

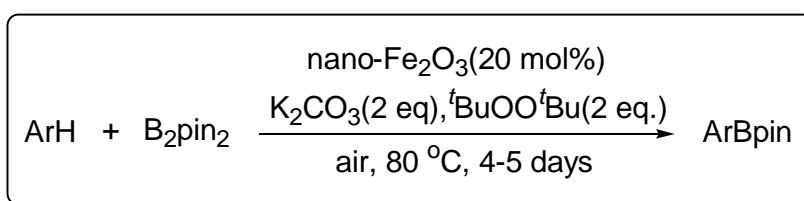
## Supporting Information for

# Nano-Fe<sub>2</sub>O<sub>3</sub>-catalyzed Direct Borylation of Arenes

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## General Information

Chemicals were either purchased or purified by standard techniques without special instructions. All solvents were distilled prior to use. For chromatography, 200-300 mesh silica gel (Qingdao, China) was employed. <sup>1</sup>H NMR (300 MHz) and <sup>13</sup>C NMR (75 MHz) were registered on Varian 300 M spectrometers; <sup>1</sup>H NMR (400 MHz) and <sup>13</sup>C NMR (100 MHz) were registered on Bruker ARX 400 M spectrometer, all with CDCl<sub>3</sub> as solvent and tetramethylsilane (TMS) as internal standard. Chemical shifts were reported in units (ppm) by assigning TMS resonance in the <sup>1</sup>H spectrum as 0.00 ppm and CDCl<sub>3</sub> resonance in the <sup>13</sup>C spectrum as 77.0 ppm. All coupling constants (*J* values) were reported in Hertz (Hz). HRMS were performed by Analytical Center of Peking University. IR spectra were recorded with a Nicolet 5MX-S infrared spectrometer. Fe<sub>2</sub>O<sub>3</sub> magnetic nanoparticles (NanoArc®) was purchased from Alfa Aesar®.

## Experimental Section

### (1) Procedure for nano-Fe<sub>2</sub>O<sub>3</sub>-catalyzed *ortho*-borylation arene with B<sub>2</sub>pin<sub>2</sub>

A reflux tube equipped with a magnetic stir bar was charged with B<sub>2</sub>pin<sub>2</sub> (254 mg, 1 mmol), K<sub>2</sub>CO<sub>3</sub> (276 mg, 2 mmol), *t*BuOO*t*Bu (292 mg, 2 mmol), Fe<sub>2</sub>O<sub>3</sub> magnetic nanoparticles (NanoArc®, Alfa Aesar®) (32 mg, 0.2 mmol) and aryl substrate (5 mL). The reaction vessel was placed in an oil bath (80 °C) under open air. The reaction progress was monitored by GC-MS. The mixture was cooled to room temperature when B<sub>2</sub>pin<sub>2</sub> disappeared completely. Yield and ratio was determined by GC using mesitylene or dodecane as the internal standard. After completion of borylation reaction, the mixture was first purified by a short silica gel column chromatography to removed iron catalyst and inorganic base. The solvent was evaporated *in vacuo*, and the residue was purified by flash column chromatography on silica gel (eluting with ethyl acetate/petroleum ether) to give pure product.

A large scale experiment: Benzene (20 mL) and B<sub>2</sub>pin<sub>2</sub> (1 g, 4 mmol) were subjected to the above reaction conditions. PhBpin was isolated in 52% yield after column chromatography

### (2) Procedure for Sequential Reactions

A reflux tube equipped with a magnetic stir bar was charged with B<sub>2</sub>pin<sub>2</sub> (254 mg, 1 mmol), K<sub>2</sub>CO<sub>3</sub> (276 mg, 2 mmol), *t*BuOO*t*Bu (292 mg, 2 mmol), Fe<sub>2</sub>O<sub>3</sub> magnetic nanoparticles (32 mg, 0.2 mmol) and benzene (5 mL). The reaction vessel was placed in oil bath (80 °C) under air. The solution was cooled to room temperature until B<sub>2</sub>pin<sub>2</sub> was disappeared. The reaction progress was monitored and analyzed by GC-MS. After the completion of the borylation reaction, benzene was evaporated under reduced pressure. To this mixture were added aryl iodide (1 mmol), PdCl<sub>2</sub>(dppf) (0.030 mmol), K<sub>3</sub>PO<sub>4</sub> (3 mmol), and DMF (5 mL), and the mixture was stirred at 60 °C under N<sub>2</sub>. After the completion of the cross-coupling reaction, the mixture was extracted with EtOAc, washed with brine, and dried over MgSO<sub>4</sub>. The residue was purified by flash column chromatography on a silica gel (eluting with ethyl acetate/petroleum ether) to give the product.

### (3) Procedure for Nano Fe<sub>2</sub>O<sub>3</sub> Catalyst preparation<sup>1-4</sup>

$\gamma$ -Fe<sub>2</sub>O<sub>3</sub> (20 nm) catalyst was prepared by co-precipitation of aqueous solutions of FeSO<sub>4</sub>·7H<sub>2</sub>O and FeCl<sub>3</sub>·6H<sub>2</sub>O by urea hydrolysis (All from Beijing Chemicals, AR grade). The cation (Fe<sup>2+</sup> + Fe<sup>3+</sup>) concentration was kept at 0.60 M with [Fe<sup>2+</sup>]/[Fe<sup>3+</sup>] ratio of 1/2 and the urea concentration was kept at 6.0 M. The mixed solution was heated to 100 °C under N<sub>2</sub> atmosphere and maintained at 100 °C for 3 h to form precipitates. After filtration and thoroughly washing with deionized water until the filtrate was neutral, the precipitates were treated in ambient air at 110 °C overnight, and then at 300 °C for 3 h. A mixed crystal Fe<sub>2</sub>O<sub>3</sub> (9 nm) with  $\alpha$  and  $\gamma$  phases was obtained when the concentrations of the cation (Fe<sup>2+</sup> + Fe<sup>3+</sup>) and urea improved to 1.20 M and 12.0 M respectively.

$\alpha$ -Fe<sub>2</sub>O<sub>3</sub> catalysts were prepared in a similar way, in which Fe(NO<sub>3</sub>)<sub>3</sub>·9H<sub>2</sub>O was used as the Fe<sup>3+</sup> precursor salt instead of FeCl<sub>3</sub>·6H<sub>2</sub>O. The average crystallite size of  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> decreased from 18 nm to 14 nm by doubling the solution concentration as described above.

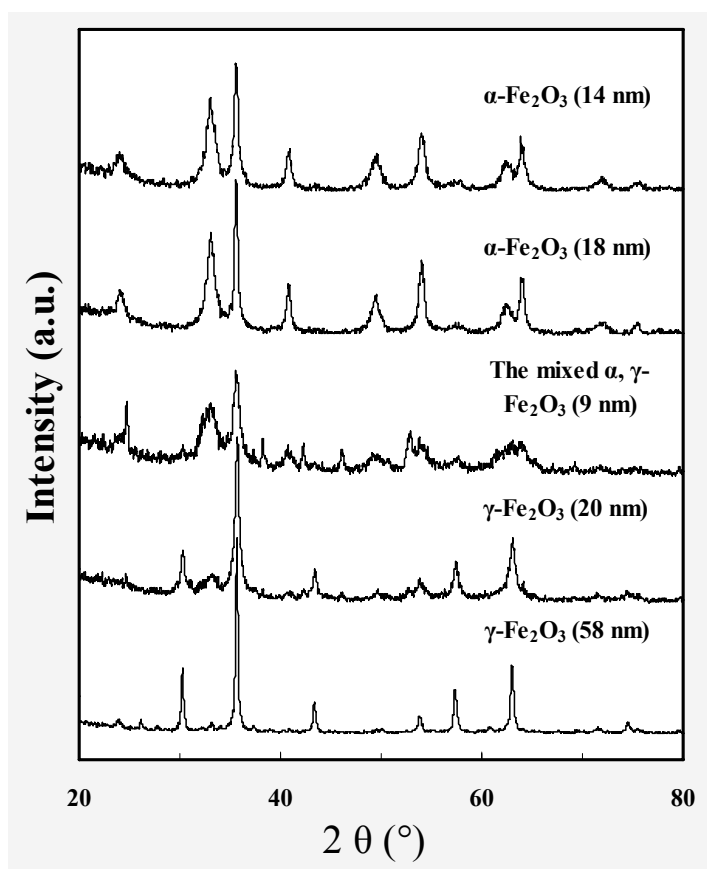
The crystalline phase of the catalysts was identified by X-ray diffraction (Rigaku D/MAX-2400 diffractometer) and the crystallite size of Fe<sub>2</sub>O<sub>3</sub> was calculated by Scherrer equation,  $d = 0.90\lambda / \beta \cos\theta$ , where  $\theta$  is the diffraction angle and  $\beta$  is the full width at half-maximum.

The X-ray diffraction patterns of Fe<sub>2</sub>O<sub>3</sub> catalysts (the crystallite size of the commercial  $\gamma$ -Fe<sub>2</sub>O<sub>3</sub> was 58 nm)

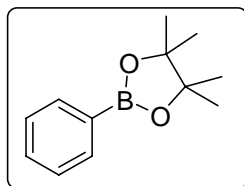
## References

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- (2) S. Laurent, D. Forge, M. Port, A. Roch, C. Robic, L. V. Elst, R. N. Muller, *Chem. Rev.* 2008, **108**, 2064.
- (3) A. C. Garade, M. Bharadwaj, S. V. Bhagwat, A. A. Athawale, C. V. Rode, *Catal. Commun.*, 2009, **10**, 485.
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## X-Ray Diffraction of Fe<sub>2</sub>O<sub>3</sub> Catalysts



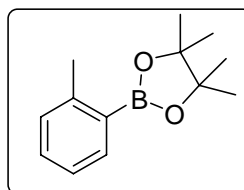
## Spectral data for the products



### 4,4,5,5-Tetramethyl-2-phenyl-1,3,2-dioxaborolane

Colorless liquid

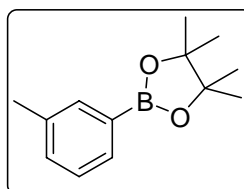
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.81 (d,  $J = 6.7$  Hz, 2H), 7.47~7.43 (m, 1H), 7.38~7.35 (m, 2H), 1.34 (s, 12H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  131.7, 131.2, 127.7, 83.7, 24.8.



### 4,4,5,5-Tetramethyl-2-*o*-tolyl-1,3,2-dioxaborolane

Colorless liquid

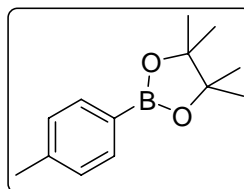
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$ : 7.77 (d,  $J = 1.4$  Hz, 1H), 7.33~7.29 (m, 1H), 7.16~7.14 (m, 2H), 2.54 (s, 3H), 1.34 (s, 12H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$ : 144.8, 135.8, 130.8, 129.7, 124.7, 83.4, 24.9, 22.2.



### 4,4,5,5-Tetramethyl-2-*m*-tolyl-1,3,2-dioxaborolane

White solid

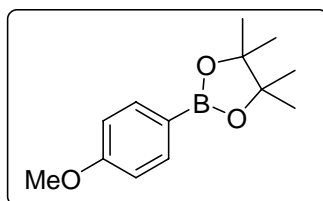
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.64~7.60 (m, 2H), 7.28~7.26 (m, 2H), 2.35 (s, 3H), 1.34 (s, 12H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  137.1, 135.3, 132.0, 131.8, 127.7, 83.7, 24.8, 21.2.



### 4,4,5,5-Tetramethyl-2-*p*-tolyl-1,3,2-dioxaborolane

White solid

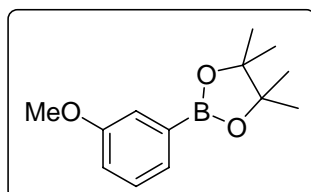
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.70 (d,  $J = 7.5$  Hz, 2H), 7.18 (d,  $J = 7.5$  Hz, 2H), 2.36 (s, 3H), 1.33 (s, 12H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  141.4, 134.8, 128.5, 83.6, 24.8, 21.7.



### 2-(4-Methoxyphenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane

Colorless liquid

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.76 (d,  $J = 1.8$  Hz, 2H), 6.89 (q,  $J = 1.8$  Hz, 2H), 3.82 (s, 3H), 1.33 (s, 12H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  162.1, 136.5, 113.3, 83.5, 55.0, 24.8.

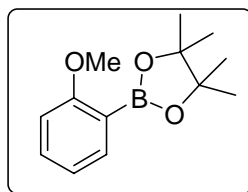


### 2-(3-Methoxyphenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane

Colorless liquid

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.40 (d,  $J = 11.2$  Hz, 1H), 7.33~7.28 (m, 2H), 7.02~6.99 (m, 1H), 3.83 (s, 3H), 1.34 (s, 12H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  159.0, 128.9, 127.1, 118.6, 117.9,

83.8, 55.2, 24.8.

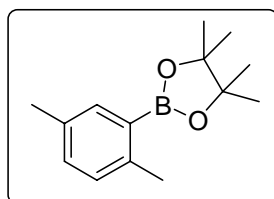


**2-(2-Methoxyphenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane**

White solid

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.69~7.66 (m, 1H), 7.41~7.37 (m, 1H), 6.94 (t,  $J = 7.4$  Hz, 1H), 6.85 (d,  $J = 8.3$  Hz, 1H), 3.83 (s, 3H), 1.35 (s, 12H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  164.1, 136.7, 132.4, 120.2, 110.4,

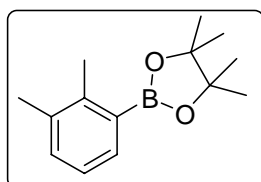
83.4, 55.8, 24.8.



**4,4,5,5-Tetramethyl-2-(2,5-dimethylphenyl)-1,3,2-dioxaborolane**

White solid

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.57 (s, 1H), 7.13~7.11 (m, 1H), 7.05 (d,  $J = 7.7$  Hz, 1H), 2.49 (s, 3H), 2.30 (s, 3H), 1.33 (s, 12H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  141.7, 136.3, 133.9, 131.5, 129.8, 83.3, 24.9, 21.7, 20.8.

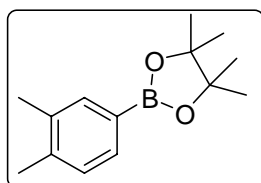


**4,4,5,5-Tetramethyl-2-(2,3-dimethylphenyl)-1,3,2-dioxaborolane**

White solid

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.60 (d,  $J = 7.4$  Hz, 1H), 7.20 (d,  $J = 7.4$  Hz, 1H), 7.08 (t,  $J = 7.4$  Hz, 1H), 2.47 (s, 3H), 2.26 (s, 3H), 1.34 (s, 12H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  143.0, 136.4, 133.5, 132.3, 124.8,

83.4, 24.8, 20.4, 18.4; IR (film): 2978, 1429, 1379, 1346, 1304, 1138, 1034, 827, 850, 728, 669  $\text{cm}^{-1}$ ; EI-MS ( $m/z$ , relative intensity): 232 ( $\text{M}^+$ , 38), 217 (20), 175 (100), 159 (5), 146 (16), 132 (98), 117 (27), 105 (27), 91 (28), 77 (14), 41(44); HRMS calcd for  $\text{C}_{14}\text{H}_{22}\text{BO}_2$  [ $\text{M}+\text{H}$ ] $^+$  233.1707, found 233.1706.

