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Supporting Information

Copper-Photocatalyzed Hydroboration of Alkynes and Alkenes

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Supporting Information

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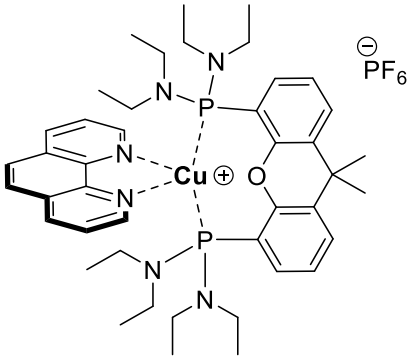
1. General information

All reactions were carried out using oven-dried glassware and magnetic stirring under an argon atmosphere unless otherwise stated. Analytical thin-layer chromatography (TLC) were performed using Merck-Kiesegel 60 F254 plates and visualized by UV light (254 nm) and/or chemical staining with alizarin solution (1M in acetone). Flash column chromatography was performed with silica gel 40 (particle size 63 μm) supplied by VWR. Yields refer to chromatographically and spectroscopically pure compounds unless otherwise stated. Copper photocatalyzed hydroboration reactions in batch were performed using a 405 nm blue LEDs. Copper photocatalyzed hydroboration reactions in continuous flow were performed using a Vapourtec E-series continuous flow system equipped with a UV-150 Photochemical flow reactor (10 mL) and a 450 nm blue LED lamp. ^{1}H NMR spectra were recorded on a Bruker DXP 300 spectrometer at 300 MHz, ^{13}C NMR spectra were recorded at 75 MHz, ^{19}F NMR and ^{11}B NMR spectra were recorded on a Bruker DXP 300 spectrometer. Chemical shifts are quoted in parts per million (ppm) relative to the residual solvent peak for C_6D_6 (δ_H = 7.16 ppm, δ_C = 128.06 ppm) or for $CDCl_3$ (δ_H = 7.26 ppm, δ_C = 77.16 ppm). The following abbreviations have been used: δ (chemical shift), *J* (coupling constant expressed in hertz), app. (apparent), br. (broad), s (singlet), d (doublet), dd (doublet of doublets), t (triplet), q (quartet) and m (multiplet). High-resolution mass spectra (HRMS) were recorded on Waters LCT Premier. Infrared spectra were recorded on a PerkinElmer Spectrum 100. Melting points were recorded on a Stuart Scientific Analogue SMP3. Absorption Spectra were recorded on UV/Visible Agilent Cary 60 spectrophotometer. Emission spectra were recorded on a Varian Cary Eclipse fluorescence spectrofluorimeter equipped with a xenon flash lamp as excitation source and a high performance R928 photomultiplier detector. Cyclic voltammetry measurements in dry acetonitrile with tetra-n-butylammonium tetrafluoroborate as the supporting electrolyte were carried out at 25 °C using a standard three-electrode cell, consisting of a Saturated Calomel Electrode (SCE) as the reference electrode, a platinum wire counter electrode and a carbon disk working electrode (area = 1 mm^2). The potential of the working electrode was controlled by a BioLogic SP-300 potentiostat with a scan rate of 200 mV·s^{-1}. Prior the measurements, all the solutions were degassed with a flow of argon for 15 minutes, which was left over the surface of the solution during the measurements. Lamps were purchased from EvoluChem, 405 nm, 18W LED.

Dichloromethane was freshly distilled from calcium hydride under argon. Acetonitrile (99.9%, Extra dry over molecular sieves in AcroSeal® bottles) was purchased from Acros Organics. Solvents were degassed with the freeze-pump-thaw technique. Tetrakis(acetonitrile)copper(I) hexafluorophosphate was purchased from Acros Organics and used as supplied. P,P′-(9,9-Dimethyl-9H-xanthene-4,5-diyl)bis[N,N,N′,N′-tetraethyl-phosphonous diamide] (97% purity) and 4,6-Bis(diphenylphosphino)-10H-phenoxazine (97% purity) were purchased from Sigma Aldrich and used as supplied. 1,10 –phenanthroline (99% purity) and 2,9-Dimethyl-1,10-phenanthroline (98% purity) were purchased from Alpha Aesar and used as supplied. Bis(pinacolato)diboron (98+% purity) was purchased from Alpha Aesar or Apollo Scientific Ltd and used as supplied. All other reagents were used as supplied.

2. Synthesis and characterization of Cu-PC-1 and Cu-PC-2



Cu-PC-1: [Cu(xantphosTEPD)(phen)]PF_6

[Cu(xantphosTEPD)(phen)]PF_6. To a solution of tetrakisacetonitrile copper(I) hexafluorophosphate (74.5 mg, 0.2 mmol) in dry dichloromethane (16 mL) was added P,P′-(9,9-Dimethyl-9H-xanthene-4,5-diyl)bis[N,N,N′,N′-tetraethyl-phosphonous diamide] (xantphosTEPD, 120 mg, 0.2 mmol). The reaction mixture was stirred at room temperature for two hours under argon atmosphere. A solution of 1,10–phenanthroline (phen, 36 mg, 0.2 mmol) in dry dichloromethane (4 mL) was then added dropwise and the resulting reaction mixture was stirred for another one hour. The reaction mixture was then concentrated under reduced pressure to one tenth of the original volume and the resulting solution was added dropwise with a syringe pump (1 drop/sec) to 100 mL of n-hexane under stirring. The yellow precipitate was collected by filtration and dried under vacuum to give the desired copper complex [Cu(xantphosTEPD)(phen)]PF_6 (183.8 mg, 0.194 mmol, 97%) as a yellow solid, mp: 264-266 °C; ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.55 (d, J = 9 Hz, 2H), 8.26 (m, 2H), 8.06 (s, 2H), 7.70 (m, 4H), 7.31-7.26 (m, 4H), 2.93 (s, 16H), 1.78 (s, 6H), 0.77 (s, 24H). ^{13}C NMR (75 MHz, $CDCl_3$): 154.5, 154.4, 154.3, 148.8, 142.9, 142.8 (2), 137.5, 135.0, 129.8, 129.3, 127.5, 126.1, 126.0, 125.9, 125.0, 124.0, 41.7, 41.6 (2), 35.8, 34.1, 22.3, 14.0. IR (ATR): ν_{max} 3060, 1556, 1499, 1481, 1461, 1434, 1391, 1300, 1259, 1215, 1094, 1026, 975, 835, 744, 694, 556, 509 cm^{-1}. HRMS (ESI) m/z calcd for $C_{43}H_{60}N_6OP_2Cu^+$ $[M\text{-}PF_6]^+$: 801.3600, found: 801.3593.

Cyclic voltammetry, absorption and emission spectra of Cu-PC-1

A solution of $(Et)_4N^+$ BF_4^- as supporting electrolyte (488 mg, 0.09 M) was prepared in HPLC-grade acetonitrile (25 mL) and degassed with N_2. A cyclic voltammogram of this solution was measured, then the [Cu(XantphosTEPD)(phen)]PF_6 (23.7 mg, 1 mM) powder was added and the solution was degassed again with N_2 for over 10 minutes. The cyclic voltammograms were measured using a silver wire reference electrode, a platinum working electrode and a platinum counter electrode using a scanning rate of 100 mV/s. Extra degassing under N_2 was necessary to see the reduction peaks that formed Cu(0). Water was avoided in these experiments to prevent its redox chemistry within the voltage limits needed to see both Cu(0) and Cu(II) formation.

To adjust the redox potentials from Ag/AgCl to SCE, the potentials were reduced by 47 mV.

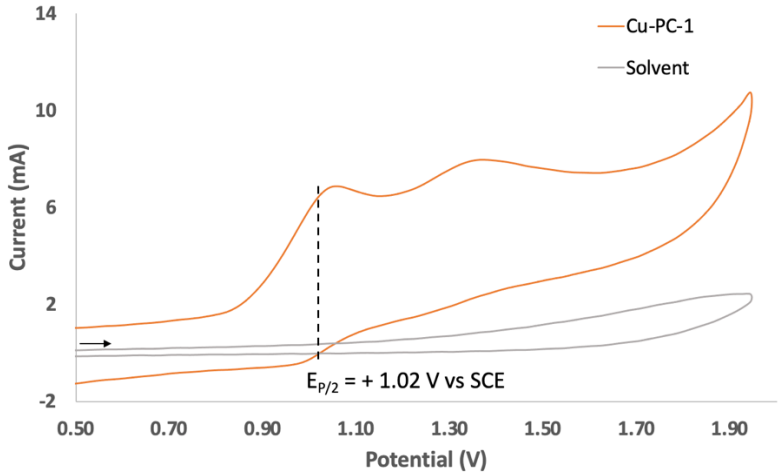


Figure S1. Cyclic voltammetry of Cu-PC-1 (1 mM) in deoxygenated acetonitrile to observe the redox peaks associated with Cu(II)/Cu(I)(orange) and solvent (grey).

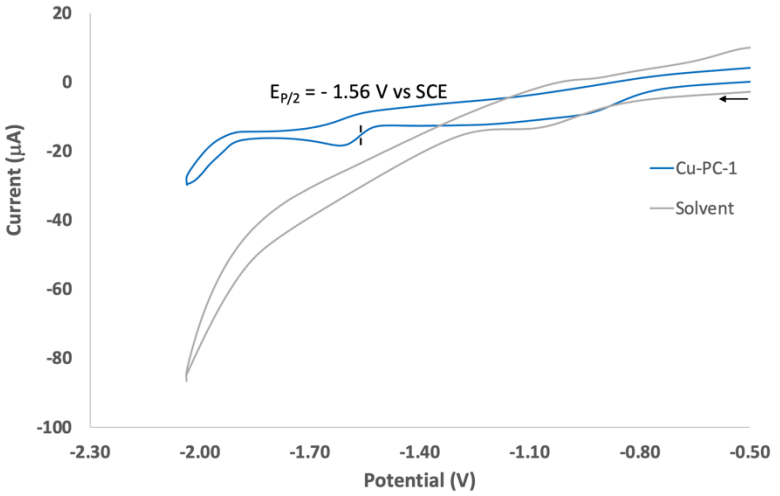


Figure S2. Cyclic voltammetry of Cu-PC-1 (1 mM) in deoxygenated acetonitrile to observe the redox peaks associated with Cu(0)/Cu(I) (blue) and solvent (grey).

The excited state redox potentials were calculated using the Rehm and Weller equation [Rehm D, Weller A. Kinetics of fluorescence quenching by electron and H-atom transfer. Israel Journal of Chemistry. 1970;8(2):259-71.]:

$$E^*_{1/2}{}^{red} = E_{1/2}{}^{red} + E_{00}$$

$$E^*_{1/2}{}^{oxi} = E_{1/2}{}^{oxi} - E_{00}$$

Where $E^*_{1/2}$ is the excited state reduction (red) or oxidation (oxi) potentials. $E_{1/2}$ is the oxidation or reduction potentials of the ground state, measured with cyclic voltammetry (Figure S1 and S1). E_{00} is the energy gap between the zeroth vibrational level of the ground and excited state, which can be calculated by finding the overlap in the normalized UV-visible spectrum and the emission spectrum (figure S3), then converting that value into eV.

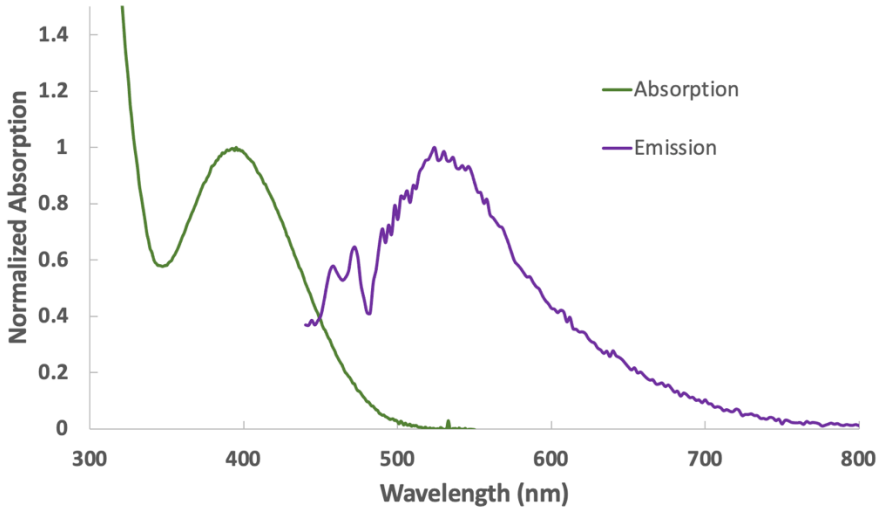


Figure S3. Normalized UV-Visible spectrum (green) and emission spectrum (solvent corrected λ_{ex} = 420 nm, purple) of Cu-PC-1.

Table S1. Summary of redox potentials and excited state redox potentials for Cu-PC-1

$E_{1/2}{}^{oxi}(Cu^{II}/Cu^{I})$ Vs SCE	$E_{1/2}{}^{red}(Cu^{I}/Cu^{0})$ Vs SCE	E_{00} eV	$E_{1/2}{}^{oxi}(Cu^{II}/Cu^{I}*)$ Vs SCE	$E_{1/2}{}^{red}(Cu^{I}*/Cu^{0})$ Vs SCE
+1.02	-1.56	2.77 (448 nm)	-1.75	+1.21

Cu-PC-1 is very weakly emissive and its measured emission spectra were found to contain Raman scattering in addition to Cu-PC-1 emission. To try and reduce the Raman scattering contribution, which increases proportional to $\frac{1}{\lambda^4}$, the excitation wavelength was tested at 360, 400 and 420 nm. When an excitation wavelength of 360 nm was used, the Raman peaks are much more intense then at 400 or 420 nm, such that the peak associated to Cu-PC-1 emission at 530 nm was no longer visible (Figure S4 to S6). An excitation wavelength of 420 nm was chosen due to the weaker Raman signal and the relatively stronger peak at 530 nm.

All spectra were collected using a slit width of 1.5 mm (6 nm resolution) with an absorption below 0.14 at 400 nm.

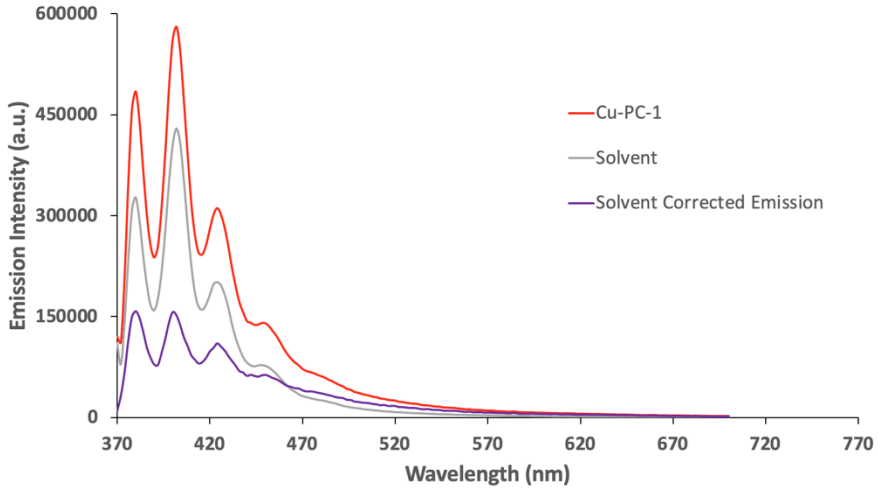


Figure S4. Solvent corrected emission spectra of Cu-PC-1 (purple) using an excitation wavelength of 360 nm.

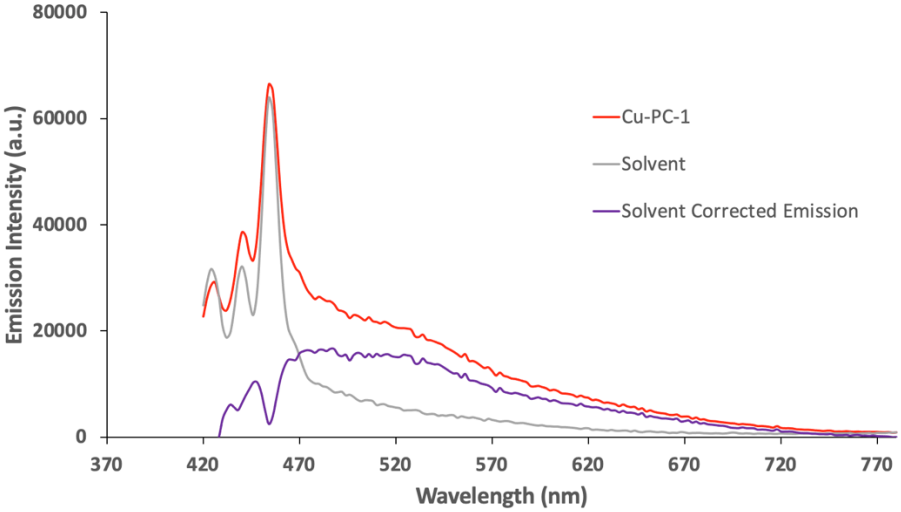


Figure S5. Solvent corrected emission spectra of Cu-PC-1 (purple) using an excitation wavelength of 400 nm.

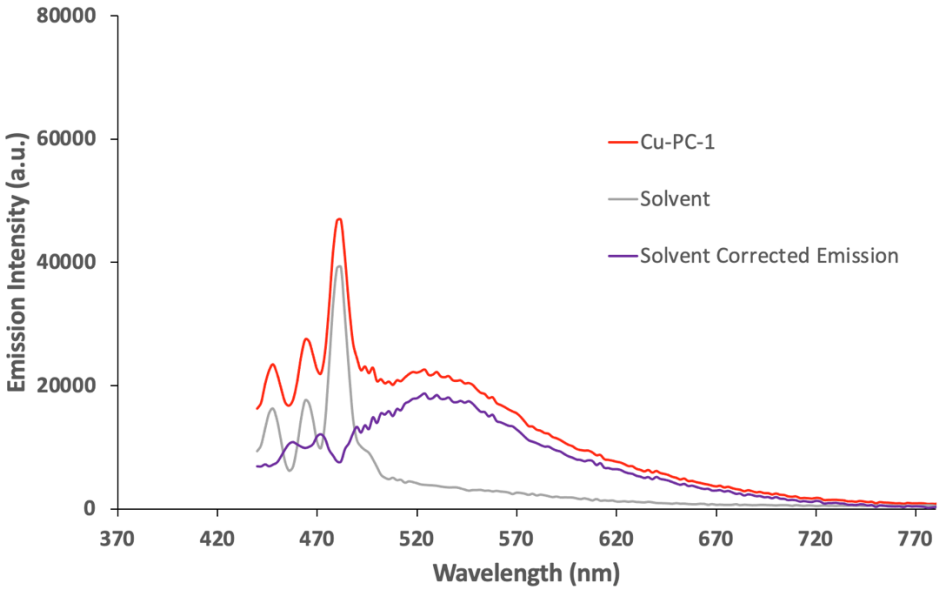
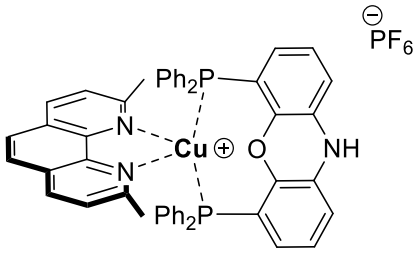


Figure S6. Solvent corrected emission spectra of Cu-PC-1 (purple) using an excitation wavelength of 420 nm.



Cu-PC-2: [Cu(N-xantphos)(dmp)]PF_6

[Cu(N-xantphos)(dmp)]PF_6. To a solution of tetrakisacetonitrile copper(I) hexafluorophosphate (74.5 mg, 0.2 mmol) in dry dichloromethane (16 mL) was added 4,6-Bis(diphenylphosphino)-10H-phenoxazine (N-xantphos, 115 mg, 0.2 mmol). The reaction mixture was stirred at room temperature for two hours under argon atmosphere. A solution of 2,9-Dimethyl-1,10-phenanthroline (dmp, 45 mg, 0.2 mmol) in dry dichloromethane (4 mL) was then added dropwise and the resulting reaction mixture was stirred for another one hour. The reaction mixture was then concentrated under reduced pressure to one tenth of the original volume and the resulting solution was added dropwise with a syringe pump (1 drop/sec) to 100 mL of diethylether under stirring. The yellow precipitate was collected by filtration and dried under vacuum to give the desired copper complex [Cu(N-xantphos)(dmp)]PF_6 (178.17 mg, 0.184 mmol, 92%) as a yellow solid, mp: 238-240 ºC; ^{1}H NMR (300 MHz, $(CD_3)_2CO$): δ 8.75 (d, J = 9 Hz, 1H), 8.53 (d, J = 9 Hz, 2H), 8.27-8.18 (m, 2H), 8.01-7.94 (m, 3H), 7.75 (d, J = 9 Hz, 2H), 7.41-7.27 (m, 5H), 7.23-7.01 (m, 15H), 6.61-6.52 (m, 2H), 2.62 (s, 3H), 2.52 (s, 3H). ^{13}C NMR (75 MHz, d_6-DMSO): 158.3, 157.7, 145.7, 145.6, 145.5, 142.3, 142.1, 138.0, 137.5, 135.3, 135.2, 135.1, 132.6, 132.5, 132.4, 131.0, 130.8, 130.5, 130.0, 128.7, 128.6, 128.5, 127.3, 127.2, 126.0, 125.8, 125.4, 122.8, 121.3, 121.1, 121.0, 116.2, 26.8, 25.2; IR (ATR): ν_{max} 3081, 1556, 1481, 1461, 1390, 1300, 1247, 1215, 1100, 1026, 962, 835, 744, 694, 556 cm^{-1}. HRMS (ESI) m/z calcd for $C_{50}H_{39}N_3OP_2Cu^+$ [M-PF_6]$^+$: 822.1859, found: 822.1843.

Cyclic voltammetry, absorption and emission spectra of Cu-PC-2

A solution of $(Et)_4N^+$ BF_4^- as supporting electrolyte (488 mg, 0.09 M) was prepared in HPLC-grade acetonitrile (25 mL) and degassed with N_2. A cyclic voltammogram of this solution was measured, then the [[Cu(N-xantphos)(dmp)]PF_6 (1 mM) powder was added and the solution was degassed again with N_2 for over 10 minutes. The cyclic voltammograms were measured using an Ag/AgCl wire reference electrode, a platinum working electrode and a platinum counter electrode using a scanning rate of 200 mV/s.

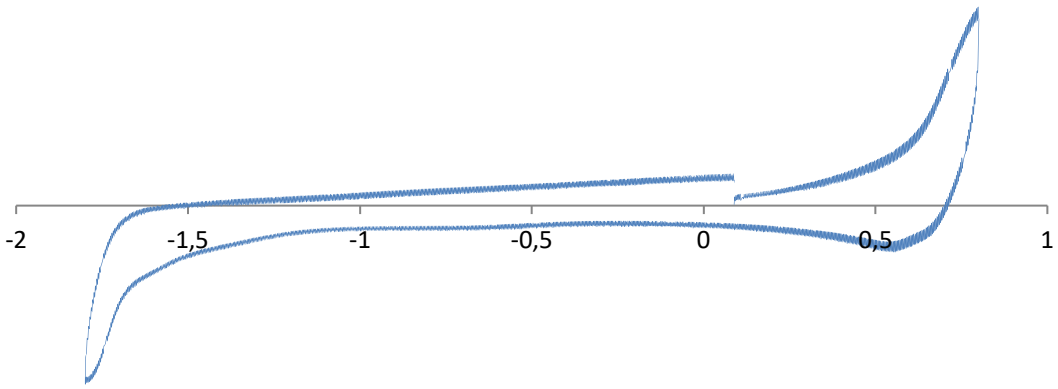


Figure S7. Cyclic voltammogram of Cu-PC-2 (1 mM) in deoxygenated acetonitrile.

The excited state redox potentials were calculated using the Rehm and Weller equation [Rehm D, Weller A. Kinetics of fluorescence quenching by electron and H-atom transfer. Israel Journal of Chemistry. 1970;8(2):259-71.]:

$$E^*_{1/2}{}^{red} = E_{1/2}{}^{red} + E_{00}$$
$$E^*_{1/2}{}^{oxi} = E_{1/2}{}^{oxi} - E_{00}$$

Where $E^*_{1/2}$ is the excited state reduction (red) or oxidation (oxi) potentials. $E_{1/2}$ is the oxidation or reduction potentials of the ground state, measured with cyclic voltammetry (figure S7). E_{00} is the energy gap between the zeroth vibrational level of the ground and excited state, which can be calculated by finding the overlap in the normalized UV-visible spectrum and the emission spectrum (figure S8), then converting that value into eV. The very weak emission spectrum was obtained by subtracting the signal due to the solvent as Raman scattering contributed significantly to the overall emission signal.

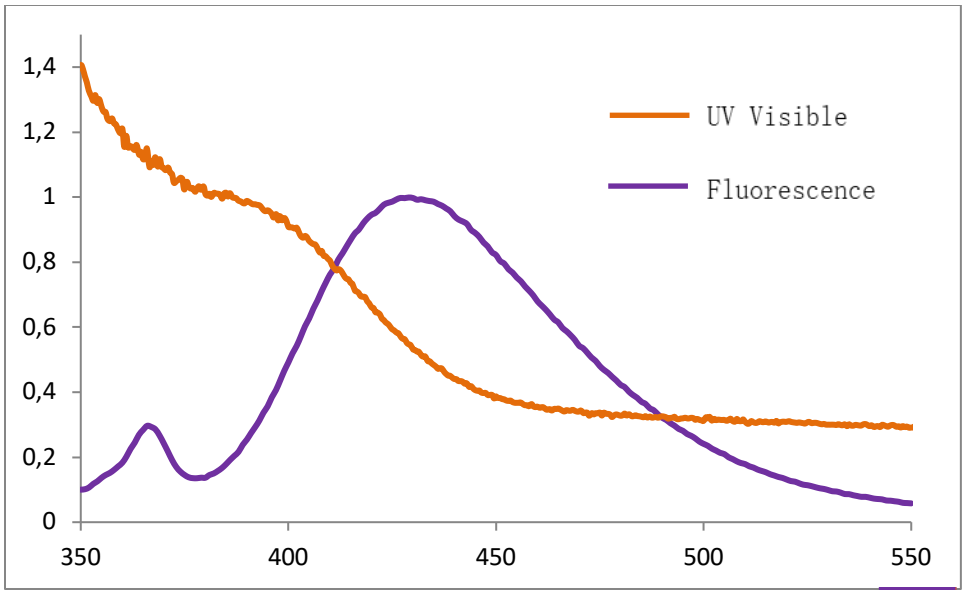
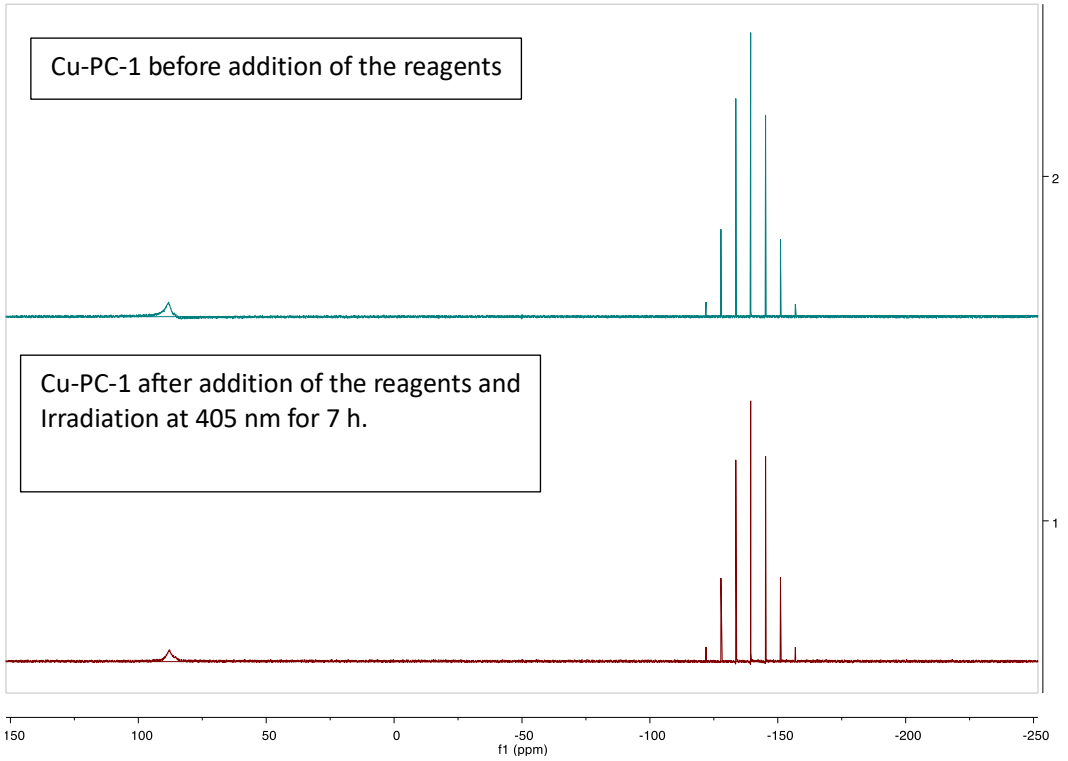


Figure S8. Normalized UV-Visible spectrum (orange) and emission spectrum (λ_{ex} = 365 nm, purple).

Table S2. Summary of redox potentials and excited state redox potentials for Cu-PC-2

$E_{1/2}^{oxi}(Cu^{II}/Cu^{I})$ Vs SCE	$E_{1/2}^{red}(Cu^{I}/Cu^{0})$ Vs SCE	E_{00} eV	$E_{1/2}^{oxi}(Cu^{II}/Cu^{I}*)$ Vs SCE	$E_{1/2}^{red}(Cu^{I}*/Cu^{0})$ Vs SCE
+0.83	-1.81	3.15 (414 nm)	-2.37	+1.34

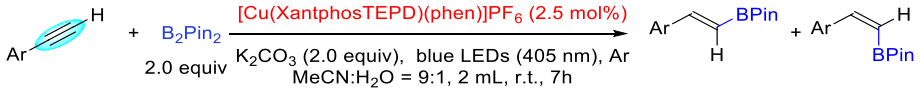
Stability of the catalyst within the reaction conditions:



Here are the ^{31}P NMR of the catalyst (green) and the ^{31}P NMR measurement after irradiation of the reaction mixture (red). No decomposition of the catalyst structure has been witnessed by ^{31}P NMR. Hence, the catalyst **Cu-PC-1** is stable within the reaction conditions. Note, that the catalyst structure cannot be witnessed by ^{1}H NMR due to its low concentration in the reaction mixture.

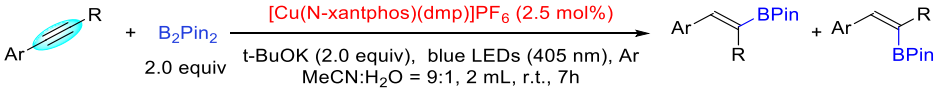
General procedures for copper-photocatalyzed hydroboration of alkynes and alkenes

General procedure 1: copper photocatalyzed hydroboration of terminal alkynes under batch conditions.



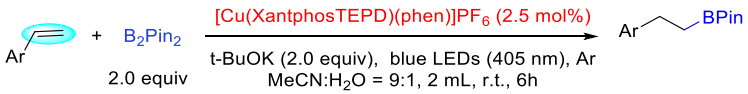
To a 10 mL vial equipped with a stir bar the alkyne (0.2 mmol), and B_2Pin_2 (120 mg, 0.4 mmol, 2.0 equiv) was added followed by [Cu(XantphosTEPD)(phen)]PF_6 (5 mg, 0.005 mmol, 2.5 mol%) and K_2CO_3 (65 mg, 0.4 mmol, 2.0 equiv). The vial was sealed with a rubber septum, then evacuated under vacuum and back filled with argon three times. A degassed solution of acetonitrile/H_2O (9:1, 2 mL) was added to the 10 mL vial and the reaction mixture was irradiated with 405 nm LEDs for 7 hours at room temperature. Additional water was added into the reaction mixture. The water was then extracted with EtOAc 3 times, the organic layer was dried with Na_2SO_4, and the solvents were removed under vacuum. The crude residue was purified via flash chromatography (pentane/EtOAc) over silica gel to produce the hydroborated product.

General procedure 2: copper photocatalyzed hydroboration of internal alkynes under batch conditions.



To a 10 mL vial equipped with a stir bar the alkyne (0.2 mmol), and B_2Pin_2 (120 mg, 0.4 mmol, 2.0 equiv) was added followed by [Cu(N-Xantphos)(dmp)]PF_6 (5 mg, 0.005 mmol, 2.5 mol%) and t-BuOK (45 mg, 0.4 mmol, 2.0 equiv). The vial was sealed with a rubber septum, then evacuated under vacuum and back filled with argon three times. A degassed solution of acetonitrile/H_2O (9:1, 2 mL) was added to the 10 mL vial and the reaction mixture was irradiated with 405 nm LEDs for 7 hours at room temperature. Additional water was then added into the reaction mixture. The water was then extracted with EtOAc 3 times, the organic layer was dried with Na_2SO_4, and the solvents were removed under vacuum. The crude residue was purified via flash chromatography (pentane/EtOAc) over silica gel to produce the hydroborated product.

General procedure 3: copper photocatalyzed hydroboration of alkenes under batch conditions:



To a 10 mL vial equipped with a stir bar the alkyne (0.2 mmol), and B_2Pin_2 (120 mg, 0.4 mmol, 2.0 equiv) was added followed by [Cu(XantphosTEPD)(phen)]PF_6 (5 mg, 0.005 mmol, 2.5 mol%) and t-BuOK (20 mg, 0.4 mmol, 2.0 equiv). The vial was sealed with a rubber septum, then evacuated under vacuum and back filled with argon three times. A degassed solution of acetonitrile/H_2O (9:1, 2 mL) was added to the 10 mL vial and the reaction mixture was irradiated with 405 nm LEDs for 6 hours at room temperature. Additional water was then added into the reaction mixture. The water was then extracted with EtOAc 3 times, the organic layer was dried with Na_2SO_4, and the solvents were removed under vacuum. The crude residue was purified via flash chromatography (pentane/EtOAc) over silica gel to produce the hydroborated product.

3. Condition Optimization of copper-photocatalyzed hydroboration of terminal alkynes, non-terminal alkynes and terminal alkenes

a) Screening of the copper-photocatalyzed hydroboration with phenylacetylene

Catalyst screening

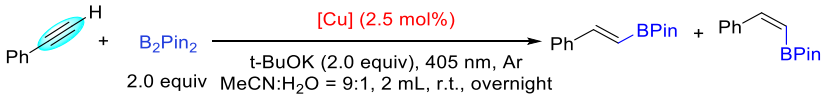


Table S3. Photocatalyst screening for copper-photocatalyzed hydroboration. Standard conditions: phenylacetylene (0.2 mmol), [Cu] (2.5 mol%), t-BuOK (2.0 equiv), B_2Pin_2 (2.0 equiv), acetonitrile/H_2O (9:1, 2.0 mL), 405 nm LEDs, overnight, room temperature. [a] NMR yield. [b] *E*/*Z* ratio determined by ^1H NMR.

Entry	[Cu]	Yield (%)[a]	*E*/*Z*[b]
1	[Cu(XantphosTEPD)(phen)]PF_6	70	99:1
2	[Cu(N-Xantphos)(dmp)]PF_6	91	1:1

Base screening

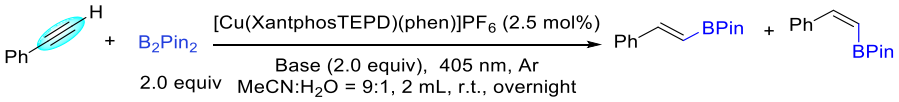


Table S4. Base screening for copper-photocatalyzed hydroboration. Standard conditions: phenylacetylene (0.2 mmol), [Cu(XantphosTEPD)(phen)]PF_6 (2.5 mol%), base (2.0 equiv), B_2Pin_2 (2.0 equiv), acetonitrile/H_2O (9:1, 2.0 mL), 405 nm LEDs, overnight, room temperature. [a] isolated yield. [b] *E*/*Z* ratio determined by ^1H NMR.

Entry	Base	Yield (%)[a]	*E*/*Z*[b]
1	^{t}BuOK	70	99:1
2	Li_2CO_3	62	99:1
3	Na_2CO_3	82	99:1
4	K_2CO_3	90	99:1
5	Cs_2CO_3	79	39:1
6	NaOH	40	39:1
7	KOH	61	7:1
8	KF	75	24:1
9	NaOMe	38	99:1
10	$NaPF_6$	n.r.	--

Solvent screening

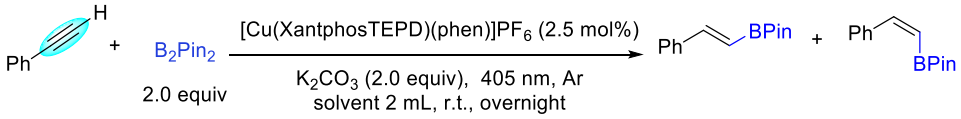


Table S5. Solvent screening for copper-photocatalyzed hydroboration of phenylacetylene. Standard conditions: phenylacetylene (0.2 mmol), [Cu(XantphosTEPD)(phen)]PF_6 (2.5 mol%), K_2CO_3 (2.0 equiv), B_2Pin_2 (2.0 equiv), solvent (2.0 mL), 405 nm blue LEDs, overnight, room temperature. [a] NMR yield. [b] *E*/*Z* ratio determined by ^1H NMR.

Entry	Solvent	Yield (%)[a]	*E*/*Z*[b]
1	MeOH	trace	99:1
2	MeOH+H_2O	12	99:1
3	DMSO	16	17:1
4	DMSO+H_2O	37	20:1
5	MeCN	70	22:1
6	MeCN+H_2O	90	99:1
7	THF	56	2:1
8	THF+H_2O	45	2:1
9	DMF	30	10:1
10	DMF+H_2O	39	5:1
11	H_2O	53	4:1

Reaction time screening

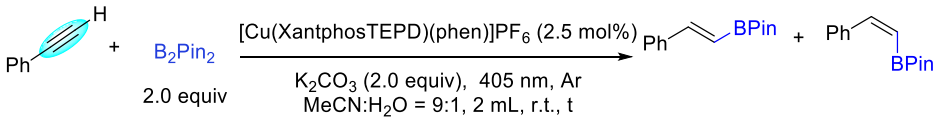


Table S6. Reaction time screening for copper-photocatalyzed hydroboration of phenylacetylene. Standard conditions: phenylacetylene (0.2 mmol), [Cu(XantphosTEPD)(phen)]PF_6 (2.5 mol%), K_2CO_3 (2.0 equiv), B_2Pin_2 (2.0 equiv), acetonitrile/H_2O (9:1, 2.0 mL), 405 nm LEDs, t, room temperature. [a] NMR yield. [b] *E*/*Z* ratio determined by ^{1}H NMR.

Entry	Time (h)	Yield (%)a	*E*/*Z*[b]
1	2	18	99:1
2	4	54	99:1
3	7	87	99:1
4	overnight	90	99:1

Catalyst loading screening

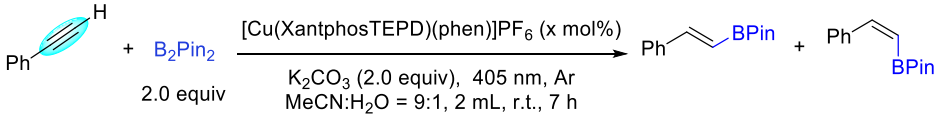


Table S7. Catalyst loading screening for copper-photocatalyzed hydroboration of phenylacetylene. Standard conditions: phenylacetylene (0.2 mmol), [Cu(XantphosTEPD)(phen)]PF_6 (x mol%), K_2CO_3 (2.0 equiv), B_2Pin_2 (2.0 equiv), acetonitrile/H_2O (9:1, 2.0 mL), 405 nm LEDs, 7 h, room temperature. [a] NMR yield. [b] *E*/*Z* ratio determined by ^{1}H NMR.

Entry	x	Yield (%)[a]	*E*/*Z*[b]
1	1 mol%	66	99:1
2	2 mol%	72	99:1
3	2.5 mol%	90	99:1

b) Optimization of the copper-photocatalyzed hydroboration of diphenylacetylene

Catalyst screening

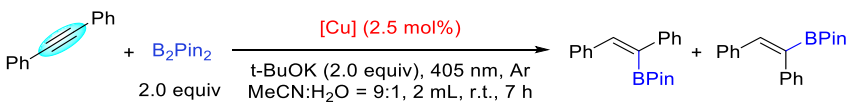


Table S8. Catalyst screening for copper-photocatalyzed hydroboration of diphenylacetylene. Standard conditions: diphenylacetylene (0.2 mmol), [Cu] (2.5 mol%), t-BuOK (2.0 equiv), B_2Pin_2 (2.0 equiv), acetonitrile/H_2O (9:1, 2.0 mL), 405 nm LEDs, 7 h, room temperature. [a] Isolated yield. [b] *E*/*Z* ratio determined by ^{1}H NMR.

Entry	[Cu]	Yield (%)[a]	*E*/*Z*[b]
1	[Cu(XantphosTEPD)(phen)]PF_6	41	1:4
2	[Cu(N-Xantphos)(dmp)]PF_6	85	1:14

Base screening

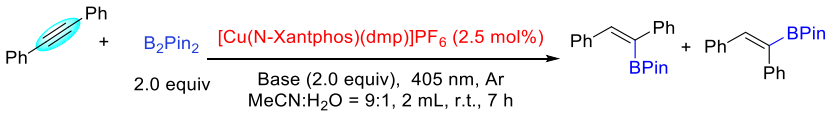


Table S9. Base screening for copper-photocatalyzed hydroboration of diphenylacetylene. Standard conditions: diphenylacetylene (0.2 mmol), [Cu(N-Xantphos)(dmp)]PF_6 (2.5 mol%), base (2.0 equiv), B_2Pin_2 (2.0 equiv), acetonitrile/H_2O (9:1, 2.0 mL), 405 nm LEDs, 7 h, room temperature. [a] Isolated yield. [b] *E*/*Z* ratio determined by ^{1}H NMR.

Entry	Base	Yield (%)[a]	*E*/*Z*[b]
1	^{t}BuOK	85(E/Z=1:14)	1:14
2	Cs_2CO_3	83(E/Z=1:3)	1:3
3	Li_2CO_3	21(E/Z=1:2)	1:2
4	Na_2CO_3	97(E/Z=1:3)	1:3
5	K_2CO_3	85(E/Z=1:1)	1:1
6	Ag_2CO_3	n.r.	--
7	NaOAc	trace	--
8	KOAc	trace	--

c) Screening of the copper-photocatalyzed hydroboration of styrene

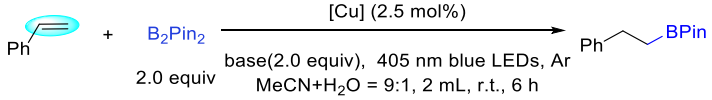


Table S10. Screening of the copper-photocatalyzed hydroboration of styrene. Standard conditions: styrene (0.2 mmol), [Cu] (2.5 mol%), base (2.0 equiv), B_2Pin_2 (2.0 equiv), acetonitrile/H_2O (9:1, 2.0 mL), 405 nm LEDs, 6 h, room temperature. [a] Isolated yield.

Entry	[Cu]	Base	Yield (%)[a]
1	[Cu(XantphosTEPD)(phen)]PF_6	K_2CO_3	25
2	[Cu(N-Xantphos)(dmp)]PF_6	t-BuOK	50
3	[Cu(XantphosTEPD)(phen)]PF_6	t-BuOK	97
4	[Cu(XantphosTEPD)(phen)]PF_6	KOH	42

4. Development of the reactions under continuous flow conditions

Screening of the copper-photocatalyzed hydroboration of phenylacetylene under continuous flow:

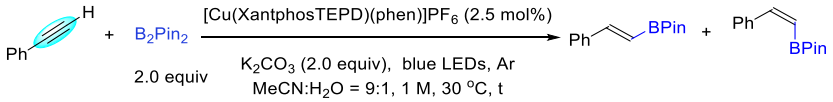
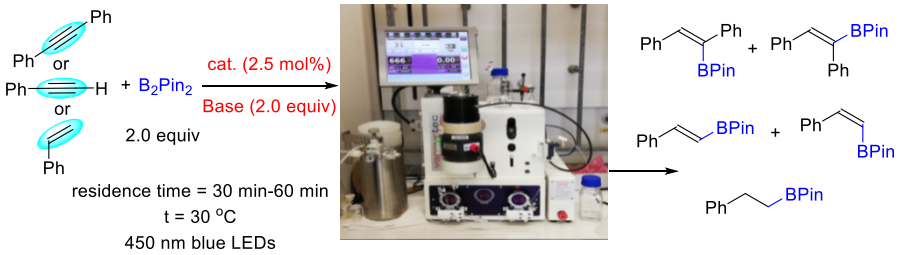


Table S11. Screening of the copper-photocatalyzed hydroboration of phenylacetylene. Standard conditions: phenylacetylene (1.0 equiv), B_2Pin_2 (2.0 equiv), [Cu(XantphosTEPD)(phen)]PF_6 (2.5 mol%), K_2CO_3 (2.0 equiv), acetonitrile/H_2O (9:1, 0.1M), blue LEDs (405 nm for batch, 450 nm for flow), 0.333 mL/min, reactor size (10 mL), room temperature. [a] NMR yield. [b] Z/E ratio determined by ^1H NMR.

Entry	Variation of standard conditions	Yield (%)[a]	*E*/*Z*[b]
1	In batch for 7 h	87	99:1
2	In flow for 30 min	91	99:1
3	In flow and 20 mmol, 0.333 mL/ min	78 (1.6 g)	99:1

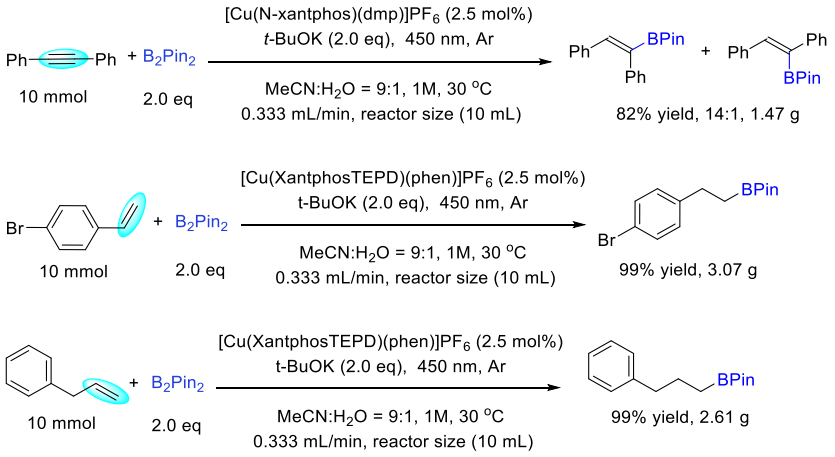
General Procedure for the copper photocatalyzed hydroboration of alkenes and alkynes under flow conditions:



Scheme S4. Copper photocatalyzed hydroboration of alkenes and alkynes under flow conditions

To a 10 mL vial equipped with a stir bar the alkene or alkyne (0. 2 mmol), and B_2Pin_2 (120 mg, 0.4 mmol, 2.0 equiv) was added followed by the Cu(I) photocatalyst (5 mg, 0.005 mmol, 2.5 mol%) and base (0.4 mmol, 2.0 equiv). The vial was sealed with a rubber septum, then evacuated under vacuum and back filled with argon three times. A degassed solution of acetonitrile/H_2O (9:1, 0.1 M) was then added to the 10 mL vial and the reaction mixture was pumped into the UV-150 photochemical flow reactor (10 mL) irradiated at 450 nm for 30 minutes (flow rate of 0.333 mL/min). Additional water was then added into the reaction mixture. The water was then extracted with EtOAc 3 times, the organic layer was dried with Na_2SO_4, and the solvents were removed under vacuum. The crude residue was purified via flash chromatography (pentane/EtOAc) over silica gel to produce the hydroborated product. This procedure could be scale up to 20 mmol.

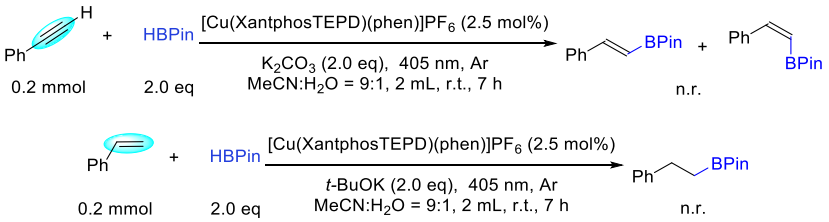
Using these optimized conditions in the flow reactor, alkenes and alkynes were tested as follow (Scheme S1):



Scheme S1. Gram-scale scope under continuous flow

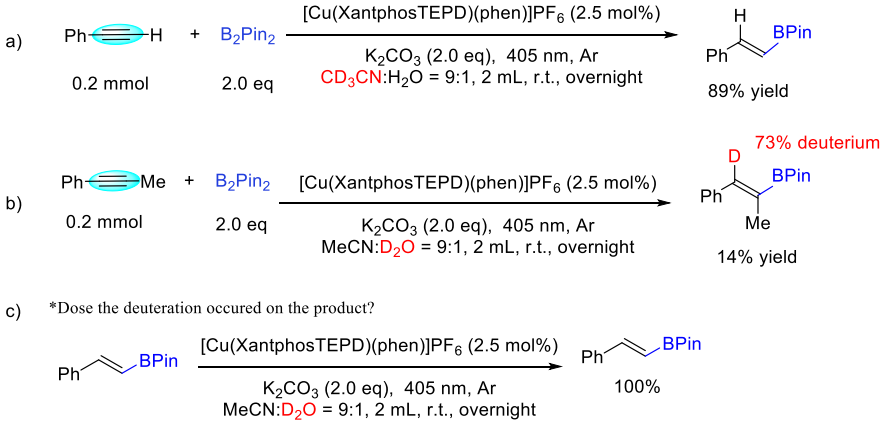
5. Mechanistic studies

6.1 HBPin *vs* B_2Pin_2



Scheme S2. HBPin replace B_2Pin_2 in the reaction

6.2 Deuterium labelling



Scheme S3. Deuterium experiments

6.3 Control experiments

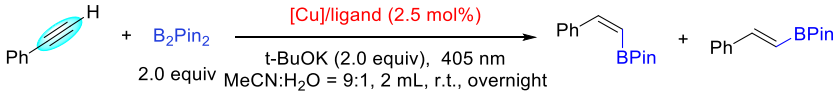
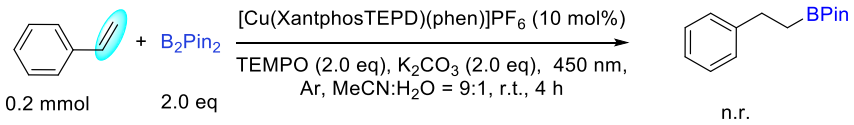


Table S12. Control experiments. Standard conditions: phenylacetylene (1.0 eq), B_2Pin_2 (2.0 eq.), [Cu]/ligand (2.5 mol%), K_2CO_3 (2.0 equiv), acetonitrile/H_2O (9:1, 2 mL), blue LEDs 405 nm, 7 h, room temperature. [a] NMR yield. [b] *E*/*Z* ratio determined by ^{1}H NMR; [c] the reaction performed in the dark.

Entry	[Cu]	Ligand	Yield (%)[a]	*E*/*Z*[b]
1	[Cu(XantphosTEPD)(phen)]PF_6	--	89(E/Z=99:1)	99:1
2	Cu(MeCN)$_4PF_6$	--	trace	--
3	Cu(MeCN)$_4PF_6$	dmp	7	--
4	Cu(MeCN)$_4PF_6$	XantphosTEPD	9	--
5[c]	[Cu(XantphosTEPD)(phen)]PF_6	--	trace	--
6[c]	Cu(MeCN)$_4PF_6$	--	trace	--
7[c]	Cu(MeCN)$_4PF_6$	dmp	trace	--
8[c]	Cu(MeCN)$_4PF_6$	XantphosTEPD	trace	--

