Electronic Supplementary Information

Catalytic hydroboration of aldehydes, ketones, alkynes and alkenes initiated by NaOH

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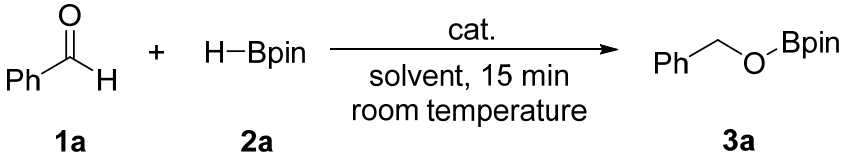
Table S1. Crystal data and structure refinement details for compound 7a

	7a
CCDC	1503838
empirical formula	$C_{18}H_{36}BNaO_5$
formula weight	366.27
temp, K	100.01(10)
cryst syst	Triclinic
space group	*P*-1
a, Å	7.5751(5)
b, Å	10.0045(7)
c, Å	13.9038(9)
α, deg	93.500(6)
β, deg	90.410(5)
γ, deg	104.176(6)
V, Å^3	1019.45(12)
Z	2
D_{calcd}, g/cm^3	1.193
μ, mm^{-1}	0.852
F(000)	400.0
2Θ range, deg	9.136–131.946
index range	$-8 \le h \le 8$
	$-11 \le k \le 11$
	$-16 \le l \le 14$
reflns collected/unique	5838 / 3440 [R(int) = 0.0776]
data/restraints/param	3440/0/250
GOF on F^2	1.025
final R indices	R1 = 0.0394,
[I >2σ(I)]	wR2 = 0.1062
R indices (all data)	R1 = 0.0420,
	wR2 = 0.1096
largest diff peak/hole,e/Å^3	0.24/-0.23

General information

All manipulations were carried out on a Schlenk line or in an argon atmosphere glovebox. THF and *n*hexane were dried by refluxing with sodium benzophenone under N_2, distilled, and stored over 3 Å sieves. Unless otherwise stated, commercial reagents were used without further purification. IR spectra were recorded on a Nicolet 330 spectrometer. ^{1}H, ^{11}B and ^{13}C NMR spectra were recorded on a Bruker AV-500M or a Bruker AV-400M spectrometer. ^{1}H and ^{13}C NMR spectroscopic chemical shifts were given relative to residual solvent peaks. HRMS were recorded on a Q-TOF mass spectrometer (Bruker micro TOF-QII, U.S.A). The single crystal diffraction data were collected on a SuperNova, Dual, Cu at zero, Atlas diffractometer. The crystal was kept at 100.01(10) K during data collection. The structure was solved with Olex2[S1] and the ShelXS[S2] structure solution program using Direct Methods and refined with the ShelXL[S3] refinement package using Least Squares minimization.

Table S2. Detailed optimization of the reaction conditions for aldehyde

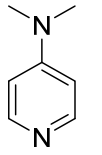


1a **2a** **3a**

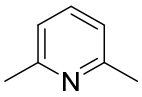
entry	catalyst	loading (mol%)	solvent	TON	TOF (h^{-1})	yield (%)[b]
1	-	-	C_6D_6	-	-	<5
2	Et_3N	5	C_6D_6	7	28	35
3	$^{i}Pr_2NEt$	5	C_6D_6	-	-	<5
4	$^{t}BuOK$	5	C_6D_6	16	66	82
5	$^{t}BuONa$	5	C_6D_6	20	79	99
6	PMe_3	5	C_6D_6	20	79	99
7	PPh_3	5	C_6D_6	18	71	89
8	py	5	C_6D_6	2	6	8
9	DMAP	5	C_6D_6	3	11	14
10	2,6-Lutidine	5	C_6D_6	-	-	<5
11	KOH[c]	5	C_6D_6	16	62	78
12	NaOH[c]	5	C_6D_6	18	74	92
13	NaH	5	C_6D_6	20	79	99
14	LiHDMS	5	C_6D_6	20	79	99
15	$LiNEt_2$	5	C_6D_6	20	78	98
16	$^{n}BuLi$	5	C_6D_6	20	79	99
17	PhLi	5	C_6D_6	20	79	99
18	**IMes**	5	C_6D_6	20	79	99
19	**IPr**	5	C_6D_6	20	79	99
20	NaOH[d]	5	C_6D_6	20	79	99
21	NaOH[e]	5	C_6D_6	20	78	98
22	NaOH[f]	5	C_6D_6	17	70	87
23	NaOH[g]	5	C_6D_6	18	72	90
24	NaOH[d]	1	C_6D_6	99	396	99

25	NaOH[d]	1	$CDCl_3$	99	396	99
26	NaOH[d]	1	acetone-d_6	72	288	72
27	NaOH[d]	1	THF-d_8	99	396	99
28	NaOH[d]	1	CD_3CN	18	72	18

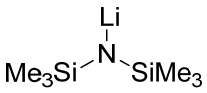
[a] Reaction conditions: benzaldehyde (1.00 mmol), HBpin (1.02 mmol), solvent (0.4 mL), room temperature. Catalyst loading relative to benzaldehyde. [b] Yields were determined by ^{1}H NMR spectroscopy using 1,3,5-trimethoxybenzene as an internal standard. [c] Alfa Aesar, beads/pellet, 99.99% (metal basis). [d] Sigma-Aldrich, powders, ACS reagent grade, 97%,. [e] Adamas-beta, pellet, 99%+. [f] Acros, micropearls, for analysis. [g] Sigma-Aldrich, pellet, semiconductor grade, 99.99% trace metals basis.



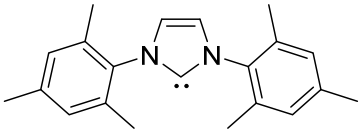
DMAP



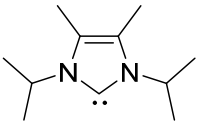
2,6-Lutidine



LiHDMS



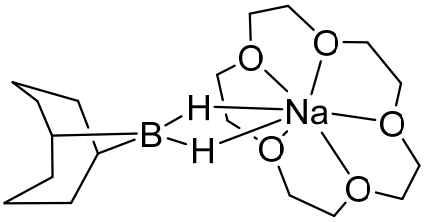
IMes



IPr

Experimental section

*Synthesis of **7a***:



In an argon atmosphere glovebox, a solution of 9-BBN (0.5 M, 8 mL, 4 mmol) in THF was added slowly to a suspension of powdered NaOH (0.080 g, 2 mmol) in THF (10 mL). The mixture was stirred at room temperature for 10 minutes and a solution of 15-Crown-5 (0.440 g, 2 mmol) in THF was added in. After stirring for additional 12 h, the solvent was removed and the residues were washed with ^{n}hexane (2 × 20 mL) to afford **7a** (0.615 g, 84%). The THF solution of **7a** was stored at -20 °C for additional 2 h, and colorless needle crystals suitable for XRD test were obtained. ^{1}H NMR (500 MHz, THF-d$_8$, ppm): δ 3.58 (s, 20H), 1.80-1.65 (m, 6H), 1.53 (br, 4H,), 1.41-1.34 (m, 2H), 0.63 (q, J = 74.1 Hz, 2H, overlapped), 0.63 (br, 2H). ^{13}C NMR (125 MHz, THF-d$_8$, ppm): δ 69.7, 36.9, 27.8 (d, J = 3.5 Hz), 24.1 (q, J = 40.6 Hz). ^{11}B NMR (160 MHz, THF-d$_8$, ppm): δ 17.88 (t, J = 74.1 Hz). IR (Nujol mull, cm^{-1}): $\tilde{\nu}$ 2833.1, 2105.8, 1463.6, 1374.5, 1354.2, 1295.4, 1250.9, 1198.2, 1117.2, 1094.9, 1044.2, 949.0, 898.4, 861.9, 722.1, 523.6. Elem. Anal. Calcd for $C_{18}H_{36}BNaO_5$: C, 59.03; H, 9.91; Found: C, 59.19; H, 9.98.

General Catalytic Procedures for the Hydroboration of Aldehydes with HBpin/HBcat:

In an argon atmosphere glovebox, aldehyde (1 mmol), 1,3,5-trimethoxybenzene (0.005 g), NaOH powder (0.01 mmol) and C_6D_6 (0.4 mL) were loaded in a dried NMR tube, then BH compound (1.05 mmol) was added in slowly. The tube was sealed securely before being brought outside of the glovebox, continually shaken and monitored by NMR spectroscopy. NMR spectra of the products were collected after filtration under argon and dried under vacuum for more than 6 hours to remove the volatiles.

General Catalytic Procedures for the Hydroboration of Aldehydes with 9-BBN:

In an argon atmosphere glovebox, aldehyde (1 mmol), 1,3,5-trimethoxybenzene (0.005 g), NaOH powder (0.01 mmol) and THF-d$_8$ (0.5 mL) were loaded in a dried Schlenk flask, then

9-BBN (0.5 M in THF, 2.2 mL, 1.1 mmol) was added in slowly. The reaction mixture was stirred in room temperature for 2 hours and monitored by NMR spectroscopy. NMR spectra of the products were collected after filtration under argon and dried under vacuum for more than 6 hours to remove the volatiles.

General Catalytic Procedures for the Hydroboration of Ketones with HBpin:

In an argon atmosphere glovebox, ketone (1 mmol), 1,3,5-trimethoxybenzene (0.005 g), NaOH powder (0.05 mmol) and C_6D_6 (0.4 mL) were loaded in a dried NMR tube, then HBpin (1.05 mmol) was added in slowly. The tube was sealed securely before being brought outside of the glovebox, continually shaken and monitored by NMR spectroscopy. NMR spectra of the products were collected after filtration under argon and dried under vacuum for more than 6 hours to remove the volatiles.

General Catalytic Procedures for the Hydroboration of Aldehydes with 9-BBN:

In an argon atmosphere glovebox, ketones (1 mmol), 1,3,5-trimethoxybenzene (0.005 g), NaOH powder (0.05 mmol) and THF-d_8 (0.5 mL) were loaded in a dried Schlenk flask, then 9-BBN (0.5 M in THF, 2.2 mL, 1.1 mmol) was added in slowly. The reaction mixture was stirred in room temperature for 2 hours and monitored by NMR spectroscopy. NMR spectra of the products were collected after filtration under argon and dried under vacuum for more than 6 hours to remove the volatiles.

General Catalytic Procedures for the Hydroboration of imine with HBpin:

In an argon atmosphere glovebox, imine (1 mmol), 1,3,5-trimethoxybenzene (0.005 g), NaOH powder (0.05 mmol) and C_6D_6 (0.4 mL) were loaded in a dried NMR tube, then HBpin compounds (1.05 mmol) was added in slowly. The tube was sealed securely before being brought outside of the glovebox, heated at 90 ºC for 6 hours and monitored by NMR spectroscopy. NMR spectra of the products were collected after filtration under argon and dried under vacuum for more than 6 hours to remove the volatiles.

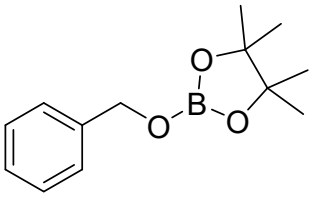
General Catalytic Procedures for the Hydroboration of Alkynes with HBpin:

In an argon atmosphere glovebox, alkyne (1 mmol), HBpin (1.2 mmol), 1,3,5-trimethoxybenzene (0.005 g), NaOH powder (0.08 mmol) and C_6D_6 (0.4 mL) were loaded in a dried NMR tube. The tube was sealed securely before being brought outside of the glove box, heated at 100 ºC and monitored by NMR spectorscopy. Then the volatiles were removed under vacuum and the residue was purified by silica gel column chromatography using a mixture of petroleum ether and ethyl acetate as eluent.

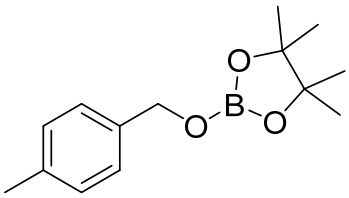
*Large-scale reaction of **1a** with HBpin:*

In an argon atmosphere glovebox, **1a** (10 mmol), HBpin (10.2 mmol), NaOH powder (0.1 mmol) and toluene (15 mL) were loaded in a dried Schlenk tube. The mixture was stirred at room temperature for 15 minutes. Then mixture was filtrated and the volatiles were removed under vacuum for 4 hours. The corresponding hydroboration product **2a** was obtained as colorless oil (94% yield).

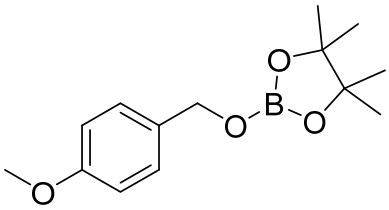
Spectral Data



2a *(CAS 95843-98-4)*: ^{1}H NMR (500 MHz, $CDCl_3$, ppm): δ 7.27-7.22 (m, 4H, Ar*H*), 7.19-7.15 (m, 1H, Ar*H*), 4.84 (s, 2H, OCH_2), 1.17 (s, 12H, CH_3). ^{13}C NMR (125 MHz, $CDCl_3$, ppm): δ 139.15, 128.20, 127.28, 126.63 (*Ar*), 82.88 (*C*$(CH_3)_2$), 66.59 (O*C*H_2), 24.53 (C(*C*$H_3)_2$). ^{11}B NMR (160 MHz, $CDCl_3$, ppm): δ 22.42. HRMS (ESI): m/z calcd for $C_{13}H_{19}BNaO_3^+$: 257.1319 $[(M+Na)]^+$; found: 257.1322.

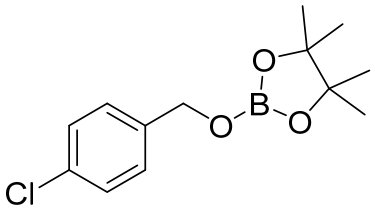


2b *(CAS 1143018-79-4)*: ^{1}H NMR (500 MHz, $CDCl_3$, ppm): δ 7.14 (d, *J* = 7.8 Hz, 2H, Ar*H*), 7.03 (d, *J* = 7.8 Hz, 2H, Ar*H*), 4.79 (s, 2H, OCH_2), 2.23 (s, 3H, ArCH_3), 1.15 (s, 12H, C(C$H_3)_2$). ^{13}C NMR (125 MHz, $CDCl_3$, ppm): δ 136.84, 136.14, 128.82, 126.73 (*Ar*), 82.75 (*C*$(CH_3)_2$), 66.46 (O*C*H_2), 24.49 (C(*C*$H_3)_2$), 21.00 (Ar*C*H_3). ^{11}B NMR (160 MHz, $CDCl_3$, ppm): δ 22.40. HRMS (ESI): m/z calcd for $C_{14}H_{21}BNaO_3^+$: 271.1476 $[(M+Na)]^+$; found: 271.1475.

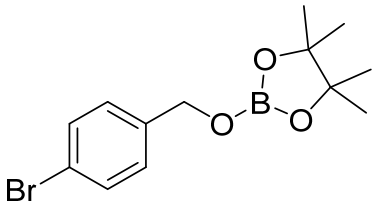


2c *(CAS 1143018-81-8)*: ^{1}H NMR (500 MHz, $CDCl_3$, ppm): δ 7.26 (d, *J* = 8.5 Hz, 2H, Ar*H*), 6.84 (d, *J* = 8.5 Hz, 2H, Ar*H*), 4.84 (s, 2H, OCH_2), 3.75 (s, 2H, OCH_3), 1.24 (s, 12H, C(C$H_3)_2$). ^{13}C NMR (125 MHz, $CDCl_3$, ppm): δ 158.87, 131.26, 128.33, 113.48 (*Ar*), 82.66 (*C*$(CH_3)_2$), 66.24 (O*C*H_2), 54.99 (O*C*H_3), 24.42 (C(*C*$H_3)_2$). ^{11}B NMR (160 MHz, $CDCl_3$, ppm): δ 22.34. HRMS (ESI): m/z calcd for $C_{14}H_{21}BNaO_4^+$: 287.1425 $[(M+Na)]^+$; found:

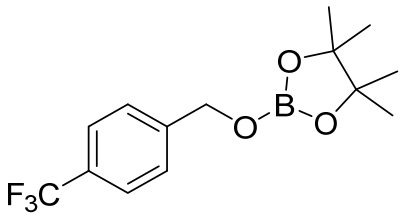
287.1428.



2d *(CAS 1143018-85-2)*: ^{1}H NMR (500 MHz, $CDCl_3$, ppm): δ 7.21 (d, *J* = 8.7 Hz, 2H, Ar*H*), 7.18 (d, *J* = 8.7 Hz, 2H, Ar*H*), 4.50 (s, 2H, OCH_2), 0.79 (s, 12H, C(CH_3)$_2$). ^{13}C NMR (125 MHz, $CDCl_3$, ppm): δ 137.64, 133.00, 128.33, 128.01 (*Ar*), 82.99 (*C*(CH$_3$)$_2$), 65.84 (O*C*H$_2$), 24.51 (C(*C*H$_3$)$_2$). ^{11}B NMR (160 MHz, $CDCl_3$, ppm): δ 22.35. HRMS (ESI): m/z calcd for $C_{13}H_{18}BClNaO_3^+$: 291.0930 $[(M+Na)]^+$; found: 291.0934.

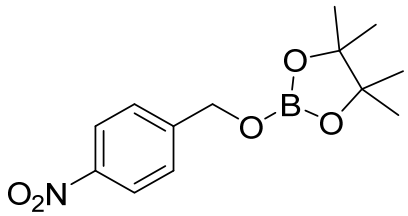


2e *(CAS 1566593-61-0)*: ^{1}H NMR (500 MHz, $CDCl_3$, ppm): δ 7.34 (d, *J* = 8.2 Hz, 2H, Ar*H*), 7.11 (d, *J* = 8.2 Hz, 2H, Ar*H*), 4.76 (s, 2H, OCH_2), 1.15 (s, 12H, C(CH_3)$_2$). ^{13}C NMR (125 MHz, $CDCl_3$, ppm): δ 138.08, 131.18, 128.23, 121.00 (*Ar*), 82.87 (*C*(CH$_3$)$_2$), 65.76 (O*C*H$_2$), 24.44 (C(*C*H$_3$)$_2$). ^{11}B NMR (160 MHz, $CDCl_3$, ppm): δ 22.38. HRMS (ESI): m/z calcd for $C_{13}H_{18}BBrNaO_3^+$: 335.0425 $[(M+Na)]^+$; found: 335.0427.

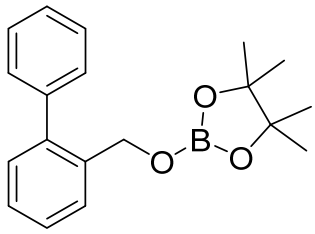


2f *(New Compound)*: ^{1}H NMR (500 MHz, $CDCl_3$, ppm): δ 7.49 (d, *J* = 8.1 Hz, 2H, Ar*H*), 7.36 (d, *J* = 8.1 Hz, 2H, Ar*H*), 4.89 (s, 2H, OCH_2), 1.17 (s, 12H, C(CH_3)$_2$). ^{13}C NMR (125 MHz, $CDCl_3$, ppm): δ 143.21 (*Ar*), 129.49 (q, *J* = 32.3 Hz, *Ar*), 126.55 (*Ar*), 125.18 (q, *J* = 3.8 Hz, *Ar*), 124.17 (q, *J* = 272.0 Hz, *C*F$_3$), 83.16 (*C*(CH$_3$)$_2$), 65.89 (O*C*H$_2$), 24.50 (C(*C*H$_3$)$_2$).

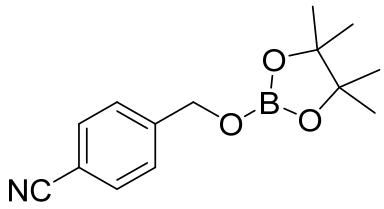
^{11}B NMR (160 MHz, $CDCl_3$, ppm): δ 22.39. HRMS (ESI): m/z calcd for $C_{14}H_{18}BF_3NaO_3^+$: 325.1193 $[(M+Na)]^+$; found: 325.1194.



2g *(1143018-83-0)*: ^{1}H NMR (500 MHz, $CDCl_3$, ppm): δ 8.09 (d, *J* = 8.4 Hz, 2H, Ar*H*), 7.42 (d, *J* = 8.4 Hz, 2H, Ar*H*), 4.94 (s, 2H, OCH_2), 1.18 (s, 12H, C(CH_3)$_2$). ^{13}C NMR (125 MHz, $CDCl_3$, ppm): δ 147.04, 146.48, 126.69, 123.38 (*Ar*), 83.20 (*C*$(CH_3)_2$), 65.36 (O*C*H_2), 24.41 (C(*C*H_3)$_2$). ^{11}B NMR (160 MHz, $CDCl_3$, ppm): δ 22.39. HRMS (ESI): m/z calcd for $C_{13}H_{18}BNNaO_5^+$: 302.1170 $[(M+Na)]^+$; found: 302.1173.

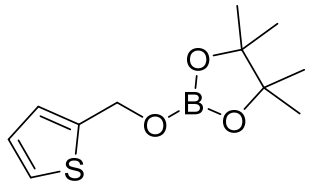


2h *(New Compound)*: ^{1}H NMR (500 MHz, $CDCl_3$, ppm): δ 7.59 (d, *J* = 7.6 Hz, 1H, Ar*H*), 7.33-7.19 (m, 8H, Ar*H*), 4.83 (s, 2H, OCH_2), 1.18 (s, 12H, C(CH_3)$_2$). ^{13}C NMR (125 MHz, $CDCl_3$, ppm): δ 140.95, 140.30, 136.05, 129.53, 128.90, 128.15, 127.80, 127.22, 127.13, 126.78 (*Ar*), 82.45 (*C*$(CH_3)_2$), 64.37 (O*C*H_2), 24.25 (C(*C*H_3)$_2$). ^{11}B NMR (160 MHz, $CDCl_3$, ppm): δ 22.45. HRMS (ESI): m/z calcd for $C_{19}H_{23}BNaO_3^+$: 333.1632 $[(M+Na)]^+$; found: 333.1633.

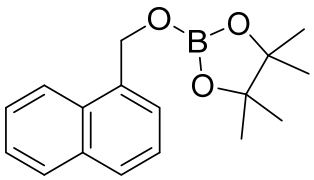


2i *(CAS 1640962-14-6)*: ^{1}H NMR (500 MHz, C_6D_6, ppm): δ 7.00-6.98 (m, 2H, Ar*H*), 6.88-6.87 (m, 2H, Ar*H*), 4.67 (s, 2H, OCH_2), 1.03 (s, 12H, C(CH_3)$_2$). ^{13}C NMR (125 MHz,

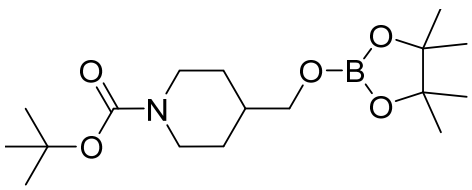
C_6D_6, ppm): δ 143.46(*C*N), 131.04, 125.69, 117.79, 110.56 (*Ar*), 82.03 (*C*$(CH_3)_2$), 64.77 (O*C*H_2), 23.58 (C(*C*$H_3)_2$). ^{11}B NMR (160 MHz, C_6D_6, ppm): δ 22.77. HRMS (ESI): m/z calcd for $C_{14}H_{18}BNaO_3^+$: 282.1272 [(M+Na)]$^+$; found: 282.1273.



2j *(CAS 1811523-11-1)*: ^{1}H NMR (500 MHz, $CDCl_3$, ppm): δ 7.15 (d, *J* = 5.1 Hz, 1H, Ar*H*), 6.92 (d, *J* = 3.4 Hz, 1H, Ar*H*), 6.86 (t, *J* = 4.5 Hz, 1H, Ar*H*), 4.95 (s, 2H, OC*H*$_2$), 1.18 (s, 12H, C(C*H*$_3)_2$). ^{13}C NMR (125 MHz, $CDCl_3$, ppm): δ 141.86, 126.46, 125.74, 125.38 (*Ar*), 82.98 (*C*$(CH_3)_2$), 61.49 (O*C*H_2), 24.50 (C(*C*$H_3)_2$). ^{11}B NMR (160 MHz, $CDCl_3$, ppm): δ 22.36. HRMS (ESI): m/z calcd for $C_{11}H_{17}BNaO_3S^+$: 263.0884 [(M+Na)]$^+$; found: 263.0886.

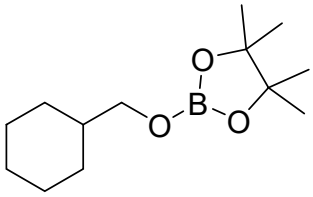


2k *(CAS 1809788-30-4)*: ^{1}H NMR (500 MHz, $CDCl_3$, ppm): δ 7.91 (d, *J* = 8.3 Hz, 1H, Ar*H*), 7.70 (d, *J* = 7.7 Hz, 1H, Ar*H*), 7.63 (d, *J* = 8.3 Hz, 1H, Ar*H*), 7.46 (d, *J* = 7.0 Hz, 1H, Ar*H*), 7.37-7.28 (d, *J* = 7.0 Hz, 1H, Ar*H*), 5.28 (s, 2H, OC*H*$_2$), 1.13 (s, 12H, C(C*H*$_3)_2$). ^{13}C NMR (125 MHz, $CDCl_3$, ppm): δ 134.52, 133.44, 130.82, 128.42, 128.04, 125.96, 125.52, 125.21, 124.71, 123.32 (*Ar*), 82.85 (*C*$(CH_3)_2$), 64.88 (O*C*H_2), 24.42 (C(*C*$H_3)_2$). ^{11}B NMR (160 MHz, $CDCl_3$, ppm): δ 22.56. HRMS (ESI): m/z calcd for $C_{17}H_{22}BNaO_3^+$: 307.1476 [(M+Na)]$^+$; found: 307.1481.

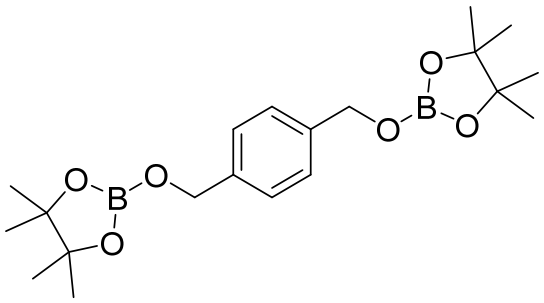


2l *(New Compound)*: ^{1}H NMR (500 MHz, $CDCl_3$, ppm): δ 4.06 (br, 2H, piperidine*H*), 3.67 (d, *J* = 6.1 Hz, 2H, OC*H*$_2$), 2.65 (br, 2H, piperidine*H*), 1.66-1.63 (m, 3H, piperidine*H*), 1.41 (s,

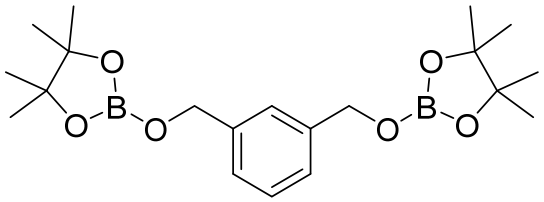
9H, ^{t}Bu*H*), 1.21 (s, 12H, C(C*H*$_3$)$_2$), 1.08 (qd, *J* = 12.6, 4.1 Hz, 2H, piperidine*H*). ^{13}C NMR (125 MHz, $CDCl_3$, ppm): δ 154.73 (*C*=O), 82.66 (*C*(CH$_3$)$_2$), 79.15 (O*C*(CH$_3$)$_3$), 69.15 (O*C*H$_2$), 43.73, 43.17 (N*C*H$_2$*C*H$_2$), 37.64 (OCH$_2$*C*H), 28.35 (C(*C*H$_3$)$_3$), 24.48 (C(*C*H$_3$)$_2$). ^{11}B NMR (160 MHz, $CDCl_3$, ppm): δ 21.99. HRMS (ESI): m/z calcd for $C_{17}H_{32}BNNaO_5^+$: 364.2266 [(M+Na)]$^+$; found: 364.2270.



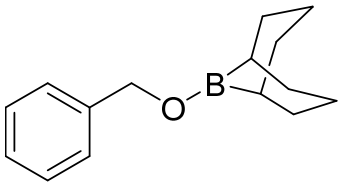
2m *(CAS 1566593-62-1)*: ^{1}H NMR (500 MHz, $CDCl_3$, ppm): δ 3.61 (d, *J* = 6.5 Hz, 2H, OC*H*$_2$), 1.70-1.65 (m, 4H, C$_6$*H*$_{11}$), 1.62-1.59 (m, 1H, C$_6$*H*$_{11}$), 1.51-1.43 (m, 1H, C$_6$*H*$_{11}$), 1.21 (s, 12H, C(C*H*$_3$)$_2$), 1.18-1.08 (m, 3H, C$_6$*H*$_{11}$), 0.94-0.85 (m, 2H, C$_6$*H*$_{11}$). ^{13}C NMR (125 MHz, $CDCl_3$, ppm): δ 82.46 (*C*(CH$_3$)$_2$), 70.27 (O*C*H$_2$), 39.22, 29.24, 26.45, 25.69 (*C*$_6$H$_{11}$), 24.47 (C(*C*H$_3$)$_2$). ^{11}B NMR (160 MHz, $CDCl_3$, ppm): δ 22.03. HRMS (ESI): m/z calcd for $C_{13}H_{25}BNaO_3^+$: 263.1789 [(M+Na)]$^+$; found: 263.1790.



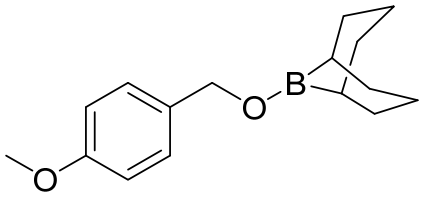
2n *(CAS 1373393-10-2)*: ^{1}H NMR (500 MHz, $CDCl_3$, ppm): δ 7.22 (s, *4*H, Ar*H*), 4.81 (s, 4H, OC*H*$_2$), 1.16 (s, 24H, C(C*H*$_3$)$_2$). ^{13}C NMR (125 MHz, $CDCl_3$, ppm): δ 138.18, 126.48 (*Ar*), 82.70 (*C*(CH$_3$)$_2$), 66.23 (O*C*H$_2$), 24.39 (C(*C*H$_3$)$_2$). ^{11}B NMR (160 MHz, $CDCl_3$, ppm): δ 22.36. HRMS (ESI): m/z calcd for $C_{20}H_{32}B_2NaO_6^+$: 413.2277 [(M+H)]$^+$; found: 413.2278.



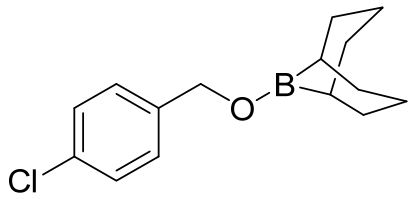
2o *(New Compound)*: ^{1}H NMR (500 MHz, $CDCl_3$, ppm): δ 7.24-7.16 (m, *4*H, Ar*H*), 4.83 (s, 4H, OC*H*$_2$), 1.17 (s, 24H, C(C*H*$_3$)$_2$). ^{13}C NMR (125 MHz, $CDCl_3$, ppm): δ 139.14, 128.14, 125.61, 124.97 (*Ar*), 82.80 (*C*(CH$_3$)$_2$), 66.43 (O*C*H$_2$), 24.46 (C(*C*H$_3$)$_2$). ^{11}B NMR (160 MHz, $CDCl_3$, ppm): δ 22.37. HRMS (ESI): m/z calcd for $C_{20}H_{32}B_2NaO_6^+$: 413.2277 $[(M+H)]^+$; found: 413.2280.



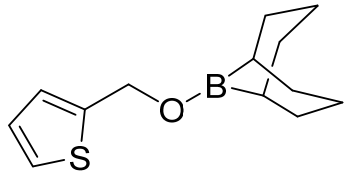
2p *(CAS 149832-59-7)*: ^{1}H NMR (500 MHz, C_6D_6, ppm): δ 7.01 (d, *J* = 7.6 Hz, 2H, Ar*H*), 6.93 (t, *J* = 7.6 Hz, 2H, Ar*H*), 6.85 (t, *J* = 7.4 Hz, 1H, Ar*H*), 4.64 (s, 2H, OC*H*$_2$), 1.67-1.52 (m, 10H, BC$_8$*H*$_{14}$), 1.19-1.03 (m, 4H, BC$_8$*H*$_{14}$). ^{13}C NMR (125 MHz, C_6D_6, ppm): δ 139.25, 127.62, 126.53, 125.88 (*Ar*), 66.82 (O*C*H$_2$), 32.80, 32.56, 22.66 (B*C*$_8$H$_{14}$). ^{11}B NMR (160 MHz, C_6D_6, ppm): δ 57.30. HRMS (ESI): m/z calcd for $C_{15}H_{23}BNaO_2^+$: 269.1683 $[(M+H_2O+Na)]^+$; found: 269.1686.



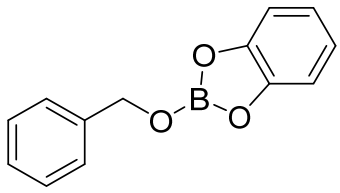
2q *(New Compound)*: ^{1}H NMR (500 MHz, $CDCl_3$, ppm): δ 7.14 (d, *J* = 8.6 Hz, 2H, Ar*H*), 6.75 (d, *J* = 8.6 Hz, 2H, Ar*H*), 4.88 (s, 2H, OC*H*$_2$), 3.64 (s, 3H, OC*H*$_3$), 1.82-1.64 (m, 10H, BC$_8$*H*$_{14}$), 1.41-1.21 (m, 4H, BC$_8$*H*$_{14}$). ^{13}C NMR (125 MHz, $CDCl_3$, ppm): δ 158.89, 131.67, 128.13, 113.64 (*Ar*), 67.27 (O*C*H$_2$), 54.87 (O*C*H$_3$), 33.29, 33.03, 23.06 (B*C*$_8$H$_{14}$). ^{11}B NMR (160 MHz, $CDCl_3$, ppm): δ 57.37. HRMS (ESI): m/z calcd for $C_{18}H_{26}BNNaO_2^+$: 322.1954 $[(M+CH_3CN+Na)]^+$; found: 322.1956.



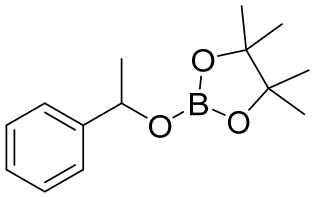
2r *(2016862-41-0)*: ^{1}H NMR (500 MHz, C_6D_6, ppm): δ 7.11 (d, *J* = 8.2 Hz, 2H, Ar*H*), 6.98 (d, *J* = 8.2 Hz, 2H, Ar*H*), 4.70 (s, 2H, OCH_2), 1.86-1.75 (m, 10H, BC$_8H_{14}$), 1.35-1.28 (m, 4H, BC$_8H_{14}$). ^{13}C NMR (125 MHz, C_6D_6, ppm): δ 138.65, 133.38, 128.78, 128.19 (*Ar*), 66.96 (O*C*H$_2$), 33.80, 33.54, 23.61 (B*C*$_8$H$_{14}$). ^{11}B NMR (160 MHz, C_6D_6, ppm): δ 57.45. HRMS (ESI): m/z calcd for $C_{15}H_{22}BClNaO_2^+$: 281.1474 [(M+ H_2O+H)]$^+$; found: 281.1478.



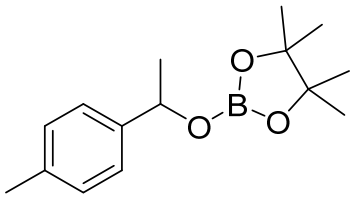
2s *(New Compound)*: ^{1}H NMR (500 MHz, C_6D_6, ppm): δ 6.90 (d, *J* = 4.6 Hz, 1H, Ar*H*), 6.76 (br, 1H, Ar*H*), 6.71-6.70 (m, 1H, Ar*H*), 4.94 (s, 2H, OCH_2), 1.86-1.79 (m, 10H, BC$_8H_{14}$), 1.38-1.24 (m, 4H, BC$_8H_{14}$). ^{13}C NMR (125 MHz, C_6D_6, ppm): δ 143.25, 128.29, 126.76, 125.42 (*Ar*), 62.89 (O*C*H$_2$), 33.80, 33.49, 23.60 (B*C*$_8$H$_{14}$). ^{11}B NMR (160 MHz, C_6D_6, ppm): δ 57.48. HRMS (ESI): m/z calcd for $C_{13}H_{19}BNaOS^+$: 257.1142 [(M+Na)]$^+$; found: 257.1142.



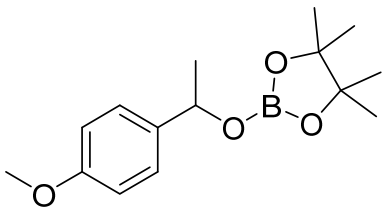
2t *(New Compound)*: ^{1}H NMR (500 MHz, $CDCl_3$, ppm): δ 7.40-7.26 (m, 4H, Ar*H*), 7.14-6.96 (m, 5H, Ar*H*), 5.15 (s, 2H, OCH_2). ^{13}C NMR (125 MHz, $CDCl_3$, ppm): δ 147.82, 137.69, 128.43, 127.91, 127.06 122.19, 111.88 (*Ar*), 67.78 (O*C*H$_2$). ^{11}B NMR (160 MHz, $CDCl_3$, ppm): δ 23.57. HRMS (ESI): m/z calcd for $C_{13}H_{11}BNaO_3^+$: 249.0693 [(M+Na)]$^+$; found: 249.0695.



4a *(CAS 1143018-72-7)*: ^{1}H NMR (500 MHz, C_6D_6, ppm): δ 7.10-7.07 (m, 2H, Ar*H*), 6.91-6.87 (m, 2H, Ar*H*), 6.80 (tt, *J* = 3.7, 1.5 Hz, 1H, Ar*H*), 5.11 (q, *J* = 6.5 Hz, 1H, OC*H*), 1.18 (d, *J* = 6.5 Hz, 3H, OCHC*H*$_3$), 0.77 (d, *J* = 13.8 Hz, 12H, C(C*H*$_3$)$_2$). ^{13}C NMR (125 MHz, C_6D_6, ppm): δ 145.27, 128.46, 127.29, 125.60 (*Ar*), 82.49 (*C*(CH$_3$)$_2$), 72.83 (O*C*H), 25.72 (OCH*C*H$_3$), 24.60 (d, *J* = 9.1 Hz, C(*C*H$_3$)$_2$). ^{11}B NMR (160 MHz, C_6D_6, ppm): δ 22.53. HRMS (ESI): m/z calcd for $C_{14}H_{21}BNaO_3^+$: 271.1476 [(M+Na)]$^+$; found: 271.1479.

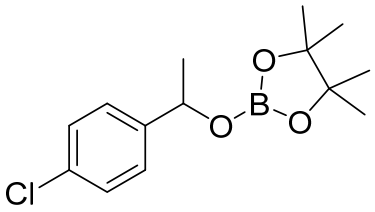


4b *(CAS 1416719-04-4)*: ^{1}H NMR (500 MHz, C_6D_6, ppm): δ 7.02 (d, *J* = 8.1 Hz, 2H, Ar*H*), 6.73 (d, *J* = 7.9 Hz, 2H, Ar*H*), 5.11 (q, *J* = 6.5 Hz, 1H, OC*H*), 1.87 (s, 3H, ArC*H*$_3$), 1.21 (d, *J* = 6.5 Hz, 3H, OCHC*H*$_3$), 0.79 (d, *J* = 12.4 Hz, 12H, C(C*H*$_3$)$_2$). ^{13}C NMR (125 MHz, C_6D_6, ppm): δ 141.40, 135.52, 128.14, 124.61 (*Ar*), 81.43 (*C*(CH$_3$)$_2$), 71.70 (O*C*H), 24.74 (OCH*C*H$_3$), 23.63 (d, *J* = 7.3 Hz, C(*C*H$_3$)$_2$), 20.04 (Ar*C*H$_3$). ^{11}B NMR (160 MHz, C_6D_6, ppm): δ 22.52. HRMS (ESI): m/z calcd for $C_{15}H_{23}BNaO_3^+$: 285.1632 [(M+Na)]$^+$; found: 285.1634.

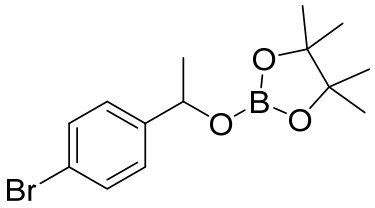


4c *(CAS 1566593-64-3)*: ^{1}H NMR (500 MHz, C_6D_6, ppm): δ 7.02 (dt, *J* = 9.4, 2.4 Hz, 2H, Ar*H*), 6.50 (dt, *J* = 9.4, 2.5 Hz, 2H, Ar*H*), 5.11 (q, *J* = 6.4 Hz, 1H, OC*H*), 3.10 (s, 3H, OC*H*$_3$), 1.21 (d, *J* = 6.5 Hz, 3H, OCHC*H*$_3$), 0.79 (d, *J* = 10.9 Hz, 12H, C(C*H*$_3$)$_2$). ^{13}C NMR (125 MHz, C_6D_6, ppm): δ 159.30, 137.36, 126.89, 113.92 (*Ar*), 82.44 (*C*(CH$_3$)$_2$), 72.52 (O*C*H), 54.76 (O*C*H$_3$), 25.65 (OCH*C*H$_3$), 24.61 (d, *J* = 9.9 Hz, C(*C*H$_3$)$_2$). ^{11}B NMR (160 MHz, C_6D_6, ppm):

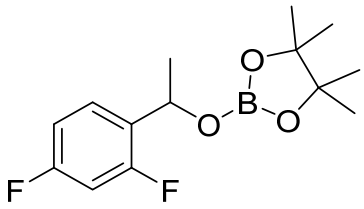
δ 22.51. HRMS (ESI): m/z calcd for $C_{15}H_{23}BNaO_4^+$: 301.1582 $[(M+Na)]^+$; 301.1582.



4d *(CAS 1416719-03-3)*: ^{1}H NMR (500 MHz, C_6D_6, ppm): δ 7.09-7.05 (m, 4H, Ar*H*), 5.25 (q, *J* = 6.0 Hz, 1H, OC*H*), 1.34 (d, *J* = 6.5 Hz, 3H, OCHC*H*$_3$), 1.00 (d, *J* = 13.5 Hz, 12H, C(C*H*$_3$)$_2$). ^{13}C NMR (125 MHz, C_6D_6, ppm): δ 143.73, 133.02, 128.62, 127.09 (*Ar*), 82.61 (*C*(CH$_3$)$_2$), 72.17 (O*C*H), 25.49 (OCH*C*H$_3$), 24.56 (d, *J* = 9.2 Hz, C(*C*H$_3$)$_2$). ^{11}B NMR (160 MHz, C_6D_6, ppm): δ 22.52. HRMS (ESI): m/z calcd for $C_{14}H_{20}BClNaO_3^+$: 305.1086 $[(M+Na)]^+$; found: 305.1087.

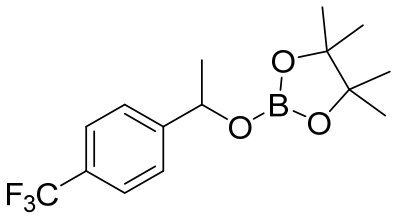


4e *(New Compound)*: ^{1}H NMR (500 MHz, C_6D_6, ppm): δ 7.23 (dt, *J* = 8.9, 2.2 Hz, 2H, Ar*H*), 7.00 (dt, *J* = 8.6, 2.2 Hz, 2H, Ar*H*), 5.20 (q, *J* = 6.5 Hz, 1H, OC*H*), 1.32 (d, *J* = 6.5 Hz, 3H, OCHC*H*$_3$), 1.01 (d, *J* = 14.2 Hz, 12H, C(C*H*$_3$)$_2$). ^{13}C NMR (125 MHz, C_6D_6, ppm): δ 144.21, 131.56, 127.44, 121.10 (*Ar*), 82.64 (*C*(CH$_3$)$_2$), 72.14 (O*C*H), 25.47 (OCH*C*H$_3$), 24.59 (d, *J* = 7.3 Hz, C(*C*H$_3$)$_2$). ^{11}B NMR (160 MHz, C_6D_6, ppm): δ 22.45. HRMS (ESI): m/z calcd for $C_{14}H_{20}BBrNaO_3^+$: 349.0581 $[(M+Na)]^+$; found: 349.0583.

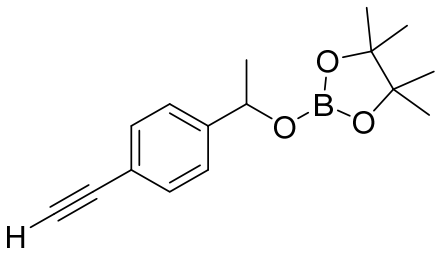


4f *(New Compound)*: ^{1}H NMR (500 MHz, C_6D_6, ppm): δ 7.38 (td, *J* = 8.5, 6.7 Hz, 1H, Ar*H*), 6.54 (tdd, *J* = 8.4, 2.5, 0.8 Hz, 1H, Ar*H*), 6.45 (ddd, *J* = 10.5, 8.9, 2.5 Hz, 1H, Ar*H*), 5.70 (q,

J = 6.4 Hz, 1H, OC*H*), 1.40 (d, *J* = 6.4 Hz, 3H, OCHC*H*$_3$), 1.01 (d, *J* = 13.0 Hz, 12H, C(C*H*$_3$)$_2$). ^{13}C NMR (125 MHz, C_6D_6, ppm): δ 162.36 (dd, *J* = 247.1, 11.9 Hz, *Ar*), 159.48 (dd, *J* = 247.9, 11.8 Hz, *Ar*), 128.39 (dd, *J* = 14.1, 3.8 Hz, *Ar*), 128.00 (d, *J* = 15.4 Hz, *Ar*), 111.37 (dd, *J* = 20.9, 3.6 Hz, *Ar*), 103.50 (t, *J* = 25.7 Hz, *Ar*), 82.75 (*C*(CH$_3$)$_2$), 66.60 (d, *J* = 2.0 Hz, O*C*H), 24.51 (d, *J* = 5.1 Hz, C(*C*H$_3$)$_2$) , 24.41 (OCH*C*H$_3$). ^{11}B NMR (160 MHz, C_6D_6, ppm): δ 22.49. HRMS (ESI): m/z calcd for $C_{14}H_{19}BF_2NaO_3^+$: 307.1288 [(M+Na)]$^+$; found: 307.1289.

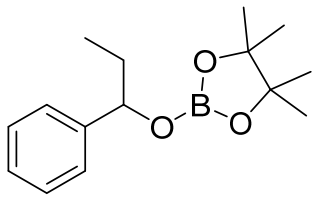


4g *(CAS 1416719-02-2)*: ^{1}H NMR (500 MHz, C_6D_6, ppm): δ 7.10 (d, *J* = 8.1 Hz, 2H, Ar*H*), 6.95 (dd, *J* = 8.1, 0.5 Hz, 2H, Ar*H*), 5.00 (q, *J* = 6.5 Hz, 1H, OC*H*), 1.08 (d, 3H, *J* = 6.5 Hz, OCHC*H*$_3$), 0.78 (d, *J* = 16.3 Hz, 12H, C(C*H*$_3$)$_2$). ^{13}C NMR (125 MHz, C_6D_6, ppm): δ 149.19 (*Ar*), 129.41 (q, *J* = 32.1 Hz, *Ar*), 125.94 (*Ar*), 125.42 (q, *J* = 3.7 Hz, *Ar*), 124.96 (q, *J* = 271.9 Hz, *C*F$_3$), 82.79 (*C*(CH$_3$)$_2$), 72.18 (O*C*H), 25.38 (OCH*C*H$_3$), 24.51 (d, *J* = 1.9 Hz, C(*C*H$_3$)$_2$). ^{11}B NMR (160 MHz, C_6D_6, ppm): δ 22.39. HRMS (ESI): m/z calcd for $C_{15}H_{20}BF_3NaO_3^+$: 339.1350 [(M+Na)]$^+$; found: 339.1351.

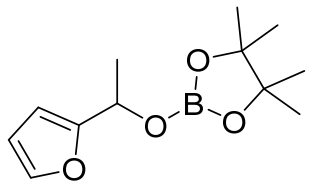


4h *(New Compound)*: ^{1}H NMR (500 MHz, C_6D_6, ppm): δ 7.13-7.11 (m, 2H, Ar*H*), 6.91-6.89 (m, 2H, Ar*H*), 5.00 (q, *J* = 6.5 Hz, 1H, OC*H*), 2.55 (s, 1H, C≡C*H*), 1.09 (d, *J* = 6.5 Hz, 3H, OCHC*H*$_3$), 0.75 (d, *J* = 14.8 Hz, 12H, C(C*H*$_3$)$_2$). ^{13}C NMR (125 MHz, C_6D_6, ppm): δ 145.93, 132.34, 125.64, 121.41 (*Ar*), 83.89 (*C*(CH$_3$)$_2$), 82.62 (*C*≡C), 77.59 (C≡*C*), 72.43 (O*C*H), 25.39 (OCH*C*H$_3$), 24.55 (d, *J* = 10.6 Hz, C(*C*H$_3$)$_2$). ^{11}B NMR (160 MHz, C_6D_6, ppm): δ

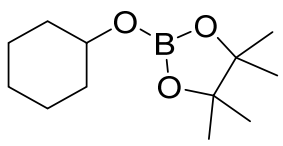
22.40. HRMS (ESI): m/z calcd for $C_{16}H_{21}BNaO_3^+$: 295.1476 [(M+Na)]$^+$; found: 295.1475.



4i *(New Compound)*: ^{1}H NMR (500 MHz, C_6D_6, ppm): δ 7.09-7.07 (m, 2H, Ar*H*), 6.92-6.89 (m, 2H, Ar*H*), 6.82 (tt, *J* = 3.7, 1.5 Hz, 1H, Ar*H*), 4.91 (dd, *J* = 7.4, 5.5 Hz, 1H, OC*H*), 1.55-1.43 (m, 2H, OCHC*H*$_2$), 0.78 (d, *J* = 16.1 Hz, 12H, C(C*H*$_3$)$_2$), 0.62 (t, *J* = 7.4 Hz, 3H, CH$_2$C*H*$_3$). ^{13}C NMR (125 MHz, C_6D_6, ppm): δ 143.03, 127.36, 126.32, 125.17 (*Ar*), 81.45 (*C*(CH$_3$)$_2$), 76.99 (O*C*H), 31.44 (OCH*C*H$_2$), 23.59 (d, *J* = 6.4 Hz, C(*C*H$_3$)$_2$), 9.00 (CH$_2$*C*H$_3$). ^{11}B NMR (160 MHz, C_6D_6, ppm): δ 22.53. HRMS (ESI): m/z calcd for $C_{15}H_{23}BNaO_3^+$: 285.1632 [(M+Na)]$^+$; found: 285.1635.

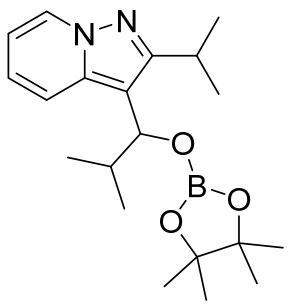


4j *(New Compound)*: ^{1}H NMR (500 MHz, C_6D_6, ppm): δ 7.07 (dd, *J* = 1.8, 0.9 Hz, 1H, Ar*H*), 6.15 (dt, *J* = 3.3, 0.8 Hz, 1H, Ar*H*), 6.05 (dd, *J* = 3.3, 1.8 Hz, 1H, Ar*H*), 5.41 (q, *J* = 6.6 Hz, 1H, OC*H*), 1.48 (d, *J* = 6.6 Hz, 3H, OCHC*H*$_3$), 1.04 (d, *J* = 3.1 Hz, 12H, C(C*H*$_3$)$_2$). ^{13}C NMR (125 MHz, C_6D_6, ppm): δ 157.06, 141.84, 110.27, 105.78 (*Ar*), 82.64 (*C*(CH$_3$)$_2$), 66.43 (O*C*H), 24.59 (d, *J* = 17.1 Hz, C(*C*H$_3$)$_2$), 21.28 (OCH*C*H$_3$). ^{11}B NMR (160 MHz, C_6D_6, ppm): δ 22.60. HRMS (ESI): m/z calcd for $C_{12}H_{19}BNaO_4^+$: 261.1269 [(M+Na)]$^+$; found: 261.1272.

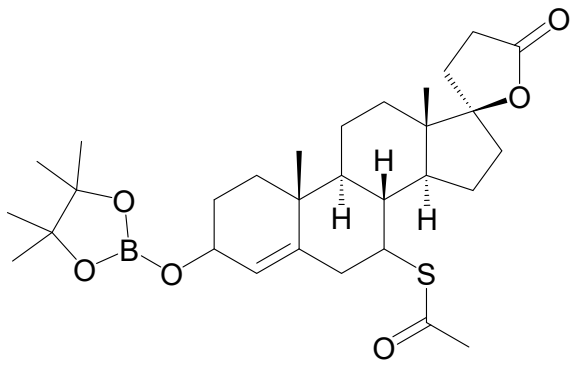


4k *(CAS 96649-78-4)*: ^{1}H NMR (500 MHz, C_6D_6, ppm): δ 4.15 (hept, *J* = 4.4 Hz, 1H, OC*H*), 1.87-1.83 (m, 2H, C*H*$_2$), 1.62-1.57 (m, 2H, C*H*$_2$), 1.47-1.391 (m, 2H, C*H*$_2$), 1.31-1.27 (m, 1H, C*H*$_2$), 1.16-1.11 (m, 3H, overlapped, C*H*$_2$), 1.07 (br, 12H, overlapped, C(C*H*$_3$)$_2$). ^{13}C NMR

(125 MHz, C_6D_6, ppm): δ 82.15 (*C*$(CH_3)_2$), 72.61 (O*C*H), 34.70, 25.74 (*C*H_2), 24.69 (C(*C*$H_3)_2$) , 24.05 (*C*H_2). ^{11}B NMR (160 MHz, C_6D_6, ppm): δ 22.27. HRMS (ESI): m/z calcd for $C_{12}H_{23}BNaO_3^+$: 249.1632 $[(M+Na)]^+$; found: 249.1636.

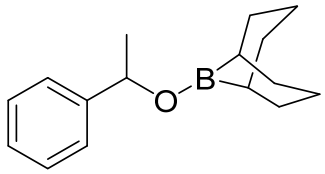


4l *(New Compound)*: ^{1}H NMR (500 MHz, C_6D_6, ppm): δ 8.10 (dt, *J* = 7.0, 1.1 Hz, 1H, Ar*H*), 7.63 (dt, *J* = 9.0, 1.2 Hz, 1H, Ar*H*), 6.51 (ddd, *J* = 9.0, 6.7, 1.2 Hz, 1H, Ar*H*), 5.99 (td, *J* = 6.9, 1.4 Hz, 1H, Ar*H*), 5.24 (d, *J* = 8.3 Hz, 1H, OC*H*), 3.38 n(hept, *J* = 6.9 Hz, 1H, ArC*H*Me_2), 2.30-2.23 (m, 1H, OCHC*H*Me_2), 1.59 (q, *J* = 7.1 Hz, 6H, ArCH(C*H*$_3)_2$), 1.16 (d, *J* = 6.6 Hz, 3H, OCHCH(C*H*$_3)_2$), 0.95 (d, *J* = 16.2 Hz, 12H, C(C*H*$_3)_2$), 0.78 (d, *J* = 6.8 Hz, 3H, OCHCH(C*H*$_3)_2$). ^{13}C NMR (125 MHz, C_6D_6, ppm): δ 158.81, 138.72, 128.45, 122.08, 118.51, 110.59, 108.82 (*Ar*), 82.38 (*C*$(CH_3)_2$), 75.92 (O*C*H), 35.59 (*C*HMe_2), 27.00 (*C*HMe_2), 24.53 (d, *J* = 25.8 Hz, C(*C*$H_3)_2$), 23.74, 23.14 (CH*Me*$_2$), 19.37 (d, *J* = 2.6 Hz, CH*Me*$_2$). ^{11}B NMR (160 MHz, C_6D_6, ppm): δ 22.66. HRMS (ESI): m/z calcd for $C_{20}H_{31}BN_2NaO_3^+$: 381.2320 $[(M+Na)]^+$; found: 381.2319.

