

# Physicochemical characterization of *B*-hydroxyphenyl phosphine borane derivatives and their evaluation as nuclear estrogen receptor ligands

Yu Miyajima, Tomomi Noguchi-Yachide, Kotaro Ochiai and Shinya Fujii

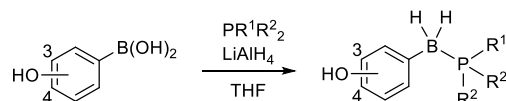
## Supplementary Information

### Table of Contents

1. Synthesis and characterization of compounds	S2
1.1 General procedure of phosphine borane derivatives <b>7-22</b>	S2
1.2 Characterization of phosphine borane derivatives <b>7-22</b>	S2
1.3 Preparation of alkane analogue <b>26</b>	S9
1.4 Preparation of silane analogues <b>30</b> and <b>31</b>	S9
2. <sup>1</sup> H, <sup>13</sup> C, <sup>11</sup> B and <sup>31</sup> P NMR Spectra	S12
3. Calculation of Log <i>P</i> ( <b>Table S1</b> )	S47
4. Calculation of p <i>K</i> <sub>a</sub> ( <b>Table S2</b> )	S48
References for Supplementary Materials	S49

## 1. Synthesis and characterization of compounds

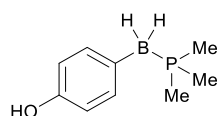
### 1.1 General procedure of phosphine borane derivatives 7-22.



A dry round-bottomed flask, equipped with a magnetic stirring bar, sealed with a septum and protected with an Ar balloon, was charged with 4- or 3-hydroxyphenylboronic acid (207 mg, 2.0 mmol) in 10 mL of THF. LiAlH<sub>4</sub> (171 mg, 6.0 mmol) was added at 0 °C. The mixture was stirred and then phosphine (2.0 mmol, 1.0 eq.) was added. Stirring was continued at room temperature with monitoring by TLC. After the change of the spots on TLC stopped, the mixture was quenched by the addition of sodium sulfate hydrate and filtered through Celite. The obtained solution was evaporated, and the residue was purified by silica gel column chromatography (eluent: hexane/ethyl acetate) to give the desired phosphine borane derivatives.

### 1.2 Characterization of phosphine borane derivatives 7-22.

#### **B-(4-Hydroxyphenyl) trimethylphosphine borane (7)**



Yield : 35.7 mg, 9.8%, white solid

R<sub>f</sub> = 0.46 (hexane/ethyl acetate = 1/1)

<sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>): δ 8.64 (s, 1H), 6.97 (dd, *J* = 8.0, 2.6 Hz, 2H), 6.54 (d, *J* = 7.5 Hz, 2H), 2.04-1.36 (br, 2H), 1.20 (d, *J* = 10.6 Hz, 9H).

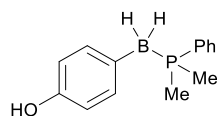
<sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>): δ 154.9 (d, *J*<sub>CP</sub> = 4.3 Hz), 136.5 (d, *J*<sub>CP</sub> = 6.9 Hz), 114.7 (d, *J*<sub>CP</sub> = 3.6 Hz), 9.9 (d, *J*<sub>CP</sub> = 36.8 Hz)

<sup>11</sup>B NMR (128 MHz, DMSO-*d*<sub>6</sub>): δ -23.8 (d, *J*<sub>BP</sub> = 50.6 Hz)

<sup>31</sup>P NMR (161 MHz, DMSO-*d*<sub>6</sub>): δ -7.0 (s)

HRMS (ESI) *m/z* calcd. C<sub>9</sub>H<sub>16</sub>BNaOP [M+Na]<sup>+</sup>: 205.0924. Found 205.0930.

#### **B-(4-Hydroxyphenyl) dimethylphenylphosphine borane (8)**



Yield : 35.4 mg, 16.1%, white solid

R<sub>f</sub> = 0.31 (hexane/ethyl acetate = 2/1)

$^1\text{H}$  NMR (400MHz, DMSO- $d_6$ ):  $\delta$  8.69 (s,1H), 7.67 (t,  $J$  = 9.1 Hz, 2H), 7.52-7.49 (m, 3H), 6.96 (dd,  $J$  = 8.2, 2.8 Hz, 2H), 6.50 (dd,  $J$  = 8.3, 0.85 Hz, 2H), 2.29-1.70 (br, 2H), 1.45 (d,  $J$  = 10.3 Hz, 6H)

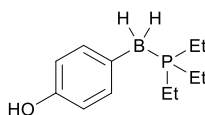
$^{13}\text{C}$  NMR (125 MHz, DMSO- $d_6$ ):  $\delta$  155.1(d,  $J_{\text{CP}}$  = 4.3 Hz), 136.9 (d,  $J_{\text{CP}}$  = 7.1 Hz), 131.5 (d,  $J_{\text{CP}}$  = 8.8 Hz), 131.4 (d,  $J_{\text{CP}}$  = 1.7 Hz), 130.9 (d,  $J_{\text{CP}}$  = 51.2 Hz), 129.2 (d,  $J_{\text{CP}}$  = 9.5 Hz), 114.8 (d,  $J_{\text{CP}}$  = 3.3 Hz), 9.7 (d,  $J_{\text{CP}}$  = 37.7 Hz)

$^{11}\text{B}$  NMR (128 MHz, DMSO- $d_6$ ):  $\delta$  -23.8(s)

$^{31}\text{P}$  NMR (161 MHz, DMSO- $d_6$ ):  $\delta$  -2.5(s)

HRMS (ESI)  $m/z$  calcd.  $\text{C}_{14}\text{H}_{18}\text{BNaOP}$  [ $\text{M}+\text{Na}$ ] $^+$ : 267.1081. Found 267.1090.

#### ***B*-(4-Hydroxyphenyl) triethylphenylphosphine borane (9)**



Yield : 20.0 mg, 8.9%, white solid

$R_f$  = 0.40 (hexane/ethyl acetate = 2/1)

$^1\text{H}$  NMR (400 MHz, DMSO- $d_6$ ):  $\delta$  8.66 (s,1H), 6.98 (dd,  $J$  = 8.1, 2.3 Hz, 2H), 6.52 (d,  $J$  = 7.6 Hz, 2H), 2.20-1.40 (br, 2H), 1.56-1.48 (m, 6H), 0.99 (quin,  $J$  = 7.5 Hz, 9H)

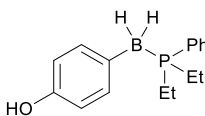
$^{13}\text{C}$  NMR (100 MHz, DMSO- $d_6$ ):  $\delta$  154.8 (d,  $J_{\text{CP}}$  = 3.9 Hz), 136.7 (d,  $J_{\text{CP}}$  = 6.7 Hz), 114.8 (d,  $J_{\text{CP}}$  = 3.2 Hz), 12.7 (d,  $J_{\text{CP}}$  = 33.4 Hz), 6.8 (d,  $J_{\text{CP}}$  = 3.5 Hz)

$^{11}\text{B}$  NMR (128 MHz, DMSO- $d_6$ ):  $\delta$  -27.4(s)

$^{31}\text{P}$  NMR (161 MHz, DMSO- $d_6$ ):  $\delta$  12.2(s)

HRMS (ESI)  $m/z$  calcd.  $\text{C}_{12}\text{H}_{22}\text{BNaOP}$  [ $\text{M}+\text{Na}$ ] $^+$ : 247.1394. Found 247.1404.

#### ***B*-(4-Hydroxyphenyl) diethylphenylphosphine borane (10)**



Yield : 65.5 mg, 24%, white solid

$R_f$  = 0.38 (hexane/ethyl acetate = 2/1)

$^1\text{H}$  NMR (400MHz, DMSO- $d_6$ ):  $\delta$  8.70 (s,1H), 7.70 (t,  $J$  = 8.0 Hz, 2H), 7.58-7.52 (m, 3H), 6.99 (d,  $J$  = 6.1 Hz, 2H), 6.51 (d,  $J$  = 7.9 Hz, 2H), 2.28-1.67 (br, 2H), 1.95-1.70 (m, 4H), 0.92 (quin,  $J$  = 7.7 Hz, 6H)

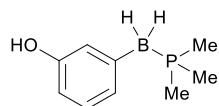
$^{13}\text{C}$  NMR (100 MHz, DMSO- $d_6$ ):  $\delta$  155.0 (d,  $J_{\text{CP}}$  = 4.0 Hz), 136.9 (d,  $J_{\text{CP}}$  = 6.9 Hz), 132.7 (d,  $J_{\text{CP}}$  = 7.5 Hz), 131.6 (d,  $J_{\text{CP}}$  = 2.1 Hz), 129.2 (d,  $J_{\text{CP}}$  = 9.0 Hz), 127.2 (d,  $J_{\text{CP}}$  = 47.7 Hz), 114.8 (d,  $J_{\text{CP}}$  = 2.9 Hz), 14.8 (d,  $J_{\text{CP}}$  = 35.2 Hz), 7.7 (d,  $J_{\text{CP}}$  = 2.8 Hz)

$^{11}\text{B}$  NMR (128 MHz, DMSO- $d_6$ ):  $\delta$  -27.6(s)

$^{31}\text{P}$  NMR (161 MHz, DMSO- $d_6$ ):  $\delta$  12.1(s)

HRMS (ESI)  $m/z$  calcd.  $C_{32}H_{44}B_2NaO_2P_2$   $[2M+Na]^+$ : 567.2895. Found 567.2909.

### ***B*-(3-Hydroxyphenyl) trimethylphosphine borane (11)**



Yield : 98.2 mg, 27%, white solid

$R_f$  = 0.40 (hexane/ethyl acetate = 1/1)

$^1H$  NMR (400MHz,  $DMSO-d_6$ ):  $\delta$  8.65 (s, 1H), 6.88 (t,  $J$  = 7.5 Hz, 1H), 6.63-6.60 (m, 2H), 6.39 (d,  $J$  = 7.9 Hz, 1H), 2.15-1.40 (br, 2H), 1.19 (d,  $J$  = 10.7 Hz, 9H)

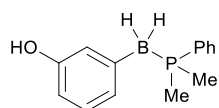
$^{13}C$  NMR (125 MHz,  $DMSO-d_6$ ):  $\delta$  156.5 (s), 128.1 (d,  $J_{CP}$  = 3.7 Hz), 126.7 (d,  $J_{CP}$  = 7.1 Hz), 122.6 (d,  $J_{CP}$  = 7.3 Hz), 111.7 (d,  $J_{CP}$  = 4.1 Hz), 10.0 (d,  $J_{CP}$  = 37.4 Hz)

$^{11}B$  NMR (128 MHz,  $DMSO-d_6$ ):  $\delta$  -23.6 (d,  $J_{BP}$  = 52.6 Hz)

$^{31}P$  NMR (161 MHz,  $DMSO-d_6$ ):  $\delta$  -6.7 (s)

HRMS (ESI)  $m/z$  calcd.  $C_9H_{16}BNaOP$   $[M+Na]^+$ : 205.0924. Found 205.0928.

### ***B*-(3-Hydroxyphenyl) dimethylphenylphosphine borane (12)**



Yield : 77.1 mg, 18%, white solid

$R_f$  = 0.29 (hexane/ethyl acetate = 2/1)

$^1H$  NMR (400 MHz,  $DMSO-d_6$ ):  $\delta$  8.65 (s, 1H), 7.70 (t,  $J$  = 8.6 Hz, 2H), 7.54-7.48 (m, 3H), 6.86 (t,  $J$  = 7.5 Hz, 1H), 6.64 (s, 1H), 6.60 (d,  $J$  = 6.6 Hz, 1H), 6.39 (d,  $J$  = 7.9 Hz, 1H), 2.31-1.67 (br, 2H), 1.49 (d,  $J$  = 10.5 Hz, 6H),

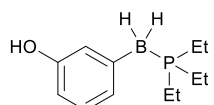
$^{13}C$  NMR (100 MHz, acetone- $d_6$ ):  $\delta$  157.2 (s), 132.1 (d,  $J_{CP}$  = 8.5 Hz), 132.0 (s), 131.5 (s), 129.7 (d,  $J_{CP}$  = 9.6 Hz), 128.7 (s), 128.3 (s), 123.6 (d,  $J_{CP}$  = 7.4 Hz), 112.4 (s), 10.3 (d,  $J_{CP}$  = 38.4 Hz)

$^{11}B$  NMR (128 MHz, acetone- $d_6$ ):  $\delta$  -24.0 (d,  $J_{BP}$  = 52.8 Hz)

$^{31}P$  NMR (161 MHz, acetone- $d_6$ ):  $\delta$  -2.7 (s)

HRMS (ESI)  $m/z$  calcd.  $C_{14}H_{18}BNaOP$   $[M+Na]^+$ : 267.1081. Found 267.1084.

### ***B*-(3-Hydroxyphenyl) triethylphosphine borane (13)**



Yield : 163.1 mg, 36%, colorless oil

$R_f = 0.37$  (hexane/ethyl acetate = 2/1)

$^1\text{H}$  NMR (400 MHz,  $\text{DMSO-}d_6$ ):  $\delta$  8.65 (s, 1H), 6.69 (t,  $J = 7.5$  Hz, 1H), 6.65-6.62 (m, 2H), 6.38 (d,  $J = 7.9$  Hz, 1H), 2.05-1.42 (br, 2H), 1.59-1.51 (m, 6H), 1.01 (quin,  $J = 7.5$  Hz, 9H)

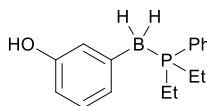
$^{13}\text{C}$  NMR (125 MHz,  $\text{DMSO-}d_6$ ):  $\delta$  156.5 (d,  $J_{\text{CP}} = 3.7$  Hz), 128.1 (d,  $J_{\text{CP}} = 3.1$  Hz), 126.9 (d,  $J_{\text{CP}} = 6.9$  Hz), 122.8 (d,  $J_{\text{CP}} = 6.8$  Hz), 111.6 (d,  $J_{\text{CP}} = 3.7$  Hz), 12.8 (d,  $J_{\text{CP}} = 34.1$  Hz), 6.8 (d,  $J_{\text{CP}} = 3.5$  Hz)

$^{11}\text{B}$  NMR (128 MHz,  $\text{DMSO-}d_6$ ):  $\delta$  -27.6(s)

$^{31}\text{P}$  NMR (161 MHz,  $\text{DMSO-}d_6$ ):  $\delta$  12.8(s)

HRMS (ESI)  $m/z$  calcd.  $\text{C}_{12}\text{H}_{22}\text{BNaOP}$   $[\text{M}+\text{Na}]^+$ : 247.1394. Found 247.1397.

### **B-(3-Hydroxyphenyl) diethylphenylphosphine borane (14)**



Yield : 65.2 mg, 12%, white solid

$R_f = 0.38$  (hexane/ethyl acetate = 2/1)

$^1\text{H}$  NMR (400MHz,  $\text{DMSO-}d_6$ ):  $\delta$  8.67 (s, 1H), 7.72 (t,  $J = 8.3$  Hz, 2H), 7.59-7.51 (m, 3H), 6.86 (t,  $J = 7.6$ , 1H), 6.68 (s, 1H), 6.64 (d,  $J = 6.9$  Hz, 1H), 6.39 (d,  $J = 7.9$  Hz, 1H), 2.27-1.70 (br, 2H), 1.98-1.87 (m, 2H), 1.85-1.71 (m, 2H), 0.92 (quin,  $J = 7.8$  Hz, 6H)

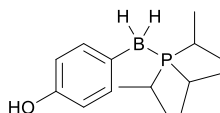
$^{13}\text{C}$  NMR (125 MHz,  $\text{DMSO-}d_6$ ):  $\delta$  156.6 (d,  $J_{\text{CP}} = 2.8$  Hz), 132.8 (d,  $J_{\text{CP}} = 7.8$  Hz), 131.7 (d,  $J_{\text{CP}} = 1.7$  Hz), 129.3 (d,  $J_{\text{CP}} = 9.1$  Hz), 128.2 (d,  $J_{\text{CP}} = 2.9$  Hz), 127.0 (d,  $J_{\text{CP}} = 48.8$  Hz), 127.0 (d,  $J_{\text{CP}} = 7.0$  Hz), 122.9 (d,  $J_{\text{CP}} = 7.2$  Hz), 111.9 (d,  $J_{\text{CP}} = 3.9$  Hz), 15.0 (d,  $J_{\text{CP}} = 35.6$  Hz), 7.1 (d,  $J_{\text{CP}} = 2.8$  Hz)

$^{11}\text{B}$  NMR (128 MHz,  $\text{DMSO-}d_6$ ):  $\delta$  -27.7(s)

$^{31}\text{P}$  NMR (161 MHz,  $\text{DMSO-}d_6$ ):  $\delta$  12.6(s)

HRMS (ESI)  $m/z$  calcd. for  $\text{C}_{16}\text{H}_{23}\text{BOP}$   $[\text{M}+\text{H}]^+$ : 273.1574. Found 273.1580.

### **B-(4-Hydroxyphenyl) triisopropylphosphine borane (15)**



Yield : 72.0 mg, 9.1% (2 steps), white solid

$R_f = 0.47$  (hexane/ethyl acetate = 2/1)

$^1\text{H}$  NMR (400 MHz,  $\text{DMSO-}d_6$ ):  $\delta$  8.66 (s, 1H), 7.05 (d,  $J = 7.9$  Hz, 2H), 6.50 (d,  $J = 6.8$  Hz, 2H), 2.30-1.50 (br, 2H), 2.21-2.12 (m, 3H), 1.15-1.10 (m, 18H)

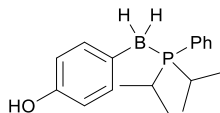
$^{13}\text{C}$  NMR (125 MHz,  $\text{DMSO-}d_6$ ):  $\delta$  154.8 (d,  $J_{\text{CP}} = 3.6$  Hz), 137.2 (d,  $J_{\text{CP}} = 6.3$  Hz), 114.7 (d,  $J_{\text{CP}} = 2.4$  Hz), 20.5 (d,  $J_{\text{CP}} = 28.3$  Hz), 18.2 (s)

$^{11}\text{B}$  NMR (128 MHz,  $\text{DMSO-}d_6$ ):  $\delta$  -28.6(s)

$^{31}\text{P}$  NMR (161 MHz, DMSO- $d_6$ ):  $\delta$  23.4(s)

HRMS (ESI)  $m/z$  calcd.  $\text{C}_{30}\text{H}_{56}\text{B}_2\text{NaO}_2\text{P}_2$   $[2\text{M}+\text{Na}]^+$ : 555.3834. Found 555.3820.

#### ***B*-(4-Hydroxyphenyl) diisopropylphenylphosphine borane (16)**



Yield : 86.7 mg, 9.6% (2 steps), white solid

$R_f$  = 0.42 (hexane/ethyl acetate = 2/1)

$^1\text{H}$  NMR (400MHz,  $\text{CD}_2\text{Cl}_2$ ):  $\delta$  7.78 (t,  $J$  = 7.9 Hz, 2H), 7.54-7.45 (m, 3H), 7.27 (d,  $J$  = 6.7 Hz, 2H), 6.61 (d,  $J$  = 7.8 Hz, 2H), 2.58-1.90 (br, 2H), 2.47-2.38 (m, 2H), 1.07-0.95 (m, 12H)

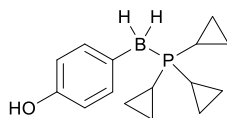
$^{13}\text{C}$  NMR (125 MHz, DMSO- $d_6$ ):  $\delta$  155.0 (d,  $J_{\text{CP}}$  = 3.6 Hz), 137.3 (d,  $J_{\text{CP}}$  = 6.8 Hz), 134.0 (d,  $J_{\text{CP}}$  = 6.5 Hz), 131.7 (s), 129.0 (d,  $J_{\text{CP}}$  = 8.4 Hz), 114.8 (d,  $J_{\text{CP}}$  = 2.5 Hz), 100.0 (s), 20.6 (d,  $J_{\text{CP}}$  = 31.3 Hz), 16.8-16.7 (m)

$^{11}\text{B}$  NMR (128 MHz, DMSO- $d_6$ ):  $\delta$  -28.5(s)

$^{31}\text{P}$  NMR (161 MHz, DMSO- $d_6$ ):  $\delta$  20.0(s)

HRMS (ESI)  $m/z$  calcd. for  $\text{C}_{36}\text{H}_{52}\text{B}_2\text{NaO}_2\text{P}_2$   $[2\text{M}+\text{Na}]^+$ : 623.3521. Found 623.3519.

#### ***B*-(4-Hydroxyphenyl) tricyclopropylphosphine borane (17)**



Yield : 92.6 mg, 24% (2 steps) , white solid

$R_f$  = 0.37 (hexane/ethyl acetate = 2/1)

$^1\text{H}$  NMR (400 MHz, DMSO- $d_6$ ):  $\delta$  8.66 (s, 1H), 7.01 (dd,  $J$  = 8.3, 2.3 Hz, 2H), 6.49 (d,  $J$  = 7.8 Hz, 2H), 1.82-1.13 (br, 2H), 0.752-0.643 (m, 15H)

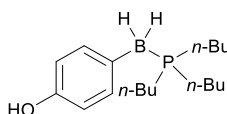
$^{13}\text{C}$  NMR (100 MHz, DMSO- $d_6$ ):  $\delta$  154.9 (d,  $J_{\text{CP}}$  = 3.8 Hz), 137.1 (d,  $J_{\text{CP}}$  = 6.7 Hz), 114.6 (d,  $J_{\text{CP}}$  = 2.8 Hz), 32.2 (d,  $J_{\text{CP}}$  = 31.2 Hz), 2.32 (s), 2.10 (d,  $J_{\text{CP}}$  = 61.9 Hz)

$^{11}\text{B}$  NMR (128 MHz, DMSO- $d_6$ ):  $\delta$  -29.1 (s)

$^{31}\text{P}$  NMR (161 MHz, DMSO- $d_6$ ):  $\delta$  15.5 (s)

HRMS (ESI)  $m/z$  calcd. for  $\text{C}_{30}\text{H}_{44}\text{B}_2\text{NaO}_2\text{P}_2$   $[2\text{M}+\text{Na}]^+$ : 543.2895. Found 543.2892.

#### ***B*-(4-Hydroxyphenyl) tributylphosphine borane (18)**



Yield : 152.0 mg, 25%, white solid

$R_f$  = 0.56 (hexane/ethyl acetate = 2/1)

$^1\text{H}$  NMR (400 MHz,  $\text{DMSO-}d_6$ ):  $\delta$  8.67 (s, 1H), 6.97 (dd,  $J$  = 8.1, 2.4 Hz, 2H), 6.52 (d,  $J$  = 7.8 Hz, 2H), 2.08-1.12 (br, 2H), 1.48-1.45 (m, 6H), 1.38-1.28 (m, 12H), 0.99 (t,  $J$  = 7.0 Hz, 9H)

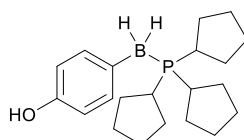
$^{13}\text{C}$  NMR (100 MHz,  $\text{DMSO-}d_6$ ):  $\delta$  154.9 (d,  $J_{\text{CP}}$  = 3.9 Hz), 136.7 (d,  $J_{\text{CP}}$  = 6.7 Hz), 114.7 (d,  $J_{\text{CP}}$  = 3.0 Hz), 24.5 (d,  $J_{\text{CP}}$  = 2.6 Hz), 24.3 (d,  $J_{\text{CP}}$  = 12.1 Hz), 20.1 (d,  $J_{\text{CP}}$  = 32.4 Hz), 13.9 (s)

$^{11}\text{B}$  NMR (128 MHz,  $\text{DMSO-}d_6$ ):  $\delta$  -26.9 (s)

$^{31}\text{P}$  NMR (161 MHz,  $\text{DMSO-}d_6$ ):  $\delta$  6.7 (s)

HRMS (ESI)  $m/z$  calcd.  $\text{C}_{36}\text{H}_{68}\text{B}_2\text{NaO}_2\text{P}_2$  [ $2\text{M}+\text{Na}$ ] $^+$ : 639.4773. Found 639.4770.

### ***B*-(4-Hydroxyphenyl) tricyclopentylphosphine borane (19)**



Yield : 175.0 mg, 25%, white solid

$R_f$  = 0.53 (hexane/ethyl acetate = 2/1)

$^1\text{H}$  NMR (400 MHz,  $\text{DMSO-}d_6$ ):  $\delta$  8.63 (s, 1H), 7.03 (dd,  $J$  = 8.1, 2.0 Hz, 2H), 6.49 (d,  $J$  = 7.9 Hz, 2H), 2.23-1.30 (br, 2H), 2.14-2.05 (m, 3H), 1.77-1.49 (m, 24H)

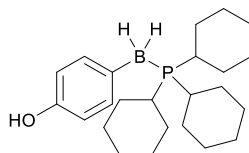
$^{13}\text{C}$  NMR (100 MHz,  $\text{DMSO-}d_6$ ):  $\delta$  154.7 (d,  $J_{\text{CP}}$  = 3.7 Hz), 137.3 (d,  $J_{\text{CP}}$  = 6.2 Hz), 114.6 (d,  $J_{\text{CP}}$  = 3.1 Hz), 32.2 (d,  $J_{\text{CP}}$  = 31.2 Hz), 28.3 (s), 26.2 (d,  $J_{\text{CP}}$  = 8.5 Hz)

$^{11}\text{B}$  NMR (128 MHz,  $\text{DMSO-}d_6$ ):  $\delta$  -28.8 (s)

$^{31}\text{P}$  NMR (161 MHz,  $\text{DMSO-}d_6$ ):  $\delta$  18.0 (s)

HRMS (ESI)  $m/z$  calcd. for  $\text{C}_{42}\text{H}_{68}\text{B}_2\text{NaO}_2\text{P}_2$  [ $2\text{M}+\text{Na}$ ] $^+$ : 711.4773. Found 711.4799.

### ***B*-(4-Hydroxyphenyl) tricyclohexylphosphine borane (20)**



Yield : 34.8 mg, 4.5%, white solid

$R_f$  = 0.61 (hexane/ethyl acetate = 2/1)

$^1\text{H}$  NMR (400 MHz,  $\text{DMSO-}d_6$ ):  $\delta$  8.67 (s, 1H), 7.02 (d,  $J$  = 6.4 Hz, 2H), 6.52 (d,  $J$  = 7.8 Hz, 2H), 1.93-1.11 (br, 2H), 1.88-1.65 (m, 19H), 1.32-1.16 (m, 16H)

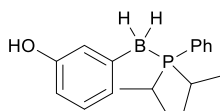
$^{13}\text{C}$  NMR (125 MHz, DMSO- $d_6$ ):  $\delta$  154.8 (d,  $J_{\text{CP}} = 3.3$  Hz), 137.2 (d,  $J_{\text{CP}} = 6.7$  Hz), 114.8 (d,  $J_{\text{CP}} = 2.8$  Hz), 30.3 (d,  $J_{\text{CP}} = 27.3$  Hz), 27.8 (d,  $J_{\text{CP}} = 1.9$  Hz), 27.3 (d,  $J_{\text{CP}} = 9.2$  Hz)

$^{11}\text{B}$  NMR (128 MHz, DMSO- $d_6$ ):  $\delta$  -28.5 (s)

$^{31}\text{P}$  NMR (161 MHz, DMSO- $d_6$ ):  $\delta$  14.7 (s)

HRMS (ESI)  $m/z$  calcd. for  $\text{C}_{48}\text{H}_{80}\text{B}_2\text{NaO}_2\text{P}_2$   $[2\text{M}+\text{Na}]^+$ : 795.5712. Found 795.5747.

### ***B*-(3-Hydroxyphenyl) diisopropylphosphine borane (21)**



Yield : 317.8 mg, 35% (2 steps), white solid

$R_f = 0.47$  (hexane/ethyl acetate = 2/1)

$^1\text{H}$  NMR (400MHz,  $\text{CD}_2\text{Cl}_2$ ):  $\delta$  7.80-7.75 (m, 2H), 7.57-7.48 (m, 3H), 6.97 (d,  $J = 5.3$  Hz, 2H), 6.87 (s, 1H), 6.51-6.48 (m, 1H), 4.50 (s, 1H), 2.60-1.80 (br, 2H), 2.60-1.80 (br, 2H), 2.49-2.39 (m, 2H), 1.07-0.97 (m, 12H)

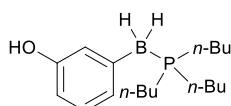
$^{13}\text{C}$  NMR (125 MHz, DMSO- $d_6$ ):  $\delta$  156.5 (d,  $J_{\text{CP}} = 2.8$  Hz), 134.0 (d,  $J_{\text{CP}} = 6.2$  Hz), 131.8 (d,  $J_{\text{CP}} = 2.5$  Hz), 129.0 (d,  $J_{\text{CP}} = 8.8$  Hz), 128.1 (d,  $J_{\text{CP}} = 2.9$  Hz), 127.5 (d,  $J_{\text{CP}} = 6.5$  Hz), 124.3 (d,  $J_{\text{CP}} = 45.8$  Hz), 123.4 (d,  $J_{\text{CP}} = 7.5$  Hz), 111.9 (d,  $J_{\text{CP}} = 3.3$  Hz), 20.7 (d,  $J_{\text{CP}} = 31.2$  Hz), 16.8-16.7 (m)

$^{11}\text{B}$  NMR (128 MHz, DMSO- $d_6$ ):  $\delta$  -28.3(s)

$^{31}\text{P}$  NMR (161 MHz, DMSO- $d_6$ ):  $\delta$  21.2(s)

HRMS (ESI)  $m/z$  calcd. for  $\text{C}_{36}\text{H}_{52}\text{B}_2\text{NaO}_2\text{P}_2$   $[2\text{M}+\text{Na}]^+$ : 623.3521. Found 623.3561.

