, 159.0, 139.3, 133.2, 114.3, 33.9, 32.8, 29.4, 29.4, 29.2, 29.2, 29.0, 28.0 ppm. **HRMS (APCI)** Calc. for $C_{13}H_{23}O$ [M+H$^+$]: 195.1743, found 195.1741.

(*E*)-3-(Tetrahydro-2H-pyran-4-yl)acrylaldehyde (S30)



Synthesized from **S19** according to general procedure C for 9 h. Yellow oil is obtained in 54% yield after flash column chromatography on silica gel (Hexane:AcOEt 98:2). **^{1}H NMR** (300 MHz, $CDCl_3$) δ 9.52 (d, *J* = 7.7 Hz, 1H), 6.75 (dd, *J* = 15.8, 6.3 Hz, 1H), 6.10 (dd, *J* = 15.8, 7.7 Hz, 1H), 4.01 (dd, *J* = 11.7, 1.9 Hz, 2H), 3.46 (td, *J* = 11.7, 2.4 Hz, 2H), 2.61 – 2.44 (m, 1H), 1.72 (d, *J* = 11.0 Hz, 2H), 1.63 – 1.47 (m, 2H) ppm. **^{13}C NMR** (75 MHz, $CDCl_3$) δ 194.0, 160.9, 131.1, 67.3, 38.1, 31.2 ppm. **HRMS (APCI)** Calc. for $C_8H_{13}O_2$ [M+H$^+$]: 141.0910, found 141.0904.

- **Synthesis of (*E*)-8-((*tert*-butyldimethylsilyl)oxy)oct-2-enal (S25).**



α,β-Unsaturated ester was synthetized via a described protocol.[18] To a suspension of NaH (60% in mineral oil, 3.75 equiv) in THF [0.13 M] at 0 °C, the phosphonate (3.75 equiv) was slowly added. After the addition, the suspension turned clear. A solution of the aldehyde (1 equiv) in THF [0.7 M] was added. The reaction mixture was stirred at 0 °C for 7 h before being quenched by saturated NH_4Cl. The product was extracted with AcOEt (2x20mL). The combined extracts were washed with brine, dried and concentrated. The residue was purified by silica gel column chromatography (Hexane/AcOEt 20:1) to afford the ester in 57% yield.

$LiAlH_4$ (3 equiv.), $AlCl_3$ (1 equiv) and α,β-unsaturated ester (1 equiv) were diluted in Et_2O [0.1 M] and stirred under argon atmosphere at -78 °C for 2 h. After this time, the reaction was quenched by the addition of ice at -78 °C and a solution of L(+)-Tartaric acid potassium sodium salt (Rochelle's salt), the mixture was stirred for 2 h. The layers were separated and the aqueous layer extracted two times with Et_2O. The combined organic layers were dried with Na_2SO_4 and the solvent was removed in vacuo.

The last step is a Dess-Martin oxidation followed by general procedure A, quenching with $Na_2S_2O_3$ (30 mL) and $NaHCO_3$ (30 mL).

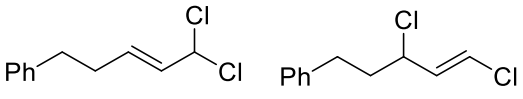
[18] Wang, Y.; Ma, J.; Cheon, H.-S.; Kishi, Y. *Angew. Chem. Int. Ed.* **2007**, *46*, 1333-1336

(*E*)-8-((*tert*-Butyldimethylsilyl)oxy)oct-2-enal (S25)

Synthesized from **S14**. Yellow oil is obtained in 63% overall yield. **^{1}H NMR** (300 MHz, $CDCl_3$) δ 9.52 (d, *J* = 7.9 Hz, 1H), 6.86 (dt, *J* = 15.6, 6.8 Hz, 1H), 6.14 (dd, *J* = 15.6, 7.9 Hz, 1H), 3.67 – 3.58 (m, 2H), 2.36 (q, *J* = 7.2 Hz, 2H), 1.54 (q, *J* = 7.3 Hz, 4H), 1.48 – 1.36 (m, 2H), 0.91 (s, 9H), 0.06 (s, 6H) ppm. **^{13}C NMR** (75 MHz, $CDCl_3$) δ 194.1, 158.8, 133.2, 63.0, 32.8, 32.6, 27.8, 26.1, 25.6, 18.5, -5.2 ppm. **HRMS (APCI)** Calc. for $C_{14}H_{29}O_2Si$ [$M+H^+$]: 257.1931, found 257.1932.

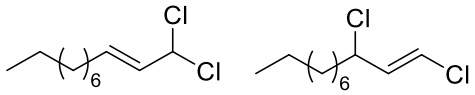
7. Synthesis and characterization of allylic *gem*-dichlorides.

(*E*)-(5,5-Dichloropent-3-en-1-yl)benzene (1) + (*E*)-(3,5-dichloropent-4-en-1-yl)benzene (1')



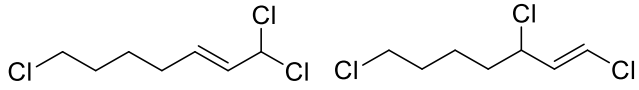
Synthesized from **S20**, prepared as reported in the literature,[19] according to general procedure E at 50 °C. Yellow oil is obtained as a 1:1 mixture of (*E*)-(5,5-Dichloropent-3-en-1-yl)benzene and (*E*)-(3,5-dichloropent-4-en-1-yl)benzene in 46% yield after flash column chromatography on silica gel (Hexane). **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.37 – 7.27 (m, 5H), 7.25 – 7.14 (m, 5H), 6.27 (d, *J* = 13.6 Hz, 1H, **1'**), 6.13 (d, *J* = 6.8 Hz, 1H, **1**), 6.03 (dd, *J* = 13.2, 8.8 Hz, 1H, **1'**), 5.97 – 5.79 (m, 2H, **1**), 4.42 – 4.27 (m, 1H, **1'**), 2.84 – 2.70 (m, 4H), 2.48 – 2.37 (m, 2H), 2.14 (hept, *J* = 6.3 Hz, 2H) ppm.**^{13}C NMR** (75 MHz, $CDCl_3$) δ 141.0, 140.3, 133.9, 133.4, 130.6, 128.7, 128.6, 128.6, 128.5, 126.4, 126.3 ,121.8, 71.2, 59.1, 39.9, 35.0, 33.2, 32.5 ppm. **HRMS (APCI)** Calc. for $C_{11}H_{13}Cl_2$ [M+H$^+$]: 215.0389, found 215.0383.

(*E*)-1,1-Dichloroundec-2-ene (26) + (*E*)-1,3-dichloroundec-1-ene (26')



Synthesized from **S21** according to general procedure E at 45 °C. Yellow oil is obtained as a 1:0.9 mixture of (*E*)-1,1-Dichloroundec-2-ene and (*E*)-1,3-dichloroundec-1-ene in 40% yield after flash column chromatography on silica gel (Hexane). **^{1}H NMR** (300 MHz, $CDCl_3$) δ 6.28 (d, *J* = 13.2 Hz, 1H, **26'**), 6.14 (d, *J* = 6.9 Hz, 1H, **26**), 6.00 (dd, *J* = 13.2, 8.9 Hz, 1H, **26'**), 5.93 – 5.77 (m, 2H, **26**), 4.40 – 4.30 (m, 1H, **26'**), 2.09 (q, *J* = 6.2 Hz, 2H), 1.90 – 1.72 (m, 2H), 1.48 – 1.35 (m, 4H), 1.27 (s, 20H), 0.88 (t, *J* = 5.9 Hz, 6H) ppm. **^{13}C NMR** (75 MHz, $CDCl_3$) δ 134.6, 134.3, 130.0, 121.3, 71.5, 60.1, 38.6, 32.0, 32.0, 31.5, 29.5, 29.5, 29.4, 29.3, 29.2, 29.1, 28.6, 26.5, 22.8, 14.2 ppm. **HRMS (APCI)** Calc. for $C_{11}H_{20}Cl$ [M+H$^+$-HCl]: 187.1248, found 187.1249

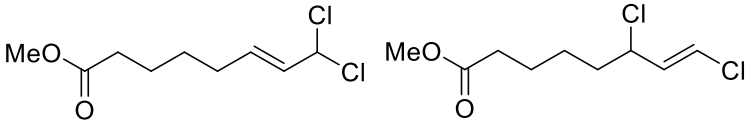
(*E*)-1,1,7-Trichlorohept-2-ene (28) + (*E*)-1,3,7-trichlorohept-1-ene (28')



Synthesized from **S22** according to general procedure E at 45 °C. Yellow oil is obtained as a 1:1 mixture of (*E*)-1,1,7-trichlorohept-2-ene and (*E*)-1,3,7-trichlorohept-1-ene in 37% yield after flash column chromatography on deactivated silica gel (Pentane). **^{1}H NMR** (300 MHz, $CDCl_3$) δ 6.30 (d, *J* = 13.2 Hz, 1H, **28'**), 6.14 (dd, *J* = 4.9, 2.2 Hz, 1H, **28**), 6.00 (dd, *J* = 13.2, 8.9 Hz, 1H **28'**), 5.92 – 5.81 (m, 2H, **28**), 4.37 (dt, *J* = 9.0, 6.7 Hz, 1H, **28'**), 3.54 (t, *J* = 6.5 Hz, 5H), 2.14 (td, *J* = 7.5, 5.3 Hz, 2H), 1.81 (dddd, *J* = 15.7, 13.0, 6.9, 3.7 Hz, 7H), 1.70 – 1.51 (m, 4H) ppm. **^{13}C NMR** (75 MHz, $CDCl_3$) δ 133.8, 133.6, 130.5, 121.7, 71.2, 59.6, 44.8, 44.6, 37.8, 32.0, 30.7, 25.8, 23.8 ppm. **HRMS (APCI)** Calc. for $C_7H_{11}Cl_2$ [M+H$^+$-HCl]: 165.0232, found 165.0236.

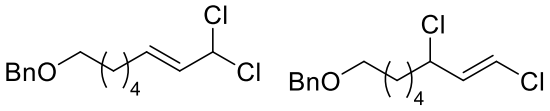
[19] Bouisseau, A.; Gao, M.; Willis, M. C. *Chem. Eur. J.* **2016**, *22*, 15624-15628

Methyl (*E*)-8,8-dichlorooct-6-enoate (29) + methyl (*E*)-6,8-dichlorooct-7-enoate (29')



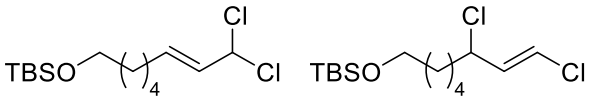
Synthesized from **S23** according to general procedure E at 40 °C. Yellow oil is obtained as a 1:1 mixture of methyl (*E*)-8,8-dichlorooct-6-enoate and methyl (*E*)-6,8-dichlorooct-7-enoate in 26% yield after flash column chromatography on silica gel (Hexane:AcOEt 95:5). **^{1}H NMR** (300 MHz, $CDCl_3$) δ 6.29 (d, *J* = 13.2 Hz, 1H, **29'**), 6.15 – 6.11 (m, 1H, **29**), 5.99 (dd, *J* = 13.2, 8.9 Hz, 1H, **29'**), 5.87 – 5.81 (m, 2H, **29**), 4.41 – 4.31 (m, 1H, **29'**), 3.67 (s, 7H), 2.33 (td, *J* = 7.4, 1.8 Hz, 5H), 2.17 – 2.08 (m, 2H), 1.89 – 1.79 (m, 2H), 1.72 – 1.59 (m, 5H), 1.51 – 1.38 (m, 3H) ppm. **^{13}C NMR** (75 MHz, $CDCl_3$) δ 173.9, 134.0, 133.8, 130.4, 121.6, 71.3, 59.7, 51.7, 38.2, 33.9, 31.1, 28.1, 26.0, 24.5, 24.4 ppm. **HRMS (APCI)** Calc. for $C_9H_{15}Cl_2O_2$ [M+H$^+$]: 225.0444, found 225.0448.

(*E*)-(((8,8-Dichlorooct-6-en-1-yl)oxy)methyl)benzene (30) + (*E*)-(((6,8-dichlorooct-7-en-1-yl)oxy)methyl)benzene (30')



Synthesized from **S24** according to general procedure E at 45 °C. Yellow oil is obtained as a 1.2:1 mixture of (*E*)-(((8,8-dichlorooct-6-en-1-yl)oxy)methyl)benzene and (*E*)-(((6,8-dichlorooct-7-en-1-yl)oxy)methyl)benzene in 35% yield after flash column chromatography on deactivated silica gel (Hexane). **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.39 – 7.27 (m, 11H), 6.28 (d, *J* = 13.3 Hz, 1H, **30'**), 6.14 (d, *J* = 6.9 Hz, 1H, **30**), 6.00 (dd, *J* = 13.2, 8.8 Hz, 1H, **30'**), 5.93 – 5.76 (m, 2H, **30**), 4.51 (s, 4H), 4.40 – 4.31 (m, 1H, **30'**), 3.48 (t, *J* = 6.5 Hz, 4H), 2.11 (q, *J* = 6.7 Hz, 3H), 1.90 – 1.74 (m, 3H), 1.63 (p, *J* = 6.7 Hz, 6H), 1.53 – 1.34 (m, 12H) ppm. **^{13}C NMR** (75 MHz, $CDCl_3$) δ 138.8, 138.7, 134.4, 134.2, 130.1, 128.5, 127.7, 127.6, 121.4, 73.0, 71.4, 70.3, 70.2, 62.4, 59.9, 38.5, 31.4, 29.7, 28.4, 26.2, 25.8, 25.7, 1.1 ppm. **HRMS (APCI)** Calc. for $C_{15}H_{19}Cl_2O$ [M+H$^+$]: 285.0807, found 285.0808.

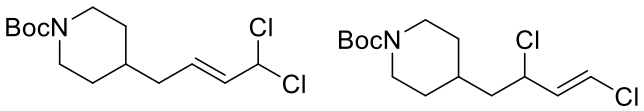
(*E*)-*Tert*-butyl((8,8-dichlorooct-6-en-1-yl)oxy)dimethylsilane (31) + (*E*)-*tert*-butyl((6,8-dichlorooct-7-en-1-yl)oxy)dimethylsilane (31')



Synthesized from **S25** according to general procedure F for 10 min. Pale yellow oil is obtained as a 1:2.4 mixture of (*E*)-*tert*-butyl((8,8-dichlorooct-6-en-1-yl)oxy)dimethylsilane + (*E*)-*tert*-butyl((6,8-dichlorooct-7-en-1-yl)oxy)dimethylsilane in 27% yield after flash column chromatography on deactivated silica gel (Hexane). **^{1}H NMR** (300 MHz, $CDCl_3$) δ 6.27 (d, *J* = 13.2 Hz, 2H, **31'**), 6.13 (d, *J* = 6.7 Hz, 1H, **31**), 5.99 (dd, *J* = 13.2, 8.9 Hz, 2H, **31'**), 5.91 – 5.76 (m, 2H, **31**), 4.40 – 4.28 (m, 2H, **31'**), 3.60 (t, *J* = 6.3 Hz, 7H), 2.08 (dd, *J* = 7.7, 5.4 Hz, 2H), 1.89 – 1.70 (m, 5H), 1.51 (p, *J* = 6.0 Hz, 8H), 1.46 – 1.29 (m, 13H), 0.89 (s, 27H), 0.04 (s, 18H) ppm. **^{13}C NMR** (75 MHz, $CDCl_3$) δ 134.4, 134.2, 130.1, 121.3, 71.4, 63.1, 63.0, 59.9, 38.6, 32.7, 31.5, 28.4, 26.3,

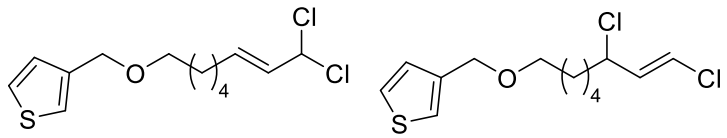
26.1, 25.4, 18.5, -5.2 ppm. **HRMS (APCI)** Calc. for $C_{14}H_{29}Cl_2OSi$ [M+H$^+$]: 311,1359, found 311,1358.

***Tert*-butyl (*E*)-4-(4,4-dichlorobut-2-en-1-yl)piperidine-1-carboxylate (32) + *tert*-butyl (*E*)-4-(2,4-dichlorobut-3-en-1-yl)piperidine-1-carboxylate (32')**



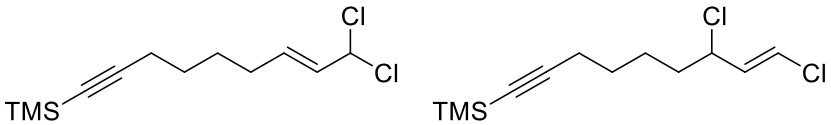
Synthesized from **S26** according to general procedure F for 20 min. Yellow oil is obtained as a 1:1.8 mixture of *tert*-butyl (*E*)-4-(4,4-dichlorobut-2-en-1-yl)piperidine-1-carboxylate and *tert*-butyl (*E*)-4-(2,4-dichlorobut-3-en-1-yl)piperidine-1-carboxylate in 35% yield after flash column chromatography on deactivated silica gel (Hexane:AcOEt 90:10). **^{1}H NMR** (300 MHz, $CDCl_3$) δ 6.28 (d, *J* = 13.2 Hz, 2H, **32'**), 6.12 (dd, *J* = 4.3, 2.6 Hz, 1H, **32**), 5.96 (dd, *J* = 13.2, 8.9 Hz, 2H, **32'**), 5.84 – 5.78 (m, 2H, **32**), 4.43 (td, *J* = 8.8, 4.8 Hz, 2H, **32'**), 4.05 (d, *J* = 14.0 Hz, 7H), 2.73 – 2.57 (m, 7H), 2.05 – 1.97 (m, 2H), 1.79 (t, *J* = 8.5 Hz, 2H), 1.72 – 1.54 (m, 14H), 1.41 (s, 34H), 1.16 – 0.99 (m, 8H) ppm. **^{13}C NMR** (75 MHz, $CDCl_3$) δ 154.9, 154.8, 134.1, 131.9, 131.6, 121.5, 79.4, 79.3, 71.0, 57.3, 45.0, 43.8, 38.4, 35.8, 33.2, 32.1, 31.9, 31.3, 29.7, 28.5 ppm. **HRMS (APCI)** Calc. for $C_{14}H_{24}Cl_2NO_2$ [M+H$^+$]: 308.1179, found 308.1171.

(*E*)-3-(((8,8-Dichlorooct-6-en-1-yl)oxy)methyl)thiophene (33) + (*E*)-3-(((6,8-dichlorooct-7-en-1-yl)oxy)methyl)thiophene (33')



Synthesized from **S27** according to general procedure E at 45 °C. Yellow oil is obtained as a 1.2:1 mixture of (*E*)-3-(((8,8-dichlorooct-6-en-1-yl)oxy)methyl)thiophene and (*E*)-3-(((6,8-dichlorooct-7-en-1-yl)oxy)methyl)thiophene in 37% yield after flash column chromatography on silica gel (Hexane). **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.30 (dd, *J* = 5.0, 3.0 Hz, 2H), 7.20 (d, *J* = 3.1 Hz, 2H), 7.07 (d, *J* = 5.0 Hz, 2H), 6.27 (d, *J* = 13.3 Hz, 1H, **33'**), 6.14 (d, *J* = 6.0 Hz, 1H, **33**), 6.00 (dd, *J* = 13.2, 8.9 Hz, 1H, **33'**), 5.92 – 5.77 (m, 2H, **33**), 4.51 (s, 4H), 4.41 – 4.29 (m, 1H, **33'**), 3.46 (t, *J* = 6.4 Hz, 4H), 2.10 (q, *J* = 6.0 Hz, 2H), 1.88 – 1.76 (m, 2H), 1.61 (q, *J* = 6.8 Hz, 5H), 1.53 – 1.32 (m, 9H) ppm. **^{13}C NMR** (75 MHz, $CDCl_3$) δ 139.9, 134.3, 134.1, 130.0, 127.4, 126.0, 122.6, 121.3, 71.4, 70.2, 70.1, 68.2, 59.9, 38.4, 31.3, 29.6, 28.3, 26.2, 25.8, 25.7 ppm. **HRMS (APCI)** Calc. for $C_{13}H_{19}Cl_2OS$ [M+H$^+$]: 293.0528 found 293.0522.

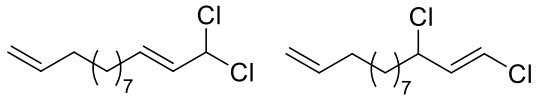
(*E*)-(9,9-Dichloronon-7-en-1-yn-1-yl)trimethylsilane (34) + (*E*)-(7,9-dichloronon-8-en-1-yn-1-yl)trimethylsilane (34')



Synthesized from **S28** according to general procedure E at 45 °C. Yellow oil is obtained as a 1.1:1 mixture of (*E*)-(9,9-Dichloronon-7-en-1-yn-1-yl)trimethylsilane and (*E*)-(7,9-dichloronon-8-en-1-yn-1-yl)trimethylsilane in 33% yield after flash column chromatography on silica gel (Pentane). **^{1}H NMR** (300 MHz, $CDCl_3$)

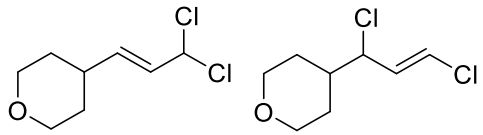
δ 6.30 (d, *J* = 13.2 Hz, 1H, **34'**), 6.18 – 6.12 (m, 1H, **34**), 6.00 (dd, *J* = 13.3, 8.9 Hz, 1H, **34'**), 5.89 – 5.83 (m, 2H, **34**), 4.42 – 4.32 (m, 1H, **34'**), 2.24 (d, *J* = 1.6 Hz, 6H), 2.12 (d, *J* = 4.8 Hz, 2H), 1.84 (d, *J* = 5.0 Hz, 2H), 1.53 (d, *J* = 3.2 Hz, 10H), 0.15 (s, 18H) ppm. **^{13}C NMR** (75 MHz, $CDCl_3$) δ 134.0, 130.2, 121.5, 107.1, 106.9, 85.2, 71.3, 59.8, 38.0, 30.9, 28.0, 27.9, 27.6, 25.6, 19.8, 0.3 ppm. **HRMS (APCI)** Calc. for $C_{12}H_{20}ClSi$ [M+H$^+$-HCl]: 227.1017, found 227.1023.

(*E*)-13,13-Dichlorotrideca-1,11-diene (35) + (*E*)-1,3-dichlorotrideca-1,12-diene (35')



Synthesized from **S29** according to general procedure E at 45 ºC. Yellow oil is obtained as a 1:1 mixture of (*E*)-13,13-Dichlorotrideca-1,11-diene + (*E*)-1,3-dichlorotrideca-1,12-diene in 37% yield after flash column chromatography on silica gel (Hexane). **^{1}H NMR** (300 MHz, $CDCl_3$) δ 6.28 (d, *J* = 13.1 Hz, 1H, **35'**), 6.14 (d, *J* = 6.1 Hz, 1H, **35**), 6.00 (dd, *J* = 13.2, 8.9 Hz, 1H, **35'**), 5.93 – 5.73 (m, 5H), 5.06 – 4.90 (m, 5H), 4.35 (q, *J* = 7.0 Hz, 1H, **35'**), 2.07 (dq, *J* = 13.5, 6.6 Hz, 7H), 1.81 (hept, *J* = 7.3 Hz, 2H), 1.40 (dd, *J* = 14.3, 7.7 Hz, 10H), 1.29 (s, 18H) ppm. **^{13}C NMR** (75 MHz, $CDCl_3$) δ 139.2, 134.5, 134.2, 130.0, 121.2, 114.3, 71.5, 60.0, 38.6, 33.9, 31.4, 29.5, 29.2, 29.0, 28.5, 26.4 ppm. **HRMS (APCI)** Calc. for $C_{13}H_{23}Cl_2$ [M+H$^+$-HCl]: 249.1171, found 249.1171

(*E*)-4-(3,3-Dichloroprop-1-en-1-yl)tetrahydro-2H-pyran (36) + (*E*)-4-(1,3-dichloroallyl)tetrahydro-2H-pyran (36')

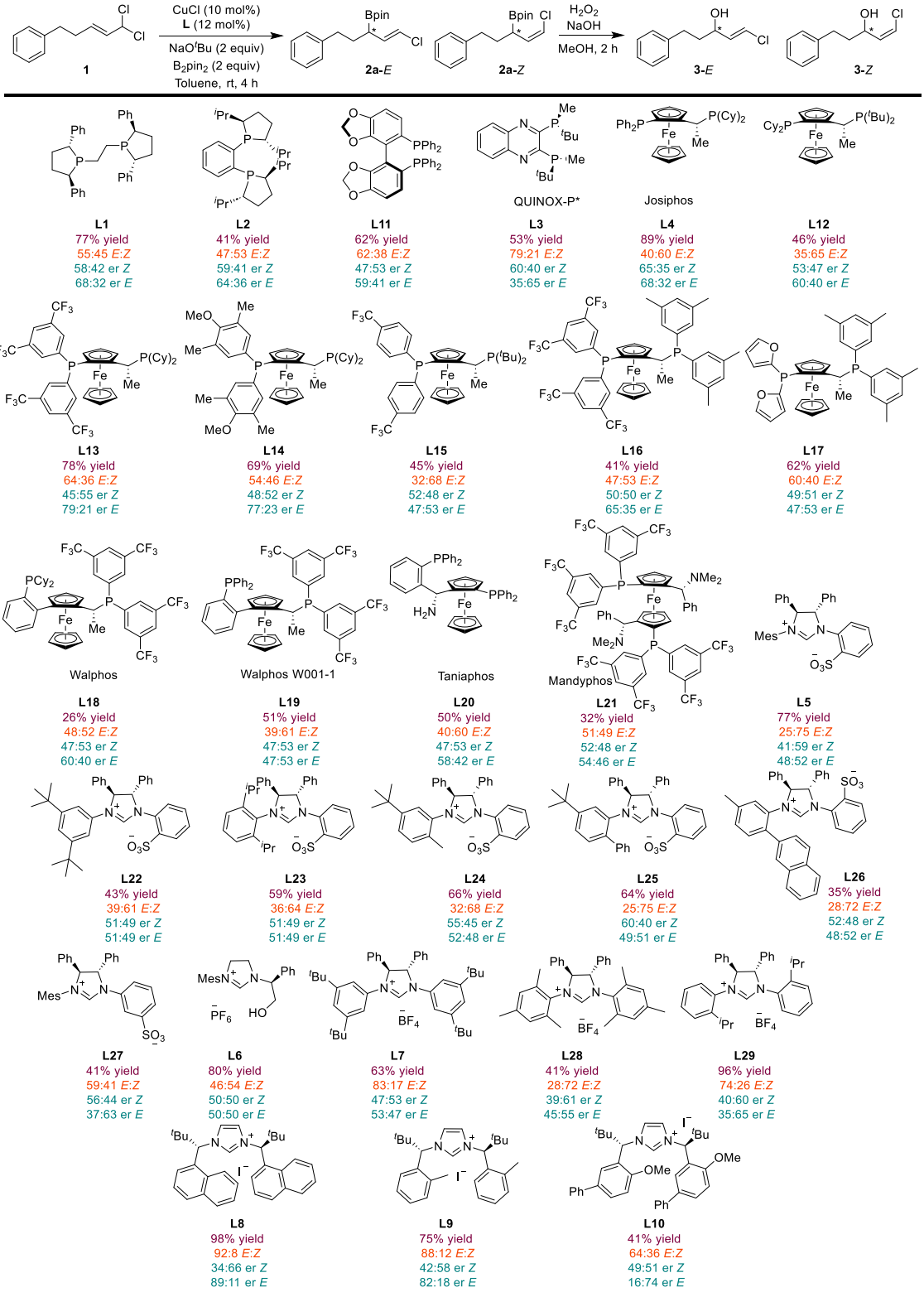


Synthesized from **S30** according to general procedure F for 40 min. Yellow oil is obtained as a 1:2.33 mixture of (*E*)-4-(3,3-Dichloroprop-1-en-1-yl)tetrahydro-2H-pyran and (*E*)-4-(1,3-dichloroallyl)tetrahydro-2H-pyran in 61% yield after flash column chromatography on silica gel (Hexane:Et_2O 97:3). **^{1}H NMR** (300 MHz, $CDCl_3$) δ 6.27 (d, *J* = 13.2 Hz, 2H, **36'**), 6.14 (dd, *J* = 4.9, 2.1 Hz, 1H, **36**), 5.98 (dd, *J* = 13.2, 9.5 Hz, 2H, **36'**), 5.84 – 5.79 (m, 2H, **36**), 4.15 (dd, *J* = 9.6, 7.0 Hz, 2H, **36'**), 4.00 (dt, *J* = 11.4, 5.9 Hz, 8H), 3.46 - 3.26 (m, 9H), 2.35 – 2.22 (m, 1H), 1.94 – 1.78 (m, 6H), 1.72 – 1.56 (m, 5H), 1.56 – 1.29 (m, 8H) ppm. **^{13}C NMR** (75 MHz, $CDCl_3$) δ 137.7, 132.1, 128.6, 122.1, 71.3, 67.6, 67.4, 67.4, 64.5, 42.1, 36.9, 31.8, 29.8, 29.8 ppm. **HRMS (APCI)** Calc. for $C_8H_{13}Cl_2O$ [M+H$^+$]: 195.0338, found 195.0336.

8. Optimization studies

8.1. Screening of chiral ligands

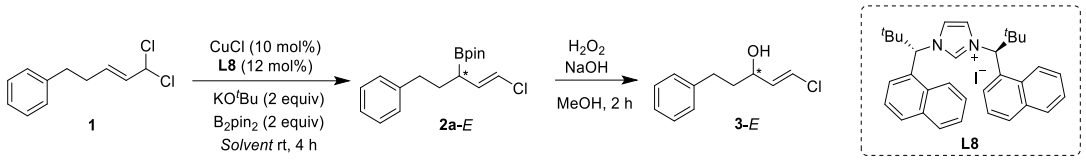
Table S1. Ligand screening



a) *E*:*Z* ratio was determined by GC-MS analysis in **2a**. b) Enantiomeric ratios were determined by SFC analysis in compound **3**.

8.2. Solvent effect

Table 1. Solvent effect on the reaction outcome.

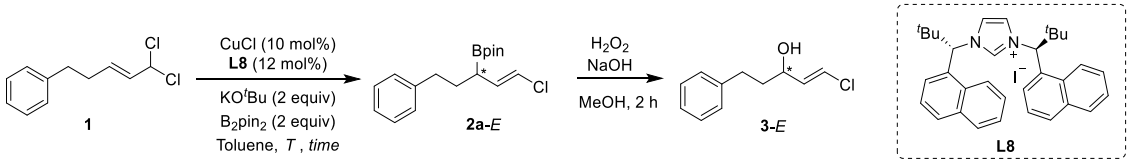


Entry	Solvent	Ratio 2a *E*:*Z*[a]	Isolated yield 3 (%)	er 3*E*[b]
1	Toluene	97:3	80	89:11
2	Dioxane	76:24	79	80:20
3	THF	89:11	83	88:12

[a] *E*:*Z* ratio was determined by GC-MS analysis **2a**. [b] Enantiomeric ratios were determined by SFC analysis in **3**.

8.3. Temperature effect

Table S3. Evaluation of temperature.

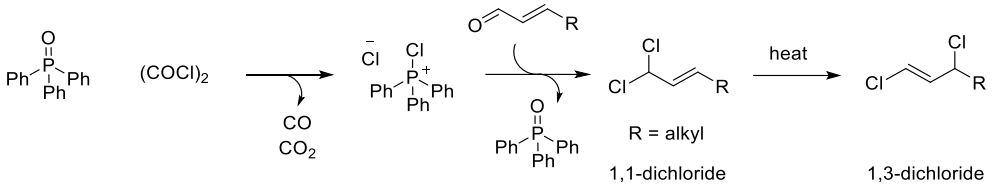


Entry	T /ºC (time)	Ratio 2a *E*:*Z*[a]	Isolated yield 3 (%)	er 3*E*[b]
1	20 (4 h)	97:3	80	89:11
2	0 (8 h)	97:3	80	90:10
3	-20 (24 h)	98:2	79	90:10
4	-40 (30 h)	97:3	75	88:12

[a] *E*:*Z* ratio was determined by GC-MS analysis in **2a**. [b] Enantiomeric ratios were determined by SFC analysis in **3**.

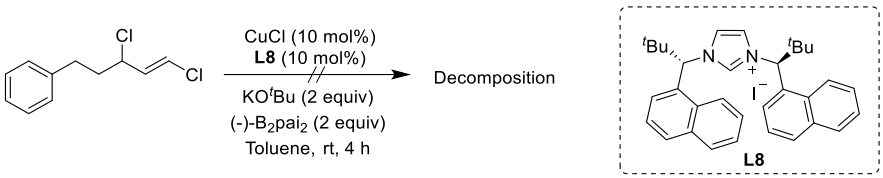
9. Attempted borylation of 1,3-dichloride

The starting allylic dichloride was used as a 1:1 mixture of 1,1- and 1,3-isomers (Scheme S1). Since both isomers can have different chemical behavior, we decided to evaluate the potential role of the 1,3-isomer in the borylation reaction outcome.



Scheme S1. Isomerization of 1,1-dichloride to 1,3-dichloride

Once we run the borylation reaction the *E*-1,3-dichloride was partially recovered. Having isolated the allylic 1,3-dichloride, we ran the reaction with this substrate under optimized and observed full consumption of the starting material, but no formation of the borylation product (Scheme S2). This result confirms that only the 1,1-dichloride is reactive towards borylation, whereas the 1,3-dichloride merely decomposes under reaction conditions.



Scheme S2. Borylation of 1,3-dichloride

10. General procedure for the Cu-catalyzed enantioselective borylation of allylic *gem*-dichlorides.

- **General procedure G: Cu-catalyzed enantioselective borylation of allylic *gem*-dichlorides.**

A screw cap vial was charged with CuCl (10 mol%, 0.01 mmol) and KO^{t}Bu (0.05 mmol) in a glovebox. The vial was removed from the glovebox, ligand **L8** (11 mol%, 0.011 mmol) was added, and the mixture was dissolved in dry toluene (0.4 mL) and stirred for 30 min at rt. The resulting solution was added to a separate flame-dried Schlenk tube equipped with a magnetic stirring bar and charged with B_2pin_2 (2.0 equiv, 0.2 mmol) and KO^{t}Bu (0.15 mmol). The allylic *gem*-dichloride (1 equiv, 0.1 mmol) was dissolved in dry toluene (0.35 mL), added to the Schlenk tube and the mixture was stirred for 4 h at rt. After this time, the mixture was diluted with CH_2Cl_2 (2 mL) and washed with saturated aqueous solution of NH_4Cl (5 mL). Then the aqueous layer was extracted with CH_2Cl_2 (2x2 mL). Combined organic layers were dried over anhydrous Na_2SO_4, filtered and solvent was removed under reduced pressure. Crude product was purified through flash column chromatography using the indicated mixture of solvents as eluent.

Note: Racemic products were synthesized by reaction at rt in toluene using chloro[1,3-bis(2,4,6-trimethylphenyl)imidazol-2-ylidene]copper(I) (IMesCuCl) (10 mol%) as catalyst and NaO^{t}Bu as base.

- **General procedure H. Oxidation with $NaBO_3 \cdot 4H_2O$**

In a screw cap vial equipped with a magnetic stirrer, the allyl boron (1 equiv) and $NaBO_3 \cdot 4H_2O$ (5 equiv) were dissolved in a THF:H_2O mixture (1:1) and the resulting solution was stirred at rt overnight. After that time, the mixture was washed with saturated aqueous solution of NH_4Cl (5 mL) and CH_2Cl_2 (2 mL). Combined organic layers were dried over anhydrous Na_2SO_4, filtered, and solvent was removed under reduced pressure. Crude product was purified through flash column chromatography using the indicated mixture of solvents as eluent.

- **General procedure I. Oxidation with H_2O_2/NaOH**

In a screw cap vial equipped with a magnetic stirrer, the allyl boron (1 equiv) and NaOH aq 2M (5 equiv) and H_2O_2 30% (8 equiv) were dissolved in a MeOH [0.2 M] and the resulting solution was stirred at rt for 2 h After that time, the mixture was washed with saturated aqueous solution of NH_4Cl (5 mL) and CH_2Cl_2 (2 mL). Combined organic layers were dried over anhydrous Na_2SO_4, filtered, and solvent was removed under reduced pressure. Crude product was purified through flash column chromatography using the indicated mixture of solvents as eluent.

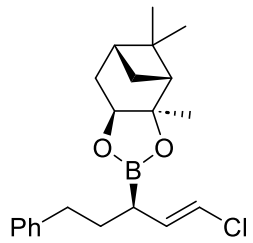
- **General procedure J. Alcohol protection with benzoyl chloride**

To an Ar-filled screw cap vial equipped with a magnetic stirrer, allylic alcohol (1 equiv), DMAP (20 mol%), Et_3N (2 equiv), benzoyl chloride (1 equiv) and CH_2Cl_2 [0.1 M] were added. The reaction was stirred for 2 h at rt. Reaction was washed with aqueous solution

of NH_4Cl (5 mL) and CH_2Cl_2 (2 mL). Combined organic layers were dried over anhydrous Na_2SO_4, filtered, and solvent was removed under reduced pressure. Crude product was purified through flash column chromatography using the indicated mixture of solvents as eluent.

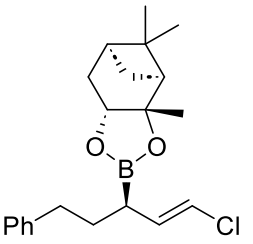
11. Characterization of borylation products.

(3a*R*,4*R*,6*R*,7a*S*)-2-((*R*,*E*)-1-Chloro-5-phenylpent-1-en-3-yl)-3a,5,5-trimethylhexahydro-4,6-methanobenzo[*d*][1,3,2]dioxaborole. (2a)



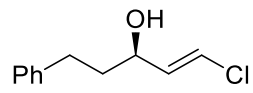
Synthesized from a 1:1 mixture of **1**:**1'** and **42** according to general procedure G. Yellow oil obtained in 97% yield with 98:2 *E*:*Z* and 91:9 er after column chromatography (Hexane:AcOEt, 98:2). **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.34 – 7.23 (m, 2H), 7.22 – 7.12 (m, 3H), 6.01 – 5.87 (m, 2H), 4.27 (d, *J* = 8.8 Hz, 1H), 2.73 – 2.51 (m, 2H), 2.34 (dd, *J* = 13.0, 10.6 Hz, 1H), 2.28 – 2.18 (m, 1H), 2.05 (t, *J* = 5.5 Hz, 1H), 1.93 (dd, *J* = 13.1, 8.6 Hz, 3H), 1.88 – 1.67 (m, 2H), 1.38 (s, 3H), 1.29 (s, 3H), 1.07 (d, *J* = 10.9 Hz, 1H), 0.84 (s, 3H) ppm. **^{13}C NMR** (75 MHz, $CDCl_3$) δ 142.2, 134.6, 128.6, 128.5, 125.9, 116.4, 86.1, 78.1, 51.4, 39.6, 38.3, 35.6, 35.2, 32.5, 28.8, 27.2, 26.6, 24.1 ppm. **^{11}B NMR** (160 MHz, $CDCl_3$) δ 32.1 ppm. **HRMS (APCI)** Calc. for $C_{21}H_{29}BClO_2$ [M+H$^+$]: 359.1944, found 359.1947. **Specific rotation:** $[\alpha]_D^{21}$ +5.9 (*c* = 0.73, $CHCl_3$).

(3a*S*,4*S*,6*S*,7a*R*)-2-((*R*,*E*)-1-Chloro-5-phenylpent-1-en-3-yl)-3a,5,5-trimethylhexahydro-4,6-methanobenzo[*d*][1,3,2]dioxaborole (2c)



Synthesized from a 1:1 mixture of **1**:**1'** and **41** according to general procedure G. Yellow oil obtained in 69% yield with 92:8 *E*:*Z* and 89:11 er after column chromatography (Hexane:AcOEt, 98:2). **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.33 – 7.26 (m, 2H), 7.24 – 7.17 (m, 3H), 6.00 – 5.93 (m, 2H), 4.30 (d, *J* = 8.7 Hz, 1H), 2.75 – 2.54 (m, 3H), 2.43 – 2.31 (m, 2H), 2.31 – 2.20 (m, 2H), 2.08 (t, *J* = 4.9 Hz, 1H), 2.01 – 1.90 (m, 4H), 1.90 – 1.69 (m, 4H), 1.40 (s, 3H), 1.32 (s, 3H), 1.10 (d, *J* = 10.8 Hz, 1H), 0.86 (s, 3H) ppm. **^{13}C NMR** (75 MHz, $CDCl_3$) δ 142.2, 134.6, 128.6, 128.5, 125., 116.4, 86.1, 78.1, 51.4, 39.6, 38.3, 35.6, 35.2, 32.5, 28.7, 27.2, 26.6, 24.1 pp,. **^{11}B NMR** (160 MHz, $CDCl_3$) δ 32.1 ppm. **HRMS (APCI)** Calc. for $C_{21}H_{29}BClO_2$ [M+H$^+$]: 359.1944, found 359.1948. **Specific rotation:** $[\alpha]_D^{21}$ +18.5 (*c* = 0.74, $CHCl_3$).

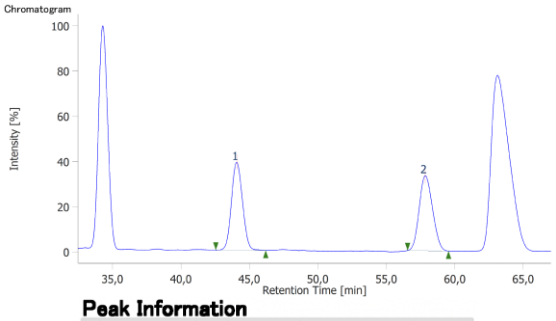
(*R*,*E*)-1-Chloro-5-phenylpent-1-en-3-ol (3)



Obtained from **2a** as yellow oil after flash column chromatography (Hexane:AcOEt 95:5) following general procedure I, in 99% yield and 91:9 er. **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.34 – 7.28 (m, 2H), 7.24 – 7.19 (m, 3H), 6.26 (d, *J* = 13.5 Hz, 1H), 6.02 (dd, *J* = 13.3, 6.9 Hz, 1H), 4.19 (q, *J* = 7.0 Hz, 1H), 2.79 – 2.68 (m, 2H), 1.97 – 1.85 (m, 2H), 1.62 (s, 1H) ppm. **^{13}C NMR** (75 MHz, $CDCl_3$) δ 141.4, 136.2, 128.6, 128.6, 126.2, 120.2, 70.6, 38.6, 31.6 ppm. **HRMS (APCI)** Calc. for $C_{11}H_{12}Cl$ [M+H$^+$-H_2O]: 179.0622, found 179.0621. **Specific rotation:** $[\alpha]_D^{21}$ –6.6 (*c* = 0.95, $CHCl_3$).

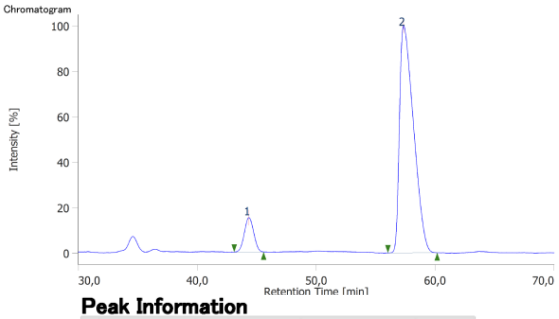
Enantiomeric purity was determined by chiral SFC analysis [Lux Cellulose-1, 100 bar, T_{oven}: 40 °C, flow: 1 mL/min; 5% MeOH, λ = 205 nm, minor enantiomer t_R = 44.32 min, major enantiomer t_R = 57.34 min].

- Oxidation of compound **2a**:



Peak Information

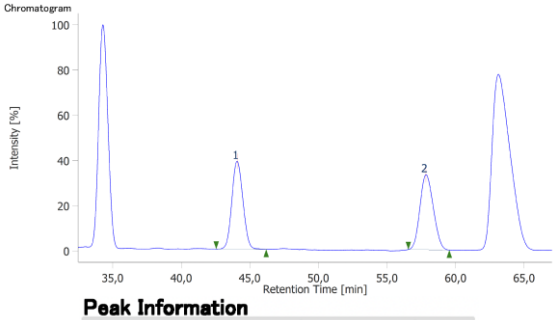
#	Peak Name	CH	tR [min]	Area [µV·sec]	Area%
1	Unknown	9	44,077	6436149	49,253
2	Unknown	9	57,817	6631349	50,747



Peak Information

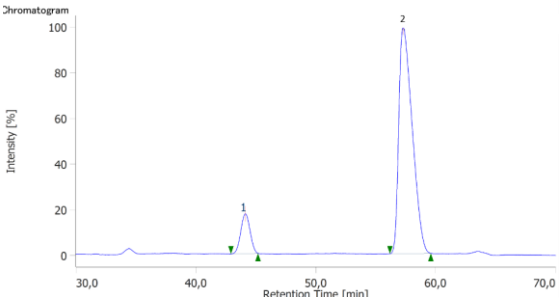
#	Peak Name	CH	tR [min]	Area [µV·sec]	Area%
1	Unknown	9	44,323	3473841	9,190
2	Unknown	9	57,337	34325939	90,810

- Oxidation of compound **2c**: Yellow oil was obtained after flash column chromatography (Hexane/AcOEt 95:5) following general procedure I, in 69% yield and 89:11 er



Peak Information

#	Peak Name	CH	tR [min]	Area [µV·sec]	Area%
1	Unknown	9	44,077	6436149	49,253
2	Unknown	9	57,817	6631349	50,747

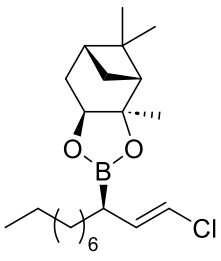


Peak Information

#	Peak Name	CH	tR [min]	Area [µV·sec]	Area%
1	Unknown	9	44,113	3315297	10,865
2	Unknown	9	57,270	27197412	89,135

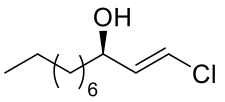
Note: Chromatogram of racemic compound (*E*:*Z* = 28:72) displays only the integrations corresponding to the *E*-isomer (44.07 and 57.81 min) for clarity.

(3a*R*,4*R*,6*R*,7a*S*)-2-((*R*,*E*)-1-Chloroundec-1-en-3-yl)-3a,5,5-trimethylhexahydro-4,6-methanobenzo[*d*][1,3,2]dioxaborole (4)



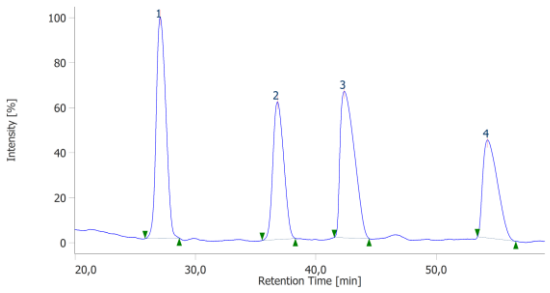
Synthesized from a 1:0.9 mixture of **26**:**26'** and **42** according to general procedure G. Yellow oil obtained in 71% yield with 98:2 *E*:*Z* and 92:8 er after column chromatography (Hexane:AcOEt, 98:2). **^{1}H NMR** (300 MHz, $CDCl_3$) δ 5.95 – 5.83 (m, 2H), 4.26 (d, *J* = 8.7 Hz, 1H), 2.33 (ddt, *J* = 13.5, 8.9, 2.5 Hz, 1H), 2.26 – 2.16 (m, 1H), 2.05 (t, *J* = 5.5 Hz, 1H), 1.94 – 1.87 (m, 2H), 1.87 – 1.79 (m, 1H), 1.37 (s, 3H), 1.29 (s, 3H), 1.26 (s, 13H), 1.07 (d, *J* = 10.9 Hz, 1H), 0.88 (t, *J* = 6.8 Hz, 3H), 0.84 (s, 3H) ppm. **^{13}C NMR** (75 MHz, $CDCl_3$) δ 135.2, 115.8, 86.0, 78.1, 51.4, 39.6, 38.3, 35.6, 32.0, 30.8, 29.7, 29.6, 29.4, 29.1, 28.8, 27.2, 26.5, 24.1, 22.8, 14.2 ppm. **^{11}B NMR** (160 MHz, $CDCl_3$) δ 33.5 ppm. **HRMS (APCI)** Calc. for $C_{21}H_{37}BClO_2$ [M+H$^+$]: 367.2570, found 367.2568. **Specific rotation:** $[\alpha]_D^{21}$ -18.9 (*c* = 0.87, $CHCl_3$).

(*R*,*E*)-1-Chloroundec-1-en-3-ol (S31)



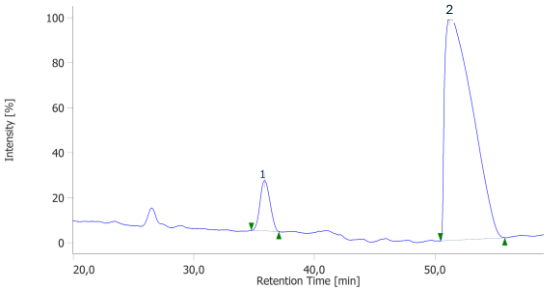
Obtained from **4** as yellow oil after flash column chromatography (Hexane:AcOEt 98:2) following general procedure I, in 85% yield and 92.5:7.5 er. **^{1}H NMR** (300 MHz, $CDCl_3$) δ 6.22 (d, *J* = 13.3 Hz, 1H), 5.96 (dd, *J* = 13.3, 6.9 Hz, 1H), 4.14 (d, *J* = 7.0 Hz, 1H), 1.56 – 1.49 (m, 3H), 1.33 – 1.21 (m, 12H), 0.93 – 0.84 (m, 3H) ppm. **^{13}C NMR** (126 MHz, $CDCl_3$) δ 136.5, 119.7, 71.4, 37.3, 32.0, 29.6, 29.6, 29.4, 25.3, 22.8, 14.2 ppm. **HRMS (APCI)** Calc. for $C_{11}H_{21}O$ [M+H$^+$-HCl]: 169.1587, found 169.1593. **Specific rotation:** $[\alpha]_D^{20}$ –12.0 (*c* = 0.68, $CHCl_3$).

Enantiomeric purity was determined by chiral SFC analysis [Lux Amylose-1, 100 bar, T_{oven}: 40 °C, flow: 1 mL/min; 2% MeOH, λ = 205 nm, minor enantiomer t_R = 35.84 min, major enantiomer t_R = 51.22 min].



Peak Information

#	Peak Name	CH	tR [min]	Area [µV·sec]	Area%
1	Unknown	9	27.080	5170717	29.837
2	Unknown	9	36.810	3630239	20.948
3	Unknown	9	42.353	5036331	29.061
4	Unknown	9	54.250	3492692	20.154

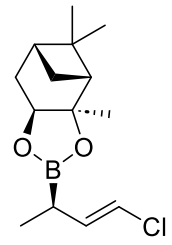


Peak Information

#	Peak Name	CH	tR [min]	Area [µV·sec]	Area%
1	Unknown	9	35.843	1776262	7.554
2	Unknown	9	51.220	21737513	92.446

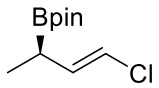
Note: Chromatogram of racemic compound (*E*:*Z* = 41:59) shows peaks for *E*-isomer (36.81 and 54.25 min), *Z*-isomer (27.08 and 42.35 min).

(3a*R*,4*R*,6*R*,7a*S*)-2-((*R*,*E*)-4-chlorobut-3-en-2-yl)-3a,5,5-trimethylhexahydro-4,6-methanobenzo[*d*][1,3,2]dioxaborole (5a)



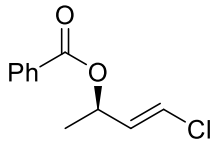
Synthesized from a 0.8:1 mixture of **27:27'** and **42** according to general procedure G. Yellow oil obtained in 99% yield with 95.5 *E*:*Z* and 88:12 er after column chromatography (Pentane:CH_2Cl_2, 90:10). **^{1}H NMR** (300 MHz, $CDCl_3$) δ 6.02 (dd, *J* = 13.3, 7.8 Hz, 1H), 5.90 (d, *J* = 13.3 Hz, 1H), 4.27 (dd, *J* = 8.7, 2.0 Hz, 1H), 2.33 (ddt, *J* = 14.4, 8.7, 2.4 Hz, 1H), 2.21 (ddt, *J* = 8.4, 6.1, 3.0 Hz, 1H), 2.04 (t, *J* = 5.6 Hz, 1H), 2.00 – 1.93 (m, 1H), 1.91 (dd, *J* = 5.5, 2.6 Hz, 1H), 1.83 (dt, *J* = 14.5, 2.7 Hz, 1H), 1.38 (s, 3H), 1.28 (s, 4H), 1.12 (d, *J* = 7.3 Hz, 3H), 1.05 (d, *J* = 10.9 Hz, 1H), 0.83 (s, 3H) ppm. **^{13}C NMR** (75 MHz, $CDCl_3$) δ 136.4, 115.3, 86.1, 78.2, 51.4, 39.6, 38.3, 35.6, 28.7, 27.2, 26.5, 24.1, 15.0 ppm. **^{11}B NMR** (160 MHz, $CDCl_3$) δ 32.3 ppm. **HRMS (APCI)** Calc. for $C_{14}H_{23}BClO_2$ [M+H$^+$]: 269.1474, found 269.1470. **Specific rotation:** $[\alpha]_D^{20}$ -9.3 (*c* = 0.86, $CHCl_3$).

(*R*,*E*)-2-(4-Chlorobut-3-en-2-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (5b)



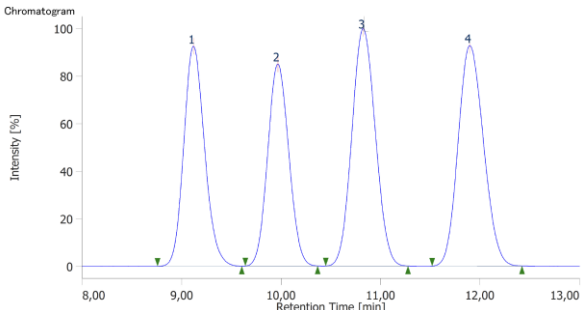
Synthesized from a 0.8:1 mixture of **27:27'** and **37** according to general procedure G. Yellow oil obtained in 69% yield with 89:11 *E*:*Z* and 84:16 er after column chromatography (Pentane:CH_2Cl_2, 85:15). **^{1}H NMR** (300 MHz, $CDCl_3$) δ 5.99 (dd, *J* = 13.3, 7.7 Hz, 1H), 5.88 (d, *J* = 13.2 Hz, 1H), 1.98 – 1.83 (m, 1H), 1.23 (s, 12H), 1.09 (d, *J* = 7.4 Hz, 3H) ppm. **^{13}C NMR** (126 MHz, $CDCl_3$) δ 136.2, 115.3, 83.7, 24.8, 24.8, 14.8 ppm. **^{11}B NMR** (160 MHz, $CDCl_3$) δ 33.0 ppm. **HRMS (APCI)** Calc. for $C_{10}H_{19}BClO_2$ [M+H$^+$]: 217.1161, found 217.1171 **Specific rotation:** $[\alpha]_D^{20}$ +3.9 (*c* = 0.88, $CHCl_3$).

(*R*,*E*)-4-Chlorobut-3-en-2-yl benzoate (S32)



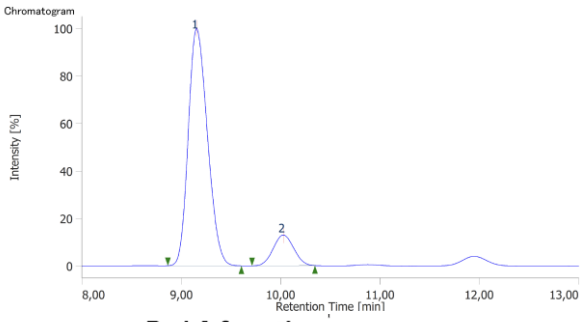
Obtained from **5a** as yellow oil after flash column chromatography (Pentane:CH_2Cl_2 85:15) following general procedure I and J, in 90% overall yield and 88:12 er. **^{1}H NMR** (300 MHz, $CDCl_3$) δ 8.08 – 8.01 (m, 2H), 7.57 (t, *J* = 7.4 Hz, 1H), 7.44 (t, *J* = 7.5 Hz, 2H), 6.39 (d, *J* = 13.3 Hz, 1H), 6.05 (dd, *J* = 13.4, 7.0 Hz, 1H), 5.68 – 5.55 (m, 1H), 1.47 (d, *J* = 6.5 Hz, 3H) ppm. **^{13}C NMR** (75 MHz, $CDCl_3$) δ 165.7, 133.2, 133.1, 130.4, 129.8, 128.5, 122.0, 69.5, 20.4 ppm. **HRMS (APCI)** Calc. for $C_{11}H_{11}ClO_2$ [M]: 210.0442 found 210.0437 **Specific rotation:** $[\alpha]_D^{21}$ -13.4 (*c* = 1.02, $CHCl_3$).

Enantiomeric purity was determined by chiral SFC analysis [Lux Amylose-1, 100 bar, T_{oven}: 40 °C, flow: 1 mL/min; 1% MeOH, λ = 220 nm, minor enantiomer t_R = 9.15 min, major enantiomer t_R = 10.03 min].



Peak Information

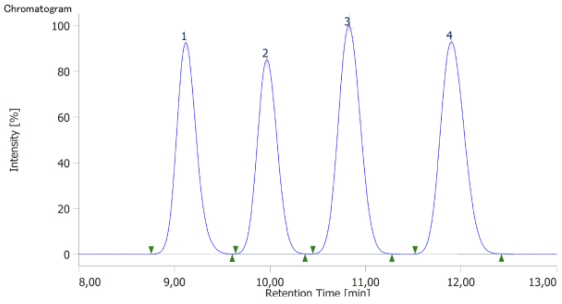
#	Peak Name	CH	tR [min]	Area [µV·sec]	Area%
1	Unknown	10	9,117	3951375	22,866
2	Unknown	10	9,967	3675056	21,267
3	Unknown	10	10,823	4819014	27,887
4	Unknown	10	11,893	4834849	27,979



Peak Information

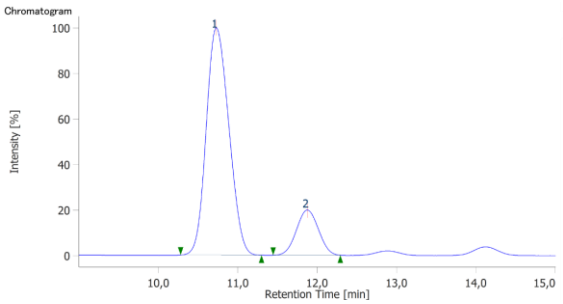
#	Peak Name	CH	tR [min]	Area [µV·sec]	Area%
1	Unknown	10	9,153	15145497	87,782
2	Unknown	10	10,027	2108079	12,218

- <u>Oxidation of compound **5b**.</u> Yellow oil was obtained after flash column chromatography (Hexane/AcOEt 95:5) following general procedure I and J, in 80% yield and 84:16 er.



Peak Information

#	Peak Name	CH	tR [min]	Area [µV·sec]	Area%
1	Unknown	10	9,117	3951375	22,866
2	Unknown	10	9,967	3675056	21,267
3	Unknown	10	10,823	4819014	27,887
4	Unknown	10	11,893	4834849	27,979

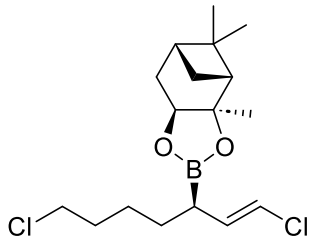


Peak Information

#	Peak Name	CH	tR [min]	Area [µV·sec]	Area%
1	Unknown	10	10,727	8673566	83,813
2	Unknown	10	11,873	1675143	16,187

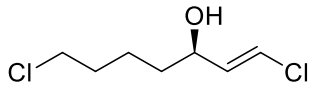
Note: Chromatogram of racemic compound (*E*:*Z* = 44:56) shows peaks for *E*-isomer (9.12 and 9.98 min), *Z*-isomer (10.82 and 11.89 min).

(3a*R*,4*R*,6*R*,7a*S*)-2-((*R*,*E*)-1,7-Dichlorohept-1-en-3-yl)-3a,5,5-trimethylhexahydro-4,6-methanobenzo[*d*][1,3,2]dioxaborole (6)



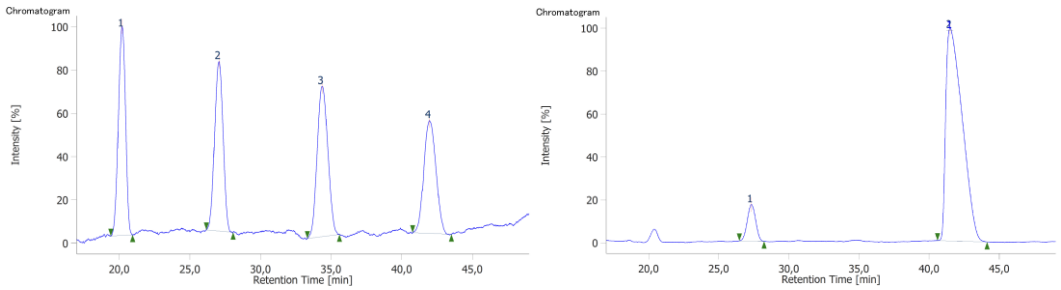
Synthesized from a 1:1 mixture of **28:28'** and **42** according to general procedure G. Yellow oil obtained in 78% yield with 96:4 *E*:*Z* and 92:8 er after column chromatography (Hexane:AcOEt, 98:2). **^{1}H NMR** (300 MHz, $CDCl_3$) δ 5.97 – 5.81 (m, 2H), 4.27 (dd, *J* = 8.7, 2.0 Hz, 1H), 3.52 (t, *J* = 6.7 Hz, 1H), 2.33 (ddt, *J* = 13.6, 8.7, 2.4 Hz, 1H), 2.21 (ddt, *J* = 8.4, 6.2, 3.1 Hz, 1H), 2.04 (t, *J* = 5.5 Hz, 1H), 1.95 – 1.83 (m, 3H), 1.83 – 1.70 (m, 3H), 1.63 – 1.54 (m, 1H), 1.53 – 1.41 (m, 3H), 1.37 (s, 3H), 1.28 (s, 3H), 1.05 (d, *J* = 10.9 Hz, 1H), 0.83 (s, 3H) ppm. **^{13}C NMR** (75 MHz, $CDCl_3$) δ 134.7, 116.2, 86.1, 78.1, 51.4, 45.0, 39.6, 38.3, 35.6, 32.7, 30.0, 28.8, 27.2, 26.6, 26.3, 24.1 ppm. **^{11}B NMR** (160 MHz, $CDCl_3$) δ 32.5 ppm. **HRMS (APCI)** Calc. for $C_{17}H_{28}BCl_2O_2$ [M+H$^+$]: 345.1554, found 345.1557. **Specific rotation:** $[\alpha]_D^{20}$ -16.1 (*c* = 0.57, $CHCl_3$).

(*R*,*E*)-1,7-Dichlorohept-1-en-3-ol (S33)



Obtained from **6** as yellow oil after flash column chromatography (Hexane:AcOEt 96:4) following general procedure I, in 43% yield and 92:8 er. **^{1}H NMR** (300 MHz, $CDCl_3$) δ 6.24 (d, *J* = 13.3 Hz, 1H), 5.96 (dd, *J* = 13.3, 7.0 Hz, 1H), 4.16 (t, *J* = 6.2 Hz, 1H), 3.54 (t, *J* = 6.6 Hz, 2H), 1.80 (p, *J* = 6.6 Hz, 2H), 1.60 – 1.50 (m, 5H) ppm. **^{13}C NMR** (126 MHz, $CDCl_3$) δ 136.1, 120.1, 71.1, 44.9, 36.3, 32.5, 22.7 ppm. **HRMS (APCI)** Calc. for $C_7H_{12}ClO$ [M+H$^+$-HCl]: 147.0571, found 147.0579. **Specific rotation:** $[\alpha]_D^{20}$ -12.0 (*c* = 0.68, $CHCl_3$).

Enantiomeric purity was determined by chiral SFC analysis [Lux Amylose-1, 100 bar, T_{oven}: 40 °C, flow: 1 mL/min; 5% MeOH, λ = 205 nm, minor enantiomer t_R = 27.33 min, major enantiomer t_R = 41.48min].



Peak Information

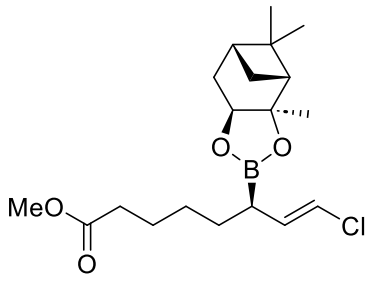
#	Peak Name	CH	tR [min]	Area [μV·sec]	Area%
1	Unknown	9	20.210	1146437	25.285
2	Unknown	9	27.070	1104071	24.351
3	Unknown	9	34.353	1234022	27.217
4	Unknown	9	41.953	1049471	23.147

Peak Information

#	Peak Name	CH	tR [min]	Area [μV·sec]	Area%
1	Unknown	9	27.333	1487191	7.984
2	Unknown	9	41.480	17139013	92.016

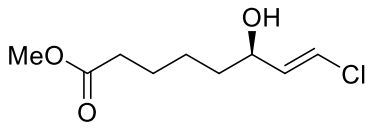
Note: Chromatogram of racemic compound (*E*:*Z* = 48:52) shows peaks for *E*-isomer (27.02 and 41.95 min) and *Z*-isomer (20.21 and 34.35 min).

Methyl (*R*,*E*)-8-chloro-6-((3a*R*,4*R*,6*R*,7a*S*)-3a,5,5-trimethylhexahydro-4,6-methanobenzo[*d*][1,3,2]dioxaborol-2-yl)oct-7-enoate (7)



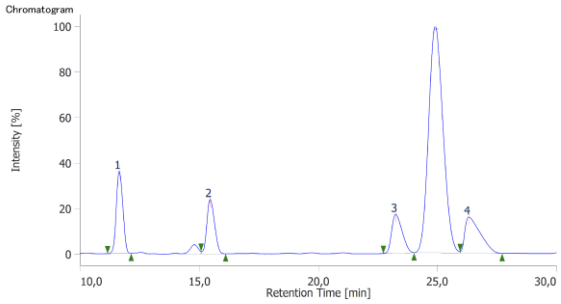
Synthesized from a 1:1 mixture of **29:29'** and **42** according to general procedure G. Yellow oil obtained in 45% yield with 99:1 *E*:*Z* and 92.5:7.5 er after column chromatography (Hexane:AcOEt, 99:1). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 5.91 (d, *J* = 13.2 Hz, 1H), 5.86 (dd, *J* = 13.2, 8.8 Hz, 1H), 4.26 (dd, *J* = 8.8, 1.9 Hz, 1H), 3.66 (s, 3H), 2.34 (dt, *J* = 9.6, 2.9 Hz, 1H), 2.30 (t, *J* = 7.4 Hz, 2H), 2.21 (dqd, *J* = 10.9, 6.5, 2.3 Hz, 2H), 2.04 (t, *J* = 5.5 Hz, 1H), 1.93 – 1.86 (m, 3H), 1.82 (ddd, *J* = 14.7, 3.5, 2.1 Hz, 2H), 1.66 – 1.54 (m, 5H), 1.37 (s, 3H), 1.28 (s, 3H), 1.05 (d, *J* = 11.0 Hz, 1H), 0.83 (s, 3H) ppm. **^{13}C NMR** (126 MHz, $CDCl_3$) δ 174.2, 134.8, 116.1, 86.1, 78.1, 51.6, 51.4, 39.6, 38.3, 35.6, 34.1, 30.3, 28.8, 28.5, 27.2, 26.5, 25.0, 24.1 ppm. **^{11}B NMR** (160 MHz, $CDCl_3$) δ 32.6 ppm. **HRMS (APCI)** Calc. for $C_{19}H_{31}BClO_4$ [M+H$^+$]: 369.1993, found 369.1998. **Specific rotation** $[\alpha]_D^{20}$ -15.7 (*c* = 0.82, $CHCl_3$).

Methyl (*R*,*E*)-8-chloro-6-hydroxyoct-7-enoate (S34)



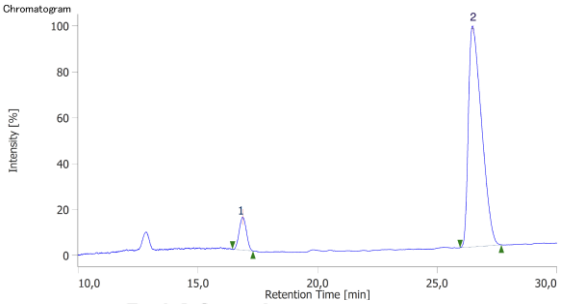
Obtained from **7** as yellow oil after flash column chromatography (Hexane:AcOEt 90:10) following general procedure H, in 76% yield and 92.5:7.5 er. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 6.22 (dd, *J* = 13.3, 1.2 Hz, 1H), 5.95 (dd, *J* = 13.3, 6.9 Hz, 1H), 4.16 (q, *J* = 6.5 Hz, 1H), 3.67 (s, 3H), 2.32 (t, *J* = 7.4 Hz, 2H), 1.73 (s, 1H), 1.69 – 1.62 (m, 2H), 1.59 – 1.52 (m, 2H), 1.48 – 1.32 (m, 2H) ppm. **^{13}C NMR** (126 MHz, $CDCl_3$) δ 174.2, 136.2, 119.9, 71.0, 51.7, 36.7, 33.9, 24.8, 24.7 ppm. **HRMS (APCI)** Calc. for $C_9H_{14}ClO_3$ [M-H$^+$]: 205.0626, found 205.0531. **Specific rotation:** $[\alpha]_D^{20}$ -5.4 (*c* = 0.32, $CHCl_3$).

Enantiomeric purity was determined by chiral SFC analysis [Lux Amylose-1, 100 bar, T_{oven}: 40 °C, flow: 1 mL/min; 10% MeOH, λ = 205 nm, minor enantiomer t_R = 16.87 min, major enantiomer t_R = 26.46 min].



Peak Information

#	Peak Name	CH	tR [min]	Area [μV·sec]	Area%
1	Unknown	9	11,637	3740033	28,138
2	Unknown	9	15,447	2894063	21,773
3	Unknown	9	23,243	2813918	21,170
4	Unknown	9	26,317	3843964	28,919

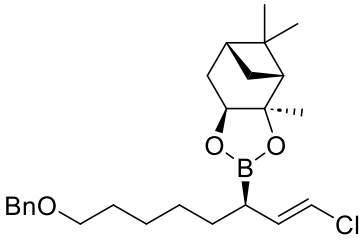


Peak Information

#	Peak Name	CH	tR [min]	Area [μV·sec]	Area%
1	Unknown	9	16,867	442208	7,532
2	Unknown	9	26,463	5428627	92,468

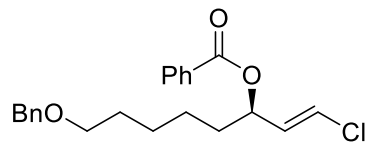
Note: Chromatogram of racemic compound (*E*:*Z* = 43:57) shows peaks for *E*-isomer (15.45 and 26.32 min), *Z*-isomer (15.45 and 23.24 min) and impurity.

(3a*R*,4*R*,6*R*,7a*S*)-2-((*R*,*E*)-8-(Benzyloxy)-1-chlorooct-1-en-3-yl)-3a,5,5-trimethylhexahydro-4,6-methanobenzo[*d*][1,3,2]dioxaborole (8)



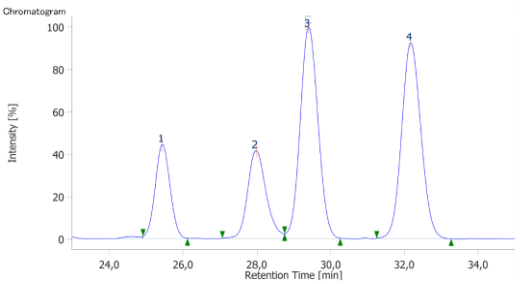
Synthesized from a 1.2:1 mixture of **30:30'**and **42** according to general procedure G. Yellow oil obtained in 65% yield with 96:4 *E*:*Z* and 91:9 er after column chromatography (Hexane:AcOEt, 99:1). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.34 (d, *J* = 3.4 Hz, 4H), 7.29 – 7.26 (m, 1H), 5.92 – 5.85 (m, 2H), 4.49 (s, 2H), 4.26 (dd, *J* = 8.8, 2.1 Hz, 1H), 3.45 (t, *J* = 6.6 Hz, 2H), 2.36 – 2.30 (m, 2H), 2.24 – 2.18 (m, 2H), 2.06 – 2.03 (m, 1H), 1.92 – 1.85 (m, 3H), 1.83 (ddd, *J* = 14.7, 3.4, 2.0 Hz, 1H), 1.65 – 1.54 (m, 5H), 1.37 (s, 3H), 1.28 (s, 3H), 1.06 (d, *J* = 11.0 Hz, 1H), 0.83 (s, 3H) ppm. **^{13}C NMR** (126 MHz, $CDCl_3$) δ 138.8, 135.0, 128.5, 127.7, 127.6, 115.9, 86.0, 78.0, 73.0, 70.5, 51.4, 39.6, 38.3, 35.6, 30.7, 29.8, 28.9, 28.8, 27.2, 26.5, 26.2, 24.1 ppm. **^{11}B NMR** (160 MHz, $CDCl_3$) δ 32.5 ppm. **HRMS (APCI)** Calc. for $C_{25}H_{37}BClO_3$ [M+H$^+$]: 431.2516, found 431.2512. **Specific rotation:** $[\alpha]_D^{20}$ -12.0 (*c* = 0.52, $CHCl_3$).

(*R*,*E*)-8-(Benzyloxy)-1-chlorooct-1-en-3-yl benzoate (S35)



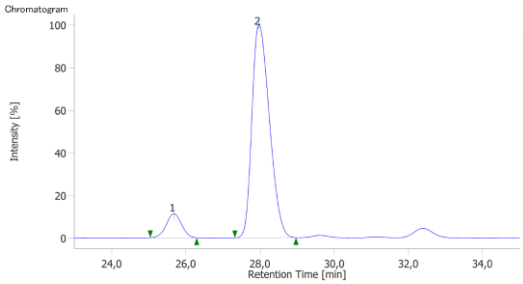
Obtained from **8** as yellow oil after flash column chromatography (Hexane:AcOEt 98:2) following general procedure I and then, the general procedure J, in 46% overall yield and 91:9 er. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.03 (d, *J* = 7.2 Hz, 2H), 7.57 (t, *J* = 7.4 Hz, 1H), 7.45 (t, *J* = 7.8 Hz, 2H), 7.37 – 7.31 (m, 4H), 7.28 (dt, *J* = 5.9, 2.8 Hz, 1H), 6.37 (d, *J* = 13.3 Hz, 1H), 5.98 (dd, *J* = 13.3, 7.6 Hz, 1H), 5.50 (q, *J* = 6.7 Hz, 1H), 4.49 (s, 2H), 3.46 (t, *J* = 6.5 Hz, 2H), 1.87 – 1.79 (m, 1H), 1.74 (ddt, *J* = 13.3, 9.1, 4.3 Hz, 1H), 1.63 (t, *J* = 7.4 Hz, 2H), 1.42 (pd, *J* = 7.6, 4.2 Hz, 4H) ppm. **^{13}C NMR** (126 MHz, $CDCl_3$) δ 165.8, 138.8, 133.2, 132.0, 130.3, 129.7, 128.6, 128.5, 127.8, 127.7, 122.5, 73.1, 70.3, 34.4, 29.7, 26.1, 25.0 ppm. **HRMS (APCI)** Calc. for $C_{22}H_{25}O_3$ [M+H$^+$-HCl]: 337.1798, found 337.1791. **Specific rotation:** $[\alpha]_D^{20}$ -5.5 (*c* = 0.73, $CHCl_3$).

Enantiomeric purity was determined by chiral SFC analysis [Lux Celulose-1, 100 bar, T_{oven}: 40 °C, flow: 1.5 mL/min; 5% MeOH, λ = 220 nm, minor enantiomer t_R = 25.68 min, major enantiomer t_R = 27.97 min].



Peak Information

#	Peak Name	CH	tR [min]	Area [µV·sec]	Area%
1	Unknown	10	25.443	1363406	13.277
2	Unknown	10	27.980	1547009	15.065
3	Unknown	10	29.400	3671863	35.758
4	Unknown	10	32.163	3686388	35.899

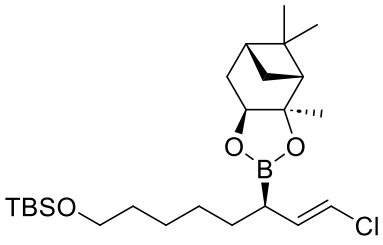


Peak Information

#	Peak Name	CH	tR [min]	Area [µV·sec]	Area%
1	Unknown	10	25.680	1321055	9.118
2	Unknown	10	27.970	13167892	90.882

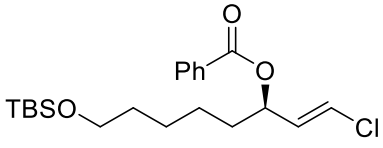
Note: Chromatogram of racemic compound (*E*:*Z* = 28:72) shows peaks for *E*-isomer (25.44 and 27.98 min) and *Z*-isomer (29.40 and 32.16 min).

Tert-butyl(((*R*,*E*)-8-chloro-6-((3a*R*,4*R*,6R,7a*S*)-3a,5,5-trimethylhexahydro-4,6-methanobenzo[*d*][1,3,2]dioxaborol-2-yl)oct-7-en-1-yl)oxy)dimethylsilane (9)



Synthesized from a 1:2.4 mixture of **31:31'** and **42** according to general procedure G. Yellow oil obtained in 45% yield with >95:5 *E*:*Z* and 91:9 er after column chromatography (Hexane:CH_2Cl_2, 95:5). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 5.88 (d, *J* = 7.3 Hz, 2H), 4.26 (dd, *J* = 8.8, 2.1 Hz, 1H), 3.58 (t, *J* = 6.6 Hz, 2H), 2.36 – 2.30 (m, 1H), 2.24 – 2.18 (m, 1H), 2.04 (t, *J* = 5.6 Hz, 1H), 1.93 – 1.86 (m, 2H), 1.83 (ddd, *J* = 14.7, 3.4, 2.0 Hz, 2H), 1.50 (t, *J* = 7.0 Hz, 2H), 1.37 (s, 3H), 1.28 (s, 3H), 1.06 (d, *J* = 11.0 Hz, 1H), 0.89 (s, 9H), 0.83 (s, 3H), 0.04 (s, 6H) ppm. **^{13}C NMR** (126 MHz, $CDCl_3$) δ 135.0, 115.8, 86.0, 78.0, 63.3, 51.4, 39.6, 38.3, 35.6, 32.9, 30.7, 28.9, 28.8, 27.2, 26.5, 26.1, 25.9, 24.1, 18.5, -5.1 ppm. **^{11}B NMR** (160 MHz, $CDCl_3$) δ 32.1 ppm. **HRMS (APCI)** Calc. for $C_{24}H_{43}BClO_3Si$ [M-H$^+$]: 452.2794, found 452.2796. **Specific rotation:** $[\alpha]_D^{20}$ -11.9 (*c* = 0.75, $CHCl_3$).

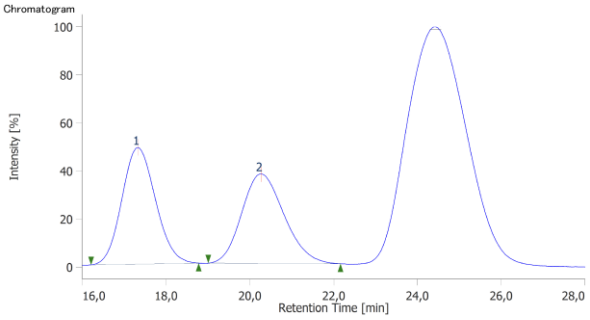
(*R*,*E*)-8-((*Tert*-butyldimethylsilyl)oxy)-1-chlorooct-1-en-3-yl benzoate (S36)



Obtained from **9** as yellow oil after flash column chromatography (Hexane:AcOEt 99:1) following general procedure I and then, the general procedure J, in 56% overall yield and 91:9 er. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.04 – 8.02 (m, 2H), 7.59 – 7.55 (m, 1H), 7.47 – 7.42 (m, 2H), 6.37 (dd, *J* = 13.3, 1.0 Hz, 1H), 5.99 (dd, *J* = 13.3, 7.7 Hz, 1H), 5.50 0 (q, *J* = 6.4 Hz, 1H), 3.59 (t, *J* = 6.5 Hz, 2H), 1.86 – 1.79 (m, 1H), 1.77 – 1.69 (m, 1H), 1.55 – 1.49 (m, 2H), 1.44 – 1.35 (m, 4H), 0.88 (s, 9H), 0.03 (s, 6H) ppm. **^{13}C NMR** (126 MHz, $CDCl_3$) δ 165.8, 133.2, 132.0, 130.3, 129.8, 128.6, 122.5, 73.1, 63.1, 34.5, 32.8, 26.1, 25.7, 25.0, 18.5, -5.1 ppm.

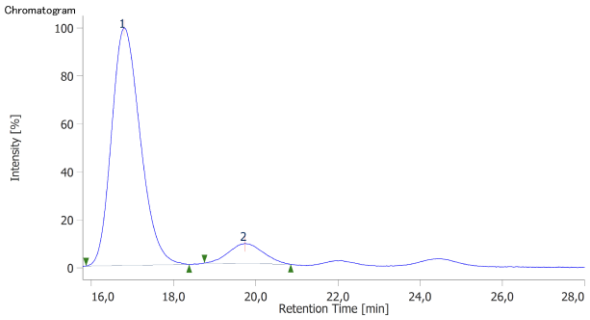
HRMS (APCI) Calc. for $C_{21}H_{34}ClO_3Si$ [M+H$^+$]: 397.1960, found 397.1949. **Specific rotation:** $[\alpha]_D^{21}$ -4.9 (c = 0.4, $CHCl_3$).

Enantiomeric purity was determined by chiral SFC analysis [Lux Amylose-1, 100 bar, T_{oven}: 40 °C, flow: 1 mL/min; 1% MeOH, λ = 220 nm, minor enantiomer t_R = 16.80 min, major enantiomer t_R = 19.74 min].



Peak Information

#	Peak Name	CH	tR [min]	Area [µV·sec]	Area%
1	Unknown	10	17.330	1452835	50.907
2	Unknown	10	20.260	1401044	49.093

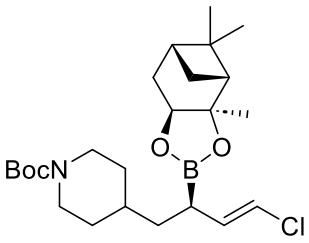


Peak Information

#	Peak Name	CH	tR [min]	Area [µV·sec]	Area%
1	Unknown	10	16.800	2113681	90.817
2	Unknown	10	19.740	213727	9.183

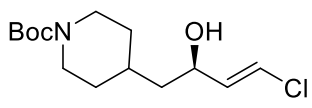
Note: Chromatogram of racemic compound shows peaks for *E*-isomer (17.33 and 20.26 min) and *Z*-isomer (not separated).

***Tert*-butyl 4-((*R*,*E*)-4-chloro-2-((3a*R*,4*R*,6*R*,7a*S*)-3a,5,5-trimethylhexahydro-4,6-methanobenzo[*d*][1,3,2]dioxaborol-2-yl)but-3-en-1-yl)piperidine-1-carboxylate (10)**



Synthesized from a 1:1.8 mixture of **32**:**32'** and **42** according to general procedure G. Colorless oil obtained in 50% yield with 97:3 *E*:*Z* and 90.5:9.5 er after column chromatography (Hexane:AcOEt, 95:5). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 5.91 (d, J = 13.2 Hz, 1H), 5.85 (dd, J = 13.3, 9.3 Hz, 1H), 4.26 (dd, J = 8.7, 2.0 Hz, 1H), 4.10 – 4.05 (m, 2H), 2.70 – 2.58 (m, 2H), 2.33 (ddt, J = 14.6, 8.8, 2.5 Hz, 1H), 2.25 – 2.18 (m, 1H), 2.05 – 1.99 (m, 2H), 1.91 (hept, J = 3.0 Hz, 1H), 1.84 – 1.78 (m, 1H), 1.67 – 1.58 (m, 2H), 1.44 (s, 9H), 1.43 – 1.39 (m, 1H), 1.37 (s, 3H), 1.28 (s, 3H), 1.12 – 0.96 (m, 4H), 0.83 (s, 3H) ppm. **^{13}C NMR** (75 MHz, $CDCl_3$) δ 155.0, 134.8, 116.0, 86.1, 79.3, 78.1, 51.4, 44.1, 39.6, 38.3, 37.2, 35.6, 34.8, 32.6, 31.6, 28.7, 28.6, 27.2, 26.5, 24.1 ppm. **^{11}B NMR** (160 MHz, $CDCl_3$) δ 33.1 ppm. **HRMS (APCI)** Calc. for $C_{24}H_{39}BClNO_4$ [M+H$^+$]: 451.2655, found 451.2662. **Specific rotation:** $[\alpha]_D^{19}$ -12.0 (c = 0.52, $CHCl_3$).

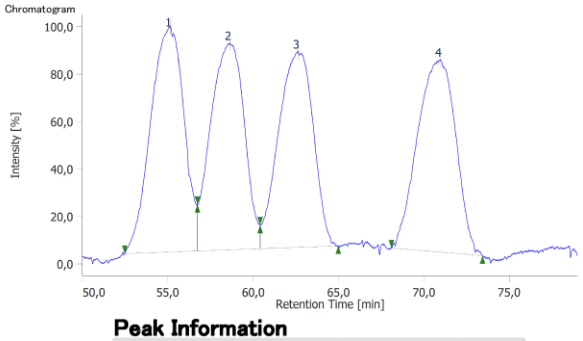
***Tert*-butyl (*R*,*E*)-4-(4-chloro-2-hydroxybut-3-en-1-yl)piperidine-1-carboxylate (S37)**



Obtained from **10** as yellow oil after flash column chromatography (Hexane:AcOEt 90:10) following method I, in 40% yield and 90.5:9.5 er. **^{1}H NMR** (300 MHz, $CDCl_3$) δ 6.24 (d, J = 13.4 Hz, 1H), 5.96 (dd, J = 13.3, 7.0 Hz, 1H), 4.26 (q, J = 7.5 Hz, 1H), 4.15 – 3.96 (m, 2H), 2.69 (t, J = 11.9 Hz, 2H), 1.74 – 1.54 (m, 5H), 1.45 (s, 9H), 1.28 (dd, J = 10.1, 7.5 Hz, 2H), 1.12 (t, J = 11.5 Hz, 1H) ppm. **^{13}C NMR** (126 MHz, $CDCl_3$) δ 155.0,

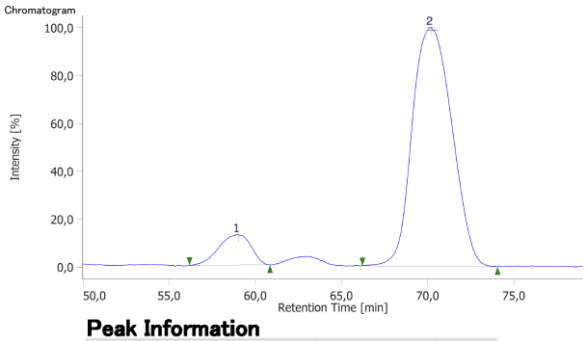
136.6, 120.0, 79.5, 68.7, 43.9, 32.5, 28.6 ppm. **HRMS (APCI)** Calc. for $C_{14}H_{25}ClNO_3$ [M+H$^+$]: 290.1517, found 290.1518. **Specific rotation:** $[\alpha]_D^{20}$ -8.5 (c = 0.53, $CHCl_3$).