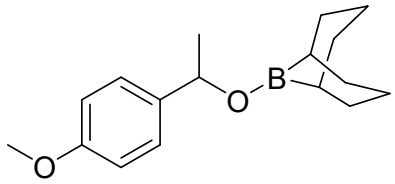


4m *(New Compound)*: ^{1}H NMR (500 MHz, C_6D_6, ppm): δ 5.57 (d, *J* = 1.4 Hz, 1H), 4.92-4.89 (m, 1H), 3.93 (q, *J* = 3.0 Hz, 1H), 2.45-2.42 (m, 1H), 2.13 (dd, *J* = 14.2, 2.7 Hz, 1H), 2.01-1.96 (m, 4H), 1.87 (s, 3H), 1.76-1.66 (m, 2H), 1.54 (td, *J* = 11.1, 3.6 Hz, 1H), 1.49-1.42

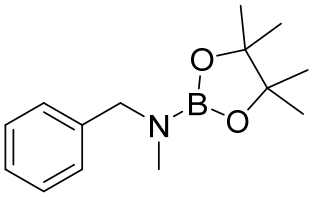
(m, 2H), 1.35-1.30 (m, 1H), 1.20-1.10 (m, overlapped, 5H), 1.07 (d, *J* = 4.8 Hz, overlapped, 12H), 1.01 (s, 2H), 0.79 (s, overlapped, 2H), 0.76 (s, overlapped, 2H), 0.81-0.64 (m, overlapped, 4H). ^{13}C NMR (125 MHz, C_6D_6, ppm): δ 192.41, 175.10, 142.12, 127.15, 94.47, 82.43, 70.40, 50.05, 46.26, 46.17, 45.54, 39.63, 39.19, 37.37, 35.34, 35.33, 31.17, 31.05, 30.80, 29.18, 28.11, 24.65 (d, *J* = 10.0 Hz), 22.53, 20.41, 18.85, 14.63. ^{11}B NMR (160 MHz, C_6D_6, ppm): δ 22.38. HRMS (ESI): m/z calcd for $C_{30}H_{45}BNaO_6S^+$: 567.2922 $[(M+Na)]^+$; found: 567.2925.



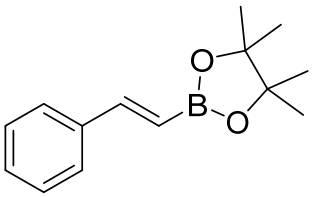
4n *(New Compound)*: ^{1}H NMR (500 MHz, C_6D_6, ppm): ^{1}H NMR (500 MHz, C_6D_6, ppm): δ 7.05 (d, *J* = 7.4 Hz, 2H, Ar*H*), 6.93 (t, *J* = 7.7 Hz, 2H, Ar*H*), 6.84 (t, *J* = 7.4 Hz, 1H, Ar*H*), 4.98 (q, *J* = 6.5 Hz, 1H, OC*H*), 1.64-1.52 (m, 10H, BC_8H_{14}), 1.21 (d, *J* = 6.5 Hz, 3H, overlapped, OCHCH_3), 1.20-1.05 (m, 4H, overlapped, BC_8H_{14}). ^{13}C NMR (125 MHz, C_6D_6, ppm): δ 145.81, 128.62, 127.37, 125.71 (*Ar*), 73.87 (O*C*H), 33.68, 33.40 (B*C*$_8$H$_{14}$), 26.35 (OCH*C*H$_3$), 23.62 (B*C*$_8$H$_{14}$). ^{11}B NMR (160 MHz, C_6D_6, ppm): δ 57.10. HRMS (ESI): m/z calcd for $C_{16}H_{25}BNaO_2^+$:283.1840 $[(M+H_2O+Na)]^+$; found: 283.1838.



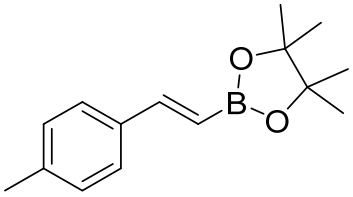
4m *(New Compound)*: ^{1}H NMR (500 MHz, C_6D_6, ppm): ^{1}H NMR (500 MHz, C_6D_6, ppm): δ 7.20 (d, *J* = 8.1 Hz, 2H, Ar*H*), 6.75 (d, *J* = 8.1 Hz, 2H, Ar*H*), 5.20 (q, *J* = 6.0 Hz, 1H, OC*H*), 3.35 (s, 3H, OCH_3) 1.86-1.65 (m, 10H, BC_8H_{14}), 1.45 (d, *J* = 6.0 Hz, 3H, overlapped, OCHCH_3), 1.41-1.25 (m, 4H, overlapped, BC_8H_{14}). ^{13}C NMR (125 MHz, C_6D_6, ppm): δ 159.31, 137.93, 126.90, 114.05 (*Ar*), 73.55 (O*C*H), 54.76 (O*C*H$_3$) 33.68, 33.42 (B*C*$_8$H$_{14}$), 26.35 (OCH*C*H$_3$), 23.64 (B*C*$_8$H$_{14}$). ^{11}B NMR (160 MHz, C_6D_6, ppm): δ 56.31. HRMS (ESI): m/z calcd for $C_{19}H_{28}BNNaO_2^+$: 336.2105 $[(M+CH_3CN+Na)]^+$; found: 336.2107.



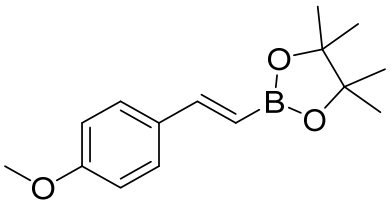
4p *(1892609-31-2)*: ^{1}H NMR (500 MHz, C_6D_6, ppm): δ 7.26-7.24 (m, 2H, Ar*H*), 7.19-7.15 (m, 2H, Ar*H*), 7.10-7.07 (m, 1H, Ar*H*), 4.13 (s, NC*H*$_2$), 2.56 (s, NC*H*$_3$), 1.14 (s, C(C*H*$_3$)$_2$). ^{13}C NMR (125 MHz, C_6D_6, ppm): δ 140.69, 128.56, 128.00, 126.95 (*Ar*), 82.35 (*C*(CH$_3$)$_2$), 53.19 (N*C*H), 33.27 (N*C*H$_3$), 24.80 (C(*C*H$_3$)$_2$). ^{11}B NMR (160 MHz, C_6D_6, ppm): δ 24.60. HRMS (ESI): m/z calcd for $C_{14}H_{23}BNaO_2^+$: 248.1816 $[(M+H)]^+$; found: 248.1816.



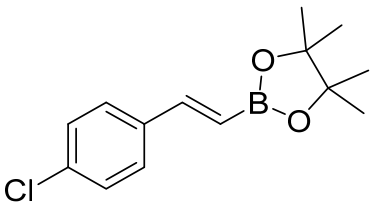
6a *(CAS 3947-56-2)*: ^{1}H NMR (500 MHz, $CDCl_3$, ppm): δ 7.51-7.49 (m, 2H, Ar*H*), 7.42 (d, *J* = 18.5 Hz, 1H, ArC*H*=), 7.37-7.33 (m, 2H, Ar*H*), 7.30 (tt, *J* = 3.6, 1.7 Hz, 2H, Ar*H*), 6.19 (d, *J* = 18.5 Hz, 1H, =C*H*B), 1.33 (s, 12H, C(C*H*$_3$)$_2$). ^{13}C NMR (125 MHz, $CDCl_3$, ppm): δ 149.48 (Ar*C*H=), 137.42, 128.85, 128.52, 127.01 (*Ar*), 116.32 (br, =*C*HB), 83.30 (*C*(CH$_3$)$_2$), 24.77 (C(*C*H$_3$)$_2$). ^{11}B NMR (160 MHz, $CDCl_3$, ppm): δ 30.06. HRMS (ESI): m/z calcd for $C_{14}H_{19}BNaO_2^+$: 253.1370 $[(M+Na)]^+$; found: 253.1373.



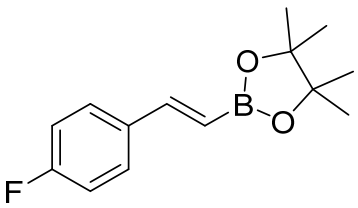
6b *(CAS 149777-84-4)*: ^{1}H NMR (500 MHz, $CDCl_3$, ppm): δ 7.39 (d, *J* = 10.1 Hz, 1H, overlapped, ArC*H*=), 7.37 (d, *J* = 8.2 Hz, 2H, overlapped, Ar*H*), 6.11 (d, *J* = 18.5 Hz, 1H, =C*H*B), 2.31 (s, 3H, ArC*H*$_3$), 1.29 (s, 12H, C(C*H*$_3$)$_2$). ^{13}C NMR (125 MHz, $CDCl_3$, ppm): δ 149.37 (Ar*C*H=), 138.76, 134.67, 129.16, 126.87 (*Ar*), 115.12 (br, =*C*HB), 83.07 (*C*(CH$_3$)$_2$), 24.67 (C(*C*H$_3$)$_2$), 21.17 (Ar*C*H$_3$). ^{11}B NMR (160 MHz, $CDCl_3$, ppm): δ 30.06. HRMS (ESI): m/z calcd for $C_{15}H_{21}BNaO_2^+$: 267.1527 $[(M+Na)]^+$; found: 267.1530.



6c *(CAS 149777-83-3)*: ^{1}H NMR (500 MHz, $CDCl_3$, ppm): δ 7.44 (dt, *J* = 9.6, 2.4 Hz, 2H, Ar*H*), 7.36 (d, *J* = 18.4 Hz, 1H, ArC*H*=), 6.87 (dt, *J* = 9.6, 2.4 Hz, 2H, Ar*H*), 6.02 (d, *J* = 18.4 Hz, 1H, =C*H*B), 3.81 (s, 3H, OCH_3), 1.33 (s, 12H, C(CH_3)$_2$). ^{13}C NMR (125 MHz, $CDCl_3$, ppm): δ 160.25 (*Ar*), 149.03 (Ar*C*H=), 130.35, 128.421 113.92 (*Ar*), 113.64 (br, =*C*HB), 83.17 (*C*(CH$_3$)$_2$), 24.76 (C(*C*H$_3$)$_2$). ^{11}B NMR (160 MHz, $CDCl_3$, ppm): δ 30.42. HRMS (ESI): m/z calcd for $C_{15}H_{22}BO_3^+$: 261.1657 $[(M+H)]^+$; found: 261.1653.

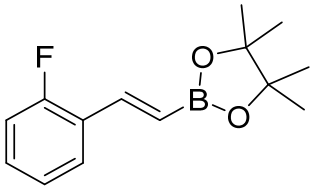


6d *(CAS 223919-54-8)*: ^{1}H NMR (500 MHz, $CDCl_3$, ppm): δ 7.35-7.32 (m, 2H, Ar*H*), 7.26 (d, *J* = 18.4 Hz, 1H, overlapped, ArC*H*=), 7.24-7.21 (m, 2H, overlapped, Ar*H*), 6.06 (d, *J* = 18.4 Hz, 1H, =C*H*B), 1.24 (s, 12H, C(CH_3)$_2$). ^{13}C NMR (125 MHz, $CDCl_3$, ppm): δ 148.00 (Ar*C*H=), 135.94, 134.59, 128.77, 128.20 (*Ar*), 117.20 (br, =*C*HB), 83.44 (*C*(CH$_3$)$_2$), 24.78 (C(*C*H$_3$)$_2$). ^{11}B NMR (160 MHz, $CDCl_3$, ppm): δ 30.05. HRMS (ESI): m/z calcd for $C_{14}H_{19}BO_2$: 265.1161 $[(M+H)]^+$; found: 265.1163.

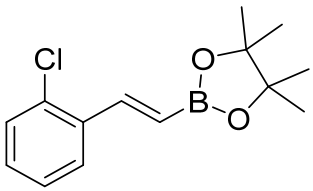


6e *(CAS 504433-86-7)*: ^{1}H NMR (500 MHz, $CDCl_3$, ppm): δ 7.48-7.44 (m, 2H, Ar*H*), 7.36 (d, *J* = 18.4 Hz, 1H, ArC*H*=), 7.02 (tt, *J* = 9.1, 2.3 Hz, 2H, Ar*H*), 6.08 (d, *J* = 18.4 Hz, 1H, =C*H*B), 1.31 (s, 12H, C(CH_3)$_2$). ^{13}C NMR (125 MHz, $CDCl_3$, ppm): δ 163.09 (d, *J* = 248.8 Hz, *Ar*), 148.11 (Ar*C*H=), 133.67 (d, *J* = 3.1 Hz, *Ar*), 128.65 (d, *J* = 8.2 Hz, *Ar*), 116.16 (br,

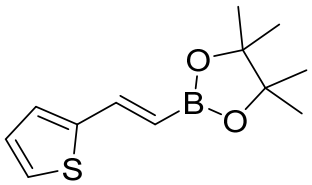
=*C*HB), 115.51 (d, *J* = 21.8 Hz, *Ar*), 83.33 (*C*(CH_3)$_2$), 24.74 (C(*C*H_3)$_2$). ^{11}B NMR (160 MHz, $CDCl_3$, ppm): δ 30.31. HRMS (ESI): m/z calcd for $C_{14}H_{19}BFO_2^+$: 249.1457 [(M+H)]$^+$; found: 249.1457.



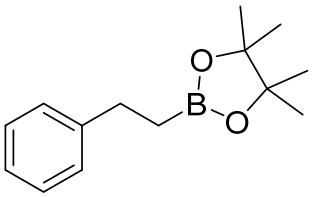
6f *(CAS 633327-38-5)*: ^{1}H NMR (500 MHz, $CDCl_3$, ppm): δ 7.61 (d, *J* = 18.6 Hz, 1H, ArC*H*=), 7.58 (td, *J* = 7.6, 1.7 Hz, 1H, Ar*H*), 7.29-7.25 (m, 1H, Ar*H*), 7.12 (t, *J* = 7.5 Hz, 1H, Ar*H*), 7.06-7.03 (m, 1H, Ar*H*), 6.26 (d, *J* = 18.6 Hz, 1H, =C*H*B), 1.33 (s, 12H, C(C*H*$_3$)$_2$). ^{13}C NMR (125 MHz, $CDCl_3$, ppm): δ 160.66 (d, *J* = 251.6 Hz, *Ar*), 141.26 (d, *J* = 4.2 Hz, Ar*C*H=), 130.13 (d, *J* = 8.4 Hz, *Ar*), 127.33 (d, *J* = 3.5 Hz, *Ar*), 125.32 (d, *J* = 11.6 Hz, *Ar*), 124.05 (d, *J* = 3.6 Hz, *Ar*), 119.04 (br, =*C*HB), 115.76 (d, *J* = 22.0 Hz, *Ar*), 83.39 (*C*(CH_3)$_2$), 24.75 (C(*C*H_3)$_2$). ^{11}B NMR (160 MHz, $CDCl_3$, ppm): δ 30.15. HRMS (ESI): m/z calcd for $C_{14}H_{18}BFNaO_2^+$: 271.1276 [(M+Na)]$^+$; found: 271.1279.



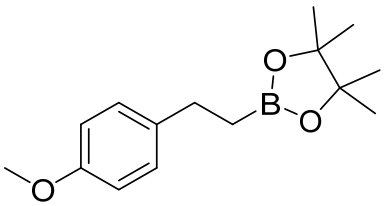
6g *(CAS 1355094-04-0)*: ^{1}H NMR (500 MHz, $CDCl_3$, ppm): δ 7.79 (d, *J* = 18.4 Hz, 1H, ArC*H*=), 7.64 (dd, *J* = 7.3, 2.2 Hz, 1H, Ar*H*), 7.36 (dd, *J* = 7.5, 1.8 Hz, 1H, Ar), 7.25-7.22 (m, 2H, Ar*H*), 6.18 (d, *J* = 18.4 Hz, 1H, =C*H*B), 1.33 (s, 12H, C(C*H*$_3$)$_2$). ^{13}C NMR (125 MHz, $CDCl_3$, ppm): δ 144.98 (Ar*C*H=), 135.63, 133.86, 132.58 (*Ar*), 129.74 (d, *J* = 15.0 Hz, *Ar*), 128.63 (d, *J* = 90.1 Hz, *Ar*), 126.9 (d, *J* = 21.7 Hz, *Ar*), 119.53 (br, =*C*HB), 83.50 (*C*(CH_3)$_2$), 24.83 (C(*C*H_3)$_2$). ^{11}B NMR (160 MHz, $CDCl_3$, ppm): δ 30.02. HRMS (ESI): m/z calcd for $C_{14}H_{18}BClNaO_2^+$: 287.0981 [(M+Na)]$^+$; found: 287.0980.



6h *(CAS 161395-82-0)*: ^{1}H NMR (500 MHz, $CDCl_3$, ppm): δ 7.48 (d, *J* = 18.1 Hz, 1H, ArC*H*=), 7.25 (d, *J* = 5.1 Hz, 1H, Ar*H*), 7.09-7.08 (m, 1H, Ar*H*), 6.99 (dd, *J* = 5.1, 3.6 Hz, 1H, Ar*H*), 5.92 (d, *J* = 18.1 Hz, 1H, =C*H*B), 1.31 (s, 12H, C(C*H*$_3$)$_2$). ^{13}C NMR (125 MHz, $CDCl_3$, ppm): δ 143.90 (Ar*C*H=), 141.78, 127.67, 127.59, 126.26 (*Ar*), 116.14 (br, =*C*HB), 83.34 (*C*(CH$_3$)$_2$), 24.76 (C(*C*H$_3$)$_2$). ^{11}B NMR (160 MHz, $CDCl_3$, ppm): δ 30.07. HRMS (ESI): m/z calcd for $C_{12}H_{17}BNaO_2S^+$: 259.0935 $[(M+Na)]^+$; found: 259.0932.

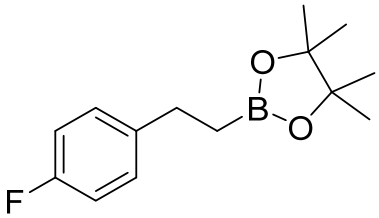


6i *(CAS 165904-22-3)*: ^{1}H NMR (500 MHz, $CDCl_3$, ppm): δ 7.16-7.10 (m, 4H, Ar*H*), 7.05-7.02 (m, 1H, Ar*H*), 2.66 (t, *J* = 8.1 Hz, 2H, C*H*$_2$), 1.10 (s, 12H, C(C*H*$_3$)$_2$), 1.05 (t, *J* = 8.1 Hz, 2H, C*H*$_2$). ^{13}C NMR (125 MHz, $CDCl_3$, ppm): δ 144.24, 128.04, 127.87, 125.36 (*Ar*), 82.90 (*C*(CH$_3$)$_2$), 29.84 (Ar*C*H$_2$), 24.68 (C(*C*H$_3$)$_2$), 12.85 (br, B*C*H$_2$). ^{11}B NMR (160 MHz, $CDCl_3$, ppm): δ 33.79. HRMS (ESI): m/z calcd for $C_{14}H_{21}BNaO_2^+$: 255.1527 $[(M+Na)]^+$; found: 255.1526.

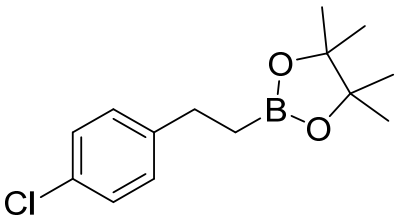


6j *(CAS 355012-39-4)*: ^{1}H NMR (500 MHz, $CDCl_3$, ppm): δ 7.18-7.15 (m, 2H, Ar*H*), 6.85-6.82 (m, 2H, Ar*H*), 3.78 (s, 3H, OC*H*$_3$), 2.73 (t, *J* = 8.1 Hz, 2H, C*H*$_2$), 1.24 (s, 12H, C(C*H*$_3$)$_2$), 1.15 (t, *J* = 8.1 Hz, 2H, C*H*$_2$). ^{13}C NMR (125 MHz, $CDCl_3$, ppm): δ 157.44, 136.36, 128.69, 113.44 (*Ar*), 82.84 (*C*(CH$_3$)$_2$), 54.98 (OCH_3), 28.91 (Ar*C*H$_2$), 24.65

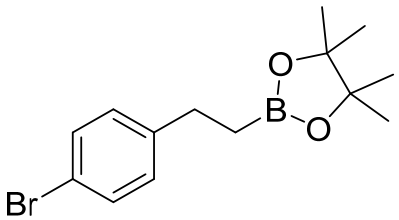
(C(CH_3)$_2$), 13.13 (br, BCH_2). ^{11}B NMR (160 MHz, $CDCl_3$, ppm): δ 33.79. HRMS (ESI): m/z calcd for $C_{15}H_{23}BNaO_3^+$: 285.1632 [(M+Na)]$^+$; found: 285.1635.



6k *(CAS 1065498-70-5)*: ^{1}H NMR (500 MHz, $CDCl_3$, ppm): δ 7.18-7.15 (m, 2H, Ar*H*), 6.95-6.91 (m, 2H, Ar*H*), 2.72 (t, *J* = 8.1 Hz, 2H, CH_2), 1.21 (s, 12H, C(CH_3)$_2$), 1.12 (t, *J* = 8.1 Hz, 2H, CH_2). ^{13}C NMR (125 MHz, $CDCl_3$, ppm): δ 161.02 (d, *J* = 242.6 Hz, *Ar*), 139.86 (d, *J* = 3.3 Hz, *Ar*), 129.23 (d, *J* = 7.5 Hz, *Ar*), 114.70 (d, *J* = 20.9 Hz, *Ar*), 83.00 (*C*(CH_3)$_2$), 29.07 (Ar*C*H$_2$), 24.68 (C(*C*H$_3$)$_2$), 13.10 (br, B*C*H$_2$). ^{11}B NMR (160 MHz, $CDCl_3$, ppm): δ 33.73. HRMS (ESI): m/z calcd for $C_{14}H_{20}BFNaO_2^+$: 273.1433 [(M+Na)]$^+$; found: 273.1436.



6l *(CAS 444094-88-6)*: ^{1}H NMR (500 MHz, $CDCl_3$, ppm): δ 7.22-7.20 (m, 2H, Ar*H*), 7.15-7.13 (m, 2H, Ar*H*), 2.71 (t, *J* = 8.1 Hz, 2H, CH_2), 1.21 (s, 12H, C(CH_3)$_2$), 1.11 (t, *J* = 8.1 Hz, 2H, CH_2). ^{13}C NMR (125 MHz, $CDCl_3$, ppm): δ 142.75, 131.08, 129.32, 128.15 (*Ar*), 83.08 (*C*(CH_3)$_2$), 29.26 (Ar*C*H$_2$), 24.73 (C(*C*H$_3$)$_2$), 12.80 (br, B*C*H$_2$). ^{11}B NMR (160 MHz, $CDCl_3$, ppm): δ 33.52. HRMS (ESI): m/z calcd for $C_{14}H_{20}BClNaO_2^+$: 289.1137 [(M+Na)]$^+$; found: 289.1140.

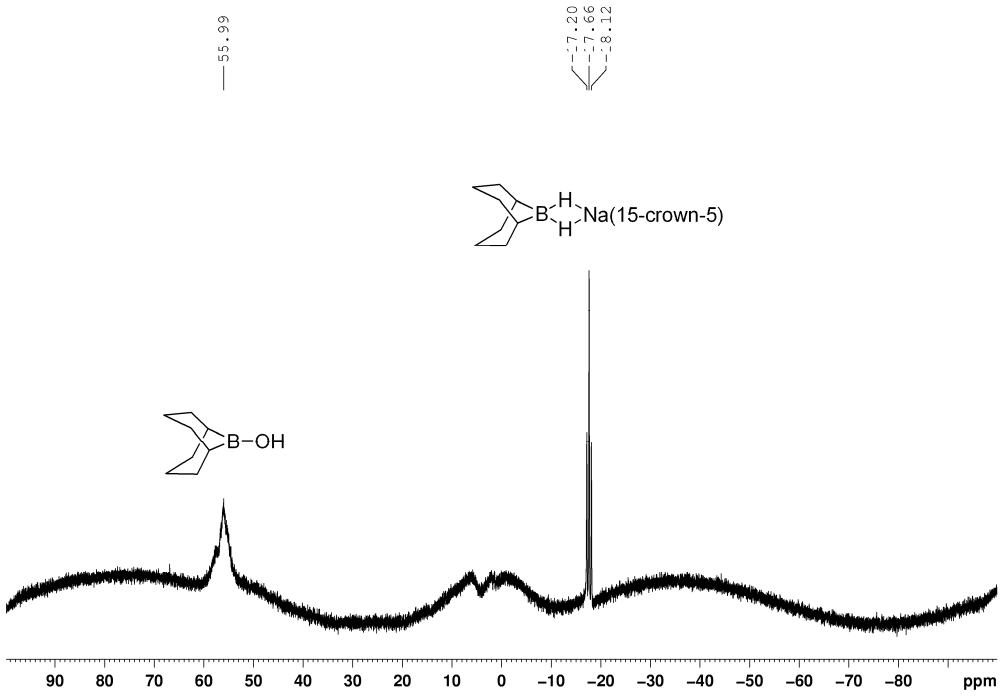


6m *(CAS 748801-42-5)*: ^{1}H NMR (500 MHz, $CDCl_3$, ppm): δ 7.39-7.36 (m, 2H, Ar*H*), 7.11-7.09 (m, 2H, Ar*H*), 2.71 (t, *J* = 8.1 Hz, 2H, CH_2), 1.23 (s, 12H, C(CH_3)$_2$), 1.12 (t, *J* =

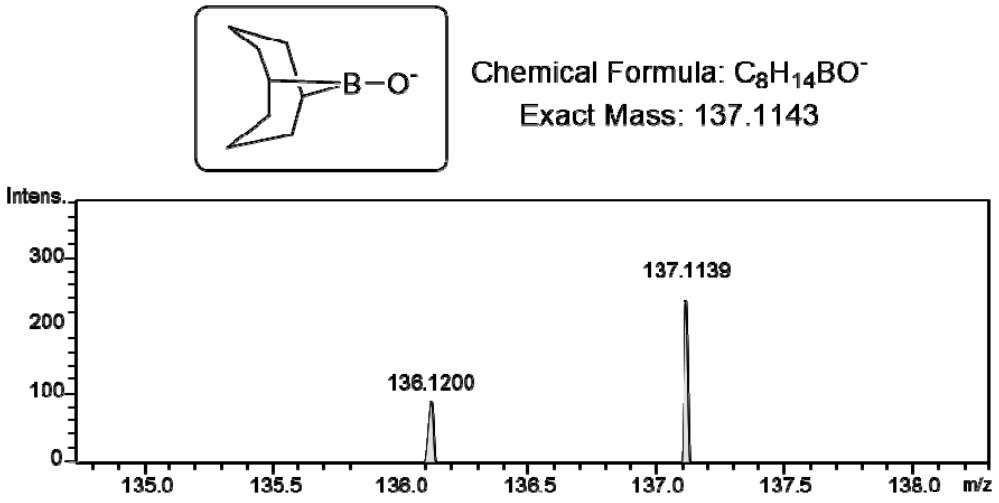
8.1 Hz, 2H, CH_2). ^{13}C NMR (125 MHz, $CDCl_3$, ppm): δ 143.28, 131.11, 129.76, 119.11 (*Ar*), 83.10 ($C(CH_3)_2$), 29.33 (ArCH_2), 24.75 (C(CH_3)$_2$), 12.75 (br, BCH_2). ^{11}B NMR (160 MHz, $CDCl_3$, ppm): δ 33.59. HRMS (ESI): m/z calcd for $C_{14}H_{20}BBrNaO_2^+$: 333.0632 $[(M+Na)]^+$; found: 233.0629.

Spectra

In situ analysis of the reaction of NaOH with 9-BBN:

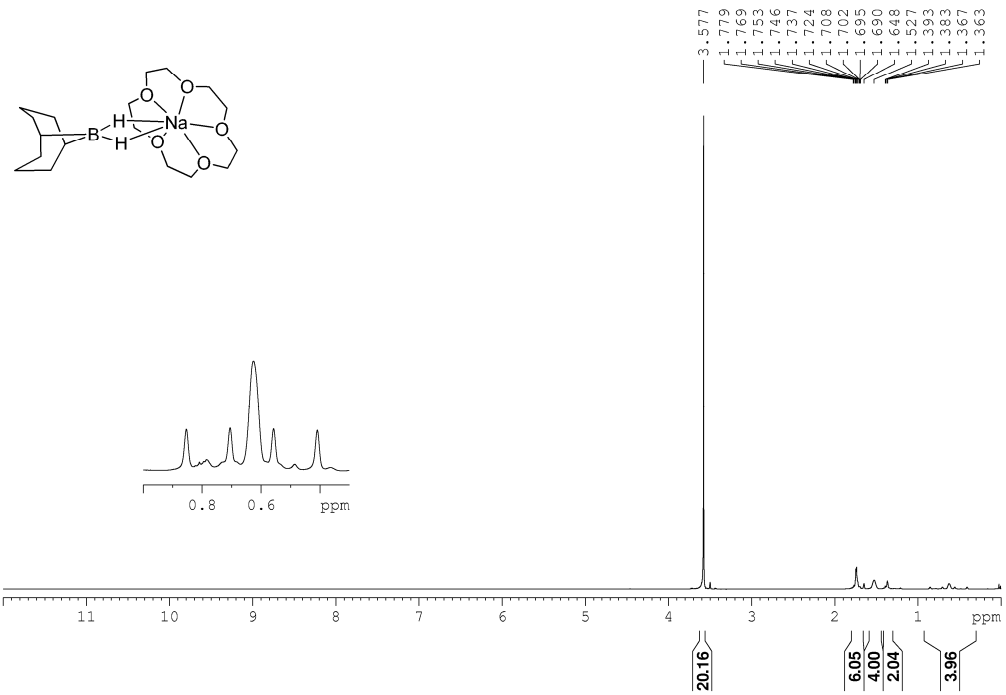


B^{11} NMR



HRMS (negative ion mode)

Compound 7a: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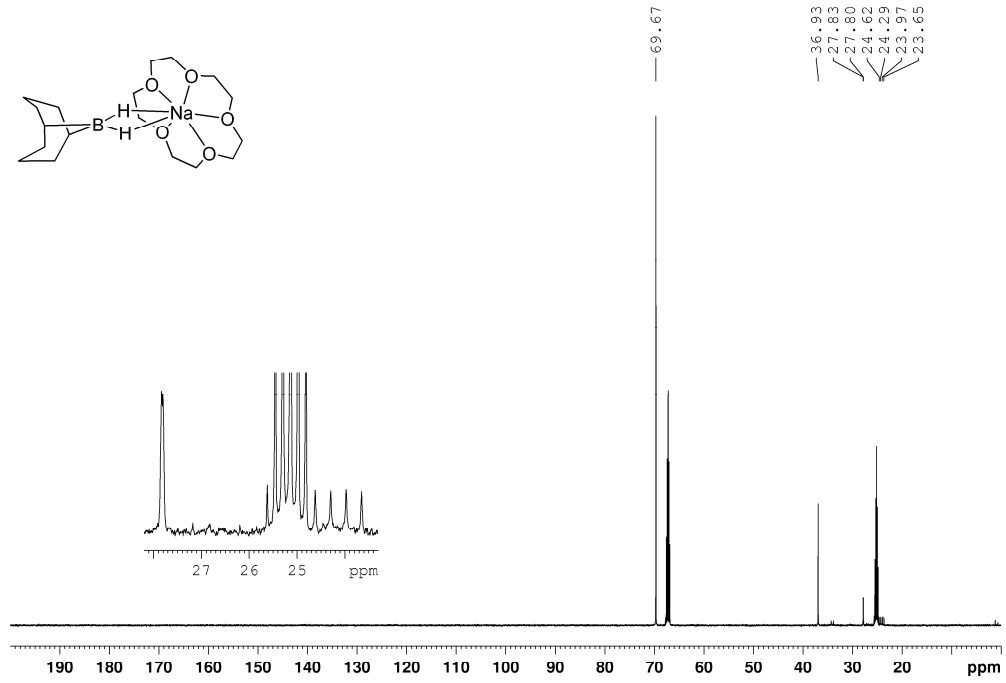
1.769
1.753
1.746
1.737
1.724
1.708
1.702
1.695
1.690
1.648
1.527
1.393
1.383
1.367
1.363
0.8
0.6
ppm
11
10
9
8
7
6
5
4
3
2
1
ppm
20.16
6.05
4.00
2.04
3.96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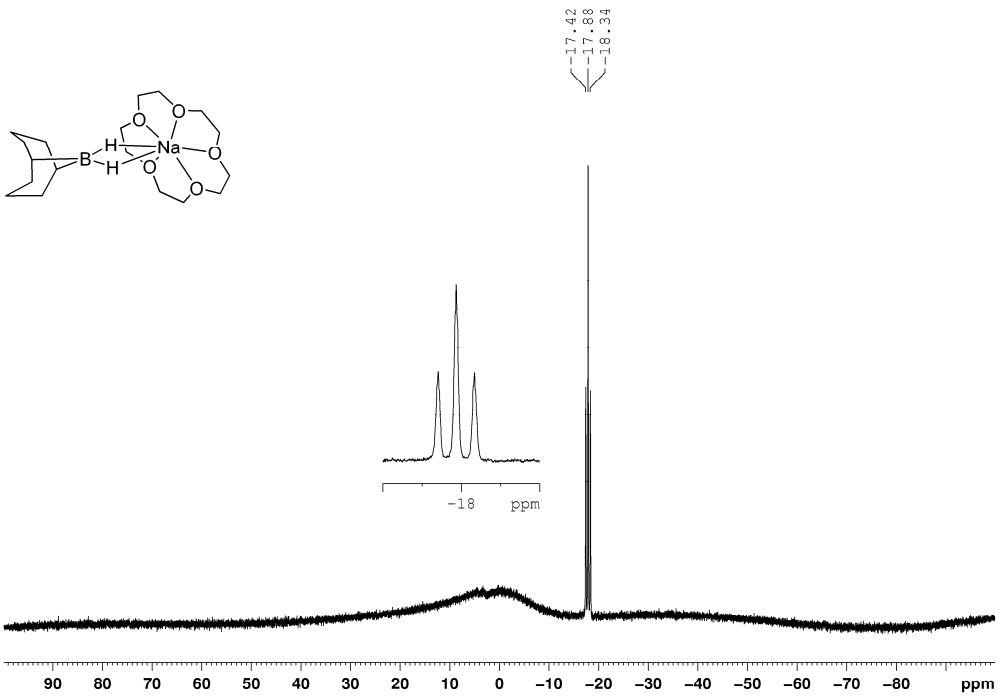
36.93
27.83
27.80
24.62
24.29
23.97
23.65
27
26
25
ppm
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm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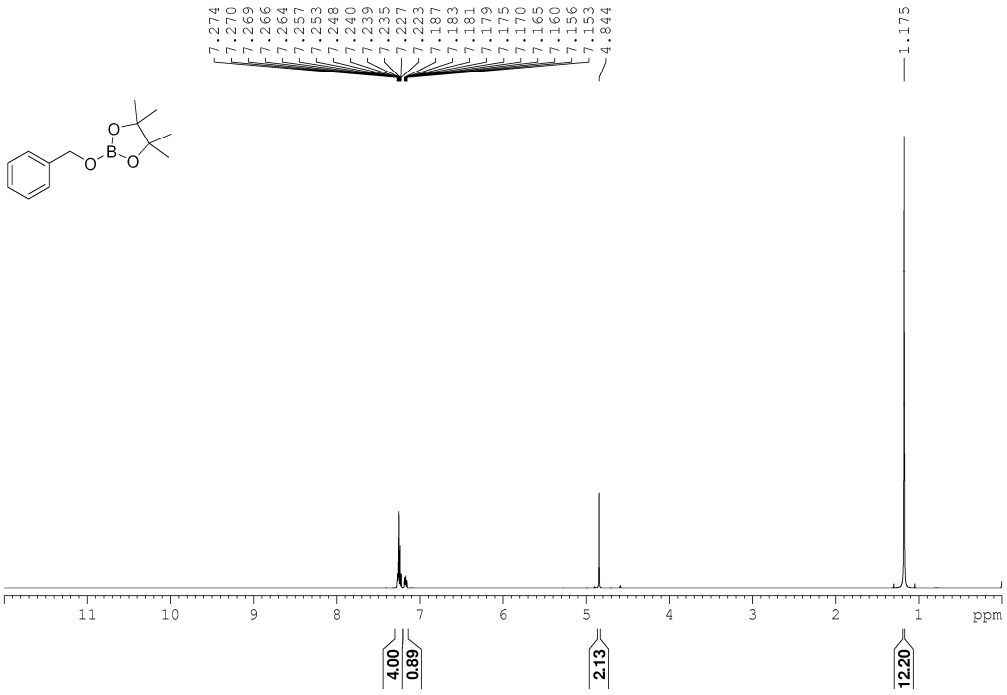
-17.88
-18.34
O
O
H
Na
O
B
H
O
O
-18
ppm
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
ppm

2a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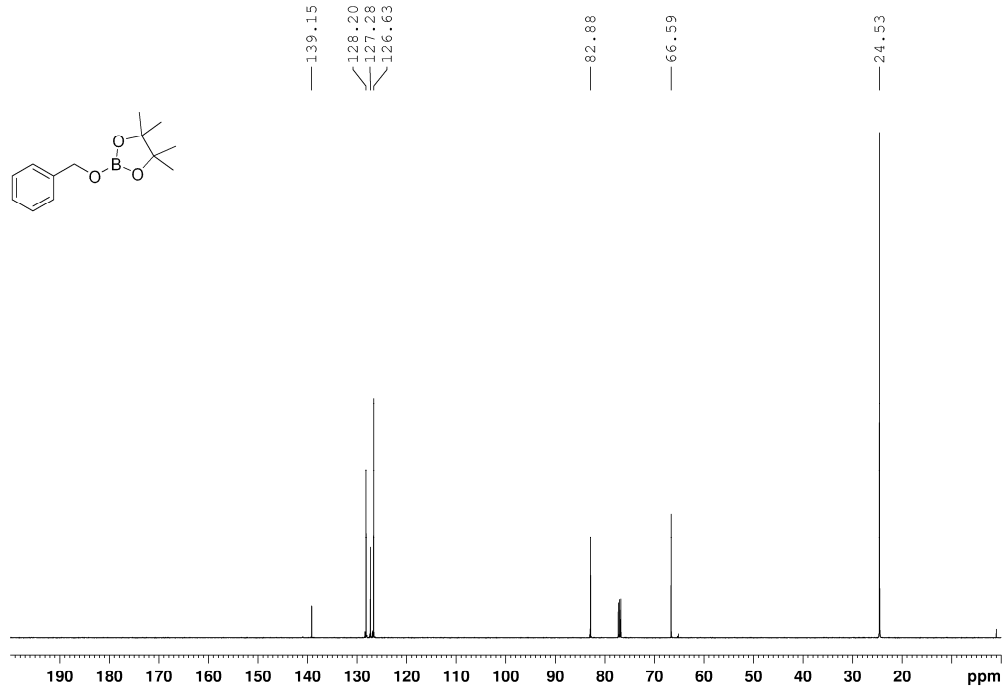
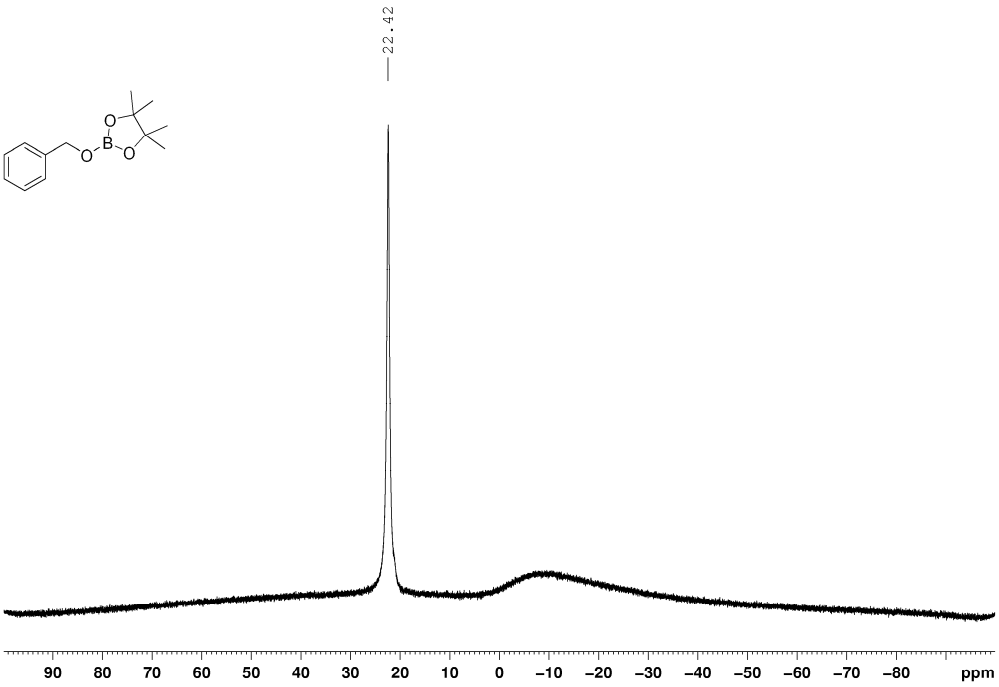
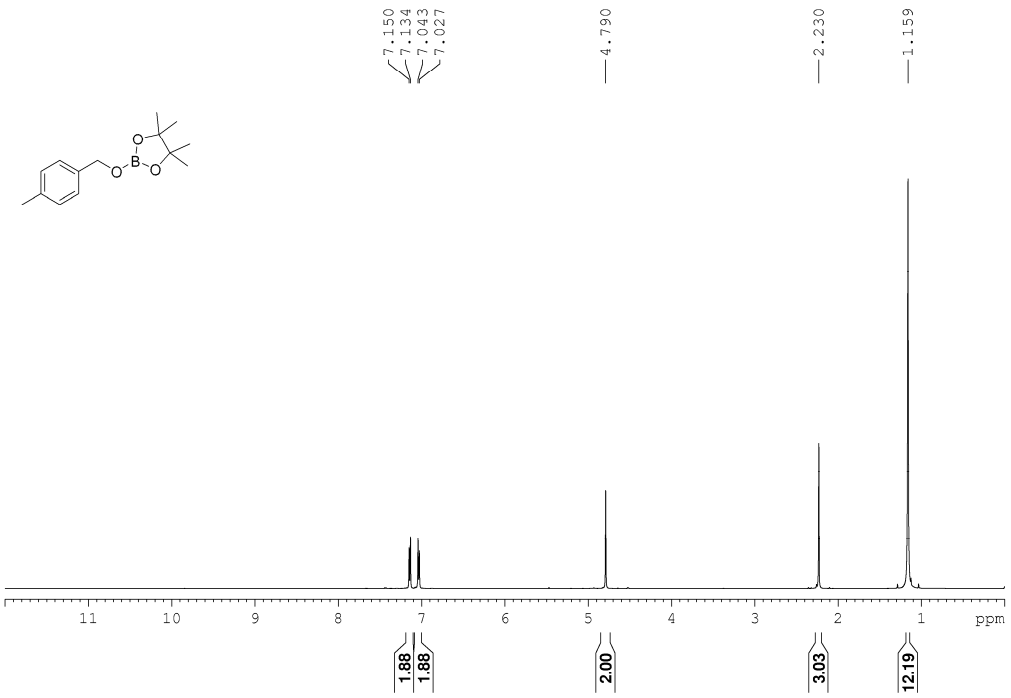
7.270
7.269
7.266
7.264
7.257
7.253
7.248
7.240
7.239
7.235
7.227
7.223
7.187
7.183
7.181
7.179
7.175
7.170
7.165
7.160
7.156
7.153
4.844
1.175
11
10
9
8
7
6
5
4
3
2
1
ppm
4.00
0.89
2.13
12.20


139.15
128.20
127.28
126.63
82.88
66.59
24.53
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


22.42
O
B
O
O
90
80
70
60
50
40
30
20
10
0
−10
−20
−30
−40
−50
−60
−70
−80
ppm

2b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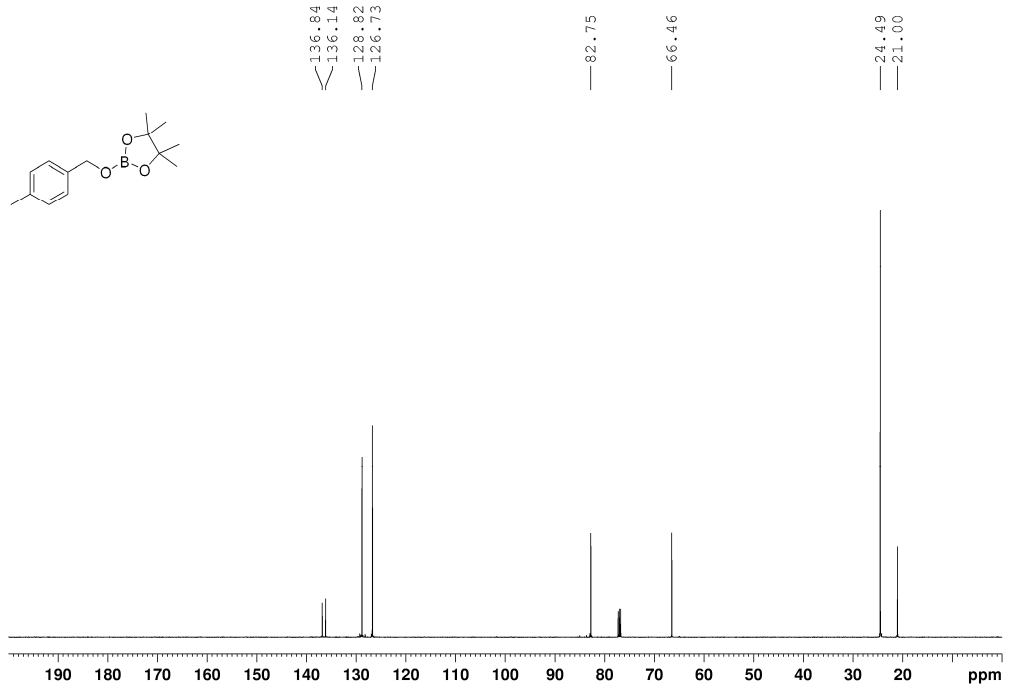
7.134
7.043
7.027
4.790
2.230
1.159
11
10
9
8
7
6
5
4
3
2
1
ppm
1.88
1.88
2.00
3.03
12.19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136.14
128.82
126.73
82.75
66.46
24.49
21.00
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160
150
140
130
120
110
100
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80
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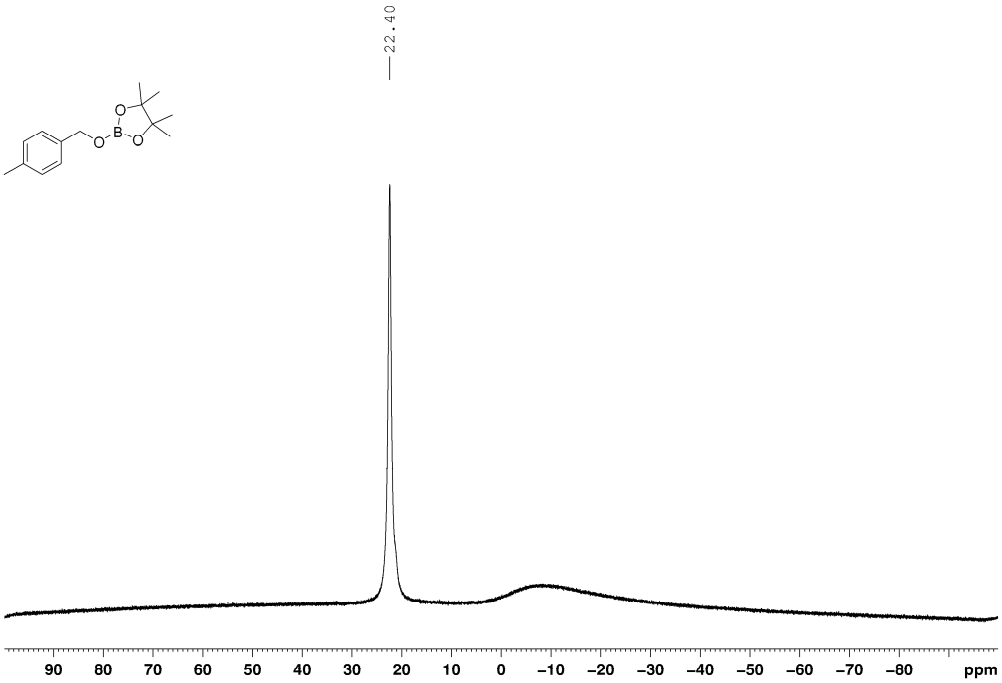
60
50
40
30
20
ppm


22.40
O
B
O
O
90
80
70
60
50
40
30
20
10
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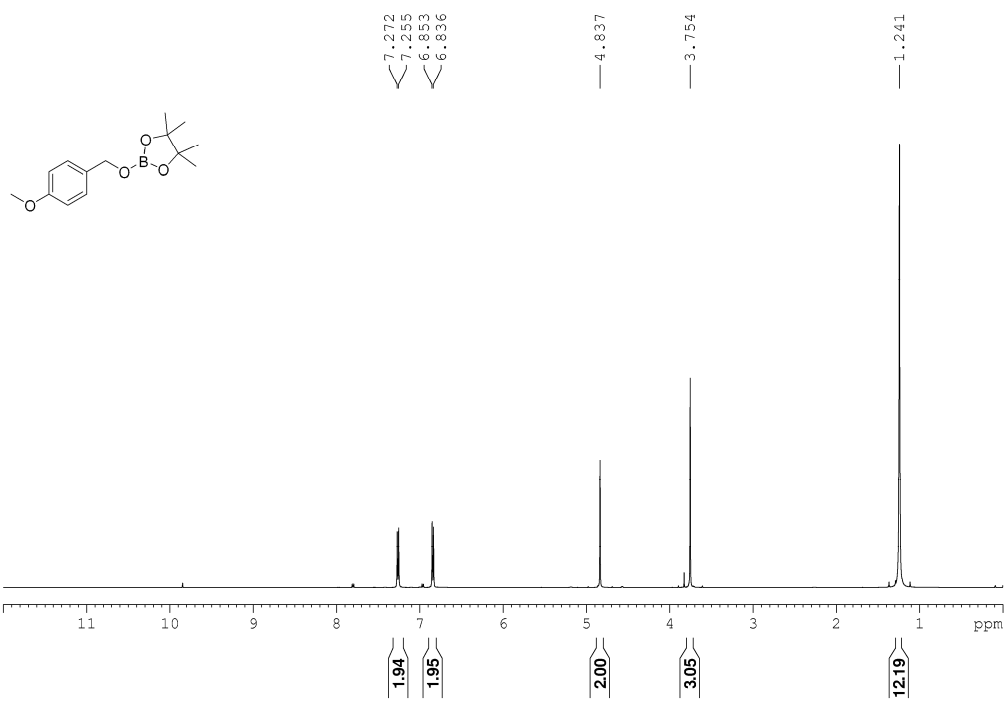
−10
−20
−30
−40
−50
−60
−70
−80
ppm

2c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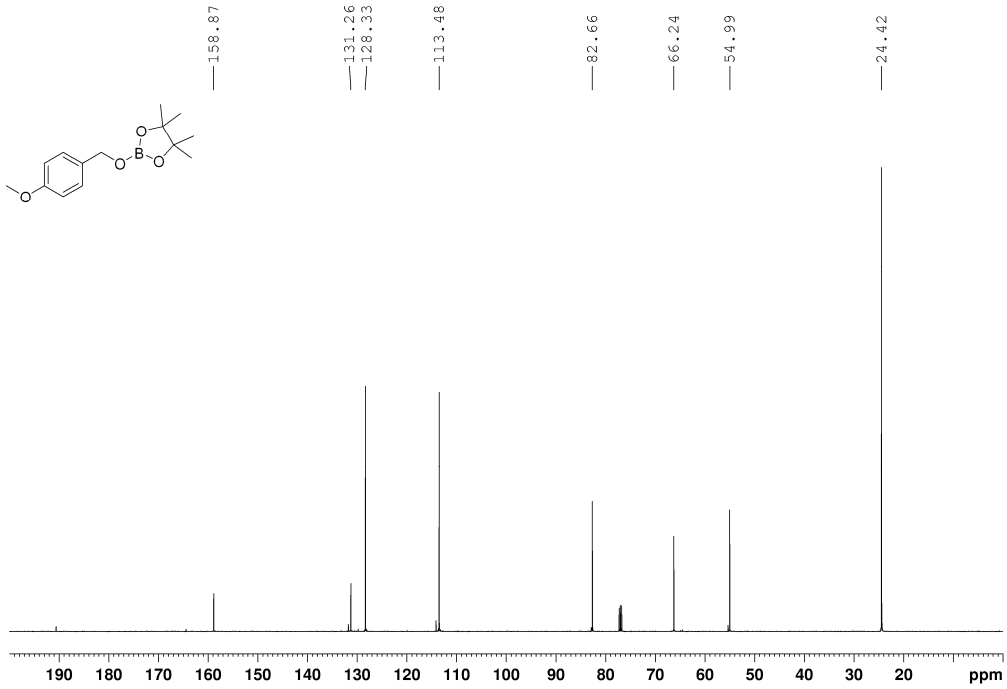
6.853
6.836
4.837
3.754
1.241
11
10
9
8
7
6
5
4
3
2
1
ppm
1.94
1.95
2.00
3.05
12.19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131.26
128.33
113.48
82.66
66.24
54.99
24.42
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160
150
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130
120
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90
80
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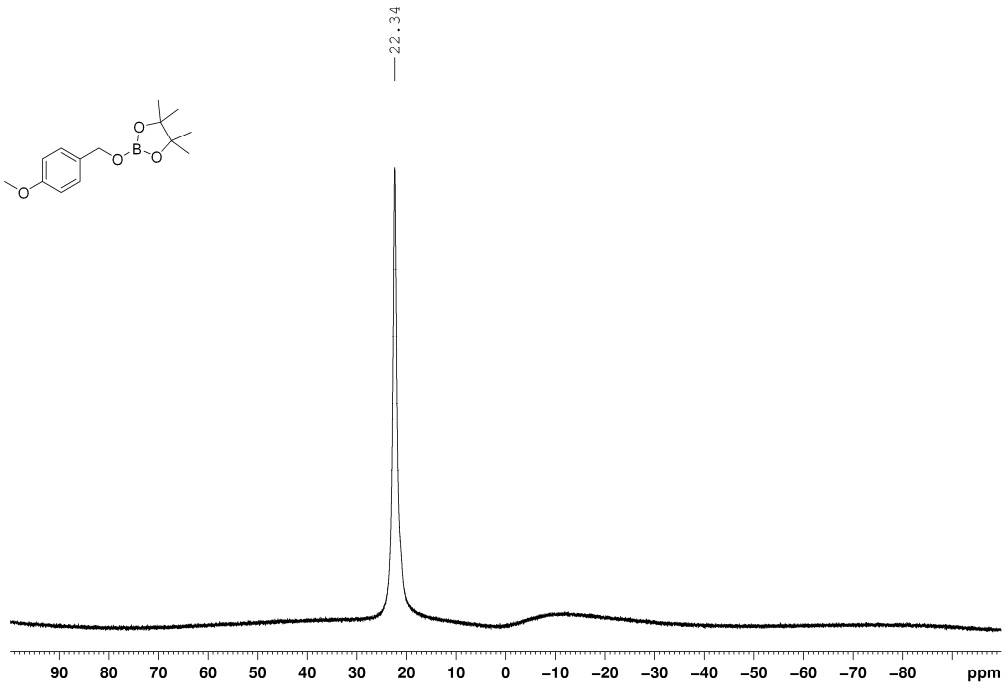
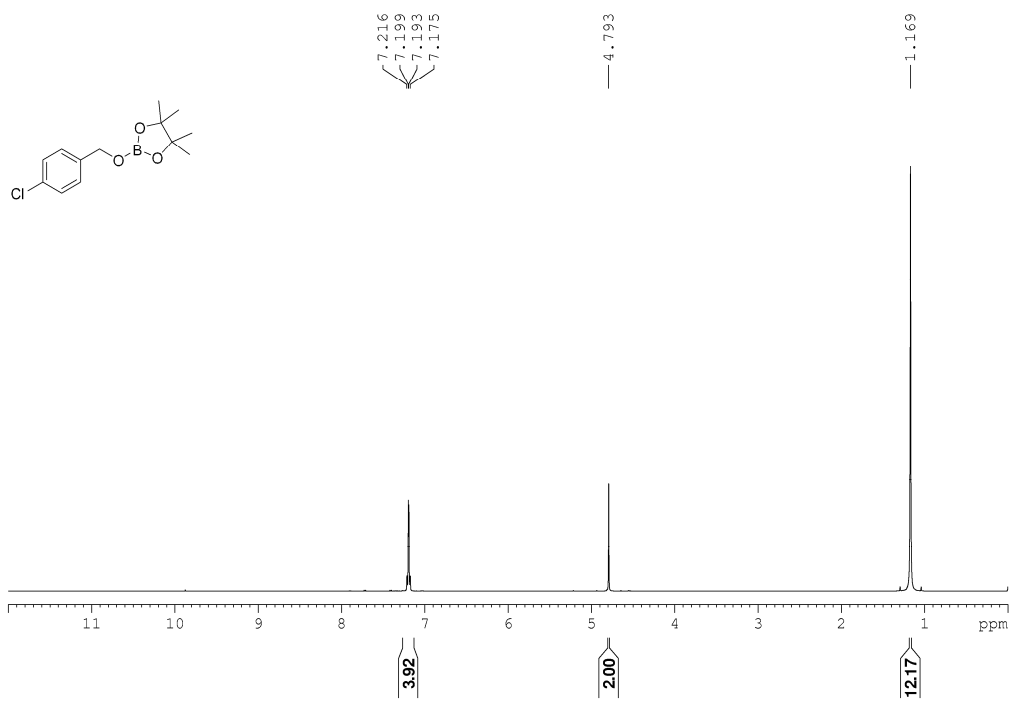
40
30
20
ppm