6.4 Effect of the radical scavengers



Scheme S4. Effect of the TEMPO (Found TEMPO-BPin, MW: 283)

```
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Operator   : tia
Acquired   :  5 Jan 2021  17:04     using AcqMethod METHODE_50_250-25°CPARMIN.M
Instrument :    GCMS
Sample Name:
Misc Info  :
Vial Number: 6
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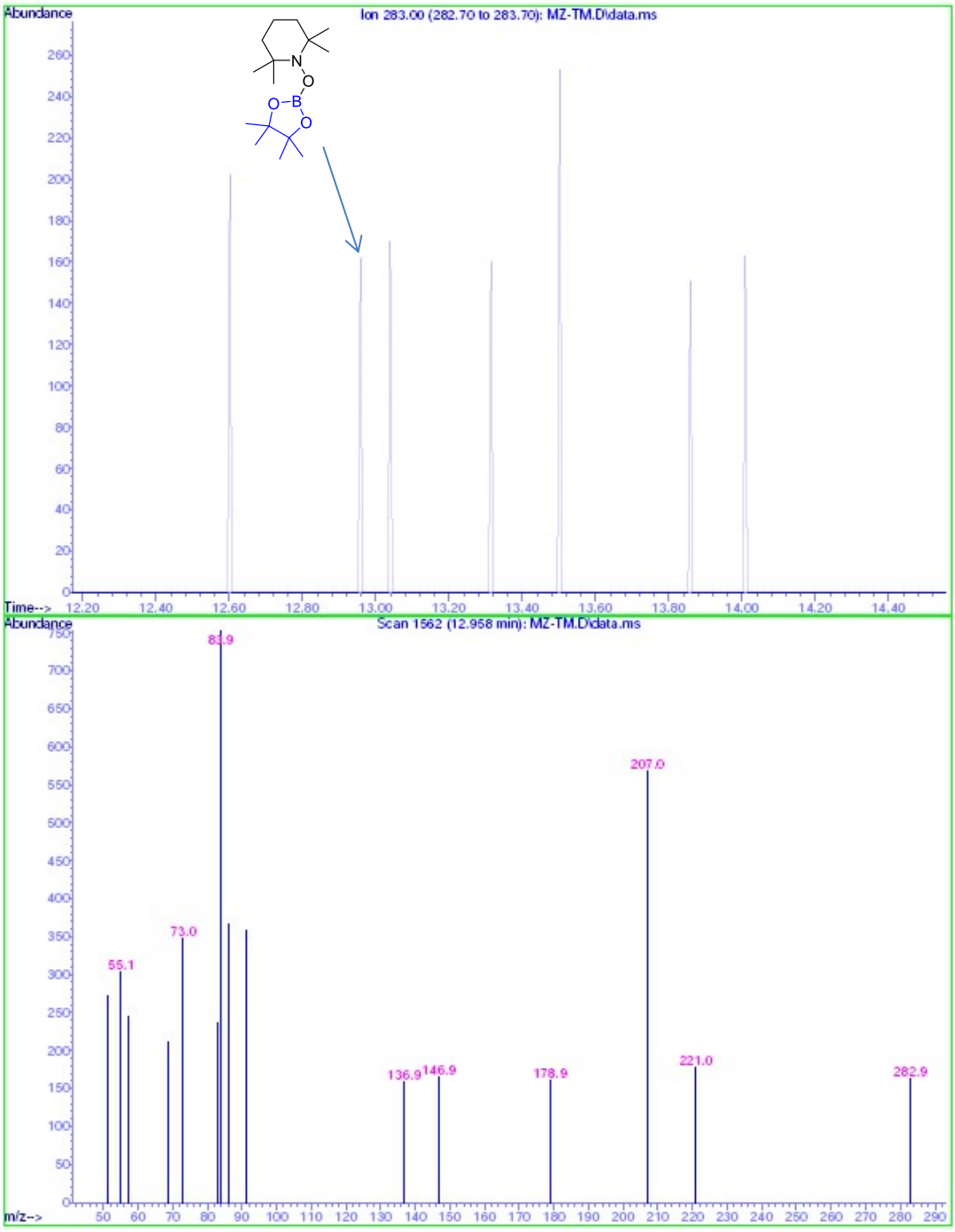
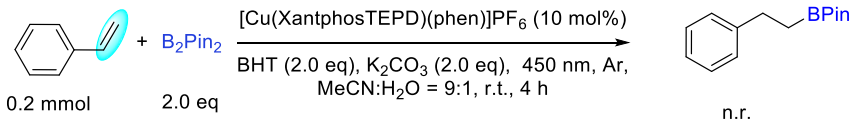
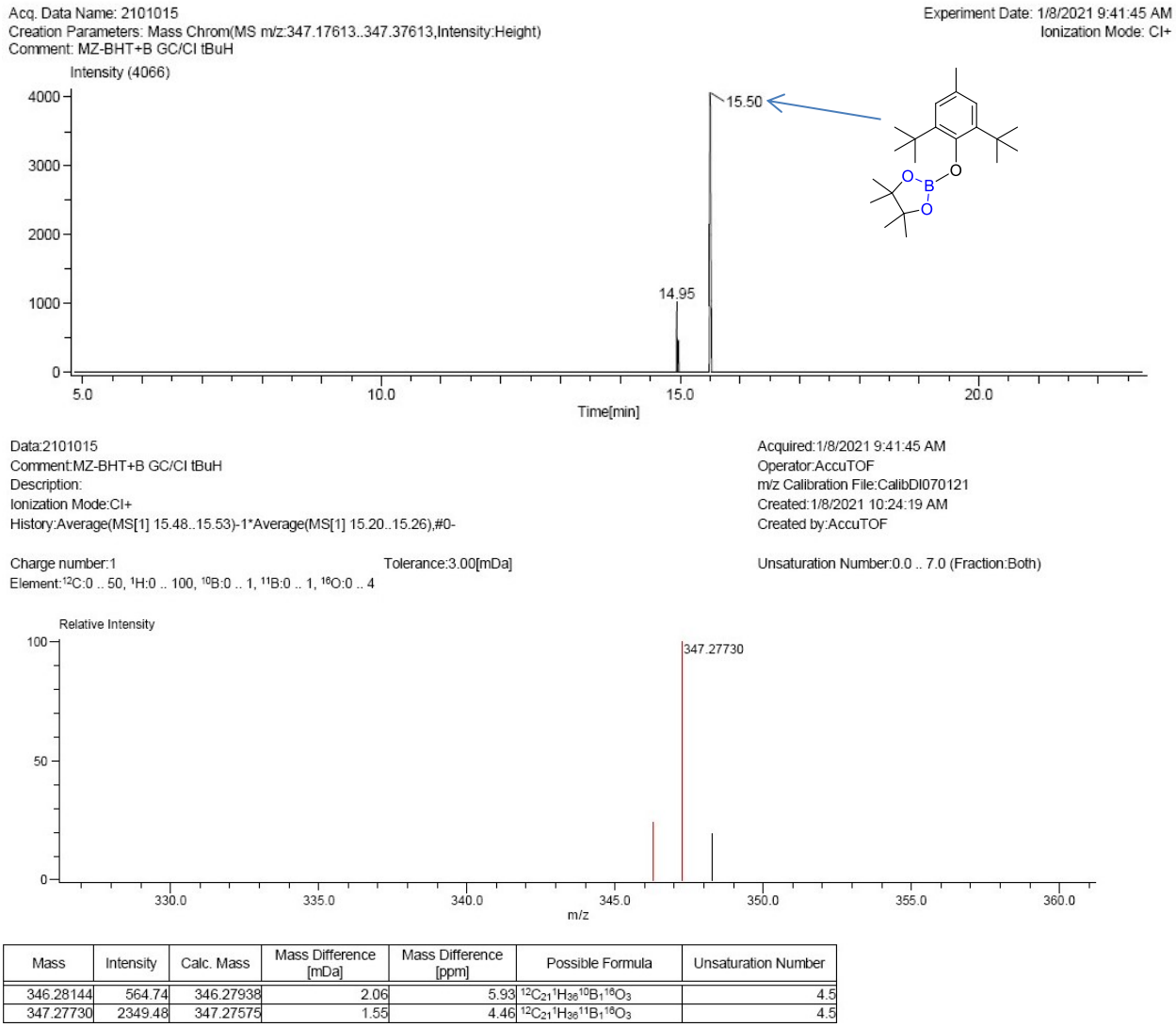




Scheme S5. Effect of the BHT (Found [BHT-BPin+H], MW: 347.2773)



Mass	Intensity	Calc. Mass	Mass Difference [mDa]	Mass Difference [ppm]	Possible Formula	Unsaturation Number
346.28144	564.74	346.27938	2.06	5.93	$^{12}C_{21}{}^{1}H_{36}{}^{10}B_{1}{}^{16}O_{3}$	4.5
347.27730	2349.48	347.27575	1.55	4.46	$^{12}C_{21}{}^{1}H_{36}{}^{11}B_{1}{}^{16}O_{3}$	4.5

6.5 Quantum yield measurements

a) Determination of the light intensity of a single blue LED at 405 nm:

Following the literature procedures from Yoon[1] and Glorius,[2] the photon flux of the LED (λmax = 405 nm) was determined by standard ferrioxalate actinometry. A solution of ferrioxalate (0.006 M) was prepared by dissolving potassium ferrioxalate hydrate (29.5 mg) in aq. H_2SO_4 (0.05 M, 10 mL). A buffered solution of 1,10-phenanthroline was prepared by dissolving 1,10-phenanthroline (20.0 mg) and sodium acetate (4.50 g) in aq. H_2SO_4 (0.5 M, 20 mL). Both solutions were stored in the dark. To determine the photon flux of the LED, 1 mL of the ferrioxalate solution was placed in a 10 mL Schlenk tube and irradiated for 90 s at λmax = 405 nm. After irradiation, 175 µL of the phenanthroline solution was added and the mixture stirred in the dark for 1 h to allow

the ferrous ions to completely coordinate to the phenanthroline. The solution was transferred to a quartz cuvette and the absorption was measured at 510 nm. A non-irradiated sample was prepared as a control and the absorption at 510 nm was measured. The actinometry experiment was done 3 times for each sample to ensure accuracy. The average of the absorption of the irradiated and non-irradiated samples was determined and used to calculate the conversion of Fe^{2+} from eq. 1.

$$(Fe^{2+}) = \frac{V \cdot \Delta A(510\ nm)}{l \cdot \varepsilon} \quad (1)$$

Where V is the total volume (0.001175 L) of the solution, ΔA is the difference in absorption at 510 nm between the irradiated and non-irradiated solutions (ΔA = 1.214), l is the path length (1.0 cm), and ε is the molar absorption coefficient of the ferrioxalate actinometer at 510 nm (11 100 L mol^{-1} cm^{-1}). The photon flux (Φq) was calculated using eq. 2,

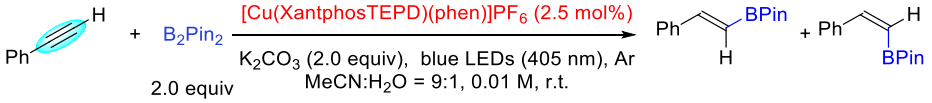
$$\Phi q = \frac{n(Fe2+)}{\Phi F \cdot t \cdot f} \quad (2)$$

Where Φ_F is the photoreaction quantum yield for the ferrioxalate actinometer (1.13 at λ_{ex} = 405 nm), t is the irradiation time (90 s), and f is the fraction of light absorbed at λ_{ex} = 405 nm by the ferrioxalate actinometer. This value is calculated using eq. 3. Where A is the absorption of the ferrioxalate solution at 405 nm. An absorption spectrum gave an A (405 nm) value of 1.2065, indicating that the fraction of absorbed light (f) is > 0.938.

$$f = 1 - 10^{-A} \quad (3)$$

The photon flux was thus calculated from an average of three experiments to be 1.37×10^{-9} Einstein's * s^{-1}.

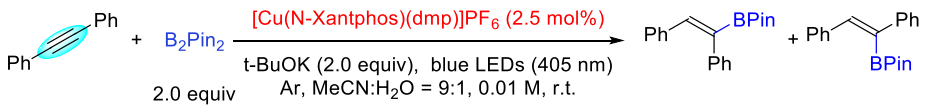
b) Determination of the reaction quantum yield:



To a dried 10 mL Schlenk tube a stir bar, phenylacetylene (0.02 mmol), [Cu(XantphosTEPD)(phen)PF_6] (2.5 mol%), B_2Pin_2 (2 equiv), and K_2CO_3 (2 equiv) in acetonitrile/H_2O (9:1, v/v, 0.01 M) was mixed together. The reaction mixture was degassed via freeze-pump-thaw 3 times. After the mixture was thoroughly degassed and filled with argon, the Schlenk tube was tightly sealed and stirred under irradiation with a single LED (λ_{max} = 405 nm) for 30 min. After irradiation, the yield was determined by proton NMR using DMF as an internal standard. The yield was determined to be 3.17% (obtained from three parallel experiments) (6.34×10^{-8} mol). The quantum yield (Φ) of the reaction was determined using eq. 4 where the photon flux (Φ_q) is 1.32×10^{-9} Einstein's * s^{-1} (determined by actinometry as described above), t is the reaction time (1800 s) and f_R is the fraction of incident light absorbed by the reaction mixture. An absorption spectrum of the reaction mixture gave a value of > 3 at 405 nm, indicating that essentially all the incident light (f_R > 0.999) is absorbed by the photocatalyst.

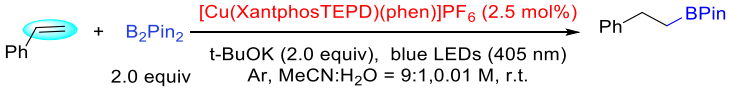
$$\Phi = \frac{n(product)}{\Phi q \cdot t \cdot fR} \quad (4)$$

The quantum yield of the reaction (Φ_R) was determined to be Φ_R = 0.31.



To a dried 10 mL Schlenk tube a stir bar, diphenylacetylene (0.02 mmol), [Cu(N-Xantphos)(dmp)PF_6] (2.5 mol%), B_2Pin_2 (2 equiv), and t-BuOK (2 equiv) in acetonitrile/H_2O (9:1, v/v, 0.01 M) was mixed together. The reaction mixture was degassed via freeze-pump-thaw 3 times. After the mixture was thoroughly degassed and filled with argon, the Schlenk tube was tightly sealed and stirred under irradiation with a single LED (λ_{max} = 405 nm) for 30 min. After irradiation, the yield was determined by proton NMR using DMF as an internal standard. The yield was determined to be 2.10% (obtained from three parallel experiments) (4.22×10^{-8} mol). The quantum yield (Φ) of the reaction was determined using eq. 4 where the photon flux (Φ_q) is 1.32×10^{-9} Einstein's * s^{-1} (determined by actinometry as described above), t is the reaction time (1800 s) and f_R is the fraction of incident light absorbed by the reaction mixture, determined using eq 3. An absorption spectrum of the reaction mixture gave an absorbance value of > 3 at 405 nm, indicating that essentially all the incident light ($f_R > 0.999$) is absorbed by the photocatalyst.

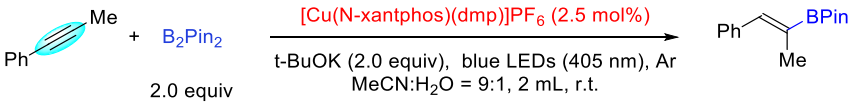
The reaction quantum yield (Φ_R) was thus determined to be $\Phi_R = 0.18$.



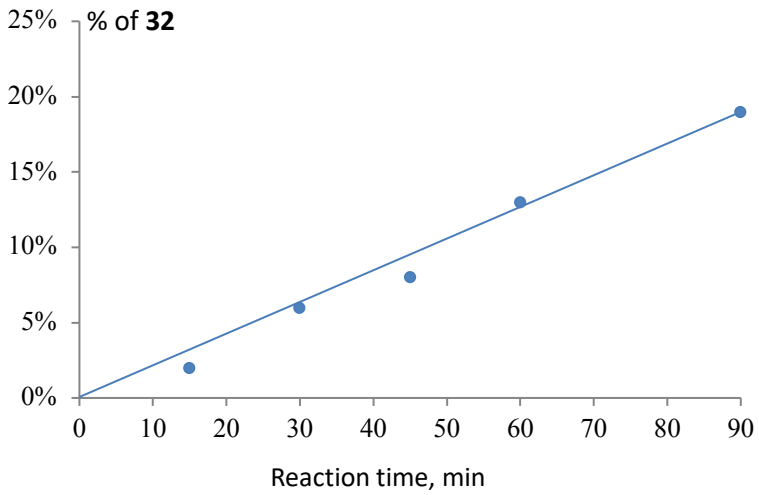
To a dried 10 mL Schlenk tube a stir bar, styrene (0.02 mmol), [Cu(XantphosTEPD)(phen)PF_6] (2.5 mol%), B_2Pin_2 (2 equiv), and K_2CO_3 (2 equiv) in MeCN:H_2O (9:1, v/v, 0.01 M) were mixed together. The reaction mixture was degassed via freeze-pump-thaw 3 times. After the mixture was thoroughly degassed and filled with argon, the Schlenk tube was tightly sealed and stirred under irradiation with a single LED (λ_{max} = 405 nm) for 30 min. After irradiation, the yield was determined by proton NMR using DMF as an internal standard. The yield was determined to be 5.75 % (obtained from three parallel experiments) (1.15×10^{-7} mol). The quantum yield (Φ) of the reaction was determined using eq. 4 where the photon flux (Φ_q) is 1.32×10^{-9} Einstein's * s^{-1} (determined by actinometry as described above), t is the reaction time (1800 s) and f_R is the fraction of incident light absorbed by the reaction mixture, determined using eq 3. An absorption spectrum of the reaction mixture gave an absorbance value of > 3 at 405 nm, indicating that essentially all the incident light ($f_R > 0.999$) is absorbed by the photocatalyst.

The reaction quantum yield (Φ_R) was thus determined to be $\Phi_R = 0.48$.

6.6 KIE determination and effect of HOBPin



a) Reaction in H_2O



y = ax + b

Figure 9. Yield of product **32** over time using H_2O.

b) Reaction in D_2O

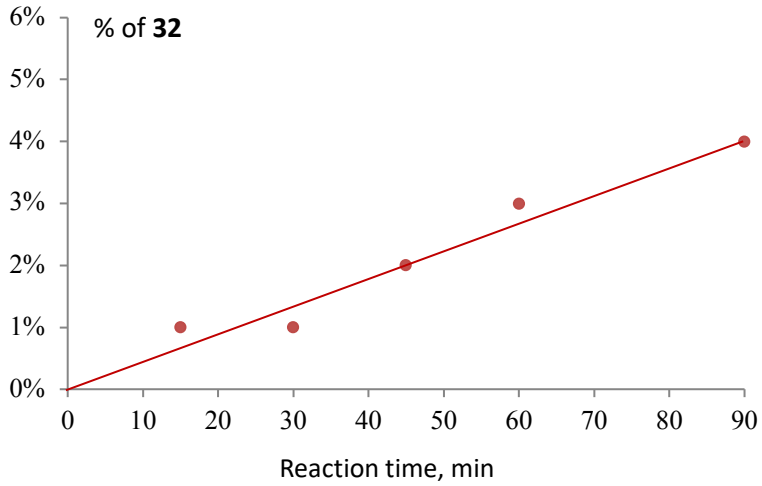


Figure 10. Yield of product **32** over reaction time using D_2O.

y = a'x + b'

KIE = $\frac{a}{a'}$ = 5.5

c) Reaction in H_2O with (green) and without HOBPin (blue)

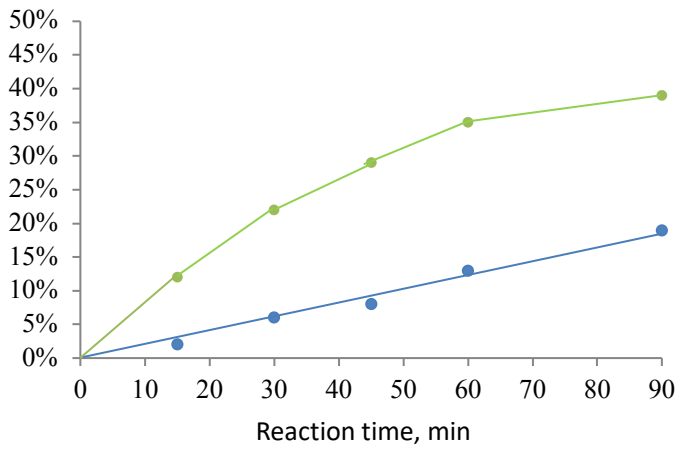


Figure 11. Reaction yield in function of reaction time using H_2O with HOBPin (green) and without HOBPin (blue).

6.7 CV measurements of B_2Pin_2 (green) and B_2Pin_2+KOH (red)

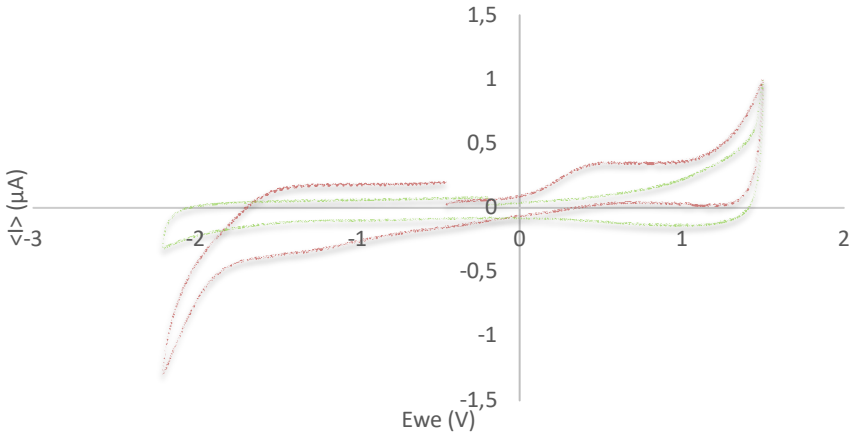


Figure 12. Cyclic voltammetry for B_2Pin_2 (green) and B_2Pin_2+KOH (red).

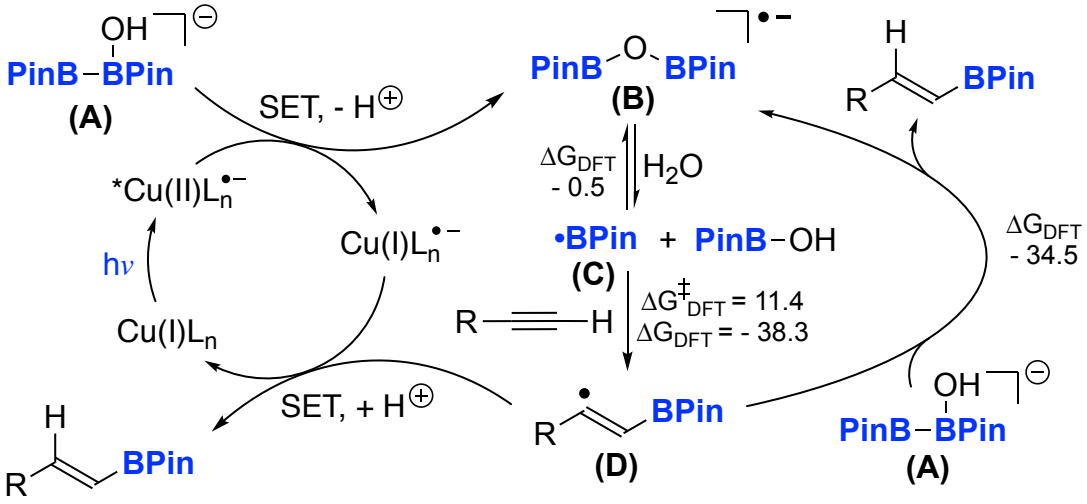
6.8 DFT Calculations

Density Functional Theory (DFT) calculations were performed using the Gaussian 16 software[3] at the B3LYP level of theory which uses Becke's 3-parameter exchange[4] and Lee, Yang and Parr's correlation function[5]. All geometry optimization and frequency calculations used the conductor-like polarizable continuum model (CPCM) to simulate the acetonitrile solvent.

Resulting outputs were verified for imaginary frequencies to ensure the optimized structures were local minima for ground states (no imaginary frequency) or saddle points for transition states (one imaginary frequency). Reaction free energies (ΔG) were calculated using the zero-point energy corrected Gibbs free energy at 298.15 K (Sum of Thermal and Free Energies in Gaussian Output), and free enthalpies (ΔH) were calculated using the zero-point energy corrected Enthalpy at 298.15K (Sum of electronic and thermal Enthalpies in Gaussian Output).

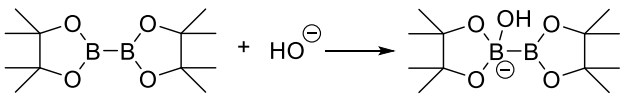
Both geometry and frequency calculations were conducted at the B3LYP/6-311+G(2d,2p) level of theory in "acetonitrile solvent", i.e., CPCM(ACN).

[#] Gaussian 09, Revision C.01, 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. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, 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. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. 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, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.
[##] Becke, A. D., Density-functional thermochemistry. I. The effect of the exchange-only gradientcorrection. *J. Chem. Phys.* **1992,** *96*, 2155-2160; Becke, A. D., Density-functional thermochemistry. III. The role of exact exchange. *J. Chem. Phys.* **1993,** *98*, 5648-5652.
[###] Lee, C.; Yang, W.; Parr. R. G., Development of the Colle-Salvetti correlation-energy formula into a functional of the electron density. *Phys. Rev. B.* **1998,** 785-789.



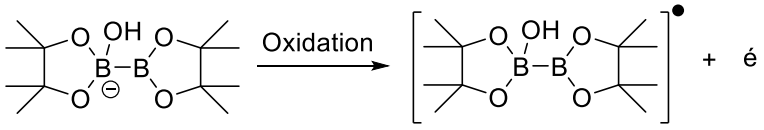
1. Forming PinB• from B2Pin2 oxidation in basic media:

Thermochemical data obtained from DFT calculations for the addition of hydroxide on the B_2Pin_2 to form borate (**A**).



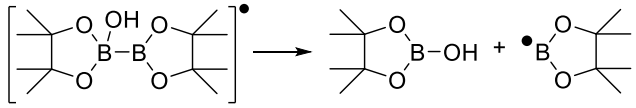
ΔG°$_{RX}$ (kcal/mol)	**ΔH°$_{RX}$ (kcal/mol)**
-6.67	-17.57

Redox potential obtained from DFT calculations for the oxidation of the B_2Pin_2-OH anion according to Nicewicz (Synlett 2016; 27(05): 714-723).



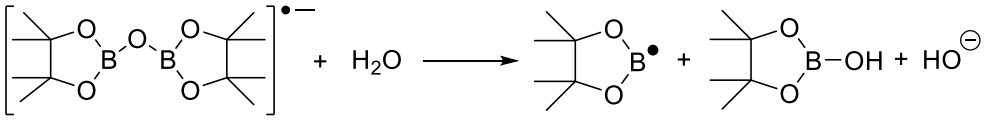
Calculated $E^0_{1/2}$ vs. SCE (V)	0.28

Thermochemical data obtained from DFT calculations for the dissociation of the B_2Pin_2-OH radical into BPin-OH and BPin radical (**C**)



$\Delta G°_{RX}$ (kcal/mol)	**$\Delta H°_{RX}$ (kcal/mol)**
-50.1	-38.5

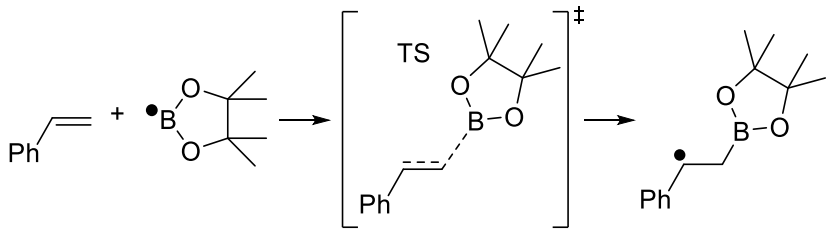
Thermochemical data obtained from DFT calculations for the dissociation of the BPin-O-BPin radical anion with H_2O for regenerate the BPin radical.



$\Delta G°_{RX}$ (kcal/mol)	**$\Delta H°_{RX}$ (kcal/mol)**
-0.5	-1.0

2. Addition reactions of PinB• onto alkenes and alkynes:

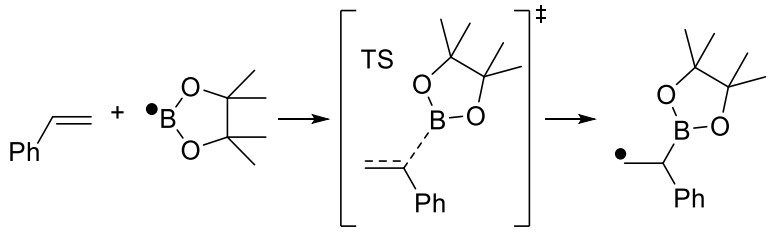
Thermochemical data obtained from DFT calculations for the anti-Markovnikov additon of the BPin radical on styrene.



$\Delta G^‡$ (kcal/mol)	**$\Delta G°_{RX}$ (kcal/mol)**
11.6	-34.2

$\Delta H^‡$ (kcal/mol)	**$\Delta H°_{RX}$ (kcal/mol)**
1.3	-45.6

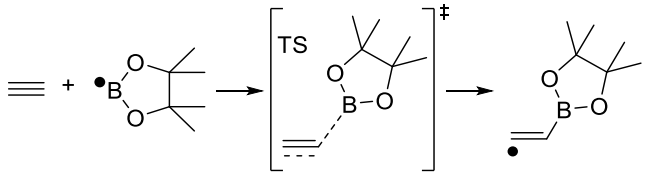
Thermochemical data obtained from DFT calculations for the Markovnikov addition of the BPin radical on the styrene.



$\Delta G^{\ddagger}$ (kcal/mol)	$\Delta G°_{RX}$ (kcal/mol)
15.5	-17.8

$\Delta H^{\ddagger}$ (kcal/mol)	$\Delta H°_{RX}$ (kcal/mol)
4.7	-29.3

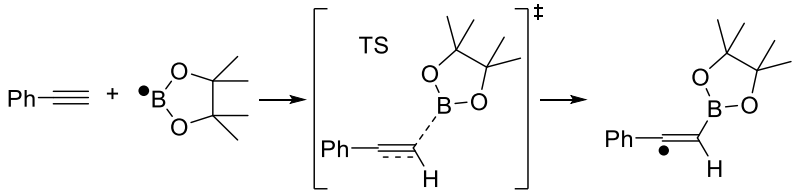
Thermochemical data obtained from DFT calculations for the addition of the BPin radical on acetylene.



$\Delta G^{\ddagger}$ (kcal/mol)	$\Delta G°_{RX}$ (kcal/mol)
11.8	-32.0

$\Delta H^{\ddagger}$ (kcal/mol)	$\Delta H°_{RX}$ (kcal/mol)
3.7	-42.2

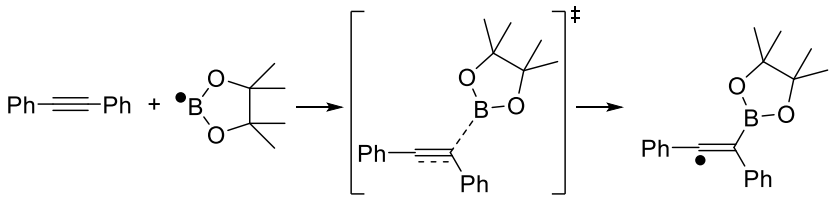
Thermochemical data obtained from DFT calculations for the addition of the BPin radical on the phenylacetylene.



$\Delta G^{\ddagger}$ (kcal/mol)	$\Delta G°_{RX}$ (kcal/mol)
11.4	-38.3

$\Delta H^{\ddagger}$ (kcal/mol)	$\Delta H°_{RX}$ (kcal/mol)
2.2	-49.6

Thermochemical data obtained from DFT calculations for the addition of the BPin radical on the diphenylacetylene.

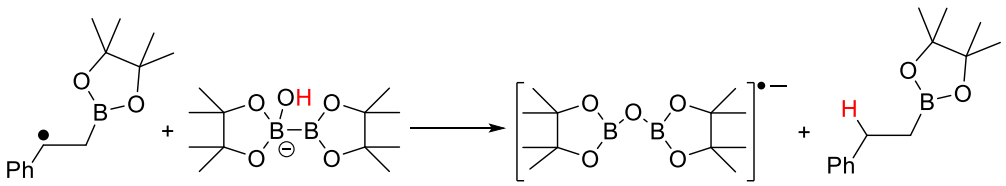


$\Delta G^{\ddagger}$ (kcal/mol)	$\Delta G°_{RX}$ (kcal/mol)
16.4	-30.5

$\Delta H^{\ddagger}$ (kcal/mol)	$\Delta H°_{RX}$ (kcal/mol)
3.5	-42.7

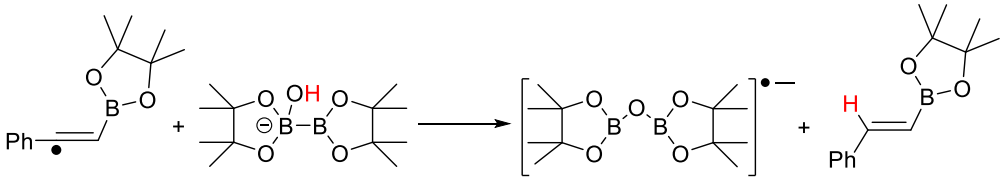
3. Formation of final product by H-atom transfer to carbon-centered radicals.

Thermochemical data obtained from DFT calculations for the HAT between the B_2Pin_2-OH anion and the BPin-CH_2-CH-Ph radical.



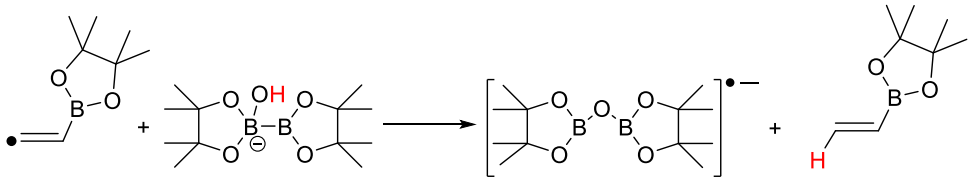
$\Delta G°_{RX}$ (kcal/mol)	$\Delta H°_{RX}$ (kcal/mol)
-23.7	-24.8

Thermochemical data obtained from DFT calculations for the HAT between the B_2Pin_2-OH anion and the BPin-CH=C-Ph radical (*E* product).



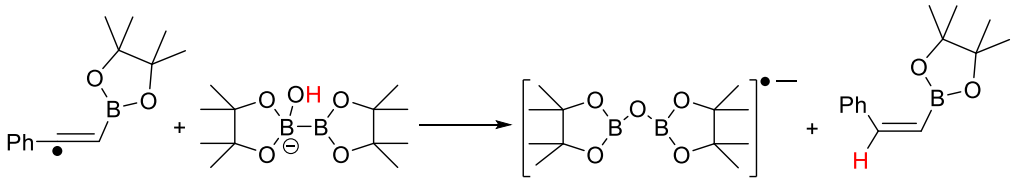
$\Delta G°_{RX}$ (kcal/mol)	$\Delta H°_{RX}$ (kcal/mol)
-39.6	-41.0

Thermochemical data obtained from DFT calculations for the HAT between the B_2Pin_2-OH anion and the BPin-CH=CH radical.



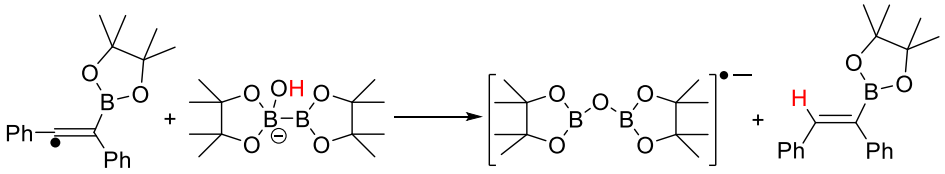
$\Delta G°_{RX}$ (kcal/mol)	$\Delta H°_{RX}$ (kcal/mol)
-48.5	-49.5

Thermochemical data obtained from DFT calculations for the HAT between the B_2Pin_2-OH anion and the BPin-CH=C-Ph radical (*Z* product).



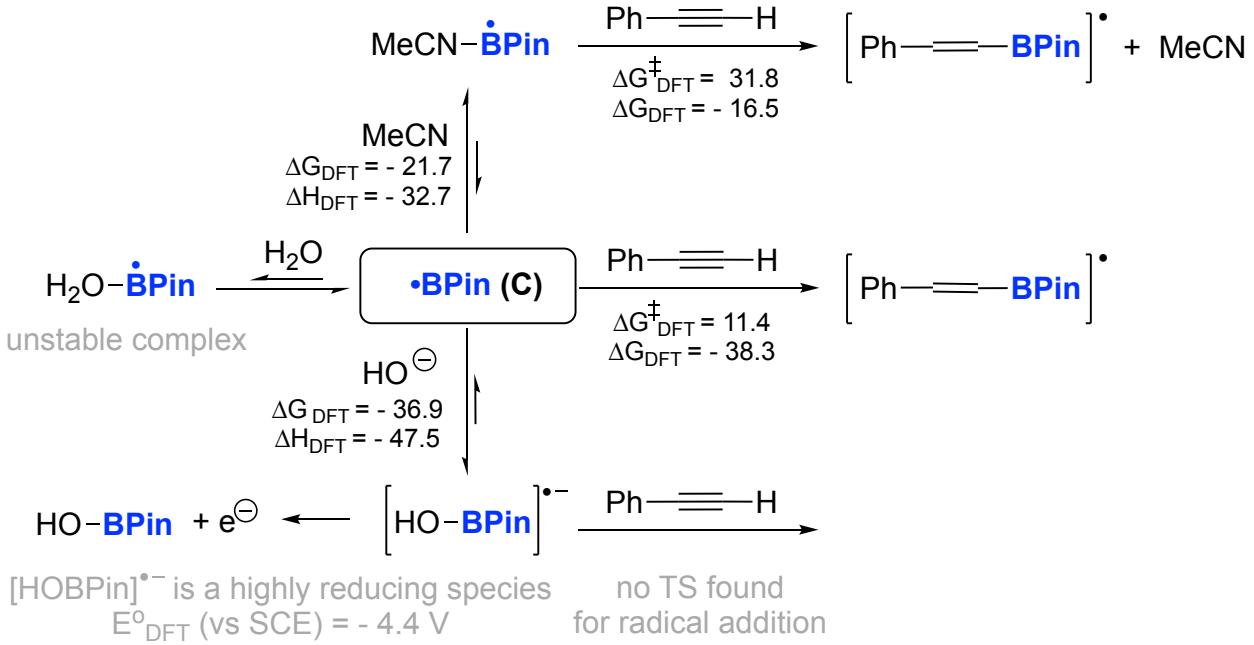
$\Delta G°_{RX}$ (kcal/mol)	$\Delta H°_{RX}$ (kcal/mol)
-34.5	-35.9

Thermochemical data obtained from DFT calculations for the HAT between the B_2Pin_2-OH anion and the BPin-CPH=C-Ph radical (*E* product).

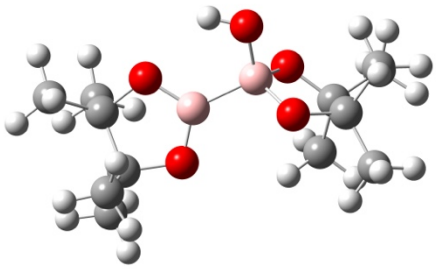


$\Delta G°_{RX}$ (kcal/mol)	$\Delta H°_{RX}$ (kcal/mol)
-35.9	-37.9

Thermodynamic data exploring the possible Lewis base interactions with boryl radical **C**.



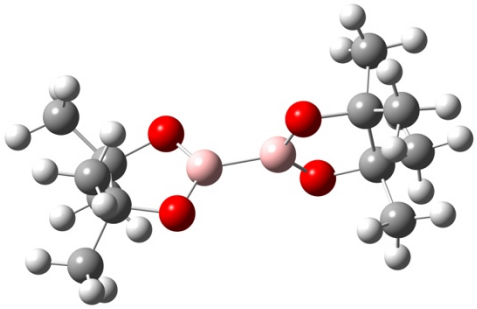
DFT energies and coordinates as obtained from 6-311++G(2d,2p)//CPCM(acetonitrile).



B_2Pin_2-OH Anion

Zero-point correction (Hartree)=	0.373224
Thermal correction to Energy=	0.394909
Thermal correction to Enthalpy=	0.395853
Thermal correction to Gibbs Free Energy=	0.324346
Sum of electronic and zero-point Energies=	-898.436504
Sum of electronic and thermal Energies=	-898.414819
Sum of electronic and thermal Enthalpies=	-898.413875
Sum of electronic and thermal Free Energies=	-898.485381

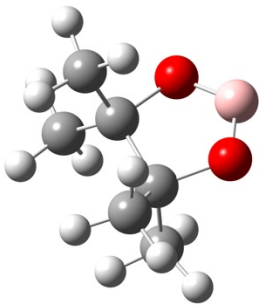
C	2.73907	-0.80912	-0.42547
C	3.04552	0.48667	0.40606
C	-2.92523	-0.14418	-0.66557
C	-2.56017	-0.37942	0.85035
B	-0.87453	0.94751	-0.219
B	0.79267	0.4328	-0.17074
O	-1.56174	0.58698	1.08723
O	-1.68018	0.21044	-1.2292
O	1.85953	1.27395	0.18432
O	1.29941	-0.84599	-0.41433
C	-3.91897	1.0216	-0.84992
H	-3.97188	1.25875	-1.91373
H	-4.92554	0.77404	-0.49997
H	-3.55894	1.9072	-0.33046
C	-3.46323	-1.37794	-1.39768
H	-4.38746	-1.74679	-0.94381
H	-3.6773	-1.1169	-2.43609
H	-2.72798	-2.1801	-1.40046
C	-3.71681	-0.15384	1.83196
H	-4.55417	-0.83013	1.63547
H	-3.36723	-0.33587	2.85054
H	-4.07336	0.87257	1.78065
C	-1.97119	-1.78581	1.09041
H	-1.54968	-1.81177	2.09702
H	-2.72263	-2.57665	1.0123
H	-1.16895	-1.98677	0.38247
C	3.17608	-0.70385	-1.8931
H	4.26183	-0.74008	-2.00258
H	2.74402	-1.53945	-2.44313
H	2.80639	0.21644	-2.34243
C	3.26921	-2.10892	0.17464
H	2.97787	-2.94543	-0.4612
H	4.35969	-2.09793	0.24256
H	2.85829	-2.28544	1.16563
C	3.14022	0.22761	1.91581
H	4.0497	-0.31364	2.18382
H	3.14413	1.18723	2.43246
H	2.27699	-0.33512	2.26705
C	4.26155	1.28686	-0.05447
H	4.36643	2.17546	0.56882
H	5.17898	0.70021	0.03474
H	4.15468	1.61349	-1.08609
O	-0.96083	2.40494	-0.46007
H	-0.19041	2.83471	-0.08656



B_2Pin_2

Zero-point correction(Hartree) =	0.361677
Thermal correction to Energy=	0.381651
Thermal correction to Enthalpy=	0.382596
Thermal correction to Gibbs Free Energy=	0.313259
Sum of electronic and zero-point Energies=	-822.460116
Sum of electronic and thermal Energies=	-822.440142
Sum of electronic and thermal Enthalpies=	-822.439198
Sum of electronic and thermal Free Energies=	-822.508534

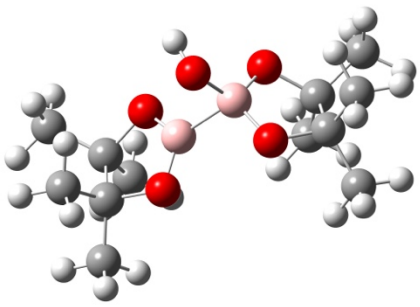
C	3.0056	0.51064	-0.59905
C	3.00558	-0.51065	0.59904
C	-3.00561	-0.59915	-0.51051
C	-3.00558	0.59916	0.51052
B	-0.85077	0.00002	-0.00007
B	0.85078	0.00002	-0.00001
O	-1.61289	1.0373	0.47354
O	-1.6129	-1.03727	-0.47361
O	1.61289	-0.47375	1.0372
O	1.6129	0.47382	-1.03719
C	-3.2896	-0.17377	-1.95298
H	-3.079	-1.01312	-2.61417
