Electronic Supplementary Material (ESI) for Chemical Science.

Mechanochemical Protocol Facilitates the Generation of Arylmanganese Nucleophiles from Unactivated Manganese Metal

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1. General and Materials

Materials were obtained from commercial suppliers and purified using standard procedures, unless otherwise noted. Solvents were purchased from commercial suppliers and further dried over molecular sieve (MS 4Å). Manganese powder (> 98%, product no. 130-06732) was purchased from Wako Pure Chemical Industries, Co., Ltd. All reactions were performed using grinding vessels in the Retsch MM 400 (Figure S1). Both jars and balls were made of stainless steel (SUS400B and SUS420J2, respectively, Figure S2), tungsten carbide, or zirconia. NMR spectra were recorded on JEOL JNM-ECZ400S and JNM-ECS400 spectrometers (^{1}H: 392, 399, or 401 MHz, ^{13}C: 99 or 100 MHz, ^{19}F: 375 or 377 MHz). Tetramethylsilane (^{1}H), $CDCl_3$ (^{13}C), and (Trifluoromethyl)benzene (^{19}F) were employed as internal standards, respectively. Multiplicity was recorded as follows: s = singlet, brs = broad singlet, d = doublet, t = triplet, q = quartet, and m = multiplet. Fluorobenzene, 1,2-difluorobenzene, and hexafluorobenzene were used as an internal standard to determine the NMR yields. Thermographic images were obtained using the InfRec Thermo GEAR (NEC Avio Infrared Technologies Co., Ltd.). Recycling preparative gel permeation chromatography (GPC) was conducted with the JAI LC-9101 using $CHCl_3$ as the eluent with the JAIGEL-1H. X-Ray photoelectron spectroscopy (XPS) was performed using JEOL JPS-9200. High-resolution mass spectra were recorded at the Global Facility Center, Hokkaido University.

Figure S1. Retsch MM400 used in this study.

Figure S2. Stainless jars and balls used in this study.

2. List of Substrates Used in This Study

Aryl halides except **1k**–**1n** were obtained from commercial suppliers and were used as received. **1k**,[1] **1l**,[2] **1m**,[3] and **1n**[4] were synthesized according to the reported procedures.

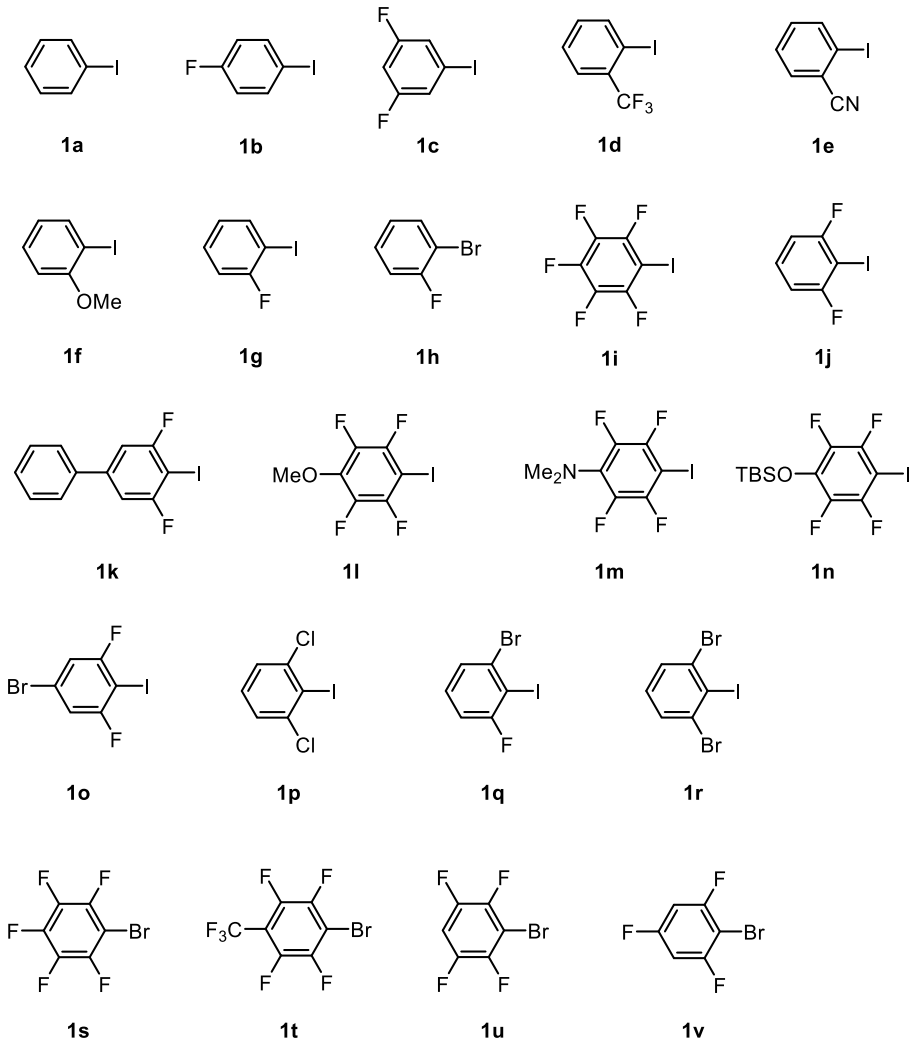


Figure S3. List of aryl halides used in this study.

All electrophiles were obtained from commercial suppliers. **2a** and **2b** were distilled before use. **2c**, **2d** and **5a**, **5b** were used as received.

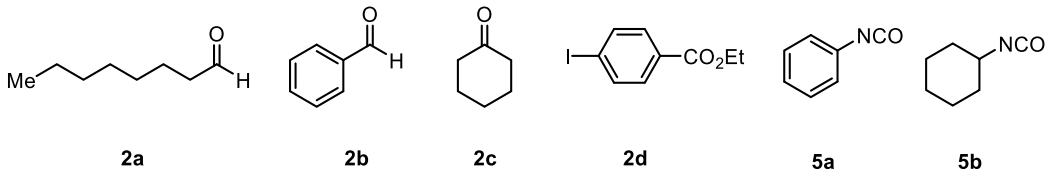
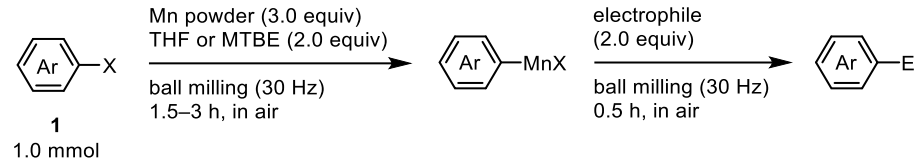


Figure S4. List of electrophiles used in this study.

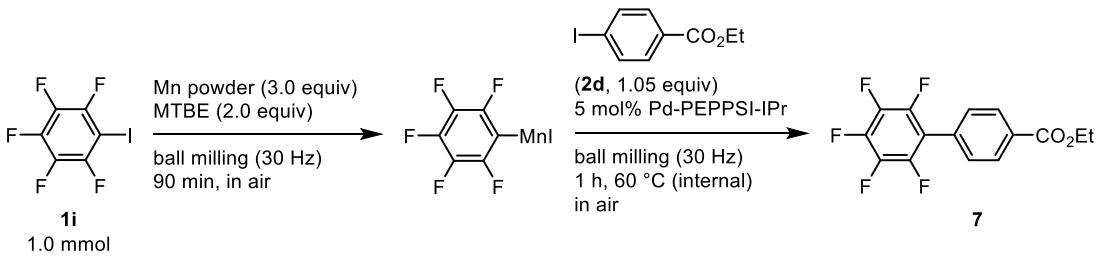
3. General Procedure for Synthesis of Organomanganese Reagents Using a Ball Mill

Procedure for the nucleophilic addition to various electrophiles (A)



All synthetic operations were carried out under atmospheric conditions. Manganese powder (3.0 mmol, 3.0 equiv) were placed in a milling jar (5 mL) with a ball (10 mm, diameter). An aryl halide (**1**, 1.0 mmol, 1.0 equiv) and liquid additive [2.0 mmol, 2.0 equiv, THF (162 μL) or MTBE (236 μL)] were added to the jar using a syringe. After the jar was closed without purging with inert gas, the jar was placed in the ball mill (Retsch MM 400, 1.5–3 h, 30 Hz). After ball milling, the jar was opened in air and charged with an electrophile (2.0 mmol, 2.0 equiv). In order to prevent undesired protonation of mechanochemically generated arylmanganese nucleophiles by atmospheric moisture, an electrophile should be added as rapidly as possible (< 1 min). The jar was then closed without purging with inert gas, and was placed in the ball mill (Retsch MM 400, 0.5 h, 30 Hz). After ball milling, the reaction mixture was quenched with 1 M HCl and extracted with ethyl acetate (30 mL×3). The solution was washed with brine and dried over $MgSO_4$. After the removal of the solvents under reduced pressure, the crude material was purified by flash column chromatography (SiO_2, hexane/ethyl acetate, 100:0 to 80:20) to give the corresponding product. In some cases, the product was further purified by recycling GPC.

Procedure for the palladium-catalyzed cross-coupling reactions (B)



The reaction was conducted based on a solution-state reaction reported by P. Knochel *et al*.[5] All synthetic operations were carried out under atmospheric conditions. Manganese powder (3.0 mmol, 3.0 equiv) were placed in a milling jar (5 mL) with a ball (10 mm, diameter). 1,2,3,4,5-Pentafluoro-6-iodobenzene (**1i**, 1.0 mmol, 1.0 equiv) and MTBE (2.0 mmol, 2.0 equiv, 236 μL) were added to the jar using a syringe. After the jar was closed without purging with inert gas, the jar was placed in the ball mill (Retsch MM 400, 90 min, 30 Hz). After ball milling, the jar was opened in air and charged with Pd-PEPPSI-IPr (0.05 mmol, 5 mol%) and ethyl 4-iodobenzoate (**2d**, 1.05 mmol, 1.05 equiv). The

jar was then closed without purging with inert gas, and was placed in the ball mill (Retsch MM 400, 1 h, 30 Hz) and a heat gun (Takagi HG-1450B). After ball milling while applying heated air to the outside of the milling jar (the preset temperature at 120 °C), the reaction mixture was quenched with 1 M HCl and extracted with ethyl acetate (30 mL×3). The solution was washed with brine and dried over $MgSO_4$. After the removal of the solvents under reduced pressure, the crude material was purified by flash column chromatography (SiO_2, hexane) and recycling GPC using $CHCl_3$ as the eluent.

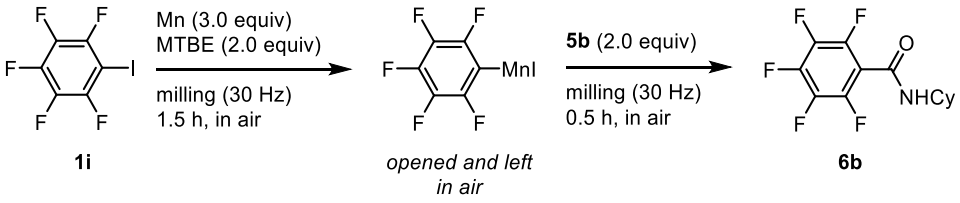
Set-up procedure for high-temperature ball-milling

The heat gun was fixed with clamps and placed directly above the ball milling jar (distance between the heat gun and ball milling jar: ca. 1 cm) (Figure S5). The mechanochemical cross-coupling reactions were conducted while applying heated air to the outside of the milling jar (the preset temperature at 120 °C). The temperature inside the milling jar after the solid-state coupling reactions was confirmed by observation with a thermography camera immediately after opening the milling jar.

Figure S5. The set-up procedure for a heat gun on MM400.

4. Air Stability of Organomanganese Reagents Prepared by Ball Milling

We conducted a number of nucleophilic addition reactions with **5b** after exposing the mechanochemically generated arylmanganese nucleophile **1i** to air for different lengths of time (5−60 min; Figure S6). The results showed that the yield of **6b** decreased when the generated arylmanganese species were exposed to air for 5 min or more.



Time (min)	<1	5	10	30	60
Yield (%)	91	61	51	38	18

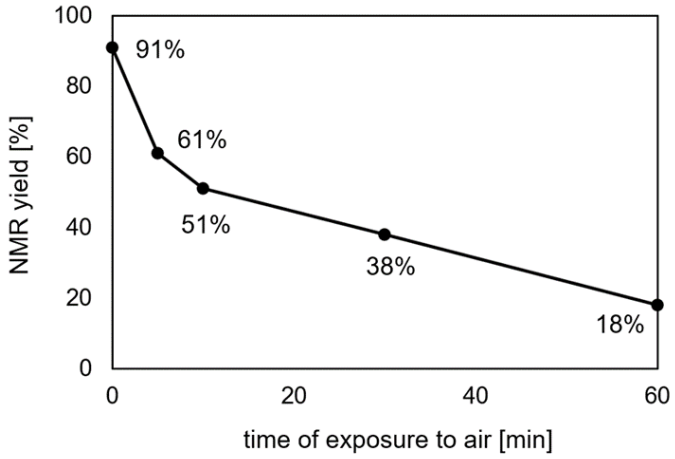
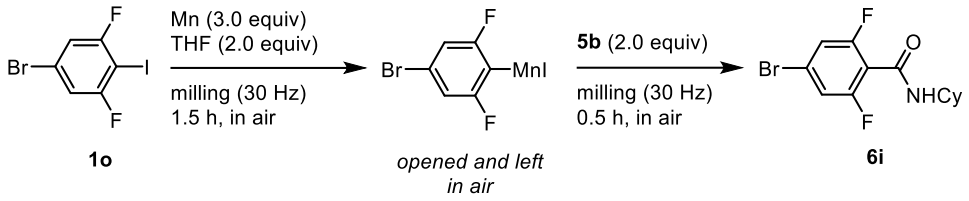


Figure S6. Stability of the mechanochemically generated organomanganese reagent in air.

We also checked the air stability of the mechanochemically generated organomanganese reagent from **1o** (Figure S7). We found that the yield of **6i** decreased when the generated arylmanganese species were exposed to air for 5 min or more, which was a result similar to that of **1i**.

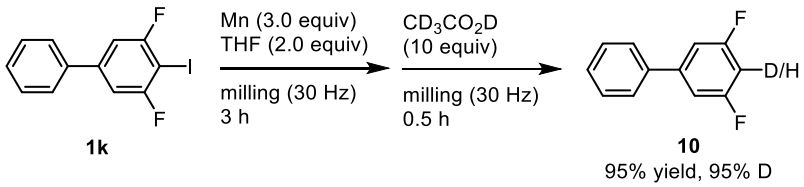


1o *opened and left in air* **6i**

Time (min)	<1	5	10	30
NMR Yield (%)	79	66	41	11

Figure S7. Stability of the mechanochemically generated organomanganese reagent from **1o** in air.

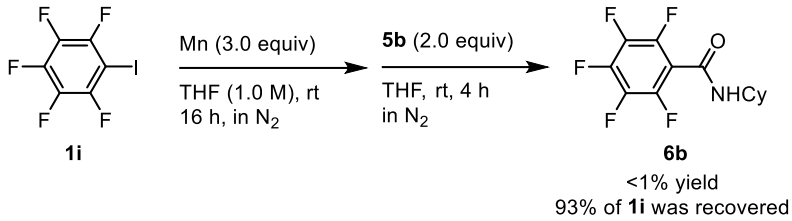
5. Deuteration Experiments



All synthetic operations were carried out under atmospheric conditions. Manganese powder (3.0 mmol, 3.0 equiv) and 3,5-difluoro-4-iodo-1,1'-biphenyl (**1k**) were placed in a milling jar (5 mL) with a ball (10 mm, diameter). THF (2.0 mmol, 2.0 equiv, 162 μL) were added to the jar using a syringe. After the jar was closed without purging with inert gas, the jar was placed in the ball mill (Retsch MM 400, 3 h, 30 Hz). After ball milling, the reaction was quenched by adding acetic acid-d_4 (10 mmol, 10 equiv) immediately after opening the jar in order to prevent undesired protonation by atmospheric moisture. The jar was then closed without purging with inert gas, and was placed in the ball mill (Retsch MM 400, 0.5 h, 30 Hz). After grinding, the reaction mixture was quenched with 1 M HCl, extracted with ethyl acetate (30 mL×3), washed with saturated aqueous Na_2CO_3, and dried over $MgSO_4$. After the removal of the solvents under reduced pressure, the resulting crude mixture was analyzed by ^1H NMR with dibromomethane as an internal standard to determine the NMR yield of 3,5-difluoro-1,1'-biphenyl (**10**, 95% yield, 95% D).

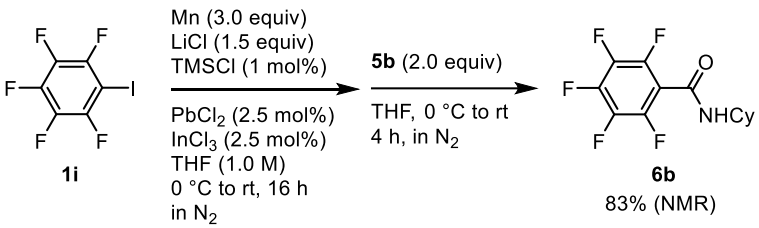
6. Details of Solution-based Reactions

Solution-based reaction without activation of manganese



An oven-dried reaction vial was charged with manganese powder (3.0 equiv) in air. After the vial was sealed with a screw cap containing a Teflon®-coated rubber septum, the vial was connected to a vacuum/nitrogen manifold through a needle. It was evacuated and then backfilled with nitrogen. This cycle was repeated three times. THF (1.0 mL) was added to the vial via syringe. **1i** was then added dropwise and the reaction mixture was stirred for 16 h. After 16 h, cyclohexyl isocyanate (**5b**, 249.8 mg, 2.0 mmol) was added to the reaction mixture. The reaction mixture was stirred at room temperature for 16 h followed by quenching with 1M HCl. The aqueous layer was extracted with ethyl acetate (30 mL×3). The combined organic phases were dried over $MgSO_4$, the solvent was removed in vacuo. The resulting crude mixture was analyzed by ^{19}F NMR with fluorobenzene as internal standards to determine the NMR yield of **6b** and the conversion of **1i**.

Solution-based reaction under the conditions reported by P. Knochel *et al.*



The reaction was conducted according to the reported procedure.[5] Mn powder (≧99.9%, product No. 463728, purchased from Aldrich), LiCl (99.9%, product No. 125-03322, purchased from Wako), $PbCl_2$ (−10 mesh, 99.999%, product No. 203440, purchased from Aldrich) and $InCl_3$ (99.999%, product No. 203440, purchased from Aldrich) were used for this reaction. An oven-dried reaction vial was charged with manganese powder (3.0 equiv), LiCl (1.5 equiv), $InCl_3$ (2.5 mol %) and $PbCl_2$ (2.5 mol %) in a glovebox under argon atmosphere. After the reaction vial was removed from the glove box, the mixture was dried for 5 min with a heat gun under high vacuum. The vial was then evacuated and backfilled with nitrogen three times and THF (4.0 mL) and TMSCl (1 mol%) were added to the mixture via syringe. **1i** (579.5 mg, 2.0 mmol) was then added dropwise at 0 °C and the reaction mixture was stirred for 16 h to give the solution of arylmanganese(II) iodide. This solution was added to a THF solution of cyclohexyl isocyanate (**5b**, 249.4 mg, 2.0 mmol, 1.3 M) at 0 °C. The reaction mixture was

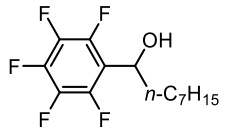
allowed to warm to room temperature and continuously stirred for 4 h, followed by quenching with brine. The aqueous layer was extracted with CH_2Cl_2 (30 mL×3). The combined organic phases were dried over $MgSO_4$, the solvent was removed in vacuo. The resulting crude mixture was analyzed by ^{19}F NMR with fluorobenzene as an internal standard to determine the NMR yield of **6b**.

7. Sample Preparation for XPS Analysis

X-Ray photoelectron spectroscopy (XPS) was used to analyze the surface of manganese metals. The ball-milled sample was prepared via the following conditions: Manganese powder (160 mg) was placed in a milling jar (5 mL) with a ball (10 mm, diameter) under atmospheric conditions. After the jar was closed without purging with inert gas, the jar was placed in the ball mill (Retsch MM 400, 1.5 h, 30 Hz). After ball milling, the jar was opened in a glove box, and the ball-milled sample was transferred to the vessel for XPS analysis.

8. Characterization of Products

1-(Perfluorophenyl)octan-1-ol (3i).

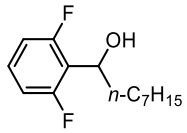


3i

The first metalation step was conducted with **1i** (293.7 mg, 1.0 mmol) and MTBE (236 μL, 2.0 mmol) for 1.5 h and the second addition step was conducted with **2a** (246.5 mg, 1.9 mmol) for 0.5 h. The product **3i** was purified by flash column chromatography (SiO_2, hexane/ethyl acetate, 100:0 to 90:10) and GPC. The product **3i** was obtained in 54% yield (160.7 mg, 0.54 mmol) as a white solid.

^{1}H NMR (399 MHz, $CDCl_3$, δ): 0.88 (t, J = 6.6 Hz, 3H), 1.17–1.37 (m, 9H), 1.39–1.50 (m, 1H), 1.77–1.88 (m, 1H), 1.96–2.06 (m, 1H), 2.10 (d, J = 7.6 Hz, 1H), 5.04 (q, J = 7.6 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 14.1 (CH_3), 22.7 (CH_2), 26.0 (CH_2), 29.26 (CH_2), 29.31 (CH_2), 31.9 (CH_2), 36.9 (CH_2), 66.5 (CH), 117.3 (t, $J_{C–F}$ = 15.3 Hz, C), 137.6 (dm, $J_{C–F}$ = 252.0 Hz, C), 140.6 (dm, $J_{C–F}$ = 254.0 Hz, C), 144.8 (dm, $J_{C–F}$ = 247.3 Hz, C). ^{19}F NMR (375 MHz, $CDCl_3$, δ): −162.8 (t, J = 23.1 Hz, 2F), −156.4 (d, J = 23.3 Hz, 1F), −145.0 (t, J = 22.9 Hz, 2F). HRMS-EI (m/z): $[M]^+$ calcd for $C_{14}H_{17}F_5O$, 296.1200; found, 296.1198.

1-(2,6-Difluorophenyl)octan-1-ol (3j).

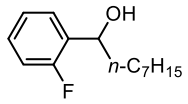


3j

The first metalation step was conducted with **1j** (240.5 mg, 1.0 mmol) and THF (165 μL, 2.0 mmol) for 3 h and the second addition step was conducted with **2a** (255.9 mg, 2.0 mmol) for 0.5 h. The product **3j** was purified by flash column chromatography (SiO_2, hexane/ethyl acetate, 100:0 to 90:10) and GPC. The product **3j** was obtained in 67% yield (96.6 mg, 0.68 mmol) as colorless oil.

^{1}H NMR (399 MHz, $CDCl_3$, δ): 0.87 (t, J = 6.8 Hz, 3H), 1.18–1.36 (m, 9H), 1.39–1.51 (m, 1H), 1.77–1.88 (m, 1H), 1.94–2.05 (m, 1H), 2.17 (dt, J = 2.4, 9.0 Hz, 1H), 5.03 (q, J = 7.8 Hz, 1H), 6.83–6.92 (m, 2H), 7.16–7.25 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 14.2 (CH_3), 22.7 (CH_2), 26.0 (CH_2), 29.3 (CH_2), 29.4 (CH_2), 31.9 (CH_2), 37.4 (CH_2), 66.6 (CH), 111.4–112.0 (m, CH), 119.9 (t, $J_{C–F}$ = 16.7 Hz, C), 128.9 (t, $J_{C–F}$ = 11.0 Hz, CH), 161.1 (dd, $J_{C–F}$ = 8.7, 248.0 Hz, C). ^{19}F NMR (377 MHz, $CDCl_3$, δ): −116.5 (s, 2F). HRMS-EI (m/z): $[M]^+$ calcd for $C_{14}H_{20}F_2O$, 242.1482; found, 242.1481.

1-(2-Fluorophenyl)octan-1-ol (3g).

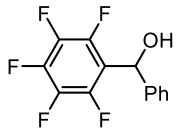


3g

The first metalation step was conducted with **1g** (222.2 mg, 1.0 mmol) and THF (162 μL, 2.0 mmol) for 3 h and the second addition step was conducted with **2a** (257.0 mg, 2.0 mmol) for 0.5 h. The product **3g** was purified by flash column chromatography (SiO_2, hexane/ethyl acetate, 100:0 to 90:10) and GPC. The product **3g** was obtained in 25% yield (55.1 mg, 0.25 mmol) as colorless oil.

^{1}H NMR (399 MHz, $CDCl_3$, δ): 0.87 (t, J = 6.8 Hz, 3H), 1.18–1.37 (m, 9H), 1.39–1.50 (m, 1H), 1.69–1.82 (m, 2H), 1.85 (d, J = 4.8 Hz, 1H), 5.01 (q, J = 5.9 Hz, 1H), 7.02 (ddd, J = 1.4, 8.2, 10.4 Hz, 1H), 7.15 (td, J = 1.1, 7.5 Hz, 1H), 7.21–7.26 (m, 1H), 7.46 (td, J = 1.9, 7.6 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 14.2 (*C*H_3), 22.8 (*C*H_2), 25.8 (*C*H_2), 29.3 (*C*H_2), 29.5 (*C*H_2), 31.9 (*C*H_2), 38.2 (*C*H_2), 68.5 (*C*H), 115.3 (d, $J_{C–F}$ = 21.9 Hz, *C*H), 124.3 (d, $J_{C–F}$ = 2.9 Hz, *C*H), 127.4 (d, $J_{C–F}$ = 4.8 Hz, *C*H), 128.8 (d, $J_{C–F}$ = 8.7 Hz, *C*H), 132.0 (d, $J_{C–F}$ = 13.3 Hz, *C*), 159.9 (d, $J_{C–F}$ = 245.2 Hz, *C*). ^{19}F NMR (377 MHz, $CDCl_3$, δ): −120.8 (s, 1F). HRMS-EI (m/z): $[M]^+$ calcd for $C_{14}H_{21}FO$, 224.1576; found, 224.1568.

(Perfluorophenyl)(phenyl)methanol (3k).

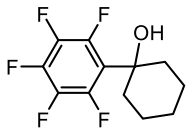


3k

The first metalation step was conducted with **1i** (293.8 mg, 1.0 mmol) and MTBE (236 μL, 2.0 mmol) for 1.5 h and the second addition step was conducted with **2b** (215.4 mg, 2.0 mmol) for 0.5 h. The product **3k** was purified by flash column chromatography (SiO_2, hexane/ethyl acetate, 100:0 to 90:10) and obtained in 60% yield (165.0 mg, 0.60 mmol) as a white solid. ^{1}H, ^{13}C, and ^{19}F NMR of the product **3k** were in agreement with the literature.[6]

^{1}H NMR (401 MHz, $CDCl_3$, δ): 2.64 (d, J = 8.0 Hz, 1H), 6.25 (d, J = 8.0 Hz, 1H), 7.30–7.42 (m, 5H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 67.6 (*C*H), 117.0 (t, $J_{C–F}$ = 13.8 Hz, *C*), 125.4 (*C*H), 128.3 (*C*H), 128.8 (*C*H), 137.7 (dm, $J_{C–F}$ = 252.7 Hz, *C*), 140.6 (*C*), 140.9 (dm, $J_{C–F}$ = 254.6 Hz, *C*), 144.7 (dm, $J_{C–F}$ = 249.8 Hz, *C*). ^{19}F NMR (377 MHz, $CDCl_3$, δ): −162.4 (t, J = 23.0 Hz, 2F), −155.5 (d, J = 34.7 Hz, 1F), −144.0 (t, J = 23.0 Hz, 2F). HRMS-EI (m/z): $[M]^+$ calcd for $C_{13}H_7F_5O$, 274.0417; found, 274.0414.

1-(Perfluorophenyl)cyclohexan-1-ol (4).

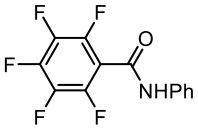


4

The first metalation step was conducted with **1i** (295.6 mg, 1.0 mmol) and MTBE (236 μL, 2.0 mmol) for 1.5 h and the second addition step was conducted with **2c** (117.0 mg, 1.2 mmol) for 0.5 h. The product **4** was purified by flash column chromatography (SiO_2, hexane/ethyl acetate, 100:0 to 90:10) and GPC. The product **4** was obtained in 45% yield (120.1 mg, 0.45 mmol) as a white solid. ^1H, ^{13}C, and ^{19}F NMR of the product **4** were in agreement with the literature.[6]

^1H NMR (392 MHz, $CDCl_3$, δ): 1.29 (qt, J = 3.8, 12.8 Hz, 1H), 1.56–1.64 (m, 2H), 1.67–1.89 (m, 3H), 1.97–2.09 (m, 4H), 2.42 (t, J = 3.4 Hz, 1H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 21.4 (CH_2), 25.1 (CH_2), 37.2 (t, $J_{C–F}$ = 4.3 Hz, CH_2), 75.3 (*C*), 121.3–121.7 (m, *C*), 137.5 (dm, $J_{C–F}$ = 248.2 Hz, *C*), 140.0 (dm, $J_{C–F}$ = 252.0 Hz, *C*), 145.1 (dm, $J_{C–F}$ = 248.8 Hz, *C*). ^{19}F NMR (377 MHz, $CDCl_3$, δ): –162.7 (t, J = 23.1 Hz, 2F), –157.1 (d, J = 23.1 Hz, 1F), –140.7 (t, J = 23.1 Hz, 2F). HRMS-EI (m/z): $[M]^+$ calcd for $C_{12}H_{11}F_5O$, 266.0730; found, 266.0728.

2,3,4,5,6-Pentafluoro-*N*-phenylbenzamide (6a).

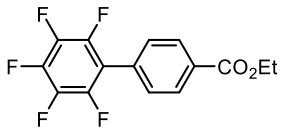


6a

The first metalation step was conducted with **1i** (293.8 mg, 1.0 mmol) and MTBE (236 μL, 2.0 mmol) for 1.5 h and the second amidation step was conducted with **5a** (237.4 mg, 2.0 mmol) for 0.5 h. The product **6a** was purified by flash column chromatography (SiO_2, hexane/ethyl acetate, 100:0 to 85:15) and obtained in 69% yield (197.0 mg, 0.69 mmol) as a white solid. ^1H and ^{19}F NMR of the product **6a** were in agreement with the literature.[7]

^1H NMR (401 MHz, DMSO-d_6, δ): 7.23 (t, J = 7.2 Hz, 1H), 7.41 (t, J = 8.0 Hz, 2H), 7.52 (brs, 1H), 7.61 (d, J = 8.8 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 112.5 (t, $J_{C–F}$ = 20.5 Hz, *C*), 119.6 (*C*H), 124.8 (*C*H), 129.1 (*C*H), 137.1 (dm, $J_{C–F}$ = 253.7 Hz, *C*), 138.0 (*C*), 141.5 (dm, $J_{C–F}$ = 250.9 Hz, *C*), 143.2 (dm, $J_{C–F}$ = 251.3 Hz, *C*), 154.9 (*C*). ^{19}F NMR (375 MHz, $CDCl_3$, δ): –160.4 (t, J = 23.1 Hz, 2F), –150.6 (t, J = 23.3 Hz, 1F), –140.9 (s, 2F). HRMS-EI (m/z): $[M]^+$ calcd for $C_{13}H_6F_5NO$, 287.0370; found, 287.0372.

Ethyl 2',3',4',5',6'-pentafluoro-[1,1'-biphenyl]-4-carboxylate (7).

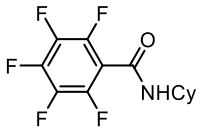


7

The reaction was conducted with **1i** (293.5 mg, 1.0 mmol) according to the general procedure B. The product **7** was purified by GPC. The product **7** was obtained in 71% yield (224.6 mg, 0.71 mmol) as a white solid. ^{1}H, ^{13}C, and ^{19}F NMR of the product **7** were in agreement with the literature.[8]

^{1}H NMR (401 MHz, $CDCl_3$, δ): 1.42 (t, J = 7.1 Hz, 3H), 4.42 (q, J = 7.0 Hz, 2H), 7.51 (d, J = 8.2 Hz, 2H), 8.17 (d, J = 8.7 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 14.2 (CH_3), 61.3 (CH_2), 114.7–115.2 (m, *C*), 129.7 (*C*H), 130.2 (*C*H), 130.7 (*C*), 131.2 (*C*), 137.8 (dm, $J_{C–F}$ = 252.2 Hz, *C*), 140.7 (dm, $J_{C–F}$ = 254.1 Hz, *C*), 144.0 (dm, $J_{C–F}$ = 249.3 Hz, *C*), 165.8 (*C*). ^{19}F NMR (377 MHz, $CDCl_3$, δ): –162.2 (t, J = 23.1 Hz, 2F), –154.8 (d, J = 34.7 Hz, 1F), –143.4 (s, 2F). HRMS-EI (m/z): $[M]^+$ calcd for $C_{15}H_9F_5O_2$, 316.0523; found, 316.0520.

***N*-Cyclohexyl-2,3,4,5,6-pentafluorobenzamide (6b).**



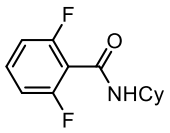
6b

For reaction with **1i**: the first metalation step was conducted with **1i** (293.3 mg, 1.0 mmol) and MTBE (236 μL, 2.0 mmol) for 1.5 h and the second amidation step was conducted with **5b** (246.4 mg, 2.0 mmol) for 0.5 h. The product **6b** was purified by flash column chromatography (SiO_2, hexane/ethyl acetate, 100:0 to 80:20) and obtained in 72% yield (210.7 mg, 0.72 mmol) as a white solid.

For the reaction with **1s**: the first metalation step was conducted with **1s** (246.8 mg, 1.0 mmol) and MTBE (236 μL, 2.0 mmol) for 1.5 h and the second arylation step was conducted with **5b** (248.2 mg, 2.0 mmol) for 0.5 h. The product **6b** was purified by flash column chromatography (SiO_2, hexane/ethyl acetate, 100:0 to 85:15) and obtained in 57% yield (168.2 mg, 0.57 mmol) as a white solid.

^{1}H NMR (392 MHz, $CDCl_3$, δ): 1.15–1.32 (m, 3H), 1.36–1.49 (m, 2H), 1.61–1.69 (m, 1H), 1.71–1.80 (m, 2H), 1.99–2.09 (m, 2H), 3.94–4.06 (m, 1H), 5.76 (brs, 1H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 24.8 (CH_2), 25.4 (CH_2), 32.7 (CH_2), 49.6 (*C*H), 112.2 (t, $J_{C–F}$ = 18.6 Hz, *C*), 137.6 (dm, $J_{C–F}$ = 255.1 Hz, *C*), 142.1 (dm, $J_{C–F}$ = 256.1 Hz, *C*), 144.0 (dm, $J_{C–F}$ = 251.7 Hz, *C*), 156.5 (*C*). ^{19}F NMR (377 MHz, $CDCl_3$, δ): –161.1 (s, 2F), –152.1 (d, J = 23.0 Hz, 1F), –141.7 (d, J = 23.4 Hz, 2F). HRMS-EI (m/z): $[M]^+$ calcd for $C_{13}H_{12}F_5NO$, 293.0839; found, 293.0833.

***N*-Cyclohexyl-2,6-difluorobenzamide (6c).**

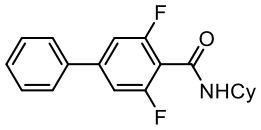


6c

The first metalation step was conducted with **1b** (242.1 mg, 1.0 mmol) and THF (162 μL, 2.0 mmol) for 1.5 h and the second amidation step was conducted with **5b** (248.9 mg, 2.0 mmol) for 0.5 h. The product **6c** was purified by flash column chromatography (SiO_2, hexane/ethyl acetate, 100:0 to 80:20) and obtained in 79% yield (191.1 mg, 0.80 mmol) as a white solid. ^1H, ^{13}C, and ^{19}F NMR of the product **6c** were in agreement with the literature.[9]

^1H NMR (392 MHz, $CDCl_3$, δ): 1.18–1.32 (m, 3H), 1.36–1.50 (m, 2H), 1.59–1.69 (m, 1H), 1.70–1.80 (m, 2H), 2.01–2.10 (m, 2H), 3.97–4.07 (m, 1H), 5.77 (brs, 1H), 6.90–6.98 (m, 2H), 7.30–7.39 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 24.8 (*C*H_2), 25.6 (*C*H_2), 33.0 (*C*H_2), 49.0 (*C*H), 111.9–112.1 (m, *C*H), 114.9 (t, $J_{C–F}$ = 20.5 Hz, *C*), 131.5 (t, $J_{C–F}$ = 10.1 Hz, *C*H), 159.5 (*C*), 160.0 (dd, $J_{C–F}$ = 6.7, 251.7 Hz, *C*). ^{19}F NMR (377 MHz, $CDCl_3$, δ): −113.6 (s, 2F). HRMS-EI (m/z): $[M]^+$ calcd for $C_{13}H_{15}F_2NO$, 239.1122; found, 239.1120.

***N*-Cyclohexyl-3,5-difluoro-[1,1'-biphenyl]-4-carboxamide (6d).**

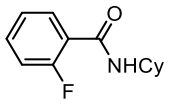


6d

The first metalation step was conducted with **1k** (316.3 mg, 1.0 mmol) and THF (162 μL, 2.0 mmol) for 3 h and the second amidation step was conducted with **5b** (247.6 mg, 2.0 mmol) for 0.5 h. The product **6d** was purified by flash column chromatography (SiO_2, CH_2Cl_2) and the obtained solid was washed with hexane. The product **6d** was obtained in 71% yield (224.0 mg, 0.71 mmol) as a white solid.

^1H NMR (401 MHz, $CDCl_3$, δ): 1.16–1.34 (m, 3H), 1.38–1.50 (m, 2H), 1.60–1.69 (m, 1H), 1.71–1.81 (m, 2H), 2.02–2.13 (m, 2H), 3.98–4.10 (m, 1H), 5.84 (brs, 1H), 7.14–7.20 (m, 2H), 7.40–7.50 (m, 3H), 7.52–7.57 (m, 2H). ^{13}C NMR (100 MHz, DMSO-d_6, δ): 24.5 (*C*H_2), 25.2 (*C*H_2), 32.2 (*C*H_2), 48.3 (*C*H), 109.8 (d, $J_{C–F}$ = 24.8 Hz, *C*H), 114.4 (t, $J_{C–F}$ = 6.2 Hz, *C*), 126.9 (*C*H), 128.9 (*C*H), 129.1 (*C*H), 137.2 (*C*H), 143.3 (t, $J_{C–F}$ = 9.6 Hz, *C*), 158.5 (*C*), 159.2 (dd, $J_{C–F}$ = 9.0, 247.5 Hz, *C*). ^{19}F NMR (377 MHz, $CDCl_3$, δ): −113.1 (s, 2F). HRMS-EI (m/z): $[M]^+$ calcd for $C_{19}H_{19}F_2NO$, 315.1435; found, 315.1430.