22.34
O
O
B
O
O
90
80
70
60
50
40
30
20
10
0
−10
−20
−30
−40
−50
−60
−70
−80
ppm

2d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7.193
7.175
4.793
1.169
Cl
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B
O
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10
9
8
7
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4
3
2
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ppm
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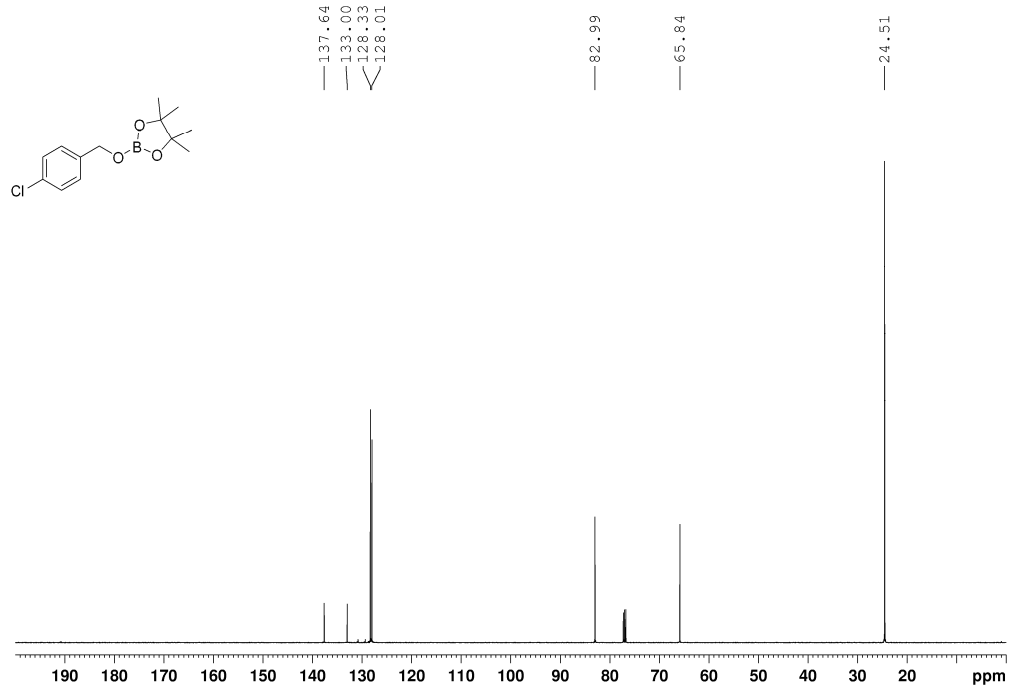
2.00
12.17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128.01
82.99
65.84
24.51
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B
O
O
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180
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160
150
140
130
120
110
100
90
80
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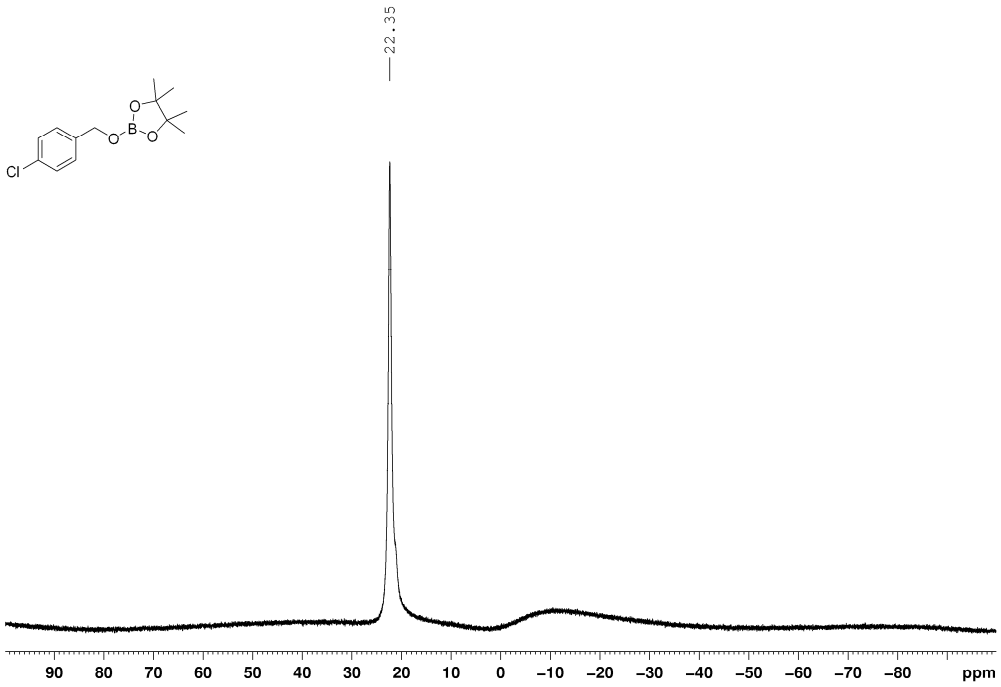
60
50
40
30
20
ppm


22.35
Cl
O
B
O
O
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80
70
60
50
40
30
20
10
0
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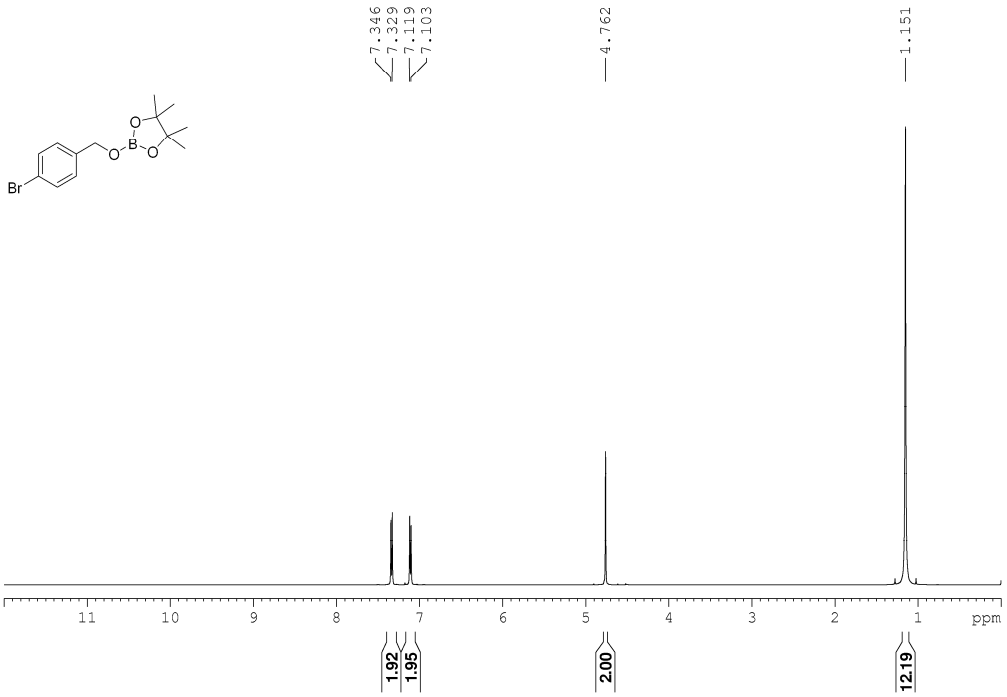
−20
−30
−40
−50
−60
−70
−80
ppm

2e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Br
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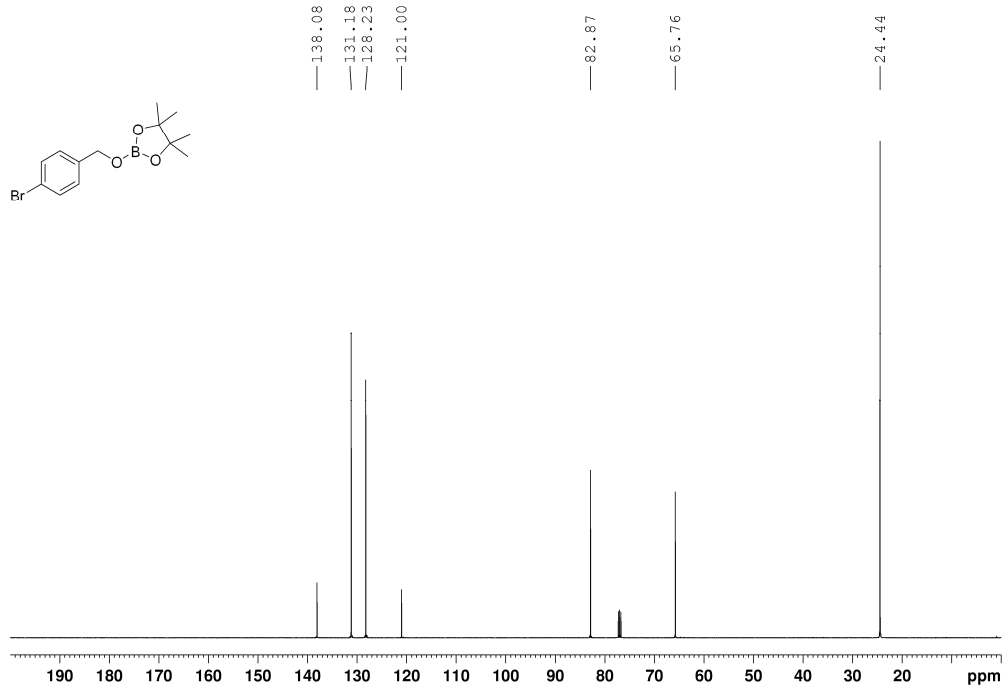
B
O
O
11
10
9
8
7
6
5
4
3
2
1
ppm
1.92
1.95
2.00
12.19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Br
O
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O
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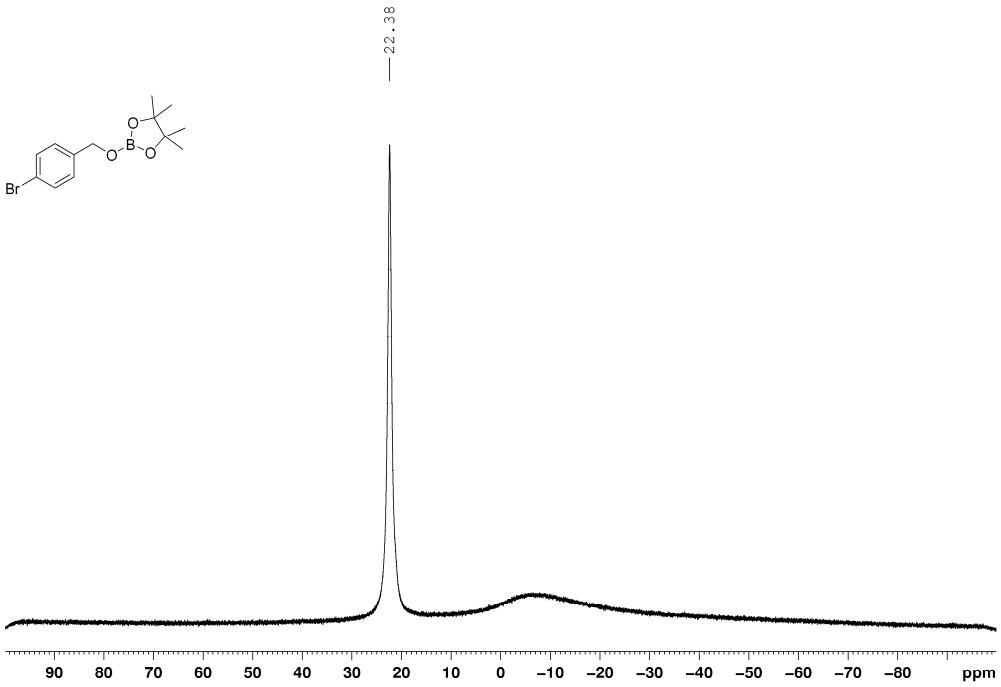
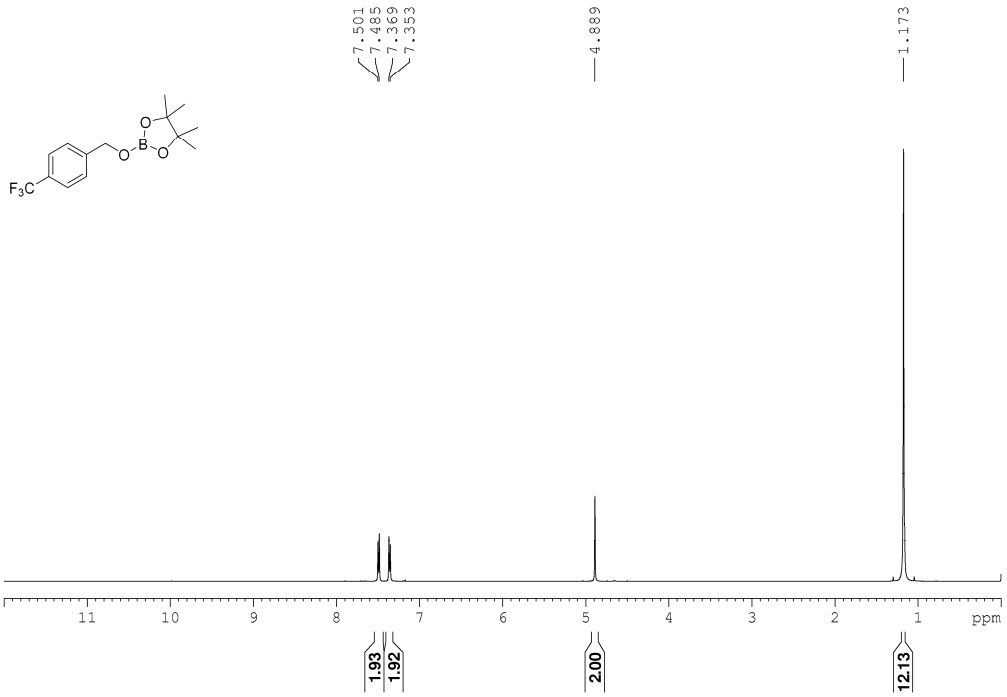
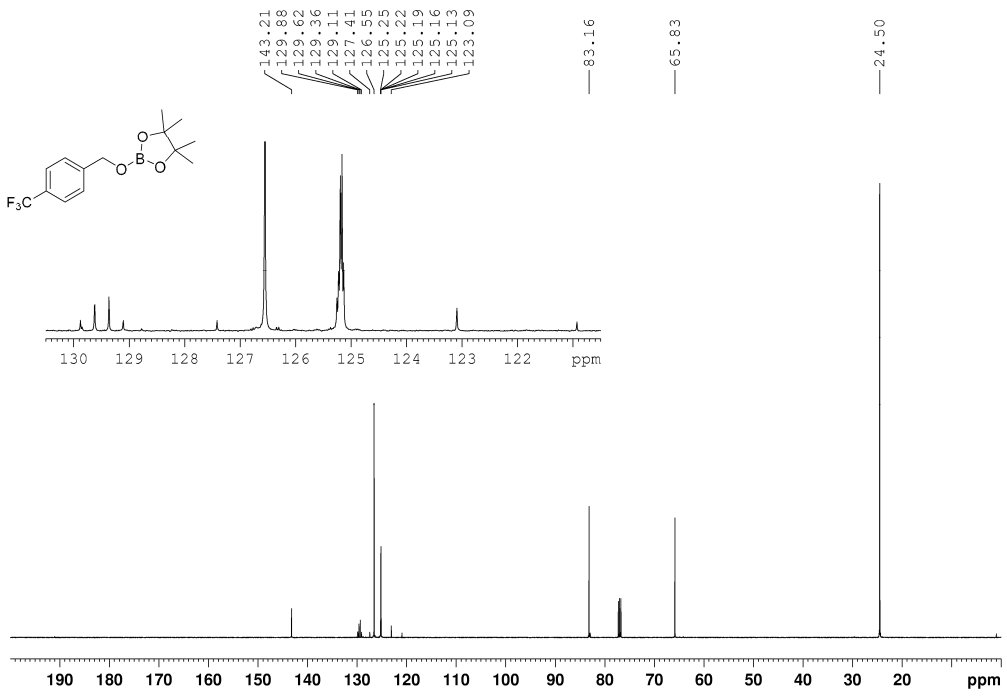
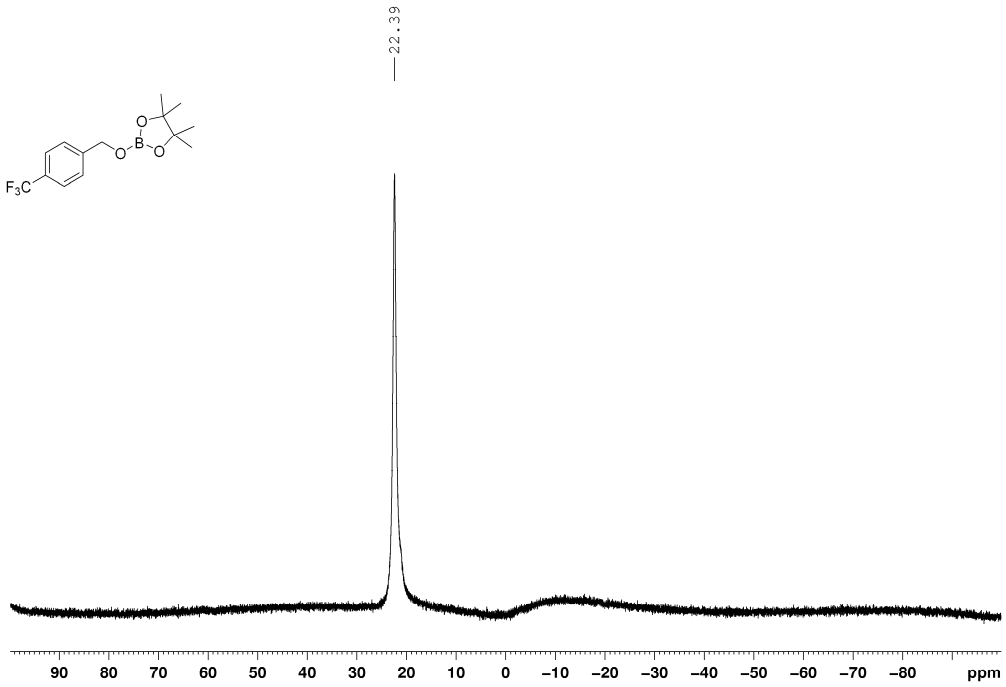
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


22.38
Br
O
B
O
O
90
80
70
60
50
40
30
20
10
0
−10
−20
−30
−40
−50
−60
−70
−80
ppm

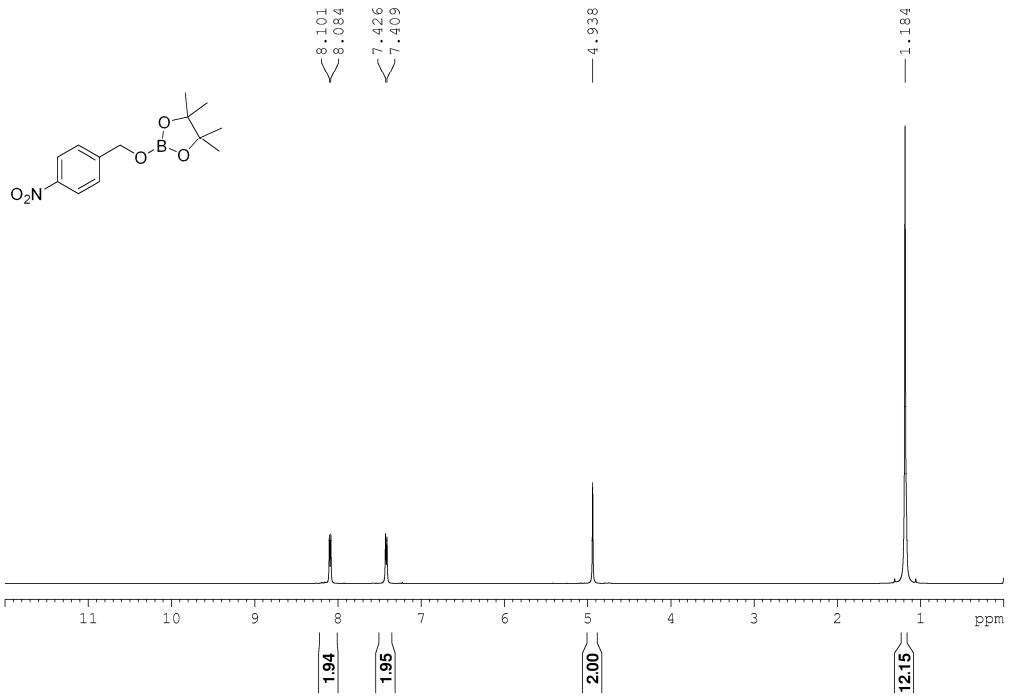
2f

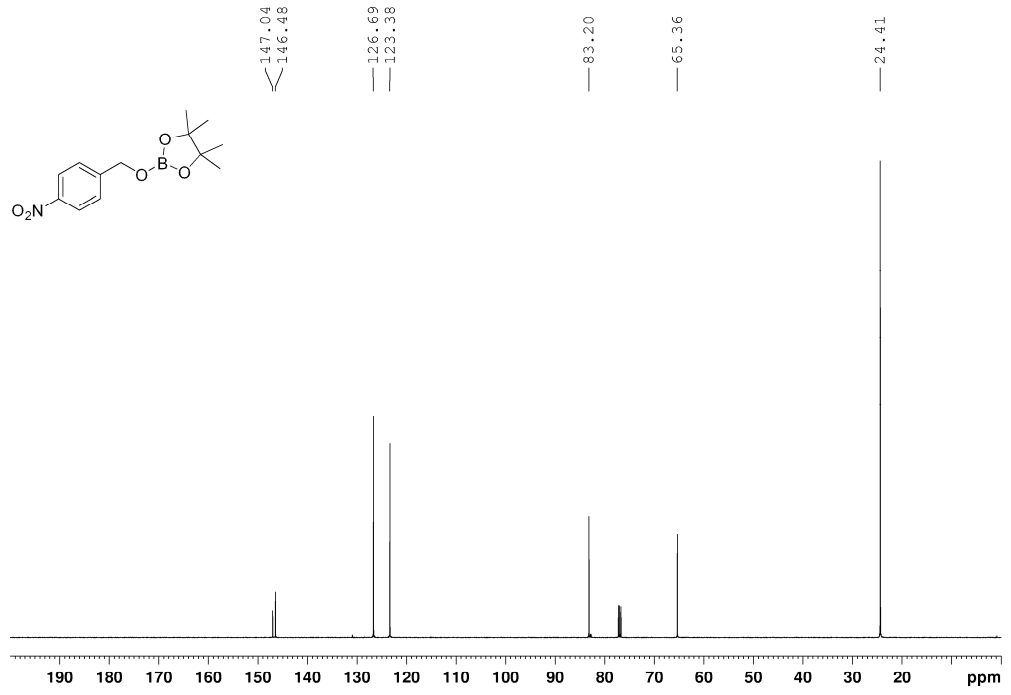

7.501
7.485
7.369
7.353
4.889
1.173
F3C
11 10 9 8 7 6 5 4 3 2 1 ppm
1.93
1.92
2.00
12.13

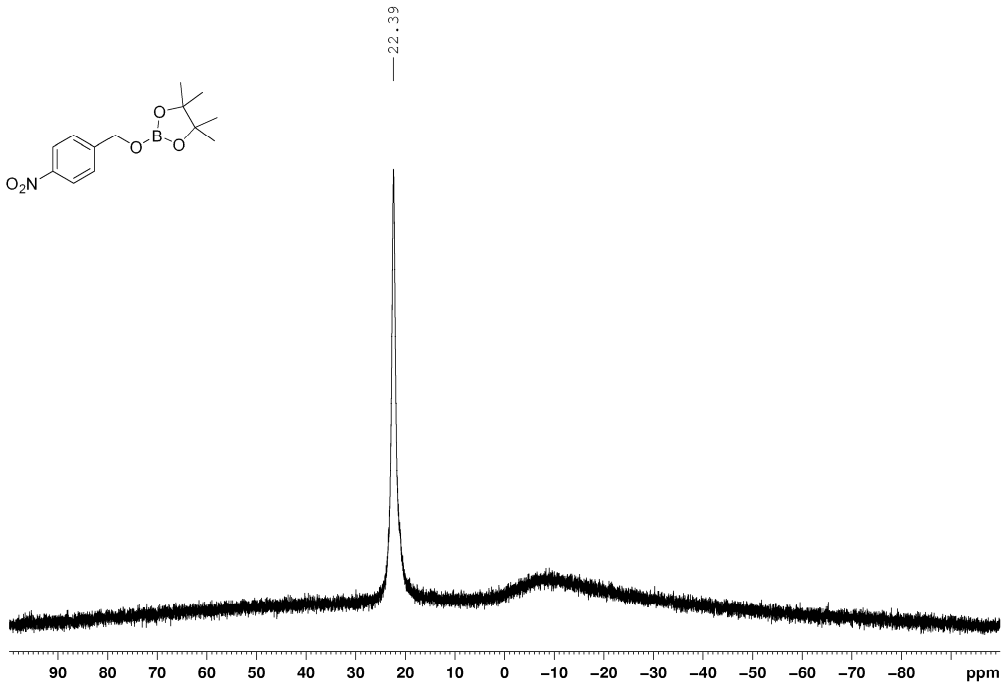

143.21
129.88
129.62
129.36
129.11
127.41
126.55
125.25
125.22
125.19
125.16
125.13
123.09
83.16
65.83
24.50
F3C
130 129 128 127 126 125 124 123 122 ppm
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


22.39
F3C
O
B
O
O
90
80
70
60
50
40
30
20
10
0
−10
−20
−30
−40
−50
−60
−70
−80
ppm

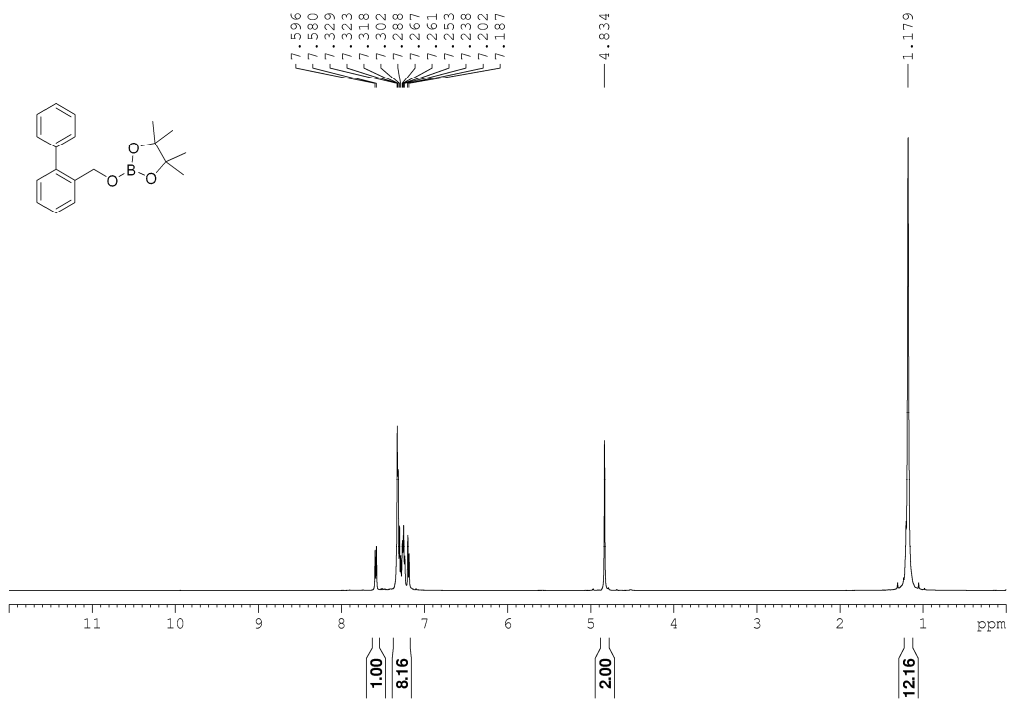
2g

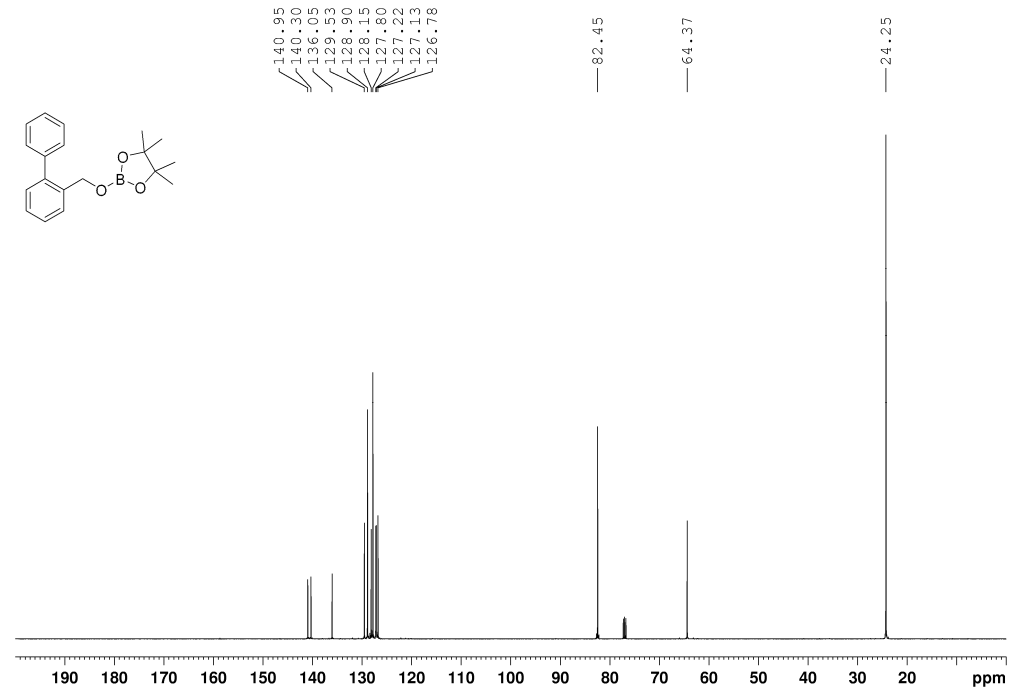

8.101
8.084
7.426
7.409
4.938
1.184
O
B
O
O
O2N
11
10
9
8
7
6
5
4
3
2
1
ppm
1.94
1.95
2.00
12.15

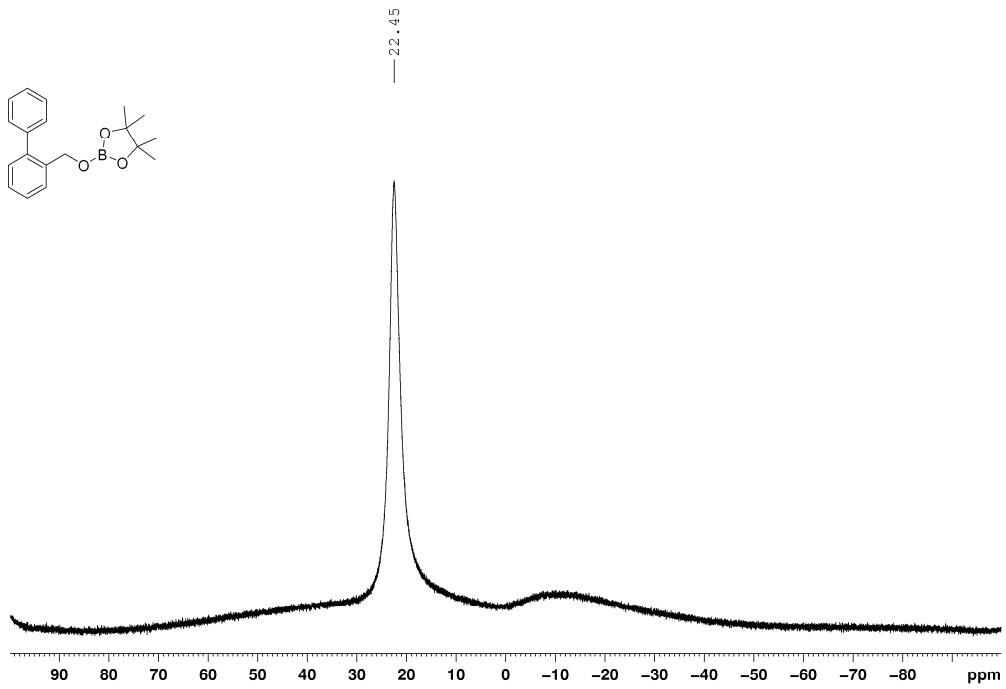

147.04
146.48
126.69
123.38
83.20
65.36
24.41
O
B
O
O
O2N
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


22.39
O
B
O
O
O2N
90
80
70
60
50
40
30
20
10
0
−10
−20
−30
−40
−50
−60
−70
−80
ppm

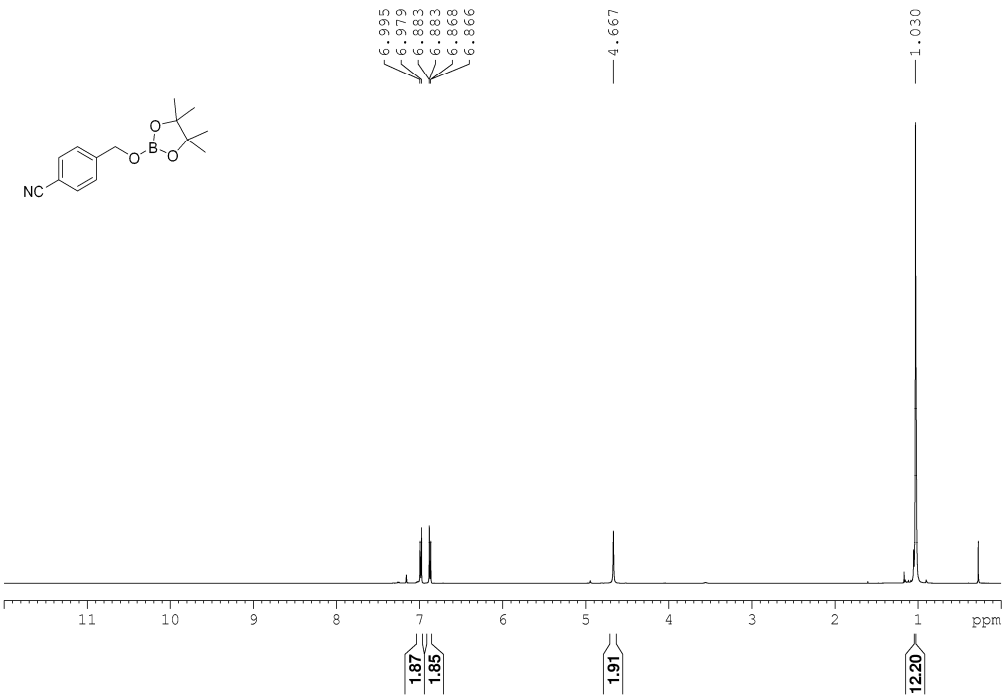
2h

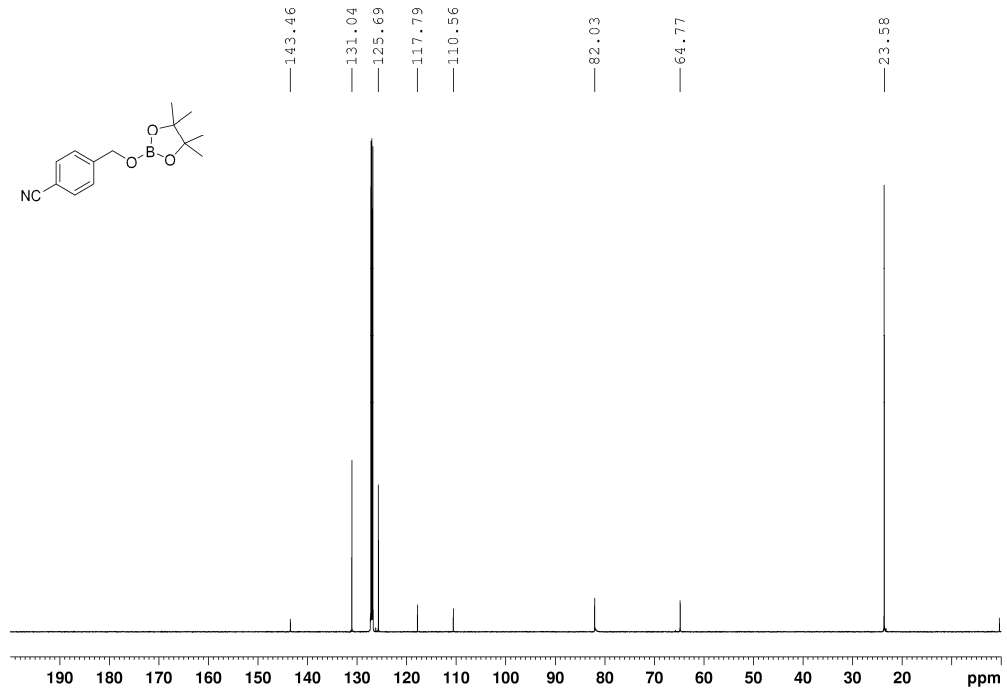

7.596
7.580
7.329
7.323
7.318
7.302
7.288
7.267
7.261
7.253
7.238
7.202
7.187
4.834
1.179
11
10
9
8
7
6
5
4
3
2
1
ppm
1.00
8.16
2.00
12.16

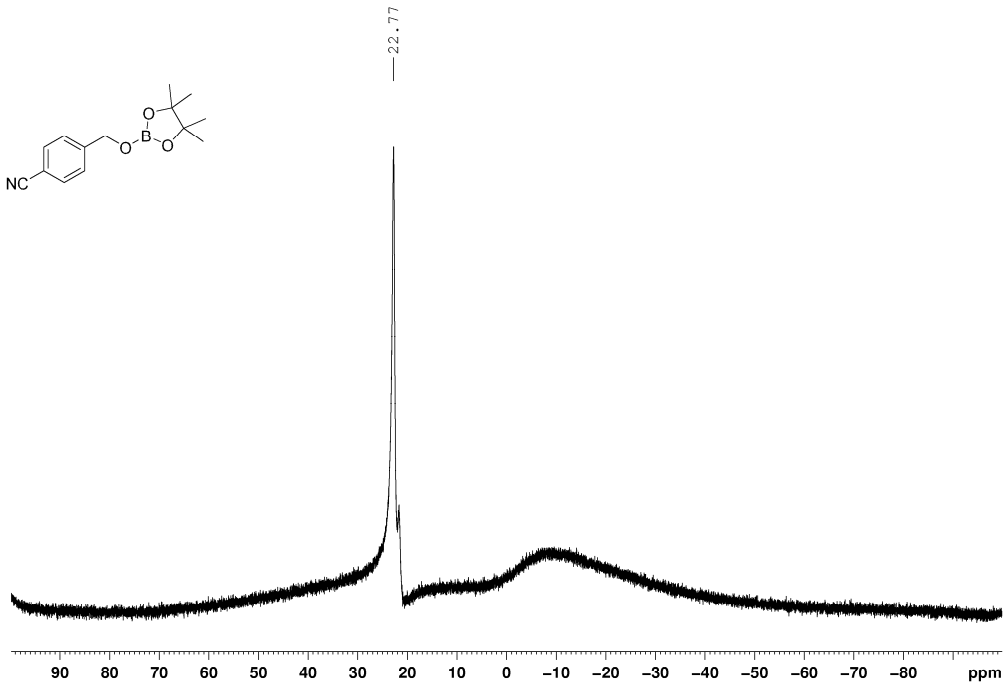

140.95
140.30
136.05
129.53
128.90
128.15
127.80
127.22
127.13
126.78
82.45
64.37
24.25
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


22.45
90
80
70
60
50
40
30
20
10
0
−10
−20
−30
−40
−50
−60
−70
−80
ppm

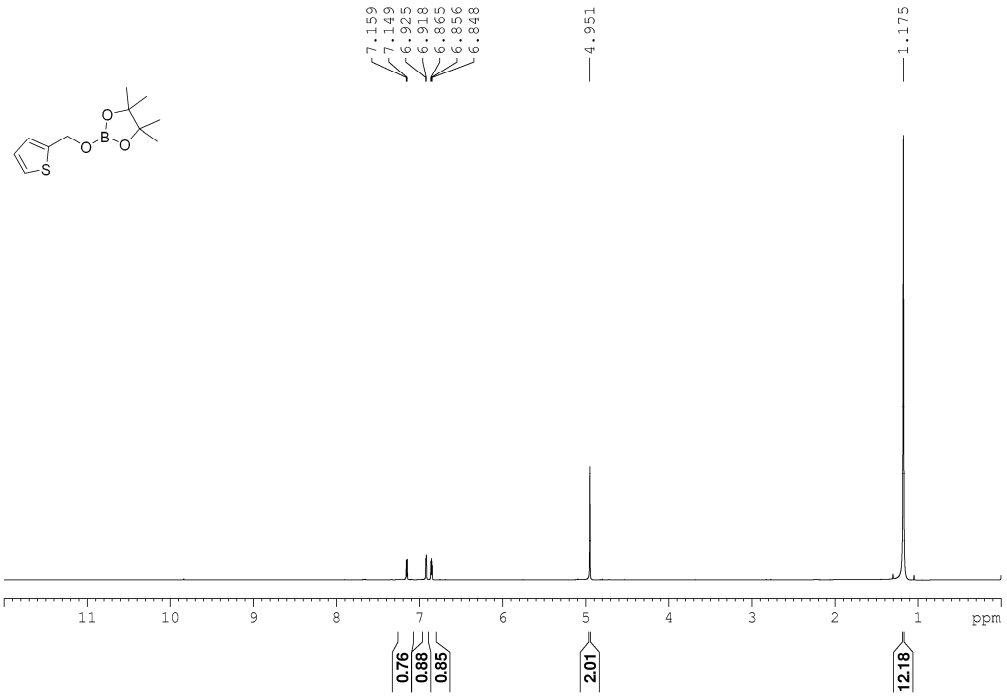
2i

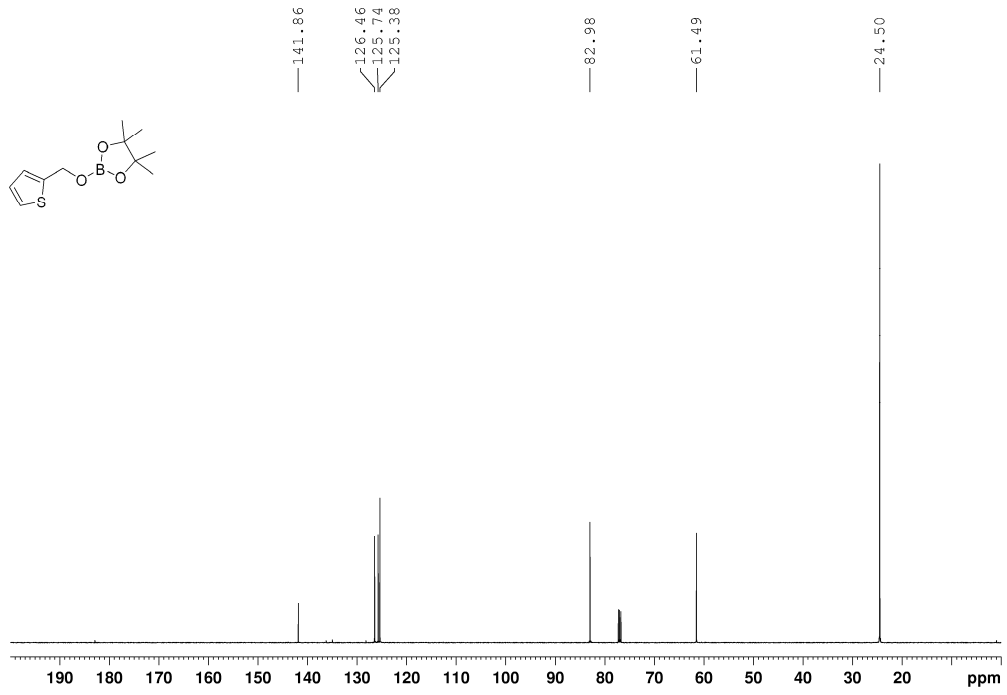

6.995
6.979
6.883
6.868
6.866
4.667
1.030
NC
11
10
9
8
7
6
5
4
3
2
1
ppm
1.87
1.85
1.91
12.20

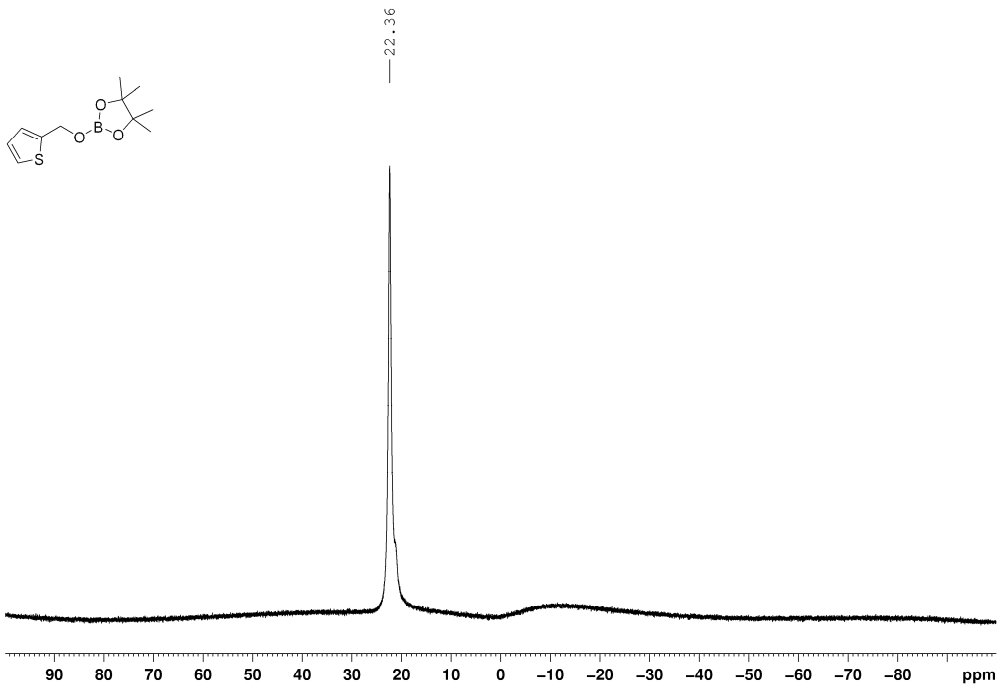

143.46
131.04
125.69
117.79
110.56
82.03
64.77
23.58
NC
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


22.77
NC
O
B
O
O
90
80
70
60
50
40
30
20
10
0
−10
−20
−30
−40
−50
−60
−70
−80
ppm

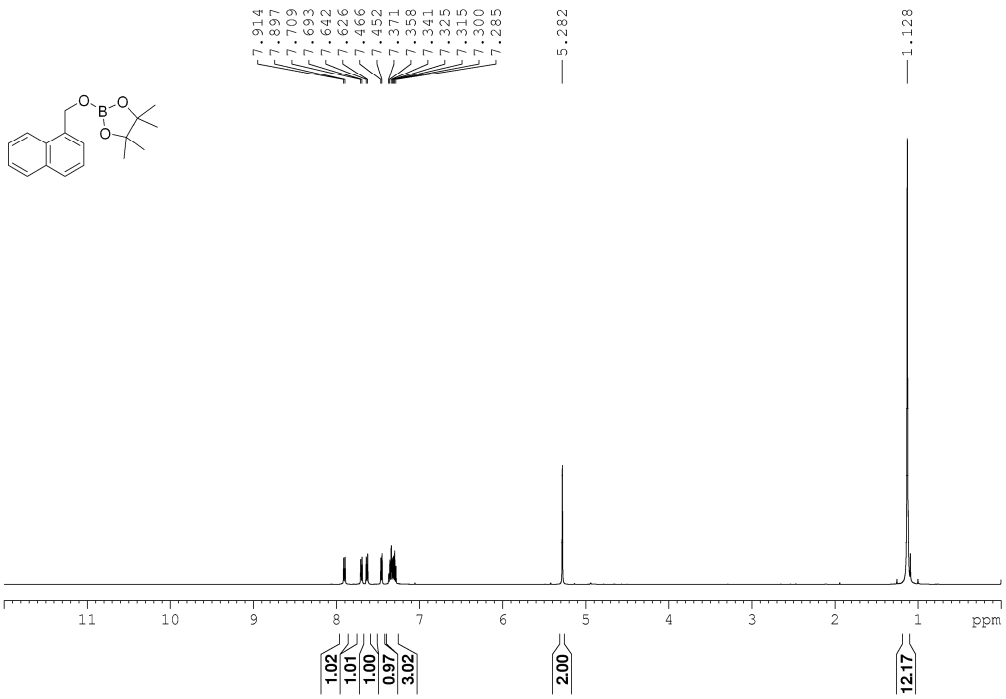
2j

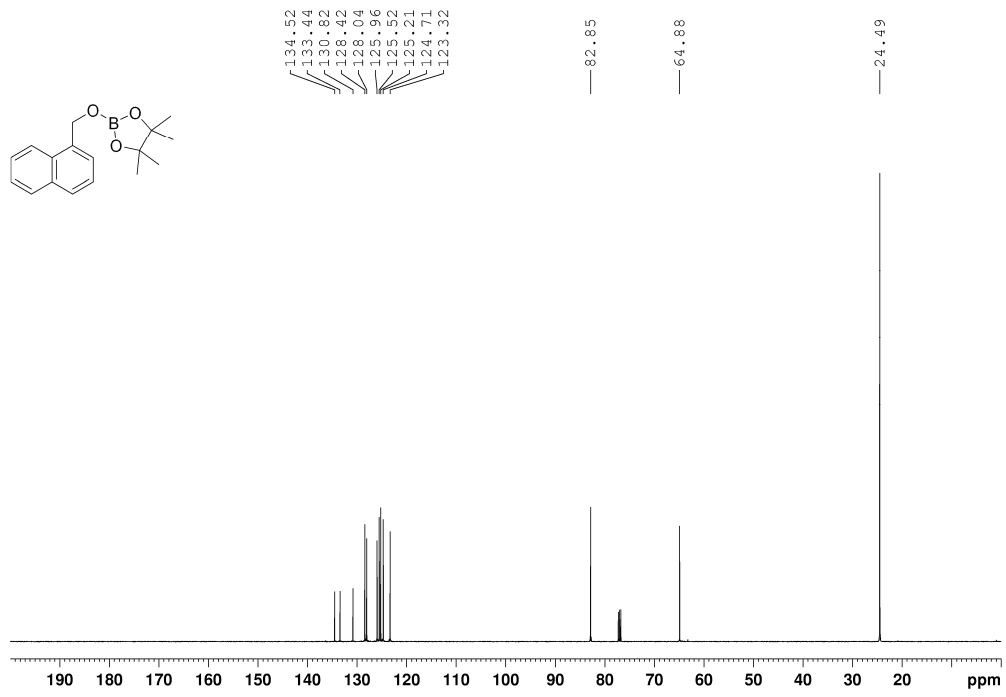

7.159
7.149
6.925
6.918
6.865
6.856
6.848
4.951
1.175
11
10
9
8
7
6
5
4
3
2
1
ppm
0.76
0.88
0.85
2.01
12.18

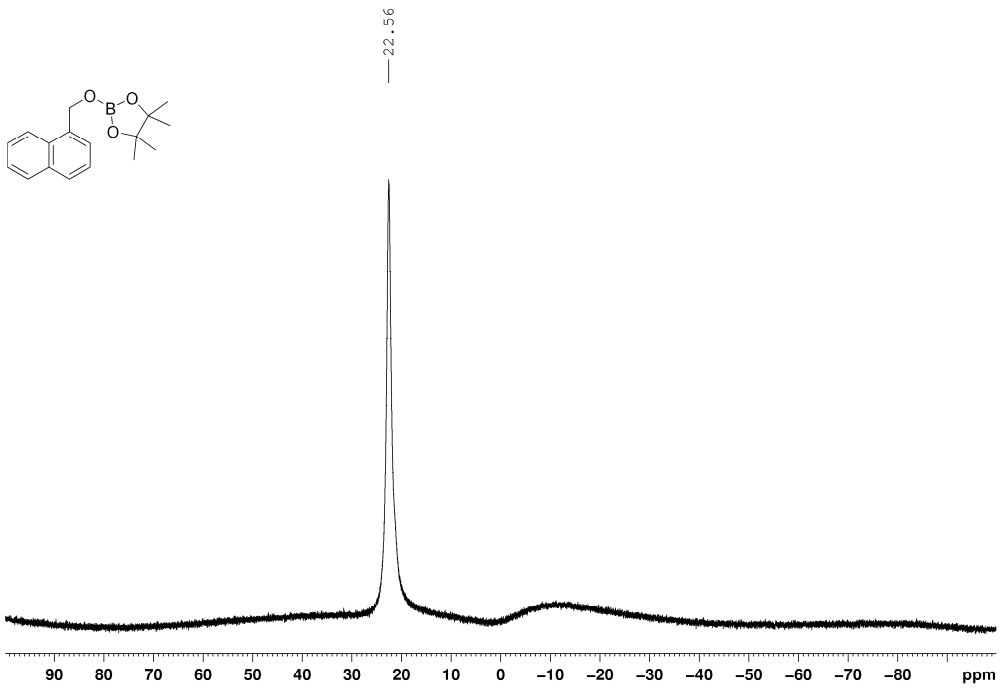

141.86
126.46
125.74
125.38
82.98
61.49
24.50
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