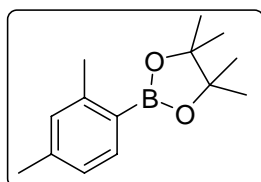


**4,4,5,5-Tetramethyl-2-(3,4-dimethylphenyl)-1,3,2-dioxaborolane**

White solid

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.58 (s, 1H), 7.5 (d,  $J = 7.4$  Hz, 1H), 7.14 (d,  $J = 7.4$  Hz, 1H), 2.27 (s, 3H), 2.26 (s, 3H), 1.33 (s, 12H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  140.1, 135.9, 135.8, 132.4, 129.1, 83.5,

24.8, 20.0, 19.4.

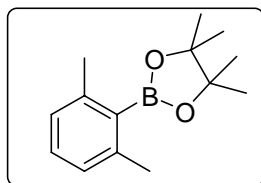


**4,4,5,5-Tetramethyl-2-(2,4-dimethylphenyl)-1,3,2-dioxaborolane**

Colorless liquid

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.66 (d,  $J = 8.1$  Hz, 1H), 6.98 (d,  $J = 7.0$  Hz, 1H), 2.50 (s, 3H), 2.30 (s, 3H), 1.34 (s, 12H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  144.9, 140.8, 136.1, 130.7, 125.5, 83.2, 24.9, 22.1, 21.5; IR

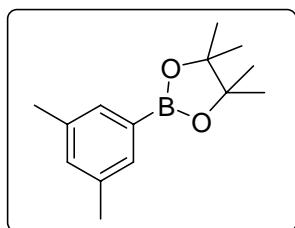
(film): 2978, 1612, 1371, 1346, 1311, 1146, 1063, 963, 860, 659  $\text{cm}^{-1}$ ; EI-MS ( $m/z$ , relative intensity): 232 ( $\text{M}^+$ , 29), 217 (26), 175 (73), 159 (6), 146 (18), 132 (100), 117 (21), 105 (25), 91 (28), 77 (14), 41 (40); HRMS calcd for  $\text{C}_{14}\text{H}_{22}\text{BO}_2$  [ $\text{M}+\text{H}$ ] $^+$  233.1707, found 233.1705.



**4,4,5,5-Tetramethyl-2-(2,6-dimethylphenyl)-1,3,2-dioxaborolane**

White solid

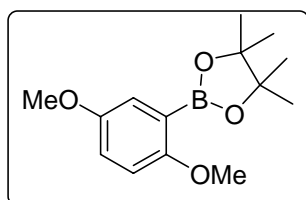
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$ : 7.12 (t,  $J = 7.6$  Hz, 1H), 6.94 (d,  $J = 7.6$  Hz, 2H), 2.39 (s, 6H), 1.34 (s, 12H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$ : 141.7, 129.1, 126.4, 83.6, 24.9, 22.2.



**4,4,5,5-Tetramethyl-2-(3,5-dimethylphenyl)-1,3,2-dioxaborolane**

White solid

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.44 (s, 2H), 7.10 (s, 1H), 2.32 (s, 6H), 1.34 (s, 12H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  137.1, 133.0, 132.4, 83.7, 24.8, 21.1.

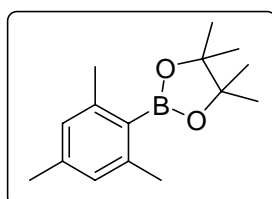


**2-(2,5-Dimethoxyphenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane**

White solid, mp 58-60 °C.

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.21 (d,  $J = 3.3$  Hz, 1H), 6.93 (q,  $J = 3.3$  Hz, 2H), 2.78 (s, 6H), 1.35 (s, 12H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  158.6, 153.3, 121.0, 118.0, 112.3, 83.5, 56.8, 55.8, 24.8;

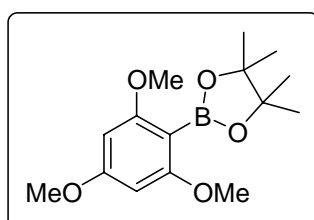
IR (film): 2978, 1585, 1494, 1408, 1344, 1220, 1139, 1066, 1048, 965, 90, 855, 812, 727, 672  $\text{cm}^{-1}$ ; EI-MS ( $m/z$ , relative intensity): 264 ( $\text{M}^+$ , 100), 249 (18), 191 (24), 164 (56), 149 (32), 135 (18), 121 (46), 105 (4), 91 (6), 77 (14), 41 (29); HRMS calcd for  $\text{C}_{14}\text{H}_{22}\text{BO}_4$  [ $\text{M}+\text{H}$ ] $^+$  265.1606, found 265.1605.



**2-Mesityl-4,4,5,5-tetramethyl-2-phenyl-1,3,2-dioxaborolane**

White solid

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  6.76 (s, 2H), 2.36 (s, 6H), 2.23 (s, 3H), 1.36 (s, 12H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  142.1, 138.9, 127.4, 83.4, 24.9, 22.1, 21.2.

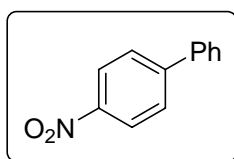


**2-(2,4,6-Trimethoxyphenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane**

White solid, mp 114-116 °C.

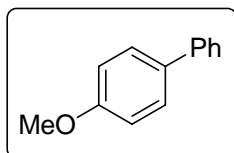
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$ : 6.04 (s, 2H), 3.79 (s, 3H), 3.74 (s, 6H), 1.36 (s, 12H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  164.5, 163.1, 90.2, 83.4, 55.6, 55.2, 24.6; IR (film): 2996, 1607, 1581, 1457,

1356, 1327, 1295, 1221, 1204, 1124, 1037, 864, 804, 733; EI-MS ( $m/z$ , relative intensity): 294 ( $\text{M}^+$ , 100), 279 (16), 236 (42), 221 (52), 194 (69), 151 (40), 135 (56), 121 (59), 105 (10), 91 (20), 77 (24), 41 (44); HRMS calcd for  $\text{C}_{15}\text{H}_{24}\text{BO}_5$  [ $\text{M}+\text{H}$ ] $^+$  295.1711, found 295.1708.



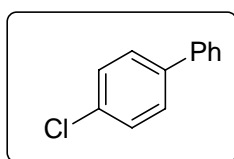
#### 4-Nitro-biphenyl

$^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ )  $\delta$  8.31 (d,  $J = 9.0$  Hz, 2H), 7.76~7.65 (m, 2H), 7.24~7.20 (m, 2H), 7.45~7.53 (m, 3H);  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ )  $\delta$  147.6, 147.1, 138.8, 129.1, 128.9, 127.8, 127.4, 124.1.



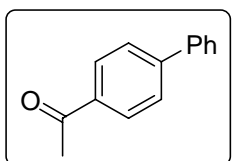
#### 4-Methoxy-biphenyl

$^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ )  $\delta$  7.57~7.52 (m, 4H), 7.44~7.39 (m, 2H), 7.33~7.28 (m, 1H), 6.98 (d,  $J = 8.7$  Hz, 2H), 3.85 (s, 3H);  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ )  $\delta$  159.2, 140.8, 133.8, 128.7, 128.1, 126.7, 126.6, 114.2, 55.3.



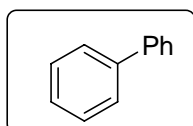
#### 4-Chloro-biphenyl

$^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ )  $\delta$  7.56~7.50 (m, 3H), 7.48~7.36 (m, 6H);  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ )  $\delta$  140.0, 139.7, 133.4, 129.0, 128.9, 128.4, 128.2, 127.0.



#### 4-Acetyl-biphenyl

$^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ )  $\delta$  8.04 (q,  $J = 1.5$  Hz, 2H), 7.70~7.62 (m, 4H), 7.50~7.40 (m, 3H), 2.64 (s, 3H);  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ )  $\delta$  197.7, 145.7, 139.8, 135.8, 128.9, 128.8, 128.2, 127.2, 127.1, 26.6.

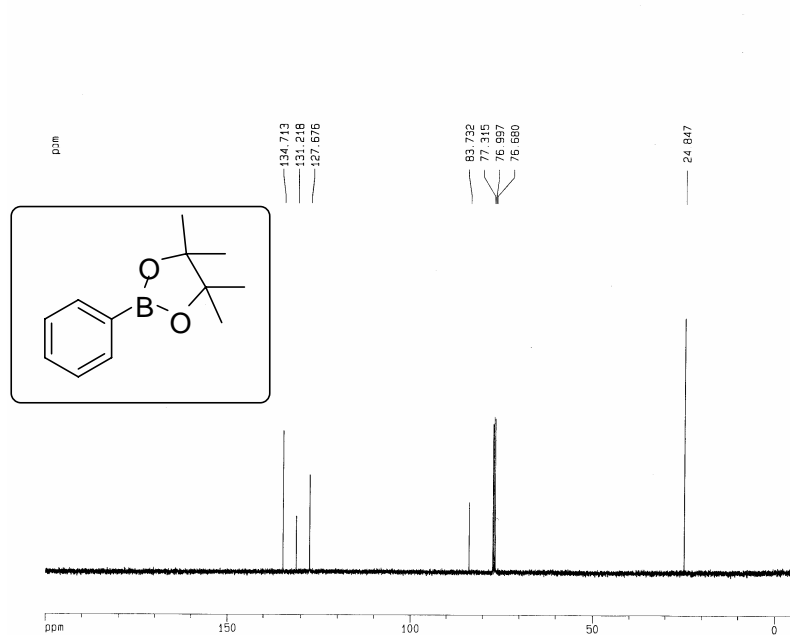
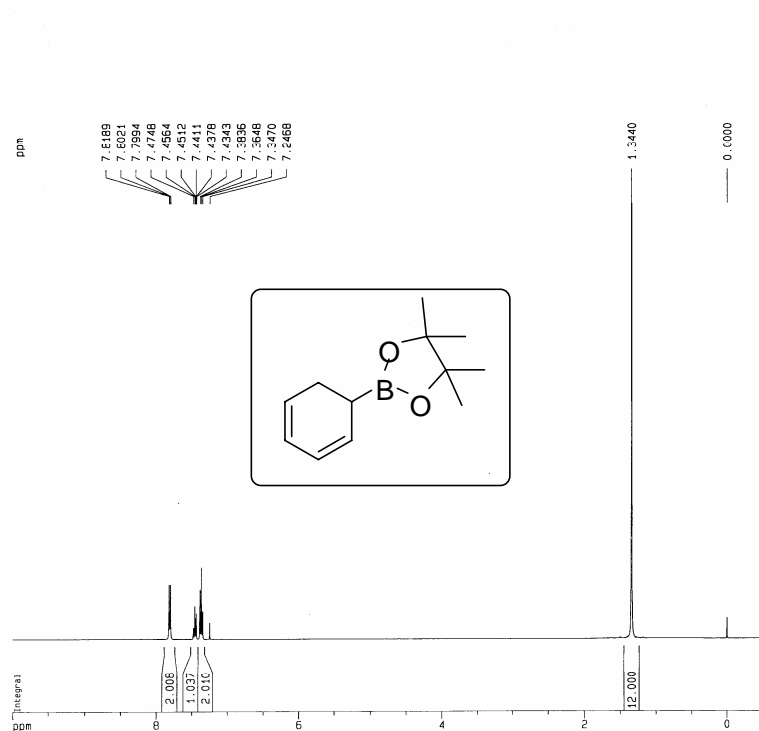


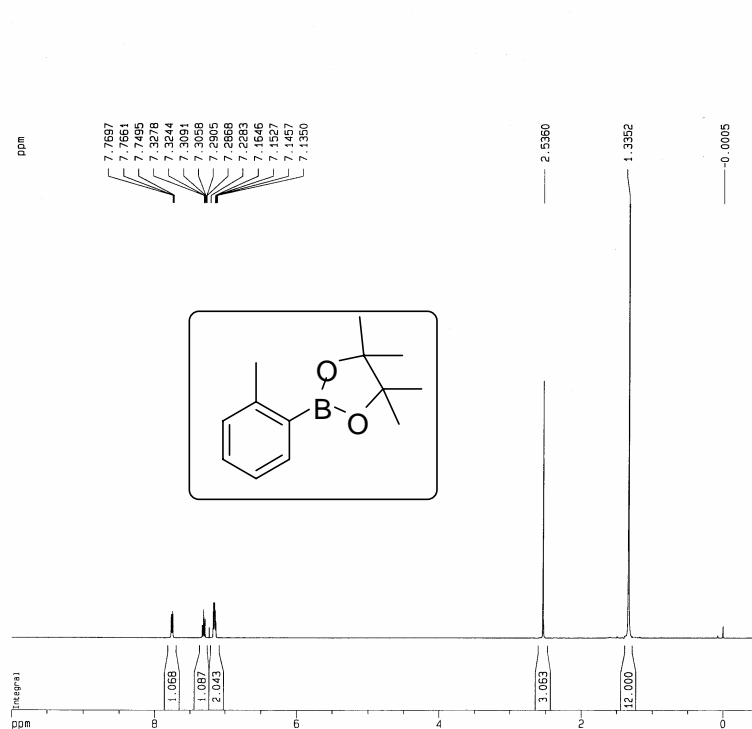
#### Biphenyl

$^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ )  $\delta$  7.60 (d,  $J = 7.5$  Hz, 4H), 7.47~7.37 (m, 4H), 7.35~7.32 (m, 2H);  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ )  $\delta$  141.2, 128.7, 127.2, 127.1.