### ***B*-(3-Hydroxyphenyl) tributylphosphine borane (22)**



Yield : 47.7 mg, 7.7%, colorless oil

$R_f = 0.64$  (hexane/ethyl acetate = 2/1)

$^1\text{H}$  NMR (400 MHz, DMSO- $d_6$ ):  $\delta$  8.65 (s, 1H), 6.86 (t,  $J = 7.5$  Hz, 1H), 6.64-6.60 (m, 2H), 6.38 (d,  $J = 7.3$  Hz, 1H), 1.98-1.22 (br, 2H), 1.39-1.29 (m, 18H), 0.86 (d,  $J = 7.3$  Hz, 9H)

$^{13}\text{C}$  NMR (125 MHz, DMSO- $d_6$ ):  $\delta$  156.6 (s), 128.1 (s), 126.8 (d,  $J_{\text{CP}} = 6.6$  Hz), 122.8 (d,  $J_{\text{CP}} = 6.5$  Hz), 111.6 (d,  $J_{\text{CP}} = 2.9$  Hz), 24.5 (d,  $J_{\text{CP}} = 2.6$  Hz), 24.3 (d,  $J_{\text{CP}} = 12.2$  Hz), 20.2 (d,  $J_{\text{CP}} = 33.2$  Hz), 14.0 (s)

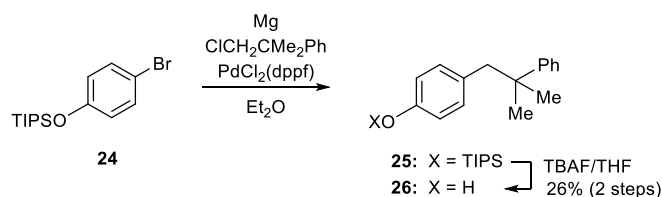
$^{11}\text{B}$  NMR (128 MHz, DMSO- $d_6$ ):  $\delta$  -26.8(s)

$^{31}\text{P}$  NMR (161 MHz, DMSO- $d_6$ ):  $\delta$  7.57(s)

HRMS (ESI)  $m/z$  calcd. for  $\text{C}_{36}\text{H}_{68}\text{B}_2\text{NaO}_2\text{P}_2$   $[2\text{M}+\text{Na}]^+$ : 639.4773. Found 639.4761.



### 1.3 Preparation of alkane analogue 26



A dry round bottom flask, equipped with a magnetic stirring bar, sealed with a septum and protected with an Ar balloon, was charged with magnesium (52.3 mg, 2.2 mmol) in 0.5 mL of Et<sub>2</sub>O. 1-Chloro-2-methyl-2-phenylpropane (0.32 mL, 2.0 mmol) was added to the mixture and then stirred under reflux for 1 h. Then, compound **24** (262 mg, 0.84 mmol) and PdCl<sub>2</sub>(dppf) (19.1 mg, 0.23 mmol) in 5.5 mL of Et<sub>2</sub>O were further added and the mixture was stirred for 4.5 h. The reaction mixture was allowed to cool to room temperature, washed with 1 % aqueous HCl at three times, water at two times and saturated brine at two times. The organic layer was dried over Na<sub>2</sub>SO<sub>4</sub>, filtered off, and concentrated under reduced pressure. The residue was purified by silica-gel column chromatography (eluent: diethyl ether) and used for the next step.

To a solution of compound **25** (131 mg, 0.30 mmol) in 1.0 mL of THF was added 1 M tetrabutylammonium fluoride in THF (0.40 mmol) at room temperature. After stirring for 15 min, the reaction was quenched by H<sub>2</sub>O and extracted with EtOAc. The organic layer was combined, washed with brine, dried over Na<sub>2</sub>SO<sub>4</sub>, and concentrated under reduced pressure. The residue was purified by silica-gel column chromatography (eluent: hexane/ethyl acetate, 8:1) to give the compound **26** (48.5 mg, 26%, 2steps).

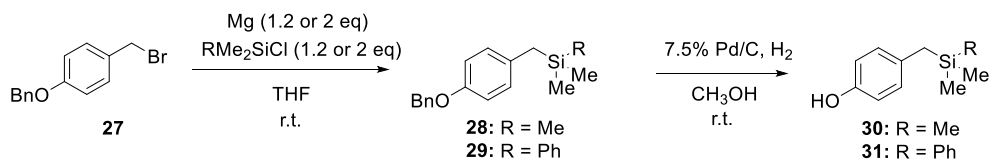
Yield : 26% (2steps), white solid

R<sub>f</sub> = 0.48 (hexane/ethyl acetate = 5/1)

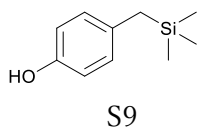
<sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>): δ 9.06 (s, 1H), 7.32-7.27 (m, 4H), 7.16 (t, *J* = 6.8 Hz, 1H), 6.61 (d, *J* = 8.5 Hz, 2H), 6.50 (d, *J* = 8.6 Hz, 2H), 2.72 (s, 2H), 1.22 (s, 6H)

<sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>): δ 155.9 (s), 149.4 (s), 131.5 (s), 129.1 (s), 128.3 (s), 126.5 (s), 125.9 (s), 114.7 (s), 49.7 (s), 38.9 (s), 28.4 (s)

### 1.4. Preparation of silane analogues 30 and 31



#### 4-[(Trimethylsilyl)methyl]phenol (30)



A dry round bottom flask, equipped with a magnetic stirring bar, sealed with a septum and protected with an Ar balloon, was charged with magnesium (12.2 mg, 0.6 mmol) trimethylsilyl chloride (76  $\mu$ L, 0.6 mmol) and THF (0.6 mL). Compound **27** (138.6 mg, 0.5 mmol) in THF (0.3 mL) was added dropwise over 20 minutes. After stirring at room temperature, the reaction was quenched with a saturated  $\text{NH}_4\text{Cl}$  solution and extracted with ethyl acetate for three times. The organic layer was combined, washed with brine and dried over  $\text{Na}_2\text{SO}_4$ . The solvent was removed under reduced pressure and the residue was purified by silica-gel column chromatography (eluent: hexane/ethyl acetate, 20:1) to give the compound **28** as a mixture. The mixture was used for next reaction without further purification. Then the mixture was hydrogenated with 7.5 % Pd/C in MeOH at room temperature. Insoluble materials were removed through Celite, and the filtrate was concentrated. The residue was purified by preparative thin-layer chromatography (eluent: dichloromethane) to give the compound **30** (11.4 mg, 13% for 2 steps).

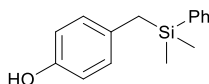
Yield : 13% (2steps), white solid

$R_f$  = 0.32 (hexane/ethyl acetate = 5/1)

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  6.86 (d,  $J$  = 8.4 Hz, 2H), 6.70 (d,  $J$  = 8.5 Hz, 2H), 4.47 (s, 1H), 1.99 (s, 2H), 0.02 (s, 9H)

$^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ):  $\delta$  152.2 (s), 132.5 (s), 128.9 (s), 115.0 (s), 25.7 (s), -2.0 (s)

#### 4-[(Dimethylphenylsilyl)methyl]phenol (**31**)



A dry round bottom flask, equipped with a magnetic stirring bar, sealed with a septum and protected with an Ar balloon, was charged with magnesium (332 mg, 13.6 mmol) dimethylphenylsilyl chloride (1.1 mL, 13.6 mmol) and THF (0.5 mL). Compound **27** (1.90 g, 6.8 mmol) in THF (8 mL) was added dropwise over 30 minutes. After stirring at room temperature, the reaction was quenched with a saturated  $\text{NH}_4\text{Cl}$  solution and extracted with ethyl acetate for three times. The organic layer was combined, washed with brine and dried over  $\text{Na}_2\text{SO}_4$ . The solvent was removed under reduced pressure and the residue was purified by silica-gel column chromatography (eluent: hexane/ethyl acetate, 11:1) to give the compound **29** as a mixture. The mixture was used for next reaction without further purification.

Then the mixture was hydrogenated with 7.5 % Pd/C in MeOH at room temperature. Insoluble materials were removed through Celite, and the filtrate was concentrated. The residue was purified by silica-gel column chromatography (eluent: hexane/ethyl acetate, 10:1) to give the compound **31**

(175 mg, 54 % for 2 steps).

Yield : 54% (2steps), white solid

$R_f$  = 0.29 (hexane/ethyl acetate = 5/1)

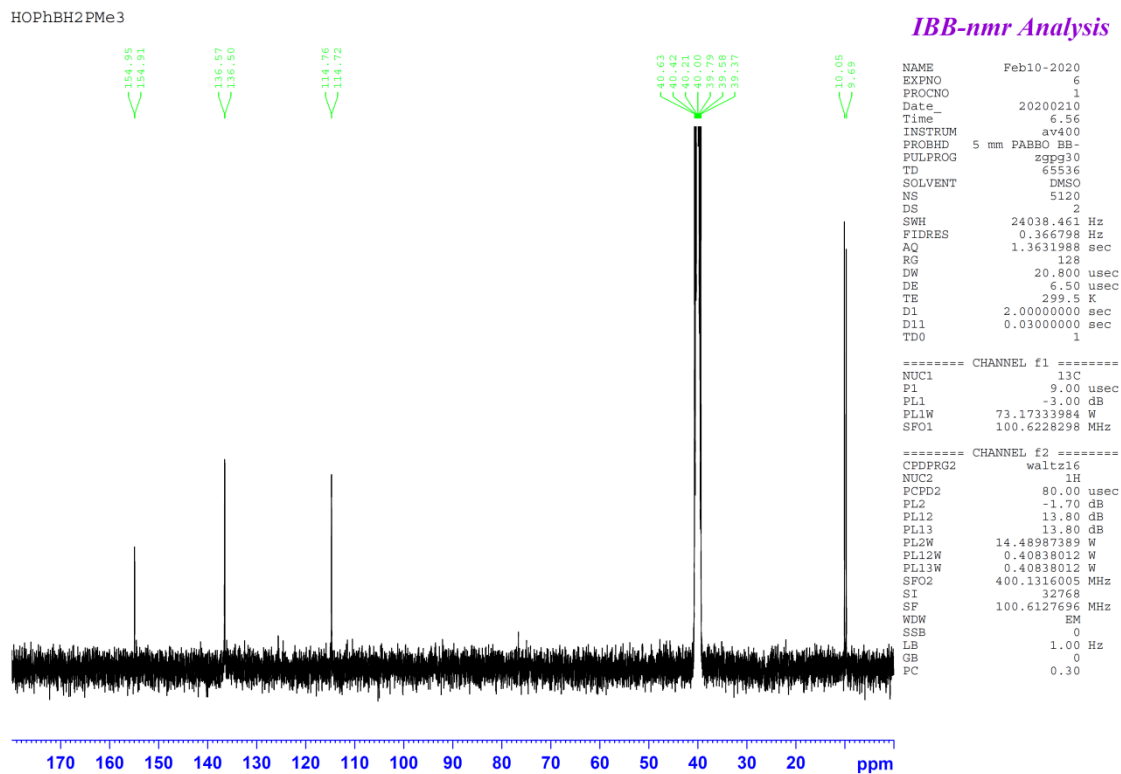
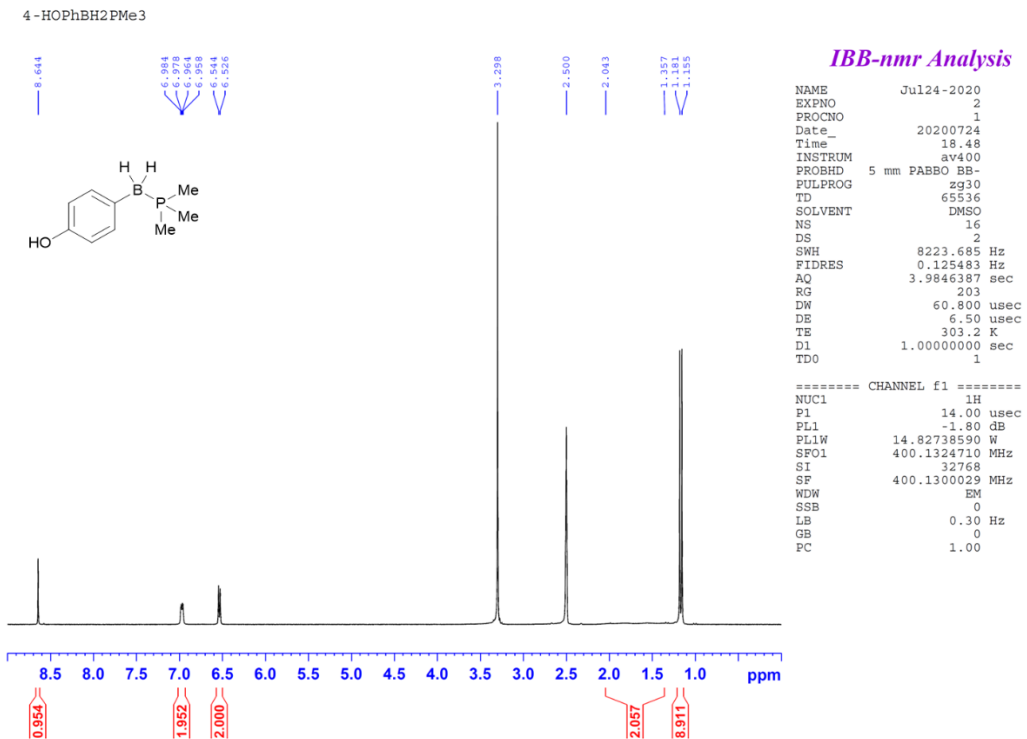
$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.46-7.44 (m, 2H), 7.37-7.32 (m, 3H), 6.80 (d,  $J$  = 8.4 Hz, 2H), 6.67 (d,  $J$  = 8.5 Hz, 2H), 4.44 (s, 1H), 2.22 (s, 2H), 0.24 (s, 6H)

$^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ):  $\delta$ =152.3 (s), 138.5 (s), 133.7 (s), 131.6 (s), 129.2 (s), 129.0 (s), 127.7 (s), 115.0 (s), 24.9 (s), -3.5 (s)

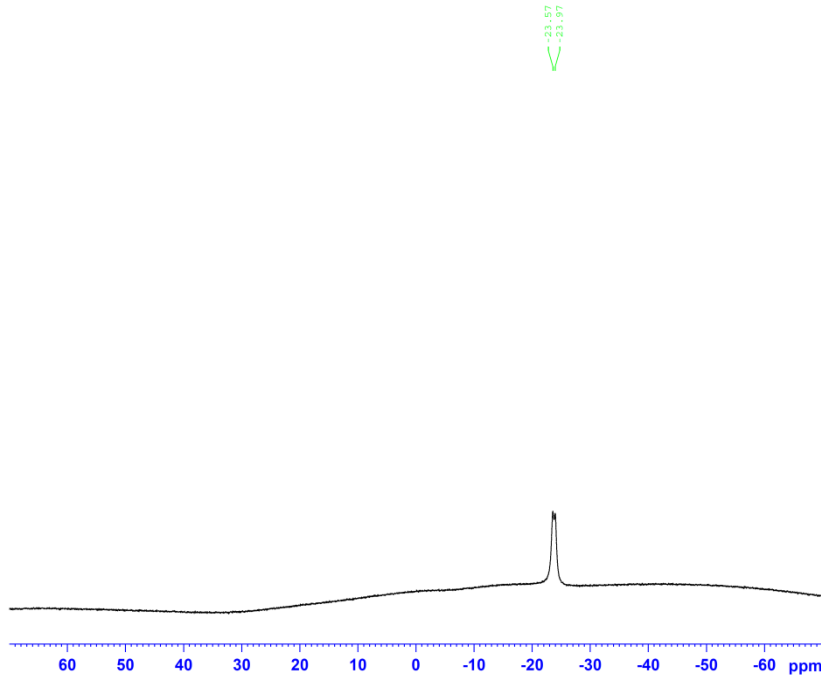
HRMS (ESI)  $m/z$  calcd. for  $\text{C}_{15}\text{H}_{17}\text{OSi}$   $[\text{M}-\text{H}]^-$  : 241.1054. Found 241.1053.

## 2. <sup>1</sup>H, <sup>13</sup>C, <sup>11</sup>B and <sup>31</sup>P NMR Spectra

### B-(4-Hydroxyphenyl) trimethylphosphine borane (7)



HOPhBH2PMe3



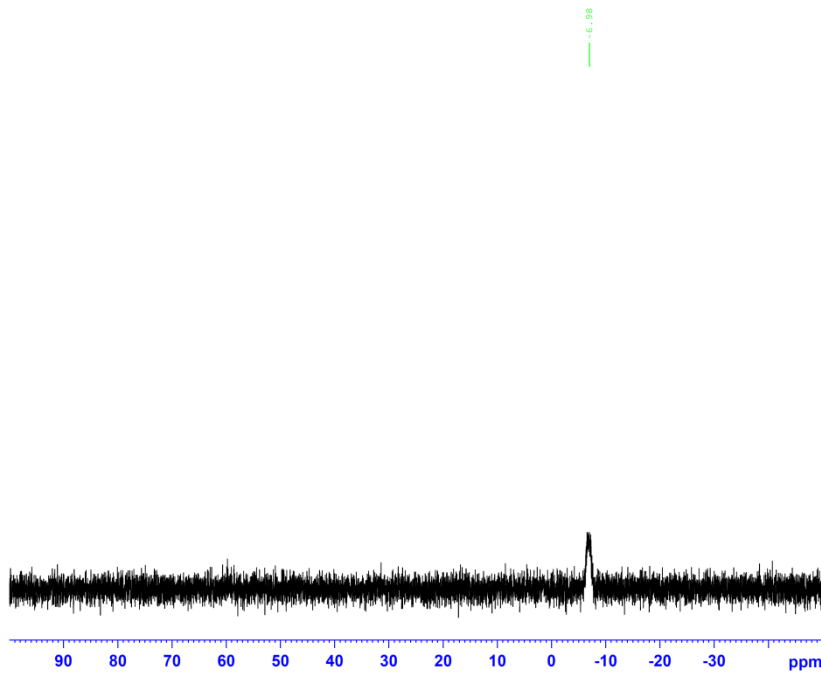
**IBB-nmr Analysis**

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NAME Feb10-2020
EXPNO 3
PROCNO 1
Date_ 20200210
Time 1.49
INSTRUM av400
PROBHD 5 mm PABBO BB-
PULPROG zgpg
TD 32768
SOLVENT DMSO
NS 256
DS 4
SWH 20000.000 Hz
FIDRES 0.610352 Hz
AQ 0.8192500 sec
RG 203
DW 25.000 usec
DE 20.00 usec
TE 298.5 K
D1 1.00000000 sec
D11 0.03000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 11B
P1 6.30 usec
PL1 -2.00 dB
SFO1 128.3776050 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -1.70 dB
PL12 13.80 dB
PL2W 14.48987389 W
PL12W 0.40838012 W
SFO2 400.1316005 MHz
SI 32768
SF 128.3776176 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40
```

HOPhBH2PMe3



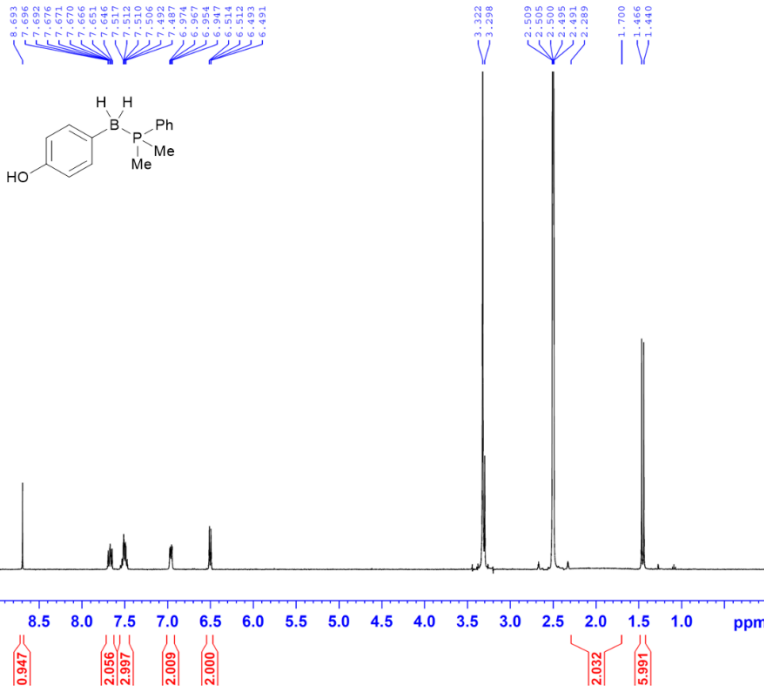
**IBB-nmr Analysis**

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NAME Feb10-2020
EXPNO 4
PROCNO 1
Date_ 20200210
Time 1.53
INSTRUM av400
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 4
SWH 64102.563 Hz
FIDRES 0.978127 Hz
AQ 0.5112308 sec
RG 203
DW 7.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 31P
P1 10.00 usec
PL1 -0.70 dB
PL1W 30.10233498 W
SFO1 161.9674942 MHz
SI 32768
SF 161.9754962 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
```

**B-(4-Hydroxyphenyl) dimethylphenylphosphine borane (8)**

HOPhBH2PPhMe2



**IBB-nmr Analysis**

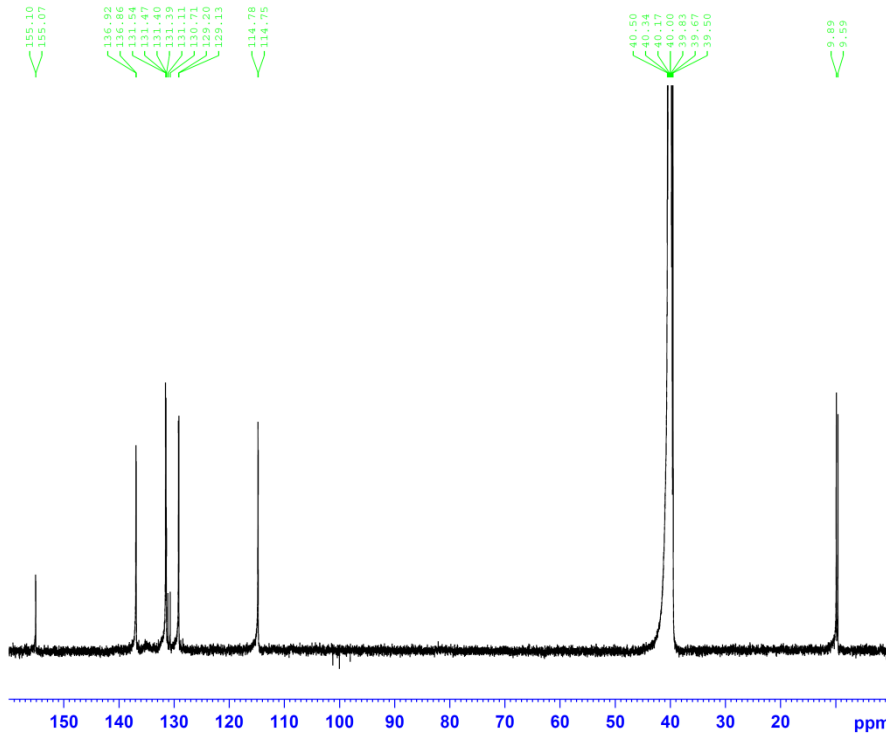
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NAME      Oct27-2019
EXPNO     2
PROCNO    1
Date_     20191027
Time      7.09
INSTRUM   av400
PROBHD    5 mm PABBO BB-
PULPROG   zg30
TD         65536
SOLVENT   DMSO
NS         16
DS         2
SWH        8223.685 Hz
FIDRES     0.125483 Hz
AQ         3.9846387 sec
RG         203
DW         60.800 usec
DE         6.50 usec
TE         297.9 K
D1         1.00000000 sec
TD0        1
    
```

```

----- CHANNEL f1 -----
NUC1      1H
P1        14.00 usec
PL1       -1.80 dB
PL1W      14.82738590 W
SFO1      400.1324710 MHz
SI         32768
SF         400.1300031 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
    
```

HOPhBH2PMe2Ph



**IBB-nmr Analysis**

```

NAME      Apr11-2020
EXPNO     4
PROCNO    1
Date_     20200411
Time      21.49
INSTRUM   av500
PROBHD    5 mm CPDCH 13C
PULPROG   zgpg30
TD         65536
SOLVENT   DMSO
NS         256
DS         4
SWH        30030.029 Hz
FIDRES     0.458222 Hz
AQ         1.0912410 sec
RG         35.9
DW         16.650 usec
DE         20.00 usec
TE         297.9 K
D1         2.00000000 sec
D11        0.03000000 sec
TD0        1
    
```

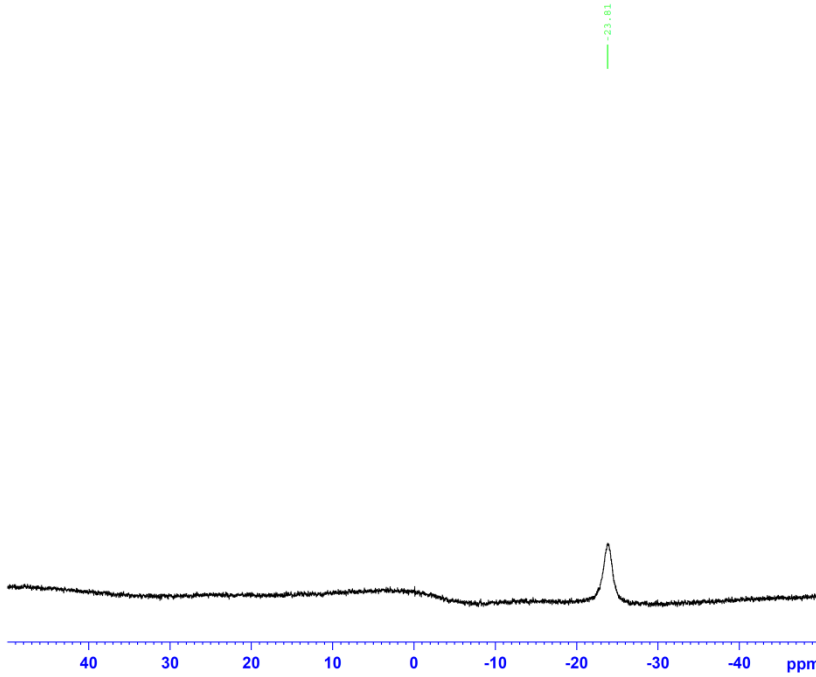
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----- CHANNEL f1 -----
NUC1      13C
P1        10.00 usec
PL1       -5.00 dB
PL1W      14.29790783 W
SFO1      125.7703643 MHz
    
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```

----- CHANNEL f2 -----
CPDPRG2   waltz16
NUC2      1H
PCPD2     90.00 usec
PL2       -4.00 dB
PL12      14.06 dB
PL13      17.00 dB
PL2W      6.30957365 W
PL12W     0.09862794 W
PL13W     0.05011872 W
SFO2      500.1320005 MHz
SI         32768
SF         125.7577866 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         0.30
    
```

4 - HOPhBH2PMe2Ph



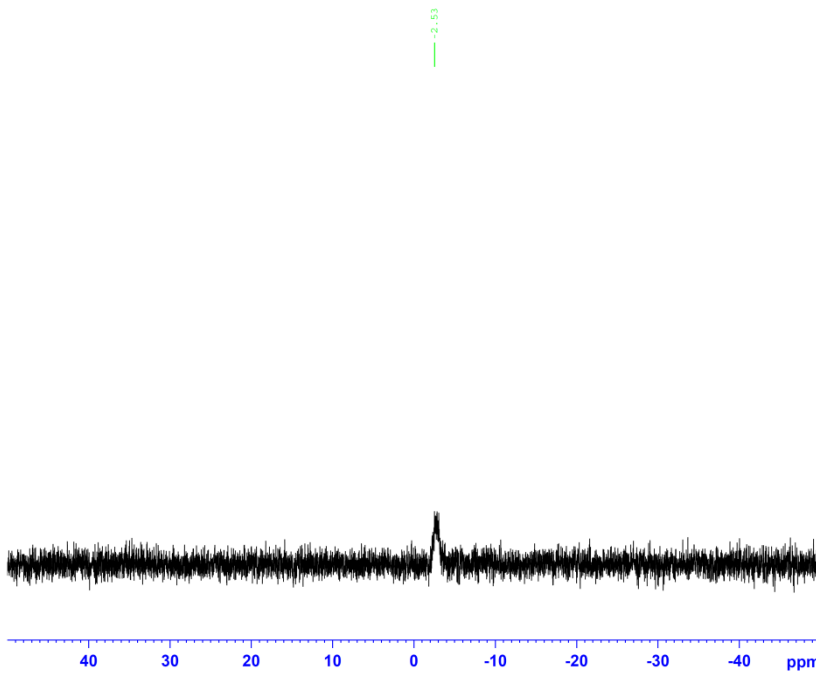
### IBB-nmr Analysis

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NAME      Apr5-2020
EXPNO     4
PROCNO    1
Date_     20200405
Time      17.38
INSTRUM   av400
PROBHD    5 mm PABBO BB-
PULPROG   zgpg
TD         32768
SOLVENT   DMSO
NS         512
DS         4
SWH        20000.000 Hz
FIDRES     0.610352 Hz
AQ         0.8192500 sec
RG         203
DW         25.000 usec
DE         20.00 usec
TE         298.3 K
D1         1.00000000 sec
D11        0.03000000 sec
TDO        1