22.36
O
B
O
O
S
90
80
70
60
50
40
30
20
10
0
−10
−20
−30
−40
−50
−60
−70
−80
ppm

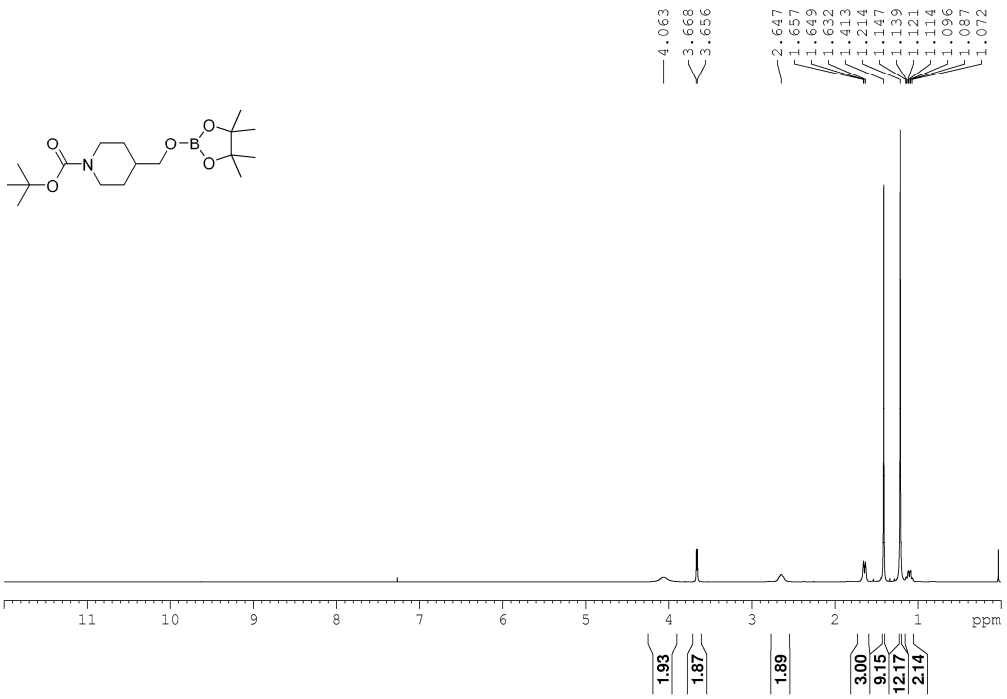
2k

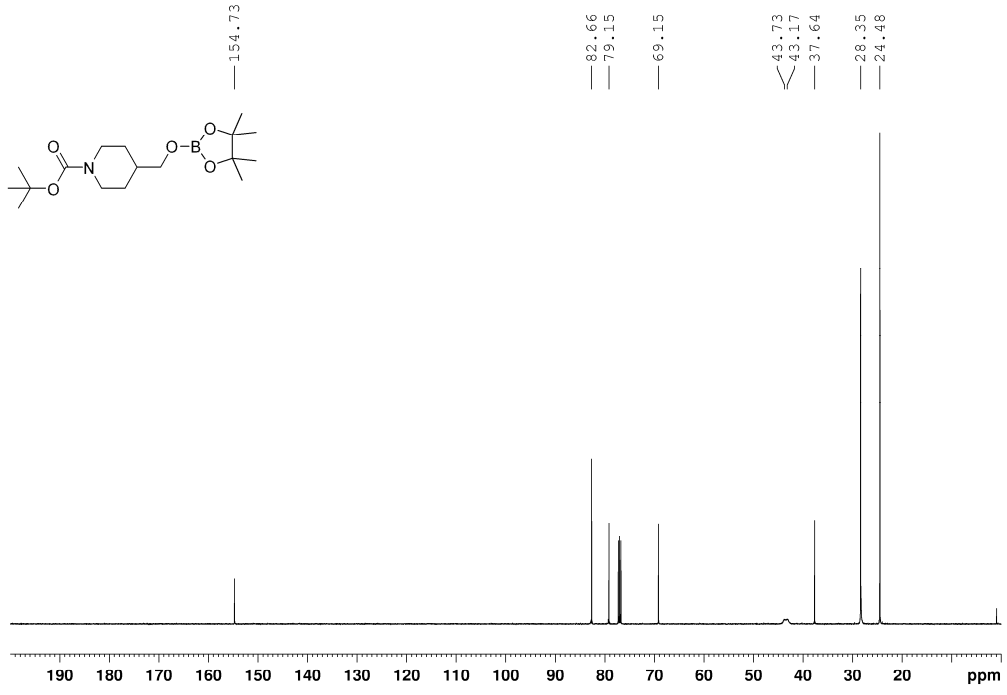

7.914
7.897
7.709
7.693
7.642
7.626
7.466
7.452
7.371
7.358
7.341
7.325
7.315
7.300
7.285
5.282
1.128
11
10
9
8
7
6
5
4
3
2
1
ppm
1.02
1.01
1.00
0.97
3.02
2.00
12.17

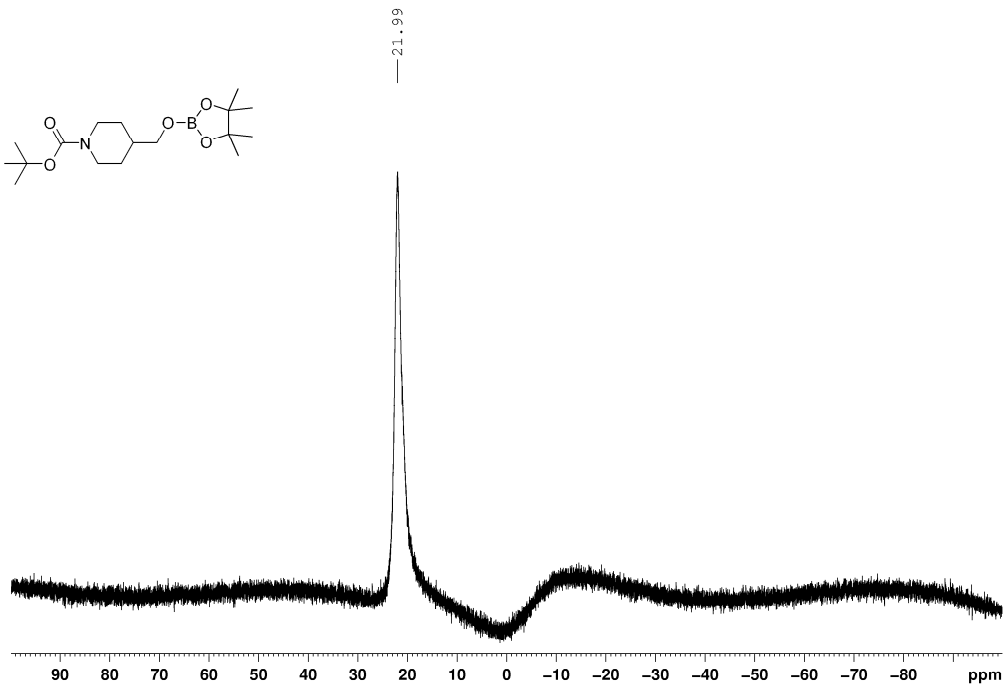

134.52
133.44
130.82
128.42
128.04
125.96
125.52
125.21
124.71
123.32
82.85
64.88
24.49
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


22.56
O
B
O
O
90
80
70
60
50
40
30
20
10
0
−10
−20
−30
−40
−50
−60
−70
−80
ppm

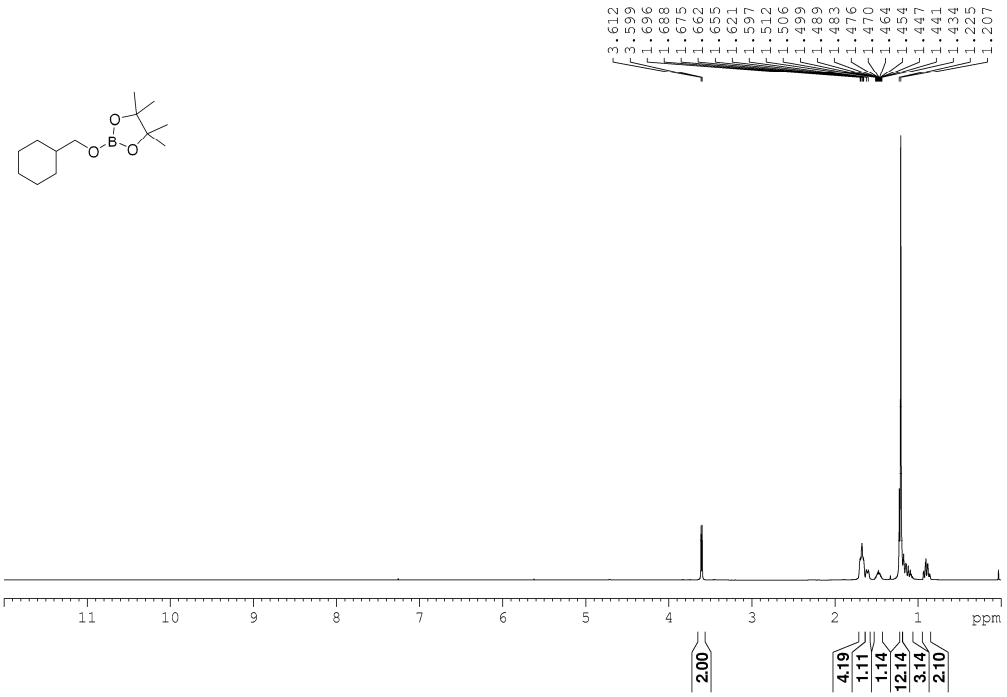
2l

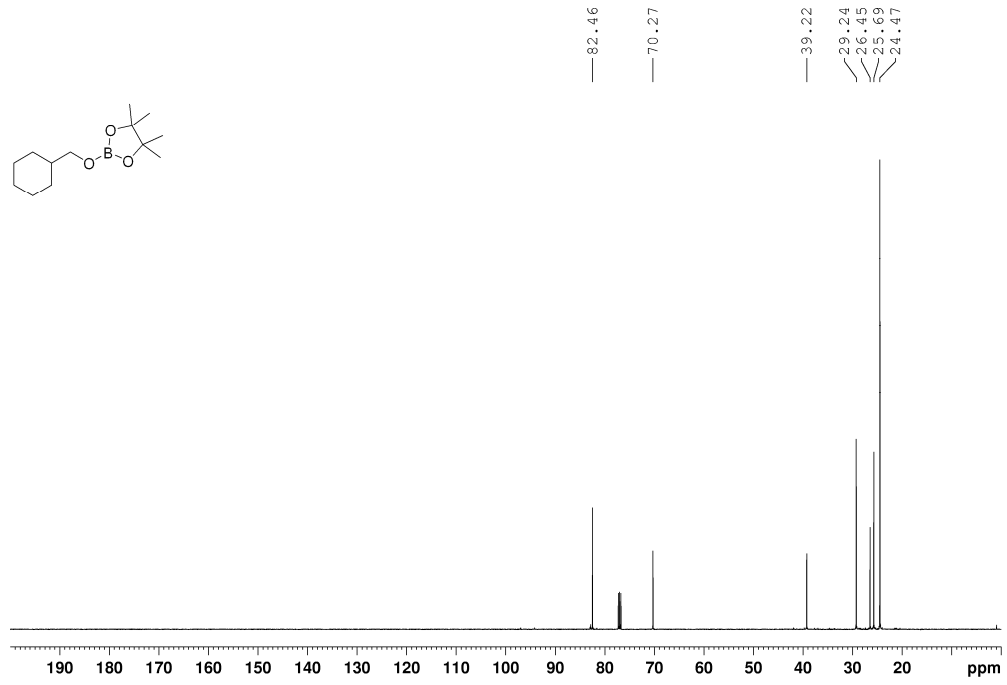

4.063
3.668
3.656
2.647
1.657
1.649
1.632
1.413
1.214
1.147
1.139
1.121
1.114
1.096
1.087
1.072
11
10
9
8
7
6
5
4
3
2
1
ppm
1.93
1.87
1.89
3.00
9.15
12.17
2.14

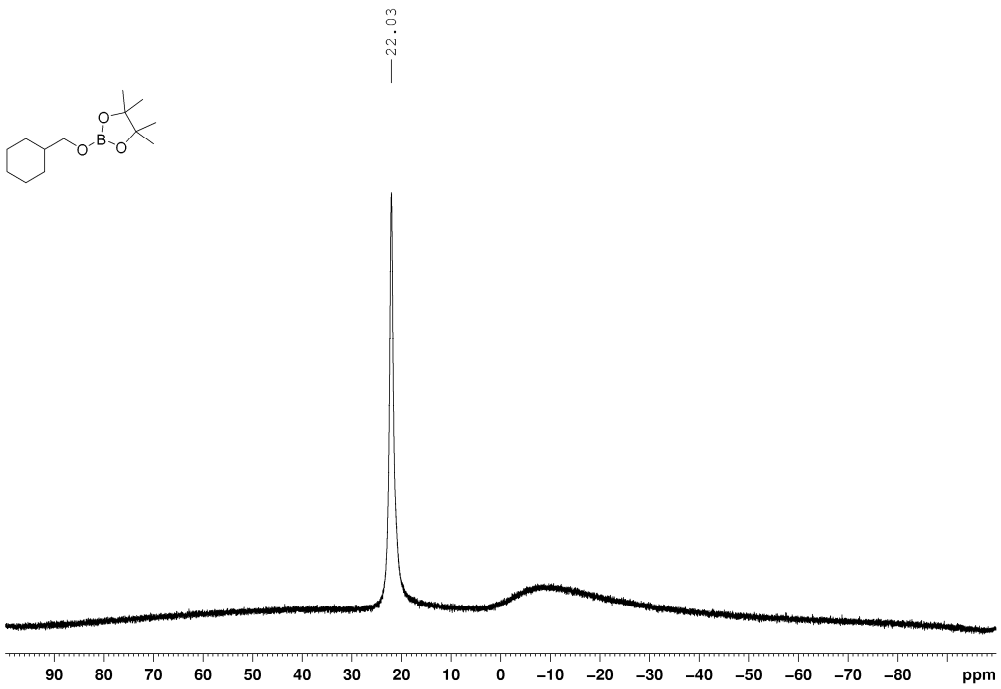

154.73
82.66
79.15
69.15
43.73
43.17
37.64
28.35
24.48
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


21.99
90
80
70
60
50
40
30
20
10
0
−10
−20
−30
−40
−50
−60
−70
−80
ppm

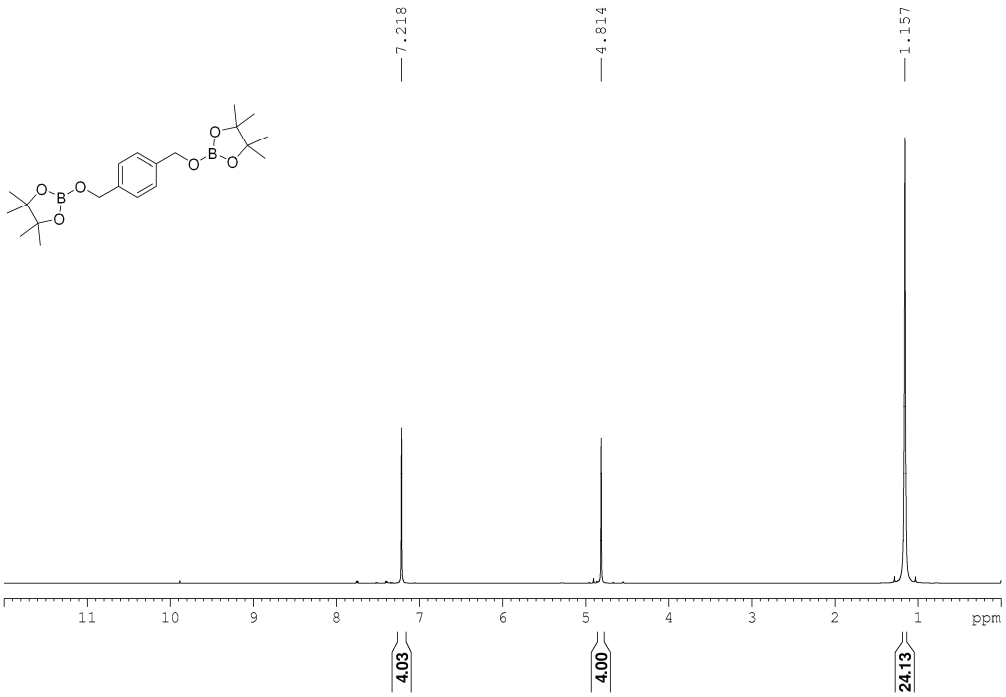
2m

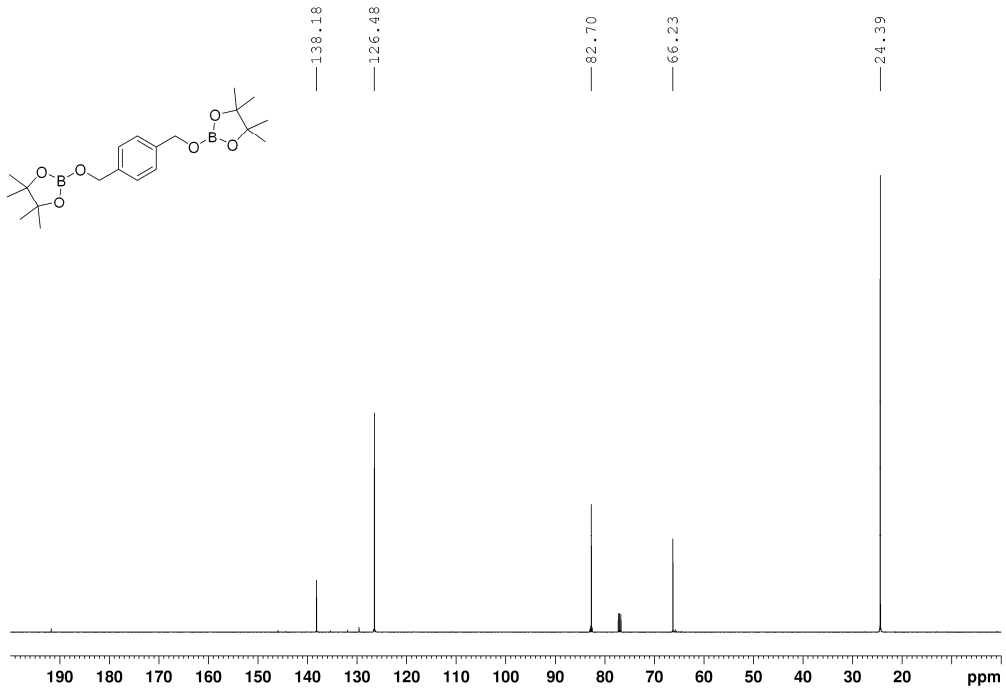

3.612
3.599
1.696
1.688
1.675
1.662
1.655
1.621
1.597
1.512
1.506
1.499
1.489
1.483
1.476
1.470
1.464
1.454
1.447
1.441
1.434
1.225
1.207
11
10
9
8
7
6
5
4
3
2
1
ppm
2.00
4.19
1.11
1.14
12.14
3.14
2.10

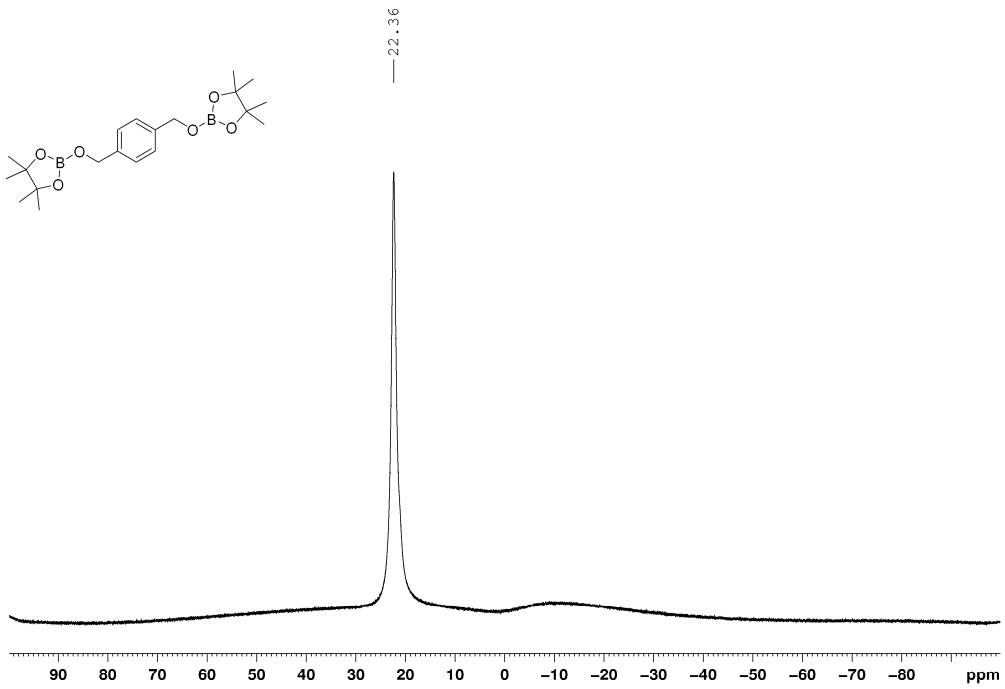

82.46
70.27
39.22
29.24
26.45
25.69
24.47
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


22.03
O
B
O
O
90
80
70
60
50
40
30
20
10
0
−10
−20
−30
−40
−50
−60
−70
−80
ppm

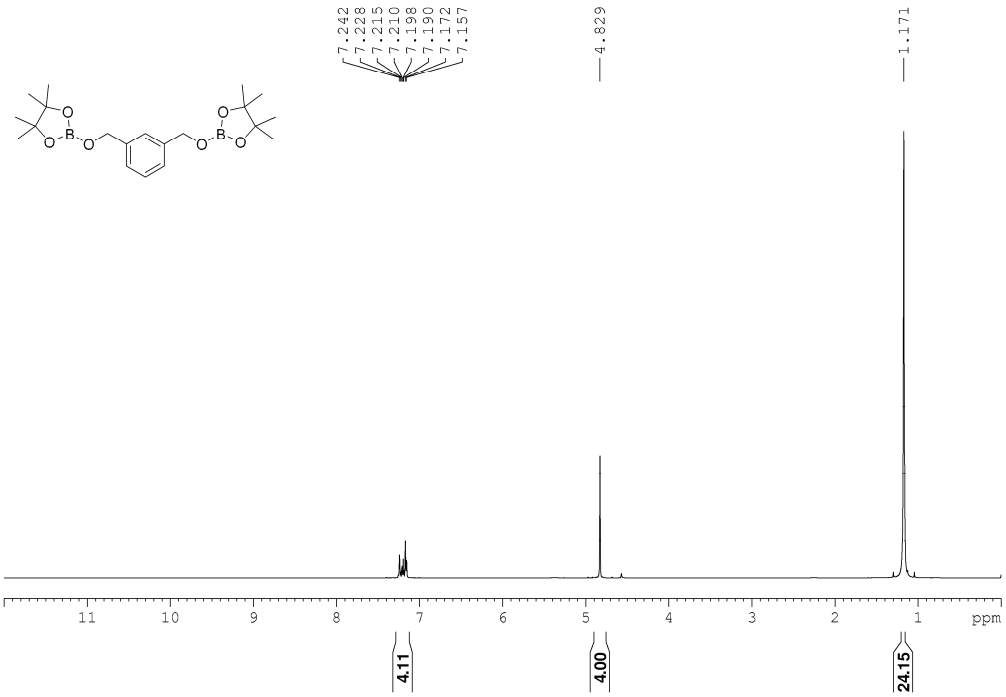
2n

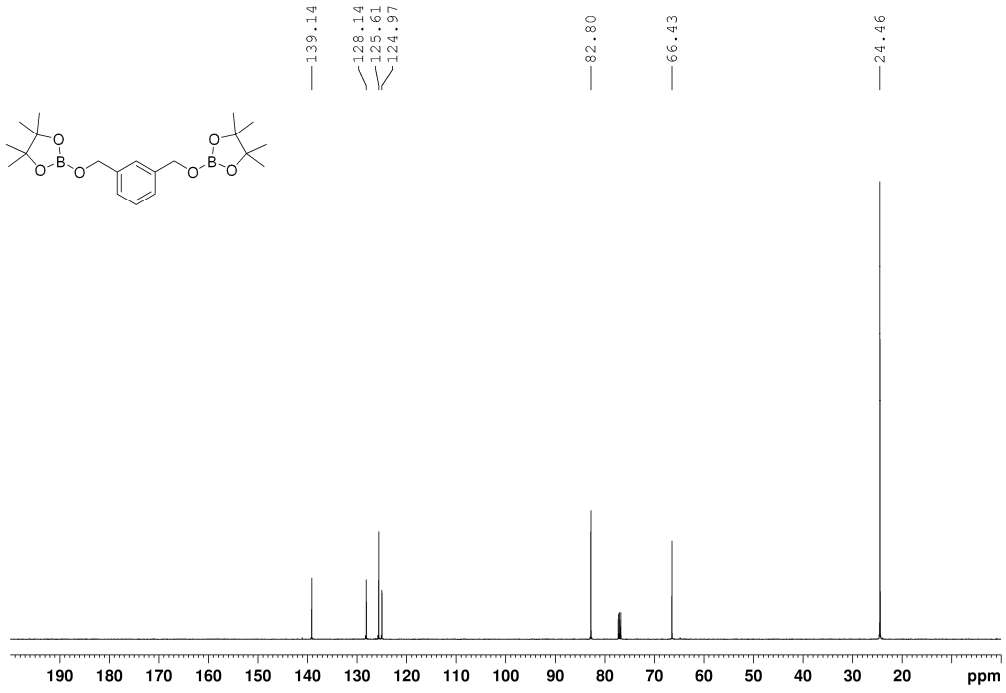

7.218
4.814
1.157
11
10
9
8
7
6
5
4
3
2
1
ppm
4.03
4.00
24.13

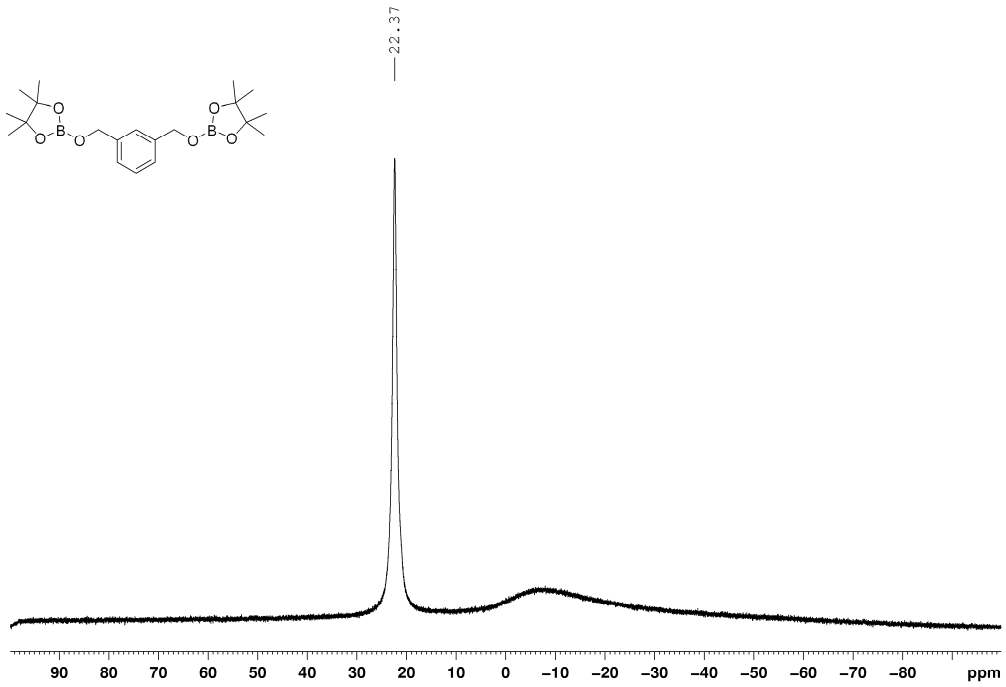

138.18
126.48
82.70
66.23
24.39
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


22.36
90
80
70
60
50
40
30
20
10
0
−10
−20
−30
−40
−50
−60
−70
−80
ppm

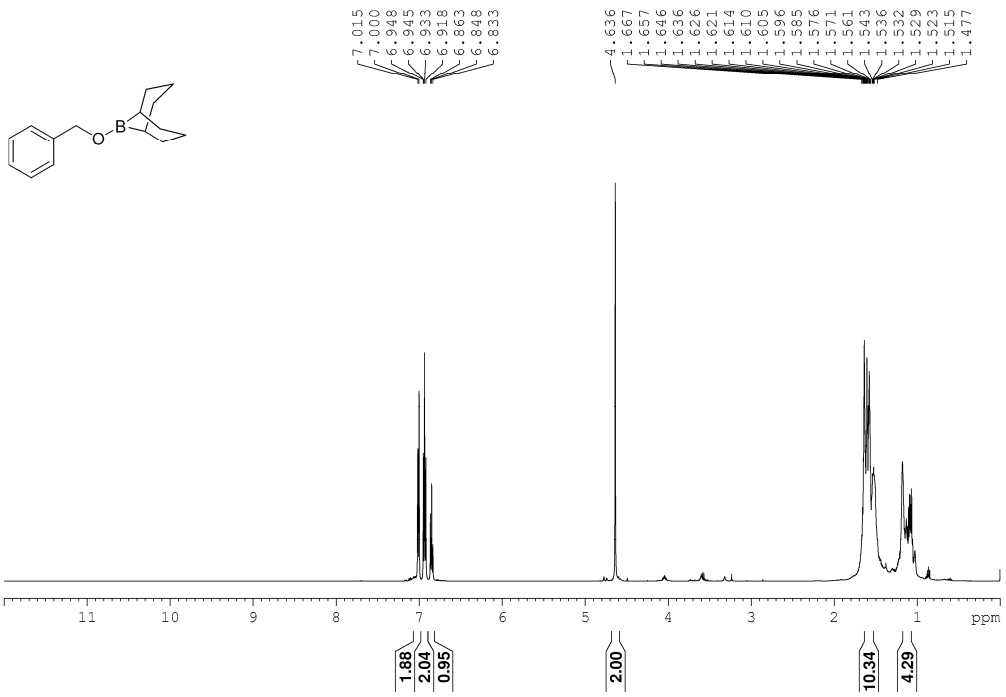
2o

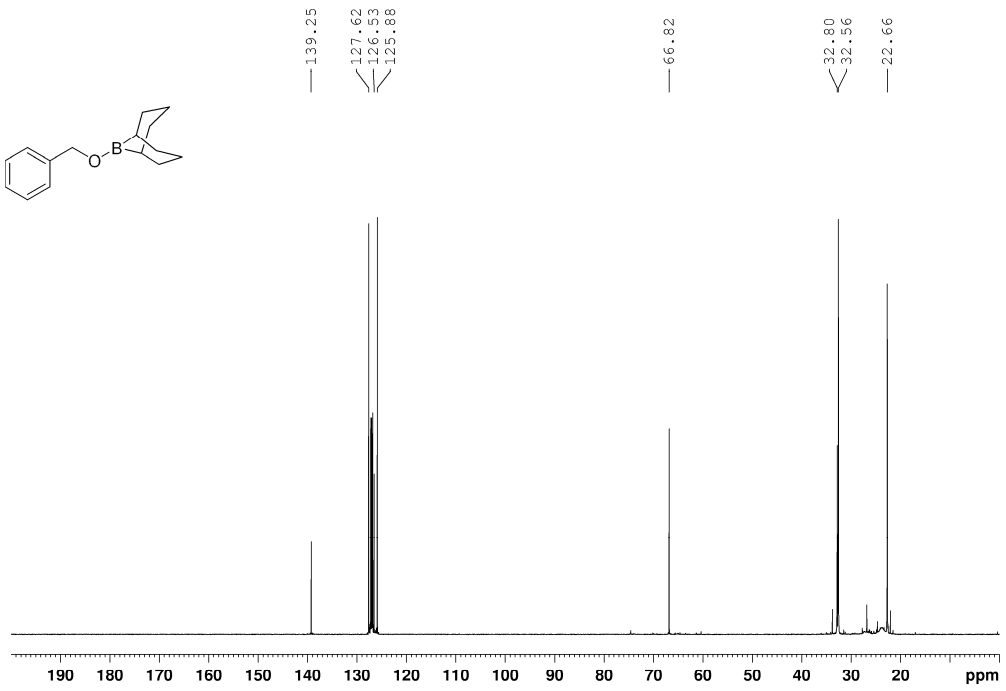

7.242
7.228
7.215
7.210
7.198
7.190
7.172
7.157
4.829
1.171
11
10
9
8
7
6
5
4
3
2
1
ppm
4.11
4.00
24.15

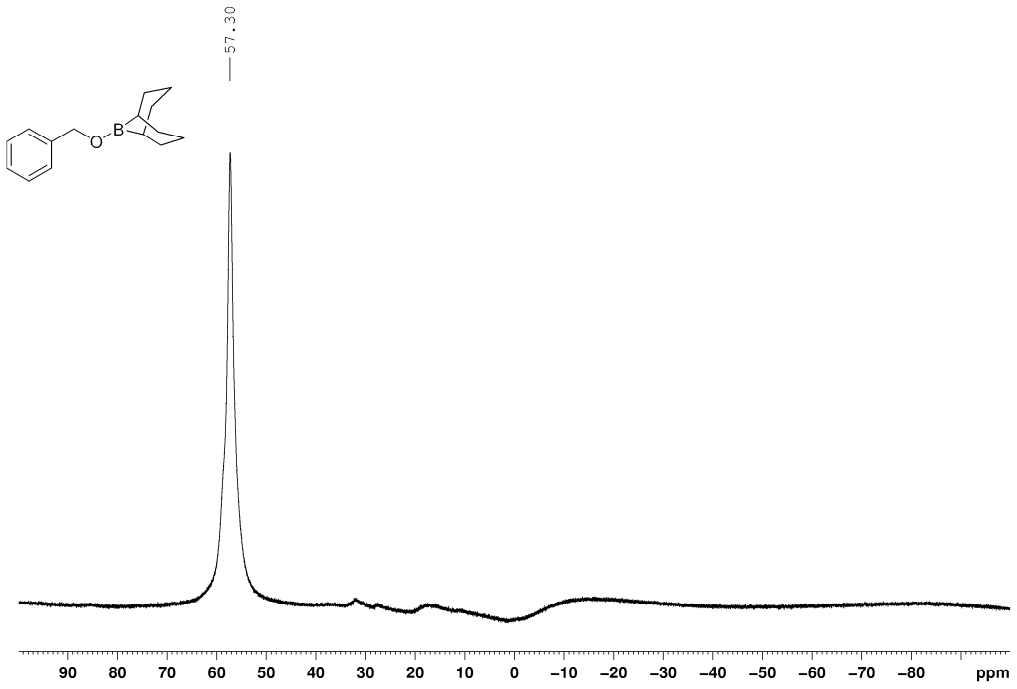

139.14
128.14
125.61
124.97
82.80
66.43
24.46
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


22.37
90
80
70
60
50
40
30
20
10
0
−10
−20
−30
−40
−50
−60
−70
−80
ppm

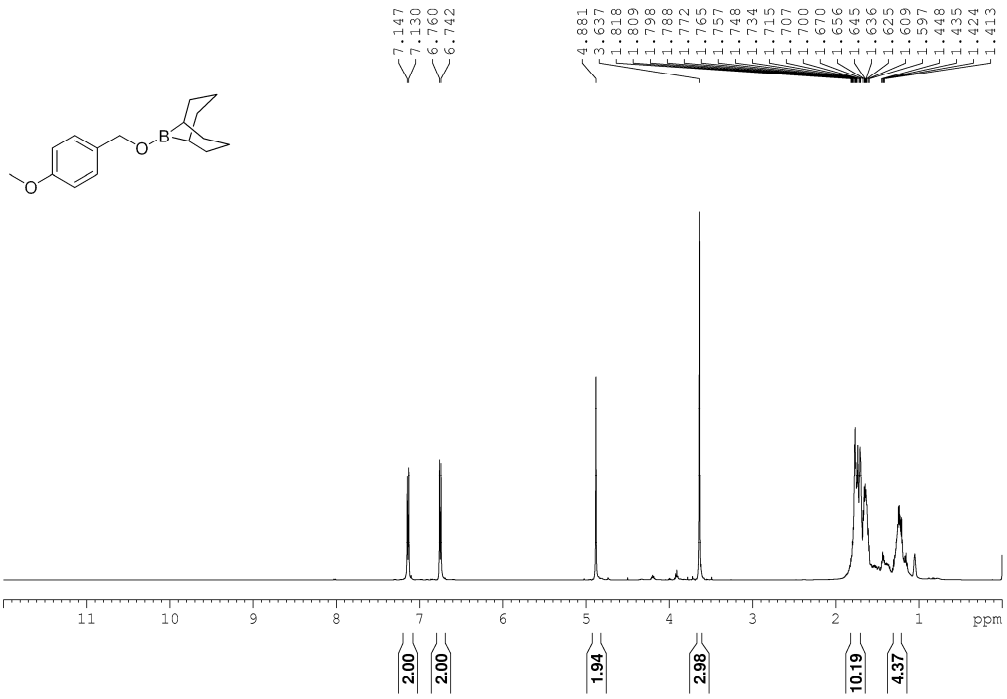
2p


7.015
7.000
6.948
6.945
6.933
6.918
6.863
6.848
6.833
4.636
1.667
1.657
1.646
1.636
1.626
1.621
1.614
1.610
1.605
1.596
1.585
1.576
1.571
1.561
1.543
1.536
1.532
1.529
1.523
1.515
1.477
O
B
11
10
9
8
7
6
5
4
3
2
1
ppm
1.88
2.04
0.95
2.00
10.34
4.29


139.25
127.62
126.53
125.88
66.82
32.80
32.56
22.66
O
B
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


57.30
O
B
90
80
70
60
50
40
30
20
10
0
−10
−20
−30
−40
−50
−60
−70
−80
ppm

2q


7.147
7.130
6.760
6.742
4.881
3.637
1.818
1.809
1.798
1.788
1.772
1.765
1.757
1.748
1.734
1.715
1.707
1.700
1.670
1.656
1.645
1.636
1.625
1.609
1.597
1.448
1.435
1.424
1.413
O
B
O
11
10
9
8
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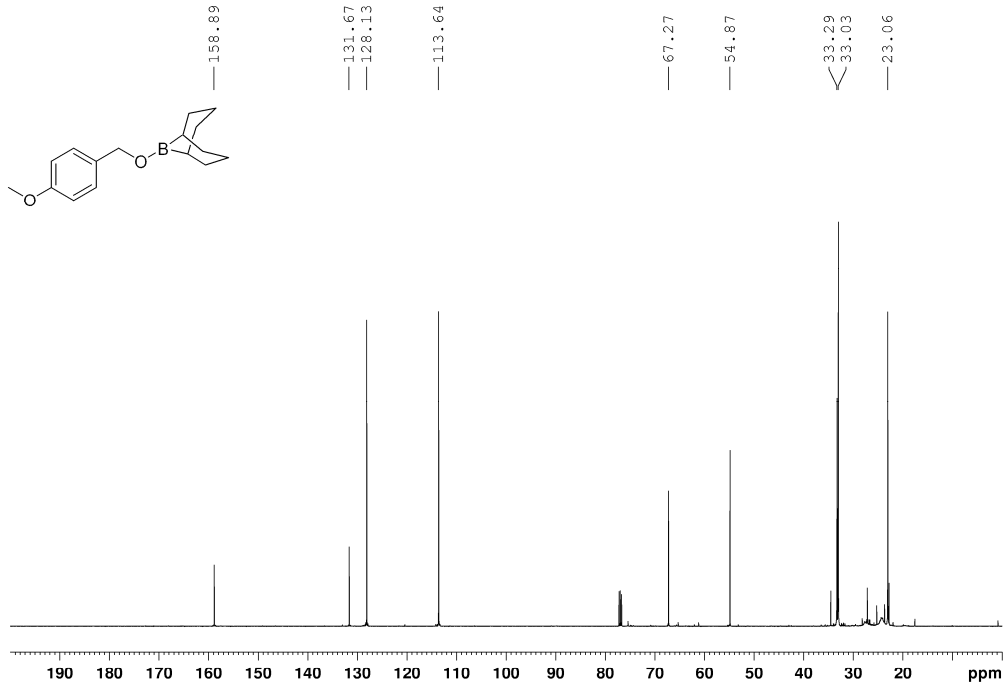
6
5
4
3
2
1
ppm
2.00
2.00
1.94
2.98
10.19
4.37


158.89
131.67
128.13
113.64
67.27
54.87
33.29
33.03
23.06
O
B
O
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160
150
140
130
120
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80
70
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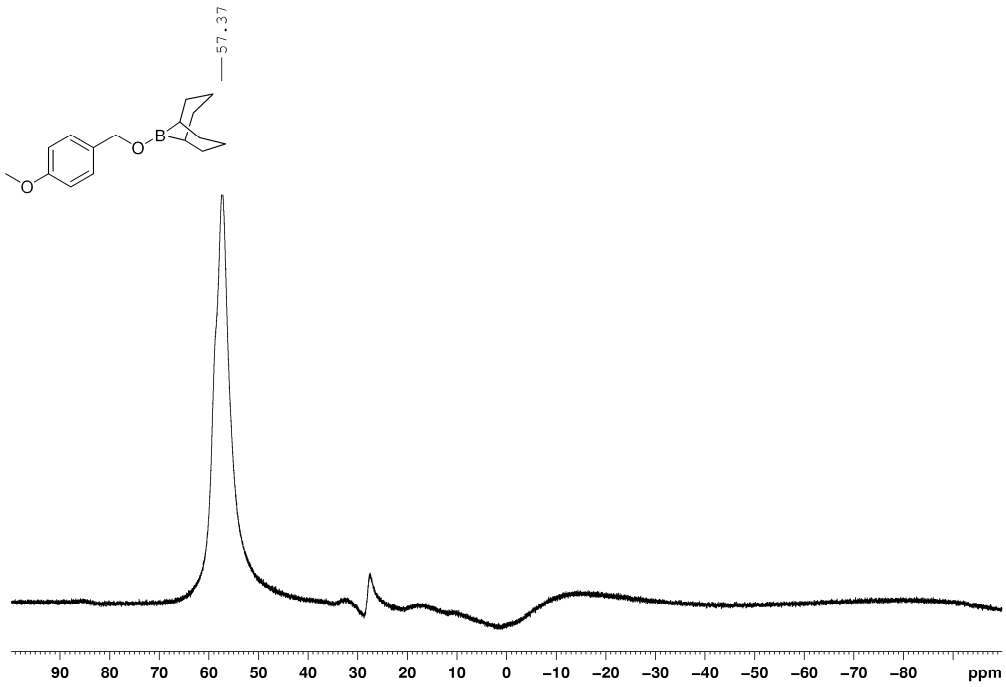
50
40
30
20
ppm


57.37
B
O
O
90
80
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60
50
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20
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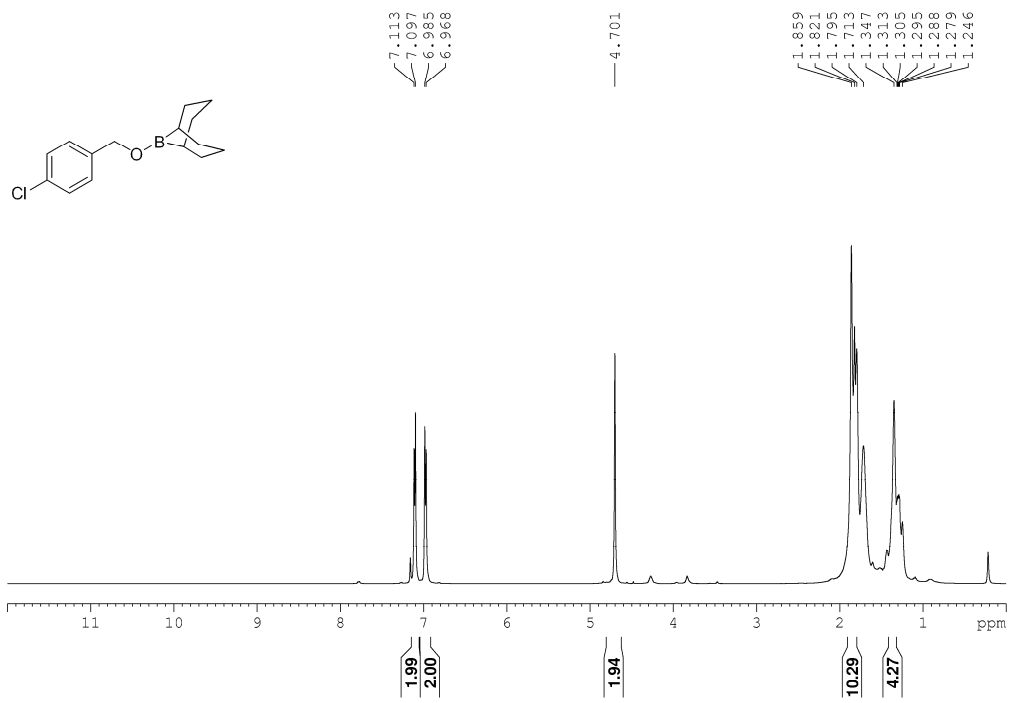
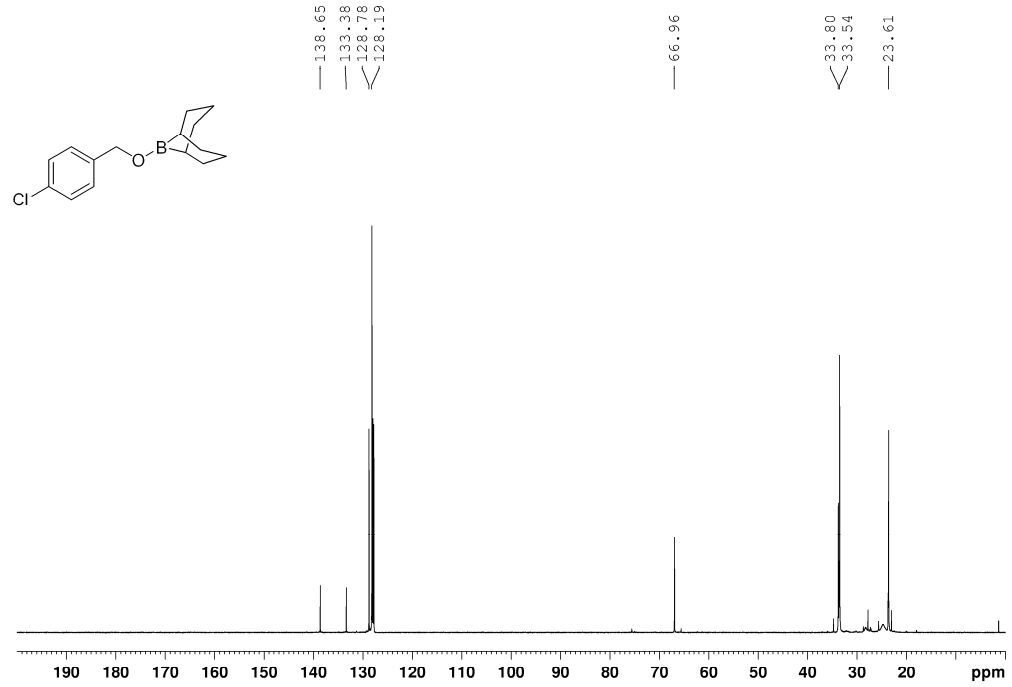
−10
−20
−30
−40
−50
−60
−70
−80
ppm

2r


7.113
7.097
6.985
6.968
4.701
1.859
1.821
1.795
1.713
1.347
1.313
1.305
1.295
1.288
1.279
1.246
O
B
Cl
11
10
9
8
7
6
5
4
3
2
1
ppm
1.99
2.00
1.94
10.29
4.27


138.65
133.38
128.78
128.19
66.96
33.80
33.54
23.61
O
B
Cl
190
180
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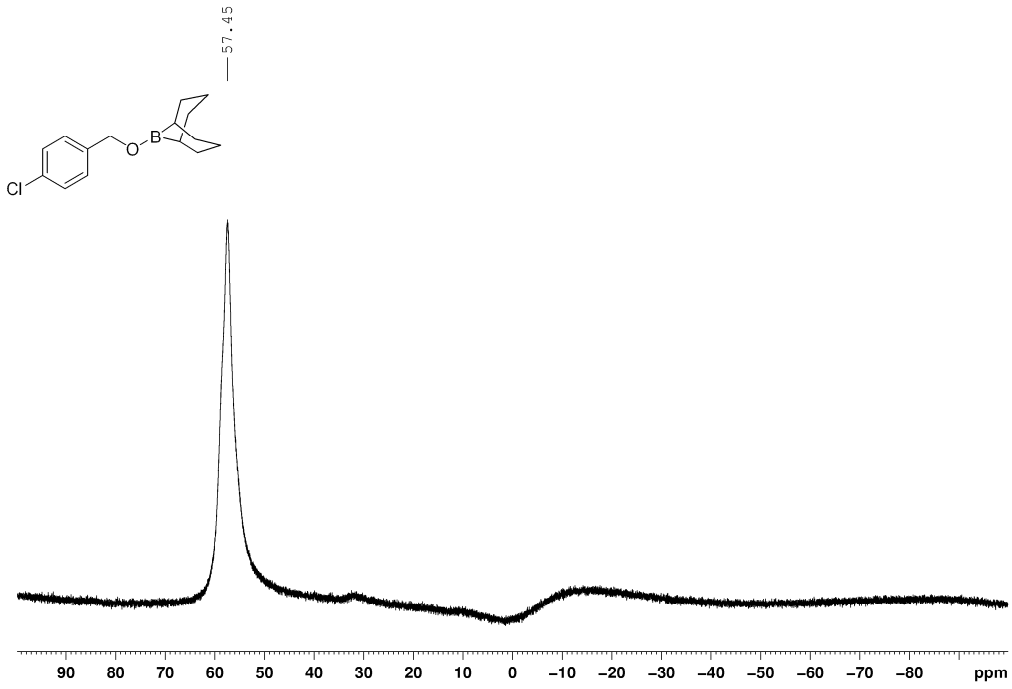
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm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Cl
O
B
90
80
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50
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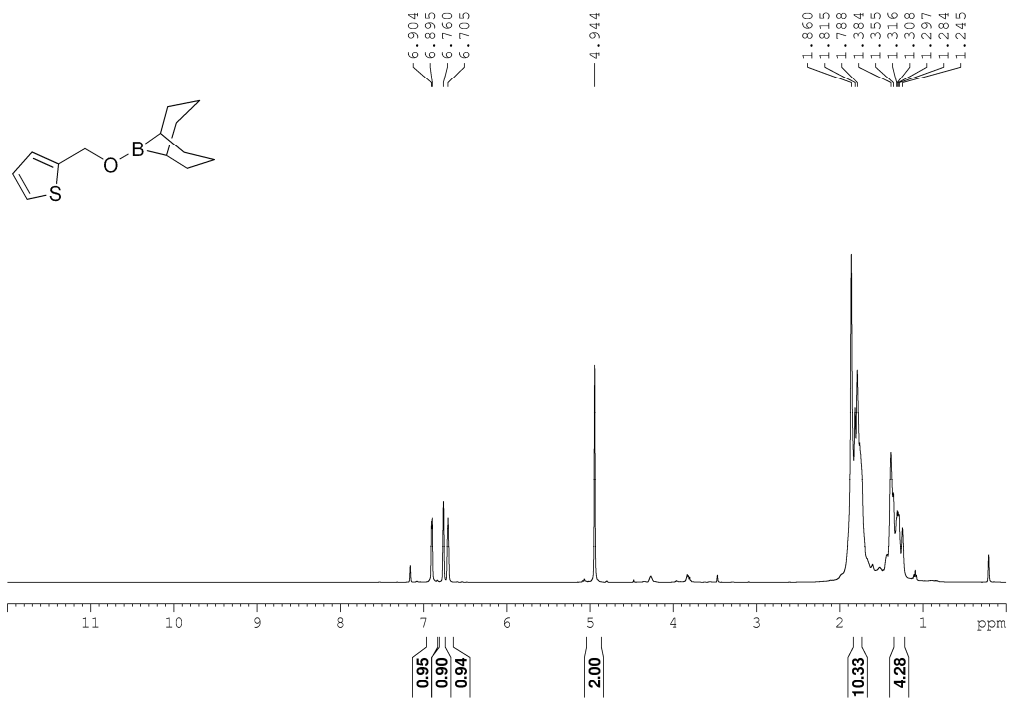
20
10
0
−10
−20
−30
−40
−50
−60
−70
−80
ppm

2s


6.904
6.895
6.760
6.705
4.944
1.860
1.815
1.788
1.384
1.355
1.316
1.308
1.297
1.284
1.245
O
B
S
11
10
9
8
7
6
5
4
3
2
1
ppm
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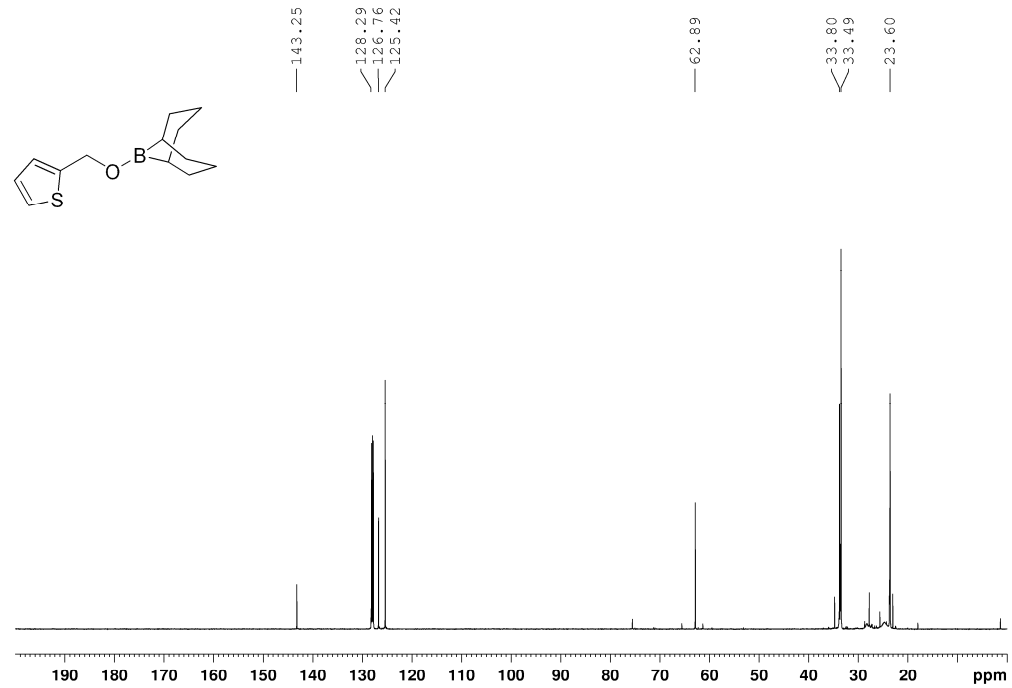
0.90
0.94
2.00
10.33
4.28


