

Electronic Supplementary Information

Ruthenium-catalyzed regio- and site-selective *ortho* C–H borylation of phenol derivatives

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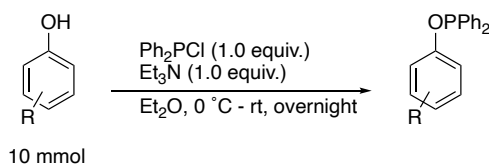
^bJST, PRESTO, Honcho, Kawaguchi, Saitama, 332-0012, Japan

Table of Contents

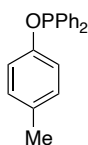
S2	General
S3-S7	Preparation of phosphinites Spectral data
S8-S16	Procedure for C–H borylation of aryl phosphinites Spectral data
S17-S18	Procedure for C–H borylation of aryl phosphites Procedure for one-pot C–H borylation of aryl phosphites
S19	Deuterium labeling experiments
S20	References
S21–97	NMR spectra

General: All operations were performed under an argon atmosphere. ^1H , ^{13}C and ^{31}P spectra were recorded on an ECS-400 (400 MHz for ^1H , 128 MHz for ^{11}B , 100 MHz for ^{13}C , and 160 MHz for ^{31}P), an ECX-400 (400 MHz for ^1H and 160 MHz for ^{31}P), or an ECZ-500 (500 MHz for ^1H , 125 MHz for ^{13}C , and 200 MHz for ^{31}P) spectrometer in CDCl_3 , C_6D_6 , acetone- d_6 , or dms- d_6 . Chemical shifts are expressed in parts per million (ppm) downfield from tetramethylsilane (δ_{H} 0.00, δ_{C} 0.00), $\text{BF}_3\cdot\text{OEt}_2$ (δ_{B} 0.00), 85% H_3PO_4 aq. (δ_{P} 0.00), or C_6F_6 (δ_{F} -163.00) and are referenced to residual solvents (δ_{H} 7.26 and δ_{C} 77.0 for chloroform, δ_{H} 7.16 and δ_{C} 128.06 for C_6H_6 , δ_{H} 7.05 and δ_{C} 206.26 for acetone- d_6 , and δ_{H} 2.50 for dms- d_6). IR spectra were recorded on an FT/IR-460 plus (JASCO Co., Ltd.) with an ATR PRO450-S accessory (JASCO Co., Ltd.). High resolution mass spectra (HRMS) were recorded on a BRUKER micrOTOF II and a JEOL JMS-T100 spectrometer. Silica Gel 60 (Kanto Chemical Co., Inc.) was used for flash column chromatography. A Merck Kieselgel 60 F₂₅₄ (0.25 mm thickness, coated on glass 20 x 20 cm²) plate was used for analytical thin layer chromatography (TLC). THF, Et₂O, hexanes and toluene were purified by solvent purification system of Glass-Contour. *n*-Octane was purchased from Tokyo Chemical Industry and degassed by freeze-pump-thaw technique and dried over 4A molecular sieves. Benzene- d_6 was purchased from ACROS chemicals and dried and degassed by benzophenone ketyl. Chloroform- d was purchased from Kanto Chemicals. Unless otherwise noted, materials were purchased from Sigma-Aldrich Corporation, FUJIFILM Wako Pure Chemical Corporation, Tokyo Chemical Industry Corporation, and Kanto Chemical Corporation.

General procedure for the synthesis of aryl diphenylphosphinites



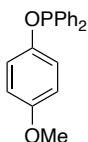
In a 100 mL two-neck flask, a phenol derivative (10.0 mmol) was dissolved in Et₂O (30.0 mL) under an argon atmosphere. The flask was cooled to 0 °C in an ice-bath, and triethylamine (10.0 mmol) and chlorodiphenylphosphine (10.0 mmol) were successively added. The flask was allowed to stand at room temperature and stirred overnight. The solution was filtered through a short pad of alumina and Celite[®], and the filtrate was concentrated under reduced pressure to give the product.



1b (colorless oil, 2.0 g, 7.0 mmol, 70%)

The spectral data were in good agreement with the literature values.¹

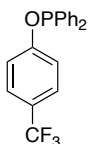
¹H NMR (CDCl₃, 400 MHz) δ = 7.61-7.56 (m, 4H), 7.42-7.32 (m, 6H), 7.10-6.98 (m, 4H), 2.28 (s, 3H).



1c (white solid, 1.6 g, 5.2 mmol, 51%)

The spectral data were in good agreement with the literature values.²

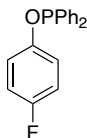
¹H NMR (CDCl₃, 400 MHz) δ = 7.61-7.55 (m, 4H), 7.43-7.34 (m, 6H), 7.05-6.90 (m, 2H), 6.82-6.76 (m, 2H), 3.75 (s, 3H).



1d (colorless oil, 1.6 g, 4.5 mmol, 45%)

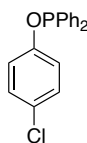
¹H NMR (C₆D₆, 500 MHz) δ = 7.58-7.52 (m, 4H), 7.20 (d, J = 8.0 Hz, 2H), 7.13-7.40 (m, 6H), 7.97 (d, J = 8.0 Hz, 2H); ³¹P NMR (C₆D₆, 200 MHz) δ = 113.3; ¹⁹F NMR (C₆D₆, 465 MHz) δ = -62.5; ¹³C NMR (C₆D₆, 125 MHz) δ = 160.2 (d, J = 10.7 Hz), 140.6 (d, J = 18.3 Hz), 131.0 (d, J = 22.8

Hz), 130.3, 128.9 (d, $J = 7.5$ Hz), 127.2 (d, $J = 3.8$ Hz), 125.0 (q, $J = 272$ Hz), 124.7 (q, $J = 32.5$ Hz), 119.1 (d, $J = 11.3$ Hz); IR (ATR) 3053.6, 1610.3, 1510.1, 1434.8, 1322.0, 1228.4, 1106.0 cm^{-1} ; HRMS (ESI): Calcd for $\text{C}_{19}\text{H}_{15}\text{F}_3\text{OP}$ $[\text{M}+\text{H}]^+$:347.0807; Found: 347.0790.



1e (colorless oil, 2.1 g, 7.1 mmol, 71%)

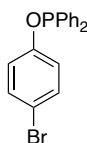
^1H NMR (C_6D_6 , 500 MHz) $\delta = 7.62\text{-}7.54$ (m, 4H), 7.14-7.02 (m, 6H), 6.92-6.86 (m, 2H), 6.68-6.60 (m, 2H); ^{31}P NMR (C_6D_6 , 200 MHz) $\delta = 114.4$; ^{19}F NMR (C_6D_6 , 465 MHz) $\delta = -112.3$; ^{13}C NMR (C_6D_6 , 125 MHz) $\delta = 158.8$ (d, $J = 241.8$ Hz), 153.9 (d, $J = 2.4$ Hz), 141.4 (d, $J = 18.0$ Hz), 130.9 (d, $J = 22.8$ Hz), 130.0, 128.8 (d, $J = 7.1$ Hz), 120.4 (dd, $J = 10.8, 8.4$ Hz), 116.2 (d, $J = 22.8$ Hz); IR (ATR) 3053.7, 1497.5, 1433.8, 1194.7, 1090.6 cm^{-1} ; HRMS (ESI): Calcd for $\text{C}_{18}\text{H}_{15}\text{FOP}$ $[\text{M}+\text{H}]^+$:297.0839; Found: 297.0831.



1f (white solid, 2.0 g, 6.5 mmol, 65%)

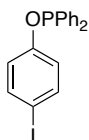
The spectral data were in good agreement with the literature values.³

^1H NMR (CDCl_3 , 400 MHz) $\delta = 7.61\text{-}7.54$ (m, 4H), 7.44-7.37 (m, 6H), 7.23-7.19 (m, 2H), 7.08-7.03 (m, 2H).



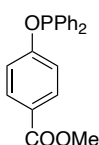
1g (white solid, 2.7 g, 5.5 mmol, 75%)

^1H NMR (C_6D_6 , 500 MHz) $\delta = 7.58\text{-}7.51$ (m, 4H), 7.11-7.01 (m, 8H), 6.84-6.78 (m, 2H); ^{31}P NMR (C_6D_6 , 200 MHz) $\delta = 113.6$; ^{13}C NMR (C_6D_6 , 125 MHz) $\delta = 156.9$ (d, $J = 9.6$ Hz), 141.1 (d, $J = 18.0$ Hz), 132.8, 131.0 (d, $J = 22.8$ Hz), 130.1, 128.8 (d, $J = 7.1$ Hz), 121.0 (d, $J = 10.8$ Hz), 115.4; IR (ATR) 3065.3, 1582.3, 1573.6, 1478.2, 1433.8, 1220.7, 1097.3 cm^{-1} ; HRMS (ESI): Calcd for $\text{C}_{18}\text{H}_{15}\text{BrOP}$ $[\text{M}+\text{H}]^+$:357.0038; Found: 357.0040.



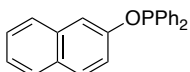
1h (white solid, 2.0 g, 4.9 mmol, 49%)

^1H NMR (C_6D_6 , 500 MHz) δ = 7.55 (t, J = 7.5 Hz, 4H), 7.25 (d, J = 8.3 Hz, 2H), 7.14-7.01 (m, 6H), 6.72 (d, J = 8.3 Hz, 2H); ^{31}P NMR (C_6D_6 , 200 MHz) δ = 113.1; ^{13}C NMR (C_6D_6 , 125 MHz) δ = 157.6 (d, J = 10.8 Hz), 141.0 (d, J = 17.9 Hz), 138.8, 130.9 (d, J = 22.8 Hz), 130.1, 128.8 (d, J = 7.1 Hz), 121.4 (d, J = 10.8 Hz), 85.7; IR (ATR) 3073.9, 1577.5, 1475.3, 1211.1, 1164.8, 1092.5 cm^{-1} ; HRMS (ESI): Calcd for $\text{C}_{18}\text{H}_{15}\text{IOP}$ $[\text{M}+\text{H}]^+$: 404.9900; Found: 404.9886.



1i (white solid, 1.1 g, 3.3 mmol, 34%)

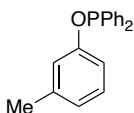
^1H NMR (C_6D_6 , 500 MHz) δ = 8.03 (d, J = 8.5, 2H), 7.55 (t, J = 7.5 Hz, 4H), 7.20-7.02 (m, 8H), 3.45 (s, 3H); ^{31}P NMR (C_6D_6 , 200 MHz) δ = 112.5; ^{13}C NMR (C_6D_6 , 125 MHz) δ = 165.9, 161.1 (d, J = 10.9 Hz), 140.4 (d, J = 16.9 Hz), 131.7, 130.7 (d, J = 22.8 Hz), 129.9, 128.5 (d, J = 6.0 Hz), 124.9, 118.5 (d, J = 12.0 Hz), 51.2; IR (ATR) 1718.3, 1598.7, 1503.2, 1431.9, 1309.4, 1271.8, 1235.2, 1167.7, 1101.2, 1009.6 cm^{-1} ; HRMS (ESI): Calcd for $\text{C}_{20}\text{H}_{18}\text{O}_3\text{P}$ $[\text{M}+\text{H}]^+$: 337.0988; Found: 337.0985.



1j (white solid, 2.3 g, 7.0 mmol, 70%)

The spectral data were in good agreement with the literature values.⁴

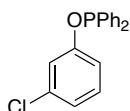
^1H NMR (CDCl_3 , 400 MHz) δ = 7.79-7.74 (m, 2H), 7.70 (d, J = 10.0 Hz, 1H), 7.64 (td, J = 10.0, 3.0 Hz, 4H), 7.51 (t, J = 3.0 Hz 1H), 7.45-7.38 (m, 7H), 7.38-7.32 (m, 2H).



1k (white solid, 1.2 g, 4.1 mmol, 41%)

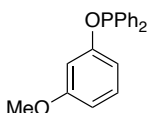
^1H NMR (C_6D_6 , 500 MHz) δ = 7.68-7.62 (m, 4H), 7.12-7.02 (m, 7H), 6.99 (t, J = 7.8 Hz, 1H), 6.67 (d, J = 7.8 Hz, 2H), 2.00 (s, 3H); ^{31}P NMR (C_6D_6 , 200 MHz) δ = 110.9; ^{13}C NMR (C_6D_6 , 125 MHz) δ = 158.0 (d, J = 9.5 Hz), 141.8 (d, J = 17.9 Hz), 139.9, 130.9 (d, J = 22.8 Hz), 129.9, 129.7, 128.8

(d, $J = 7.1$ Hz), 123.8, 120.1 (d, $J = 10.8$ Hz), 116.3 (d, $J = 12.0$ Hz), 21.3; IR (ATR) 3052.8, 1603.5, 1582.3, 1484.0, 1433.8, 1250.6, 1145.5, 1094.4 cm^{-1} ; HRMS (ESI): Calcd for $\text{C}_{19}\text{H}_{18}\text{OP}$ $[\text{M}+\text{H}]^+$: 293.1090; Found: 293.1088.



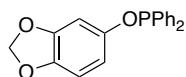
1l (colorless oil, 1.9 g, 6.2 mmol, 62%)

^1H NMR (C_6D_6 , 500 MHz) $\delta = 7.56\text{-}7.51$ (m, 4H), 7.30 (dd, $J = 4.0, 2.3$ Hz 1H), 7.10-7.00 (m, 6H), 6.93 (br d, $J = 8.0$ Hz, 1H), 6.79 (dd, $J = 8.0, 2.3$ Hz, 1H), 6.68 (t, $J = 8.0$ Hz, 1H); ^{31}P NMR (C_6D_6 , 200 MHz) $\delta = 113.6$; ^{13}C NMR (C_6D_6 , 125 MHz) $\delta = 158.5$ (d, $J = 10.8$ Hz), 140.8 (d, $J = 18.0$ Hz), 135.2, 130.9 (d, $J = 22.8$ Hz), 130.7, 130.1, 128.8 (d, $J = 7.3$ Hz), 123.0, 119.8 (d, $J = 10.8$ Hz), 117.3 (d, $J = 11.9$ Hz); IR (ATR) 3055.7, 1586.2, 1472.4, 1433.8, 1215.9, 1088.6 cm^{-1} ; HRMS (ESI): Calcd for $\text{C}_{18}\text{H}_{15}\text{ClOP}$ $[\text{M}+\text{H}]^+$: 313.0544; Found: 313.0534.



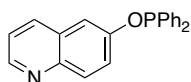
1m (colorless oil, 1.9 g, 6.3 mmol, 63%)

^1H NMR (C_6D_6 , 500 MHz) $\delta = 7.67\text{-}7.61$ (m, 4H), 7.11-7.01 (m, 6H), 6.98-6.89 (m, 3H), 6.51 (dd, $J = 8.5, 2.0$ Hz, 1H), 3.20 (s, 3H); ^{31}P NMR (C_6D_6 , 200 MHz) $\delta = 111.3$; ^{13}C NMR (C_6D_6 , 125 MHz) $\delta = 161.5, 159.4$ (d, $J = 10.8$ Hz), 141.5 (d, $J = 21.6$ Hz), 131.0 (d, $J = 22.8$ Hz), 130.4, 129.9, 128.8 (d, $J = 7.3$ Hz), 111.3 (d, $J = 12.0$ Hz), 109.0, 105.4 (d, $J = 10.8$ Hz), 54.8; IR (ATR) 3071.1, 3053.7, 3002.6, 2957.3, 2938.0, 2832.9, 1598.7, 1588.1, 1487.8, 1433.8, 1261.2, 1191.8, 1138.8 cm^{-1} ; HRMS (ESI): Calcd for $\text{C}_{19}\text{H}_{18}\text{O}_2\text{P}$ $[\text{M}+\text{H}]^+$: 309.1039; Found: 309.1034.



1n (white solid, 2.3 g, 7.0 mmol, 70%)

^1H NMR (C_6D_6 , 500 MHz) $\delta = 7.64\text{-}7.56$ (m, 4H), 7.12-7.01 (m, 6H), 6.81 (s, 1H), 6.59 (dt, $J = 8.5, 2.5$ Hz, 1H), 6.46 (d, $J = 8.5$ Hz, 1H), 5.22 (s, 2H); ^{31}P NMR (C_6D_6 , 200 MHz) $\delta = 114.4$; ^{13}C NMR (C_6D_6 , 125 MHz) $\delta = 153.0$ (d, $J = 9.6$ Hz), 148.8, 143.6, 141.7 (d, $J = 18.0$ Hz), 131.0 (d, $J = 21.6$ Hz), 129.9, 128.7 (d, $J = 6.0$ Hz), 111.4 (d, $J = 12.0$ Hz), 108.3, 102.1 (d, $J = 9.5$ Hz), 101.3; IR (ATR) 2909.1, 1624.7, 1500.4, 1483.0, 1240.0, 1183.1, 1122.4, 1094.4 cm^{-1} ; HRMS (ESI): Calcd for $\text{C}_{19}\text{H}_{16}\text{O}_3\text{P}$ $[\text{M}+\text{H}]^+$: 323.0832; Found: 323.0819.

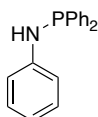


1o (beige solid, 1.2 g, 3.8 mmol, 38%)

1o was synthesized according to the slightly modified procedure as follows.

In a 100 mL two-neck flask, 6-hydroxyquinoline (1.45 g, 10.0 mmol) was dissolved in THF (30.0 mL) under an argon atmosphere. The flask was cooled to 0 °C in an ice-bath, and triethylamine (2.77 mL, 20.0 mmol) and chlorodiphenylphosphine (1.84 mL, 10.0 mmol) were successively added. The flask was allowed to stand at room temperature and stirred for 2 h. The solution was filtered through a short pad of Celite[®]. After the filtrate was concentrated under reduced pressure, the resulting solid was precipitated from hexane/ dichloromethane to give **1o**.

¹H NMR (CDCl₃, 500 MHz) δ = 8.79 (dd, J = 4.0, 1.5 Hz, 1H), 8.04-8.00 (m, 2H), 7.68-7.60 (m, 4H), 7.57 (dd, J = 9.0, 2.5 Hz 1H), 7.47 (t, J = 2.5 Hz, 1H) 7.45-7.38(m, 6H), 7.32 (dd, J = 8.5, 4.0 Hz 1H); ³¹P NMR (CDCl₃ 200 MHz) δ = 112.4; ¹³C NMR (CDCl₃ 125 MHz) δ = 155.4 (d, J = 9.5 Hz), 148.9, 145.0, 140.4 (d, J = 16.8 Hz), 135.3, 131.1, 130.7 (d, J = 22.8 Hz), 130.1, 129.2, 128.7 (d, J = 7.3 Hz), 124.2 (d, J = 7.1 Hz), 121.5, 113.1 (d, J = 13.0 Hz); IR (ATR) 3067.2, 2351.8, 2320.0, 1619.9, 1592.9, 1497.5, 1376.0, 1319.1, 1220.7, 1160.0 cm⁻¹; HRMS (ESI+) Calcd for C₂₁H₁₇NOP [M+H]⁺: 330.1048; Found: 330.1057.



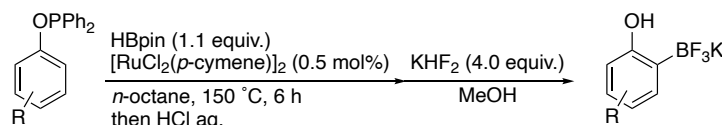
4 (white solid, 1.3 g, 4.7 mmol, 47%)

The spectral data were in good agreement with the literature values⁵

¹H NMR (C₆D₆, 500 MHz) δ = 7.48-7.42 (m, 4H), 7.40-7.33 (m, 6H), 7.19 (t, J = 7.9 Hz, 2H), 7.04-6.98 (m, 2H), 6.81 (t, J = 7.9 Hz, 1H), 4.37 (d, J = 7.4 Hz, 1H).

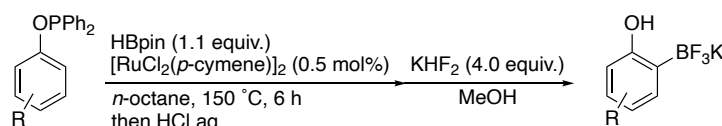
General procedure for C–H borylation of aryl diphenylphosphinites

Procedure A



A solution of [RuCl₂(*p*-cymene)]₂ (0.9 mg, 1.5 μmol) and aryl diphenylphosphinite **1** (0.30 mmol) in *n*-octane (1.5 mL) was placed in a glass tube (inside diameter = 1.7 cm, length = 18 cm) equipped with a three-way stop cock under Ar. HBpin (47.4 μL, 0.33 mmol) was added to the solution at room temperature, and the glass tube was closed. Then the mixture was stirred at 150 °C in the closed system for 6 h. 1N HCl aq. was added to the solution at room temperature, and the mixture was stirred for 24 h. The mixture was extracted with AcOEt three times, and the combined organic layers were washed with brine and dried over MgSO₄. After filtration to remove the drying agent, the filtrate was evaporated to give a crude product. To a MeOH solution (1.5 mL) of the crude product was added KHF₂ (93.7 mg, 1.2 mmol) at room temperature, and the mixture was stirred for 24 h. The suspension was evaporated at 40 °C for 20 min, and residual white solids were dissolved in acetone (5.0 mL). After insoluble salts were filtered off, the filtrate was concentrated to ca. 1 mL volume. Then, toluene (ca. 1 mL) was added, and the remaining acetone was removed under reduced pressure to give the suspension in toluene. The resulting beige solids were collected by filtration and rinsed with excess *n*-hexane and a small amount of cold MeOH (ca. 0 °C) to give aryl trifluoroborate **2**.

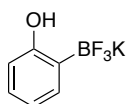
Procedure B



A solution of [RuCl₂(*p*-cymene)]₂ (0.9 mg, 1.5 μmol) and aryl diphenylphosphinite **1** (0.30 mmol) in *n*-octane (1.5 mL) was placed in a glass tube (inside diameter = 1.7 cm, length = 18 cm) equipped with a three-way stop cock under Ar. HBpin (47.4 μL, 0.33 mmol) was added to the solution at room temperature, and the glass tube was closed. Then the mixture was stirred at 150 °C in the closed system for 6 h. 1N HCl aq. was added to the solution at room temperature, and the mixture was stirred for 24 h. The mixture was extracted with AcOEt three times, and the combined organic layers were washed with brine and dried over MgSO₄. After filtration to remove the drying agent, the filtrate was evaporated to give a crude product. To a MeOH solution (1.5 mL) of the crude product was added KHF₂ (93.7 mg, 1.2 mmol) at room temperature, and the mixture was stirred for 24 h. After the suspension was evaporated at 40 °C for 20 min, the resulting beige solid

was collected by filtration and rinsed with a small amount of cold MeOH (ca. 0°C) to give aryl trifluoroborate **2**.

This reaction should be conducted inside an explosion proof wall. This reaction is performed in a sealed glass tube at 150 °C which is over the boiling point of *n*-octane. Furthermore, H₂ is generated during the reaction. The volume of the dead space inside the glass ware is ca. 34.5 cm³.

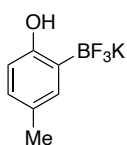


Synthesized according to the procedure A.

2a (white solid, 46 mg, 0.23 mmol, 77%)

The spectral data were in good agreement with the literature values.⁶

¹H NMR (acetone-*d*₆, 500 MHz) δ = 7.41 (q, *J* = 10.5 Hz, 1H), 7.27 (br d, *J* = 7.0 Hz, 1H), 6.93-6.88 (m, 1H), 6.63-6.57 (m, 1H), 6.52 (d, *J* = 8.5 Hz, 1H).

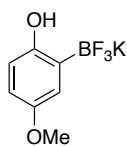


Synthesized according to the procedure A.

2b (white solid, 49 mg, 0.23 mmol, 76%)

The spectral data were in good agreement with the literature values.⁶

¹H NMR (acetone-*d*₆, 500 MHz) δ = 7.23 (q, *J* = 10.5 Hz, 1H), 7.08 (br s, 1H), 6.71 (dd, *J* = 8.0, 2.5 Hz, 1H), 6.41 (d, *J* = 8.0 Hz, 1H), 2.13 (s, 3H).

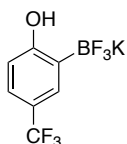


Synthesized according to the procedure B.

2c (white solid, 68 mg, 0.29 mmol, 96%)

The spectral data were in good agreement with the literature values.⁷

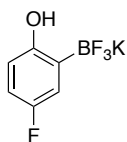
¹H NMR (acetone-*d*₆, 500 MHz) δ = 7.07 (q, *J* = 11.0 Hz, 1H), 6.84 (br s, 1H), 6.45 (dd, *J* = 8.5, 3.5 Hz, 1H), 6.40 (d, *J* = 8.5 Hz, 1H), 3.61 (s, 3H).



Synthesized according to the procedure A.

2d (white solid, 46 mg, 0.17 mmol, 57%)

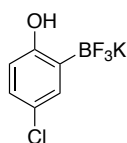
^1H NMR (acetone- d_6 , 500 MHz) δ = 8.02 (q, J = 11.5 Hz, 1H), 7.59 (br s, 1H), 7.24 (dd, J = 8.5, 2.0 Hz, 1H), 6.66 (d, J = 8.5 Hz, 1H); ^{13}C NMR (acetone- d_6 , 125 MHz) δ = 164.2, 131.2, 126.8 (q, J = 271.6 Hz), 124.9 (d, J = 3.6 Hz), 120.6 (q, J = 31.1 Hz), 114.3, 1C(C-B) is missing.; ^{19}F NMR (acetone- d_6 , 465 MHz), δ = -62.3 (s), -139.2 (m); ^{11}B NMR (acetone- d_6 , 158 MHz) δ = 3.06 (q, J = 52.8 Hz); IR (ATR) 1329.7, 1239.0, 1181.2, 1113.7, 1079.0 cm^{-1} ; HRMS (ESI): Calcd for $\text{C}_7\text{H}_4\text{BF}_6\text{O}$ [M-K] $^-$: 229.0265; Found: 229.0255.



Synthesized according to the procedure A.

2e (white solid, 52 mg, 0.24 mmol, 80%)

^1H NMR (acetone- d_6 , 500 MHz) δ = 7.28 (q, J = 10.5 Hz 1H), 6.93 (br d, J = 7.5 Hz, 1H), 6.62 (td, J = 8.5, 3.5 Hz, 1H), 6.49 (dd, J = 8.5, 4.0 Hz 1H); ^{13}C NMR (acetone- d_6 , 125 MHz) δ = 157.4 (d, J = 234.6 Hz), 156.9, 119.1 (d, J = 19.1 Hz), 114.6, 113.2 (d, J = 24.0 Hz), 1C(C-B) is missing.; ^{19}F NMR (acetone- d_6 , 465 MHz), δ = -131.0 (s), -139.7 (m); ^{11}B NMR (acetone- d_6 , 158 MHz) δ = 2.99 (q, J = 54.2 Hz); IR (ATR) 3565.7, 1487.8, 1417.4, 1265.1, 1187.0, 1144.6 cm^{-1} ; HRMS (ESI): Calcd for $\text{C}_6\text{H}_4\text{BF}_4\text{O}$ [M-K] $^-$: 179.0297; Found: 179.0294.

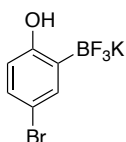


Synthesized according to the procedure A.

2f (white solid, 69 mg, 0.29 mmol, 98%)

The spectral data were in good agreement with literature values.⁶

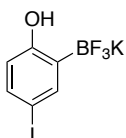
^1H NMR (acetone- d_6 , 500 MHz) δ = 7.54 (q, J = 11.0 Hz, 1H), 7.19 (br s, 1H), 6.85 (dd, J = 8.8, 3.0 Hz, 1H), 6.48 (d, J = 8.8 Hz 1H).



Synthesized according to the procedure A.

2g (white solid, 74 mg, 0.26 mmol, 88%)

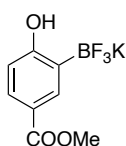
^1H NMR (acetone- d_6 , 500 MHz) δ = 7.55 (q, J = 11.0 Hz 1H), 7.36 (br s, 1H), 7.02 (dd, J = 8.5, 3.0 Hz, 1H), 6.47 (d, J = 8.5 Hz 1H); ^{13}C NMR (acetone- d_6 , 125 MHz) δ = 160.4, 136.6, 130.1, 116.5, 111.6, 1C(C-B) is missing.; ^{19}F NMR (acetone- d_6 , 465 MHz), δ = -139.3 (m); ^{11}B NMR (acetone- d_6 , 158 MHz) δ = 2.85 (q, J = 52.8 Hz); IR (ATR) 3523.3, 1600.6, 1482.0, 1390.4, 1241.0, 1121.4 cm^{-1} ; HRMS (ESI): Calcd for $\text{C}_6\text{H}_4\text{BBrF}_3\text{O} [\text{M-K}]^-$: 238.9496; Found: 238.9502.



Synthesized according to the procedure B.

2h (white solid, 95 mg, 0.29 mmol, 97%)

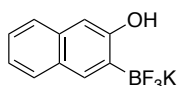
^1H NMR (acetone- d_6 , 500 MHz) δ = 7.60-7.51 (m, 2H), 7.21 (dd, J = 8.5, 2.5 Hz, 1H), 6.39 (d, J = 8.5 Hz, 1H); ^{13}C NMR (acetone- d_6 , 125 MHz) δ = 160.1, 142.8, 136.2, 117.3, 82.1, 1C(C-B) is missing.; ^{19}F NMR (acetone- d_6 , 465 MHz), δ = -137.9 (m); ^{11}B NMR (acetone- d_6 , 158 MHz) δ = 2.71 (q, J = 54.2 Hz); IR (ATR) 3505.0, 1595.8, 1478.2, 1381.8, 1245.8, 1177.3, 1120.4 cm^{-1} ; HRMS (ESI): Calcd for $\text{C}_6\text{H}_4\text{BF}_3\text{IO} [\text{M-K}]^-$: 286.9358; Found: 286.9361.



Synthesized according to the procedure B.

2i (white solid, 58 mg, 0.22 mmol, 75%)

^1H NMR (acetone- d_6 , 500 MHz) δ = 8.12-8.02 (m, 2H), 7.65 (dd, J = 8.5, 2.5 Hz, 1H), 6.59 (d, J = 8.5 Hz 1H), 3.76 (s, 3H); ^{13}C NMR (acetone- d_6 , 125 MHz) δ = 168.2, 165.8, 136.7, 130.1, 121.1, 114.2, 51.4, 1C(C-B) is missing.; ^{19}F NMR (acetone- d_6 , 465 MHz), δ = -138.7 (m); ^{11}B NMR (acetone- d_6 , 158 MHz) δ = 3.22 (q, J = 52.8 Hz); IR (ATR) 3512.7, 1700.0, 1613.2, 1438.6, 1313.3, 1229.4, 1163.8 cm^{-1} ; HRMS (ESI): Calcd for $\text{C}_8\text{H}_7\text{BF}_3\text{O}_3 [\text{M-K}]^-$: 219.0446; Found: 219.0445.

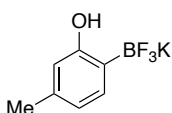


Synthesized according to the procedure B.

2j (white solid, 65 mg, 0.26 mmol, 86%)

The spectral data were in good agreement with literature values.⁸

¹H NMR (dms-*d*₆, 500 MHz) δ = 7.68-7.52 (m, 4H), 7.24 (t, J = 7.5 Hz, 1H), 7.14 (d, J = 7.5 Hz, 1H), 6.88 (s, 1H)

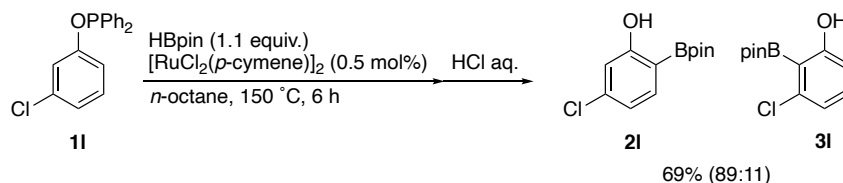


Synthesized according to the procedure A.

2k (white solid, 55 mg, 0.26 mmol, 85%)

The spectral data were in good agreement with literature values.⁶

¹H NMR (acetone-*d*₆, 500 MHz) δ = 7.40 (q, J = 10.5 Hz, 1H), 7.14 (d, J = 6.5 Hz, 1H), 6.43 (d, J = 6.5 Hz, 1H), 6.35 (s, 1H), 2.15 (s, 3H).

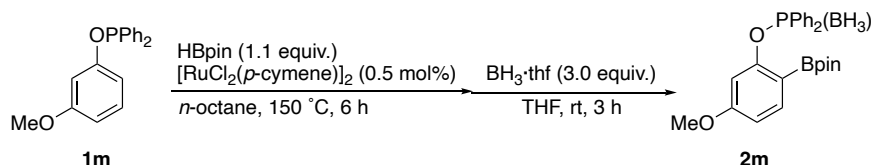


Borylation of 11: A solution of $[\text{RuCl}_2(p\text{-cymene})]_2$ (0.9 mg, 1.5 μmol) and **11** (93.8 mg, 0.30 mmol) in *n*-octane (1.5 mL) was placed in a glass tube (inside diameter = 1.7 cm, length = 18 cm) equipped with a three-way stop cock under Ar. HBpin (47.4 μL , 0.33 mmol) was added to the solution at room temperature, and the glass tube was closed. Then the mixture was stirred at 150 $^\circ\text{C}$ in the closed system for 6 h. 1N HCl aq. was added to the solution at room temperature, and the mixture was stirred for 24 h. The mixture was extracted with AcOEt three times, and the combined organic layers were washed with brine and dried over MgSO_4 . After filtration to remove the drying agent, the filtrate was evaporated to give a crude product. The crude mixture was passed through a short pad of silica gel using CH_2Cl_2 as an eluent to afford a mixture of the borylation products **21** and **31** as colorless oil (53 mg, 0.21 mmol, 69%, **21:31** = 89:11). These regioisomers were inseparable by column chromatography, and the ratio was determined by ¹H NMR.

The spectral data were in good agreement with literature values.⁹

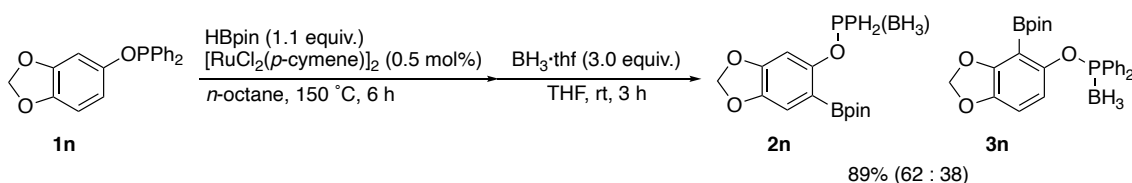
2l: $^1\text{H NMR}$ (CDCl_3 , 500 MHz) δ = 7.91 (s, 1H), 7.51 (d, J = 10.0 Hz, 1H), 6.91-6.82 (m, 2H), 1.36 (s, 12H).

3l: $^1\text{H NMR}$ (CDCl_3 , 500 MHz) δ = 8.63 (s, 1H), 7.23 (t, J = 10.8 Hz, 1H), 6.77(d, J = 10.8 Hz, 1H), 1.40 (s, 12H), a phenolic *OH* is missing.



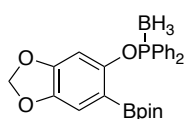
Borylation of 1m: A solution of $[\text{RuCl}_2(p\text{-cymene})]_2$ (0.9 mg, 1.5 μmol) and **1m** (92.5 mg, 0.30 mmol) in *n*-octane (1.5 mL) was placed in a glass tube (inside diameter = 1.7 cm, length = 18 cm) equipped with a three-way stop cock under Ar. HBpin (47.4 μL , 0.33 mmol) was added to the solution at room temperature, and the glass tube was closed. Then the mixture was stirred at 150 $^\circ\text{C}$ in the closed system. After 6 h, the solvent was removed under reduced pressure, and the obtained crude material was suspended in THF (1.0 mL). $\text{BH}_3\cdot\text{thf}$ (0.9 M solution in THF, 1.5 mL, 1.4 mmol) was added to the solution at room temperature, and then the mixture was stirred for 3 h. The reaction was quenched by adding H_2O at 0 $^\circ\text{C}$, and the obtained crude material was purified by silica gel chromatography (hexane: ethyl acetate = 5:1) to give the borylation product **2m** containing a small amount of **1m**. These compounds were inseparable, and the yield of **2m** was calculated to be 68% (0.21 mmol) by $^1\text{H NMR}$.

$^1\text{H NMR}$ (CDCl_3 , 500 MHz) δ = 8.06-7.98 (m, 4H), 7.65 (d, J = 8.8 Hz 1H), 7.58-7.42 (m, 6H), 6.71(s, 1H), 6.63 (d, J = 8.8 Hz, 1H), 3.67 (s, 1H), 1.27 (s, 12H), BH_3 are missing.; $^{13}\text{C NMR}$ (CDCl_3 , 100 MHz) δ =163.0, 158.8 (d J = 4.7 Hz), 138.2, 132.6, 132.3, 132.1, 132.0, 128.5 (d, J = 10.4 Hz) 110.4, 106.0 (d, J = 4.8 Hz), 83.5, 55.4, 25.0; $^{31}\text{P NMR}$ (CDCl_3 , 200 MHz) δ = 107.6 (br), $^{11}\text{B NMR}$ (CDCl_3 , 158 MHz) δ = 29.9 (br), -39.3 (br); IR (ATR) 2975.6, 2929.3, 2384.6, 1605.5, 1416.5, 1349.9, 1238.1, 1131.1, 1074.2 cm^{-1} ; HRMS (FD): Calcd for $\text{C}_{25}\text{H}_{31}\text{B}_2\text{O}_4\text{P}$ $[\text{M}]^+$:448.2146; Found: 448.2138.



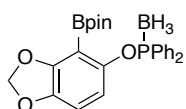
Borylation of 1n: A solution of $[\text{RuCl}_2(p\text{-cymene})]_2$ (0.9 mg, 1.5 μmol) and **1n** (96.7 mg, 0.30 mmol) in *n*-octane (1.5 mL) was placed in a glass tube (inside diameter = 1.7 cm, length = 18 cm)

equipped with a three-way stop cock under Ar. HBpin (47.4 μ L, 0.33 mmol) was added to the solution at room temperature, and the glass tube was closed. Then the mixture was stirred at 150 $^{\circ}$ C in the closed system. After 6 h, the solvent was removed under reduced pressure, and the obtained crude material was suspended in THF (1.0 mL). $\text{BH}_3\cdot\text{thf}$ (0.9 M solution in THF, 1.5 mL, 1.4 mmol) was added to the solution at room temperature, and then the mixture was stirred for 3 h. The reaction was quenched by adding H_2O at 0 $^{\circ}$ C, and the obtained crude material was purified by silica gel chromatography using toluene as an eluent to give a fraction of **2n** containing a small amount of **3n** (**2n:3n** = 93:7) and a fraction of **3n** containing a small amount of **1n** and **2n** (**1n:2n:3n** = 14:3:83). The yields were calculated to be 55% for **2n** (0.16 mmol) and 34% for **3n** (0.10 mmol) by ^1H NMR.



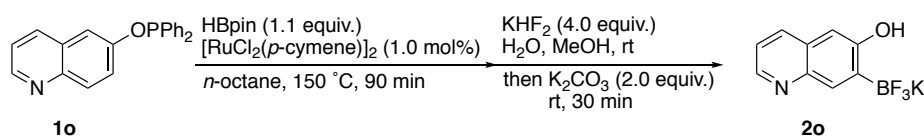
2n (white solid, 0.16 mmol, 55%)

^1H NMR (CDCl_3 , 500 MHz) δ = 8.00-7.94 (m, 4H), 7.54-7.43 (m, 2H), 7.48-7.42 (m, 4H), 7.13 (s, 1H), 6.48 (s, 1H), 5.92 (s, 2H), 1.21 (s, 12H). BH_3 are missing.; ^{13}C NMR (CDCl_3 , 100 MHz) δ = 152.9 (d, J = 4.8 Hz), 150.6, 144.3, 132.7, 132.2, 132.1, 132.0, 128.6 (d, J = 10.8 Hz), 114.4, 102.9, 101.9, 83.7, 24.9; ^{31}P NMR (CDCl_3 , 200 MHz) δ = 109.2 (br); ^{11}B NMR (CDCl_3 , 158 MHz) δ = 30.1 (br), -39.8 (br); IR (ATR) 3059.5, 2975.6, 2385.5, 1725.0, 1619.9, 1485.9, 1424.2, 1370.2, 1315.2, 1241.9, 1110.8, 1037.5 cm^{-1} ; HRMS (FD): Calcd for $\text{C}_{25}\text{H}_{29}\text{B}_2\text{O}_5\text{P}$ $[\text{M}]^+$: 462.1939; Found: 462.1928.



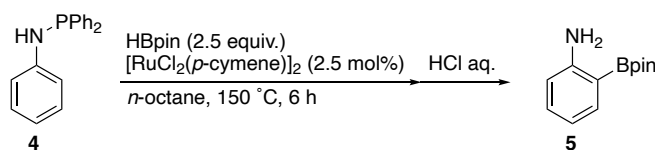
3n (white solid, 0.1 mmol, 34%)

^1H NMR (CDCl_3 , 500 MHz) δ = 7.98-7.90 (m, 4H), 7.54-7.43 (m, 6H), 6.60 (d, J = 8.5 Hz, 1H), 6.33 (d, J = 8.5, 1.0 Hz, 1H), 5.99 (s, 2H), 1.21 (s, 12H); ^{13}C NMR (CDCl_3 , 100 MHz) δ = 153.7, 151.1 (d J = 4.8 Hz), 144.0, 132.8, 132.3, 132.0, 131.9, 128.5 (d, J = 10.8 Hz) 112.7 (d, J = 4.8 Hz), 109.9, 101.7, 83.8, 24.9; ^{31}P NMR (CDCl_3 , 200 MHz) δ = 108.6 (br); ^{11}B NMR (CDCl_3 , 158 MHz) δ = 29.3 (br), -40.2 (br); IR (ATR) 2974.7, 2917.8, 2397.1, 1638.2, 1437.7, 1329.7, 1209.2, 1135.9, 1050.1 cm^{-1} ; HRMS (FD): Calcd for $\text{C}_{25}\text{H}_{29}\text{B}_2\text{O}_5\text{P}$ $[\text{M}]^+$: 462.1939; Found: 462.1956.



Borylation of 1o: A solution of $[\text{RuCl}_2(p\text{-cymene})]_2$ (1.8 mg, 3.0 μmol) and **1o** (98.8 mg, 0.30 mmol) in *n*-octane (1.5 mL) was placed in a glass tube (inside diameter = 1.7 cm, length = 18 cm) equipped with a three-way stop cock under Ar. HBpin (47.4 μL , 0.33 mmol) was added to the solution at room temperature, and the glass tube was closed. Then the mixture was stirred at 150 °C in the closed system for 90 min. After removal of the solvent under reduced pressure, H_2O (1.0 mL), KHF_2 (93.7 mg, 1.2 mmol), and MeOH (1.0 mL) were successively added and then stirred at room temperature. After 24 h, K_2CO_3 (80.5 mg, 0.6 mmol) was added to the solution, and the mixture was stirred for 30 min. The suspension was evaporated at 40 °C for 20 min, and the resulting beige solids were collected by filtration, which were rinsed with a small amount of cold MeOH to give **2o** containing small amounts of KBF_4 and $\text{K}[\text{HOBF}_3]$ (ca. **2o**: KBF_4 : $\text{K}[\text{HOBF}_3]$ = 100:2:5 in ^{19}F NMR) (60.3 mg). The yield of **2o** was calculated to be 78%.

^1H NMR (dms- d_6 , 500 MHz) δ = 8.55 (dd, J = 4.5, 1.5 Hz, 1H), 7.99 (d, J = 8.0 Hz, 1H), 7.88-7.78 (m, 2H), 7.25 (dd, J = 8.0, 4.0 Hz, 1H), 6.92 (s, 1H; ^{13}C NMR (dms- d_6 , 100 MHz) δ = 158.7, 146.1, 143.7, 133.4, 133.1, 128.3, 120.1, 106.2, 1C(C-B) is missing.; ^{19}F NMR (dms- d_6 , 465 MHz), δ = -136.1; ^{11}B NMR (dms- d_6 , 158 MHz) δ = 2.26 (br); IR (ATR) 3045.2, 2926.0, 1625.1, 1440.6, 1416.4, 1349.3, 1330.7, 1222.6, 1157.3, 1114.5 cm^{-1} ; HRMS (ESI-) Calcd for $\text{C}_9\text{H}_6\text{BF}_3\text{NO} [\text{M}-\text{K}]^-$: 212.0495; Found: 212.0504.



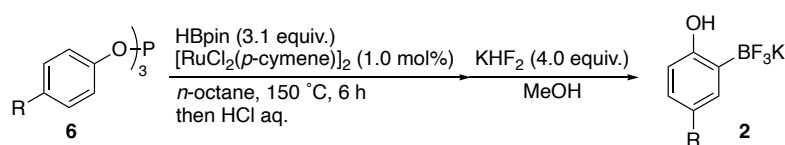
Borylation of 4: A solution of $[\text{RuCl}_2(p\text{-cymene})]_2$ (0.9 mg, 1.5 μmol) and **4** (83.2 mg, 0.30 mmol) in *n*-octane (1.5 mL) was placed in a glass tube (inside diameter = 1.7 cm, length = 18 cm) equipped with a three-way stop cock under Ar. HBpin (47.4 μL , 0.33 mmol) was added to the solution at room temperature, and the glass tube was closed. Then the mixture was stirred at 150 °C in the closed system for 6 h. 1N HCl aq. was added to the solution at room temperature, and the mixture was stirred for 24 h. The mixture was extracted with AcOEt three times, and the combined organic layers were washed with brine and dried over MgSO_4 . After the filtration of the drying

agent, the filtrate was evaporated to give a crude product. The crude product was purified by silica gel chromatography (hexane: ethyl acetate = 20:1) to give the borylation products **5** as a colorless oil (30 mg, 0.14 mmol, 46%).

The spectral data were in good agreement with the literature values.¹⁰

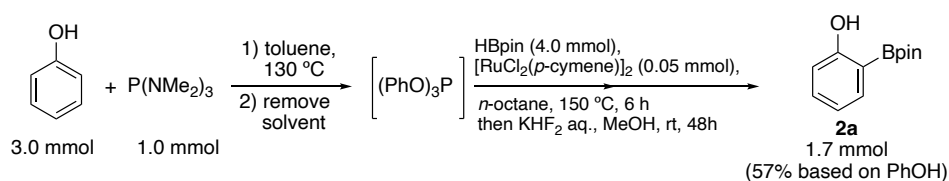
¹H NMR (CDCl₃, 400 MHz) δ = 7.61 (dd, J = 7.6, 1.6 Hz, 1H), 7.24-7.18 (m, 1H), 6.67 (t, J = 7.6 Hz, 1H), 6.59 (d, J = 7.6 Hz, 1H), 4.73 (br s, 2H), 1.34 (s, 12H).

Procedure for C–H borylation of aryl phosphites (Scheme 3)



A solution of $[\text{RuCl}_2(p\text{-cymene})]_2$ (1.8 mg, 3.0 μmol) and aryl phosphite **6** (0.30 mmol) in n -octane (1.5 mL) was placed in a glass tube (inside diameter = 1.7 cm, length = 18 cm) equipped with a three-way stop cock under Ar. HBpin (133.7 μL , 0.93 mmol) was added to the solution at room temperature, and the glass tube was closed. Then the mixture was stirred at 150 °C in the closed system for 6 h. 4N HCl aq. was added to the solution at room temperature, and the mixture was stirred for 48 h. The mixture was extracted with AcOEt three times, and the combined organic layers were washed with brine and dried over MgSO_4 . After filtration to remove the drying agent, the filtrate was evaporated to give a crude product. To a MeOH solution (1.5 mL) of the crude product was added KHF_2 (281 mg, 3.6 mmol) at room temperature, and the mixture was stirred for 24 h. The suspension was evaporated at 40 °C for 20 min, and residual white solids were dissolved in acetone (5.0 mL). After insoluble salts were filtered off, the filtrate was concentrated to ca. 1 mL volume. Then, toluene (ca. 1 mL) was added, and the remaining acetone was removed under reduced pressure to give suspension in toluene. The resulting beige solids were collected by filtration and rinsed with excess n -hexane and a small amount of cold MeOH (ca. 0 °C) to give aryl trifluoroborate **2**.

Procedure for one-pot borylation of phenol (Scheme 4)

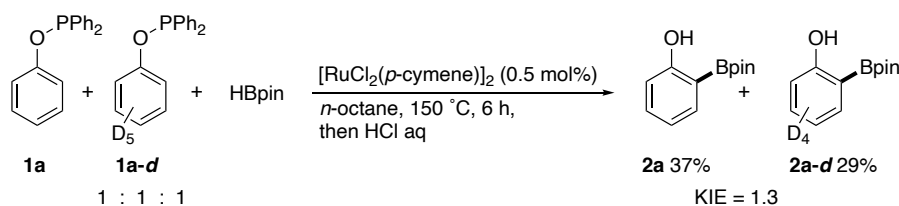


A solution of phenol (282 mg, 3.0 mmol) and $\text{P}(\text{NMe}_2)_3$ (181.3 μL , 1.0 mmol) in toluene (1.0 mL) was placed in a 50 mL Schlenk flask under Ar, and the glass tube was closed. Then the mixture was stirred at 130 °C in the closed system. After 8 h, the solvent was removed under reduced pressure at 100 °C for 1 h to give triphenyl phosphite **6a**. To the same flask was added $[\text{RuCl}_2(p\text{-cymene})]_2$ (30.6 mg, 50 μmol), n -octane (5.0 mL) and HBpin (575.2 μL , 4.0 mmol) under Ar, and then the mixture was stirred at 150 °C in the closed system. After 6 h, KHF_2 (937 mg, 12 mmol), MeOH (3.0 mL) and H_2O (2.0 mL) were added at room temperature, and the solution was stirred for 24 h. After removal of volatile materials, the residual white solids were dissolved in acetone (10~15 mL). After insoluble salts were filtered off, the filtrate was concentrated to ca. 1 mL volume. Then, toluene (ca.

3 mL) was added, and the remaining acetone was removed under reduced pressure to give suspension in toluene. The resulting beige solids were collected by filtration and rinsed with excess *n*-hexane and a small amount of cold MeOH (ca. 0°C) to give aryl trifluoroborate **2a** as white solids (342 mg, 1.7 mmol, 57% based on phenol).

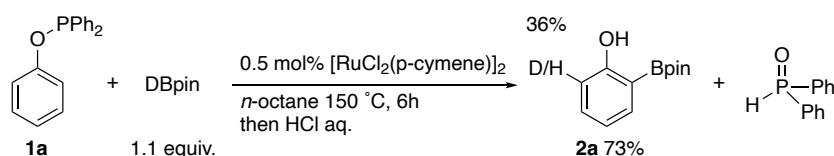
Deuterium labeling experiments

1. Intermolecular competition experiment (Scheme 5a)



A solution of $[RuCl_2(p\text{-cymene})]_2$ (0.9 mg, 1.5 μmol), **1a** (41.7 mg, 0.15 mmol) and **1a-d** (42.5 mg, 0.15 mmol) in *n*-octane (1.5 mL) was placed in a glass tube (inside diameter = 1.7 cm, length = 18 cm) equipped with a three-way stop cock under Ar. HBpin (21.6 μL , 0.15 mmol) was added to the solution at room temperature, and the glass tube was closed. Then the mixture was stirred at 150 °C in the closed system for 6 h. 1N HCl aq. was added to the solution at room temperature, and the mixture was stirred for 24 h. The mixture was extracted with AcOEt three times, and the combined organic layers were washed with brine and dried over $MgSO_4$. After the filtration of the drying agent, the filtrate was evaporated to give a pale-yellow oil. The yields of borylation products were determined to be **2a** = 37% and **2a-d** = 29% by 1H NMR using tetrachloroethane (10 μL , 0.095 mmol) as an internal standard. Therefore, the intermolecular KIE was calculated to be KIE = 1.3.

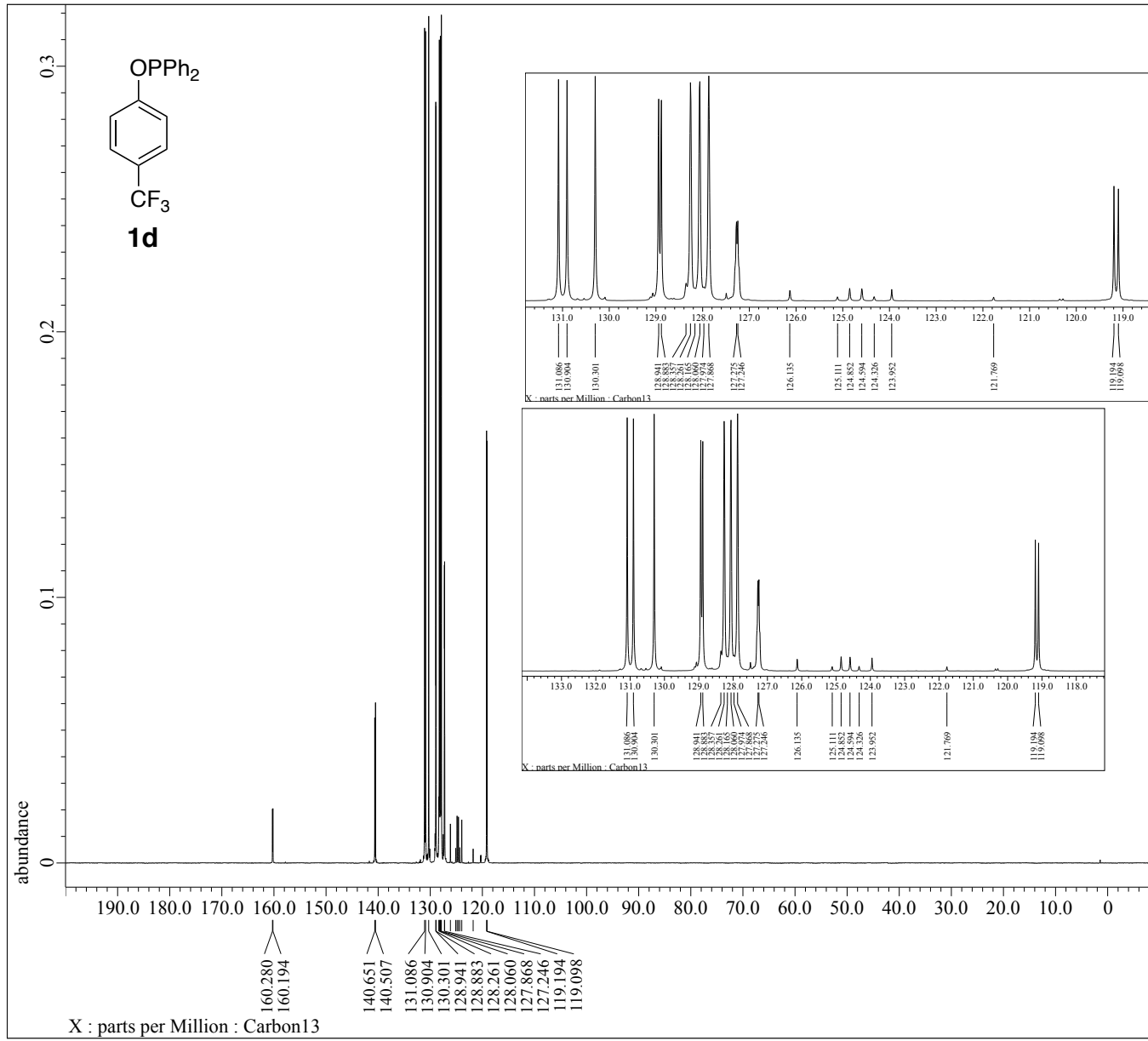
2. Reaction of **1a** with DBpin (Scheme 5b)



A solution of $[RuCl_2(p\text{-cymene})]_2$ (0.9 mg, 1.5 μmol) and **1a** (83.5 mg, 0.3 mmol) in *n*-octane (1.5 mL) was placed in a glass tube (inside diameter = 1.7 cm, length = 18 cm) equipped with a three-way stop cock under Ar. DBpin (47.8 μL , 0.33 mmol) was added to the solution at room temperature, and the glass tube was closed. Then the mixture was stirred at 150 °C in the closed system for 6 h. 1N HCl aq. was added to the solution at room temperature, and the mixture was stirred for 24 h. The mixture was extracted with AcOEt three times, and the combined organic layers were washed with brine and dried over $MgSO_4$. After the filtration of the drying agent, the filtrate was evaporated to give a pale-yellow oil. The yields of **2a** was determined to be 73% with 36% deuterium incorporation by 1H NMR using tetrachloroethane (10 μL , 0.095 mmol) as an internal standard.