***N*-Cyclohexyl-2-fluorobenzamide (6e).**

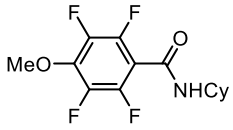


6e

The first metalation step was conducted with **1g** (221.3 mg, 1.0 mmol) and 1,2-dimethoxyethane (207 μL, 2.0 mmol) for 3 h and the second amidation step was conducted with **5b** (253 μL, 2.0 mmol) for 0.5 h. The product **6e** was purified by flash column chromatography (SiO_2, hexane/ethyl acetate, 100:0 to 80:20) and obtained in 38% yield (84.1 mg, 0.38 mmol) as a white solid. ^{1}H, ^{13}C, and ^{19}F NMR of the product **6e** were in agreement with the literature.[10]

^{1}H NMR (401 MHz, $CDCl_3$, δ): 1.18–1.34 (m, 3H), 1.38–1.51 (m, 2H), 1.60–1.69 (m, 1H), 1.71–1.80 (m, 2H), 1.98–2.09 (m, 2H), 3.96–4.09 (m, 1H), 6.62 (brs, 1H), 7.10 (dd, J = 8.6, 11.4 Hz, 1H), 7.22–7.29 (m, 1H), 7.40–7.50 (m, 1H), 8.09 (dt, J = 3.9, 11.3 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 24.8 (*C*H_2), 25.6 (*C*H_2), 33.0 (*C*H_2), 48.6 (*C*H), 115.9 (d, $J_{C–F}$ = 24.8 Hz, *C*H), 121.6 (d, $J_{C–F}$ = 12.3 Hz, *C*), 124.7 (d, $J_{C–F}$ = 2.8 Hz, *C*H), 132.0 (*C*H), 133.0 (d, $J_{C–F}$ = 8.7 Hz, *C*H), 160.5 (d, $J_{C–F}$ = 247.0 Hz, *C*), 162.3 (d, $J_{C–F}$ = 2.9 Hz, *C*). ^{19}F NMR (377 MHz, $CDCl_3$, δ): −114.9 (s, 1F). HRMS-EI (m/z): $[M]^+$ calcd for $C_{13}H_{16}FNO$, 221.1216; found, 221.1216.

***N*-Cyclohexyl-2,3,5,6-tetrafluoro-4-methoxybenzamide (6f).**

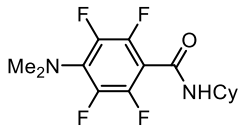


6f

The first metalation step was conducted with **1l** (308.7 mg, 1.0 mmol) and THF (162 μL, 2.0 mmol) for 1.5 h and the second amidation step was conducted with **5b** (249.4 mg, 2.0 mmol) for 0.5 h. The product **6f** was purified by flash column chromatography (SiO_2, hexane/ethyl acetate, 100:0 to 80:20) and obtained in 70% yield (215.2 mg, 0.70 mmol) as a white solid.

^{1}H NMR (401 MHz, $CDCl_3$, δ): 1.18–1.30 (m, 3H), 1.36–1.49 (m, 2H), 1.60–1.68 (m, 1H), 1.70–1.79 (m, 2H), 1.98–2.09 (m, 2H), 3.94–4.04 (m, 1H), 4.10–4.12 (m, 3H), 5.77 (brs, 1H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 24.7 (*C*H_2), 25.4 (*C*H_2), 32.5 (*C*H_2), 49.3 (*C*H), 62.0 (t, $J_{C–F}$ = 3.8 Hz, *C*H_3), 110.0 (t, $J_{C–F}$ = 19.6 Hz, *C*), 138.9–139.5 (m, *C*), 140.4 (dm, $J_{C–F}$ = 239.9 Hz, *C*), 143.9 (dm, $J_{C–F}$ = 249.8 Hz, *C*), 157.3 (*C*). ^{19}F NMR (377 MHz, $CDCl_3$, δ): −157.9 (s, 2F), −143.6 (d, J = 23.4 Hz, 2F). HRMS-EI (m/z): $[M]^+$ calcd for $C_{14}H_{15}F_4NO_2$, 305.1039; found, 305.1039.

***N*-Cyclohexyl-4-(dimethylamino)-2,3,5,6-tetrafluorobenzamide (6g).**

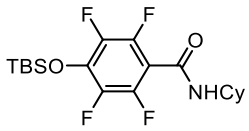


6g

The first metalation step was conducted with **1m** (318.1 mg, 1.0 mmol) and THF (162 μL, 2.0 mmol) for 1.5 h and the second amidation step was conducted with **5b** (249.2 mg, 2.0 mmol) for 0.5 h. The product **6g** was purified by flash column chromatography (SiO_2, hexane/ethyl acetate, 100:0 to 80:20) and obtained in 69% yield (220.5 mg, 0.69 mmol) as a white solid.

^{1}H NMR (401 MHz, $CDCl_3$, δ): 1.16–1.30 (m, 3H), 1.35–1.48 (m, 2H), 1.59–1.68 (m, 1H), 1.69–1.79 (m, 2H), 1.98–2.08 (m, 2H), 2.99 (t, J = 2.2 Hz, 6H), 3.93–4.05 (m, 1H), 5.78 (brs, 1H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 24.8 (*C*H_2), 25.5 (*C*H_2), 32.8 (*C*H_2), 43.1 (t, $J_{C–F}$ = 4.3 Hz, *C*H_3), 49.1 (*C*H), 107.1 (t, $J_{C–F}$ = 18.1 Hz, *C*), 132.9 (t, $J_{C–F}$ = 8.6 Hz, *C*), 141.2 (dm, $J_{C–F}$ = 244.1 Hz, *C*), 144.8 (dm, $J_{C–F}$ = 245.1 Hz, *C*), 158.0 (*C*). ^{19}F NMR (377 MHz, $CDCl_3$, δ): −152.5 (d, J = 23.0 Hz, 2F), −144.6 (s, 2F). HRMS-EI (m/z): $[M]^+$ calcd for $C_{15}H_{18}F_4N_2O_1$, 318.1355; found, 318.1346.

4-[(*tert*-Butyldimethylsilyl)oxy]-*N*-cyclohexyl-2,3,5,6-tetrafluorobenzamide (6h).

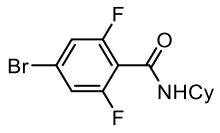


6h

The first metalation step was conducted with **1n** (406.6 mg, 1.0 mmol) and THF (162 μL, 2.0 mmol) for 90 min and the second amidation step was conducted with **5b** (248.7 mg, 2.0 mmol) for 30 min. The product **6h** was purified by flash column chromatography (SiO_2, hexane/ethyl acetate, 100:0 to 80:20) and obtained in 28% yield (113.4 mg, 0.28 mmol) as a white solid.

^{1}H NMR (401 MHz, $CDCl_3$, δ): 0.23 (s, 6H), 1.01 (s, 9H), 1.15–1.31 (m, 3H), 1.36–1.49 (m, 2H), 1.60–1.68 (m, 1H), 1.70–1.79 (m, 2H), 2.00–2.08 (m, 2H), 3.94–4.06 (m, 1H), 5.78 (brs, 1H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): −4.9 (*C*H_3), 18.5 (*C*), 24.8 (*C*H_2), 25.3 (*C*H_3), 25.5 (*C*H_2), 32.8 (*C*H_2), 49.3 (*C*H), 108.6 (t, $J_{C–F}$ = 18.6 Hz, *C*), 136.1–136.5 (m, *C*), 140.7 (dm, $J_{C–F}$ = 248.4 Hz, *C*), 144.3 (dm, $J_{C–F}$ = 251.7 Hz, *C*), 157.7 (*C*). ^{19}F NMR (377 MHz, $CDCl_3$, δ): −157.6 (d, J = 23.0 Hz, 2F), −144.4 (s, 2F). HRMS-EI (m/z): $[M]^+$ calcd for $C_{19}H_{27}F_4NO_2Si$, 405.1747; found, 405.1740.

4-Bromo-*N*-cyclohexyl-2,6-difluorobenzamide (6i).

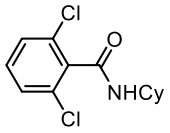


6i

The first step was conducted with **1o** (319.1 mg, 1.0 mmol) and THF (162 μL, 2.0 mmol) for 1.5 h and the second amidation step was conducted with **5b** (247.6 mg, 2.0 mmol) for 0.5 h. The product **6i** was purified by flash column chromatography (SiO_2, hexane/ethyl acetate, 100:0 to 80:20) and obtained in 75% yield (237.9 mg, 0.75 mmol) as a white solid.

^{1}H NMR (401 MHz, $CDCl_3$, δ): 1.14–1.30 (m, 3H), 1.35–1.49 (m, 2H), 1.60–1.69 (m, 1H), 1.70–1.79 (m, 2H), 1.98–2.10 (m, 2H), 3.93–4.06 (m, 1H), 5.73 (brs, 1H), 7.11–7.17 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 24.8 (*C*H_2), 25.5 (*C*H_2), 32.9 (*C*H_2), 49.1 (*C*H), 114.2 (t, $J_{C–F}$ = 21.0 Hz, *C*), 116.0 (d, $J_{C–F}$ = 28.6 Hz, *C*H), 123.8 (t, $J_{C–F}$ = 11.9 Hz, *C*), 158.6 (*C*), 159.8 (dd, $J_{C–F}$ = 8.6, 255.6 Hz, *C*). ^{19}F NMR (377 MHz, $CDCl_3$, δ): −111.7 (s, 2F). HRMS-ESI (m/z): $[M+Na]^+$ calcd for $C_{13}H_{14}BrF_2NONa$, 340.0119; found, 340.0122.

2,6-Dichloro-*N*-cyclohexylbenzamide (6j).

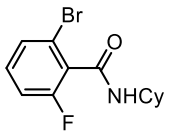


6j

The first metalation step was conducted with **1p** (273.3 mg, 1.0 mmol) and THF (162 μL, 2.0 mmol) for 1.5 h and the second amidation step was conducted with **5b** (248.5 mg, 2.0 mmol) for 0.5 h. The product **6j** was purified by flash column chromatography (SiO_2, hexane/ethyl acetate, 100:0 to 80:20) and obtained in 55% yield (149.4 mg, 0.55 mmol) as a white solid.

^{1}H NMR (401 MHz, $CDCl_3$, δ): 1.13–1.33 (m, 3H), 1.37–1.51 (m, 2H), 1.61–1.69 (m, 1H), 1.71–1.82 (m, 2H), 2.01–2.16 (m, 2H), 3.98–4.12 (m, 1H), 5.60 (brs, 1H), 7.21–7.26 (m, 1H), 7.29–7.33 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 24.8 (*C*H_2), 25.4 (*C*H_2), 32.6 (*C*H_2), 48.7 (*C*H), 127.8 (*C*H), 130.3 (*C*H), 132.1 (*C*), 136.2 (*C*), 163.4 (*C*). HRMS-EI (m/z): $[M]^+$ calcd for $C_{13}H_{15}Cl_2NO$, 271.0531; found, 271.0531.

2-Bromo-*N*-cyclohexyl-6-fluorobenzamide (6k).

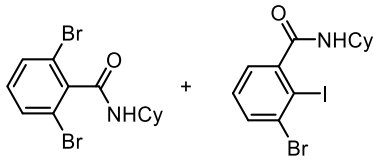


6k

The first metalation step was conducted with **1q** (299.0 mg, 1.0 mmol) and THF (162 μL, 2.0 mmol) for 1.5 h and the second amidation step was conducted with **5b** (249.7 mg, 2.0 mmol) for 0.5 h. The product **6k** was purified by flash column chromatography (SiO_2, hexane/ethyl acetate, 100:0 to 80:20) and obtained in 69% yield (208.4 mg, 0.69 mmol) as a white solid.

^{1}H NMR (401 MHz, $CDCl_3$, δ): 1.13–1.32 (m, 3H), 1.37–1.50 (m, 2H), 1.60–1.69 (m, 1H), 1.71–1.81 (m, 2H), 2.04–2.15 (m, 2H), 3.97–4.10 (m, 1H), 5.64 (brs, 1H), 7.07 (td, J = 0.8, 8.6 Hz, 1H), 7.23 (td, J = 5.9, 8.2 Hz, 1H), 7.37 (d, J = 8.0 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 24.9 (*C*H_2), 25.5 (*C*H_2), 32.7 (*C*H_2), 48.9 (*C*H), 114.9 (d, $J_{C–F}$ = 22.0 Hz, *C*H), 120.6 (d, $J_{C–F}$ = 4.8 Hz, *C*), 127.8 (d, $J_{C–F}$ = 21.9 Hz, *C*), 128.5 (d, $J_{C–F}$ = 3.8 Hz, *C*H), 131.1 (d, $J_{C–F}$ = 8.6 Hz, *C*H), 159.2 (d, $J_{C–F}$ = 251.7 Hz, *C*), 162.4 (*C*). ^{19}F NMR (377 MHz, $CDCl_3$, δ): −113.4 (s, 1F). HRMS-EI (m/z): $[M]^+$ calcd for $C_{13}H_{15}BrFNO$, 299.0321; found, 299.0313.

2,6-Dibromo-*N*-cyclohexylbenzamide (6m).

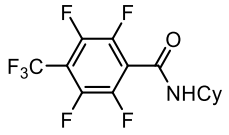


6m **6n**

The first metalation step was conducted with **1r** (361.7 mg, 1.0 mmol) and THF (162 μL, 2.0 mmol) for 1.5 h and the second amidation step was conducted with **5b** (249.7 mg, 2.0 mmol) for 0.5 h. The product **6m** and the byproduct **6n** were obtained in 54% NMR yield (**6m**:**6n** = 78:22).

^{1}H NMR for **6m** (401 MHz, $CDCl_3$, δ): 1.14–1.34 (m, 3H), 1.37–1.51 (m, 2H), 1.60–1.69 (m, 1H), 1.72–1.82 (m, 2H), 2.03–2.17 (m, 2H), 3.98–4.11 (m, 1H), 5.56 (brs, 1H), 7.09 (t, J = 8.0 Hz, 1H), 7.52 (d, J = 7.6 Hz, 2H). ^{13}C NMR for **6m** (100 MHz, $CDCl_3$, δ): 24.9 (*C*H_2), 25.6 (*C*H_2), 32.8 (*C*H_2), 48.8 (*C*H), 120.5 (*C*), 131.2 (*C*H), 131.8 (*C*H), 140.0 (*C*), 165.3 (*C*). HRMS-EI (m/z): $[M]^+$ calcd for $C_{13}H_{15}Br_2NO$, 358.9520; found, 358.9517.

***N*-Cyclohexyl-2,3,5,6-tetrafluoro-4-(trifluoromethyl)benzamide (6o).**

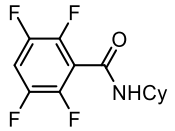


6o

The first step was conducted with **1t** (296.2 mg, 1.0 mmol) and MTBE (236 μL, 2.0 mmol) for 1.5 h and the second amidation step was conducted with **5b** (249.2 mg, 2.0 mmol) for 0.5 h. The product **6o** was purified by flash column chromatography (SiO_2, hexane/ethyl acetate, 100:0 to 80:20) and obtained in 69% yield (235.1 mg, 0.68 mmol) as a white solid.

^{1}H NMR (401 MHz, $CDCl_3$, δ): 1.18–1.32 (m, 3H), 1.37–1.50 (m, 2H), 1.62–1.70 (m, 1H), 1.72–1.80 (m, 2H), 1.99–2.10 (m, 2H), 3.95–4.07 (m, 1H), 5.80 (brs, 1H). ^{13}C NMR (100 MHz, DMSO-d_6, δ): 24.2 (CH_2), 25.1 (CH_2), 32.0 (CH_2), 48.7 (*C*H), 108.0–109.3 (m, *C*), 120.4 (d, $J_{C–F}$ = 229.8 Hz, *C*), 121.9 (d, $J_{C–F}$ = 21.9 Hz, *C*), 143.3 (dm, $J_{C–F}$ = 262.3 Hz, *C*), 155.1 (*C*). ^{19}F NMR (377 MHz, $CDCl_3$, δ): −139.1 (s, 2F), −138.5 (q, *J* = 23.1 Hz, 2F), −56.6 (t, *J* = 23.2 Hz, 3F). HRMS-EI (m/z): $[M]^+$ calcd for $C_{14}H_{12}F_7NO$, 343.0807; found, 343.0799.

***N*-Cyclohexyl-2,3,5,6-tetrafluorobenzamide (6p).**

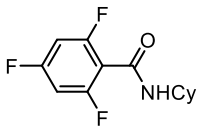


6p

The first metalation step was conducted with **1u** (229.1 mg, 1.0 mmol) and THF (162 μL, 2.0 mmol) for 90 min and the second amidation step was conducted with **5b** (249.7 mg, 2.0 mmol) for 30 min. The product **6p** was purified by flash column chromatography (SiO_2, hexane/ethyl acetate, 100:0 to 80:20) and obtained in 45% yield (124.6 mg, 0.45 mmol) as a white solid.

^{1}H NMR (392 MHz, $CDCl_3$, δ): 1.14–1.32 (m, 3H), 1.36–1.49 (m, 2H), 1.61–1.70 (m, 1H), 1.71–1.81 (m, 2H), 2.01–2.11 (m, 2H), 3.96–4.07 (m, 1H), 5.77 (brs, 1H), 7.07–7.17 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 24.8 (CH_2), 25.5 (CH_2), 32.8 (CH_2), 49.4 (*C*H), 107.2 (t, $J_{C–F}$ = 22.4 Hz, *C*H), 117.7 (t, $J_{C–F}$ = 19.1 Hz, *C*), 144.6 (dm, $J_{C–F}$ = 495.4 Hz, *C*), 144.5–145.0 (m, *C*), 157.3 (*C*). ^{19}F NMR (377 MHz, $CDCl_3$, δ): −142.5 (s, 2F), −138.3 (s, 2F). HRMS-EI (m/z): $[M]^+$ calcd for $C_{13}H_{13}F_4NO$, 275.0933; found, 275.0932.

***N*-Cyclohexyl-2,4,6-trifluorobenzamide (6q).**



6q

The first metalation step was conducted with **1v** (211.4 mg, 1.0 mmol) and THF (162 μL, 2.0 mmol) for 3 h and the second amidation step was conducted with **5b** (250.4 mg, 2.0 mmol) for 0.5 h. The product **6q** was purified by flash column chromatography (SiO_2, hexane/ethyl acetate, 100:0 to 85:15) and obtained in 39% yield (101.4 mg, 0.39 mmol) as a white solid.

^{1}H NMR (401 MHz, $CDCl_3$, δ): 1.14–1.32 (m, 3H), 1.35–1.49 (m, 2H), 1.60–1.69 (m, 1H), 1.70–1.80 (m, 2H), 1.99–2.09 (m, 2H), 3.94–4.05 (m, 1H), 5.74 (brs, 1H), 6.66–6.75 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 24.8 (*C*H_2), 25.5 (*C*H_2), 32.8 (*C*H_2), 49.1 (*C*H), 100.7 (td, $J_{C–F}$ = 3.5, 26.2 Hz, *C*H), 111.7 (td, $J_{C–F}$ = 4.1, 21.2 Hz, *C*), 158.7 (*C*), 160.4 (ddd, $J_{C–F}$ = 9.8, 15.1, 253.0 Hz, *C*), 163.2 (dt, $J_{C–F}$ = 15.3, 252.7 Hz, *C*). ^{19}F NMR (377 MHz, $CDCl_3$, δ): −110.1 (s, 2F), −105.4 (s, 1F). HRMS-EI (m/z): $[M]^+$ calcd for $C_{13}H_{14}F_3NO$, 257.1028; found, 257.1025.

9. References

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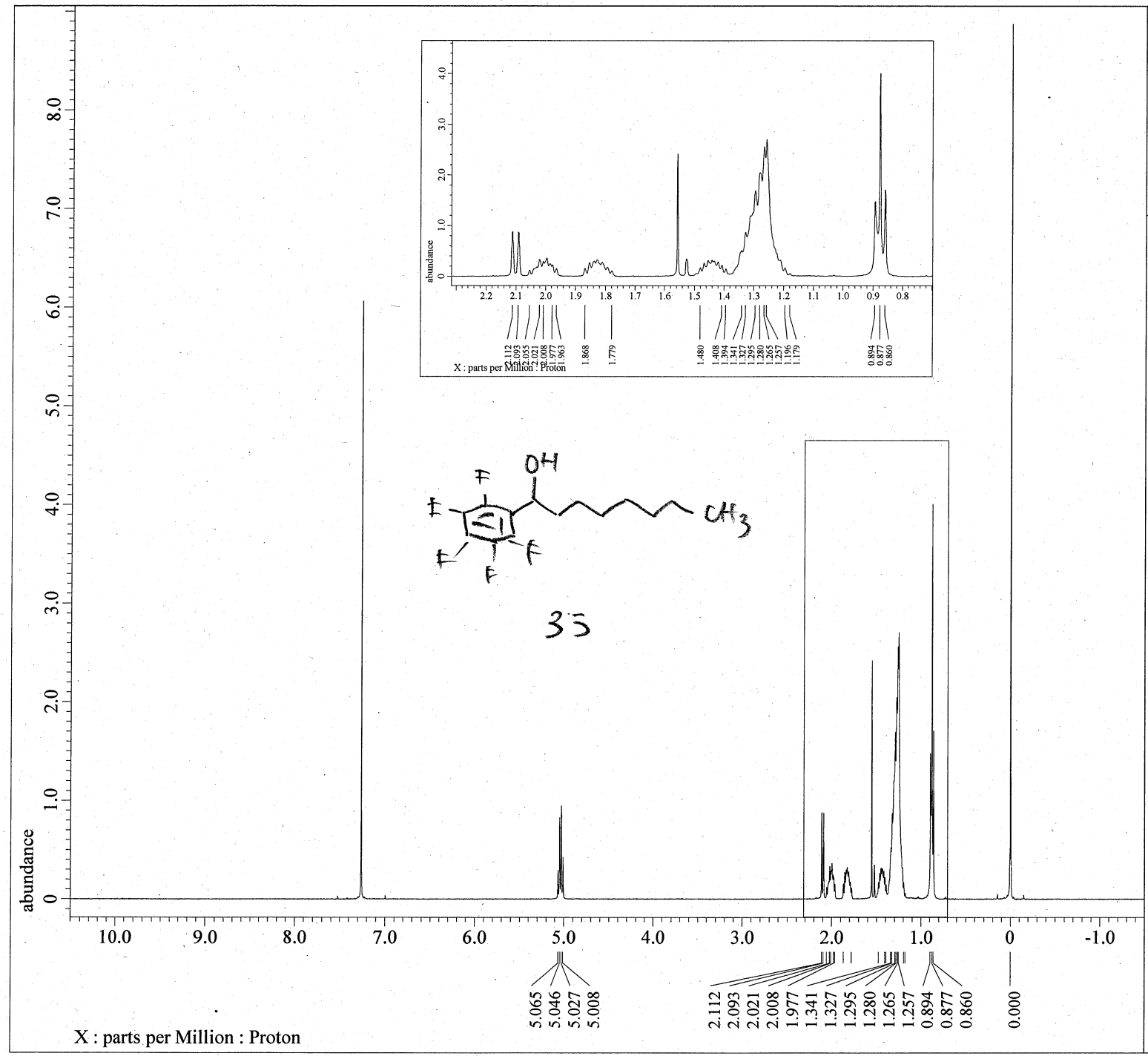


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trapezoid( 0[%], 0[%], 80[%], 100[%] )
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fft( 1, TRUE, TRUE )
machinephase
ppm

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X_Sweep	= 7.48502994[kHz]
X_Sweep_Clipped	= 5.98802395[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.03472754[MHz]
Irr_Offset	= 5.0[ppm]
Tri_Domain	= Proton
Tri_Freq	= 399.03472754[MHz]
Tri_Offset	= 5.0[ppm]
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Total_Scans	= 8
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Recvr_Gain	= 50
Temp_Get	= 18.4[dC]
X_90_Width	= 6.6[us]
X_Acq_Time	= 2.1889024[s]
X_Angle	= 45[deg]
X_Atn	= 1[dB]
X_Pulse	= 3.3[us]
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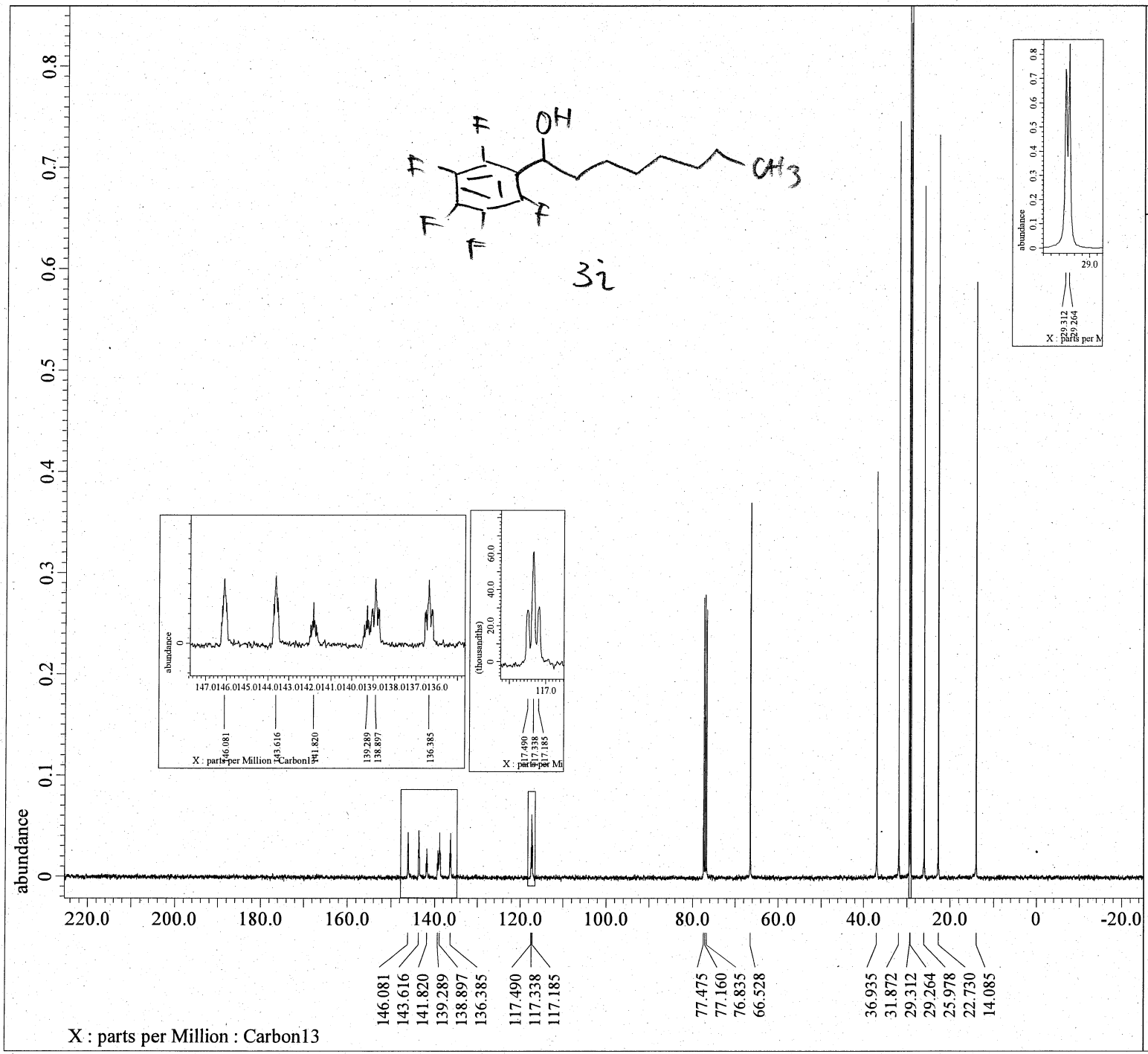
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.1889024[s]

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fft( 1, TRUE, TRUE )
machinephase
ppm

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Author	= element
Experiment	= carbon.jxp
Sample_Id	= TKH-1577
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 8-MAR-2022 20:56:59
Revision_Time	= 11-MAR-2022 10:20:17
Comment	= single pulse decoupled ga
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Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
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X_Offset	= 100.0[ppm]
X_Points	= 32768
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X_Resolution	= 0.95846665[Hz]
X_Sweep	= 31.40703518[kHz]
X_Sweep_Clipped	= 25.12562814[kHz]
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Irr_Freq	= 399.03472754[MHz]
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Clipped	= FALSE
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Recvr_Gain	= 50
Temp_Get	= 18.2[dC]
X_90_Width	= 10.9[us]
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X_Angle	= 30[deg]
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Irr_Atn_Noe	= 25.823[dB]
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Initial_Wait	= 1[s]
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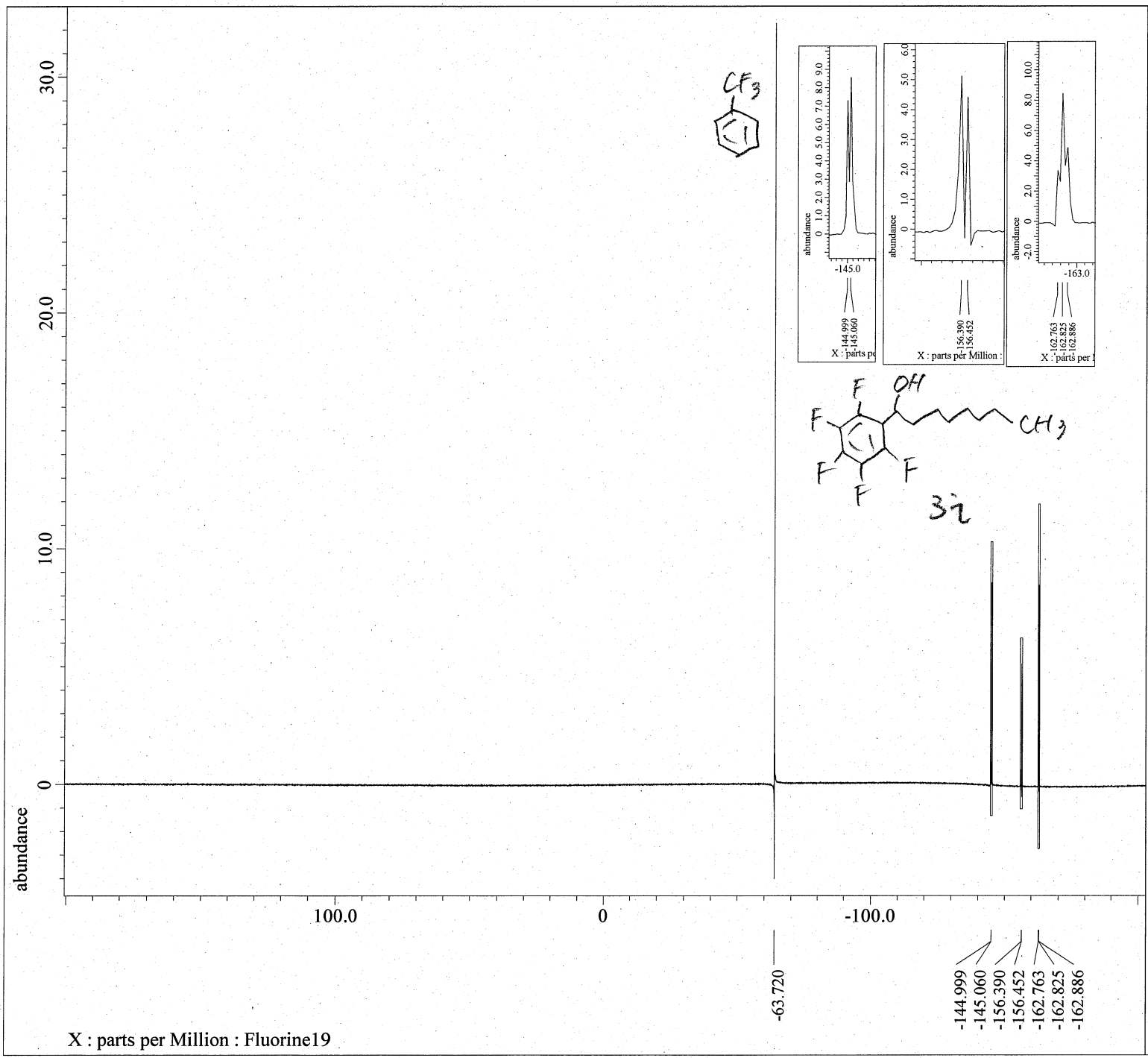
Repetition_Time	= 3.04333312[s]

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sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
phase( 68, 0, 50[%] )

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Author	= element
Experiment	= proton.jxp
Sample_Id	= TKH-1577_F_standard
Solvent	= CHLOROFORM-D
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X_Offset	= 0[ppm]
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X_Resolution	= 11.55968868[Hz]
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X_Sweep_Clipped	= 151.51515152[kHz]
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Tri_Freq	= 375.46772873[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
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Relaxation_Delay	= 5[s]
Recvr_Gain	= 50
Temp_Get	= 18.2[dC]
X_90_Width	= 7.6[us]
X_Acq_Time	= 86.50752[ms]
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X_Atn	= 2.5[dB]
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Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
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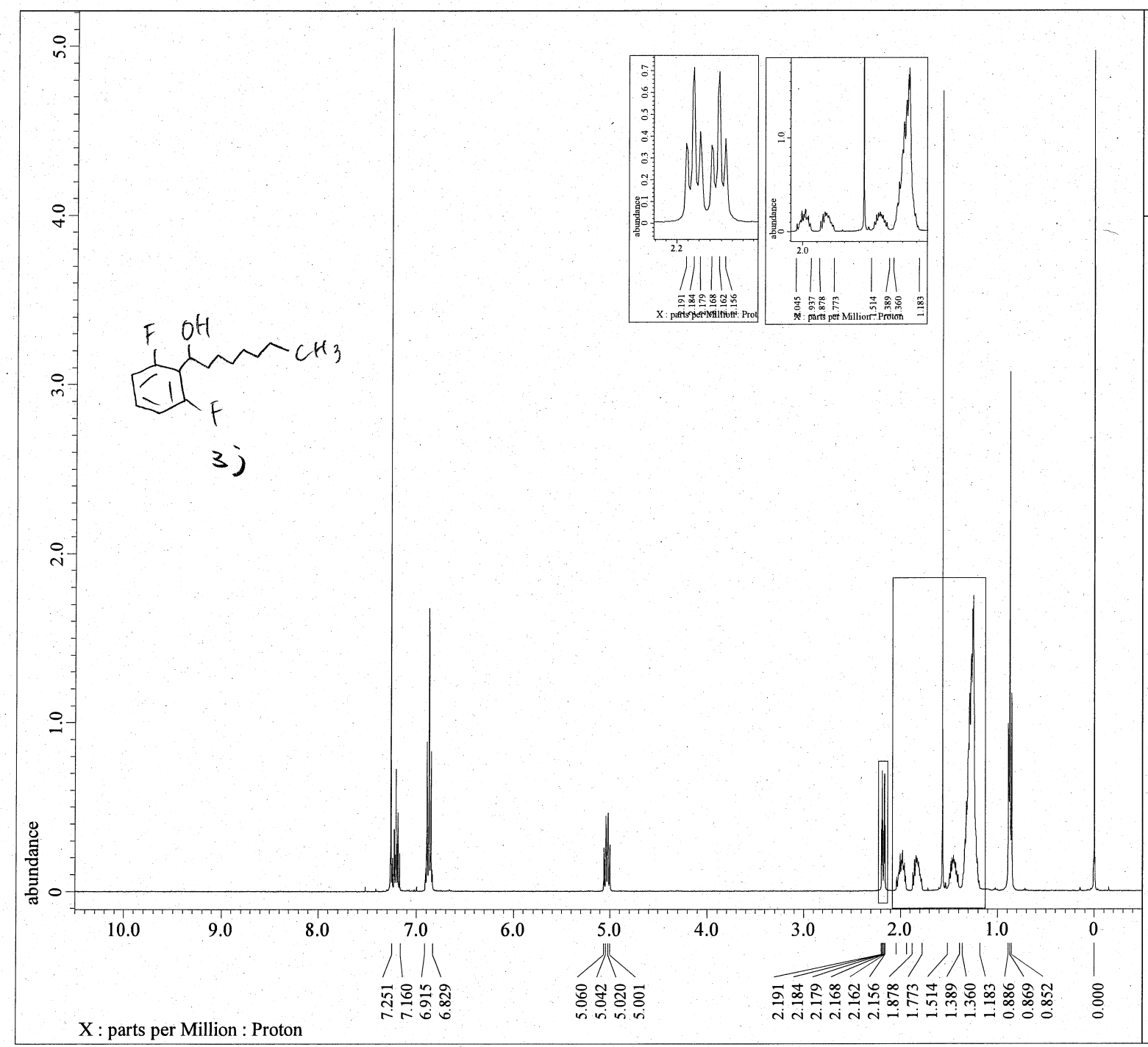


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---- PROCESSING PARAMETERS ----
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sexp( 0.2[Hz], 0.0[s] )
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fft( 1, TRUE, TRUE )
machinephase
ppm

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Dim_Units           = [ppm]
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Spectrometer        = DELTA2_NMR

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X_Sweep_Clipped     = 5.98802395[kHz]
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Relaxation_Delay    = 5[s]
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X_Angle             = 45[deg]
X_Atn               = 1[dB]
X_Pulse             = 3.3[us]
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Tri_Mode            = Off
Dante_Presat        = FALSE
Initial_Wait        = 1[s]
Repetition_Time     = 7.1889024[s]
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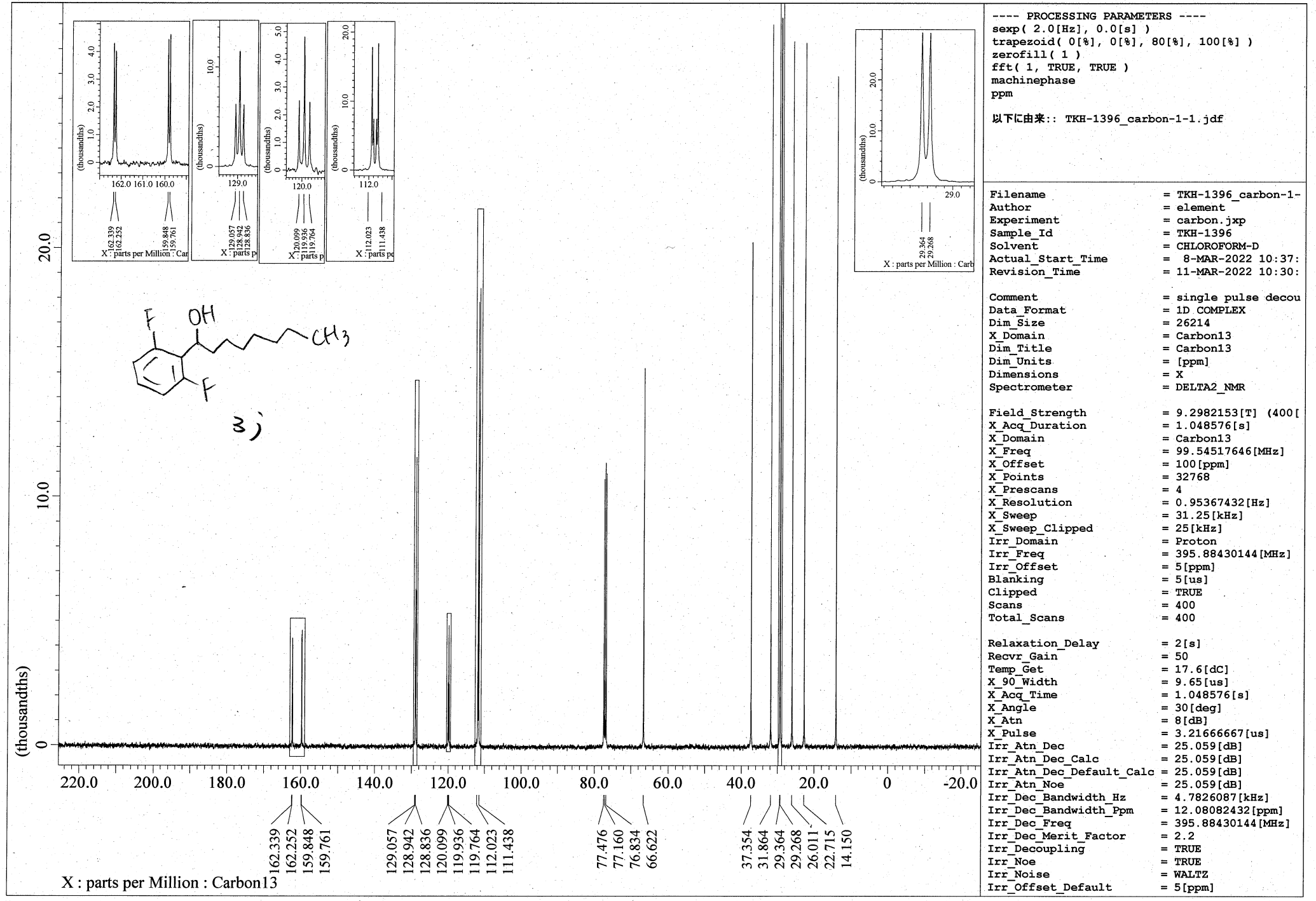


