

## Catalyst-free and Solvent-free Hydroboration of Carboxylic Acids

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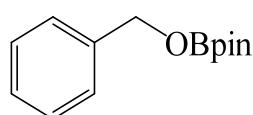
References

## EXPERIMENTAL SECTION

**General Information.** All reactions were performed under an atmosphere of nitrogen using glovebox technique.  $^1\text{H}$ ,  $^{13}\text{C}\{^1\text{H}\}$ ,  $^{11}\text{B}\{^1\text{H}\}$ , and  $^{19}\text{F}\{^1\text{H}\}$  NMR spectra were recorded at  $25^\circ\text{C}$  on Bruker Avance III 600 MHz spectrometer in deuterated solvents and were referenced to the resonances of the solvent used. Chemicals were purchased from Sigma-Aldrich, Alfa Aesar, and Acros and used without further purification.

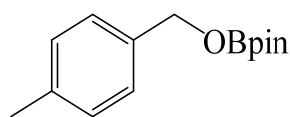
**General Procedure for Hydroboration of Carboxylic Acids.** Carboxylic acids (0.4 mmol) and HBpin (1.6 mmol) were placed in a 10 ml Schlenk flask equipped with a magnetic stir bar inside the glove box. Then the reaction mixture was stirred at  $25^\circ\text{C}$  for 6 hours or  $60^\circ\text{C}$  for 1 hour. The progress of the reaction was monitored by  $^1\text{H}$  NMR,  $^{13}\text{C}$  NMR,  $^{11}\text{B}$  NMR, and  $^{19}\text{F}$  NMR using mesitylene (0.4 mmol) as an internal standard. Two examples were selected to purify to get pure products: upon completion of the reaction, the combined organic layers were dried, evaporated and purified by column chromatography over silica-gel (100-200 mesh) using ethyl acetate/hexane (1:4) mixture as eluents to obtain the pure products (**1a**, **1g**).

### Spectroscopic Data for Acid Hydroboration Products



**1a**<sup>[S1-3]</sup>

$^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.25–7.14 (m, 5 H), 4.83 (s, 2 H), 1.16 (s-overlap, 48 H).  $^{13}\text{C}\{^1\text{H}\}$  NMR (151 MHz,  $\text{CDCl}_3$ ):  $\delta$  139.19, 128.23, 127.32, 126.87, 82.99, 82.86, 66.61, 24.56, 24.49.  $^{11}\text{B}\{^1\text{H}\}$  NMR (193 MHz,  $\text{CDCl}_3$ ):  $\delta$  22.50.

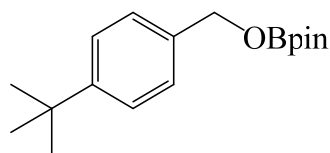


**1b**<sup>[S3]</sup>

$^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.12 (d, 2 H,  $^3J_{\text{HH}} = 7.8$  Hz), 7.01 (d, 2 H,  $^3J_{\text{HH}} = 7.8$  Hz), 4.77 (s, 2 H), 2.22 (s, 3 H), 1.15 (s-overlap, 48 H).  $^{13}\text{C}\{^1\text{H}\}$  NMR (151 MHz,

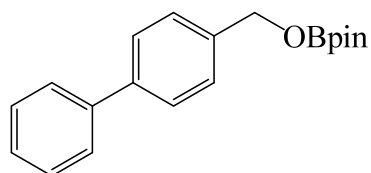
CDCl<sub>3</sub>):  $\delta$  136.86, 136.39, 128.91, 126.90, 82.96, 82.77, 66.57, 24.58, 24.51, 21.02.

<sup>11</sup>B{<sup>1</sup>H} NMR (193 MHz, CDCl<sub>3</sub>):  $\delta$  22.44.



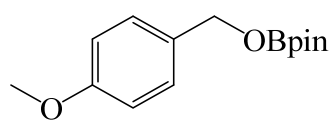
**1c**<sup>[S1]</sup>

<sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>):  $\delta$  7.24 (d, 2 H, <sup>3</sup>J<sub>HH</sub> = 7.8 Hz), 7.17 (d, 2 H, <sup>3</sup>J<sub>HH</sub> = 8.4 Hz), 4.79 (s, 2 H), 1.21 (s, 9 H), 1.15 (s-overlap, 48 H). <sup>13</sup>C{<sup>1</sup>H} NMR (151 MHz, CDCl<sub>3</sub>):  $\delta$  150.16, 136.26, 126.86, 125.10, 82.93, 82.74, 66.43, 34.40, 31.31, 24.55, 24.48. <sup>11</sup>B{<sup>1</sup>H} NMR (193 MHz, CDCl<sub>3</sub>):  $\delta$  22.50.



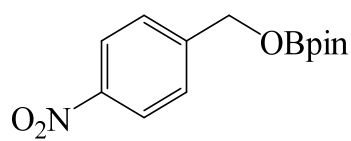
**1d**<sup>[S4]</sup>

<sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>):  $\delta$  7.64–7.61 (m, 4 H), 7.49–7.36 (m, 5 H), 5.04 (s, 2 H), 1.32 (s-overlap, 48 H). <sup>13</sup>C{<sup>1</sup>H} NMR (151 MHz, CDCl<sub>3</sub>):  $\delta$  140.89, 140.30, 138.31, 128.71, 127.18, 127.16, 127.01, 126.99, 82.98, 82.90, 66.39, 24.58, 24.50. <sup>11</sup>B{<sup>1</sup>H} NMR (193 MHz, CDCl<sub>3</sub>):  $\delta$  22.48.



**1e**<sup>[S3]</sup>

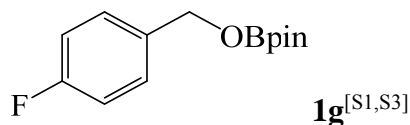
<sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>):  $\delta$  7.17 (d, 2 H, <sup>3</sup>J<sub>HH</sub> = 8.4 Hz), 6.75 (d, 2 H, <sup>3</sup>J<sub>HH</sub> = 8.4 Hz), 4.74 (s, 2 H), 3.66 (s, 3 H), 1.16 (s-overlap, 48 H). <sup>13</sup>C{<sup>1</sup>H} NMR (151 MHz, CDCl<sub>3</sub>):  $\delta$  159.03, 131.40, 128.44, 113.60, 82.94, 82.72, 66.35, 55.04, 24.53, 24.46. <sup>11</sup>B{<sup>1</sup>H} NMR (193 MHz, CDCl<sub>3</sub>):  $\delta$  22.38.



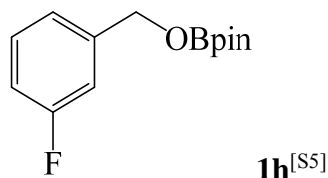
**1f**<sup>[S3]</sup>

<sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>):  $\delta$  8.07 (d, 2 H, <sup>3</sup>J<sub>HH</sub> = 9.0 Hz), 7.39 (d, 2 H, <sup>3</sup>J<sub>HH</sub> = 8.4

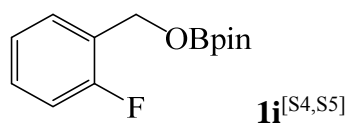
Hz), 4.91 (s, 2 H), 1.16 (s-overlap, 48 H).  $^{13}\text{C}\{^1\text{H}\}$  NMR (151 MHz,  $\text{CDCl}_3$ ):  $\delta$  147.17, 146.58, 126.79, 123.45, 83.13, 82.93, 65.45, 24.51, 24.44.  $^{11}\text{B}\{^1\text{H}\}$  NMR (193 MHz,  $\text{CDCl}_3$ ):  $\delta$  22.44.



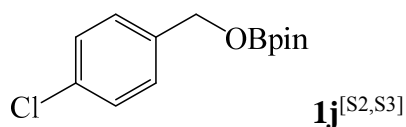
$^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.22–7.19 (m, 2 H), 6.91–6.88 (m, 2 H), 4.76 (s, 2 H), 1.16 (s-overlap, 48 H).  $^{13}\text{C}\{^1\text{H}\}$  NMR (151 MHz,  $\text{CDCl}_3$ ):  $\delta$  162.96, 161.33, 135.03, 135.01, 128.61, 128.56, 115.09, 114.94, 82.94, 82.89, 65.96, 24.52, 24.46.  $^{11}\text{B}\{^1\text{H}\}$  NMR (193 MHz,  $\text{CDCl}_3$ ):  $\delta$  22.40.  $^{19}\text{F}\{^1\text{H}\}$  NMR (565 MHz,  $\text{CDCl}_3$ ):  $\delta$  -115.23.



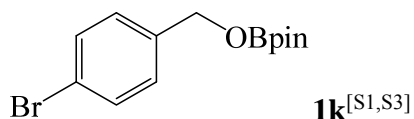
$^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.17–7.14 (m, 1 H), 6.97 (t, 2 H,  $^3J_{\text{HH}} = 8.4$  Hz), 6.83–6.80 (m, 1 H), 4.79 (s, 2 H), 1.15 (s-overlap, 48 H).  $^{13}\text{C}\{^1\text{H}\}$  NMR (151 MHz,  $\text{CDCl}_3$ ):  $\delta$  163.68, 162.05, 141.90, 141.86, 129.76, 129.71, 121.94, 121.92, 114.11, 113.97, 113.45, 113.30, 82.95, 82.91, 65.82, 65.81, 24.49, 24.44.  $^{11}\text{B}\{^1\text{H}\}$  NMR (193 MHz,  $\text{CDCl}_3$ ):  $\delta$  22.44.  $^{19}\text{F}\{^1\text{H}\}$  NMR (565 MHz,  $\text{CDCl}_3$ ):  $\delta$  -113.30.



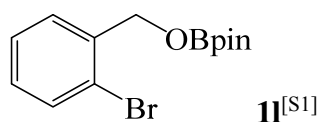
$^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.35–7.32 (m, 1 H), 7.14–7.10 (m, 1 H), 7.00–6.98 (m, 1 H), 6.88 (t, 1 H,  $^3J_{\text{HH}} = 9.6$  Hz), 4.89 (s, 2 H), 1.15 (s-overlap, 48 H).  $^{13}\text{C}\{^1\text{H}\}$  NMR (151 MHz,  $\text{CDCl}_3$ ):  $\delta$  161.04, 159.41, 129.00, 128.95, 128.85, 128.82, 126.51, 126.41, 123.94, 123.92, 115.00, 114.86, 82.93, 60.73, 60.70, 24.52, 24.48.  $^{11}\text{B}\{^1\text{H}\}$  NMR (193 MHz,  $\text{CDCl}_3$ ):  $\delta$  22.47.  $^{19}\text{F}\{^1\text{H}\}$  NMR (565 MHz,  $\text{CDCl}_3$ ):  $\delta$  -119.30.



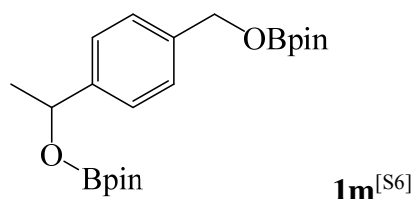
<sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>): δ 7.18–7.15 (m, 4 H), 4.77 (s, 2 H), 1.15 (s-overlap, 48 H). <sup>13</sup>C{<sup>1</sup>H} NMR (151 MHz, CDCl<sub>3</sub>): δ 137.74, 133.02, 128.34, 128.04, 82.93, 65.84, 24.52, 24.46. <sup>11</sup>B{<sup>1</sup>H} NMR (193 MHz, CDCl<sub>3</sub>): δ 22.43.



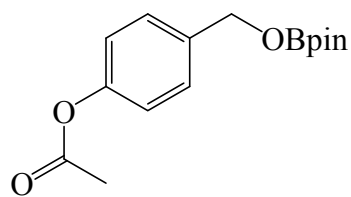
<sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>): δ 7.33 (d, 2 H, <sup>3</sup>J<sub>HH</sub> = 8.4 Hz), 7.11 (d, 2 H, <sup>3</sup>J<sub>HH</sub> = 8.4 Hz), 4.76 (s, 2 H), 1.16 (s-overlap, 48 H). <sup>13</sup>C{<sup>1</sup>H} NMR (151 MHz, CDCl<sub>3</sub>): δ 138.26, 131.32, 128.37, 121.13, 82.97, 82.96, 65.88, 24.55, 24.49. <sup>11</sup>B{<sup>1</sup>H} NMR (193 MHz, CDCl<sub>3</sub>): δ 22.40.



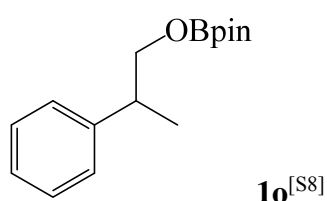
<sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>): δ 7.40–7.37 (m, 2 H), 7.18 (t, 1 H, <sup>3</sup>J<sub>HH</sub> = 7.2 Hz), 7.01–6.99 (m, 1 H), 4.86 (s, 2 H), 1.14 (s-overlap, 48 H). <sup>13</sup>C{<sup>1</sup>H} NMR (151 MHz, CDCl<sub>3</sub>): δ 138.25, 132.17, 128.56, 127.72, 127.27, 121.43, 82.95, 82.88, 66.16, 24.49, 24.43. <sup>11</sup>B{<sup>1</sup>H} NMR (193 MHz, CDCl<sub>3</sub>): δ 22.47.



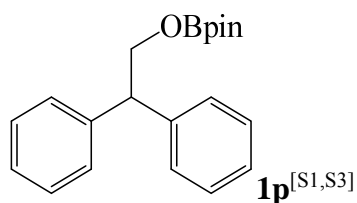
<sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>): δ 7.23–7.19 (m, 4 H), 5.14 (q, 1 H, <sup>3</sup>J<sub>HH</sub> = 6.6 Hz), 4.80 (s, 2 H), 1.37 (d, 3 H, <sup>3</sup>J<sub>HH</sub> = 6.6 Hz), 1.16 (s-overlap, 48 H). <sup>13</sup>C{<sup>1</sup>H} NMR (151 MHz, CDCl<sub>3</sub>): δ 143.73, 138.04, 126.60, 125.20, 82.92, 82.78, 82.58, 72.28, 66.40, 25.35, 24.52, 24.45, 24.43. <sup>11</sup>B{<sup>1</sup>H} NMR (193 MHz, CDCl<sub>3</sub>): δ 22.34.



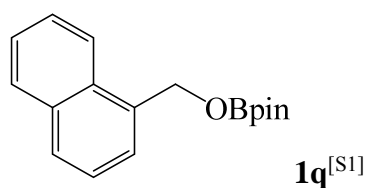
<sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>): δ 7.23 (d, 2 H, <sup>3</sup>J<sub>HH</sub> = 8.4 Hz), 6.93 (d, 2 H, <sup>3</sup>J<sub>HH</sub> = 8.4 Hz), 4.79 (s, 2 H), 2.13 (s, 3 H), 1.14 (s-overlap, 48 H). <sup>13</sup>C{<sup>1</sup>H} NMR (151 MHz, CDCl<sub>3</sub>): δ 169.00, 149.85, 136.69, 127.60, 121.26, 82.80, 82.75, 65.89, 24.42, 24.35, 20.79. <sup>11</sup>B{<sup>1</sup>H} NMR (193 MHz, CDCl<sub>3</sub>): δ 22.36.



<sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>): δ 7.16–7.05 (m, 5 H), 3.87–3.75 (m, 2 H), 2.88–2.83 (m, 1 H), 1.17 (d, 3 H, <sup>3</sup>J<sub>HH</sub> = 7.2 Hz), 1.14 (s-overlap, 48 H). <sup>13</sup>C{<sup>1</sup>H} NMR (151 MHz, CDCl<sub>3</sub>): δ 143.58, 128.13, 127.41, 126.19, 82.80, 82.35, 70.19, 41.23, 24.38, 24.35, 17.39. <sup>11</sup>B{<sup>1</sup>H} NMR (193 MHz, CDCl<sub>3</sub>): δ 22.08.

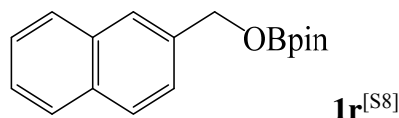


<sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>): δ 7.13–7.03 (m, 10 H), 4.29 (d, 2 H, <sup>3</sup>J<sub>HH</sub> = 7.2 Hz), 4.11 (t, 1 H, <sup>3</sup>J<sub>HH</sub> = 7.2 Hz), 1.13 (s-overlap, 48 H). <sup>13</sup>C{<sup>1</sup>H} NMR (151 MHz, CDCl<sub>3</sub>): δ 141.64, 128.37, 128.25, 126.35, 82.87, 82.49, 67.68, 52.46, 24.42, 24.39. <sup>11</sup>B{<sup>1</sup>H} NMR (193 MHz, CDCl<sub>3</sub>): δ 22.07.



<sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>): δ 7.90 (d, 1 H, <sup>3</sup>J<sub>HH</sub> = 8.4 Hz), 7.69 (d, 1 H, <sup>3</sup>J<sub>HH</sub> = 7.8

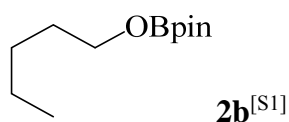
Hz), 7.62 (d, 1 H,  $^3J_{\text{HH}} = 7.8$  Hz), 7.44 (d, 1 H,  $^3J_{\text{HH}} = 7.2$  Hz), 7.36–7.27 (m, 3 H), 5.26 (s, 2 H), 1.11 (s-overlap, 48 H).  $^{13}\text{C}\{^1\text{H}\}$  NMR (151 MHz,  $\text{CDCl}_3$ ):  $\delta$  134.58, 133.51, 130.90, 128.46, 128.08, 125.97, 125.54, 125.21, 124.75, 123.34, 82.87, 82.79, 64.87, 24.50, 24.41.  $^{11}\text{B}\{^1\text{H}\}$  NMR (193 MHz,  $\text{CDCl}_3$ ):  $\delta$  22.55.



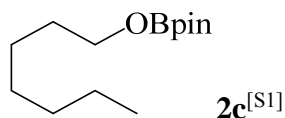
$^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.68–7.65 (m, 4 H), 7.33–7.28 (m, 3 H), 4.96 (s, 2 H), 1.12 (s-overlap, 48 H).  $^{13}\text{C}\{^1\text{H}\}$  NMR (151 MHz,  $\text{CDCl}_3$ ):  $\delta$  136.65, 133.29, 132.79, 127.92, 127.80, 127.58, 125.94, 125.63, 125.07, 124.76, 82.92, 82.87, 66.64, 24.52, 24.43.  $^{11}\text{B}\{^1\text{H}\}$  NMR (193 MHz,  $\text{CDCl}_3$ ):  $\delta$  22.53.



$^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ):  $\delta$  3.80 (q, 2 H,  $^3J_{\text{HH}} = 7.2$  Hz), 1.17 (s-overlap, 48 H), 1.12 (t, 3 H,  $^3J_{\text{HH}} = 6.6$  Hz).  $^{13}\text{C}\{^1\text{H}\}$  NMR (151 MHz,  $\text{CDCl}_3$ ):  $\delta$  82.90, 82.41, 60.48, 24.48, 24.43, 17.11.  $^{11}\text{B}\{^1\text{H}\}$  NMR (193 MHz,  $\text{CDCl}_3$ ):  $\delta$  22.06.

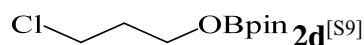


$^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ):  $\delta$  3.73 (t, 2 H,  $^3J_{\text{HH}} = 6.6$  Hz), 1.49–1.44 (m, 2 H), 1.25–1.22 (m, 4 H), 1.16 (s-overlap, 48 H), 0.80 (t, 3 H,  $^3J_{\text{HH}} = 7.2$  Hz).  $^{13}\text{C}\{^1\text{H}\}$  NMR (151 MHz,  $\text{CDCl}_3$ ):  $\delta$  82.78, 82.29, 64.68, 31.04, 27.66, 24.40, 24.36, 22.22, 13.85.  $^{11}\text{B}\{^1\text{H}\}$  NMR (193 MHz,  $\text{CDCl}_3$ ):  $\delta$  22.09.

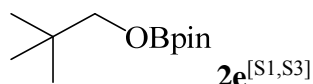


$^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ):  $\delta$  3.74 (t, 2 H,  $^3J_{\text{HH}} = 6.6$  Hz), 1.49–1.44 (m, 2 H), 1.28–1.21 (m, 8 H), 1.17 (s-overlap, 48 H), 0.79 (t, 3 H,  $^3J_{\text{HH}} = 6.6$  Hz).  $^{13}\text{C}\{^1\text{H}\}$  NMR (151 MHz,  $\text{CDCl}_3$ ):  $\delta$  82.88, 82.37, 64.79, 31.77, 31.41, 28.91, 25.50, 24.46, 24.42,

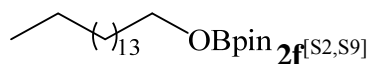
22.52, 13.97.  $^{11}\text{B}\{^1\text{H}\}$  NMR (193 MHz,  $\text{CDCl}_3$ ):  $\delta$  22.06.



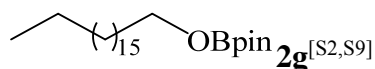
$^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ):  $\delta$  3.90 (t, 2 H,  $^3J_{\text{HH}} = 6.0$  Hz), 3.53 (t, 2 H,  $^3J_{\text{HH}} = 6.6$  Hz), 1.93–1.88 (m, 2 H), 1.17 (s-overlap, 48 H).  $^{13}\text{C}\{^1\text{H}\}$  NMR (151 MHz,  $\text{CDCl}_3$ ):  $\delta$  82.93, 82.74, 61.38, 41.13, 34.19, 24.51, 24.46.  $^{11}\text{B}\{^1\text{H}\}$  NMR (193 MHz,  $\text{CDCl}_3$ ):  $\delta$  22.11.



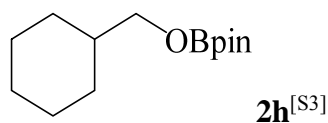
$^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ):  $\delta$  3.42 (s, 2 H), 1.17 (s-overlap, 48 H), 0.81 (s, 9 H).  $^{13}\text{C}\{^1\text{H}\}$  NMR (151 MHz,  $\text{CDCl}_3$ ):  $\delta$  82.89, 82.40, 74.78, 32.23, 25.92, 24.78, 24.45.  $^{11}\text{B}\{^1\text{H}\}$  NMR (193 MHz,  $\text{CDCl}_3$ ):  $\delta$  22.12.



$^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ):  $\delta$  3.74 (t, 2 H,  $^3J_{\text{HH}} = 6.6$  Hz), 1.49–1.45 (m, 2 H), 1.18, 1.16 (s-overlap, 74 H), 0.80 (t, 3 H,  $^3J_{\text{HH}} = 7.2$  Hz).  $^{13}\text{C}\{^1\text{H}\}$  NMR (151 MHz,  $\text{CDCl}_3$ ):  $\delta$  82.98, 82.48, 64.91, 31.95, 31.50, 29.72, 29.63, 29.39, 29.35, 25.63, 24.56, 24.52, 22.70, 14.10.  $^{11}\text{B}\{^1\text{H}\}$  NMR (193 MHz,  $\text{CDCl}_3$ ):  $\delta$  22.06.



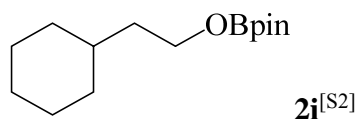
$^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ):  $\delta$  3.74 (t, 2 H,  $^3J_{\text{HH}} = 6.6$  Hz), 1.49–1.45 (m, 2 H), 1.17, 1.16, 1.14 (s-overlap, 78 H), 0.80 (t, 3 H,  $^3J_{\text{HH}} = 6.6$  Hz).  $^{13}\text{C}\{^1\text{H}\}$  NMR (151 MHz,  $\text{CDCl}_3$ ):  $\delta$  82.44, 81.82, 64.88, 31.93, 31.49, 30.51, 30.30, 30.28, 29.67, 29.39, 25.64, 24.84, 24.50, 24.47, 22.66, 14.09.  $^{11}\text{B}\{^1\text{H}\}$  NMR (193 MHz,  $\text{CDCl}_3$ ):  $\delta$  22.24.



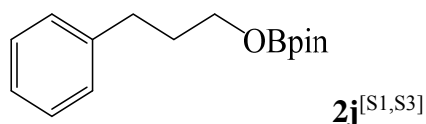
$^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ):  $\delta$  3.56 (d, 2 H,  $^3J_{\text{HH}} = 6.6$  Hz), 1.65–1.40 (m, 7 H), 1.36 (q, 2 H,  $^3J_{\text{HH}} = 6.6$  Hz), 1.33–1.27 (m, 2 H), 1.17 (s-overlap, 48 H), 1.10–1.05 (m, 2 H),



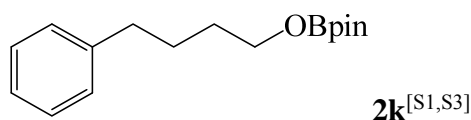
0.89–0.81 (m, 2 H).  $^{13}\text{C}\{^1\text{H}\}$  NMR (151 MHz,  $\text{CDCl}_3$ ):  $\delta$  82.90, 82.40, 70.24, 39.30, 29.28, 26.48, 25.73, 24.48, 24.45.  $^{11}\text{B}\{^1\text{H}\}$  NMR (193 MHz,  $\text{CDCl}_3$ ):  $\delta$  22.05.



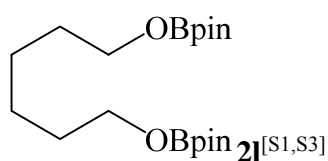
$^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ):  $\delta$  3.90 (t, 2 H,  $^3J_{\text{HH}} = 6.0$  Hz), 1.65–1.54 (m, 5 H), 1.36 (q, 2 H,  $^3J_{\text{HH}} = 6.6$  Hz), 1.33–1.27 (m, 2 H), 1.17 (s-overlap, 48 H), 1.09–1.04 (m, 2 H), 0.84–0.77 (m, 2 H).  $^{13}\text{C}\{^1\text{H}\}$  NMR (151 MHz,  $\text{CDCl}_3$ ):  $\delta$  82.93, 82.43, 62.68, 38.94, 33.86, 33.18, 26.56, 26.24, 24.52, 24.47.  $^{11}\text{B}\{^1\text{H}\}$  NMR (193 MHz,  $\text{CDCl}_3$ ):  $\delta$  22.07.



$^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.16–7.13 (m, 2 H), 7.08–7.04 (m, 3 H), 3.76 (t, 2 H,  $^3J_{\text{HH}} = 6.6$  Hz), 2.58 (t, 2 H,  $^3J_{\text{HH}} = 7.2$  Hz), 1.80–1.75 (m, 2 H), 1.15 (s-overlap, 48 H).  $^{13}\text{C}\{^1\text{H}\}$  NMR (151 MHz,  $\text{CDCl}_3$ ):  $\delta$  141.71, 128.37, 128.22, 125.67, 82.88, 82.50, 63.98, 33.08, 31.79, 24.49, 24.43.  $^{11}\text{B}\{^1\text{H}\}$  NMR (193 MHz,  $\text{CDCl}_3$ ):  $\delta$  22.18.

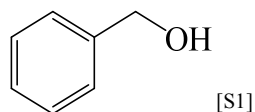


$^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.15–7.12 (m, 2 H), 7.06–7.02 (m, 3 H), 3.75 (t, 2 H,  $^3J_{\text{HH}} = 6.0$  Hz), 2.51 (t, 2 H,  $^3J_{\text{HH}} = 7.8$  Hz), 1.60–1.55 (m, 2 H), 1.52–1.47 (m, 2 H), 1.15 (s-overlap, 48 H).  $^{13}\text{C}\{^1\text{H}\}$  NMR (151 MHz,  $\text{CDCl}_3$ ):  $\delta$  142.16, 128.26, 128.10, 125.53, 82.82, 82.37, 64.48, 35.38, 30.89, 27.32, 24.43, 24.39.  $^{11}\text{B}\{^1\text{H}\}$  NMR (193 MHz,  $\text{CDCl}_3$ ):  $\delta$  22.10.

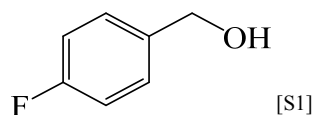


$^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ):  $\delta$  3.72 (t, 4 H,  $^3J_{\text{HH}} = 6.6$  Hz), 1.53–1.42 (m, 4 H), 1.28–1.25 (m, 4 H), 1.17 (s-overlap, 84 H).  $^{13}\text{C}\{^1\text{H}\}$  NMR (151 MHz,  $\text{CDCl}_3$ ):  $\delta$  82.72,

82.25, 64.51, 31.24, 25.11, 24.36, 24.32.  $^{11}\text{B}\{^1\text{H}\}$  NMR (193 MHz,  $\text{CDCl}_3$ ):  $\delta$  22.40.

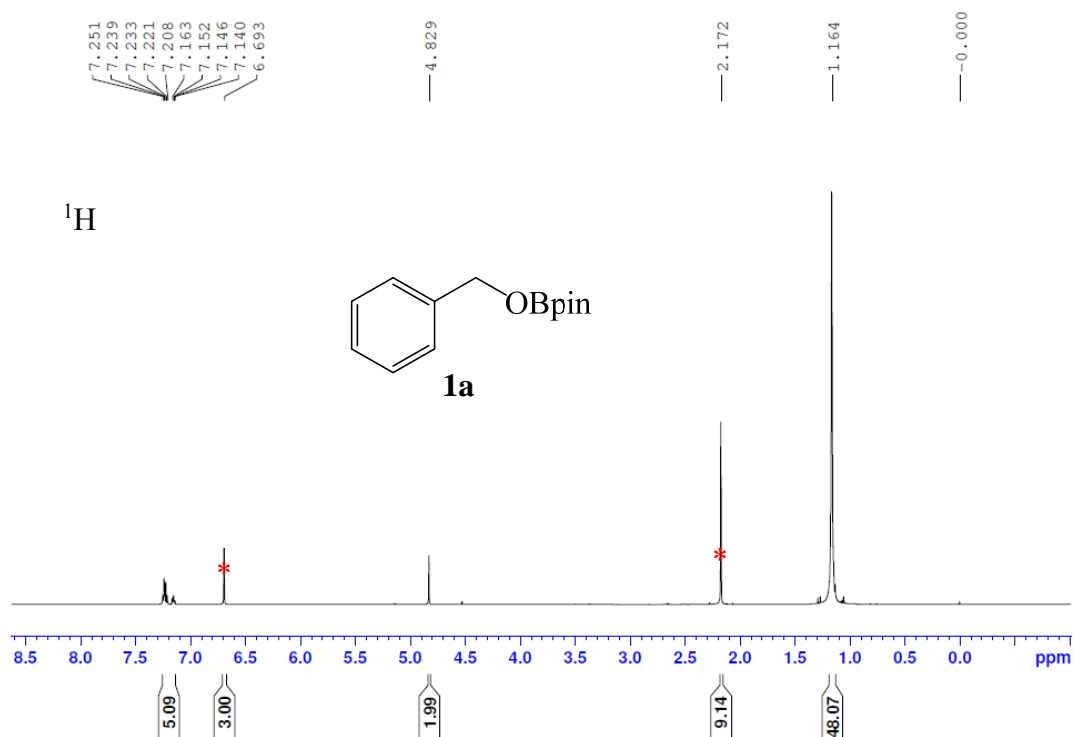


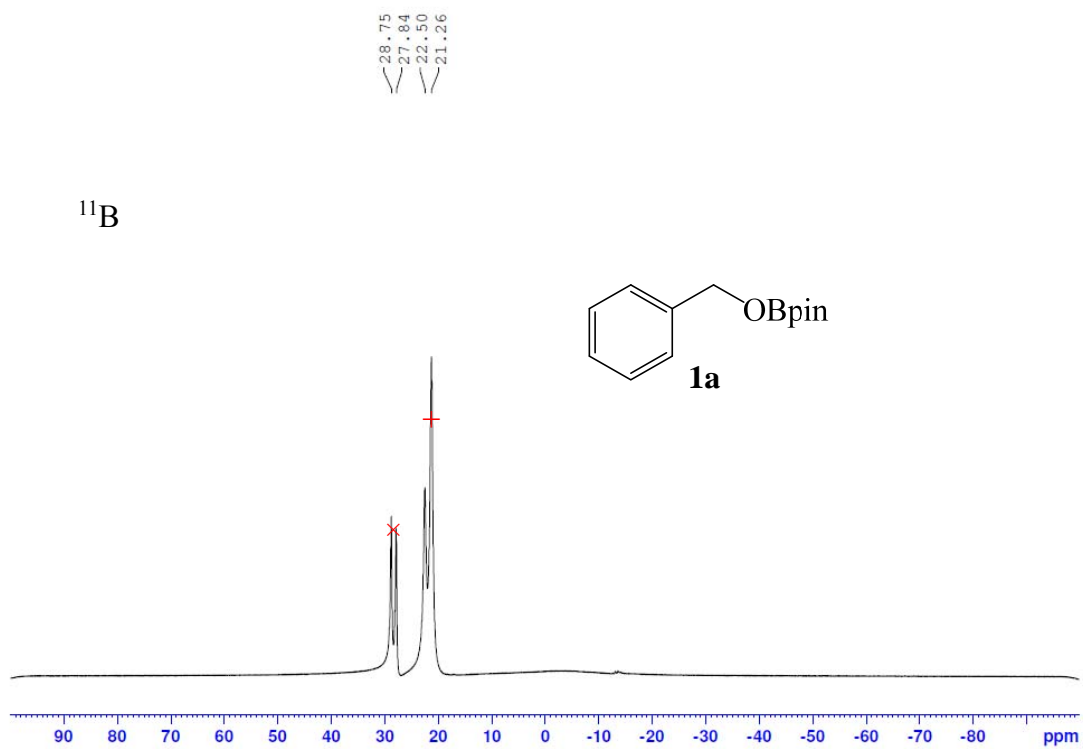
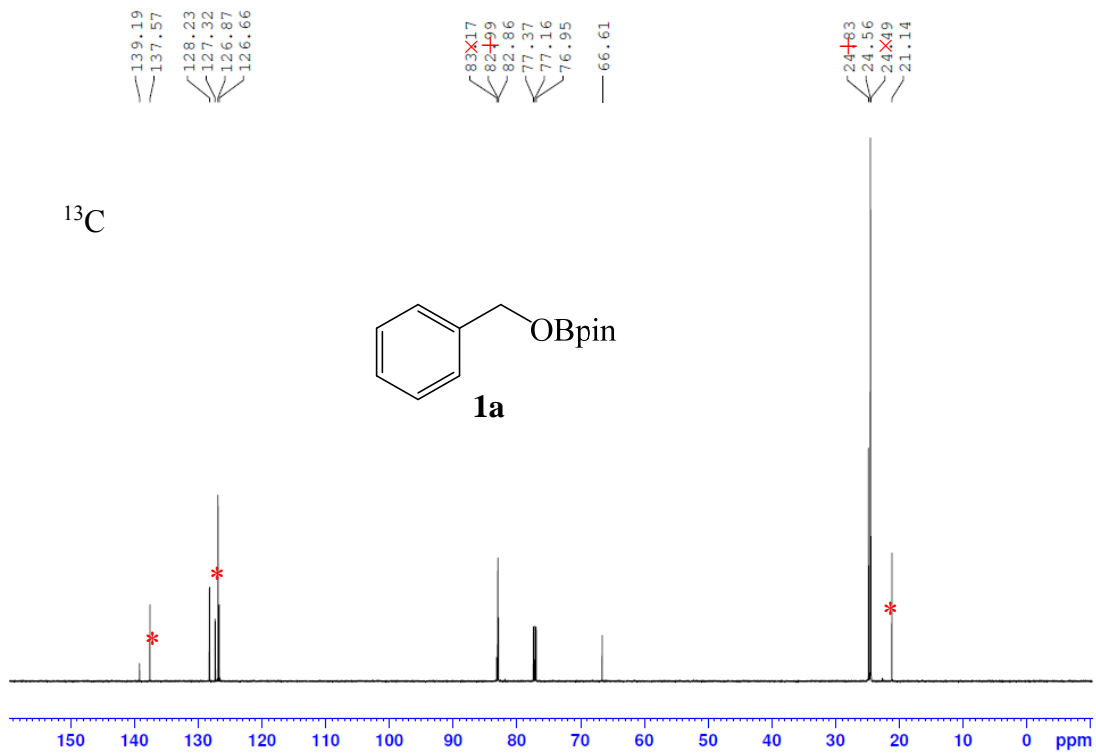
$^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.22–7.15 (m, 5 H), 4.44 (s, 2 H), 2.95 (s, 1 H).  $^{13}\text{C}\{^1\text{H}\}$  NMR (151 MHz,  $\text{CDCl}_3$ ):  $\delta$  140.91, 128.49, 127.52, 127.00, 64.94.