Enantiomeric purity was determined by chiral SFC analysis [Lux Cellulose-5, 100 bar, T_{oven}: 40 °C, flow: 0.8 mL/min; 5% MeOH, λ = 205 nm, minor enantiomer t_R = 59.00 min, major enantiomer t_R = 70.18 min].



Peak Information

#	Peak Name	CH	tR [min]	Area [µV·sec]	Area%
1	Unknown	9	55,137	3011421	26,133
2	Unknown	9	58,610	2808803	24,375
3	Unknown	9	62,613	2740497	23,782
4	Unknown	9	70,937	2962761	25,711

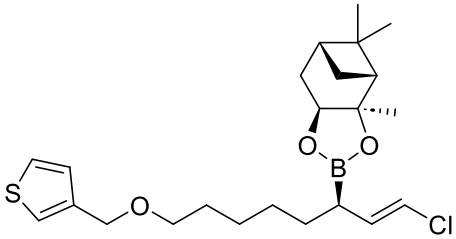


Peak Information

#	Peak Name	CH	tR [min]	Area [µV·sec]	Area%
1	Unknown	9	59,000	3121364	9,406
2	Unknown	9	70,187	30062614	90,594

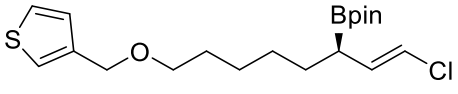
Note: Chromatogram of racemic compound (*E*:*Z* = 50:50) shows peaks for *E*-isomer (58.61 and 70.94 min) and *Z*-isomer (55.14 and 62.61 min).

(3a*R*,4*R*,6*R*,7a*S*)-2-((*R*,*E*)-1-Chloro-8-(thiophen-3-ylmethoxy)oct-1-en-3-yl)-3a,5,5-trimethylhexahydro-4,6-methanobenzo[*d*][1,3,2]dioxaborole (11a)



Synthesized from a 1.2:1 mixture of **33:33'** and **42** according to general procedure G. Yellow oil obtained in 62% yield with >95:5 *E*:*Z* and 94:6 er after column chromatography (Hexane:AcOEt, 99:1). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.29 (dd, J = 5.0, 3.0 Hz, 1H), 7.20 – 7.18 (m, 1H), 7.06 (dd, J = 5.0, 1.2 Hz, 1H), 5.92 – 5.84 (m, 2H), 4.49 (s, 2H), 4.26 (dd, J = 8.8, 2.1 Hz, 1H), 3.44 (t, J = 6.7 Hz, 2H), 2.36 – 2.29 (m, 2H), 2.24 – 2.16 (m, 2H), 2.04 (t, J = 5.5 Hz, 1H), 1.93 – 1.85 (m, 3H), 1.82 (ddd, J = 14.7, 3.4, 2.0 Hz, 1H), 1.63 – 1.53 (m, 6H), 1.37 (s, 3H), 1.28 (s, 3H), 1.06 (d, J = 11.0 Hz, 1H), 0.83 (s, 3H) ppm. **^{13}C NMR** (126 MHz, $CDCl_3$) δ 140.0, 135.0, 127.5, 126.0, 122.6, 115.9, 86.0, 78.0, 70.5, 68.3, 51.4, 39.6, 38.3, 35.6, 30.7, 29.7, 28.9, 28.8, 27.2, 26.5, 26.2, 24.1 ppm. **^{11}B NMR** (160 MHz, $CDCl_3$) δ 32.3 ppm. **HRMS (APCI)** Calc. for $C_{23}H_{35}BClO_3S$ [M+H$^+$]: 437.2083, found 437.2089. **Specific rotation:** $[\alpha]_D^{20}$ -17.8 (c = 1.1, $CHCl_3$).

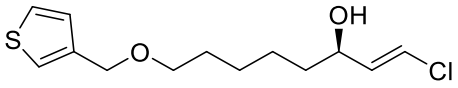
(*R*,*E*)-2-(1-Chloro-8-(thiophen-3-ylmethoxy)oct-1-en-3-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (11b)



Synthesized from a mixture of **33:33'** and **37** according to general procedure G. Yellow oil obtained in 57% yield with 94:6 *E*:*Z* and 93:7 er after column chromatography (Hexane:AcOEt, 99:1). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.31

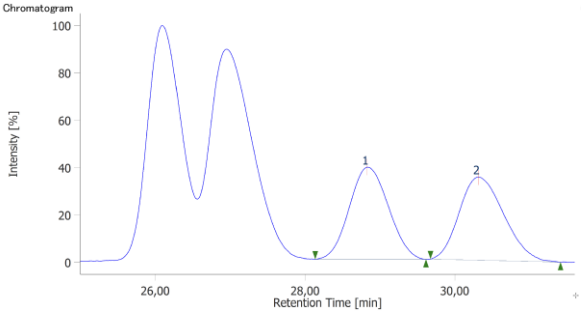
– 7.27 (m, 1H), 7.21 - 7.17 (m, 1H), 7.06 (d, J = 5.0 Hz, 1H), 5.91 – 5.82 (m, 2H), 4.49 (s, 2H), 3.44 (t, J = 6.6 Hz, 2H), 1.82 (q, J = 7.7 Hz, 1H), 1.62 – 1.56 (m, 3H), 1.55 – 1.49 (m, 1H), 1.44 – 1.38 (m, 1H), 1.38 – 1.30 (m, J = 4.3 Hz, 4H), 1.23 (s, 12H) ppm. **^{13}C NMR** (126 MHz, $CDCl_3$) δ 140.0, 134.8, 127.5, 126.0, 122.6, 115.8, 83.6, 70.5, 68.3, 30.6, 29.7, 28.8, 26.2, 25.2, 24.9, 24.8 ppm. **^{11}B NMR** (160 MHz, $CDCl_3$) δ 32.9 ppm. **HRMS (APCI)** Calc. for $C_{19}H_{31}BClO_3S$ [M+H$^+$]: 385.1770, found 385.1772. **Specific rotation:** $[\alpha]_D^{19}$ -7.6 (c = 0.73, $CHCl_3$).

(*R*,*E*)-1-Chloro-8-(thiophen-3-ylmethoxy)oct-1-en-3-ol (S38)



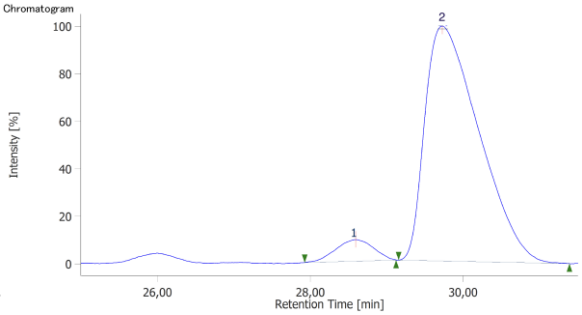
Obtained from **11a** as yellow oil after flash column chromatography (Hexane:AcOEt 95:5) following general procedure I in 95% yield and 94:6 er. **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.30 (dd, J = 5.0, 3.0 Hz, 1H), 7.20 (d, J = 3.1 Hz, 1H), 7.11 – 7.04 (m, 1H), 6.21 (d, J = 13.3 Hz, 1H), 5.94 (dd, J = 13.3, 6.9 Hz, 1H), 4.50 (s, 2H), 4.12 (t, J = 6.8 Hz, 1H), 3.45 (t, J = 6.5 Hz, 2H), 1.67 – 1.52 (m, 5H), 1.45 – 1.33 (m, 3H) ppm. **^{13}C NMR** (75 MHz, $CDCl_3$) δ 139.9, 136.4, 127.4, 126.0, 122.7, 119.7, 71.2, 70.3, 68.3, 37.1, 29.1, 26.2, 25.1 ppm. **HRMS (APCI)** Calc. for $C_{13}H_{19}ClO_2S$ [M+]: 274.0789, found 274.0785. **Specific rotation:** $[\alpha]_D^{20}$ -4.4 (c = 0.67, $CHCl_3$).

Enantiomeric purity was determined by chiral SFC analysis [Lux Cellulose-5 100 bar, T_{oven}: 40 °C, flow: 2 mL/min; 5% MeOH, λ = 220 nm, minor enantiomer t_R = 28.59 min, major enantiomer t_R = 29.72 min].



Peak Information

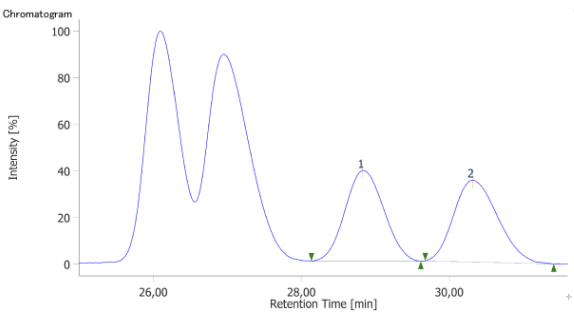
#	Peak Name	CH	tR [min]	Area [µV·sec]	Area%
1	Unknown	10	28,827	837568	49,304
2	Unknown	10	30,310	861225	50,696



Peak Information

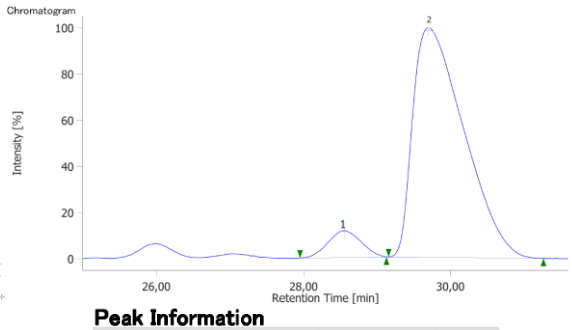
#	Peak Name	CH	tR [min]	Area [µV·sec]	Area%
1	Unknown	10	28,590	280719	6,011
2	Unknown	10	29,723	4389568	93,989

- Oxidation of compound **11b**: Yellow oil was obtained after flash column chromatography (Hexane/AcOEt 95:5) following general procedure I, in 60% yield and 93:7 er.



Peak Information

#	Peak Name	CH	tR [min]	Area [µV·sec]	Area%
1	Unknown	10	28,827	837568	49,304
2	Unknown	10	30,310	861225	50,696

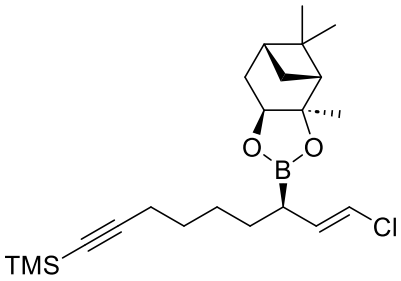


Peak Information

#	Peak Name	CH	tR [min]	Area [µV·sec]	Area%
1	Unknown	10	28,557	380511	7,006
2	Unknown	10	29,700	5050884	92,994

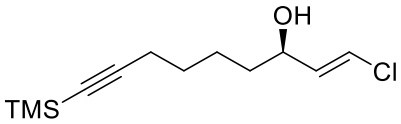
Note: Chromatogram of racemic compound shows peaks for *E*-isomer (28.83 and 30.31 min) and *Z*-isomer (not separated).

((*R*,*E*)-9-Chloro-7-((3a*R*,4*R*,6*R*,7a*S*)-3a,5,5-trimethylhexahydro-4,6-methanobenzo[*d*][1,3,2]dioxaborol-2-yl)non-8-en-1-yn-1-yl)trimethylsilane (12)



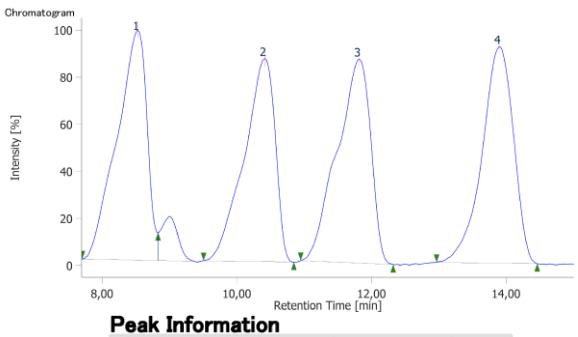
Synthesized from a 1.1:1 mixture of **34:34'** and **42** according to general procedure G. Yellow oil obtained in 77% yield with 99:1 *E*:*Z* and 91:9 er after column chromatography (Hexane:AcOEt, 98:2). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 5.91 (d, *J* = 13.2 Hz, 1H), 5.87 (dd, *J* = 13.2, 8.5 Hz, 1H), 4.26 (dd, *J* = 8.7, 2.0 Hz, 1H), 2.33 (ddt, *J* = 14.6, 8.8, 2.5 Hz, 1H), 2.20 (t, *J* = 6.9 Hz, 3H), 2.06 – 2.02 (m, 1H), 1.92 – 1.85 (m, 2H), 1.82 (ddd, *J* = 14.7, 3.4, 2.1 Hz, 1H), 1.61 – 1.39 (m, 7H), 1.37 (s, 3H), 1.28 (s, 3H), 1.05 (d, *J* = 11.0 Hz, 1H), 0.83 (s, 3H), 0.14 (s, 9H) ppm. **^{13}C NMR** (75 MHz, $CDCl_3$) δ 134.8, 116.0, 107.6, 86.0, 84.6, 78.1, 51.4, 39.6, 38.3, 35.6, 30.2, 28.8, 28.7, 28.2, 27.2, 26.6, 24.1, 19.9, 0.3 ppm. **^{11}B NMR** (160 MHz, $CDCl_3$) δ 32.2 ppm. **HRMS (APCI)** Calc. for $C_{22}H_{37}BClO_2Si$ [M+H$^+$]: 407.2339, found 407.2350. **Specific rotation:** $[\alpha]_D^{20}$ -21.5 (*c* = 0.55, $CHCl_3$).

(*R*,*E*)-1-Chloro-9-(trimethylsilyl)non-1-en-8-yn-3-ol (S39)



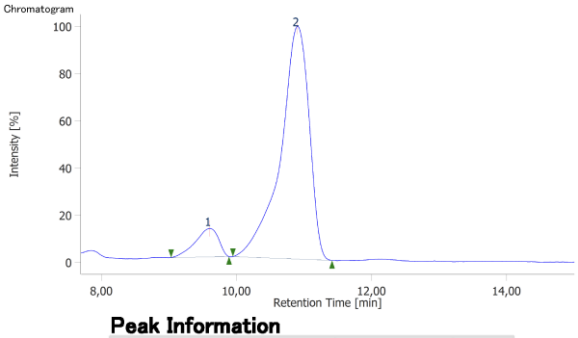
Obtained from **12** as yellow oil after flash column chromatography (Hexane:AcOEt 98:2) following general procedure H, in 78% yield and 91:9 er. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 6.23 (dd, *J* = 13.3, 1.1 Hz, 1H), 5.96 (dd, *J* = 13.3, 6.9 Hz, 1H), 4.19 – 4.14 (m, 1H), 2.24 (t, *J* = 6.9 Hz, 2H), 1.62 – 1.51 (m, 7H), 1.51 – 1.39 (m, 2H), 0.14 (s, 9H) ppm. **^{13}C NMR** (126 MHz, $CDCl_3$) δ 136.3, 119.9, 107.2, 84.9, 71.2, 36.6, 28.4, 24.5, 19.9, 0.3 ppm. **HRMS (APCI)** Calc. for $C_{12}H_{22}ClOSi$ [M-H$^+$]: 245.1123, found 245.1122. **Specific rotation:** $[\alpha]_D^{20}$ -5.6 (*c* = 0.94, $CHCl_3$).

Enantiomeric purity was determined by chiral SFC analysis [Lux Amylose 1, 100 bar, T_{oven}: 40 °C, flow: 1 mL/min; 5% MeOH, λ = 205 nm, minor enantiomer t_R = 9.60 min, major enantiomer t_R = 10.90 min].



Peak Information

#	Peak Name	CH	tR [min]	Area [µV·sec]	Area%
1	Unknown	9	8,530	4238603	25,749
2	Unknown	9	10,410	3859609	23,447
3	Unknown	9	11,813	4192239	25,468
4	Unknown	9	13,893	4170631	25,336

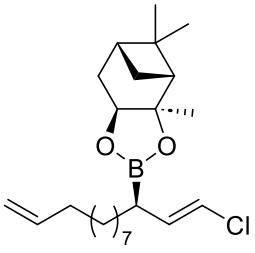


Peak Information

#	Peak Name	CH	tR [min]	Area [µV·sec]	Area%
1	Unknown	9	9,603	580667	9,045
2	Unknown	9	10,903	5839045	90,955

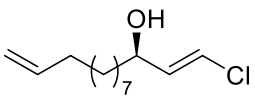
Note: Chromatogram of racemic compound (*E*:*Z* = 50:50) shows peaks for *E*-isomer (10.41 and 11.81 min), *Z*-isomer (8.53 and 13.89 min) and impurity.

(3a*R*,4*R*,6*R*,7a*S*)-2-((*R*,*E*)-1-Chlorotrideca-1,12-dien-3-yl)-3a,5,5-trimethylhexahydro-4,6-methanobenzo[*d*][1,3,2]dioxaborole (13)



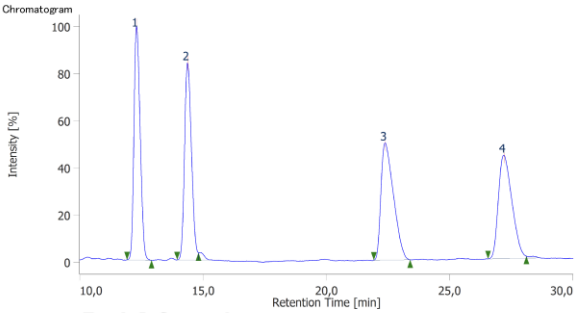
Synthesized from a 1:1 mixture of **35:35'** and **42** according to general procedure G. Yellow oil obtained in 84% yield with 94:6 *E*:*Z* and 91:9 er after column chromatography (Hexane:AcOEt, 98:2). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 5.92 – 5.85 (m, 2H), 5.81 (ddt, *J* = 16.9, 10.2, 6.7 Hz, 1H), 4.99 (dq, *J* = 17.1, 1.7 Hz, 1H), 4.92 (ddt, *J* = 10.2, 2.5, 1.3 Hz, 1H), 4.27 (dd, *J* = 8.8, 2.1 Hz, 1H), 2.33 (ddt, *J* = 13.9, 8.8, 2.5 Hz, 1H), 2.24 – 2.18 (m, 1H), 2.06 – 2.00 (m, 4H), 1.91 (dt, *J* = 5.6, 2.9 Hz, 1H), 1.88 (dd, *J* = 8.4, 1.8 Hz, 1H), 1.83 (ddd, *J* = 14.6, 3.4, 2.0 Hz, 1H), 1.59 – 1.51 (m, 2H), 1.46 – 1.39 (m, 2H), 1.37 (s, 3H), 1.28 (s, 3H), 1.26 (s, 11H), 1.07 (d, *J* = 11.0 Hz, 1H), 0.84 (s, 3H) ppm. **^{13}C NMR** (75 MHz, $CDCl_3$) δ 139.4, 135.2, 115.8, 114.2, 86.0, 78.1, 51.4, 39.6, 38.3, 35.6, 34.0, 30.8, 29.6, 29.6, 29.3, 29.1, 29.0, 28.8, 27.2, 26.6, 24.1 ppm. **^{11}B NMR** (160 MHz, $CDCl_3$) δ 32.6 ppm. **HRMS (APCI)** Calc. for $C_{23}H_{39}BClO_2$ [M+H$^+$]: 393.2726, found 393.2725. **Specific rotation:** $[\alpha]_D^{21}$ -21.4 (*c* = 0.83, $CHCl_3$).

(*R*,*E*)-1-Chlorotrideca-1,12-dien-3-ol (S40)



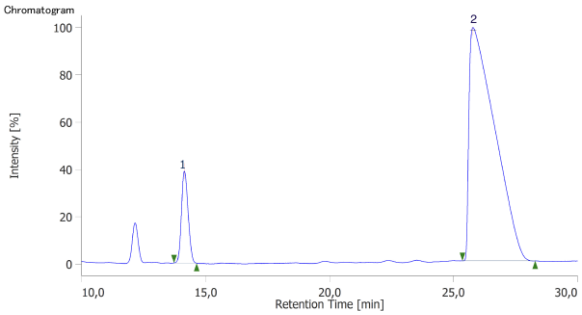
Obtained from **13** as yellow oil after flash column chromatography (Hexane:AcOEt 98:2) following general procedure H, in 70% yield and 91:9 er. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 6.22 (dd, *J* = 13.3, 1.2 Hz, 1H), 5.96 (dd, *J* = 13.3, 6.9 Hz, 1H), 5.81 (ddt, *J* = 16.9, 10.2, 6.7 Hz, 1H), 4.99 (dq, *J* = 17.2, 1.7 Hz, 1H), 4.95 – 4.91 (m, 1H), 4.14 (q, *J* = 6.7 Hz, 1H), 2.06 – 2.01 (m, 2H), 1.60 – 1.48 (m, 3H), 1.39 – 1.35 (m, 3H), 1.29 (d, *J* = 7.0 Hz, 9H) ppm. **^{13}C NMR** (75 MHz, $CDCl_3$) δ 139.3, 136.5, 119.7, 114.3, 71.4, 37.3, 33.9, 29.6, 29.5, 29.5, 29.2, 29.1, 25.3 ppm. **HRMS (APCI)** Calc. for $C_{13}H_{23}O$ [M+H$^+$-HCl]: 195.1743 found 195.1744. **Specific rotation:** $[\alpha]_D^{20}$ -2.8 (*c* = 0.52, $CHCl_3$).

Enantiomeric purity was determined by chiral SFC analysis [Lux Amylose-1, 100 bar, T_{oven}: 40 °C, flow: 1 mL/min; 10% MeOH, λ = 205 nm, minor enantiomer t_R = 14.13 min, major enantiomer t_R = 25.77 min].



Peak Information

#	Peak Name	CH	tR [min]	Area [µV·sec]	Area%
1	Unknown	9	12,307	1989493	25,429
2	Unknown	9	14,363	1890553	24,164
3	Unknown	9	22,373	2012301	25,720
4	Unknown	9	27,190	1931427	24,687

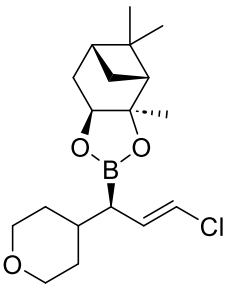


Peak Information

#	Peak Name	CH	tR [min]	Area [µV·sec]	Area%
1	Unknown	9	14,133	1722921	9,255
2	Unknown	9	25,773	16892264	90,745

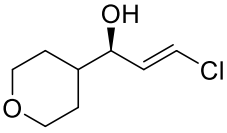
Note: Chromatogram of racemic compound (*E*:*Z* = 49:51) shows peaks for *E*-isomer (14.36 and 27.19 min) and *Z*-isomer (12.31 and 22.37 min).

(3a*R*,4*R*,6*R*,7a*S*)-2-((*R*,*E*)-3-Chloro-1-(tetrahydro-2H-pyran-4-yl)allyl)-3a,5,5-trimethylhexahydro-4,6-methanobenzo[*d*][1,3,2]dioxaborole (14)



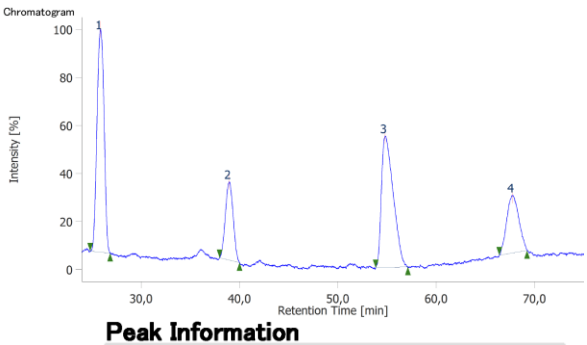
Synthesized from a 1:2.3 mixture of **36:36'** and **42** according to general procedure G. Colorless oil obtained in 51% yield with 99:1 *E*:*Z* and 91.5:8.5 er after column chromatography (Hexane:AcOEt, 98:2). **^{1}H NMR** (300 MHz, $CDCl_3$) δ 5.93 (d, *J* = 13.2 Hz, 1H), 5.87 (dd, *J* = 13.2, 9.3 Hz, 1H), 4.28 (d, *J* = 8.8 Hz, 1H), 3.99 – 3.88 (m, 2H), 3.43 – 3.30 (m, 2H), 2.40 – 2.28 (m, 1H), 2.27 – 2.16 (m, 1H), 2.04 (t, *J* = 5.7 Hz, 1H), 1.91 (s, 1H), 1.87 – 1.73 (m, 3H), 1.69 – 1.53 (m, 3H), 1.37 (s, 4H), 1.28 (s, 3H), 1.05 (d, *J* = 11.0 Hz, 1H), 0.84 (s, 3H) ppm. **^{13}C NMR** (75 MHz, $CDCl_3$) δ 132.9, 117.0, 86.3, 78.1, 68.3, 68.3, 51.4, 39.6, 38.3, 36.6, 35.6, 32.8, 32.5, 28.9, 27.2, 26.6, 24.3 ppm. **^{11}B NMR** (160 MHz, $CDCl_3$) δ 32.1 ppm. **HRMS (APCI)** Calc. for $C_{18}H_{29}BClO_3$ [M+H$^+$]: 339.1893, found 339.1890. **Specific rotation:** $[\alpha]_D^{19}$ -16.0 (*c* = 0.51, $CHCl_3$).

(*R*,*E*)-3-Chloro-1-(tetrahydro-2H-pyran-4-yl)prop-2-en-1-ol (15)



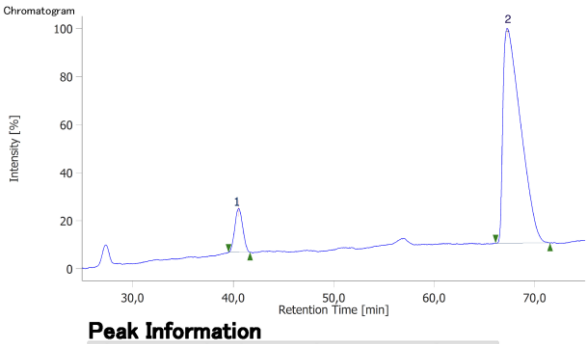
Obtained from **14** as white solid after flash column chromatography (Hexane:AcOEt 90:10) following general procedure I, in 71% yield and 91:9 er. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 6.15 (dd, *J* = 13.3, 1.0 Hz, 1H), 5.88 (dd, *J* = 13.3, 7.5 Hz, 1H), 3.92 (tdd, *J* = 12.5, 4.4, 1.8 Hz, 2H), 3.83 (td, *J* = 7.1, 2.8 Hz, 1H), 3.29 (tt, *J* = 11.6, 2.8 Hz, 2H), 1.68 (ddq, *J* = 13.1, 4.0, 2.2 Hz, 1H), 1.59 (tdd, *J* = 12.0, 7.2, 3.7 Hz, 2H), 1.45 (ddt, *J* = 13.3, 4.1, 2.2 Hz, 1H), 1.30 (dqd, *J* = 13.3, 11.8, 4.7 Hz, 3H) ppm. **^{13}C NMR** (75 MHz, $CDCl_3$) δ 134.5, 120.9, 75.2, 67.9, 67.7, 41.1, 28.8 ppm. **HRMS (APCI)** Calc. for $C_8H_{14}ClO_2$ [M+H$^+$]: 177.0677, found 177.0679. **Specific rotation:** $[\alpha]_D^{20}$ -6.9 (*c* = 0.50, $CHCl_3$). **Mp (°C):** 85.9-88.4.

Enantiomeric purity was determined by chiral SFC analysis [Lux Amylose-1, 100 bar, T_{oven}: 40 °C, flow: 1 mL/min; 5% MeOH, λ = 205 nm, minor enantiomer t_R = 40.54 min, major enantiomer t_R = 67.22 min].



Peak Information

#	Peak Name	CH	tR [min]	Area [μV·sec]	Area%
1	Unknown	9	25,877	1517963	35,623
2	Unknown	9	38,960	582871	13,679
3	Unknown	9	54,797	1490512	34,979
4	Unknown	9	67,707	669847	15,720



Peak Information

#	Peak Name	CH	tR [min]	Area [μV·sec]	Area%
1	Unknown	9	40,537	1253168	8,501
2	Unknown	9	67,220	13487464	91,499

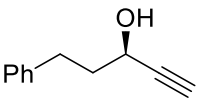
Note: Chromatogram of racemic compound (*E*:*Z* = 29:71) shows peaks for *E*-isomer (38.96 and 67.71 min) and *Z*-isomer (25.88 and 54.79 min).

12. Synthetic modifications.

- **General procedure K. LDA-mediated dehydrochlorination of alkenyl chlorides.**[20]

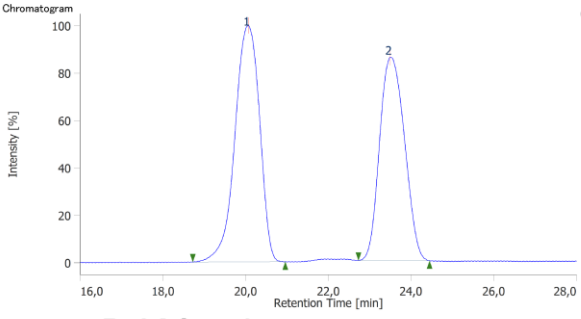
In an Ar-filled vial equipped with a stirring bar, the corresponding alkenyl chloride (1 equiv) was dissolved in THF [0.1 M] (Solution 1). In a separate oven-dried Schlenk equipped with a magnetic stirring bar, a solution of ^{n}BuLi (2.5 M in hexanes; 3.5-10 equiv) was added to a solution of $^{i}Pr_2NH$ (3.7-10 equiv) in THF (same volume as solution 1) at -78 °C, and was stirred for 30 min. Then, solution 1 was added to the preformed LDA at -78 °C, and the reaction was stirred for 30 min. The reaction was then quenched with saturated aqueous solution of NH_4Cl (5 mL) and allowed to get to room temperature. The mixture was extracted with CH_2Cl_2 (2 x 5 mL). Combined organic layers were dried over Na_2SO_4, filtered, and concentrated in vacuo. The crude product was purified through flash column chromatography.

(*R*)-5-Phenylpent-1-yn-3-ol (16)



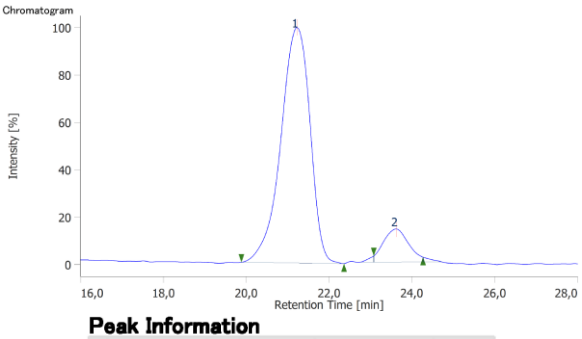
Obtained from **3** as yellow oil after flash column chromatography (Hexane:AcOEt 98:2) following general procedure K using ^{n}BuLi (3.5 equiv) and $^{i}Pr_2NH$ (3.7 equiv), in 52% yield and 89:11 er. **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.34 – 7.27 (m, 2H), 7.24 – 7.16 (m, 3H), 4.37 (q, J = 5.4 Hz, 1H), 2.81 (t, J = 7.8 Hz, 2H), 2.51 (d, J = 2.1 Hz, 1H), 2.10 – 2.00 (m, 2H), 1.82 (d, J = 5.5 Hz, 1H) ppm. **^{13}C NMR** (126 MHz, $CDCl_3$) δ 141.2, 128.6, 126.2, 84.8, 73.5, 61.7, 39.2, 31.4 ppm. **HRMS (APCI)** Calc. for $C_{11}H_{11}$ [M+H$^+$-H_2O]: 143.0855 found 143.0873. **Specific rotation:** $[\alpha]_D^{19}$ -6.5 (c = 0.65, $CHCl_3$).

Enantiomeric purity was determined by chiral SFC analysis [Lux Amylose-1, 100 bar, T_{oven}: 40 °C, flow: 1 mL/min; 5% MeOH, λ = 205 nm, minor enantiomer t_R = 23.62 min, major enantiomer t_R = 21.22 min].



Peak Information

#	Peak Name	CH	tR [min]	Area [µV·sec]	Area%
1	Unknown	9	20,063	37422037	53,514
2	Unknown	9	23,493	32507288	46,486

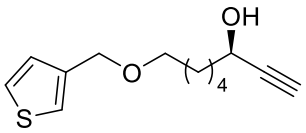


Peak Information

#	Peak Name	CH	tR [min]	Area [µV·sec]	Area%
1	Unknown	9	21,217	70921959	89,198
2	Unknown	9	23,617	8588823	10,802

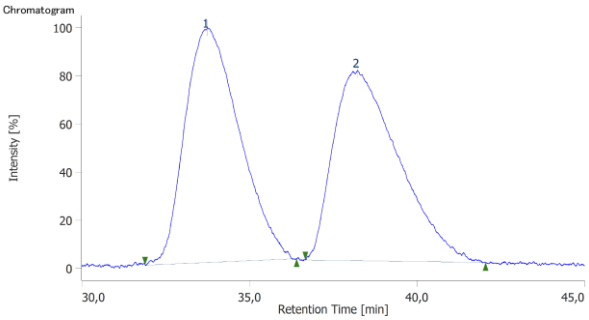
[20] Álvarez-Constantino, A. M.; Chaves-Pouso, A.; Fañanás-Mastral, M. *Angew. Chem. Int. Ed.* **2024**, *63*, e202407813

(*R*)-8-(Thiophen-3-ylmethoxy)oct-1-yn-3-ol (17)



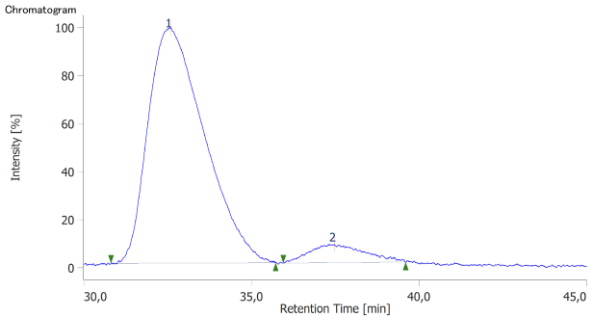
Obtained from **S38** as yellow oil after flash column chromatography (Hexane:AcOEt 100:0 to 95:5) following general procedure K using ^{n}BuLi (10 equiv) and $^{i}Pr_2NH$ (10 equiv), in 56% yield and 93:7 er. **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.29 (dd, *J* = 5.0, 3.0 Hz, 1H), 7.22 – 7.17 (m, 1H), 7.07 (d, *J* = 4.9 Hz, 1H), 4.50 (s, 2H), 4.36 (td, *J* = 6.6, 2.2 Hz, 1H), 3.46 (t, *J* = 6.5 Hz, 2H), 2.45 (d, *J* = 2.1 Hz, 1H), 1.87 (s, 1H), 1.78 – 1.67 (m, 2H), 1.61 (p, *J* = 6.9 Hz, 2H), 1.54 – 1.35 (m, 4H) ppm. **^{13}C NMR** (75 MHz, $CDCl_3$) δ 140.0, 127.5, 126.0, 122.7, 85.1, 73.0, 70.3, 68.3, 62.4, 37.7, 29.7, 26.0, 25.0 ppm. **HRMS (APCI)** Calc. for $C_{13}H_{19}O_2S$ [M+H$^+$]: 239.1100 found 239.1102. **Specific rotation:** $[\alpha]_D^{19}$ +3.7 (*c* = 0.39, $CHCl_3$).

Enantiomeric purity was determined by chiral SFC analysis [Lux Amylose-2, 100 bar, T_{oven}: 40 °C, flow: 2 mL/min; 3% MeOH, λ = 220 nm, minor enantiomer t_R = 32.59 min, major enantiomer t_R = 37.47 min].



Peak Information

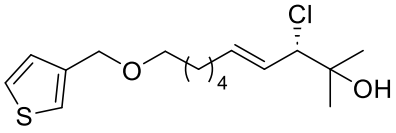
#	Peak Name	CH	tR [min]	Area [µV·sec]	Area%
1	Unknown	10	33.743	2108114	50.616
2	Unknown	10	38.227	2056787	49.384



Peak Information

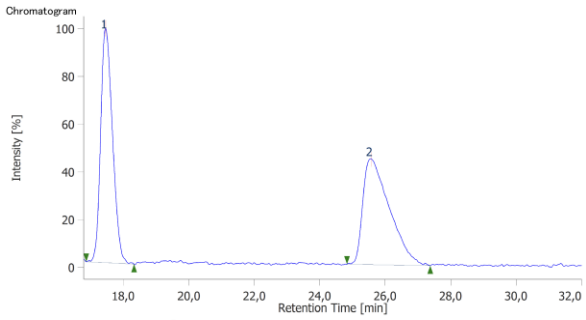
#	Peak Name	CH	tR [min]	Area [µV·sec]	Area%
1	Unknown	10	32.587	2660970	92.895
2	Unknown	10	37.470	203524	7.105

(*S*,*E*)-3-Chloro-2-methyl-10-(thiophen-3-ylmethoxy)dec-4-en-2-ol (18)



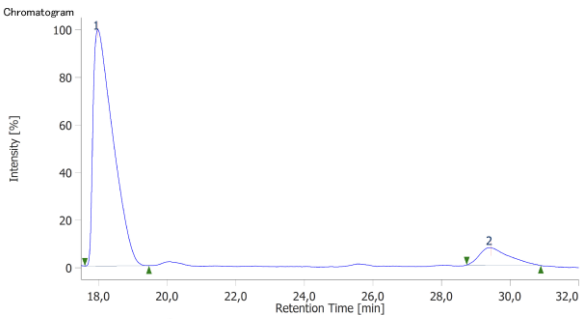
To a mixture of **11b** (1 equiv, 0.1 mmol), $NaIO_4$ (3.1 equiv) and NH_4OAc (3.5 equiv) was diluted in Acetone (0.66 mL) and H_2O (0.33 mL). The reaction was stirred for 14 h at rt. After this time, the mixture was diluted with CH_2Cl_2 (2 mL) and washed with saturated aqueous solution of NH_4Cl (5 mL). Then the aqueous layer was extracted with CH_2Cl_2 (2 mL). The combined organic layer was dried over anhydrous Na_2SO_4, filtered and solvent was removed under reduced pressure. Crude product was purified through flash column chromatography (Hexane:AcOEt 90:10) obtaining a yellow oil in a 78% yield and 90:10 er. **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.29 (dd, *J* = 5.0, 2.9 Hz, 1H), 7.19 (d, *J* = 3.2 Hz, 1H), 7.06 (d, *J* = 4.9 Hz, 1H), 5.75 (dt, *J* = 15.4, 6.7 Hz, 1H), 5.57 (dd, *J* = 15.3, 9.6 Hz, 1H), 4.50 (s, 2H), 4.31 (d, *J* = 9.4 Hz, 1H), 3.45 (t, *J* = 6.5 Hz, 2H), 2.19 (s, 1H), 2.07 (q, *J* = 6.6 Hz, 2H), 1.60 (p, *J* = 6.9 Hz, 2H), 1.39 (h, *J* = 4.8 Hz, 4H), 1.27 (s, 3H), 1.26 (s, 3H) ppm. **^{13}C NMR** (75 MHz, $CDCl_3$) δ 139.9, 136.5, 127.4, 127.3, 126.0, 122.6, 74.2, 72.6, 70.3, 68.3, 32.1, 29.6, 28.7, 26.9, 25.8, 25.2 ppm. **HRMS (APCI)** Calc. for $C_{16}H_{26}ClO_2S$ [M+H$^+$]: 317.1337 found 317.1326. **Specific rotation:** $[\alpha]_D^{19}$ -17.9 (*c* = 1.0, $CHCl_3$).

Enantiomeric purity was determined by chiral SFC analysis [Lux Cellulose-1, 100 bar, T_{oven}: 40 °C, flow: 2 mL/min; 5% MeOH, λ = 220 nm, minor enantiomer t_R = 17.98 min, major enantiomer t_R = 29.43 min].



Peak Information

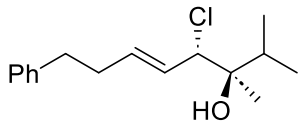
#	Peak Name	CH	tR [min]	Area [µV·sec]	Area%
1	Unknown	10	17,463	2994214	49,626
2	Unknown	10	25,560	3039293	50,374



Peak Information

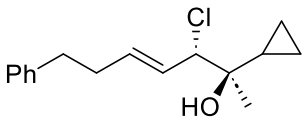
#	Peak Name	CH	tR [min]	Area [µV·sec]	Area%
1	Unknown	10	17,983	5168020	90,097
2	Unknown	10	29,433	568031	9,903

(3*R*,4*S*,*E*)-4-Chloro-2,3-dimethyl-8-phenyloct-5-en-3-ol (19)



To a mixture of **2b** (1 equiv, 0.1 mmol), $NaIO_4$ (3.1 equiv) and NH_4OAc (3.5 equiv) was diluted in THF (0.66 mL) and H_2O (0.33 mL). 3-methylbutan-2-one (5 equiv) was added, and the reaction was stirred for 14 h at rt. After this time, the mixture was diluted with CH_2Cl_2 (2 mL) and washed with saturated aqueous solution of NH_4Cl (5 mL). Then the aqueous layer was extracted with CH_2Cl_2 (2 mL). The combined organic layer was dried over anhydrous Na_2SO_4, filtered and solvent was removed under reduced pressure. Crude product was purified through flash column chromatography (Hexane:AcOEt 98:02) obtaining a colorless oil in a 54% yield. Enantiomeric ratio was determined in epoxide **22**. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.30 – 7.27 (m, 2H), 7.21 – 7.15 (m, 3H), 5.79 – 5.65 (m, 2H), 4.43 (d, *J* = 9.2 Hz, 1H), 2.80 – 2.66 (m, 2H), 2.46 – 2.36 (m, 2H), 1.79 – 1.72 (m, 1H), 1.13 (s, 3H), 0.95 (d, *J* = 6.8 Hz, 3H), 0.77 (d, *J* = 6.8 Hz, 3H) ppm. **^{13}C NMR** (126 MHz, $CDCl_3$) δ 141.4, 134.8, 128.6, 128.5, 127.7, 126.1, 76.1, 72.0, 35.3, 33.9, 33.7, 31.5, 19.8, 17.3, 17.1 ppm. **HRMS (APCI)** Calc. for $C_{16}H_{23}O$ [M+H-HCl]: 231.1743 found 231.1742. **Specific rotation:** $[\alpha]_D^{22}$ -2.8 (*c* = 0.5, $CHCl_3$).

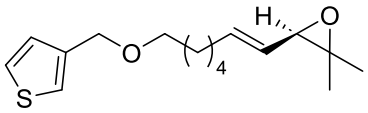
(2*R*,3*S*,*E*)-3-Chloro-2-cyclopropyl-7-phenylhept-4-en-2-ol (20)



To a mixture of **2b** (1 equiv, 0.1 mmol), $NaIO_4$ (3.1 equiv) and NH_4OAc (3.5 equiv) was diluted in THF (0.66 mL) and H_2O (0.33 mL). 1-cyclopropylethan-1-one (5 equiv) was added, and the reaction was stirred for 14 h at rt. After this time, the mixture was diluted with CH_2Cl_2 (2 mL) and washed with saturated aqueous solution of NH_4Cl (5 mL). Then the aqueous layer was extracted with CH_2Cl_2 (2 mL). The combined organic layer was dried over anhydrous Na_2SO_4, filtered and solvent was removed under reduced pressure. Crude product was purified through flash column chromatography (Hexane:AcOEt 98:02) obtaining a colorless oil in a 79% yield. Enantiomeric ratio was determined in compound **24**. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.23 – 7.16 (m, 2H), 7.13 – 7.07 (m, 3H), 5.69 (dt, *J* = 15.3, 6.7 Hz, 1H), 5.59 (ddt, *J* = 15.3, 9.5, 1.3 Hz, 1H), 4.27

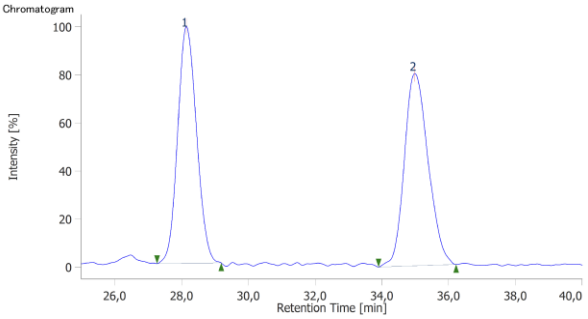
(d, J = 9.4 Hz, 1H), 2.73 – 2.58 (m, 2H), 2.42 – 2.28 (m, 2H), 0.99 (s, 3H), 0.89 (tt, J = 8.5, 5.5 Hz, 1H), 0.41 – 0.36 (m, 1H), 0.32 – 0.26 (m, 2H), 0.23 – 0.17 (m, 1H) ppm. **^{13}C NMR** (126 MHz, $CDCl_3$) δ 141.4, 134.9, 128.6, 128.5, 128.1, 126.1, 73.5, 72.8, 35.3, 33.9, 23.4, 17.6, 1.3, 1.0 ppm. **HRMS (APCI)** Calc. for $C_{16}H_{20}Cl$ [M+H-H_2O]: 247.1248 found 247.1242. **Specific rotation:** $[\alpha]_D^{21}$ -21.7 (c = 0.63, $CHCl_3$).

(*R*,*E*)-2,2-Dimethyl-3-(7-(thiophen-3-ylmethoxy)hept-1-en-1-yl)oxirane (21)



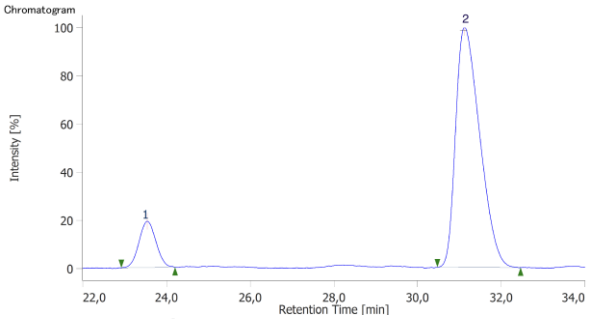
18 (1 equiv) and K_2CO_3 (3 equiv) were dissolved in MeCN [0.1 M]. The reaction mixture was heated to 80 °C and stirred for 16 h. After this time, the mixture was diluted with CH_2Cl_2 (2 mL) and washed with H_2O (5 mL). Then the aqueous layer was extracted with CH_2Cl_2 (2 mL). The combined organic layer was dried over anhydrous Na_2SO_4, filtered and solvent was removed under reduced pressure. Yellow oil was obtained after flash column chromatography (Hexane:AcOEt 95:5) in 95% yield and 88:12 er. **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.29 (dd, J = 4.9, 2.9 Hz, 1H), 7.22 - 7.17 (m, 1H), 7.07 (d, J = 4.9 Hz, 1H), 5.89 (dt, J = 15.5, 6.9 Hz, 1H), 5.32 (dd, J = 15.5, 7.9 Hz, 1H), 4.50 (s, 2H), 3.45 (t, J = 6.6 Hz, 2H), 3.16 (d, J = 7.9 Hz, 1H), 2.08 (q, J = 7.0 Hz, 1H), 1.66 – 1.55 (m, 3H), 1.40 (d, J = 3.4 Hz, 4H), 1.34 (s, 3H), 1.28 (s, 3H) ppm. **^{13}C NMR** (126 MHz, $CDCl_3$) δ 140.0, 137.6, 127.5, 126.0, 125.4, 122.7, 70.4, 68.3, 64.5, 60.2, 32.7, 29.7, 29.0, 25.9, 24.8, 19.1 ppm. **HRMS (APCI)** Calc. for $C_{16}H_{25}O_2S$ [M+H^+]: 281.1570 found 281.1564. **Specific rotation:** $[\alpha]_D^{19}$ +4.0 (c = 0.75, $CHCl_3$).

Enantiomeric purity was determined by chiral SFC analysis [Lux Amylose-1, 100 bar, T_{oven}: 40 °C, flow: 1 mL/min; 5% MeOH, λ = 205 nm, minor enantiomer t_R = 23.54 min, major enantiomer t_R = 31.12 min].



Peak Information

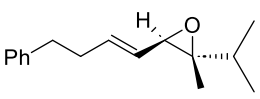
#	Peak Name	CH	tR [min]	Area [µV·sec]	Area%
1	Unknown	9	28,140	33050316	49,195
2	Unknown	9	34,980	34131546	50,805



Peak Information

#	Peak Name	CH	tR [min]	Area [µV·sec]	Area%
1	Unknown	10	23,543	462914	11,968
2	Unknown	10	31,117	3405160	88,032

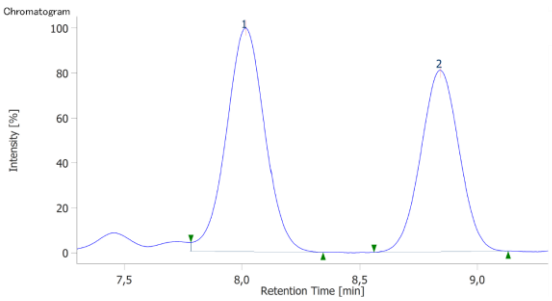
(2*R*,3*R*)-2-Isopropyl-2-methyl-3-((*E*)-4-phenylbut-1-en-1-yl)oxirane (22)



19 (1 equiv) and K_2CO_3 (3 equiv) were dissolved in MeCN [0.1 M]. The reaction mixture was heated to 80 °C and stirred for 16 h. After this time, the mixture was diluted with CH_2Cl_2 (2 mL) and washed with H_2O (5 mL). Then the aqueous layer was extracted with CH_2Cl_2 (2 mL). The combined organic layer was dried over anhydrous Na_2SO_4, filtered and solvent was removed under reduced pressure. Colorless oil was obtained after flash column

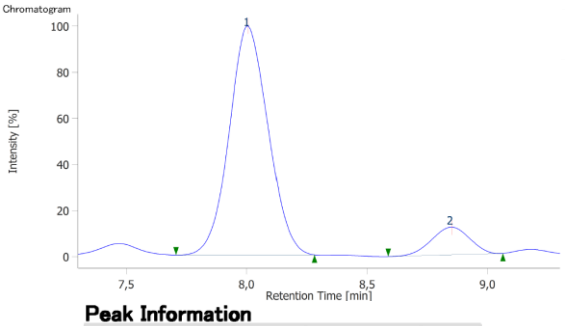
chromatography (Hexane:AcOEt 98:02) in 74% yield and 89:11 er. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.29 (d, *J* = 6.3 Hz, 2H), 7.21 – 7.15 (m, 3H), 5.94 – 5.87 (m, 1H), 5.38 (dd, *J* = 15.4, 7.6 Hz, 1H), 3.14 (d, *J* = 7.7 Hz, 1H), 2.75 – 2.69 (m, 2H), 2.45 – 2.38 (m, 2H), 1.46 (p, *J* = 6.9 Hz, 1H), 1.13 (s, 3H), 1.00 (d, *J* = 6.9 Hz, 3H), 0.93 (d, *J* = 7.0 Hz, 3H). ppm. **^{13}C NMR** (126 MHz, $CDCl_3$) δ 141.7, 136.2, 128.6, 128.5, 126.1, 126.0, 66.2, 63.3, 36.3, 35.6, 34.5, 31.1, 18.6, 17.8 ppm. **HRMS (APCI)** Calc. for $C_{16}H_{23}O$ [M+H]: 231.1743 found 231.1738. **Specific rotation:** $[\alpha]_D^{23}$ +1.0 (*c* = 0.5, $CHCl_3$).

Enantiomeric purity was determined by chiral SFC analysis [Lux Amylose-1, 100 bar, T_{oven}: 40 °C, flow: 1 mL/min; 5% MeOH, λ = 205 nm, minor enantiomer t_R = 8.85 min, major enantiomer t_R = 8.01 min].



Peak Information

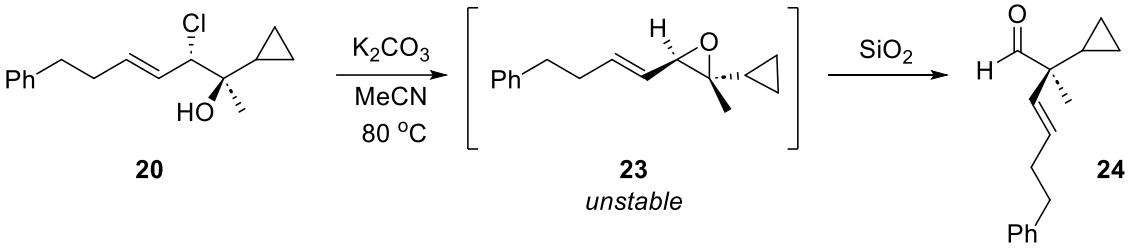
#	Peak Name	CH	tR [min]	Area [µV·sec]	Area%
1	Unknown	9	8,017	1831410	55,177
2	Unknown	9	8,843	1487769	44,823



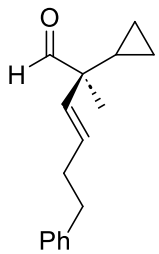
Peak Information

#	Peak Name	CH	tR [min]	Area [µV·sec]	Area%
1	Unknown	9	8,007	19047595	89,455
2	Unknown	9	8,850	2245287	10,545

(*S*,*E*)-2-Cyclopropyl-2-methyl-6-phenylhex-3-enal (24)



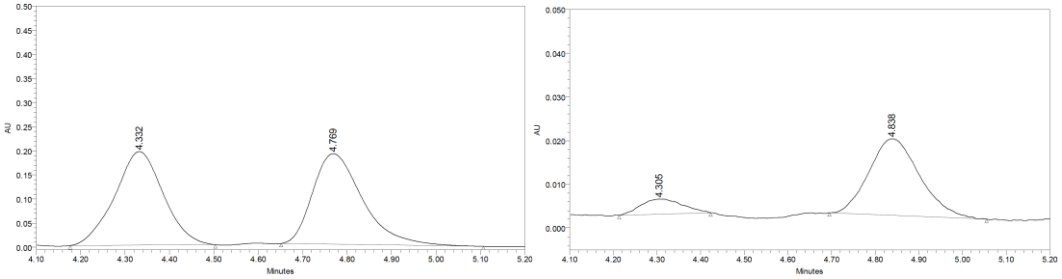
20 **23** *unstable* **24**



20 (1 equiv) and K_2CO_3 (3 equiv) were dissolved in MeCN [0.1 M]. The reaction mixture was heated to 80 °C and stirred for 16 h. After this time, the mixture was diluted with CH_2Cl_2 (2 mL) and washed with H_2O (5 mL). Then the aqueous layer was extracted with CH_2Cl_2 (2 mL). The combined organic layer was dried over anhydrous Na_2SO_4, filtered and solvent was removed under reduced pressure to afford crude product **23**. Attempted purification of **23** by flash column chromatography (Hexane:AcOEt 98:02) in SiO_2 led to product **24**, which was obtained as a colorless oil in 98% yield and with 86:14 er. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 9.43 (s, 1H), 7.31 – 7.26 (m, 2H), 7.21 – 7.13 (m, 3H), 5.57 (dt, *J* = 15.8, 6.8 Hz, 1H), 5.28 (d, *J* = 16.0 Hz, 1H), 2.71 – 2.66 (m, 2H), 2.41 – 2.35 (m, 2H), 1.00 (s, 3H), 0.90 (tt, *J* = 8.5, 5.4 Hz, 1H), 0.47 – 0.36 (m, 2H), 0.26 (td, *J* = 9.5, 5.4 Hz, 1H), 0.19 (tt, *J* = 9.8, 4.7 Hz, 1H) ppm. **^{13}C NMR** (126 MHz, $CDCl_3$) δ 202.9, 141.6, 132.6, 129.5, 128.6, 128.5, 126.0, 50.8, 35.9, 34.9, 17.7, 15.8, 0.1, -0.5

ppm. **HRMS (APCI)** Calc. for $C_{16}H_{21}O$ [M+H]: 229,1586 found 229.1579. **Specific rotation:** $[\alpha]_D^{21}$ +4.7 (c = 0.52, $CHCl_3$).

Enantiomeric purity was determined by chiral uHPLC [Lux i-Amylose-3, T_{oven}: 40 °C, flow: 1 mL/min; 98% ^{n}Hexane, 2% ^{i}PrOH, λ = 209 nm, minor enantiomer t_R = 4. 33min, major enantiomer t_R = 4.77 min].



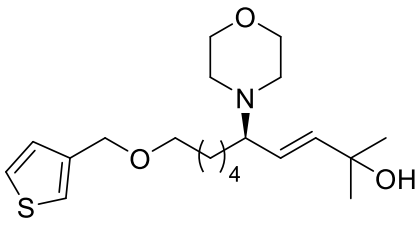
Unknown Peak Results

	Peak Type	RT	Area	% Area	Height
1	Unknown	4.332	1475853	50.25	194102
2	Unknown	4.769	1461289	49.75	187678

Unknown Peak Results

	Peak Type	RT	Area	% Area	Height
1	Unknown	4.305	23243	14.15	3472
2	Unknown	4.838	141034	85.85	17505

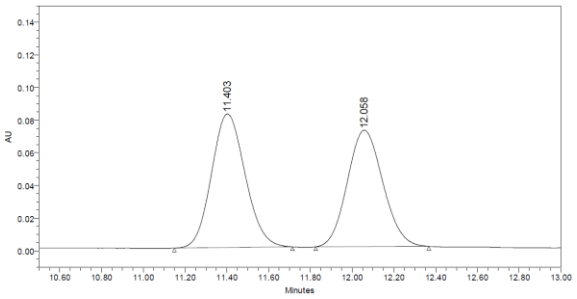
(*R*,*E*)-2-Methyl-5-morpholino-7-(thiophen-3-ylmethoxy)hept-3-en-2-ol (25)



25 was synthetized from **18** via a modified literature protocol.[21] **18** (1 equiv) was dissolved in MeCN (0.1 M) and morpholine (5 equiv) was added to the resulting solution. The reaction mixture was heated to 80 °C and stirred for 16 h. After this time, the mixture was cooled to rt and diluted with CH_2Cl_2 (2 mL) and washed with saturated aqueous solution of H_2O (5 mL). Then the aqueous layer was extracted with CH_2Cl_2 (2 mL). Combined organic layer were dried over anhydrous Na_2SO_4, filtered and solvent was removed under reduced pressure. Crude product was purified through flash column chromatography (AcOEt:MeOH 90:10) obtaining a colorless oil in a 59% yield and 87:13 er. **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.32 – 7.27 (m, 1H), 7.21 – 7.17 (m, 1H), 7.08 – 7.04 (m, 1H), 5.71 (d, J = 15.7 Hz, 1H), 5.48 (dd, J = 15.6, 9.0 Hz, 1H), 4.49 (s, 2H), 3.79 – 3.65 (m, 4H), 3.44 (t, J = 6.5 Hz, 2H), 2.73 (td, J = 9.3, 4.8 Hz, 1H), 2.63 – 2.53 (m, 2H), 2.53 – 2.42 (m, 2H), 1.58 (p, J = 6.6 Hz, 3H), 1.49 – 1.20 (m, 13H) ppm. **^{13}C NMR** (126 MHz, $CDCl_3$) δ 140.0, 127.5, 126.0, 122.7, 70.9, 70.4, 68.3, 67.8, 67.1, 50.3, 31.6, 30.2, 30.1, 29.8, 26.3, 26.3 ppm. **HRMS (APCI)** Calc. for $C_{20}H_{34}NO_3S$ [M+H$^+$]: 368.2254 found 368.2265. **Specific rotation:** $[\alpha]_D^{21}$ +1.4 (c = 1, $CHCl_3$).

Enantiomeric purity was determined by chiral HPLC analysis [Lux i-cellulose-5, T_{oven}: 40 °C, flow: 1 mL/min; 91% ^{n}Hexane, 9% ^{i}PrOH, λ = 220 nm, minor enantiomer t_R = 12.10 min, major enantiomer t_R = 11.45 min].

[21] Zhang, Y.; Goetzke, F. W.; Christensen, K. E.; Fletcher, S. P. *ACS Catal.* **2022**, *12*, 8995-9002



Unknown Peak Results

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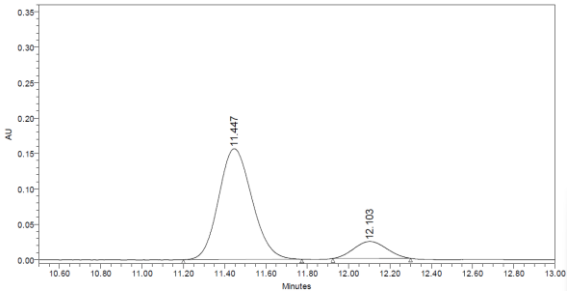


Unknown Peak Results

	Peak Type	RT	Area	% Area	Height
1	Unknown	11.447	1752904	87.00	156385
2	Unknown	12.103	261951	13.00	23903

13. X-Ray diffraction of compound 15.

Product **15** was dissolved in in CH_2Cl_2 exposed in hexane atmosphere and left to slow evaporation for 6 h to yield plate, clear colorless type of crystals of an approximate dimensions 0.050 × 0.100 × 0.140 mm. The X-ray intensity data were measured on a Bruker D8 VENTURE PHOTON-III-14 κ-geometry diffractometer system equipped with a Incoatec IμS 3.0 microfocus sealed tube (Cu Kα, λ = 1.54178 Å) and a multilayer mirror monochromator. The structure was solved and refined using the Bruker SAINT Software Package.

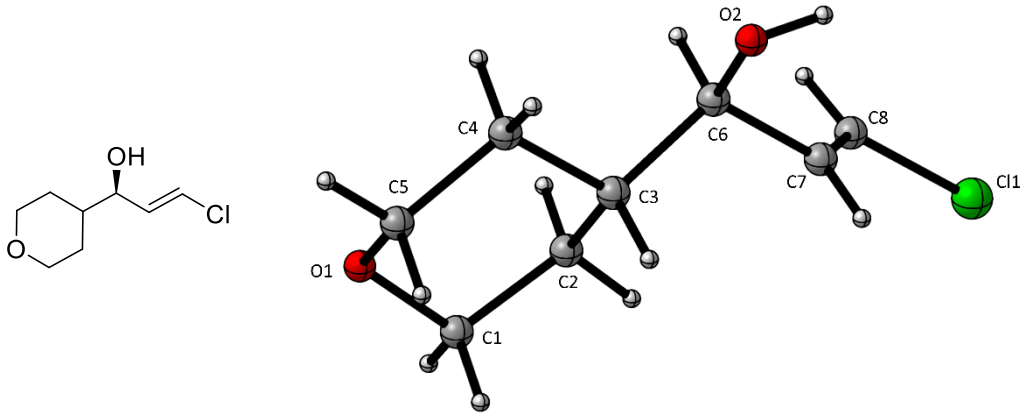


Figure S1. ORTEP plot of **15** with 30% ellipsoids. Selected bond distances (Å) and angles (°): C6-O2 (1.436), C6-C7 (1.506), C7-C8 (1.321), C8-Cl1 (1.743), C7-C8-Cl1 (122.47).

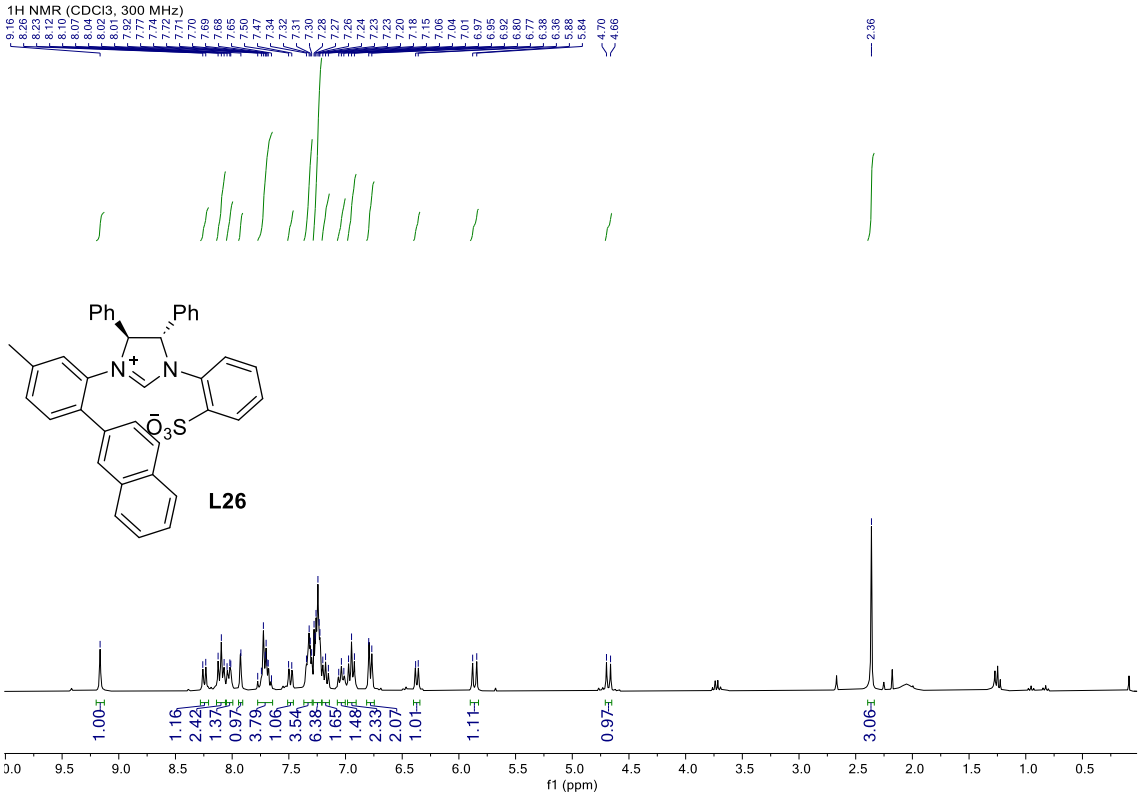
Table S4. Crystal data for product **15**.

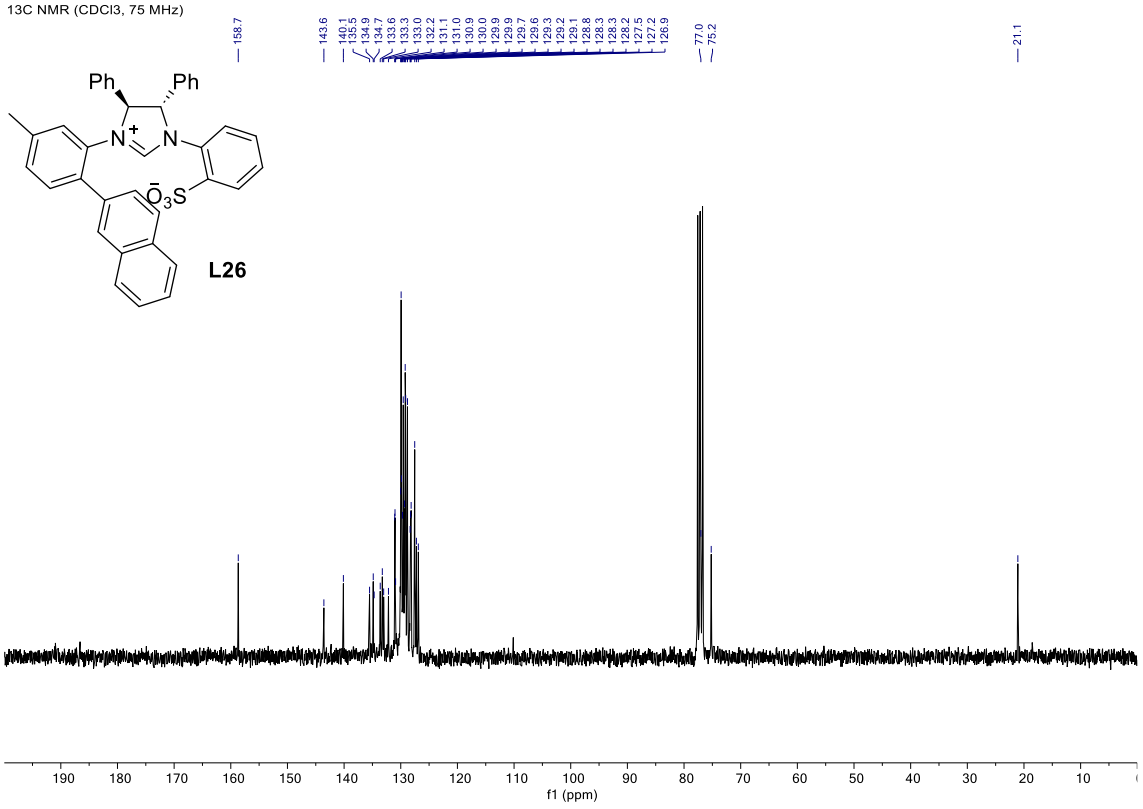
Chemical formula	$C_8H_{13}BlO_2$	
Formula Weight	176.63	
Temperature	100 K	
Wavelength	1.54178 Å	
Crystal size	0.050 × 0.100 × 0.140 mm	
Crystal habit	colorless plate	
Crystal system	Orthorhombic	
Space group	$P2_12_12_1$	
Unit cell dimensions	a = 5.8095 (1) Å	α =90º
	b = 7.8048 (2) Å	β =90 º
	c = 19.3744 (5) Å	γ =90º
Volume	878.48 (4) $Å^3$	
Z	4	
Density (calculated)	1.336 g cm^{-3}	
Absorption coefficient	3.449 mm^{-1}	
F(000)	376	

Table S5. Data collection and structure refinement for product **15**.

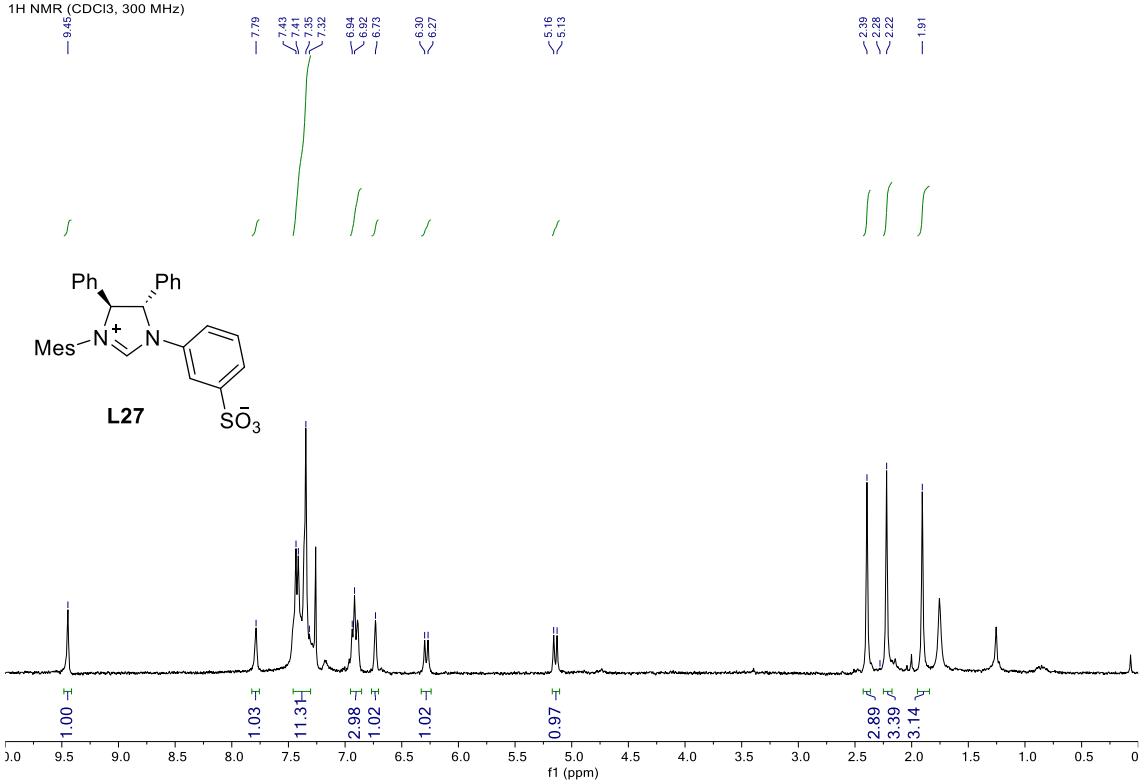
Diffractometer	Bruker D8 Venture PhotonIII-14
Radiation source	Incoatec IμS 3.0 microfocus sealed tube
Theta range for data collection	4.56 to 74.60°
Index ranges	-7< = h < = 7, -8< = k <= 9, -24 <= I< = 24
Reflections collected	13087
Independent reflections	1793 [R(int) = 0.047]
Coverage of independent reflections	99.8%
Absorption correction	Multi-Scan
Max. and min. transmission	0.8460 and 0.6440
Structure solution technique	direct methods
Structure solution program	SHELXT 2018/2 (Sheldrick, 2015)
Refinement method	Full-matrix least-squares on F^2
Refinement program	SHELXL-2019/1 (Sheldrick, 2019)
Function minimized	$\Sigma w(F_o^2 - F_c^2)^2$
Data / restraints / parameters	1793 / 0 / 109
Goodness-of-fit on F^2	1.083
Final R indices	1741 data; I>2σ(I) R1 = 0.0646
	all data wR2 = 0.0656
Weighting scheme	$w = 1/[\sigma^2(F_o^2) + (0.0222P)^2 + 0.4114P]$ where $P = (F_o^2 + 2F_c^2)/3$
Largest diff. peak and hole	0.231 and -0.159 $e^-/Å^3$
R.M.S. deviation from mean	0.040 $e^-/Å^3$
Absolute structure	Flack x determined using 691 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons, Flack and Wagner, Acta Cryst. B69 (2013) 249-259).
Absolute structure parameter	0.009 (9)

14. NMR spectra of the starting materials



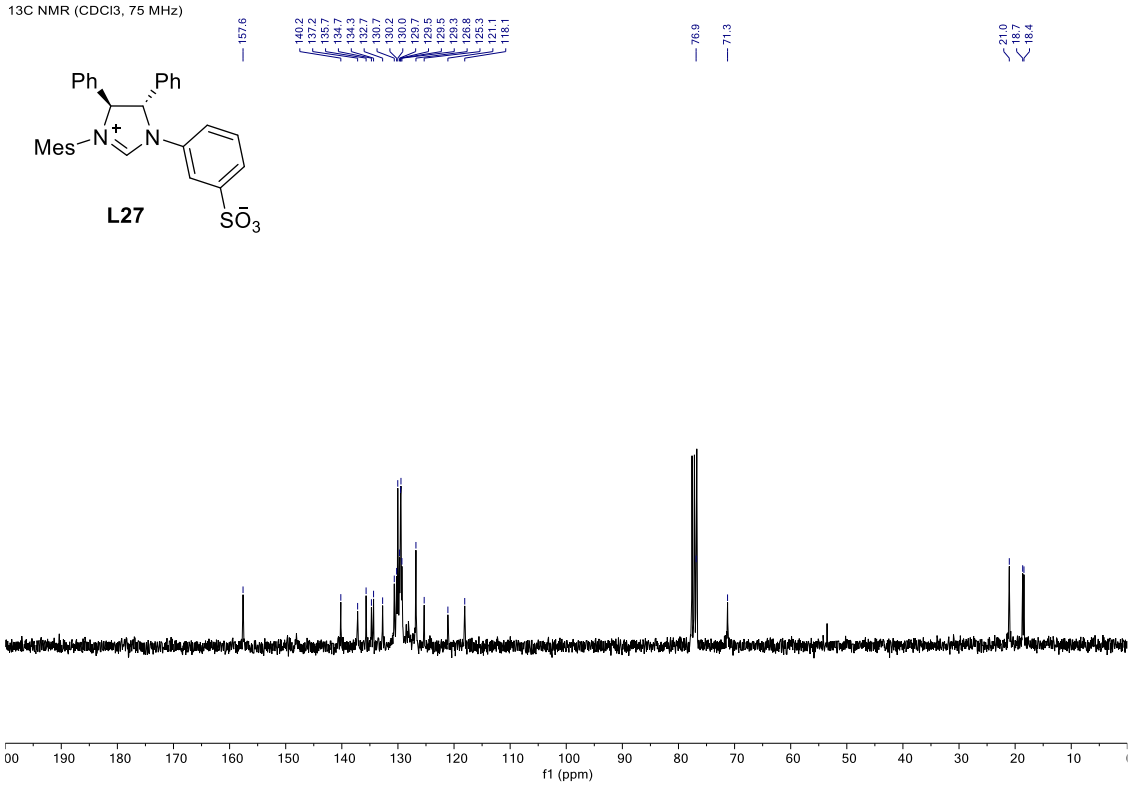


1H NMR (CDCl3, 300 MHz)



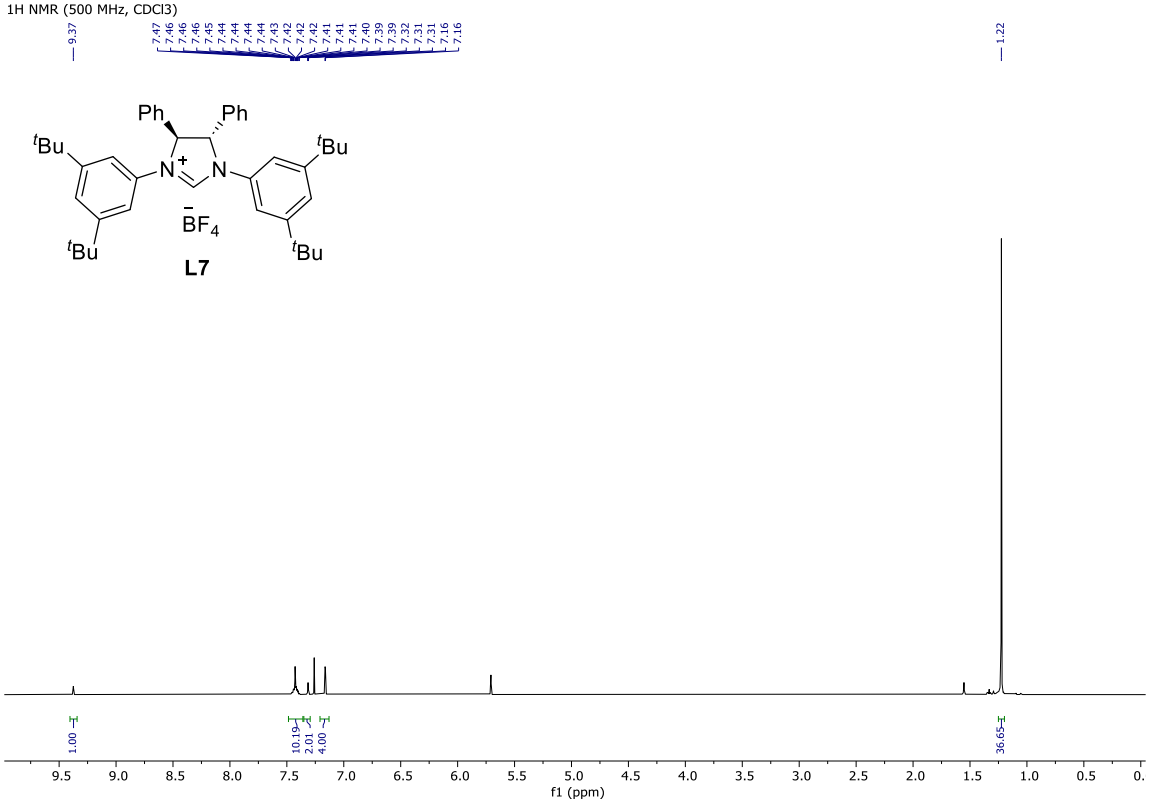
L27

13C NMR (CDCl3, 75 MHz)



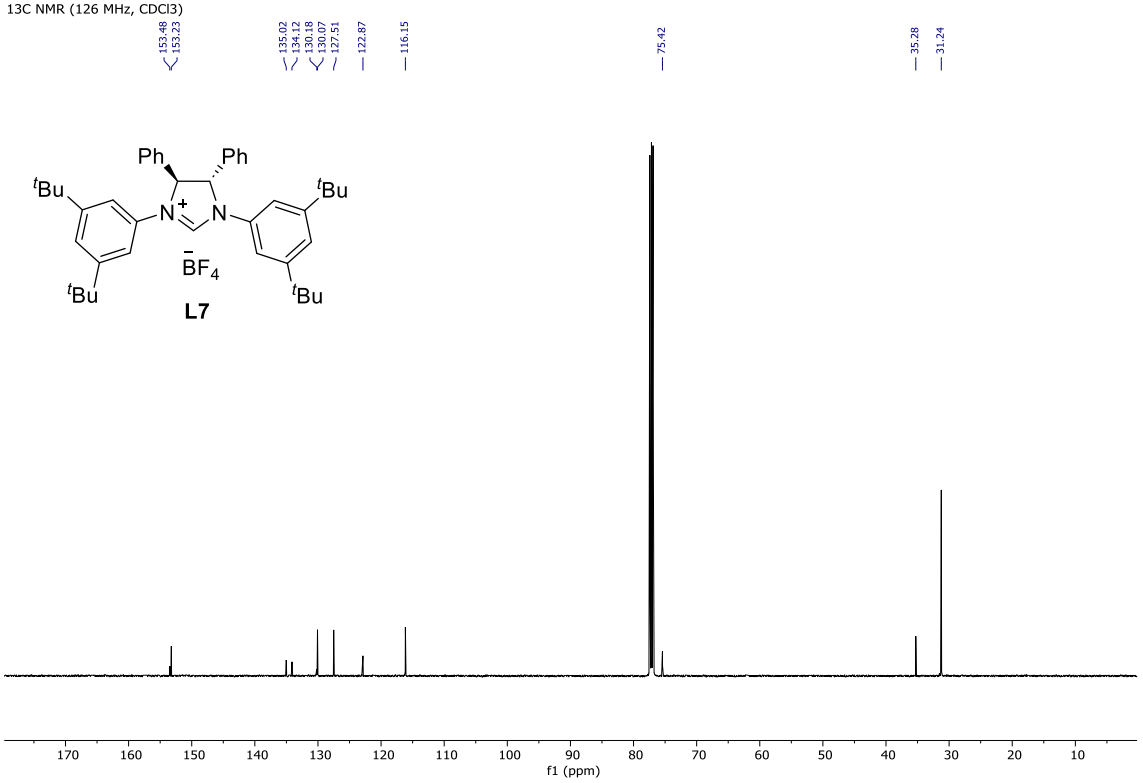
L27

1H NMR (500 MHz, CDCl3)



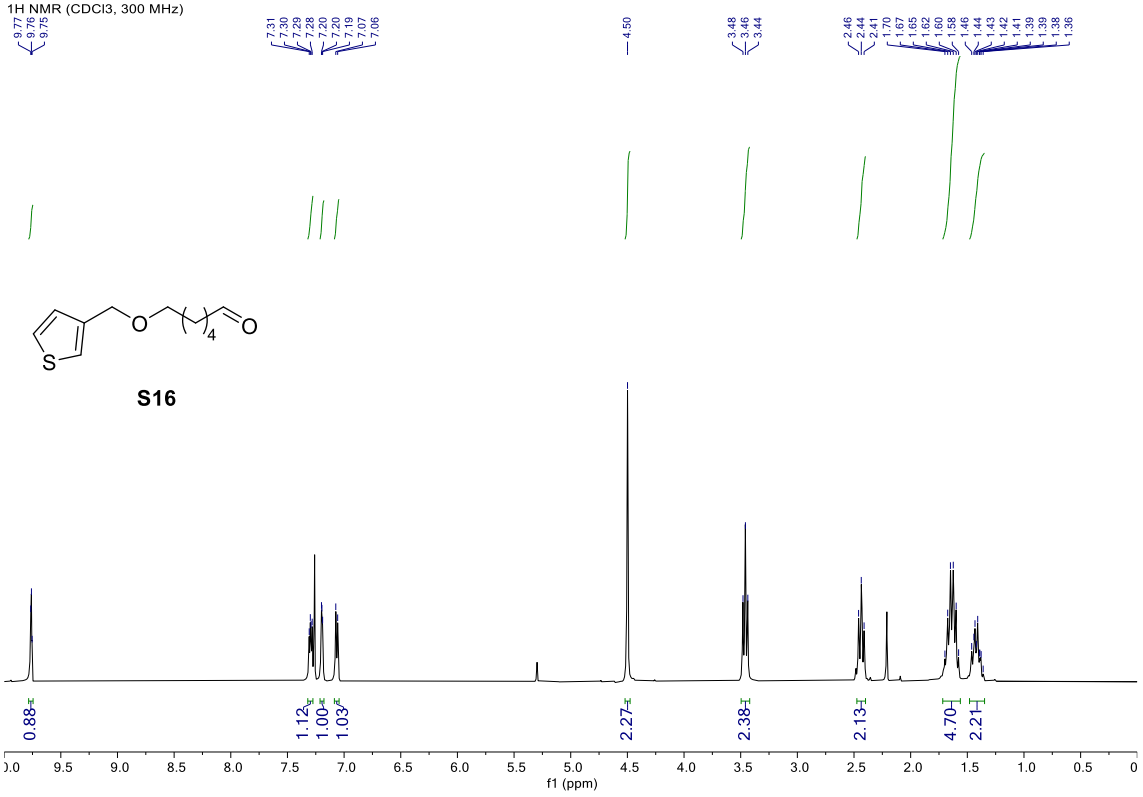
L7

13C NMR (126 MHz, CDCl3)