H	-4.33156	0.11608	-2.08806
H	-2.65506	0.65852	-2.25356
C	-3.89111	-1.77794	-0.12793
H	-4.93851	-1.47639	-0.08173
H	-3.79865	-2.56086	-0.87972
H	-3.60735	-2.19922	0.83284
C	-3.89114	1.77793	0.128
H	-4.93853	1.47632	0.08187
H	-3.79868	2.56087	0.87976
H	-3.60745	2.19919	-0.83279
C	-3.28947	0.17377	1.95301
H	-3.07884	1.01312	2.61419
H	-4.33141	-0.11611	2.08817
H	-2.65488	-0.65851	2.25354
C	3.28956	1.95302	-0.17333
H	4.33151	2.08806	0.11656
H	3.07894	2.6144	-1.01253
H	2.65499	2.25339	0.65902
C	3.89116	0.12834	-1.77789
H	3.79879	0.88032	-2.56063
H	4.93853	0.08202	-1.47626
H	3.60739	-0.83232	-2.19941
C	3.28945	-1.95305	0.17335
H	4.3314	-2.08818	-0.11651
H	3.07876	-2.61441	1.01255
H	2.6549	-2.25339	-0.65903
C	3.89116	-0.12838	1.77788
H	3.79875	-0.88035	2.56063
H	4.93853	-0.08211	1.47625
H	3.60743	0.8323	2.19938



BPin Radical

Zero-point correction (Hartree)=	0.178843
Thermal correction to Energy=	0.188325
Thermal correction to Enthalpy=	0.189269
Thermal correction to Gibbs Free Energy=	0.145083
Sum of electronic and zero-point Energies=	-411.149948
Sum of electronic and thermal Energies=	-411.140466
Sum of electronic and thermal Enthalpies=	-411.139522
Sum of electronic and thermal Free Energies=	-411.183708

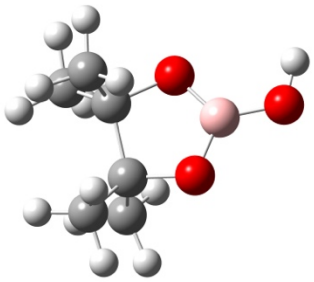
C	-0.49012	1.59094	0.50636
C	-1.07337	2.58038	-0.63857
B	-2.19711	1.16444	-0.05922
C	-0.54984	2.08752	-2.00041
H	-0.948	2.70328	-2.77964
H	0.51866	2.14276	-2.01297
H	-0.85643	1.07408	-2.15482
C	-0.63187	4.04038	-0.42627
H	-0.99012	4.38727	0.52043
H	0.43649	4.09634	-0.4456
H	-1.03523	4.65196	-1.20612
C	1.04752	1.51482	0.4682
H	1.45711	2.48913	0.63512
H	1.39067	0.84811	1.23151
H	1.36315	1.15434	-0.48853
C	-0.93088	2.11248	1.88669
H	-0.58229	1.44601	2.64774
H	-0.51775	3.08613	2.04865
H	-1.99885	2.16767	1.92275
O	-2.5429	2.45739	-0.62168
O	-1.10108	0.27403	0.26896



B_2Pin_2-OH Radical

Zero-point correction (Hartree)=	0.374815
Thermal correction to Energy=	0.396599
Thermal correction to Enthalpy=	0.397543
Thermal correction to Gibbs Free Energy=	0.324930
Sum of electronic and zero-point Energies=	-898.262787
Sum of electronic and thermal Energies=	-898.241003
Sum of electronic and thermal Enthalpies=	-898.240059
Sum of electronic and thermal Free Energies=	-898.312671

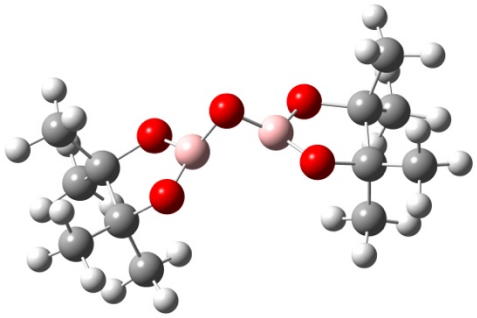
C	-2.77638	-0.62901	-0.51857
C	-2.74955	0.77954	0.19353
C	2.82405	-0.57344	-0.46704
C	2.53224	0.89103	0.03849
B	0.92295	-0.5504	0.86401
B	-0.71085	-0.22585	0.34232
O	1.61255	0.65861	1.13919
O	1.58937	-1.27544	-0.15239
O	-1.47114	0.72674	0.93863
O	-1.33539	-0.96048	-0.60827
C	3.93391	-1.27013	0.32745
H	3.95497	-2.32416	0.05346
H	4.91044	-0.84102	0.10464
H	3.76045	-1.19891	1.40021
C	3.09344	-0.6958	-1.9613
H	3.98021	-0.1268	-2.24174
H	3.27131	-1.74037	-2.21584
H	2.25262	-0.3406	-2.55192
C	3.74602	1.63353	0.58666
H	4.50552	1.75096	-0.1866
H	3.44641	2.62778	0.91697
H	4.18803	1.11245	1.43192
C	1.82321	1.76187	-1.00312
H	1.46945	2.6724	-0.52135
H	2.49998	2.04372	-1.80868
H	0.96643	1.25229	-1.44173
C	-3.41926	-1.73018	0.3214
H	-4.49623	-1.58681	0.39625
H	-3.23645	-2.69162	-0.15618
H	-3.00303	-1.76402	1.32691
C	-3.34728	-0.62944	-1.92746
H	-3.29461	-1.63569	-2.3411
H	-4.39438	-0.32648	-1.91334
H	-2.80119	0.04062	-2.58607
C	-2.63992	1.95607	-0.77329
H	-3.56776	2.09626	-1.32604
H	-2.44191	2.86375	-0.20519
H	-1.8298	1.81677	-1.48712
C	-3.86724	1.0161	1.19718
H	-3.74686	1.99875	1.65135
H	-4.83676	0.99268	0.69935
H	-3.86549	0.2707	1.98798
O	0.38453	-1.32274	1.95987
H	0.08943	-0.75573	2.6824



BPin-OH

Zero-point correction (Hartree)=	0.195514
Thermal correction to Energy=	0.206197
Thermal correction to Enthalpy=	0.207141
Thermal correction to Gibbs Free Energy=	0.160926
Sum of electronic and zero-point Energies=	-487.133146
Sum of electronic and thermal Energies=	-487.122463
Sum of electronic and thermal Enthalpies=	-487.121519
Sum of electronic and thermal Free Energies=	-487.167735

C	-0.5592	-0.55451	-0.48488
C	0.5592	0.55451	-0.48488
B	0.	0.	1.72189
O	1.03364	0.51116	0.87271
O	-1.03364	-0.51116	0.87271
C	0.	-1.96078	-0.73939
H	-0.78382	-2.69215	-0.54171
H	0.32994	-2.08827	-1.77051
H	0.83939	-2.17628	-0.07886
C	-1.72529	-0.29142	-1.43363
H	-1.38484	-0.23832	-2.46875
H	-2.44768	-1.10529	-1.36128
H	-2.23722	0.63691	-1.19043
C	1.72529	0.29142	-1.43363
H	1.38484	0.23832	-2.46875
H	2.44768	1.10529	-1.36128
H	2.23722	-0.63691	-1.19043
C	0.	1.96078	-0.73939
H	0.78382	2.69215	-0.54171
H	-0.32994	2.08827	-1.77051
H	-0.83939	2.17628	-0.07886
O	0.	0.	3.01814
H	0.9051	0.	3.33814

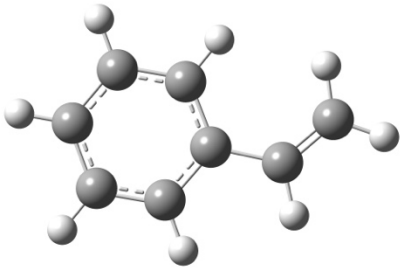


BPin-O-BPin Radical Anion

Zero-point correction (Hartree)=	0.362626
Thermal correction to Energy=	0.383575
Thermal correction to Enthalpy=	0.384520
Thermal correction to Gibbs Free Energy=	0.313949
Sum of electronic and zero-point Energies=	-897.843993
Sum of electronic and thermal Energies=	-897.823044
Sum of electronic and thermal Enthalpies=	-897.822099
Sum of electronic and thermal Free Energies=	-897.892670

C	-3.16658	0.70918	0.26115
C	-2.98898	-0.83198	-0.0187
C	3.16658	0.70919	0.26112
C	2.98898	-0.83197	-0.0187
B	1.00941	0.26534	-0.51159
B	-1.00945	0.26539	-0.5118
O	1.81595	-0.8563	-0.85722
O	1.80622	1.1954	0.21943
O	-1.81602	-0.85627	-0.85732
O	-1.80623	1.19541	0.21932
C	3.94684	1.42732	-0.84753
H	3.86717	2.50335	-0.69315
H	5.00436	1.16095	-0.83848
H	3.53865	1.19421	-1.83009
C	3.77666	1.04924	1.61757
H	4.7814	0.63398	1.70974
H	3.85177	2.13186	1.72444
H	3.16927	0.67008	2.43615
C	4.14491	-1.4834	-0.77166
H	5.07237	-1.40929	-0.20192
H	3.9312	-2.54153	-0.92566
H	4.29882	-1.02408	-1.74524
C	2.68779	-1.63917	1.25095
H	2.39642	-2.64958	0.9635
H	3.5592	-1.70967	1.90186
H	1.86628	-1.19675	1.81242
C	-3.94695	1.42732	-0.84742
H	-5.00446	1.16092	-0.83828

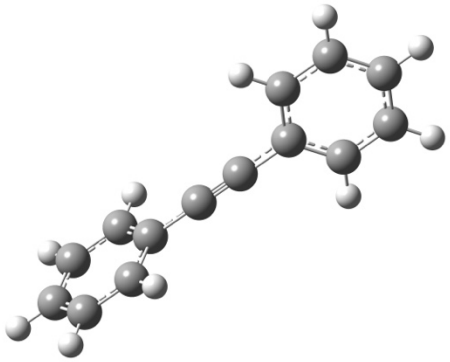
H	-3.86729	2.50334	-0.69303
H	-3.53885	1.19422	-1.83002
C	-3.77654	1.04921	1.61765
H	-3.85166	2.13184	1.72454
H	-4.78126	0.63394	1.70991
H	-3.16907	0.67007	2.43617
C	-2.68765	-1.63919	1.2509
H	-3.55901	-1.70972	1.90189
H	-2.39628	-2.64959	0.9634
H	-1.86611	-1.19676	1.81231
C	-4.14495	-1.48342	-0.77157
H	-3.93123	-2.54154	-0.9256
H	-5.07237	-1.40933	-0.20177
H	-4.29895	-1.0241	-1.74514
O	-0.00001	0.70247	-1.40092



Styrene

Zero-point correction (Hartree)=	0.133067
Thermal correction to Energy=	0.139815
Thermal correction to Enthalpy=	0.140760
Thermal correction to Gibbs Free Energy=	0.101767
Sum of electronic and zero-point Energies=	-309.613881
Sum of electronic and thermal Energies=	-309.607133
Sum of electronic and thermal Enthalpies=	-309.606188
Sum of electronic and thermal Free Energies=	-309.645181

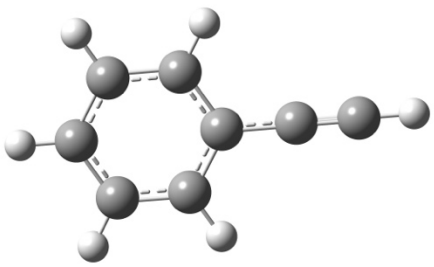
C	0.5674	-0.32982	-0.60507
C	1.96534	-0.23452	-0.62946
C	2.60172	0.87903	-0.0647
C	1.84015	1.89728	0.52444
C	0.44221	1.80198	0.54884
C	-0.19417	0.68843	-0.01592
H	0.08151	-1.18004	-1.03628
H	2.54681	-1.01198	-1.07929
H	2.32604	2.7475	0.95565
H	-0.13927	2.57944	0.99867
H	-1.26153	0.61567	0.0027
C	4.13792	0.98375	-0.09151
H	4.62381	1.83397	0.3397
C	4.87438	-0.00094	-0.66123
H	4.38849	-0.85116	-1.09244
H	5.94174	0.07183	-0.67986



Diphenylacetylene

Zero-point correction (Hartree)=	0.191069
Thermal correction to Energy=	0.202130
Thermal correction to Enthalpy=	0.203075
Thermal correction to Gibbs Free Energy=	0.151308
Sum of electronic and zero-point Energies=	-539.431542
Sum of electronic and thermal Energies=	-539.420480
Sum of electronic and thermal Enthalpies=	-539.419536
Sum of electronic and thermal Free Energies=	-539.471303

C	4.13459	0.85286	0.84952
C	2.74644	0.85573	0.85223
C	2.03214	-0.00007	-0.00019
C	2.74674	-0.85579	-0.85244
C	4.13488	-0.85278	-0.84932
C	4.83386	0.00008	0.0002
H	4.67163	1.51783	1.51202
H	2.20263	1.5173	1.51123
H	2.20315	-1.51742	-1.51157
H	4.67218	-1.51771	-1.51165
H	5.91511	0.0001	0.00034
C	0.60374	-0.00015	-0.00027
C	-0.60376	0.00021	0.00001
C	-2.03214	0.00012	-0.00003
C	-2.74647	-0.85565	0.8524
C	-2.7467	0.85578	-0.85237
C	-4.1346	-0.85287	0.8495
H	-2.20267	-1.51725	1.51138
C	-4.13486	0.85271	-0.8494
H	-2.2031	1.51753	-1.51136
C	-4.83386	-0.00015	0.00007
H	-4.67169	-1.51795	1.51184
H	-4.67212	1.5177	-1.51171
H	-5.91511	-0.00026	0.00012

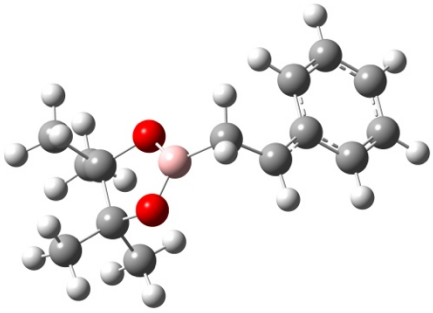


Phenylacetylene

Zero-point correction (Hartree)=	0.109146
Thermal correction to Energy=	0.115584
Thermal correction to Enthalpy=	0.116528
Thermal correction to Gibbs Free Energy=	0.078707
Sum of electronic and zero-point Energies=	-308.383730

Sum of electronic and thermal Energies= -308.377292
Sum of electronic and thermal Enthalpies= -308.376348
Sum of electronic and thermal Free Energies= -308.414168

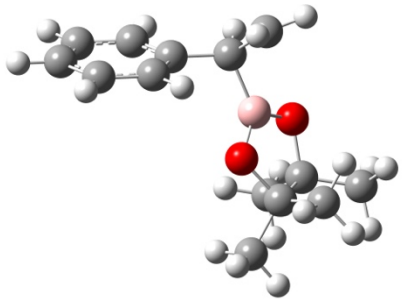
C	2.38048	-1.00375	0.00068
C	3.77564	-1.00375	0.00068
C	4.47318	0.204	0.00068
C	3.77552	1.41251	-0.00052
C	2.3807	1.41243	-0.001
C	1.6831	0.20423	0.
H	1.83072	-1.95607	0.00113
H	4.32515	-1.95626	0.002
H	4.32572	2.36465	-0.00058
H	1.83058	2.36471	-0.00195
H	0.58349	0.20441	-0.00018
C	6.01318	0.20411	0.00157
C	7.21438	0.2042	0.00226
H	8.28438	0.20428	0.00288



BPin-CH_2-CPh Radical

Zero-point correction (Hartree)= 0.314146
Thermal correction to Energy= 0.331165
Thermal correction to Enthalpy= 0.332109
Thermal correction to Gibbs Free Energy= 0.267053
Sum of electronic and zero-point Energies= -720.836265
Sum of electronic and thermal Energies= -720.819246
Sum of electronic and thermal Enthalpies= -720.818302
Sum of electronic and thermal Free Energies= -720.883358

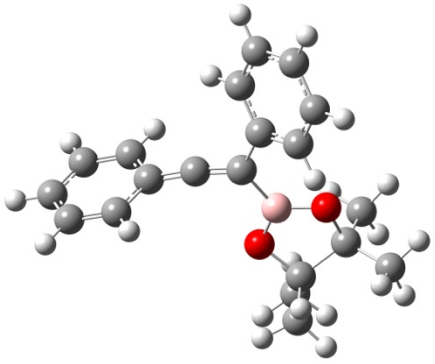
C	-5.53407	-0.1001	-0.47793
C	-4.89121	1.13099	-0.64328
C	-3.56714	1.28231	-0.28201
C	-2.81782	0.19759	0.24754
C	-3.49277	-1.04525	0.40566
C	-4.82265	-1.17994	0.05361
H	-6.57273	-0.21395	-0.75511
H	-5.43086	1.97209	-1.05716
H	-3.08053	2.24086	-0.41195
H	-2.96771	-1.89263	0.82194
H	-5.31562	-2.13163	0.19885
C	-1.47755	0.38099	0.60027
H	-1.11297	1.40201	0.59458
C	-0.54038	-0.68148	1.05342
H	-0.8806	-1.66377	0.72251
H	-0.51417	-0.72507	2.15705
C	2.91612	0.6336	0.34963
C	2.83168	-0.5168	-0.71135
B	0.92647	-0.43112	0.5567
O	1.41405	-0.9019	-0.60474
O	1.80706	0.28003	1.24916
C	3.63919	-1.72204	-0.29925
H	3.37469	-2.55346	-0.94981
H	4.71147	-1.52947	-0.38486
H	3.41206	-2.00191	0.72976
C	3.13663	-0.10041	-2.14555
H	4.15641	0.27501	-2.26509
H	3.03152	-0.97095	-2.7934
H	2.4481	0.66368	-2.48528
C	2.60695	2.02226	-0.17765
H	2.49664	2.6936	0.67192
H	3.40969	2.39449	-0.81549
H	1.67402	2.03951	-0.74241
C	4.20795	0.5924	1.15055
H	5.09115	0.76988	0.53117
H	4.17551	1.37008	1.91374
H	4.32321	-0.37254	1.63828



BPin-CHPh-CH_2 Radical

Zero-point correction (Hartree)= 0.312554
Thermal correction to Energy= 0.330109
Thermal correction to Enthalpy= 0.331053
Thermal correction to Gibbs Free Energy= 0.266226
Sum of electronic and zero-point Energies= -720.810847
Sum of electronic and thermal Energies= -720.793292
Sum of electronic and thermal Enthalpies= -720.792347
Sum of electronic and thermal Free Energies= -720.857174

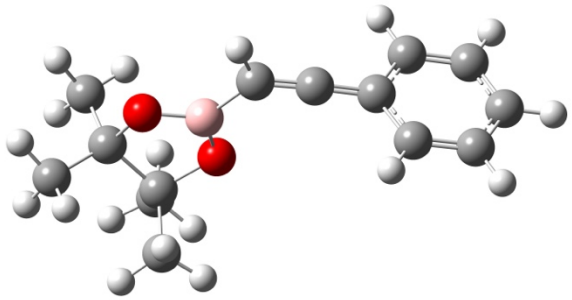
C	-4.41853	-1.06248	-0.38898
C	-3.99471	-0.17896	-1.377
C	-2.88472	0.63329	-1.15981
C	-2.1749	0.58251	0.04366
C	-2.61116	-0.31084	1.02727
C	-3.72067	-1.12367	0.8146
H	-5.28157	-1.69315	-0.55275
H	-4.52866	-0.11682	-2.31584
H	-2.56787	1.32012	-1.93456
H	-2.0804	-0.38112	1.96671
H	-4.03925	-1.80664	1.59085
C	-0.95811	1.46846	0.23605
C	-0.85761	2.14613	1.56257
H	-1.25986	1.6948	2.45689
H	-0.22483	3.01454	1.67271
C	2.54962	0.216	-0.64256
C	2.08285	-0.85328	0.41871
B	0.41785	0.67722	0.06222
O	1.51865	1.25253	-0.51219
O	0.63947	-0.59736	0.5025
C	2.48243	-0.28485	-2.08567
H	2.64072	0.5564	-2.75921
H	3.25392	-1.02797	-2.28252
H	1.51187	-0.72405	-2.31207
C	2.28991	-2.30393	0.00769
H	3.35042	-2.51525	-0.12995
H	1.91586	-2.9614	0.79176
H	1.76648	-2.54107	-0.91491
C	2.64954	-0.61341	1.81831
H	2.14521	-1.27463	2.52176
H	3.71658	-0.82836	1.85451
H	2.4914	0.41385	2.14378
C	3.90621	0.84897	-0.36724
H	4.6924	0.09422	-0.38907
H	4.12741	1.58598	-1.1385
H	3.93114	1.34773	0.59819
H	-0.956	2.23165	-0.54701



BPin-CPh=CPh Radical

Zero-point correction (Hartree)=	0.371434
Thermal correction to Energy=	0.393095
Thermal correction to Enthalpy=	0.394039
Thermal correction to Gibbs Free Energy=	0.317564
Sum of electronic and zero-point Energies=	-950.649725
Sum of electronic and thermal Energies=	-950.628064
Sum of electronic and thermal Enthalpies=	-950.627120
Sum of electronic and thermal Free Energies=	-950.703595

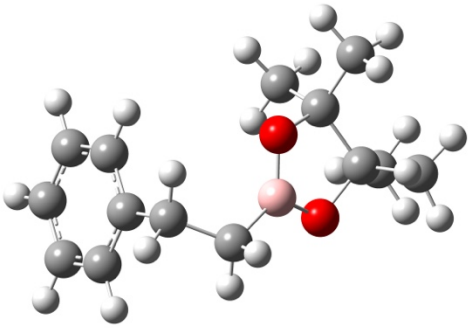
C	-0.90571	4.31431	-0.5958
C	-0.85997	2.92386	-0.5702
C	0.24379	2.25476	-0.03087
C	1.292	3.02269	0.49304
C	1.24375	4.40944	0.47139
C	0.1431	5.06392	-0.07612
H	-1.76691	4.81106	-1.02247
H	-1.6868	2.35576	-0.96775
H	2.1482	2.52125	0.92384
H	2.06371	4.9807	0.88578
H	0.10321	6.14455	-0.09231
C	0.32595	0.75861	-0.03228
C	1.4831	0.14027	-0.02064
C	2.58668	-0.66523	-0.02062
C	3.19357	-1.09383	1.2029
C	3.19189	-1.09353	-1.245
C	4.31679	-1.89316	1.18662
H	2.75286	-0.78396	2.13952
C	4.31582	-1.89174	-1.23011
H	2.75125	-0.78047	-2.18041
C	4.89169	-2.30071	-0.02217
H	4.75651	-2.20842	2.12352
H	4.75555	-2.20508	-2.16764
H	5.77306	-2.92599	-0.02284
B	-0.94343	-0.16849	-0.00973
O	-2.23926	0.27653	0.02895
O	-0.85121	-1.53547	-0.00539
C	-3.09853	-0.87663	0.28776
C	-2.192	-2.07586	-0.18347
C	-3.38181	-0.87928	1.79147
H	-3.83227	0.07328	2.06627
H	-4.07115	-1.67706	2.06649
H	-2.46599	-0.99803	2.36854
C	-4.39478	-0.69426	-0.49043
H	-5.0392	-1.56689	-0.3767
H	-4.93124	0.17237	-0.10608
H	-4.21017	-0.53469	-1.54958
C	-2.33927	-2.40488	-1.67104
H	-3.30115	-2.86971	-1.88588
H	-2.23953	-1.51296	-2.2881
H	-1.55126	-3.10066	-1.95534
C	-2.31402	-3.3459	0.6481
H	-2.06468	-3.16918	1.69094
H	-3.32601	-3.74942	0.59386
H	-1.62934	-4.09957	0.26132



BPin-CH=CPh Radical

Zero-point correction (Hartree)=	0.290391
Thermal correction to Energy=	0.307215
Thermal correction to Enthalpy=	0.308160
Thermal correction to Gibbs Free Energy=	0.244214
Sum of electronic and zero-point Energies=	-719.612671
Sum of electronic and thermal Energies=	-719.595847
Sum of electronic and thermal Enthalpies=	-719.594903
Sum of electronic and thermal Free Energies=	-719.658848

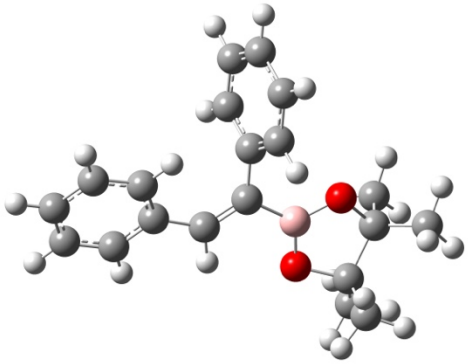
C	2.35703	0.94334	-0.67219
C	3.5993	0.33724	-0.8987
C	4.70056	0.68867	-0.09637
C	4.56351	1.64795	0.92039
C	3.3224	2.25504	1.14312
C	2.21995	1.89844	0.34904
H	1.51425	0.6737	-1.28057
H	3.7049	-0.38978	-1.68298
H	5.40364	1.91719	1.52793
H	3.21799	2.98693	1.91712
H	1.27382	2.36065	0.52388
C	6.0736	0.03132	-0.3219
C	6.23695	-0.90619	-1.29167
H	5.40421	-1.1977	-1.90057
C	9.59036	-2.73634	-1.10048
C	9.63436	-2.19493	-2.53667
B	7.71811	-1.58695	-1.52204
O	8.19855	-2.89546	-0.83811
O	8.79637	-1.04113	-2.49149
C	10.20754	-1.69947	-0.14151
H	10.13099	-2.05475	0.86545
H	11.23277	-1.55568	-0.39118
H	9.6845	-0.77163	-0.23614
C	10.36438	-4.06144	-0.93493
H	11.39189	-3.90665	-1.17305
H	10.28149	-4.40237	0.08023
H	9.95565	-4.7944	-1.59743
C	9.05349	-3.24123	-3.5029
H	9.03863	-2.83946	-4.49401
H	9.66171	-4.12001	-3.48369
H	8.05811	-3.49163	-3.20309
C	11.0619	-1.84853	-2.99474
H	11.66108	-2.73079	-2.98265
H	11.03503	-1.44732	-3.9833
H	11.48311	-1.12241	-2.33342



BPin-CH_2-CH_2-Ph

Zero-point correction (Hartree)=	0.327597
Thermal correction to Energy=	0.344647
Thermal correction to Enthalpy=	0.345591
Thermal correction to Gibbs Free Energy=	0.281318
Sum of electronic and zero-point Energies=	-721.467606
Sum of electronic and thermal Energies=	-721.450557
Sum of electronic and thermal Enthalpies=	-721.449613
Sum of electronic and thermal Free Energies=	-721.513886

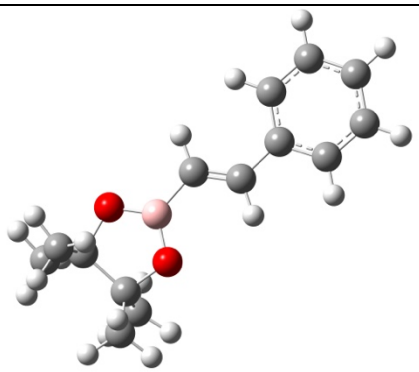
C	3.44241	-0.97469	1.31769
C	3.39398	0.396	1.60542
C	2.8097	1.25153	0.73177
C	2.25394	0.76553	-0.45939
C	2.30237	-0.60516	-0.74712
C	2.88665	-1.46069	0.12653
H	3.90372	-1.65018	2.00748
H	3.81832	0.76707	2.51489
H	2.77273	2.29808	0.95145
H	1.87804	-0.97623	-1.65659
H	2.92362	-2.50724	-0.09315
C	1.58999	1.73772	-1.45217
H	1.17608	2.56662	-0.91691
C	0.46865	1.00709	-2.214
H	0.88256	0.17819	-2.74926
H	0.00733	1.68258	-2.90379
C	-2.22711	0.48562	0.45359
C	-1.96514	-0.95471	-0.00423
B	-0.65967	0.46086	-1.14115
O	-0.61274	-0.92626	-0.46427
O	-1.89268	1.27378	-0.69026
C	-2.91632	-1.31465	-1.16064
H	-2.69306	-2.30017	-1.5125
H	-3.92807	-1.28034	-0.8141
H	-2.78872	-0.61354	-1.9588
C	-2.16578	-1.97804	1.12897
H	-3.18123	-1.94408	1.46455
H	-1.94252	-2.95977	0.76665
H	-1.513	-1.7413	1.94305
C	-1.30013	0.83385	1.63301
H	-1.4479	1.85591	1.91309
H	-1.52725	0.19978	2.46444
H	-0.28117	0.6878	1.34098
C	-3.68517	0.70595	0.89755
H	-3.90248	0.0752	1.73411
H	-3.82193	1.72955	1.17762
H	-4.34419	0.46619	0.0894
H	2.32169	2.09195	-2.1479



BPin-CPh=CH-Ph

Zero-point correction (Hartree)=	0.385490
Thermal correction to Energy=	0.406833