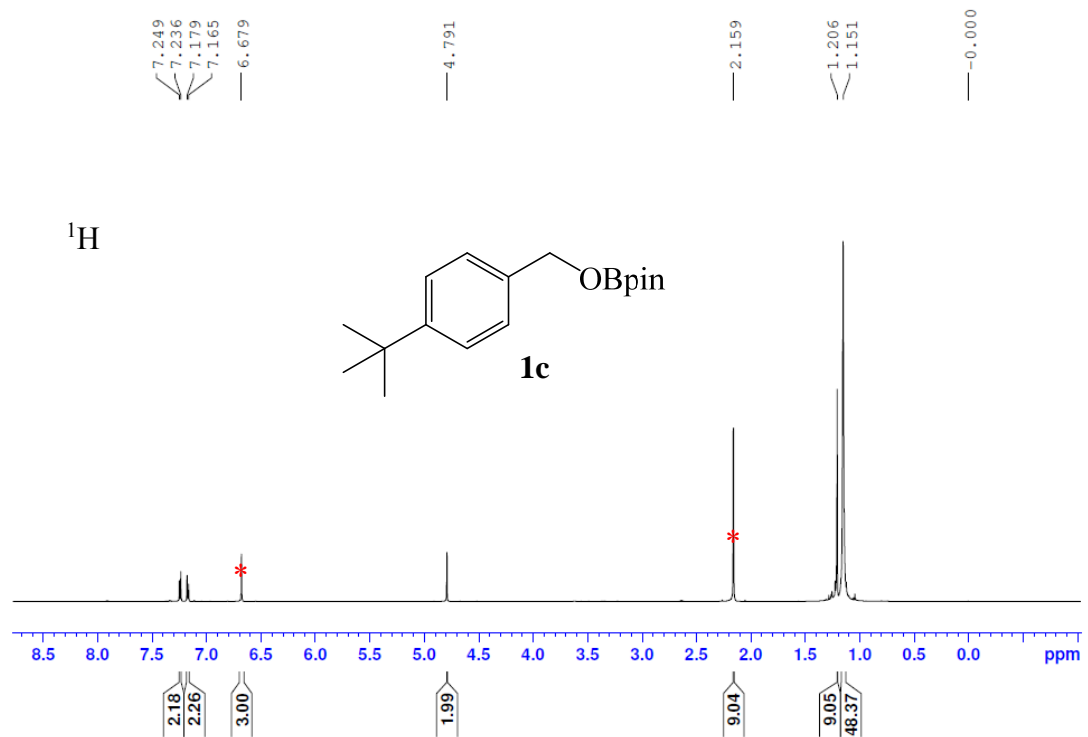
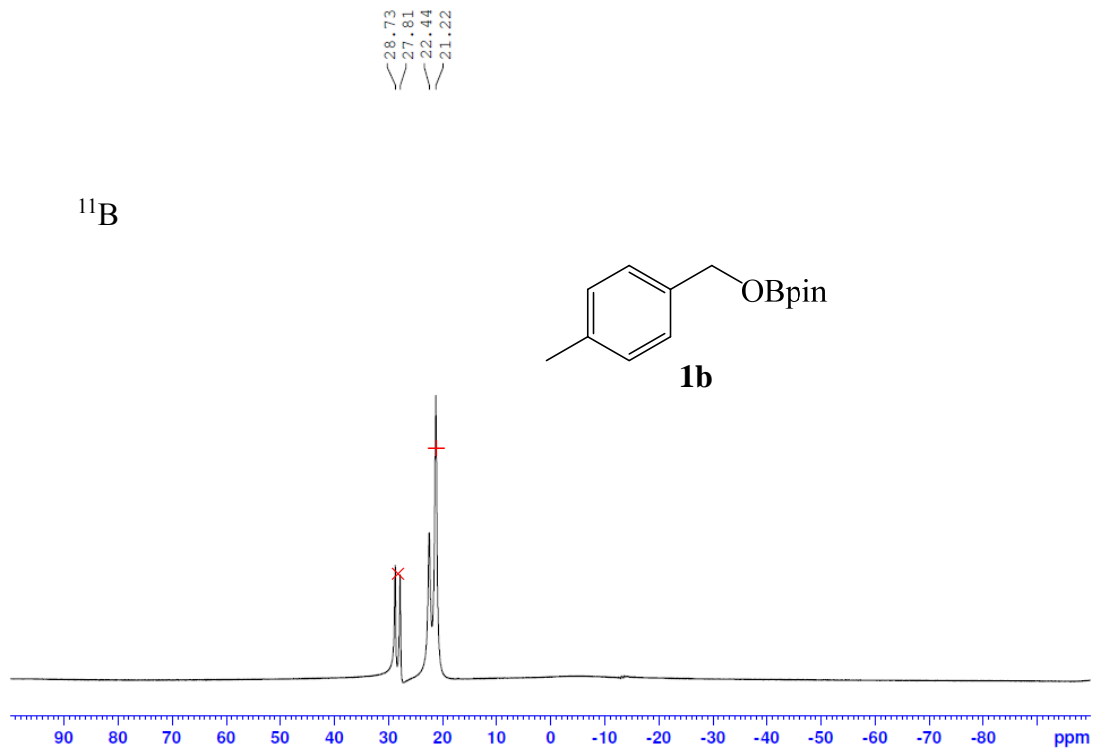
$^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.14–7.11 (m, 2 H), 6.90–6.87 (m, 2 H), 4.40 (s, 2 H), 3.15 (s, 1 H).  $^{13}\text{C}\{^1\text{H}\}$  NMR (151 MHz,  $\text{CDCl}_3$ ):  $\delta$  163.07, 161.45, 136.60, 136.58, 128.77, 128.72, 115.36, 115.22, 64.21.  $^{11}\text{B}\{^1\text{H}\}$  NMR (193 MHz,  $\text{CDCl}_3$ ):  $\delta$  22.40.  $^{19}\text{F}\{^1\text{H}\}$  NMR (565 MHz,  $\text{CDCl}_3$ ):  $\delta$  -115.01.

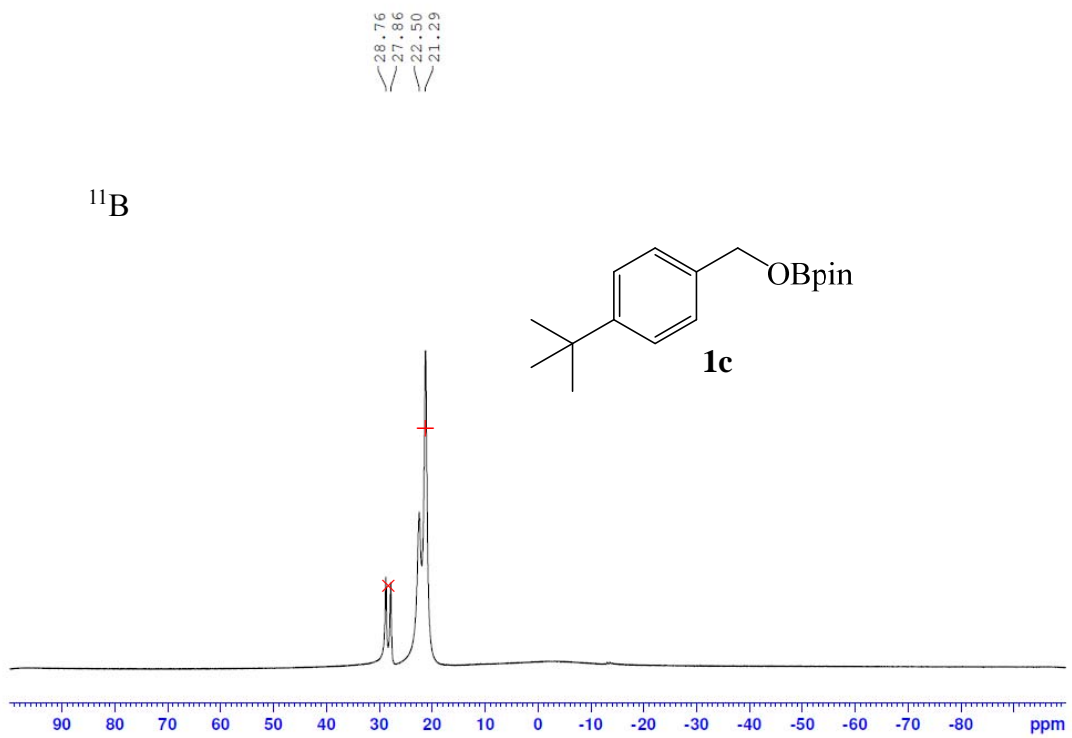
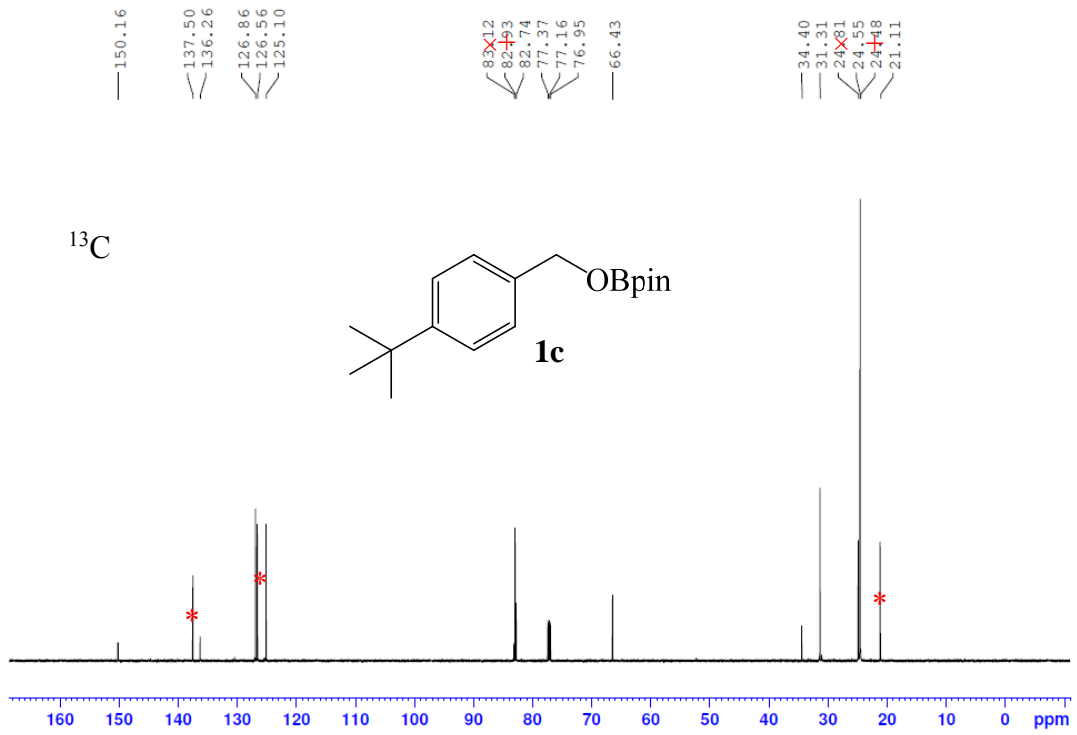
**NMR Spectra of Acid Hydroboration Products** (mesitylene (\*), excess HBpin (x),  $\text{O}(\text{Bpin})_2(+)$ )

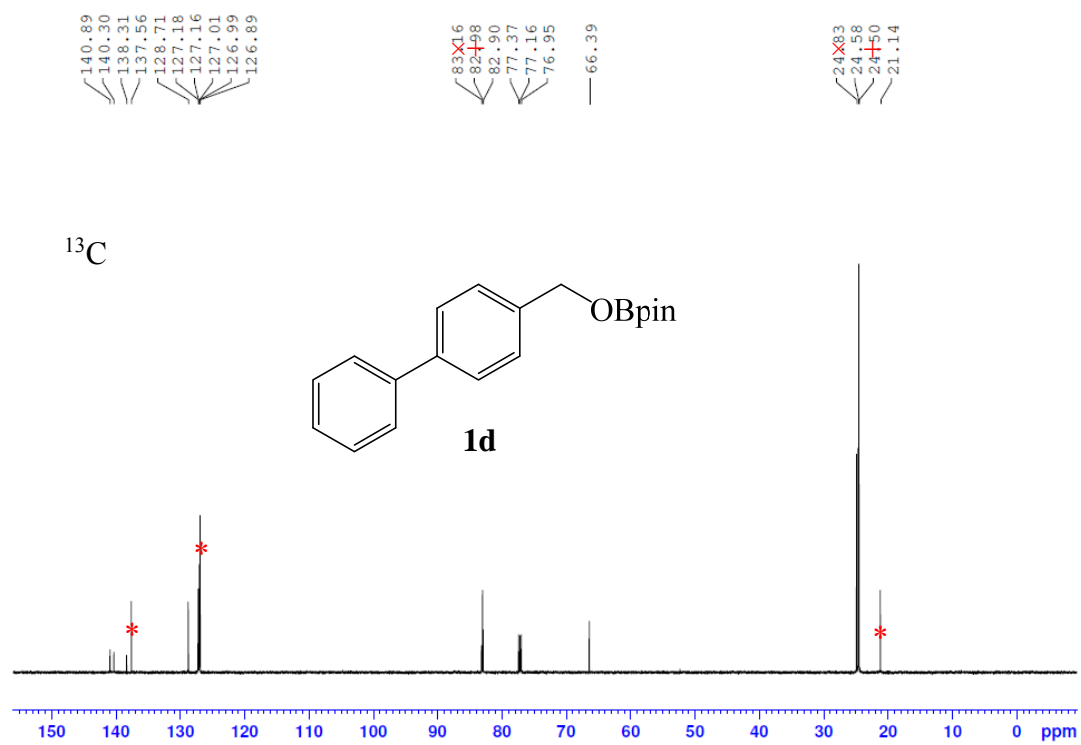
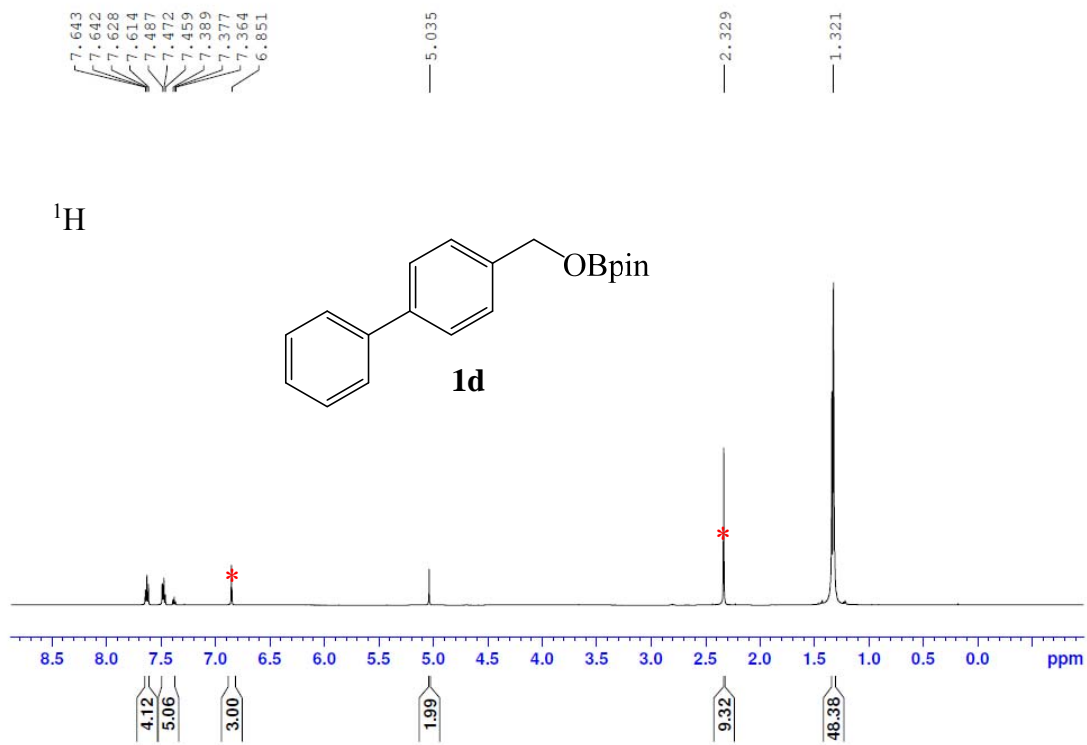






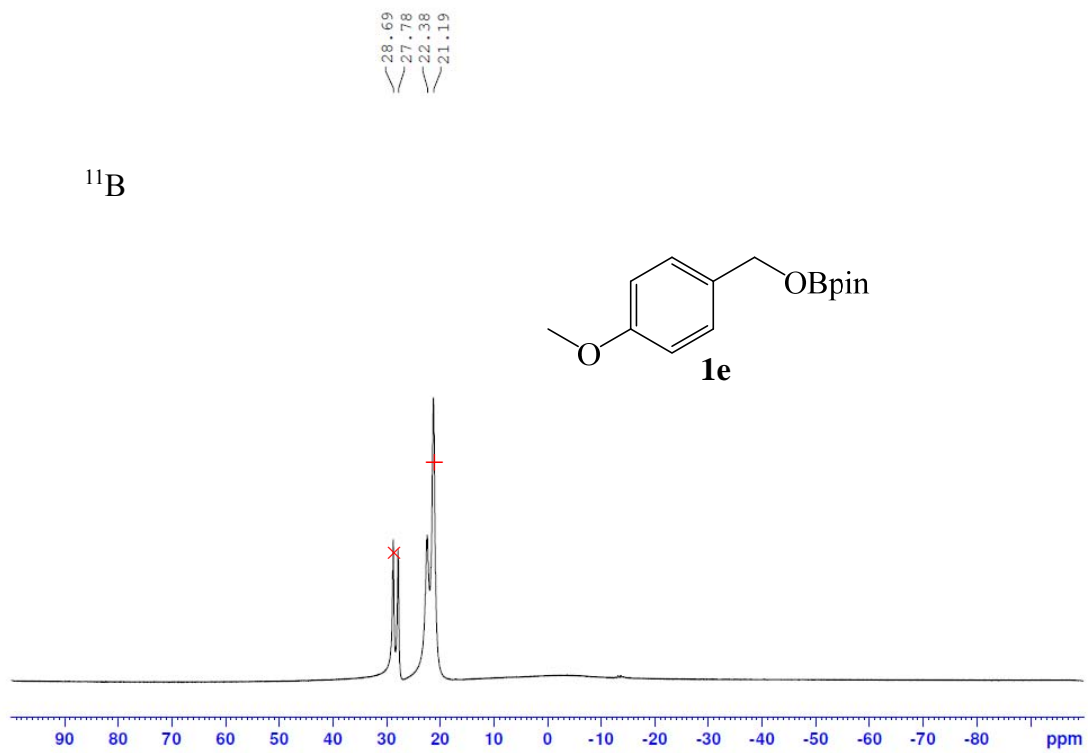
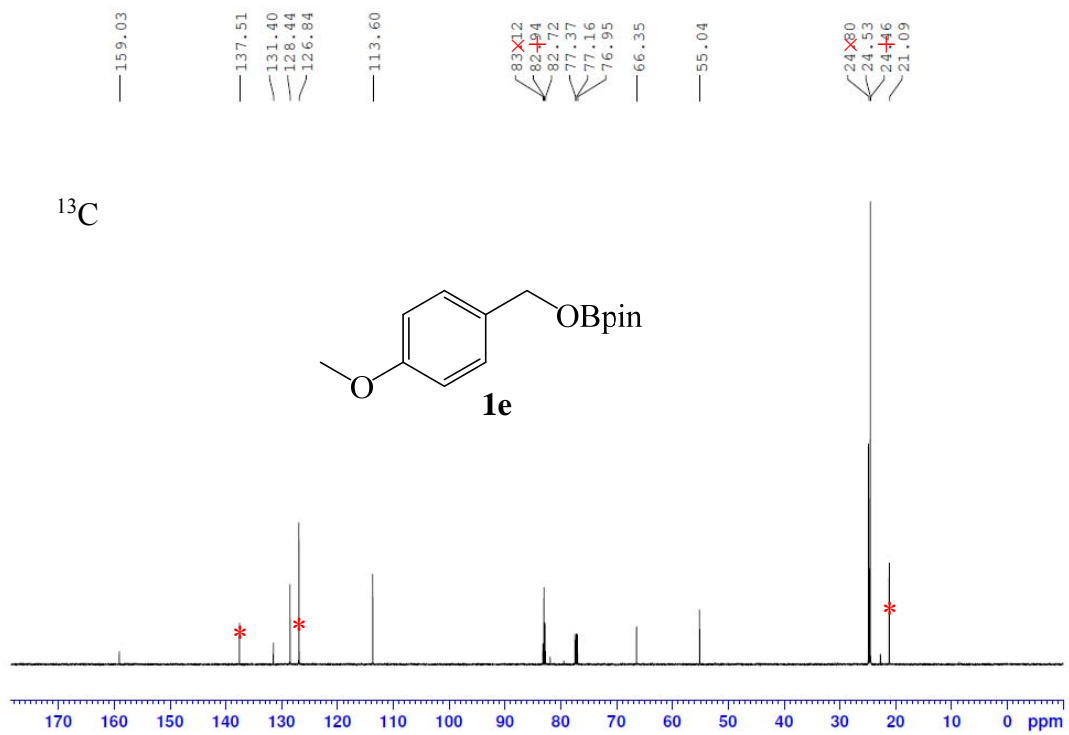


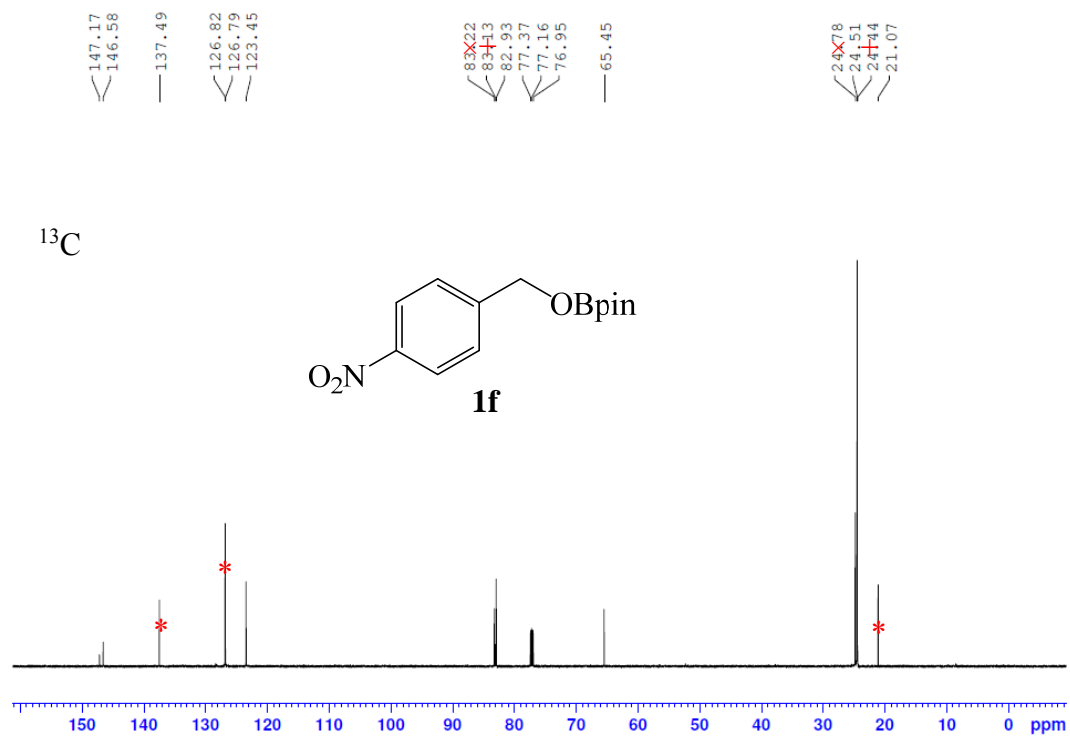
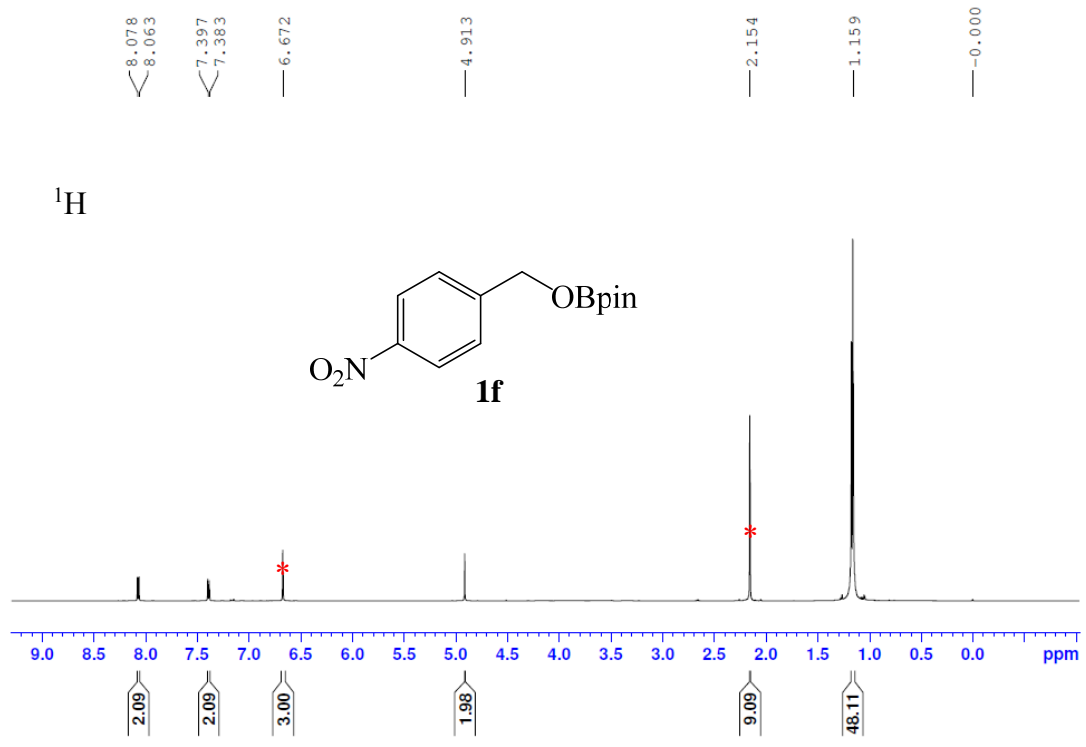




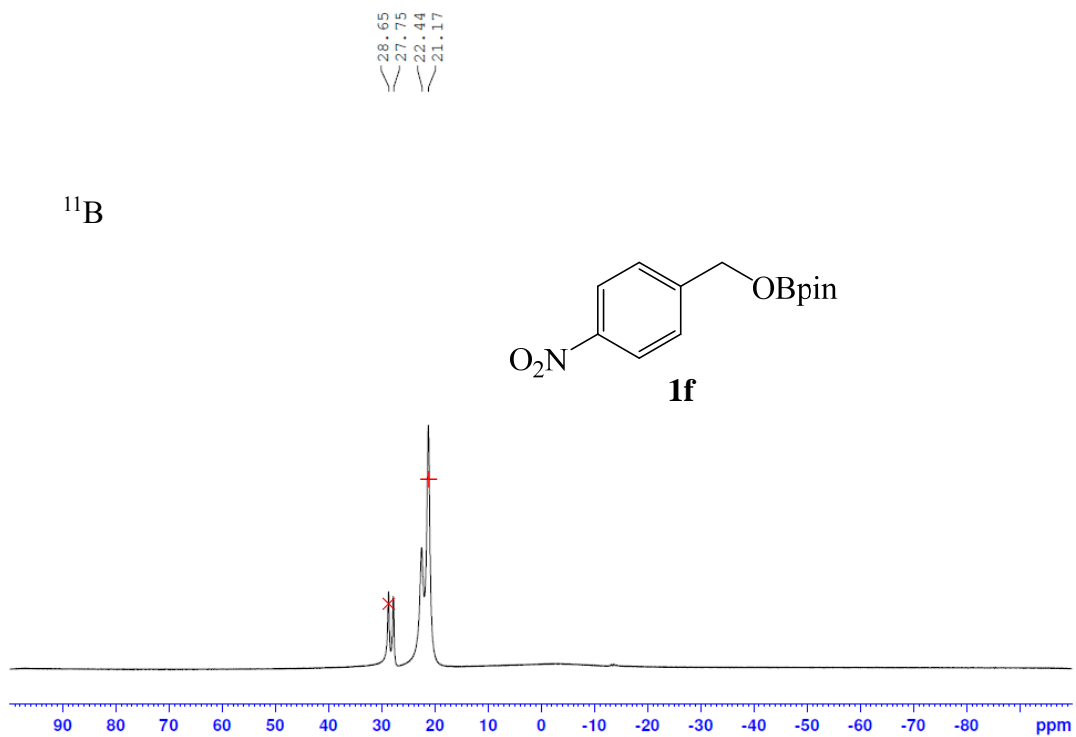




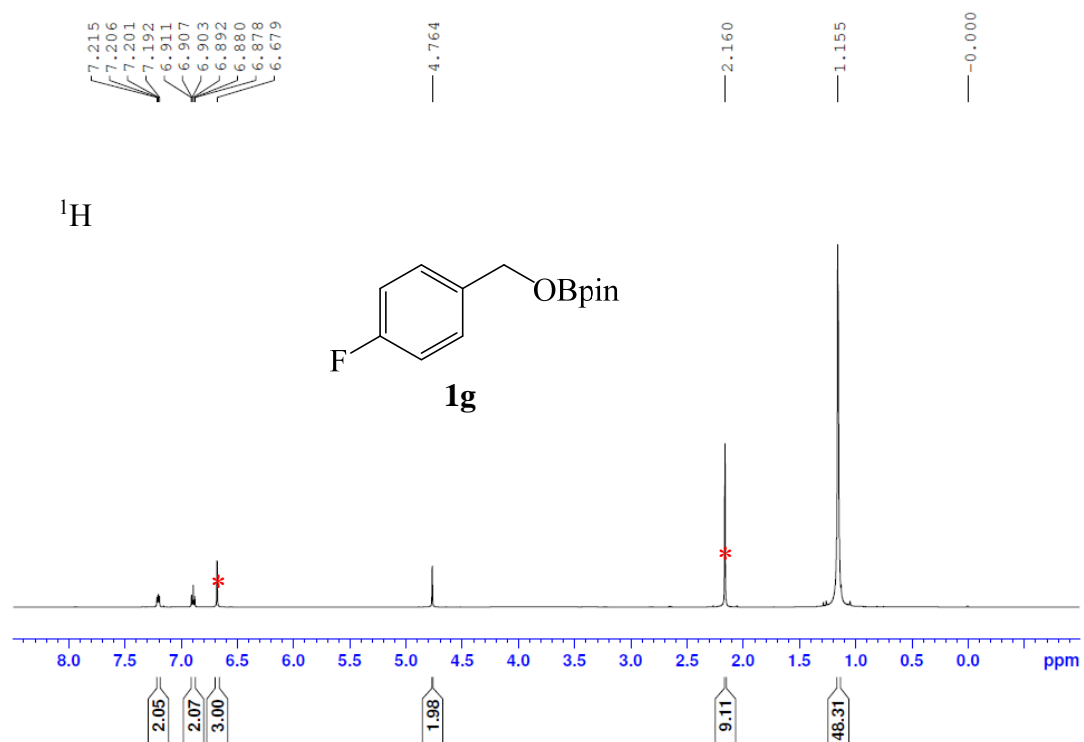




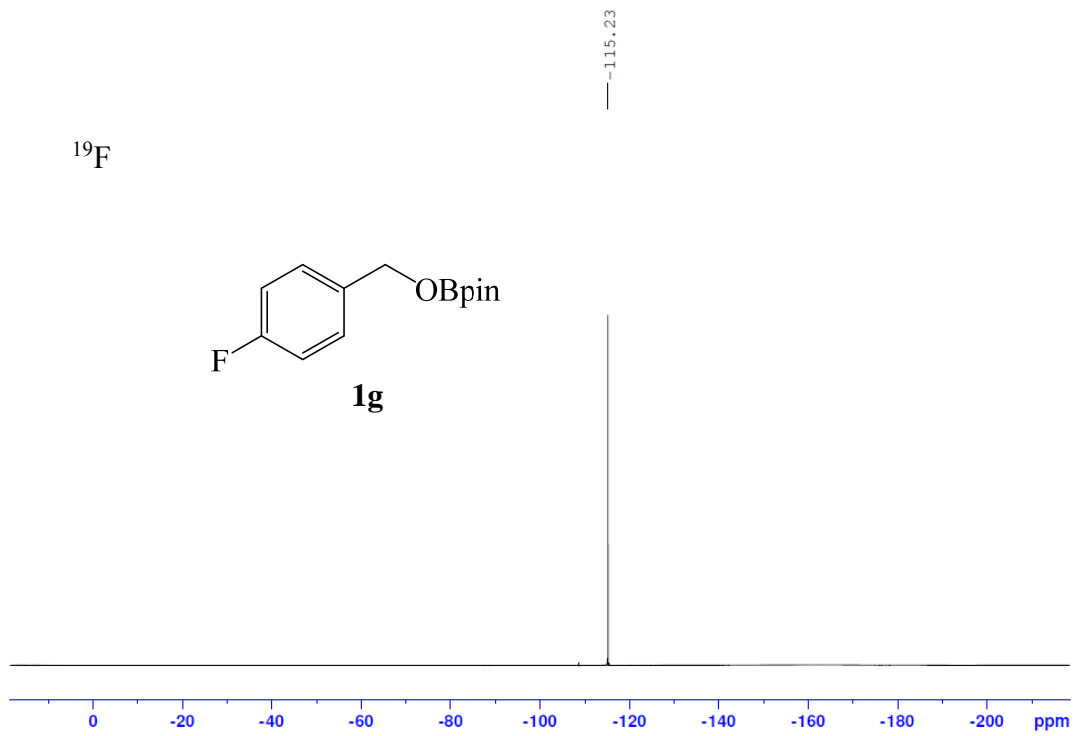
$^{11}\text{B}$



$^1\text{H}$







7.174  
7.161  
7.151  
7.138  
6.983  
6.969  
6.947  
6.833  
6.830  
6.819  
6.816  
6.805  
6.802  
6.671