# <sup>1</sup>H and <sup>13</sup>C NMR spectra



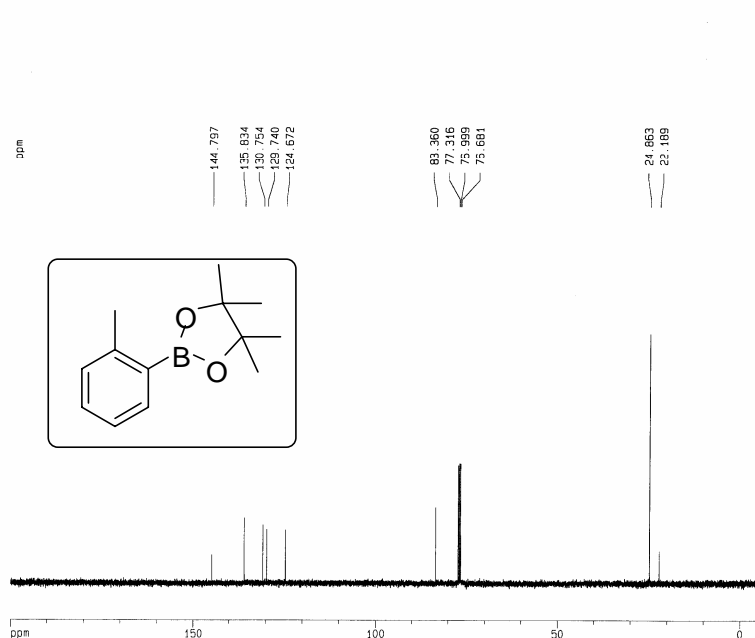


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 EXPNO 1  
 PROCNO 1

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 PULPROG zg  
 TO 32768  
 SOLVENT CDCl3  
 NS 16  
 DS 0  
 SWH 8064.516 Hz  
 FIDRES 0.246110 Hz  
 AQ 2.0316660 sec  
 RG 90  
 DW 62.000 usec  
 DE 88.57 usec  
 TE 300.0 K  
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 NUCLEUS 1H

F2 - Processing parameters  
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 WDW no  
 SSB 0  
 LB 0.00 Hz  
 GB 0  
 PC 4.00

1D NMR plot parameters  
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 F2 -200.07 Hz  
 PPMCM 0.52500 ppm/cm  
 HZCM 210.06827 Hz/cm

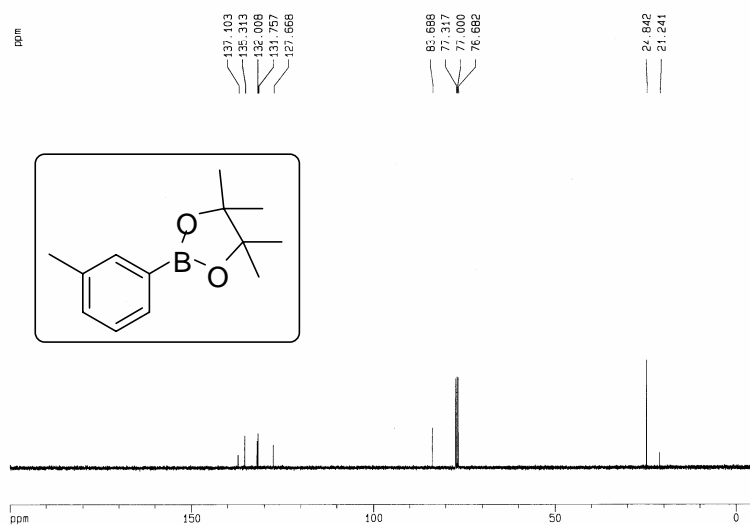
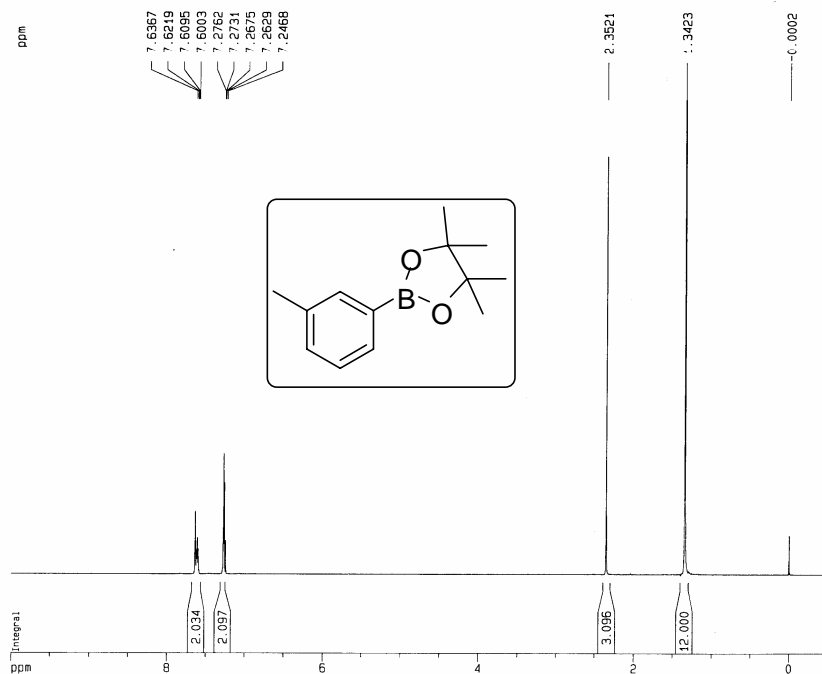


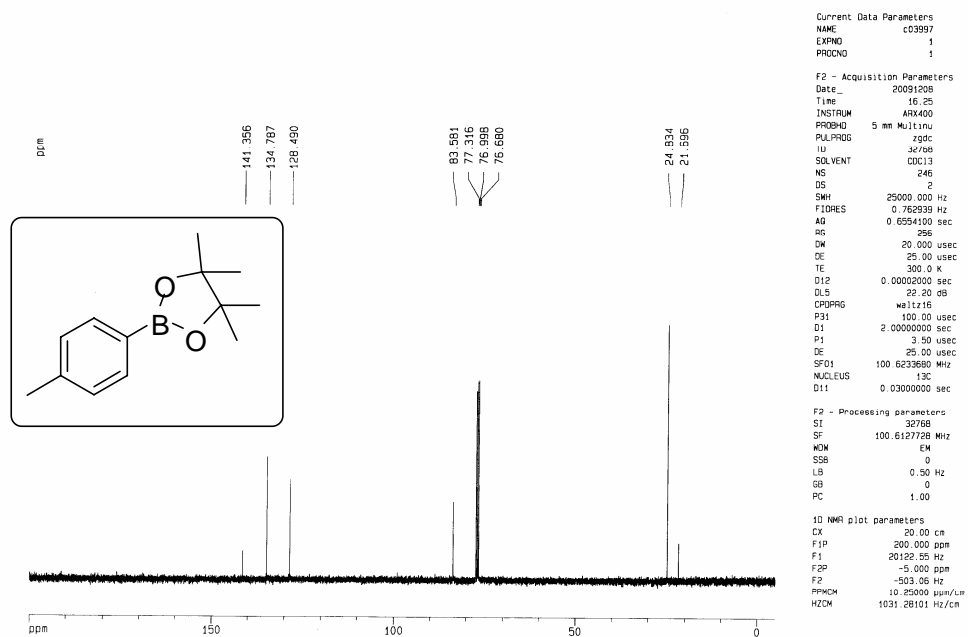
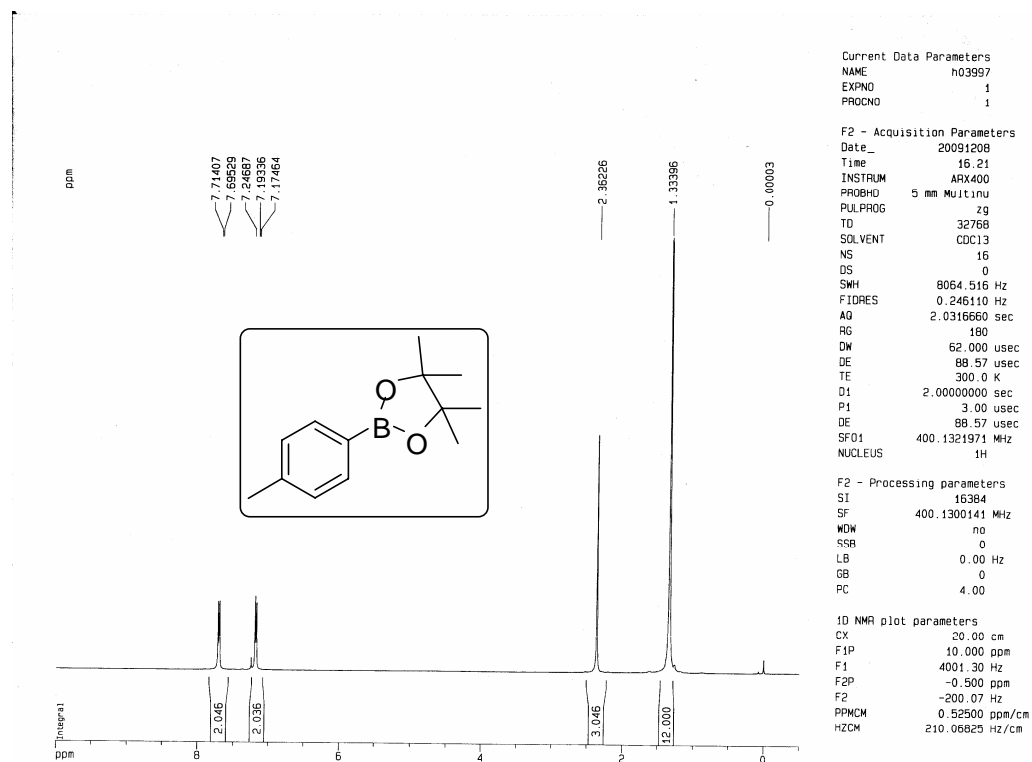
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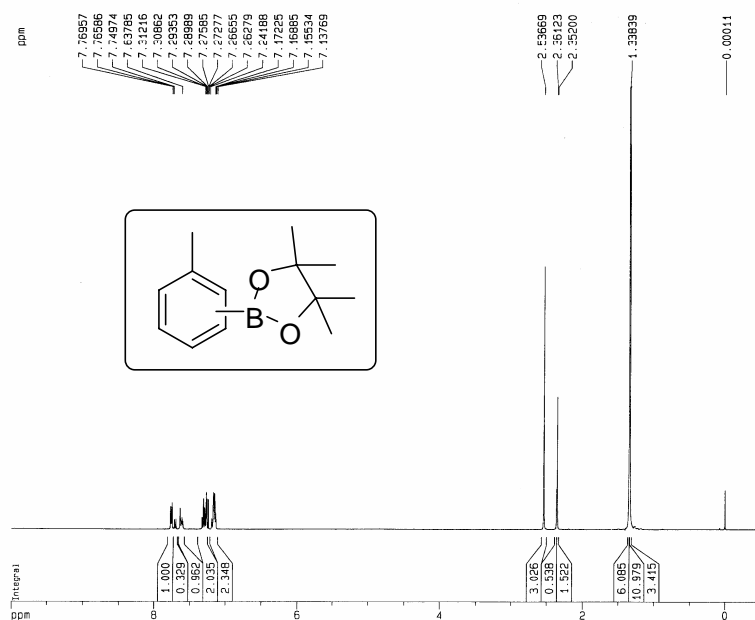
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 NS 70  
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 SWH 25000.000 Hz  
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 AQ 0.6554100 sec  
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 DE 25.00 usec  
 TE 300.0 K  
 D1P 0.00002000 sec  
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 CPDPRG walz16  
 P31 100.00 usec  
 D1 2.00000000 sec  
 P1 3.50 usec  
 DE 25.00 usec  
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 NUCLEUS 13C  
 D11 0.03000000 sec

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1D NMR plot parameters  
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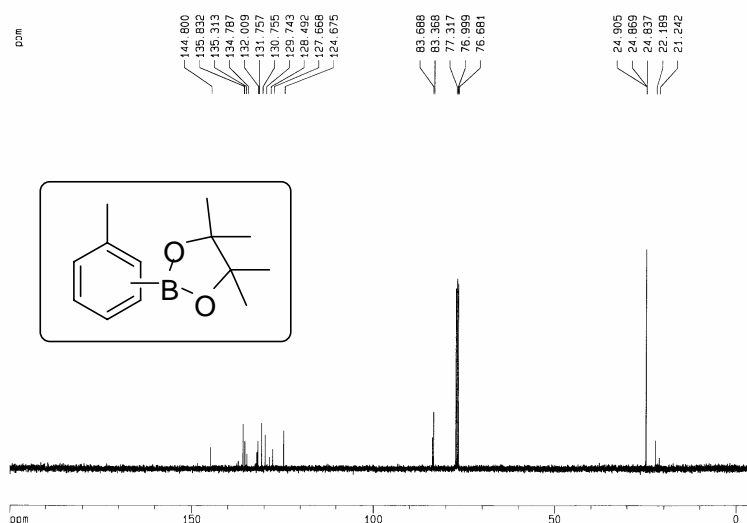


Current Data Parameters  
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EXPNO 1  
PROCNO 1

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PROBHD 5 mm Multinu  
PULPROG zg  
TD 32768  
SOLVENT CDCl3  
NS 16  
DS 0  
SWH 8064.516 Hz  
FIDRES 0.246110 Hz  
AQ 2.0316660 sec  
RG 128  
DW 62.000 usec  
DE 88.57 usec  
TE 300.0 K  
D1 2.00000000 sec  
P1 3.00 usec  
DE 88.57 usec  
SFO1 400.1321971 MHz  
NUCLEUS 1H

F2 - Processing parameters  
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SF 400.1300166 MHz  
WDW no  
SSB 0  
LB 0.00 Hz  
GB 0  
PC 4.00

1D NMR plot parameters  
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F1P 10.000 ppm  
F1 4001.30 Hz  
F2P -0.500 ppm  
F2 -200.07 Hz  
PPMCM 0.52500 ppm/cm  
HZCM 210.06825 Hz/cm

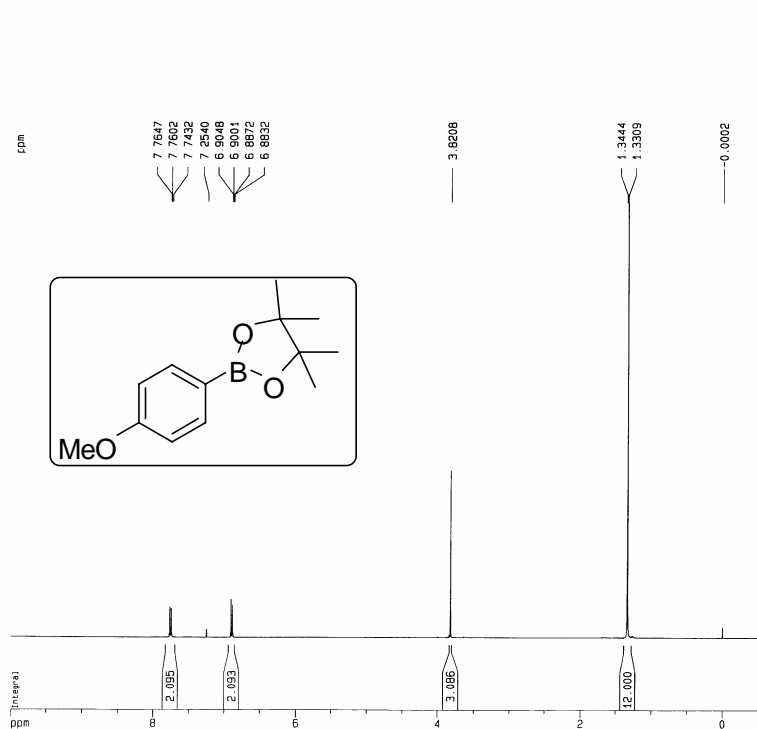


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PROCNO 1

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PULPROG zgpg  
TD 32768  
SOLVENT CDCl3  
NS 181  
DS 2  
SWH 25000.000 Hz  
FIDRES 0.762938 Hz  
AQ 0.6554100 sec  
RG 256  
DW 20.000 usec  
DE 25.00 usec  
TE 300.0 K  
D12 0.00002000 sec  
DLS 22.20 dB  
CPDPRG waltz16  
P31 100.00 usec  
D1 2.00000000 sec  
P1 3.50 usec  
DE 25.00 usec  
SFO1 100.6233680 MHz  
NUCLEUS 13C  
D11 0.03000000 sec