===== CHANNEL f1 =====
NUC1       11B
P1         6.30 usec
PL1        -2.00 dB
SFO1       128.3776050 MHz

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2       1H
PCPD2      80.00 usec
PL2        -1.70 dB
PL12       13.80 dB
PL2W       14.48987389 W
PL12W      0.40838012 W
SFO2       400.1316005 MHz
SI         32768
SF         128.3776183 MHz
WDW        EM
SSB         0
LB          2.00 Hz
GB          0
PC          1.40
```

4 - HOPhBH2PMe2Ph

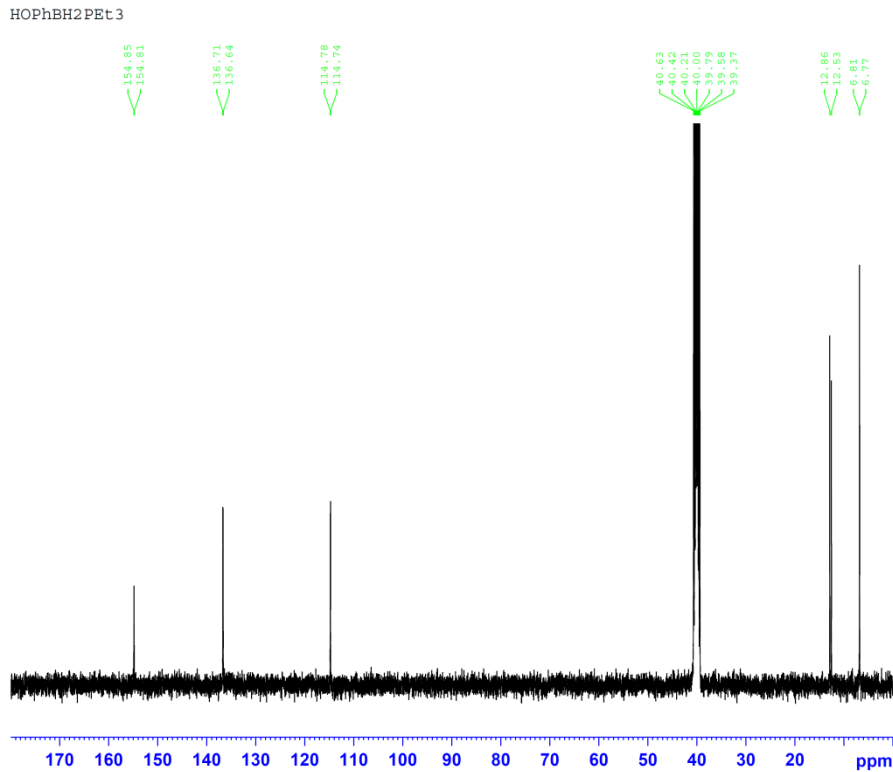
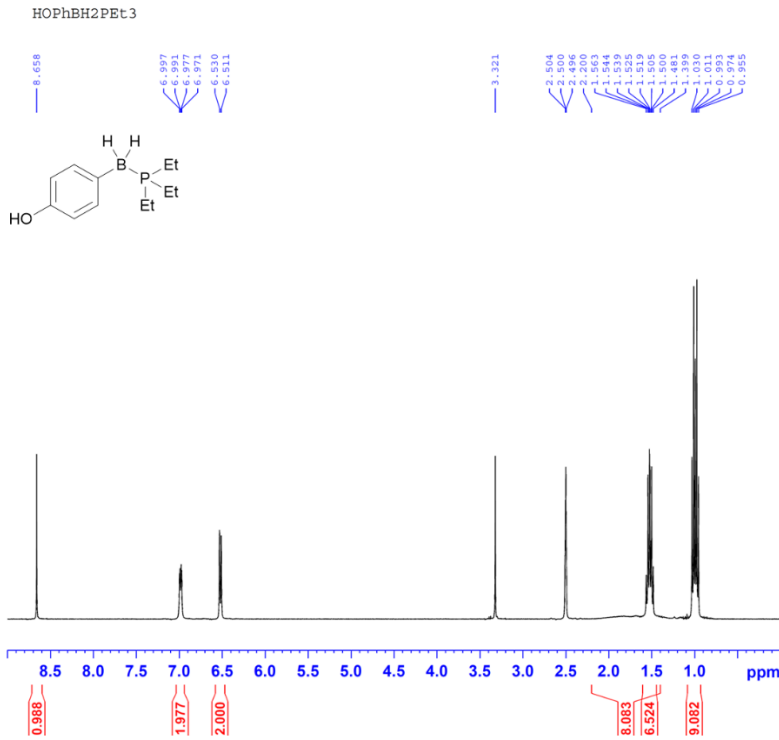


### IBB-nmr Analysis

```
NAME      Apr5-2020
EXPNO     3
PROCNO    1
Date_     20200405
Time      17.18
INSTRUM   av400
PROBHD    5 mm PABBO BB-
PULPROG   zg30
TD         65536
SOLVENT   DMSO
NS         64
DS         4
SWH        64102.563 Hz
FIDRES     0.978127 Hz
AQ         0.5112308 sec
RG         203
DW         7.800 usec
DE         6.50 usec
TE         298.2 K
D1         2.00000000 sec
TDO        1

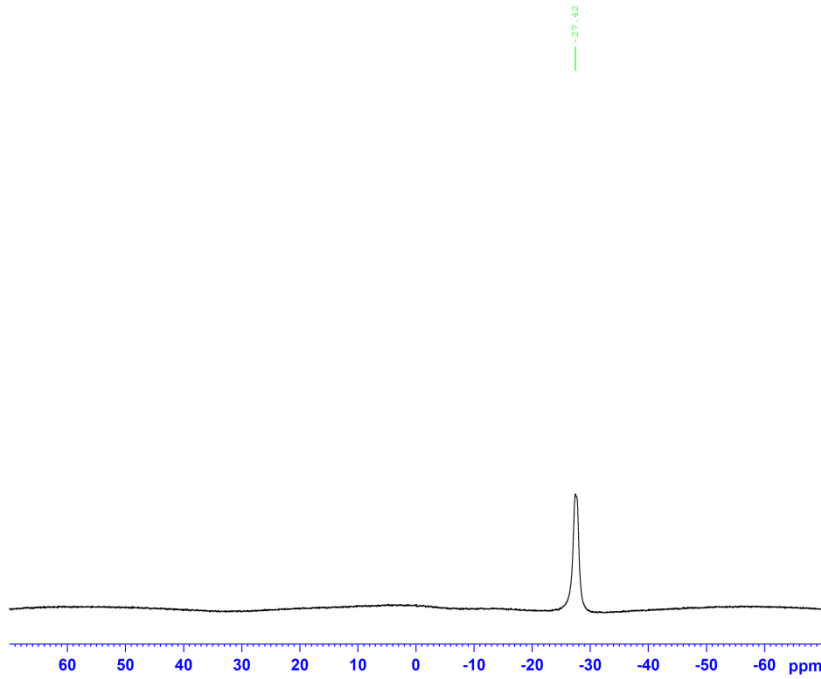
===== CHANNEL f1 =====
NUC1       31P
P1         10.00 usec
PL1        -0.70 dB
PL1W       30.10233498 W
SFO1       161.9674942 MHz
SI         32768
SF         161.9754962 MHz
WDW        EM
SSB         0
LB          1.00 Hz
GB          0
PC          1.40
```

**B-(4-Hydroxyphenyl) triethylphenylphosphine borane (9)**





HOPhBH2PEt3



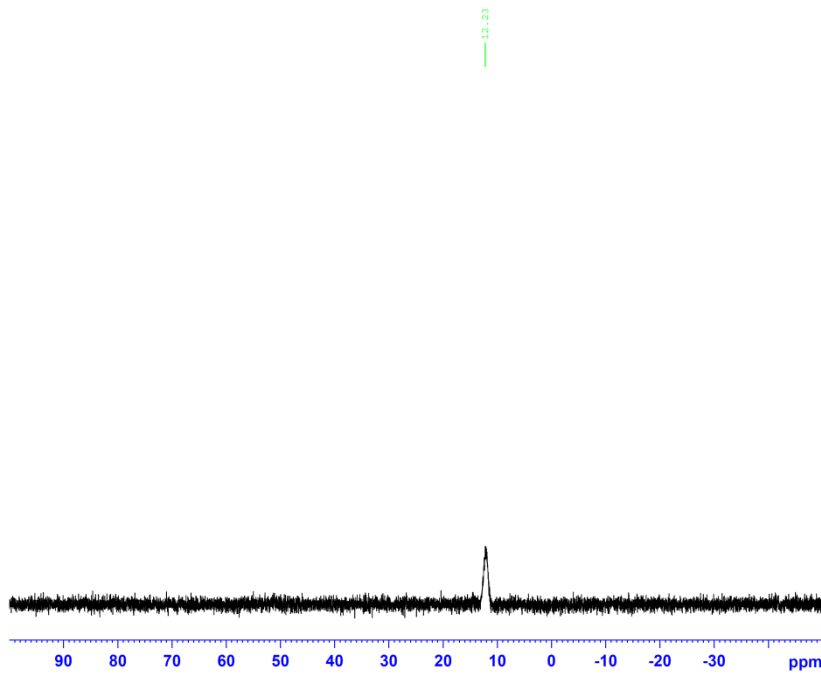
**IBB-nmr Analysis**

```
NAME          Feb9-2020
EXPNO         6
PROCNO        1
Date_         20200210
Time_         0.48
INSTRUM       av400
PROBHD        5 mm PABBO BB-
PULPROG       zgpg
TD            32768
SOLVENT       DMSO
NS            256
DS            4
SWH           20000.000 Hz
FIDRES        0.610352 Hz
AQ            0.8192500 sec
RG            203
DW            25.000 usec
DE            20.00 usec
TE            298.7 K
D1            1.0000000 sec
D11           0.0300000 sec
TDO           1

===== CHANNEL f1 =====
NUC1          11B
P1            6.30 usec
PL1           -2.00 dB
SFO1         128.3776050 MHz

===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2          1H
PCPD2         80.00 usec
PL2           -1.70 dB
PL12          13.80 dB
PL2W          14.48987389 W
PL12W         0.40838012 W
SFO2         400.1316005 MHz
SI            32768
SF            128.3776179 MHz
WDW           EM
SSB           0
LB            2.00 Hz
GB            0
PC            1.40
```

HOPhBH2PEt3



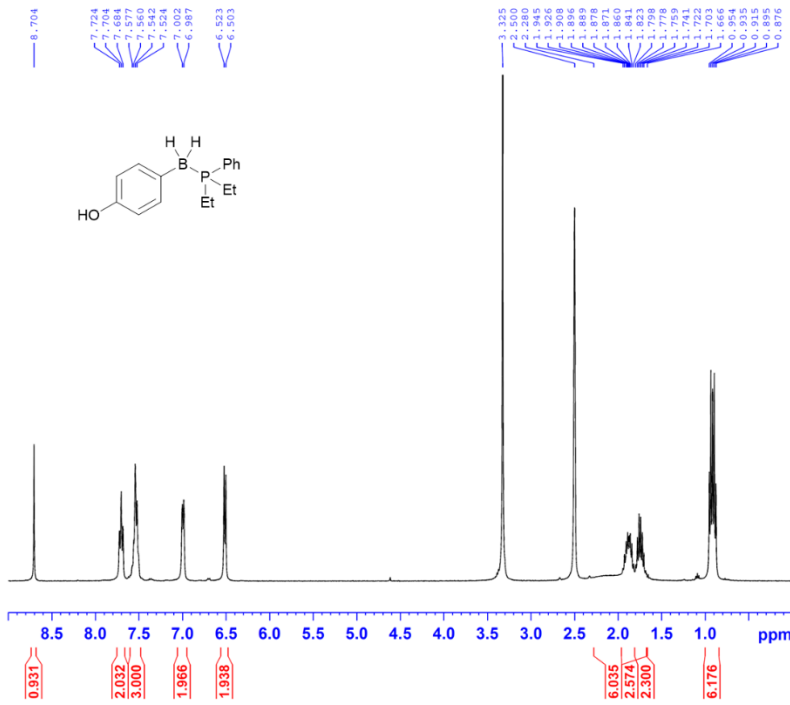
**IBB-nmr Analysis**

```
NAME          Feb9-2020
EXPNO         9
PROCNO        1
Date_         20200210
Time_         1.01
INSTRUM       av400
PROBHD        5 mm PABBO BB-
PULPROG       zg30
TD            65536
SOLVENT       DMSO
NS            16
DS            4
SWH           64102.563 Hz
FIDRES        0.978127 Hz
AQ            0.5112308 sec
RG            203
DW            7.800 usec
DE            6.50 usec
TE            298.0 K
D1            2.0000000 sec
TDO           1

===== CHANNEL f1 =====
NUC1          31P
P1            10.00 usec
PL1           -0.70 dB
PL1W          30.10233498 W
SFO1         161.9674942 MHz
SI            32768
SF            161.9754962 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
```

# B-(4-Hydroxyphenyl) diethylphenylphosphine borane (10)

4 -HOPhBH2PPhEt2



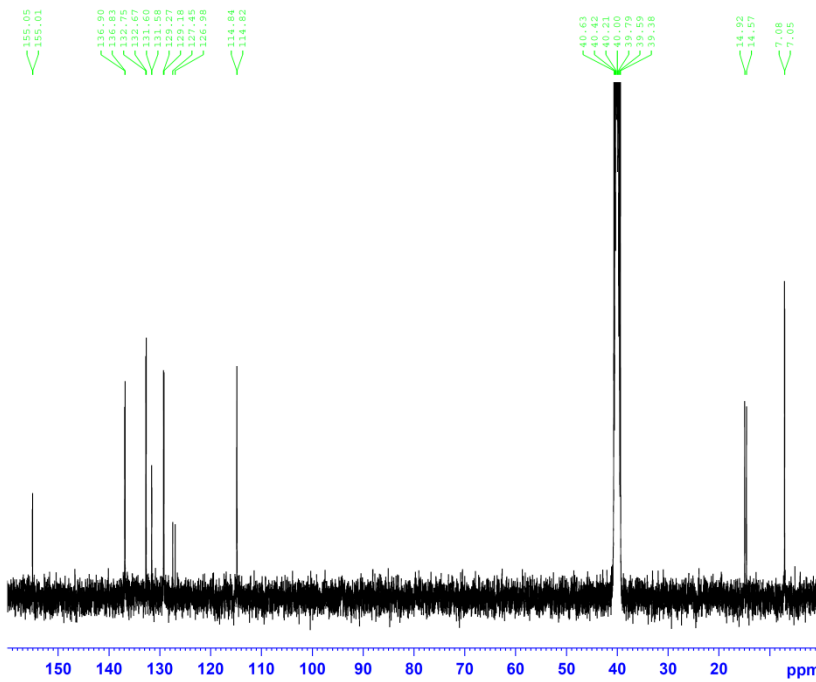
## IBB-nmr Analysis

```

NAME      Dec20-2020
EXPNO    2
PROCNO   1
Date_    20201220
Time     14.59
INSTRUM  av400
PROBHD   5 mm PABBO BB-
PULPROG  zg30
TD       65536
SOLVENT  DMSO
NS       16
DS       2
SWH      8223.685 Hz
FIDRES   0.125483 Hz
AQ       3.9846387 sec
RG       203
DW       60.800 usec
DE       6.50 usec
TE       297.8 K
D1       1.00000000 sec
TDO      1

===== CHANNEL f1 =====
NUC1     1H
P1       14.00 usec
PL1      -1.80 dB
PL1W     14.82738590 W
SFO1     400.1324710 MHz
SI       32768
SF       400.1300023 MHz
WDW      EM
SSB      0
LB       0.30 Hz
GB       0
PC       1.00
    
```

4 -HOPhBH2PPhEt2



## IBB-nmr Analysis

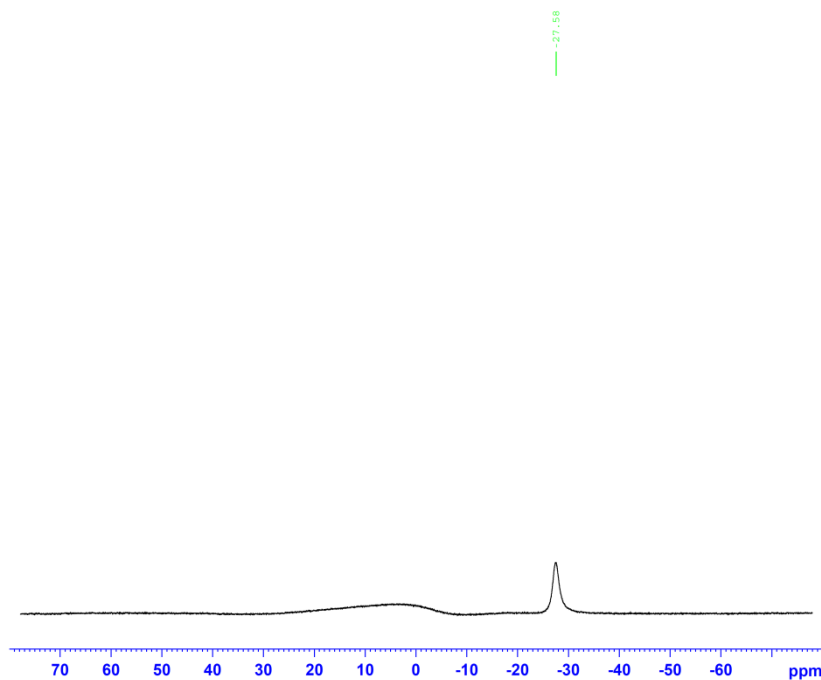
```

NAME      Feb29-2020
EXPNO    5
PROCNO   1
Date_    20200223
Time     2.38
INSTRUM  av400
PROBHD   5 mm PABBO BB-
PULPROG  zgpg30
TD       65536
SOLVENT  DMSO
NS       2048
DS       2
SWH      24038.461 Hz
FIDRES   0.366798 Hz
AQ       1.3631988 sec
RG       128
DW       20.800 usec
DE       6.50 usec
TE       299.7 K
D1       2.00000000 sec
D11      0.03000000 sec
TDO      1

===== CHANNEL f1 =====
NUC1     13C
P1       9.00 usec
PL1      -3.00 dB
PL1W     73.17333984 W
SFO1     100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2  waltz16
NUC2     1H
FCPD2    80.00 usec
PL2      -1.70 dB
PL12     13.80 dB
PL13     13.80 dB
PL2W     14.48987389 W
PL12W    0.40838012 W
PL13W    0.40838012 W
SFO2     400.1316005 MHz
SI       32768
SF       100.6127696 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       0.30
    
```

4-HOPhBH2PPhEt2



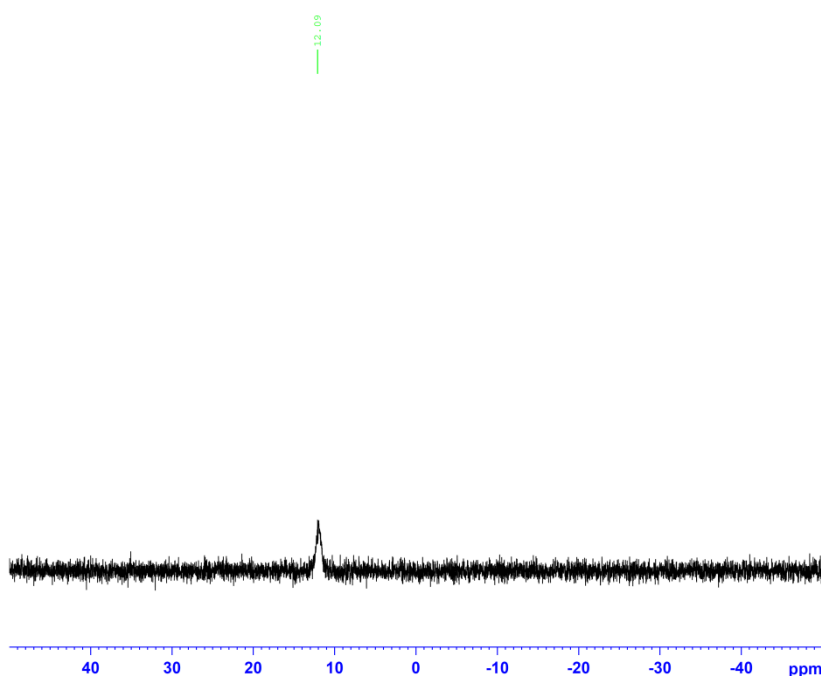
### IBB-nmr Analysis

```
NAME Feb29-2020
EXPNO 4
PROCNO 1
Date_ 20200229
Time 0.36
INSTRUM av400
PROBHD 5 mm PABBO BB-
PULPROG zgpg
TD 32768
SOLVENT DMSO
NS 256
DS 4
SWH 20000.000 Hz
FIDRES 0.610352 Hz
AQ 0.8192500 sec
RG 203
DW 25.000 usec
DE 20.00 usec
TE 299.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 11B
P1 6.30 usec
PL1 -2.00 dB
SFO1 128.3776050 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -1.70 dB
PL12 13.80 dB
PL2W 14.48987389 W
PL12W 0.40838012 W
SFO2 400.1316005 MHz
SI 32768
SF 128.3776180 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40
```

4HOPhBH2PEt2Ph

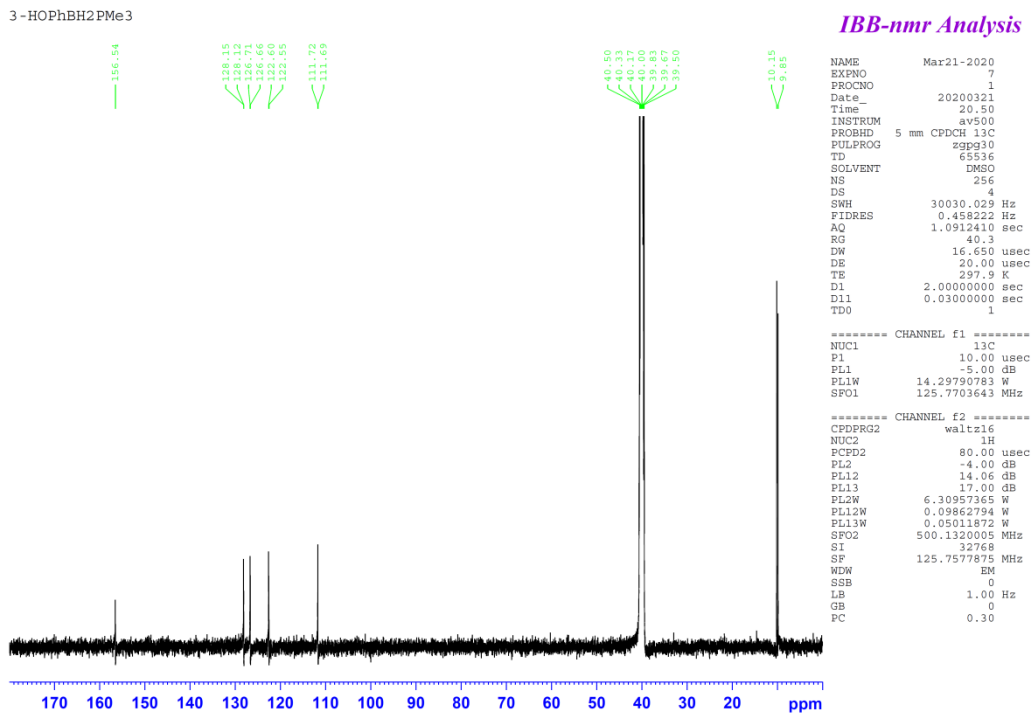
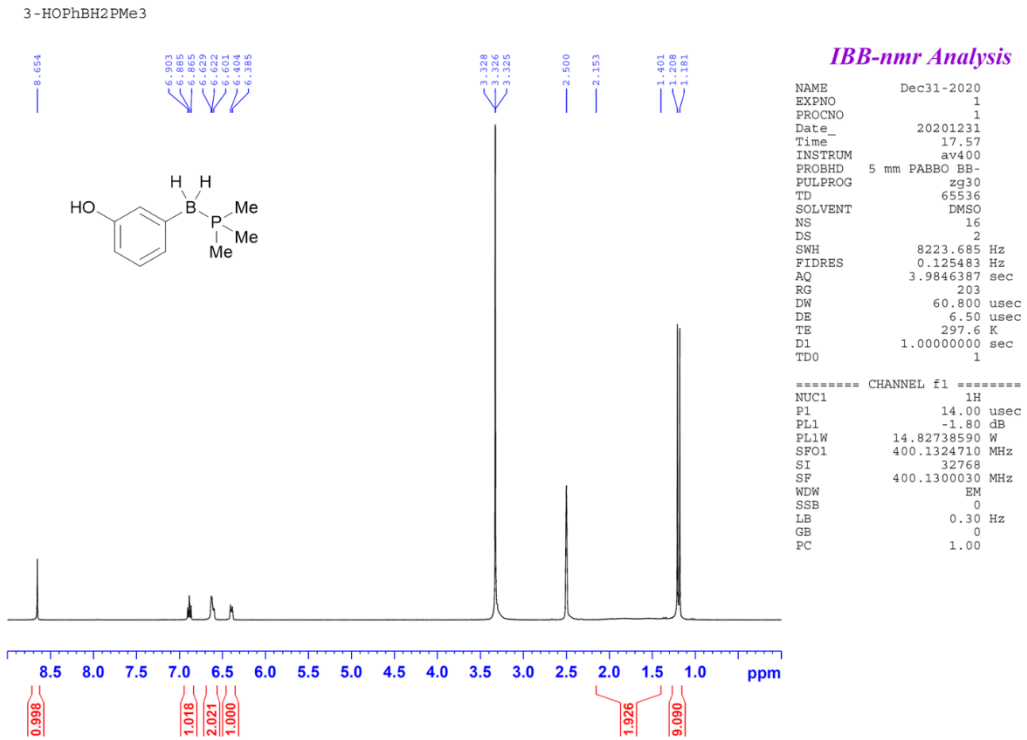


### IBB-nmr Analysis

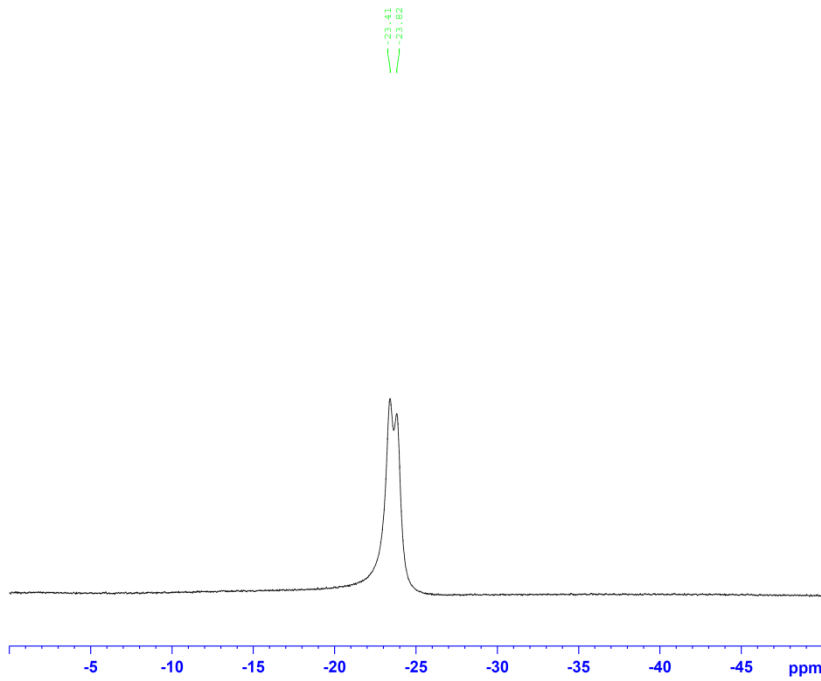
```
NAME Feb29-2020
EXPNO 2
PROCNO 1
Date_ 20200229
Time 0.01
INSTRUM av400
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 8
DS 4
SWH 64102.563 Hz
FIDRES 0.978127 Hz
AQ 0.5112308 sec
RG 203
DW 7.800 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 31P
P1 10.00 usec
PL1 -0.70 dB
PL1W 30.10233498 W
SFO1 161.9674942 MHz
SI 32768
SF 161.9754962 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
```

**B-(3-Hydroxyphenyl) trimethylphosphine borane (11)**



3HOPhBH2PMe3



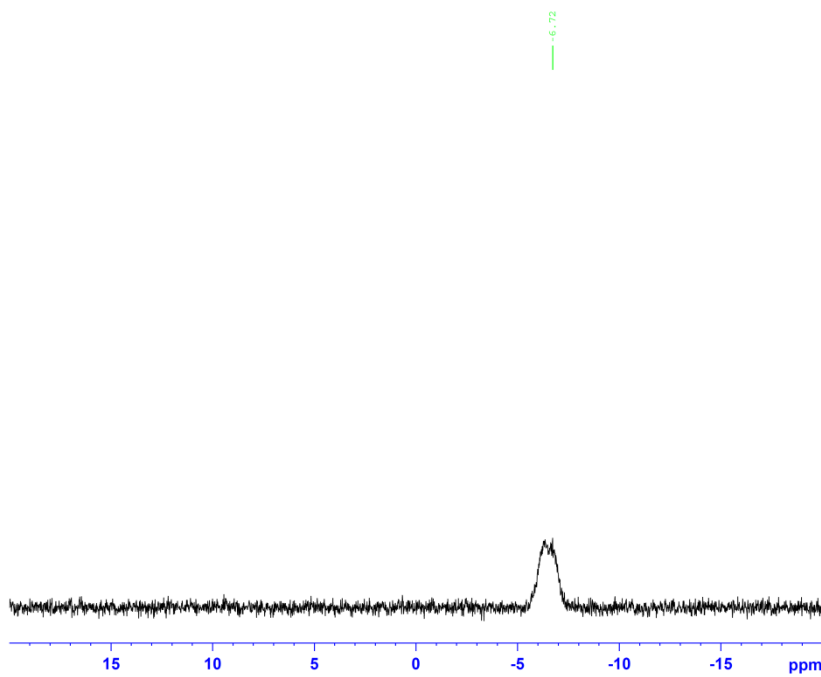
### IBB-nmr Analysis