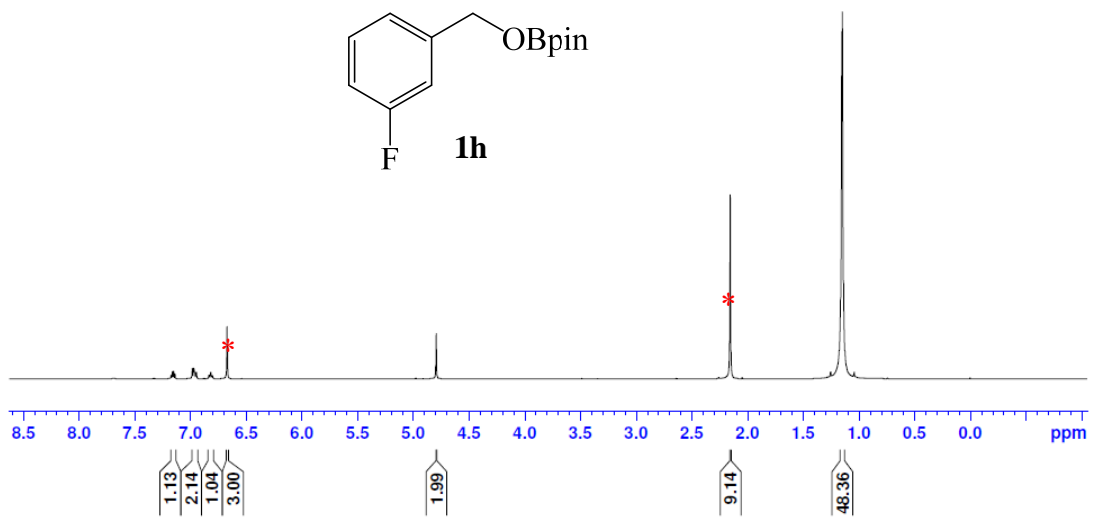
— 4.793

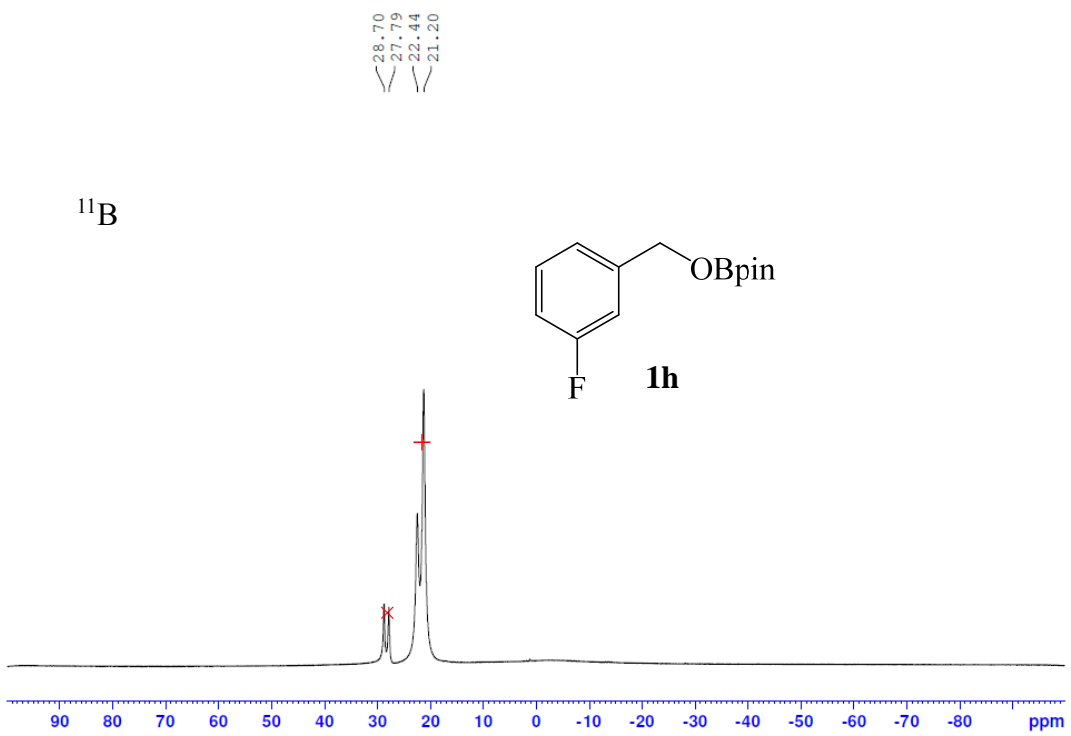
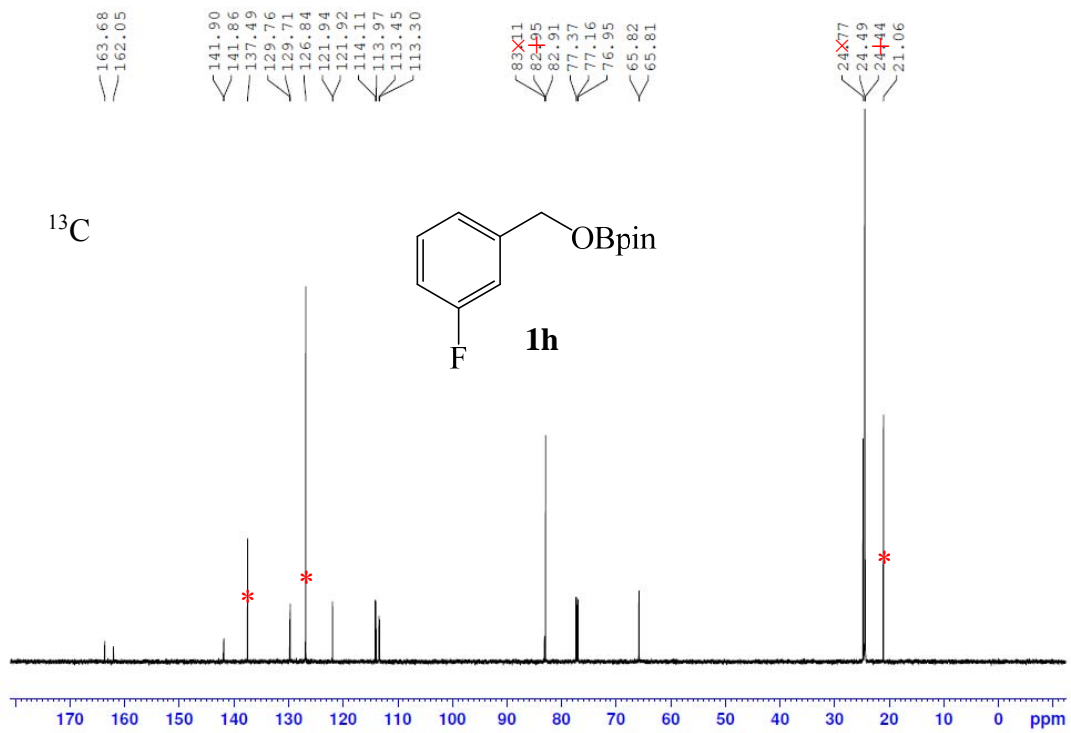
— 2.153

— 1.150

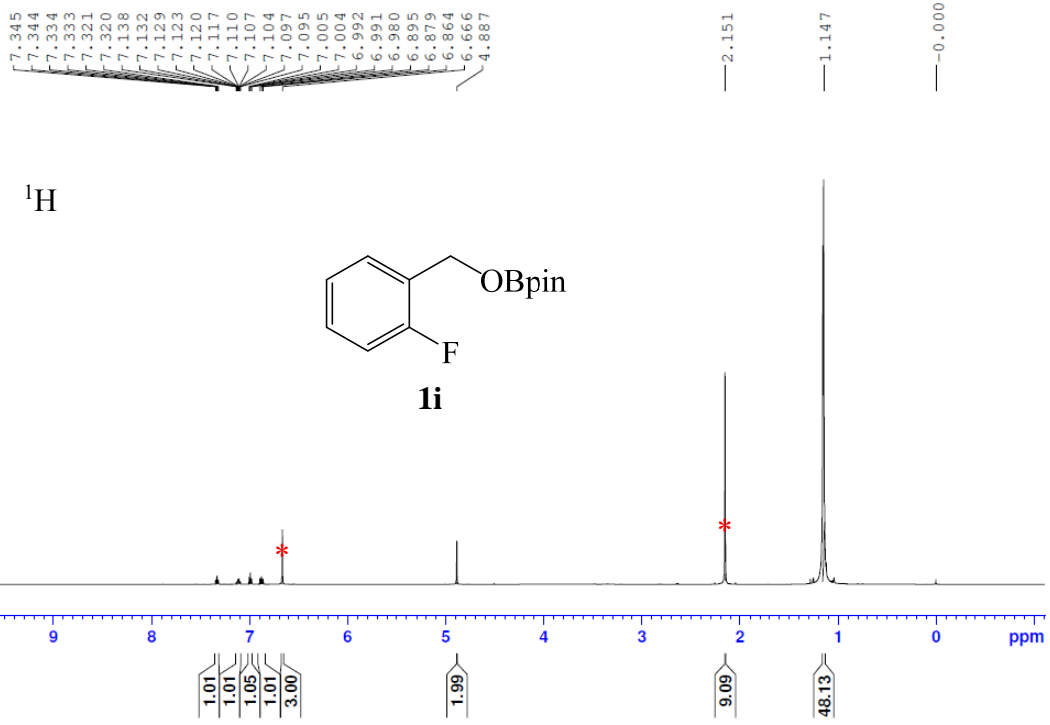
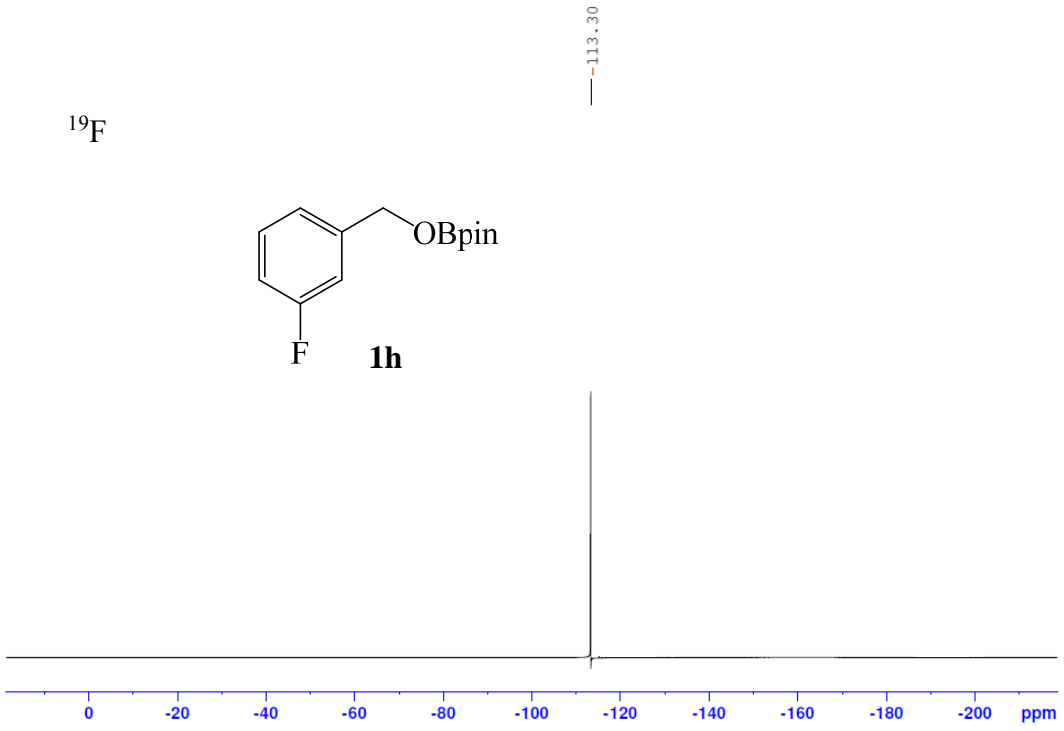
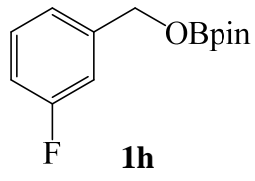
— 0.000

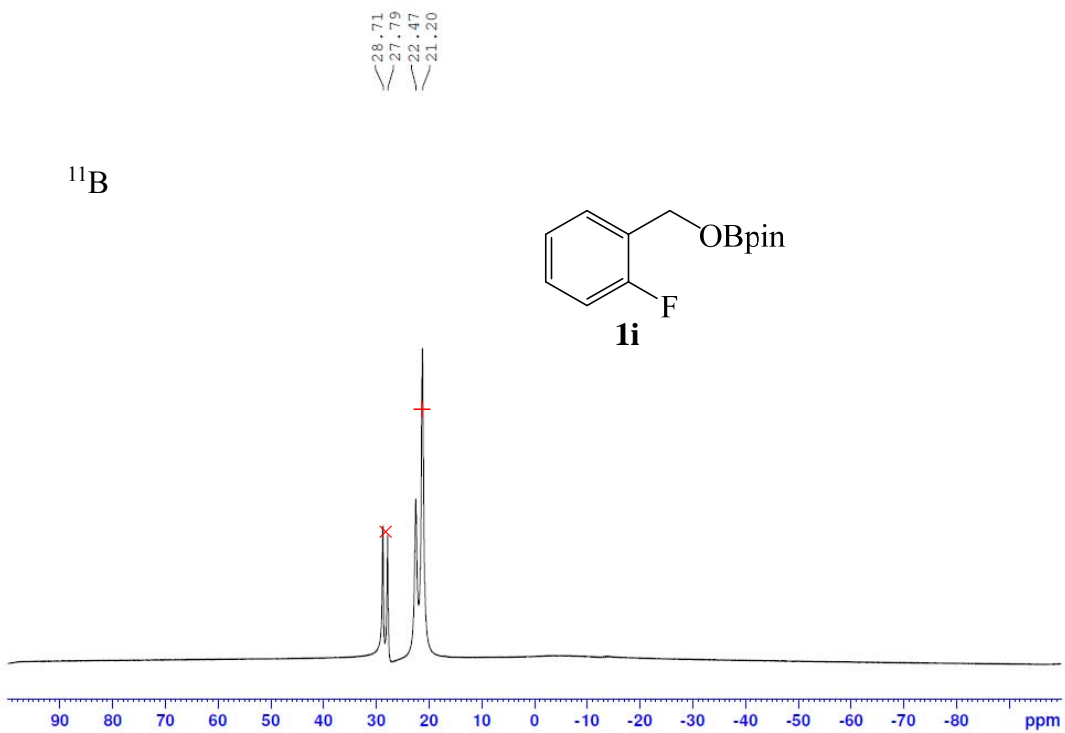
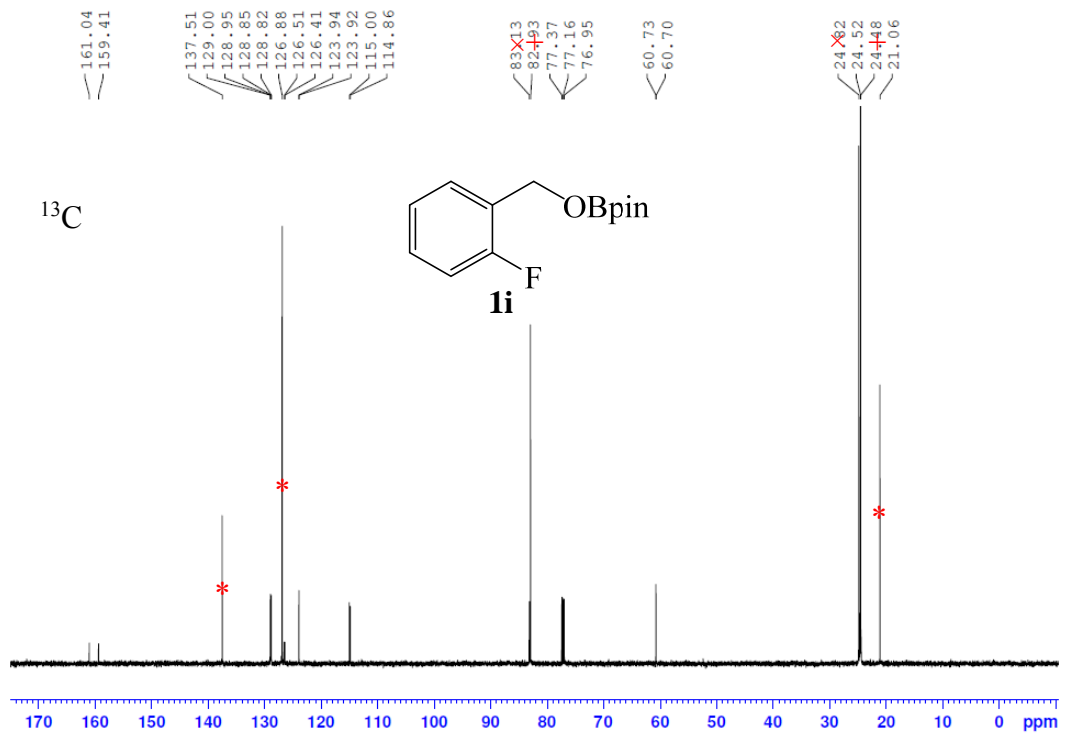
$^1\text{H}$



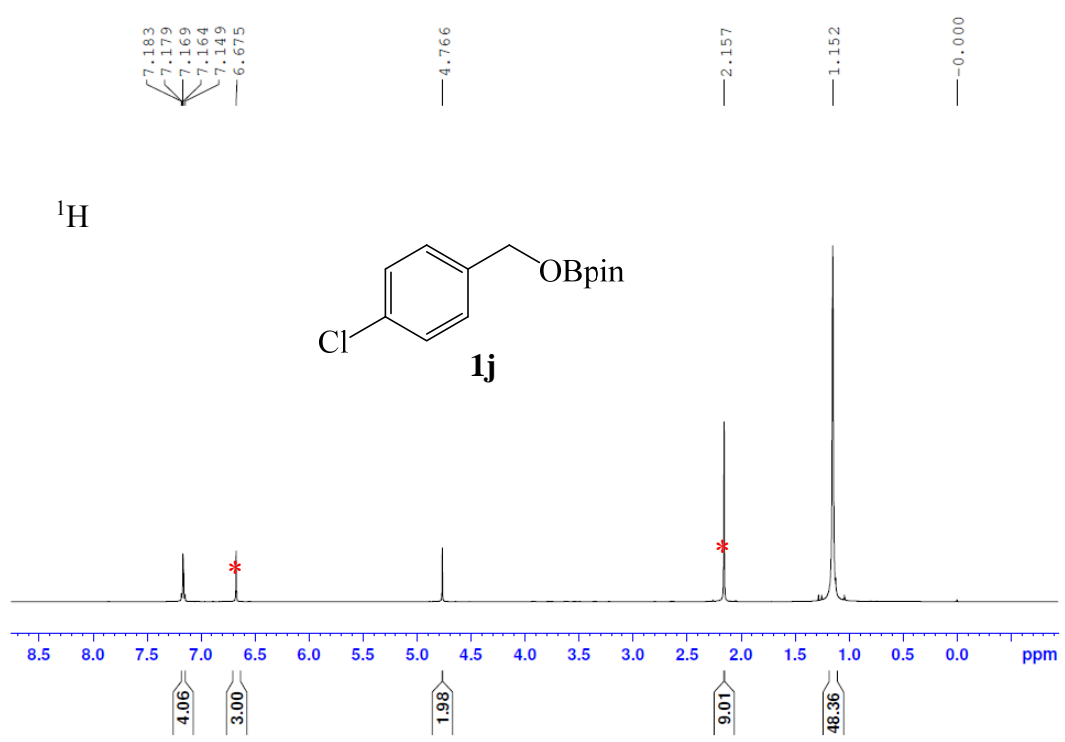
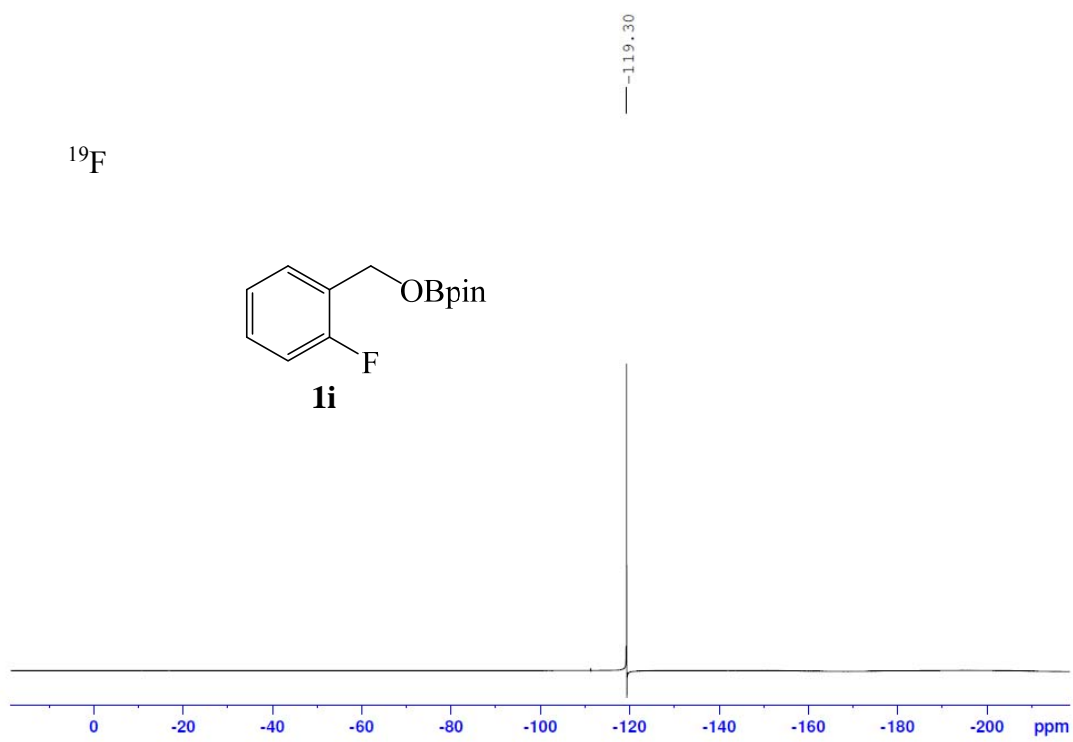


$^{19}\text{F}$

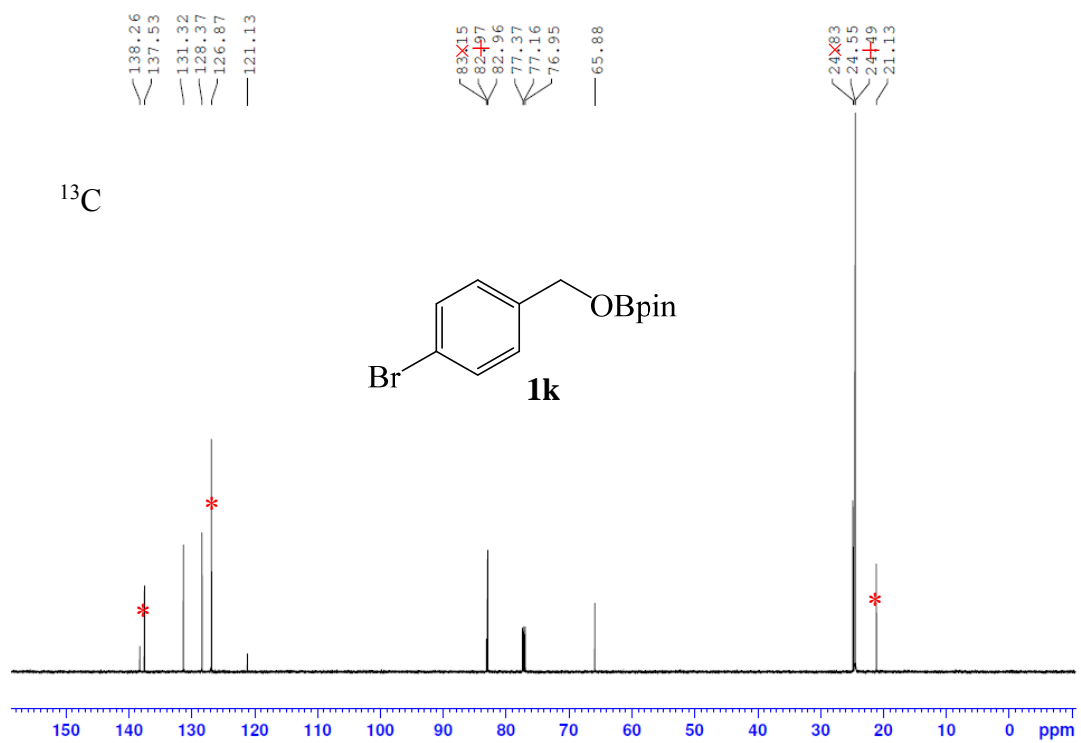
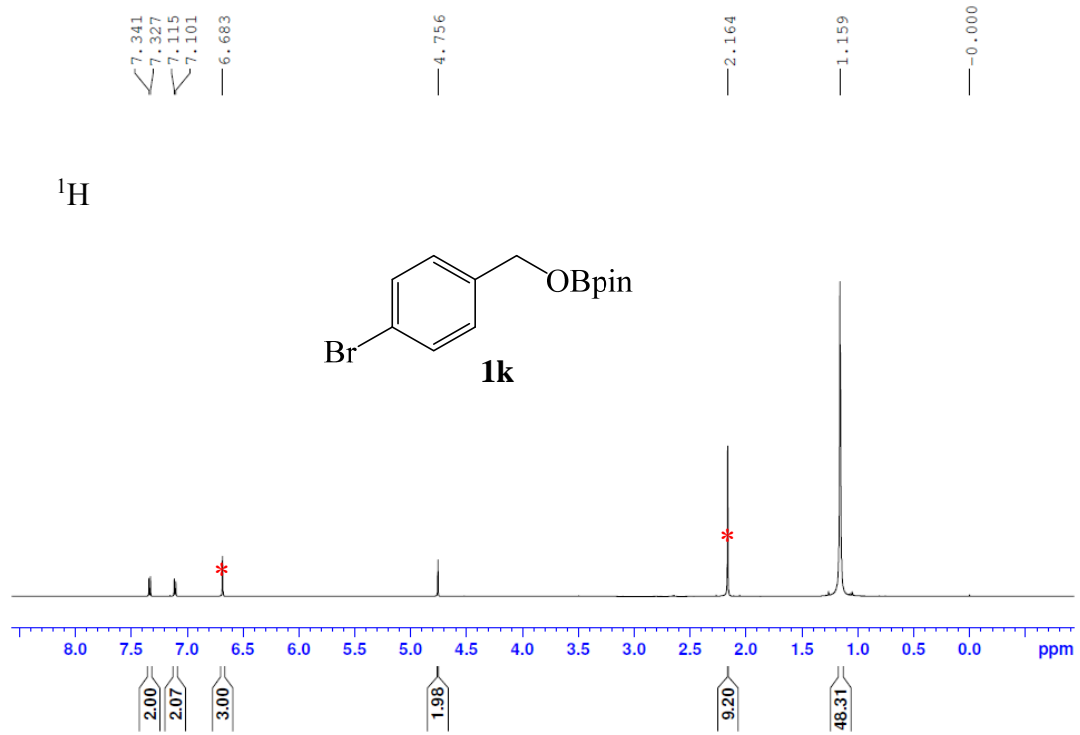


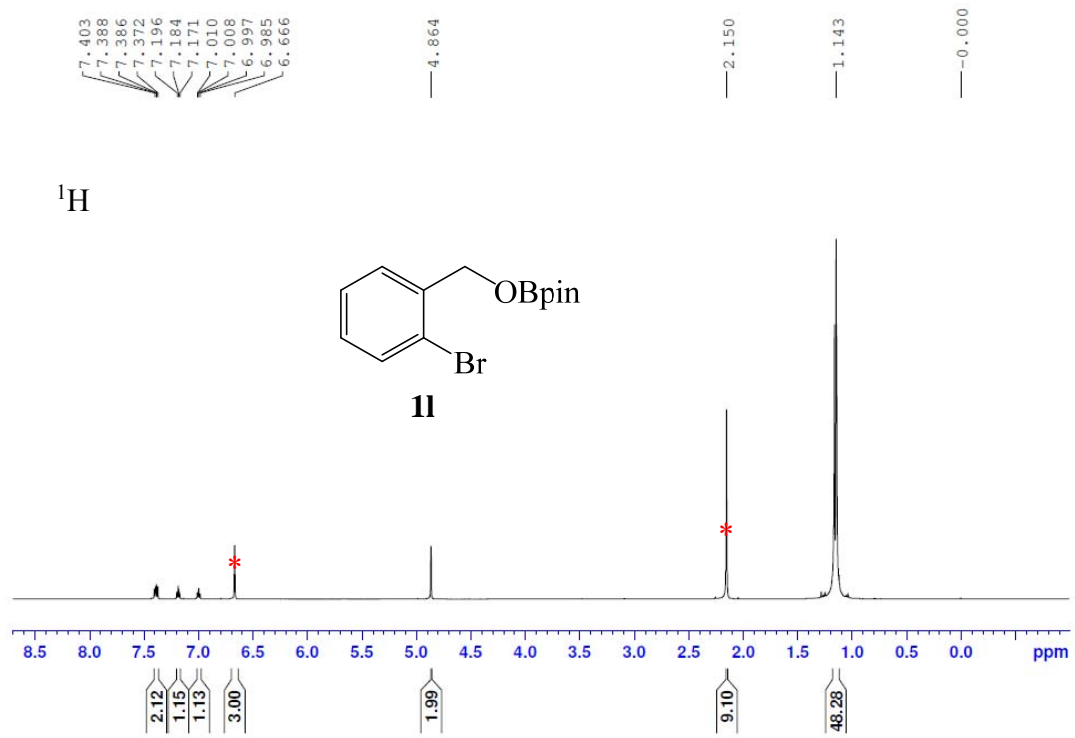
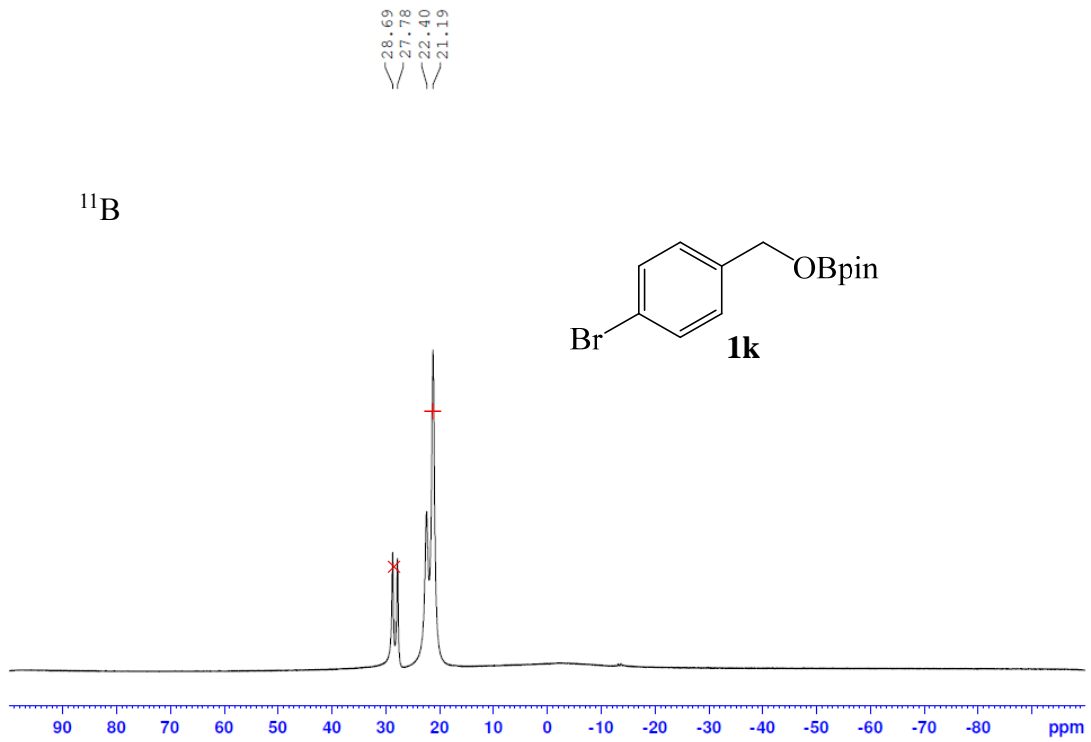


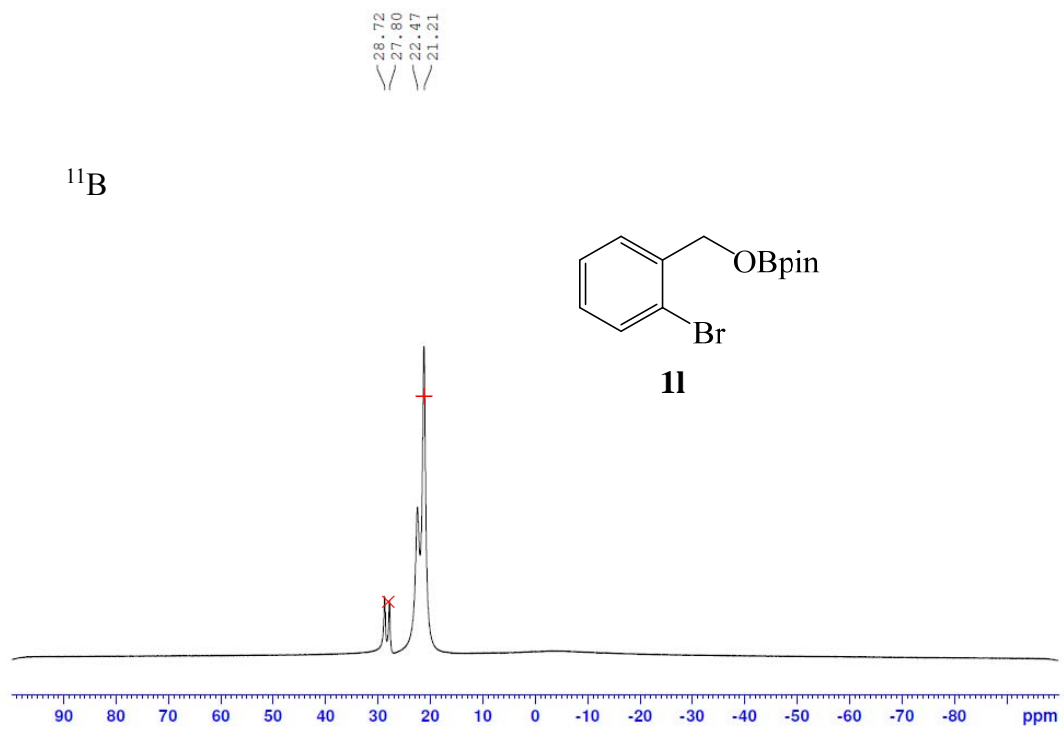
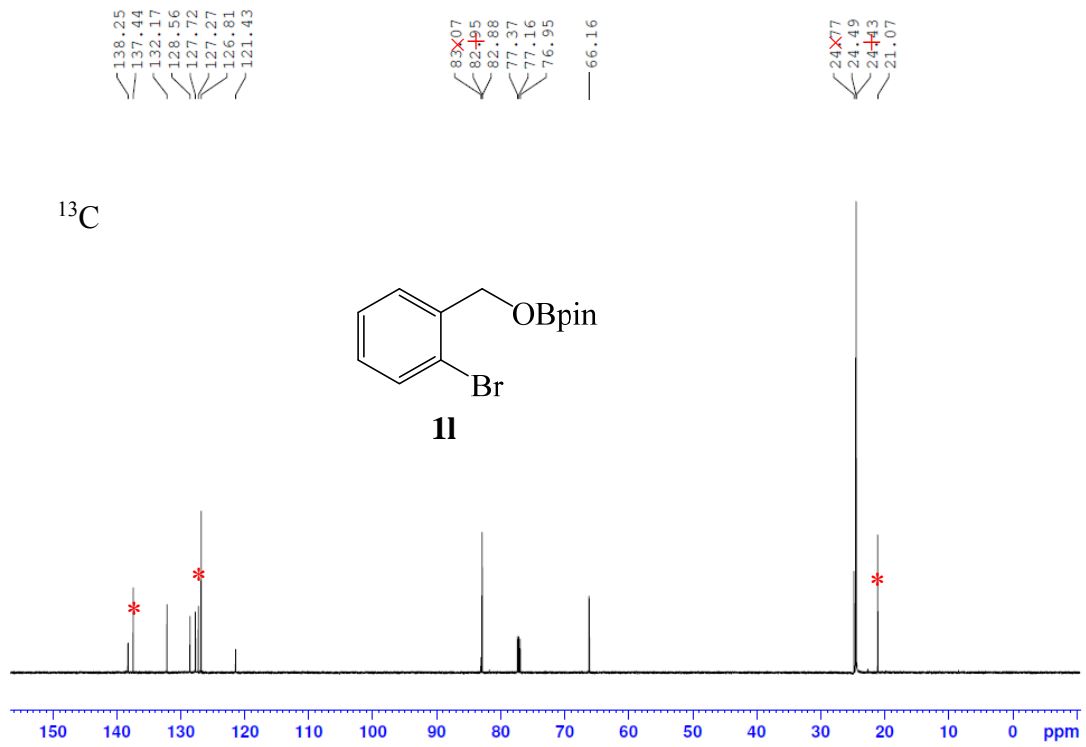


