

## Supporting Information

### Merging Norrish Type I Reaction and Transition Metal Catalysis: Photo- and Rh-promoted Borylation of C–C σ-Bonds of Arylketones

Yuki Fujimaki, Nobuharu Iwasawa, Jun Takaya\*

Department of Chemistry, School of Science, Tokyo Institute of Technology, 2-12-1, O-okayama, Meguro-ku,  
Tokyo 152-8551, Japan  
E-mail: takayajun@chem.titech.ac.jp

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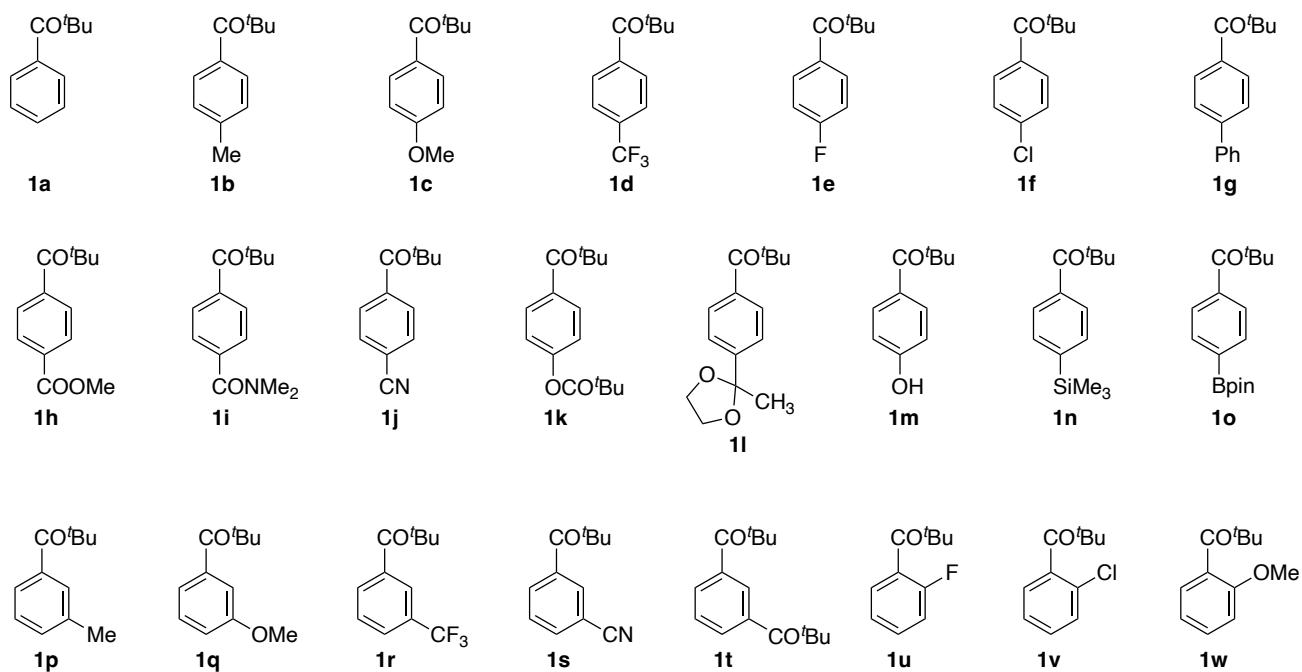
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## **General methods**

All operations were performed under an argon atmosphere.  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra were recorded on a JEOL ECX-500 or a JEOL ECZ-500 (500 MHz for  $^1\text{H}$  and 125 MHz for  $^{13}\text{C}$ ) spectrometer in  $\text{CDCl}_3$  or  $\text{C}_6\text{D}_6$ . Chemical shifts are expressed in parts per million (ppm) downfield from tetramethylsilane ( $\delta_{\text{H}} = 0.00$ ,  $\delta_{\text{C}} = 0.00$ ) and are referenced to residual solvents ( $\delta_{\text{H}} 7.26$  and  $\delta_{\text{C}} 77.0$  for  $\text{CDCl}_3$  and  $\delta_{\text{H}} 7.15$  and  $\delta_{\text{C}} 128.1$  for  $\text{C}_6\text{D}_6$ ). IR spectra were recorded on an IRTtracer-100 (SHIMADZU Co., Ltd.) with an ATR QATR10 accessory. High resolution mass spectra (HRMS) were recorded on a BRUKER micrOTOF II and a JEOL JMS-T100 spectrometer. Gas chromatography (GC) analyses were conducted on a SHIMADZU GC-2010 equipped with an Agilent DB-1 column. EI-MS analyses ( $\text{EI}^+$ ) were performed on a Shimadzu GCMS-QP2020. Silica Gel 60 (Kanto Chemical Co., Inc.) was used for flash column chromatography. Photoirradiation was carried out using a LED (365 nm, HDL-120U6-NWPSC/PSCC-60048(A), CCS). During the photoirradiation, the reaction temperature was kept at a constant temperature using a water bath equipped with a low temperature circulator (CTP-1000, EYELA). Merck Kieselgel 60 F254 (0.25 mm thickness, coated on glass 20x20 cm<sup>2</sup>) plate was used for analytical thin layer chromatography (TLC). THF, Et<sub>2</sub>O and hexane were purified by solvent purification system of Glass-Contour. Benzene-*d*<sub>6</sub> was purchased from Kanto chemicals and dried and degassed by benzophenone ketyl. All commercially available reagents were obtained from chemical suppliers and used after proper purification if necessary.

### **General procedures for the preparation of pivalophenone derivatives**

Pivalophenone derivatives **1a-c**, **1e-g**, **1l**, **1n**, **1p-1q**, **1t** and **1u-1w** were synthesized by the general procedure **A**. **1h-k** and **1s** were synthesized by the general procedure **B**. **1d**, **1m**, **1o** and **1r** were synthesized according to a literature procedure.<sup>S1-S3</sup> All analytical data of **1h**, **1j**, and **1m** are listed below. Other ketones are known compounds in literatures as referenced, and spectral data were in good agreement with literature values.



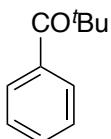
**Figure S1.** List of pivalophenone derivatives

### **General procedure A**

Under a nitrogen atmosphere, a THF solution of Grignard reagent (ArMgBr, 20 mmol), which was prepared from Mg (20 mmol) and ArBr (21 mmol) in THF (40 mL), was added slowly to a solution of pivaloyl chloride (6.0 mL, 49 mmol) in THF (40 mL) at 0 °C. After stirring for 3 hours, the mixture was diluted with saturated aq. NH<sub>4</sub>Cl (30 mL) and extracted with ethyl acetate three times. The combined organic layers were washed with saturated aq. Na<sub>2</sub>CO<sub>3</sub> (30 mL) and brine (30 mL) and dried over anhydrous Na<sub>2</sub>SO<sub>4</sub>. After the solvent was removed under reduced pressure, the residue was purified by flash column chromatography followed by distillation to give pivalophenone derivatives in 22-72% yields.

### General procedure B

Under a nitrogen atmosphere, a solution of  $^i\text{PrMgCl} \bullet \text{LiCl}$  (1.3 M in THF, 15.4 mL, 20 mmol) was added slowly to a solution of aryl iodide (20 mmol) in THF (10 mL) at  $-40^\circ\text{C}$ . The solution of Grignard reagent ( $\text{ArMgX}$ ) was added slowly to a solution of pivaloyl chloride (6.0 mL, 20 mmol) in THF (40 mL) at  $-40^\circ\text{C}$ . After stirring for 3 hours, the mixture was diluted with saturated aq.  $\text{NH}_4\text{Cl}$  (30 mL) and extracted with ethyl acetate three times. The combined organic layers were washed with saturated aq.  $\text{Na}_2\text{CO}_3$  (30 mL) and brine (30 mL) and dried over anhydrous  $\text{Na}_2\text{SO}_4$ . After the solvent was removed under reduced pressure, the residue was purified by flash column chromatography followed by distillation to give pivalophenone derivatives in 36-70% yields.

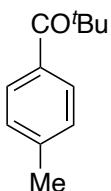


**1a** (colorless oil, 3.97 g, 24.5 mmol, 49%)

Synthesized according to the procedure A using 50 mmol of commercially available  $\text{PhMgBr}$ .

**$^1\text{H NMR}$**  (500 MHz,  $\text{CDCl}_3$ )  $\delta$  = 7.69 (d,  $J$  = 7.0 Hz, 2H), 7.46 (t,  $J$  = 7.5 Hz, 1H), 7.40 (t,  $J$  = 7.5 Hz, 2H), 1.35 (s, 9H).

Spectral data were in good agreement with literature values.<sup>S1</sup>

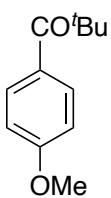


**1b** (colorless oil, 1.05 g, 5.94 mmol, 56%)

Synthesized according to the procedure A using 10 mmol of Mg.

**$^1\text{H NMR}$**  (500 MHz,  $\text{CDCl}_3$ )  $\delta$  = 7.66 (d,  $J$  = 8.5 Hz, 2H), 7.20 (d,  $J$  = 8.5 Hz, 2H), 2.39 (s, 3H), 1.35 (s, 9H).

Spectral data were in good agreement with literature values.<sup>S5</sup>

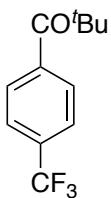


**1c** (colorless oil, 1.63 g, 8.50 mmol, 43%)

Synthesized according to the procedure A.

**<sup>1</sup>H NMR** (500 MHz, CDCl<sub>3</sub>) δ = 7.86 (d, *J* = 8.0 Hz, 2H), 6.90 (d, *J* = 8.0 Hz, 2H), 3.86 (s, 3H), 1.37 (s, 9H).

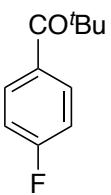
Spectral data were in good agreement with literature values.<sup>51</sup>



**1d** (colorless oil, 3.33 g, 14.5 mmol, 72%)

**<sup>1</sup>H NMR** (500 MHz, CDCl<sub>3</sub>) δ = 7.72 (d, *J* = 8.0 Hz, 2H), 7.67 (d, *J* = 8.5 Hz, 2H), 1.34 (s, 9H).

Spectral data were in good agreement with literature values.<sup>51</sup>

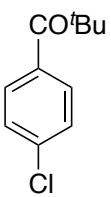


**1e** (colorless oil, 1.04 g, 5.78 mmol, 58%)

Synthesized according to the procedure A using 10 mmol of Mg.

**<sup>1</sup>H NMR** (500 MHz, CDCl<sub>3</sub>) δ = 7.82-7.76 (m, 2H), 7.08 (t, *J* = 8.5 Hz, 2H), 1.36 (s, 9H).

Spectral data were in good agreement with literature values.<sup>56</sup>

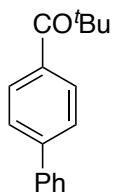


**1f** (colorless oil, 1.04 g, 5.21 mmol, 52%)

Synthesized according to the procedure A using 10 mmol of Mg.

**<sup>1</sup>H NMR** (500 MHz, CDCl<sub>3</sub>) δ = 7.67 (d, *J* = 9.0 Hz, 2H), 7.38 (d, *J* = 8.5 Hz, 2H), 1.34 (s, 9H).

Spectral data were in good agreement with literature values.<sup>S6</sup>

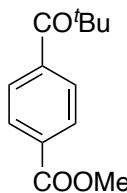


**1g** (white solids, 1.03 g, 4.33 mmol, 22%)

Synthesized according to the procedure A.

**<sup>1</sup>H NMR** (500 MHz, CDCl<sub>3</sub>) δ = 7.82 (d, *J* = 9.0 Hz, 2H), 7.65-7.60 (m, 4H), 7.49-7.44 (m, 2H), 7.39 (t, *J* = 7.5 Hz, 1H), 1.40 (s, 9H).

Spectral data were in good agreement with literature values.<sup>S7</sup>

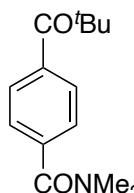


**1h** (white solids, 0.863 g, 3.91 mmol, 39%)

Synthesized according to the procedure B using 10 mmol of methyl 4-iodobenzoate.

**<sup>1</sup>H NMR** (500 MHz, CDCl<sub>3</sub>) δ = 8.07 (d, *J* = 8.5 Hz, 2H), 7.66 (d, *J* = 8.5 Hz, 2H), 3.94 (s, 3H), 1.33 (s, 9H).

Spectral data were in good agreement with literature values.<sup>S1</sup>



**1i** (white solids, 1.68 g, 7.21 mmol, 36%)

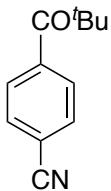
Synthesized according to the procedure B.

**<sup>1</sup>H NMR** (500 MHz, CDCl<sub>3</sub>) δ = 7.69 (d, *J* = 8.5 Hz, 2H), 7.45 (d, *J* = 8.5 Hz, 2H), 3.13 (s, 3H), 2.97 (s, 3H), 1.34 (s, 9H).

**<sup>13</sup>C NMR** (125 MHz, CDCl<sub>3</sub>) δ = 209.0, 170.7, 139.7, 138.5, 127.8, 126.8, 44.3, 39.4, 35.3, 27.9.

**IR** (ATR) 2933.7, 1669.4, 1621.2, 1508.3, 1392.6, 1262.4, 1168.9.

**HRMS** (FD) Calcd for C<sub>14</sub>H<sub>19</sub>NO<sub>2</sub> [M]<sup>+</sup>:233.1416; Found: 233.1410

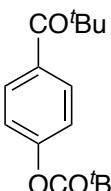


**1j** (pale yellow oil, 1.32 g, 7.03 mmol, 70%)

Synthesized according to the procedure **B**.

**<sup>1</sup>H NMR** (500 MHz, CDCl<sub>3</sub>) δ = 7.71 (s, 4H), 1.33 (s, 9H).

Spectral data were in good agreement with literature values.<sup>55</sup>

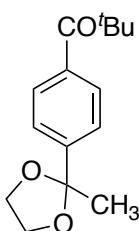


**1k** (white solids, 4.29 g, 16.3 mmol, 82%)

Synthesized according to the procedure **B**.

**<sup>1</sup>H NMR** (500 MHz, CDCl<sub>3</sub>) δ = 7.79 (dd, *J* = 8.5, 2.5 Hz, 2H), 7.10 (dd, *J* = 9.5, 2.3 Hz, 2H), 1.37 (s, 9H). 1.36 (s, 9H).

Spectral data were in good agreement with literature values.<sup>58</sup>



**1l** (white solid, 1.28 g, 5.14 mmol, 26%)

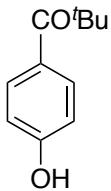
Synthesized according to the procedure **A**.

**<sup>1</sup>H NMR** (500 MHz, CDCl<sub>3</sub>) δ = 7.68 (d, *J* = 8.0 Hz, 2H), 7.51 (d, *J* = 8.0 Hz, 2H), 4.00-4.09 (m, 2H), 3.81-3.75 (m, 2H), 1.66 (s, 3H), 1.35 (s, 9H).

**<sup>13</sup>C NMR** (125 MHz, CDCl<sub>3</sub>) δ = 208.9, 146.1, 138.1, 128.0, 125.0, 108.5, 64.5, 44.2, 28.0, 27.4.

**IR** (ATR) 2971.3, 2935.7, 2883.6, 1669.4, 1605.7, 1568.1, 1465.9, 1401.3, 1369.5, 1273.0, 1242.2, 1220.0, 1191.0, 1175.6, 1142.8.

**HRMS** (ESI) Calcd for C<sub>15</sub>H<sub>20</sub>NaO<sub>3</sub> [M+Na]<sup>+</sup>: 271.1305; Found: 271.1317

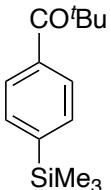


**1m** (white solids, 1.87 g, 10.5 mmol, 52%)

Synthesized according to the procedure A.

**<sup>1</sup>H NMR** (500 MHz, CDCl<sub>3</sub>) δ = 7.71 (dt, *J* = 8.5 Hz, 2H), 6.82 (d, *J* = 8.5 Hz, 2H), 4.86 (s, 1H), 1.33 (s, 9H).

Spectral data were in good agreement with literature values.<sup>S4</sup>

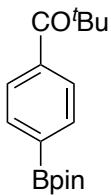


**1n** (colorless oil, 1.27 g, 5.42 mmol, 27%)

Synthesized according to the procedure A.

**<sup>1</sup>H NMR** (500 MHz, CDCl<sub>3</sub>) δ = 7.66 (d, *J* = 8.5 Hz, 2H), 7.55 (d, *J* = 8.0 Hz, 2H), 1.35 (s, 9H). 0.28 (s, 9H).

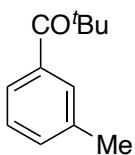
Spectral data were in good agreement with literature values.<sup>S9</sup>



**1o** (pale yellow solids, 0.820 g, 2.85 mmol, 14%)

**1H NMR** (500 MHz,  $\text{CDCl}_3$ )  $\delta$  = 7.83 (d,  $J$  = 8.0 Hz, 2H), 7.61 (d,  $J$  = 9.0 Hz, 2H), 1.35 (s, 12H), 1.33 (s, 9H).

Spectral data were in good agreement with literature values.<sup>S10</sup>

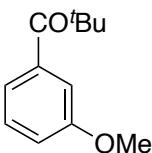


**1p** (colorless oil, 0.654 g, 3.71 mmol, 37%)

Synthesized according to the procedure A using 10 mmol of Mg.

**1H NMR** (500 MHz,  $\text{CDCl}_3$ )  $\delta$  = 7.50-7.45 (m, 2H), 7.30-7.25 (m, 2H), 2.39 (s, 3H), 1.34 (s, 9H).

Spectral data were in good agreement with literature values.<sup>S11</sup>

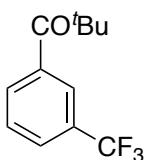


**1q** (colorless oil, 2.85 g, 14.8 mmol, 74%)

Synthesized according to the procedure A.

**1H NMR** (500 MHz,  $\text{CDCl}_3$ )  $\delta$  = 7.33-7.26 (m, 2H), 7.19 (s, 1H), 7.00 (d,  $J$  = 8.0 Hz, 1H), 3.84 (s, 3H), 1.35 (s, 9H).

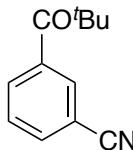
Spectral data were in good agreement with literature values.<sup>S6</sup>



**1r** (colorless oil, 1.28 g, 5.56 mmol, 56%)

**<sup>1</sup>H NMR** (500 MHz, CDCl<sub>3</sub>) δ = 7.93 (s, 1H), 7.87 (d, *J* = 8.0 Hz, 1H), 7.73 (d, *J* = 8.0 Hz, 1H), 7.55 (t, *J* = 8.0, 1H), 1.36 (s, 9H).

Spectral data were in good agreement with literature values.<sup>S12</sup>



**1s** (pale yellow oil, 2.82 g, 15.0 mmol, 69%)

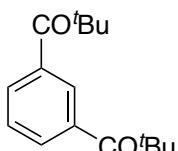
Synthesized according to the procedure **B** using 21.8 mmol of 3-iodobenzonitrile.

**<sup>1</sup>H NMR** (500 MHz, CDCl<sub>3</sub>) δ = 7.95 (s, 1H), 7.90 (d, *J* = 8.0 Hz, 1H), 7.75 (d, *J* = 8.0 Hz, 1H), 7.55 (t, *J* = 8.0, 1H), 1.35 (s, 9H).

**<sup>13</sup>C NMR** (125 MHz, CDCl<sub>3</sub>) δ = 207.1, 139.5, 134.0, 131.9, 131.4, 129.1, 118.1, 112.6, 44.4, 27.8.

**IR** (ATR) 2972.3, 2873.9, 2231.6, 1680.0, 1477.5, 1367.5, 1276.9, 1215.2, 1149.6

The satisfactory data for HRMS analysis was not obtained by ESI- and FD-MS.

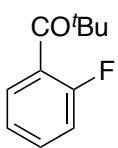


**1t** (white solids, 1.35 g, 15.0 mmol, 69%)

Synthesized according to the procedure **A** using 40 mmol of Mg and 10 mL of pivaloyl chloride.

**<sup>1</sup>H NMR** (500 MHz, CDCl<sub>3</sub>) δ = 8.03 (s, 1H), 7.79 (dd, *J* = 8.0, 2.0 Hz, 2H), 7.46 (t, *J* = 8.0 Hz, 1H), 1.37 (s, 18H).

Spectral data were in good agreement with literature values.<sup>S13</sup>

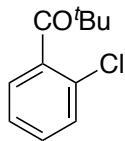


**1u** (colorless oil, 1.48 g, 8.22 mmol, 41%)

Synthesized according to the procedure **A**.

**<sup>1</sup>H NMR** (500 MHz, CDCl<sub>3</sub>) δ = 7.40-7.34 (m, 1H), 7.21-7.13 (m, 2H), 7.09 (t, *J* = 9.0 Hz, 1H), 1.23 (s, 9H).

Spectral data were in good agreement with literature values.<sup>S14</sup>

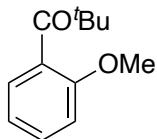


**1v** (colorless oil, 2.10 g, 10.7 mmol, 54%)

Synthesized according to the procedure **B**.

**$^1\text{H NMR}$**  (500 MHz,  $\text{CDCl}_3$ )  $\delta$  = 7.39 (dd,  $J$  = 7.8, 1.4 Hz, 1H), 7.31 (td,  $J$  = 7.9, 2.0 Hz, 1H), 7.27 (td,  $J$  = 7.6, 1.5 Hz, 1H), 7.15 (dd,  $J$  = 7.5, 1.7 Hz, 1H), 1.27 (s, 9H).

Spectral data were in good agreement with literature values.<sup>S15</sup>



**1w** (colorless oil, 2.10 g, 10.7 mmol, 54%)

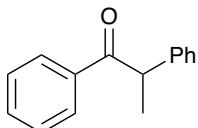
Synthesized according to the procedure **A**.

**$^1\text{H NMR}$**  (500 MHz,  $\text{CDCl}_3$ )  $\delta$  = 7.31 (,  $J$  = 8.0 Hz, 1H), 7.02 (d,  $J$  = 7.5 Hz, 1H), 6.94 (t,  $J$  = 7.5 Hz, 1H), 6.90 (d,  $J$  = 8.5 Hz, 1H), 3.78 (s, 3H), 1.21 (s, 9H).

Spectral data were in good agreement with literature values.<sup>S11</sup>

### **General procedures for the preparation of alkyl phenyl ketones**

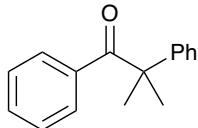
Alkyl phenyl ketones **3a**, **3b**, **3f** and **3g** were obtained from chemical suppliers and used after proper recrystallization or distillation. **3c-e** and **3h** were synthesized according to literature procedures. All ketones are known compounds in literatures as referenced, and spectral data were in good agreement with literature values.



**3c** (pale yellow solids, 1.38 g, 6.56 mmol, 33%)<sup>S16</sup>

**<sup>1</sup>H NMR** (500 MHz, CDCl<sub>3</sub>) δ = 7.95 (d, *J* = 7.5 Hz, 2H), 7.47 (t, *J* = 7.5 Hz, 1H), 7.38 (t, *J* = 8.0 Hz, 2H), 7.32-7.27 (m, 4H), 7.23-7.17 (m, 1H), 4.69 (q, *J* = 7.0 Hz, 1H), 1.53 (d, *J* = 7.0 Hz, 3H).

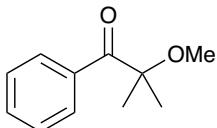
Spectral data were in good agreement with literature values.<sup>S16</sup>



**3d** (white solids, 1.52 g, 6.78 mmol, 33%)<sup>S17</sup>

**<sup>1</sup>H NMR** (500 MHz, CDCl<sub>3</sub>) δ = 7.48 (d, *J* = 7.5 Hz, 2H), 7.38-7.30 (m, 5H), 7.29-7.25 (m, 1H), 7.22 (t, *J* = 7.5 Hz, 2H), 1.61 (s, 6H).

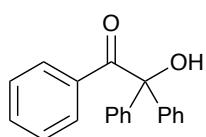
Spectral data were in good agreement with literature values.<sup>S17</sup>



**3e** (white solids, 3.27 g, 18.3 mmol, 80%)<sup>S18</sup>

**<sup>1</sup>H NMR** (500 MHz, CDCl<sub>3</sub>) δ = 8.28 (dd, *J* = 8.5, 1.0 Hz, 2H), 7.55 (t, *J* = 7.5 Hz, 1H), 7.44 (t, *J* = 7.5 Hz, 2H), 3.20 (s, 3H), 1.52 (s, 6H).

Spectral data were in good agreement with literature values.<sup>S18</sup>

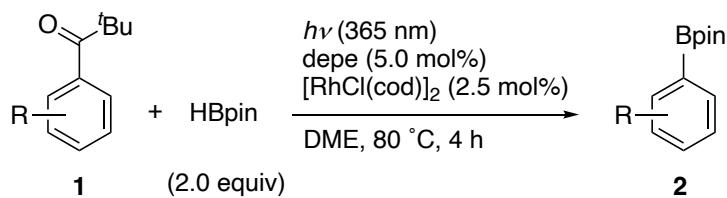


**3h** (white solids, 3.91 g, 13.6 mmol, 36%)<sup>S19</sup>

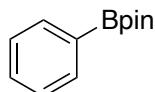
**<sup>1</sup>H NMR** (500 MHz, CDCl<sub>3</sub>) δ = 7.71 (dd, *J* = 8.5, 1.0 Hz, 2H), 7.47-7.38 (m, 5H), 7.37-7.27 (m, 8H), 4.98 (s, 1H).

Spectral data were in good agreement with literature values.<sup>S19</sup>

**A general procedure for the borylation of pivalophenone derivatives (Table 2)**



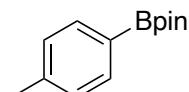
A solution of  $[\text{RhCl}(\text{cod})]_2$  (6.2 mg, 0.0125 mmol), depe (5.9  $\mu\text{L}$ , 0.025 mmol), a pivalophenone derivative (0.5 mmol) and HBpin (145.0  $\mu\text{L}$ , 1.0 mmol) in DME (5 mL) was placed in a sealed glass tube. The solution was photoirradiated at 365 nm with stirring at 80 °C. After 4 h, the solvent was removed under reduced pressure to give a crude mixture, in which the yields of arylboronates were determined by  $^1\text{H}$  NMR using tetrachloroethane as an internal standard or GC analysis using dodecane as an internal standard. The crude product was purified by silica gel column chromatography or PTLC to afford arylboronates **2a-w**.



**2a** (white solids, 59.2 mg, 0.29 mmol, 58%) (NMR yield = 68%)

$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  = 7.81 (d,  $J$  = 6.9 Hz, 2H), 7.46 (t,  $J$  = 7.4 Hz, 1H), 7.37 (t,  $J$  = 7.4 Hz, 2H), 1.35 (s, 12H).

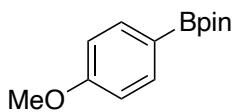
Spectral data were in good agreement with literature values.<sup>S20</sup>



**2b** (white solids, 67.6 mg, 0.31 mmol, 62%) (NMR yield = 83%)

$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  = 7.70 (d,  $J$  = 7.5 Hz, 2H), 7.18 (d,  $J$  = 8.0 Hz, 2H), 2.36 (s, 3H), 1.33 (s, 12H).

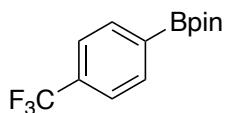
Spectral data were in good agreement with literature values.<sup>S20</sup>



**2c** (white solids, 82.7 mg, 0.35 mmol, 71%) (NMR yield = 81%)

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ = 7.75 (d, *J* = 8.0 Hz, 2H), 6.90 (d, *J* = 8.5 Hz, 2H), 3.83 (s, 3H), 1.33 (s, 12H).

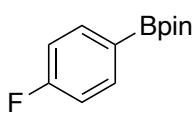
Spectral data were in good agreement with literature values.<sup>S20</sup>



**2d** (white solids, 73.2 mg, 0.27 mmol, 55%) (NMR yield = 72%)

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ = 7.91 (d, *J* = 8.0 Hz, 2H), 7.61 (d, *J* = 8.0 Hz, 2H), 1.36 (s, 12H).

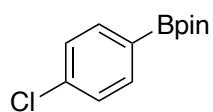
Spectral data were in good agreement with literature values.<sup>S20</sup>



**2e** (colorless oil, 69.7 mg, 0.31 mmol, 63%) (NMR yield = 84%)

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ = 7.80 (dd, *J* = 8.0, 6.0 Hz, 2H), 7.04 (t, *J* = 9.0 Hz, 2H), 1.33 (s, 12H).

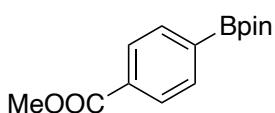
Spectral data were in good agreement with literature values.<sup>S20</sup>



**2f** (white solids, 65.9 mg, 0.28 mmol, 55%) (NMR yield = 71%)

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ = 7.73 (d, *J* = 8.5 Hz, 2H), 7.33 (d, *J* = 8.5 Hz, 2H), 1.33 (s, 12H).

Spectral data were in good agreement with literature values.<sup>S20</sup>

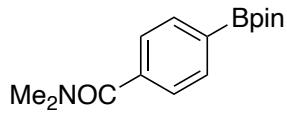


**2h**

**2h** (white solids, 59.4 mg, 0.23 mmol, 45%) (NMR yield = 66%)

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ = 8.02 (d, *J* = 8.0 Hz, 2H), 7.87 (d, *J* = 8.5 Hz, 2H), 3.92 (s, 3H), 1.36 (s, 12H).

Spectral data were in good agreement with literature values.<sup>S20</sup>

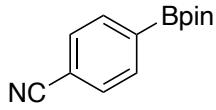


**2i**

**2i** (white solids, 110.4 mg, 0.4012 mmol, 80%) (NMR yield = 89%)

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ = 7.84 (d, *J* = 8.0 Hz, 2H), 7.40 (d, *J* = 8.0 Hz, 2H), 3.11 (s, 3H), 2.95 (s, 3H), 1.35 (s, 12H).

Spectral data were in good agreement with literature values.<sup>S23</sup>

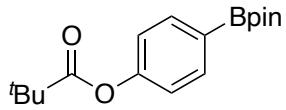


**2j**

**2j** was obtained as an inseparable mixture with **1j** (52.7 mg). The amount of **2j** was calculated to be 0.209 mmol (42%) from the <sup>1</sup>H NMR. (NMR yield = 58%)

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ = 7.86 (d, *J* = 8.5 Hz, 2H), 7.62 (d, *J* = 9.0 Hz, 2H), 1.33 (s, 12H).

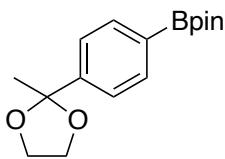
Spectral data were in good agreement with literature values.<sup>S20</sup>



**2k** (white solids, 76.0 mg, 0.250 mmol, 50%) (NMR yield = 53%)

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ = 7.83 (d, *J* = 8.5 Hz, 2H), 7.06 (d, *J* = 8.5 Hz, 2H), 1.35 (s, 9H), 1.34 (s, 12H).

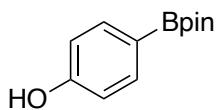
Spectral data were in good agreement with literature values.<sup>S8</sup>



**2l** (white solids, 71.7 mg, 0.25 mmol, 50%) (NMR yield = 76%)

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ = 7.80 (d, *J* = 8.0 Hz, 2H), 7.49 (d, *J* = 8.0 Hz, 2H), 4.05-4.02 (m, 2H), 3.78-3.72 (m, 2H), 1.64 (s, 3H), 1.34 (s, 12H).

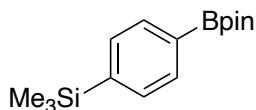
Spectral data were in good agreement with literature values.<sup>S24</sup>



**2m** (white solids, 94.9 mg, 0.43 mmol, 86%) (NMR yield = 76%)

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ = 7.69 (d, *J* = 8.5 Hz, 2H), 6.82 (d, *J* = 8.5 Hz, 2H), 6.48 (s, 1H), 1.34 (s, 12H).

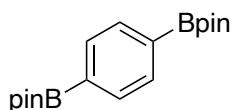
Spectral data were in good agreement with literature values.<sup>S20</sup>



**2n** (white solids, 77.6 mg, 0.28 mmol, 56%) (NMR yield = 53%)

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ = 7.83 (d, *J* = 8.0 Hz, 2H), 7.57 (d, *J* = 8.0 Hz, 2H), 1.37 (s, 12H), 0.30 (s, 9H).

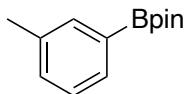
Spectral data were in good agreement with literature values.<sup>S22</sup>



**2o** (white solids, 108.8 mg, 0.33 mmol, 66%) (NMR yield = quant.)

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ = 7.80 (s, 4H), 1.35 (s, 24H).

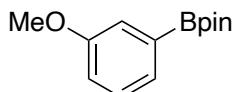
Spectral data were in good agreement with literature values.<sup>S20</sup>



**2p** (white solids, 68.8 mg, 0.32 mmol, 63%) (NMR yield = 78%)

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ = 7.64 (s, 1H), 7.65–7.60 (m, 1H), 7.27–7.25 (m, 2H), 2.35 (s, 3H), 1.34 (s, 12H).

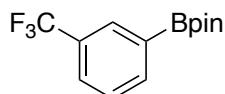
Spectral data were in good agreement with literature values.<sup>S20</sup>



**2q** (white solids, 73.6 mg, 0.31 mmol, 63%) (NMR yield = 76%)

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ = 7.40 (d, *J* = 7.0 Hz, 1H), 7.33 (d, *J* = 2.5 Hz, 1H), 7.29 (t, *J* = 8.0 Hz, 1H), 8.01 (ddd, *J* = 8.0, 3.0, 1.0 Hz, 1H), 3.83 (s, 3H), 1.35 (s, 12H).

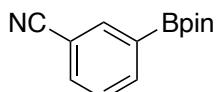
Spectral data were in good agreement with literature values.<sup>S22</sup>



**2r** (white solids, 110.2 mg, 0.41 mmol, 81%) (NMR yield = 76%)

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ = 8.06 (s, 1H), 7.97 (d, *J* = 7.0 Hz, 1H), 7.70 (d, *J* = 8.0 Hz, 1H), 7.49 (t, *J* = 7.5 Hz, 1H), 1.36 (s, 12H).

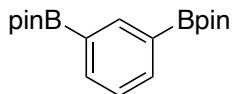
Spectral data were in good agreement with literature values.<sup>S24</sup>



**2s** (white solids, 52.4 mg, 0.229 mmol, 46%) (NMR yield = 57%)

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ = 8.10 (s, 1H), 8.01 (d, *J* = 7.5 Hz, 1H), 7.72 (d, *J* = 7.5 Hz, 1H), 7.47 (t, *J* = 8.0 Hz, 1H), 1.36 (s, 12H).

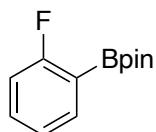
Spectral data were in good agreement with literature values.<sup>S20</sup>



**2t** (white solids, 35.7 mg, 0.108 mmol, 22%) (NMR yield = 49%)

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ = 8.29 (s, 1H), 7.90 (dd, *J* = 7.5, 2.0 Hz, 2H), 7.38 (t, *J* = 7.5 Hz, 1H), 1.34 (s, 24H).

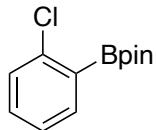
Spectral data were in good agreement with literature values.<sup>S20</sup>



**2u** (white solids, 71.3 mg, 0.321 mmol, 64%) (NMR yield = 79%)

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ = 7.76–7.72 (m, 1H), 7.46–7.41 (m, 1H), 7.14 (t, *J* = 7.5 Hz, 1H), 7.03 (t, *J* = 8.5 Hz, 1H), 1.37 (s, 12H).