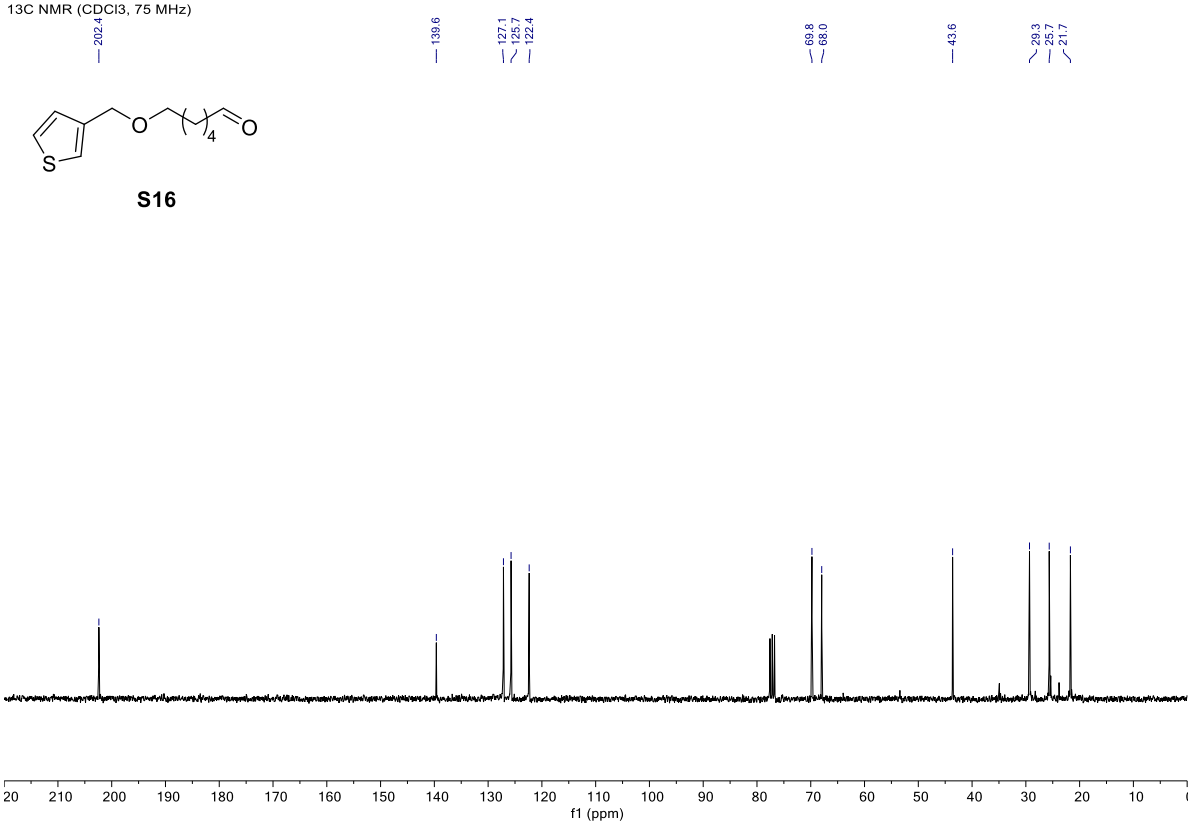
L7

1H NMR (CDCl3, 300 MHz)



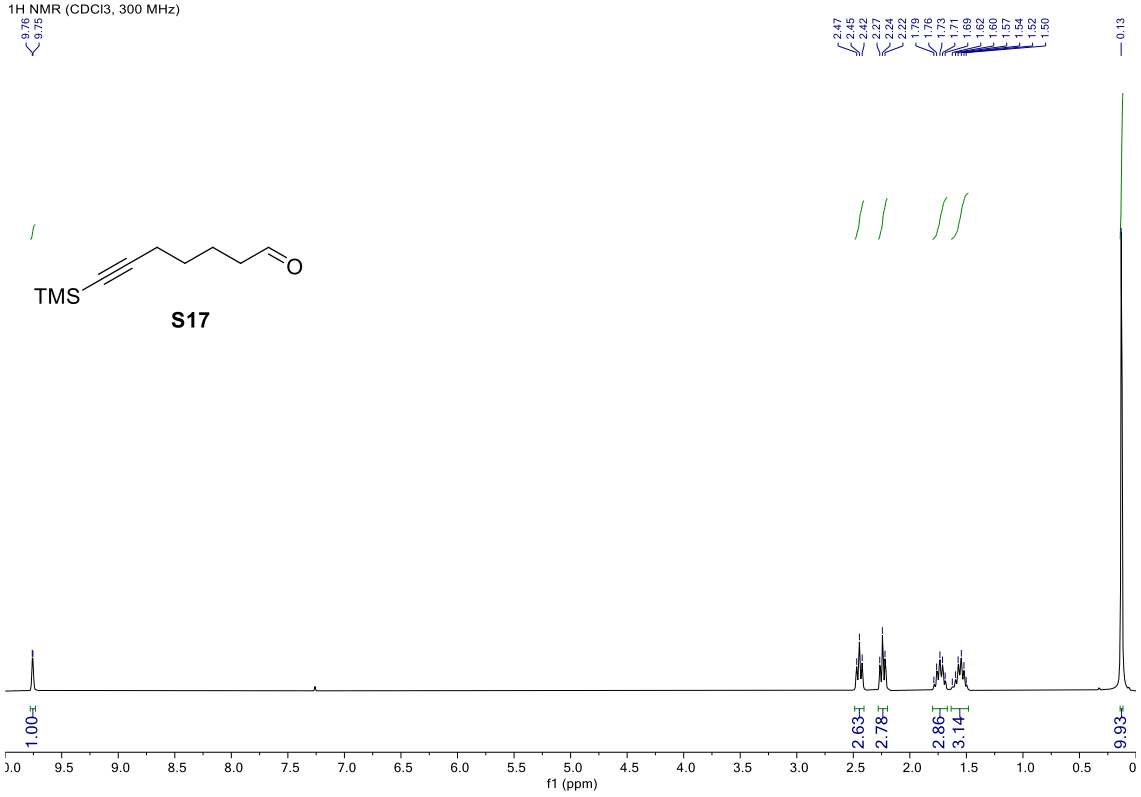
S16

13C NMR (CDCl3, 75 MHz)



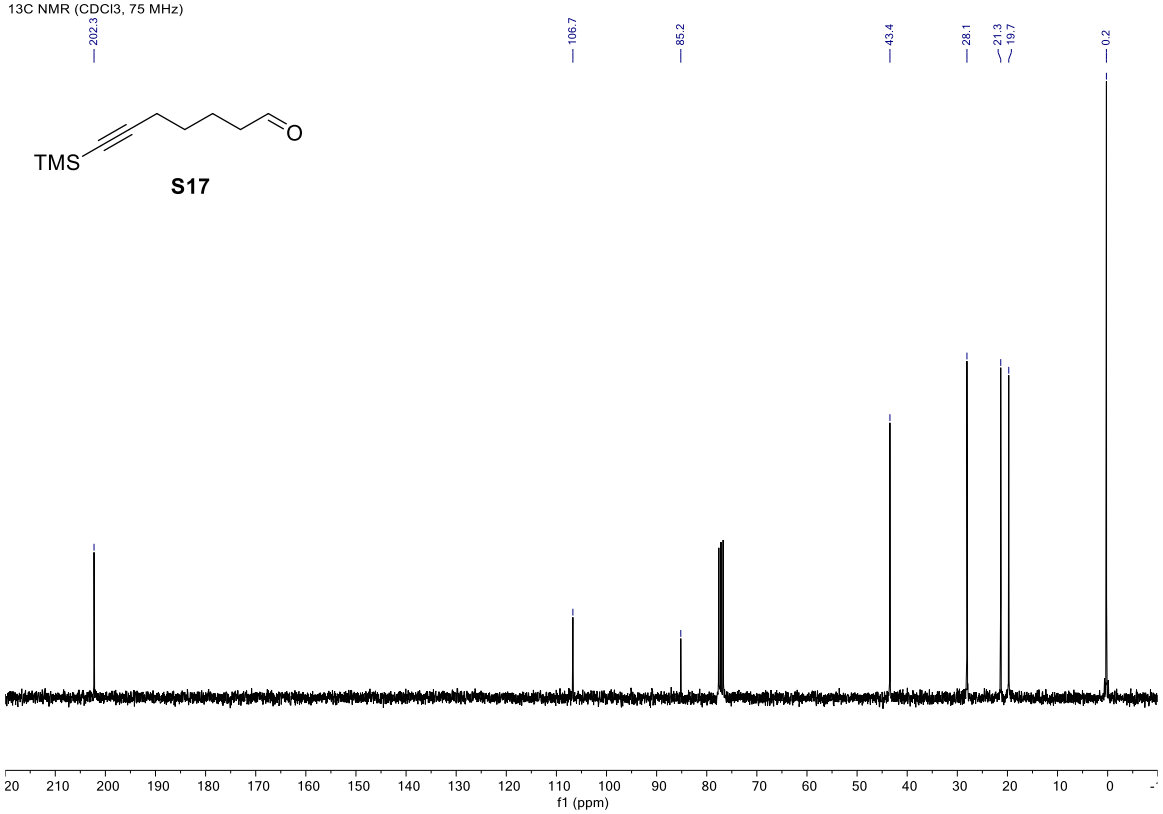
S16

1H NMR (CDCl3, 300 MHz)



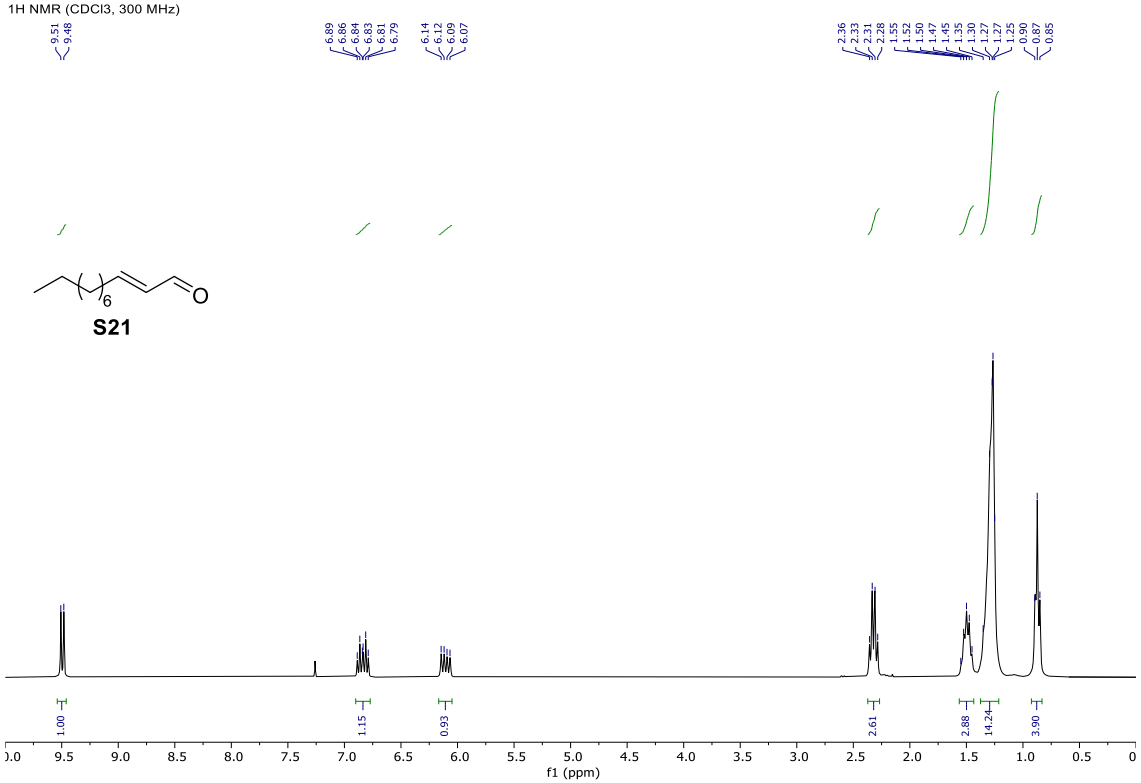
S17

13C NMR (CDCl3, 75 MHz)



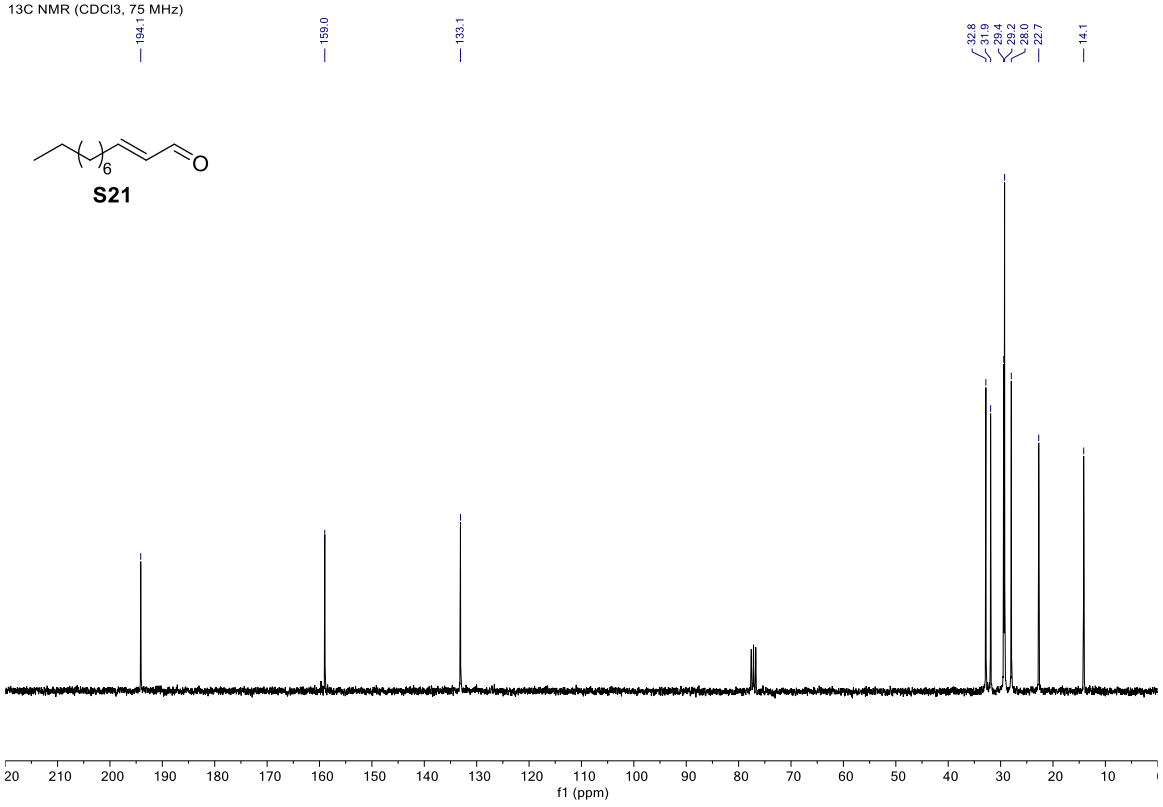
S17

1H NMR (CDCl3, 300 MHz)



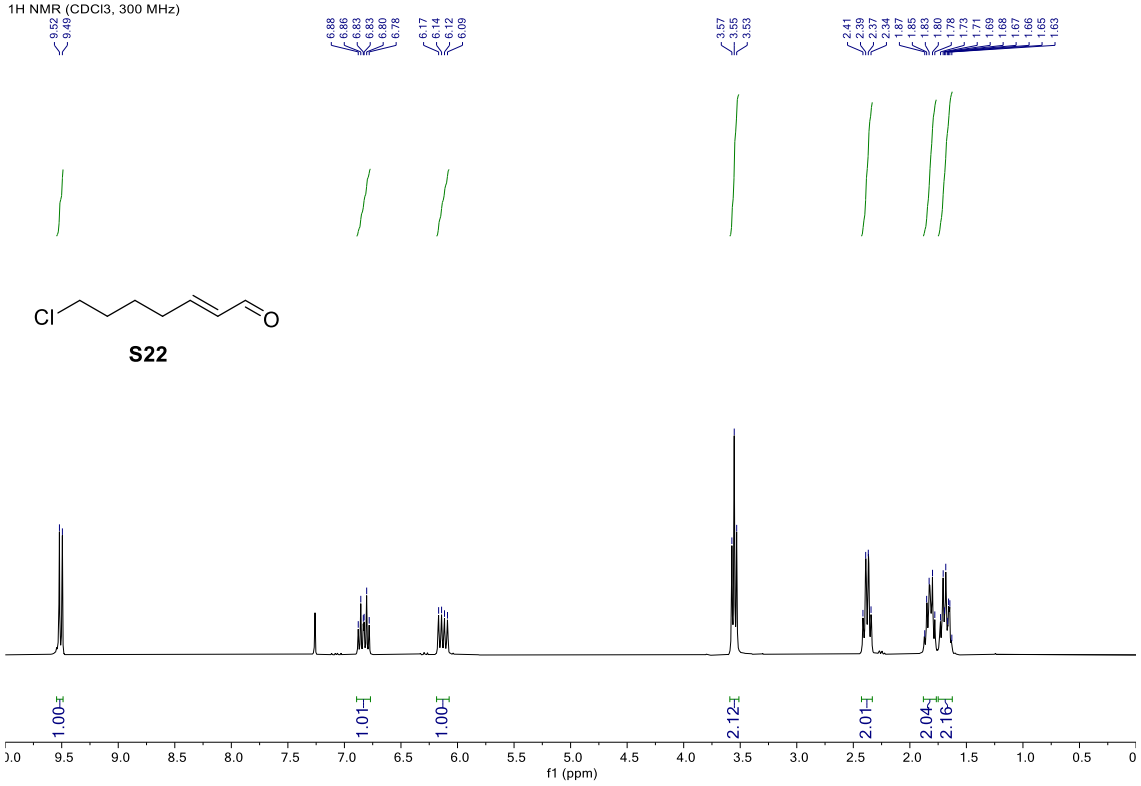
S21

13C NMR (CDCl3, 75 MHz)



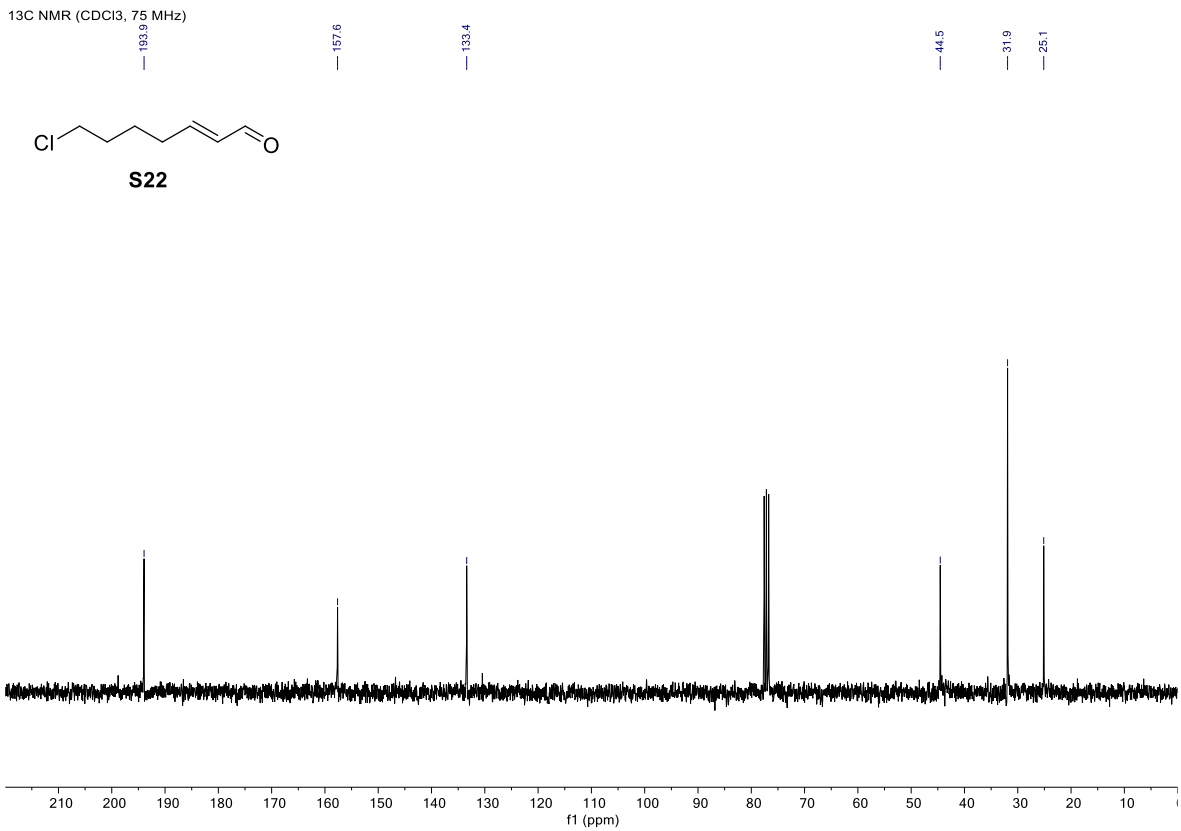
S21

1H NMR (CDCl3, 300 MHz)



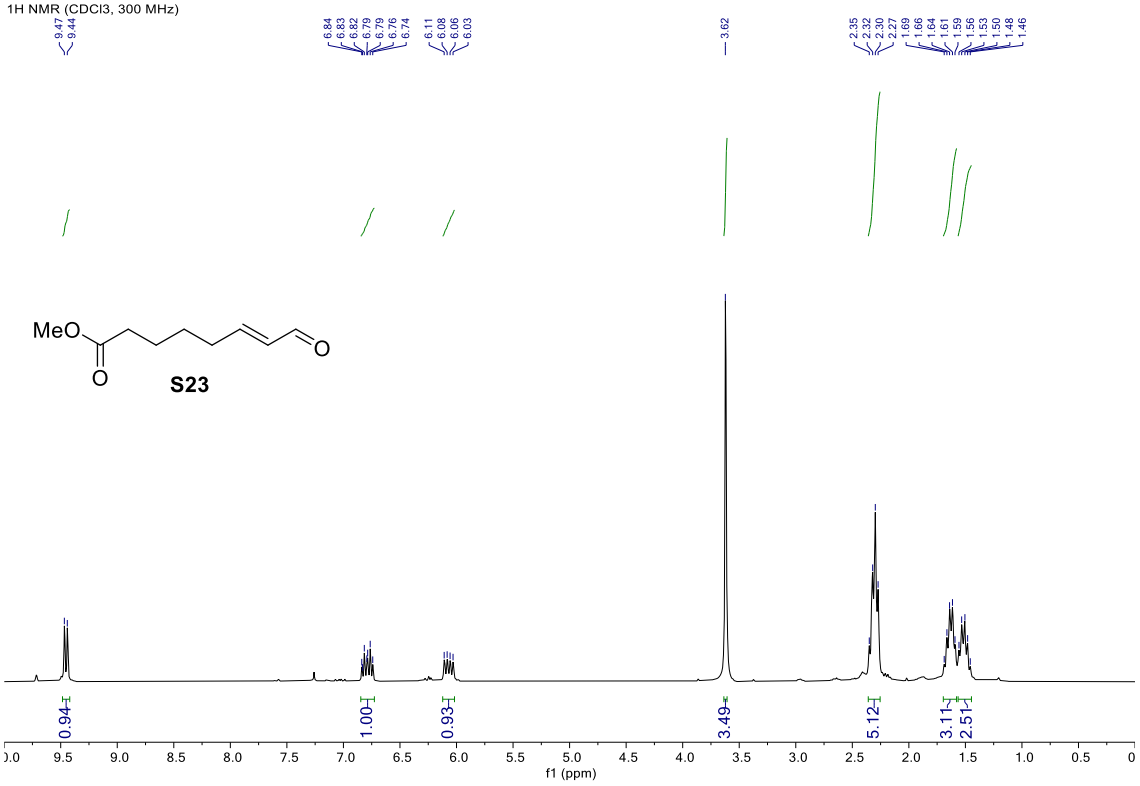
S22

13C NMR (CDCl3, 75 MHz)



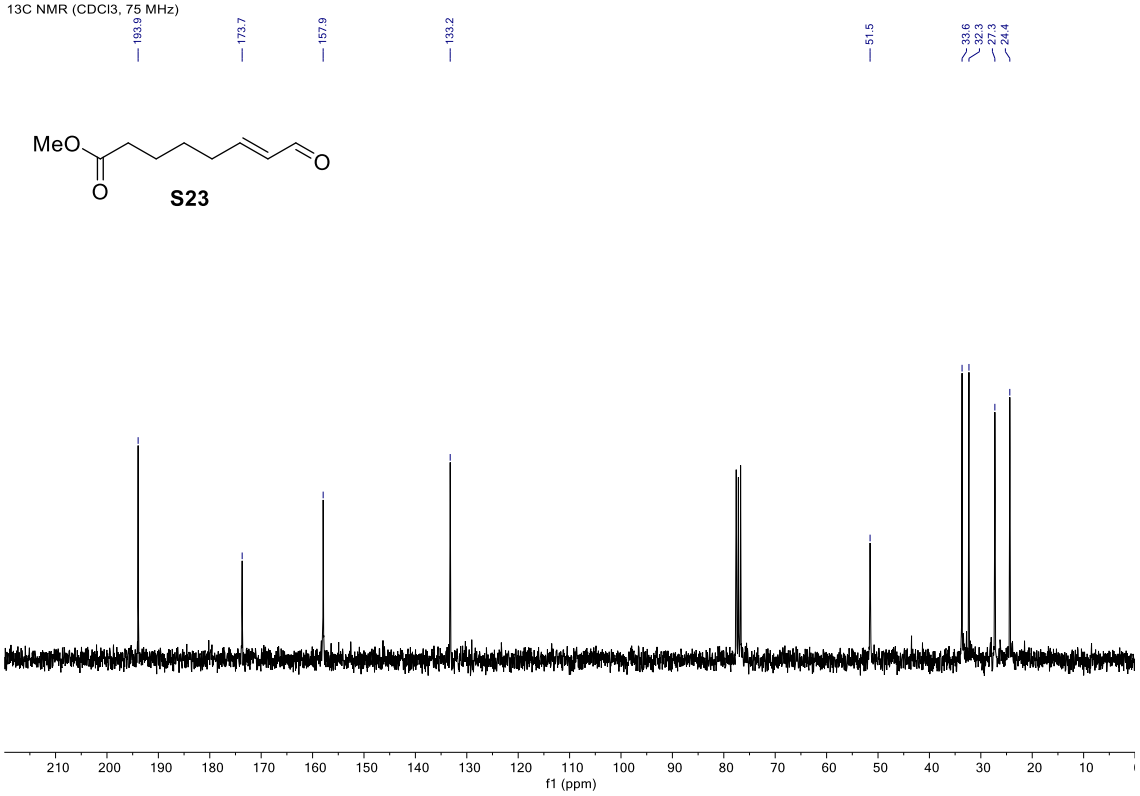
S22

1H NMR (CDCl3, 300 MHz)



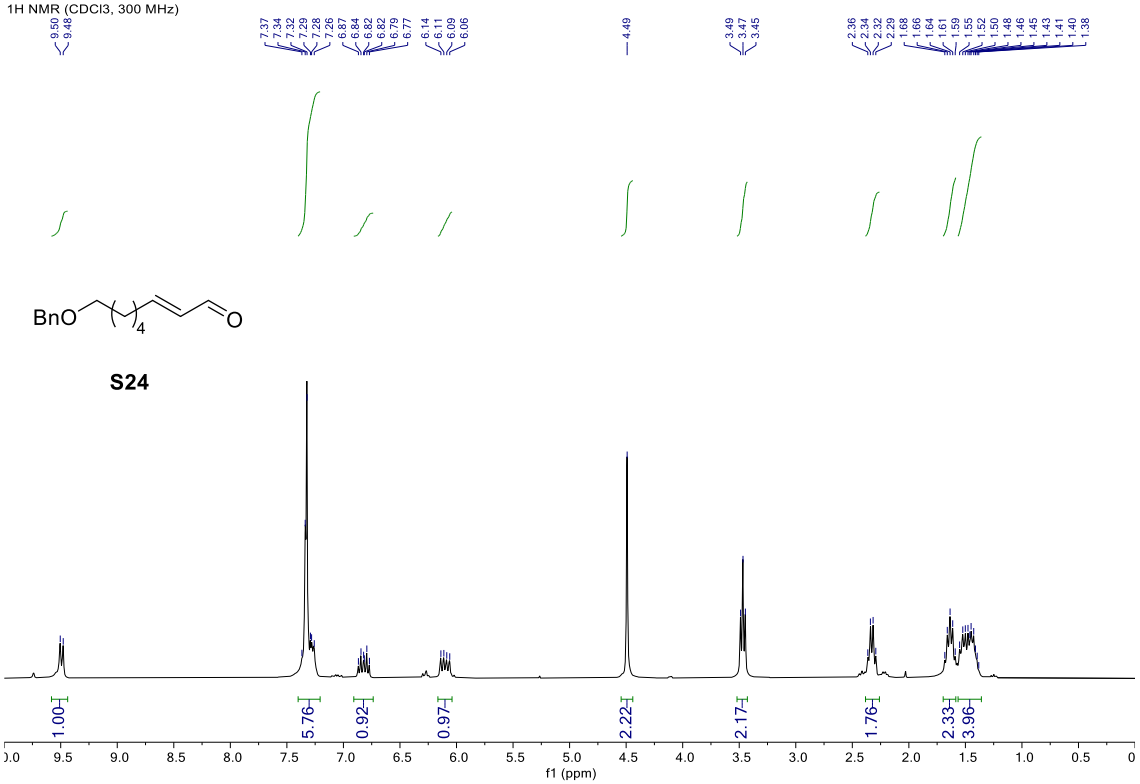
S23

13C NMR (CDCl3, 75 MHz)



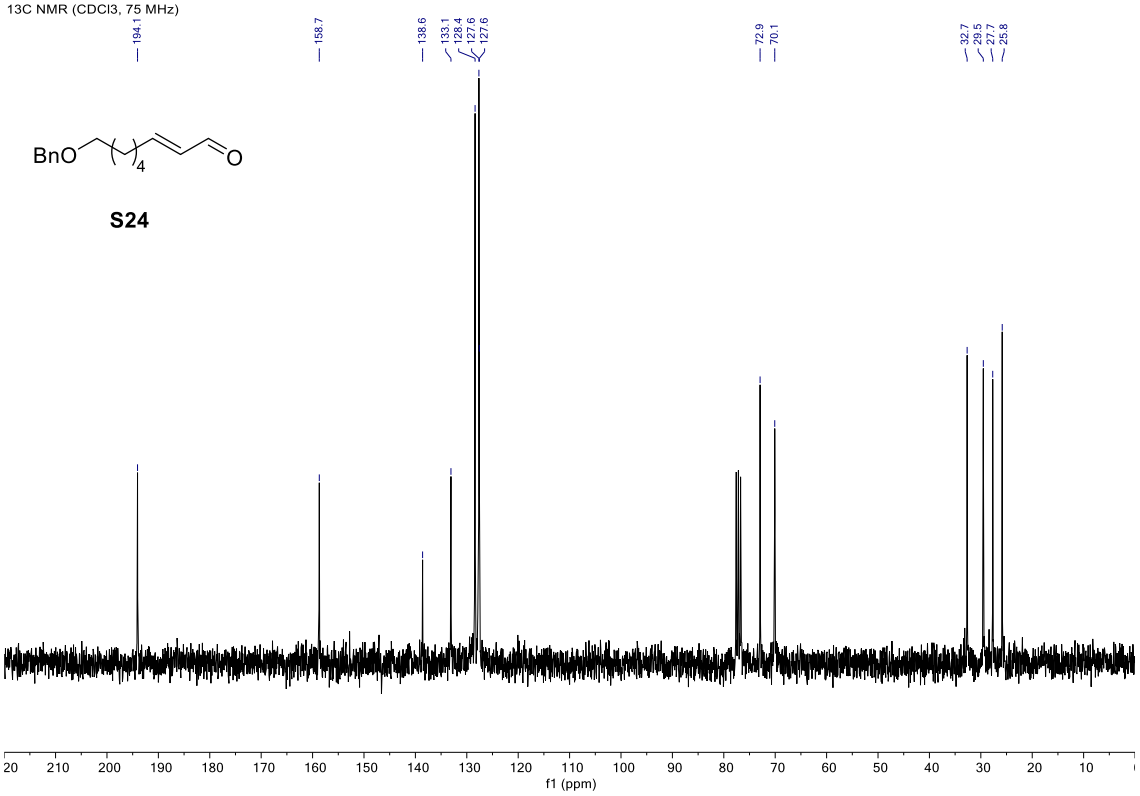
S23

1H NMR (CDCl3, 300 MHz)



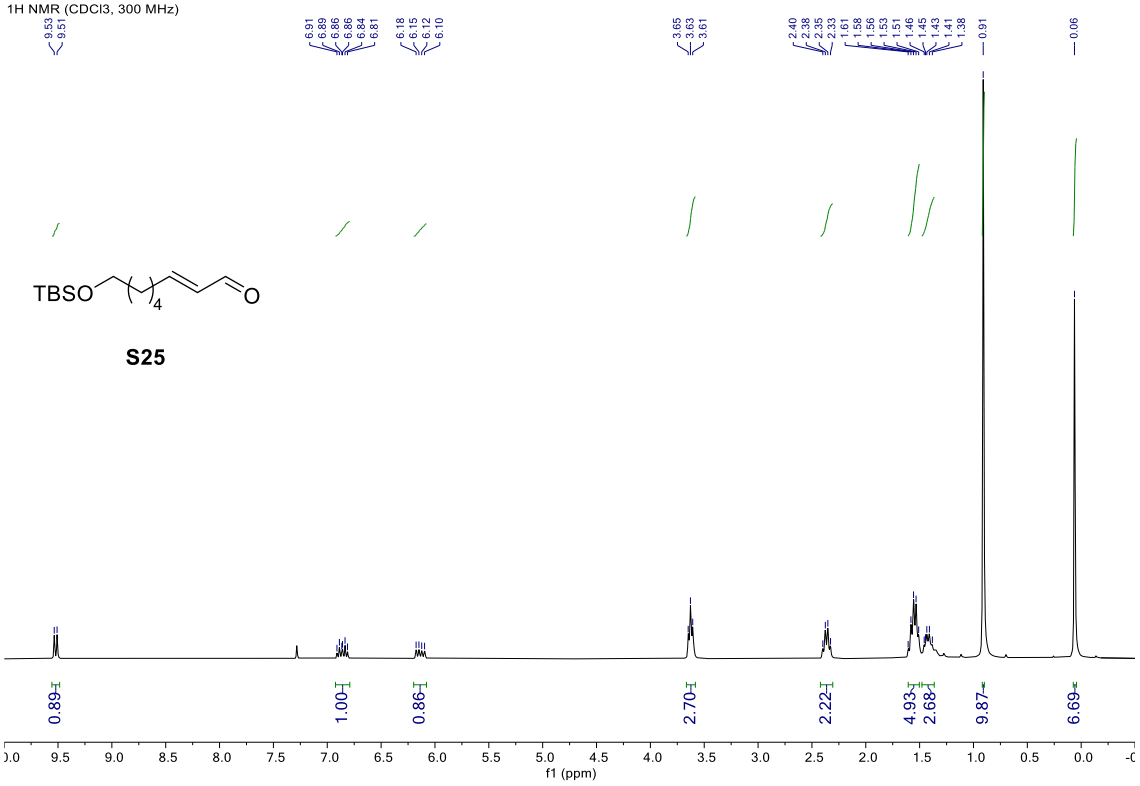
S24

13C NMR (CDCl3, 75 MHz)



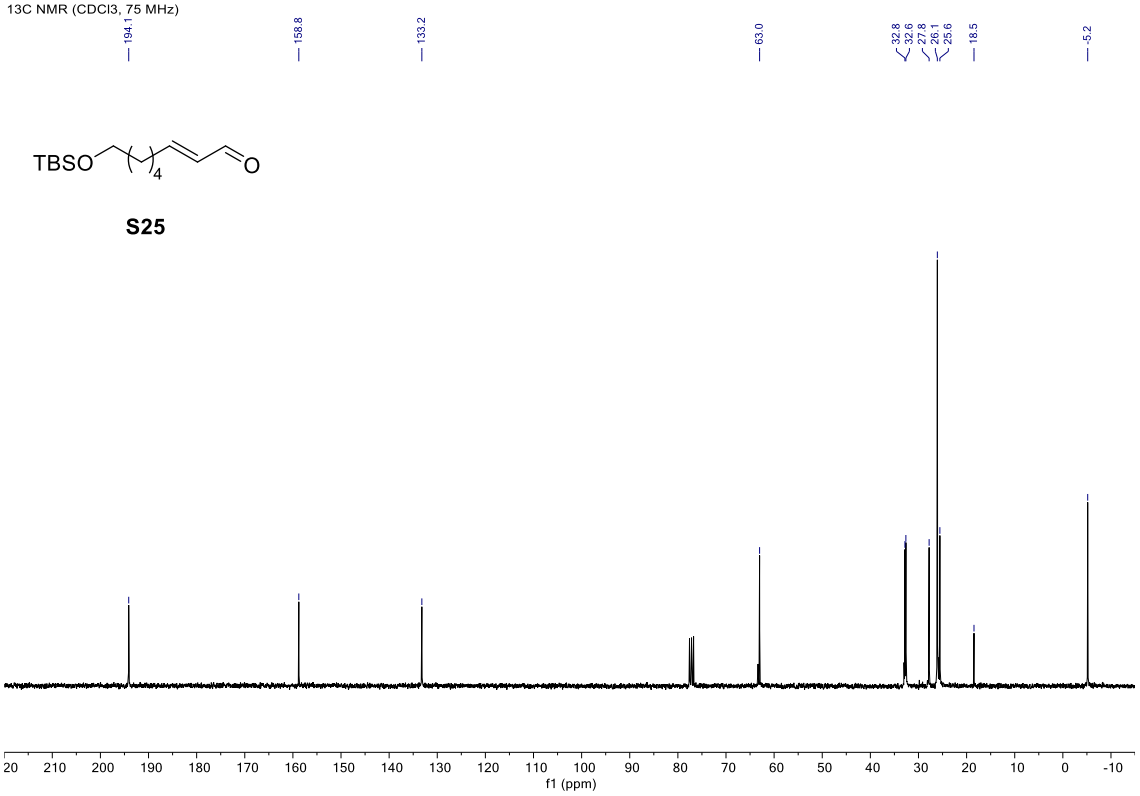
S24

1H NMR (CDCl3, 300 MHz)



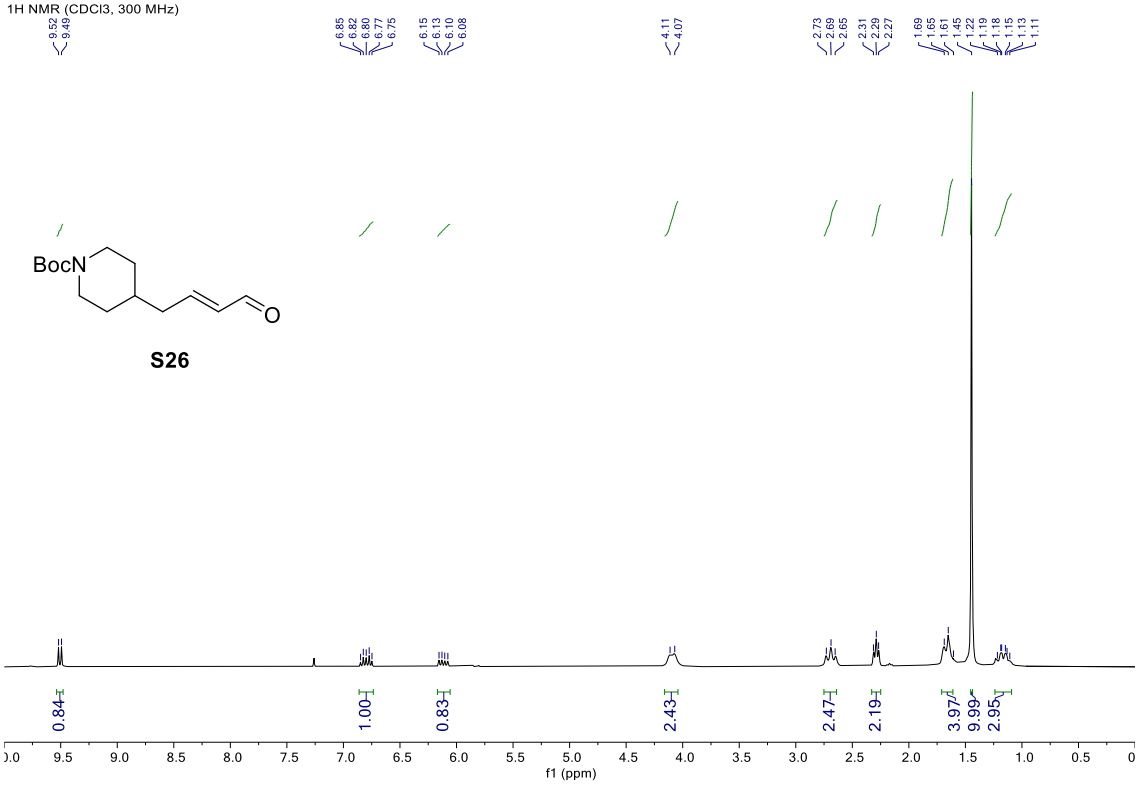
S25

13C NMR (CDCl3, 75 MHz)



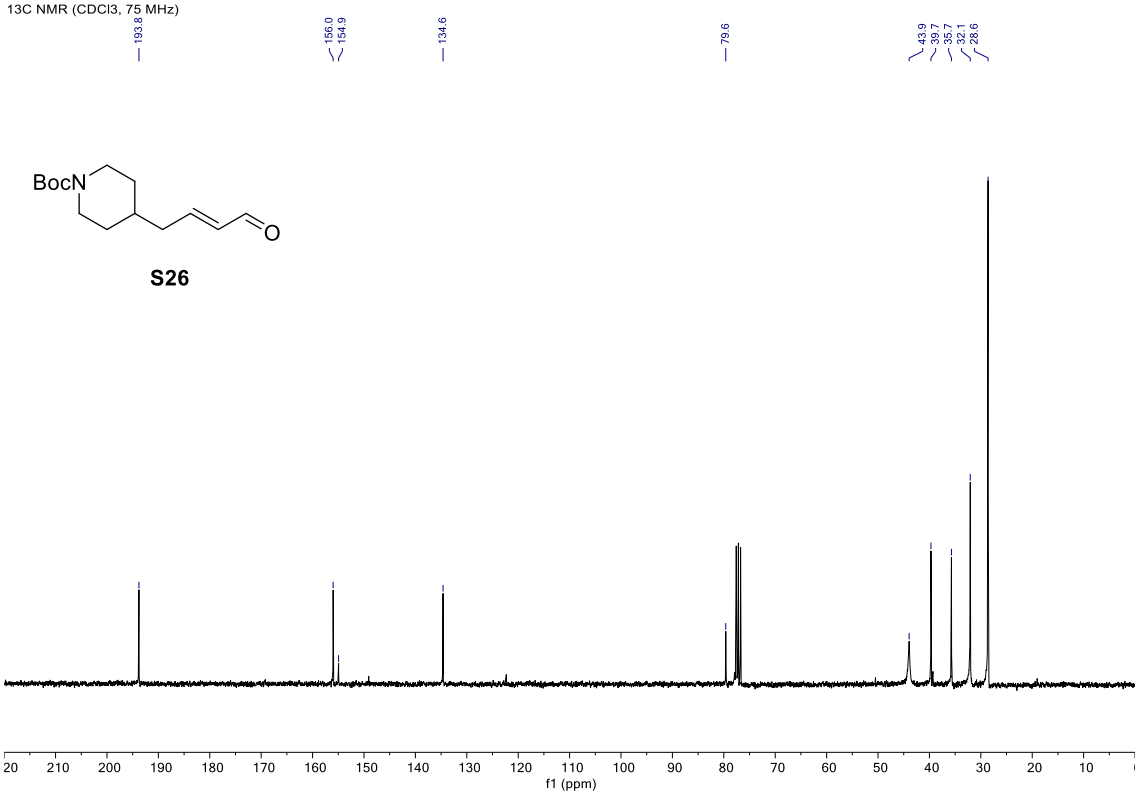
S25

1H NMR (CDCl3, 300 MHz)



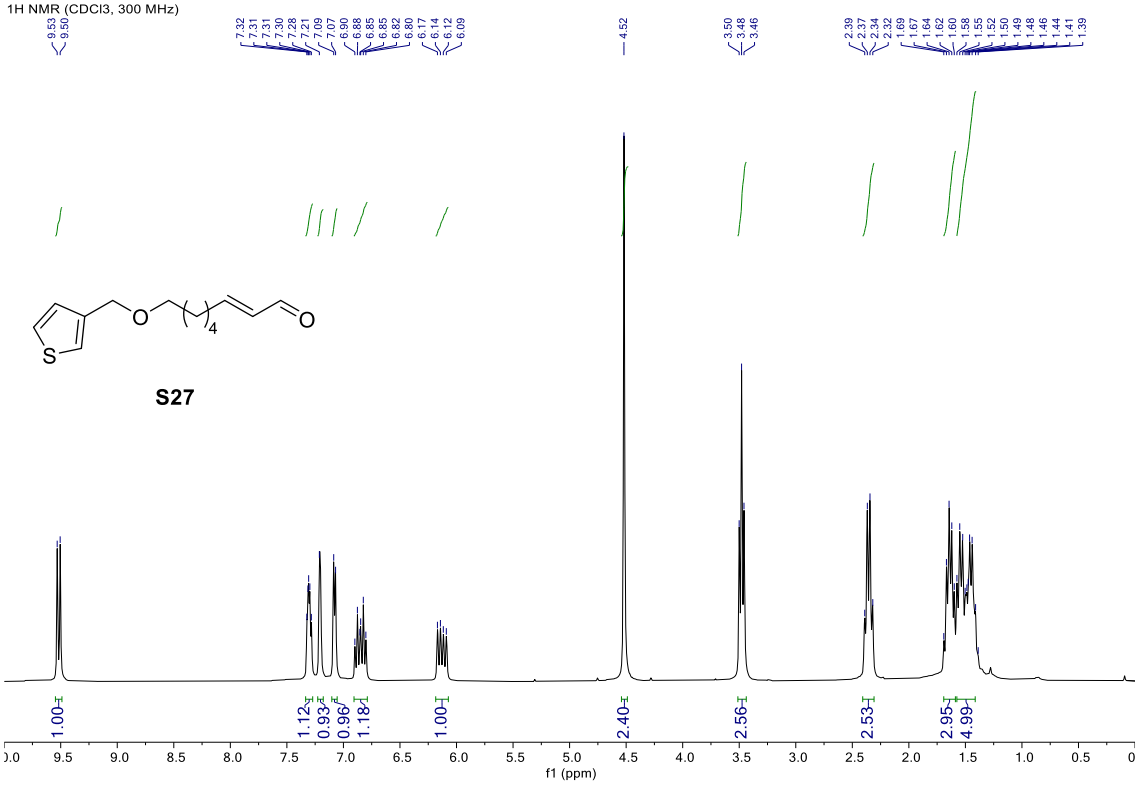
S26

13C NMR (CDCl3, 75 MHz)



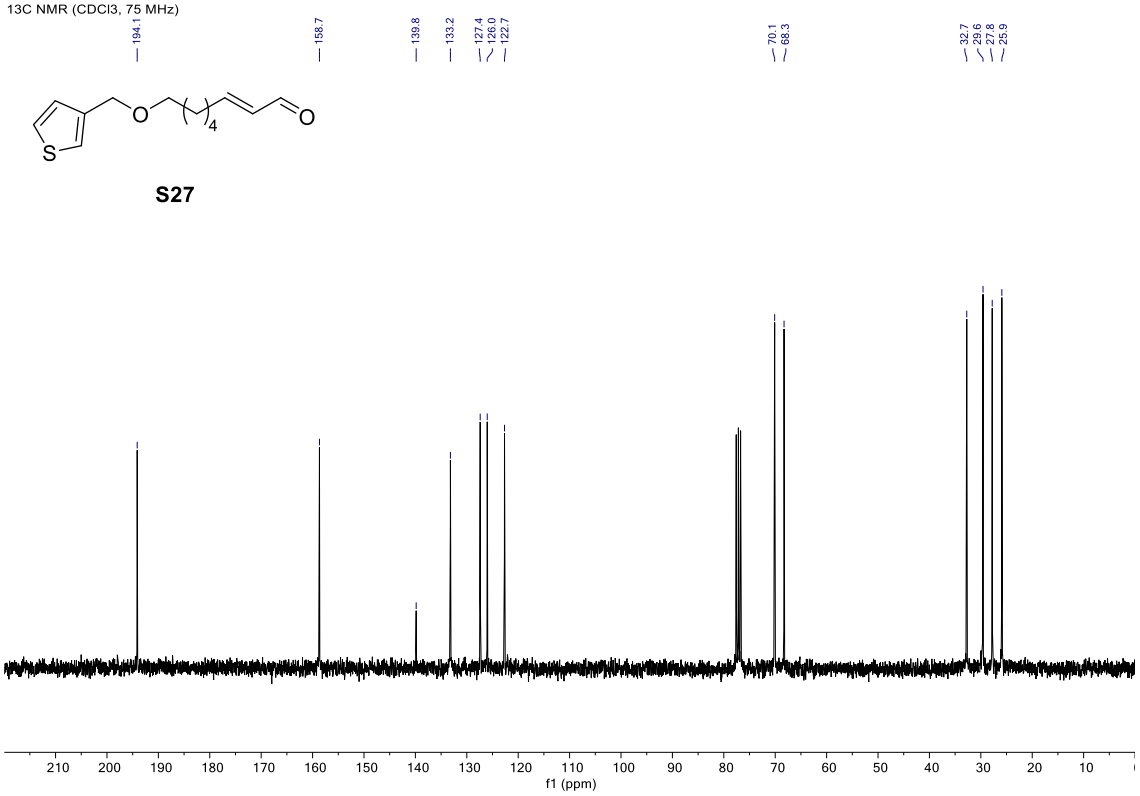
S26

1H NMR (CDCl3, 300 MHz)



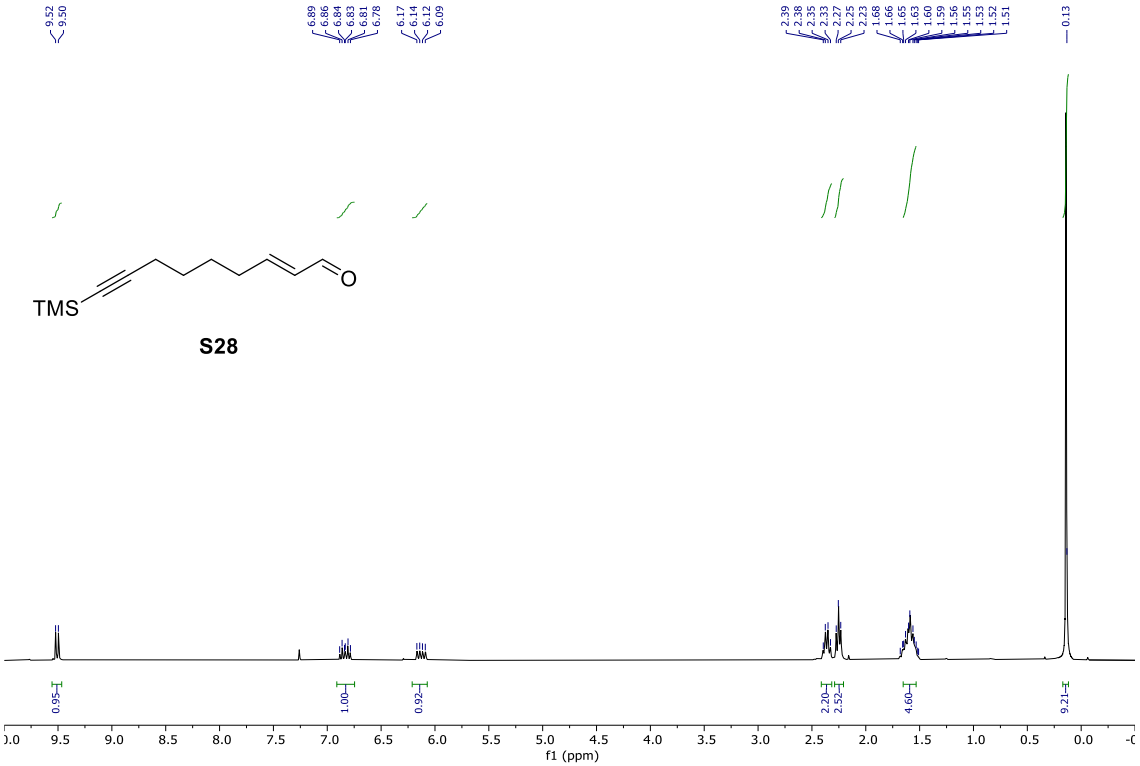
S27

13C NMR (CDCl3, 75 MHz)



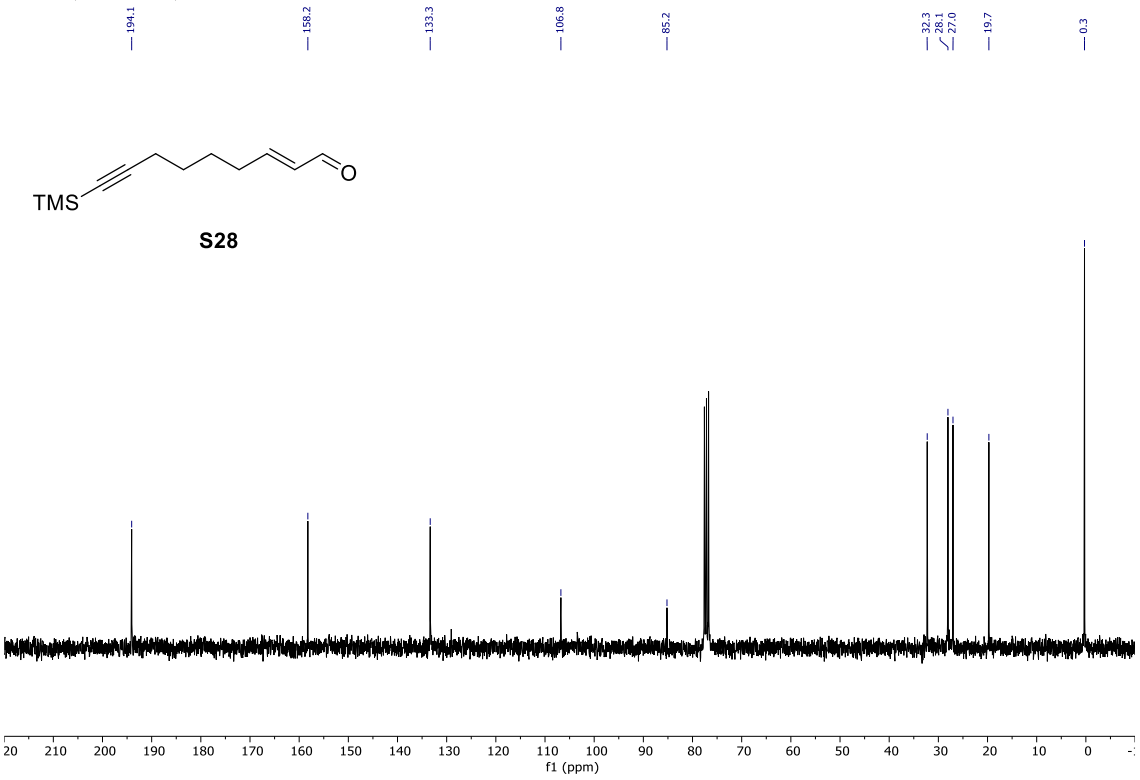
S27

1H NMR (CDCl3, 300 MHz)



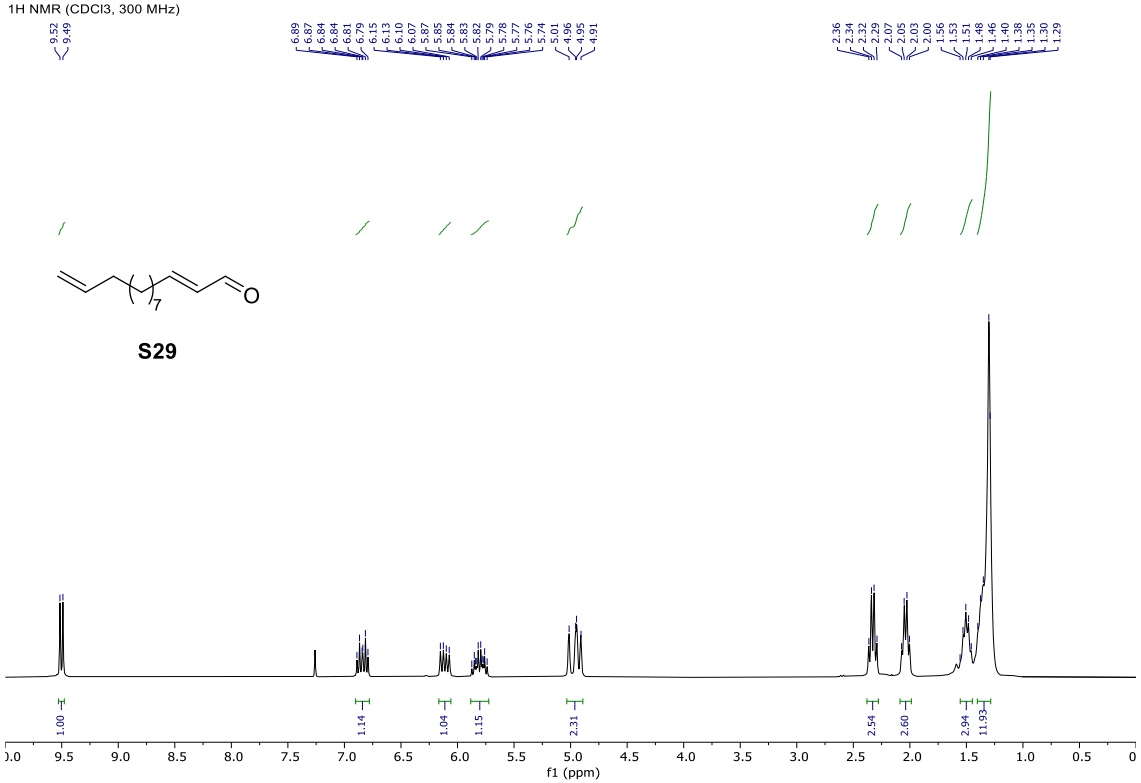
S28

13C NMR (CDCl3, 75 MHz)



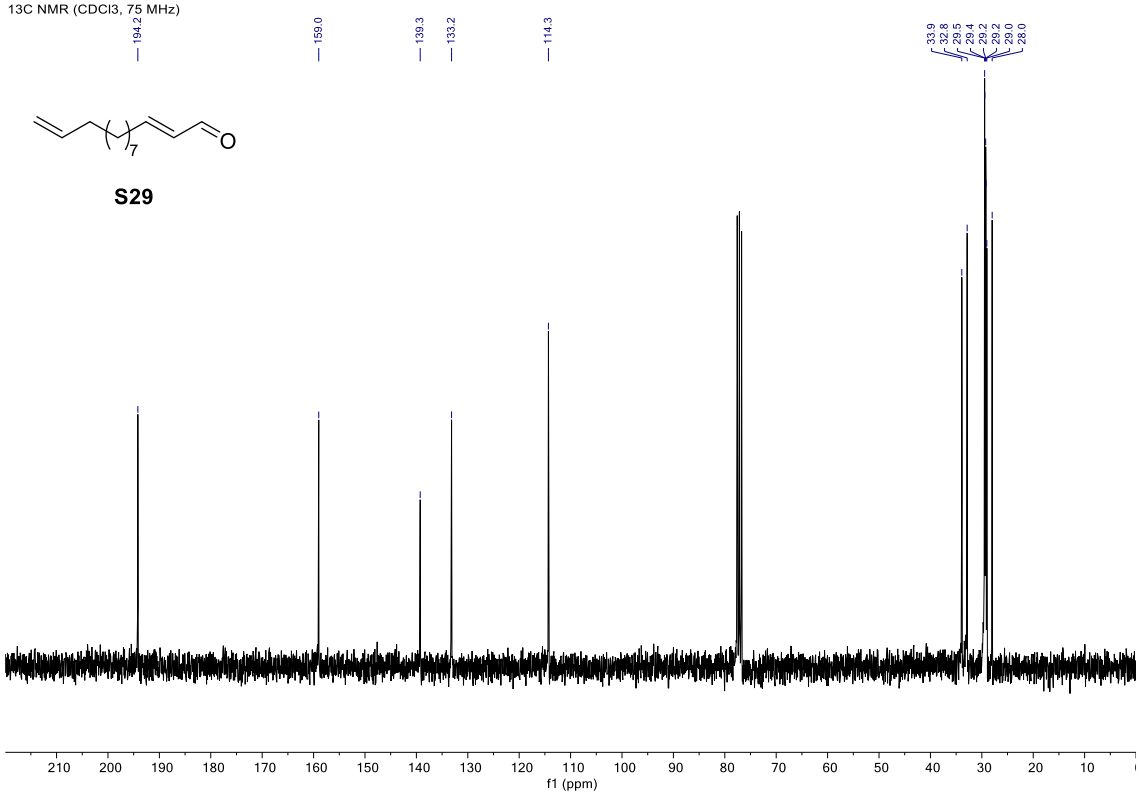
S28

1H NMR (CDCl3, 300 MHz)



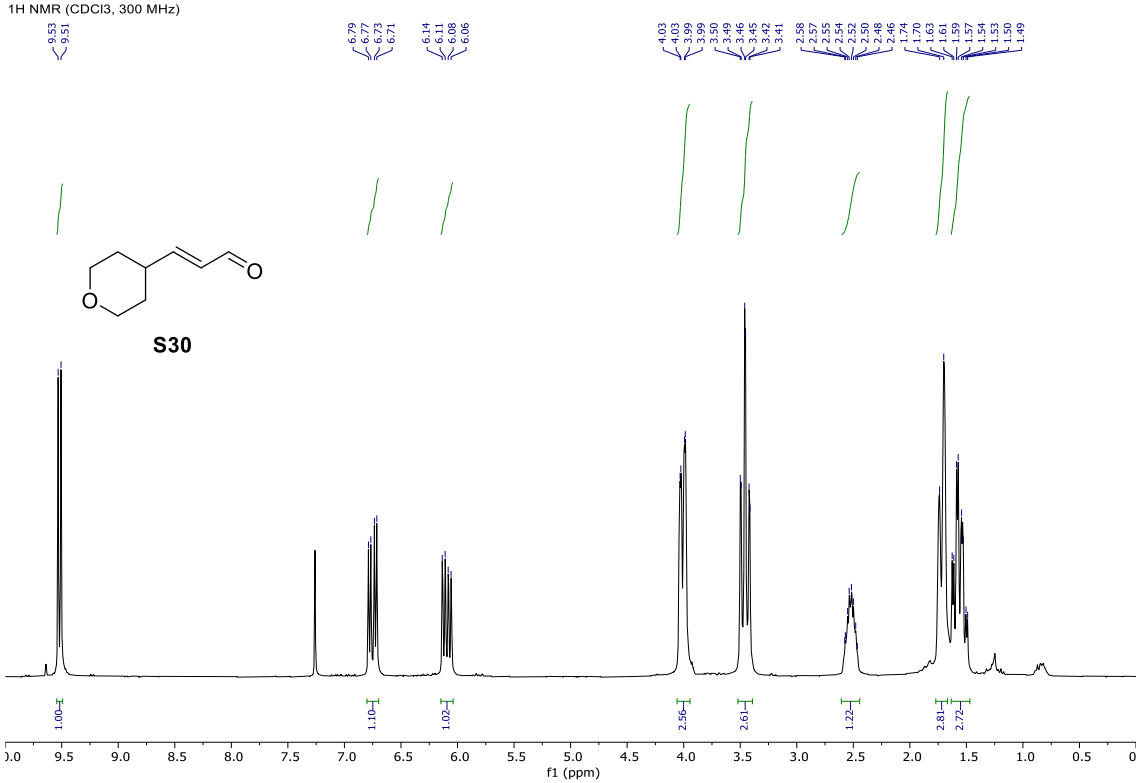
S29

13C NMR (CDCl3, 75 MHz)



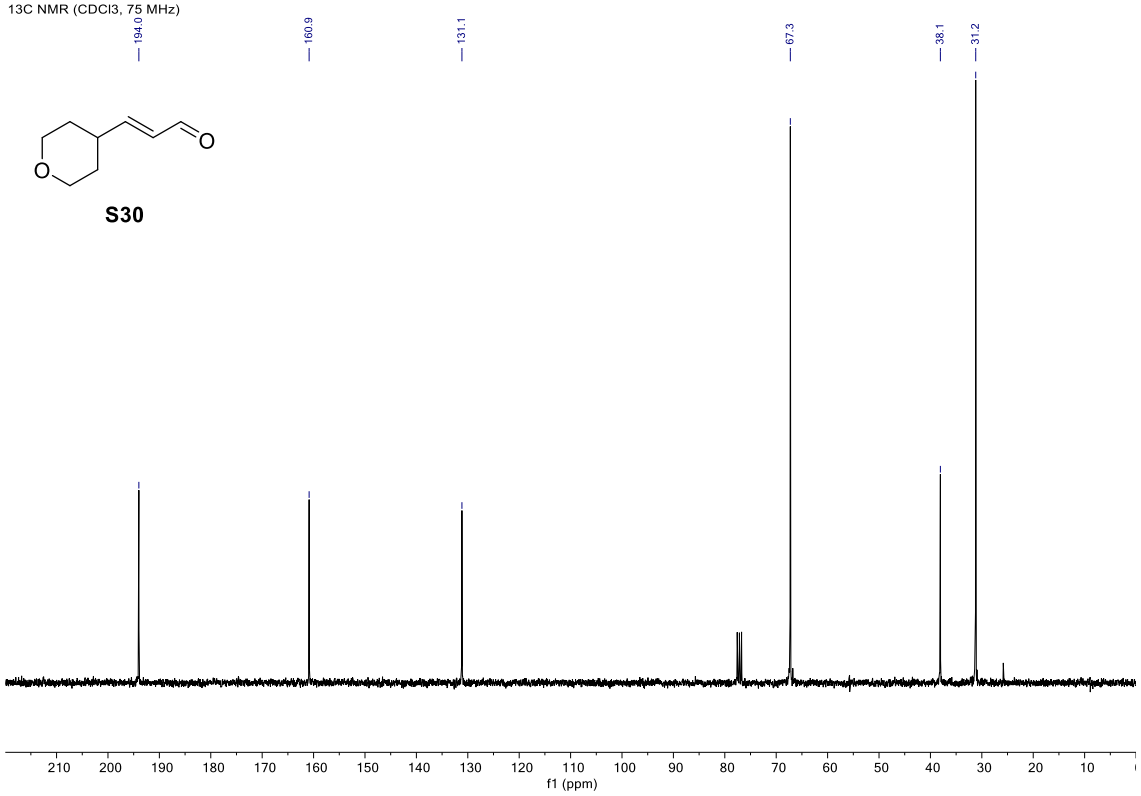
S29

1H NMR (CDCl3, 300 MHz)



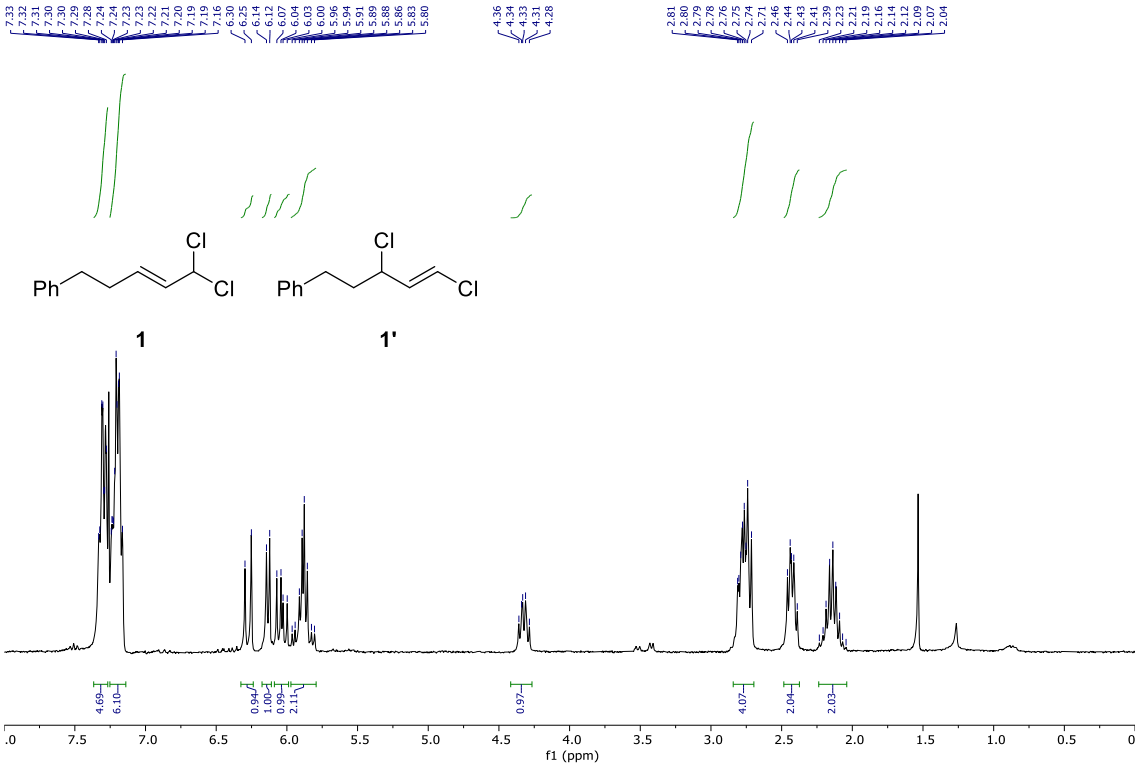
S30

13C NMR (CDCl3, 75 MHz)

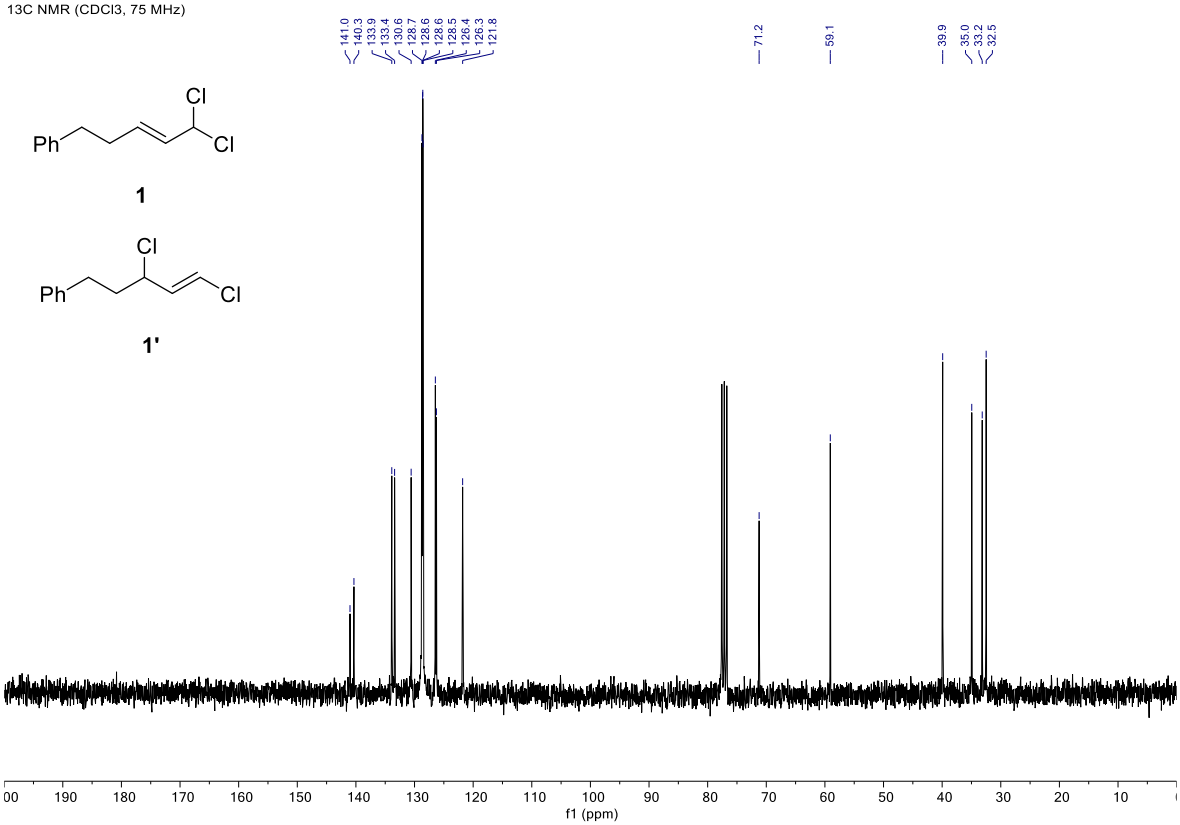


S30

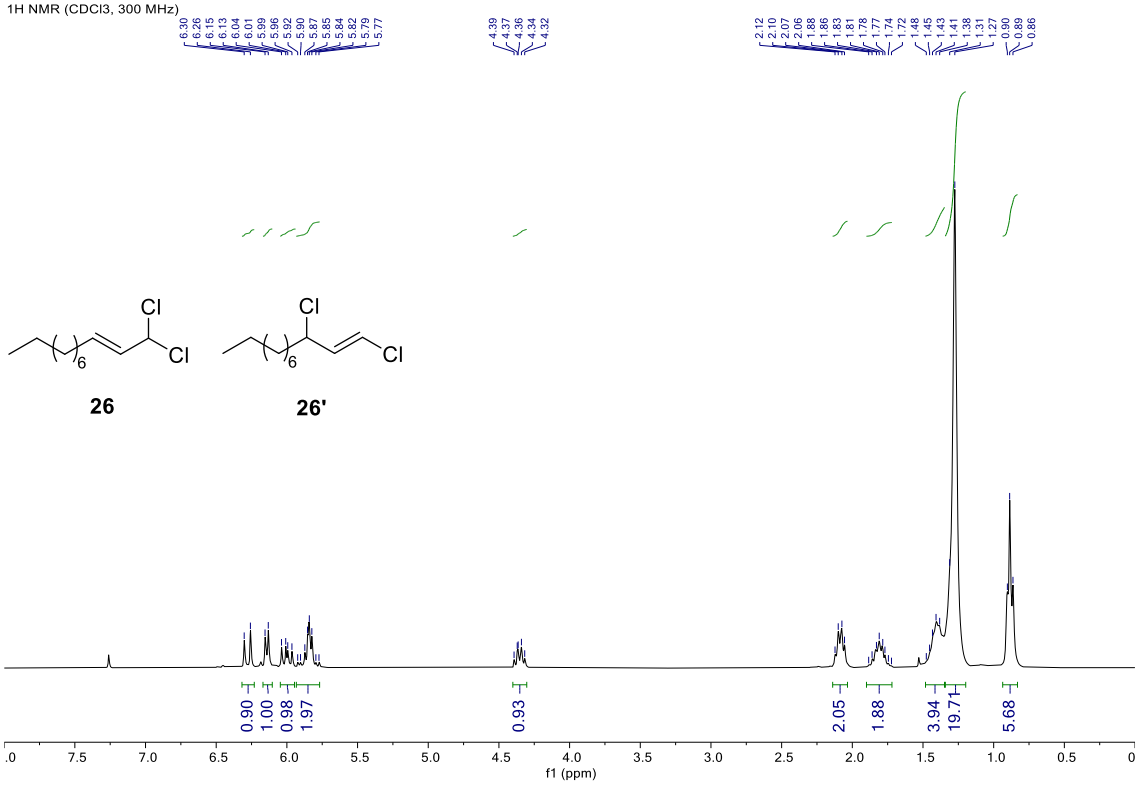
1H NMR (CDCl3, 300 MHz)



13C NMR (CDCl3, 75 MHz)

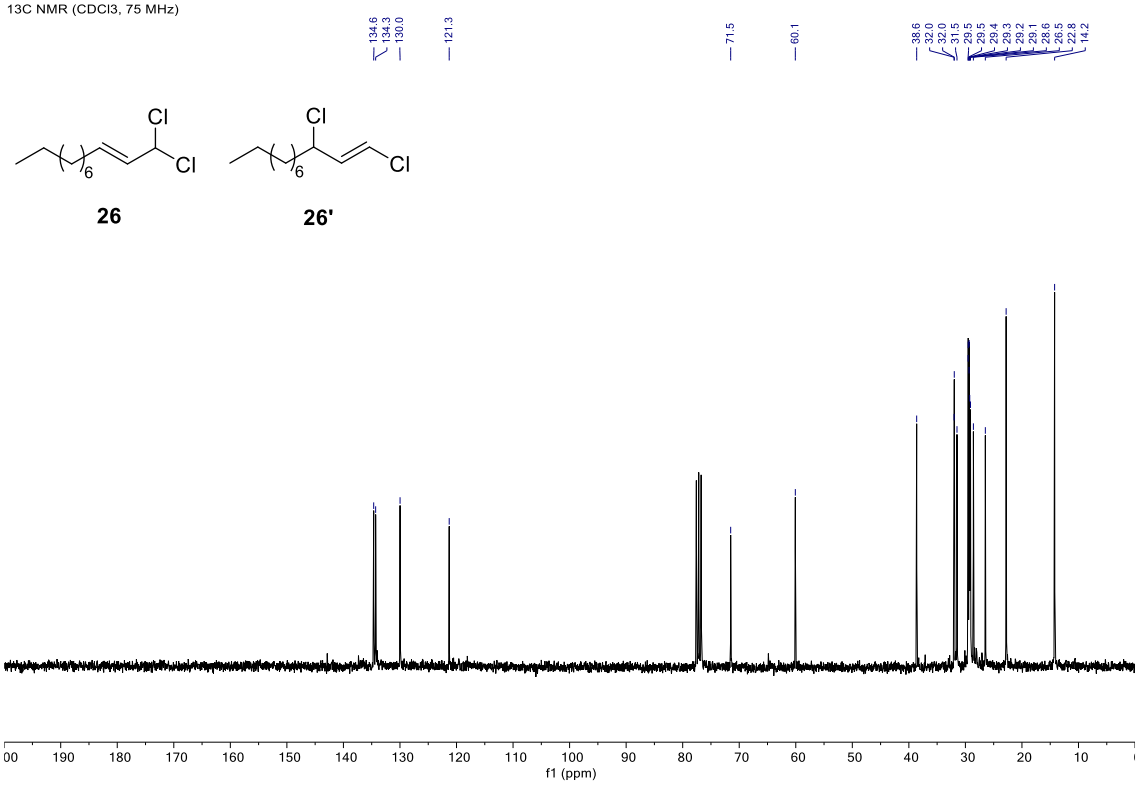


1H NMR (CDCl3, 300 MHz)



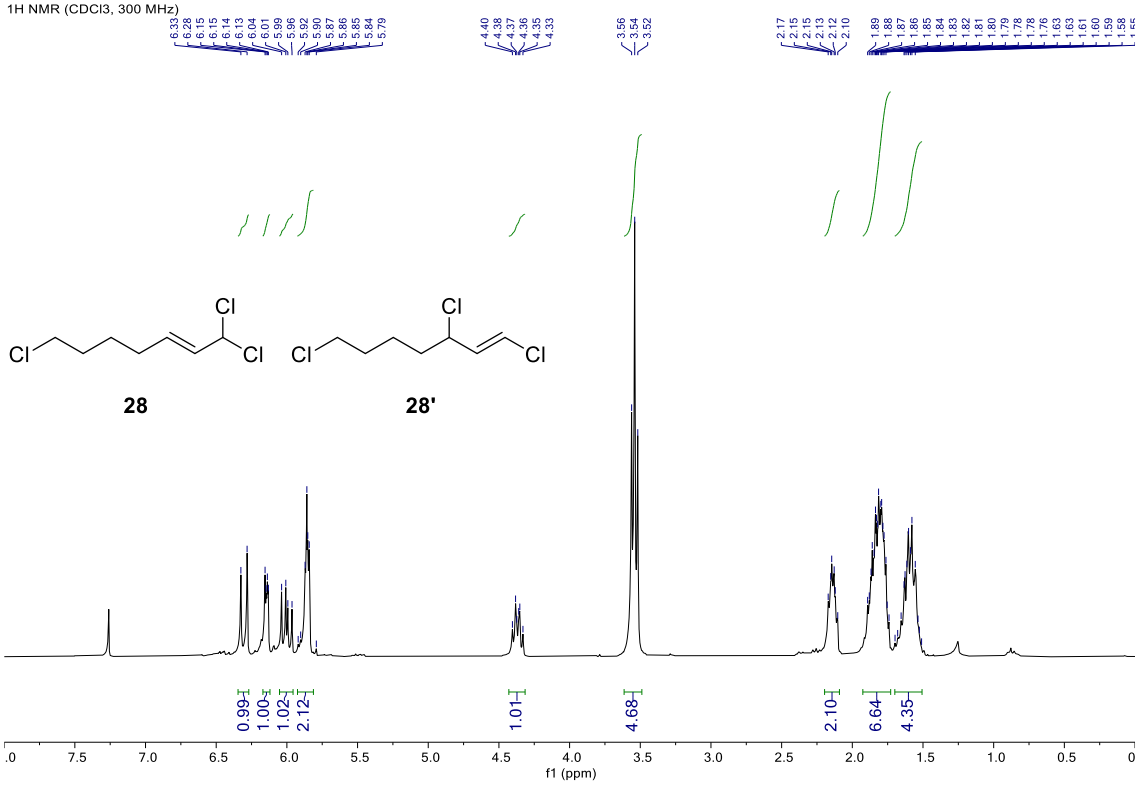
26 **26'**

13C NMR (CDCl3, 75 MHz)

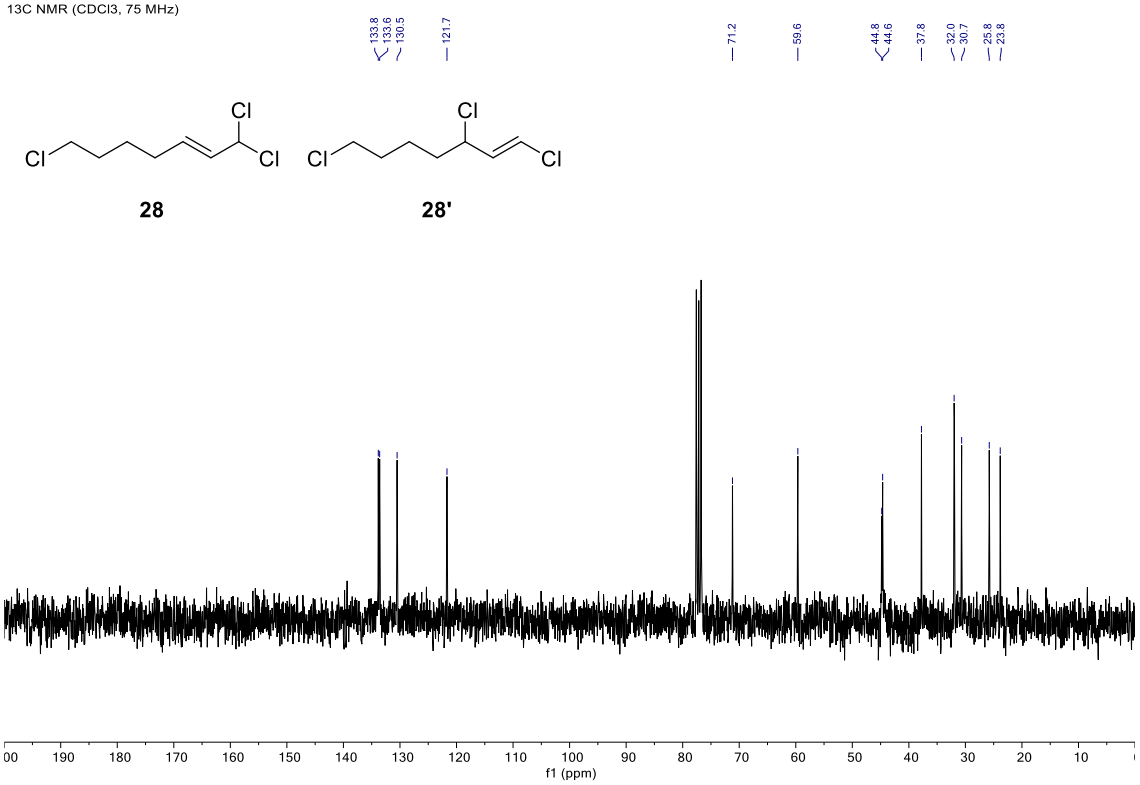


26 **26'**

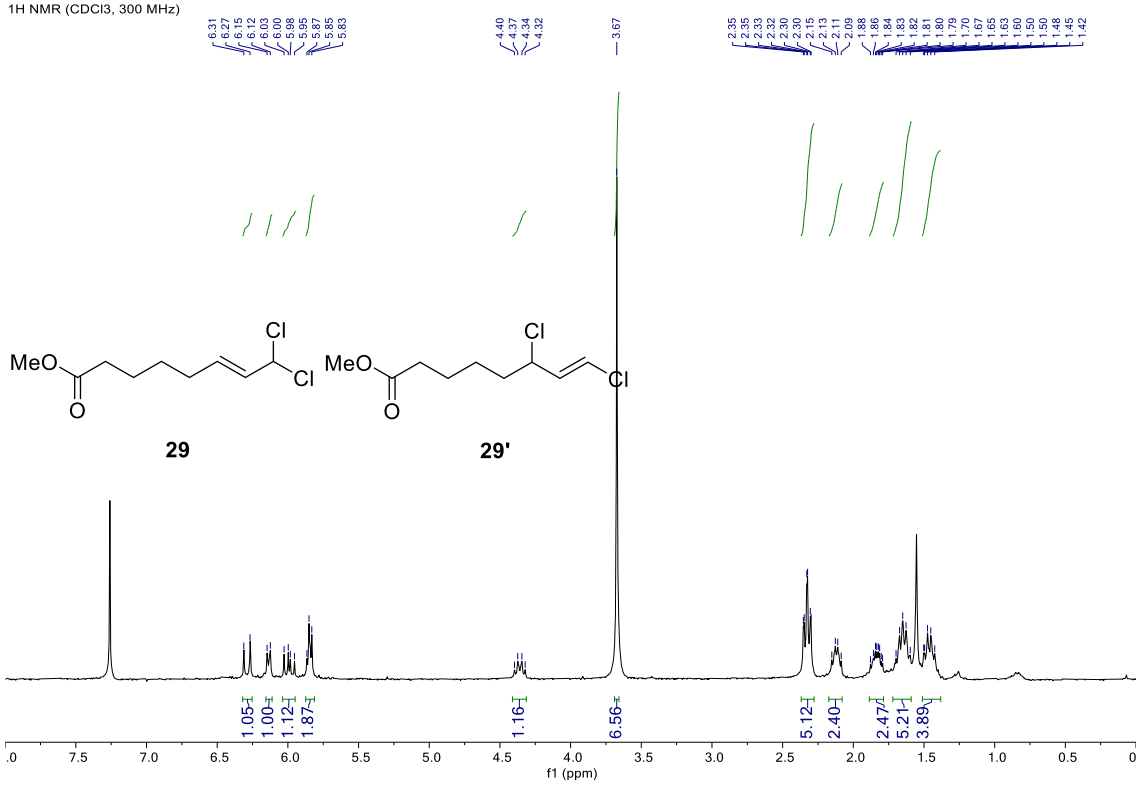
1H NMR (CDCl3, 300 MHz)



13C NMR (CDCl3, 75 MHz)