References

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```

---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
phase( 0.75, 0, 50[%] )
base_correct( Akima, 5, 0, FALSE, 3, None, FA
Derived from: YH(S-p-CF3)_Carbon-1-1.jdf

```

```

Filename      = YH(S-p-CF3)_Carbon
Author        = delta
Experiment    = carbon.jxp
Sample Id     = YH(S-p-CF3)
Solvent       = BENZENE-D6
Actual_Start_Time = 4-APR-2020 18:22:
Revision_Time  = 9-APR-2020 14:01:

```

```

Comment       = single pulse decou
Data Format    = 1D REAL
Dim Size      = 26214
X Domain      = Carbon13
Dim Title     = Carbon13
Dim Units     = [ppm]
Dimensions    = X
Spectrometer  = JNM-ECZ500R/S1

```

```

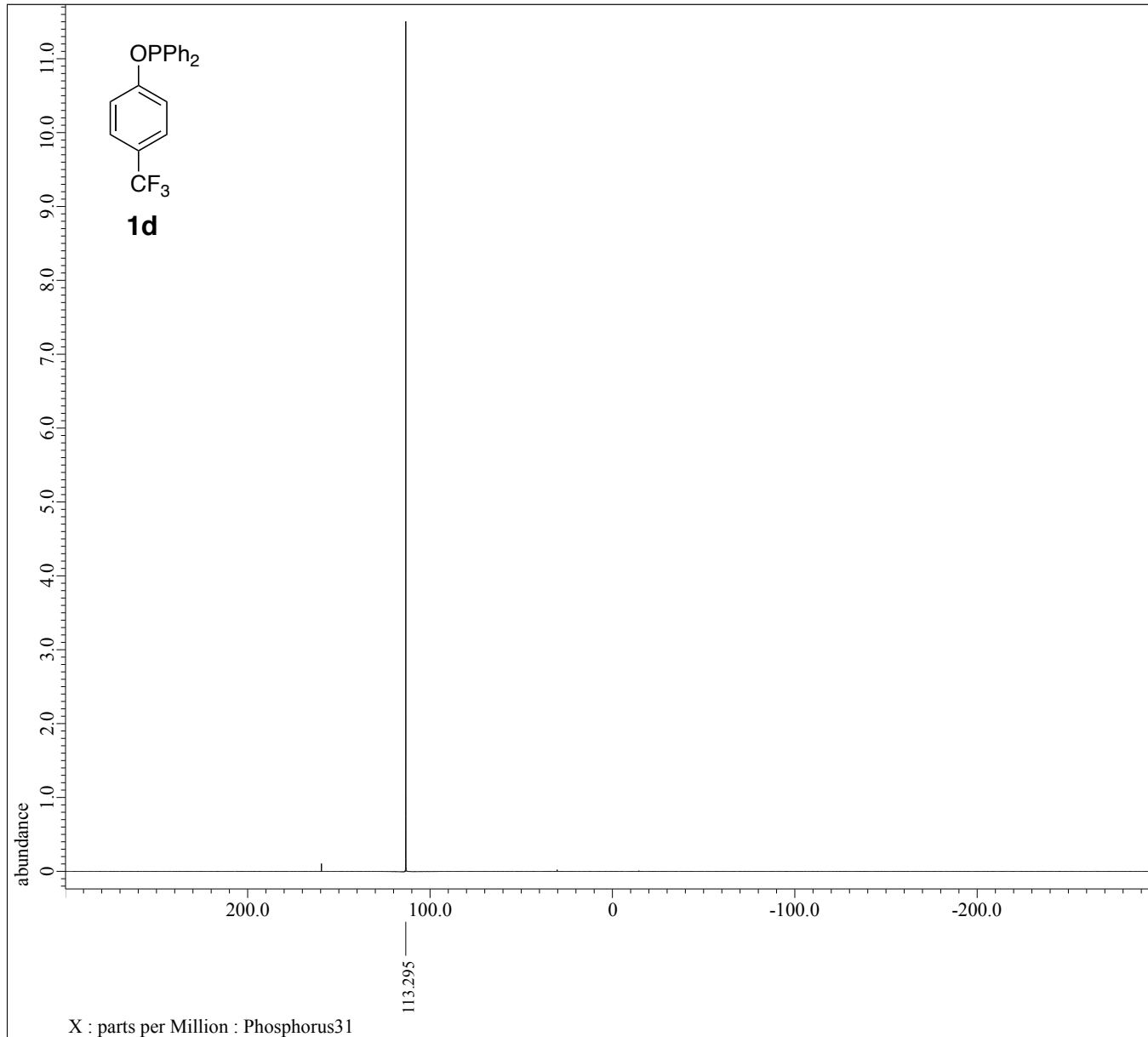
Field Strength = 11.62926421[T] (50
X Acq Duration = 0.8388608[s]
X Domain       = 13C
X Freq        = 124.5010059[MHz]
X Offset      = 100[ppm]
X Points      = 32768
X Prescans    = 4
X Resolution  = 1.1920929[Hz]
X Sweep       = 39.0625[kHz]
X Sweep Clipped = 31.25[kHz]
Irr Domain    = Proton
Irr Freq     = 495.13191398[MHz]
Irr Offset    = 5[ppm]
Clipped      = FALSE
Scans        = 1668
Total_Scans  = 1668

```

```

Relaxation_Delay = 2[s]
Recvr Gain       = 56
Temp_Get        = 20.8[dC]
X 90_Width      = 9.61[us]
X Acq Time      = 0.8388608[s]
X Angle         = 30[deg]
X Atn           = 10[dB]
X Pulse         = 3.20333333[us]
Irr Atn Dec     = 23.948[dB]
Irr Atn Dec Calc = 23.948[dB]
Irr Atn Dec Default_Calc = 23.948[dB]
Irr Atn Noe     = 23.948[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

```



```

---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
phase( -91, 0, 50[%] )
base_correct( Akima, 5, 0, FALSE, 3, None, FA
Derived from: YH(S-p-CF3)_31P_1Hdec-1-1.jdf

```

```

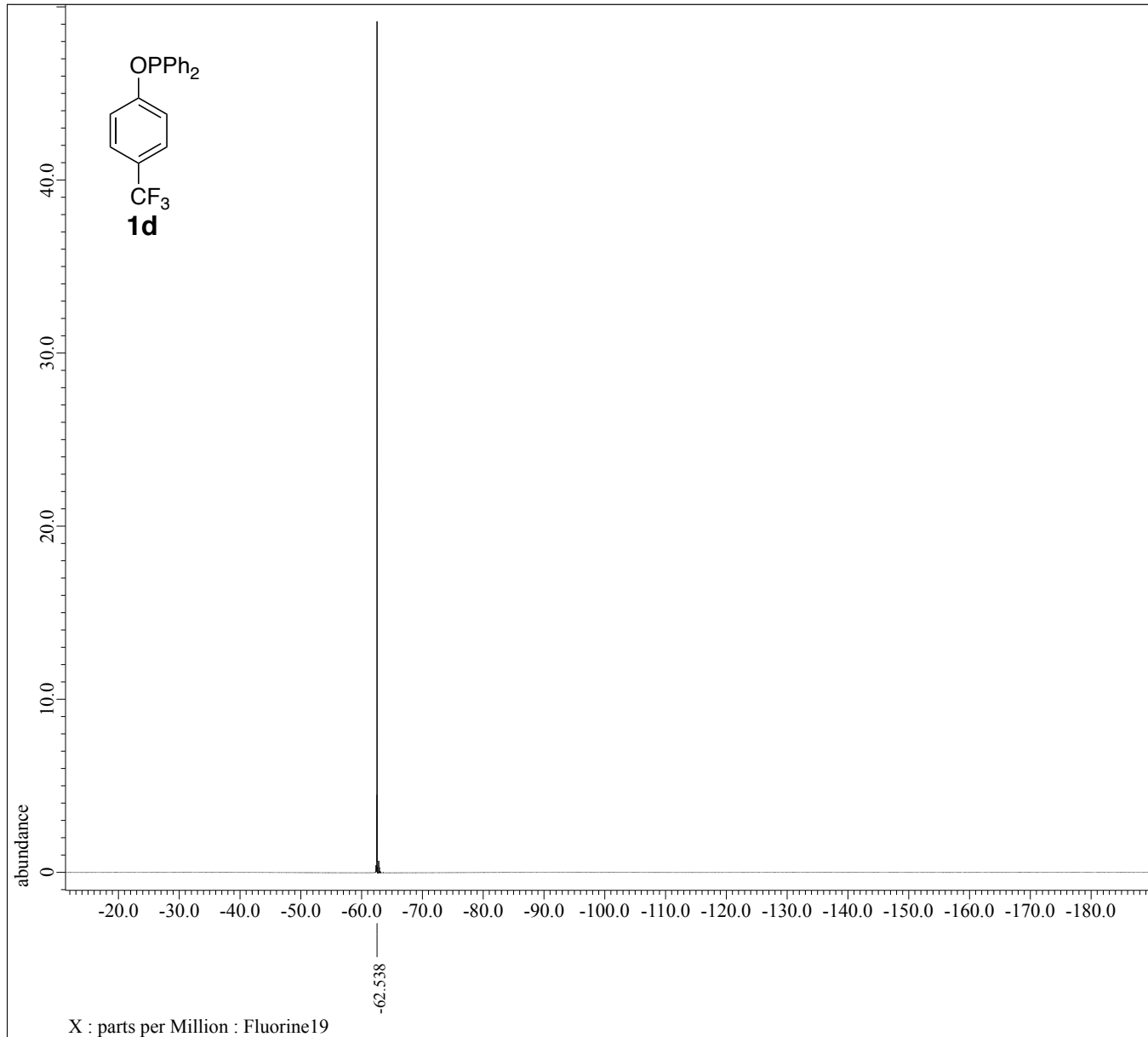
Filename           = YH(S-p-CF3)_31P_1H
Author             = delta
Experiment         = single_pulse_decou
Sample_Id          = YH(S-p-CF3)
Solvent            = BENZENE-D6
Actual_Start_Time  = 3-APR-2020 19:21:
Revision_Time      = 7-APR-2020 12:36:

Comment           = single_pulse decou
Data_Format       = 1D REAL
Dim_Size          = 26214
X_Domain          = Phosphorus31
Dim_Title         = Phosphorus31
Dim_Units         = [ppm]
Dimensions        = X
Spectrometer      = JNM-ECZ500R/S1

Field_Strength    = 11.62926421[T] (50
X_Acq_Duration    = 0.18874368[s]
X_Domain          = 31P
X_Freq            = 200.43293989[MHz]
X_Offset          = 0[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 5.29819065[Hz]
X_Sweep           = 173.61111111[kHz]
X_Sweep_Clipped   = 138.88888889[kHz]
Irr_Domain        = Proton
Irr_Freq          = 495.13191398[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 64
Total_Scans       = 64

Relaxation_Delay  = 1[s]
Recvr_Gain        = 56
Temp_Get          = 20.3[dC]
X_90_Width        = 19.78[us]
X_Acq_Time        = 0.18874368[s]
X_Angle           = 30[deg]
X_Atn             = 9.4[dB]
X_Pulse           = 6.59333333[us]
Irr_Atn_Dec       = 23.948[dB]
Irr_Atn_Dec_Calc = 23.948[dB]
Irr_Atn_Dec_Default_Calc = 23.948[dB]
Irr_Atn_Noise    = 23.948[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_Noise        = TRUE
Irr_Noise        = WALTZ

```



```

---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
phase( 12.76831, 0, 50[%] )

Derived from: YH(S-p-CF3)_19F-1-1.jdf

```

```

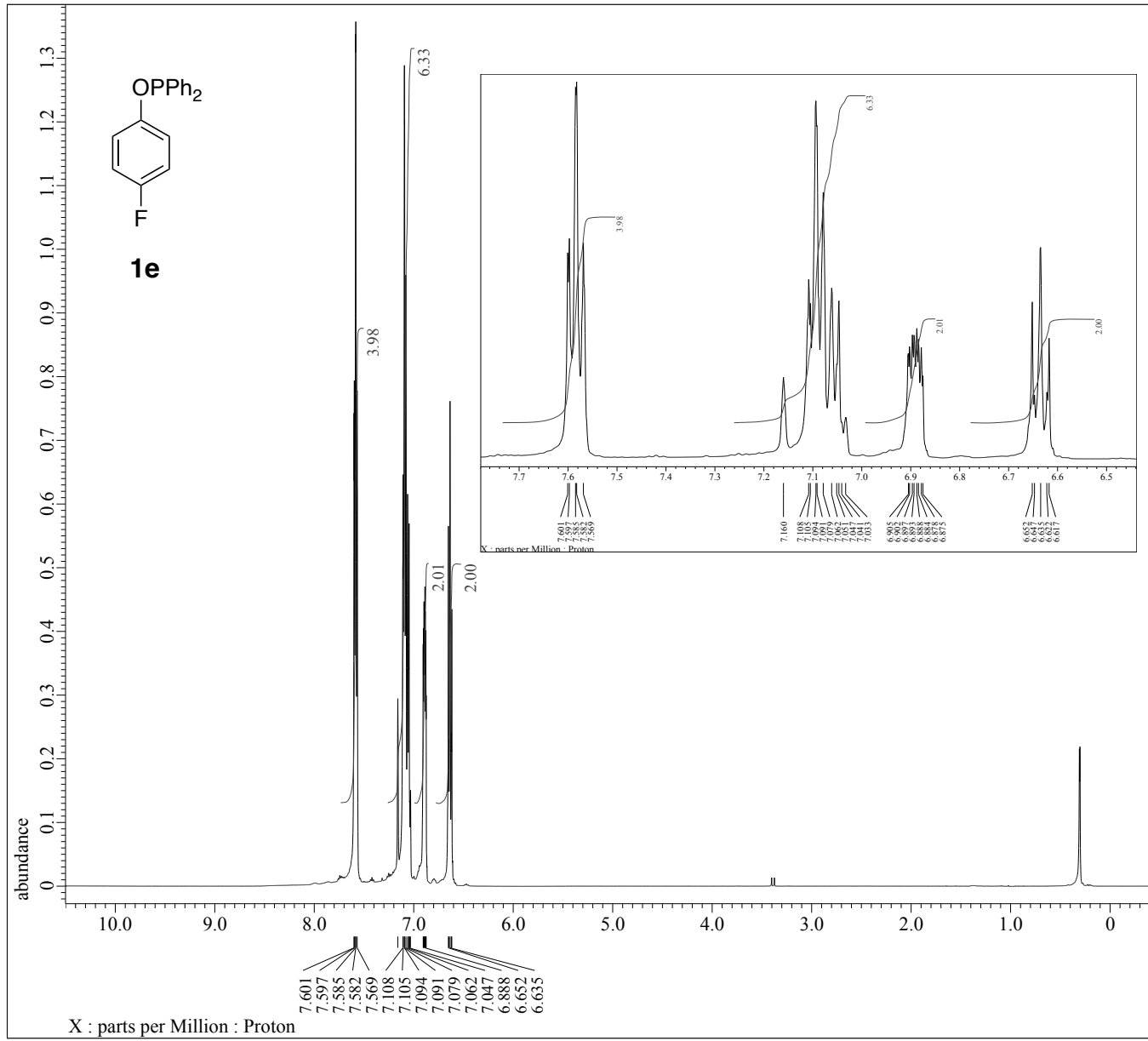
Filename      = YH(S-p-CF3)_19F-1-2.j
Author       = delta
Experiment    = single_pulse.jxp
Sample_Id     = YH(S-p-CF3)
Solvent       = BENZENE-D6
Actual_Start_Time = 3-APR-2020 19:26:29
Revision_Time = 7-APR-2020 14:33:15

Comment      = single_pulse
Data_Format   = 1D COMPLEX
Dim_Size     = 26214
X_Domain     = Fluorine19
Dim_Title    = Fluorine19
Dim_Units    = [ppm]
Dimensions   = X
Spectrometer = JNM-ECZ500R/s1

Field_Strength = 11.62926421[T] (500[M]
X_Acq_Duration = 0.28311552[s]
X_Domain      = 19F
X_Freq       = 465.88941346[MHz]
X_Offset     = -100[ppm]
X_Points     = 32768
X_Prescans   = 1
X_Resolution = 3.5321271[Hz]
X_Sweep      = 115.74074074[kHz]
X_Sweep_Clip = 92.59259259[kHz]
Irr_Domain   = Fluorine19
Irr_Freq    = 465.88941346[MHz]
Irr_Offset  = 5[ppm]
Tri_Domain   = Fluorine19
Tri_Freq    = 465.88941346[MHz]
Tri_Offset  = 5[ppm]
Clipped     = FALSE
Scans       = 8
Total_Scans = 8

Relaxation_Delay = 5[s]
Recvr_Gain       = 36
Temp_Get         = 20.2[dC]
X_90_Width      = 11[us]
X_Acq_Time      = 0.28311552[s]
X_Angle         = 45[deg]
X_Atn           = 3.7[dB]
X_Pulse         = 5.5[us]
Irr_Mode        = Off
Tri_Mode        = Off
Dante_Loop     = 500
Dante_Preset   = FALSE
Decimation_Rate = 0
Initial_Wait    = 1[s]
Phase           = {0, 90, 270, 180, 180}
Preset_Time     = 5[s]

```

```

---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
phase( 27.60676, 0, 50[%] )
base_correct( Akima, 5, 0, FALSE, 3, None, FA

Derived from: YH(S-p-F)_Proton-1-1.jdf
  
```

```

Filename      = YH(S-p-F)_Proton-1-2.
Author        = delta
Experiment    = proton.jxp
Sample_Id     = YH(S-p-F)
Solvent       = BENZENE-D6
Actual_Start_Time = 2-APR-2020 04:31:53
Revision_Time = 10-APR-2020 19:12:01
  
```

```

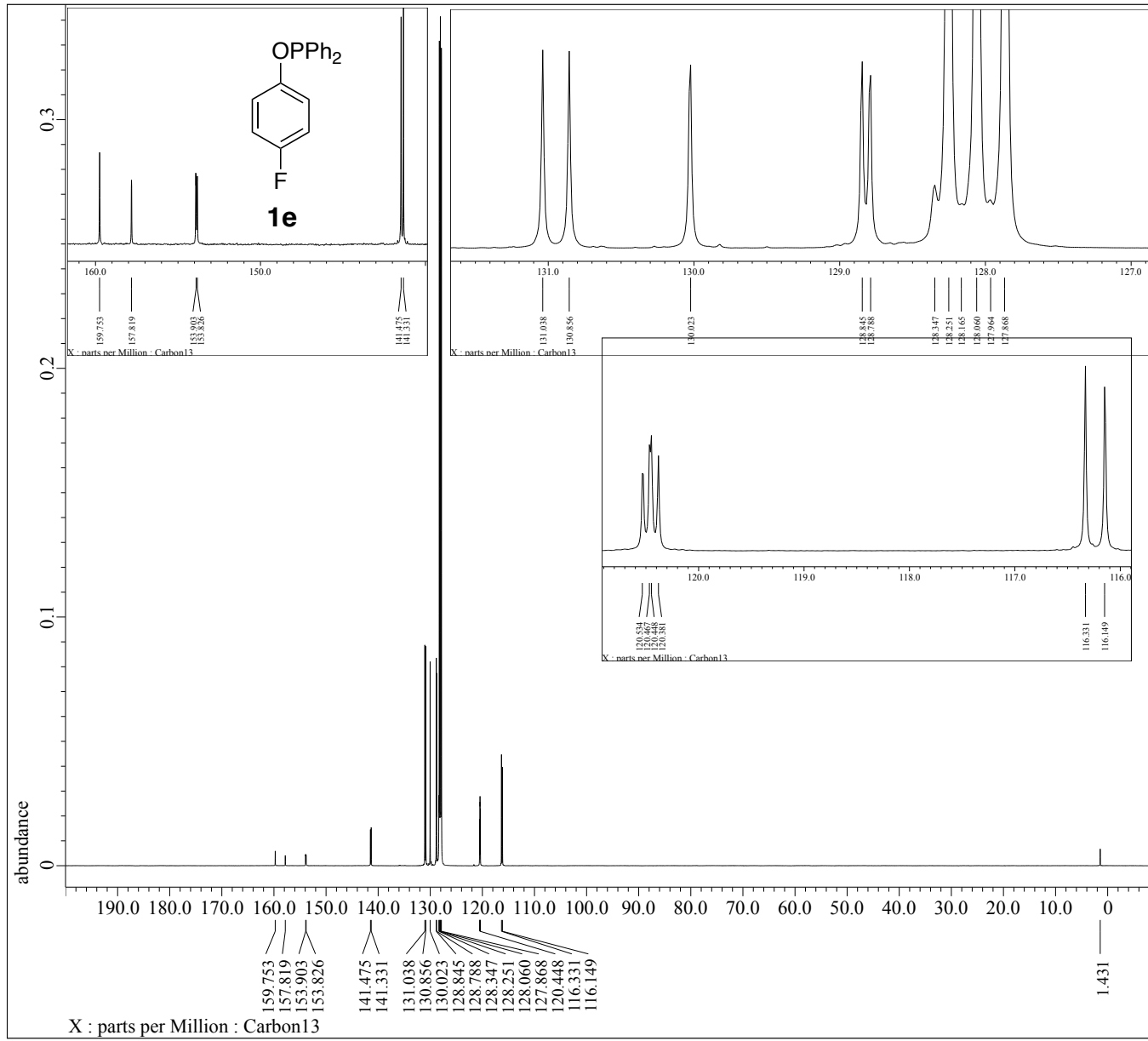
Comment      = single pulse
Data Format   = 1D REAL
Dim Size     = 13107
X Domain     = Proton
Dim Title    = Proton
Dim Units    = [ppm]
Dimensions   = X
Spectrometer = JNM-ECZ500R/s1
  
```

```

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     = 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]
Recvr Gain       = 36
Temp_Get         = 20.9[dC]
X 90 Width      = 9.58[us]
X Acq Time       = 1.76422912[s]
X Angle          = 45[deg]
X Atn            = 4.3[dB]
X Pulse         = 4.79[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]
  
```



```

---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
phase( -1.5, -1, 50[%] )
base_correct( Akima, 5, 0, FALSE, 3, None, FA
Derived from: YH(S-p-F)_Carbon-1-1.jdf

```

```

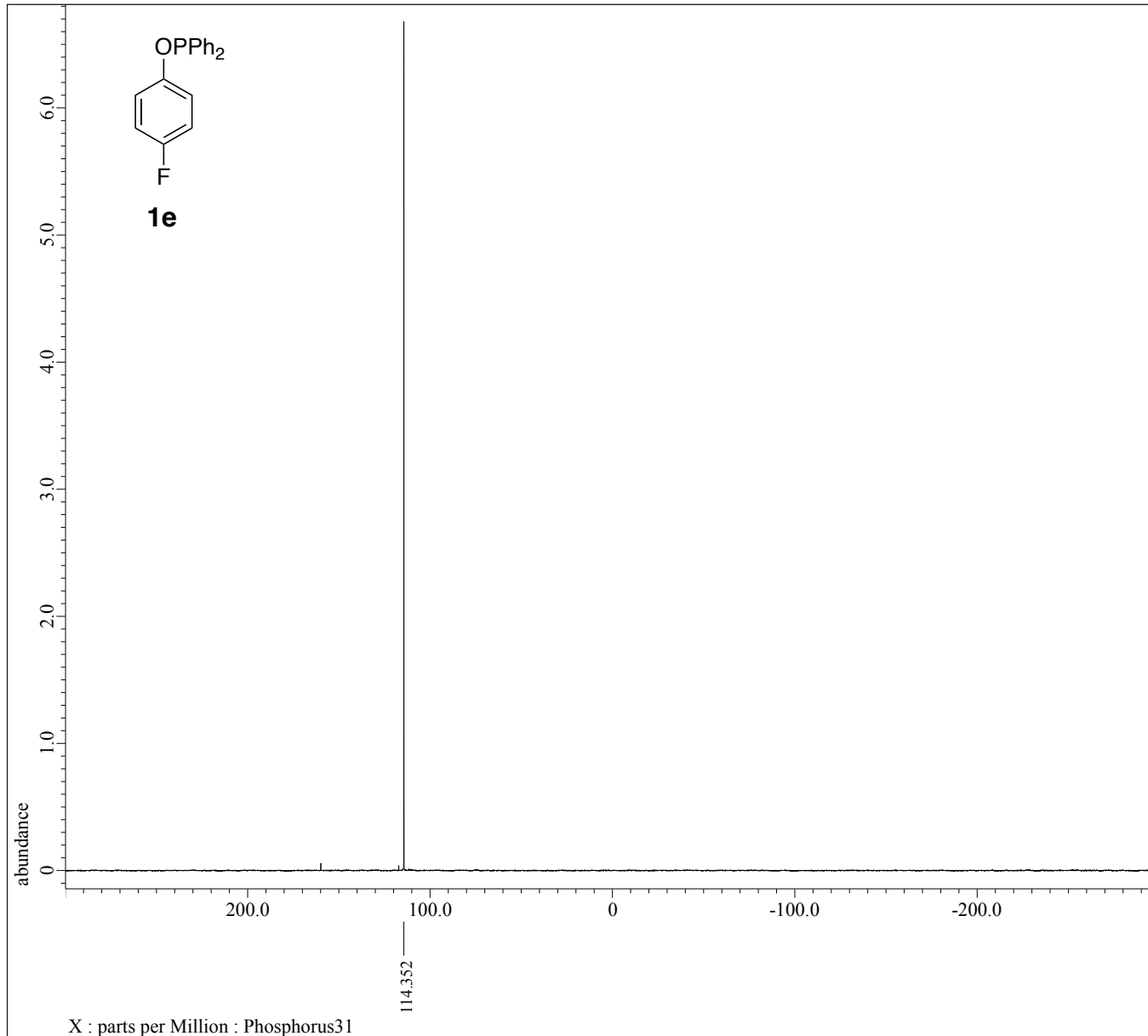
Filename      = YH(S-p-F)_Carbon-1
Author        = delta
Experiment    = carbon.jxp
Sample Id     = YH(S-p-F)
Solvent       = BENZENE-D6
Actual_Start_Time = 4-APR-2020 12:36:
Revision_Time  = 10-APR-2020 19:28:

Comment       = single pulse decou
Data Format    = 1D REAL
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          = 5000
Total_Scans    = 5000

Relaxation_Delay = 2[s]
Recvr Gain       = 56
Temp_Get         = 19.6[dC]
X 90_Width      = 9.61[us]
X Acq Time       = 0.8388608[s]
X Angle          = 30[deg]
X Atn            = 10[dB]
X Pulse         = 3.20333333[us]
Irr Atn Dec     = 23.948[dB]
Irr Atn Dec Calc = 23.948[dB]
Irr Atn Dec Default_Calc = 23.948[dB]
Irr Atn Noe     = 23.948[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

```



```

---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
phase( 27, 0, 50[%] )
ibase_correct( , FALSE, FALSE, FALSE )
base_correct( Akima, 5, 0, FALSE, 3, None, FA
base_correct( Akima, 5, 0, FALSE, 3, None, FA
Derived from: YH(S-p-F)_31P_1Hdec-1-1.jdf

```

```

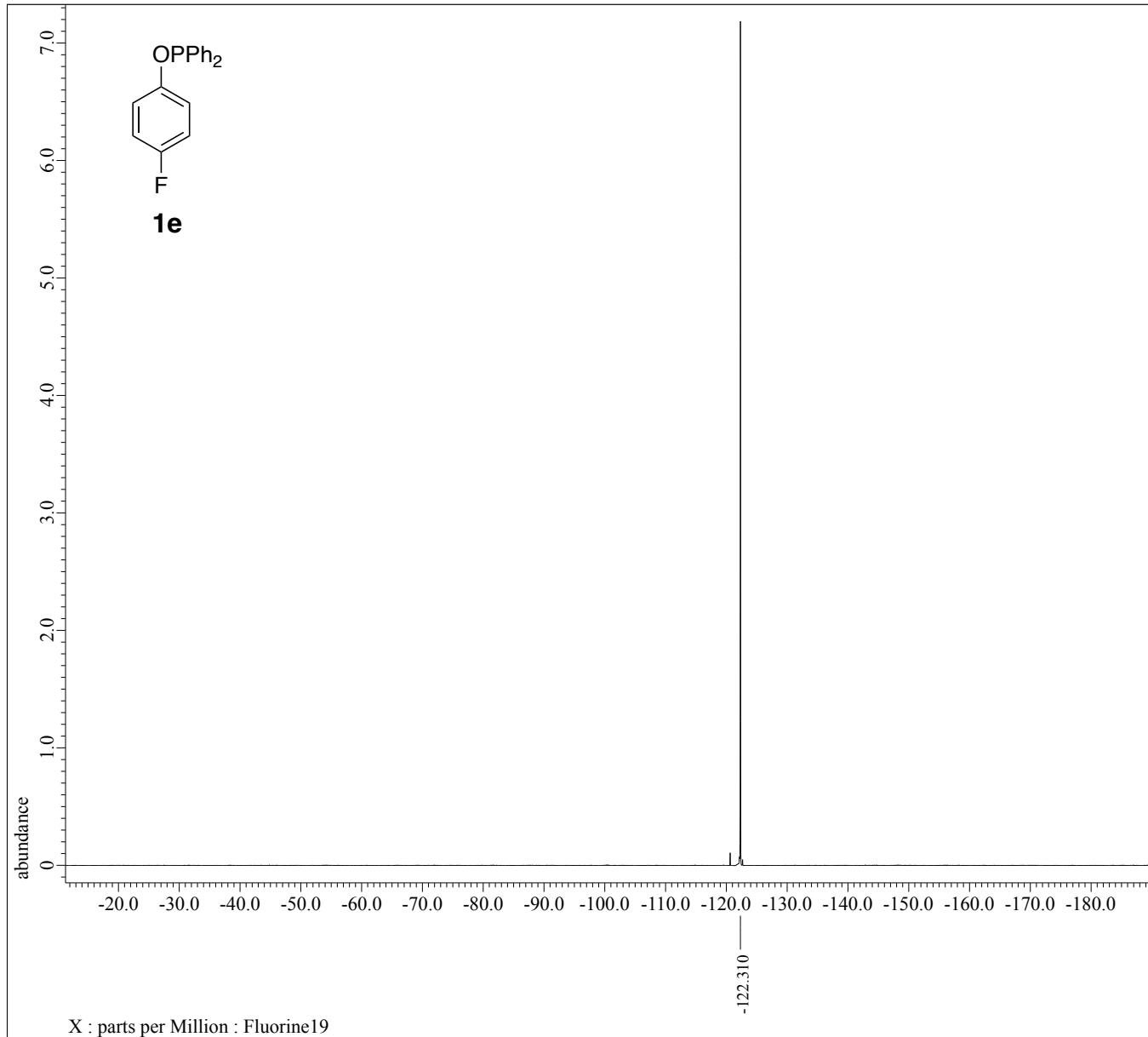
Filename           = YH(S-p-F)_31P_1Hdec
Author             = delta
Experiment         = single_pulse_decou
Sample_Id          = YH(S-p-F)
Solvent            = BENZENE-D6
Actual_Start_Time  = 2-APR-2020 11:55:
Revision_Time      = 7-APR-2020 12:34:

Comment           = single_pulse decou
Data_Format       = 1D REAL
Dim_Size          = 26214
X_Domain          = Phosphorus31
Dim_Title         = Phosphorus31
Dim_Units         = [ppm]
Dimensions        = X
Spectrometer      = JNM-ECZ500R/S1

Field_Strength    = 11.62926421[T] (50
X_Acq_Duration    = 0.18874368[s]
X_Domain          = 31P
X_Freq            = 200.43293989[MHz]
X_Offset          = 0[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 5.29819065[Hz]
X_Sweep           = 173.61111111[kHz]
X_Sweep_Clipped   = 138.88888889[kHz]
Irr_Domain        = Proton
Irr_Freq          = 495.13191398[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 64
Total_Scans       = 64

Relaxation_Delay  = 1[s]
Recvr_Gain        = 66
Temp_Get          = 20.2[dC]
X_90_Width        = 19.78[us]
X_Acq_Time        = 0.18874368[s]
X_Angle           = 30[deg]
X_Atn             = 9.4[dB]
X_Pulse           = 6.59333333[us]
Irr_Atn_Dec       = 23.948[dB]
Irr_Atn_Dec_Calc = 23.948[dB]
Irr_Atn_Dec_Default_Calc = 23.948[dB]
Irr_Atn_Noise    = 23.948[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_Noise         = TRUE
Irr_Noise         = WALTZ

```



```

---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
phase( 0.75, 0, 50[%] )
base_correct( Akima, 5, 0, FALSE, 3, None, FA
Derived from: YH(S-p-F)_19F-1-1.jdf

```

```

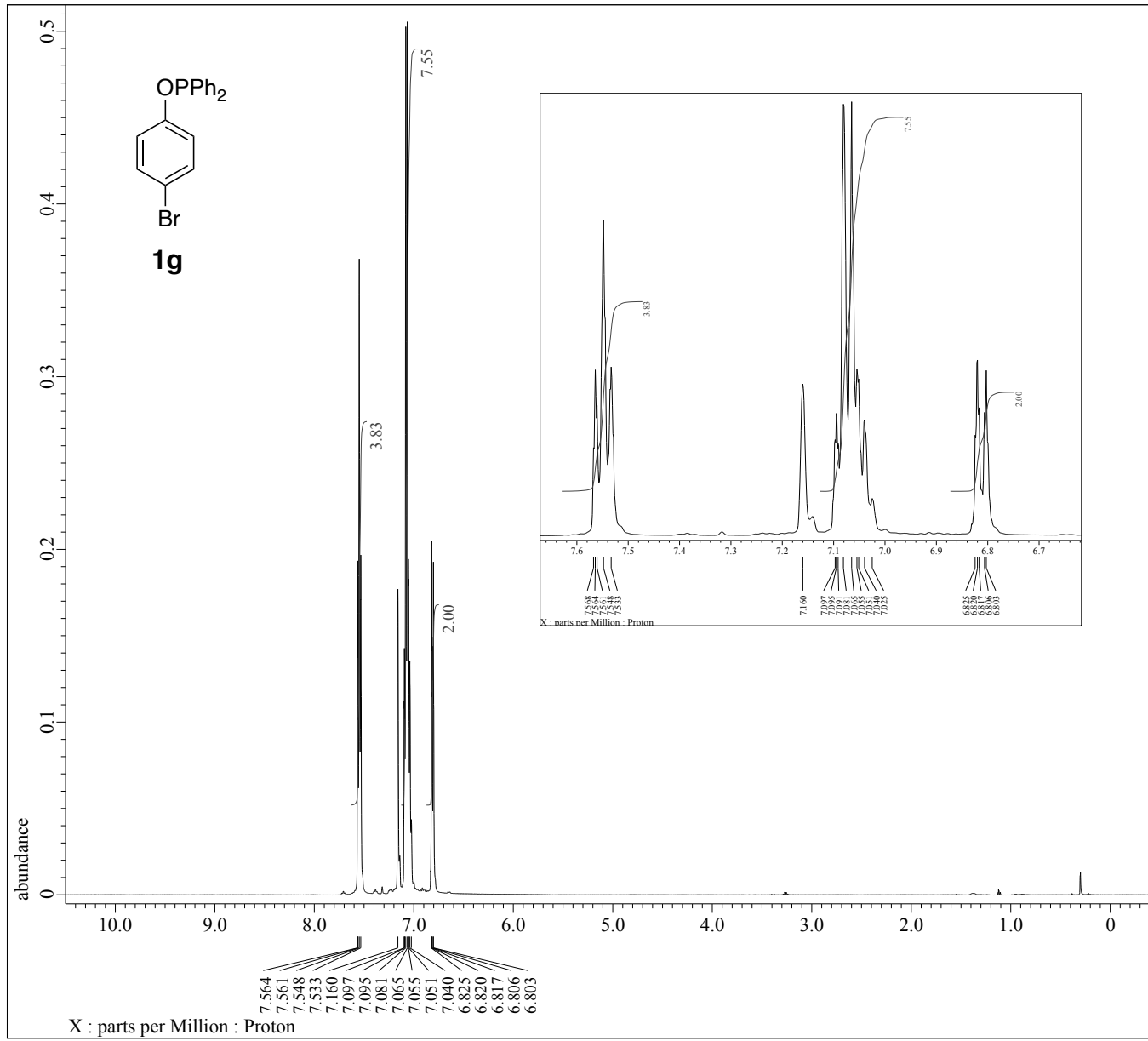
Filename      = YH(S-p-F)_19F-1-2.jdf
Author       = delta
Experiment   = single_pulse.jxp
Sample_Id    = YH(S-p-F)
Solvent      = BENZENE-D6
Actual_Start_Time = 3-APR-2020 20:06:10
Revision_Time   = 7-APR-2020 14:31:23

Comment      = single_pulse
Data_Format  = 1D_REAL
Dim_Size     = 26214
X_Domain     = Fluorine19
Dim_Title    = Fluorine19
Dim_Units    = [ppm]
Dimensions   = X
Spectrometer = JNM-ECZ500R/s1

Field_Strength = 11.62926421[T] (500[M]
X_Acq_Duration = 0.28311552[s]
X_Domain       = 19F
X_Freq         = 465.88941346[MHz]
X_Offset       = -100[ppm]
X_Points       = 32768
X_Prescans     = 1
X_Resolution   = 3.5321271[Hz]
X_Sweep        = 115.74074074[kHz]
X_Sweep_Clipped = 92.59259259[kHz]
Irr_Domain     = Fluorine19
Irr_Freq       = 465.88941346[MHz]
Irr_Offset     = 5[ppm]
Tri_Domain     = Fluorine19
Tri_Freq       = 465.88941346[MHz]
Tri_Offset     = 5[ppm]
Clipped        = FALSE
Scans          = 8
Total_Scans    = 8

Relaxation_Delay = 5[s]
Recvr_Gain       = 56
Temp_Get         = 20.6[dC]
X_90_Width       = 11[us]
X_Acq_Time       = 0.28311552[s]
X_Angle          = 45[deg]
X_Atn            = 3.7[dB]
X_Pulse          = 5.5[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]

```



```

---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
phase( 20.03359, 0, 35.06791[%] )
base_correct( Akima, 5, 0, FALSE, 3, None, FA
Derived from: YH-p-Br-2_Proton-1-1.jdf

```

```

Filename      = YH-p-Br-2_Proton-1-10
Author       = delta
Experiment   = proton.jxp
Sample Id    = YH-p-Br-2
Solvent      = BENZENE-D6
Actual_Start_Time = 1-APR-2020 14:25:52
Revision_Time   = 6-APR-2020 22:20:58

```

```

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

```

```

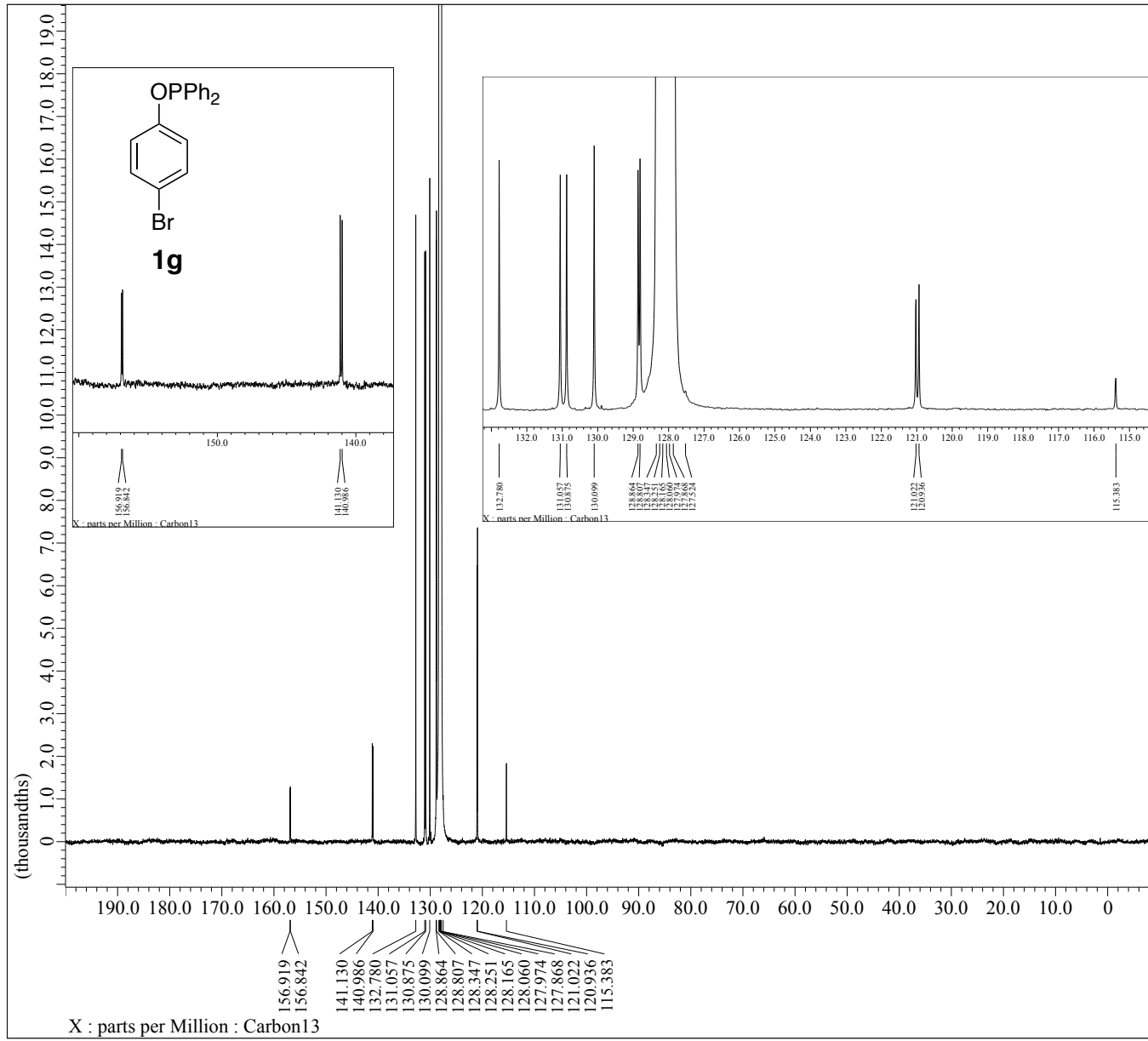
Field Strength = 11.62926421[T] (500[M
X_Acq_Duration = 1.76422912[s]
X_Domain       = 1H
X_Freq         = 495.13191398[MHz]
X_Offset       = 5[ppm]
X_Points       = 16384
X_Prescans     = 1
X_Resolution   = 0.5668198[Hz]
X_Sweep        = 9.28677563[kHz]
X_Sweep_Clippped = 7.42942051[kHz]
Irr_Domain     = 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]
Recvr Gain       = 36
Temp_Get         = 21[dC]
X_90_Width       = 9.58[us]
X_Acq_Time       = 1.76422912[s]
X_Angle          = 45[deg]
X_Atn            = 4.3[dB]
X_Pulse          = 4.79[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]

```



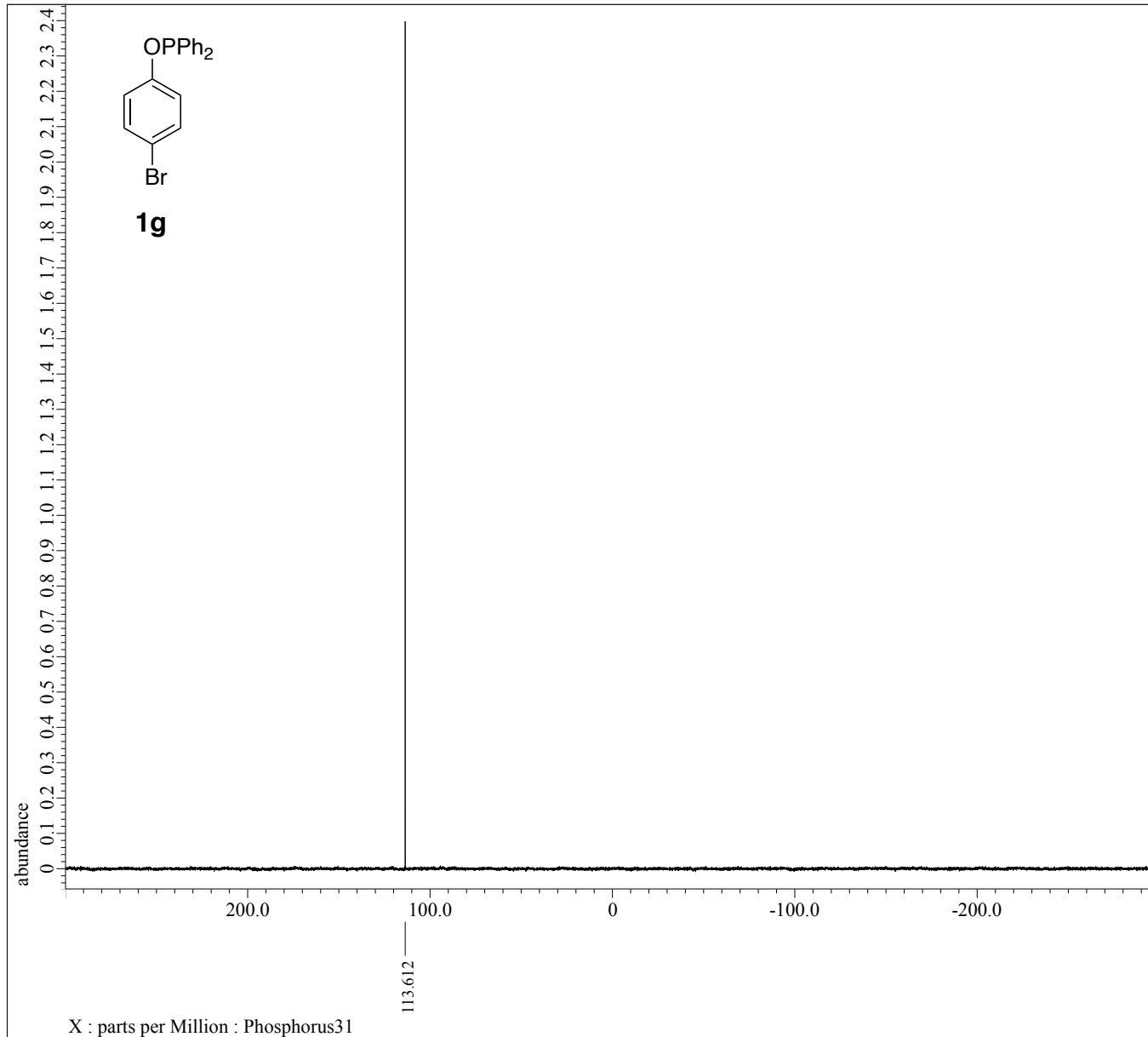
---- PROCESSING PARAMETERS ----
 sexp(2.0[Hz], 0.0[s])
 trapezoid(0[%], 0[%], 80[%], 100[%])
 zerofill(1, TRUE)
 fft(1, TRUE, TRUE)
 machinephase
 ppm
 phase(-2.25, 0, 50[%])
 base_correct(Akima, 5, 0, FALSE, 3, None, FA
 Derived from: YH-p-Br-2_Carbon-1-1.jdf

Filename = YH-p-Br-2_Carbon-1
 Author = delta
 Experiment = carbon.jxp
 Sample_Id = YH-p-Br-2
 Solvent = BENZENE-D6
 Actual_Start_Time = 2-APR-2020 00:07:
 Revision_Time = 9-APR-2020 13:44:

Comment = single pulse decou
 Data Format = 1D REAL
 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_Clippped = 31.25[kHz]
 Irr_Domain = Proton
 Irr_Freq = 495.13191398[MHz]
 Irr_Offset = 5[ppm]
 Clipped = FALSE
 Scans = 5000
 Total_Scans = 5000

Relaxation_Delay = 2[s]
 Recvr Gain = 56
 Temp_Get = 20.9[dC]
 X_90_Width = 9.61[us]
 X_Acq_Time = 0.8388608[s]
 X_Angle = 30[deg]
 X_Atn = 10[dB]
 X_Pulse = 3.20333333[us]
 Irr_Atn_Dec = 23.948[dB]
 Irr_Atn_Dec_Calc = 23.948[dB]
 Irr_Atn_Dec_Default_Calc = 23.948[dB]
 Irr_Atn_Noise = 23.948[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_Noise = TRUE
 Irr_Noise = WALTZ



```

---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
phase( -12.5, 0, 50[%] )
base_correct( Akima, 5, 0, FALSE, 3, None, FA
Derived from: YH-p-Br-2_31P_1Hdec-1-1.jdf

```

```

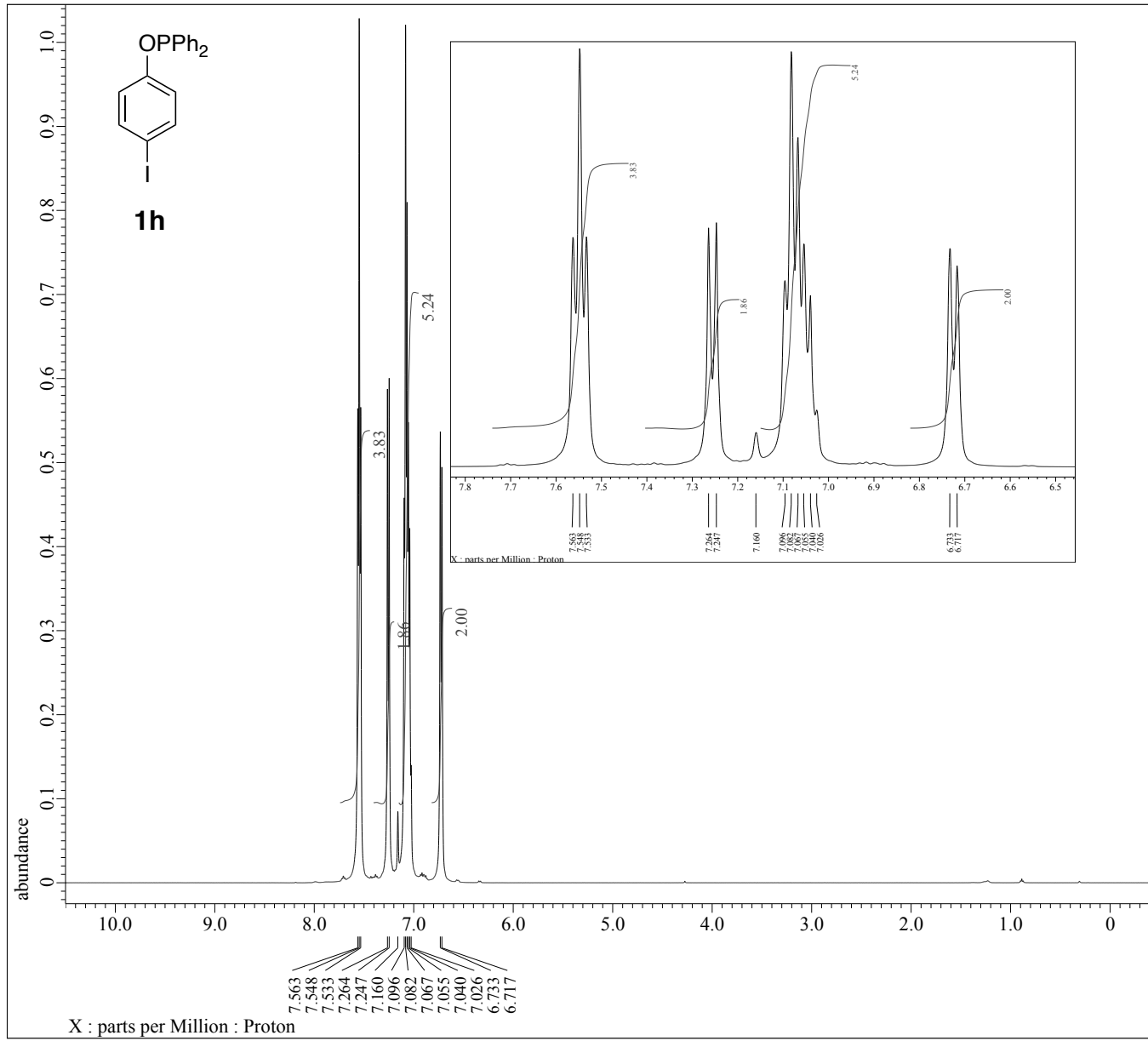
Filename           = YH-p-Br-2_31P_1Hde
Author            = delta
Experiment        = single_pulse_decou
Sample_Id         = YH-p-Br-2
Solvent           = BENZENE-D6
Actual_Start_Time = 1-APR-2020 14:30:
Revision_Time     = 7-APR-2020 12:52:

Comment          = single_pulse decou
Data_Format      = 1D REAL
Dim_Size         = 26214
X_Domain         = Phosphorus31
Dim_Title        = Phosphorus31
Dim_Units        = [ppm]
Dimensions       = X
Spectrometer     = JNM-ECZ500R/S1

Field_Strength   = 11.62926421[T] (50
X_Acq_Duration   = 0.18874368[s]
X_Domain         = 31P
X_Freq           = 200.43293989[MHz]
X_Offset         = 0[ppm]
X_Points         = 32768
X_Prescans       = 4
X_Resolution     = 5.29819065[Hz]
X_Sweep          = 173.61111111[kHz]
X_Sweep_Clipped = 138.88888889[kHz]
Irr_Domain       = Proton
Irr_Freq         = 495.13191398[MHz]
Irr_Offset       = 5[ppm]
Clipped          = FALSE
Scans            = 64
Total_Scans      = 64

Relaxation_Delay = 1[s]
Recvr_Gain       = 66
Temp_Get         = 20.6[dC]
X_90_Width       = 19.78[us]
X_Acq_Time       = 0.18874368[s]
X_Angle          = 30[deg]
X_Atn            = 9.4[dB]
X_Pulse          = 6.59333333[us]
Irr_Atn_Dec      = 23.948[dB]
Irr_Atn_Dec_Calc = 23.948[dB]
Irr_Atn_Dec_Default_Calc = 23.948[dB]
Irr_Atn_Noise   = 23.948[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_Noise        = TRUE
Irr_Noise        = WALTZ

```



```

---- 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
Derived from: YH(S-p-I)_Proton-1-1.jdf

```