143.25
128.29
126.76
125.42
62.89
33.80
33.49
23.60
O
B
S
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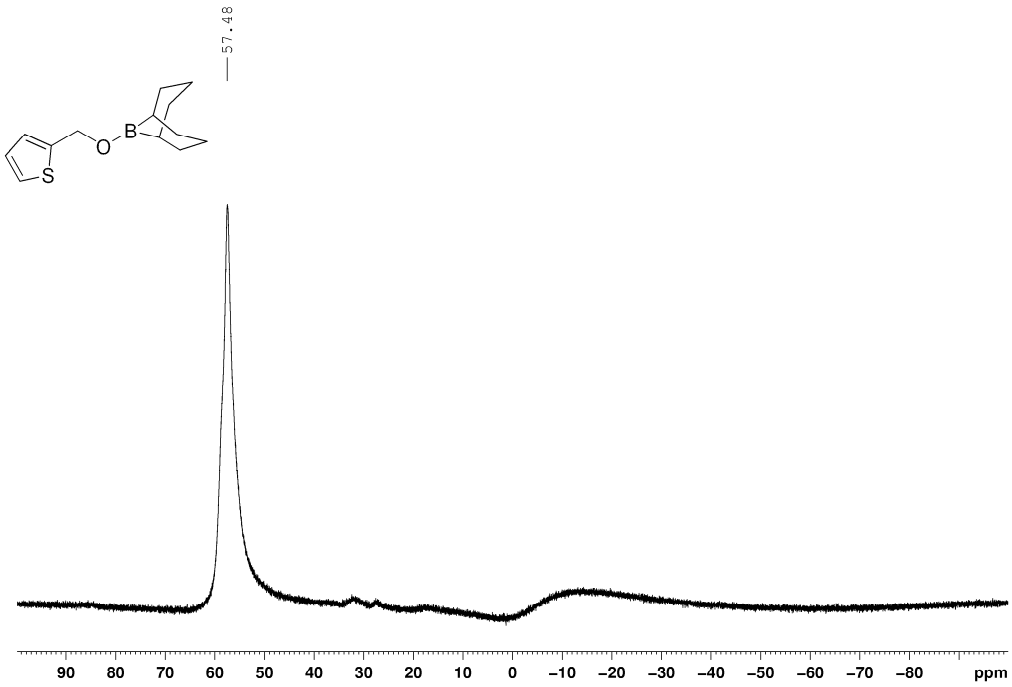
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


57.48
B
O
S
90
80
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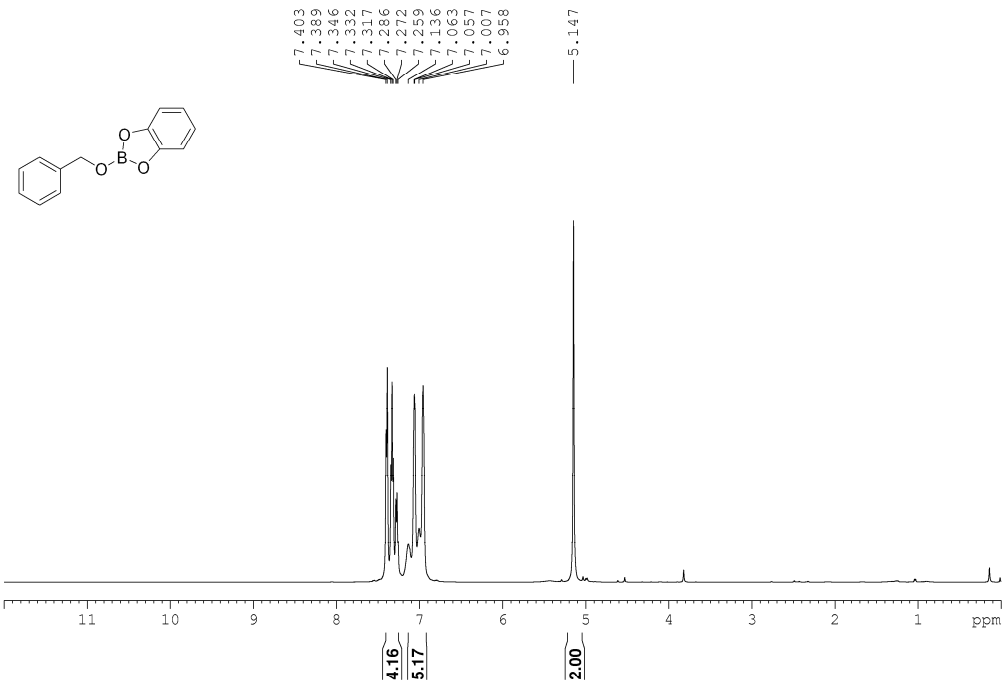
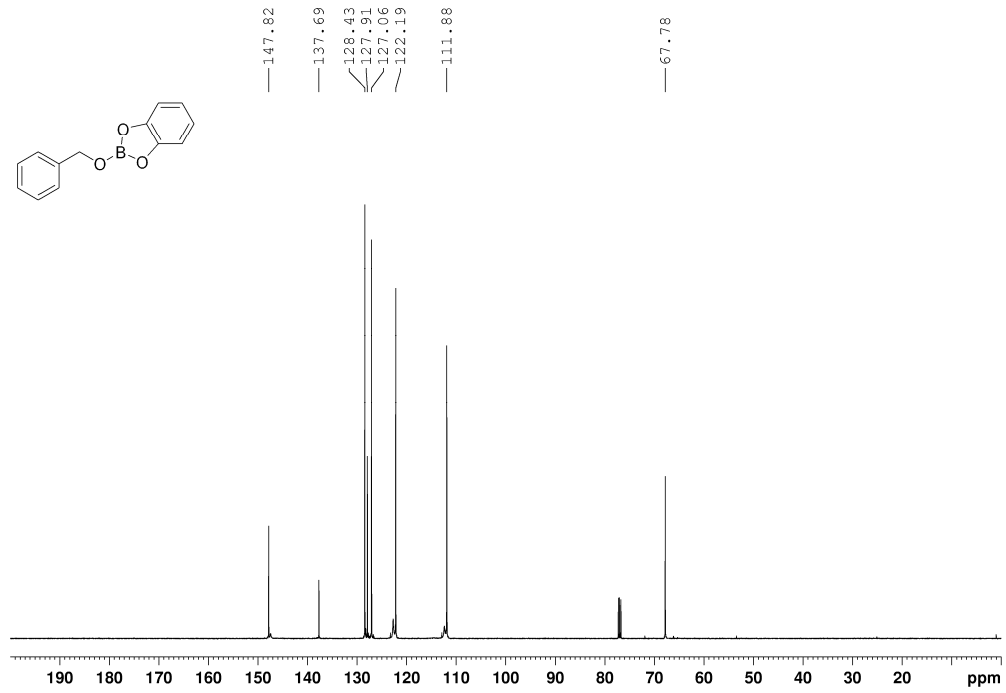
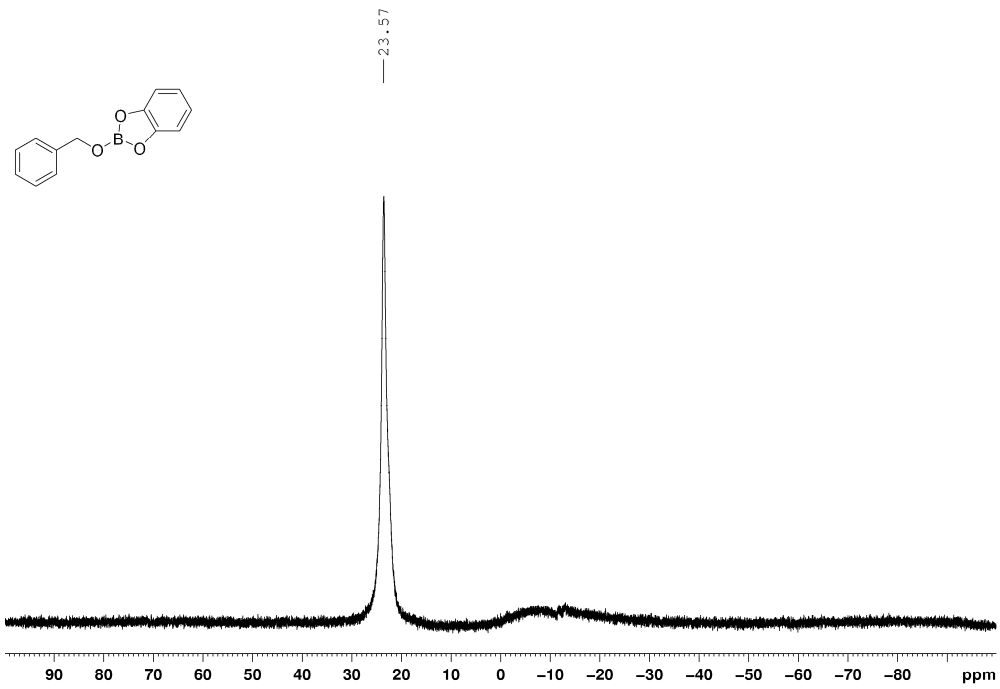
20
10
0
−10
−20
−30
−40
−50
−60
−70
−80
ppm

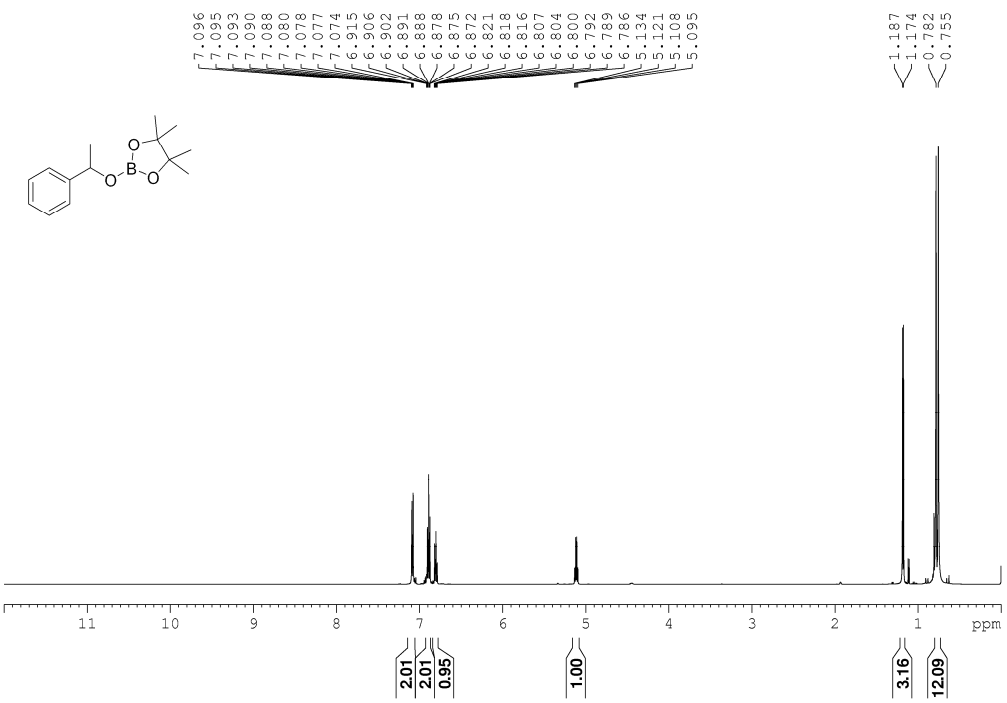
2t

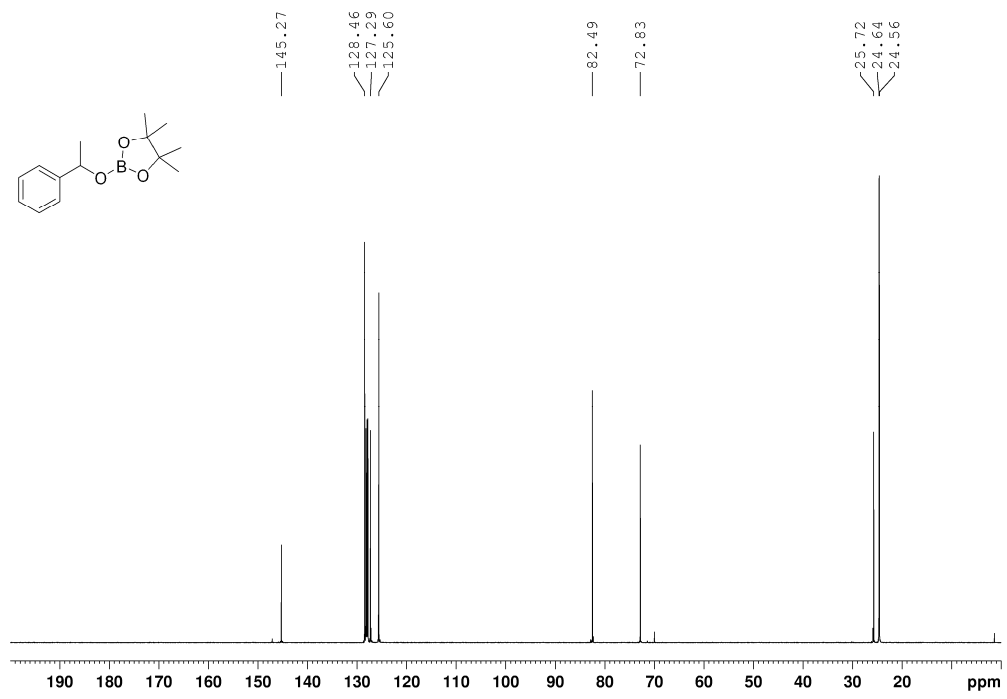

7.403
7.389
7.346
7.332
7.317
7.286
7.272
7.259
7.136
7.063
7.057
7.007
6.958
5.147
O
B
O
O
11
10
9
8
7
6
5
4
3
2
1
ppm
4.16
5.17
2.00

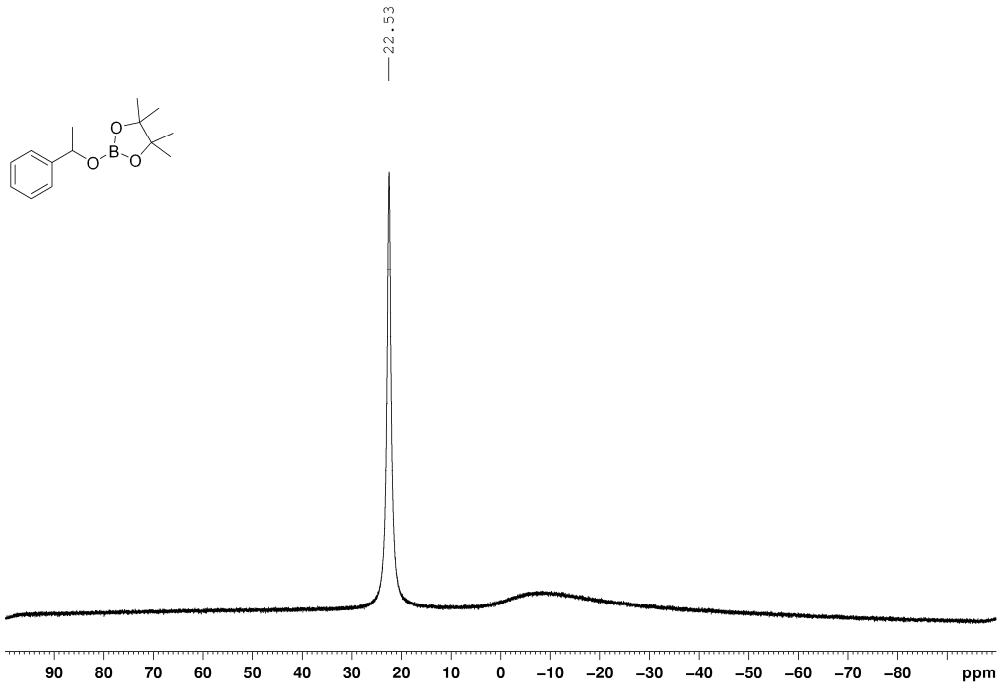

147.82
137.69
128.43
127.91
127.06
122.19
111.88
67.78
O
B
O
O
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


23.57
O
B
O
O
90
80
70
60
50
40
30
20
10
0
−10
−20
−30
−40
−50
−60
−70
−80
ppm

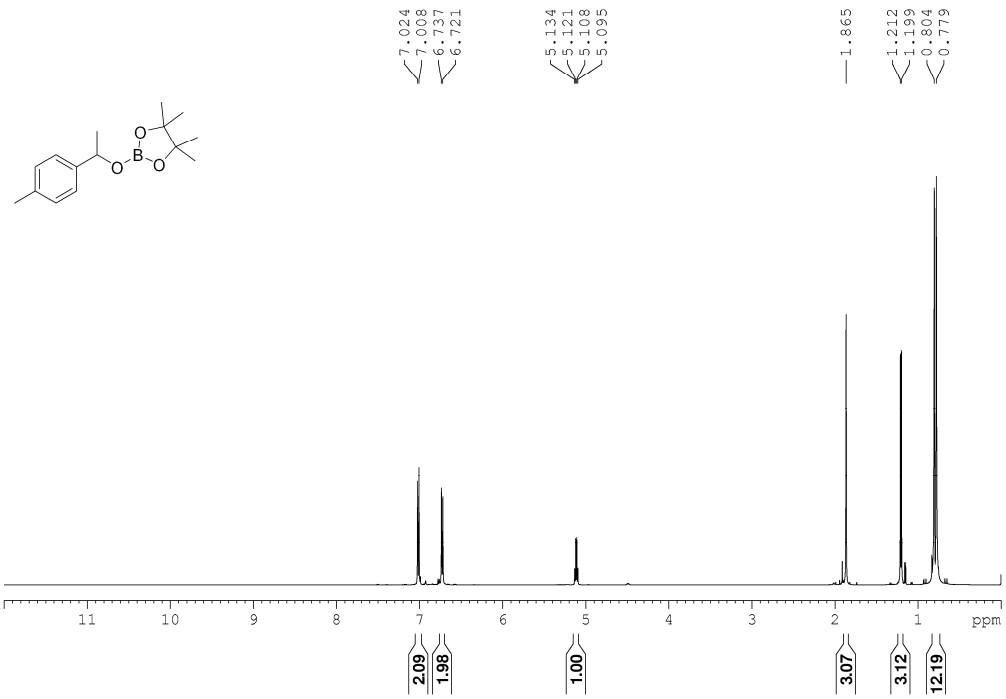
4a

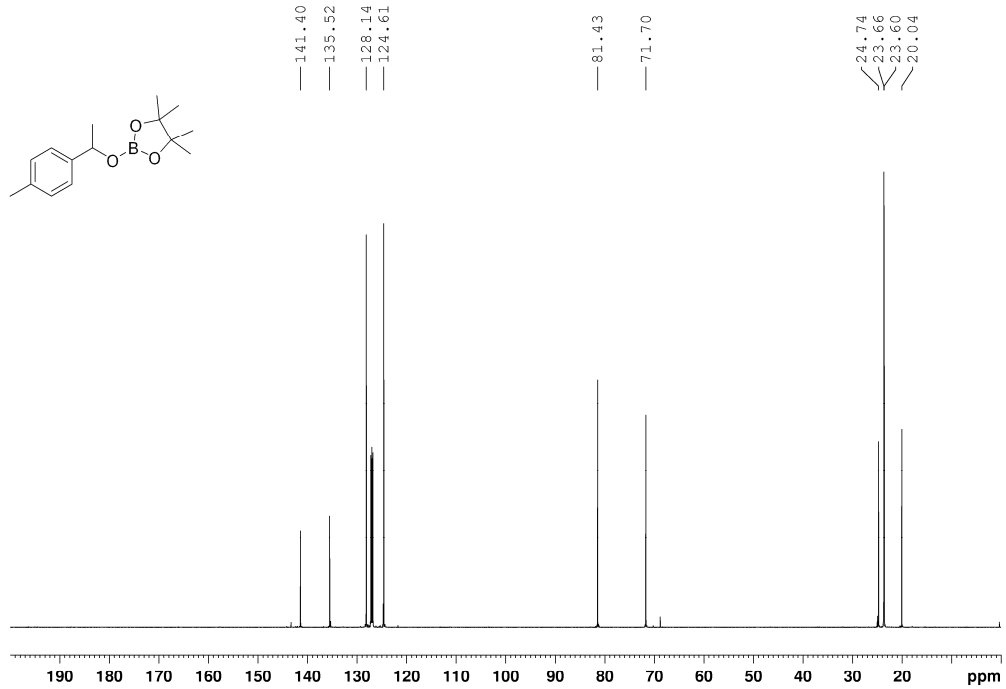

7.096
7.095
7.093
7.090
7.088
7.080
7.078
7.077
7.074
6.915
6.906
6.902
6.891
6.888
6.878
6.875
6.872
6.821
6.818
6.816
6.807
6.804
6.800
6.792
6.789
6.786
5.134
5.121
5.108
5.095
1.187
1.174
0.782
0.755
O
B
O
O
11
10
9
8
7
6
5
4
3
2
1
ppm
2.01
2.01
0.95
1.00
3.16
12.09

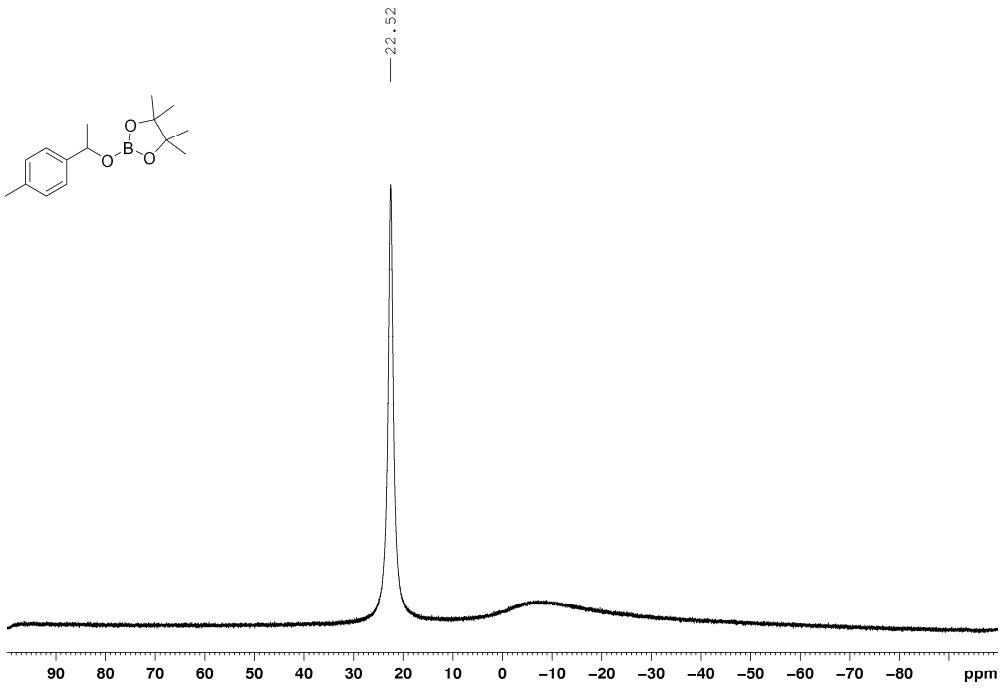

145.27
128.46
127.29
125.60
82.49
72.83
25.72
24.64
24.56
O
B
O
O
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


22.53
O
B
O
O
90
80
70
60
50
40
30
20
10
0
−10
−20
−30
−40
−50
−60
−70
−80
ppm

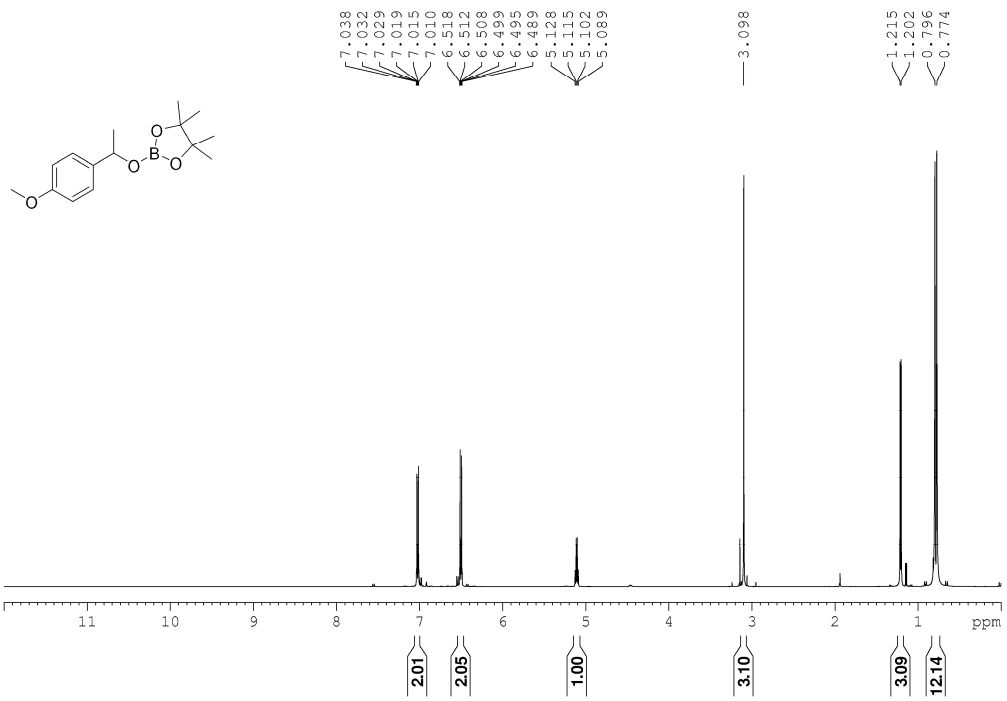
4b

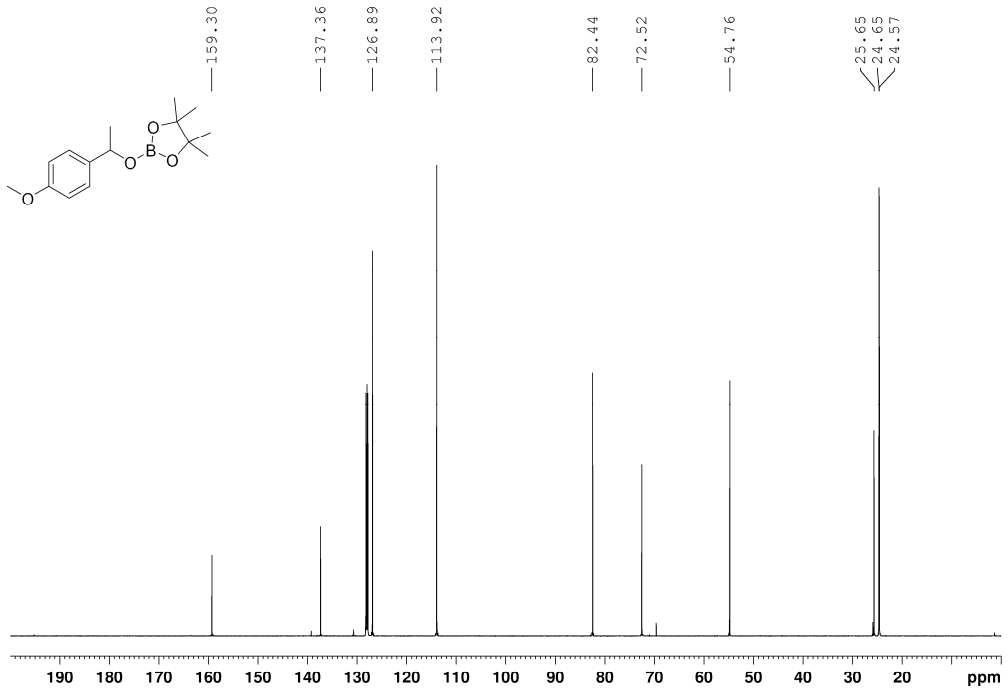

7.024
7.008
6.737
6.721
5.134
5.121
5.108
5.095
1.865
1.212
1.199
0.804
0.779
11
10
9
8
7
6
5
4
3
2
1
ppm
2.09
1.98
1.00
3.07
3.12
12.19

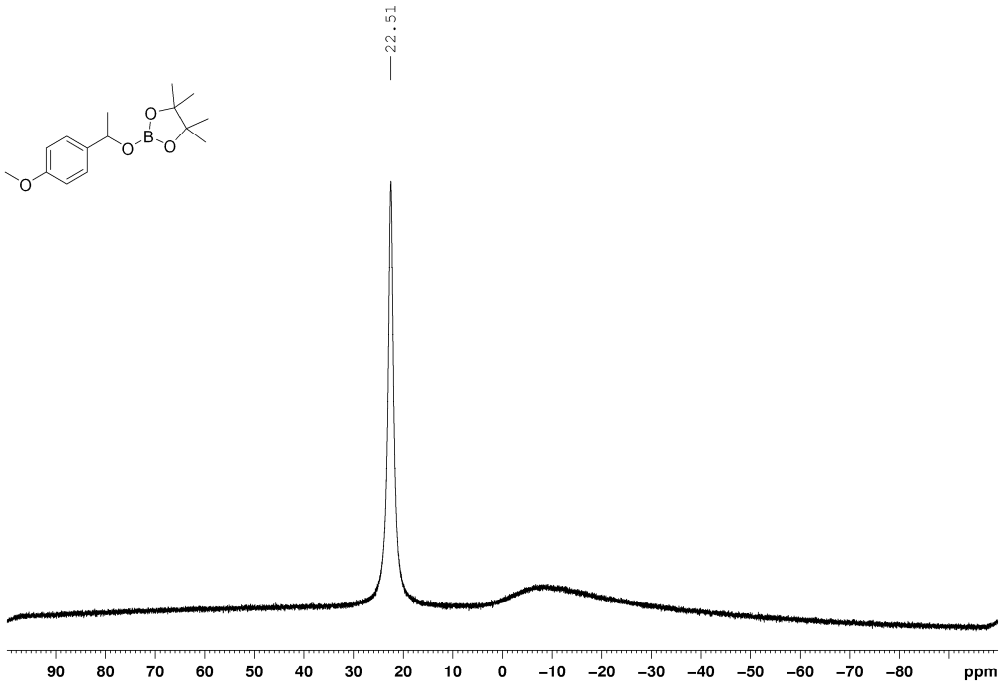

141.40
135.52
128.14
124.61
81.43
71.70
24.74
23.66
23.60
20.04
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


22.52
O
B
O
O
90
80
70
60
50
40
30
20
10
0
−10
−20
−30
−40
−50
−60
−70
−80
ppm

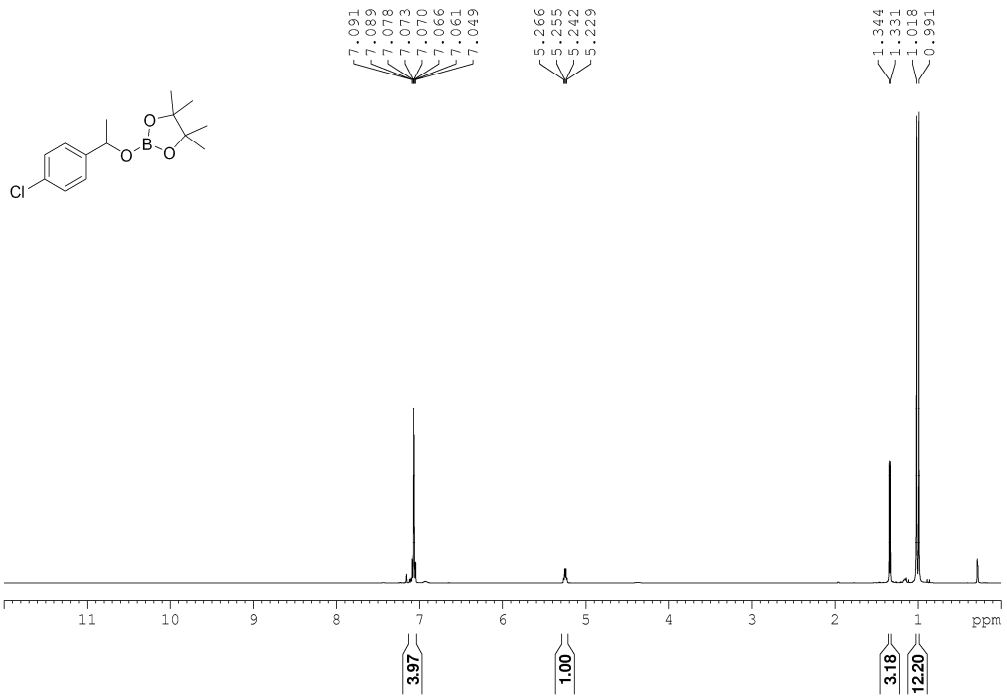
4c

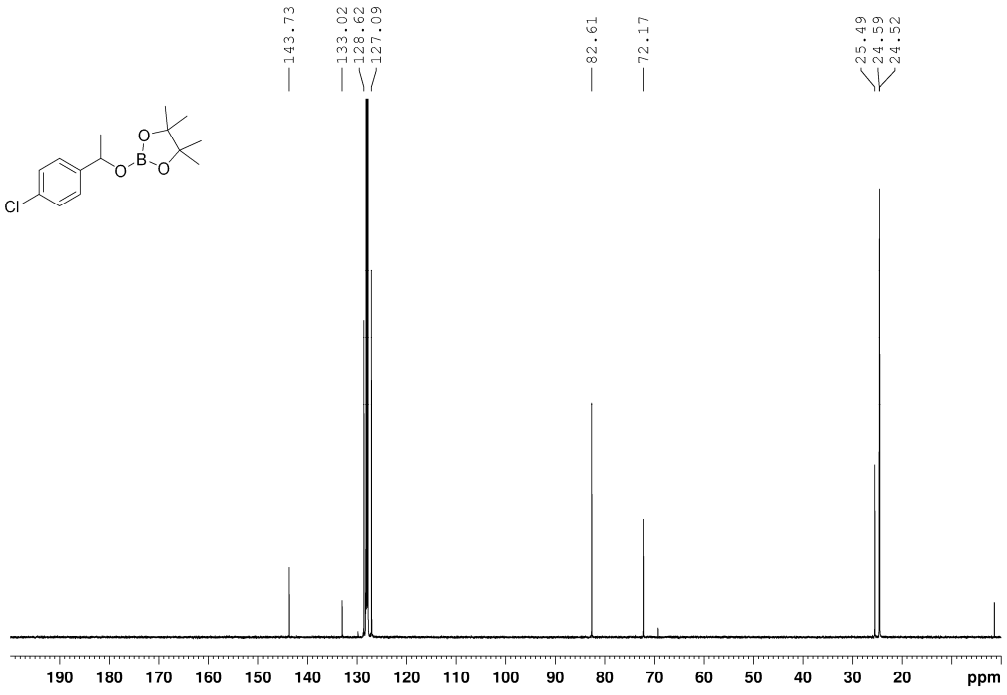

7.038
7.032
7.029
7.019
7.015
7.010
6.518
6.512
6.508
6.499
6.495
6.489
5.128
5.115
5.102
5.089
3.098
1.215
1.202
0.796
0.774
ppm
2.01
2.05
1.00
3.10
3.09
12.14


159.30
137.36
126.89
113.92
82.44
72.52
54.76
25.65
24.65
24.57
ppm


22.51
O
B
O
O
90
80
70
60
50
40
30
20
10
0
−10
−20
−30
−40
−50
−60
−70
−80
ppm

4d


7.091
7.089
7.078
7.073
7.070
7.066
7.061
7.049
5.266
5.255
5.242
5.229
1.344
1.331
1.018
0.991
Cl
O
B
O
O
11
10
9
8
7
6
5
4
3
2
1
ppm
3.97
1.00
3.18
12.20


143.73
133.02
128.62
127.09
82.61
72.17
25.49
24.59
24.52
Cl
O
B
O
O
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160
150
140
130
120
110
100
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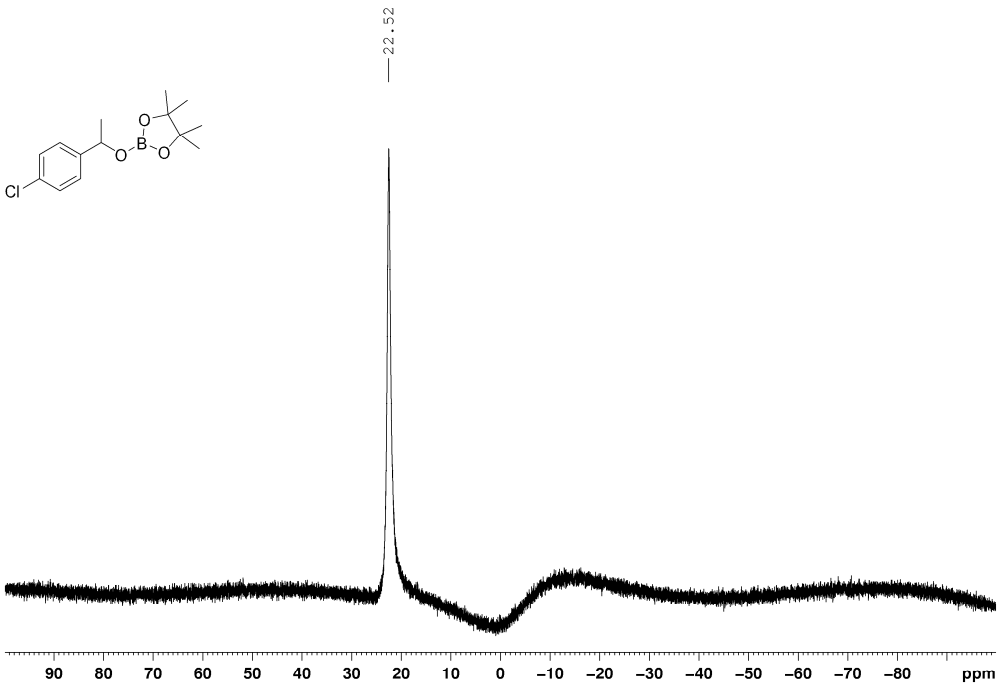
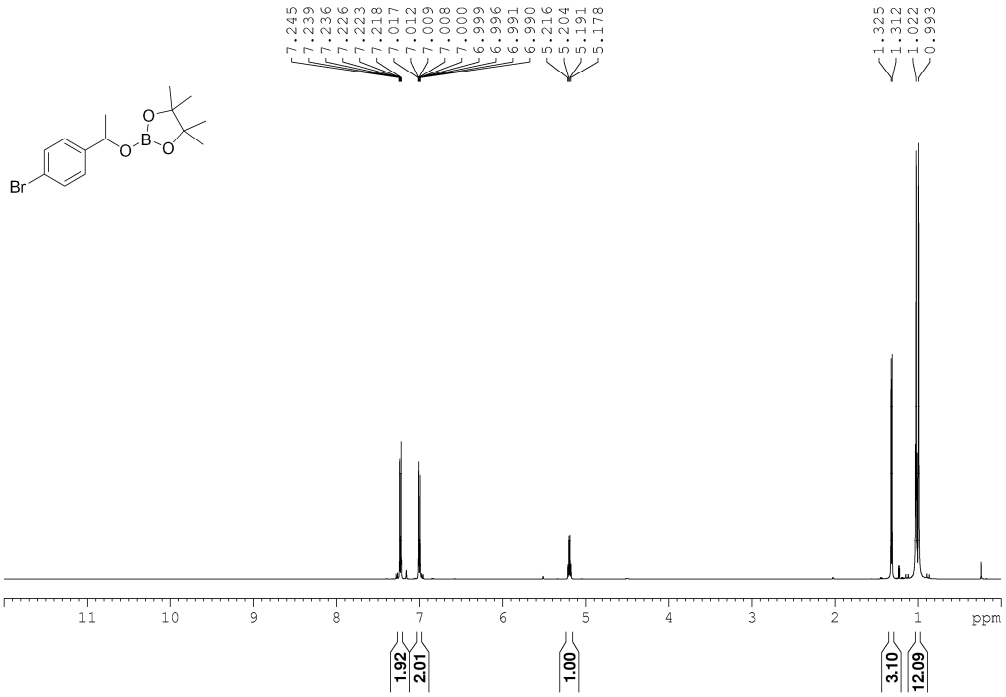
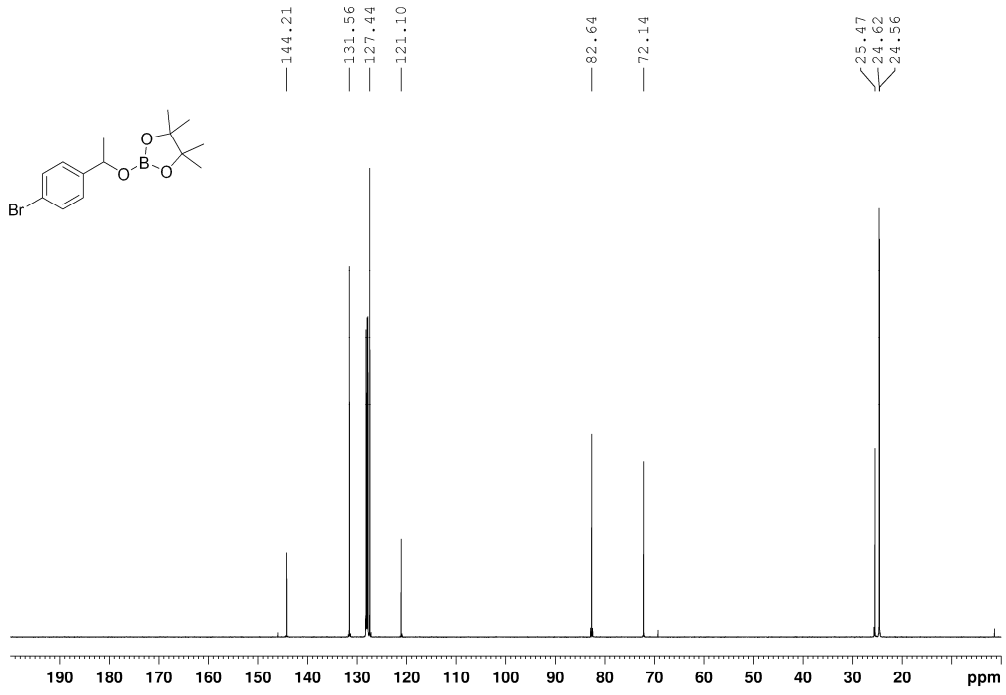
80
70
60
50
40
30
20
ppm


22.52
O
B
O
O
Cl
90
80
70
60
50
40
30
20
10
0
−10
−20
−30
−40
−50
−60
−70
−80
ppm

4e


7.245
7.239
7.236
7.226
7.223
7.218
7.017
7.012
7.009
7.008
7.000
6.999
6.996
6.991
6.990
5.216
5.204
5.191
5.178
1.325
1.312
1.022
0.993
Br
11
10
9
8
7
6
5
4
3
2
1
ppm
1.92
2.01
1.00
3.10
12.09


144.21
131.56
127.44
121.10
82.64
72.14
25.47
24.62
24.56
Br
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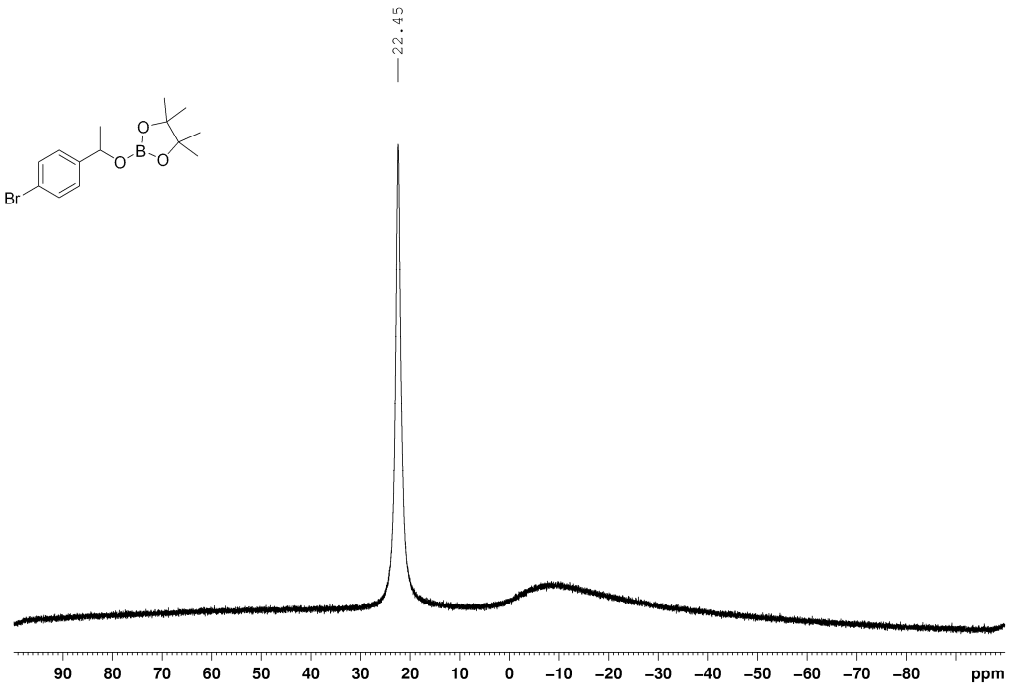
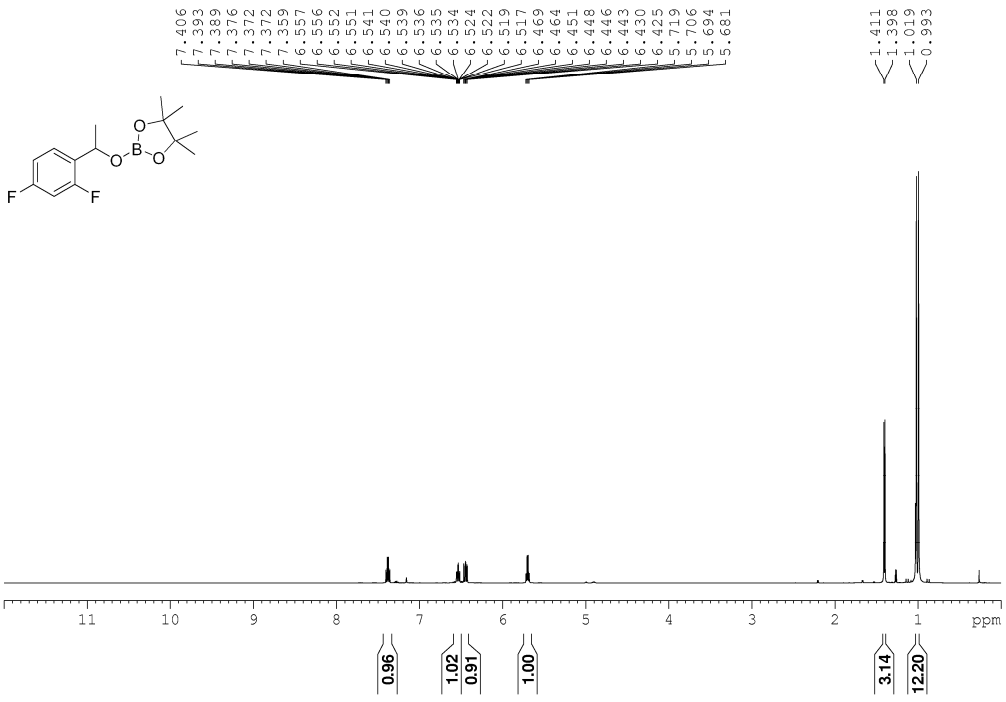
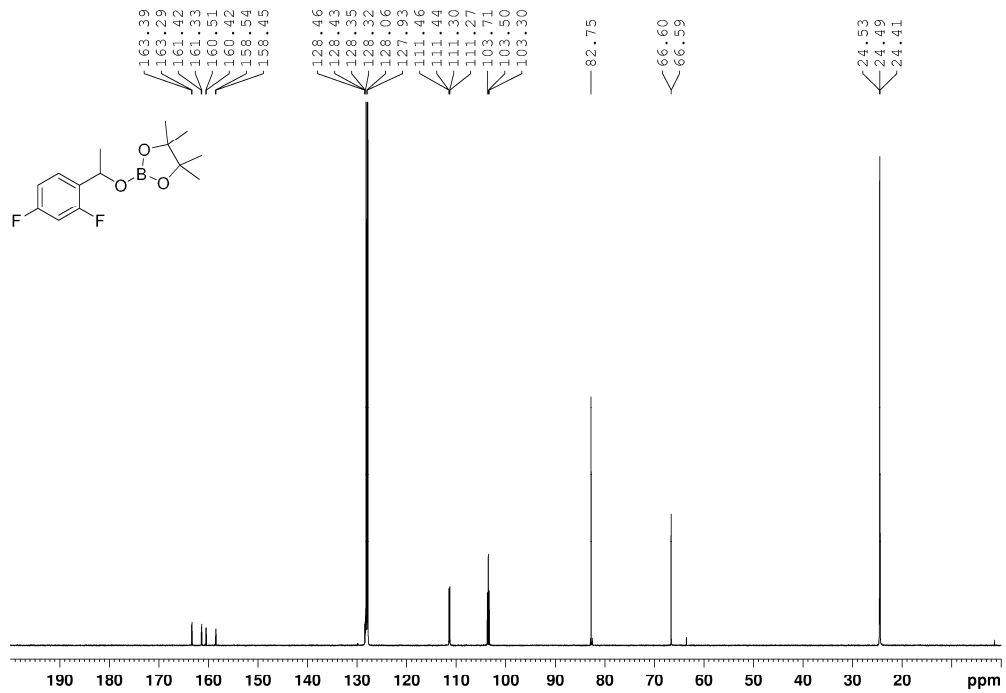
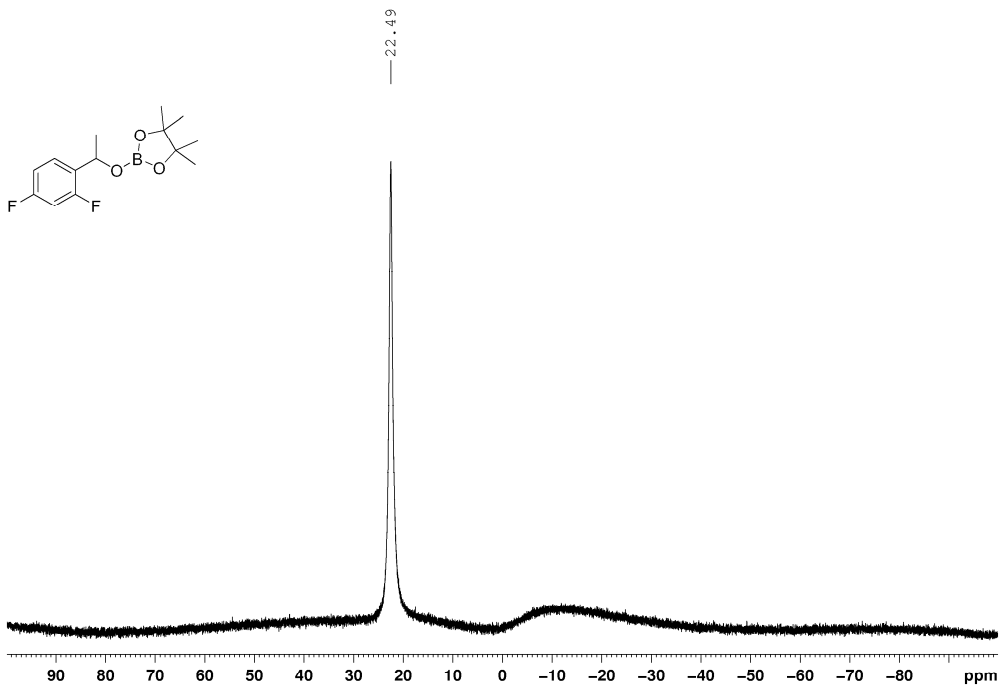
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


22.45
O
B
O
O
Br
90
80
70
60
50
40
30
20
10
0
−10
−20
−30
−40
−50
−60
−70
−80
ppm

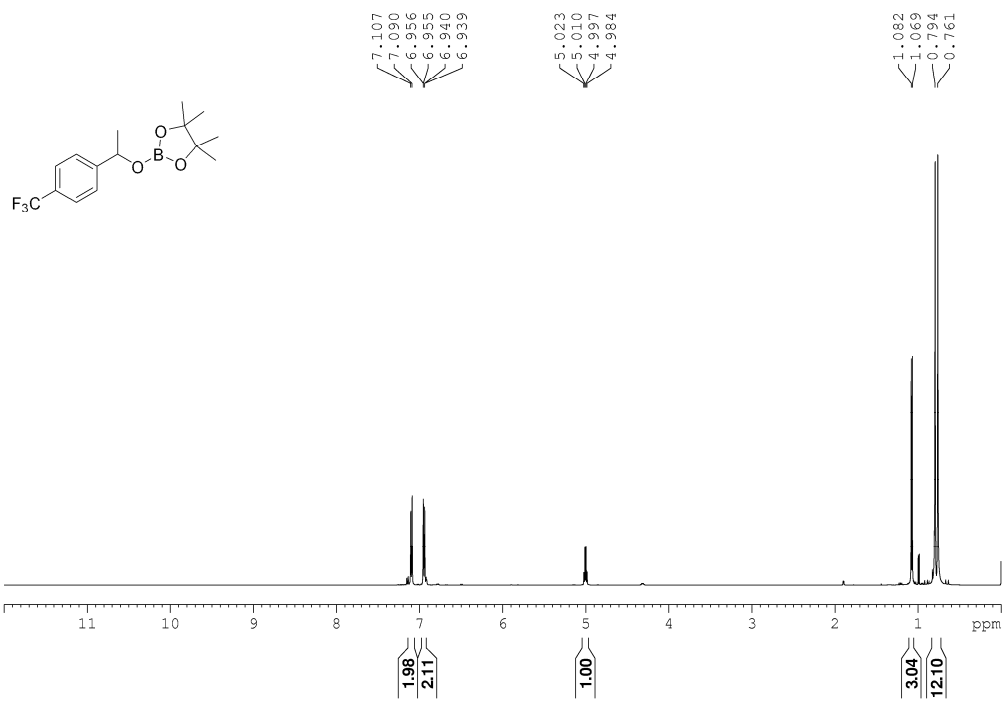
4f

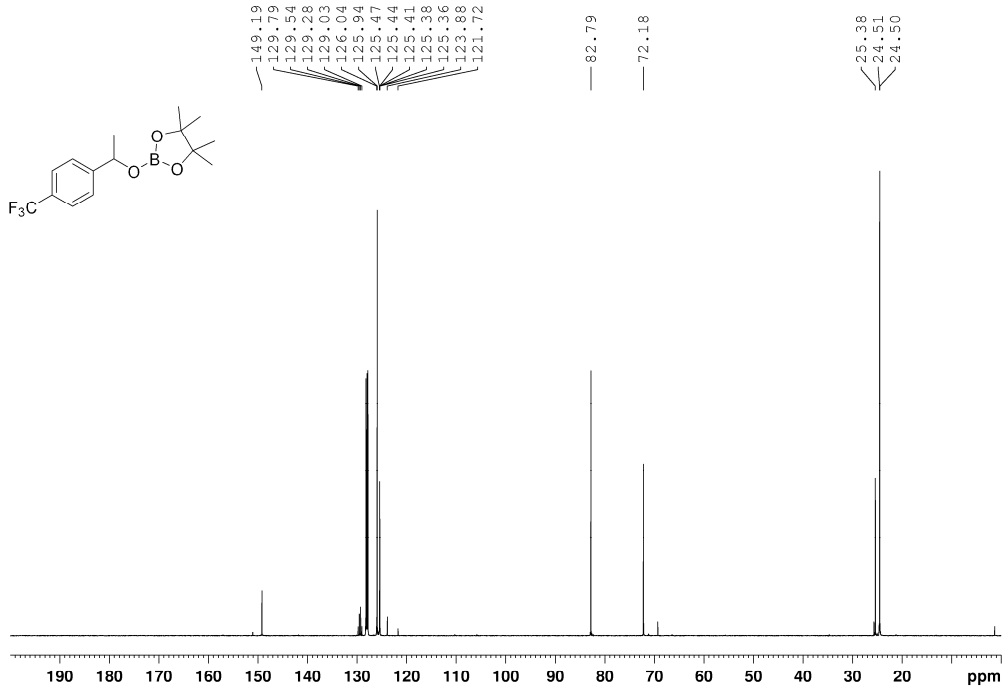

7.406
7.393
7.389
7.376
7.372
7.372
7.359
6.557
6.556
6.552
6.551
6.541
6.540
6.539
6.536
6.535
6.534
6.524
6.522
6.519
6.517
6.469
6.464
6.451
6.448
6.446
6.443
6.430
6.425
5.719
5.706
5.694
5.681
1.411
1.398
1.019
0.993
O
B
O
O
F
F
11
10
9
8
7
6
5
4
3
2
1
ppm
0.96
1.02
0.91
1.00
3.14
12.20