Thermal correction to Enthalpy=	0.407778
Thermal correction to Gibbs Free Energy=	0.333461
Sum of electronic and zero-point Energies=	-951.301534
Sum of electronic and thermal Energies=	-951.280191
Sum of electronic and thermal Enthalpies=	-951.279247
Sum of electronic and thermal Free Energies=	-951.353564

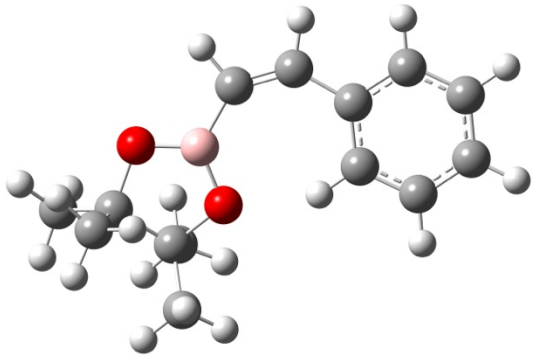
C	0.71791	0.83182	0.02659
C	0.95249	-0.72768	-0.01299
B	-1.2892	-0.26338	-0.06133
O	-0.3757	-1.23099	-0.3803
O	-0.71838	0.92312	0.30973
C	1.28242	-1.3311	1.35244
H	1.24737	-2.41709	1.27659
H	2.28086	-1.04515	1.68039
H	0.56576	-1.01961	2.11101
C	1.95302	-1.20359	-1.05648
H	2.94278	-0.79495	-0.8523
H	2.02506	-2.29017	-1.02276
H	1.65839	-0.91231	-2.06135
C	0.93998	1.51748	-1.32189
H	0.58171	2.5441	-1.25875
H	1.99676	1.54184	-1.58394
H	0.396	1.01591	-2.1211
C	1.47221	1.56954	1.12363
H	2.54841	1.46519	0.98509
H	1.22986	2.63089	1.08167
H	1.21204	1.1992	2.11185
C	-2.82374	-0.52525	-0.12425
C	-3.74699	0.36339	0.13977
H	-3.46803	1.35793	0.41901
C	-3.27611	-1.9424	-0.52256
C	-3.49023	-2.90843	0.46054
C	-3.47227	-2.25979	-1.86688
C	-3.90026	-4.19216	0.09948
H	-3.33596	-2.65825	1.52014
C	-3.88174	-3.54334	-2.22797
H	-3.30376	-1.4978	-2.64177
C	-4.09545	-4.50991	-1.24446
H	-4.06824	-4.95376	0.87472
H	-4.03577	-3.79408	-3.28754
H	-4.41804	-5.52192	-1.52917
C	-5.23519	-0.02202	0.04864
C	-5.89681	-0.52004	1.17105
C	-5.92179	0.12752	-1.15661
C	-7.24511	-0.86893	1.08833
H	-5.35581	-0.63761	2.12112
C	-7.26964	-0.22171	-1.23951
H	-5.39998	0.5206	-2.0413
C	-7.93138	-0.72042	-0.11674
H	-7.76622	-1.26225	1.97319
H	-7.81097	-0.10466	-2.18954
H	-8.99396	-0.99599	-0.18219



BPin-CH=CPH-h (*Z*)

Zero-point correction (Hartree)=	0.304502
Thermal correction to Energy=	0.321238
Thermal correction to Enthalpy=	0.322182
Thermal correction to Gibbs Free Energy=	0.259462
Sum of electronic and zero-point Energies=	-720.269696
Sum of electronic and thermal Energies=	-720.252959
Sum of electronic and thermal Enthalpies=	-720.252015
Sum of electronic and thermal Free Energies=	-720.314736

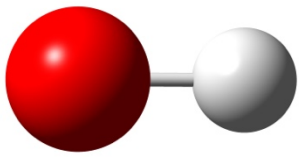
C	2.35703	0.94334	-0.67219
C	3.5993	0.33724	-0.8987
C	4.70056	0.68867	-0.09637
C	4.56351	1.64795	0.92039
C	3.3224	2.25504	1.14312
C	2.21995	1.89844	0.34904
H	1.51425	0.6737	-1.28057
H	3.7049	-0.38978	-1.68298
H	5.40364	1.91719	1.52793
H	3.21799	2.98693	1.91712
H	1.27382	2.36065	0.52388
C	6.0736	0.03132	-0.3219
H	6.905	0.30977	0.28561
C	6.23695	-0.90619	-1.29167
H	5.40421	-1.1977	-1.90057
C	9.59036	-2.73634	-1.10048
C	9.63436	-2.19493	-2.53667
B	7.71811	-1.58695	-1.52204
O	8.19855	-2.89546	-0.83811
O	8.79637	-1.04113	-2.49149
C	10.20754	-1.69947	-0.14151
H	10.13099	-2.05475	0.86545
H	11.23277	-1.55568	-0.39118
H	9.6845	-0.77163	-0.23614
C	10.36438	-4.06144	-0.93493
H	11.39189	-3.90665	-1.17305
H	10.28149	-4.40237	0.08023
H	9.95565	-4.7944	-1.59743
C	9.05349	-3.24123	-3.5029
H	9.03863	-2.83946	-4.49401
H	9.66171	-4.12001	-3.48369
H	8.05811	-3.49163	-3.20309
C	11.0619	-1.84853	-2.99474
H	11.66108	-2.73079	-2.98265
H	11.03503	-1.44732	-3.9833
H	11.48311	-1.12241	-2.33342



BPin-CH=CH-Ph (*E*)

Zero-point correction (Hartree)=	0.305093
Thermal correction to Energy=	0.321611
Thermal correction to Enthalpy=	0.322555
Thermal correction to Gibbs Free Energy=	0.259957
Sum of electronic and zero-point Energies=	-720.261364
Sum of electronic and thermal Energies=	-720.244845
Sum of electronic and thermal Enthalpies=	-720.243901
Sum of electronic and thermal Free Energies=	-720.306500

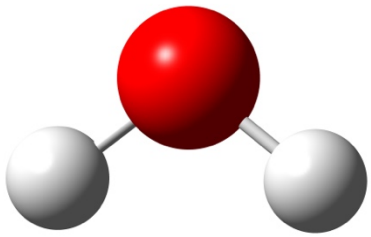
C	3.19648	-1.53672	-0.55126
C	2.30662	-0.47759	-0.68307
C	2.609	0.78272	-0.14999
C	3.84584	0.94984	0.49242
C	4.72988	-0.11259	0.63768
C	4.40709	-1.3625	0.11625
H	2.94837	-2.4996	-0.97704
H	1.3777	-0.62458	-1.21072
H	4.10897	1.92306	0.88648
H	5.67188	0.03697	1.14746
H	5.09697	-2.18915	0.21667
C	1.726	1.95478	-0.27755
H	2.27616	2.89152	-0.31699
C	0.37755	2.04076	-0.33705
H	0.00186	3.05234	-0.46918
C	-1.95595	-0.93699	0.15668
C	-2.93519	0.29116	0.03119
B	-0.75587	0.99178	-0.17213
O	-0.65678	-0.28082	0.32672
O	-2.05068	1.33808	-0.48031
C	-1.86068	-1.77397	-1.12019
H	-1.03922	-2.48197	-1.01896
H	-2.7763	-2.33824	-1.29175
H	-1.66833	-1.15207	-1.99342
C	-2.20066	-1.83906	1.35821
H	-3.18837	-2.29649	1.29887
H	-1.46082	-2.63879	1.37015
H	-2.12717	-1.29278	2.29504
C	-3.46632	0.78797	1.37712
H	-3.97761	1.73783	1.22595
H	-4.1773	0.08365	1.80684
H	-2.65947	0.94575	2.09151
C	-4.08403	0.10434	-0.95024
H	-4.72886	-0.71601	-0.63475
H	-4.68674	1.01145	-0.98222
H	-3.7266	-0.10271	-1.95569



OH Anion

Zero-point correction (Hartree)=	0.008693
Thermal correction to Energy=	0.011054
Thermal correction to Enthalpy=	0.011998
Thermal correction to Gibbs Free Energy=	-0.007554
Sum of electronic and zero-point Energies=	-75.949974
Sum of electronic and thermal Energies=	-75.947614
Sum of electronic and thermal Enthalpies=	-75.946670
Sum of electronic and thermal Free Energies=	-75.966221

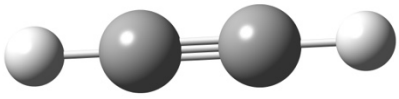
O	0.	0.	0.10689
H	0.	0.	-0.85513



H_2O

Zero-point correction (Hartree)=	0.021259
Thermal correction to Energy=	0.024094
Thermal correction to Enthalpy=	0.025038
Thermal correction to Gibbs Free Energy=	0.003614
Sum of electronic and zero-point Energies=	-76.447648
Sum of electronic and thermal Energies=	-76.444812
Sum of electronic and thermal Enthalpies=	-76.443868
Sum of electronic and thermal Free Energies=	-76.465293

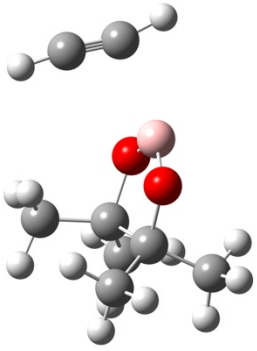
O	-1.5912	0.07945	1.16018
H	-0.6312	0.07945	1.16018
H	-1.91166	0.98438	1.16018



Acetylene

Zero-point correction(Hartree)=	0.026880
Thermal correction to Energy=	0.029673
Thermal correction to Enthalpy=	0.030617
Thermal correction to Gibbs Free Energy=	0.007933
Sum of electronic and zero-point Energies=	-77.335890
Sum of electronic and thermal Energies=	-77.333096
Sum of electronic and thermal Enthalpies=	-77.332152
Sum of electronic and thermal Free Energies=	-77.354837

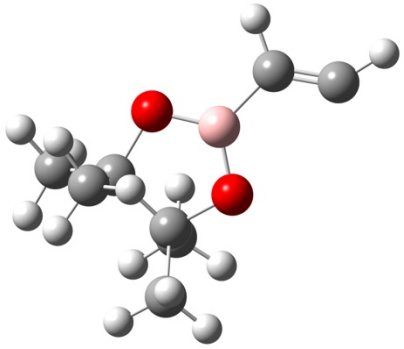
C	0.	0.	0.59804
H	0.	0.	1.65895
C	0.	0.	-0.59804
H	0.	0.	-1.65895



BPin Radical----Acetylene(TS)

Zero-point correction (Hartree)=	0.205808
Thermal correction to Energy=	0.218831
Thermal correction to Enthalpy=	0.219775
Thermal correction to Gibbs Free Energy=	0.165773
Sum of electronic and zero-point Energies=	-488.479772
Sum of electronic and thermal Energies=	-488.466749
Sum of electronic and thermal Enthalpies=	-488.465805
Sum of electronic and thermal Free Energies=	-488.519807

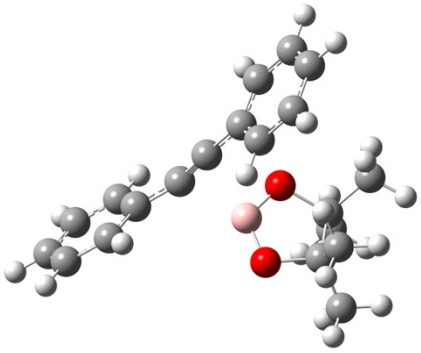
C	-0.81763	0.79817	0.11085
C	-0.90491	-0.77352	0.01563
B	1.03941	-0.03794	-0.91226
O	0.47039	-1.14199	-0.36351
O	0.30903	1.10119	-0.7937
C	-1.81314	-1.27216	-1.10843
H	-1.66433	-2.34395	-1.23061
H	-2.86445	-1.09602	-0.88065
H	-1.57674	-0.78985	-2.0554
C	-1.2413	-1.48313	1.31937
H	-2.23196	-1.19322	1.67319
H	-1.24404	-2.56015	1.15655
H	-0.51627	-1.26158	2.09801
C	-0.41105	1.3086	1.49259
H	-0.18791	2.37218	1.42346
H	-1.2124	1.17306	2.21896
H	0.48008	0.80086	1.85685
C	-2.04233	1.54782	-0.39143
H	-2.91792	1.30534	0.21296
H	-1.86842	2.62049	-0.31629
H	-2.26107	1.31423	-1.42978
C	3.43898	0.30258	-0.4486
C	3.68568	-0.38946	0.51093
H	3.51485	1.0053	-1.24181
H	3.75249	-1.064	1.32812



BPin-CH=CH Radical

Zero-point correction(Hartree)=	0.209487
Thermal correction to Energy=	0.221686
Thermal correction to Enthalpy=	0.222631
Thermal correction to Gibbs Free Energy=	0.171898
Sum of electronic and zero-point Energies=	-488.545319
Sum of electronic and thermal Energies=	-488.533120
Sum of electronic and thermal Enthalpies=	-488.532176
Sum of electronic and thermal Free Energies=	-488.582908

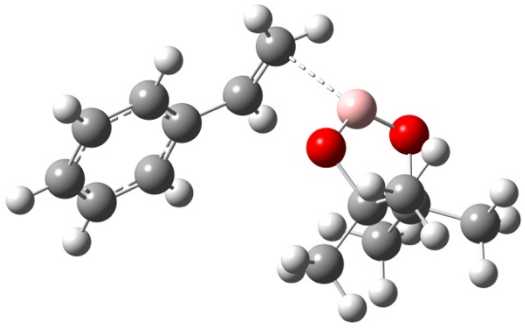
C	-0.76376	0.70882	0.39515
C	-0.8133	-0.77248	0.00013
B	1.22854	0.05534	-0.38227
O	0.53614	-1.21393	0.15994
O	0.25544	1.25264	-0.44564
C	-1.24897	-0.90478	-1.47102
H	-1.2293	-1.93552	-1.75751
H	-2.24159	-0.52182	-1.58486
H	-0.57872	-0.3489	-2.09285
C	-1.79041	-1.58186	0.87293
H	-2.78167	-1.19896	0.7476
H	-1.76513	-2.60988	0.57723
H	-1.50335	-1.4991	1.90037
C	-0.36207	0.83964	1.87607
H	-0.27573	1.87497	2.13209
H	-1.10909	0.38151	2.49006
H	0.57769	0.35335	2.03503
C	-2.11581	1.41753	0.19199
H	-2.85559	0.95982	0.81498
H	-2.01963	2.4508	0.45276
H	-2.41163	1.33439	-0.83294
C	2.81294	0.12382	-0.83778
C	3.76481	0.45461	0.06836
H	3.08885	-0.09296	-1.84861
H	4.51636	0.7158	0.7838



BPin Radical----Diphenylacetylene

Zero-point correction (Hartree)=	0.369506
Thermal correction to Energy=	0.390696
Thermal correction to Enthalpy=	0.391640
Thermal correction to Gibbs Free Energy=	0.316322
Sum of electronic and zero-point Energies=	-950.575652
Sum of electronic and thermal Energies=	-950.554462
Sum of electronic and thermal Enthalpies=	-950.553518
Sum of electronic and thermal Free Energies=	-950.628836

C	-1.31035	2.36722	0.89402
C	-1.66002	2.36795	-0.64382
B	0.29009	1.23226	-0.28307
O	-0.71905	1.35473	-1.1832
O	0.09134	1.87204	0.89703
C	-1.32901	3.68104	-1.35025
H	-1.42793	3.53891	-2.42553
H	-2.01259	4.47361	-1.04813
H	-0.31006	4.00275	-1.14151
C	-3.07423	1.92344	-0.98303
H	-3.80382	2.60979	-0.55218
H	-3.20799	1.92694	-2.06414
H	-3.28101	0.92191	-0.6158
C	-2.12289	1.36684	1.71235
H	-1.6994	1.3023	2.71371
H	-3.16094	1.68514	1.80273
H	-2.10217	0.37314	1.26908
C	-1.32602	3.73429	1.55987
H	-2.32739	4.16459	1.52474
H	-1.04183	3.63262	2.60662
H	-0.63551	4.42565	1.08408
C	1.38042	-1.02176	-0.13247
C	0.35424	-1.68176	-0.09413
C	-0.89759	-2.34763	-0.08249
C	-1.59724	-2.5808	-1.28189
C	-1.46024	-2.79482	1.12821
C	-2.81975	-3.23697	-1.26417
H	-1.17298	-2.24311	-2.21652
C	-2.68305	-3.45042	1.13374
H	-0.92979	-2.62282	2.05385
C	-3.36782	-3.6741	-0.05954
H	-3.347	-3.40832	-2.19253
H	-3.10362	-3.78808	2.07091
H	-4.32017	-4.18559	-0.05083
C	2.78219	-0.69739	-0.09707
C	3.5572	-1.08551	1.00619
C	3.4023	-0.02246	-1.15851
C	4.91884	-0.80792	1.04089
H	3.08636	-1.60388	1.8293
C	4.7648	0.24234	-1.12162
H	2.80883	0.29129	-2.00524
C	5.52789	-0.14599	-0.02183
H	5.50358	-1.11093	1.89857
H	5.23157	0.75731	-1.95001
H	6.58731	0.06781	0.00674

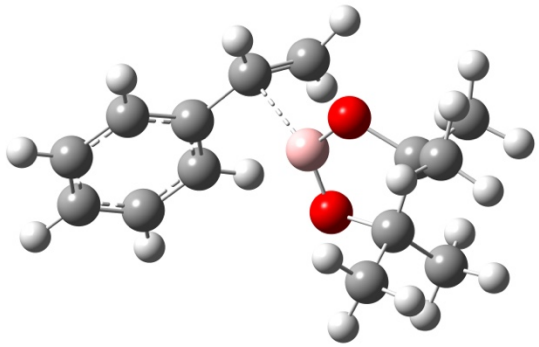


BPin Radical----CH_2=CH-Ph (TS)

Imaginary frequency = -96.91

Zero-point correction (Hartree)=	0.312262
Thermal correction to Energy=	0.329749
Thermal correction to Enthalpy=	0.330693
Thermal correction to Gibbs Free Energy=	0.263825
Sum of electronic and zero-point Energies=	-720.762009
Sum of electronic and thermal Energies=	-720.744522
Sum of electronic and thermal Enthalpies=	-720.743578
Sum of electronic and thermal Free Energies=	-720.810446

C	-2.6701	0.23964	0.59298
C	-2.23253	-0.95736	-0.33566
B	-1.33483	0.99845	-1.09642
O	-1.15418	-0.34297	-1.1551
O	-2.26821	1.42482	-0.21228
C	-3.31335	-1.40464	-1.31726
H	-2.87491	-2.09735	-2.03417
H	-4.1244	-1.91797	-0.80203
H	-3.72964	-0.56272	-1.86794
C	-1.6446	-2.15656	0.39088
H	-2.38717	-2.60237	1.05337
H	-1.34704	-2.91211	-0.3352
H	-0.77249	-1.88643	0.98015
C	-1.887	0.32425	1.90061
H	-2.1215	1.26663	2.3936
H	-2.15928	-0.48779	2.57379
H	-0.81264	0.28739	1.72918
C	-4.16356	0.33887	0.85899
H	-4.51436	-0.54209	1.39731
H	-4.36562	1.21197	1.47826
H	-4.73444	0.43281	-0.06097
C	1.02265	2.42481	-0.99535
C	1.64024	1.87727	0.06496
H	1.21173	2.10717	-2.01045
H	0.38471	3.28711	-0.87311
H	1.42589	2.28784	1.04571
C	2.57573	0.74897	0.06303
C	3.12549	0.32109	1.28125
C	2.95456	0.06682	-1.10531
C	4.01963	-0.74253	1.33482
H	2.84588	0.83226	2.19353
C	3.84613	-0.99519	-1.05225
H	2.55016	0.36712	-2.06168
C	4.3844	-1.40638	0.1675
H	4.42973	-1.05221	2.28649
H	4.12369	-1.50634	-1.9642
H	5.07883	-2.23435	0.20444

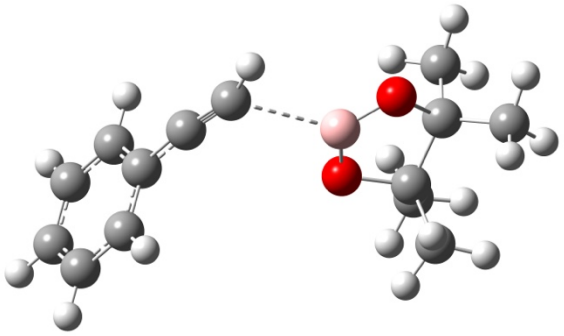


BPin Radical----CHPh=CH_2 (TS)

Imaginary frequency = -237.82

Zero-point correction (Hartree)=	0.311789
Thermal correction to Energy=	0.329234
Thermal correction to Enthalpy=	0.330179
Thermal correction to Gibbs Free Energy=	0.264263
Sum of electronic and zero-point Energies=	-720.756625
Sum of electronic and thermal Energies=	-720.739181
Sum of electronic and thermal Enthalpies=	-720.738236
Sum of electronic and thermal Free Energies=	-720.804151

C	-2.78987	0.37193	-0.30512
C	-2.23547	-1.0026	0.23185
B	-0.52164	0.27679	-0.57027
O	-0.77188	-0.75936	0.27032
O	-1.622	0.90938	-1.05111
C	-2.45206	-2.17131	-0.7273
H	-1.88514	-3.03042	-0.37136
H	-3.50322	-2.45351	-0.77285
H	-2.11247	-1.93257	-1.73385
C	-2.68716	-1.37673	1.63492
H	-3.76956	-1.5052	1.66585
H	-2.22928	-2.32171	1.92495
H	-2.40677	-0.62265	2.36562
C	-3.10069	1.38315	0.79543
H	-3.30408	2.35128	0.33975
H	-3.97956	1.08538	1.36606
H	-2.26425	1.49883	1.4826
C	-3.95696	0.26401	-1.27353
H	-4.82038	-0.18571	-0.78228
H	-4.24412	1.25951	-1.61011
H	-3.70577	-0.3326	-2.14655
C	1.40252	1.68725	-0.00776
C	0.85727	2.24511	1.09888
H	1.22146	2.16977	-0.96003
H	0.14526	3.05264	1.0122
H	1.06762	1.88442	2.09571
C	2.48669	0.67993	-0.02502
C	2.84832	-0.06738	1.10346
C	3.20445	0.47626	-1.21016
C	3.89272	-0.98196	1.04653
H	2.3079	0.05779	2.03128
C	4.2527	-0.43579	-1.26829
H	2.93657	1.04145	-2.09366
C	4.60142	-1.17077	-0.13884
H	4.15368	-1.55101	1.92863
H	4.79445	-0.57301	-2.1943
H	5.41358	-1.88342	-0.18041

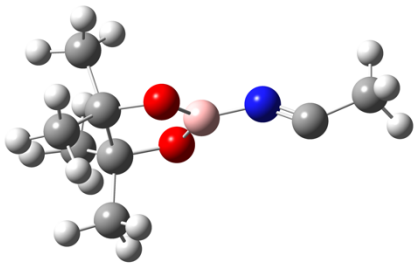


BPin Radical----CHΞCPh (TS)

Imaginary frequency = -355.60

Zero-point correction (Hartree)=	0.287495
Thermal correction to Energy=	0.304850
Thermal correction to Enthalpy=	0.305794
Thermal correction to Gibbs Free Energy=	0.238461
Sum of electronic and zero-point Energies=	-719.530713
Sum of electronic and thermal Energies=	-719.513358
Sum of electronic and thermal Enthalpies=	-719.512413
Sum of electronic and thermal Free Energies=	-719.579747

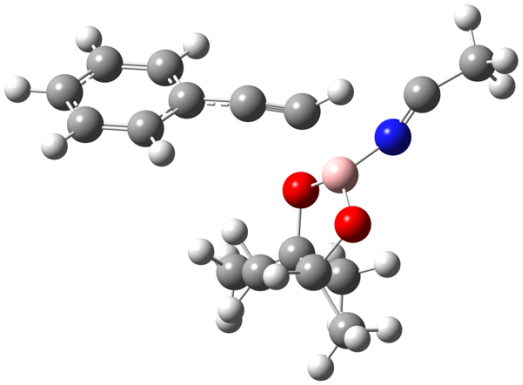
C	1.97878	1.65939	-0.31066
C	0.96349	2.32913	-0.46851
H	0.44597	3.24633	-0.63512
C	3.01673	0.7205	-0.11106
C	3.60977	0.05909	-1.206
C	3.48529	0.43132	1.18701
C	4.63005	-0.85823	-1.00314
H	3.26102	0.27415	-2.20603
C	4.50582	-0.48857	1.37632
H	3.04055	0.93394	2.03408
C	5.08374	-1.13733	0.28558
H	5.07389	-1.35833	-1.85302
H	4.85285	-0.70103	2.37824
H	5.87971	-1.85261	0.43828
C	-2.38564	-0.9642	-0.15396
C	-3.2618	0.28389	0.24676
B	-1.15136	0.9459	-0.31462
O	-1.01154	-0.39048	-0.1745
O	-2.41215	1.42181	-0.20871
C	-4.60254	0.38768	-0.46152
H	-5.23867	-0.4583	-0.19891
H	-5.11066	1.29854	-0.14746
H	-4.48965	0.41419	-1.54202
C	-3.43431	0.46053	1.75302
H	-3.88323	1.43363	1.94627
H	-4.09165	-0.30445	2.16465
H	-2.47987	0.41551	2.27495
C	-2.65301	-1.48	-1.56533
H	-1.89148	-2.21403	-1.82444
H	-3.62666	-1.9645	-1.62729
H	-2.61686	-0.67729	-2.29996
C	-2.39868	-2.1102	0.84441
H	-3.40209	-2.5277	0.93198
H	-1.73595	-2.90182	0.49718
H	-2.06708	-1.79428	1.82986



CH3CN-BPin Radical

Zero-point correction (Hartree)=	0.226660
Thermal correction to Energy=	0.240492
Thermal correction to Enthalpy=	0.241436
Thermal correction to Gibbs Free Energy=	0.186258
Sum of electronic and zero-point Energies=	-543.965947
Sum of electronic and thermal Energies=	-543.952115
Sum of electronic and thermal Enthalpies=	-543.951171
Sum of electronic and thermal Free Energies=	-544.006350

C	-0.52593	2.50687	0.13341
C	-1.77728	1.63952	0.13341
B	0.14864	0.19732	0.13342
O	0.65063	1.53671	0.13342
O	-1.28173	0.19732	0.13342
C	-0.48267	3.41524	1.37623
H	0.41535	3.99683	1.36186
H	-1.33048	4.068	1.3706
H	-0.50284	2.81203	2.25977
C	-0.48267	3.41524	-1.10941
H	-1.32864	4.07036	-1.10198
H	0.417	3.99431	-1.09681
H	-0.50633	2.81217	-1.99295
C	-2.64304	1.91781	-1.10941
H	-3.50721	1.28712	-1.09059
H	-2.94958	2.94296	-1.10827
H	-2.07388	1.7167	-1.99287
C	-2.64304	1.91781	1.37623
H	-2.95195	2.94224	1.3736
H	-3.50575	1.28509	1.35889
H	-2.07296	1.71945	2.25973
C	1.77288	-2.14601	0.13342
N	1.08859	-1.15877	0.13342
C	2.65017	-3.41169	0.13342
H	3.26169	-3.4218	-0.74456
H	3.2741	-3.41319	1.00268
H	2.02428	-4.27949	0.14213

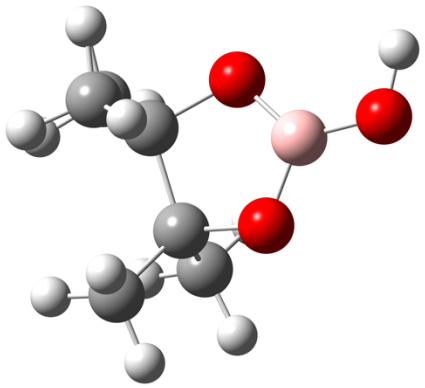


CH3CN-BPin Radical + CHΞCPh (TS)

Imaginary frequency = -601.7020

Zero-point correction (Hartree)=	0.334648
Thermal correction to Energy=	0.355970
Thermal correction to Enthalpy=	0.356915
Thermal correction to Gibbs Free Energy=	0.282834
Sum of electronic and zero-point Energies=	-852.318071
Sum of electronic and thermal Energies=	-852.296749
Sum of electronic and thermal Enthalpies=	-852.295805
Sum of electronic and thermal Free Energies=	-852.369885

C	1.26003	1.16507	-0.88061
C	0.09099	1.4608	-1.16411
C	2.50792	0.71439	-0.41964
C	3.0946	1.28147	0.73386
C	3.20845	-0.29975	-1.10996
C	4.33092	0.84179	1.17715
H	2.56595	2.05857	1.26671
C	4.44417	-0.72947	-0.65531
H	2.7718	-0.73344	-1.99792
C	5.00999	-0.1632	0.48741
H	4.76919	1.28067	2.0626
H	4.97104	-1.5066	-1.19119
H	5.97474	-0.5023	0.83769
H	-0.44165	2.15226	-1.80089
B	-1.35571	0.58407	-0.14446
O	-0.80781	-0.13336	0.93597