```
NAME Mar21-2020
EXPNO 6
PROCNO 1
Date_ 20200321
Time 20.38
INSTRUM av400
PROBHD 5 mm PABBO BB-
PULPROG zgpg
TD 32768
SOLVENT DMSO
NS 256
DS 4
SWH 20000.000 Hz
FIDRES 0.610352 Hz
AQ 0.8192500 sec
RG 203
DW 25.000 usec
DE 20.00 usec
TE 299.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 11B
P1 6.30 usec
PL1 -2.00 dB
SFO1 128.3776050 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -1.70 dB
PL12 13.80 dB
PL2W 14.48987389 W
PL12W 0.40838012 W
SFO2 400.1316005 MHz
SI 32768
SF 128.3776183 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40
```

3HOPhBH2PMe3



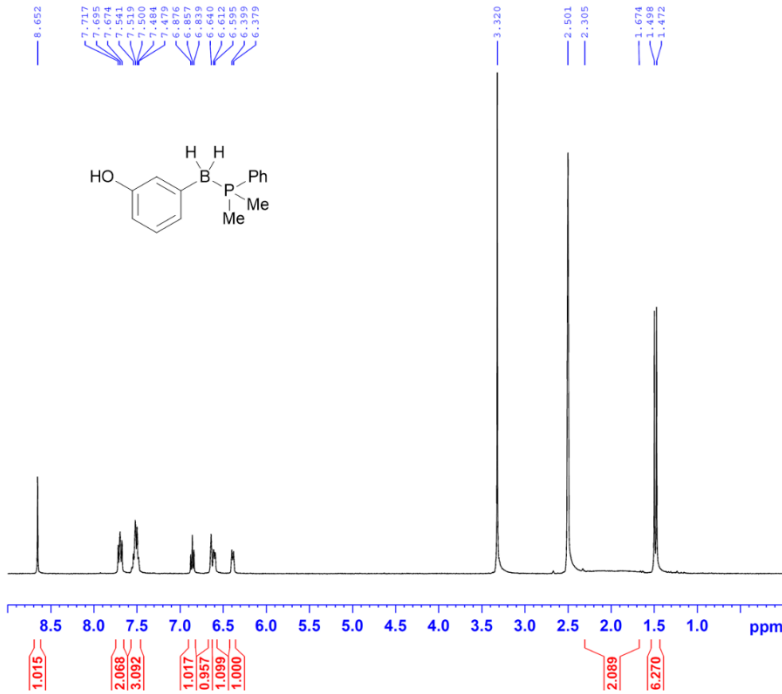
### IBB-nmr Analysis

```
NAME Mar21-2020
EXPNO 5
PROCNO 1
Date_ 20200321
Time 20.26
INSTRUM av400
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 4
SWH 64102.563 Hz
FIDRES 0.978127 Hz
AQ 0.5112308 sec
RG 203
DW 7.800 usec
DE 6.50 usec
TE 298.4 K
D1 2.00000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 31P
P1 10.00 usec
PL1 -0.70 dB
PL1W 30.10233498 W
SFO1 161.9674942 MHz
SI 32768
SF 161.9754962 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
```

### B-(3-Hydroxyphenyl) dimethylphenylphosphine borane (12)

3-HOPhBH2PPhMe2 redried



#### IBB-nmr Analysis

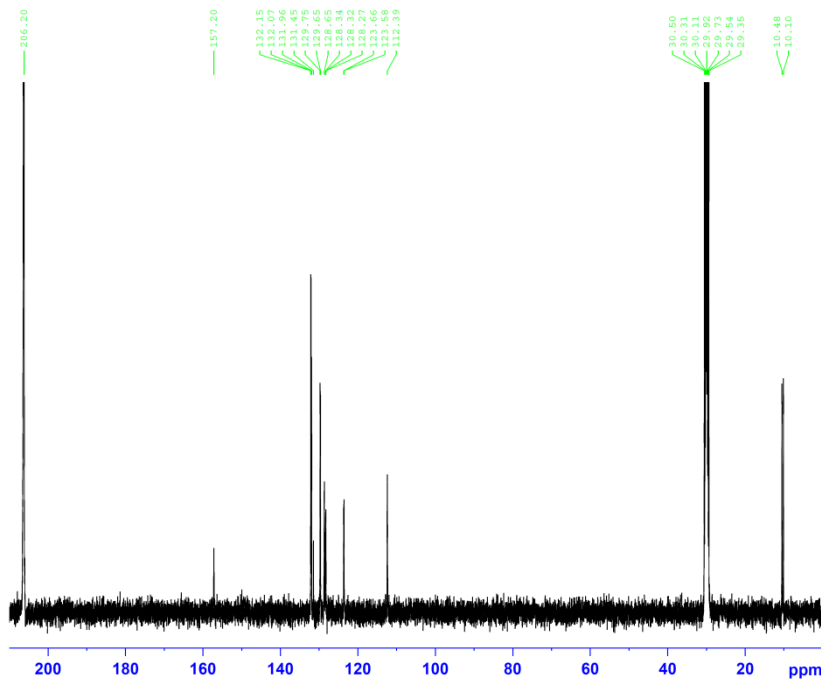
```

NAME      Dec27-2020
EXPNO     1
PROCNO    1
Date_     20201227
Time      18.36
INSTRUM   av400
PROBHD    5 mm PABBO BB-
PULPROG   zg30
TD         65536
SOLVENT   DMSO
NS         16
DS         2
SWH        8223.685 Hz
FIDRES     0.125483 Hz
AQ         3.9846387 sec
RG         203
DW         60.800 usec
DE         6.50 usec
TE         297.9 K
D1         1.00000000 sec
TD0        1
  
```

```

===== CHANNEL f1 =====
NUC1      1H
P1        14.00 usec
PL1       -1.80 dB
PL1W      14.82738590 W
SF01      400.1324710 MHz
SI        32768
SF        400.1300025 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB        0
PC        1.00
  
```

3HOPhBH2PPhMe2



#### IBB-nmr Analysis

```

NAME      Feb23-2020
EXPNO     4
PROCNO    1
Date_     20200223
Time      19.35
INSTRUM   av400
PROBHD    5 mm PABBO BB-
PULPROG   zgpg30
TD         65536
SOLVENT   Acetone
NS         1024
DS         2
SWH        24038.461 Hz
FIDRES     0.366798 Hz
AQ         1.3631988 sec
RG         128
DW         20.800 usec
DE         6.50 usec
TE         299.6 K
D1         2.00000000 sec
D11       0.03000000 sec
TD0        1
  
```

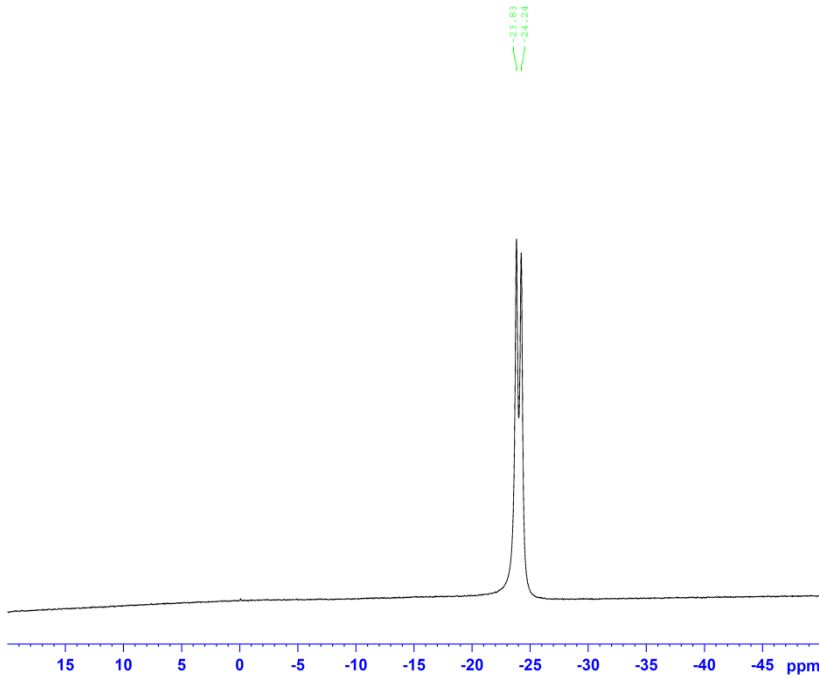
```

===== CHANNEL f1 =====
NUC1      13C
P1        9.00 usec
PL1       -3.00 dB
PL1W      73.17333984 W
SF01      100.6228298 MHz
  
```

```

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2      1H
FPCPD2    80.00 usec
PL2       -1.70 dB
PL12      13.80 dB
PL13      13.80 dB
PL2W      14.48987389 W
PL12W     0.40838012 W
PL13W     0.40838012 W
SF02      400.1316005 MHz
SI        32768
SF        100.6126687 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        0.30
  
```

3-HOPhBH2PMe2Ph



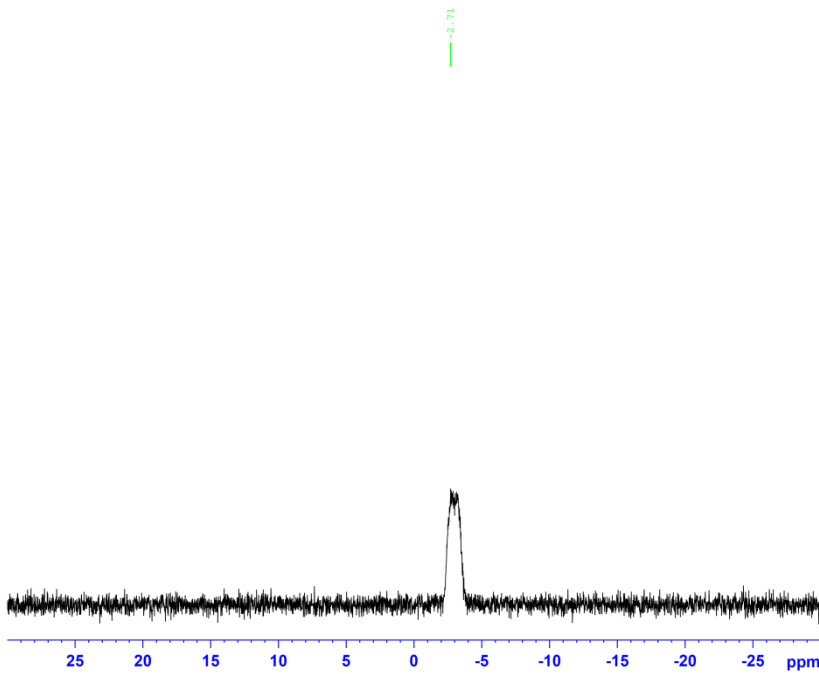
**IBB-nmr Analysis**

```
NAME Feb23-2020
EXPNO 7
PROCNO 1
Date_ 20200223
Time 20.03
INSTRUM av400
PROBHD 5 mm PABBO BB-
PULPROG zgpg
TD 32768
SOLVENT Acetone
NS 128
DS 4
SWH 20000.000 Hz
FIDRES 0.610352 Hz
AQ 0.8192500 sec
RG 203
DW 25.000 usec
DE 20.00 usec
TE 299.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 11B
P1 6.30 usec
PL1 -2.00 dB
SFO1 128.3776050 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -1.70 dB
PL12 13.80 dB
PL2W 14.48987389 W
PL12W 0.40838012 W
SFO2 400.1316005 MHz
SI 32768
SF 128.3776179 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40
```

3HOPhBH2PPhMe2



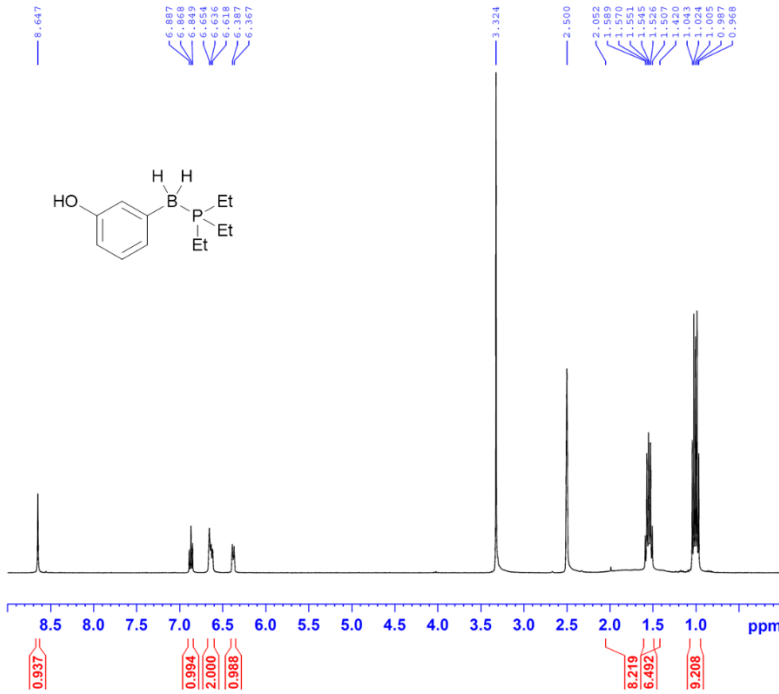
**IBB-nmr Analysis**

```
NAME Feb23-2020
EXPNO 5
PROCNO 1
Date_ 20200223
Time 19.39
INSTRUM av400
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT Acetone
NS 8
DS 4
SWH 64102.563 Hz
FIDRES 0.978127 Hz
AQ 0.5112308 sec
RG 203
DW 7.800 usec
DE 6.50 usec
TE 298.9 K
D1 2.00000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 31P
P1 10.00 usec
PL1 -0.70 dB
PL1W 30.10233498 W
SFO1 161.9674942 MHz
SI 32768
SF 161.9754962 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
```

**B-(3-Hydroxyphenyl) triethylphosphine borane (13)**

3-HOPhBH2PEt3 5-20Fr



**IBB-nmr Analysis**

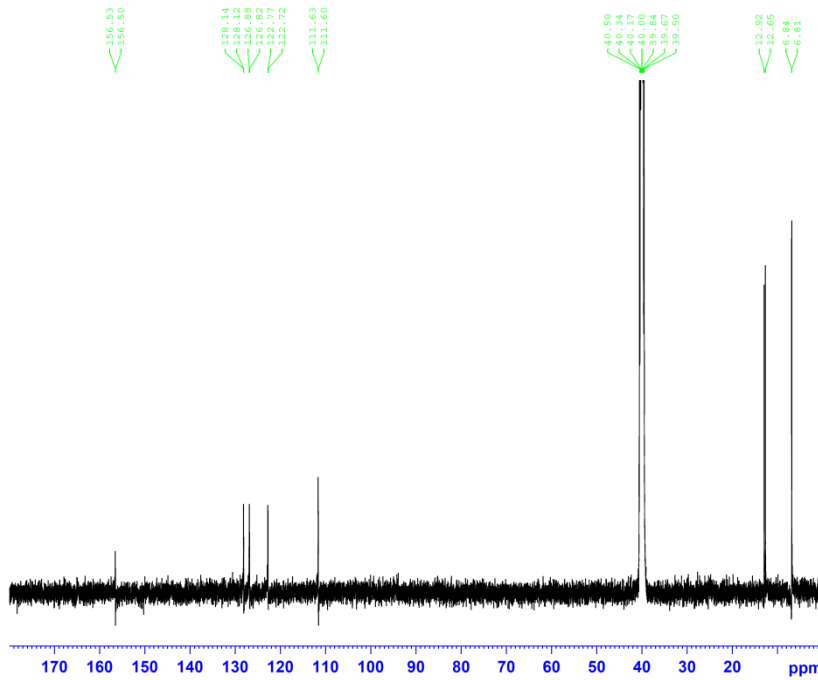
```

NAME      Dec6-2020
EXPNO     3
PROCNO    1
Date_     20201206
Time      20.35
INSTRUM   av400
PROBHD    5 mm PABBO BB-
PULPROG   zg30
TD         65536
SOLVENT   DMSO
NS         16
DS         2
SWH        8223.685 Hz
FIDRES     0.125483 Hz
AQ         3.9846387 sec
RG         203
DW         60.800 usec
DE         6.50 usec
TE         297.8 K
D1         1.0000000 sec
TD0        1
    
```

```

----- CHANNEL f1 -----
NUC1      1H
P1         14.00 usec
PL1        -1.80 dB
PL1W      14.82738590 W
SFO1      400.1324710 MHz
SI         32768
SF         400.1300031 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
    
```

3-HOPhBH2PEt3 5-20Fr



**IBB-nmr Analysis**

```

NAME      Dec6-2020
EXPNO     2
PROCNO    1
Date_     20201206
Time      16.05
INSTRUM   av500
PROBHD    5 mm CPBCH 13C
PULPROG   zgpg30
TD         65536
SOLVENT   DMSO
NS         64
DS         4
SWH        30030.029 Hz
FIDRES     0.458222 Hz
AQ         1.0912410 sec
RG         90.5
DW         16.650 usec
DE         20.00 usec
TE         298.0 K
D1         2.0000000 sec
D11        0.0300000 sec
TD0        1
    
```

```

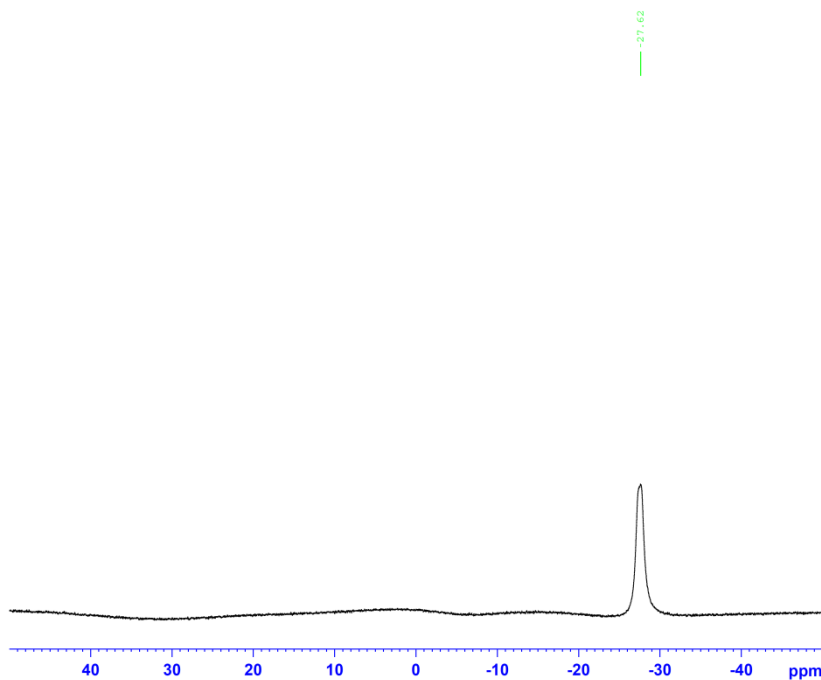
----- CHANNEL f1 -----
NUC1      13C
P1         10.00 usec
PL1         -5.00 dB
PL1W      14.29790783 W
SFO1      125.7703643 MHz
    
```

```

----- CHANNEL f2 -----
CPDPRG2   waltz16
NUC2      1H
FPCPD2    80.00 usec
PL2        -4.00 dB
PL12      14.06 dB
PL13      17.00 dB
PL2W      6.30957365 W
PL12W     0.09862794 W
PL13W     0.05011872 W
SFO2      500.1320005 MHz
SI         32768
SF         125.7577866 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         0.30
    
```



3-HOPhBH2PEt3 5-20Fr



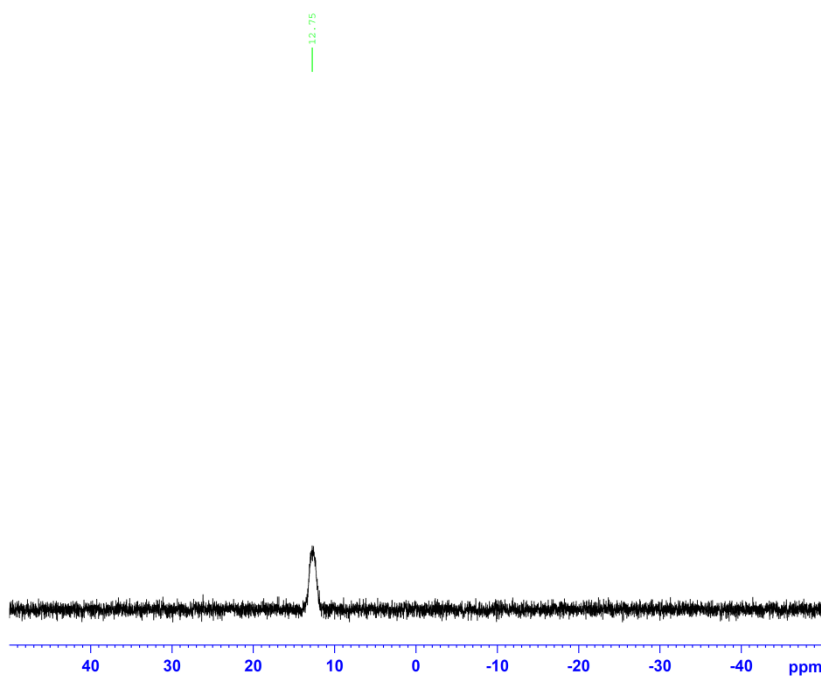
### IBB-nmr Analysis

```
NAME      Dec5-2020
EXPNO     2
PROCNO    1
Date_     20201205
Time      22.26
INSTRUM   av400
PROBHD    5 mm PABBO BB-
PULPROG   zgpg
TD         32768
SOLVENT   DMSO
NS         512
DS         4
SWH        20000.000 Hz
FIDRES     0.610352 Hz
AQ         0.8192500 sec
RG         203
DW         25.000 usec
DE         20.00 usec
TE         298.4 K
D1         1.00000000 sec
D11        0.03000000 sec
TDO        1

===== CHANNEL f1 =====
NUC1       11B
P1         6.30 usec
PL1        -2.00 dB
SFO1       128.3776050 MHz

===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2        1H
PCPD2       80.00 usec
PL2         -1.70 dB
PL12        13.80 dB
PL2W        14.48987389 W
PL12W       0.40838012 W
SFO2        400.1316005 MHz
SI          32768
SF          128.3776183 MHz
WDW         EM
SSB         0
LB          2.00 Hz
GB          0
PC          1.40
```

3-HOPhBH2PEt3 5-20Fr



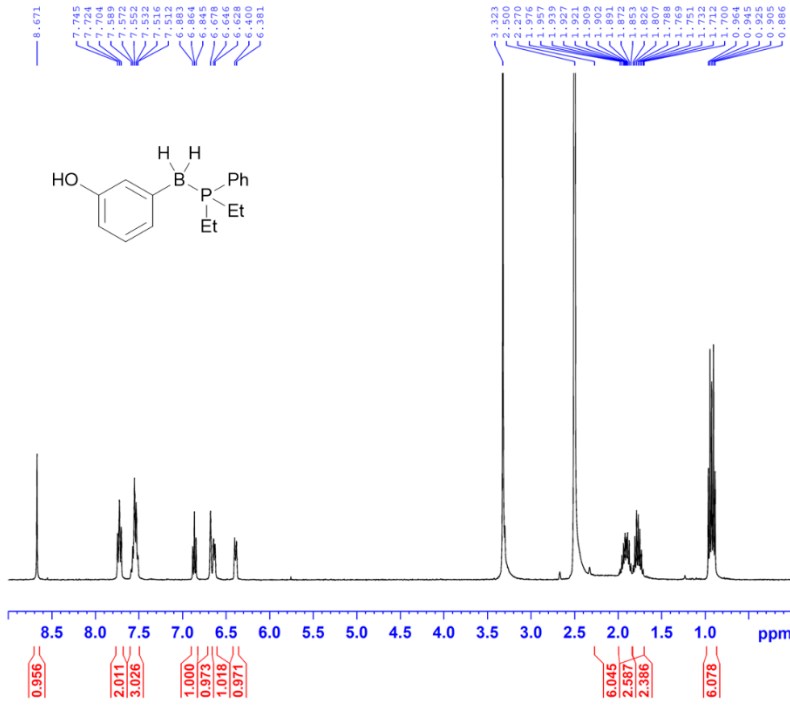
### IBB-nmr Analysis

```
NAME      Dec5-2020
EXPNO     5
PROCNO    1
Date_     20201205
Time      22.46
INSTRUM   av400
PROBHD    5 mm PABBO BB-
PULPROG   zg30
TD         65536
SOLVENT   DMSO
NS         64
DS         4
SWH        64102.563 Hz
FIDRES     0.978127 Hz
AQ         0.5112308 sec
RG         203
DW         7.800 usec
DE         6.50 usec
TE         297.7 K
D1         2.00000000 sec
TDO        1

===== CHANNEL f1 =====
NUC1       31P
P1         10.00 usec
PL1        -0.70 dB
PL1W       30.10233498 W
SFO1       161.9674942 MHz
SI          32768
SF         161.9754962 MHz
WDW         EM
SSB         0
LB          1.00 Hz
GB          0
PC          1.40
```

**B-(3-Hydroxyphenyl) diethylphenylphosphine borane (14)**

3-HOPhBH2PEt2Ph redried



**IBB-nmr Analysis**

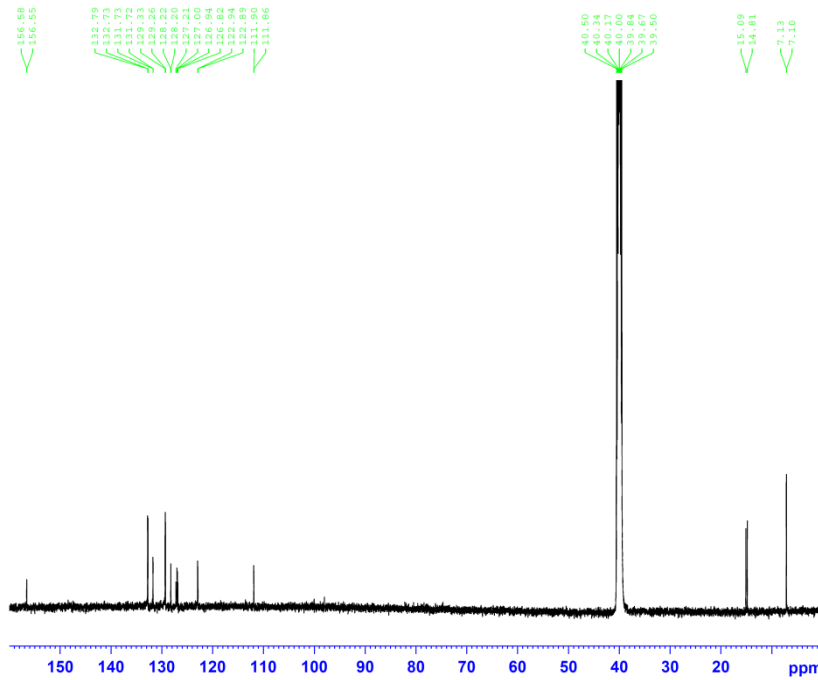
```