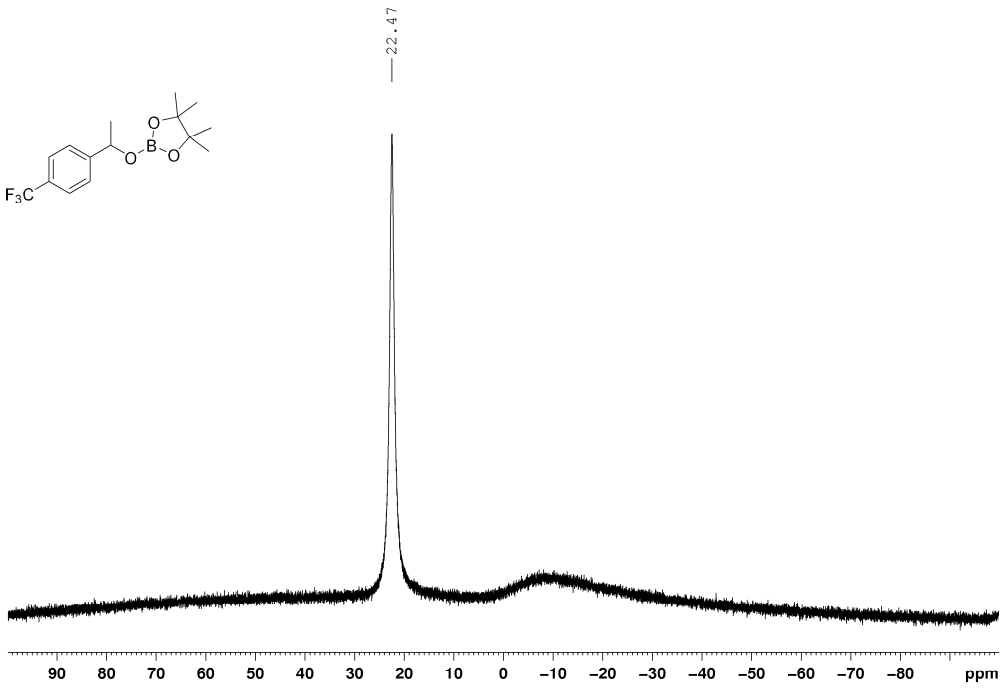

163.39
163.29
161.42
161.33
160.51
160.42
158.54
158.45
128.46
128.43
128.35
128.32
128.06
127.93
111.46
111.44
111.30
111.27
103.71
103.50
103.30
82.75
66.60
66.59
24.53
24.49
24.41
O
B
O
O
F
F
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


22.49
O
B
O
O
F
F
90
80
70
60
50
40
30
20
10
0
−10
−20
−30
−40
−50
−60
−70
−80
ppm

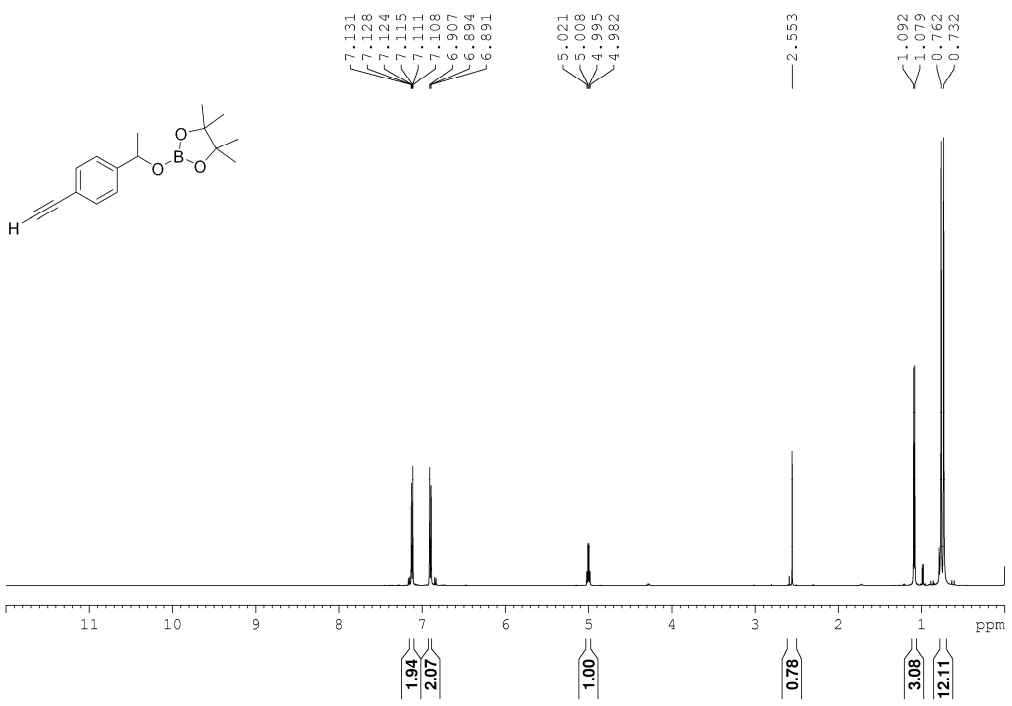
4g

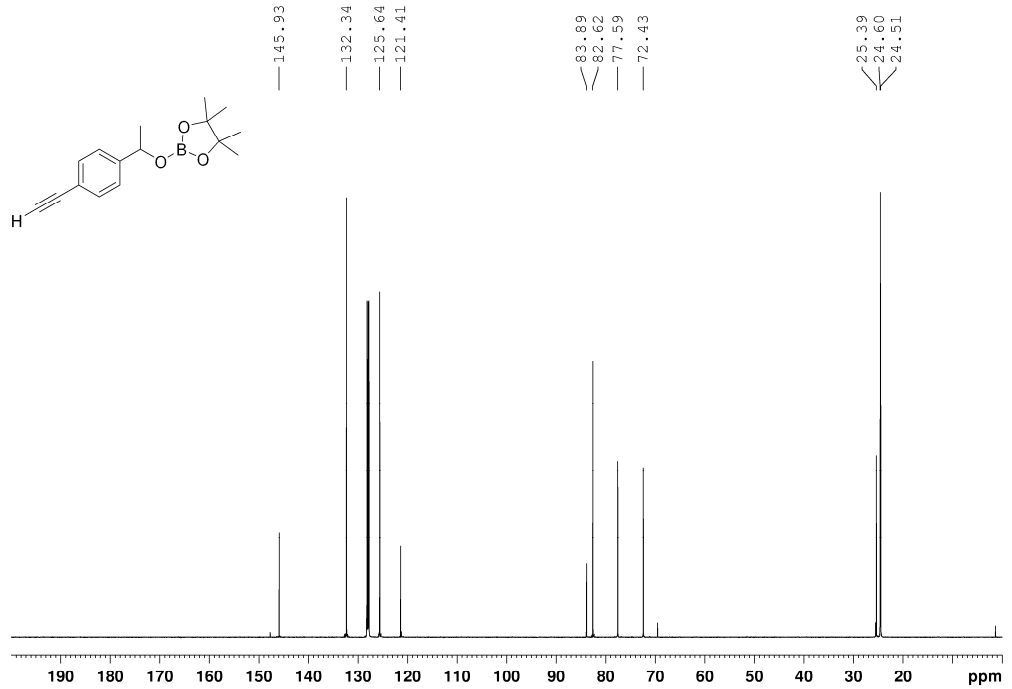

7.107
7.090
6.956
6.955
6.940
6.939
5.023
5.010
4.997
4.984
1.082
1.069
0.794
0.761
F3C
ppm
1.98
2.11
1.00
3.04
12.10

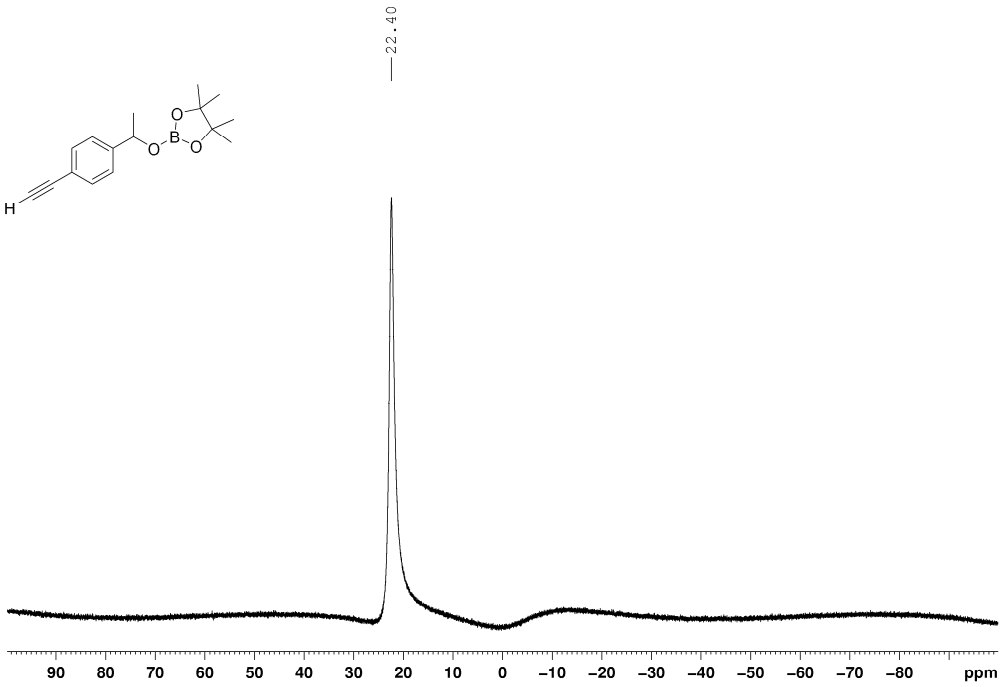

149.19
129.79
129.54
129.28
129.03
126.04
125.94
125.47
125.44
125.41
125.38
125.36
123.88
121.72
82.79
72.18
25.38
24.51
24.50
F3C
ppm


22.47
O
B
O
O
F3C
90
80
70
60
50
40
30
20
10
0
−10
−20
−30
−40
−50
−60
−70
−80
ppm

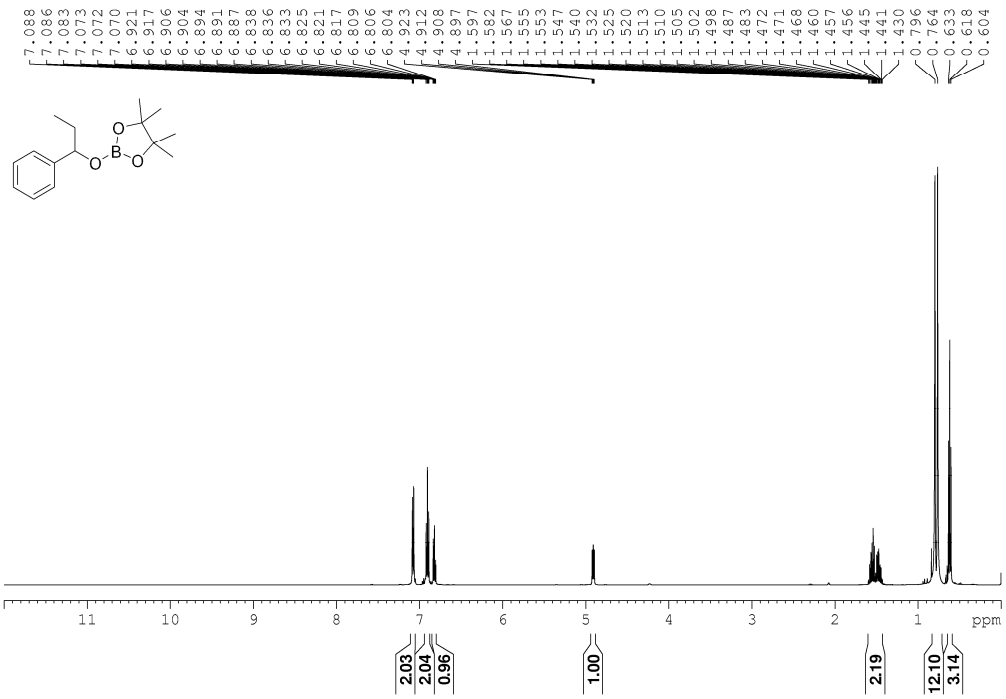
4h

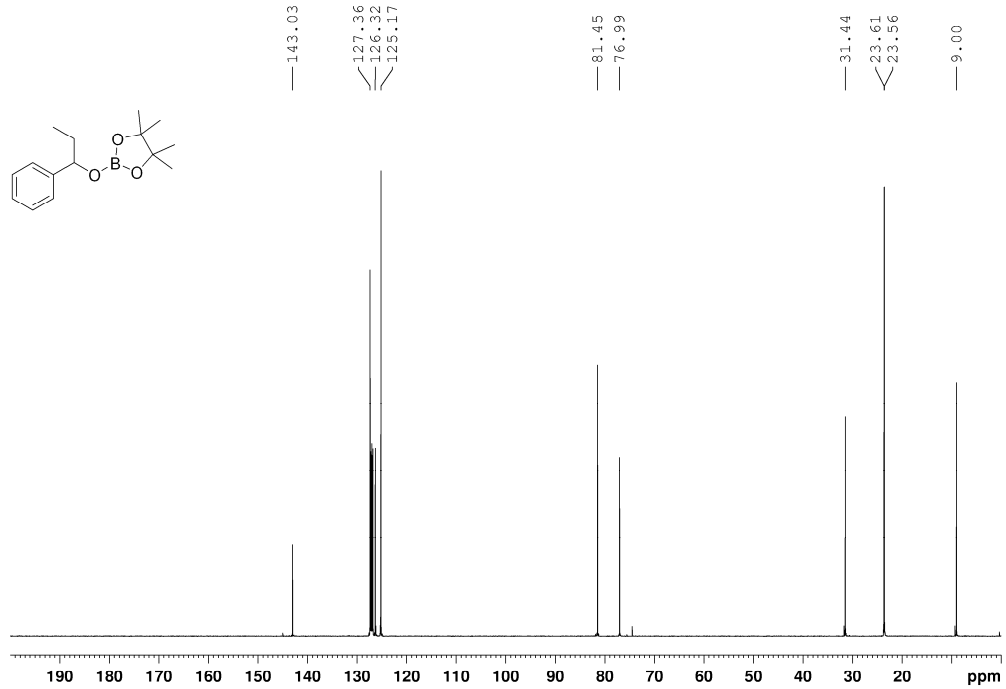

7.131
7.128
7.124
7.115
7.111
7.108
6.907
6.894
6.891
5.021
5.008
4.995
4.982
2.553
1.092
1.079
0.762
0.732
O
B
O
O
H
11
10
9
8
7
6
5
4
3
2
1
ppm
1.94
2.07
1.00
0.78
3.08
12.11

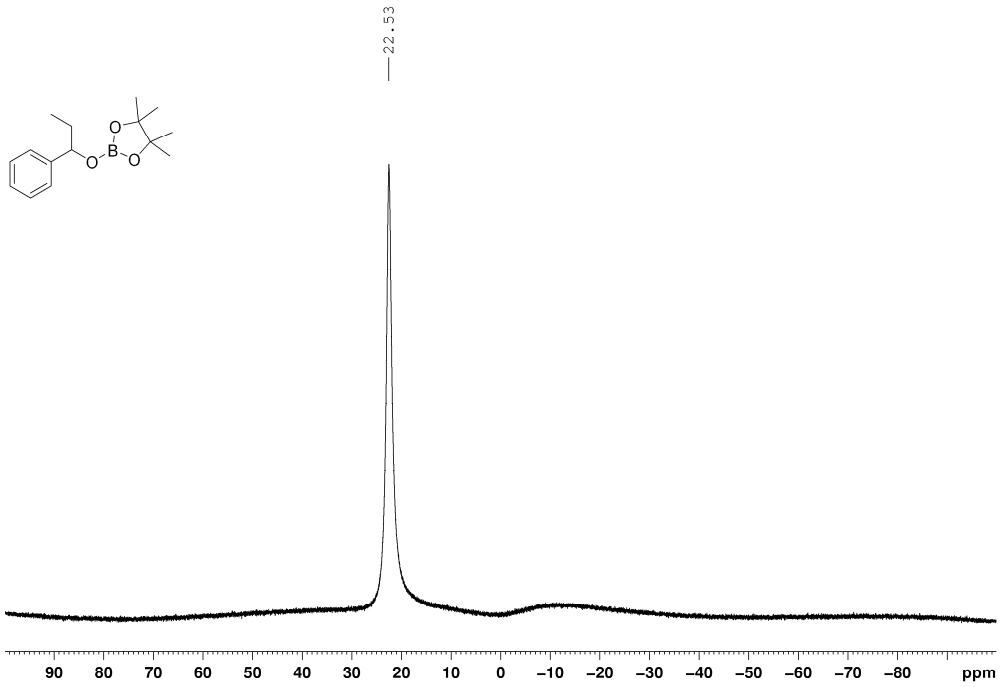

145.93
132.34
125.64
121.41
83.89
82.62
77.59
72.43
25.39
24.60
24.51
O
B
O
O
H
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


22.40
O
B
O
O
H
90
80
70
60
50
40
30
20
10
0
−10
−20
−30
−40
−50
−60
−70
−80
ppm

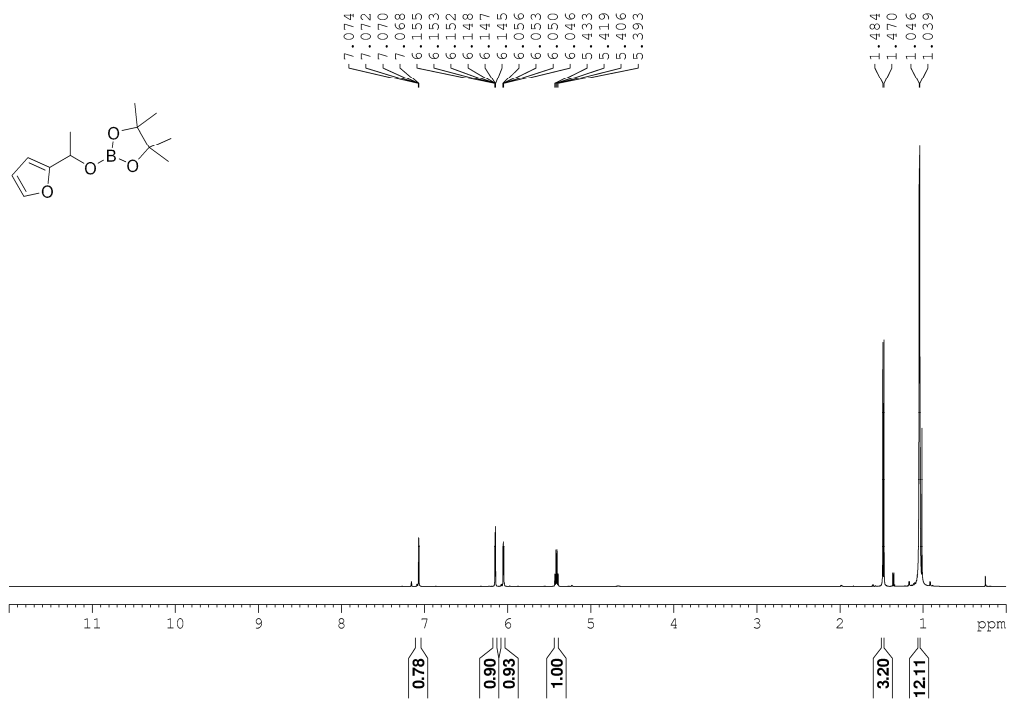
4i

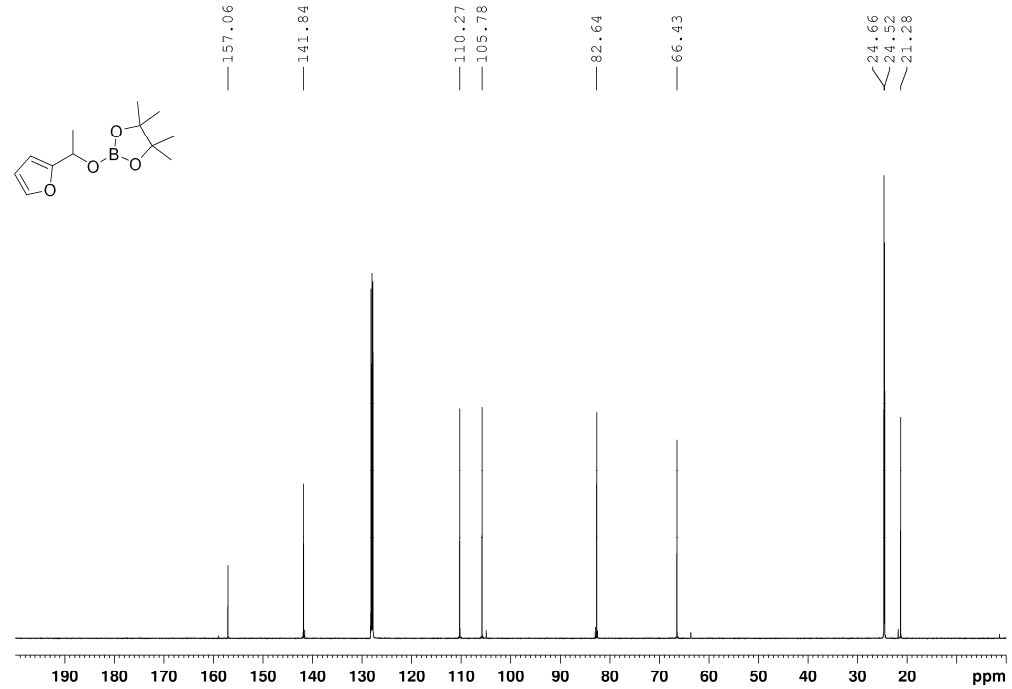

7.088
7.086
7.083
7.073
7.072
7.070
6.921
6.917
6.906
6.904
6.894
6.891
6.887
6.838
6.836
6.833
6.825
6.821
6.817
6.809
6.806
6.804
4.923
4.912
4.908
4.897
1.597
1.582
1.567
1.555
1.553
1.547
1.540
1.532
1.525
1.520
1.513
1.510
1.505
1.502
1.498
1.487
1.483
1.472
1.471
1.468
1.460
1.457
1.456
1.445
1.441
1.430
0.796
0.764
0.633
0.618
0.604
O
B
O
O
11
10
9
8
7
6
5
4
3
2
1
ppm
2.03
2.04
0.96
1.00
2.19
12.10
3.14

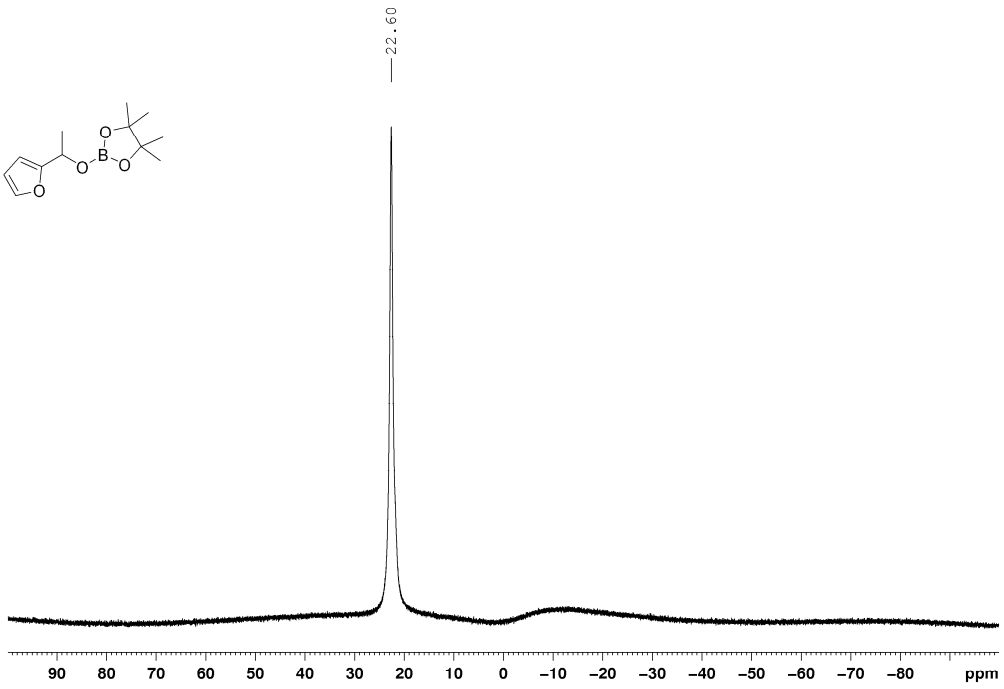

143.03
127.36
126.32
125.17
81.45
76.99
31.44
23.61
23.56
9.00
O
B
O
O
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


22.53
O
B
O
O
90
80
70
60
50
40
30
20
10
0
−10
−20
−30
−40
−50
−60
−70
−80
ppm

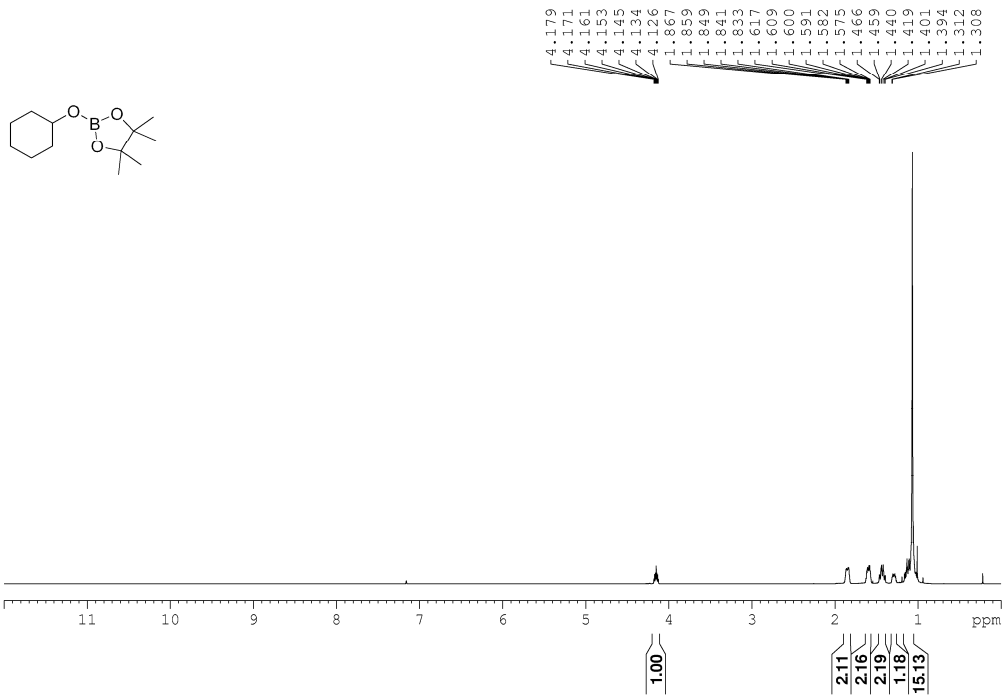
4j

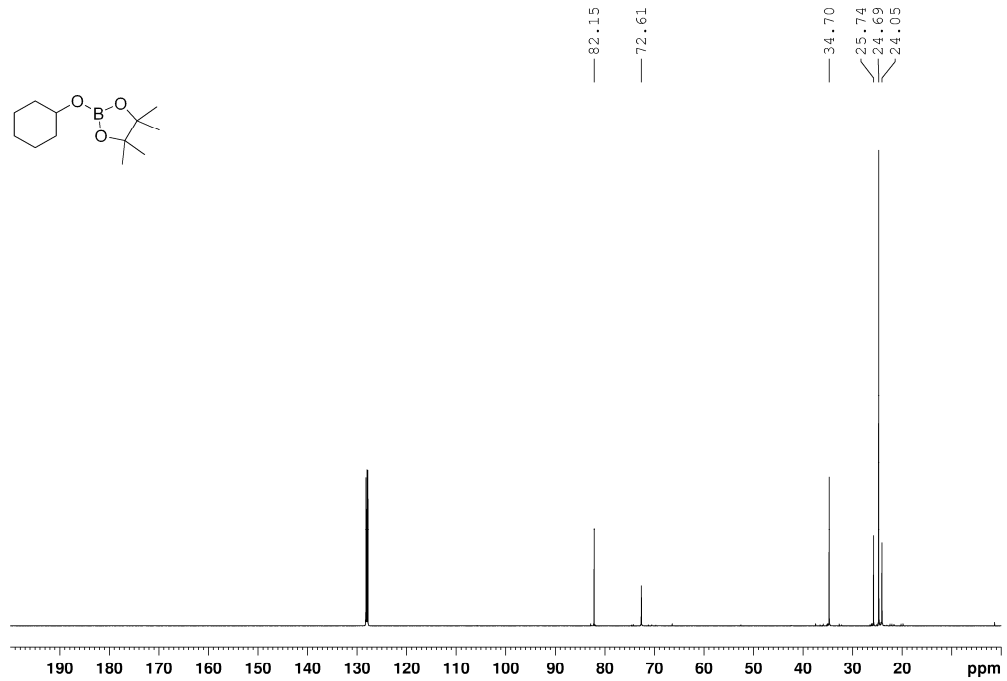

7.074
7.072
7.070
7.068
6.155
6.153
6.152
6.148
6.147
6.145
6.056
6.053
6.050
6.046
5.433
5.419
5.406
5.393
1.484
1.470
1.046
1.039
O
B
O
O
11
10
9
8
7
6
5
4
3
2
1
ppm
0.78
0.90
0.93
1.00
3.20
12.11

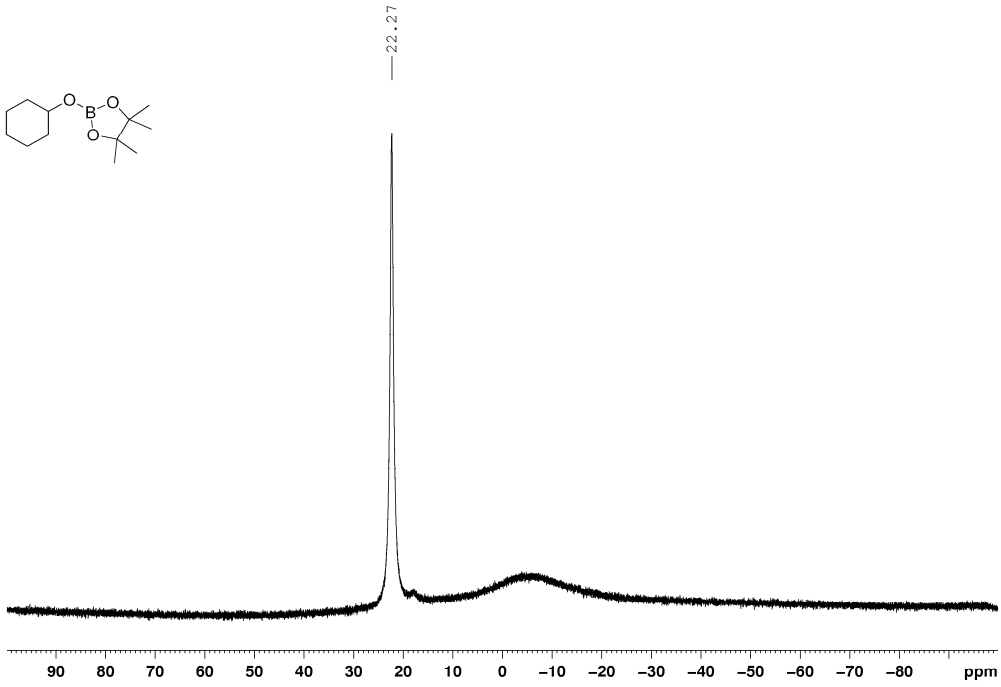

157.06
141.84
110.27
105.78
82.64
66.43
24.66
24.52
21.28
O
B
O
O
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


22.60
O
B
O
O
90
80
70
60
50
40
30
20
10
0
−10
−20
−30
−40
−50
−60
−70
−80
ppm

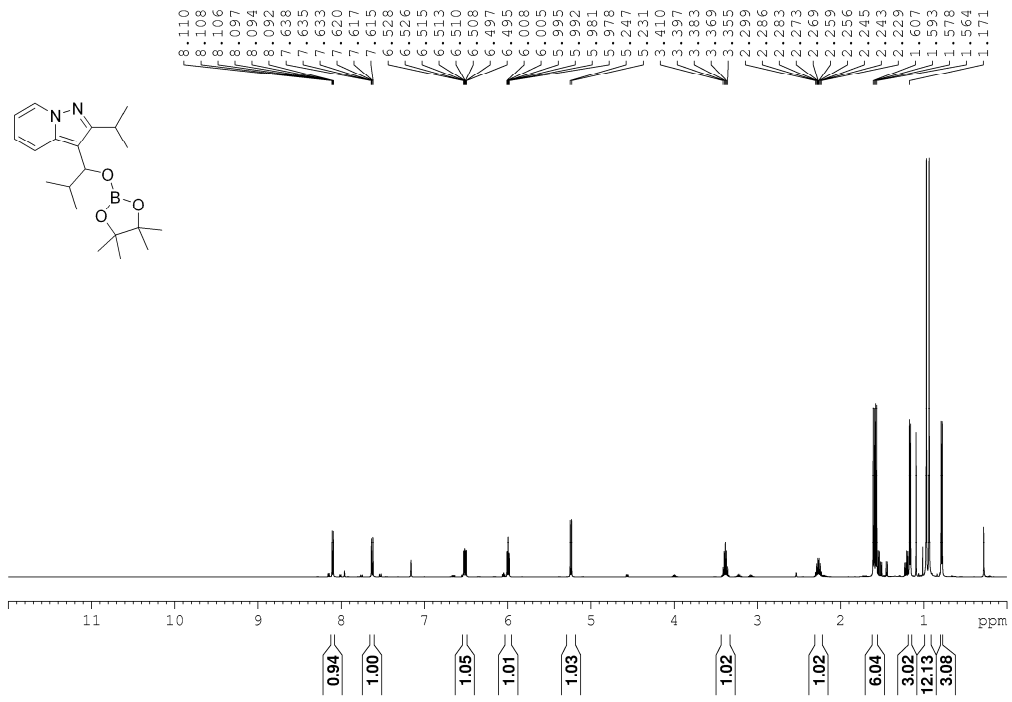
4k

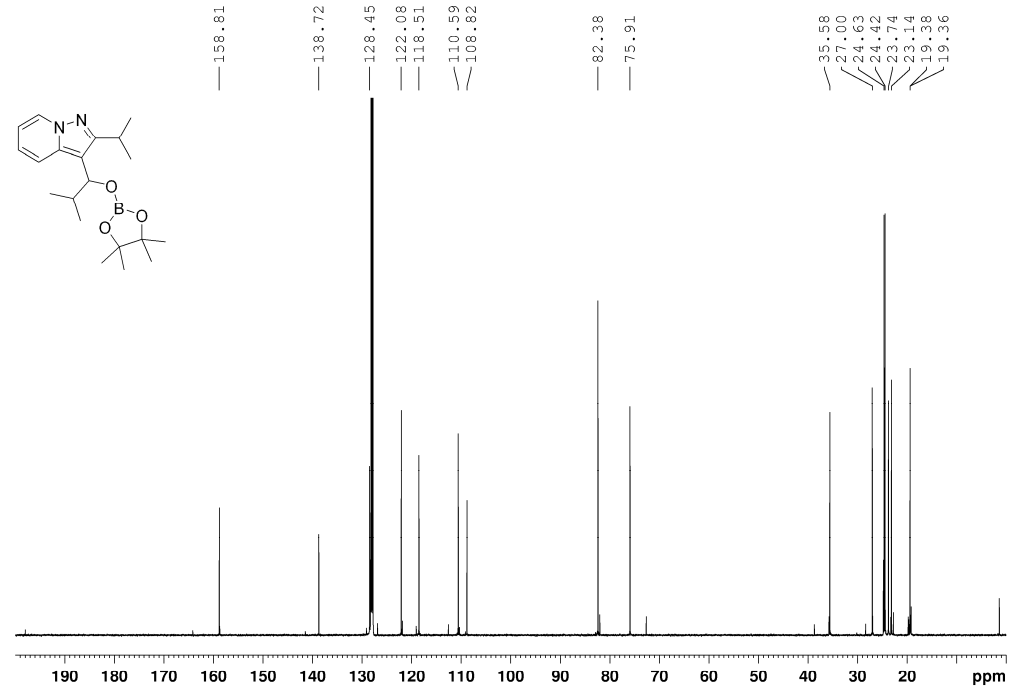

4.179
4.171
4.161
4.153
4.145
4.134
4.126
1.867
1.859
1.849
1.841
1.833
1.617
1.609
1.600
1.591
1.582
1.575
1.466
1.459
1.440
1.419
1.401
1.394
1.312
1.308
11
10
9
8
7
6
5
4
3
2
1
ppm
1.00
2.11
2.16
2.19
1.18
15.13

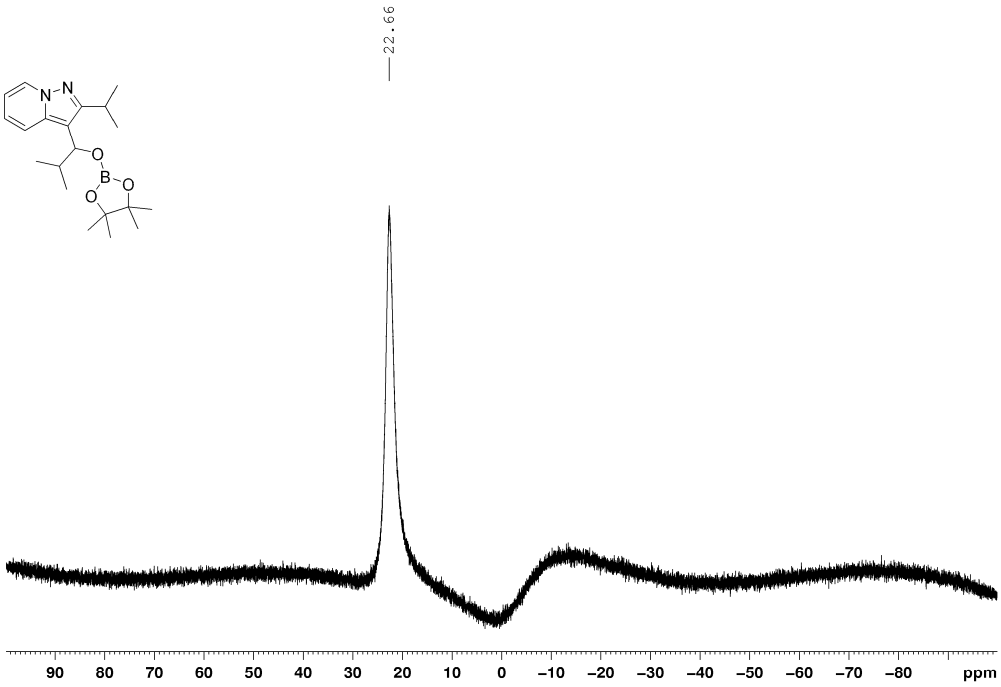

82.15
72.61
34.70
25.74
24.69
24.05
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


22.27
O
B
O
O
90
80
70
60
50
40
30
20
10
0
−10
−20
−30
−40
−50
−60
−70
−80
ppm

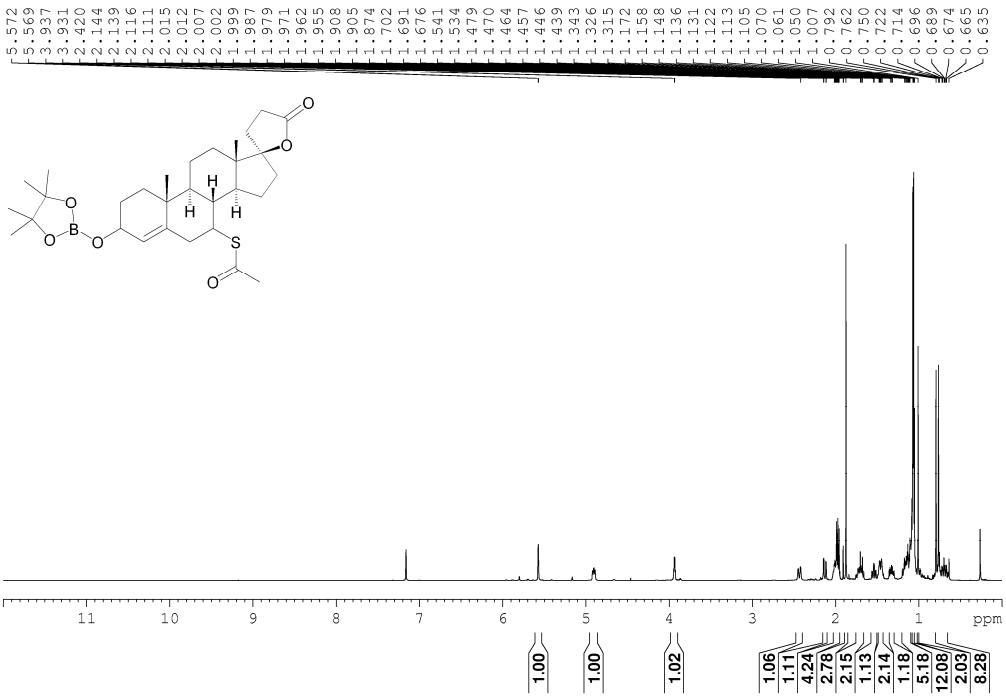
4l

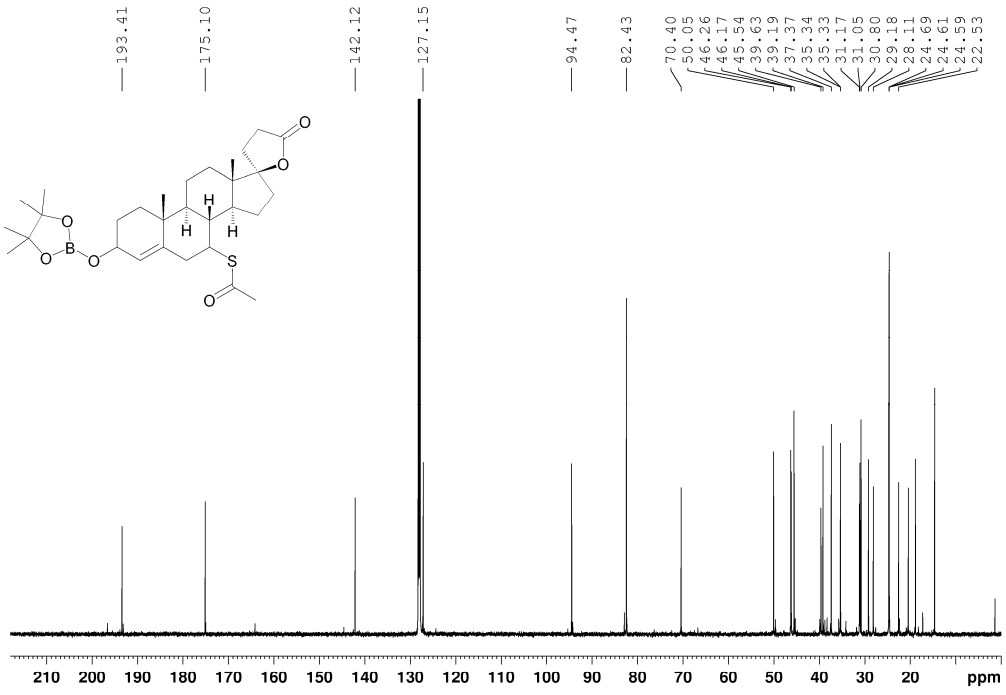

8.110
8.108
8.106
8.097
8.094
8.092
7.638
7.635
7.633
7.620
7.617
7.615
6.528
6.526
6.515
6.513
6.510
6.508
6.497
6.495
6.008
6.005
5.995
5.992
5.981
5.978
5.247
5.231
3.410
3.397
3.383
3.369
3.355
2.299
2.286
2.283
2.273
2.269
2.259
2.256
2.245
2.243
2.229
1.607
1.593
1.578
1.564
1.171
11
10
9
8
7
6
5
4
3
2
1
ppm
0.94
1.00
1.05
1.01
1.03
1.02
1.02
6.04
3.02
12.13
3.08

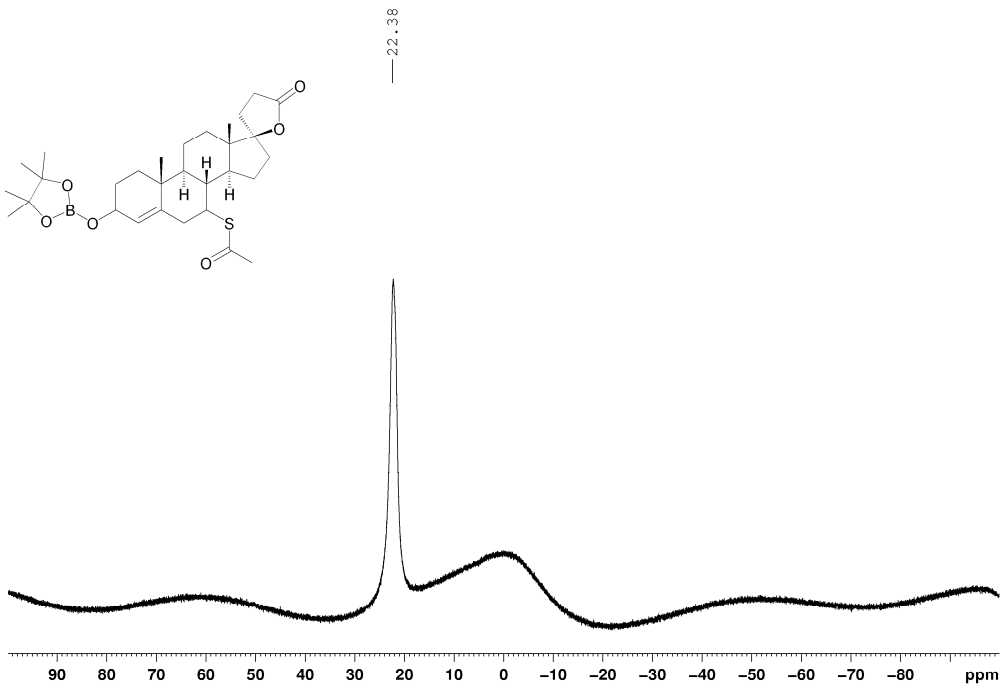

158.81
138.72
128.45
122.08
118.51
110.59
108.82
82.38
75.91
35.58
27.00
24.63
24.42
23.74
23.14
19.38
19.36
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


22.66
N
N
O
B
O
O
90
80
70
60
50
40
30
20
10
0
−10
−20
−30
−40
−50
−60
−70
−80
ppm

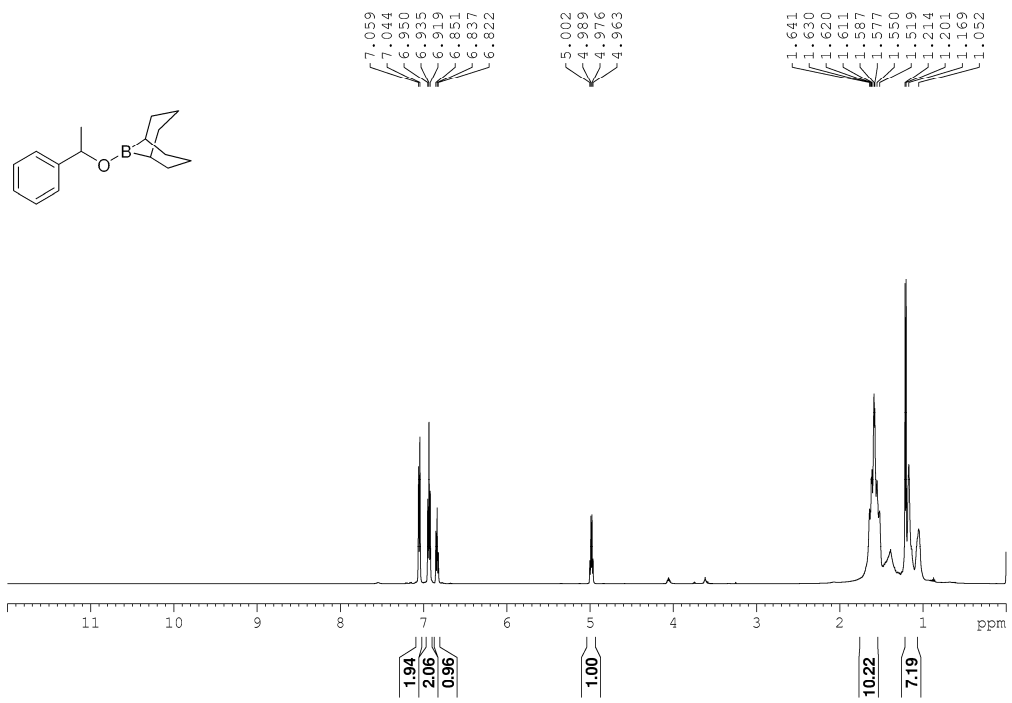
4m


5.572
5.569
3.937
3.931
2.420
2.144
2.139
2.116
2.111
2.015
2.012
2.007
2.002
1.999
1.987
1.979
1.971
1.962
1.955
1.908
1.905
1.874
1.702
1.691
1.676
1.541
1.534
1.479
1.470
1.464
1.457
1.446
1.439
1.343
1.326
1.315
1.172
1.158
1.148
1.136
1.131
1.122
1.113
1.105
1.070
1.061
1.050
1.007
0.792
0.762
0.750
0.722
0.714
0.696
0.689
0.674
0.665
0.635
ppm
1.00
1.00
1.02
1.06
1.11
4.24
2.78
2.15
1.13
2.14
1.18
5.18
12.08
2.03
8.28


193.41
175.10
142.12
127.15
94.47
82.43
70.40
50.05
46.26
46.17
45.54
39.63
39.19
37.37
35.34
35.33
31.17
31.05
30.80
29.18
28.11
24.69
24.61
24.59
22.53
ppm