```

Filename      = YH(S-p-I)_Proton-1-2.
Author       = delta
Experiment   = proton.jxp
Sample_Id    = YH(S-p-I)
Solvent      = BENZENE-D6
Actual_Start_Time = 3-APR-2020 19:08:47
Revision_Time   = 7-APR-2020 09:56:14

```

```

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

```

```

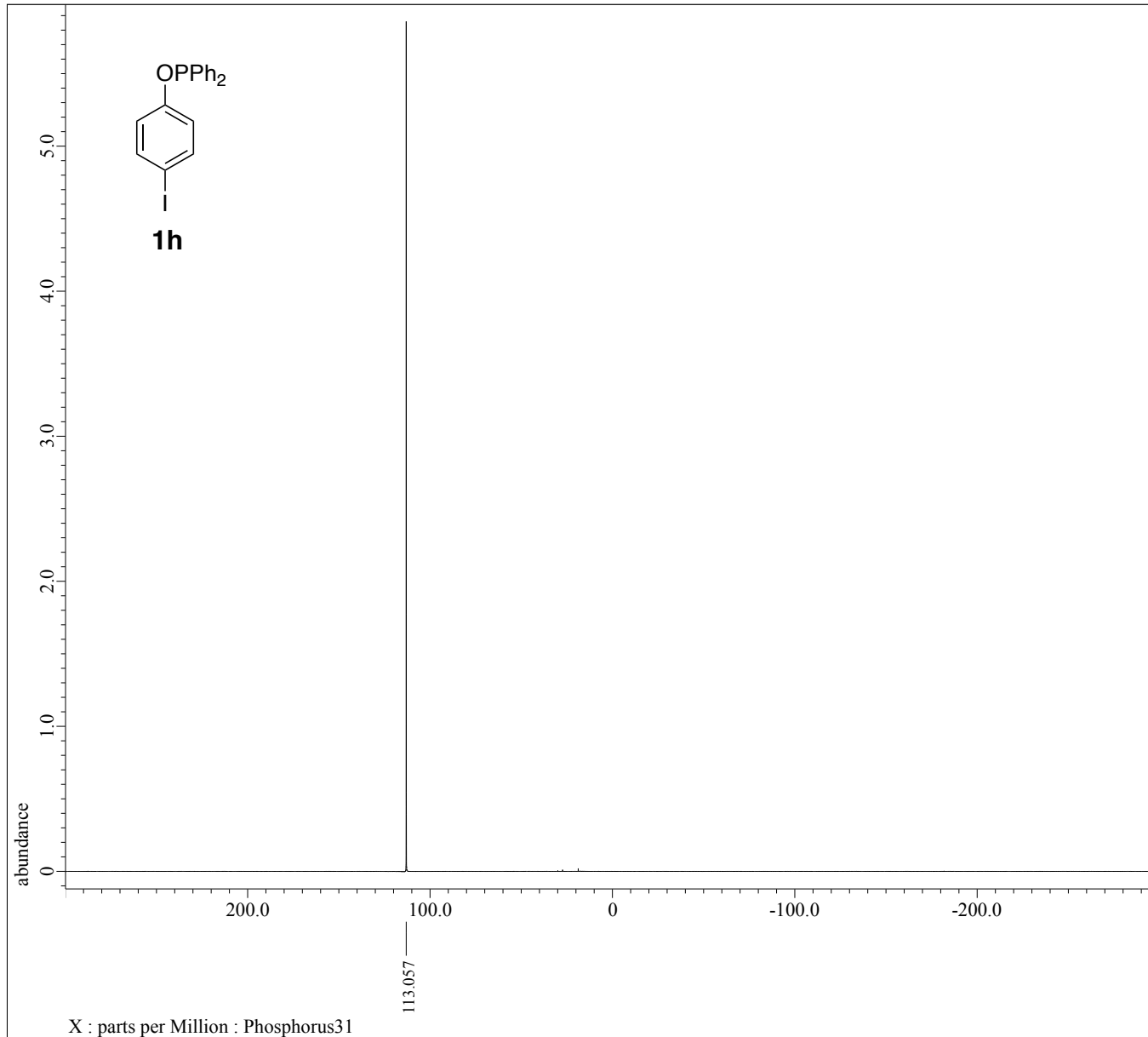
Field Strength = 11.62926421[T] (500[M]
X_Acq_Duration = 1.76422912[s]
X_Domain       = 1H
X_Freq        = 495.13191398[MHz]
X_Offset      = 5[ppm]
X_Points      = 16384
X_Prescans    = 1
X_Resolution  = 0.5668198[Hz]
X_Sweep       = 9.28677563[kHz]
X_Sweep_Clip  = 7.42942051[kHz]
Irr_Domain    = Proton
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]
Recvr_Gain       = 26
Temp_Get         = 19.1[dC]
X_90_Width      = 9.58[us]
X_Acq_Time      = 1.76422912[s]
X_Angle         = 45[deg]
X_Atn           = 4.3[dB]
X_Pulse         = 4.79[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]

```

```

---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
phase( 6.75, 0, 33.97551[%] )
base_correct( Akima, 5, 0, FALSE, 3, None, FA
Derived from: YH(S-p-I)_31P_1Hdec-1-1.jdf

```

```

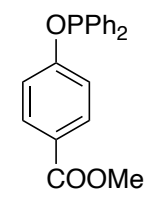
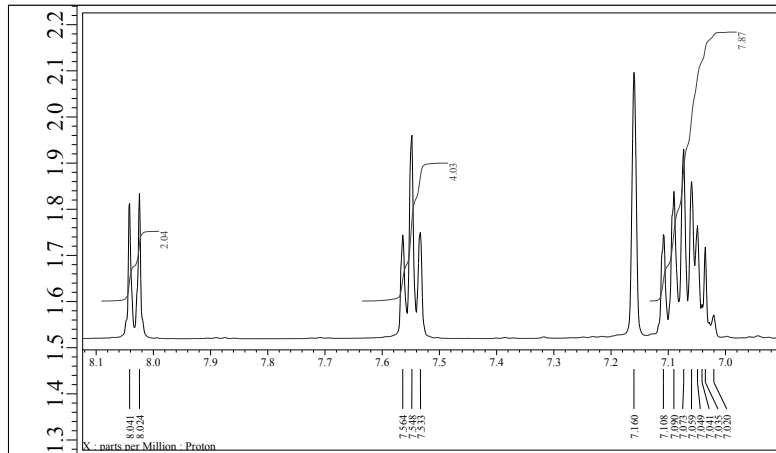
Filename           = YH(S-p-I)_31P_1Hdec
Author             = delta
Experiment         = single_pulse_decou
Sample_Id          = YH(S-p-I)
Solvent            = BENZENE-D6
Actual_Start_Time  = 3-APR-2020 19:12:
Revision_Time      = 7-APR-2020 12:32:

Comment           = single_pulse decou
Data_Format       = 1D REAL
Dim_Size          = 26214
X_Domain          = Phosphorus31
Dim_Title         = Phosphorus31
Dim_Units         = [ppm]
Dimensions        = X
Spectrometer      = JNM-ECZ500R/S1

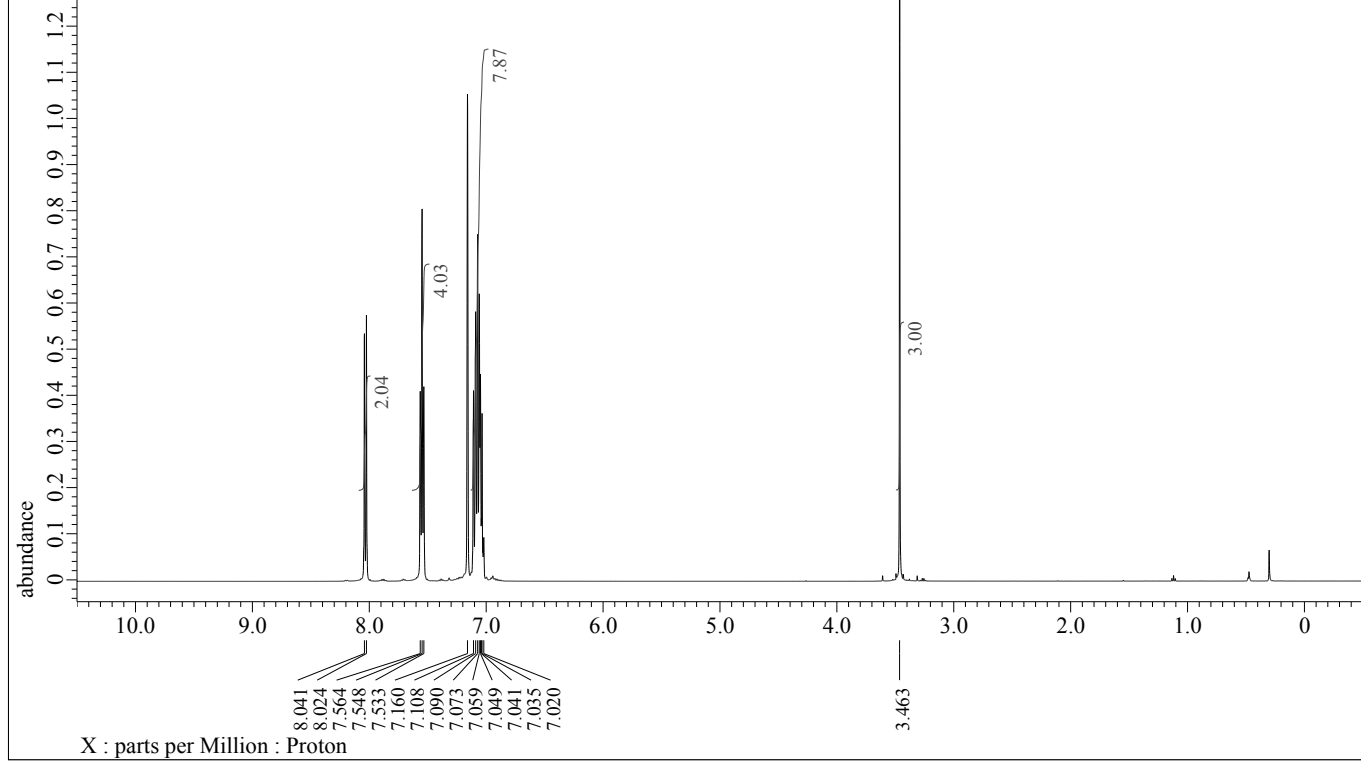
Field_Strength    = 11.62926421[T] (50
X_Acq_Duration    = 0.18874368[s]
X_Domain          = 31P
X_Freq            = 200.43293989[MHz]
X_Offset          = 0[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 5.29819065[Hz]
X_Sweep           = 173.61111111[kHz]
X_Sweep_Clippped = 138.88888889[kHz]
Irr_Domain        = Proton
Irr_Freq          = 495.13191398[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 64
Total_Scans       = 64

Relaxation_Delay  = 1[s]
Recvr_Gain        = 56
Temp_Get          = 20[dC]
X_90_Width        = 19.78[us]
X_Acq_Time        = 0.18874368[s]
X_Angle           = 30[deg]
X_Atn             = 9.4[dB]
X_Pulse           = 6.59333333[us]
Irr_Atn_Dec       = 23.948[dB]
Irr_Atn_Dec_Calc  = 23.948[dB]
Irr_Atn_Dec_Default_Calc = 23.948[dB]
Irr_Atn_Noise     = 23.948[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_Noise         = TRUE
Irr_Noise         = WALTZ

```

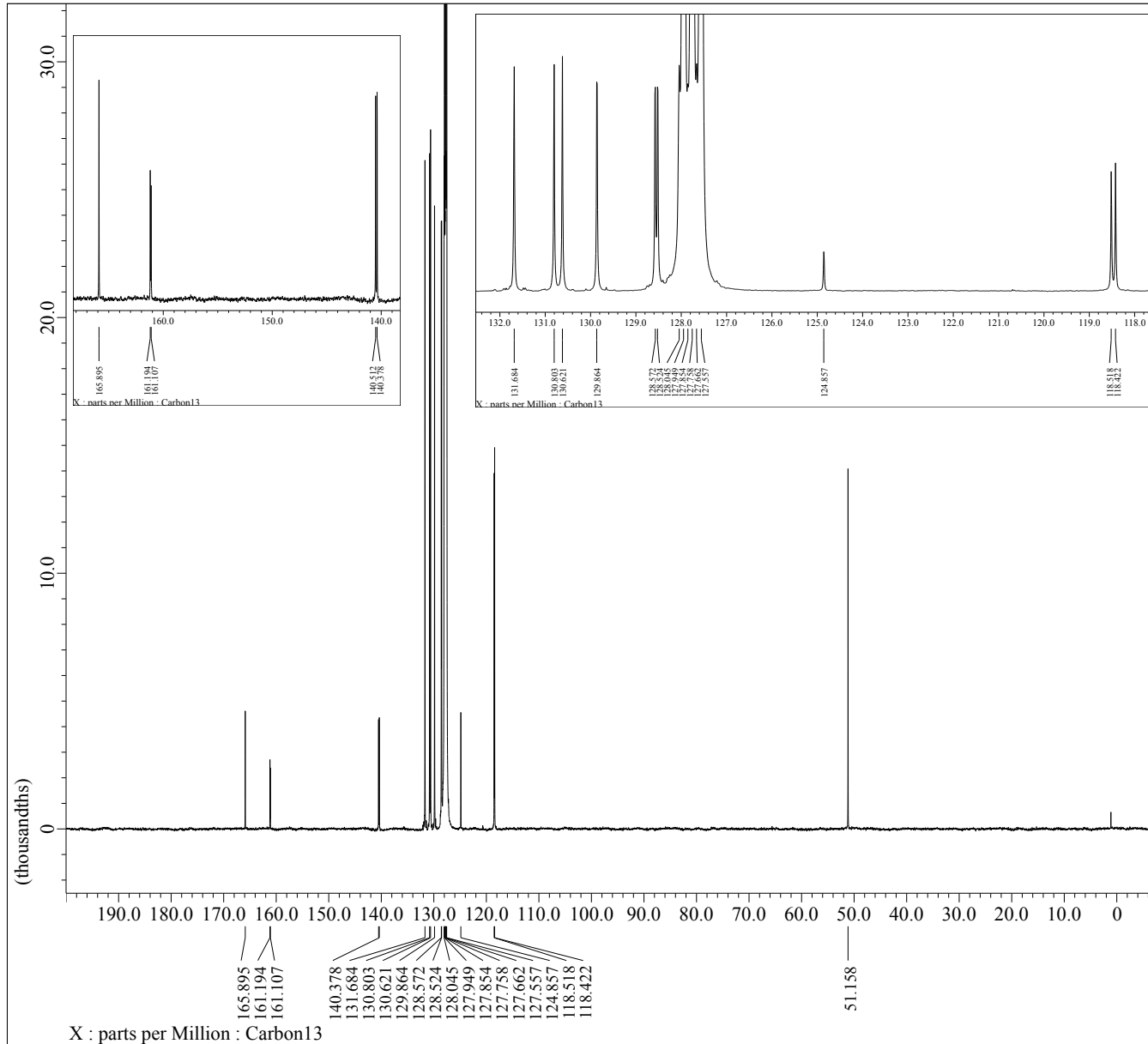


1i



---- PROCESSING PARAMETERS ----
 sexp(0.2[Hz], 0.0[s])
 trapezoid(0[%], 0[%], 80[%], 100[%])
 zerofill(1, TRUE)
 fft(1, TRUE, TRUE)
 machinephase
 ppm
 reference(7.09954[ppm], 7.16[ppm])
 Derived from: YH(CO2Me)_Proton-1-1.jdf

Filename = YH(CO2Me)_Proton-1-2.
 Author = delta
 Experiment = proton.jsp
 Sample_Id = YH(CO2Me)
 Solvent = BENZENE-D6
 Actual_Start_Time = 2-APR-2020 19:13:05
 Revision_Time = 7-APR-2020 10:13:17
 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_Clippped = 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]
 Recvr_Gain = 36
 Temp_Get = 20[dC]
 X_90_Width = 9.58[us]
 X_Acq_Time = 1.76422912[s]
 X_Angle = 45[deg]
 X_Atn = 4.3[dB]
 X_Pulse = 4.79[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]



---- PROCESSING PARAMETERS ----

```

sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
phase( -1.75, 0, 50[%] )
base_correct( Akima, 5, 0, FALSE, 3, None, FA
Derived from: YH(CO2Me)_Carbon-1-1.jdf

```

```

Filename      = YH(CO2Me)_Carbon-1
Author        = delta
Experiment    = carbon.jxp
Sample Id     = YH(CO2Me)
Solvent       = BENZENE-D6
Actual_Start_Time = 3-APR-2020 03:30:
Revision_Time = 9-APR-2020 13:42:

```

```

Comment       = single pulse decou
Data Format    = 1D REAL
Dim Size      = 26214
X Domain      = Carbon13
Dim Title     = Carbon13
Dim Units     = [ppm]
Dimensions    = X
Spectrometer  = JNM-ECZ500R/S1

```

```

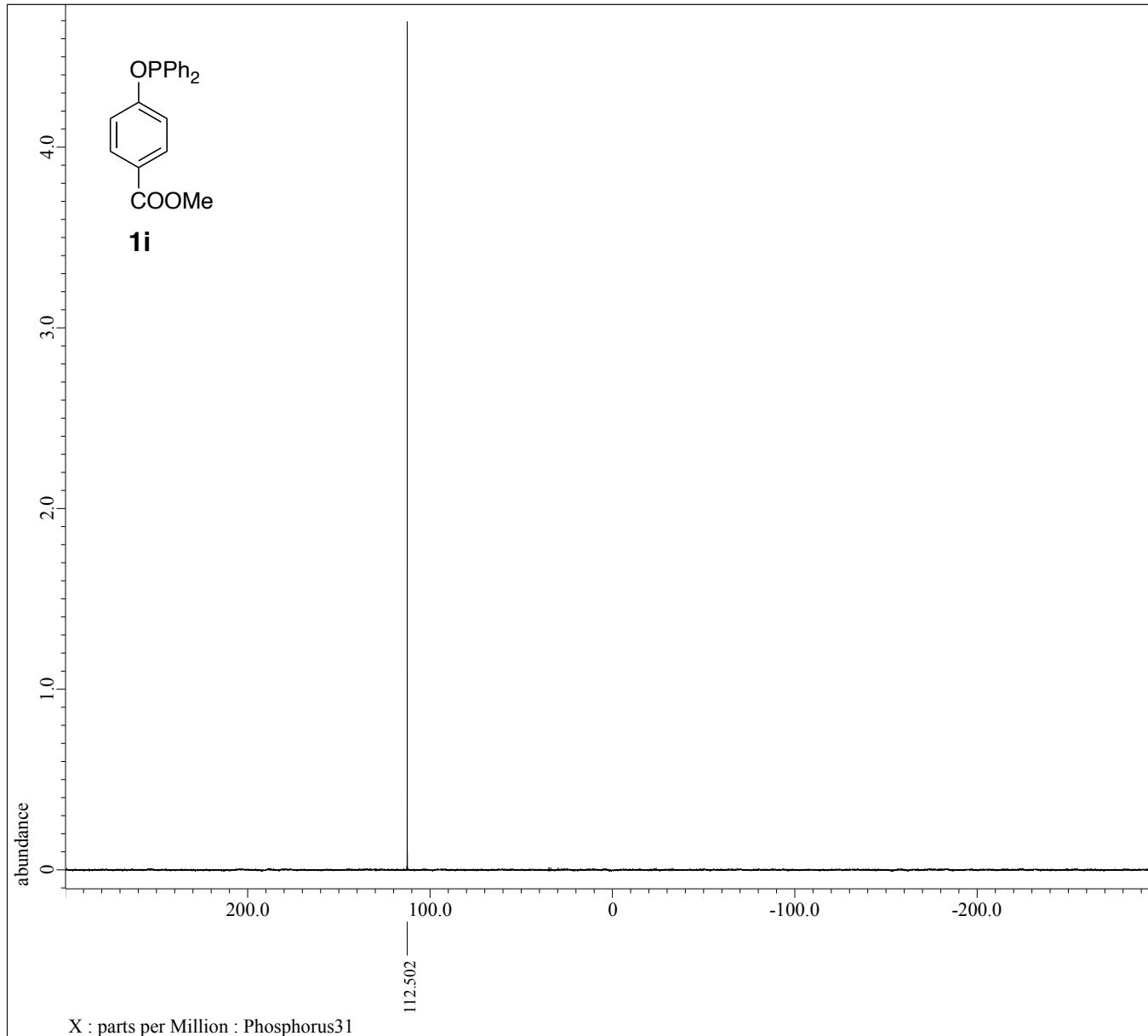
Field Strength = 11.62926421[T] (50
X Acq Duration = 0.8388608[s]
X Domain       = 13C
X Freq         = 124.5010059[MHz]
X Offset       = 100[ppm]
X Points       = 32768
X Prescans     = 4
X Resolution   = 1.1920929[Hz]
X Sweep        = 39.0625[kHz]
X Sweep Clipped = 31.25[kHz]
Irr Domain     = Proton
Irr Freq       = 495.13191398[MHz]
Irr Offset     = 5[ppm]
Clipped        = FALSE
Scans          = 5000
Total_Scans    = 5000

```

```

Relaxation_Delay = 2[s]
Recvr Gain       = 56
Temp_Get         = 20.7[dC]
X 90 Width      = 9.61[us]
X Acq Time       = 0.8388608[s]
X Angle         = 30[deg]
X Atn           = 10[dB]
X Pulse         = 3.20333333[us]
Irr Atn Dec     = 23.948[dB]
Irr Atn Dec Calc = 23.948[dB]
Irr Atn Dec Default_Calc = 23.948[dB]
Irr Atn Noe     = 23.948[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

```



```

---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
phase( -30, 0, 50[%] )
base_correct( Akima, 5, 0, FALSE, 3, None, FA
Derived from: YH(CO2Me)_31P_1Hdec-1-1.jdf

```

```

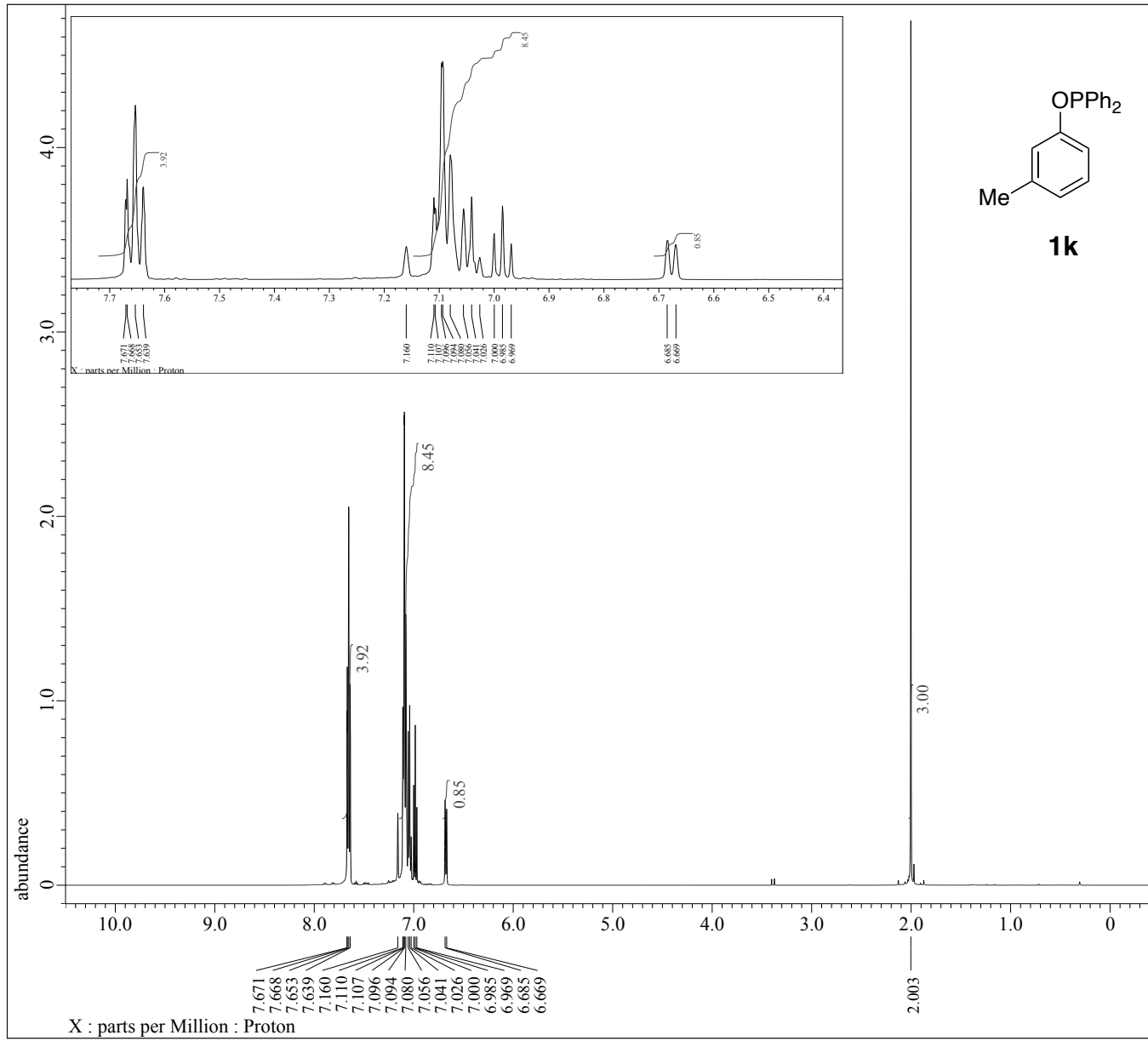
Filename           = YH(CO2Me)_31P_1Hdec
Author             = delta
Experiment         = single_pulse_decou
Sample_Id          = YH(CO2Me)
Solvent            = BENZENE-D6
Actual_Start_Time  = 2-APR-2020 19:16:
Revision_Time      = 7-APR-2020 12:50:

Comment           = single_pulse decou
Data_Format       = 1D REAL
Dim_Size          = 26214
X_Domain          = Phosphorus31
Dim_Title         = Phosphorus31
Dim_Units         = [ppm]
Dimensions        = X
Spectrometer      = JNM-ECZ500R/S1

Field_Strength    = 11.62926421[T] (50
X_Acq_Duration    = 0.18874368[s]
X_Domain          = 31P
X_Freq            = 200.43293989[MHz]
X_Offset          = 0[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 5.29819065[Hz]
X_Sweep           = 173.61111111[kHz]
X_Sweep_Clippped = 138.88888889[kHz]
Irr_Domain        = Proton
Irr_Freq          = 495.13191398[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans              = 64
Total_Scans       = 64

Relaxation_Delay  = 1[s]
Recvr_Gain        = 66
Temp_Get          = 20[dC]
X_90_Width        = 19.78[us]
X_Acq_Time        = 0.18874368[s]
X_Angle           = 30[deg]
X_Atn             = 9.4[dB]
X_Pulse           = 6.59333333[us]
Irr_Atn_Dec       = 23.948[dB]
Irr_Atn_Dec_Calc = 23.948[dB]
Irr_Atn_Dec_Default_Calc = 23.948[dB]
Irr_Atn_Noise    = 23.948[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_Noise        = TRUE
Irr_Noise        = WALTZ

```



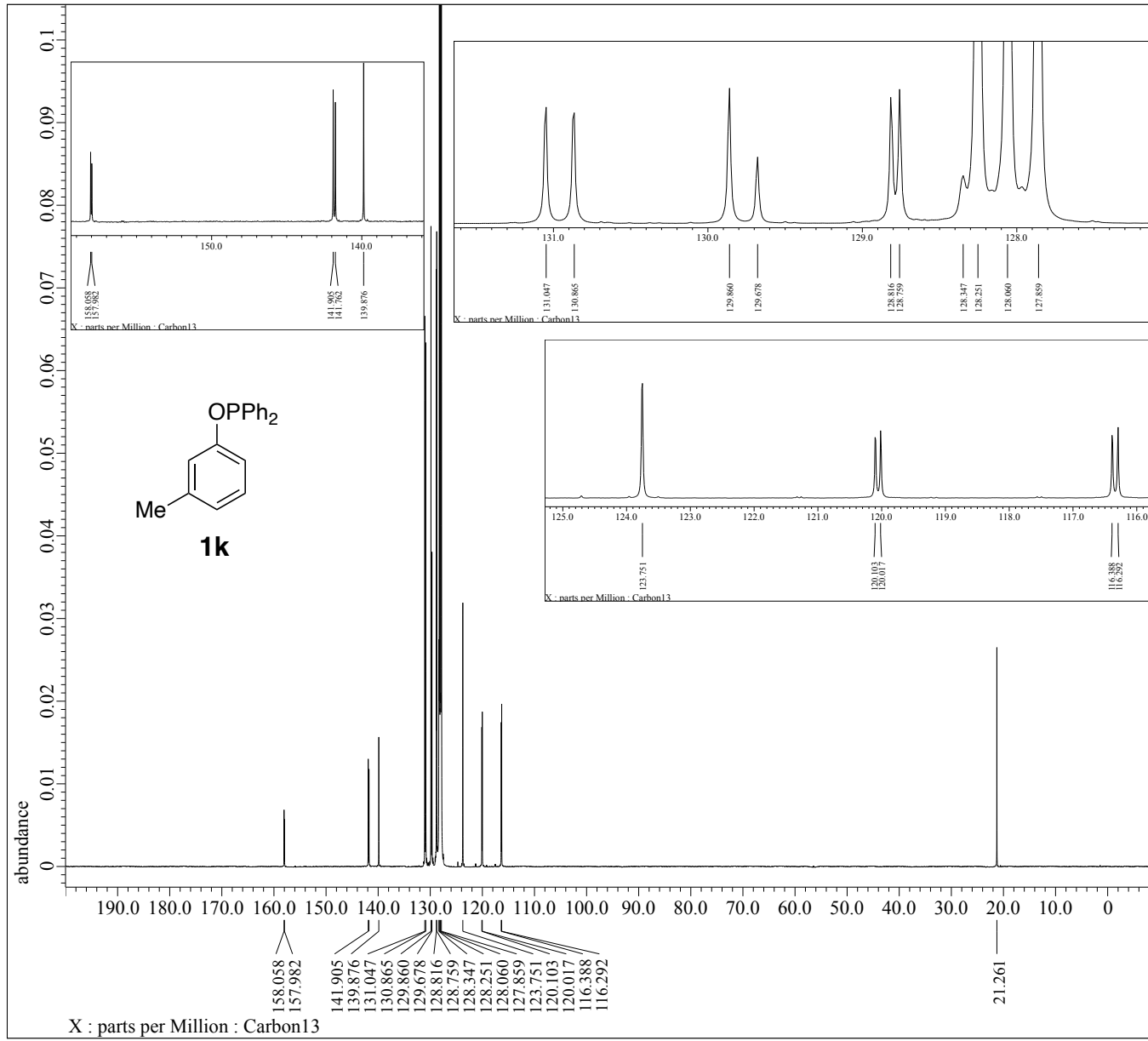
---- PROCESSING PARAMETERS ----
 sexp(0.2[Hz], 0.0[s])
 trapezoid(0[%], 0[%], 80[%], 100[%])
 zerofill(1, TRUE)
 fft(1, TRUE, TRUE)
 machinephase
 ppm
 base_correct(Akima, 5, 0, FALSE, 3, None, FA
 Derived from: YH(S-m-Me)_Proton-1-1.jdf

Filename = YH(S-m-Me)_Proton-1-4
 Author = delta
 Experiment = proton.jxp
 Sample_Id = YH(S-m-Me)
 Solvent = BENZENE-D6
 Actual_Start_Time = 2-APR-2020 04:26:51
 Revision_Time = 7-APR-2020 12:28:56

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_Clippped = 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]
 Recvr_Gain = 36
 Temp_Get = 20.8 [dC]
 X_90_Width = 9.58 [us]
 X_Acq_Time = 1.76422912 [s]
 X_Angle = 45 [deg]
 X_Atn = 4.3 [dB]
 X_Pulse = 4.79 [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]



```

---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
phase( -1.25, 0, 50[%] )
base_correct( Akima, 5, 0, FALSE, 3, None, FA
reference( 127.75783[ppm], 128.06[ppm] )

Derived from: YH(S-m-Me)_Carbon-1-1.jdf

```

```

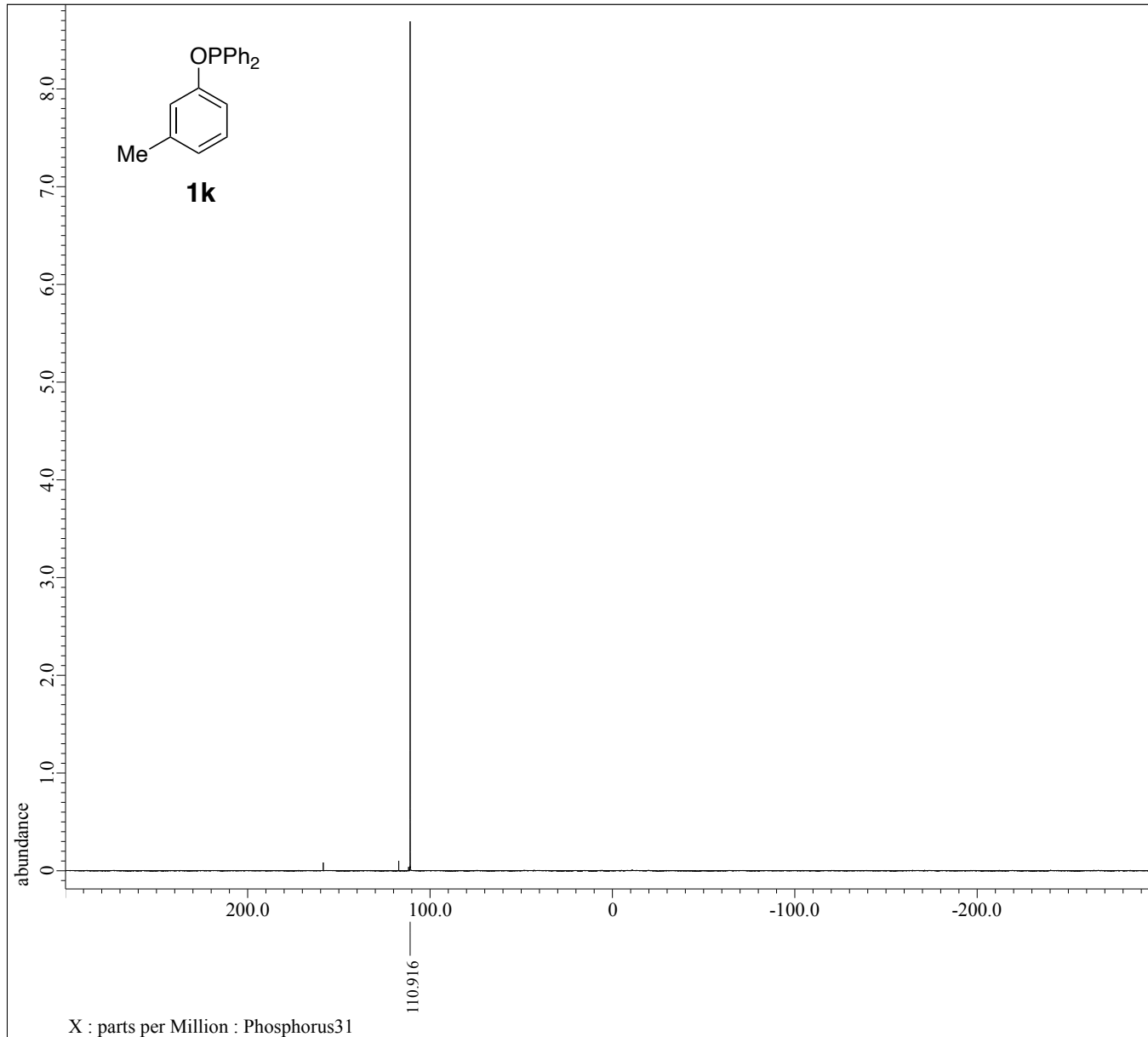
Filename      = YH(S-m-Me)_Carbon-
Author        = delta
Experiment    = carbon.jxp
Sample_Id     = YH(S-m-Me)
Solvent       = BENZENE-D6
Actual_Start_Time = 3-APR-2020 07:33:
Revision_Time  = 9-APR-2020 13:49:

Comment       = single pulse decou
Data Format    = 1D REAL
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_Clippped = 31.25[kHz]
Irr_Domain     = Proton
Irr_Freq       = 495.13191398[MHz]
Irr_Offset     = 5[ppm]
Clipped        = FALSE
Scans          = 5000
Total_Scans    = 5000

Relaxation_Delay = 2[s]
Recvr Gain       = 56
Temp_Get         = 20.4[dC]
X_90_Width      = 9.61[us]
X_Acq_Time      = 0.8388608[s]
X_Angle         = 30[deg]
X_Atn           = 10[dB]
X_Pulse         = 3.20333333[us]
Irr_Atn_Dec     = 23.948[dB]
Irr_Atn_Dec_Calc = 23.948[dB]
Irr_Atn_Dec_Default_Calc = 23.948[dB]
Irr_Atn_Noise   = 23.948[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_Noise       = TRUE
Irr_Noise       = WALTZ

```



```

---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
phase( 4, 0, 50[%] )
base_correct( Akima, 5, 0, FALSE, 3, None, FA
Derived from: YH(S-m-Me)_31P_1Hdec-1-1.jdf

```

```

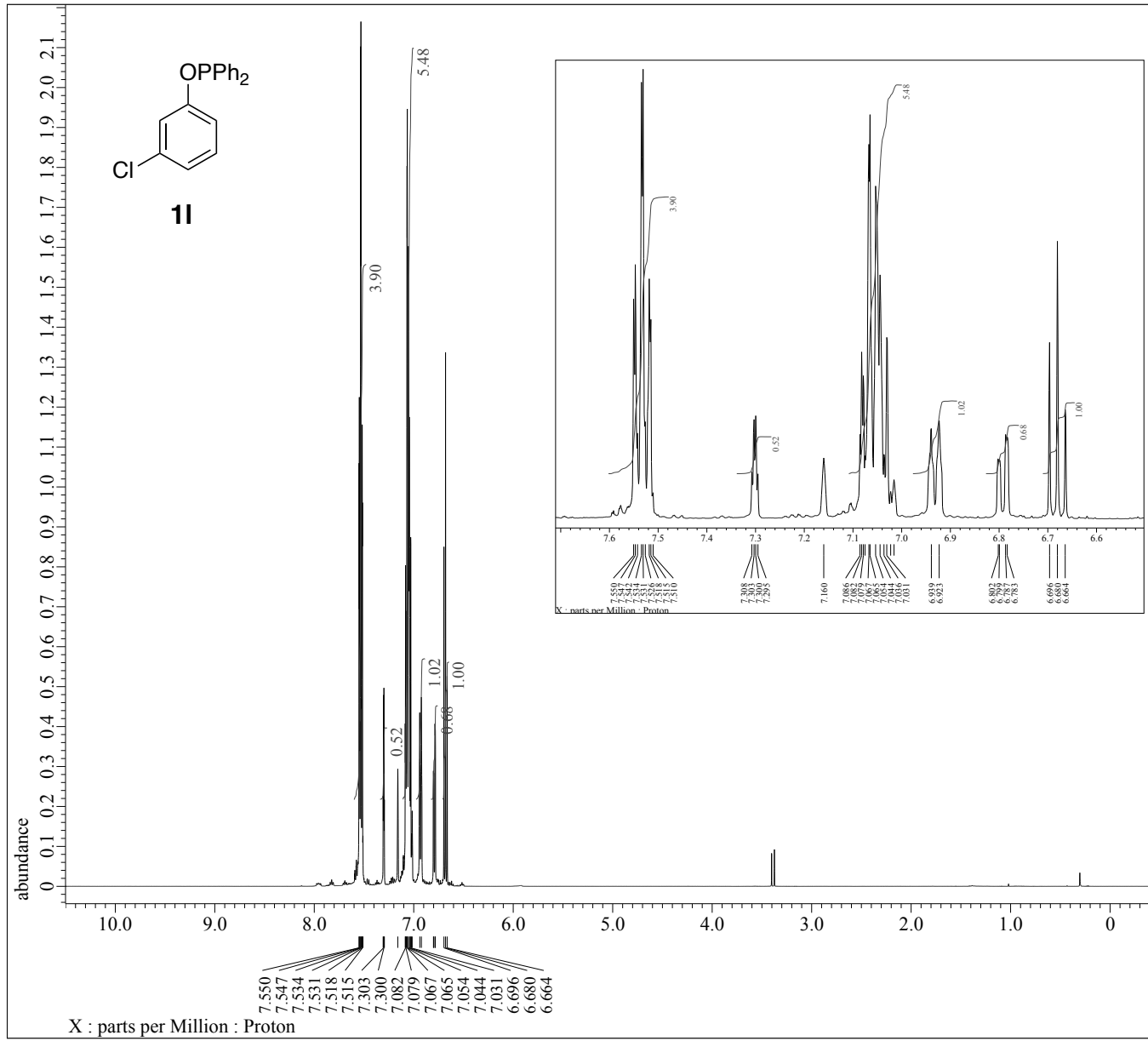
Filename           = YH(S-m-Me)_31P_1Hd
Author             = delta
Experiment         = single_pulse_decou
Sample_Id          = YH(S-m-Me)
Solvent            = BENZENE-D6
Actual_Start_Time  = 2-APR-2020 11:47:
Revision_Time      = 7-APR-2020 12:44:

Comment           = single_pulse decou
Data_Format       = 1D REAL
Dim_Size          = 26214
X_Domain          = Phosphorus31
Dim_Title         = Phosphorus31
Dim_Units         = [ppm]
Dimensions        = X
Spectrometer      = JNM-ECZ500R/S1

Field_Strength    = 11.62926421[T] (50
X_Acq_Duration    = 0.18874368[s]
X_Domain          = 31P
X_Freq            = 200.43293989[MHz]
X_Offset          = 0[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 5.29819065[Hz]
X_Sweep           = 173.61111111[kHz]
X_Sweep_Clipped   = 138.88888889[kHz]
Irr_Domain        = Proton
Irr_Freq          = 495.13191398[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 64
Total_Scans       = 64

Relaxation_Delay  = 1[s]
Recvr_Gain        = 66
Temp_Get          = 20.3[dC]
X_90_Width        = 19.78[us]
X_Acq_Time        = 0.18874368[s]
X_Angle           = 30[deg]
X_Atn             = 9.4[dB]
X_Pulse           = 6.59333333[us]
Irr_Atn_Dec       = 23.948[dB]
Irr_Atn_Dec_Calc  = 23.948[dB]
Irr_Atn_Dec_Default_Calc = 23.948[dB]
Irr_Atn_Noise     = 23.948[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_Noise         = TRUE
Irr_Noise         = WALTZ

```

```

---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
reference( 7.0961[ppm], 7.16[ppm] )
base_correct( Akima, 5, 0, FALSE, 3, None, FA
Derived from: YH(S-m-Cl)_Proton-1-1.jdf

```

```

Filename      = YH(S-m-Cl)_Proton-1-2
Author       = delta
Experiment   = proton.jxp
Sample_Id    = YH(S-m-Cl)
Solvent      = BENZENE-D6
Actual_Start_Time = 2-APR-2020 04:12:54
Revision_Time   = 7-APR-2020 10:10:10

```

```

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

```

```

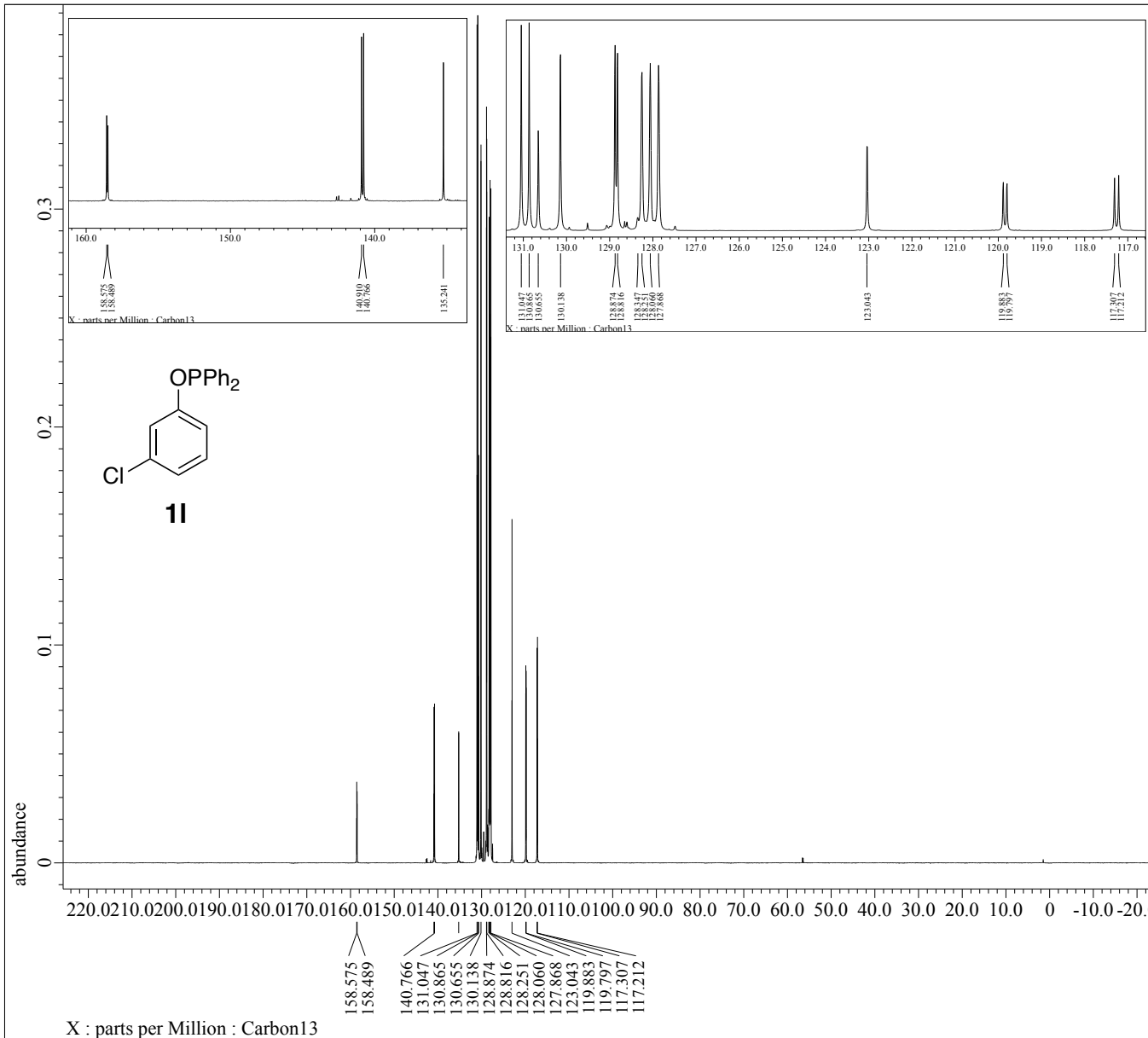
Field Strength = 11.62926421[T] (500[M]
X_Acq_Duration = 1.76422912[s]
X_Domain       = 1H
X_Freq         = 495.13191398[MHz]
X_Offset       = 5[ppm]
X_Points       = 16384
X_Prescans     = 1
X_Resolution   = 0.5668198[Hz]
X_Sweep        = 9.28677563[kHz]
X_Sweep_Clippped = 7.42942051[kHz]
Irr_Domain     = 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

```

```

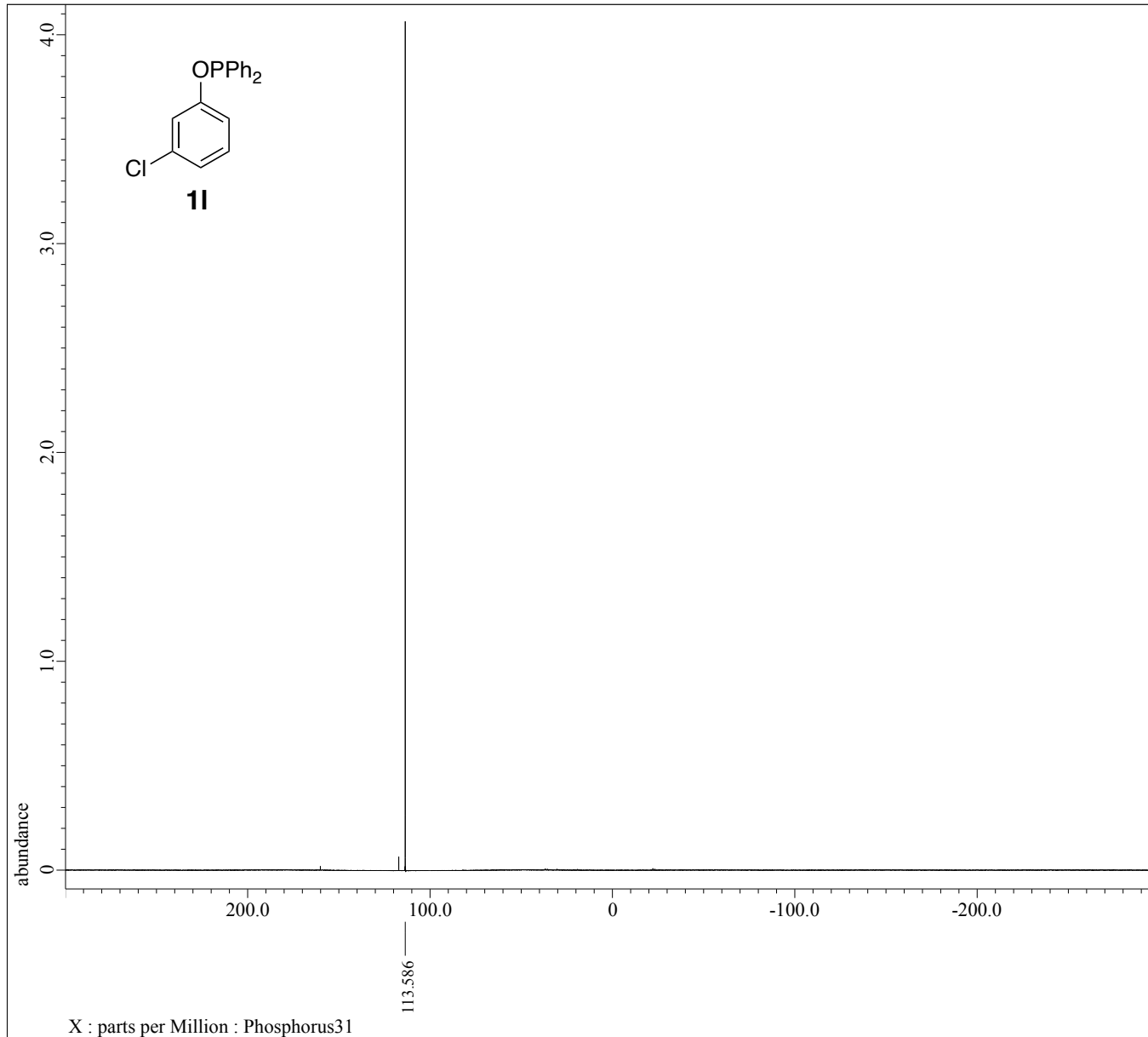
Relaxation_Delay = 5[s]
Recvr_Gain       = 36
Temp_Get         = 21.3[dC]
X_90_Width       = 9.58[us]
X_Acq_Time       = 1.76422912[s]
X_Angle          = 45[deg]
X_Atn           = 4.3[dB]
X_Pulse         = 4.79[us]
Irr_Mode        = Off
Tri_Mode        = Off
Dante_Loop      = FALSE
Dante_Presat    = FALSE
Decimation_Rate = 0
Initial_Wait    = 1[s]
Phase           = {0, 90, 270, 180, 180}
Presat_Time     = 5[s]

```



---- PROCESSING PARAMETERS ----
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
phase(2.72465, 0, 50[%])
base_correct(Akima, 5, 0, FALSE, 3, None, FA
Derived from: YH(m-Cl-2)_Carbon-1-1.jdf

Filename = YH(m-Cl-2)_Carbon-
Author = delta
Experiment = carbon.jxp
Sample_Id = YH(m-Cl-2)
Solvent = BENZENE-D6
Actual_Start_Time = 7-APR-2020 01:00:
Revision_Time = 9-APR-2020 13:40:
Comment = single pulse decou
Data_Format = 1D REAL
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_Clippped = 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]
Recvr_Gain = 56
Temp_Get = 21.2[dC]
X_90_Width = 9.61[us]
X_Acq_Time = 0.8388608[s]
X_Angle = 30[deg]
X_Atn = 10[dB]
X_Pulse = 3.20333333[us]
Irr_Atn_Dec = 23.948[dB]
Irr_Atn_Dec_Calc = 23.948[dB]
Irr_Atn_Dec_Default_Calc = 23.948[dB]
Irr_Atn_No = 23.948[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_No = TRUE
Irr_Noise = WALTZ



```

---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
phase( 1, 0, 50[%] )

Derived from: YH(S-m-Cl)_31P_1Hdec-1-1.jdf

```

```

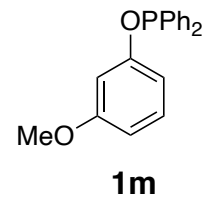
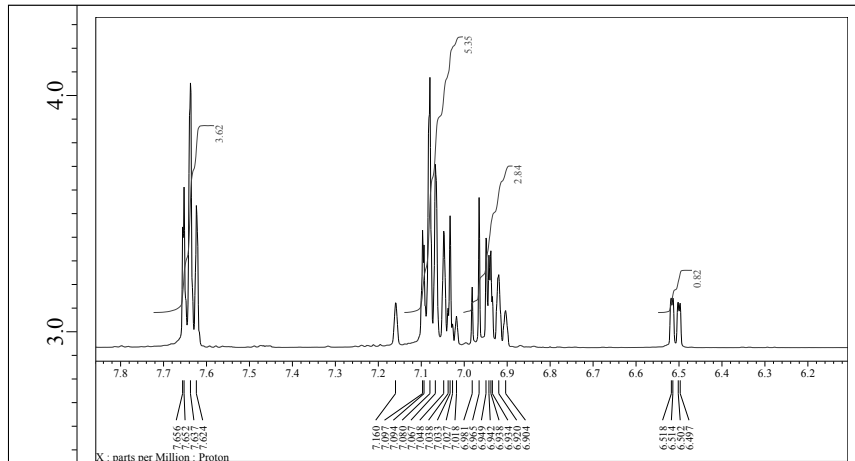
Filename           = YH(S-m-Cl)_31P_1Hd
Author             = delta
Experiment         = single_pulse_decou
Sample_Id          = YH(S-m-Cl)
Solvent            = BENZENE-D6
Actual_Start_Time  = 2-APR-2020 11:25:
Revision_Time      = 7-APR-2020 12:46:

Comment           = single_pulse decou
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
X_Domain          = Phosphorus31
Dim_Title         = Phosphorus31
Dim_Units         = [ppm]
Dimensions        = X
Spectrometer      = JNM-ECZ500R/S1

Field_Strength    = 11.62926421[T] (50
X_Acq_Duration    = 0.18874368[s]
X_Domain          = 31P
X_Freq            = 200.43293989[MHz]
X_Offset          = 0[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 5.29819065[Hz]
X_Sweep           = 173.61111111[kHz]
X_Sweep_Clipped   = 138.88888889[kHz]
Irr_Domain        = Proton
Irr_Freq          = 495.13191398[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 64
Total_Scans       = 64