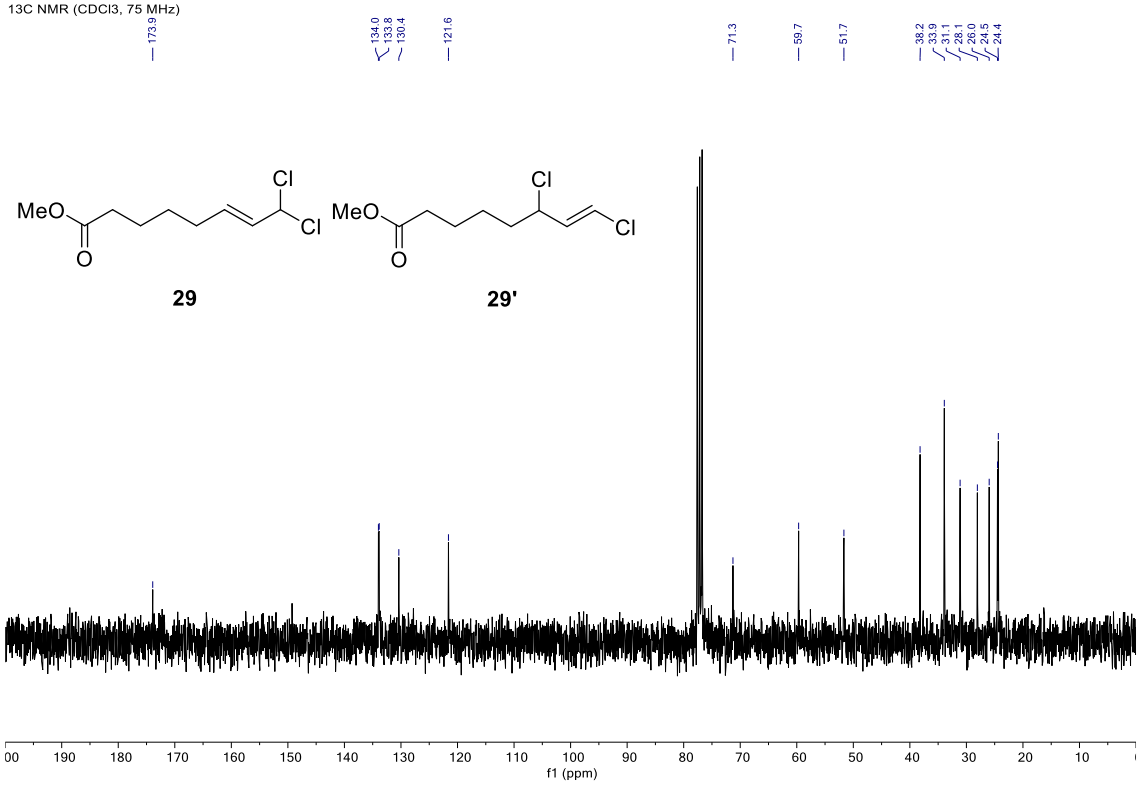


1H NMR (CDCl3, 300 MHz)

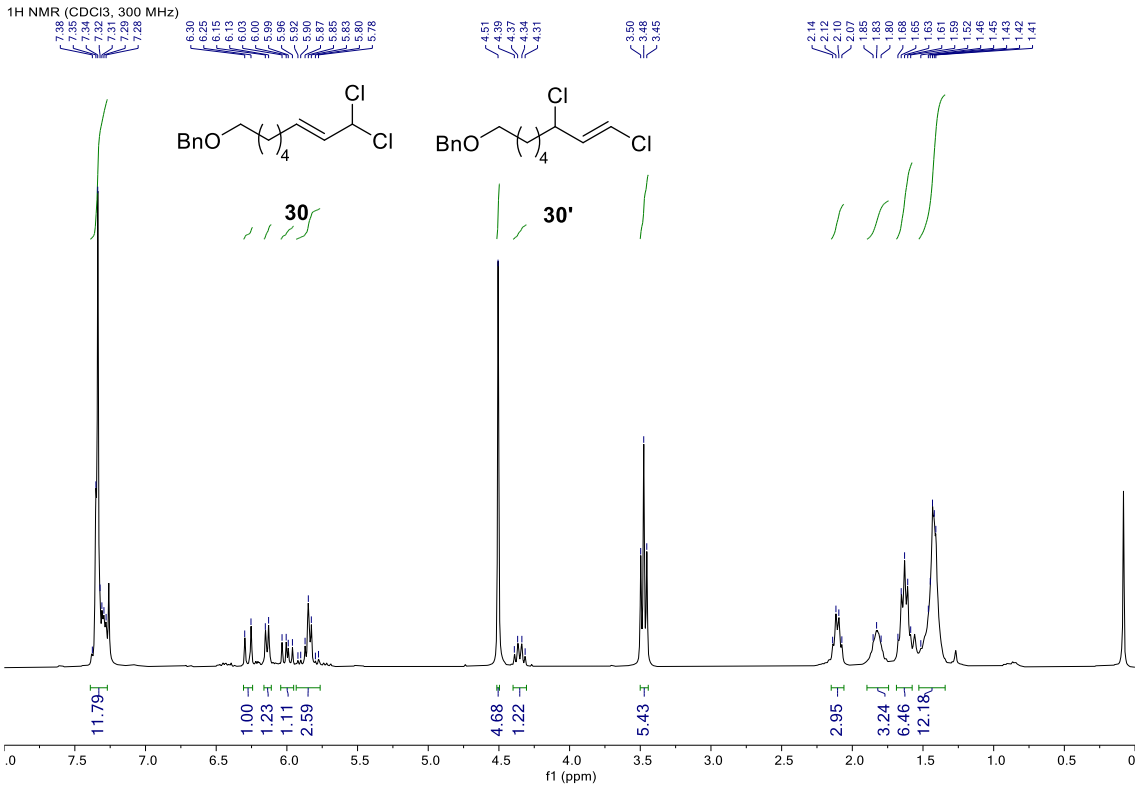


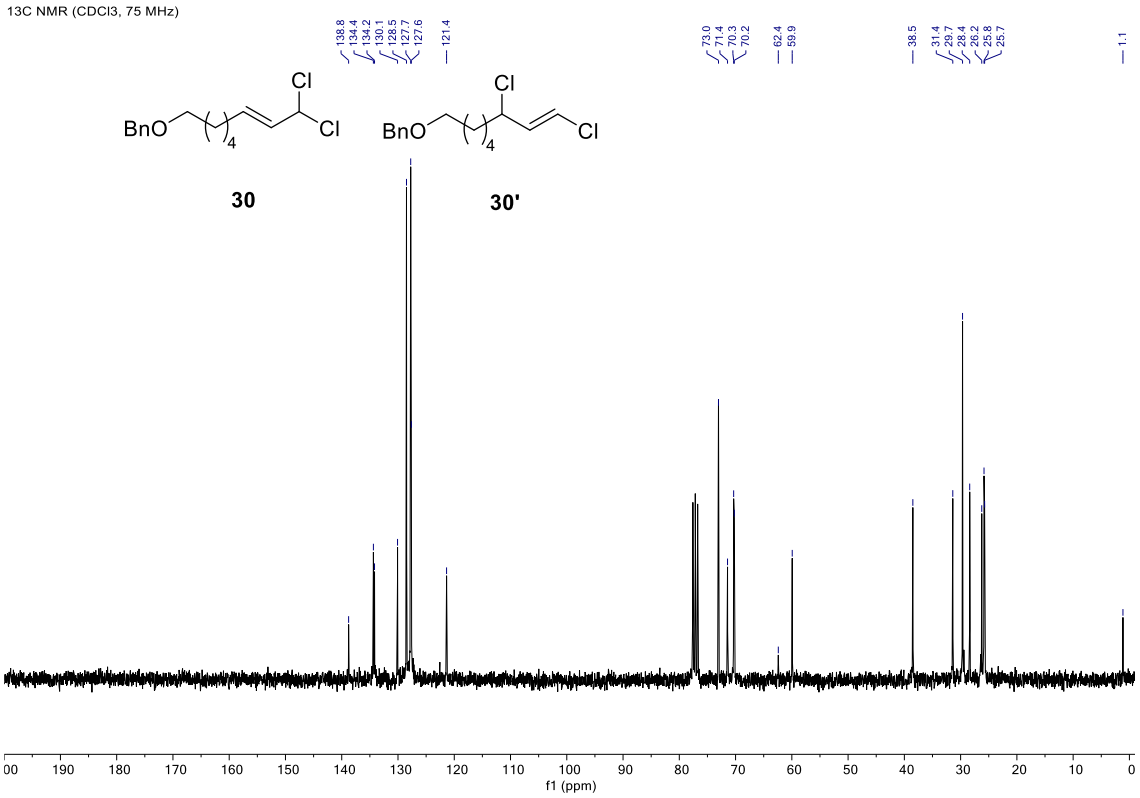
29 **29'**

13C NMR (CDCl3, 75 MHz)

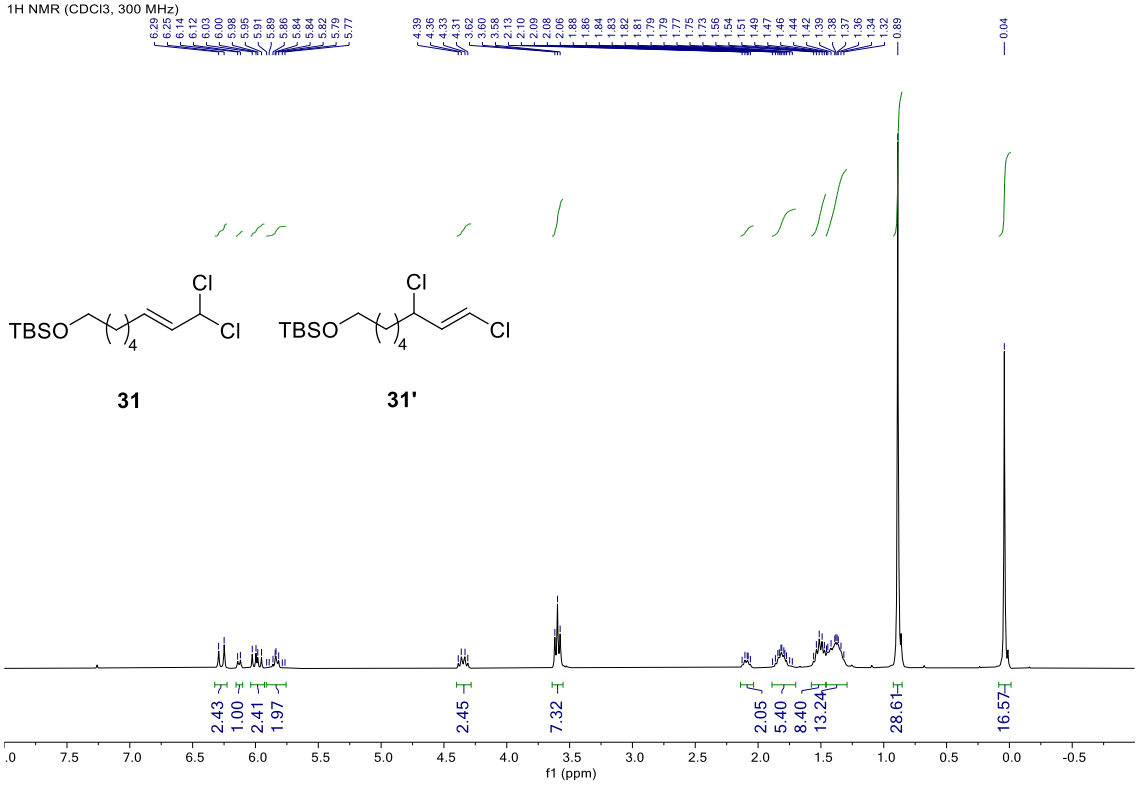


29 **29'**


1H NMR (CDCl3, 300 MHz)
7.38
7.35
7.34
7.32
7.31
7.29
7.28
6.30
6.25
6.15
6.13
6.03
6.00
5.99
5.96
5.92
5.90
5.87
5.85
5.83
5.80
5.78
4.51
4.39
4.37
4.34
4.31
3.50
3.48
3.45
2.14
2.12
2.10
2.07
1.85
1.83
1.80
1.68
1.65
1.63
1.61
1.59
1.52
1.46
1.45
1.43
1.42
1.41
BnO
Cl
Cl
4
30
30'
11.79
1.00
1.23
1.11
2.59
4.68
1.22
5.43
2.95
3.24
6.46
12.18
f1 (ppm)


13C NMR (CDCl3, 75 MHz)
138.8
134.4
134.2
130.1
129.5
127.7
127.6
121.4
73.0
71.4
70.3
70.2
62.4
59.9
38.5
31.4
29.7
28.4
26.2
25.8
25.7
1.1
BnO
Cl
Cl
4
30
30'
f1 (ppm)

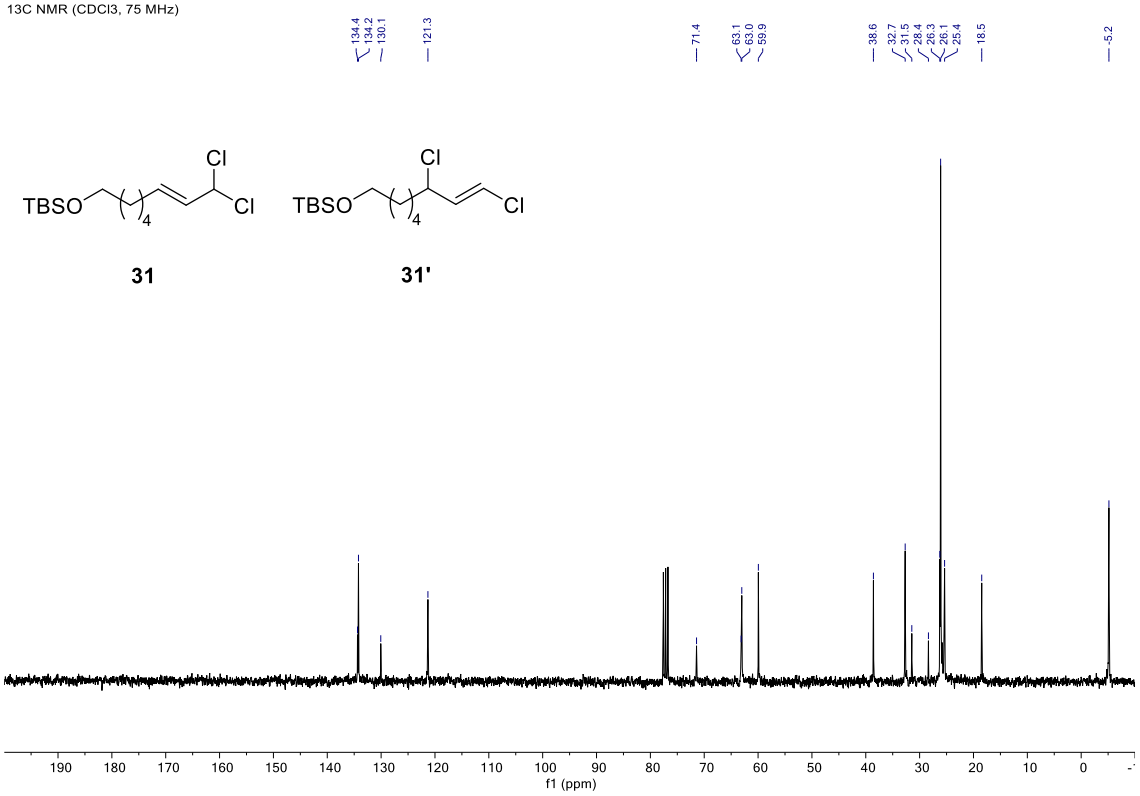
1H NMR (CDCl3, 300 MHz)



31

31'

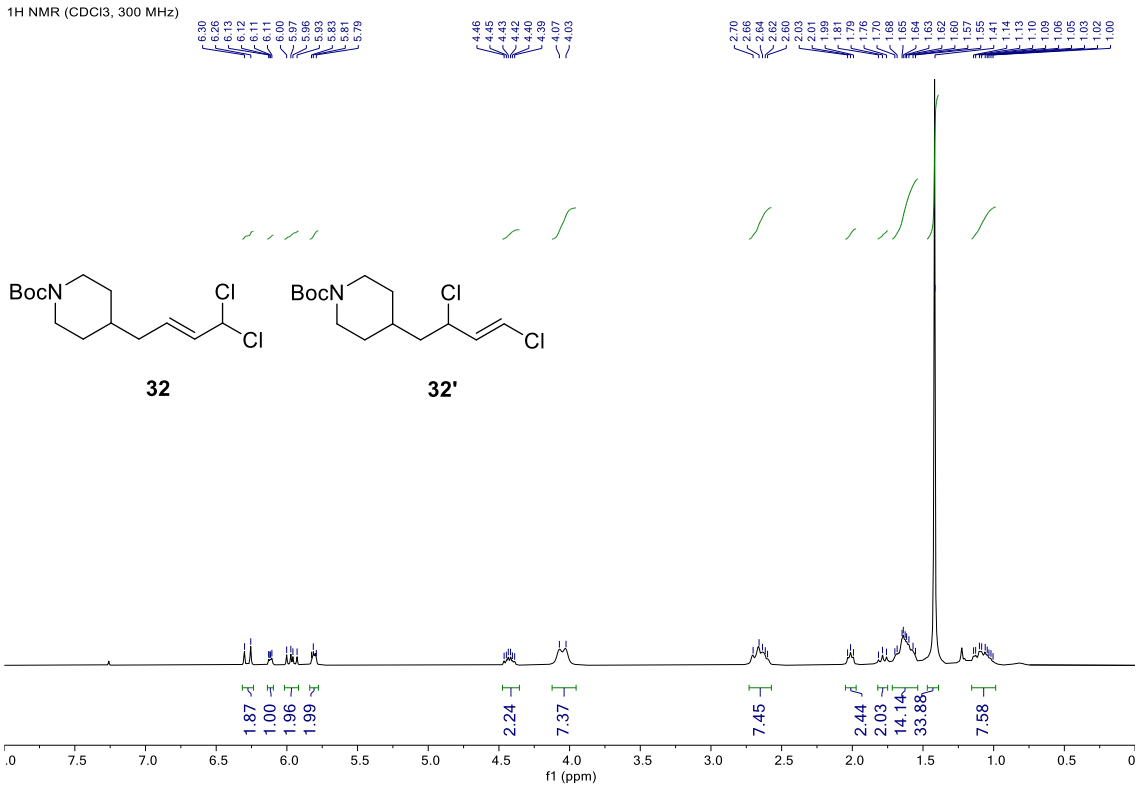
13C NMR (CDCl3, 75 MHz)



31

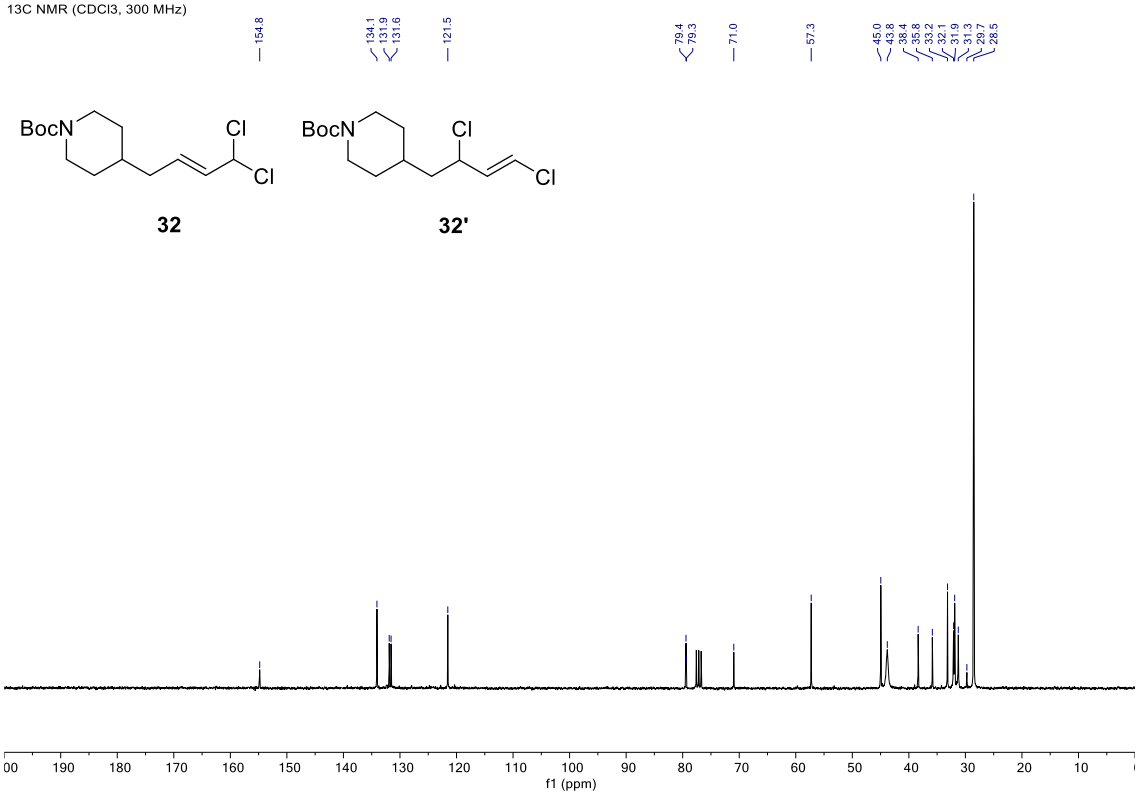
31'

1H NMR (CDCl3, 300 MHz)



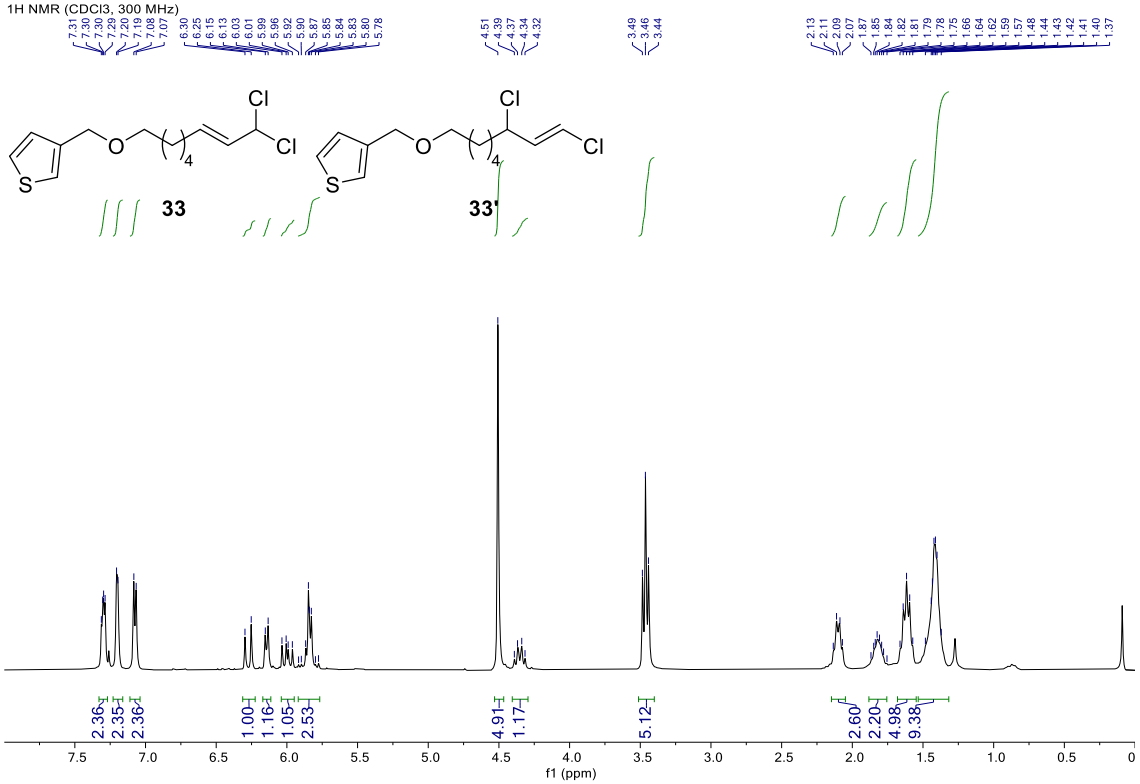
32 **32'**

13C NMR (CDCl3, 300 MHz)

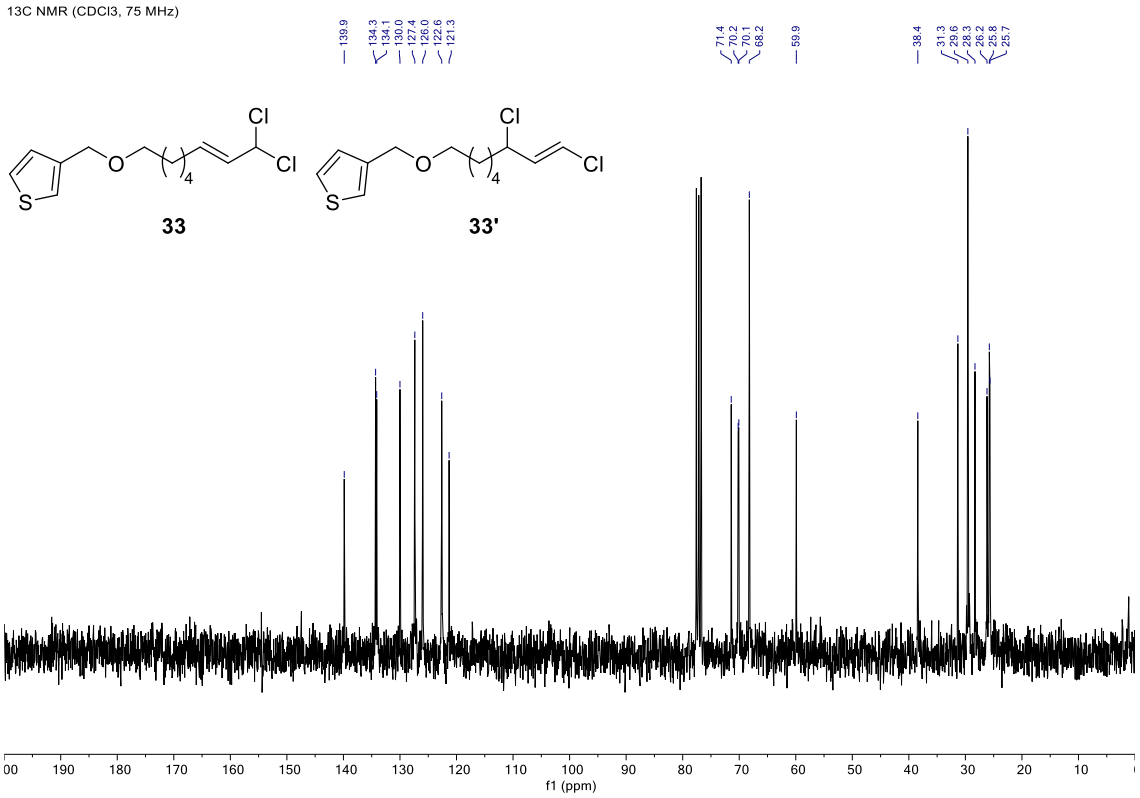


32 **32'**

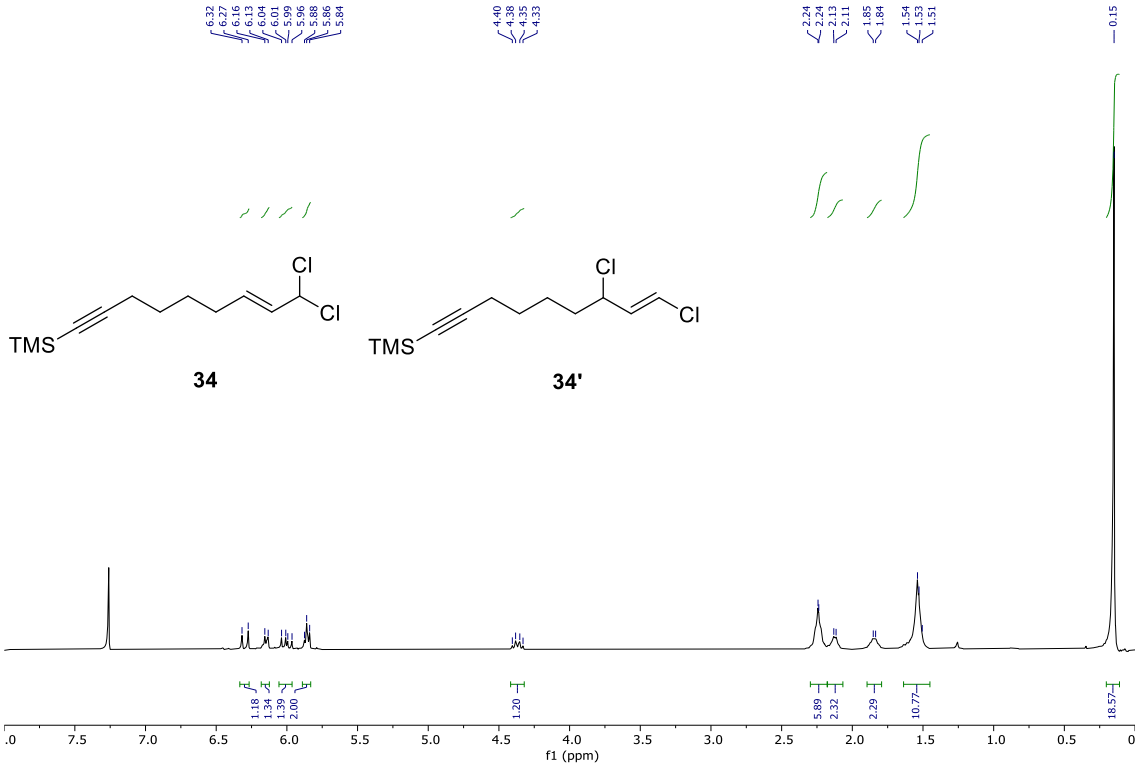
1H NMR (CDCl3, 300 MHz)



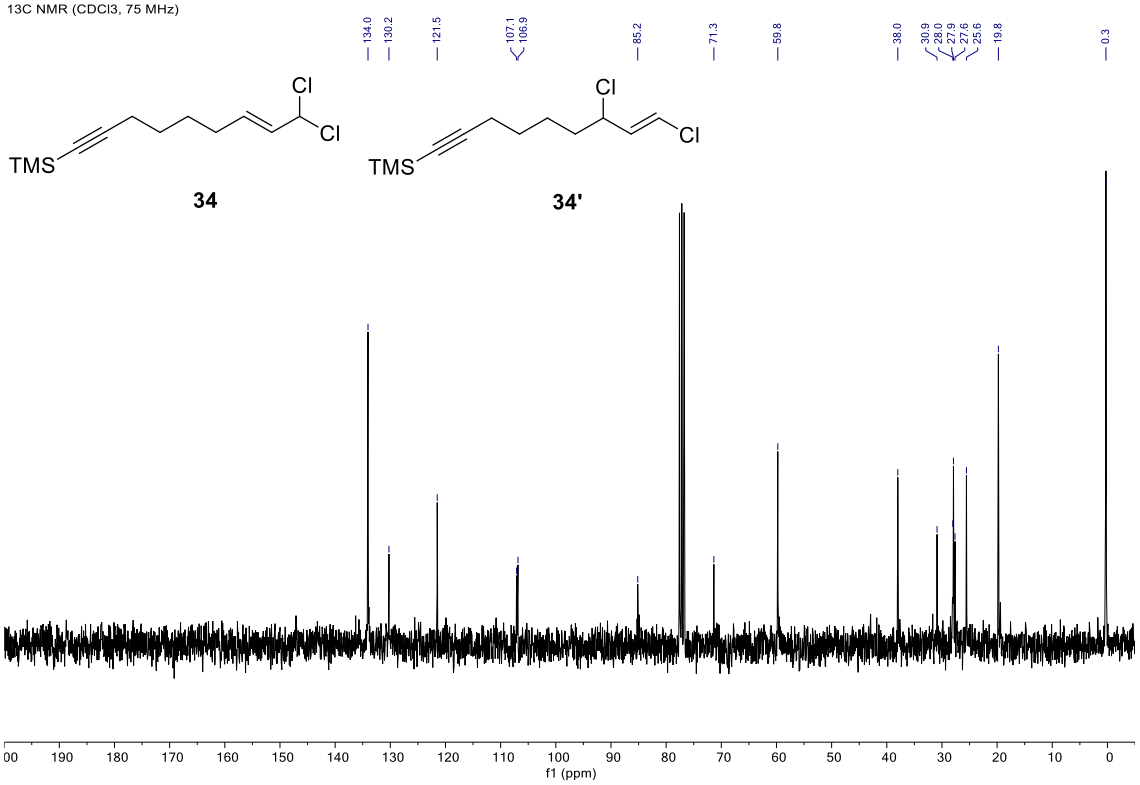
13C NMR (CDCl3, 75 MHz)



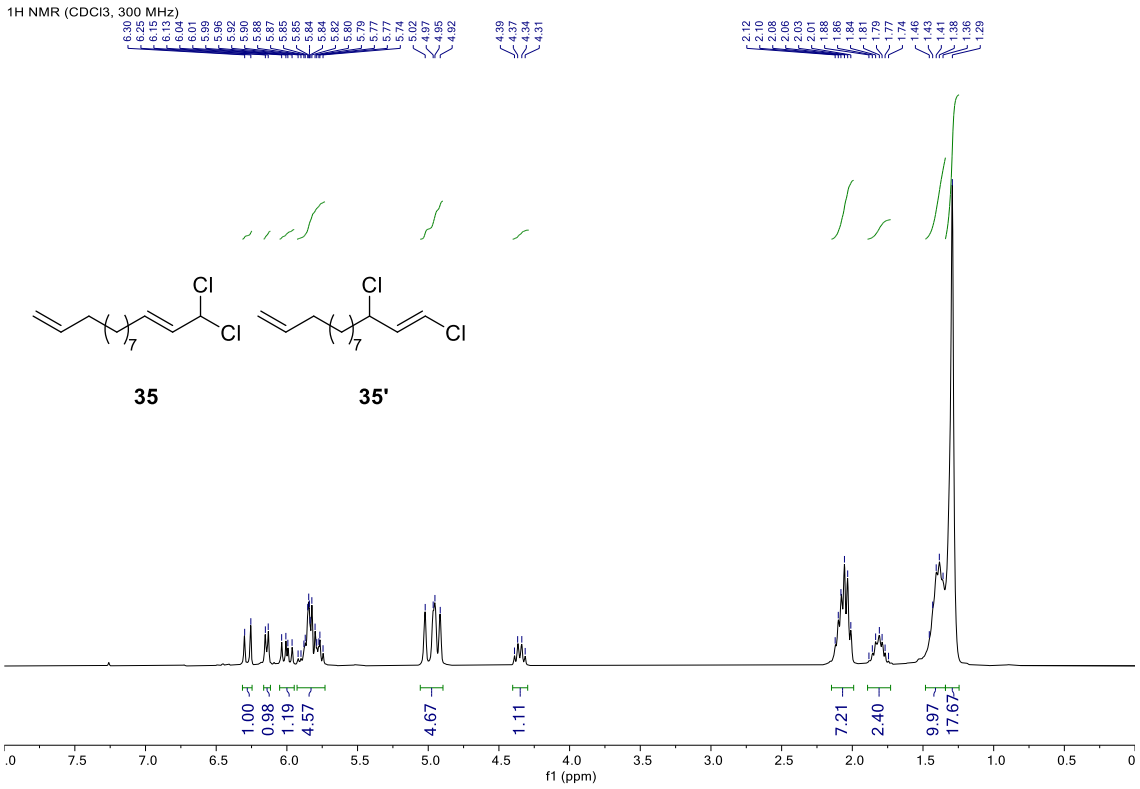
1H NMR (CDCl3, 300 MHz)



13C NMR (CDCl3, 75 MHz)

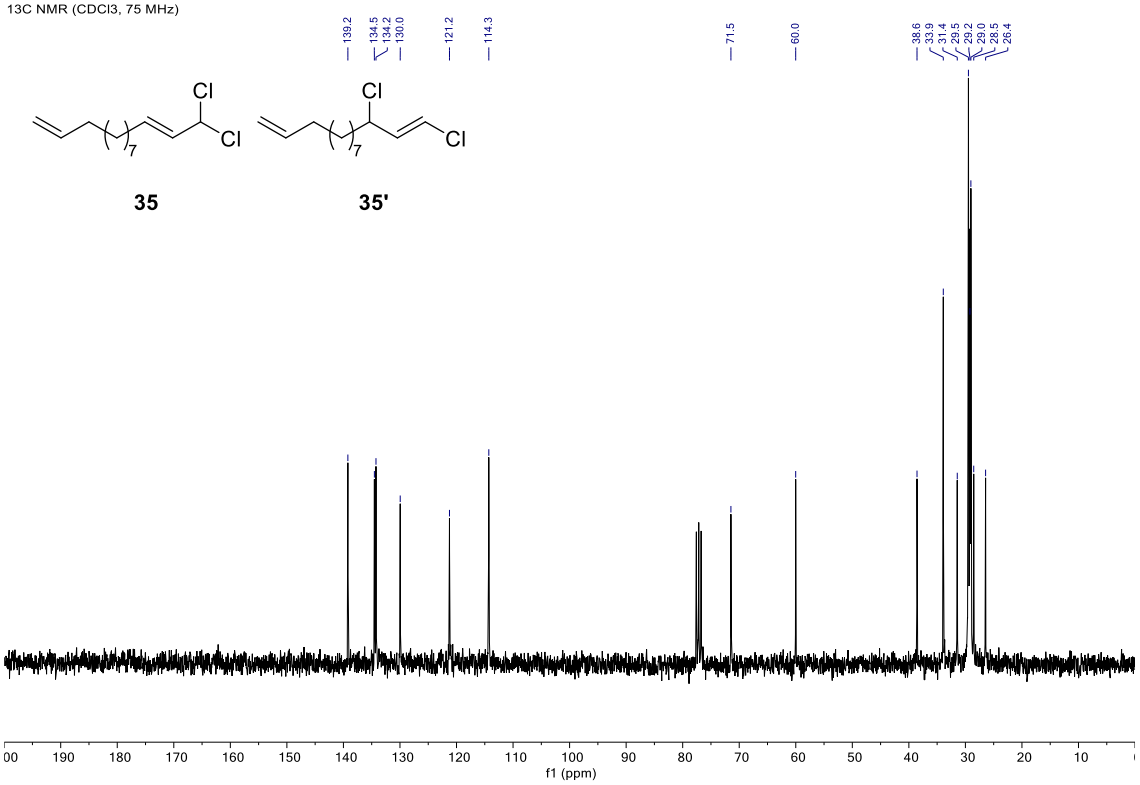


1H NMR (CDCl3, 300 MHz)



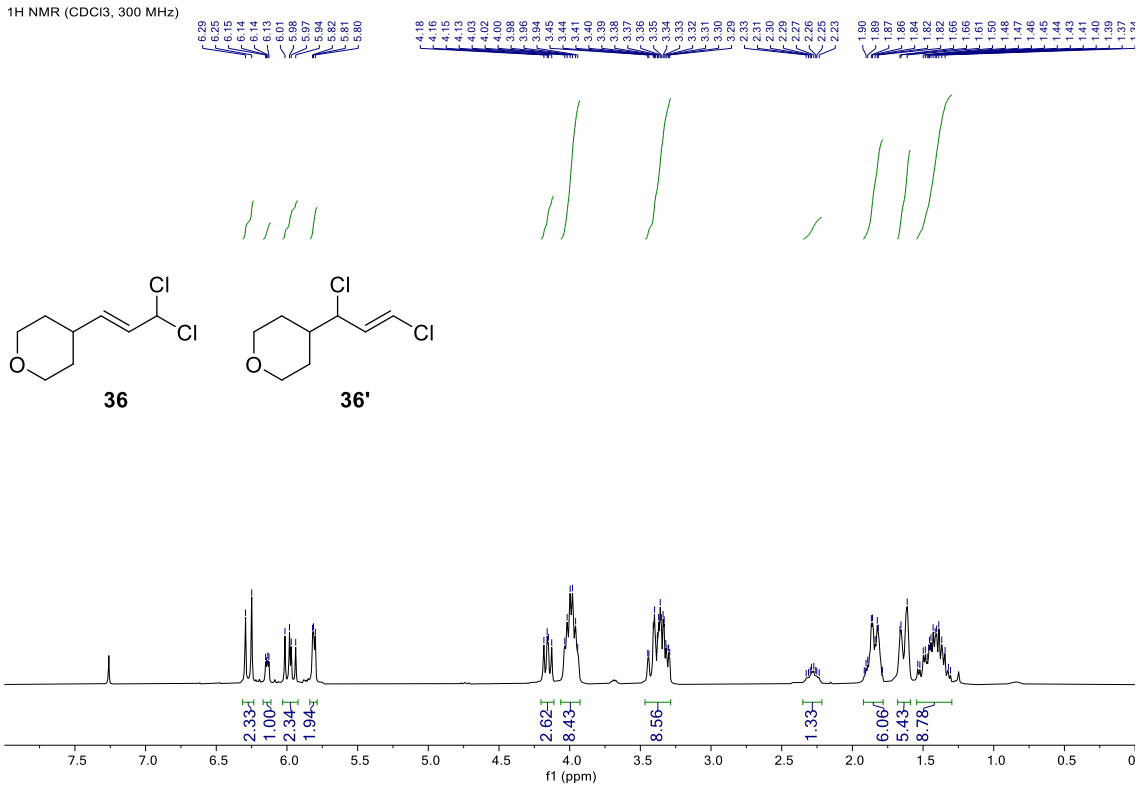
35 **35'**

13C NMR (CDCl3, 75 MHz)

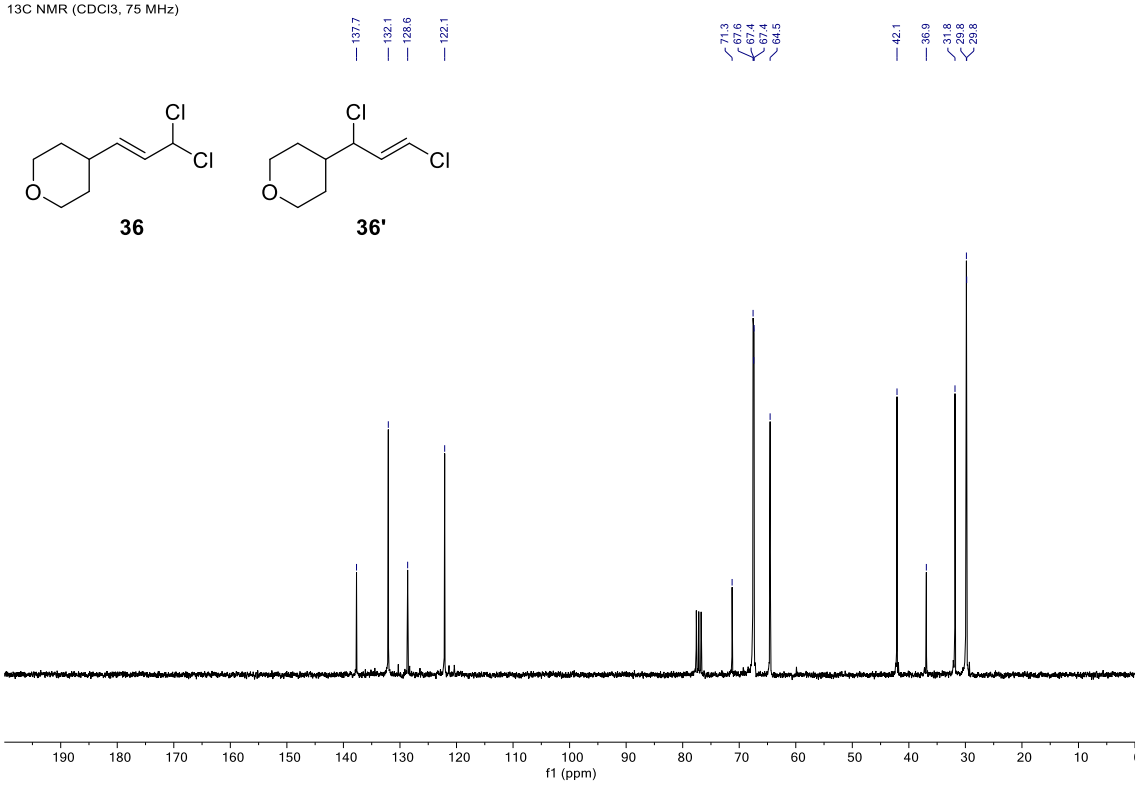


35 **35'**

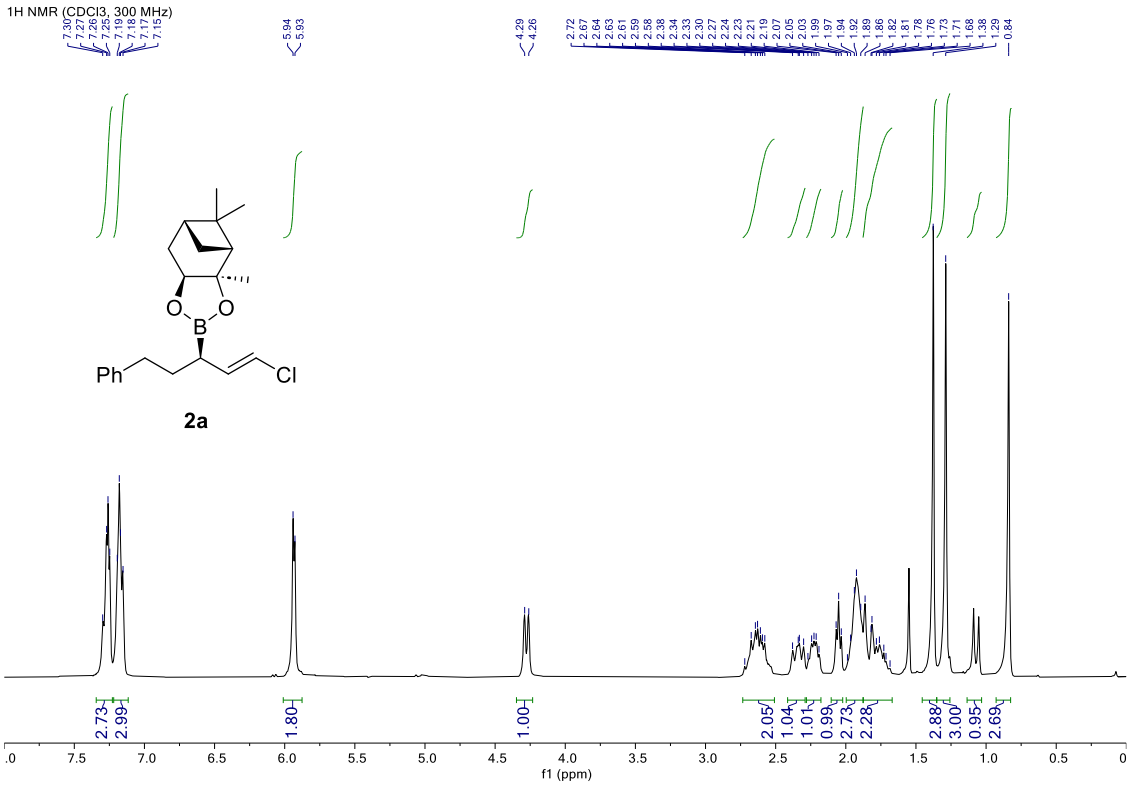
1H NMR (CDCl3, 300 MHz)

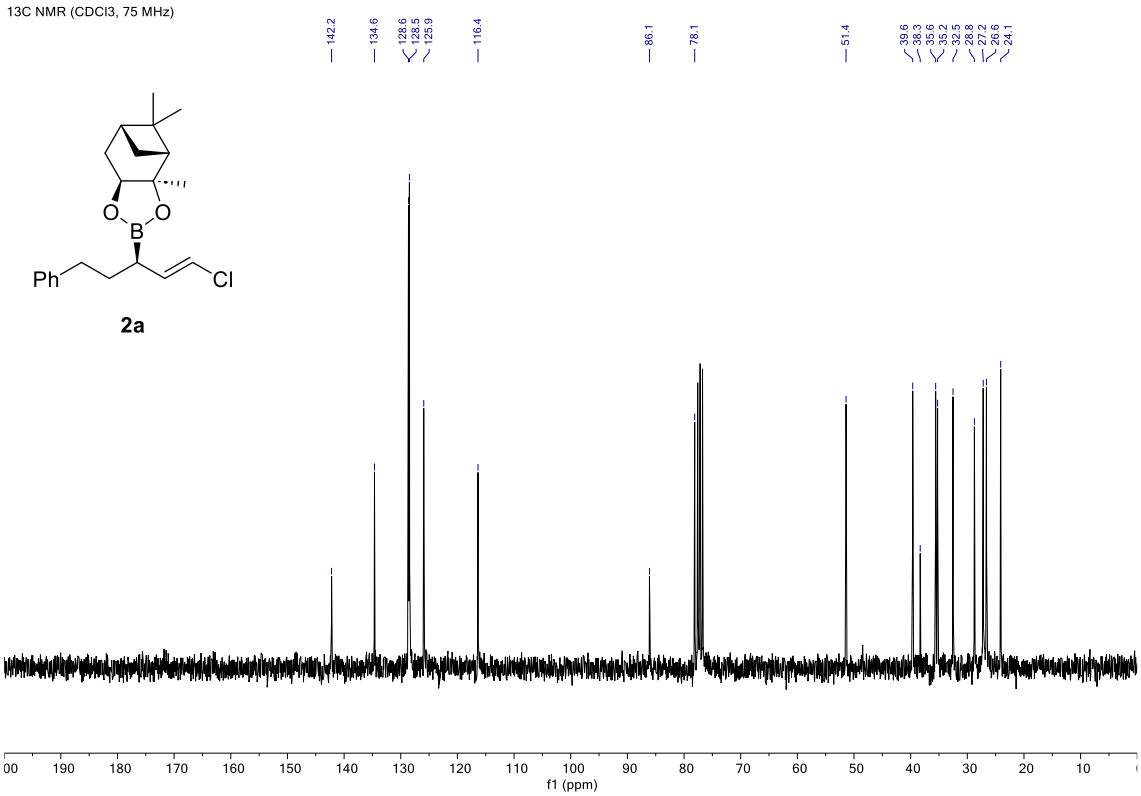


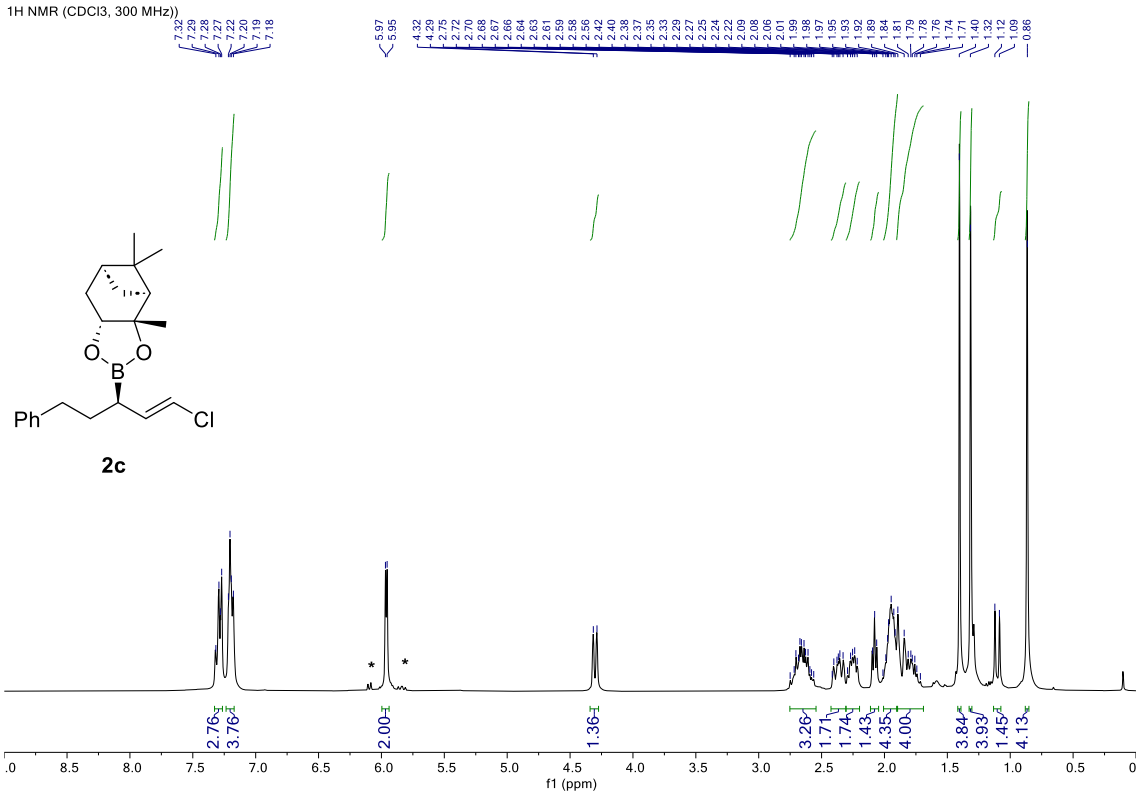
13C NMR (CDCl3, 75 MHz)



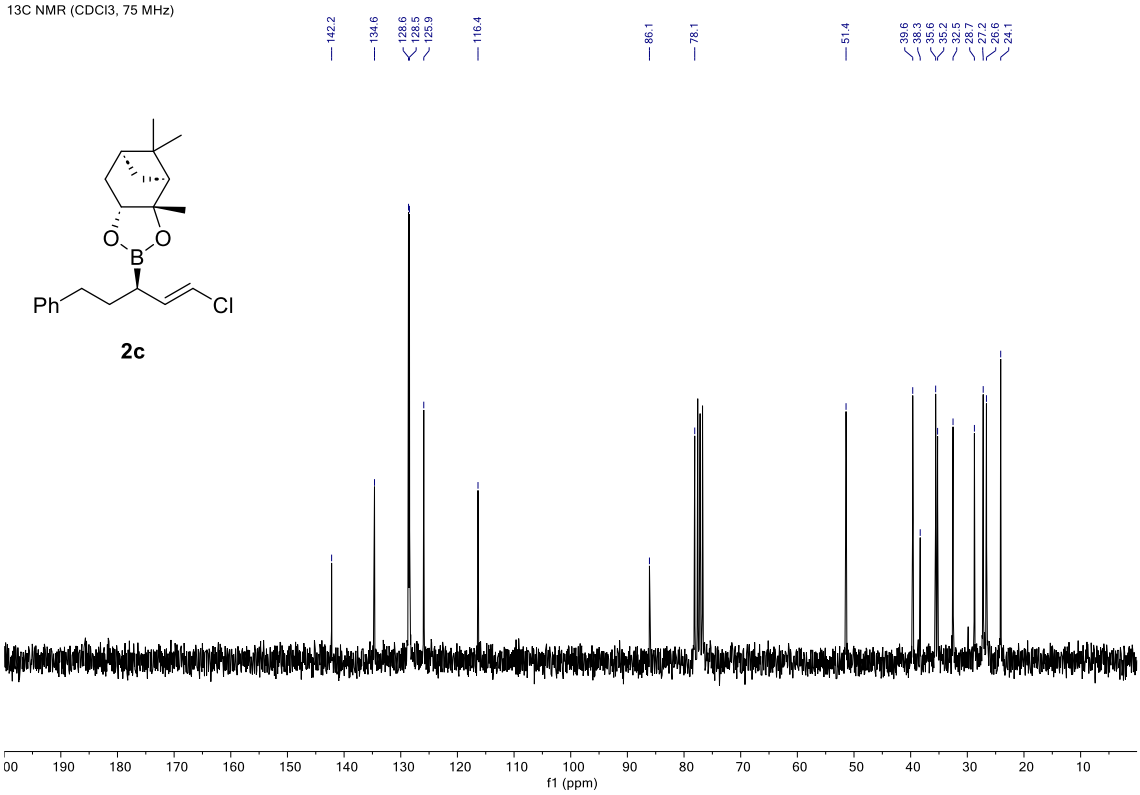
15. NMR spectra for the borylation products



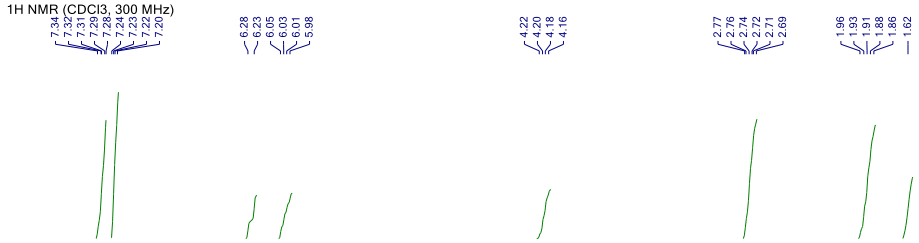


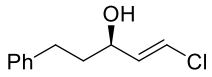


*The signals that correspond to the *Z*-isomer.

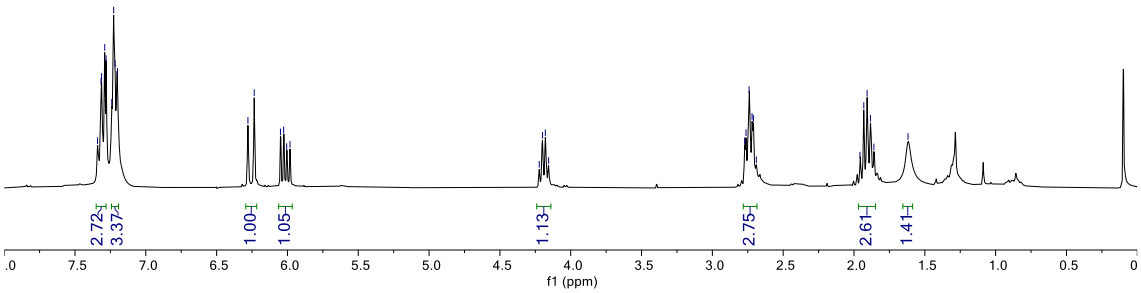


1H NMR (CDCl3, 300 MHz)

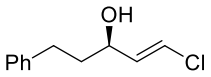




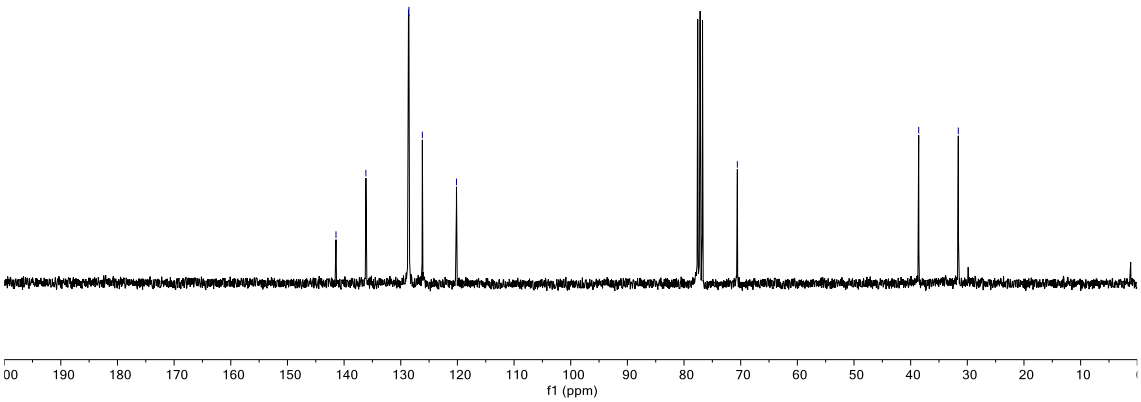
3



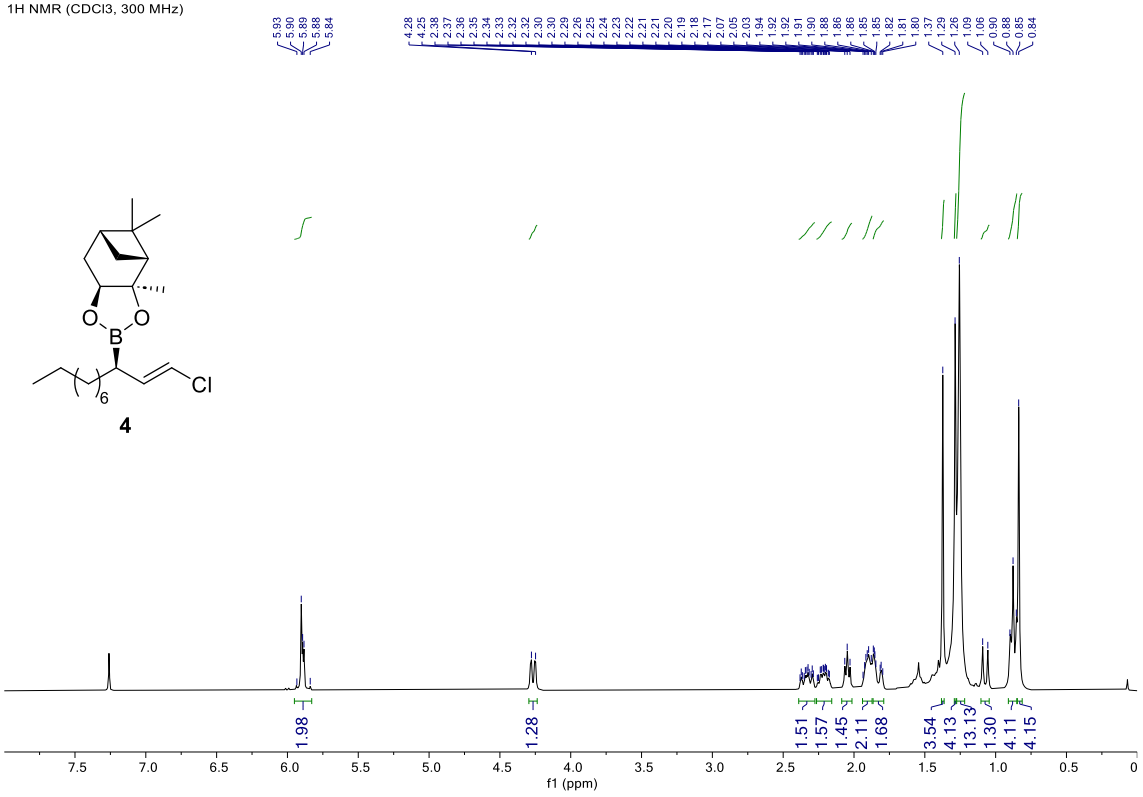
13C NMR (CDCl3, 75 MHz)



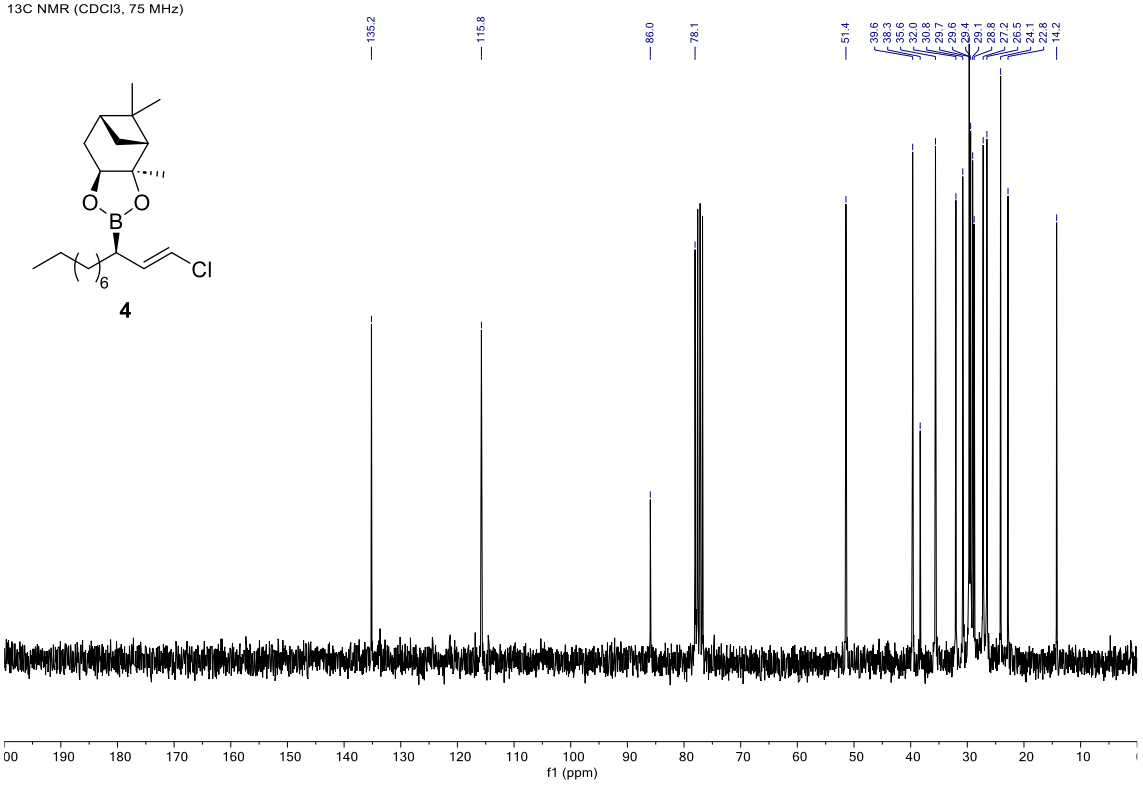
3



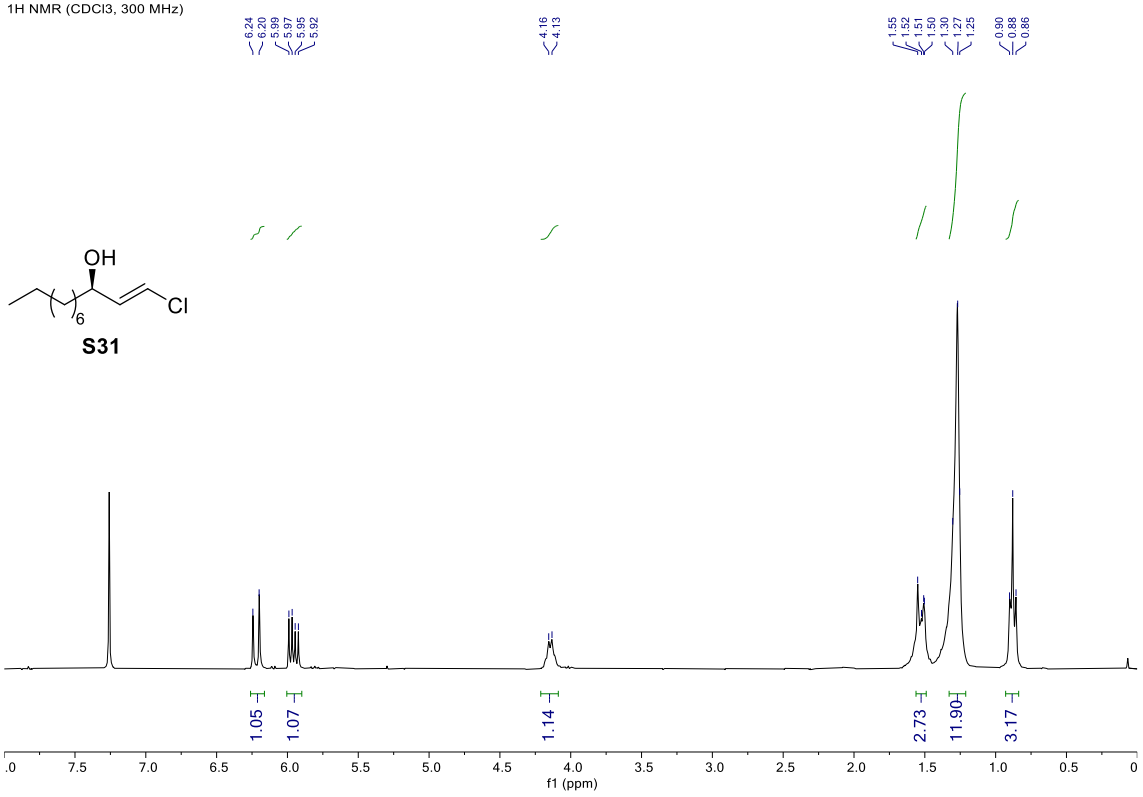
1H NMR (CDCl3, 300 MHz)



13C NMR (CDCl3, 75 MHz)

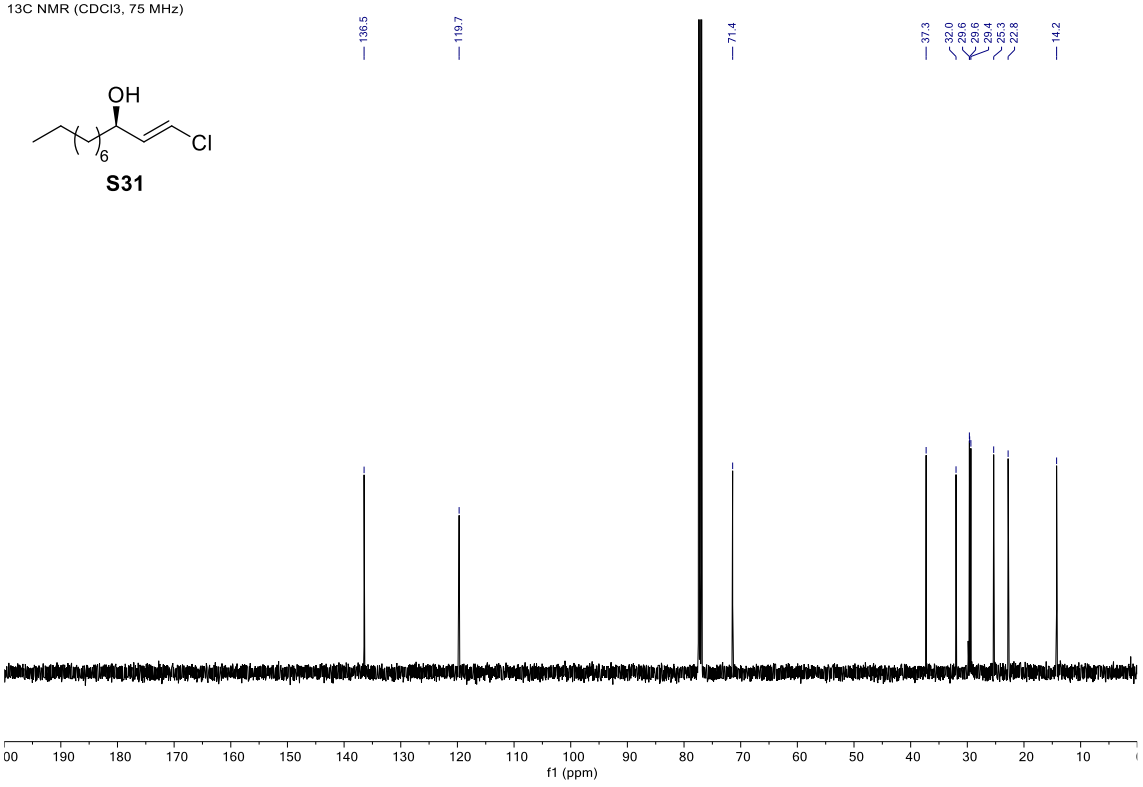


1H NMR (CDCl3, 300 MHz)



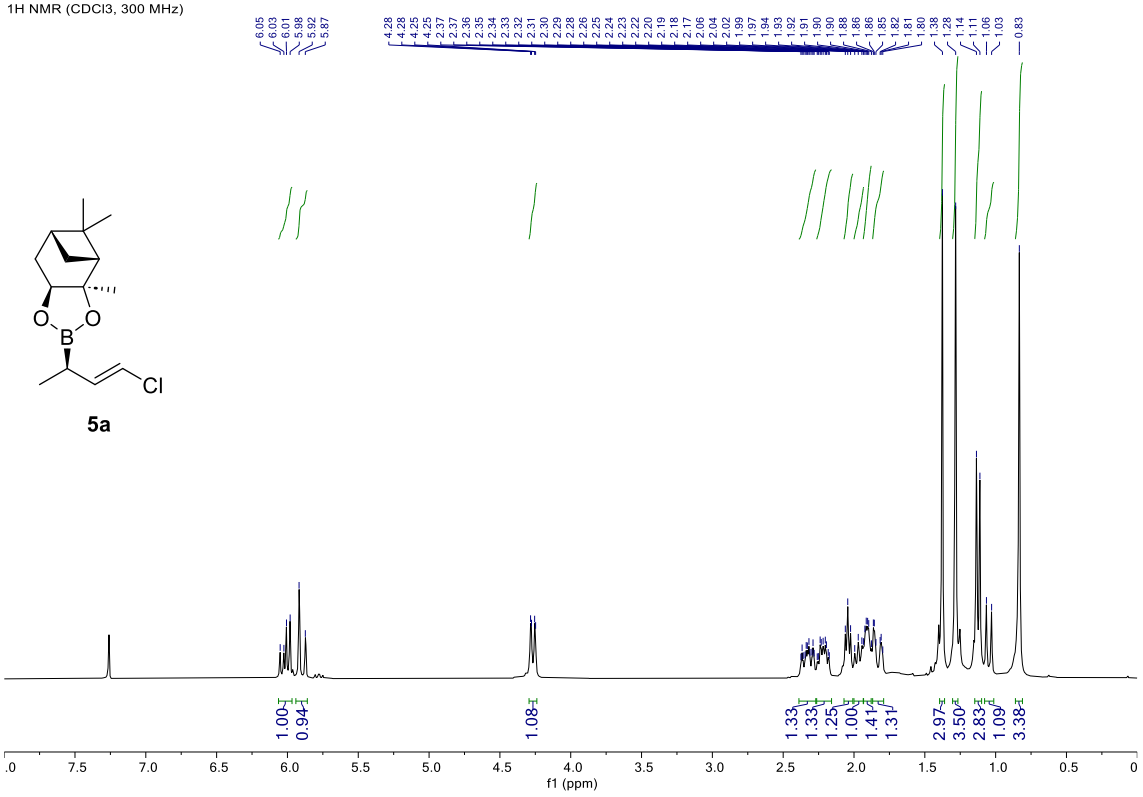
S31

13C NMR (CDCl3, 75 MHz)



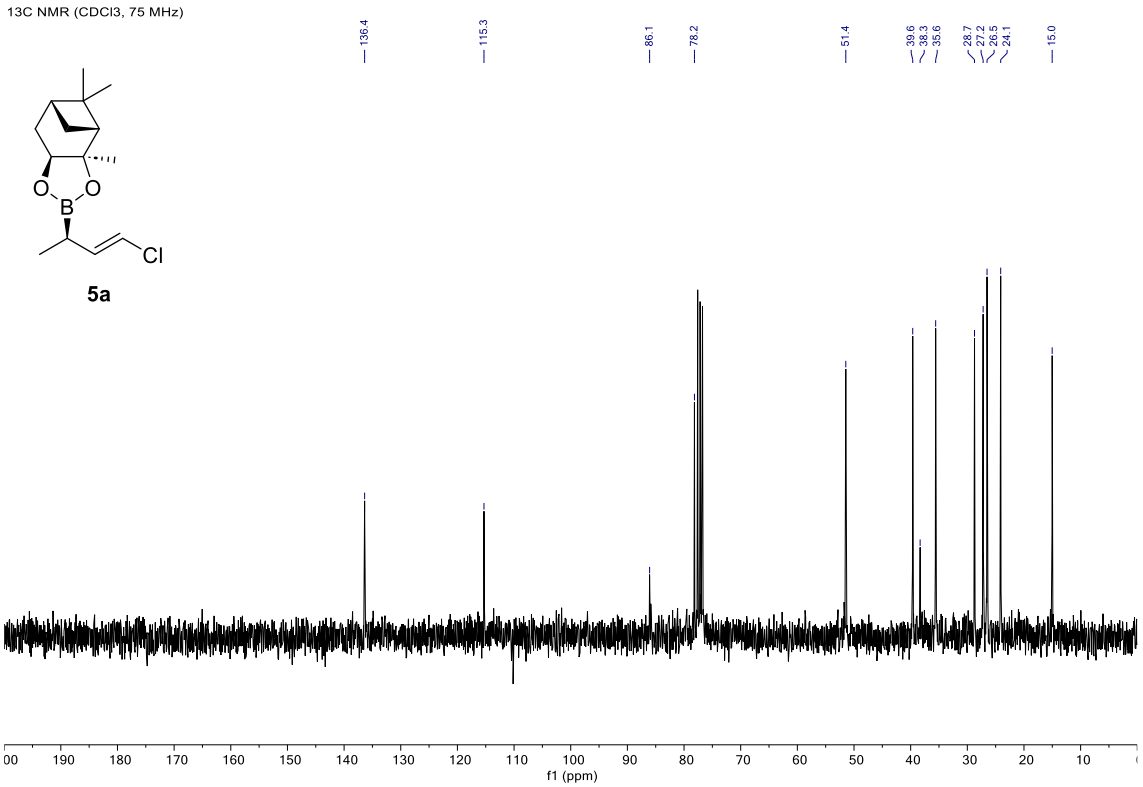
S31

1H NMR (CDCl3, 300 MHz)



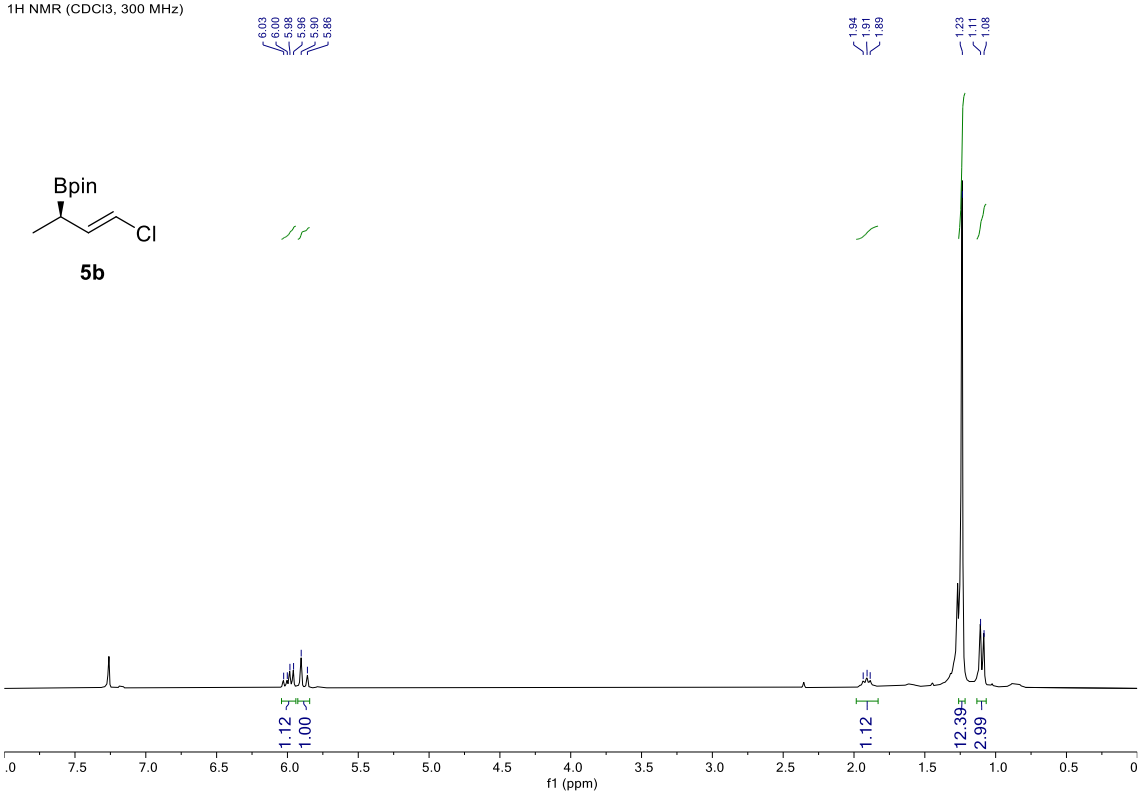
5a

13C NMR (CDCl3, 75 MHz)

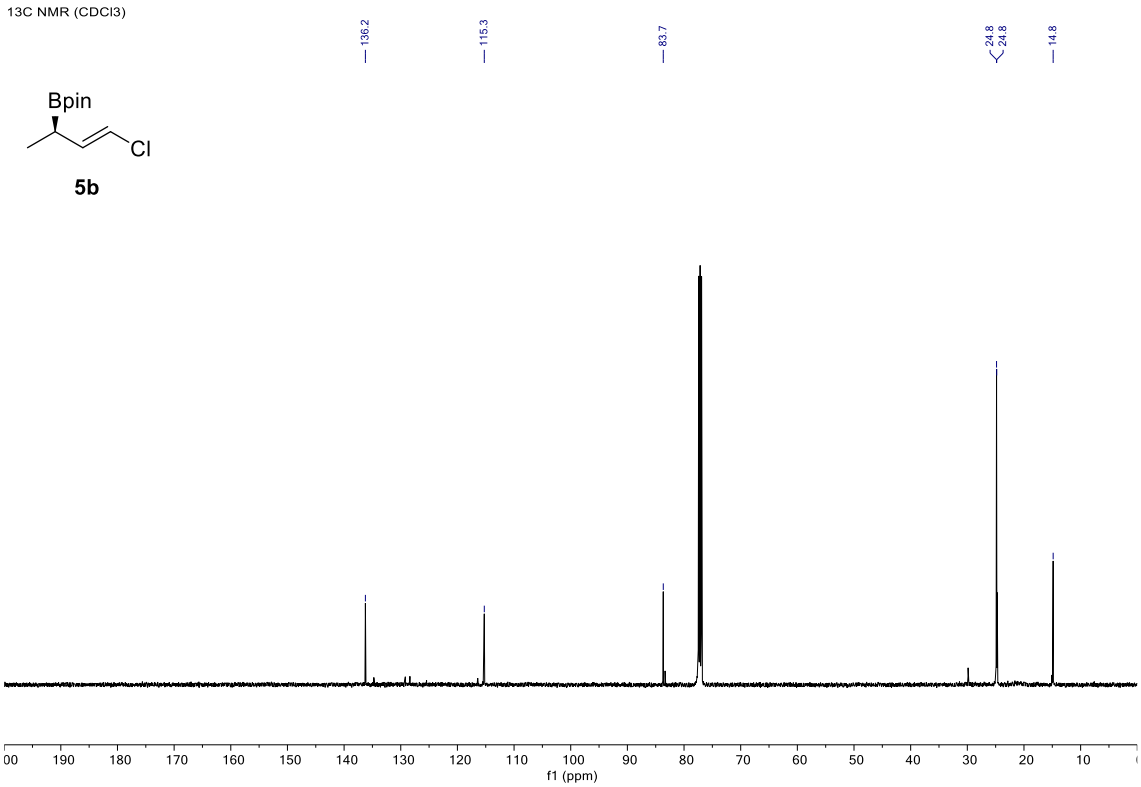


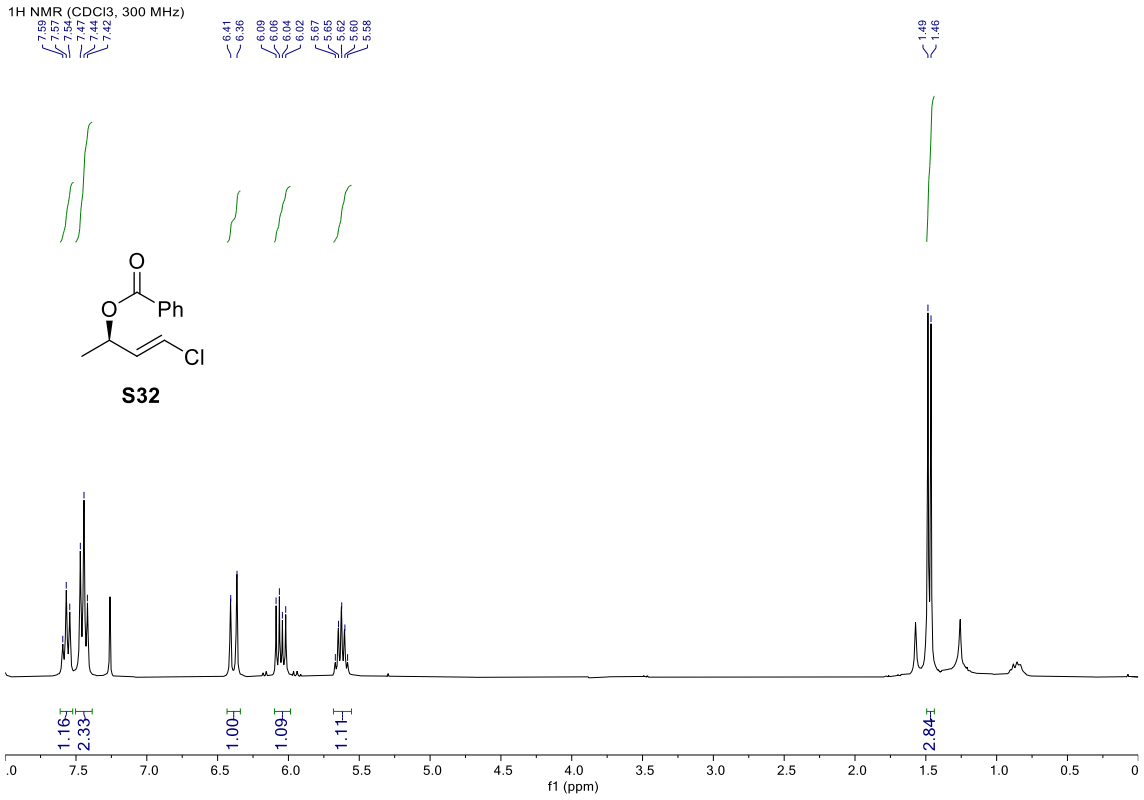
5a

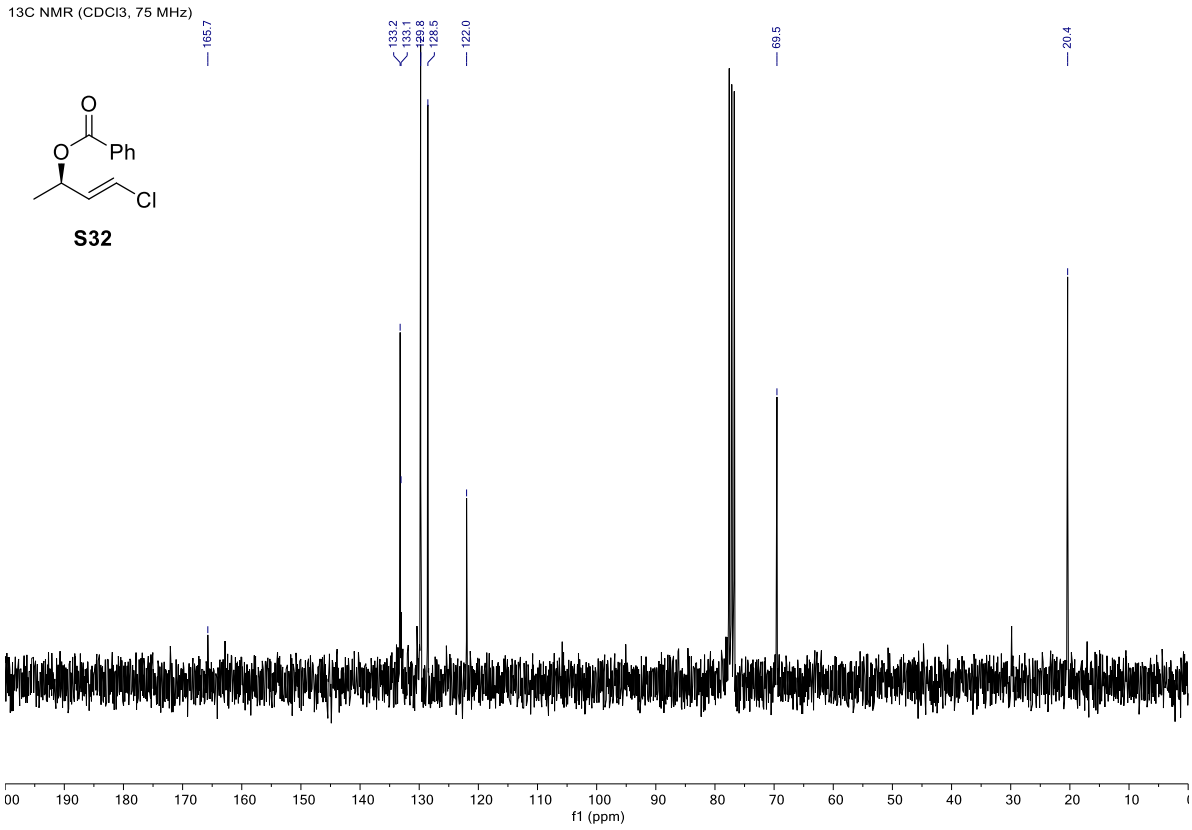
1H NMR (CDCl3, 300 MHz)