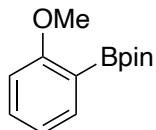
Spectral data were in good agreement with literature values.<sup>S20</sup>



**2v** (white solids, 74.5 mg, 0.312 mmol, 62%) (NMR yield = 80%)

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ = 7.68 (d, *J* = 8.0 Hz, 1H), 7.40–7.29 (m, 2H), 7.24–7.19 (m, 1H), 1.36 (s, 12H).

Spectral data were in good agreement with literature values.<sup>S25</sup>

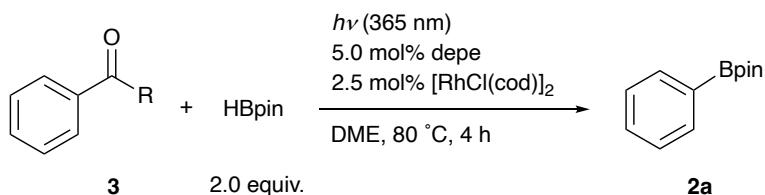


**2w** (white solids, 65.1 mg, 0.28 mmol, 56%) (NMR yield = 80%)

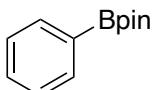
<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ = 7.68 (dd, *J* = 9.0, 1.7 Hz, 1H), 7.41–7.37 (m, 1H), 6.94 (t, *J* = 8.0 Hz, 1H), 6.85 (dd, *J* = 8.0, 1 H), 3.82 (s, 3H), 1.35 (s, 12H).

Spectral data were in good agreement with literature values.<sup>S20</sup>

**A general procedure for the borylation of alkyl phenyl ketones (Table 3)**



A solution of  $[\text{RhCl}(\text{cod})]_2$  (6.2 mg, 0.0125 mmol), depe (5.9  $\mu\text{L}$ , 0.025 mmol), an alkyl phenyl ketone (0.50 mmol) and HBpin (145.0  $\mu\text{L}$ , 1.0 mmol) in DME (5 mL) was placed in a sealed glass tube. The solution was photoirradiated at 365 nm with stirring at 80 °C. After 4 h, the solvent was removed under reduced pressure to give a crude mixture, in which the yield of phenylboronic acid pinacol ester **2a** was determined by  $^1\text{H}$  NMR using tetrachloroethane as an internal standard. The crude product was purified by silica gel column chromatography to afford phenylboronic acid pinacol ester **2a**. For the reaction of **3g** and **3h**, separation of **2a** from **3** was difficult. Therefore, the crude mixture was treated with  $\text{KHF}_2$  to convert **2a** to  $\text{PhBF}_3\text{K}$  **2a'**, which was isolated by washing with hexanes and a small amount of cold MeOH (ca. –20 °C).



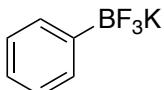
**2a** from **3b** (white solids, 16.3 mg, 0.080 mmol, 16%) (NMR yield = 30%)

**2a** from **3c** (white solids, 48.6 mg, 0.238 mmol, 48%) (NMR yield = 45%)

**2a** from **3d** (white solids, 47.0 mg, 0.230 mmol, 46%) (NMR yield = 59%)

**2a** from **3e** (white solids, 37.6 mg, 0.184 mmol, 37%) (NMR yield = 43%)

**2a** from **3f** (white solids, 10.2 mg, 0.050 mmol, 10%) (NMR yield = 17%)



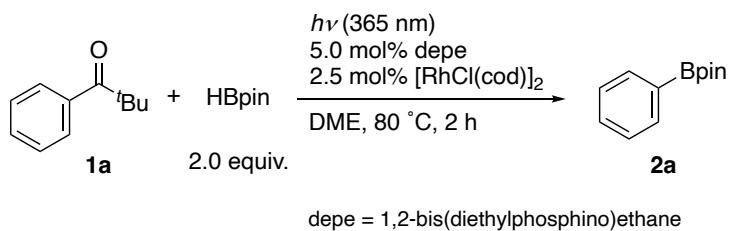
**2a'** from **3g** (white solids, 5.8 mg, 0.032 mmol, 6%) (NMR yield = 16%)

**2a'** from **3h** (white solids, 13.8 mg, 0.075 mmol, 15%) (NMR yield = 26%)

$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  = 7.81 (d,  $J$  = 6.9 Hz, 2H), 7.46 (t,  $J$  = 7.4 Hz, 1H), 7.37 (t,  $J$  = 7.4 Hz, 2H), 1.35 (s, 12H).

Spectral data were in good agreement with literature values.<sup>S21</sup>

## Optimization of reaction conditions



**Table S1.** Optimization of reaction conditions.

entry	variation from the standard conditions	yield of <b>2a</b> <sup>a</sup>
1	—	68% (58%) <sup>b</sup>
2	dmpe instead of depe	19%
3	dippe instead of depe	12%
4	dtbpe instead of depe	12%
5	dppp instead of depe	54%
6	dppbz instead of depe	19%
7	depbz instead of depe	19%
8	DMA instead of DME	41%
9	toluene instead of DME	61%
10	[Rh(cod)I] <sub>2</sub> instead of [Rh(cod)Cl] <sub>2</sub>	58%
11	[Rh(ethylene) <sub>2</sub> Cl] <sub>2</sub> instead of [Rh(cod)Cl] <sub>2</sub>	53%
12	[Rh(coe) <sub>2</sub> Cl] <sub>2</sub> instead of [Rh(cod)Cl] <sub>2</sub>	50%

<sup>a</sup> Determined by NMR using 1,1,2,2-tetrachloroethane as an internal standard. <sup>b</sup> Isolated yield.

dmpe = 1,2-bis(dimethylphosphino)ethane

dippe = 1,2-bis(di-*i*-propylphosphino)ethane

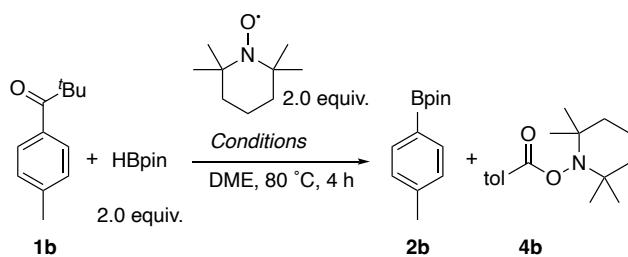
dtbpe = 1,2-bis(di-*tert*-butylphosphino)ethane

dppe = 1,2-bis(diphenylphosphino)ethane

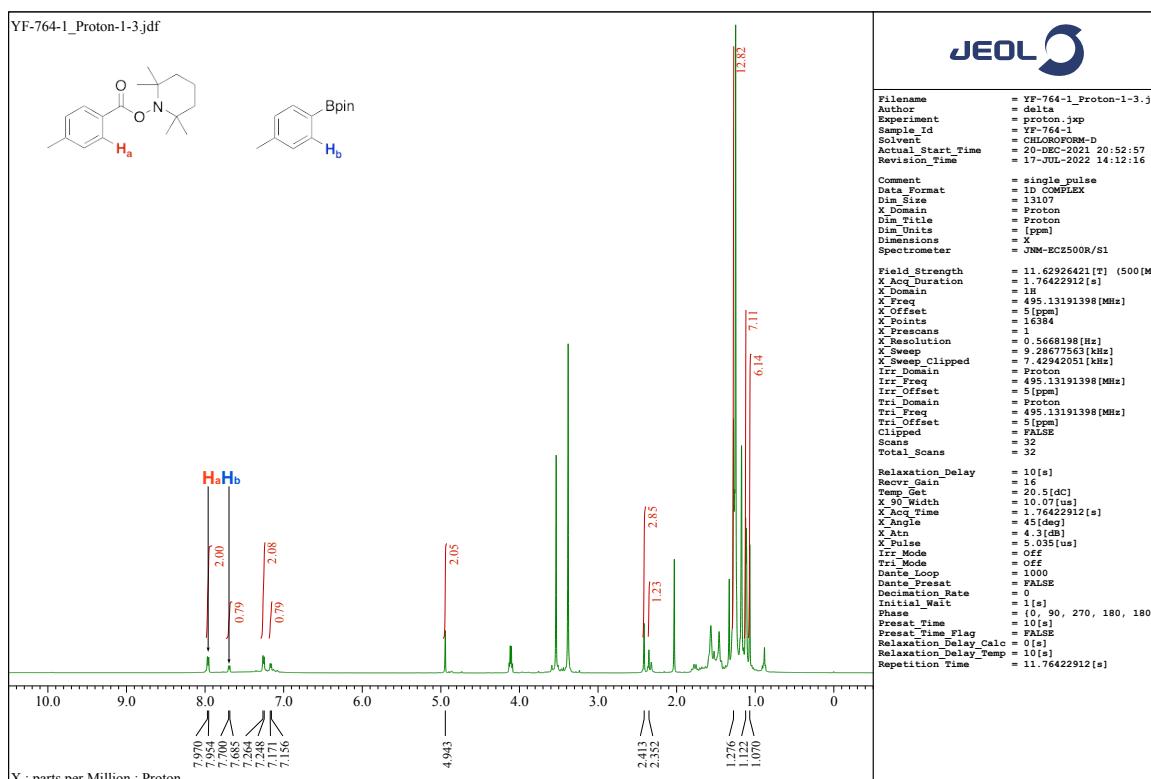
dppbz = 1,2-bis(diphenylphosphino)benzene

depbz = 1,2-bis(diethylphosphino)benzene

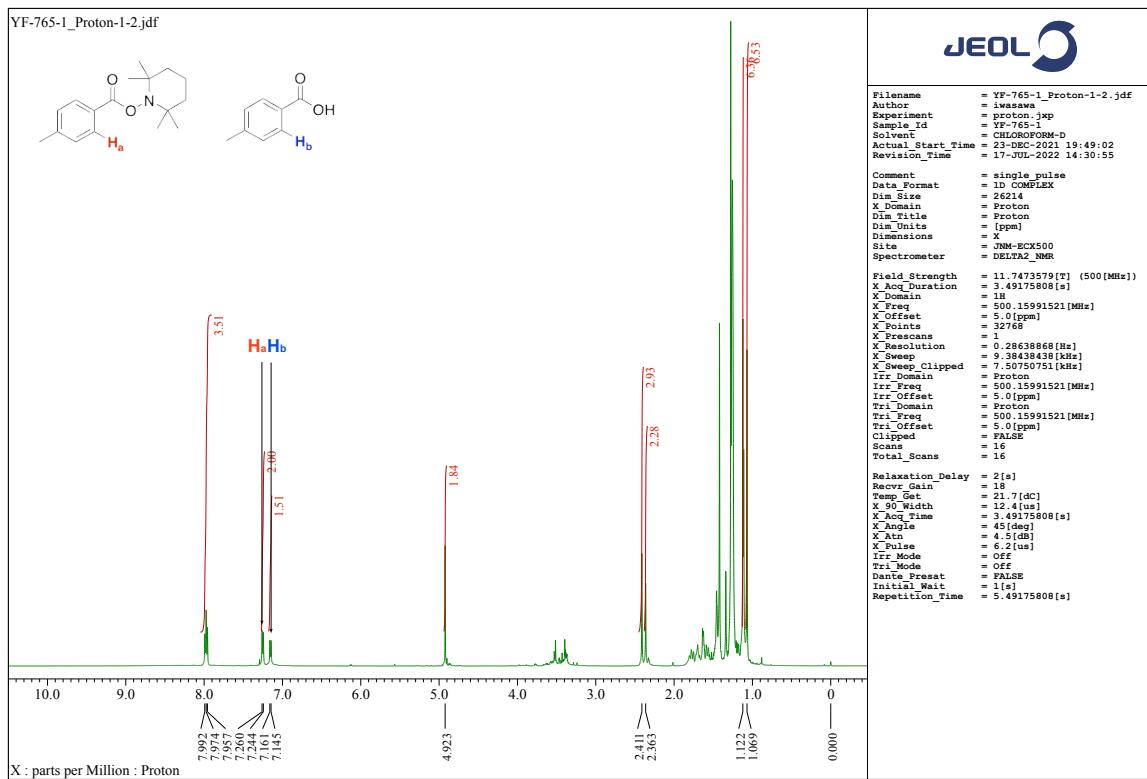
## Procedures for radical trapping experiments (Table 4)



For the experiment in entry 1, a solution of  $[\text{RhCl}(\text{cod})]_2$  (2.5 mg, 0.0050 mmol), depe (2.4  $\mu\text{L}$ , 0.01 mmol),  $t$ -butyl *p*-tolyl ketone **1b** (35.3 mg, 0.20 mmol), TEMPO (62.5 mg, 0.40 mmol) and HBpin (58.0  $\mu\text{L}$ , 0.4 mmol) in DME (2.0 mL) was placed in a sealed glass tube. The solution was photoirradiated at 365 nm with stirring at 80  $^\circ\text{C}$  for 4 hours. After removal of the solvent and volatile compounds, the crude mixture was analyzed by  $^1\text{H}$  NMR in  $\text{CDCl}_3$  to determine the yield of **2b** and **4b** using dibromomethane (14.0  $\mu\text{L}$ , 0.20 mmol) as an internal standard. Spectral data were in good agreement with literature values.<sup>S20, S25</sup> Other radical trapping experiments in the absence of the Rh catalyst (entry 2) or without photoirradiation (entry 3) were also conducted according to the same procedure.

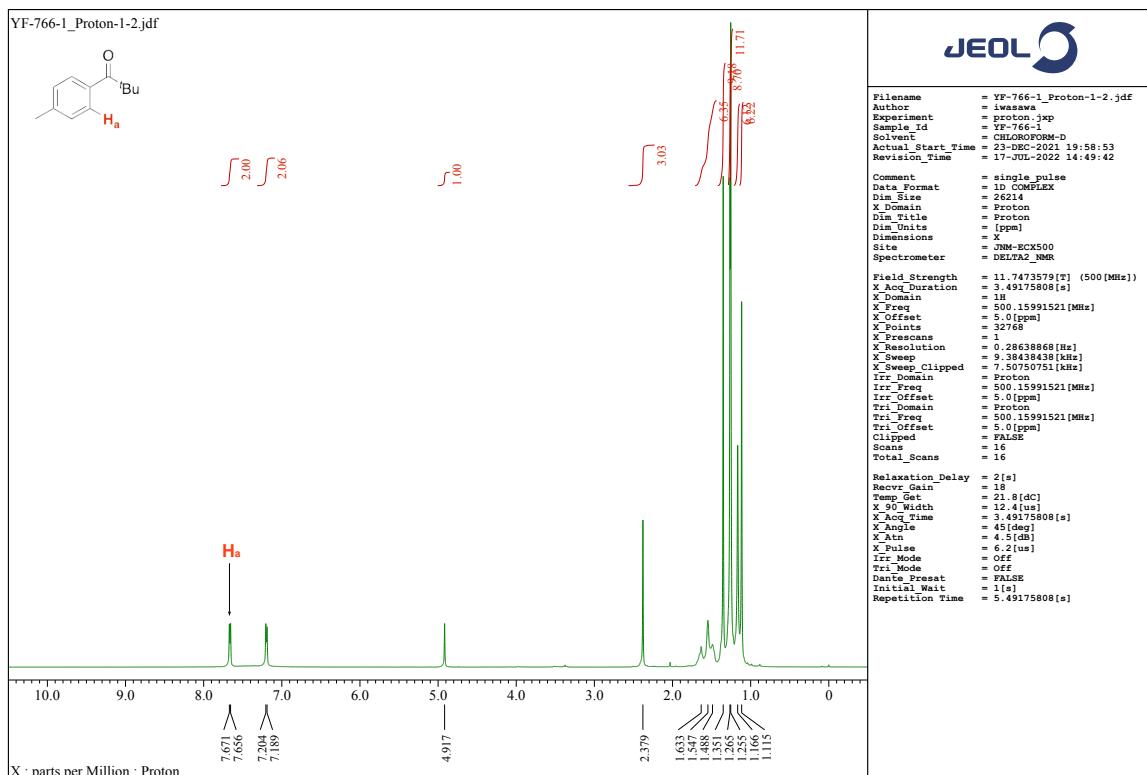


**Figure S2.** The radical trapping experiment under the standard conditions (entry 1).



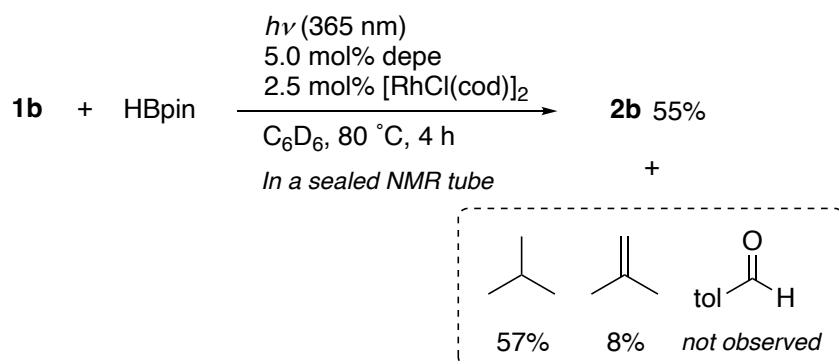
**Figure S3.** The radical trapping experiment without  $[\text{RhCl}(\text{cod})_2]$  and depe (entry 2).<sup>a</sup>

<sup>a</sup> We confirmed that **4b** further reacted with HBpin to generate *p*-methylbenzoic acid under the reaction conditions. Therefore, the yield of the radical-TEMPO adduct was calculated to be the combined yield of **4b** and *p*-methylbenzoic acid.

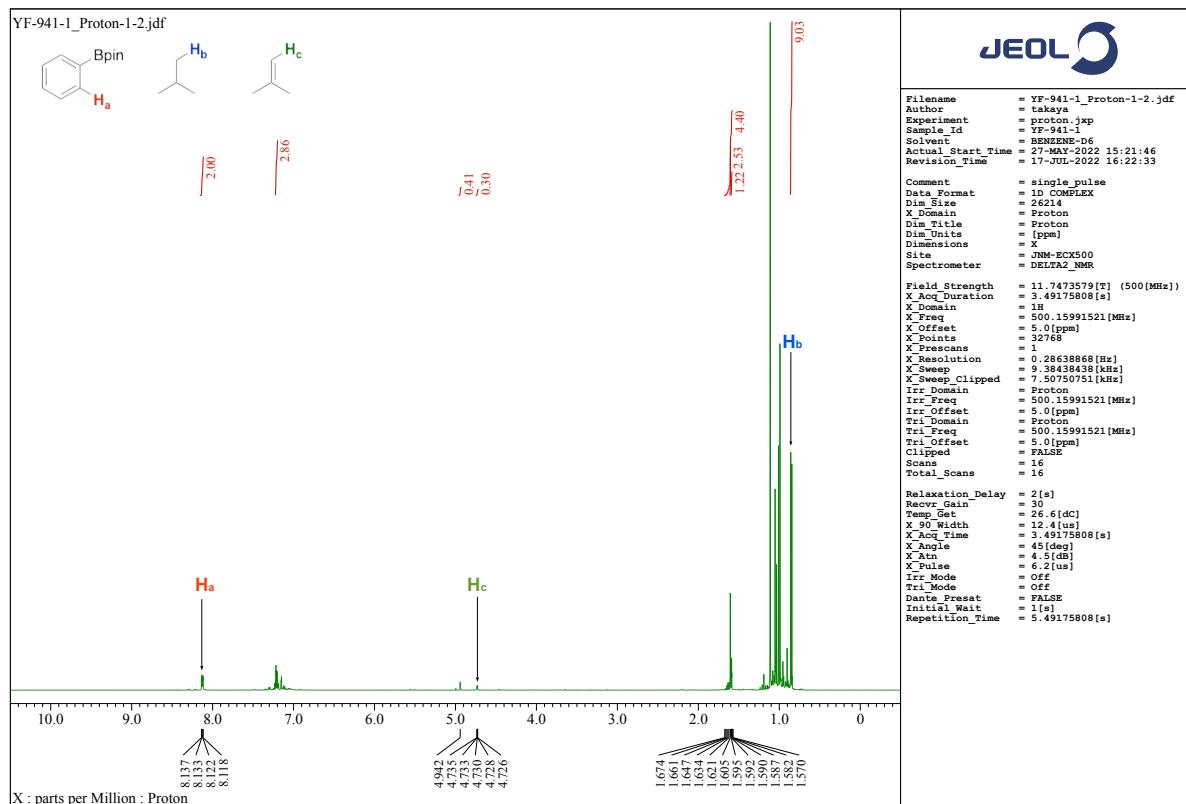


**Figure S4.** The radical trapping experiment without  $h\nu$  (entry 3).

## An NMR experiment in a sealed NMR tube (Scheme 1)

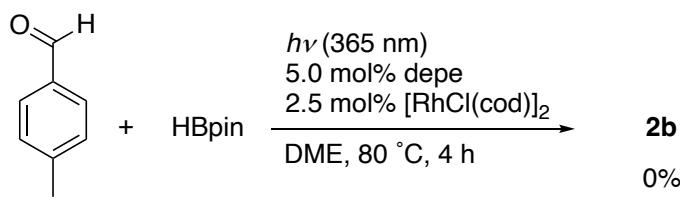


A solution of  $[\text{RhCl}(\text{cod})]_2$  (1.2 mg, 0.0025 mmol), depe (1.2  $\mu\text{L}$ , 0.005 mmol), pivalophenone **1a** (16.7 mg, 0.10 mmol), and HBpin (58  $\mu\text{L}$ , 0.20 mmol) in  $\text{C}_6\text{D}_6$  (0.5 mL) was placed in a sealed NMR tube. The solution was photoirradiated at 365 nm without stirring at 80  $^\circ\text{C}$  for 4 hours. The solution was analyzed by  $^1\text{H}$  NMR, demonstrating the formation of 2-methylpropane and 2-methylpropene as major by-products. The yields were determined after adding 1,1,2,2-teetrachloroethane quickly into the NMR tube as an internal standard.

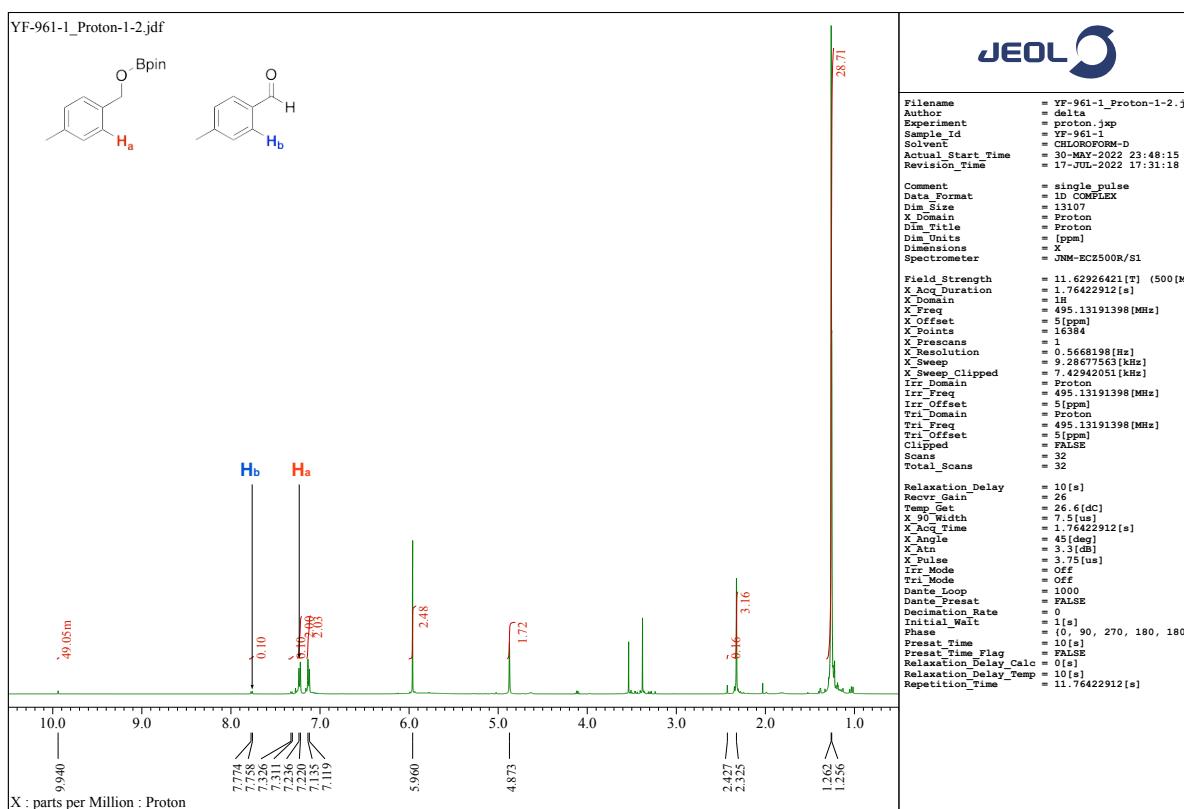


**Figure S5.**  $^1\text{H}$  NMR after the reaction (NMR experiment in  $\text{C}_6\text{D}_6$ )

### A reaction of aldehyde (Scheme 2)

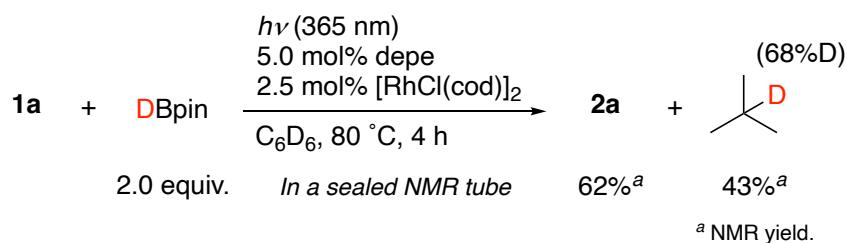


A solution of  $[\text{RhCl(cod)}]_2$  (6.2 mg, 0.012 mmol), depe (2.4  $\mu\text{L}$ , 0.025 mmol), *p*-tolualdehyde (59.6 mg, 0.496 mmol) and HBpin (145  $\mu\text{L}$ , 1.0 mmol) in DME (5.0 mL) was placed in a sealed glass tube. The solution was photoirradiated at 365 nm with stirring at 80  $^\circ\text{C}$  for 4 hours. After removal of the solvent and volatile compounds, the crude mixture was analyzed by  $^1\text{H}$  NMR with 1,1,2,2-tetrachloroethane as an internal standard (50.0  $\mu\text{L}$ , 0.472 mmol), supporting no formation of *p*-tolylboronate **2b** and formation of hydroboration product in 71% yield.



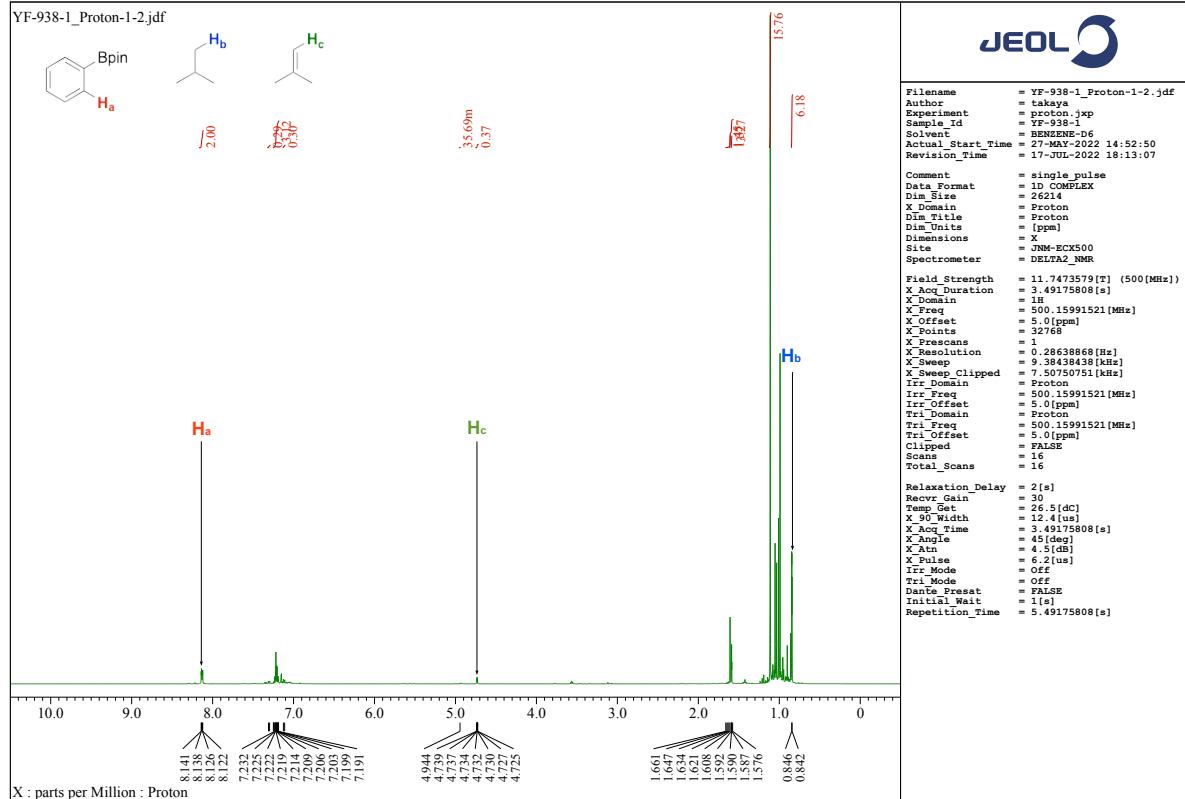
**Figure S6.**  $^1\text{H}$  NMR of the reaction of *p*-tolualdehyde under the standard conditions

### A deuterium labeling experiment (Scheme 3)



<sup>a</sup> NMR yield.

A solution of  $[\text{RhCl}(\text{cod})_2$  (1.2 mg, 0.0025 mmol), depe (1.2  $\mu\text{L}$ , 0.0050 mmol), pivalophenone **1a** (16.7 mg, 0.10 mmol), and DBpin (51.6 mg, 0.20 mmol) in  $\text{C}_6\text{D}_6$  (0.5 mL) was placed in a sealed NMR tube. The solution was photoirradiated at 365 nm without stirring at 80 °C for 4 hours. The solution was analyzed by  $^1\text{H}$  NMR after adding 1,1,2,2-tetrachloroethane quickly, demonstrating the formation of **2a** in 62% yield and 2-methylpropane in 43% yield. The incorporation of a deuterium at the methine carbon was confirmed by  $^1\text{H}$  NMR. The D-content of 2-methylpropane was determined to be 68% by EI-MS, in which the relative abundance of non-labeled 2-methylpropane ( $m/z$  58) to D-labeled one ( $m/z$  59, including a natural isotope of non-labeled 2-methylprpopane) was 126628:268735.