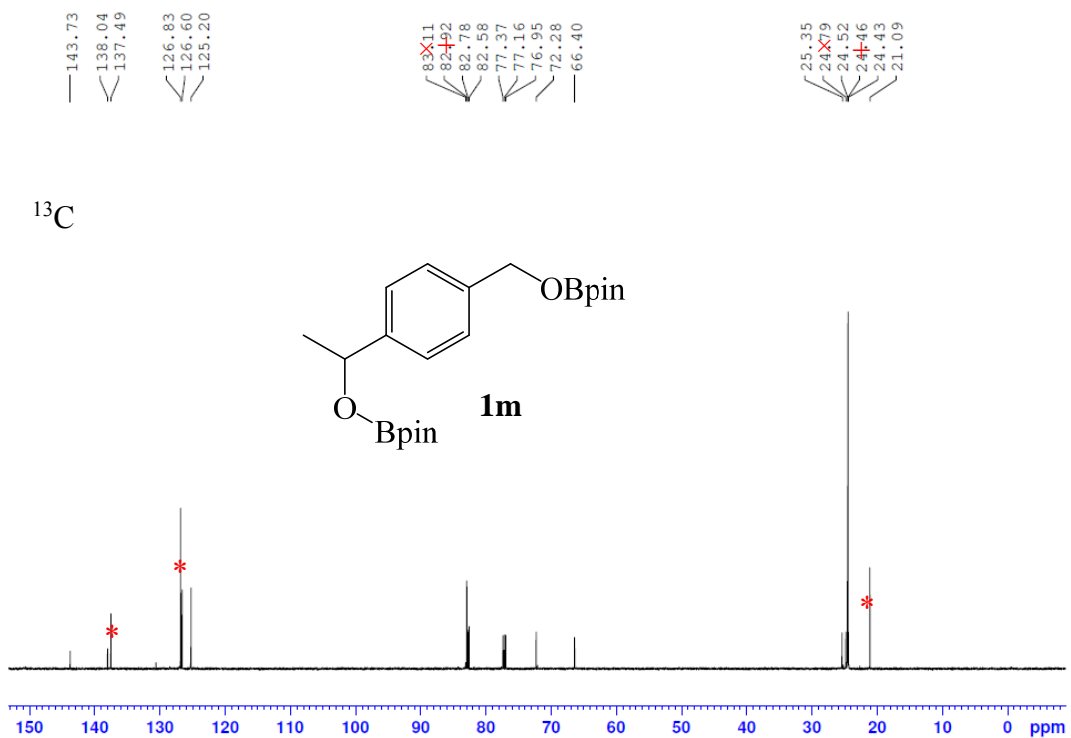
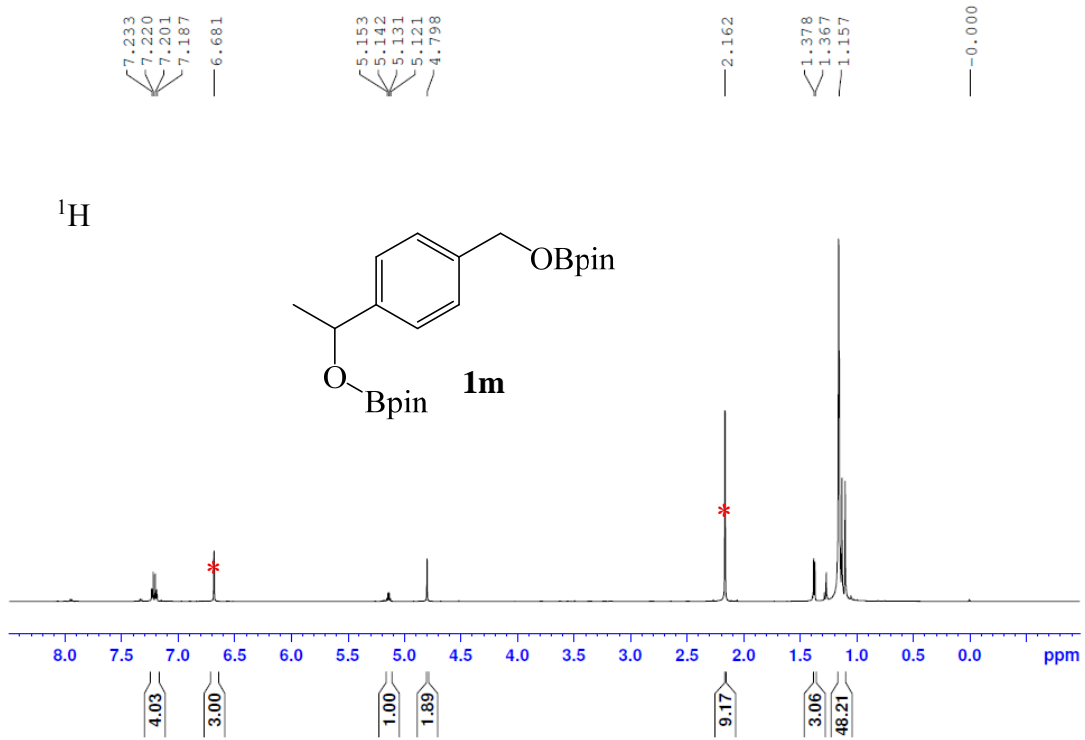


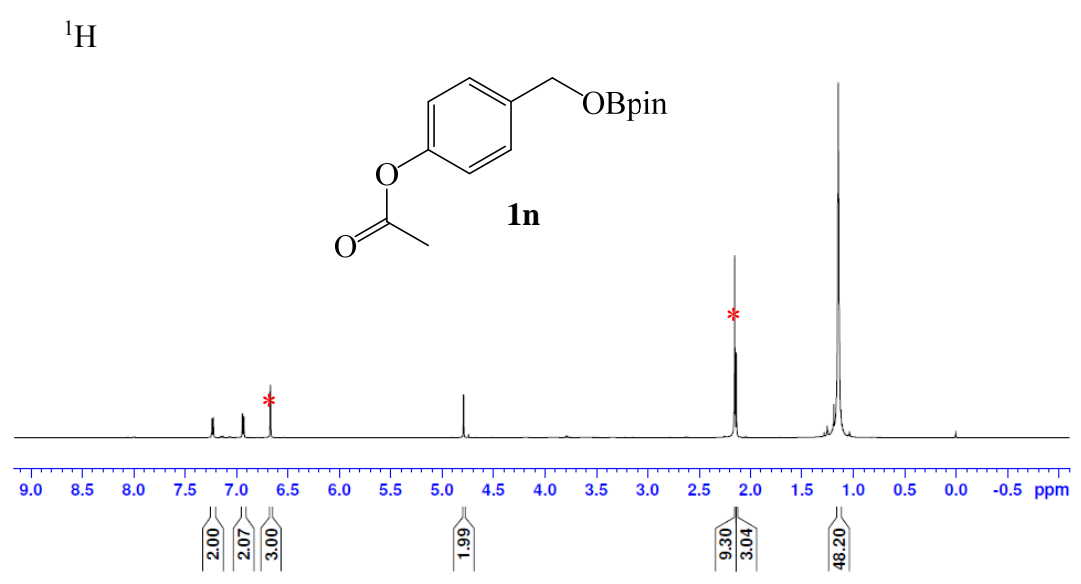
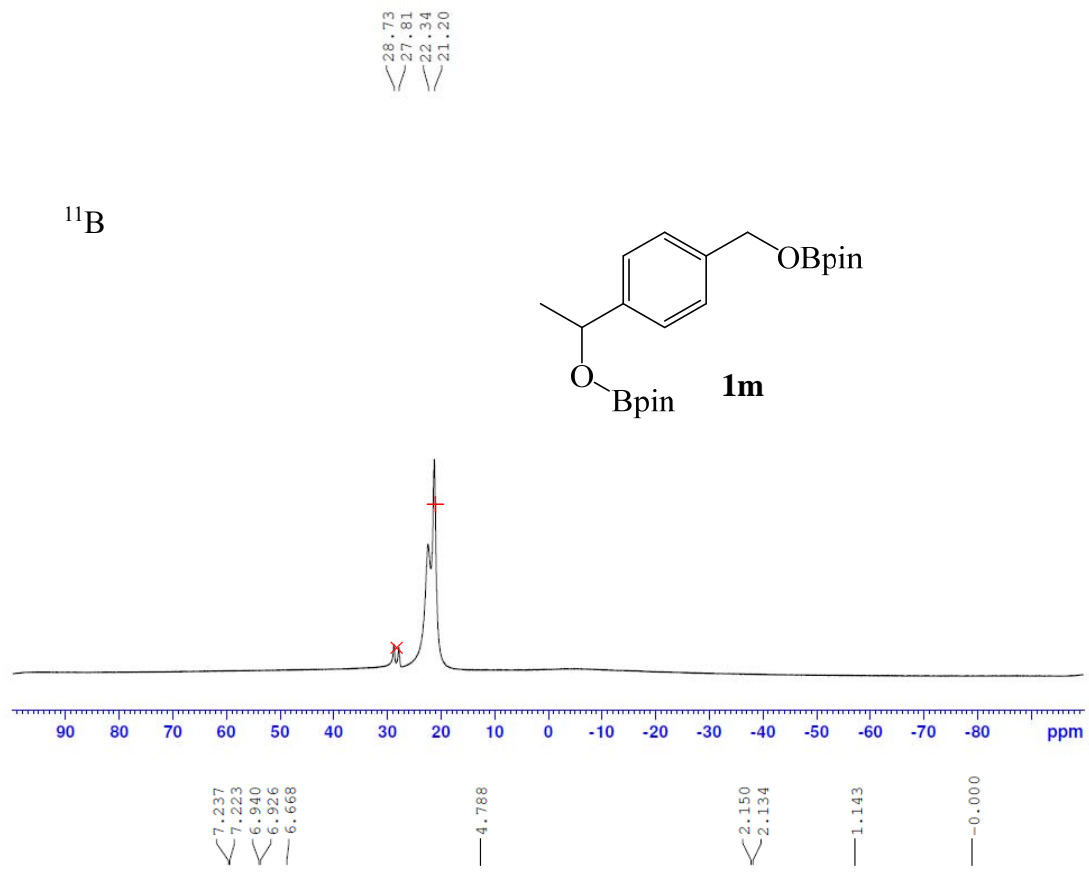


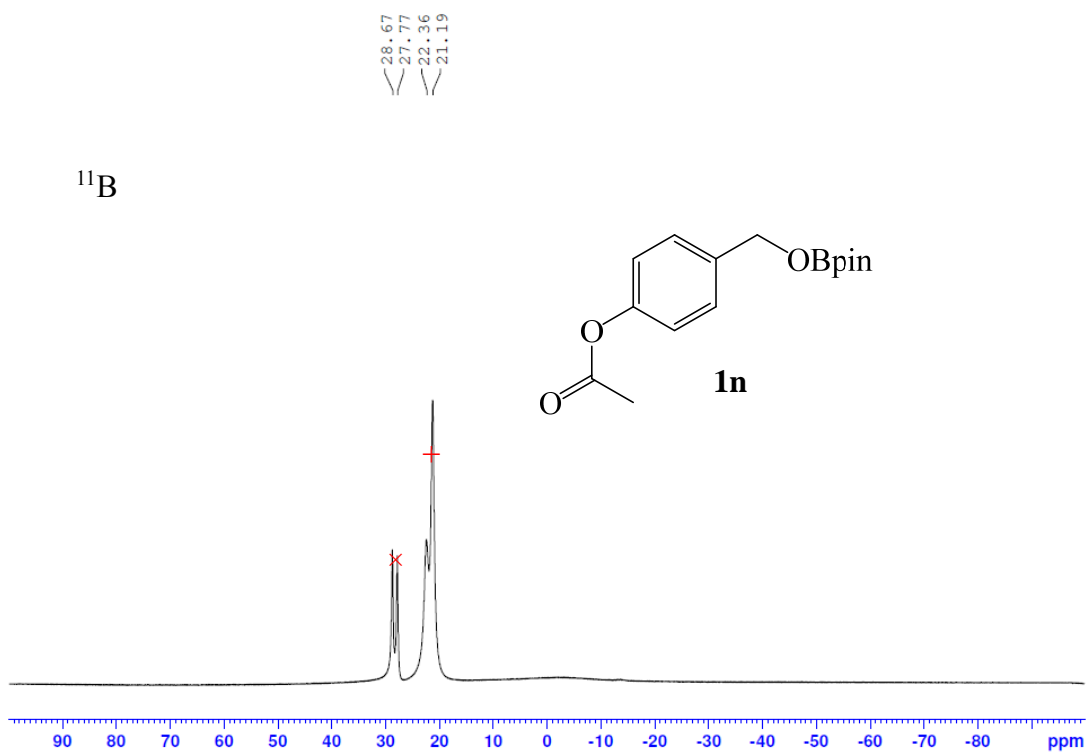
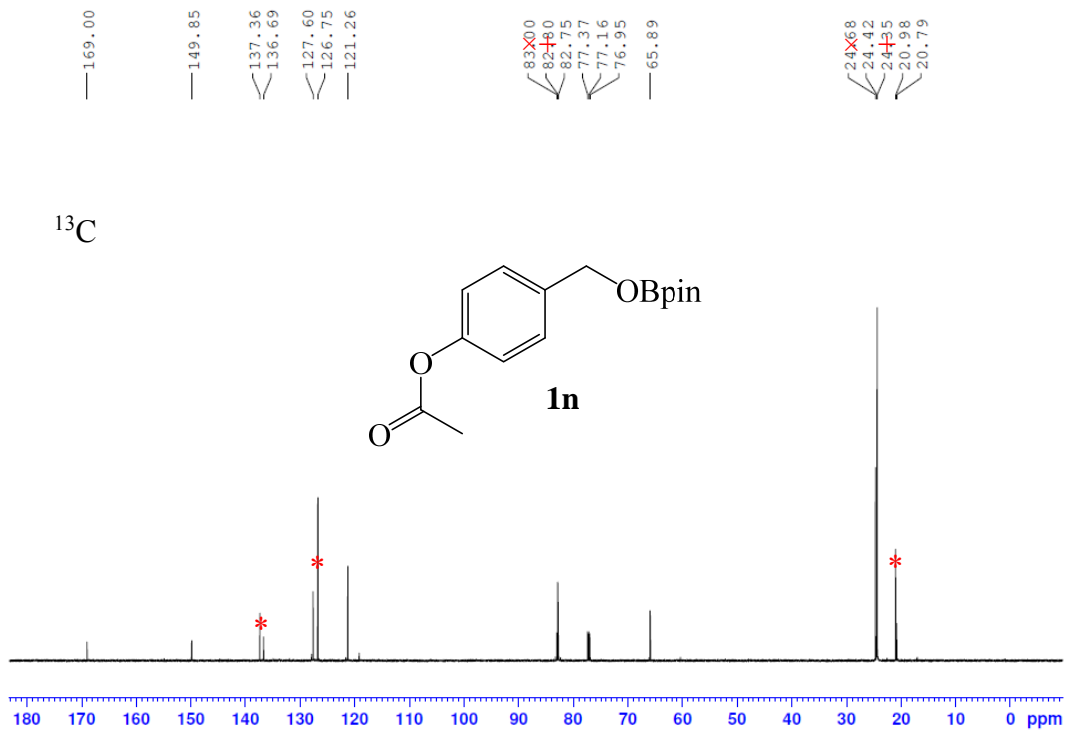




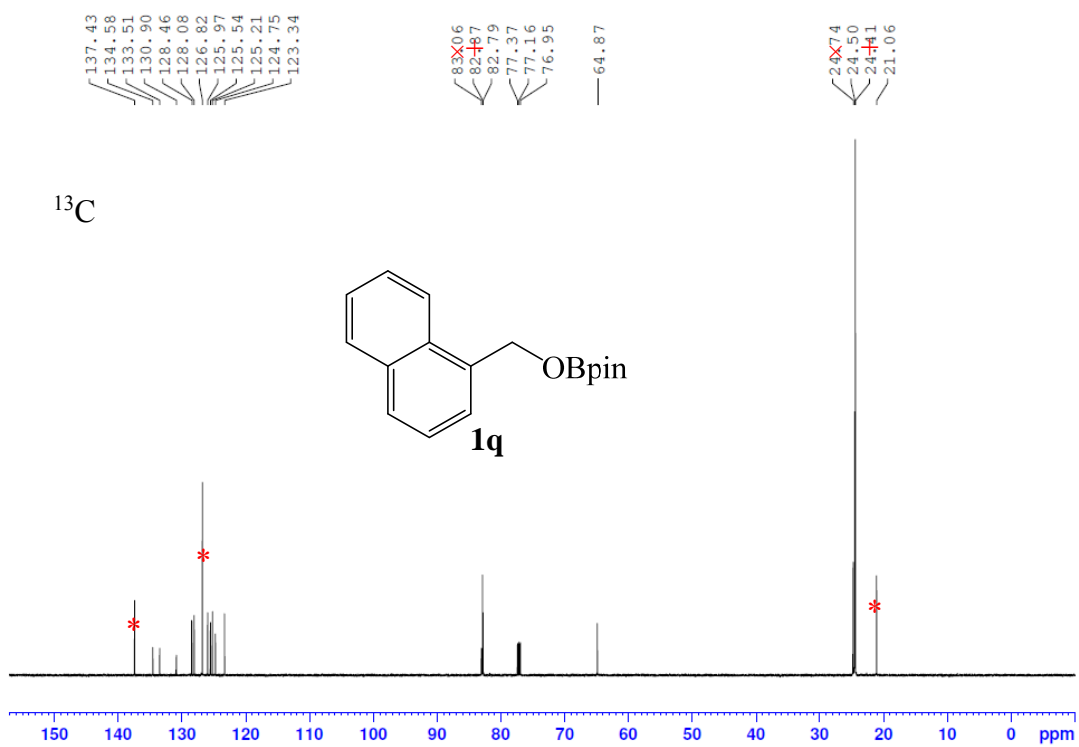
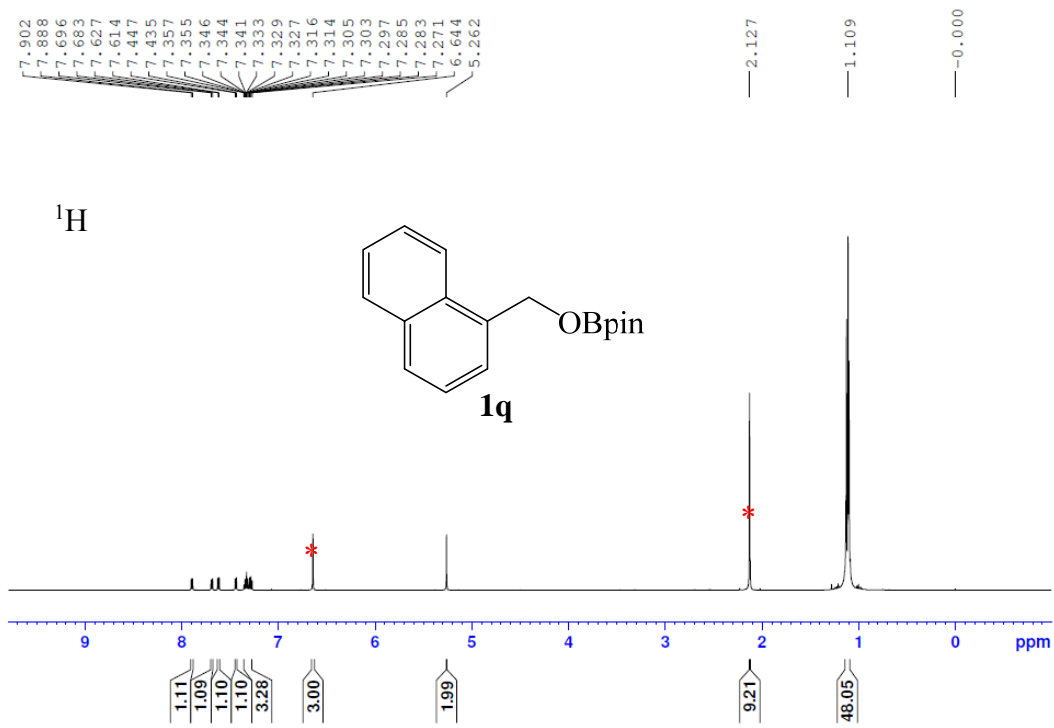


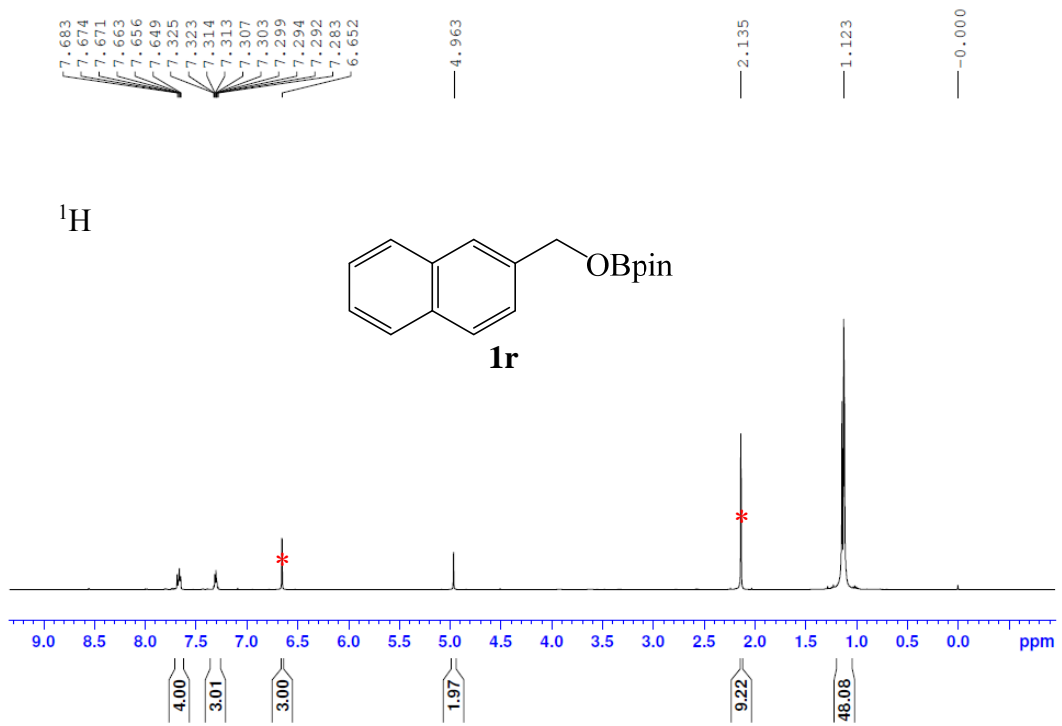
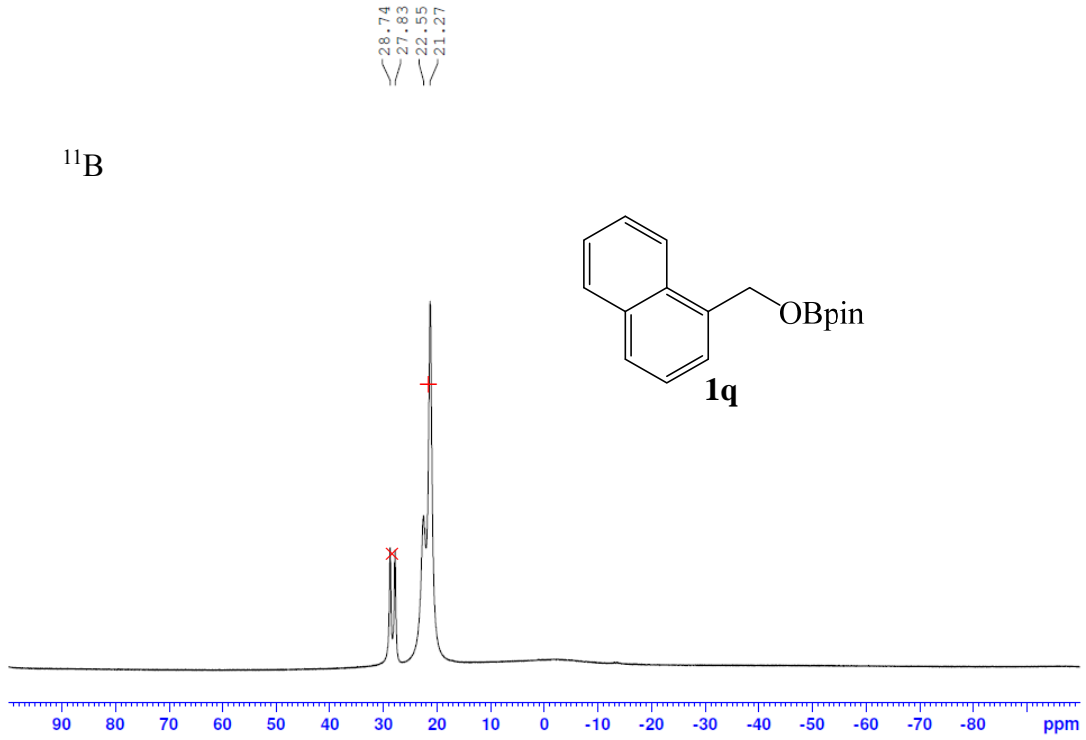


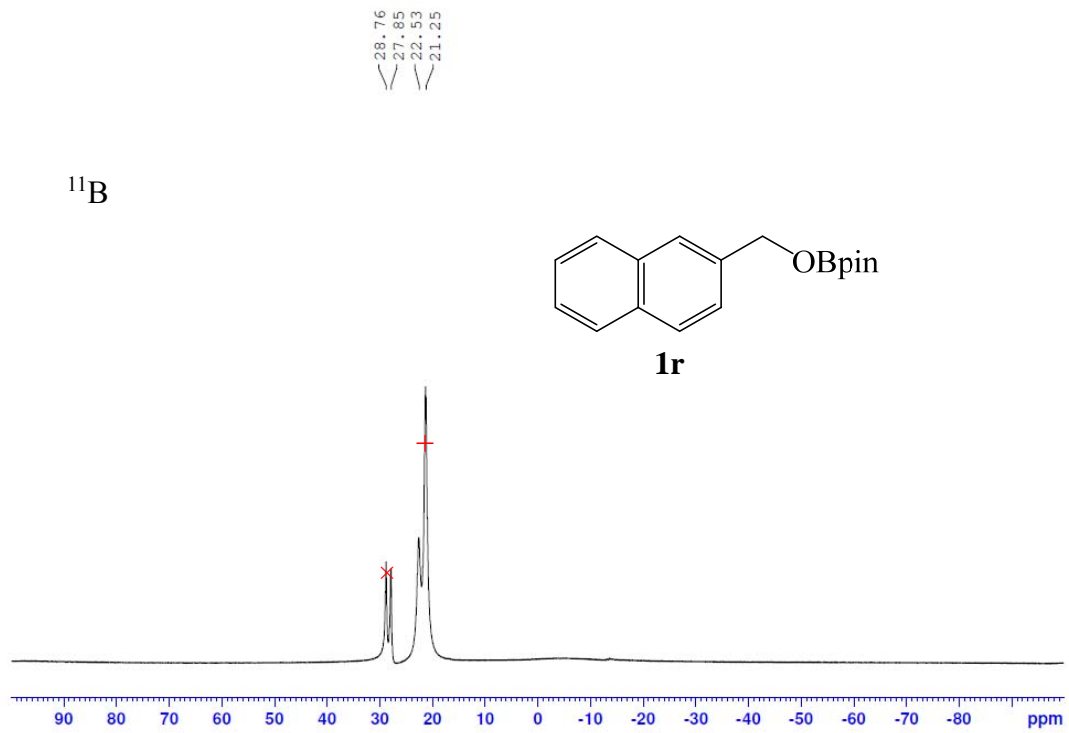
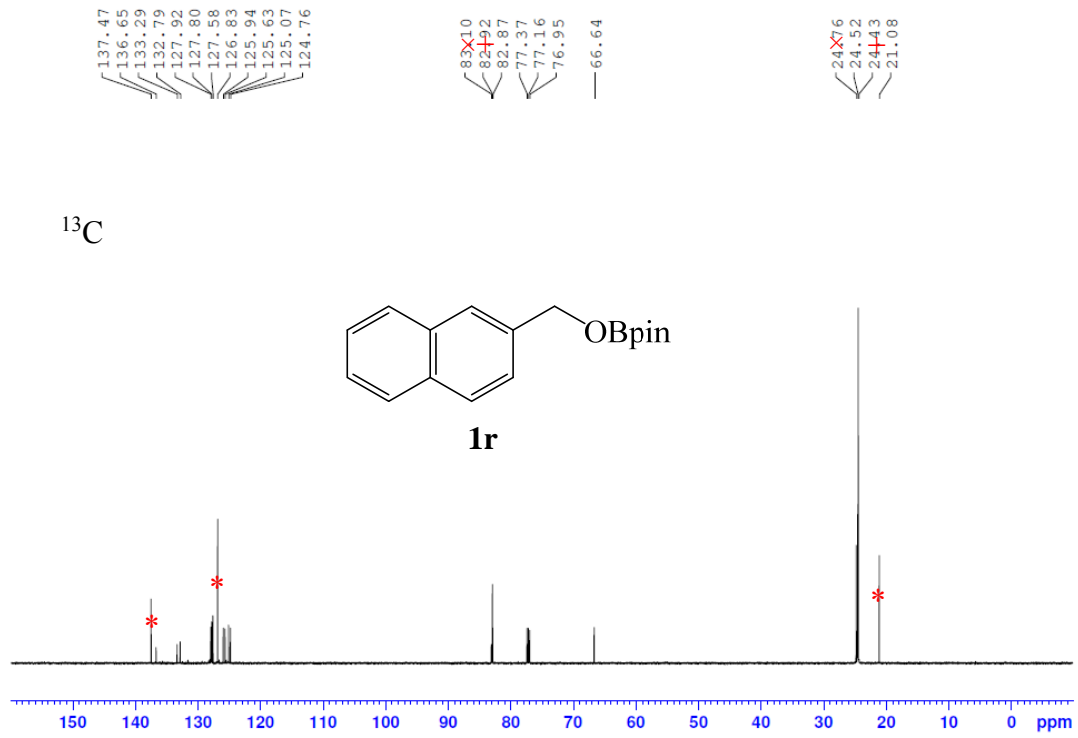


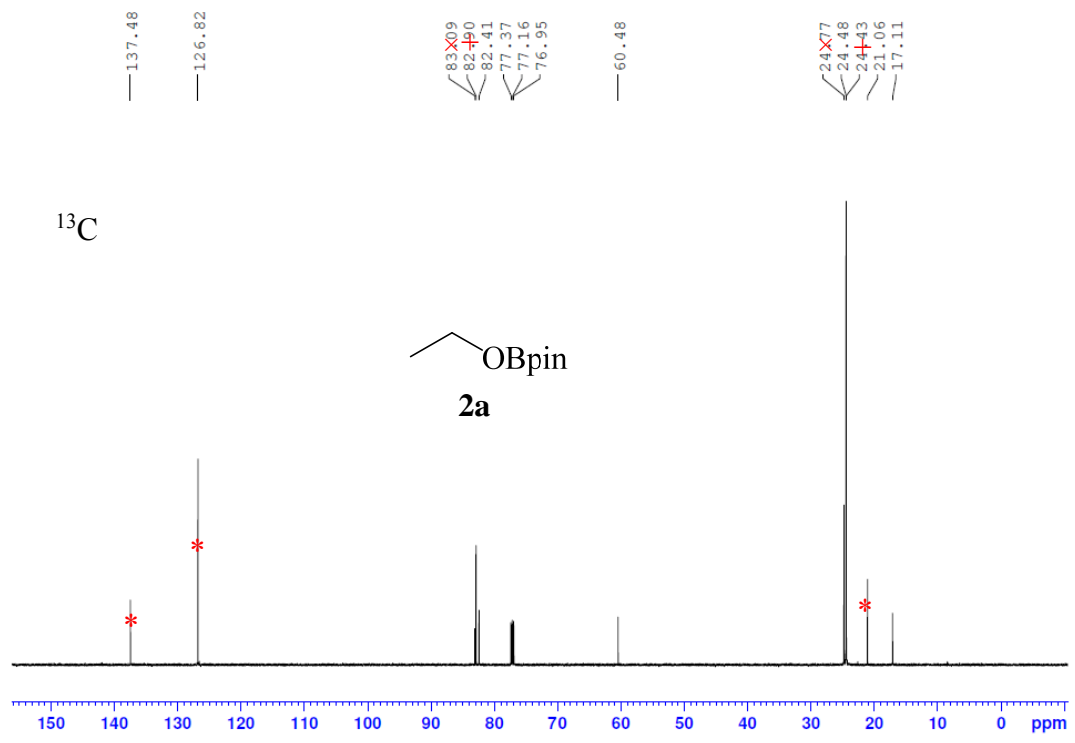
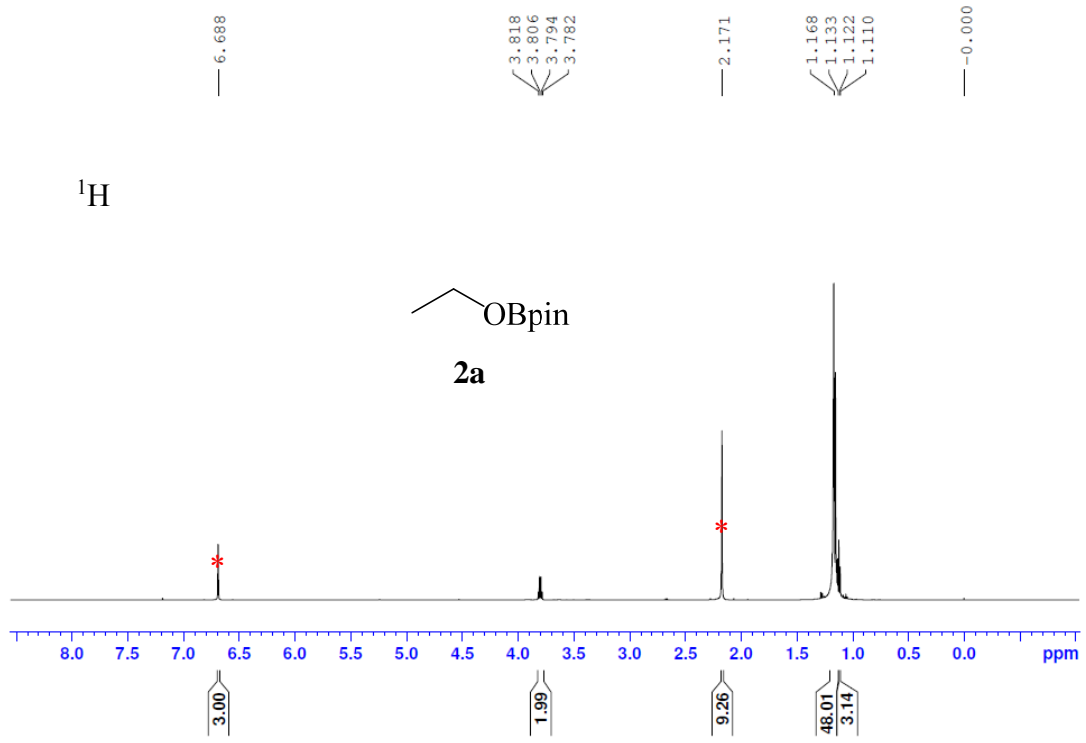