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machinephase
ppm

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Revision_Time	= 11-MAR-2022 10:30:
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Blanking	= 5[us]
Clipped	= TRUE
Scans	= 400
Total_Scans	= 400
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 17.6[dC]
X_90_Width	= 9.65[us]
X_Acq_Time	= 1.048576[s]
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X_Pulse	= 3.21666667[us]
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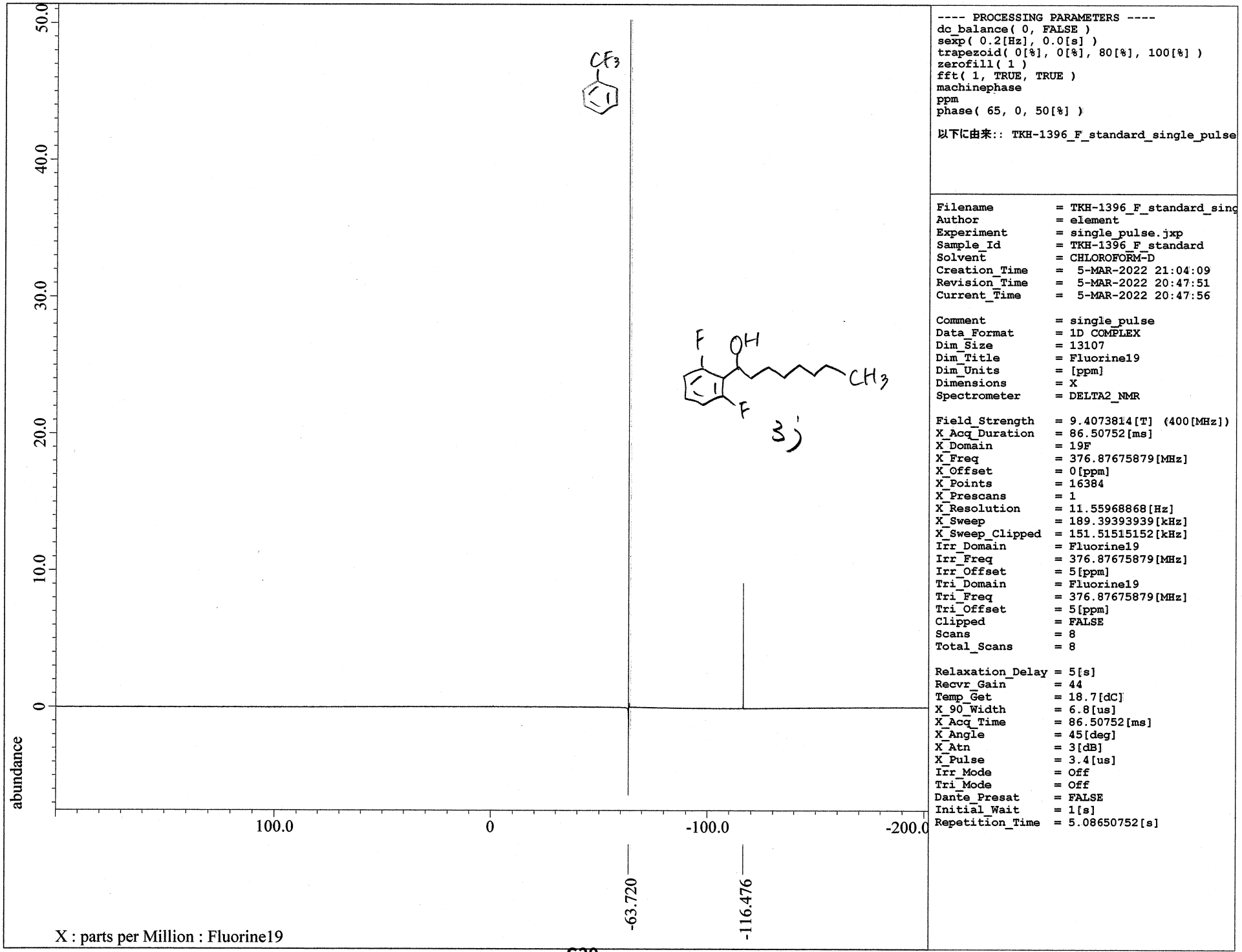


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fft( 1, TRUE, TRUE )
machinephase
ppm
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X_Sweep_Clipped   = 151.51515152[kHz]
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Tri_Offset        = 5[ppm]
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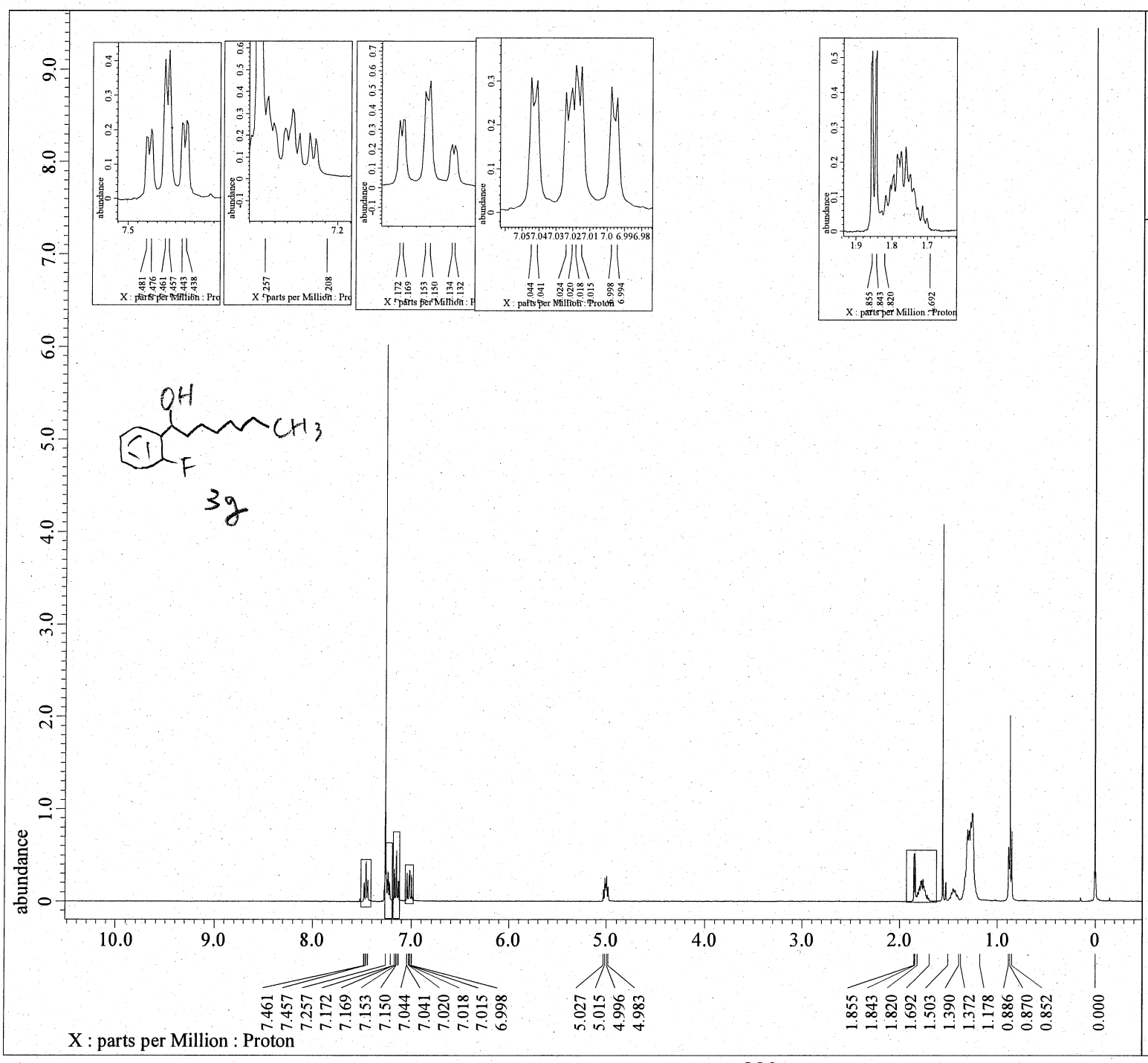
Scans             = 8
Total_Scans       = 8

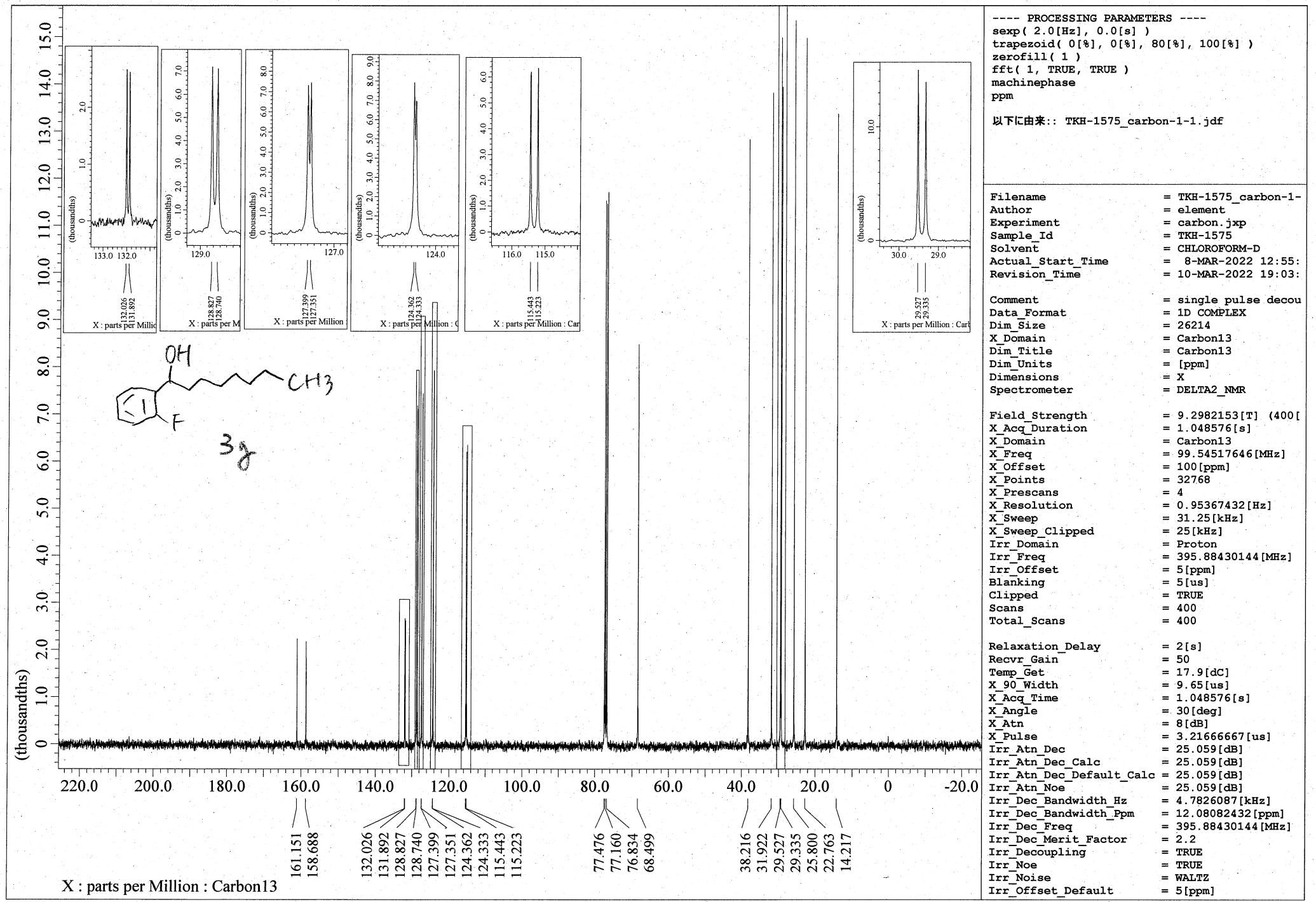
Relaxation_Delay = 5[s]
Recvr_Gain        = 44
Temp_Get          = 18.7[dC]
X_90_Width        = 6.8[us]
X_Acq_Time        = 86.50752[ms]
X_Angle           = 45[deg]
X_Atn             = 3[dB]
X_Pulse           = 3.4[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 5.08650752[s]
```




```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
phase( 2, 0, 50[%] )

以下に由来:: TKH-1575GPC_Proton-1-1.jdf
```

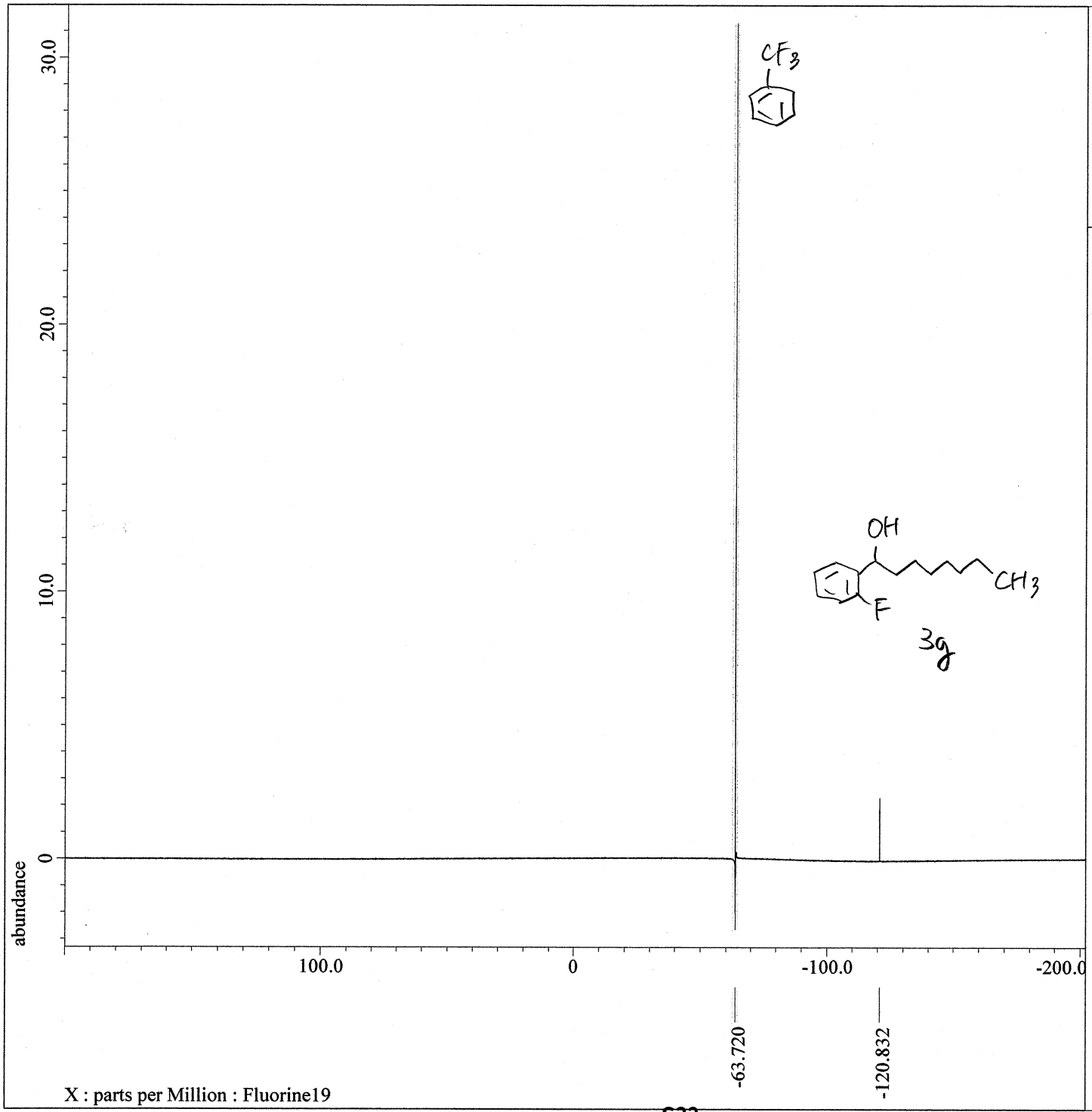
Filename	= TKH-1575GPC_Proton-1-2.jd
Author	= element
Experiment	= proton.jxp
Sample_Id	= TKH-1575GPC
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 4-MAR-2022 22:00:25
Revision_Time	= 11-MAR-2022 10:42:16
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECS400
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.37221[T] (400[MHz])
X_Acq_Duration	= 2.1889024[s]
X_Domain	= 1H
X_Freq	= 399.03472754[MHz]
X_Offset	= 5.0[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45684997[Hz]
X_Sweep	= 7.48502994[kHz]
X_Sweep_Clipped	= 5.98802395[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.03472754[MHz]
Irr_Offset	= 5.0[ppm]
Tri_Domain	= Proton
Tri_Freq	= 399.03472754[MHz]
Tri_Offset	= 5.0[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 46
Temp_Get	= 17.6[dC]
X_90_Width	= 6.6[us]
X_Acq_Time	= 2.1889024[s]
X_Angle	= 45[deg]
X_Atn	= 1[dB]
X_Pulse	= 3.3[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.1889024[s]




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

以下に由来:: TKH-1575_carbon-1-1.jdf
```

Filename	= TKH-1575_carbon-1-
Author	= element
Experiment	= carbon.jxp
Sample_Id	= TKH-1575
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 8-MAR-2022 12:55:
Revision_Time	= 10-MAR-2022 19:03:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.2982153[T] (400[
X_Acq_Duration	= 1.048576[s]
X_Domain	= Carbon13
X_Freq	= 99.54517646[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.95367432[Hz]
X_Sweep	= 31.25[kHz]
X_Sweep_Clipped	= 25[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 5[us]
Clipped	= TRUE
Scans	= 400
Total_Scans	= 400
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 17.9[dC]
X_90_Width	= 9.65[us]
X_Acq_Time	= 1.048576[s]
X_Angle	= 30[deg]
X_Atn	= 8[dB]
X_Pulse	= 3.21666667[us]
Irr_Atn_Dec	= 25.059[dB]
Irr_Atn_Dec_Calc	= 25.059[dB]
Irr_Atn_Dec_Default_Calc	= 25.059[dB]
Irr_Atn_Noe	= 25.059[dB]
Irr_Dec_Bandwidth_Hz	= 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.08082432[ppm]
Irr_Dec_Freq	= 395.88430144[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]




```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
phase( -35, 0, 50[%] )

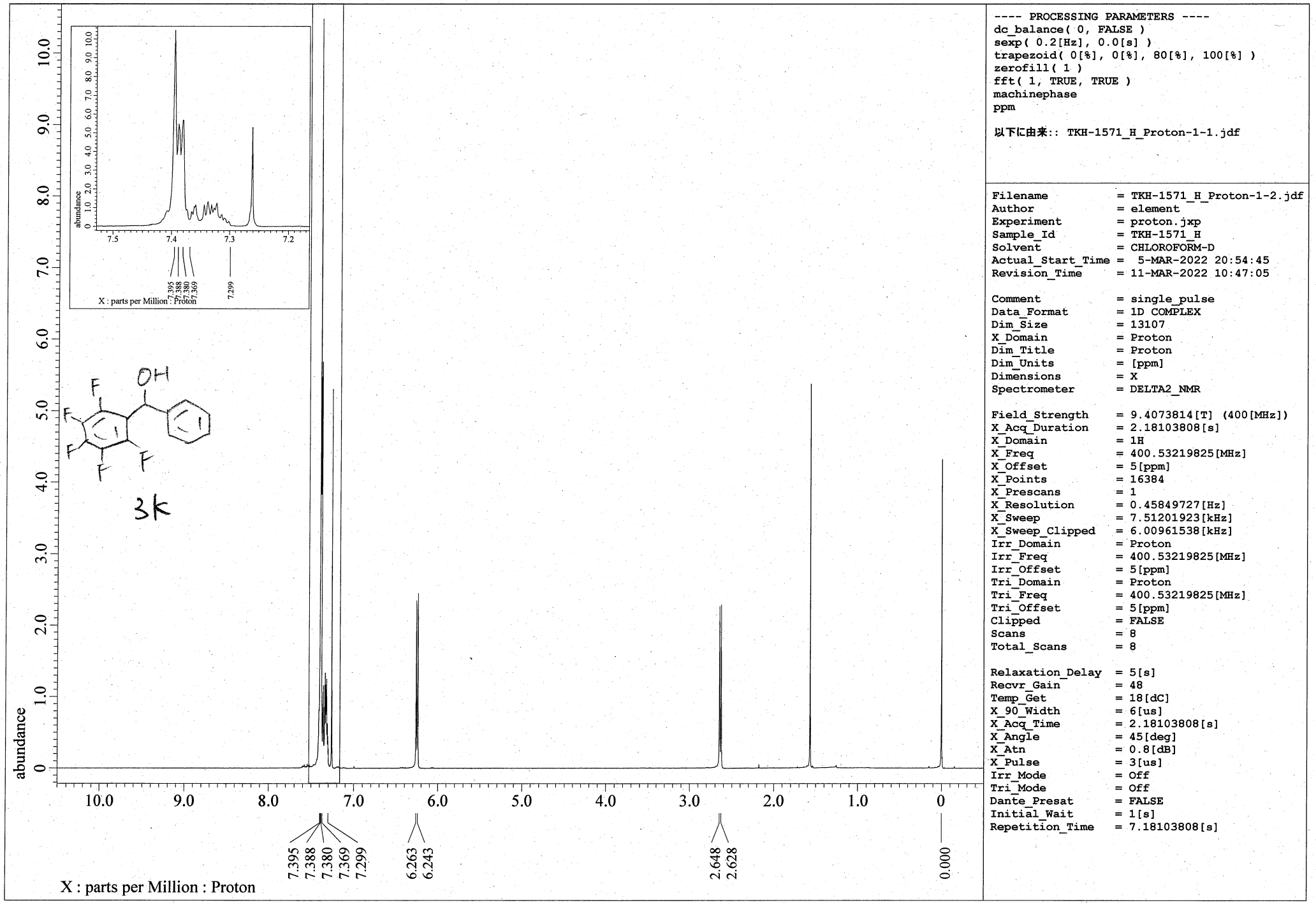
以下に由来:: TKH-1575_F_standard_single_pulse
```

```
Filename          = TKH-1575_F_standard_sing
Author            = element
Experiment        = single_pulse.jxp
Sample_Id         = TKH-1575_F_standard
Solvent           = CHLOROFORM-D
Creation_Time     =  5-MAR-2022 15:59:13
Revision_Time     =  5-MAR-2022 18:54:50
Current_Time      =  5-MAR-2022 18:54:54

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = Fluorine19
Dim_Units         = [ppm]
Dimensions        = X
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.4073814[T] (400[MHz])
X_Acq_Duration    = 86.50752[ms]
X_Domain          = 19F
X_Freq            = 376.87675879[MHz]
X_Offset          = 0[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 11.55968868[Hz]
X_Sweep           = 189.39393939[kHz]
X_Sweep_Clipped   = 151.51515152[kHz]
Irr_Domain        = Fluorine19
Irr_Freq          = 376.87675879[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = Fluorine19
Tri_Freq          = 376.87675879[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

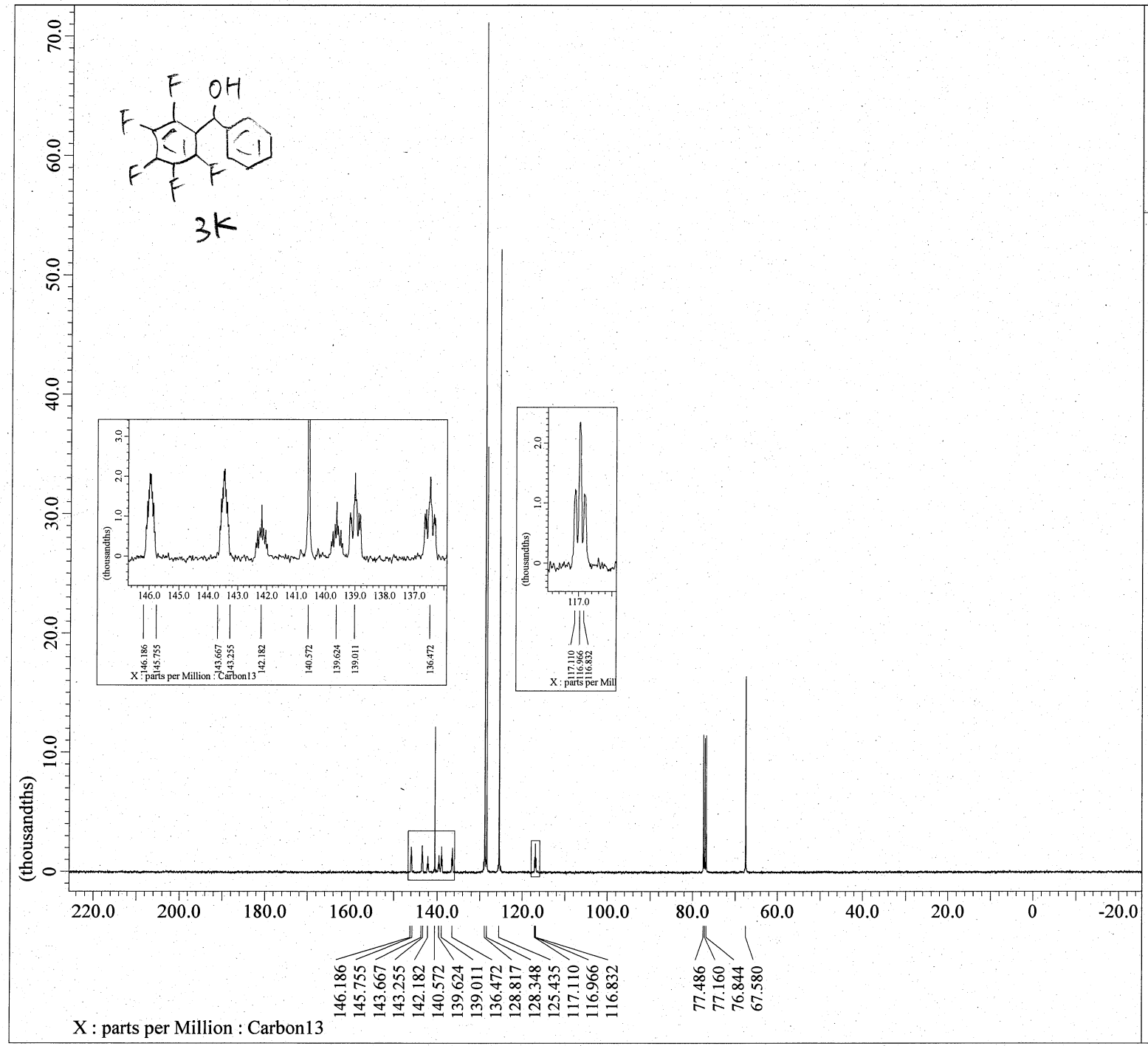
Relaxation_Delay = 5[s]
Recvr_Gain        = 44
Temp_Get          = 18.8[dC]
X_90_Width        = 6.8[us]
X_Acq_Time        = 86.50752[ms]
X_Angle           = 45[deg]
X_Atn             = 3[dB]
X_Pulse           = 3.4[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 5.08650752[s]
```




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

以下に由来:: TKH-1571_H_Proton-1-1.jdf
```

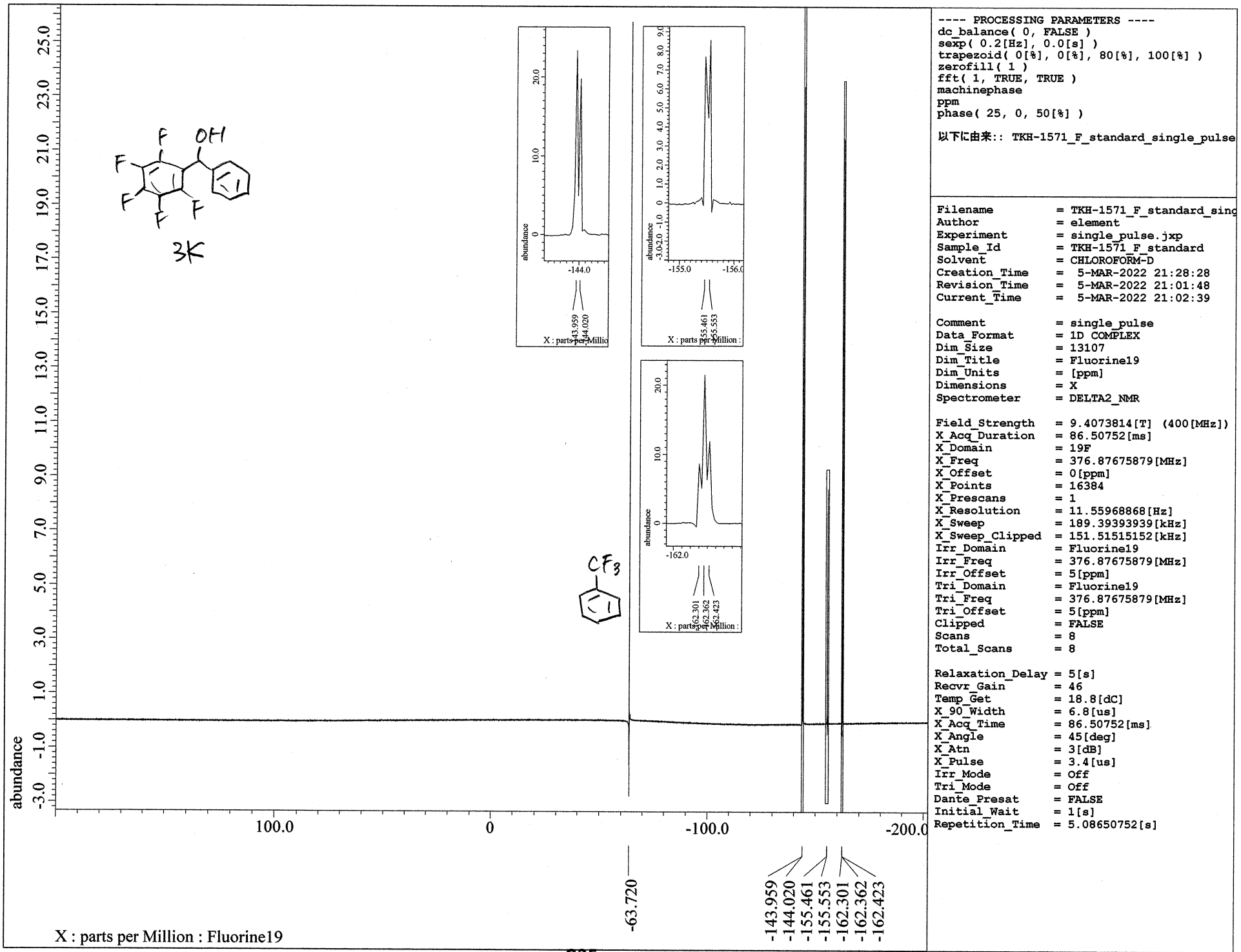
Filename	= TKH-1571_H_Proton-1-2.jdf
Author	= element
Experiment	= proton.jxp
Sample_Id	= TKH-1571_H
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 5-MAR-2022 20:54:45
Revision_Time	= 11-MAR-2022 10:47:05
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.4073814[T] (400[MHz])
X_Acq_Duration	= 2.18103808[s]
X_Domain	= 1H
X_Freq	= 400.53219825[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45849727[Hz]
X_Sweep	= 7.51201923[kHz]
X_Sweep_Clipped	= 6.00961538[kHz]
Irr_Domain	= Proton
Irr_Freq	= 400.53219825[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 400.53219825[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 48
Temp_Get	= 18[dC]
X_90_Width	= 6[us]
X_Acq_Time	= 2.18103808[s]
X_Angle	= 45[deg]
X_Atn	= 0.8[dB]
X_Pulse	= 3[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.18103808[s]




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

以下に由来:: TKH-1571_carbon-1-1.jdf
```

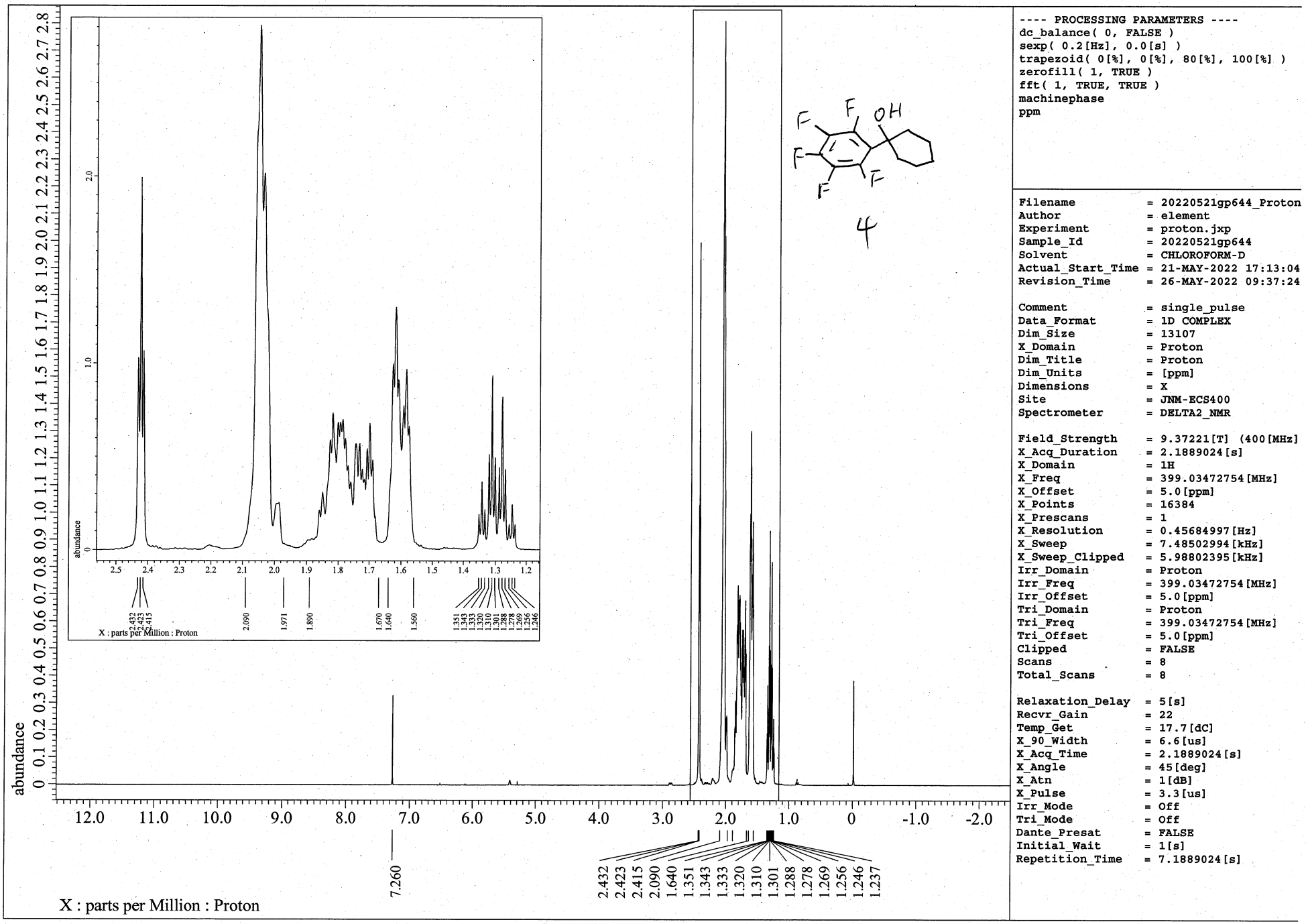
Filename	= TKH-1571_carbon-1-
Author	= element
Experiment	= carbon.jxp
Sample_Id	= TKH-1571
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 8-MAR-2022 13:31:
Revision_Time	= 11-MAR-2022 10:49:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.2982153[T] (400[
X_Acq_Duration	= 1.048576[s]
X_Domain	= Carbon13
X_Freq	= 99.54517646[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.95367432[Hz]
X_Sweep	= 31.25[kHz]
X_Sweep_Clipped	= 25[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 5[us]
Clipped	= TRUE
Scans	= 400
Total_Scans	= 400
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 17.9[dC]
X_90_Width	= 9.65[us]
X_Acq_Time	= 1.048576[s]
X_Angle	= 30[deg]
X_Atn	= 8[dB]
X_Pulse	= 3.21666667[us]
Irr_Atn_Dec	= 25.059[dB]
Irr_Atn_Dec_Calc	= 25.059[dB]
Irr_Atn_Dec_Default_Calc	= 25.059[dB]
Irr_Atn_Noe	= 25.059[dB]
Irr_Dec_Bandwidth_Hz	= 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.08082432[ppm]
Irr_Dec_Freq	= 395.88430144[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]




```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
phase( 25, 0, 50[%] )

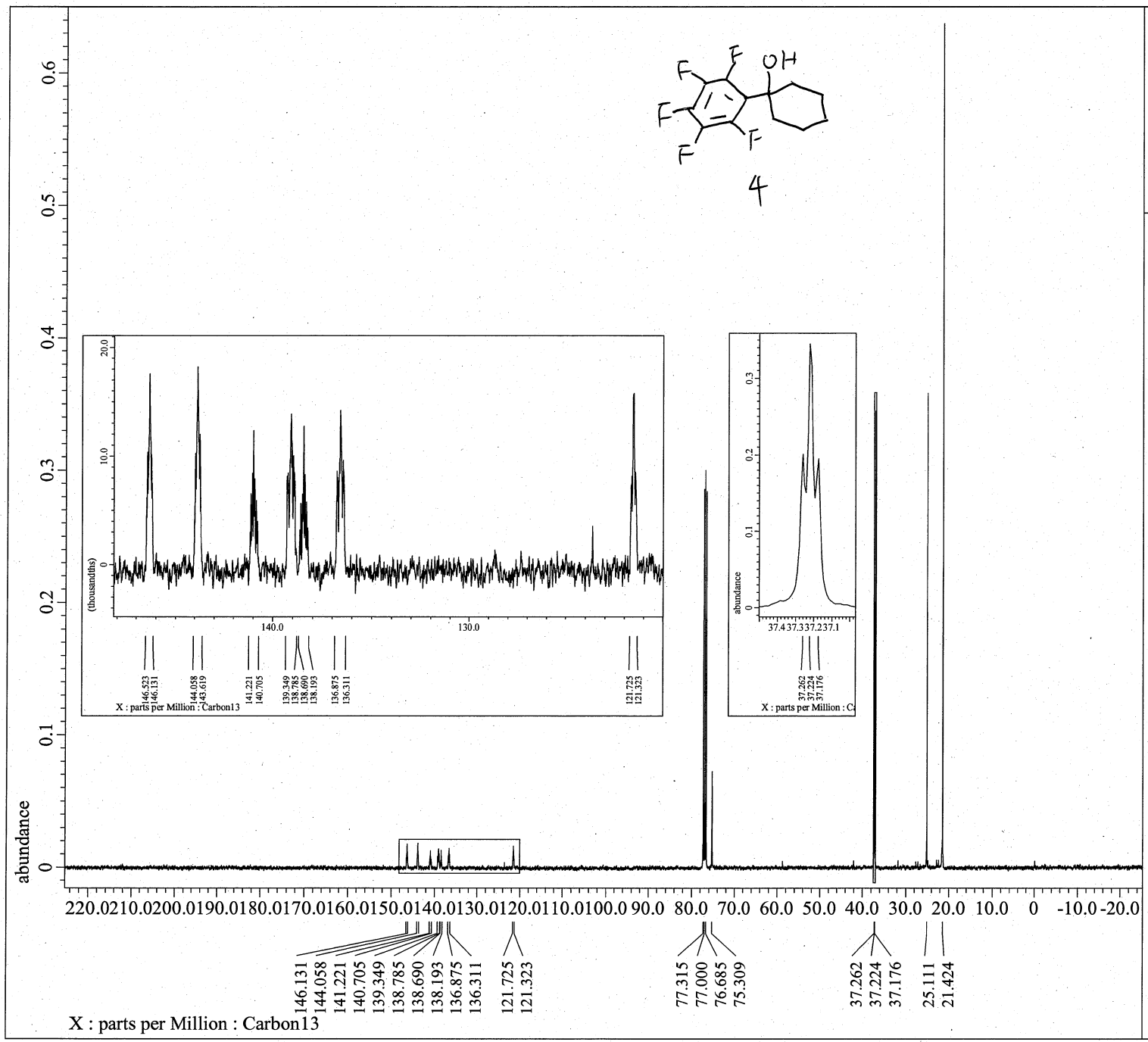
以下に由来:: TKH-1571_F_standard_single_pulse
```