22.38
O
O
H
H
H
O
B
O
O
S
O
90
80
70
60
50
40
30
20
10
0
−10
−20
−30
−40
−50
−60
−70
−80
ppm

4n


7.059
7.044
6.950
6.935
6.919
6.851
6.837
6.822
5.002
4.989
4.976
4.963
1.641
1.630
1.620
1.611
1.587
1.577
1.550
1.519
1.214
1.201
1.169
1.052
B
O
11
10
9
8
7
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5
4
3
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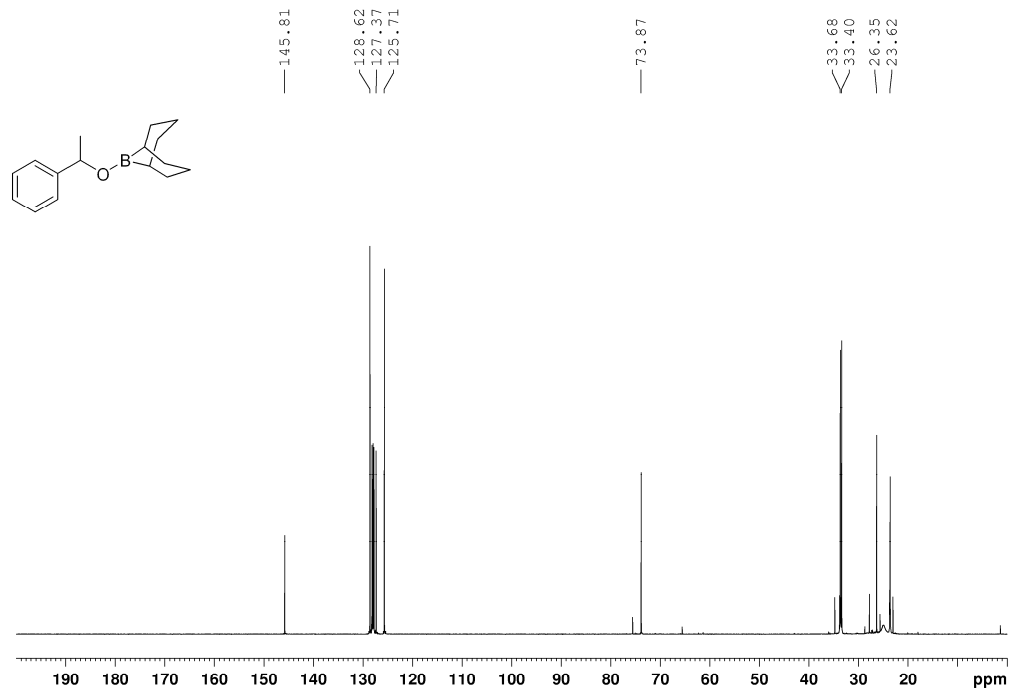
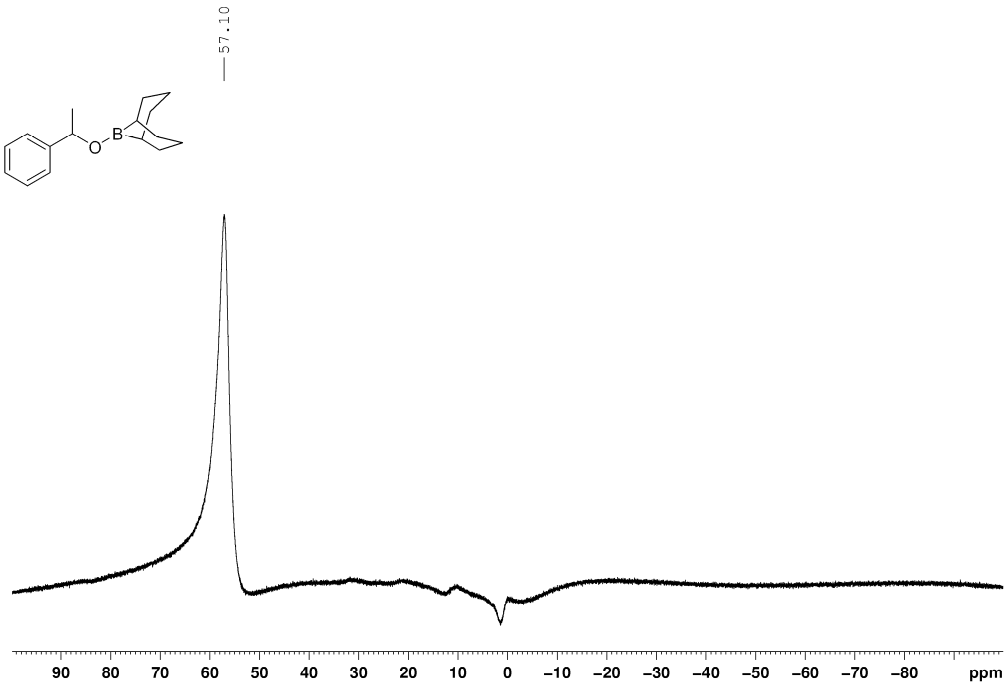
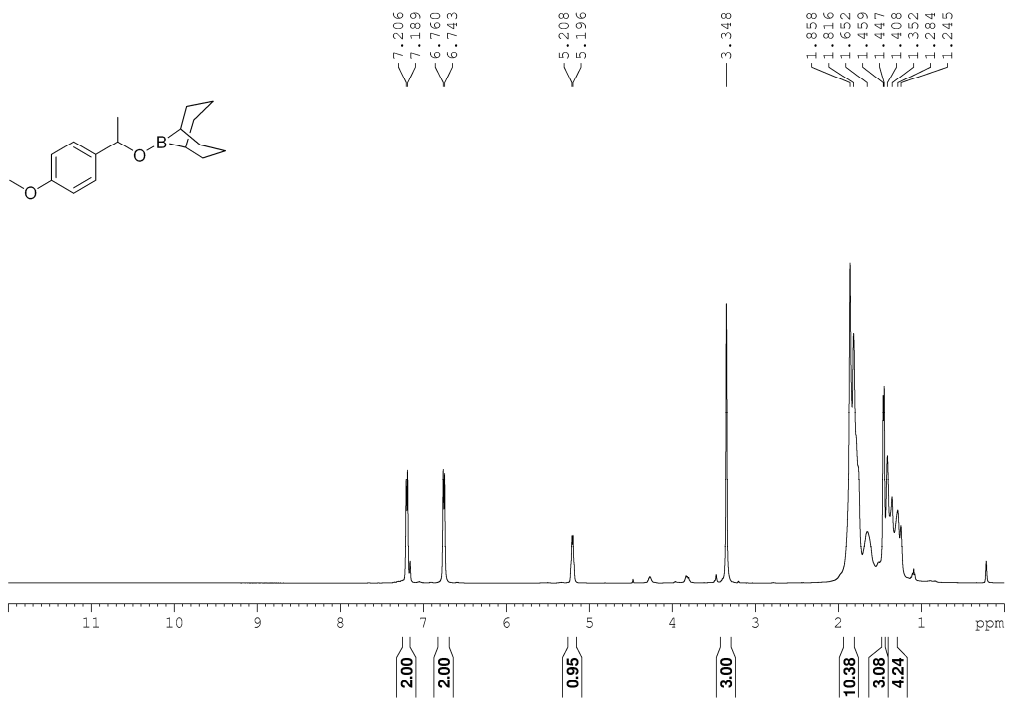
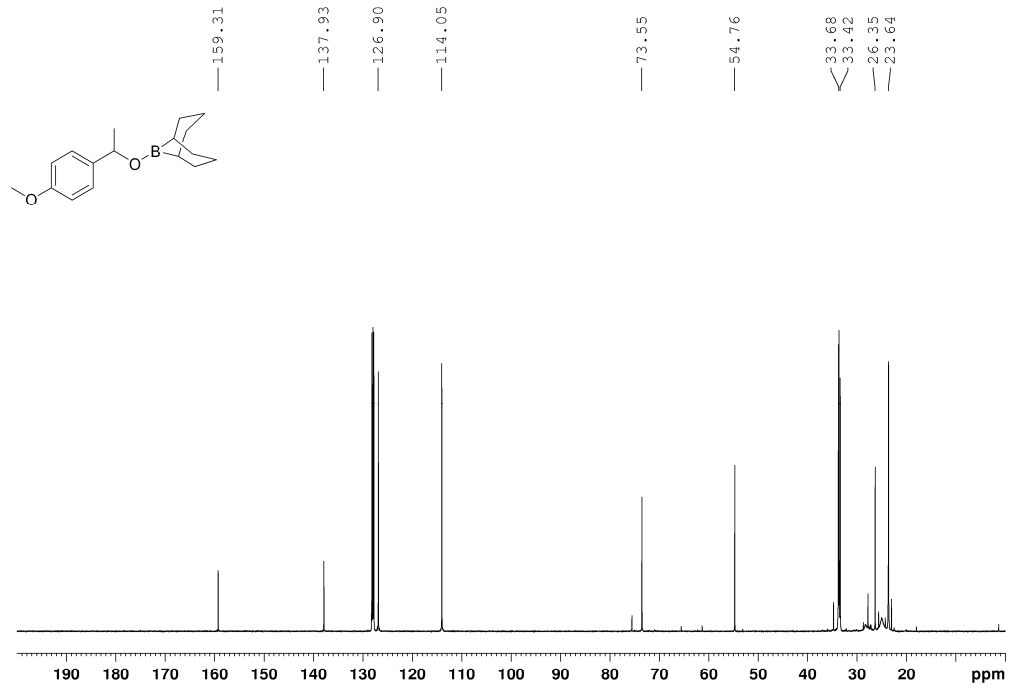
ppm
1.94
2.06
0.96
1.00
10.22
7.19

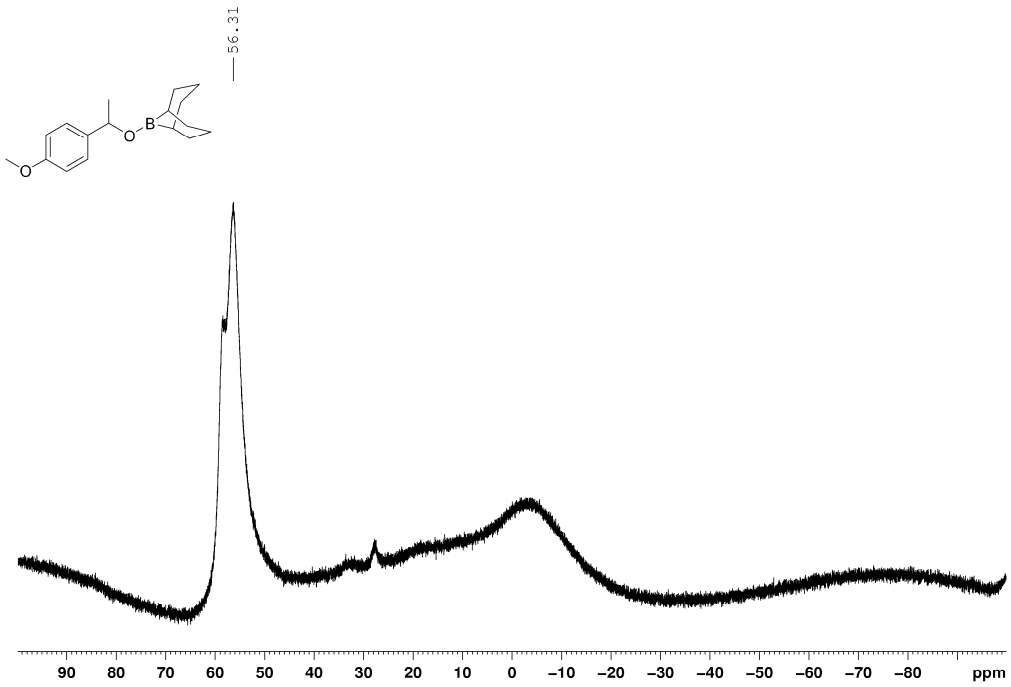

145.81
128.62
127.37
125.71
73.87
33.68
33.40
26.35
23.62
B
O
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


57.10
B
O
90
80
70
60
50
40
30
20
10
0
−10
−20
−30
−40
−50
−60
−70
−80
ppm

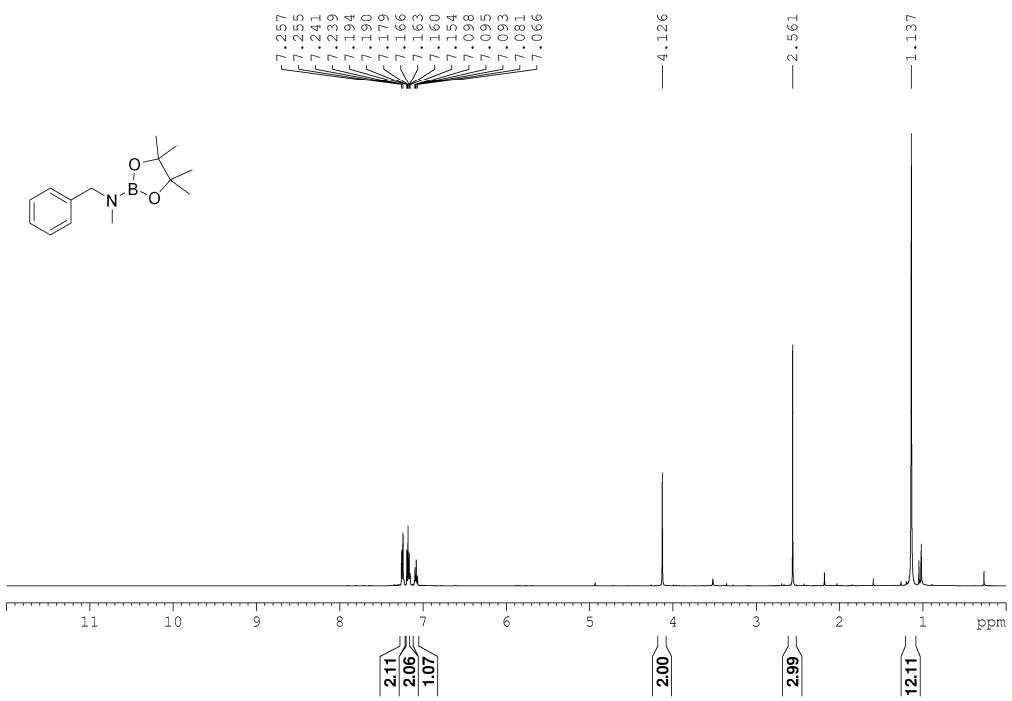
4o

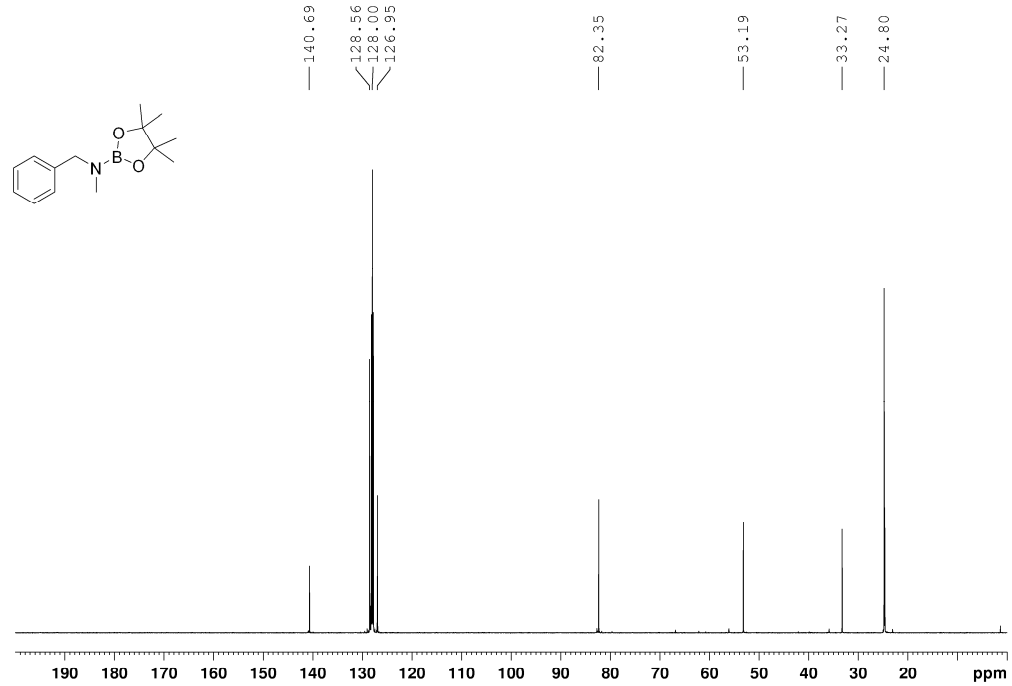

7.206
7.189
6.760
6.743
5.208
5.196
3.348
1.858
1.816
1.652
1.459
1.447
1.408
1.352
1.284
1.245
O
B
O
11
10
9
8
7
6
5
4
3
2
1
ppm
2.00
2.00
0.95
3.00
10.38
3.08
4.24

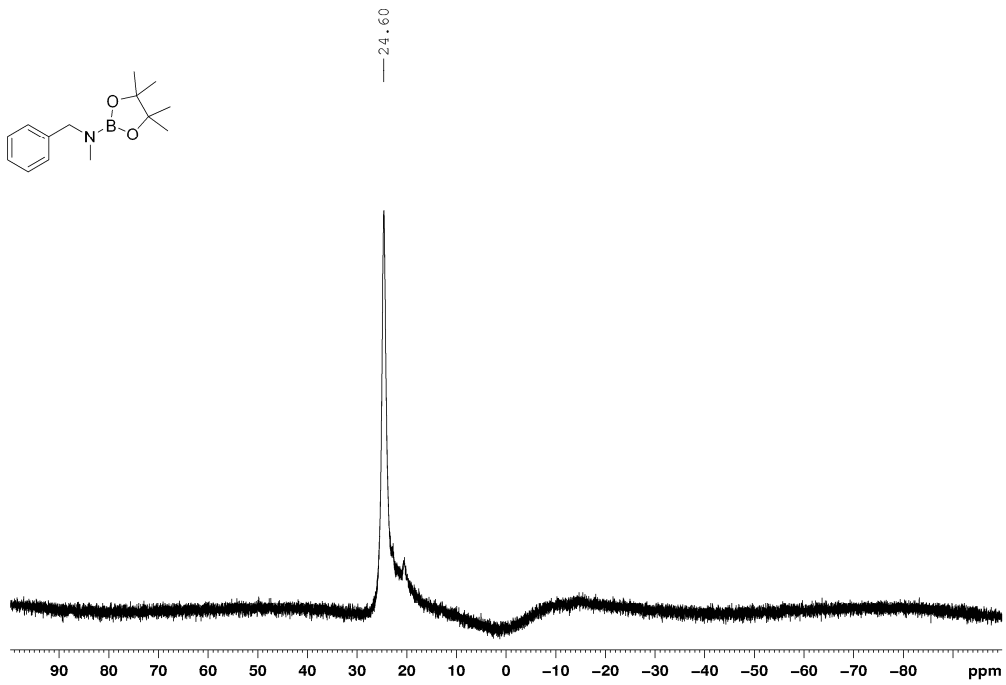

159.31
137.93
126.90
114.05
73.55
54.76
33.68
33.42
26.35
23.64
O
B
O
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


56.31
O
B
O
90
80
70
60
50
40
30
20
10
0
−10
−20
−30
−40
−50
−60
−70
−80
ppm

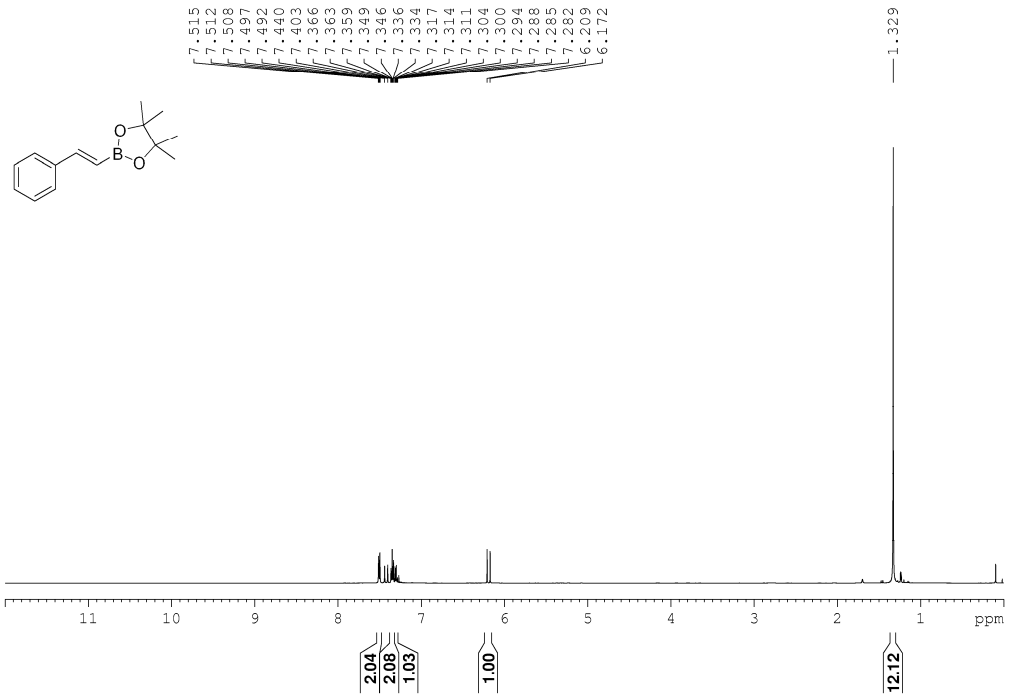
4p

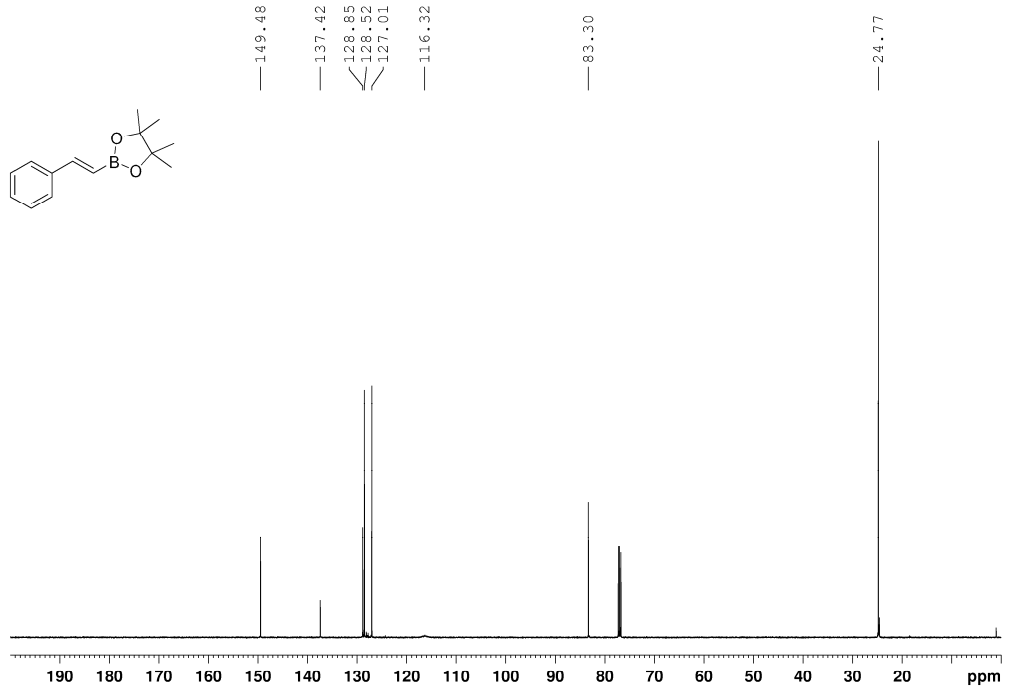

7.257
7.255
7.241
7.239
7.194
7.190
7.179
7.166
7.163
7.160
7.154
7.098
7.095
7.093
7.081
7.066
4.126
2.561
1.137
11
10
9
8
7
6
5
4
3
2
1
ppm
2.11
2.06
1.07
2.00
2.99
12.11


140.69
128.56
128.00
126.95
82.35
53.19
33.27
24.80
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


24.60
O
B
O
N
90
80
70
60
50
40
30
20
10
0
−10
−20
−30
−40
−50
−60
−70
−80
ppm

6a


7.515
7.512
7.508
7.497
7.492
7.440
7.403
7.366
7.363
7.359
7.349
7.346
7.336
7.334
7.317
7.314
7.311
7.304
7.300
7.294
7.288
7.285
7.282
6.209
6.172
1.329
O
B
O
11
10
9
8
7
6
5
4
3
2
1
ppm
2.04
2.08
1.03
1.00
12.12


149.48
137.42
128.85
128.52
127.01
116.32
83.30
24.77
O
B
O
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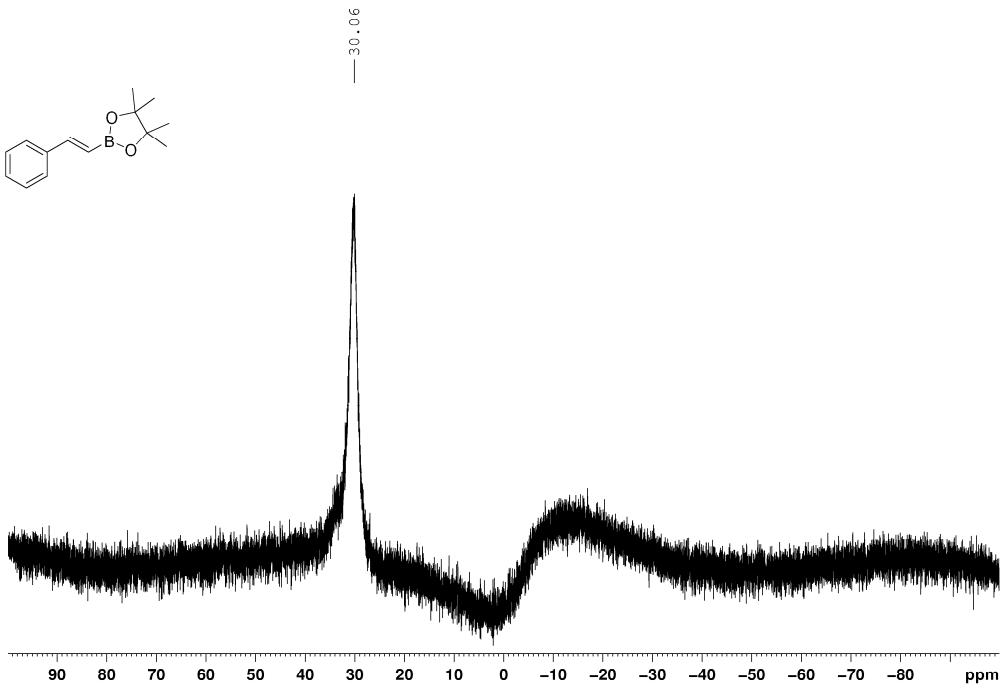
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


30.06
O
B
O
90
80
70
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50
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30
20
10
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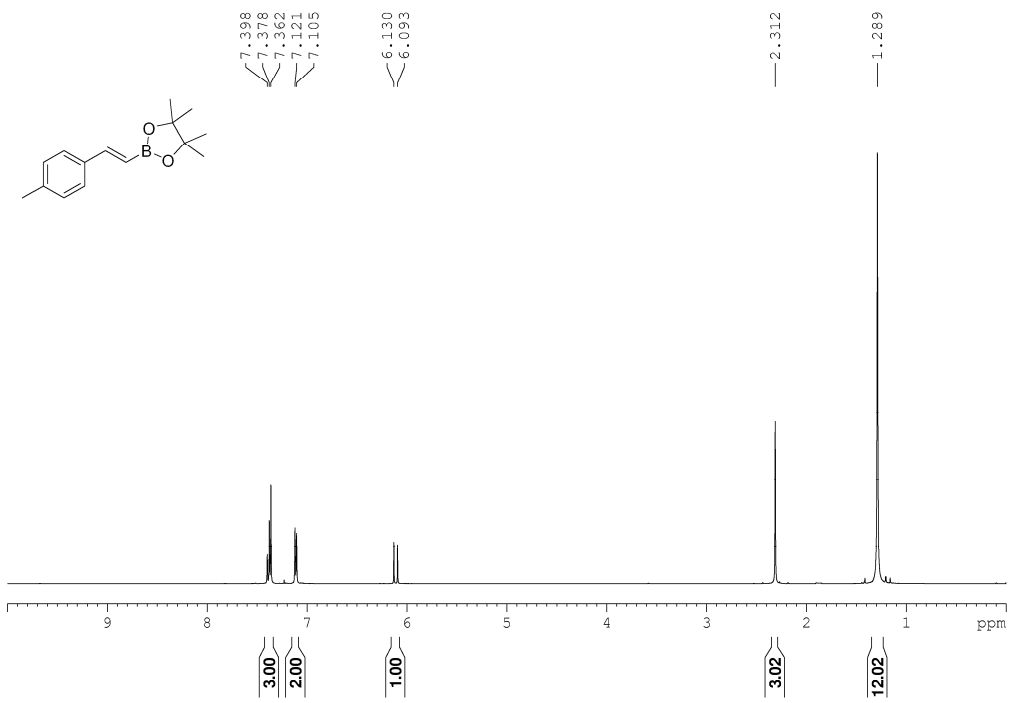
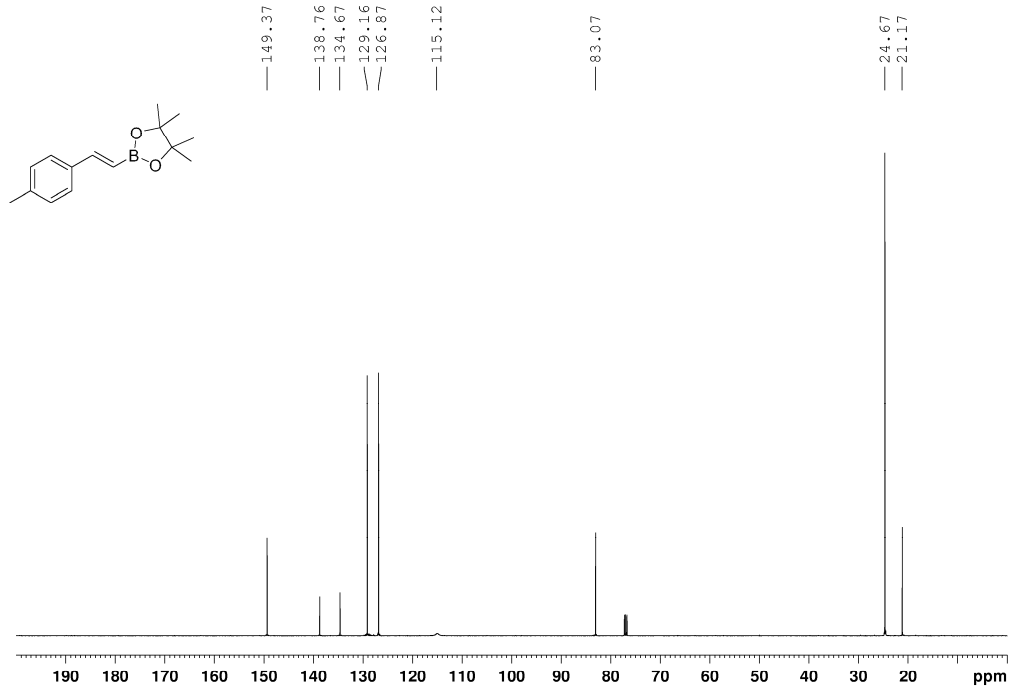
−20
−30
−40
−50
−60
−70
−80
ppm

6b


7.398
7.378
7.362
7.121
7.105
6.130
6.093
2.312
1.289
O
B
O
9
8
7
6
5
4
3
2
1
ppm
3.00
2.00
1.00
3.02
12.02


149.37
138.76
134.67
129.16
126.87
115.12
83.07
24.67
21.17
O
B
O
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180
170
160
150
140
130
120
110
100
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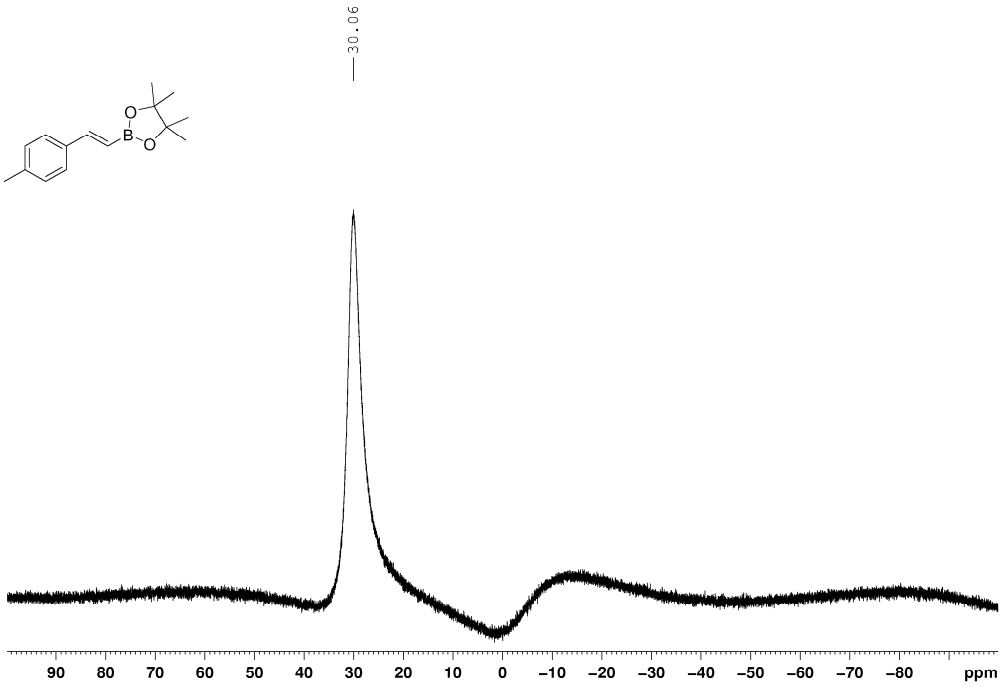
80
70
60
50
40
30
20
ppm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O
B
O
90
80
70
60
50
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30
20
10
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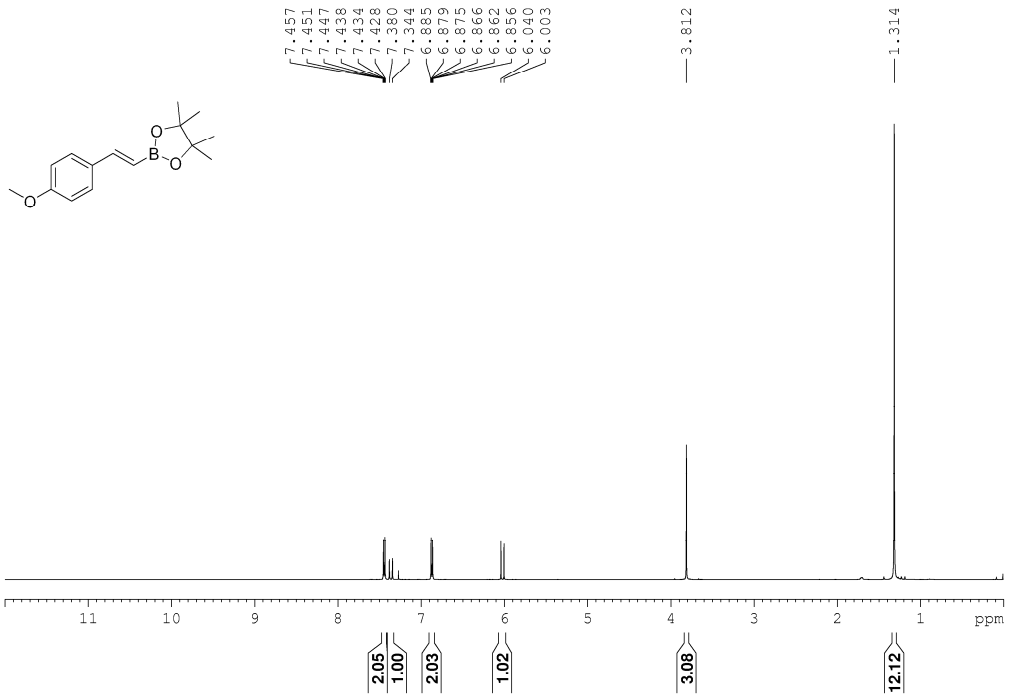
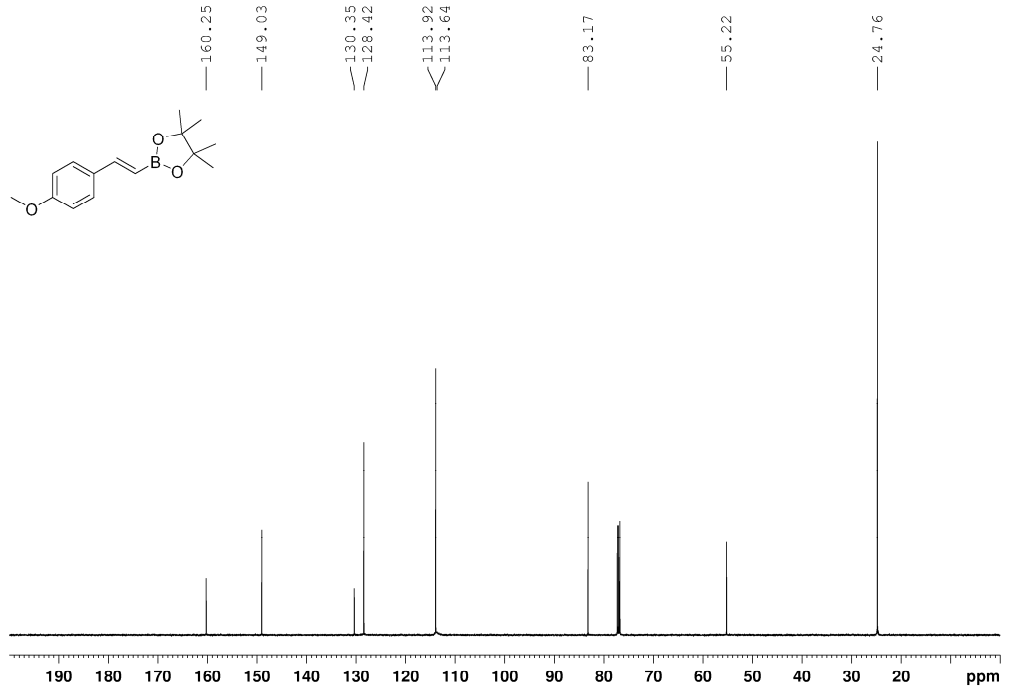
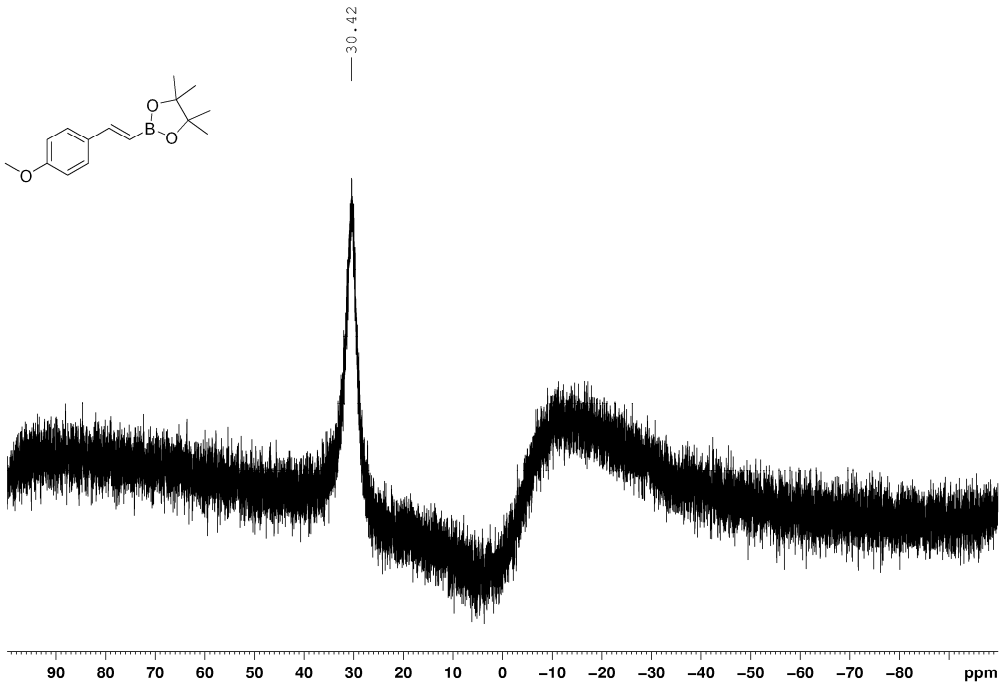
−10
−20
−30
−40
−50
−60
−70
−80
ppm

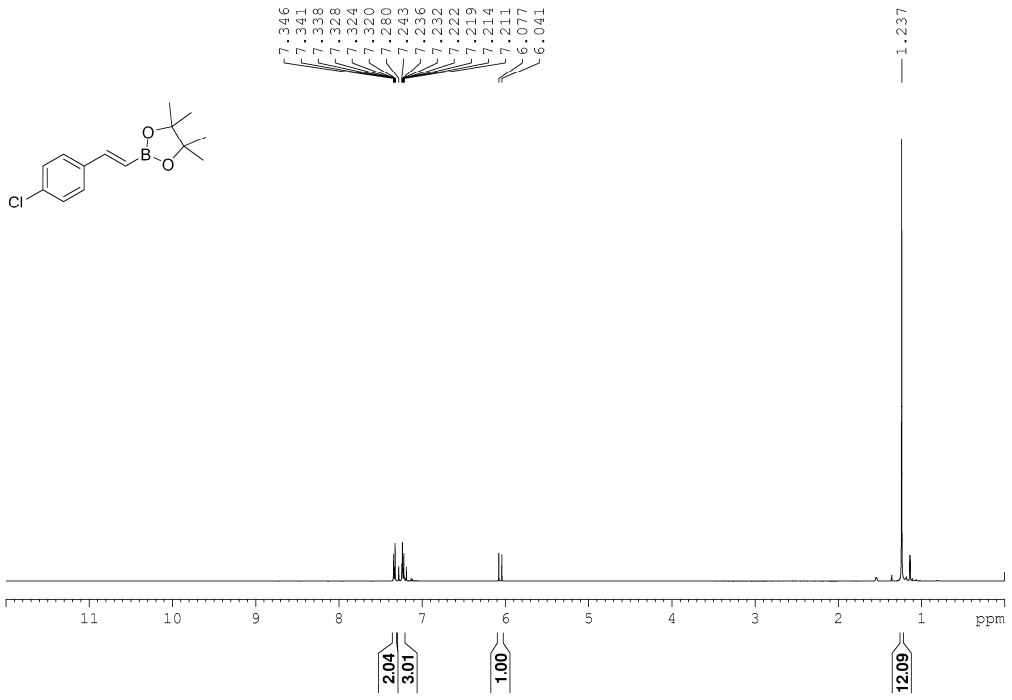
6c


7.457
7.451
7.447
7.438
7.434
7.428
7.380
7.344
6.885
6.879
6.875
6.866
6.862
6.856
6.040
6.003
3.812
1.314
O
B
O
O
11
10
9
8
7
6
5
4
3
2
1
ppm
2.05
1.00
2.03
1.02
3.08
12.12


160.25
149.03
130.35
128.42
113.92
113.64
83.17
55.22
24.76
O
B
O
O
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


30.42
O
B
O
O
90
80
70
60
50
40
30
20
10
0
−10
−20
−30
−40
−50
−60
−70
−80
ppm

6d


7.346
7.341
7.338
7.328
7.324
7.320
7.280
7.243
7.236
7.232
7.222
7.219
7.214
7.211
6.077
6.041
1.237
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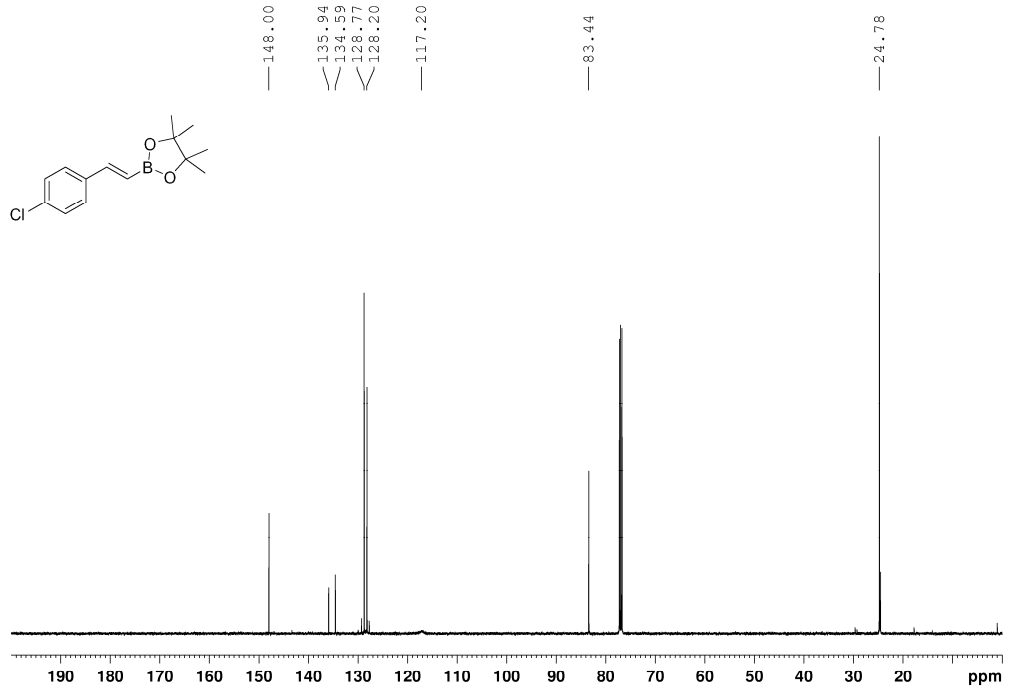
3.01
1.00
12.09


148.00
135.94
134.59
128.77
128.20
117.20
83.44
24.78
Cl
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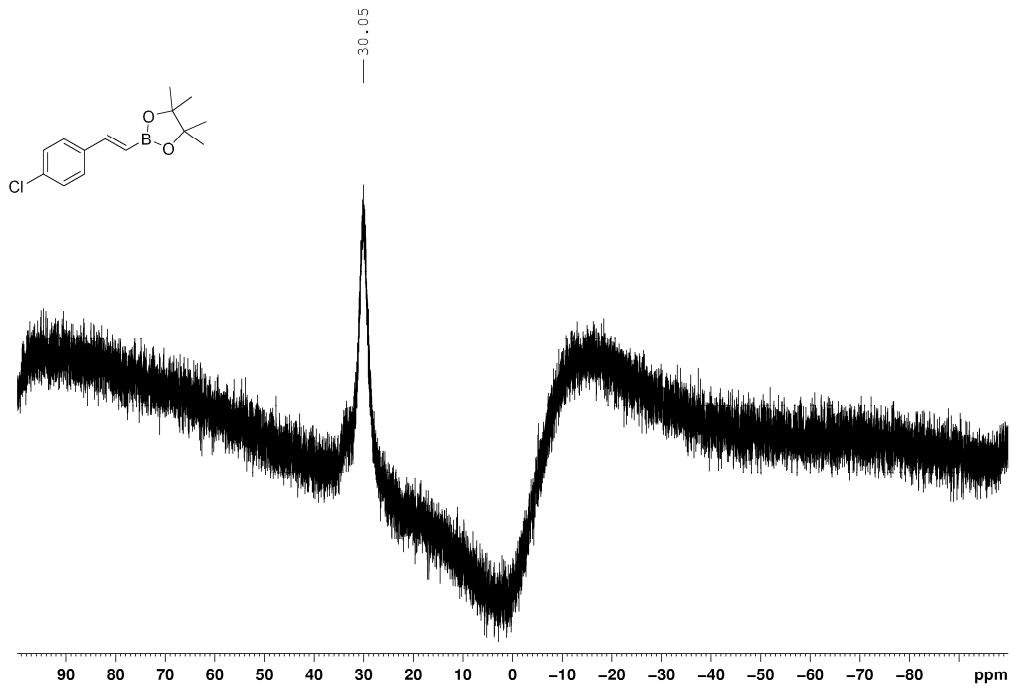
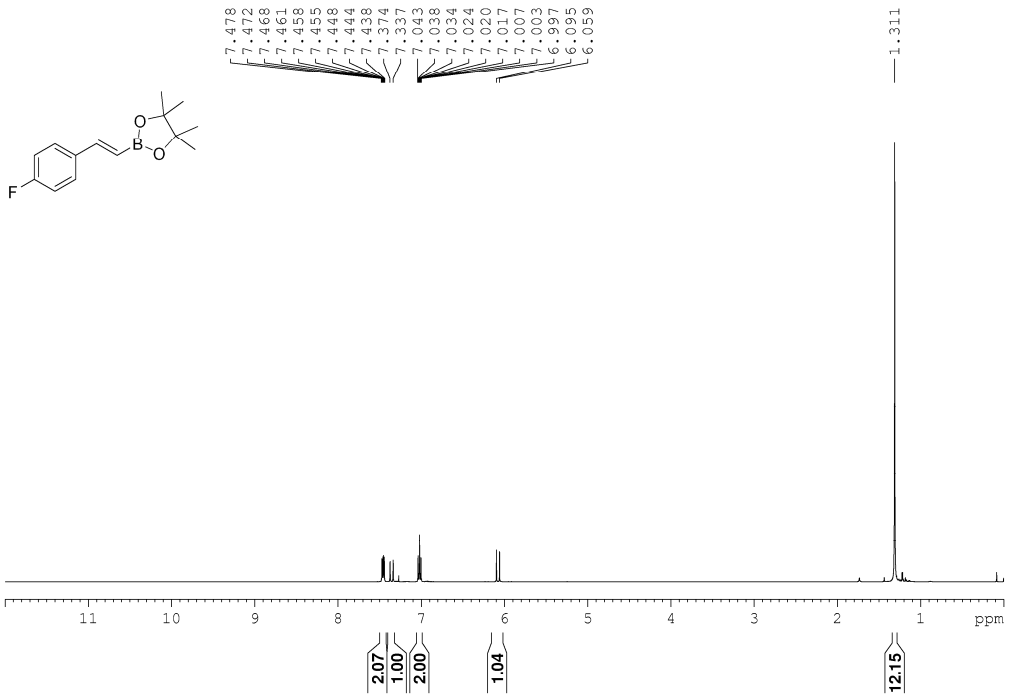
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


30.05
O
B
O
Cl
90
80
70
60
50
40
30
20
10
0
−10
−20
−30
−40
−50
−60
−70
−80
ppm

6e


7.478
7.472
7.468
7.461
7.458
7.455
7.448
7.444
7.438
7.374
7.337
7.043
7.038
7.034
7.024
7.020
7.017
7.007
7.003
6.997
6.095
6.059
1.311
O
B
O
F
11
10
9
8
7
6
5
4
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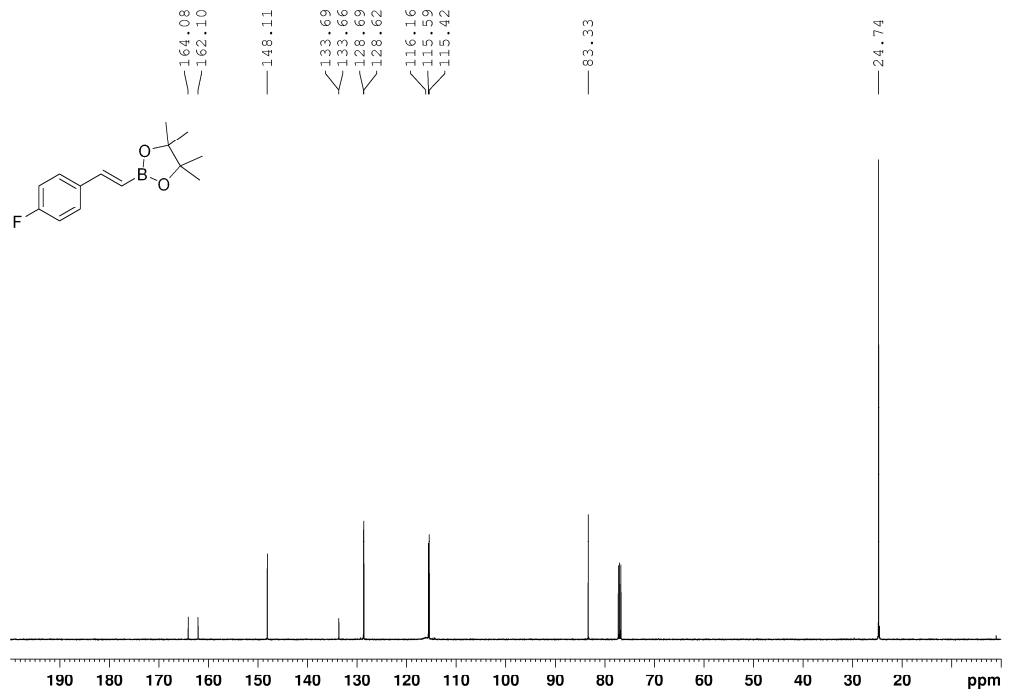
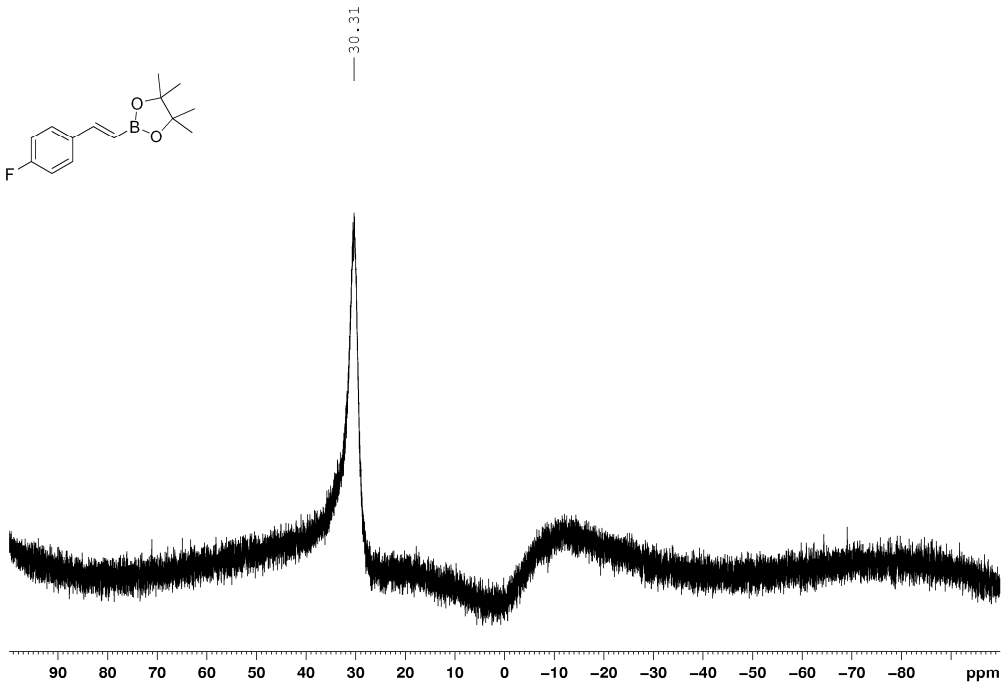
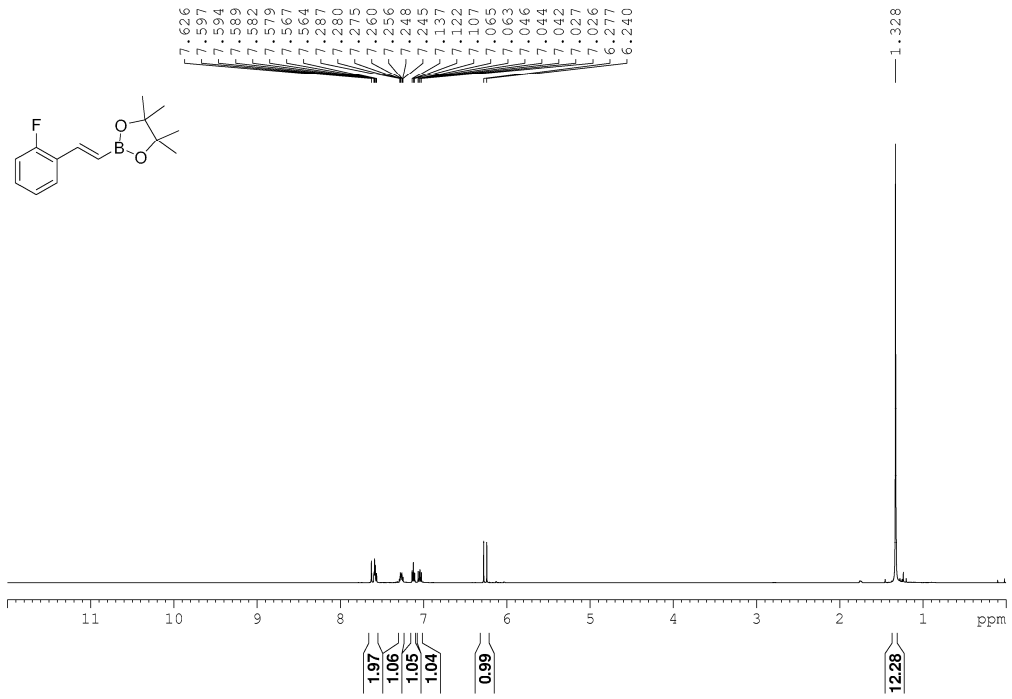
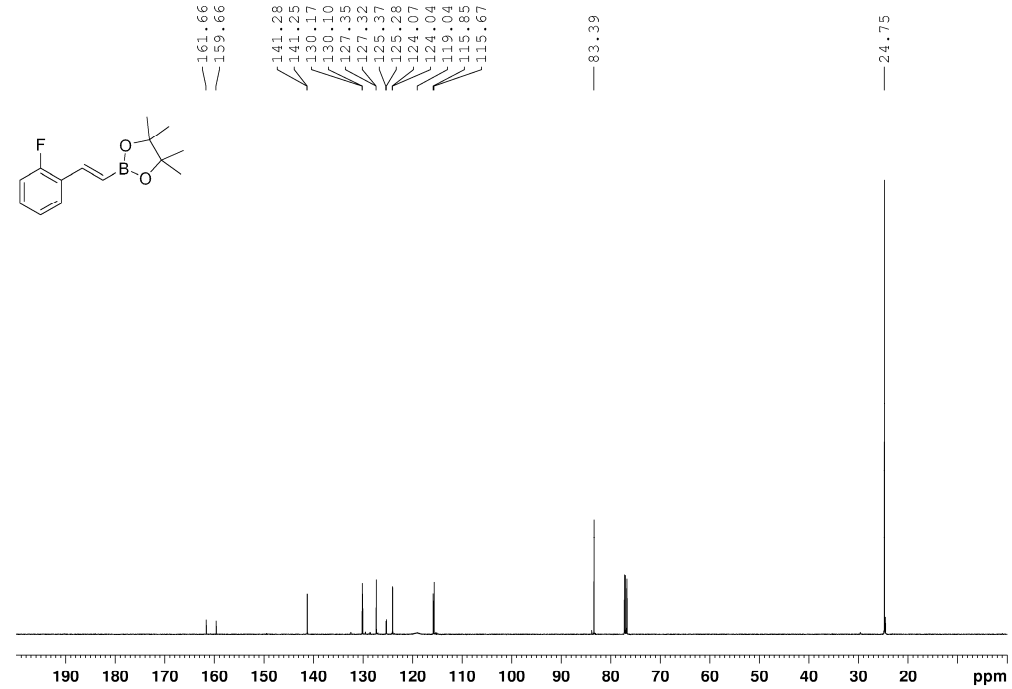
2.00
1.04
12.15