**Figure S7.**  $^1\text{H}$  NMR of the deuterium labeling experiment before adding an internal standard

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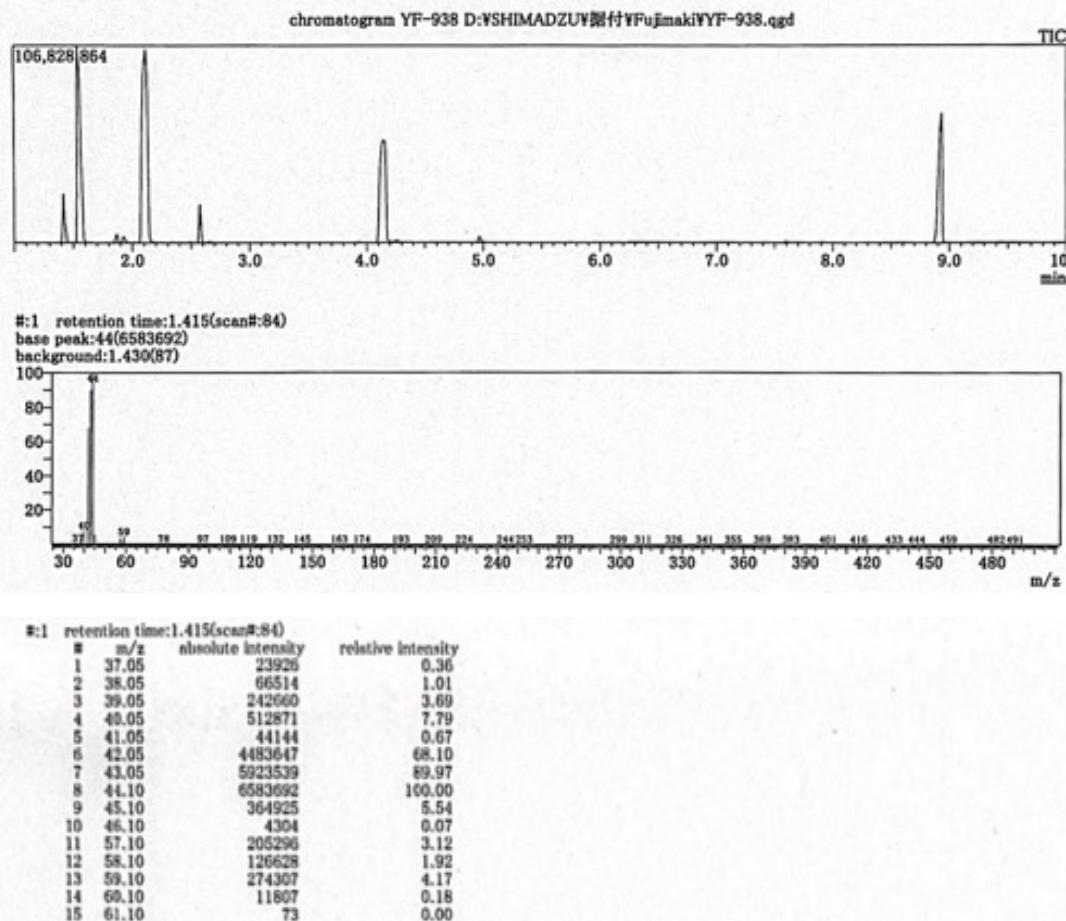
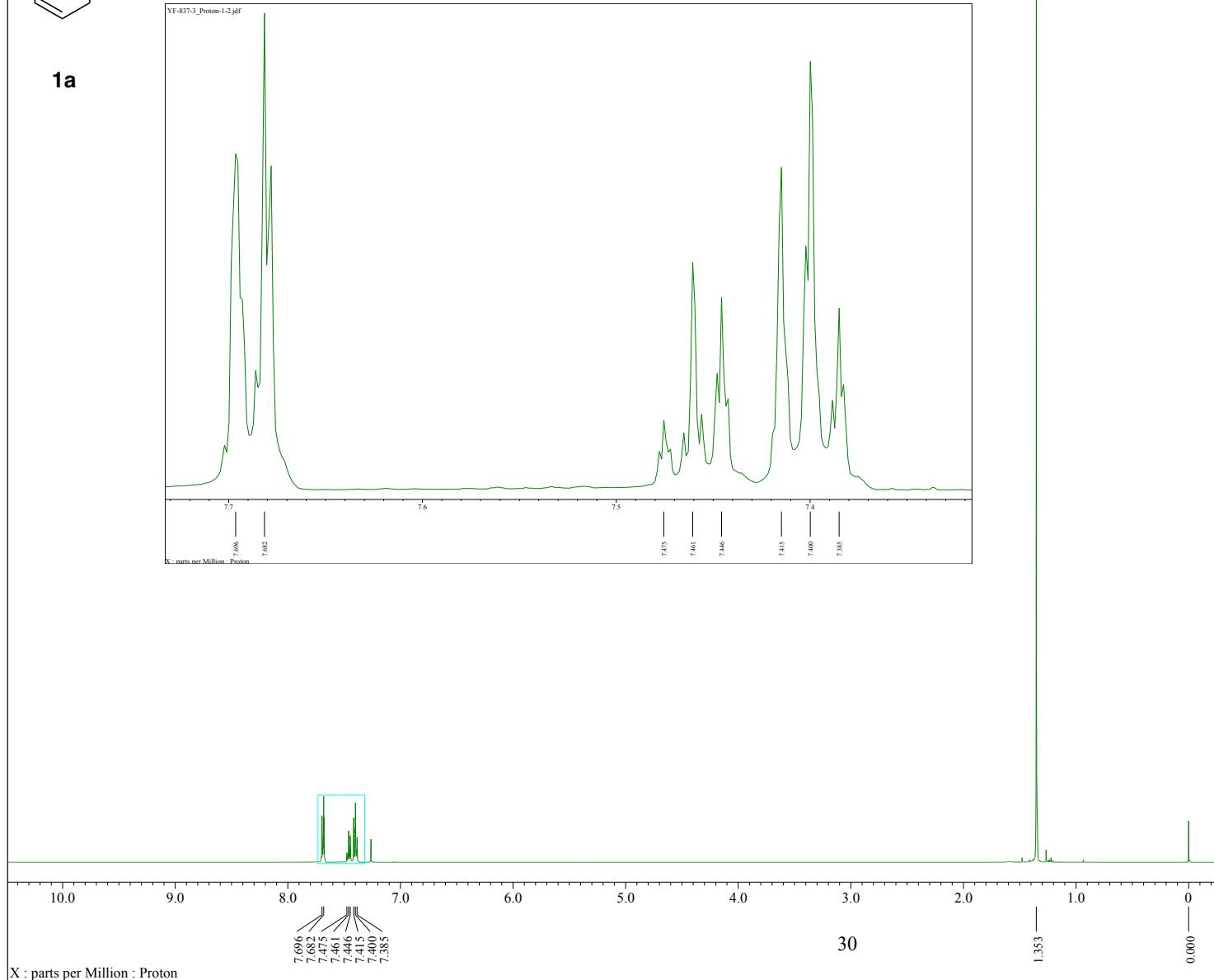
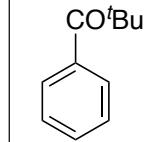


Figure S8. EI-MS spectra

## References

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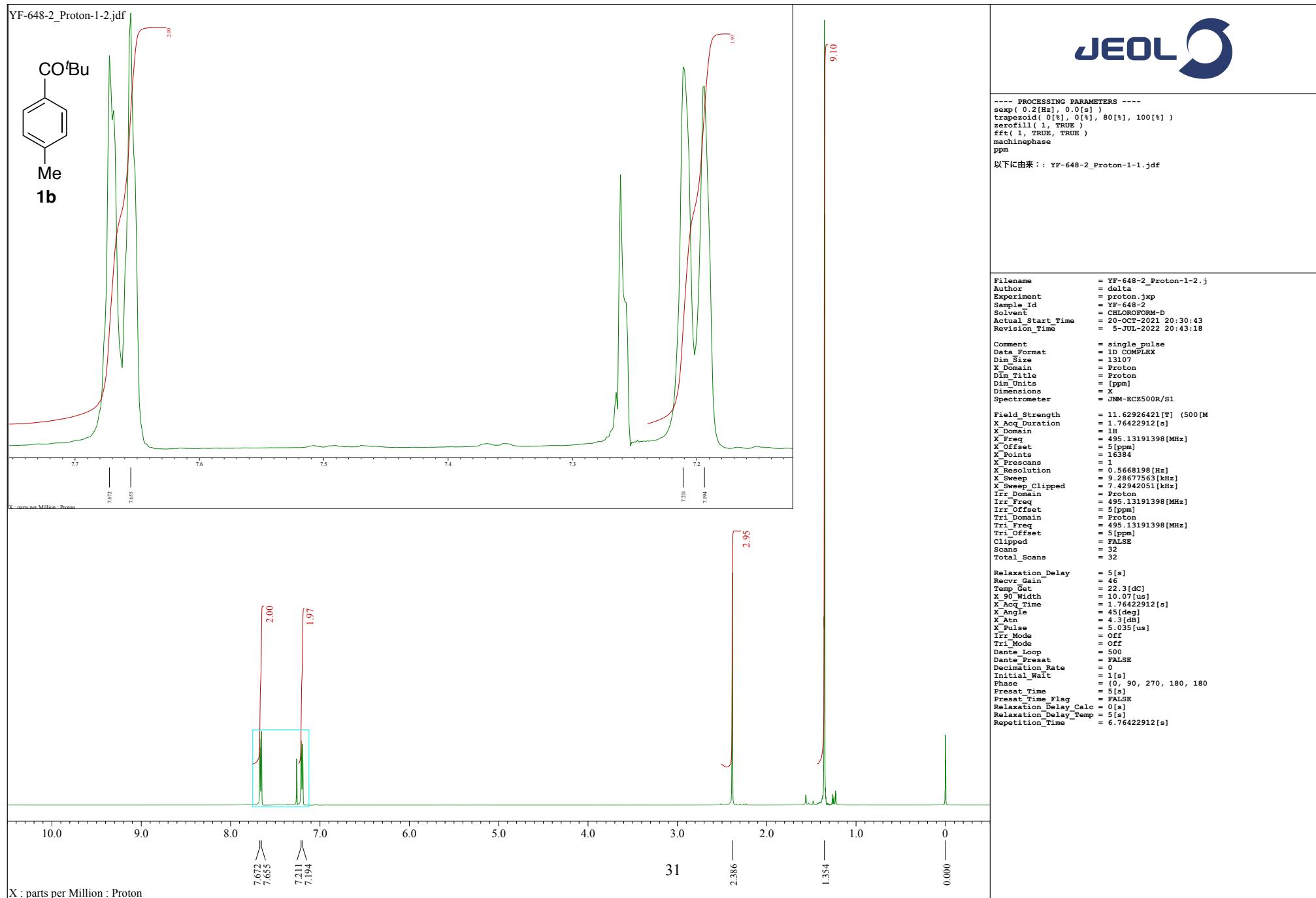
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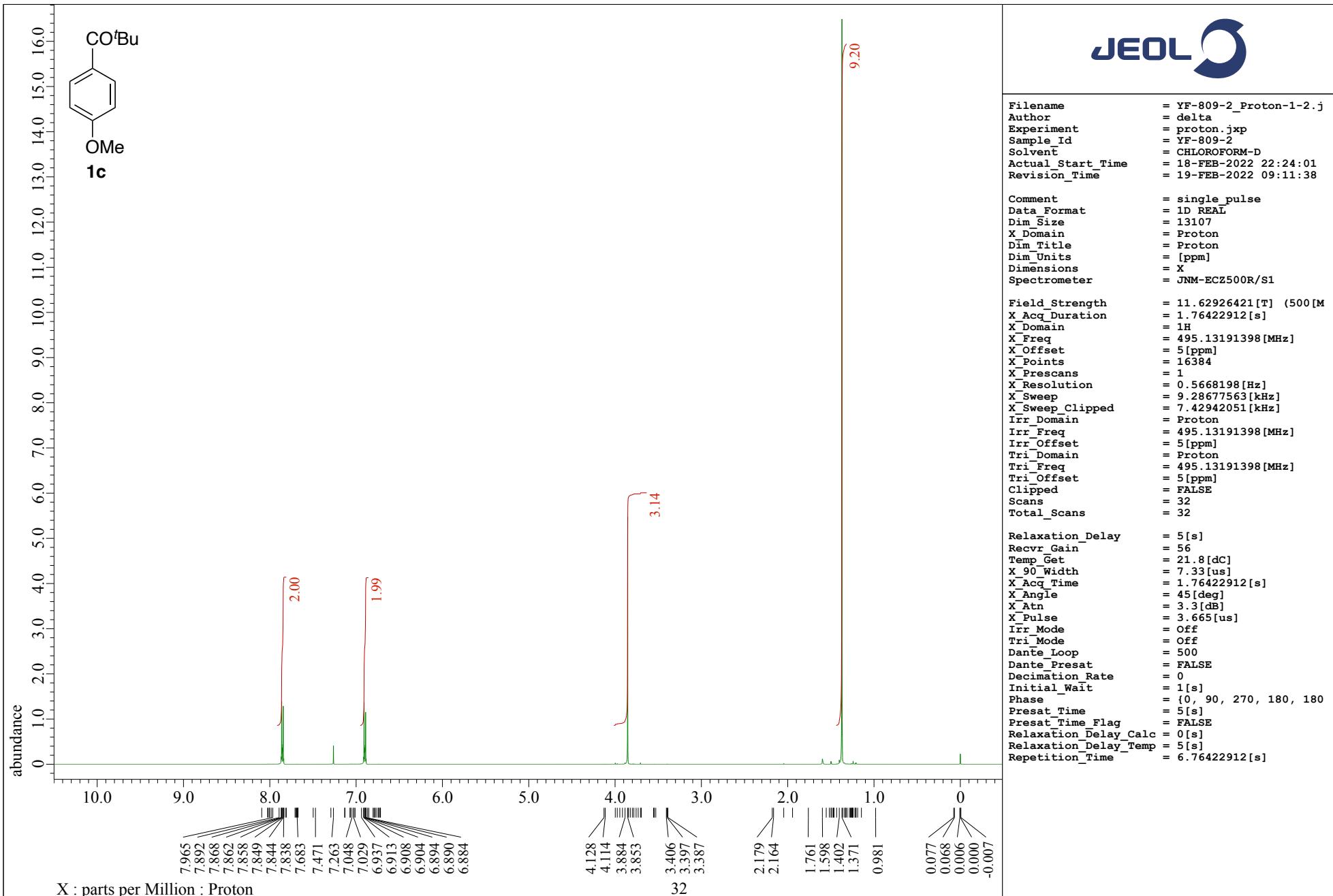


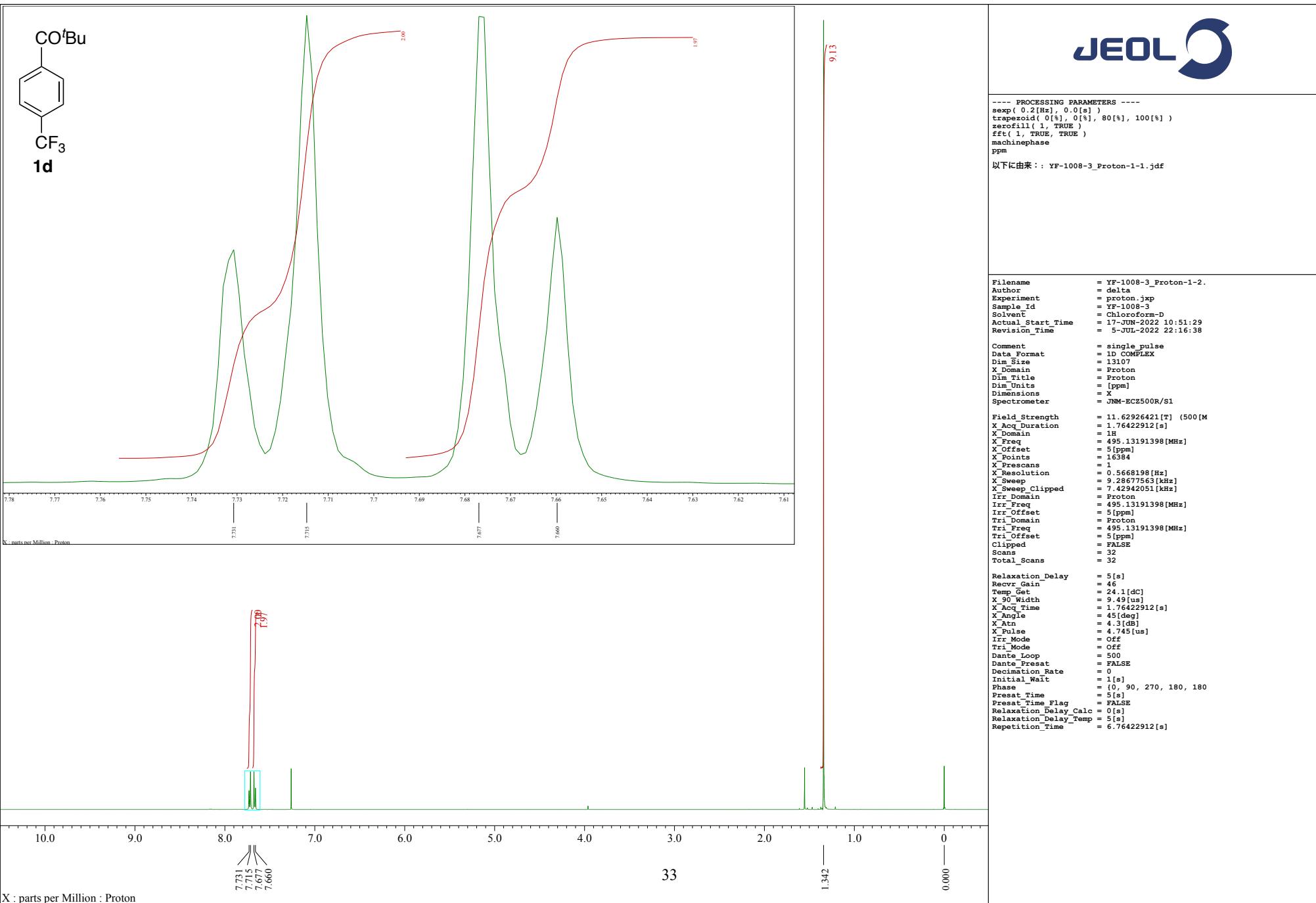
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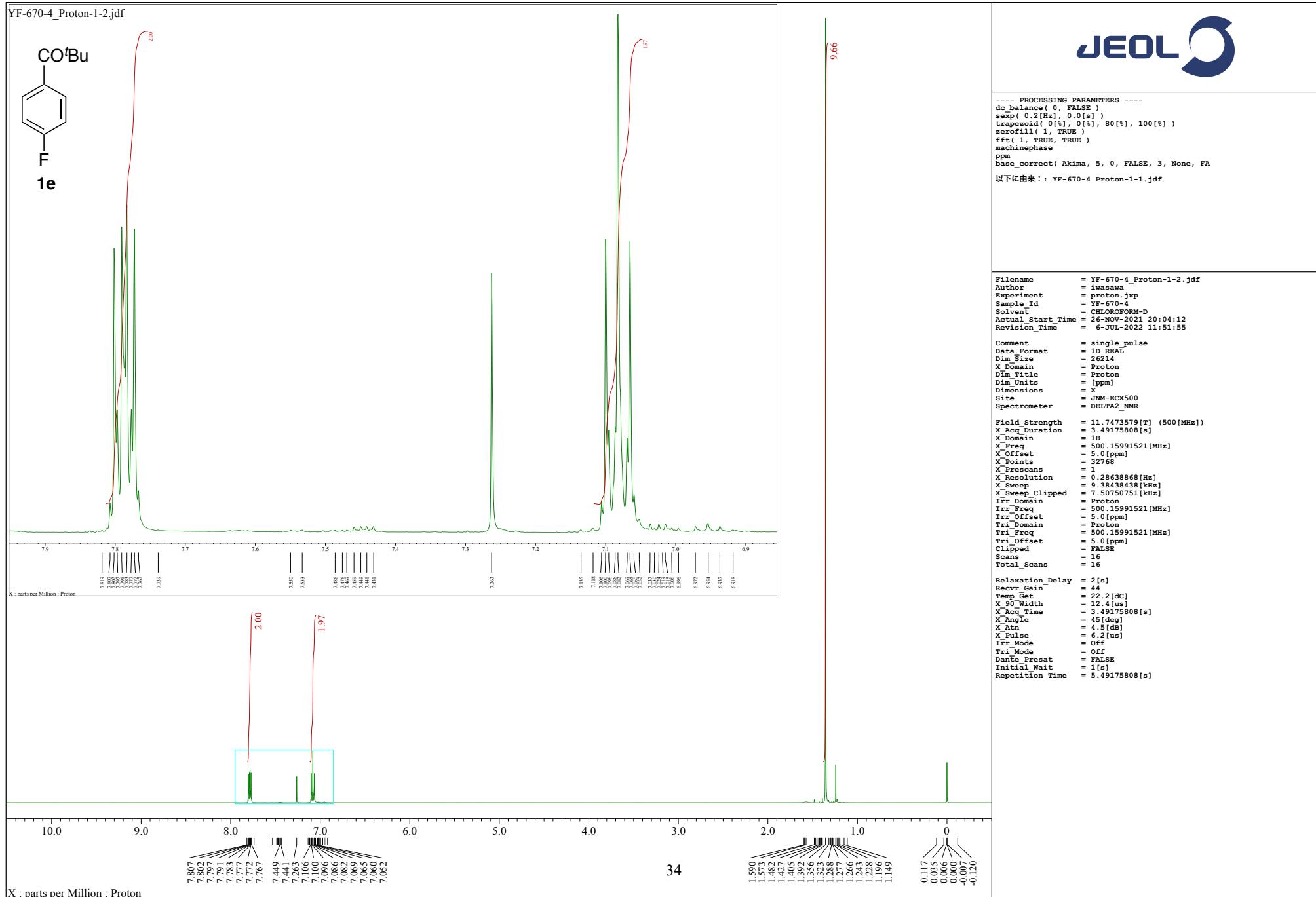
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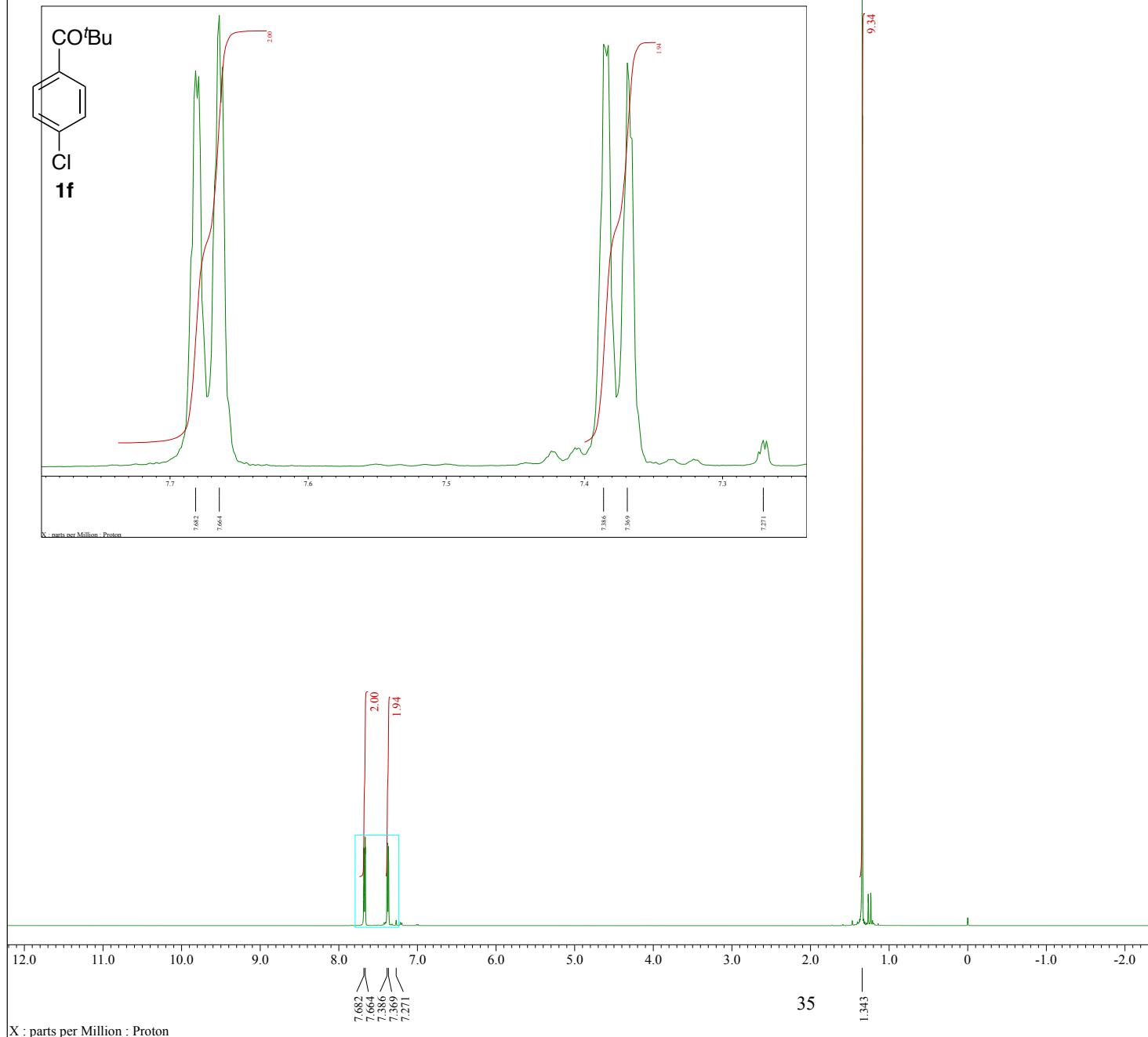
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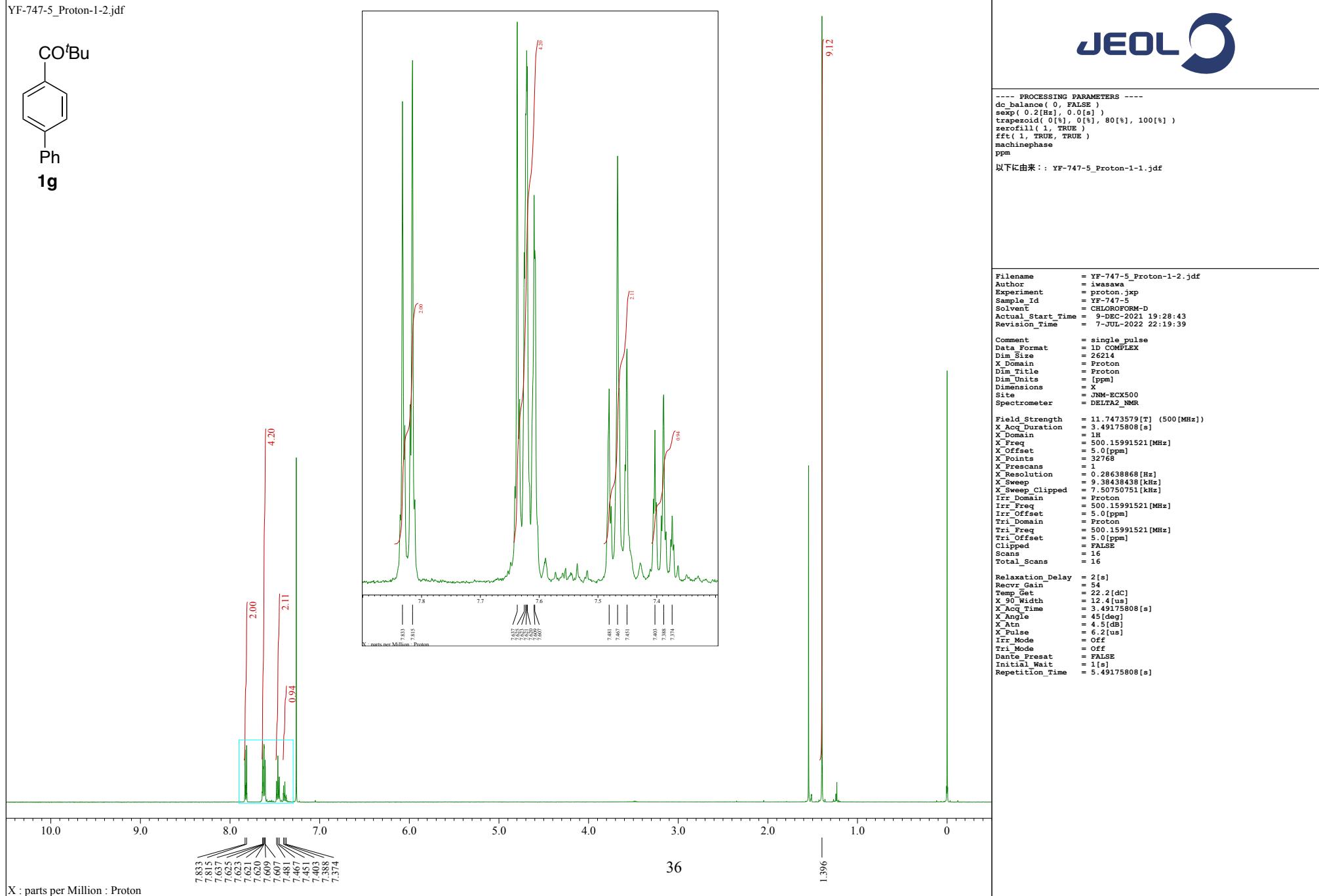
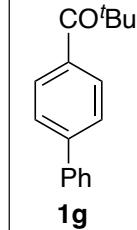




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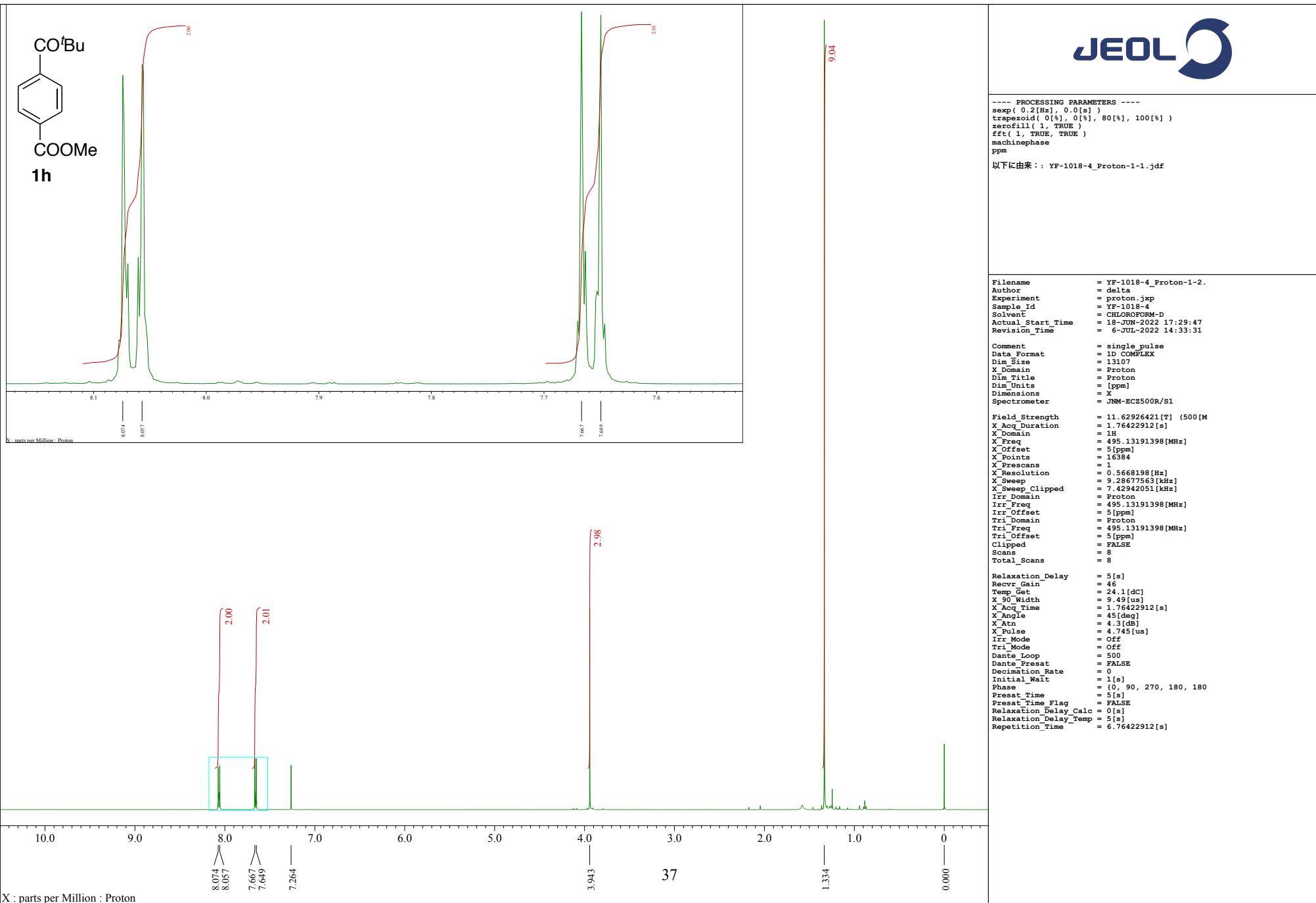
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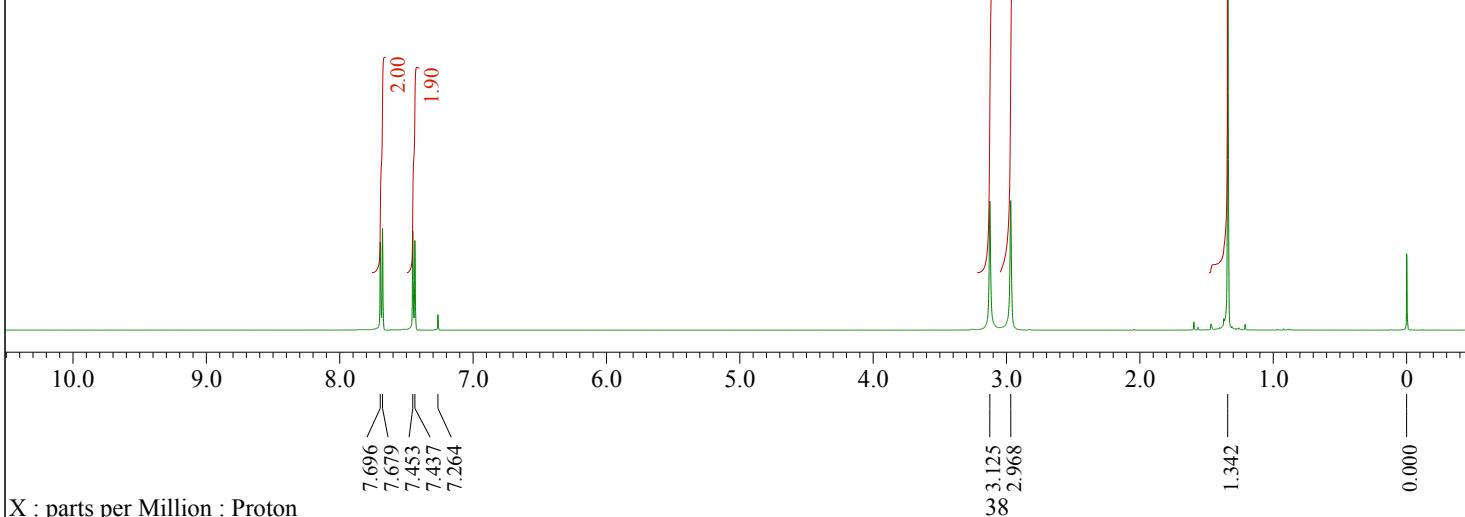
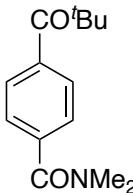
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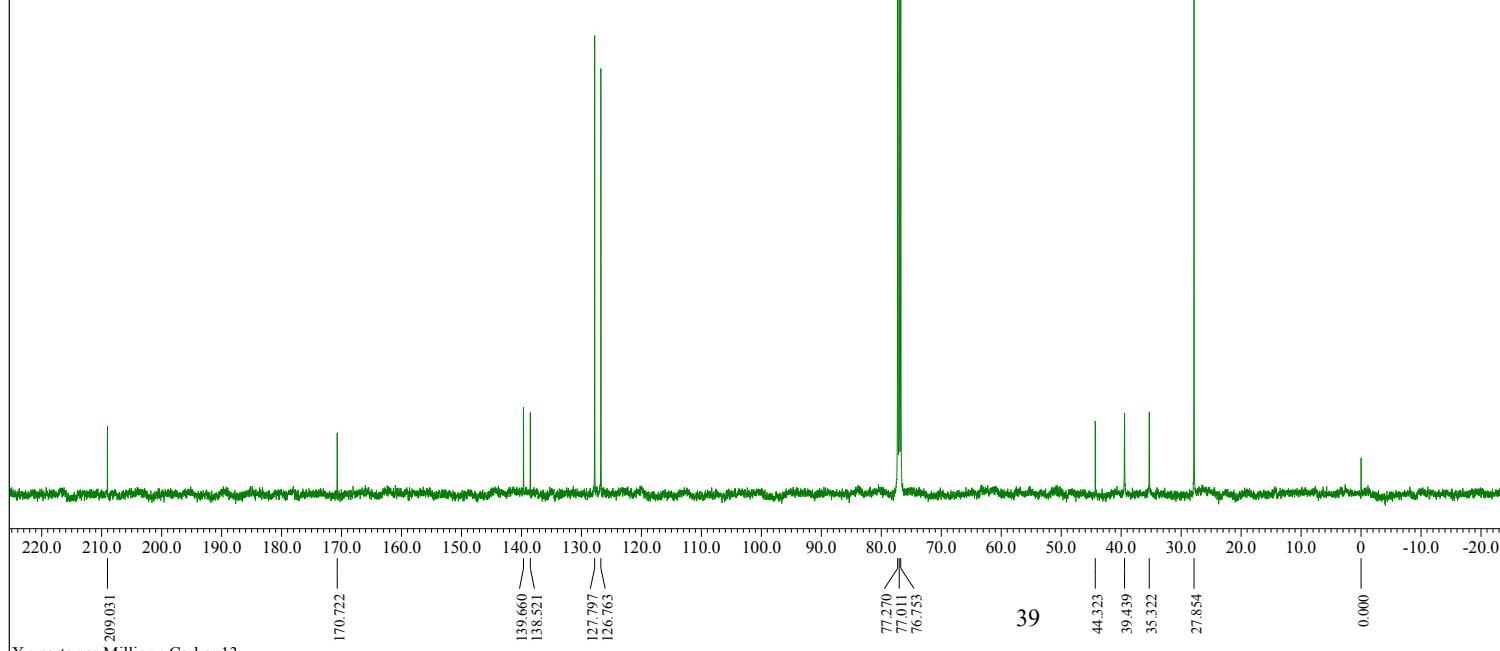
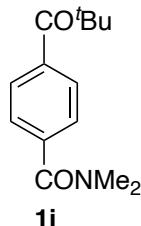
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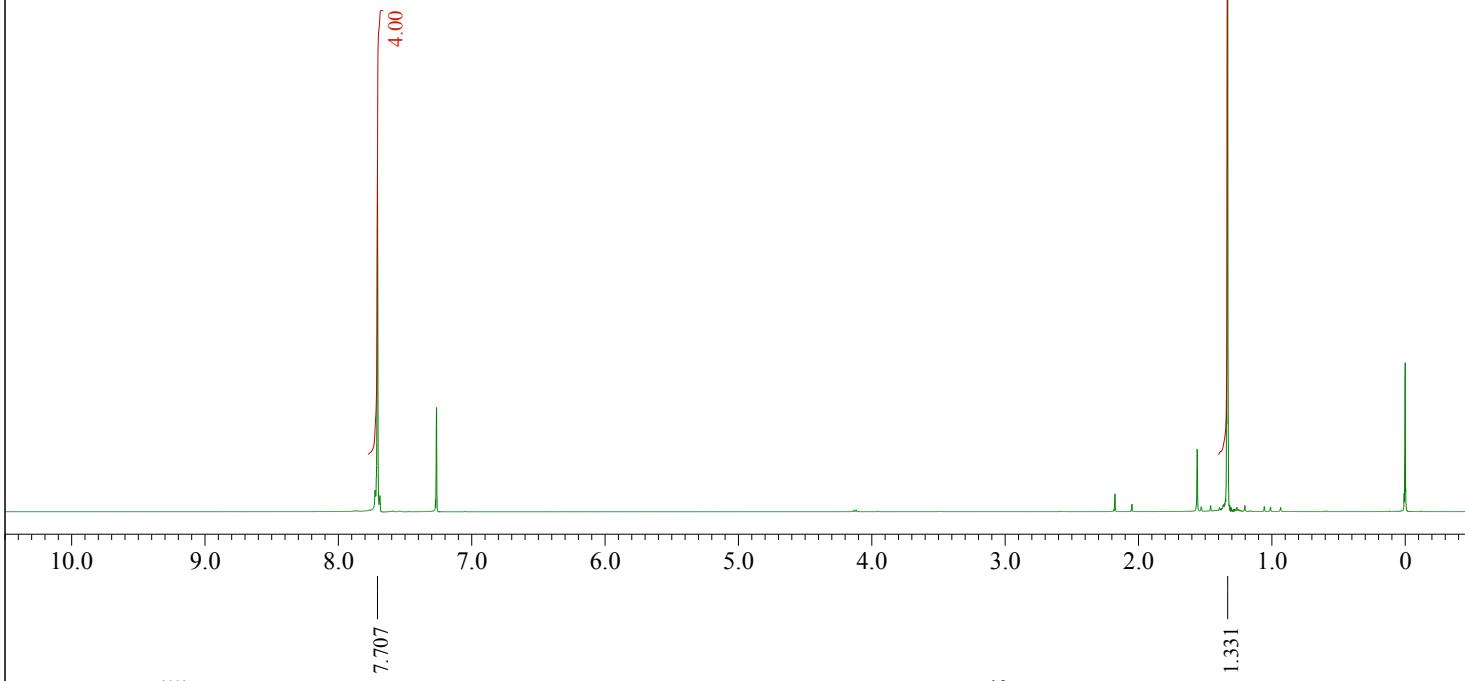
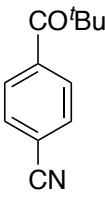