Relaxation_Delay  = 1[s]
Recvr_Gain        = 56
Temp_Get          = 20.4[dC]
X_90_Width        = 19.78[us]
X_Acq_Time        = 0.18874368[s]
X_Angle           = 30[deg]
X_Atn             = 9.4[dB]
X_Pulse           = 6.59333333[us]
Irr_Atn_Dec       = 23.948[dB]
Irr_Atn_Dec_Calc = 23.948[dB]
Irr_Atn_Dec_Default_Calc = 23.948[dB]
Irr_Atn_Noise     = 23.948[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_Noise         = TRUE
Irr_Noise         = WALTZ

```



```

---- 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
Derived from: YH(S-m-OMe)_Proton-1-1.jdf

```

```

Filename      = YH(S-m-OMe)_Proton-1-
Author       = delta
Experiment   = proton.jxp
Sample Id    = YH(S-m-OMe)
Solvent      = BENZENE-D6
Actual_Start_Time = 7-APR-2020 19:20:09
Revision_Time   = 7-APR-2020 20:38:20

```

```

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

```

```

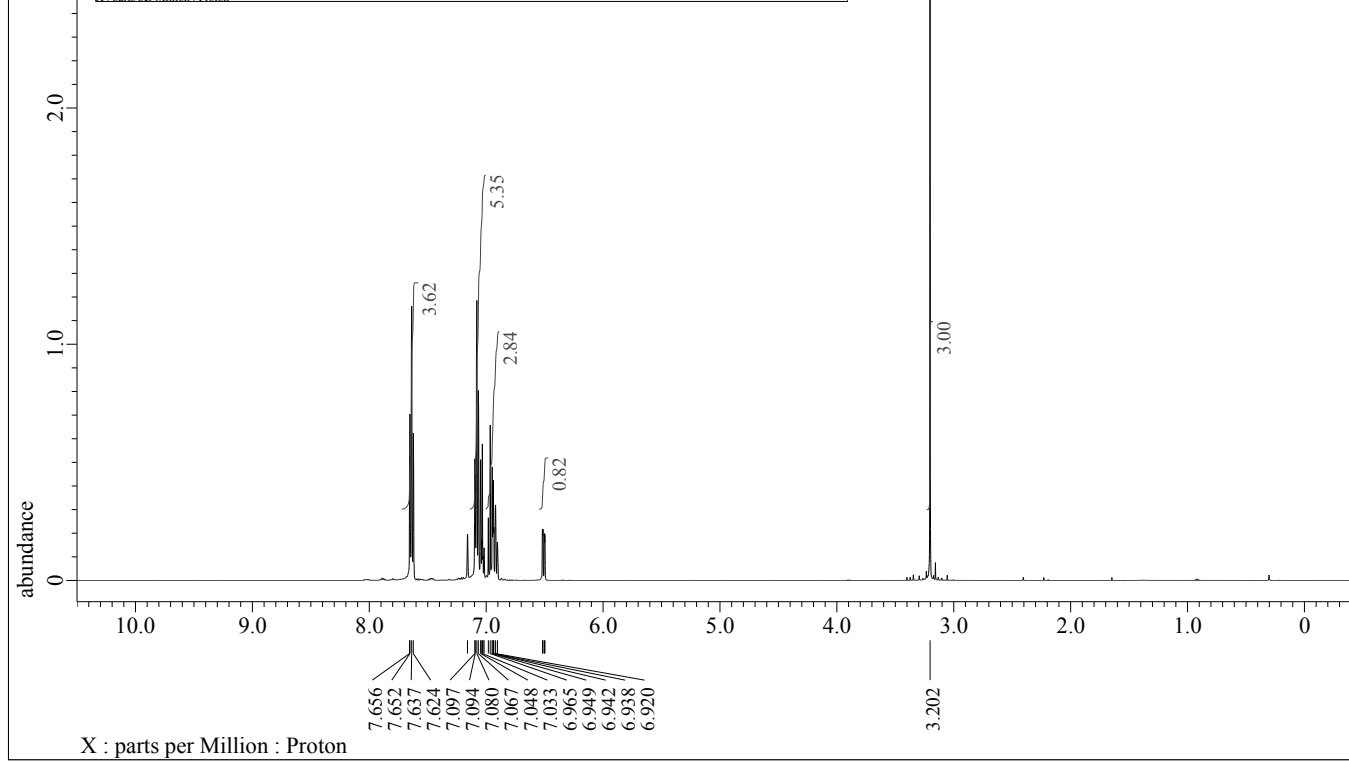
Field Strength = 11.62926421[T] (500[M]
X Acq Duration = 1.76422912[s]
X Domain       = 1H
X Freq         = 495.13191398[MHz]
X Offset       = 5[ppm]
X Points       = 16384
X Prescans     = 1
X Resolution   = 0.5668198 [Hz]
X Sweep       = 9.28677563 [kHz]
X Sweep Clipped = 7.42942051 [kHz]
Irr Domain     = Proton
Irr Freq       = 495.13191398[MHz]
Irr Offset     = 5[ppm]
Tri Domain     = Proton
Tri Freq       = 495.13191398[MHz]
Tri Offset     = 5[ppm]
Clipped        = FALSE
Scans          = 8
Total_Scans    = 8

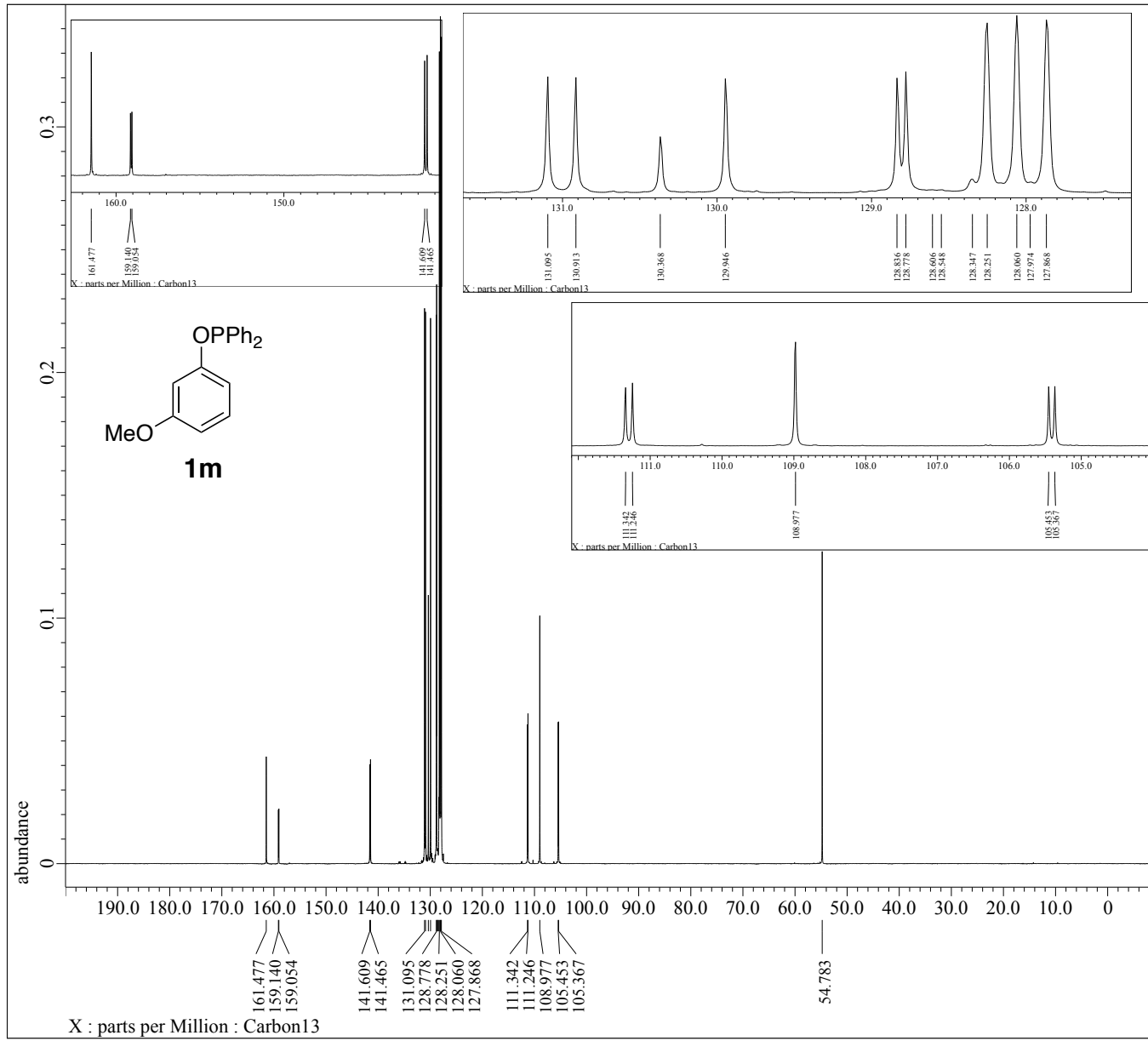
```

```

Relaxation_Delay = 5[s]
Recvr Gain       = 36
Temp_Get         = 20.2 [dC]
X 90 Width      = 9.58 [us]
X Acq Time       = 1.76422912[s]
X Angle         = 45 [deg]
X Atn           = 4.3 [dB]
X Pulse         = 4.79 [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]

```





```

---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
phase( -2, 0, 50[%] )
base_correct( Akima, 5, 0, FALSE, 3, None, FA
Derived from: YH(S-m-OMe)-c_Carbon-1-1.jdf

```

```

Filename      = YH(S-m-OMe)-c_Carb
Author        = delta
Experiment    = carbon.jxp
Sample_Id     = YH(S-m-OMe)-c
Solvent       = BENZENE-D6
Actual_Start_Time = 8-APR-2020 00:05:
Revision_Time = 9-APR-2020 14:15:

```

```

Comment      = single pulse decou
Data Format   = 1D REAL
Dim Size     = 26214
X Domain     = Carbon13
Dim Title    = Carbon13
Dim Units    = [ppm]
Dimensions   = X
Spectrometer = JNM-ECZ500R/S1

```

```

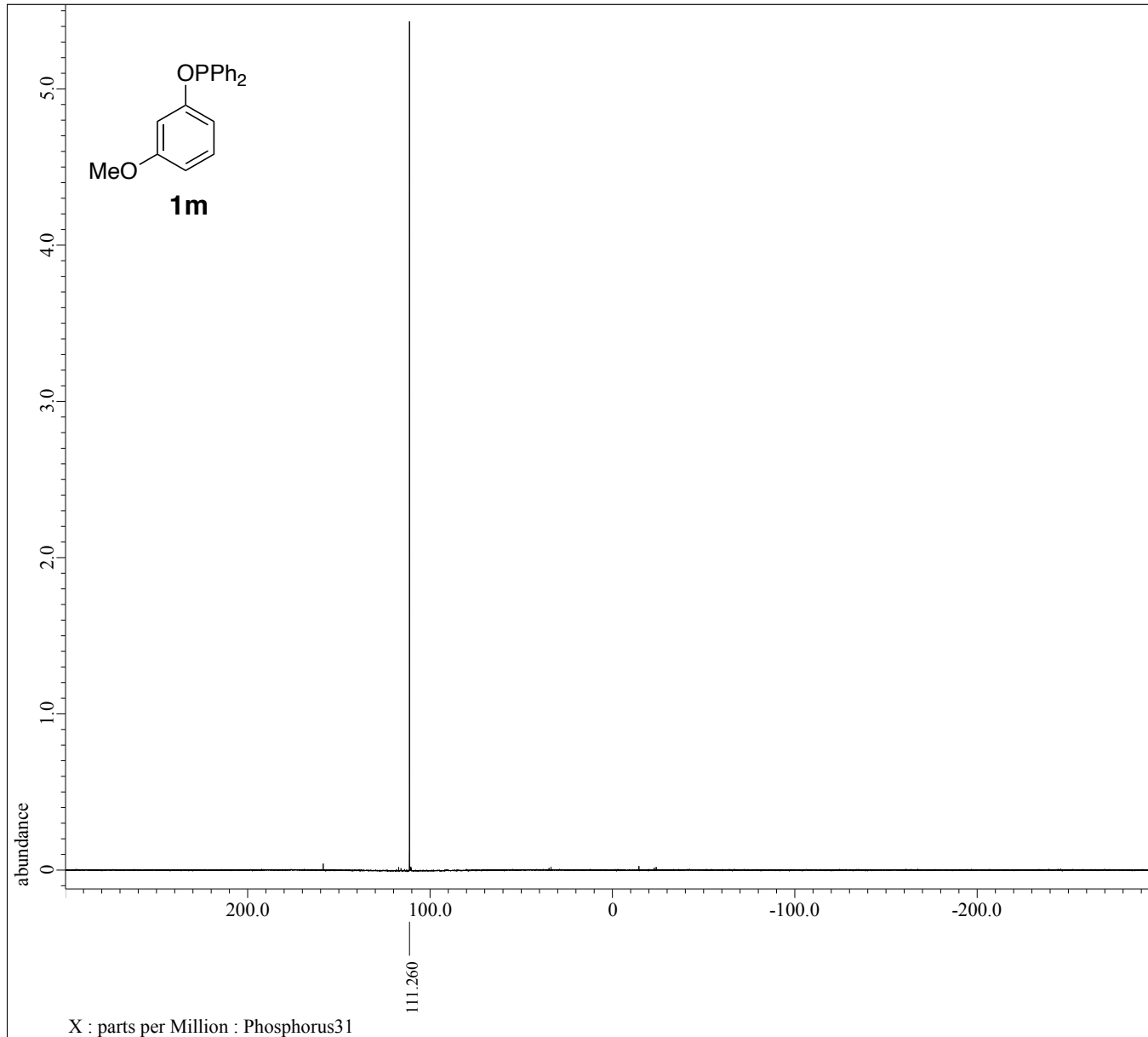
Field Strength = 11.62926421[T] (50
X Acq Duration = 0.8388608[s]
X Domain       = 13C
X Freq         = 124.5010059[MHz]
X Offset       = 100[ppm]
X Points       = 32768
X Prescans     = 4
X Resolution   = 1.1920929[Hz]
X Sweep        = 39.0625[kHz]
X Sweep Clipped = 31.25[kHz]
Irr Domain     = Proton
Irr Freq       = 495.13191398[MHz]
Irr Offset     = 5[ppm]
Clipped        = FALSE
Scans          = 1000
Total_Scans    = 1000

```

```

Relaxation_Delay = 2[s]
Recvr Gain        = 56
Temp_Get          = 20.7[dC]
X 90_Width       = 9.61[us]
X Acq Time        = 0.8388608[s]
X Angle           = 30[deg]
X Atn             = 10[dB]
X Pulse           = 3.20333333[us]
Irr Atn Dec       = 23.948[dB]
Irr Atn Dec Calc  = 23.948[dB]
Irr Atn Dec Default_Calc = 23.948[dB]
Irr Atn Noe       = 23.948[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

```



```

---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
phase( -89.40637, 0, 50[%] )

Derived from: YH(S-m-OMe)_31P_1Hdec-1-1.jdf

```

```

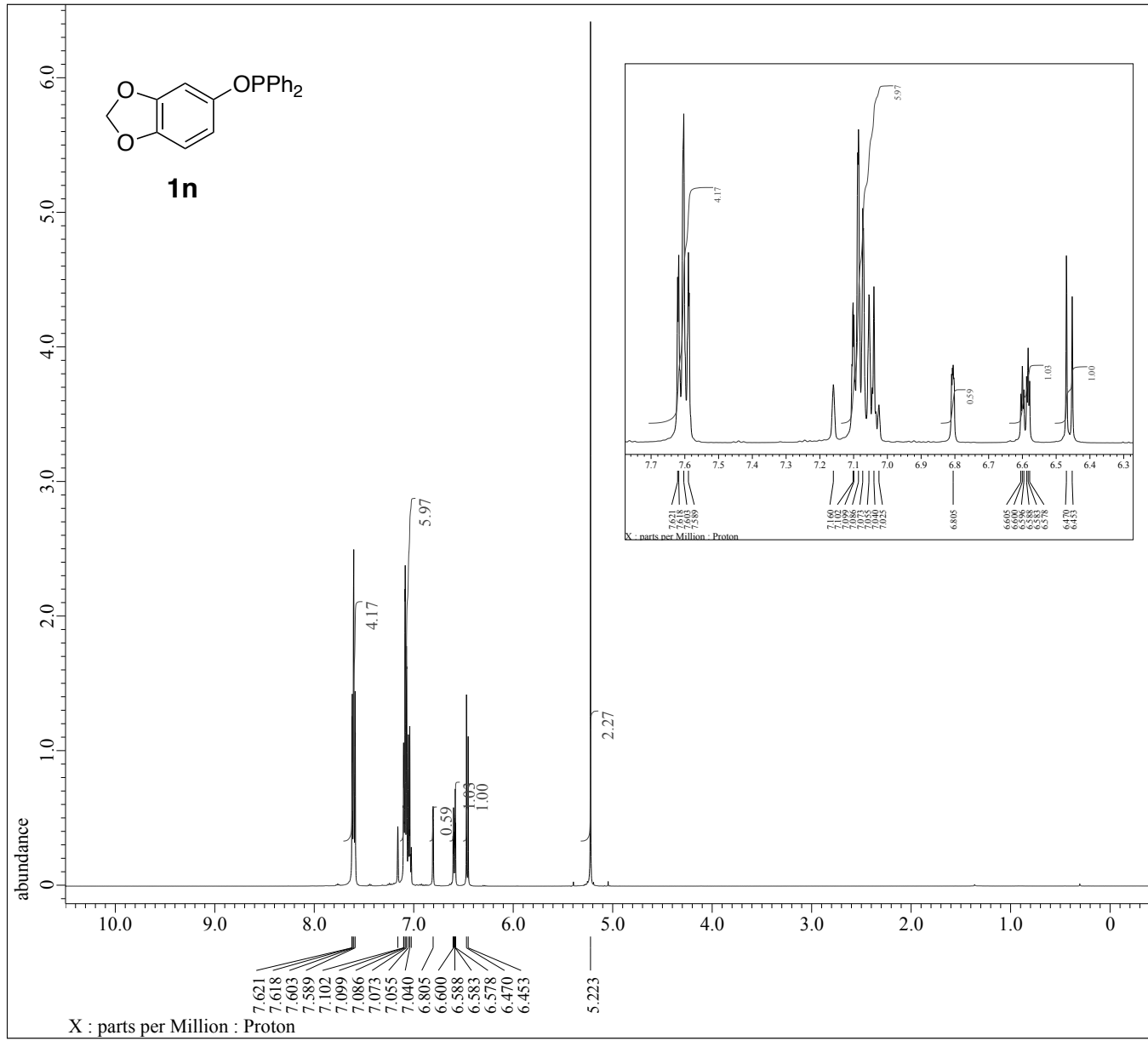
Filename           = YH(S-m-OMe)_31P_1H
Author             = delta
Experiment         = single_pulse_decou
Sample_Id          = YH(S-m-OMe)
Solvent            = BENZENE-D6
Actual_Start_Time  = 7-APR-2020 22:12:
Revision_Time      = 8-APR-2020 11:51:

Comment           = single_pulse decou
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
X_Domain          = Phosphorus31
Dim_Title         = Phosphorus31
Dim_Units         = [ppm]
Dimensions        = X
Spectrometer      = JNM-ECZ500R/S1

Field_Strength    = 11.62926421[T] (50
X_Acq_Duration    = 0.18874368[s]
X_Domain          = 31P
X_Freq            = 200.43293989[MHz]
X_Offset          = 0[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 5.29819065[Hz]
X_Sweep           = 173.61111111[kHz]
X_Sweep_Clippped = 138.88888889[kHz]
Irr_Domain        = Proton
Irr_Freq          = 495.13191398[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 64
Total_Scans       = 64

Relaxation_Delay  = 1[s]
Recvr_Gain        = 66
Temp_Get          = 20.5[dC]
X_90_Width        = 19.78[us]
X_Acq_Time        = 0.18874368[s]
X_Angle           = 30[deg]
X_Atn             = 9.4[dB]
X_Pulse           = 6.59333333[us]
Irr_Atn_Dec       = 23.948[dB]
Irr_Atn_Dec_Calc = 23.948[dB]
Irr_Atn_Dec_Default_Calc = 23.948[dB]
Irr_Atn_Noise     = 23.948[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_Noise         = TRUE
Irr_Noise         = WALTZ

```



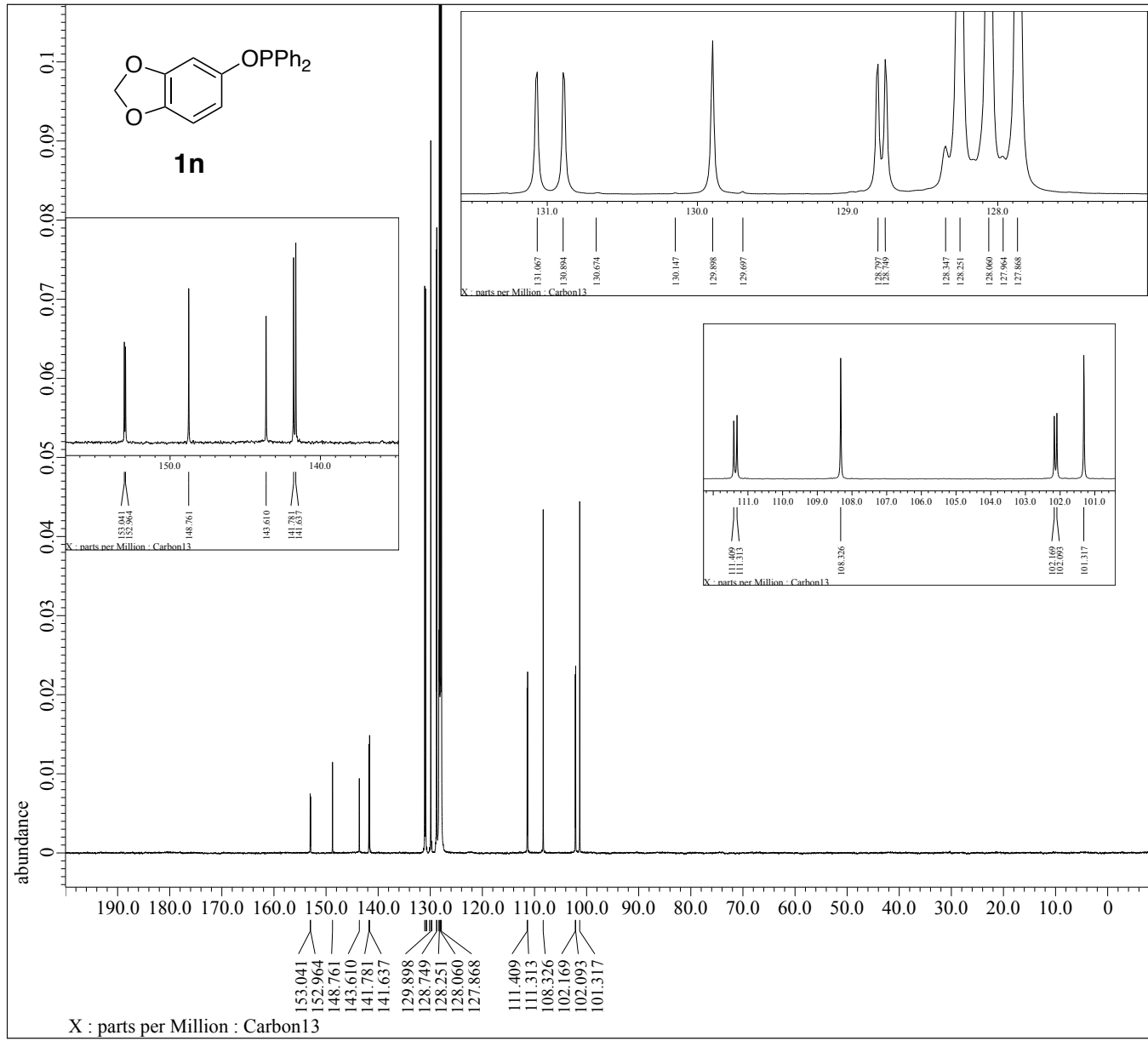
---- PROCESSING PARAMETERS ----
 sexp(0.2[Hz], 0.0[s])
 trapezoid(0[%], 0[%], 80[%], 100[%])
 zerofill(1, TRUE)
 fft(1, TRUE, TRUE)
 machinephase
 ppm
 Derived from: YH(OMO)_Proton-1-1.jdf

Filename = YH(OMO)_Proton-1-2.jd
 Author = delta
 Experiment = proton.jxp
 Sample Id = YH(OMO)
 Solvent = BENZENE-D6
 Actual_Start_Time = 6-APR-2020 22:17:15
 Revision_Time = 7-APR-2020 10:19:25

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 = 8
 Total_Scans = 8

Relaxation_Delay = 5[s]
 Recvr Gain = 36
 Temp_Get = 21.4 [dC]
 X 90 Width = 9.58 [us]
 X Acq Time = 1.76422912 [s]
 X Angle = 45 [deg]
 X Atn = 4.3 [dB]
 X Pulse = 4.79 [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]



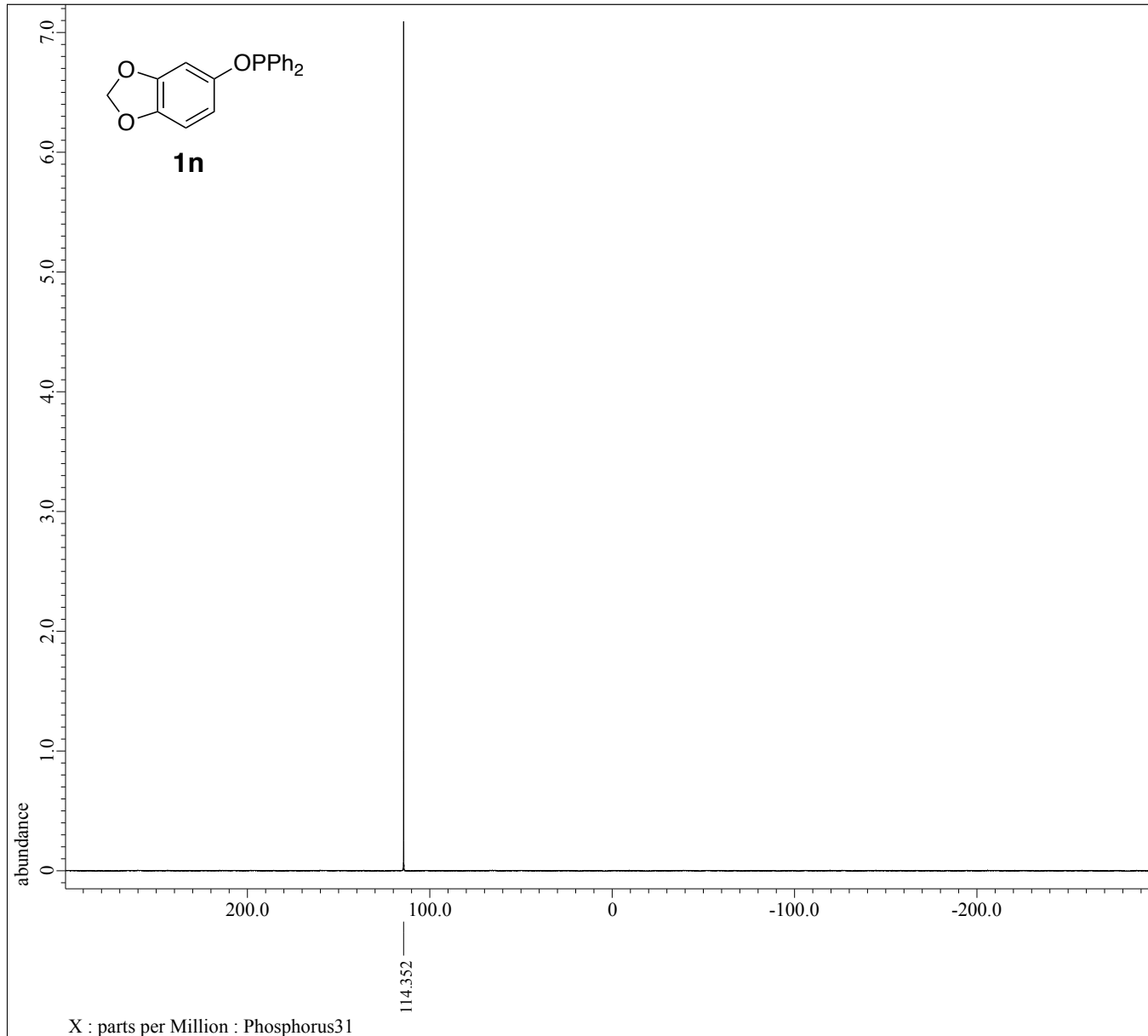
---- PROCESSING PARAMETERS ----
 sexp(2.0[Hz], 0.0[s])
 trapezoid(0[%], 0[%], 80[%], 100[%])
 zerofill(1, TRUE)
 fft(1, TRUE, TRUE)
 machinephase
 ppm
 phase(-1.25, 0, 50[%])
 base_correct(Akima, 5, 0, FALSE, 3, None, FA)
 Derived from: YH(OMO)_Carbon-1-1.jdf

Filename = YH(OMO)_Carbon-1-2
 Author = delta
 Experiment = carbon.jxp
 Sample_Id = YH(OMO)
 Solvent = BENZENE-D6
 Actual_Start_Time = 7-APR-2020 00:06:
 Revision_Time = 9-APR-2020 13:36:

Comment = single pulse decou
 Data Format = 1D REAL
 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_Clippped = 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]
 Recvr_Gain = 56
 Temp_Get = 20.9[dC]
 X_90_Width = 9.61[us]
 X_Acq_Time = 0.8388608[s]
 X_Angle = 30[deg]
 X_Atn = 10[dB]
 X_Pulse = 3.20333333[us]
 Irr_Atn_Dec = 23.948[dB]
 Irr_Atn_Dec_Calc = 23.948[dB]
 Irr_Atn_Dec_Default_Calc = 23.948[dB]
 Irr_Atn_Noise = 23.948[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_Noise = TRUE
 Irr_Noise = WALTZ



```

---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
phase( -43.60394, 0, 50[%] )
base_correct( Akima, 5, 0, FALSE, 3, None, FA
Derived from: YH(S-OMO)_31P_1Hdec-1-1.jdf

```

```

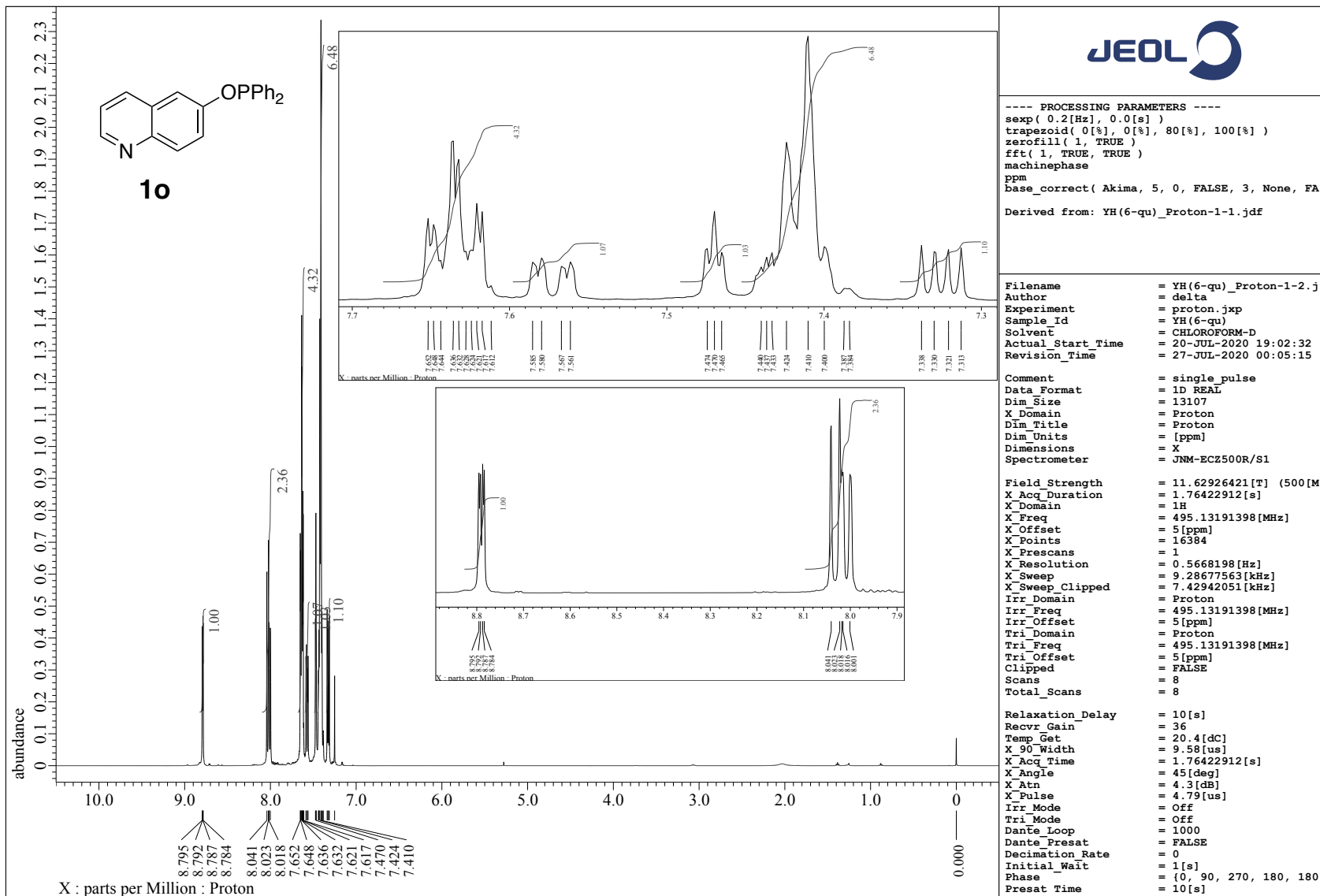
Filename           = YH(S-OMO)_31P_1Hde
Author            = delta
Experiment        = single_pulse_decou
Sample_Id         = YH(S-OMO)
Solvent           = BENZENE-D6
Actual_Start_Time = 7-APR-2020 22:34:
Revision_Time     = 8-APR-2020 09:38:

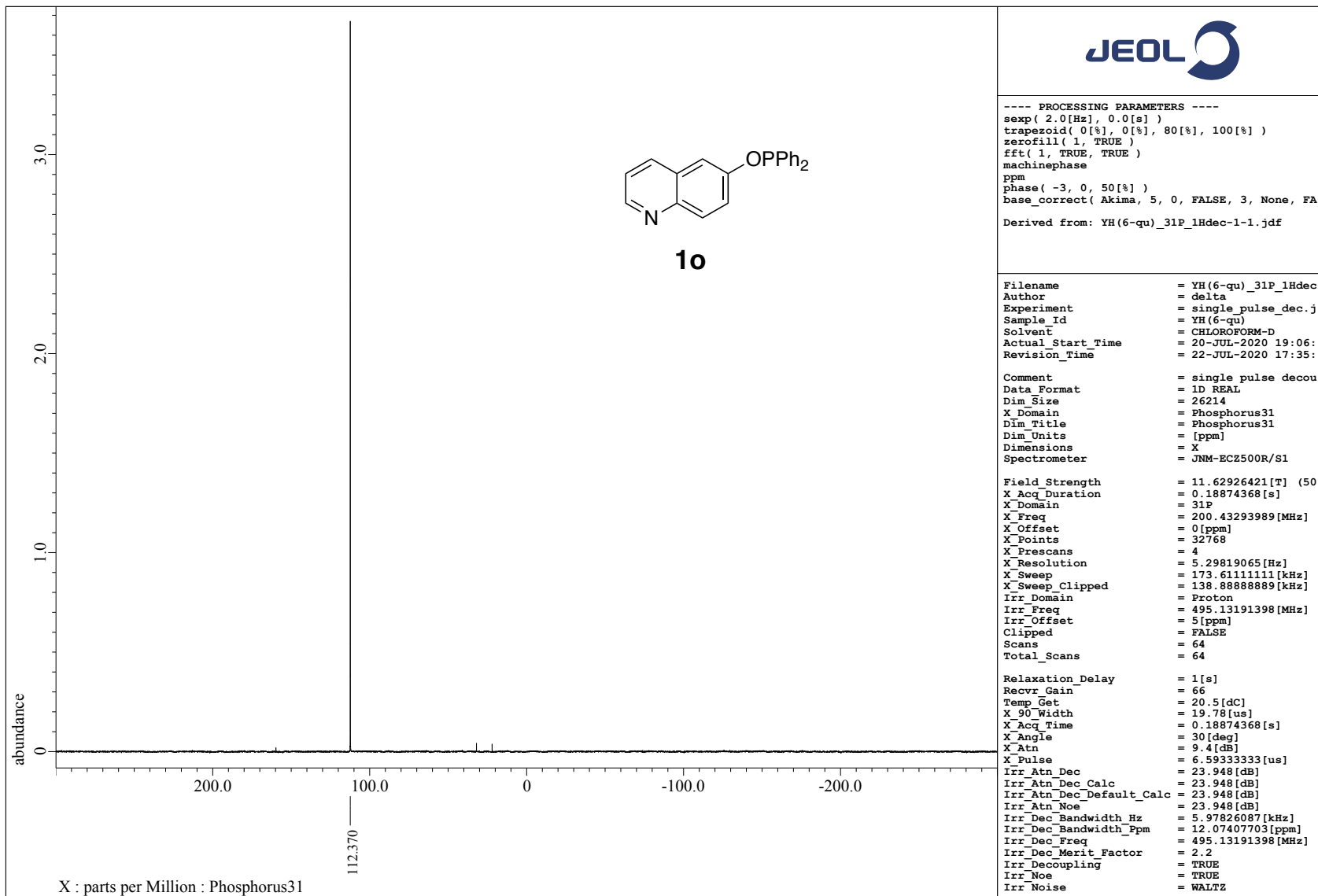
Comment           = single_pulse decou
Data_Format       = 1D REAL
Dim_Size          = 26214
X_Domain          = Phosphorus31
Dim_Title         = Phosphorus31
Dim_Units         = [ppm]
Dimensions        = X
Spectrometer      = JNM-ECZ500R/S1

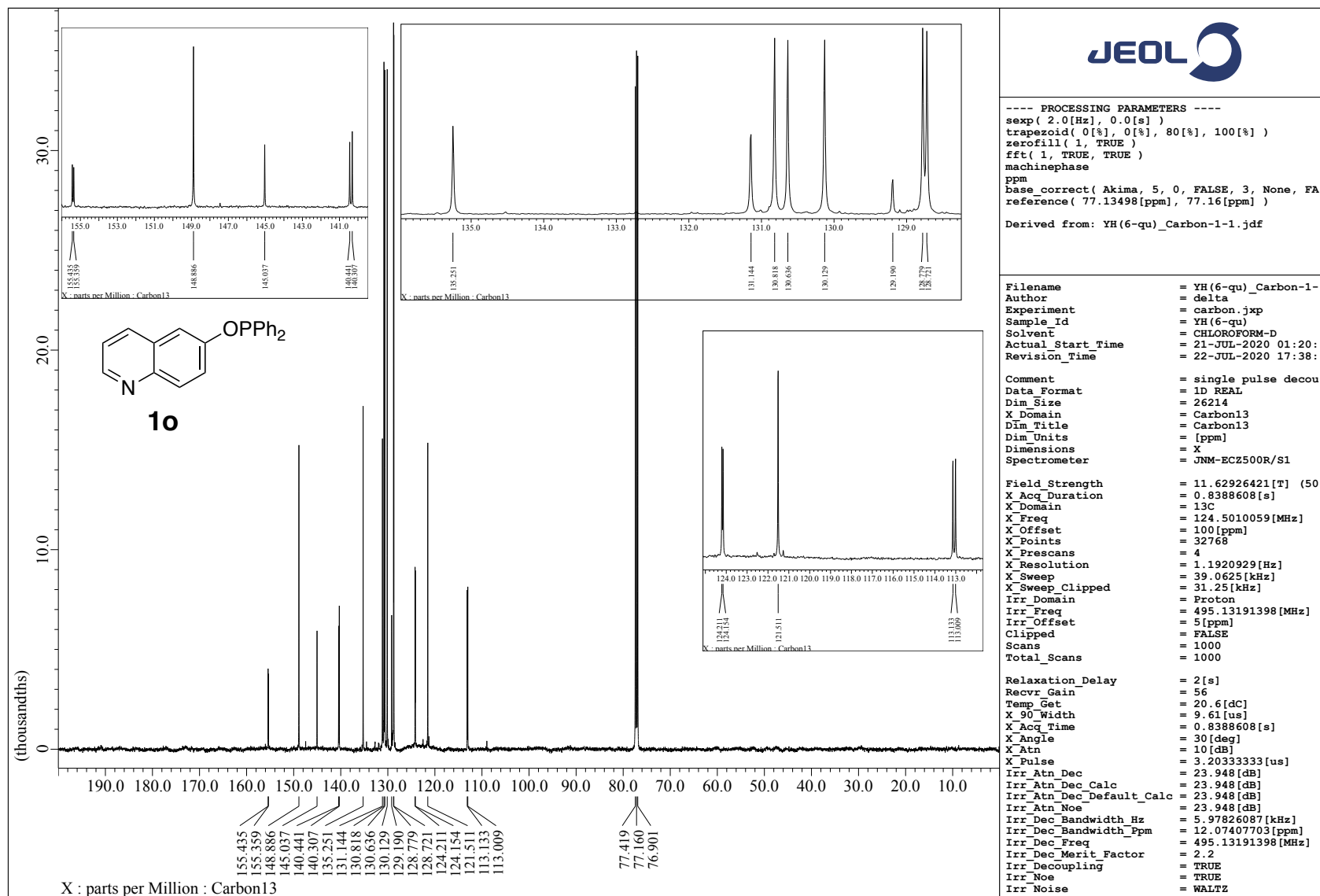
Field_Strength    = 11.62926421[T] (50
X_Acq_Duration    = 0.18874368[s]
X_Domain          = 31P
X_Freq            = 200.43293989[MHz]
X_Offset          = 0[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 5.29819065[Hz]
X_Sweep           = 173.61111111[kHz]
X_Sweep_Clippped = 138.88888889[kHz]
Irr_Domain        = Proton
Irr_Freq          = 495.13191398[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 64
Total_Scans       = 64

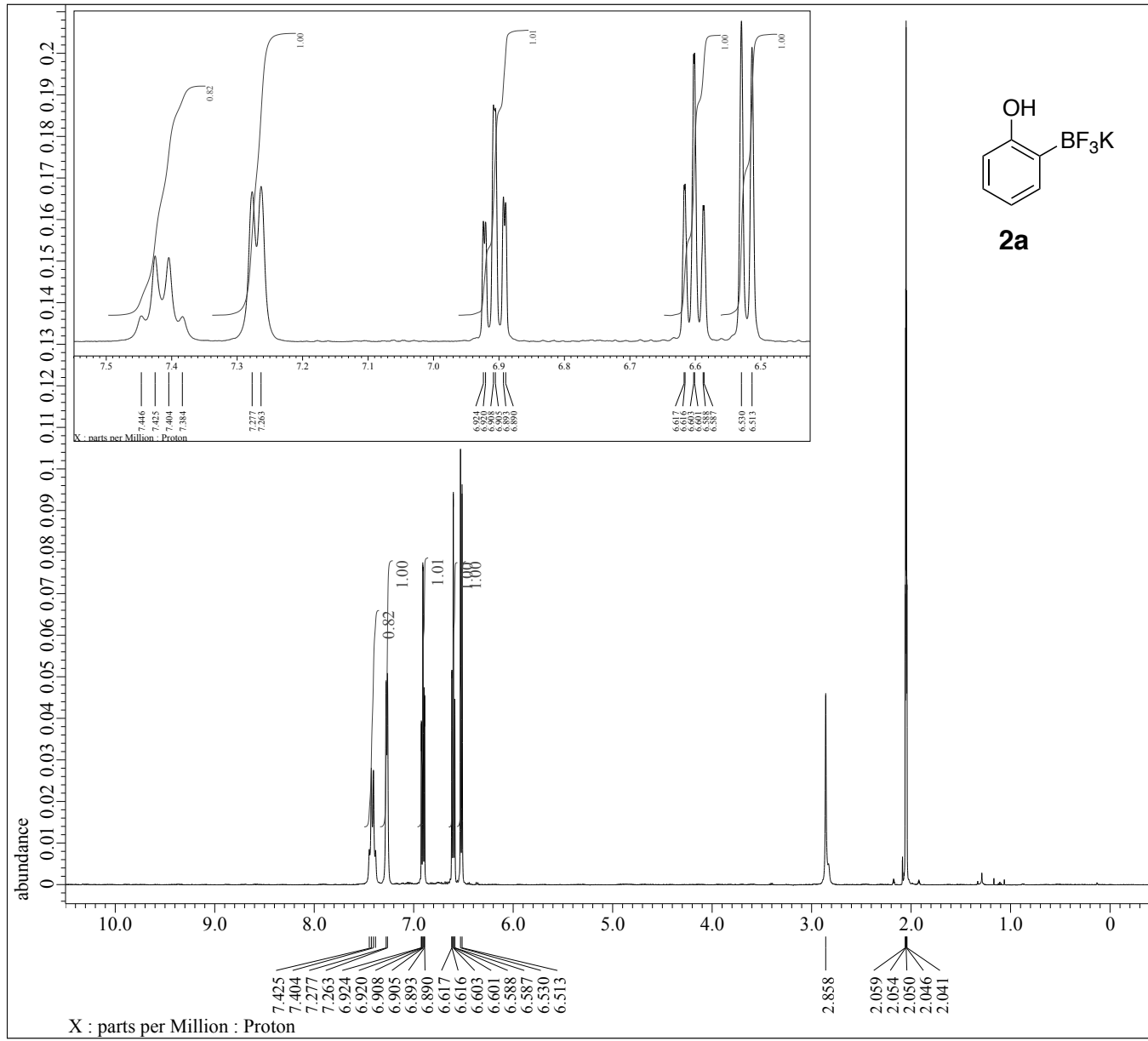
Relaxation_Delay  = 1[s]
Recvr_Gain        = 66
Temp_Get          = 20.4[dC]
X_90_Width        = 19.78[us]
X_Acq_Time        = 0.18874368[s]
X_Angle           = 30[deg]
X_Atn             = 9.4[dB]
X_Pulse           = 6.59333333[us]
Irr_Atn_Dec       = 23.948[dB]
Irr_Atn_Dec_Calc = 23.948[dB]
Irr_Atn_Dec_Default_Calc = 23.948[dB]
Irr_Atn_Noise    = 23.948[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_Noise        = TRUE
Irr_Noise        = WALTZ

```









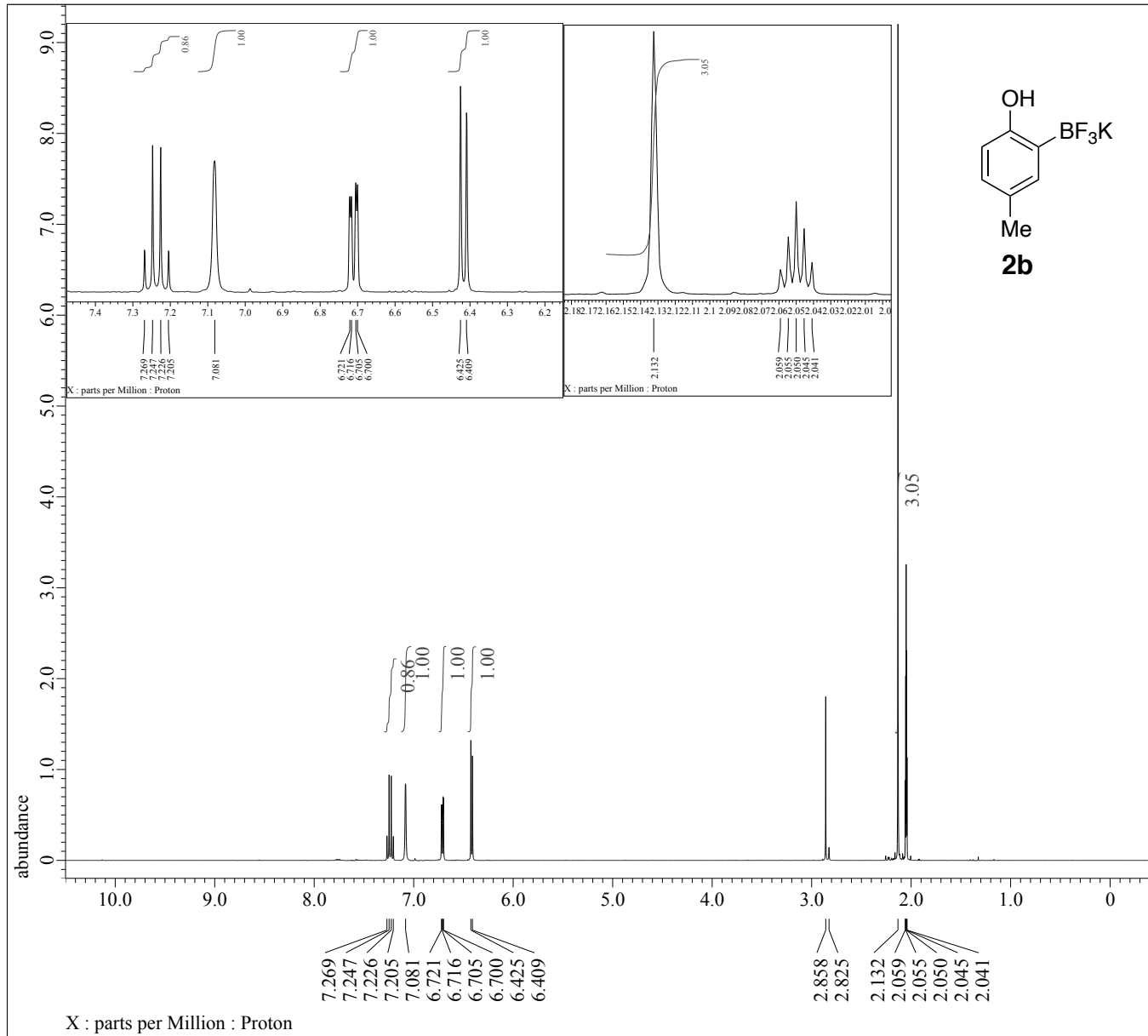
---- PROCESSING PARAMETERS ----
 sexp(0.2[Hz], 0.0[s])
 trapezoid(0[%], 0[%], 80[%], 100[%])
 zerofill(1, TRUE)
 fft(1, TRUE, TRUE)
 machinphase
 ppm
 base_correct(Akima, 5, 0, FALSE, 3, None, FA
 Derived from: YH-225-(H)_Proton-1-1.jdf

Filename = YH-225-(H)_Proton-1-3
 Author = delta
 Experiment = proton.jxp
 Sample Id = YH-225-(H)
 Solvent = ACETONE-D6
 Actual_Start_Time = 22-FEB-2020 17:29:44
 Revision_Time = 13-APR-2020 12:26:36

Comment = single pulse
 Data Format = 1D REAL
 Dim_Size = 104858
 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 = 14.11383296[s]
 X_Domain = 1H
 X_Freq = 495.13191398[MHz]
 X_Offset = 5[ppm]
 X_Points = 131072
 X_Prescans = 1
 X_Resolution = 70.85247522[mHz]
 X_Sweep = 9.28677563[kHz]
 X_Sweep_Clippped = 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 = 3[s]
 Recvr Gain = 56
 Temp_Get = 21.3[dC]
 X_90_Width = 7.12[us]
 X_Acq_Time = 14.11383296[s]
 X_Angle = 45[deg]
 X_Atn = 3.3[dB]
 X_Pulse = 3.56[us]
 Irr_Mode = Off
 Tri_Mode = Off
 Dante Loop = 299
 Dante_Presat = FALSE
 Decimation_Rate = 0
 Initial_Wait = 1[s]
 Phase = {0, 90, 270, 180, 180
 Presat_Time = 3[s]



```

---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
phase( 2.25, -23, 69.74668[%] )
base_correct( None, 0, Smooth )
以下に由来 : YH-161(p-Me)_Proton-1-1.jdf

```

```

Filename      = YH-161(p-Me)_Proton-1
Author       = delta
Experiment   = proton.jxp
Sample Id    = YH-161(p-Me)
Solvent      = ACETONE-D6
Creation Time = 10-MAR-2020 22:25:05
Revision Time = 11-MAR-2020 11:49:15
Current Time  = 11-MAR-2020 11:49:27

```

```

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
Decimation_Reg = r : 1346 ( 1345 ), g : 52
Scans          = 8
Total_Scans    = 8

```

```

Relaxation_Delay = 5[s]
Recvr Gain       = 66
Temp Get         = 21.9[dC]
X 90_Width       = 7.12[us]
X Acq Time       = 1.76422912[s]
X Angle          = 45[deg]
X Atn            = 3.3[dB]
X Pulse         = 3.56[us]
Irr Mode         = Off
Tri Mode         = Off
Comment 1       = *** Pulse ***
Comment 111     = *** presat time ***
Comment 201     = *** obs_dante presatu
Comment 202     = *** irr_ preaturation
Comment 203     = *** tri_ preaturation

```

```

---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
phase( 2.5, -21, 69.8535[%] )
base_correct( None, 0, Smooth )

```

以下に由来 : YH-54 (p-MeO)_Proton-1-1.jdf

```

Filename      = YH-54 (p-MeO)_Proton-1
Author       = delta
Experiment   = proton.jxp
Sample_Id    = YH-54 (p-MeO)
Solvent      = ACETONE-D6
Creation_Time = 10-MAR-2020 22:02:19
Revision_Time = 11-MAR-2020 12:52:33
Current_Time  = 11-MAR-2020 12:53:26

```

```

Comment       = single pulse
Data Format    = 1D REAL
Dim Size      = 13107
Dim Title     = Proton
Dim Units     = [ppm]
Dimensions    = X
Spectrometer  = JNM-ECZ500R/s1

```