Filename	= TKH-1571_F_standard_sing
Author	= element
Experiment	= single_pulse.jxp
Sample_Id	= TKH-1571_F_standard
Solvent	= CHLOROFORM-D
Creation_Time	= 5-MAR-2022 21:28:28
Revision_Time	= 5-MAR-2022 21:01:48
Current_Time	= 5-MAR-2022 21:02:39
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
Dim_Title	= Fluorine19
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.4073814[T] (400[MHz])
X_Acq_Duration	= 86.50752[ms]
X_Domain	= 19F
X_Freq	= 376.87675879[MHz]
X_Offset	= 0[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 11.55968868[Hz]
X_Sweep	= 189.39393939[kHz]
X_Sweep_Clipped	= 151.51515152[kHz]
Irr_Domain	= Fluorine19
Irr_Freq	= 376.87675879[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Fluorine19
Tri_Freq	= 376.87675879[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 46
Temp_Get	= 18.8[dC]
X_90_Width	= 6.8[us]
X_Acq_Time	= 86.50752[ms]
X_Angle	= 45[deg]
X_Atn	= 3[dB]
X_Pulse	= 3.4[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 5.08650752[s]




```
---- 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
```

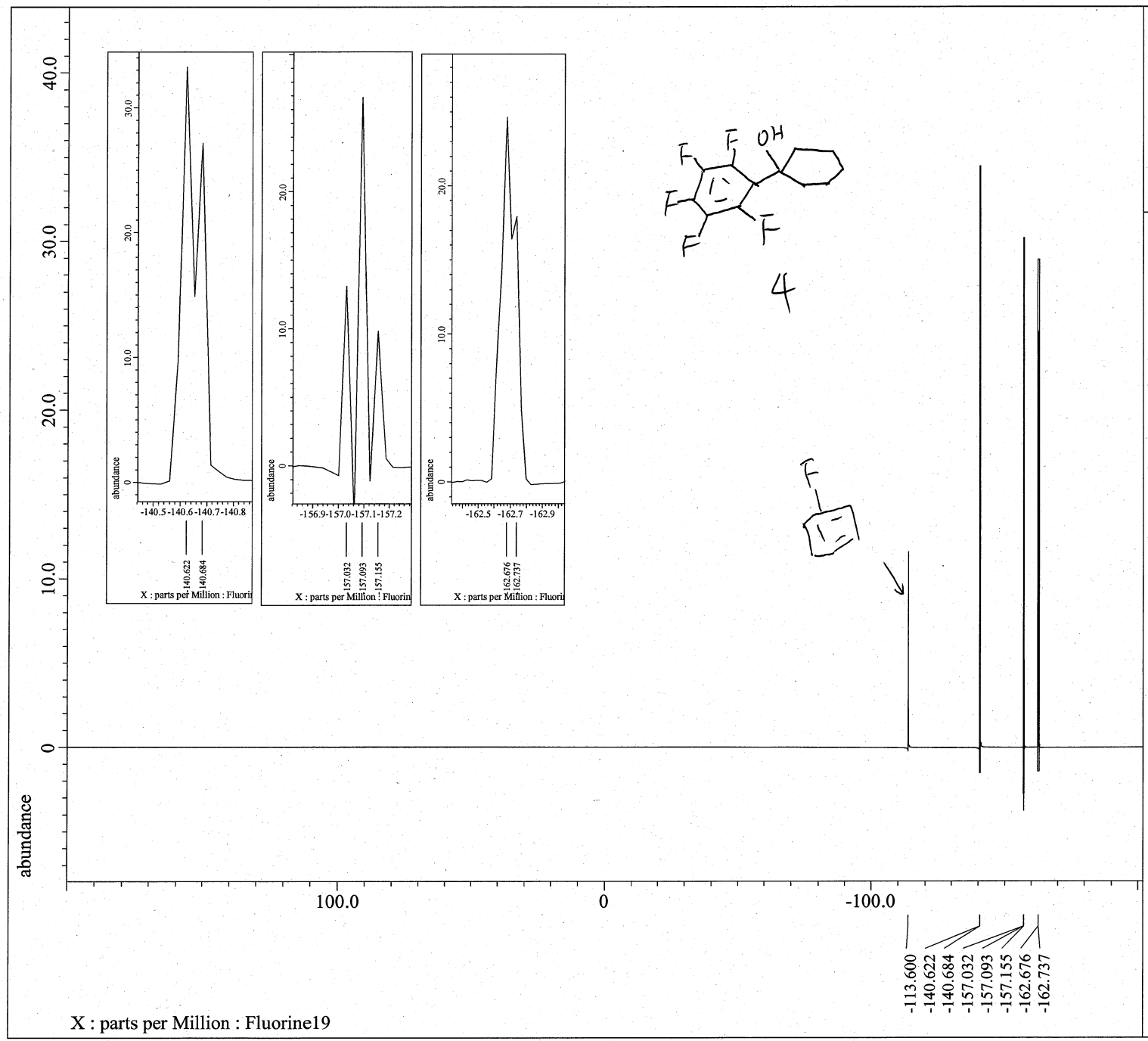
Filename	= 20220521gp644_Proton
Author	= element
Experiment	= proton.jxp
Sample_Id	= 20220521gp644
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 21-MAY-2022 17:13:04
Revision_Time	= 26-MAY-2022 09:37:24
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECS400
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.37221[T] (400[MHz]
X_Acq_Duration	= 2.1889024[s]
X_Domain	= 1H
X_Freq	= 399.03472754[MHz]
X_Offset	= 5.0[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45684997[Hz]
X_Sweep	= 7.48502994[kHz]
X_Sweep_Clipped	= 5.98802395[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.03472754[MHz]
Irr_Offset	= 5.0[ppm]
Tri_Domain	= Proton
Tri_Freq	= 399.03472754[MHz]
Tri_Offset	= 5.0[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 22
Temp_Get	= 17.7[dC]
X_90_Width	= 6.6[us]
X_Acq_Time	= 2.1889024[s]
X_Angle	= 45[deg]
X_Atn	= 1[dB]
X_Pulse	= 3.3[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.1889024[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

数据来源：20220521gp644_Carbon-1-1.jdf
```

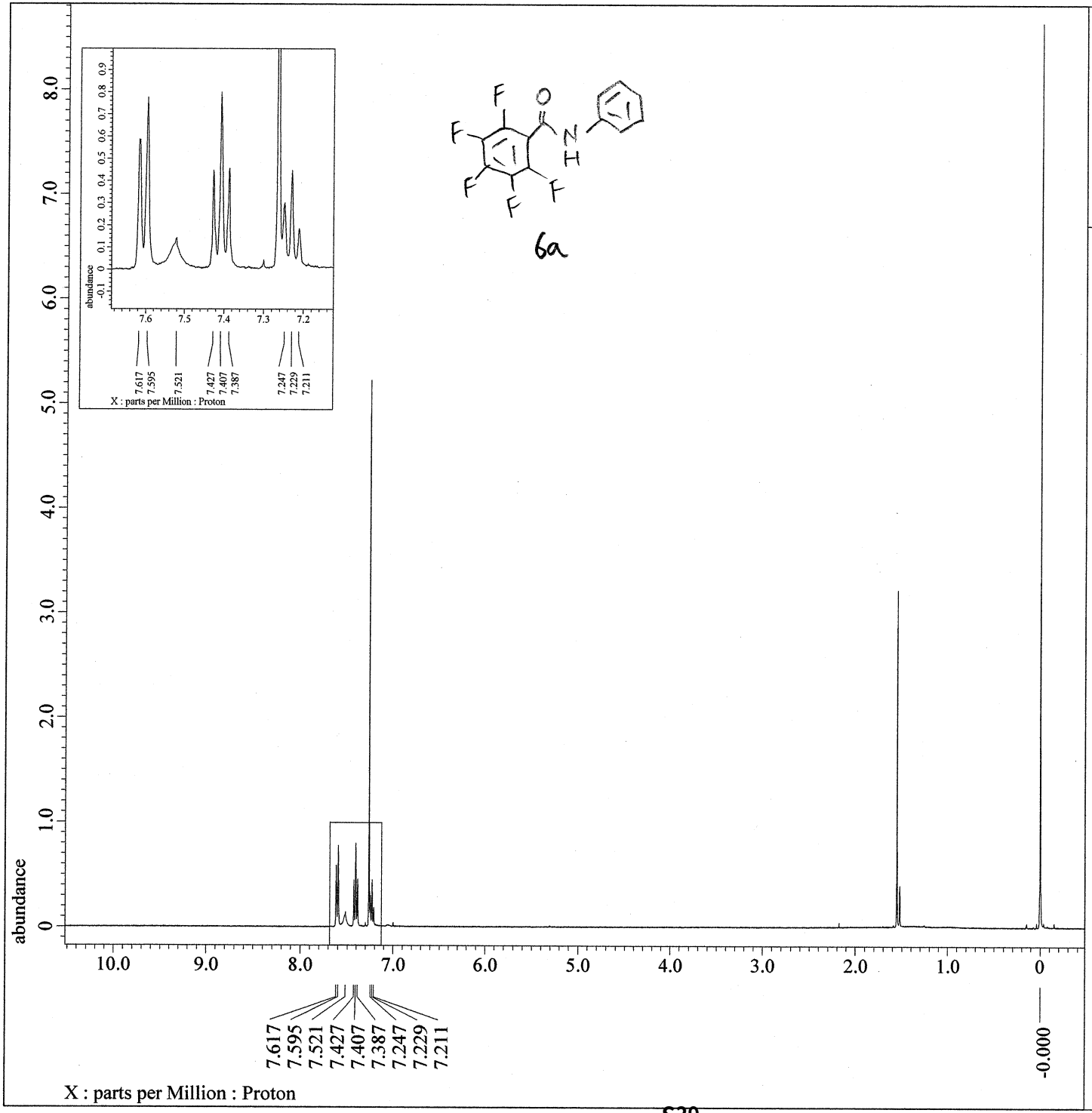
Filename	= 20220521gp644_Carbon
Author	= element
Experiment	= carbon.jxp
Sample_Id	= 20220521gp644
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 21-MAY-2022 17:14:24
Revision_Time	= 25-MAY-2022 19:57:28
Comment	= single pulse decoupl
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECS400
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.37221[T] (400[MHz]
X_Acq_Duration	= 1.04333312[s]
X_Domain	= 13C
X_Freq	= 100.33735165[MHz]
X_Offset	= 100.0[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.95846665[Hz]
X_Sweep	= 31.40703518[kHz]
X_Sweep_Clipped	= 25.12562814[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.03472754[MHz]
Irr_Offset	= 5.0[ppm]
Clipped	= FALSE
Scans	= 1024
Total_Scans	= 1024
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 17.7[dC]
X_90_Width	= 10.9[us]
X_Acq_Time	= 1.04333312[s]
X_Angle	= 30[deg]
X_Atn	= 5.4[dB]
X_Pulse	= 3.63333333[us]
Irr_Atn_Dec	= 25.823[dB]
Irr_Atn_Noe	= 25.823[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 ----
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

数据来源: 20220521gp644_single_pulse-1-1
```

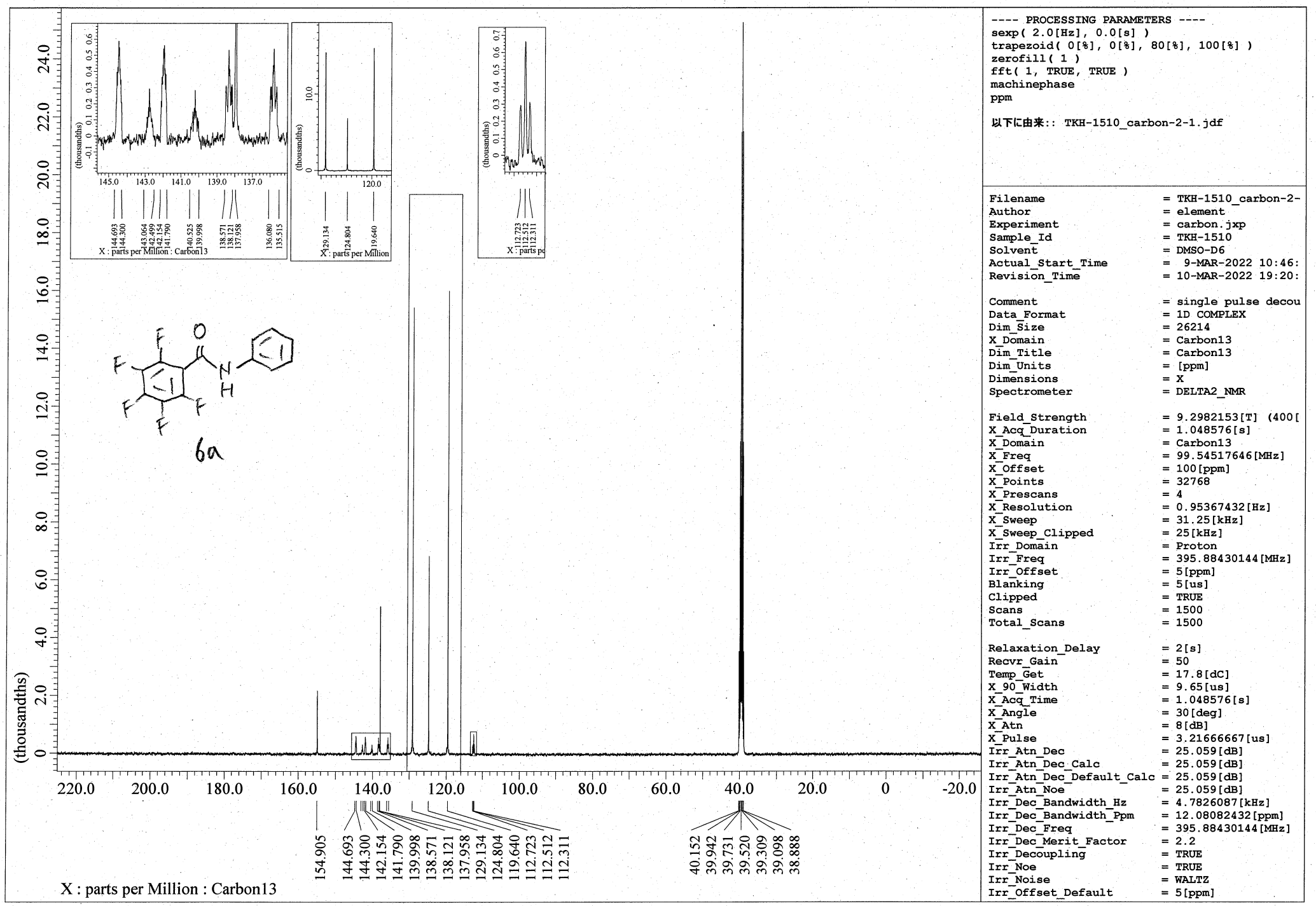
Filename	= 20220521gp644_single
Author	= element
Experiment	= single_pulse.jxp
Sample_Id	= 20220521gp644
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 21-MAY-2022 18:05:28
Revision_Time	= 25-MAY-2022 20:46:00
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Fluori
Dim_Title	= Fluorine19
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.4073814[T] (400[MH
X_Acq_Duration	= 86.50752[ms]
X_Domain	= 19F
X_Freq	= 376.87675879[MHz]
X_Offset	= 0[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 11.55968868[Hz]
X_Sweep	= 189.39393939[kHz]
X_Sweep_Clipped	= 151.51515152[kHz]
Irr_Domain	= Fluorine19
Irr_Freq	= 376.87675879[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Fluorine19
Tri_Freq	= 376.87675879[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 30
Temp_Get	= 19.1[dC]
X_90_Width	= 6.8[us]
X_Acq_Time	= 86.50752[ms]
X_Angle	= 45[deg]
X_Atn	= 3[dB]
X_Pulse	= 3.4[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 5.08650752[s]




```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
phase( 3, 0, 50[%] )

以下に由来:: TKH-1510_H_proton-1-1.jdf
```

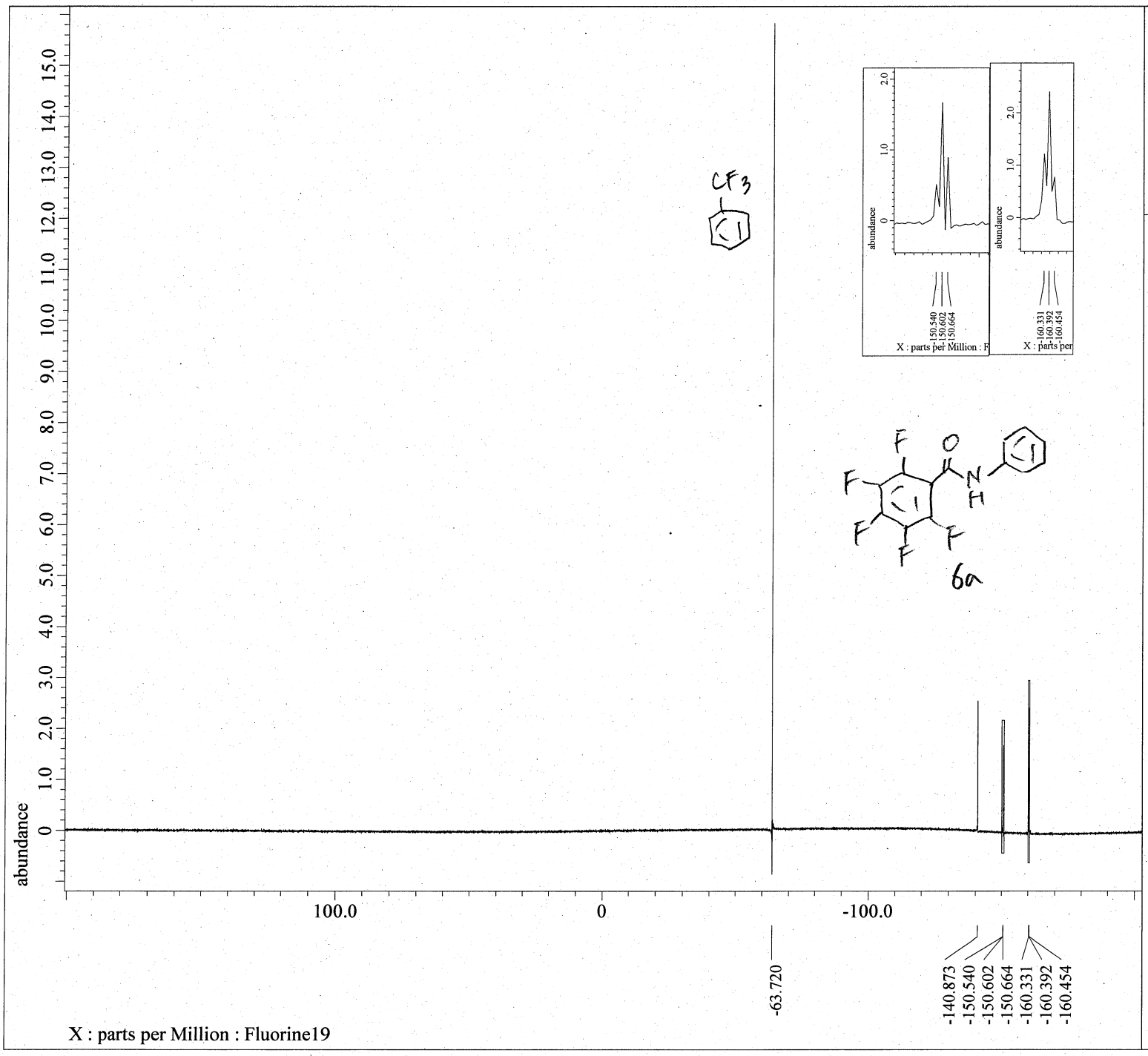
Filename	= TKH-1510_H_proton-1-4.jd
Author	= element
Experiment	= proton.jxp
Sample_Id	= TKH-1510_H
Solvent	= CHLOROFORM-D
Creation_Time	= 14-MAR-2022 15:26:11
Revision_Time	= 14-MAR-2022 15:02:38
Current_Time	= 14-MAR-2022 15:02:40
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.4073814[T] (400[MHz])
X_Acq_Duration	= 2.18103808[s]
X_Domain	= 1H
X_Freq	= 400.53219825[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45849727[Hz]
X_Sweep	= 7.51201923[kHz]
X_Sweep_Clipped	= 6.00961538[kHz]
Irr_Domain	= Proton
Irr_Freq	= 400.53219825[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 400.53219825[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 50
Temp_Get	= 18.7[dC]
X_90_Width	= 6[us]
X_Acq_Time	= 2.18103808[s]
X_Angle	= 45[deg]
X_Atn	= 0.8[dB]
X_Pulse	= 3[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.18103808[s]




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

以下に由来:: TKH-1510_carbon-2-1.jdf
```

Filename	= TKH-1510_carbon-2-
Author	= element
Experiment	= carbon.jxp
Sample_Id	= TKH-1510
Solvent	= DMSO-D6
Actual_Start_Time	= 9-MAR-2022 10:46:
Revision_Time	= 10-MAR-2022 19:20:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.2982153[T] (400[
X_Acq_Duration	= 1.048576[s]
X_Domain	= Carbon13
X_Freq	= 99.54517646[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.95367432[Hz]
X_Sweep	= 31.25[kHz]
X_Sweep_Clipped	= 25[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 5[us]
Clipped	= TRUE
Scans	= 1500
Total_Scans	= 1500
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 17.8[dC]
X_90_Width	= 9.65[us]
X_Acq_Time	= 1.048576[s]
X_Angle	= 30[deg]
X_Atn	= 8[dB]
X_Pulse	= 3.21666667[us]
Irr_Atn_Dec	= 25.059[dB]
Irr_Atn_Dec_Calc	= 25.059[dB]
Irr_Atn_Dec_Default_Calc	= 25.059[dB]
Irr_Atn_Noe	= 25.059[dB]
Irr_Dec_Bandwidth_Hz	= 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.08082432[ppm]
Irr_Dec_Freq	= 395.88430144[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]




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

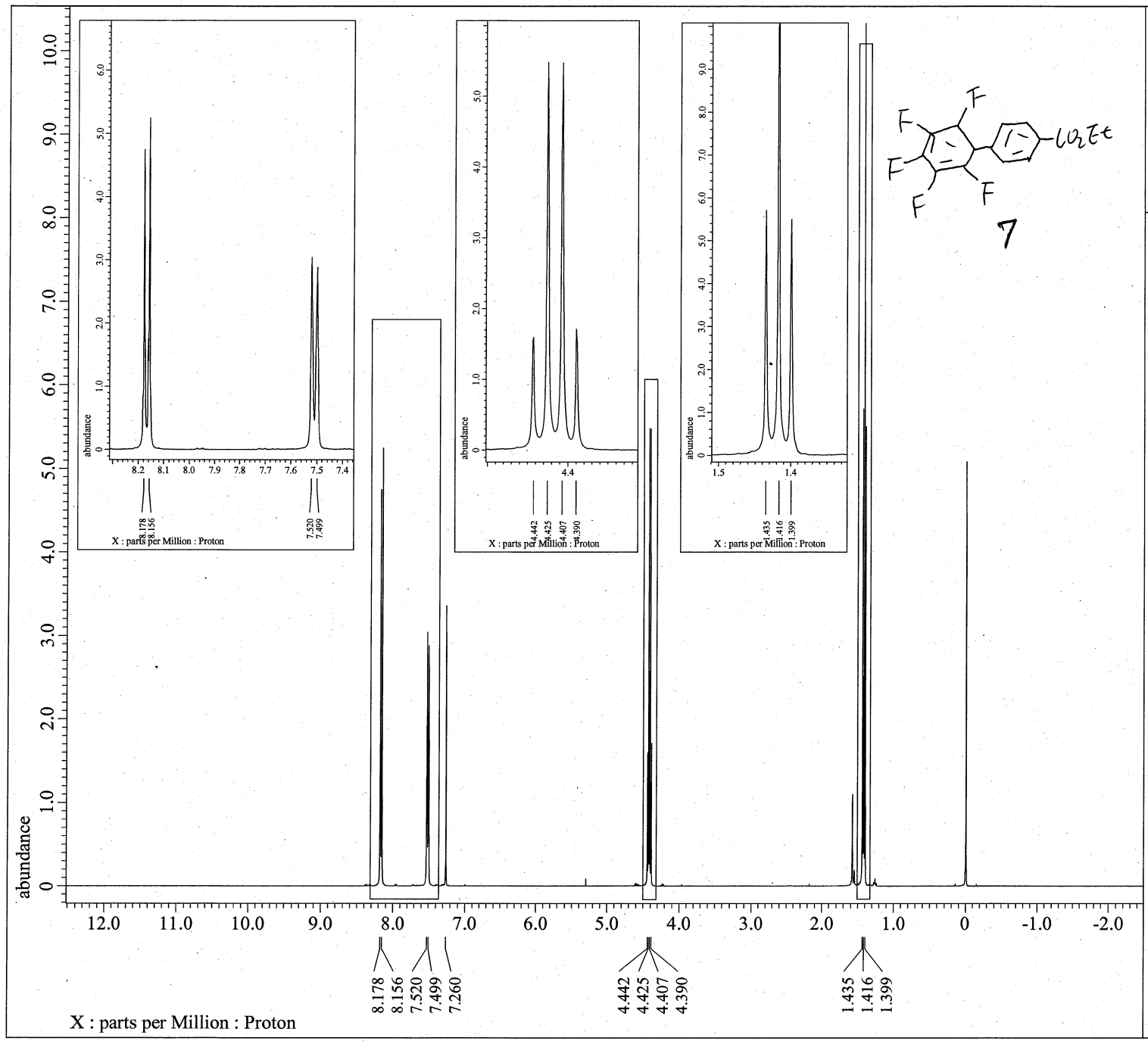
以下に由来:: TKH-1510_F_standard_Proton-1-1.jdf
```

```
Filename            = TKH-1510_F_standard_Proto
Author              = element
Experiment          = proton.jxp
Sample_Id           = TKH-1510_F_standard
Solvent             = CHLOROFORM-D
Actual_Start_Time   =  7-MAR-2022 15:56:17
Revision_Time       = 11-MAR-2022 13:59:02

Comment             = single_pulse
Data_Format         = 1D COMPLEX
Dim_Size            = 13107
X_Domain            = Fluori
Dim_Title           = Fluorine19
Dim_Units           = [ppm]
Dimensions          = X
Site                = JNM-ECS400
Spectrometer        = DELTA2_NMR

Field_Strength      = 9.37221[T] (400[MHz])
X_Acq_Duration      = 86.50752[ms]
X_Domain            = 19F
X_Freq              = 375.46772873[MHz]
X_Offset            = 0[ppm]
X_Points            = 16384
X_Prescans          = 1
X_Resolution        = 11.55968868[Hz]
X_Sweep             = 189.39393939[kHz]
X_Sweep_Clipped     = 151.51515152[kHz]
Irr_Domain          = Fluorine19
Irr_Freq            = 375.46772873[MHz]
Irr_Offset          = 5[ppm]
Tri_Domain          = Fluorine19
Tri_Freq            = 375.46772873[MHz]
Tri_Offset          = 5[ppm]
Clipped             = FALSE
Scans               = 8
Total_Scans         = 8

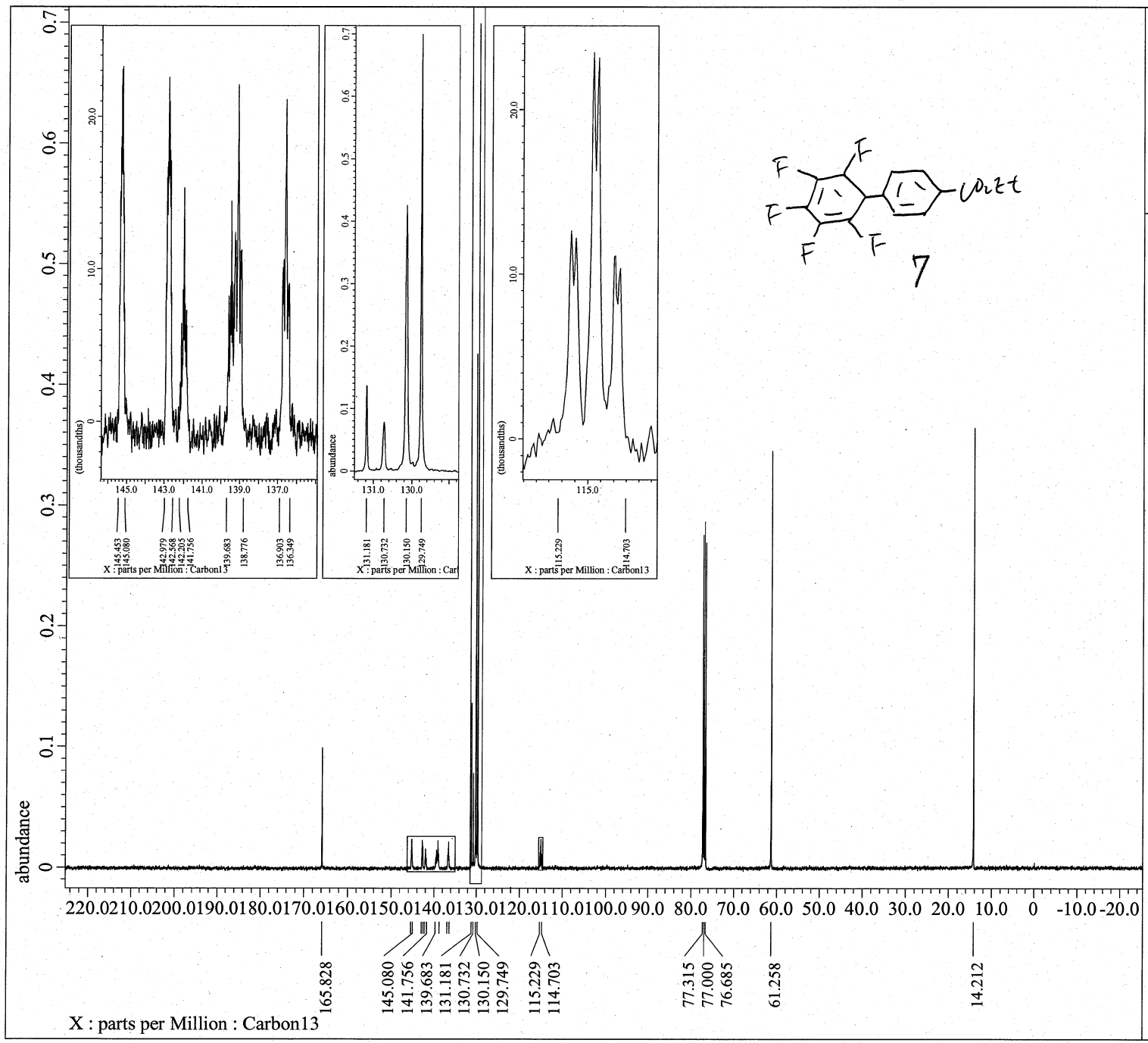
Relaxation_Delay    = 5[s]
Recvr_Gain          = 46
Temp_Get            = 18[dC]
X_90_Width          = 7.6[us]
X_Acq_Time          = 86.50752[ms]
X_Angle             = 45[deg]
X_Atn               = 2.5[dB]
X_Pulse             = 3.8[us]
Irr_Mode            = Off
Tri_Mode            = Off
Dante_Presat        = FALSE
Initial_Wait        = 1[s]
Repetition_Time     = 5.08650752[s]
```




```
---- 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

数据来源：20220521gp641_Proton-1-1.jdf
```

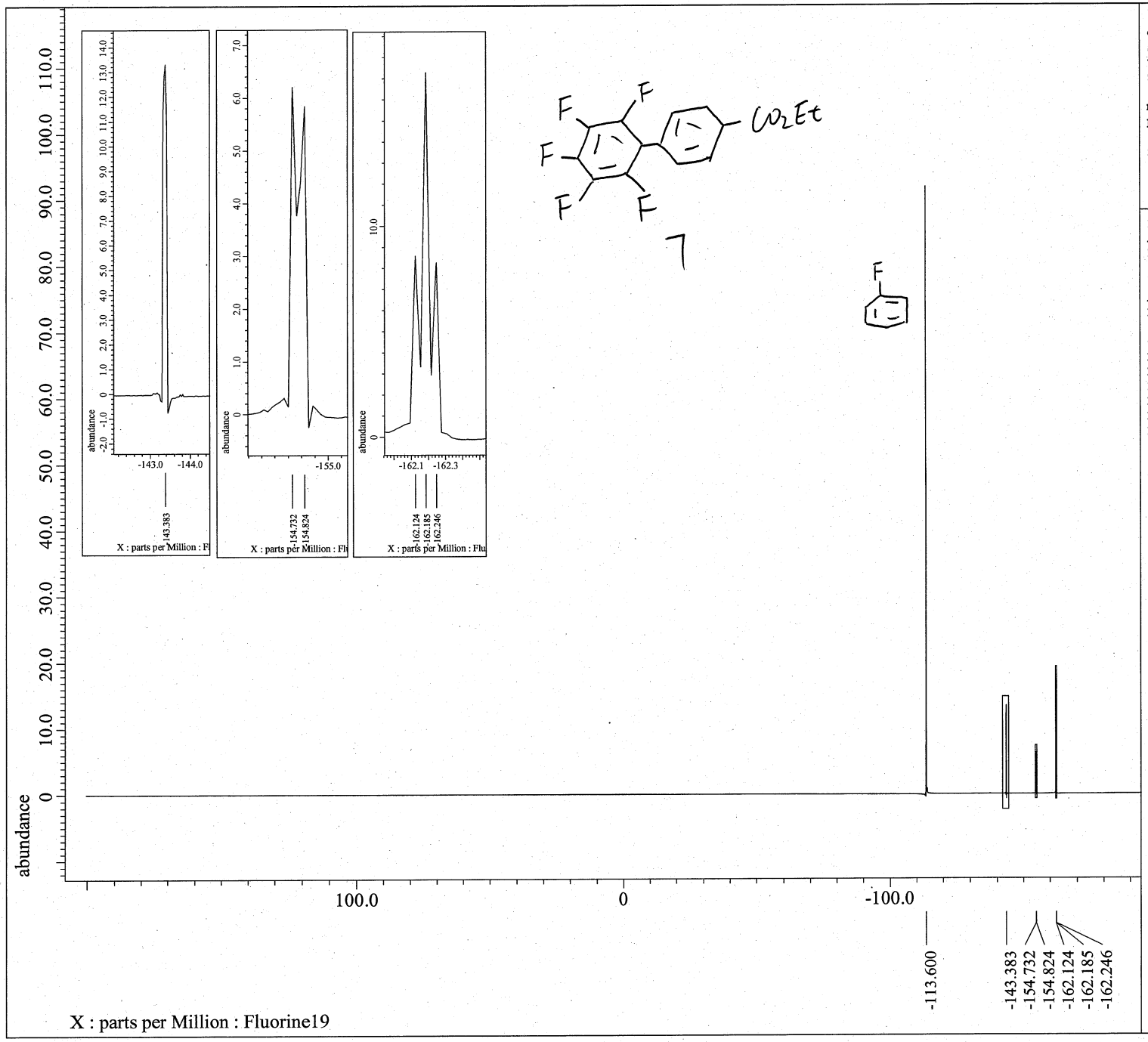
Filename	= 20220521gp641_Proton
Author	= element
Experiment	= proton.jxp
Sample_Id	= 20220521gp641
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 21-MAY-2022 14:59:06
Revision_Time	= 26-MAY-2022 09:41:20
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECS400
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.37221[T] (400[MHz]
X_Acq_Duration	= 2.1889024[s]
X_Domain	= 1H
X_Freq	= 399.03472754[MHz]
X_Offset	= 5.0[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45684997[Hz]
X_Sweep	= 7.48502994[kHz]
X_Sweep_Clipped	= 5.98802395[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.03472754[MHz]
Irr_Offset	= 5.0[ppm]
Tri_Domain	= Proton
Tri_Freq	= 399.03472754[MHz]
Tri_Offset	= 5.0[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 42
Temp_Get	= 17.4[dC]
X_90_Width	= 6.6[us]
X_Acq_Time	= 2.1889024[s]
X_Angle	= 45[deg]
X_Atn	= 1[dB]
X_Pulse	= 3.3[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.1889024[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