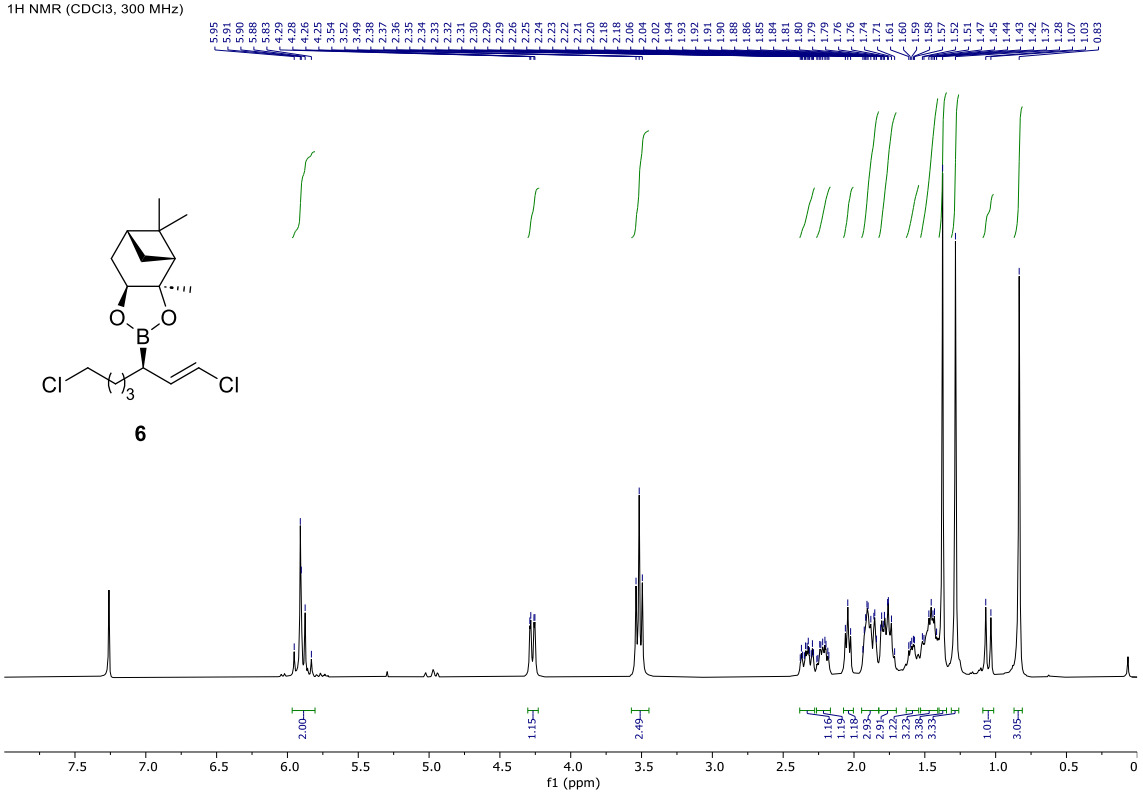
13C NMR (CDCl3)




1H NMR (CDCl3, 300 MHz)
7.59
7.57
7.54
7.47
7.44
7.42
6.41
6.36
6.09
6.06
6.04
6.02
5.67
5.65
5.62
5.60
5.58
1.49
1.46
O
O
Ph
Cl
S32
1.16
2.33
1.00
1.09
1.11
2.84
f1 (ppm)

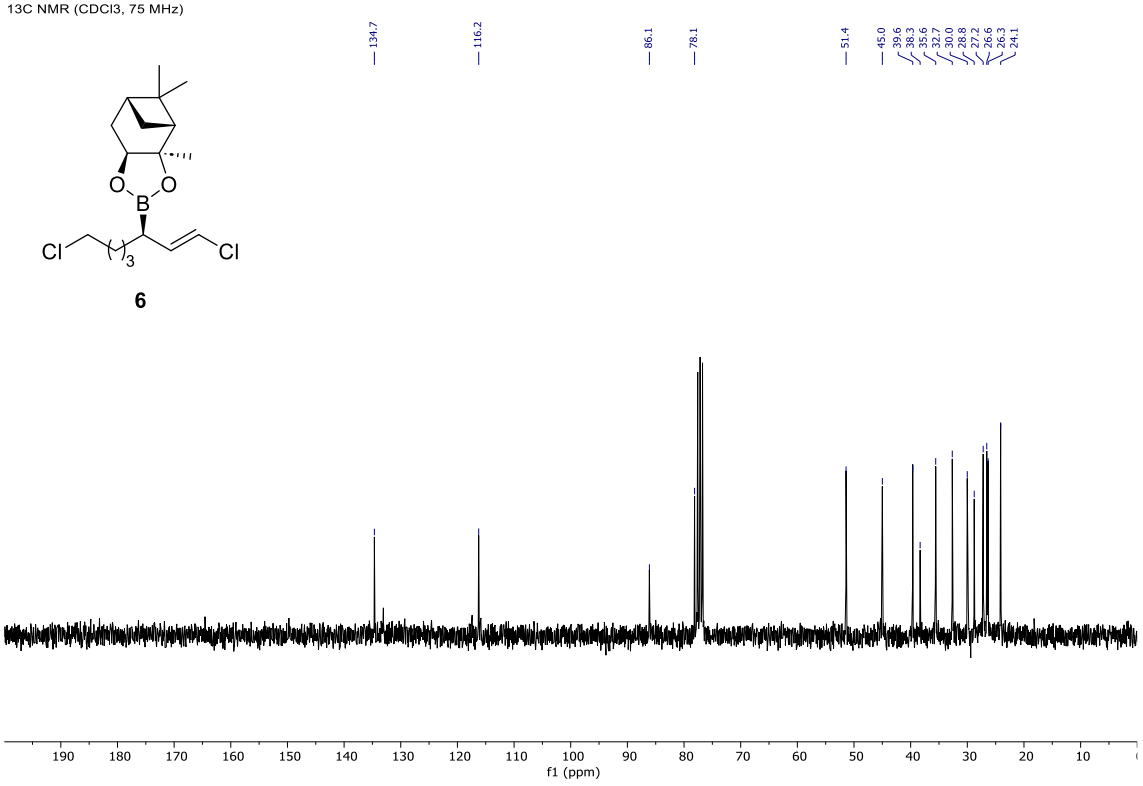

13C NMR (CDCl3, 75 MHz)
165.7
133.2
133.1
129.8
128.5
122.0
69.5
20.4
O
O
Ph
Cl
S32
f1 (ppm)

1H NMR (CDCl3, 300 MHz)



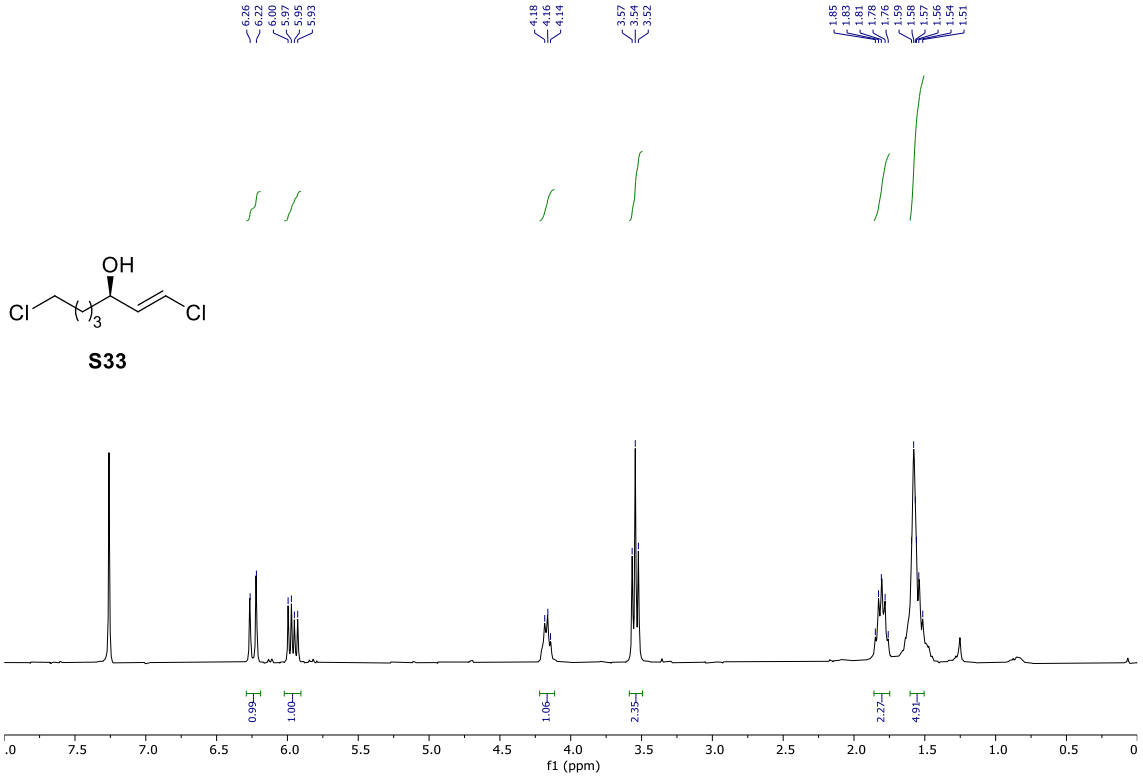
6

13C NMR (CDCl3, 75 MHz)



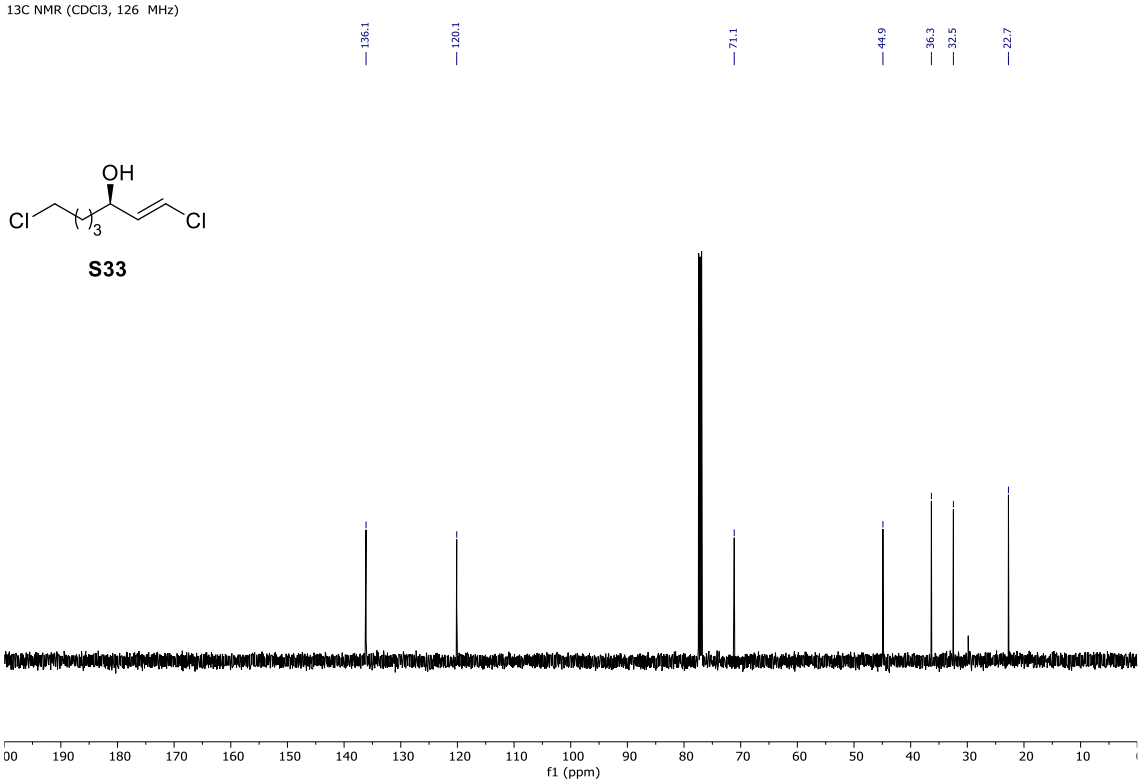
6

1H NMR (CDCl3, 300 MHz)

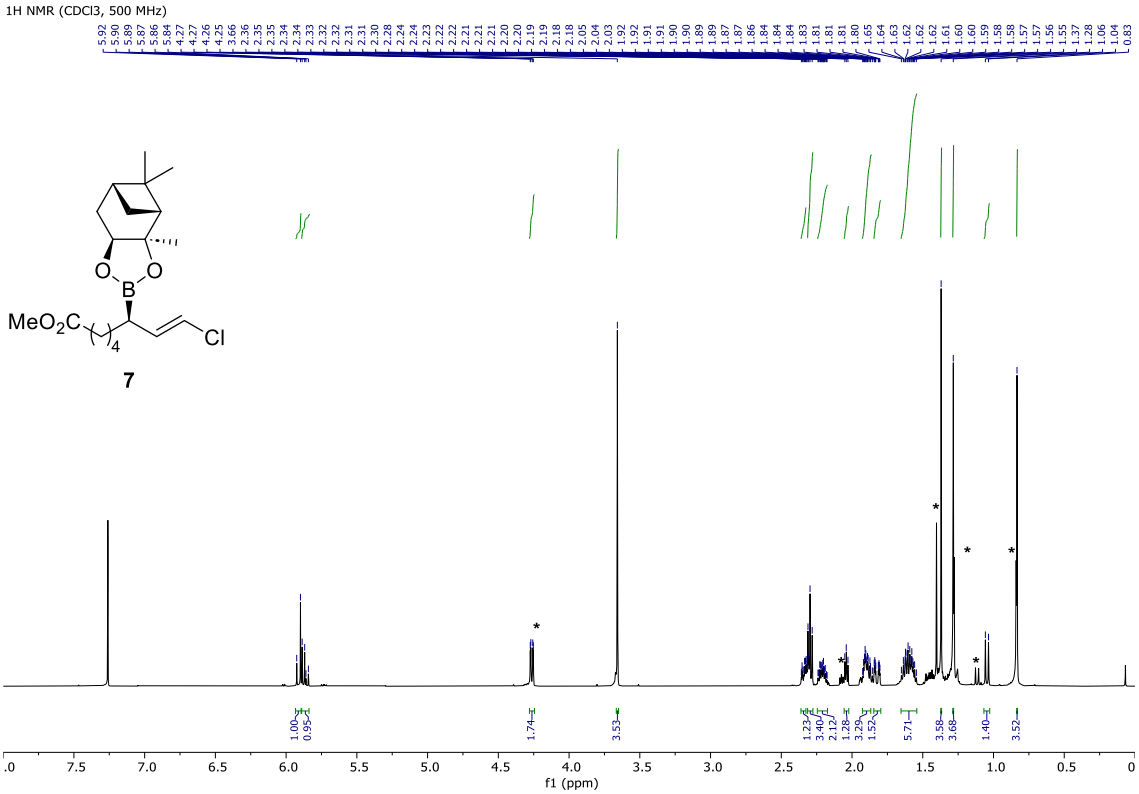


S33

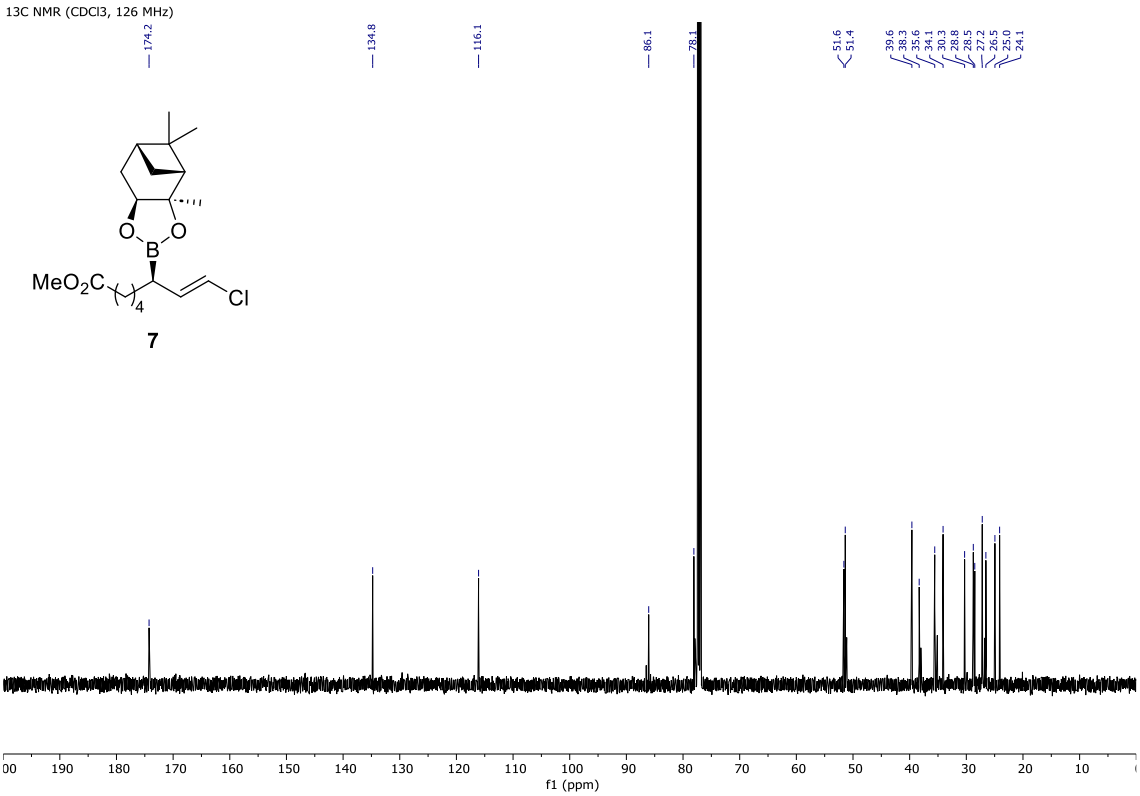
13C NMR (CDCl3, 126 MHz)



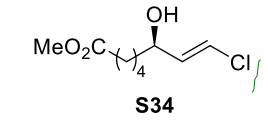
S33



* These signals belong (+)-Bpai impurity.

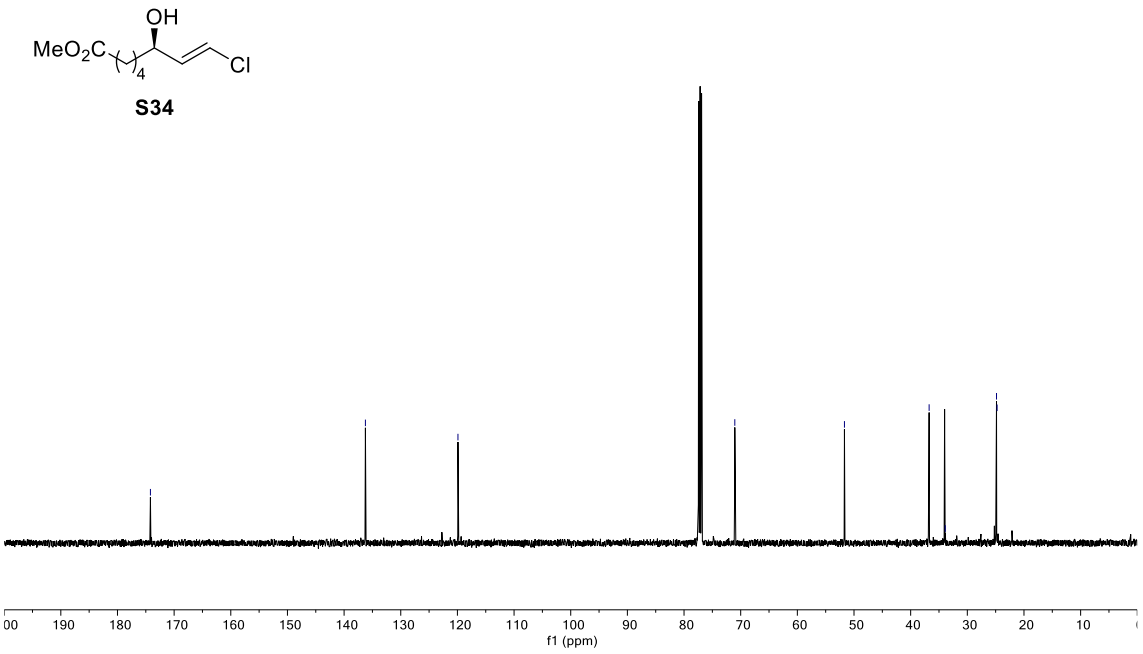


1H NMR (CDCl3, 500 MHz)

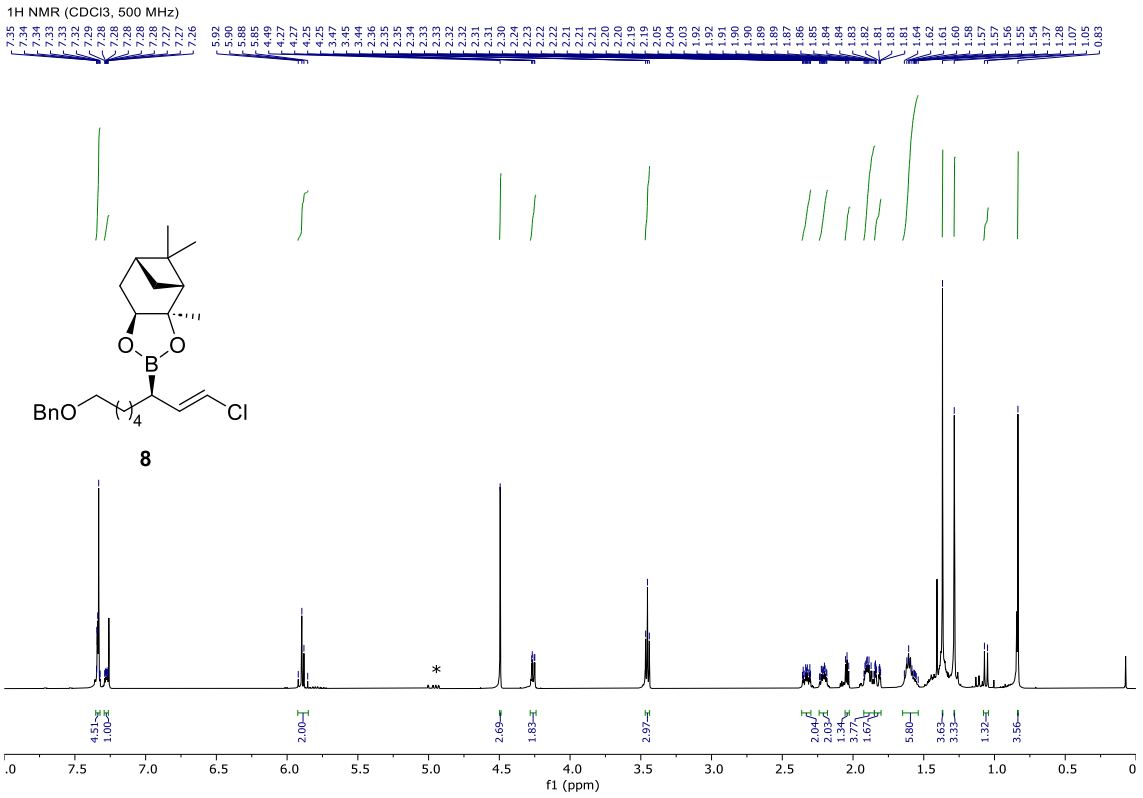


S34

13C NMR (CDCl3, 126 MHz)

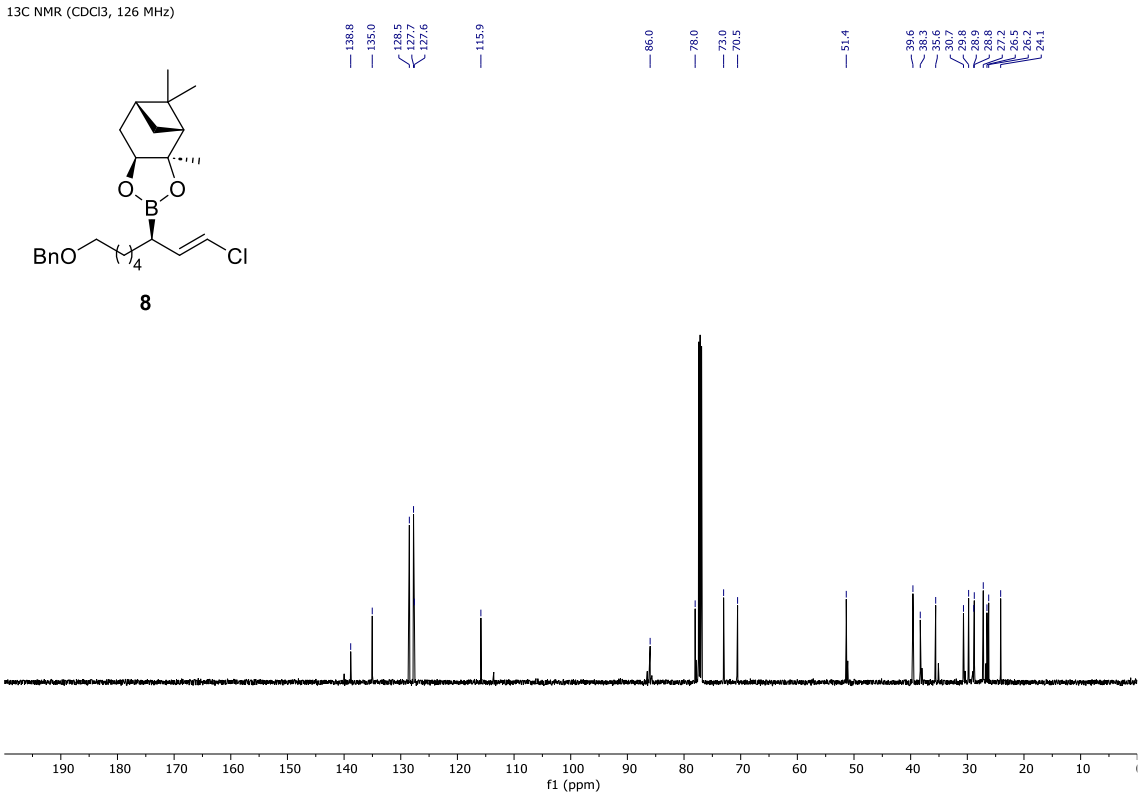


1H NMR (CDCl3, 500 MHz)

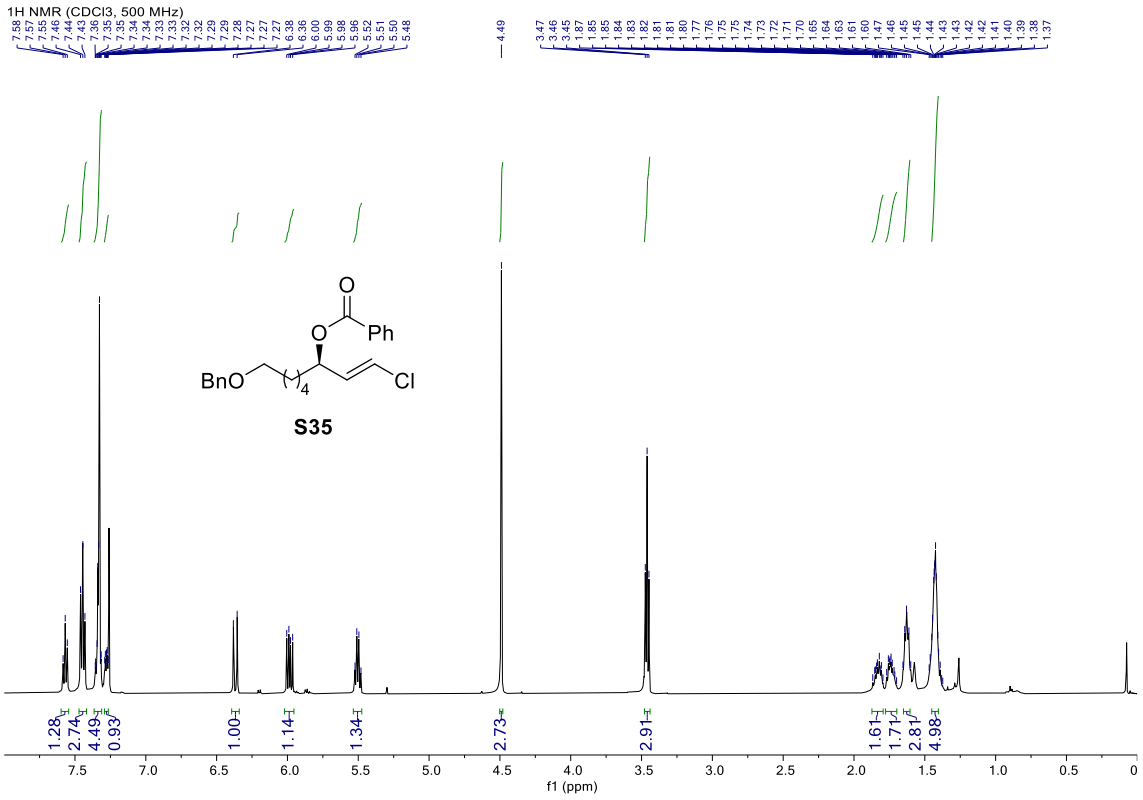


*These signals belong to the dechlorinated product.

13C NMR (CDCl3, 126 MHz)

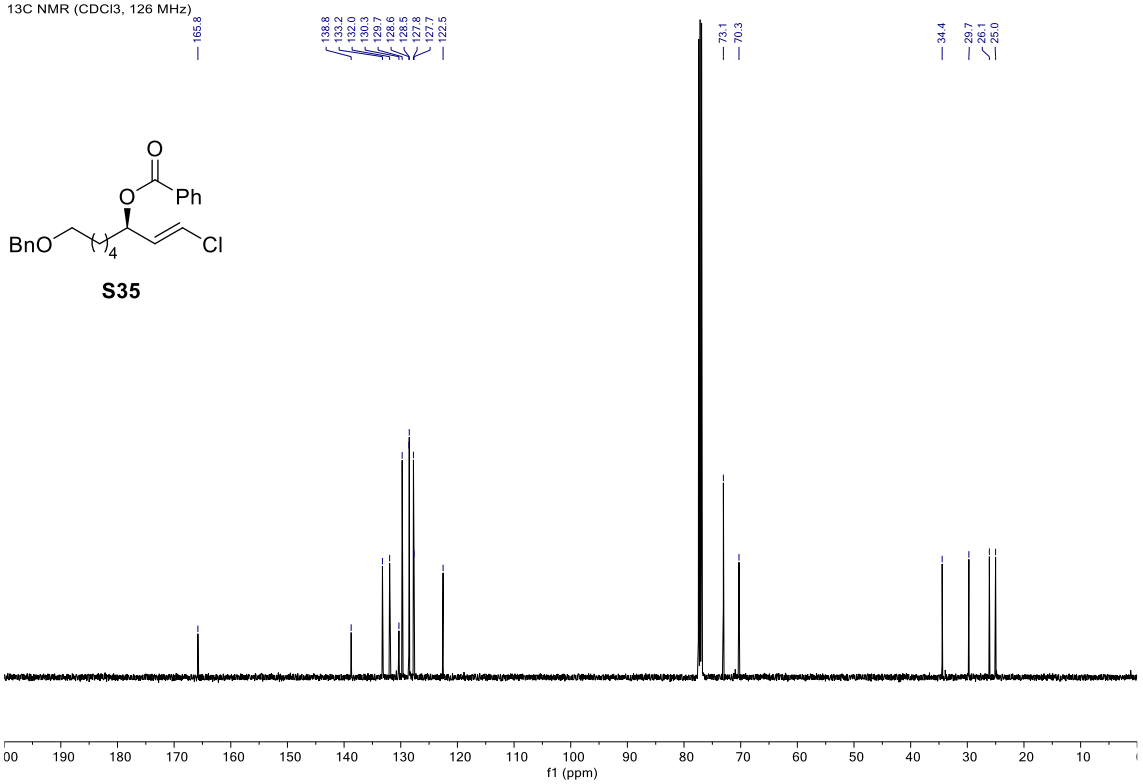


1H NMR (CDCl3, 500 MHz)



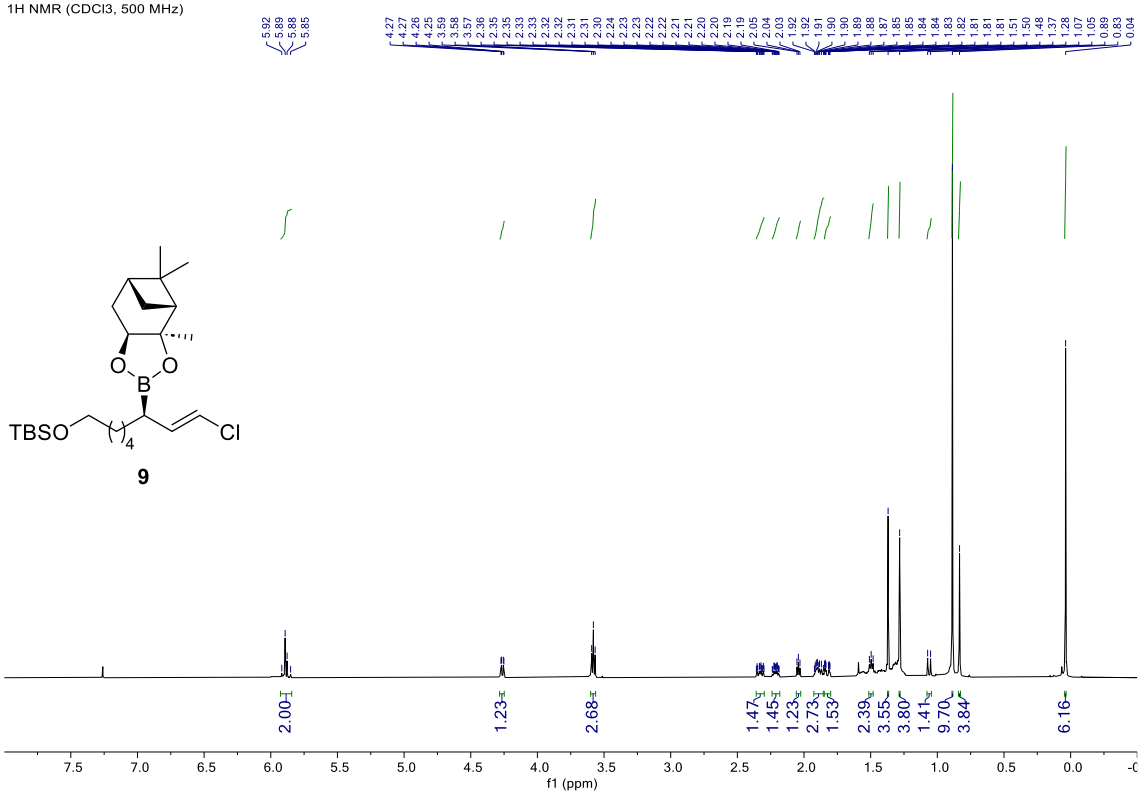
S35

13C NMR (CDCl3, 126 MHz)

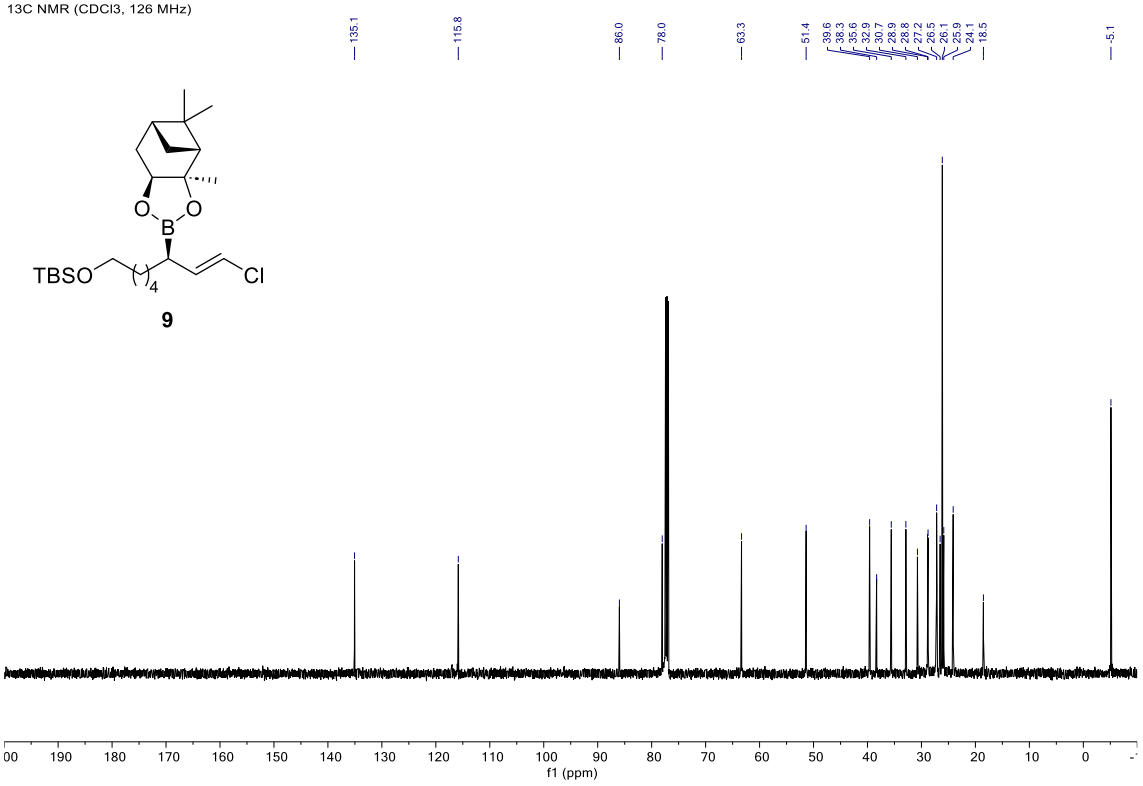


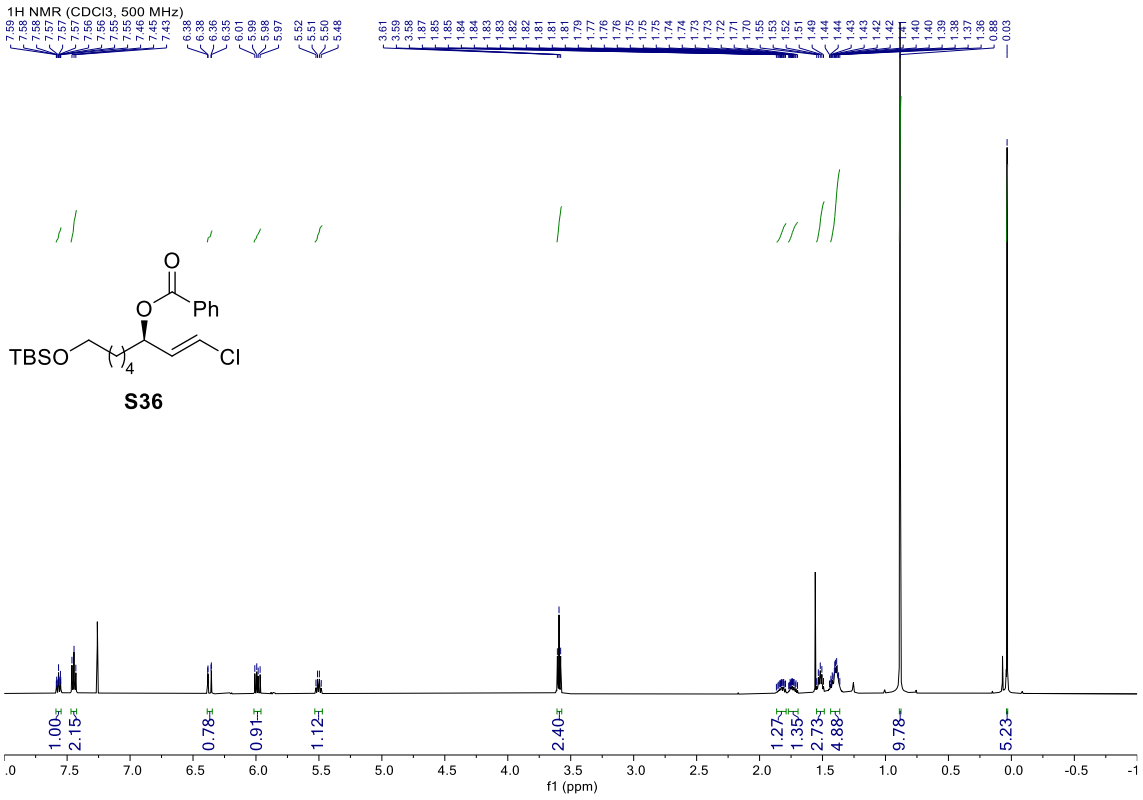
S35

1H NMR (CDCl3, 500 MHz)

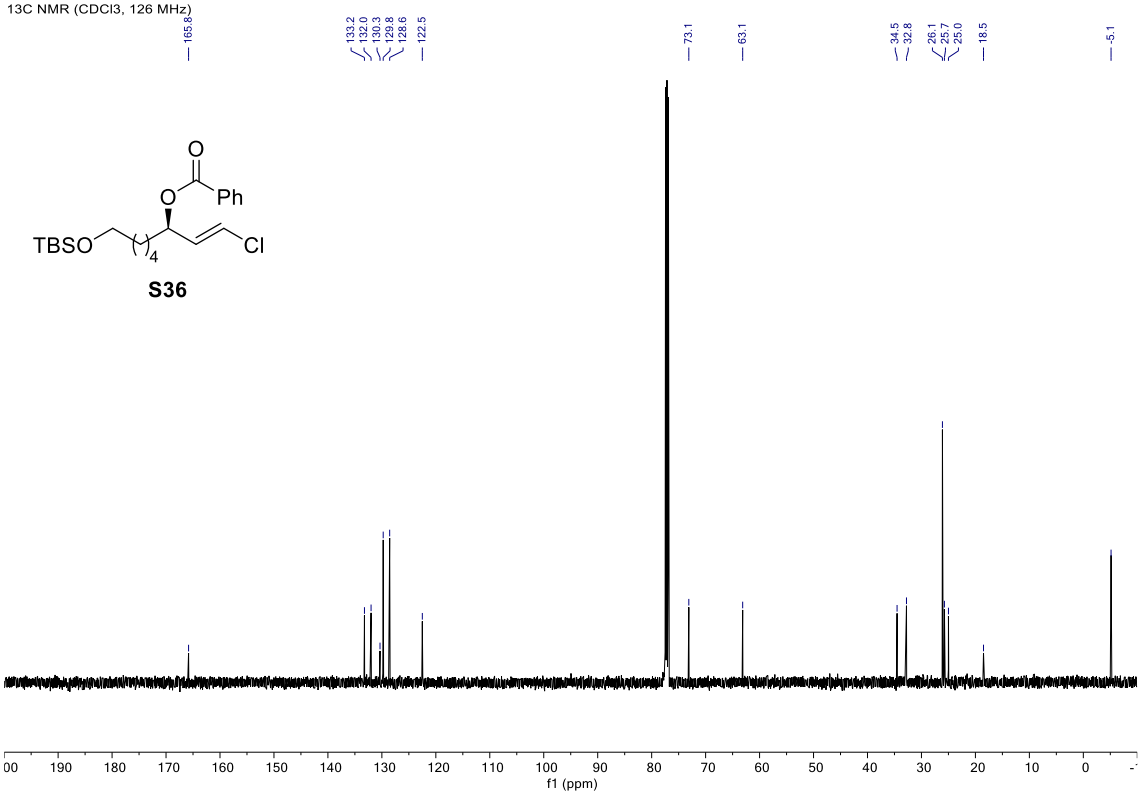


13C NMR (CDCl3, 126 MHz)



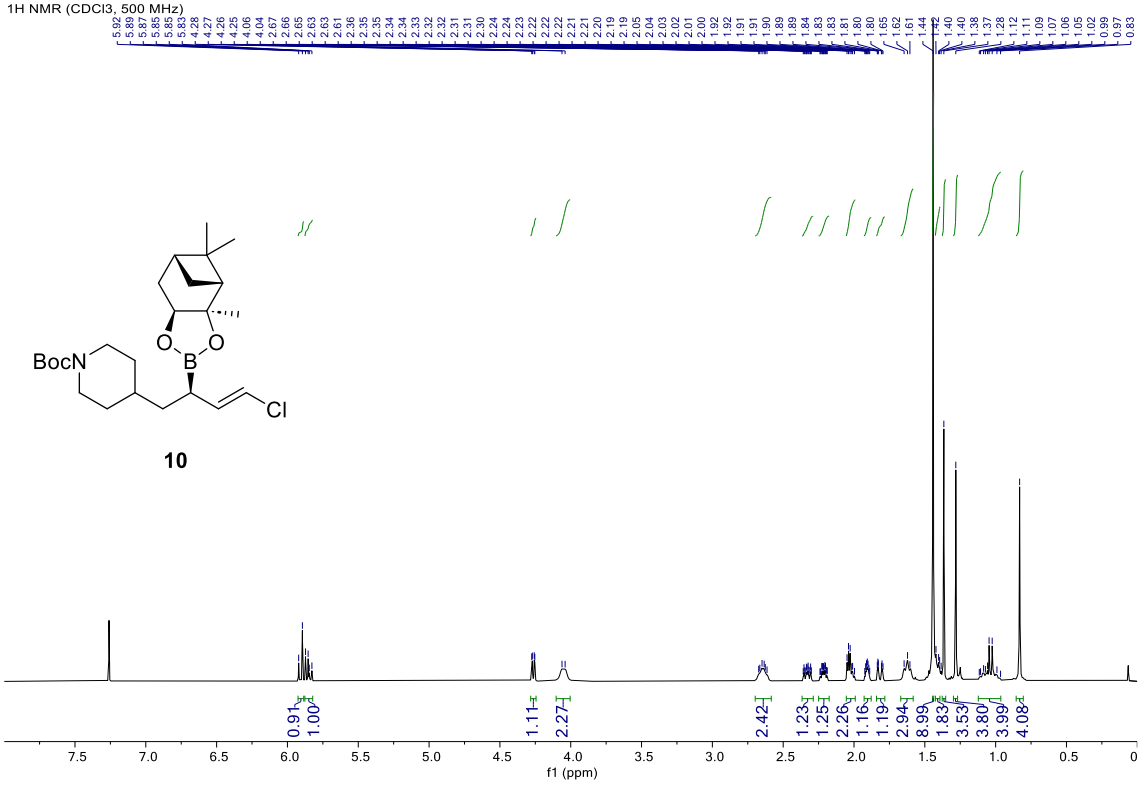

1H NMR (CDCl3, 500 MHz)
O
O
Ph
TBSO
4
Cl
1.00
2.15
0.78
0.91
1.12
2.40
1.27
1.35
2.73
4.88
9.78
5.23
f1 (ppm)

S36


13C NMR (CDCl3, 126 MHz)
165.8
133.2
132.0
130.3
129.8
128.6
122.5
73.1
63.1
34.5
32.8
26.1
25.7
25.0
18.5
-5.1
O
O
Ph
TBSO
4
Cl
f1 (ppm)

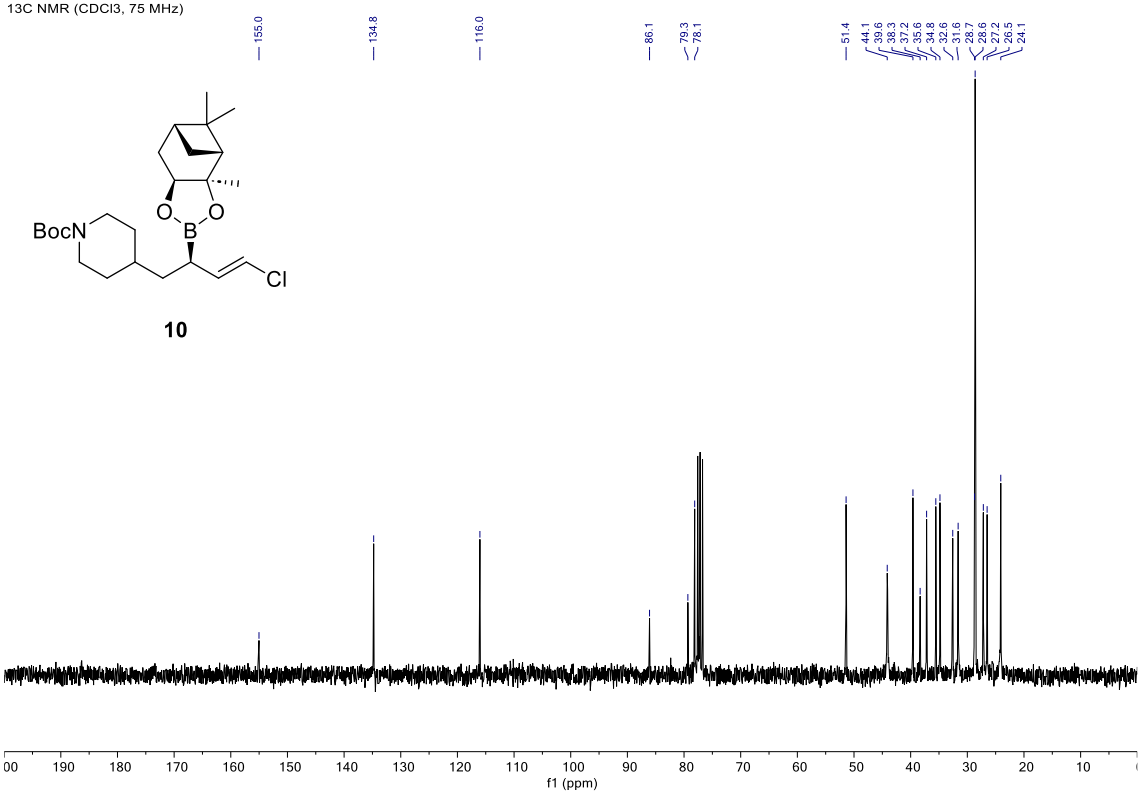
S36

1H NMR (CDCl3, 500 MHz)



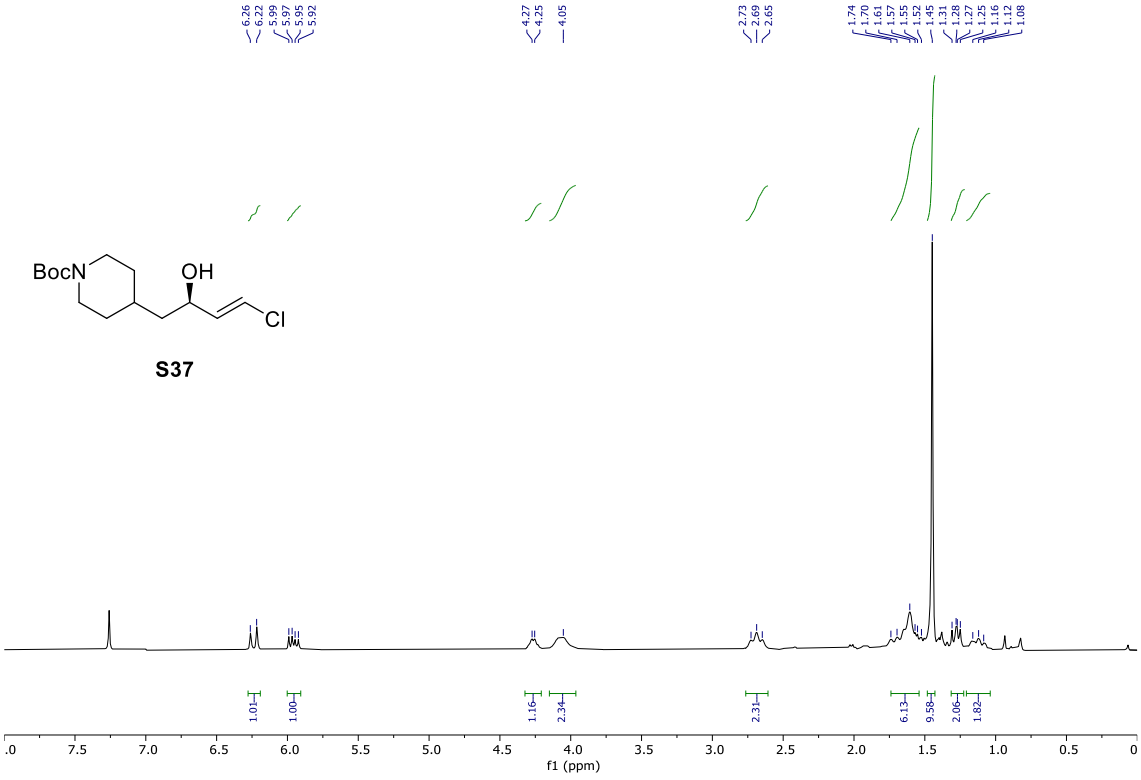
10

13C NMR (CDCl3, 75 MHz)



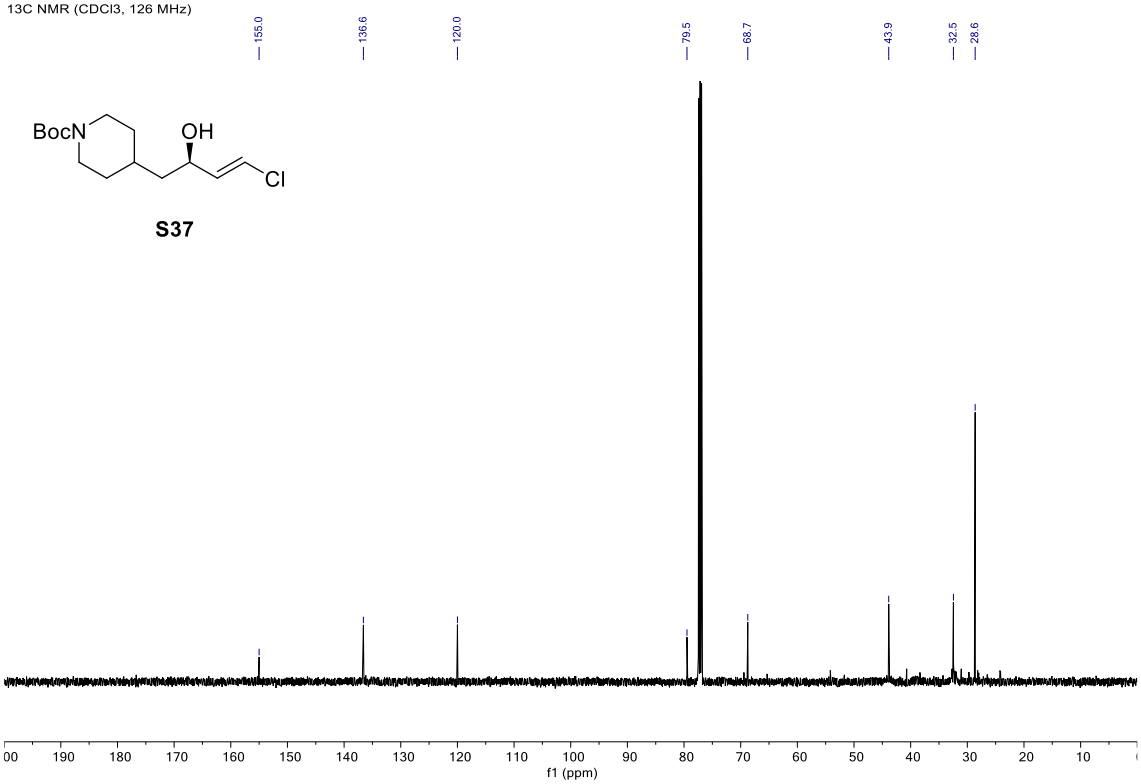
10

1H NMR (CDCl3, 300 MHz)

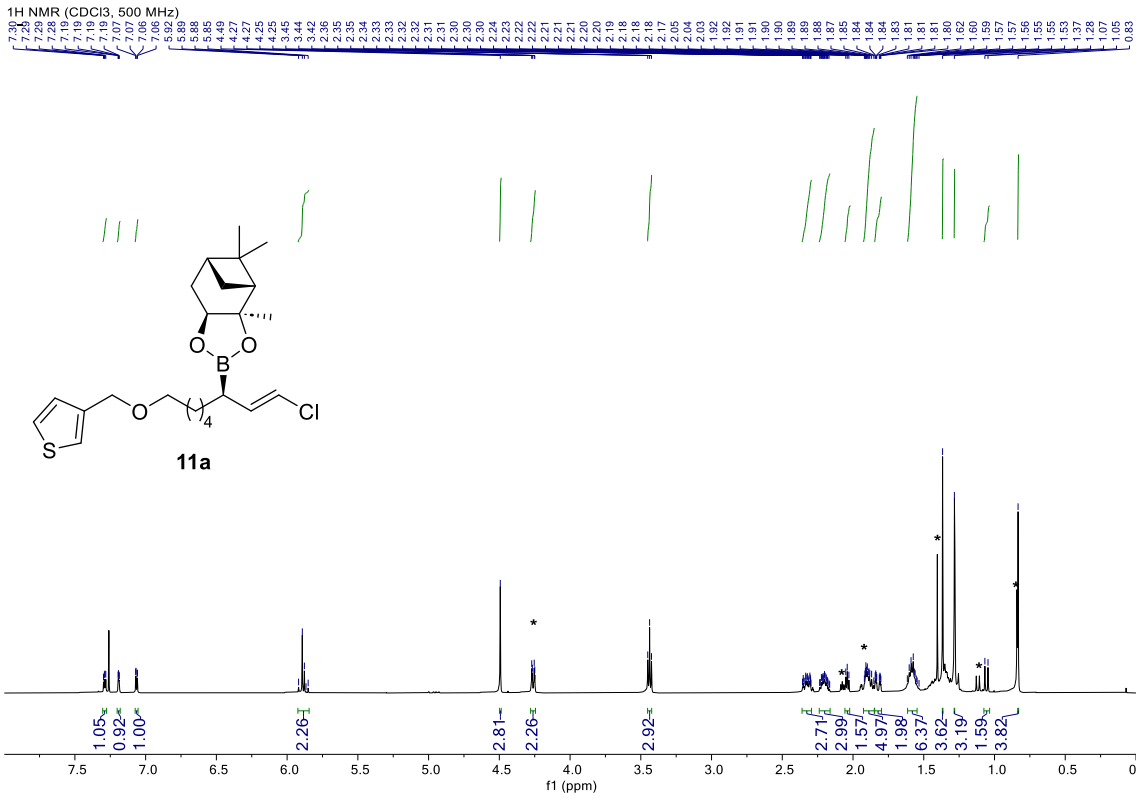


S37

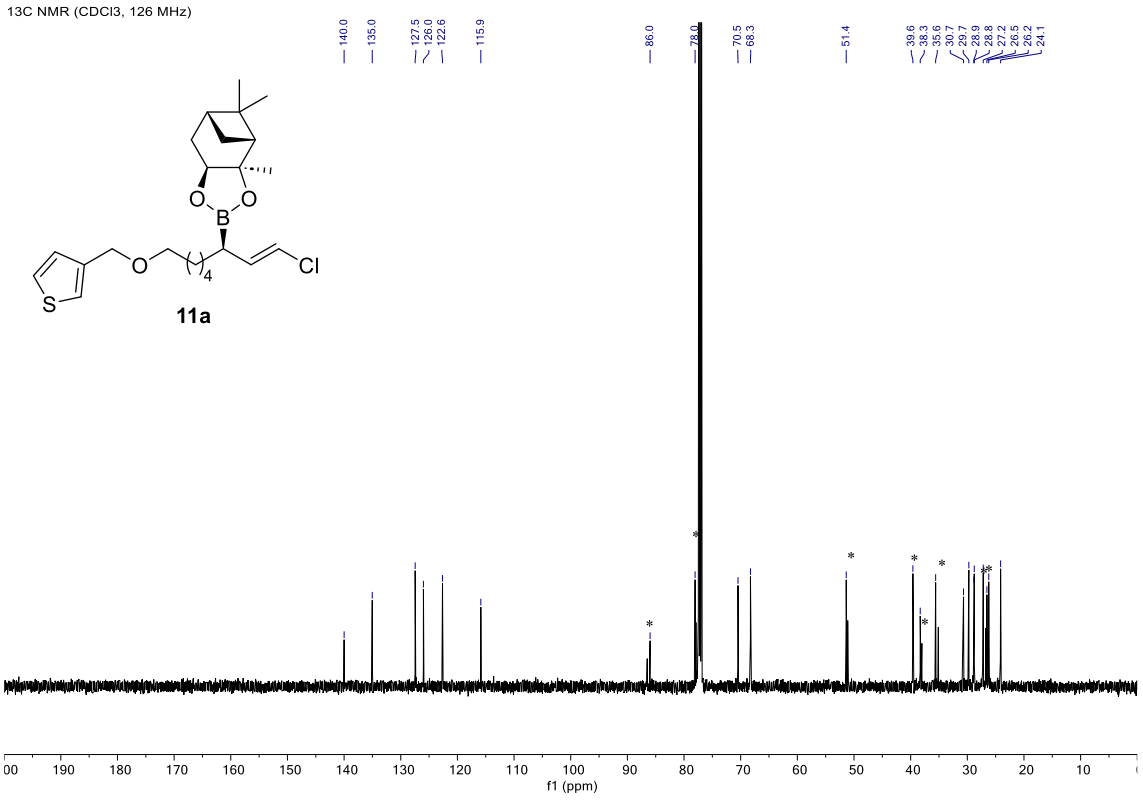
13C NMR (CDCl3, 126 MHz)



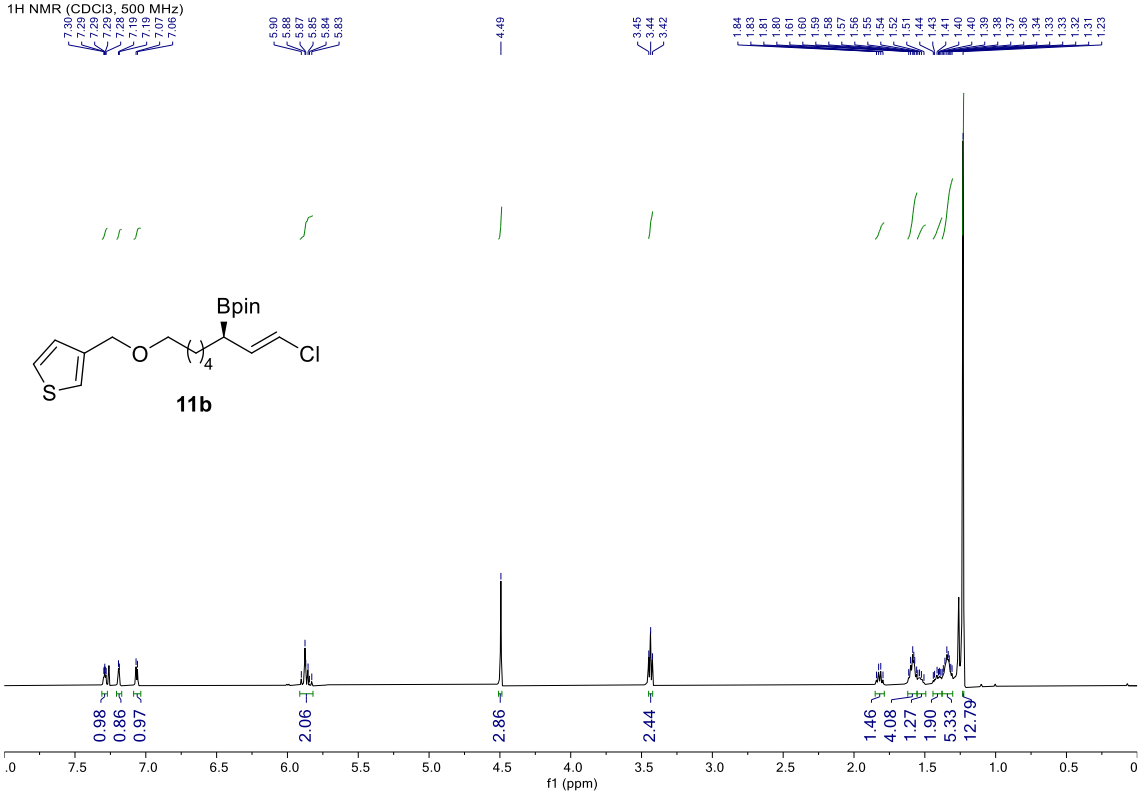
S37



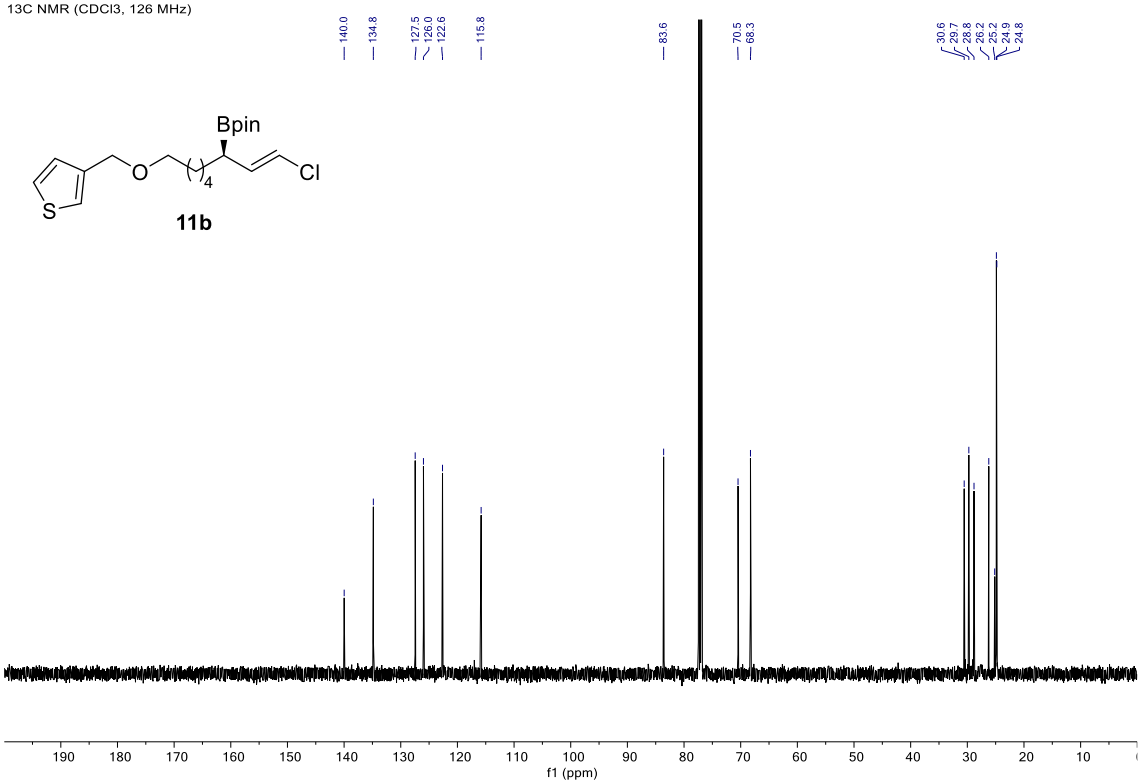
*These signals belong (+)-Bpai impurity.



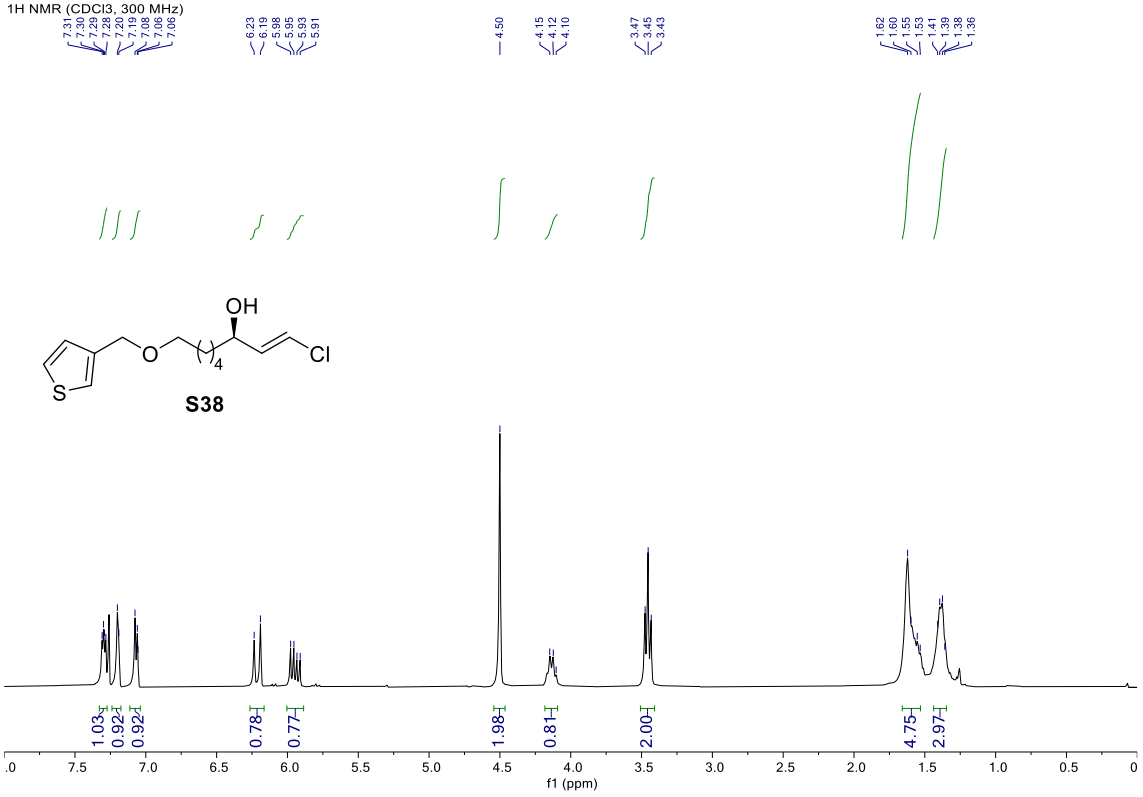
1H NMR (CDCl3, 500 MHz)



13C NMR (CDCl3, 126 MHz)

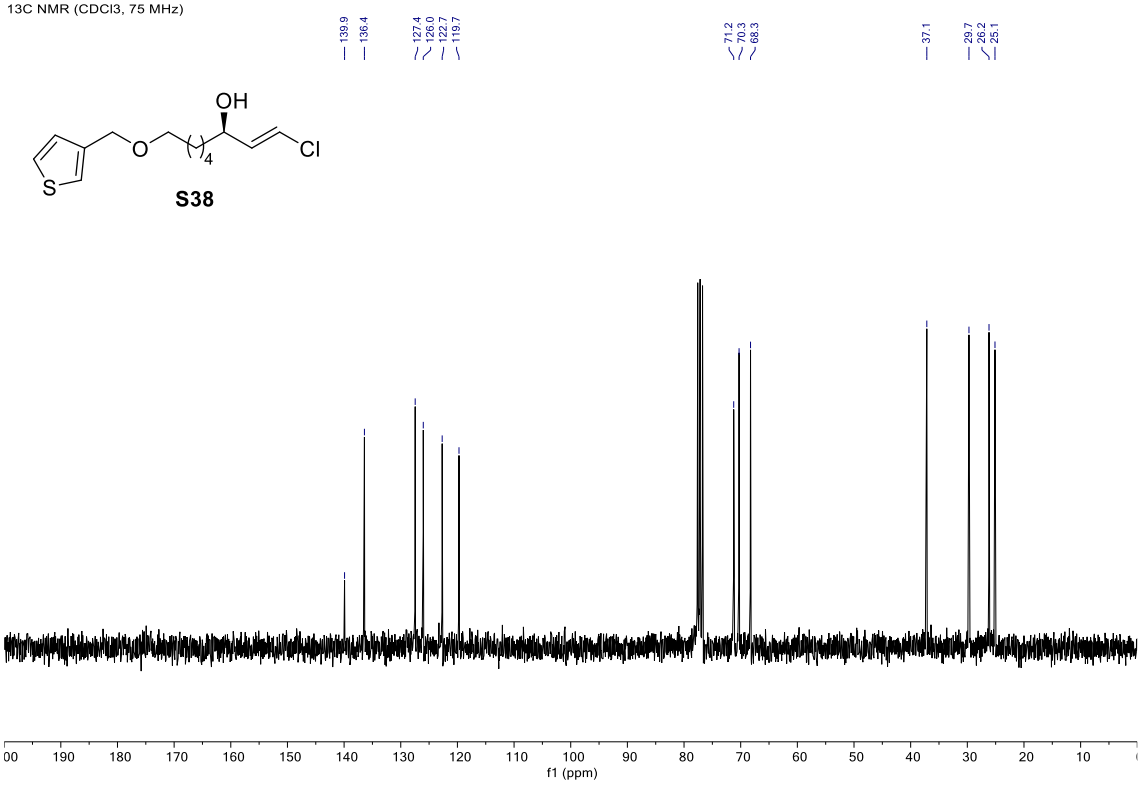


1H NMR (CDCl3, 300 MHz)



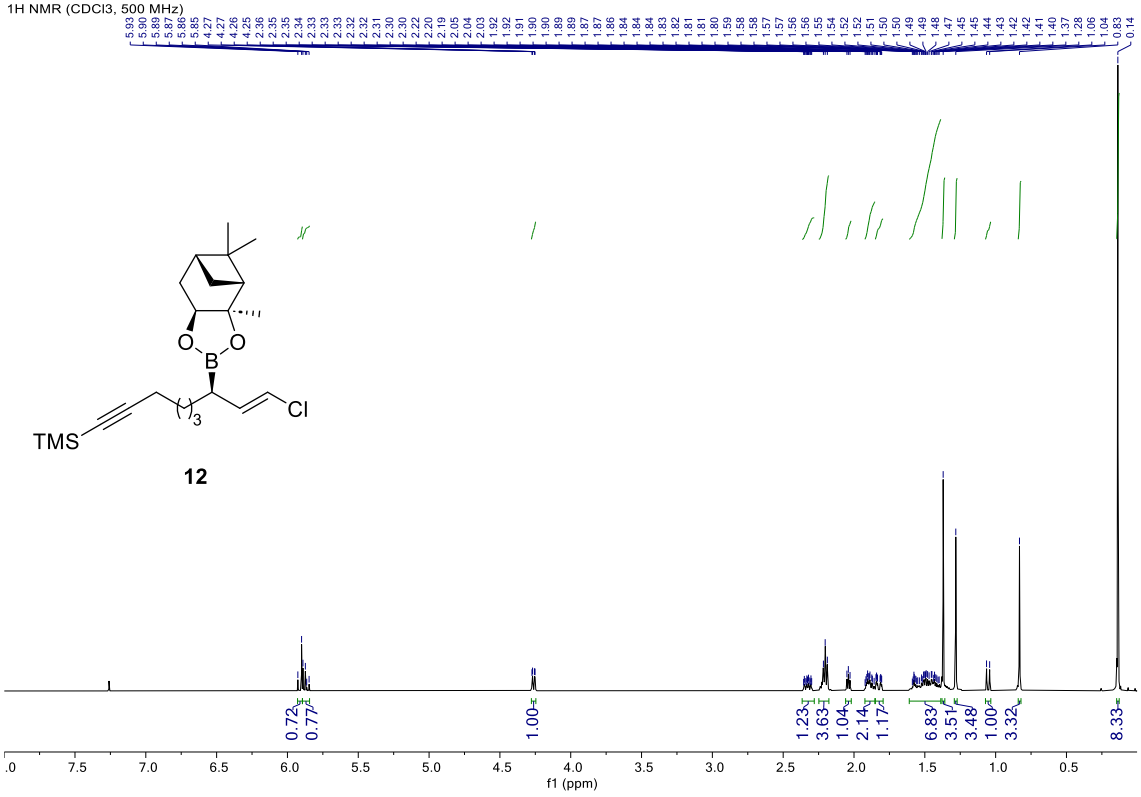
S38

13C NMR (CDCl3, 75 MHz)



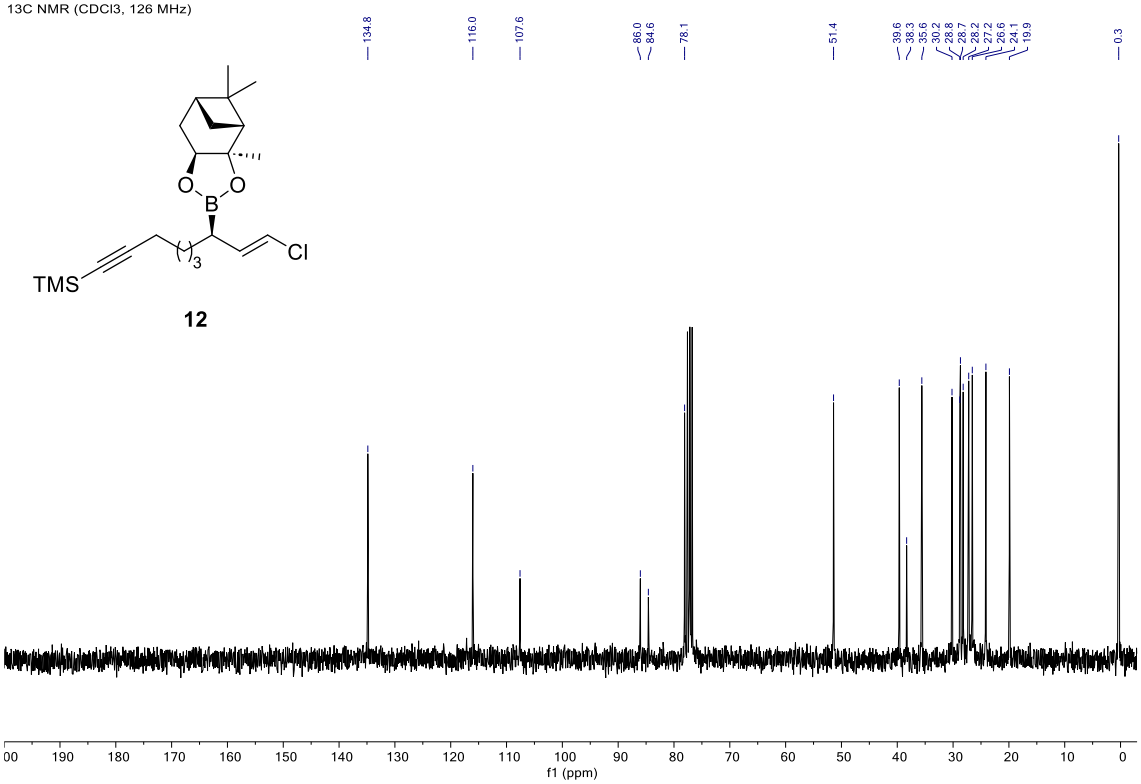
S38

1H NMR (CDCl3, 500 MHz)



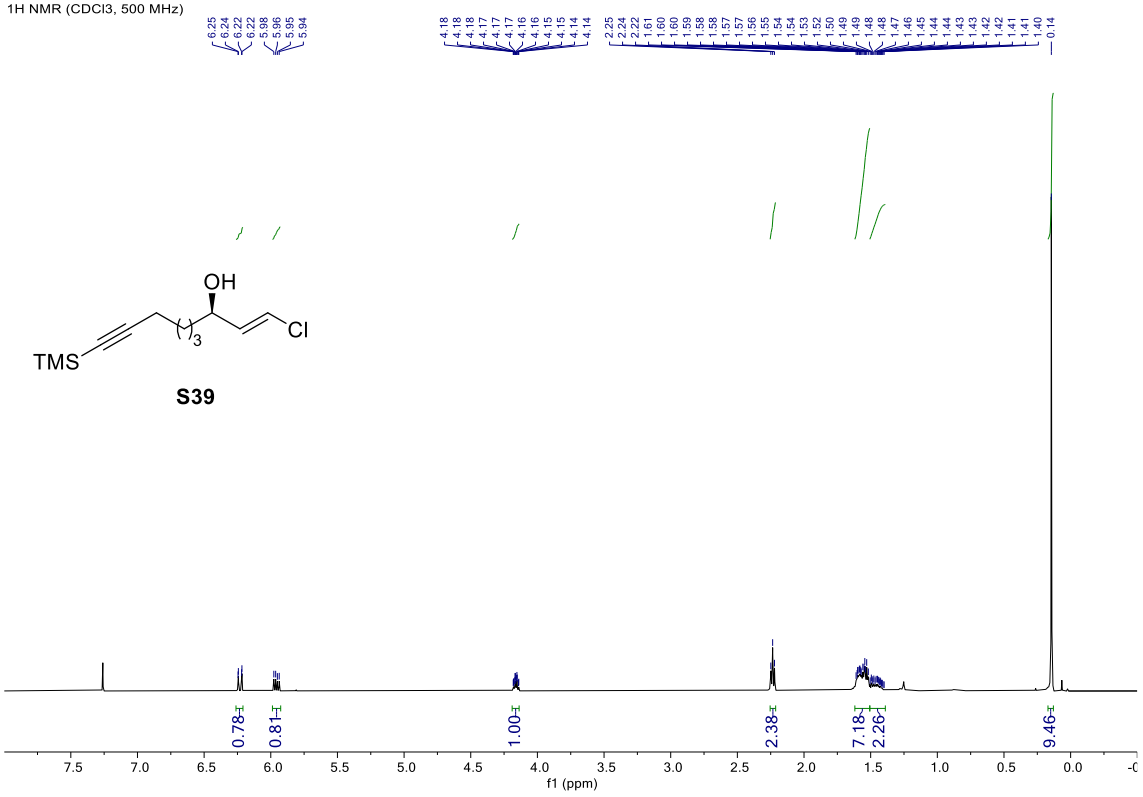
12

13C NMR (CDCl3, 126 MHz)



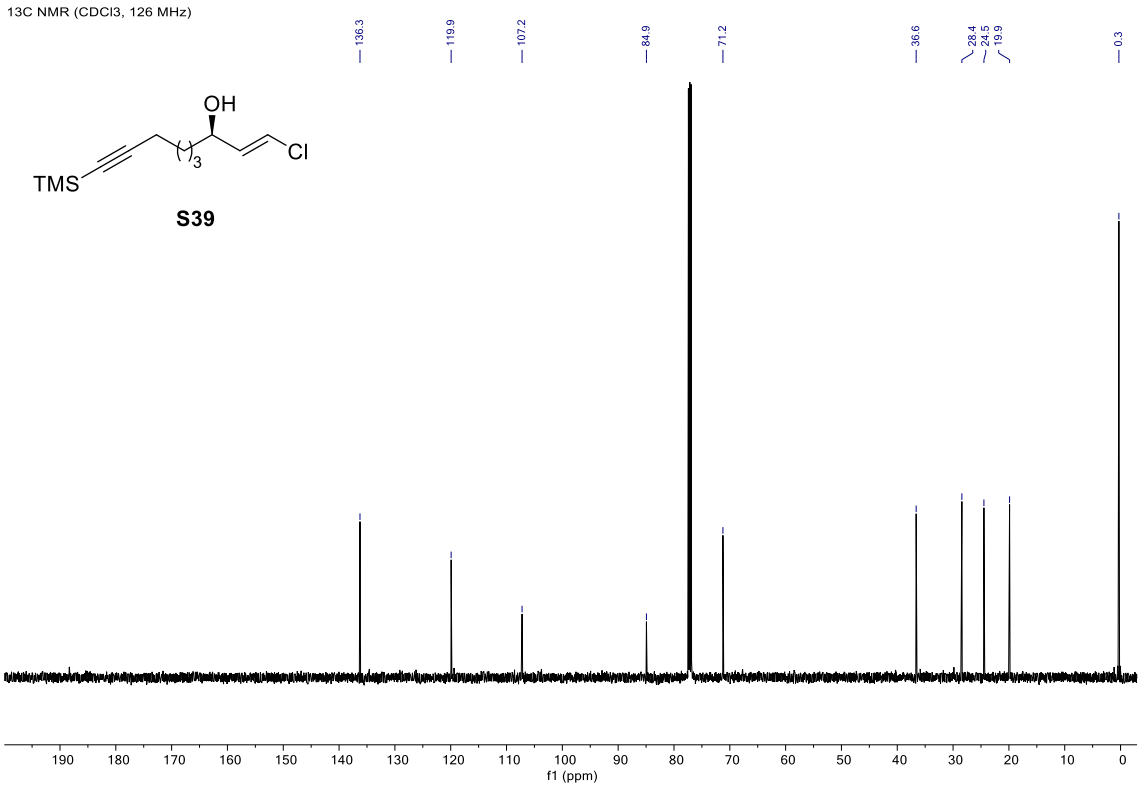
12

1H NMR (CDCl3, 500 MHz)



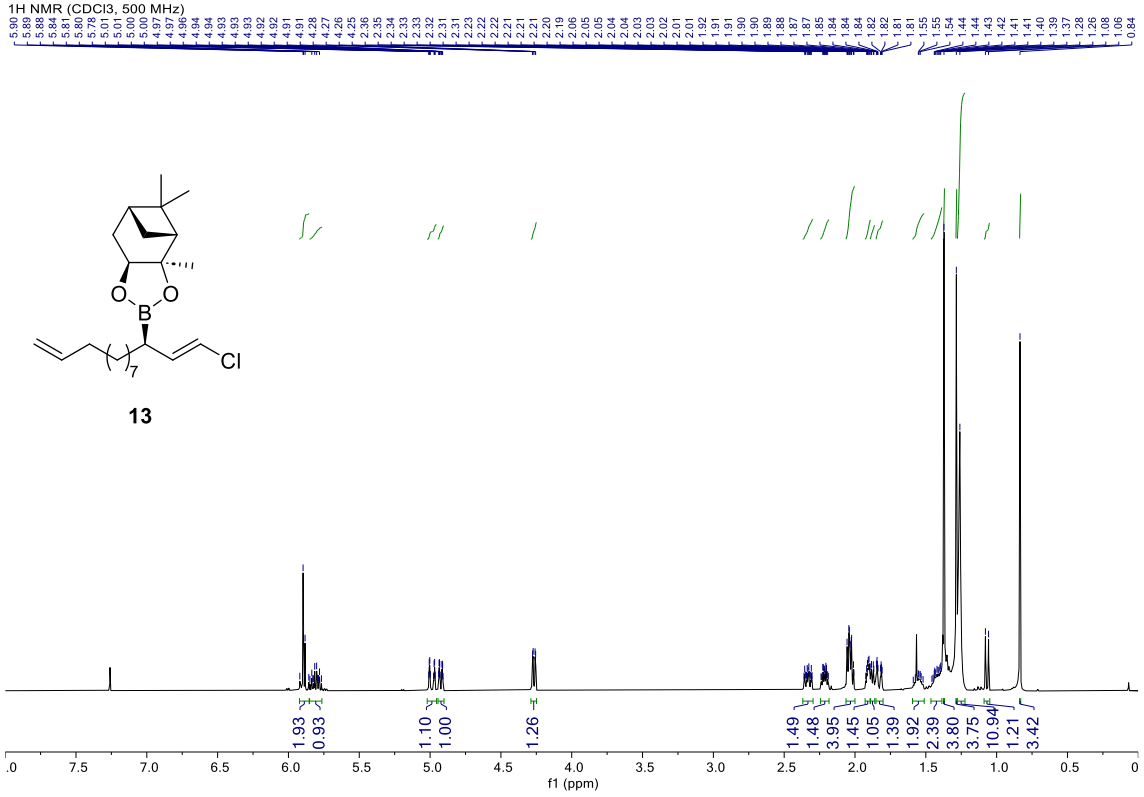
S39

13C NMR (CDCl3, 126 MHz)