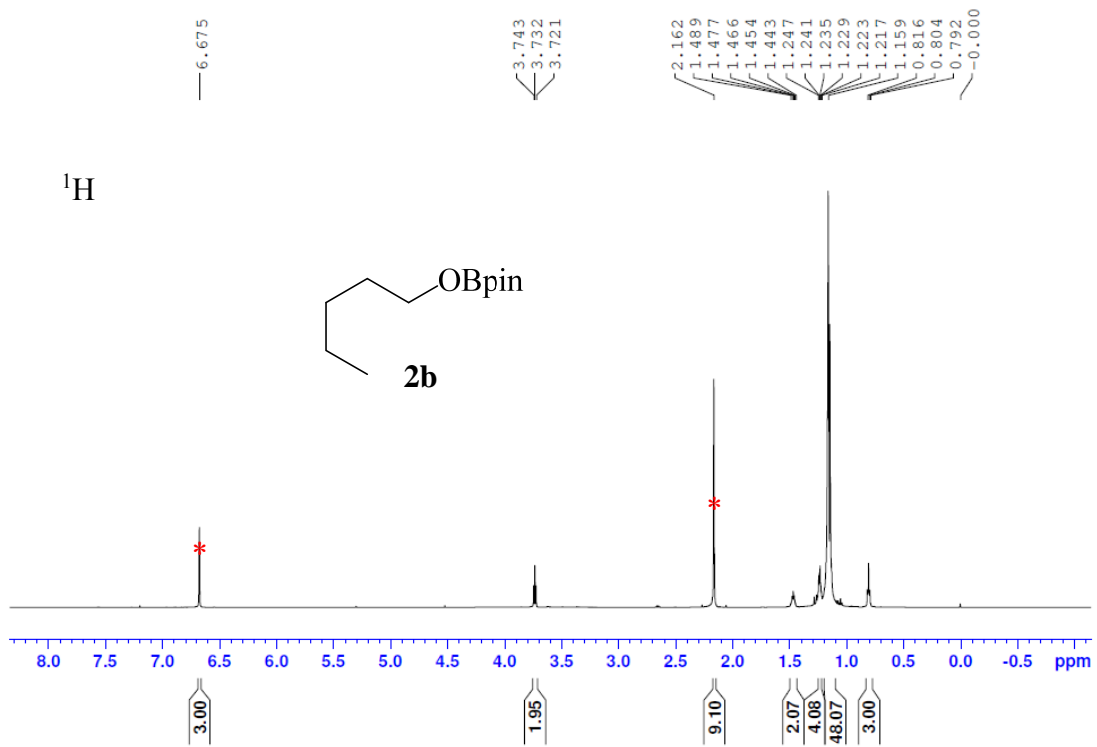
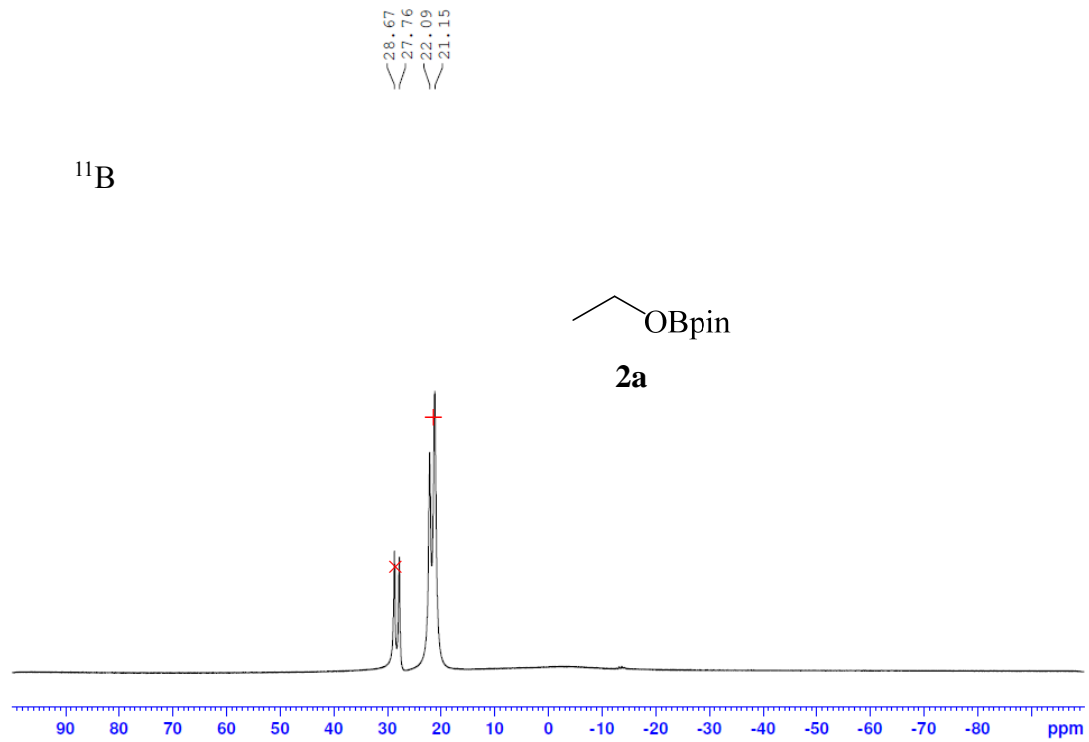


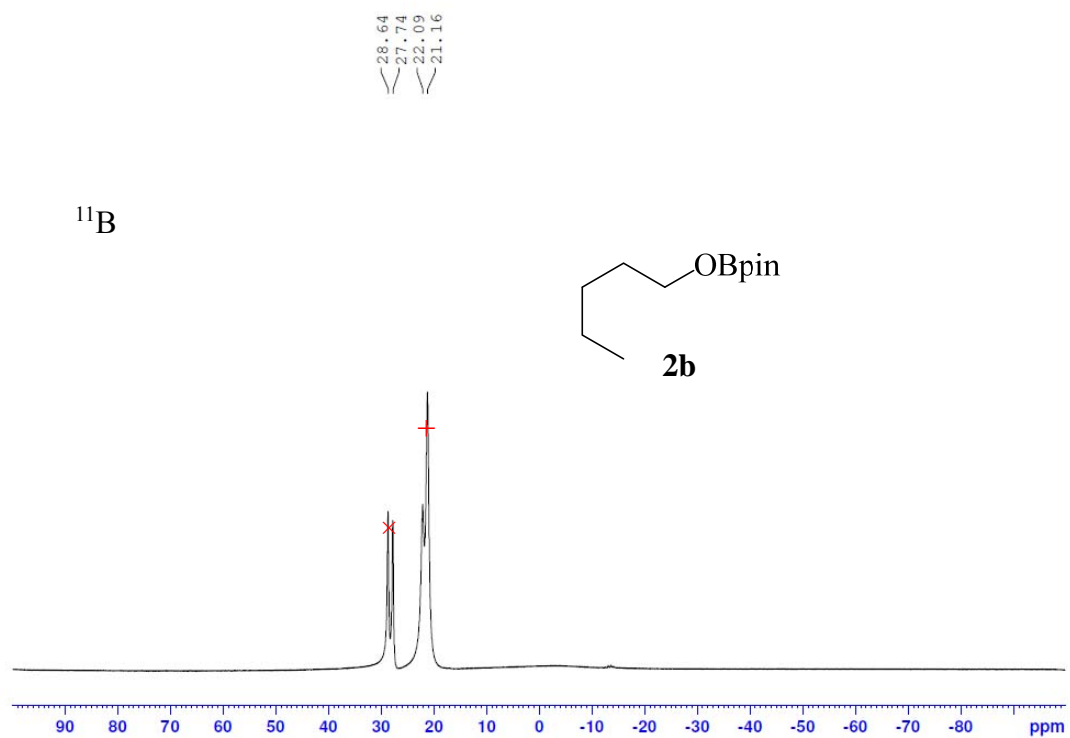
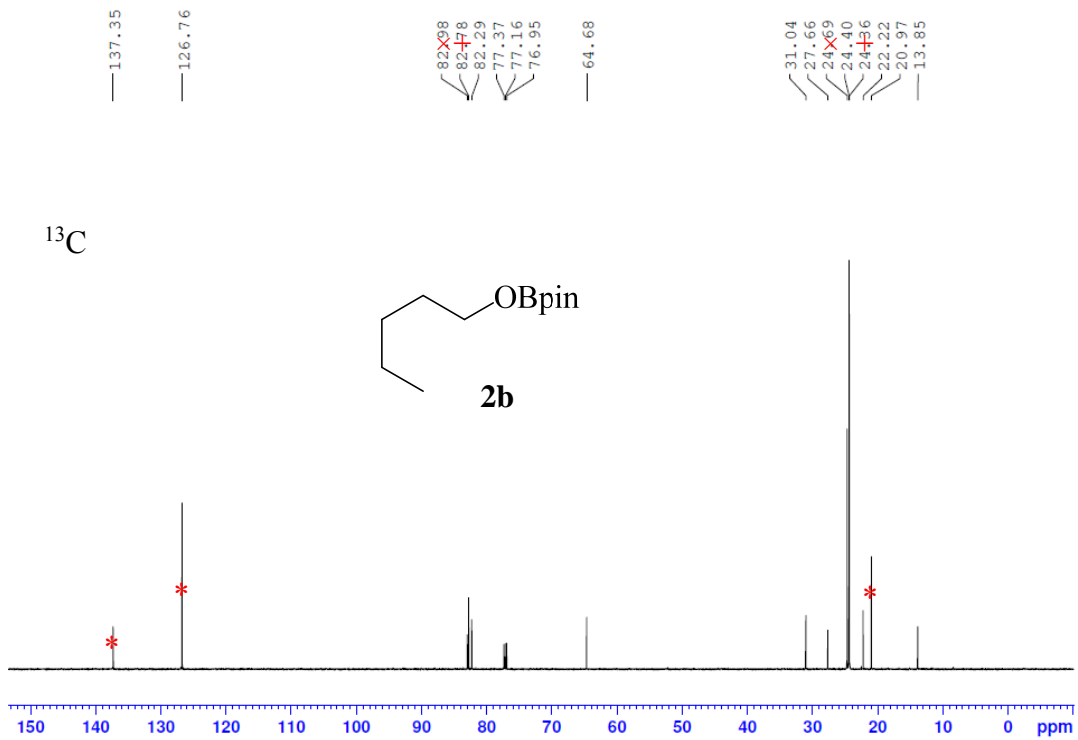


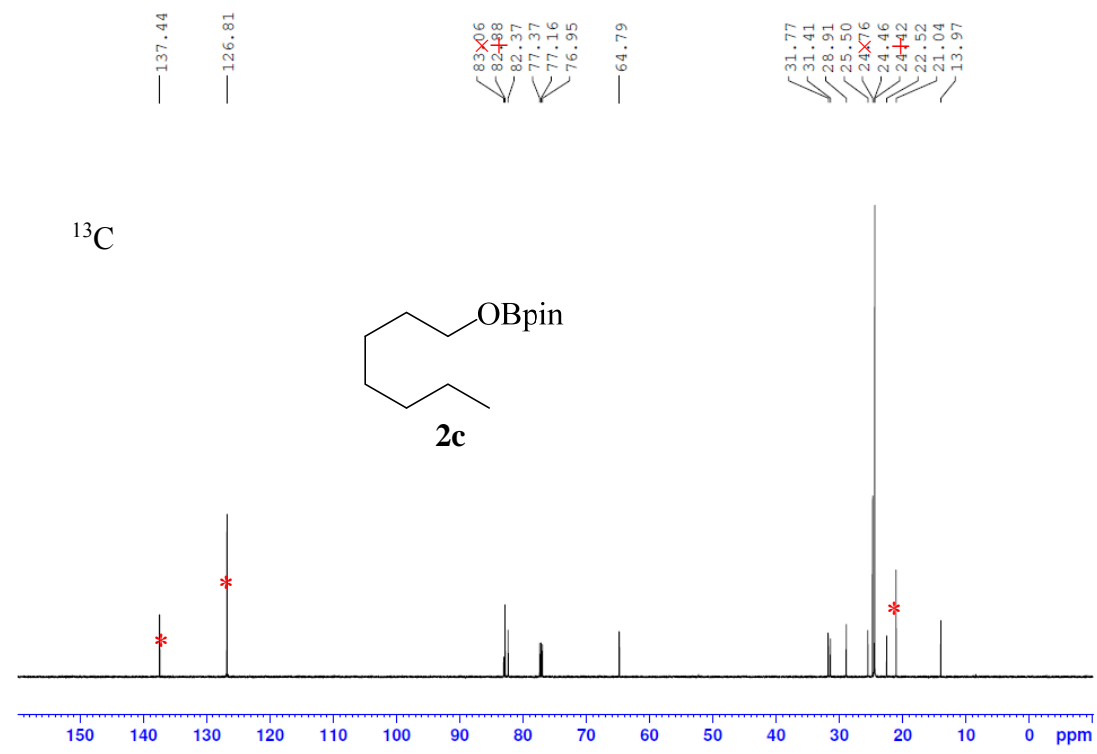
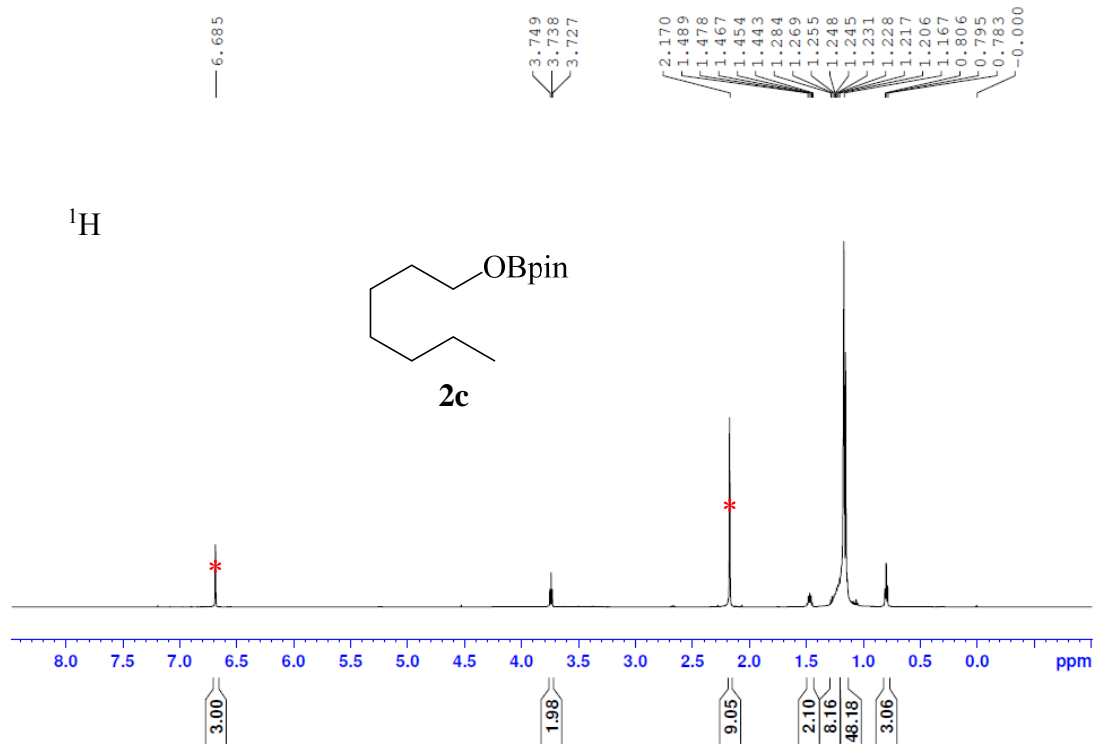


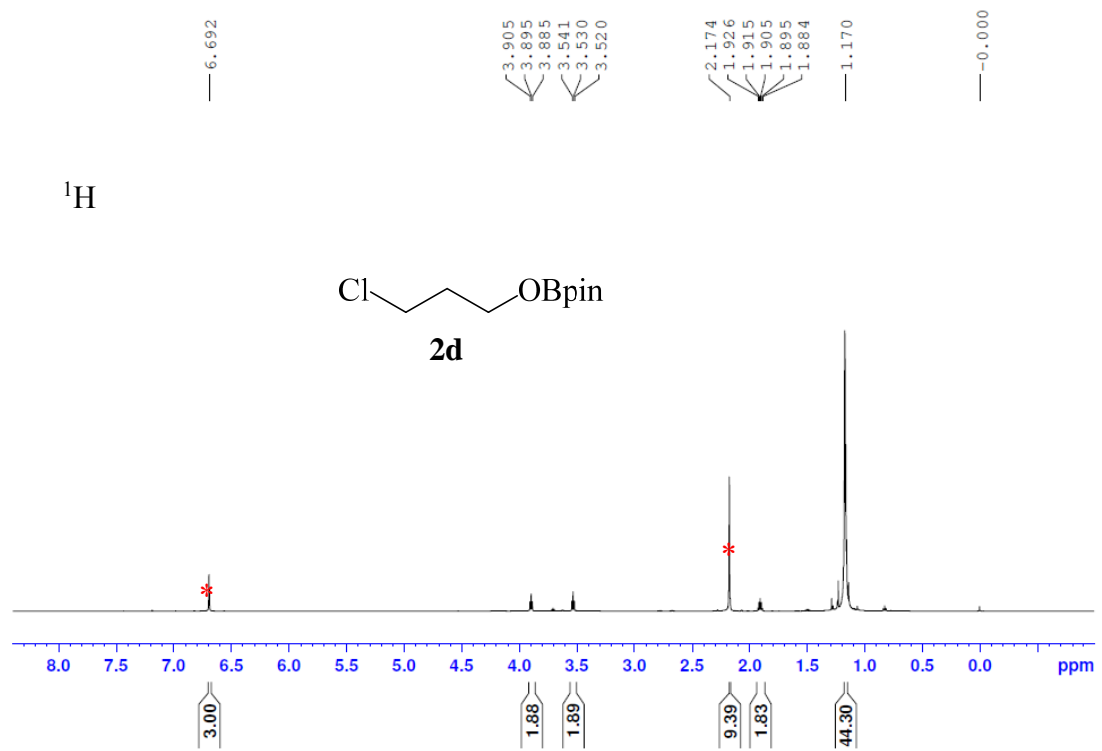
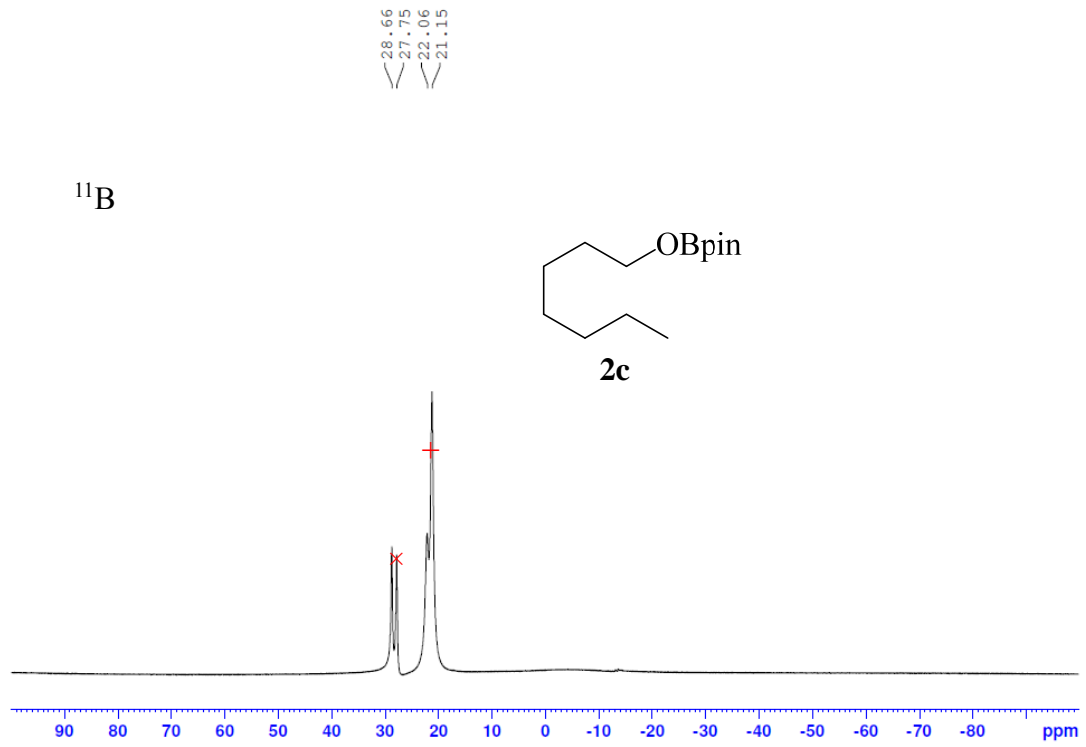






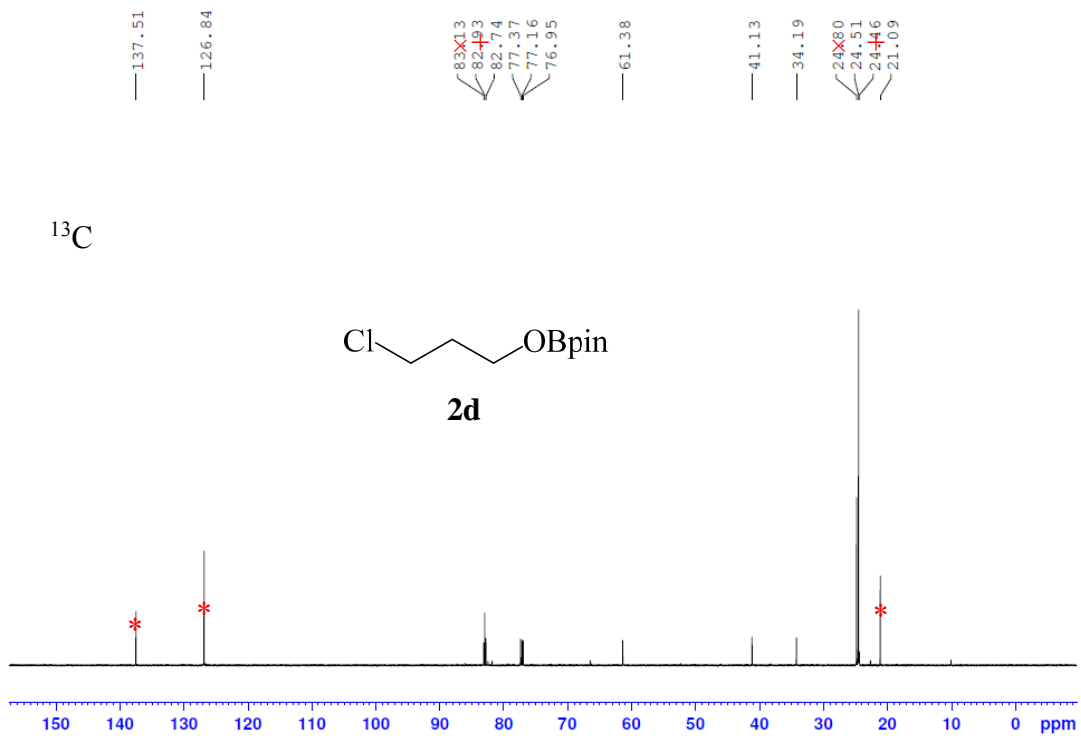




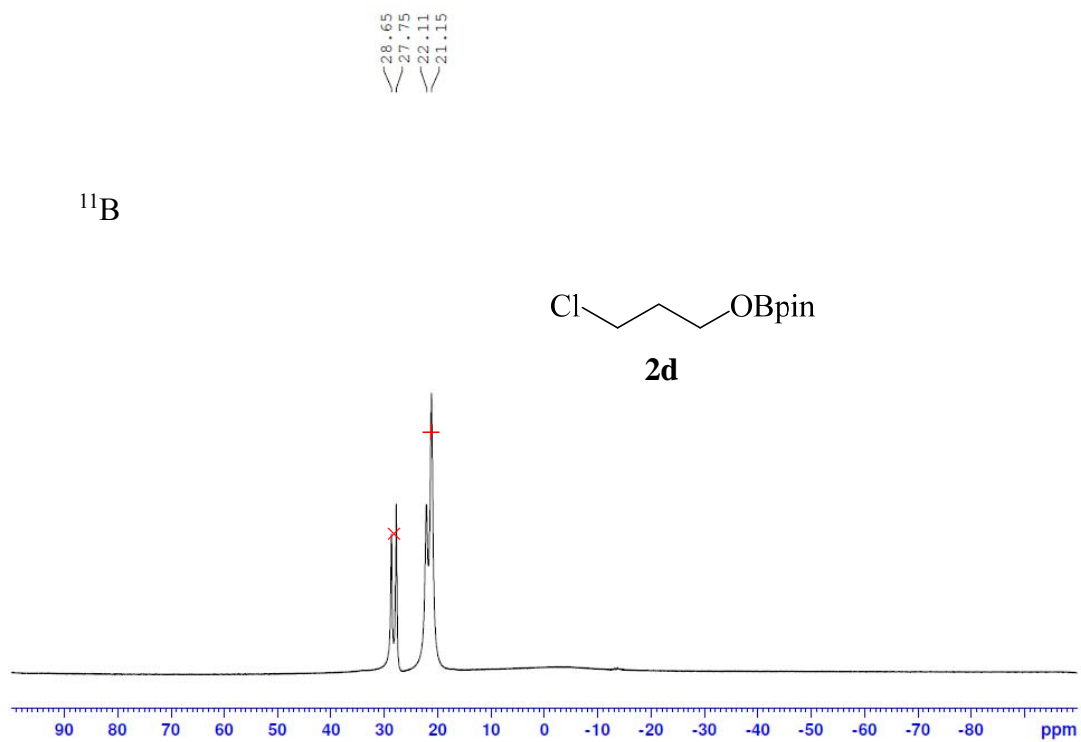




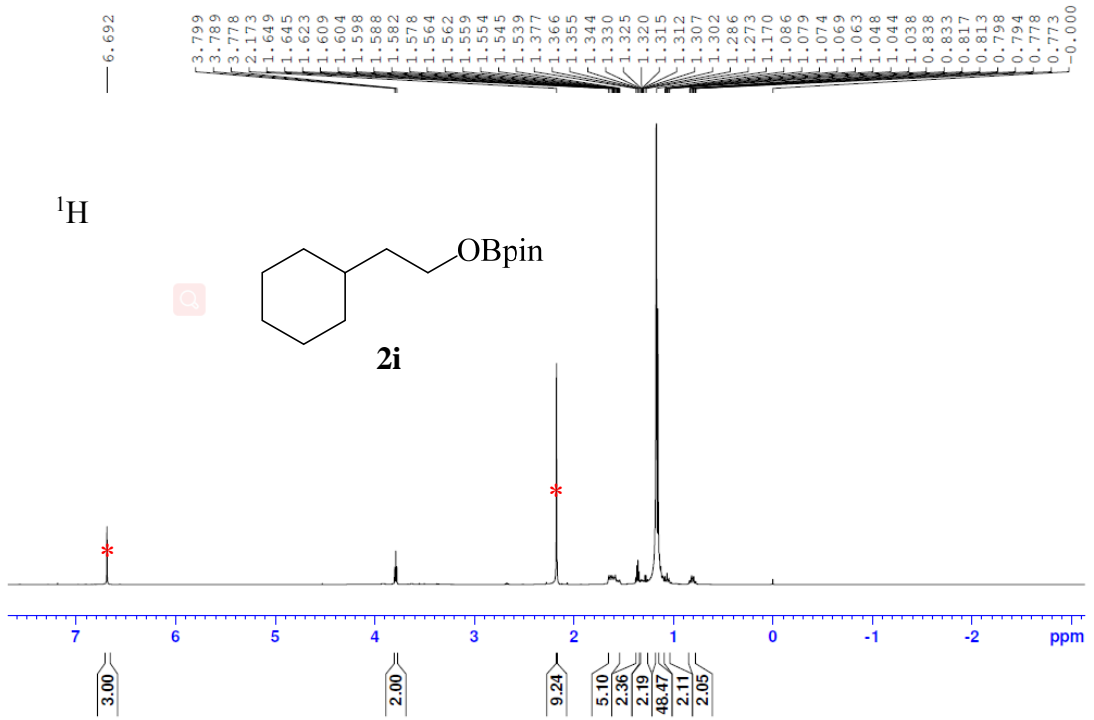
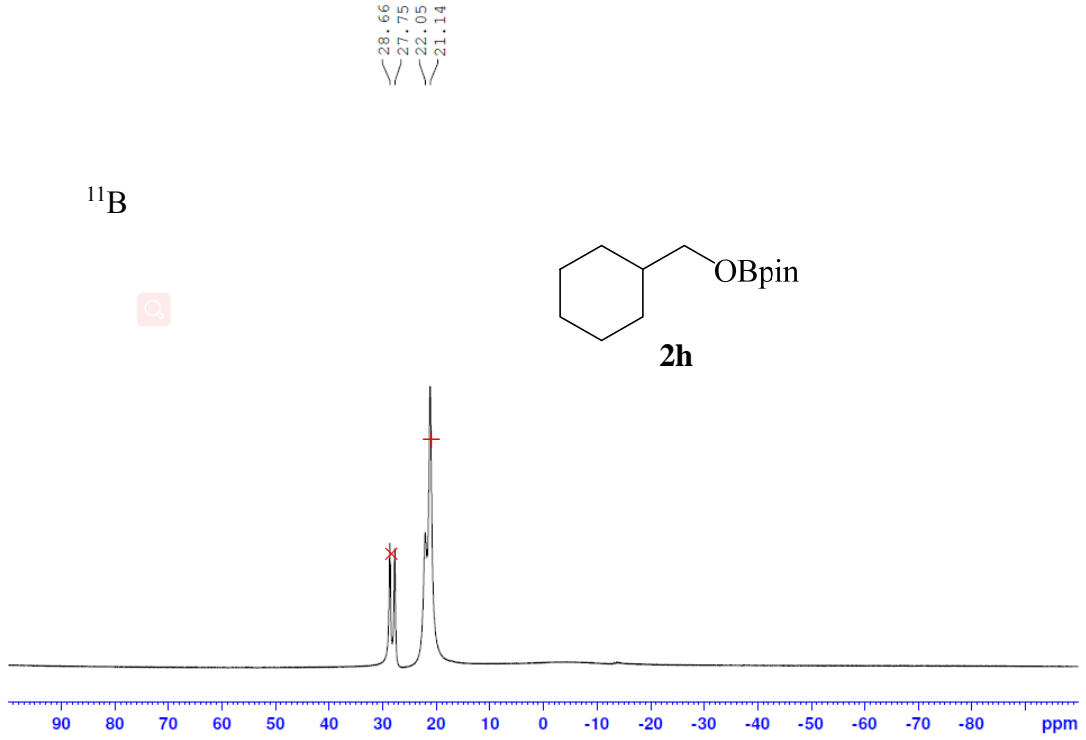
$^{13}\text{C}$

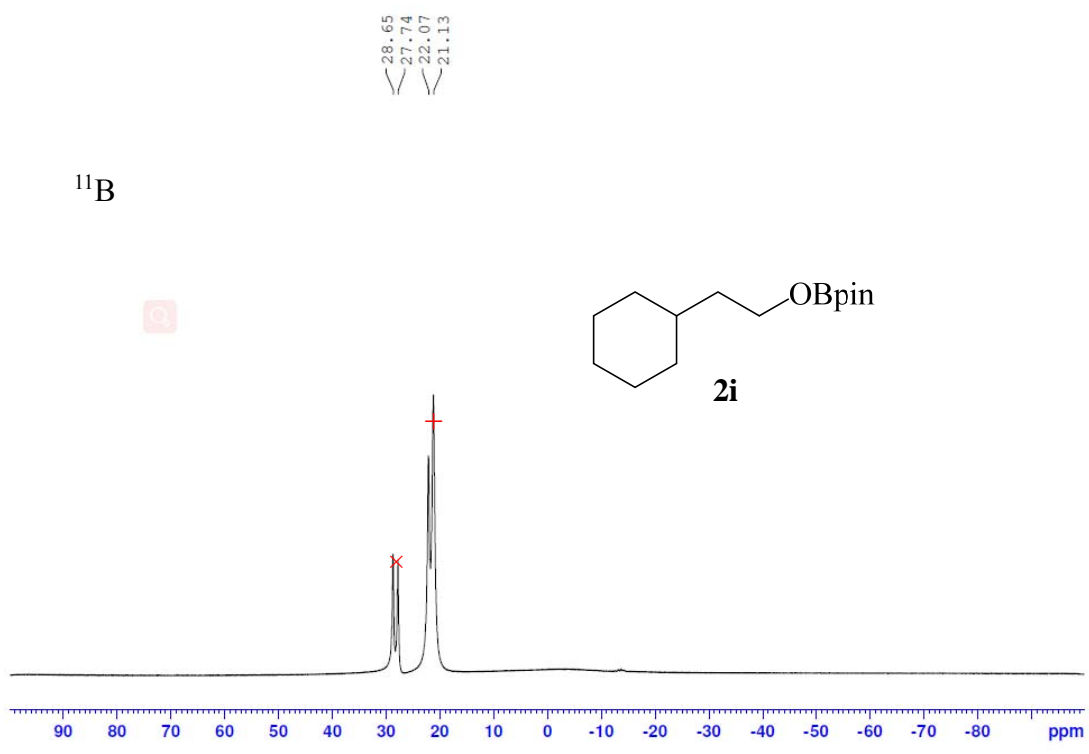
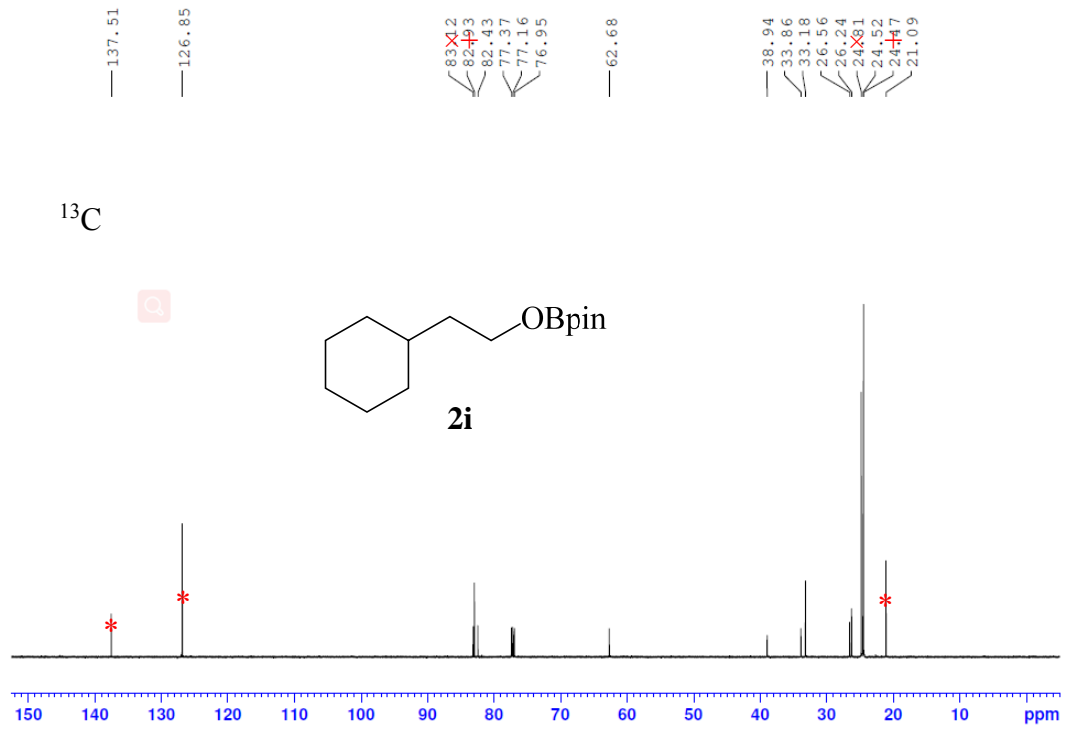