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**JEOL**

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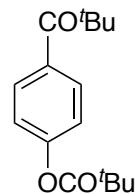
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Data_Format = 1D COMPLEX
Dim_Size = 13107
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1

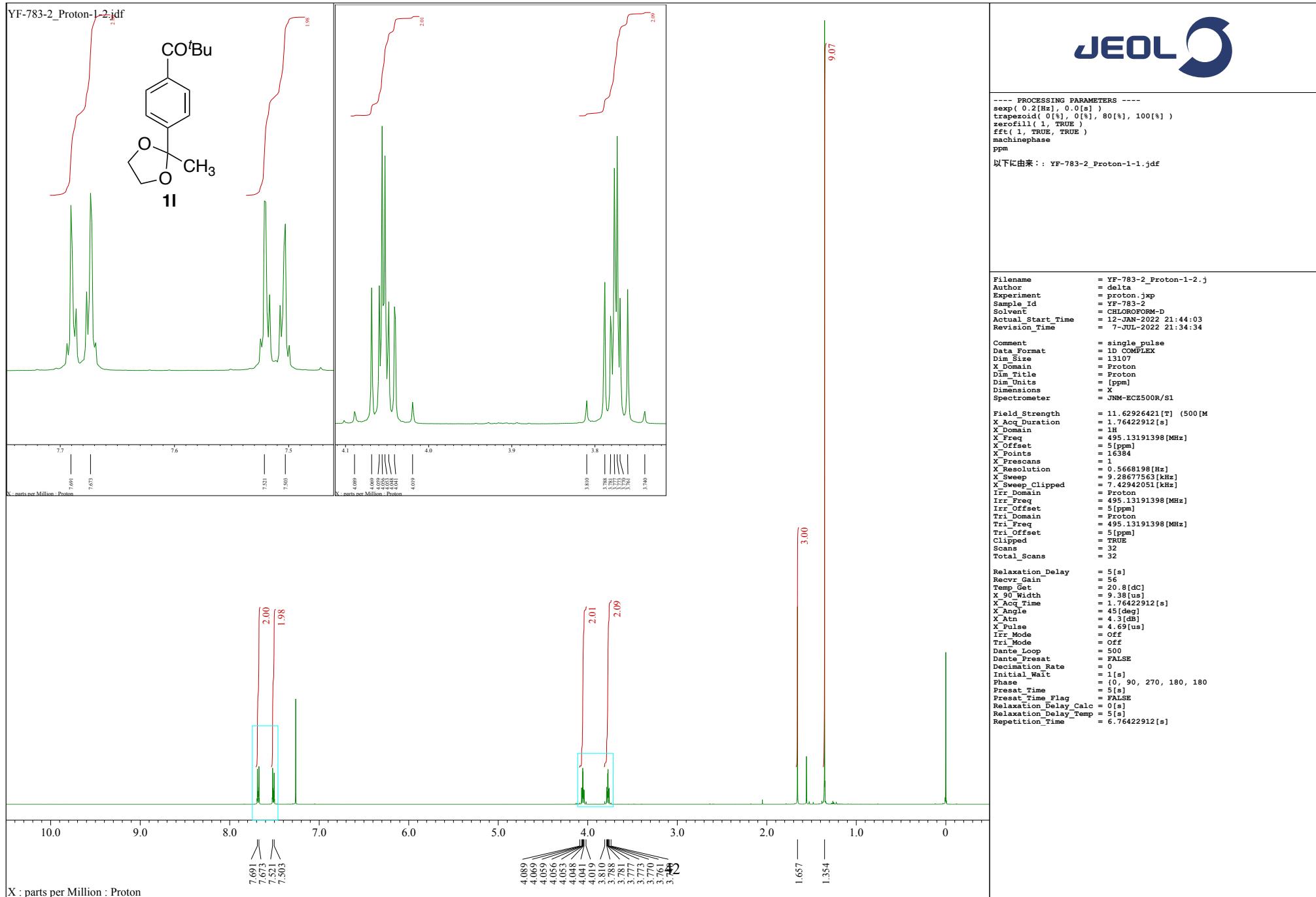
Field_Strength = 11.62926421[T] (500[M
X_Acq_Duration = 1.76422912[s]
X_Domain = 1H
X_Freq = 495.13191398[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.5668198[Hz]
X_Sweep = 9.28677563[kHz]
X_Sweep_Clipped = 7.42942051[kHz]
Irr_Domain = Proton
Irr_Freq = 495.13191398[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 495.13191398[MHz]
Tri_Offset = 5[ppm]
Clipped = TRUE
Scans = 32
Total_Scans = 32

Relaxation_Delay = 5[s]
Recvr_Gain = 56
Temp_Get = 20.5[dC]
X_90_Width = 9.38[us]
X_Acq_Time = 1.76422912[s]
X_Angle = 45[deg]
X_Atn = 4.3[dB]
X_Pulse = 4.69[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = {0, 90, 270, 180, 180
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 6.76422912[s]
```

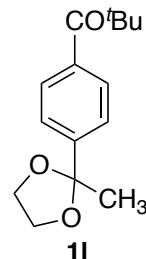
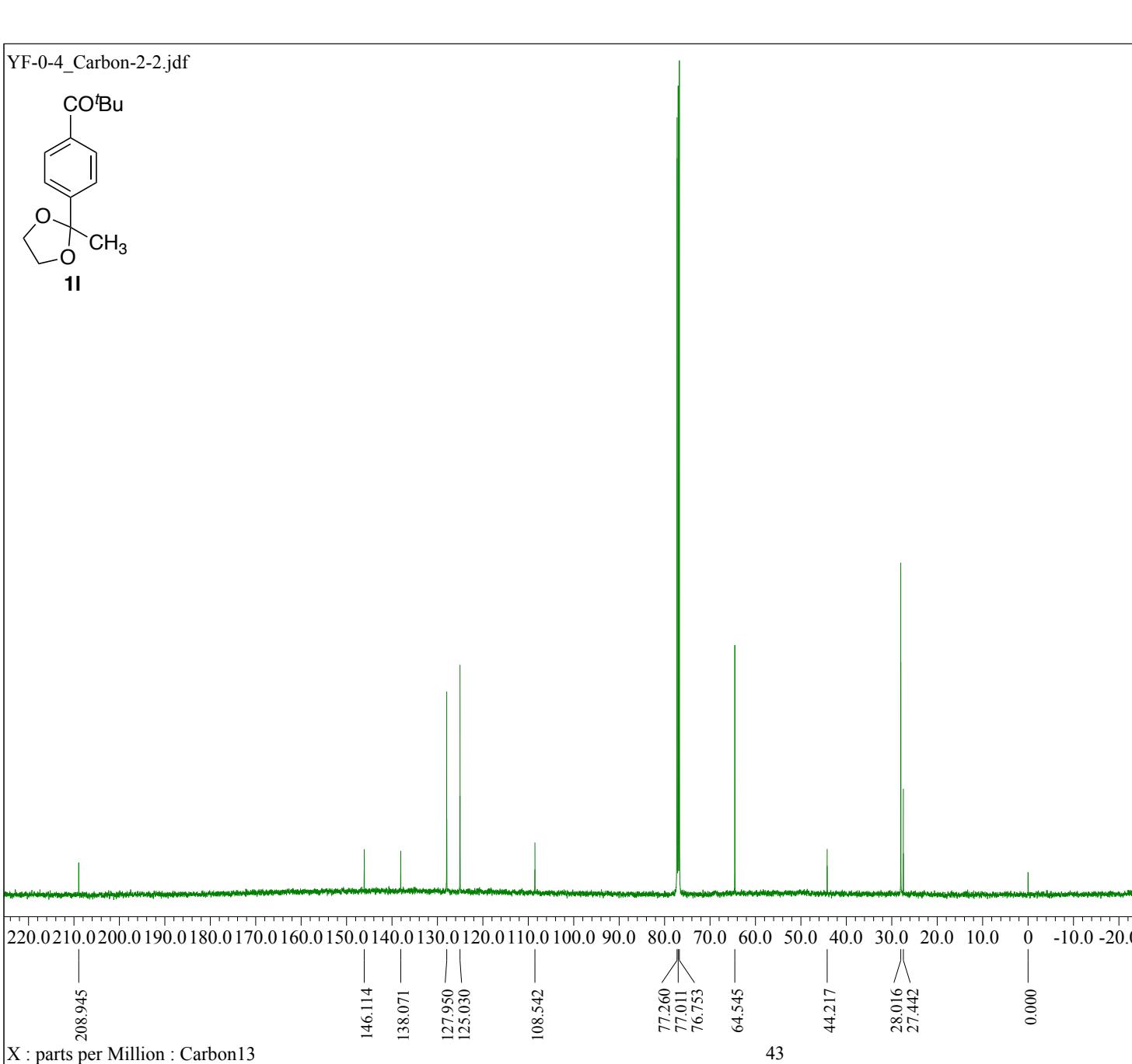
YF-1164-4\_Proton-1-2.jdf



&lt;/div



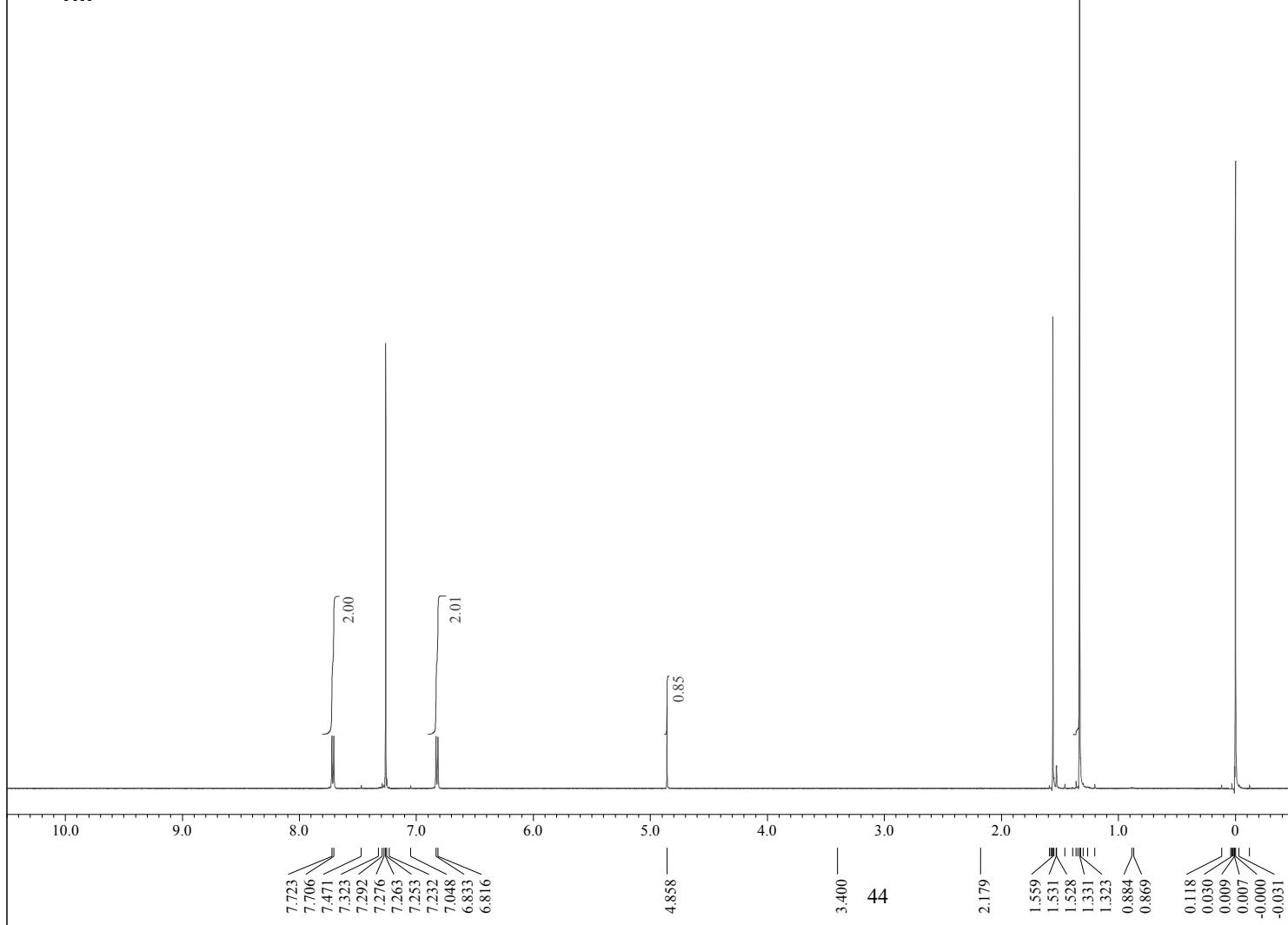
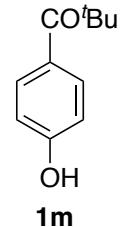
YF-0-4\_Carbon-2-2.jdf

**II**

X : parts per Million : Carbon13



Filename	= YF-0-4_Carbon-2-2.
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= YF-0-4
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 22-MAY-2022 06:44:
Revision_Time	= 23-MAY-2022 15:57:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ500R/S1
Field_Strength	= 11.62926421[T] (50
X_Acq_Duration	= 0.8388608[s]
X_Domain	= 13C
X_Freq	= 124.5010059[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 1.1920929[Hz]
X_Sweep	= 39.0625[kHz]
X_Sweep_Clipped	= 31.25[kHz]
Irr_Domain	= Proton
Irr_Freq	= 495.13191398[MHz]
Irr_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 4096
Total_Scans	= 4096
Relaxation_Delay	= 2[s]
Recv_Gain	= 56
Temp_Get	= 24.8[dC]
X_90_Width	= 14[us]
X_Acq_Time	= 0.8388608[s]
X_Angle	= 30[deg]
X_Atn	= 11[dB]
X_Pulse	= 4.6666667[us]
Irr_Atn_Dec	= 25.8[dB]
Irr_Atn_Dec_Calc	= 25.8[dB]
Irr_Atn_Dec_Default_Calc	= 25.8[dB]
Irr_Atn_Noe	= 25.8[dB]
Irr_Dec_Bandwidth_Hz	= 5.97826087[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.07407703[ppm]
Irr_Dec_Freq	= 495.13191398[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 92[us]
Irr_Pwidth_Default	= 92[us]
Irr_Pwidth_Default_Calc	= 92[us]
Irr_Pwidth_Templ	= 92[us]
Irr_Wurst	= FALSE
Decimation_Rate	= 0
Initial_Wait	= 1[s]
Noe_Time	= 2[s]
Noe_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 2[s]
Repetition_Time	= 2.8388608[s]



```

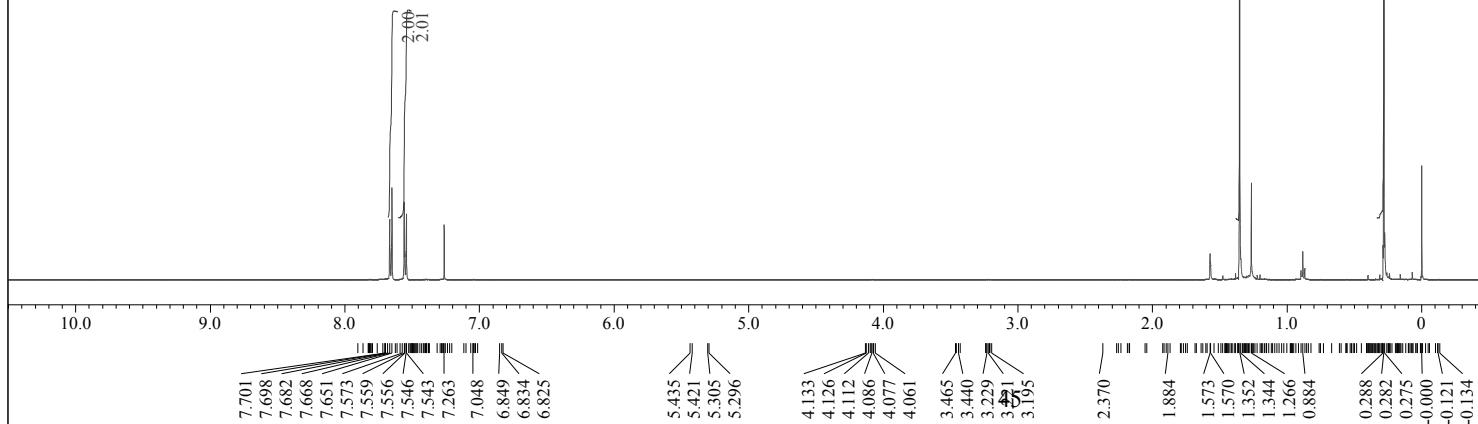
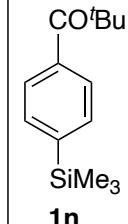
Filename      = YF-0-p-OH_Proton-1-5.
Author       = delta
Experiment   = proton.jxp
Sample_Id    = YF-0-p-OH
Solvent      = CHLOROFORM-D
Actual_Start_Time = 11-NOV-2022 19:34:07
Revision_Time = 11-NOV-2022 18:35:33

Comment      = single_pulse
Data_Format  = 1D REAL
Dim_Size     = 13107
Dim_Title    = Proton
Dim_Units    = [ppm]
Dimensions   = X
Spectrometer = JNM-ECZ500R/S1

Field_Strength = 11.62926421[T] (500[M
X_Acc_Duration = 1.76422912[s]
X_Domain     = 1H
X_Freq        = 495.13191398[MHz]
X_Offset      = 5[ppm]
X_Points      = 16384
X_Prescans   = 1
X_Resolution  = 0.5668198[Hz]
X_Sweep       = 9.28677563[kHz]
X_Sweep_Clipped = 7.42942051[kHz]
Irr_Domain   = Proton
Irr_Freq     = 495.13191398[MHz]
Irr_Offset   = 5[ppm]
Tri_Domain   = Proton
Tri_Freq     = 495.13191398[MHz]
Tri_Offset   = 5[ppm]
Clipped      = FALSE
Scans        = 8
Total_Scans  = 8

Relaxation_Delay = 5[s]
Recvs_Gain      = 50
Temp_Get        = 19.91[do]
X_Acc_Width    = 8.7[us]
X_Acc_Time     = 1.76422912[s]
X_Angle        = 45[deg]
X_Atn          = 4.3[dB]
X_Pulse        = 4.35[us]
Irr_Mode       = Off
Tri_Mode       = Off
Dante_Loop    = 500
Dante_Presat  = FALSE
Decimation_Rate = 0
Initial_Wait   = 1[s]
Phase          = {0, 90, 270, 180, 180
Presat_Time    = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 6.76422912[s]

```



**JEOL**

```

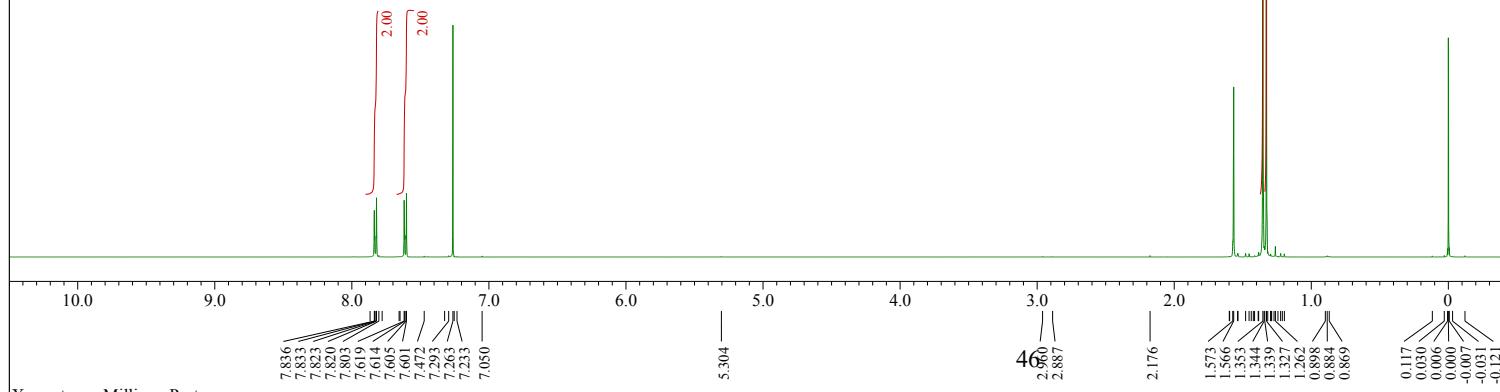
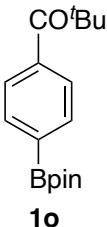
Filename      = YF-1183-4_Proton-1-4.
Author       = delta
Experiment   = proton.jpx
Sample_Id    = YF-1183-4
Solvent      = CHLOROFORM-D
Actual_Start_Time = 26-OCT-2022 21:49:09
Revision_Time = 26-OCT-2022 20:51:44

Comment      = single_pulse
Data_Format  = 1D REAL
Dim_Size     = 13107
Dim_Title    = Proton
Dim_Units    = [ppm]
Dimensions   = X
Spectrometer = JNM-ECZ500R/S1

Field_Strength = 11.62926421[T] (500[M
X_Acc_Duration = 1.76422912[s]
X_Domain     = 1H
X_Freq        = 495.13191398[MHz]
X_Offset      = 5[ppm]
X_Points      = 16384
X_Prescans   = 1
X_Resolution  = 0.5668198[Hz]
X_Sweep       = 9.28677563[kHz]
X_Sweep_Clipped = 7.42942051[kHz]
Irr_Domain   = Proton
Irr_Freq     = 495.13191398[MHz]
Irr_Offset   = 5[ppm]
Tri_Domain   = Proton
Tri_Freq     = 495.13191398[MHz]
Tri_Offset   = 5[ppm]
Clipped      = FALSE
Scans        = 8
Total_Scans  = 8

Relaxation_Delay = 5[s]
Recv_Gain        = 40
Temp_Get         = 19.01[do]
X_Acc_Width     = 8.7[us]
X_Acc_Time      = 1.76422912[s]
X_Angle         = 45[deg]
X_Atn          = 4.3[dB]
X_Pulse         = 4.35[us]
Irr_Mode        = Off
Tri_Mode        = Off
Dante_Loop     = 500
Dante_Presat   = FALSE
Decimation_Rate = 0
Initial_Wait   = 1[s]
Phase          = {0, 90, 270, 180, 180
Presat_Time    = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 6.76422912[s]

```



**JEOL**

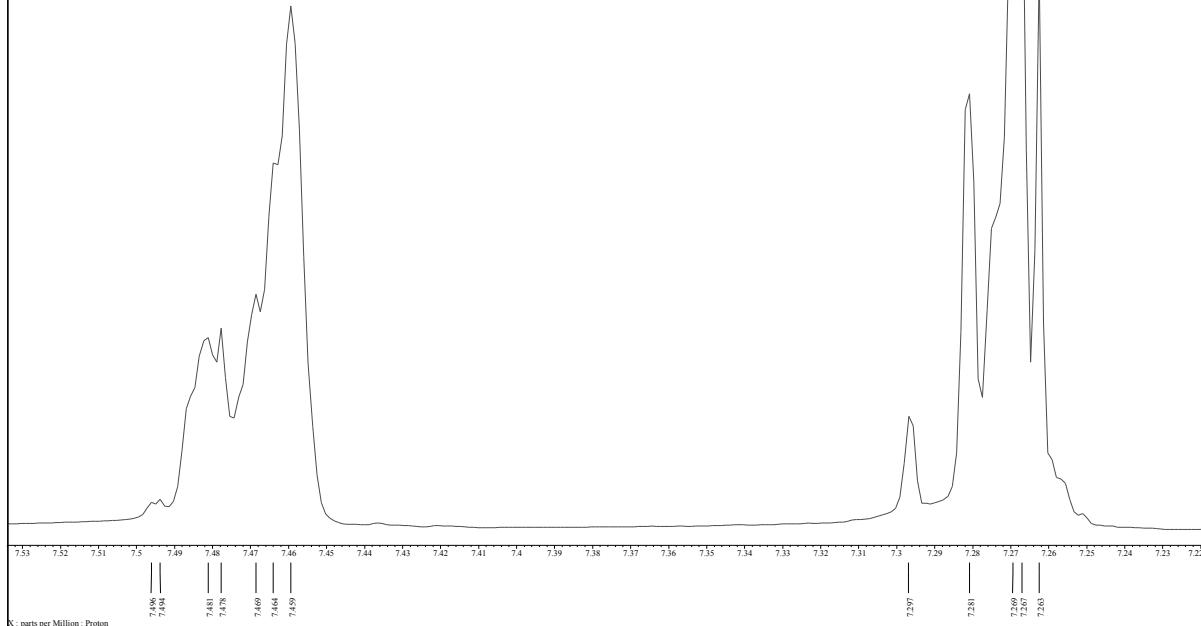
```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
ppm
base_correct( Akima, 5, 0, FALSE, 3, None, FA
以下に由来 : YF-1187-2_Proton-1-1.jdf
```

```
Filename = YF-1187-2_Proton-1-2.
Author = delta
Experiment = proton.jpx
Sample_Id = YF-1187-2
Solvent = CHLOROFORM-D
Actual_Start_Time = 28-OCT-2022 20:02:12
Revision_Time = 29-OCT-2022 15:18:43

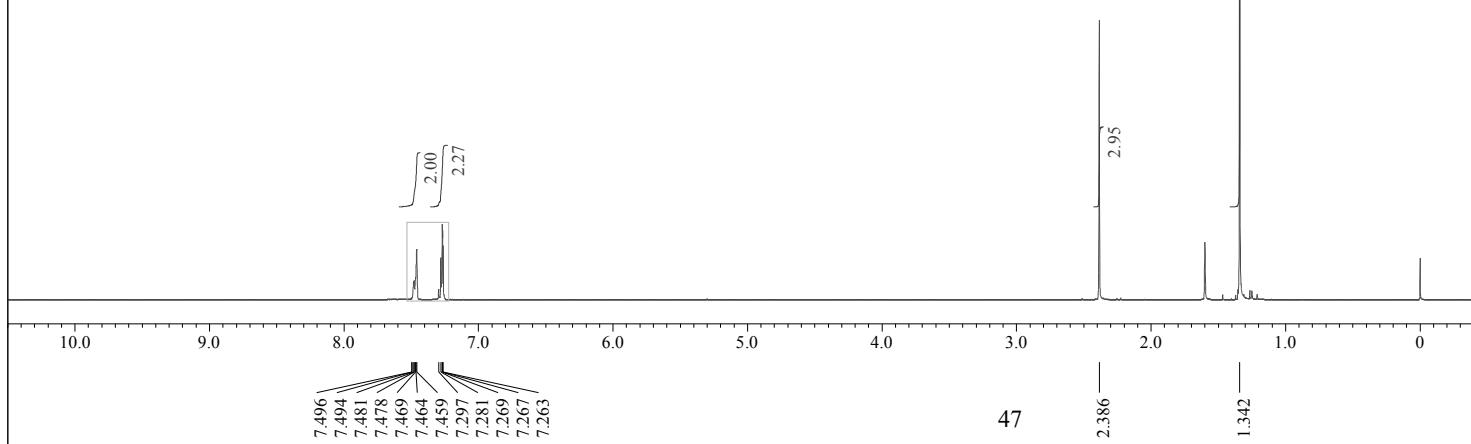
Comment = single_pulse
Data_Format = delta
Dim_Size = 13107
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1

Field_Strength = 11.62926421[T] (500[M
X_Acq_Duration = 1.76422912[s]
X_Domain = 1H
X_Freq = 495.13191398[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.5668198[Hz]
X_Sweep = 9.28677563[kHz]
X_Sweep_Clipped = 7.42942051[kHz]
Irr_Domain = Proton
Irr_Freq = 495.13191398[MHz]
Irr_Offset = 8[ppm]
Tri_Domain = proton
Tri_Freq = 495.13191398[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8

Relaxation_Delay = 5[s]
Recvr_Gain = 56
Temp_Get = 19.1[dC]
X_90_Width = 8.7[us]
X_Acq_Time = 1.76422912[s]
X_Angle = 45[deg]
X_Atri = 4.3[dB]
X_Pulse = 4.35[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = {0, 90, 270, 180, 180
Preset_Time = 5[s]
Preset_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 6.76422912[s]
```

**1p**

X : parts per Million : Proton



X : parts per Million : Proton



```

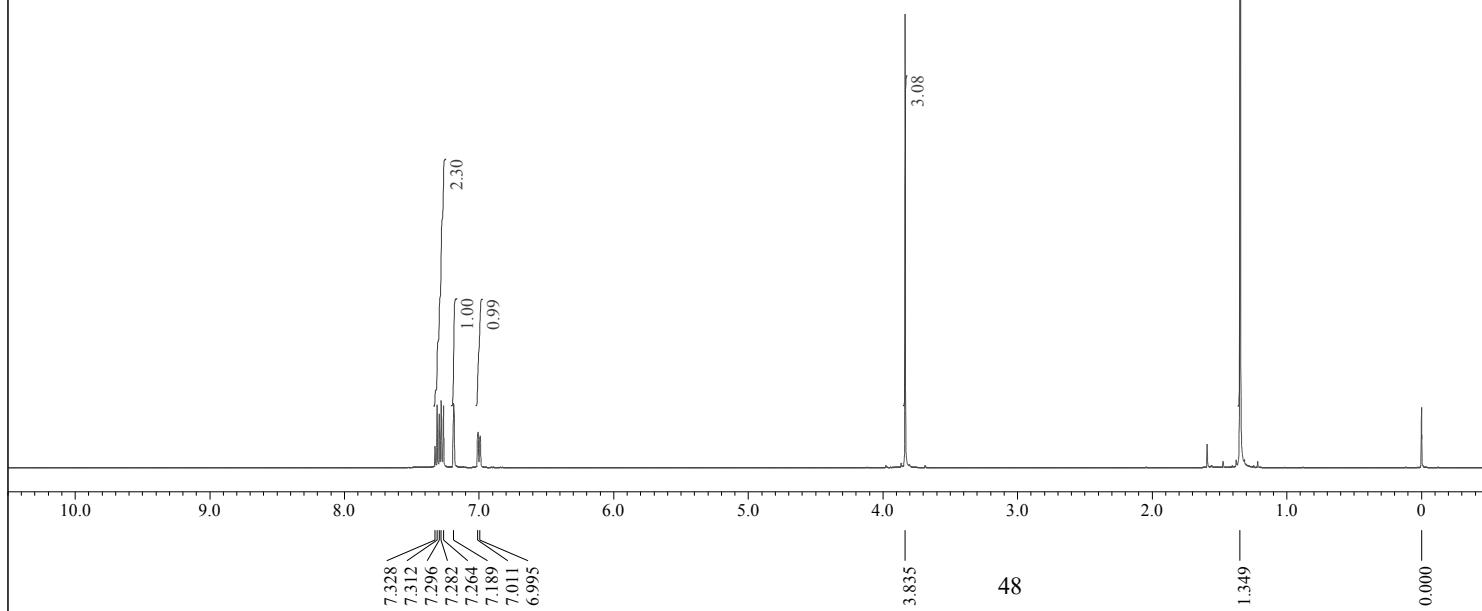
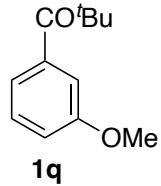
Filename = YF-0-m-Me_Proton-4-3.
Author = delta
Experiment = proton.npx
Sample_Id = YF-0-m-Me
Solvent = CHLOROFORM-D
Actual_Start_Time = 8-JUL-2022 15:19:07
Revision_Time = 8-JUL-2022 14:38:13

Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/SI

Field_Strength = 11.62926421[T] (500[M
X_Acq_Duration = 1.76422912[s]
X_Domain = 1H
X_Freq = 495.13191398[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.5668198[Hz]
X_Sweep = 9.28677563[kHz]
X_Sweep_Clipped = 7.42942051[kHz]
Irr_Domain = Proton
Irr_Freq = 495.13191398[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 495.13191398[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 32
Total_Scans = 32

Relaxation_Delay = 51[s]
Recvr_Gain = 30
Tau_Get = 20.2[dG]
X_90_Width = 9.49[us]
X_Acq_Time = 1.76422912[s]
X_Angle = 45[deg]
X_Atn = 4.3[dB]
X_Pulse = 4.745[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = {0, 90, 270, 180, 180
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 6.76422912[s]

```



**JEOL**

```

Filename      = YF-0-m-OMe_Proton-2-2
Author       = delta
Experiment   = proton.jxp
Sample_Id    = YF-0-m-OMe
Solvent      = CHLOROFORM-D
Actual_Start_Time = 23-NOV-2022 17:48:44
Revision_Time = 23-NOV-2022 16:55:42