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WDW EM  
SSB 0  
LB 0.50 Hz  
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PC 1.00

1D NMR plot parameters  
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HZCM 1031.28101 Hz/cm

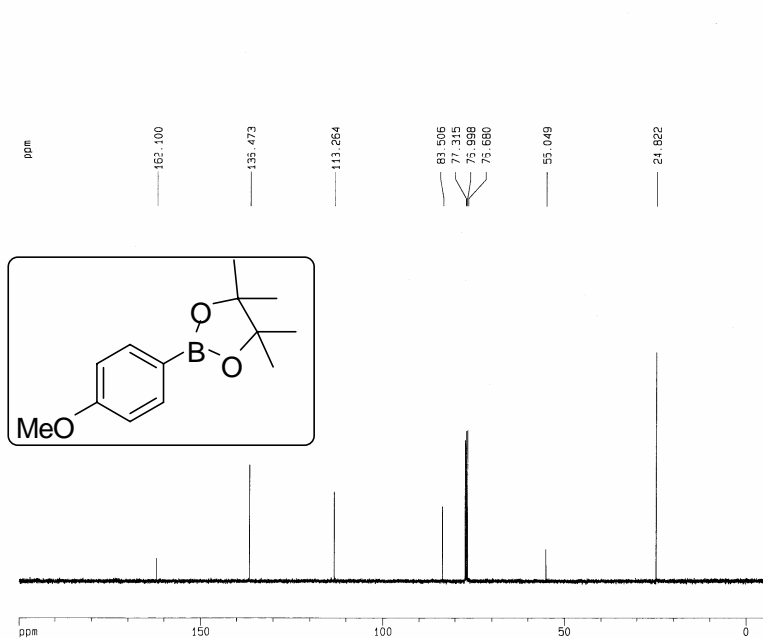


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EXPNO 1  
PROCNO 1

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Time 11.16  
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PULPROG zg  
TD 32768  
SOLVENT CDCl3  
NS 16  
DS 0  
SWH 8054.516 Hz  
FIDRES 0.246110 Hz  
AQ 2.0316660 sec  
RG 180  
DW 62.000 usec  
DE 88.57 usec  
TE 300.0 K  
D1 2.00000000 sec  
P1 3.00 usec  
DE 88.57 usec  
SF01 400.1321971 MHz  
NUCLEUS 1H

F2 - Processing parameters  
SI 16384  
SF 400.1300117 MHz  
WDW no  
SSB 0  
LB 0.00 Hz  
GB 0  
PC 4.00

1D NMR plot parameters  
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F1P 10.000 ppm  
F1 4001.30 Hz  
F2P -0.500 ppm  
F2 -200.07 Hz  
PPMCM 0.52500 ppm/cm  
HZCM 210.06825 Hz/cm

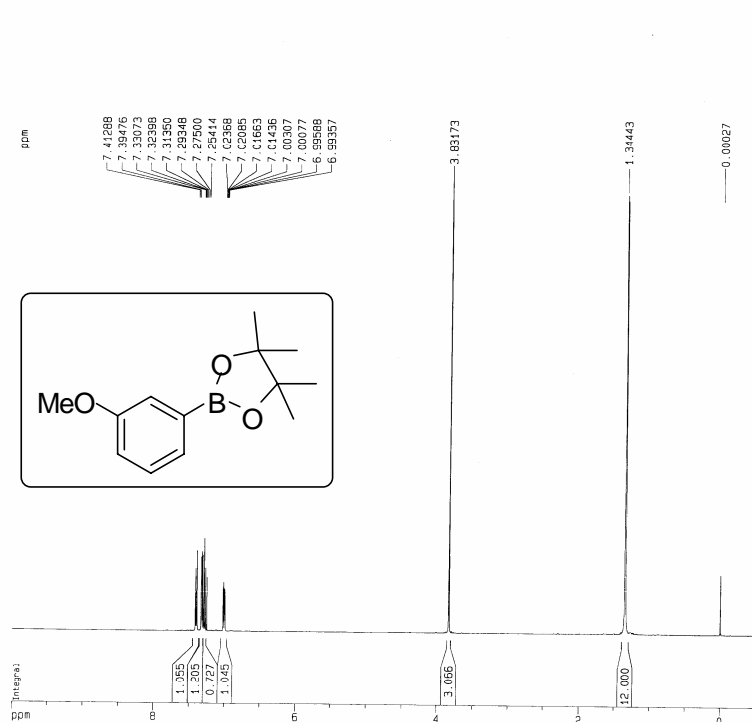


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NAME c04007  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
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PULPROG zgpg  
TD 32768  
SOLVENT CDCl3  
NS 243  
DS 2  
SWH 25000.000 Hz  
FIDRES 0.762935 Hz  
AQ 0.6554100 sec  
RG 256  
DW 20.000 usec  
DE 25.00 usec  
TE 300.0 K  
D12 0.00000000 sec  
DLS 22.20 dB  
CPDPRG waltz16  
P31 100.00 usec  
D1 2.00000000 sec  
P1 3.00 usec  
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F2 - Processing parameters  
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GB 0  
PC 1.00

1D NMR plot parameters  
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F2P -5.000 ppm  
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HZCM 1031.28101 Hz/cm

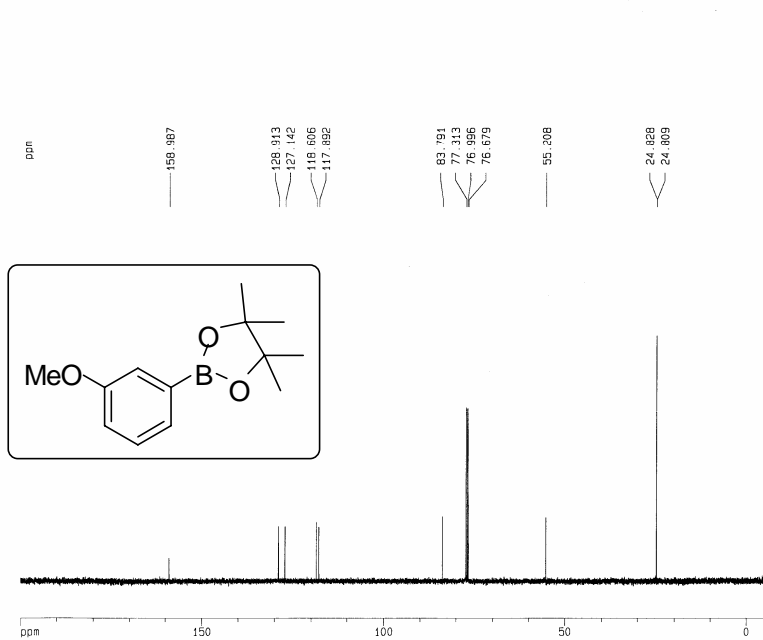


Current Data Parameters  
NAME n04009  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
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Time 13.58  
INSTRUM ARX400  
PROBHD 5 mm Multinu  
PULPROG zg  
TO 32768  
SOLVENT CDCl3  
NS 16  
DS 0  
SWH 8064.516 Hz  
FIDRES 0.246110 Hz  
AQ 2.0316660 sec  
RG 180  
DM 62.000 usec  
DE 88.57 usec  
TE 300.0 K  
D1 2.00000000 sec  
P1 3.00 usec  
DE 88.57 usec  
SFO1 400.1321974 MHz  
NUCLEUS 1H

F2 - Processing parameters  
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WDW no  
SSB 0  
LB 0.00 Hz  
GB 0  
PC 4.00

1D NMR plot parameters  
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F1P 10.000 ppm  
F1 4001.30 Hz  
F2P -0.500 ppm  
F2 -200.07 Hz  
PPMCM 0.52500 ppm/cm  
HZCM 210.06825 Hz/cm

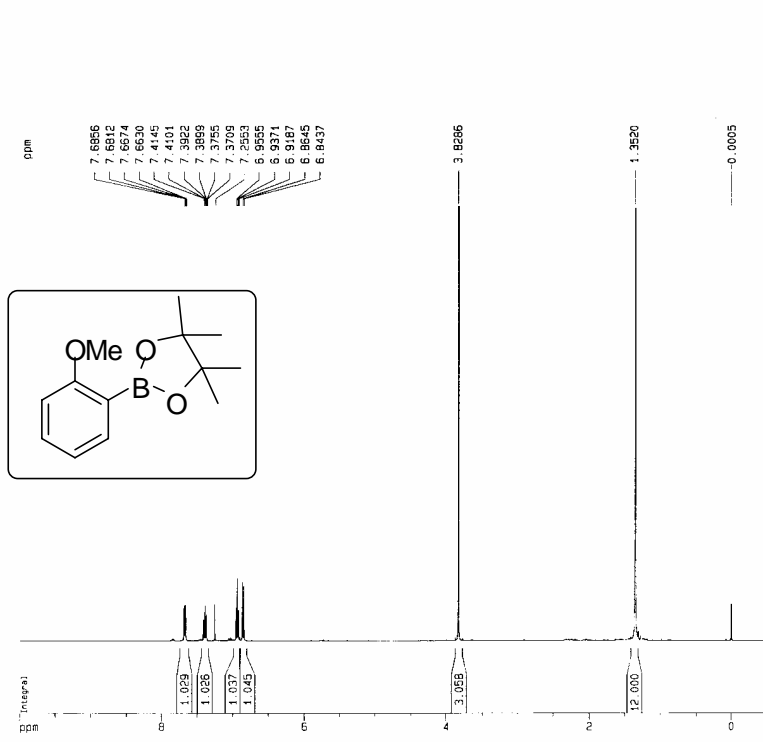


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EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
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INSTRUM ARX400  
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PULPROG zgpg  
TO 32768  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 25000.000 Hz  
FIDRES 0.762939 Hz  
AQ 0.6554100 sec  
RG 256  
DM 20.000 usec  
DE 25.00 usec  
TE 300.0 K  
D12 0.00000000 sec  
DL5 22.20 dB  
CPRPRG waltz16  
P31 100.00 usec  
D1 2.00000000 sec  
P1 3.50 usec  
DE 25.00 usec  
SFO1 100.6233680 MHz  
NUCLEUS 13C  
D11 0.03000000 sec

F2 - Processing parameters  
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SF 100.6127743 MHz  
WDW EM  
SSB 0  
LB 0.50 Hz  
GB 0  
PC 1.00

1D NMR plot parameters  
CX 20.00 cm  
F1P 200.000 ppm  
F1 20122.56 Hz  
F2P -5.000 ppm  
F2 -503.06 Hz  
PPMCM 10.25000 ppm/cm  
HZCM 1031.28101 Hz/cm

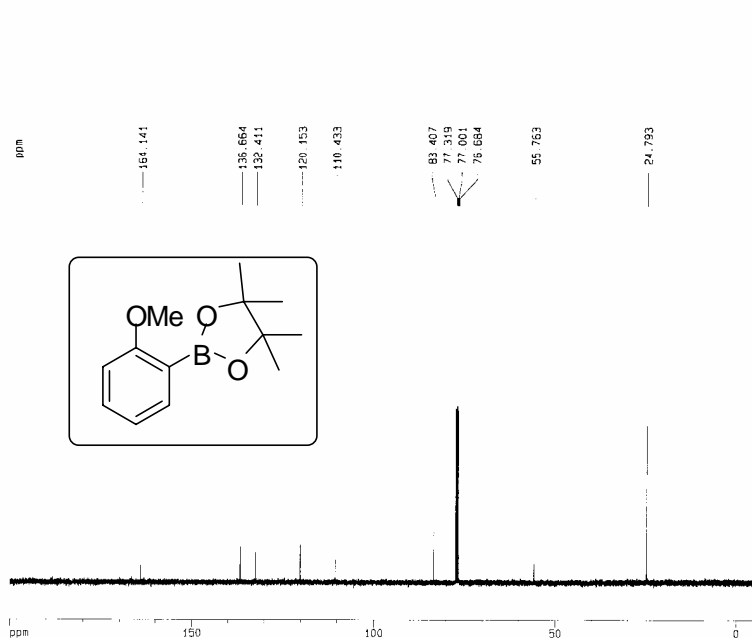


Current Data Parameters  
NAME h04066  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
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Time 10.06  
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PROBHD 5 mm Multinu  
PULPROG zg  
TD 32768  
SOLVENT CDCl3  
NS 16  
DS 0  
SWH 8064.516 Hz  
FIDRES 0.246110 Hz  
AQ 2.0316650 sec  
RG 256  
DM 62.000 usec  
DE 88.57 usec  
TE 300.0 K  
D1 2.0000000 sec  
P1 3.00 usec  
DE 88.57 usec  
SFO1 400.1321971 MHz  
NUCLEUS 1H

F2 - Processing parameters  
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SF 400.1300112 MHz  
WDW no  
SSB 0  
LB 0.00 Hz  
GB 0  
PC 4.00

1D NMR plot parameters  
CX 20.00 cm  
F1P 10.000 ppm  
F1 4001.30 Hz  
F2P -0.500 ppm  
F2 -200.07 Hz  
P1MCM 0.52500 ppm/cm  
HZCM 210.06825 Hz/cm



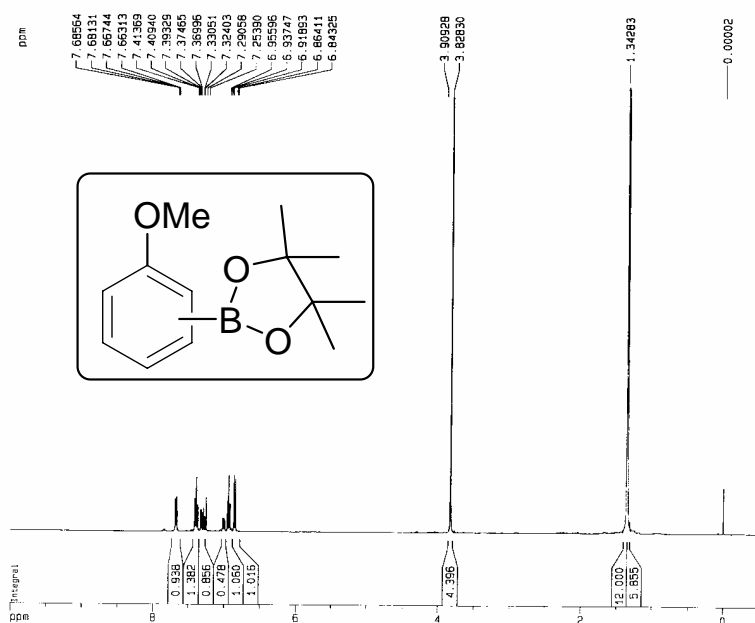
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NAME c04066  
EXPNO 1  
PROCNO 1