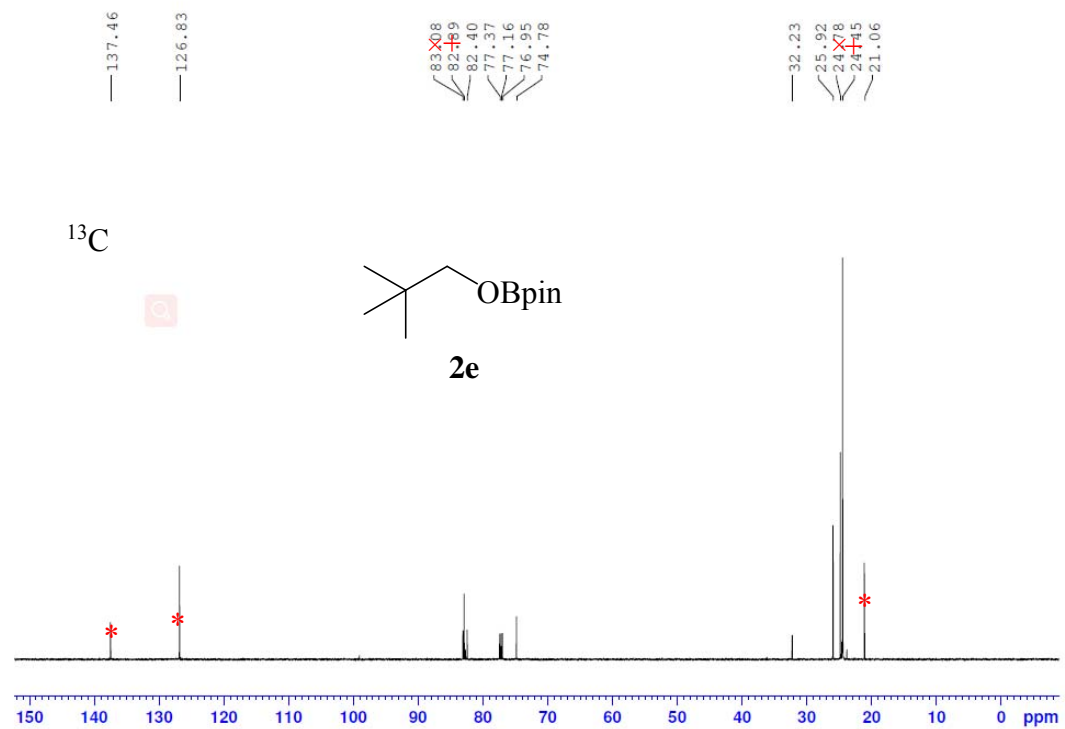
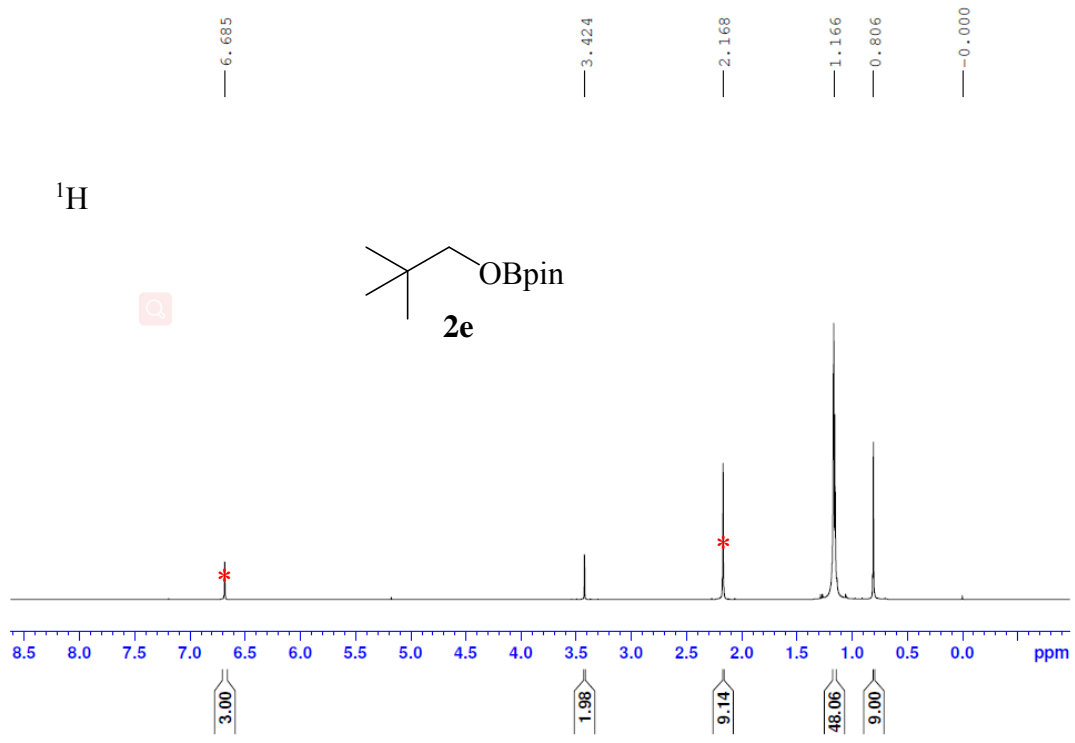
$^{11}\text{B}$

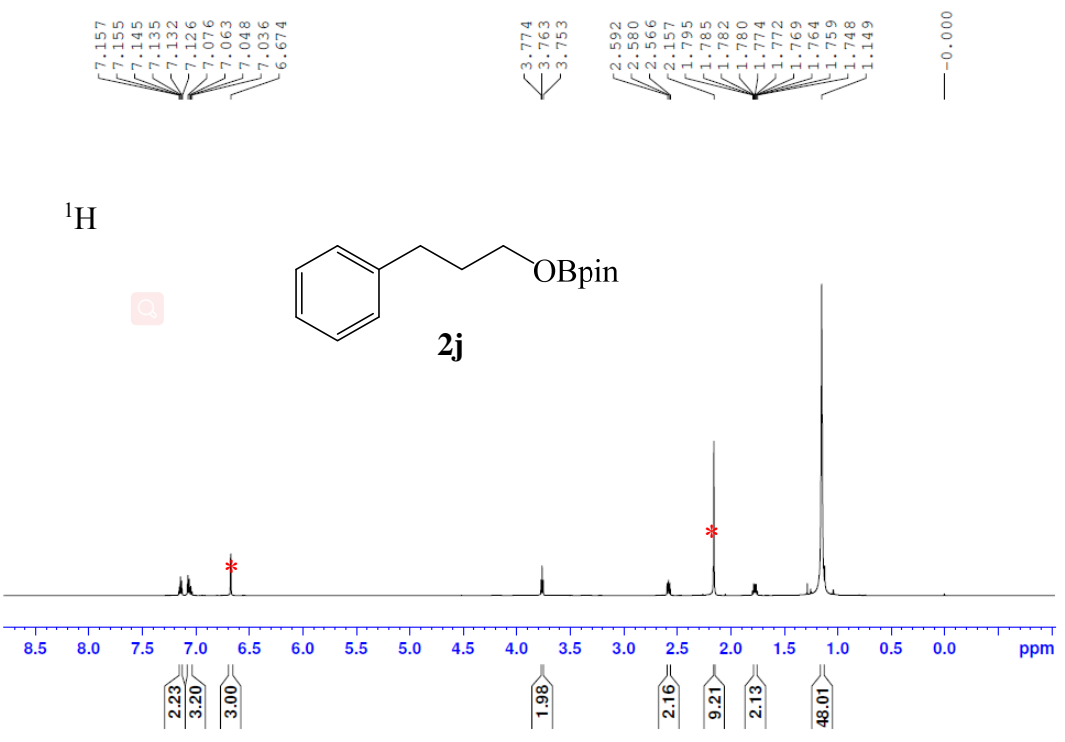
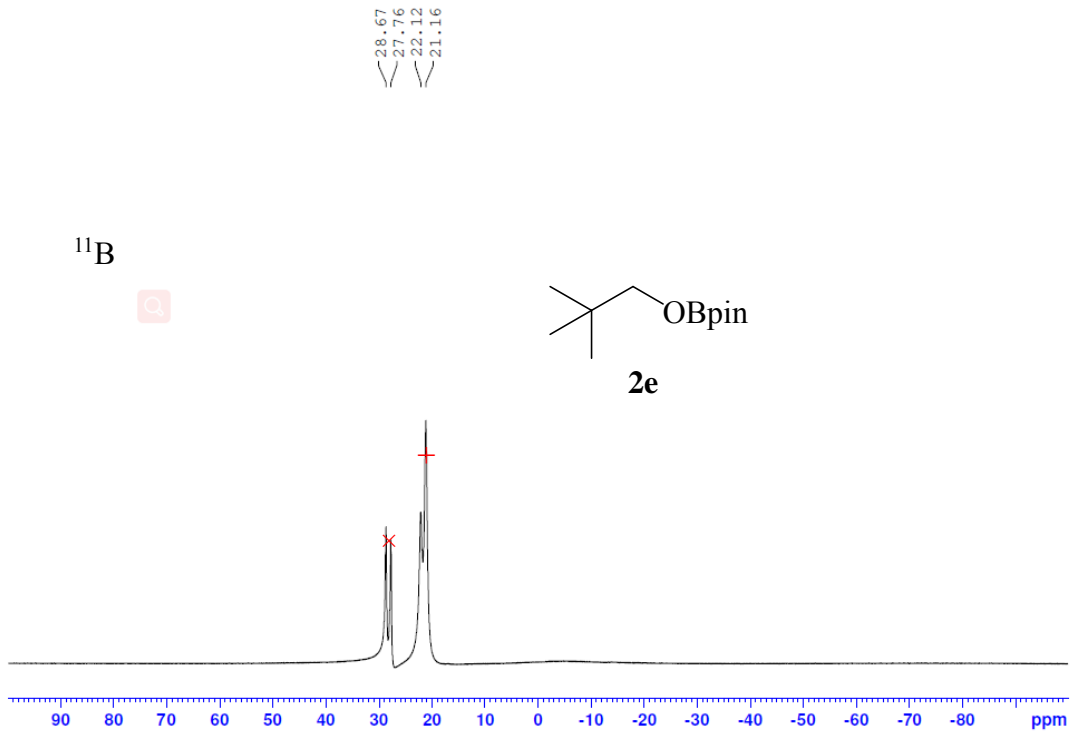


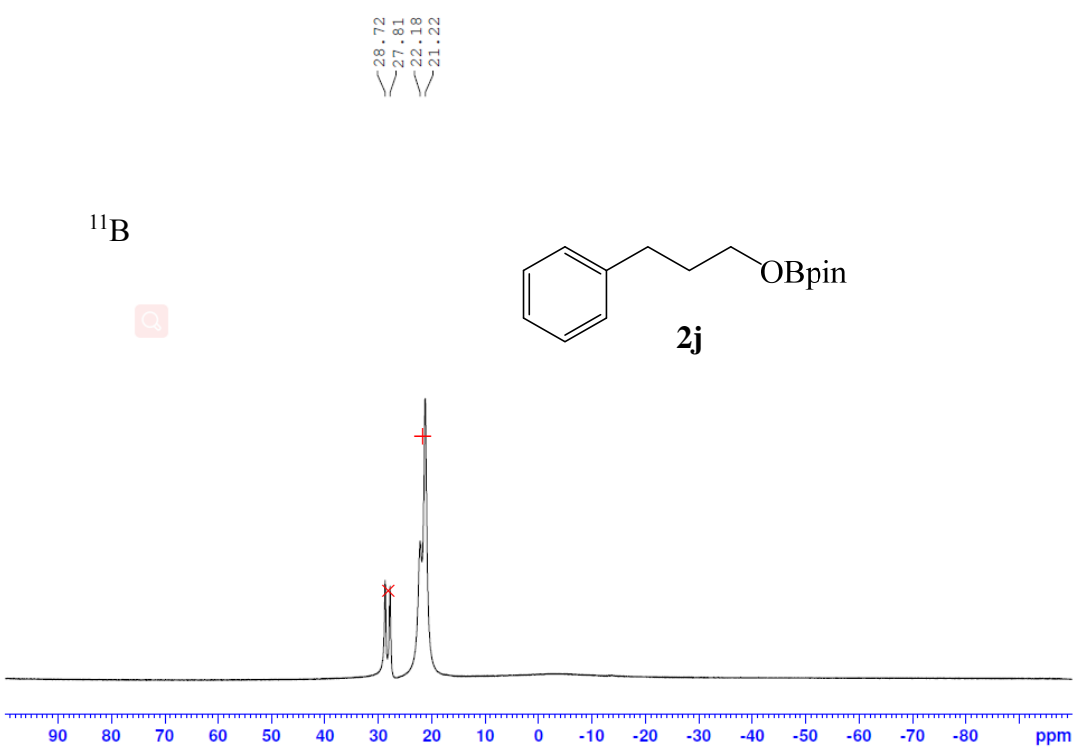
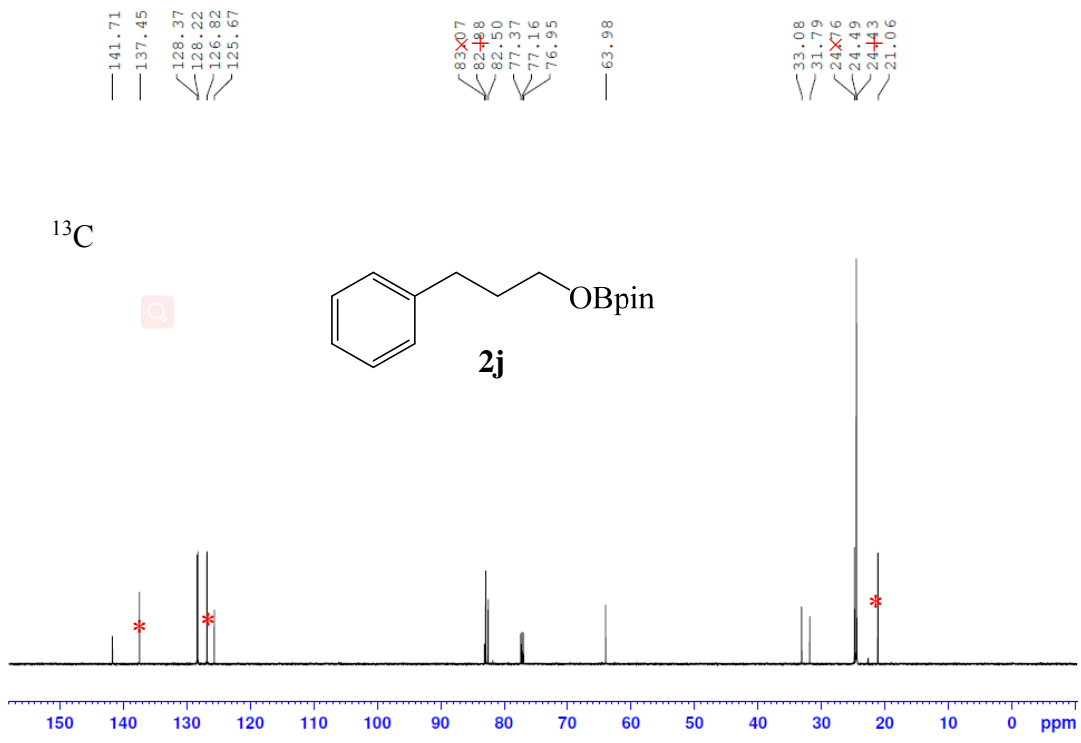


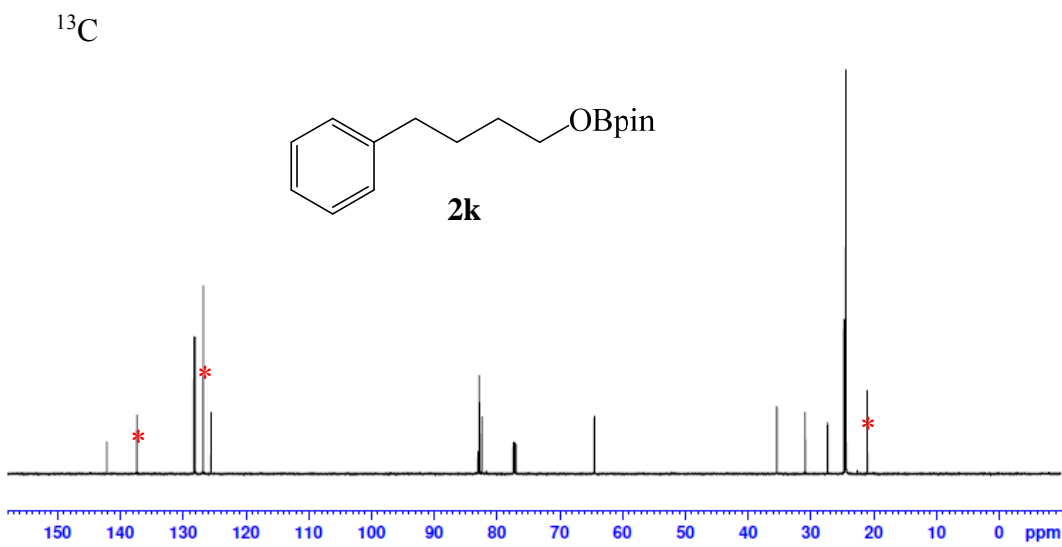
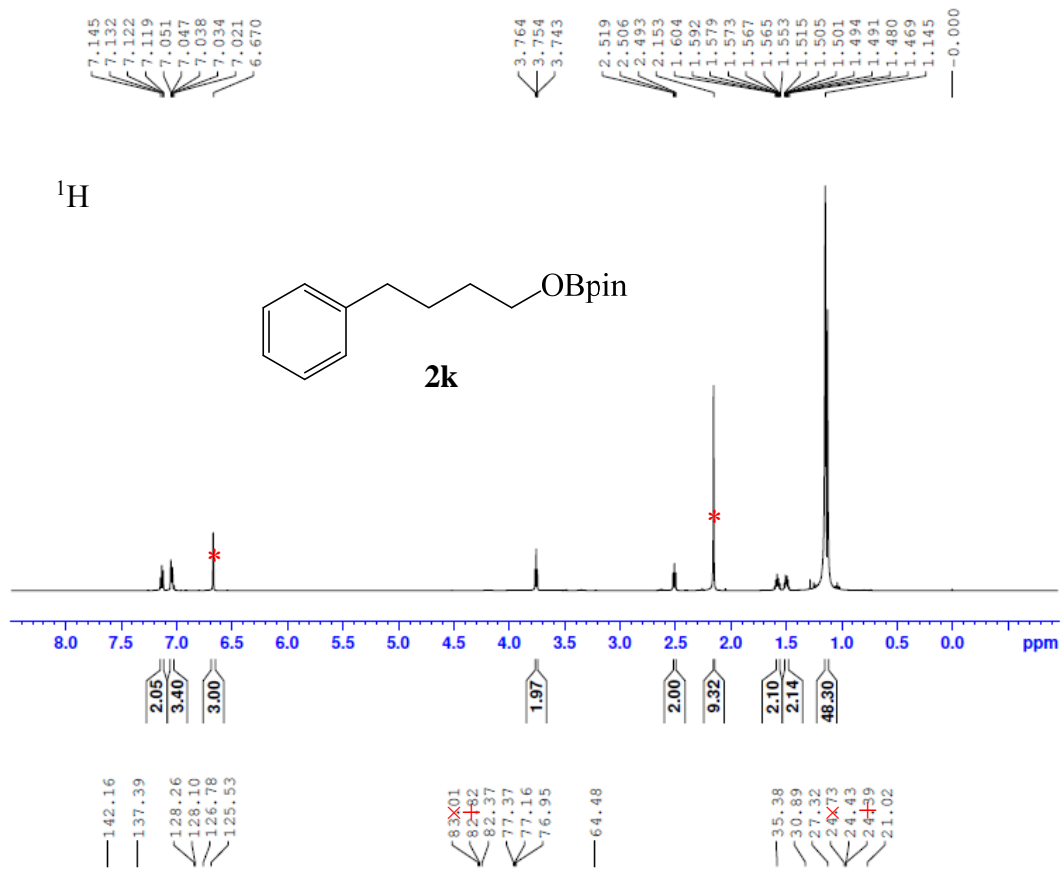




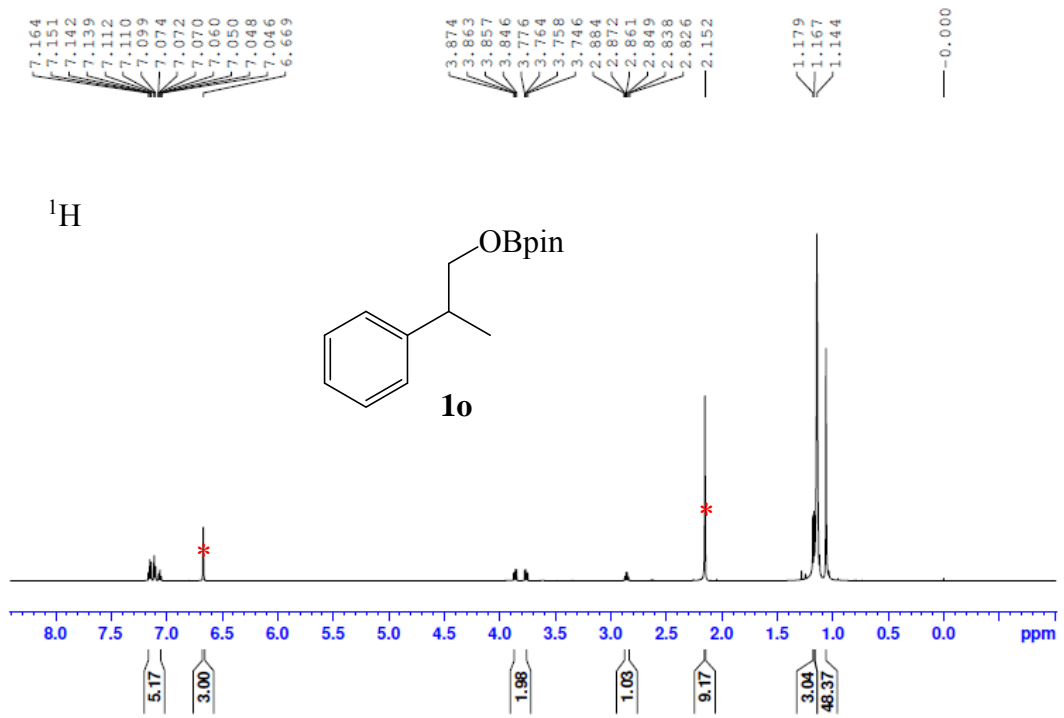
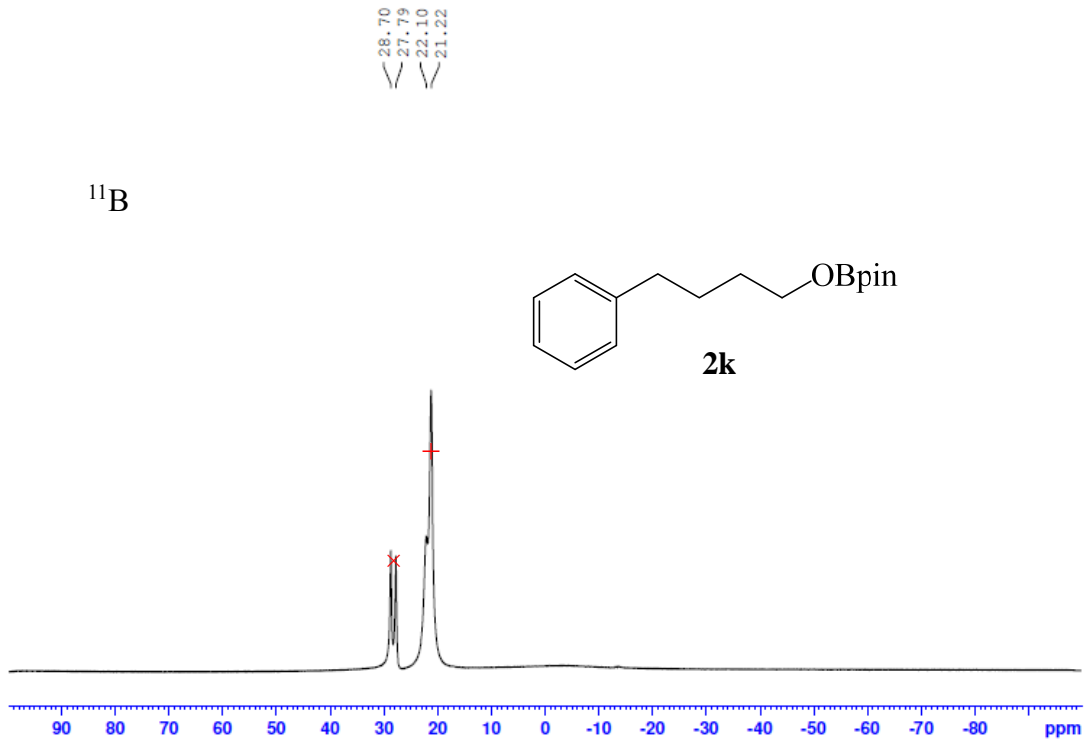


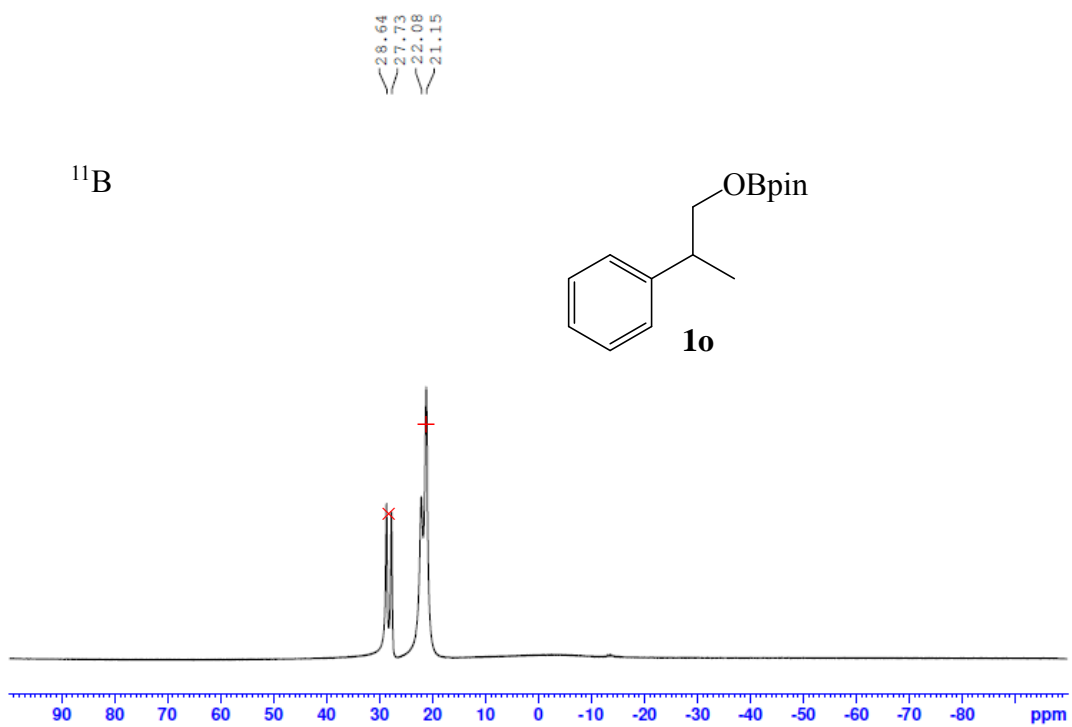
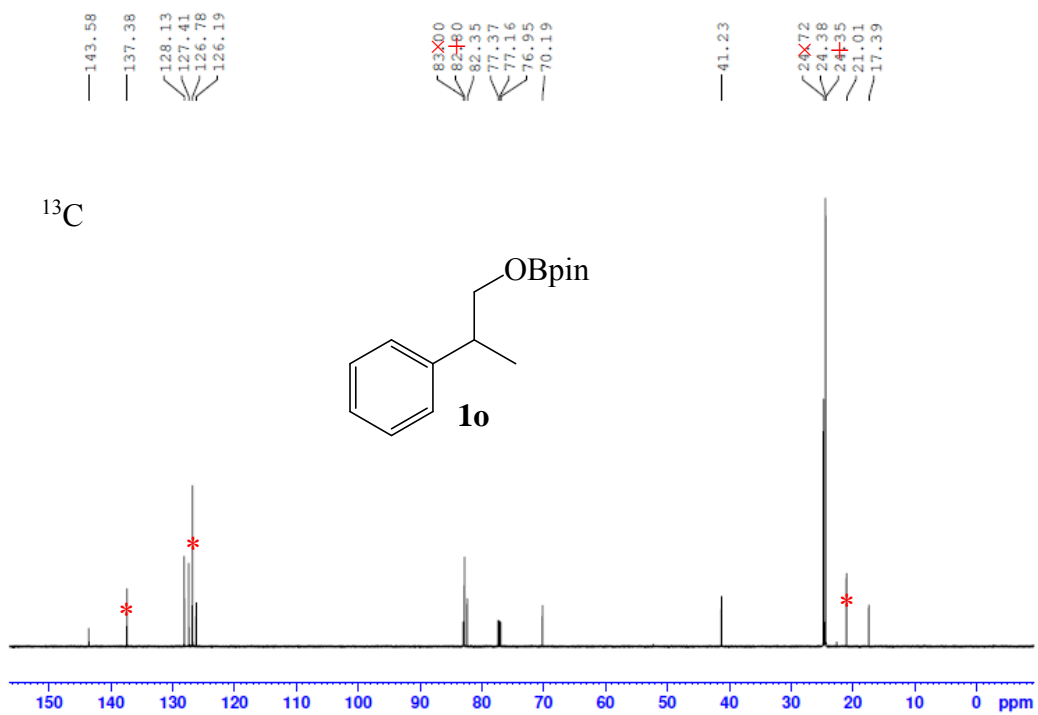


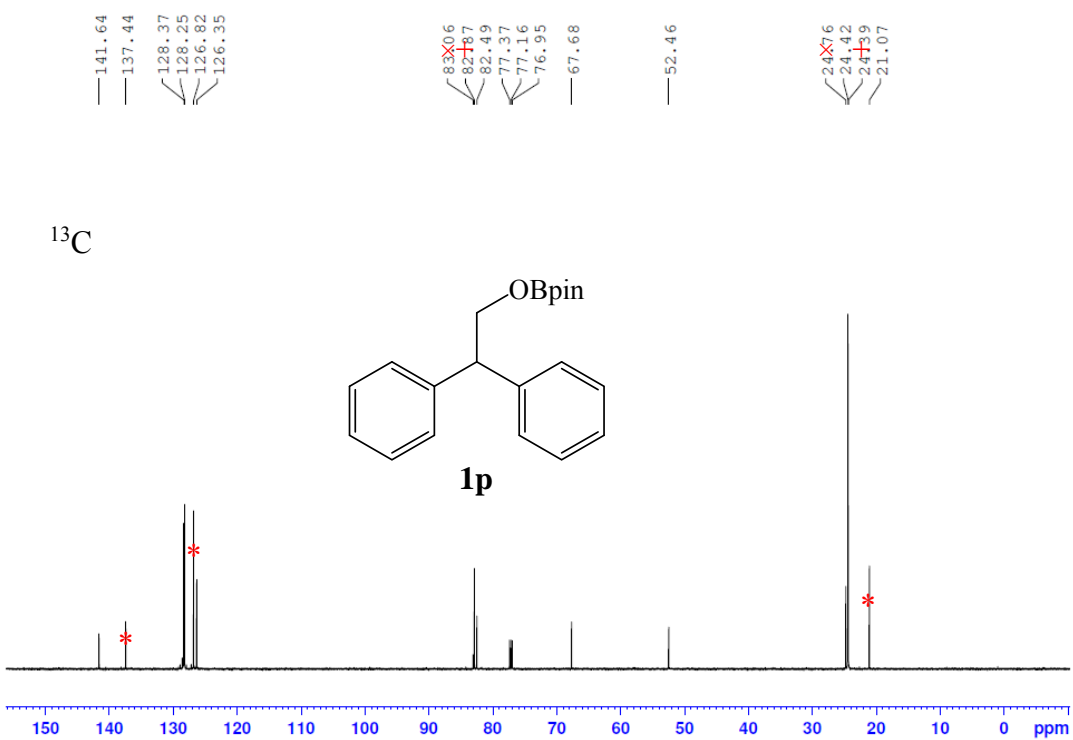
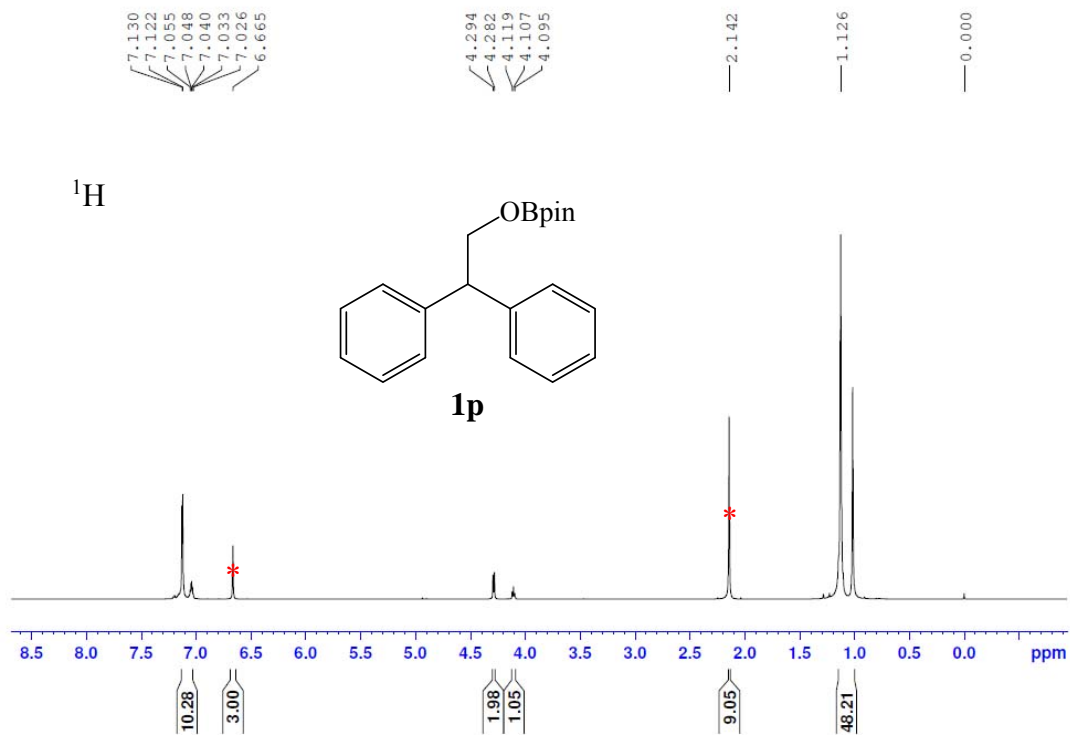