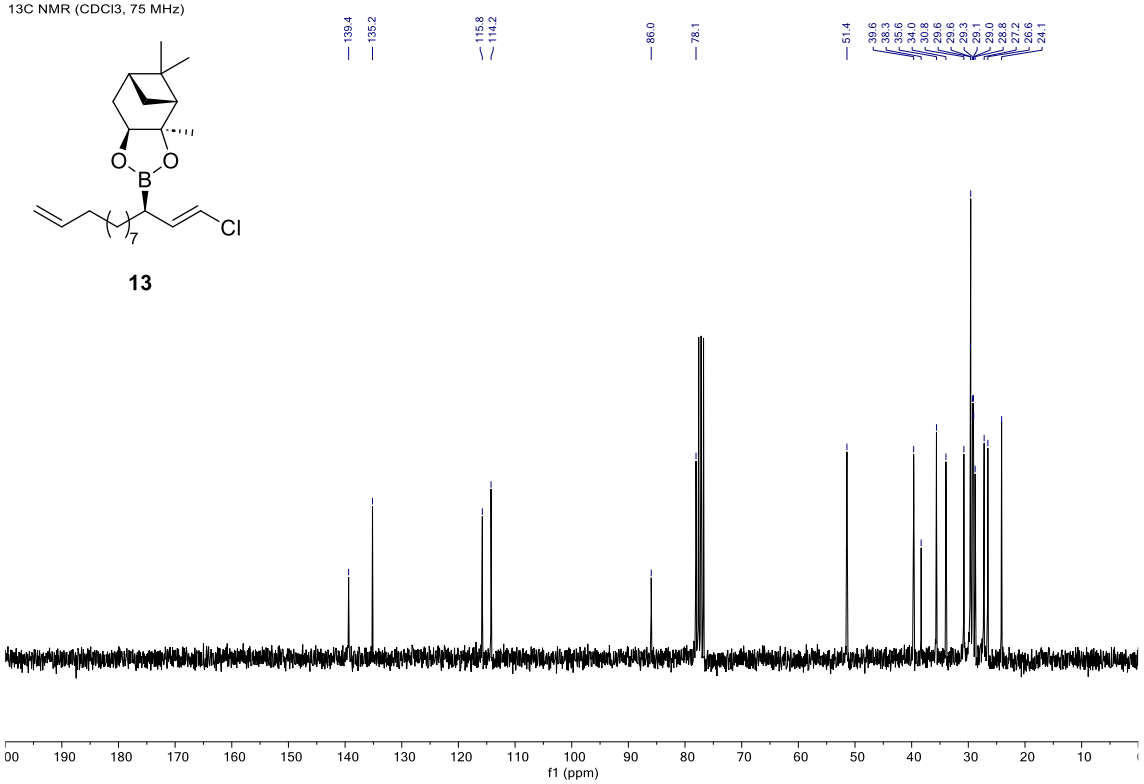
S39

1H NMR (CDCl3, 500 MHz)



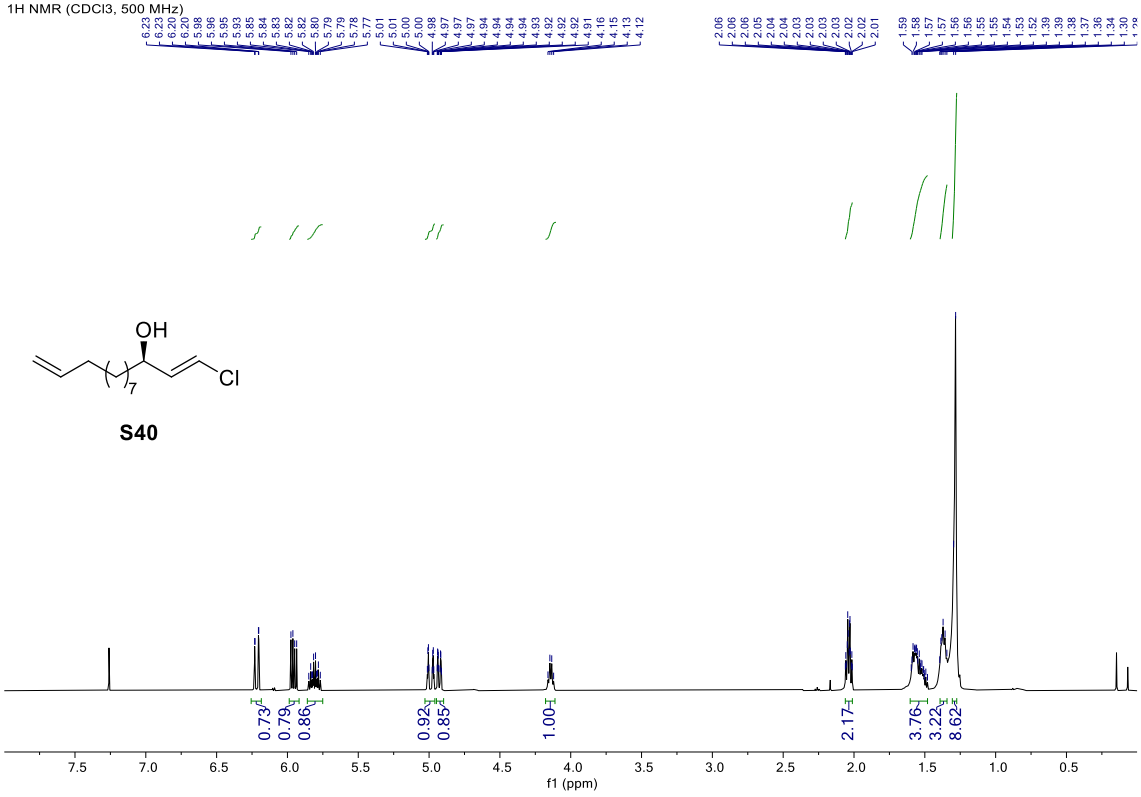
13

13C NMR (CDCl3, 75 MHz)



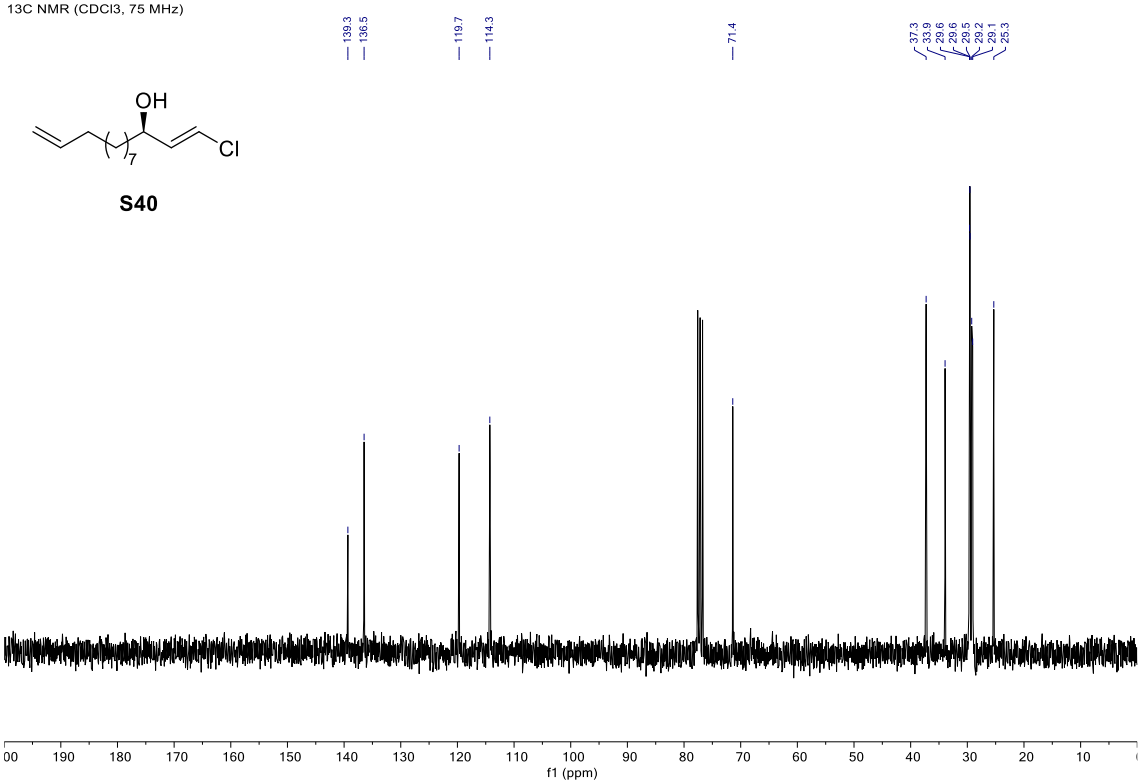
13

1H NMR (CDCl3, 500 MHz)



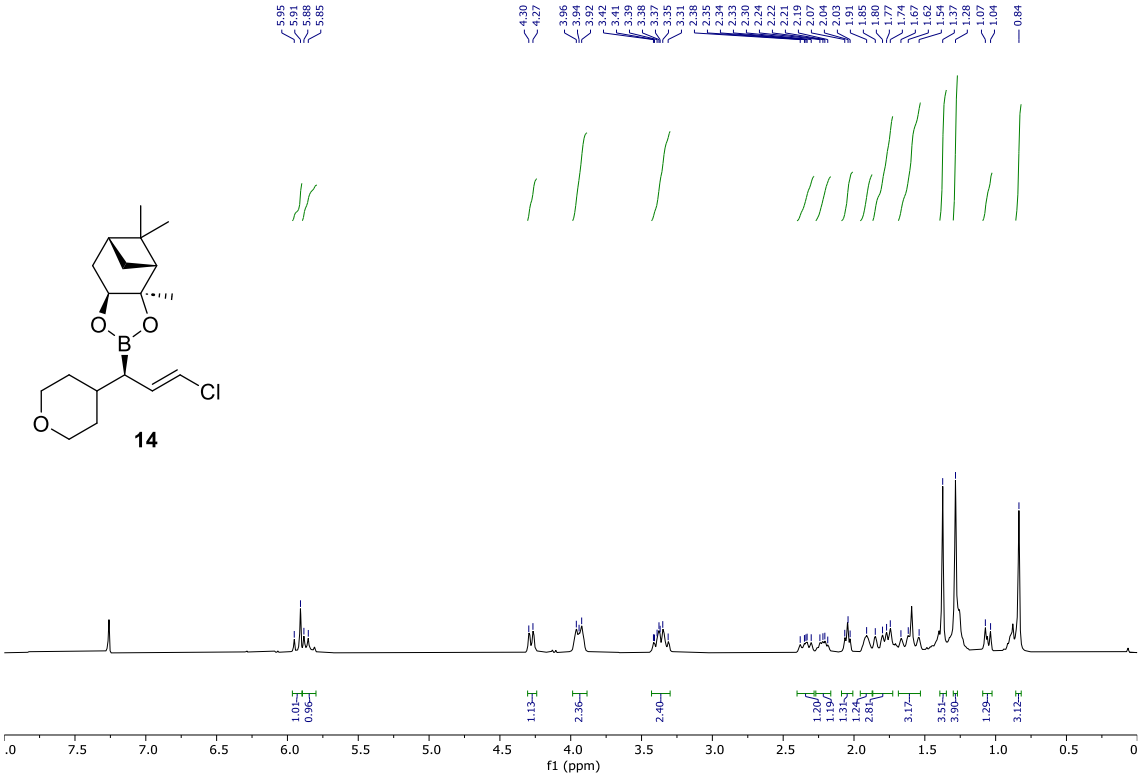
S40

13C NMR (CDCl3, 75 MHz)

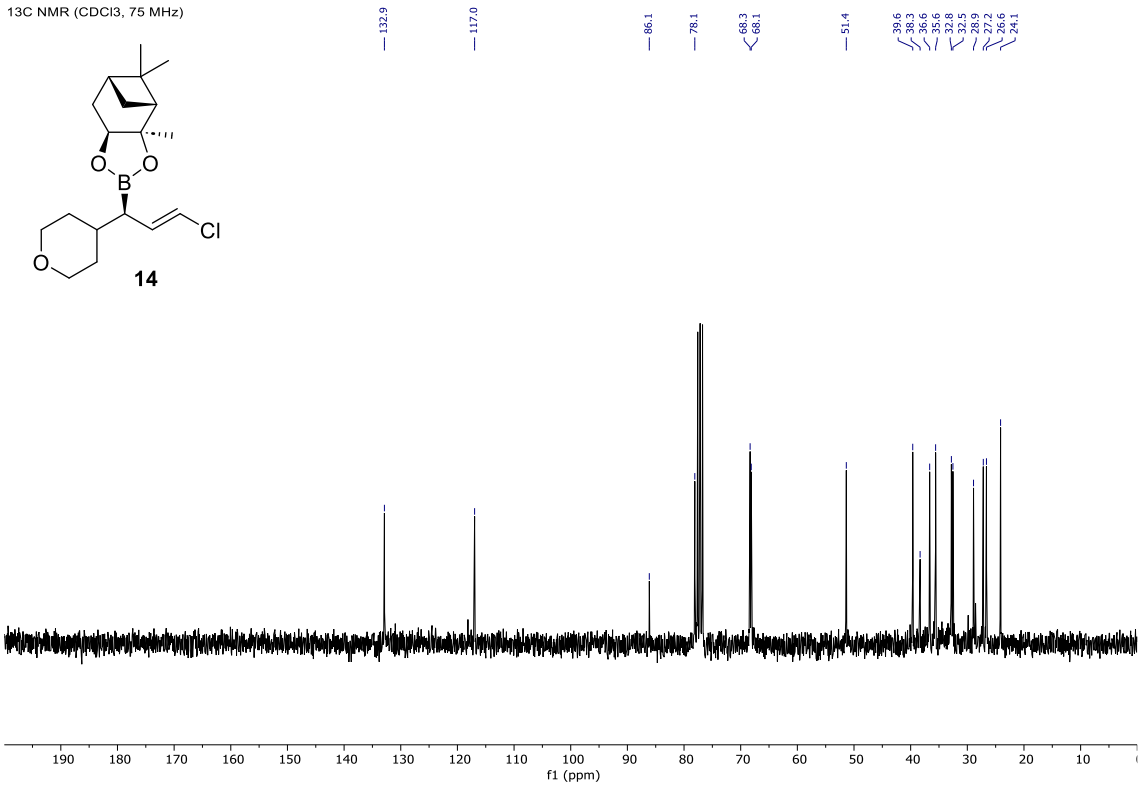


S40

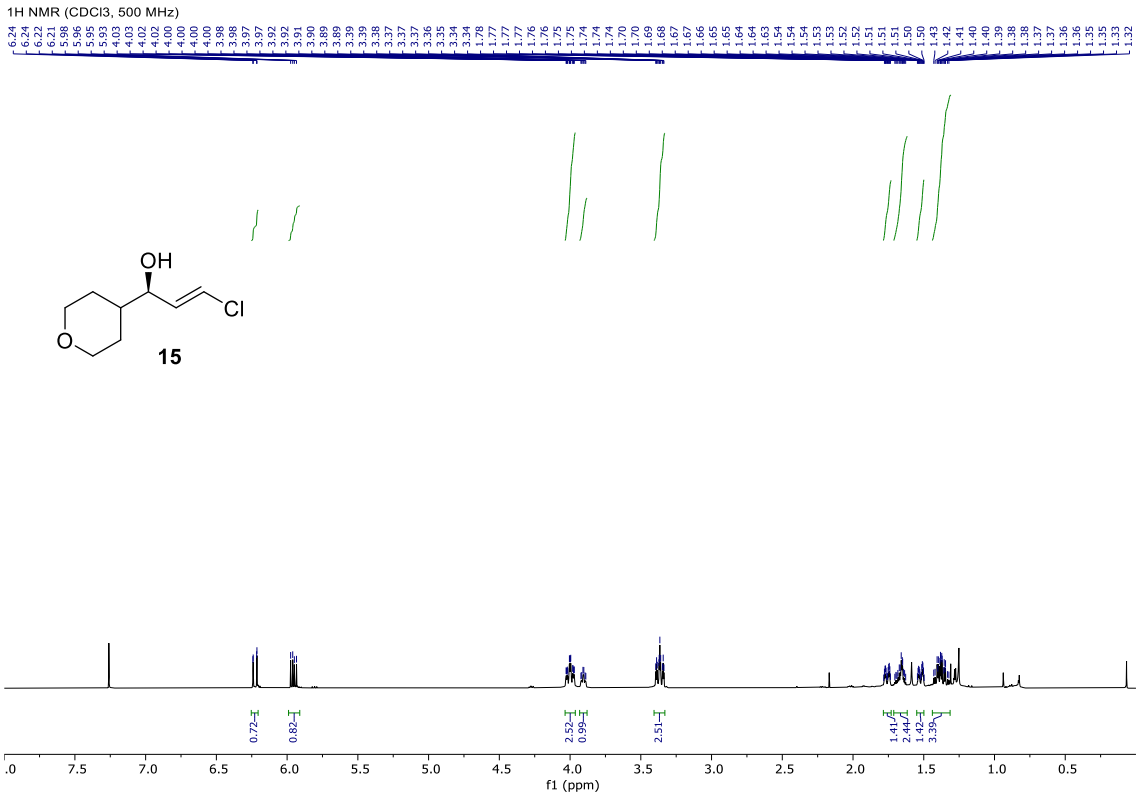
1H NMR (CDCl3, 300 MHz)



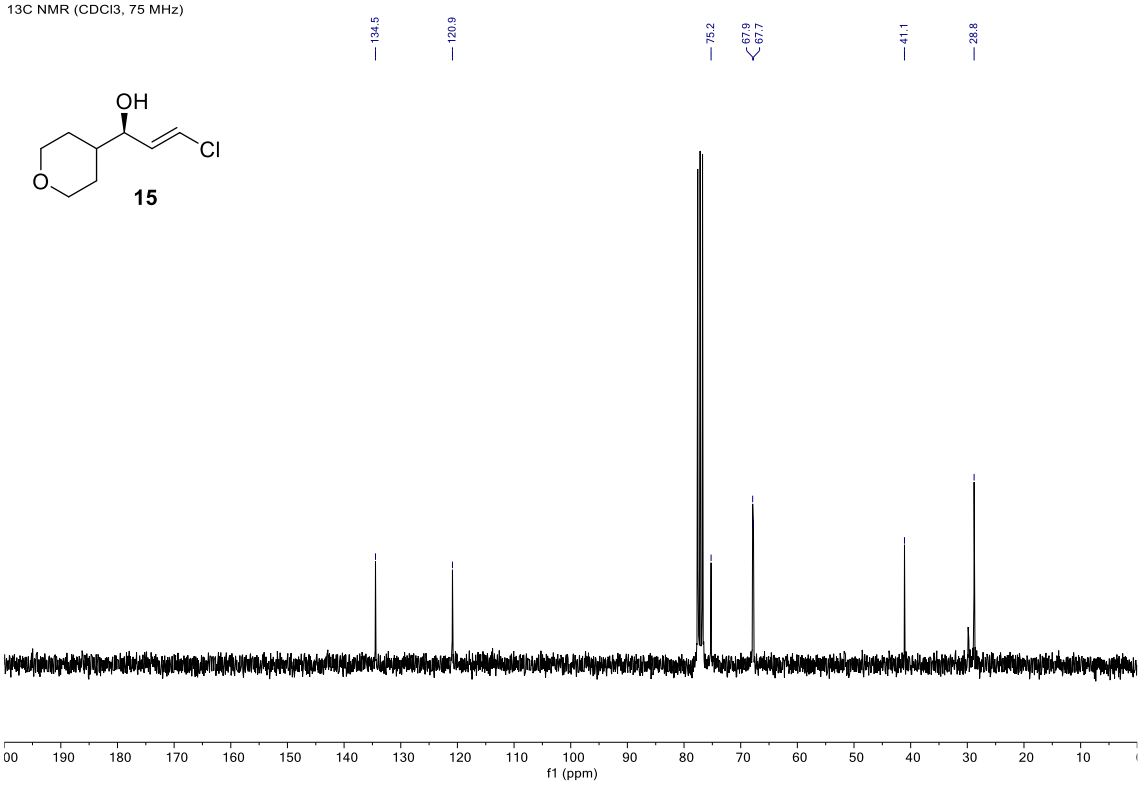
13C NMR (CDCl3, 75 MHz)



1H NMR (CDCl3, 500 MHz)

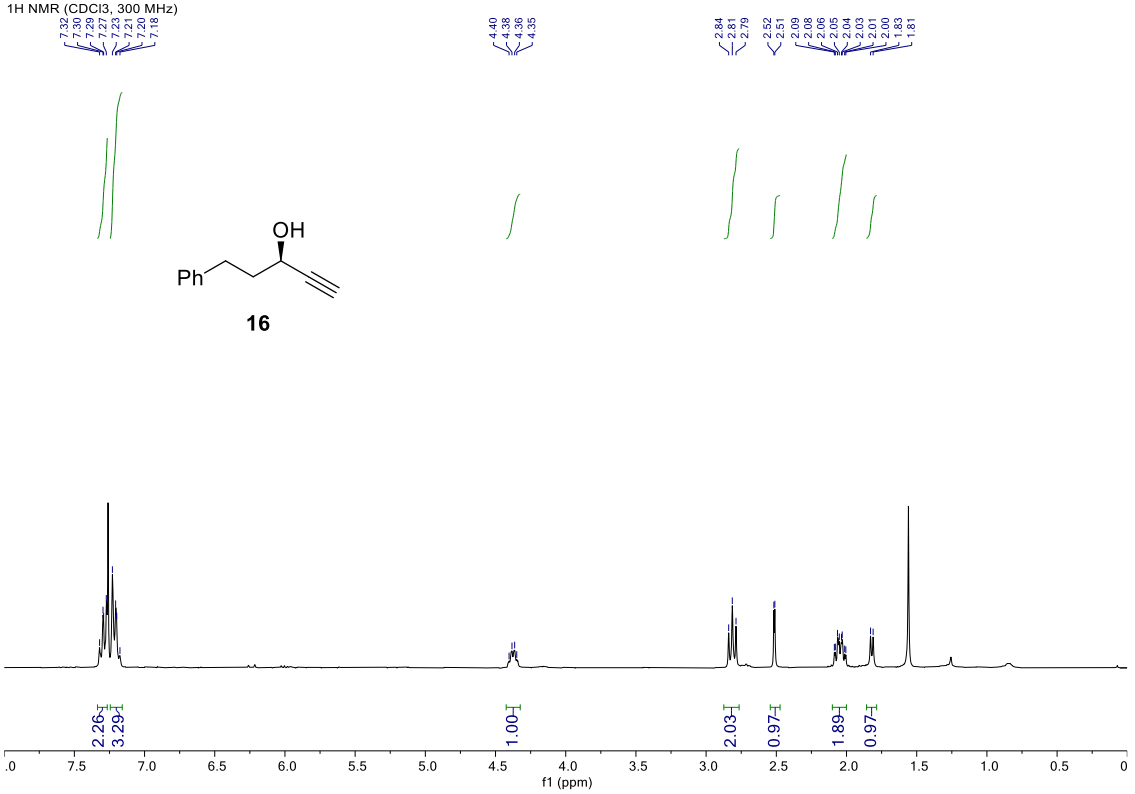


13C NMR (CDCl3, 75 MHz)

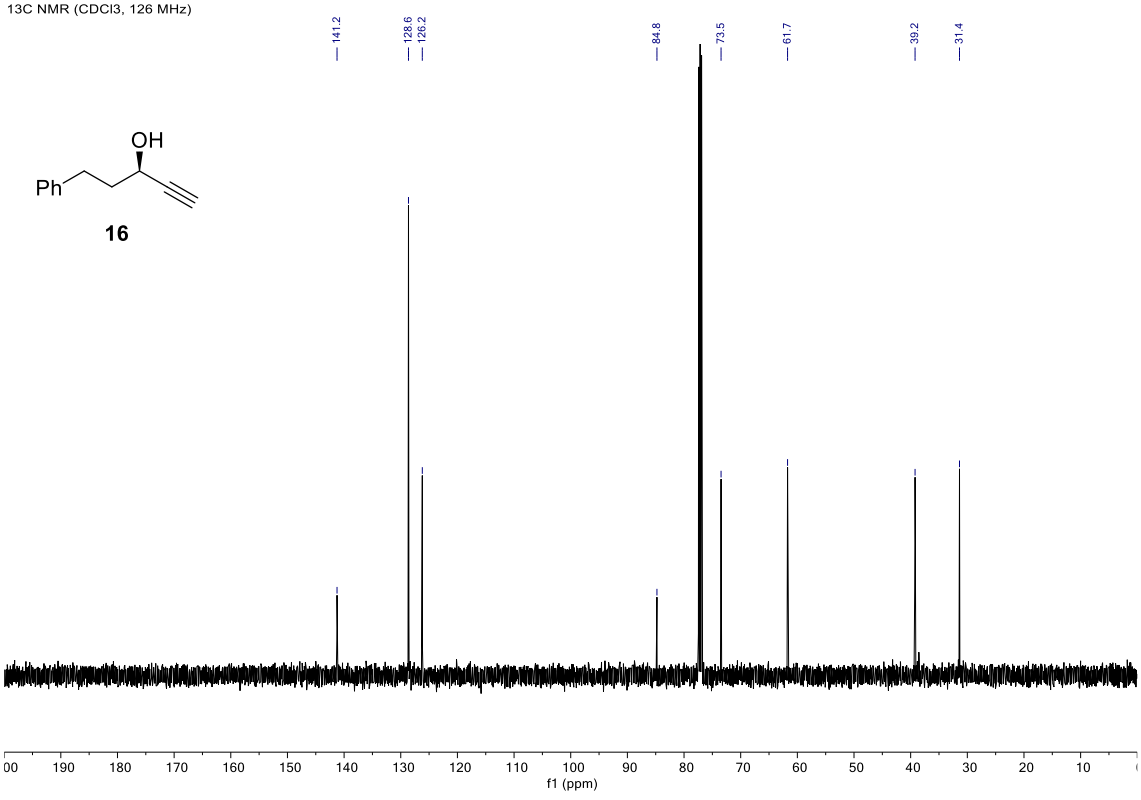


16. NMR spectra of the synthetic applications

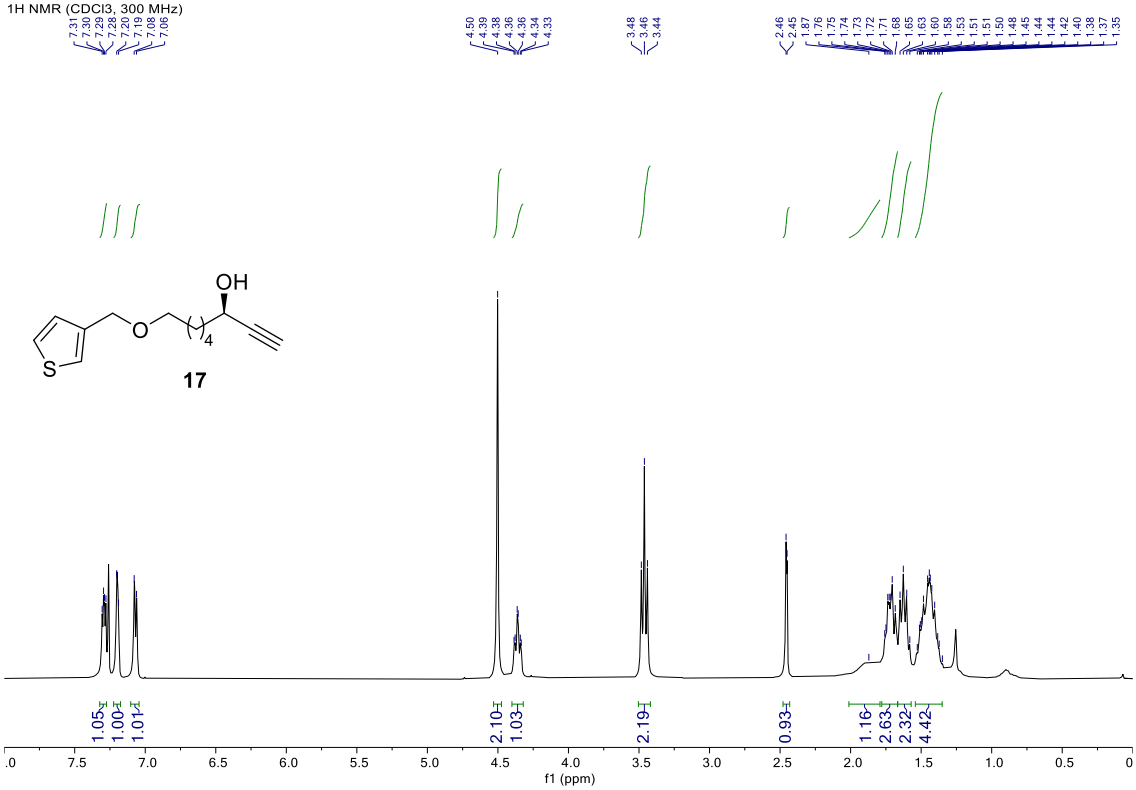
1H NMR (CDCl3, 300 MHz)



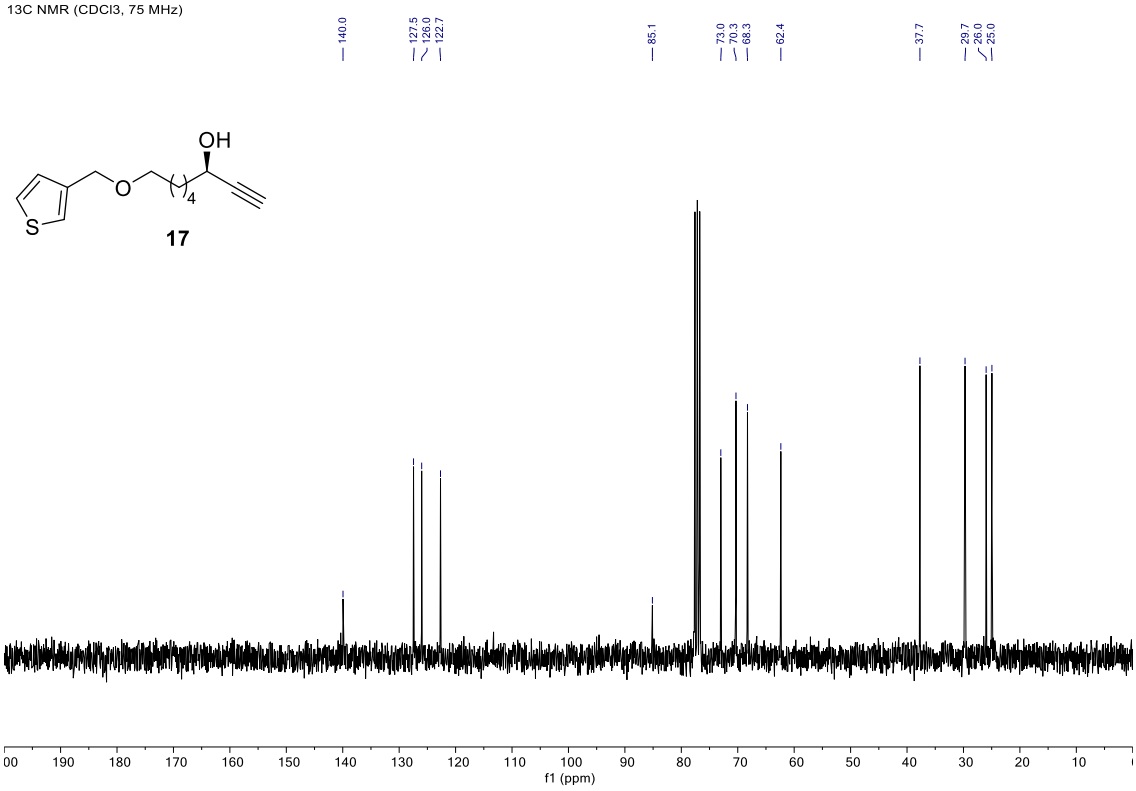
13C NMR (CDCl3, 126 MHz)



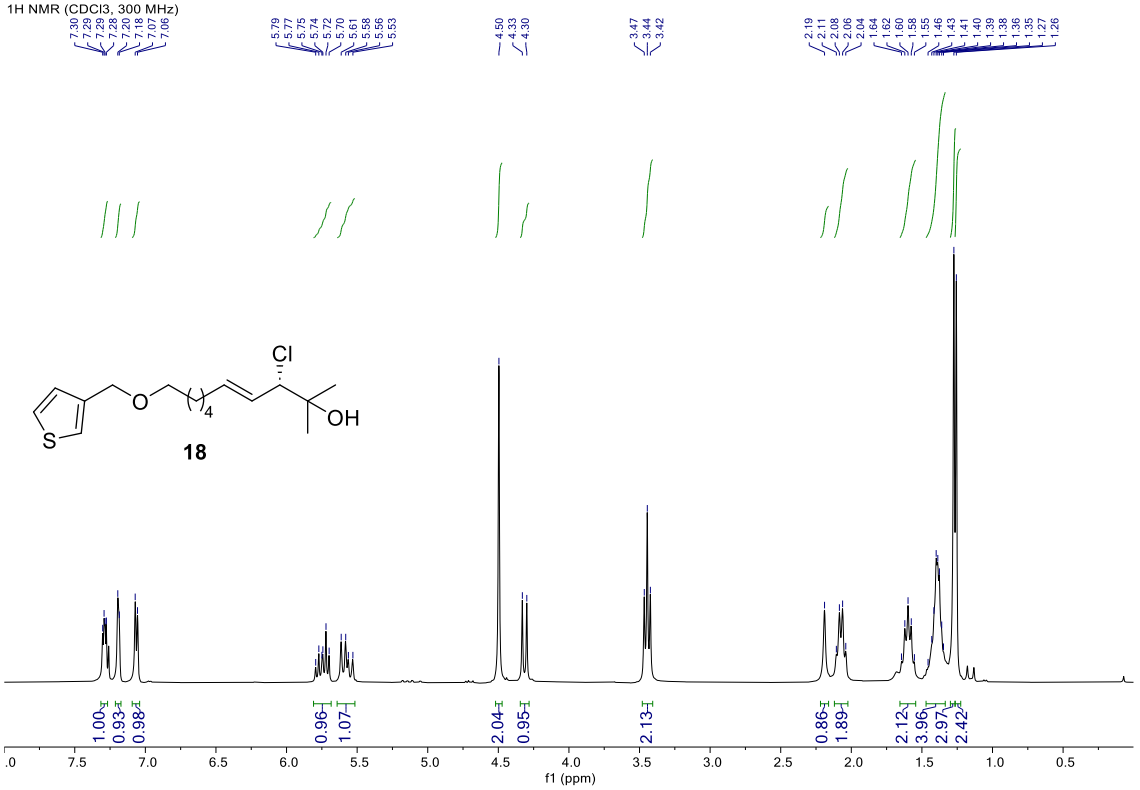
1H NMR (CDCl3, 300 MHz)



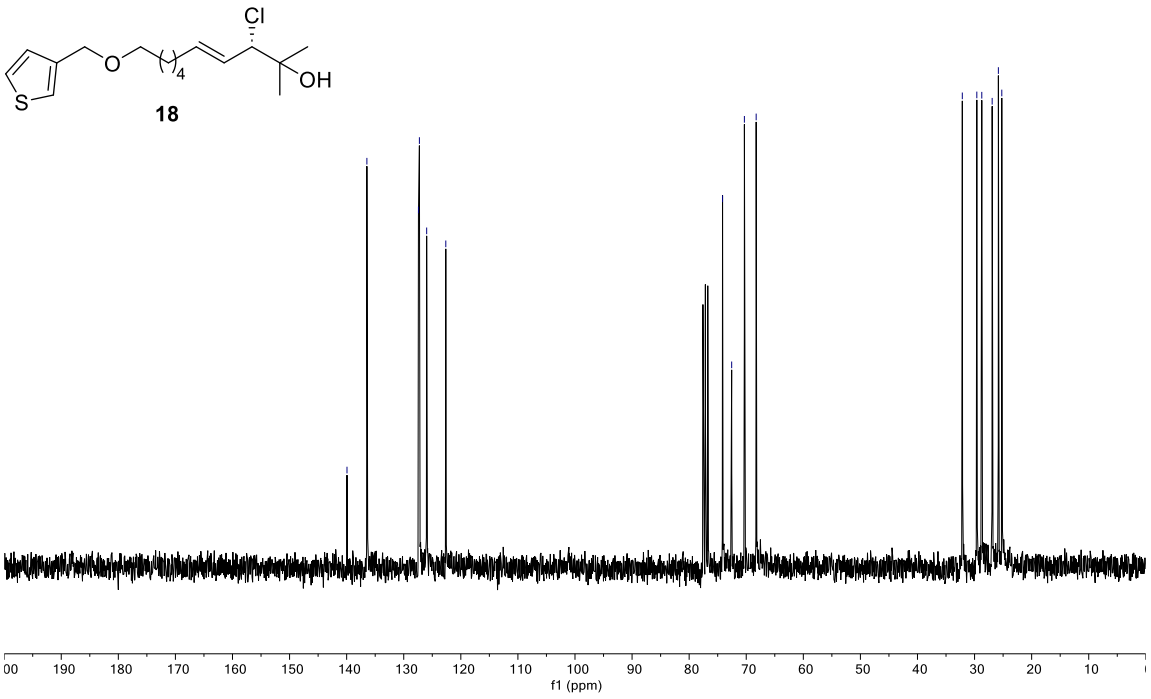
13C NMR (CDCl3, 75 MHz)



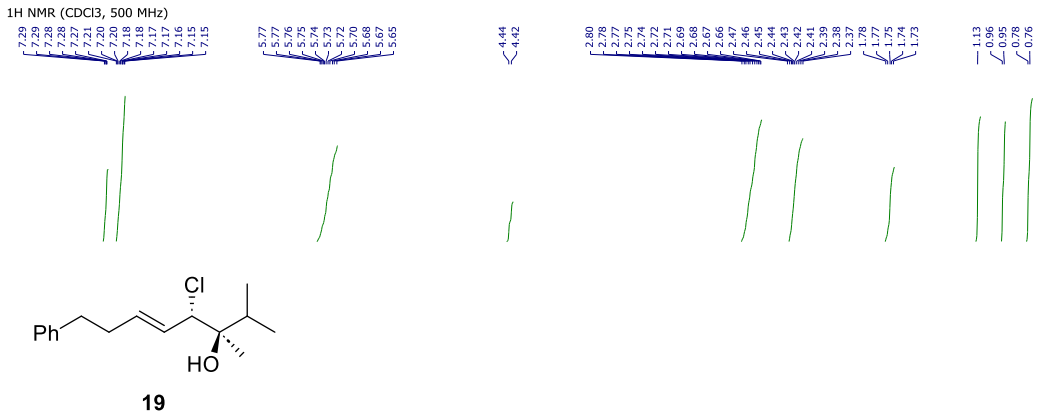
1H NMR (CDCl3, 300 MHz)



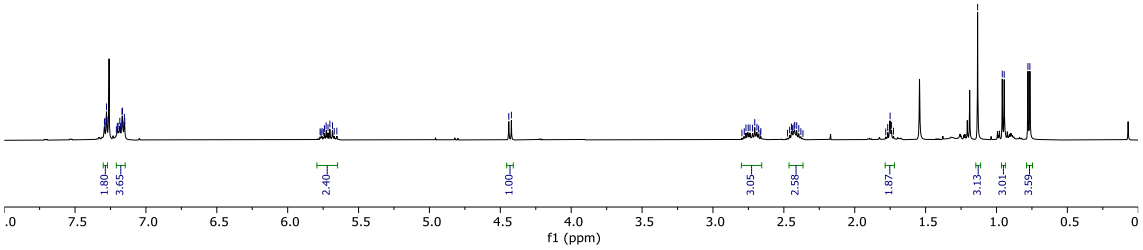
13C NMR (CDCl3, 75 MHz)



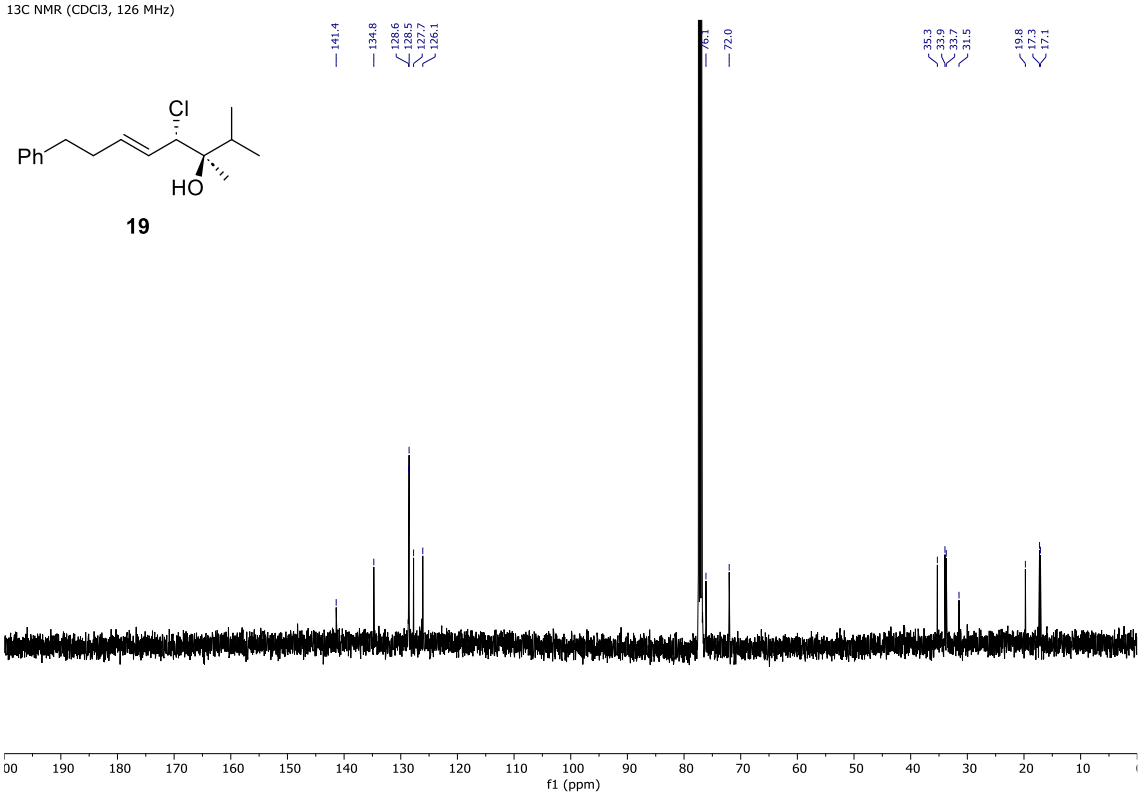
1H NMR (CDCl3, 500 MHz)



19

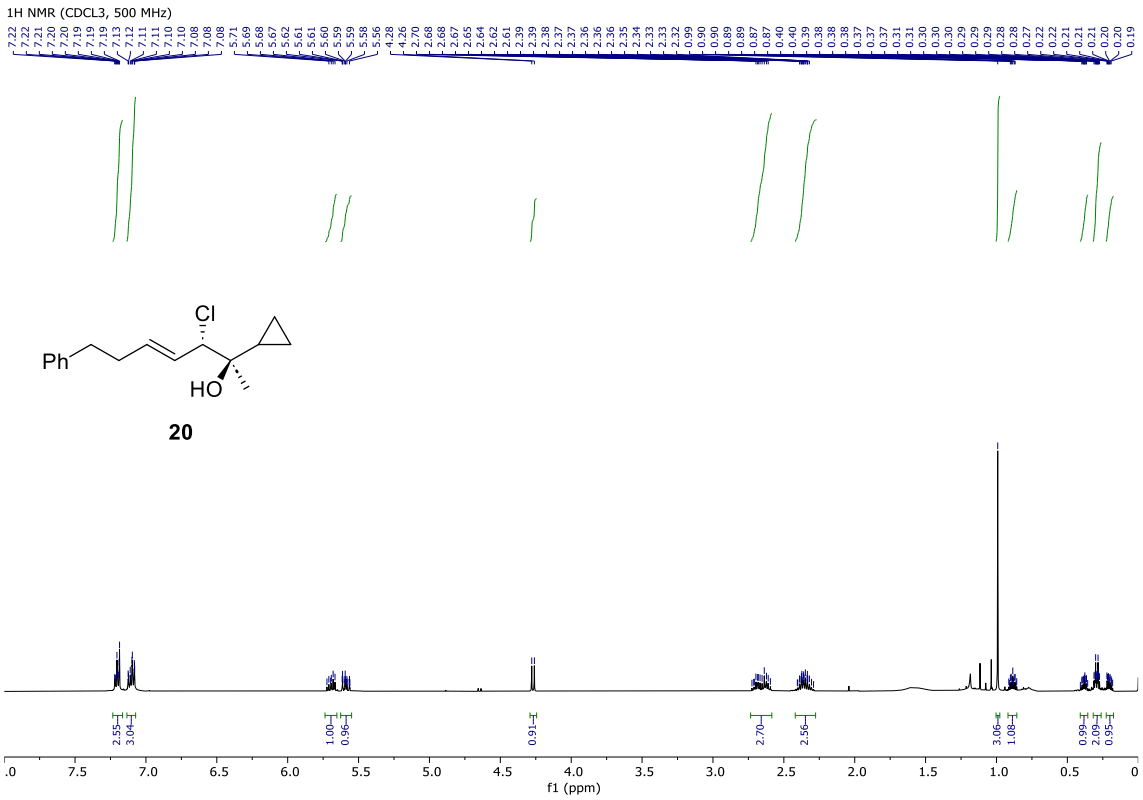


13C NMR (CDCl3, 126 MHz)

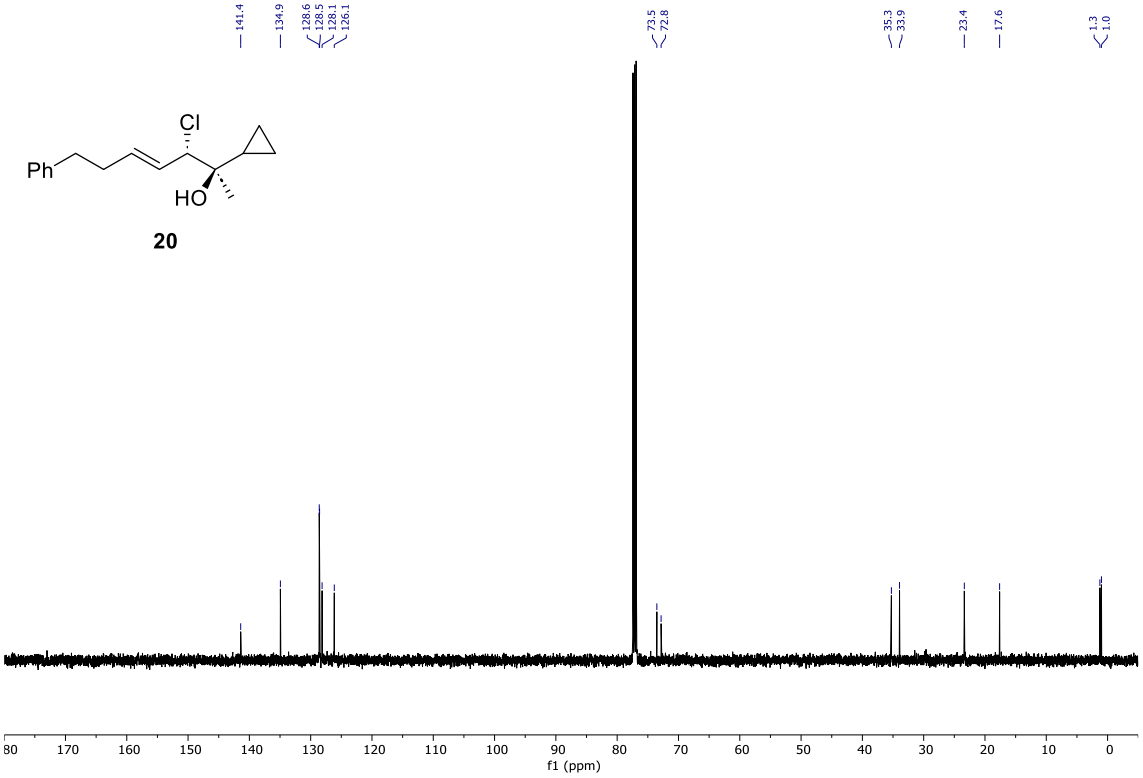


19

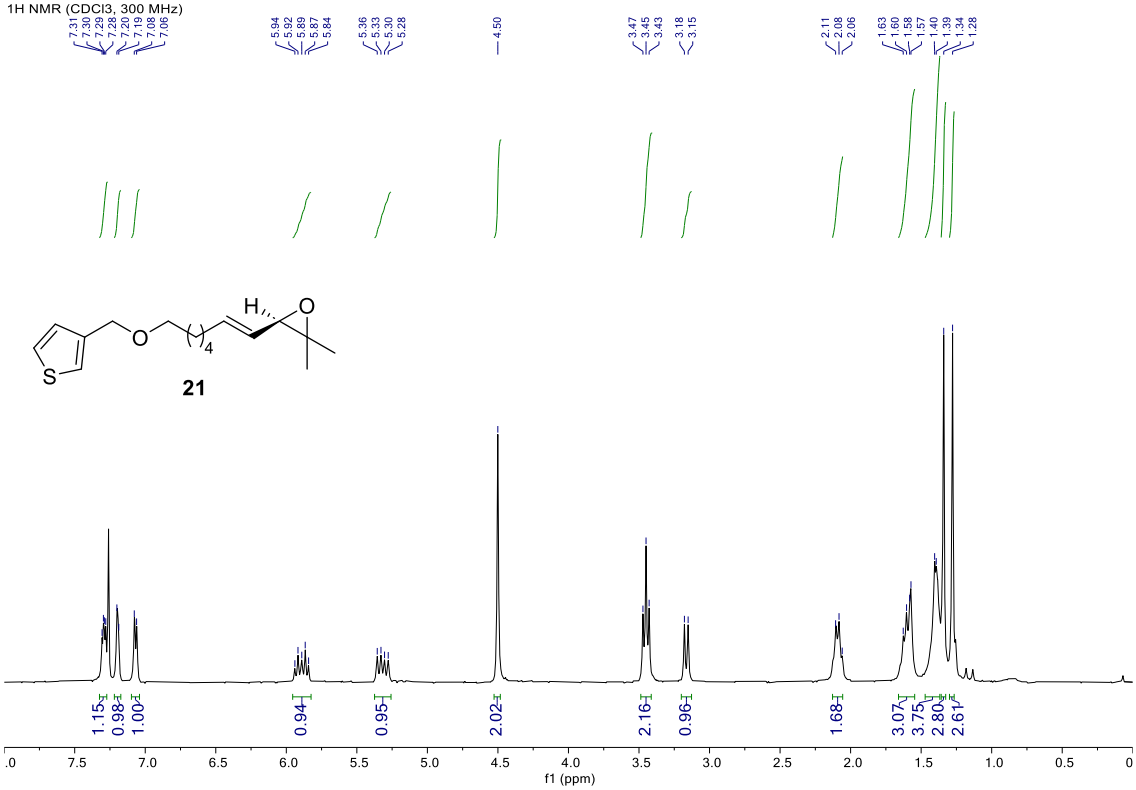
1H NMR (CDCL3, 500 MHz)



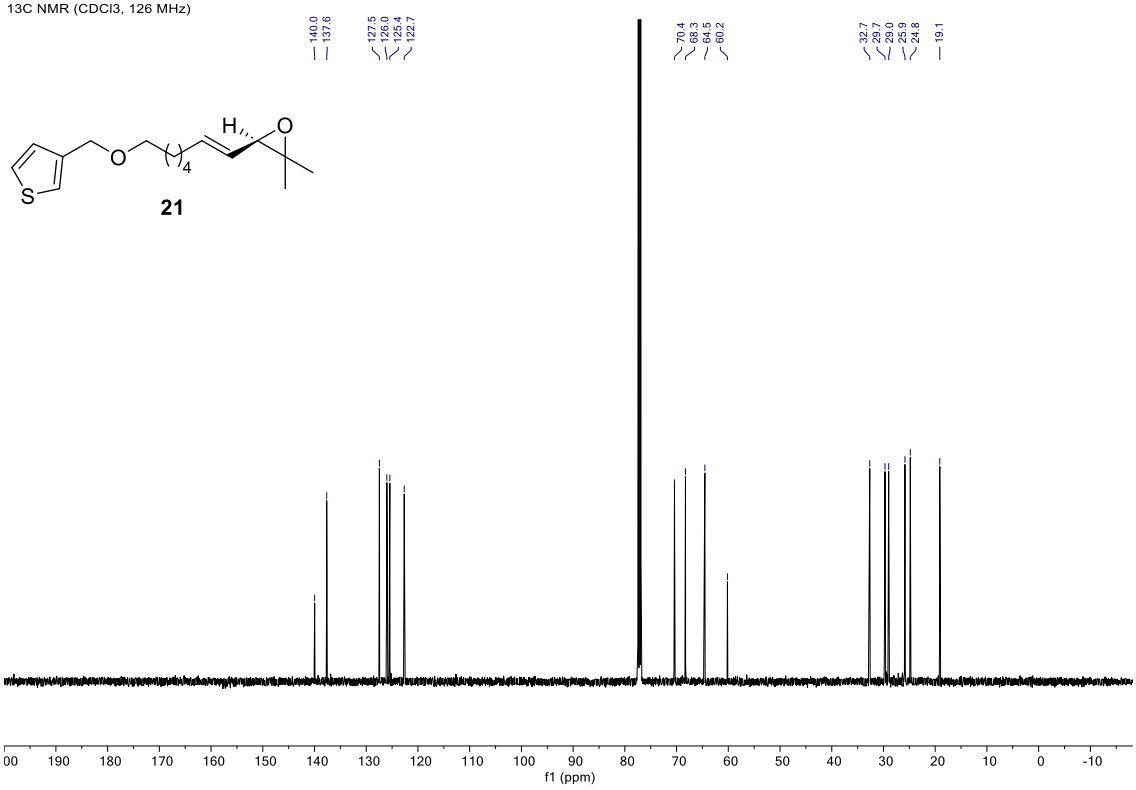
13C NMR (CDCl3, 126 MHz)



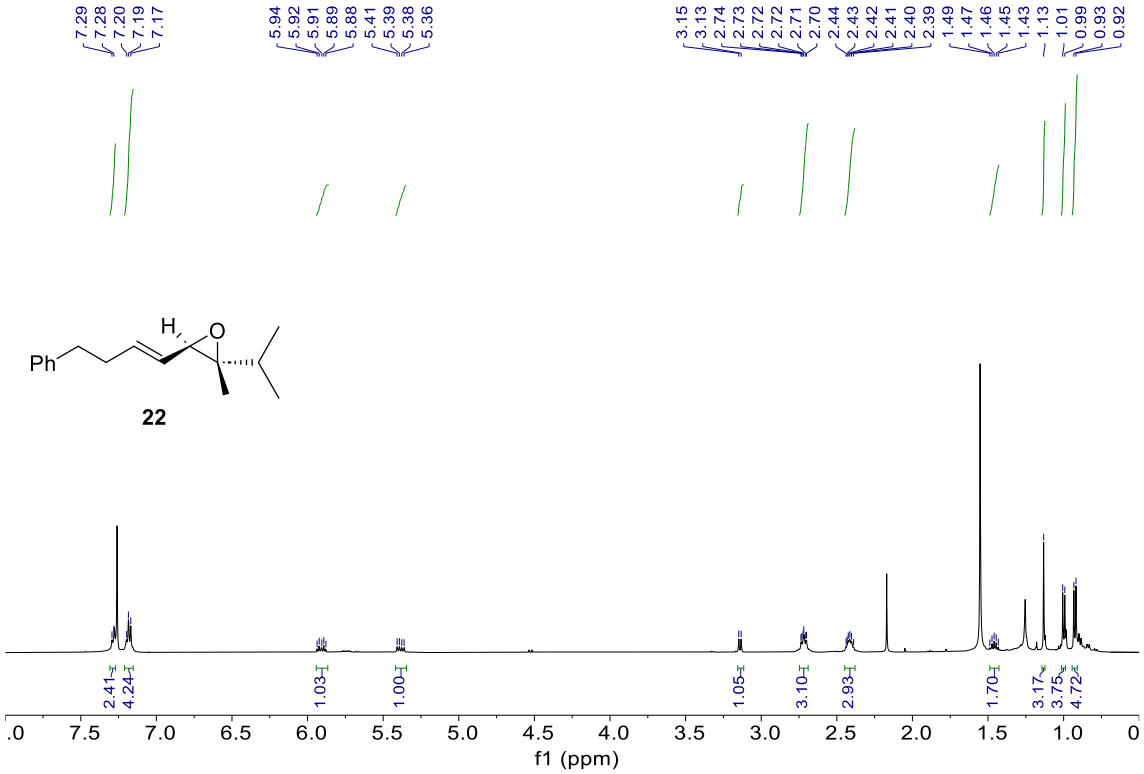
1H NMR (CDCl3, 300 MHz)



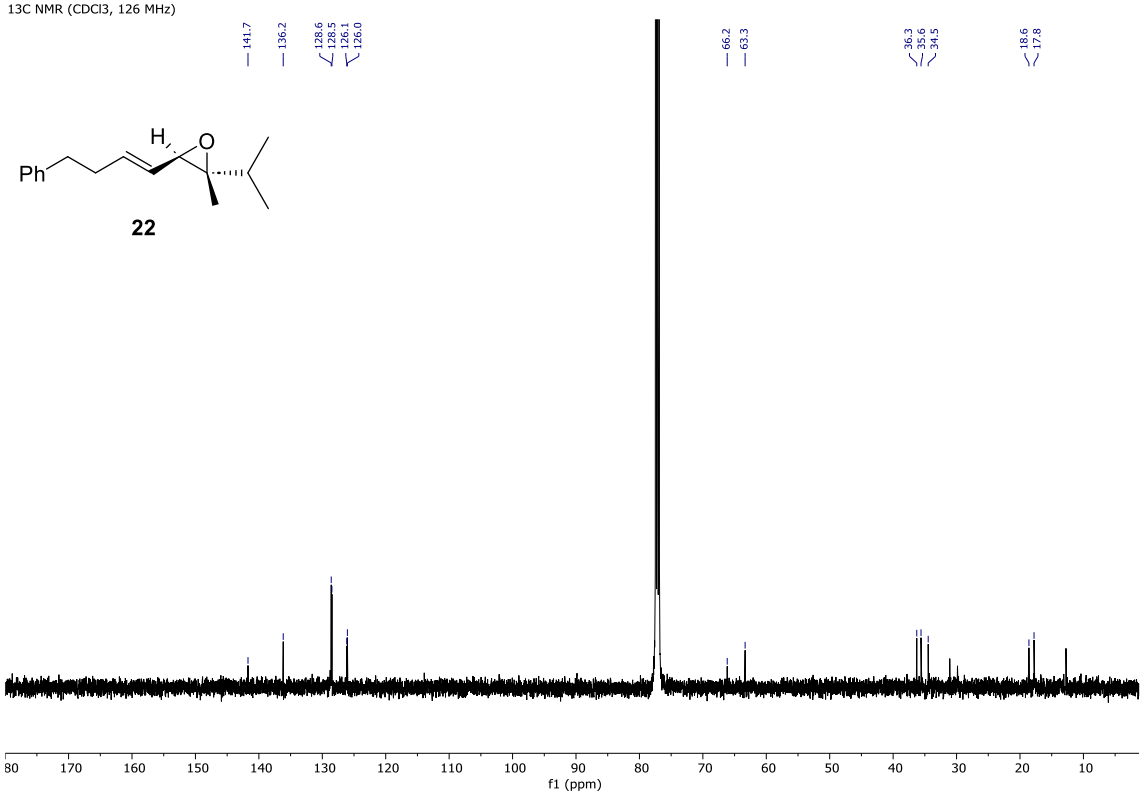
13C NMR (CDCl3, 126 MHz)

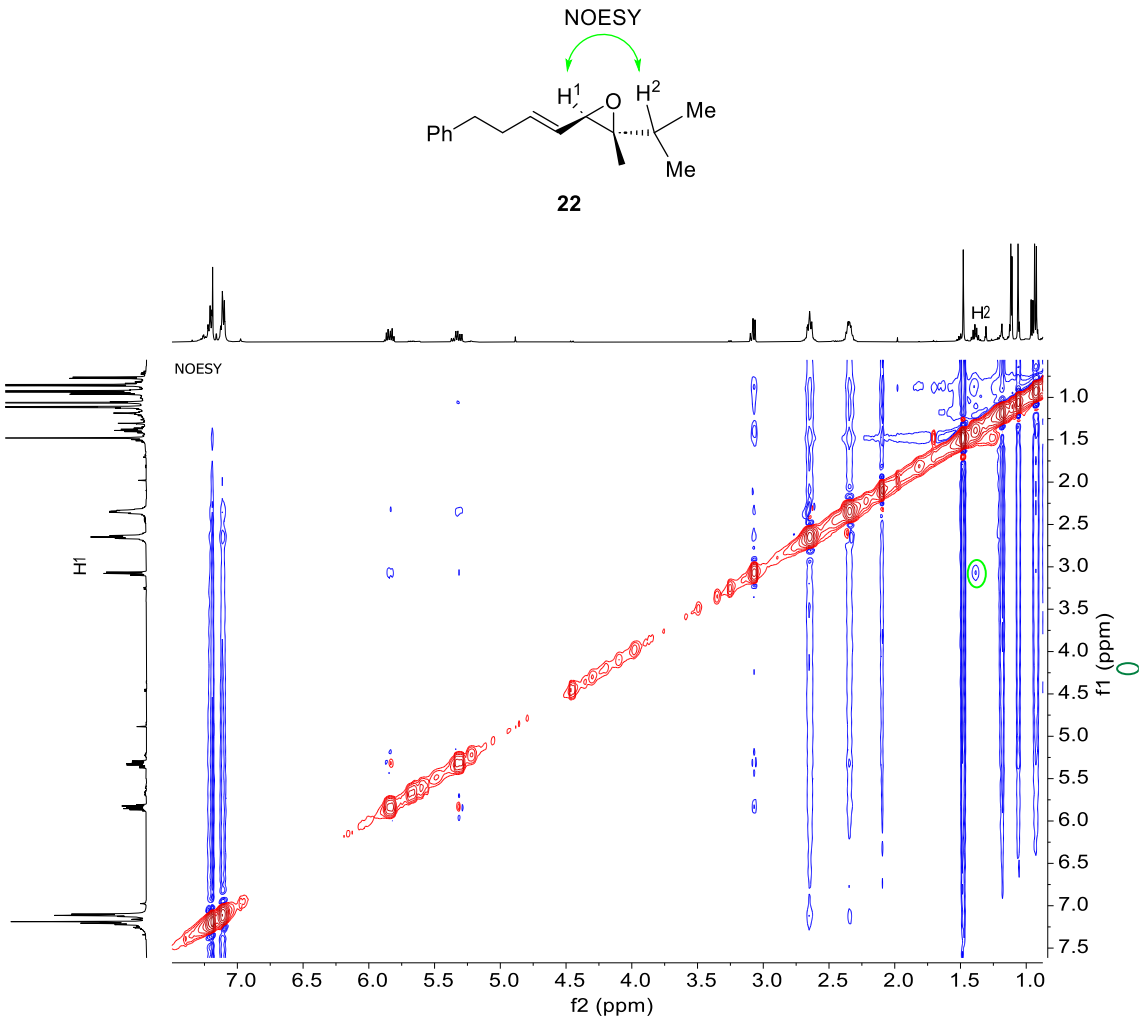


1H NMR (CDCl3, 500 MHz)

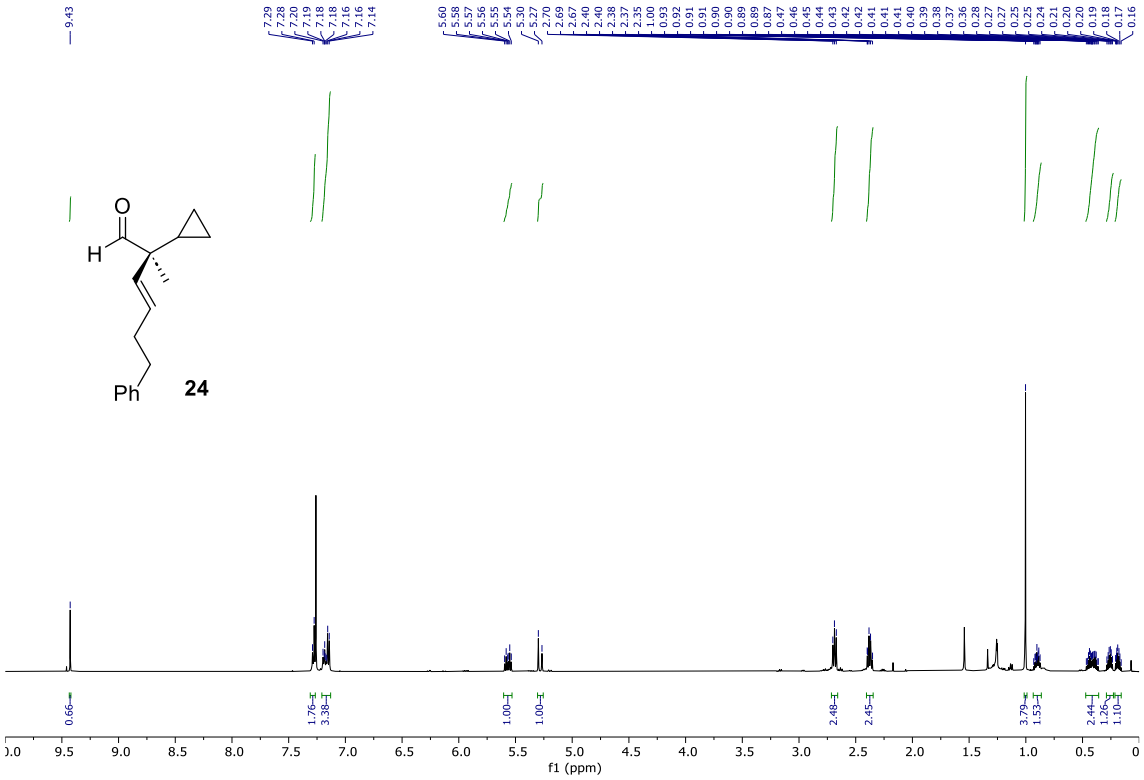


13C NMR (CDCl3, 126 MHz)

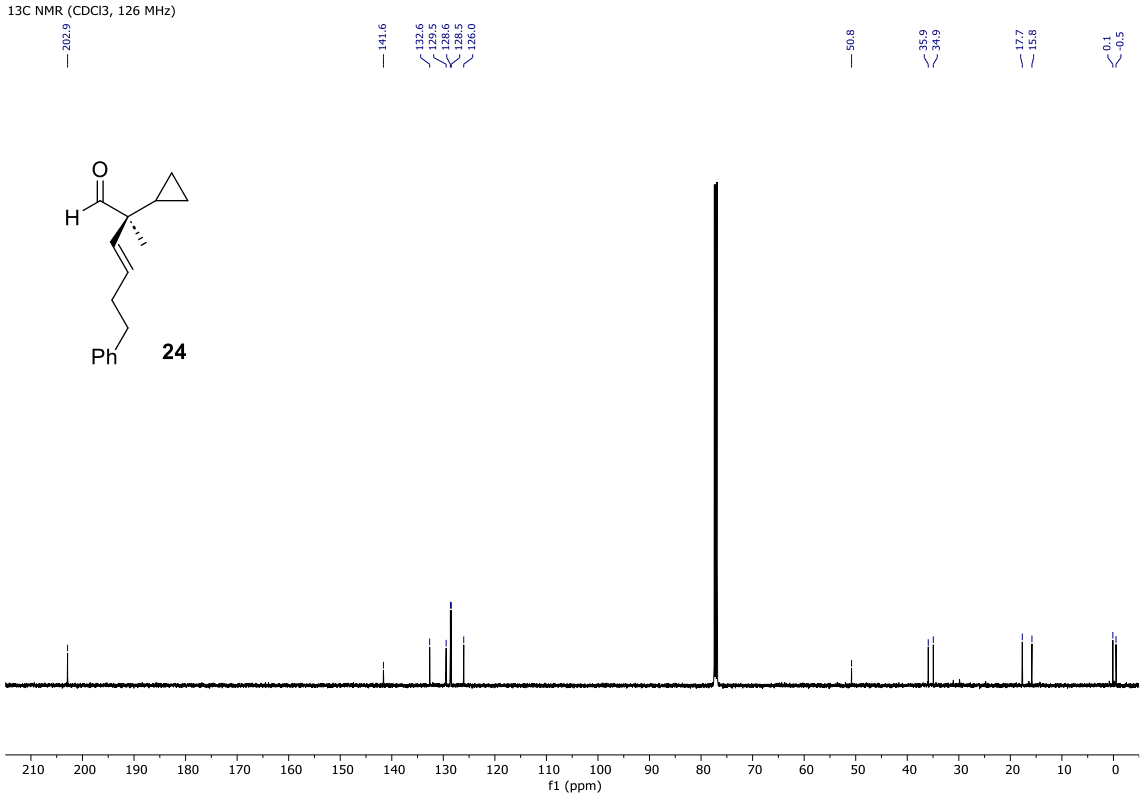



NOESY
H1
O
H2
Ph
Me
Me
22
NOESY
H1
H2
f2 (ppm)
f1 (ppm)

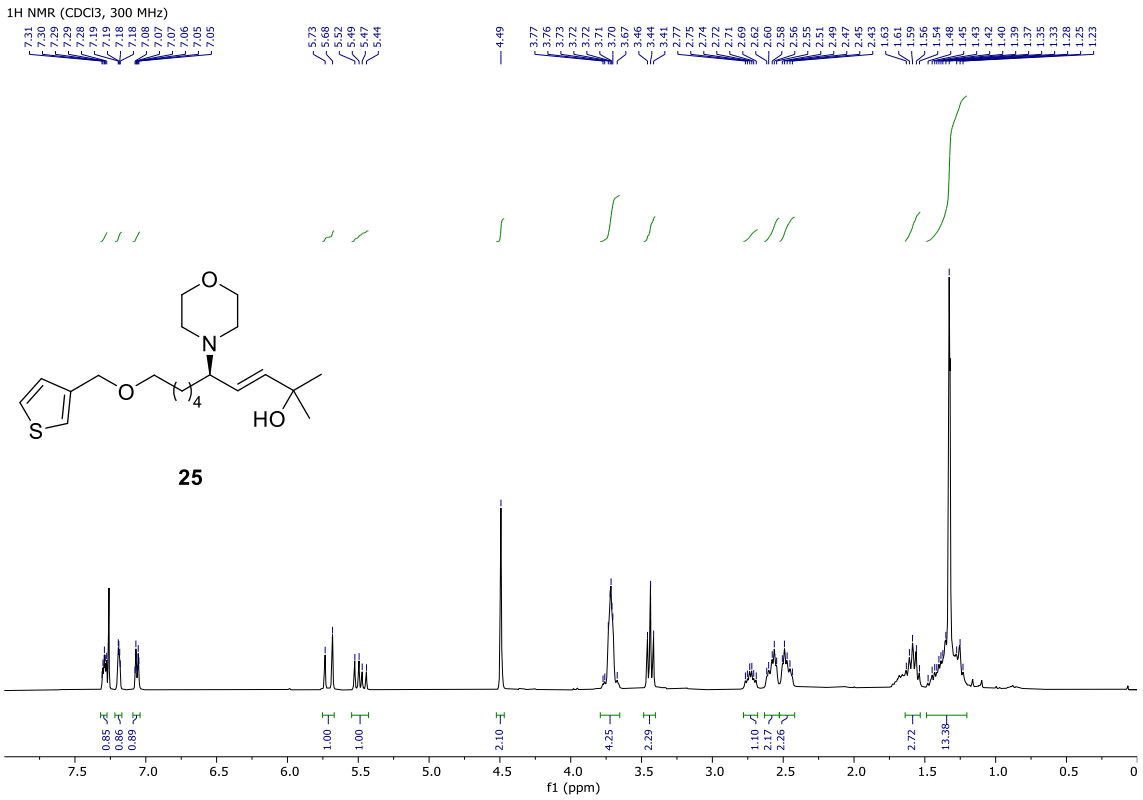
1H NMR (CDCl3, 500 MHz)



13C NMR (CDCl3, 126 MHz)

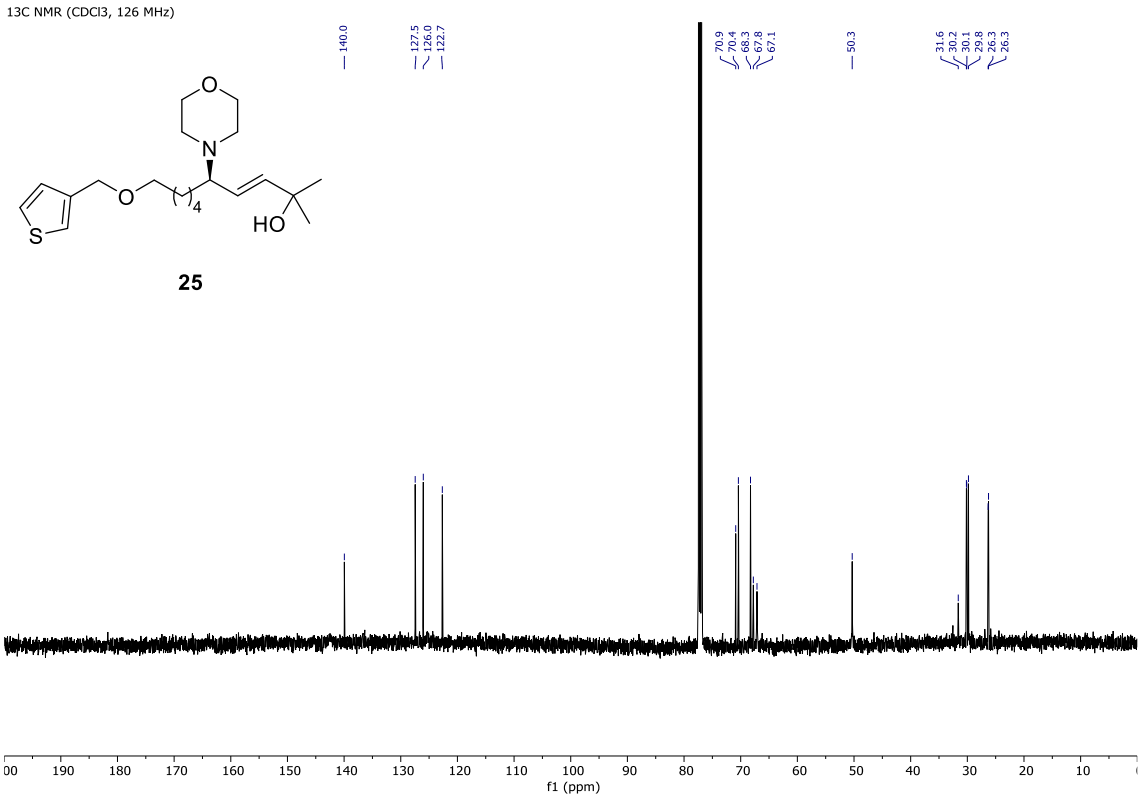


1H NMR (CDCl3, 300 MHz)



25

13C NMR (CDCl3, 126 MHz)



25

17. Computational details.

Theoretical mechanistic calculations were performed at DFT level of theory using Gaussian16 Revision C.01 software.[22] The structures of all the intermediates and transition states were optimized using the ωB97XD functional.[23] Geometric optimizations of all intermediates and transition states were used with basis set BS1. BS1 includes the 6-31G(d,p) basis set for the main group elements[2425262728293031] and the scalar relativistic Stuttgart-Dresden SDD pseudopotential and its associated double-ζ basis set,[32] complemented with a set of *f* polarization functions, for the copper atom. Nature of the optimized geometries, whether the stationary points are minimal (zero imaginary frequencies) or transition state (one imaginary frequency), was confirmed by frequency calculations at the same theoretical level. Connection of transition states with the corresponding intermediates was confirmed using intrinsic reaction coordinate (IRC) calculations and subsequent optimization to minimum.

Final Gibbs energies were calculated using the ωB97XD functional within the self-consistent reaction field (SCRF) using the PCM model (toluene)[333435363738] and a larger basis set BS2. BS2 consists of the *def2*-TZVP basis set for the main group elements and the quadruple-ζ *def2*-QZVP basis set for Cu.[3940] The final Gibbs energies were obtained

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[22] M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, Williams, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, D. J. Fox, *Gaussian 16 Rev. C.01*, **2016**,

[23] J.-D. Chai, M. Head-Gordon, *Phys. Chem. Chem. Phys.* **2008**, *10*, 6615-6620.

[24] R. Ditchfield, W. J. Hehre, J. A. Pople, *J. Chem. Phys.* **1971**, *54*, 724-728

[25] W. J. Hehre, R. Ditchfield, J. A. Pople, *J. Chem. Phys.* **1972**, *56*, 2257-2261

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[27] J. D. Dill, J. A. Pople, *J. Chem. Phys.* **1975**, *62*, 2921-2923

[28] M. M. Francl, W. J. Pietro, W. J. Hehre, J. S. Binkley, M. S. Gordon, D. J. DeFrees, J. A. Pople, *J. Chem. Phys.* **1982**, *77*, 3654-3665.

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[30] V. A. Rassolov, J. A. Pople, M. A. Ratner, T. L. Windus, *J. Chem. Phys.* **1998**, *109*, 1223-1229

[31] V. A. Rassolov, M. A. Ratner, J. A. Pople, P. C. Redfern, L. A. Curtiss, *J. Comput. Chem.* **2001**, *22*, 976-984.

[32] D. Andrae, U. Häußermann, M. Dolg, H. Stoll, H. Preuß, *Theor. Chim. Acta* **1990**, *77*, 123-141

[33] R. Improta, V. Barone, G. Scalmani, M. J. Frisch, *J. Chem. Phys.* **2006**, *125*.

[34] R. Improta, G. Scalmani, M. J. Frisch, V. Barone, *J. Chem. Phys.* **2007**, *127*

[35] G. Scalmani, M. J. Frisch, *J. Chem. Phys.* **2010**, *132*.

[36] D. M. York, M. Karplus, *The Journal of Physical Chemistry A* **1999**, *103*, 11060-11079

[37] S. Miertuš, J. Tomasi, *Chem. Phys.* **1982**, *65*, 239-245.

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[39] F. Weigend, R. Ahlrichs, *Phys. Chem. Chem. Phys.* **2005**, *7*, 3297-3305.

[40] D. Rappoport, F. Furche, *J. Chem. Phys.* **2010**, *133*.

adding the thermal and entropic corrections computed at the BS1 level to the electronic energy computed at BS2 level. The reaction profiles were built up in terms of ΔG_{sol}.

All 3D chemical structures were prepared using CYLview20.[41]

17.1 Conformer sampling details.

Conformational samplings were performed using meta-dynamics CREST package[42][43] with `--nci` and `--ewin 5` keywords. Analysis of the obtained conformers was performed through a custom-built Python script (ChemConf-Analysis),[44] based on root mean square deviation (RMSD) threshold and geometrical constrains. The script was build based on the following Python modules: `itertools`, `os`, `sys` and `shutil`. Moreover, the following packages were also included: `ChemCoord`,[45] `Pandas`,[46] `Numpy`[47] and `rmsd-1.6.3`.[48][49]

ChemConf-Analysis details:

ChemConf-Analysis is a combined Python/Linux script for conformational analysis of a *.xyz* file containing multiple structures (Figure S2).

The function of the script is as follows:

1. Get your `crest_conformers.xyz` file with multiple structures. Make sure the `.xyz` file saved the geometries in the proper format, including atom number and energy. This is crucial for line counting and slicing the document.
2. A new folder called "conformers" is created within the main directory. The `crest_conformers.xyz` file is sliced into *N* files containing one conformer each called "`conformer_N.xyz`", by using `islice()` iterator from `itertools` module.
3. Once each conformer is stored in independent files, rmsd-1.6.3 program is run through the bash terminal. `calculate_rmsd` functionality is implemented in a `for` loop comparing all the conformers, while storing rmsd values in "`raw_rmsd.csv`" file.
4. The first refinement step, based on RMSD threshold (1 Å), takes place by

[41] C. Y. Legault, *CYLview, 1.0b*, Université de Sherbrooke, **2009**, (http://www.cylview.org)
[42] S. Grimme, J. Antony, S. Ehrlich, H. Krieg, *J. Chem. Phys.* **2010**, *132*.
[43] S. Grimme, *Journal of Chemical Theory and Computation* **2019**, *15*, 2847-2862.
[44] A. M. Álvarez-Constantino, *ChemConf-Analysis (v1.0.0)* **2024**, Zenodo (https://doi.org/10.5281/zenodo.14266368)
[45] O. Weser, B. Hein-Janke, R. A. Mata, *J. Comput. Chem.* **2023**, *44*, 710-726.
[46] *pandas-dev/pandas: Pandas (v2.2.3)*, The pandas development team, **2024**, Zenodo (https://doi.org/10.5281/zenodo.13819579)
[47] C. R. Harris, K. J. Millman, S. J. van der Walt, R. Gommers, P. Virtanen, D. Cournapeau, E. Wieser, J. Taylor, S. Berg, N. J. Smith, R. Kern, M. Picus, S. Hoyer, M. H. van Kerkwijk, M. Brett, A. Haldane, J. F. del Río, M. Wiebe, P. Peterson, P. Gérard-Marchant, K. Sheppard, T. Reddy, W. Weckesser, H. Abbasi, C. Gohlke, T. E. Oliphant, *Nature* **2020**, *585*, 357-362.
[48] J. C. Kromann, *Calculate Root-mean-square deviation (RMSD) of Two Molecules Using Rotation. (v1.6.3).* , **2025**, GitHub (http://github.com/charnley/rmsd)
[49] D. F. Crouse, *IEEE Transactions on Aerospace and Electronic Systems* **2016**, *52*, 1679-1696.

combining a series of `for` and `if/else` loops that goes through the "`raw_rmsd.csv`" file. When the rmsd between two structures is lower than the indicated threshold (1 Å) the structure is moved apart and excluded in the next steps. The remained conformers are stored in "`clean_conf_list`" variable.

5. The second refinement step, based on geometrical constraint focused on distance of between the Cu and the *gem*-dichloride olefine (5 Å), takes place by combining a series of `for` and `if/else` loops. The loops go through the geometries stored in "`clean_conf_list`". If the Cu-C distance is equal or higher than the indicated threshold (5 Å) the structure is moved apart and excluded in the next steps. The remained conformers are stored in "`n_clean_conf_list`" variable.
6. The last refinement step, based on geometrical constraint focused on C-C bond distance (6.5 Å), takes place by combining a series of `for` and `if/else` loops. The loops go through the geometries stored in "`n_clean_conf_list`". If the C-C distance is equal or lower than the indicated threshold (6.5 Å) the structure is moved apart and excluded in the next step. The remained conformers are stored in "`nn_clean_conf_list`" variable.
7. The resulting structures were checked manually, and redundant structures were discarded.

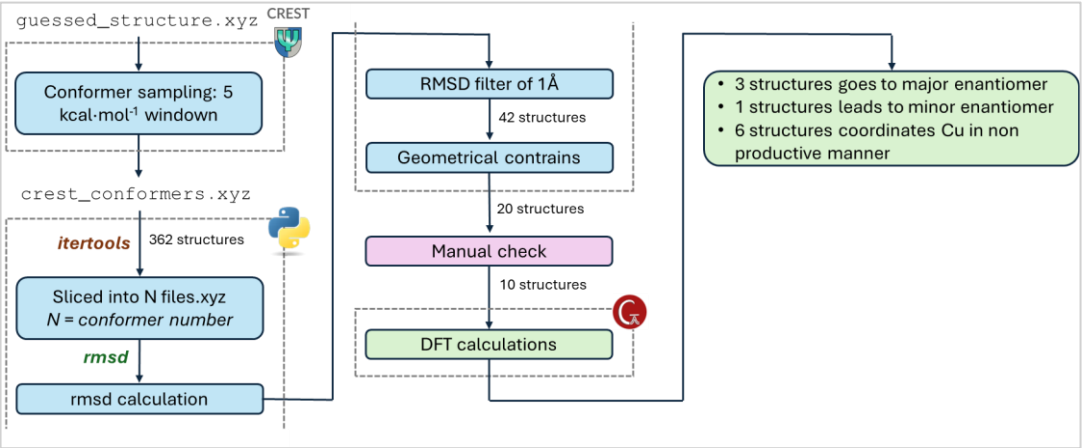

Figure S2. Schematic script work-flow chart.

This study revealed 362 possible structures within a 5 kcal·mol^{-1} energy window, and after several filters and geometrical constraints the number was reduced to 10. Six of these ten geometries were found not to evolve into the product. Out of the resulting four, three structures go to the major enantiomer and one to the minor enantiomer.

17.2. Energy profiles.

17.2.1. Formation of **(*R*)-5b-*E*** versus **(*S*)-5b-*E***

DFT calculations showed that two of the intermediates leading to the major enantiomer (**II-*E*,*R*** and **II'-*E*,*R***, black and red pathways in Figure S3) converged into the same pathway, while the other led to a more energetically demanding insertion step (**II"-*E*,*R***, green pathway). The major difference between them is the spatial orientation of the chiral ligand arms.