O	-2.04759	-0.28434	-1.01201
N	-2.08159	1.86791	0.15693
C	-1.38025	-1.46666	0.9157
C	-1.76824	-1.64804	-0.60136
C	-2.22987	3.01993	-0.11622
C	-0.33827	-2.45131	1.43338
C	-2.59639	-1.4616	1.84871
C	-3.01964	-2.48458	-0.84762
C	-0.61834	-2.18178	-1.46099
C	-3.0923	4.17842	0.18242
H	-0.12344	-2.23831	2.48063
H	-0.70675	-3.47566	1.36896
H	0.59192	-2.38106	0.87531
H	-3.0456	-2.45092	1.931
H	-2.27455	-1.15075	2.84236
H	-3.35803	-0.76297	1.505
H	-3.21599	-2.54001	-1.9184
H	-2.88377	-3.50189	-0.47913
H	-3.8931	-2.0539	-0.3644
H	-0.41993	-3.23231	-1.25044
H	-0.89386	-2.09266	-2.51162
H	0.29627	-1.6163	-1.30036
H	-3.85119	3.92474	0.92732
H	-2.48418	5.00513	0.54593
H	-3.57864	4.51053	-0.73383

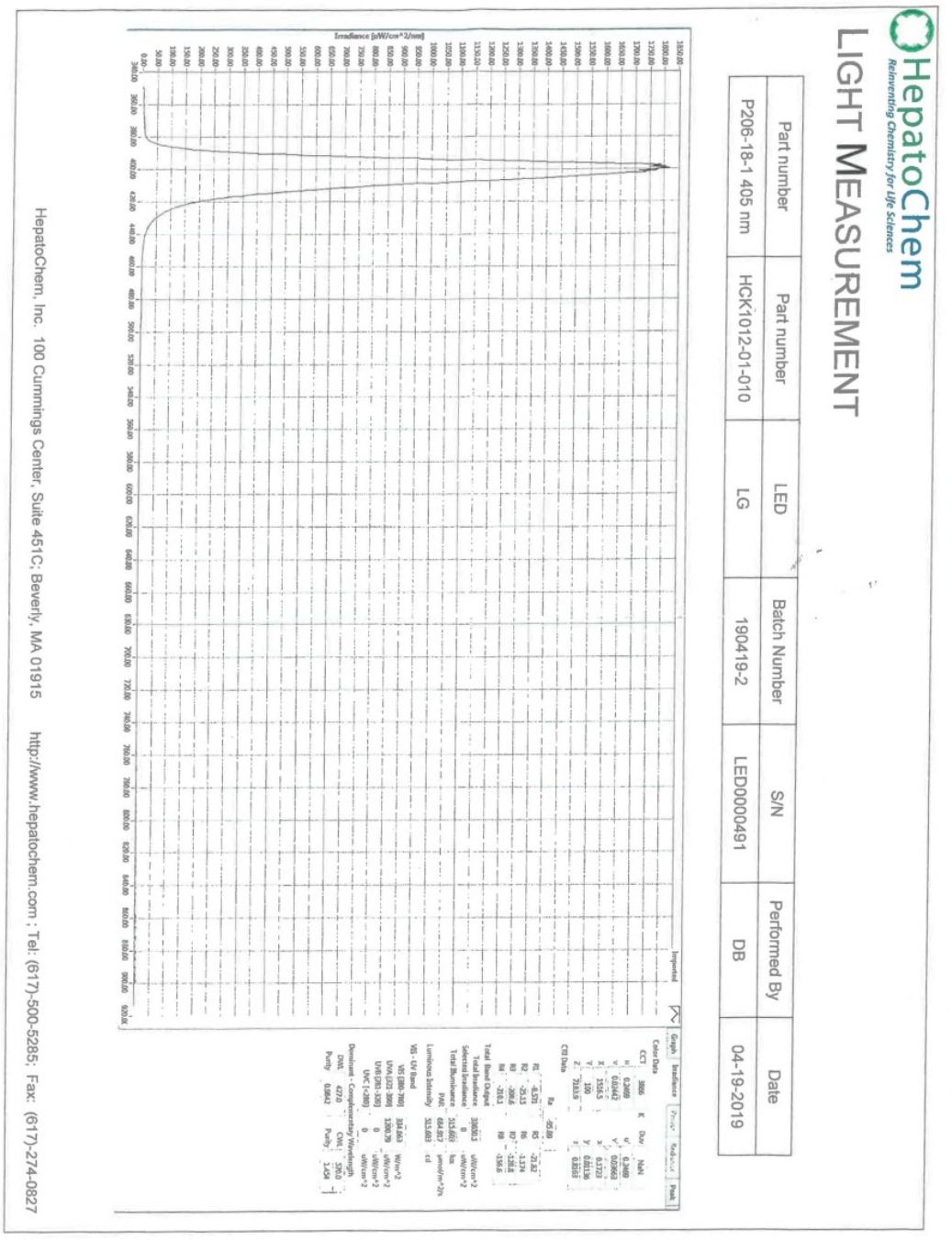


HOBPin Radical Anion

Zero-point correction (Hartree) =	0.192475
Thermal correction to Energy=	0.203179
Thermal correction to Enthalpy=	0.204124
Thermal correction to Gibbs Free Energy=	0.157238
Sum of electronic and zero-point Energies=	-487.173510
Sum of electronic and thermal Energies=	-487.162805
Sum of electronic and thermal Enthalpies=	-487.161861
Sum of electronic and thermal Free Energies=	-487.208747

C	0.51062	-0.79652	-0.04838
C	0.55523	0.77923	0.04641
B	-1.60428	0.05334	0.01545
O	-0.87926	-1.04302	-0.39599
O	-0.81063	1.10687	0.41984
O	-2.95923	0.13298	0.03037
H	-3.3755	-0.69974	-0.24076
C	0.76364	-1.48382	1.29569
H	0.51678	-2.54085	1.20197
H	1.80935	-1.40123	1.60114
H	0.13411	-1.06095	2.08
C	1.40074	-1.40389	-1.12441
H	2.45292	-1.1741	-0.9365
H	1.29112	-2.48823	-1.11878
H	1.13691	-1.04566	-2.1181
C	0.82696	1.44899	-1.30309
H	0.65238	2.52032	-1.20683
H	1.85858	1.29752	-1.62771
H	0.15898	1.06479	-2.07542
C	1.50125	1.33046	1.10488
H	2.53257	1.03048	0.90253
H	1.46367	2.41986	1.09789
H	1.23183	0.98968	2.10293

6. Special data of the LEDs used



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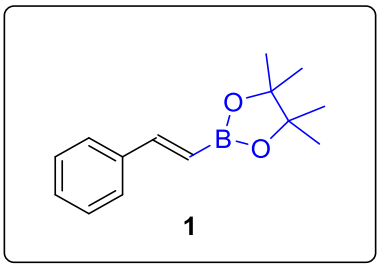
LIGHT MEASUREMENT

Part number	Part number	LED	Batch Number	S/N	Performed By	Date
P206-18-1 405 nm	HCK1012-01-010	LG	190419-2	LED0000491	DB	04-19-2019

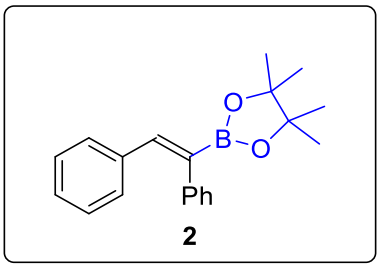
HepatoChem, Inc. 100 Cummings Center, Suite 451C; Beverly, MA 01915 http://www.hepatochem.com ; Tel: (617)-500-5285; Fax: (617)-274-0827

7. Experimental data for hydroboration products



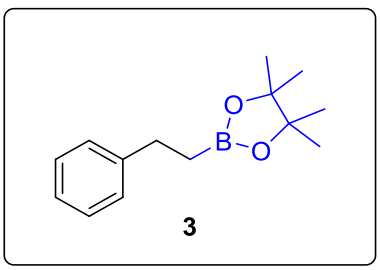
1

(*E*)-4,4,5,5-tetramethyl-2-styryl-1,3,2-dioxaborolane: Purification by silica gel column chromatography, eluent: Pentane/EtOAc from 150:1 to 120:1. Yield: 87% (40.0 mg), E/Z = 99:1. Pale yellow oil. ^{1}H NMR (300 MHz, C_6D_6): δ 7.76 (d, *J* = 18 Hz, 1H), 7.34-7.31 (m, 2H), 7.03-7.01 (m, 3H), 6.46 (d, *J* = 18 Hz, 1H), 1.12 (s, 12H). ^{13}C NMR (75.5 MHz, C_6D_6): δ 150.3, 138.1, 129.0, 128.9, 127.4, 83.2, 25.0. The carbon signal attached to B was not observed due to low intensity. ^{11}B NMR (96.3 MHz, C_6D_6): δ 30.4. IR (ATR): ν_{max} = 2978, 1622, 1450, 1370, 1349, 1320, 1209, 1141, 969, 850, 747, 692 cm^{-1}. HRMS (EI): m/z Calculated for $C_{14}H_{20}BO_2$ $[M+H]^+$: 231.1560, found 231.1556.



2

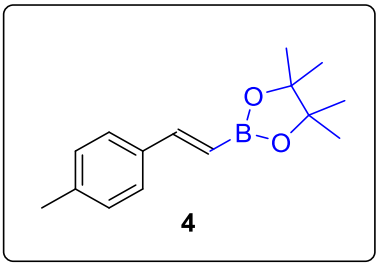
(*Z*)-2-(1,2-diphenylvinyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane: Purification by silica gel column chromatography, eluent: Pentane/EtOAc = 80:1. Yield: 85% (40.0 mg), E/Z = 1:14. Pale yellow solid, mp: 68-70 °C (Pentane/EtOAc).[3] ^{1}H NMR (300 MHz, C_6D_6): δ 7.87 (s, 1H), 7.44-7.41 (m, 2H), 7.21-7.16 (m, 3H), 7.12 (s, 1H), 7.05-7.00 (m, 1H), 6.93-6.83 (m, 3H), 1.08 (s, 12H). ^{13}C NMR (75.5 MHz, C_6D_6): δ 144.0, 143.5(minor), 141.1, 141.1(minor), 139.6(minor), 137.4, 130.3, 129.2, 128.7, 128.6(minor), 127.4, 127.0, 126.5, 83.6, 24.7, 24.4(minor). The carbon signal attached to B was not observed due to low intensity. ^{11}B NMR (96.3 MHz, C_6D_6): 30.4. iiIR (ATR): ν = 2980, 1622, 1450, 1371, 1349, 1209, 1141, 969, 850, 755, 690 cm^{-1}. HRMS (ESI): m/z Calculated for $C_{20}H_{23}BO_2$ $[M]^+$: 306.1791, found 306.1803.



3

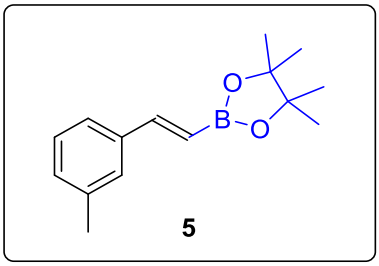
4,4,5,5-tetramethyl-2-phenethyl-1,3,2-dioxaborolane: Purification by silica gel column chromatography, eluent: Pentane/EtOAc = 120:1). Yield: 97% (45.0 mg). Colorless oil. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.21-7.05 (m, 5H), 2.67 (t, *J* = 8.2 Hz, 2H), 1.14-1.04 (m, 14H). ^{13}C NMR (75.5 MHz, $CDCl_3$): δ 144.4, 128.2, 128.0, 125.5, 83.1, 29.9, 24.8. The carbon signal attached to B was not observed due to low intensity. ^{11}B NMR (96.3 MHz, C_6D_6): 33.7. IR (ATR): ν_{max} = 2978,

2931, 1370, 1316, 1143, 743, 698 cm^{-1}. HRMS (ESI): m/z Calculated for $C_{14}H_{21}BO_2$ $[M]^+$: 232.1635, found 232.1630. These spectroscopic data match those previously reported.[4]



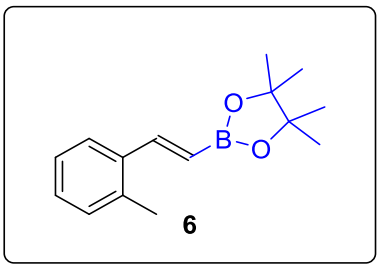
4

(*E*)-4,4,5,5-tetramethyl-2-(4-methylstyryl)-1,3,2-dioxaborolane: Purification by silica gel column chromatography, eluent: Pentane/EtOAc = 100:1. Yield: 90% (43.9 mg), E/Z = 99:1. Colorless oil. ^{1}H NMR (300 MHz, C_6D_6): δ 7.78 (d, *J* = 18 Hz, 1H), 7.28 (d, *J* = 9 Hz, 2H), 6.86 (d, *J* = 9 Hz, 2H), 6.44 (d, *J* = 18 Hz, 1H), 2.02 (s, 3H), 1.13 (s, 12H). ^{13}C NMR (75.5 MHz, C_6D_6): δ 150.3, 138.8, 135.4, 129.6, 127.4, 83.1, 24.9, 21.2. The carbon signal attached to B was not observed due to low intensity. ^{11}B NMR (96.3 MHz, C_6D_6): 30.3. IR (ATR): ν_{max} = 2978, 1625, 1511, 1347, 1319, 1141, 995, 969, 854, 798 cm^{-1}. HRMS (EI): m/z Calculated for $C_{14}H_{18}BBrO_2$ $[M]^+$: 244.1639, found 244.1634.



5

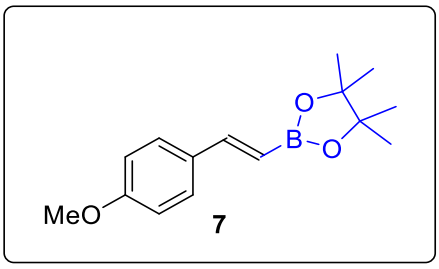
(*E*)-4,4,5,5-tetramethyl-2-(3-methylstyryl)-1,3,2-dioxaborolane: Purification by silica gel column chromatography, eluent: Pentane/EtOAc = 120:1. Yield: 92% (44.9 mg), E/Z = 99:1. Colorless oil. ^{1}H NMR (300 MHz, C_6D_6): δ 7.79 (d, *J* = 18 Hz, 1H), 7.23-7.18 (m, 2H), 7.00 (t, *J* = 7.5 Hz, 1H), 6.85 (d, *J* = 7.5 Hz, 1H), 6.50 (d, *J* = 18 Hz, 1H), 2.01 (s, 3H), 1.13 (s, 12H). ^{13}C NMR (75.5 MHz, C_6D_6): δ 150.2, 137.8, 129.5, 128.4, 127.9, 127.5, 124.3, 82.8, 24.6, 20.9. The carbon signal attached to B was not observed due to low intensity. ^{11}B NMR (96.3 MHz, C_6D_6): 30.4. IR (ATR): ν_{max} = 2978, 2927, 1449, 1369, 1319, 1143, 967, 850, 804 cm^{-1}. HRMS (EI): m/z Calculated for $C_{15}H_{21}BO_2$ $[M]^+$: 244.1638, found 244.1634.



6

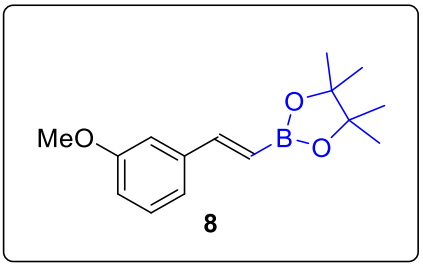
(*E*)-4,4,5,5-tetramethyl-2-(2-methylstyryl)-1,3,2-dioxaborolane: Purification by silica gel column chromatography, eluent: Pentane/EtOAc = 120:1. Yield: 89% (43.5 mg), E/Z = 99:1. Colorless oil. ^{1}H NMR (300 MHz, C_6D_6): δ 8.04 (d, *J* = 18 Hz, 1H), 7.56 (m, 1H), 6.98 (m, 2H), 6.88 (m, 1H), 6.43 (t, *J* = 18 Hz, 1H), 2.11 (s, 3H), 1.13 (s, 12H). ^{13}C NMR (75.5 MHz, C_6D_6): δ 147.7, 137.0, 136.4, 130.7, 128.8, 126.5, 126.0, 83.2, 24.9, 19.5. The carbon signal attached to B was not observed

due to low intensity. ^{11}B NMR (96.3 MHz, C_6D_6): 30.4. IR (ATR): ν_{max} = 2978, 2927, 1449, 1369, 1319, 1143, 967, 850, 804 cm^{-1}. HRMS (EI): m/z Calculated for $C_{15}H_{21}BO_2$ $[M]^+$: 244.1635, found 244.1634.



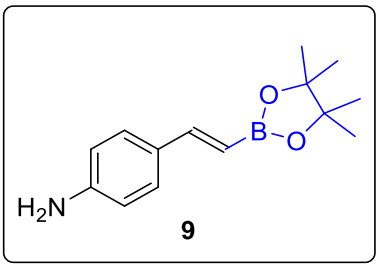
7

(*E*)-4,4,5,5-tetramethyl-2-(2-methylstyryl)-1,3,2-dioxaborolane: Purification by silica gel column chromatography, eluent: Pentane/EtOAc = 120:1. Yield: 89% (43.5 mg), E/Z = 99:1. Off-white solid; mp: 64-66 ºC (Pentane/EtOAc).[5] NMR (300 MHz, C_6D_6): δ 7.73 (d, *J* = 18 Hz, 1H), 7.28 (d, *J* = 8.7 Hz, 2H), 6.61 (d, *J* = 8.7 Hz, 2H), 6.32 (d, *J* = 18 Hz, 1H), 3.24 (s, 3H), 1.14 (s, 12H). ^{13}C NMR (75.5 MHz, C_6D_6): δ 160.7, 149.9, 130.8, 128.8, 114.3, 83.1, 54.7, 24.9. The carbon signal attached to B was not observed due to low intensity. ^{11}B NMR (96.3 MHz, C_6D_6): 30.1. IR (ATR): ν_{max} = 2977, 1624, 1603, 1510, 1352, 1250, 1140, 813 cm^{-1}. HRMS (ESI): m/z Calculated for $C_{15}H_{22}BO_3$ $[M+H]^+$: 261.1666, found 261.1672.



8

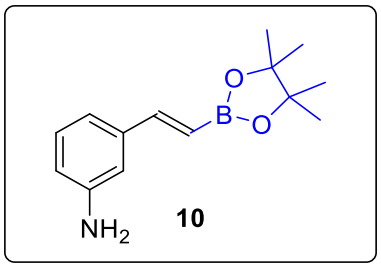
(*E*)-4,4,5,5-tetramethyl-2-(2-methylstyryl)-1,3,2-dioxaborolane: Purification by silica gel column chromatography, eluent: Pentane/EtOAc = 120/1. Yield: 89% (43.5 mg), E/Z = 99/1. Off-white solid; mp: 68-70 ºC (Pentane/EtOAc). NMR (300 MHz, C_6D_6): δ 7.76 (d, *J* = 18 Hz, 1H), 7.02-6.96 (m, 3H), 6.72-6.69 (m, 1H), 6.47 (d, *J* = 18 Hz, 1H), 3.25 (s, 3H), 1.13 (s, 12H). ^{13}C NMR (75.5 MHz, C_6D_6): δ 160.3, 150.2, 139.4, 129.7, 119.9, 115.4, 112.0, 83.1, 54.5, 24.8. The carbon signal attached to B was not observed due to low intensity. ^{11}B NMR (96.3 MHz, C_6D_6): 30.1. IR (ATR): ν_{max} = 2978, 2930, 1624, 1603, 1371, 1352, 1250, 1045, 807 cm^{-1}. HRMS (EI): m/z Calculated for $C_{15}H_{21}BO_2$ $[M+H]^+$: 261.1662, found 260.1667.



9

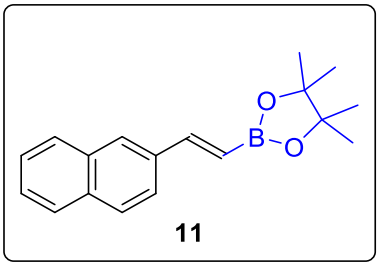
(*E*)-4-(2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)vinyl)aniline: Purification by silica gel column chromatography, eluent: Pentane/EtOAc = 150:1. Yield: 78% (38.2 mg), E/Z = 99:1. Orange oil. ^{1}H NMR (300 MHz, C_6D_6): δ 7.80 (d, *J* = 18 Hz, 1H), 7.26 (d, *J* = 9 Hz, 2H), 6.34 (d, *J* = 18 Hz, 1H), 6.16 (d, *J* = 9 Hz, 2H), 2.87 (br, 2H), 1.14 (s, 12H). ^{13}C NMR (75.5 MHz, C_6D_6): δ

150.7, 148.0, 128.9, 128.3, 114.8, 82.9, 25.0. The carbon signal attached to B was not observed due to low intensity. ^{11}B NMR (96.3 MHz, C_6D_6): 30.3. IR (ATR): ν_{max} = 3369, 2977, 1622, 1590, 1320, 1140, 969, 848, 776, 650 cm^{-1}. HRMS (ESI): m/z Calculated for $C_{14}H_{22}BNO_2$ $[M+H]^+$: 246.1666, found 246.1665.



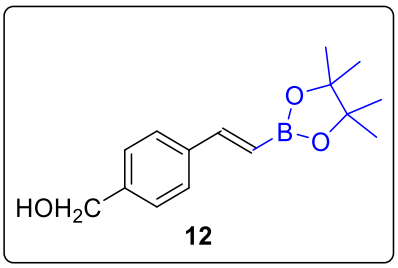
10

(*E*)-3-(2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)vinyl)aniline: Purification by silica gel column chromatography, eluent: Pentane/EtOAc from 100:1 to 60:1. Yield: 75% (36.8 mg), E/Z = 99:1. Yellow oil. ^{1}H NMR (300 MHz, C_6D_6): δ 7.78 (d, *J* = 18 Hz, 1H), 6.96-6.86 (m, 2H), 6.54-6.46 (m, 2H), 6.23-6.20 (m, 1H), 2.72 (br, 2H), 1.13 (s, 12H). ^{13}C NMR (75.5 MHz, C_6D_6): δ 150.9, 147.4, 139.0, 129.6, 117.8, 115.8, 113.3, 83.1, 24.9. The carbon signal attached to B was not observed due to low intensity. ^{11}B NMR (96.3 MHz, C_6D_6): 30.3. IR (ATR): ν_{max} = 3369, 2977, 1622, 1590, 1320, 1140, 969, 848, 776, 650 cm^{-1}. HRMS (ESI): m/z Calculated for $C_{14}H_{21}BNO_2$ $[M+H]^+$: 246.1666, found 246.1665.



11

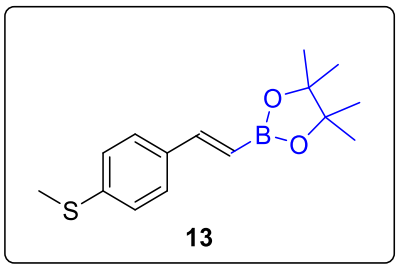
(*E*)-4,4,5,5-tetramethyl-2-(2-(naphthalen-2-yl)vinyl)-1,3,2-dioxaborolane: Purification by silica gel column chromatography, eluent: Pentane/EtOAc = 120:1. Yield: 91% (50.9 mg), E/Z = 99:1. Colorless oil. ^{1}H NMR (300 MHz, C_6D_6): δ 7.58 (d, *J* = 18 Hz, 1H), 7.54-7.48 (m, 5H), 7.19-7.16 (m, 2H), 6.55 (d, *J* = 18 Hz, 1H), 1.14 (s, 12H). ^{13}C NMR (75.5 MHz, C_6D_6): δ 150.3, 135.5, 134.2, 134.0, 128.7, 128.6, 128.5, 127.9, 126.5, 126.4, 123.7, 83.2, 25.0. The carbon signal attached to B was not observed due to low intensity. ^{11}B NMR (96.3 MHz, C_6D_6): 30.3. IR (ATR): ν_{max} = 3055, 2965, 1620, 1610, 1365, 1320, 1141 cm^{-1}. HRMS (EI): m/z Calculated for $C_{18}H_{21}BO_2$ $[M]^+$: 280.1635, found 280.1650.



12

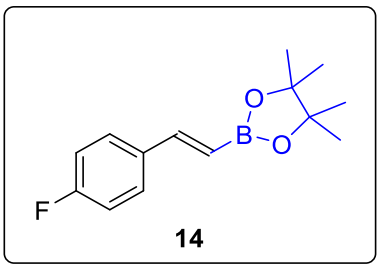
(*E*)-(4-(2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)vinyl)phenyl)methanol: Purification by silica gel column chromatography, eluent: Pentane/EtOAc = 70:1. Yield: 92% (47.9 mg), E/Z = 99:1. Off-white solid; mp: 102-104 ºC (Pentane/EtOAc). ^{1}H NMR (300 MHz, C_6D_6): δ 7.76 (d, *J* =

18 Hz, 1H), 7.30 (d, J = 9 Hz, 2H), 7.05 (d, J = 9 Hz, 2H), 6.43 (d, J = 18 Hz, 1H), 4.29 (s, 2H), 1.13 (s, 12H). ^{13}C NMR (75.5 MHz, C_6D_6): δ 150.0, 142.6, 136.9, 127.3, 127.1, 83.1, 64.5, 24.8. The carbon signal attached to B was not observed due to low intensity. ^{11}B NMR (96.3 MHz, C_6D_6): 29.9. IR (ATR): ν_{max} = 3286, 2873, 1505, 1411, 1207, 1013, 817 cm^{-1}. HRMS (APCI): m/z Calculated for $C_{15}H_{22}BO_3$ $[M+H]^+$: 261.1783, found 261.1782.



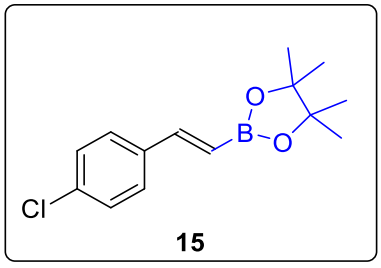
13

(*E*)-4,4,5,5-tetramethyl-2-(4-(methylthio)styryl)-1,3,2-dioxaborolane: Purification by silica gel column chromatography, eluent: Pentane/EtOAc = 120:1. Yield: 77% (42.5 mg), E/Z = 99:1. Colorless oil. ^{1}H NMR (300 MHz, C_6D_6): δ 7.72 (d, J = 18 Hz, 1H), 7.17 (d, J = 9 Hz, 2H), 6.91 (d, J = 9 Hz, 2H), 6.41 (d, J = 18 Hz, 1H), 1.89 (s, 3H), 1.13 (s, 12H). ^{13}C NMR (75.5 MHz, C_6D_6): δ 149.7, 140.3, 134.6, 127.8, 126.4, 83.2, 24.9, 14.8. The carbon signal attached to B was not observed due to low intensity. ^{11}B NMR (96.3 MHz, C_6D_6): 29.9. IR (ATR): ν_{max} = 2977, 2924, 1618, 1493, 1352, 1313, 1213, 1144, 1090, 970, 850, 798 cm^{-1}. HRMS (APCI): m/z Calculated for $C_{15}H_{22}BO_2S$ $[M]^+$: 277.1432, found 277.1428.



14

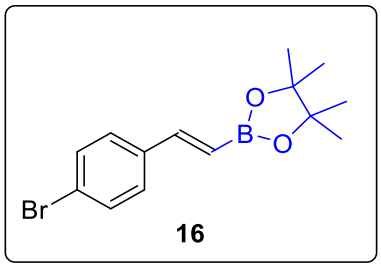
(*E*)-2-(4-fluorostyryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane: Purification by silica gel column chromatography, eluent: Pentane/EtOAc = 150:1. yield: 69% (34.2 mg), E/Z = 99:1. Colorless oil. ^{1}H NMR (300 MHz, C_6D_6): δ 7.62 (d, J = 18 Hz, 1H), 7.07-7.03 (m, 2H), 6.66-6.61 (m, 2H), 6.28 (d, J = 18 Hz, 1H), 1.13 (s, 12H). ^{13}C NMR (75.5 MHz, C_6D_6): δ 163.3 (d, J = 248 Hz), 148.7, 134.1, 129.0 (d, J = 8.3 Hz), 115.5 (d, J = 8.3 Hz), 83.1, 24.8. The carbon signal attached to B was not observed due to low intensity. ^{11}B NMR (96.3 MHz, C_6D_6): δ 30.1. ^{19}F NMR (282.5 MHz, C_6D_6): δ -112.5. IR (ATR): ν_{max} = 2970, 2921, 1621, 1530, 1439, 1366, 1315, 1259, 1217, 1055, 966, 841, 737 cm^{-1}. HRMS (EI): m/z Calculated for $C_{14}H_{19}BFO_2$ $[M+H]^+$: 249.1460, found 249.1457.



15

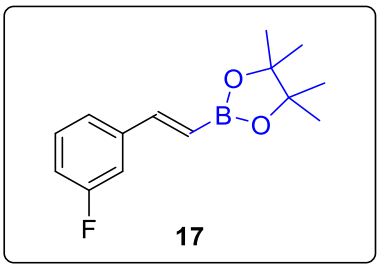
(*E*)-2-(4-chlorostyryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane: Purification by silica gel column chromatography, eluent: Pentane/EtOAc = 150:1. Yield: 77% (41.2 mg), E/Z = 99:1. Colorless oil.

^{1}H NMR (300 MHz, C_6D_6): δ 7.67 (d, *J* = 18 Hz, 1H), 6.95 (m, 4H), 6.30 (d, *J* = 18 Hz, 1H), 1.12 (s, 12H). ^{13}C NMR (75.5 MHz, C_6D_6): δ 148.6, 136.2, 134.6, 128.9, 128.5, 83.2, 24.8. The carbon signal attached to B was not observed due to low intensity. ^{11}B NMR (96.3 MHz, C_6D_6): 30.1. IR (ATR): ν_{max} = 2976, 1631, 1623, 1492, 1489, 1411, 1352, 1270, 1210, 1142, 1087, 993, 803, 640, 491; cm^{-1}. HRMS (EI): m/z Calculated for $C_{14}H_{18}BClO_2$ $[M]^+$: 264.1088, found 264.1088.



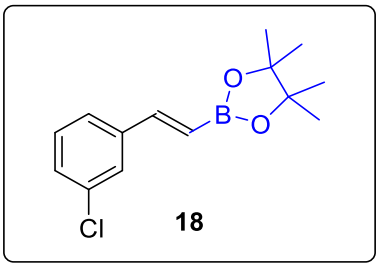
16

(*E*)-2-(4-bromostyryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane: Purification by silica gel column chromatography, eluent: Pentane/EtOAc = 150:1. Yield: 83% (51.1 mg), E/Z = 99:1. Pale yellow solid; mp: 76-78 °C (Pentane/EtOAc).[6] ^{1}H NMR (300 MHz, C_6D_6): δ 7.53 (d, *J* = 18 Hz, 1H), 7.10 (d, *J* = 9 Hz, 2H), 6.88 (d, *J* = 9 Hz, 2H), 6.30 (d, *J* = 18 Hz, 1H), 1.12 (s, 12H). ^{13}C NMR (75.5 MHz, C_6D_6): δ 148.7, 136.7, 132.0, 128.8, 123.1, 83.3, 24.9. The carbon signal attached to B was not observed due to low intensity. ^{11}B NMR (96.3 MHz, C_6D_6): 30.3. IR (ATR): ν_{max} = 2973, 1625, 1487, 1402, 1318, 1140, 1067, 1006, 969, 734, 490 cm^{-1}. HRMS (EI): m/z Calculated for $C_{14}H_{18}BBrO_2$ $[M]^+$: 308.0583, found 308.0585.



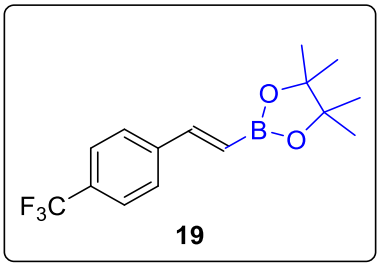
17

(*E*)-2-(3-fluorostyryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane: Purification by silica gel column chromatography, eluent: Pentane/EtOAc = 150:1. Yield: 71% (35.2 mg), E/Z = 99:1. Colorless oil. ^{1}H NMR (300 MHz, C_6D_6): δ 7.55 (d, *J* = 18 Hz, 1H), 7.01 (d, *J* = 9.9 Hz, 1H), 6.92 (d, *J* = 7.6 Hz, 1H), 6.81-6.74 (m, 1H), 6.69-6.63 (m, 1H), 6.30 (d, *J* = 18 Hz, 1H), 1.11 (s, 12H). ^{13}C NMR (75.5 MHz, C_6D_6): δ 163.4 (d, *J* = 246 Hz), 148.5 (d, *J* = 2.5 Hz), 140.3 (d, *J* = 6.5 Hz), 130.1 (d, *J* = 8.2 Hz), 123.1 (d, *J* = 2.7 Hz), 115.6 (d, *J* = 21.3 Hz), 113.5 (d, *J* = 21.4 Hz), 83.2, 24.8. The carbon signal attached to B was not observed due to low intensity. ^{11}B NMR (96.3 MHz, C_6D_6): 30.3. ^{19}F NMR (282.5 MHz, C_6D_6): -113.2. IR (ATR): ν_{max} = 2981, 2926, 2854, 1583, 1745, 1367, 1346, 1231, 1140, 1064, 953, 841, 782, 687 cm^{-1}. HRMS (EI): m/z Calculated for $C_{15}H_{21}BO_2$ $[M]^+$: 248.1384, found 248.1388.



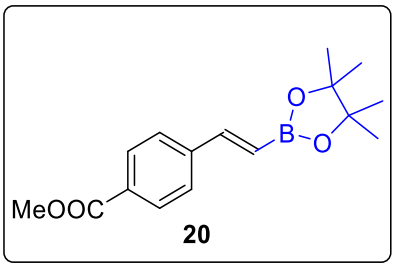
18

(*E*)-2-(3-chlorostyryl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane: Purification by silica gel column chromatography, eluent: Pentane/EtOAc = 120:1). Yield: 83% (43.8 mg), E/Z = 99:1. Pale yellow oil. ^{1}H NMR (300 MHz, C_6D_6): δ 7.52 (d, *J* = 18 Hz, 1H), 7.31 (s, 1H), 7.00-6.91 (m, 2H), 6.71 (t, *J* = 9 Hz, 1H), 6.30 (d, *J* = 18 Hz, 1H), 1.13 (s, 12H). ^{13}C NMR (75.5 MHz, C_6D_6): δ 148.3, 139.7, 134.8, 129.9, 128.7, 127.2, 125.2, 83.2, 24.8. The carbon signal attached to B was not observed due to low intensity. ^{11}B NMR (96.3 MHz, C_6D_6): 30.3. IR (ATR): ν_{max} = 2978, 2931, 1491, 1370, 1316, 1142, 1091, 967, 839, 802, 487 cm^{-1}. HRMS (EI): m/z Calculated for $C_{14}H_{18}BClO_2$ $[M]^+$: 264.1088, found 264.1088.