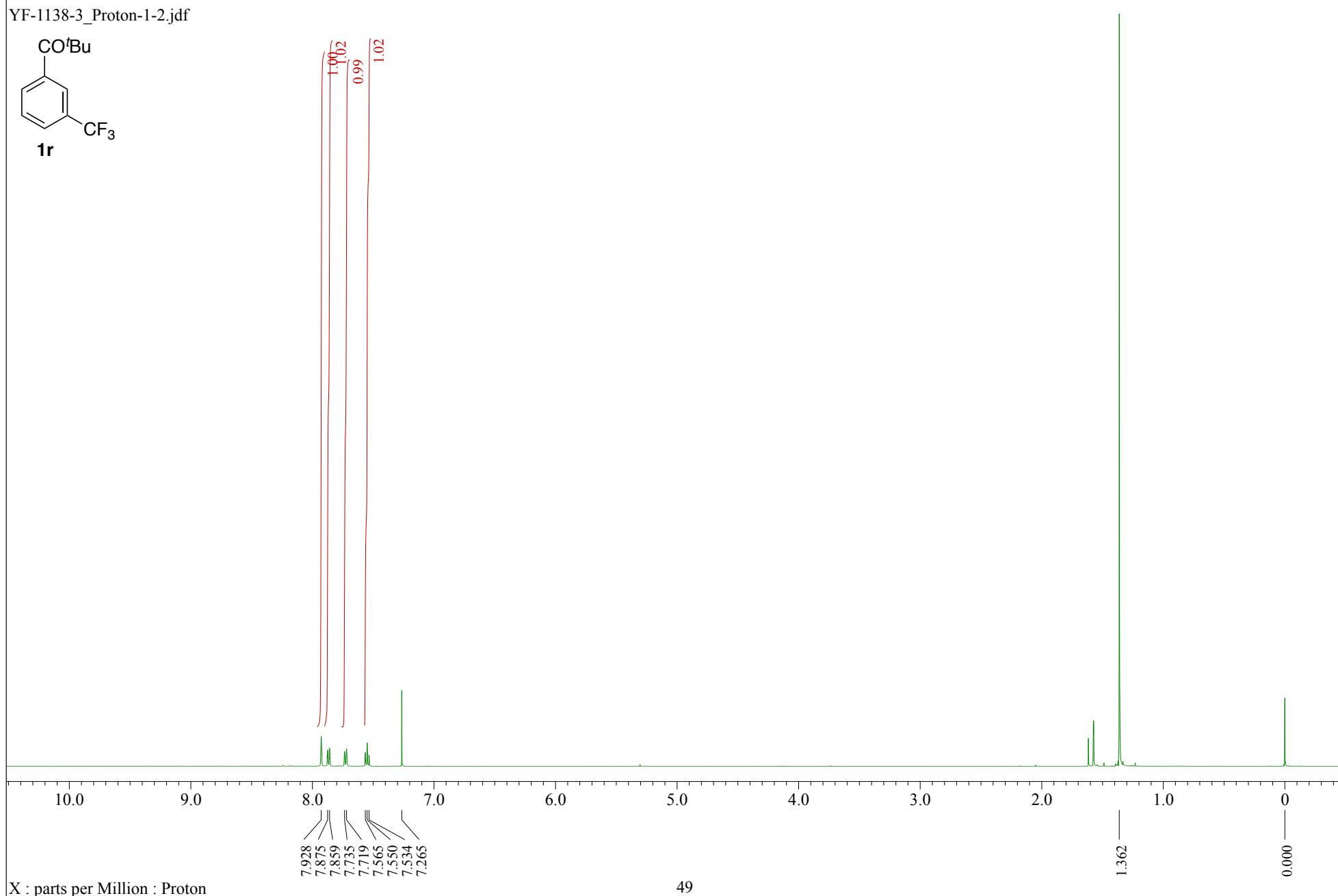
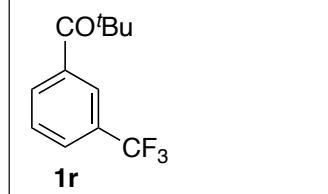
Comment      = single_pulse
Data_Format  = 1D COMPLEX
Dim_Size     = 13107
Dim_Title    = Proton
Dim_Units    = [ppm]
Dimensions   = X
Spectrometer = JNM-ECZ500R/S1

Field_Strength = 11.62926421[T] (500[M
X_Acq_Duration = 1.76422912[s]
X_Domain     = 1H
X_Freq        = 495.13191398[MHz]
X_Offset      = 5[ppm]
X_Points      = 16384
X_Prescans   = 1
X_Resolution  = 0.5668198[Hz]
X_Sweep       = 9.28677563[kHz]
X_Sweep_Clipped = 7.42942051[kHz]
Irr_Domain   = Proton
Irr_Freq     = 495.13191398[MHz]
Irr_Offset   = 5[ppm]
Tri_Domain   = Proton
Tri_Freq     = 495.13191398[MHz]
Tri_Offset   = 5[ppm]
Clipped      = FALSE
Scans        = 8
Total_Scans  = 8

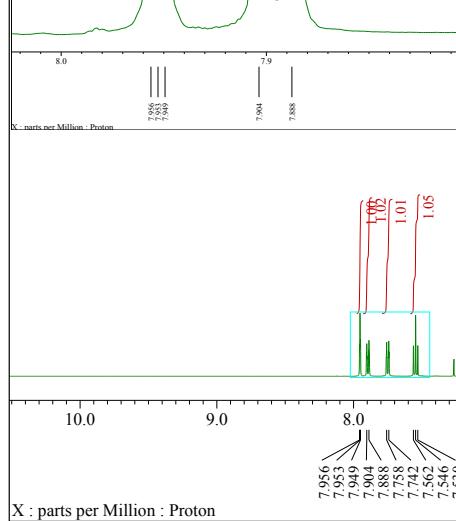
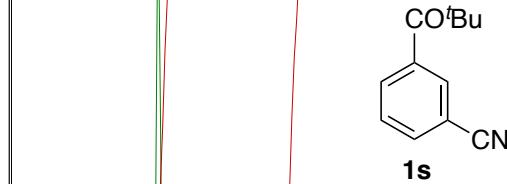
Relaxation_Delay = 5[s]
Recvs_Gain      = 30
Temp_Get        = 19.6[do]
X_Acc_Width    = 8.7[us]
X_Acc_Time     = 1.76422912[s]
X_Angle        = 45[deg]
X_Atn          = 4.3[dB]
X_Pulse        = 4.35[us]
Irr_Mode       = Off
Tri_Mode       = Off
Dante_Loop    = 500
Dante_Presat  = FALSE
Decimation_Rate = 0
Initial_Wait   = 1[s]
Phase          = {0, 90, 270, 180, 180
Presat_Time    = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 6.76422912[s]

```

YF-1138-3\_Proton-1-2.jdf



YF-0-3\_Proton-1-2.jdf

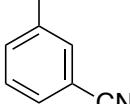
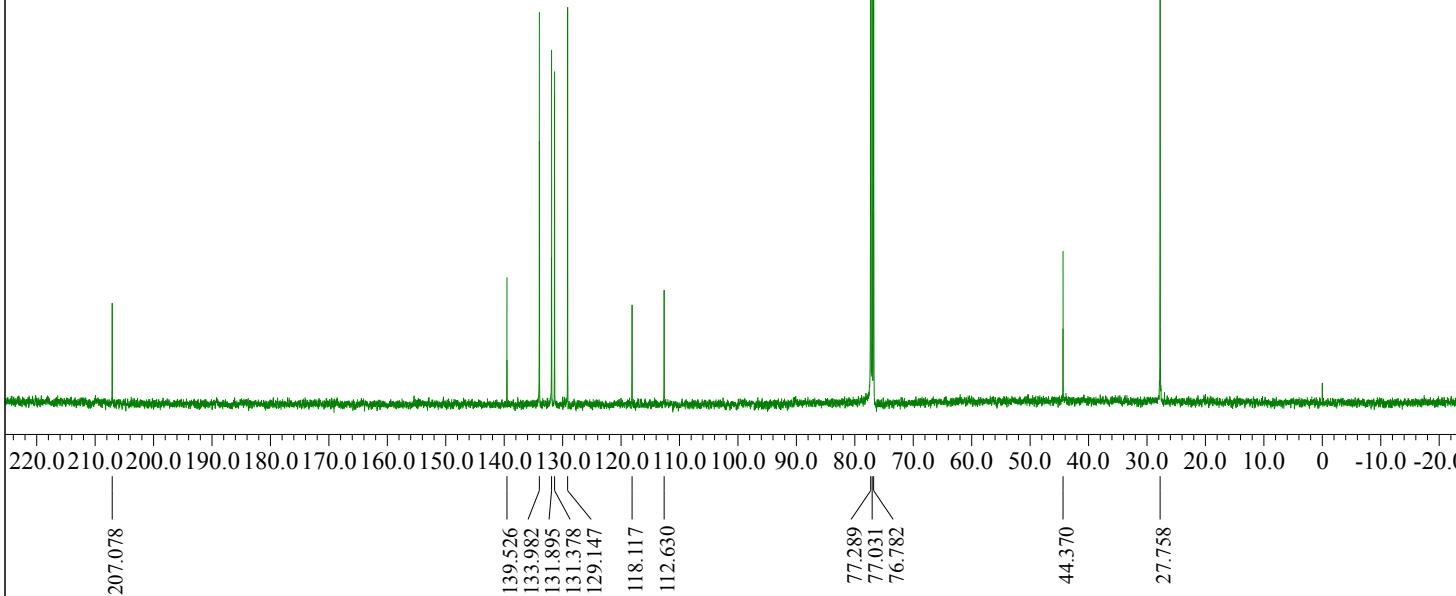


**JEOL**

---- PROCESSING PARAMETERS ----  
 sepx( 0.2[Hz], 0.0[s] )  
 trapezoid( 0[s] , 0[%] , 80[%] , 100[%] )  
 zerofill( 1, TRUE )  
 fft( 1, TRUE, TRUE )  
 machinephase  
 ppm  
 以下に由来 : YF-0-3\_Proton-1-1.jdf

Filename = YF-0-3\_Proton-1-2.jdf  
 Author = delta  
 Experiment = proton.jxp  
 Sample\_Id = YF-0-3  
 Solvent = CHLOROFORM-D  
 Actual\_Start\_Time = 21-MAY-2022 11:35:31  
 Revision\_Time = 8-JUL-2022 15:42:19  
 Comment = single\_pulse  
 Data\_Format = 1D\_COMPLEX  
 Dim\_Size = 13107  
 X\_Domain = Proton  
 Dim\_Title = Proton  
 Dim\_Units = [ppm]  
 Dimensions = X  
 Spectrometer = JNM-EC2500R/S1  
 Field\_Strength = 11.62926421[T] (500[M  
 X\_Acq\_Duration = 1.76422912[s]  
 X\_Domain = 1H  
 X\_Freq = 495.13191398[MHz]  
 X\_Kickset = 5384  
 X\_Points = 13384  
 X\_Prescans = 1  
 X\_Resolution = 0.5668198[Hz]  
 X\_Sweep = 9.28677563[kHz]  
 X\_Sweep\_Clipped = 7.42942051[kHz]  
 Irr\_Domain = Proton  
 Irr\_Freq = 495.13191398[MHz]  
 Irr\_Offset = 5  
 Tri\_Domain = Proton  
 Tri\_Freq = 495.13191398[MHz]  
 Tri\_Offset = 5[ppm]  
 Clipped = FALSE  
 Scans = 32  
 Total\_Scans = 32  
 Relaxation\_Delay = 5[s]  
 Recvr\_Gain = 46  
 Temp\_Get = 25[dC]  
 X\_90\_Width = 7.5[us]  
 X\_Acq\_Time = 1.76422912[s]  
 X\_Angle = 45[deg]  
 X\_BW = 3.75[dB]  
 X\_Pulse = 7.75[us]  
 Irr\_Mode = Off  
 Tri\_Mode = Off  
 Dancs\_Loop = 500  
 Dancs\_Presat = FALSE  
 Decimation\_Rate = 0  
 Initial\_Wait = 1[s]  
 Dmtr = { 90, 270, 180, 180 }  
 Preset\_Time = 5[s]  
 Preset\_Time\_Flag = FALSE  
 Relaxation\_Delay\_Calc = 0[s]  
 Relaxation\_Delay\_Temp = 5[s]  
 Repetition\_Time = 6.76422912[s]

YF-0-3\_Carbon-1-2.jdf

CO<sup>t</sup>Bu**1s**
**JEOL**

```

Filename = YF-0-3_Carbon-1-2.
Author = delta
Experiment = carbon.jxp
Sample_Id = YF-0-3
Solvent = CHLOROFORM-D
Actual_Start_Time = 21-MAY-2022 03:58:
Revision_Time = 23-MAY-2022 15:48:

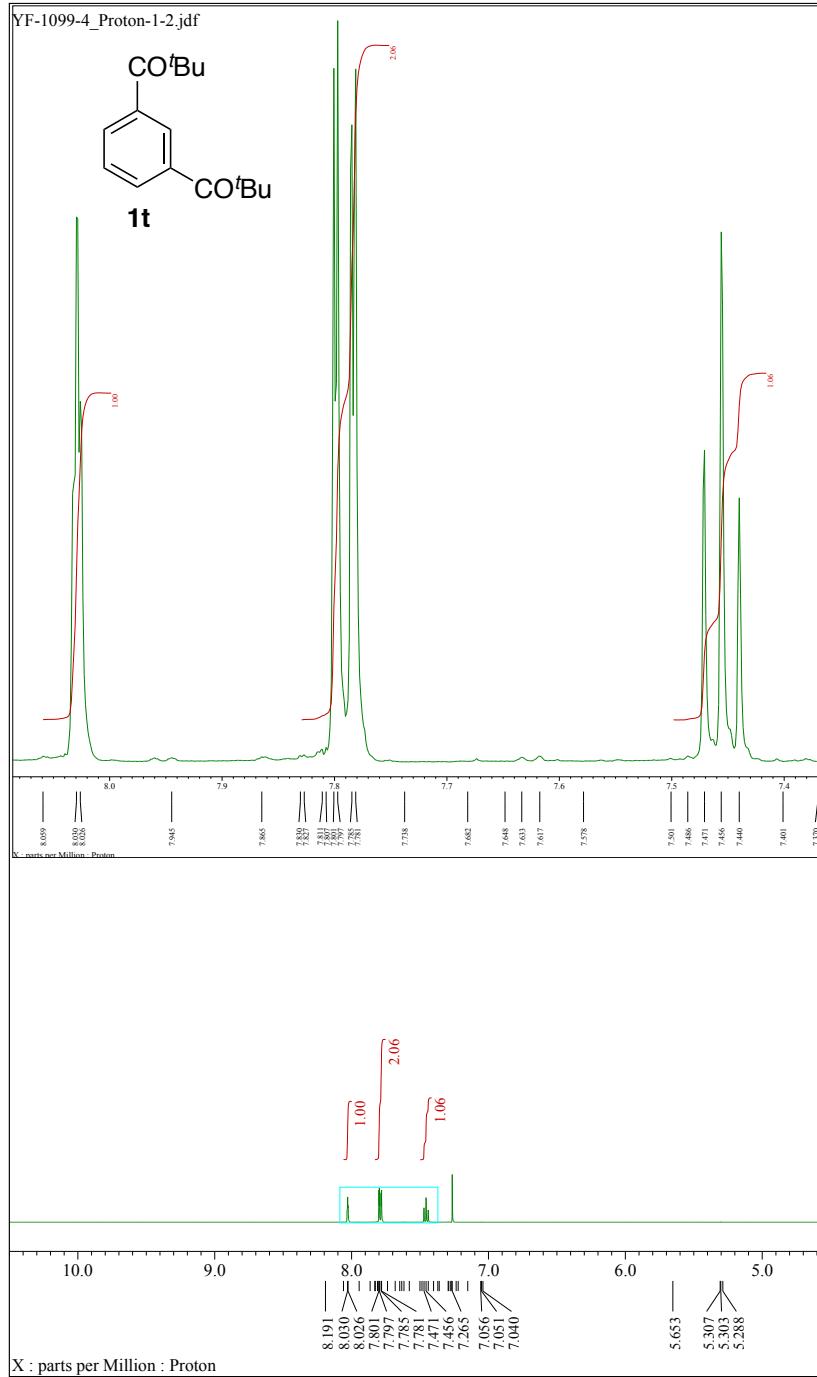
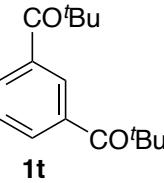
Comment = single pulse decou
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1

Field_Strength = 11.62926421[T] (50
X_Acq_Duration = 0.8388608[s]
X_Domain = 13C
X_Freq = 124.5010059[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.1920929[Hz]
X_Sweep = 39.0625[kHz]
X_Sweep_Clipped = 31.25[kHz]
Irr_Domain = Proton
Irr_Freq = 495.13191398[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 1024
Total_Scans = 1024

Relaxation_Delay = 2[s]
Recv_Gain = 56
Temp_Get = 25.3[dC]
X_90_Width = 14[us]
X_Acq_Time = 0.8388608[s]
X_Angle = 30[deg]
X_Atn = 11[dB]
X_Pulse = 4.66666667[us]
Irr_Atn_Dec = 25.8[dB]
Irr_Atn_Dec_Calc = 25.8[dB]
Irr_Atn_Dec_Default_Calc = 25.8[dB]
Irr_Atn_Noe = 25.8[dB]
Irr_Dec_Bandwidth_Hz = 5.97826087[kHz]
Irr_Dec_Bandwidth_Ppm = 12.07407703[ppm]
Irr_Dec_Freq = 495.13191398[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 92[us]
Irr_Pwidth_Default = 92[us]
Irr_Pwidth_Default_Calc = 92[us]
Irr_Pwidth_Templ = 92[us]
Irr_Wurst = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Noe_Time = 2[s]
Noe_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 2[s]
Repetition_Time = 2.8388608[s]

```

YF-1099-4\_Proton-1-2.jdf

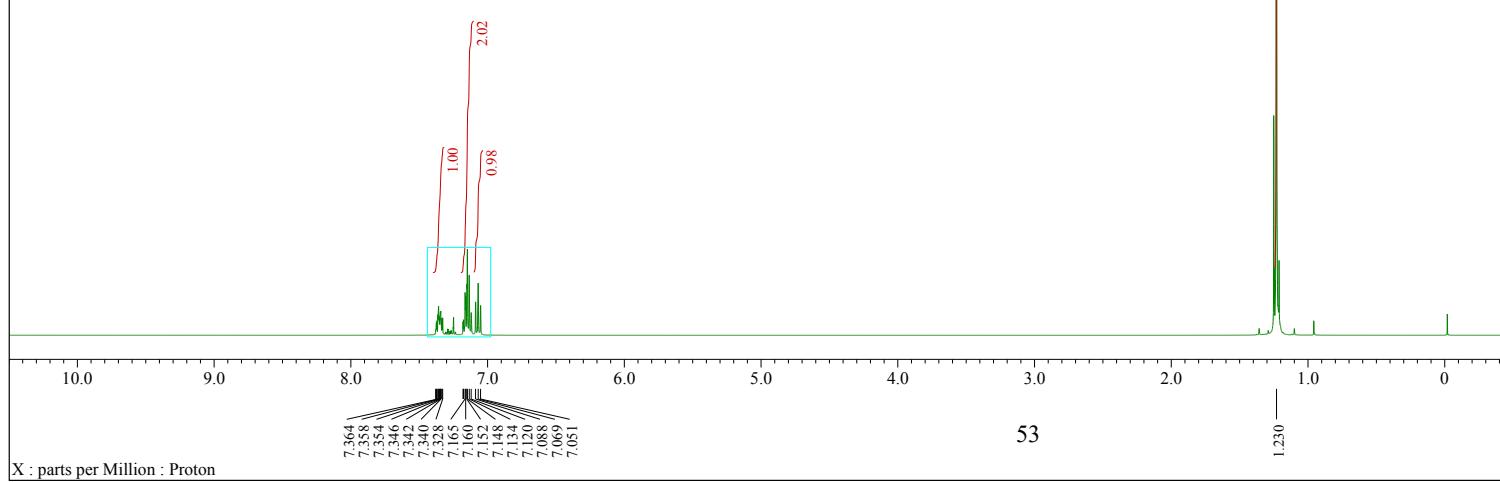
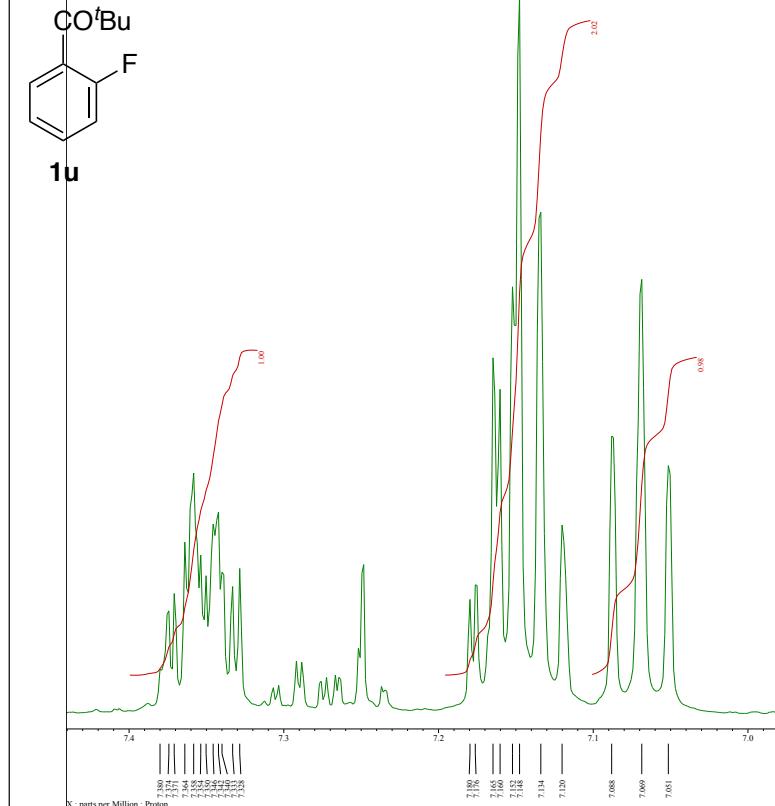


**JEOL**

---- PROCESSING PARAMETERS ----  
 sexp( 0.2[Hz], 0.0[s] )  
 trapezoid( 0[%], 0[%], 80[%], 100[%] )  
 zerofill( 1, TRUE )  
 fft( 1, TRUE, TRUE )  
 machinephase  
 ppm  
 base\_correct( Akima, 5, 0, FALSE, 3, None, FA  
 以下に由来 : YF-1099-4\_Proton-1-1.jdf

Filename = YF-1099-4\_Proton-1-2.  
 Author = delta  
 Experiment = proton.jpx  
 Sample\_Id = YF-1099-4  
 Solvent = CHLOROFORM-D  
 Actual\_Start\_Time = 11-OCT-2022 15:10:30  
 Revision\_Time = 11-OCT-2022 20:28:03  
 Comment = single\_pulse  
 Data\_Format = 1D REAL  
 Dim\_Size = 13107  
 X\_Domain = Proton  
 Dim\_Title = Proton  
 Dim\_Units = [ppm]  
 Dimensions = X  
 Spectrometer = JNM-ECZ500R/S1  
 Field\_Strength = 11.62926421[T] (500[M  
 X\_Acq\_Duration = 1.76422912[s]  
 X\_Domain = 1H  
 X\_Freq = 495.13191398[MHz]  
 X\_Offset = 5 [ppm]  
 X\_Points = 16384  
 X\_Prescans = 1  
 X\_Resolution = 0.5668198[Hz]  
 X\_Sweep = 9.28677563[kHz]  
 X\_Sweep\_Clipped = 7.42942051[kHz]  
 Irr\_Domain = Proton  
 Irr\_Freq = 495.13191398[MHz]  
 Irr\_Offset = 8 [ppm]  
 Tri\_Domain = proton  
 Tri\_Freq = 495.13191398[MHz]  
 Tri\_Offset = 5 [ppm]  
 Clipped = FALSE  
 Scans = 8  
 Total\_Scans = 8  
 Relaxation\_Delay = 5[s]  
 Recvr\_Gain = 46  
 Temp\_Get = 20.1[dC]  
 X\_90\_Width = 8.7[us]  
 X\_Acq\_Time = 1.76422912[s]  
 X\_Angle = 45[deg]  
 X\_Arr = 4.3[dB]  
 X\_Pulse = 4.35[us]  
 Irr\_Mode = Off  
 Tri\_Mode = Off  
 DanTe Loop = 500  
 DanTe\_Presat = FALSE  
 Decimation\_Rate = 0  
 Initial\_Wait = 1[s]  
 Phase = { 0, 90, 270, 180, 180  
 Presat\_Time = 5[s]  
 Presat\_Time\_Flag = FALSE  
 Relaxation\_Delay\_Calc = 0[s]  
 Relaxation\_Delay\_Temp = 5[s]  
 Repetition\_Time = 6.76422912[s]

X : parts per Million : Proton



**JEOL**

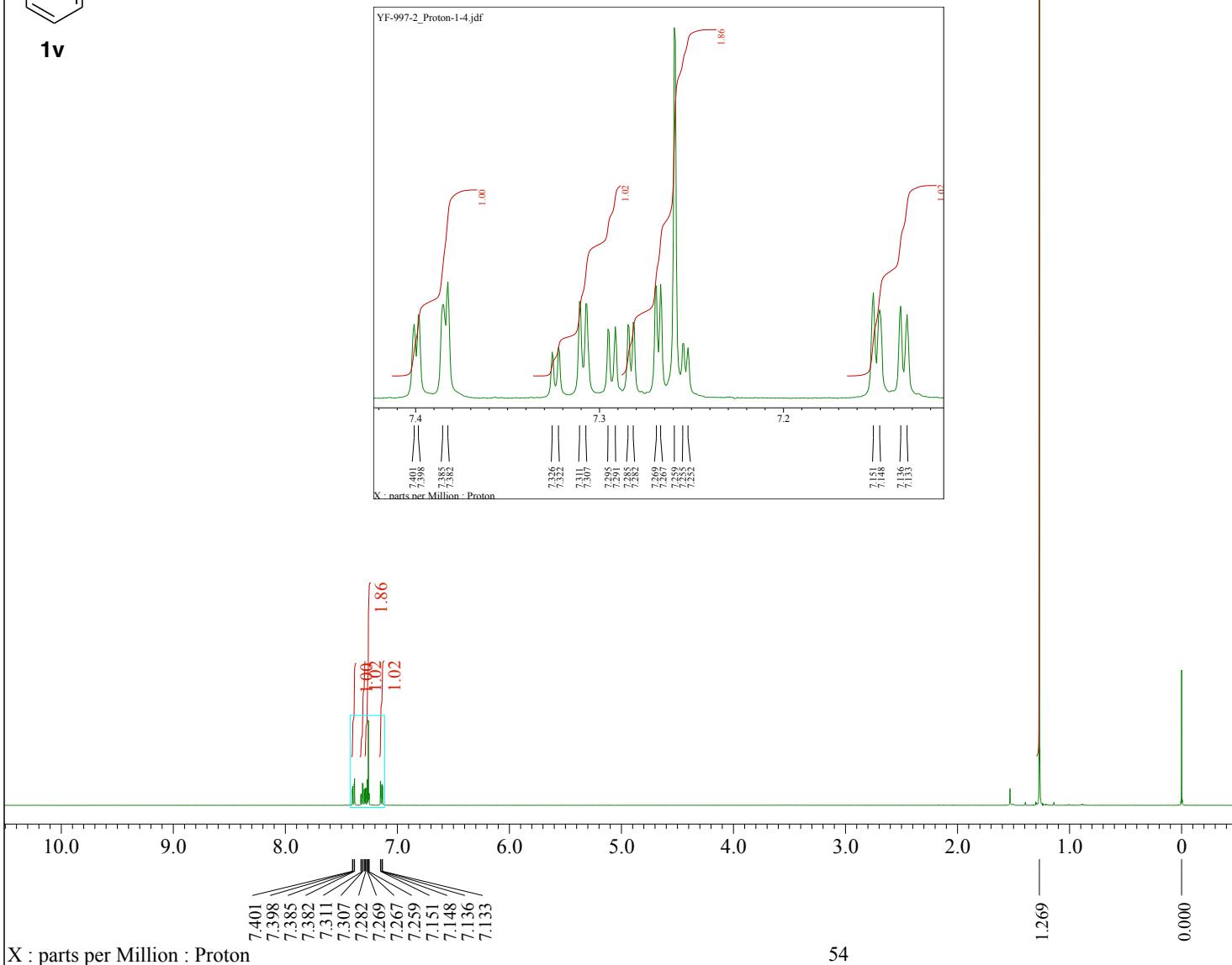
---- PROCESSING PARAMETERS ----  
 sexp( 0.2[Hz], 0.0[s] )  
 trapezoid( 0[s] , 0[%] , 80[%] )  
 zerofill( 1, TRUE )  
 fft( 1, TRUE, TRUE )  
 machinephase  
 ppm  
 以下に由来 : YF-816-3\_Proton-1-1.jdf

Filename = YF-816-3\_Proton-1-2.j  
 Author = delta  
 Experiment = proton.jxp  
 Sample\_Id = YF-816-3  
 Solvent = CHLOROFORM-D  
 Actual\_Start\_Time = 7-MAR-2022 22:07:59  
 Revision\_Time = 9-JUL-2022 11:54:30  
 Comment = single\_pulse  
 Data\_Format = 1D COMPLEX  
 Dim\_Size = 13107  
 X\_Domain = Proton  
 Dim\_Title = Proton  
 Dim\_Units = [ppm]  
 Dimensions = X  
 Spectrometer = JNM-EC2500R/S1  
 Field\_Strength = 11.62926421[T] (500[M  
 X\_Acq\_Duration = 1.76422912[s]  
 X\_Domain = 1H  
 X\_Freq = 495.13191398[MHz]  
 X\_KOffset = 5384  
 X\_Points = 13384  
 X\_Prescans = 1  
 X\_Resolution = 0.5668198[Hz]  
 X\_Sweep = 9.28677563[kHz]  
 X\_Sweep\_Clipped = 7.42942051[kHz]  
 Irr\_Domain = Proton  
 Irr\_Freq = 495.13191398[MHz]  
 Irr\_Offset = 5  
 Tri\_Domain = Proton  
 Tri\_Freq = 495.13191398[MHz]  
 Tri\_Offset = 5[ppm]  
 Clipped = FALSE  
 Scans = 32  
 Total\_Scans = 32  
 Relaxation\_Delay = 5[s]  
 Recvr\_Gain = 26  
 Temp\_Get = 20.4[dC]  
 X\_90\_Width = 9.47[us]  
 X\_Acq\_Time = 1.76422912[s]  
 X\_Angle = 45[deg]  
 X\_K = 4 [dB]  
 X\_Pulse = 4.735[us]  
 Irr\_Mode = Off  
 Tri\_Mode = Off  
 Danto\_Loop = 500  
 Danto\_Presat = FALSE  
 Decimation\_Rate = 0  
 Initial\_Wait = 1 [s]  
 Dnu = {10, 90, 270, 180, 180  
 Presat\_Time = 5[s]  
 Presat\_Time\_Flag = FALSE  
 Relaxation\_Delay\_Calc = 0[s]  
 Relaxation\_Delay\_Temp = 5[s]  
 Repetition\_Time = 6.76422912[s]

8.82

1.230

YF-997-2\_Proton-1-4.jdf

**1v**
**JEOL**

```

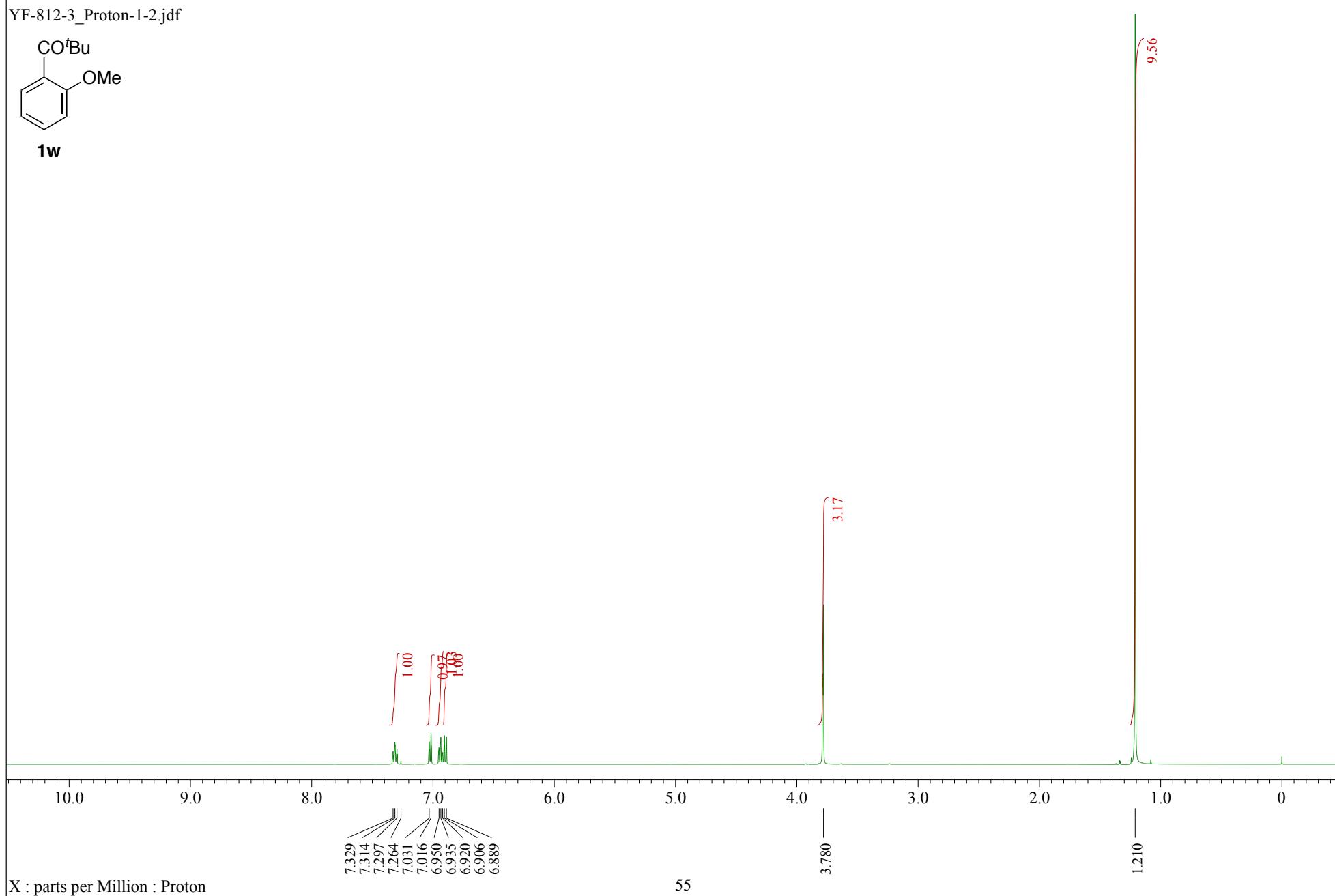
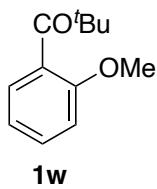
Filename      = YF-997-2_Proton-1-4.jdf
Author        = takaya
Experiment   = proton.jxp
Sample_Id    = YF-997-2
Solvent       = CHLOROFORM-D
Actual_Start_Time = 13-JUN-2022 20:41:57
Revision_Time = 19-JUL-2022 22:32:42

Comment       = single pulse
Data_Format  = 1D COMPLEX
Dim_Size     = 26214
X_Domain    = Proton
Dim_Title   = Proton
Dim_Units   = [ppm]
Dimensions  = X
Site          = JNM-ECX500
Spectrometer = DELTA2_NMR