数据来源：20220521gp641_Carbon-2-1.jdf
```

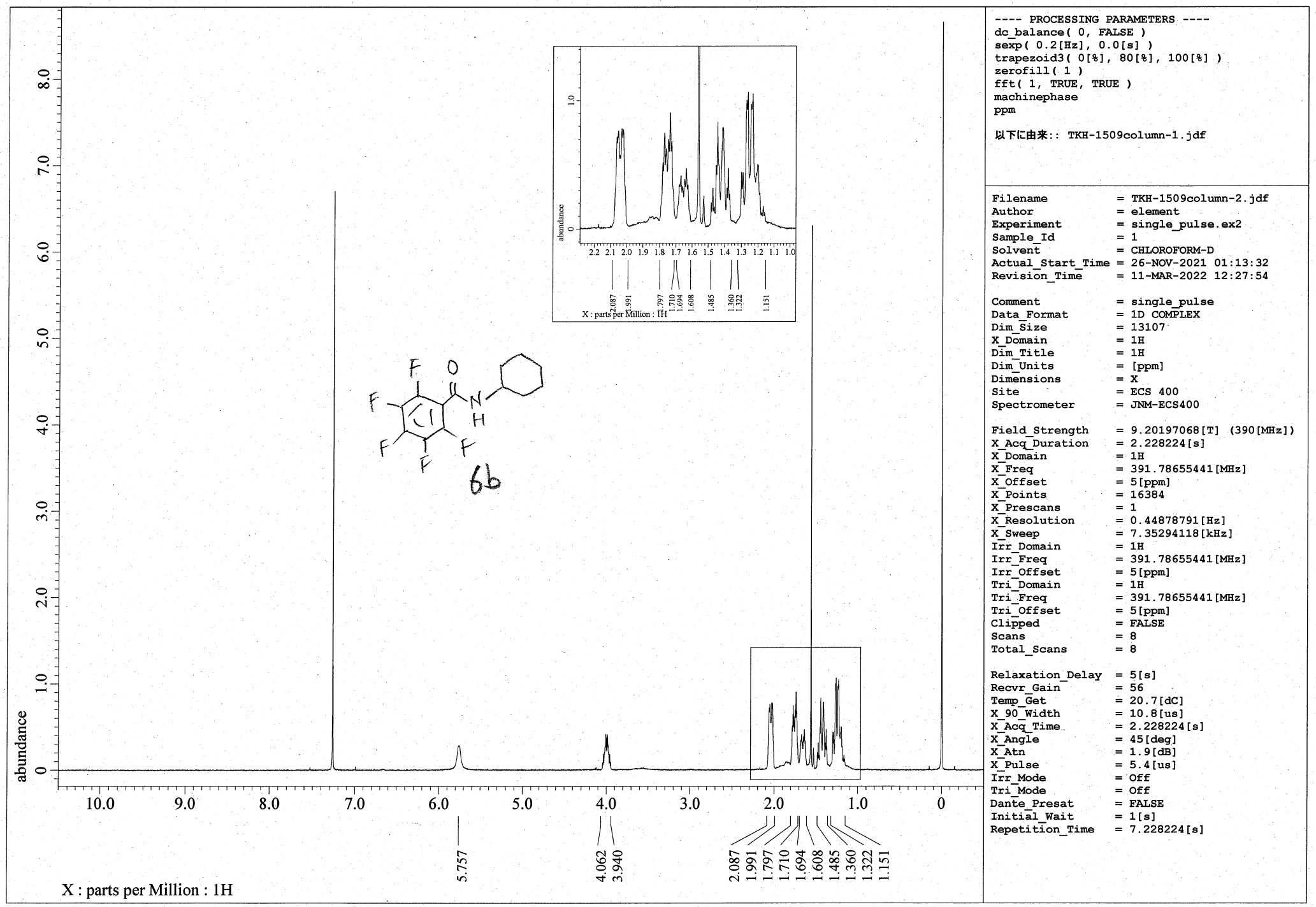
Filename	= 20220521gp641_Carbon
Author	= element
Experiment	= carbon.jxp
Sample_Id	= 20220521gp641
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 21-MAY-2022 16:02:57
Revision_Time	= 26-MAY-2022 10:08:10
Comment	= single pulse decoupl
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECS400
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.37221[T] (400[MHz]
X_Acq_Duration	= 1.04333312[s]
X_Domain	= 13C
X_Freq	= 100.33735165[MHz]
X_Offset	= 100.0[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.95846665[Hz]
X_Sweep	= 31.40703518[kHz]
X_Sweep_Clipped	= 25.12562814[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.03472754[MHz]
Irr_Offset	= 5.0[ppm]
Clipped	= FALSE
Scans	= 1024
Total_Scans	= 1024
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 17.6[dC]
X_90_Width	= 10.9[us]
X_Acq_Time	= 1.04333312[s]
X_Angle	= 30[deg]
X_Atn	= 5.4[dB]
X_Pulse	= 3.63333333[us]
Irr_Atn_Dec	= 25.823[dB]
Irr_Atn_Noe	= 25.823[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 ----
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

数据来源：20220523gp641_single_pulse-1-1
```

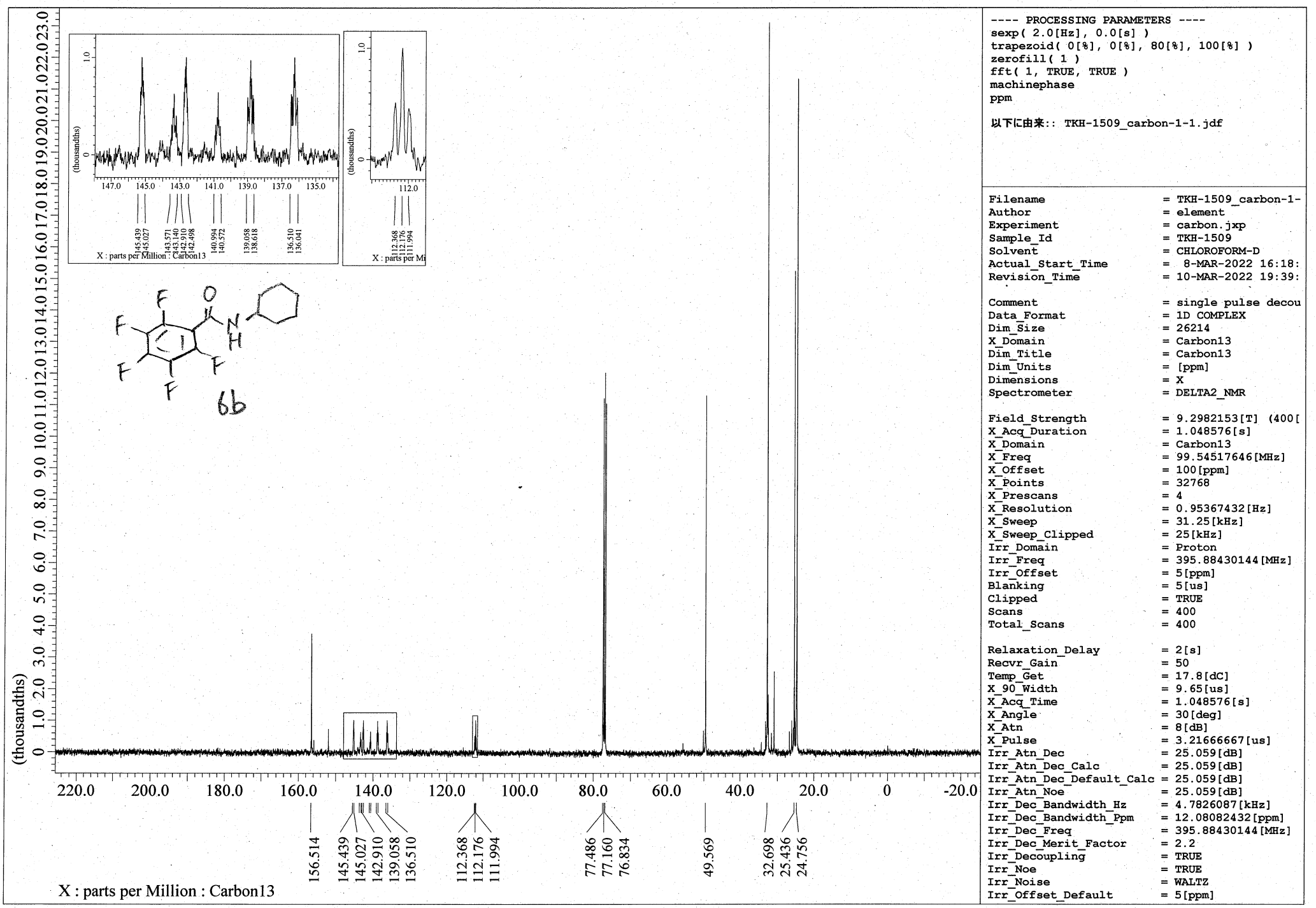
Filename	= 20220523gp641_single
Author	= element
Experiment	= single_pulse.jxp
Sample_Id	= 20220523gp641
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 23-MAY-2022 13:53:44
Revision_Time	= 26-MAY-2022 12:42:19
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Fluori
Dim_Title	= Fluorine19
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.4073814[T] (400[MH
X_Acq_Duration	= 86.50752[ms]
X_Domain	= 19F
X_Freq	= 376.87675879[MHz]
X_Offset	= 0[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 11.55968868[Hz]
X_Sweep	= 189.39393939[kHz]
X_Sweep_Clipped	= 151.51515152[kHz]
Irr_Domain	= Fluorine19
Irr_Freq	= 376.87675879[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Fluorine19
Tri_Freq	= 376.87675879[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 38
Temp_Get	= 18.9[dC]
X_90_Width	= 6.8[us]
X_Acq_Time	= 86.50752[ms]
X_Angle	= 45[deg]
X_Atn	= 3[dB]
X_Pulse	= 3.4[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 5.08650752[s]




```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

以下に由来:: TKH-1509column-1.jdf
```

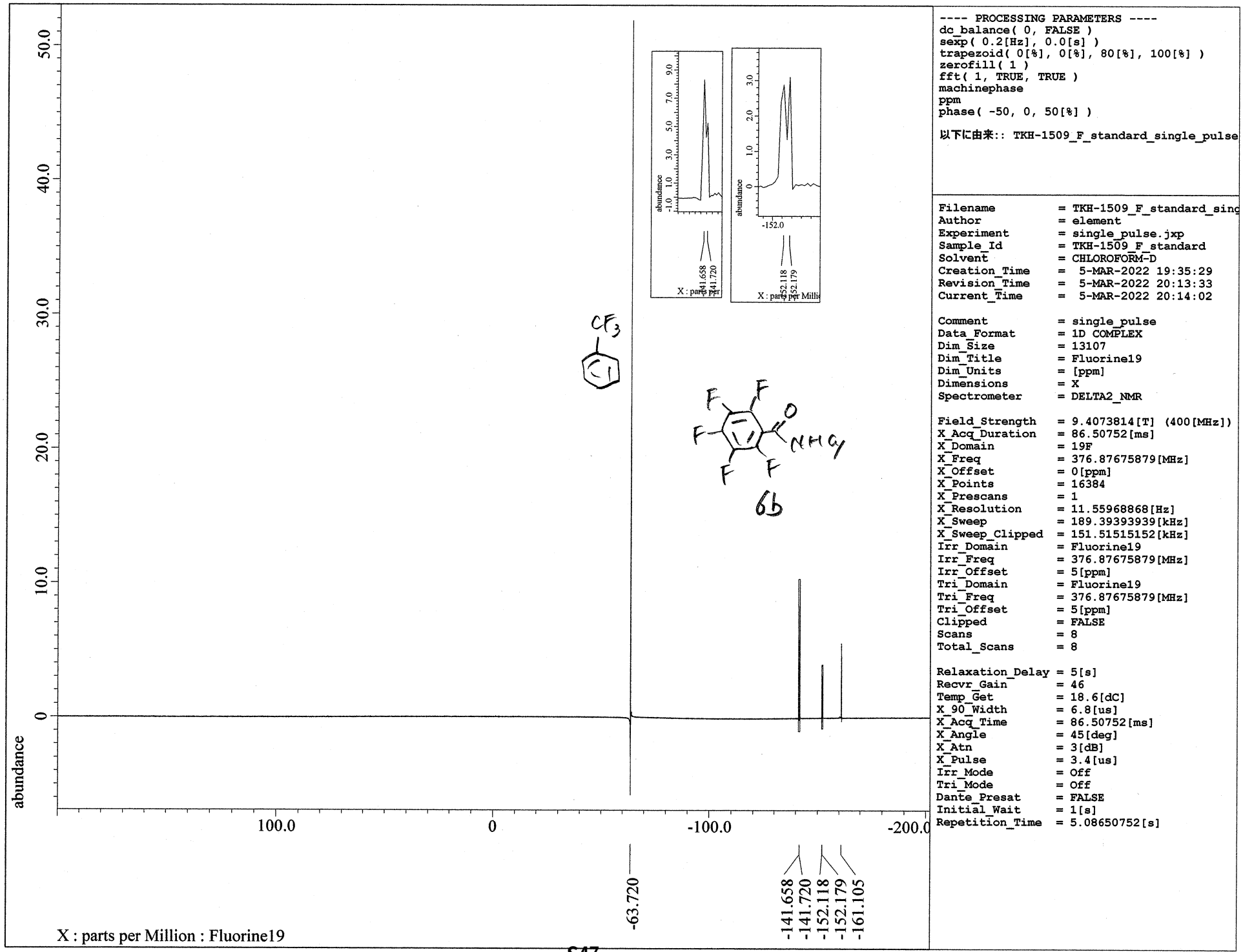
Filename	= TKH-1509column-2.jdf
Author	= element
Experiment	= single_pulse.ex2
Sample_Id	= 1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 26-NOV-2021 01:13:32
Revision_Time	= 11-MAR-2022 12:27:54
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= 1H
Dim_Title	= 1H
Dim_Units	= [ppm]
Dimensions	= X
Site	= ECS 400
Spectrometer	= JNM-ECS400
Field_Strength	= 9.20197068[T] (390[MHz])
X_Acq_Duration	= 2.228224[s]
X_Domain	= 1H
X_Freq	= 391.78655441[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.44878791[Hz]
X_Sweep	= 7.35294118[kHz]
Irr_Domain	= 1H
Irr_Freq	= 391.78655441[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= 1H
Tri_Freq	= 391.78655441[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 56
Temp_Get	= 20.7[dC]
X_90_Width	= 10.8[us]
X_Acq_Time	= 2.228224[s]
X_Angle	= 45[deg]
X_Atn	= 1.9[dB]
X_Pulse	= 5.4[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.228224[s]




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

以下に由来:: TKH-1509_carbon-1-1.jdf
```

Filename	= TKH-1509_carbon-1-
Author	= element
Experiment	= carbon.jxp
Sample_Id	= TKH-1509
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 8-MAR-2022 16:18:
Revision_Time	= 10-MAR-2022 19:39:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.2982153[T] (400[
X_Acq_Duration	= 1.048576[s]
X_Domain	= Carbon13
X_Freq	= 99.54517646[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.95367432[Hz]
X_Sweep	= 31.25[kHz]
X_Sweep_Clipped	= 25[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 5[us]
Clipped	= TRUE
Scans	= 400
Total_Scans	= 400
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 17.8[dC]
X_90_Width	= 9.65[us]
X_Acq_Time	= 1.048576[s]
X_Angle	= 30[deg]
X_Atn	= 8[dB]
X_Pulse	= 3.21666667[us]
Irr_Atn_Dec	= 25.059[dB]
Irr_Atn_Dec_Calc	= 25.059[dB]
Irr_Atn_Dec_Default_Calc	= 25.059[dB]
Irr_Atn_Noe	= 25.059[dB]
Irr_Dec_Bandwidth_Hz	= 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.08082432[ppm]
Irr_Dec_Freq	= 395.88430144[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]




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

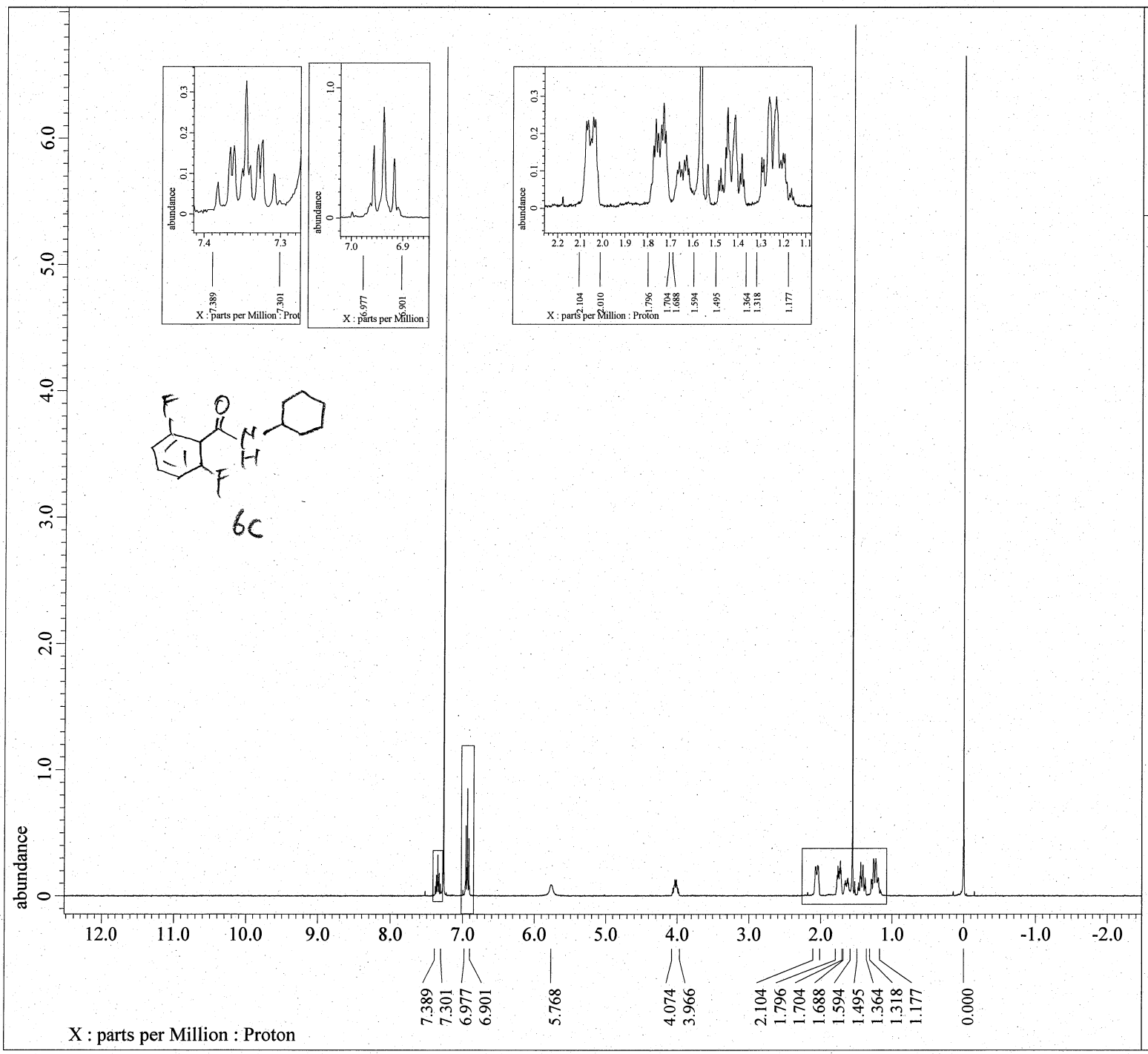
以下に由来:: TKH-1509_F_standard_single_pulse
```

```
Filename          = TKH-1509_F_standard_sing
Author            = element
Experiment        = single_pulse.jxp
Sample_Id         = TKH-1509_F_standard
Solvent           = CHLOROFORM-D
Creation_Time     =  5-MAR-2022 19:35:29
Revision_Time     =  5-MAR-2022 20:13:33
Current_Time      =  5-MAR-2022 20:14:02

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = Fluorine19
Dim_Units         = [ppm]
Dimensions        = X
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.4073814[T] (400[MHz])
X_Acq_Duration    = 86.50752[ms]
X_Domain          = 19F
X_Freq            = 376.87675879[MHz]
X_Offset          = 0[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 11.55968868[Hz]
X_Sweep           = 189.39393939[kHz]
X_Sweep_Clipped   = 151.51515152[kHz]
Irr_Domain        = Fluorine19
Irr_Freq          = 376.87675879[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = Fluorine19
Tri_Freq          = 376.87675879[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

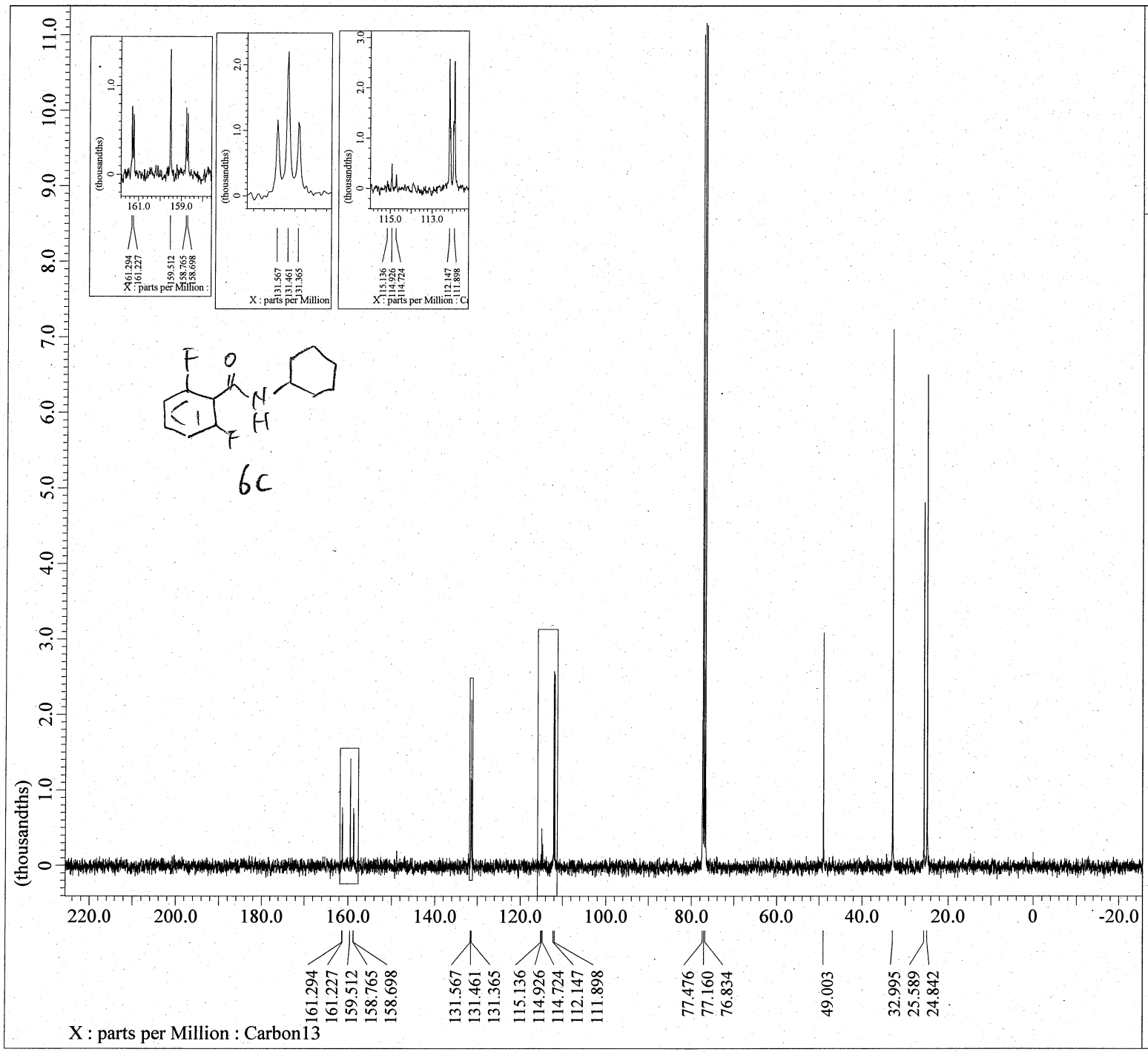
Relaxation_Delay = 5[s]
Recvr_Gain        = 46
Temp_Get          = 18.6[dC]
X_90_Width        = 6.8[us]
X_Acq_Time        = 86.50752[ms]
X_Angle           = 45[deg]
X_Atn             = 3[dB]
X_Pulse           = 3.4[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 5.08650752[s]
```




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

以下に由来:: TKH-1511_H_Proton-1-1.jdf
```

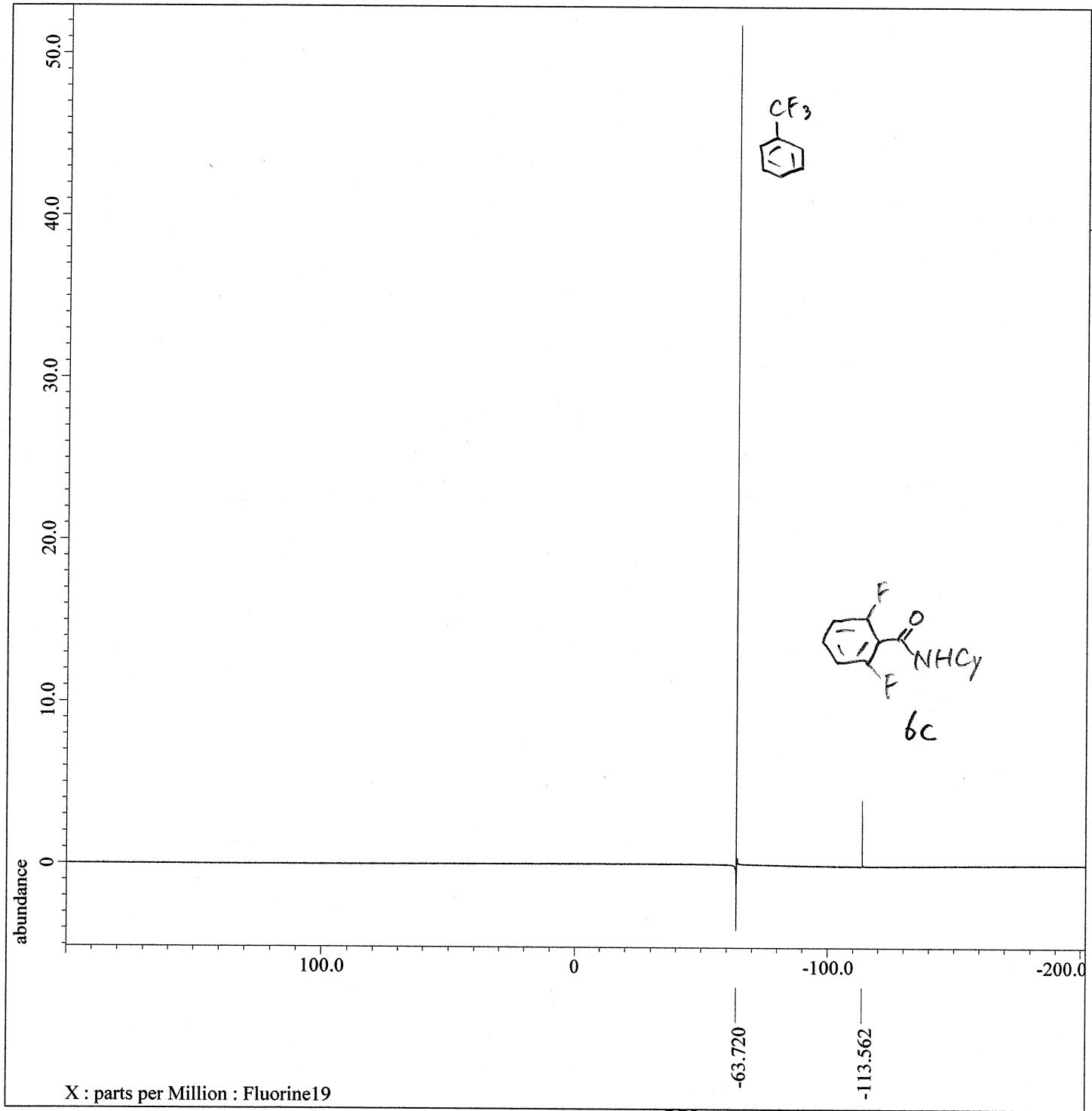
Filename	= TKH-1511_H_Proton-1-2.jdf
Author	= element
Experiment	= proton.jxp
Sample_Id	= TKH-1511_H
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 5-MAR-2022 20:59:13
Revision_Time	= 11-MAR-2022 12:32:38
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECS400
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.37221[T] (400[MHz])
X_Acq_Duration	= 2.1889024[s]
X_Domain	= 1H
X_Freq	= 399.03472754[MHz]
X_Offset	= 5.0[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45684997[Hz]
X_Sweep	= 7.48502994[kHz]
X_Sweep_Clipped	= 5.98802395[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.03472754[MHz]
Irr_Offset	= 5.0[ppm]
Tri_Domain	= Proton
Tri_Freq	= 399.03472754[MHz]
Tri_Offset	= 5.0[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 52
Temp_Get	= 17.8[dC]
X_90_Width	= 6.6[us]
X_Acq_Time	= 2.1889024[s]
X_Angle	= 45[deg]
X_Atn	= 1[dB]
X_Pulse	= 3.3[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.1889024[s]




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

以下に由来:: TKH-1511_carbon-1-1.jdf
```

Filename	= TKH-1511_carbon-1-
Author	= element
Experiment	= carbon.jxp
Sample_Id	= TKH-1511
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 9-MAR-2022 13:57:
Revision_Time	= 10-MAR-2022 19:45:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.2982153[T] (400[
X_Acq_Duration	= 1.048576[s]
X_Domain	= Carbon13
X_Freq	= 99.54517646[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.95367432[Hz]
X_Sweep	= 31.25[kHz]
X_Sweep_Clipped	= 25[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 5[us]
Clipped	= TRUE
Scans	= 400
Total_Scans	= 400
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 18[dC]
X_90_Width	= 9.65[us]
X_Acq_Time	= 1.048576[s]
X_Angle	= 30[deg]
X_Atn	= 8[dB]
X_Pulse	= 3.21666667[us]
Irr_Atn_Dec	= 25.059[dB]
Irr_Atn_Dec_Calc	= 25.059[dB]
Irr_Atn_Dec_Default_Calc	= 25.059[dB]
Irr_Atn_Noe	= 25.059[dB]
Irr_Dec_Bandwidth_Hz	= 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.08082432[ppm]
Irr_Dec_Freq	= 395.88430144[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]




```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
phase( -45, 0, 50[%] )

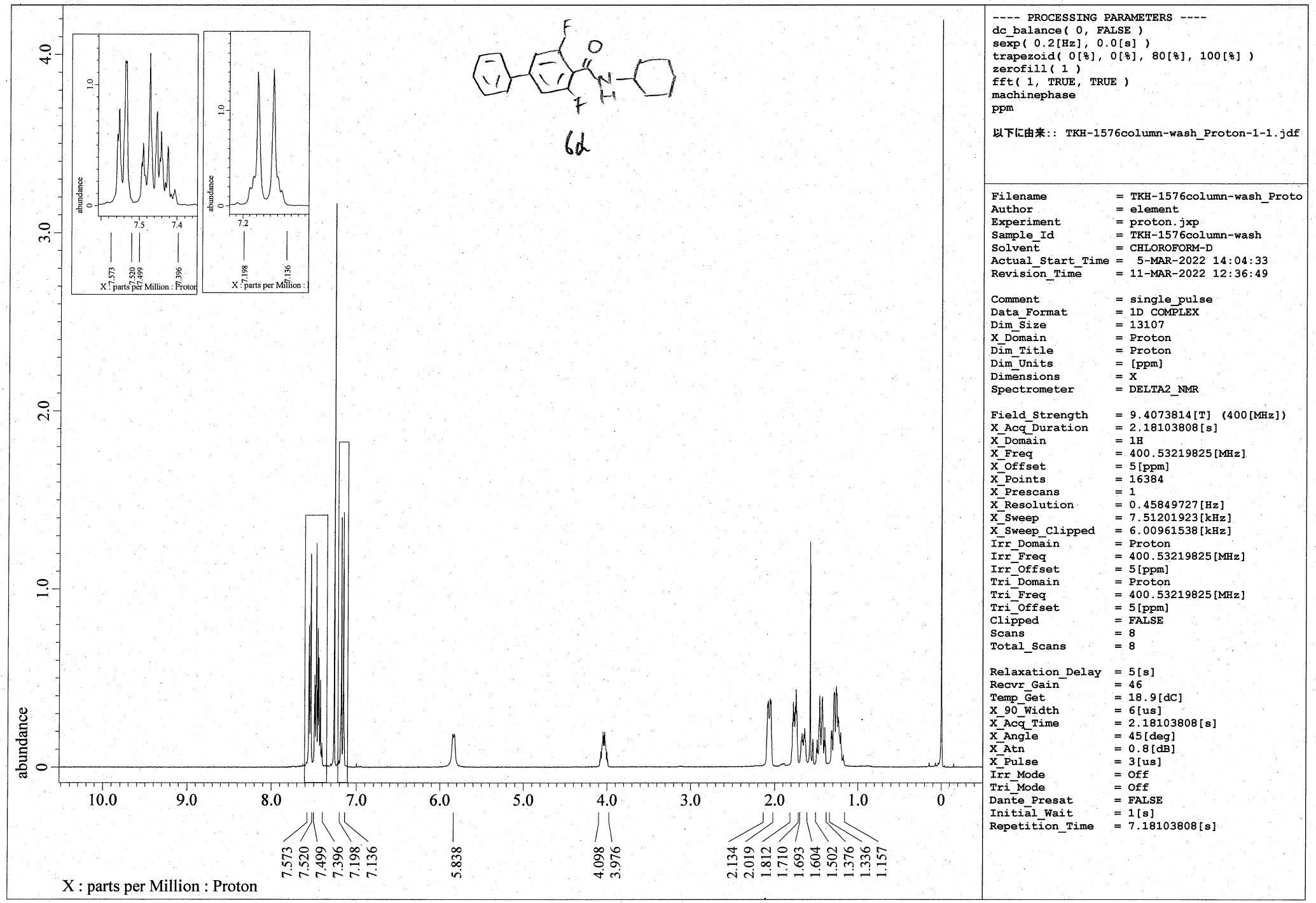
以下に由来:: TKH-1511_F_standard_single_pulse
```

```
Filename          = TKH-1511_F_standard_sing
Author            = element
Experiment        = single_pulse.jxp
Sample_Id         = TKH-1511_F_standard
Solvent           = CHLOROFORM-D
Creation_Time     =  5-MAR-2022 21:21:13
Revision_Time     =  5-MAR-2022 20:54:20
Current_Time      =  5-MAR-2022 20:54:24

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = Fluorine19
Dim_Units         = [ppm]
Dimensions        = X
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.4073814[T] (400[MHz])
X_Acq_Duration    = 86.50752[ms]
X_Domain          = 19F
X_Freq            = 376.87675879[MHz]
X_Offset          = 0[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 11.55968868[Hz]
X_Sweep           = 189.39393939[kHz]
X_Sweep_Clipped   = 151.51515152[kHz]
Irr_Domain        = Fluorine19
Irr_Freq          = 376.87675879[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = Fluorine19
Tri_Freq          = 376.87675879[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

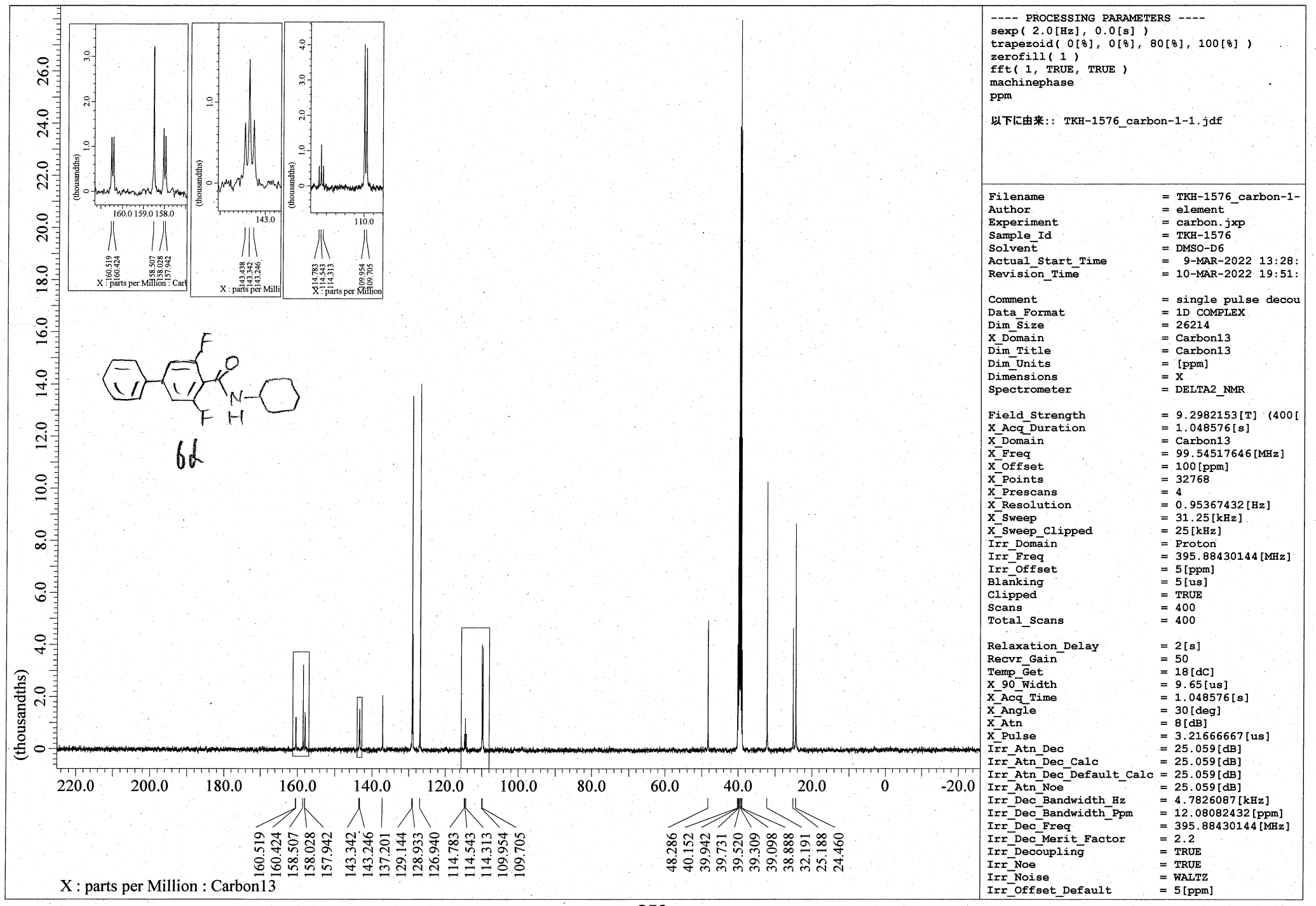
Relaxation_Delay = 5[s]
Recvr_Gain        = 46
Temp_Get          = 19.3[dC]
X_90_Width        = 6.8[us]
X_Acq_Time        = 86.50752[ms]
X_Angle           = 45[deg]
X_Atn             = 3[dB]
X_Pulse           = 3.4[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 5.08650752[s]
```

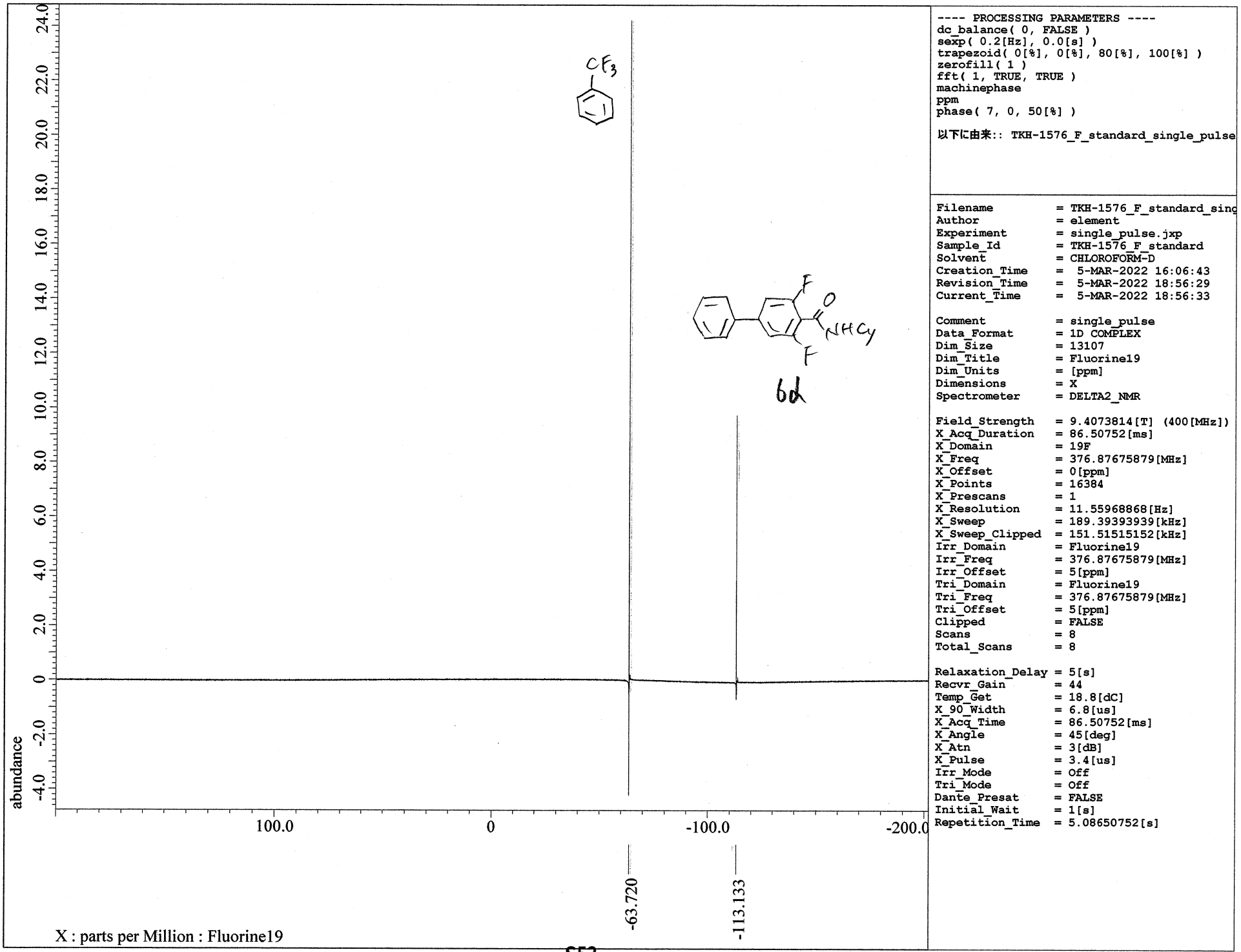



```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

以下に由来:: TKH-1576column-wash_Proton-1-1.jdf
```