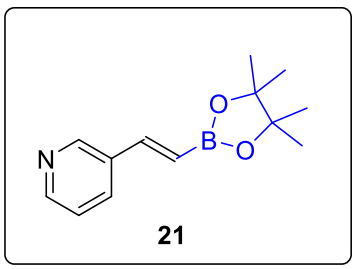
19

(*E*)-4,4,5,5-tetramethyl-2-(4-(trifluoromethyl)styryl)-1,3,2-dioxaborolane: Purification by silica gel column chromatography, eluent: Pentane/EtOAc = 150:1. Yield: 80% (47.7 mg), E/Z = 99:1. Colorless oil. ^{1}H NMR (300 MHz, C_6D_6): δ 7.54 (d, *J* = 18 Hz, 1H), 7.17 (d, *J* = 8.5 Hz, 2H), 7.03 (d, *J* = 8.1 Hz, 2H), 6.34 (d, *J* = 18 Hz, 1H), 1.11 (s, 12H). ^{13}C NMR (75.5 MHz, C_6D_6): δ 148.0, 140.8, 129.5 (q, *J* = 32 Hz), 127.2, 125.4 (q, *J* = 7.5 Hz), 124.6 (q, *J* = 272 Hz), 83.2, 24.6. The carbon signal attached to B was not observed due to low intensity. ^{11}B NMR (96.3 MHz, C_6D_6): 30.3. ^{19}F NMR (282.5 MHz, C_6D_6): -62.4. IR (ATR): ν_{max} = 2980, 2926, 2225, 1371, 1328, 1138, 967, 850, 546 cm^{-1}. HRMS (EI): m/z Calculated for $C_{15}H_{18}BF_3O_2$ $[M]^+$: 298.1341, found 298.1352.



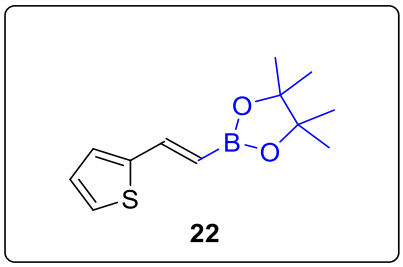
20

Methyl (*E*)-4-(2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)vinyl)benzoate: Purification by silica gel column chromatography, eluent: Pentane/EtOAc = 50:1. Yield: 77% (44.4 mg), E/Z = 99:1. Colorless oil. ^{1}H NMR (300 MHz, C_6D_6): δ 7.95 (d, *J* = 8.1 Hz, 2H), 7.61 (d, *J* = 18 Hz, 1H), 7.26 (d, *J* = 8.1 Hz, 2H), 6.40 (d, *J* = 18 Hz, 1H), 3.47 (s, 3H), 1.12 (s, 12H). ^{13}C NMR (75.5 MHz, C_6D_6): δ 166.4, 148.9, 142.0, 130.8, 130.3, 127.3, 83.4, 51.6, 25.0. The carbon signal attached to B was not observed due to low intensity. ^{11}B NMR (96.3 MHz, C_6D_6): 29.9. IR (ATR): ν_{max} = 2976, 2929, 1713, 1567, 1441, 1350, 1275, 1148, 1112, 973, 845, 759, 652 cm^{-1}. HRMS (APCI): m/z Calculated for $C_{16}H_{22}BO_4$ $[M+H]^+$: 289.1604, found 289.1605.



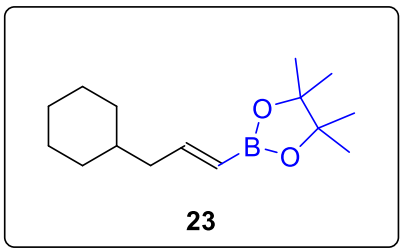
21

(*E*)-3-(2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)vinyl)pyridine: Purification by silica gel column chromatography, eluent: DCM/MeOH = 80:1. Yield: 72% (33.3 mg), E/Z = 99:1. Colorless oil. ^{1}H NMR (300 MHz, C_6D_6): δ 8.67 (br, 1H), 8.38 (br, 1H), 7.54 (d, *J* = 18 Hz, 1H), 7.24 (d, *J* = 9 Hz, 1H), 6.59-6.55 (m, 1H), 6.34 (d, *J* = 18 Hz, 1H), 1.11 (s, 12H). ^{13}C NMR (75.5 MHz, C_6D_6): δ 149.8, 149.4, 146.2, 132.7, 132.3, 123.1, 83.0, 24.6. The carbon signal attached to B was not observed due to low intensity. ^{11}B NMR (96.3 MHz, C_6D_6): 29.9. IR (ATR): ν_{max} = 2980, 1590, 1470, 1325, 1311, 1247, 1141, 836, 531 cm^{-1}. HRMS (ESI): m/z Calculated for $C_{13}H_{19}BNO_2$ $[M+H]^+$: 232.1514, found 232.1509.



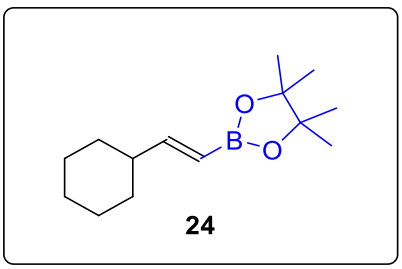
22

(*E*)-4,4,5,5-tetramethyl-2-(2-(thiophen-2-yl)vinyl)-1,3,2-dioxaborolane: Purification by silica gel column chromatography, eluent: Pentane/EtOAc = 80:1). Yield: 88% (41.6 mg), E/Z = 7:1. Colorless oil. ^{1}H NMR (300 MHz, C_6D_6): δ 7.77 (d, *J* = 18 Hz, 1H), 6.74-6.79 (m, 2H), 6.58-6.57 (m, 1H), 6.28 (d, *J* = 18 Hz, 1H), 1.10 (s, 12H). ^{13}C NMR (75.5 MHz, C_6D_6): δ 144.4, 142.5, 140.5 (minor), 130.1 (minor), 127.8, 127.3 (minor), 127.2, 126.4, 83.4 (minor), 83.2, 24.9. The carbon signal attached to B was not observed due to low intensity. ^{11}B NMR (96.3 MHz, C_6D_6): 29.9. IR (ATR): ν_{max} = 2978, 1615, 1371, 1323, 1236, 1140, 969, 847, 698 cm^{-1}. HRMS (ESI): m/z Calculated for $C_{12}H_{17}BO_2SNa$ $[M+Na]^+$: 259.0933, found 259.0935.



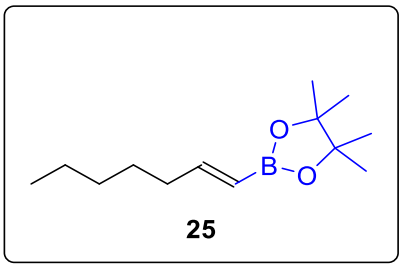
23

(*E*)-2-(3-cyclohexylprop-1-en-1-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane: Purification by silica gel column chromatography, eluent: Pentane/EtOAc = 120:1. Yield: 79% (39.5 mg), E/Z = 99:1. Colorless oil. ^{1}H NMR (300 MHz, C_6D_6): δ 6.65-6.54 (m, 1H), 5.239 (d, *J* = 18 Hz, 1H), 2.06-2.01 (m, 2H), 1.68-1.64 (m, 6H), 1.26-1.15 (m, 15H), 0.93-0.86 (m, 2H). ^{13}C NMR (75.5 MHz, C_6D_6): δ 153.4, 82.9, 44.0, 37.1, 33.1, 26.4, 26.2, 24.7. The carbon signal attached to B was not observed due to low intensity. ^{11}B NMR (96.3 MHz, C_6D_6): 29.9. IR (ATR): ν_{max} = 2979, 2921, 2852, 1638, 1359, 1316, 1143, 997, 971, 850, 647 cm^{-1}. HRMS (ESI): m/z Calculated for $C_{15}H_{27}BO_2$ $[M^+]$: 250.2104, found 250.2110.



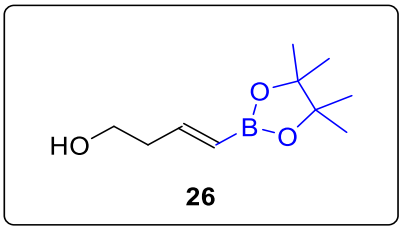
24

(*E*)-2-(2-cyclohexylvinyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane: Purification by silica gel column chromatography, eluent: Pentane/EtOAc = 120:1. Yield: 65% (30.4 mg), E/Z = 99:1. Colorless oil. ^{1}H NMR (300 MHz, C_6D_6): δ 6.46 (dd, *J* = 18 Hz, *J* = 6.2 Hz, 1H), 5.25 (dd, *J* = 18 Hz, *J* = 1.4 Hz, 1H), 1.93-1.88 (m, 1H), 1.64-1.51 (m, 6H), 1.21-1.03 (m, 16H). ^{13}C NMR (75.5 MHz, C_6D_6): δ 159.8, 82.9, 43.2, 31.9, 26.1, 25.9, 24.7. The carbon signal attached to B was not observed due to low intensity. ^{11}B NMR (96.3 MHz, C_6D_6): 29.9. IR (ATR): ν_{max} = 2980, 2920, 2855, 1650, 1389, 1300, 997, 971, 850, 597 cm^{-1}. HRMS (ESI): m/z Calculated for $C_{14}H_{25}BO_2$ $[M]^+$: 236.1948, found 236.1955.



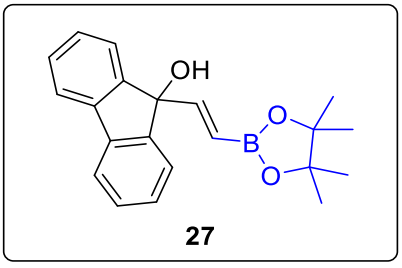
25

(*E*)-2-(hept-1-en-1-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane: Purification by silica gel column chromatography, eluent: Pentane/EtOAc = 150:1. Yield: 91% (40.8 mg), E/Z = 99:1. Colorless oil. ^{1}H NMR (300 MHz, C_6D_6): δ 7.03-6.93 (m, 1H), 5.80 (d, *J* = 18 Hz, 1H), 2.08-2.01(m, 2H), 1.15-1.07 (m, 18H), 0.79 (m, 3H). ^{13}C NMR (75.5 MHz, C_6D_6): δ 154.9, 82.7, 36.0, 31.5, 28.3, 24.8, 22.7, 14.0. The carbon signal attached to B was not observed due to low intensity. ^{11}B NMR (96.3 MHz, C_6D_6): 30.3. These spectroscopic data match those previously reported. IR (ATR): ν_{max} = 3658, 2974, 2927, 1638, 1462, 847 cm^{-1}. HRMS (ESI): m/z Calculated for $C_{13}H_{25}BO_2$ $[M]^+$: 224.1948, found 224.1946.



26

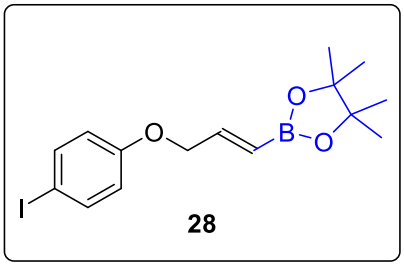
(*E*)-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)but-3-en-1-ol: Purification by silica gel column chromatography, eluent: Pentane/EtOAc = 120:1. Yield: 75% (29.7 mg), E/Z = 99:1. Pale yellow oil. ^{1}H NMR (300 MHz, C_6D_6): δ 6.92-6.82 (m, 1H), 5.76 (d, *J* = 18 Hz, 1H), 3.42 (t, *J* = 6.4 Hz, 2H), 2.24-2.17 (m, 2H), 1.90 (s, 1H) 1.08 (s, 12H). ^{13}C NMR (75.5 MHz, C_6D_6): δ 151.2, 82.9, 61.2, 39.5, 24.8. The carbon signal attached to B was not observed due to low intensity. ^{11}B NMR (96.3 MHz, C_6D_6): 30.3. IR (ATR): ν_{max} = 3388, 2978, 1639, 1440, 1367, 1317, 1259, 1140 cm^{-1}. HRMS (ESI): m/z Calculated for $C_{10}H_{20}BO_3$ $[M+H]^+$: 199.1789, found 199.1800.



27

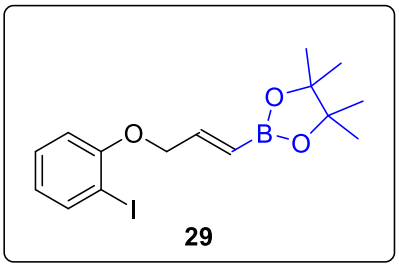
(*E*)-9-(2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)vinyl)-9H-fluoren-9-ol: Purification by

silica gel column chromatography, eluent: Pentane/EtOAc = 80:1. Yield: 75% (48.1 mg), E/Z = 99:1. Yellow oil. ^{1}H NMR (300 MHz, C_6D_6): δ 7.35 (m, 4H), 7.12-7.08 (m, 2H), 7.02-6.96 (m, 3H), 6.49 (d, *J* = 18 Hz, 1H), 1.88 (s, 1H), 0.98 (s, 12H). ^{13}C NMR (75.5 MHz, C_6D_6): δ 153.8, 148.6, 139.9, 129.0, 128.2, 125.1, 120.0, 83.4, 83.0, 24.7. The carbon signal attached to B was not observed due to low intensity. ^{11}B NMR (96.3 MHz, C_6D_6): 30.0. IR (ATR): ν_{max} = 3388, 2978, 1639, 1440, 1367, 1317, 1259, 1140, 975, 869, 583 cm^{-1}. HRMS (ESI): m/z Calculated for $C_{10}H_{20}BO_3$ $[M+H]^+$: 199.1789, found 199.1800.



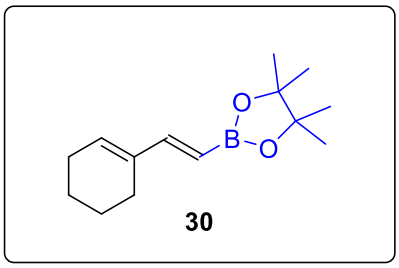
28

(*E*)-2-(3-(4-iodophenoxy)prop-1-en-1-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane: Purification by silica gel column chromatography, eluent: Pentane/EtOAc = 50:1. Yield: 92% (71.0 mg), E/Z = 99:1. Colorless oil. ^{1}H NMR (300 MHz, C_6D_6): δ 7.29 (d, *J* = 9 Hz, 2H), 6.87-6.80 (m, 1H), 6.28 (d, *J* = 9 Hz, 2H), 6.00 (d, *J* = 18 Hz, 1H), 4.00 (m, 2H), 1.06 (s, 12H). ^{13}C NMR (75.5 MHz, C_6D_6): δ 158.7, 147.4, 138.4, 117.3, 83.3, 83.1, 69.1, 24.9. The carbon signal attached to B was not observed due to low intensity. ^{11}B NMR (96.3 MHz, C_6D_6): 29.8. IR (ATR): ν_{max} = 2980, 1625, 1487, 1140, 1067, 1006, 734, 490 cm^{-1}. HRMS (ESI): m/z Calculated for $C_{15}H_{20}BINO_3$ $[M]^+$: 386.0550, found 386.0559.



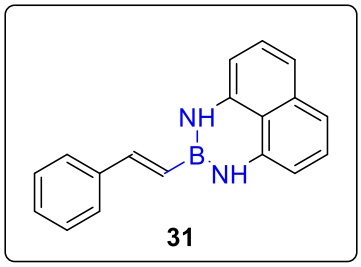
29

(*E*)-2-(3-(2-iodophenoxy)prop-1-en-1-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane: Purification by silica gel column chromatography, eluent: Pentane/EtOAc = 50:1. Yield: 90% (69.5 mg), E/Z = 99:1. Colorless oil. ^{1}H NMR (300 MHz, C_6D_6): δ 7.64 (d, *J* = 9 Hz, 1H), 6.90-6.82 (m, 2H), 6.36-6.18 (m, 3H), 4.08-4.03 (m, 2H), 1.07 (s, 12H). ^{13}C NMR (75.5 MHz, C_6D_6): δ 157.4, 147.0, 139.8, 129.3, 122.6, 112.4, 86.9, 83.2, 69.9, 24.9. The carbon signal attached to B was not observed due to low intensity. ^{11}B NMR (96.3 MHz, C_6D_6): 29.9. IR (ATR): ν_{max} = 2980, 1625, 1487, 1140, 1067, 1006, 734, 490 cm^{-1}. HRMS (ESI): m/z Calculated for $C_{15}H_{20}BINO_3$ $[M]^+$: 386.0550, found 386.0553.



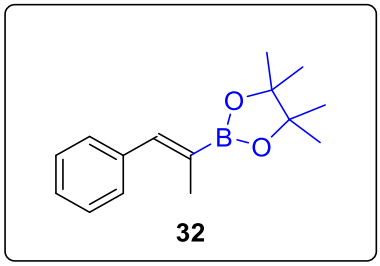
30

(*E*)-2-(2-(cyclohex-1-en-1-yl)vinyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane: Purification by silica gel column chromatography, eluent: Pentane/EtOAc = 200:1. Yield: 80% (37.5 mg), E/Z = 99:1. Colorless oil. ^{1}H NMR (300 MHz, C_6D_6): δ 7.43 (d, *J* = 9 Hz, 1H), 5.79-5.73 (m, 2H), 2.06 (m, 2H), 1.87-1.86 (m, 2H), 1.43-1.26 (m, 6H), 1.11 (s, 12H), 0.89-0.82 (m, 2H). ^{13}C NMR (75.5 MHz, C_6D_6): δ 153.8, 137.5, 133.8, 82.6, 26.4, 24.8, 24.6, 24.4, 24.0. The carbon signal attached to B was not observed due to low intensity. ^{11}B NMR (96.3 MHz, C_6D_6): 29.9. IR (ATR): ν_{max} = 2977, 2927, 2858, 2831, 1628, 1598, 1434, 1370, 1298, 1141, 1107, 1004, 966, 918, 845, 775 cm^{-1}. HRMS (EI): m/z Calculated for $C_{14}H_{23}BO_2$ $[M+H]^+$: 235.1866, found 235.1871.



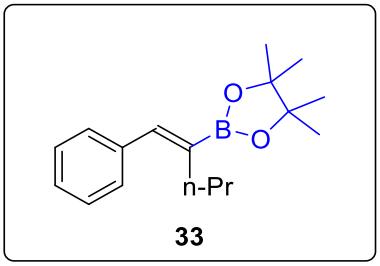
31

(*E*)-2-styryl-2,3-dihydro-1H-naphtho[1,8-de][1,3,2]diazaborinine: Purification by silica gel column chromatography, eluent: DCM/MeOH 100:1. Yield: 91% (49.1 mg), E/Z = 99:1. Orange oil. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.53 (m, 2H), 7.42-7.33 (m, 3H), 7.18-7.04 (m, 5H), 6.39-6.29 (m, 3H), 5.86 (s, 2H). ^{13}C NMR (75.5 MHz, C_6D_6): δ 143.7, 141.2, 137.6, 136.4, 128.7 (2), 127.6, 126.8, 119.9, 117.6, 105.8. The carbon signal attached to B was not observed due to low intensity. ^{11}B NMR (96.3 MHz, C_6D_6): δ 27.5. IR (ATR): ν_{max} = 3410, 1556, 1436, 1142, 981, 825, 750 cm^{-1}. HRMS (EI): m/z Calculated for $C_{18}H_{15}BN_2$ $[M]^+$: 270.1322, found 270.1330.



32

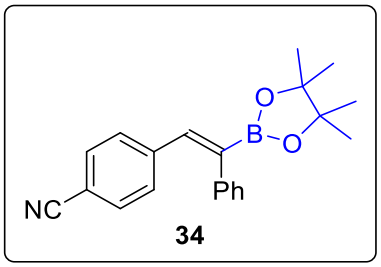
(*Z*)-4,4,5,5-tetramethyl-2-(1-phenylprop-1-en-2-yl)-1,3,2-dioxaborolane: Purification by silica gel column chromatography, eluent: Pentane/EtOAc = 120:1. Yield: 81% (40.0 mg), E/Z = 99:1. Colorless oil. ^{1}H NMR (300 MHz, C_6D_6): δ 7.77 (s, 1H), 7.38 (d, *J* = 7.4 Hz, 2H), 7.20-7.13 (m, 2H), 7.08-7.03 (m, 1H), 2.22 (d, *J* = 1.5 Hz, 3H), 1.15 (s, 12H). ^{13}C NMR (75.5 MHz, C_6D_6): δ 143.1, 138.1, 129.4, 128.1, 127.1, 83.1, 24.6, 15.9. The carbon signal attached to B was not observed due to low intensity. ^{11}B NMR (96.3 MHz, C_6D_6): 30.8. IR (ATR): ν_{max} = 2977, 1616, 1384, 1369, 1310, 1145, 1035, 865, 752, 699, 668 cm^{-1}. HRMS (EI): m/z Calculated for $C_{15}H_{21}BO_2$ $[M]^+$: 244.1635, found 244.1641.



33

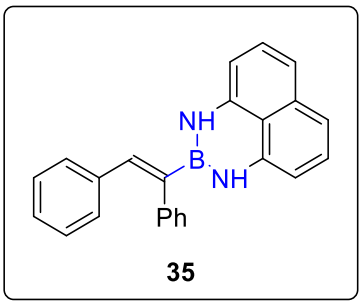
(*Z*)-4,4,5,5-tetramethyl-2-(1-phenylpent-1-en-2-yl)-1,3,2-

dioxaborolane: Purification by silica gel column chromatography, eluent: Pentane/EtOAc = 120:1. Yield: 89% (48.4 mg), E/Z = 1:99. Colorless oil. ^{1}H NMR (300 MHz, C_6D_6): δ 7.82 (s, 1H), 7.40 (d, *J* = 7.5 Hz, 2H), 7.21-7.16 (m, 2H), 7.10-7.05 (m, 1H), 2.71 (t, *J* = 7.8 Hz, 2H), 1.88-1.75 (m, 2H), 1.17 (s, 12H), 1.01 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (75.5 MHz, C_6D_6): δ 142.8, 138.2, 129.0, 128.2, 127.0, 83.0, 31.7, 24.6, 23.5, 14.2. The carbon signal attached to B was not observed due to low intensity. ^{11}B NMR (96.3 MHz, C_6D_6): 31.1. IR (ATR): ν_{max} = 2977, 2871, 1615, 1493, 1405, 1374, 1351, 1310, 1270, 1231, 1146 cm^{-1}. HRMS (ESI): m/z Calculated for $C_{17}H_{25}BO_2$ $[M]^+$: 272.1948, found 272.1950.



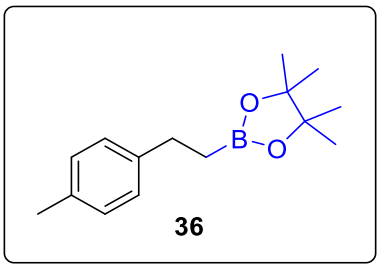
34

(*Z*)-4-(2-phenyl-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)vinyl)benzonitrile: Purification by silica gel column chromatography, eluent: Pentane/EtOAc = 120:1. Yield: 88% (58.3 mg), E/Z = 1:99. White solid, mp: 102-104 ºC (Pentane/EtOAc). ^{1}H NMR (300 MHz, C_6D_6): δ 7.54 (s, 1H), 7.25-7.22 (m, 2H), 7.12-7.08 (m, 2H), 7.03-7.00 (m, 1H), 6.74-6.65 (m, 4H), 1.06 (s, 12H). ^{13}C NMR (75.5 MHz, C_6D_6): δ 141.7, 141.1, 139.9, 131.6, 130.2, 128.9, 128.7, 127.0, 118.6, 111.4, 84.0, 24.7. The carbon signal attached to B was not observed due to low intensity. ^{11}B NMR (96.3 MHz, C_6D_6): 30.4. These spectroscopic data match those previously reported. IR (ATR): ν_{max} = 2978, 2956, 2250, 1601, 1302, 1140, 982, 849, 708 cm^{-1}. HRMS (ESI): m/z Calculated for $C_{21}H_{22}BNO_2$ $[M]^+$: 331.1744, found 331.1744.



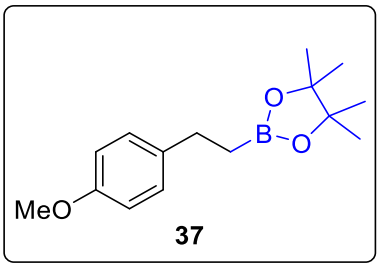
35

(*Z*)-2-(1,2-diphenylvinyl)-2,3-dihydro-1H-naphtho[1,8-de][1,3,2]diazaborinine: Purification by silica gel column chromatography, eluent: DCM/MeOH = 100:1. Yield: 78% (53.9 mg), E/Z = 1:99. Orange oil. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.95-7.89 (m, 4H), 7.60-7.35 (m, 6H), 7.09-6.92 (m, 6H), 6.21 (d, *J* = 7.1 Hz, 1H), 5.61 (s, 1H), 4.20 (s, 1H). ^{13}C NMR (75.5 MHz, C_6D_6): δ 194.6, 141.1, 137.4, 134.9, 133.0, 129.9, 129.5, 129.1, 128.6, 128.1, 127.6, 126.9, 126.8, 117.7, 105.9, 100.0. The carbon signal attached to B was not observed due to low intensity. ^{11}B NMR (96.3 MHz, C_6D_6): δ 28.1. IR (ATR): ν_{max} = 3412, 1556, 1429, 1142, 920, 825, 751 cm^{-1}. HRMS (EI): m/z Calculated for $C_{24}H_{19}BN_2$ $[M]^+$: 346.1641, found 346.1635.



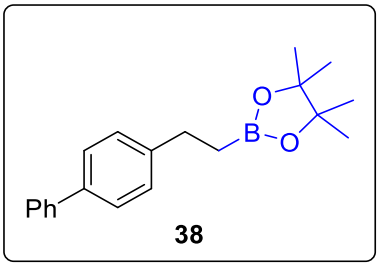
36

4,4,5,5-tetramethyl-2-(4-methylphenethyl)-1,3,2-dioxaborolane: Purification by silica gel column chromatography, eluent: Pentane/EtOAc = 150:1. Yield: 95% (46.8 mg). Colorless oil. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.13 (d, *J* = 8.6 Hz, 2H), 6.81 (d, *J* = 8.6 Hz, 2H), 3.77 (s, 3H), 2.70 (t, *J* = 8.1 Hz, 2H), 1.22 (s, 12H), 1.12 (t, *J* = 8.1 Hz, 2H). ^{13}C NMR (75.5 MHz, $CDCl_3$): δ 141.3, 134.7, 128.8, 127.8, 83.0, 29.4, 24.8, 20.9. The carbon signal attached to B was not observed due to low intensity. ^{11}B NMR (96.3 MHz, $CDCl_3$): 33.9. IR (ATR): ν_{max} = 2978, 2926, 1369, 1319, 1143, 967, 804 cm^{-1}. HRMS (ESI): m/z Calculated for $C_{12}H_{23}BO_2$ $[M]^+$: 246.1791, found 246.1792. These spectroscopic data match those previously reported. [7]



37

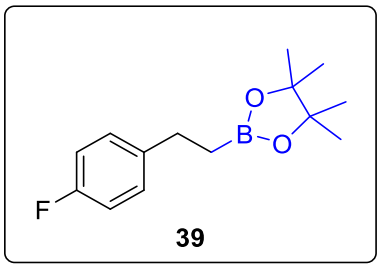
2-(4-methoxyphenethyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane: Purification by silica gel column chromatography, eluent: Pentane/EtOAc = 150:1. Yield: 90% (47.2 mg). Colorless oil. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.13 (d, *J* = 8.5 Hz, 2H), 6.81 (d, *J* = 8.5 Hz, 2H), 3.78 (s, 3H), 2.69 (t, *J* = 8.1 Hz, 2H), 1.22 (s, 12H), 1.11 (t, *J* = 8.1 Hz, 2H). ^{13}C NMR (75.5 MHz, $CDCl_3$): δ 157.6, 136.6, 128.9, 113.6, 83.1, 55.2, 29.1, 24.8. ^{11}B NMR (96.3 MHz, $CDCl_3$): 33.9. IR (ATR): ν_{max} = 2980, 2934, 2360, 1640, 1515, 1455, 1378, 1230, 1146, 968, 839, 680, 546 cm^{-1}. HRMS (EI): m/z Calculated for $C_{15}H_{23}BNaO_3$ $[M+Na]^+$: 286.1632, found 286.1635. These spectroscopic data match those previously reported.[7]



38

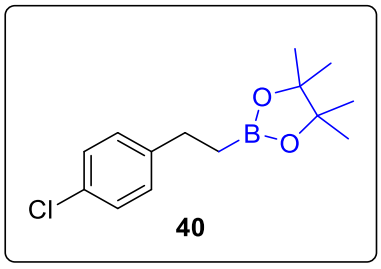
2-(2-([1,1'-biphenyl]-4-yl)ethyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane: Purification by silica gel column chromatography, eluent: Pentane/EtOAc = 80:1. Yield: 97% (59.8 mg). Colorless solid, mp: 54-56 °C (Pentane/EtOAc). ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.62 (d, *J* = 9 Hz, 2H), 7.54 (d, *J* = 9 Hz, 2H), 7.45 (t, *J* = 7.5 Hz, 2H), 7.37-7.32 (m, 3H), 2.83 (t, *J* = 7.5 Hz, 2H), 1.21-1.20 (m, 14H). ^{13}C NMR (75.5 MHz, $CDCl_3$): δ 143.6, 141.3, 138.5, 128.7, 128.5, 127.0, 127.0, 127.0, 83.2, 29.7, 24.9. The carbon signal attached to B was not observed due to low intensity. ^{11}B NMR (96.3 MHz, $CDCl_3$): 33.6. IR (ATR): ν_{max} = 2981, 2923, 1371, 1314, 1140, 830, 762, 698 cm^{-1}. HRMS (EI): m/z

Calculated for $C_{20}H_{25}BO_2$ $[M]^+$: 308.1948, found 308.1950. These spectroscopic data match those previously reported.[8]



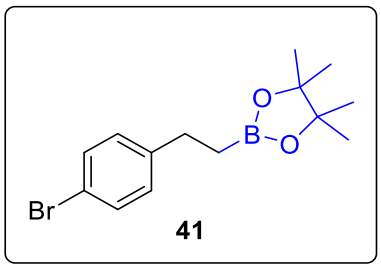
39