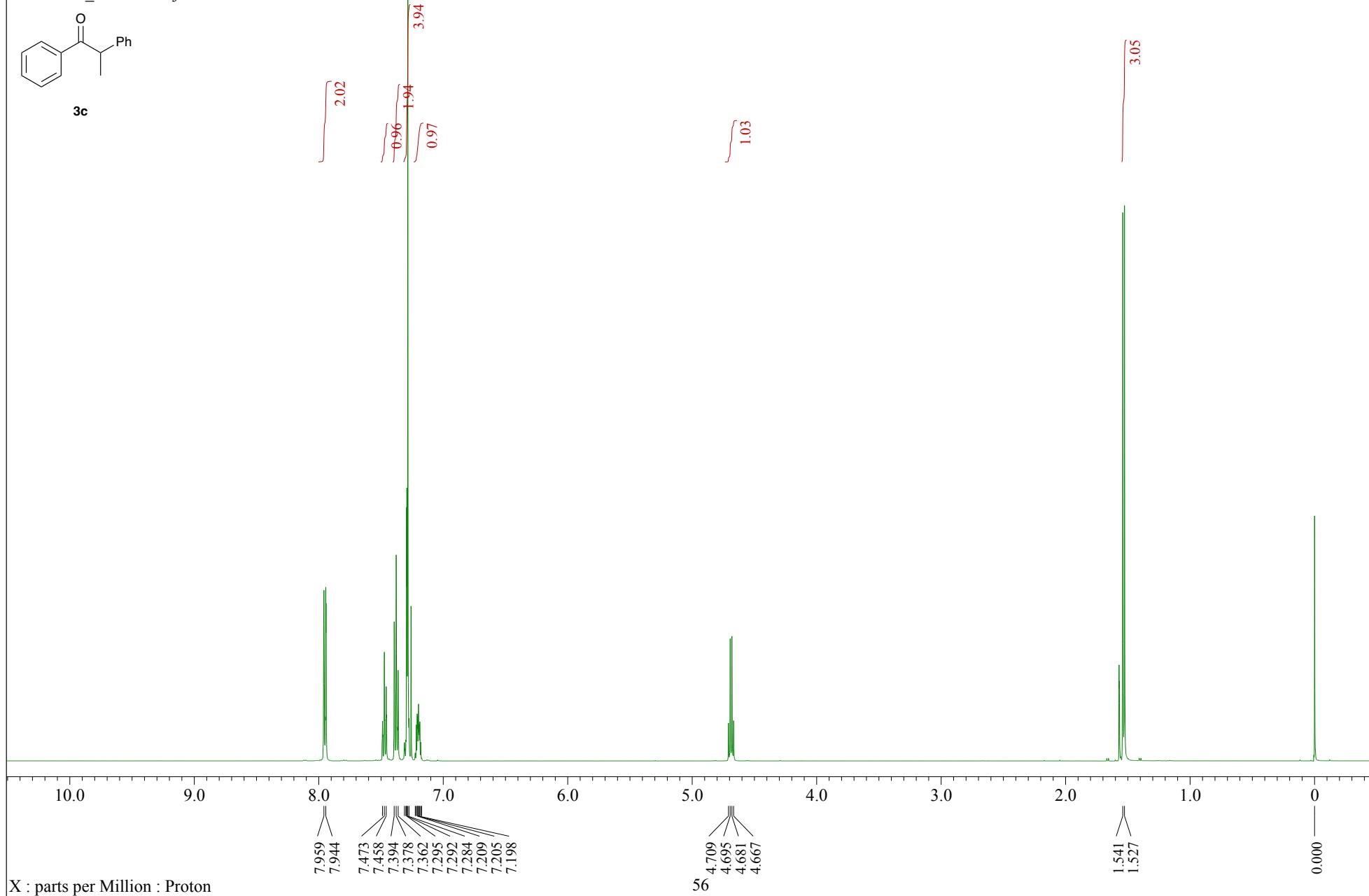
Field_Strength = 11.7473579[T] (500[MHz])
X_Acq_Duration = 3.49175808[s]
X_Domain     = 1H
X_Freq        = 500.15991521[MHz]
X_Offset      = 5.0[ppm]
X_Points      = 32768
X_Prescans   = 1
X_Resolution  = 0.28638868[Hz]
X_Sweep       = 9.38438438[kHz]
X_Sweep_Clipped = 7.50750751[kHz]
Irr_Domain   = Proton
Irr_Freq      = 500.15991521[MHz]
Irr_Offset    = 5.0[ppm]
Tri_Domain   = Proton
Tri_Freq      = 500.15991521[MHz]
Tri_Offset    = 5.0[ppm]
Clipped      = FALSE
Scans         = 8
Total_Scans   = 8

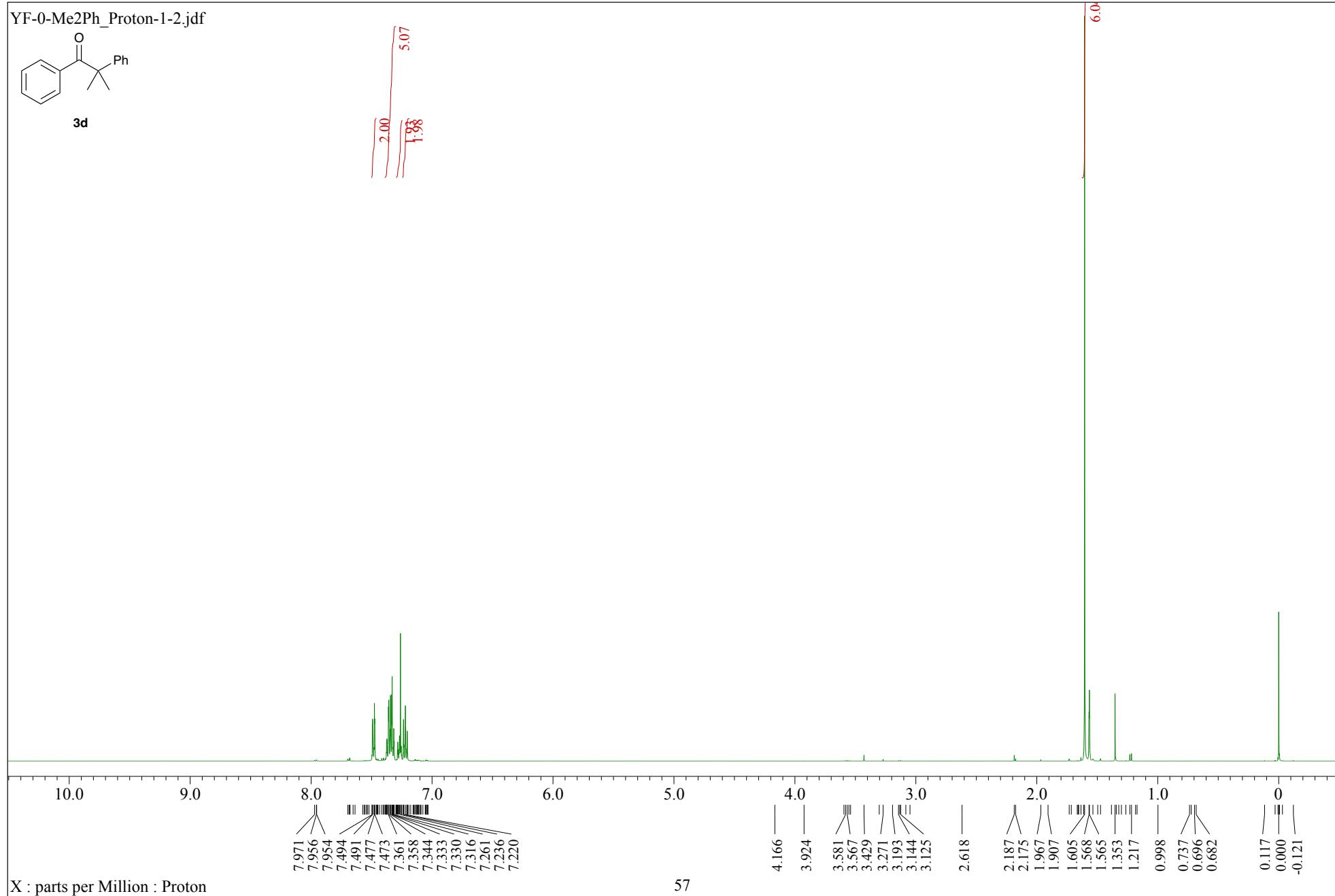
Relaxation_Delay = 2[s]
Recvr_Gain      = 58
Temp_Get         = 26.5[dC]
X_90_Width      = 12.4[us]
X_Acq_Time      = 3.49175808[s]
X_Angle          = 45[deg]
X_Atn            = 4.5[dB]
X_Pulse          = 6.2[us]
Irr_Mode         = Off
Tri_Mode         = Off
Dante_Presat    = FALSE
Initial_Wait    = 1[s]
Repetition_Time = 5.49175808[s]

```

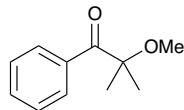


YF-1109-8\_Proton-1-2.jdf

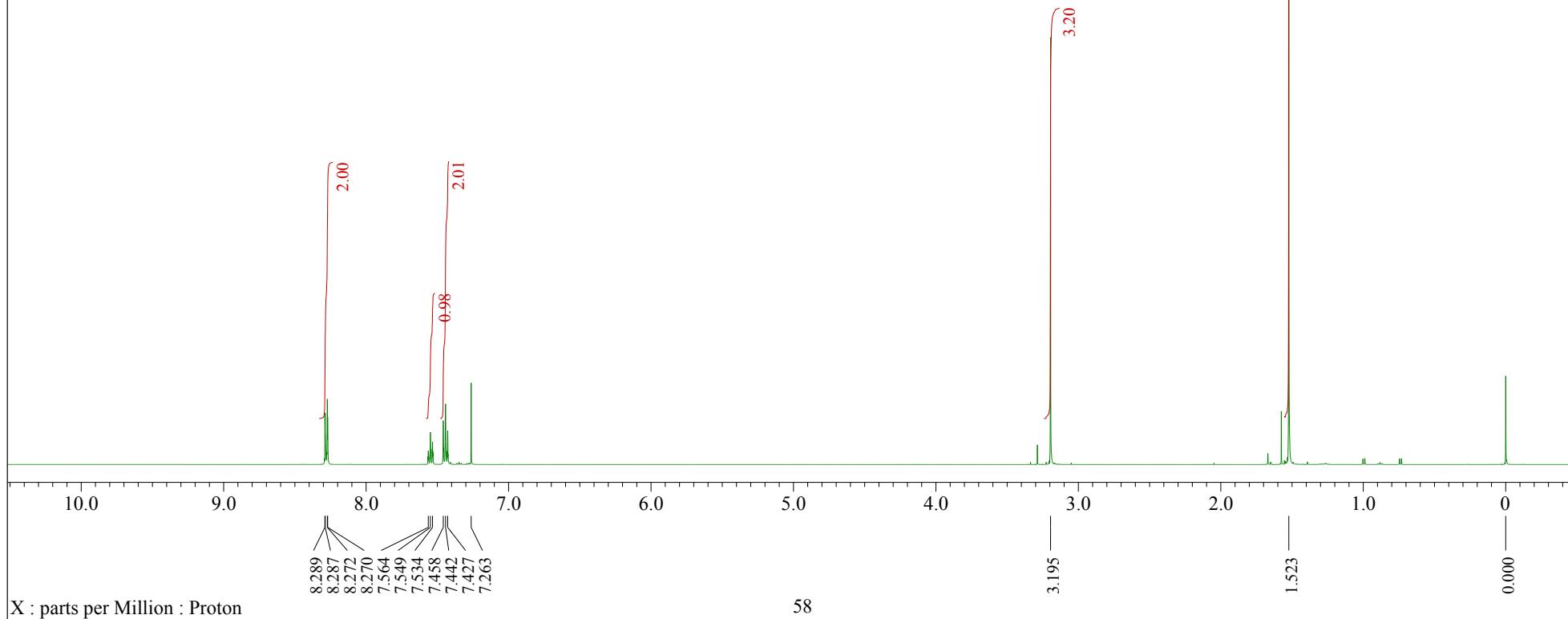




YF-1200-2\_Proton-1-2.jdf

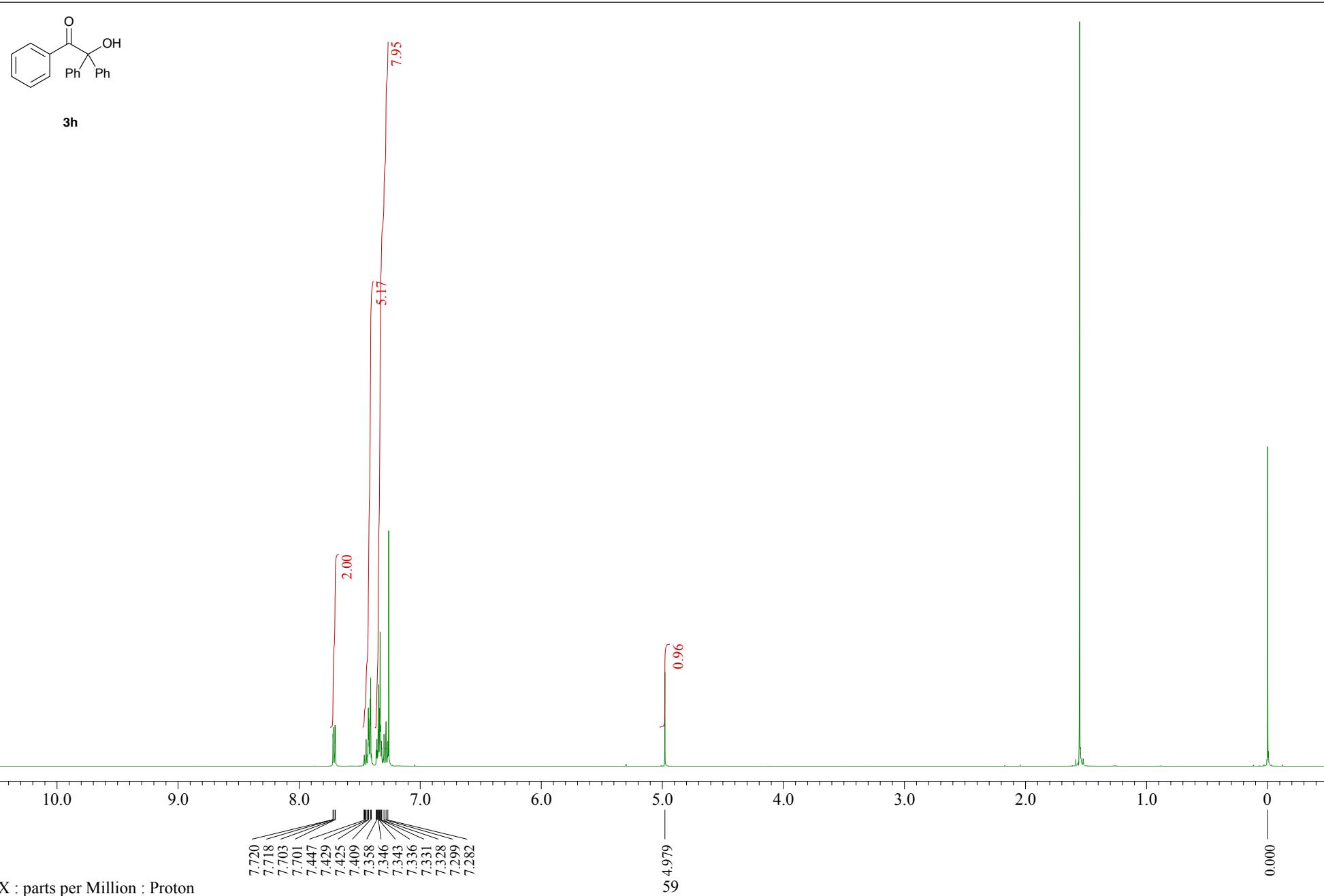


3e

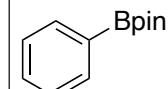


X : parts per Million : Proton

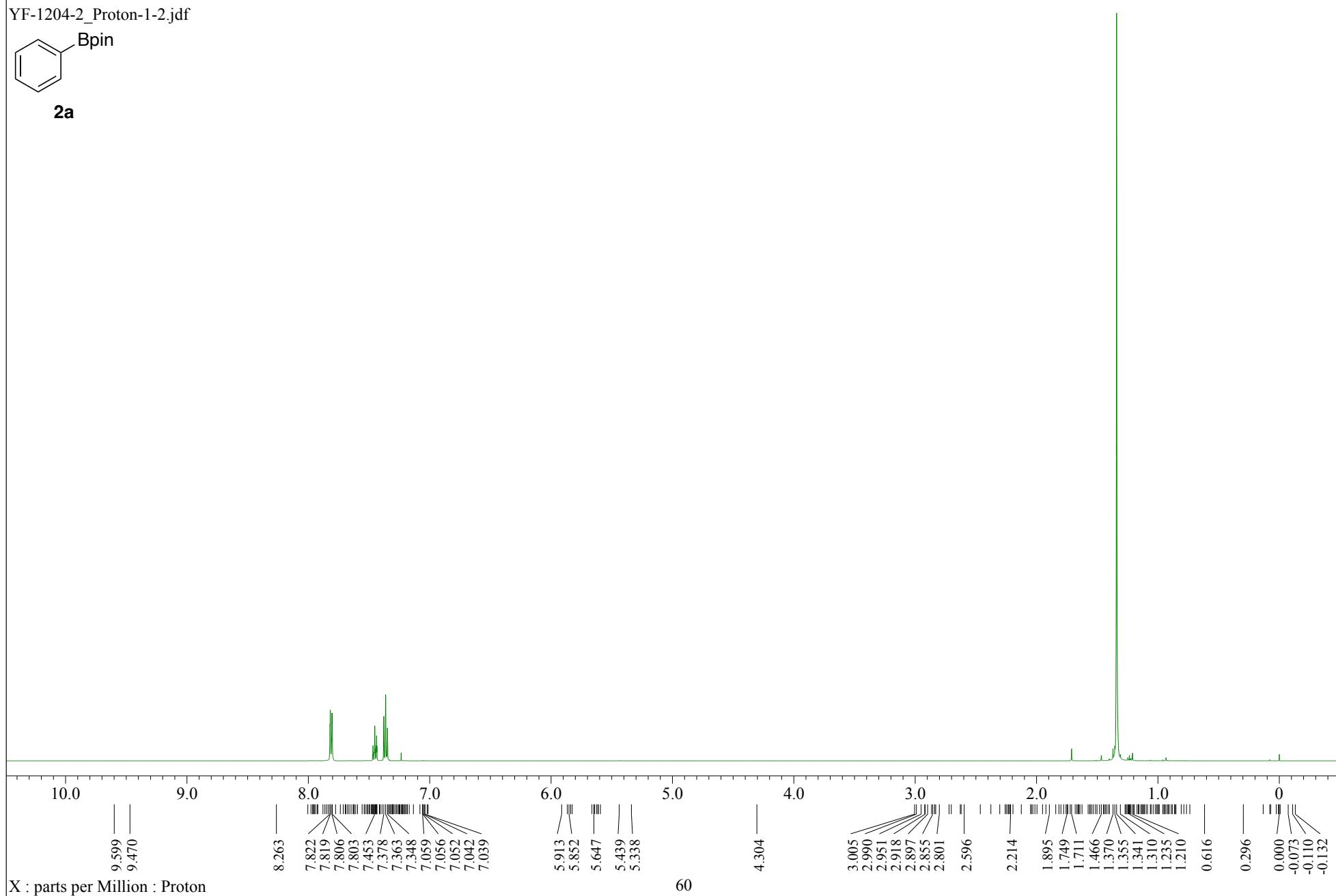
58

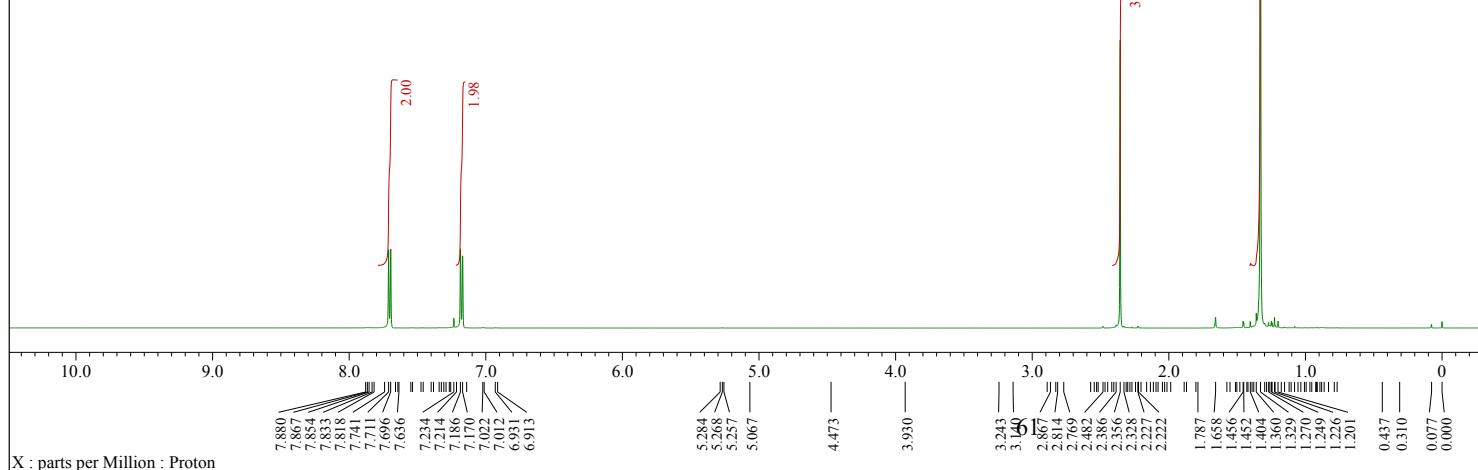
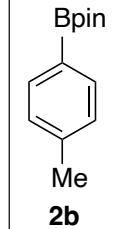


YF-1204-2\_Proton-1-2.jdf



**2a**

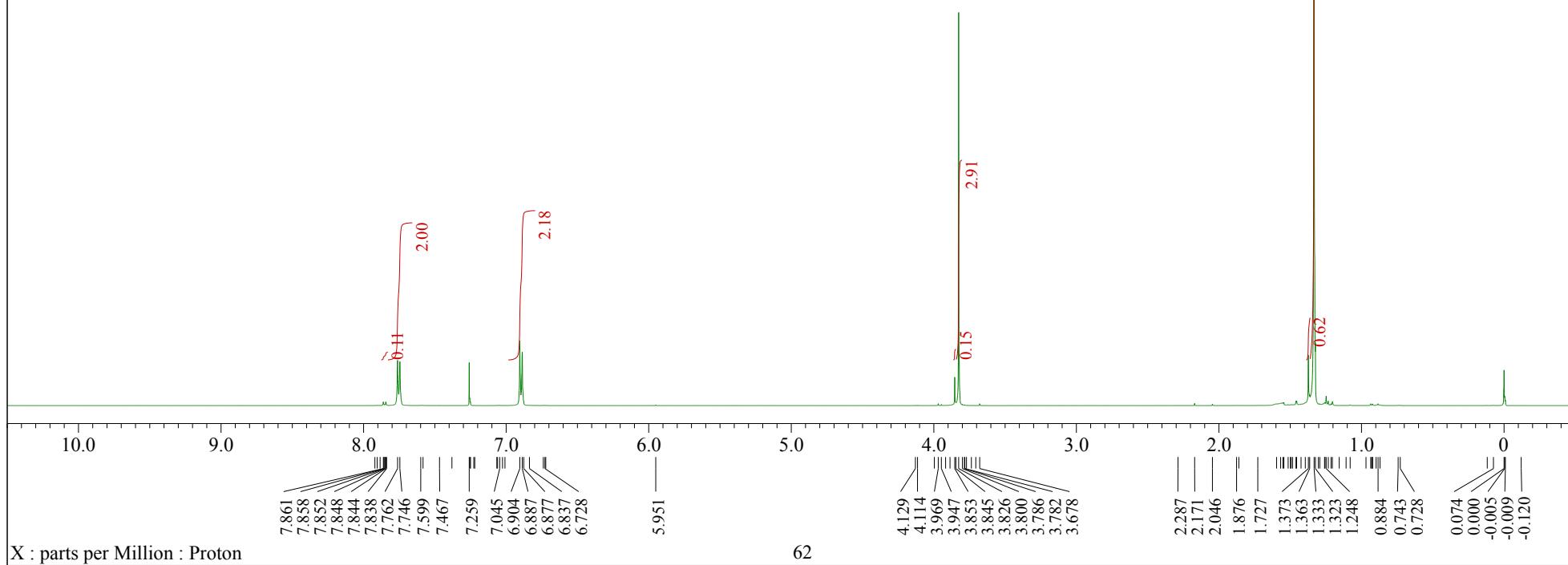
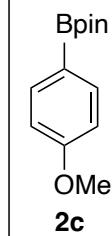




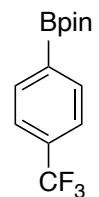
**JEOL**

---- PROCESSING PARAMETERS ----  
sepx( 0.2[Hz], 0.0[s] )  
trapezoid( 0[s] , 0[%] , 80[%] , 100[%] )  
zerofill( 1, TRUE )  
fft( 1, TRUE, TRUE )  
machinephase  
ppm  
base\_correct( Akima, 5, 0, FALSE, 3, None, FA  
以下に由来 : YF-965-2\_Proton-2-1.jdf

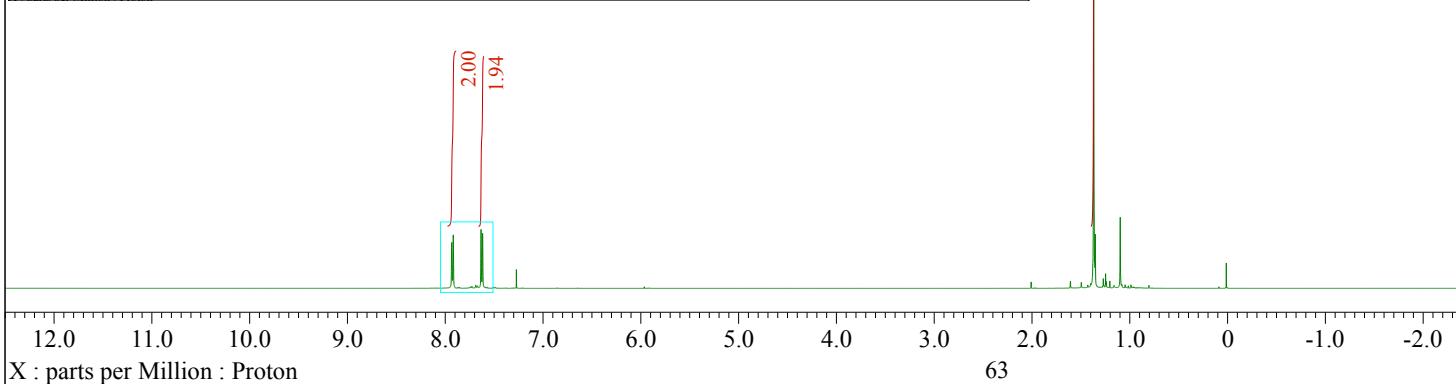
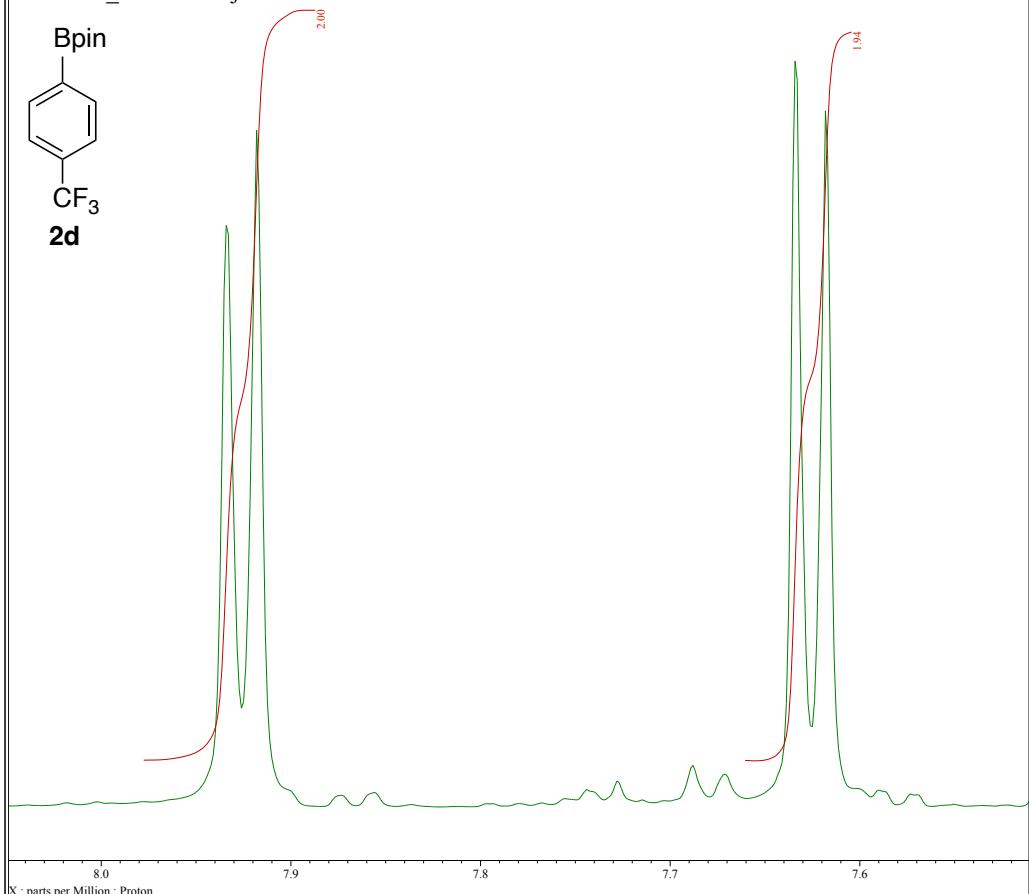
Filename = YF-965-2\_Proton-2-2.j  
Author = delta  
Experiment = proton.jxp  
Sample\_Id = YF-965-2  
Solvent = CHLOROFORM-D  
Actual\_Start\_Time = 2-JUN-2022 17:10:48  
Revision\_Time = 2-JUN-2022 19:57:33  
Comment = single\_pulse  
Data\_Format = 1D REAL  
Dim\_Size = 13107  
X\_Domain = Proton  
Dim\_Title = Proton  
Dim\_Units = [ppm]  
Dimensions = X  
Spectrometer = JNM-ECZ500R/S1  
Field\_Strength = 11.62926421[T] (500[M  
X\_Acq\_Duration = 1.76422912[s]  
X\_Domain = 1H  
X\_Freq = 495.13191398[MHz]  
X\_KOffset = 5 [ppm]  
X\_Points = 13384  
X\_Prescans = 1  
X\_Resolution = 0.5668198[Hz]  
X\_Sweep = 9.28677563[kHz]  
X\_Sweep\_Clipped = 7.42942051[kHz]  
Irr\_Domain = Proton  
Irr\_Freq = 495.13191398[MHz]  
Irr\_Offset = 5 [ppm]  
Tri\_Domain = Proton  
Tri\_Freq = 495.13191398[MHz]  
Tri\_Offset = 5 [ppm]  
Clipped = FALSE  
Scans = 32  
Total\_Scans = 32  
Relaxation\_Delay = 10[s]  
Recvr\_Gain = 36  
Temp\_Get = 27[dC]  
X\_90\_Width = 7.5[us]  
X\_Acq\_Time = 1.76422912[s]  
X\_Angle = 45[deg]  
X\_K = 3.75 [dB]  
X\_Pulse = 3.75[us]  
Irr\_Mode = Off  
Tri\_Mode = Off  
Dante\_Loop = 1000  
Dante\_Presat = FALSE  
Decimation\_Rate = 0  
Initial\_Wait = 1 [s]  
Dith = (180, 90, 270, 180, 180  
Presat\_Time = 10[s]  
Presat\_Time\_Flag = FALSE  
Relaxation\_Delay\_Calc = 0[s]  
Relaxation\_Delay\_Temp = 10[s]  
Repetition\_Time = 11.76422912[s]



YF-868-2\_Proton-1-2.jdf  
YF-868-2\_Proton-1-2.jdf



**2d**

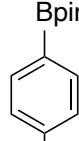


**JEOL**

Filename = YF-868-2\_Proton-1-2.j  
Author = delta  
Experiment = proton.jxp  
Sample\_Id = YF-868-2  
Solvent = CHLOROFORM-D  
Actual\_Start\_Time = 21-MAR-2022 18:02:13  
Revision\_Time = 22-MAR-2022 10:46:54  
  
Comment = single\_pulse  
Data\_Format = 1D COMPLEX  
Dim\_Size = 13107  
X\_Domain = Proton  
Dim\_Title = Proton  
Dim\_Units = [ppm]  
Dimensions = X  
Spectrometer = JNM-ECZ500R/S1  
  
Field\_Strength = 11.62926421[T] (500[M  
X\_Acq\_Duration = 1.76422912[s]  
X\_Domain = 1H  
X\_Freq = 495.13191398[MHz]  
X\_Offset = 5[ppm]  
X\_Points = 16384  
X\_Prescans = 1  
X\_Resolution = 0.5668198[Hz]  
X\_Sweep = 9.28677563[kHz]  
X\_Sweep\_Clipped = 7.42942051[kHz]  
Irr\_Domain = Proton  
Irr\_Freq = 495.13191398[MHz]  
Irr\_Offset = 5[ppm]  
Tri\_Domain = Proton  
Tri\_Freq = 495.13191398[MHz]  
Tri\_Offset = 5[ppm]  
Clipped = FALSE  
Scans = 32  
Total\_Scans = 32  
  
Relaxation\_Delay = 5[s]  
Recvr\_Gain = 36  
Temp\_Get = 20.8[dC]  
X\_90\_Width = 9.47[us]  
X\_Acq\_Time = 1.76422912[s]  
X\_Angle = 45[deg]  
X\_Atn = 4.3[dB]  
X\_Pulse = 4.735[us]  
Irr\_Mode = Off  
Tri\_Mode = Off  
Dante\_Loop = 500  
Dante\_Presat = FALSE  
Decimation\_Rate = 0  
Initial\_Wait = 1[s]  
Phase = {0, 90, 270, 180, 180  
Presat\_Time = 5[s]  
Presat\_Time\_Flag = FALSE  
Relaxation\_Delay\_Calc = 0[s]  
Relaxation\_Delay\_Temp = 5[s]  
Repetition\_Time = 6.76422912[s]

YF-813-2\_Proton-1-2.jdf

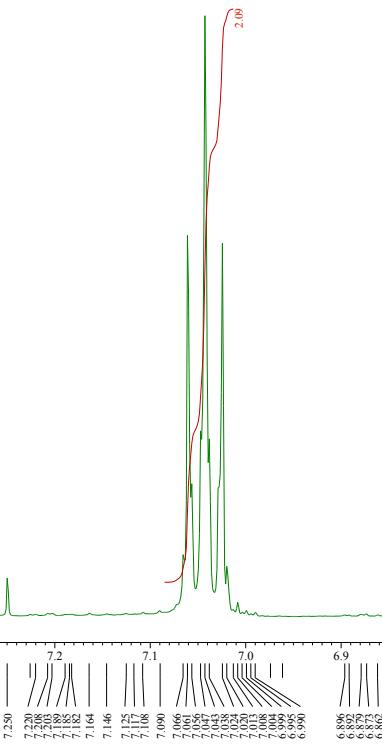
Bpin

**2e**

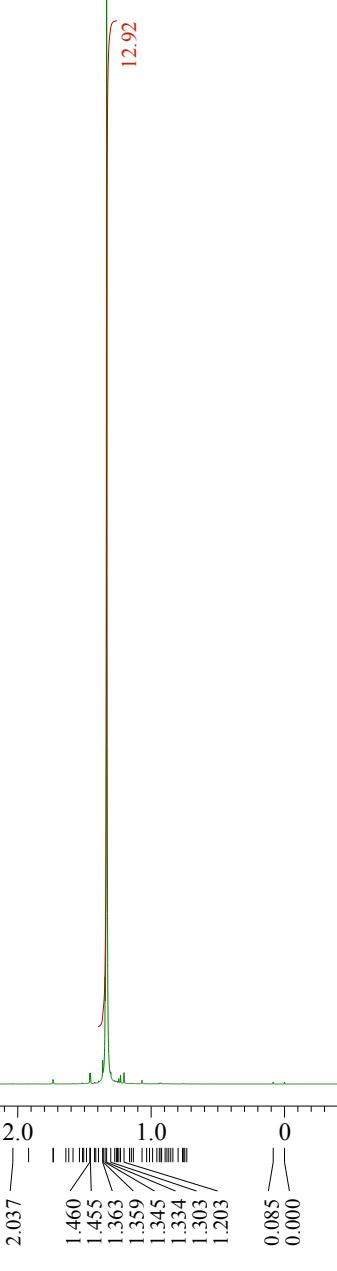
X : parts per Million : Proton

7.973  
7.961  
7.918  
7.905  
7.844  
7.814  
7.801  
7.791  
7.785  
7.785  
7.750  
7.061  
7.056  
7.047  
7.043  
7.038  
7.024  
7.020

X : parts per Million

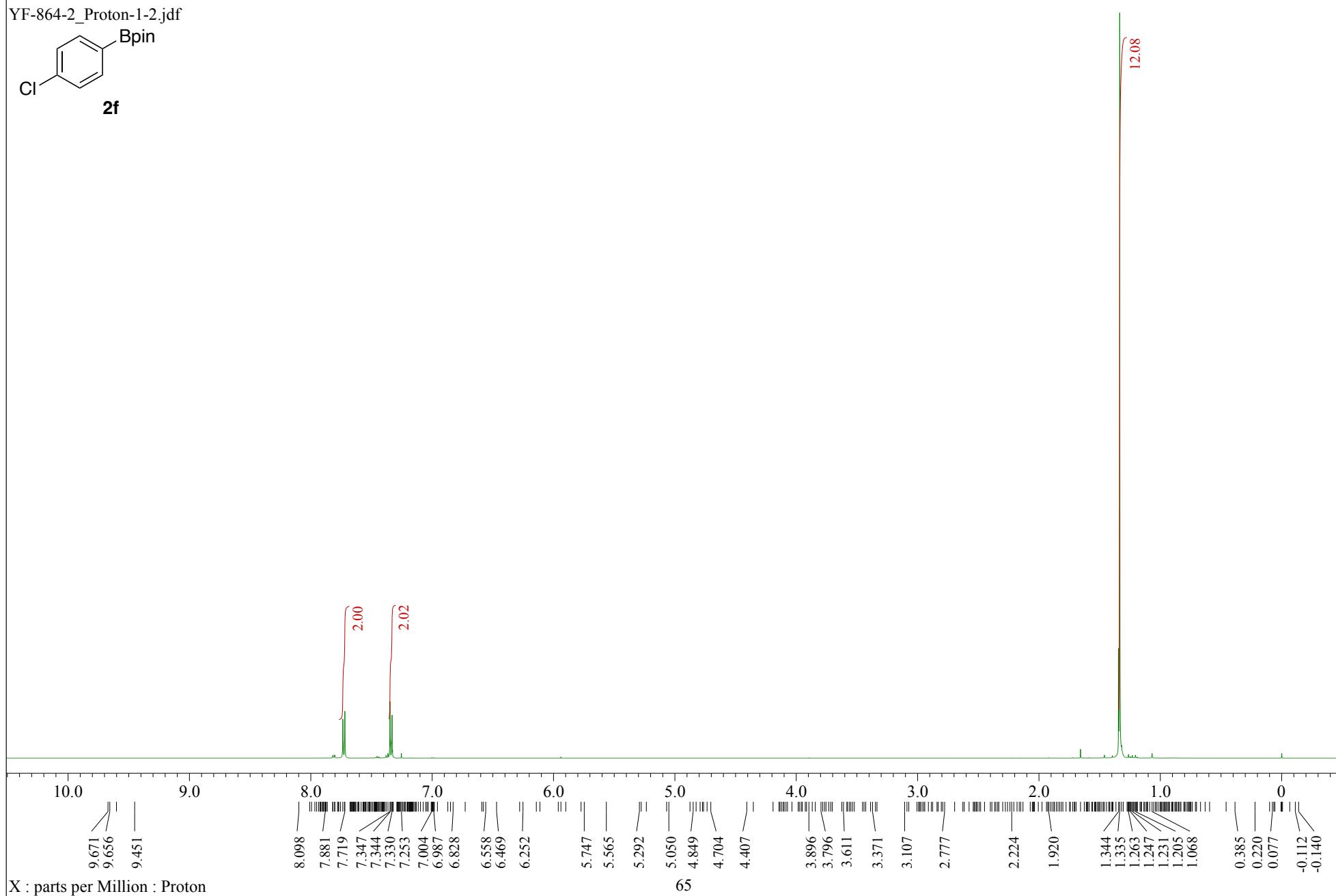
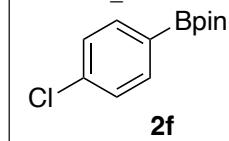
7.973  
7.961  
7.918  
7.905  
7.844  
7.814  
7.801  
7.791  
7.785  
7.785  
7.750  
7.061  
7.056  
7.047  
7.043  
7.038  
7.024  
7.020

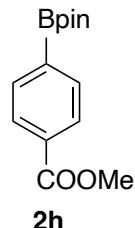
64


**JEOL**

Filename	= YF-813-2_Proton-1-2.j
Author	= delta
Experiment	= proton.jxp
Sample_Id	= YF-813-2
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 21-FEB-2022 23:40:31
Revision_Time	= 22-FEB-2022 10:27:30
Comment	= single_pulse
Data_Format	= 1D REAL
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ500R/S1
Field_Strength	= 11.62926421[T] (500[M
X_Acc_Duration	= 1.76422912[s]
X_Domain	= 1H
X_Freq	= 495.13191398[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.5668198[Hz]
X_Sweep	= 9.28677563[kHz]
X_Sweep_Clipped	= 7.42942051[kHz]
Irr_Domain	= Proton
Irr_Freq	= 495.13191398[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 495.13191398[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 32
Total_Scans	= 32
Relaxation_Delay	= 5[s]
Recv_Gain	= 26
Temp_Get	= 22.1[dC]
X_90_Width	= 7.33[us]
X_Acq_Time	= 1.76422912[s]
X_Angle	= 45[deg]
X_Atn	= 3.3[dB]
X_Pulse	= 3.665[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 500
Dante_Presat	= FALSE
Decimation_Rate	= 0
Initial_Wait	= 1[s]
Phase	= {0, 90, 270, 180, 180}
Presat_Time	= 5[s]
Presat_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 5[s]
Repetition_Time	= 6.76422912[s]

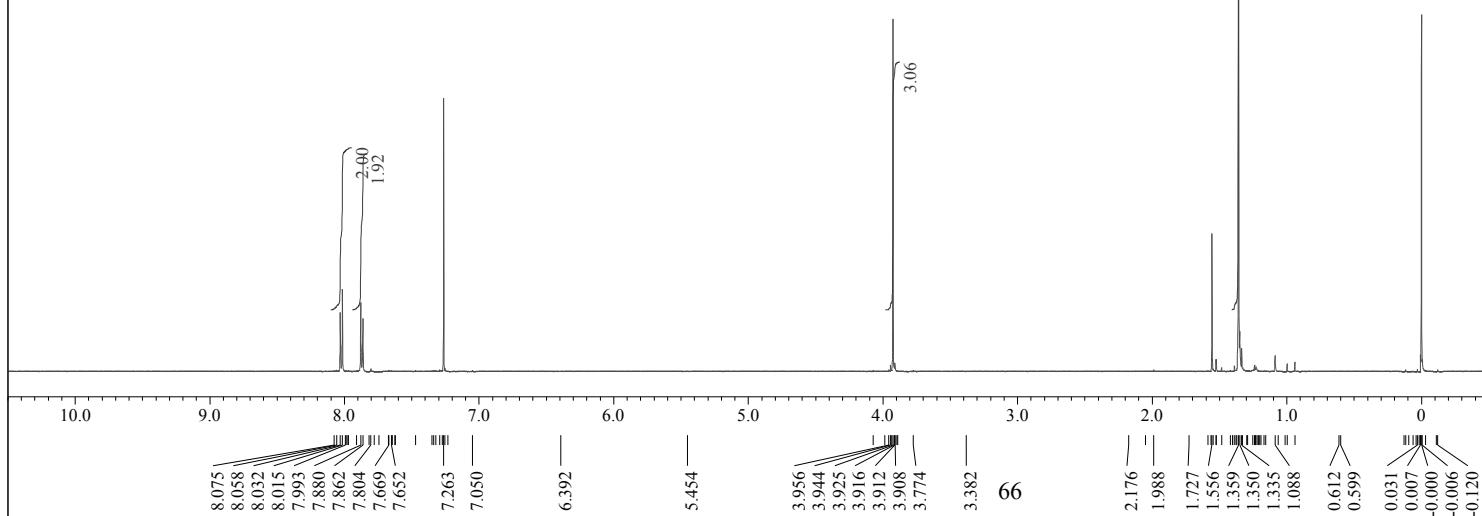
YF-864-2\_Proton-1-2.jdf





**2h**

**2h**



X : parts per Million : Proton