```

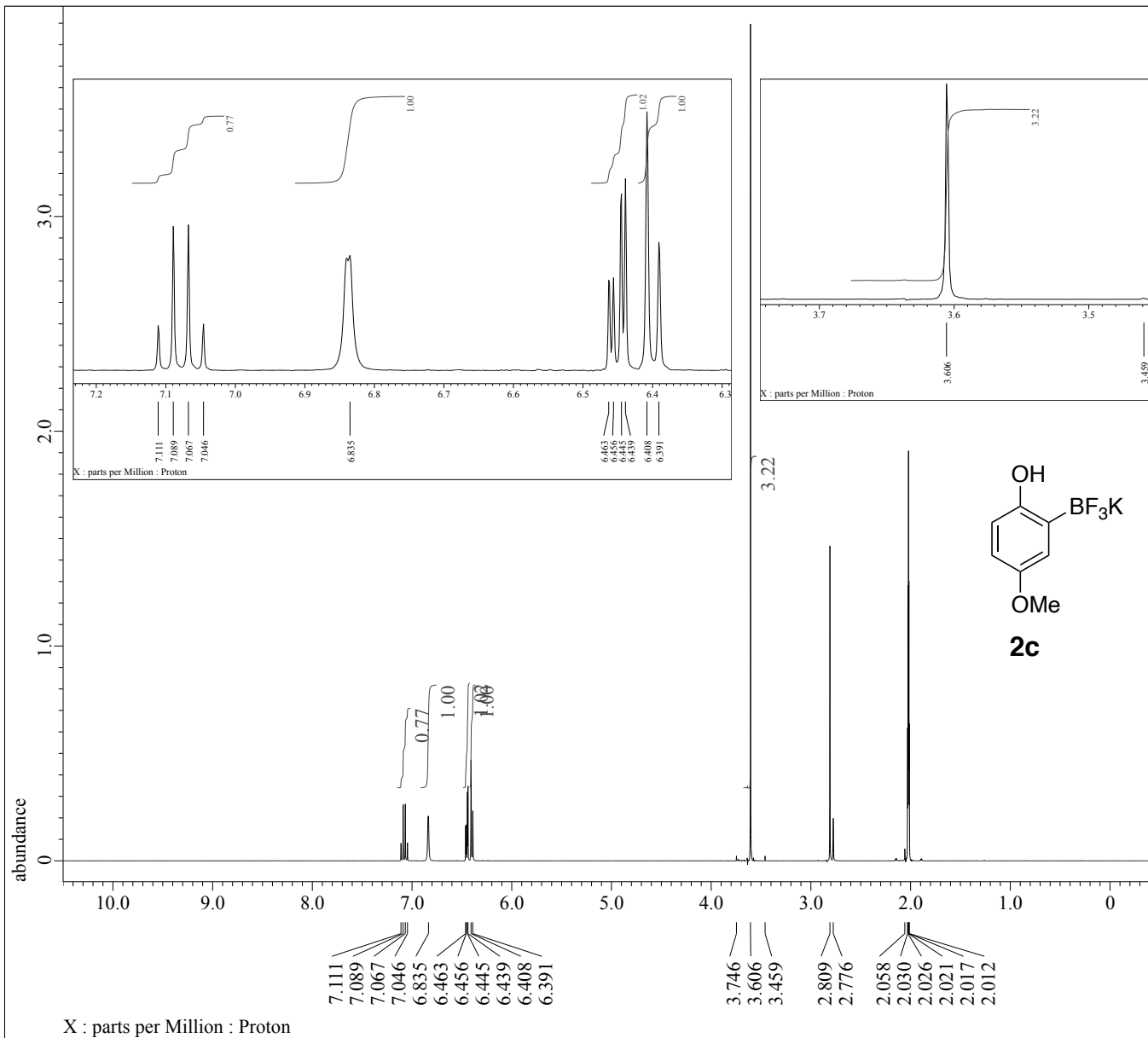
Field Strength = 11.62926421[T] (500[M
X_Acq_Duration = 1.76422912[s]
X_Domain       = 1H
X_Freq         = 495.13191398[MHz]
X_Offset       = 5[ppm]
X_Points       = 16384
X_Prescans     = 1
X_Resolution   = 0.5668198[Hz]
X_Sweep        = 9.28677563[kHz]
X_Sweep_Clippped = 7.42942051[kHz]
Irr_Domain     = Proton
Irr_Freq       = 495.13191398[MHz]
Irr_Offset     = 5[ppm]
Tri_Domain     = Proton
Tri_Freq       = 495.13191398[MHz]
Tri_Offset     = 5[ppm]
Clipped        = FALSE
Decimation_Reg = r : 1346( 1345), g : 52
Scans          = 8
Total_Scans    = 8

```

```

Relaxation_Delay = 5[s]
Recvr_Gain       = 56
Temp_Get         = 21.8[dC]
X_90_Width      = 7.12[us]
X_Acq_Time      = 1.76422912[s]
X_Angle         = 45[deg]
X_Atn           = 3.3[dB]
X_Pulse         = 3.56[us]
Irr_Mode        = Off
Tri_Mode        = Off
Comment_1       = *** Pulse ***
Comment_111    = *** presat time ***
Comment_201    = *** obs_dante presatu
Comment_202    = *** irr_preaturation
Comment_203    = *** tri_preaturation

```



```

---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
phase( 0, -25, 69.64533[%] )
base_correct( None, 0, Smooth )

```

以下に由来 : YH-88 (CF3)_Proton-1-1.jdf

```

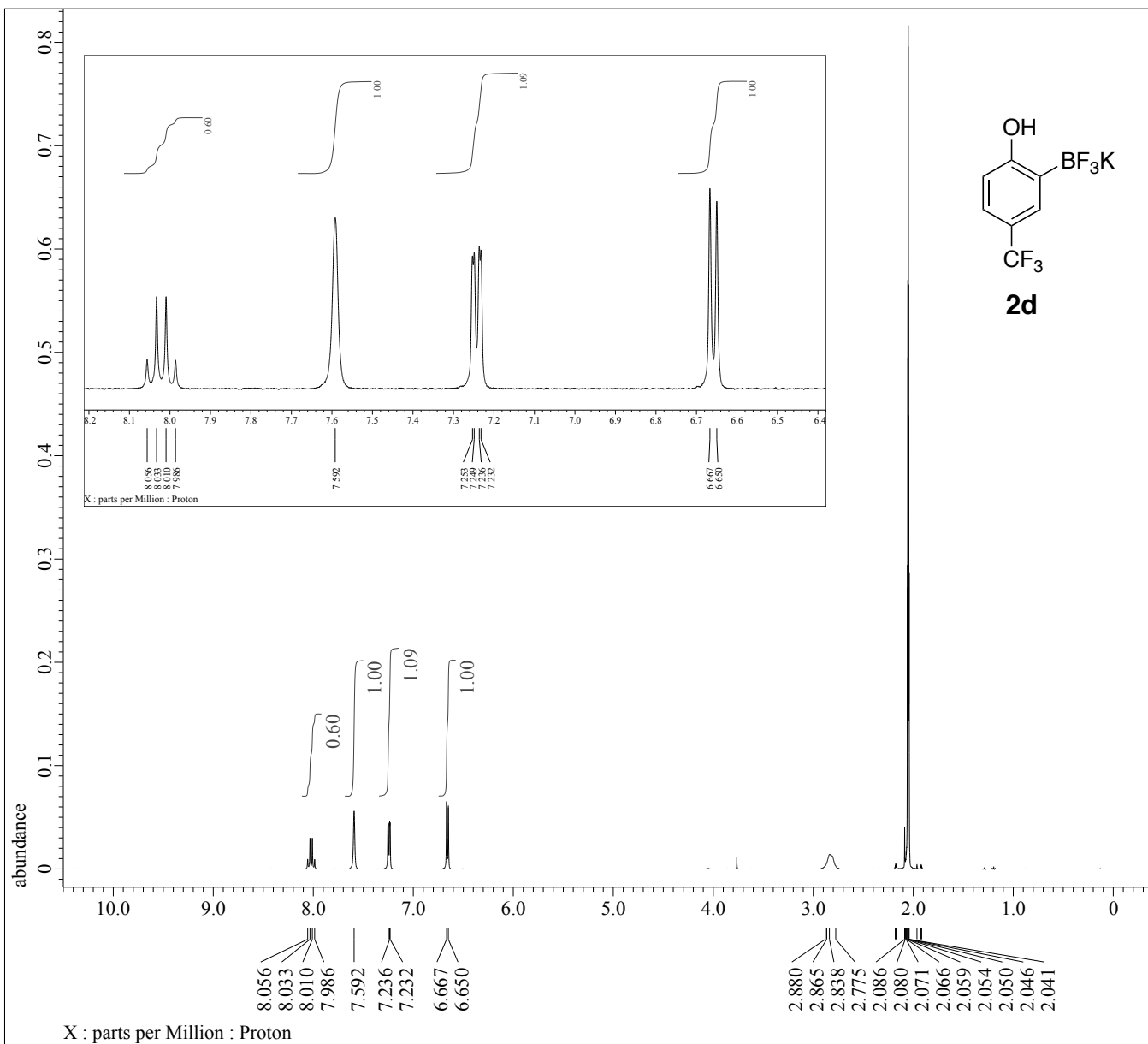
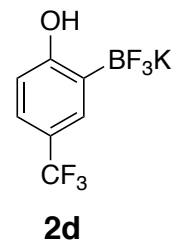
Filename      = YH-88 (CF3)_Proton-1-8
Author        = delta
Experiment    = proton.jxp
Sample_Id     = YH-88 (CF3)
Solvent       = ACETONE-D6
Creation_Time = 22-FEB-2020 13:29:51
Revision_Time = 9-MAR-2020 13:08:30
Current_Time  = 9-MAR-2020 13:09:10

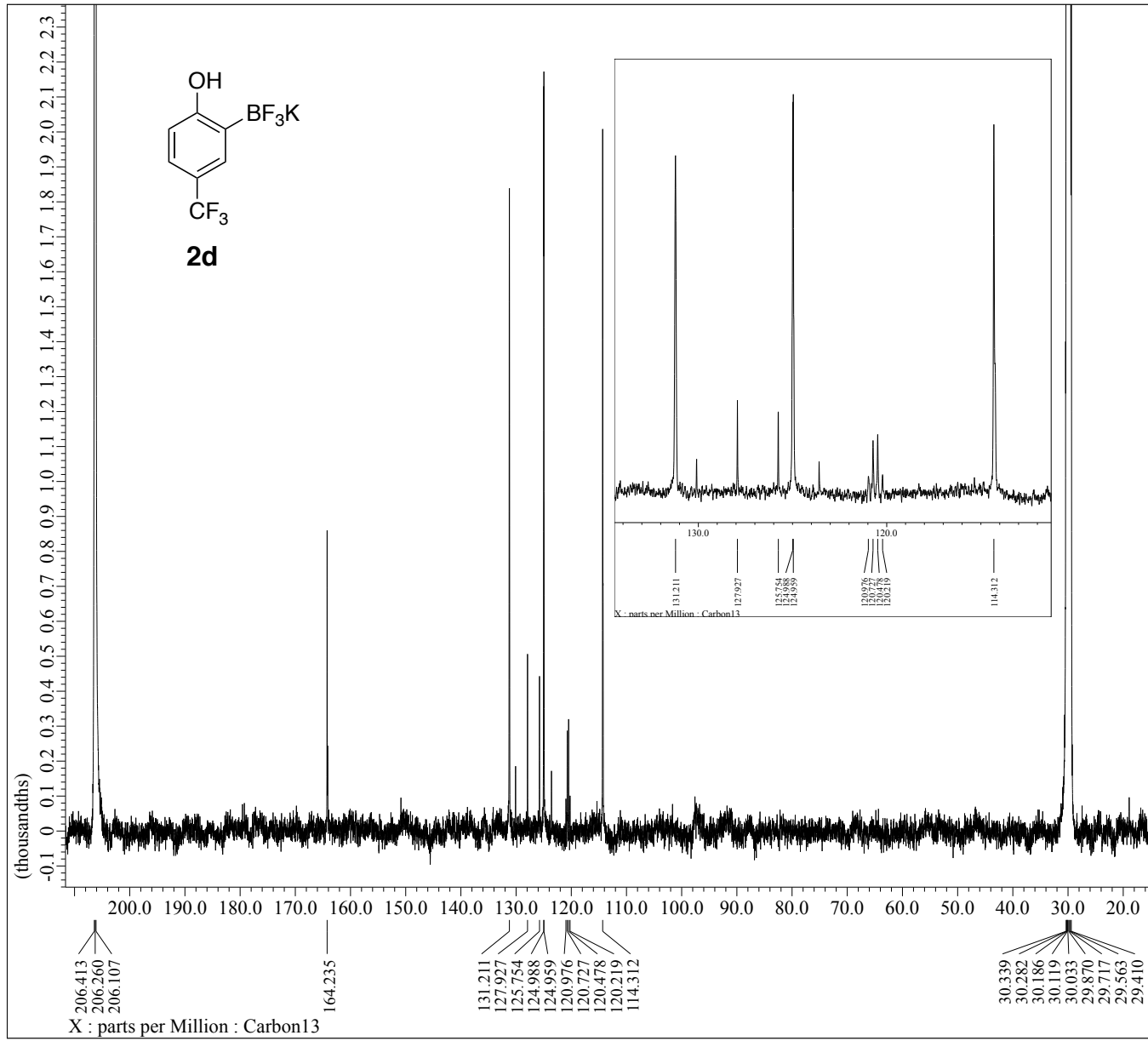
Comment       = single pulse
Data Format   = 1D REAL
Dim Size     = 104858
Dim Title    = Proton
Dim Units    = [ppm]
Dimensions   = X
Spectrometer = JNM-ECZ500R/s1

Field Strength = 11.62926421[T] (500[M]
X_Acq_Duration = 14.11383296[s]
X_Domain       = 1H
X_Freq        = 495.13191398[MHz]
X_Offset      = 5[ppm]
X_Points      = 131072
X_Prescans    = 1
X_Resolution  = 70.85247522[mHz]
X_Sweep       = 9.28677563[kHz]
X_Sweep_Clip  = 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
Decimation_Reg = r: 1346( 1345),g: 52
Scans         = 8
Total_Scans   = 8

Relaxation_Delay = 3[s]
Recvr Gain       = 66
Temp_Get        = 21.9[dC]
X_90_Width     = 7.12[us]
X_Acq_Time     = 14.11383296[s]
X_Angle        = 45[deg]
X_Atn          = 3.3[dB]
X_Pulse        = 3.56[us]
Irr_Mode       = Off
Tri_Mode       = Off
Comment_1      = *** Pulse ***
Comment_111    = *** presat time ***
Comment_201    = *** obs_dante presatu
Comment_202    = *** irr_preaturation
Comment_203    = *** tri_preaturation

```





```

---- PROCESSING PARAMETERS ----
sexp( 2.0[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
Derived from: YH(p-CF3)_Carbon-1-1.jdf

```

```

Filename      = YH(p-CF3)_Carbon-1
Author        = delta
Experiment    = carbon.jxp
Sample_Id     = YH(p-CF3)
Solvent       = ACETONE-D6
Actual_Start_Time = 8-APR-2020 00:58:
Revision_Time  = 9-APR-2020 14:12:

```

```

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

```

```

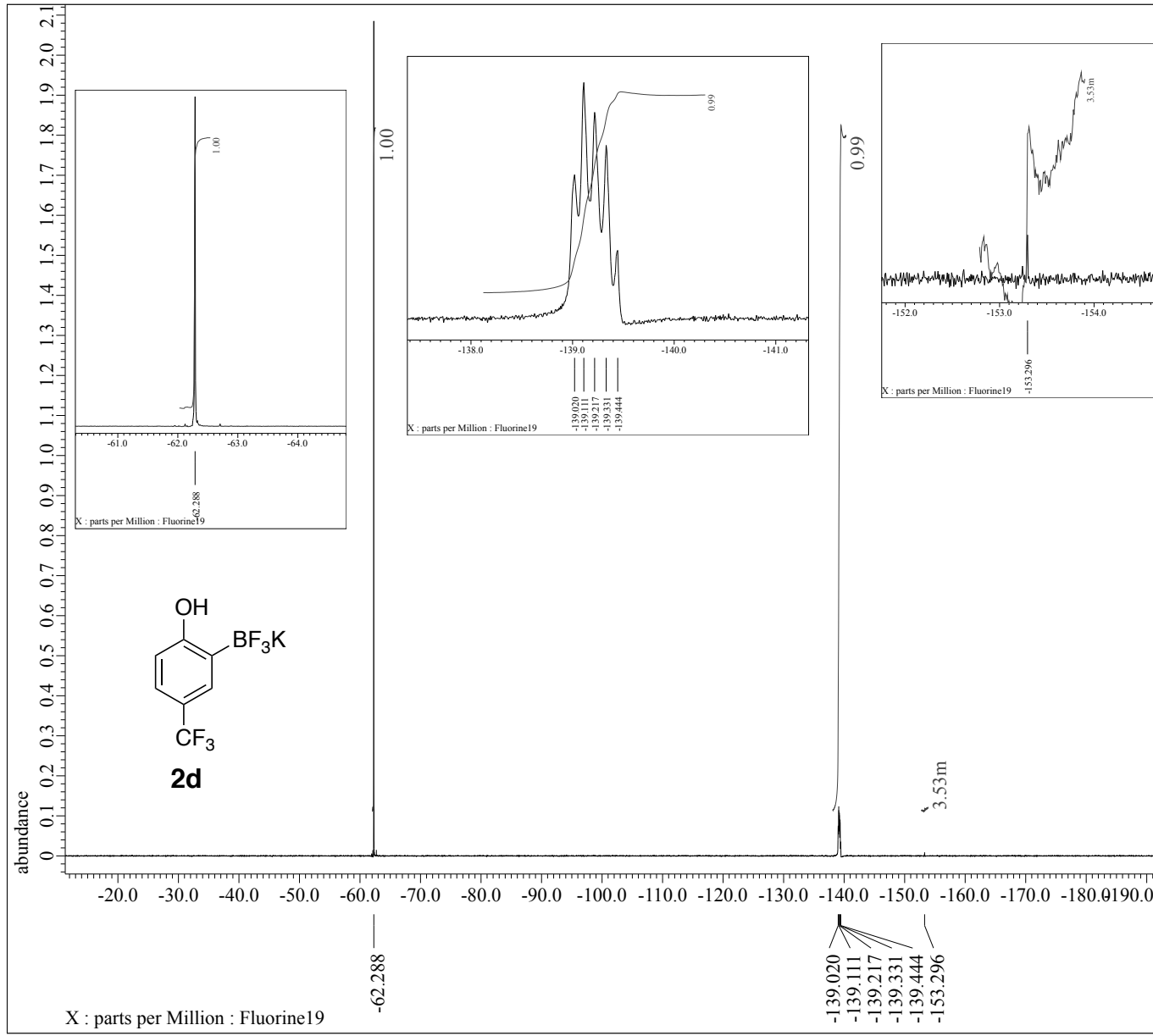
Field Strength = 11.62926421[T] (50
X_Acq_Duration = 0.8388608[s]
X_Domain        = 13C
X_Freq          = 124.5010059[MHz]
X_Offset        = 100[ppm]
X_Points        = 32768
X_Prescans      = 4
X_Resolution    = 1.1920929[Hz]
X_Sweep         = 39.0625[kHz]
X_Sweep_Clippped = 31.25[kHz]
Irr_Domain      = Proton
Irr_Freq        = 495.13191398[MHz]
Irr_Offset      = 5[ppm]
Clipped         = FALSE
Scans           = 10000
Total_Scans     = 10000

```

```

Relaxation_Delay = 2[s]
Recvr Gain       = 56
Temp_Get         = 20.7[dC]
X_90_Width       = 9.61[us]
X_Acq_Time       = 0.8388608[s]
X_Angle          = 30[deg]
X_Atn            = 10[dB]
X_Pulse          = 3.20333333[us]
Irr_Atn_Dec      = 23.948[dB]
Irr_Atn_Dec_Calc = 23.948[dB]
Irr_Atn_Dec_Default_Calc = 23.948[dB]
Irr_Atn_Noise    = 23.948[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_Noise        = TRUE
Irr_Noise        = WALTZ

```



```

---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
base_correct( None, 0, Smooth )
以下に由来 : YH-88 (CF3)_19F-1-1.jdf

```

```

Filename      = YH-88 (CF3)_19F-1-7.jd
Author       = delta
Experiment   = single pulse.jxp
Sample Id    = YH-88 (CF3)
Solvent      = ACETONE-D6
Creation Time = 22-FEB-2020 13:34:20
Revision Time = 22-FEB-2020 19:15:30
Current Time  = 22-FEB-2020 19:17:31

```

```

Comment      = single pulse
Data Format   = 1D REAL
Dim Size     = 26214
Dim Title    = Fluorine19
Dim Units    = [ppm]
Dimensions   = X
Spectrometer = JNM-ECZ500R/s1

```

```

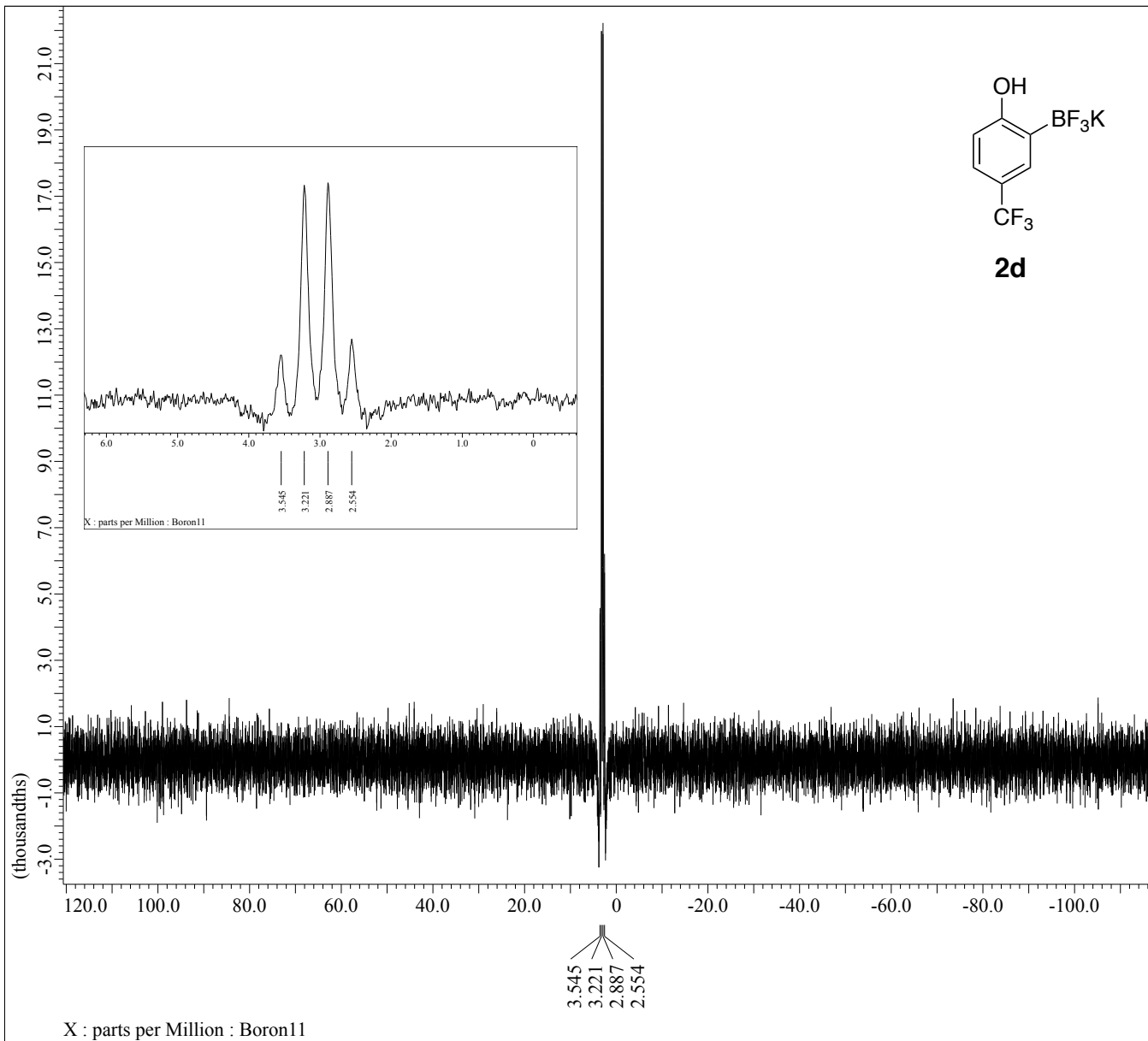
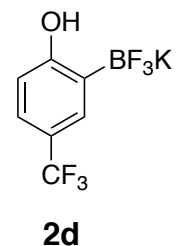
Field Strength = 11.62926421[T] (500[M]
X Acq Duration = 0.28311552[s]
X Domain       = 19F
X Freq         = 465.88941346[MHz]
X Offset       = -100[ppm]
X Points       = 32768
X Prescans     = 1
X Resolution   = 3.5321271[Hz]
X Sweep        = 115.74074074[kHz]
X Sweep Clipped = 92.59259259[kHz]
Irr Domain     = Fluorine19
Irr Freq       = 465.88941346[MHz]
Irr Offset     = 5[ppm]
Tri Domain     = Fluorine19
Tri Freq       = 465.88941346[MHz]
Tri Offset     = 5[ppm]
Clipped        = FALSE
Decimation_Reg = r : 54 ( 53 ), g : 29
Scans          = 8
Total_Scans    = 8

```

```

Relaxation_Delay = 5[s]
Recvr Gain       = 56
Temp Get         = 21.9[dC]
X 90_Width       = 7.81[us]
X Acq Time       = 0.28311552[s]
X Angle          = 45[deg]
X Atn            = 3.7[dB]
X Pulse         = 3.905[us]
Irr Mode         = Off
Tri Mode         = Off
Comment 1       = *** Pulse ***
Comment 111     = *** presat time ***
Comment 201     = *** obs_dante presatu
Comment 202     = *** irr_preaturation
Comment 203     = *** tri_preaturation

```



```

---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
phase( 25.83806, 0, 50[%] )
phase( 4.18643, 0, 50[%] )
ibase_correct( , FALSE, FALSE )
base_correct( None, 0, Smooth )
phase( 1.1835, 0, 50[%] )

```

以下に由来 : YH-88 (CF3)_11B_1Hdec-1-1.jdf

```

Filename           = YH-88 (CF3)_11B_1Hd
Author             = delta
Experiment         = single_pulse_dec.j
Sample_Id          = YH-88 (CF3)
Solvent            = ACETONE-D6
Creation_Time      = 22-FEB-2020 13:38:
Revision_Time     = 9-MAR-2020 13:14:
Current_Time       = 9-MAR-2020 13:15:

Comment           = single pulse decou
Data Format        = 1D REAL
Dim Size          = 26214
Dim Title         = Boron11
Dim Units         = [ppm]
Dimensions        = X
Spectrometer      = JNM-ECZ500R/S1

Field Strength    = 11.62926421[T] (50
X_Acq_Duration   = 0.66060288[s]
X_Domain         = 11B
X_Freq           = 158.85814241[MHz]
X_Offset         = 0[ppm]
X_Points         = 32768
X_Prescans       = 4
X_Resolution     = 1.51376876[Hz]
X_Sweep          = 49.6031746[kHz]
X_Sweep_Clipped = 39.68253968[kHz]
Irr_Domain       = Proton
Irr_Freq         = 495.13191398[MHz]
Irr_Offset       = 5[ppm]
Clipped          = FALSE
Decimation_Reg   = r: 252( 251),g: 40
Scans            = 100
Total_Scans      = 100

Relaxation_Delay  = 2[s]
Recvr Gain        = 56
Temp_Get          = 22.6[dC]
X_90_Width       = 15.74[us]
X_Acq_Time       = 0.66060288[s]
X_Angle          = 30[deg]
X_Atn            = 10.4[dB]
X_Pulse          = 5.24666667[us]
Irr_Atn_Dec      = 26.4[dB]
Irr_Atn_Dec_Calc = 26.4[dB]
Irr_Atn_Dec_Default_Calc = 26.4[dB]
Irr_Atn_Noise    = 26.4[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_Noise        = TRUE

```

```

---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
phase( 6, -26, 69.3926[%] )
base_correct( None, 0, Smooth )
reference( 2.02113[ppm], 2.05[ppm] )

```

以下に由来: YH-189(p-F)_Proton-1-1.jdf

```

Filename      = YH-189(p-F)_Proton-1-
Author        = delta
Experiment    = proton.jxp
Sample_Id     = YH-189(p-F)
Solvent       = ACETONE-D6
Creation_Time = 22-FEB-2020 16:27:38
Revision_Time = 9-MAR-2020 13:37:11
Current_Time  = 9-MAR-2020 13:37:42

```

```

Comment       = single pulse
Data Format    = 1D REAL
Dim Size      = 104858
Dim Title     = Proton
Dim Units     = [ppm]
Dimensions    = X
Spectrometer  = JNM-ECZ500R/s1

```

```

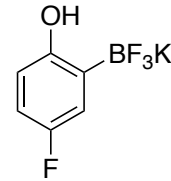
Field Strength = 11.62926421[T] (500[M]
X_Acq_Duration = 14.11383296[s]
X_Domain       = 1H
X_Freq         = 495.13191398[MHz]
X_Offset       = 5[ppm]
X_Points       = 131072
X_Prescans     = 1
X_Resolution   = 70.85247522[mHz]
X_Sweep        = 9.28677563[kHz]
X_Sweep_Clippped = 7.42942051[kHz]
Irr_Domain     = Proton
Irr_Freq       = 495.13191398[MHz]
Irr_Offset     = 5[ppm]
Tri_Domain     = Proton
Tri_Freq       = 495.13191398[MHz]
Tri_Offset     = 5[ppm]
Clipped        = FALSE
Decimation_Reg = r: 1346( 1345),g: 52
Scans          = 8
Total_Scans    = 8

```

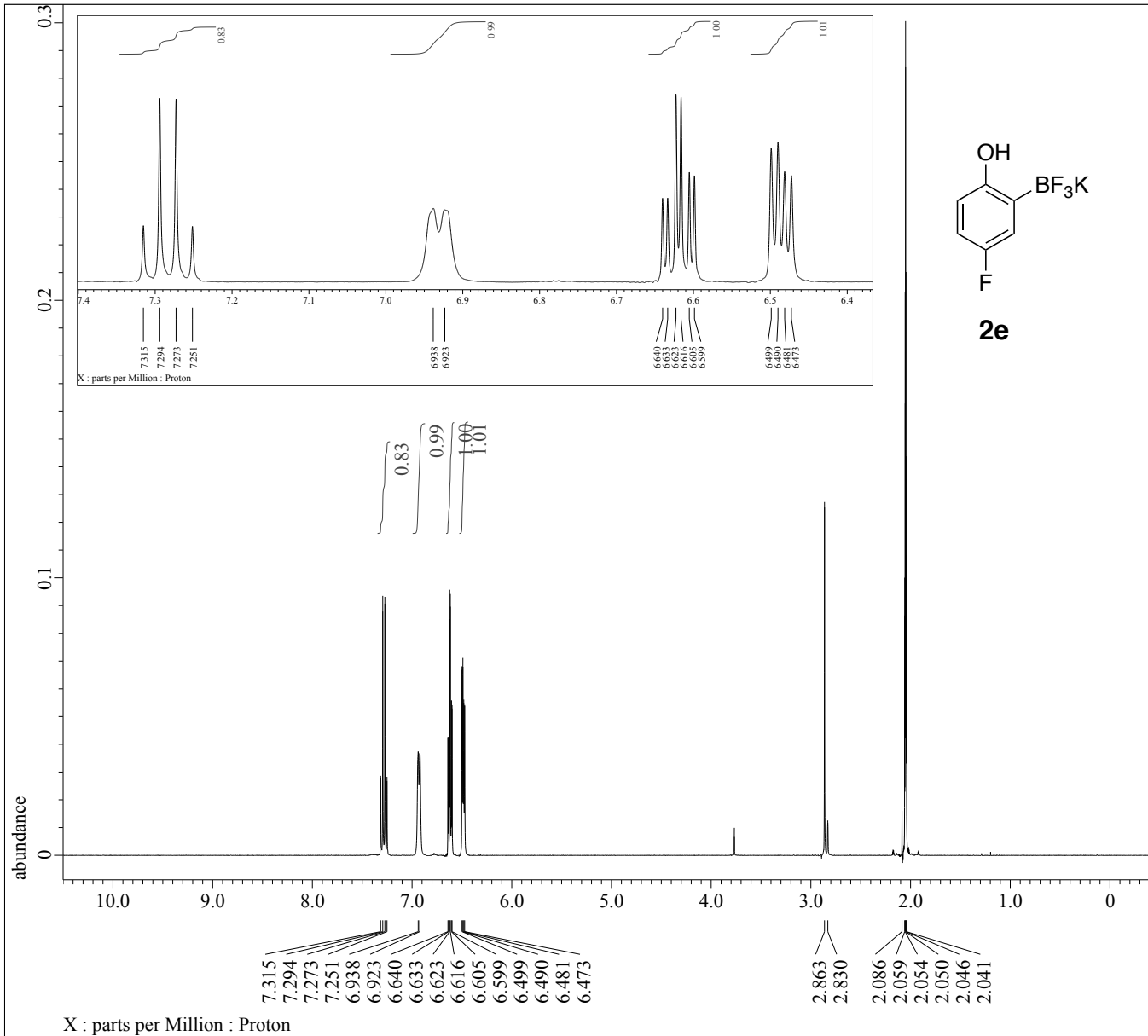
```

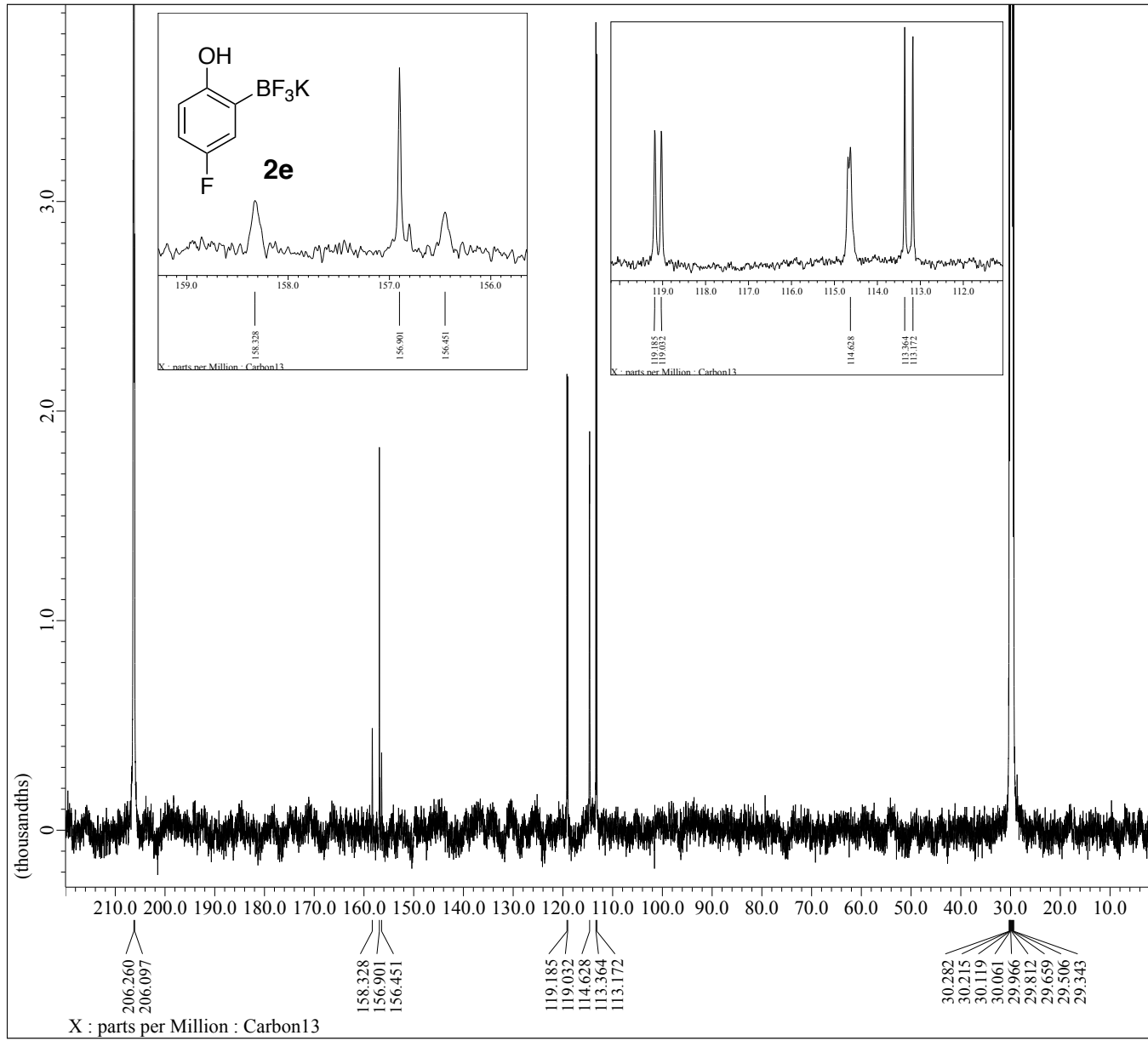
Relaxation_Delay = 3[s]
Recvr Gain       = 56
Temp_Get         = 21.9[dC]
X_90_Width       = 7.12[us]
X_Acq_Time       = 14.11383296[s]
X_Angle          = 45[deg]
X_Atn            = 3.3[dB]
X_Pulse          = 3.56[us]
Irr_Mode         = Off
Tri_Mode         = Off
Comment_1        = *** Pulse ***
Comment_111     = *** presat time ***
Comment_201     = *** obs_dante presatu
Comment_202     = *** irr_ preaturation
Comment_203     = *** tri_ preaturation

```



2e





```

---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
phase( 3, 7, 7.81673[%] )
base_correct( Akima, 5, 0, FALSE, 3, None, FA
Derived from: YH-189 (p-F)_Carbon-1-1.jdf

```

```

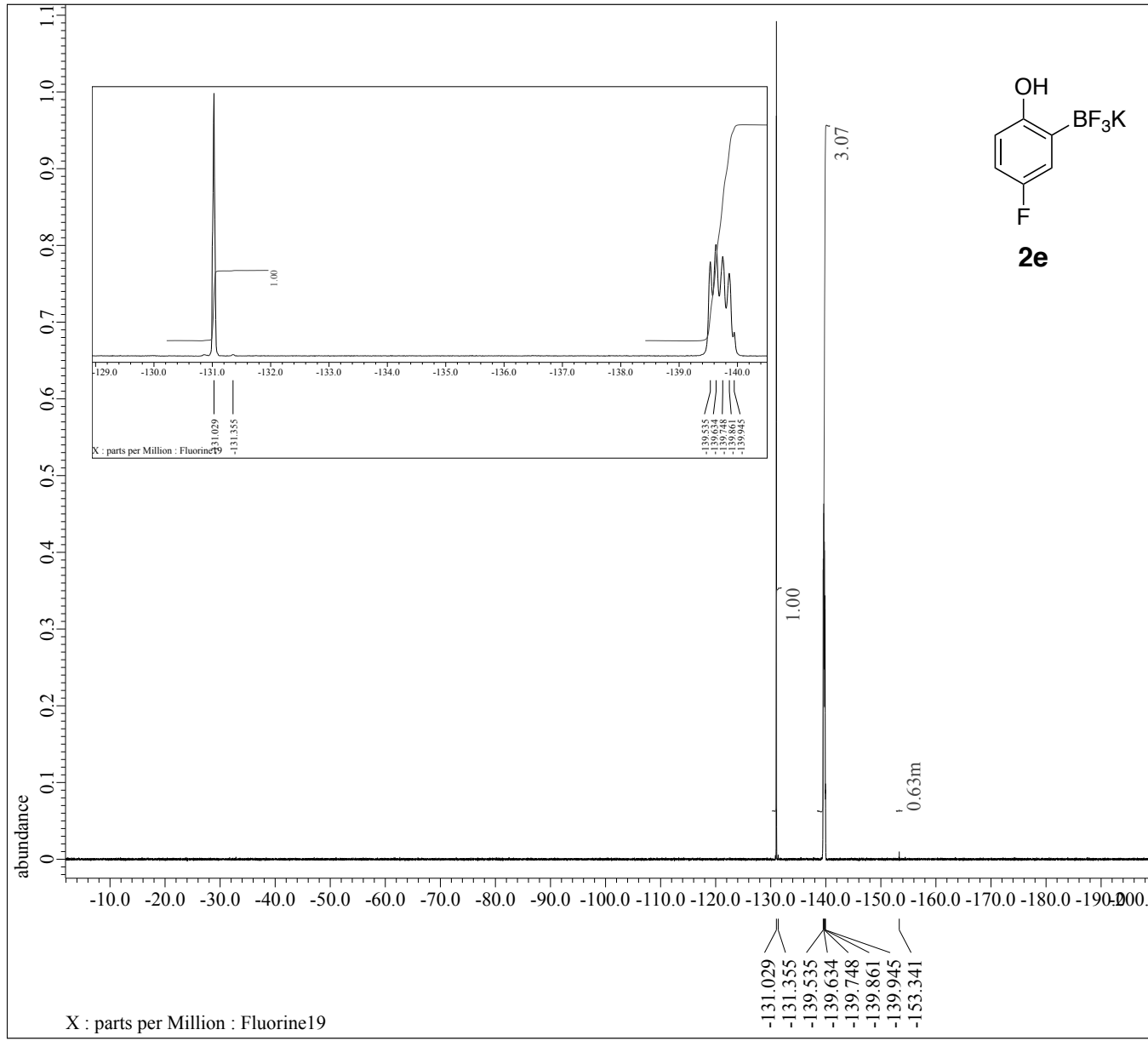
Filename      = YH-189 (p-F)_Carbon
Author       = delta
Experiment   = carbon.jxp
Sample Id    = YH-189 (p-F)
Solvent      = ACETONE-D6
Actual_Start_Time = 25-FEB-2020 06:03:
Revision_Time   = 9-APR-2020 14:27:

Comment      = single pulse decou
Data Format   = 1D REAL
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          = 5000
Total_Scans    = 5000

Relaxation_Delay = 2[s]
Recvr Gain       = 56
Temp_Get         = 22.2[dC]
X 90 Width      = 13.48[us]
X Acq Time      = 0.8388608[s]
X Angle         = 30[deg]
X Atn           = 11[dB]
X Pulse         = 4.49333333[us]
Irr Atn Dec     = 26.4[dB]
Irr Atn Dec Calc = 26.4[dB]
Irr Atn Dec Default_Calc = 26.4[dB]
Irr Atn Noe     = 26.4[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

```



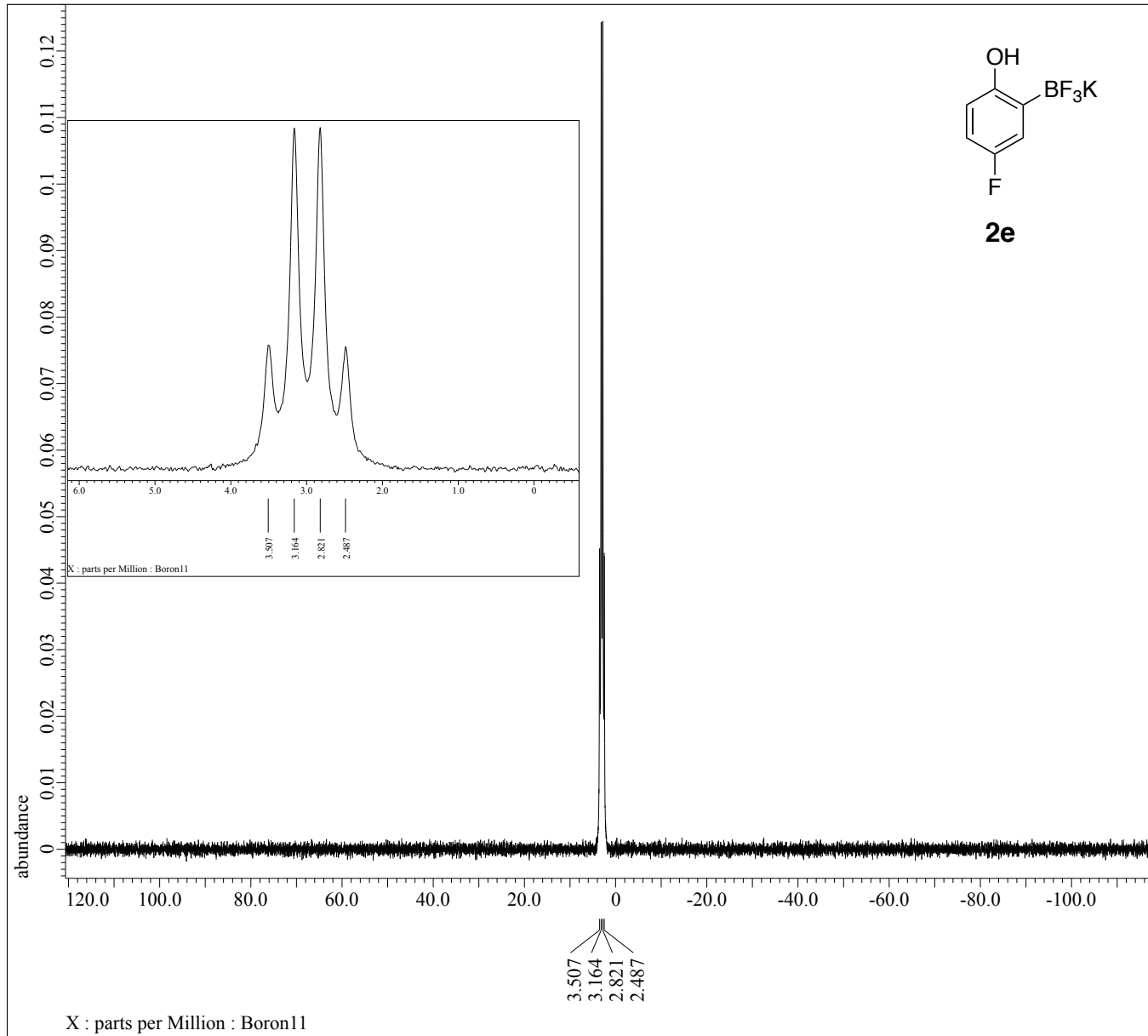
---- PROCESSING PARAMETERS ----
 sexp(0.2[Hz], 0.0[s])
 trapezoid(0[%], 0[%], 80[%], 100[%])
 zerofill(1)
 fft(1, TRUE, TRUE)
 machinephase
 ppm
 phase(-1.25, -21, 64.94487[%])
 base_correct(None, 0, Smooth)
 以下に由来 : YH-189(p-F)_19F-1-1.jdf

Filename = YH-189(p-F)_19F-1-12.
 Author = delta
 Experiment = single_pulse.jxp
 Sample_Id = YH-189(p-F)
 Solvent = ACETONE-D6
 Creation_Time = 22-FEB-2020 16:34:26
 Revision_Time = 7-MAR-2020 16:49:36
 Current_Time = 7-MAR-2020 16:50:05

Comment = single_pulse
 Data_Format = 1D_REAL
 Dim_Size = 26214
 Dim_Title = Fluorine19
 Dim_Units = [ppm]
 Dimensions = X
 Spectrometer = JNM-ECZ500R/s1

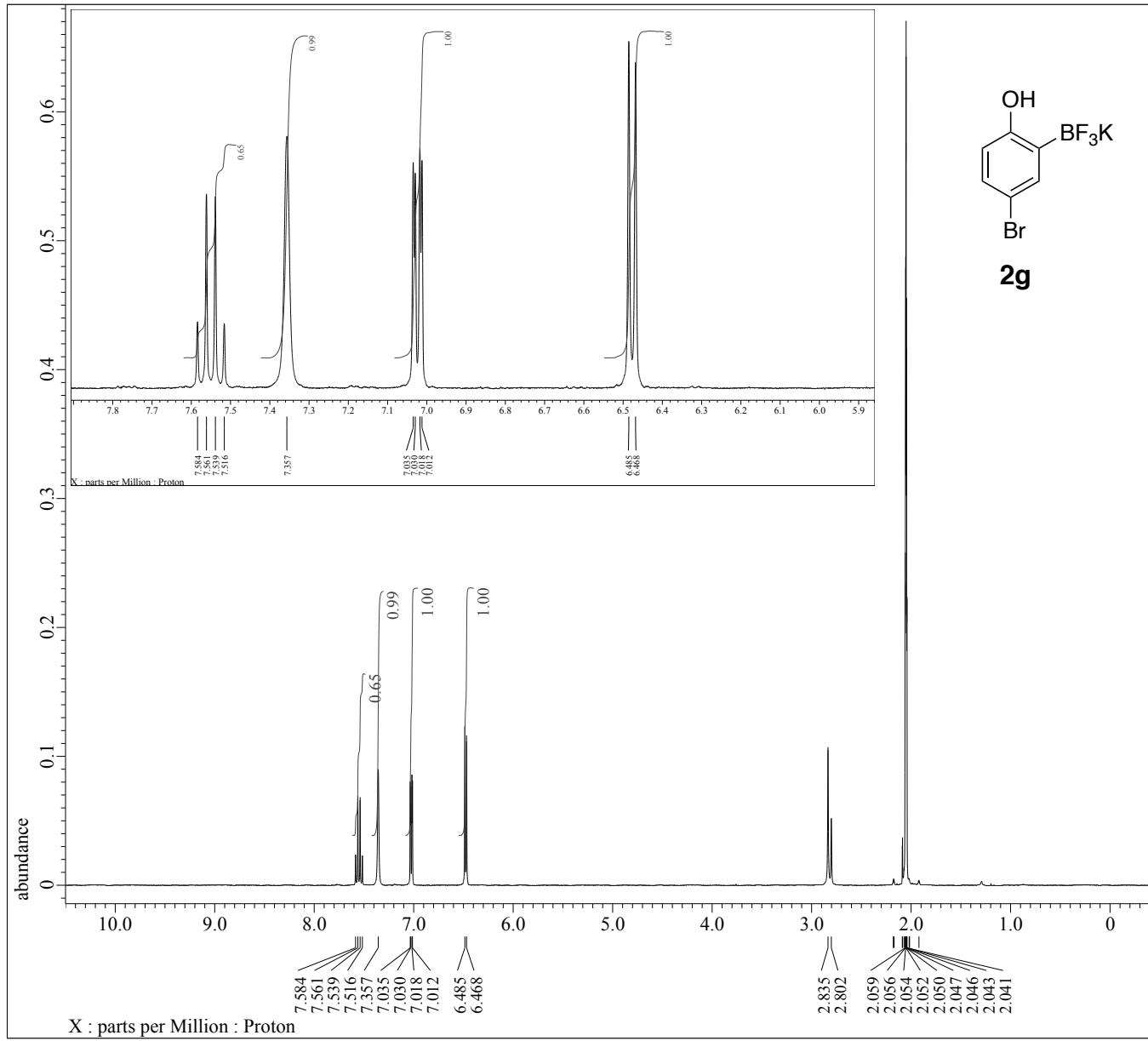
Field_Strength = 11.62926421[T] (500[M]
 X_Acq_Duration = 0.28311552[s]
 X_Domain = 19F
 X_Freq = 465.88941346[MHz]
 X_Offset = -100[ppm]
 X_Points = 32768
 X_Prescans = 1
 X_Resolution = 3.5321271[Hz]
 X_Sweep = 115.74074074[kHz]
 X_Sweep_Clippped = 92.59259259[kHz]
 Irr_Domain = Fluorine19
 Irr_Freq = 465.88941346[MHz]
 Irr_Offset = 5[ppm]
 Tri_Domain = Fluorine19
 Tri_Freq = 465.88941346[MHz]
 Tri_Offset = 5[ppm]
 Clipped = FALSE
 Decimation_Reg = r: 54(53),g: 29
 Scans = 8
 Total_Scans = 8

Relaxation_Delay = 5[s]
 Recvr_Gain = 56
 Temp_Get = 21.9[dC]
 X_90_Width = 7.81[us]
 X_Acq_Time = 0.28311552[s]
 X_Angle = 45[deg]
 X_Atn = 3.7[dB]
 X_Pulse = 3.905[us]
 Irr_Mode = Off
 Tri_Mode = Off
 Comment_1 = *** Pulse ***
 Comment_111 = *** presat time ***
 Comment_201 = *** obs_dante presatu
 Comment_202 = *** irr_preaturation
 Comment_203 = *** tri_preaturation



---- PROCESSING PARAMETERS ----
 sexp(2.0[Hz], 0.0[s])
 trapezoid(0[%], 0[%], 80[%], 100[%])
 zerofill(1)
 fft(1, TRUE, TRUE)
 machinephase
 ppm
 phase(12.5, 0, 49.12448[%])
 base_correct(None, 0, Smooth)
 以下に由来 : YH-189(p-F)_11B_1Hdec-1-1.jdf

Filename	= YH-189(p-F)_11B_1H
Author	= delta
Experiment	= single_pulse_dec.j
Sample_Id	= YH-189(p-F)
Solvent	= ACETONE-D6
Creation_Time	= 22-FEB-2020 16:37:
Revision_Time	= 9-MAR-2020 13:25:
Current_Time	= 9-MAR-2020 13:26:
Comment	= single pulse decou
Data_Format	= 1D_REAL
Dim_Size	= 26214
Dim_Title	= Boron11
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ500R/S1
Field_Strength	= 11.62926421[T] (50
X_Acq_Duration	= 0.66060288[s]
X_Domain	= 11B
X_Freq	= 158.85814241[MHz]
X_Offset	= 0[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 1.51376876[Hz]
X_Sweep	= 49.6031746[kHz]
X_Sweep_Clippped	= 39.68253968[kHz]
Irr_Domain	= Proton
Irr_Freq	= 495.13191398[MHz]
Irr_Offset	= 5[ppm]
Clipped	= FALSE
Decimation_Reg	= r: 252(251),g: 40
Scans	= 100
Total_Scans	= 100
Relaxation_Delay	= 2[s]
Recvr_Gain	= 56
Temp_Get	= 21.9[dC]
X_90_Width	= 15.74[us]
X_Acq_Time	= 0.66060288[s]
X_Angle	= 30[deg]
X_Atn	= 10.4[dB]
X_Pulse	= 5.24666667[us]
Irr_Atn_Dec	= 26.4[dB]
Irr_Atn_Dec_Calc	= 26.4[dB]
Irr_Atn_Dec_Default_Calc	= 26.4[dB]
Irr_Atn_No	= 26.4[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_No	= TRUE



```

---- 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
Derived from: YH-170-(p-Br)_Proton-1-1.jdf

```

```

Filename      = YH-170-(p-Br)_Proton-
Author       = delta
Experiment   = proton.jxp
Sample Id    = YH-170-(p-Br)
Solvent      = ACETONE-D6
Actual_Start_Time = 21-FEB-2020 18:30:09
Revision_Time   = 13-APR-2020 19:51:07

```

```

Comment      = single pulse
Data Format   = 1D REAL
Dim Size     = 104858
X Domain     = Proton
Dim Title    = Proton
Dim Units    = [ppm]
Dimensions   = X
Spectrometer = JNM-ECZ500R/s1

```