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Time 10.08  
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PULPROG zgpg  
TD 32768  
SOLVENT CDCl3  
NS 149  
DS 2  
SWH 25000.000 Hz  
FIDRES 0.782938 Hz  
AQ 0.6554100 sec  
RG 256  
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DE 25.00 usec  
TE 300.0 K  
D12 0.0002000 sec  
DLS 22.50 dB  
CPDPRG waltz16  
P31 100.00 usec  
D1 2.0000000 sec  
P1 3.50 usec  
DE 25.00 usec  
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NUCLEUS 13C  
D11 0.03000000 sec

F2 - Processing parameters  
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WDW EM  
SSB 0  
LB 0.50 Hz  
GB 0  
PC 1.00

1D NMR plot parameters  
CX 20.00 cm  
F1P 200.000 ppm  
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F2P -5.000 ppm  
F2 -503.05 Hz  
P1MCM 10.25000 ppm/cm  
HZCM 1031.28101 Hz/cm





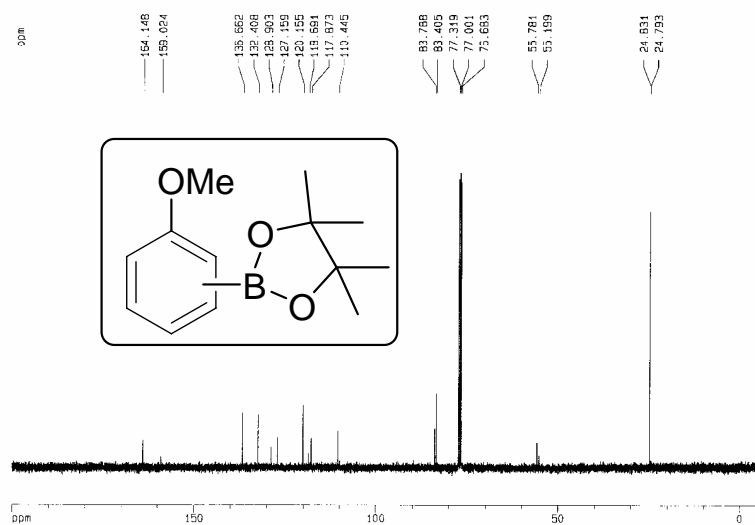
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EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
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PULPROG  zg
TD        32768
SOLVENT  CDCl3
NS        16
DS        0
SWH       8064.516 Hz
FIDRES   0.246110 Hz
AQ        2.0316660 sec
RG         180
DM        62.000 usec
DE        88.57 usec
TE        300.0 K
D1        2.00000000 sec
P1        3.00 usec
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SFO1     400.1321971 MHz
NUCLEUS  1H

F2 - Processing parameters
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SF        400.1300117 MHz
WDW       no
SSB       0
LB        0.00 Hz
GB        0
PC        4.00

1D NMR plot parameters
CX        20.00 cm
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PPMCM    0.52500 ppm/cm
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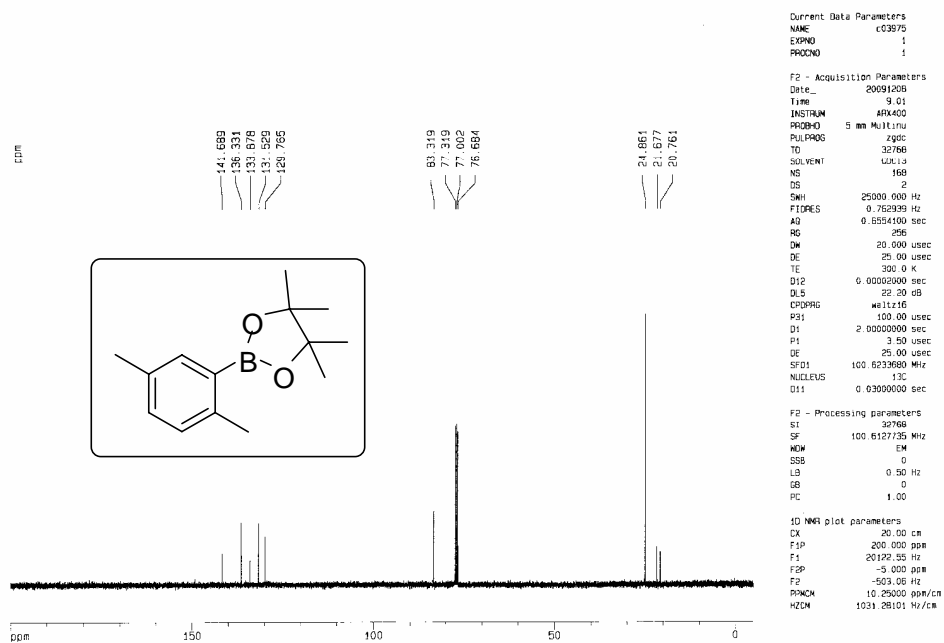
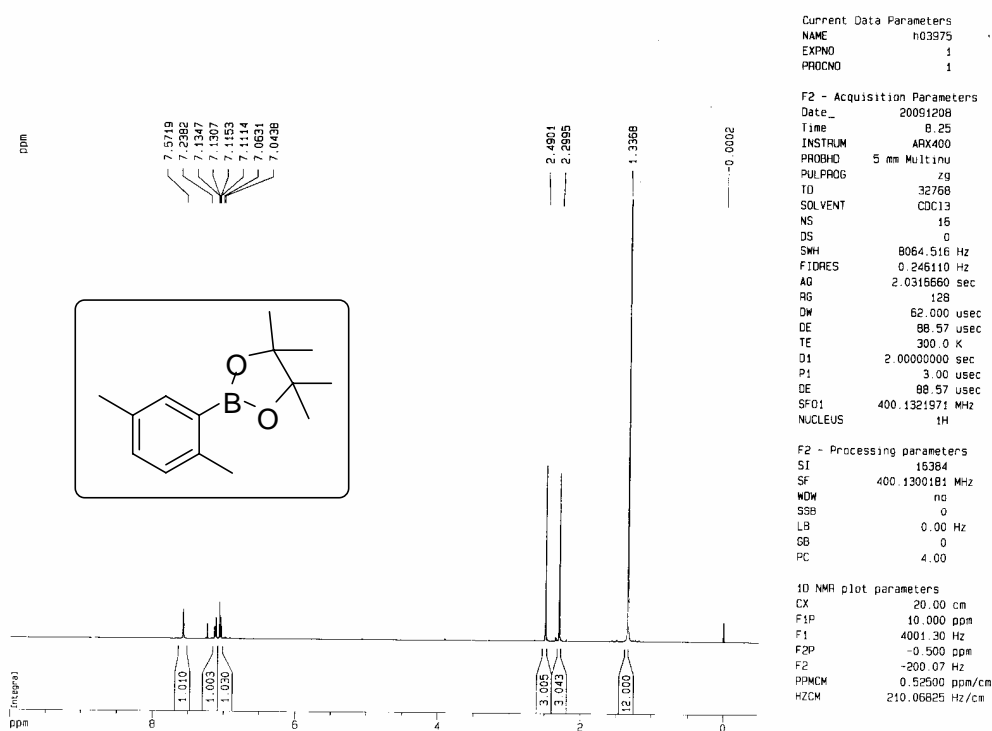
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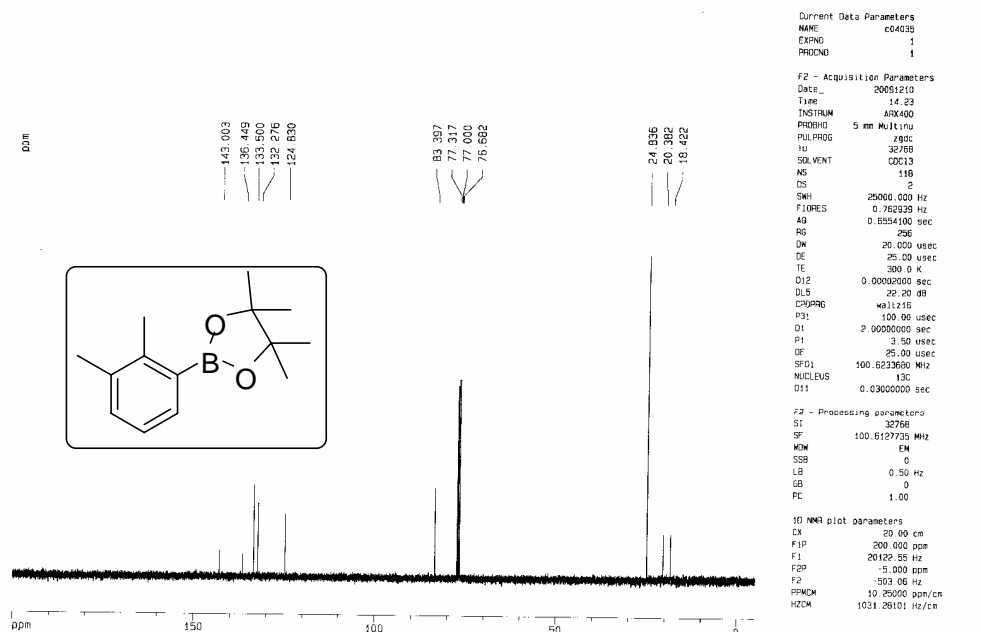
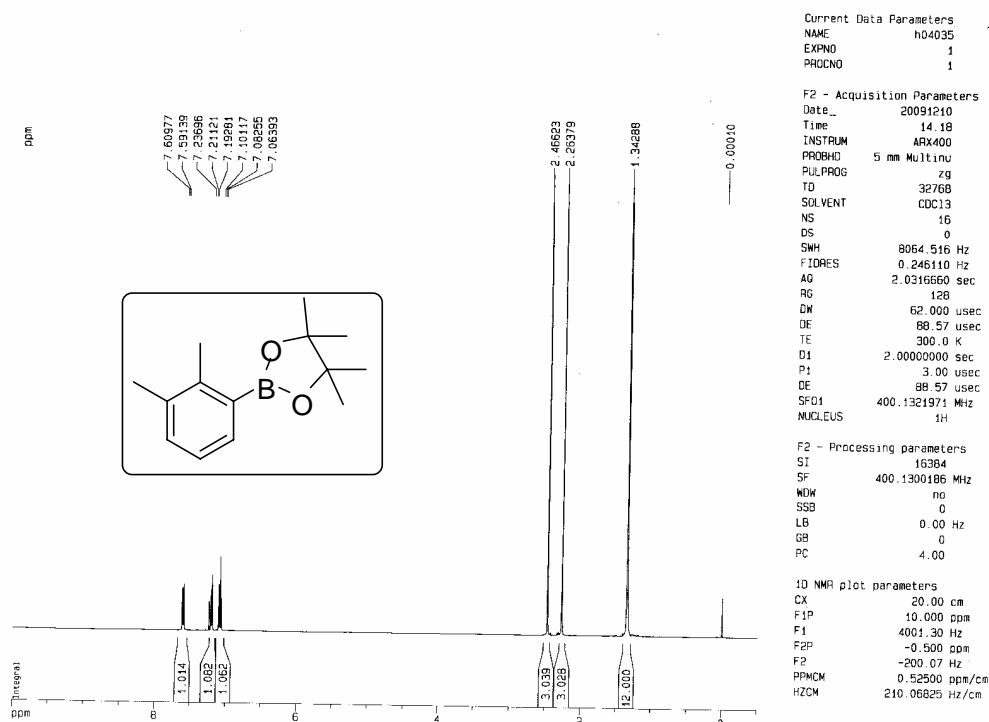
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EXPNO    1
PROCNO   1

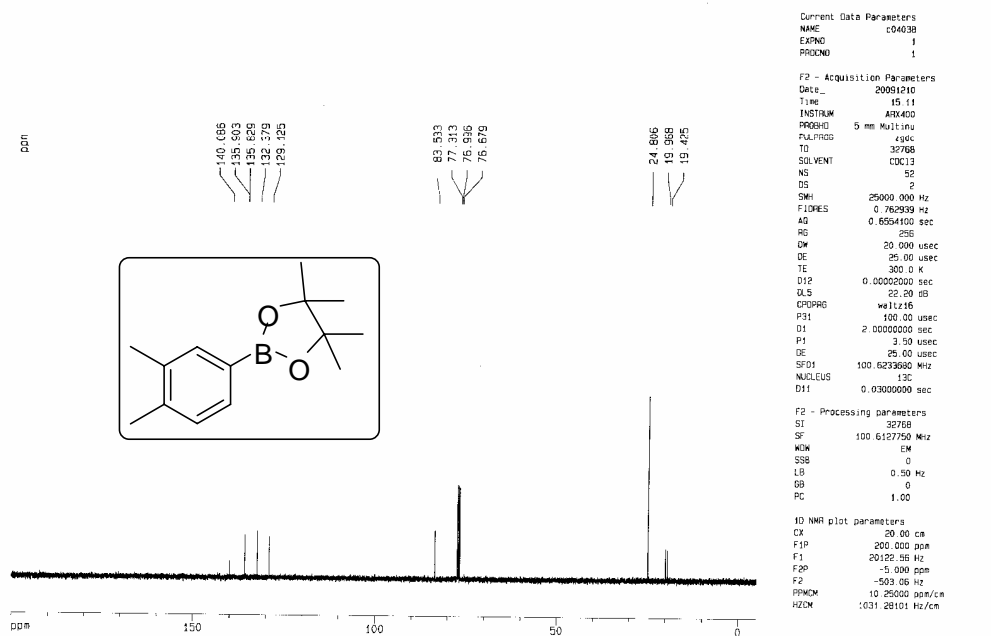
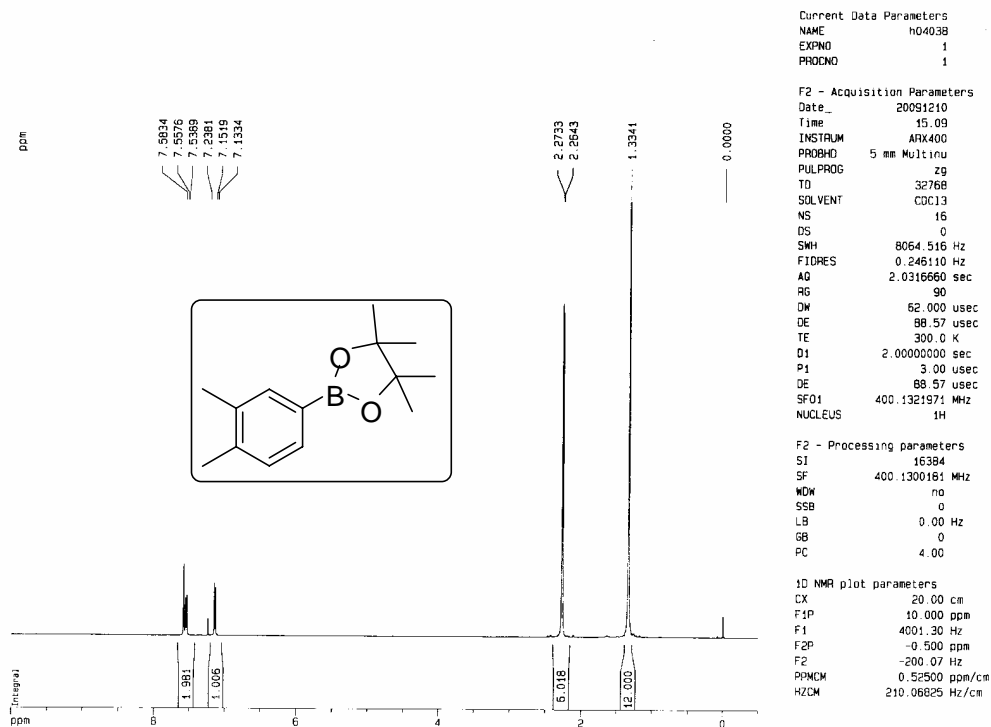
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PROBHD   5 mm Multinu
PULPROG  zgpg
TD        32768
SOLVENT  CDCl3
NS        2
DS        2
SWH       25000.000 Hz
FIDRES   0.762939 Hz
AQ        0.6594100 sec
RG         256
DM        20.000 usec
DE        20.00 usec
TE        300.0 K
D12       0.00002000 sec
DL5       22.20 dB
CPDPRG   waltz16
F21       100.00 usec
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NUCLEUS  13C
D11       0.03000000 sec