```

Filename      = YF-1219-2_Proton-1-5.
Author       = delta
Experiment   = proton.jpx
Sample_Id    = YF-1219-2
Solvent      = CHLOROFORM-D
Actual_Start_Time = 9-NOV-2022 14:05:18
Revision_Time = 9-NOV-2022 13:07:20

Comment      = single_pulse
Data_Format  = 1D REAL
Dim_Size     = 13107
Dim_Title    = Proton
Dim_Units    = [ppm]
Dimensions   = X
Spectrometer = JNM-ECZ500R/S1

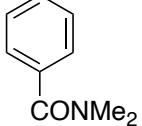
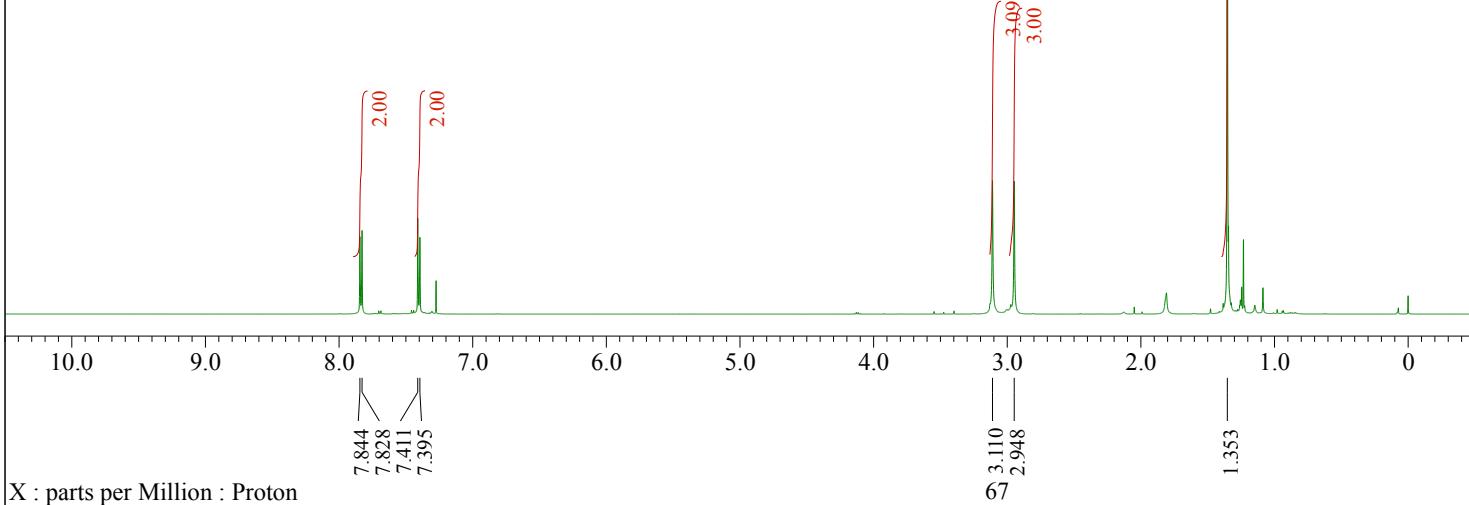
Field_Strength = 11.62926421[T] (500[M
X_Acc_Duration = 1.76422912[s]
X_Domain     = 1H
X_Freq        = 495.13191398[MHz]
X_Offset      = 5[ppm]
X_Points      = 16384
X_Prescans   = 1
X_Resolution  = 0.5668198[Hz]
X_Sweep       = 9.28677563[kHz]
X_Sweep_Clipped = 7.42942051[kHz]
Irr_Domain   = Proton
Irr_Freq     = 495.13191398[MHz]
Irr_Offset   = 5[ppm]
Tri_Domain   = Proton
Tri_Freq     = 495.13191398[MHz]
Tri_Offset   = 5[ppm]
Clipped      = FALSE
Scans        = 8
Total_Scans  = 8

Relaxation_Delay = 5[s]
Recv_Gain        = 50
Temp_Get         = 20.1[deg]
X_Acc_Width     = 8.7[us]
X_Acc_Time      = 1.76422912[s]
X_Angle         = 45[deg]
X_Atn          = 4.3[dB]
X_Pulse         = 4.35[us]
Irr_Mode        = Off
Tri_Mode        = Off
Dante_Loop     = 500
Dante_Presat   = FALSE
Decimation_Rate = 0
Initial_Wait   = 1[s]
Phase          = {0, 90, 270, 180, 180
Presat_Time    = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 6.76422912[s]

```

YF-1068-4\_Proton-1-2.jdf

Bpin

**2i**

```

Filename          = YF-1068-4_Proton-1-2.
Author           = delta
Experiment       = proton.jxp
Sample_Id        = YF-1068-4
Solvent          = CHLOROFORM-D
Actual_Start_Time = 14-JUL-2022 00:35:08
Revision_Time    = 14-JUL-2022 14:55:05

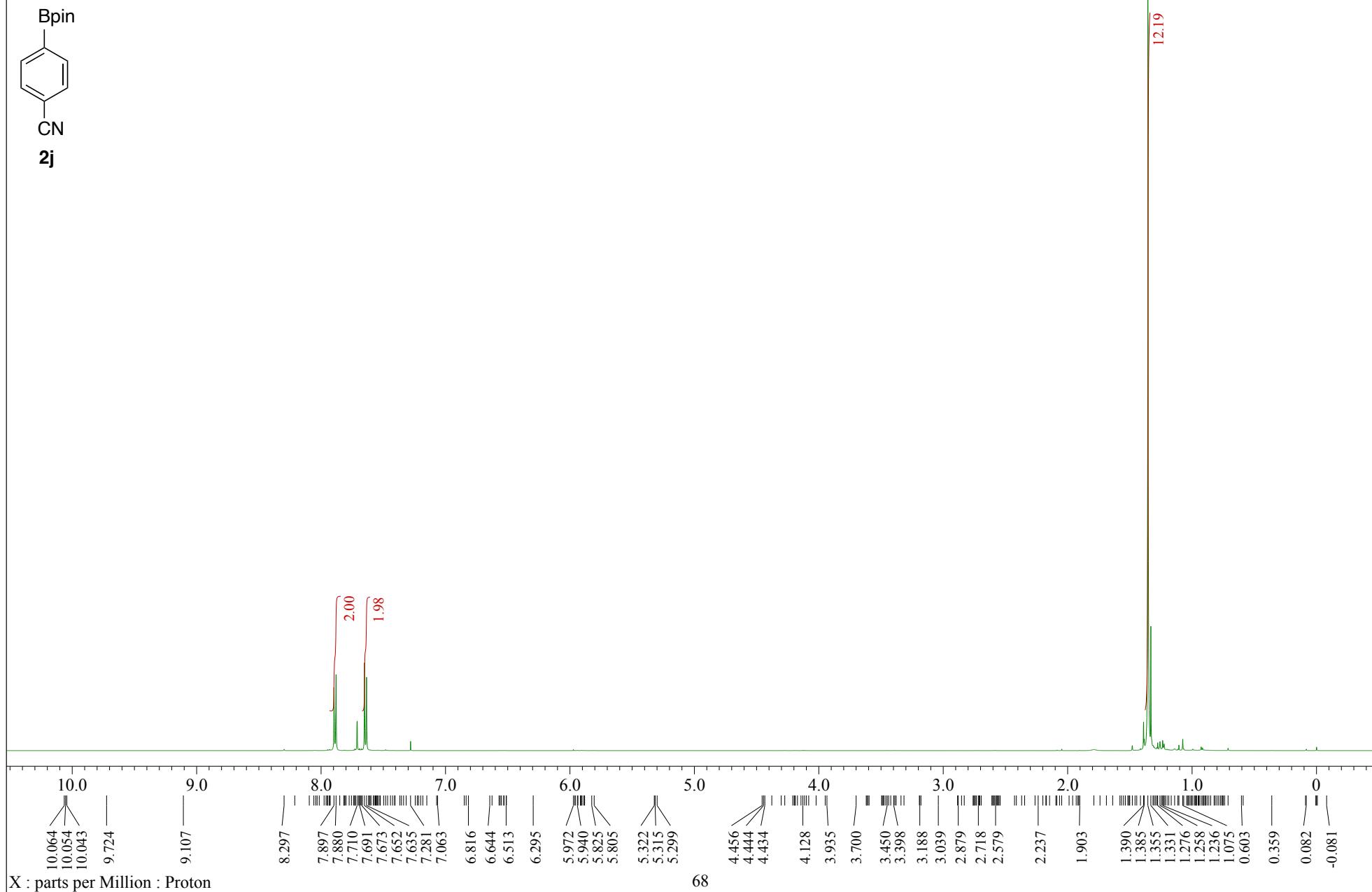
Comment          = single_pulse
Data_Format      = 1D COMPLEX
Dim_Size         = 13107
X_Domain         = Proton
Dim_Title        = Proton
Dim_Units        = [ppm]
Dimensions       = X
Spectrometer     = JNM-ECZ500R/S1

Field_Strength   = 11.62926421[T] (500[M]
X_Acq_Duration  = 1.76422912[s]
X_Domain         = 1H
X_Freq           = 495.13191398[MHz]
X_Offset         = 5[ppm]
X_Points         = 16384
X_Prescans       = 1
X_Resolution     = 0.5668198[Hz]
X_Sweep          = 9.28677563[kHz]
X_Sweep_Clipped = 7.42942051[kHz]
Irr_Domain       = Proton
Irr_Freq         = 495.13191398[MHz]
Irr_Offset       = 5[ppm]
Tri_Domain       = Proton
Tri_Freq         = 495.13191398[MHz]
Tri_Offset       = 5[ppm]
Clipped          = FALSE
Scans            = 32
Total_Scans      = 32

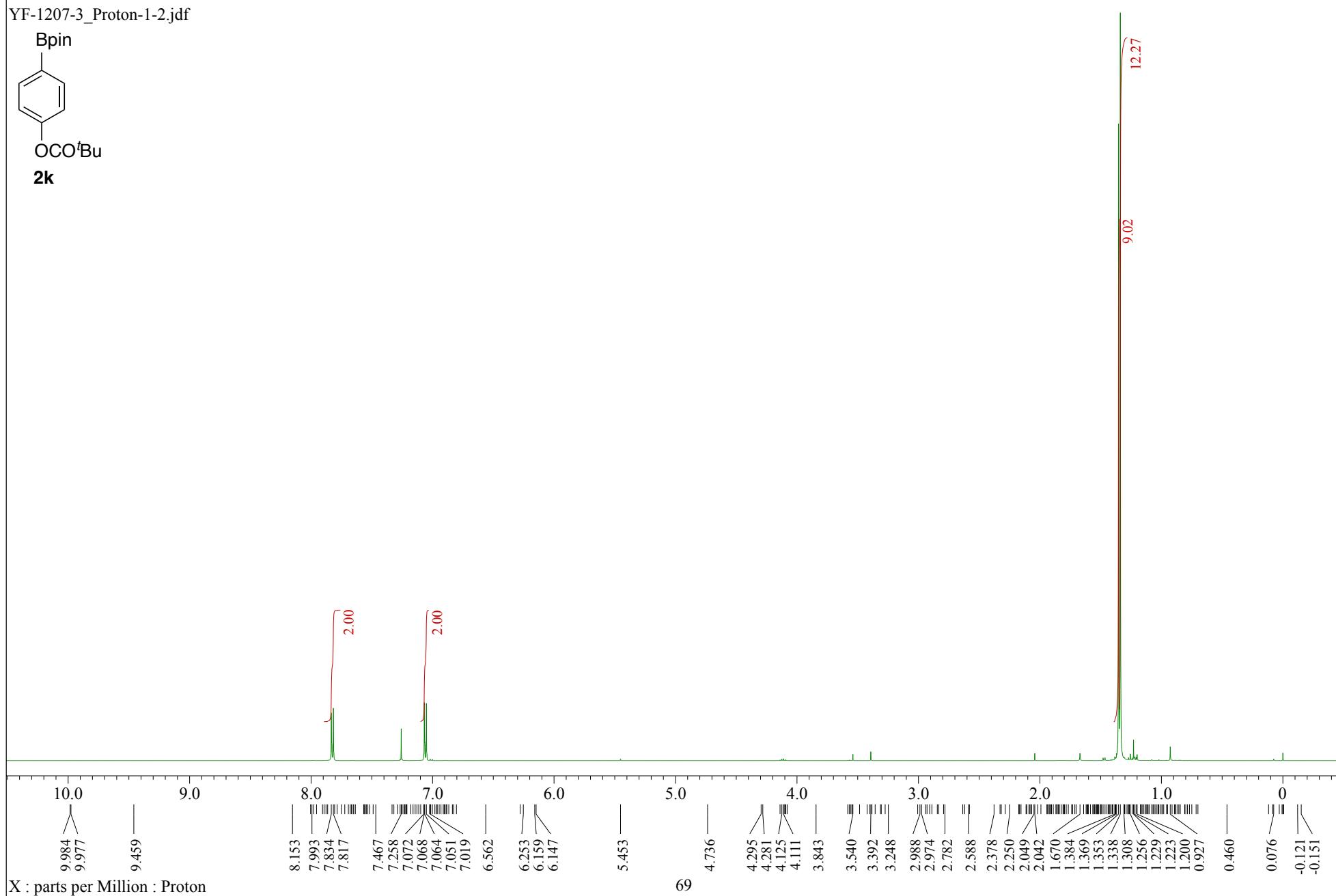
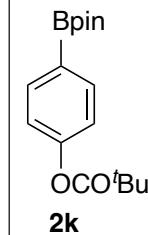
Relaxation_Delay = 10[s]
Recvr_Gain       = 36
Temp_Get          = 18.9[dC]
X_90_Width        = 9.49[us]
X_Acq_Time        = 1.76422912[s]
X_Angle           = 45[deg]
X_Atn             = 4.3[dB]
X_Pulse           = 4.745[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Loop        = 1000
Dante_Presat      = FALSE
Decimation_Rate   = 0
Initial_Wait      = 1[s]
Phase             = {0, 90, 270, 180, 180
Presat_Time       = 10[s]
Presat_Time_Flag  = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 10[s]
Repetition_Time   = 11.76422912[s]

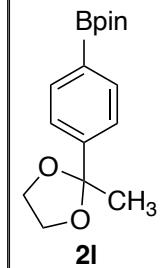
```

YF-1211-2\_Proton-1-2.jdf



YF-1207-3\_Proton-1-2.jdf





**JEOL**

```

Filename = YF-971-2_Proton-2-5.j
Author = delta
Experiment = proton.jxp
Sample_Id = YF-971-2
Solvent = CHLOROFORM-D
Actual_Start_Time = 3-JUN-2022 09:08:41
Revision_Time = 3-JUN-2022 09:10:45

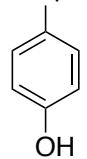
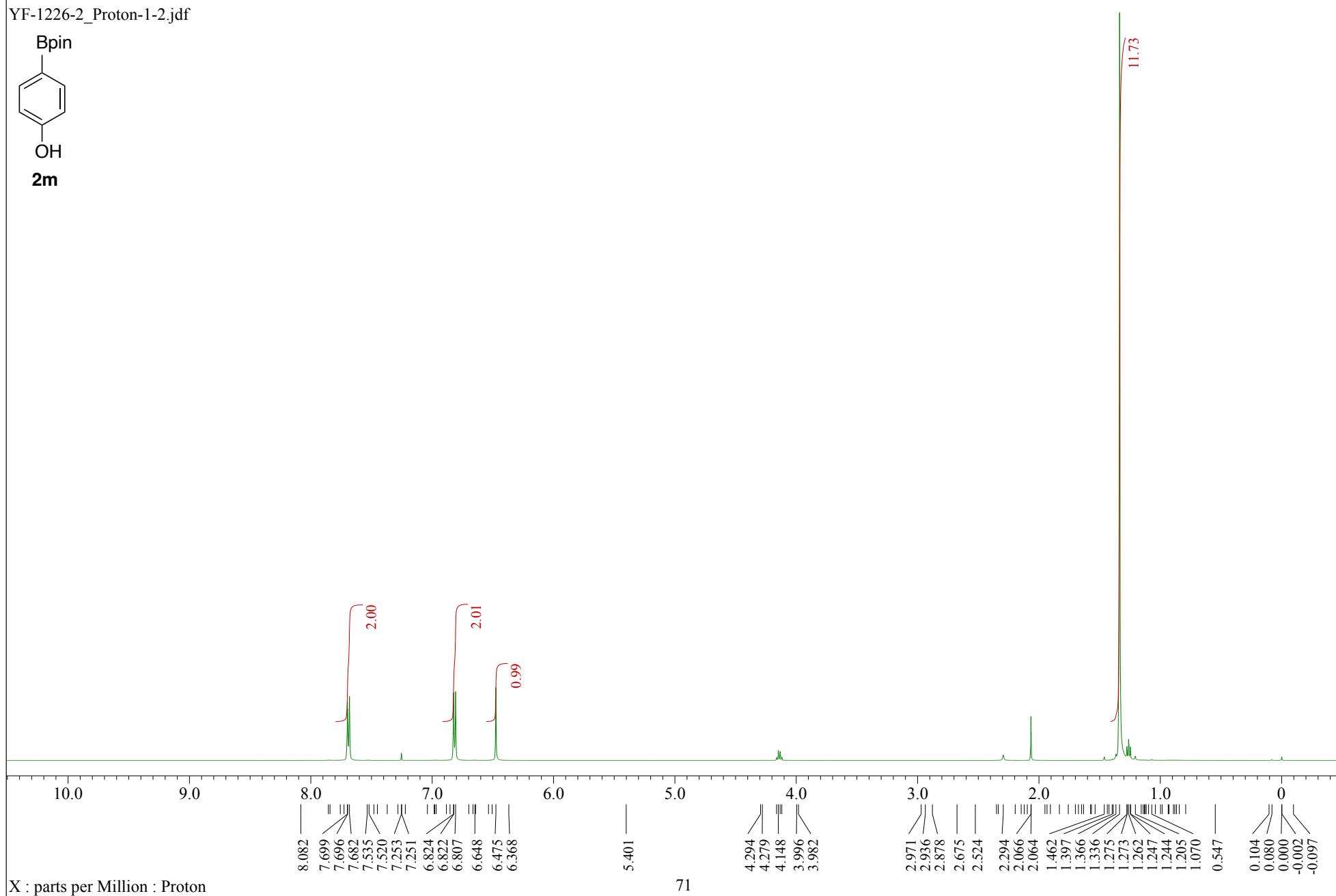
Comment = single_pulse
Data_Format = 1D_REAL
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1

Field_Strength = 11.62926421[T] (500[M
X_Acq_Duration = 1.76422912[s]
X_Domain = 1H
X_Freq = 495.13191398[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.5668198[Hz]
X_Sweep = 9.28677563[kHz]
X_Sweep_Clipped = 7.42942051[kHz]
Irr_Domain = Proton
Irr_Freq = 495.13191398[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 495.13191398[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 32
Total_Scans = 32

Relaxation_Delay = 10[s]
Recv_Gain = 66
Tau_Get = 26.7[4C]
X_90_Width = 7.5[us]
X_Acq_Time = 1.76422912[s]
X_Angle = 45[deg]
X_Atn = 3.3[dB]
X_Pulse = 3.75[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 1000
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = {0, 90, 270, 180, 180
Presat_Time = 10[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 10[s]
Repetition_Time = 11.76422912[s]

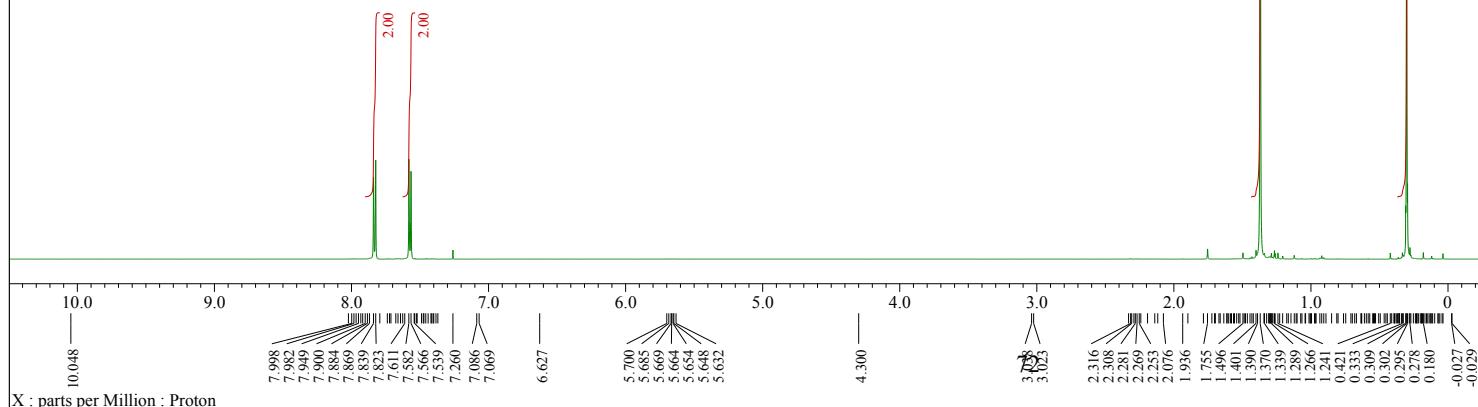
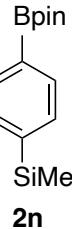
```

Bpin

**2m**

X : parts per Million : Proton

71



**JEOL**

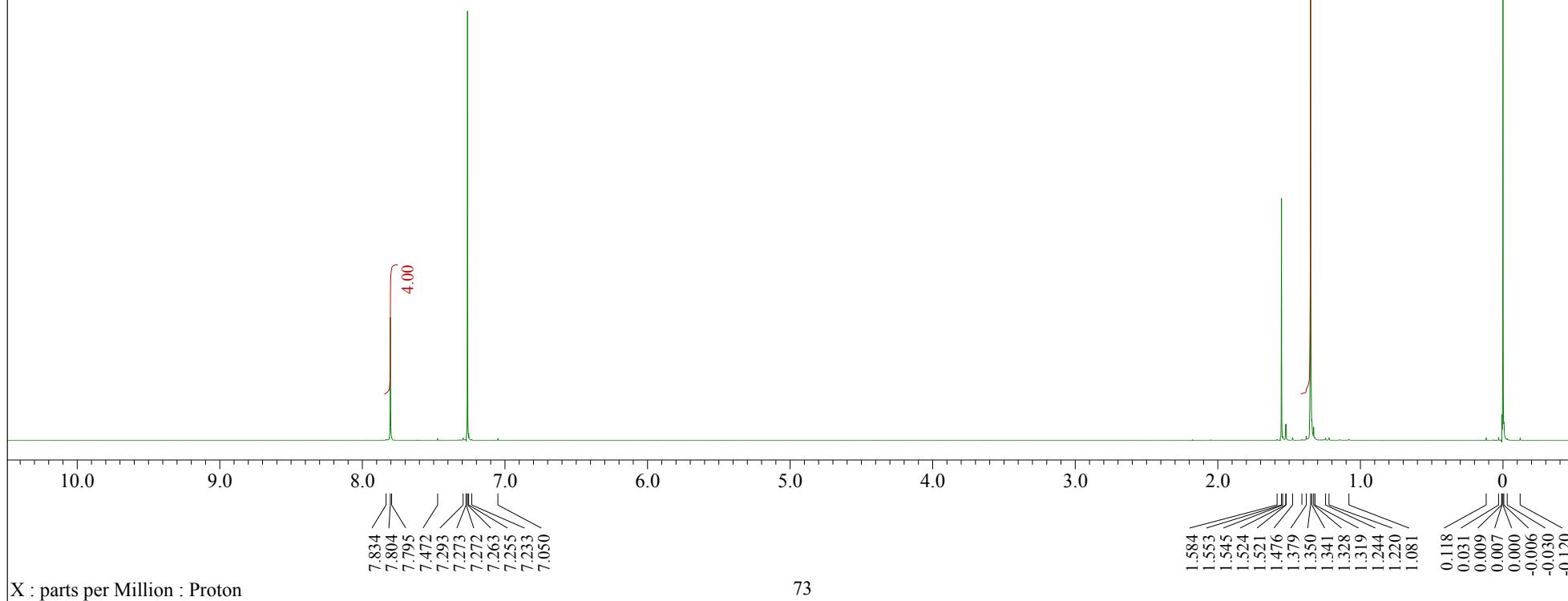
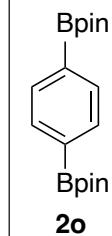
```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
ppm
base_correct( Akima, 5, 0, FALSE, 3, None, FA
以下に由来 : YF-1190-2_Proton-1-1.jdf
```

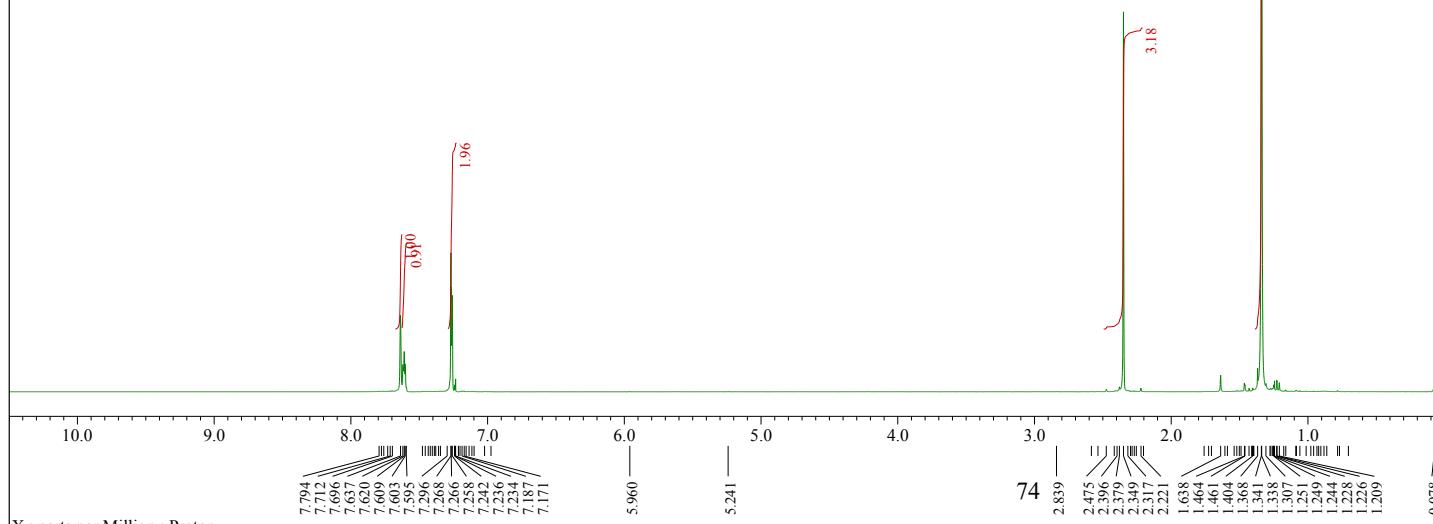
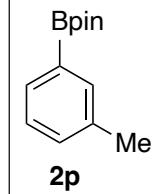
```
Filename = YF-1190-2_Proton-1-2.
Author = delta
Experiment = proton.jpx
Sample_Id = YF-1190-2
Solvent = CHLOROFORM-D
Actual_Start_Time = 28-OCT-2022 20:25:39
Revision_Time = 29-OCT-2022 15:11:32