NAME      Jan2-2021
EXPNO     1
PROCNO    1
Date_     20210102
Time      15.13
INSTRUM   av400
PROBHD    5 mm FAPBO BB-
PULPROG   zg30
TD         65536
SOLVENT   DMSO
NS         16
DS         2
SWH        8223.685 Hz
FIDRES     0.125483 Hz
AQ         3.9846387 sec
RG         203
DW         60.800 usec
DE         6.500 usec
TE         297.7 K
D1         1.00000000 sec
TDO        1
    
```

```

===== CHANNEL f1 =====
NUC1      1H
P1        14.00 usec
PL1       -1.80 dB
PL1W      14.82738590 W
SFO1      400.1324710 MHz
SI        32768
SF        400.1300034 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB        0
PC        1.00
    
```

3-HOPhBH2PEt2Ph redried



**IBB-nmr Analysis**

```

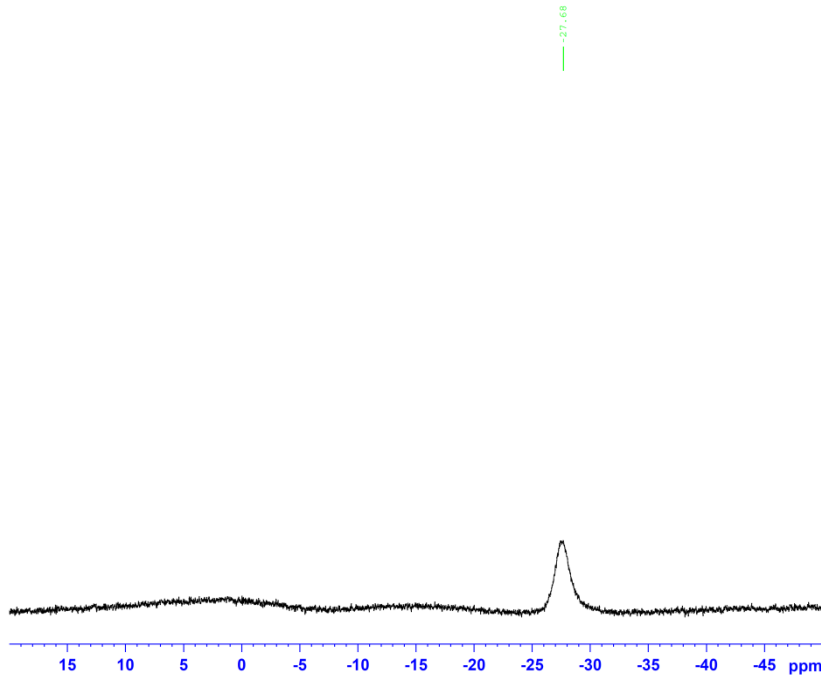
NAME      Jan2-2021
EXPNO     6
PROCNO    1
Date_     20210102
Time      17.08
INSTRUM   av500
PROBHD    5 mm CPDCH 13C
PULPROG   zgpg30
TD         65536
SOLVENT   DMSO
NS         256
DS         4
SWH        30030.029 Hz
FIDRES     0.458222 Hz
AQ         1.0912410 sec
RG         40.3
DW         16.650 usec
DE         20.00 usec
TE         298.0 K
D1         2.00000000 sec
D11        0.03000000 sec
TDO        1
    
```

```

===== CHANNEL f1 =====
NUC1      13C
P1        10.00 usec
PL1       -5.00 dB
PL1W      14.29790783 W
SFO1      125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2      1H
F2CD2     80.00 usec
PL2       -4.00 dB
PL12      14.06 dB
PL13      17.00 dB
PL2W      6.30957365 W
PL12W     0.09862794 W
PL13W     0.05011872 W
SFO2      500.1320005 MHz
SI        32768
SF        125.7577866 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        0.30
    
```

3-HOPhBH2PEt2Ph redried



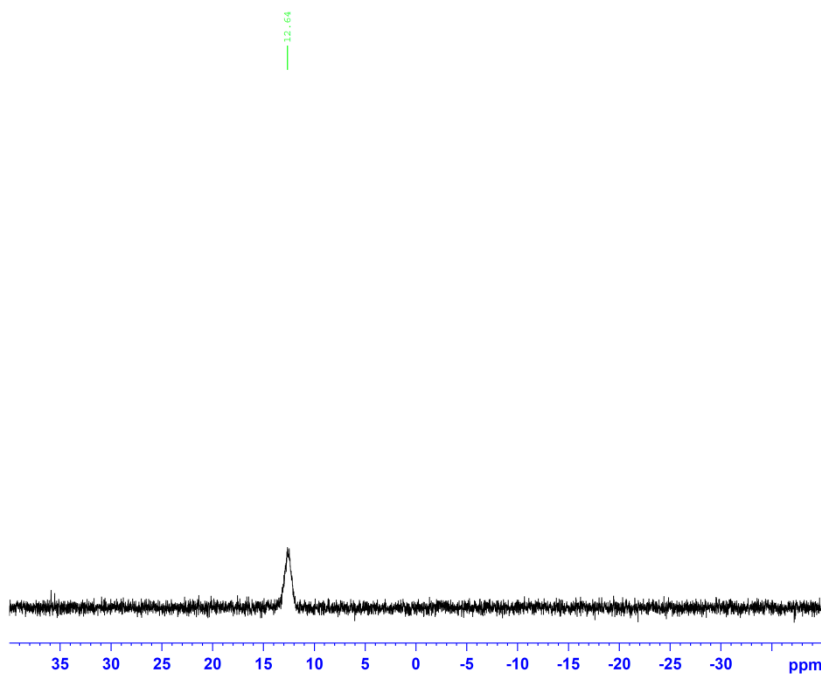
### IBB-nmr Analysis

```
NAME          Jan2-2021
EXPNO         4
PROCNO        1
Date_         20210102
Time         16.38
INSTRUM       av400
PROBHD        5 mm PABBO BB-
PULPROG       zgpg
TD            32768
SOLVENT       DMSO
NS            256
DS            4
SWH           20000.000 Hz
FIDRES        0.610352 Hz
AQ            0.8192500 sec
RG            203
DW            25.000 usec
DE            20.00 usec
TE            298.1 K
D1            1.00000000 sec
D11           0.03000000 sec
TDO           1

===== CHANNEL f1 =====
NUC1          11B
P1            6.30 usec
PL1           -2.00 dB
SFO1         128.3776050 MHz

===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2          1H
PCPD2         80.00 usec
PL2           -1.70 dB
PL12          13.80 dB
PL2W          14.48987389 W
PL12W         0.40838012 W
SFO2         400.1316005 MHz
SI            32768
SF           128.3776183 MHz
WDW           EM
SSB           0
LB            2.00 Hz
GB            0
PC            1.40
```

3-HOPhBH2PEt2Ph



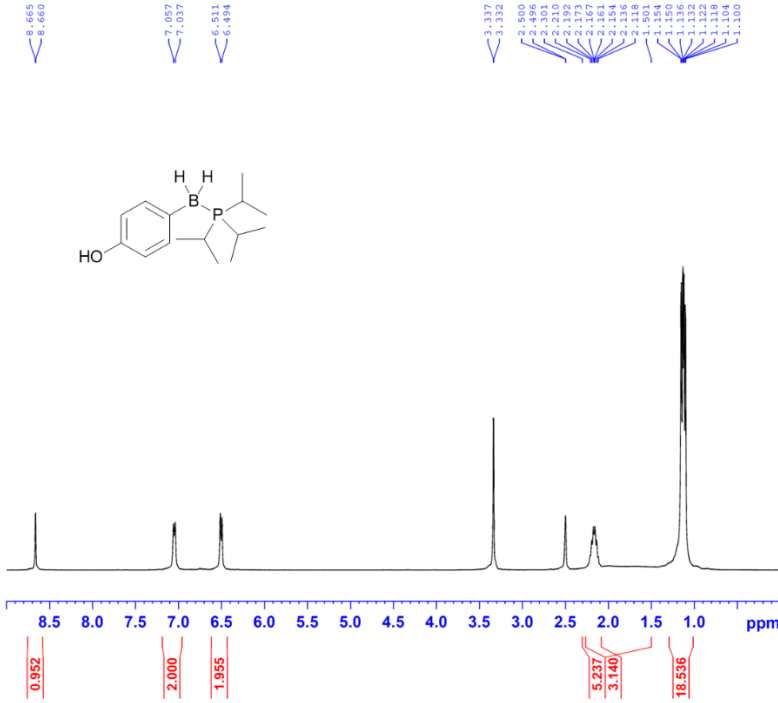
### IBB-nmr Analysis

```
NAME          Jan1-2021
EXPNO         2
PROCNO        1
Date_         20210101
Time         17.17
INSTRUM       av400
PROBHD        5 mm PABBO BB-
PULPROG       zg30
TD            65536
SOLVENT       DMSO
NS            16
DS            4
SWH           64102.563 Hz
FIDRES        0.978127 Hz
AQ            0.5112308 sec
RG            203
DW            7.800 usec
DE            6.50 usec
TE            297.7 K
D1            2.00000000 sec
TDO           1

===== CHANNEL f1 =====
NUC1          31P
P1            10.00 usec
PL1           -0.70 dB
PL1W          30.10233498 W
SFO1         161.9674942 MHz
SI            32768
SF           161.9754962 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
```

**B-(4-Hydroxyphenyl) triisopropylphosphine borane (15)**

4HOPhBH2P(i-Pr)3



**IBB-nmr Analysis**

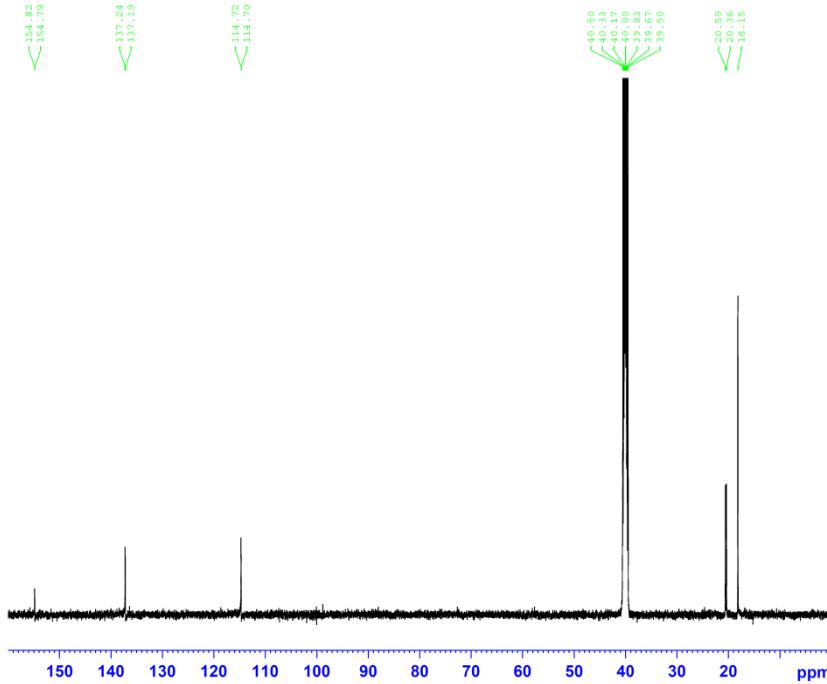
```

NAME      Apr16-2022
EXPNO    1
PROCNO   1
Date_    20220416
Time     22.59
INSTRUM  av400
PROBHD   5 mm PABBO BB-
PULPROG  zg30
TD       65536
SOLVENT  DMSO
NS       16
DS       2
SWH      8223.685 Hz
FIDRES   0.125483 Hz
AQ       3.9846387 sec
RG       128
DW       60.800 usec
DE       6.50 usec
TE       295.8 K
D1       1.00000000 sec
TD0      1
    
```

```

===== CHANNEL f1 =====
NUC1     1H
P1       14.00 usec
PL1      -1.80 dB
PL1W     14.82738590 W
SFO1     400.1324710 MHz
SI       32768
SF       400.1300032 MHz
WDW      EM
SSB      0
LB       0.30 Hz
GB       0
PC       1.00
    
```

4HOPhBH2P(i-Pr)3



**IBB-nmr Analysis**

```

NAME      Nov16-2021
EXPNO    1
PROCNO   1
Date_    20211116
Time     22.32
INSTRUM  av500
PROBHD   5 mm CPDCH 13C
PULPROG  zgpg30
TD       65536
SOLVENT  DMSO
NS       128
DS       4
SWH      30030.029 Hz
FIDRES   0.458222 Hz
AQ       1.0912410 sec
RG       40.3
DW       16.650 usec
DE       20.00 usec
TE       298.1 K
D1       2.00000000 sec
D11     0.03000000 sec
TD0      1
    
```

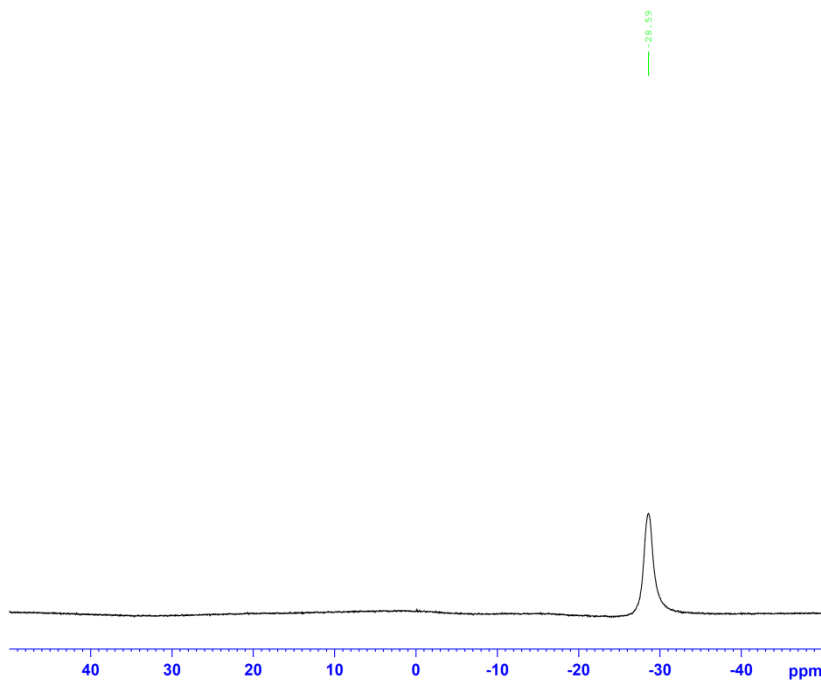
```

===== CHANNEL f1 =====
NUC1     13C
P1       10.00 usec
PL1      -5.00 dB
PL1W     14.29790783 W
SFO1     125.7703643 MHz
    
```

```

===== CHANNEL f2 =====
CPDPRG2  waltz16
NUC2     1H
PCPD2    80.00 usec
PL2      -4.00 dB
PL12     14.06 dB
PL13     17.00 dB
PL2W     6.30957365 W
PL12W    0.09862794 W
PL13W    0.05011872 W
SFO2     500.1320005 MHz
SI       32768
SF       125.7577875 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       0.30
    
```

4HOPhBH2P (i-Pr) 3



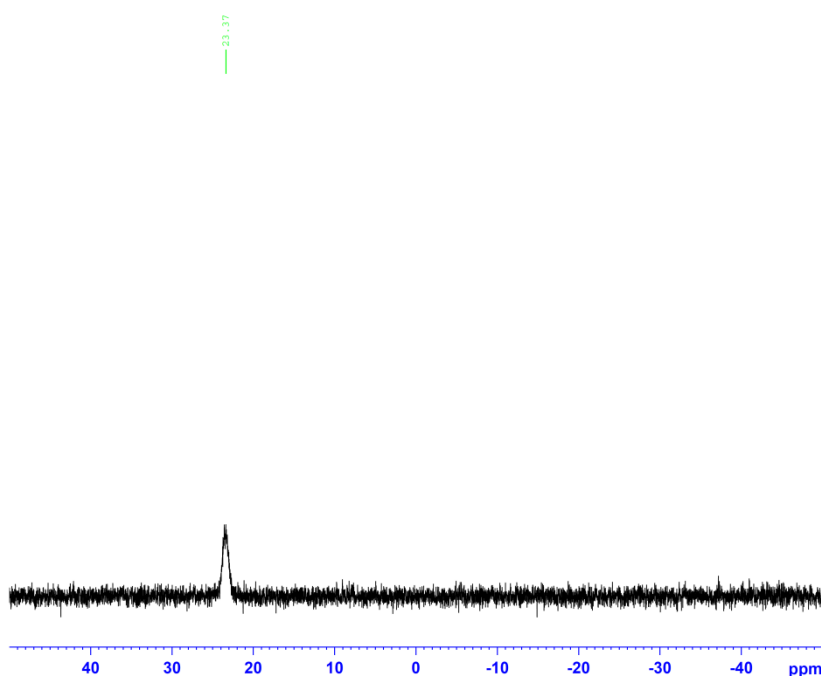
### IBB-nmr Analysis

```
NAME          Dec1-2021
EXPNO         3
PROCNO        1
Date_         20211201
Time_         20.54
INSTRUM       av400
PROBHD        5 mm PABBO BB-
PULPROG       zgpg
TD            32768
SOLVENT       DMSO
NS            256
DS            4
SWH           20000.000 Hz
FIDRES        0.610352 Hz
AQ            0.8192500 sec
RG            203
DW            25.000 usec
DE            20.00 usec
TE            297.3 K
D1            1.00000000 sec
D11           0.03000000 sec
TDO           1

===== CHANNEL f1 =====
NUC1          11B
P1            6.30 usec
PL1           -2.00 dB
SFO1         128.3776050 MHz

===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2          1H
PCPD2         80.00 usec
PL2           -1.70 dB
PL12          13.80 dB
PL2W          14.48987389 W
PL12W         0.40838012 W
SFO2          400.1316005 MHz
SI            32768
SF            128.3776183 MHz
WDW           EM
SSB           0
LB            2.00 Hz
GB            0
PC            1.40
```

4HOPhBH2P (i-Pr) 3



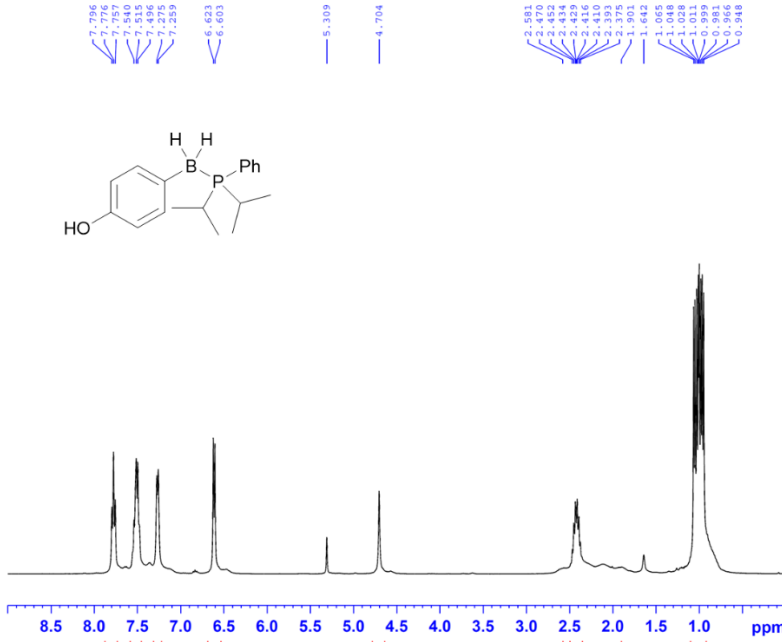
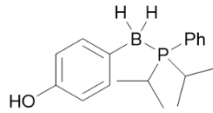
### IBB-nmr Analysis

```
NAME          Dec1-2021
EXPNO         2
PROCNO        1
Date_         20211201
Time_         20.43
INSTRUM       av400
PROBHD        5 mm PABBO BB-
PULPROG       zg30
TD            65536
SOLVENT       DMSO
NS            8
DS            4
SWH           64102.563 Hz
FIDRES        0.978127 Hz
AQ            0.5112308 sec
RG            203
DW            7.800 usec
DE            6.50 usec
TE            296.7 K
D1            2.00000000 sec
TDO           1

===== CHANNEL f1 =====
NUC1          31P
P1            10.00 usec
PL1           -0.70 dB
PL1W          30.10233498 W
SFO1         161.9674942 MHz
SI            32768
SF            161.9754962 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
```

# B-(4-Hydroxyphenyl) diisopropylphenylphosphine borane (16)

4HOPhBH2PPh(i-Pr)2 16-37Fr



## IBB-nmr Analysis

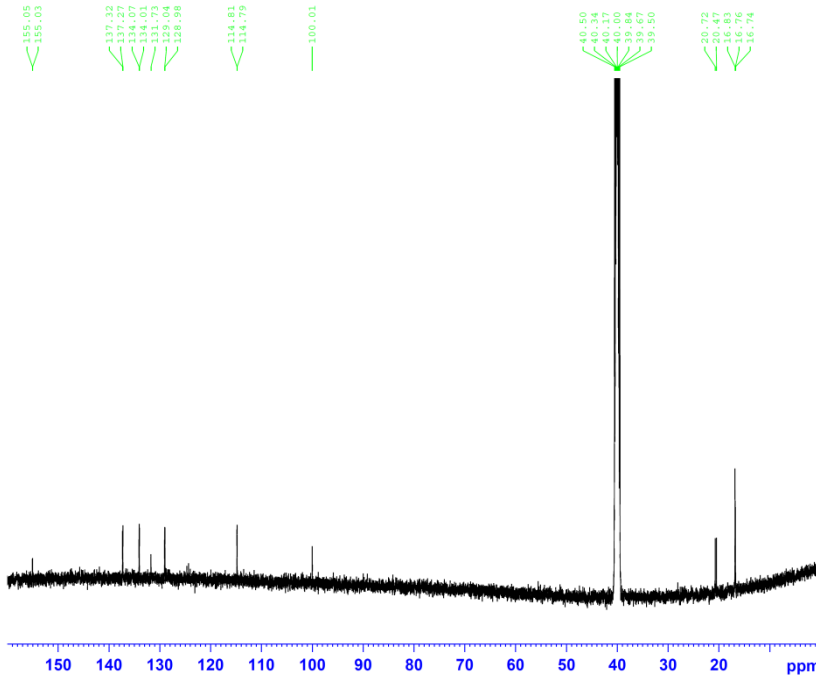
```

NAME      Apr17-2022
EXPNO     7
PROCNO    1
Date_     20220418
Time      0.38
INSTRUM   av400
PROBHD    5 mm PABBO BB-
PULPROG   zg30
TD         65536
SOLVENT   CD2Cl2
NS         16
DS         2
SWH        8223.685 Hz
FIDRES     0.125483 Hz
AQ         3.9846387 sec
RG         128
DW         60.800 usec
DE         6.50 usec
TE         295.8 K
D1         1.00000000 sec
D10        1
    
```

```

===== CHANNEL f1 =====
NUC1      1H
P1        14.00 usec
PL1       -1.80 dB
PL1W      14.82738590 W
SFO1      400.1324710 MHz
SI        32768
SF        400.1300199 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB        0
PC        1.00
    
```

4HOPhBH2PPh(i-Pr)2 16-37Fr



## IBB-nmr Analysis

```

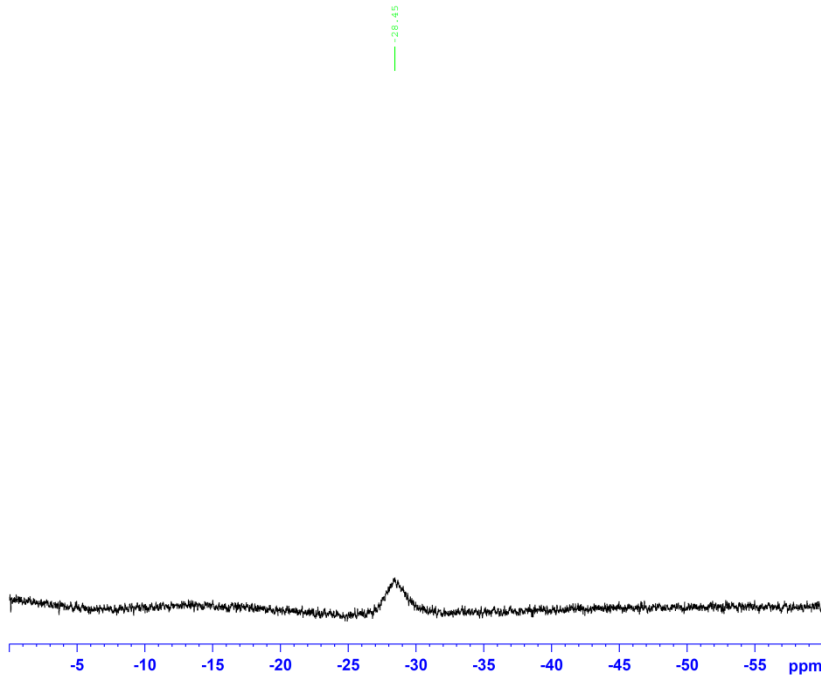
NAME      Apr17-2022
EXPNO     4
PROCNO    1
Date_     20220417
Time      22.03
INSTRUM   av500
PROBHD    5 mm CPDCH 13C
PULPROG   zgpg30
TD         65536
SOLVENT   DMSO
NS         128
DS         4
SWH        30030.029 Hz
FIDRES     0.458222 Hz
AQ         1.0912410 sec
RG         35.9
DW         16.650 usec
DE         20.00 usec
TE         297.9 K
D1         2.00000000 sec
D11        0.03000000 sec
D10        1
    
```

```

===== CHANNEL f1 =====
NUC1      13C
P1        10.00 usec
PL1       -5.00 dB
PL1W      14.29790783 W
SFO1      125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2      1H
FPCPD2    80.00 usec
PL2       -4.00 dB
PL12      14.06 dB
PL13      17.00 dB
PL2W      6.30957365 W
PL12W     0.09862794 W
PL13W     0.05011872 W
SFO2      500.1320005 MHz
SI        32768
SF        125.7577866 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        0.30
    
```

4HOPhBH2PPh(i-Pr)2 16-37Fr



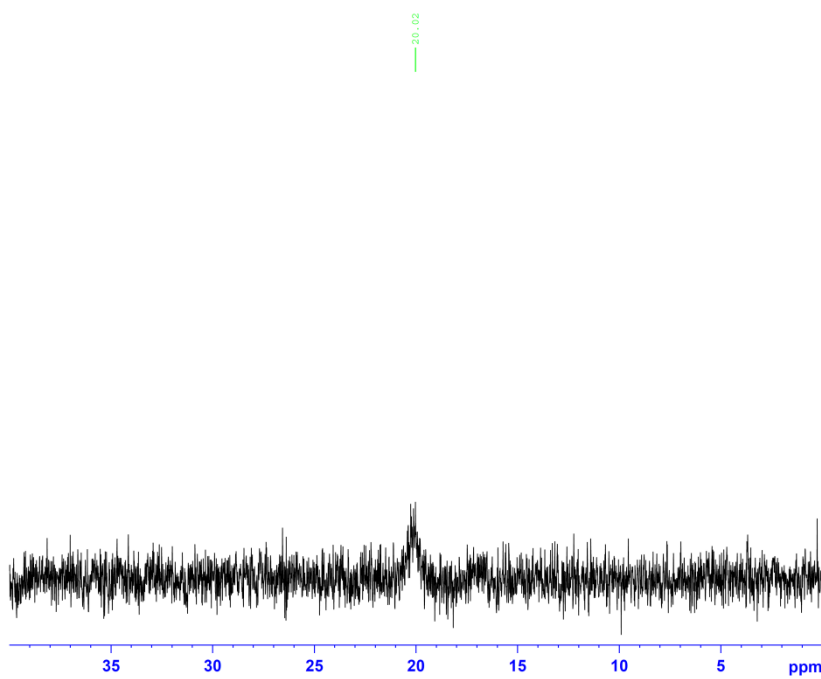
### IBB-nmr Analysis

```
NAME      Apr17-2022
EXPNO     3
PROCNO    1
Date_     20220417
Time      21.44
INSTRUM   av400
PROBHD    5 mm PABBO BB-
PULPROG   zgpg
TD         32768
SOLVENT   DMSO
NS         128
DS         4
SWH        20000.000 Hz
FIDRES     0.610352 Hz
AQ         0.8192500 sec
RG         203
DW         25.000 usec
DE         20.00 usec
TE         296.3 K
D1         1.00000000 sec
D11        0.03000000 sec
TDO        1

===== CHANNEL f1 =====
NUC1      11B
P1         6.30 usec
PL1        -2.00 dB
SFO1      128.3776050 MHz