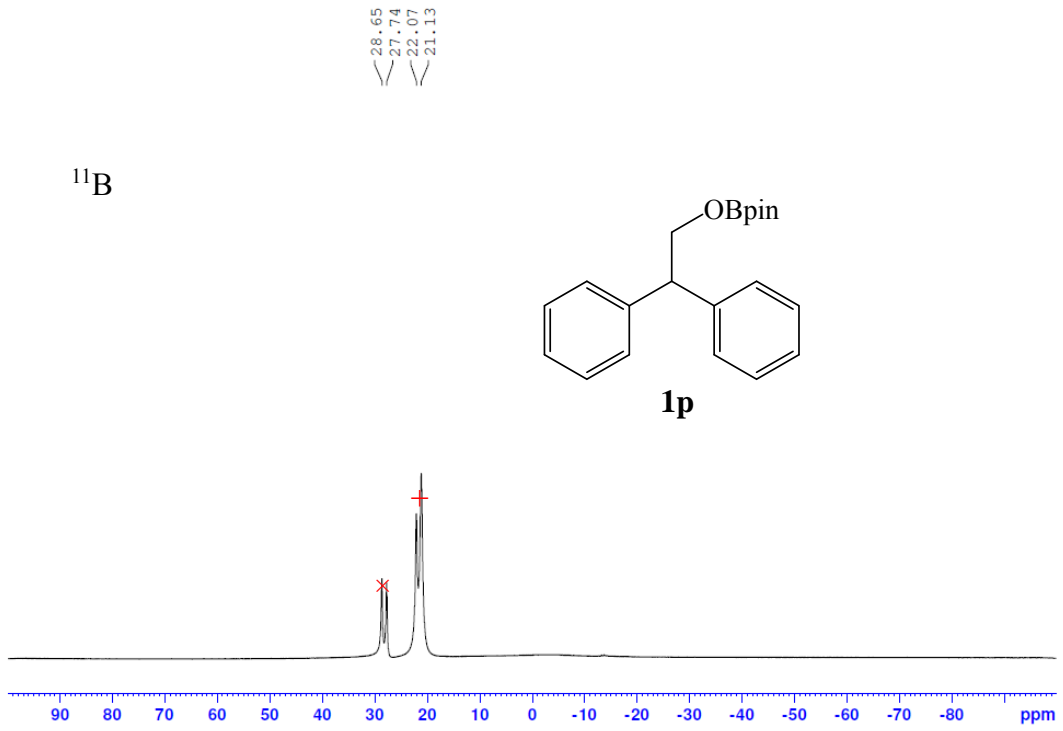




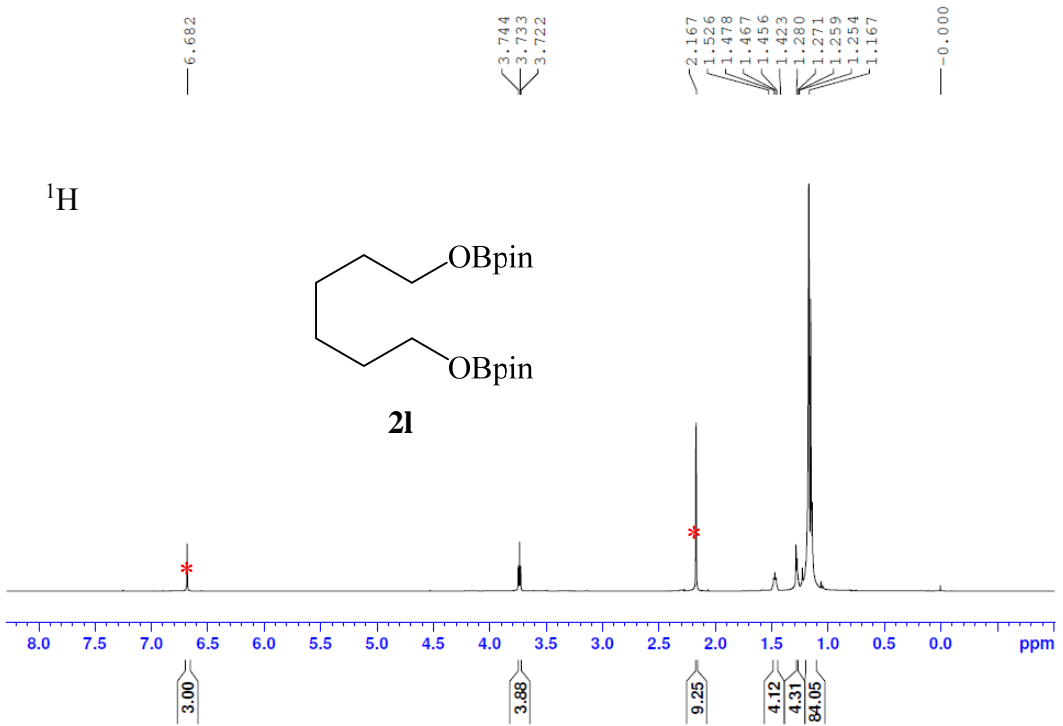


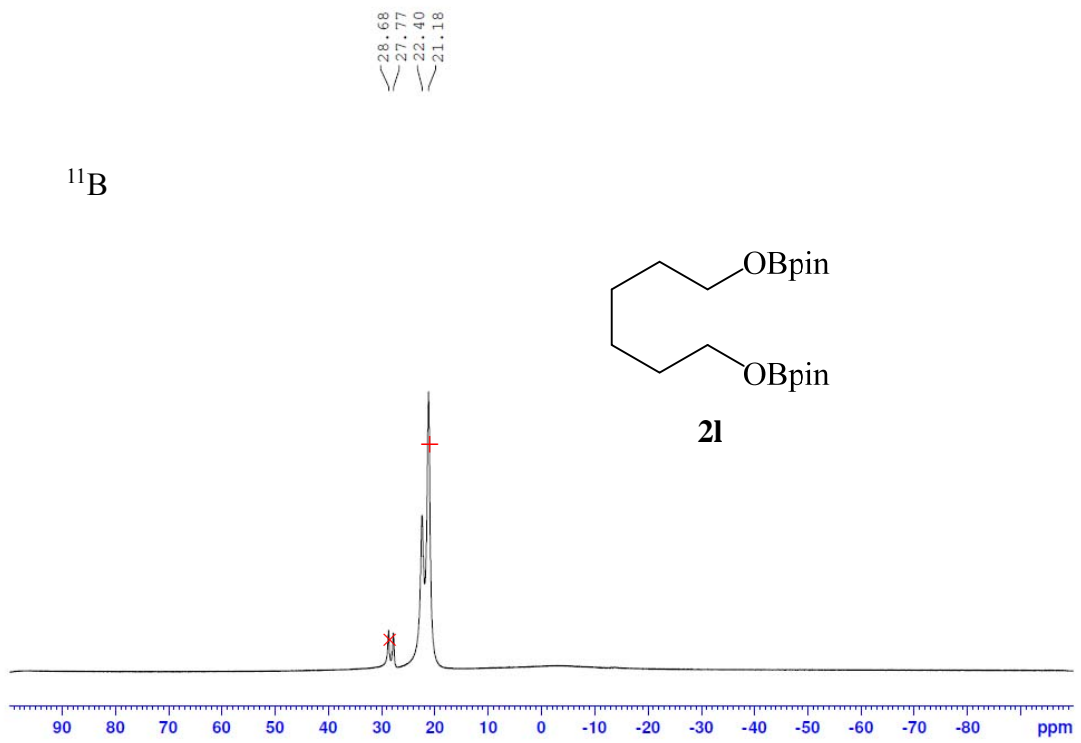
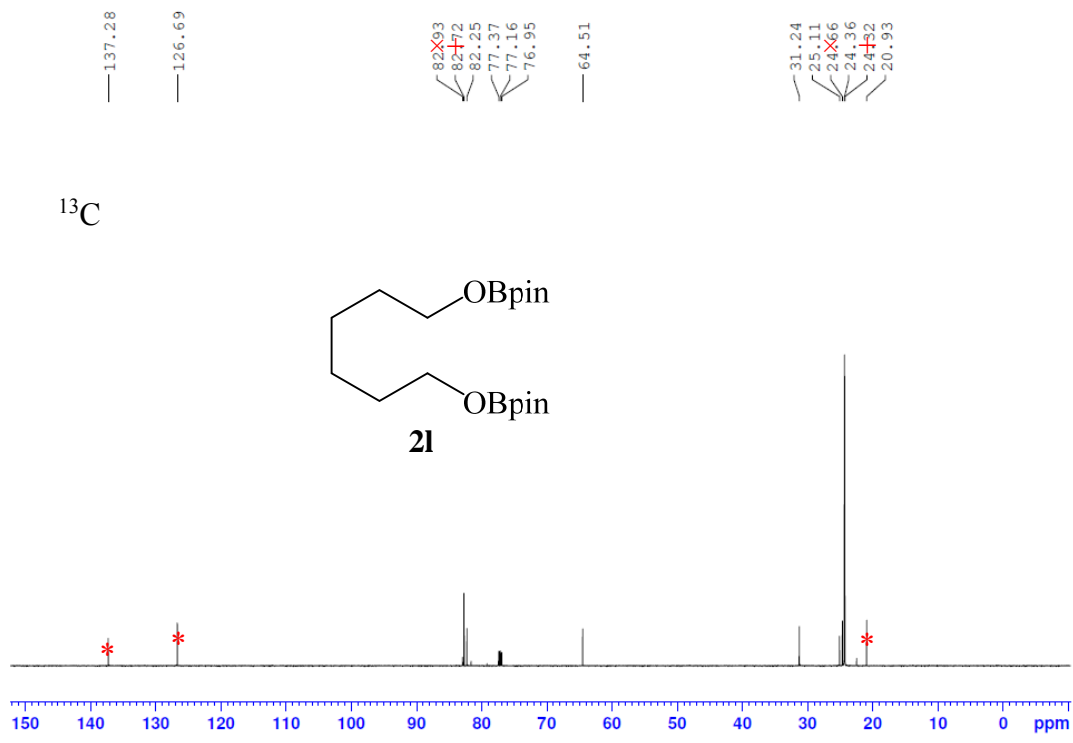


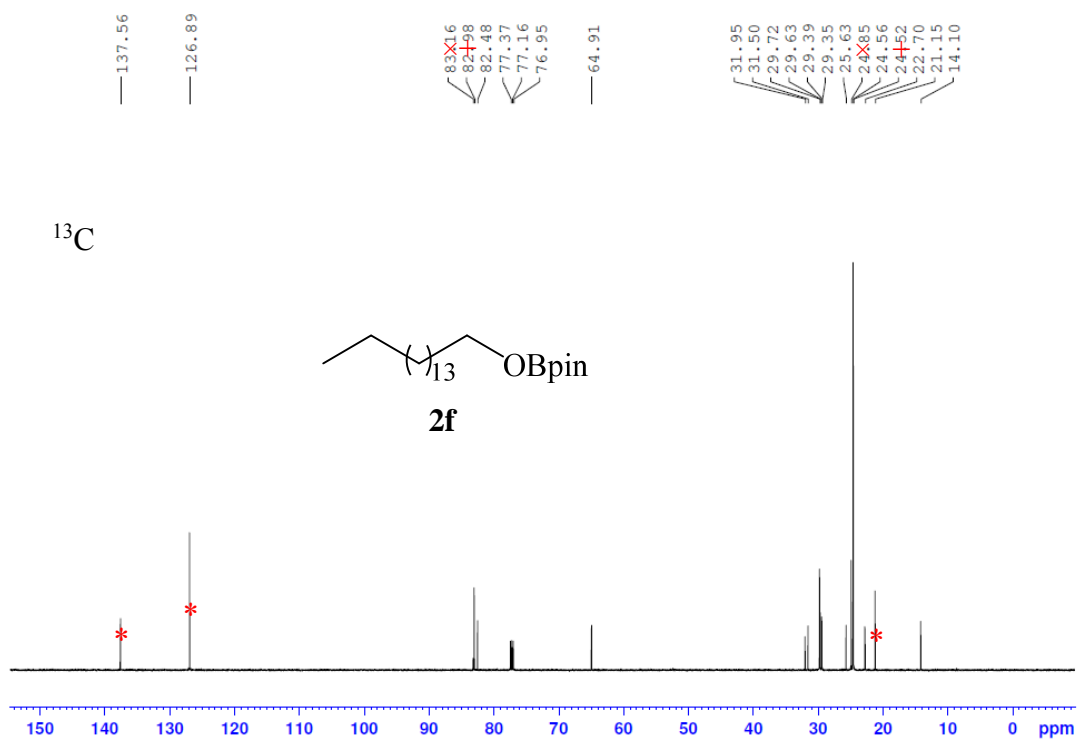
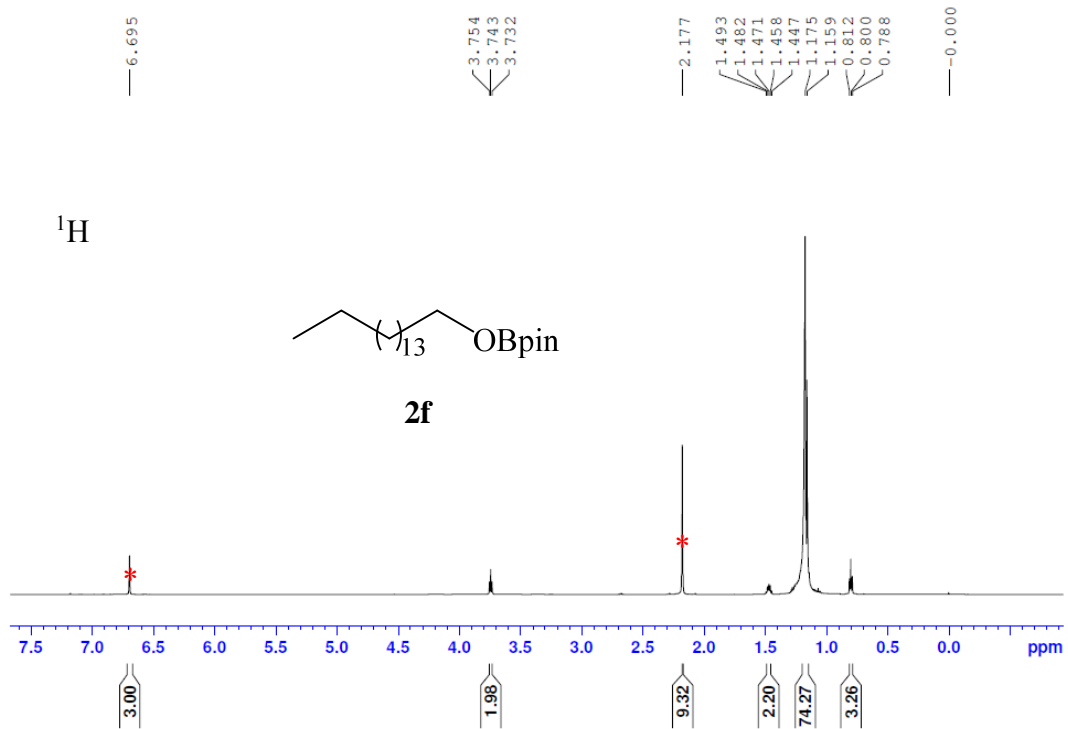
$^{11}\text{B}$



$^1\text{H}$

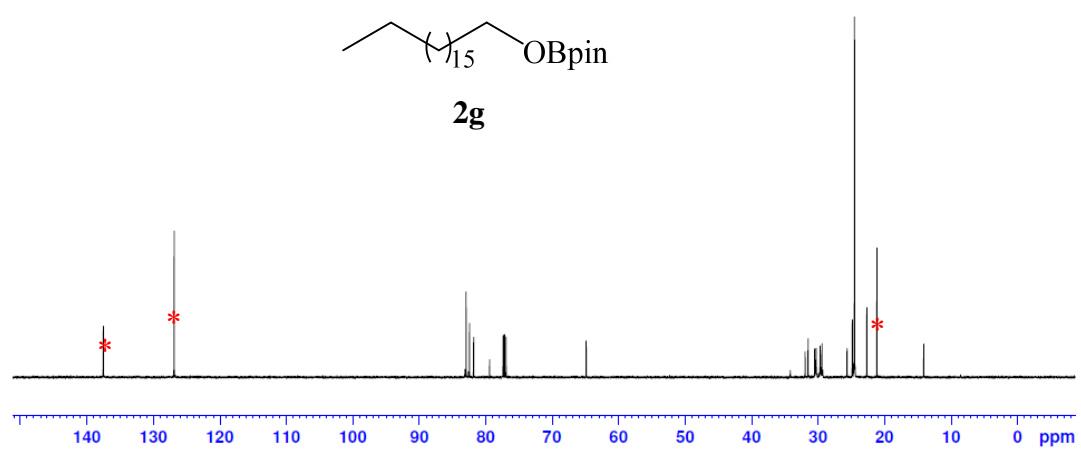






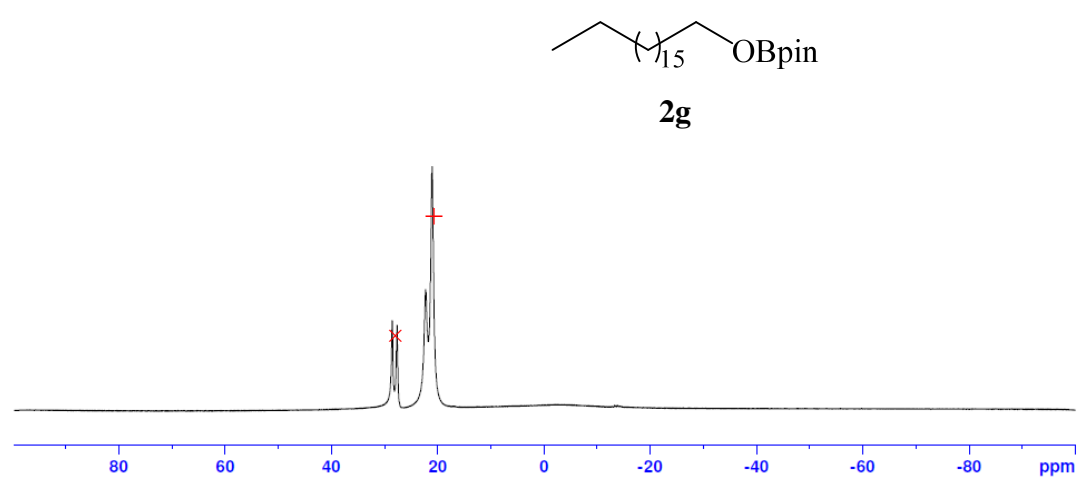


$^{13}\text{C}$   
 — 137.53  
 — 126.87  
 — 82.95  
 — 82.84  
 — 81.82  
 — 77.37  
 — 77.16  
 — 76.95  
 — 64.88  
 — 31.93  
 — 31.49  
 — 30.51  
 — 30.30  
 — 30.28  
 — 29.67  
 — 29.39  
 — 25.64  
 — 24.84  
 — 24.54  
 — 24.50  
 — 24.47  
 — 22.66  
 — 21.13  
 — 14.09

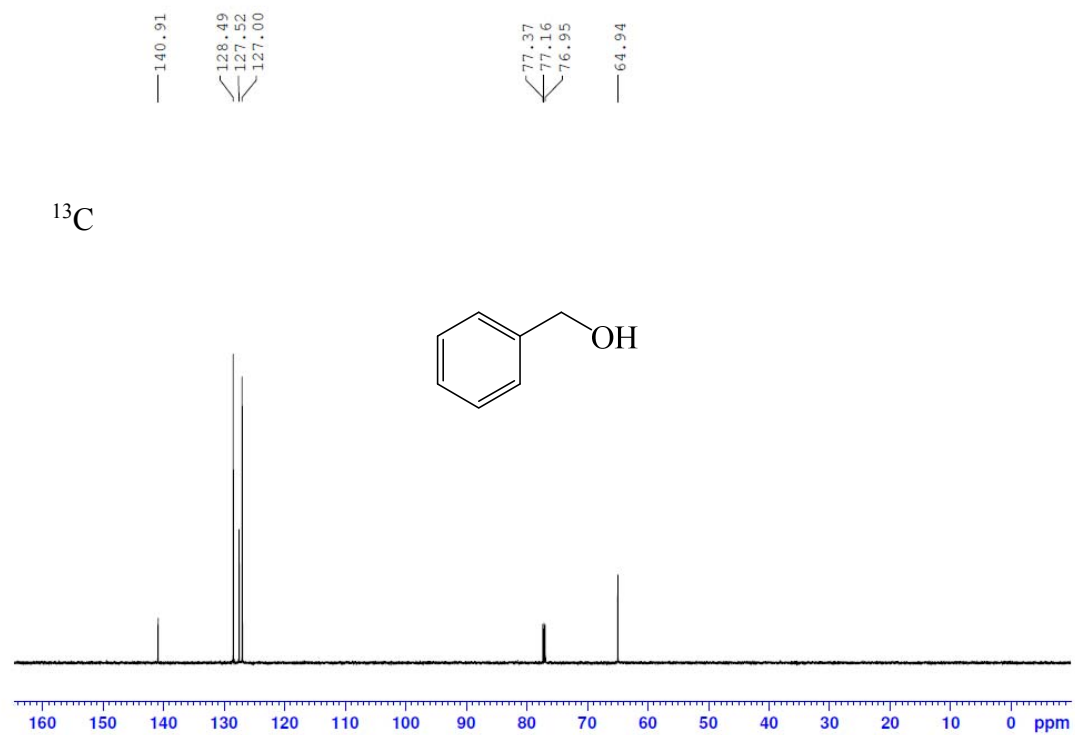
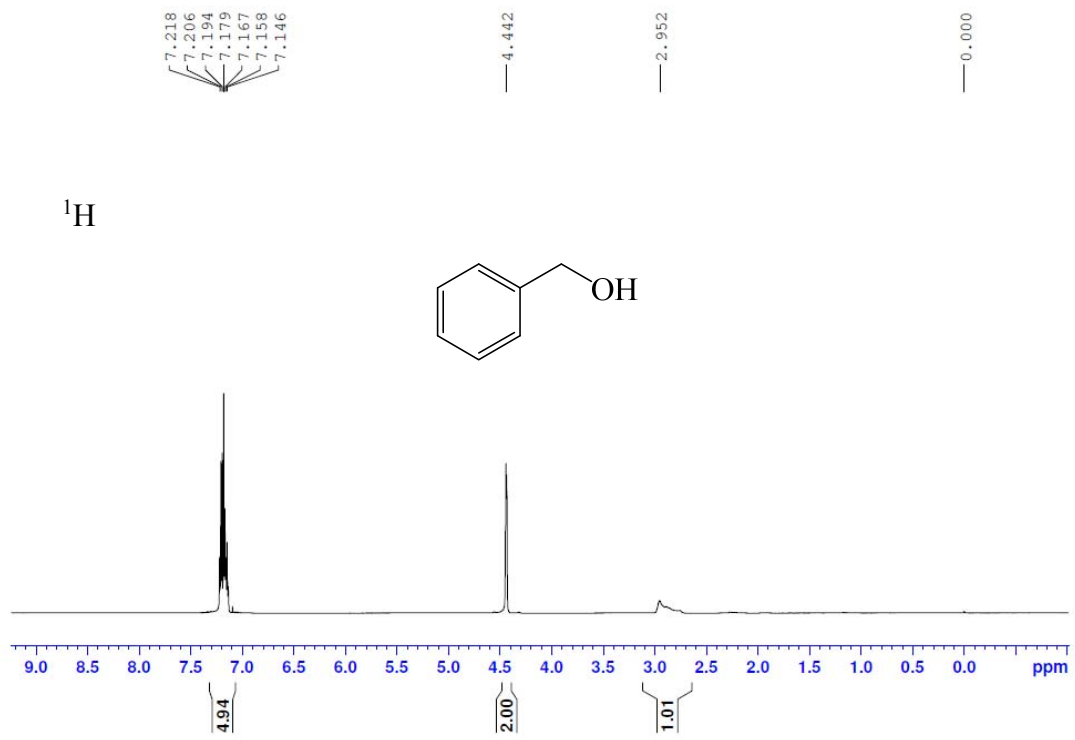


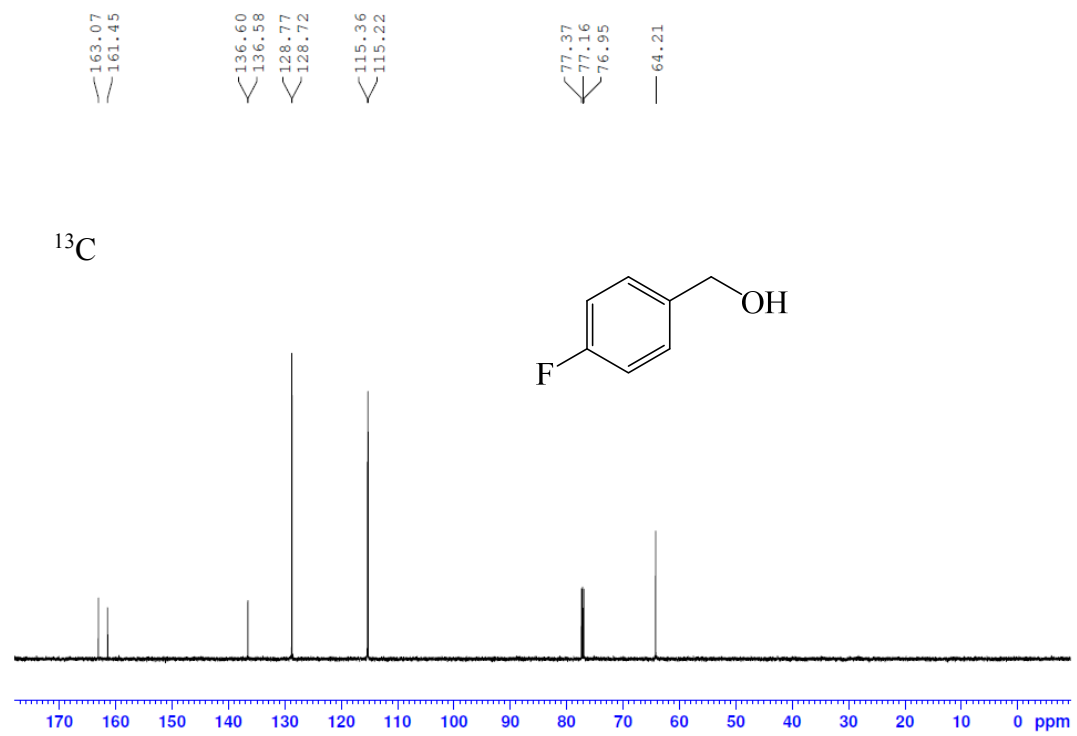
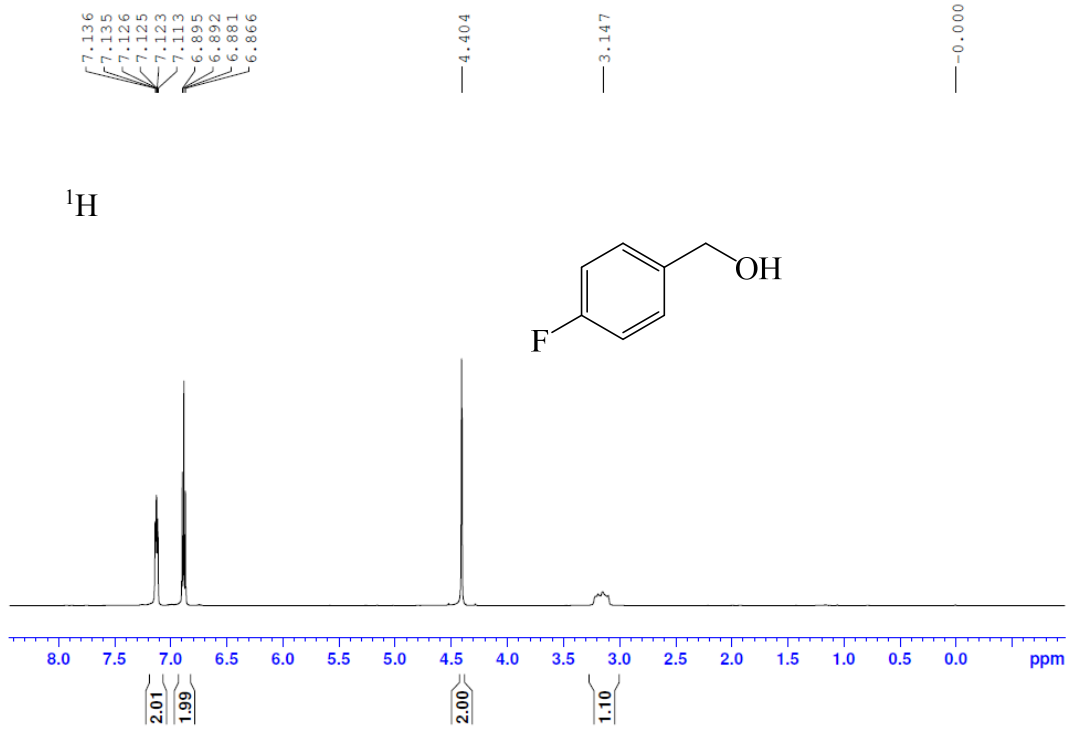
— 28.54  
 — 27.63  
 — 22.24  
 — 21.03

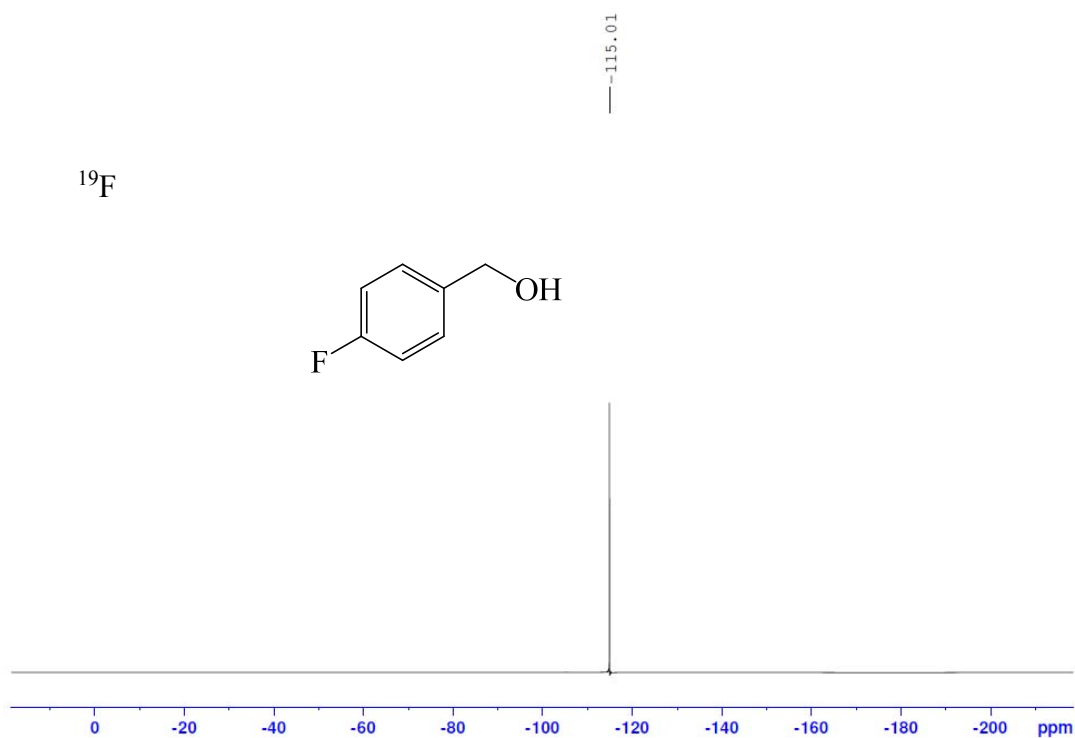
$^{11}\text{B}$











### Experimental Observations

(1)

HBpin (2.0 mmol) was added dropwise to Acetic acid (2.0 mmol) in a 10 ml Schlenk flask equipped with a magnetic stir bar inside the glove box. Hydrogen evolution was observed as the reaction progressed. Then the reaction mixture was stirred at 25°C for 3 hours. The progress of the reaction was monitored by  $^1\text{H}$  NMR,  $^{13}\text{C}$  NMR, and  $^{11}\text{B}$  NMR.

(2)

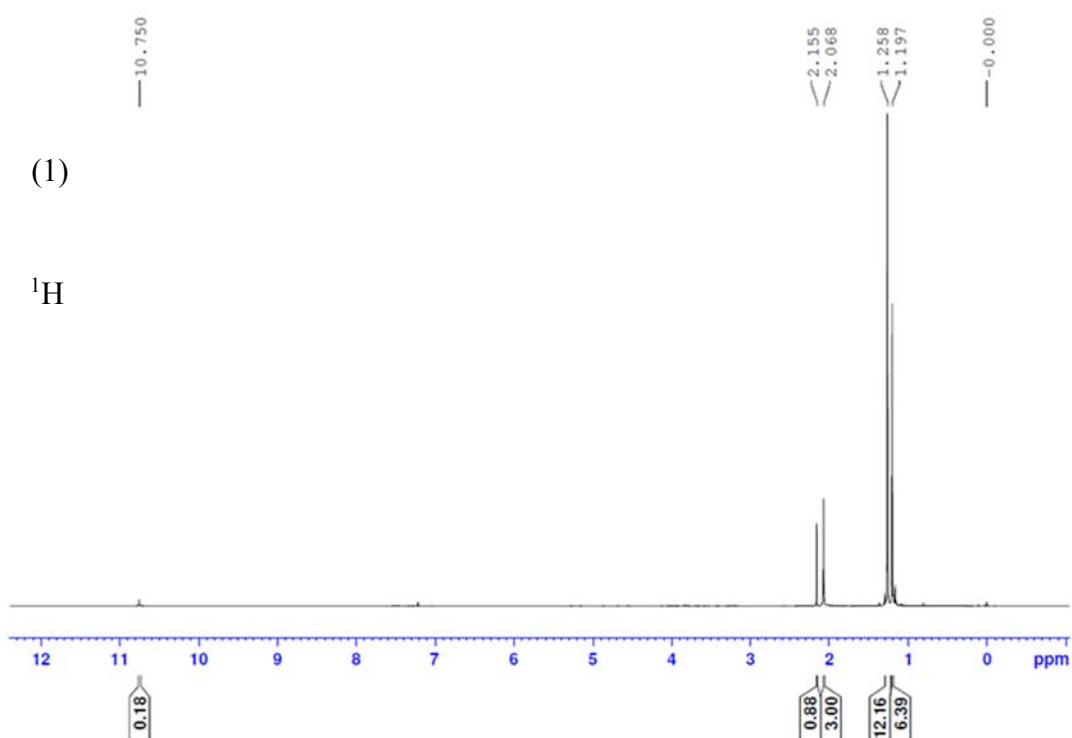
HBpin (4.0 mmol) was added dropwise to Acetic acid (2.0 mmol) in a 10 ml Schlenk flask equipped with a magnetic stir bar inside the glove box. Hydrogen evolution was observed as the reaction progressed. Then the reaction mixture was stirred at 25°C for 6 hours. The progress of the reaction was monitored by  $^1\text{H}$  NMR,  $^{13}\text{C}$  NMR, and  $^{11}\text{B}$  NMR.

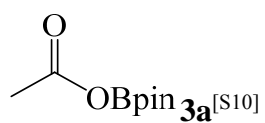
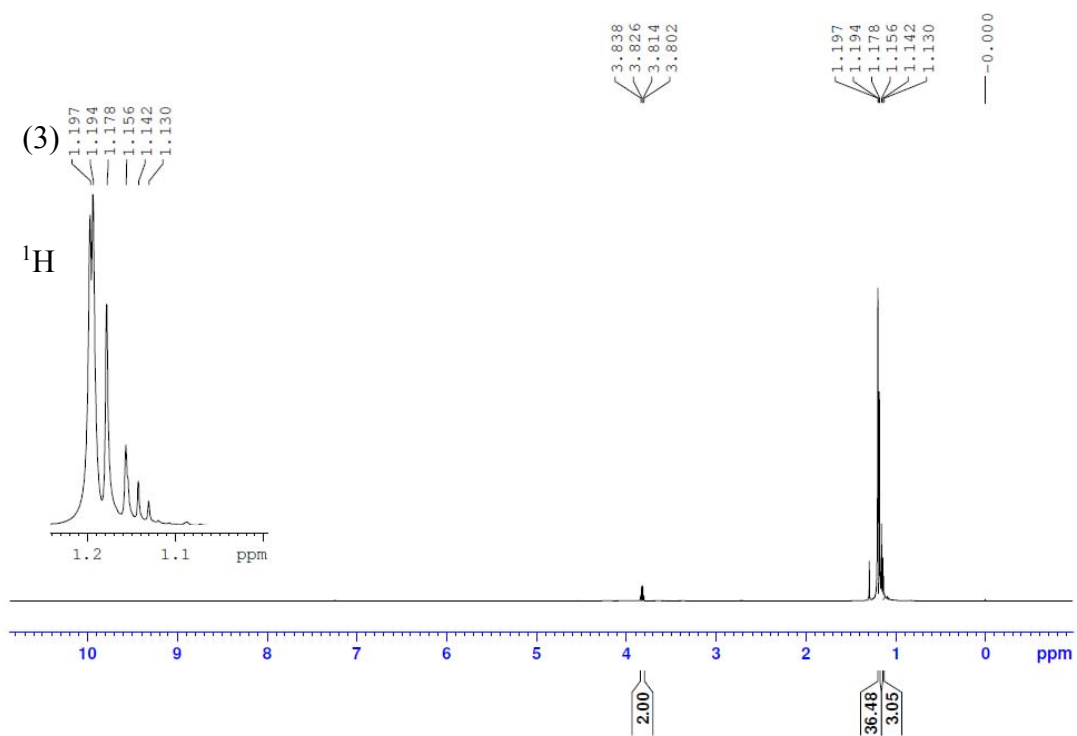
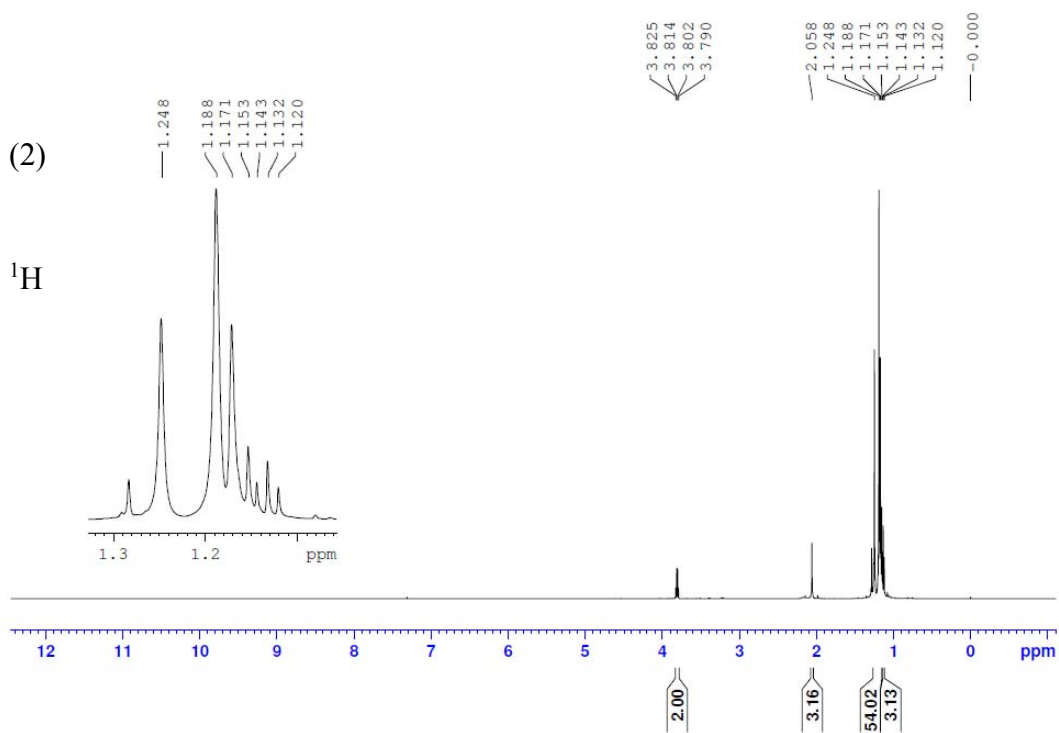
(3)

HBpin (6.0 mmol) was added dropwise to Acetic acid (2.0 mmol) in a 10 ml Schlenk flask equipped with a magnetic stir bar inside the glove box. Hydrogen evolution was

observed as the reaction progressed. Then the reaction mixture was stirred at 25°C for 12 hours. The progress of the reaction was monitored by  $^1\text{H}$  NMR,  $^{13}\text{C}$  NMR, and  $^{11}\text{B}$  NMR.