Comment = single_pulse
Data_Format = delta
Dim_Size = 13107
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1

Field_Strength = 11.62926421[T] (500[M
X_Acq_Duration = 1.76422912[s]
X_Domain = 1H
X_Freq = 495.13191398[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.5668198[Hz]
X_Sweep = 9.28677563[kHz]
X_Sweep_Clipped = 7.42942051[kHz]
Irr_Domain = Proton
Irr_Freq = 495.13191398[MHz]
Irr_Offset = 8[ppm]
Tri_Domain = proton
Tri_Freq = 495.13191398[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8

Relaxation_Delay = 5[s]
Recvr_Gain = 26
Temp_Get = 19.9[dC]
X_90_Width = 8.7[us]
X_Acq_Time = 1.76422912[s]
X_Angle = 45[deg]
X_Alt = 4.3[dB]
X_Pulse = 4.35[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = { 90, 270, 180, 180
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 6.76422912[s]
```





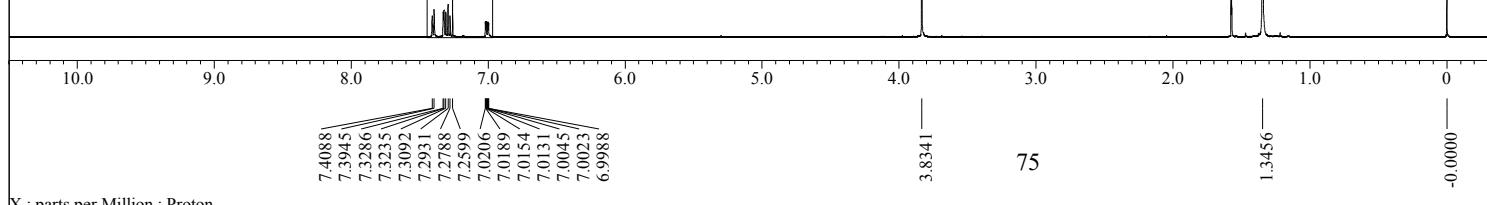
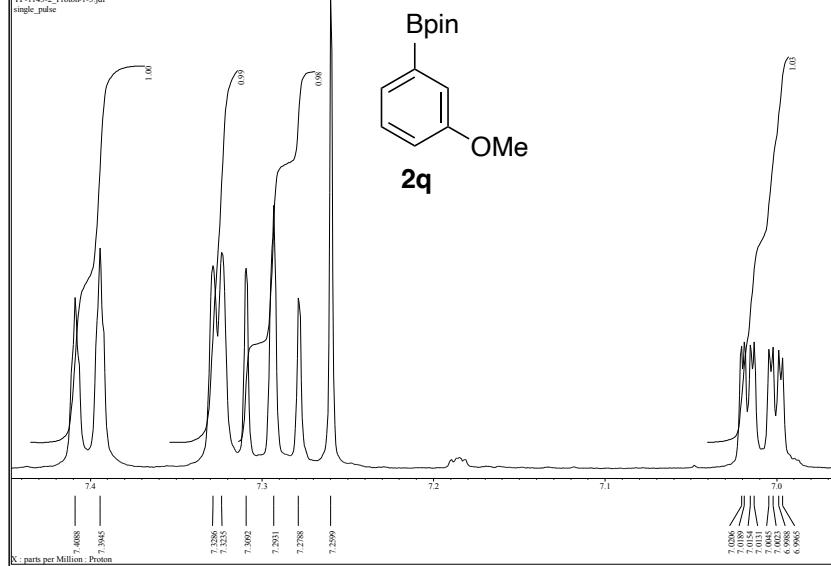
**JEOL**

---- PROCESSING PARAMETERS ----  
 sexp( 0.2[Hz], 0.0[s] )  
 trapezoid( 0[s] , 0[%] , 80[%] , 100[%] )  
 zerofill( 1, TRUE )  
 fft( 1, TRUE, TRUE )  
 machinephase  
 ppm  
 base\_correct( Akima, 5, 0, FALSE, 3, None, FA  
 以下に由来 : YF-964-2\_Proton-1-1.jdf

Filename = YF-964-2\_Proton-1-2.j  
 Author = delta  
 Experiment = proton.jxp  
 Sample\_Id = YF-964-2  
 Solvent = CHLOROFORM-D  
 Actual\_Start\_Time = 2-JUN-2022 04:15:45  
 Revision\_Time = 2-JUN-2022 11:35:10  
 Comment = single\_pulse  
 Data\_Format = 1D REAL  
 Dim\_Size = 13107  
 X\_Domain = Proton  
 Dim\_Title = Proton  
 Dim\_Units = [ppm]  
 Dimensions = X  
 Spectrometer = JNM-ECZ500R/S1  
 Field\_Strength = 11.62926421[T] (500[M  
 X\_Acq\_Duration = 1.76422912[s]  
 X\_Domain = 1H  
 X\_Freq = 495.13191398[MHz]  
 X\_KOffset = 5 [ppm]  
 X\_Points = 13384  
 X\_Prescans = 1  
 X\_Resolution = 0.5668198[Hz]  
 X\_Sweep = 9.28677563[kHz]  
 X\_Sweep\_Clipped = 7.42942051[kHz]  
 Irr\_Domain = Proton  
 Irr\_Freq = 495.13191398[MHz]  
 Irr\_Offset = 5 [ppm]  
 Tri\_Domain = Proton  
 Tri\_Freq = 495.13191398[MHz]  
 Tri\_Offset = 5 [ppm]  
 Clipped = FALSE  
 Scans = 32  
 Total\_Scans = 32  
 Relaxation\_Delay = 10[s]  
 Recvr\_Gain = 36  
 Temp\_Get = 26.7[dC]  
 X\_90\_Width = 7.5[us]  
 X\_Acq\_Time = 1.76422912[s]  
 X\_Angle = 45[deg]  
 X\_K = 3.75[dB]  
 X\_Pulse = 3.75[us]  
 Irr\_Mode = Off  
 Tri\_Mode = Off  
 Danto\_Loop = 1000  
 Danto\_Presat = FALSE  
 Decimation\_Rate = 0  
 Initial\_Wait = 1 [s]  
 Dnu = ( 10, 90, 270, 180, 180  
 Presat\_Time = 10[s]  
 Presat\_Time\_Flag = FALSE  
 Relaxation\_Delay\_Calc = 0[s]  
 Relaxation\_Delay\_Temp = 10[s]  
 Repetition\_Time = 11.76422912[s]

YF-1143-2\_Proton-1-3.jdf  
single\_pulse

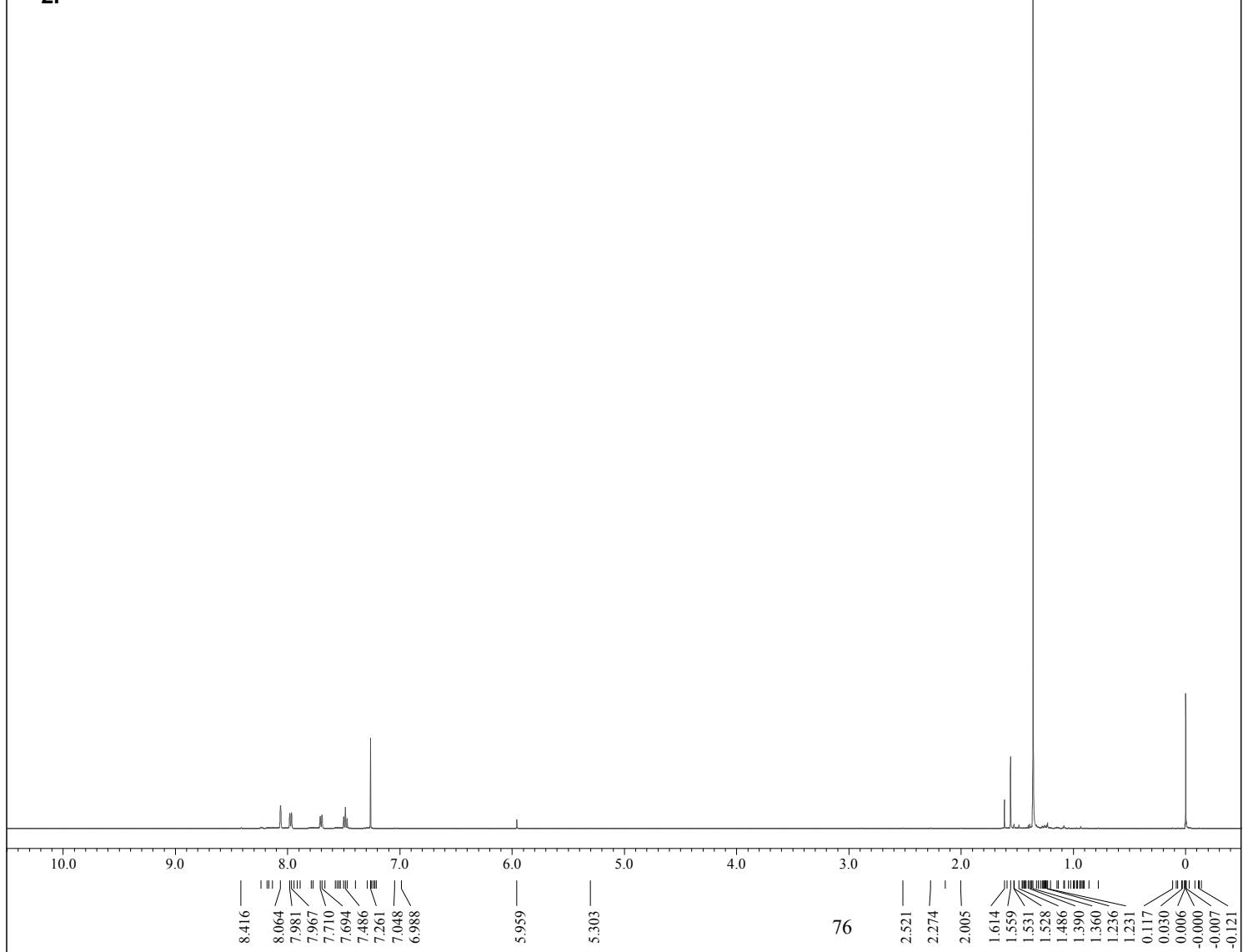
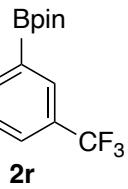
YF-1143-2\_Proton-1-3.jdf  
single\_pulse



---- PROCESSING PARAMETERS ----  
dc\_balance( 0, FALSE )  
secp( 0.2[Hz], 0.0[s] )  
trapezoid( 0[%], 0[%], 80[%], 100[%] )  
zerofill( 1 )  
fft( 1, TRUE, TRUE )  
machinephase  
ppm  
以下に由来:: YF-1143-2\_Proton-1-1.jdf

Filename = YF-1143-2\_Proton-1-3.jdf  
Author = tsukamoto  
Experiment = proton.jxp  
Sample\_Id = YF-1143-2  
Solvent = CHLOROFORM-D  
Creation\_Time = 7-OCT-2022 20:36:08  
Revision\_Time = 7-OCT-2022 21:07:19  
Current\_Time = 7-OCT-2022 21:08:04  
Comment = single\_pulse  
Data\_Format = 1H\_COMPLEX  
Dim\_Size = 26214  
Dim\_Title = Proton  
Dim\_Units = [ppm]  
Dimensions = X  
Site = JNM-ECA500  
Spectrometer = DELTA2\_NMR  
Field\_Strength = 11.7473579[T] (500[MHz])  
X\_Acq\_Duration = 3.49175808[s]  
X\_Domain = 1H  
X\_Freq = 500.15991521[MHz]  
X\_Offset = 5.0[ppm]  
X\_Points = 32768  
X\_Prescans = 1  
X\_Resolution = 0.28638868[Hz]  
X\_Sweep = 9.38438438[kHz]  
X\_Sweep\_Clipped = 7.50750751[kHz]  
Irr\_Domain = Proton  
Irr\_Freq = 500.15991521[MHz]  
Irr\_Offset = 5.0[ppm]  
Tri\_Domain = Proton  
Tri\_Freq = 500.15991521[MHz]  
Tri\_Offset = 5.0[ppm]  
Clipped = FALSE  
Scans = 8  
Total\_Scans = 8  
Relaxation\_Delay = 2[s]  
Recv\_Gain = 46  
Temp\_Get = 21.9[dC]  
X\_90\_Width = 12.4[us]  
X\_Acq\_Time = 3.49175808[s]  
X\_Angle = 45[deg]  
X\_BW = 4.0[MHz]  
X\_Pulse = 6.2[us]  
Irr\_Mode = Off  
Tri\_Mode = Off  
Dante\_Presat = FALSE  
Initial\_Wait = 1[s]  
Repetition\_Time = 5.49175808[s]

YF-1163-2\_Proton-1-6.jdf



**JEOL**

```

Filename      = YF-1163-2_Proton-1-6.
Author       = delta
Experiment   = proton.jpx
Sample_Id    = YF-1163-2
Solvent      = CHLOROFORM-D
Actual_Start_Time = 14-OCT-2022 21:52:35
Revision_Time = 14-OCT-2022 20:56:09

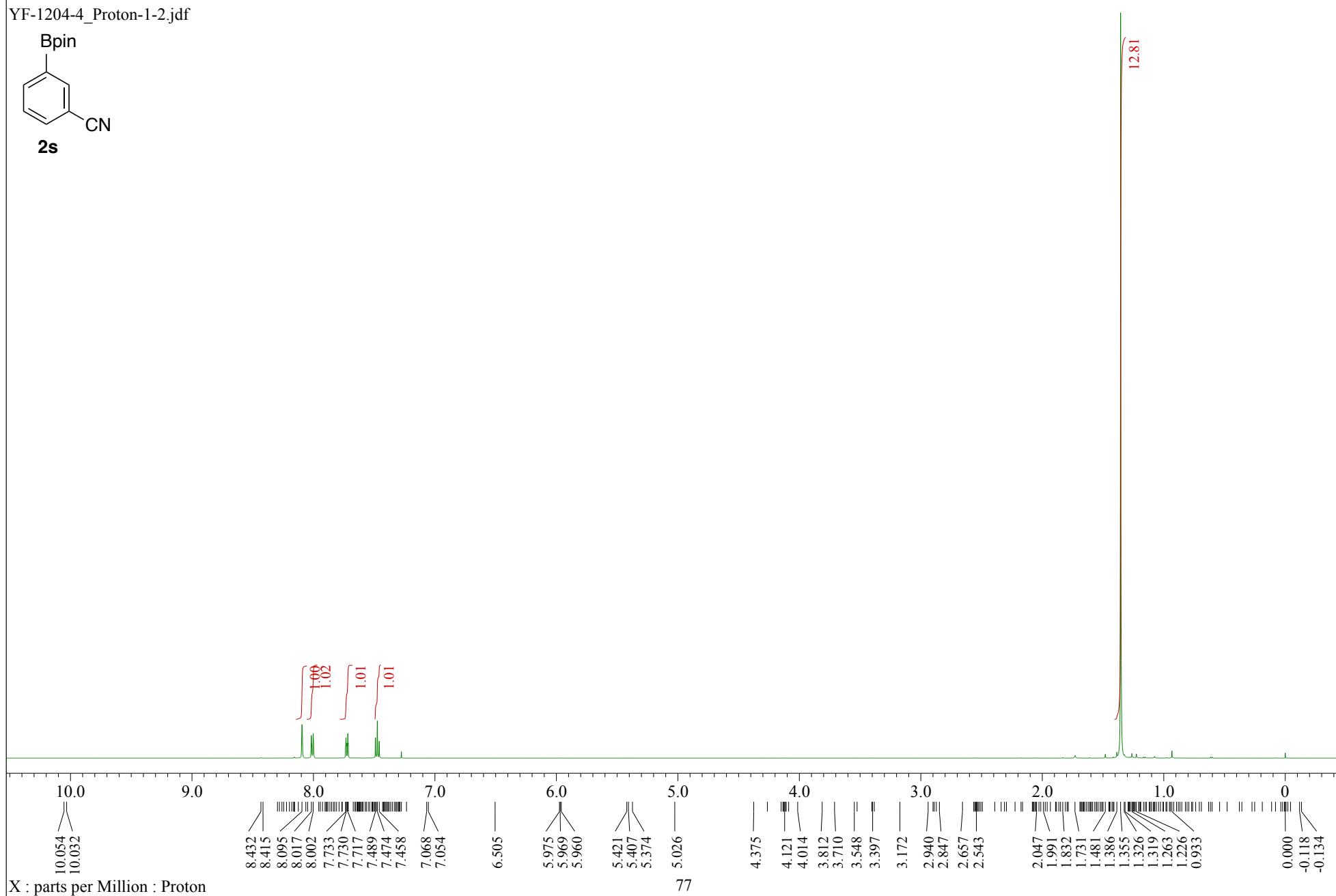
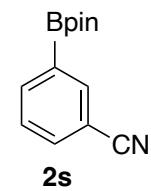
Comment      = single_pulse
Data_Format  = 1D REAL
Dim_Size     = 13107
Dim_Title    = Proton
Dim_Units    = [ppm]
Dimensions   = X
Spectrometer = JNM-ECZ500R/S1

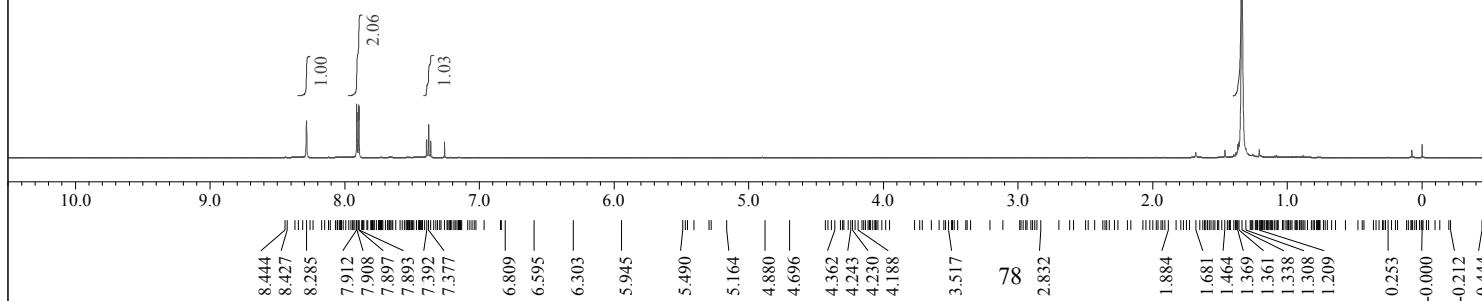
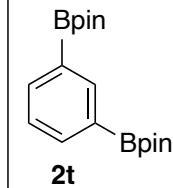
Field_Strength = 11.62926421[T] (500[M
X_Acc_Duration = 1.76422912[s]
X_Domain     = 1H
X_Freq        = 495.13191398[MHz]
X_Offset      = 5[ppm]
X_Points      = 16384
X_Prescans   = 1
X_Resolution  = 0.5668198[Hz]
X_Sweep       = 9.28677563[kHz]
X_Sweep_Clipped = 7.42942051[kHz]
Irr_Domain   = Proton
Irr_Freq     = 495.13191398[MHz]
Irr_Offset   = 5[ppm]
Tri_Domain   = Proton
Tri_Freq     = 495.13191398[MHz]
Tri_Offset   = 5[ppm]
Clipped      = FALSE
Scans        = 8
Total_Scans  = 8

Relaxation_Delay = 5[s]
Recvs_Gain      = 50
Temp_Get        = 20[dB]
X_Acc_Width    = 8.7[us]
X_Acc_Time     = 1.76422912[s]
X_Angle        = 45[deg]
X_Atn          = 4.3[dB]
X_Pulse        = 4.35[us]
Irr_Mode       = Off
Tri_Mode       = Off
Dante_Loop    = 500
Dante_Presat  = FALSE
Decimation_Rate = 0
Initial_Wait   = 1[s]
Phase          = {0, 90, 270, 180, 180}
Presat_Time    = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 6.76422912[s]

```

YF-1204-4\_Proton-1-2.jdf





**JEOL**

```

Filename      = YF-1180-4_Proton-1-4.
Author       = delta
Experiment   = proton.jpx
Sample_Id    = YF-1180-4
Solvent      = CHLOROFORM-D
Actual_Start_Time = 26-OCT-2022 21:44:12
Revision_Time = 26-OCT-2022 20:46:45

Comment      = single_pulse
Data_Format  = 1D REAL
Dim_Size     = 13107
Dim_Title    = Proton
Dim_Units    = [ppm]
Dimensions   = X
Spectrometer = JNM-ECZ500R/S1

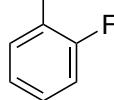
Field_Strength = 11.62926421[T] (500[M
X_Acc_Duration = 1.76422912[s]
X_Domain     = 1H
X_Freq        = 495.13191398[MHz]
X_Offset      = 5[ppm]
X_Points      = 16384
X_Prescans   = 1
X_Resolution  = 0.5668198[Hz]
X_Sweep       = 9.28677563[kHz]
X_Sweep_Clipped = 7.42942051[kHz]
Irr_Domain   = Proton
Irr_Freq     = 495.13191398[MHz]
Irr_Offset   = 5[ppm]
Tri_Domain   = Proton
Tri_Freq     = 495.13191398[MHz]
Tri_Offset   = 5[ppm]
Clipped      = FALSE
Scans        = 8
Total_Scans  = 8

Relaxation_Delay = 5[s]
Recvs_Gain      = 20
Temp_Get        = 19.01[dB]
X_Acc_Width    = 8.7[us]
X_Acc_Time     = 1.76422912[s]
X_Angle        = 45[deg]
X_Atn          = 4.3[dB]
X_Pulse        = 4.35[us]
Irr_Mode       = Off
Tri_Mode       = Off
Dante_Loop    = 500
Dante_Presat  = FALSE
Decimation_Rate = 0
Initial_Wait   = 1[s]
Phase          = {0, 90, 270, 180, 180
Presat_Time    = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 6.76422912[s]

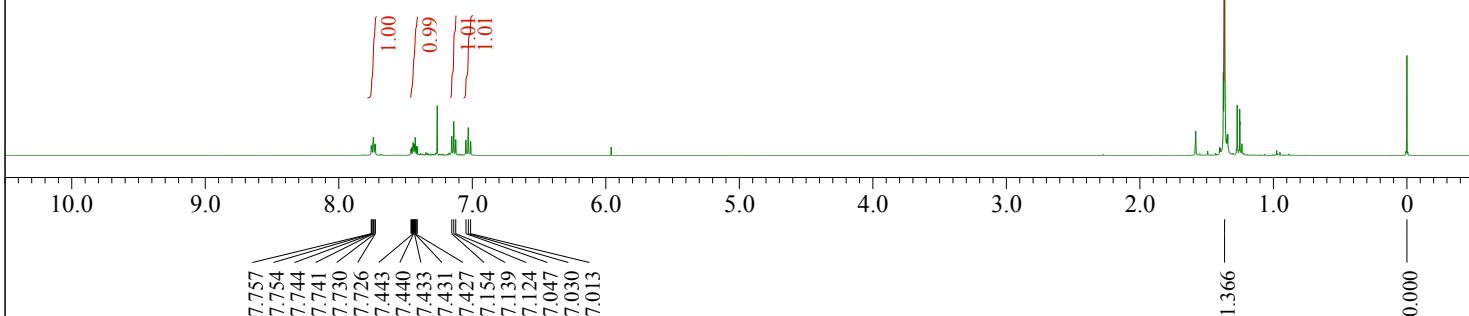
```

YF-1036-2\_Proton-1-2.jdf

Bpin



**2u**

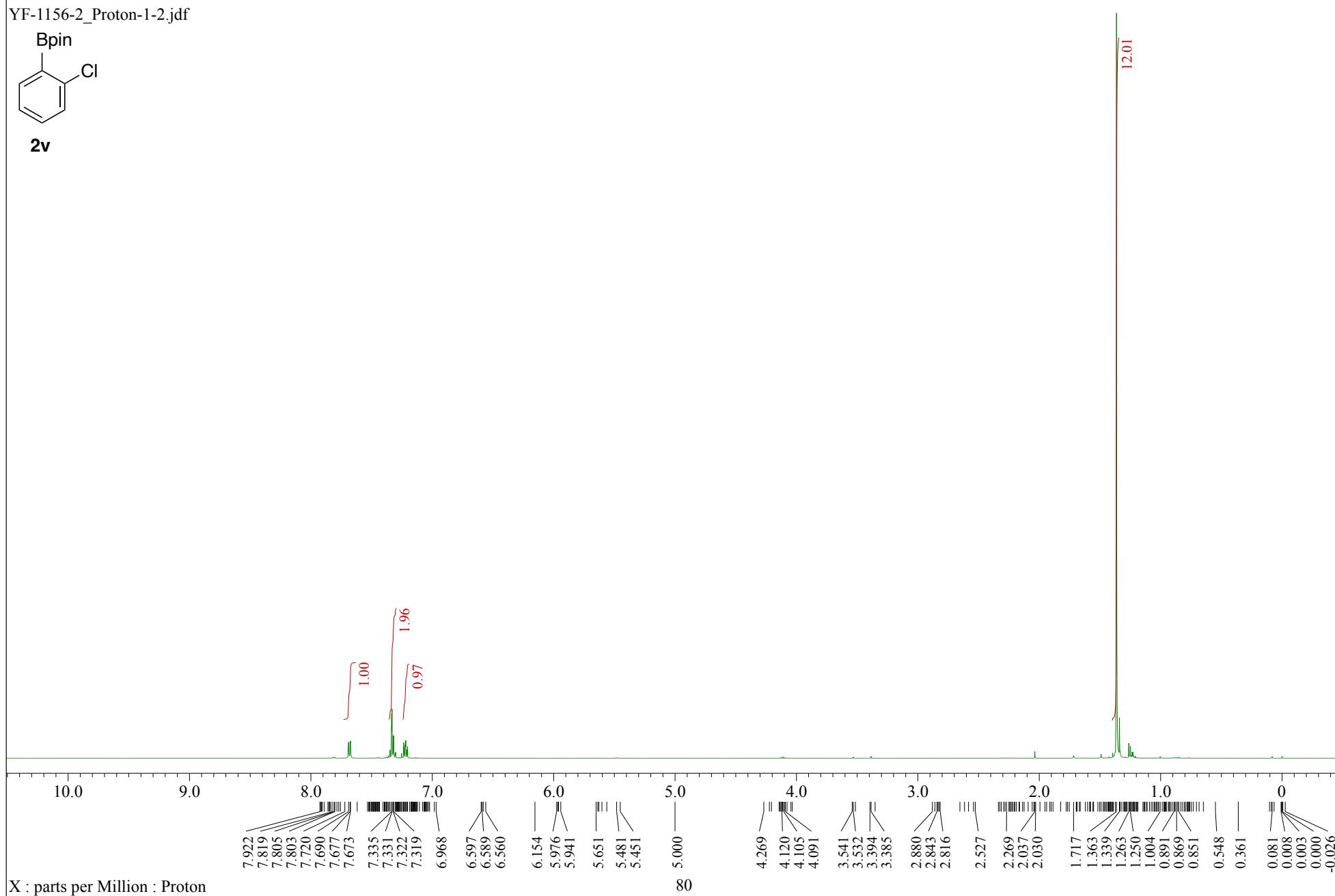
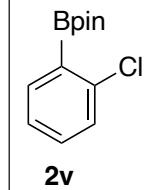


X : parts per Million : Proton

**JEOL**

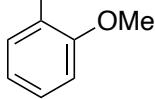
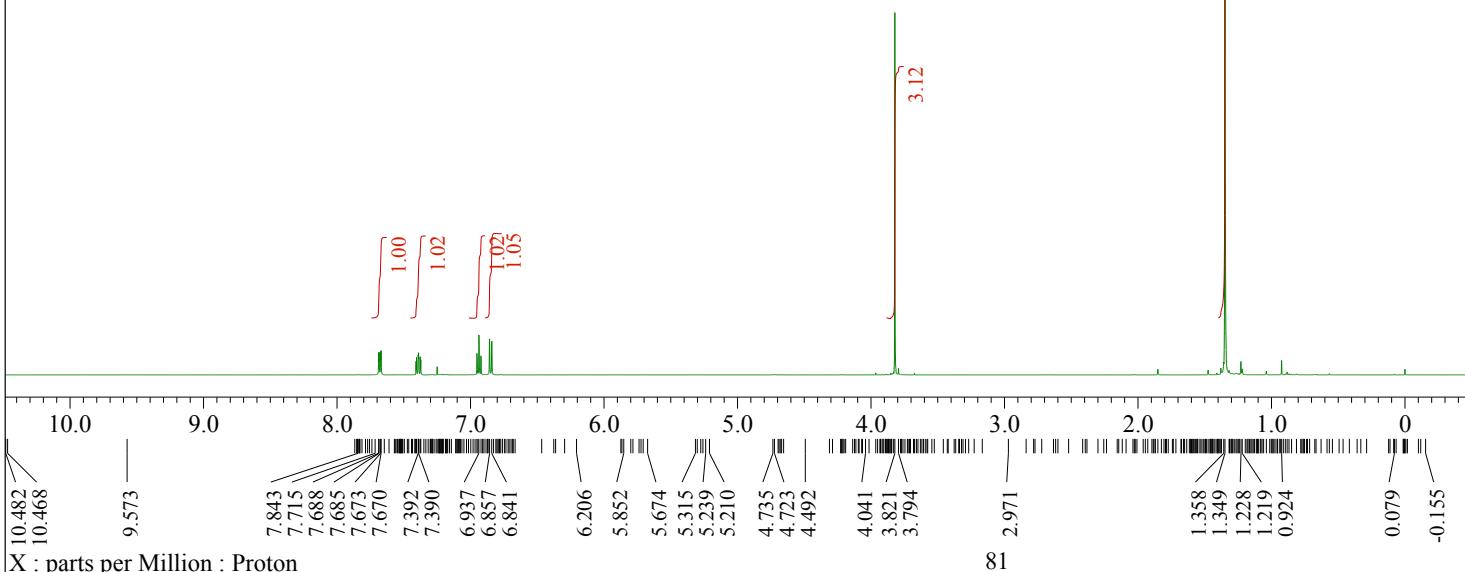
Filename = YF-1036-2\_Proton-1-2.  
Author = delta  
Experiment = proton.jxp  
Sample\_Id = YF-1036-2  
Solvent = CHLOROFORM-D  
Actual\_Start\_Time = 28-JUN-2022 19:23:37  
Revision\_Time = 18-JUL-2022 19:35:21  
  
Comment = single\_pulse  
Data\_Format = 1D COMPLEX  
Dim\_Size = 13107  
X\_Domain = Proton  
Dim\_Title = Proton  
Dim\_Units = [ppm]  
Dimensions = X  
Spectrometer = JNM-ECZ500R/S1  
  
Field\_Strength = 11.62926421[T] (500[M  
X\_Acq\_Duration = 1.76422912[s]  
X\_Domain = 1H  
X\_Freq = 495.13191398[MHz]  
X\_Offset = 5[ppm]  
X\_Points = 16384  
X\_Prescans = 1  
X\_Resolution = 0.5668198[Hz]  
X\_Sweep = 9.28677563[kHz]  
X\_Sweep\_Clipped = 7.42942051[kHz]  
Irr\_Domain = Proton  
Irr\_Fred = 495.13191398[MHz]  
Irr\_Offset = 5[ppm]  
Tri\_Domain = Proton  
Tri\_Fred = 495.13191398[MHz]  
Tri\_Offset = 5[ppm]  
Clipped = FALSE  
Scans = 32  
Total\_Scans = 32  
  
Relaxation\_Delay = 5[s]  
Recvr\_Gain = 46  
Temp\_Get = 18.5[dC]  
X\_90\_Width = 9.49[us]  
X\_Acq\_Time = 1.76422912[s]  
X\_Angle = 45[deg]  
X\_Atn = 4.3[dB]  
X\_Pulse = 4.745[us]  
Irr\_Mode = Off  
Tri\_Mode = Off  
Danfe\_Loop = 500  
Danfe\_Presat = FALSE  
Decimation\_Rate = 0  
Initial\_Wait = 1[s]  
Phase = {0, 90, 270, 180, 180  
Presat\_Time = 5[s]  
Presat\_Time\_Flag = FALSE  
Relaxation\_Delay\_Calc = 0[s]  
Relaxation\_Delay\_Temp = 5[s]  
Repetition\_Time = 6.76422912[s]

YF-1156-2\_Proton-1-2.jdf



YF-1173-5\_Proton-1-2.jdf

Bpin

**2w**
**JEOL**

```

Filename          = YF-1173-5_Proton-1-2.
Author           = delta
Experiment       = proton.jxp
Sample_Id        = YF-1173-5
Solvent          = CHLOROFORM-D
Actual_Start_Time = 20-OCT-2022 15:53:42
Revision_Time    = 20-OCT-2022 19:53:36

Comment          = single_pulse
Data_Format      = 1D REAL
Dim_Size         = 13107
X_Domain         = Proton
Dim_Title        = Proton
Dim_Units        = [ppm]
Dimensions       = X
Spectrometer     = JNM-ECZ500R/S1

Field_Strength   = 11.62926421[T] (500[M]
X_Acq_Duration  = 1.76422912[s]
X_Domain         = 1H
X_Freq           = 495.13191398[MHz]
X_Offset         = 5[ppm]
X_Points         = 16384
X_Prescans       = 1
X_Resolution     = 0.5668198[Hz]
X_Sweep          = 9.28677563[kHz]
X_Sweep_Clipped = 7.42942051[kHz]
Irr_Domain       = Proton
Irr_Fred         = 495.13191398[MHz]
Irr_Offset       = 5[ppm]
Tri_Domain       = Proton
Tri_Fred         = 495.13191398[MHz]
Tri_Offset       = 5[ppm]
Clipped          = FALSE
Scans            = 8
Total_Scans      = 8

Relaxation_Delay = 5[s]
Recvr_Gain       = 36
Temp_Get          = 20.5[dC]
X_90_Width        = 8.7[us]
X_Acq_Time        = 1.76422912[s]
X_Angle           = 45[deg]
X_Atn             = 4.3[dB]
X_Pulse           = 4.35[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Loop        = 500
Dante_Presat      = FALSE
Decimation_Rate   = 0
Initial_Wait      = 1[s]
Phase             = {0, 90, 270, 180, 180}
Presat_Time        = 5[s]
Presat_Time_Flag  = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time   = 6.76422912[s]

```