```

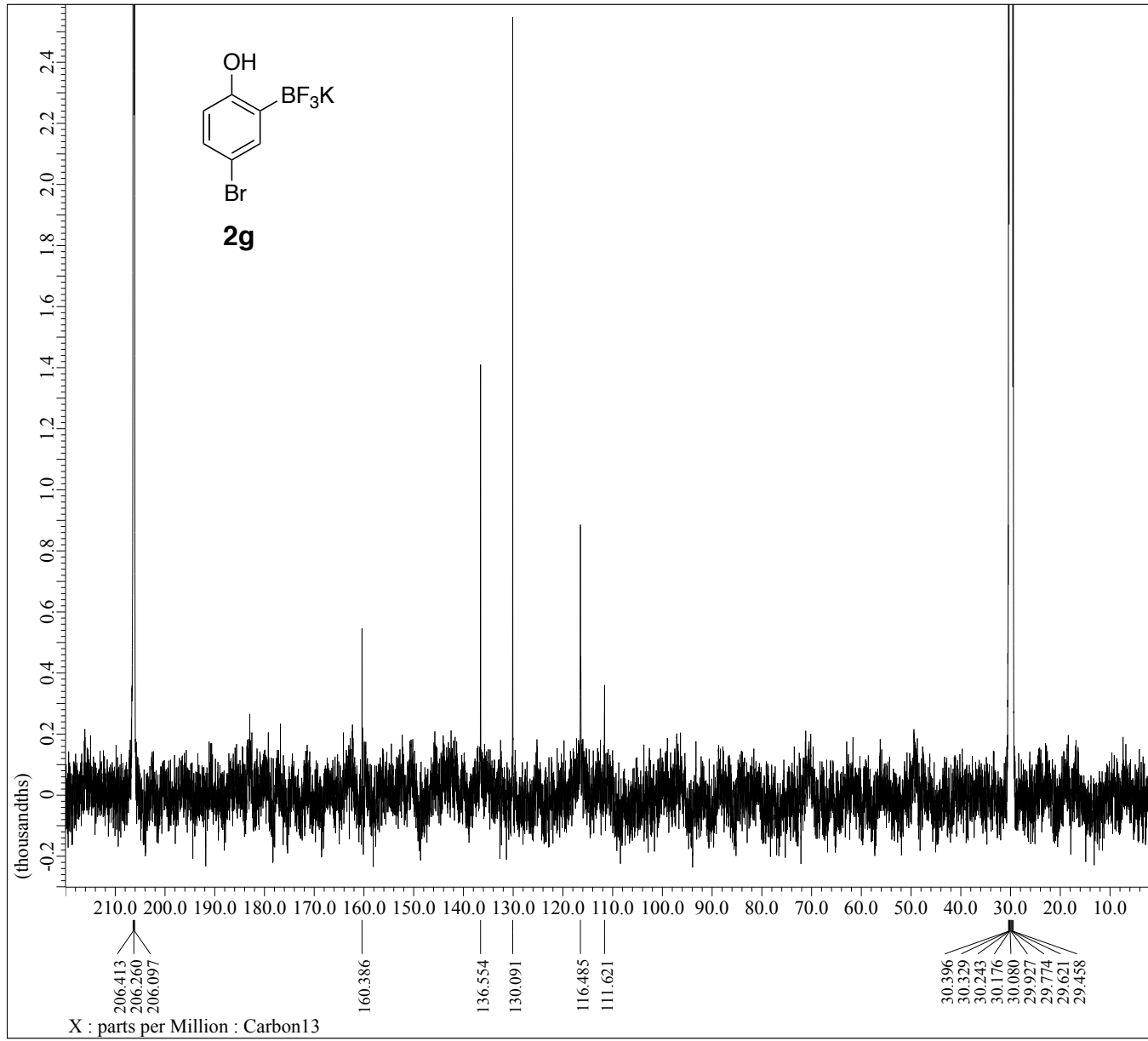
Field Strength = 11.62926421[T] (500[M]
X Acq Duration = 14.11383296[s]
X Domain       = 1H
X Freq         = 495.13191398[MHz]
X Offset       = 5[ppm]
X Points       = 131072
X Prescans     = 1
X Resolution   = 70.85247522[mHz]
X Sweep        = 9.28677563[kHz]
X Sweep Clipped = 7.42942051[kHz]
Irr Domain     = 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 = 3[s]
Recvr Gain       = 66
Temp_Get         = 21.9[dC]
X 90 Width      = 7.12[us]
X Acq Time       = 14.11383296[s]
X Angle          = 45[deg]
X Atn            = 3.3[dB]
X Pulse         = 3.56[us]
Irr Mode        = Off
Tri Mode        = Off
Dante Loop      = 299
Dante_Preset    = FALSE
Decimation Rate = 0
Initial_Wait    = 1[s]
Phase           = {0, 90, 270, 180, 180
Preset_Time     = 3[s]

```

```

---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
phase( 3, 6, 7.76714[%] )
base_correct( Akima, 5, 0, FALSE, 3, None, FA
Derived from: YH-170-(p-Br)_Carbon-1-1.jdf

```

```

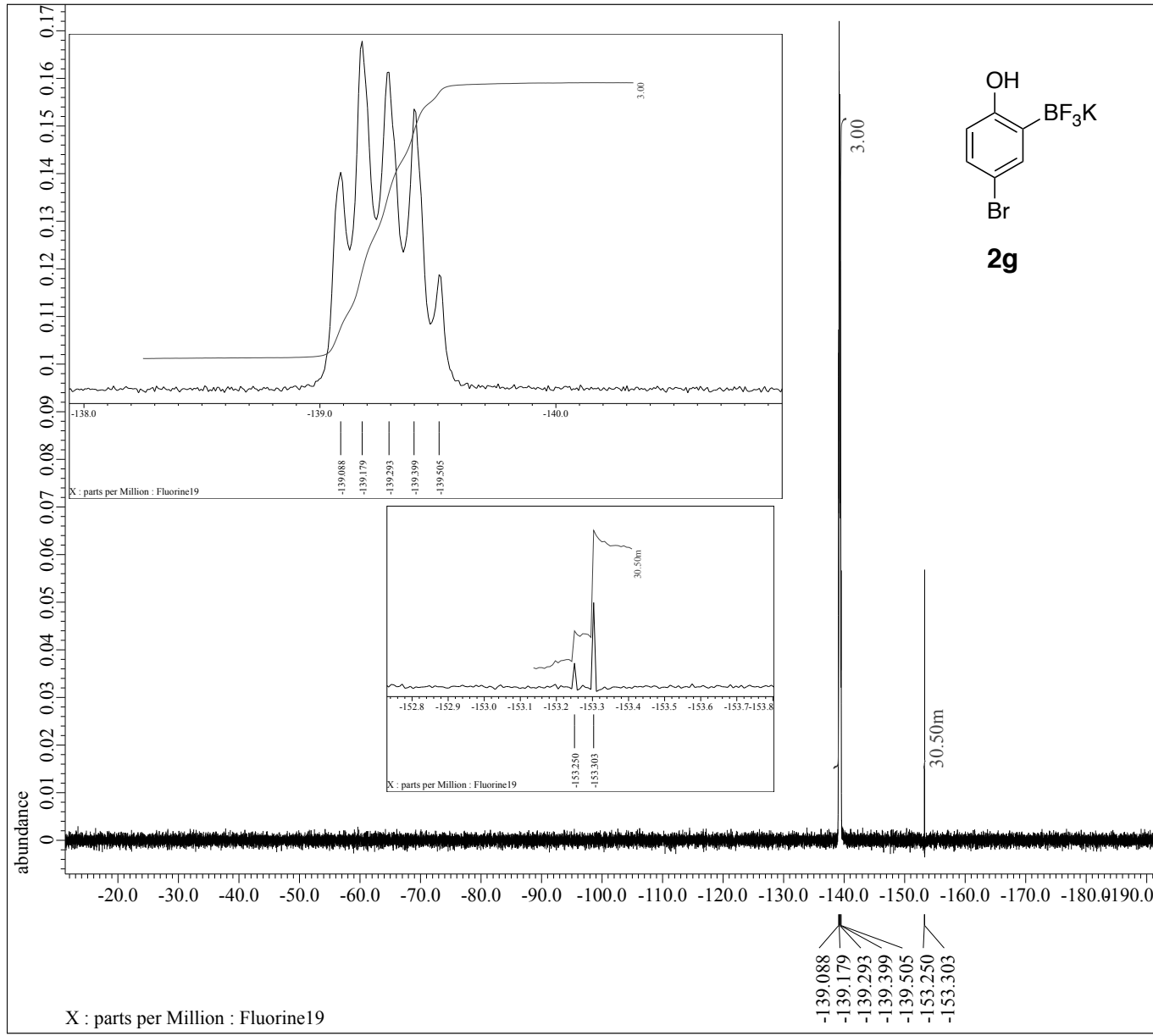
Filename           = YH-170-(p-Br)_Carb
Author             = delta
Experiment         = carbon.jxp
Sample_Id          = YH-170-(p-Br)
Solvent            = ACETONE-D6
Actual_Start_Time  = 22-FEB-2020 00:05:
Revision_Time      = 9-APR-2020 14:25:

Comment           = single pulse decou
Data_Format       = 1D REAL
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             = 3000
Total_Scans       = 3000

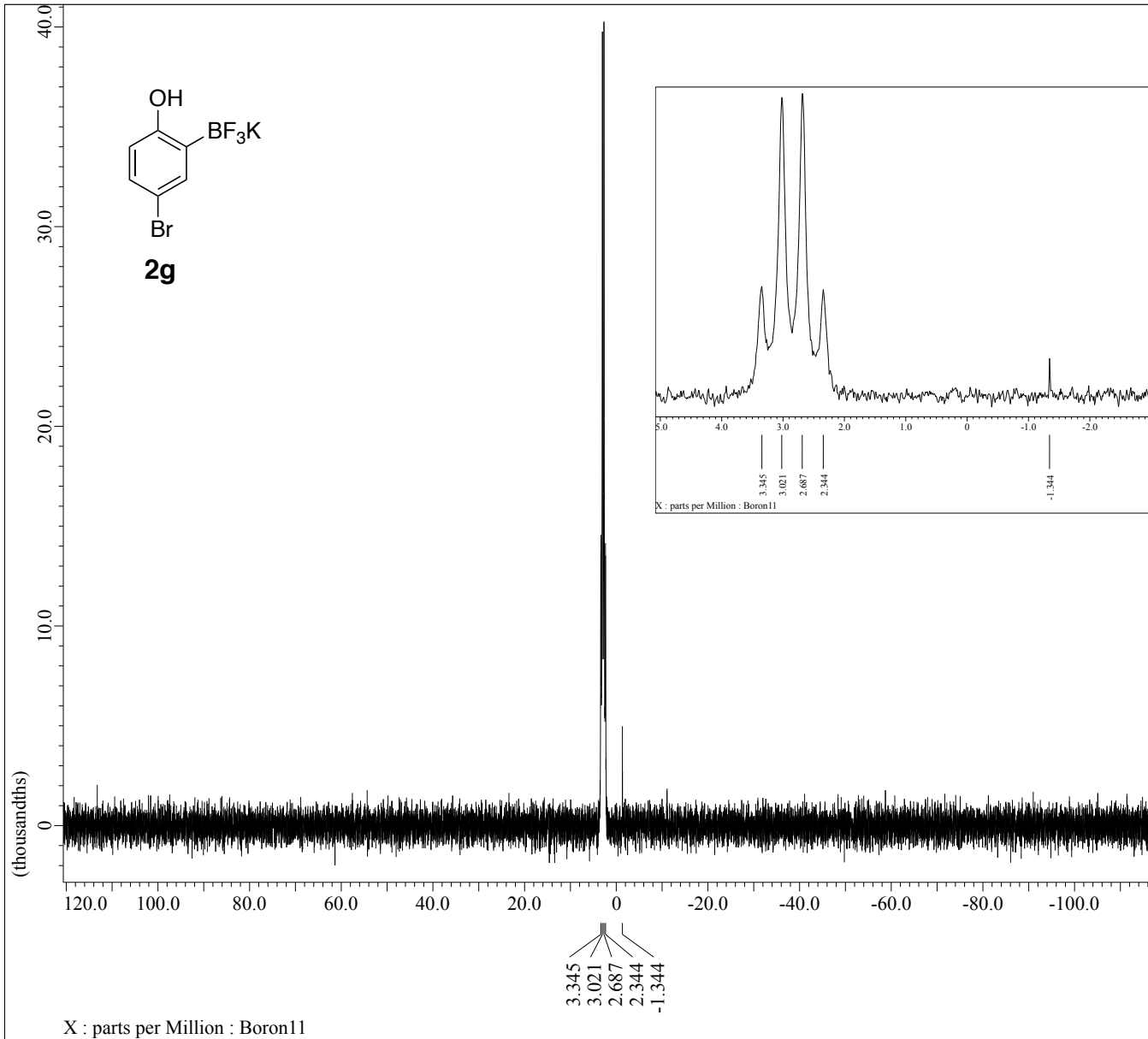
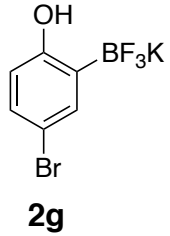
Relaxation_Delay  = 2[s]
Recvr Gain        = 56
Temp_Get          = 22.4[dC]
X_90_Width        = 13.48[us]
X_Acq_Time        = 0.8388608[s]
X_Angle           = 30[deg]
X_Atn             = 11[dB]
X_Pulse           = 4.49333333[us]
Irr_Atn_Dec       = 26.4[dB]
Irr_Atn_Dec_Calc = 26.4[dB]
Irr_Atn_Dec_Default_Calc = 26.4[dB]
Irr_Atn_Noise    = 26.4[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_Noise        = TRUE
Irr_Noise        = WALTZ

```



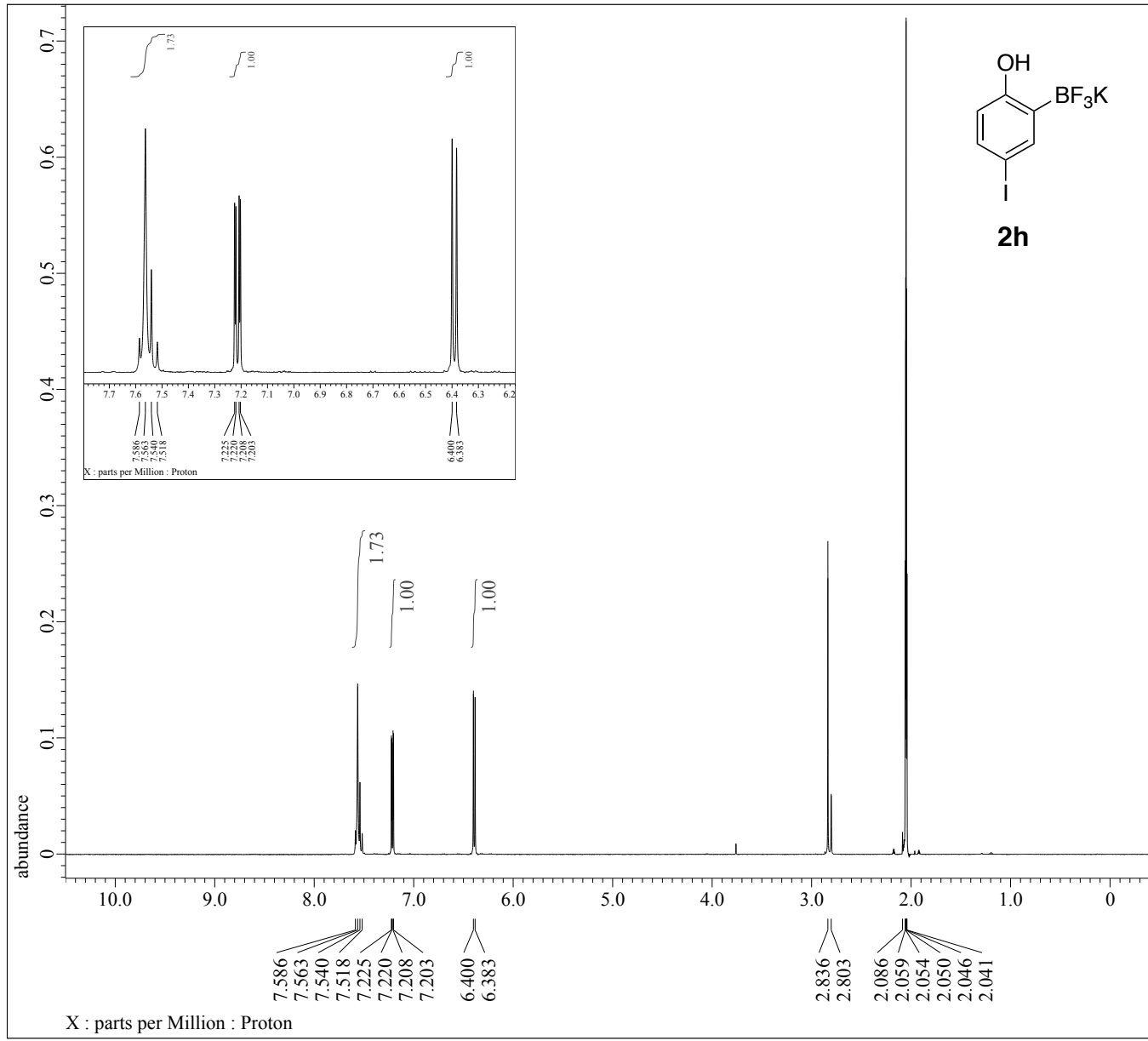
---- PROCESSING PARAMETERS ----
 sexp(0.2[Hz], 0.0[s])
 trapezoid(0[%], 0[%], 80[%], 100[%])
 zerofill(1)
 fft(1, TRUE, TRUE)
 machinephase
 ppm
 phase(-1.90826, 0, 50[%])
 base_correct(None, 0, Smooth)
 以下に由来 : YH-170-(p-Br)_19F-1-1.jdf

Filename	= YH-170-(p-Br)_19F-1-1
Author	= delta
Experiment	= single_pulse.jxp
Sample_Id	= YH-170-(p-Br)
Solvent	= ACETONE-D6
Creation_Time	= 21-FEB-2020 18:36:18
Revision_Time	= 22-FEB-2020 19:06:16
Current_Time	= 22-FEB-2020 19:06:53
Comment	= single_pulse
Data_Format	= 1D_REAL
Dim_Size	= 26214
Dim_Title	= Fluorine19
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ500R/s1
Field_Strength	= 11.62926421[T] (500[M
X_Acq_Duration	= 0.28311552[s]
X_Domain	= 19F
X_Freq	= 465.88941346[MHz]
X_Offset	= -100[ppm]
X_Points	= 32768
X_Prescans	= 1
X_Resolution	= 3.5321271[Hz]
X_Sweep	= 115.74074074[kHz]
X_Sweep_Clippped	= 92.59259259[kHz]
Irr_Domain	= Fluorine19
Irr_Freq	= 465.88941346[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Fluorine19
Tri_Freq	= 465.88941346[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Decimation_Reg	= r : 54 (53), g : 29
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 56
Temp_Get	= 21.8[dC]
X_90_Width	= 7.81[us]
X_Acq_Time	= 0.28311552[s]
X_Angle	= 45[deg]
X_Atn	= 3.7[dB]
X_Pulse	= 3.905[us]
Irr_Mode	= Off
Tri_Mode	= Off
Comment_1	= *** Pulse ***
Comment_111	= *** presat time ***
Comment_201	= *** obs_dante presatu
Comment_202	= *** irr_preaturation
Comment_203	= *** tri_preaturation



---- PROCESSING PARAMETERS ----
 sexp(2.0[Hz], 0.0[s])
 trapezoid(0[%], 0[%], 80[%], 100[%])
 zerofill(1)
 fft(1, TRUE, TRUE)
 machinephase
 ppm
 phase(27.63086, 0, 50[%])
 base_correct(None, 0, Smooth)
 以下に由来 : YH-170-(p-Br)_11B_1Hdec-1-1.jdf

Filename = YH-170-(p-Br)_11B_
 Author = delta
 Experiment = single_pulse_dec.j
 Sample_Id = YH-170-(p-Br)
 Solvent = ACETONE-D6
 Creation_Time = 21-FEB-2020 18:40:
 Revision_Time = 7-MAR-2020 15:07:
 Current_Time = 7-MAR-2020 15:08:
 Comment = single_pulse_decou
 Data_Format = 1D_REAL
 Dim_Size = 26214
 Dim_Title = Boron11
 Dim_Units = [ppm]
 Dimensions = X
 Spectrometer = JNM-ECZ500R/S1
 Field_Strength = 11.62926421[T] (50
 X_Acq_Duration = 0.66060288[s]
 X_Domain = 11B
 X_Freq = 158.85814241[MHz]
 X_Offset = 0[ppm]
 X_Points = 32768
 X_Prescans = 4
 X_Resolution = 1.51376876[Hz]
 X_Sweep = 49.6031746[kHz]
 X_Sweep_Clippped = 39.68253968[kHz]
 Irr_Domain = Proton
 Irr_Freq = 495.13191398[MHz]
 Irr_Offset = 5[ppm]
 Clipped = FALSE
 Decimation_Reg = r: 252(251),g: 40
 Scans = 100
 Total_Scans = 100
 Relaxation_Delay = 2[s]
 Recvr_Gain = 56
 Temp_Get = 21.8[dC]
 X_90_Width = 15.74[us]
 X_Acq_Time = 0.66060288[s]
 X_Angle = 30[deg]
 X_Atn = 10.4[dB]
 X_Pulse = 5.24666667[us]
 Irr_Atn_Dec = 26.4[dB]
 Irr_Atn_Dec_Calc = 26.4[dB]
 Irr_Atn_Dec_Default_Calc = 26.4[dB]
 Irr_Atn_No = 26.4[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_No = TRUE



```

---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
phase( 3, -20, 69.89901[%] )
以下に由来 : YH-14 (p-I)_Proton-1-1.jdf

```

```

Filename      = YH-14 (p-I)_Proton-1-6
Author        = delta
Experiment    = proton.jxp
Sample_Id     = YH-14 (p-I)
Solvent       = ACETONE-D6
Creation_Time = 22-FEB-2020 13:47:18
Revision_Time = 7-MAR-2020 14:57:00
Current_Time  = 7-MAR-2020 14:58:06

```

```

Comment       = single pulse
Data Format    = 1D COMPLEX
Dim Size      = 104858
Dim Title     = Proton
Dim Units     = [ppm]
Dimensions    = X
Spectrometer  = JNM-ECZ500R/s1

```

```

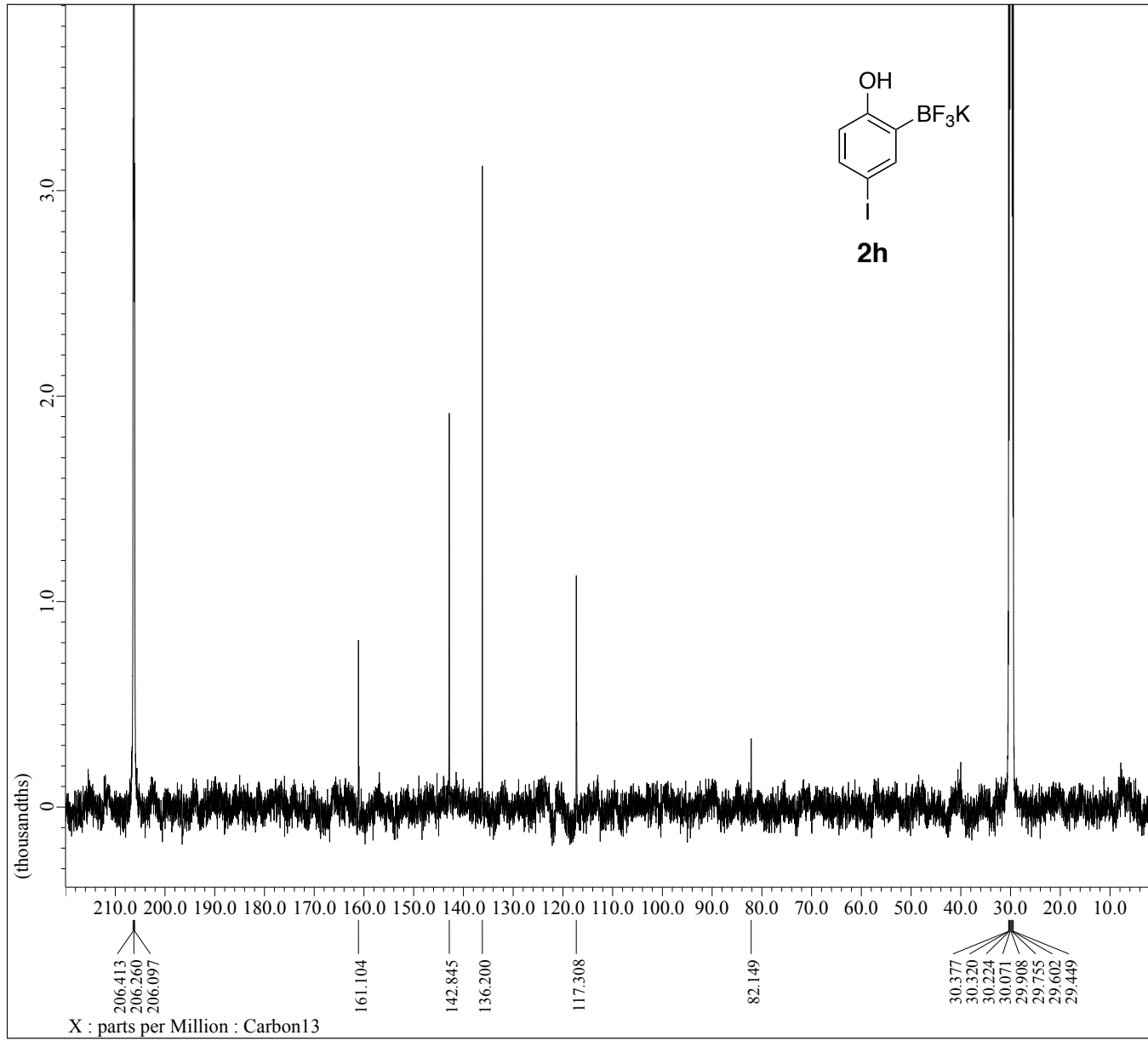
Field Strength = 11.62926421[T] (500[M]
X_Acq_Duration = 14.11383296[s]
X_Domain       = 1H
X_Freq         = 495.13191398[MHz]
X_Offset       = 5[ppm]
X_Points       = 131072
X_Prescans     = 1
X_Resolution   = 70.85247522[mHz]
X_Sweep        = 9.28677563[kHz]
X_Sweep_Clippped = 7.42942051[kHz]
Irr_Domain     = Proton
Irr_Freq       = 495.13191398[MHz]
Irr_Offset     = 5[ppm]
Tri_Domain     = Proton
Tri_Freq       = 495.13191398[MHz]
Tri_Offset     = 5[ppm]
Clipped        = FALSE
Decimation_Reg = r : 1346 ( 1345 ), g : 52
Scans          = 8
Total_Scans    = 8

```

```

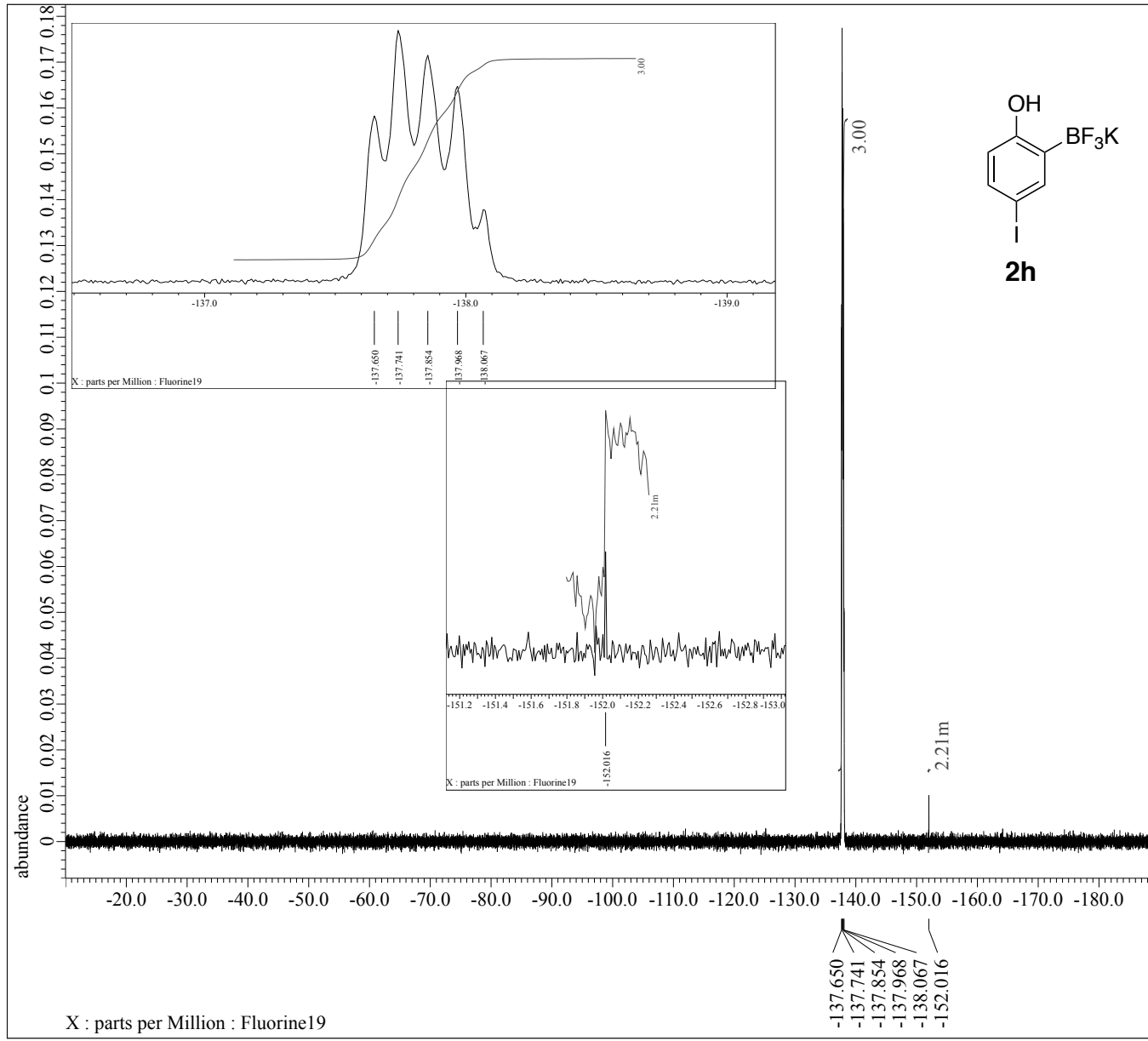
Relaxation_Delay = 3[s]
Recvr Gain       = 66
Temp_Get         = 22[dC]
X_90_Width       = 7.12[us]
X_Acq_Time       = 14.11383296[s]
X_Angle          = 45[deg]
X_Atn            = 3.3[dB]
X_Pulse          = 3.56[us]
Irr_Mode         = Off
Tri_Mode         = Off
Comment_1        = *** Pulse ***
Comment_111      = *** presat time ***
Comment_201      = *** obs_dante presatu
Comment_202      = *** irr_ preaturation
Comment_203      = *** tri_ preaturation

```



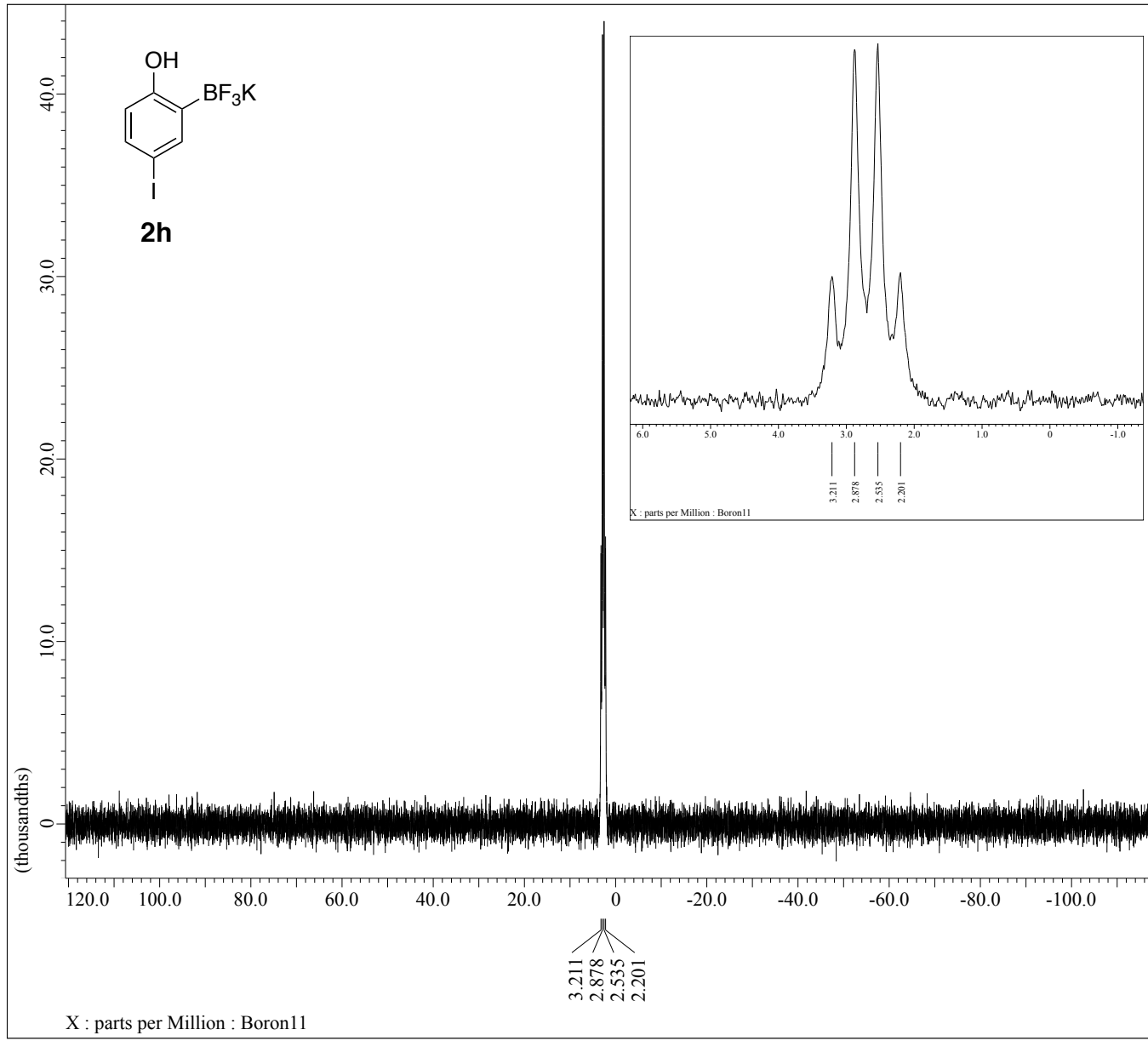
---- PROCESSING PARAMETERS ----
 sexp(2.0[Hz], 0.0[s])
 trapezoid(0[%], 0[%], 80[%], 100[%])
 zerofill(1, TRUE)
 fft(1, TRUE, TRUE)
 machinephase
 ppm
 phase(4, 7, 7.81673[%])
 base_correct(Akima, 5, 0, FALSE, 3, None, FA)
 Derived from: YH-14(p-I)_Carbon-1-1.jdf

Filename	= YH-14(p-I)_Carbon-
Author	= delta
Experiment	= carbon.jxp
Sample Id	= YH-14(p-I)
Solvent	= ACETONE-D6
Actual_Start_Time	= 24-FEB-2020 21:57:
Revision_Time	= 9-APR-2020 14:19:
Comment	= single pulse decou
Data Format	= 1D REAL
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	= 5000
Total_Scans	= 5000
Relaxation_Delay	= 2[s]
Recvr Gain	= 56
Temp_Get	= 22[dC]
X 90_Width	= 13.48[us]
X Acq Time	= 0.8388608[s]
X Angle	= 30[deg]
X Atn	= 11[dB]
X Pulse	= 4.49333333[us]
Irr Atn Dec	= 26.4[dB]
Irr Atn Dec Calc	= 26.4[dB]
Irr Atn Dec Default_Calc	= 26.4[dB]
Irr Atn Noe	= 26.4[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



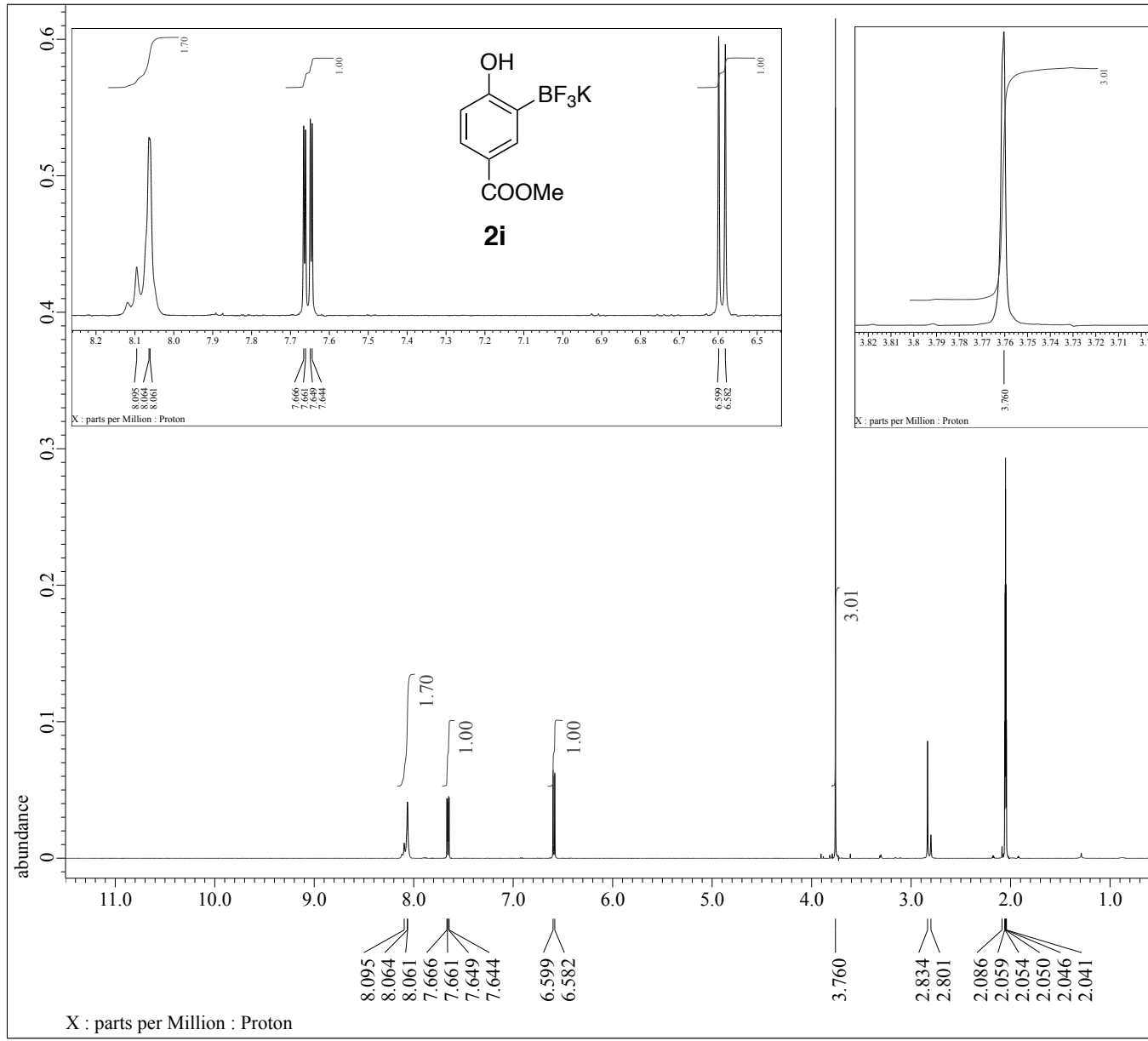
---- PROCESSING PARAMETERS ----
 sexp(0.2[Hz], 0.0[s])
 trapezoid(0[%], 0[%], 80[%], 100[%])
 zerofill(1)
 fft(1, TRUE, TRUE)
 machinephase
 ppm
 phase(-0.73926, 0, 50[%])
 base_correct(None, 0, Smooth)
 以下に由来 : YH-14 (p-I)_19F-1-1.jdf

Filename	= YH-14 (p-I)_19F-1-6.jd
Author	= delta
Experiment	= single pulse.jxp
Sample Id	= YH-14 (p-I)
Solvent	= ACETONE-D6
Creation Time	= 22-FEB-2020 13:51:46
Revision Time	= 22-FEB-2020 19:23:29
Current Time	= 22-FEB-2020 19:23:43
Comment	= single pulse
Data Format	= 1D REAL
Dim Size	= 26214
Dim Title	= Fluorine19
Dim Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ500R/s1
Field Strength	= 11.62926421[T] (500[M
X Acq Duration	= 0.28311552[s]
X Domain	= 19F
X Freq	= 465.88941346[MHz]
X Offset	= -100 [ppm]
X Points	= 32768
X Prescans	= 1
X Resolution	= 3.5321271 [Hz]
X Sweep	= 115.74074074 [kHz]
X Sweep Clipped	= 92.59259259 [kHz]
Irr Domain	= Fluorine19
Irr Freq	= 465.88941346[MHz]
Irr Offset	= 5 [ppm]
Tri Domain	= Fluorine19
Tri Freq	= 465.88941346[MHz]
Tri Offset	= 5 [ppm]
Clipped	= FALSE
Decimation_Reg	= r : 54 (53), g : 29
Scans	= 8
Total_Scans	= 8
Relaxation Delay	= 5 [s]
Recvr Gain	= 56
Temp Get	= 21.9 [dC]
X 90_Width	= 7.81 [us]
X Acq Time	= 0.28311552 [s]
X Angle	= 45 [deg]
X Atn	= 3.7 [dB]
X Pulse	= 3.905 [us]
Irr Mode	= Off
Tri Mode	= Off
Comment_1	= *** Pulse ***
Comment_111	= *** presat time ***
Comment_201	= *** obs_dante presatu
Comment_202	= *** irr_preaturation
Comment_203	= *** tri_preaturation



---- PROCESSING PARAMETERS ----
 sexp(2.0[Hz], 0.0[s])
 trapezoid(0[%], 0[%], 80[%], 100[%])
 zerofill(1)
 fft(1, TRUE, TRUE)
 machinephase
 ppm
 phase(14.75953, 0, 50[%])
 base_correct(None, 0, Smooth)
 以下に由来 : YH-14 (p-I)_11B_1Hdec-1-1. jdf

Filename	= YH-14 (p-I)_11B_1Hd
Author	= delta
Experiment	= single_pulse_dec.j
Sample Id	= YH-14 (p-I)
Solvent	= ACETONE-D6
Creation Time	= 22-FEB-2020 13:55:
Revision Time	= 22-FEB-2020 18:57:
Current Time	= 22-FEB-2020 18:59:
Comment	= single pulse decou
Data Format	= 1D REAL
Dim Size	= 26214
Dim Title	= Boron11
Dim Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ500R/S1
Field Strength	= 11.62926421[T] (50
X Acq Duration	= 0.66060288[s]
X Domain	= 11B
X Freq	= 158.85814241[MHz]
X Offset	= 0[ppm]
X Points	= 32768
X Prescans	= 4
X Resolution	= 1.51376876[Hz]
X Sweep	= 49.6031746[kHz]
X Sweep Clipped	= 39.68253968[kHz]
Irr Domain	= Proton
Irr Freq	= 495.13191398[MHz]
Irr Offset	= 5[ppm]
Clipped	= TRUE
Decimation_Reg	= r: 252(251),g: 40
Scans	= 100
Total_Scans	= 100
Relaxation_Delay	= 2[s]
Recvr Gain	= 56
Temp_Get	= 22.2[dC]
X 90 Width	= 15.74[us]
X Acq Time	= 0.66060288[s]
X Angle	= 30[deg]
X Atn	= 10.4[dB]
X Pulse	= 5.24666667[us]
Irr Atn Dec	= 26.4[dB]
Irr Atn Dec Calc	= 26.4[dB]
Irr Atn Dec_Default_Calc	= 26.4[dB]
Irr Atn Noe	= 26.4[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



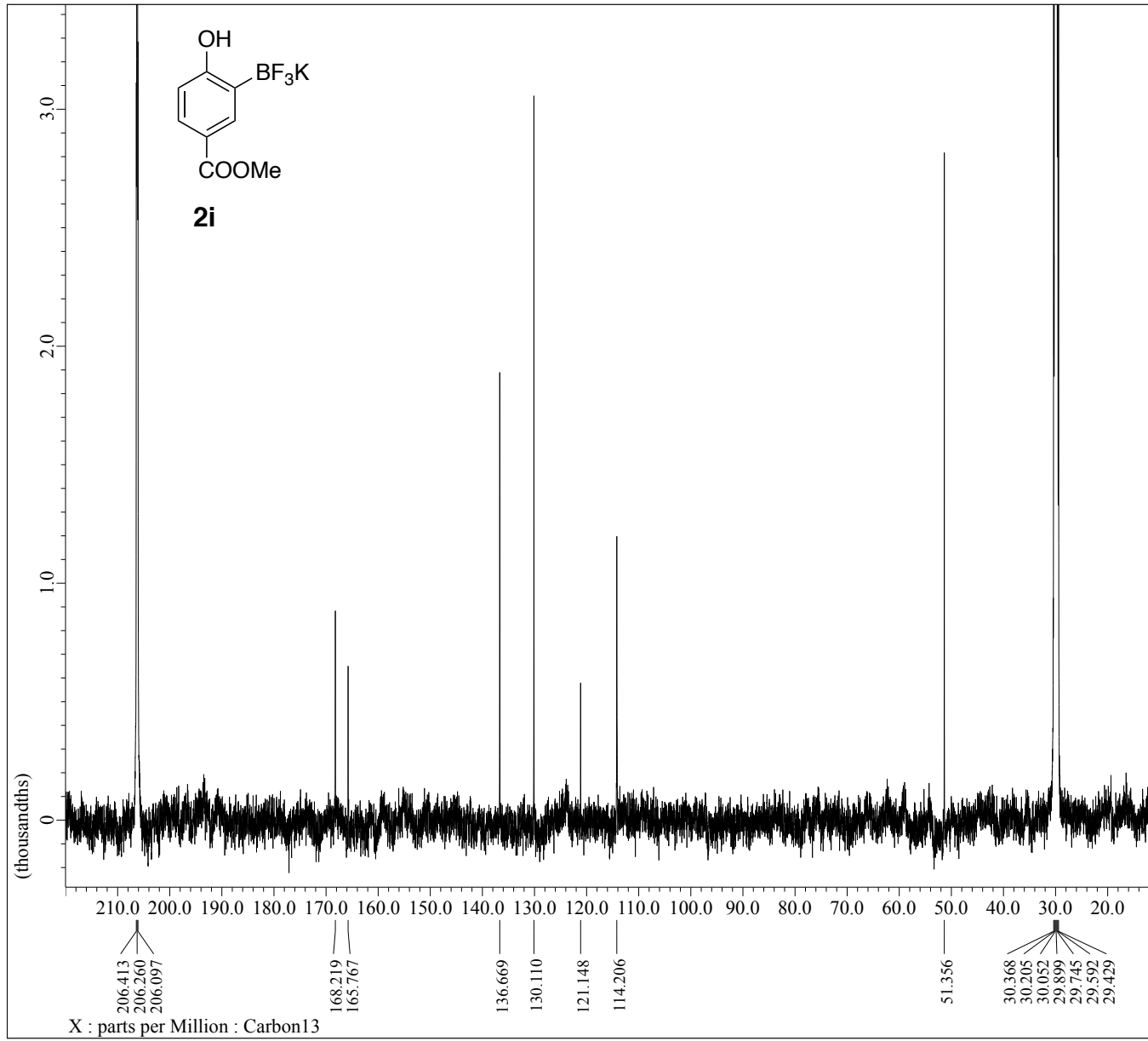
---- PROCESSING PARAMETERS ----
 sexp(0.2[Hz], 0.0[s])
 trapezoid(0[%], 0[%], 80[%], 100[%])
 zerofill(1)
 fft(1, TRUE, TRUE)
 machinephase
 ppm
 phase(3.5, -24, 69.66154[%])
 base_correct(None, 0, Smooth)
 以下に由来 : YH-78 (CO2Me)_Proton-1-1.jdf

Filename = YH-78 (CO2Me)_Proton-1
 Author = delta
 Experiment = proton.jxp
 Sample_Id = YH-78 (CO2Me)
 Solvent = ACETONE-D6
 Creation_Time = 22-FEB-2020 14:03:56
 Revision_Time = 9-MAR-2020 21:00:38
 Current_Time = 9-MAR-2020 21:00:59

Comment = single pulse
 Data_Format = 1D REAL
 Dim_Size = 104858
 Dim_Title = Proton
 Dim_Units = [ppm]
 Dimensions = X
 Spectrometer = JNM-ECZ500R/s1

Field_Strength = 11.62926421[T] (500[M]
 X_Acq_Duration = 14.11383296[s]
 X_Domain = 1H
 X_Freq = 495.13191398[MHz]
 X_Offset = 5[ppm]
 X_Points = 131072
 X_Prescans = 1
 X_Resolution = 70.85247522[mHz]
 X_Sweep = 9.28677563[kHz]
 X_Sweep_Clippped = 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
 Decimation_Reg = r : 1346 (1345), g : 52
 Scans = 8
 Total_Scans = 8

Relaxation_Delay = 3[s]
 Recvr_Gain = 56
 Temp_Get = 22.4[dC]
 X_90_Width = 7.12[us]
 X_Acq_Time = 14.11383296[s]
 X_Angle = 45[deg]
 X_Atn = 3.3[dB]
 X_Pulse = 3.56[us]
 Irr_Mode = Off
 Tri_Mode = Off
 Comment_1 = *** Pulse ***
 Comment_111 = *** presat time ***
 Comment_201 = *** obs_dante presatu
 Comment_202 = *** irr_preaturation
 Comment_203 = *** tri_preaturation



```

---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
phase( 3.25, 8, 7.98077[%] )
base_correct( Akima, 5, 0, FALSE, 3, None, FA
phase( 0, 0, 8.20204[%] )
reference( 205.3725[ppm], 206.26[ppm] )

Derived from: YH-78(CO2Me)_Carbon-1-1.jdf

```

```

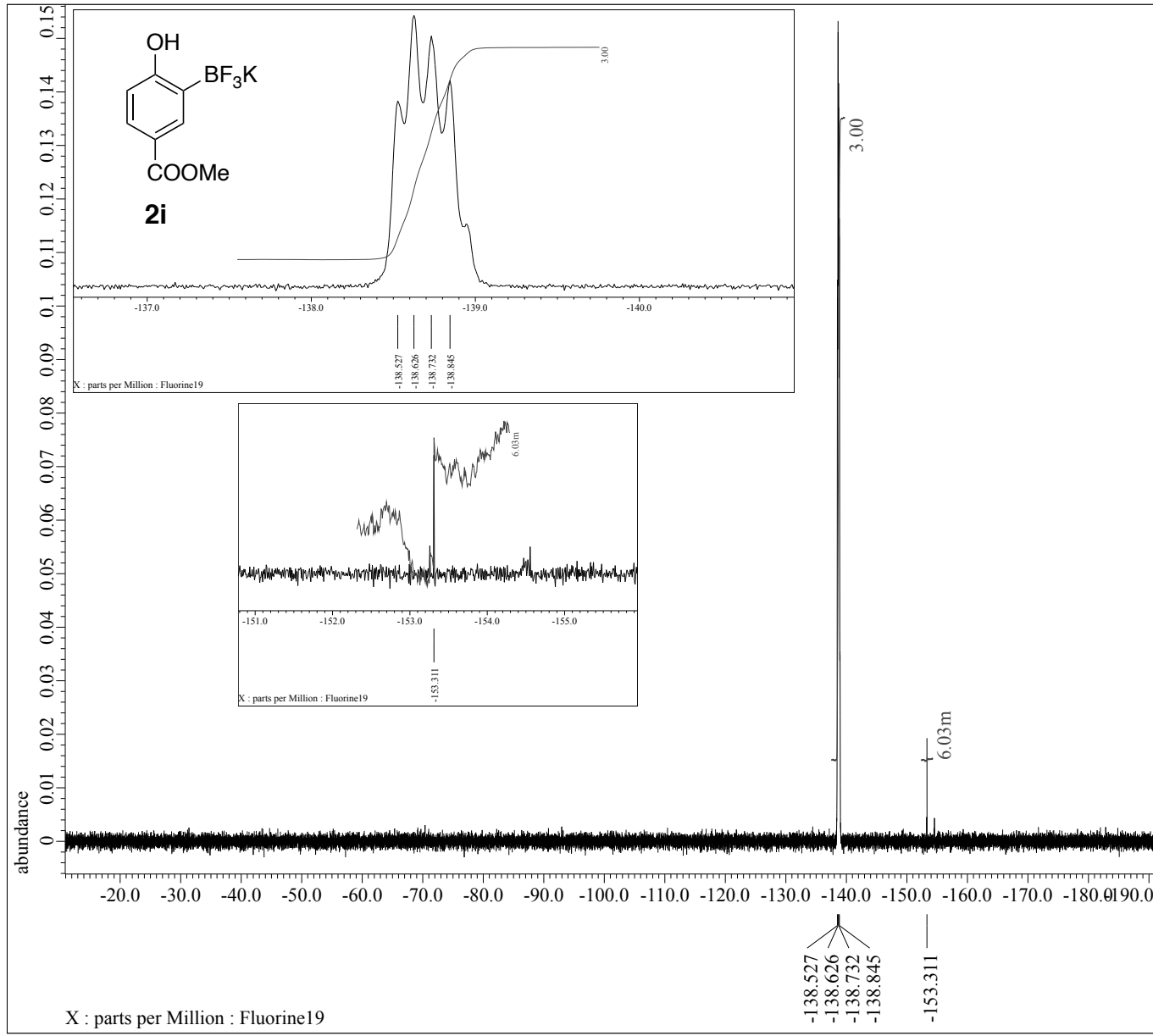
Filename           = YH-78(CO2Me)_Carbo
Author             = delta
Experiment         = carbon.jxp
Sample_Id          = YH-78(CO2Me)
Solvent            = ACETONE-D6
Actual_Start_Time  = 25-FEB-2020 02:00:
Revision_Time      = 13-APR-2020 17:49:

Comment           = single pulse decou
Data_Format       = 1D REAL
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             = 5000
Total_Scans       = 5000