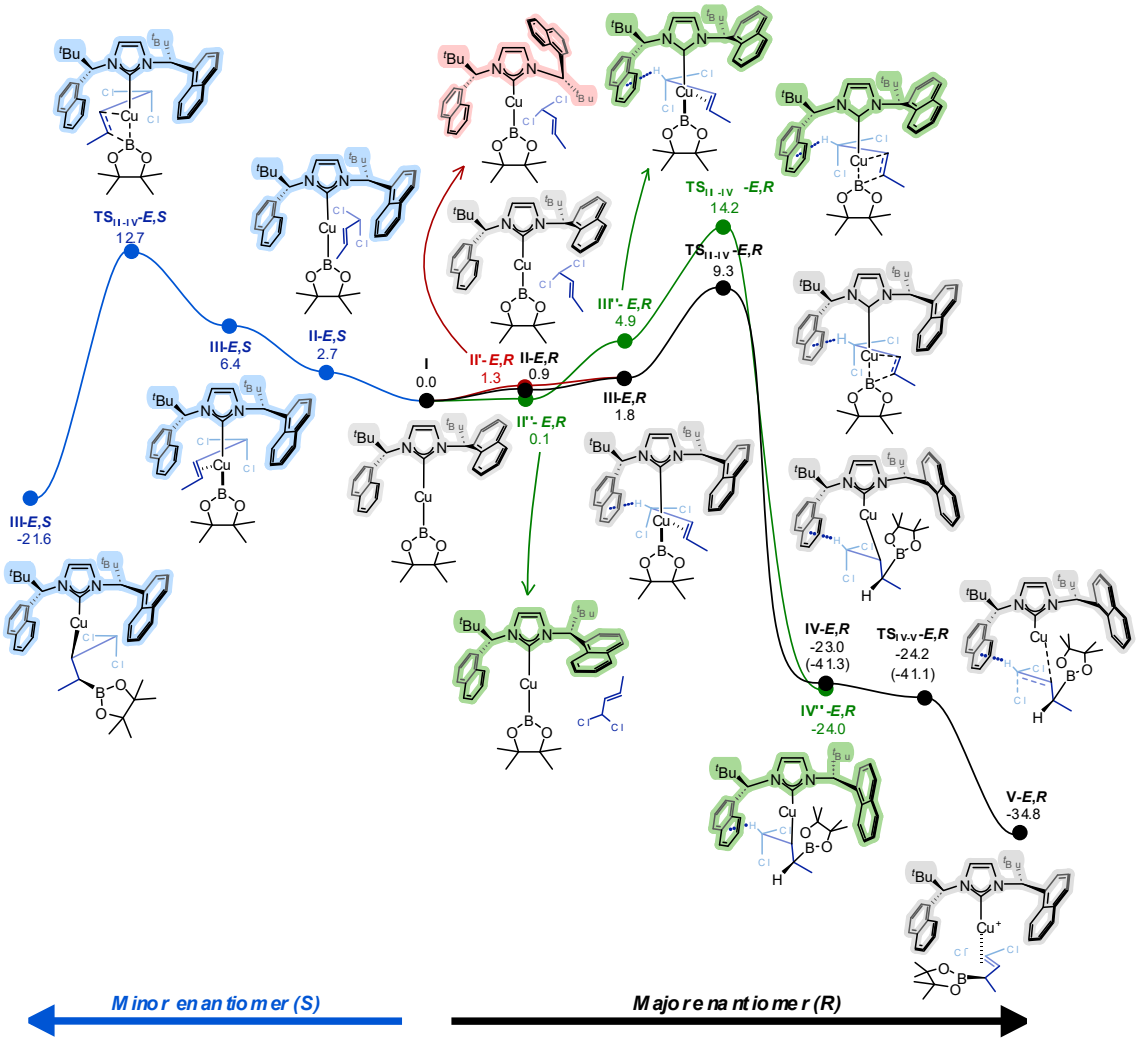

Figure S3. Free energy profile computed at the ωB97XD/def2-TZVP/def2-QZVP (Cu) (scrf=smd, toluene) //ωB97XD/6-31G(d,p)/SDD+f (Cu) level for the pathways associated to the formation of **(*R*)-5b -*E*** (black, red and green pathways) and **(*S*)-5b -*E*** (blue pathway). The numbers are Gibbs energies in kcal·mol^{-1} and are relative to complex **I** combined with those of the relevant substrates. Numbers in parentheses are Enthalpy energies in kcal·mol^{-1} and are relative to complex **I** combined with those of the relevant substrates.

After olefin insertion into the borylcopper complex, reaction profile energetically falls to a minimum from where the resulting σ-Cu(I) complex **IV-*E*,*R*** would undergo β-Cl elimination (**TS$_{IV-V}$-*E*,*R***), leading to the chiral allylboron product π-coordinated to the NHC-Cu-Cl catalyst. At the light of the energy profile, insertion behaves as the enantiodetermining step as long as **TS$_{III-IV}$-*E*,*R*** is 3.4 kcal·mol^{-1} lower in energy than competing enantiomer **TS$_{III-IV}$-*E*,*S*** (blue pathway), and the process is irreversible.

17.2.2. Formation of **(*R*)-5b-*E*** versus **(*R*)-5b-*Z***

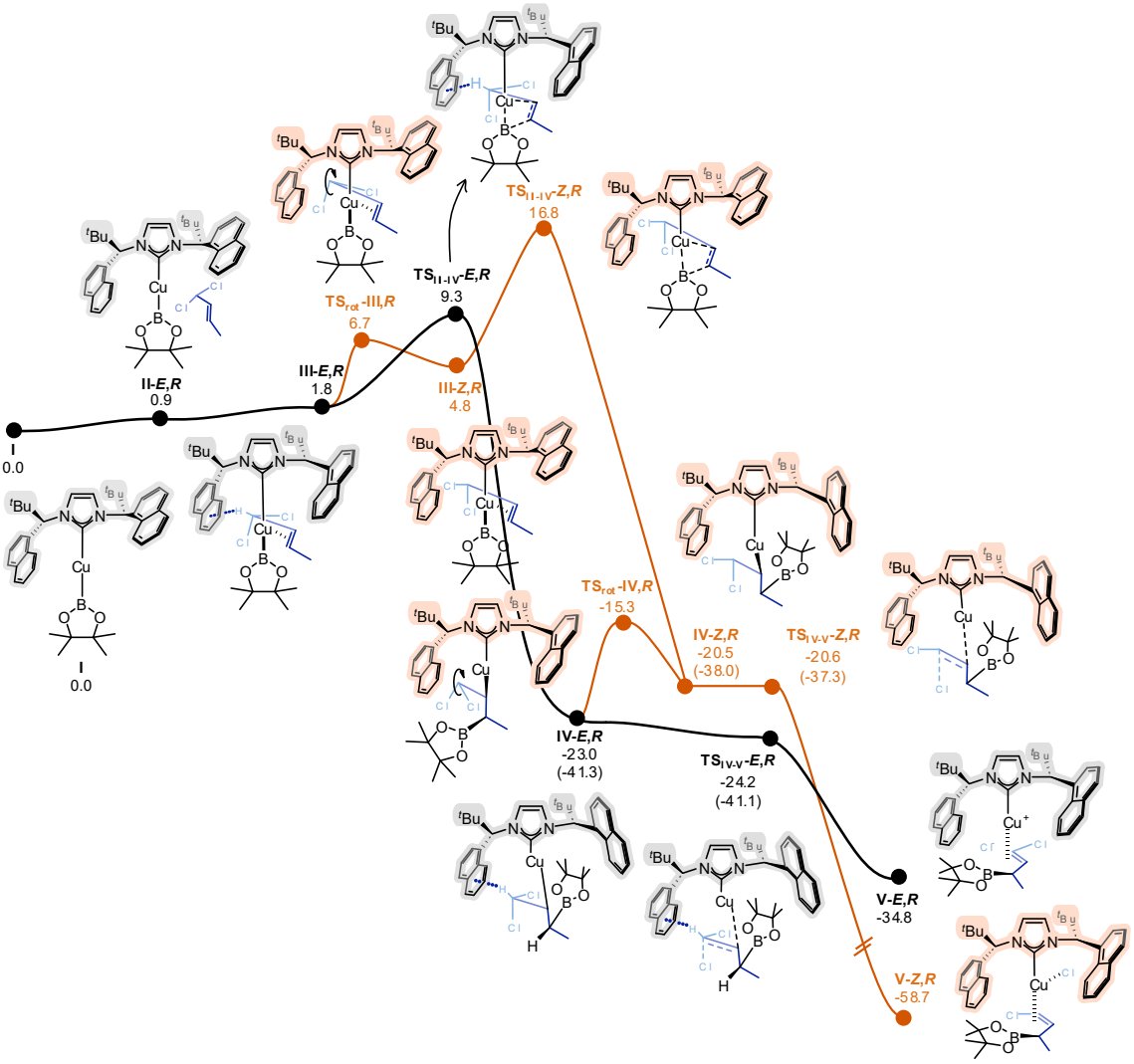

Figure S4. Free energy profile computed at the ωB97XD/def2-TZVP/def2-QZVP (Cu) (scrf=smd, toluene) //ωB97XD/6-31G(d,p)/SDD+f (Cu) level for the pathways associated to the formation of **(*R*)-5b -*E*** (black pathway) and **(*R*)-5b -*Z*** (orange pathway). The numbers are Gibbs energies in kcal·mol^{-1} and are relative to complex **I** combined with those of the relevant substrates. Numbers in parentheses are Enthalpy energies in kcal·mol^{-1} and are relative to complex **I** combined with those of the relevant substrates.

17.2.3. Formation of **(*S*)-5b-*E*** versus **(*S*)-5b-*Z***

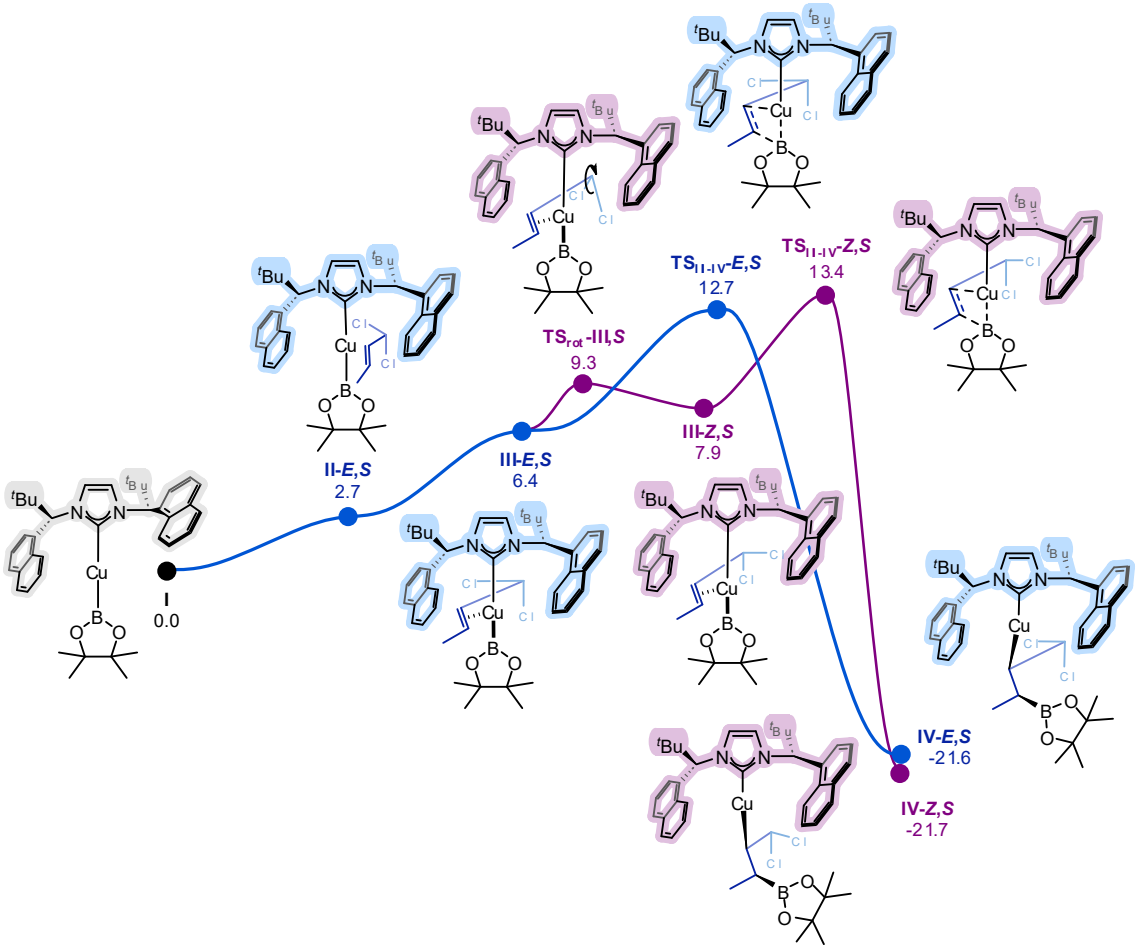

Figure S5. Free energy profile computed at the ωB97XD/def2-TZVP/def2-QZVP (Cu) (scrf=smd, toluene) //ωB97XD/6-31G(d,p)/SDD+f (Cu) level for the pathways associated to the formation of **(*S*)-5b-*E*** (blue pathway) and **(*S*)-5b-*Z*** (purple pathway). The numbers are Gibbs energies in kcal·mol^{-1} and are relative to complex **I** combined with those of the relevant substrates.

For the sake of completeness, the isomerization from the minor enantiomer was also studied (Figure S5). Intermediate **III-*E*,*S*** was found to easily rotate towards the pro-*Z* disposition. From there, subsequent insertion (**TS$_{III-IV}$-*Z*,*S***; pink pathway) features similar energy barrier than the pro-*E* transition state **TS$_{III-IV}$-*E*,*S*** (blue pathway) ($\Delta\Delta G^{\ddagger}$ = -0.7 kcal·mol^{-1}). This is in contrast to the major enantiomer pathway, where the formation of the *E* conformation is far more favored than the *Z* one ($\Delta\Delta G^{\ddagger}$ = -7.5 kcal·mol^{-1}, **TS$_{III-IV}$-*E*,*S*** *vs* **TS$_{III-IV}$-*Z*,*S***).

17.3. Non-covalent interaction (NCI) analysis.

In order to rationalize the origins of enantioselectivity and *Z* selectivity, we analyzed the structures of the corresponding stereodetermining transitions states involved in the formation of **(*R*)-5b-*E***, **(*S*)-5b-*E***, **(*R*)-5b-*Z*** and **(*S*)-5b-*Z*** (i.e. **TS$_{III-IV}$-*E*,*R***, **TS$_{III-IV}$-*E*,*S***, **TS$_{III-IV}$-*Z*,*R*** and **TS$_{III-IV}$-*Z*,*S***) by performing a NCI plot analysis of these structures.

Non-Covalent Interaction (NCI) analysis was performed using NCI theory[50] embedded in Multiwfn 3.8 software.[51] Attractive forces (blue) and weak attractive Van der Waals interactions (green) were plotted with at iso-surfaces of s(r) = 0.40. Repulsive forces (red) and weak repulsive Van der Waals interactions (brownish green) were plotted with at iso-surfaces of s(r) = 0.30. Color code corresponds with sign(λ2)ρ in a.u.. NCI surfaces were plotted using VMD software.[52]

Note: Regarding non-stabilizing distorsion interactions, similar plots were obtained for all the structures.

[50] E. R. Johnson, S. Keinan, P. Mori-Sánchez, J. Contreras-García, A. J. Cohen, W. Yang, *J. Am. Chem. Soc.* **2010**, *132*, 6498-6506.
[51] T. Lu, F. Chen, *J. Comput. Chem.* **2012**, *33*, 580-592.
[52] W. Humphrey, A. Dalke, K. Schulten, *J. Mol. Graph.* **1996**, *14*, 33-38.

17.3.1. NCI plots for **$TS_{III\text{-}IV}$- *E,R***

Analysis of the NCI plots derived from the transition state involved in the insertion step that leads to the major enantiomer **(*R*)-5b-*E*** (Figure S6), revealed that the Cα(sp^3)-H establishes a strong interaction with the second ring of the naphthyl moiety (red circle), combined with the Csp^2-H···π interaction (orange circle).
Geometrical parameters are summarized in Table S6 (see section 17.3.5) and are in agreement with literature values (Table S7).

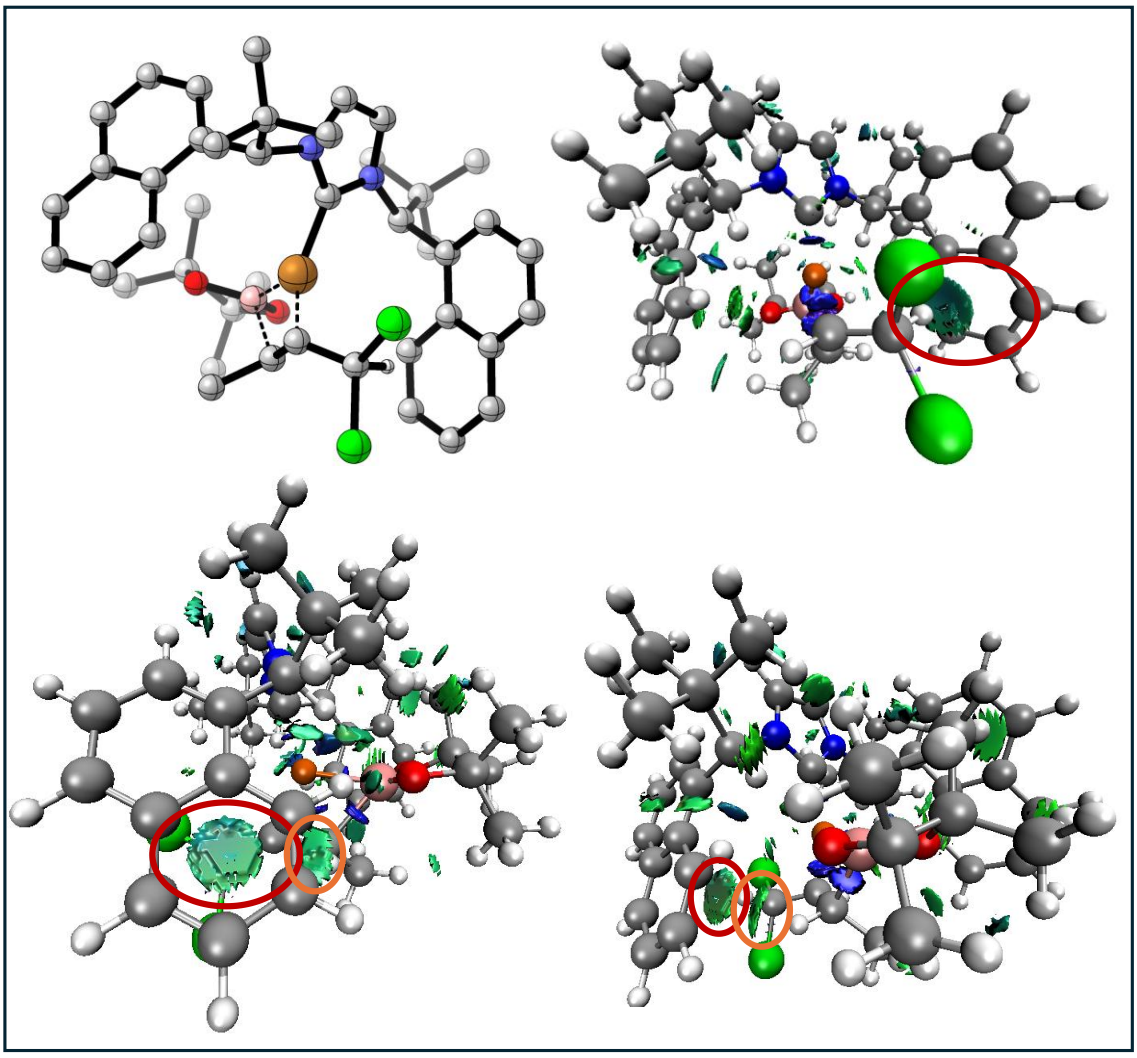

Figure S6. Attractive interactions for **$TS_{III\text{-}IV}$-*E,R*** visualized from different angles. The explicit hydrogens are the ones involved in indicated interactions.

In addition to those, NCI plots also revealed that Bpin unit engenders weak attractive sp^3-CH ···π interactions between the Me groups − from the Bpin unit − and the closer naphthyl ring, while stablishing lone pair···π (O···Naphthyl) interactions (Figure S6). Geometrical parameters are summarized in Table S7 and are in agreement with literature values (Table S7).

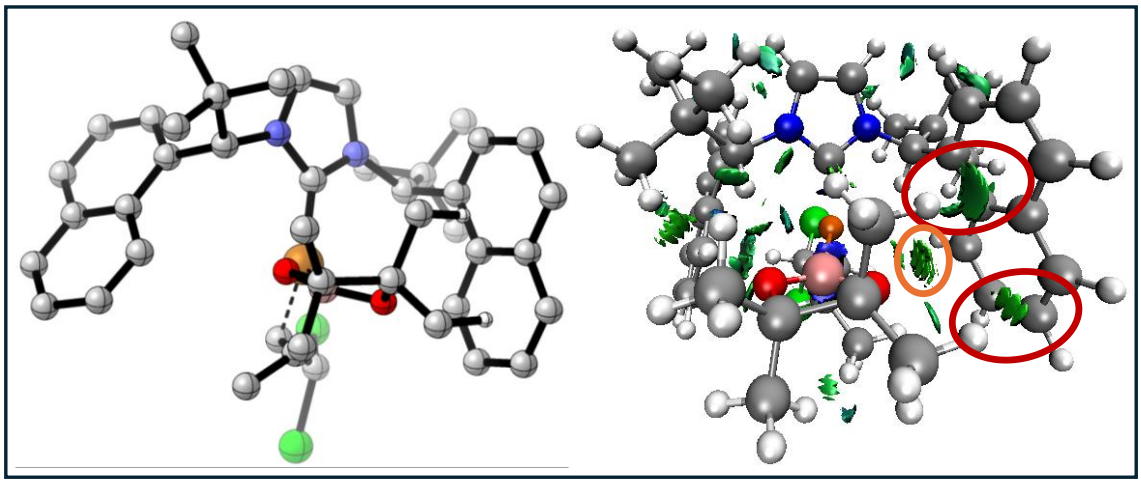

Figure S7. Attractive interactions for **TS$_{III\text{-}IV}$-*E*,*R*** focused in the Bpin region. The explicit hydrogens are the ones involved in indicated interactions.

17.3.2. NCI plots for **$TS_{III\text{-}IV}$-*E*,*S***

Analysis of the NCI plots derived from the transition state involved in the insertion step that leads to the minor enantiomer **(*S*)-5b-*E*** (Figure S8), revealed that the Cα(sp^3)-H···π interaction is absent. However, combined with the Cγ(sp^2)-H···π interaction (orange circle). In addition to those, NCI plots also revealed that interactions involving Bpin unit are present (green and blue circles), similar to the ones observed in **(*R*)-5b-*E*** (Figure S7). Geometrical parameters are summarized in Table S6 and are in agreement with literature values (Table S7).

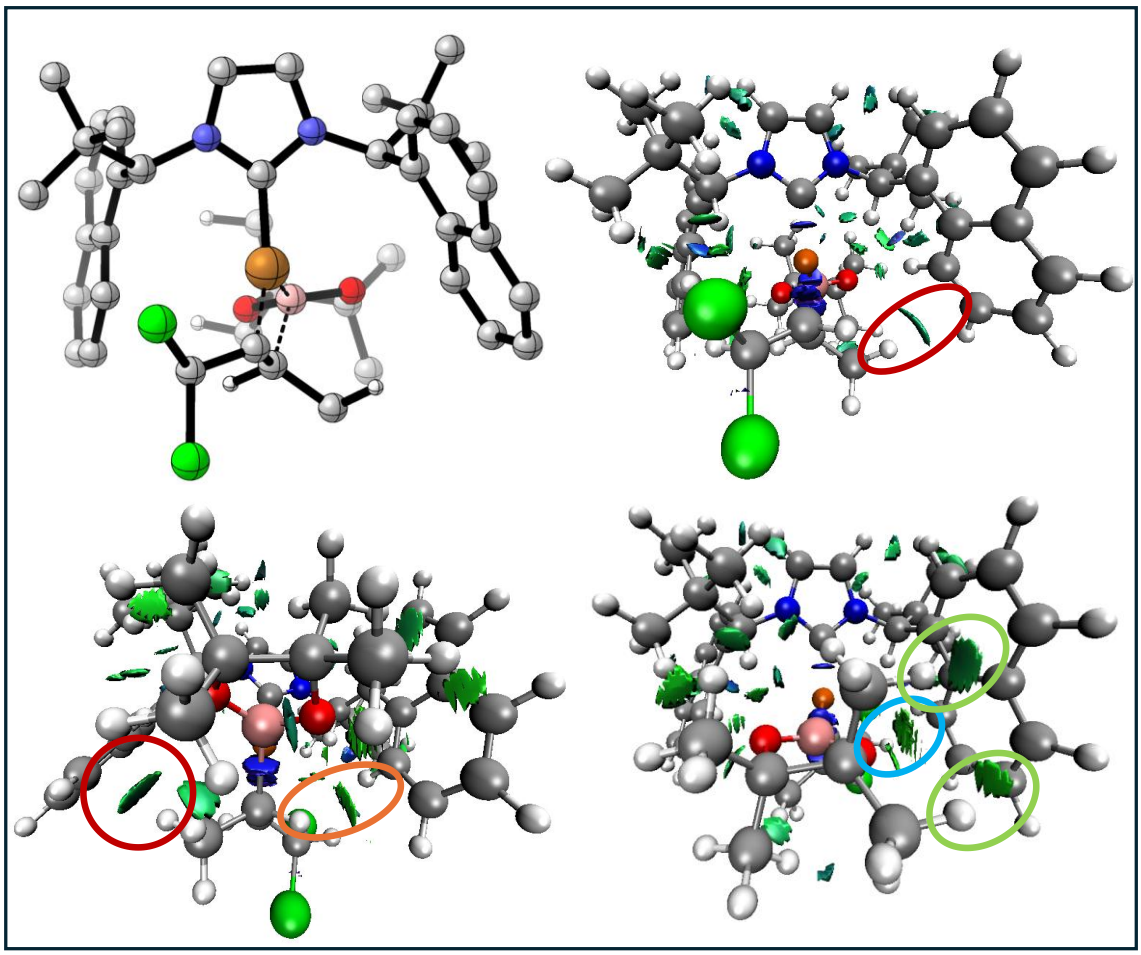

Figure S8. Attractive interactions for **$TS_{III\text{-}IV}$-*E*,*S*** visualized from different angles. The explicit hydrogens are the ones involved in indicated interactions.

17.3.3. NCI plots for **TS$_{III-IV}$-*Z*,*R***

Analysis of the NCI plots derived from the transition state involved in the insertion step that leads to the minor *Z*-isomer **(*R*)-5b-*Z***, derived from rotation at **II-*E*,*R*** step (Figure S9). it could be clearly appreciated that the adopted geometry does not allow to stablish any kind of attractive forces between the allylic *gem*-dichloride and the ligand.

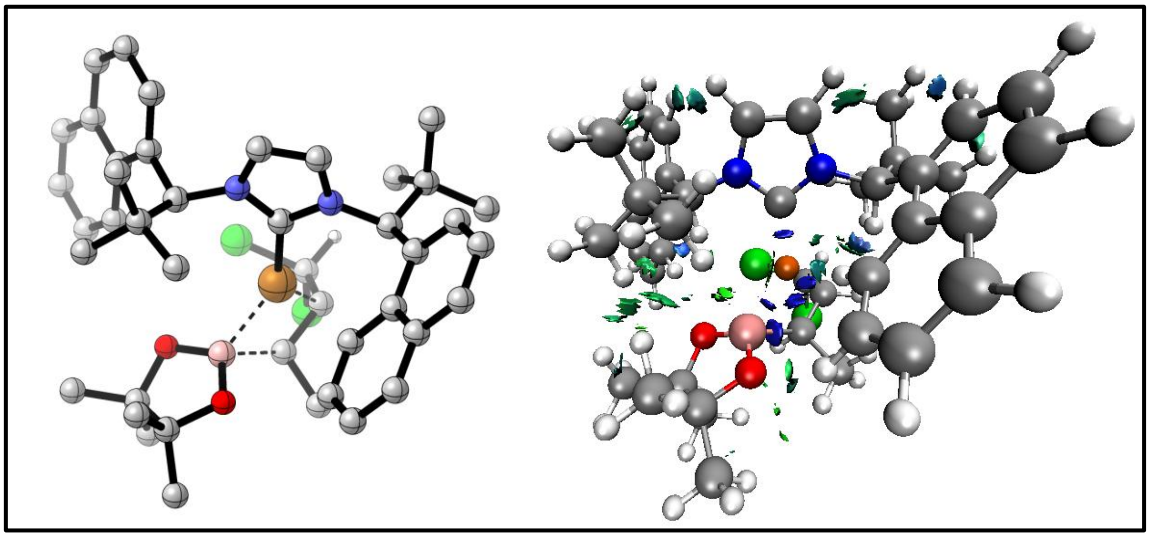

Figure S9. General view of attractive interactions for **TS$_{III-IV}$-*E*,*S***.

17.3.4.NCI plots for **$TS_{III\text{-}IV}$-*Z*,*S***

Analysis of the NCI plots derived from the transition state involved in the insertion step that leads to the minor minor *Z*-isomer **(*S*)-5b-*Z***, derived from rotation at **II-*E*,*S*** stage (Figure S10), revealed that the Cα(sp^3)-H ···π interaction is absent while one Cγ(sp^2)-H···π interaction was observed (red circle). In addition to those, NCI plots also revealed that interactions involving Bpin unit are present (green and blue circles), similar to the ones observed in **$TS_{III\text{-}IV}$-*E*,*R*** (Figure S7). Geometrical parameters are summarized in Table S6 and agree with literature values (Table S7).

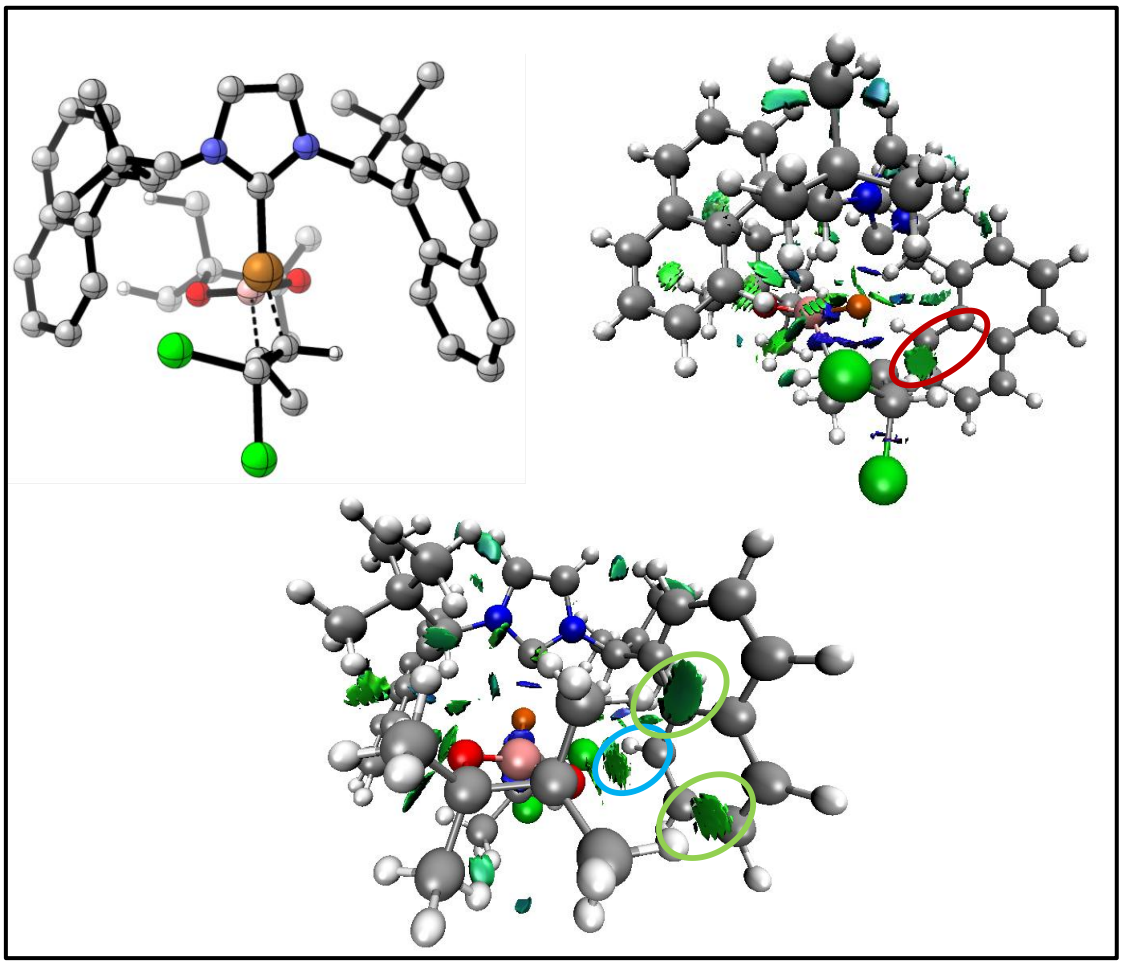

Figure S10. Attractive interactions for **$TS_{III\text{-}IV}$-*Z*,*S*** visualized from different angles. The explicit hydrogens are the ones involved in indicated interactions.

17.3.5. Geometrical parameters of the observed NCI

In Table S6, displayed interactions in Figures S6-S10 are summarized, including the geometrical parameters distance (**d**) and angle (**α**). For the sake of comparison, literature values are included in Table S7.[53]

Table S6. Compiled observed interactions involving π-orbitals from ligand naphthyl rings.

Structure	Interactions	d / Å	α / º	Energy / kcal·mol^{-1}
TS$_{III-IV}$-*E*,*R*	$RCl_2CH\cdots\pi$	2.40	178	9.3
	sp^2-CH$\cdots\pi$	2.67	144	
	Ln(O)$\cdots\pi$	3.43	-	
	sp^3-CH$\cdots\pi$	2.80	163	
	sp^3-CH$\cdots\pi$	3.23	137	
TS$_{III-IV}$-*E*,*S*	sp^3-CH$\cdots\pi$	2.59	157	12.7
	sp^2-CH$\cdots\pi$	3.14	127	
	Ln(O)$\cdots\pi$	3.28	-	
	sp^3-CH$\cdots\pi$	2.61	157	
	sp^3-CH$\cdots\pi$	3.14	139	
TS$_{III-IV}$-*Z*,*S*	sp^2-CH$\cdots\pi$	2.96	151	13.4
	Ln(O)$\cdots\pi$	3.23	-	
	sp^3-CH$\cdots\pi$	2.58	168	
	sp^3-CH$\cdots\pi$	3.00	149	

Table S7. Data extracted from literature[53]

Interactions	d / Å	α / º	Energy / kcal·mol^{-1}
$RCl_2CH\cdots\pi$	2.62 ± 0.15	151 ± 13	3.6 - 4.0
sp^2-CH$\cdots\pi$	2.73 ± 0.13	148 ± 11	1.2 - 1.6
sp^3-CH$\cdots\pi$	2.75 ± 0.10	148 ± 13	1.03 – 1.13

Further support for the presence of interactions involving π-orbitals of the ligand with the substrate was achieved by adding (and subtracting) the energies in the Table S7 to **TS$_{III-IV}$-*E*,*R*** energy, according to the establishment (or lack) of interactions (Figure S11). This further validates the observed iso-surfaces regarding non-covalent interactions.

[53] S. Tsuzuki; A. Fujii. "Nature and physical origin of CH/π interaction: significant difference from conventional hydrogen bonds." *Phys. Chem. Chem. Phys.* **2008**, *10*, 2584-2594

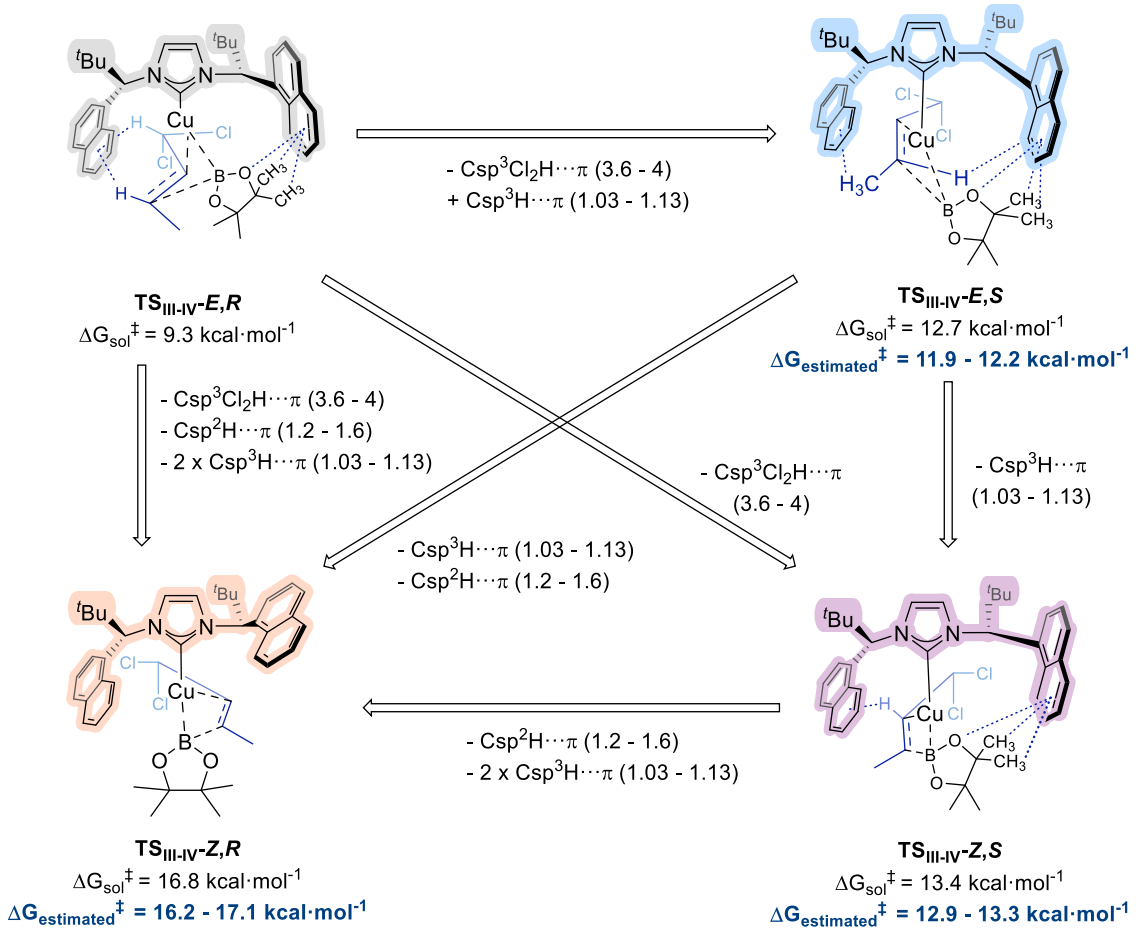

Figure S11. Influence of the presence and absence of supramolecular interactions with ligand, and calculation of estimated $\Delta G^{\ddagger}$ ($\Delta G_{estimated}^{\ddagger}$) by adding and subtracting corresponding interaction energy to **TS$_{III-IV}$-*E*,*R*** energy. Number ins parentheses refer to energy displayed by indicated interactions (in kcal·mol^{-1}).

17.4. Cartesian coordinates

1

Electronic Energy BS1 = -1076.32616532 Hartree
Electronic Energy BS2 = -1076.45550939 Hartree
Zero-point Energy Correction = 0.091507 Hartree
Thermal Correction to Enthalpy = 0.099665 Hartree
Thermal Correction to Free Energy = 0.058889 Hartree

Chemical symbol X, Y, Z

C	3.362720	-0.000053	-0.189598
H	3.927904	0.880076	0.135244
H	3.322216	0.000089	-1.281465
H	3.927753	-0.880374	0.135003
C	1.993279	-0.000027	0.412807
H	1.942678	0.000047	1.501898
C	0.858600	-0.000119	-0.283790
H	0.857012	-0.000196	-1.371204
C	-0.477053	-0.000129	0.372339
H	-0.402662	-0.000016	1.458355
Cl	-1.411655	1.470858	-0.072013
Cl	-1.411885	-1.470720	-0.072009

I

Electronic Energy BS1 = -1996.86379721 Hartree
Electronic Energy BS2 = -3440.73808633 Hartree
Zero-point Energy Correction = 0.802454 Hartree
Thermal Correction to Enthalpy = 0.846834 Hartree
Thermal Correction to Free Energy = 0.724043 Hartree

Chemical symbol X, Y, Z

C	-5.494359	-1.846792	1.346622

C	-5.112539	-3.159822	1.271635
C	-3.877833	-3.530221	0.676397
C	-3.019224	-2.522319	0.140573
C	-3.456549	-1.169891	0.232356
C	-4.650920	-0.844182	0.821185
H	-4.156124	-5.645309	1.029854
H	-6.438620	-1.575900	1.808682
H	-5.749294	-3.944634	1.671158
C	-3.490063	-4.892872	0.616576
C	-1.771246	-2.922460	-0.452512
H	-2.867324	-0.344827	-0.148730
H	-4.928502	0.203041	0.879844
C	-1.446456	-4.260006	-0.482404
C	-2.298238	-5.250868	0.050874
H	-0.513858	-4.582524	-0.930074
H	-1.999144	-6.293122	0.005190
C	-0.835556	-1.867682	-1.019971
H	-1.256731	-0.895955	-0.769703
C	-0.692475	-1.807968	-2.574313
C	0.232161	-0.632023	-2.929796
H	0.247880	-0.487190	-4.014829
H	-0.115385	0.298767	-2.466608
H	1.261517	-0.804069	-2.600132
C	-2.097225	-1.525694	-3.131969
H	-2.793564	-2.334648	-2.891448
H	-2.504681	-0.594474	-2.723751
H	-2.054193	-1.426858	-4.221153
C	-0.149048	-3.087313	-3.222540
H	0.852043	-3.340210	-2.859460
H	-0.813351	-3.939946	-3.060414
H	-0.066725	-2.935375	-4.303634
N	0.454527	-1.812609	-0.310886
C	0.827729	-0.674115	0.327463
C	1.469044	-2.752273	-0.273354
C	2.497626	-2.189175	0.401691
H	1.391416	-3.730260	-0.713417
H	3.479190	-2.566976	0.635670
N	2.082622	-0.923242	0.767500
C	2.911464	0.076174	1.461900
H	2.390839	1.022356	1.289225
C	4.244326	0.165216	0.721448
C	4.255845	0.789220	-0.576726
C	5.411741	-0.378894	1.201718
C	5.474022	0.823565	-1.316610
C	3.104464	1.372755	-1.176760
C	6.619648	-0.332656	0.468648
H	5.430253	-0.857956	2.170983
C	5.500624	1.423741	-2.602380
C	6.650621	0.253956	-0.764049
C	3.160508	1.941533	-2.424033
H	2.150027	1.372986	-0.663442
H	7.516363	-0.770377	0.895170
C	4.370181	1.969042	-3.150566
H	6.441152	1.440093	-3.146296
H	7.571564	0.291656	-1.339170
H	2.261336	2.374893	-2.850352
H	4.401295	2.423120	-4.135787
C	2.860930	-0.100484	3.014167
C	3.204655	-1.516386	3.506154
H	2.500119	-2.251795	3.106642
H	4.213727	-1.844414	3.248028
H	3.124335	-1.545868	4.597355
C	1.415904	0.193258	3.463488
H	1.098297	1.198807	3.166270
H	0.703255	-0.518490	3.038359
H	1.347456	0.126041	4.553862
C	3.771577	0.950504	3.670019
H	3.539421	1.952749	3.293745
H	3.605864	0.955754	4.751785
H	4.832943	0.768048	3.493839
Cu	-0.307401	0.921902	0.420465
C	-3.733265	3.240673	-0.349051
C	-2.862063	4.335011	0.345457
C	-5.166799	3.140652	0.157277
H	-5.705608	4.079842	-0.008102
H	-5.693661	2.348359	-0.383205
H	-5.196928	2.904479	1.222834
C	-3.728907	3.348223	-1.877208
H	-4.171323	2.439071	-2.293827
H	-4.307777	4.208410	-2.227685
H	-2.706971	3.433231	-2.256845
C	-2.799159	5.666701	-0.391983
H	-3.797805	6.107783	-0.483146
H	-2.167153	6.365116	0.163342
H	-2.374755	5.549412	-1.390577
C	-3.250654	4.567669	1.808842
H	-2.477199	5.176542	2.284003
H	-4.208458	5.089969	1.898203
H	-3.313444	3.619277	2.349537
B	-1.688216	2.351428	0.265285
O	-1.557233	3.734731	0.344318
O	-3.028893	2.037422	-0.009020

II'-E,R

Electronic Energy BS1 = -3073.22004048 Hartree
Electronic Energy BS2 = -4517.17750709 Hartree
Zero-point Energy Correction = 0.895369 Hartree
Thermal Correction to Enthalpy = 0.948531 Hartree
Thermal Correction to Free Energy = 0.808032 Hartree

Chemical symbol X, Y, Z

C	5.859150	1.191252	-0.862594
C	6.177605	-0.105930	-1.165075
C	5.349466	-1.180399	-0.745508
C	4.178374	-0.909607	0.025983
C	3.886405	0.452266	0.321181
C	4.691996	1.469850	-0.118918
H	6.560331	-2.702293	-1.689791
H	6.493613	2.004512	-1.200885
H	7.067377	-0.335498	-1.745181
C	5.664184	-2.515377	-1.104560
C	3.350276	-2.011378	0.426662
H	2.996191	0.727047	0.872894
H	4.399452	2.492312	0.093207
C	3.685952	-3.284386	0.025976
C	4.843600	-3.546072	-0.736338
H	3.044719	-4.117990	0.294368

H	5.075027	-4.566274	-1.025116
C	2.090872	-1.782171	1.250077
H	1.896066	-0.710964	1.278906
C	2.173232	-2.184769	2.754159
C	2.655238	-3.616149	3.030460
H	1.990520	-4.379805	2.616825
H	3.660803	-3.787658	2.638876
H	2.685114	-3.778254	4.112697
C	0.797636	-1.964203	3.395792
H	0.872134	-2.053124	4.484496
H	0.411675	-0.968649	3.156606
H	0.056797	-2.688914	3.048696
C	3.180922	-1.215748	3.399016
H	4.170553	-1.297833	2.939701
H	2.847791	-0.176621	3.302679
H	3.282361	-1.438389	4.465675
N	0.908847	-2.272372	0.517643
C	0.271353	-1.434577	-0.334652
C	0.369627	-3.541688	0.447802
C	-0.633865	-3.490799	-0.462098
H	0.711783	-4.366233	1.048173
H	-1.321334	-4.258281	-0.771935
N	-0.668767	-2.196687	-0.941614
C	-1.538480	-1.610555	-1.974024
H	-1.149565	-0.596752	-2.027745
C	-2.977561	-1.514327	-1.497529
C	-3.528093	-0.229757	-1.159716
C	-3.746815	-2.639256	-1.310535
C	-4.852130	-0.169821	-0.627666
C	-2.817559	0.999332	-1.282963
C	-5.061000	-2.571634	-0.800877
H	-3.339283	-3.617169	-1.539430
C	-5.398239	1.081447	-0.235923
C	-5.601173	-1.362668	-0.463454
C	-3.367379	2.192222	-0.885525
H	-1.805641	1.036742	-1.667733
H	-5.629079	-3.486191	-0.665883
C	-4.674247	2.238820	-0.353027
H	-6.401209	1.098353	0.180450
H	-6.604315	-1.297608	-0.052294
H	-2.764937	3.089778	-0.979954
H	-5.098122	3.185033	-0.032599
C	-1.271851	-2.153976	-3.410966
C	-2.026257	-1.221159	-4.372254
H	-3.105873	-1.259552	-4.198666
H	-1.700392	-0.182072	-4.253712
H	-1.837126	-1.516525	-5.408933
C	-1.720317	-3.597675	-3.673364
H	-2.805071	-3.708990	-3.605216
H	-1.427689	-3.882978	-4.689067
H	-1.243492	-4.310184	-2.993395
C	0.237968	-2.045166	-3.680837
H	0.448301	-2.281441	-4.728663
H	0.607286	-1.033521	-3.479137
H	0.811237	-2.738031	-3.057246
Cu	0.556791	0.483865	-0.545369
C	0.164519	4.706139	-0.763376
C	1.690062	4.572851	-0.447385
C	-0.673521	5.057237	0.469179
H	-0.505954	6.088000	0.795830
H	-1.733640	4.943162	0.225941
H	-0.444719	4.386056	1.300460
C	-0.175285	5.657645	-1.903762
H	-1.258328	5.678465	-2.055239
H	0.155593	6.675960	-1.672918
H	0.288895	5.340974	-2.839065
C	2.577841	4.775421	-1.678713
H	3.599023	4.472317	-1.431844
H	2.236707	4.154102	-2.510961
H	2.595213	5.821136	-2.000972
C	2.187149	5.442917	0.700314
H	3.258499	5.279651	0.848712
H	2.032783	6.504836	0.481271
H	1.677256	5.199624	1.634464
B	0.745628	2.466084	-0.624278
O	1.804837	3.192931	-0.067748
O	-0.187063	3.367618	-1.149839
C	0.290760	2.230317	2.975216
H	1.086088	2.270043	2.223673
H	0.635315	1.664472	3.845862
H	0.108932	3.263515	3.296175
C	-0.951019	1.636803	2.386110
H	-1.245957	1.997753	1.400378
C	-1.694116	0.705493	2.984266
H	-1.439340	0.316078	3.967694
C	-2.905160	0.130676	2.345686
H	-3.089478	0.544438	1.356930
Cl	-2.729292	-1.649626	2.130362
Cl	-4.380794	0.466760	3.324936

II-E,R

Electronic Energy BS1 = -3073.22068098 Hartree
Electronic Energy BS2 = -4517.21269879 Hartree
Zero-point Energy Correction = 0.895788 Hartree
Thermal Correction to Enthalpy = 0.948863 Hartree
Thermal Correction to Free Energy = 0.808452 Hartree

Chemical symbol X, Y, Z

C	5.560766	1.901690	-2.495666
C	6.475644	1.165752	-1.790603
C	6.102952	0.471942	-0.609994
C	4.758405	0.544784	-0.141080
C	3.838075	1.323549	-0.897922
C	4.227375	1.977863	-2.039320
H	8.078437	-0.341189	-0.264835
H	5.855834	2.425515	-3.399175
H	7.506733	1.098249	-2.126696
C	7.057359	-0.298512	0.103772
C	4.395352	-0.173326	1.052863
H	2.800832	1.405352	-0.594976
H	3.497244	2.558352	-2.594408
C	5.358555	-0.914038	1.695769
C	6.692227	-0.976470	1.231657
H	5.108982	-1.470762	2.588951
H	7.417717	-1.569315	1.779213
C	2.935163	-0.139241	1.498950
H	2.567338	0.870608	1.298397

C	2.550881	-0.387963	2.992366
C	1.103861	0.104202	3.170100
H	0.784477	-0.043807	4.207269
H	1.009278	1.170849	2.936480
H	0.409592	-0.442351	2.528916
C	3.449346	0.469793	3.898148
H	4.482483	0.120328	3.935495
H	3.462571	1.510962	3.557392
H	3.053721	0.459650	4.918566
C	2.578660	-1.865204	3.417888
H	2.303715	-1.938823	4.474736
H	1.847532	-2.448077	2.850482
H	3.555095	-2.341962	3.304234
N	2.171052	-0.992049	0.570467
C	1.107012	-0.556747	-0.144136
C	2.525526	-2.275050	0.200740
C	1.658993	-2.653061	-0.766564
H	3.362038	-2.793832	0.638443
H	1.591092	-3.583500	-1.300938
N	0.803623	-1.586810	-0.973595
C	-0.234068	-1.424218	-2.004619
H	-0.596643	-0.422386	-1.784078
C	-1.398624	-2.377972	-1.803930
C	-2.694885	-1.854093	-1.470787
C	-1.232211	-3.741417	-1.880817
C	-3.753787	-2.770779	-1.189767
C	-2.988650	-0.463115	-1.372268
C	-2.286059	-4.641849	-1.617440
H	-0.263973	-4.155864	-2.135103
C	-5.029906	-2.278284	-0.807706
C	-3.518971	-4.166803	-1.269385
C	-4.233451	-0.019748	-1.003733
H	-2.241200	0.297260	-1.562452
H	-2.103646	-5.709661	-1.679190
C	-5.269244	-0.933072	-0.710804
H	-5.812451	-2.996014	-0.579426
H	-4.334193	-4.848075	-1.044052
H	-4.395191	1.050070	-0.931907
H	-6.245548	-0.570037	-0.406469
C	0.341490	-1.286533	-3.449333
C	-0.816620	-0.802205	-4.336677
H	-1.630086	-1.533386	-4.366749
H	-1.225997	0.145945	-3.971883
H	-0.463672	-0.644445	-5.360556
C	0.914247	-2.577904	-4.046877
H	0.148772	-3.349802	-4.159759
H	1.314296	-2.365325	-5.043559
H	1.740347	-2.977284	-3.450799
C	1.441744	-0.213167	-3.426131
H	1.771500	0.005180	-4.446914
H	1.076863	0.718747	-2.978997
H	2.316729	-0.534777	-2.853182
Cu	0.081074	1.107027	-0.051261
C	-1.832471	4.903157	-0.032664
C	-3.010068	3.980581	-0.490609
C	-1.169154	5.650250	-1.193706
H	-0.244455	6.107902	-0.833011
H	-0.910781	4.961892	-2.003085
H	-1.815144	6.438164	-1.593317
C	-2.180202	5.883993	1.080429
H	-2.507777	5.364015	1.982609
H	-1.297460	6.476647	1.335161
H	-2.972207	6.570470	0.762295
C	-4.017070	3.699470	0.627524
H	-3.509513	3.355384	1.530933
H	-4.606181	4.587653	0.874779
H	-4.706020	2.913338	0.306400
C	-3.748877	4.449870	-1.738089
H	-4.209618	5.429620	-1.572526
H	-3.079368	4.517768	-2.596961
H	-4.542769	3.738875	-1.985142
B	-1.099441	2.713129	-0.124529
O	-2.335619	2.746227	-0.786263
O	-0.871616	3.957471	0.462418
C	-2.053602	1.857710	3.272754
H	-1.412058	2.521040	2.682621
H	-1.530678	1.580618	4.192120
H	-2.946696	2.430792	3.550000
C	-2.430621	0.653081	2.468908
H	-2.811788	0.834324	1.463584
C	-2.312878	-0.600254	2.907583
H	-1.924973	-0.820250	3.899815
C	-2.673907	-1.771421	2.070837
H	-3.033908	-1.484481	1.086283
Cl	-1.238183	-2.832173	1.798367
Cl	-3.987573	-2.743040	2.830978

III-E,R

Electronic Energy BS1 = -3073.22557395 Hartree
Electronic Energy BS2 = -4517.21382252 Hartree
Zero-point Energy Correction = 0.896709 Hartree
Thermal Correction to Enthalpy = 0.948684 Hartree
Thermal Correction to Free Energy = 0.813475 Hartree

Chemical symbol X, Y, Z

C	-5.052436	0.517074	-2.255918
C	-5.448620	0.573336	-0.947776
C	-4.765225	-0.161423	0.056900
C	-3.648348	-0.975239	-0.299146
C	-3.273761	-1.011156	-1.671029
C	-3.951170	-0.288339	-2.616626
H	-6.024434	0.551528	1.662360
H	-5.577819	1.087294	-3.015231
H	-6.295209	1.187875	-0.652681
C	-5.173319	-0.075176	1.410592
C	-2.959864	-1.690279	0.734364
H	-2.430364	-1.613406	-1.987682
H	-3.632731	-0.326417	-3.653098
C	-3.388652	-1.558901	2.036181
C	-4.495573	-0.758023	2.382932
H	-2.853900	-2.069485	2.830396
H	-4.798559	-0.685496	3.422449
C	-1.722480	-2.534436	0.436233
H	-1.359588	-2.281635	-0.560984
C	-1.938503	-4.078238	0.395291
C	-2.679760	-4.662259	1.607697
H	-2.143534	-4.524987	2.550391

H	-3.675450	-4.225838	1.718682
H	-2.799195	-5.741176	1.466616
C	-0.578020	-4.769672	0.224594
H	-0.724694	-5.836072	0.025669
H	-0.017522	-4.339234	-0.611100
H	0.047332	-4.677429	1.116705
C	-2.793838	-4.365981	-0.851837
H	-3.755852	-3.846353	-0.811576
H	-2.276993	-4.058155	-1.767146
H	-2.991913	-5.439443	-0.928269
N	-0.613764	-2.066970	1.282542
C	0.080783	-0.970820	0.893991
C	-0.281240	-2.420136	2.578174
C	0.644481	-1.528651	2.999511
H	-0.701462	-3.267929	3.089414
H	1.166632	-1.473202	3.937832
N	0.837423	-0.631788	1.963967
C	1.679650	0.575462	1.915030
H	1.214129	1.129331	1.101745
C	3.096012	0.219576	1.496035
C	3.671171	0.804196	0.319593
C	3.807749	-0.732293	2.187845
C	4.948861	0.342413	-0.119783
C	3.016349	1.796776	-0.467795
C	5.086669	-1.156596	1.771815
H	3.368115	-1.199992	3.062878
C	5.500190	0.848462	-1.326915
C	5.641878	-0.637177	0.635160
C	3.580412	2.264718	-1.627856
H	2.051114	2.195319	-0.177721
H	5.612015	-1.913412	2.345059
C	4.831284	1.782022	-2.072534
H	6.463538	0.468389	-1.654599
H	6.613088	-0.976108	0.286583
H	3.051259	3.012240	-2.211316
H	5.256898	2.150625	-3.000088
C	1.523353	1.529728	3.140696
C	2.106926	2.886621	2.706714
H	3.167511	2.804572	2.448934
H	1.565519	3.278526	1.841133
H	2.013716	3.608487	3.524530
C	2.254346	1.086977	4.415701
H	3.325687	0.957972	4.240065
H	2.132883	1.858201	5.183272
H	1.858936	0.159726	4.839389
C	0.023382	1.715713	3.420307
H	-0.122326	2.509322	4.160779
H	-0.496503	2.001507	2.500568
H	-0.440973	0.804173	3.808142
Cu	0.027533	-0.041151	-0.819632
C	-0.996477	4.034100	-0.155389
C	-2.402499	3.425897	-0.460319
C	-0.388329	4.772276	-1.350338
H	-0.894954	5.723023	-1.542221
H	0.664814	4.977706	-1.138392
H	-0.440447	4.157610	-2.253581
C	-0.928292	4.907809	1.089776
H	0.089100	5.287552	1.222111
H	-1.601622	5.766566	0.996990
H	-1.198298	4.346797	1.986444
C	-3.214314	3.135198	0.804466
H	-4.089710	2.544527	0.527234
H	-2.632506	2.546926	1.519987
H	-3.549941	4.055897	1.291809
C	-3.249555	4.215489	-1.448972
H	-4.193774	3.688648	-1.612870
H	-3.473434	5.215368	-1.061899
H	-2.748129	4.315649	-2.413322
B	-0.807486	1.774311	-0.613761
O	-2.065275	2.160869	-1.051738
O	-0.202743	2.851361	0.055119
C	-0.576014	0.328870	-3.728748
H	-1.129836	1.247683	-3.523716
H	-1.285713	-0.501990	-3.704336
H	-0.161942	0.379140	-4.743342
C	0.538574	0.113842	-2.735336
H	1.325547	0.867904	-2.759376
C	0.907034	-1.172066	-2.286009
H	0.290446	-2.026219	-2.566471
C	2.332479	-1.486439	-2.014931
H	2.890077	-0.630322	-1.644327
Cl	2.551872	-2.800635	-0.806722
Cl	3.211463	-1.974424	-3.543945

TSinx-E,R

Imaginary Freq = -177.0776 (cm^{-1})
Electronic Energy BS1 = -3073.21086461 Hartree
Electronic Energy BS2 = -4517.16941585 Hartree
Zero-point Energy Correction = 0.895719 Hartree
Thermal Correction to Enthalpy = 0.947170 Hartree
Thermal Correction to Free Energy = 0.812717 Hartree

Chemical symbol X, Y, Z

C	-4.884550	0.321303	-2.746563
C	-5.420183	0.577089	-1.513636
C	-4.861393	0.005800	-0.339891
C	-3.713344	-0.836150	-0.441567
C	-3.181644	-1.071264	-1.740528
C	-3.755676	-0.519560	-2.855905
H	-6.310243	0.908071	0.987322
H	-5.322026	0.758799	-3.638039
H	-6.291551	1.218725	-1.412367
C	-5.434202	0.267971	0.929663
C	-3.159584	-1.393158	0.757167
H	-2.303731	-1.692665	-1.869764
H	-3.331688	-0.725883	-3.833537
C	-3.746128	-1.095163	1.966466
C	-4.885896	-0.270823	2.061880
H	-3.319379	-1.492411	2.881768
H	-5.318135	-0.066088	3.035983
C	-1.907566	-2.261858	0.719604
H	-1.415931	-2.120911	-0.245505
C	-2.121673	-3.803808	0.821634
C	-3.000889	-4.256226	1.996748
H	-2.568969	-4.025688	2.974312
H	-3.995622	-3.805344	1.949853
H	-3.121958	-5.343311	1.955426

C	-0.746282	-4.487185	0.886297
H	-0.863359	-5.569062	0.768196
H	-0.089056	-4.125194	0.088196
H	-0.241721	-4.308202	1.839884
C	-2.821368	-4.240467	-0.477892
H	-3.783373	-3.736419	-0.610361
H	-2.198540	-4.029595	-1.353194
H	-3.006026	-5.318735	-0.454424
N	-0.900013	-1.714222	1.640354
C	-0.039898	-0.771483	1.189351
C	-0.715227	-1.930521	2.993368
C	0.288833	-1.113186	3.386570
H	-1.287716	-2.638483	3.565402
H	0.736779	-0.995556	4.357020
N	0.676709	-0.388840	2.274180
C	1.766144	0.590909	2.110740
H	1.370255	1.240033	1.327846
C	3.001887	-0.121678	1.575105
C	3.672859	0.337939	0.395411
C	3.438813	-1.271603	2.191059
C	4.768524	-0.426426	-0.109301
C	3.285423	1.500732	-0.330524
C	4.533822	-2.011593	1.700366
H	2.913465	-1.642460	3.066091
C	5.414964	-0.019340	-1.306436
C	5.182907	-1.599487	0.569362
C	3.934301	1.865990	-1.482923
H	2.449576	2.107042	-0.003227
H	4.841918	-2.916061	2.214419
C	5.008831	1.098912	-1.984010
H	6.230146	-0.627769	-1.686650
H	6.012906	-2.171503	0.165444
H	3.603000	2.747119	-2.023660
H	5.495734	1.386691	-2.909374
C	1.996866	1.539213	3.328826
C	2.782630	2.750737	2.794343
H	3.741533	2.451907	2.361479
H	2.209826	3.281208	2.026410
H	2.984743	3.451088	3.610796
C	2.810437	0.923389	4.476808
H	3.804566	0.619979	4.139398
H	2.934615	1.667551	5.270021
H	2.332870	0.050428	4.930119
C	0.642063	2.048464	3.845293
H	0.797261	2.875382	4.545514
H	0.031324	2.416986	3.015736
H	0.066617	1.277331	4.363033
Cu	0.134073	-0.166004	-0.597159
C	-0.727451	3.945192	-0.259081
C	-2.101815	3.195286	-0.229484
C	-0.517415	4.770878	-1.528437
H	-1.143391	5.668074	-1.530579
H	0.530128	5.078715	-1.581796
H	-0.745683	4.186030	-2.422884
C	-0.433175	4.797159	0.966928
H	0.550241	5.265069	0.865266
H	-1.179157	5.591932	1.069634
H	-0.432842	4.202686	1.881635
C	-2.525950	2.770778	1.178663
H	-3.380215	2.094459	1.098667
H	-1.720877	2.224768	1.679068
H	-2.812493	3.628245	1.795035
C	-3.246481	3.910624	-0.931208
H	-4.140982	3.283338	-0.886221
H	-3.465667	4.866481	-0.443885
H	-3.017810	4.093430	-1.982519
B	-0.456527	1.733409	-0.794822
O	-1.801709	1.990447	-0.952165
O	0.213072	2.846622	-0.302088
C	-0.494585	1.131571	-3.464849
H	-0.643777	2.213692	-3.422423
H	-1.475779	0.663223	-3.376311
H	-0.068436	0.878053	-4.441539
C	0.457349	0.621271	-2.391014
H	1.384173	1.198051	-2.363444
C	0.693384	-0.845471	-2.380952
H	-0.031678	-1.439580	-2.937585
C	2.071029	-1.315740	-2.486663
H	2.787863	-0.736323	-1.912544
Cl	2.281070	-3.035682	-1.981637
Cl	2.779688	-1.184876	-4.230590

IV-E,R

Electronic Energy BS1 = -3073.26851571 Hartree
Electronic Energy BS2 = -4517.25604892 Hartree
Zero-point Energy Correction = 0.897538 Hartree
Thermal Correction to Enthalpy = 0.949272 Hartree
Thermal Correction to Free Energy = 0.814866 Hartree

Chemical symbol X, Y, Z

C	-4.414816	2.621693	-1.260818
C	-4.971948	2.029882	-0.160187
C	-4.616236	0.708401	0.218811
C	-3.665904	-0.018240	-0.560579
C	-3.122496	0.628218	-1.705522
C	-3.481688	1.906424	-2.041868
H	-5.900902	0.682261	1.957387
H	-4.683538	3.636679	-1.534510
H	-5.693542	2.566328	0.450187
C	-5.178657	0.114797	1.376879
C	-3.292466	-1.336397	-0.135863
H	-2.394195	0.124562	-2.327956
H	-3.031555	2.375699	-2.910619
C	-3.858774	-1.860852	1.003997
C	-4.807705	-1.144829	1.762632
H	-3.557152	-2.844883	1.349022
H	-5.230313	-1.595788	2.654601
C	-2.222404	-2.125606	-0.880061
H	-1.698950	-1.439482	-1.546081
C	-2.721180	-3.268084	-1.816251
C	-3.692284	-4.263722	-1.164255
H	-3.247629	-4.828389	-0.340403
H	-4.586688	-3.761149	-0.787478
H	-4.009097	-4.996623	-1.912951
C	-1.502395	-4.008578	-2.389201
H	-1.820788	-4.689196	-3.184984
H	-0.779749	-3.303652	-2.814232

H	-0.983941	-4.601221	-1.630327
C	-3.466820	-2.585092	-2.977187
H	-4.310744	-1.987662	-2.619687
H	-2.800226	-1.929387	-3.546625
H	-3.855878	-3.342147	-3.664777
N	-1.147268	-2.503124	0.057348
C	-0.143342	-1.628197	0.300169
C	-1.028529	-3.617371	0.864141
C	0.083406	-3.438096	1.615991
H	-1.714319	-4.445261	0.841564
H	0.519339	-4.088780	2.351673
N	0.603721	-2.204590	1.272869
C	1.826949	-1.512825	1.735988
H	1.496067	-0.476616	1.822021
C	2.882915	-1.582452	0.640503
C	3.534582	-0.398576	0.162614
C	3.176446	-2.795044	0.062097
C	4.489589	-0.523301	-0.890628
C	3.259179	0.908430	0.654015
C	4.122124	-2.912685	-0.977447
H	2.652353	-3.686430	0.395636
C	5.136035	0.638396	-1.391392
C	4.767724	-1.799413	-1.441567
C	3.896708	2.010897	0.146968
H	2.509993	1.075427	1.417152
H	4.323750	-3.887188	-1.409904
C	4.852704	1.879294	-0.884843
H	5.851677	0.523836	-2.200354
H	5.490380	-1.873922	-2.248886
H	3.635182	2.991222	0.531029
H	5.340090	2.760465	-1.288370
C	2.317585	-1.893469	3.167294
C	3.347864	-0.825517	3.580884
H	4.197625	-0.795997	2.893942
H	2.902906	0.173810	3.611823
H	3.729013	-1.052356	4.581241
C	3.019854	-3.257919	3.258314
H	3.919380	-3.277958	2.638257
H	3.320726	-3.438404	4.295140
H	2.392322	-4.099102	2.954075
C	1.142695	-1.821702	4.158862
H	1.521810	-1.872298	5.184252
H	0.593567	-0.880653	4.050327
H	0.424407	-2.634438	4.032700
Cu	0.167156	-0.002972	-0.672061
C	-0.013956	3.019200	2.653199
C	-1.374513	2.414168	2.157031
C	-0.094556	4.520838	2.936064
H	-0.679217	4.731285	3.836215
H	0.916991	4.909574	3.078634
H	-0.546126	5.052849	2.093993
C	0.619845	2.298901	3.834324
H	1.567566	2.778410	4.094974
H	-0.034601	2.331918	4.711080
H	0.824040	1.254019	3.593585
C	-1.481943	0.909449	2.402632
H	-2.344597	0.518244	1.860425
H	-0.597327	0.384659	2.034319
H	-1.609125	0.686996	3.466862
C	-2.620565	3.108505	2.690715
H	-3.506826	2.614879	2.283815
H	-2.660797	3.046523	3.783305
H	-2.651017	4.158439	2.394830
B	0.019758	2.784933	0.387170
O	-1.302295	2.630444	0.738376
O	0.835773	2.856496	1.504283
C	-0.242761	4.057238	-1.807050
H	-0.100304	5.026019	-1.312298
H	-1.316423	3.839909	-1.800713
H	0.083389	4.155384	-2.845749
C	0.528164	2.933627	-1.088942
H	1.588314	3.215221	-1.042291
C	0.415696	1.561937	-1.820505
H	-0.472102	1.583008	-2.467512
C	1.607448	1.256391	-2.661069
H	2.537519	1.187979	-2.103511
Cl	1.436996	-0.331410	-3.526901
Cl	2.033624	2.520297	-3.965808

TSelim-E,R

Imaginary Freq = -169.5364 (cm^{-1})
Electronic Energy BS1 = -3073.25547861 Hartree
Electronic Energy BS2 = -4517.25587937 Hartree
Zero-point Energy Correction = 0.896309 Hartree
Thermal Correction to Enthalpy = 0.948286 Hartree
Thermal Correction to Free Energy = 0.811642 Hartree

Chemical symbol X, Y, Z

C	-4.968731	2.357231	-0.996805
C	-5.592884	1.477897	-0.153041
C	-5.066909	0.177373	0.070559
C	-3.875756	-0.227017	-0.603668
C	-3.275144	0.705846	-1.496133
C	-3.795952	1.960542	-1.677241
H	-6.603722	-0.383205	1.483529
H	-5.370691	3.353354	-1.148955
H	-6.499150	1.766345	0.372208
C	-5.695810	-0.706553	0.982349
C	-3.330709	-1.523449	-0.321083
H	-2.384649	0.440713	-2.052473
H	-3.302053	2.653450	-2.350940
C	-3.973673	-2.337002	0.583908
C	-5.159521	-1.939283	1.235438
H	-3.562992	-3.313078	0.818749
H	-5.635335	-2.614549	1.938976
C	-2.032035	-1.972119	-0.972248
H	-1.559864	-1.097671	-1.418507
C	-2.153568	-2.981647	-2.160056
C	-3.008099	-4.222749	-1.865987
H	-2.585837	-4.859583	-1.083535
H	-4.027550	-3.952651	-1.579126
H	-3.066730	-4.836736	-2.770032
C	-0.742452	-3.405861	-2.597928
H	-0.799411	-3.963667	-3.537614
H	-0.099059	-2.534925	-2.759813
H	-0.258240	-4.048970	-1.856983
C	-2.817366	-2.214004	-3.317170

H	-3.805804	-1.836573	-3.038329
H	-2.201743	-1.366528	-3.635642
H	-2.941015	-2.876743	-4.178723
N	-1.032268	-2.356037	0.041728
C	-0.033596	-1.508293	0.381987
C	-0.891987	-3.558907	0.702996
C	0.226927	-3.461830	1.459147
H	-1.571744	-4.383900	0.587948
H	0.676548	-4.192058	2.106506
N	0.733709	-2.192786	1.266084
C	2.041017	-1.621968	1.673303
H	1.780987	-0.602516	1.964370
C	2.925947	-1.567202	0.429499
C	3.546338	-0.345941	0.009190
C	3.044318	-2.689929	-0.357629
C	4.260411	-0.334181	-1.228687
C	3.449059	0.878738	0.727267
C	3.769453	-2.679025	-1.566660
H	2.539323	-3.605810	-0.063657
C	4.819695	0.880164	-1.705383
C	4.360916	-1.522323	-1.995593
C	4.009825	2.032580	0.241025
H	2.892748	0.934515	1.653863
H	3.835025	-3.585327	-2.159614
C	4.693841	2.043185	-0.993421
H	5.308922	0.883959	-2.673926
H	4.899524	-1.489855	-2.937842
H	3.896388	2.955458	0.800830
H	5.075386	2.973077	-1.397698
C	2.706070	-2.259404	2.933616
C	3.813250	-1.282340	3.372552
H	4.544513	-1.114839	2.577374
H	3.396772	-0.311322	3.660949
H	4.342298	-1.689465	4.239396
C	3.371270	-3.622295	2.680062
H	4.182052	-3.537229	1.953079
H	3.796255	-3.992724	3.618182
H	2.680763	-4.386683	2.314130
C	1.698579	-2.368977	4.091403
H	2.231128	-2.620196	5.013879
H	1.178679	-1.421885	4.253688
H	0.939530	-3.138239	3.936259
Cu	0.260829	0.219577	-0.418677
C	-0.163123	2.248217	3.001435
C	-1.561148	2.653597	2.422930
C	0.458571	3.326675	3.889345
H	-0.063779	3.409266	4.846605
H	1.502506	3.067435	4.084920
H	0.438403	4.301848	3.395286
C	-0.130508	0.901517	3.705650
H	0.879278	0.720483	4.086665
H	-0.819512	0.886604	4.555871
H	-0.395940	0.090531	3.022938
C	-2.404672	1.456143	1.987943
H	-3.250387	1.821167	1.401738
H	-1.832449	0.770956	1.354217
H	-2.790346	0.895096	2.844260
C	-2.381440	3.573085	3.316246
H	-3.332558	3.800259	2.828095
H	-2.595955	3.088061	4.274055
H	-1.864498	4.515043	3.506247
B	0.042254	2.934210	0.838674
O	-1.198650	3.366943	1.225448
O	0.650884	2.163662	1.814535
C	0.187449	4.486166	-1.243905
H	0.500668	5.354593	-0.654804
H	-0.905770	4.511806	-1.312296
H	0.618346	4.564594	-2.245341
C	0.659001	3.181618	-0.581350
H	1.751478	3.189299	-0.515386
C	0.267143	1.989425	-1.458542
H	-0.739886	2.047071	-1.873972
C	1.219721	1.368344	-2.251343
H	2.263343	1.277991	-1.993658
Cl	0.716544	0.222280	-3.480081
Cl	2.375822	3.069827	-3.690867

V-E,R

Electronic Energy BS1 = -3073.27187911 Hartree
Electronic Energy BS2 = -4517.27270633 Hartree
Zero-point Energy Correction = 0.896309 Hartree
Thermal Correction to Enthalpy = 0.948286 Hartree
Thermal Correction to Free Energy = 0.811642 Hartree

Chemical symbol X, Y, Z

C	-4.527230	3.099431	-0.676712
C	-5.017803	2.414307	0.401886
C	-4.638908	1.067845	0.651105
C	-3.746230	0.407331	-0.246767
C	-3.250466	1.157739	-1.351089
C	-3.625379	2.460936	-1.557353
H	-5.801147	0.899959	2.466633
H	-4.820839	4.128528	-0.854937
H	-5.704907	2.893816	1.093454
C	-5.129071	0.380494	1.789507
C	-3.389149	-0.958163	0.012254
H	-2.566644	0.706990	-2.059139
H	-3.226499	3.001876	-2.409858
C	-3.892256	-1.576670	1.134184
C	-4.757743	-0.914388	2.029305
H	-3.611499	-2.601390	1.353691
H	-5.126969	-1.441110	2.903145
C	-2.443161	-1.714145	-0.913159
H	-1.885396	-0.988012	-1.505259
C	-3.120049	-2.645187	-1.972556
C	-4.162829	-3.617735	-1.400492
H	-3.740199	-4.362766	-0.721776
H	-4.958140	-3.086789	-0.870907
H	-4.621758	-4.172366	-2.224663
C	-2.024573	-3.414790	-2.727578
H	-2.462331	-3.938408	-3.582835
H	-1.257037	-2.731435	-3.106270
H	-1.531892	-4.160489	-2.097481
C	-3.846621	-1.731395	-2.975973
H	-4.619176	-1.127142	-2.491834
H	-3.147459	-1.058134	-3.481179
H	-4.331321	-2.342283	-3.743209

N	-1.370794	-2.356206	-0.129940
C	-0.210692	-1.704142	0.110268
C	-1.369752	-3.588212	0.492103
C	-0.180139	-3.705044	1.124600
H	-2.179794	-4.291568	0.426415
H	0.194946	-4.533162	1.694172
N	0.523647	-2.538304	0.888786
C	1.867812	-2.110700	1.380688
H	1.648588	-1.257165	2.027353
C	2.683335	-1.609764	0.194690
C	3.402536	-0.369416	0.256268
C	2.700009	-2.340207	-0.973004
C	4.087767	0.078158	-0.911207
C	3.466022	0.458949	1.412721
C	3.381783	-1.891271	-2.121962
H	2.131508	-3.264895	-1.028464
C	4.781370	1.319714	-0.894774
C	4.051836	-0.696711	-2.098627
C	4.159989	1.640928	1.407954
H	2.962833	0.160808	2.321189
H	3.343449	-2.480911	-3.031753
C	4.825473	2.081884	0.242050
H	5.214004	1.669778	-1.825649
H	4.509876	-0.284957	-2.991793
H	4.190749	2.247733	2.308855
H	5.348222	3.032448	0.241647
C	2.606997	-3.151521	2.283458
C	3.952072	-2.536657	2.717812
H	4.586189	-2.292094	1.863283
H	3.813077	-1.628137	3.310300
H	4.487237	-3.258429	3.342320
C	2.941335	-4.463222	1.552066
H	3.643519	-4.274688	0.736014
H	3.419835	-5.156035	2.251163
H	2.076446	-4.973417	1.123766
C	1.813510	-3.398586	3.582454
H	2.403054	-4.024149	4.259621
H	1.621944	-2.448992	4.095064
H	0.850465	-3.890557	3.442893
Cu	0.275436	0.041485	-0.568841
C	-0.220679	1.607723	2.591706
C	-0.645853	3.117216	2.513834
C	0.854945	1.345691	3.643424
H	0.461908	1.502154	4.651324
H	1.185843	0.305956	3.573084
H	1.722002	1.995211	3.497308
C	-1.365099	0.618593	2.752782
H	-0.970417	-0.402065	2.757091
H	-1.890112	0.787369	3.698071
H	-2.083367	0.694998	1.936257
C	-2.030293	3.302577	1.894597
H	-2.187392	4.362834	1.683239
H	-2.120815	2.754405	0.952199
H	-2.822030	2.958224	2.565479
C	-0.537127	3.883469	3.822639
H	-0.849360	4.918701	3.665556
H	-1.189770	3.440983	4.581908
H	0.487210	3.892418	4.198658
B	0.719028	2.652049	0.766482
O	0.301352	3.669177	1.570538
O	0.375134	1.410919	1.287659
C	1.452406	4.153023	-1.268805
H	2.098927	4.756561	-0.625480
H	0.483225	4.659557	-1.335993
H	1.907049	4.085864	-2.261592
C	1.306504	2.737932	-0.690001
H	2.290165	2.256494	-0.729663
C	0.355583	1.917543	-1.547116
H	-0.687740	2.238351	-1.569021
C	0.778132	0.985010	-2.441850
H	1.836155	0.838553	-2.696850
Cl	-0.314280	0.317329	-3.651708
Cl	3.395519	2.144262	-3.797765

II''-E,R

Electronic Energy BS1 = -3073.21852602 Hartree
Electronic Energy BS2 = -4517.17587062 Hartree
Zero-point Energy Correction = 0.895142 Hartree
Thermal Correction to Enthalpy = 0.948672 Hartree
Thermal Correction to Free Energy = 0.804413 Hartree

Chemical symbol X, Y, Z

C	6.033941	-0.057848	-1.590638
C	6.093607	-1.364144	-1.996957
C	5.108241	-2.302653	-1.591515
C	4.037389	-1.883799	-0.744496
C	4.015042	-0.518398	-0.339281
C	4.978921	0.364116	-0.752971
H	6.000169	-3.950449	-2.670794
H	6.791096	0.651213	-1.910371
H	6.898722	-1.706363	-2.641581
C	5.178590	-3.650537	-2.026171
C	3.049001	-2.851980	-0.351832
H	3.240018	-0.121087	0.304584
H	4.912294	1.396167	-0.425185
C	3.168039	-4.147004	-0.803222
C	4.227776	-4.554275	-1.641403
H	2.436709	-4.892449	-0.513800
H	4.279649	-5.586101	-1.973650
C	1.892064	-2.427206	0.537068
H	1.943217	-1.344447	0.634714
C	1.913835	-2.925126	2.017356
C	0.701815	-2.322478	2.746491
H	0.760236	-2.549697	3.815788
H	0.673510	-1.232707	2.630822
H	-0.244881	-2.722533	2.370267
C	3.202180	-2.371628	2.648093
H	4.093361	-2.764599	2.149703
H	3.234027	-1.278447	2.588810
H	3.251575	-2.654143	3.704336
C	1.896018	-4.449528	2.185067
H	0.993401	-4.901102	1.762039
H	2.774307	-4.919056	1.734793
H	1.903343	-4.693684	3.252269
N	0.582407	-2.594143	-0.116809
C	-0.199125	-1.509508	-0.349546
C	-0.082225	-3.759023	-0.456278

C	-1.304175	-3.393403	-0.908827
H	0.346685	-4.740016	-0.357500
H	-2.136353	-3.986029	-1.251358
N	-1.351974	-2.014830	-0.843316
C	-2.522051	-1.184897	-1.172951
H	-2.300675	-0.215599	-0.715396
C	-3.721866	-1.761939	-0.423267
C	-3.757334	-1.617572	1.010301
C	-4.741693	-2.446877	-1.039834
C	-4.844504	-2.183278	1.737436
C	-2.764596	-0.916737	1.751304
C	-5.818189	-3.006556	-0.313994
H	-4.743896	-2.566018	-2.114203
C	-4.899344	-2.038621	3.148404
C	-5.868227	-2.880618	1.044704
C	-2.845260	-0.791790	3.114924
H	-1.916148	-0.465930	1.250157
H	-6.600483	-3.534886	-0.849077
C	-3.922925	-1.359927	3.827923
H	-5.738382	-2.477931	3.680944
H	-6.690211	-3.306611	1.613082
H	-2.068538	-0.249966	3.645450
H	-3.975689	-1.255013	4.906753
C	-2.594972	-0.862893	-2.700296
C	-2.599766	-2.097675	-3.617224
H	-1.694970	-2.696073	-3.474636
H	-3.461616	-2.754389	-3.482432
H	-2.607954	-1.765576	-4.660035
C	-1.339000	-0.043830	-3.054357
H	-1.261468	0.858675	-2.439617
H	-0.421008	-0.623000	-2.923147
H	-1.388966	0.274308	-4.100236
C	-3.814497	0.035539	-2.964343
H	-3.762971	0.938063	-2.346213
H	-3.813145	0.354938	-4.010985
H	-4.766292	-0.460423	-2.764104
Cu	0.335611	0.320271	0.100101
C	2.835080	3.283698	1.752379
C	1.718577	4.209530	1.175354
C	4.257414	3.692679	1.392886
H	4.492711	4.681276	1.801071
H	4.964510	2.972413	1.814683
H	4.402997	3.721131	0.311231
C	2.719884	3.072946	3.264534
H	3.391655	2.262095	3.559096
H	2.996329	3.972955	3.822148
H	1.701073	2.787601	3.540640
C	1.221913	5.294706	2.120242
H	2.034628	5.981433	2.380081
H	0.430586	5.869376	1.631353
H	0.814610	4.869319	3.039137
C	2.089995	4.822310	-0.177672
H	1.207266	5.300383	-0.610032
H	2.870746	5.581839	-0.073293
H	2.435600	4.053463	-0.874351
B	1.188668	1.994631	0.758860
O	0.649605	3.270721	0.940502
O	2.537625	2.023978	1.125452
C	-4.430829	1.847115	0.343481
H	-4.449162	0.785471	0.077905
H	-5.229617	2.348887	-0.209365
H	-4.655331	1.902545	1.413508
C	-3.096899	2.462739	0.052319
H	-2.247319	2.130874	0.651485
C	-2.900106	3.397917	-0.878047
H	-3.719687	3.762565	-1.494584
C	-1.574675	4.034488	-1.097274
H	-0.798165	3.657201	-0.429415
Cl	-0.993643	3.773744	-2.782319
Cl	-1.685854	5.810263	-0.779016

III''-E,R

Electronic Energy BS1 = -3073.22198693 Hartree
Electronic Energy BS2 = -4517.17811519 Hartree
Zero-point Energy Correction = 0.897241 Hartree
Thermal Correction to Enthalpy = 0.949023 Hartree
Thermal Correction to Free Energy = 0.814371 Hartree

Chemical symbol X, Y, Z

C	5.649234	0.696730	-0.348804
C	5.793399	-0.454755	0.377846
C	4.743931	-0.938278	1.203758
C	3.510956	-0.222086	1.268453
C	3.406553	0.987356	0.519555
C	4.443082	1.427085	-0.264829
H	5.847815	-2.668382	1.883435
H	6.454324	1.048222	-0.985652
H	6.715412	-1.026776	0.326379
C	4.902237	-2.137332	1.942833
C	2.434878	-0.770525	2.042371
H	2.502921	1.584099	0.542650
H	4.328092	2.347408	-0.829709
C	2.642107	-1.937221	2.740495
C	3.875232	-2.620349	2.705438
H	1.830910	-2.371841	3.314612
H	3.992440	-3.540937	3.267803
C	1.066315	-0.111061	2.029456
H	1.041010	0.606021	1.210054
C	0.694292	0.750954	3.283231
C	-0.745245	1.260785	3.107389
H	-0.964237	2.027684	3.857839
H	-0.878289	1.703414	2.116041
H	-1.482590	0.461019	3.222140
C	1.647714	1.959615	3.285823
H	2.693194	1.647671	3.373387
H	1.534038	2.543017	2.368604
H	1.418458	2.607344	4.138422
C	0.844001	0.040111	4.636118
H	0.139158	-0.784172	4.771166
H	1.858380	-0.341349	4.780724
H	0.640501	0.757135	5.438122
N	0.010420	-1.058294	1.629990
C	-0.526140	-1.021905	0.381783
C	-0.678841	-1.948600	2.436047
C	-1.684473	-2.451750	1.692598
H	-0.419197	-2.143759	3.460409
H	-2.471702	-3.138034	1.953350

N	-1.576978	-1.880991	0.435493
C	-2.609588	-2.012449	-0.608852
H	-2.326899	-1.271699	-1.358698
C	-3.941596	-1.558789	-0.011071
C	-4.248017	-0.154415	0.031554
C	-4.833433	-2.445155	0.546815
C	-5.472872	0.268388	0.630151
C	-3.392907	0.853281	-0.493071
C	-6.041385	-2.022561	1.144083
H	-4.623364	-3.506763	0.530542
C	-5.798321	1.649668	0.668541
C	-6.356270	-0.693681	1.182978
C	-3.737201	2.180207	-0.448328
H	-2.431335	0.604295	-0.925219
H	-6.713584	-2.762619	1.566265
C	-4.953871	2.588837	0.138553
H	-6.737708	1.946493	1.127191
H	-7.283603	-0.354985	1.636605
H	-3.051440	2.902388	-0.878316
H	-5.215647	3.642054	0.168559
C	-2.541345	-3.372127	-1.381395
C	-2.413321	-4.624068	-0.497683
H	-1.492503	-4.598490	0.091664
H	-3.252565	-4.774434	0.185547
H	-2.364893	-5.507686	-1.141781
C	-1.280799	-3.317301	-2.257893
H	-1.351660	-2.506221	-2.991801
H	-0.384844	-3.156724	-1.654476
H	-1.156468	-4.255794	-2.807126
C	-3.760864	-3.487659	-2.309443
H	-3.894885	-2.570872	-2.894375
H	-3.608085	-4.312463	-3.012640
H	-4.690179	-3.672519	-1.767481
Cu	0.225928	0.104488	-1.047651
C	0.276618	4.225141	0.085481
C	-0.281739	4.343675	-1.367173
C	1.490378	5.095280	0.384449
H	1.248626	6.156179	0.260716
H	1.810446	4.938840	1.418606
H	2.329236	4.848722	-0.268935
C	-0.792604	4.433815	1.159977
H	-0.380650	4.150211	2.132126
H	-1.110067	5.479591	1.213111
H	-1.669389	3.807315	0.971033
C	-1.437698	5.320690	-1.533571
H	-1.116031	6.341220	-1.300348
H	-1.789007	5.301399	-2.568661
H	-2.278794	5.069013	-0.884854
C	0.805936	4.645977	-2.402200
H	0.383895	4.526143	-3.403573
H	1.186624	5.667291	-2.307725
H	1.643083	3.948498	-2.302737
B	-0.024970	2.111216	-0.832944
O	-0.745377	3.005374	-1.627029
O	0.676664	2.843042	0.134161
C	0.584977	0.903888	-3.861949
H	0.245818	1.926597	-3.690361
H	-0.297424	0.286152	-4.057516
H	1.213360	0.880589	-4.760695
C	1.366889	0.374161	-2.684273
H	2.228186	0.971738	-2.384759
C	1.393672	-0.995292	-2.381353
H	0.771789	-1.670765	-2.961841
C	2.608777	-1.605675	-1.783982
H	3.147498	-0.922633	-1.133477
Cl	2.263146	-3.074357	-0.805042
Cl	3.819470	-2.059882	-3.075112