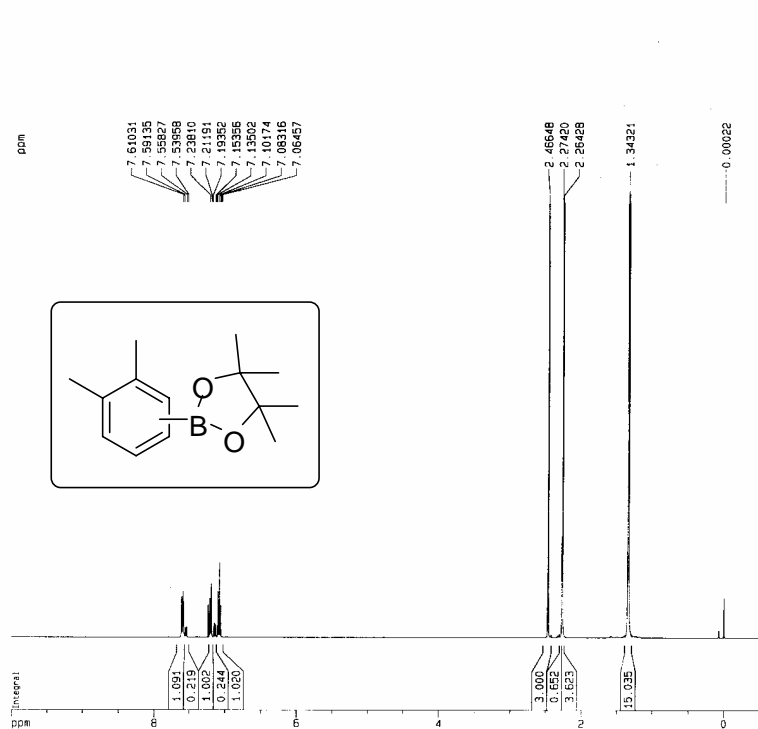
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SF        100.6127728 MHz
WDW       EM
SSB       0
LB        0.50 Hz
GB        0
PC        1.00

1D NMR plot parameters
CX        20.00 cm
F1P       200.000 ppm
F1        20122.55 Hz
F2P       -5.000 ppm
F2        -503.05 Hz
PPMCM    10.25000 ppm/cm
HZCM     1031.28191 Hz/cm
    
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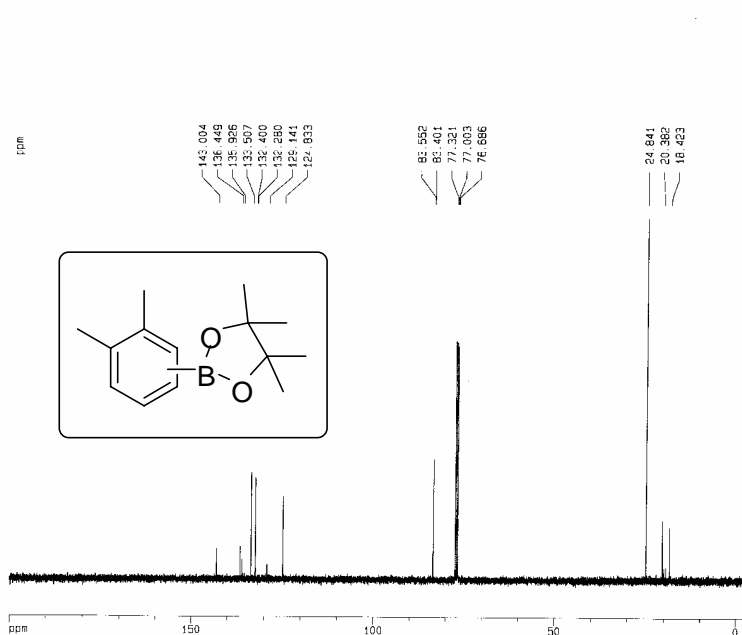


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 EXPNO 1  
 PROCNO 1

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 PULPROG zg  
 TD 32768  
 SOLVENT CDCl3  
 NS 16  
 DS 0  
 SWH 8064.516 Hz  
 FIDRES 0.246110 Hz  
 AQ 2.0316660 sec  
 RG 128  
 DW 62.000 usec  
 DE 88.57 usec  
 TE 300.0 K  
 D1 2.00000000 sec  
 P1 3.00 usec  
 DE 88.57 usec  
 SF01 400.1321971 MHz  
 NUCLEUS 1H

F2 - Processing parameters  
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 WDW no  
 SSB 0  
 LB 0.00 Hz  
 GB 0  
 PC 4.00

1D NMR plot parameters  
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 F1P 10.000 ppm  
 F1 4001.30 Hz  
 F2P -0.500 ppm  
 F2 -200.07 Hz  
 PPMCM 0.52500 ppm/cm  
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Current Data Parameters  
 NAME c04937  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
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 Time 14.59  
 INSTRUM ARX400  
 PROBHD 5 mm Multinu  
 PULPROG zgpgc  
 TD 32768  
 SOLVENT CDCl3  
 NS 256  
 DS 2  
 SWH 25000.000 Hz  
 FIDRES 0.762398 Hz  
 AQ 0.6954100 sec  
 RG 256  
 DW 20.000 usec  
 DE 25.00 usec  
 TE 300.0 K  
 D12 0.0002000 sec  
 D15 22.20 usec  
 CQPRP w21216  
 P31 100.00 usec  
 D1 2.00000000 sec  
 P1 3.50 usec  
 DE 25.00 usec  
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 NUCLEUS 13C  
 D11 0.03060000 sec

F2 - Processing parameters  
 SI 32768  
 SF 100.6127726 MHz  
 WDW EM  
 SSB 0  
 LB 0.50 Hz  
 GB 0  
 PC 1.00

1D NMR plot parameters  
 CX 20.00 cm  
 F1P 200.000 ppm  
 F1 20122.55 Hz  
 F2P -5.000 ppm  
 F2 -503.06 Hz  
 PPMCM 10.25000 ppm/cm  
 HZCM 1031.26101 Hz/cm

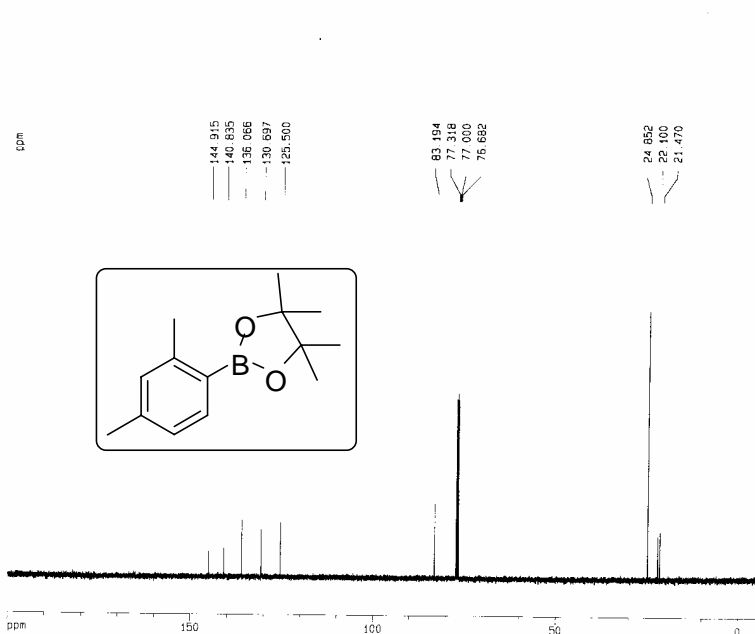


Current Data Parameters  
 NAME h04010  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20091209  
 Time 14.12  
 INSTRUM AX400  
 PROBHD 5 mm Multinu  
 PULPROG zgpg30  
 TO 32768  
 SOLVENT CDCl3  
 NS 16  
 DS 0  
 SWH 8064.516 Hz  
 FIDRES 0.246110 Hz  
 AQ 2.0316660 sec  
 RG 180  
 DW 62.000 usec  
 DE 88.57 usec  
 TE 300.0 K  
 D1 2.00000000 sec  
 P1 3.00 usec  
 DE 88.57 usec  
 SFO1 400.1321971 MHz  
 NUCLEUS 1H

F2 - Processing parameters  
 SI 16384  
 SF 400.1300166 MHz  
 NHX no  
 SSB 0  
 LB 0.00 Hz  
 GB 0  
 PC 4.00

1D NMR plot parameters  
 CX 20.00 cm  
 F1P 10.000 ppm  
 F1 4001.30 Hz  
 F2P -0.500 ppm  
 F2 -200.07 Hz  
 PPMCM 0.52500 ppm/cm  
 HZCM 210.05825 Hz/cm

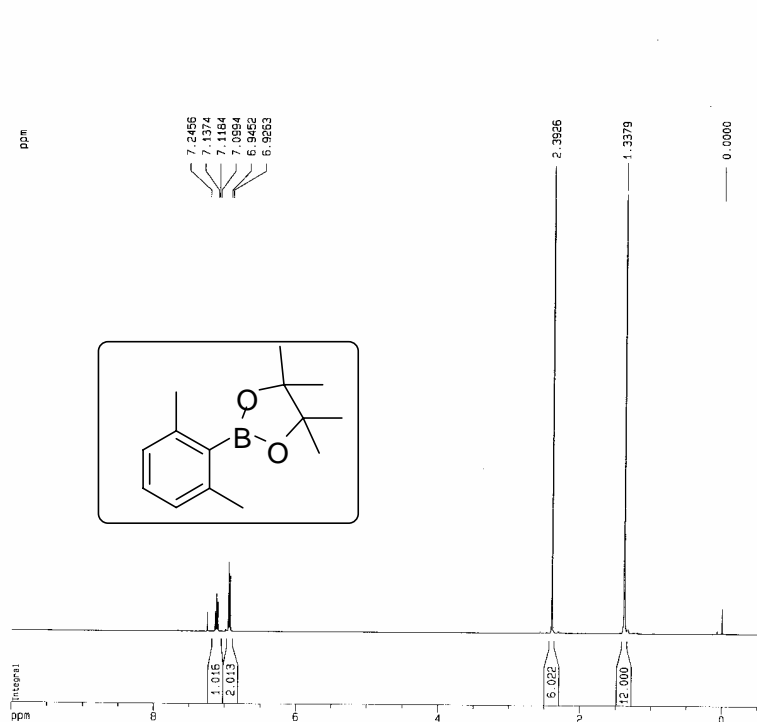


Current Data Parameters  
 NAME c04010  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20091209  
 Time 14.17  
 INSTRUM AX400  
 PROBHD 5 mm Multinu  
 PULPROG zgpg30  
 TO 32768  
 SOLVENT CDCl3  
 NS 160  
 DS 2  
 SWH 25000.000 Hz  
 FIDRES 0.762959 Hz  
 AQ 0.6554100 sec  
 RG 256  
 DW 20.000 usec  
 DE 25.00 usec  
 TE 300.0 K  
 D12 0.00002000 sec  
 DLS 22.20 dB  
 CPDPRG waltz16  
 P31 100.00 usec  
 D1 2.00000000 sec  
 P1 3.50 usec  
 DE 25.00 usec  
 SFO1 100.6233660 MHz  
 NUCLEUS 13C  
 D11 0.03000000 sec

F2 - Processing parameters  
 SI 32768  
 SF 100.6127743 MHz  
 NHX EM  
 SSB 0  
 LB 0.50 Hz  
 GB 0  
 PC 1.00

1D NMR plot parameters  
 CX 20.00 cm  
 F1P 200.000 ppm  
 F1 20122.56 Hz  
 F2P -5.000 ppm  
 F2 -503.06 Hz  
 PPMCM 10.25000 ppm/cm  
 HZCM 1031.28101 Hz/cm