2-(4-fluorophenethyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane: Purification by silica gel column chromatography, eluent: Pentane/EtOAc = 120/1). Yield: 90% (45.0 mg). Colorless oil. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.18-7.13 (m, 2H), 6.93 (m, 2H), 2.74 (t, J = 8.0 Hz, 2H), 1.21 (s, 12H), 1.11 (t, J = 8.0 Hz, 2H). ^{13}C NMR (75.5 MHz, $CDCl_3$): δ 161.4 (d, J = 241 Hz), 139.9 (d, J = 3.0 Hz), 129.3 (d, J = 7.7 Hz), 114.8 (d, J = 20.9 Hz), 83.1, 29.2, 24.8. The carbon signal attached to B was not observed due to low intensity. ^{11}B NMR (96.3 MHz, C_6D_6): 33.6. ^{19}F NMR (282.5 MHz, $CDCl_3$): -118.4. IR (ATR): ν_{max} = 2978, 2927, 1370, 1319, 1143, 967, 804 cm^{-1}. HRMS (EI): m/z Calculated for $C_{14}H_{20}BFO_2$ $[M]^+$: 250.1540, found 250.1544. These spectroscopic data match those previously reported.[6]



40

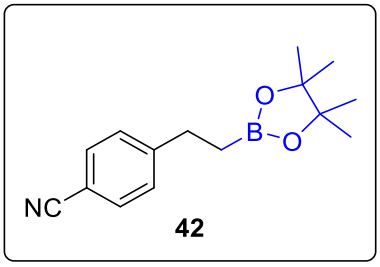
2-(4-chlorophenethyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane: Purification by silica gel column chromatography, eluent: Pentane/EtOAc = 120:1. Yield: 91% (48.3 mg). Colorless oil. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.22 (d, J = 8.4 Hz, 2H), 7.13 (d, J = 8.5 Hz, 2H), 2.71 (t, J = 8.1 Hz, 2H), 1.21 (s, 12H), 1.11 (t, J = 8.1 Hz, 2H). ^{13}C NMR (75.5 MHz, $CDCl_3$): δ 142.8, 131.1, 129.4, 128.2, 83.2, 29.3, 24.8. The carbon signal attached to B was not observed due to low intensity. ^{11}B NMR (96.3 MHz, $CDCl_3$): 33.7. IR (ATR): ν_{max} = 2979, 2931, 1492, 1370, 1316, 1143, 967, 802, 487 cm^{-1}. HRMS (EI): m/z Calculated for $C_{14}H_{20}BClO_2$ $[M]^+$: 266.1245, found 266.1245. These spectroscopic data match those previously reported.[6]



41

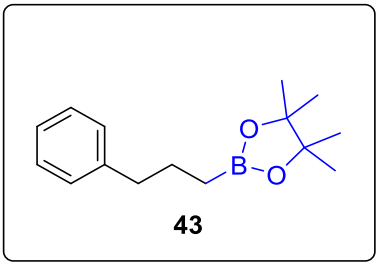
2-(4-bromophenethyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane: Purification by silica gel column chromatography, eluent: Pentane/EtOAc = 120:1. Yield: 95% (58.9 mg). Colorless oil. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.36 (d, J = 8.3 Hz, 2H), 7.08 (d, J = 8.3 Hz, 2H), 2.69 (t, J = 8.1 Hz, 2H), 1.21 (s, 12H), 1.11 (t, J = 8.1 Hz, 2H). ^{13}C NMR (75.5 MHz, $CDCl_3$): δ 143.3, 131.2, 129.8, 119.2,

83.2, 29.4, 24.8. The carbon signal attached to B was not observed due to low intensity. ^{11}B NMR (96.3 MHz, $CDCl_3$): 33.8. IR (ATR): ν_{max} = 2978, 2927, 1488, 1369, 1320, 1140, 1010, 848, 797, 485 cm^{-1}. HRMS (ESI): m/z Calculated for $C_{14}H_{20}BBrO_2$ $[M]^+$: 310.0740, found 310.0741. These spectroscopic data match those previously reported.[9]



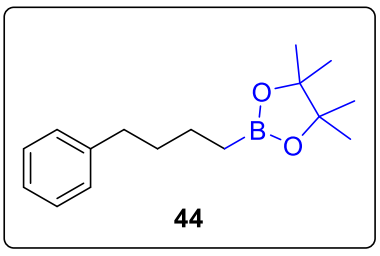
42

4-(2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)ethyl)benzonitrile: Purification by silica gel column chromatography, eluent: Pentane/EtOAc = 80:1. Yield: 99% (50.9 mg). Pale yellow solid; mp: 68-70 ºC (Pentane/EtOAc). ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.52 (d, J = 7.9 Hz, 2H), 7.30 (d, J = 7.9 Hz, 2H), 2.78 (t, J = 8.0 Hz, 2H), 1.19-1.09 (m, 14H). ^{13}C NMR (75.5 MHz, $CDCl_3$): δ 150.0, 132.0, 128.8, 119.2, 109.3, 83.3, 30.1, 24.7. The carbon signal attached to B was not observed due to low intensity. ^{11}B NMR (96.3 MHz, $CDCl_3$): 33.4. IR (ATR): ν_{max} = 2974, 2934, 2361, 2338, 1364, 1276, 1217, 965, 767 cm^{-1}. HRMS (ESI): m/z Calculated for $C_{15}H_{20}BNNaO_2$ $[M+Na]^+$: 280.1479, found 280.1482. These spectroscopic data match those previously reported.[6]



43

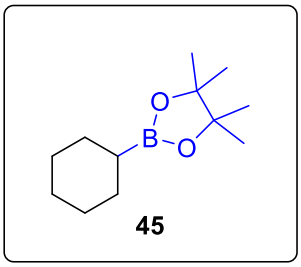
4,4,5,5-tetramethyl-2-(3-phenylpropyl)-1,3,2-dioxaborolane: Purification by silica gel column chromatography, eluent: Pentane/EtOAc = 120:1. Yield: 71% (35.0 mg). Colorless oil. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.32-7.27 (m, 2H), 7.23-7.16 (m, 3H), 2.64 (t, J = 7.5 Hz, 2H), 1.81-1.71 (m, 2H), 1.27 (s, 12H), 0.86 (t, J = 7.5 Hz, 2H). ^{13}C NMR (75.5 MHz, $CDCl_3$): δ 142.7, 128.6, 128.2, 125.6, 82.9, 38.6, 26.1, 24.9. The carbon signal attached to B was not observed due to low intensity. ^{11}B NMR (96.3 MHz, $CDCl_3$): 34.3. IR (ATR): ν_{max} = 2980, 1362, 1306, 1142, 968, 841 cm^{-1}. HRMS (ESI): m/z Calculated for $C_{15}H_{23}BO_2$ $[M]^+$: 246.1791, found 246.1801. These spectroscopic data match those previously reported.[9]



44

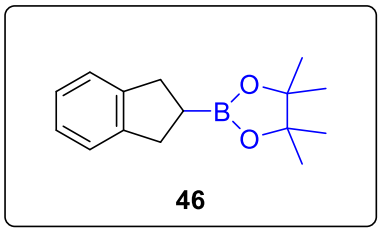
4,4,5,5-tetramethyl-2-(3-phenylpropyl)-1,3,2-dioxaborolane: Purification by silica gel column chromatography, eluent: Pentane/EtOAc = 150:1. Yield: 71% (35.0 mg). Colorless oil. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.29-7.24 (m, 5H), 2.60 (t, J = 7.6 Hz, 2H), 1.66-1.15 (m, 4H), 1.24 (s, 12H),

0.81 (t, J = 7.6 Hz, 2H). ^{13}C NMR (75.5 MHz, $CDCl_3$): δ 142.9, 128.4, 128.2, 125.5, 82.9, 35.8, 34.2, 24.8, 23.8. The carbon signal attached to B was not observed due to low intensity. ^{11}B NMR (96.3 MHz, $CDCl_3$): 33.6. IR (ATR): ν_{max} = 3032, 2956, 1646, 1368, 1247, 1108, 747 cm^{-1}. HRMS (EI): m/z Calculated for $C_{16}H_{25}BO_2$ $[M]^+$: 260.1942, found 260.1948. These spectroscopic data match those previously reported.[9]



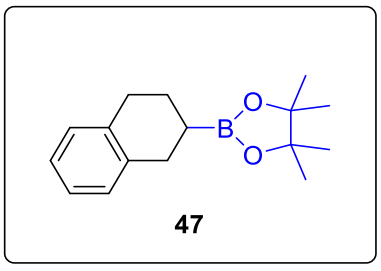
45

2-cyclohexyl-4,4,5,5-tetramethyl-1,3,2-dioxaborolane: Purification by silica gel column chromatography, eluent: Pentane/EtOAc = 150:1. Yield: 43% (18.1 mg). Colorless oil. ^{1}H NMR (300 MHz, $CDCl_3$): δ 1.86-1.58 (m, 6H), 1.30-1.23 (m, 16H), 1.01-0.97 (m, 1H). ^{13}C NMR (75.5 MHz, $CDCl_3$): δ 82.7, 28.0, 27.1, 26.8, 24.8. The carbon signal attached to B was not observed due to low intensity. ^{11}B NMR (96.3 MHz, $CDCl_3$): 33.6. IR (ATR): ν_{max} = 2979, 2928, 2851, 2353, 1415, 1382, 1310, 1258, 1146, 968, 854, 750 cm^{-1}. HRMS (EI): m/z Calculated for $C_{12}H_{23}BO_2$ $[M]^+$: 210.1791, found 210.1792. These spectroscopic data match those previously reported.[10]



46

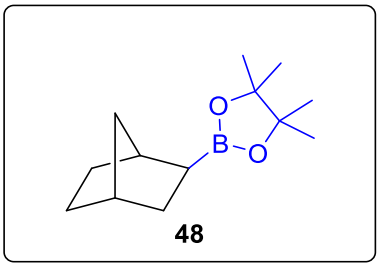
2-(2,3-dihydro-1H-inden-2-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane: Purification by silica gel column chromatography, eluent: Pentane/EtOAc = 150:1. Yield: 60% (29.3 mg). Colorless oil. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.15-7.11 (m, 2H), 7.06-7.01 (m, 2H), 3.03-2.85 (m, 4H), 1.87-1.73 (m, 1H), 1.18 (s, 12H). ^{13}C NMR (75.5 MHz, $CDCl_3$): δ 144.4, 125.8, 124.1, 83.2, 35.1, 24.7. The carbon signal attached to B was not observed due to low intensity. ^{11}B NMR (96.3 MHz, $CDCl_3$): 33.6. IR (ATR): ν_{max} = 2976, 2932, 2845, 1414, 1371, 1314, 1261, 1140, 1108, 970, 856, 740 cm^{-1}. HRMS (ESI): m/z Calculated for $C_{15}H_{21}BO_2$ $[M+H]^+$: 245.1713, found 245.1715. These spectroscopic data match those previously reported.[11]



47

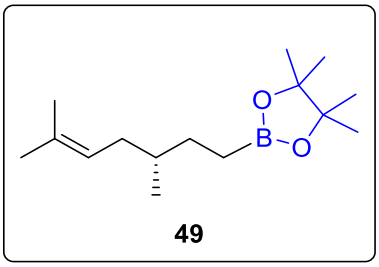
4,4,5,5-tetramethyl-2-(1,2,3,4-tetrahydronaphthalen-2-yl)-1,3,2-dioxaborolane: Purification by silica gel column chromatography, eluent: Pentane/EtOAc = 100:1. Yield: 85% (43.9 mg). Colorless oil. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.19 (m, 4H), 3.05-2.84 (m, 4H), 2.20-2.17 (m, 1H), 1.84-1.75 (m, 1H), 1.53-1.38 (m, 13H). ^{13}C NMR (75.5 MHz, $CDCl_3$): δ 137.1, 136.6, 128.9, 128.7, 125.1,

82.8, 30.5, 29.5, 24.6, 24.6, 24.5. The carbon signal attached to B was not observed due to low intensity. ^{11}B NMR (96.3 MHz, $CDCl_3$): 33.5. IR (ATR): ν_{max} = 2977, 2920, 1382, 1315, 1142, 969, 853, 740 cm^{-1}. HRMS (ESI): m/z Calculated for $C_{16}H_{23}BO_2$ $[M]^+$: 258.1791, found 258.1774. These spectroscopic data match those previously reported.[11]



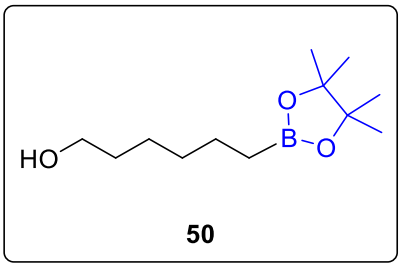
48

2-((1S,4S)-bicyclo[2.2.1]heptan-2-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane: Purification by silica gel column chromatography, eluent: Pentane/EtOAc = 150:1. Yield: 39% (17.3 mg). Colorless oil. ^{1}H NMR (300 MHz, $CDCl_3$): δ 2.24 (m, 2H), 1.58-1.42 (m, 3H), 1.37-1.11 (m, 17H), 0.89-0.84 (m, 1H). ^{13}C NMR (75.5 MHz, $CDCl_3$): δ 82.7, 38.7, 38.1, 36.6, 32.2, 32.2, 29.2, 24.7. The carbon signal attached to B was not observed due to low intensity. ^{11}B NMR (96.3 MHz, $CDCl_3$): 33.6. IR (ATR): ν_{max} = 2946, 2868, 1370, 1308, 1224, 1144, 980, 859 cm^{-1}. HRMS (ESI): m/z Calculated for $C_{13}H_{23}BO_2$ $[M]^+$: 222.1791, found 222.1791. These spectroscopic data match those previously reported.[10]



49

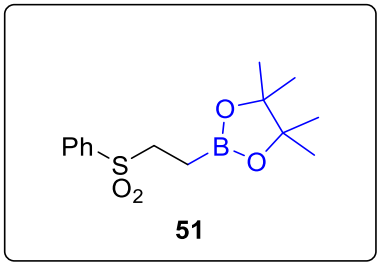
(S)-2-(3,6-dimethylhept-5-en-1-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane: Purification by silica gel column chromatography, eluent: Pentane/EtOAc = 200/1). Yield: 79% (39.8 mg). Colorless oil. ^{1}H NMR (300 MHz, $CDCl_3$): δ 5.11-5.06 (m, 1H), 1.98-1.88 (m, 2H), 1.67 (s, 3H), 1.59 (s, 3H), 1.44-1.39 (m, 1H), 1.24-1.08 (m, 14H), 0.91-0.71 (m, 5H). ^{13}C NMR (75.5 MHz, $CDCl_3$): δ 130.9, 125.1, 82.8, 36.7, 34.6, 30.9, 25.7, 25.6, 24.8, 24.8, 19.1, 17.6. ^{11}B NMR (96.3 MHz, $CDCl_3$): 34.7. IR (ATR): ν_{max} = 2922, 2868, 1370, 1308, 1220, 980, 862 cm^{-1}. HRMS (ESI): m/z Calculated for $C_{15}H_{29}BO_2$ $[M]^+$: 252.2261, found 252.2262.



50

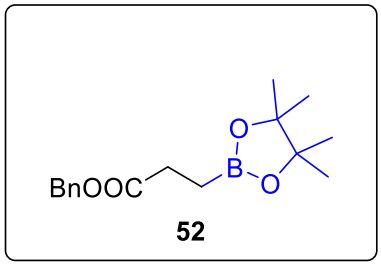
6-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)hexan-1-ol: Purification by silica gel column chromatography, eluent: Pentane/EtOAc = 60:1. Yield: 84% (38.3 mg). Colorless oil. ^{1}H NMR (300 MHz, $CDCl_3$): δ 3.59 (t, J = 6.6 Hz, 2H), 1.55 (s, 1H), 1.42-1.22 (m, 18H), 0.75 (t, J = 7.5 Hz, 2H). ^{13}C NMR (75.5 MHz, $CDCl_3$): δ 82.9, 62.9, 32.6, 32.1, 25.4, 24.8, 23.9. The carbon signal attached

to B was not observed due to low intensity. ^{11}B NMR (96.3 MHz, $CDCl_3$): 33.9. IR (ATR): ν_{max} = 3447, 2928, 2858, 1628, 1459, 1385, 1371, 1325, 1297, 1145 cm^{-1}. HRMS (ESI): m/z Calculated for $C_{12}H_{25}BO_3$ $[M]^+$: 228.1897, found 228.1895. These spectroscopic data match those previously reported.[10]



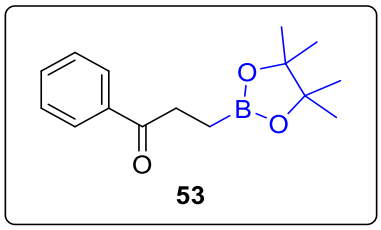
51

4,4,5,5-tetramethyl-2-(2-(phenylsulfonyl)ethyl)-1,3,2-dioxaborolane: Purification by silica gel column chromatography, eluent: Pentane/EtOAc = 80:1. Yield: 95% (56.3 mg). Colorless solid, mp: 62-64 ºC (Pentane/EtOAc). ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.91-7.88 (m, 2H), 7.66-7.51 (m, 3H), 3.19-3.08 (m, 2H), 1.29-1.15 (m, 14H). ^{13}C NMR (75.5 MHz, $CDCl_3$): δ 138.7, 133.5, 129.2, 128.3, 83.9, 52.0, 24.8. The carbon signal attached to B was not observed due to low intensity. ^{11}B NMR (96.3 MHz, $CDCl_3$): 32.7. IR (ATR): ν = 2938, 1448, 1366, 1305, 1142, 1084, 733, 534 cm^{-1}. HRMS (ESI): m/z Calculated for $C_{14}H_{21}BO_4S$ $[M]^+$: 296.1254, found 296.1258. These spectroscopic data match those previously reported.[12]



52

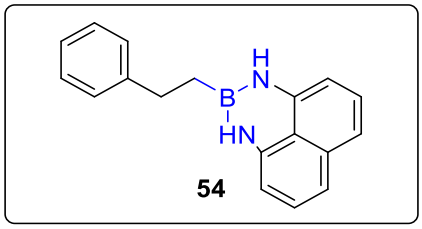
Benzyl 3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)propanoate: Purification by silica gel column chromatography, eluent: Pentane/EtOAc = 100:1. Yield: 83% (48.2 mg). Colorless oil. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.34 (m, 5H), 5.11 (s, 2H), 2.50 (t, J = 7.5 Hz, 2H), 1.22 (s, 12H), 1.05 (t, J = 7.5 Hz, 2H). ^{13}C NMR (75.5 MHz, $CDCl_3$): δ 174.5, 136.2, 128.5, 128.1, 128.1, 83.3, 66.1, 28.4, 24.8. The carbon signal attached to B was not observed due to low intensity. ^{11}B NMR (96.3 MHz, $CDCl_3$): 33.5. IR (ATR): ν_{max} = 2978, 1738, 1381, 1319, 1142, 970, 698 cm^{-1}. HRMS (ESI): m/z Calculated for $C_{16}H_{24}BO_4$ $[M+H]^+$: 291.1755, found 291.1756. These spectroscopic data match those previously reported. [13]



53

1-phenyl-3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)propan-1-one: Purification by silica gel column chromatography, eluent: Pentane/EtOAc = 150:1. Yield: 88% (45.8 mg). Colorless oil. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.97 (d, J = 7.3 Hz, 2H), 7.53 (t, J = 7.3 Hz, 1H), 7.43 (t, J = 7.4 Hz, 2H), 3.15 (t, J = 6.9 Hz, 2H), 1.25 (s, 12H), 1.07 (t, J = 6.9 Hz, 2H). ^{13}C NMR (75.5 MHz, $CDCl_3$):

δ 200.6, 137.0, 132.8, 128.5, 128.0, 83.1, 33.7, 24.8. The carbon signal attached to B was not observed due to low intensity. ^{11}B NMR (96.3 MHz, $CDCl_3$): 33.7. IR (ATR): ν_{max} = 2980, 1684, 1381, 1320, 1421 cm^{-1}. HRMS (EI): m/z Calculated for $C_{15}H_{21}BO_3$ $[M]^+$: 260.1584, found 260.1591. These spectroscopic data match those previously reported.[14]



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2-phenethyl-2,3-dihydro-1H-naphtho[1,8-de][1,3,2]diazaborinine: Purification by silica gel column chromatography, eluent: DCM/MeOH = 100:1. Yield: 95% (54.3 mg). Orange oil. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.25-7.10 (m, 5H), 7.03-6.98 (m, 3H), 6.93-6.90 (m, 2H), 6.16 (d, J = 7.2 Hz, 2H), 5.47 (s, 2H), 2.70 (t, J = 8.1 Hz, 2H), 1.15 (t, J = 8.1 Hz, 2H). ^{13}C NMR (75.5 MHz, $CDCl_3$): δ 143.9, 141.1, 136.3, 128.5, 128.0, 127.6, 125.9, 119.6, 117.5, 105.5, 30.8. The carbon signal attached to B was not observed due to low intensity. ^{11}B NMR (96.3 MHz, $CDCl_3$): 31.5. IR (ATR): ν_{max} = 3402, 2924, 1627, 1600, 1504, 1413, 1374, 1139, 1035 cm^{-1}. HRMS (EI): m/z Calculated for $C_{18}H_{17}BN_2$ $[M]^+$: 272.1485, found 272.1479. These spectroscopic data match those previously reported.[15]

8. References

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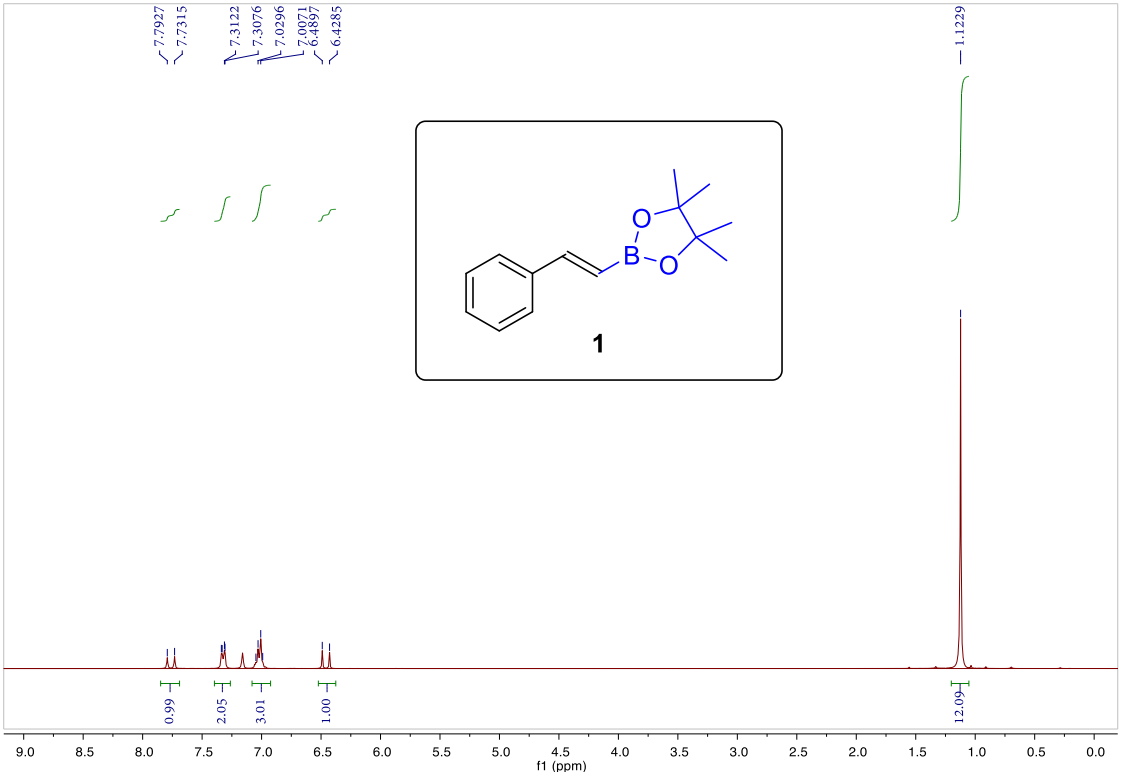
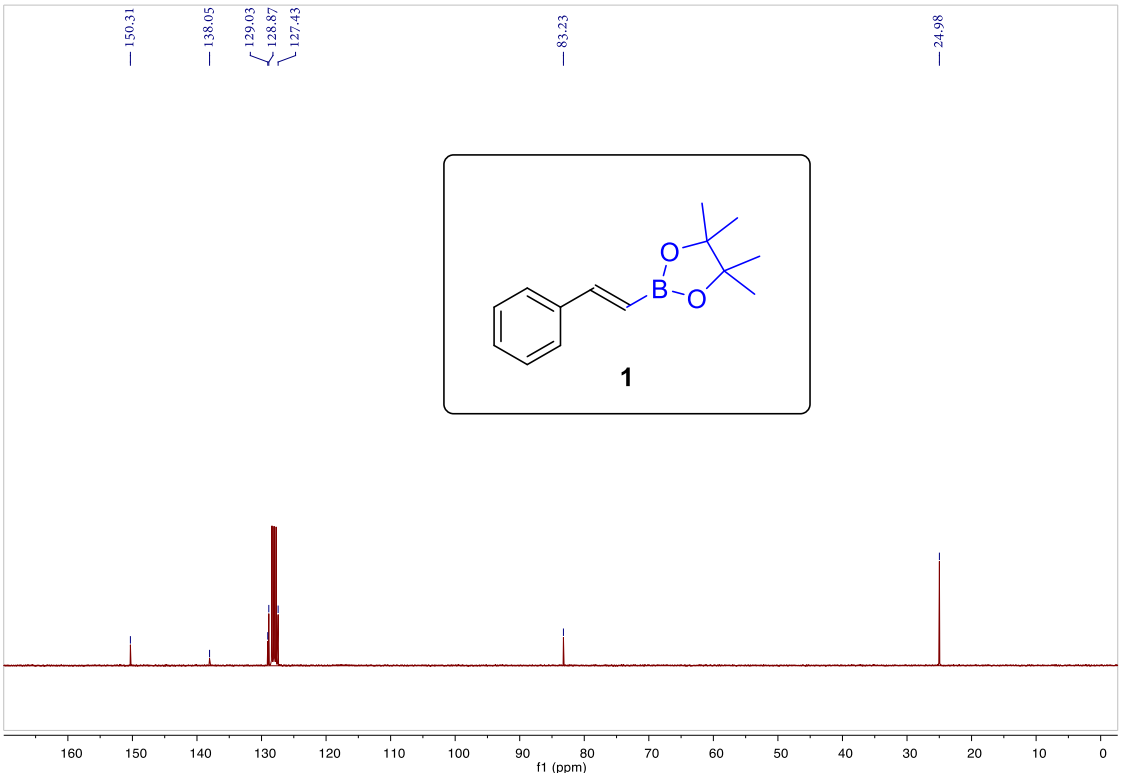
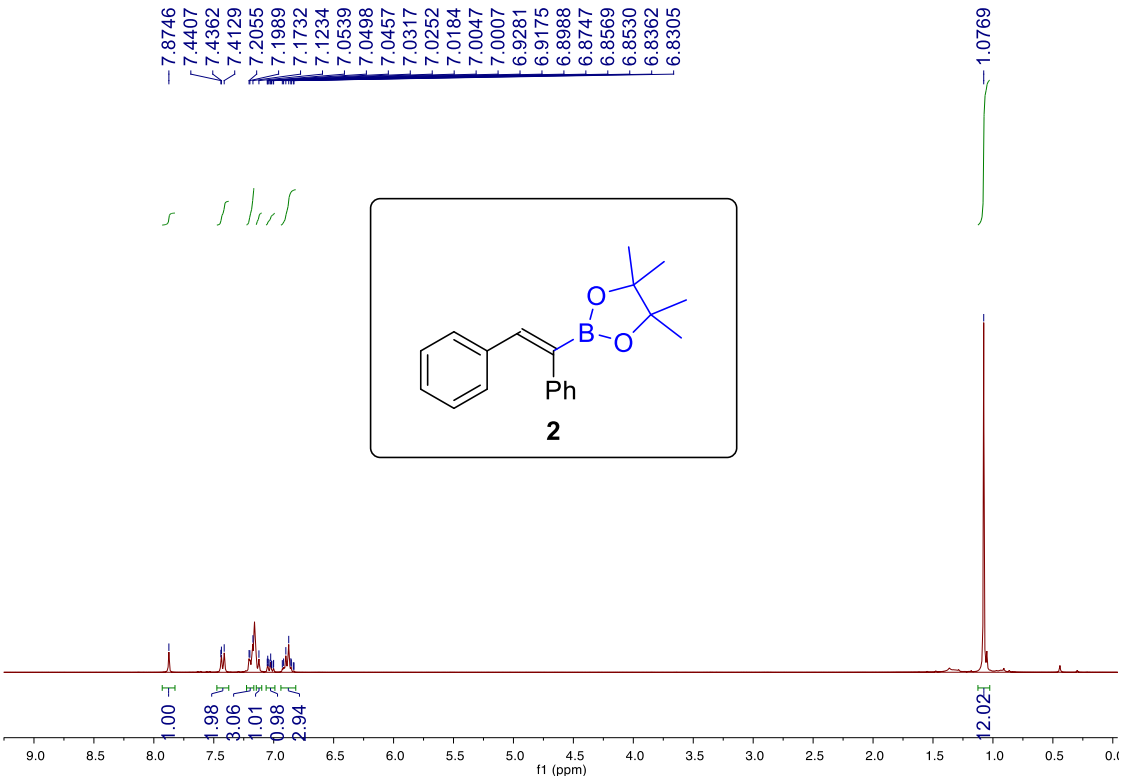
9. NMR spectra



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Ph
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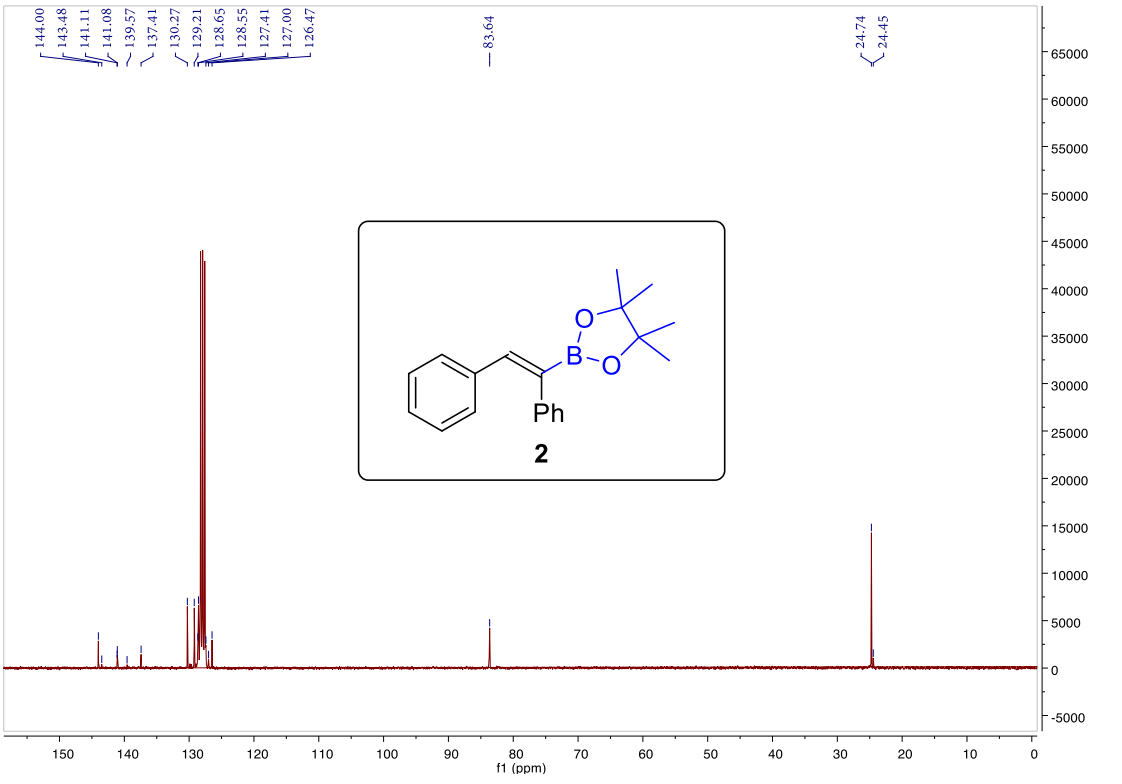
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Ph
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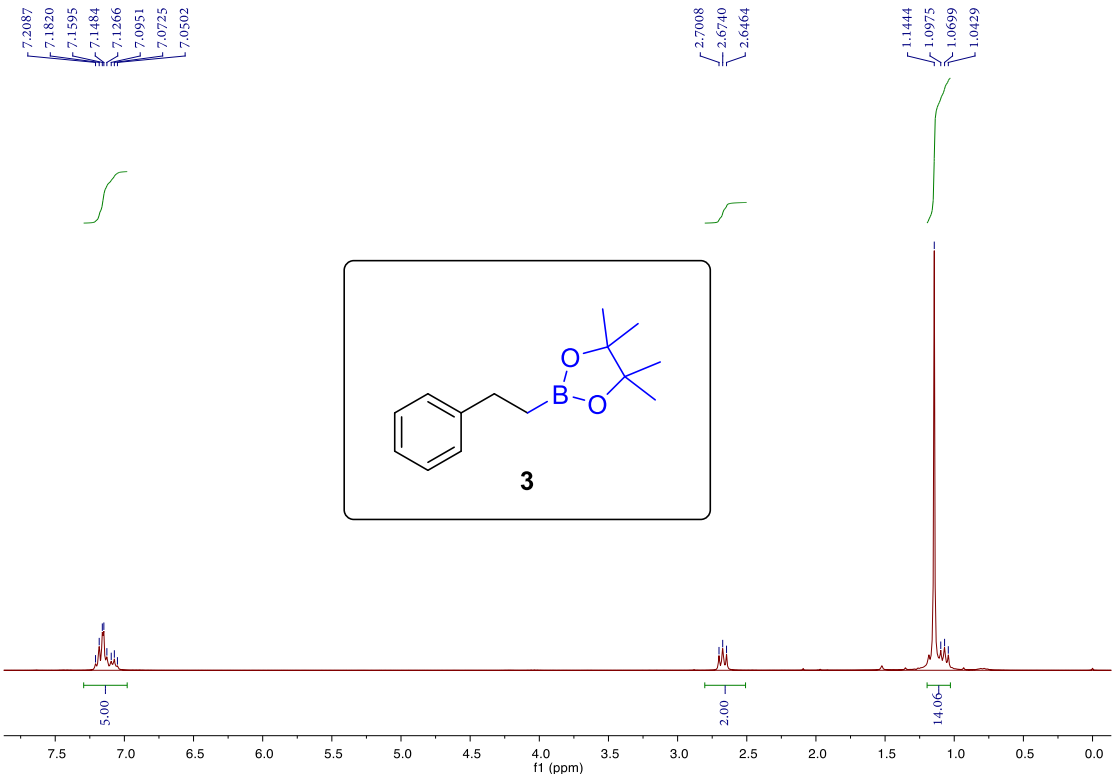
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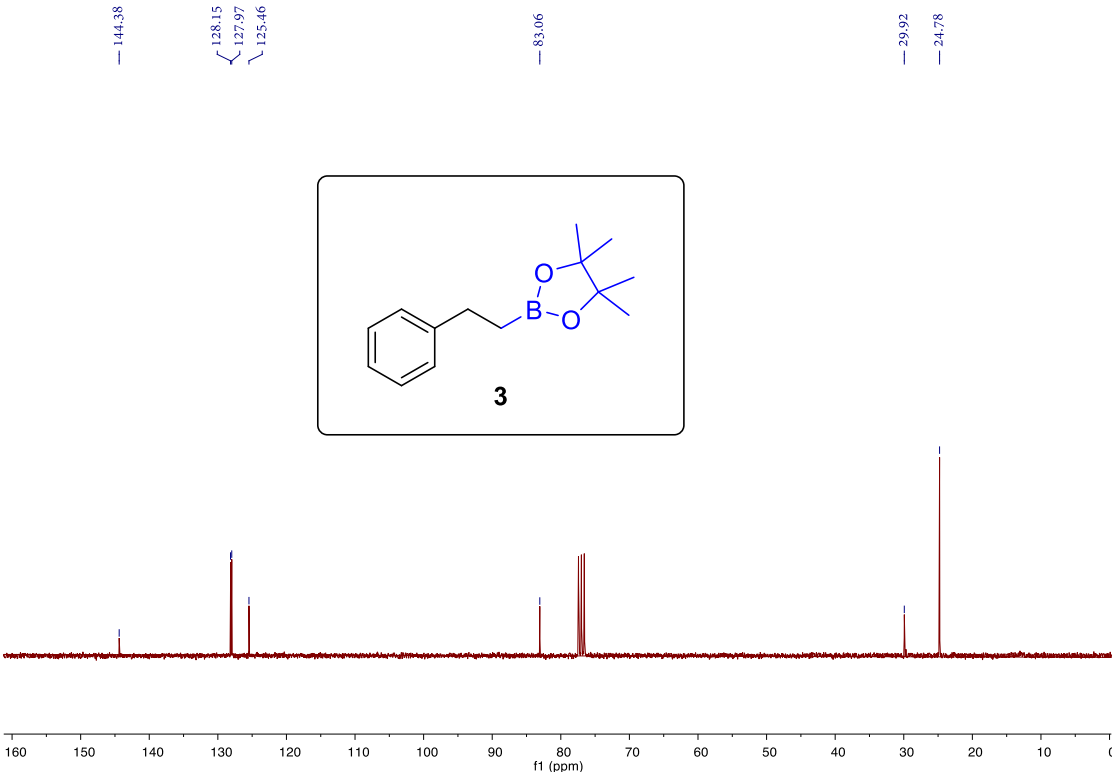
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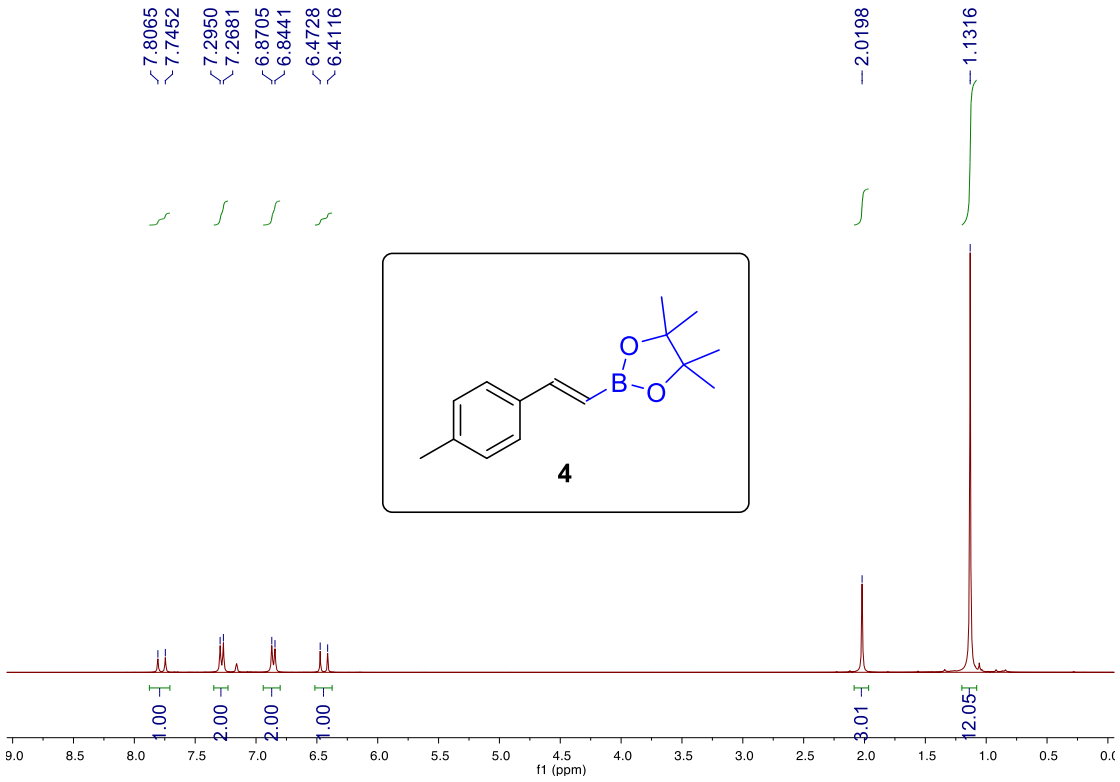
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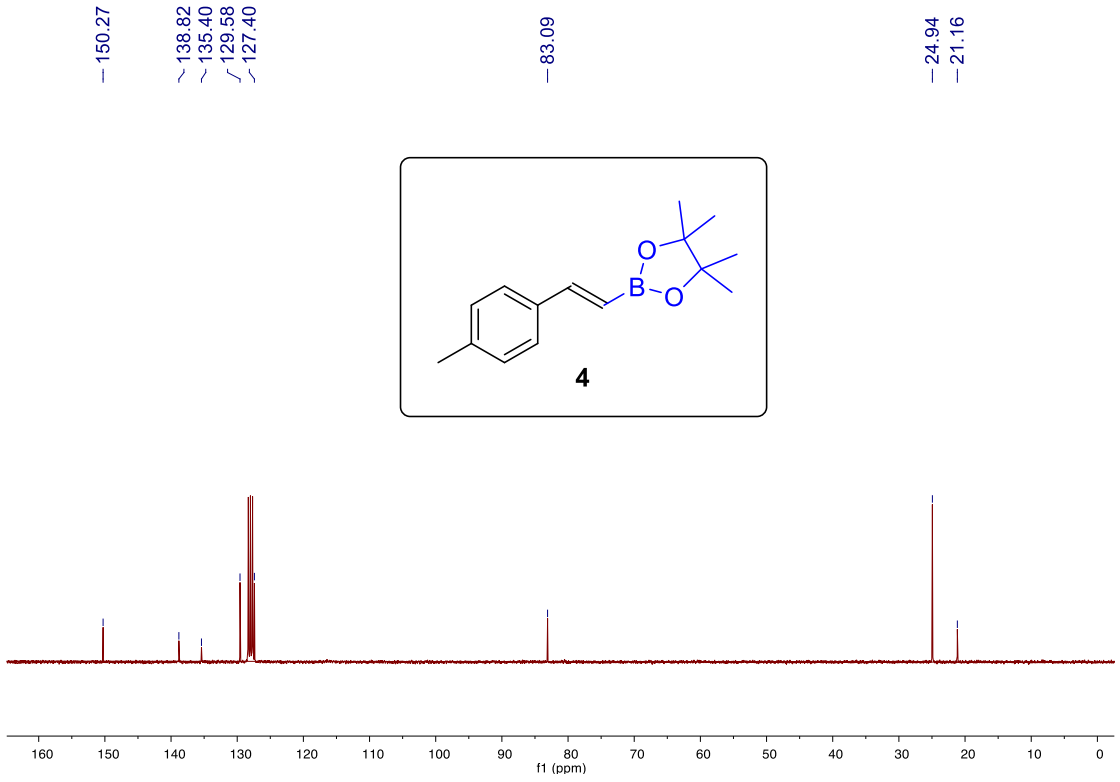
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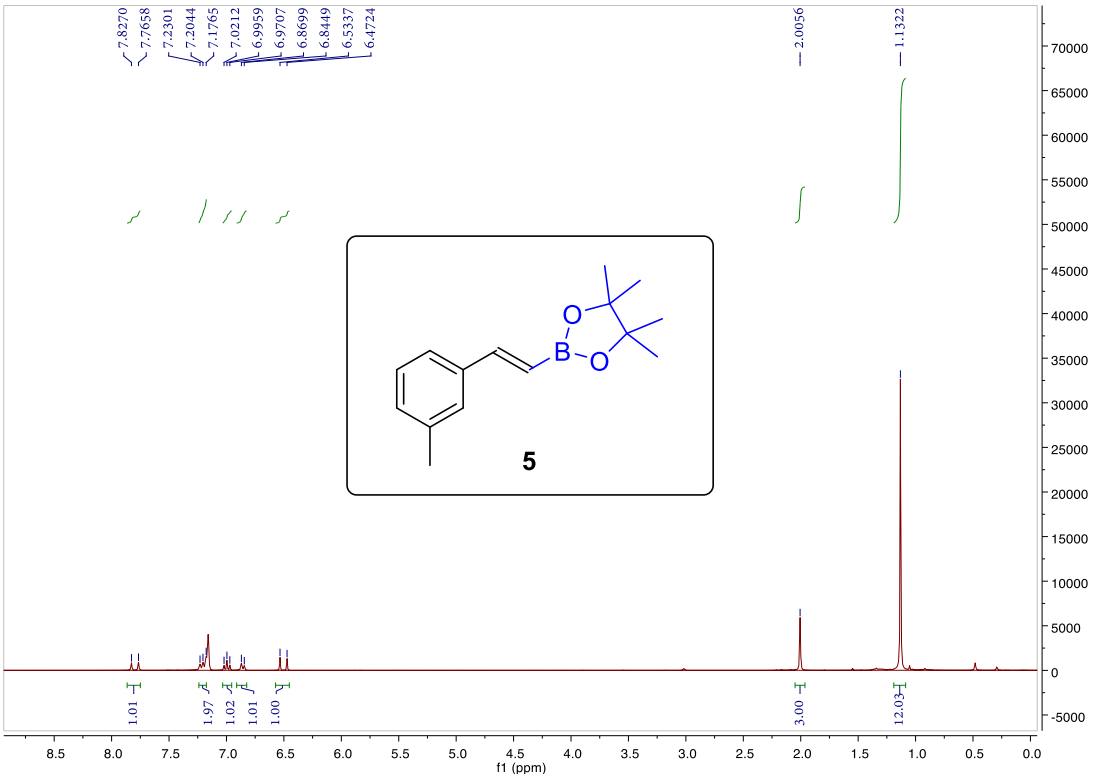
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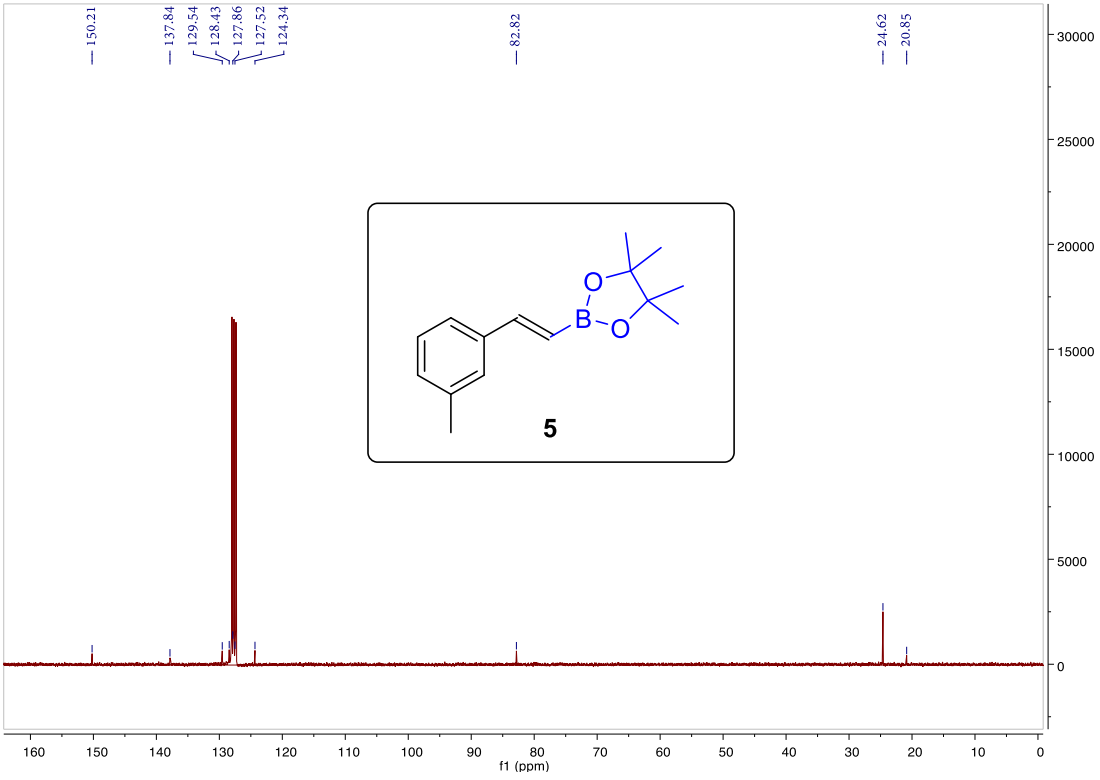
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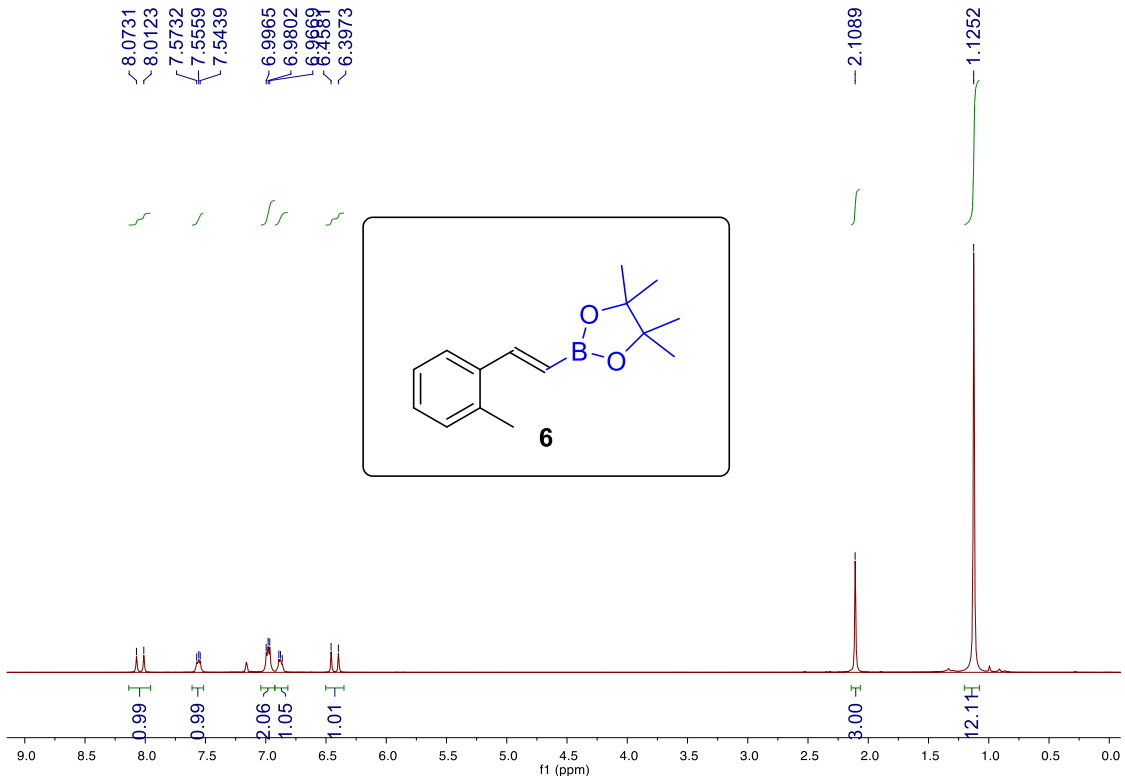
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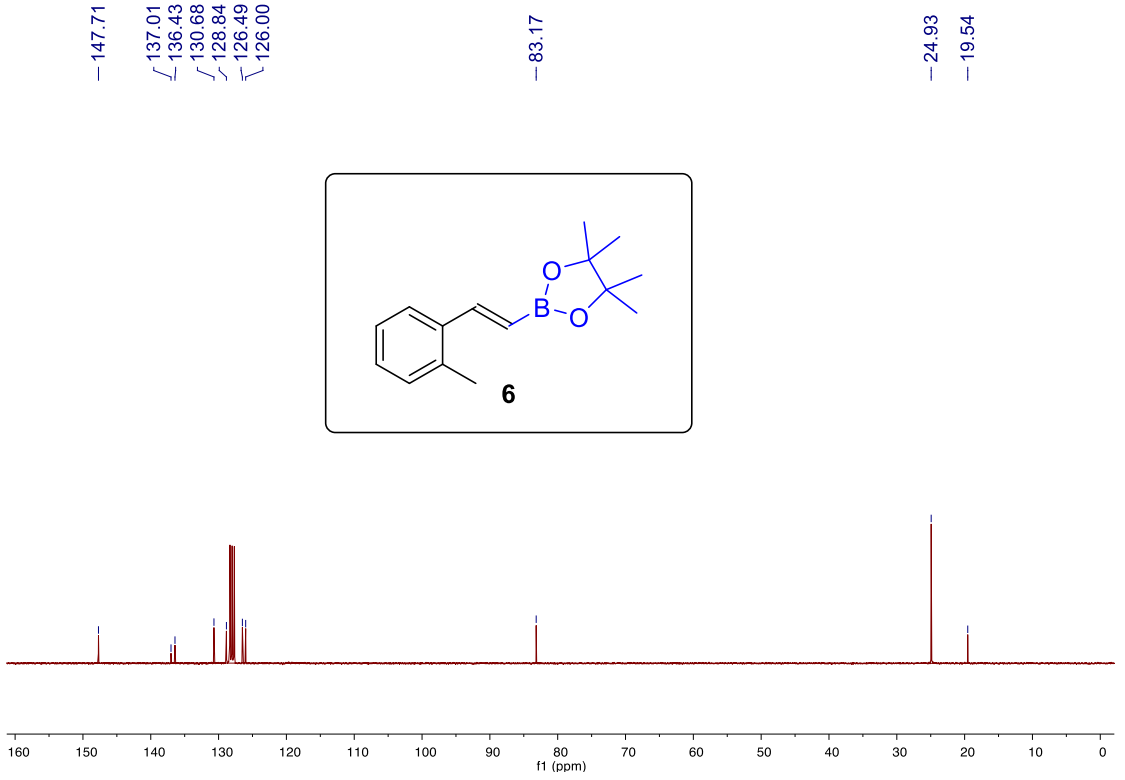
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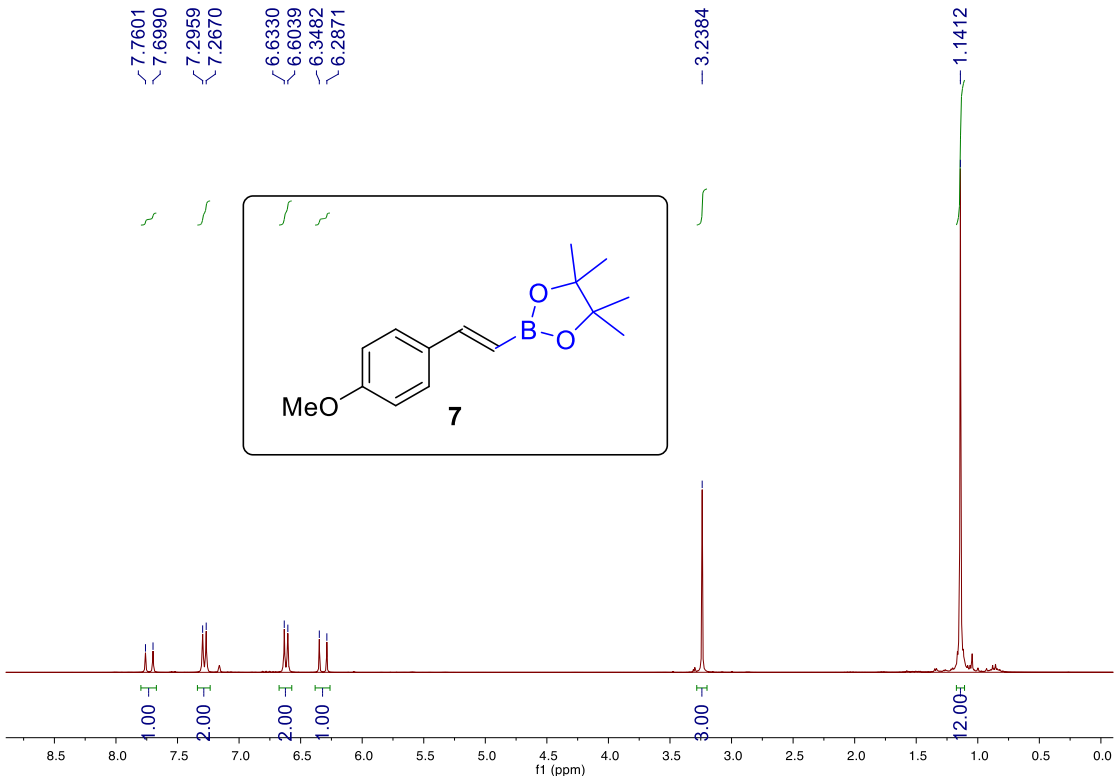
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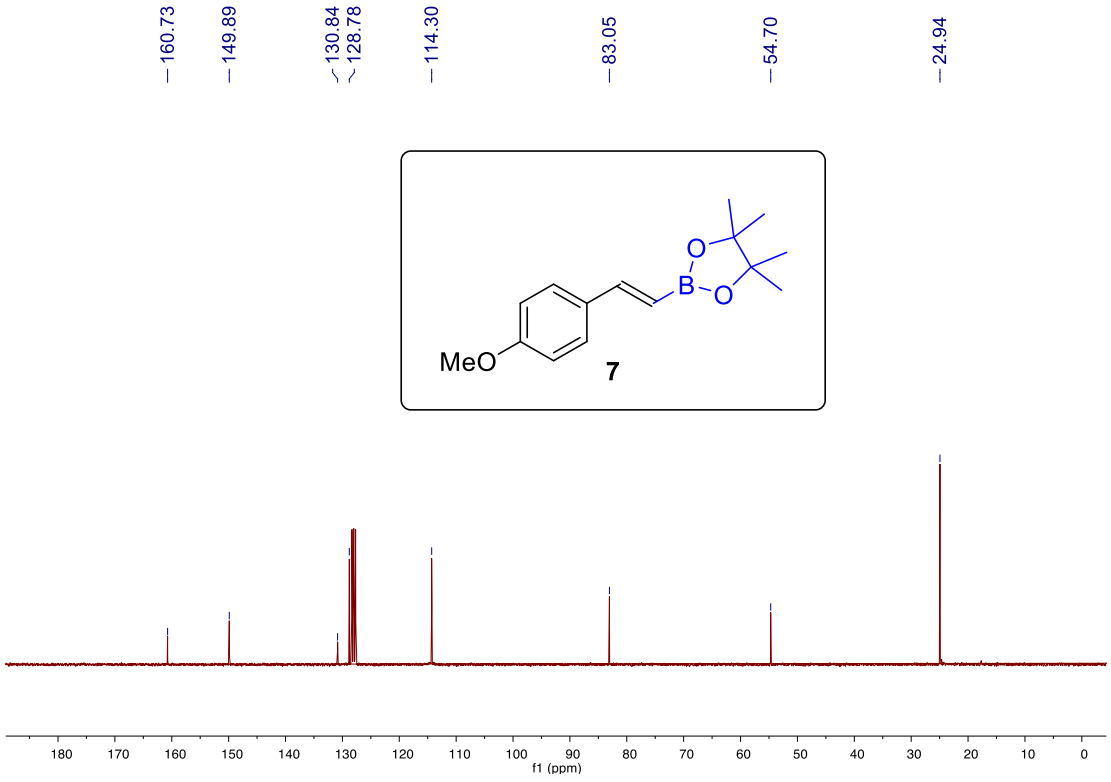
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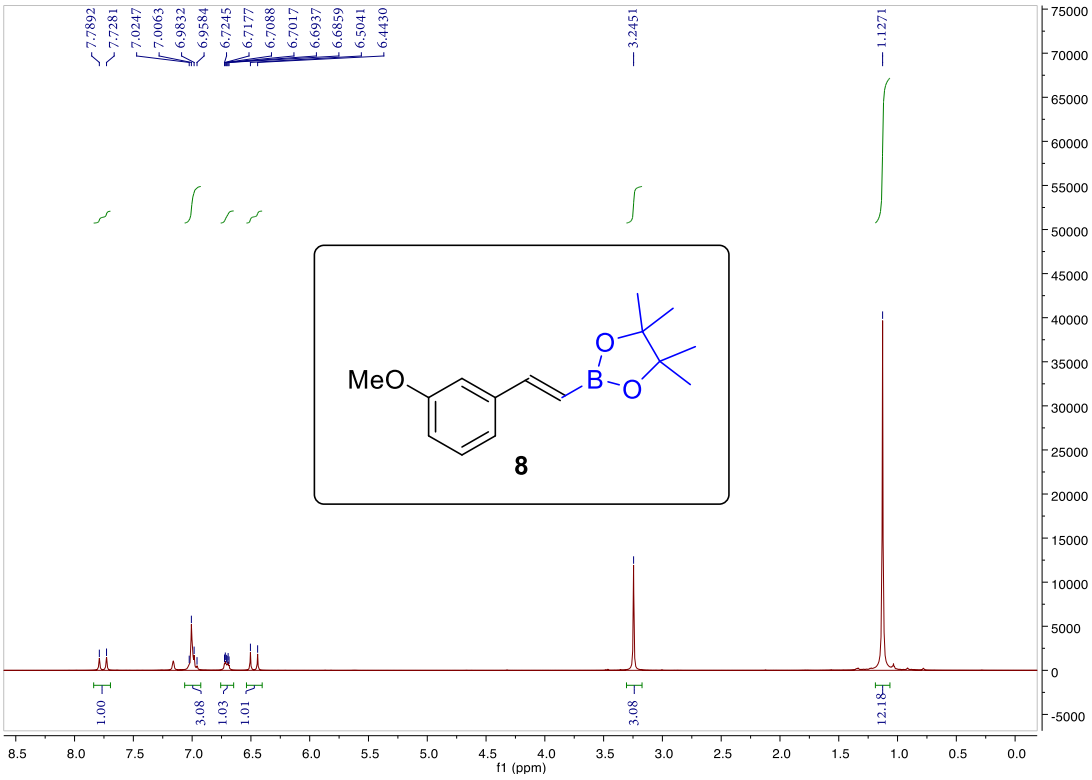
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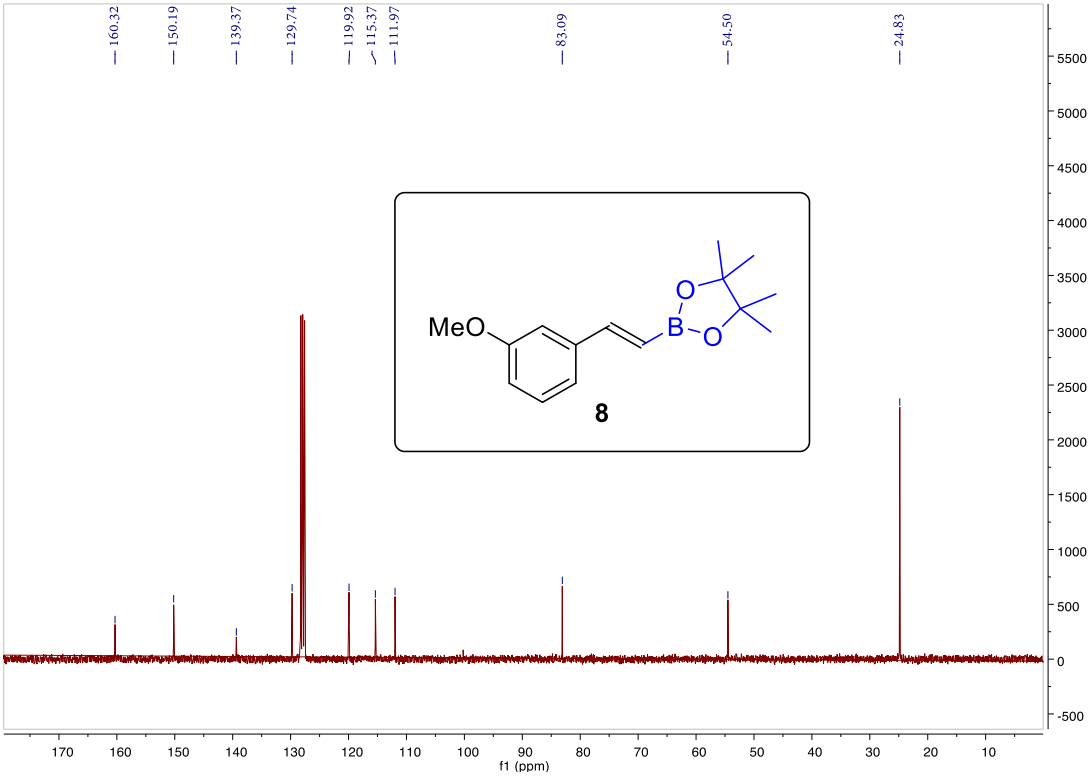
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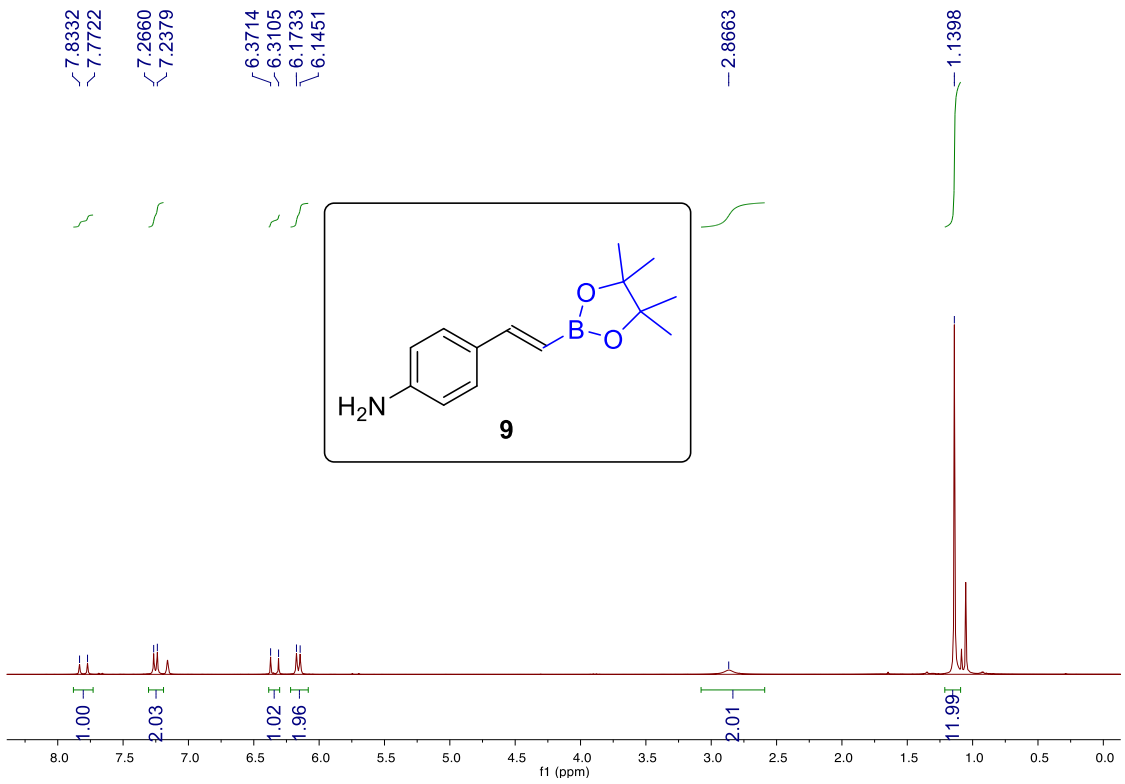
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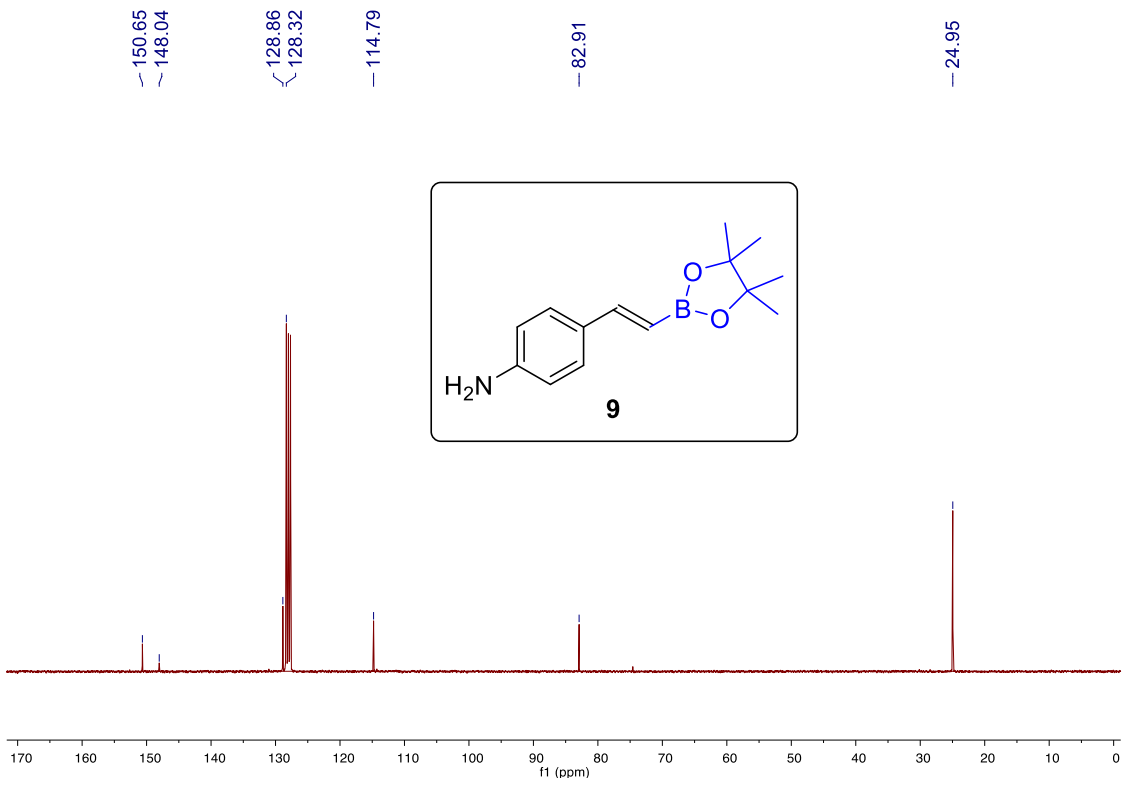
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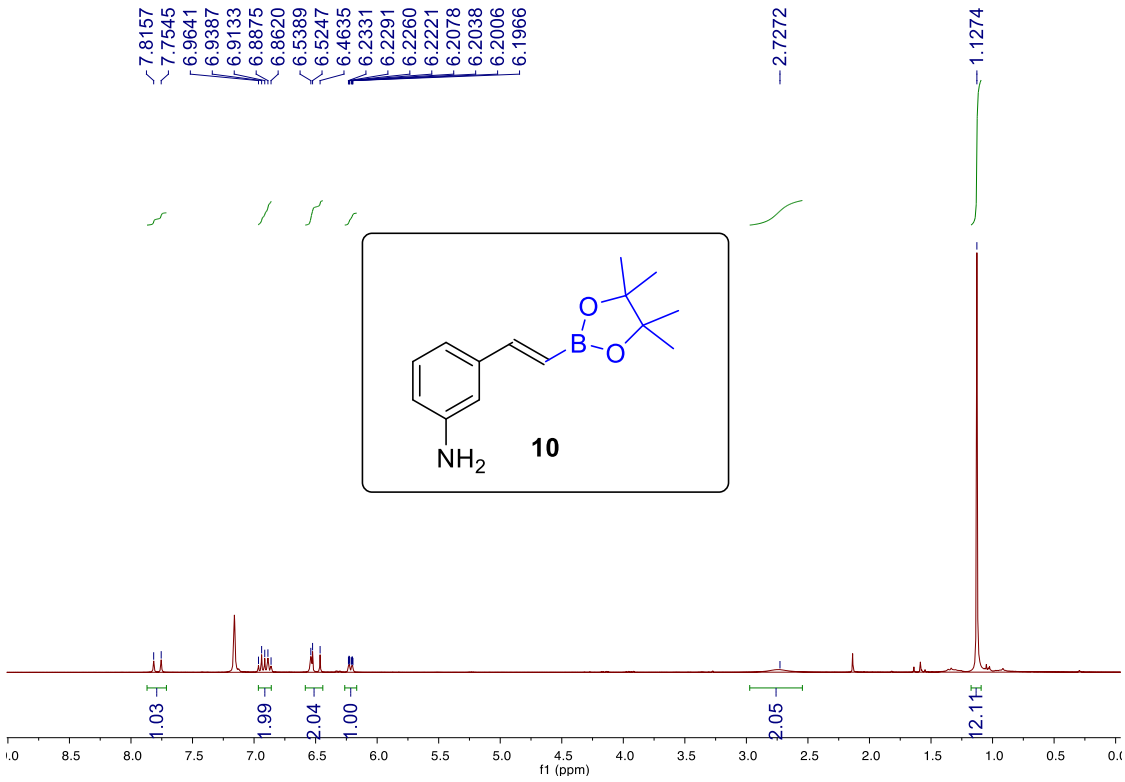
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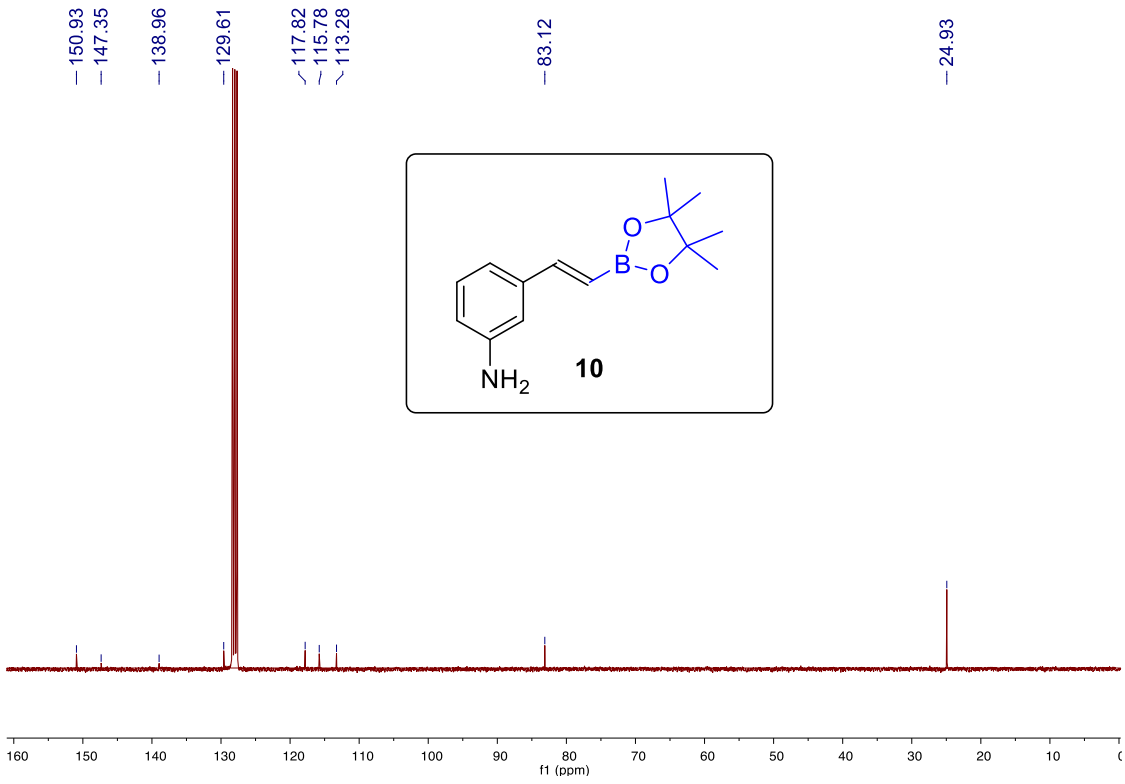
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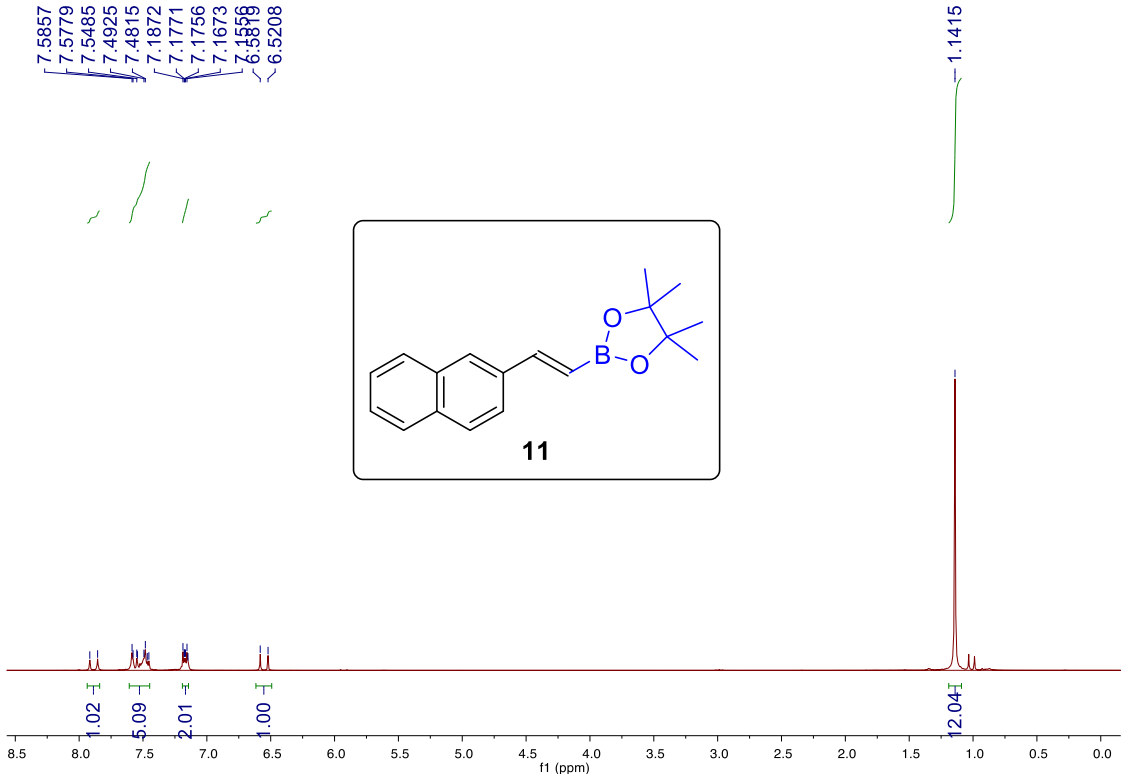
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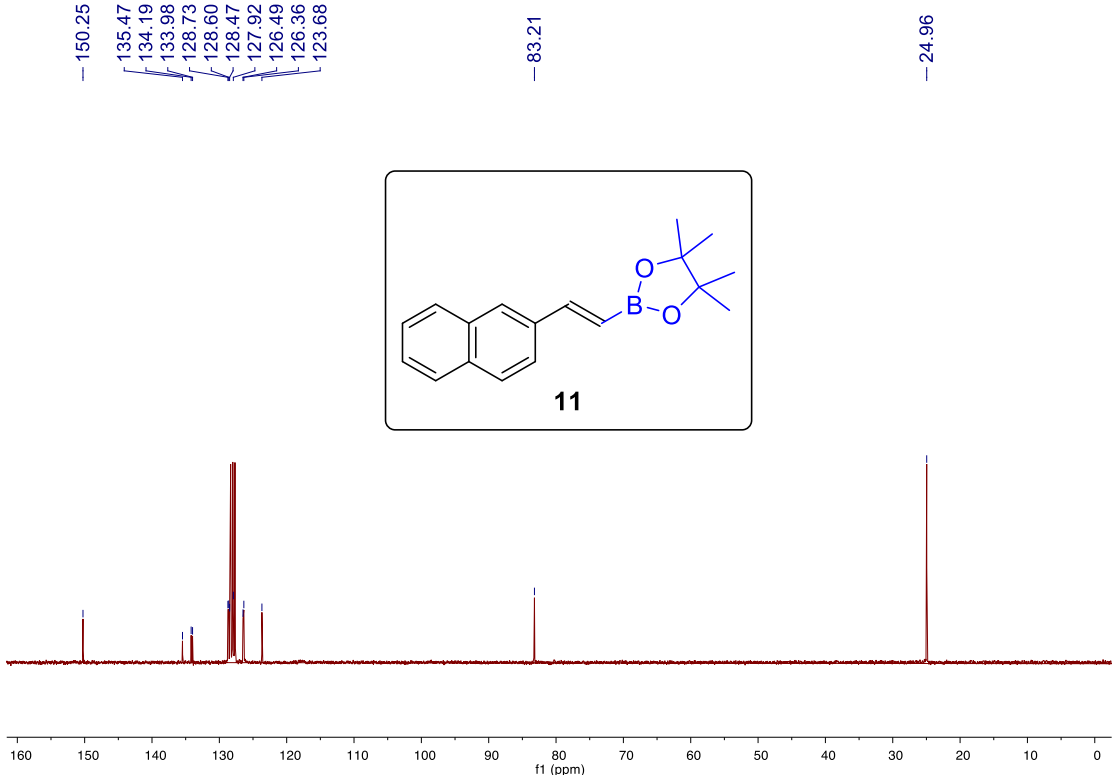
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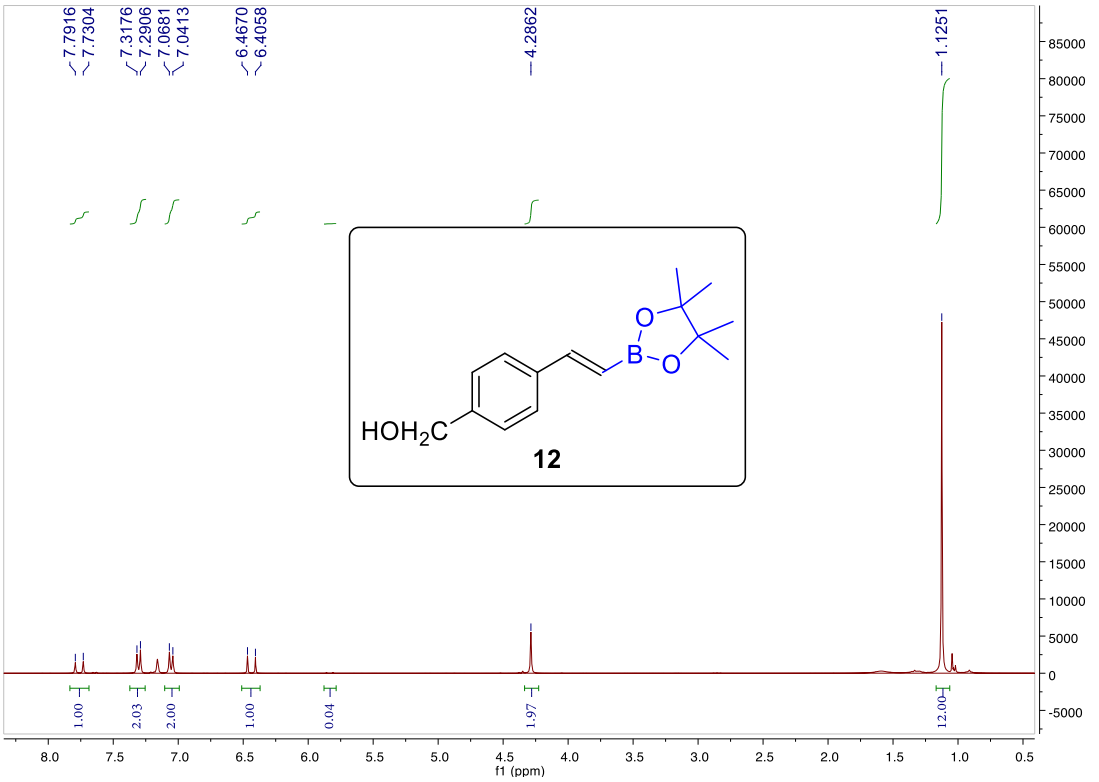
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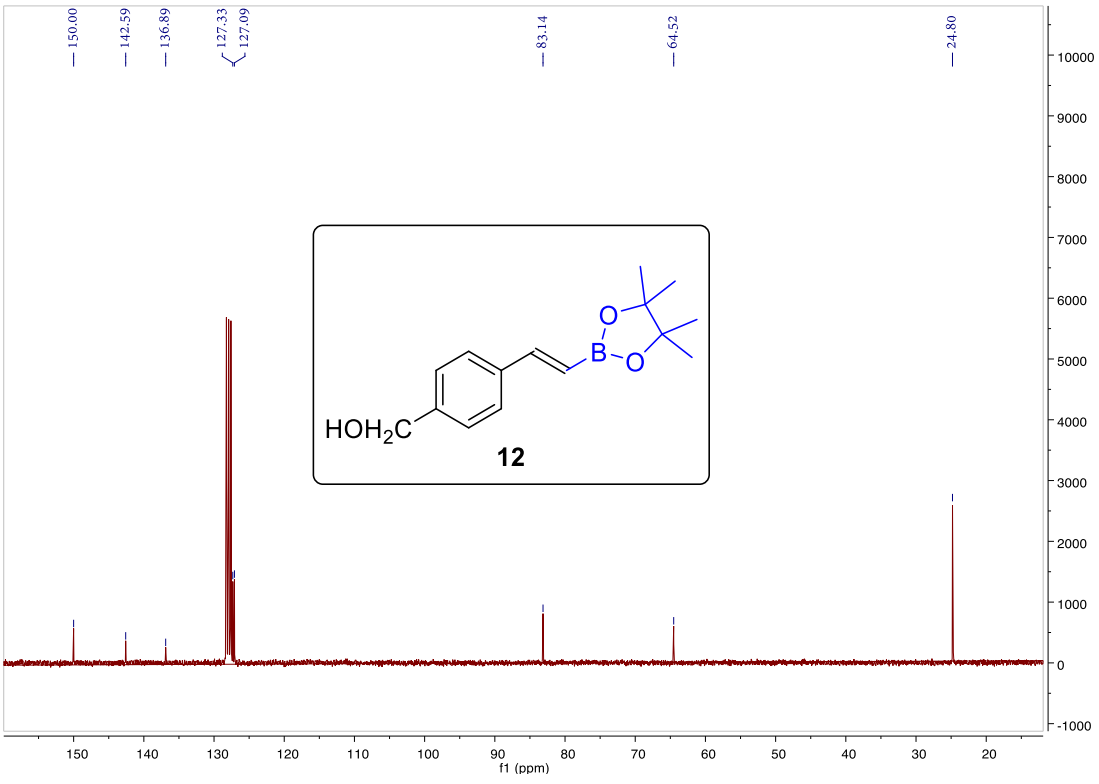
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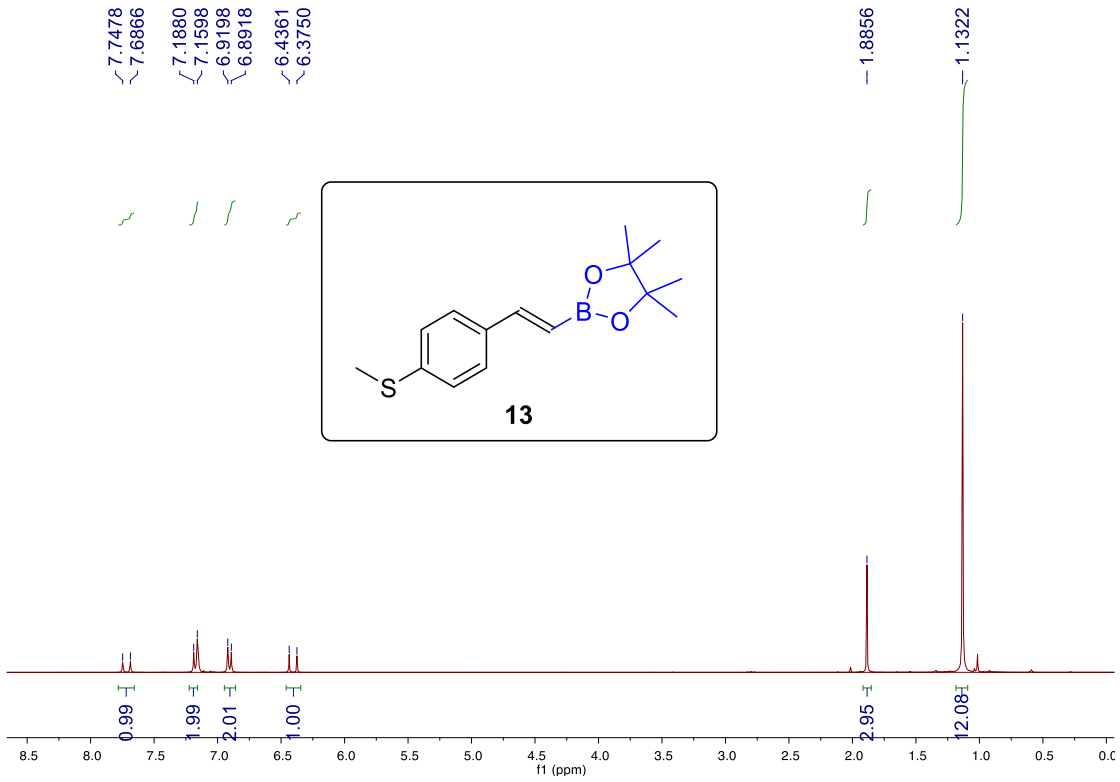
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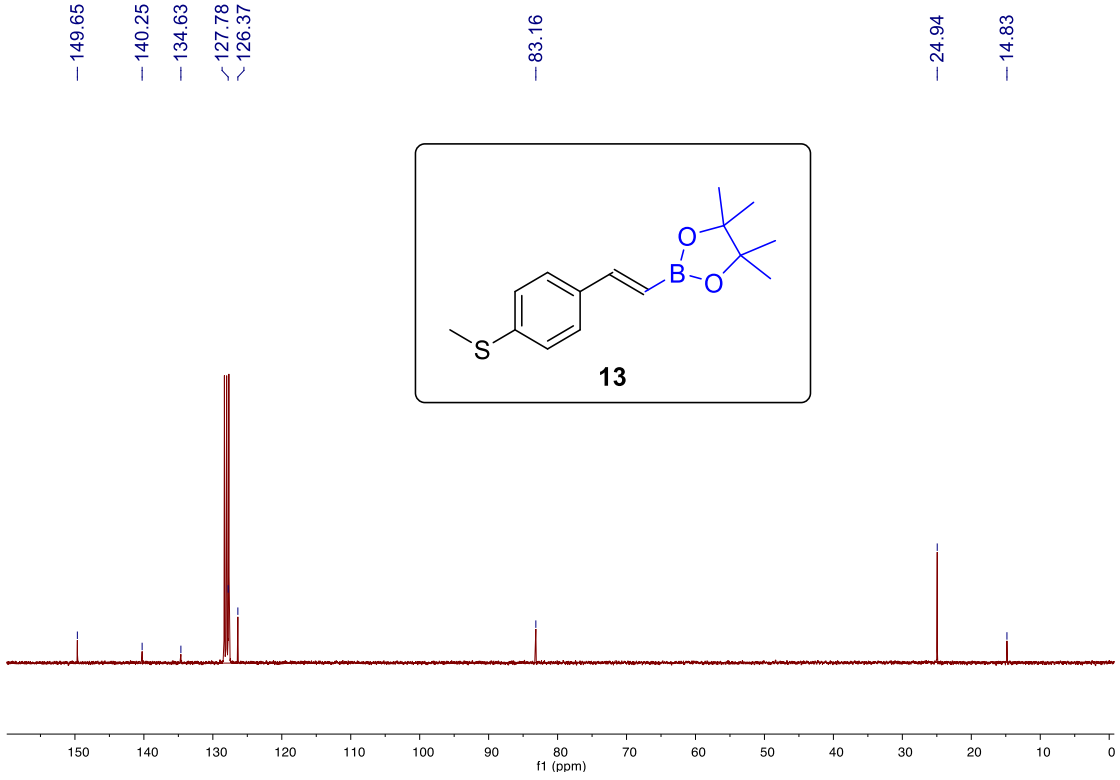
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13
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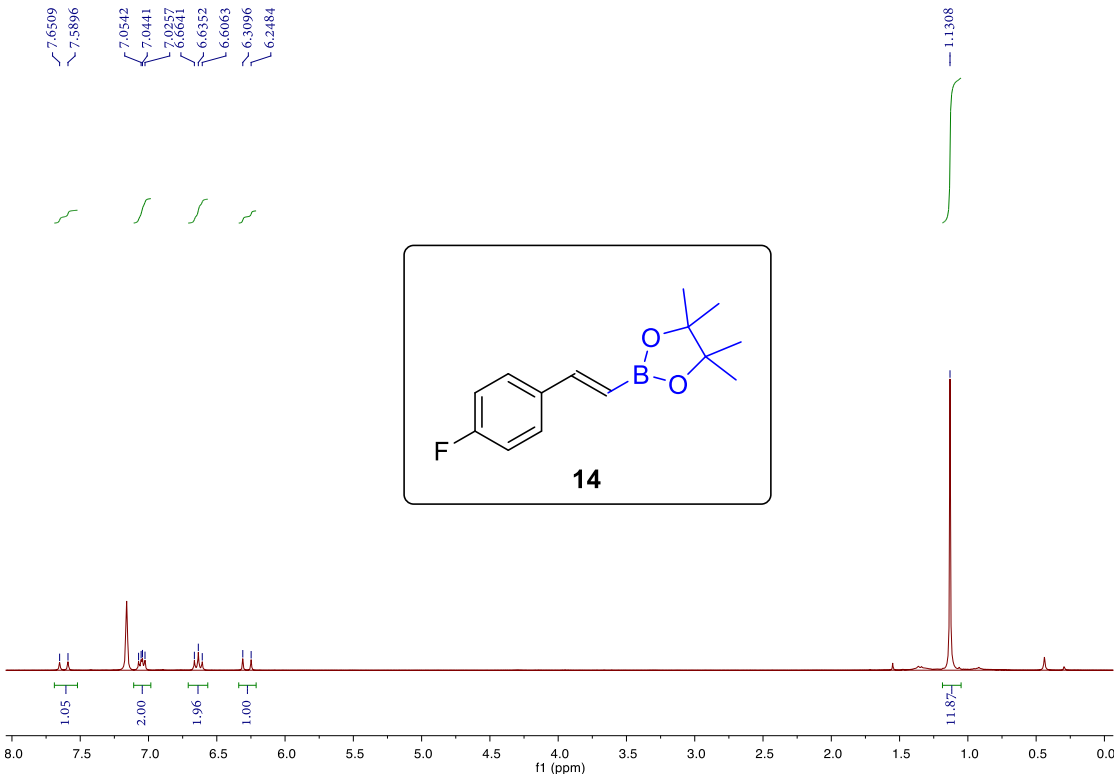
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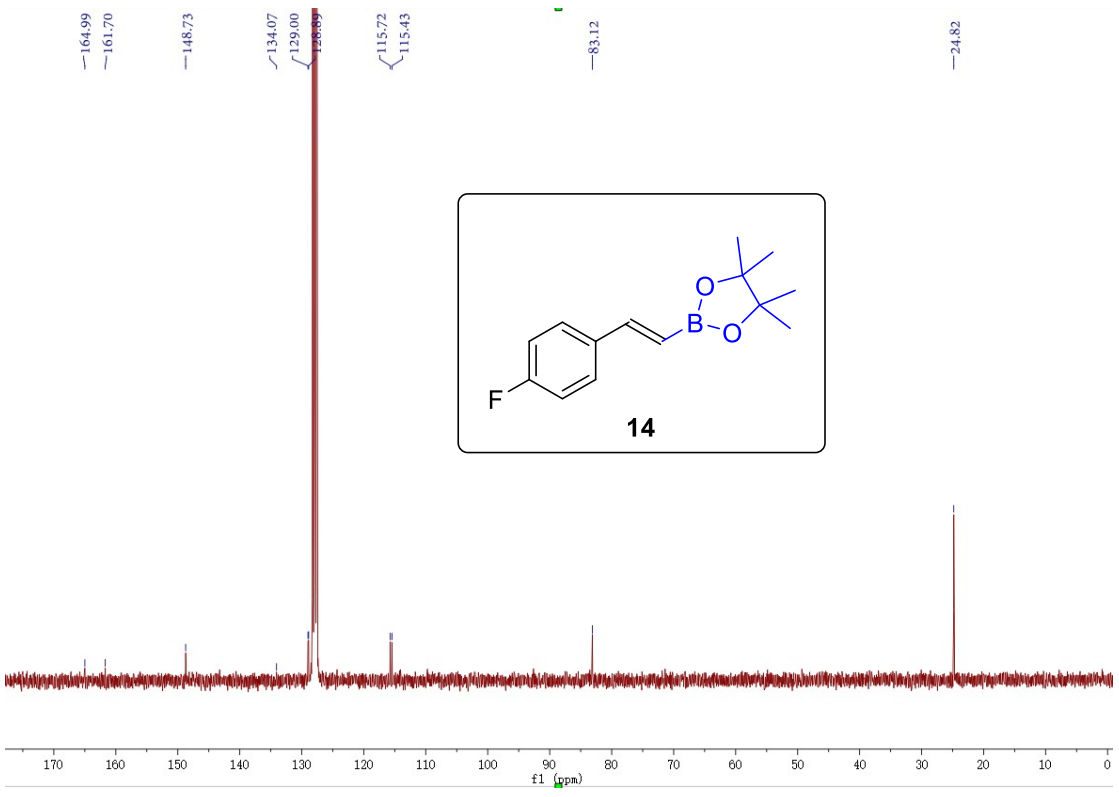
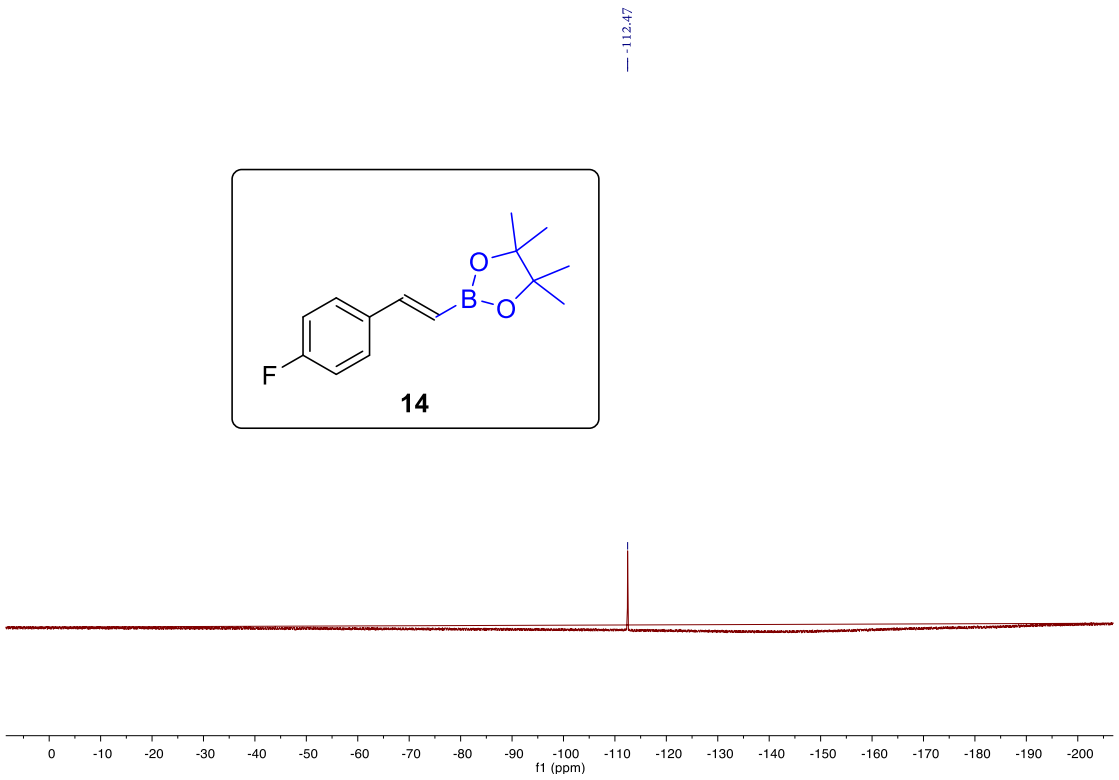
7.5896
7.0542
7.0441
7.0257
6.6641
6.6352
6.6063
6.3096
6.2484
1.1308
O
B
O
F
14
1.05
2.00
1.96
1.00
11.87
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


164.99
161.70
148.73
134.07
129.00
128.89
115.72
115.43
83.12
24.82
O
B
O
F
14
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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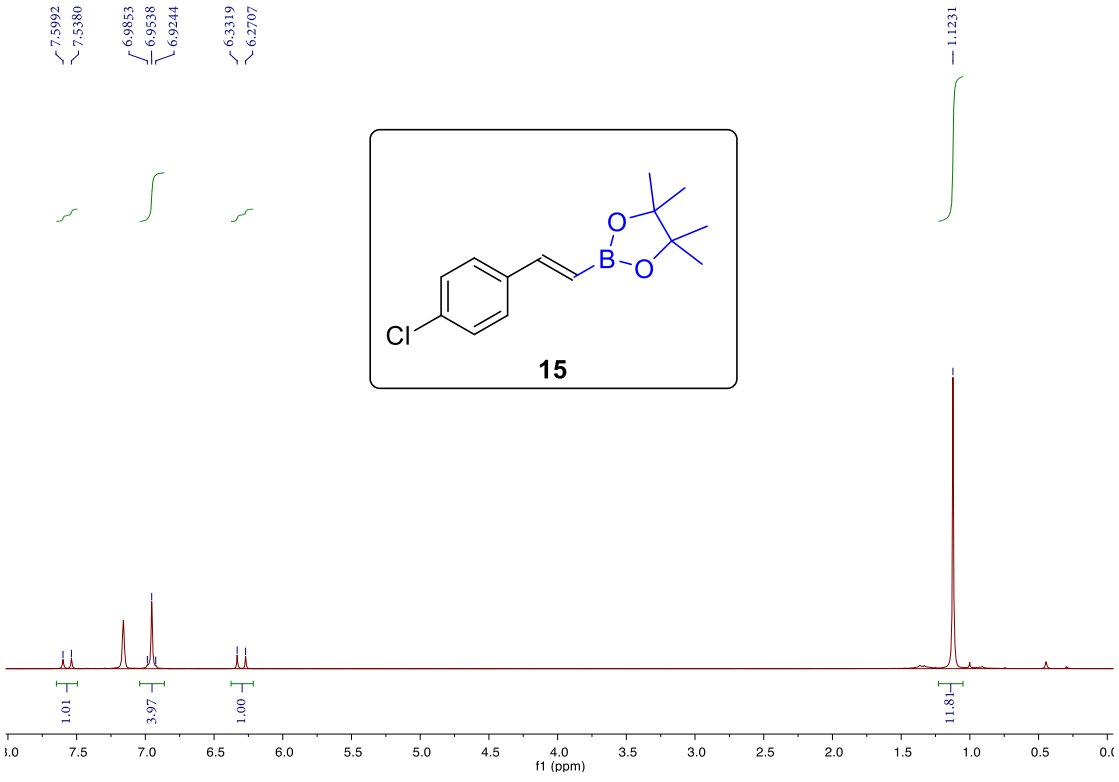
F
14
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
f1 (ppm)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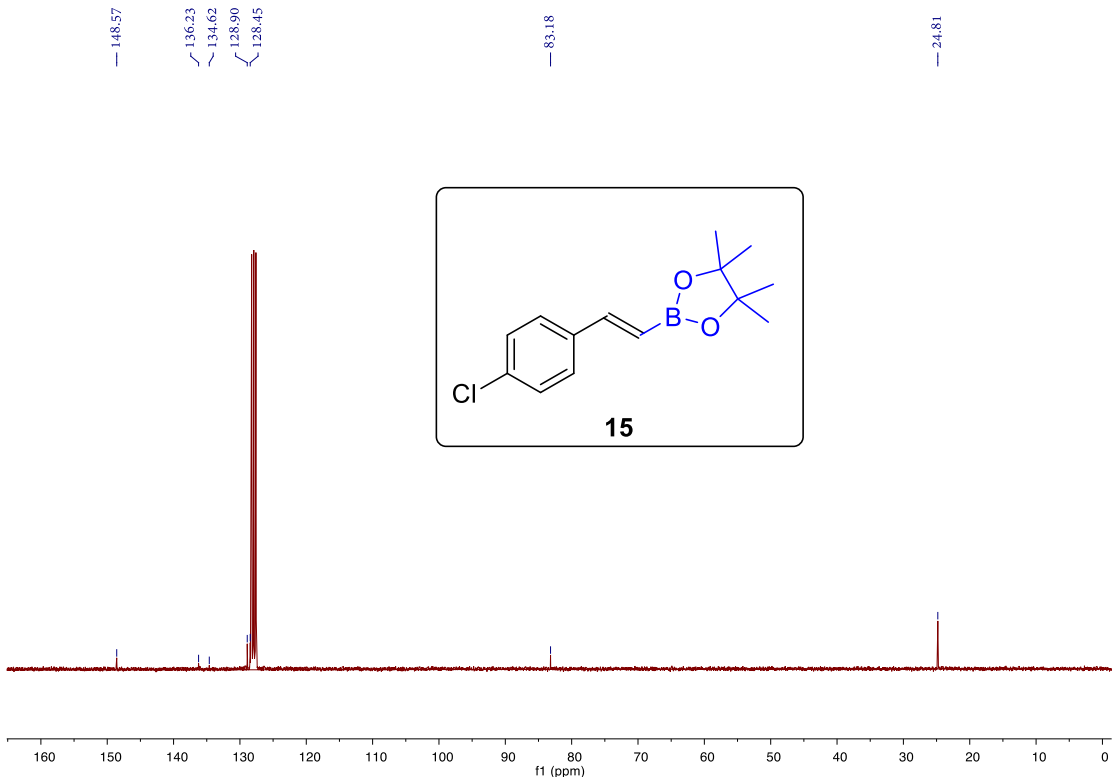
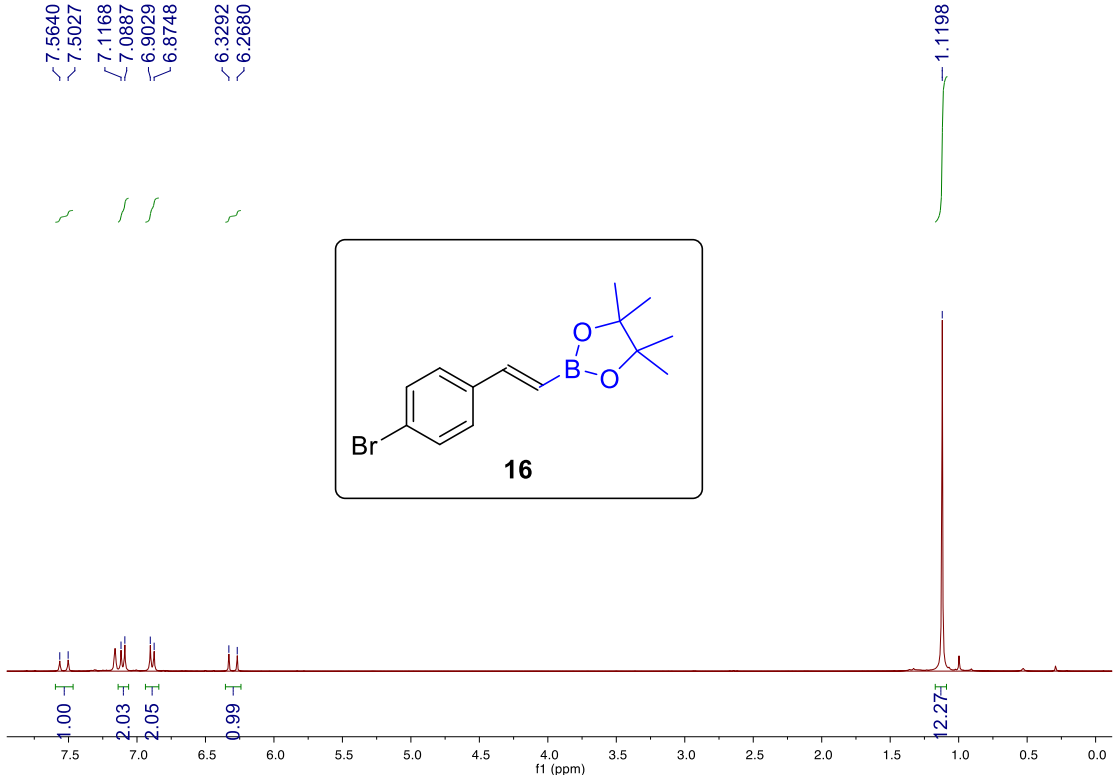
6.9853
6.9538
6.9244
6.3319
6.2707
1.1231
Cl
15
1.01
3.97
1.00
11.81
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)


148.57
136.23
134.62
128.90
128.45
83.18
24.81
Cl
O
B
O
15
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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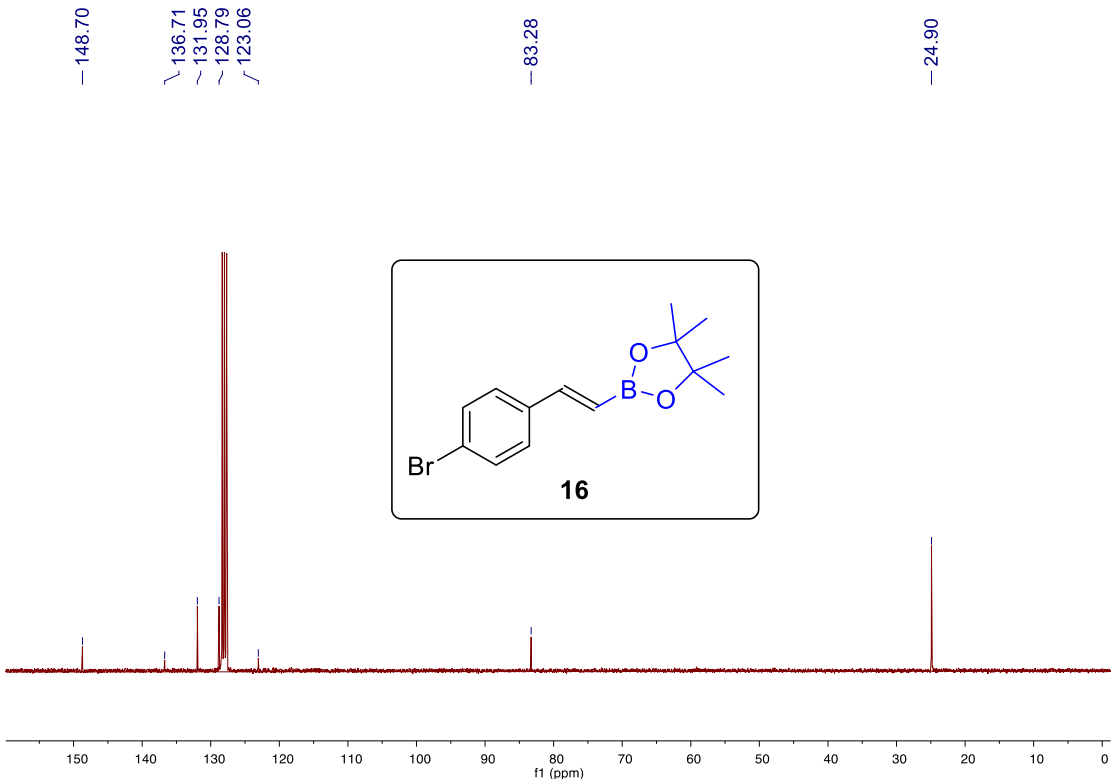