Filename	= TKH-1576column-wash_Proto
Author	= element
Experiment	= proton.jxp
Sample_Id	= TKH-1576column-wash
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 5-MAR-2022 14:04:33
Revision_Time	= 11-MAR-2022 12:36:49
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.4073814[T] (400[MHz])
X_Acq_Duration	= 2.18103808[s]
X_Domain	= 1H
X_Freq	= 400.53219825[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45849727[Hz]
X_Sweep	= 7.51201923[kHz]
X_Sweep_Clipped	= 6.00961538[kHz]
Irr_Domain	= Proton
Irr_Freq	= 400.53219825[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 400.53219825[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 46
Temp_Get	= 18.9[dC]
X_90_Width	= 6[us]
X_Acq_Time	= 2.18103808[s]
X_Angle	= 45[deg]
X_Atn	= 0.8[dB]
X_Pulse	= 3[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.18103808[s]

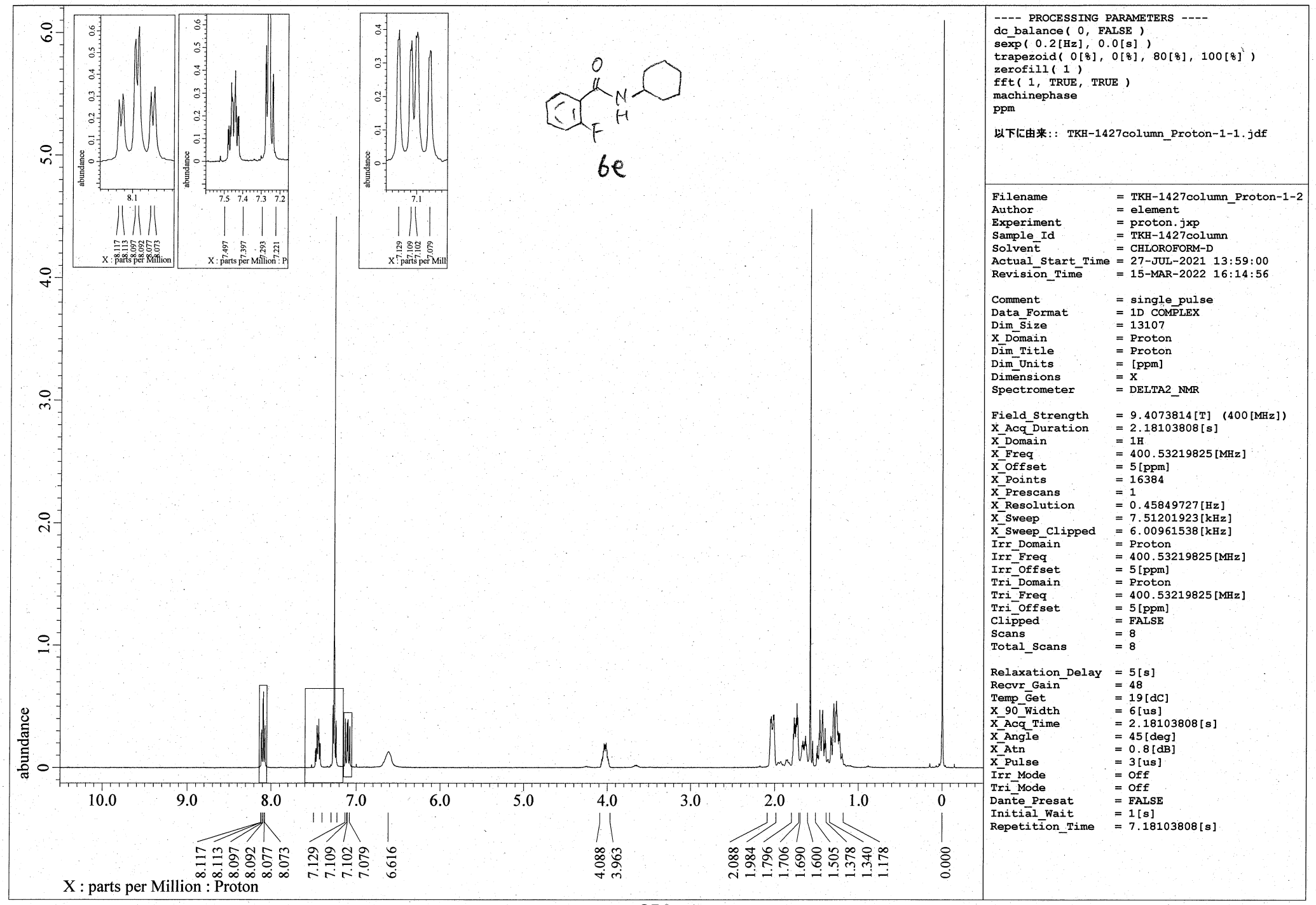

---- PROCESSING PARAMETERS ----
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
以下に由来:: TKH-1576_carbon-1-1.jdf
Filename = TKH-1576_carbon-1-
Author = element
Experiment = carbon.jxp
Sample_Id = TKH-1576
Solvent = DMSO-D6
Actual_Start_Time = 9-MAR-2022 13:28:
Revision_Time = 10-MAR-2022 19:51:
Comment = single pulse decou
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = DELTA2_NMR
Field_Strength = 9.2982153[T] (400[
X_Acq_Duration = 1.048576[s]
X_Domain = Carbon13
X_Freq = 99.54517646[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95367432[Hz]
X_Sweep = 31.25[kHz]
X_Sweep_Clipped = 25[kHz]
Irr_Domain = Proton
Irr_Freq = 395.88430144[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = TRUE
Scans = 400
Total_Scans = 400
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 18[dC]
X_90_Width = 9.65[us]
X_Acq_Time = 1.048576[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 3.21666667[us]
Irr_Atn_Dec = 25.059[dB]
Irr_Atn_Dec_Calc = 25.059[dB]
Irr_Atn_Dec_Default_Calc = 25.059[dB]
Irr_Atn_Noe = 25.059[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm = 12.08082432[ppm]
Irr_Dec_Freq = 395.88430144[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
(thousandths)
X : parts per Million : Carbon13
160.519
160.424
158.507
158.028
157.942
143.342
143.246
137.201
129.144
128.933
126.940
114.783
114.543
114.313
109.954
109.705
48.286
40.152
39.942
39.731
39.520
39.309
39.098
38.888
32.191
25.188
24.460




```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
phase( 7, 0, 50[%] )

以下に由来:: TKH-1576_F_standard_single_pulse
```

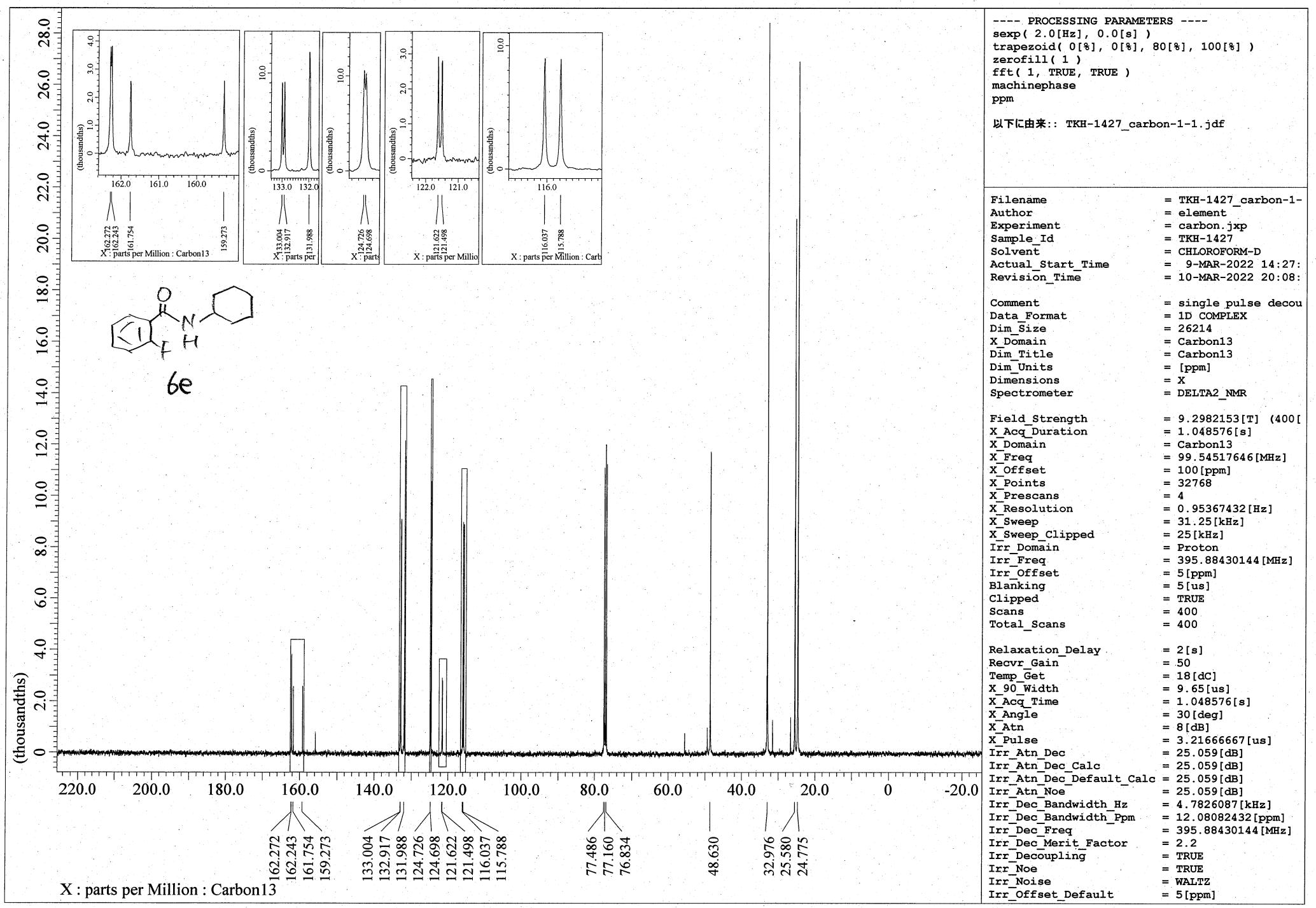
Filename	= TKH-1576_F_standard_sing
Author	= element
Experiment	= single_pulse.jxp
Sample_Id	= TKH-1576_F_standard
Solvent	= CHLOROFORM-D
Creation_Time	= 5-MAR-2022 16:06:43
Revision_Time	= 5-MAR-2022 18:56:29
Current_Time	= 5-MAR-2022 18:56:33
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
Dim_Title	= Fluorine19
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.4073814[T] (400[MHz])
X_Acq_Duration	= 86.50752[ms]
X_Domain	= 19F
X_Freq	= 376.87675879[MHz]
X_Offset	= 0[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 11.55968868[Hz]
X_Sweep	= 189.39393939[kHz]
X_Sweep_Clipped	= 151.51515152[kHz]
Irr_Domain	= Fluorine19
Irr_Freq	= 376.87675879[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Fluorine19
Tri_Freq	= 376.87675879[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 44
Temp_Get	= 18.8[dC]
X_90_Width	= 6.8[us]
X_Acq_Time	= 86.50752[ms]
X_Angle	= 45[deg]
X_Atn	= 3[dB]
X_Pulse	= 3.4[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 5.08650752[s]




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

以下に由来:: TKH-1427column_Proton-1-1.jdf
```

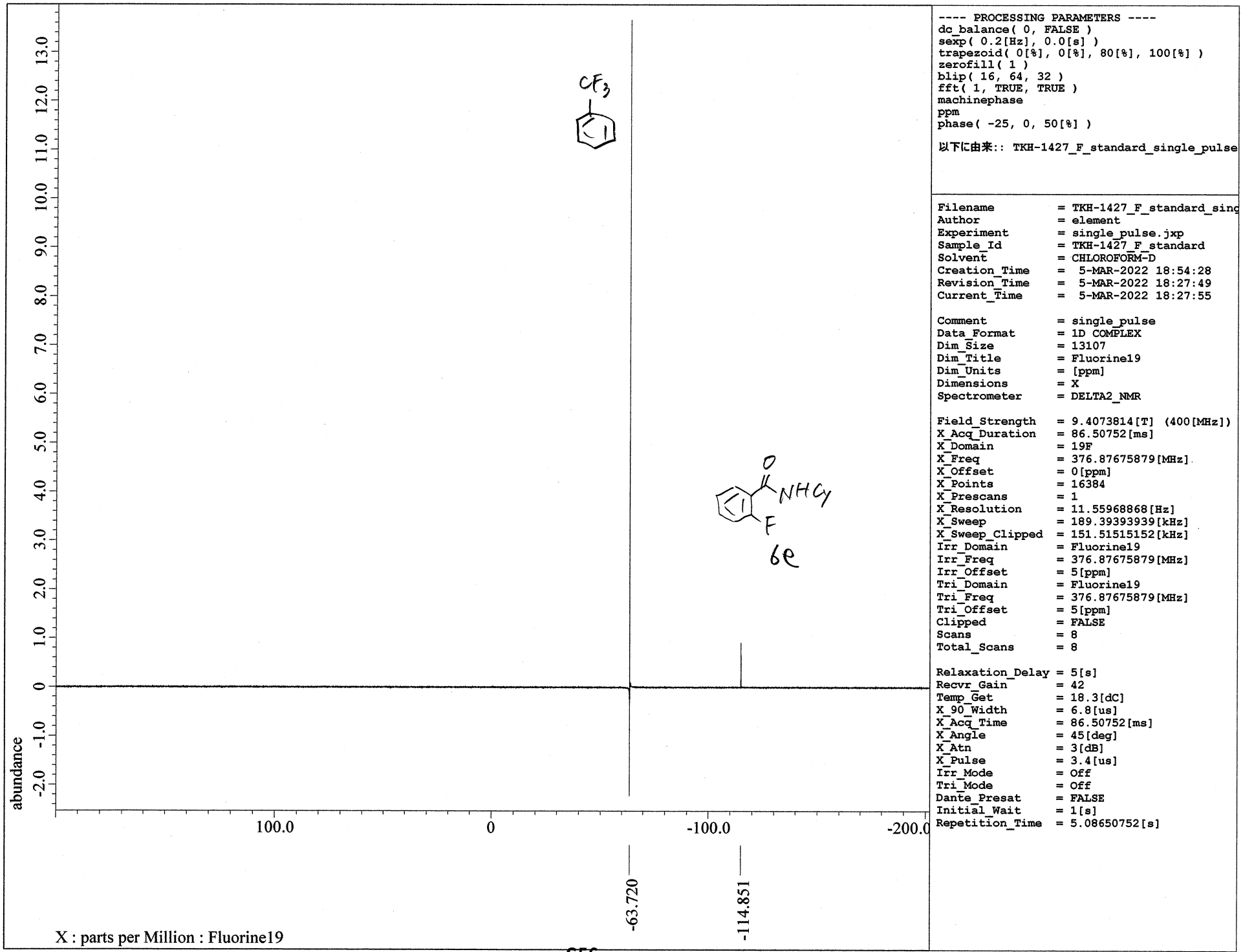
Filename	= TKH-1427column_Proton-1-2
Author	= element
Experiment	= proton.jxp
Sample_Id	= TKH-1427column
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 27-JUL-2021 13:59:00
Revision_Time	= 15-MAR-2022 16:14:56
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.4073814[T] (400[MHz])
X_Acq_Duration	= 2.18103808[s]
X_Domain	= 1H
X_Freq	= 400.53219825[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45849727[Hz]
X_Sweep	= 7.51201923[kHz]
X_Sweep_Clipped	= 6.00961538[kHz]
Irr_Domain	= Proton
Irr_Freq	= 400.53219825[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 400.53219825[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 48
Temp_Get	= 19[dC]
X_90_Width	= 6[us]
X_Acq_Time	= 2.18103808[s]
X_Angle	= 45[deg]
X_Atn	= 0.8[dB]
X_Pulse	= 3[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.18103808[s]




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

以下に由来:: TKH-1427_carbon-1-1.jdf
```

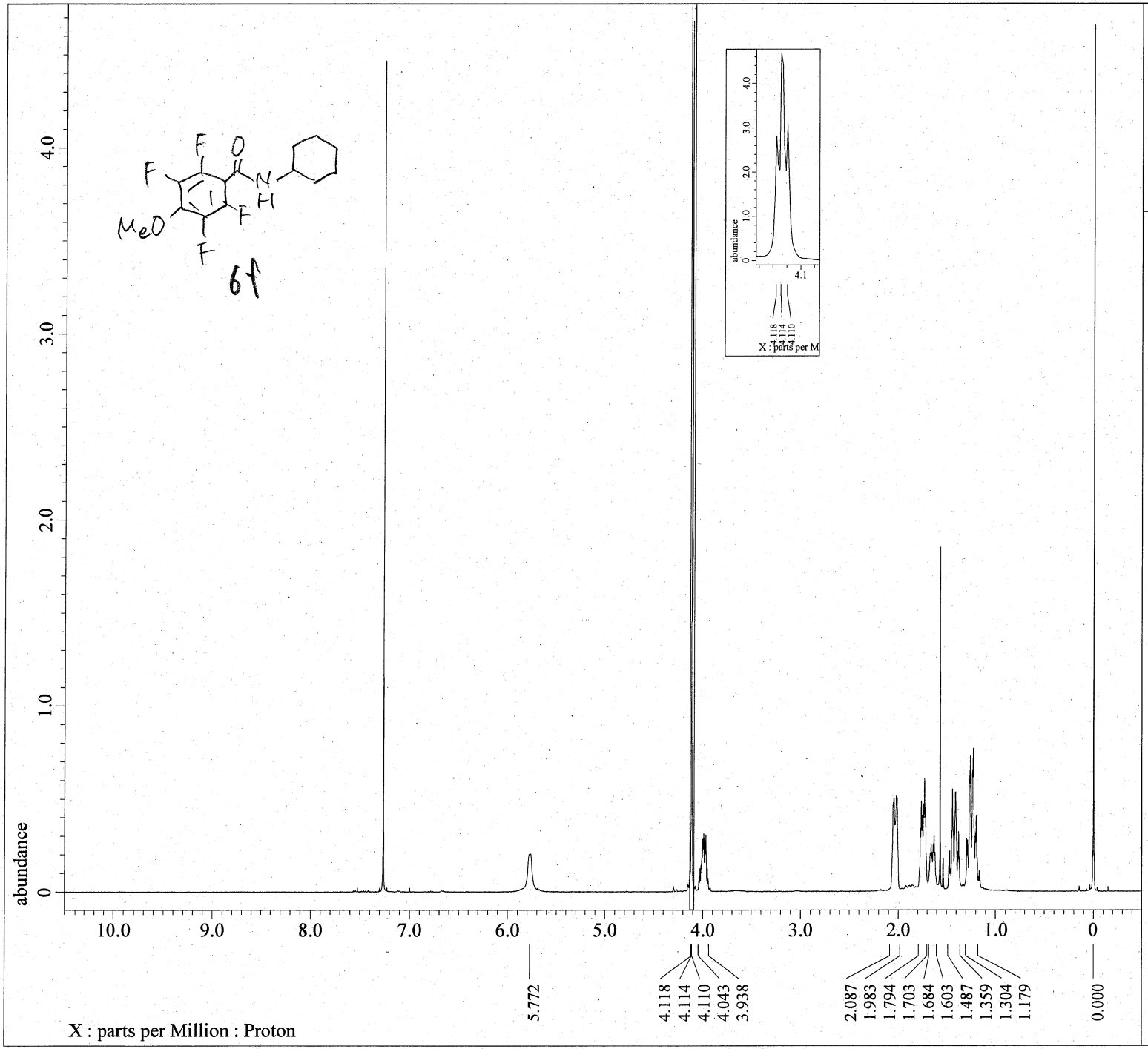
Filename	= TKH-1427_carbon-1-
Author	= element
Experiment	= carbon.jxp
Sample_Id	= TKH-1427
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 9-MAR-2022 14:27:
Revision_Time	= 10-MAR-2022 20:08:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.2982153[T] (400[
X_Acq_Duration	= 1.048576[s]
X_Domain	= Carbon13
X_Freq	= 99.54517646[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.95367432[Hz]
X_Sweep	= 31.25[kHz]
X_Sweep_Clipped	= 25[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 5[us]
Clipped	= TRUE
Scans	= 400
Total_Scans	= 400
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 18[dC]
X_90_Width	= 9.65[us]
X_Acq_Time	= 1.048576[s]
X_Angle	= 30[deg]
X_Atn	= 8[dB]
X_Pulse	= 3.21666667[us]
Irr_Atn_Dec	= 25.059[dB]
Irr_Atn_Dec_Calc	= 25.059[dB]
Irr_Atn_Dec_Default_Calc	= 25.059[dB]
Irr_Atn_Noe	= 25.059[dB]
Irr_Dec_Bandwidth_Hz	= 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.08082432[ppm]
Irr_Dec_Freq	= 395.88430144[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]




```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
blip( 16, 64, 32 )
fft( 1, TRUE, TRUE )
machinephase
ppm
phase( -25, 0, 50[%] )

以下に由来:: TKH-1427_F_standard_single_pulse
```

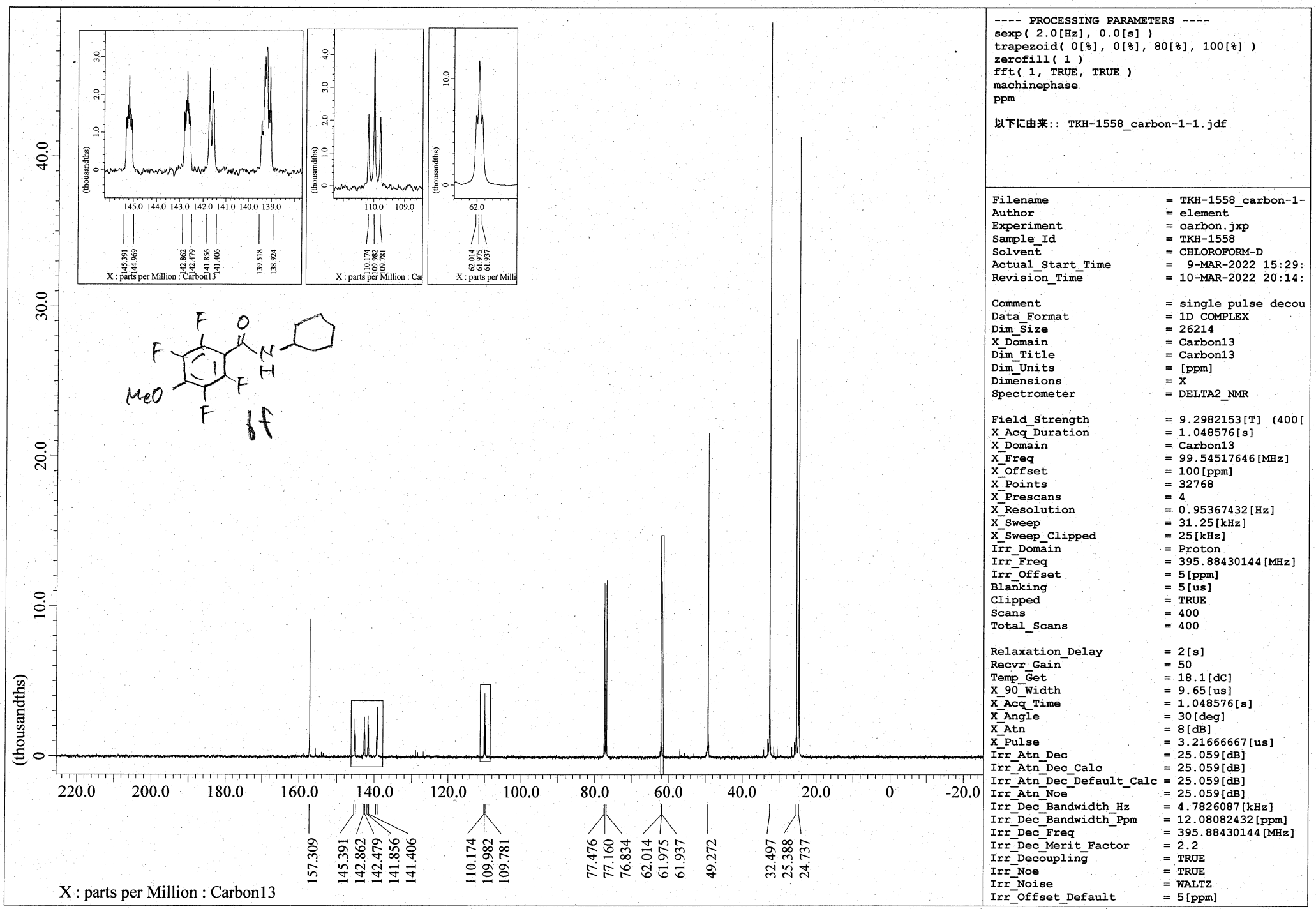
Filename	= TKH-1427_F_standard_sing
Author	= element
Experiment	= single_pulse.jxp
Sample_Id	= TKH-1427_F_standard
Solvent	= CHLOROFORM-D
Creation_Time	= 5-MAR-2022 18:54:28
Revision_Time	= 5-MAR-2022 18:27:49
Current_Time	= 5-MAR-2022 18:27:55
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
Dim_Title	= Fluorine19
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.4073814[T] (400[MHz])
X_Acq_Duration	= 86.50752[ms]
X_Domain	= 19F
X_Freq	= 376.87675879[MHz]
X_Offset	= 0[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 11.55968868[Hz]
X_Sweep	= 189.39393939[kHz]
X_Sweep_Clipped	= 151.51515152[kHz]
Irr_Domain	= Fluorine19
Irr_Freq	= 376.87675879[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Fluorine19
Tri_Freq	= 376.87675879[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 42
Temp_Get	= 18.3[dC]
X_90_Width	= 6.8[us]
X_Acq_Time	= 86.50752[ms]
X_Angle	= 45[deg]
X_Atn	= 3[dB]
X_Pulse	= 3.4[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 5.08650752[s]

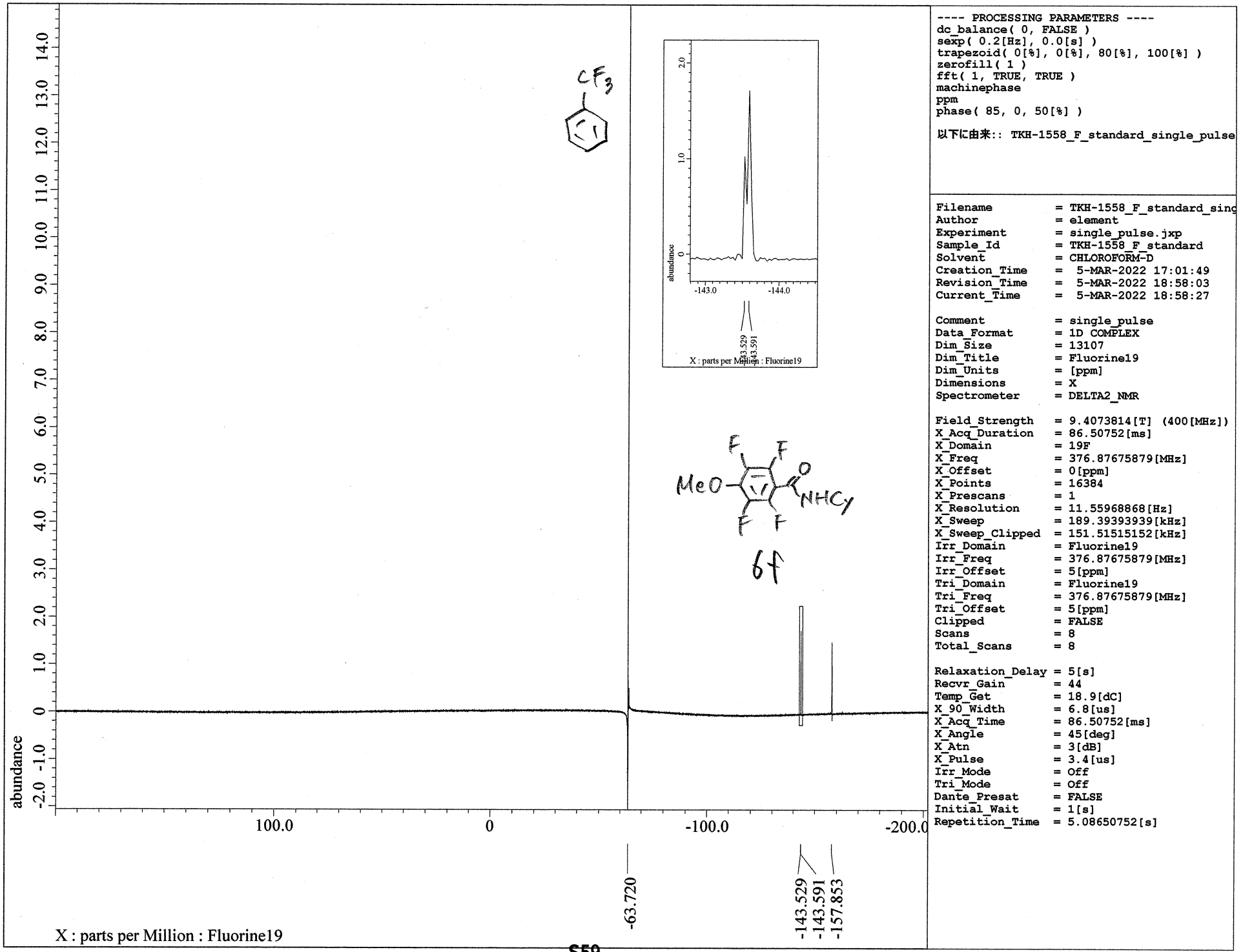



```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

以下に由来:: TKH-1558column_Proton-1-1.jdf
```

Filename	= TKH-1558column_Proton-1-2
Author	= element
Experiment	= proton.jxp
Sample_Id	= TKH-1558column
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 14-FEB-2022 20:48:43
Revision_Time	= 11-MAR-2022 12:47:28
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.4073814[T] (400[MHz])
X_Acq_Duration	= 2.18103808[s]
X_Domain	= 1H
X_Freq	= 400.53219825[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45849727[Hz]
X_Sweep	= 7.51201923[kHz]
X_Sweep_Clipped	= 6.00961538[kHz]
Irr_Domain	= Proton
Irr_Freq	= 400.53219825[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 400.53219825[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 46
Temp_Get	= 19.1[dC]
X_90_Width	= 6[us]
X_Acq_Time	= 2.18103808[s]
X_Angle	= 45[deg]
X_Atn	= 0.8[dB]
X_Pulse	= 3[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.18103808[s]


---- PROCESSING PARAMETERS ----
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
以下に由来:: TKH-1558_carbon-1-1.jdf
Filename = TKH-1558_carbon-1-
Author = element
Experiment = carbon.jxp
Sample_Id = TKH-1558
Solvent = CHLOROFORM-D
Actual_Start_Time = 9-MAR-2022 15:29:
Revision_Time = 10-MAR-2022 20:14:
Comment = single pulse decou
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = DELTA2_NMR
Field_Strength = 9.2982153[T] (400[
X_Acq_Duration = 1.048576[s]
X_Domain = Carbon13
X_Freq = 99.54517646[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95367432[Hz]
X_Sweep = 31.25[kHz]
X_Sweep_Clipped = 25[kHz]
Irr_Domain = Proton
Irr_Freq = 395.88430144[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = TRUE
Scans = 400
Total_Scans = 400
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 18.1[dC]
X_90_Width = 9.65[us]
X_Acq_Time = 1.048576[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 3.21666667[us]
Irr_Atn_Dec = 25.059[dB]
Irr_Atn_Dec_Calc = 25.059[dB]
Irr_Atn_Dec_Default_Calc = 25.059[dB]
Irr_Atn_Noe = 25.059[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm = 12.08082432[ppm]
Irr_Dec_Freq = 395.88430144[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
(thousandths)
X : parts per Million : Carbon13
157.309
145.391
142.862
142.479
141.856
141.406
110.174
109.982
109.781
77.476
77.160
76.834
62.014
61.975
61.937
49.272
32.497
25.388
24.737
MeO




```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
phase( 85, 0, 50[%] )

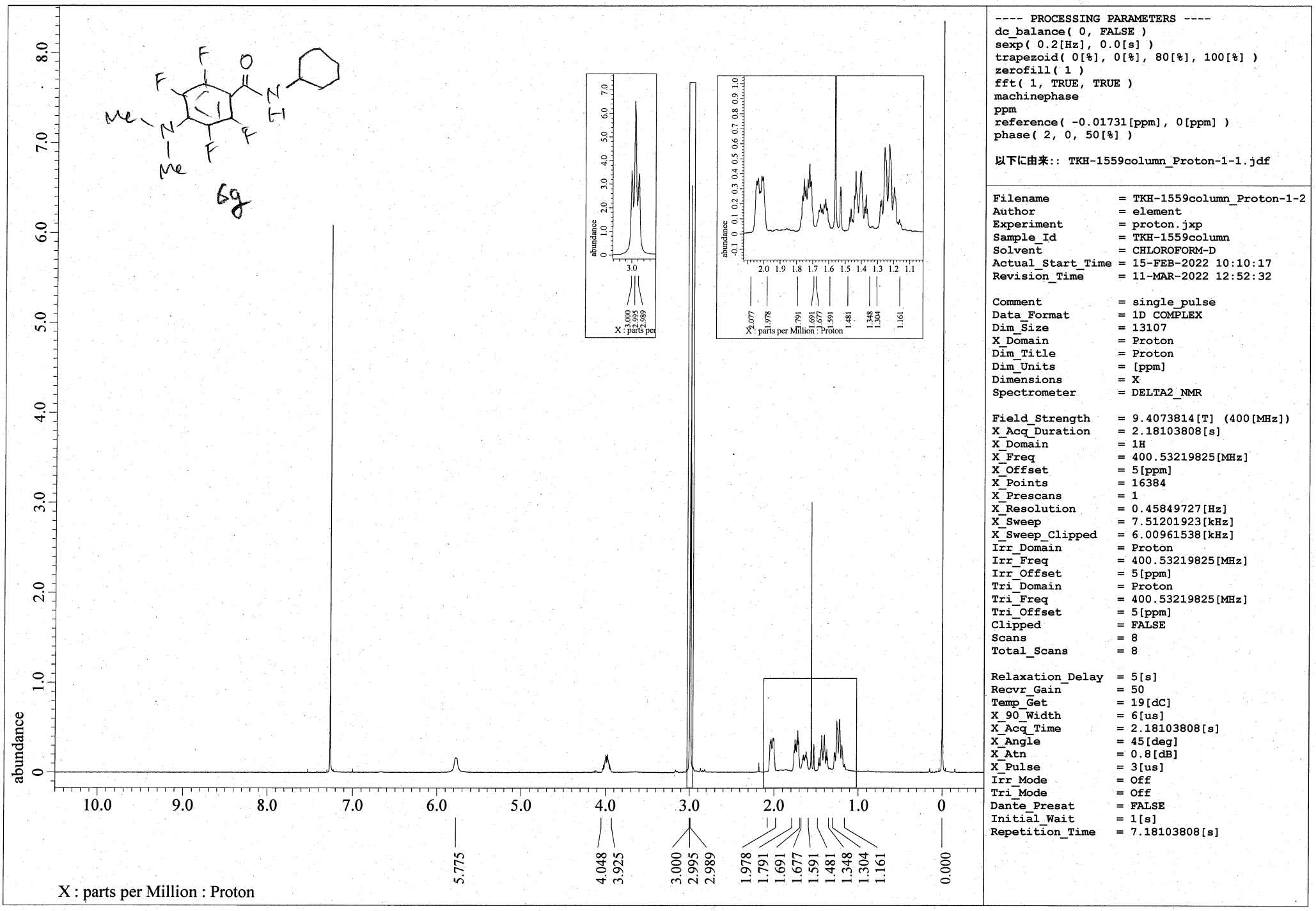
以下に由来:: TKH-1558_F_standard_single_pulse
```

```
Filename          = TKH-1558_F_standard_sing
Author            = element
Experiment        = single_pulse.jxp
Sample_Id         = TKH-1558_F_standard
Solvent           = CHLOROFORM-D
Creation_Time     =  5-MAR-2022 17:01:49
Revision_Time     =  5-MAR-2022 18:58:03
Current_Time      =  5-MAR-2022 18:58:27

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = Fluorine19
Dim_Units         = [ppm]
Dimensions        = X
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.4073814[T] (400[MHz])
X_Acq_Duration    = 86.50752[ms]
X_Domain          = 19F
X_Freq            = 376.87675879[MHz]
X_Offset          = 0[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 11.55968868[Hz]
X_Sweep           = 189.39393939[kHz]
X_Sweep_Clipped   = 151.51515152[kHz]
Irr_Domain        = Fluorine19
Irr_Freq          = 376.87675879[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = Fluorine19
Tri_Freq          = 376.87675879[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

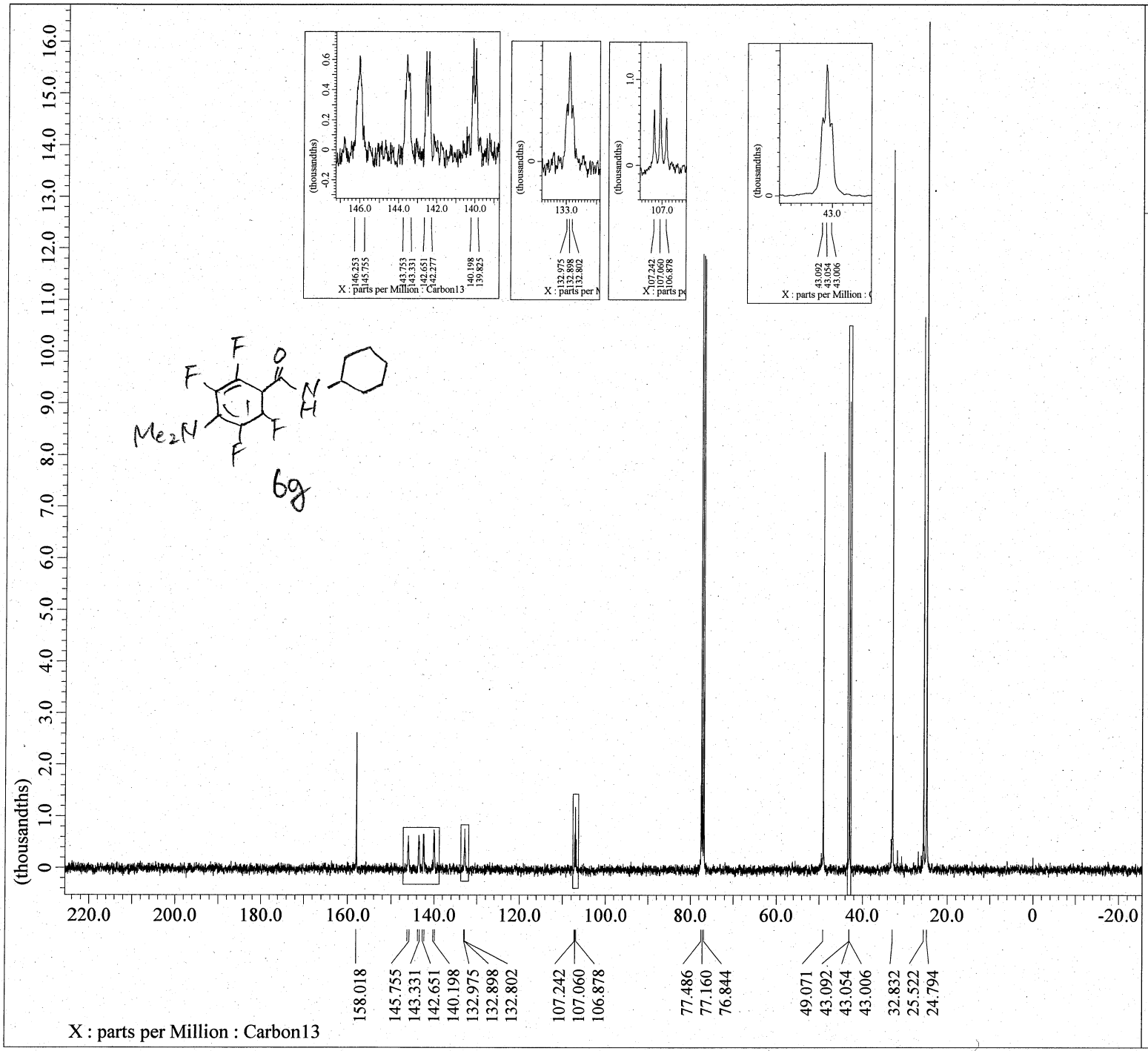
Relaxation_Delay = 5[s]
Recvr_Gain        = 44
Temp_Get          = 18.9[dC]
X_90_Width        = 6.8[us]
X_Acq_Time        = 86.50752[ms]
X_Angle           = 45[deg]
X_Atn             = 3[dB]
X_Pulse           = 3.4[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 5.08650752[s]
```




```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
reference( -0.01731[ppm], 0[ppm] )
phase( 2, 0, 50[%] )

以下に由来:: TKH-1559column_Proton-1-1.jdf
```