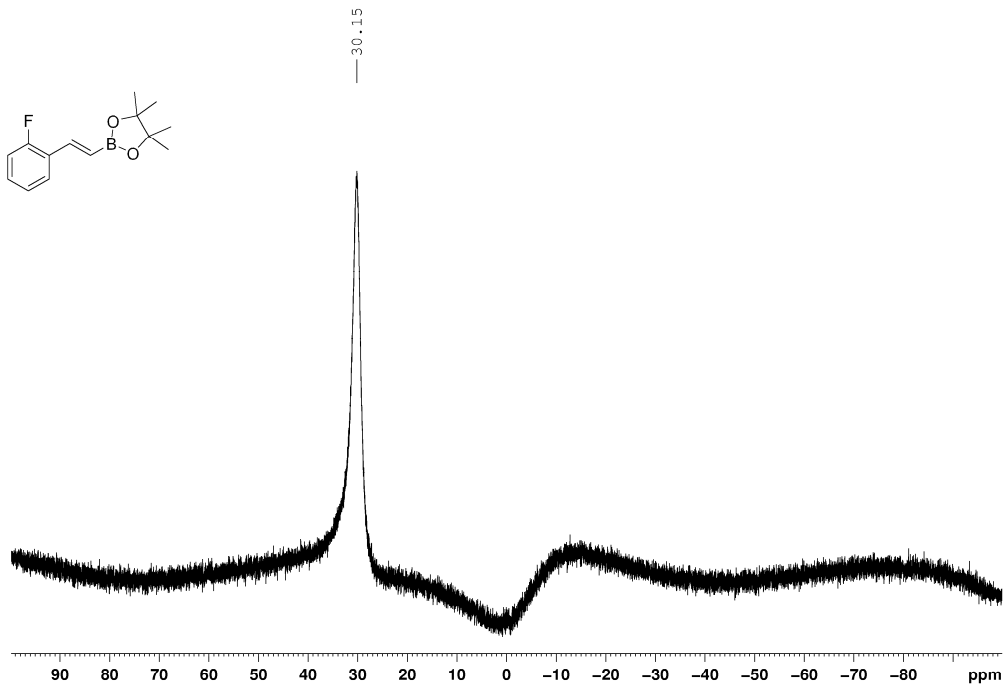

164.08
162.10
148.11
133.69
133.66
128.69
128.62
116.16
115.59
115.42
83.33
24.74
O
B
O
F
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


30.31
O
B
O
F
90
80
70
60
50
40
30
20
10
0
−10
−20
−30
−40
−50
−60
−70
−80
ppm

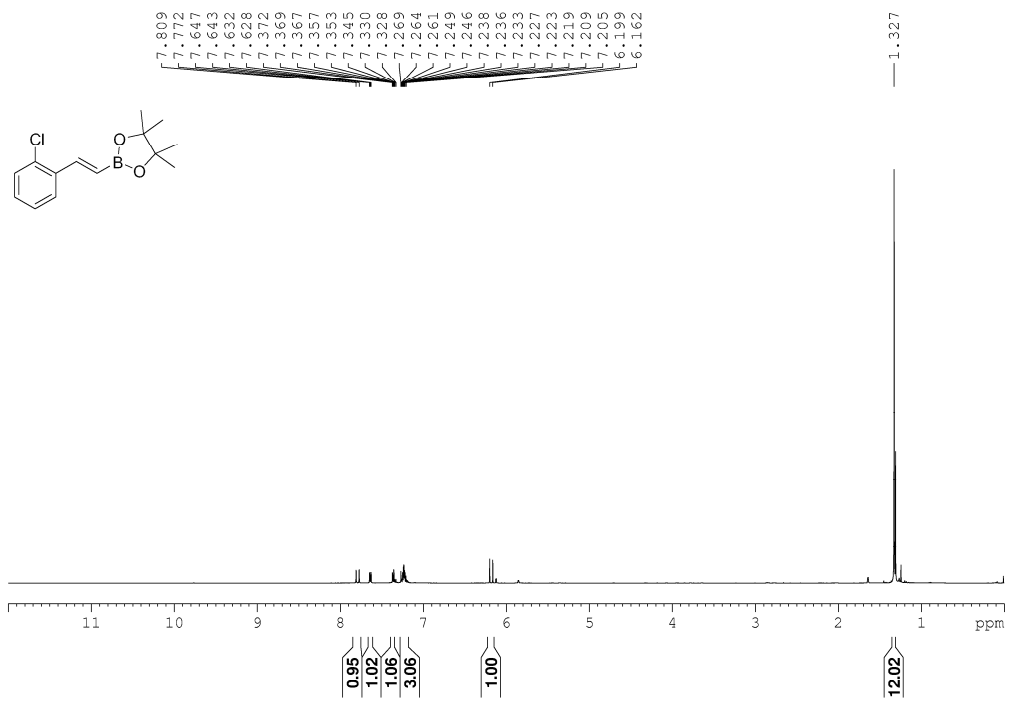
6f

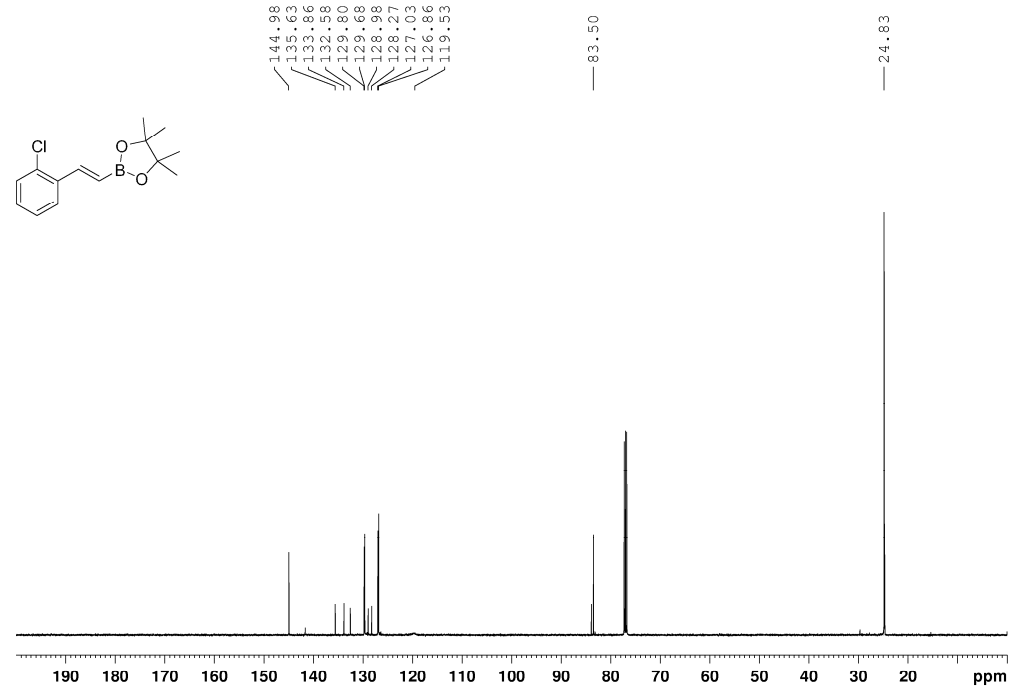

7.626
7.597
7.594
7.589
7.582
7.579
7.567
7.564
7.287
7.280
7.275
7.260
7.256
7.248
7.245
7.137
7.122
7.107
7.065
7.063
7.046
7.044
7.042
7.027
7.026
6.277
6.240
1.328
F
O
B
O
11
10
9
8
7
6
5
4
3
2
1
ppm
1.97
1.06
1.05
1.04
0.99
12.28


161.66
159.66
141.28
141.25
130.17
130.10
127.35
127.32
125.37
125.28
124.07
124.04
119.04
115.85
115.67
83.39
24.75
F
O
B
O
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


30.15
F
O
B
O
90
80
70
60
50
40
30
20
10
0
−10
−20
−30
−40
−50
−60
−70
−80
ppm

6g


7.809
7.772
7.647
7.643
7.632
7.628
7.372
7.369
7.367
7.357
7.353
7.345
7.330
7.328
7.269
7.264
7.261
7.249
7.246
7.238
7.236
7.233
7.227
7.223
7.219
7.209
7.205
6.199
6.162
1.327
Cl
O
B
O
11
10
9
8
7
6
5
4
3
2
1
ppm
0.95
1.02
1.06
3.06
1.00
12.02


144.98
135.63
133.66
132.58
129.80
129.68
128.98
128.27
127.03
126.86
119.53
83.50
24.83
Cl
O
B
O
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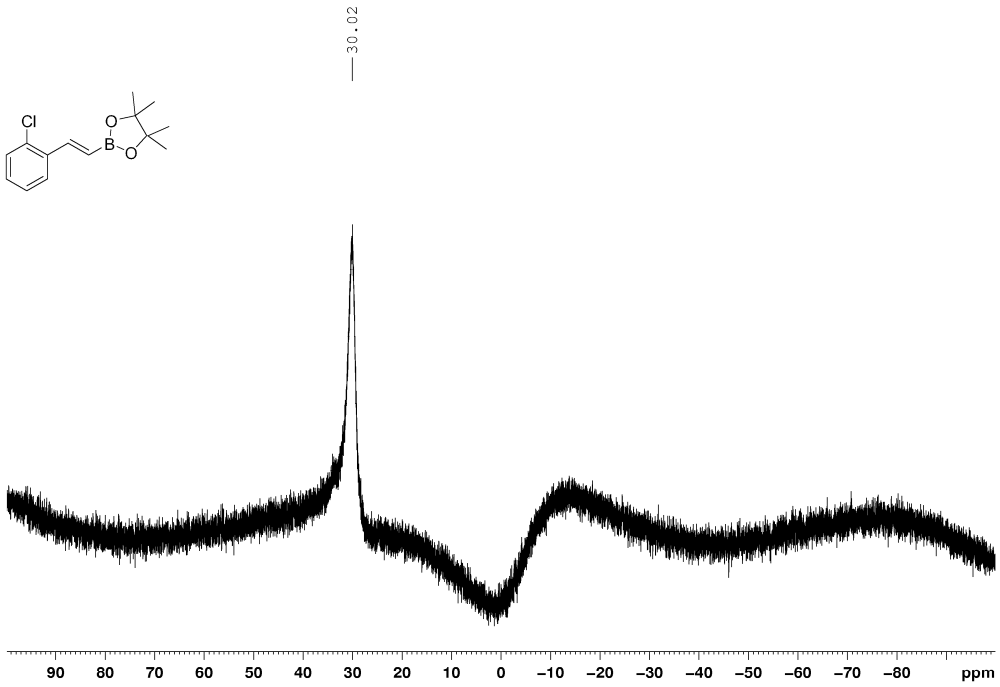
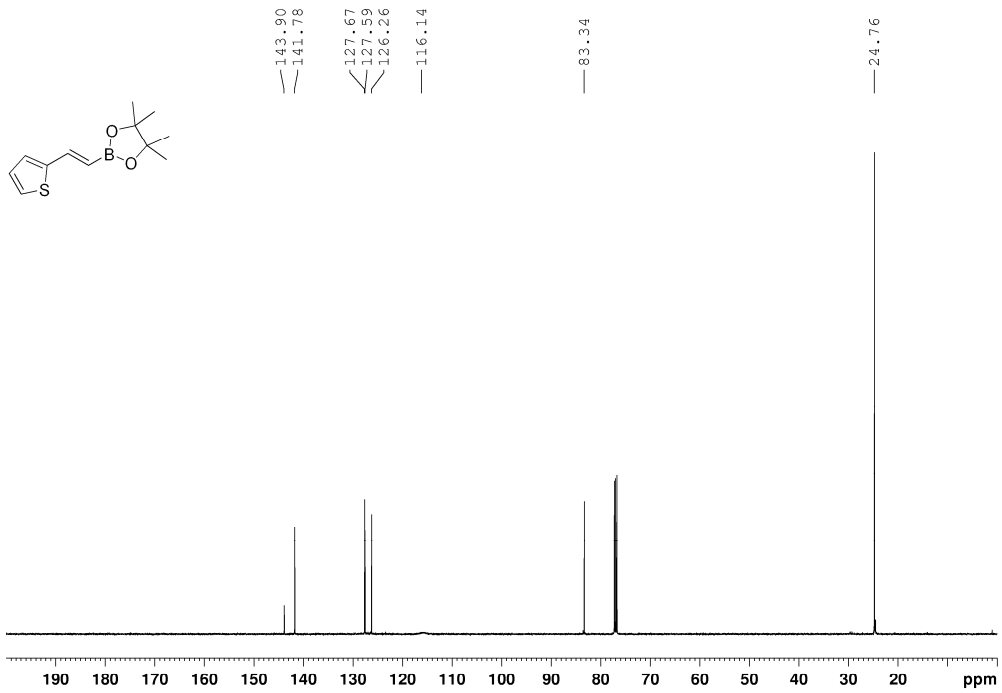
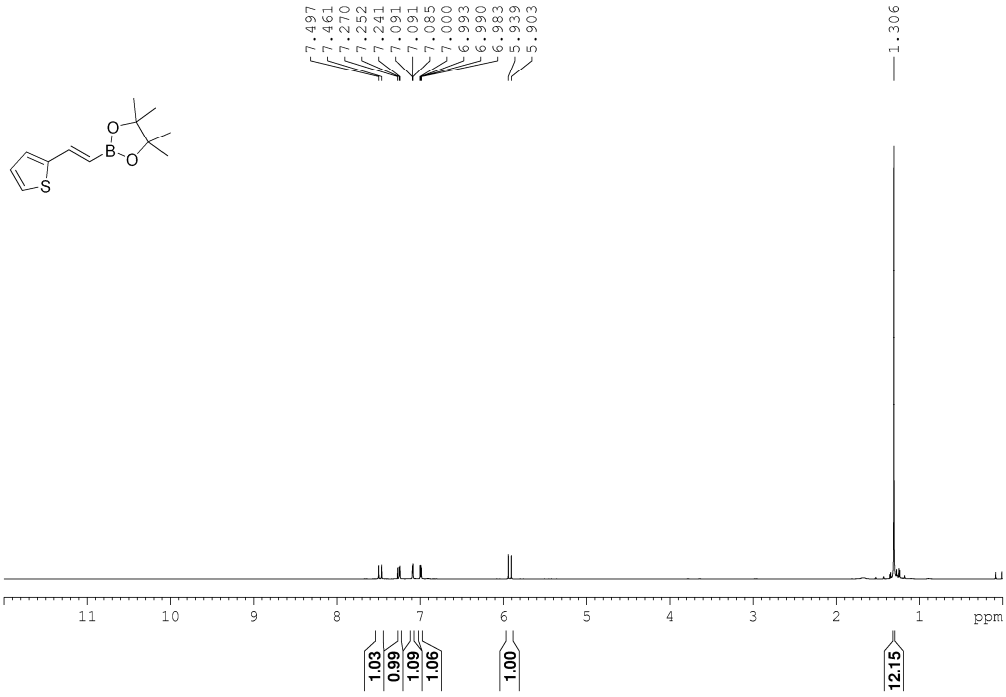
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


30.02
Cl
O
B
O
90
80
70
60
50
40
30
20
10
0
−10
−20
−30
−40
−50
−60
−70
−80
ppm

6h


143.90
141.78
127.67
127.59
126.26
116.14
83.34
24.76
O
B
O
S
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm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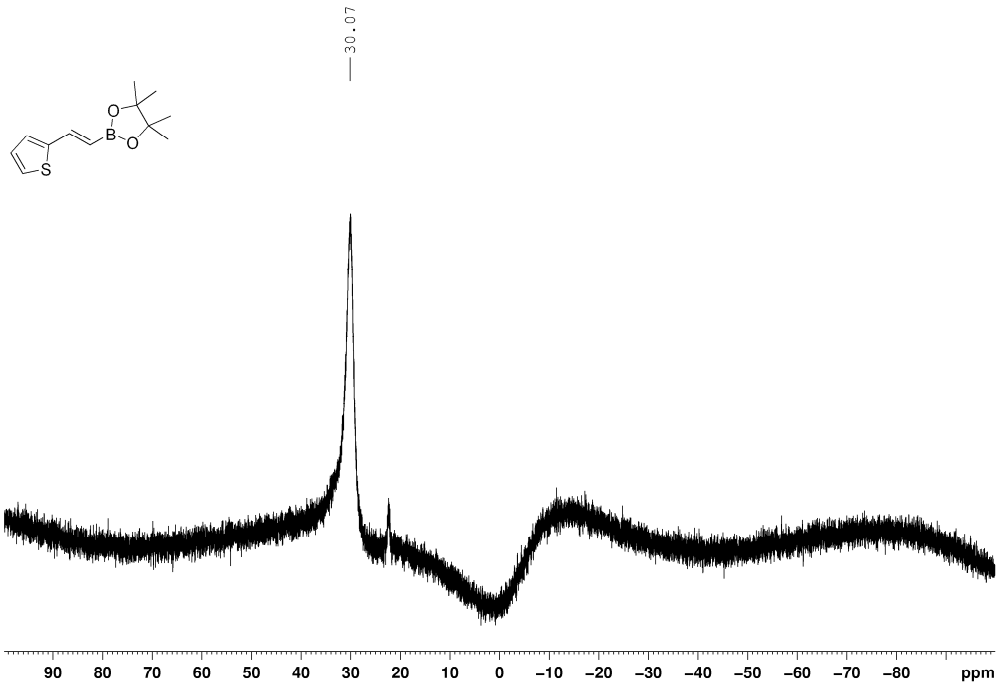
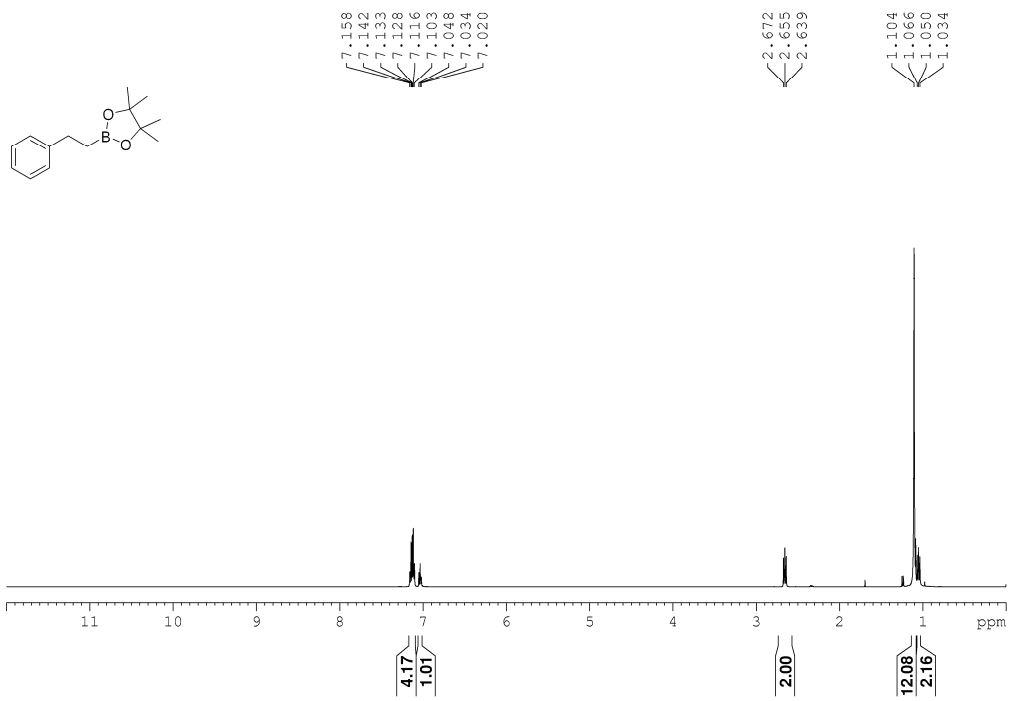
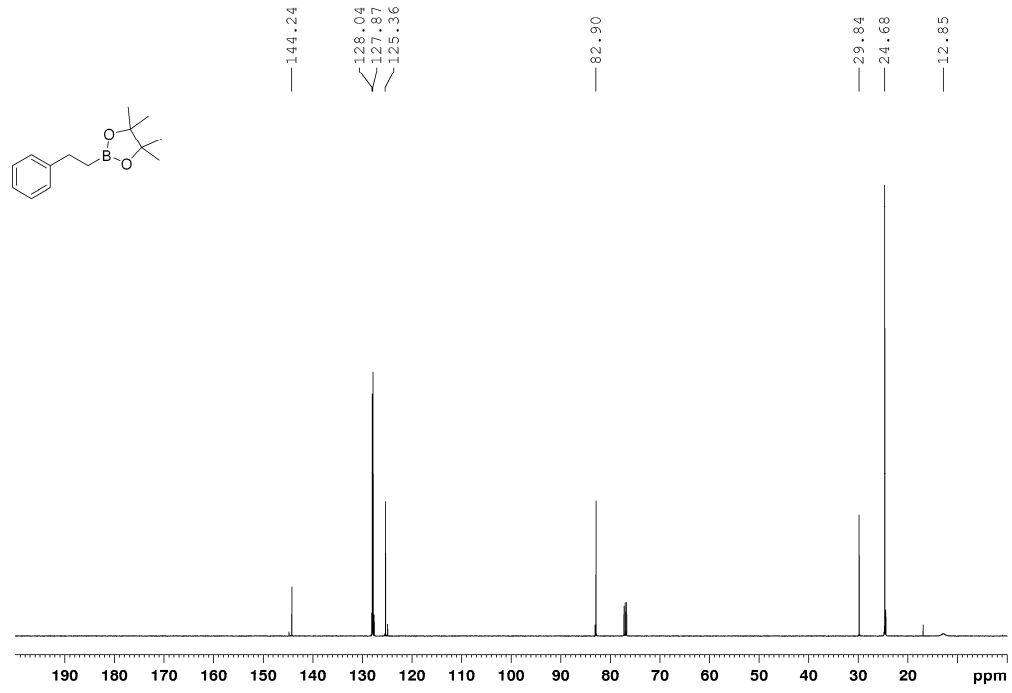
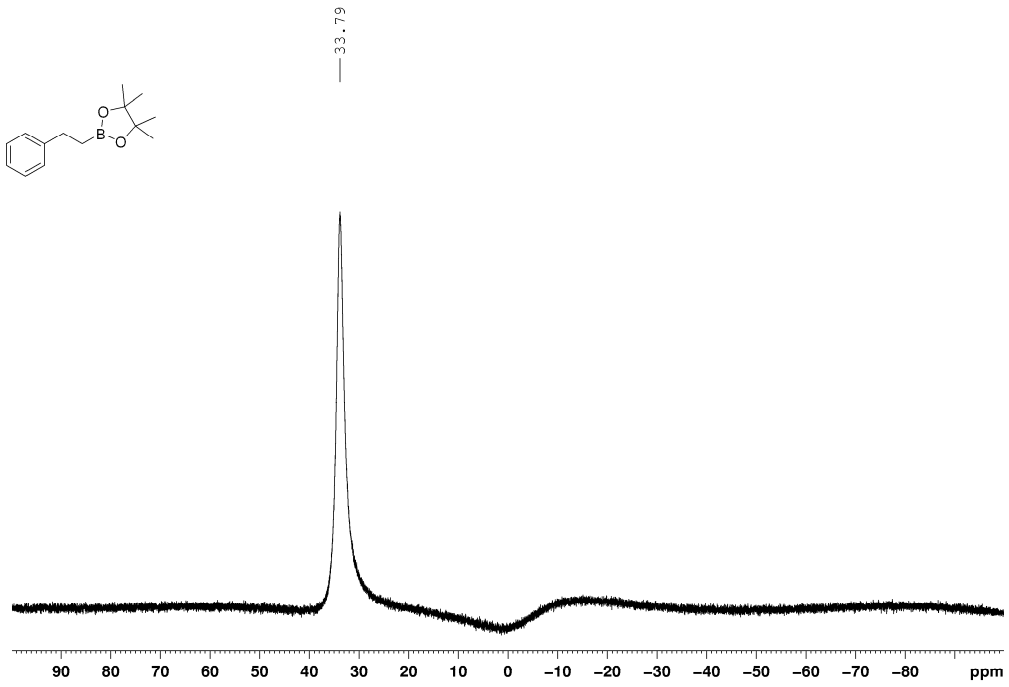
7.461
7.270
7.252
7.241
7.091
7.085
7.000
6.993
6.990
6.983
5.939
5.903
1.306
O
B
O
S
11 10 9 8 7 6 5 4 3 2 1 ppm
1.03
0.99
1.09
1.06
1.00
12.15


30.07
O
B
O
S
90
80
70
60
50
40
30
20
10
0
−10
−20
−30
−40
−50
−60
−70
−80
ppm

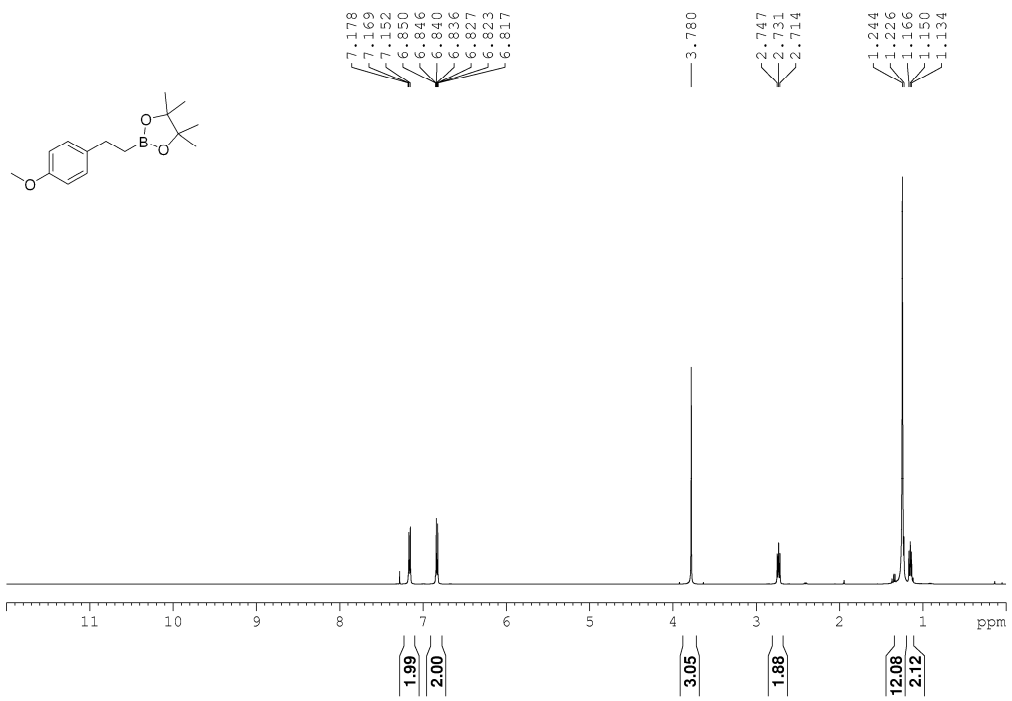
6i

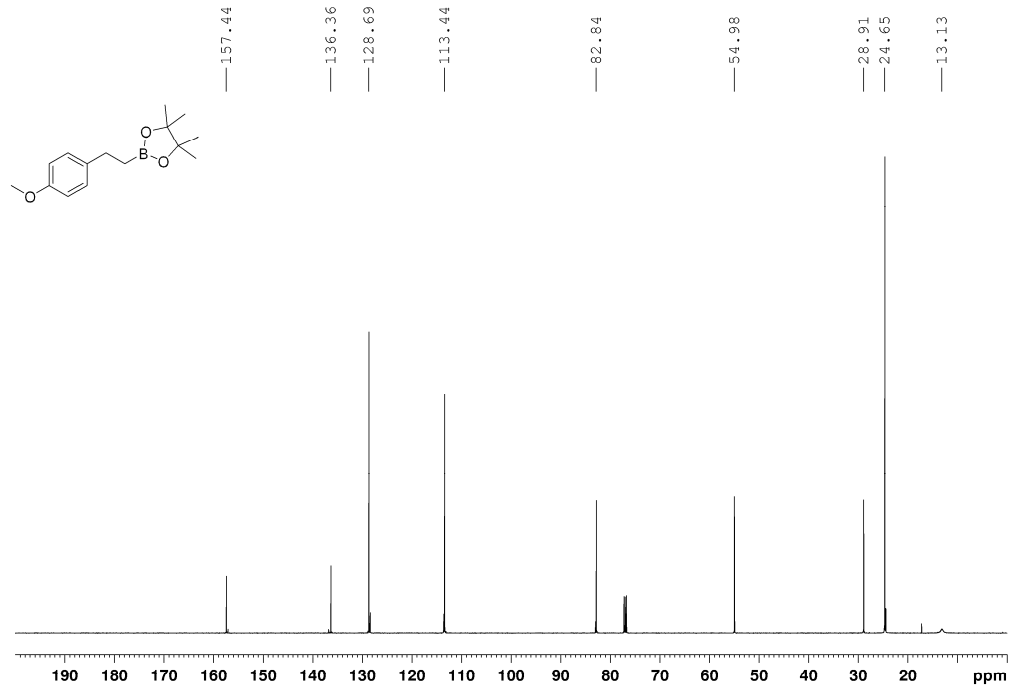

7.158
7.142
7.133
7.128
7.116
7.103
7.048
7.034
7.020
2.672
2.655
2.639
1.104
1.066
1.050
1.034
11
10
9
8
7
6
5
4
3
2
1
ppm
4.17
1.01
2.00
12.08
2.16

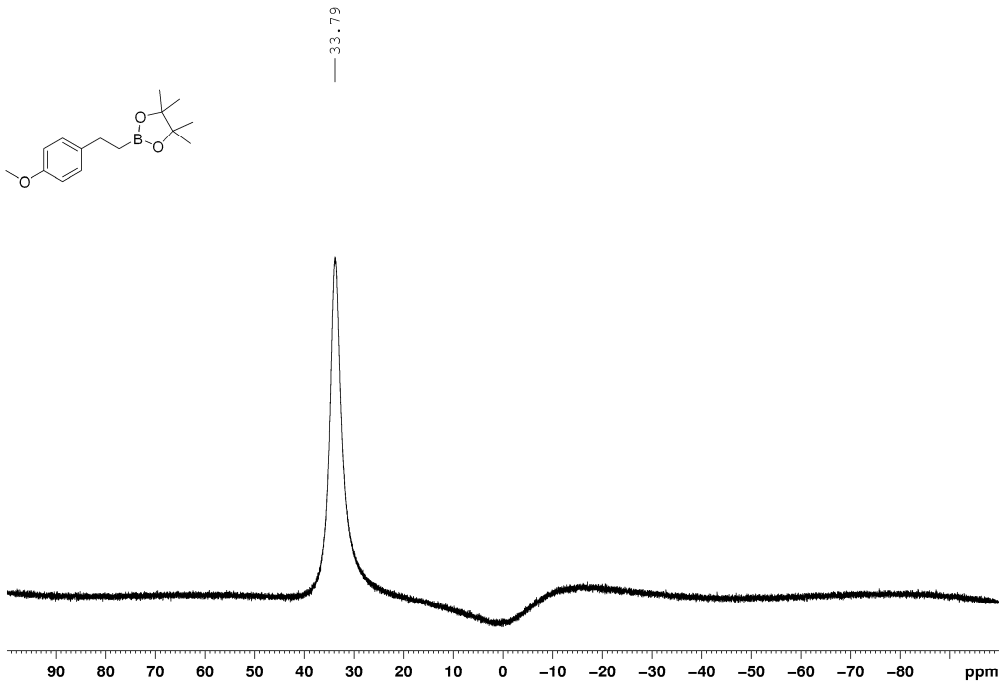

144.24
128.04
127.87
125.36
82.90
29.84
24.68
12.85
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


33.79
O
B
O
90
80
70
60
50
40
30
20
10
0
−10
−20
−30
−40
−50
−60
−70
−80
ppm

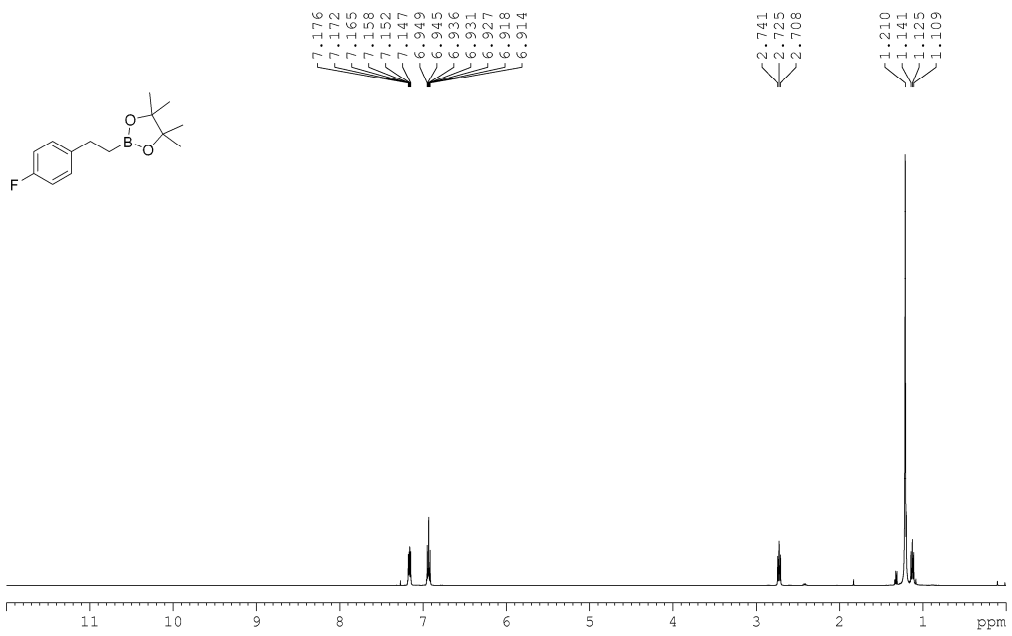
6j

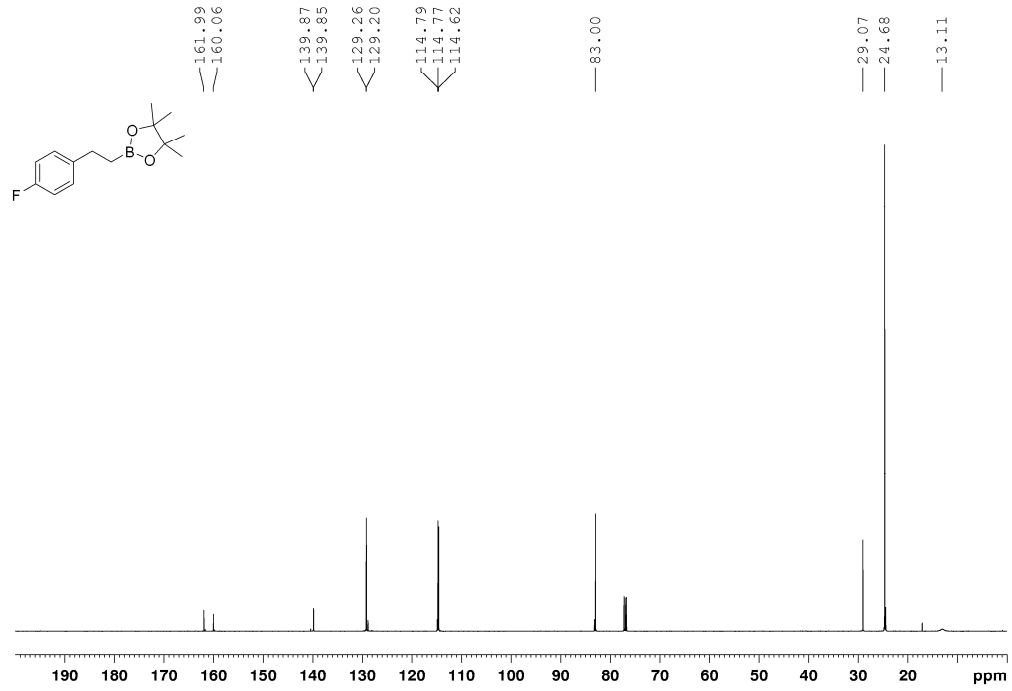

7.178
7.169
7.152
6.850
6.846
6.840
6.836
6.827
6.823
6.817
3.780
2.747
2.731
2.714
1.244
1.226
1.166
1.150
1.134
ppm
1.99
2.00
3.05
1.88
12.08
2.12

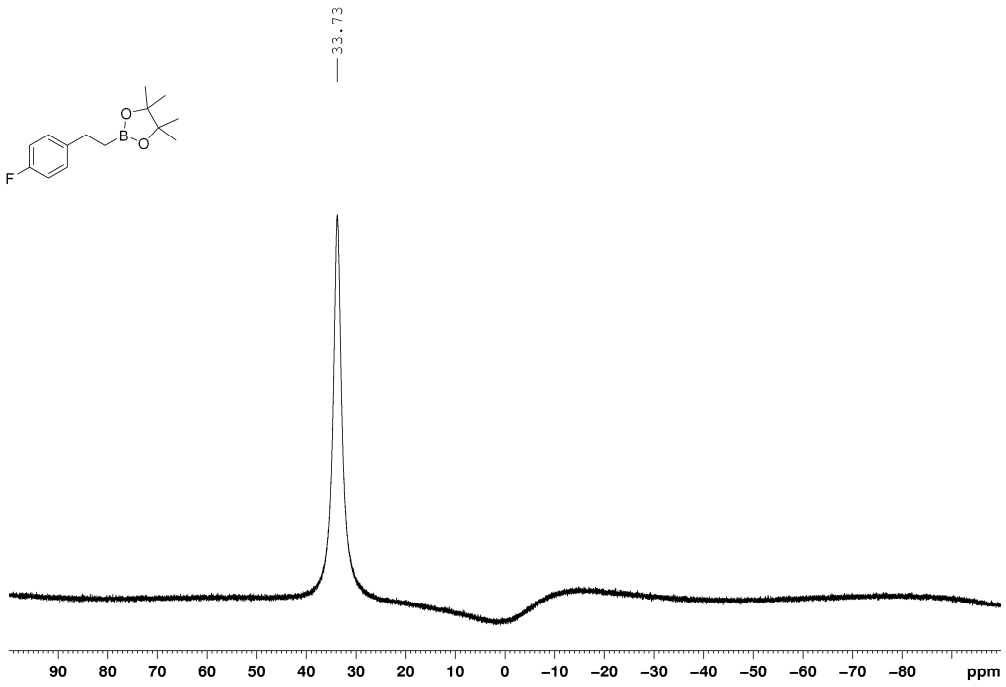

157.44
136.36
128.69
113.44
82.84
54.98
28.91
24.65
13.13
ppm


33.79
O
B
O
O
90
80
70
60
50
40
30
20
10
0
−10
−20
−30
−40
−50
−60
−70
−80
ppm

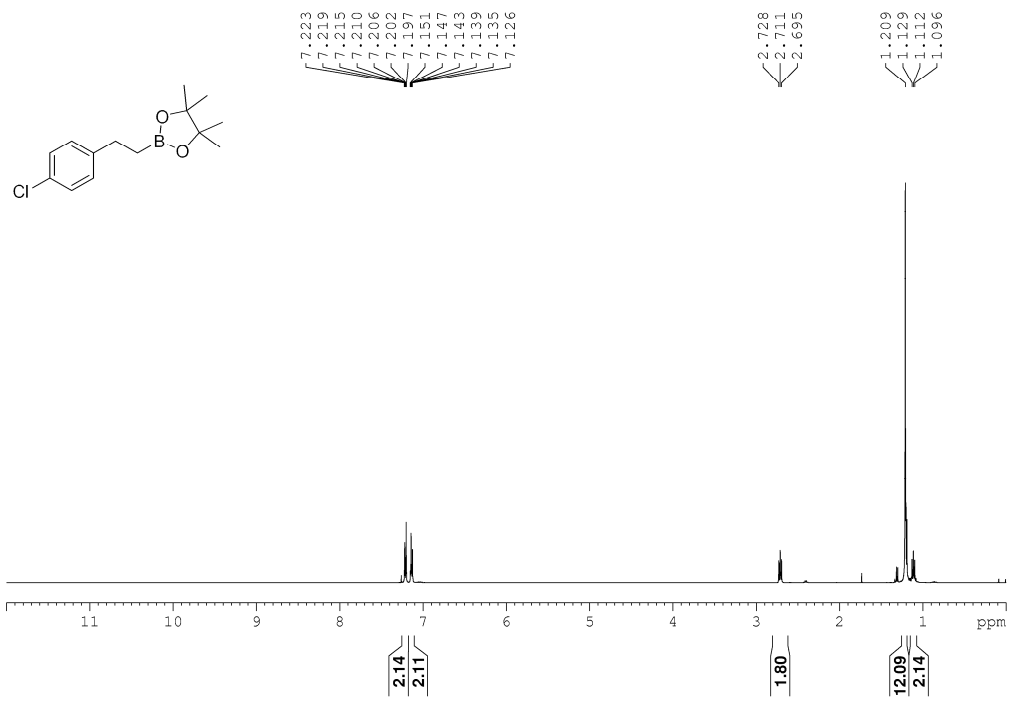
6k


7.176
7.172
7.165
7.158
7.152
7.147
6.949
6.945
6.936
6.931
6.927
6.918
6.914
2.741
2.725
2.708
1.210
1.141
1.125
1.109
O
B
O
F
11
10
9
8
7
6
5
4
3
2
1
ppm


161.99
160.06
139.87
139.85
129.26
129.20
114.79
114.77
114.62
83.00
29.07
24.68
13.11
O
B
O
F
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


33.73
O
B
O
F
90
80
70
60
50
40
30
20
10
0
−10
−20
−30
−40
−50
−60
−70
−80
ppm

6l


7.223
7.219
7.215
7.210
7.206
7.202
7.197
7.151
7.147
7.143
7.139
7.135
7.126
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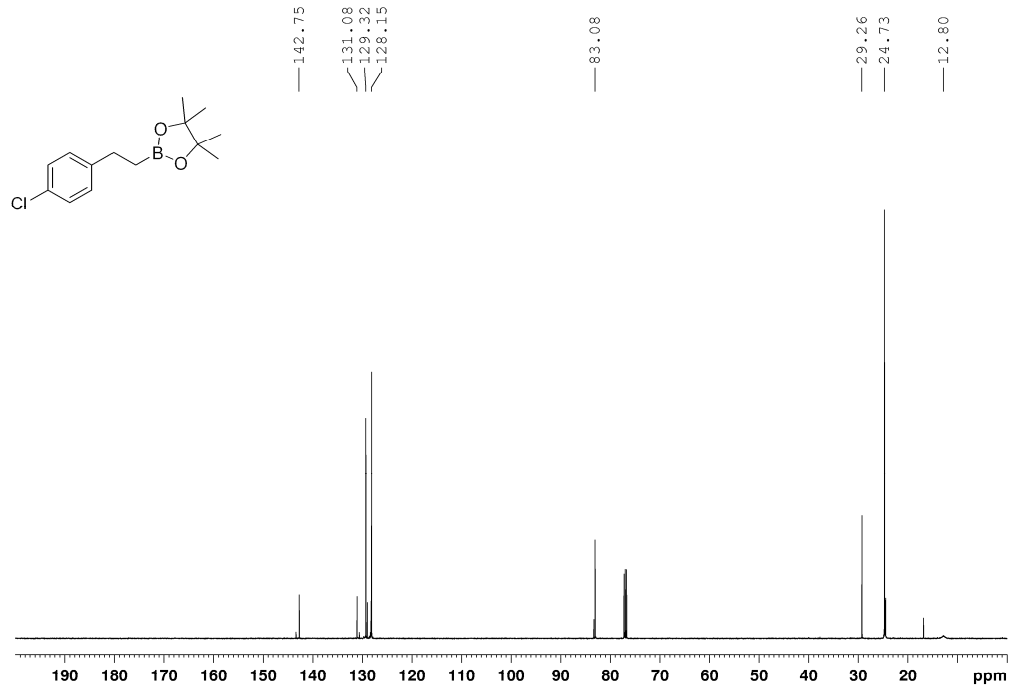
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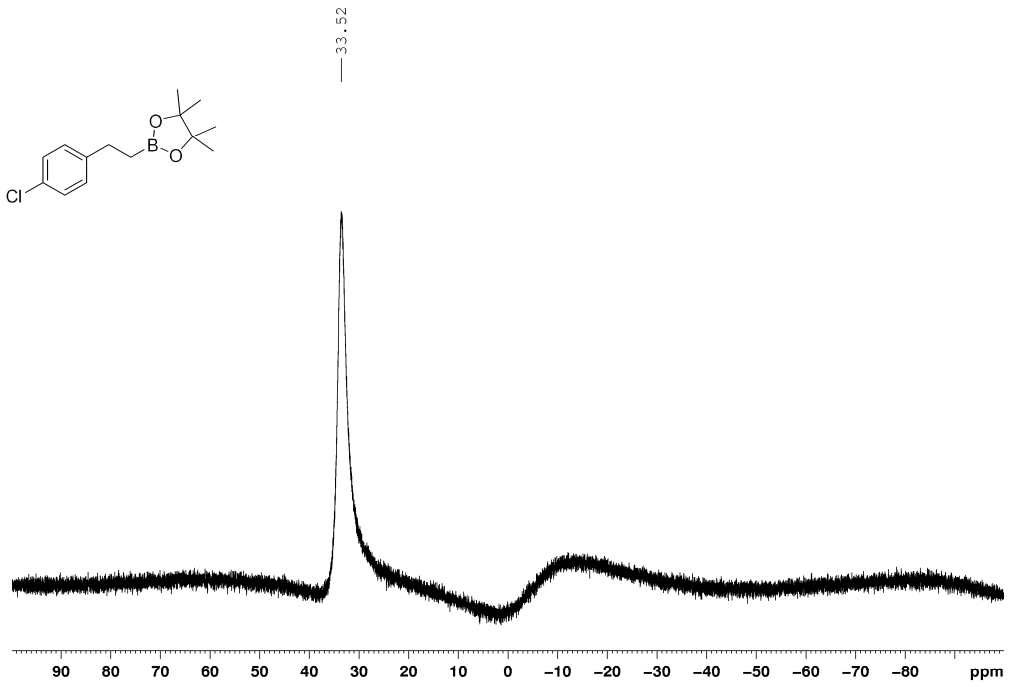
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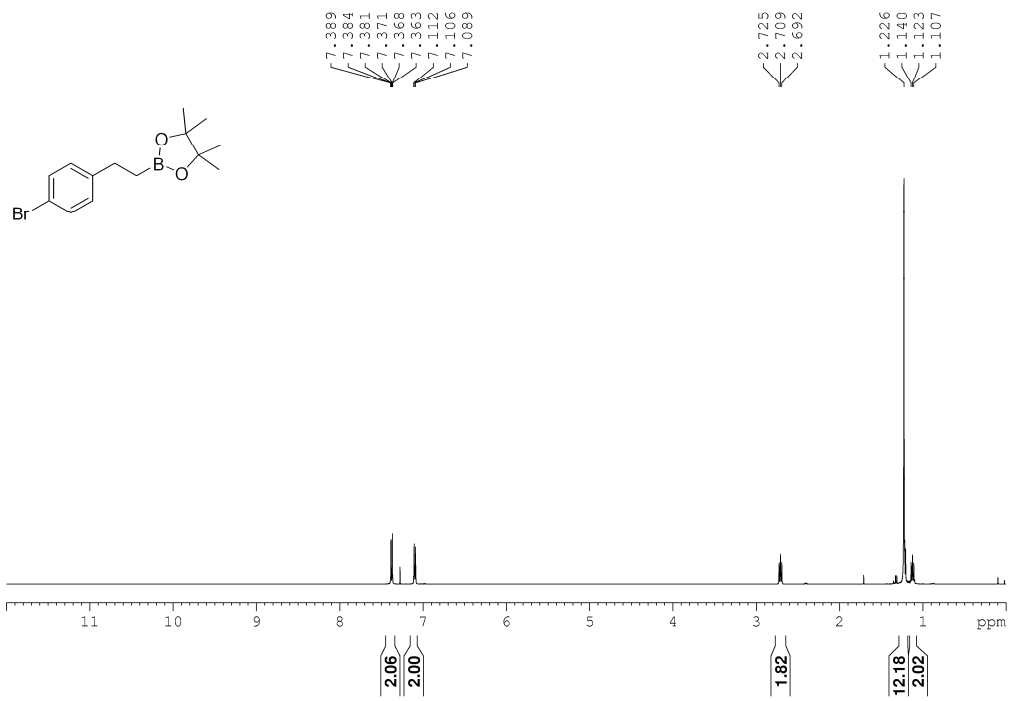
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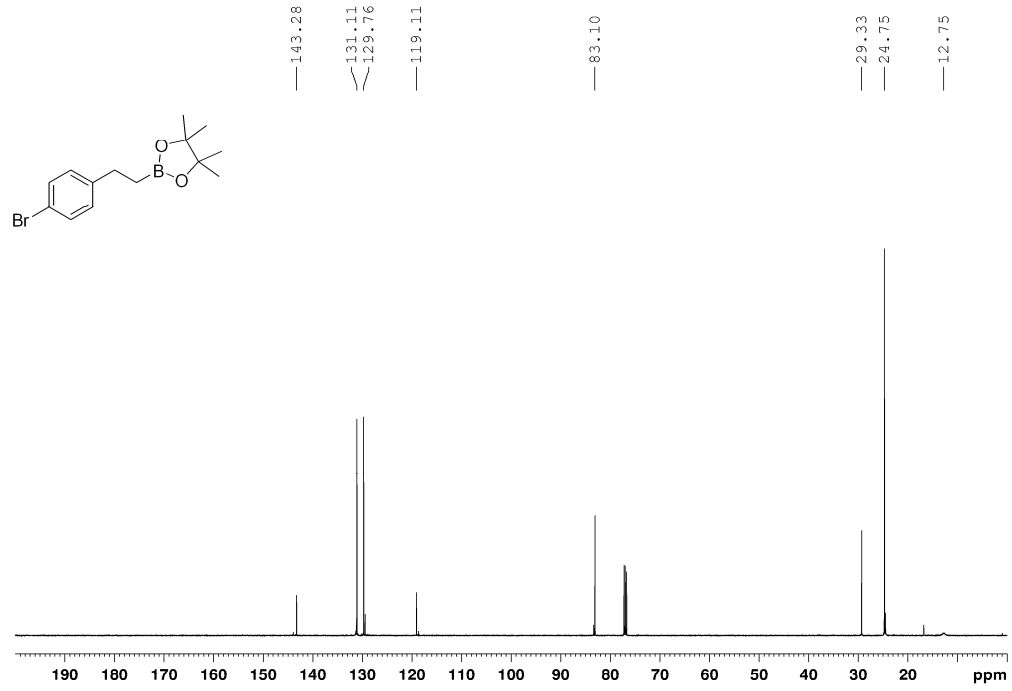
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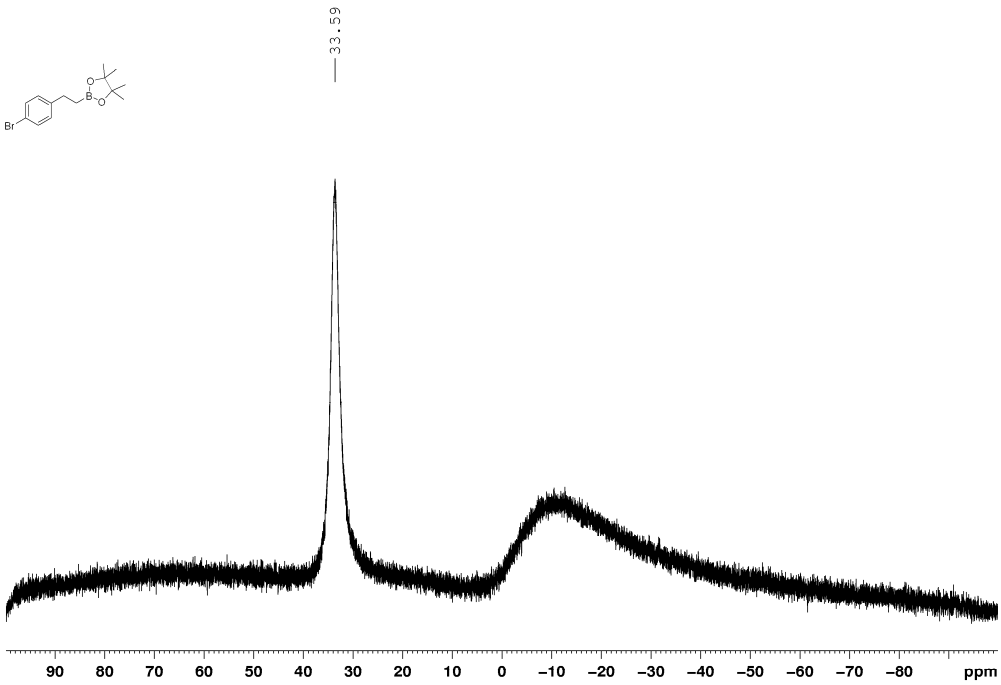
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ppm

Computational details

All the DFT calculations were performed with the Gaussian 09 software package.[S4] Optimizations of structures with frequency calculations were carried out with the M06-2X functional[S5] employing the basis set of 6-31G(d)[S6] for all atoms. Transition states with only one imaginary frequency were examined by vibrational analysis and then submitted to intrinsic reaction coordinate (IRC)[S7] calculations to ensure that such structures indeed connected two minima. Energies in solution (THF) were calculated by means of single-point calculations (SMD method[S8] with the Bondi radii[S9]) with the same functional using the basis set of 6-311++G(2d,p) for all atoms. The free energy correction from the frequency calculation was added to the single-point energy to obtain the free energy in solution. All of the solution-phase free energies reported herein correspond to the reference state of 1 mol/L, 298 K. NBO calculations were carried out using the NBO 5.9 program[S10] at the M06/TZVP level of theory.

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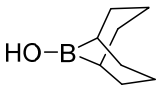
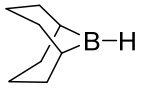
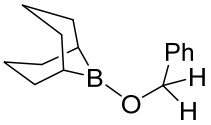
Energies of intermediates and transition states

Species	Solvation Energies (Hartree)	Thermal Correction of Gibbs Free Energies (Hartree)
9-BBN dimer	-677.3749727	0.405637
NaOH•2thf	-702.9921601	0.209718
	-413.9720623	0.194529
TS1	-1380.368932	0.639657
IN1	-966.448967	0.417829
1a	-345.539616	0.080819
IN2	-1312.001918	0.522908
TS2	-1311.965686	0.521759
IN3	-1312.053327	0.527645
	-338.6621382	0.188329
	-684.2845525	0.297308

TheCartesian coordinates for the optimized structures

9-BBN dimer

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6	1.300355	2.621863	1.293999
6	1.558634	3.414692	0.000000
6	-1.557642	3.415739	0.000000
6	-1.300159	2.622654	1.293970
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1	-0.000284	1.194047	2.234141
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1	2.140339	1.929375	1.450408
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1	0.957704	4.326699	0.000000
1	-2.599856	3.756880	0.000000
1	-0.955781	4.327151	0.000000
1	-1.313689	3.314430	2.147116
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6	-1.300364	-2.621876	-1.294006
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NaOH•2thf

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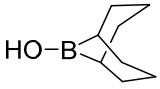

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TS1

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IN1

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IN2

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TS2

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1	-3.389369	-3.568966	2.619179
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1	-0.174363	0.066268	-4.761540
1	-0.665557	-1.259138	-2.206032
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IN3

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6	2.394395	-2.256249	0.669223
1	1.833234	-3.059293	1.174520
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1	2.718016	-1.371834	2.592694
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1	2.661260	1.143805	1.233732
6	2.383342	0.022288	-0.575649
1	1.842805	0.883787	-1.019601
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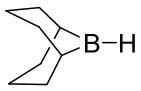

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6	0.609234	-0.365702	-1.303316
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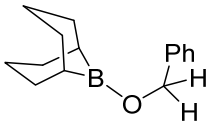

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