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2       1H
PCPD2      80.00 usec
PL2         -1.70 dB
PL12       13.80 dB
PL2W       14.48987389 W
PL12W      0.40838012 W
SFO2       400.1316005 MHz
SI         32768
SF         128.3776183 MHz
WDW        EM
SSB         0
LB          2.00 Hz
GB          0
PC          1.40
```

4HOPhBH2PPh(i-Pr)2 16-37Fr

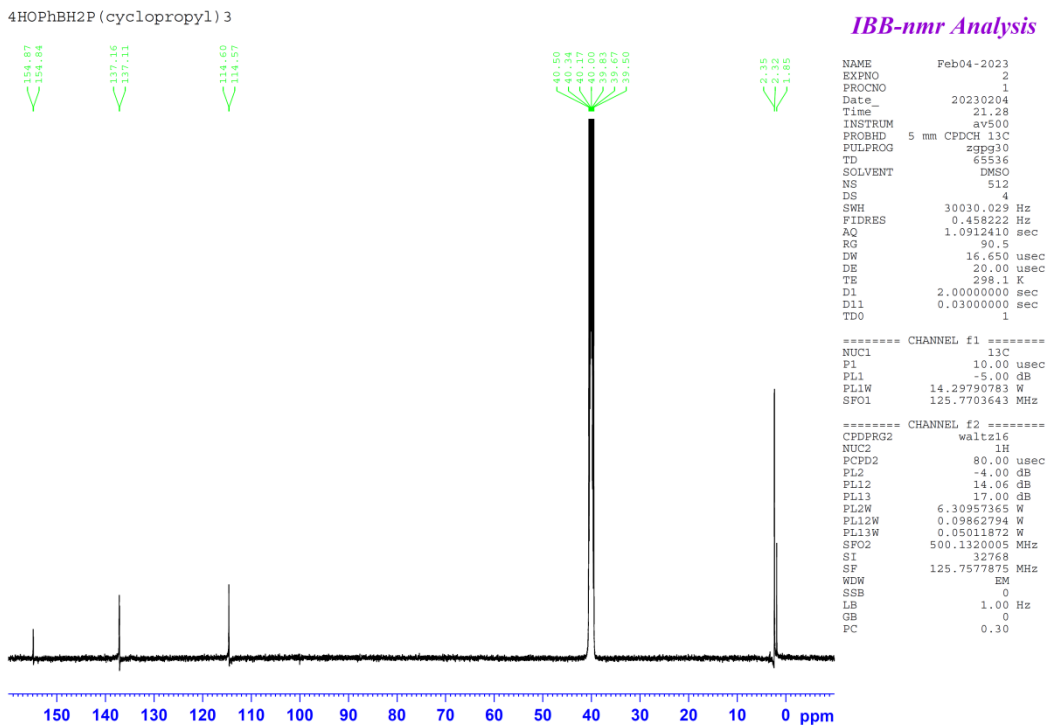
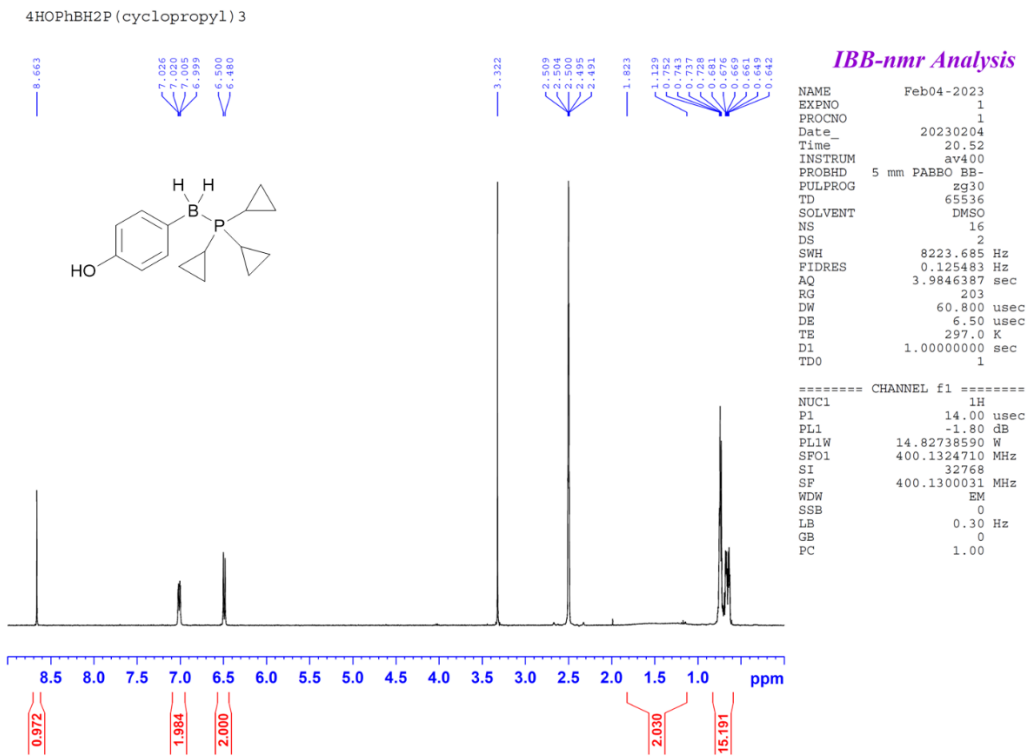


### IBB-nmr Analysis

```
NAME      Apr17-2022
EXPNO     2
PROCNO    1
Date_     20220417
Time      21.37
INSTRUM   av400
PROBHD    5 mm PABBO BB-
PULPROG   zg30
TD         65536
SOLVENT   DMSO
NS         16
DS         4
SWH        64102.563 Hz
FIDRES     0.978127 Hz
AQ         0.5112308 sec
RG         203
DW         7.800 usec
DE         6.50 usec
TE         295.7 K
D1         2.00000000 sec
TDO        1

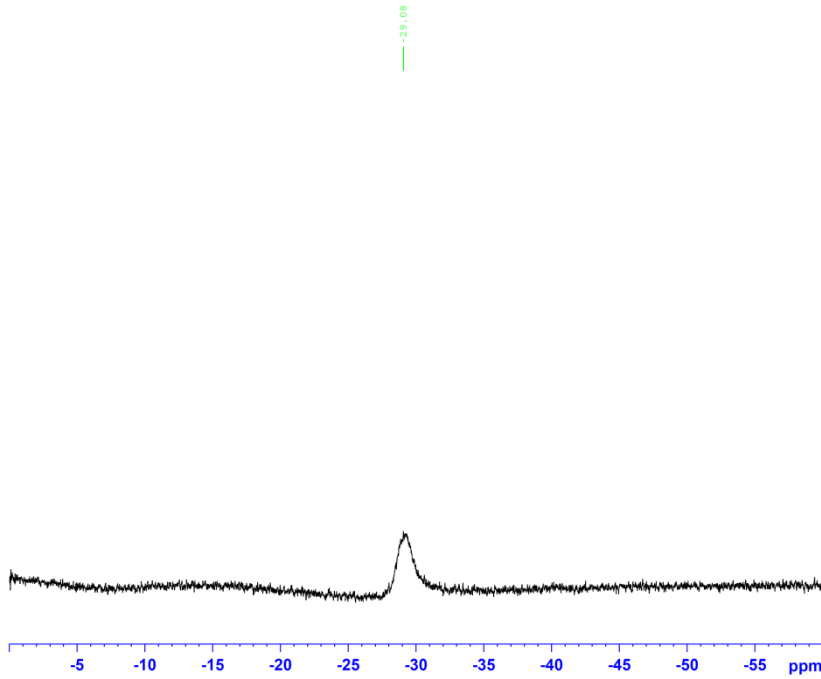
===== CHANNEL f1 =====
NUC1      13C
P1         10.00 usec
PL1         -0.70 dB
PL1W       30.10233498 W
SFO1      161.9674942 MHz
SI         32768
SF         161.9754962 MHz
WDW        EM
SSB         0
LB          1.00 Hz
GB          0
PC          1.40
```

**B-(4-Hydroxyphenyl) tricyclopropylphosphine borane (17)**





4HOPhBH2P (cyclopropyl) 3



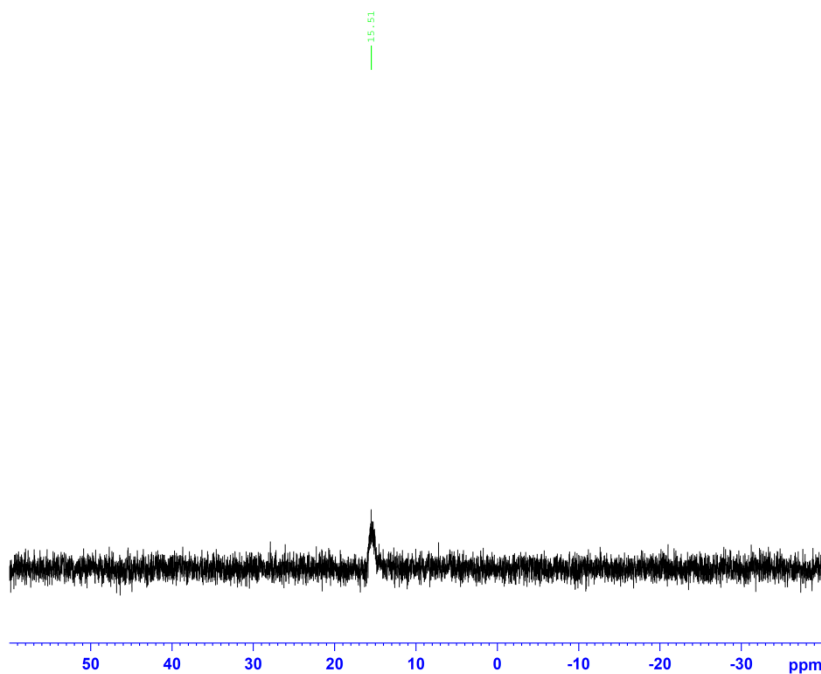
### IBB-nmr Analysis

```
NAME      Feb04-2023
EXPNO     3
PROCNO    1
Date_     20230204
Time      21.55
INSTRUM   av400
PROBHD    5 mm PABBO BB-
PULPROG   zgpg
TD        32768
SOLVENT   DMSO
NS        128
DS        4
SWH       20000.000 Hz
FIDRES    0.610352 Hz
AQ        0.8192500 sec
RG        203
DW        25.000 usec
DE        20.00 usec
TE        297.5 K
D1        1.00000000 sec
D11       0.03000000 sec
TDO       1

===== CHANNEL f1 =====
NUC1      11B
P1        6.30 usec
PL1       -2.00 dB
SFO1     128.3776050 MHz

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2      1H
PCPD2     80.00 usec
PL2       -1.70 dB
PL12     13.80 dB
PL2W     14.48987389 W
PL12W    0.40838012 W
SFO2     400.1316005 MHz
SI        32768
SF        128.3776183 MHz
WDW       EM
SSB       0
LB        2.00 Hz
GB        0
PC        1.40
```

4HOPhBH2P (cyclopropyl) 3

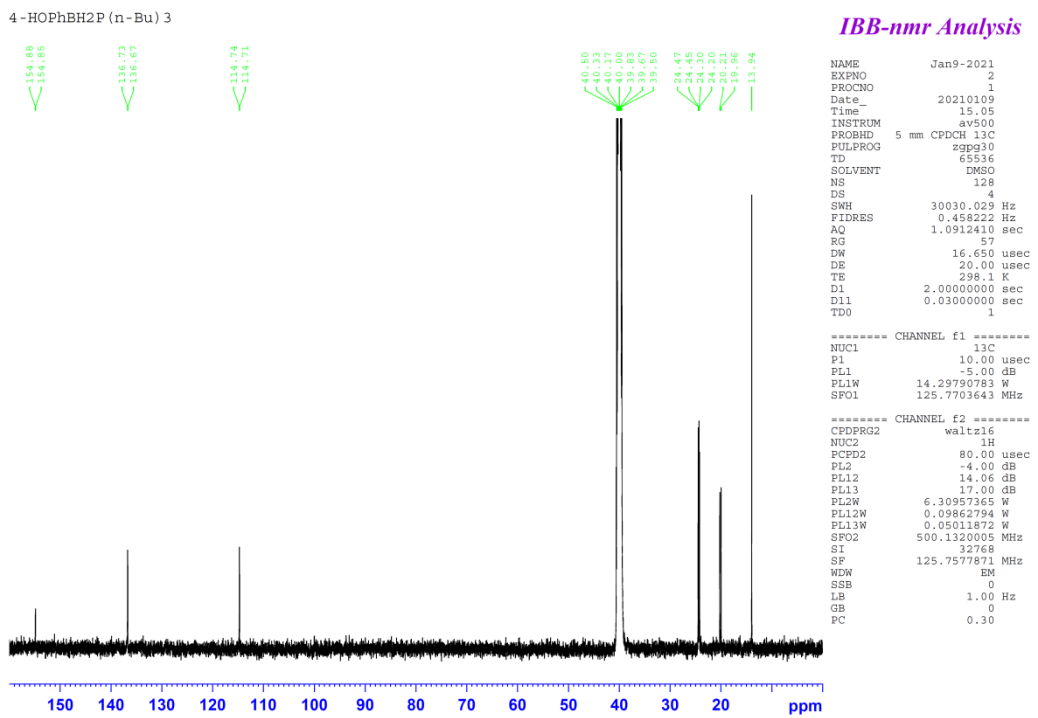
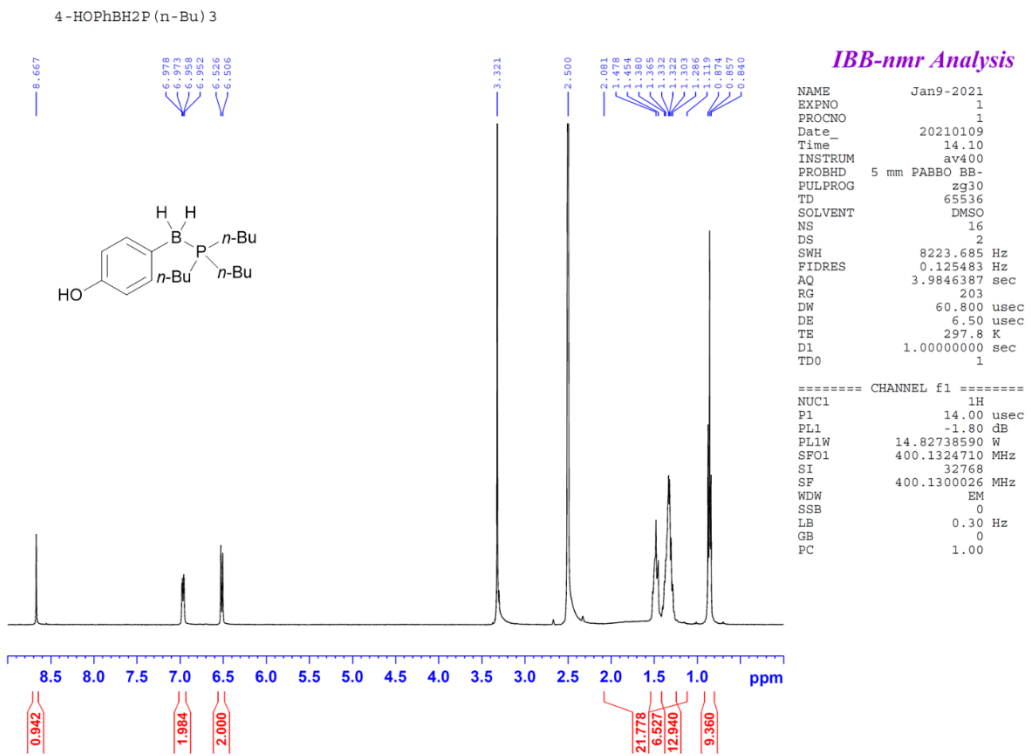


### IBB-nmr Analysis

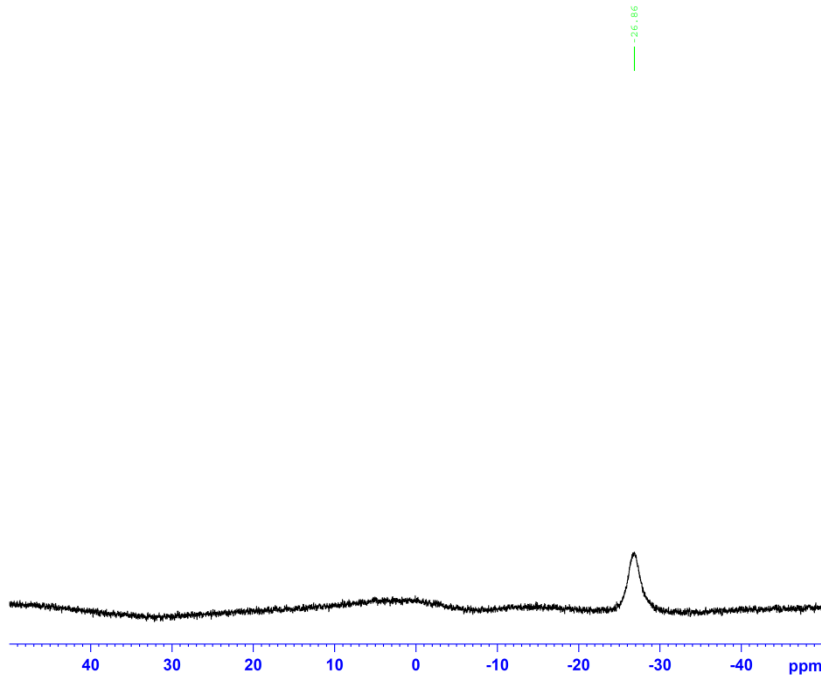
```
NAME      Feb04-2023
EXPNO     4
PROCNO    1
Date_     20230204
Time      22.02
INSTRUM   av400
PROBHD    5 mm PABBO BB-
PULPROG   zg30
TD        65536
SOLVENT   DMSO
NS        64
DS        4
SWH       64102.563 Hz
FIDRES    0.978127 Hz
AQ        0.5112308 sec
RG        203
DW        7.800 usec
DE        6.50 usec
TE        297.0 K
D1        2.00000000 sec
TDO       1

===== CHANNEL f1 =====
NUC1      31P
P1        10.00 usec
PL1       -0.70 dB
PL1W     30.10233498 W
SFO1     161.9674942 MHz
SI        32768
SF        161.9754962 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40
```

# B-(4-Hydroxyphenyl) tributylphosphine borane (18)



4-HOPhBH2P (n-Bu) 3



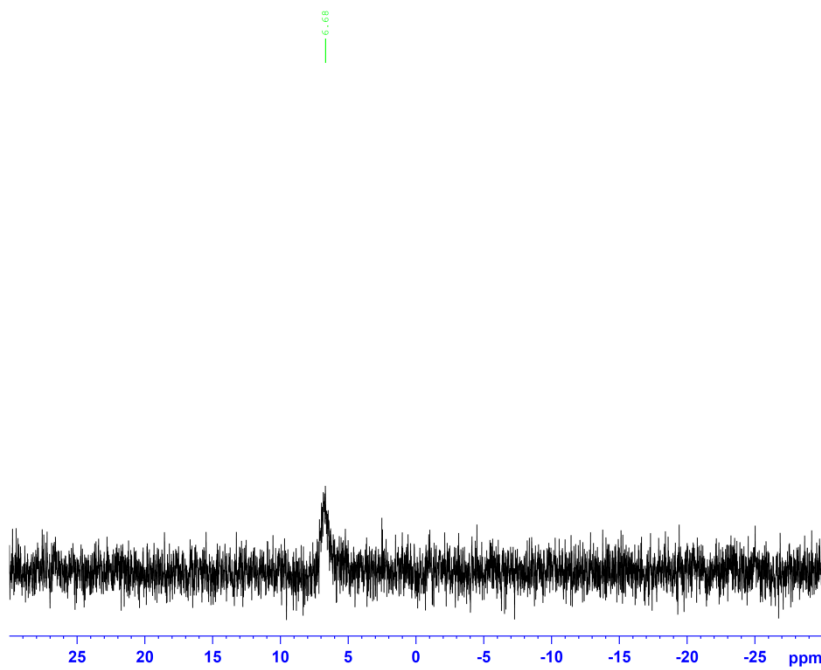
### IBB-nmr Analysis

```
NAME          Jan9-2021
EXPNO         5
PROCNO       1
Date_        20210109
Time         19.26
INSTRUM      av400
PROBHD       5 mm PABBO BB-
PULPROG      zgpg
TD           32768
SOLVENT      DMSO
NS           256
DS           4
SWH          20000.000 Hz
FIDRES       0.610352 Hz
AQ           0.8192500 sec
RG           203
DW           25.000 usec
DE           20.00 usec
TE           300.0 K
D1           1.00000000 sec
D11          0.03000000 sec
TDO          1

===== CHANNEL f1 =====
NUC1         11B
P1           6.30 usec
PL1          -2.00 dB
SFO1        128.3776050 MHz

===== CHANNEL f2 =====
CPDPRG2      waltz16
NUC2         1H
PCPD2        80.00 usec
PL2          -1.70 dB
PL12         13.80 dB
PL2W         14.48987389 W
PL12W        0.40838012 W
SFO2         400.1316005 MHz
SI           32768
SF           128.3776183 MHz
WDW          EM
SSB          0
LB           2.00 Hz
GB           0
PC           1.40
```

4-HOPhBH2P (n-Bu) 3

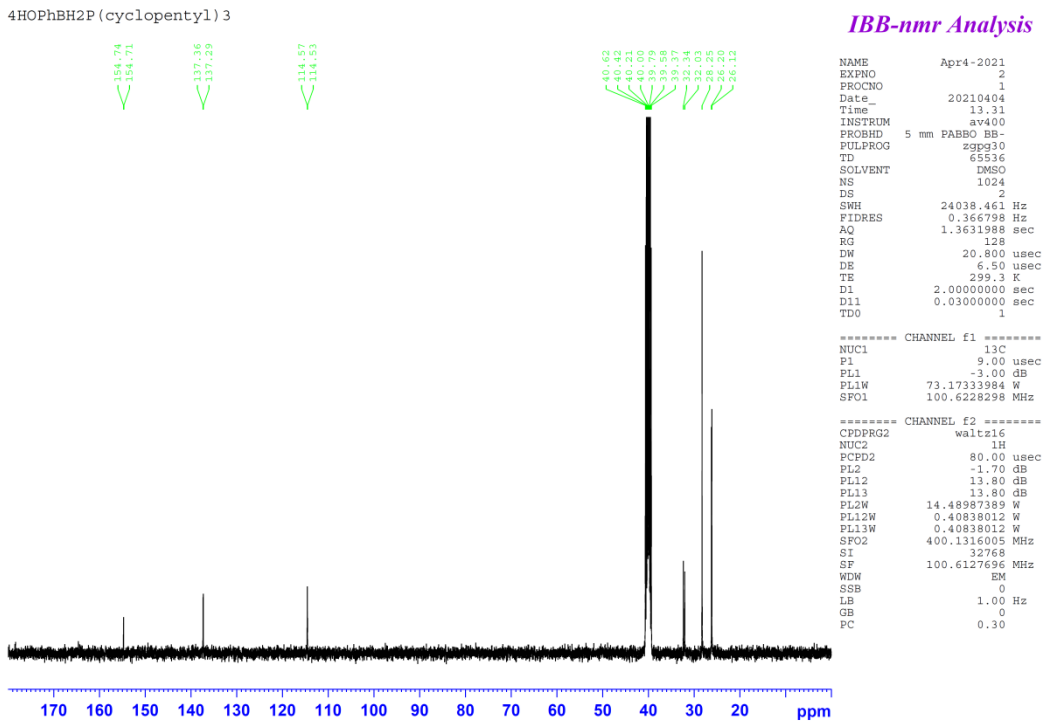
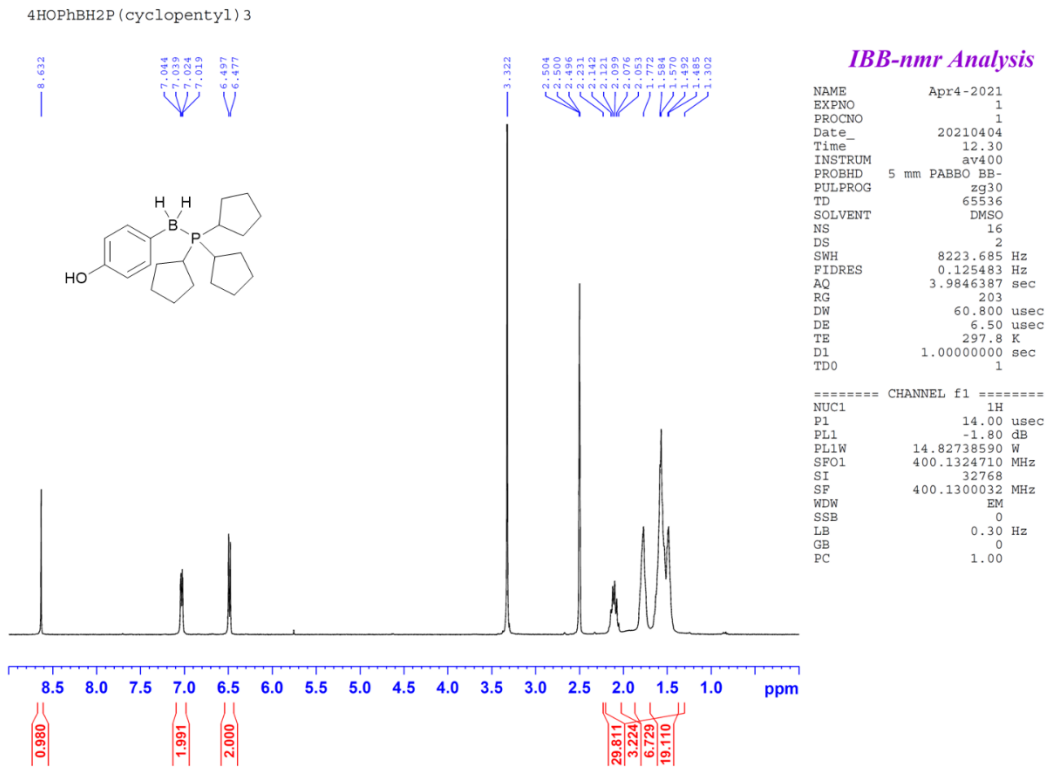


### IBB-nmr Analysis

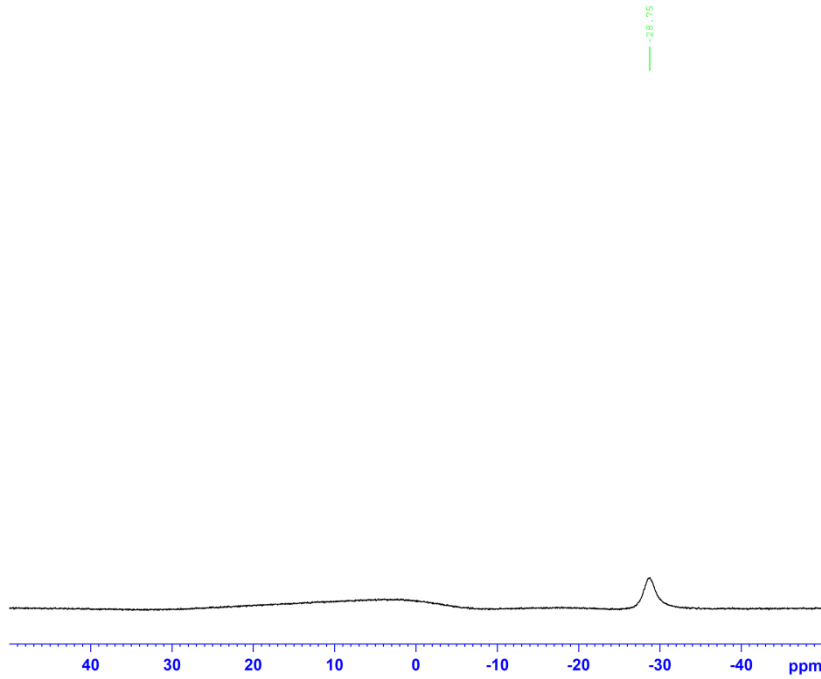
```
NAME          Jan9-2021
EXPNO         4
PROCNO       1
Date_        20210109
Time         19.13
INSTRUM      av400
PROBHD       5 mm PABBO BB-
PULPROG      zg30
TD           65536
SOLVENT      DMSO
NS           16
DS           4
SWH          64102.563 Hz
FIDRES       0.978127 Hz
AQ           0.5112308 sec
RG           203
DW           7.800 usec
DE           6.50 usec
TE           299.4 K
D1           2.00000000 sec
TDO          1