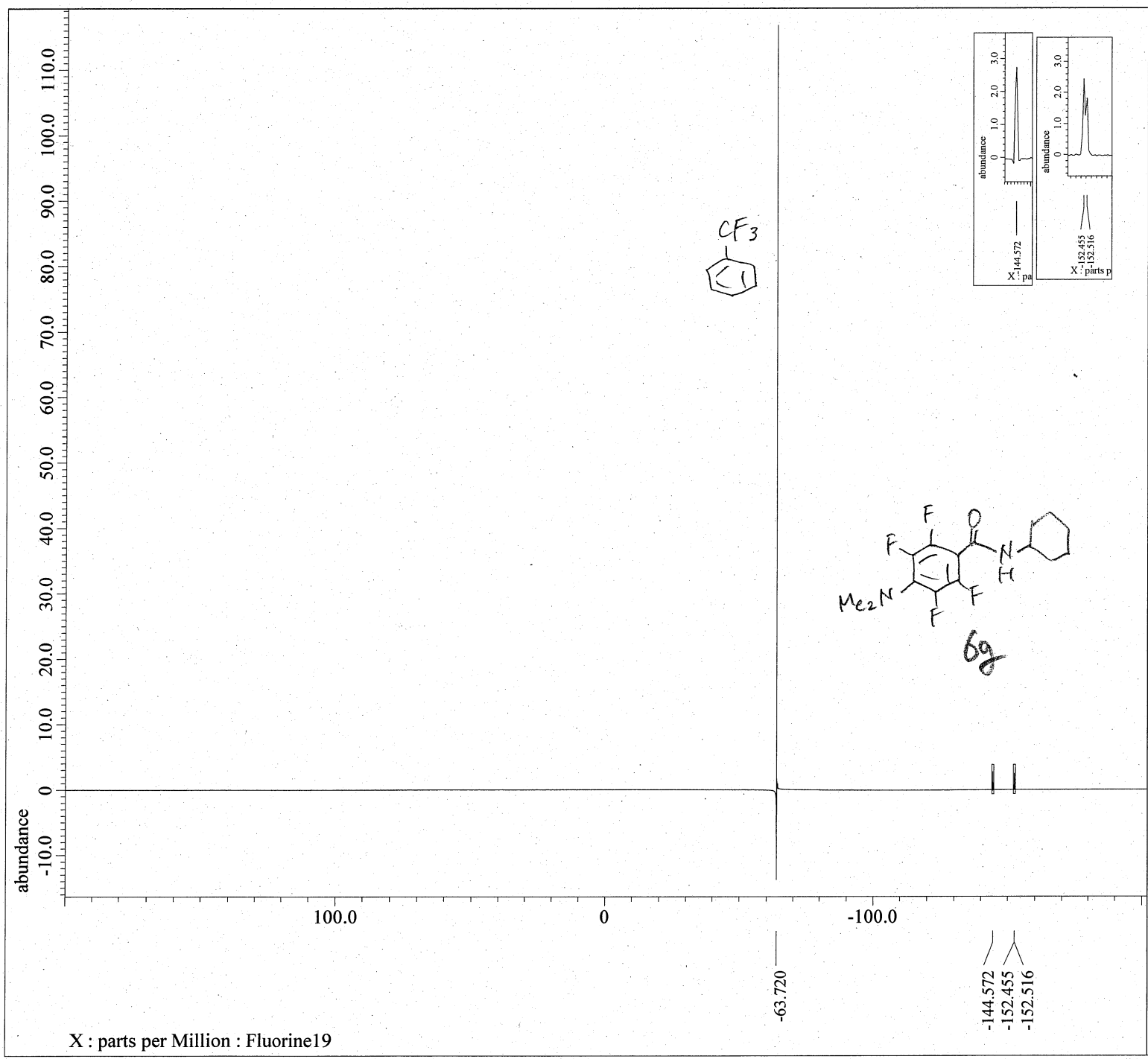
Filename	= TKH-1559column_Proton-1-2
Author	= element
Experiment	= proton.jxp
Sample_Id	= TKH-1559column
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 15-FEB-2022 10:10:17
Revision_Time	= 11-MAR-2022 12:52:32
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.4073814[T] (400[MHz])
X_Acq_Duration	= 2.18103808[s]
X_Domain	= 1H
X_Freq	= 400.53219825[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45849727[Hz]
X_Sweep	= 7.51201923[kHz]
X_Sweep_Clipped	= 6.00961538[kHz]
Irr_Domain	= Proton
Irr_Freq	= 400.53219825[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 400.53219825[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 50
Temp_Get	= 19[dC]
X_90_Width	= 6[us]
X_Acq_Time	= 2.18103808[s]
X_Angle	= 45[deg]
X_Atn	= 0.8[dB]
X_Pulse	= 3[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.18103808[s]




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

以下に由来:: TKH-1559_carbon-1-1.jdf
```

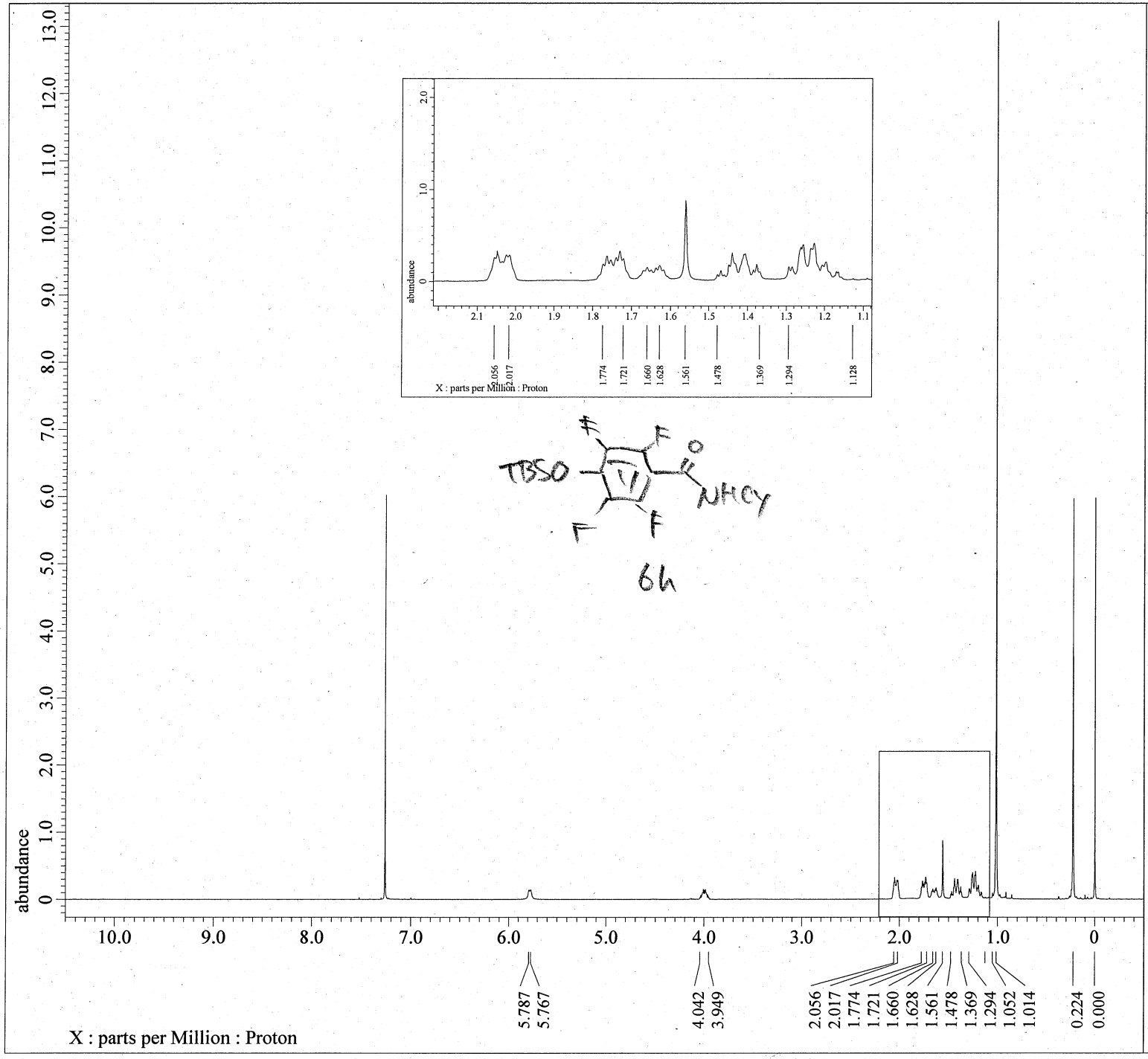
Filename	= TKH-1559_carbon-1-
Author	= element
Experiment	= carbon.jxp
Sample_Id	= TKH-1559
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 9-MAR-2022 16:27:
Revision_Time	= 10-MAR-2022 20:21:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.2982153[T] (400[
X_Acq_Duration	= 1.048576[s]
X_Domain	= Carbon13
X_Freq	= 99.54517646[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.95367432[Hz]
X_Sweep	= 31.25[kHz]
X_Sweep_Clipped	= 25[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 5[us]
Clipped	= TRUE
Scans	= 400
Total_Scans	= 400
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 18[dC]
X_90_Width	= 9.65[us]
X_Acq_Time	= 1.048576[s]
X_Angle	= 30[deg]
X_Atn	= 8[dB]
X_Pulse	= 3.21666667[us]
Irr_Atn_Dec	= 25.059[dB]
Irr_Atn_Dec_Calc	= 25.059[dB]
Irr_Atn_Dec_Default_Calc	= 25.059[dB]
Irr_Atn_Noe	= 25.059[dB]
Irr_Dec_Bandwidth_Hz	= 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.08082432[ppm]
Irr_Dec_Freq	= 395.88430144[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]




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

以下に由来:: TKH-1559_F_standard_single_pulse-1-
```

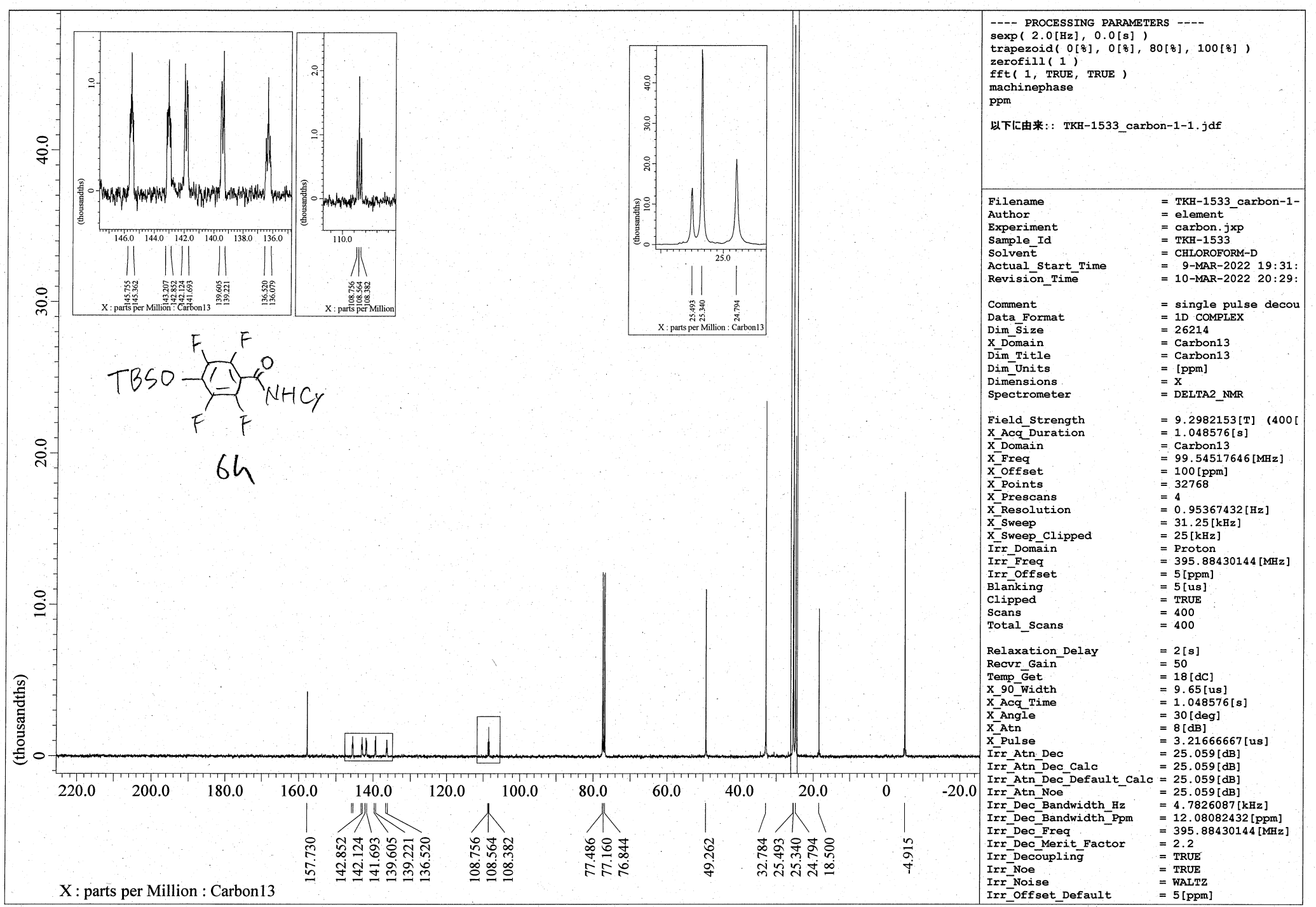
Filename	= TKH-1559_F_standard_singl
Author	= element
Experiment	= single_pulse.jxp
Sample_Id	= TKH-1559_F_standard
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 5-MAR-2022 16:54:24
Revision_Time	= 11-MAR-2022 14:01:15
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Fluori
Dim_Title	= Fluorine19
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.4073814[T] (400[MHz])
X_Acq_Duration	= 86.50752[ms]
X_Domain	= 19F
X_Freq	= 376.87675879[MHz]
X_Offset	= 0[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 11.55968868[Hz]
X_Sweep	= 189.39393939[kHz]
X_Sweep_Clipped	= 151.51515152[kHz]
Irr_Domain	= Fluorine19
Irr_Freq	= 376.87675879[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Fluorine19
Tri_Freq	= 376.87675879[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 46
Temp_Get	= 18.9[dC]
X_90_Width	= 6.8[us]
X_Acq_Time	= 86.50752[ms]
X_Angle	= 45[deg]
X_Atn	= 3[dB]
X_Pulse	= 3.4[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 5.08650752[s]




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

Derived from: TKH-1533column11-15_Proton-1-2.
```

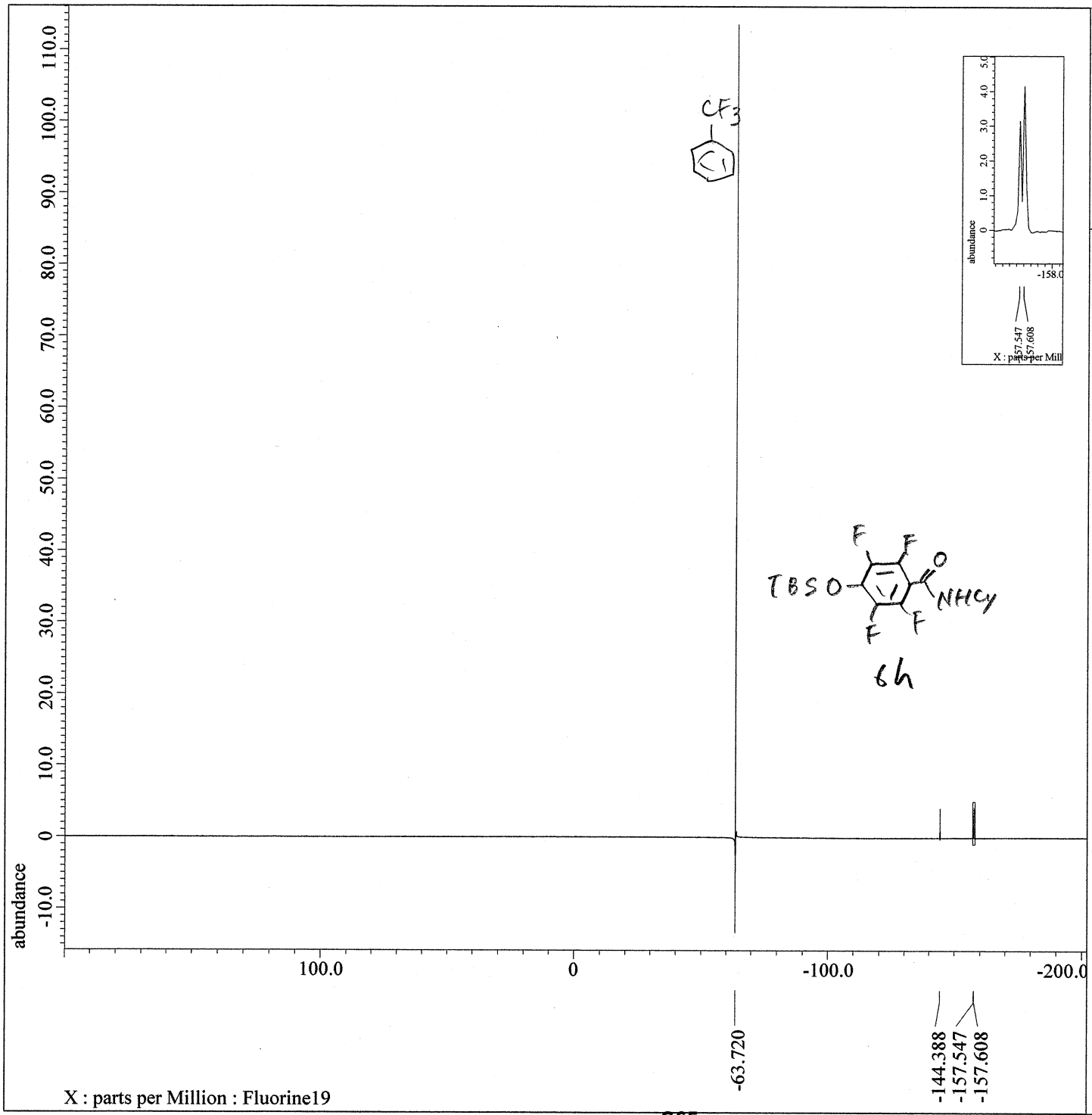
Filename	= TKH-1533column11-15_Proto
Author	= element
Experiment	= proton.jxp
Sample_Id	= TKH-1533column11-15
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 14-JAN-2022 11:07:44
Revision_Time	= 6-SEP-2022 15:02:51
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.4073814[T] (400[MHz])
X_Acq_Duration	= 2.18103808[s]
X_Domain	= 1H
X_Freq	= 400.53219825[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45849727[Hz]
X_Sweep	= 7.51201923[kHz]
X_Sweep_Clipped	= 6.00961538[kHz]
Irr_Domain	= Proton
Irr_Freq	= 400.53219825[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 400.53219825[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 46
Temp_Get	= 18.5[dC]
X_90_Width	= 6[us]
X_Acq_Time	= 2.18103808[s]
X_Angle	= 45[deg]
X_Atn	= 0.8[dB]
X_Pulse	= 3[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.18103808[s]




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

以下に由来:: TKH-1533_carbon-1-1.jdf
```

Filename	= TKH-1533_carbon-1-
Author	= element
Experiment	= carbon.jxp
Sample_Id	= TKH-1533
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 9-MAR-2022 19:31:
Revision_Time	= 10-MAR-2022 20:29:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.2982153[T] (400[
X_Acq_Duration	= 1.048576[s]
X_Domain	= Carbon13
X_Freq	= 99.54517646[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.95367432[Hz]
X_Sweep	= 31.25[kHz]
X_Sweep_Clipped	= 25[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 5[us]
Clipped	= TRUE
Scans	= 400
Total_Scans	= 400
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 18[dC]
X_90_Width	= 9.65[us]
X_Acq_Time	= 1.048576[s]
X_Angle	= 30[deg]
X_Atn	= 8[dB]
X_Pulse	= 3.21666667[us]
Irr_Atn_Dec	= 25.059[dB]
Irr_Atn_Dec_Calc	= 25.059[dB]
Irr_Atn_Dec_Default_Calc	= 25.059[dB]
Irr_Atn_Noe	= 25.059[dB]
Irr_Dec_Bandwidth_Hz	= 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.08082432[ppm]
Irr_Dec_Freq	= 395.88430144[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]




```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
phase( -73, 0, 50[%] )

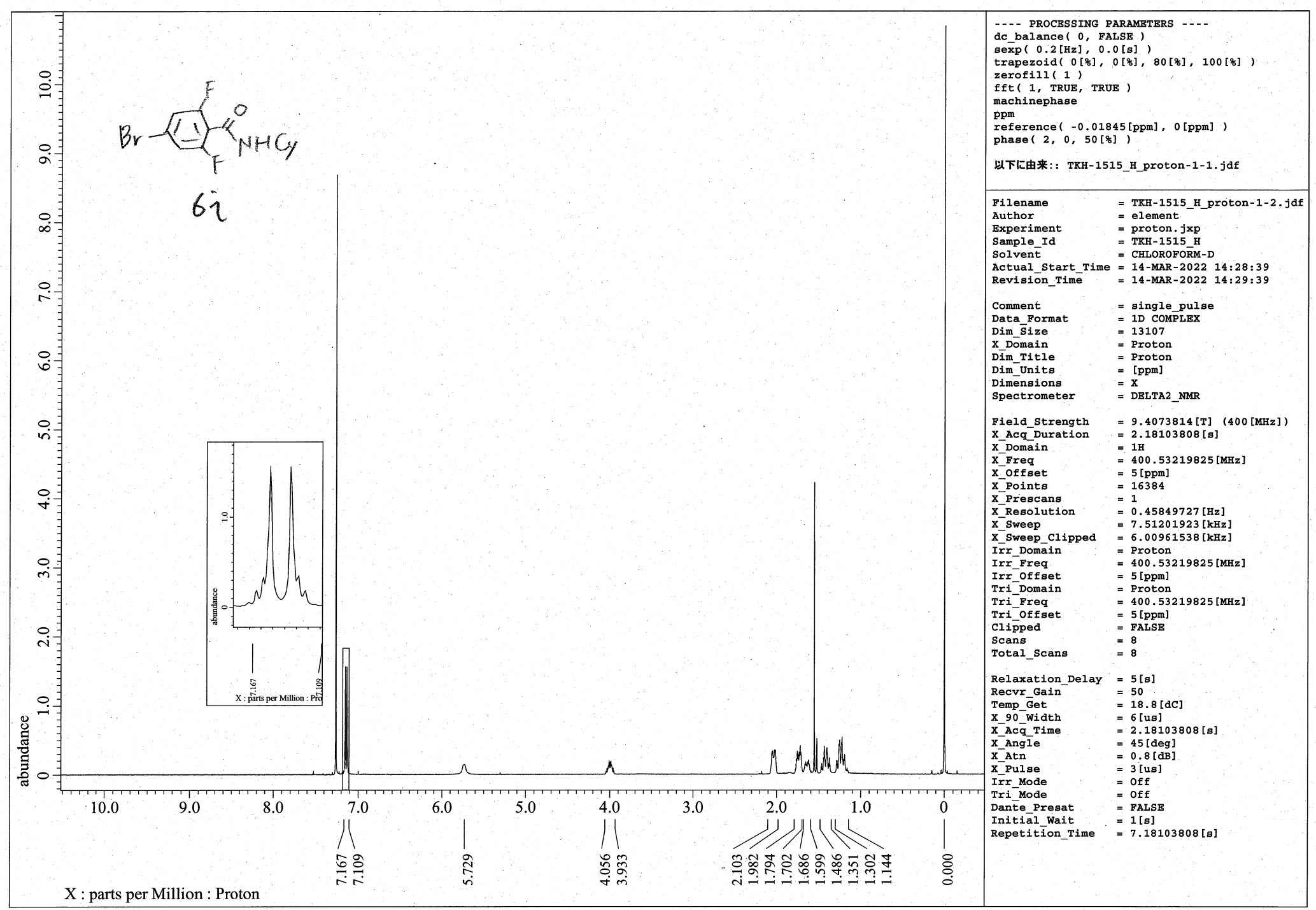
以下に由来:: TKH-1533_F_standard_single_pulse
```

```
Filename          = TKH-1533_F_standard_sing
Author            = element
Experiment        = single_pulse.jxp
Sample_Id         = TKH-1533_F_standard
Solvent           = CHLOROFORM-D
Creation_Time     =  5-MAR-2022 18:46:58
Revision_Time     =  5-MAR-2022 19:03:14
Current_Time      =  5-MAR-2022 19:03:31

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = Fluorine19
Dim_Units         = [ppm]
Dimensions        = X
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.4073814[T] (400[MHz])
X_Acq_Duration    = 86.50752[ms]
X_Domain          = 19F
X_Freq            = 376.87675879[MHz]
X_Offset          = 0[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 11.55968868[Hz]
X_Sweep           = 189.39393939[kHz]
X_Sweep_Clipped   = 151.51515152[kHz]
Irr_Domain        = Fluorine19
Irr_Freq          = 376.87675879[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = Fluorine19
Tri_Freq          = 376.87675879[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay = 5[s]
Recvr_Gain        = 46
Temp_Get          = 18.2[dC]
X_90_Width        = 6.8[us]
X_Acq_Time        = 86.50752[ms]
X_Angle           = 45[deg]
X_Atn             = 3[dB]
X_Pulse           = 3.4[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 5.08650752[s]
```




```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
reference( -0.01845[ppm], 0[ppm] )
phase( 2, 0, 50[%] )

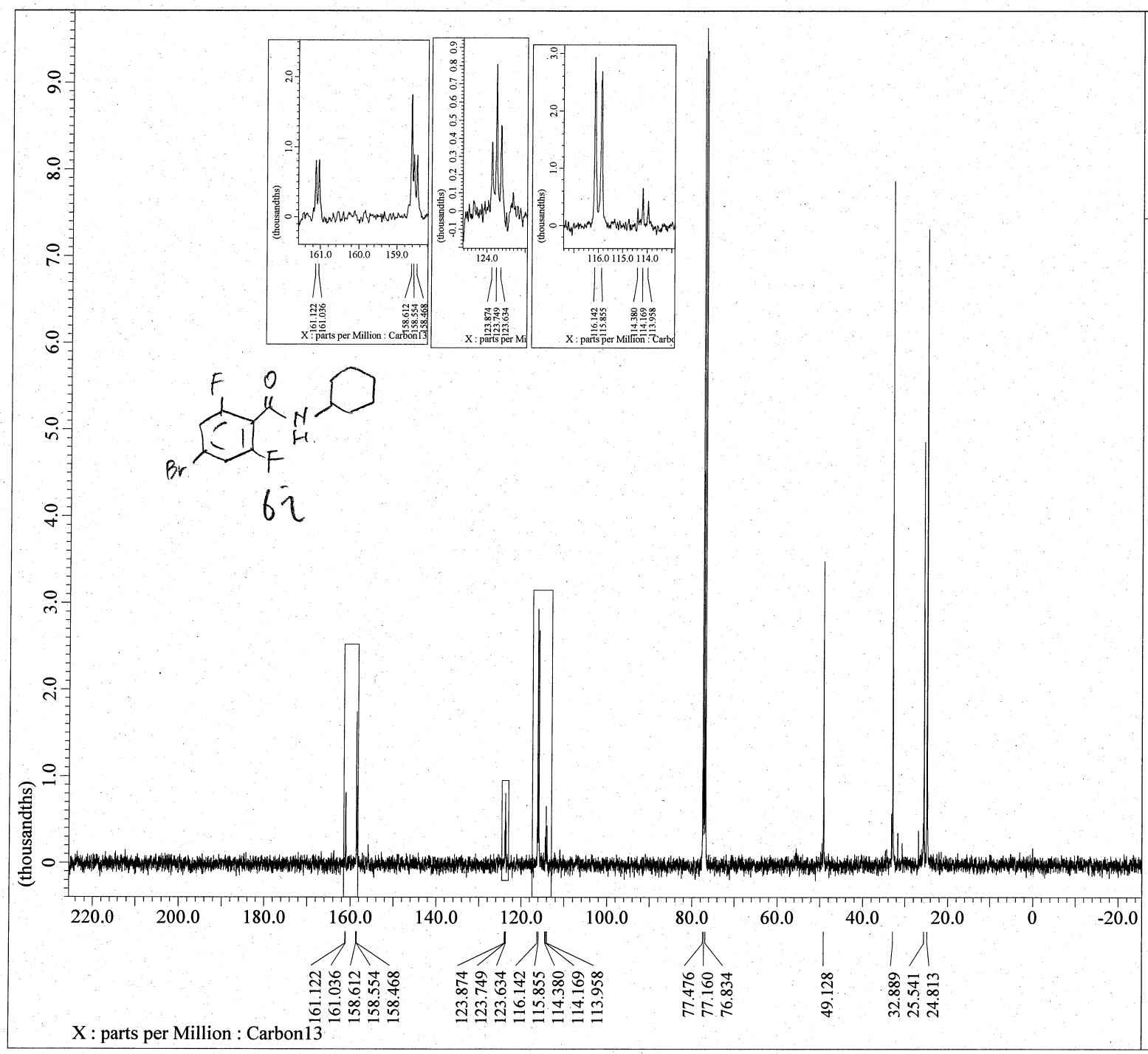
以下に由来:: TKH-1515_H_proton-1-1.jdf
```

```
Filename            = TKH-1515_H_proton-1-2.jdf
Author              = element
Experiment          = proton.jxp
Sample_Id           = TKH-1515_H
Solvent             = CHLOROFORM-D
Actual_Start_Time   = 14-MAR-2022 14:28:39
Revision_Time       = 14-MAR-2022 14:29:39

Comment             = single_pulse
Data_Format         = 1D COMPLEX
Dim_Size            = 13107
X_Domain            = Proton
Dim_Title           = Proton
Dim_Units           = [ppm]
Dimensions          = X
Spectrometer        = DELTA2_NMR

Field_Strength      = 9.4073814[T] (400[MHz])
X_Acq_Duration      = 2.18103808[s]
X_Domain            = 1H
X_Freq              = 400.53219825[MHz]
X_Offset            = 5[ppm]
X_Points            = 16384
X_Prescans          = 1
X_Resolution        = 0.45849727[Hz]
X_Sweep             = 7.51201923[kHz]
X_Sweep_Clipped     = 6.00961538[kHz]
Irr_Domain          = Proton
Irr_Freq            = 400.53219825[MHz]
Irr_Offset          = 5[ppm]
Tri_Domain          = Proton
Tri_Freq            = 400.53219825[MHz]
Tri_Offset          = 5[ppm]
Clipped             = FALSE
Scans               = 8
Total_Scans         = 8

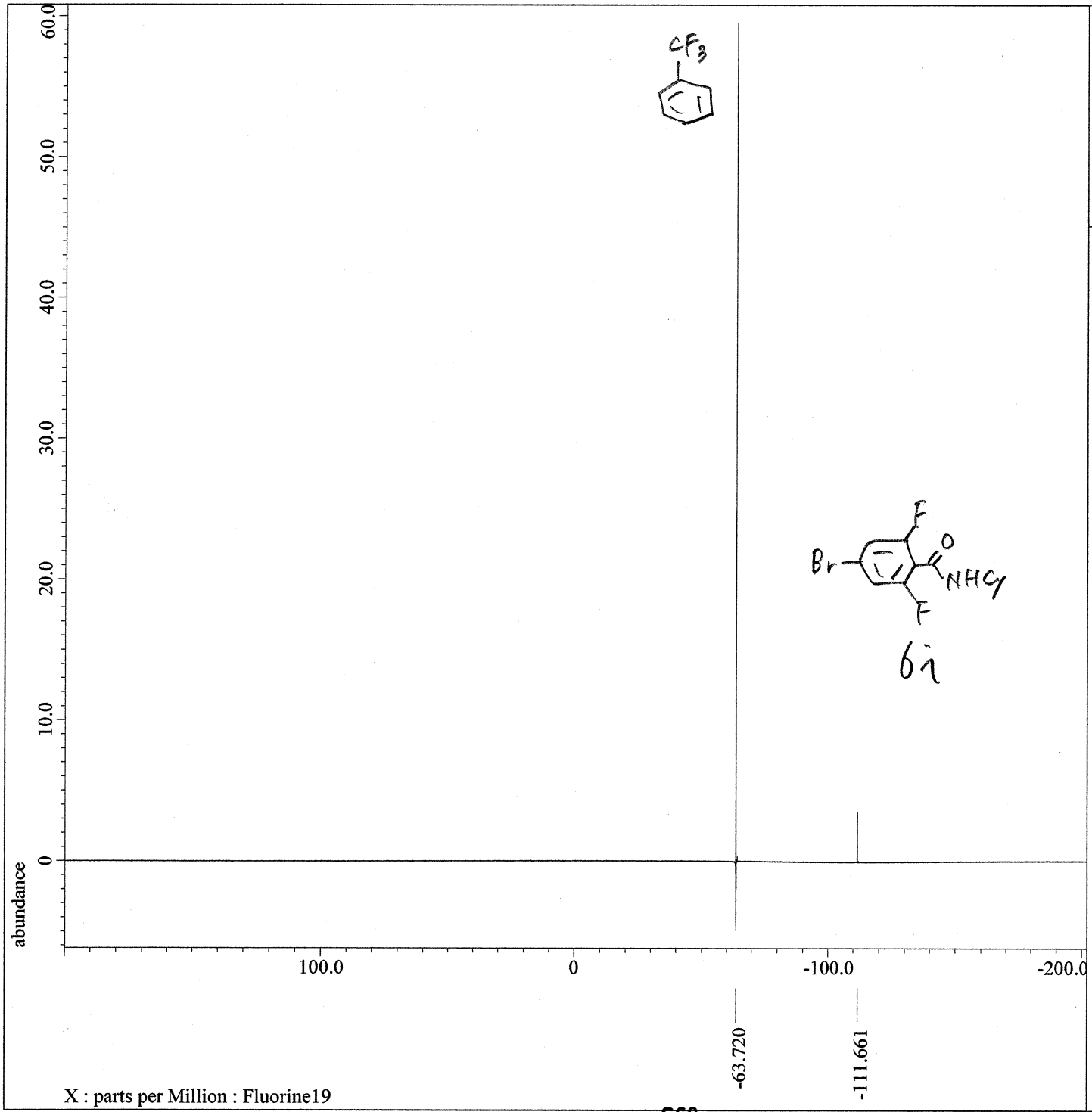
Relaxation_Delay    = 5[s]
Recvr_Gain          = 50
Temp_Get            = 18.8[dC]
X_90_Width          = 6[us]
X_Acq_Time          = 2.18103808[s]
X_Angle             = 45[deg]
X_Atn               = 0.8[dB]
X_Pulse             = 3[us]
Irr_Mode            = Off
Tri_Mode            = Off
Dante_Presat        = FALSE
Initial_Wait        = 1[s]
Repetition_Time     = 7.18103808[s]
```




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

以下に由来:: TKH-1515_carbon-1-1.jdf
```

Filename	= TKH-1515_carbon-1-
Author	= element
Experiment	= carbon.jxp
Sample_Id	= TKH-1515
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 9-MAR-2022 20:01:
Revision_Time	= 10-MAR-2022 20:36:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.2982153[T] (400[
X_Acq_Duration	= 1.048576[s]
X_Domain	= Carbon13
X_Freq	= 99.54517646[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.95367432[Hz]
X_Sweep	= 31.25[kHz]
X_Sweep_Clipped	= 25[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 5[us]
Clipped	= TRUE
Scans	= 400
Total_Scans	= 400
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 17.9[dC]
X_90_Width	= 9.65[us]
X_Acq_Time	= 1.048576[s]
X_Angle	= 30[deg]
X_Atn	= 8[dB]
X_Pulse	= 3.21666667[us]
Irr_Atn_Dec	= 25.059[dB]
Irr_Atn_Dec_Calc	= 25.059[dB]
Irr_Atn_Dec_Default_Calc	= 25.059[dB]
Irr_Atn_Noe	= 25.059[dB]
Irr_Dec_Bandwidth_Hz	= 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.08082432[ppm]
Irr_Dec_Freq	= 395.88430144[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]




```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
phase( 75, 0, 50[%] )