Relaxation_Delay  = 2[s]
Recvr_Gain        = 56
Temp_Get          = 20.7[dC]
X_90_Width        = 13.48[us]
X_Acq_Time        = 0.8388608[s]
X_Angle           = 30[deg]
X_Atn             = 11[dB]
X_Pulse           = 4.49333333[us]
Irr_Atn_Dec       = 26.4[dB]
Irr_Atn_Dec_Calc = 26.4[dB]
Irr_Atn_Dec_Default_Calc = 26.4[dB]
Irr_Atn_Noise    = 26.4[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_Noise        = TRUE
Irr_Noise        = WALTZ

```



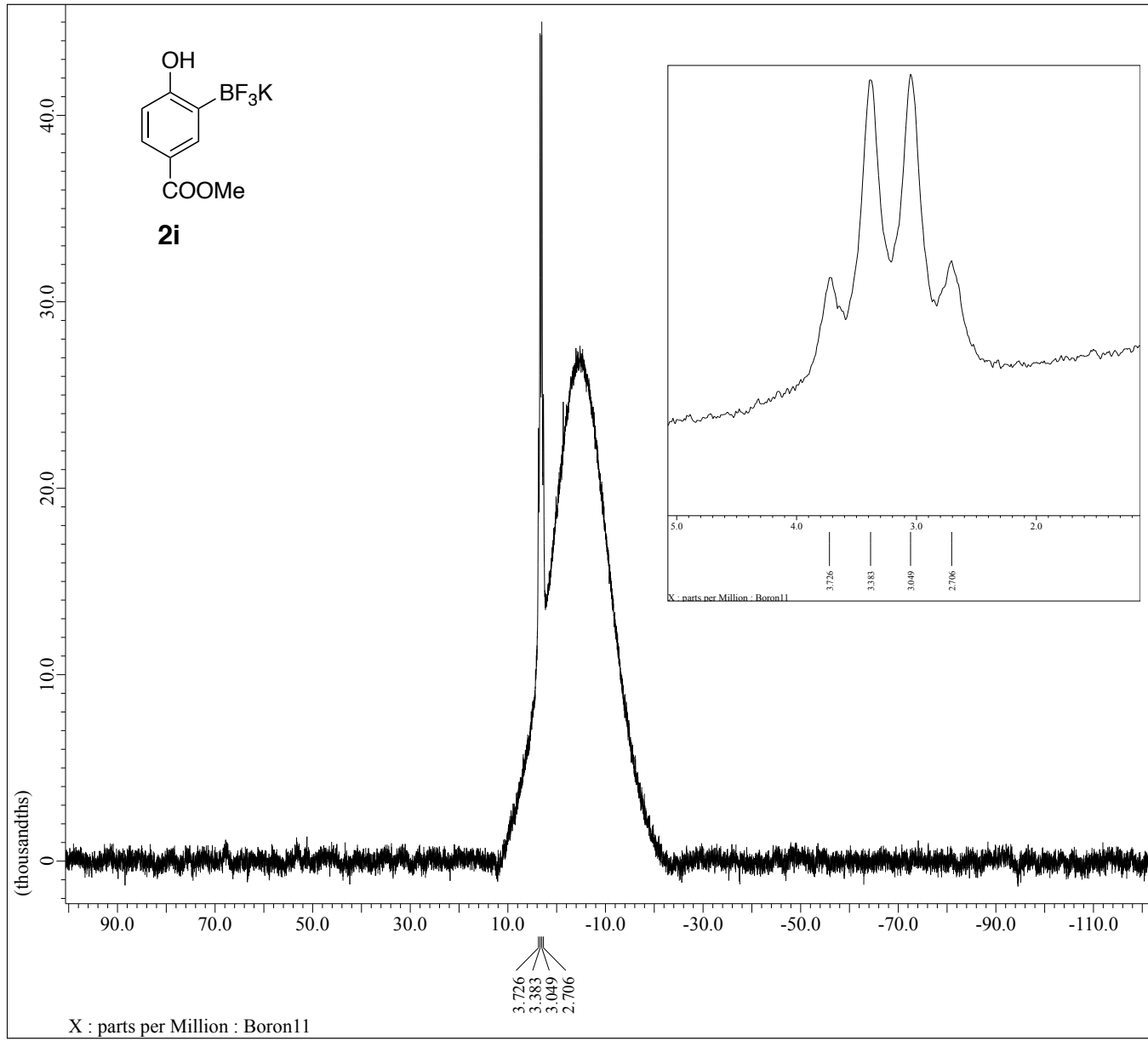
---- PROCESSING PARAMETERS ----
 sexp(0.2[Hz], 0.0[s])
 trapezoid(0[%], 0[%], 80[%], 100[%])
 zerofill(1)
 fft(1, TRUE, TRUE)
 machinephase
 ppm
 phase(-4.689, 0, 50[%])
 base_correct(None, 0, Smooth)
 以下に由来 : YH-78 (CO2Me)_19F-1-1.jdf

Filename = YH-78 (CO2Me)_19F-1-5.
 Author = delta
 Experiment = single pulse.jxp
 Sample Id = YH-78 (CO2Me)
 Solvent = ACETONE-D6
 Creation Time = 22-FEB-2020 14:08:23
 Revision Time = 22-FEB-2020 19:09:35
 Current Time = 22-FEB-2020 19:11:11

Comment = single pulse
 Data Format = 1D REAL
 Dim Size = 26214
 Dim Title = Fluorine19
 Dim Units = [ppm]
 Dimensions = X
 Spectrometer = JNM-ECZ500R/s1

Field Strength = 11.62926421[T] (500[M]
 X Acq Duration = 0.28311552[s]
 X Domain = 19F
 X Freq = 465.88941346[MHz]
 X Offset = -100[ppm]
 X Points = 32768
 X Prescans = 1
 X Resolution = 3.5321271[Hz]
 X Sweep = 115.74074074[kHz]
 X Sweep Clipped = 92.59259259[kHz]
 Irr Domain = Fluorine19
 Irr Freq = 465.88941346[MHz]
 Irr Offset = 5[ppm]
 Tri Domain = Fluorine19
 Tri Freq = 465.88941346[MHz]
 Tri Offset = 5[ppm]
 Clipped = FALSE
 Decimation_Reg = r: 54 (53),g: 29
 Scans = 8
 Total_Scans = 8

Relaxation Delay = 5[s]
 Recvr Gain = 56
 Temp Get = 22.1[dC]
 X 90_Width = 7.81[us]
 X Acq Time = 0.28311552[s]
 X Angle = 45[deg]
 X Atn = 3.7[dB]
 X Pulse = 3.905[us]
 Irr Mode = Off
 Tri Mode = Off
 Comment_1 = *** Pulse ***
 Comment_111 = *** presat time ***
 Comment_201 = *** obs_dante presatu
 Comment_202 = *** irr_preaturation
 Comment_203 = *** tri_preaturation



```

---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
phase( 12.08005, 0, 50[%] )
base_correct( Akima, 5, 0, FALSE, 3, None, FA
Derived from: YH-78(CO2Me)_11B_1Hdec-1-1 (2) .

```

```

Filename      = YH-78(CO2Me)_11B_1
Author        = delta
Experiment    = single pulse dec.j
Sample_Id     = YH-78(CO2Me)
Solvent       = ACETONE-D6
Actual_Start_Time = 22-FEB-2020 20:19:
Revision_Time = 7-APR-2020 13:13:

```

```

Comment       = single pulse decou
Data_Format   = 1D REAL
Dim_Size      = 26214
X_Domain      = Boron11
Dim_Title     = Boron11
Dim_Units     = [ppm]
Dimensions    = X
Spectrometer  = JNM-ECZ500R/S1

```

```

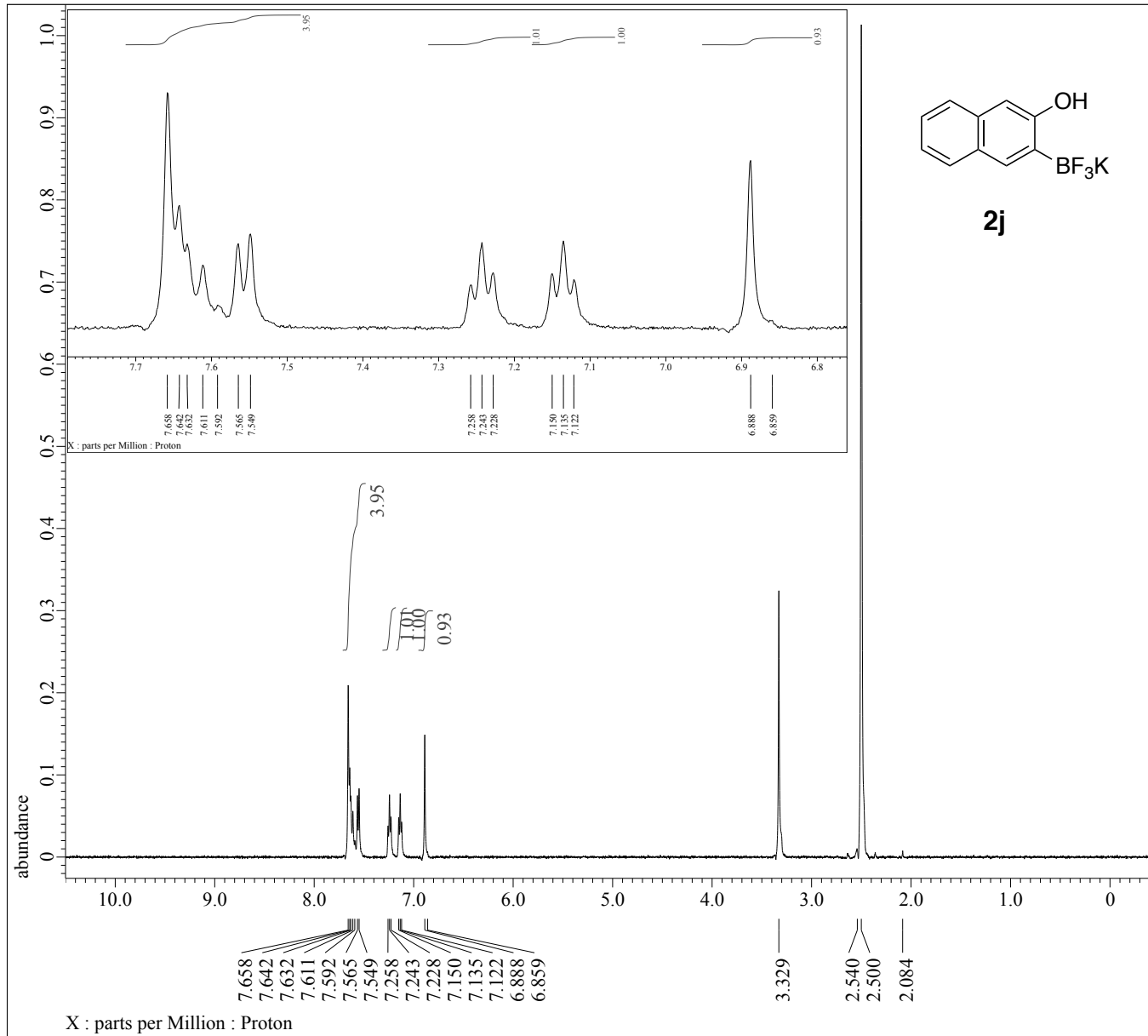
Field Strength = 11.62926421[T] (50
X_Acq_Duration = 0.66060288[s]
X_Domain       = 11B
X_Freq         = 158.85814241[MHz]
X_Offset       = 0[ppm]
X_Points       = 32768
X_Prescans     = 4
X_Resolution   = 1.51376876[Hz]
X_Sweep        = 49.6031746[kHz]
X_Sweep_Clippped = 39.68253968[kHz]
Irr_Domain     = Proton
Irr_Freq       = 495.13191398[MHz]
Irr_Offset     = 5[ppm]
Clipped        = TRUE
Scans          = 300
Total_Scans    = 300

```

```

Relaxation_Delay = 2[s]
Recvr_Gain       = 56
Temp_Get         = 21.8[dC]
X_90_Width      = 15.74[us]
X_Acq_Time       = 0.66060288[s]
X_Angle          = 30[deg]
X_Atn            = 10.4[dB]
X_Pulse          = 5.24666667[us]
Irr_Atn_Dec      = 26.4[dB]
Irr_Atn_Dec_Calc = 26.4[dB]
Irr_Atn_Dec_Default_Calc = 26.4[dB]
Irr_Atn_Noise    = 26.4[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_Noise        = TRUE
Irr_Noise        = WALTZ

```



```

---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
phase( -3, -17, 40.67603[%] )
base_correct( None, 0, Smooth )

```

以下に由来 : YH-134-(Np)_Proton-1-1.jdf

```

Filename      = YH-134-(Np)_Proton-1-
Author        = delta
Experiment    = proton.jxp
Sample_Id     = YH-134-(Np)
Solvent       = ACETONE-D6
Creation_Time = 22-FEB-2020 18:03:07
Revision_Time = 9-MAR-2020 19:56:49
Current_Time  = 9-MAR-2020 19:57:32

```

```

Comment       = single pulse
Data Format    = 1D REAL
Dim Size      = 13107
Dim Title     = Proton
Dim Units     = [ppm]
Dimensions    = X
Spectrometer  = JNM-ECZ500R/s1

```

```

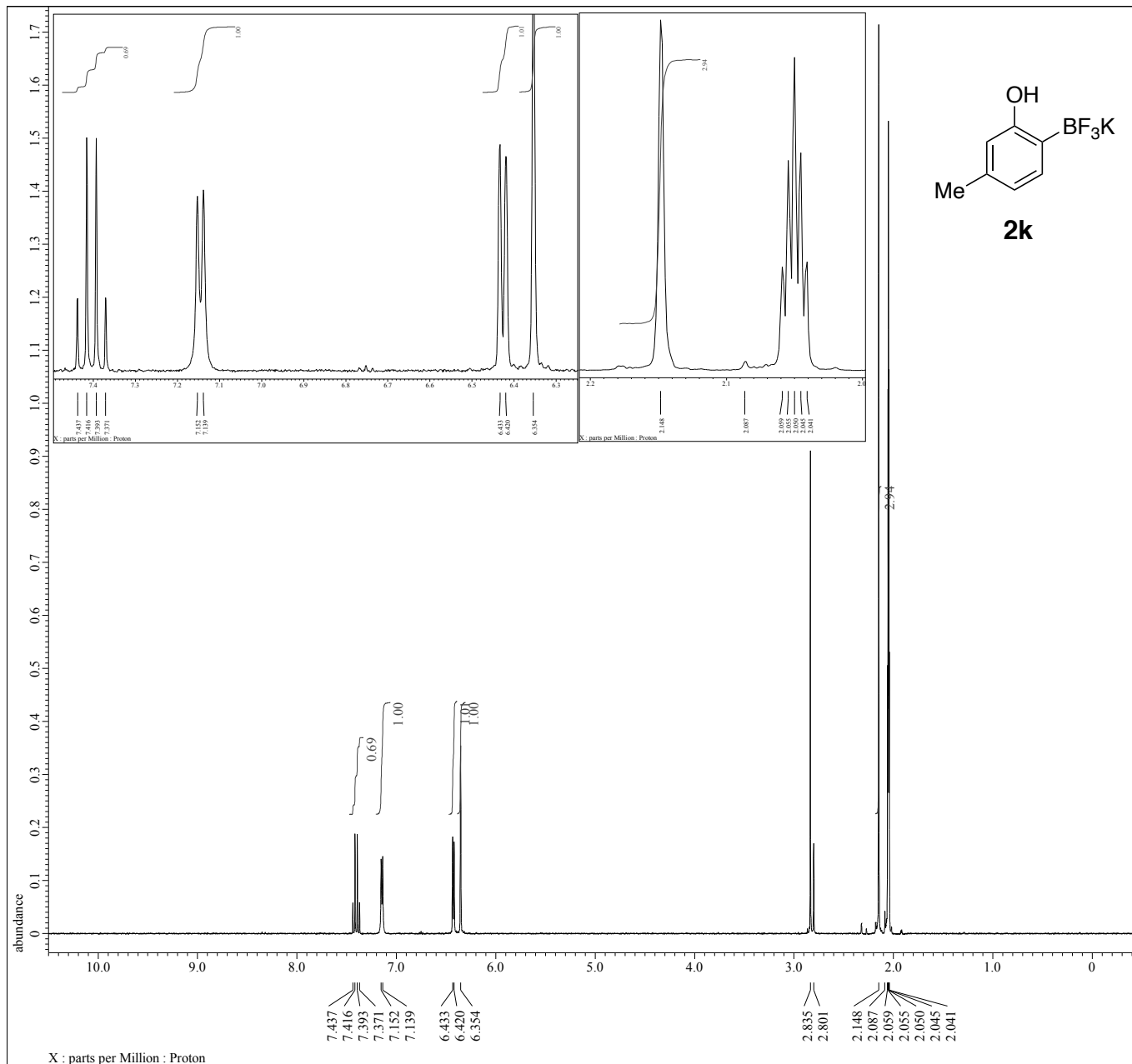
Field Strength = 11.62926421[T] (500[M]
X_Acq_Duration = 1.76422912[s]
X_Domain       = 1H
X_Freq         = 495.13191398[MHz]
X_Offset       = 5[ppm]
X_Points       = 16384
X_Prescans     = 1
X_Resolution   = 0.5668198[Hz]
X_Sweep        = 9.28677563[kHz]
X_Sweep_Clippped = 7.42942051[kHz]
Irr_Domain     = Proton
Irr_Freq       = 495.13191398[MHz]
Irr_Offset     = 5[ppm]
Tri_Domain     = Proton
Tri_Freq       = 495.13191398[MHz]
Tri_Offset     = 5[ppm]
Clipped        = FALSE
Decimation_Reg = r : 1346( 1345),g : 52
Scans          = 1
Total_Scans    = 1

```

```

Relaxation_Delay = 5[s]
Recvr Gain       = 56
Temp_Get         = 21.8[dC]
X_90_Width       = 7.12[us]
X_Acq_Time       = 1.76422912[s]
X_Angle          = 45[deg]
X_Atn            = 3.3[dB]
X_Pulse         = 3.56[us]
Irr_Mode         = Off
Tri_Mode         = Off
Comment_1        = *** Pulse ***
Comment_111      = *** presat time ***
Comment_201      = *** obs_dante_presatu
Comment_202      = *** irr_preaturation
Comment_203      = *** tri_preaturation

```



```

---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zeroFill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
base_correct( None, 0, Smooth )

```

以下に由来: YH-110(m-Me)_Proton-1-1.jdf

```

Filename      = YH-110(m-Me)_Proton-1
Author        = delta
Experiment     = proton.jxp
Sample_Id     = YH-110(m-Me)
Solvent       = ACETONE-D6
Actual_Start_Time = 10-MAR-2020 22:20:20
Revision_Time = 11-MAR-2020 11:31:23

```

```

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

```

```

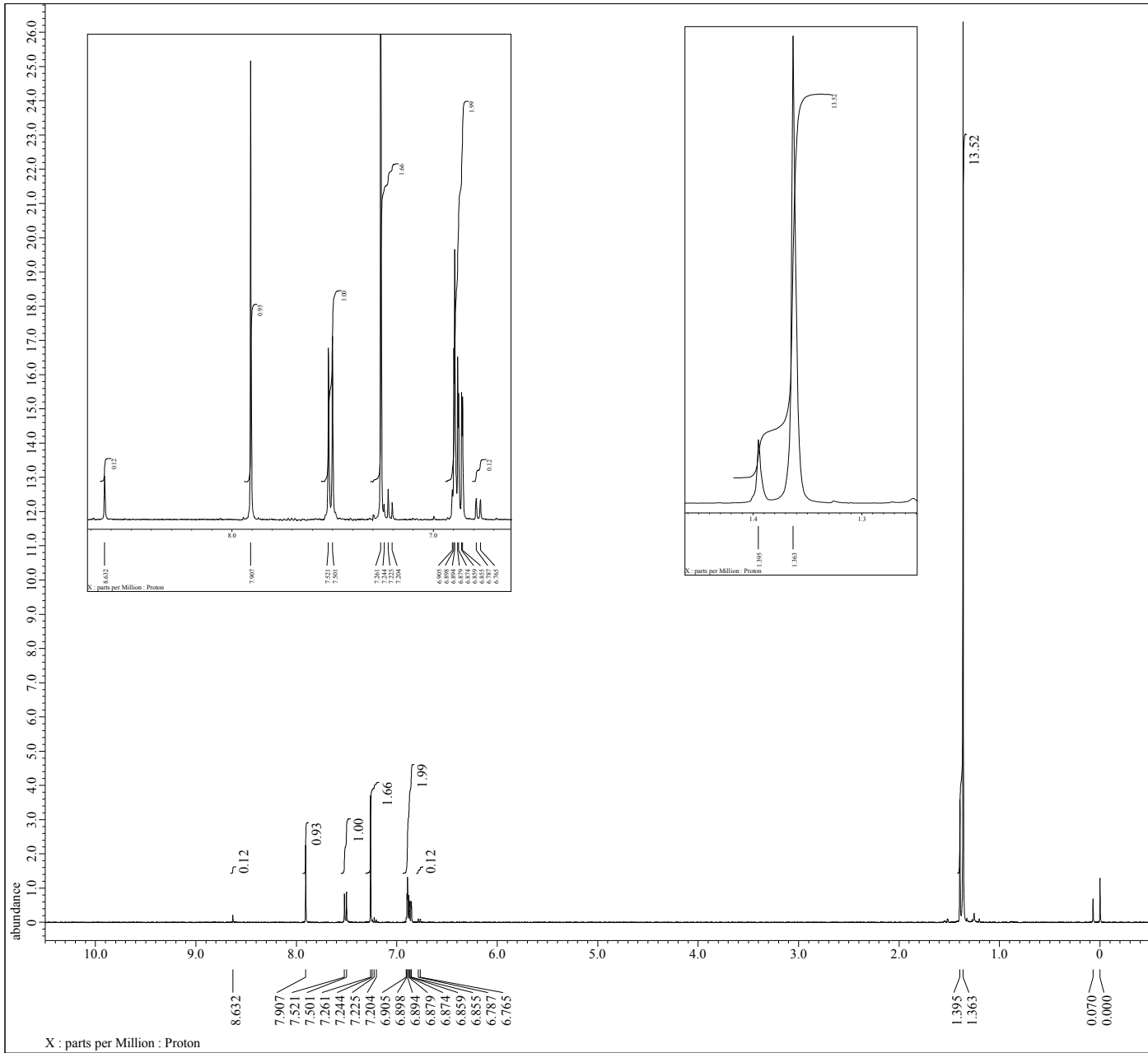
Field_Strength = 11.62926421[T] (500[M]
X_Acq_Duration = 1.76422912[s]
X_Domain       = 1H
X_Freq         = 495.13191398[MHz]
X_Offset       = 5[ppm]
X_Points       = 16384
X_Prescans     = 1
X_Resolution   = 0.5668198[Hz]
X_Sweep        = 9.28677563[kHz]
X_Sweep_Clipped = 7.42942051[kHz]
Irr_Domain     = 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          = 8
Total_Scans    = 8

```

```

Relaxation_Delay = 5[s]
Recvr_Gain       = 66
Temp_Get         = 21.8[dc]
X_90_Width       = 7.12[us]
X_Acq_Time       = 1.76422912[s]
X_Angle          = 45[deg]
X_Attn           = 3.3[dB]
X_Pulse          = 3.56[us]
Irr_Mode         = Off
Tri_Mode         = Off
Dante_Loop       = 500
Dante_Preset    = FALSE
Decimation_Rate = 0
Initial_Wait     = 1[s]
Phase            = (0, 90, 270, 180, 180)
Preset_Time      = 5[s]
Preset_Time_Plug = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time  = 6.76422912[s]

```



```

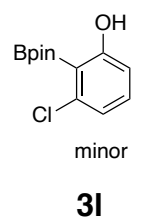
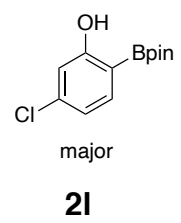
Filename = YH-254(m-Cl)_Proton-1-11.j
Author = iwawawa
Experiment = proton.jpg
Sample_Id = YH-254(m-Cl)
Solvent = CHLOROFORM-D
Creation_Time = 24-MAR-2020 20:20:36
Revision_Time = 8-APR-2020 12:15:58
Current_Time = 8-APR-2020 12:16:40

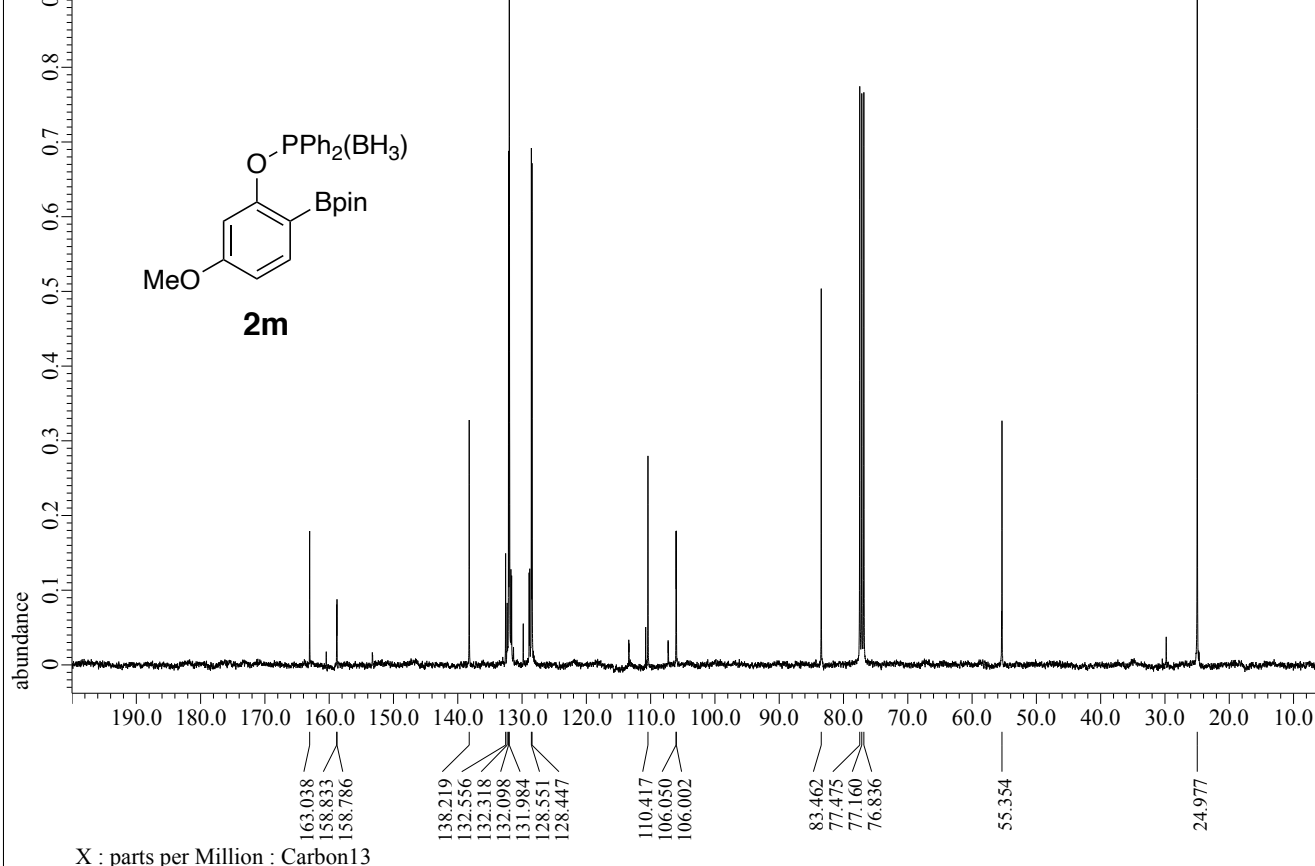
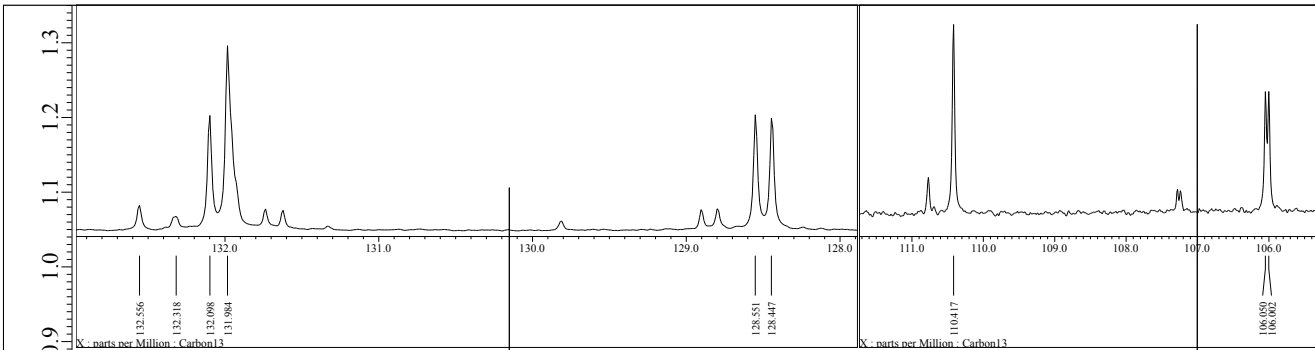
Comment = single_pulse
Data_Format = 1D_REAL
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR

Field_Strength = 9.389766[T] (400 [MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain = 1h
X_Freq = 399.78219838 [MHz]
X_Offset = 5 [ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45794685 [Hz]
X_Sweep = 7.5030012 [kHz]
X_Sweep_Clipped = 6.00240096 [kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838 [MHz]
Irr_Offset = 5 [ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838 [MHz]
Tri_Offset = 5 [ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8

Relaxation_Delay = 3 [s]
Recvr_Gain = 48
Temp_Get = 20.1 [dc]
X_90_Width = 6.1 [us]
X_Acq_Time = 2.18365952 [s]
X_Angle = 45 [deg]
X_Atn = 1 [dB]
X_Pulse = 3.05 [us]
Irr_Mode = Off
Tri_Mode = Off
Date_Presat = FALSE
Initial_Wait = 1 [s]
Repetition_Time = 5.18365952 [s]

```





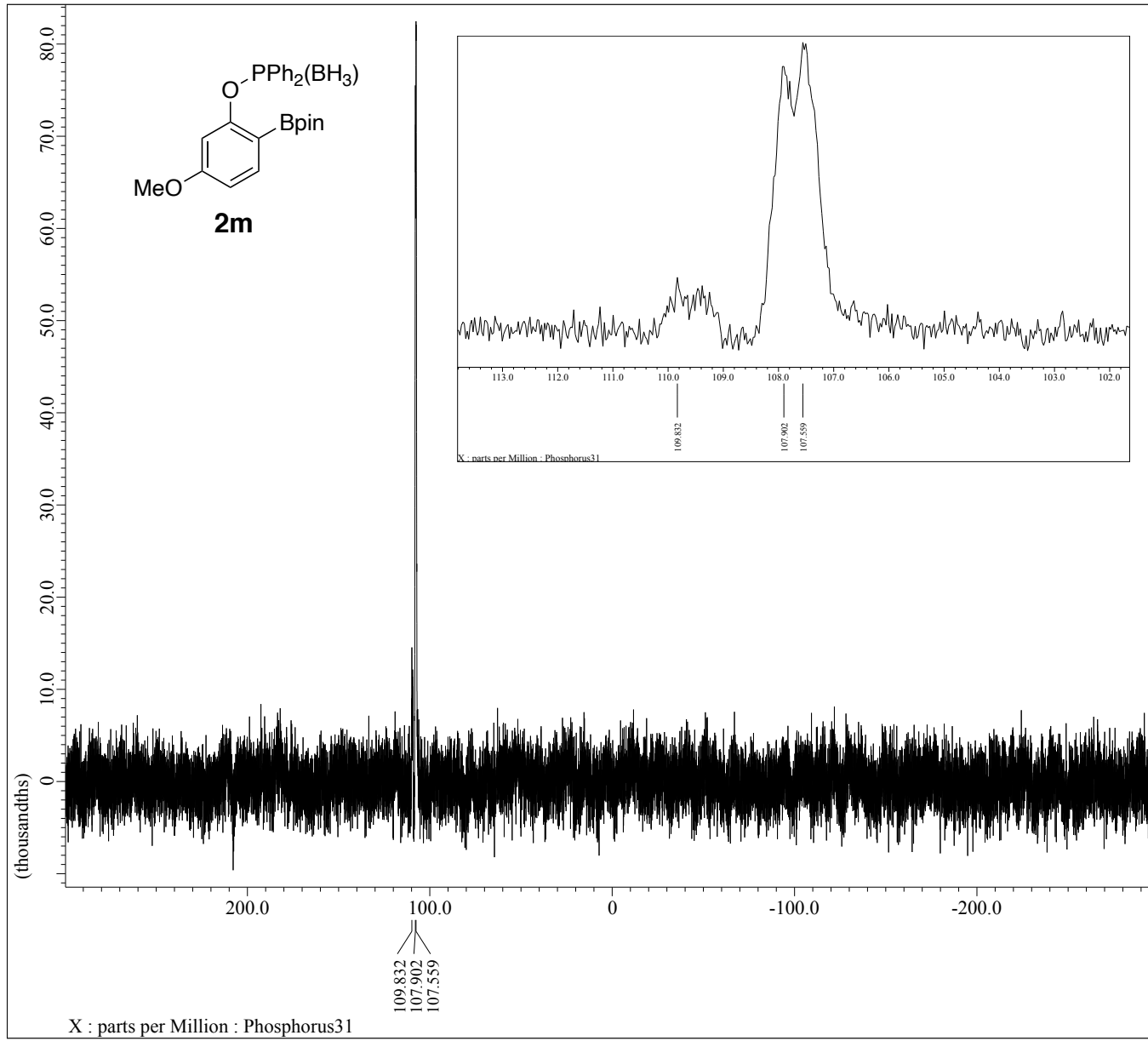
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
base_correct(Akima, 5, 0, FALSE, 3, None, FA
Derived from: YH(m-Ome)_Carbon-1-1.jdf

Filename = YH(m-Ome)_Carbon-1-2.jdf
Author = iwasawa
Experiment = carbon.jxp
Sample Id = YH(m-Ome)
Solvent = CHLOROFORM-D
Actual_Start_Time = 8-APR-2020 13:07:10
Revision_Time = 9-APR-2020 15:03:44

Comment = single pulse decoupled ga
Data Format = 1D REAL
Dim Size = 26214
X Domain = Carbon
Dim Title = Carbon13
Dim Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR

Field Strength = 9.389766[T] (400[MHz])
X Acq_Duration = 1.0433312[s]
X Domain = 13C
X Freq = 100.52530333[MHz]
X Offset = 100[ppm]
X Points = 32768
X Prescans = 4
X Resolution = 0.95846665[Hz]
X Sweep = 31.40703518[kHz]
X Sweep_Clippped = 25.12562814[kHz]
Irr Domain = Proton
Irr Freq = 399.78219838[MHz]
Irr Offset = 5[ppm]
Clipped = TRUE
Scans = 1024
Total_Scans = 1024

Relaxation_Delay = 2[s]
Recvr Gain = 60
Temp Get = 22[dC]
X 90_Width = 11.1[us]
X Acq_Time = 1.0433312[s]
X Angle = 30[deg]
X Atn = 4.5[dB]
X Pulse = 3.7[us]
Irr Atn Dec = 26.507[dB]
Irr Atn Noe = 26.507[dB]
Irr Noise = WALTZ
Irr Pwidth = 0.115[ms]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe Time = 2[s]
Repetition_Time = 3.04333312[s]



```

---- PROCESSING PARAMETERS ----
sexp( 2.0[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
Derived from: YH(m-OMe)_31P_1Hdec-1-1.jdf

```

```

Filename      = YH(m-OMe)_31P_1Hdec
Author        = delta
Experiment    = single_pulse_dec.j
Sample_Id     = YH(m-OMe)
Solvent       = CHLOROFORM-D
Actual_Start_Time = 7-APR-2020 22:03:
Revision_Time = 8-APR-2020 11:56:

```

```

Comment       = single pulse decou
Data Format    = 1D REAL
Dim Size      = 26214
X Domain      = Phosphorus31
Dim Title     = Phosphorus31
Dim Units     = [ppm]
Dimensions    = X
Spectrometer  = JNM-ECZ500R/S1

```

```

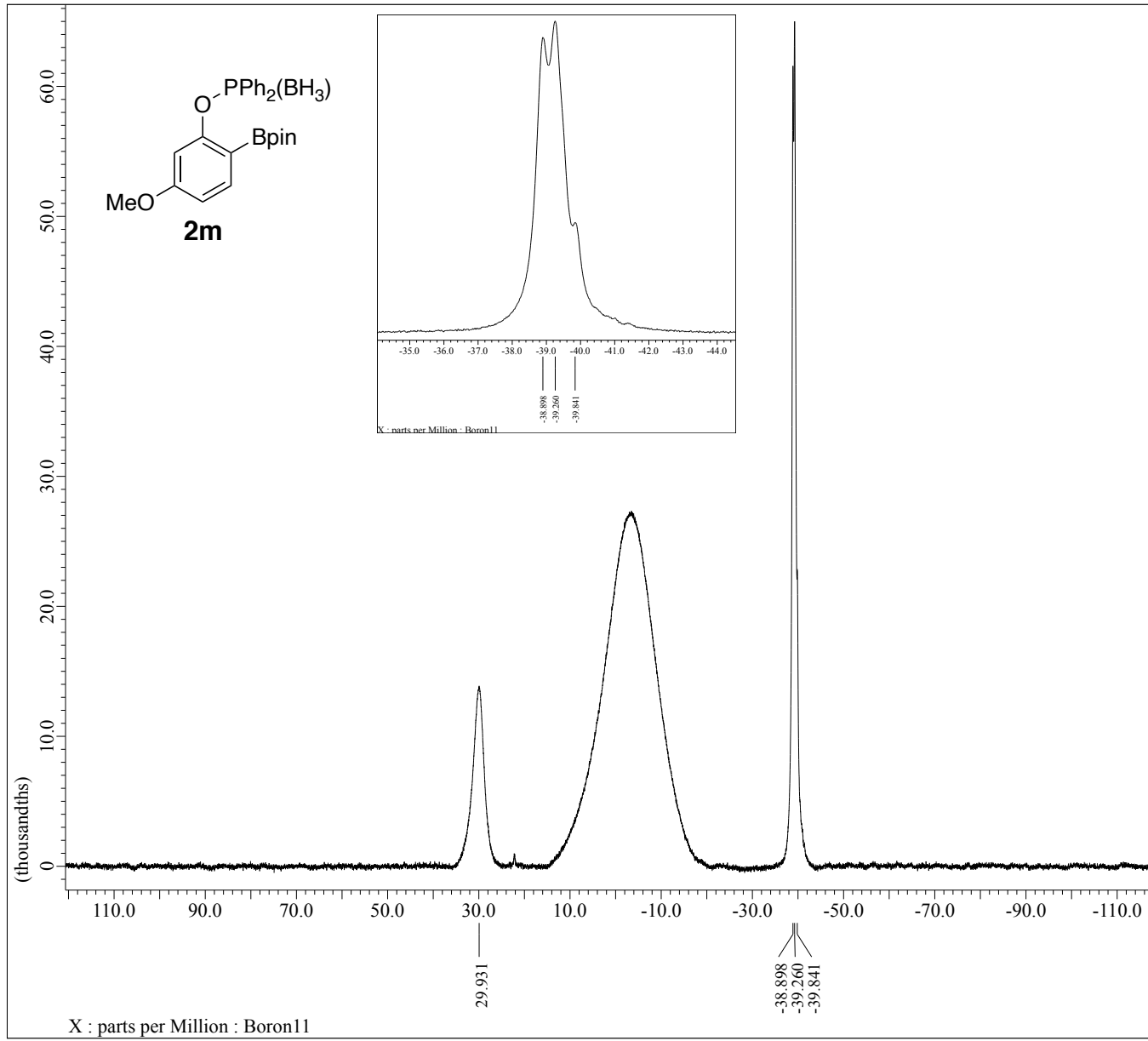
Field Strength = 11.62926421[T] (50
X Acq Duration = 0.18874368[s]
X Domain       = 31P
X Freq         = 200.43293989[MHz]
X Offset       = 0[ppm]
X Points       = 32768
X Prescans     = 4
X Resolution   = 5.29819065[Hz]
X Sweep       = 173.61111111[kHz]
X Sweep Clipped = 138.88888889[kHz]
Irr Domain     = Proton
Irr Freq       = 495.13191398[MHz]
Irr Offset     = 5[ppm]
Clipped        = FALSE
Scans          = 64
Total_Scans    = 64

```

```

Relaxation_Delay = 1[s]
Recvr Gain       = 66
Temp_Get         = 20.5[dC]
X 90 Width      = 19.78[us]
X Acq Time       = 0.18874368[s]
X Angle         = 30[deg]
X Atn            = 9.4[dB]
X Pulse         = 6.59333333[us]
Irr Atn Dec     = 23.948[dB]
Irr Atn Dec Calc = 23.948[dB]
Irr Atn Dec Default_Calc = 23.948[dB]
Irr Atn Noe     = 23.948[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

```



```

---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
phase( 17.25, 0, 38.11849[%] )
base_correct( Akima, 5, 0, FALSE, 3, None, FA
Derived from: YH(m-OMe)_11B_1Hdec-1-1.jdf

```

```

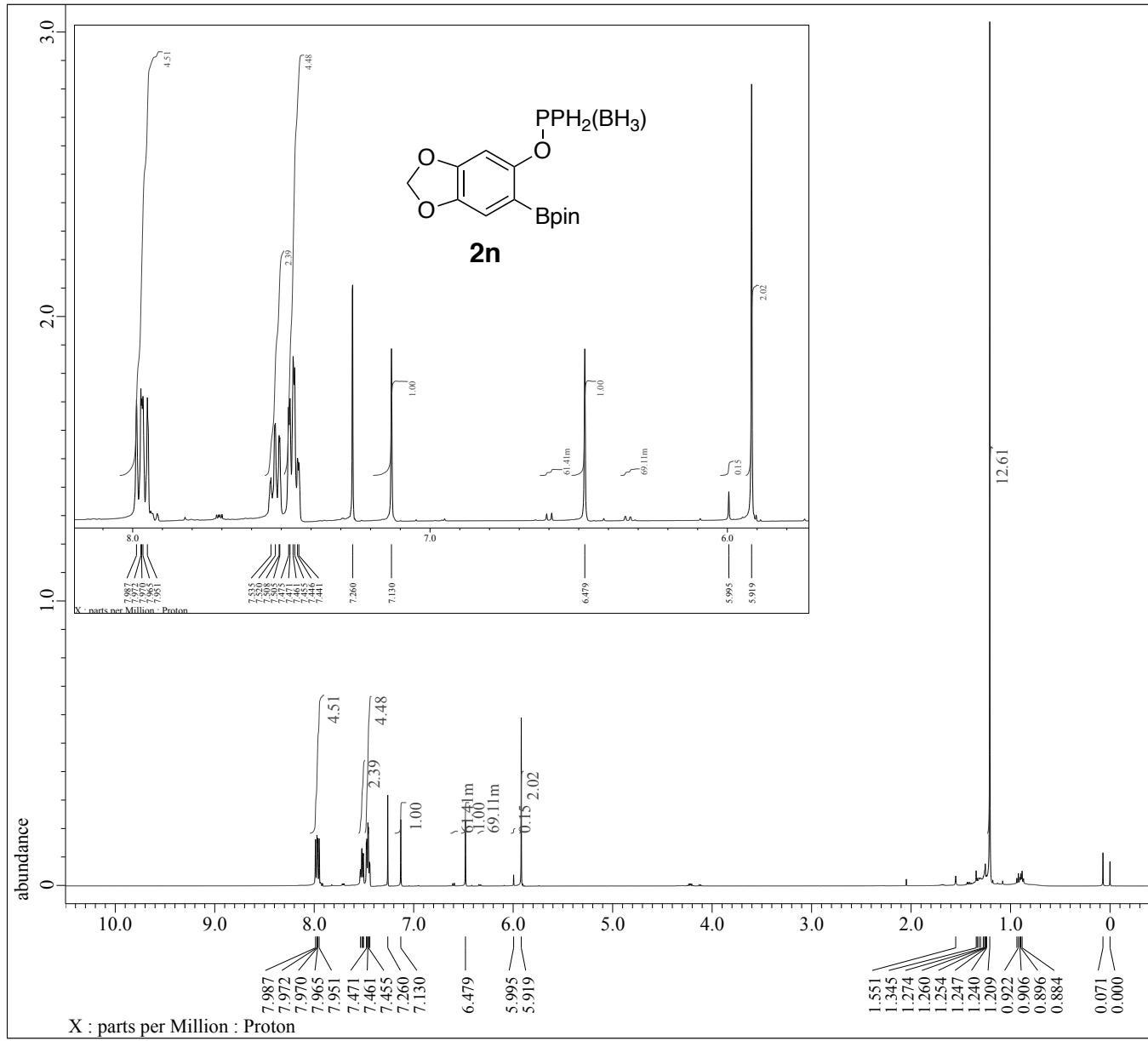
Filename           = YH(m-OMe)_11B_1Hde
Author             = delta
Experiment         = single_pulse_dec.j
Sample_Id          = YH(m-OMe)
Solvent            = CHLOROFORM-D
Actual_Start_Time  = 8-APR-2020 10:34:
Revision_Time      = 8-APR-2020 12:00:

Comment           = single_pulse decou
Data_Format       = 1D REAL
Dim_Size          = 26214
X_Domain          = Boron11
Dim_Title         = Boron11
Dim_Units         = [ppm]
Dimensions        = X
Spectrometer      = JNM-ECZ500R/S1

Field_Strength    = 11.62926421[T] (50
X_Acq_Duration    = 0.66060288[s]
X_Domain          = 11B
X_Freq            = 158.85814241[MHz]
X_Offset          = 0[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 1.51376876[Hz]
X_Sweep           = 49.6031746[kHz]
X_Sweep_Clippped  = 39.68253968[kHz]
Irr_Domain        = Proton
Irr_Freq          = 495.13191398[MHz]
Irr_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 300
Total_Scans       = 300

Relaxation_Delay  = 2[s]
Recvr_Gain        = 56
Temp_Get          = 20.8[dC]
X_90_Width        = 36.17[us]
X_Acq_Time        = 0.66060288[s]
X_Angle           = 30[deg]
X_Atn             = 12[dB]
X_Pulse           = 12.05666667[us]
Irr_Atn_Dec       = 23.948[dB]
Irr_Atn_Dec_Calc  = 23.948[dB]
Irr_Atn_Dec_Default_Calc = 23.948[dB]
Irr_Atn_Noise     = 23.948[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_Noise         = TRUE
Irr_Noise         = WALTZ

```



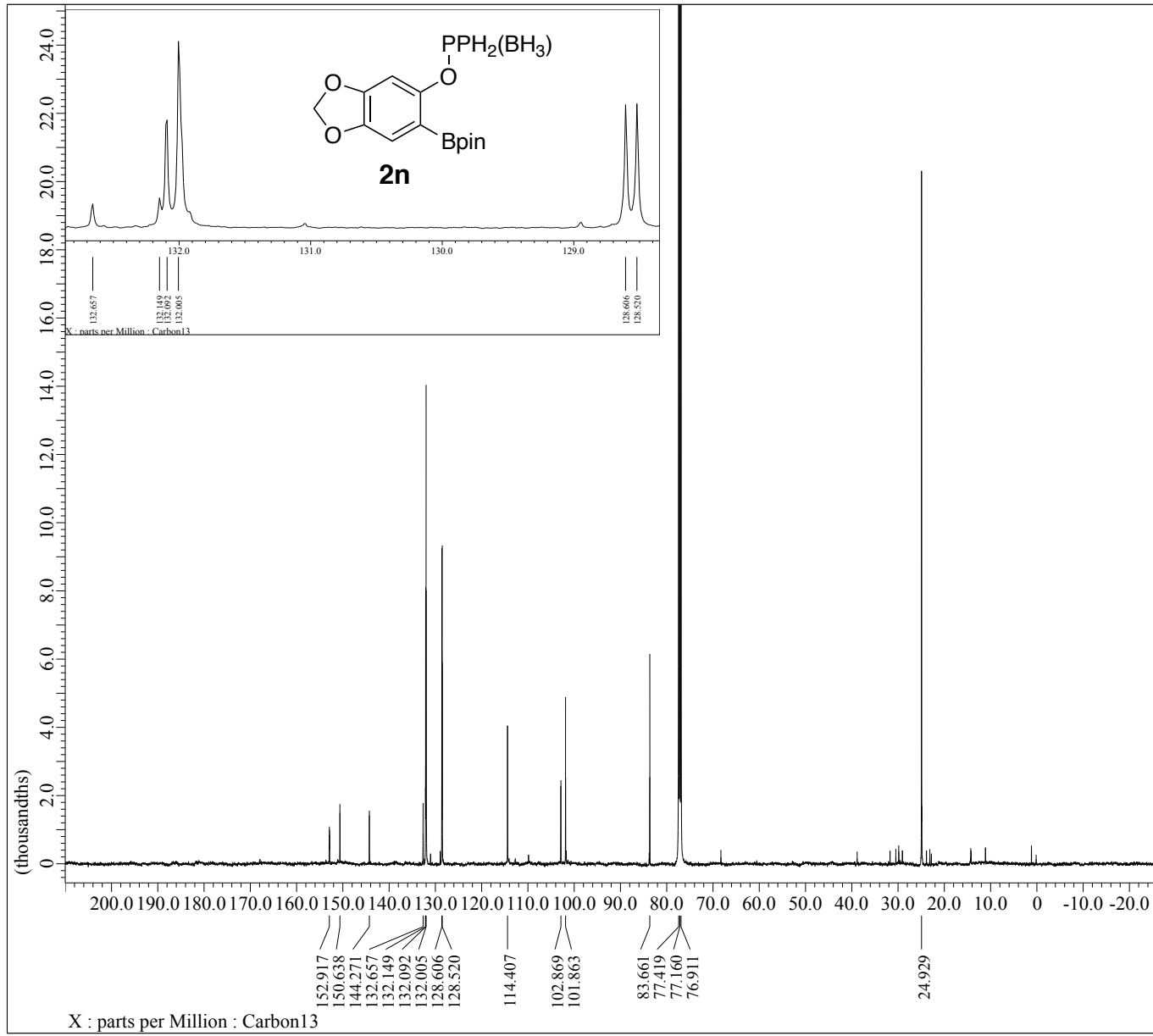
---- PROCESSING PARAMETERS ----
 sexp(0.2[Hz], 0.0[s])
 trapezoid(0[%], 0[%], 80[%], 100[%])
 zerofill(1, TRUE)
 fft(1, TRUE, TRUE)
 machinephase
 ppm
 Derived from: YH-295-f1_Proton-1-1.jdf

Filename = YH-295-f1_Proton-1-2.
 Author = delta
 Experiment = proton.jxp
 Sample_Id = YH-295-f1
 Solvent = CHLOROFORM-D
 Actual_Start_Time = 2-APR-2020 21:18:43
 Revision_Time = 7-APR-2020 10:29:22

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_Clippped = 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]
 Recvr_Gain = 36
 Temp_Get = 20.8 [dC]
 X_90_Width = 9.58 [us]
 X_Acq_Time = 1.76422912[s]
 X_Angle = 45 [deg]
 X_Atn = 4.3 [dB]
 X_Pulse = 4.79 [us]
 Irr_Mode = Off
 Tri_Mode = Off
 Dante_Loop = FALSE
 Dante_Presat = FALSE
 Decimation_Rate = 0
 Initial_Wait = 1[s]
 Phase = {0, 90, 270, 180, 180
 Presat_Time = 5[s]



```

---- PROCESSING PARAMETERS ----
sexp( 2.0[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
Derived from: YH-295-f1_Carbon-1-1.jdf

```

```

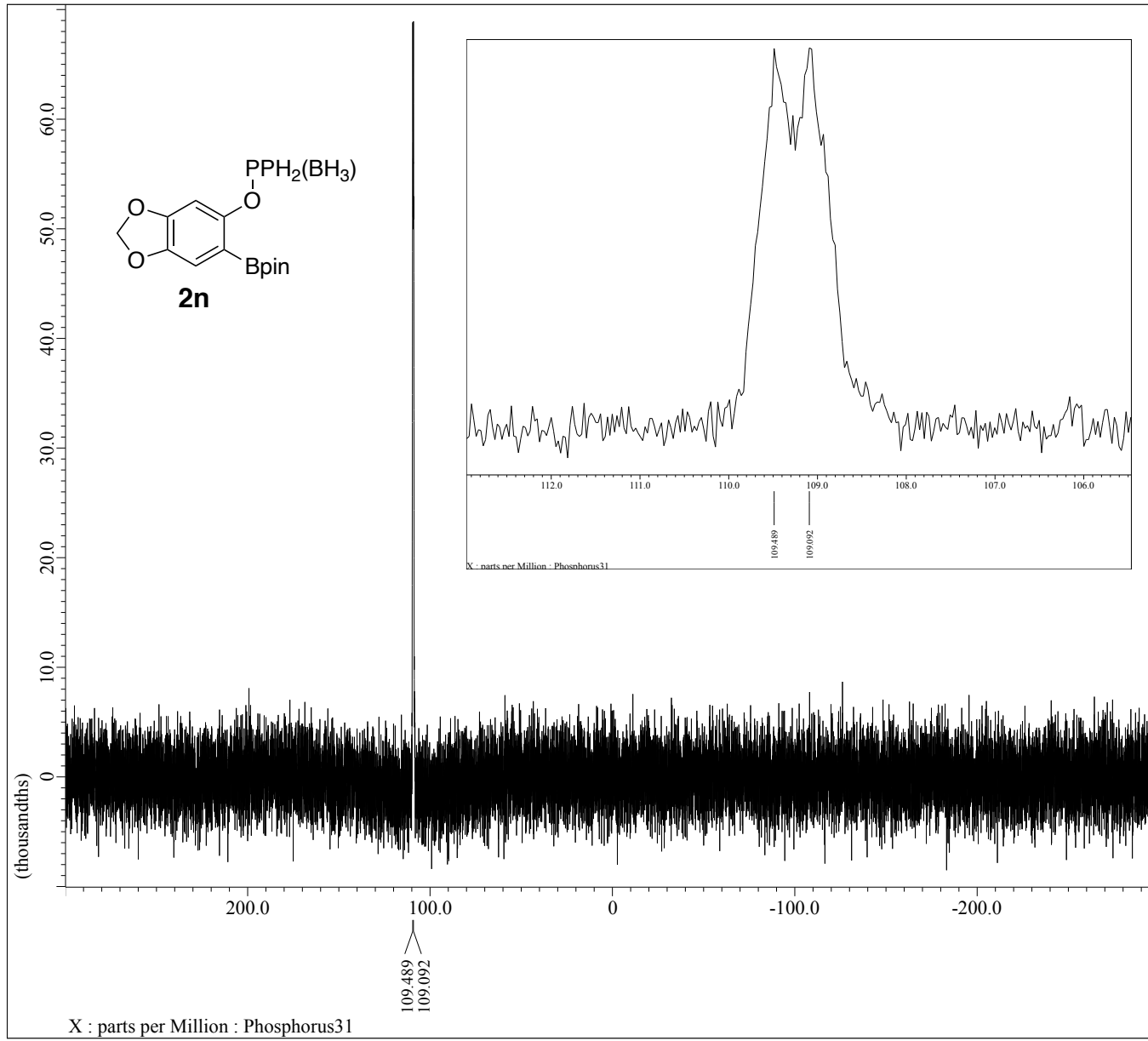
Filename           = YH-295-f1_Carbon-1
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = YH-295-f1
Solvent           = CHLOROFORM-D
Actual_Start_Time = 5-APR-2020 00:51:
Revision_Time     = 9-APR-2020 10:39:

Comment          = single pulse decou
Data_Format      = 1D REAL
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            = 5000
Total_Scans      = 5000