Acetic acid (0.4 mmol) and HBpin (1.6 mmol) were placed in a 10 ml Schlenk flask equipped with a magnetic stir bar inside the glove box. Hydrogen evolution was observed as the reaction progressed. Then the reaction mixture was stirred at 0°C for 5 hours, 7 hours, 12 hours and 18 hours. The progress of the reaction was monitored by  $^1\text{H}$  NMR,  $^{13}\text{C}$  NMR, and  $^{11}\text{B}$  NMR.

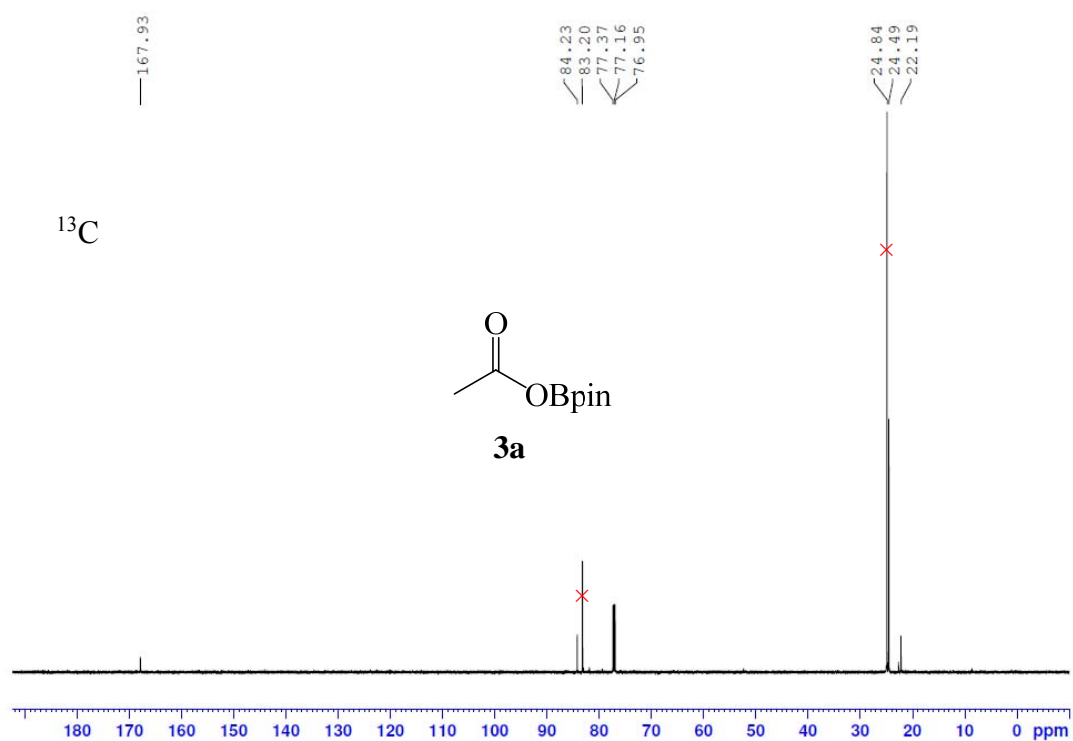
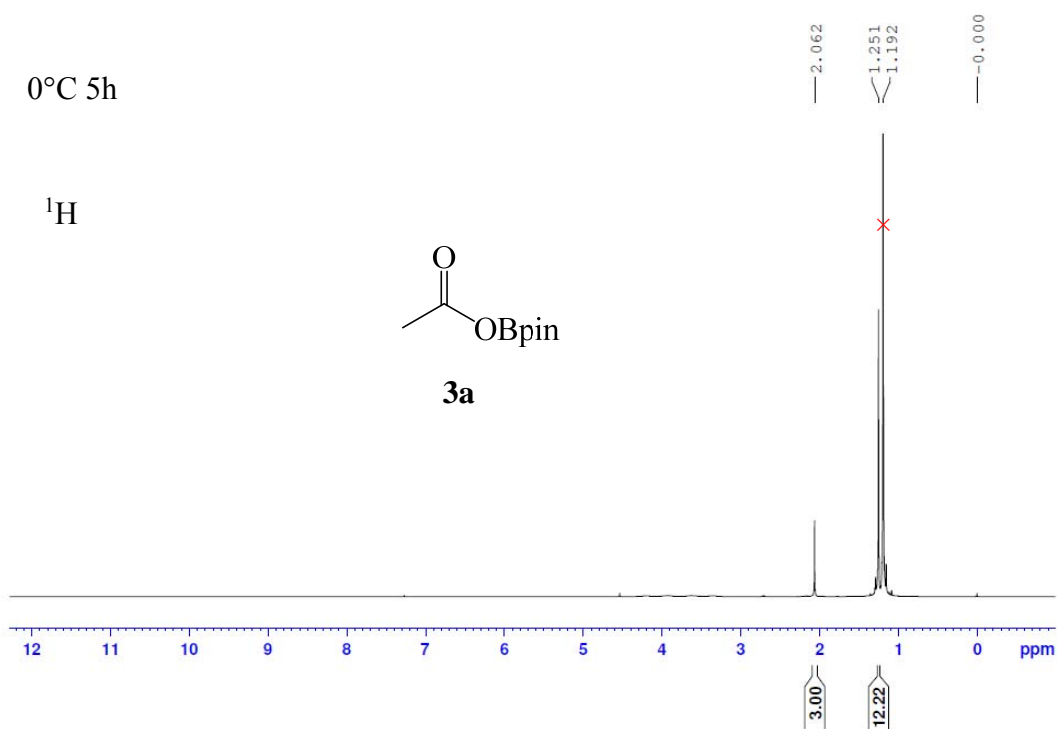




$^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ):  $\delta$  2.06 (s, 3 H), 1.25 (s, 12 H).  $^{13}\text{C}\{^1\text{H}\}$  NMR (151 MHz,

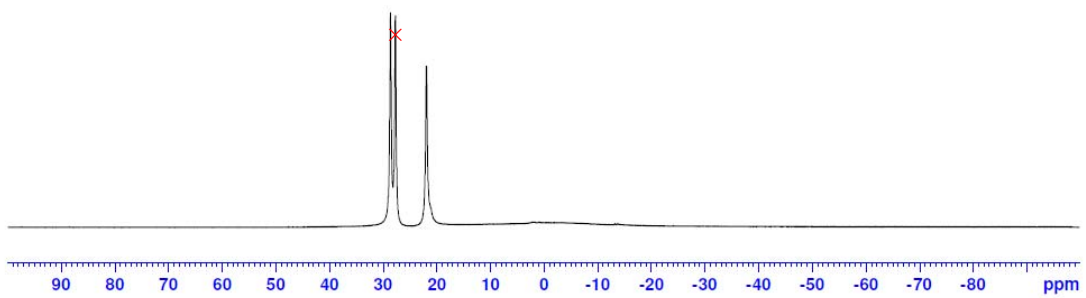
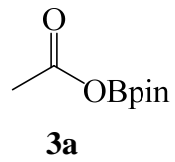
CDCl<sub>3</sub>): δ 167.93, 84.23, 24.49, 22.19. <sup>11</sup>B{<sup>1</sup>H} NMR (193 MHz, CDCl<sub>3</sub>): δ 21.91.

HRMS (ESI): m/z Calcd. For C<sub>8</sub>H<sub>15</sub>BO<sub>4</sub> [M<sup>+</sup>+Na]: 209.0961; Found 209.1049.



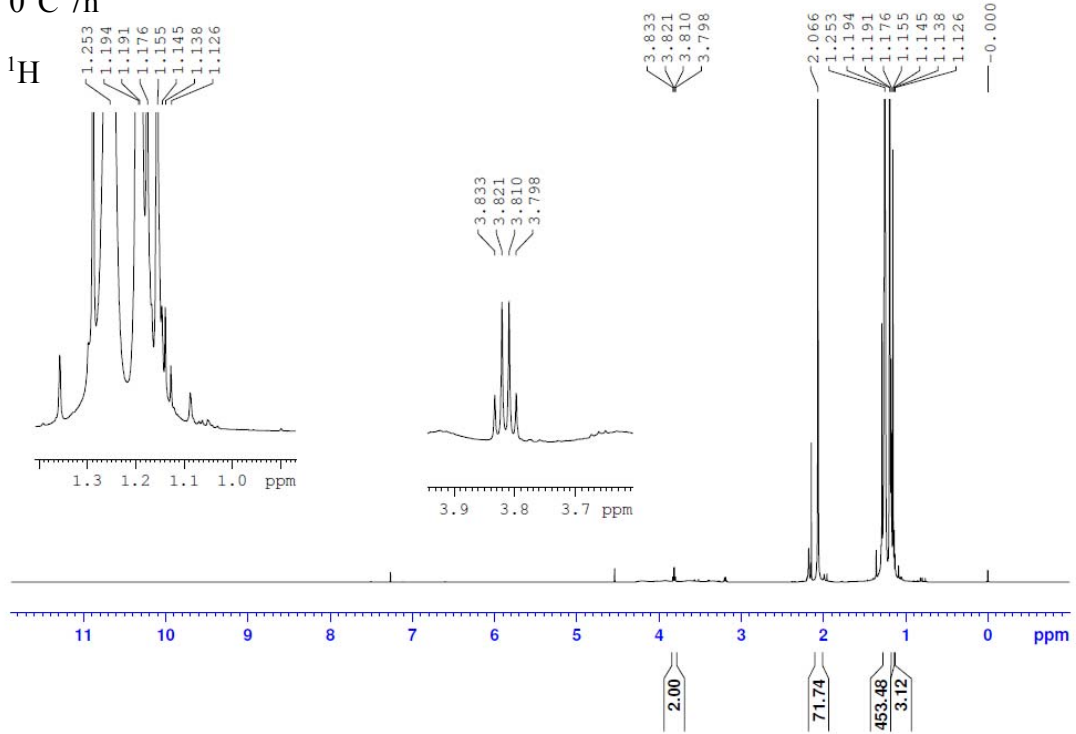
28.59  
27.68  
21.91

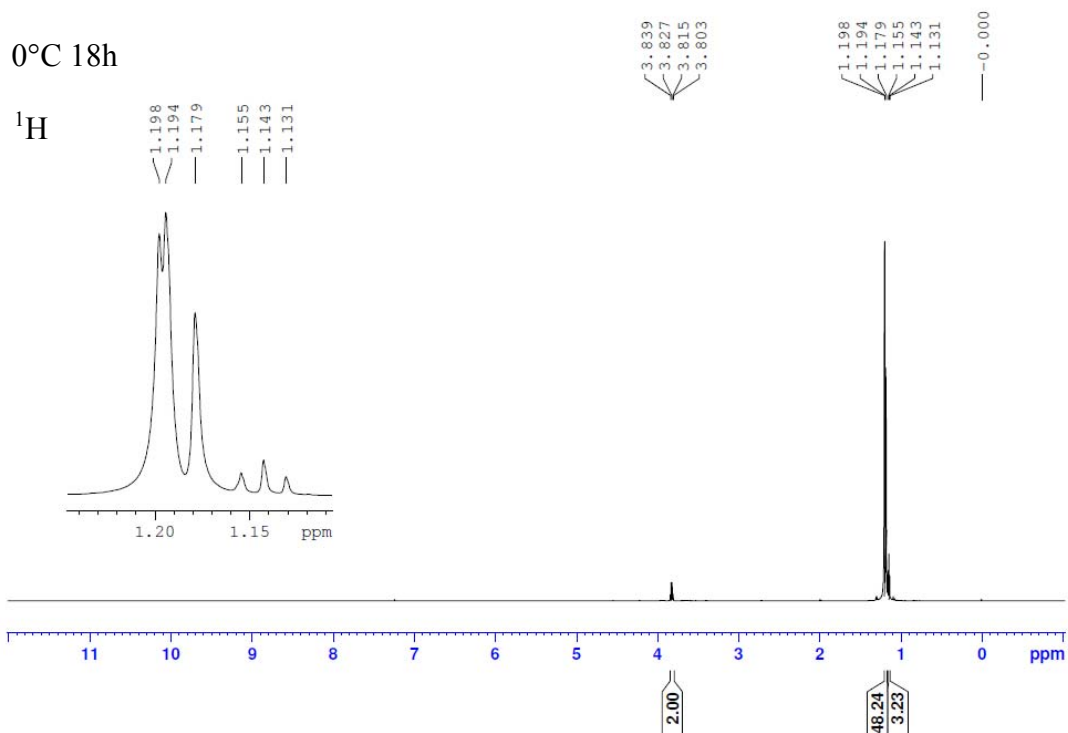
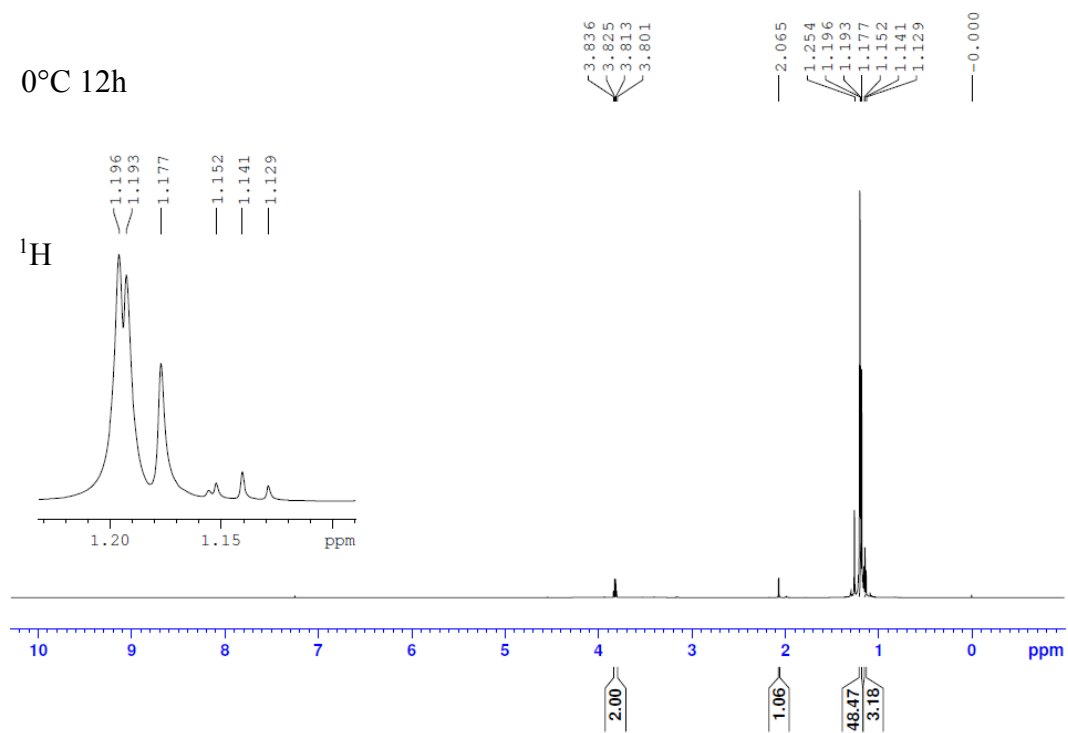
$^{11}\text{B}$



0°C 7h

$^1\text{H}$





### Computational Studies

All structures were initially optimized using density functional theory (DFT) by using the B3LYP<sup>[S11]</sup> functional as implemented in Gaussian 09<sup>[S12]</sup>. Optimizations were carried out in a solvent model (SMD, solvent = acetic acid)<sup>[S13]</sup> by using the 6-



31G\*<sup>[S14]</sup> basis set for C, H, O, B. The critical stationary points were characterized by frequency calculations in order to verify that they have the right number of imaginary frequencies, and the intrinsic reaction coordinates (IRC)<sup>[S15]</sup> were followed to verify the energy profiles connecting the key transition structures to the correct associated local minima. The energies showed in the manuscript have been refined by single-point calculations with the M06<sup>[S16]</sup> functional and def2-TZVP<sup>[S17]</sup> basis set on the previously optimized structures. The values correspond to Free Gibbs energies and are given in kcal/mol. These energies are relative to the acetic acid and HBpin, marked as G = 0.0 kcal/mol in the figure 1.

Table S1: E<sub>el</sub> represents the single point energies at def2-TZVP. Thermal corrections to enthalpy (H<sub>corr</sub>) and Gibbs free energy (G<sub>corr</sub>) were calculated at 298.15K and 1atm. ΔG<sub>sol</sub> are calculated by employing the SMD model at M06-2X/def2-TZVP level. The optimized cartesian coordinates are also given.

HBpin (B3LYP)

E<sub>el</sub> = -412.032005

H<sub>corr</sub> = 0.201984

G<sub>corr</sub> = 0.158359

ΔG<sub>sol</sub> = -0.01219

B	-0.00007100	1.94494200	-0.00035500
H	-0.00025200	3.13486700	-0.00032600
O	-1.08610200	1.20090400	-0.36752200
O	1.08622900	1.20116200	0.36656500
C	-0.78923700	-0.19149000	-0.04498300
C	0.78924100	-0.19149200	0.04502600
C	-1.37972600	-1.07413000	-1.14309000
H	-1.14054600	-2.12925900	-0.96739700
H	-2.46942100	-0.97057400	-1.14828500
H	-1.01063100	-0.79279000	-2.13191900
C	-1.48003700	-0.48320900	1.29355200
H	-2.54921100	-0.27221400	1.19415500
H	-1.36098600	-1.53070600	1.58961600
H	-1.08481000	0.15102900	2.09318000
C	1.48004300	-0.48415600	-1.29329100
H	2.54929600	-0.27361500	-1.19385600

H	1.36053400	-1.53174500	-1.58884600
H	1.08522900	0.14988100	-2.09328300
C	1.37967700	-1.07329600	1.14380000
H	1.14084900	-2.12860900	0.96870900
H	2.46934500	-0.96942500	1.14926300
H	1.01017500	-0.79143500	2.13233400

Acetic acid (B3LYP)

Eel = -229.189

Hcorr = 0.067541

Gcorr = 0.034765

$\Delta G_{sol}$  = -0.010132

C	-1.39723200	-0.11031600	-0.00000900
H	-1.68433800	-0.69114800	0.88271800
H	-1.91783600	0.84742900	-0.00126500
H	-1.68409500	-0.69346100	-0.88128600
C	0.09227200	0.12593400	-0.00003700
O	0.64504000	1.20236100	0.00000800
O	0.77900000	-1.04660300	-0.00000300
H	1.72370600	-0.80259200	0.00007200

H<sub>2</sub> (B3LYP)

Eel = -1.17965

Hcorr = 0.013450

Gcorr = -0.001342

$\Delta G_{sol}$  = -0.000393

H	0.00000000	0.00000000	0.37139400
H	0.00000000	0.00000000	-0.37139400

TS1 (B3LYP)

Eel = -641.148

Hcorr = 0.264868

Gcorr = 0.207945

$\Delta G_{sol}$  = -0.019291

C	2.91058400	1.15273500	0.79625200
H	2.70612500	0.96567400	1.85467600
H	3.84829600	1.69765200	0.67862000
H	2.08395400	1.74849800	0.39559300
C	2.98059600	-0.14187800	0.03481000

O	3.84332400	-0.46885700	-0.73660600
O	1.93107900	-1.00853900	0.32369600
H	1.59612400	-1.73234700	-0.62789000
B	0.40572400	-0.86356300	-0.27206000
H	0.72627400	-1.85323100	-1.17353300
O	0.09500700	0.32589900	-0.91714700
O	-0.55513700	-1.26366000	0.64072700
C	-1.16636200	0.79364100	-0.35163000
C	-1.75617600	-0.51989100	0.30364600
C	-2.00167600	1.38496300	-1.48645400
H	-2.98919300	1.69380900	-1.12444600
H	-1.49852200	2.26879000	-1.89195000
H	-2.13566700	0.67184000	-2.30272300
C	-0.84104000	1.88286100	0.67888500
H	-0.26838300	2.67856700	0.19111900
H	-1.75183900	2.32796500	1.09355000
H	-0.24473000	1.48501500	1.50539000
C	-2.57106300	-1.37342300	-0.67975200
H	-2.76735500	-2.34754100	-0.22135200
H	-3.53165200	-0.90651800	-0.92197100
H	-2.02520400	-1.54392900	-1.61296400
C	-2.55550400	-0.30222500	1.58734200
H	-3.43872200	0.31894600	1.39862600
H	-2.89728300	-1.26810700	1.97272800
H	-1.95118200	0.17329000	2.36286700

Int1 (B3LYP)

Eel=-640.059

Hcorr=0.250238

Gcorr= 0.194125

$\Delta G_{sol}$ =-0.020574

C	-3.01777700	1.24079100	-0.40851600
H	-2.73539200	1.31482100	-1.46493500
H	-4.01254700	1.66335300	-0.26365900
H	-2.27961600	1.80358500	0.16908300
C	-3.03353600	-0.20731900	0.02495800
O	-3.98923600	-0.77623700	0.47965400
O	-1.87174000	-0.91425200	-0.19528100
B	-0.57161600	-0.48402100	-0.11309700
O	-0.15602600	0.66995200	0.50638600
O	0.44295800	-1.23627900	-0.63790400
C	1.26597800	0.81748200	0.20595800
C	1.68815300	-0.66704700	-0.14065500

C	1.95286300	1.42204100	1.42760800
H	3.03458000	1.49577800	1.26848700
H	1.56801400	2.43152700	1.60436000
H	1.77194500	0.82970000	2.32700200
C	1.36626000	1.77379800	-0.98862300
H	0.87438500	2.71746200	-0.73262500
H	2.40827200	1.98979500	-1.24530900
H	0.87114300	1.36132800	-1.87359800
C	2.08754600	-1.48840700	1.09194800
H	2.16469500	-2.54151500	0.80555000
H	3.05376100	-1.16803300	1.49519700
H	1.33675700	-1.40963100	1.88474300
C	2.74731700	-0.80260200	-1.23213300
H	3.69014200	-0.33836400	-0.92121100
H	2.93937400	-1.86287000	-1.42401600
H	2.42410200	-0.34471500	-2.16969700

TS2 (B3LYP)

Eel=-1052.04

Hcorr=0.451469

Gcorr= 0.373436

$\Delta G_{sol}$ =-0.03109

C	-0.12621600	-2.52730200	-0.28171700
H	-0.43632900	-3.21260100	-1.08260200
H	0.79193600	-2.90693400	0.16770700
H	-0.92141100	-2.45218600	0.46003500
C	0.16376800	-1.20202400	-0.93864300
O	1.27461400	-1.00423600	-1.54972200
O	-0.87224400	-0.45130800	-1.33606400
B	-2.06144400	-0.19398300	-0.66916800
O	-2.29355900	-0.46583800	0.64807900
O	-3.08738700	0.40665100	-1.33018100
C	-3.70980600	-0.17106800	0.88660900
C	-4.05395400	0.80765400	-0.30936100
C	-3.83993800	0.43428500	2.28103100
H	-4.87685100	0.72717600	2.48038600
H	-3.54696200	-0.30586200	3.03218600
H	-3.19913200	1.30994900	2.40267000
C	-4.45147400	-1.51085600	0.81387200
H	-4.02058200	-2.19752800	1.54912100
H	-5.51595000	-1.39223600	1.03985200
H	-4.35871300	-1.96925600	-0.17602600
C	-3.76802900	2.28088100	0.00523000

H	-3.84098700	2.86029800	-0.91984600
H	-4.48814500	2.68517400	0.72382400
H	-2.75989500	2.41738700	0.40902700
C	-5.45565300	0.65155100	-0.89208000
H	-6.21729500	0.89721900	-0.14358200
H	-5.57744900	1.33718000	-1.73626200
H	-5.63435100	-0.36334500	-1.25375200
B	1.85736200	-0.33689100	-0.20768600
H	0.75448900	-0.39316600	0.47145900
O	2.90035600	-1.13880300	0.31779400
O	2.26632300	1.00515500	-0.36564100
C	3.94891500	-0.23357500	0.72149500
C	3.70399000	1.00489800	-0.22691400
C	5.29173300	-0.93906500	0.52985500
H	6.12709900	-0.26380100	0.75081600
H	5.35988500	-1.79470000	1.21065500
H	5.40328800	-1.31268600	-0.49054900
C	3.74116400	0.10234800	2.20755100
H	3.70252100	-0.83197800	2.77735300
H	4.55537700	0.71610500	2.60928200
H	2.79709300	0.63431400	2.36198000
C	4.31864300	0.81516600	-1.62351900
H	3.92790700	1.59284700	-2.28752900
H	5.41170200	0.89432700	-1.60470900
H	4.04495200	-0.15650600	-2.04498100
C	4.12650800	2.35585100	0.35041700
H	5.20526700	2.38215700	0.54628100
H	3.89357100	3.15111000	-0.36581900
H	3.59664000	2.57647700	1.28023600

Int2(B3LYP)

Eel = -1052.14

Hcorr = 0.457566

Gcorr = 0.379395

$\Delta G_{sol}$  = -0.028009

C	-0.35728100	-3.83179100	-0.02626200
H	-0.16839600	-4.17430700	-1.04792700
H	0.23463300	-4.43704500	0.66693000
H	-1.41906000	-3.96068200	0.20471700
C	0.02760100	-2.36971500	0.09425000
O	1.40862800	-2.25966500	-0.18901000
O	-0.69025300	-1.60138400	-0.86152700
B	-1.65432700	-0.72428100	-0.47329100

O	-2.11508600	-0.58426500	0.81943100
O	-2.28773700	0.09486000	-1.37765300
C	-3.29947100	0.25702400	0.75453500
C	-3.08229300	1.03361200	-0.60520200
C	-3.34028800	1.13213400	2.00553800
H	-4.18187300	1.83324500	1.96493500
H	-3.46822700	0.50150100	2.89137500
H	-2.41610000	1.70107500	2.12892000
C	-4.51144200	-0.68412500	0.72755500
H	-4.47474900	-1.33510100	1.60670700
H	-5.45564800	-0.12984000	0.74924200
H	-4.50299200	-1.31886900	-0.16436000
C	-2.23677600	2.30429100	-0.44106800
H	-1.95761900	2.67373200	-1.43286000
H	-2.78737500	3.09506400	0.07956900
H	-1.31753300	2.09415600	0.11519600
C	-4.35710200	1.34488100	-1.38631400
H	-5.01495700	2.00920600	-0.81424400
H	-4.09833500	1.84869400	-2.32318000
H	-4.90837200	0.43547200	-1.63520100
B	2.04972600	-1.06224400	-0.08805100
H	-0.17480700	-1.97920600	1.09716200
O	1.49064000	0.10061400	0.40010100
O	3.36720200	-0.93080800	-0.45539300
C	2.44699900	1.16560100	0.13095700
C	3.80743600	0.36916800	0.01876400
C	2.37755600	2.17752500	1.27230900
H	3.13281800	2.96155500	1.14484700
H	1.39293700	2.65664300	1.28101000
H	2.52879100	1.70129000	2.24368300
C	2.02245600	1.82165600	-1.18937900
H	0.98845700	2.16807100	-1.09997100
H	2.65449300	2.68165000	-1.43507500
H	2.06622400	1.10910300	-2.01878900
C	4.48804500	0.14370700	1.37606100
H	5.30047700	-0.57835800	1.24938400
H	4.90928000	1.07147200	1.77760300
H	3.78528400	-0.26407700	2.10984500
C	4.80980800	0.93552200	-0.98476600
H	5.12673100	1.94406000	-0.69505400
H	5.69843200	0.29678700	-1.01416900
H	4.39185900	0.97556800	-1.99303700

TS3 (B3LYP)

Eel=-1464.09  
Hcorr=0.657009  
Gcorr= 0.555  
 $\Delta G_{sol}=-0.042564$

C	0.23838600	1.07804700	3.16146900
H	0.00020400	1.99890700	3.69509000
H	0.51964500	0.25923600	3.83636200
H	1.12874300	1.21816700	2.48594600
C	-0.81815500	0.64144900	2.27110100
O	-1.88367600	1.33957000	2.10344600
O	0.16909400	0.20336500	-0.32226100
B	0.63908500	-1.04936700	-0.27142900
O	0.17044600	-1.95228700	0.69789800
O	1.55816700	-1.65670900	-1.11104000
C	1.02690100	-3.11879300	0.66252000
C	1.58093200	-3.07129600	-0.81568800
C	0.19562300	-4.35388700	1.00589700
H	0.79784800	-5.26662700	0.92864600
H	-0.16964300	-4.27867200	2.03588800
H	-0.67126400	-4.45155900	0.34828600
C	2.12012400	-2.90383800	1.72042200
H	1.64609600	-2.77343500	2.69949700
H	2.80093000	-3.75923300	1.78463100
H	2.70301100	-2.00307500	1.50406200
C	0.65245100	-3.75526100	-1.83012200
H	0.98643500	-3.49970200	-2.84042500
H	0.66482400	-4.84575000	-1.72688000
H	-0.37972600	-3.40724100	-1.71839800
C	3.01057100	-3.58278200	-0.98863200
H	3.08652700	-4.64268800	-0.71836600
H	3.31202500	-3.47817700	-2.03591900
H	3.71646100	-3.01449500	-0.37869400
B	-2.79595000	0.98092500	1.05805600
H	-0.73705000	-0.31593500	1.75425500
O	-3.10437000	-0.30486100	0.79532800
O	-3.37954500	1.93653800	0.31463300
C	-4.13507000	-0.25457600	-0.25783900
C	-3.96276900	1.21463500	-0.83474000
C	-5.47360000	-0.48981700	0.44770300
H	-6.29889200	-0.52523200	-0.27034800
H	-5.43612200	-1.44740200	0.97581400
H	-5.68691400	0.29494400	1.18059800
C	-3.84071300	-1.37380400	-1.25047600

H	-3.94948300	-2.34264800	-0.75312000
H	-4.54600100	-1.34030400	-2.08823400
H	-2.82446400	-1.30278400	-1.64255100
C	-5.26132800	1.91529200	-1.21807300
H	-5.03844000	2.93093800	-1.55806400
H	-5.75605300	1.38496300	-2.03942300
H	-5.95494300	1.98251600	-0.37689200
C	-2.93120500	1.31503800	-1.96255200
H	-3.29986800	0.83576100	-2.87552500
H	-2.74753900	2.37130100	-2.17955300
H	-1.97400700	0.86412700	-1.68264900
B	0.92699500	1.48685900	-0.04350500
H	0.10091800	2.19577400	0.55000300
O	2.08727600	1.14636500	0.83056000
O	1.48008000	2.16105800	-1.19011500
C	3.19880400	1.95244900	0.41492500
C	2.90381400	2.17934800	-1.12383300
C	4.49184300	1.19104900	0.71891800
H	5.37082100	1.74029300	0.36016200
H	4.59953300	1.05695900	1.80197900
H	4.48714700	0.20220600	0.25354800
C	3.17382200	3.26427000	1.22234200
H	3.21199500	3.02776400	2.29251100
H	4.02940800	3.90846100	0.99057700
H	2.25419800	3.82429100	1.02823600
C	3.45744000	1.05456700	-2.01859200
H	3.05484300	1.19125600	-3.02811600
H	4.55275900	1.07830900	-2.08260400
H	3.14003500	0.07024100	-1.66806100
C	3.39469700	3.52831400	-1.66657000
H	4.48371500	3.62944200	-1.57575900
H	3.13737900	3.60450000	-2.72873100
H	2.91907600	4.36577100	-1.15005500

nipBOBpin (B3LYP)

Eel = -898.233

Hcorr = 0.392264

Gcorr = 0.322277

$\Delta G_{sol}$  = -0.024935

O	-0.00000100	-1.24015100	0.00003400
B	1.24138600	-0.68037300	-0.00463600
O	2.34267200	-1.37220100	0.43650600
O	1.52909100	0.57874600	-0.47576100



C	3.44770200	-0.42852500	0.47092200
C	2.97755800	0.68054400	-0.55332000
C	4.72745500	-1.16812800	0.08666600
H	5.57943100	-0.47972100	0.04475600
H	4.94728300	-1.93379200	0.83752400
H	4.63103900	-1.66472800	-0.88137500
C	3.54618800	0.08183400	1.91523900
H	3.67067700	-0.77501900	2.58453400
H	4.40053300	0.75320400	2.05177700
H	2.63630000	0.61285200	2.21276500
C	3.36535700	0.36983100	-2.00550900
H	2.83704500	1.06164900	-2.66886000
H	4.44140600	0.48713200	-2.17142200
H	3.08075800	-0.64963700	-2.28516800
C	3.38082800	2.10971500	-0.19656800
H	4.47158300	2.21747200	-0.18625600
H	2.97972000	2.80086800	-0.94487600
H	2.98995000	2.40767600	0.77880800
B	-1.24137600	-0.68036400	0.00465300
O	-1.52905600	0.57883300	0.47558900
O	-2.34269000	-1.37225500	-0.43632700
C	-2.97751400	0.68066400	0.55319400
C	-3.44773200	-0.42861300	-0.47081200
C	-3.38078600	2.10976300	0.19618700
H	-4.47153800	2.21754500	0.18596600
H	-2.97959100	2.80106000	0.94431500
H	-2.98999600	2.40751700	-0.77928600
C	-3.36526200	0.37023700	2.00546100
H	-2.83690100	1.06216100	2.66866300
H	-4.44130000	0.48761000	2.17139300
H	-3.08070100	-0.64918900	2.28531300
C	-3.54636300	0.08146800	-1.91522000
H	-3.67101100	-0.77552300	-2.58431100
H	-4.40066900	0.75287900	-2.05180200
H	-2.63646400	0.61233600	-2.21297800
C	-4.72744100	-1.16815100	-0.08629000
H	-5.57940700	-0.47973500	-0.04437900
H	-4.94735900	-1.93392800	-0.83700800
H	-4.63091100	-1.66461400	0.88180900

CH<sub>3</sub>CH<sub>2</sub>OBpin(B3LYP)

Eel = -565.996

Hcorr = 0.268987

Gcorr = 0.214946

$\Delta G_{sol} = -0.016724$

C	3.71666600	-0.14586300	0.86164500
H	2.97161500	-0.49432700	1.58473400
H	4.58048600	-0.81968300	0.90752900
H	4.04416200	0.85729800	1.15418400
C	3.13085700	-0.12903100	-0.54409500
O	2.06036900	0.81544900	-0.64815700
B	0.78700700	0.44663000	-0.36765600
O	0.40854400	-0.81138900	0.06230600
O	-0.26665200	1.32275300	-0.49661900
C	-1.04427800	-0.85215700	0.00800600
C	-1.42375900	0.67960400	0.09854300
C	-1.54744800	-1.71840200	1.16068100
H	-2.64280200	-1.71981300	1.19958900
H	-1.21340400	-2.75130100	1.01772800
H	-1.16440800	-1.37148100	2.12302500
C	-1.42143500	-1.48975700	-1.33642500
H	-0.94714200	-2.47350700	-1.40851400
H	-2.50423200	-1.62160100	-1.43312400
H	-1.07032600	-0.88177100	-2.17642200
C	-1.52704000	1.19208600	1.54213100
H	-1.58175200	2.28488200	1.52535400
H	-2.42029000	0.80899600	2.04692900
H	-0.64796000	0.90785700	2.12949500
C	-2.66436900	1.08971700	-0.69264800
H	-3.55780300	0.58029000	-0.31341400
H	-2.82180900	2.16839300	-0.59213400
H	-2.55741700	0.86443100	-1.75609100
H	3.88616400	0.18484800	-1.27255800
H	2.77862900	-1.12833800	-0.82530600

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