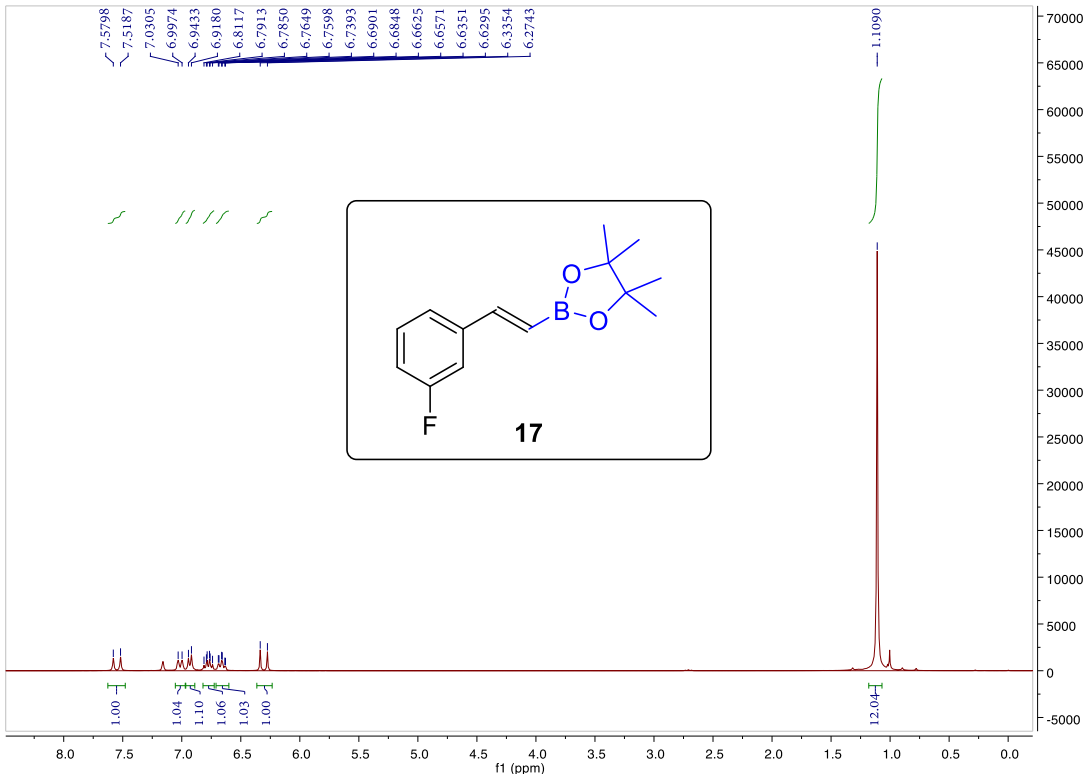
7.5027
7.1168
7.0887
6.9029
6.8748
6.3292
6.2680
1.1198
Br
O
B
O
16
1.00
2.03
2.05
0.99
12.27
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


148.70
136.71
131.95
128.79
123.06
83.28
24.90
Br
O
B
O
16
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.0305
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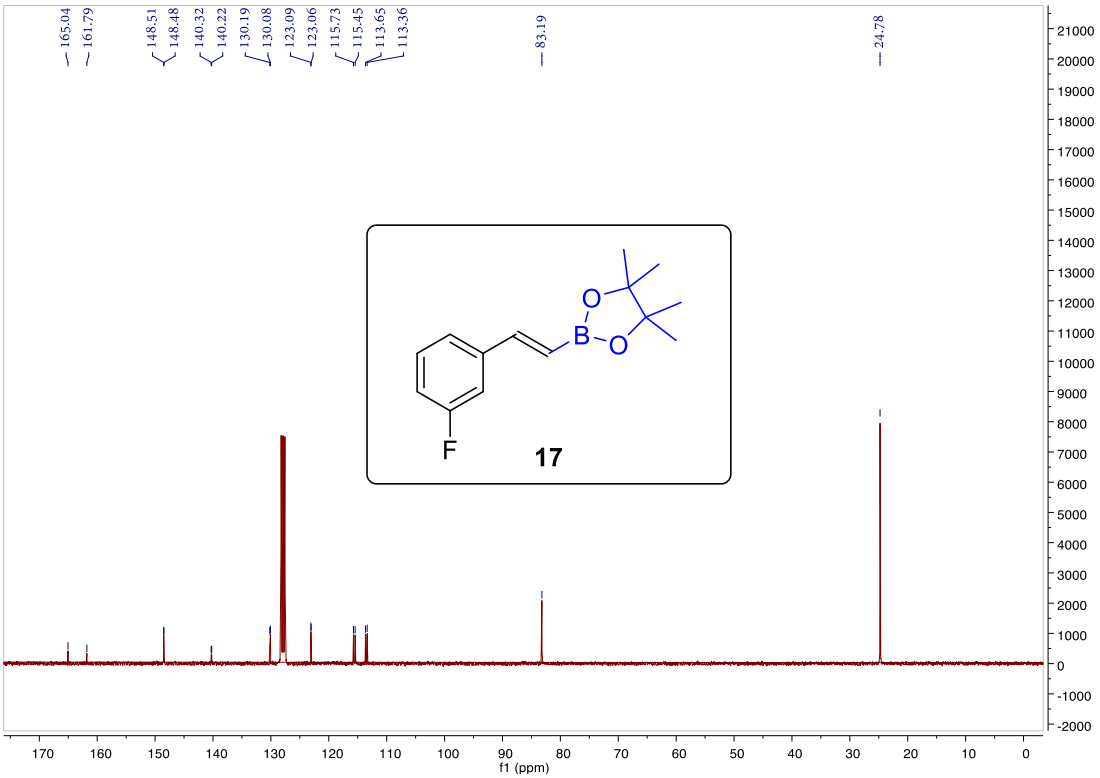
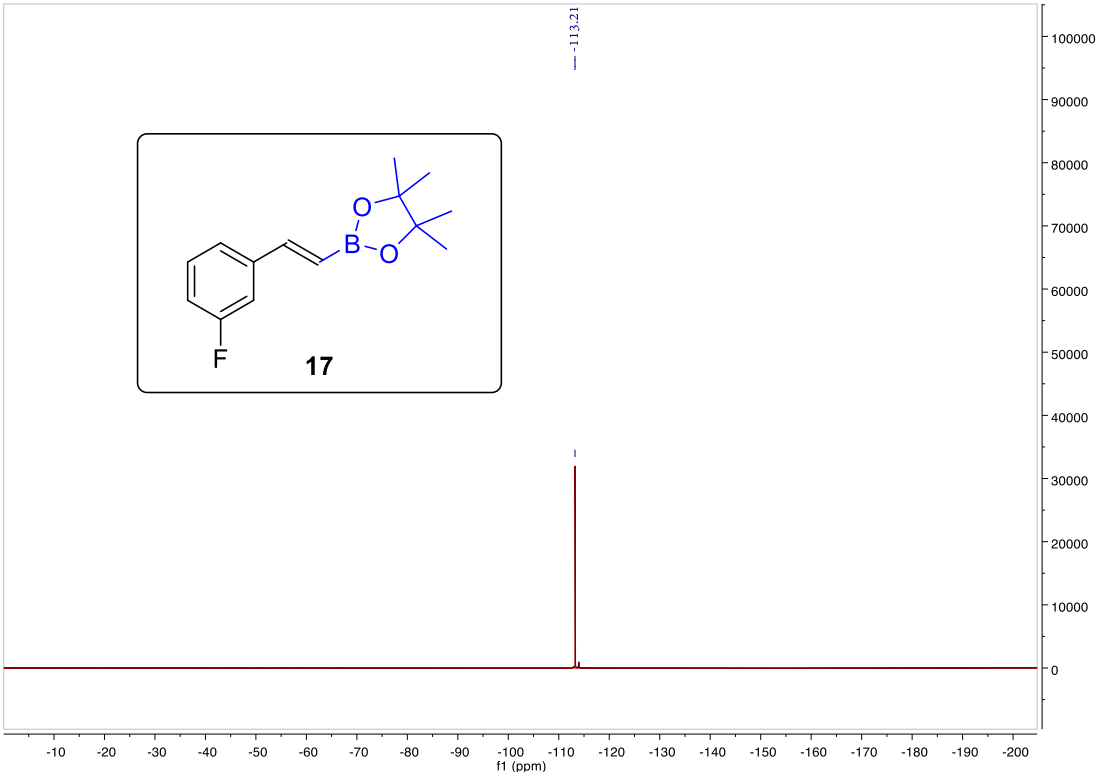
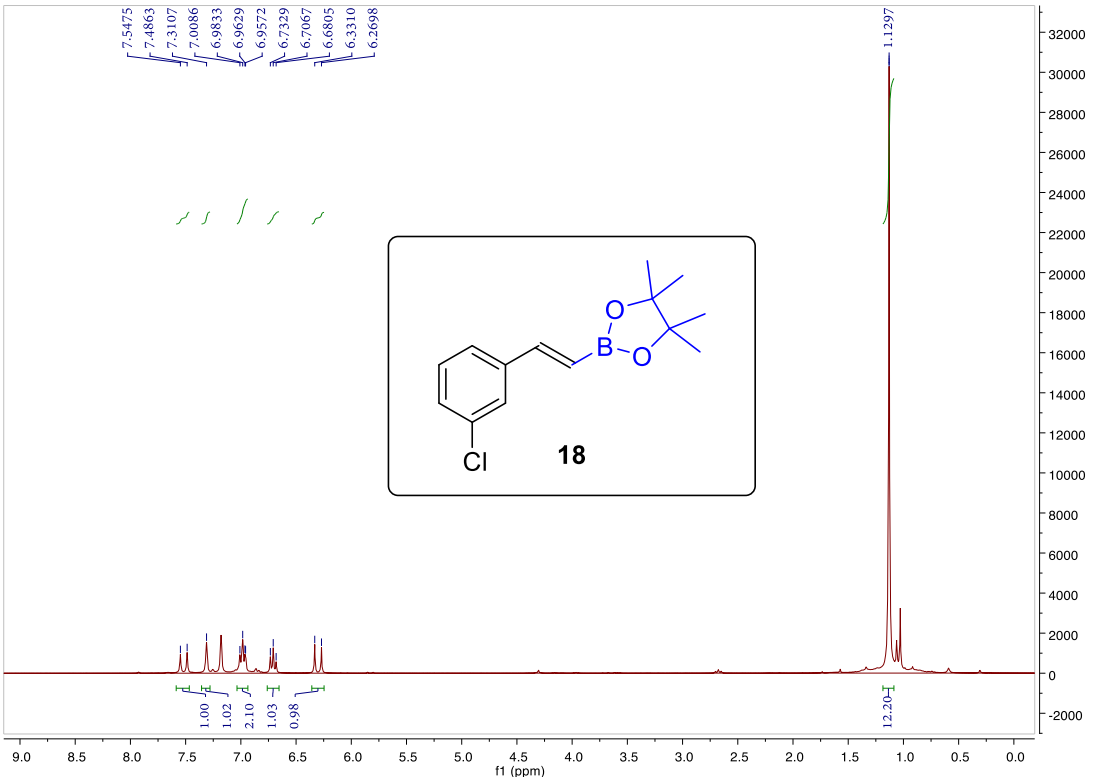
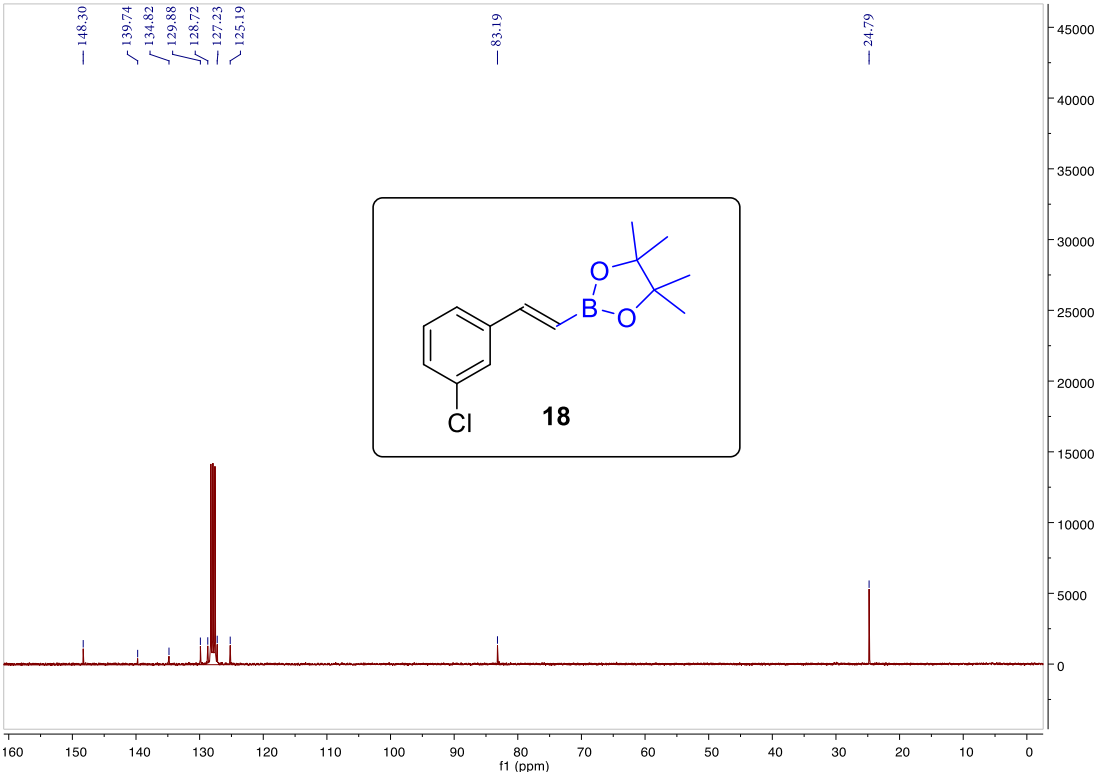
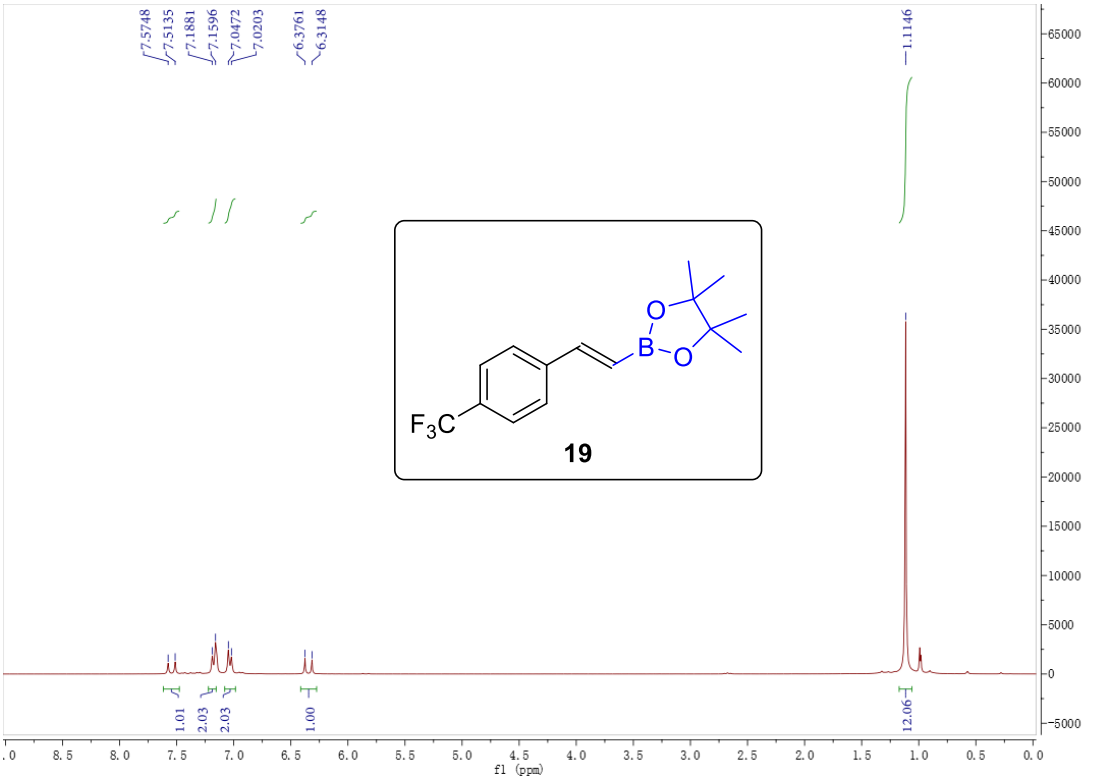
6.9433
6.9180
6.8117
6.7913
6.7850
6.7649
6.7598
6.7393
6.6901
6.6848
6.6625
6.6571
6.6351
6.6295
6.3354
6.2743
1.1090
F
O
B
O
17
1.00
1.04
1.10
1.06
1.03
1.00
12.04
70000
65000
60000
55000
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
-5000
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

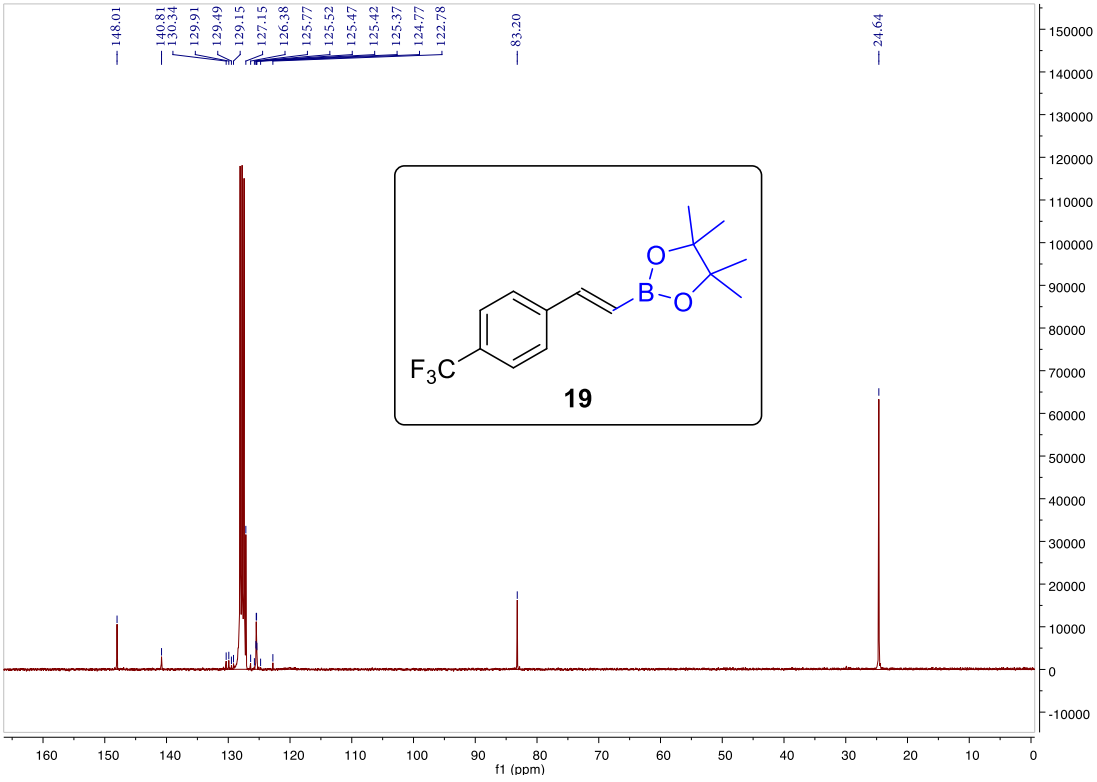

165.04
161.79
148.51
148.48
140.32
140.22
130.19
130.08
123.09
123.06
115.73
115.45
113.65
113.36
83.19
24.78
O
B
O
F
17
f1 (ppm)

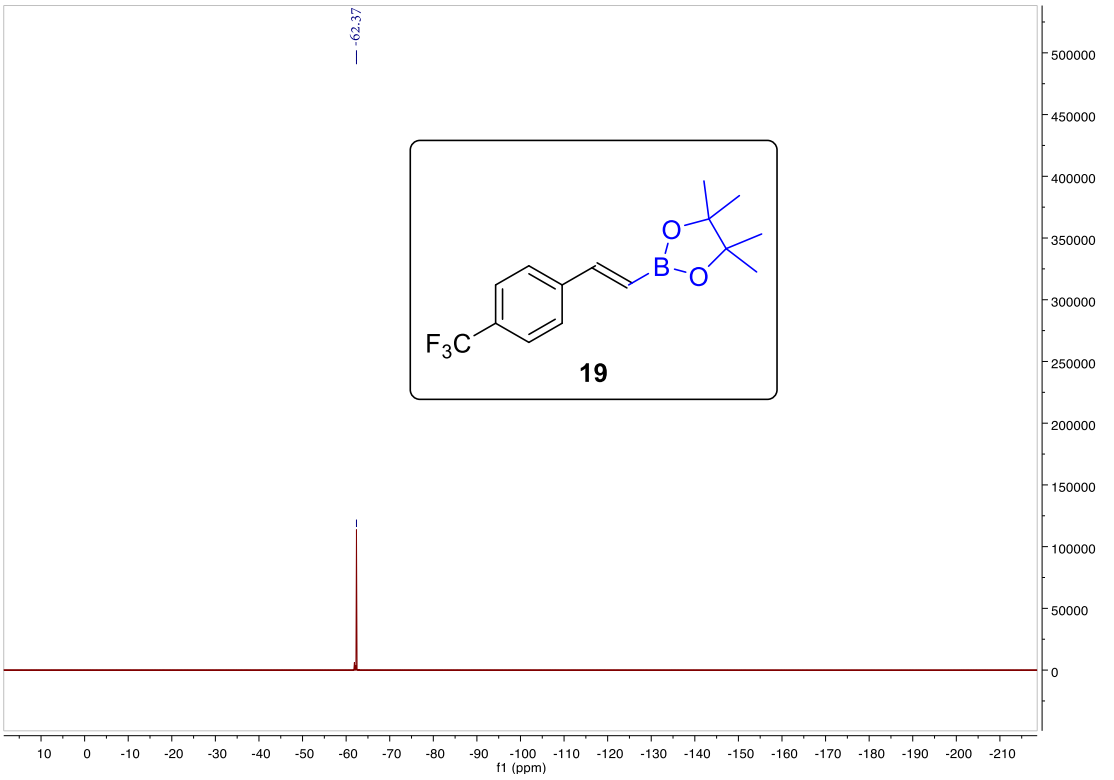

-113.21
O
B
O
F
17
f1 (ppm)


7.5475
7.4863
7.3107
7.0086
6.9833
6.9629
6.9572
6.7329
6.7067
6.6805
6.3310
6.2698
1.1297
1.00
1.02
2.10
1.03
0.98
12.20
O
B
O
Cl
18
f1 (ppm)


148.30
139.74
134.82
129.88
128.72
127.23
125.19
83.19
24.79
O
B
O
Cl
18
f1 (ppm)


7.5748
7.5135
7.1881
7.1596
7.0472
7.0203
6.3761
6.3148
1.1146
1.01
2.03
2.03
1.00
12.06
F3C
19
f1 (ppm)


148.01
140.81
130.34
129.91
129.49
129.15
127.15
126.38
125.77
125.52
125.47
125.42
125.37
124.77
122.78
83.20
24.64
F3C
19
f1 (ppm)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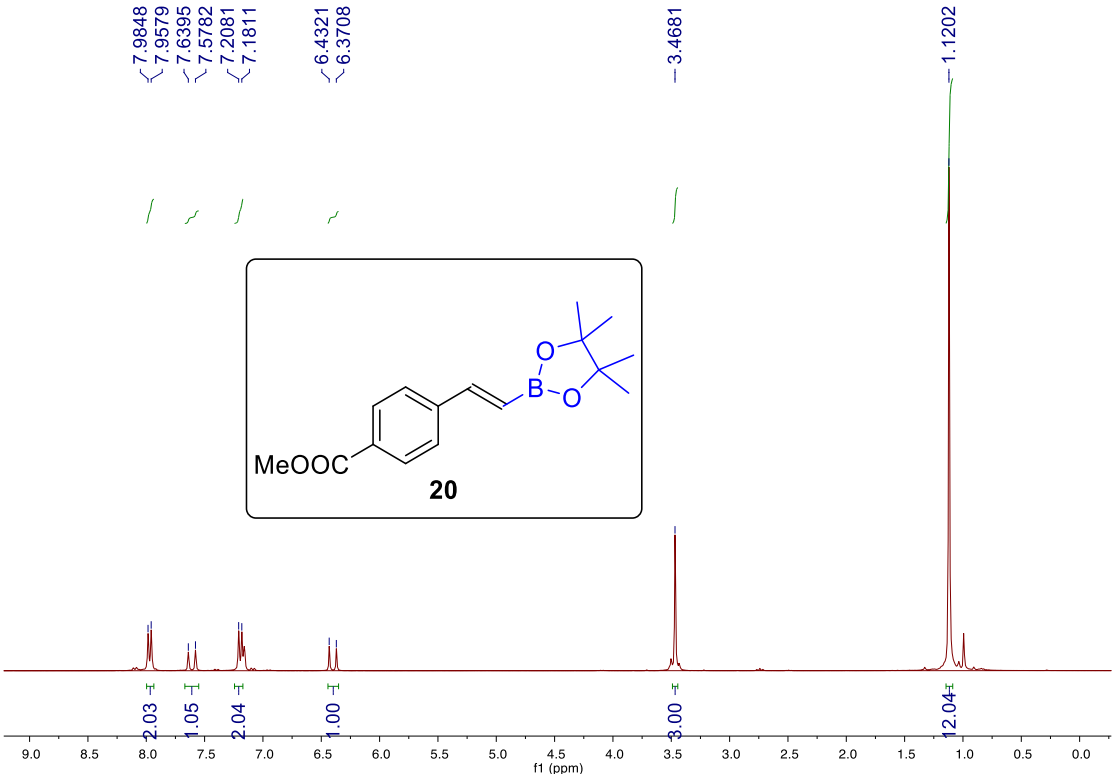
500000
450000
400000
350000
300000
250000
200000
150000
100000
50000
0
O
B
O
F3C
19
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)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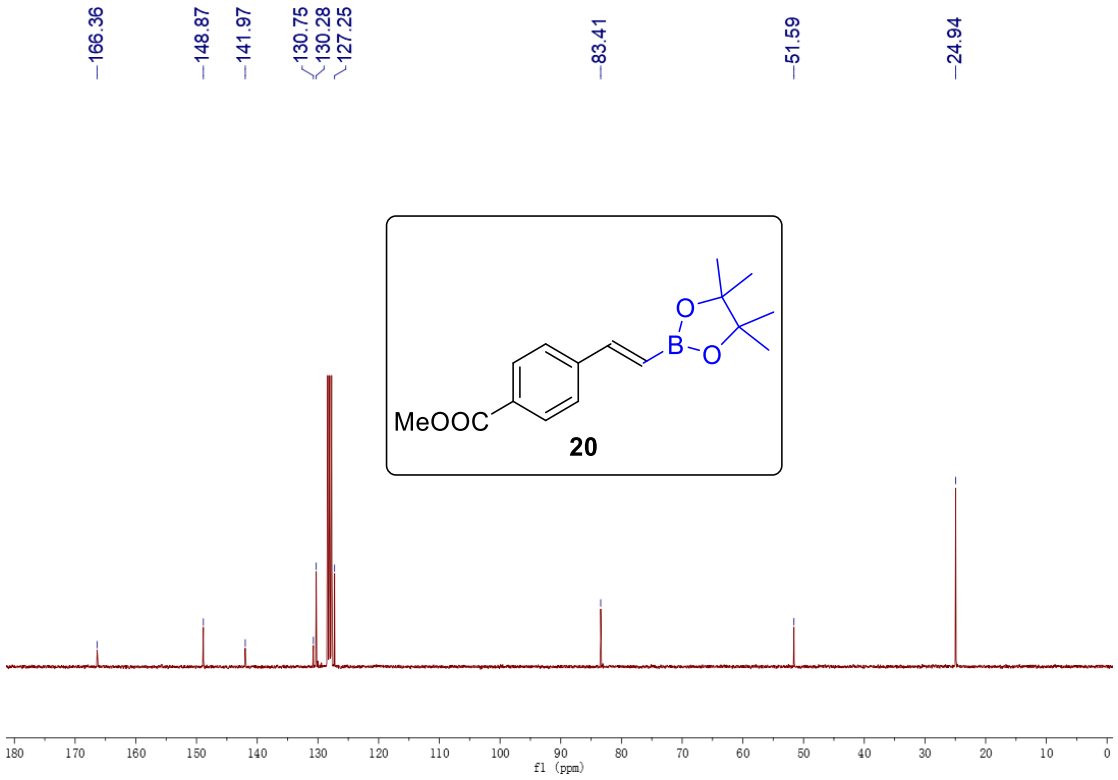
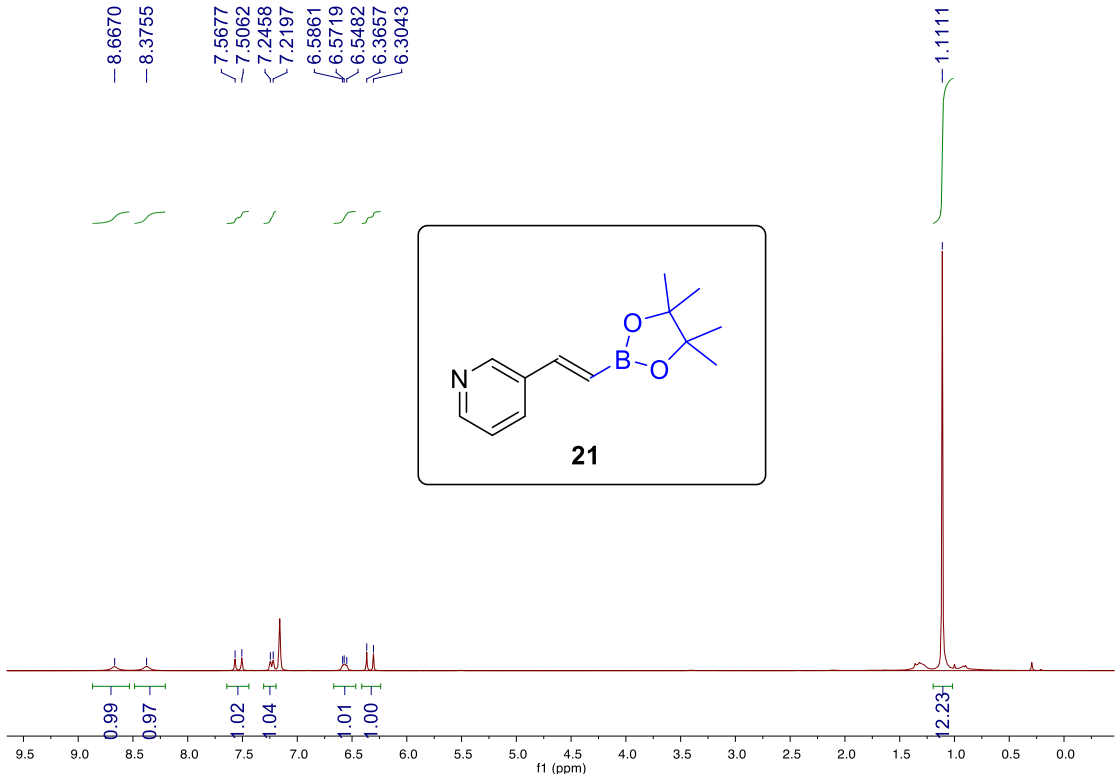
7.9579
7.6395
7.5782
7.2081
7.1811
6.4321
6.3708
3.4681
1.1202
O
B
O
MeOOC
20
2.03
1.05
2.04
1.00
3.00
12.04
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


166.36
148.87
141.97
130.75
130.28
127.25
83.41
51.59
24.94
MeOOC
B
O
O
20
f1 (ppm)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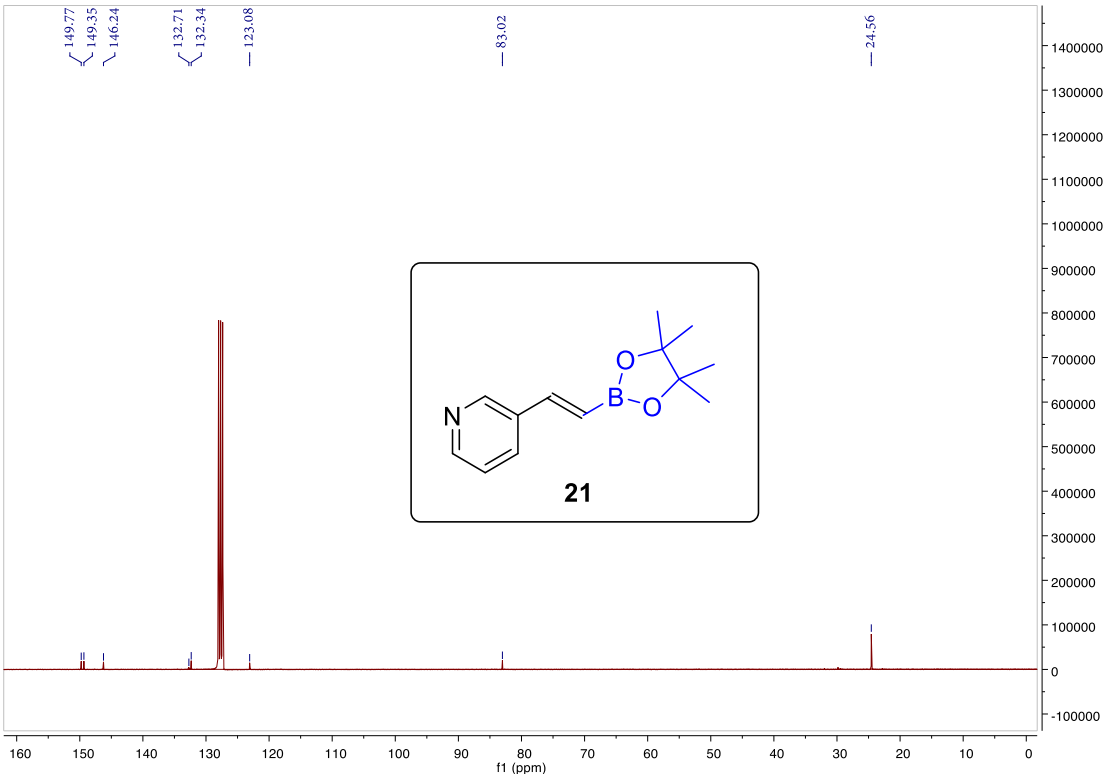
7.2458
7.2197
6.5861
6.5719
6.5482
6.3657
6.3043
1.1111
N
B
O
O
21
0.99
0.97
1.02
1.04
1.01
1.00
12.23
f1 (ppm)


149.77
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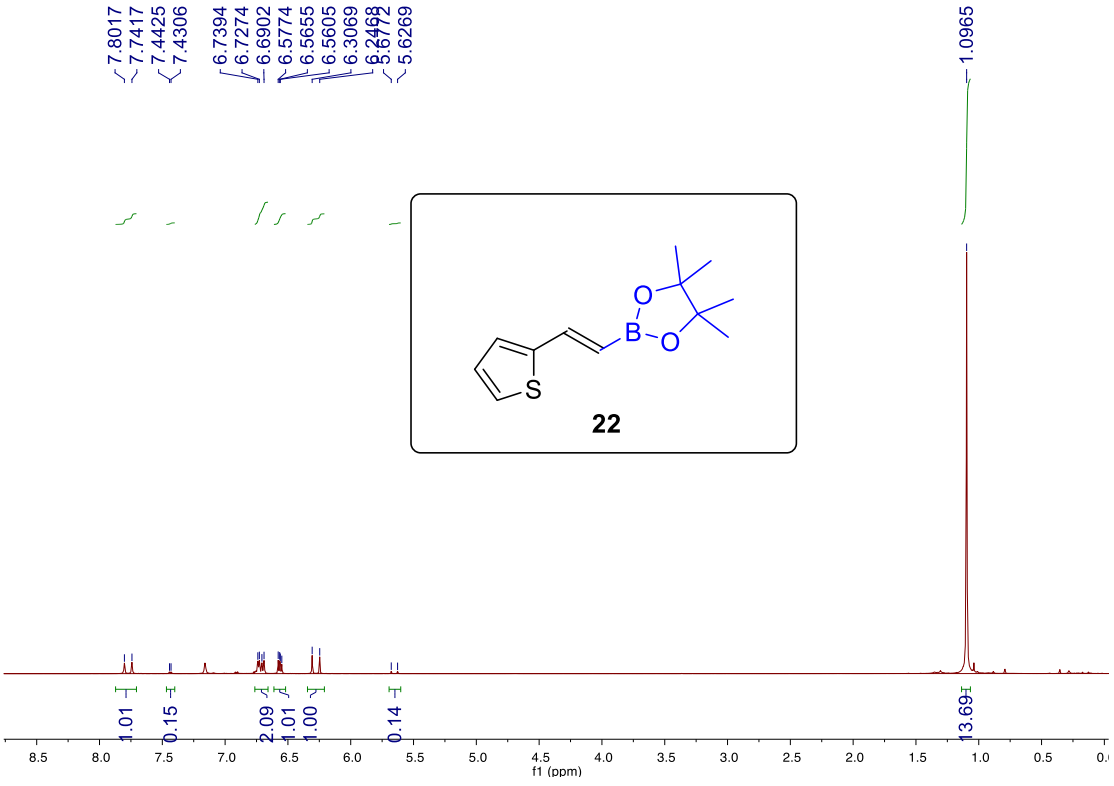
132.71
132.34
123.08
83.02
24.56
N
O
B
O
21
f1 (ppm)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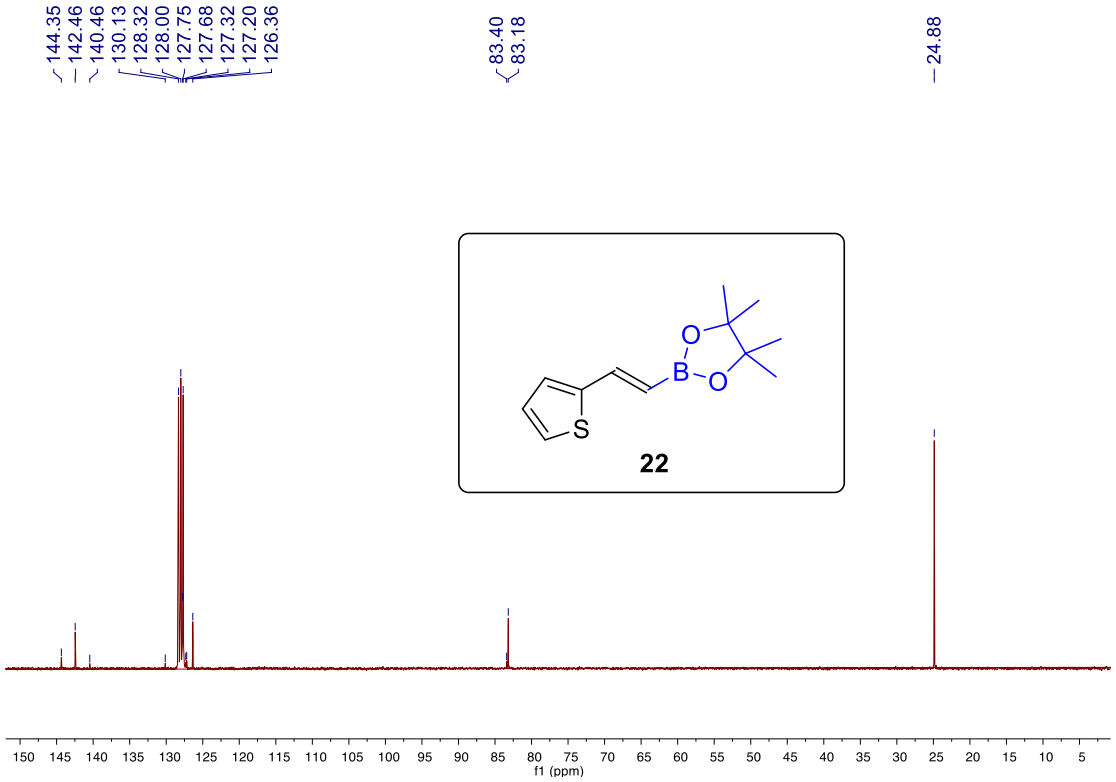
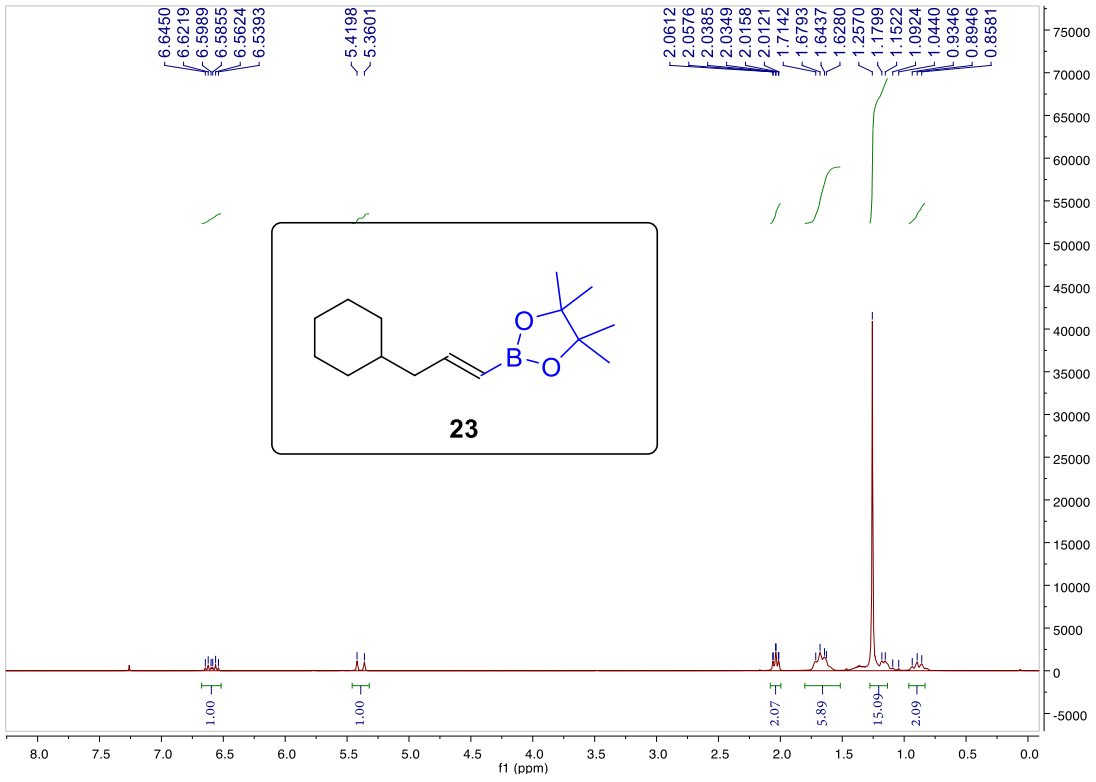
7.4425
7.4306
6.7394
6.7274
6.6902
6.5774
6.5655
6.5605
6.3069
5.6772
5.6269
1.0965
S
O
B
O
22
1.01
0.15
2.09
1.01
1.00
0.14
13.69
f1 (ppm)


144.35
142.46
140.46
130.13
128.32
128.00
127.75
127.68
127.32
127.20
126.36
83.40
83.18
24.88
O
B
O
S
22
150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5
f1 (ppm)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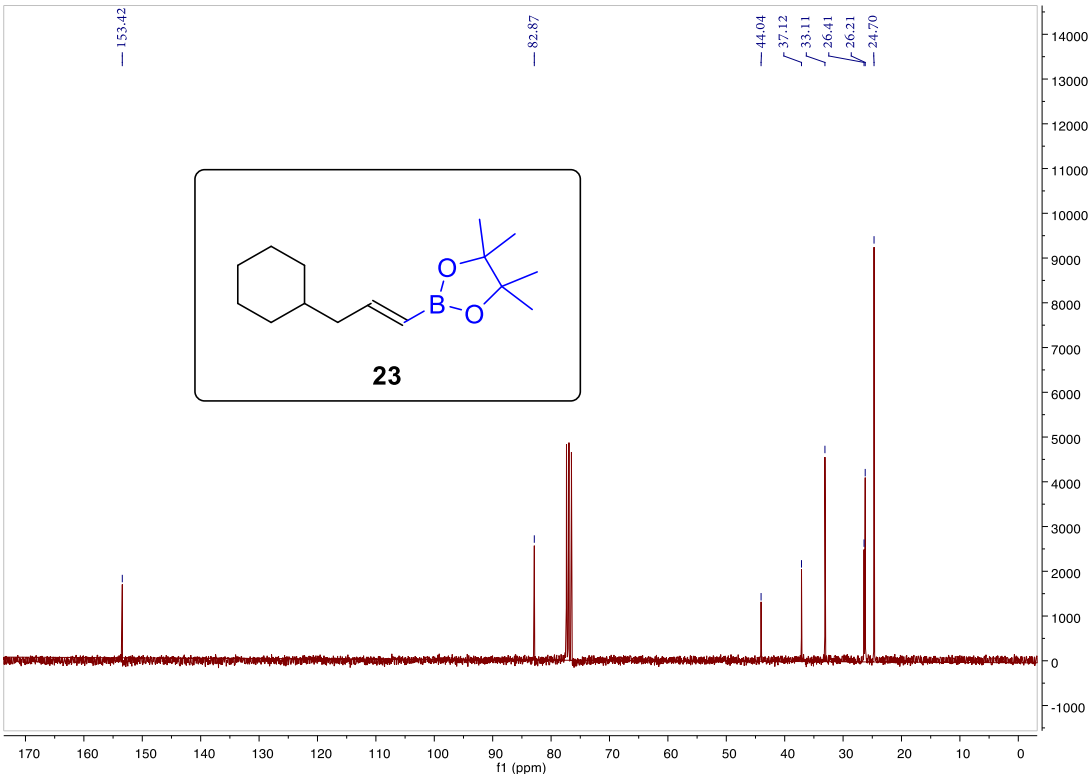
5.4198
5.3601
2.0612
2.0576
2.0385
2.0349
2.0158
2.0121
1.7142
1.6793
1.6437
1.6280
1.2570
1.1799
1.1522
1.0924
1.0440
0.9346
0.8946
0.8581
O
B
O
23
1.00
1.00
2.07
5.89
15.09
2.09
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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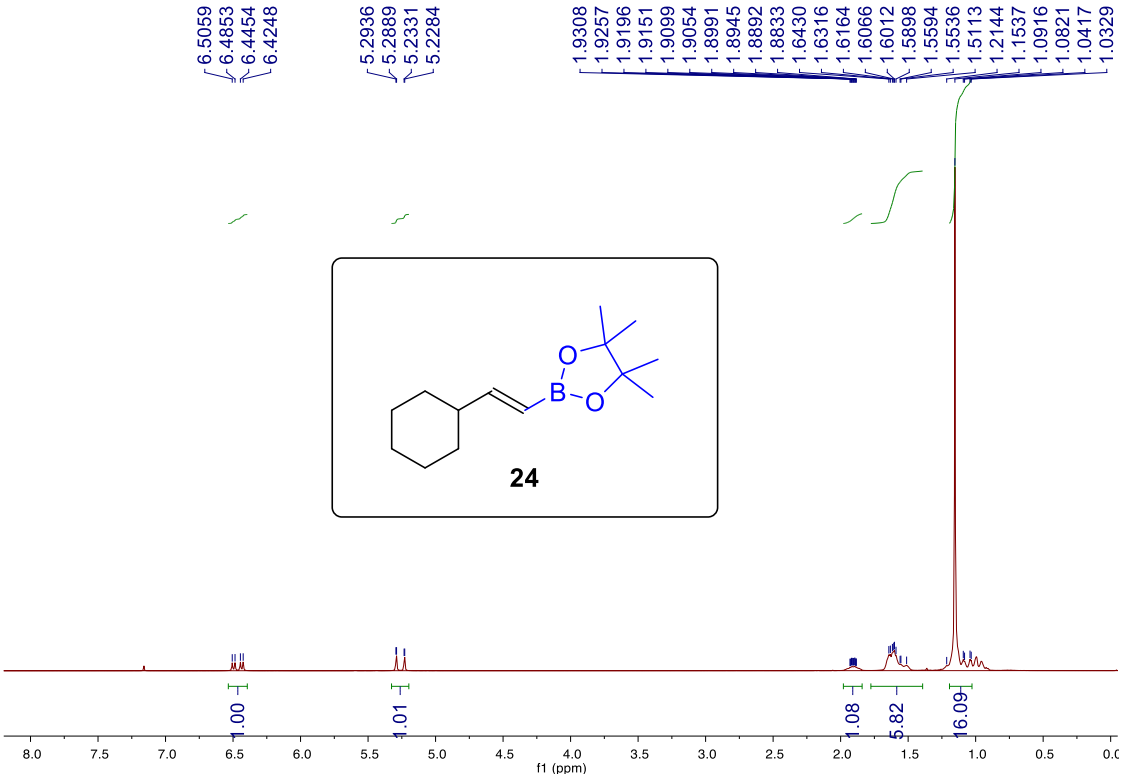
82.87
44.04
37.12
33.11
26.41
26.21
24.70
23
f1 (ppm)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6.4454
6.4248
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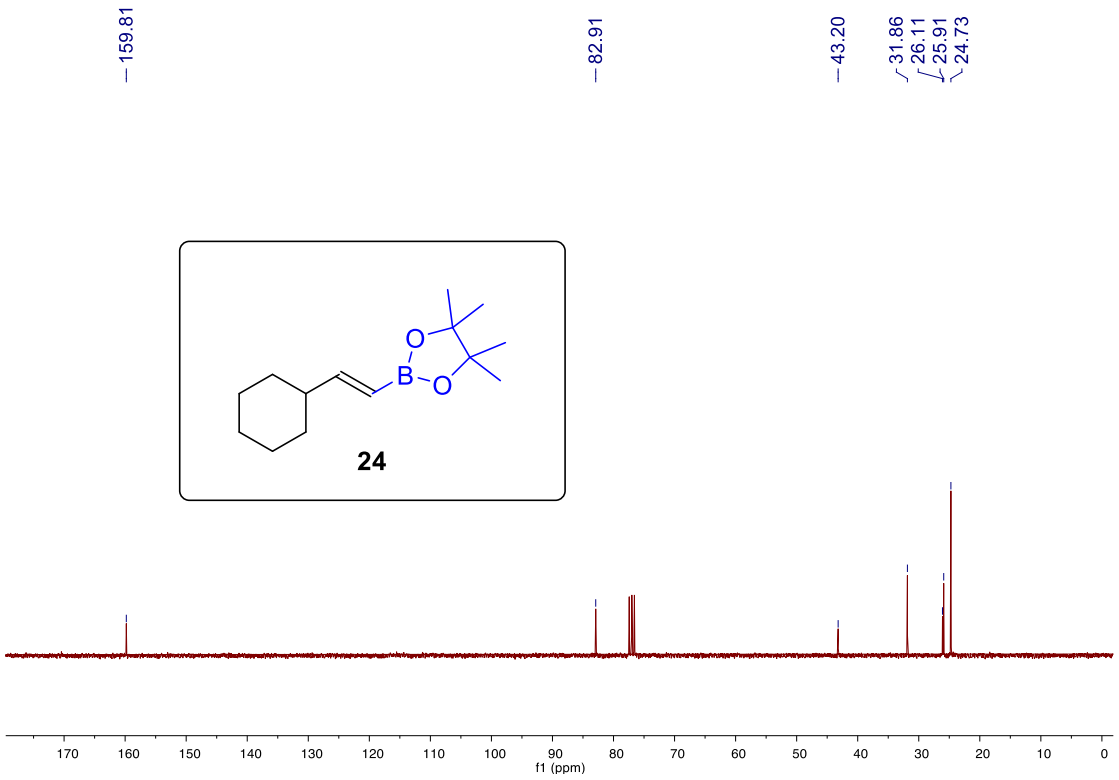
5.2889
5.2331
5.2284
1.9308
1.9257
1.9196
1.9151
1.9099
1.9054
1.8991
1.8945
1.8892
1.8833
1.6430
1.6316
1.6164
1.6066
1.6012
1.5898
1.5594
1.5536
1.5113
1.2144
1.1537
1.0916
1.0821
1.0417
1.0329
24
1.00
1.01
1.08
5.82
16.09
f1 (ppm)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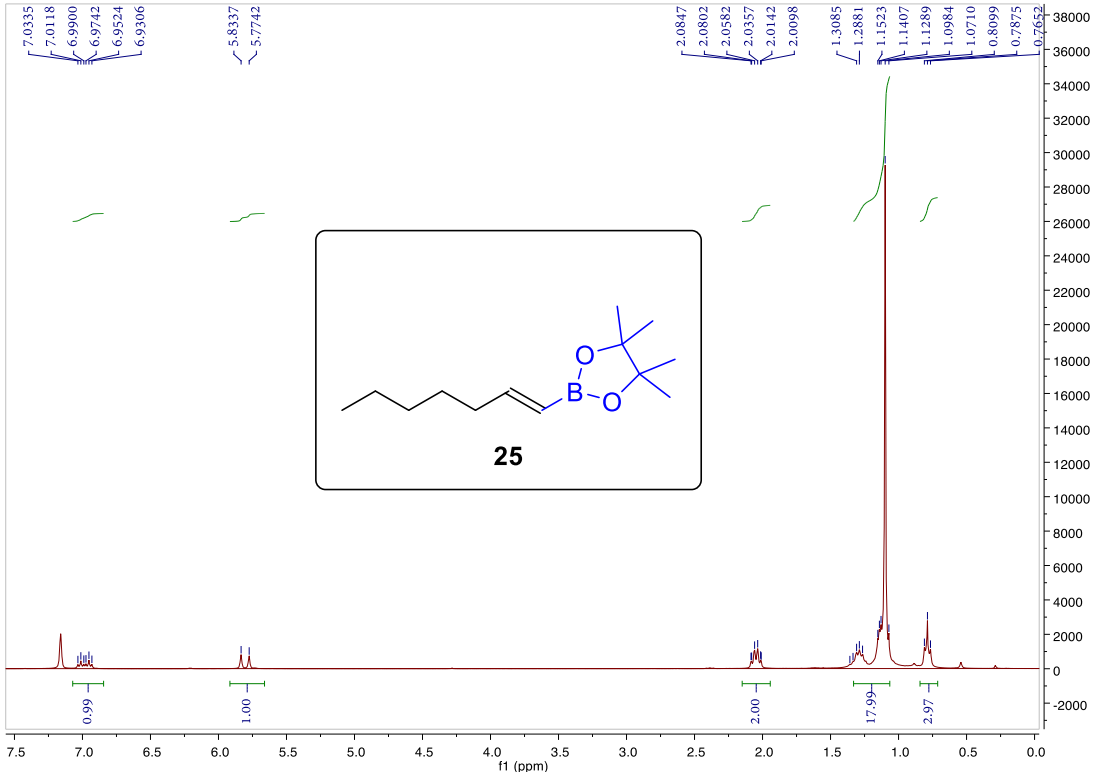
26.11
25.91
24.73
24
f1 (ppm)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6.9524
6.9306
5.8337
5.7742
2.0847
2.0802
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2.0357
2.0142
2.0098
1.3085
1.2881
1.1523
1.1407
1.1289
1.0984
1.0710
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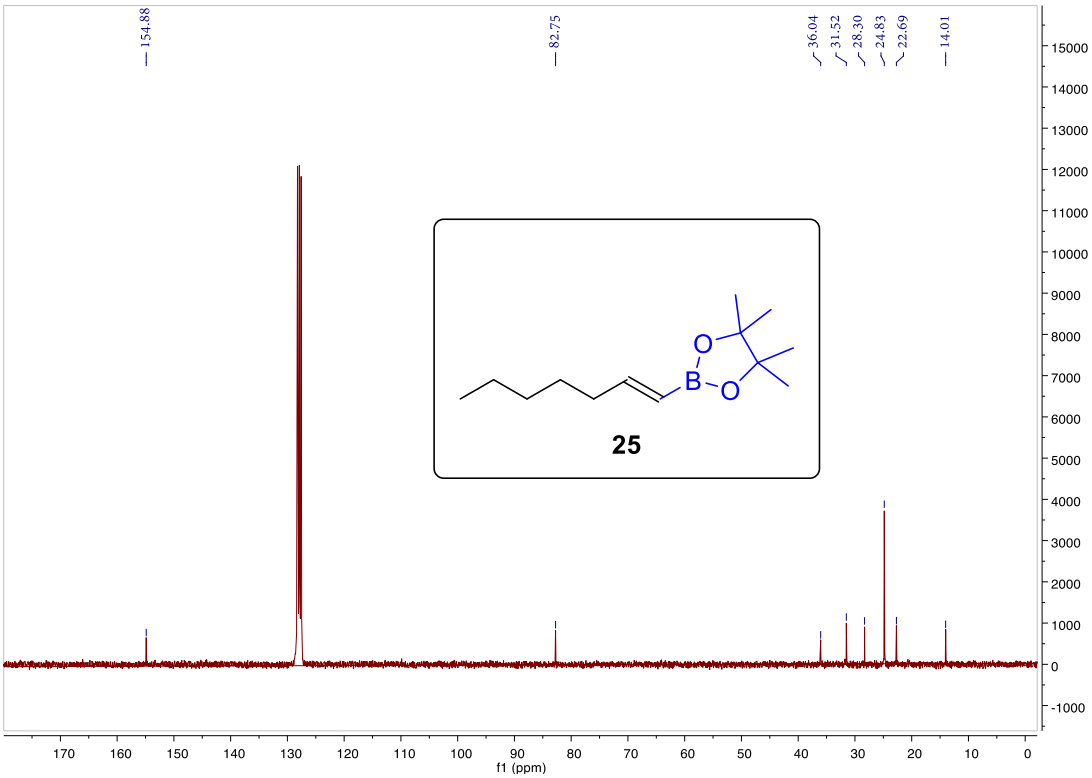
0.7875
0.7652
25
0.99
1.00
2.00
17.99
2.97
f1 (ppm)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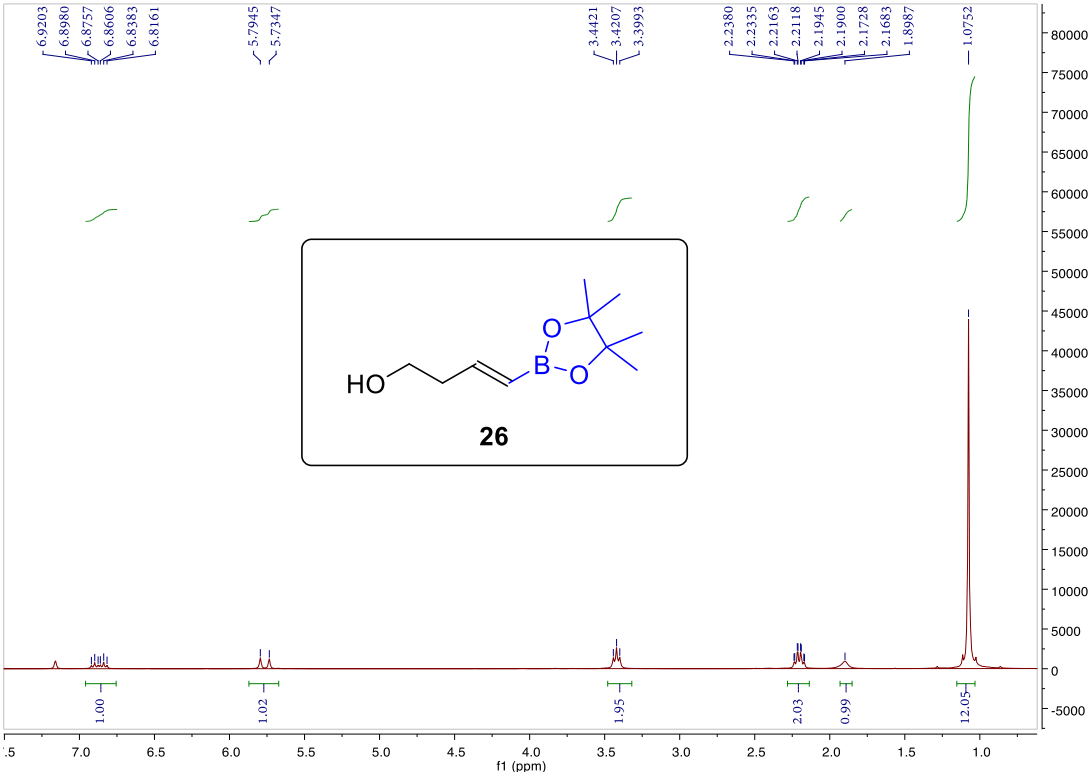
36.04
31.52
28.30
24.83
22.69
14.01
O
B
O
25
f1 (ppm)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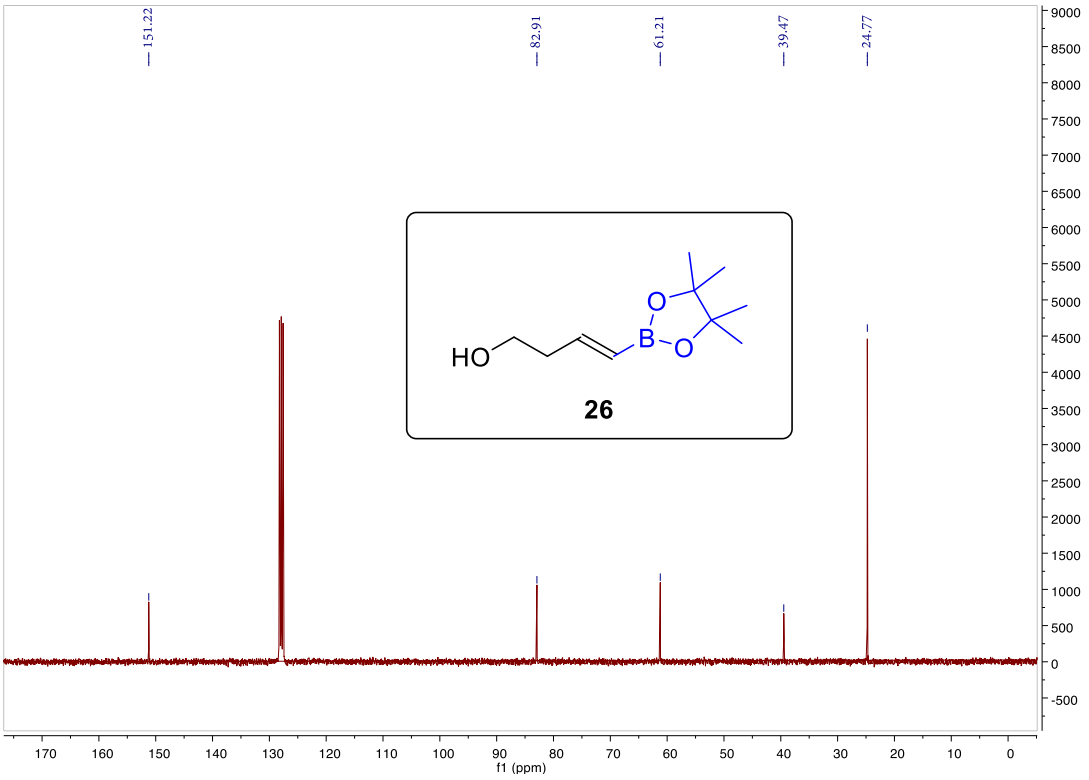
6.8757
6.8606
6.8383
6.8161
5.7945
5.7347
3.4421
3.4207
3.3993
2.2380
2.2335
2.2163
2.2118
2.1945
2.1900
2.1728
2.1683
1.8987
1.0752
HO
O
B
O
26
1.00
1.02
1.95
2.03
0.99
12.05
f1 (ppm)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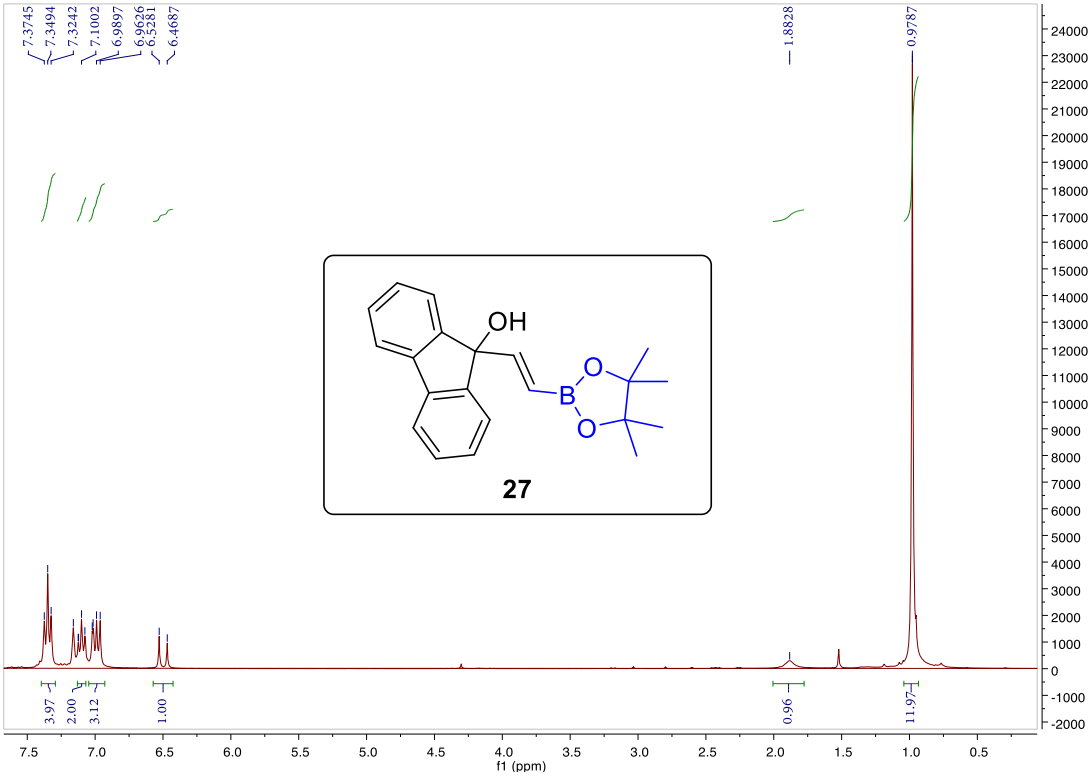
61.21
39.47
24.77
HO
O
B
O
26
f1 (ppm)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7.3494
7.3242
7.1002
6.9897
6.9626
6.5281
6.4687
1.8828
0.9787
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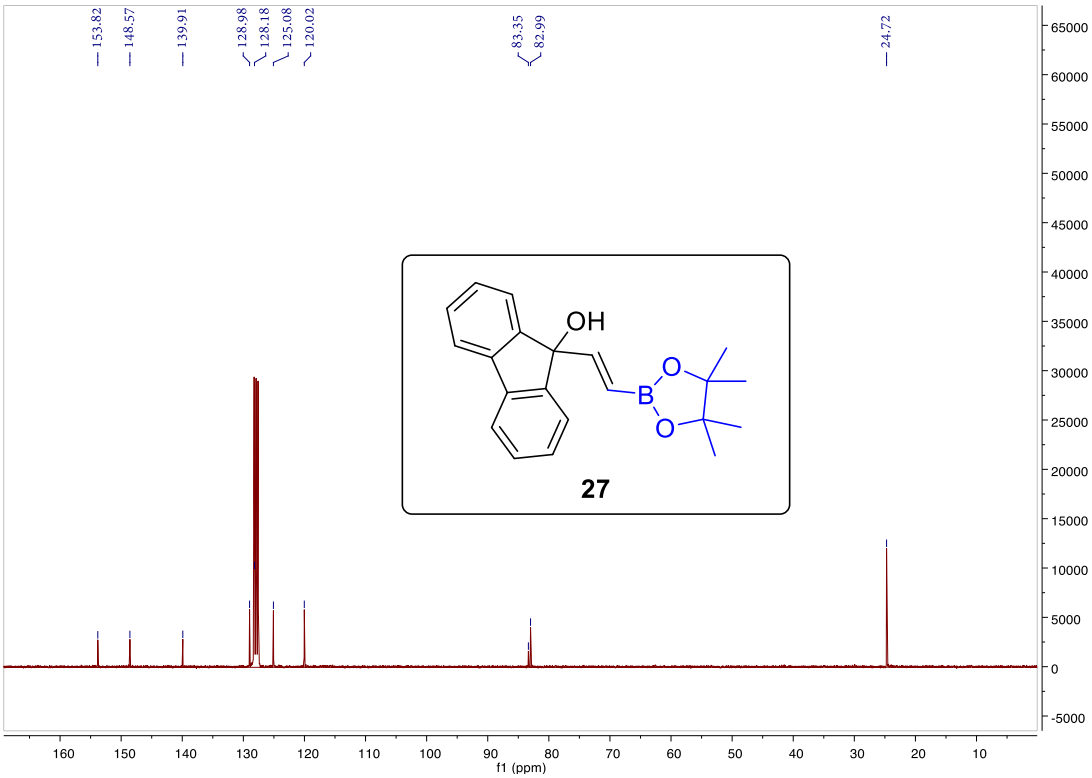
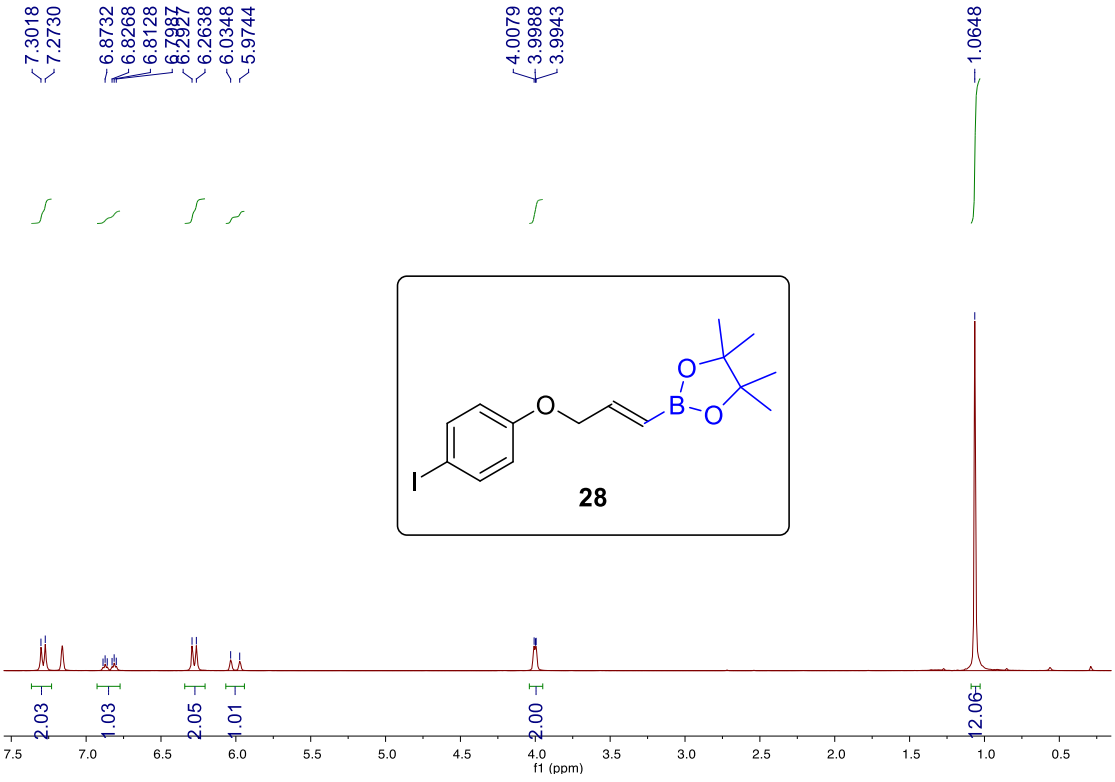
O
B
O
27
3.97
2.00
3.12
1.00
0.96
11.97
f1 (ppm)


153.82
148.57
139.91
128.98
128.18
125.08
120.02
83.35
82.99
24.72
OH
O
B
O
27
f1 (ppm)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6.8128
6.2638
6.0348
5.9744
4.0079
3.9988
3.9943
1.0648
O
B
O
O
I
28
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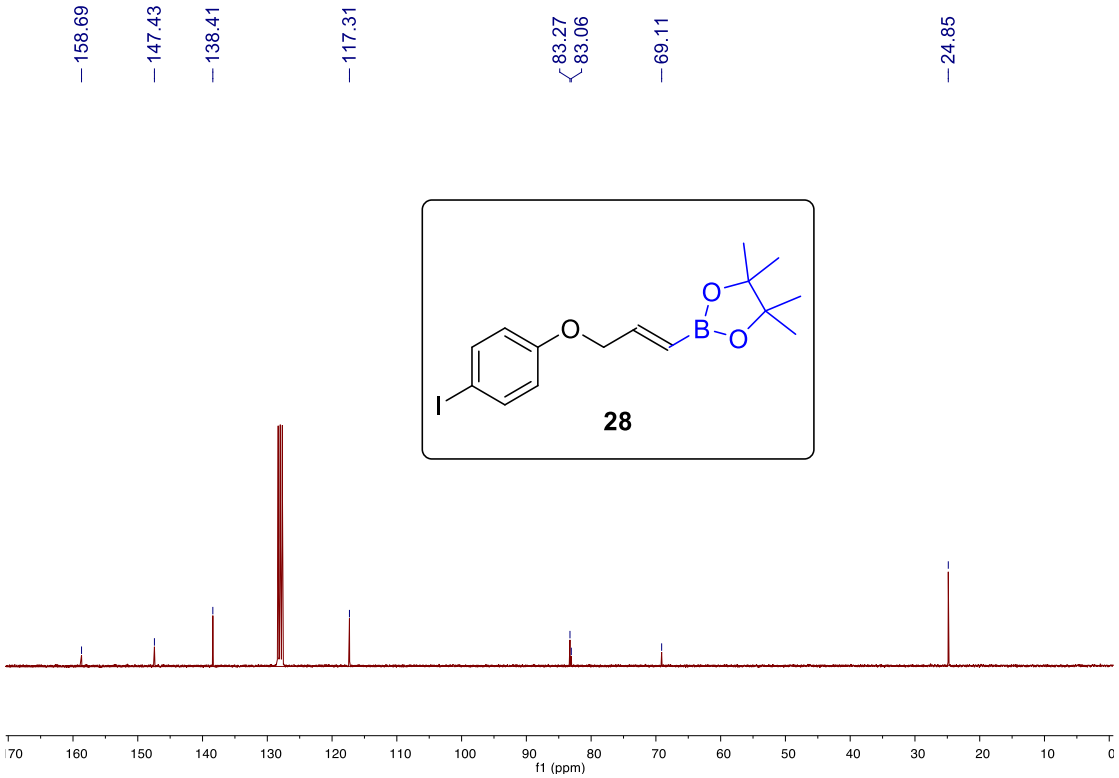
1.03
2.05
1.01
2.00
12.06
f1 (ppm)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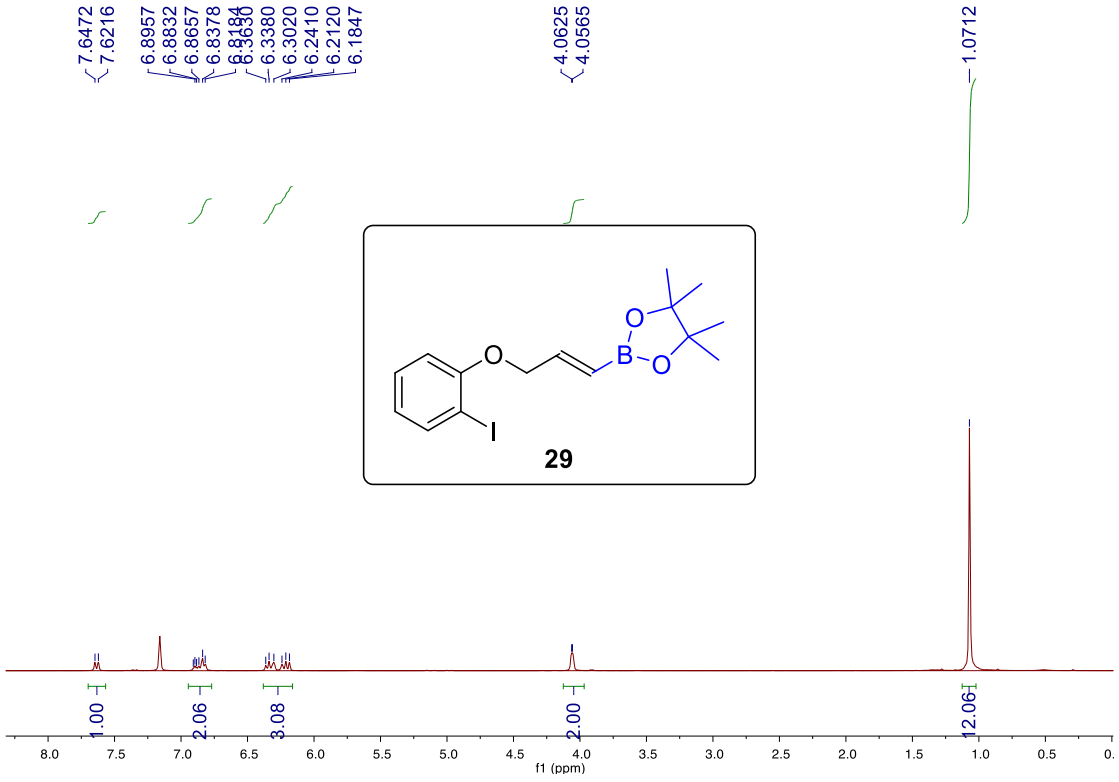
117.31
83.27
83.06
69.11
24.85
28
f1 (ppm)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6.8957
6.8832
6.8657
6.8378
6.3380
6.3020
6.2410
6.2120
6.1847
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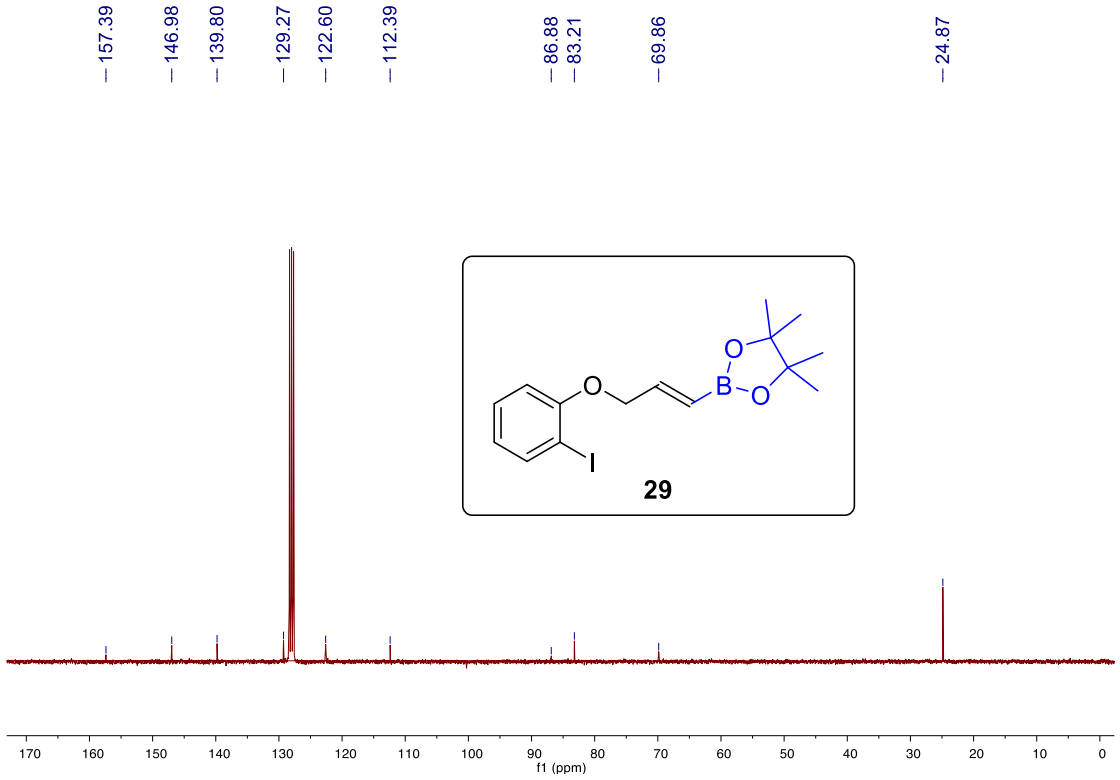
4.0565
1.0712
29
1.00
2.06
3.08
2.00
12.06
f1 (ppm)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139.80
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112.39
86.88
83.21
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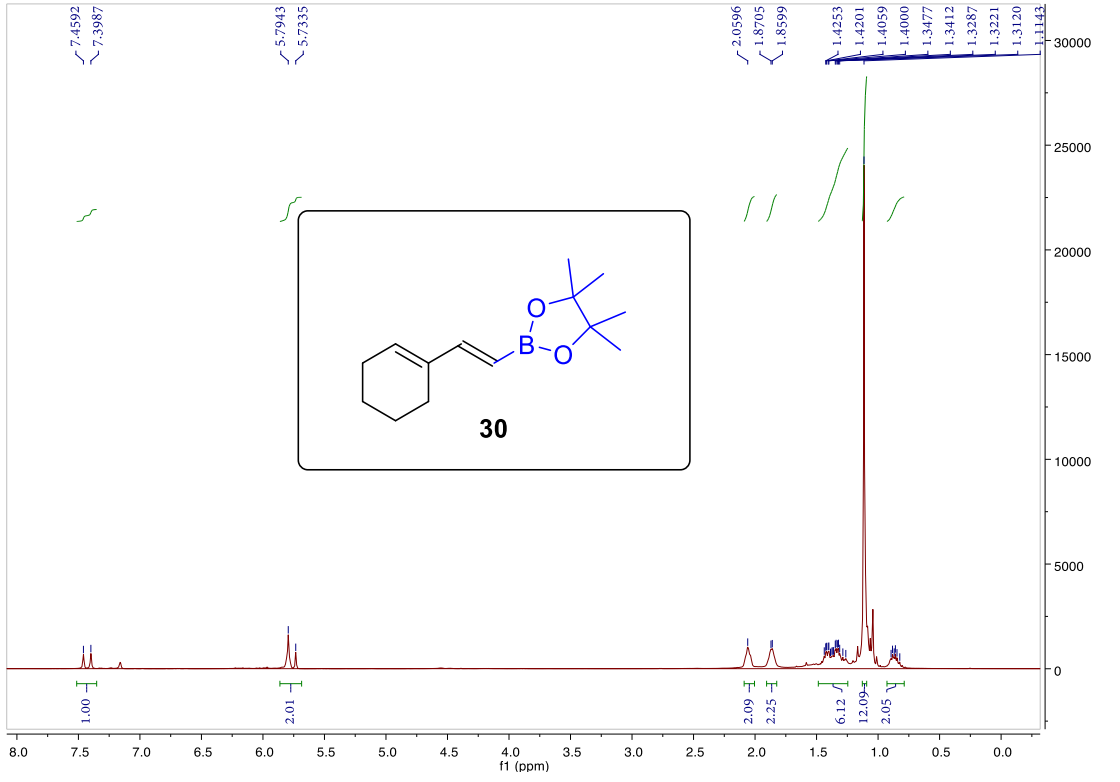
24.87
O
B
O
O
I
29
f1 (ppm)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2.0596
1.8705
1.8599
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1.4201
1.4059
1.4000
1.3477
1.3412
1.3287
1.3221
1.3120
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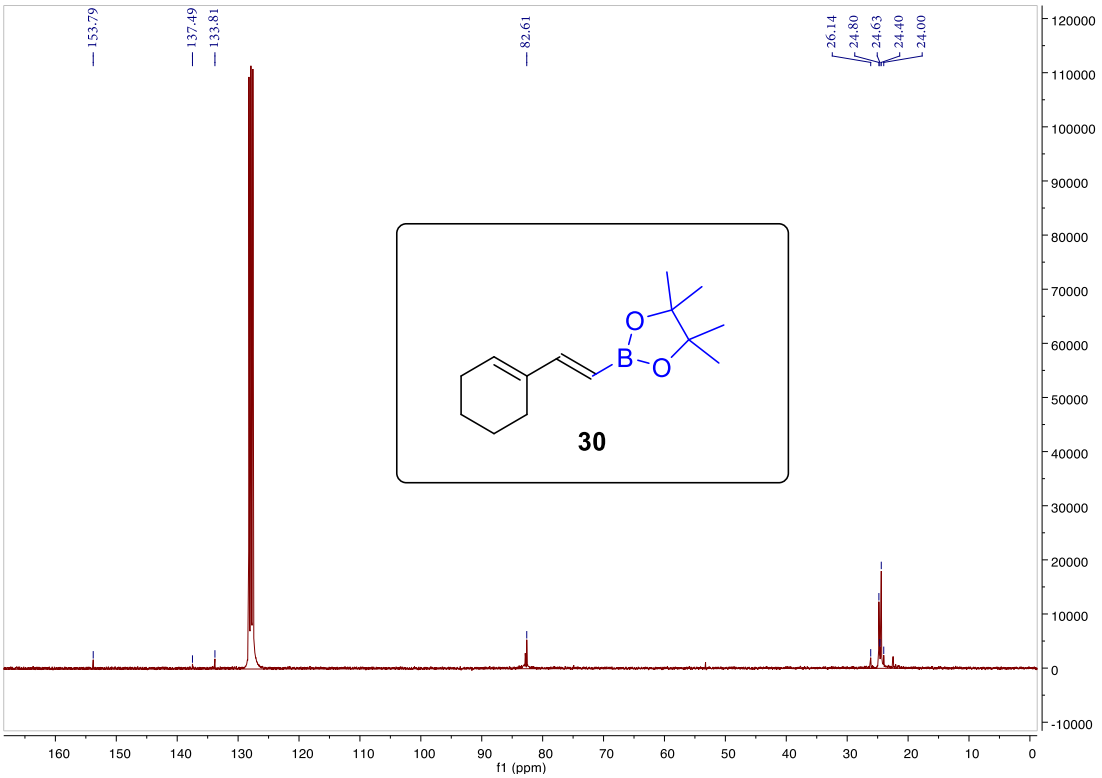
B
O
30
1.00
2.01
2.09
2.25
6.12
12.09
2.05
f1 (ppm)


153.79
137.49
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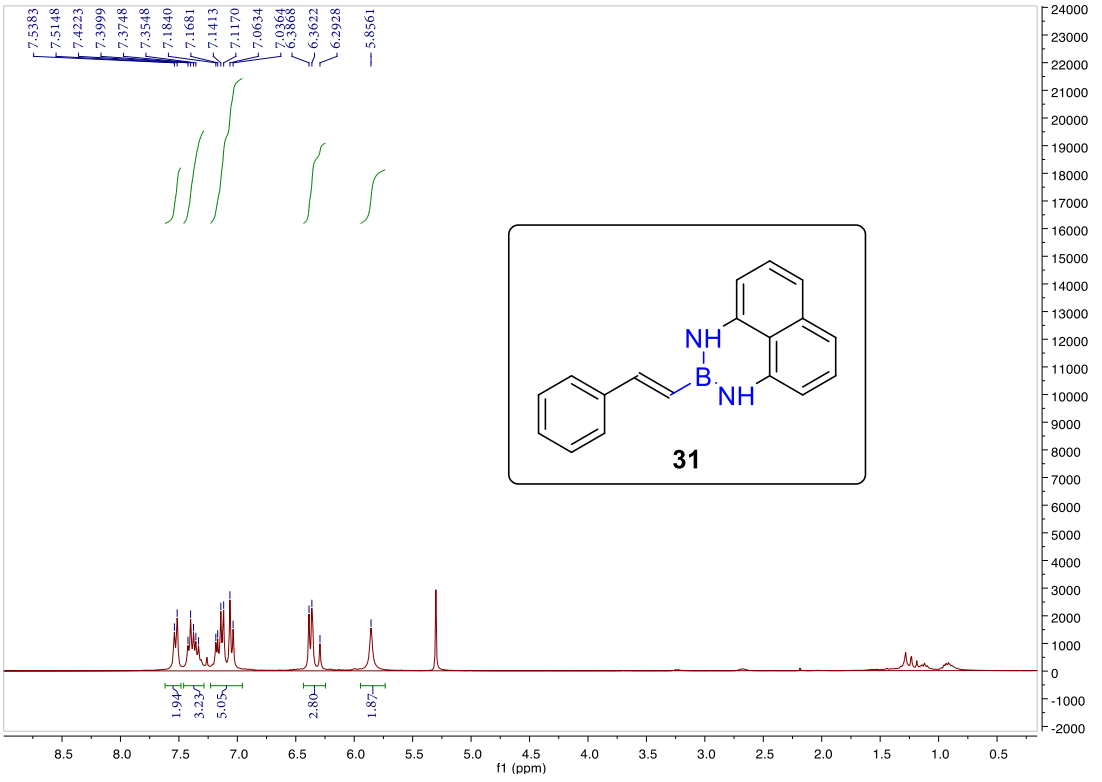
26.14
24.80
24.63
24.40
24.00
O
B
O
30
f1 (ppm)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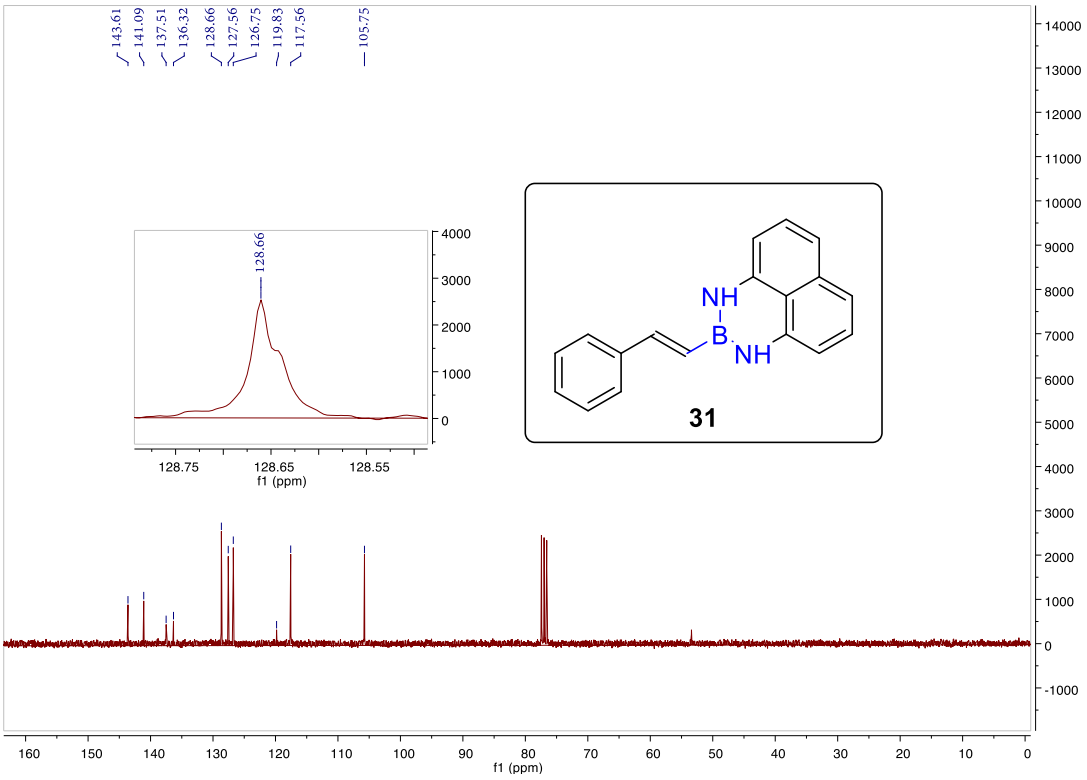
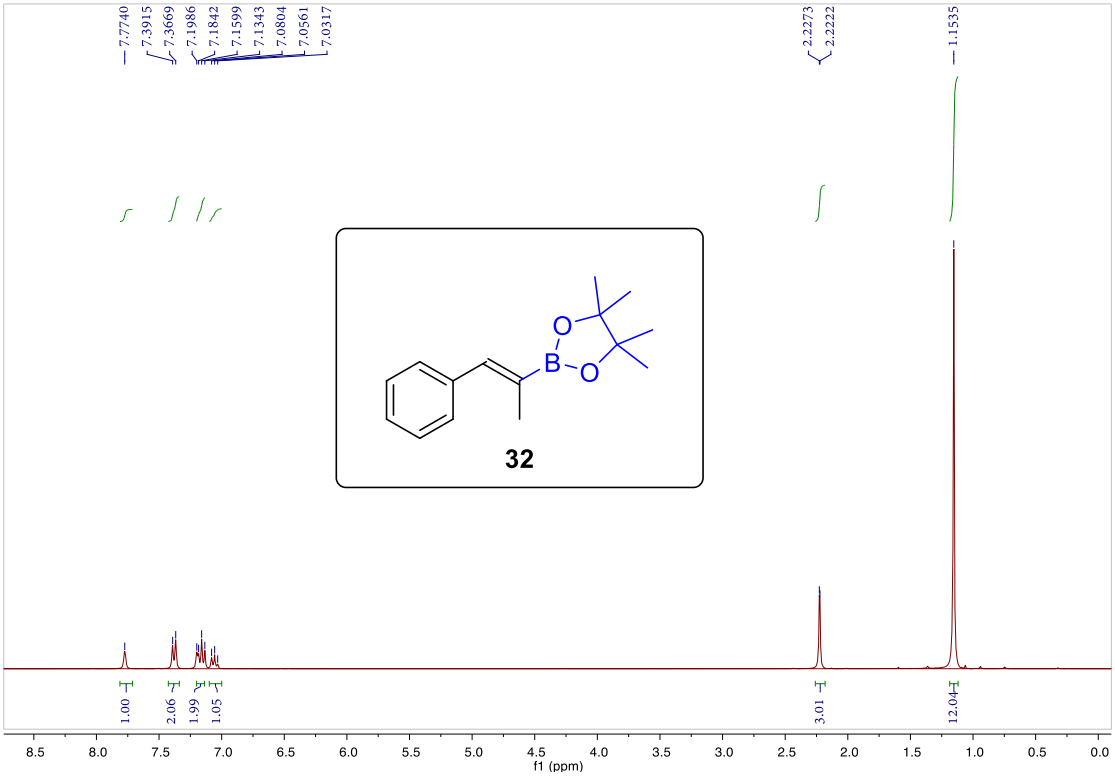
7.4223
7.3999
7.3748
7.3548
7.1840
7.1681
7.1413
7.1170
7.0634
7.0364
6.3868
6.3622
6.2928
5.8561
NH
B
NH
31
1.94
3.23
5.05
2.80
1.87
f1 (ppm)


143.61
141.09
137.51
136.32
128.66
127.56
126.75
119.83
117.56
105.75
128.66
128.75
128.65
128.55
f1 (ppm)
NH
B
NH
31
f1 (ppm)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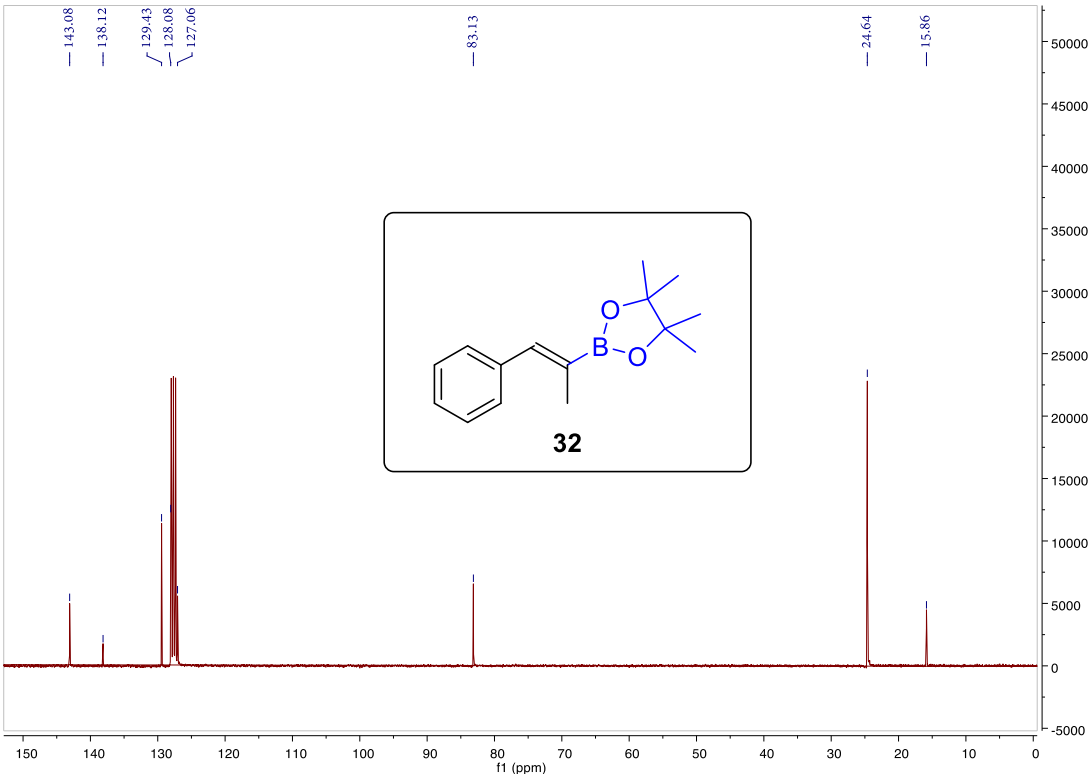
7.3915
7.3669
7.1986
7.1842
7.1599
7.1343
7.0804
7.0561
7.0317
2.2273
2.2222
1.1535
O
B
O
32
1.00
2.06
1.99
1.05
3.01
12.04
f1 (ppm)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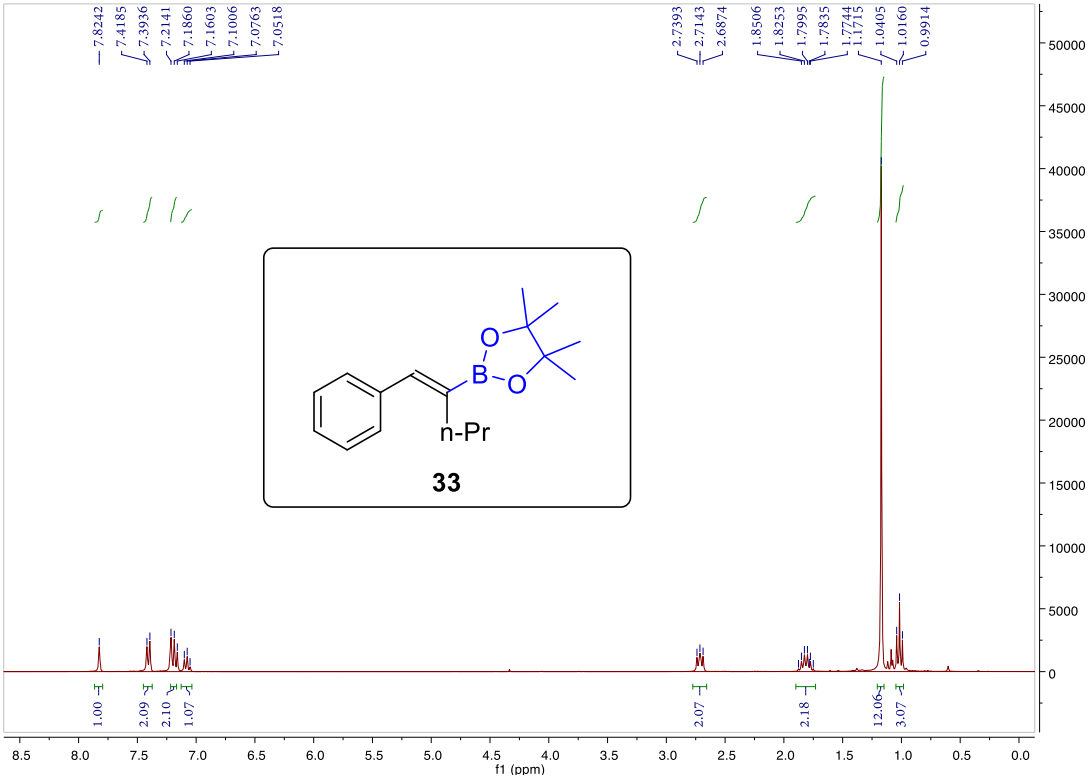
128.08
127.06
83.13
24.64
15.86
O
B
O
32
f1 (ppm)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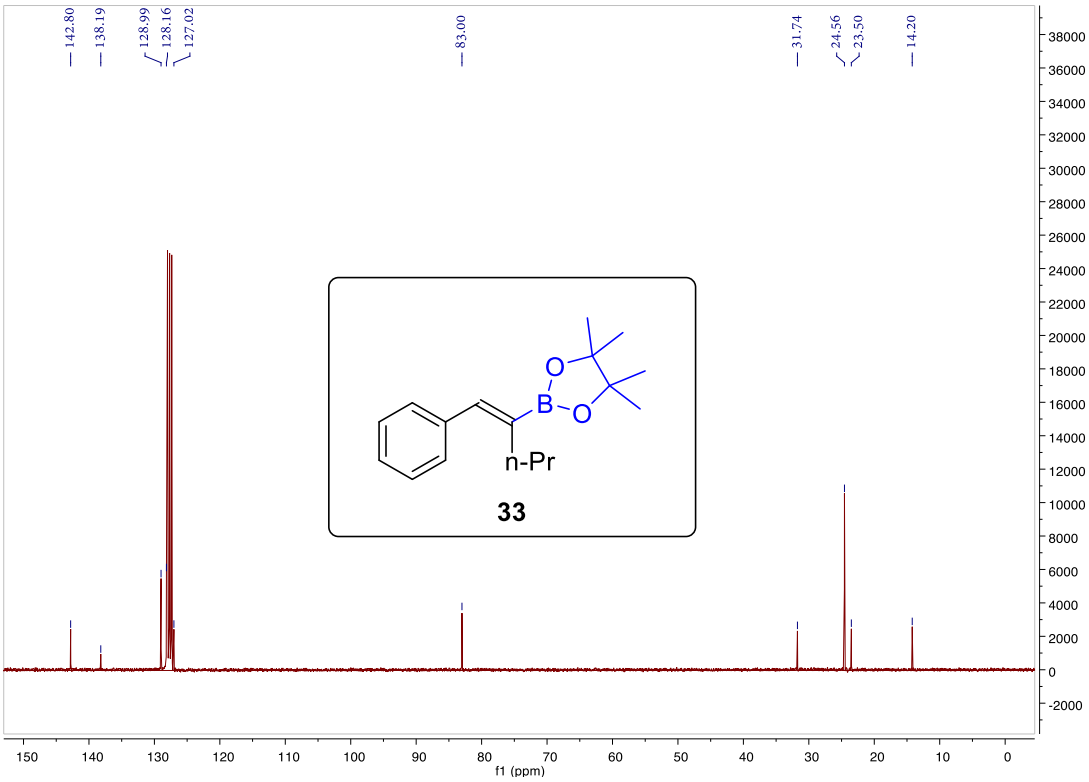
7.3936
7.2141
7.1860
7.1603
7.1006
7.0763
7.0518
2.7393
2.7143
2.6874
1.8506
1.8253
1.7995
1.7835
1.7744
1.1715
1.0405
1.0160
0.9914
O
B
O
n-Pr
33
1.00
2.09
2.10
1.07
2.07
2.18
12.06
3.07
f1 (ppm)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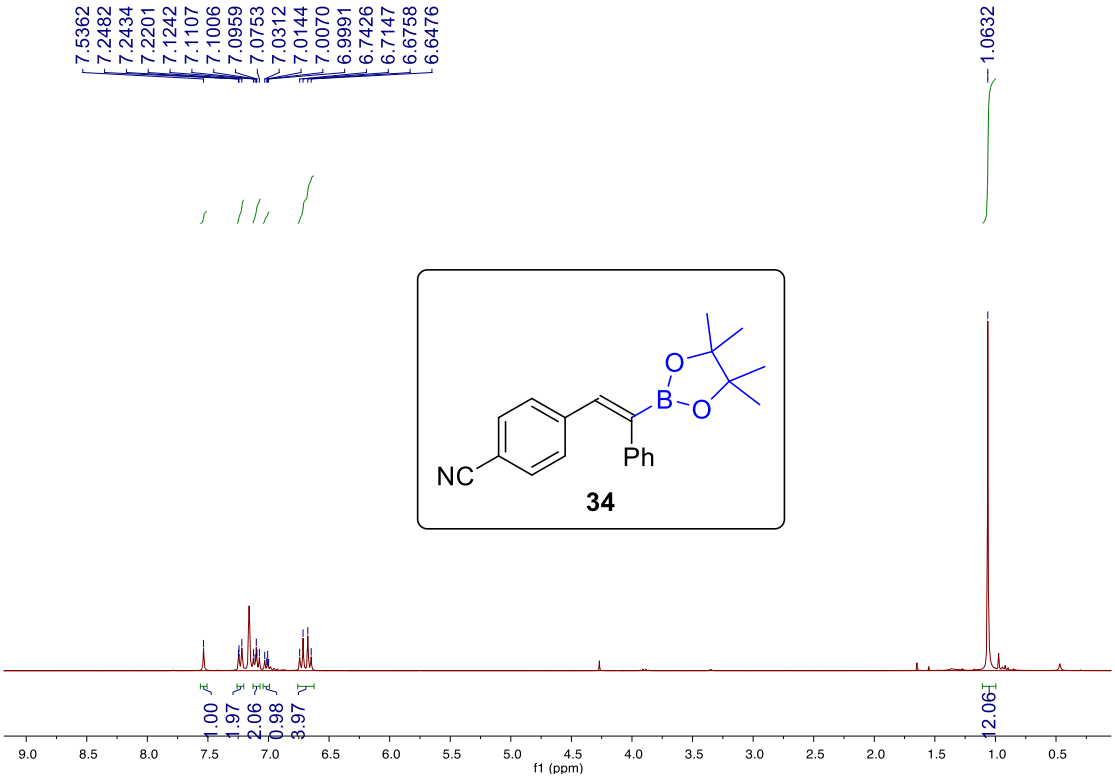
128.16
127.02
83.00
31.74
24.56
23.50
14.20
n-Pr
33
f1 (ppm)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7.2482
7.2434
7.2201
7.1242
7.1107
7.1006
7.0959
7.0753
7.0312
7.0144
7.0070
6.9991
6.7426
6.7147
6.6758
6.6476
1.0632
NC
Ph
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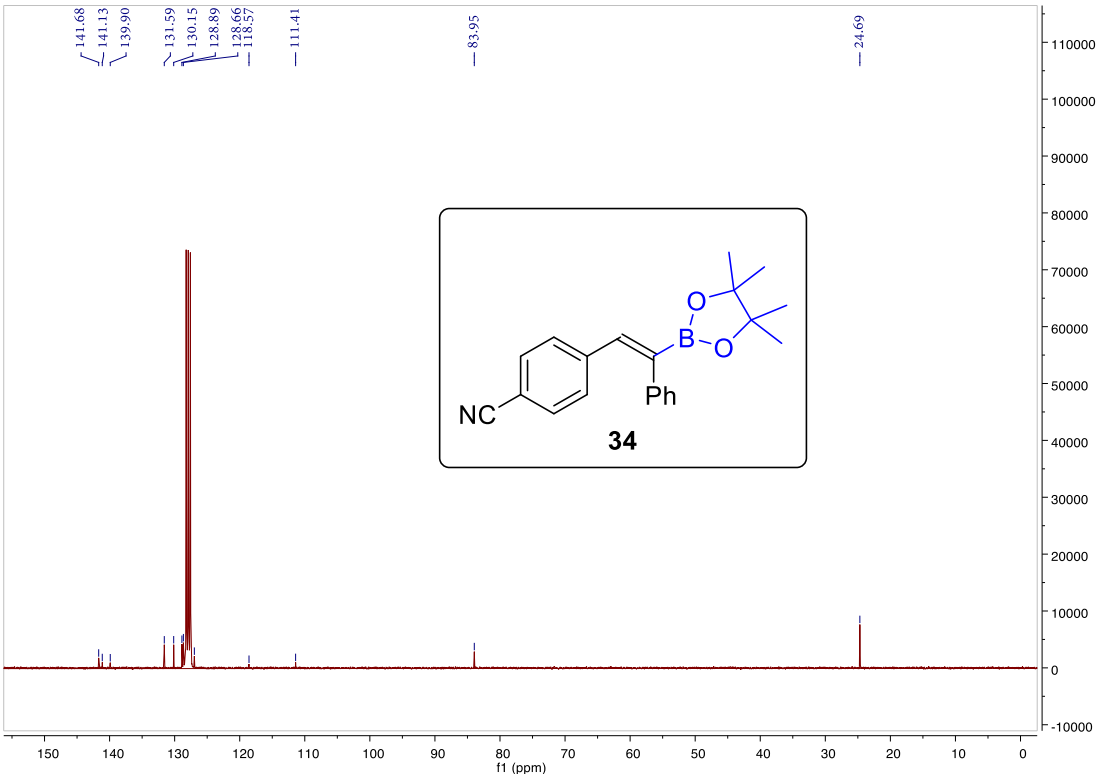
1.97
2.06
0.98
3.97
12.06
f1 (ppm)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139.90
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118.57
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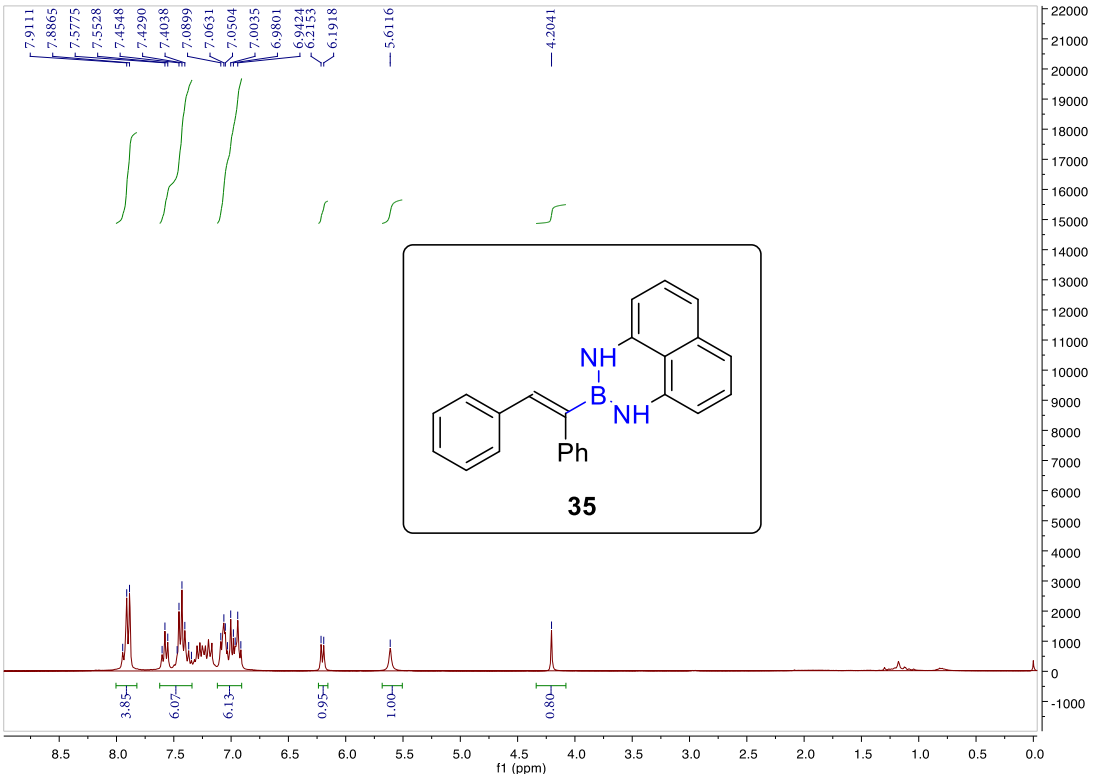
83.95
24.69
NC
Ph
O
B
O
34
f1 (ppm)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7.4290
7.4038
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7.0631
7.0504
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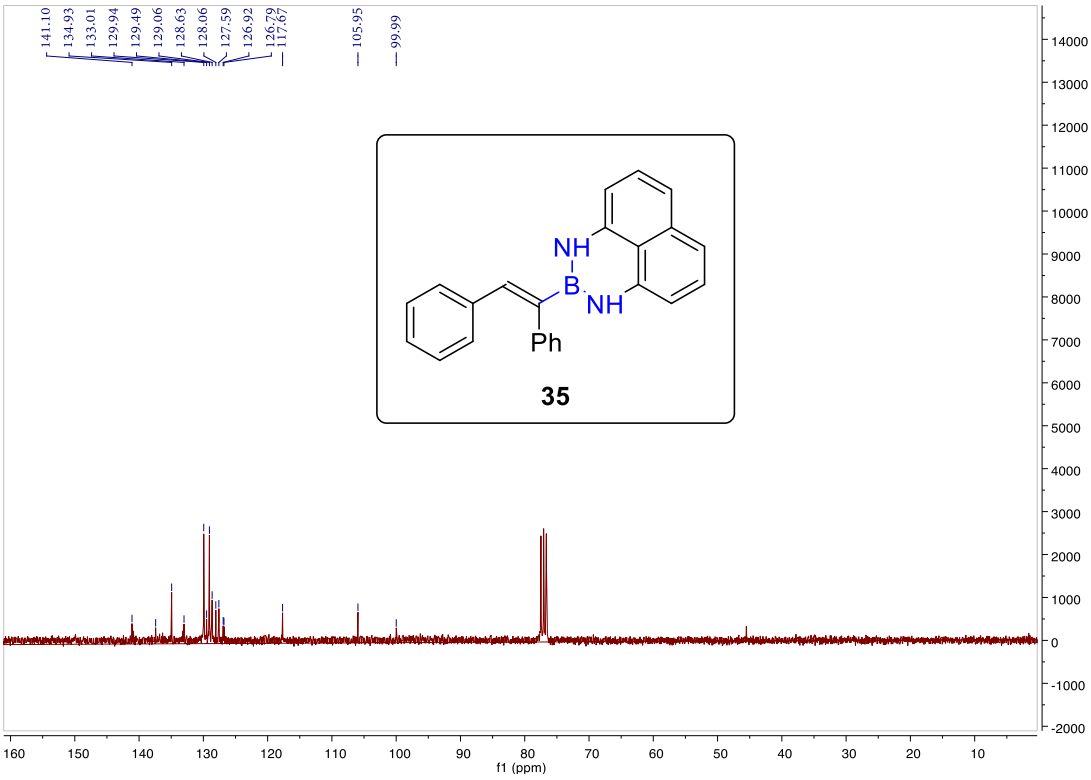
6.9801
6.9424
6.2153
6.1918
5.6116
4.2041
NH
B
NH
Ph
35
3.85
6.07
6.13
0.95
1.00
0.80
f1 (ppm)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129.49
129.06
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128.06
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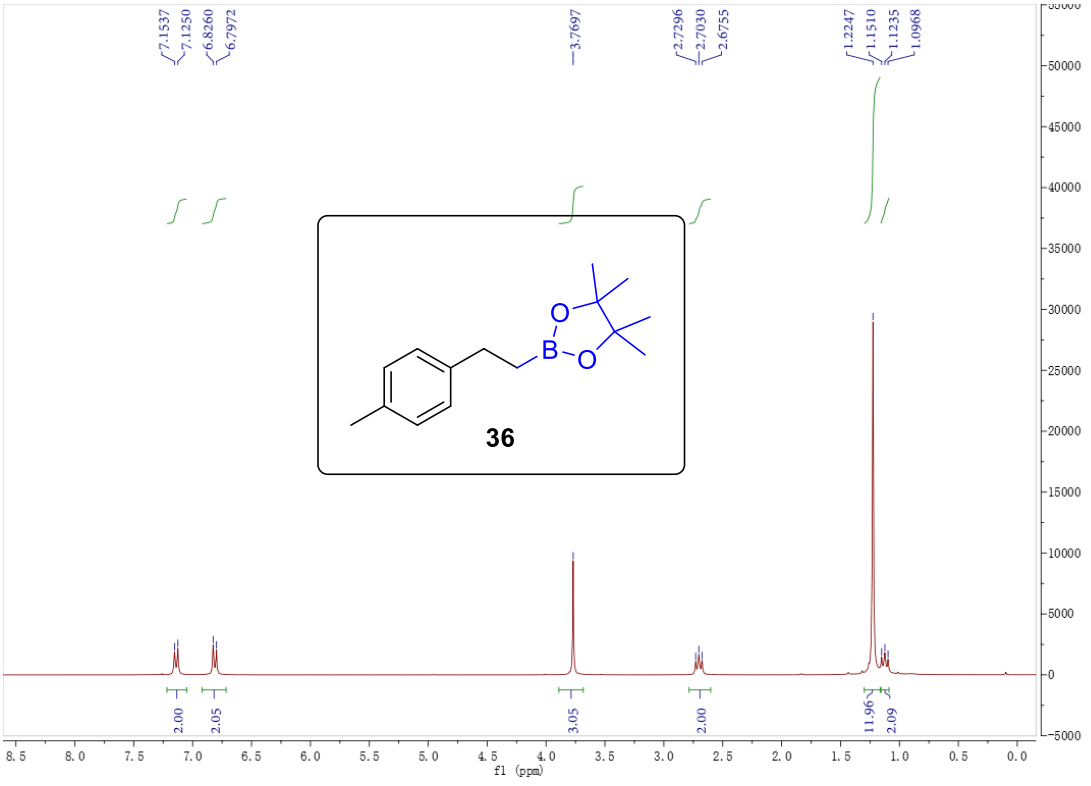
126.79
117.67
105.95
99.99
NH
B
NH
Ph
35
f1 (ppm)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2.7296
2.7030
2.6755
1.2247
1.1510
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1.0968
O
B
O
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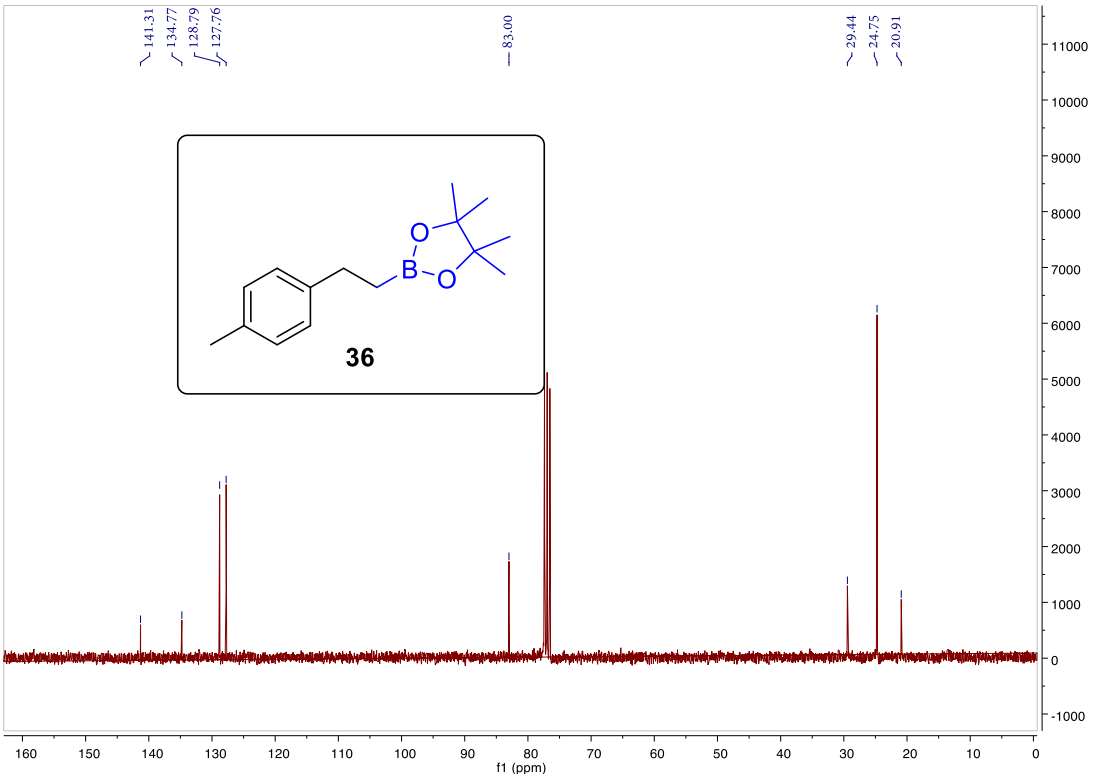
2.00
2.05
3.05
2.00
11.96
2.09
f1 (ppm)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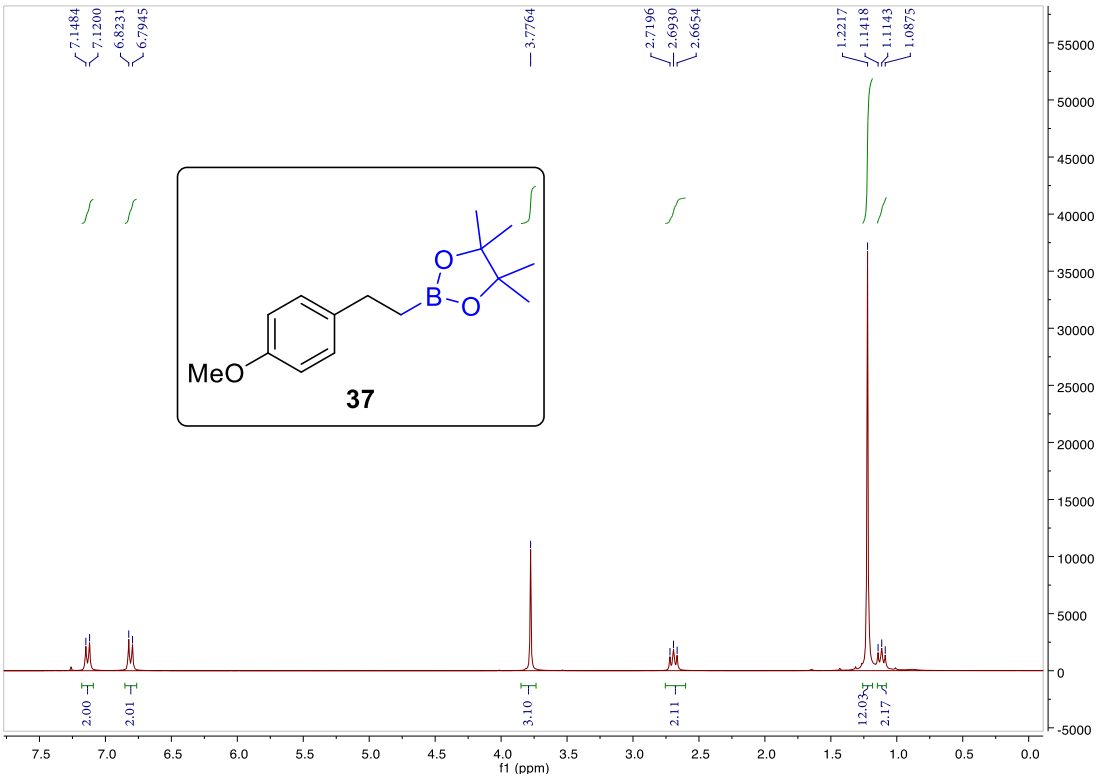
B
O
36
f1 (ppm)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3.7764
2.7196
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2.6654
1.2217
1.1418
1.1143
1.0875
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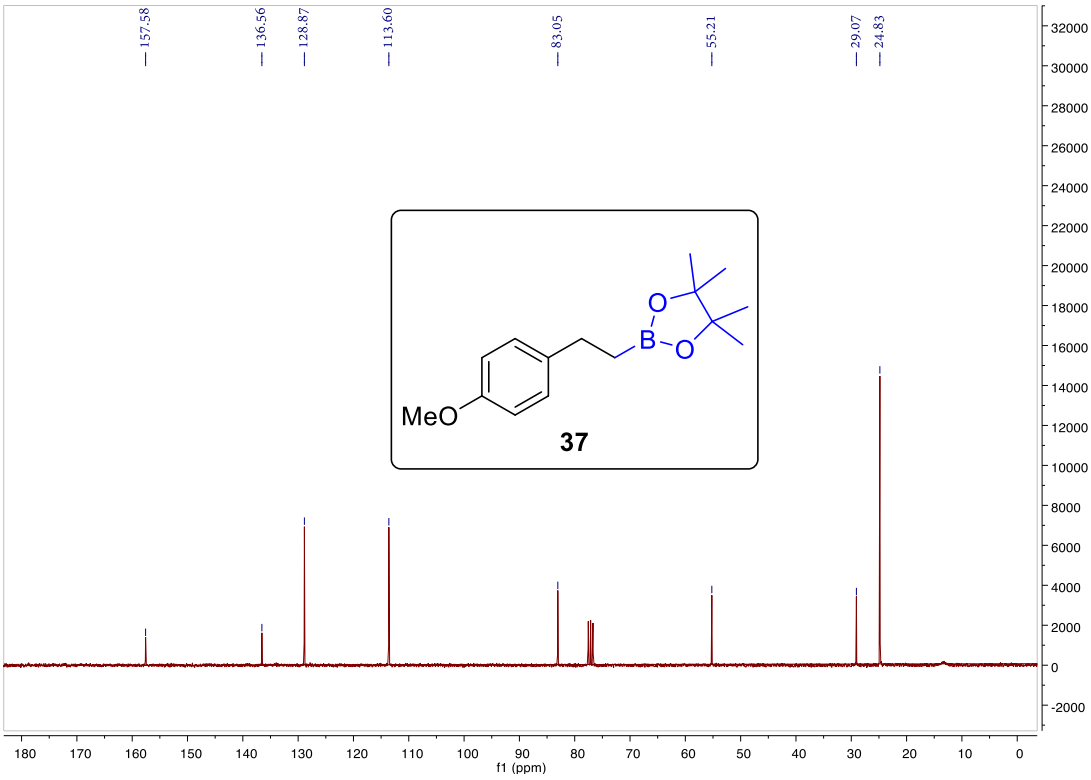
B
O
MeO
37
2.00
2.01
3.10
2.11
12.03
2.17
f1 (ppm)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113.60
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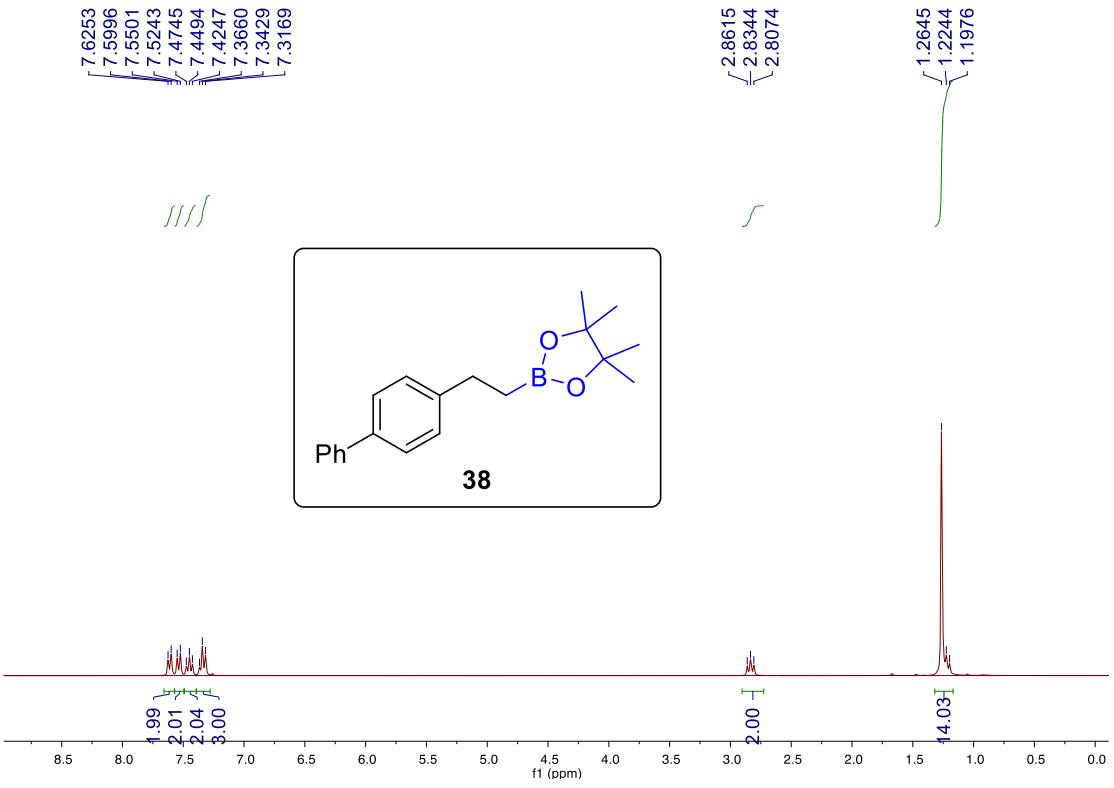
55.21
29.07
24.83
MeO
37
f1 (ppm)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7.3660
7.3429
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2.8615
2.8344
2.8074
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Ph
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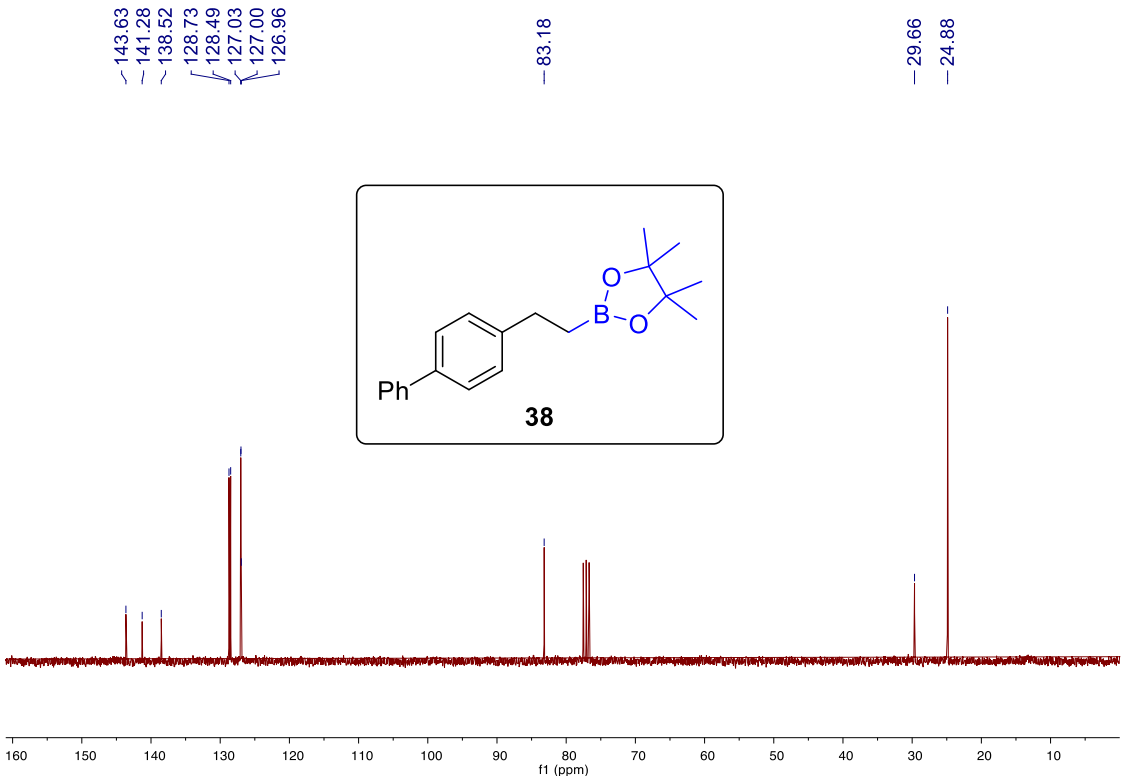
1.99
2.01
2.04
3.00
2.00
14.03
f1 (ppm)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127.00
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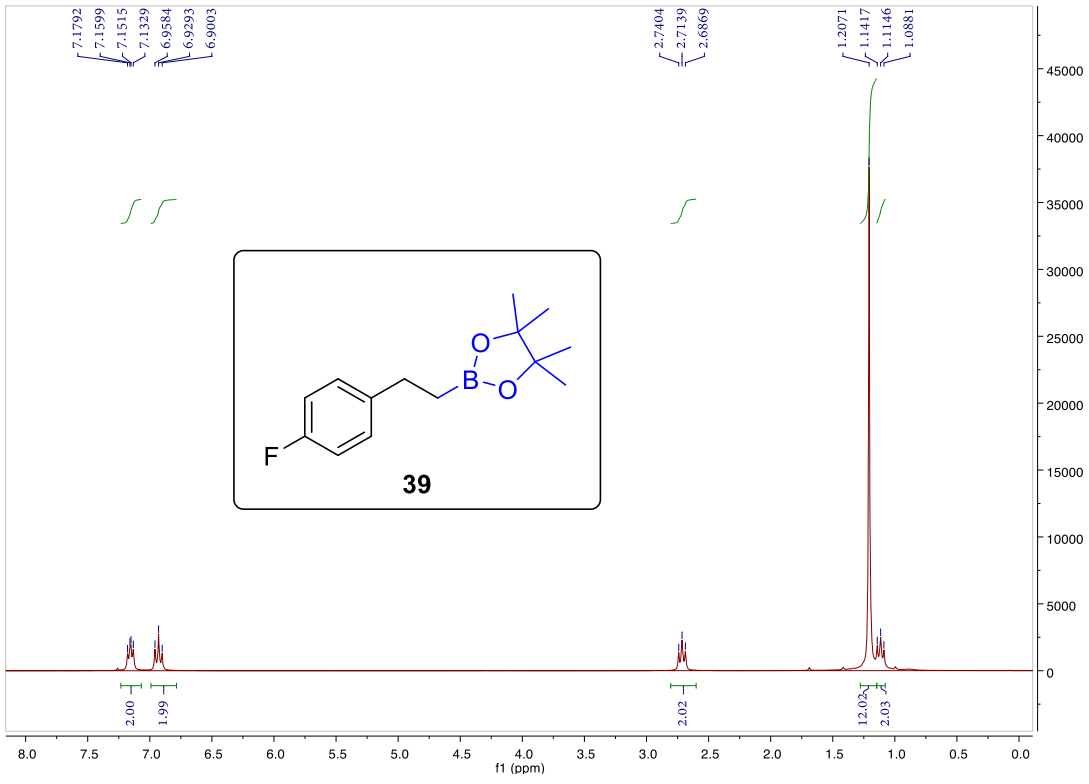
Ph
38
f1 (ppm)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2.6869
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1.0881
F
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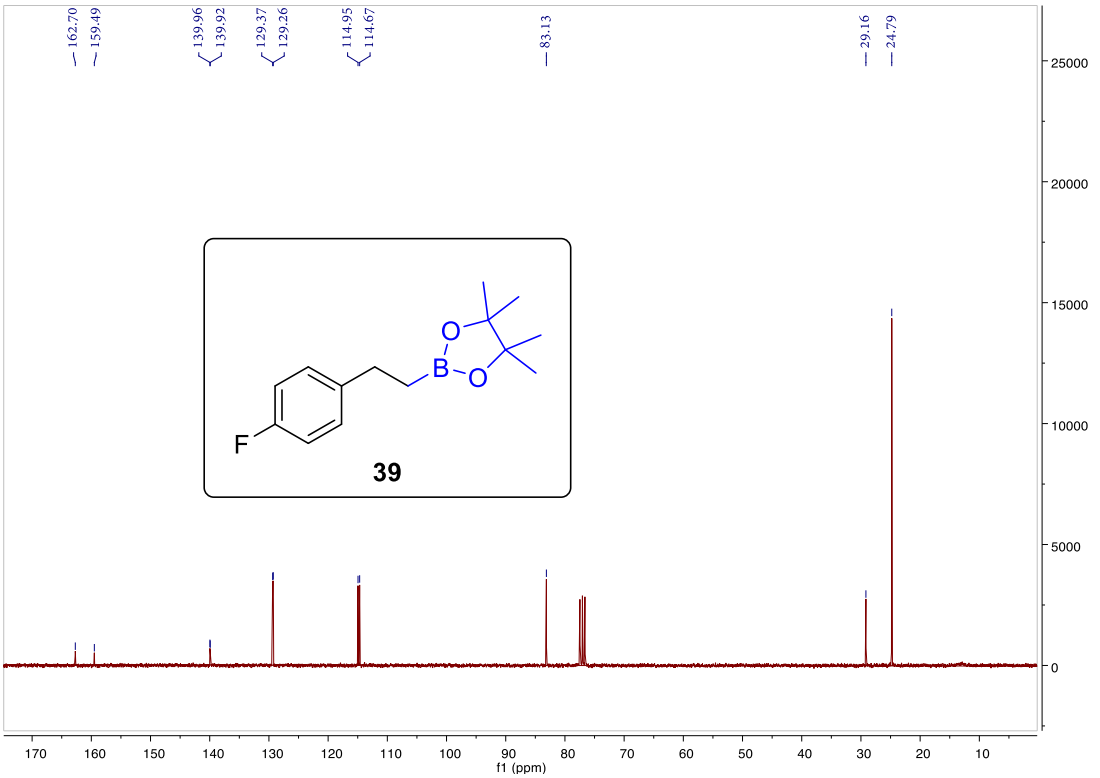
1.99
2.02
12.02
2.03
f1 (ppm)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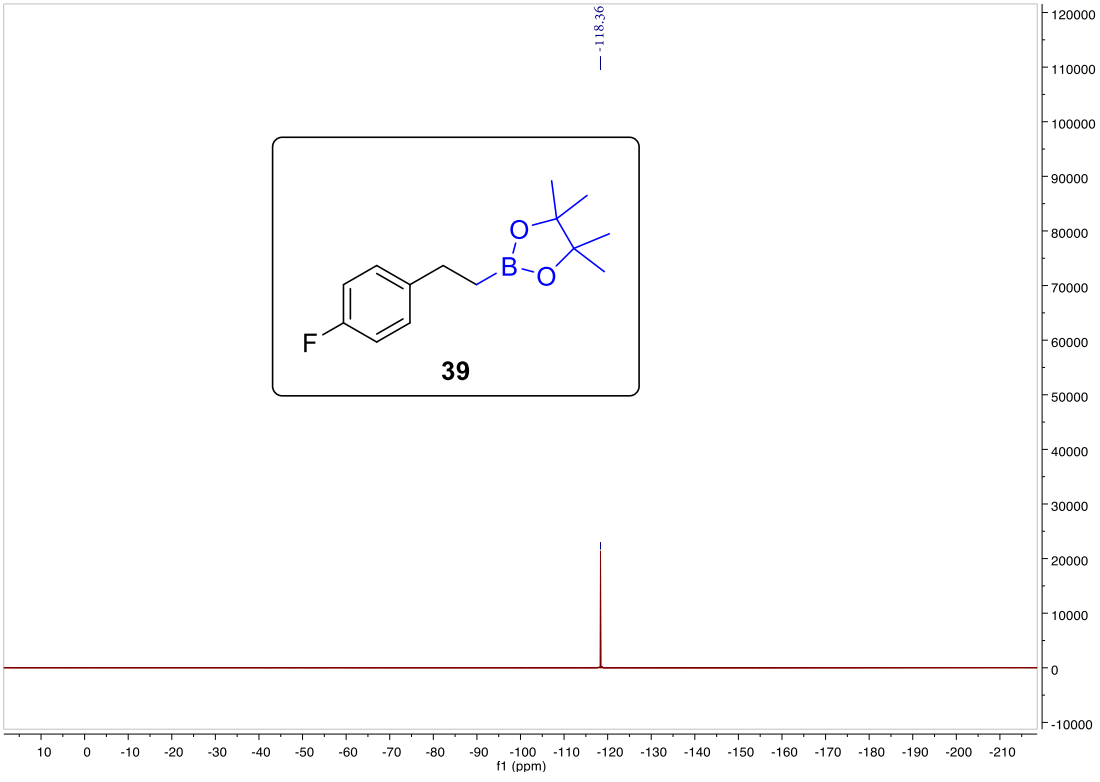
O
B
O
F
39
f1 (ppm)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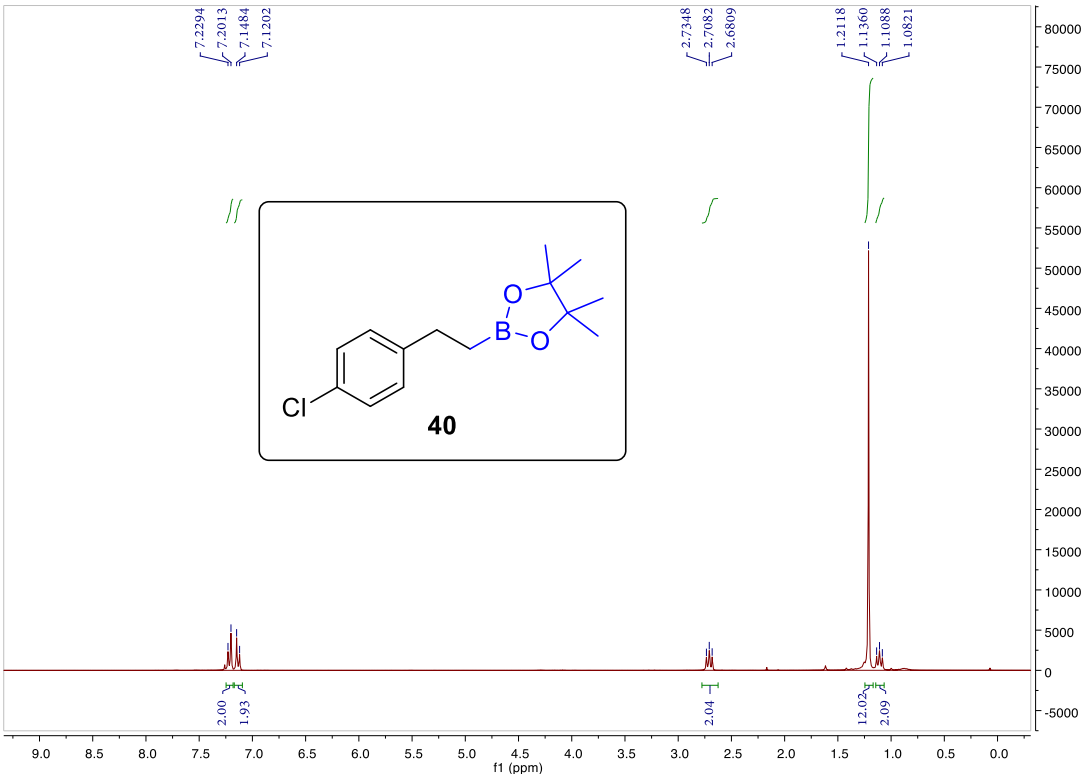
O
F
39
f1 (ppm)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2.6809
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1.1360
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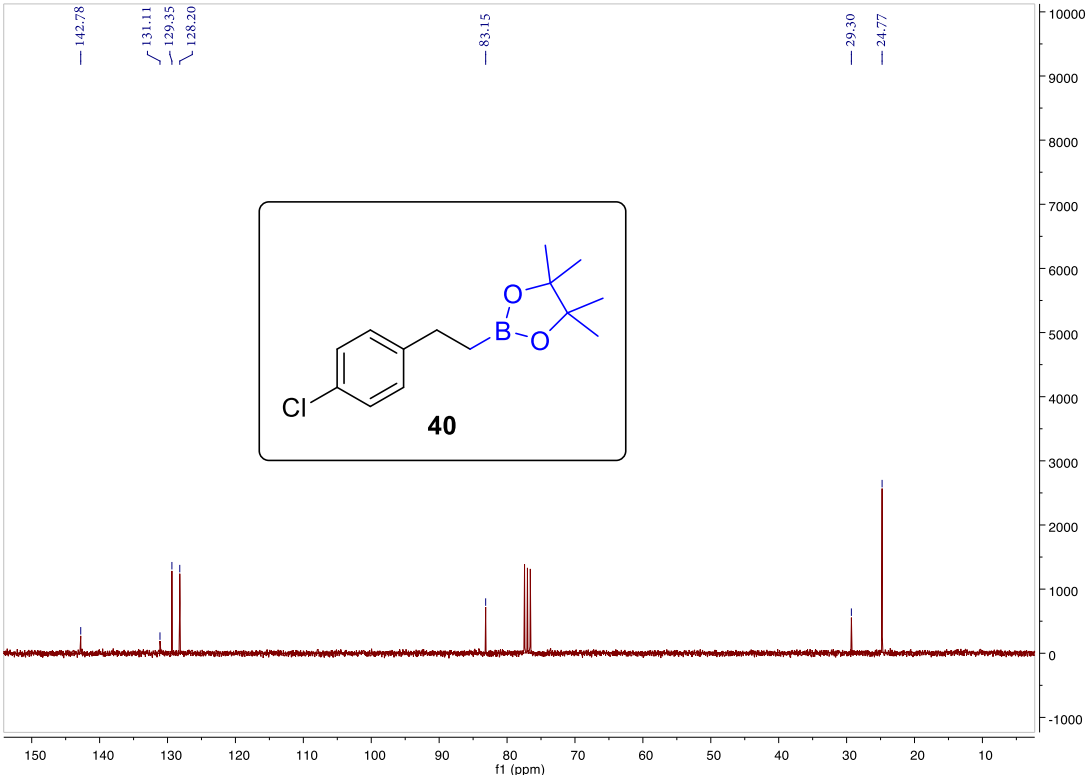
Cl
O
B
O
40
2.00
1.93
2.04
12.02
2.09
f1 (ppm)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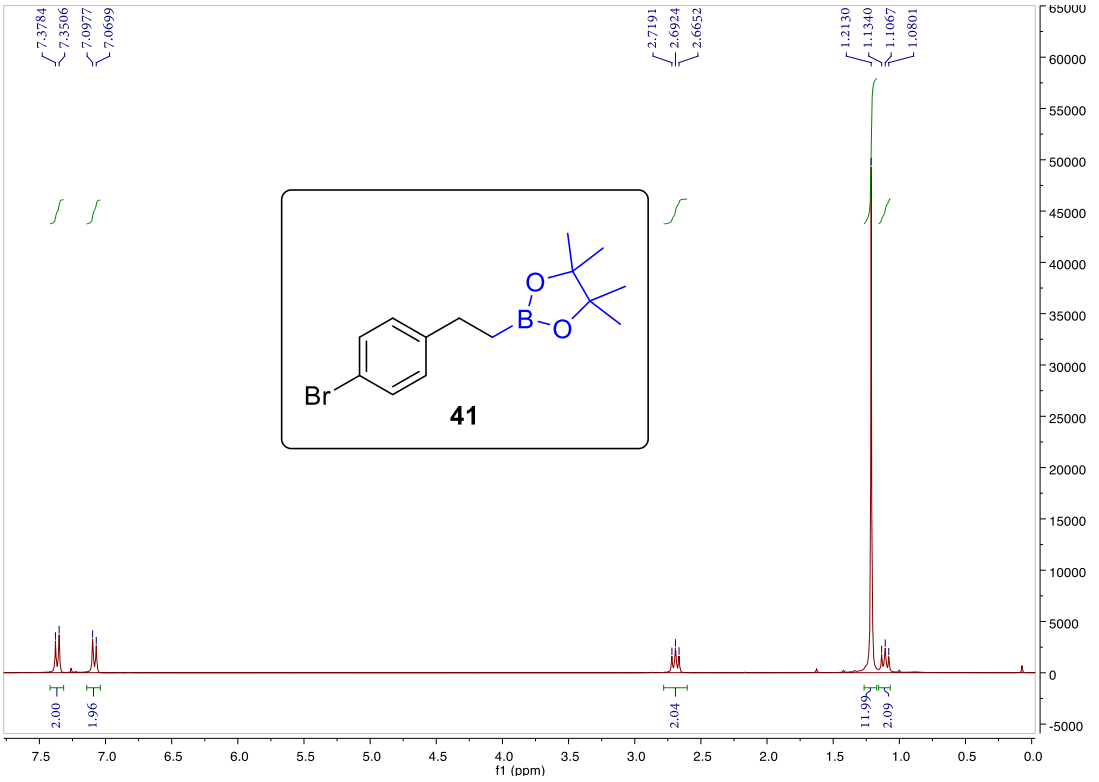
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Br
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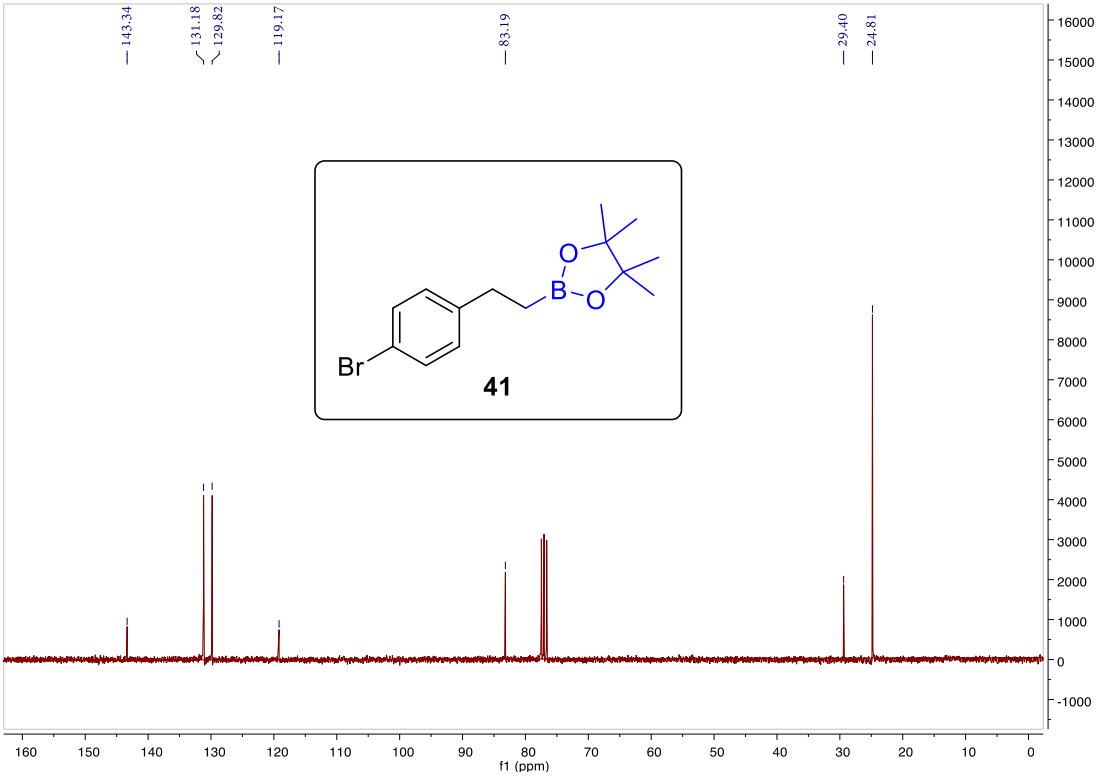
2.09
f1 (ppm)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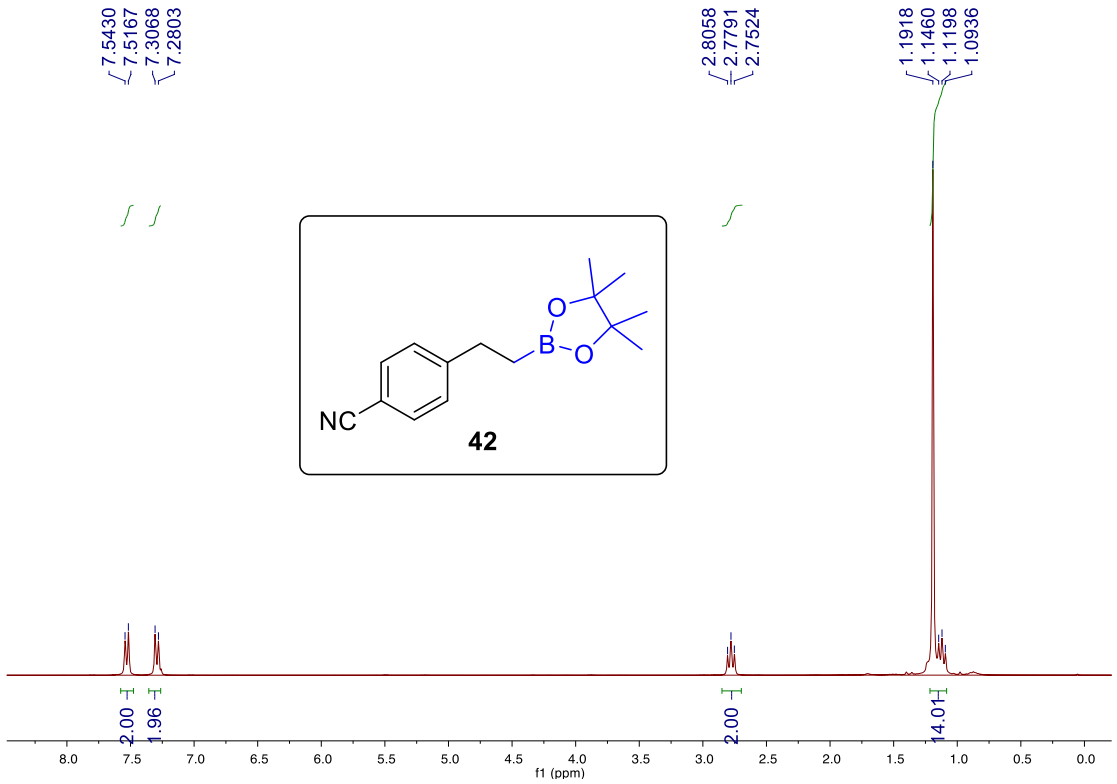
f1 (ppm)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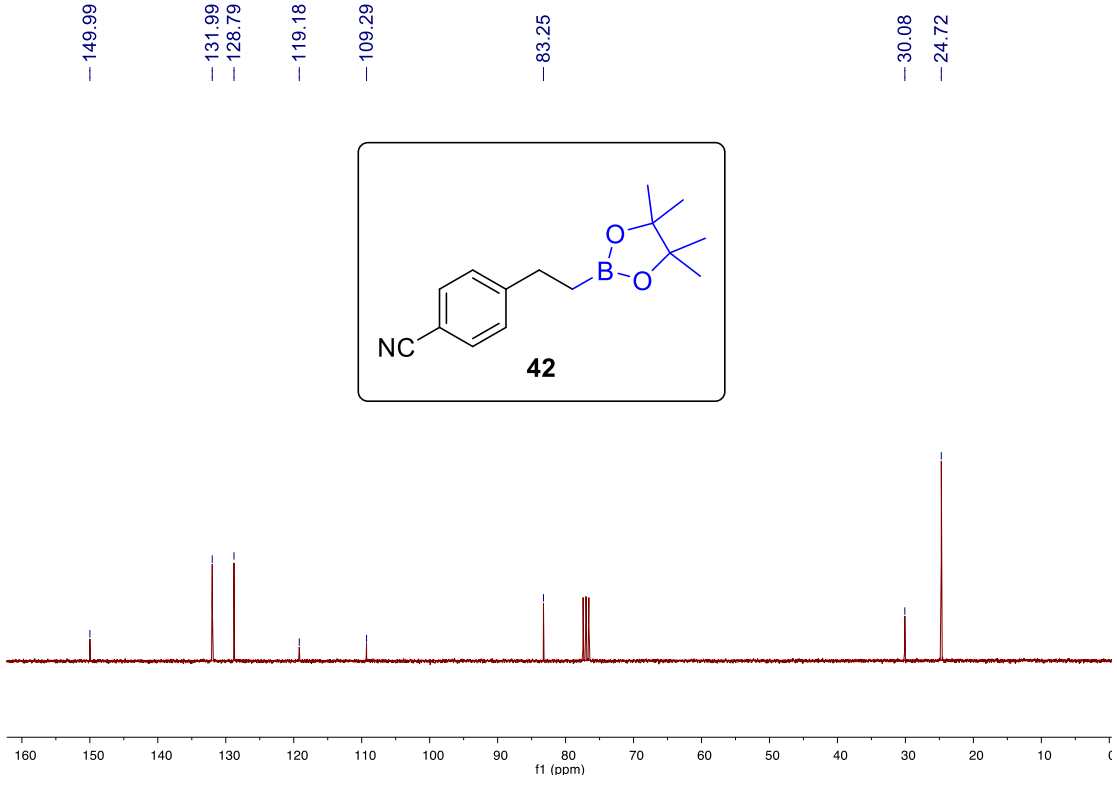
14.01
f1 (ppm)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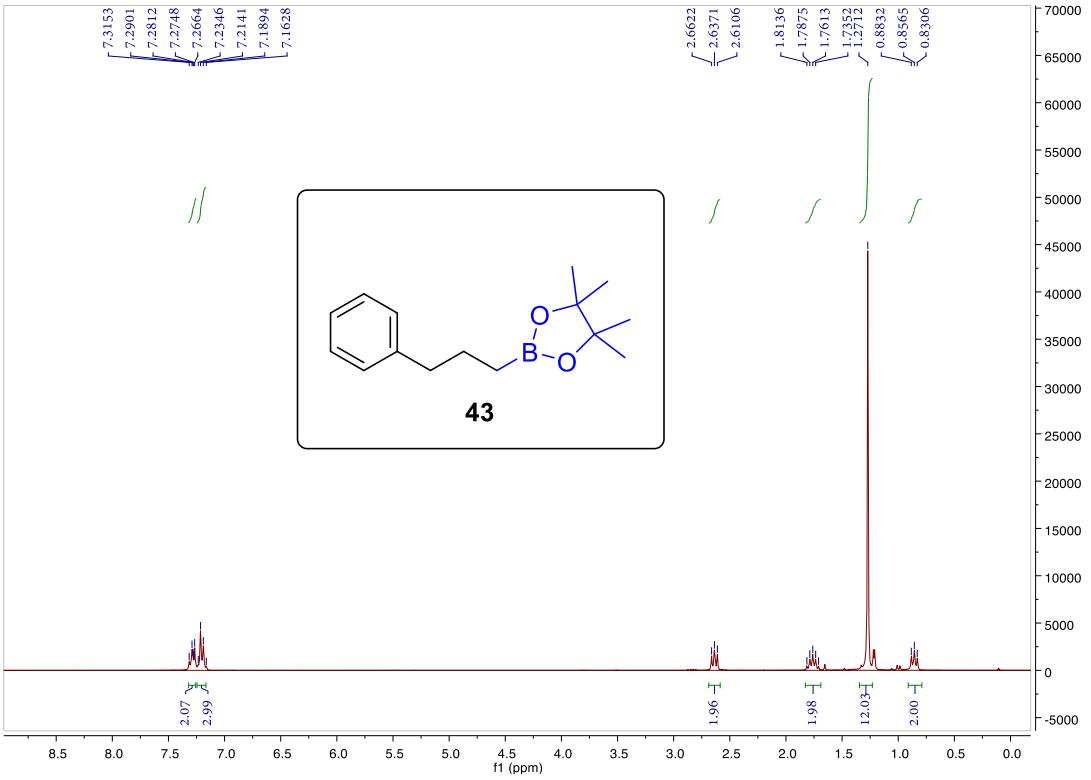
30.08
24.72
NC
42
f1 (ppm)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2.6106
1.8136
1.7875
1.7613
1.7352
1.2712
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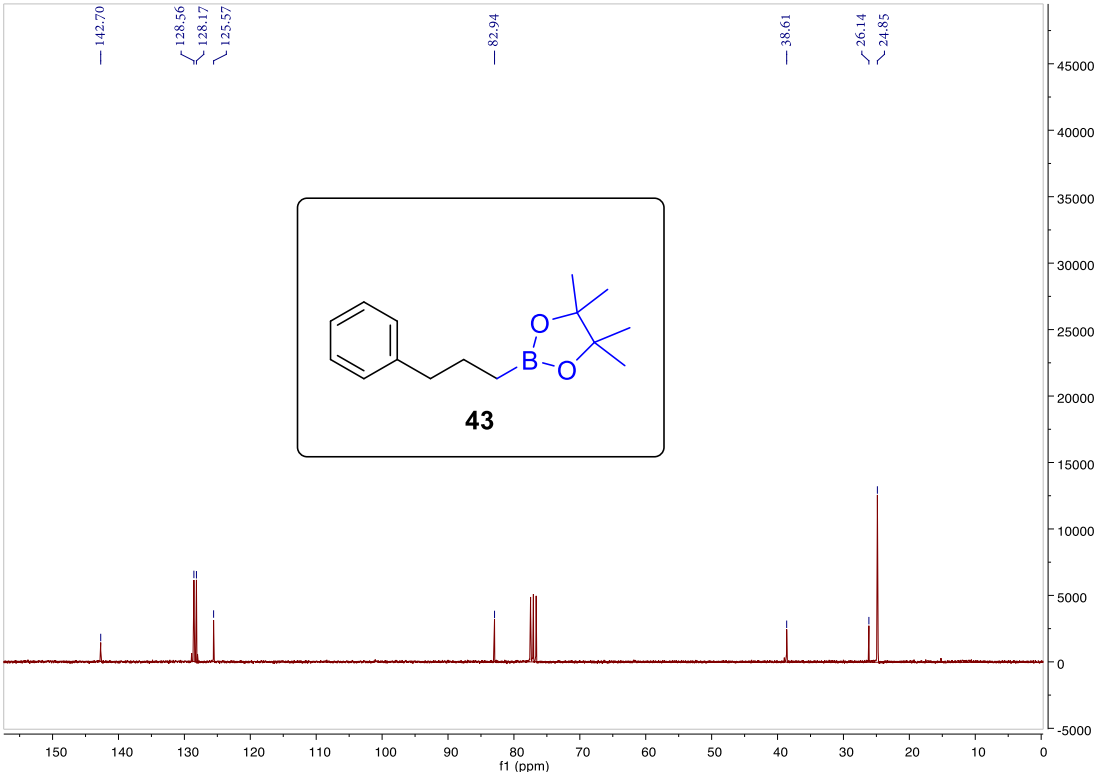
f1 (ppm)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38.61
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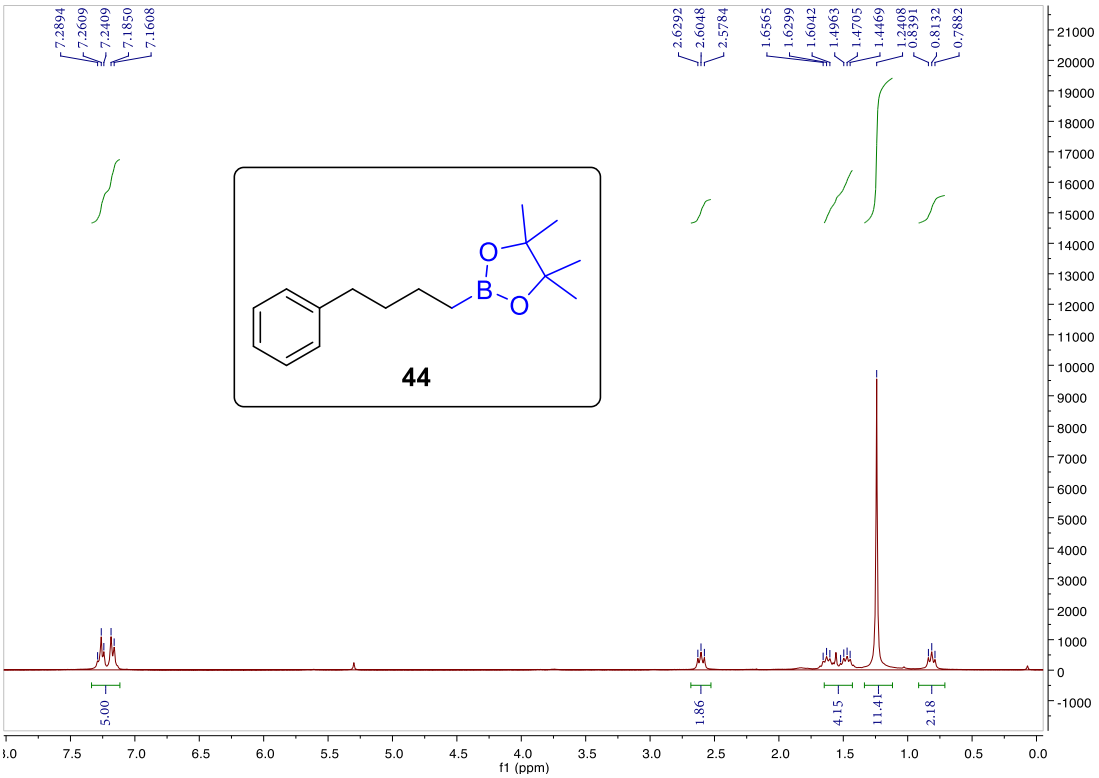
24.85
43
f1 (ppm)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1.4963
1.4705
1.4469
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0.8132
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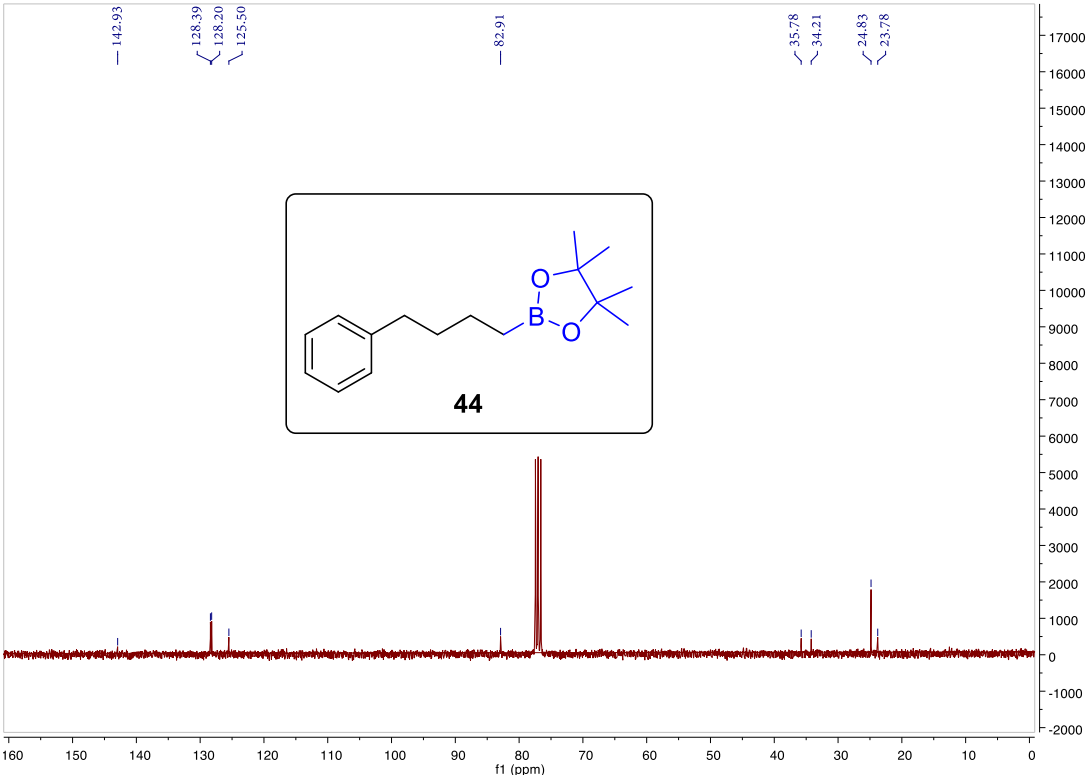
2.18
f1 (ppm)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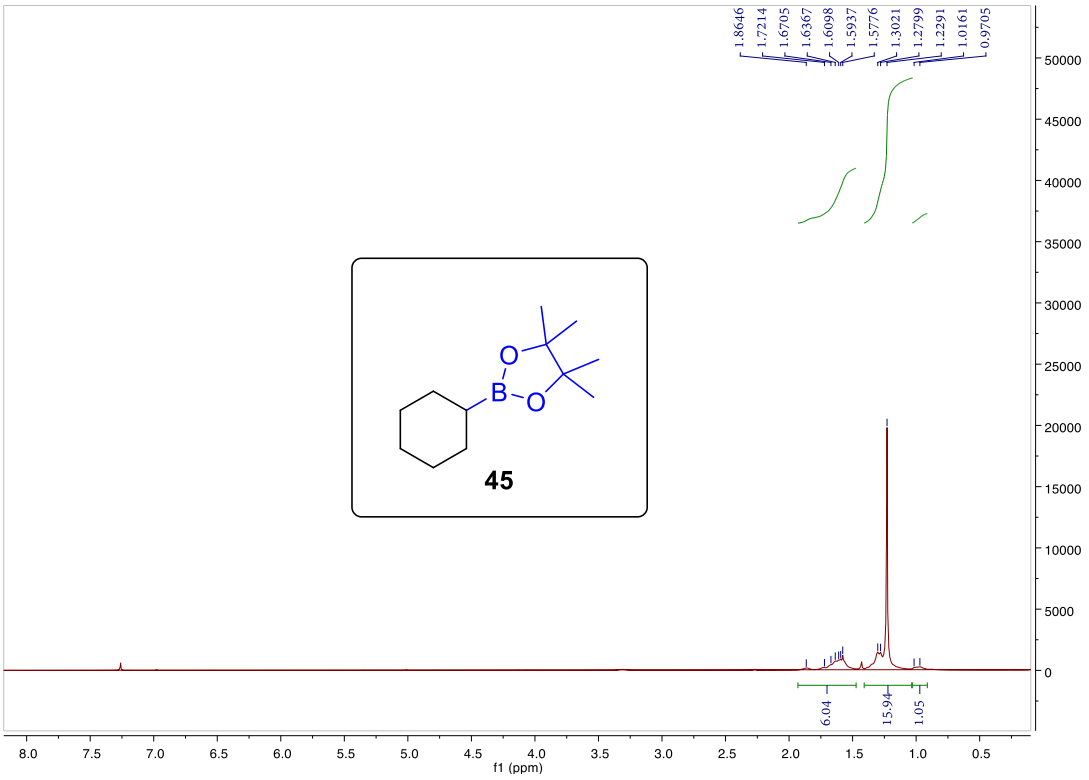
82.91
35.78
34.21
24.83
23.78
44
f1 (ppm)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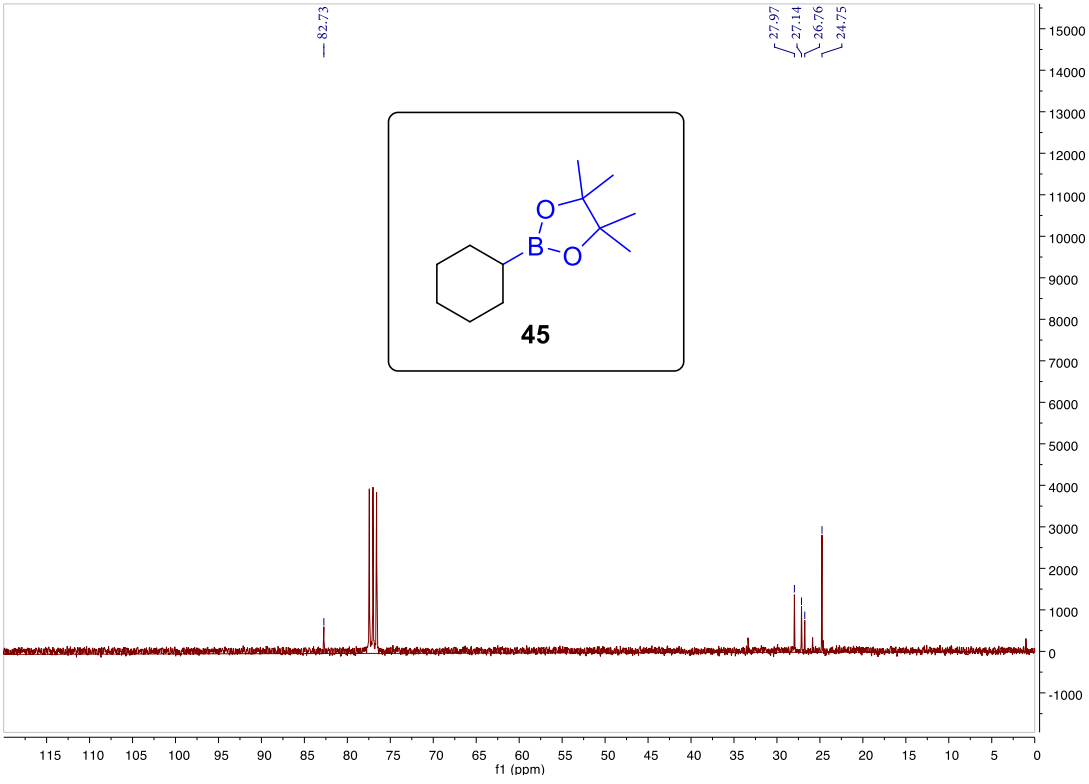
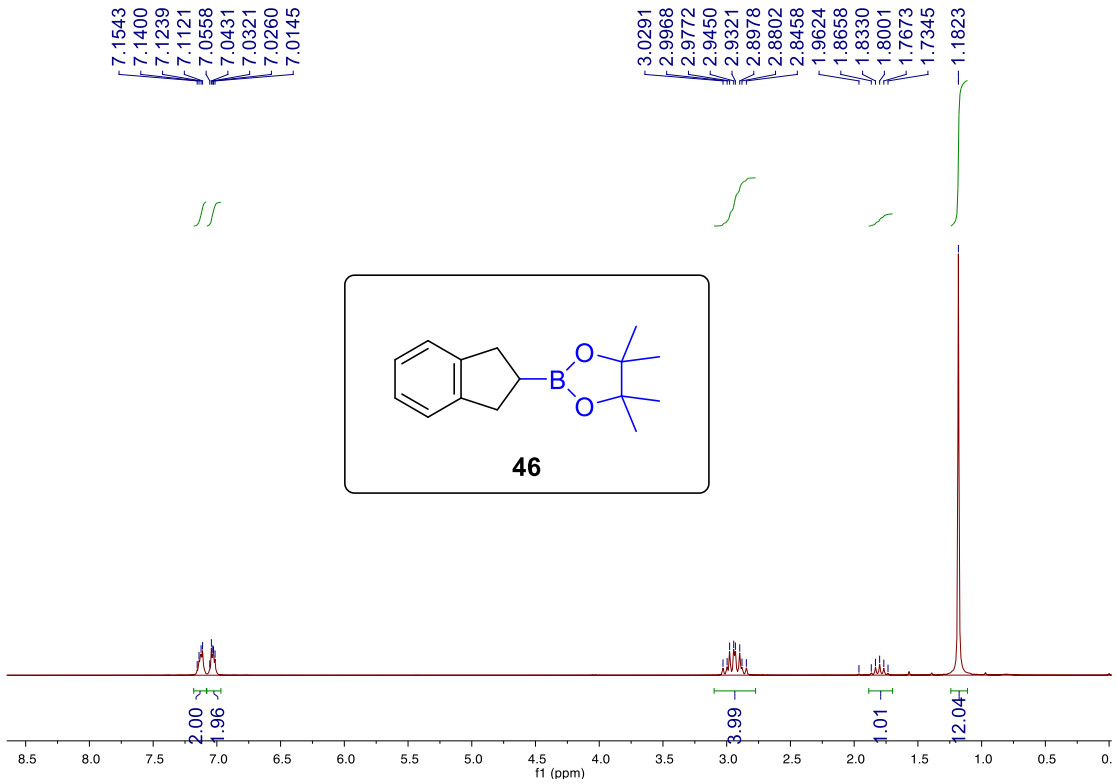
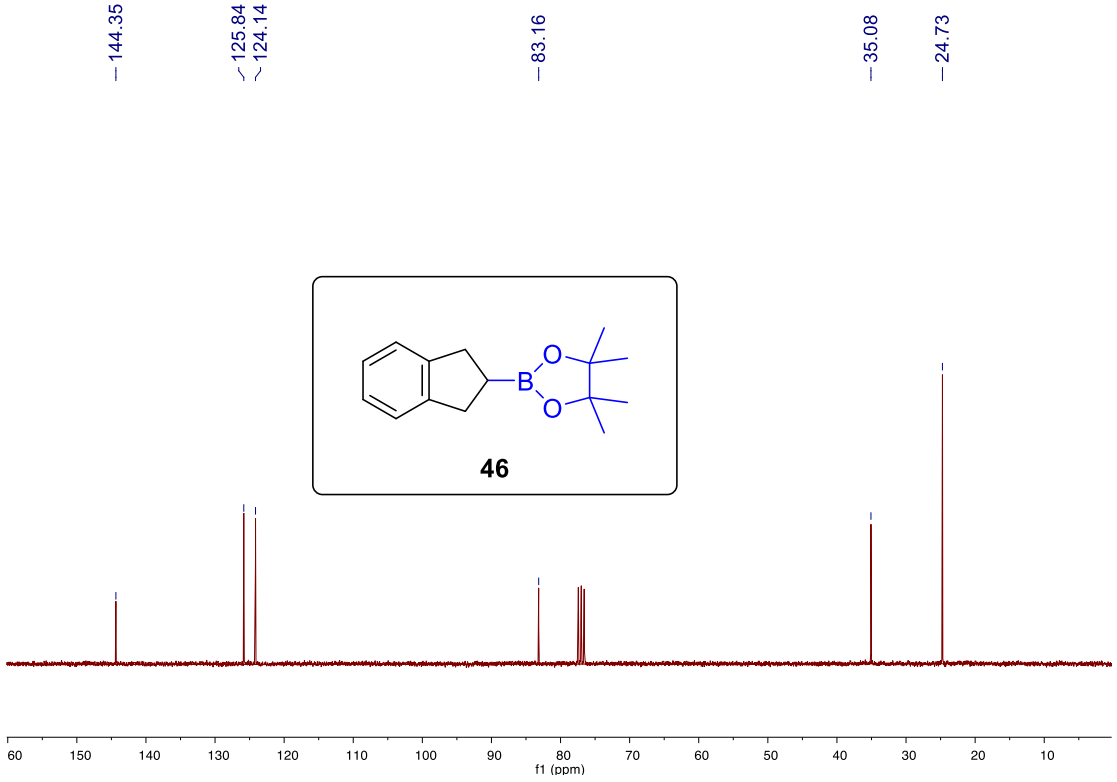
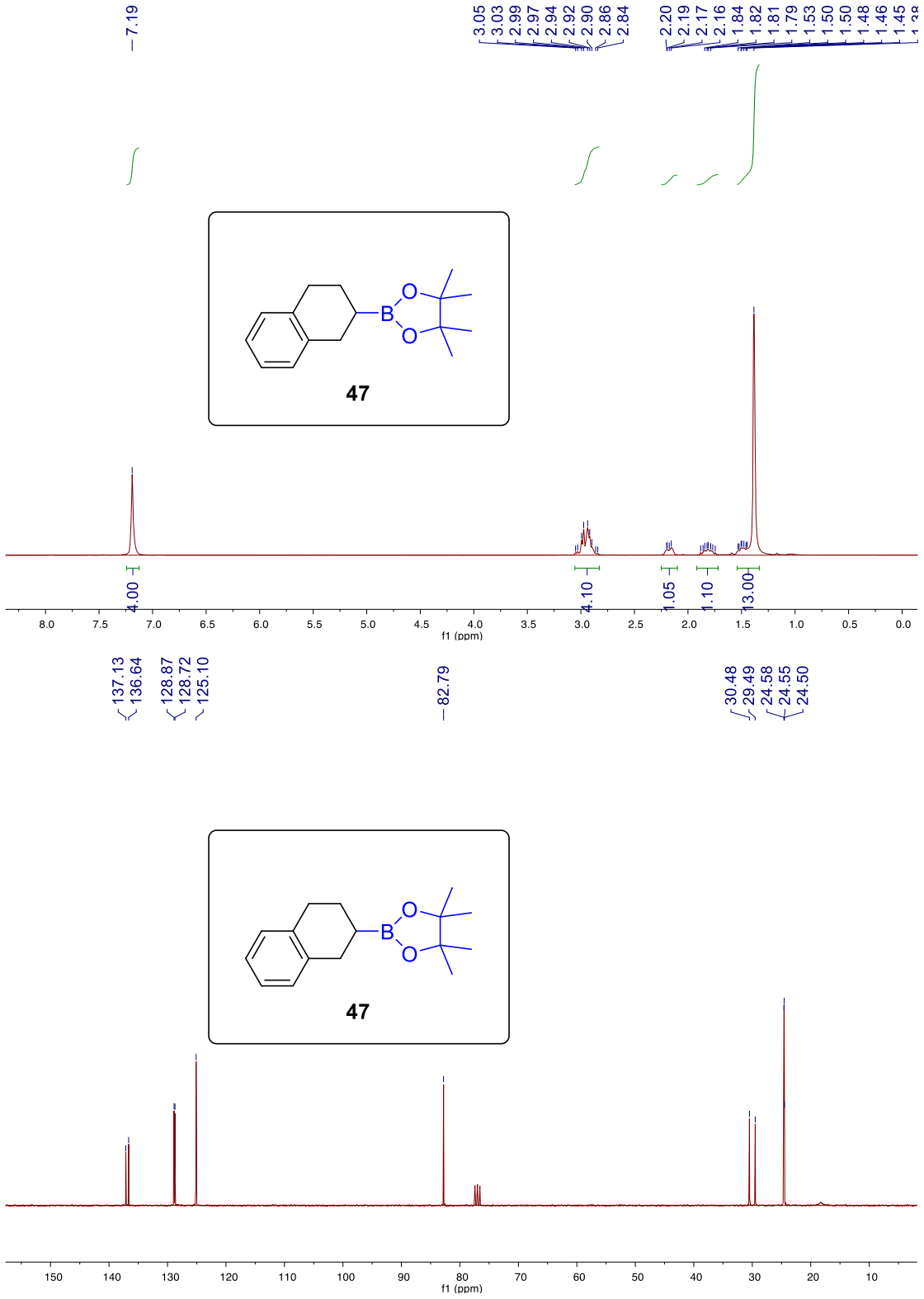
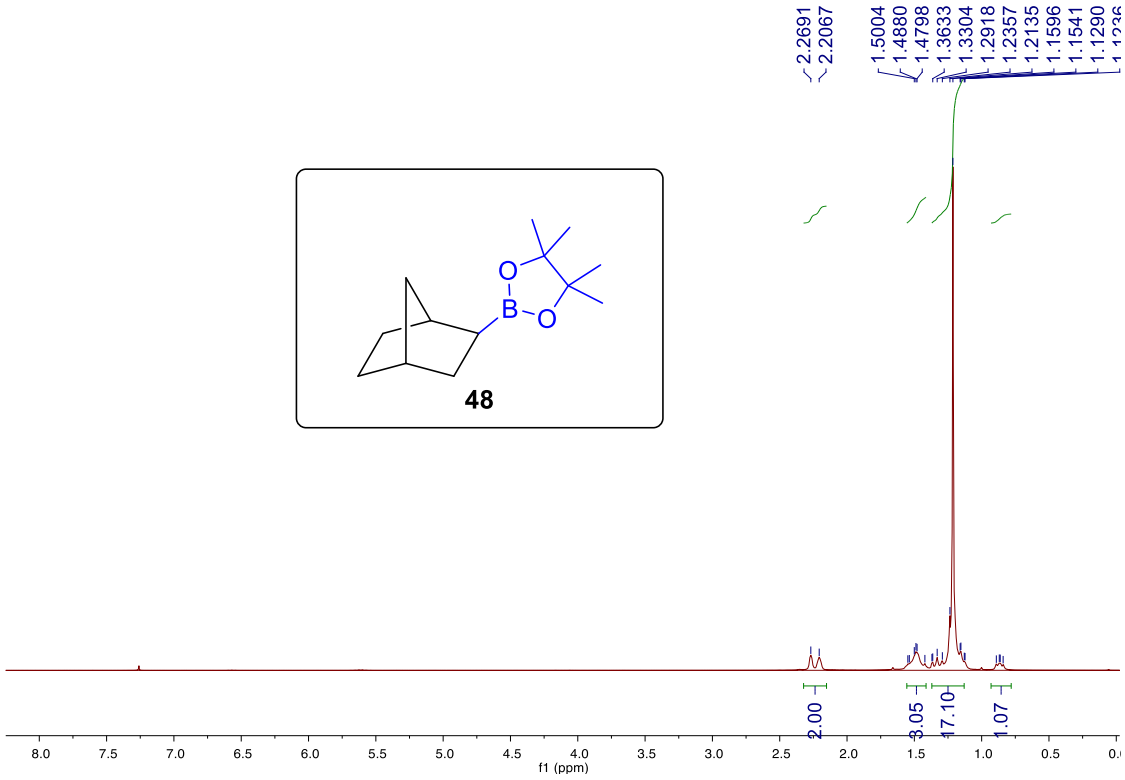
1.05
f1 (ppm)

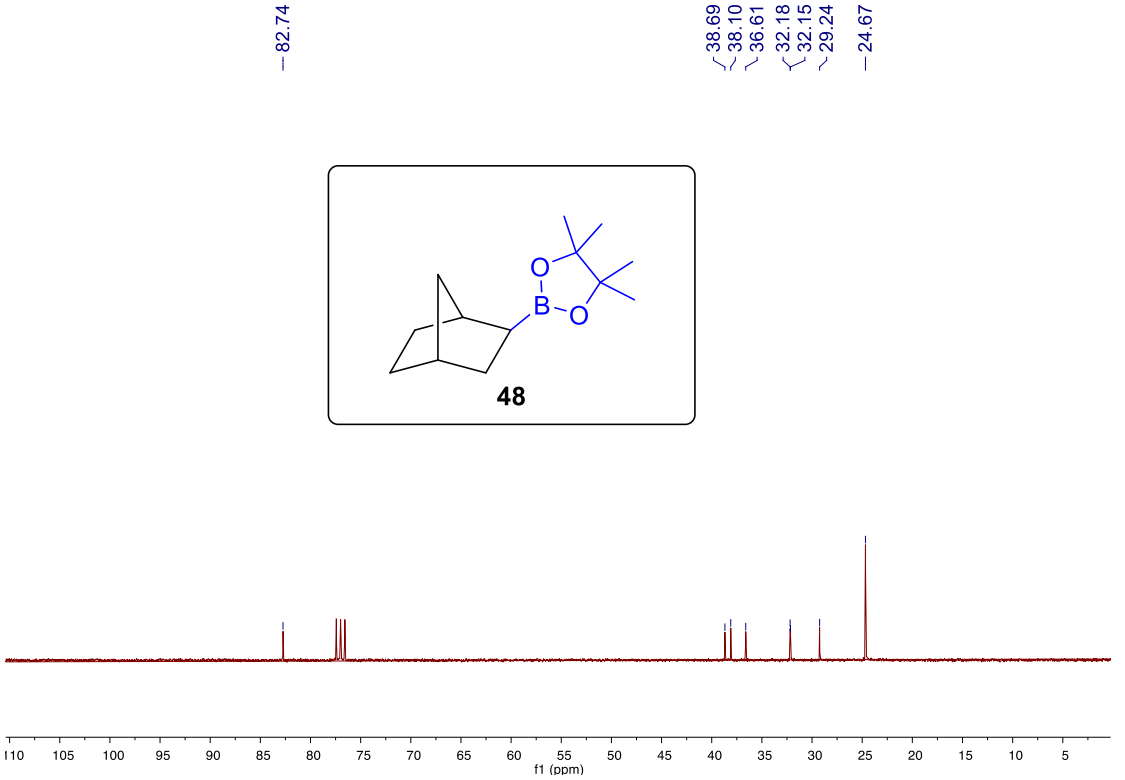

82.73
27.97
27.14
26.76
24.75
O
B
O
45
f1 (ppm)

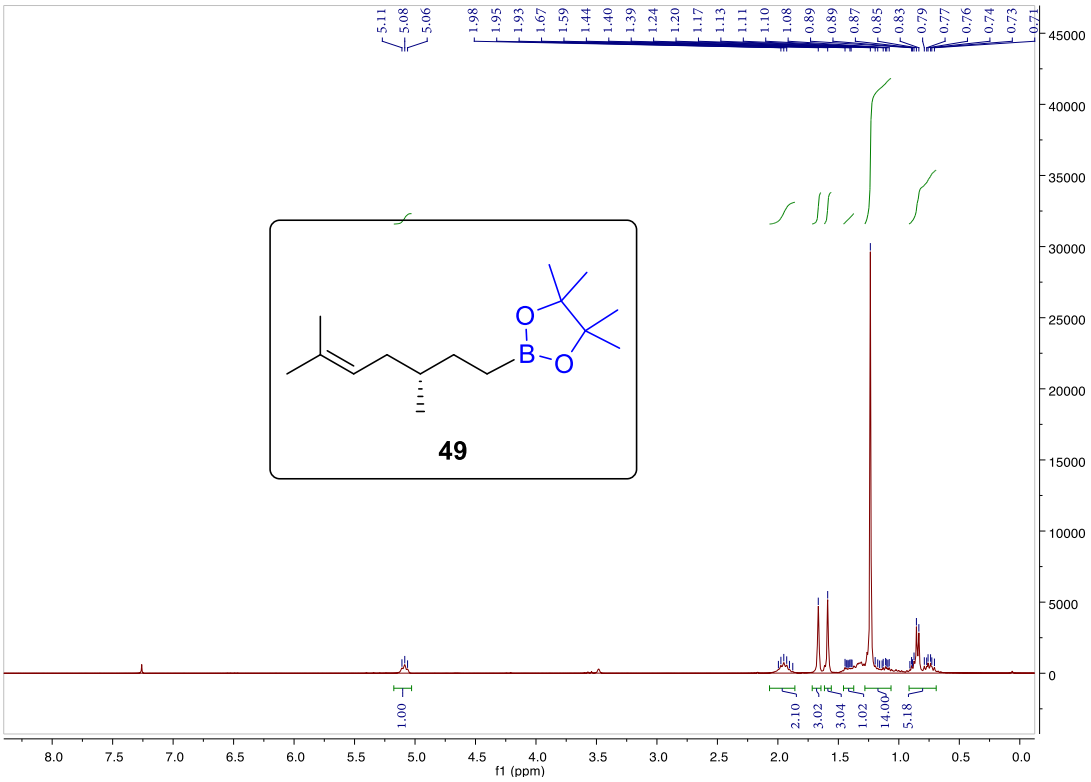

7.1543
7.1400
7.1239
7.1121
7.0558
7.0431
7.0321
7.0260
7.0145
3.0291
2.9968
2.9772
2.9450
2.9321
2.8978
2.8802
2.8458
1.9624
1.8658
1.8330
1.8001
1.7673
1.7345
1.1823
46
2.00
1.96
3.99
1.01
12.04
f1 (ppm)

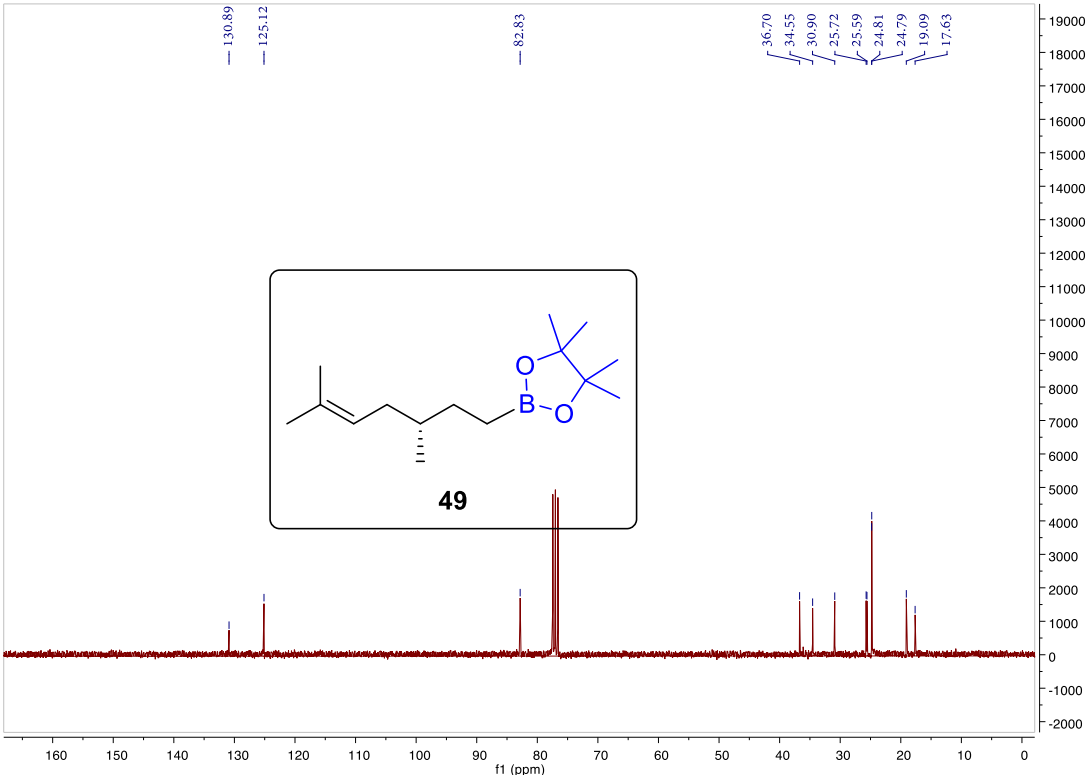

144.35
125.84
124.14
83.16
35.08
24.73
46
f1 (ppm)

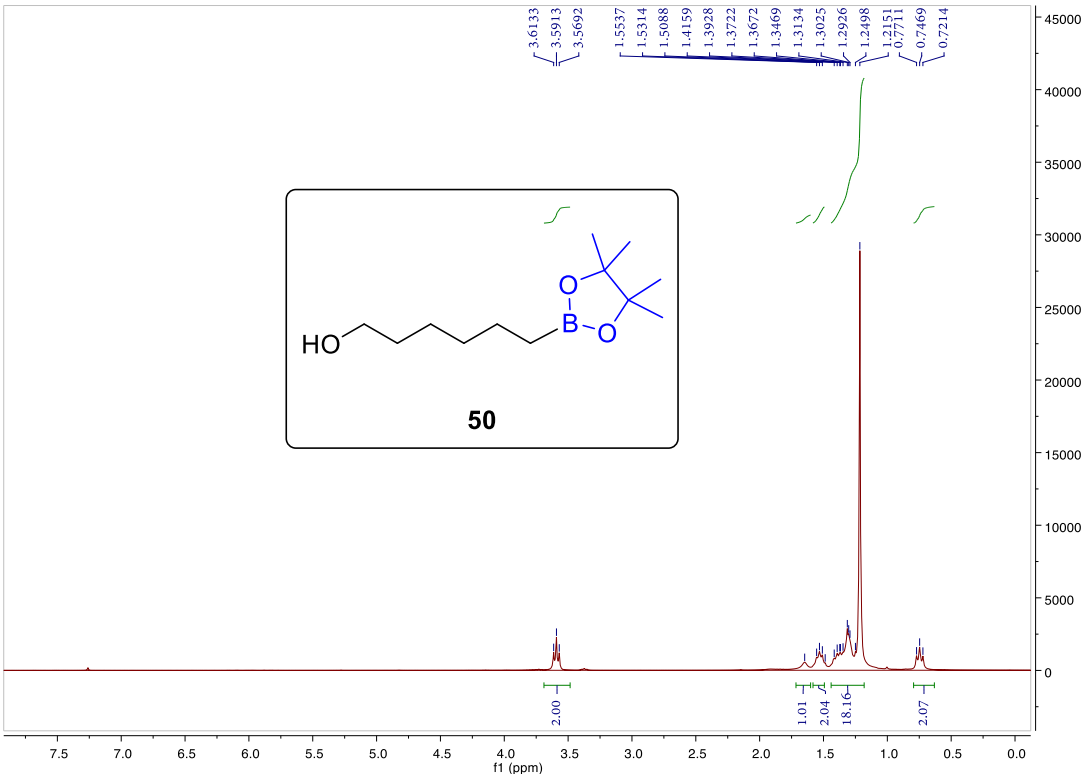

7.19
3.05
3.03
2.99
2.97
2.94
2.92
2.90
2.86
2.84
2.20
2.19
2.17
2.16
1.84
1.82
1.81
1.79
1.53
1.50
1.50
1.48
1.46
1.45
47
4.00
4.10
1.05
1.10
13.00
f1 (ppm)
137.13
136.64
128.87
128.72
125.10
82.79
30.48
29.49
24.58
24.55
24.50
47
f1 (ppm)

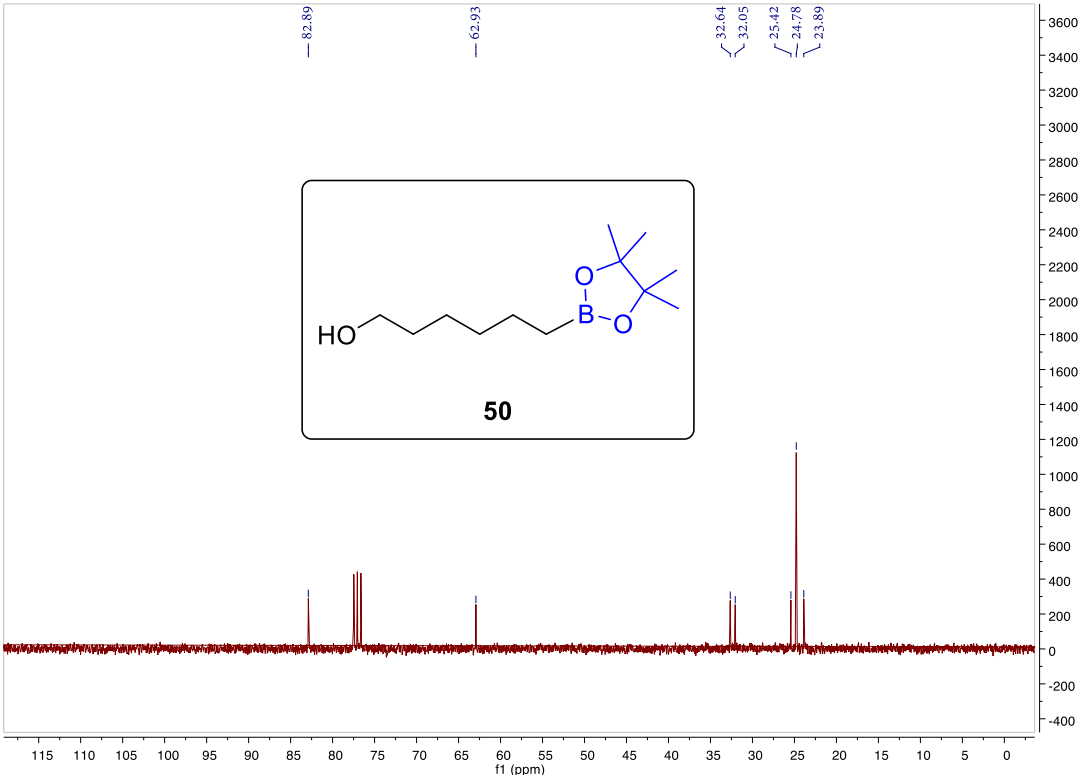

2.2691
2.2067
1.5004
1.4880
1.4798
1.3633
1.3304
1.2918
1.2357
1.2135
1.1596
1.1541
1.1290
O
B
O
48
2.00
3.05
17.10
1.07
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

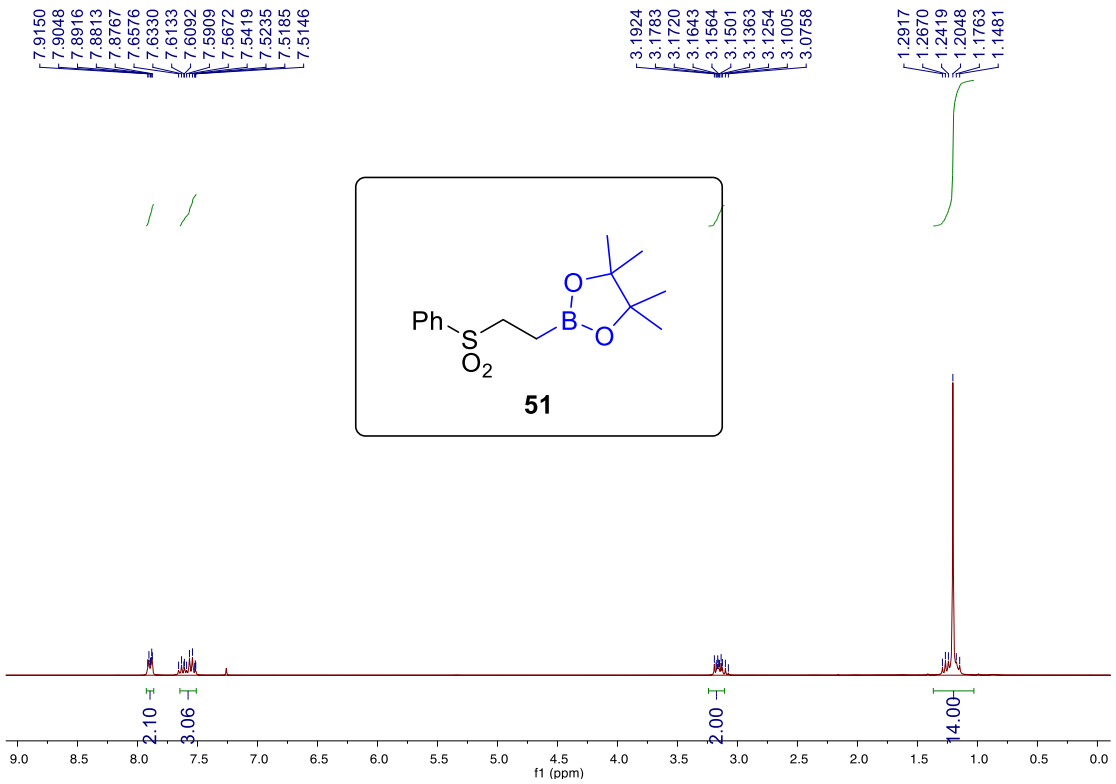

82.74
38.69
38.10
36.61
32.18
32.15
29.24
24.67
O
B
O
48
110
105
100
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
5
f1 (ppm)

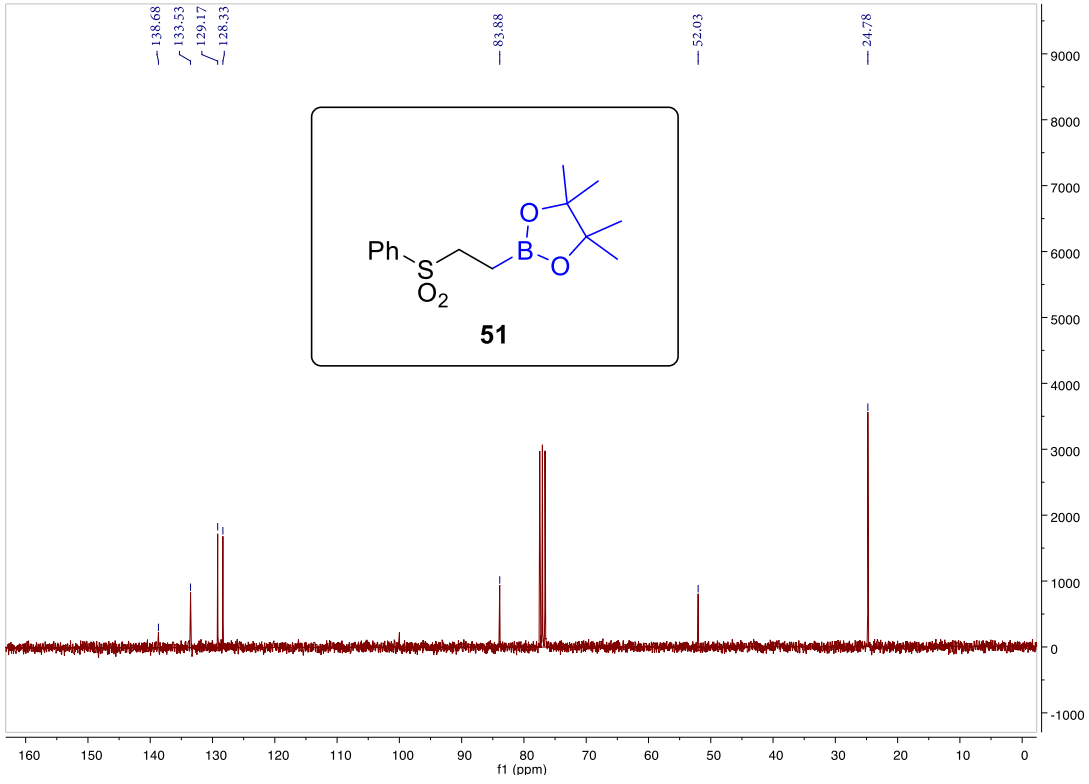

5.11
5.08
5.06
1.98
1.95
1.93
1.67
1.59
1.44
1.40
1.39
1.24
1.20
1.17
1.13
1.11
1.10
1.08
0.89
0.89
0.87
0.85
0.83
0.79
0.77
0.76
0.74
0.73
0.71
O
B
O
49
1.00
2.10
3.02
3.04
1.02
14.00
5.18
f1 (ppm)

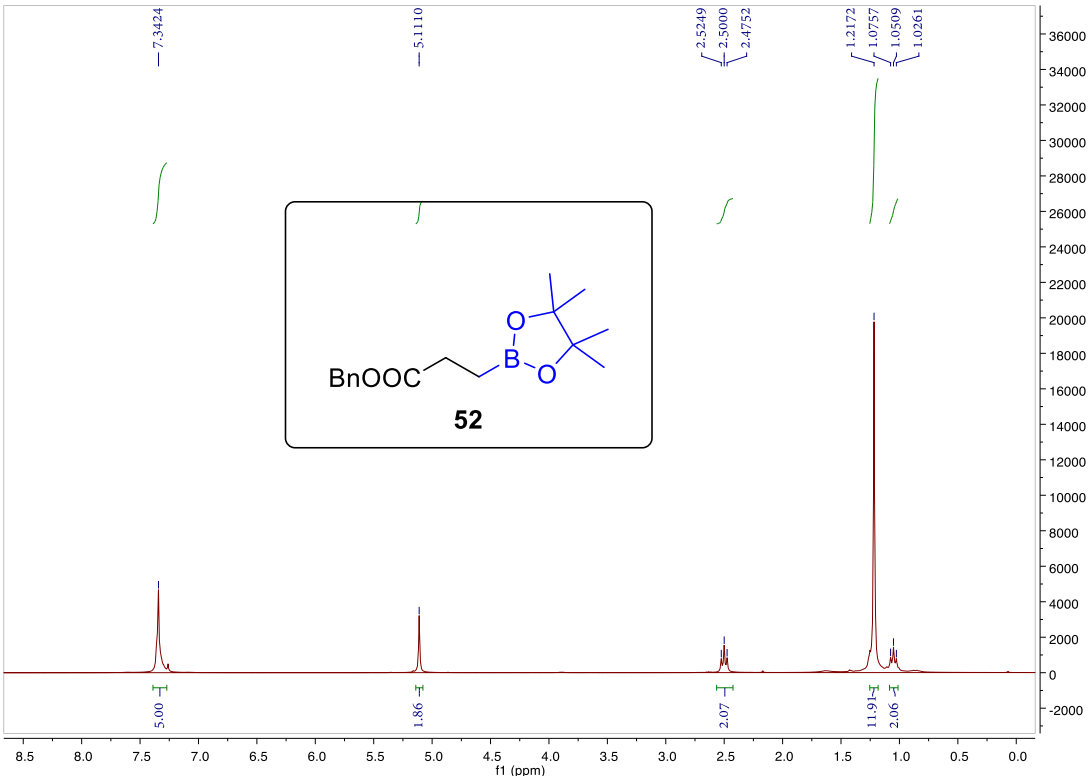

130.89
125.12
82.83
36.70
34.55
30.90
25.72
25.59
24.81
24.79
19.09
17.63
O
B
O
49
f1 (ppm)

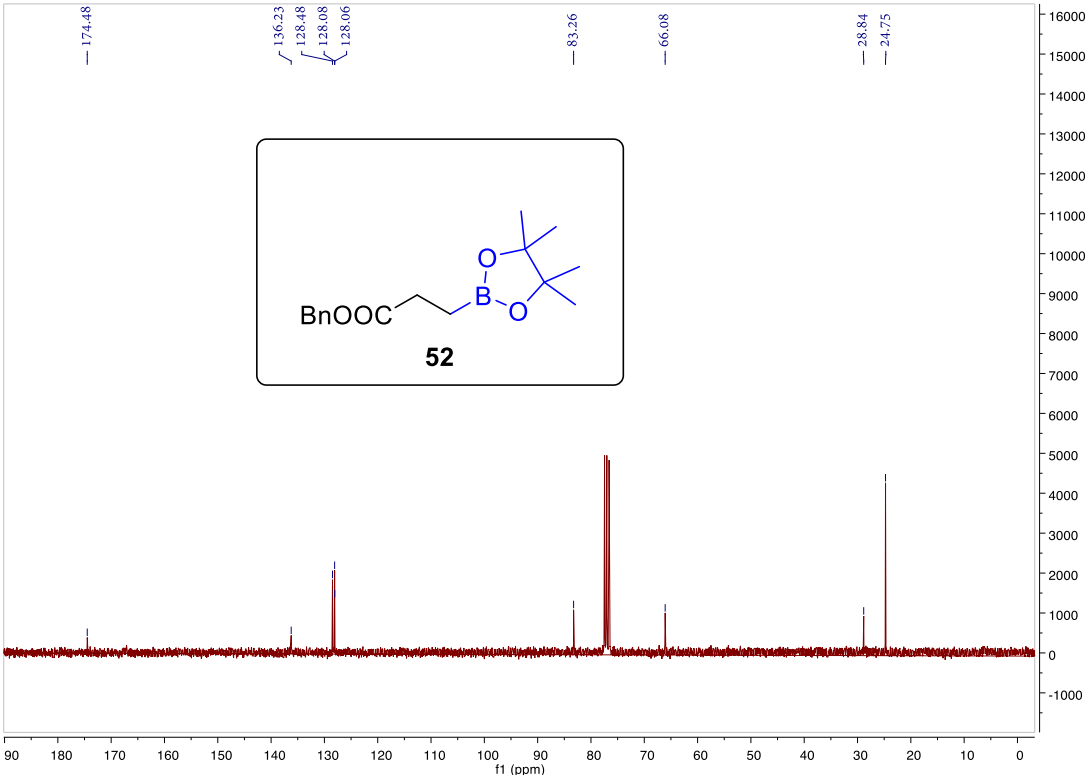

3.6133
3.5913
3.5692
1.5537
1.5314
1.5088
1.4159
1.3928
1.3722
1.3672
1.3469
1.3134
1.3025
1.2926
1.2498
1.2151
0.7711
0.7469
0.7214
HO
O
B
O
50
2.00
1.01
2.04
18.16
2.07
f1 (ppm)

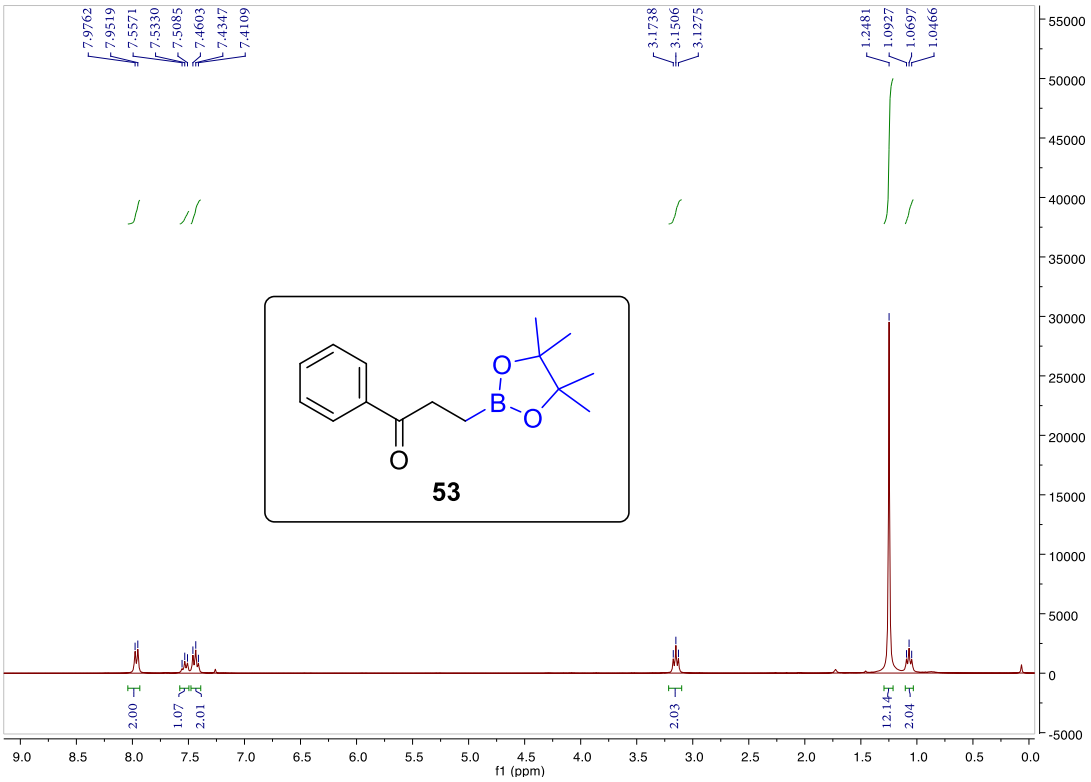

82.89
62.93
32.64
32.05
25.42
24.78
23.89
HO
O
B
O
50
f1 (ppm)

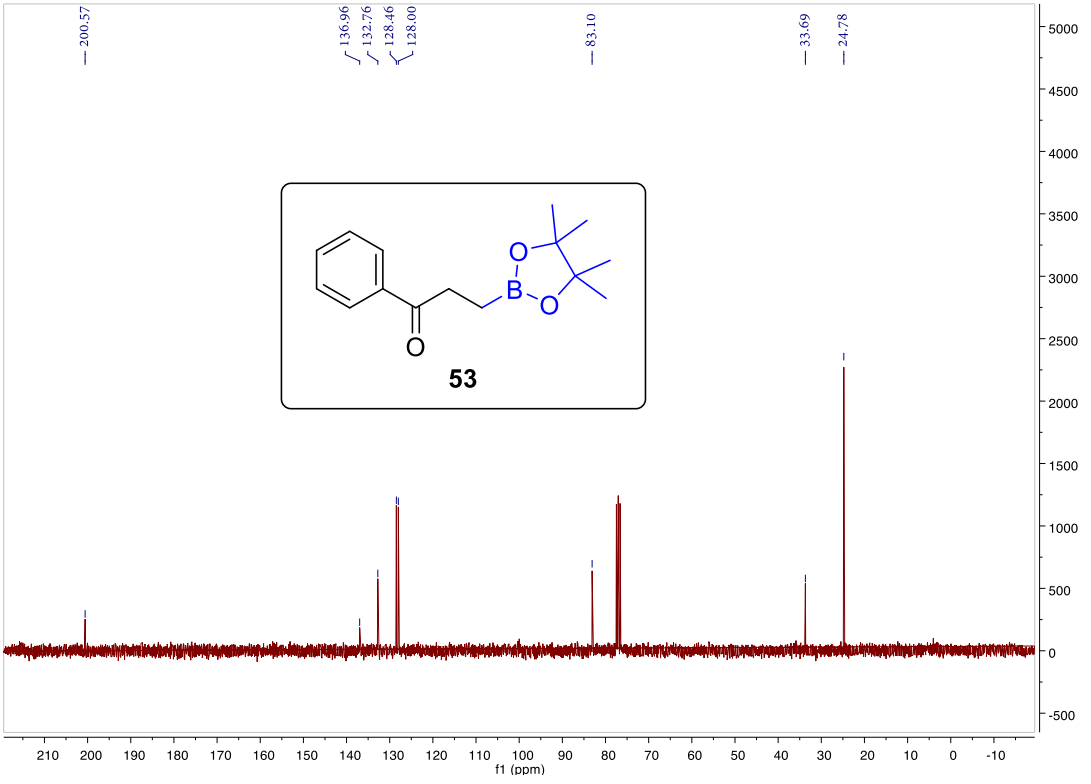

7.9150
7.9048
7.8916
7.8813
7.8767
7.6576
7.6330
7.6133
7.6092
7.5909
7.5672
7.5419
7.5235
7.5185
7.5146
3.1924
3.1783
3.1720
3.1643
3.1564
3.1501
3.1363
3.1254
3.1005
3.0758
1.2917
1.2670
1.2419
1.2048
1.1763
1.1481
Ph
S
O2
O
B
O
51
2.10
3.06
2.00
14.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

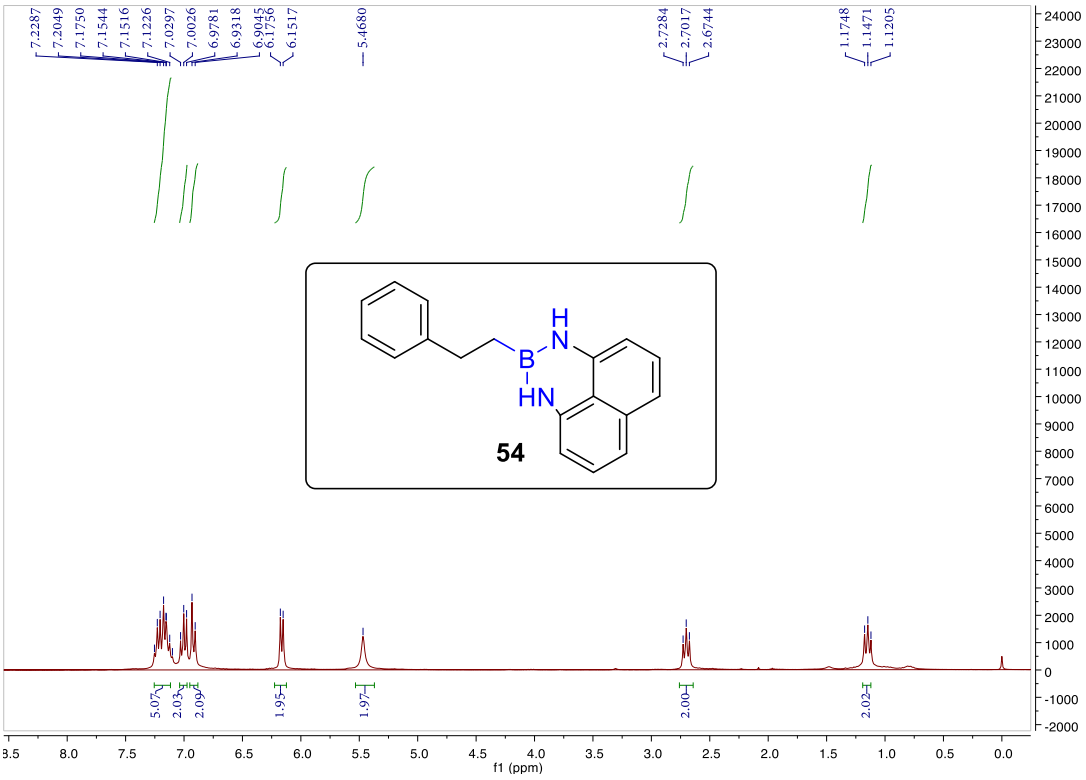

138.68
133.53
129.17
128.33
83.88
52.03
24.78
Ph
S
O2
O
B
O
51
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

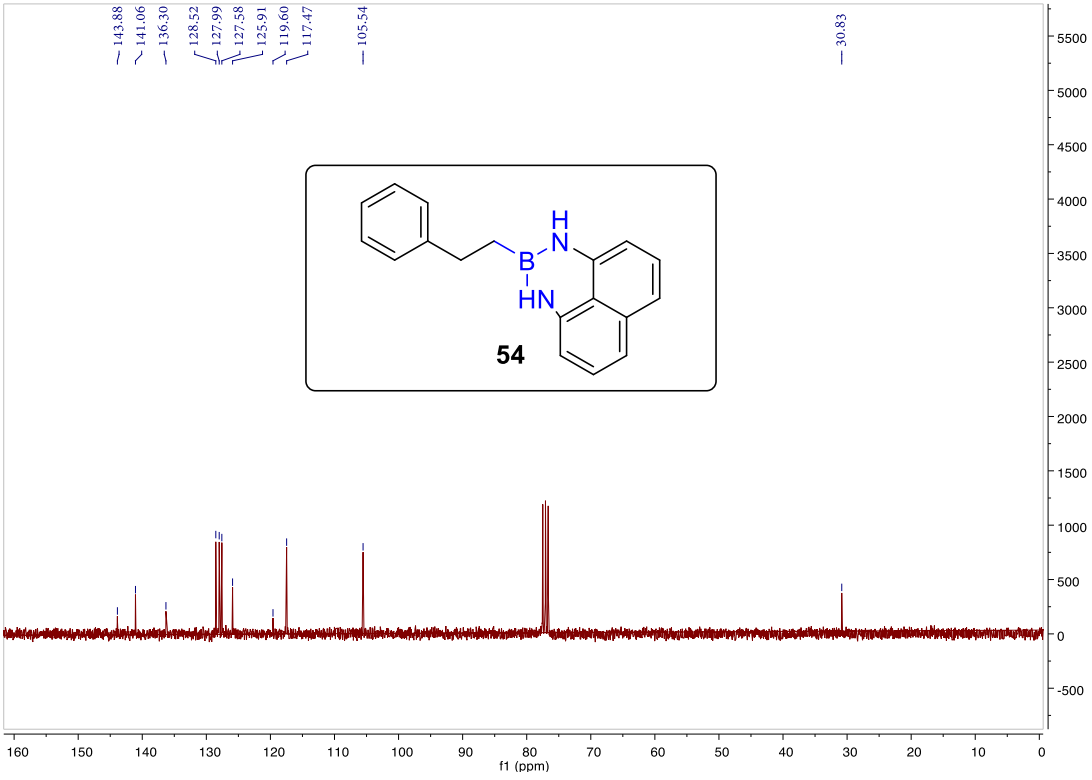

7.3424
5.1110
2.5249
2.5000
2.4752
1.2172
1.0757
1.0509
1.0261
BnOOC
O
B
O
52
5.00
1.86
2.07
11.91
2.06
f1 (ppm)

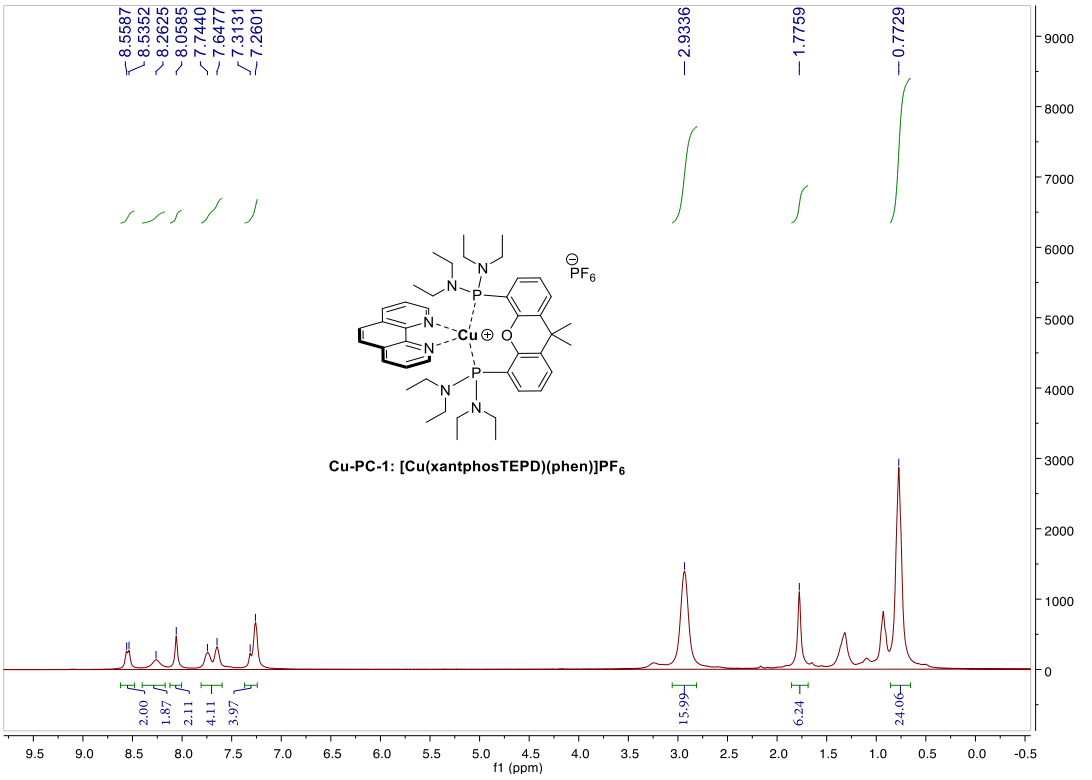

174.48
136.23
128.48
128.08
128.06
83.26
66.08
28.84
24.75
BnOOC
O
B
O
52
f1 (ppm)

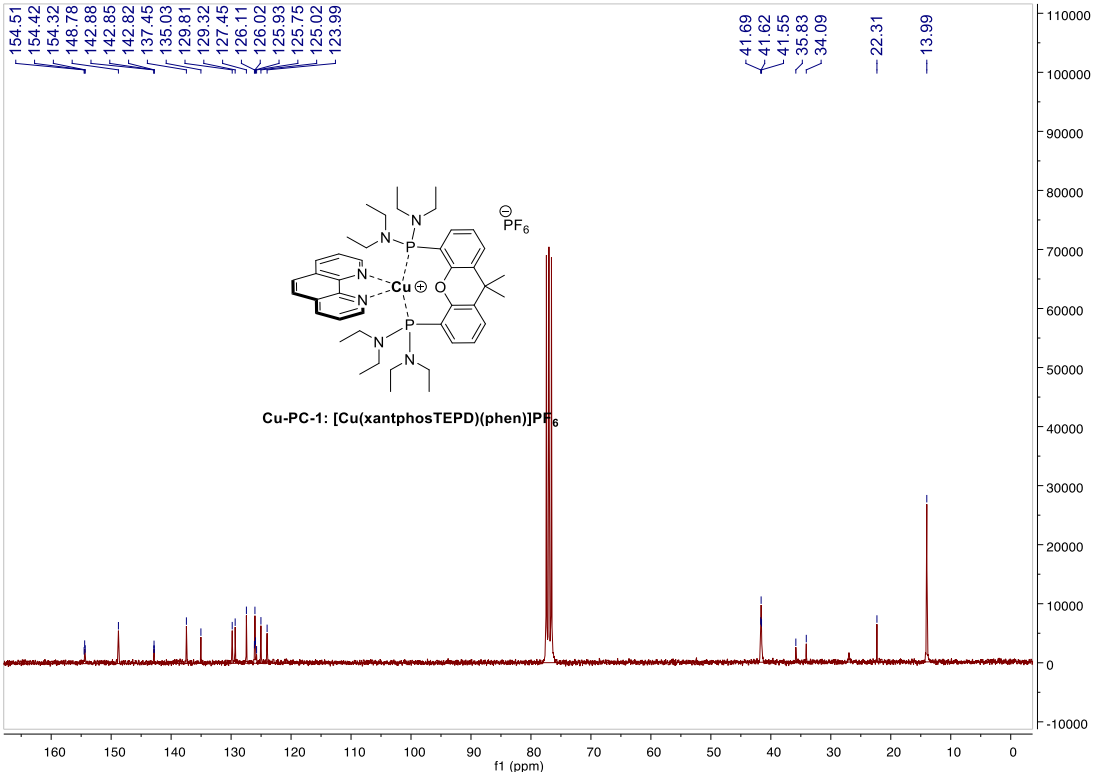

7.9762
7.9519
7.5571
7.5330
7.5085
7.4603
7.4347
7.4109
3.1738
3.1506
3.1275
1.2481
1.0927
1.0697
1.0466
O
B
O
O
53
2.00
1.07
2.01
2.03
12.14
2.04
f1 (ppm)

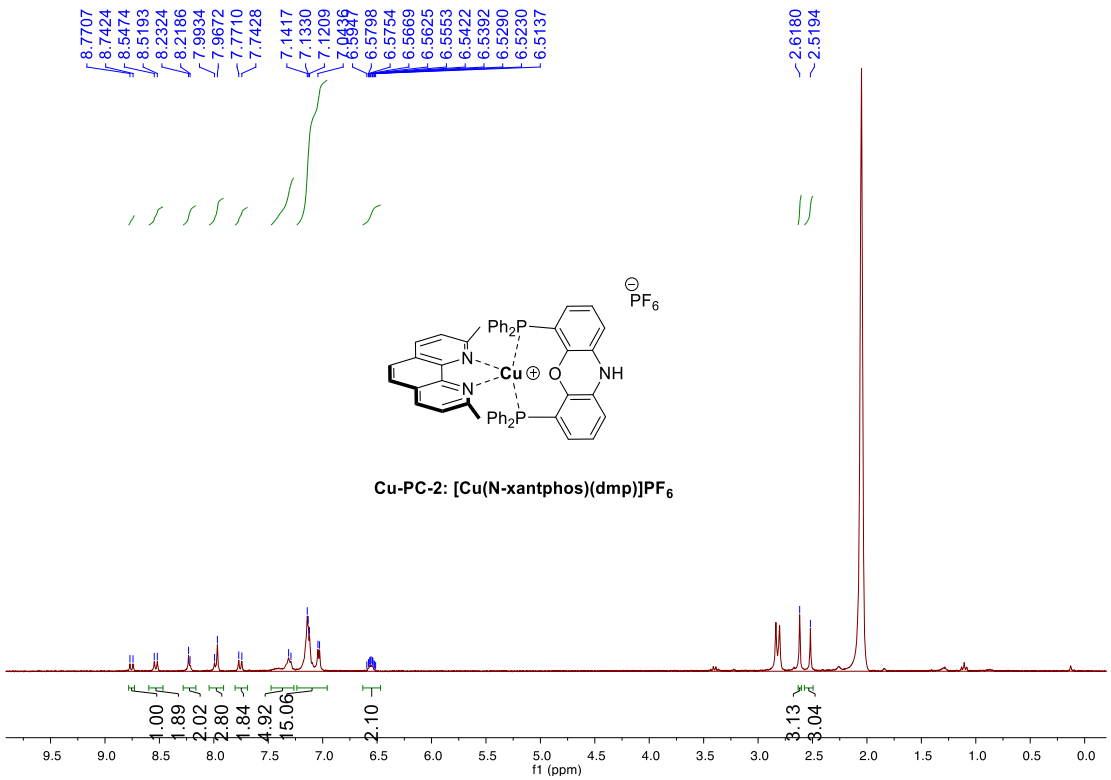

200.57
136.96
132.76
128.46
128.00
83.10
33.69
24.78
O
B
O
O
53
f1 (ppm)


7.2287
7.2049
7.1750
7.1544
7.1516
7.1226
7.0297
7.0026
6.9781
6.9318
6.9045
6.1756
6.1517
5.4680
2.7284
2.7017
2.6744
1.1748
1.1471
1.1205
H
N
B
HN
54
5.07
2.03
2.09
1.95
1.97
2.00
2.02
f1 (ppm)

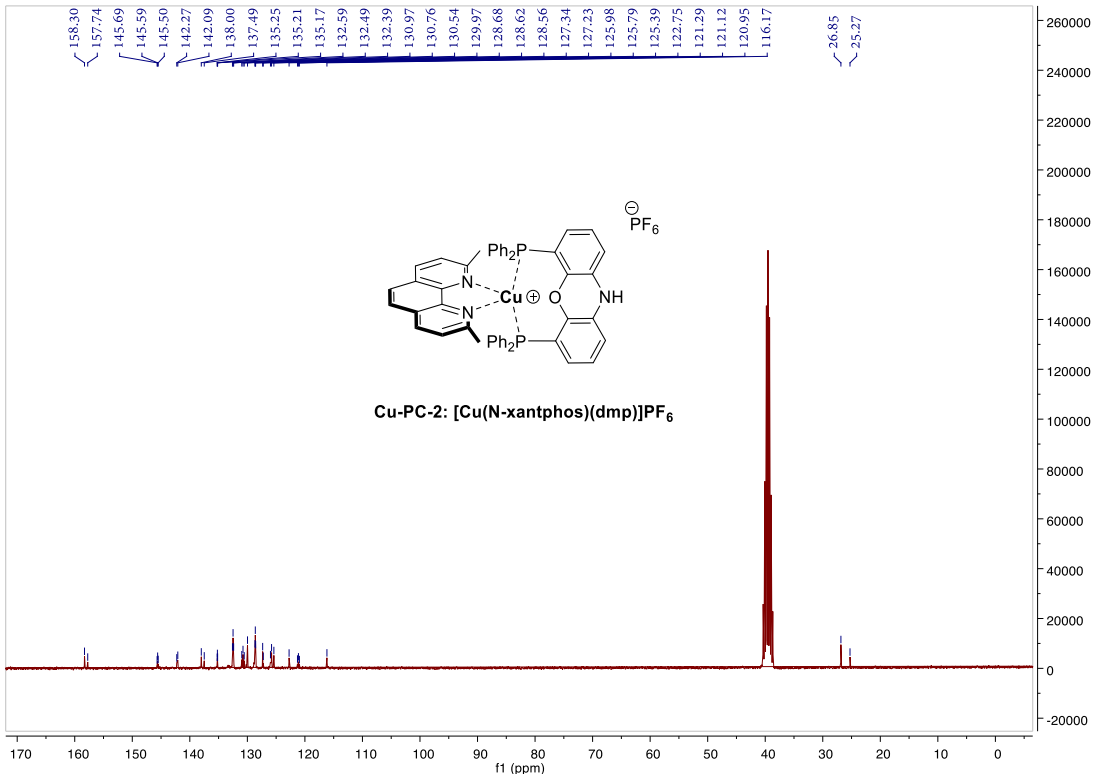

143.88
141.06
136.30
128.52
127.99
127.58
125.91
119.60
117.47
105.54
30.83
H
N
B
HN
54
f1 (ppm)


8.5587
8.5352
8.2625
8.0585
7.7440
7.6477
7.3131
7.2601
2.9336
1.7759
0.7729
Cu-PC-1: [Cu(xantphosTEPD)(phen)]PF6
2.00
1.87
2.11
4.11
3.97
15.99
6.24
24.06
f1 (ppm)


154.51
154.42
154.32
148.78
142.88
142.85
142.82
137.45
135.03
129.81
129.32
127.45
126.11
126.02
125.93
125.75
125.02
123.99
41.69
41.62
41.55
35.83
34.09
22.31
13.99
Cu-PC-1: [Cu(xantphosTEPD)(phen)]PF6
f1 (ppm)



Cu-PC-2: [Cu(N-xantphos)(dmp)]PF_6



Cu-PC-2: [Cu(N-xantphos)(dmp)]PF_6