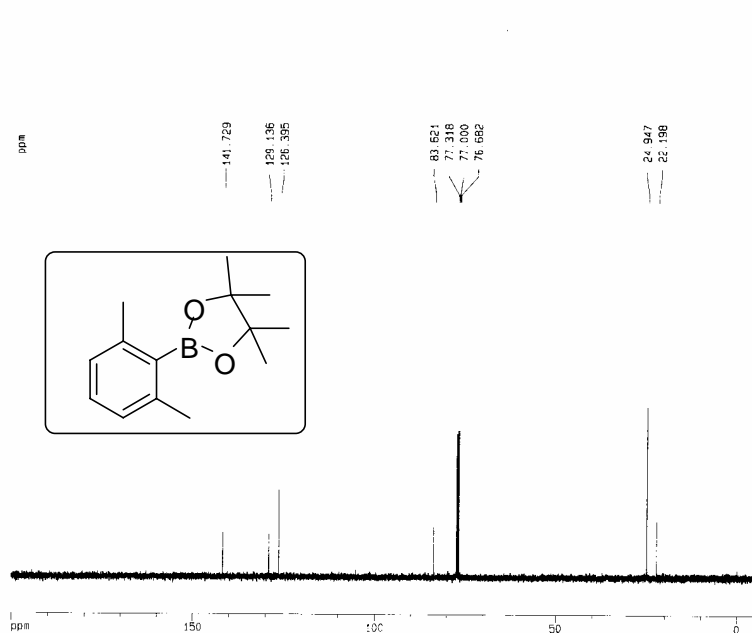


Current Data Parameters  
NAME h04039  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20091210  
Time 15.22  
INSTRUM ARX400  
PROBHD 5 mm Multinu  
PULPROG zg  
TD 32768  
SOLVENT CDCl3  
NS 16  
DS 0  
SWH 8064.616 Hz  
FIDRES 0.246110 Hz  
AQ 2.0316660 sec  
RG 128  
DW 62.000 usec  
DE 68.57 usec  
TE 300.0 K  
D1 2.00000000 sec  
P1 3.00 usec  
DE 68.57 usec  
SFO1 400.1321971 MHz  
NUCLEUS 1H

F2 - Processing parameters  
SI 15384  
SF 400.1300151 MHz  
WDW no  
SSB 0  
LB 0.00 Hz  
GB 0  
PC 4.00

1D NMR plot parameters  
CX 20.00 cm  
F1P 10.000 ppm  
F1 4001.30 Hz  
F2P -0.500 ppm  
F2 -200.07 Hz  
PQCM 0.52500 ppm/cm  
HZCM 210.06825 Hz/cm

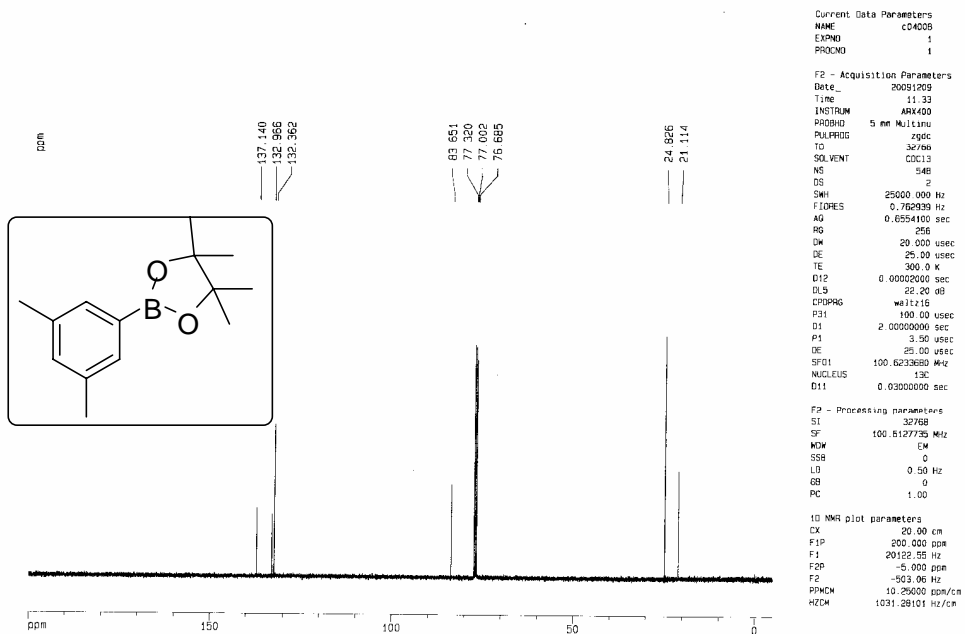
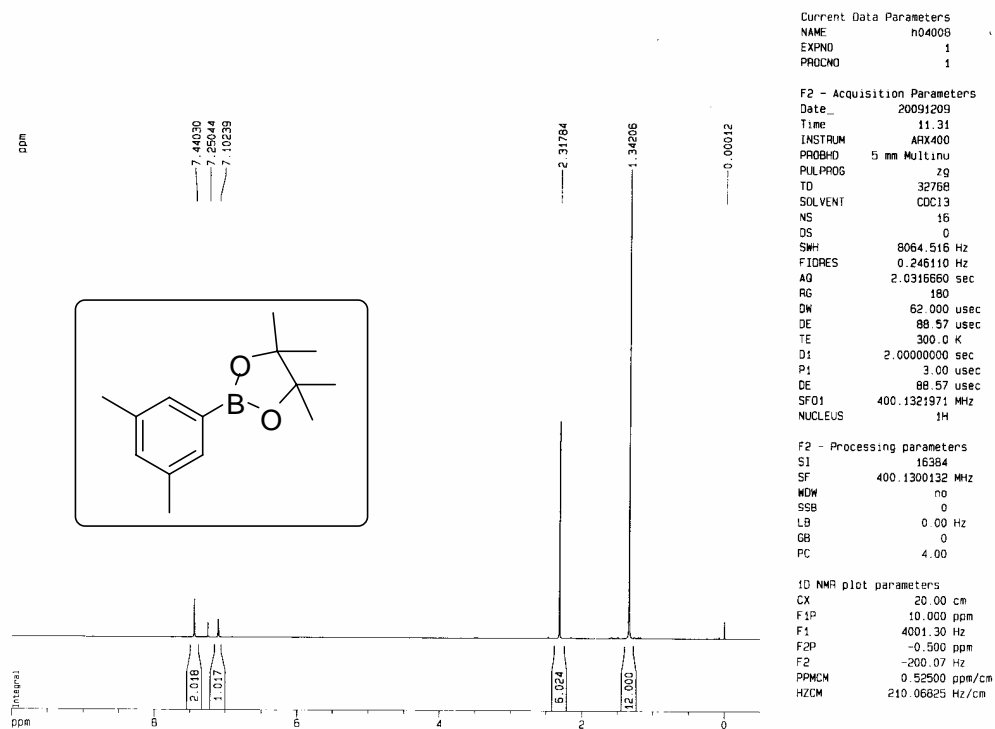


Current Data Parameters  
NAME c04039  
EXPNO 1  
PROCNO 1

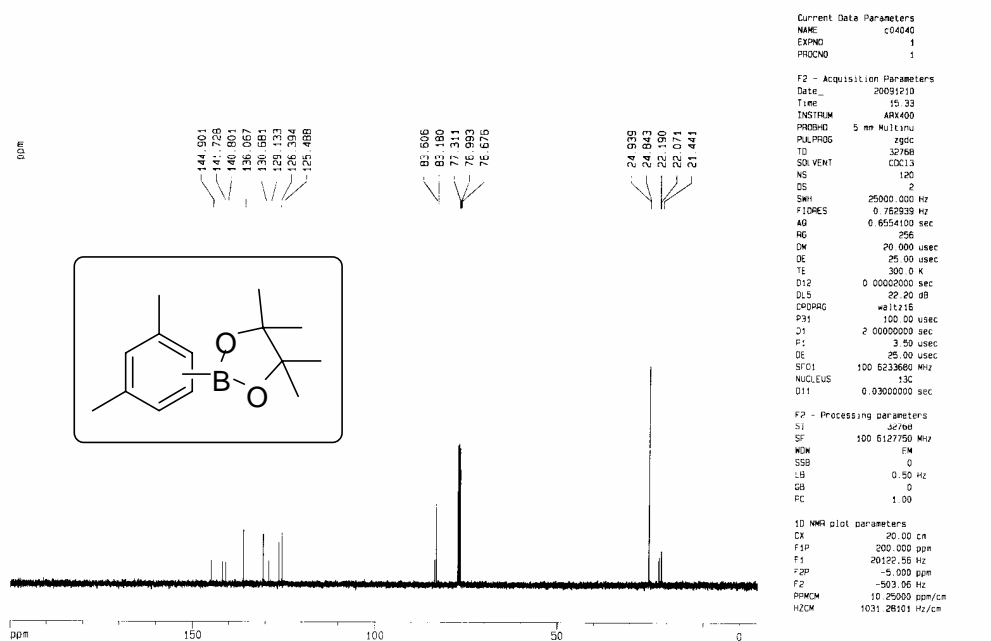
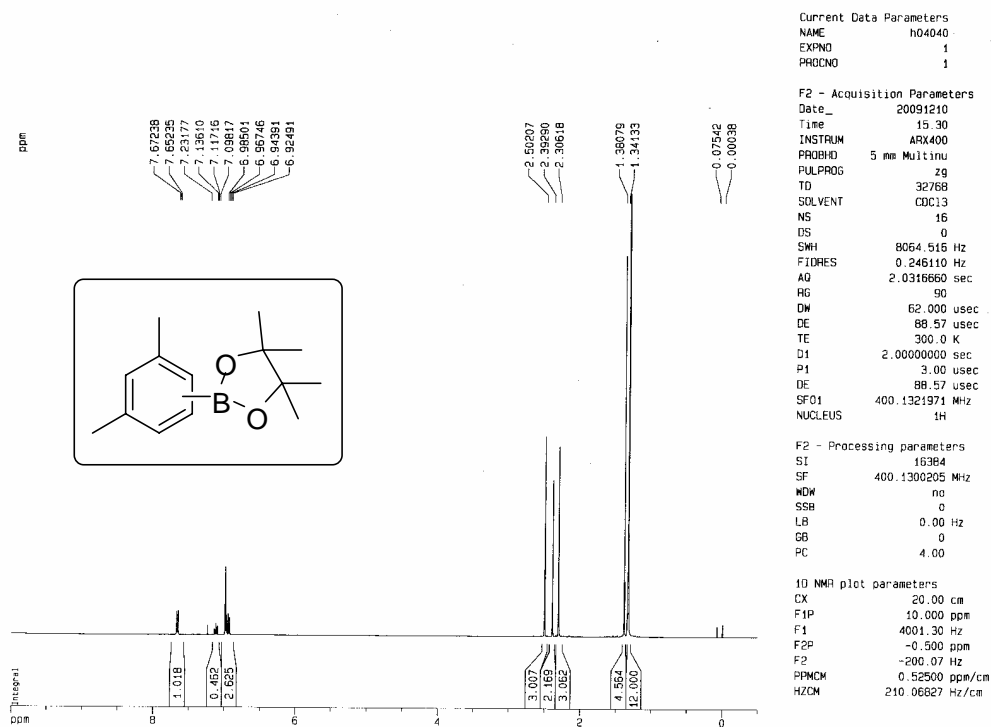
F2 - Acquisition Parameters  
Date\_ 20091210  
Time 15.24  
INSTRUM ARX400  
PROBHD 5 mm Multinu  
PULPROG zgpg  
TD 32768  
SOLVENT CDCl3  
NS 72  
DS 2  
SWH 25000.000 Hz  
FIDRES 0.762939 Hz  
AQ 0.6554100 sec  
RG 256  
DW 20.000 usec  
DE 25.00 usec  
TE 300.0 K  
D12 0.00000000 sec  
D13 22.00 usec  
CPDPRG waltz16  
P31 100.00 usec  
D1 2.00000000 sec  
P1 3.50 usec  
DE 25.00 usec  
SFO1 100.6233690 MHz  
NUCLEUS 13C  
D11 0.03000000 sec

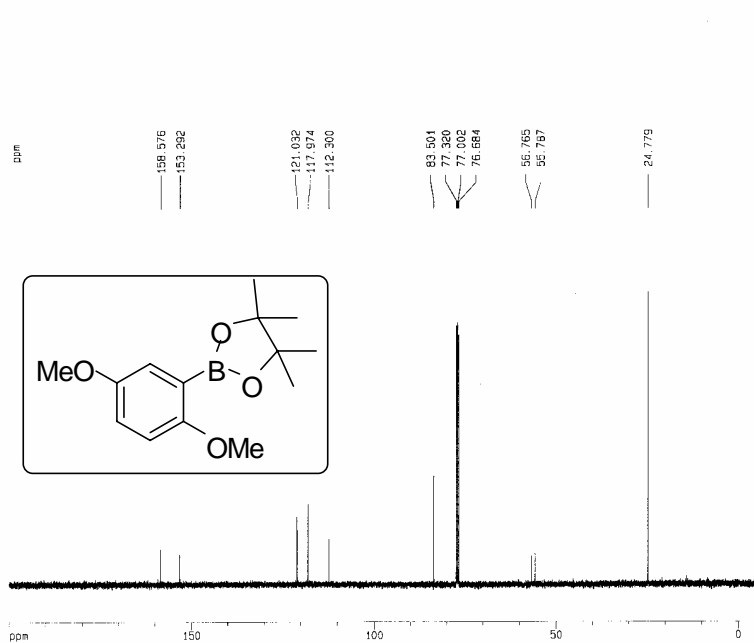
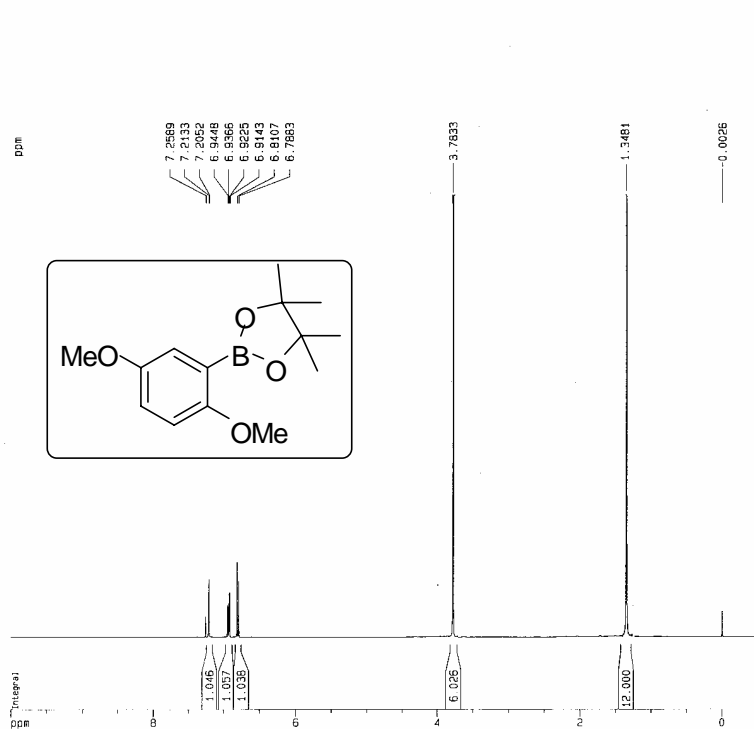
F2 - Processing parameters  
SI 32768  
SF 100.6127735 MHz  
WDW EM  
SSB 0  
LB 0.50 Hz  
GB 0  
PC 1.00