TSinx''-E,R

Imaginary Freq = -214.9693 (cm^{-1})
Electronic Energy BS1 = -3073.20425535 Hartree
Electronic Energy BS2 = -4517.16274244 Hartree
Zero-point Energy Correction = 0.896514 Hartree
Thermal Correction to Enthalpy = 0.947722 Hartree
Thermal Correction to Free Energy = 0.813728 Hartree

Chemical symbol X, Y, Z

C	5.577289	0.414533	-0.417968
C	5.550088	-0.921255	-0.117912
C	4.481685	-1.484902	0.628758
C	3.418023	-0.645915	1.078108
C	3.483351	0.738782	0.751987
C	4.527458	1.249862	0.023917
H	5.258170	-3.499278	0.539531
H	6.386538	0.827037	-1.010707
H	6.338442	-1.580310	-0.469337
C	4.443905	-2.875661	0.896214
C	2.325306	-1.240744	1.788383
H	2.685331	1.412600	1.032720
H	4.531324	2.305002	-0.230666
C	2.325436	-2.600224	2.000667
C	3.383728	-3.423226	1.564154
H	1.484888	-3.063038	2.509070
H	3.342892	-4.491044	1.752547
C	1.154912	-0.403397	2.293805
H	1.120741	0.535106	1.735793
C	1.257632	0.018033	3.799074
C	-0.053552	0.684126	4.250019
H	0.105465	1.208273	5.197749
H	-0.398420	1.413691	3.513385
H	-0.862440	-0.033240	4.403687
C	2.383956	1.064378	3.891738
H	3.344482	0.654180	3.569149
H	2.169267	1.941265	3.272815
H	2.490923	1.400419	4.927707
C	1.628328	-1.123745	4.760152
H	0.908642	-1.946140	4.765934
H	2.606462	-1.545491	4.517261
H	1.673036	-0.730132	5.780698
N	-0.115756	-1.048073	1.914508
C	-0.607038	-0.915114	0.653922
C	-0.900003	-1.917638	2.653929
C	-1.912016	-2.311019	1.852764
H	-0.698225	-2.171198	3.678235
H	-2.759749	-2.944245	2.051503
N	-1.710303	-1.704281	0.627616
C	-2.577413	-1.906191	-0.545269

H	-2.220824	-1.174519	-1.272220
C	-4.003915	-1.510308	-0.172938
C	-4.387434	-0.126602	-0.250557
C	-4.927997	-2.426905	0.272127
C	-5.721800	0.240860	0.098763
C	-3.506938	0.913067	-0.659555
C	-6.241838	-2.056665	0.634570
H	-4.662381	-3.473642	0.338028
C	-6.128071	1.597203	0.000034
C	-6.633132	-0.751017	0.543105
C	-3.929676	2.214529	-0.750951
H	-2.468346	0.706872	-0.890637
H	-6.934764	-2.819159	0.975368
C	-5.256374	2.565451	-0.422160
H	-7.150754	1.851016	0.265636
H	-7.643736	-0.453427	0.808619
H	-3.218204	2.964535	-1.074772
H	-5.578922	3.599138	-0.499606
C	-2.316041	-3.281083	-1.254664
C	-2.308088	-4.514868	-0.335575
H	-1.504075	-4.453778	0.403058
H	-3.247035	-4.688519	0.195048
H	-2.120140	-5.403039	-0.946857
C	-0.922139	-3.204138	-1.899721
H	-0.868098	-2.405873	-2.644884
H	-0.134336	-3.009561	-1.167882
H	-0.688886	-4.148219	-2.401865
C	-3.352495	-3.456790	-2.375959
H	-3.401668	-2.561722	-3.005979
H	-3.061347	-4.296406	-3.014595
H	-4.357470	-3.651179	-1.995420
Cu	0.171929	0.087317	-0.767190
C	0.537766	3.978840	0.669871
C	-0.453502	4.339493	-0.481266
C	1.678482	4.964634	0.877560
H	1.292289	5.953249	1.146163
H	2.319654	4.617420	1.692749
H	2.292841	5.059188	-0.019305
C	-0.176888	3.710725	1.993637
H	0.540110	3.302424	2.709548
H	-0.594529	4.627393	2.419227
H	-0.984590	2.984948	1.859003
C	-1.699702	5.094185	-0.039034
H	-1.425932	6.041657	0.436451
H	-2.321939	5.322560	-0.909180
H	-2.296908	4.507663	0.661315
C	0.222221	5.077687	-1.638344
H	-0.470248	5.126913	-2.482698
H	0.493250	6.099081	-1.356048
H	1.125307	4.556278	-1.968666
B	0.175074	2.141199	-0.661966
O	-0.836884	3.035310	-0.963363
O	1.088951	2.729793	0.210117
C	0.145727	1.780881	-3.398168
H	-0.067649	2.840949	-3.266762
H	-0.812583	1.261527	-3.499811
H	0.706246	1.639535	-4.327739
C	0.966331	1.172564	-2.262228
H	1.892991	1.722934	-2.070054
C	1.196703	-0.288038	-2.443986
H	0.619241	-0.729756	-3.255217
C	2.568266	-0.777757	-2.370852
H	3.138469	-0.421567	-1.520292
Cl	2.671671	-2.570892	-2.361490
Cl	3.654712	-0.183267	-3.809585

IV''-E,R

Electronic Energy BS1 = -3073.26838072 Hartree
Electronic Energy BS2 = -4517.22250048 Hartree
Zero-point Energy Correction = 0.897486 Hartree
Thermal Correction to Enthalpy = 0.949344 Hartree
Thermal Correction to Free Energy = 0.812623 Hartree

Chemical symbol X, Y, Z

C	5.083435	2.023715	-0.399085
C	5.361132	0.811499	-0.971989
C	4.655046	-0.359609	-0.587697
C	3.640208	-0.274579	0.412785
C	3.361862	1.007603	0.967270
C	4.067401	2.117238	0.578007
H	5.702482	-1.645758	-1.972542
H	5.620293	2.913574	-0.709729
H	6.120379	0.727813	-1.743982
C	4.935999	-1.604336	-1.204343
C	2.940422	-1.470031	0.780462
H	2.554801	1.139861	1.677329
H	3.822317	3.082846	1.008639
C	3.241605	-2.650777	0.142341
C	4.239542	-2.727139	-0.850430
H	2.683637	-3.548793	0.392377
H	4.443053	-3.677359	-1.333111
C	1.837386	-1.455024	1.832657
H	1.485380	-0.427682	1.952154
C	2.283076	-1.907252	3.259307
C	1.084940	-1.887237	4.224466
H	1.435873	-2.048049	5.248617
H	0.579039	-0.917176	4.195775
H	0.337158	-2.652692	4.008722
C	3.293245	-0.860291	3.764983
H	4.168925	-0.792136	3.114660
H	2.839836	0.134103	3.829602
H	3.636386	-1.137152	4.766562
C	2.985982	-3.274182	3.297385
H	2.371930	-4.096875	2.923129
H	3.906071	-3.258425	2.708308
H	3.252150	-3.513313	4.331807
N	0.648518	-2.145826	1.282271
C	-0.035357	-1.551550	0.274156
C	0.099399	-3.380270	1.575801
C	-0.966063	-3.541661	0.755340
H	0.482965	-4.043610	2.329152
H	-1.657008	-4.362821	0.684618
N	-1.032591	-2.411746	-0.035958
C	-2.011086	-2.047571	-1.073439
H	-1.540430	-1.165403	-1.503305
C	-3.333735	-1.612447	-0.460828
C	-3.828942	-0.279780	-0.674089

C	-4.064395	-2.477744	0.321203
C	-5.087919	0.082691	-0.105013
C	-3.127370	0.721475	-1.405292
C	-5.297986	-2.107770	0.897611
H	-3.694411	-3.479671	0.507614
C	-5.605692	1.388259	-0.316454
C	-5.804865	-0.856963	0.678245
C	-3.640358	1.982486	-1.566192
H	-2.151834	0.518956	-1.830073
H	-5.840236	-2.824562	1.505723
C	-4.901997	2.320122	-1.031216
H	-6.571094	1.637193	0.115628
H	-6.758894	-0.561894	1.106159
H	-3.061373	2.727385	-2.101194
H	-5.300297	3.319316	-1.173825
C	-2.077521	-3.039927	-2.274263
C	-2.809343	-4.359090	-1.994535
H	-2.319427	-4.954994	-1.218614
H	-3.850960	-4.193505	-1.707549
H	-2.809448	-4.967269	-2.904692
C	-0.639321	-3.334092	-2.729066
H	-0.080217	-2.408768	-2.904784
H	-0.091307	-3.919723	-1.984350
H	-0.653175	-3.905775	-3.662281
C	-2.820079	-2.304312	-3.402777
H	-2.300010	-1.382750	-3.684377
H	-2.875276	-2.941422	-4.290661
H	-3.841333	-2.043594	-3.108460
Cu	0.336646	0.093648	-0.636588
C	-0.897200	1.991112	2.538759
C	-1.818439	3.166941	2.058383
C	-0.379757	2.123617	3.964709
H	-1.208018	2.116524	4.680269
H	0.276265	1.279457	4.196979
H	0.194955	3.041098	4.100914
C	-1.547782	0.622159	2.341825
H	-0.811765	-0.162528	2.529125
H	-2.385114	0.478886	3.030690
H	-1.913437	0.499848	1.319238
C	-3.310790	2.886037	2.154311
H	-3.605439	2.723125	3.196406
H	-3.869290	3.743843	1.770584
H	-3.594695	2.014214	1.564271
C	-1.490051	4.502947	2.729288
H	-2.025706	5.298828	2.206098
H	-1.791761	4.512909	3.780703
H	-0.419895	4.721646	2.669403
B	-0.190966	2.783213	0.510634
O	-1.453230	3.299655	0.675961
O	0.225797	2.091711	1.639154
C	0.221696	4.296052	-1.506740
H	0.272878	5.167863	-0.844021
H	-0.821799	4.200048	-1.827025
H	0.829674	4.498346	-2.389810
C	0.674108	3.015746	-0.782061
H	1.711250	3.146453	-0.440988
C	0.637563	1.734525	-1.668588
H	-0.177080	1.832731	-2.401141
C	1.914405	1.481806	-2.399432
H	2.775737	1.376821	-1.745932
Cl	1.851373	-0.050715	-3.373938
Cl	2.492329	2.806354	-3.577864

II-E,S

Electronic Energy BS1 = -3073.21611083 Hartree
Electronic Energy BS2 = -4517.17529307 Hartree
Zero-point Energy Correction = 0.895689 Hartree
Thermal Correction to Enthalpy = 0.948809 Hartree
Thermal Correction to Free Energy = 0.808066 Hartree

Chemical symbol X, Y, Z

C	5.419353	-0.536423	0.704754
C	5.207203	-1.860859	0.980033
C	3.954045	-2.315103	1.469437
C	2.883837	-1.386997	1.652016
C	3.143209	-0.018083	1.351008
C	4.374064	0.391341	0.904322
H	4.587957	-4.376075	1.625691
H	6.382466	-0.198407	0.336110
H	5.999454	-2.589637	0.833974
C	3.764257	-3.685293	1.780400
C	1.620354	-1.879374	2.127973
H	2.377777	0.741528	1.460755
H	4.536932	1.443144	0.694735
C	1.501992	-3.213963	2.441182
C	2.567098	-4.123155	2.271473
H	0.561485	-3.601265	2.814177
H	2.420782	-5.169529	2.518347
C	0.427221	-0.942786	2.213819
H	0.732879	0.009878	1.784466
C	-0.086786	-0.552343	3.634422
C	-1.241222	0.449219	3.467068
H	-1.538738	0.841330	4.444912
H	-0.942234	1.295322	2.837602
H	-2.121150	-0.012417	3.008549
C	1.082912	0.144360	4.348358
H	1.939657	-0.526961	4.461950
H	1.413660	1.029846	3.795329
H	0.771878	0.469375	5.346065
C	-0.560135	-1.728987	4.497021
H	-0.914076	-1.348191	5.460489
H	-1.397392	-2.265605	4.040601
H	0.248410	-2.435724	4.701128
N	-0.647620	-1.340669	1.289227
C	-1.000863	-0.520103	0.269888
C	-1.470062	-2.451978	1.332672
C	-2.363224	-2.315475	0.325598
H	-1.366928	-3.243112	2.053245
H	-3.187563	-2.940922	0.025612
N	-2.057921	-1.130818	-0.314897
C	-2.848446	-0.522266	-1.399132
H	-2.525745	0.522818	-1.410991
C	-4.311205	-0.525840	-0.959245
C	-4.707328	0.386288	0.082574
C	-5.245559	-1.401602	-1.458861
C	-6.052184	0.355240	0.554806
C	-3.819247	1.321212	0.685450

C	-6.580540	-1.421696	-0.994189
H	-4.972657	-2.103213	-2.235255
C	-6.455932	1.238922	1.589372
C	-6.975962	-0.562933	-0.008851
C	-4.237487	2.157959	1.689098
H	-2.783743	1.384348	0.372080
H	-7.282345	-2.127488	-1.426548
C	-5.570733	2.120510	2.150660
H	-7.486739	1.198985	1.930781
H	-7.998012	-0.571592	0.359479
H	-3.530149	2.853746	2.129311
H	-5.889345	2.788787	2.944234
C	-2.433634	-1.058880	-2.806595
C	-2.424264	-2.592030	-2.923474
H	-1.697490	-3.031614	-2.234416
H	-3.394120	-3.057373	-2.734669
H	-2.124863	-2.872568	-3.938586
C	-0.993353	-0.579162	-3.066512
H	-0.920451	0.514283	-3.056324
H	-0.299927	-0.962109	-2.314265
H	-0.660846	-0.929735	-4.050313
C	-3.333523	-0.422519	-3.878366
H	-3.368173	0.665951	-3.759173
H	-2.925467	-0.634770	-4.871580
H	-4.359989	-0.791685	-3.852298
Cu	-0.115675	1.175690	-0.131538
C	1.594497	4.914466	-1.197324
C	2.295751	4.638626	0.172687
C	0.446931	5.923161	-1.091949
H	-0.237004	5.650641	-0.283581
H	0.812739	6.939824	-0.917497
H	-0.116838	5.912349	-2.028362
C	2.532983	5.314517	-2.329365
H	1.956238	5.478203	-3.243831
H	3.061300	6.243259	-2.088263
H	3.269922	4.534613	-2.531168
C	3.726993	4.115657	0.018741
H	4.410714	4.891378	-0.339234
H	4.078694	3.769414	0.995013
H	3.757473	3.272582	-0.677328
C	2.280568	5.809077	1.148421
H	2.786058	5.522430	2.074838
H	2.804737	6.673683	0.726949
H	1.260773	6.105378	1.399091
B	0.844417	2.907264	-0.326775
O	1.509162	3.565459	0.712558
O	1.008544	3.640352	-1.505813
C	3.158948	1.092155	-2.542139
H	3.755419	1.410273	-3.405301
H	3.808596	1.046273	-1.665235
H	2.392753	1.856336	-2.371444
C	2.530762	-0.236545	-2.809145
H	1.867405	-0.291166	-3.673087
C	2.730057	-1.336854	-2.082462
H	3.380155	-1.338285	-1.211392
C	2.101975	-2.632824	-2.446579
H	1.451115	-2.546180	-3.315314
Cl	3.354222	-3.859660	-2.872610
Cl	1.077793	-3.279728	-1.114462

III-E,S

Electronic Energy BS1 = -3073.21764116 Hartree
Electronic Energy BS2 = -4517.17454823 Hartree
Zero-point Energy Correction = 0.896719 Hartree
Thermal Correction to Enthalpy = 0.948596 Hartree
Thermal Correction to Free Energy = 0.813216 Hartree

Chemical symbol X, Y, Z

C	-5.128843	0.693603	2.410873
C	-5.443530	-0.536063	1.898369
C	-4.782448	-1.041680	0.747252
C	-3.770593	-0.258289	0.115261
C	-3.448142	1.002615	0.695328
C	-4.116306	1.466139	1.799493
H	-5.881648	-2.903452	0.722801
H	-5.644431	1.071742	3.287814
H	-6.210073	-1.148481	2.365196
C	-5.115710	-2.316343	0.224131
C	-3.129911	-0.776919	-1.057155
H	-2.653944	1.612219	0.280138
H	-3.850622	2.433993	2.214728
C	-3.485114	-2.022451	-1.520024
C	-4.475537	-2.799275	-0.884218
H	-2.981628	-2.432270	-2.390443
H	-4.721824	-3.779543	-1.279159
C	-2.046503	0.016377	-1.770763
H	-1.641854	0.756902	-1.081471
C	-2.512249	0.861089	-3.002303
C	-1.280650	1.513379	-3.654009
H	-1.604022	2.254027	-4.393041
H	-0.679334	2.022208	-2.893749
H	-0.643315	0.788629	-4.167440
C	-3.402272	1.994175	-2.459139
H	-4.289261	1.609024	-1.948371
H	-2.841082	2.620826	-1.760158
H	-3.738745	2.624626	-3.288501
C	-3.338713	0.084289	-4.038254
H	-3.661505	0.770441	-4.827957
H	-2.785500	-0.721101	-4.527884
H	-4.232967	-0.352063	-3.585137
N	-0.874844	-0.840713	-2.021595
C	0.071856	-0.974002	-1.063995
C	-0.538188	-1.569431	-3.147899
C	0.660448	-2.142282	-2.899818
H	-1.155170	-1.626622	-4.026018
H	1.255619	-2.779111	-3.528249
N	1.018058	-1.779049	-1.612821
C	2.304759	-1.949853	-0.913693
H	1.994608	-2.123348	0.117841
C	3.065040	-0.626455	-0.983763
C	3.572166	0.016985	0.190029
C	3.193509	0.003138	-2.200593
C	4.192196	1.294855	0.059302
C	3.473833	-0.532825	1.498502
C	3.833520	1.251973	-2.330374
H	2.769830	-0.458302	-3.087527
C	4.657722	1.970373	1.217325

C	4.325211	1.884585	-1.221208
C	3.929314	0.144675	2.599171
H	3.039692	-1.514607	1.640739
H	3.920505	1.709292	-3.310712
C	4.525282	1.417665	2.461739
H	5.119873	2.946244	1.094462
H	4.806121	2.855097	-1.303617
H	3.830993	-0.302056	3.583782
H	4.876845	1.948430	3.340318
C	3.138412	-3.212172	-1.303655
C	3.886776	-3.091349	-2.641665
H	3.230426	-2.925100	-3.499204
H	4.611049	-2.273389	-2.618097
H	4.433426	-4.020782	-2.829709
C	2.244321	-4.462576	-1.296666
H	1.693629	-4.543568	-0.355267
H	1.511098	-4.469417	-2.105939
H	2.865978	-5.357012	-1.405771
C	4.201977	-3.395585	-0.204814
H	3.739077	-3.586386	0.769379
H	4.832776	-4.257220	-0.443335
H	4.849453	-2.519131	-0.112866
Cu	0.072349	-0.034704	0.651426
C	0.959268	4.170697	0.574578
C	-0.456681	4.072290	-0.081396
C	2.073428	4.426761	-0.441876
H	2.025715	3.706698	-1.263173
H	2.027949	5.441383	-0.849742
H	3.035608	4.294984	0.059748
C	1.063892	5.166981	1.722087
H	2.080031	5.153578	2.125474
H	0.844710	6.183536	1.377993
H	0.377229	4.914896	2.532419
C	-1.599555	4.355545	0.898596
H	-1.642097	5.410819	1.184109
H	-2.548731	4.090747	0.422021
H	-1.494384	3.748976	1.803347
C	-0.639179	4.900838	-1.346337
H	-1.650186	4.760031	-1.739831
H	-0.502342	5.966921	-1.135947
H	0.068624	4.603127	-2.122028
B	0.336002	1.952548	0.419582
O	-0.533294	2.677521	-0.419096
O	1.153226	2.846250	1.095571
C	-0.789449	1.097612	3.336646
H	-0.850880	0.876729	4.409902
H	-1.808237	1.169318	2.951218
H	-0.288830	2.060388	3.209047
C	-0.019039	0.004478	2.642246
H	1.039907	-0.030076	2.908222
C	-0.606029	-1.199385	2.210868
H	-1.693106	-1.265548	2.169314
C	0.089416	-2.496525	2.351519
H	1.166102	-2.424133	2.211124
Cl	-0.080679	-3.189765	4.044069
Cl	-0.514466	-3.730660	1.191277

TSinx-E,S

Imaginary Freq = -175.5743 (cm^{-1})
Electronic Energy BS1 = -3073.20663025 Hartree
Electronic Energy BS2 = -4517.16502217 Hartree
Zero-point Energy Correction = 0.896427 Hartree
Thermal Correction to Enthalpy = 0.947662 Hartree
Thermal Correction to Free Energy = 0.813632 Hartree

Chemical symbol X, Y, Z

C	-5.624799	0.166914	2.471788
C	-5.937676	-0.953455	1.750929
C	-5.221527	-1.289088	0.571548
C	-4.158830	-0.445963	0.125911
C	-3.844295	0.696074	0.917366
C	-4.561673	0.993978	2.047772
H	-6.358934	-3.088689	0.195849
H	-6.179881	0.415670	3.370450
H	-6.742962	-1.608896	2.070878
C	-5.552473	-2.455346	-0.162626
C	-3.469089	-0.790281	-1.083322
H	-3.023328	1.351078	0.647033
H	-4.297645	1.871635	2.629634
C	-3.823751	-1.939172	-1.752418
C	-4.861012	-2.779103	-1.297368
H	-3.292934	-2.220131	-2.656084
H	-5.105474	-3.677038	-1.855451
C	-2.364976	0.099779	-1.634700
H	-1.971079	0.715008	-0.824483
C	-2.815656	1.130956	-2.725729
C	-1.568210	1.820256	-3.298321
H	-1.860969	2.691254	-3.893435
H	-0.925264	2.162837	-2.482836
H	-0.976540	1.160312	-3.937917
C	-3.661658	2.202181	-2.014543
H	-4.558991	1.775186	-1.558645
H	-3.081405	2.702087	-1.233286
H	-3.979981	2.958925	-2.738659
C	-3.669962	0.538766	-3.856129
H	-3.967754	1.341825	-4.537971
H	-3.141603	-0.205169	-4.458069
H	-4.578629	0.072688	-3.466870
N	-1.185151	-0.693887	-2.015276
C	-0.164916	-0.879686	-1.140941
C	-0.915065	-1.329016	-3.213945
C	0.306608	-1.894439	-3.093360
H	-1.590389	-1.328752	-4.050342
H	0.869169	-2.471292	-3.804932
N	0.751044	-1.619286	-1.814404
C	2.064987	-1.889143	-1.207595
H	1.817061	-1.909680	-0.144669
C	2.994328	-0.708964	-1.476639
C	3.643774	-0.016152	-0.404623
C	3.172138	-0.258276	-2.765261
C	4.449616	1.121401	-0.704415
C	3.516991	-0.393026	0.959934
C	3.996948	0.846176	-3.062735
H	2.658931	-0.754279	-3.582918
C	5.047638	1.853608	0.355259
C	4.627339	1.520714	-2.052455
C	4.102116	0.334656	1.962210

H	2.956517	-1.281777	1.218225
H	4.119033	1.159247	-4.094600
C	4.869495	1.481248	1.660448
H	5.651874	2.722411	0.107202
H	5.255303	2.381154	-2.266759
H	3.979507	0.025569	2.996129
H	5.324129	2.054047	2.462104
C	2.655562	-3.305544	-1.498085
C	3.314164	-3.466840	-2.877172
H	2.622188	-3.331547	-3.712795
H	4.144162	-2.768346	-3.010024
H	3.714028	-4.482218	-2.961792
C	1.549778	-4.356199	-1.309838
H	1.038341	-4.216418	-0.352440
H	0.798196	-4.314584	-2.103091
H	1.987918	-5.359195	-1.318449
C	3.745025	-3.550274	-0.437792
H	3.322687	-3.550637	0.571722
H	4.209148	-4.527134	-0.604474
H	4.532878	-2.792299	-0.486013
Cu	-0.066263	-0.265844	0.656712
C	1.227914	3.634669	0.198088
C	-0.289363	3.952664	0.417380
C	1.596852	3.435898	-1.272509
H	0.951787	2.690169	-1.743907
H	1.532039	4.370873	-1.836805
H	2.620096	3.061740	-1.330621
C	2.194857	4.616393	0.845241
H	3.218909	4.276956	0.668177
H	2.080017	5.616148	0.413542
H	2.044359	4.678723	1.924101
C	-0.568669	4.638773	1.755065
H	-0.247492	5.684426	1.739999
H	-1.643702	4.608807	1.952046
H	-0.055728	4.132733	2.576756
C	-0.951030	4.734321	-0.708103
H	-2.006155	4.901444	-0.472962
H	-0.471209	5.711359	-0.826469
H	-0.895135	4.203021	-1.659033
B	0.136454	1.736555	0.836272
O	-0.869371	2.627219	0.477182
O	1.366619	2.359516	0.848133
C	-1.093922	1.206652	3.266252
H	-0.986290	0.970529	4.330448
H	-2.077761	0.860529	2.945456
H	-1.060639	2.290915	3.143147
C	0.001639	0.466308	2.510007
H	1.001959	0.795270	2.803502
C	-0.133966	-1.015359	2.508871
H	-1.126762	-1.395654	2.748239
C	0.956108	-1.767673	3.111786
H	1.932597	-1.323391	2.945340
Cl	0.884426	-1.836923	4.987495
Cl	1.082266	-3.488884	2.554546

III-E,S

Electronic Energy BS1 = -3073.26652403 Hartree

Electronic Energy BS2 = -4517.22084876 Hartree

Zero-point Energy Correction = 0.897618 Hartree

Thermal Correction to Enthalpy = 0.949322 Hartree

Thermal Correction to Free Energy = 0.814922 Hartree

Chemical symbol X, Y, Z

C	-4.612178	2.257782	1.245936
C	-4.884772	1.096954	1.919095
C	-4.399905	-0.152947	1.450538
C	-3.616845	-0.201092	0.259026
C	-3.352030	1.026976	-0.408492
C	-3.833845	2.216890	0.068284
H	-5.265692	-1.292456	3.070140
H	-4.976941	3.208302	1.621256
H	-5.470570	1.114356	2.833800
C	-4.669457	-1.347900	2.163849
C	-3.108776	-1.468387	-0.175418
H	-2.725562	1.060465	-1.289812
H	-3.583479	3.132738	-0.456249
C	-3.382824	-2.597072	0.561155
C	-4.171529	-2.546291	1.729039
H	-2.961048	-3.550344	0.254537
H	-4.366658	-3.458251	2.283793
C	-2.203973	-1.572778	-1.395459
H	-1.848670	-0.570455	-1.637960
C	-2.890796	-2.074302	-2.702719
C	-1.860597	-2.133944	-3.844569
H	-2.375260	-2.288775	-4.797971
H	-1.300041	-1.195774	-3.914859
H	-1.134017	-2.940673	-3.727679
C	-3.946360	-1.017178	-3.079803
H	-4.693662	-0.893251	-2.291734
H	-3.490169	-0.040824	-3.269625
H	-4.464192	-1.326468	-3.992822
C	-3.628162	-3.416145	-2.563849
H	-4.069062	-3.684822	-3.529028
H	-2.985336	-4.246120	-2.261250
H	-4.437548	-3.343964	-1.833301
N	-0.957775	-2.271988	-1.009897
C	-0.084419	-1.644687	-0.183302
C	-0.515530	-3.547274	-1.304764
C	0.672162	-3.705628	-0.674444
H	-1.053205	-4.239222	-1.926391
H	1.331916	-4.554595	-0.658375
N	0.917261	-2.533882	0.013489
C	2.115497	-2.122680	0.769369
H	1.706801	-1.352565	1.423974
C	3.108067	-1.462005	-0.181071
C	3.586808	-0.132305	0.059282
C	3.494614	-2.115623	-1.329677
C	4.434270	0.478694	-0.912868
C	3.254870	0.628811	1.214296
C	4.350694	-1.517209	-2.276956
H	3.117101	-3.112501	-1.533291
C	4.887372	1.809286	-0.712558
C	4.807443	-0.242850	-2.074406
C	3.713413	1.908667	1.381743
H	2.631724	0.196673	1.987104
H	4.631170	-2.068937	-3.168296
C	4.533045	2.513988	0.404642

H	5.523305	2.258605	-1.470551
H	5.456829	0.235989	-2.802233
H	3.441513	2.466182	2.272993
H	4.879276	3.532536	0.545377
C	2.686431	-3.198212	1.743776
C	3.545902	-4.283202	1.078127
H	2.993298	-4.895676	0.360397
H	4.407123	-3.850997	0.562333
H	3.922350	-4.963761	1.848332
C	1.522294	-3.838242	2.516400
H	0.874340	-3.070064	2.951427
H	0.904640	-4.478170	1.880096
H	1.912700	-4.454992	3.331952
C	3.578733	-2.446571	2.748251
H	2.995377	-1.728670	3.334150
H	4.030632	-3.157007	3.447104
H	4.387310	-1.906661	2.246286
Cu	-0.242634	0.067428	0.676096
C	1.112334	2.081366	-2.573485
C	-0.277905	2.771153	-2.816629
C	1.056290	0.559323	-2.697317
H	0.246961	0.144388	-2.092477
H	0.920479	0.247868	-3.737953
H	1.991440	0.135113	-2.327067
C	2.254852	2.620145	-3.425043
H	3.171492	2.078230	-3.177840
H	2.045893	2.476261	-4.490311
H	2.426793	3.681598	-3.239041
C	-0.155362	4.229672	-3.263372
H	0.227482	4.309827	-4.284859
H	-1.142973	4.696189	-3.222947
H	0.508366	4.787106	-2.596549
C	-1.212835	2.017840	-3.752226
H	-2.165297	2.549709	-3.830692
H	-0.780955	1.935212	-4.754639
H	-1.415389	1.011483	-3.380742
B	0.183781	2.720108	-0.586713
O	-0.854429	2.787132	-1.500335
O	1.375642	2.405394	-1.199480
C	-0.839457	4.268552	1.196632
H	-0.891350	4.514945	2.259508
H	-1.859150	4.084080	0.845066
H	-0.460403	5.147157	0.660186
C	0.040833	3.032799	0.944214
H	1.060540	3.250457	1.294617
C	-0.449046	1.742508	1.673896
H	-1.535776	1.799135	1.827736
C	0.221758	1.574267	2.992102
H	1.303767	1.655837	2.928084
Cl	-0.191459	2.830646	4.295924
Cl	-0.082264	-0.054553	3.756964

TSrot-III,R

Imaginary Freq = -34.8808 (cm^{-1})
Electronic Energy BS1 = -3073.21517766 Hartree
Electronic Energy BS2 = -4517.17228286 Hartree
Zero-point Energy Correction = 0.895991 Hartree
Thermal Correction to Enthalpy = 0.947369 Hartree
Thermal Correction to Free Energy = 0.811326 Hartree

Chemical symbol X, Y, Z

C	-5.109402	1.403553	-1.889869
C	-5.534123	1.345114	-0.589767
C	-4.939256	0.447260	0.335634
C	-3.896784	-0.426509	-0.098327
C	-3.489250	-0.335617	-1.458031
C	-4.066802	0.556030	-2.322179
H	-6.157053	1.095461	1.999845
H	-5.563232	2.101771	-2.585794
H	-6.330468	1.996022	-0.239115
C	-5.363865	0.422156	1.687169
C	-3.307077	-1.323560	0.852867
H	-2.694128	-0.969119	-1.830963
H	-3.710574	0.618720	-3.344737
C	-3.746659	-1.294227	2.157152
C	-4.774629	-0.427710	2.582340
H	-3.287964	-1.944854	2.893828
H	-5.089549	-0.441290	3.620732
C	-2.168433	-2.258536	0.457051
H	-1.818202	-1.970704	-0.532775
C	-2.529165	-3.768014	0.306717
C	-3.283927	-4.385104	1.493174
H	-2.704259	-4.377992	2.420587
H	-4.232499	-3.875113	1.678002
H	-3.504791	-5.433413	1.268426
C	-1.240063	-4.558890	0.042541
H	-1.482805	-5.589446	-0.234627
H	-0.663141	-4.120626	-0.777834
H	-0.592298	-4.592703	0.923198
C	-3.437671	-3.869248	-0.931593
H	-4.345047	-3.268686	-0.814880
H	-2.917730	-3.528652	-1.833718
H	-3.737347	-4.909008	-1.093667
N	-0.985394	-1.968784	1.279503
C	-0.119282	-1.006943	0.873694
C	-0.695816	-2.377416	2.568356
C	0.377983	-1.660633	2.970547
H	-1.247643	-3.140686	3.088023
H	0.916938	-1.696508	3.899937
N	0.707683	-0.810829	1.929455
C	1.715277	0.265009	1.889335
H	1.335354	0.891976	1.084368
C	3.079899	-0.265518	1.483767
C	3.824773	0.367003	0.433231
C	3.613447	-1.366200	2.115406
C	5.117066	-0.143148	0.108662
C	3.334383	1.468248	-0.327444
C	4.886141	-1.874169	1.781132
H	3.045100	-1.866779	2.893026
C	5.868418	0.461693	-0.933398
C	5.627770	-1.266469	0.805273
C	4.081953	2.020569	-1.334984
H	2.353855	1.886281	-0.133915
H	5.269291	-2.744711	2.303743
C	5.366162	1.518983	-1.643137
H	6.850175	0.057757	-1.164853
H	6.610095	-1.645855	0.538408

H	3.675865	2.852086	-1.903258
H	5.946449	1.967944	-2.443065
C	1.690279	1.206517	3.140760
C	2.472257	2.476203	2.758031
H	3.521257	2.256356	2.539150
H	2.024611	2.953846	1.883054
H	2.443668	3.187460	3.589954
C	2.338073	0.625911	4.406486
H	3.366468	0.304128	4.221164
H	2.365278	1.400544	5.179686
H	1.782771	-0.214740	4.830536
C	0.231988	1.607245	3.419063
H	0.202890	2.389758	4.184693
H	-0.231922	1.997631	2.507987
H	-0.367106	0.765543	3.779169
Cu	-0.023704	-0.077302	-0.857351
C	-0.189977	4.122375	-0.134693
C	-1.570181	3.888080	-0.823579
C	0.863254	4.715193	-1.074501
H	0.667748	5.769196	-1.294265
H	1.844266	4.637715	-0.595977
H	0.898916	4.159913	-2.016281
C	-0.245477	4.921171	1.160554
H	0.761904	5.038268	1.570499
H	-0.656724	5.920195	0.980516
H	-0.859127	4.420530	1.911682
C	-2.718902	3.743142	0.178520
H	-3.597168	3.364748	-0.349645
H	-2.466284	3.020248	0.959810
H	-2.972660	4.698837	0.648026
C	-1.934482	4.905081	-1.896033
H	-2.908230	4.651240	-2.324091
H	-1.999887	5.912370	-1.470828
H	-1.201012	4.912334	-2.704496
B	-0.419296	1.895402	-0.733892
O	-1.385303	2.603196	-1.439981
O	0.220523	2.775134	0.157236
C	-0.667004	0.217429	-3.754143
H	-0.976977	1.245490	-3.555883
H	-1.544957	-0.428777	-3.660691
H	-0.317067	0.143992	-4.791076
C	0.435478	-0.217950	-2.819237
H	1.373572	0.322600	-2.927314
C	0.487073	-1.503080	-2.270337
H	-0.370516	-2.156678	-2.423341
C	1.737874	-2.263531	-1.904208
H	1.894125	-2.389340	-0.834735
Cl	1.620450	-3.964680	-2.542297
Cl	3.245193	-1.512312	-2.516311

III-Z,R

Electronic Energy BS1 = -3073.21671942 Hartree
Electronic Energy BS2 = -4517.21696380 Hartree
Zero-point Energy Correction = 0.896031 Hartree
Thermal Correction to Enthalpy = 0.948317 Hartree
Thermal Correction to Free Energy = 0.810258 Hartree

Chemical symbol X, Y, Z

C	-5.084387	1.822755	-1.481727
C	-5.410395	1.746472	-0.154170
C	-4.817573	0.771509	0.690878
C	-3.884655	-0.162222	0.146287
C	-3.575536	-0.047950	-1.237555
C	-4.145630	0.918412	-2.022850
H	-5.846084	1.447581	2.467978
H	-5.534987	2.579470	-2.115941
H	-6.123899	2.441550	0.279990
C	-5.135763	0.727750	2.071107
C	-3.298194	-1.139228	1.017855
H	-2.860360	-0.720844	-1.694010
H	-3.861872	0.997211	-3.066690
C	-3.628780	-1.124436	2.354102
C	-4.546930	-0.197059	2.888704
H	-3.165548	-1.834794	3.030382
H	-4.778500	-0.224546	3.948496
C	-2.276631	-2.147167	0.499494
H	-1.986328	-1.849003	-0.505621
C	-2.779970	-3.613547	0.329866
C	-3.425888	-4.239623	1.574932
H	-2.726298	-4.361577	2.406227
H	-4.280080	-3.654820	1.924188
H	-3.788988	-5.240780	1.321975
C	-1.609995	-4.490040	-0.139981
H	-1.959360	-5.507730	-0.339073
H	-1.177203	-4.106077	-1.069503
H	-0.814117	-4.548290	0.608450
C	-3.845706	-3.576281	-0.780207
H	-4.692400	-2.941263	-0.503116
H	-3.430022	-3.195852	-1.719568
H	-4.224860	-4.585066	-0.969302
N	-1.011729	-1.980578	1.231241
C	-0.123176	-1.044683	0.805986
C	-0.663756	-2.451984	2.483973
C	0.467188	-1.803997	2.841857
H	-1.220058	-3.206186	3.011517
H	1.059055	-1.905476	3.733287
N	0.777684	-0.931318	1.813194
C	1.801112	0.131754	1.792562
H	1.475337	0.732088	0.945001
C	3.191007	-0.403216	1.489453
C	3.988794	0.198456	0.457966
C	3.699600	-1.475664	2.185057
C	5.289104	-0.329871	0.201044
C	3.540903	1.279726	-0.354912
C	4.985630	-1.995227	1.926207
H	3.102072	-1.954309	2.953078
C	6.086590	0.235158	-0.829573
C	5.767148	-1.429567	0.957679
C	4.333805	1.796331	-1.346969
H	2.557586	1.712773	-0.217086
H	5.344325	-2.844383	2.498998
C	5.623867	1.274934	-1.590045
H	7.073310	-0.183481	-1.007952
H	6.758380	-1.820322	0.745494
H	3.957828	2.613306	-1.955645
H	6.239491	1.694027	-2.379687
C	1.693556	1.107550	3.015459

C	2.547830	2.343033	2.681770
H	3.606309	2.086666	2.578231
H	2.207129	2.808199	1.754291
H	2.455899	3.078878	3.487383
C	2.196909	0.536587	4.349443
H	3.214620	0.145392	4.264618
H	2.211199	1.337440	5.095803
H	1.548223	-0.246903	4.749717
C	0.227676	1.550838	3.153050
H	0.146916	2.332471	3.916033
H	-0.136310	1.954728	2.203824
H	-0.426070	0.724898	3.450782
Cu	-0.078188	-0.110321	-0.927962
C	0.190706	4.120570	-0.356323
C	-1.267756	3.960444	-0.886464
C	1.172099	4.615292	-1.421601
H	1.020019	5.673267	-1.656275
H	2.191226	4.487573	-1.044597
H	1.073090	4.032296	-2.341705
C	0.324444	4.958038	0.908653
H	1.376860	5.036747	1.195998
H	-0.057871	5.970873	0.742588
H	-0.220064	4.509872	1.741940
C	-2.309441	3.927294	0.235632
H	-3.262899	3.596043	-0.182190
H	-2.024127	3.212939	1.013583
H	-2.446591	4.912227	0.692941
C	-1.678627	4.965877	-1.953040
H	-2.706766	4.764950	-2.266890
H	-1.633822	5.988154	-1.562417
H	-1.036480	4.898182	-2.833220
B	-0.247670	1.896179	-0.838946
O	-1.234410	2.647860	-1.468988
O	0.543665	2.757239	-0.061919
C	-0.841375	0.293088	-3.813832
H	-0.919874	1.368526	-3.645288
H	-1.826743	-0.148219	-3.636964
H	-0.584721	0.112491	-4.864858
C	0.203854	-0.333130	-2.924580
H	1.221677	0.022589	-3.075926
C	0.037382	-1.600855	-2.358111
H	-0.935967	-2.080645	-2.471857
C	1.104543	-2.598165	-2.052679
H	0.907365	-3.146663	-1.134124
Cl	1.143448	-3.904467	-3.339464
Cl	2.731252	-1.893947	-1.871584

TSinx-Z,R

Imaginary Freq = -211.9829 (cm^{-1})

Electronic Energy BS1 = -3073.20049844 Hartree

Electronic Energy BS2 = -4517.15795312 Hartree

Zero-point Energy Correction = 0.896195 Hartree

Thermal Correction to Enthalpy = 0.947398 Hartree

Thermal Correction to Free Energy = 0.813085 Hartree

Chemical symbol X, Y, Z

C	4.323894	2.834364	-1.906476
C	5.381146	1.969974	-2.014348
C	5.366688	0.708474	-1.363752
C	4.239118	0.331571	-0.575666
C	3.165607	1.259595	-0.490444
C	3.200022	2.470645	-1.134059
H	7.316056	0.121530	-2.097464
H	4.347413	3.794924	-2.411552
H	6.253512	2.235733	-2.605335
C	6.464237	-0.180820	-1.494673
C	4.238151	-0.951489	0.078496
H	2.275568	1.019134	0.077825
H	2.344430	3.132373	-1.042863
C	5.327363	-1.773602	-0.092012
C	6.443538	-1.396029	-0.872217
H	5.357118	-2.741733	0.387980
H	7.279772	-2.080982	-0.968366
C	3.005967	-1.366185	0.883929
H	2.618430	-0.469185	1.373859
C	3.139118	-2.394899	2.059640
C	3.331145	-3.866148	1.648486
H	2.451448	-4.246546	1.121921
H	4.205766	-4.053624	1.022693
H	3.450864	-4.469003	2.554214
C	1.832667	-2.339452	2.873419
H	1.888185	-3.048563	3.705571
H	1.661187	-1.339373	3.276154
H	0.961294	-2.597646	2.264750
C	4.282019	-1.935746	2.980328
H	5.268098	-2.054391	2.527488
H	4.163359	-0.880154	3.248554
H	4.262966	-2.517491	3.907113
N	1.943556	-1.747591	-0.063517
C	0.726114	-1.151520	-0.151091
C	2.070018	-2.751528	-1.001546
C	0.895714	-2.813405	-1.664543
H	2.979258	-3.315133	-1.125802
H	0.600408	-3.458570	-2.471285
N	0.078121	-1.830996	-1.130994
C	-1.238011	-1.392909	-1.617874
H	-1.402321	-0.493908	-1.024598
C	-2.354899	-2.378104	-1.300313
C	-3.569960	-1.924073	-0.681026
C	-2.233874	-3.711213	-1.621841
C	-4.614947	-2.867809	-0.443100
C	-3.795853	-0.577503	-0.278185
C	-3.263791	-4.642218	-1.371688
H	-1.326749	-4.078085	-2.086098
C	-5.827023	-2.439426	0.160032
C	-4.434291	-4.227315	-0.800591
C	-4.975256	-0.198198	0.308894
H	-3.036139	0.183611	-0.400223
H	-3.118702	-5.683339	-1.641416
C	-6.009644	-1.133770	0.527859
H	-6.607601	-3.175908	0.330210
H	-5.238812	-4.931545	-0.607934
H	-5.099583	0.832990	0.624081
H	-6.937122	-0.818994	0.995368
C	-1.180102	-0.881535	-3.098300
C	-2.436530	-0.024506	-3.316547
H	-3.349756	-0.622345	-3.245165

H	-2.499371	0.768601	-2.567127
H	-2.409394	0.437836	-4.308673
C	-1.170268	-1.984711	-4.165280
H	-2.040554	-2.640264	-4.078281
H	-1.197441	-1.521255	-5.156890
H	-0.265328	-2.597489	-4.131442
C	0.073196	-0.003887	-3.257032
H	0.029745	0.544978	-4.203288
H	0.163136	0.721935	-2.442679
H	0.988659	-0.603015	-3.261961
Cu	0.171741	0.361987	0.881111
C	-2.310903	3.472948	-0.675676
C	-0.955126	3.898949	-1.338811
C	-2.686273	4.336174	0.532262
H	-3.000174	5.338837	0.228955
H	-3.512685	3.857001	1.063176
H	-1.851999	4.434543	1.232888
C	-3.496858	3.381845	-1.624306
H	-4.370915	3.011830	-1.081711
H	-3.738109	4.370782	-2.027049
H	-3.307999	2.707153	-2.459570
C	-0.832945	3.488158	-2.804206
H	0.208577	3.599644	-3.117887
H	-1.118223	2.447031	-2.953633
H	-1.458808	4.116781	-3.444488
C	-0.612891	5.377407	-1.194188
H	0.349063	5.579079	-1.673455
H	-1.371694	5.998472	-1.681051
H	-0.537907	5.674361	-0.146879
B	-0.638439	2.130147	0.111496
O	0.007372	3.138612	-0.580402
O	-2.002387	2.158772	-0.164300
C	0.928835	3.139609	2.102317
H	0.712251	4.014625	1.489233
H	1.915064	2.767961	1.805769
H	0.982605	3.440929	3.153129
C	-0.129218	2.040621	1.980869
H	-1.137900	2.411555	2.193427
C	0.209174	0.858085	2.827877
H	1.156796	0.943729	3.358838
C	-0.820525	0.225710	3.639115
H	-0.469119	-0.642799	4.190172
Cl	-1.504749	1.324494	5.024577
Cl	-2.256062	-0.313948	2.682359

TSrot-IV,R

Imaginary Freq = -48.8037 (cm^{-1})
Electronic Energy BS1 = -3073.25615189 Hartree
Electronic Energy BS2 = -4517.21089032 Hartree
Zero-point Energy Correction = 0.897678 Hartree
Thermal Correction to Enthalpy = 0.948594 Hartree
Thermal Correction to Free Energy = 0.814875 Hartree

Chemical symbol X, Y, Z

C	5.182789	-2.099404	-0.152749
C	5.676889	-1.070384	0.604329
C	5.067383	0.212494	0.584494
C	3.922660	0.436514	-0.237840
C	3.456513	-0.652084	-1.027961
C	4.059324	-1.881656	-0.980631
H	6.449120	1.077089	2.005057
H	5.650117	-3.078270	-0.121193
H	6.544181	-1.220711	1.241451
C	5.574049	1.264106	1.388939
C	3.291395	1.725993	-0.205010
H	2.600196	-0.538821	-1.679722
H	3.659615	-2.691682	-1.581852
C	3.821048	2.709389	0.598705
C	4.965841	2.489044	1.393533
H	3.347413	3.684050	0.643497
H	5.350563	3.294049	2.011252
C	2.021727	1.973902	-1.004405
H	1.640950	1.002194	-1.318150
C	2.164130	2.772028	-2.338278
C	2.819591	4.152317	-2.193418
H	2.211620	4.851558	-1.612748
H	3.809265	4.081640	-1.734234
H	2.944278	4.596468	-3.185993
C	0.769823	2.915860	-2.968281
H	0.855824	3.348262	-3.969880
H	0.280725	1.940040	-3.063965
H	0.115944	3.563434	-2.376345
C	3.040154	1.922368	-3.275512
H	4.032198	1.743515	-2.850335
H	2.576575	0.953320	-3.486923
H	3.170620	2.441704	-4.229753
N	0.923004	2.442554	-0.139153
C	-0.060884	1.586981	0.231378
C	0.678982	3.707438	0.358628
C	-0.487169	3.639973	1.044282
H	1.330640	4.547765	0.199477
H	-1.013528	4.413658	1.573343
N	-0.918475	2.329982	0.972463
C	-2.200700	1.723799	1.391524
H	-1.896569	0.731019	1.725617
C	-3.090955	1.572672	0.162200
C	-3.689565	0.315230	-0.175034
C	-3.288764	2.656894	-0.662136
C	-4.517459	0.243039	-1.336100
C	-3.483032	-0.881668	0.566762
C	-4.096140	2.577010	-1.815292
H	-2.802670	3.600541	-0.431090
C	-5.130222	-0.989359	-1.684127
C	-4.706646	1.395593	-2.139057
C	-4.081488	-2.057560	0.196696
H	-2.811391	-0.904753	1.415260
H	-4.228061	3.455525	-2.438595
C	-4.925146	-2.115177	-0.933949
H	-5.755138	-1.023953	-2.571935
H	-5.334085	1.319872	-3.022625
H	-3.882961	-2.956275	0.771630
H	-5.386303	-3.055218	-1.218137
C	-2.891868	2.378034	2.629850
C	-3.944853	1.367358	3.121695
H	-4.686154	1.147884	2.348656
H	-3.480993	0.422031	3.421759
H	-4.470605	1.774395	3.990795

C	-3.626656	3.695211	2.331472
H	-4.428470	3.545982	1.604739
H	-4.074717	4.071737	3.256453
H	-2.974930	4.483705	1.946203
C	-1.872729	2.586978	3.762578
H	-2.397121	2.882376	4.676768
H	-1.325090	1.665101	3.974353
H	-1.138339	3.364123	3.539460
Cu	-0.190459	-0.226704	-0.395337
C	-0.099494	-2.193633	3.098137
C	1.365031	-2.494664	2.615542
C	-0.687133	-3.294168	3.982501
H	-0.208918	-3.321915	4.965791
H	-1.755134	-3.105112	4.120664
H	-0.575564	-4.274424	3.511231
C	-0.280555	-0.834096	3.756953
H	-1.329725	-0.703923	4.041341
H	0.328955	-0.749509	4.662237
H	-0.003593	-0.029466	3.071489
C	2.163151	-1.237010	2.269839
H	3.094004	-1.535880	1.783517
H	1.615845	-0.595625	1.571442
H	2.409333	-0.654546	3.162774
C	2.177940	-3.375751	3.555388
H	3.171042	-3.538352	3.128639
H	2.299797	-2.892194	4.530182
H	1.708083	-4.349775	3.701663
B	-0.106353	-2.882823	0.918713
O	1.143718	-3.208418	1.388243
O	-0.847786	-2.201969	1.870796
C	-0.052272	-4.516879	-1.082884
H	-0.447824	-5.367857	-0.515314
H	1.040227	-4.548487	-1.006135
H	-0.320864	-4.660780	-2.132858
C	-0.585657	-3.180257	-0.543283
H	-1.680851	-3.180791	-0.555798
C	-0.076945	-1.943826	-1.326287
H	1.001429	-2.103241	-1.443979
C	-0.622537	-1.710731	-2.736106
H	-0.996563	-0.708458	-2.924396
Cl	0.706040	-1.861677	-4.008532
Cl	-2.029204	-2.744242	-3.233914

IV-Z,R

Electronic Energy BS1 = -3073.26221495 Hartree

Electronic Energy BS2 = -4517.21696380 Hartree

Zero-point Energy Correction = 0.897597 Hartree

Thermal Correction to Enthalpy = 0.949403 Hartree

Thermal Correction to Free Energy = 0.812768 Hartree

Chemical symbol X, Y, Z

C	4.712645	3.027777	-0.033167
C	5.675977	2.136012	-0.425084
C	5.441125	0.736790	-0.379283
C	4.187161	0.244305	0.093111
C	3.207770	1.204647	0.473446
C	3.461346	2.551903	0.414774
H	7.389752	0.217429	-1.161451
H	4.904238	4.095581	-0.071643
H	6.640950	2.486470	-0.781060
C	6.441594	-0.174613	-0.804228
C	3.977399	-1.178180	0.149272
H	2.216536	0.901201	0.792114
H	2.671007	3.242689	0.689940
C	4.978921	-2.013902	-0.287532
C	6.212558	-1.521316	-0.766857
H	4.837891	-3.086909	-0.257122
H	6.974676	-2.220722	-1.094912
C	2.642763	-1.709267	0.656406
H	2.182244	-0.905055	1.229553
C	2.614181	-2.910264	1.662481
C	2.851592	-4.302417	1.055960
H	2.112175	-4.539015	0.285618
H	3.850483	-4.430612	0.633458
H	2.746898	-5.052366	1.846359
C	1.215872	-2.930767	2.308390
H	1.159072	-3.729618	3.054043
H	0.998474	-1.985052	2.815958
H	0.424903	-3.100983	1.571651
C	3.655223	-2.630557	2.756393
H	4.676436	-2.688691	2.371903
H	3.514795	-1.632848	3.186785
H	3.551070	-3.360678	3.564836
N	1.716492	-1.894318	-0.472357
C	0.509580	-1.283345	-0.543591
C	1.923675	-2.710695	-1.565151
C	0.809757	-2.625128	-2.328250
H	2.838477	-3.256882	-1.720999
H	0.583687	-3.108529	-3.260481
N	-0.042304	-1.736330	-1.697190
C	-1.429516	-1.348513	-2.033647
H	-1.444999	-0.279058	-1.815949
C	-2.383952	-2.047635	-1.074176
C	-3.396918	-1.317995	-0.372203
C	-2.251825	-3.400462	-0.859500
C	-4.274849	-2.034290	0.495255
C	-3.567352	0.091252	-0.471384
C	-3.113108	-4.100793	0.009910
H	-1.458883	-3.946731	-1.363082
C	-5.294938	-1.334182	1.192028
C	-4.111181	-3.431580	0.665321
C	-4.556026	0.738388	0.222134
H	-2.903765	0.697223	-1.076008
H	-2.978556	-5.168177	0.152315
C	-5.439199	0.020478	1.057871
H	-5.954066	-1.897228	1.846918
H	-4.783721	-3.958909	1.335906
H	-4.639794	1.816914	0.136703
H	-6.214839	0.546292	1.604850
C	-1.817859	-1.460727	-3.543063
C	-3.141197	-0.691946	-3.720323
H	-3.941612	-1.118952	-3.110884
H	-3.037063	0.362338	-3.447216
H	-3.452323	-0.737123	-4.768462
C	-2.066854	-2.897442	-4.031947
H	-2.898836	-3.356523	-3.492753
H	-2.326069	-2.873126	-5.095107

H	-1.203414	-3.558328	-3.926121
C	-0.754528	-0.771049	-4.415672
H	-1.127070	-0.671818	-5.439912
H	-0.530148	0.232468	-4.042212
H	0.188822	-1.319006	-4.460652
Cu	-0.151410	-0.045486	0.773989
C	-1.205239	3.633178	-1.922744
C	0.300425	3.370532	-1.580629
C	-1.607781	5.099801	-1.755134
H	-1.183034	5.727286	-2.543818
H	-2.697179	5.174635	-1.799604
H	-1.280648	5.487001	-0.785922
C	-1.657105	3.116239	-3.279445
H	-2.720676	3.326973	-3.420733
H	-1.100481	3.602601	-4.086756
H	-1.512169	2.037861	-3.359246
C	0.832264	2.072764	-2.190204
H	1.811655	1.850209	-1.761692
H	0.173010	1.231886	-1.958474
H	0.935296	2.154261	-3.276642
C	1.241312	4.521501	-1.909712
H	2.267929	4.238404	-1.661933
H	1.202553	4.755849	-2.978589
H	0.986819	5.419147	-1.343613
B	-1.024550	2.803794	0.188223
O	0.253857	3.194977	-0.152449
O	-1.884020	2.892629	-0.891334
C	-1.577568	3.676722	2.487123
H	-2.172466	4.440297	1.968657
H	-0.586284	4.099719	2.683925
H	-2.051875	3.483010	3.450683
C	-1.465963	2.390271	1.633328
H	-2.467935	1.953790	1.547106
C	-0.507791	1.300309	2.156197
H	0.474088	1.756707	2.361015
C	-0.880858	0.575263	3.409613
H	-0.170140	-0.209120	3.657870
Cl	-0.863578	1.578192	4.985089
Cl	-2.488744	-0.238121	3.314243

TSelim-Z,R

Imaginary Freq = -198.2462 (cm^{-1})
Electronic Energy BS1 = -3073.25184241 Hartree
Electronic Energy BS2 = -4517.21519862 Hartree
Zero-point Energy Correction = 0.895686 Hartree
Thermal Correction to Enthalpy = 0.947793 Hartree
Thermal Correction to Free Energy = 0.810751 Hartree

Chemical symbol X, Y, Z

C	5.267998	-1.527910	-0.349204
C	5.497125	-0.721234	0.734295
C	4.724620	0.450717	0.953645
C	3.701914	0.804169	0.022089
C	3.517103	-0.048586	-1.102123
C	4.262450	-1.185334	-1.280919
H	5.725579	0.970944	2.797295
H	5.856770	-2.427171	-0.498203
H	6.270966	-0.971170	1.455238
C	4.941894	1.254774	2.100352
C	2.909379	1.971883	0.283167
H	2.776843	0.173720	-1.860455
H	4.052226	-1.809062	-2.146390
C	3.154250	2.711515	1.417712
C	4.171957	2.362515	2.329778
H	2.545927	3.584563	1.632769
H	4.333973	2.975033	3.210799
C	1.777149	2.370216	-0.653551
H	1.514465	1.494782	-1.248406
C	2.102747	3.477406	-1.708581
C	2.740107	4.746643	-1.122830
H	2.078652	5.297540	-0.449108
H	3.661319	4.516125	-0.581875
H	2.992179	5.429266	-1.940141
C	0.820625	3.827615	-2.480880
H	1.065729	4.466255	-3.334765
H	0.335928	2.924160	-2.867380
H	0.092239	4.360576	-1.863506
C	3.111363	2.872006	-2.702159
H	4.032872	2.556077	-2.205804
H	2.694372	2.007687	-3.228990
H	3.375252	3.619710	-3.455874
N	0.530778	2.601583	0.108676
C	-0.347494	1.591967	0.315785
C	0.076985	3.761520	0.703183
C	-1.116210	3.470949	1.274444
H	0.613933	4.692270	0.675233
H	-1.786530	4.109789	1.820386
N	-1.353495	2.131383	1.043301
C	-2.564109	1.321382	1.301888
H	-2.145582	0.347352	1.558946
C	-3.346861	1.189797	-0.000474
C	-3.715493	-0.092718	-0.522468
C	-3.661111	2.323719	-0.714316
C	-4.438337	-0.147299	-1.752432
C	-3.377689	-1.326331	0.101808
C	-4.369118	2.263995	-1.932044
H	-3.346878	3.294945	-0.343036
C	-4.814868	-1.406721	-2.288755
C	-4.757536	1.052285	-2.435739
C	-3.747064	-2.526060	-0.449117
H	-2.789165	-1.351228	1.009860
H	-4.598806	3.181756	-2.463350
C	-4.481558	-2.572795	-1.654078
H	-5.365043	-1.426282	-3.225261
H	-5.302314	0.991169	-3.373419
H	-3.455848	-3.447596	0.044712
H	-4.764221	-3.529907	-2.079749
C	-3.408688	1.737787	2.547757
C	-4.323113	0.539270	2.864024
H	-4.974979	0.295442	2.020766
H	-3.740125	-0.354842	3.109169
H	-4.956110	0.773312	3.725193
C	-4.314325	2.961058	2.331849
H	-5.053559	2.776268	1.549243
H	-4.852676	3.174097	3.260690
H	-3.767839	3.868823	2.062564
C	-2.492721	1.971166	3.761381

H	-3.100004	2.047792	4.668587
H	-1.792967	1.142430	3.895412
H	-1.905752	2.888957	3.682985
Cu	-0.162137	-0.171140	-0.412820
C	-0.147980	-2.494337	2.852645
C	1.360048	-2.779278	2.539119
C	-0.842820	-3.643665	3.582356
H	-0.507118	-3.721676	4.620231
H	-1.921647	-3.465580	3.579349
H	-0.653960	-4.597014	3.081545
C	-0.411578	-1.177102	3.564857
H	-1.484459	-1.076230	3.756119
H	0.107198	-1.141575	4.527901
H	-0.084927	-0.328485	2.958352
C	2.173749	-1.510109	2.278432
H	3.134394	-1.792397	1.841595
H	1.673019	-0.848063	1.563832
H	2.360741	-0.945802	3.196667
C	2.069847	-3.659017	3.557385
H	3.108813	-3.804521	3.251471
H	2.067093	-3.184097	4.543860
H	1.599421	-4.640386	3.637435
B	0.122490	-3.084788	0.666252
O	1.278695	-3.481645	1.284366
O	-0.727568	-2.421225	1.533829
C	0.590965	-4.350623	-1.570479
H	0.139814	-5.297286	-1.253448
H	1.654312	-4.379144	-1.316095
H	0.520037	-4.267464	-2.657512
C	-0.098171	-3.159885	-0.884299
H	-1.168594	-3.159076	-1.116109
C	0.495745	-1.828469	-1.343414
H	1.543529	-1.696356	-1.057137
C	0.258785	-1.256931	-2.597029
H	0.721826	-0.333744	-2.911104
Cl	1.975590	-2.047769	-4.116850
Cl	-1.233858	-1.552536	-3.440110

V-Z,R

Electronic Energy BS1 = -3073.31751039 Hartree
Electronic Energy BS2 = -4517.27642095 Hartree
Zero-point Energy Correction = 0.897946 Hartree
Thermal Correction to Enthalpy = 0.950469 Hartree
Thermal Correction to Free Energy = 0.811275 Hartree

Chemical symbol X, Y, Z

C	5.452638	2.835905	-1.791666
C	6.098985	1.671478	-2.109008
C	5.726853	0.440148	-1.507849
C	4.658895	0.407799	-0.559563
C	4.022321	1.642359	-0.245297
C	4.405547	2.814873	-0.844934
H	7.221168	-0.710618	-2.566036
H	5.745953	3.771390	-2.257707
H	6.913263	1.669478	-2.828681
C	6.409821	-0.755479	-1.844757
C	4.286877	-0.853405	0.023899
H	3.222362	1.698254	0.483081
H	3.895633	3.734260	-0.574777
C	4.990294	-1.980846	-0.338918
C	6.051662	-1.941451	-1.267946
H	4.736688	-2.941313	0.091802
H	6.574452	-2.858716	-1.519387
C	3.105156	-0.931511	0.985990
H	2.700995	0.072050	1.092842
C	3.401573	-1.349290	2.459338
C	3.980894	-2.756857	2.652137
H	3.318384	-3.535518	2.260693
H	4.969153	-2.863280	2.198223
H	4.095483	-2.948952	3.723823
C	2.090870	-1.237358	3.252985
H	2.280352	-1.438527	4.312626
H	1.670887	-0.230045	3.165145
H	1.340928	-1.953410	2.901434
C	4.402111	-0.316997	3.004504
H	5.351899	-0.354781	2.462074
H	3.998690	0.698005	2.924907
H	4.606157	-0.517041	4.061084
N	1.977278	-1.650018	0.359810
C	0.823415	-1.017892	0.007752
C	1.964945	-2.962553	-0.059502
C	0.791595	-3.159378	-0.695369
H	2.773624	-3.650105	0.108398
H	0.427511	-4.047243	-1.176506
N	0.096959	-1.961319	-0.654014
C	-1.140635	-1.631474	-1.384772
H	-1.260510	-0.568590	-1.164285
C	-2.377070	-2.359798	-0.857118
C	-3.632882	-1.666089	-0.744524
C	-2.332076	-3.681648	-0.477125
C	-4.773830	-2.362457	-0.246189
C	-3.808948	-0.297552	-1.088011
C	-3.462230	-4.367430	0.017282
H	-1.402882	-4.231631	-0.519394
C	-6.015502	-1.684017	-0.120800
C	-4.661365	-3.723571	0.130258
C	-5.018733	0.332872	-0.958009
H	-2.963181	0.281530	-1.426141
H	-3.364140	-5.407591	0.310327
C	-6.143746	-0.367146	-0.470564
H	-6.867388	-2.236780	0.265237
H	-5.537883	-4.238784	0.512288
H	-5.105917	1.386214	-1.208944
H	-7.096937	0.140646	-0.365733
C	-0.912915	-1.727557	-2.941685
C	-2.152722	-1.197929	-3.680427
H	-3.041985	-1.797064	-3.467835
H	-2.375455	-0.160005	-3.425456
H	-1.970534	-1.236917	-4.758711
C	-0.666089	-3.159740	-3.445367
H	-1.416143	-3.858439	-3.060977
H	-0.733309	-3.173689	-4.537476
H	0.330467	-3.524851	-3.189180
C	0.291178	-0.844432	-3.304865
H	0.416472	-0.809133	-4.391649
H	0.152317	0.180958	-2.944179
H	1.221832	-1.222899	-2.872257

Cu	0.469428	0.762254	0.633457
C	-1.404339	3.052912	-1.137466
C	-2.148155	4.166014	-0.313204
C	-2.136495	2.656090	-2.418271
H	-2.100438	3.459525	-3.158521
H	-1.644322	1.780199	-2.849457
H	-3.184890	2.407915	-2.230666
C	0.051941	3.360103	-1.456547
H	0.494955	2.521743	-2.003676
H	0.115500	4.250085	-2.091336
H	0.638950	3.518524	-0.551392
C	-1.213347	4.992420	0.567984
H	-1.819339	5.604511	1.241031
H	-0.561611	4.352067	1.169182
H	-0.588957	5.657655	-0.035382
C	-3.036487	5.081985	-1.144362
H	-3.517303	5.812495	-0.489170
H	-2.440614	5.627543	-1.882724
H	-3.819388	4.526974	-1.664624
B	-2.458476	2.148117	0.695310
O	-2.989684	3.397123	0.574414
O	-1.469303	1.908377	-0.242847
C	-4.246163	1.524626	2.450311
H	-5.035933	1.630494	1.700938
H	-4.140919	2.485840	2.962028
H	-4.564955	0.775903	3.180964
C	-2.923974	1.099890	1.784598
H	-3.082594	0.139481	1.286309
C	-1.850626	0.901652	2.818345
H	-1.427535	1.787182	3.289004
C	-1.348259	-0.253107	3.244746
H	-0.575782	-0.321773	3.999110
Cl	1.167791	2.438690	1.909749
Cl	-1.835315	-1.821560	2.642823

TSrot-III,S

Imaginary Freq = -40.4964 (cm^{-1})
Electronic Energy BS1 = -3073.21257092 Hartree
Electronic Energy BS2 = -4517.16915440 Hartree
Zero-point Energy Correction = 0.895704 Hartree
Thermal Correction to Enthalpy = 0.947155 Hartree
Thermal Correction to Free Energy = 0.812350 Hartree

Chemical symbol X, Y, Z

C	5.131669	0.568417	-2.553084
C	5.488375	-0.600082	-1.935343
C	4.861286	-1.012596	-0.729557
C	3.840823	-0.198466	-0.152520
C	3.476294	0.996589	-0.838165
C	4.111085	1.370276	-1.994985
H	6.009455	-2.836411	-0.554872
H	5.621060	0.875486	-3.471832
H	6.262599	-1.233959	-2.358865
C	5.236655	-2.224994	-0.097659
C	3.234151	-0.623356	1.074731
H	2.676400	1.625707	-0.464780
H	3.811265	2.287466	-2.493357
C	3.628588	-1.812157	1.643128
C	4.628556	-2.619711	1.062620
H	3.150461	-2.150697	2.557699
H	4.908009	-3.552645	1.541290
C	2.142427	0.204506	1.732906
H	1.719331	0.880303	0.990663
C	2.600730	1.154797	2.886675
C	1.362508	1.843938	3.486138
H	1.677964	2.654761	4.151148
H	0.747689	2.270754	2.687251
H	0.740084	1.160139	4.069200
C	3.472256	2.248818	2.242575
H	4.360220	1.832372	1.758636
H	2.898347	2.807015	1.497351
H	3.806837	2.951291	3.012672
C	3.441177	0.480091	3.980933
H	3.745580	1.232753	4.715388
H	2.905082	-0.298015	4.530399
H	4.346924	0.030797	3.564899
N	0.986628	-0.650722	2.058842
C	0.048573	-0.881736	1.111122
C	0.644194	-1.269675	3.247582
C	-0.550609	-1.869590	3.047576
H	1.256147	-1.240376	4.130793
H	-1.150719	-2.447909	3.727141
N	-0.899207	-1.633613	1.728271
C	-2.192165	-1.850423	1.057806
H	-1.901180	-1.932895	0.012733
C	-3.043890	-0.591509	1.187775
C	-3.578669	0.060717	0.029274
C	-3.238555	-0.026326	2.427085
C	-4.305486	1.275559	0.201801
C	-3.408051	-0.419925	-1.299391
C	-3.967200	1.169279	2.593791
H	-2.803873	-0.495559	3.304282
C	-4.819461	1.953306	-0.935038
C	-4.492340	1.805742	1.502157
C	-3.905245	0.263318	-2.377409
H	-2.877101	-1.344656	-1.489600
H	-4.098971	1.581037	3.589181
C	-4.620001	1.467720	-2.198326
H	-5.372433	2.876064	-0.779482
H	-5.045639	2.734025	1.614309
H	-3.744481	-0.128637	-3.376917
H	-5.008122	2.000668	-3.060194
C	-2.903175	-3.201747	1.381286
C	-3.675238	-3.211083	2.709981
H	-3.039266	-3.049426	3.584294
H	-4.457619	-2.448398	2.720519
H	-4.153620	-4.186981	2.839540
C	-1.879043	-4.348092	1.359724
H	-1.305163	-4.359568	0.427022
H	-1.164800	-4.290283	2.184533
H	-2.400006	-5.307580	1.435037
C	-3.920168	-3.445491	0.251278
H	-3.422842	-3.543965	-0.720033
H	-4.467464	-4.374224	0.438917
H	-4.648867	-2.632735	0.181172
Cu	0.019628	-0.105578	-0.685641
C	-1.065779	4.044977	-0.806694

C	0.389998	4.066907	-0.240101
C	-2.129433	4.254031	0.273636
H	-1.978502	3.566063	1.110403
H	-2.130942	5.281843	0.649999
H	-3.108784	4.037678	-0.159401
C	-1.314029	4.992247	-1.972922
H	-2.350503	4.894259	-2.307008
H	-1.146211	6.032586	-1.673865
H	-0.664869	4.760428	-2.819338
C	1.450969	4.364354	-1.304232
H	1.419502	5.406977	-1.634478
H	2.440781	4.167353	-0.880364
H	1.320253	3.714580	-2.174884
C	0.596870	4.969628	0.968826
H	1.637360	4.912649	1.302152
H	0.378211	6.012700	0.716289
H	-0.041141	4.670403	1.802363
B	-0.293197	1.882683	-0.600898
O	0.572154	2.697944	0.157530
O	-1.193720	2.692654	-1.275062
C	0.831438	0.671608	-3.482253
H	0.838001	0.364991	-4.536017
H	1.866375	0.717225	-3.137604
H	0.391823	1.669996	-3.417844
C	0.024562	-0.313557	-2.674508
H	-1.038166	-0.322398	-2.916759
C	0.577774	-1.480579	-2.129409
H	1.662434	-1.567562	-2.115363
C	-0.134829	-2.795414	-1.976459
H	-0.703602	-2.915435	-1.060854
Cl	-1.377068	-3.110061	-3.276164
Cl	1.048745	-4.149823	-1.929665

III-Z,S

Electronic Energy BS1 = -3073.21630815 Hartree
Electronic Energy BS2 = -4517.17297508 Hartree
Zero-point Energy Correction = 0.896977 Hartree
Thermal Correction to Enthalpy = 0.948772 Hartree
Thermal Correction to Free Energy = 0.814018 Hartree

Chemical symbol X, Y, Z

C	5.354888	0.973050	-2.107822
C	5.756826	-0.151512	-1.439078
C	5.043895	-0.623194	-0.304711
C	3.888907	0.084202	0.145604
C	3.482518	1.233217	-0.593568
C	4.201759	1.666773	-1.677710
H	6.342505	-2.321609	0.017819
H	5.909498	1.326441	-2.971109
H	6.632703	-0.704807	-1.766369
C	5.465846	-1.791424	0.378867
C	3.193721	-0.398835	1.302719
H	2.583911	1.776248	-0.321698
H	3.868491	2.547042	-2.219668
C	3.639743	-1.541858	1.925171
C	4.774032	-2.245158	1.468595
H	3.102221	-1.924625	2.787612
H	5.091183	-3.144073	1.987303
C	1.964830	0.322380	1.831153
H	1.549723	0.938725	1.034180
C	2.213241	1.335101	2.998902
C	0.858472	1.896801	3.463729
H	1.022564	2.744021	4.137860
H	0.281737	2.246760	2.601604
H	0.258710	1.156594	3.999946
C	3.026267	2.504990	2.415221
H	3.998557	2.178869	2.035325
H	2.476564	2.986223	1.601862
H	3.203588	3.251814	3.195754
C	3.010118	0.767998	4.183290
H	3.184554	1.565719	4.912481
H	2.494647	-0.035402	4.715467
H	3.983670	0.387975	3.861854
N	0.871708	-0.634331	2.077882
C	-0.002408	-0.921605	1.084230
C	0.515961	-1.287873	3.244664
C	-0.623050	-1.966111	2.982089
H	1.081286	-1.226208	4.156716
H	-1.211145	-2.593207	3.627321
N	-0.926413	-1.739386	1.650265
C	-2.180019	-2.009453	0.922903
H	-1.838262	-2.086816	-0.108821
C	-3.096455	-0.794060	1.042385
C	-3.635050	-0.148097	-0.117709
C	-3.372815	-0.274439	2.286681
C	-4.470929	0.993725	0.058553
C	-3.361026	-0.564035	-1.450535
C	-4.196909	0.857125	2.456336
H	-2.936143	-0.733368	3.168273
C	-5.003144	1.655655	-1.079531
C	-4.743462	1.472927	1.363451
C	-3.872902	0.107807	-2.528517
H	-2.726119	-1.420444	-1.635641
H	-4.390480	1.232651	3.456016
C	-4.708340	1.231345	-2.346116
H	-5.645063	2.518581	-0.921659
H	-5.377582	2.347721	1.478416
H	-3.628713	-0.225928	-3.532102
H	-5.110223	1.753588	-3.208395
C	-2.848834	-3.388690	1.218805
C	-3.624448	-3.467489	2.543760
H	-2.999445	-3.328843	3.429316
H	-4.426773	-2.726585	2.580095
H	-4.079235	-4.459448	2.630093
C	-1.778788	-4.490236	1.164032
H	-1.222155	-4.444462	0.222398
H	-1.061777	-4.416318	1.986149
H	-2.254407	-5.474296	1.222688
C	-3.862085	-3.636845	0.086172
H	-3.367504	-3.676259	-0.888587
H	-4.366526	-4.595043	0.244154
H	-4.625454	-2.854179	0.051384
Cu	0.030041	-0.167986	-0.718681
C	-1.388704	3.884527	-0.923916
C	0.053835	4.013487	-0.337457
C	-2.478507	4.039346	0.139235
H	-2.298366	3.370254	0.985544

H	-2.546596	5.068905	0.504437
H	-3.436764	3.760356	-0.304092
C	-1.683155	4.795698	-2.108007
H	-2.704112	4.618563	-2.457010
H	-1.595192	5.849403	-1.821886
H	-1.004351	4.599236	-2.940056
C	1.108508	4.376527	-1.387134
H	1.007098	5.410958	-1.729019
H	2.102042	4.257123	-0.943171
H	1.041916	3.710700	-2.252497
C	0.176448	4.941585	0.864182
H	1.214251	4.971736	1.208922
H	-0.120914	5.961415	0.597424
H	-0.445251	4.602187	1.694604
B	-0.474589	1.782121	-0.682055
O	0.325630	2.664136	0.076289
O	-1.419946	2.520430	-1.374242
C	1.051015	0.772749	-3.400761
H	1.312704	0.471065	-4.423214
H	1.970032	1.072692	-2.894763
H	0.379397	1.633095	-3.455799
C	0.379800	-0.374845	-2.689804
H	-0.602210	-0.634260	-3.087408
C	1.073609	-1.382197	-2.005759
H	2.124744	-1.205252	-1.772588
C	0.760831	-2.838409	-1.967148
H	0.888122	-3.277241	-0.979903
Cl	-0.913612	-3.254168	-2.480495
Cl	1.923572	-3.774738	-3.024895

TSinx-Z,S

Imaginary Freq = -151.2590 (cm^{-1})
Electronic Energy BS1 = -3073.20489085 Hartree
Electronic Energy BS2 = -4517.16304968 Hartree
Zero-point Energy Correction = 0.896116 Hartree
Thermal Correction to Enthalpy = 0.947432 Hartree
Thermal Correction to Free Energy = 0.812841 Hartree

Chemical symbol X, Y, Z

C	5.446960	-0.369679	-2.181276
C	5.753388	-1.124053	-1.081427
C	5.044394	-0.961703	0.138303
C	3.990918	-0.001995	0.219953
C	3.686205	0.750171	-0.951336
C	4.400310	0.575821	-2.108941
H	6.172862	-2.477877	1.187145
H	5.995301	-0.500848	-3.108363
H	6.548070	-1.863736	-1.123570
C	5.370256	-1.750466	1.269874
C	3.292304	0.143699	1.462287
H	2.868538	1.462547	-0.956652
H	4.149151	1.164445	-2.985709
C	3.639296	-0.654469	2.527832
C	4.678652	-1.603017	2.441140
H	3.092046	-0.567522	3.461671
H	4.920789	-2.212769	3.305537
C	2.150538	1.138496	1.613561
H	1.780250	1.403447	0.621822
C	2.525936	2.508984	2.265898
C	1.245192	3.324515	2.508055
H	1.501414	4.369638	2.708508
H	0.602966	3.294841	1.623059
H	0.659475	2.958005	3.354109
C	3.378838	3.271531	1.235754
H	4.286706	2.721730	0.972978
H	2.810961	3.456503	0.318138
H	3.678865	4.239465	1.649305
C	3.345975	2.397306	3.559664
H	3.560087	3.402030	3.937964
H	2.829599	1.858283	4.358561
H	4.298895	1.892451	3.382542
N	0.980896	0.472168	2.212678
C	0.134387	-0.229351	1.420650
C	0.573558	0.405762	3.532804
C	-0.571820	-0.312019	3.553397
H	1.107729	0.867743	4.343525
H	-1.199835	-0.575001	4.385000
N	-0.830950	-0.695752	2.249272
C	-2.017123	-1.369043	1.694386
H	-1.645793	-1.718248	0.730863
C	-3.134007	-0.359961	1.444983
C	-3.756521	-0.249652	0.157150
C	-3.550381	0.472266	2.459673
C	-4.807017	0.700080	-0.019774
C	-3.373169	-1.024509	-0.971402
C	-4.592620	1.405982	2.282130
H	-3.069128	0.421035	3.430406
C	-5.416775	0.842290	-1.294655
C	-5.216900	1.509822	1.069195
C	-3.977985	-0.863573	-2.189249
H	-2.575486	-1.750878	-0.895105
H	-4.892918	2.035789	3.113340
C	-5.012678	0.081661	-2.358964
H	-6.213806	1.572530	-1.408118
H	-6.021539	2.224162	0.918157
H	-3.647523	-1.463819	-3.030949
H	-5.482652	0.202907	-3.329748
C	-2.433590	-2.678235	2.439131
C	-3.137591	-2.470074	3.788720
H	-2.486378	-2.038902	4.553473
H	-4.024507	-1.839089	3.689505
H	-3.462429	-3.442696	4.171656
C	-1.179888	-3.545416	2.630185
H	-0.660758	-3.696077	1.678119
H	-0.474382	-3.092129	3.332933
H	-1.461755	-4.527545	3.022772
C	-3.417298	-3.420881	1.517646
H	-2.960702	-3.655379	0.552324
H	-3.716167	-4.365285	1.982549
H	-4.321503	-2.832865	1.335105
Cu	0.315331	-0.494136	-0.452358
C	-1.668745	2.937715	-1.590259
C	-0.201212	3.384820	-1.892116
C	-2.085911	3.212474	-0.143441
H	-1.350745	2.808904	0.559234
H	-2.207877	4.283217	0.045623
H	-3.036406	2.713195	0.051894

C	-2.723411	3.465981	-2.550176
H	-3.697624	3.055659	-2.270956
H	-2.777527	4.558687	-2.502898
H	-2.515700	3.167257	-3.578980
C	0.079780	3.560491	-3.384462
H	-0.363186	4.486806	-3.762292
H	1.160960	3.602309	-3.540677
H	-0.316481	2.727283	-3.967718
C	0.263643	4.623564	-1.140084
H	1.302162	4.846791	-1.401774
H	-0.348558	5.488788	-1.414626
H	0.206701	4.489951	-0.059550
B	-0.297134	1.137949	-1.427268
O	0.554229	2.240969	-1.427105
O	-1.584221	1.506728	-1.738381
C	1.016177	0.009838	-3.555630
H	1.291352	-0.720756	-4.323835
H	1.923576	0.517436	-3.226064
H	0.352332	0.749011	-4.010188
C	0.348775	-0.741167	-2.413039
H	-0.656512	-1.076340	-2.685320
C	1.142740	-1.786470	-1.737253
H	2.223177	-1.636150	-1.785057
C	0.830131	-3.205604	-1.845649
H	1.475408	-3.835264	-1.239970
Cl	-0.866377	-3.675008	-1.405928
Cl	1.098003	-3.909791	-3.580199

IV-Z,S

Electronic Energy BS1 = -3073.26611684 Hartree
Electronic Energy BS2 = -4517.22026529 Hartree
Zero-point Energy Correction = 0.897893 Hartree
Thermal Correction to Enthalpy = 0.949555 Hartree
Thermal Correction to Free Energy = 0.814074 Hartree

Chemical symbol X, Y, Z

C	4.839038	2.291852	-0.192164
C	5.131013	1.383750	-1.174469
C	4.573901	0.077504	-1.154038
C	3.698773	-0.297519	-0.091231
C	3.422208	0.674272	0.910469
C	3.970109	1.928694	0.860087
H	5.529942	-0.545835	-2.989863
H	5.255723	3.292819	-0.229927
H	5.786238	1.654151	-1.997662
C	4.859647	-0.847579	-2.189980
C	3.111806	-1.605356	-0.117231
H	2.724590	0.464797	1.710093
H	3.696164	2.655049	1.617660
C	3.405608	-2.459656	-1.154296
C	4.288105	-2.091315	-2.190994
H	2.927610	-3.434592	-1.194127
H	4.497817	-2.793894	-2.990968
C	2.108303	-2.036104	0.943726
H	1.756369	-1.140288	1.457164
C	2.676672	-2.943473	2.078201
C	1.558169	-3.296837	3.074748
H	1.991553	-3.763278	3.964875
H	1.022996	-2.396536	3.395310
H	0.818500	-3.988526	2.666732
C	3.724303	-2.104824	2.835038
H	4.534205	-1.778185	2.177694
H	3.276717	-1.215533	3.289422
H	4.161136	-2.705203	3.638791
C	3.388758	-4.211610	1.580348
H	3.747250	-4.784450	2.441339
H	2.750904	-4.876918	0.993752
H	4.253290	-3.956452	0.962497
N	0.879478	-2.529171	0.279372
C	0.073168	-1.639103	-0.351437
C	0.370931	-3.808086	0.160647
C	-0.791773	-3.705537	-0.525720
H	0.848298	-4.683269	0.561296
H	-1.484268	-4.474841	-0.816571
N	-0.959719	-2.369256	-0.831113
C	-2.117880	-1.686325	-1.440040
H	-1.681461	-0.729338	-1.728081
C	-3.177597	-1.416097	-0.377355
C	-3.681748	-0.089680	-0.164136
C	-3.624095	-2.439250	0.428694
C	-4.631909	0.123162	0.880125
C	-3.277669	1.040246	-0.926259
C	-4.562932	-2.224149	1.458943
H	-3.237292	-3.443142	0.290698
C	-5.135323	1.429757	1.115900
C	-5.056321	-0.967190	1.680310
C	-3.787634	2.287104	-0.679363
H	-2.539575	0.945979	-1.711570
H	-4.883939	-3.059623	2.072646
C	-4.726902	2.490325	0.353896
H	-5.855392	1.569332	1.917907
H	-5.777406	-0.785932	2.472736
H	-3.447560	3.126004	-1.278174
H	-5.116241	3.485241	0.544143
C	-2.611803	-2.310103	-2.781495
C	-3.447930	-3.589123	-2.629032
H	-2.878119	-4.429692	-2.223428
H	-4.320821	-3.424088	-1.992183
H	-3.806459	-3.902117	-3.614702
C	-1.390912	-2.579224	-3.674458
H	-0.772445	-1.680209	-3.771558
H	-0.761080	-3.381432	-3.278576
H	-1.718833	-2.873373	-4.676357
C	-3.494197	-1.250241	-3.464509
H	-2.928216	-0.336949	-3.673140
H	-3.866187	-1.637845	-4.417829
H	-4.357564	-0.984442	-2.847637
Cu	0.399530	0.222952	-0.680030
C	-1.286931	1.217443	2.946436
C	0.110439	1.784602	3.386552
C	-1.265225	-0.285210	2.664826
H	-0.459393	-0.545000	1.973778
H	-1.144339	-0.862135	3.587236
H	-2.207701	-0.575925	2.196361
C	-2.440641	1.542677	3.886290
H	-3.362495	1.118827	3.479353
H	-2.267853	1.110192	4.877379

H	-2.581115	2.619795	3.990310
C	0.005953	3.075254	4.202058
H	-0.402113	2.892518	5.200287
H	1.003543	3.509604	4.306462
H	-0.628012	3.806979	3.693546
C	1.009342	0.787571	4.104883
H	1.972387	1.254321	4.331429
H	0.556636	0.459053	5.045773
H	1.194811	-0.093543	3.487035
B	-0.302350	2.335200	1.214432
O	0.716364	2.134151	2.131820
O	-1.510865	1.895327	1.700217
C	0.458229	4.465273	0.040168
H	0.487295	5.036955	-0.888971
H	1.477385	4.424925	0.440302
H	-0.158250	5.020889	0.758766
C	-0.089873	3.038150	-0.175464
H	-1.076930	3.104362	-0.648775
C	0.797427	2.104501	-1.030786
H	1.839975	2.196050	-0.696087
C	0.853768	2.305441	-2.505298
H	1.503626	1.581803	-2.990838
Cl	-0.754468	2.132793	-3.343866
Cl	1.573934	3.919005	-3.10593