===== CHANNEL f1 =====
NUC1         31P
P1           10.00 usec
PL1          -0.70 dB
PL1W         30.10233498 W
SFO1        161.9674942 MHz
SI           32768
SF           161.9754962 MHz
WDW          EM
SSB          0
LB           1.00 Hz
GB           0
PC           1.40
```

**B-(4-Hydroxyphenyl) tricyclopentylphosphine borane (19)**



4-HOPhBH2P(cyclopentyl)3



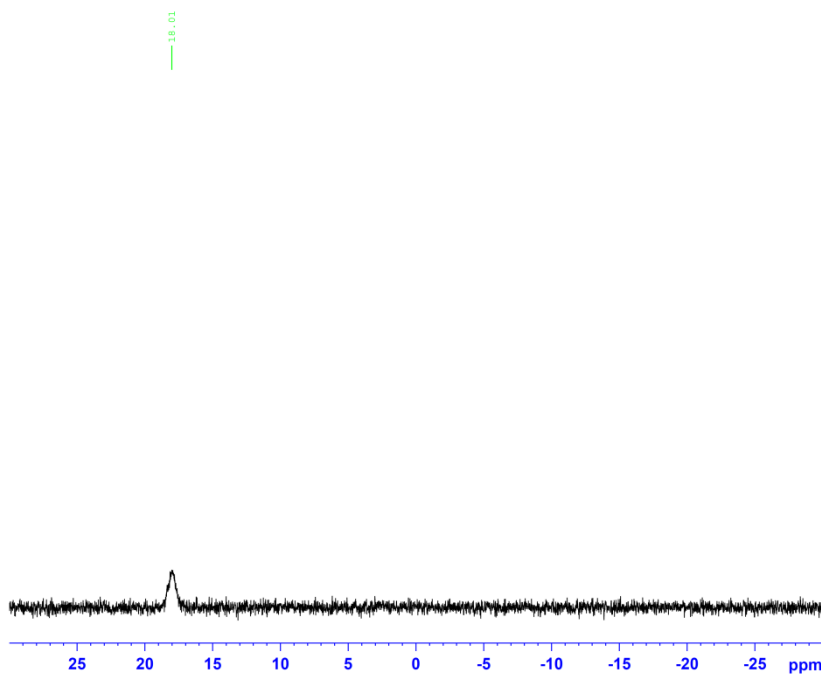
### IBB-nmr Analysis

```
NAME      Apr4-2021
EXPNO     3
PROCNO    1
Date_     20210404
Time      13.46
INSTRUM   av400
PROBHD    5 mm PABBO BB-
PULPROG   zgpg
TD         32768
SOLVENT   DMSO
NS         256
DS         4
SWH        20000.000 Hz
FIDRES     0.610352 Hz
AQ         0.8192500 sec
RG         203
DW         25.000 usec
DE         20.00 usec
TE         298.4 K
D1         1.00000000 sec
D11        0.03000000 sec
TDO        1

===== CHANNEL f1 =====
NUC1       11B
P1         6.30 usec
PL1        -2.00 dB
SFO1       128.3776050 MHz

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2       1H
PCPD2     80.00 usec
PL2        -1.70 dB
PL12       13.80 dB
PL2W       14.48987389 W
PL12W      0.40838012 W
SFO2       400.1316005 MHz
SI         32768
SF         128.3776183 MHz
WDW        EM
SSB        0
LB         2.00 Hz
GB         0
PC         1.40
```

4-HOPhBH2P(cyclopentyl)3



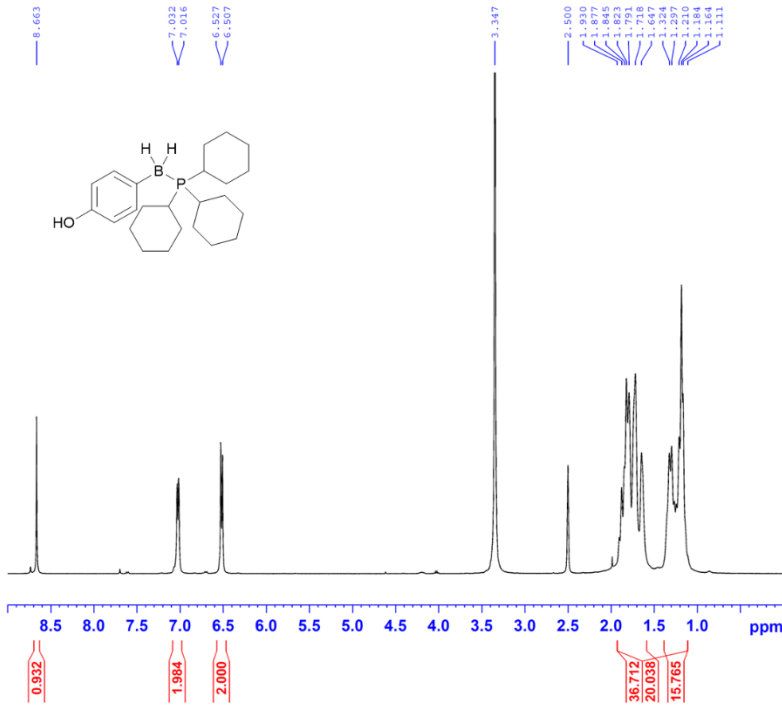
### IBB-nmr Analysis

```
NAME      Apr4-2021
EXPNO     4
PROCNO    1
Date_     20210404
Time      13.54
INSTRUM   av400
PROBHD    5 mm PABBO BB-
PULPROG   zg30
TD         65536
SOLVENT   DMSO
NS         16
DS         4
SWH        64102.563 Hz
FIDRES     0.978127 Hz
AQ         0.5112308 sec
RG         203
DW         7.800 usec
DE         6.50 usec
TE         298.0 K
D1         2.00000000 sec
TDO        1

===== CHANNEL f1 =====
NUC1       31P
P1         10.00 usec
PL1        -0.70 dB
PL1W       30.10233498 W
SFO1       161.9674942 MHz
SI         32768
SF         161.9754962 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
```

**B-(4-Hydroxyphenyl) tricyclohexylphosphine borane (20)**

4HOPhBH2cyclohexyl3 6-10Fr



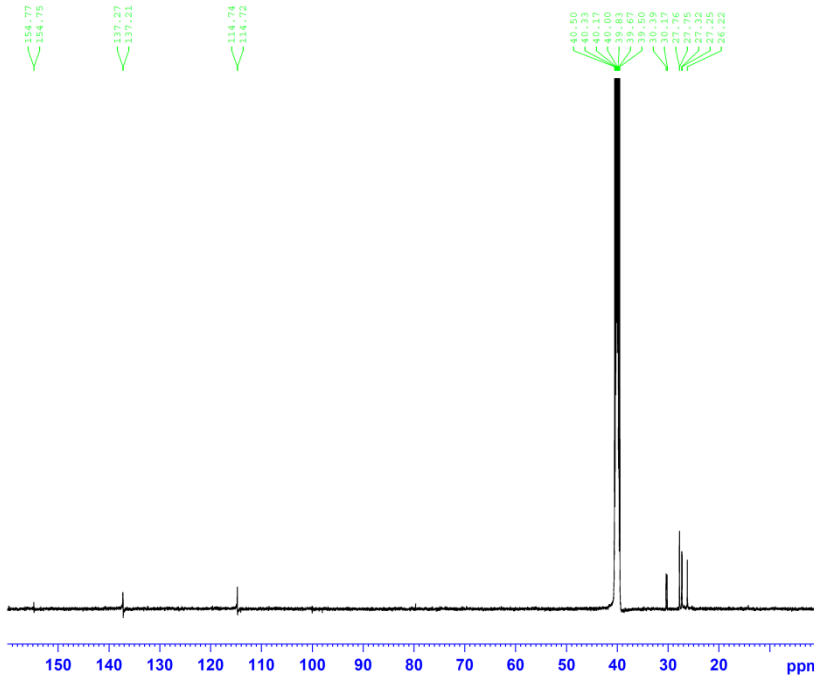
**IBB-nmr Analysis**

```

NAME      Sep21-2021
EXPNO     1
PROCNO    1
Date_     20210921
Time      8.32
INSTRUM   av400
PROBHD    5 mm PABBO BB-
PULPROG   zg30
TD         65536
SOLVENT   DMSO
NS         16
DS         2
SWH        8223.685 Hz
FIDRES     0.125483 Hz
AQ         3.9846387 sec
RG         128
DW         60.800 usec
DE         6.50 usec
TE         299.3 K
D1         1.00000000 sec
TD0        1

===== CHANNEL f1 =====
NUC1      1H
P1         14.00 usec
PL1        -1.80 dB
PL1W       14.82738590 W
SFO1       400.1324710 MHz
SI         32768
SF         400.1300036 MHz
WDW        EM
SSB         0
LB         0.30 Hz
GB         0
PC         1.00
    
```

4HOPhBH2cyclohexyl3 6-10Fr



**IBB-nmr Analysis**

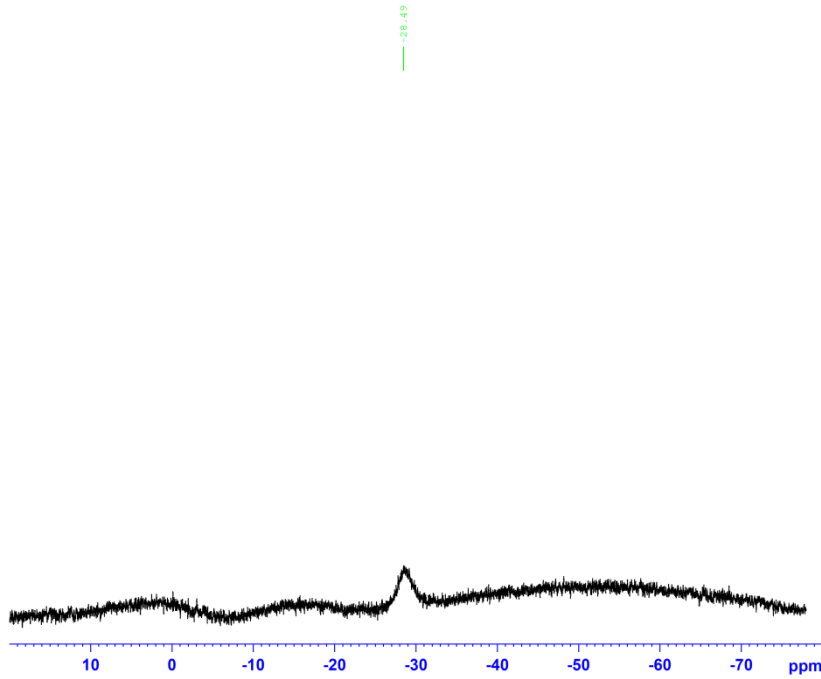
```

NAME      Sep19-2021
EXPNO     7
PROCNO    1
Date_     20210919
Time      22.08
INSTRUM   av500
PROBHD    5 mm CPDCH 13C
PULPROG   zgpg30
TD         65536
SOLVENT   DMSO
NS         1024
DS         4
SWH        30030.029 Hz
FIDRES     0.458222 Hz
AQ         1.0912410 sec
RG         35.9
DW         16.650 usec
DE         20.00 usec
TE         298.0 K
D1         2.00000000 sec
D11        0.03000000 sec
TD0        1

===== CHANNEL f1 =====
NUC1      13C
P1         10.00 usec
PL1         -5.00 dB
PL1W       14.29790783 W
SFO1       125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2      1H
FCPD2     80.00 usec
PL2        -4.00 dB
PL12       14.06 dB
PL13       17.00 dB
PL2W       6.30957365 W
PL12W      0.09862794 W
PL13W      0.05011872 W
SFO2       500.1320005 MHz
SI         32768
SF         125.7577875 MHz
WDW        EM
SSB         0
LB         1.00 Hz
GB         0
PC         0.30
    
```

4HOPhBH2cyclohexyl3 6-10Fr



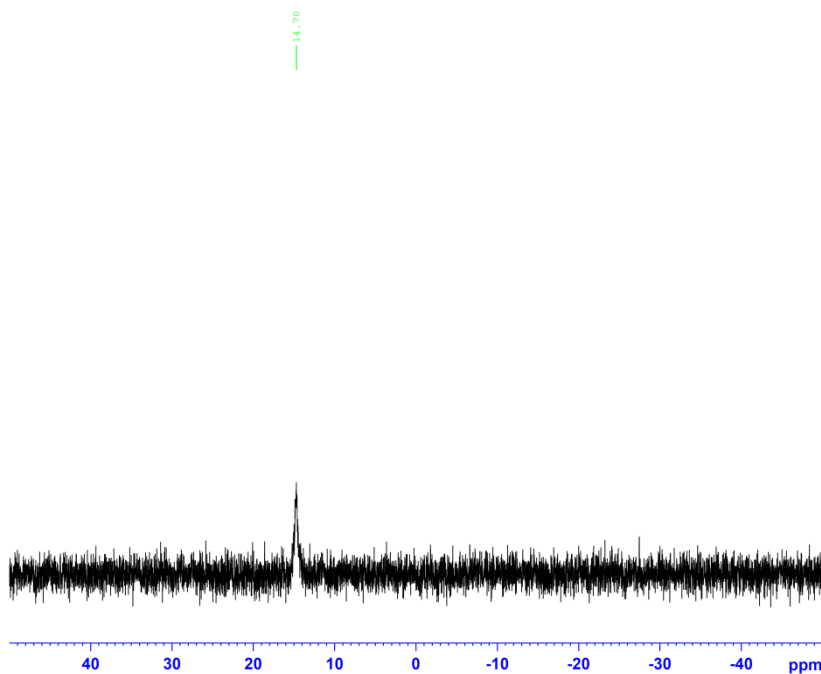
### IBB-nmr Analysis

```
NAME Sep19-2021
EXPNO 4
PROCNO 1
Date_ 20210919
Time 20.38
INSTRUM av400
PROBHD 5 mm PABBO BB-
PULPROG zgpg
TD 32768
SOLVENT DMSO
NS 256
DS 4
SWH 20000.000 Hz
FIDRES 0.610352 Hz
AQ 0.8192500 sec
RG 203
DW 25.000 usec
DE 20.00 usec
TE 300.1 K
D1 1.00000000 sec
D11 0.03000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 11B
P1 6.30 usec
PL1 -2.00 dB
SFO1 128.3776050 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -1.70 dB
PL12 13.80 dB
PL2W 14.48987389 W
PL12W 0.40838012 W
SFO2 400.1316005 MHz
SI 32768
SF 128.3776183 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40
```

4HOPhBH2cyclohexyl3 6-10Fr



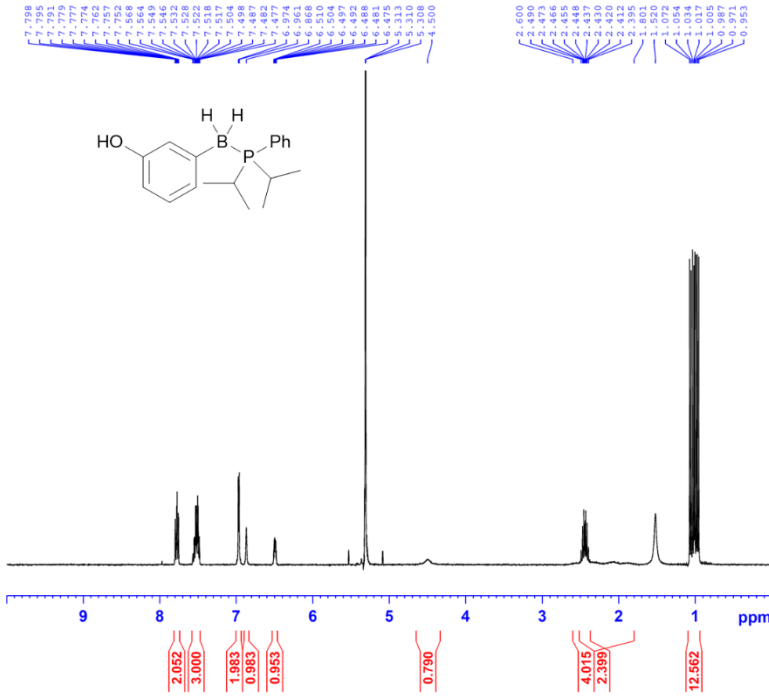
### IBB-nmr Analysis

```
NAME Sep19-2021
EXPNO 3
PROCNO 1
Date_ 20210919
Time 20.26
INSTRUM av400
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 128
DS 4
SWH 64102.563 Hz
FIDRES 0.978127 Hz
AQ 0.5112308 sec
RG 203
DW 7.800 usec
DE 6.50 usec
TE 299.5 K
D1 2.00000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 31P
P1 10.00 usec
PL1 -0.70 dB
PL1W 30.10233498 W
SFO1 161.9674942 MHz
SI 32768
SF 161.9754962 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
```

**B-(3-Hydroxyphenyl) diisopropylphenylphosphine borane (21)**

3HOPhBH2PPh(i-Pr)2



**IBB-nmr Analysis**

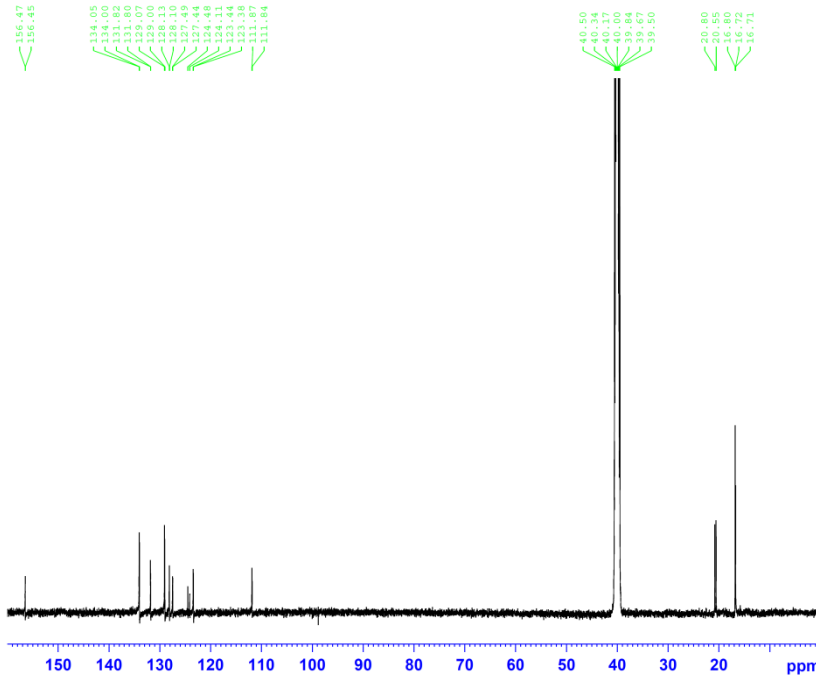
```

NAME      Nov24-2022
EXPNO    5
PROCNO   1
Date_    20221124
Time     23.36
INSTRUM  av400
PROBHD   5 mm PABBO BB-
PULPROG  zg30
TD       65536
SOLVENT  CD2Cl2
NS       16
DS       2
SWH      8223.685 Hz
FIDRES   0.125483 Hz
AQ       3.9846387 sec
RG       203
DW       60.800 usec
DE       6.50 usec
TE       297.3 K
D1       1.00000000 sec
TD0      1
    
```

```

----- CHANNEL f1 -----
NUC1     1H
P1       14.00 usec
PL1      -1.80 dB
PL1W     14.82738590 W
SFO1     400.1324710 MHz
SI       32768
SF       400.1300194 MHz
WDW      EM
SSB      0
LB       0.30 Hz
GB       0
PC       1.00
    
```

3HOPhBH2PPh(i-Pr)2



**IBB-nmr Analysis**

```

NAME      Nov24-2022
EXPNO    4
PROCNO   1
Date_    20221124
Time     23.20
INSTRUM  av500
PROBHD   5 mm CPDCH 13C
PULPROG  zgpg30
TD       65536
SOLVENT  DMSO
NS       1024
DS       4
SWH      30030.029 Hz
FIDRES   0.458222 Hz
AQ       1.0912410 sec
RG       35.9
DW       16.650 usec
DE       20.00 usec
TE       298.0 K
D1       2.00000000 sec
D11      0.03000000 sec
TD0      1
    
```

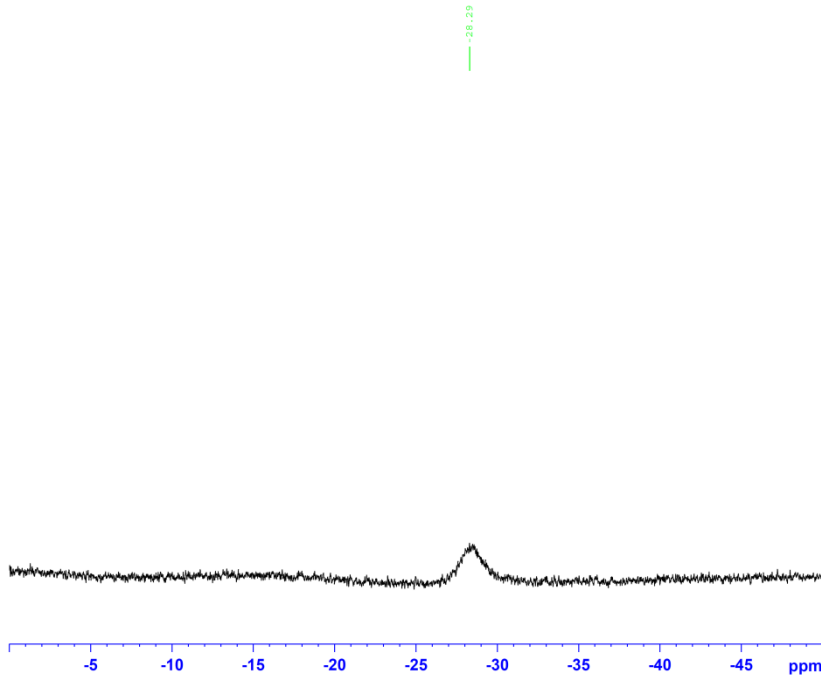
```

----- CHANNEL f1 -----
NUC1     13C
P1       10.00 usec
PL1      -5.00 dB
PL1W     14.29790783 W
SFO1     125.7703643 MHz

----- CHANNEL f2 -----
CPDPRG2  waltz16
NUC2     1H
FPCPD2   80.00 usec
PL2      -4.00 dB
PL12     14.06 dB
PL13     17.00 dB
PL2W     6.30957365 W
PL12W    0.09862794 W
PL13W    0.05011872 W
SFO2     500.1320005 MHz
SI       32768
SF       125.7577875 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       0.30
    
```



3HOPhBH2PPh(i-Pr)2



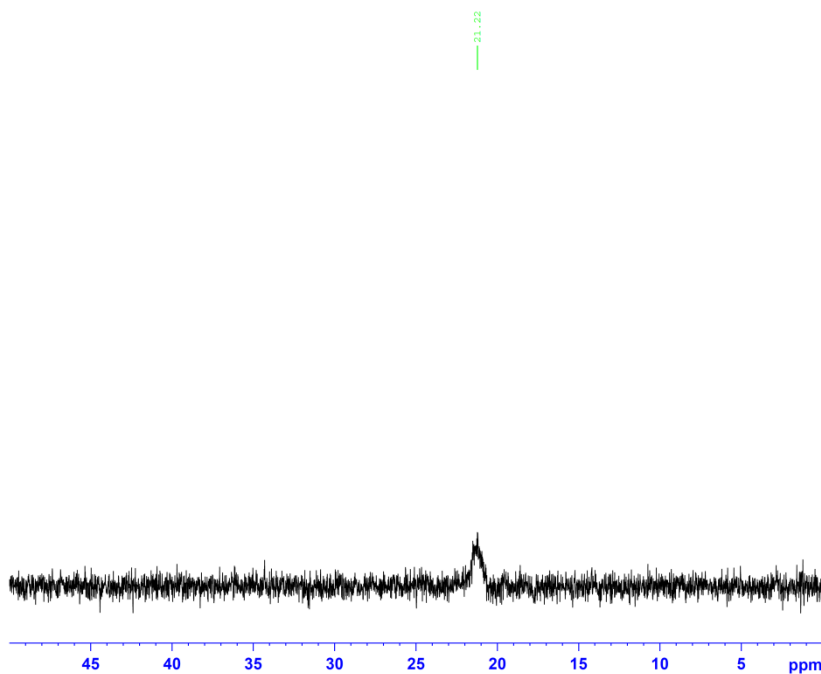
### IBB-nmr Analysis

```
NAME      Nov24-2022
EXPNO     3
PROCNO    1
Date_     20221124
Time      22.08
INSTRUM   av400
PROBHD    5 mm PABBO BB-
PULPROG   zgpg
TD         32768
SOLVENT   DMSO
NS         128
DS         4
SWH        20000.000 Hz
FIDRES     0.610352 Hz
AQ         0.8192500 sec
RG         203
DW         25.000 usec
DE         20.00 usec
TE         297.3 K
D1         1.00000000 sec
D11        0.03000000 sec
TDO        1

===== CHANNEL f1 =====
NUC1       11B
P1         6.30 usec
PL1        -2.00 dB
SFO1       128.3776050 MHz

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2       1H
PCPD2     80.00 usec
PL2        -1.70 dB
PL12       13.80 dB
PL2W       14.48987389 W
PL12W      0.40838012 W
SFO2       400.1316005 MHz
SI         32768
SF         128.3776183 MHz
WDW        EM
SSB        0
LB         2.00 Hz
GB         0
PC         1.40
```

3HOPhBH2PPh(i-Pr)2



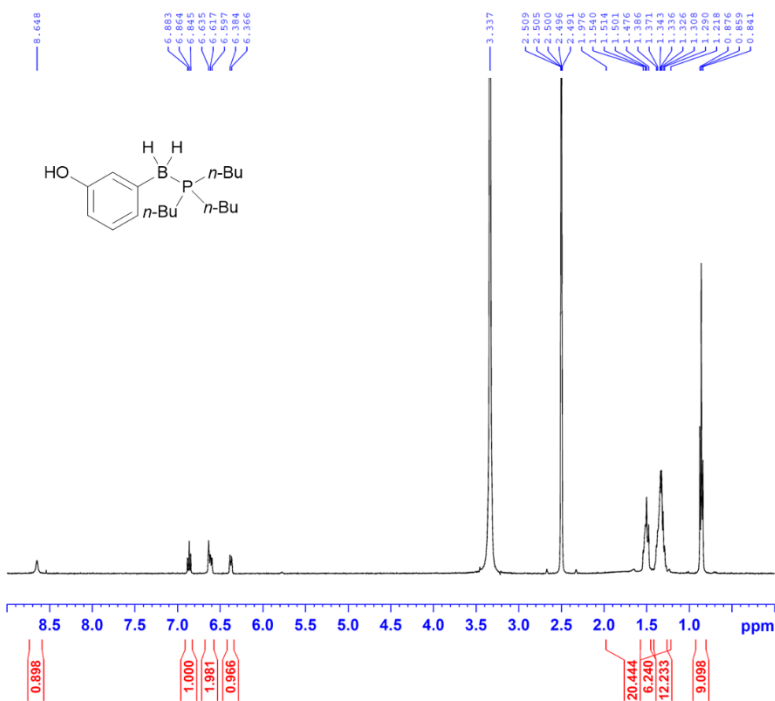
### IBB-nmr Analysis

```
NAME      Nov24-2022
EXPNO     2
PROCNO    1
Date_     20221124
Time      22.01
INSTRUM   av400
PROBHD    5 mm PABBO BB-
PULPROG   zg30
TD         65536
SOLVENT   DMSO
NS         64
DS         4
SWH        64102.563 Hz
FIDRES     0.978127 Hz
AQ         0.5112308 sec
RG         203
DW         7.800 usec
DE         6.50 usec
TE         297.3 K
D1         2.00000000 sec
TDO        1

===== CHANNEL f1 =====
NUC1       31P
P1         10.00 usec
PL1        -0.70 dB
PL1W       30.10233498 W
SFO1       161.9674942 MHz
SI         32768
SF         161.9754962 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
```

### B-(3-Hydroxyphenyl) tributylphosphine borane (22)

3HOPhBH2P(n-Bu)3 21-31Fr



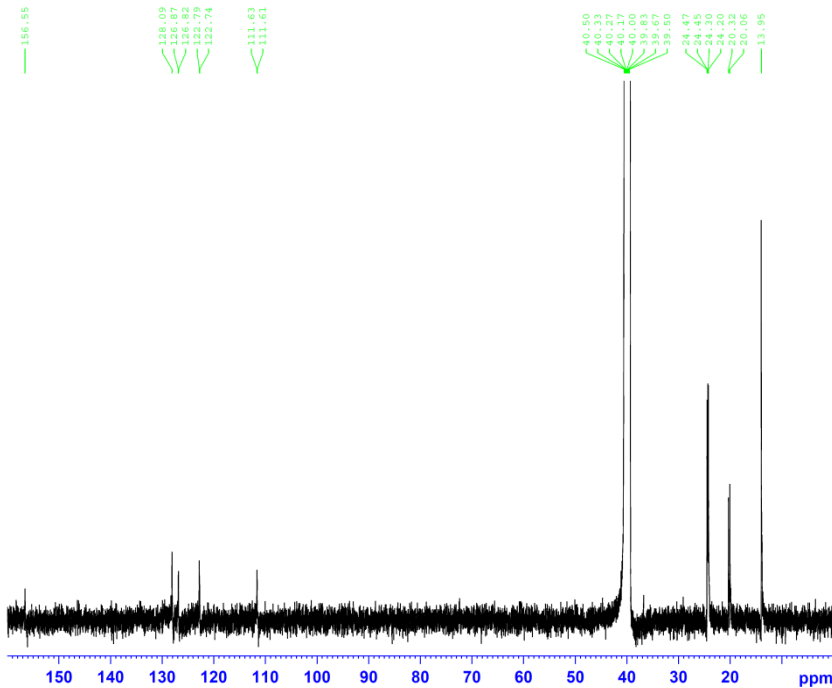
#### IBB-nmr Analysis