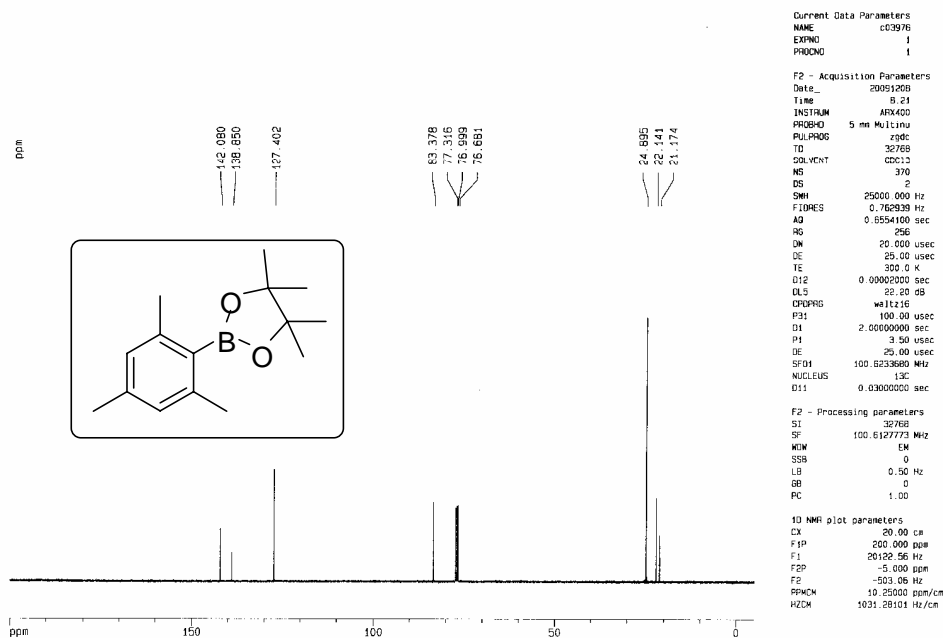
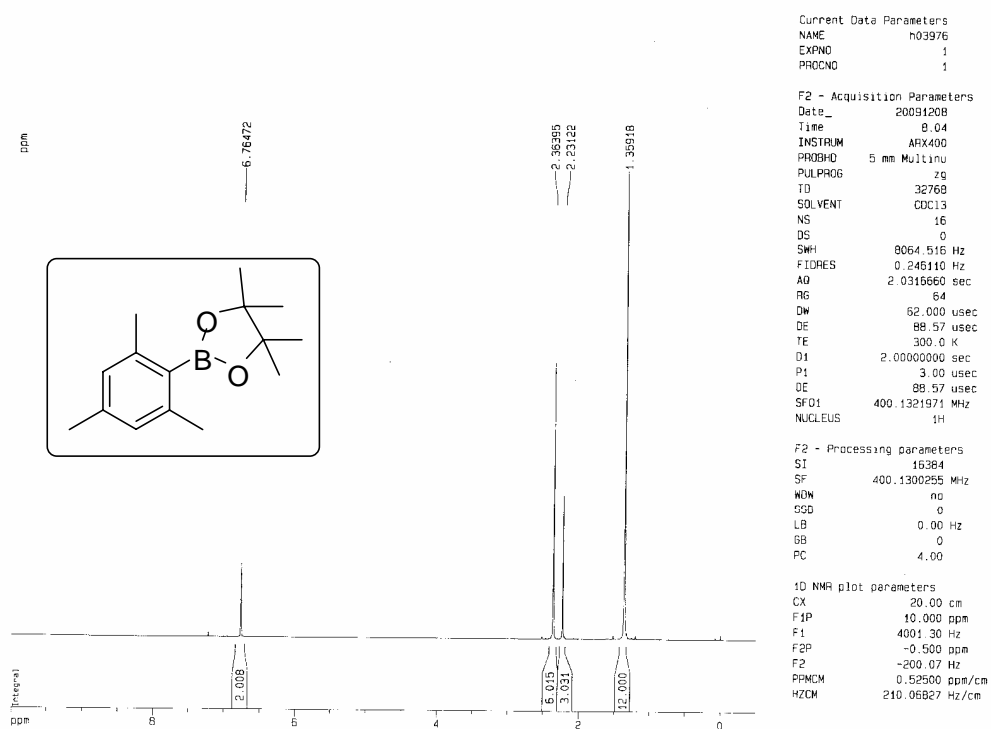
1D NMR plot parameters  
CX 20.00 cm  
F1P 200.000 ppm  
F1 20122.55 Hz  
F2P -5.000 ppm  
F2 -503.06 Hz  
PQCM 10.25000 ppm/cm  
HZCM 1031.28101 Hz/cm

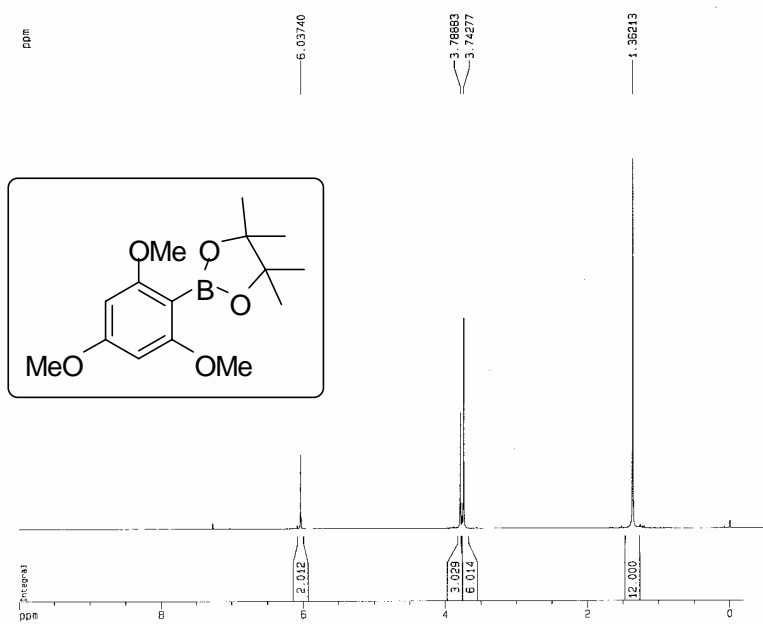












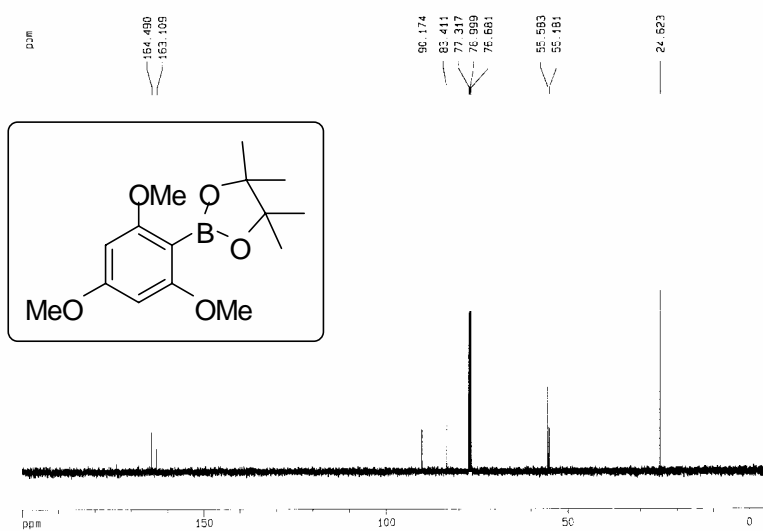
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Current Data Parameters
NAME      h03984
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    20091208
Time     9.26
INSTRUM  ARX400
PROBHD   5 mm Multinu
PULPROG  zg
TD        32768
SOLVENT  CDCl3
NS        16
DS        0
SWH       8064.516 Hz
FIDRES   0.246110 Hz
AQ        2.0316650 sec
RG         128
DW        62.000 usec
DE        88.57 usec
TE        300.0 K
O1        2.0000000 sec
P1         3.00 usec
DE        88.57 usec
SFO1     400.1321971 MHz
NUCLEUS  1H

F2 - Processing parameters
SI        16384
SF        400.1300058 MHz
WDW       no
SSB       0
LB        0.00 Hz
GB        0
PC        4.00

1D NMR plot parameters
CX        20.00 cm
F1P       10.000 ppm
F1        4001.30 Hz
F2P       -0.500 ppm
F2        -200.07 Hz
PPMCM    0.52500 ppm/cm
HZCM     210.06625 Hz/cm
    
```



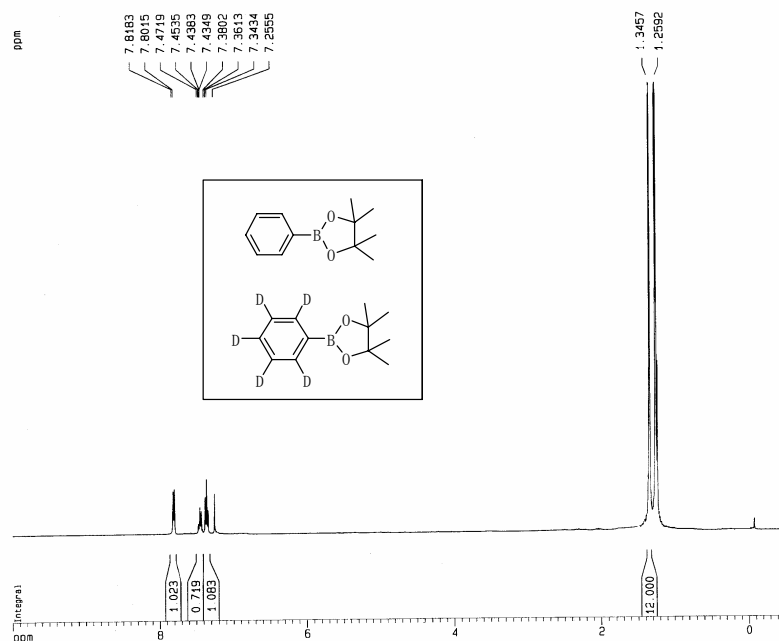
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Current Data Parameters
NAME      c03984
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    20091208
Time     9.26
INSTRUM  ARX400
PROBHD   5 mm Multinu
PULPROG  zgpg30
TD        32768
SOLVENT  CDCl3
NS        76
DS        2
SWH       25000.000 Hz
FIDRES   0.752939 Hz
AQ        0.6554100 sec
RG         256
DW        20.000 usec
DE        25.00 usec
TE        300.0 K
O1P       0.0000000 sec
DLS       22.20 dB
CPDPRG   waltz16
P31       100.00 usec
O1        2.0000000 sec
P1         3.50 usec
DE        25.00 usec
SFO1     100.6233650 MHz
NUCLEUS  13C
D11       0.0300000 sec

F2 - Processing parameters
SI        32768
SF        100.6127751 MHz
WDW       EM
SSB       0
LB        0.50 Hz
GB        0
PC        1.00

1D NMR plot parameters
CX        20.00 cm
F1P       200.000 ppm
F1        20122.56 Hz
F2P       -5.000 ppm
F2        -503.06 Hz
PPMCM    10.25000 ppm/cm
HZCM     1031.28101 Hz/cm
    
```

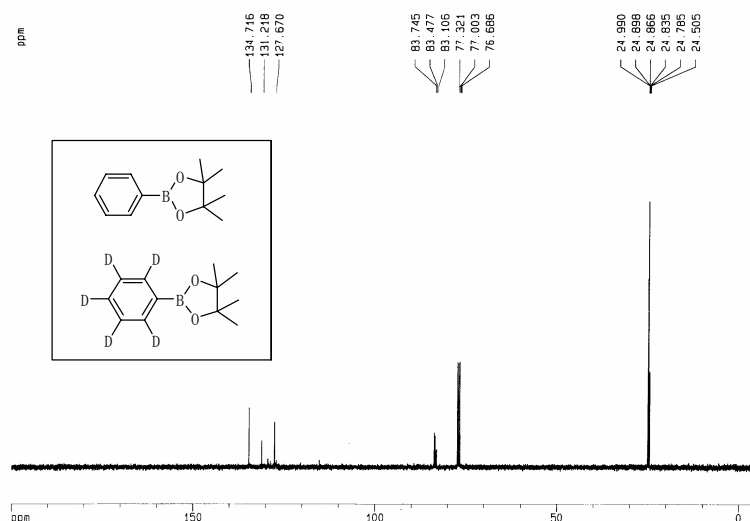


Current Data Parameters  
 NAME n02140  
 EXPNO 1  
 PROCNU 1

F2 - Acquisition Parameters  
 Date\_ 20090615  
 Time 10.01  
 INSTRUM ARX400  
 PROBHD 5 mm Multinu  
 PULPROG zg  
 TD 32768  
 SOLVENT CDCl3  
 NS 9  
 DS 0  
 SWH 7246.377 Hz  
 FIDRES 0.221142 Hz  
 AQ 2.2610421 sec  
 RG 180  
 DW 69.000 usec  
 DE 98.57 usec  
 TE 300.0 K  
 U1 1.50000000 sec  
 P1 3.00 usec  
 DE 98.57 usec  
 SF01 400.1318844 MHz  
 NUCLEUS 1H

F2 - Processing parameters  
 SI 16384  
 SF 400.1300122 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 4.00

1D NMR plot parameters  
 CX 20.00 cm  
 F1P 10.000 ppm  
 F1 4001.30 Hz  
 F2P -0.500 ppm  
 F2 -200.07 Hz  
 PPMCM 0.52500 ppm/cm  
 HZCM 210.06825 Hz/cm



Current Data Parameters  
 NAME l02140  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20090615  
 Time 10.03  
 INSTRUM ARX400  
 PROBHD 5 mm Multinu  
 PULPROG zgpg  
 TD 32768  
 SOLVENT CDCl3  
 NS 138  
 DS 2  
 SWH 25000.000 Hz  
 FIDRES 0.162530 Hz  
 AQ 0.6554100 sec  
 RG 1024  
 DW 20.000 usec  
 DE 25.00 usec  
 TE 300.0 K  
 D12 0.00002000 sec  
 DL5 22.20 dB  
 CPOPRG waltz16  
 P31 100.00 usec  
 D1 2.00000000 sec  
 P1 2.50 usec  
 DE 25.00 usec  
 SF01 100.6233680 MHz  
 NUCLEUS 13C  
 D11 0.03000000 sec

F2 - Processing parameters  
 SI 32768  
 SF 100.6127728 MHz  
 WDW EM  
 SSB 0  
 LB 0.50 Hz  
 GB 0  
 PC 1.00

1D NMR plot parameters  
 CX 20.00 cm  
 F1P 200.000 ppm  
 F1 20122.55 Hz  
 F2P -5.000 ppm  
 F2 -503.06 Hz  
 PPMCM 10.25000 ppm/cm  
 HZCM 1031.28101 Hz/cm