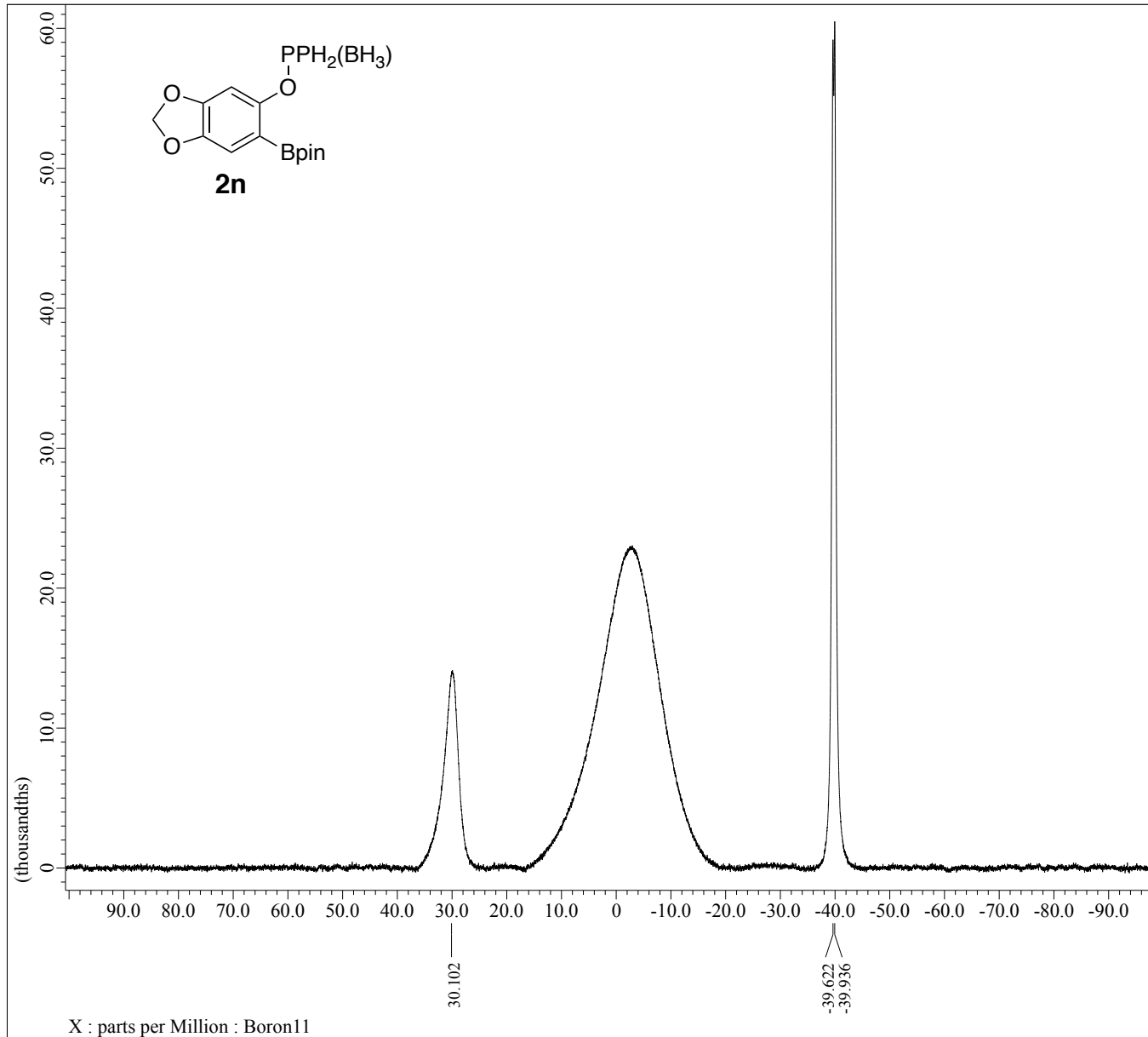
Relaxation_Delay = 2[s]
Recvr_Gain       = 56
Temp_Get         = 20.3[dC]
X_90_Width      = 9.61[us]
X_Acq_Time       = 0.8388608[s]
X_Angle         = 30[deg]
X_Atn           = 10[dB]
X_Pulse         = 3.20333333[us]
Irr_Atn_Dec     = 23.948[dB]
Irr_Atn_Dec_Calc = 23.948[dB]
Irr_Atn_Dec_Default_Calc = 23.948[dB]
Irr_Atn_Noise   = 23.948[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_Noise       = TRUE
Irr_Noise       = WALTZ

```



---- PROCESSING PARAMETERS ----
 sexp(2.0[Hz], 0.0[s])
 trapezoid(0[%], 0[%], 80[%], 100[%])
 zerofill(1, TRUE)
 fft(1, TRUE, TRUE)
 machinephase
 ppm
 Derived from: YH-295-f1_31P_1Hdec-1-1.jdf

Filename	= YH-295-f1_31P_1Hdec
Author	= delta
Experiment	= single_pulse_dec.j
Sample Id	= YH-295-f1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 3-APR-2020 12:45:
Revision_Time	= 7-APR-2020 21:40:
Comment	= single_pulse decou
Data Format	= 1D COMPLEX
Dim Size	= 26214
X Domain	= Phosphorus31
Dim Title	= Phosphorus31
Dim Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ500R/S1
Field Strength	= 11.62926421[T] (50
X Acq Duration	= 0.18874368[s]
X Domain	= 31P
X Freq	= 200.43293989[MHz]
X Offset	= 0[ppm]
X Points	= 32768
X Prescans	= 4
X Resolution	= 5.29819065[Hz]
X Sweep	= 173.61111111[kHz]
X Sweep Clipped	= 138.88888889[kHz]
Irr Domain	= Proton
Irr Freq	= 495.13191398[MHz]
Irr Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 64
Total_Scans	= 64
Relaxation_Delay	= 1[s]
Recvr Gain	= 66
Temp_Get	= 20.7[dC]
X 90_Width	= 19.78[us]
X Acq Time	= 0.18874368[s]
X Angle	= 30[deg]
X Atn	= 9.4[dB]
X Pulse	= 6.59333333[us]
Irr Atn Dec	= 23.948[dB]
Irr Atn Dec Calc	= 23.948[dB]
Irr Atn Dec Default_Calc	= 23.948[dB]
Irr Atn Noe	= 23.948[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



```

---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
phase( 0, -40, 38.22531[%] )
base_correct( Akima, 5, 0, FALSE, 3, None, FA
Derived from: YH-295-f1_11B_1Hdec-1-1.jdf

```

```

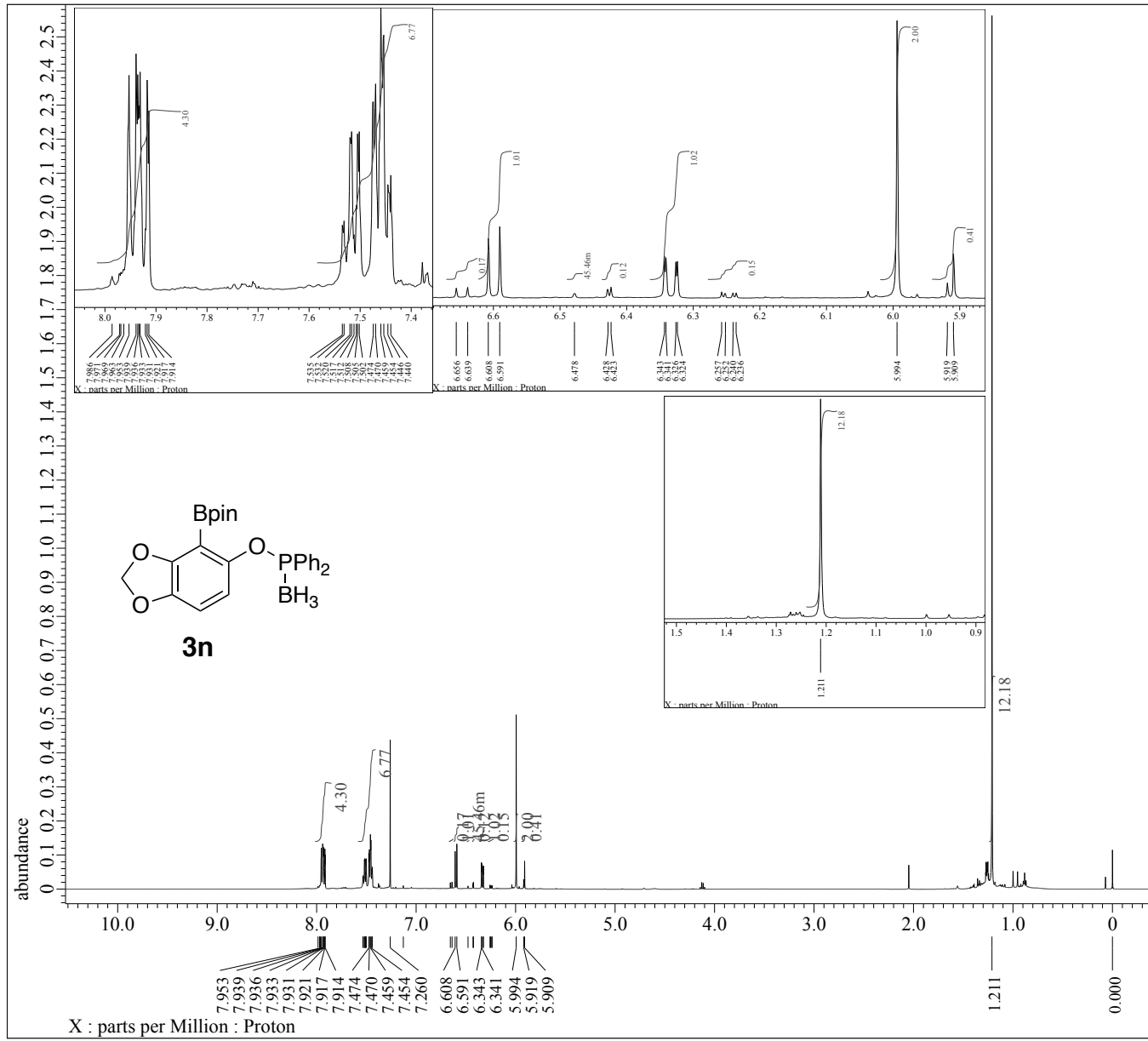
Filename      = YH-295-f1_11B_1Hde
Author        = delta
Experiment    = single_pulse_decou
Sample_Id     = YH-295-f1
Solvent       = CHLOROFORM-D
Actual_Start_Time = 3-APR-2020 13:04:
Revision_Time  = 7-APR-2020 13:01:

Comment       = single_pulse decou
Data_Format   = 1D REAL
Dim_Size      = 26214
X_Domain      = Boron11
Dim_Title     = Boron11
Dim_Units     = [ppm]
Dimensions    = X
Spectrometer  = JNM-ECZ500R/S1

Field Strength = 11.62926421[T] (50
X_Acq_Duration = 0.66060288[s]
X_Domain       = 11B
X_Freq         = 158.85814241[MHz]
X_Offset       = 0[ppm]
X_Points       = 32768
X_Prescans     = 4
X_Resolution   = 1.51376876[Hz]
X_Sweep        = 49.6031746[kHz]
X_Sweep_Clippped = 39.68253968[kHz]
Irr_Domain     = Proton
Irr_Freq       = 495.13191398[MHz]
Irr_Offset     = 5[ppm]
Clipped        = TRUE
Scans          = 500
Total_Scans    = 500

Relaxation_Delay = 2[s]
Recvr Gain       = 56
Temp_Get         = 20.6[dC]
X_90_Width      = 36.17[us]
X_Acq_Time      = 0.66060288[s]
X_Angle         = 30[deg]
X_Atn           = 12[dB]
X_Pulse         = 12.05666667[us]
Irr_Atn_Dec     = 23.948[dB]
Irr_Atn_Dec_Calc = 23.948[dB]
Irr_Atn_Dec_Default_Calc = 23.948[dB]
Irr_Atn_Noise  = 23.948[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_Noise      = TRUE
Irr_Noise      = WALTZ

```



```

---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
phase( 22.5, 0, 74.75202[%] )
base_correct( Akima, 5, 0, FALSE, 3, None, FA
Derived from: YH-295-f2_Proton-1-1.jdf

```

```

Filename      = YH-295-f2_Proton-1-2.
Author        = delta
Experiment    = proton.jxp
Sample Id     = YH-295-f2
Solvent       = CHLOROFORM-D
Actual_Start_Time = 2-APR-2020 21:24:39
Revision_Time = 14-APR-2020 16:14:47

```

```

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

```

```

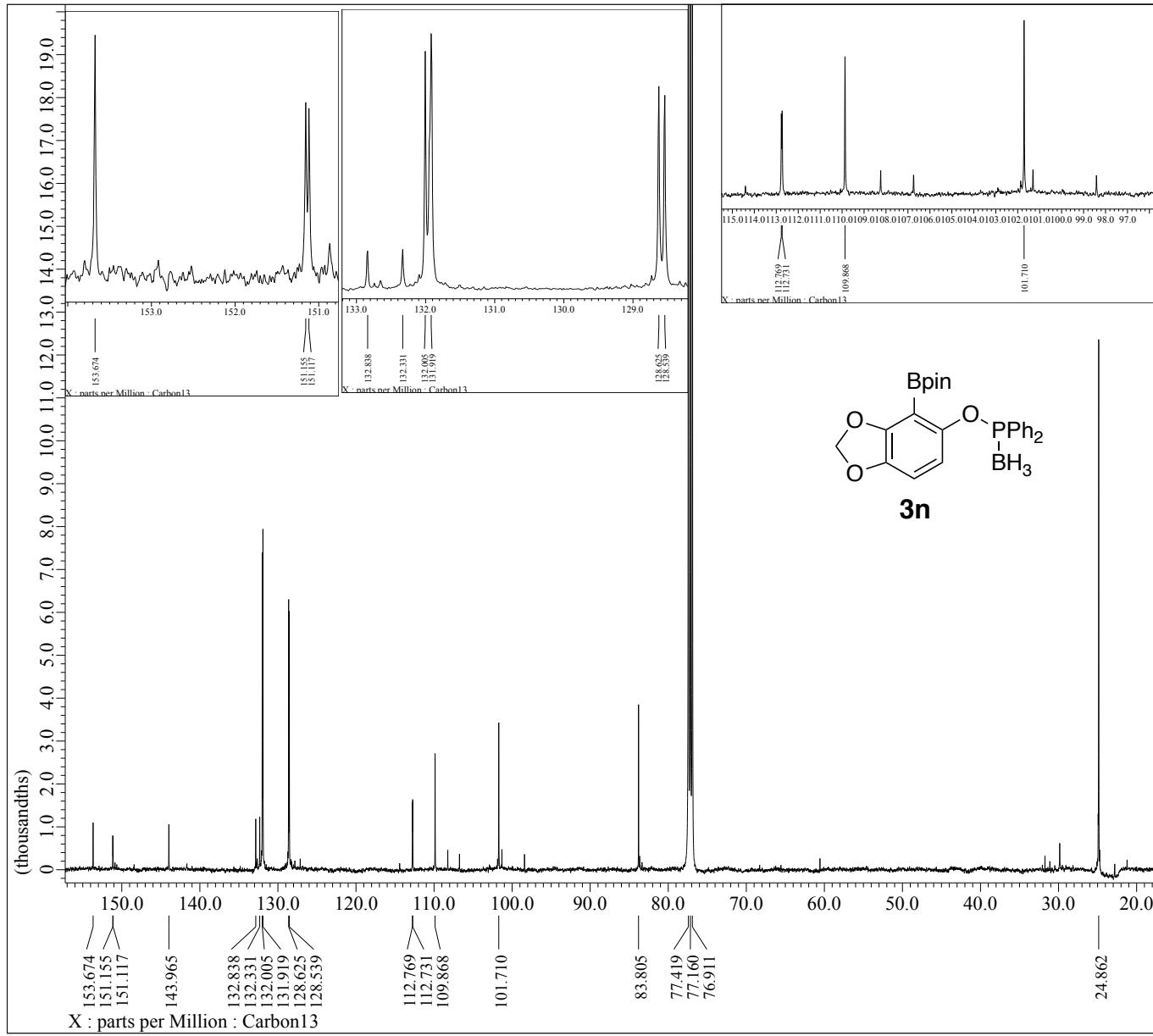
Field Strength = 11.62926421[T] (500[M
X Acq Duration = 1.76422912[s]
X Domain       = 1H
X Freq         = 495.13191398[MHz]
X Offset       = 5[ppm]
X Points       = 16384
X Prescans     = 1
X Resolution   = 0.5668198 [Hz]
X Sweep       = 9.28677563[kHz]
X Sweep Clipped = 7.42942051[kHz]
Irr Domain     = Proton
Irr Freq       = 495.13191398[MHz]
Irr Offset     = 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]
Recvr Gain       = 36
Temp_Get         = 20.7 [dC]
X 90 Width      = 9.58 [us]
X Acq Time      = 1.76422912[s]
X Angle         = 45 [deg]
X Atn           = 4.3 [dB]
X Pulse         = 4.79 [us]
Irr Mode        = Off
Tri Mode        = Off
Dante Loop      = FALSE
Dante_Presat   = FALSE
Decimation Rate = 0
Initial_Wait    = 1[s]
Phase           = {0, 90, 270, 180, 180
Presat_Time     = 5[s]

```



```

---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
reference( 77.10626[ppm], 77.16[ppm] )
base_correct( Akima, 5, 0, FALSE, 3, None, FA
Derived from: YH-295-f2_Carbon-1-1.jdf

```

```

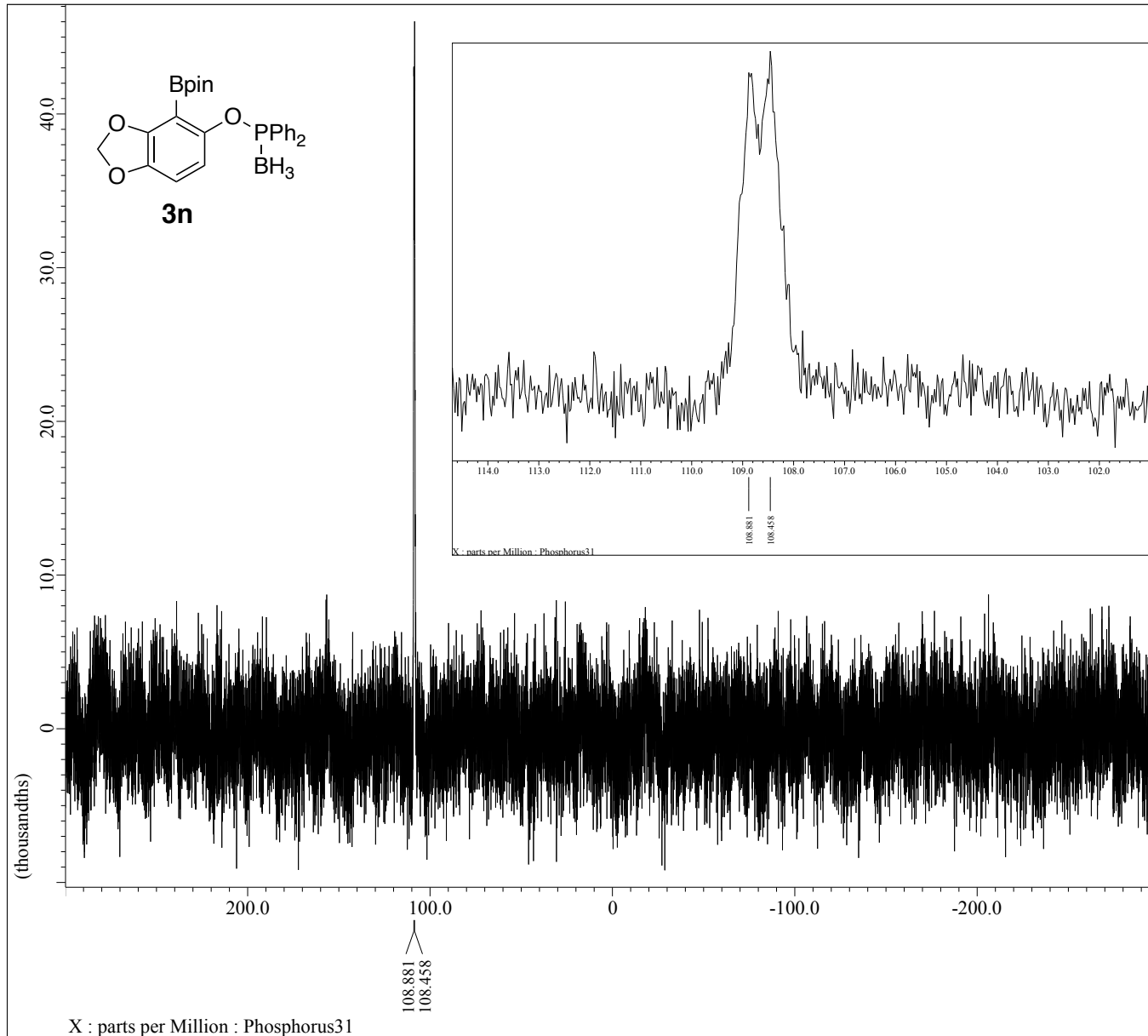
Filename           = YH-295-f2_Carbon-1
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = YH-295-f2
Solvent           = CHLOROFORM-D
Actual_Start_Time = 5-APR-2020 04:55:
Revision_Time     = 9-APR-2020 10:49:

Comment           = single pulse decou
Data Format       = 1D REAL
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            = 5000
Total_Scans      = 5000

Relaxation_Delay = 2[s]
Recvr Gain       = 56
Temp_Get         = 20.5[dC]
X_90_Width       = 9.61[us]
X_Acq_Time       = 0.8388608[s]
X_Angle          = 30[deg]
X_Atn            = 10[dB]
X_Pulse          = 3.20333333[us]
Irr_Atn_Dec      = 23.948[dB]
Irr_Atn_Dec_Calc = 23.948[dB]
Irr_Atn_Dec_Default_Calc = 23.948[dB]
Irr_Atn_Noise   = 23.948[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_Noise       = TRUE
Irr_Noise       = WALTZ

```

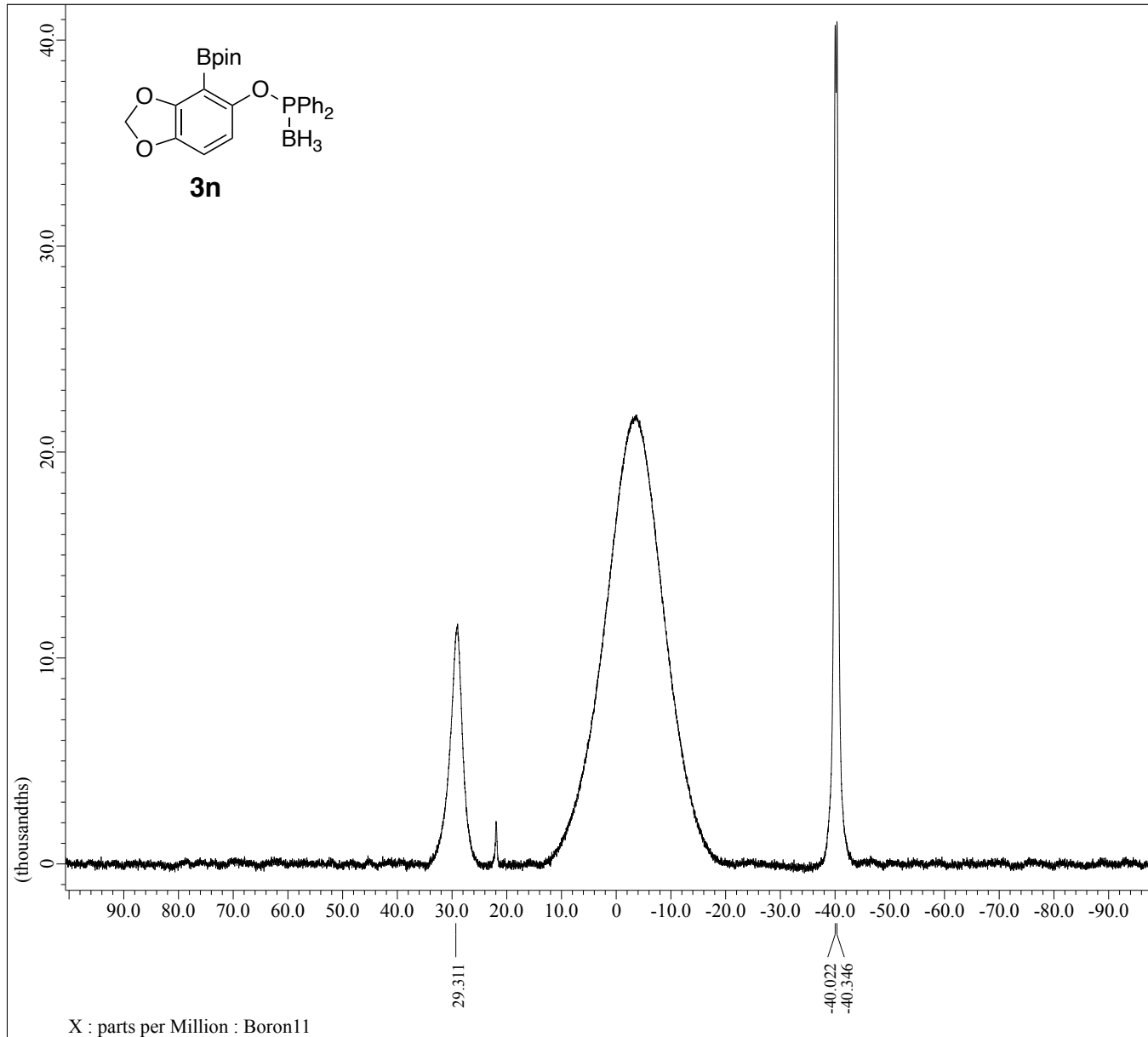
---- PROCESSING PARAMETERS ----
 sexp(2.0[Hz], 0.0[s])
 trapezoid(0[%], 0[%], 80[%], 100[%])
 zerofill(1, TRUE)
 fft(1, TRUE, TRUE)
 machinephase
 ppm
 phase(-21.42682, 0, 50[%])
 base_correct(Akima, 5, 0, FALSE, 3, None, FA
 Derived from: YH-295-f2_31P_1Hdec-1-1.jdf

Filename = YH-295-f2_31P_1Hdec
 Author = delta
 Experiment = single_pulse_dec.j
 Sample_Id = YH-295-f2
 Solvent = CHLOROFORM-D
 Actual_Start_Time = 3-APR-2020 12:54:
 Revision_Time = 7-APR-2020 21:38:

Comment = single pulse decou
 Data Format = 1D REAL
 Dim Size = 26214
 X Domain = Phosphorus31
 Dim Title = Phosphorus31
 Dim Units = [ppm]
 Dimensions = X
 Spectrometer = JNM-ECZ500R/S1

Field Strength = 11.62926421[T] (50
 X Acq Duration = 0.18874368[s]
 X Domain = 31P
 X Freq = 200.43293989[MHz]
 X Offset = 0[ppm]
 X Points = 32768
 X Prescans = 4
 X Resolution = 5.29819065[Hz]
 X Sweep = 173.61111111[kHz]
 X Sweep Clipped = 138.88888889[kHz]
 Irr Domain = Proton
 Irr Freq = 495.13191398[MHz]
 Irr Offset = 5[ppm]
 Clipped = FALSE
 Scans = 64
 Total_Scans = 64

Relaxation_Delay = 1[s]
 Recvr Gain = 66
 Temp_Get = 20.7[dC]
 X 90_Width = 19.78[us]
 X Acq Time = 0.18874368[s]
 X Angle = 30[deg]
 X Atn = 9.4[dB]
 X Pulse = 6.59333333[us]
 Irr Atn Dec = 23.948[dB]
 Irr Atn Dec Calc = 23.948[dB]
 Irr Atn Dec Default_Calc = 23.948[dB]
 Irr Atn Noe = 23.948[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



```

---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
phase( 15, 0, 38.85477[%] )
base_correct( Akima, 5, 0, FALSE, 3, None, FA
Derived from: YH-295-f2_11B_1Hdec-1-1.jdf

```

```

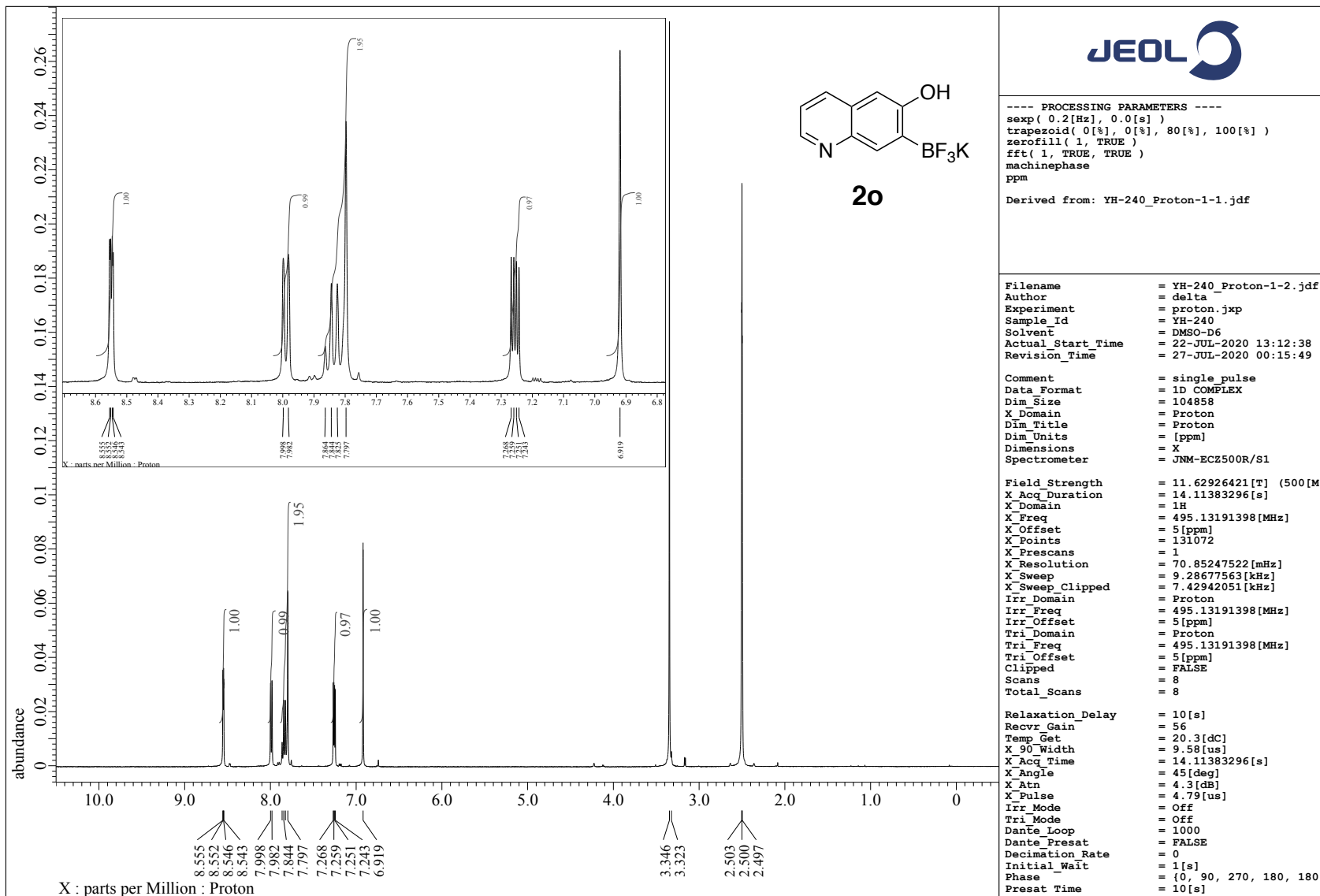
Filename      = YH-295-f2_11B_1Hde
Author        = delta
Experiment    = single_pulse_decou
Sample_Id     = YH-295-f2
Solvent       = CHLOROFORM-D
Actual_Start_Time = 3-APR-2020 13:34:
Revision_Time  = 7-APR-2020 12:59:

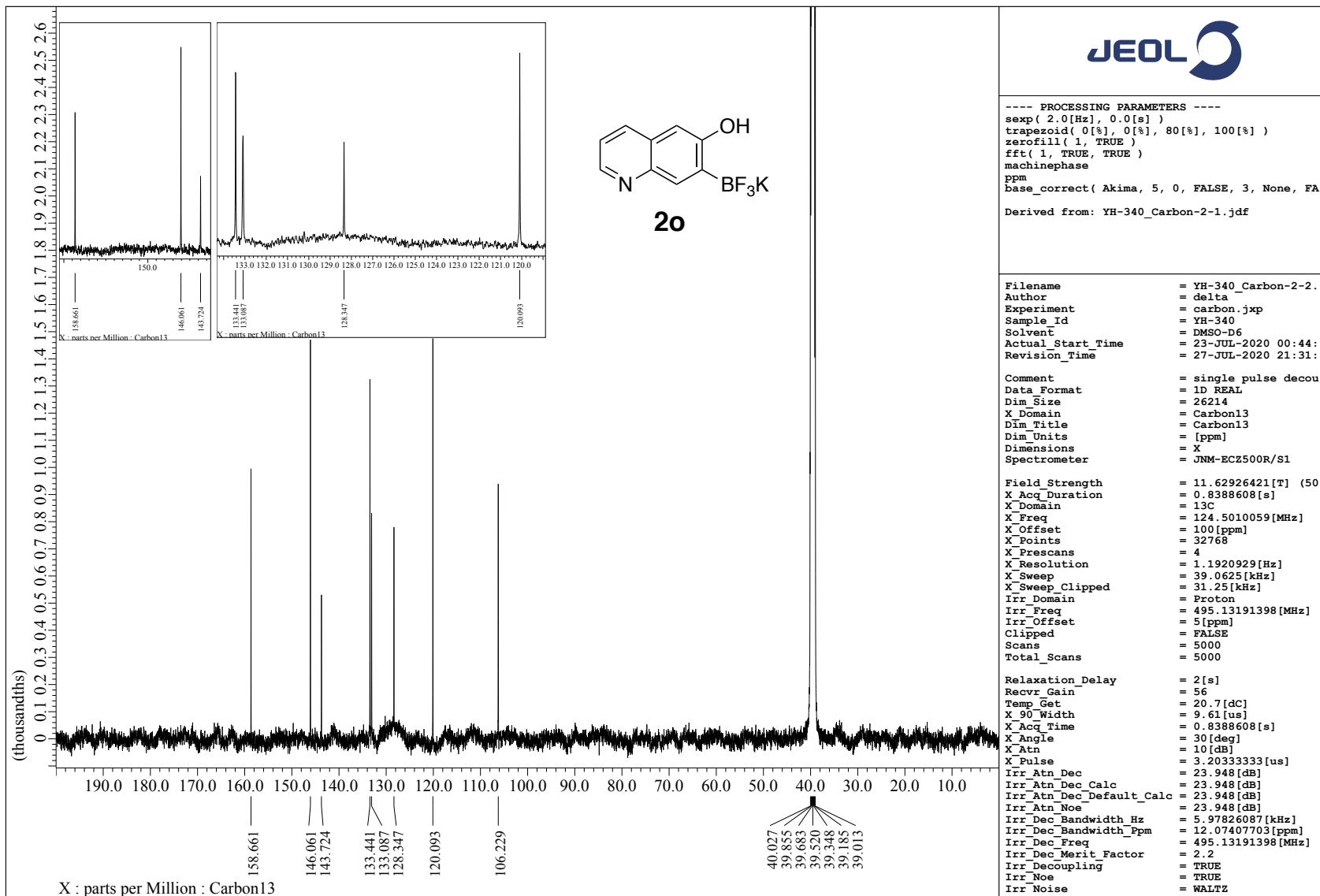
Comment       = single_pulse decou
Data_Format   = 1D REAL
Dim_Size      = 26214
X_Domain      = Boron11
Dim_Title     = Boron11
Dim_Units     = [ppm]
Dimensions    = X
Spectrometer  = JNM-ECZ500R/S1

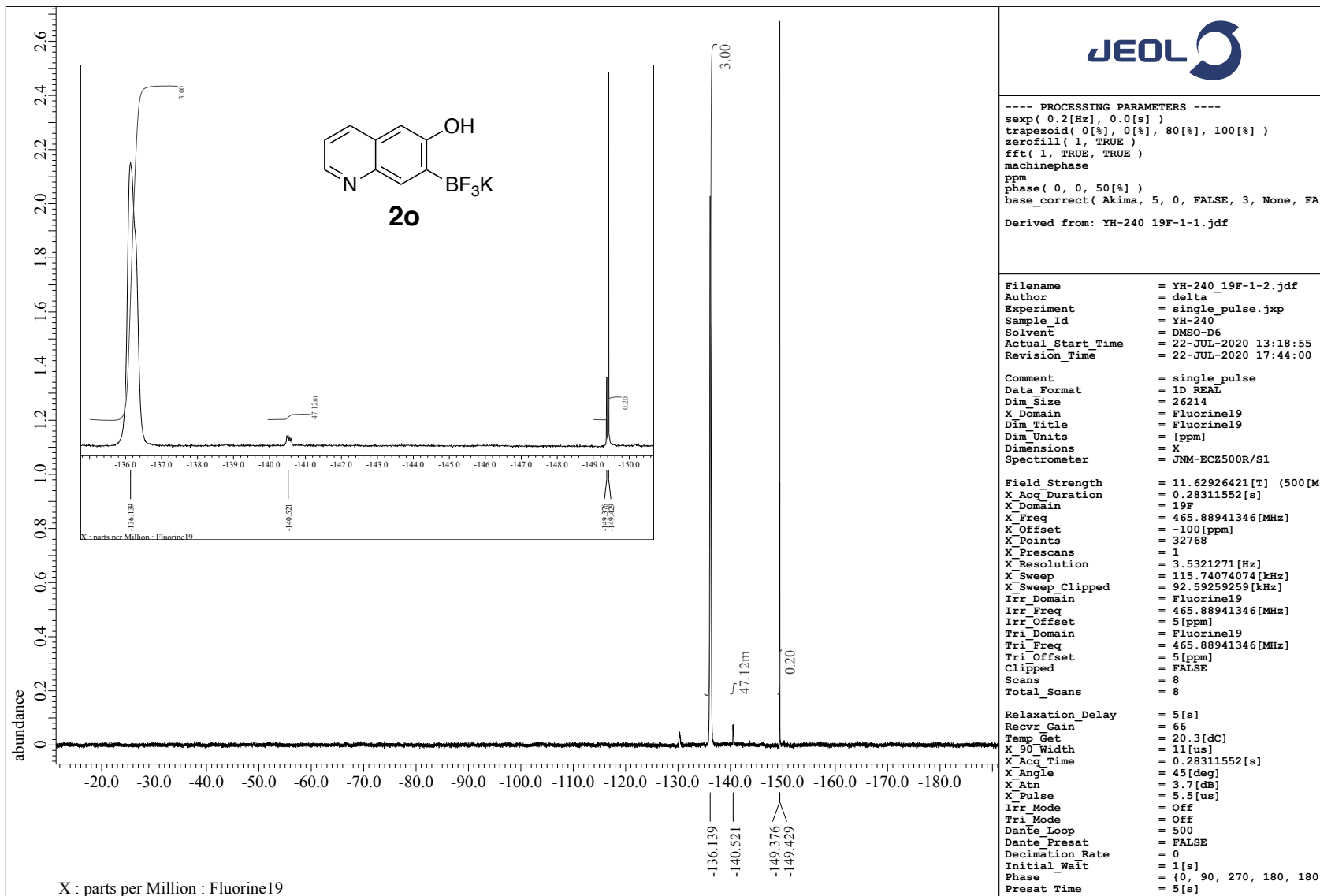
Field Strength = 11.62926421[T] (50
X_Acq_Duration = 0.66060288[s]
X_Domain       = 11B
X_Freq         = 158.85814241[MHz]
X_Offset       = 0[ppm]
X_Points       = 32768
X_Prescans     = 4
X_Resolution   = 1.51376876[Hz]
X_Sweep        = 49.6031746[kHz]
X_Sweep_Clipped = 39.68253968[kHz]
Irr_Domain     = Proton
Irr_Freq       = 495.13191398[MHz]
Irr_Offset     = 5[ppm]
Clipped        = FALSE
Scans          = 500
Total_Scans    = 500

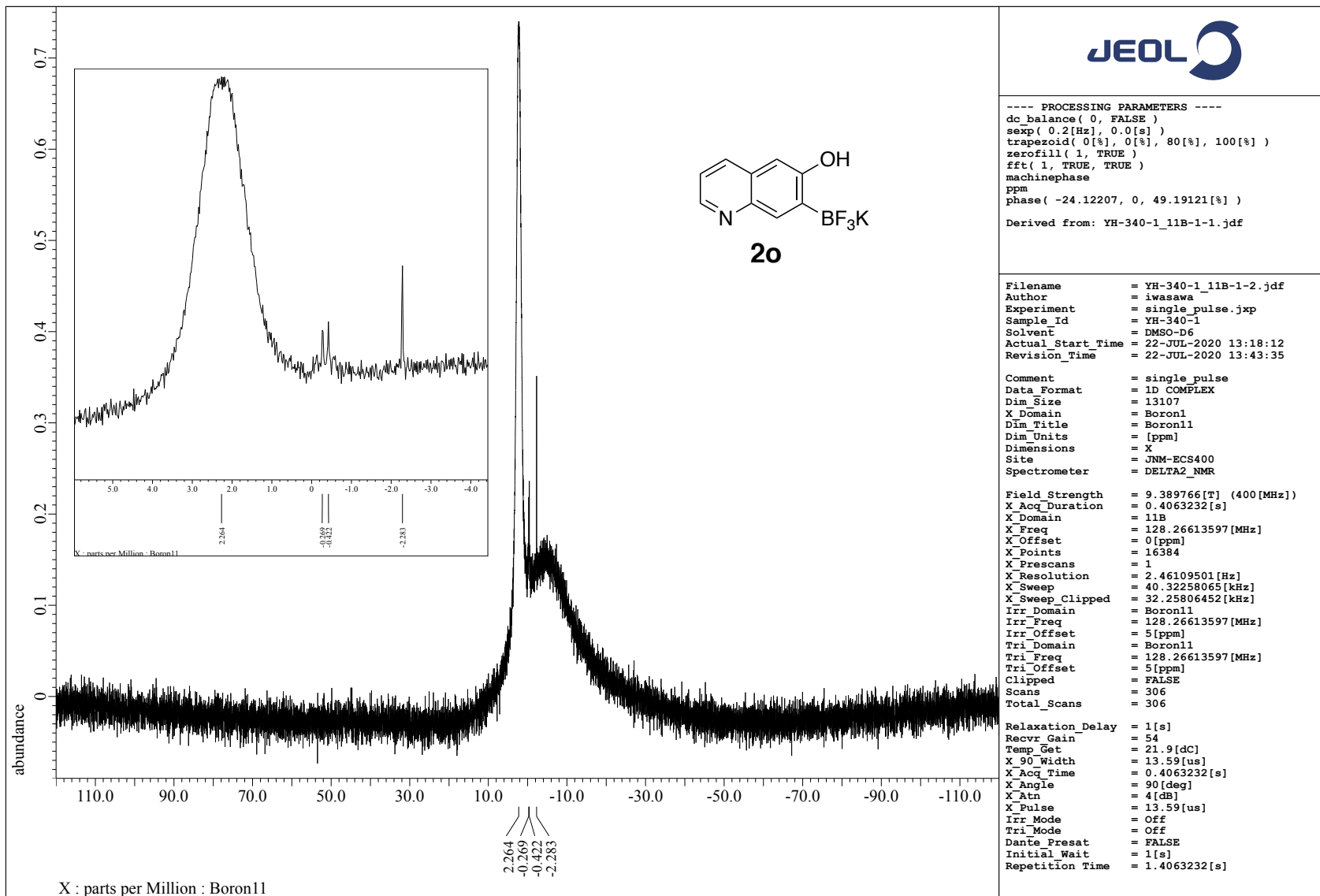
Relaxation_Delay = 2[s]
Recvr Gain       = 56
Temp_Get         = 21[dC]
X_90_Width      = 36.17[us]
X_Acq_Time       = 0.66060288[s]
X_Angle         = 30[deg]
X_Atn           = 12[dB]
X_Pulse         = 12.05666667[us]
Irr_Atn_Dec     = 23.948[dB]
Irr_Atn_Dec_Calc = 23.948[dB]
Irr_Atn_Dec_Default_Calc = 23.948[dB]
Irr_Atn_Noise  = 23.948[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_Noise      = TRUE
Irr_Noise      = WALTZ

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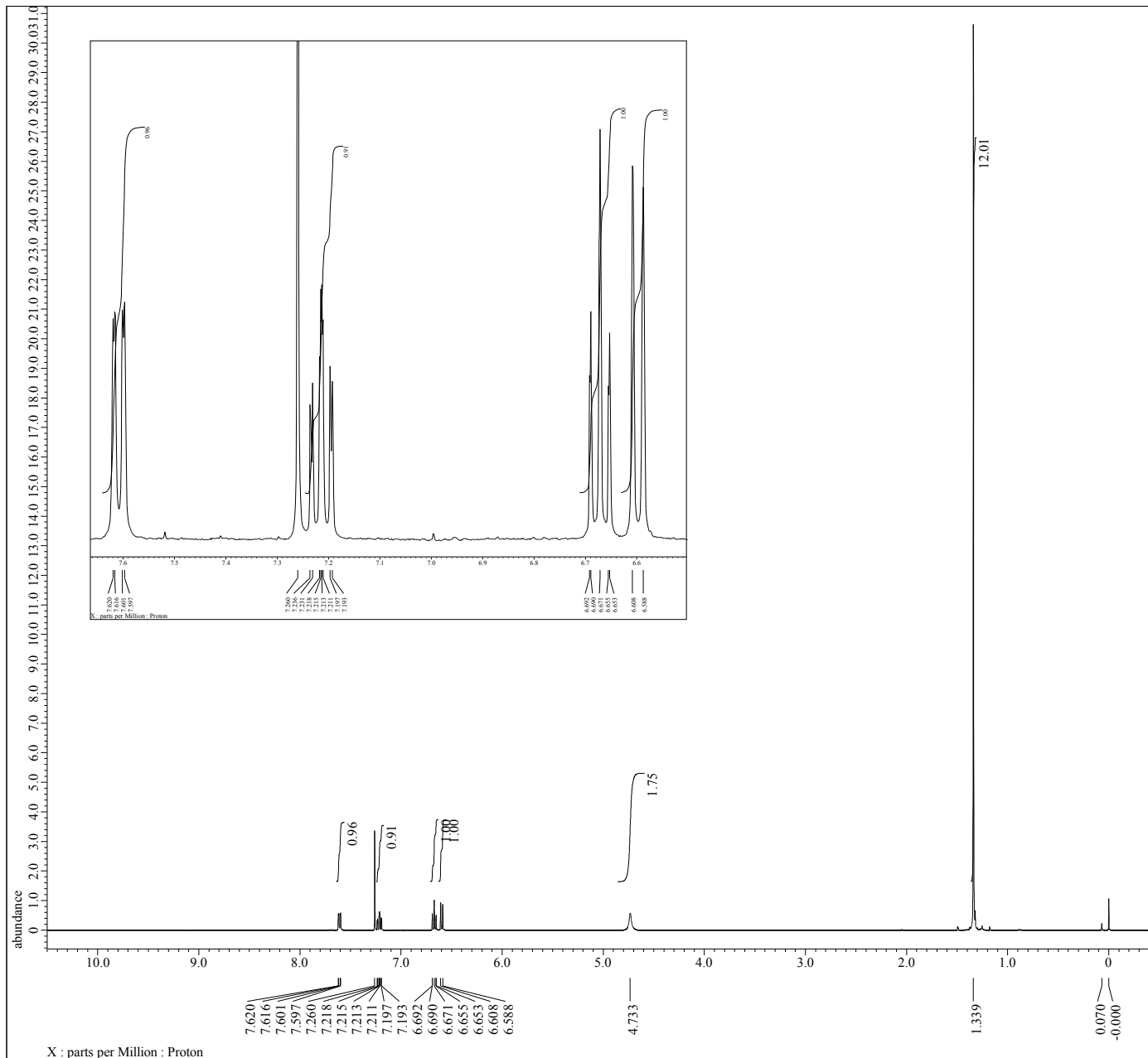
---- PROCESSING PARAMETERS ----
 dc balance(0, FALSE)
 sexp(0.2[Hz], 0.0[s])
 trapezoid(0[%], 0[%], 80[%], 100[%])
 zerofill(1, TRUE)
 fft(1, TRUE, TRUE)
 machinephase
 ppm
 phase(-24.12207, 0, 49.19121[%])
 Derived from: YH-340-1_11B-1-1.jdf

Filename = YH-340-1_11B-1-2.jdf
 Author = iwasawa
 Experiment = single_pulse.jxp
 Sample Id = YH-340-1
 Solvent = DMSO-D6
 Actual Start Time = 22-JUL-2020 13:18:12
 Revision_Time = 22-JUL-2020 13:43:35

Comment = single_pulse
 Data Format = 1D COMPLEX
 Dim Size = 13107
 X_Domain = Boron1
 Dim Title = Boron11
 Dim Units = [ppm]
 Dimensions = X
 Site = JNM-ECS400
 Spectrometer = DELTA2_NMR

Field Strength = 9.389766[T] (400[MHz])
 X_Acq_Duration = 0.4063232[s]
 X_Domain = 11B
 X_Freq = 128.26613597[MHz]
 X_Offset = 0[ppm]
 X_Points = 16384
 X_Prescans = 1
 X_Resolution = 2.46109501[Hz]
 X_Sweep = 40.32258065[kHz]
 X_Sweep_Clippped = 32.25806452[kHz]
 Irr_Domain = Boron11
 Irr_Freq = 128.26613597[MHz]
 Irr_Offset = 5[ppm]
 Tri_Domain = Boron11
 Tri_Freq = 128.26613597[MHz]
 Tri_Offset = 5[ppm]
 Clipped = FALSE
 Scans = 306
 Total_Scans = 306

Relaxation_Delay = 1[s]
 Recvr_Gain = 54
 Temp_Get = 21.9[dC]
 X_90_Width = 13.59[us]
 X_Acq_Time = 0.4063232[s]
 X_Angle = 90[deg]
 X_Atn = 4[dB]
 X_Pulse = 13.59[us]
 Irr_Mode = Off
 Tri_Mode = Off
 Dante_Presat = FALSE
 Initial_Wait = 1[s]
 Repetition_Time = 1.4063232[s]



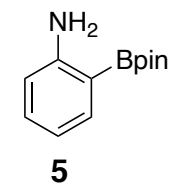
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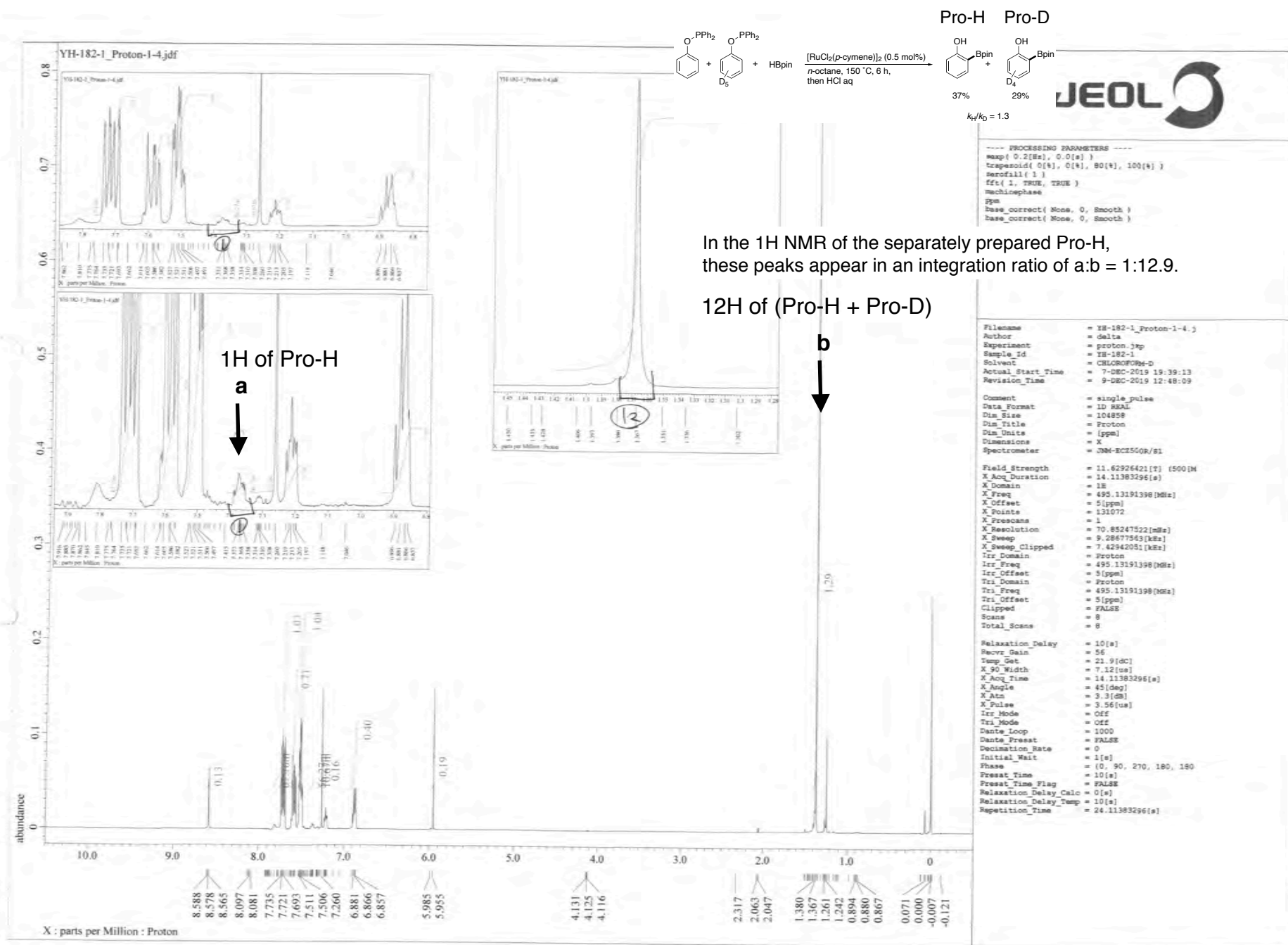
Filename      = YH-196(aniline)_Proton-1-6
Author       = iwawata
Experiment   = proton.jpg
Sample_Id    = YH-196(aniline)
Solvent      = CHLOROFORM-D
Creation_Time = 24-MAR-2020 20:17:58
Revision_Time = 8-APR-2020 12:09:55
Current_Time = 8-APR-2020 12:11:16

Comment      = single_pulse
Data_Format  = 1D_REAL
Dim_Size     = 13107
Dim_Title    = Proton
Dim_Units    = [ppm]
Dimensions   = X
Site         = JNM-ECS400
Spectrometer = DELTA2_NMR

Field_Strength = 9.389766[T] (400 [MHz])
X_Acq_Duration = 2.18365952[s]
X_Domain       = 1h
X_Freq         = 399.78219838 [MHz]
X_Offset       = 5 [ppm]
X_Points       = 16384
X_Prescans     = 1
X_Resolution   = 0.45794685 [Hz]
X_Sweep        = 7.5030012 [kHz]
X_Sweep_Clipped = 6.00240096 [kHz]
Irr_Domain     = Proton
Irr_Freq       = 399.78219838 [MHz]
Irr_Offset     = 5 [ppm]
Tri_Domain     = Proton
Tri_Freq       = 399.78219838 [MHz]
Tri_Offset     = 5 [ppm]
Clipped        = FALSE
Scans          = 8
Total_Scans    = 8

Relaxation_Delay = 3 [s]
Recvr_Gain       = 44
Temp_Get         = 19.9 [dc]
X_90_Width      = 6.1 [us]
X_Acq_Time      = 2.18365952 [s]
X_Angle         = 45 [deg]
X_Attn          = 1 [dB]
X_Pulse         = 3.05 [us]
Irr_Mode        = Off
Tri_Mode        = Off
Date_Preset     = FALSE
Initial_Wait    = 1 [s]
Repetition_Time = 5.18365952 [s]
  
```







Filename = YH-317_Proton-1-6.jdf
Author = delta
Experiment = proton_jmp
Sample_Id = YH-317
Solvent = CHLOROFORM-D
Actual_Start_Time = 7-APR-2020 21:51:23
Revision_Time = 7-APR-2020 21:41:06
Comment = single_pulse
Data_Format = 1D_REAL
Dim_Size = 104858
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/si
Field_Strength = 11.62926421[T] (500[M]
X_Acq_Duration = 14.11383296[s]
X_Domain = 18
X_Freq = 495.13191398[MHz]
X_Offset = 5[ppm]
X_Points = 131072
X_Prescans = 1
X_Resolution = 70.85247522[mHz]
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 = 10[s]
Recvr_Gain = 36
Temp_Get = 20.9[degC]
X_90_Width = 9.58[us]
X_Acq_Time = 14.11383296[s]
X_Angle = 45[deg]
X_Atn = 4.3[dB]
X_Pulse = 4.79[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 1000
Dante_Preset = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = 10, 90, 270, 180, 180
Preset_Time = 10[s]
Preset_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]