```

NAME      Oct9-2021
EXPNO     4
PROCNO    1
Date_     20211009
Time      20.18
INSTRUM   av400
PROBHD    5 mm PABBO BB-
PULPROG   zg30
TD         65536
SOLVENT   DMSO
NS         16
DS         2
SWH        8223.685 Hz
FIDRES     0.125483 Hz
AQ         3.9846387 sec
RG         203
DW         60.800 usec
DE         6.50 usec
TE         297.3 K
D1         1.0000000 sec
TD0        1

===== CHANNEL f1 =====
NUC1      1H
P1        14.00 usec
PL1       -1.80 dB
PL1W      14.82738590 W
SFO1      400.1324710 MHz
SI        32768
SF        400.1300029 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB        0
PC        1.00
    
```

3HOPhBH2P(n-Bu)3 21-31Fr



#### IBB-nmr Analysis

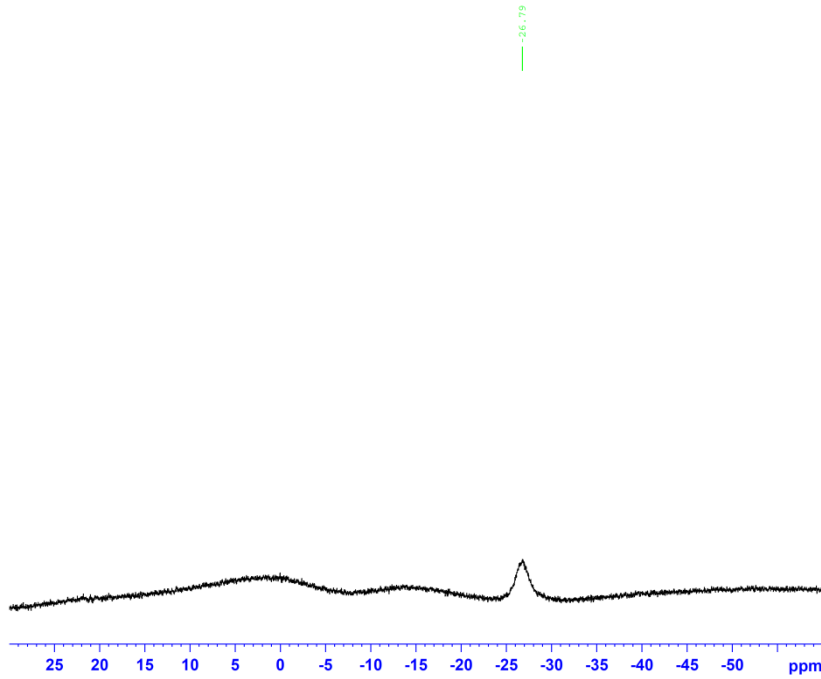
```

NAME      Oct9-2021
EXPNO     7
PROCNO    1
Date_     20211009
Time      22.02
INSTRUM   av500
PROBHD    5 mm CPDCH 13C
PULPROG   zgpg30
TD         65536
SOLVENT   DMSO
NS         1024
DS         4
SWH        30030.029 Hz
FIDRES     0.458222 Hz
AQ         1.0912410 sec
RG         90.5
DW         16.650 usec
DE         20.00 usec
TE         298.0 K
D1         2.0000000 sec
D11        0.0300000 sec
TD0        1

===== CHANNEL f1 =====
NUC1      13C
P1        10.00 usec
PL1       -5.00 dB
PL1W      14.29790783 W
SFO1      125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2      1H
PCPD2     80.00 usec
PL2       -4.00 dB
PL12      14.06 dB
PL13      17.00 dB
PL2W      6.30957365 W
PL12W     0.09862794 W
PL13W     0.05011872 W
SFO2      500.1320005 MHz
SI        32768
SF        125.7577857 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        0.30
    
```

3HOPhBH2P (n-Bu) 3 21-31Fr



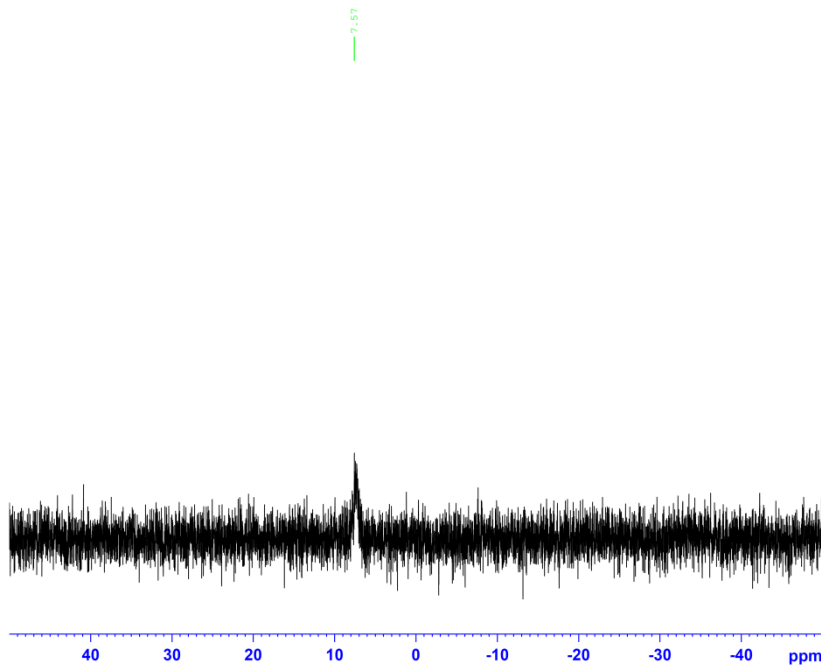
### IBB-nmr Analysis

```
NAME          Oct9-2021
EXPNO         6
PROCNO        1
Date_         20211009
Time_         20.58
INSTRUM       av400
PROBHD        5 mm PABBO BB-
PULPROG       zgpg
TD            32768
SOLVENT       DMSO
NS            1024
DS            4
SWH           20000.000 Hz
FIDRES        0.610352 Hz
AQ            0.8192500 sec
RG            203
DW            25.000 usec
DE            20.00 usec
TE            297.3 K
D1            1.00000000 sec
D11           0.03000000 sec
TDO           1

===== CHANNEL f1 =====
NUC1           11B
P1             6.30 usec
PL1            -2.00 dB
SFO1          128.3776050 MHz

===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2           1H
PCPD2          80.00 usec
PL2            -1.70 dB
PL12           13.80 dB
PL2W           14.48987389 W
PL12W          0.40838012 W
SFO2           400.1316005 MHz
SI            32768
SF            128.3776183 MHz
WDW            EM
SSB            0
LB             2.00 Hz
GB             0
PC             1.40
```

3HOPhBH2P (n-Bu) 3 21-31Fr



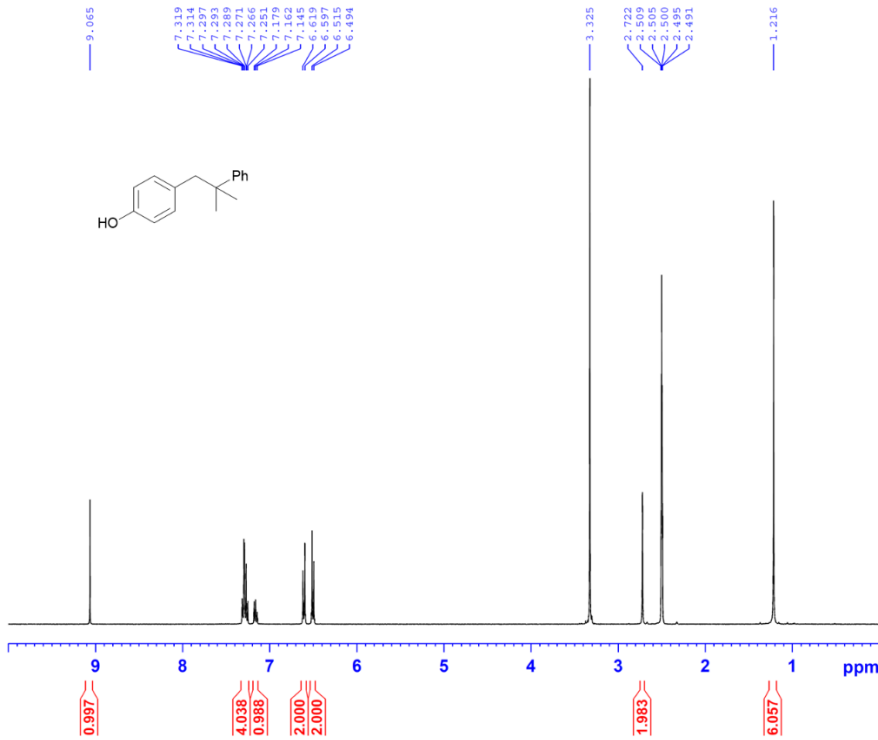
### IBB-nmr Analysis

```
NAME          Oct9-2021
EXPNO         5
PROCNO        1
Date_         20211009
Time_         20.23
INSTRUM       av400
PROBHD        5 mm PABBO BB-
PULPROG       zg30
TD            65536
SOLVENT       DMSO
NS            64
DS            4
SWH           64102.563 Hz
FIDRES        0.978127 Hz
AQ            0.5112308 sec
RG            203
DW            7.800 usec
DE            6.50 usec
TE            297.2 K
D1            2.00000000 sec
TDO           1

===== CHANNEL f1 =====
NUC1           31P
P1            10.00 usec
PL1            -0.70 dB
PL1W           30.10233498 W
SFO1          161.9674942 MHz
SI            32768
SF            161.9754962 MHz
WDW            EM
SSB            0
LB             1.00 Hz
GB             0
PC             1.40
```

# 4-(2-Methyl-2-phenylpropyl)phenol (26)

4HOPhCH2CMe2Ph



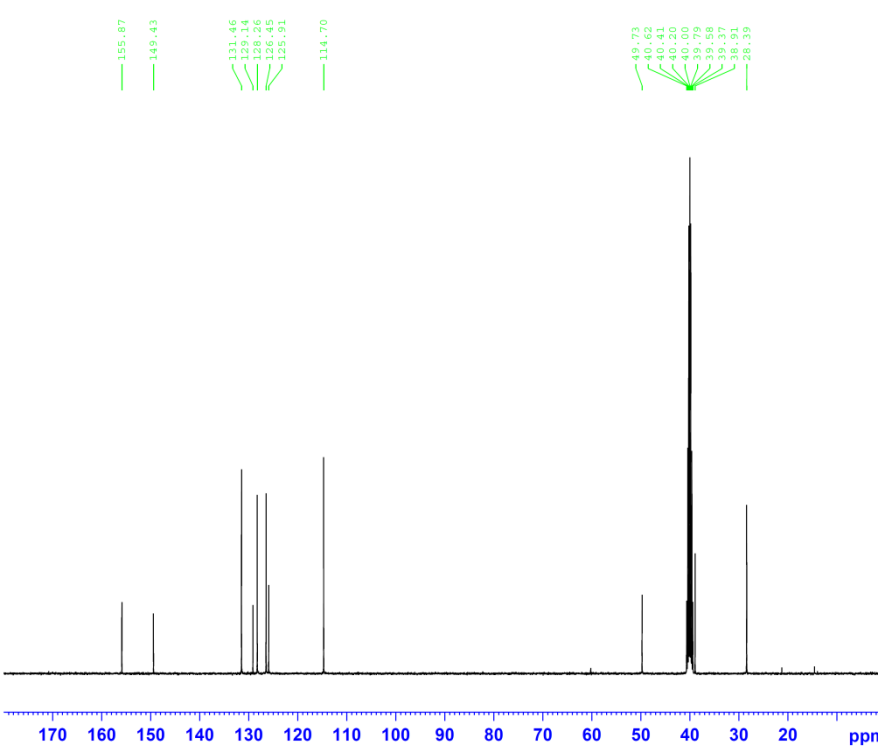
## IBB-nmr Analysis

```

NAME      May15-2021
EXPNO    4
PROCNO   1
Date_    20210515
Time     16.33
INSTRUM  av400
PROBHD   5 mm PABBO BB-
PULPROG  zg30
TD        65536
SOLVENT  DMSO
NS        16
DS        2
SWH       8223.685 Hz
FIDRES   0.125483 Hz
AQ        3.9846387 sec
RG        203
DW        60.800 usec
DE        6.50 usec
TE        297.3 K
D1        1.00000000 sec
TDO       1

===== CHANNEL f1 =====
NUC1      1H
P1        14.00 usec
PL1       -1.80 dB
PL1W     14.82738590 W
SFO1     400.1324710 MHz
SI        32768
SF        400.1300036 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB        0
PC        1.00
    
```

4HOPhCH2CMe2Ph



## IBB-nmr Analysis

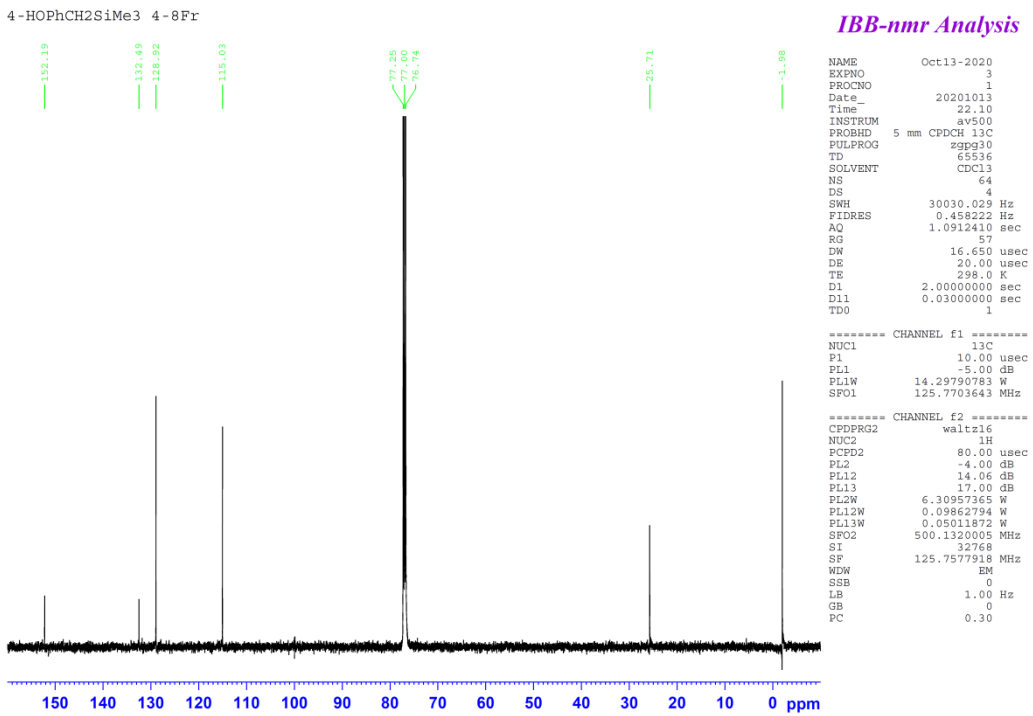
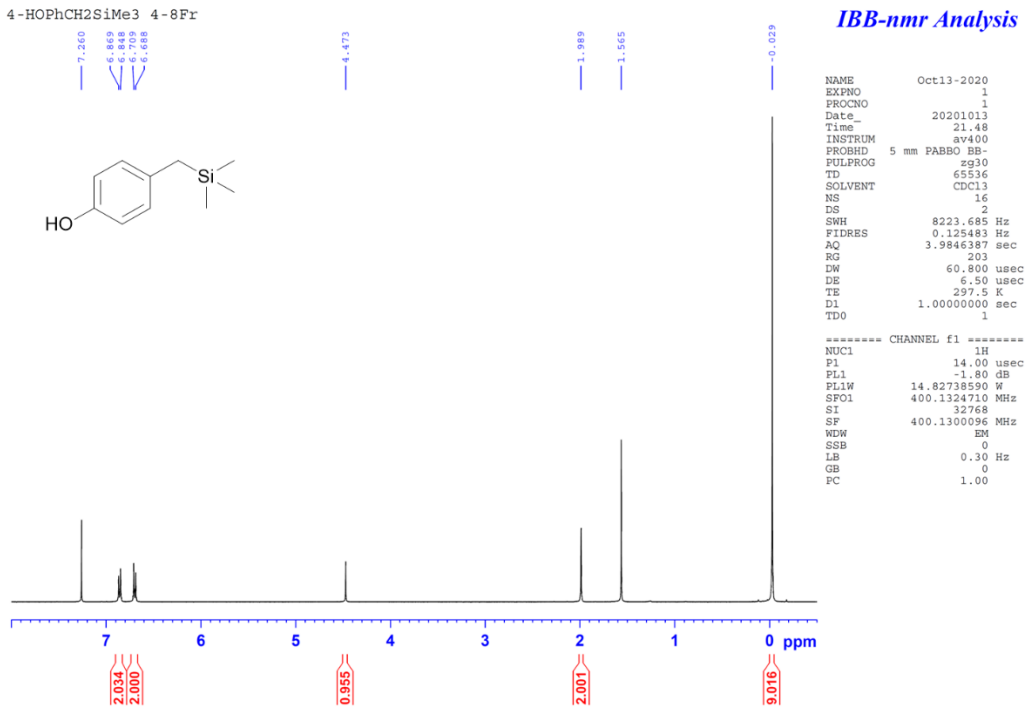
```

NAME      Apr25-2021
EXPNO    3
PROCNO   1
Date_    20210425
Time     19.32
INSTRUM  av400
PROBHD   5 mm PABBO BB-
PULPROG  zgpg30
TD        65536
SOLVENT  DMSO
NS        1024
DS        2
SWH       24038.461 Hz
FIDRES   0.366798 Hz
AQ        1.3631988 sec
RG        128
DW        20.800 usec
DE        6.50 usec
TE        299.2 K
D1        2.00000000 sec
D11      0.03000000 sec
TDO       1

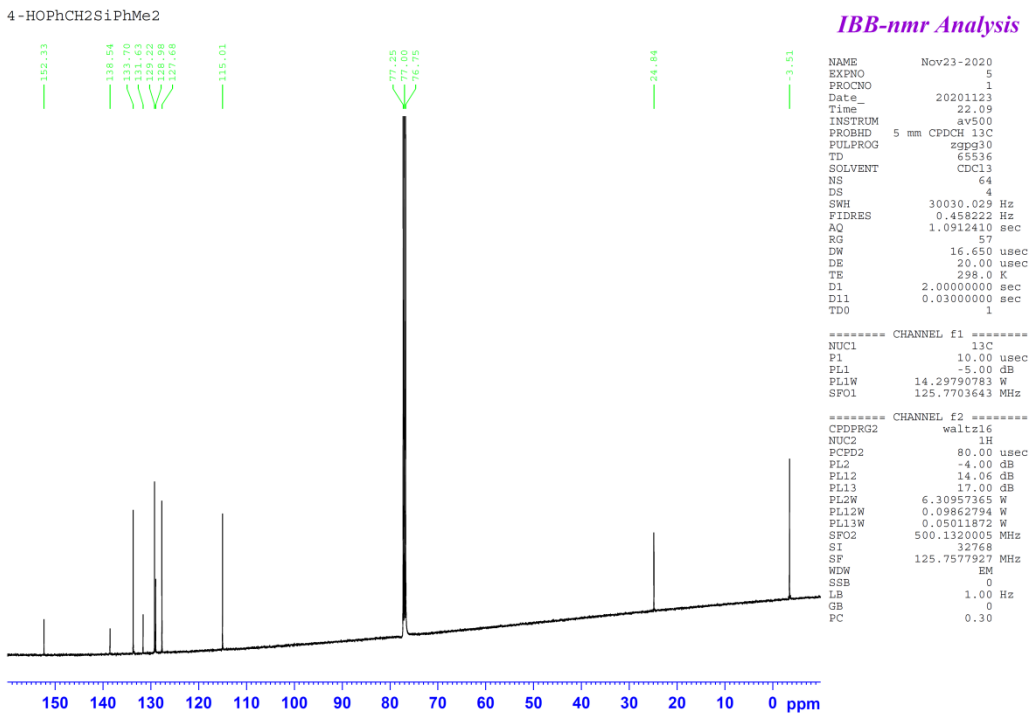
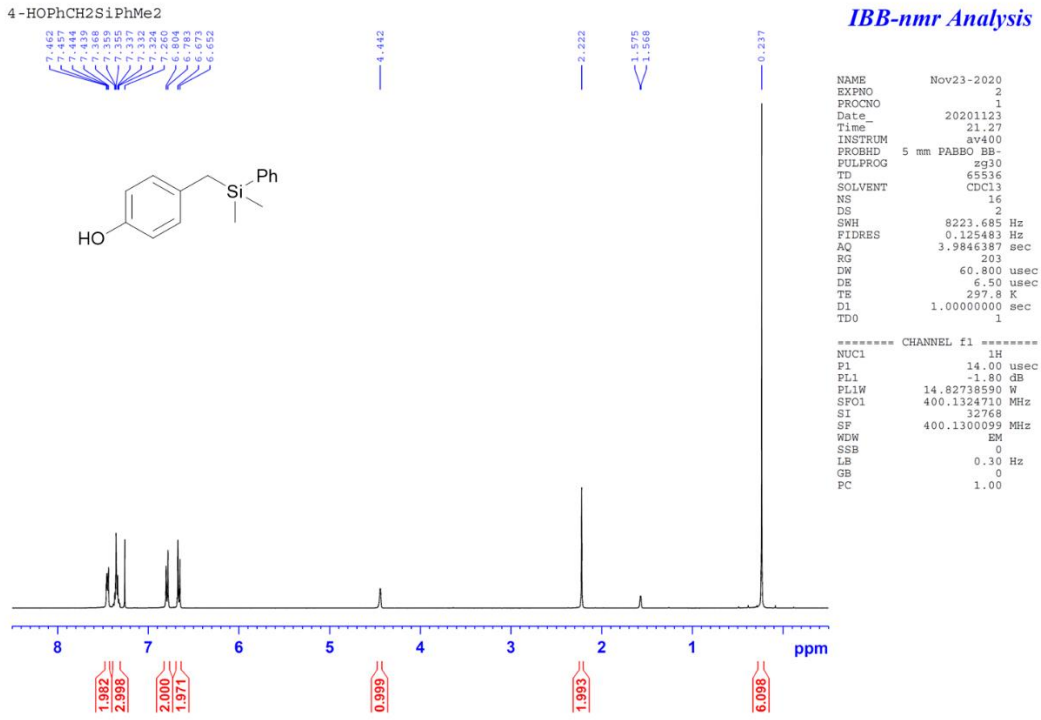
===== CHANNEL f1 =====
NUC1      13C
P1        9.00 usec
PL1       -3.00 dB
PL1W     73.17333984 W
SFO1     100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2  waltz16
NUC2      1H
PCPD2    90.00 usec
PL2       -1.70 dB
PL12     13.80 dB
PL13     13.80 dB
PL2W     14.48987389 W
PL12W    0.40838012 W
PL13W    0.40838012 W
SFO2     400.1316005 MHz
SI        32768
SF        100.6127690 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        0.30
    
```

4-[(trimethylsilyl)methyl]phenol (30)



4-[(dimethylphenylsilyl)methyl]phenol (31)



### 3. Calculation of Log*P*

**Table S1.** Experimental and calculated Log*P* values of phosphine boranes. Differences between experimental values and calculated values are noted in parentheses.

Cmpd	X-Y		R <sup>1</sup>	R <sup>2</sup>	Log <i>P</i>			
					experimental	Calculated by ChemDraw <sup>a</sup>	Calculated by ALOGPS <sup>b</sup>	
Phenol	-	-	-	-	1.46	1.48 (+0.02)	1.39 (-0.07)	
<b>7</b>	-BH <sub>2</sub> -P	4-OH	Me	Me	2.44	2.13 (-0.31)	3.05 (+0.61)	
<b>8</b>			Ph	Me	3.18	4.03 (+0.31)	4.41 (+1.23)	
<b>9</b>			Et	Et	3.28	3.72 (+0.31)	4.85 (+1.57)	
<b>10</b>			Ph	Et	4.11	5.09 (+0.98)	5.42 (+1.31)	
<b>11</b>		3-OH	Me	Me	2.55	2.13 (-0.42)	2.98 (+0.43)	
<b>12</b>			Ph	Me	3.27	4.03 (+0.76)	4.39 (+1.12)	
<b>13</b>			Et	Et	3.47	3.72 (+0.25)	4.81 (+1.34)	
<b>14</b>			Ph	Et	4.19	5.09 (+0.90)	5.39 (+1.20)	
<b>23</b>		-CH <sub>2</sub> -C	4-OH	Me	Me	4.36	3.83 (-0.53)	3.79 (-0.57)
<b>26</b>				Ph	Me	5.26	4.72 (-0.54)	4.64 (-0.62)
<b>30</b>	-CH <sub>2</sub> -Si	Me		Me	4.91	3.47 (-1.44)	3.31 (-1.60)	
<b>31</b>		Ph		Me	5.74	5.62 (-0.12)	5.41 (-0.33)	

<sup>a</sup>ChemDraw 22.2.0

<sup>b</sup>ALOGPS 2.1 program<sup>1,2</sup>

#### 4. Calculation of pK<sub>a</sub> values

**Table S2.** Experimental and calculated LogP values of phosphine boranes. Differences between experimental values and calculated values are noted in parentheses.

Cmpd	X-Y		R <sup>1</sup>	R <sup>2</sup>	pK <sub>a</sub>		
					experimental	Calculated by ChemDraw <sup>a</sup>	DFT-based calibration method <sup>b</sup>
Phenol	-	-	-	-	10.44	9.97 (-0.47)	9.85 (-0.59)
<b>7</b>	-BH <sub>2</sub> -P	4-OH	Me	Me	11.28	11.40 (+0.12)	10.46 (-0.82)
<b>8</b>			Ph	Me	11.22	11.29 (+0.07)	10.38 (-0.84)
<b>9</b>			Et	Et	11.02	11.32 (+0.30)	10.13 (-0.89)
<b>10</b>			Ph	Et	11.05	11.24 (+0.19)	10.04 (-1.01)
<b>11</b>		3-OH	Me	Me	11.26	12.60 (+1.34)	10.55 (-0.71)
<b>12</b>			Ph	Me	11.33	12.45 (+1.12)	10.51 (-0.82)
<b>13</b>			Et	Et	11.33	12.53 (+1.20)	10.57 (-0.76)
<b>14</b>			Ph	Et	11.29	12.41 (+1.12)	10.53 (-0.80)
<b>23</b>	-CH <sub>2</sub> -C	4-OH	Me	Me	10.77	9.76 (-1.01)	10.12 (-0.65)
<b>26</b>			Ph	Me	10.69	9.65 (-1.04)	10.10 (-0.59)
<b>30</b>	-CH <sub>2</sub> -Si		Me	Me	10.74	9.66 (-1.08)	10.26 (-0.48)
<b>31</b>			Ph	Me	10.89	9.54 (-1.35)	10.27 (-0.62)

<sup>a</sup>Calculated by ChemDraw 22.2.0

<sup>b</sup>The detailed method is noted below.

**Calculation of pK<sub>a</sub> by DFT-based calibration:** All density functional theory (DFT) calculations were performed with the Spartan' 18 programs, Wavefunction, Inc., Irvine, CA. The geometry optimization of compounds were carried out at the B3LYP/6-311++G\* level of theory. The Gibbs energy of the protonated and the deprotonated forms of each compound was approximated by essentially a combination of the gas phase and solution phase DFT energies.<sup>3,4</sup> For the reference compounds (phenol, 4-methylphenol, 4-methoxyphenol, 4-chlorophenol, 4-phenylphenol, 2-nitrophenol), the differences of calculated Gibbs energy between the protonated and the deprotonated forms were plotted against the actual pK<sub>a</sub> values to prepare a calibration curve. The pK<sub>a</sub> values of test compounds were obtained by interpolation of the calculated Gibbs energy of the calibration curve.



#### References for Supplementary Information

1. I. V. Tetko, J. Gasteiger, R. Todeschini, A. Mauri, D. Livingstone, P. Ertl, V. A. Palyulin, E. V. Radchenko, N. S. Zefirov, A. S. Makarenko, V. Y. Tanchuk, and V. V. Prokopenko, *J. Comput. Aid. Mol. Des.*, 2005, **19**, 453–463.
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3. M. D. Liptak, K. C. Gross, P. G. Seybold, S. Feldgus, and G. C. Shields, *J. Am. Chem. Soc.* 2002, **124**, 6421–6427.
4. J. J. Kličić, R. A. Friesner, S.-Y. Liu, and W. C. Guida, *J. Phys. Chem. A* 2002, **106**, 1327–1335.