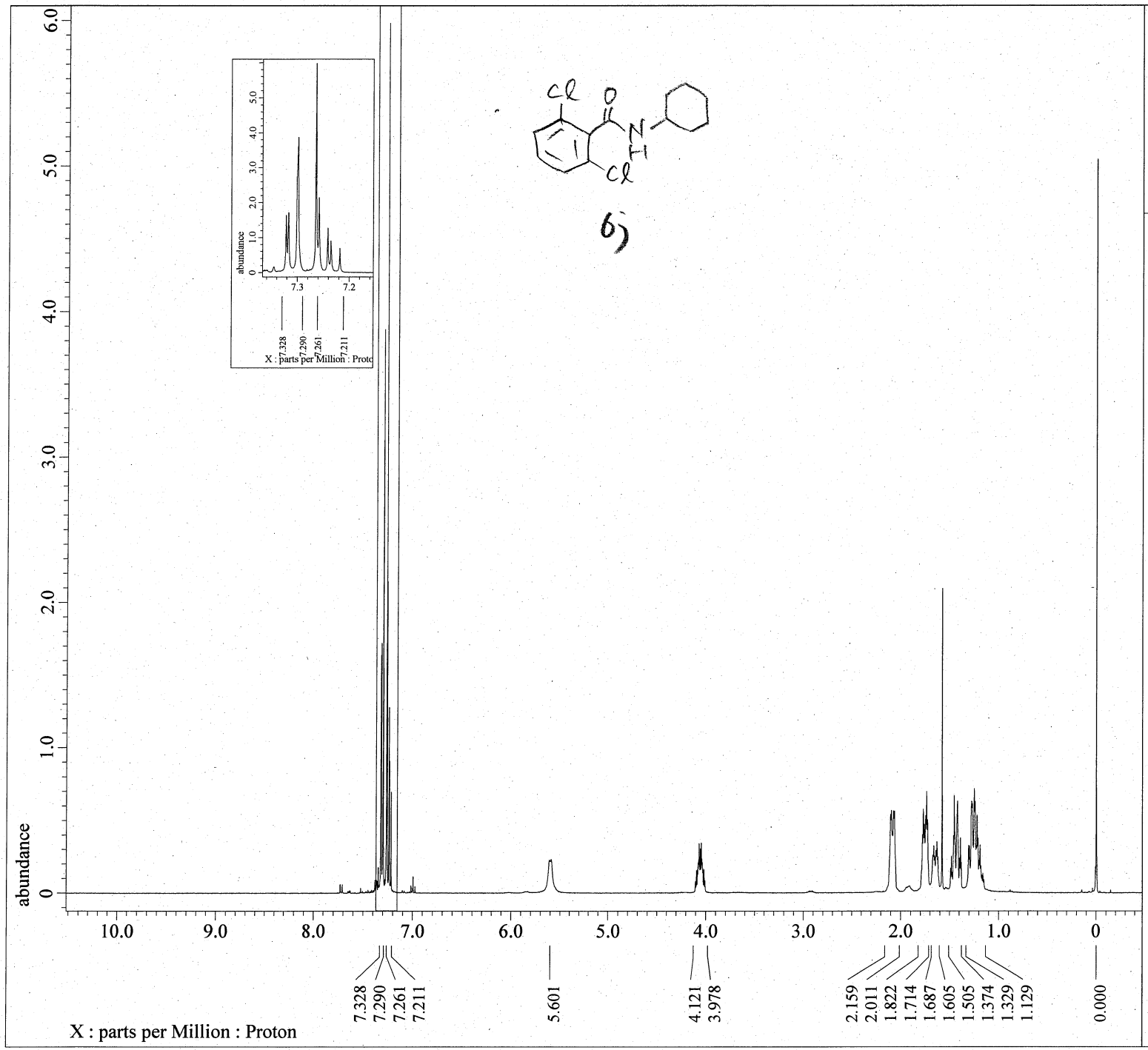
以下に由来:: TKH-1515_F_standard_single_pulse
```

```
Filename          = TKH-1515_F_standard_sing
Author            = element
Experiment        = single_pulse.jxp
Sample_Id         = TKH-1515_F_standard
Solvent           = CHLOROFORM-D
Creation_Time     =  5-MAR-2022 16:46:49
Revision_Time     =  5-MAR-2022 19:05:28
Current_Time      =  5-MAR-2022 19:05:32

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = Fluorine19
Dim_Units         = [ppm]
Dimensions        = X
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.4073814[T] (400[MHz])
X_Acq_Duration    = 86.50752[ms]
X_Domain          = 19F
X_Freq            = 376.87675879[MHz]
X_Offset          = 0[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 11.55968868[Hz]
X_Sweep           = 189.39393939[kHz]
X_Sweep_Clipped   = 151.51515152[kHz]
Irr_Domain        = Fluorine19
Irr_Freq          = 376.87675879[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = Fluorine19
Tri_Freq          = 376.87675879[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

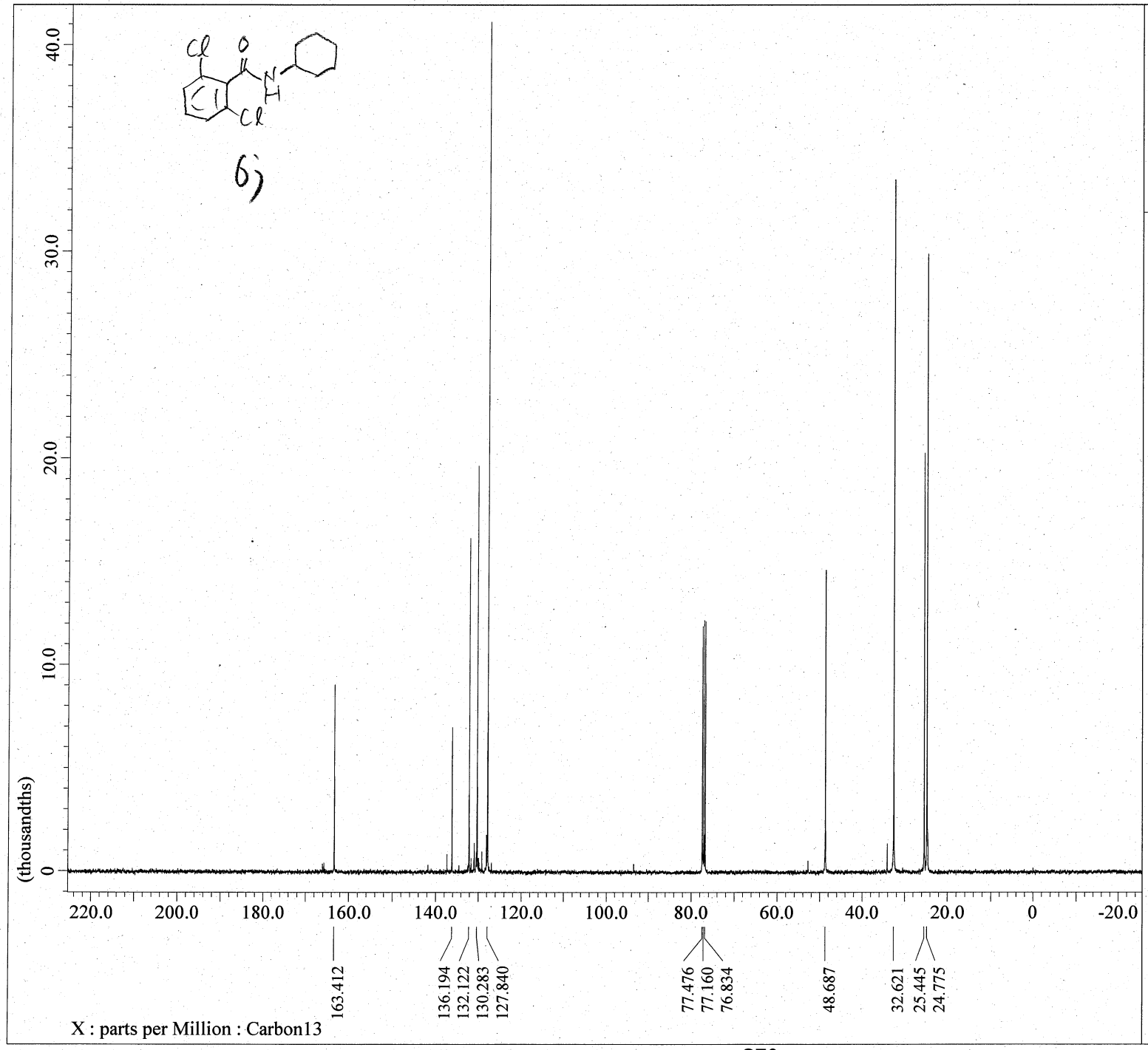
Relaxation_Delay = 5[s]
Recvr_Gain        = 44
Temp_Get          = 18.7[dC]
X_90_Width        = 6.8[us]
X_Acq_Time        = 86.50752[ms]
X_Angle           = 45[deg]
X_Atn             = 3[dB]
X_Pulse           = 3.4[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 5.08650752[s]
```




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

以下に由来:: TKH-1532column_Proton-1-1.jdf
```

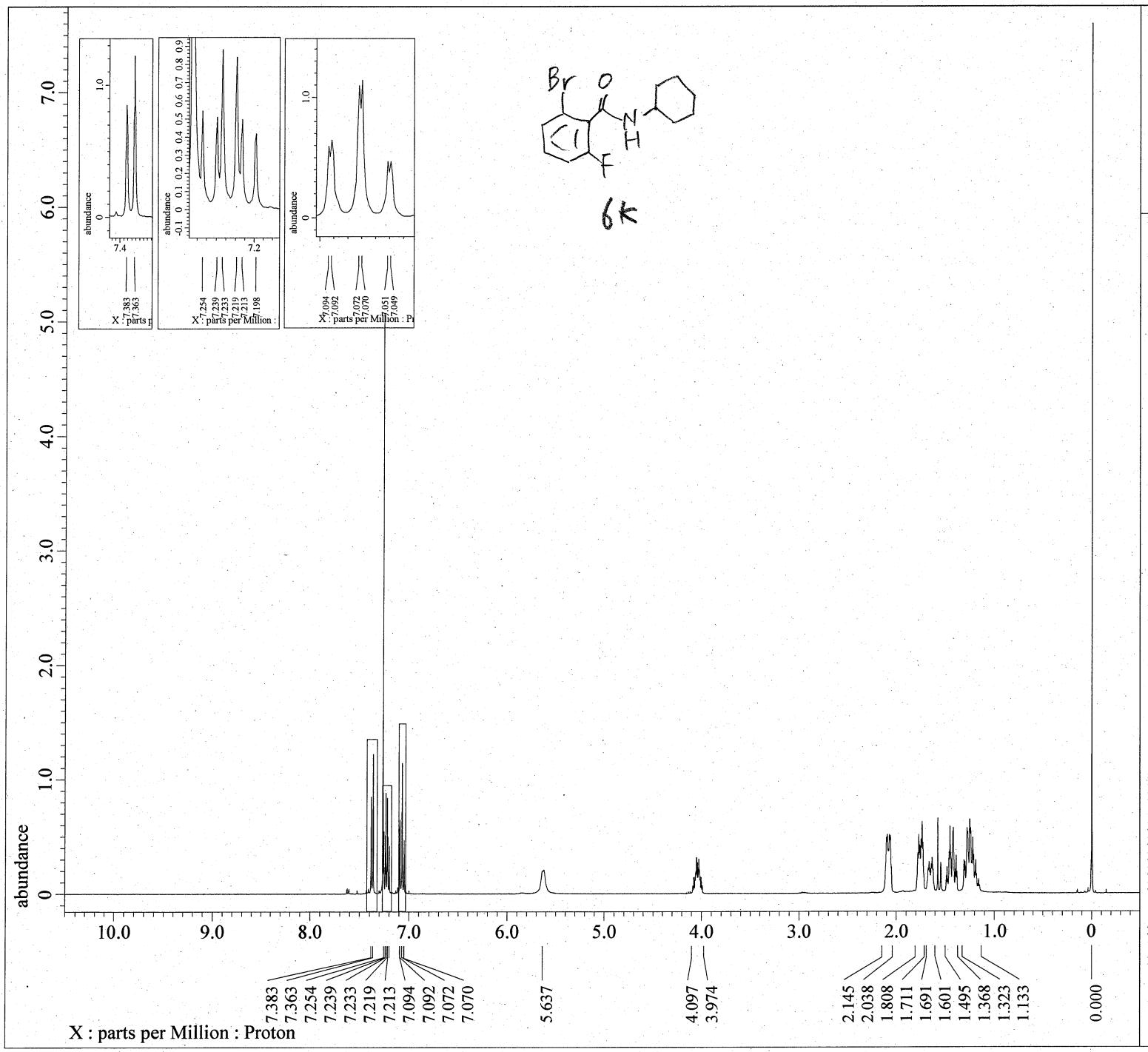
Filename	= TKH-1532column_Proton-1-2
Author	= element
Experiment	= proton.jxp
Sample_Id	= TKH-1532column
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 11-JAN-2022 20:26:52
Revision_Time	= 11-MAR-2022 13:06:31
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.4073814[T] (400[MHz])
X_Acq_Duration	= 2.18103808[s]
X_Domain	= 1H
X_Freq	= 400.53219825[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45849727[Hz]
X_Sweep	= 7.51201923[kHz]
X_Sweep_Clipped	= 6.00961538[kHz]
Irr_Domain	= Proton
Irr_Freq	= 400.53219825[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 400.53219825[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 48
Temp_Get	= 18.3[dC]
X_90_Width	= 6[us]
X_Acq_Time	= 2.18103808[s]
X_Angle	= 45[deg]
X_Atn	= 0.8[dB]
X_Pulse	= 3[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.18103808[s]




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

以下に由来:: TKH-1532_carbon-1-1.jdf
```

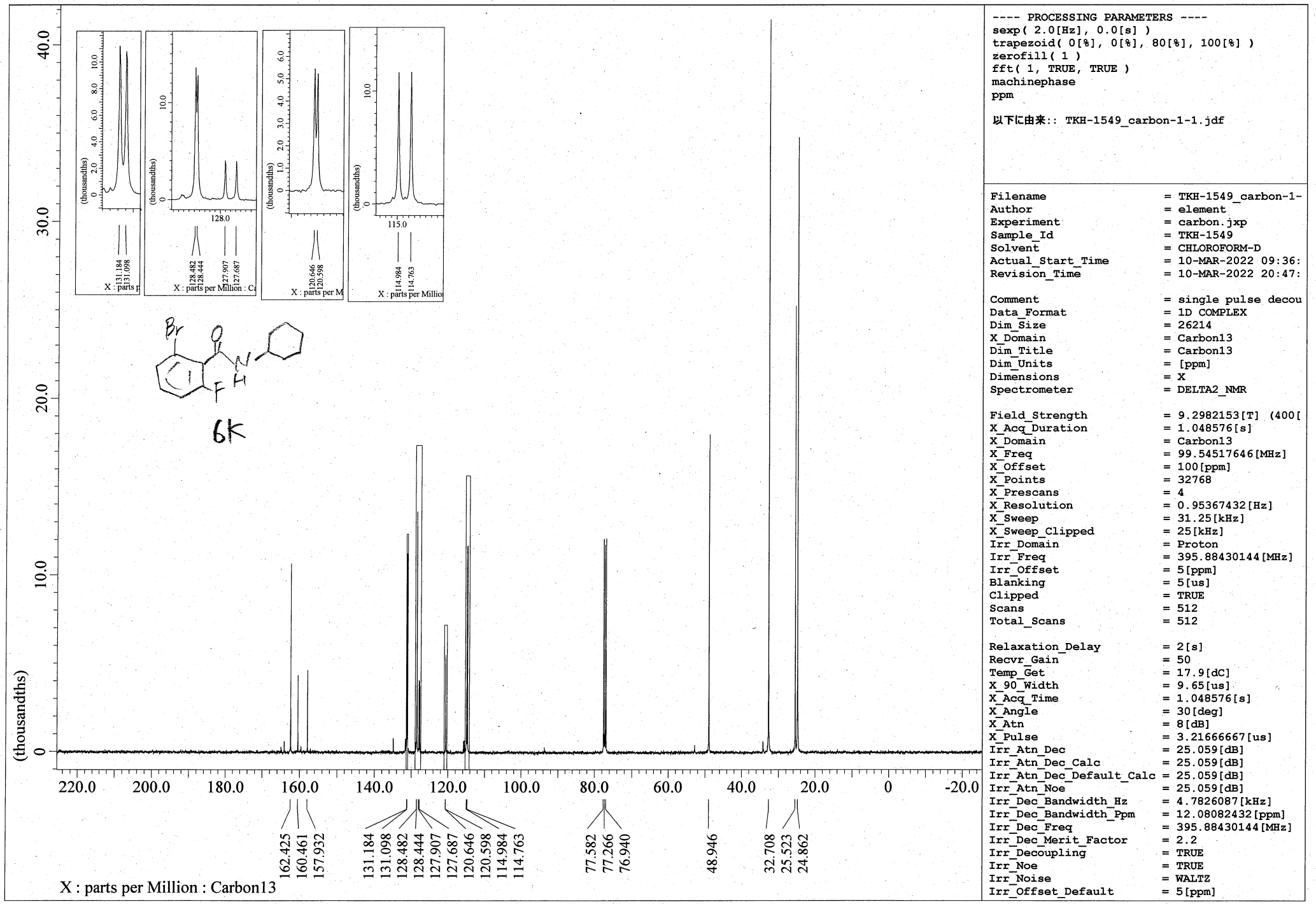
Filename	= TKH-1532_carbon-1-
Author	= element
Experiment	= carbon.jxp
Sample_Id	= TKH-1532
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 9-MAR-2022 20:29:
Revision_Time	= 10-MAR-2022 20:44:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.2982153[T] (400[
X_Acq_Duration	= 1.048576[s]
X_Domain	= Carbon13
X_Freq	= 99.54517646[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.95367432[Hz]
X_Sweep	= 31.25[kHz]
X_Sweep_Clipped	= 25[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 5[us]
Clipped	= TRUE
Scans	= 400
Total_Scans	= 400
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 17.9[dC]
X_90_Width	= 9.65[us]
X_Acq_Time	= 1.048576[s]
X_Angle	= 30[deg]
X_Atn	= 8[dB]
X_Pulse	= 3.21666667[us]
Irr_Atn_Dec	= 25.059[dB]
Irr_Atn_Dec_Calc	= 25.059[dB]
Irr_Atn_Dec_Default_Calc	= 25.059[dB]
Irr_Atn_Noe	= 25.059[dB]
Irr_Dec_Bandwidth_Hz	= 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.08082432[ppm]
Irr_Dec_Freq	= 395.88430144[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]

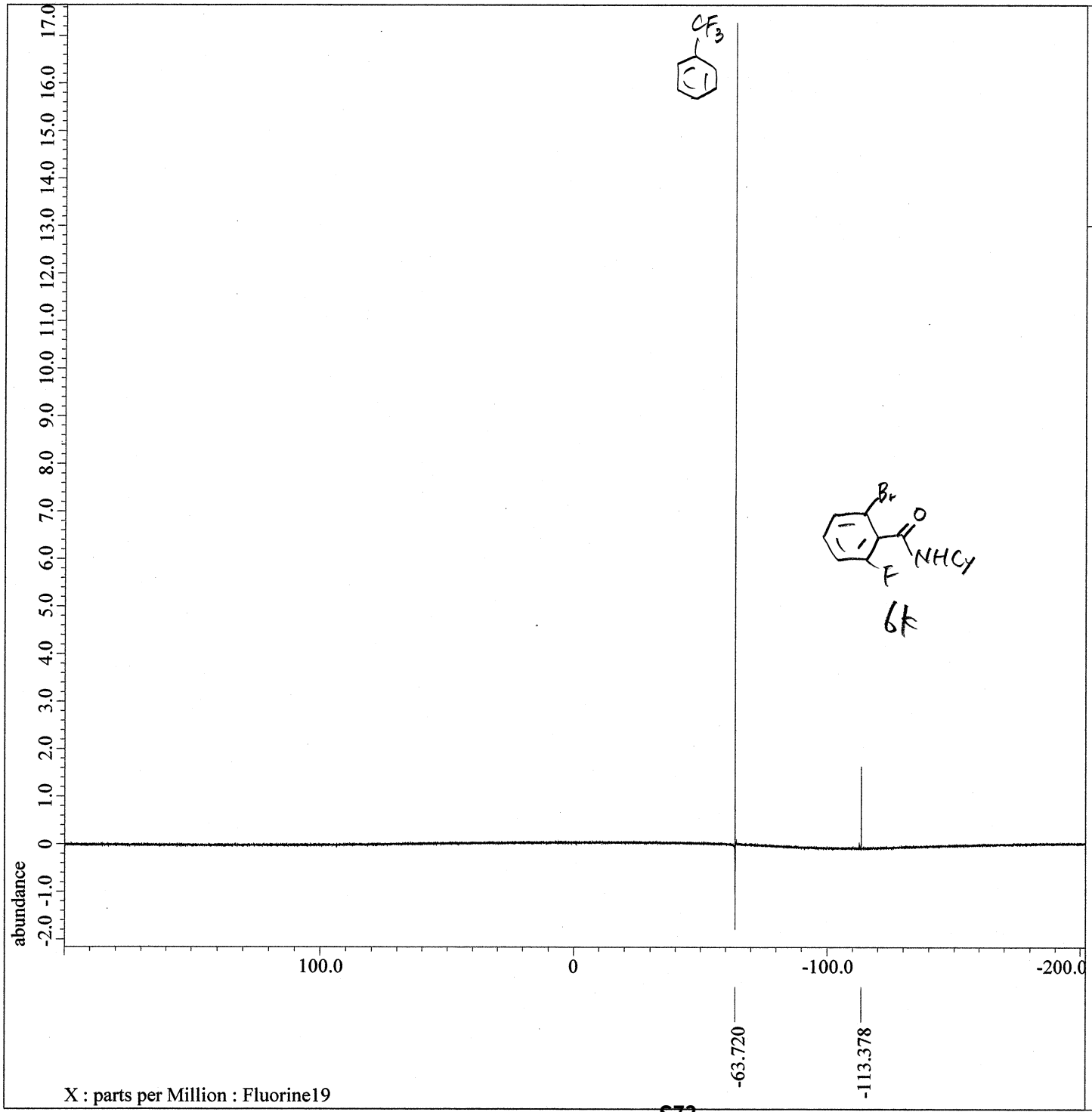



```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

以下に由来:: TKH-1549column_Proton-1-1.jdf
```

Filename	= TKH-1549column_Proton-1-2
Author	= element
Experiment	= proton.jxp
Sample_Id	= TKH-1549column
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 2-FEB-2022 19:40:07
Revision_Time	= 11-MAR-2022 13:11:45
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.4073814[T] (400[MHz])
X_Acq_Duration	= 2.18103808[s]
X_Domain	= 1H
X_Freq	= 400.53219825[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45849727[Hz]
X_Sweep	= 7.51201923[kHz]
X_Sweep_Clipped	= 6.00961538[kHz]
Irr_Domain	= Proton
Irr_Freq	= 400.53219825[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 400.53219825[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 46
Temp_Get	= 17.9[dC]
X_90_Width	= 6[us]
X_Acq_Time	= 2.18103808[s]
X_Angle	= 45[deg]
X_Atn	= 0.8[dB]
X_Pulse	= 3[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.18103808[s]


---- PROCESSING PARAMETERS ----
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
以下に由来:: TKH-1549_carbon-1-1.jdf
Filename = TKH-1549_carbon-1-
Author = element
Experiment = carbon.jxp
Sample_Id = TKH-1549
Solvent = CHLOROFORM-D
Actual_Start_Time = 10-MAR-2022 09:36:
Revision_Time = 10-MAR-2022 20:47:
Comment = single pulse decou
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = DELTA2_NMR
Field_Strength = 9.2982153[T] (400[
X_Acq_Duration = 1.048576[s]
X_Domain = Carbon13
X_Freq = 99.54517646[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95367432[Hz]
X_Sweep = 31.25[kHz]
X_Sweep_Clipped = 25[kHz]
Irr_Domain = Proton
Irr_Freq = 395.88430144[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = TRUE
Scans = 512
Total_Scans = 512
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 17.9[dC]
X_90_Width = 9.65[us]
X_Acq_Time = 1.048576[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 3.21666667[us]
Irr_Atn_Dec = 25.059[dB]
Irr_Atn_Dec_Calc = 25.059[dB]
Irr_Atn_Dec_Default_Calc = 25.059[dB]
Irr_Atn_Noe = 25.059[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm = 12.08082432[ppm]
Irr_Dec_Freq = 395.88430144[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
(thousandths)
X : parts per Million : Carbon13
162.425
160.461
157.932
131.184
131.098
128.482
128.444
127.907
127.687
120.646
120.598
114.984
114.763
77.582
77.266
76.940
48.946
32.708
25.523
24.862
6K




```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
phase( 61, 0, 50[%] )

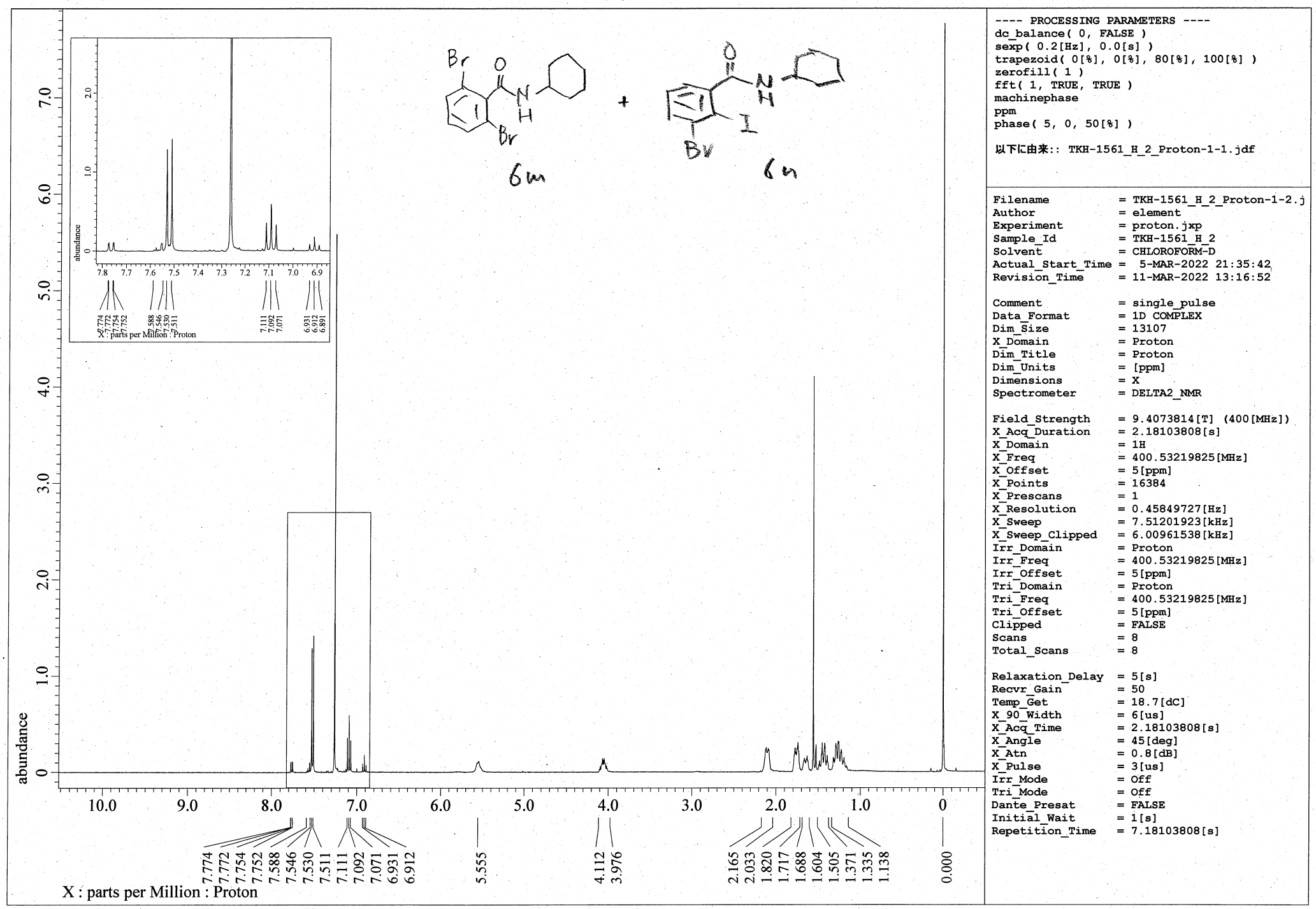
以下に由来:: TKH-1549_F_standard_single_pulse
```

```
Filename          = TKH-1549_F_standard_sinc
Author            = element
Experiment        = single_pulse.jxp
Sample_Id         = TKH-1549_F_standard
Solvent           = CHLOROFORM-D
Creation_Time     =  5-MAR-2022 16:38:05
Revision_Time     =  5-MAR-2022 19:06:15
Current_Time      =  5-MAR-2022 19:06:19

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = Fluorine19
Dim_Units         = [ppm]
Dimensions        = X
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.4073814[T] (400[MHz])
X_Acq_Duration    = 86.50752[ms]
X_Domain          = 19F
X_Freq            = 376.87675879[MHz]
X_Offset          = 0[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 11.55968868[Hz]
X_Sweep           = 189.39393939[kHz]
X_Sweep_Clipped   = 151.51515152[kHz]
Irr_Domain        = Fluorine19
Irr_Freq          = 376.87675879[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = Fluorine19
Tri_Freq          = 376.87675879[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay = 5[s]
Recvr_Gain        = 46
Temp_Get          = 18.9[dC]
X_90_Width        = 6.8[us]
X_Acq_Time        = 86.50752[ms]
X_Angle           = 45[deg]
X_Atn             = 3[dB]
X_Pulse           = 3.4[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 5.08650752[s]
```




```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
phase( 5, 0, 50[%] )

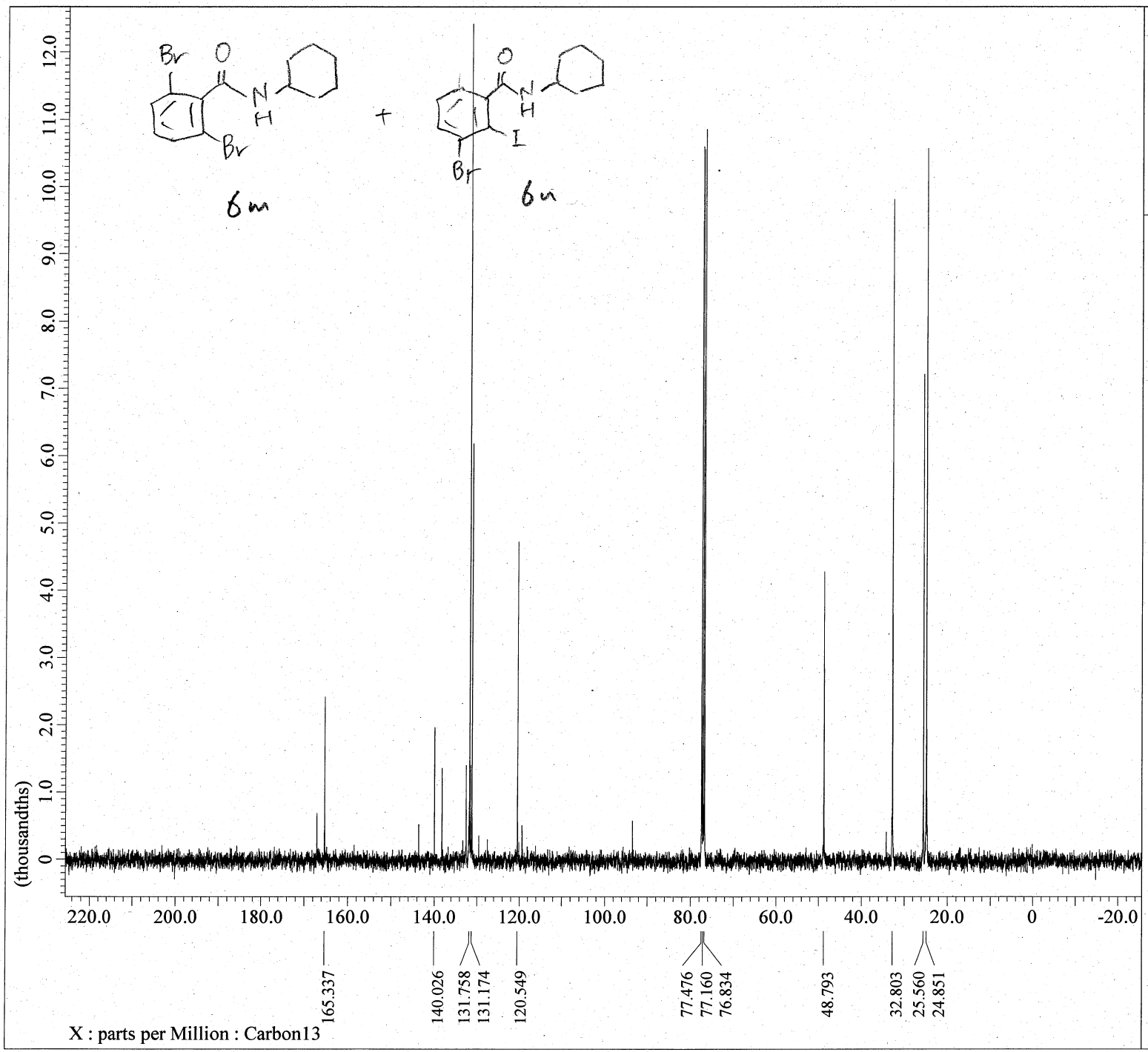
以下に由来:: TKH-1561_H_2_Proton-1-1.jdf
```

```
Filename            = TKH-1561_H_2_Proton-1-2.j
Author              = element
Experiment          = proton.jxp
Sample_Id           = TKH-1561_H_2
Solvent             = CHLOROFORM-D
Actual_Start_Time   =  5-MAR-2022 21:35:42
Revision_Time       = 11-MAR-2022 13:16:52

Comment             = single_pulse
Data_Format         = 1D COMPLEX
Dim_Size            = 13107
X_Domain            = Proton
Dim_Title           = Proton
Dim_Units           = [ppm]
Dimensions          = X
Spectrometer        = DELTA2_NMR

Field_Strength      = 9.4073814[T] (400[MHz])
X_Acq_Duration      = 2.18103808[s]
X_Domain            = 1H
X_Freq              = 400.53219825[MHz]
X_Offset            = 5[ppm]
X_Points            = 16384
X_Prescans          = 1
X_Resolution        = 0.45849727[Hz]
X_Sweep             = 7.51201923[kHz]
X_Sweep_Clipped     = 6.00961538[kHz]
Irr_Domain          = Proton
Irr_Freq            = 400.53219825[MHz]
Irr_Offset          = 5[ppm]
Tri_Domain          = Proton
Tri_Freq            = 400.53219825[MHz]
Tri_Offset          = 5[ppm]
Clipped             = FALSE
Scans               = 8
Total_Scans         = 8

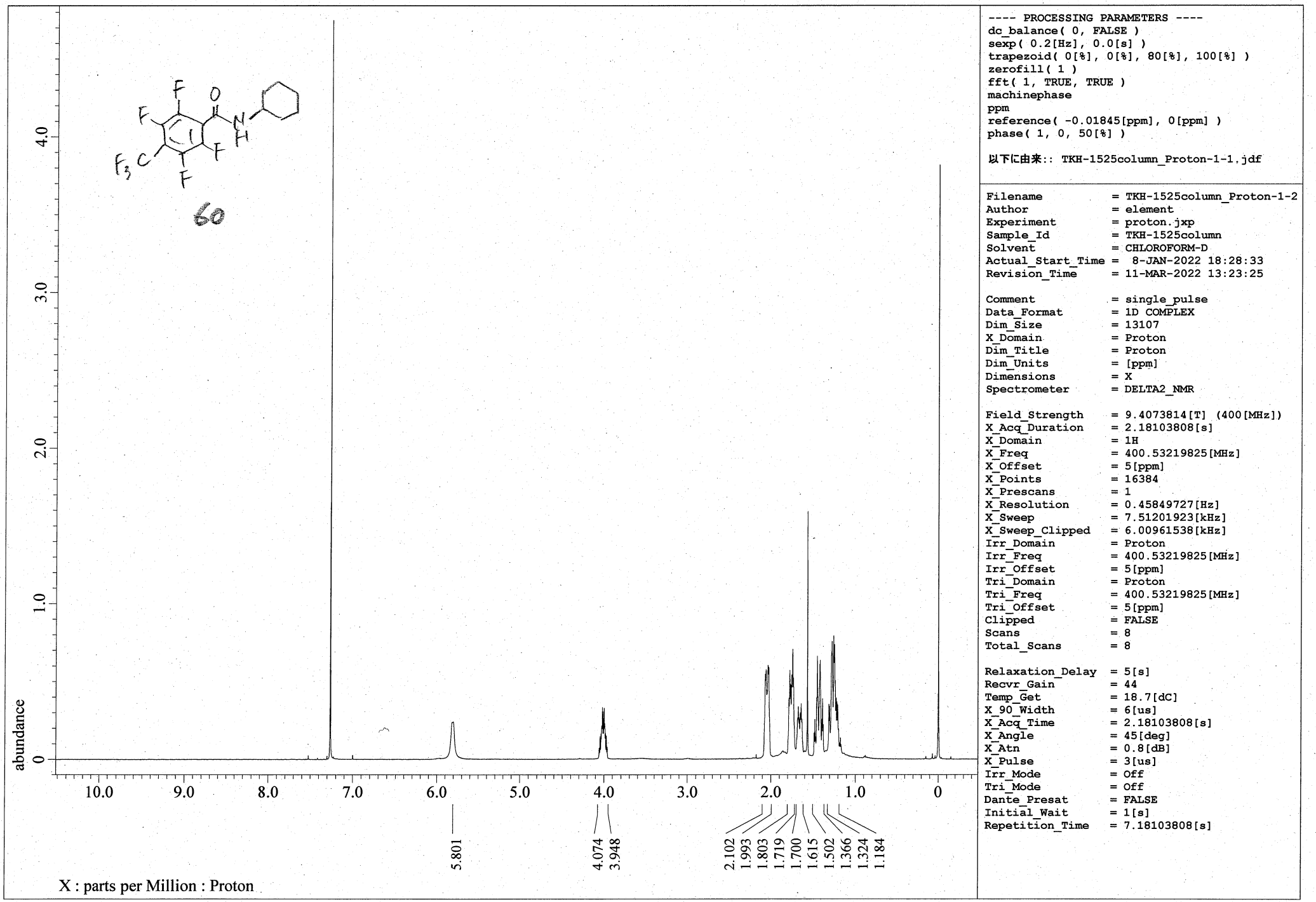
Relaxation_Delay    = 5[s]
Recvr_Gain          = 50
Temp_Get            = 18.7[dC]
X_90_Width          = 6[us]
X_Acq_Time          = 2.18103808[s]
X_Angle             = 45[deg]
X_Atn               = 0.8[dB]
X_Pulse             = 3[us]
Irr_Mode            = Off
Tri_Mode            = Off
Dante_Presat        = FALSE
Initial_Wait        = 1[s]
Repetition_Time     = 7.18103808[s]
```




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

以下に由来:: TKH-1561_carbon-1-1.jdf
```

Filename	= TKH-1561_carbon-1-
Author	= element
Experiment	= carbon.jxp
Sample_Id	= TKH-1561
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 10-MAR-2022 09:19:
Revision_Time	= 10-MAR-2022 20:57:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.2982153[T] (400[
X_Acq_Duration	= 1.048576[s]
X_Domain	= Carbon13
X_Freq	= 99.54517646[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.95367432[Hz]
X_Sweep	= 31.25[kHz]
X_Sweep_Clipped	= 25[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 5[us]
Clipped	= TRUE
Scans	= 200
Total_Scans	= 200
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 17.8[dC]
X_90_Width	= 9.65[us]
X_Acq_Time	= 1.048576[s]
X_Angle	= 30[deg]
X_Atn	= 8[dB]
X_Pulse	= 3.21666667[us]
Irr_Atn_Dec	= 25.059[dB]
Irr_Atn_Dec_Calc	= 25.059[dB]
Irr_Atn_Dec_Default_Calc	= 25.059[dB]
Irr_Atn_Noe	= 25.059[dB]
Irr_Dec_Bandwidth_Hz	= 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.08082432[ppm]
Irr_Dec_Freq	= 395.88430144[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]




```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
reference( -0.01845[ppm], 0[ppm] )
phase( 1, 0, 50[%] )

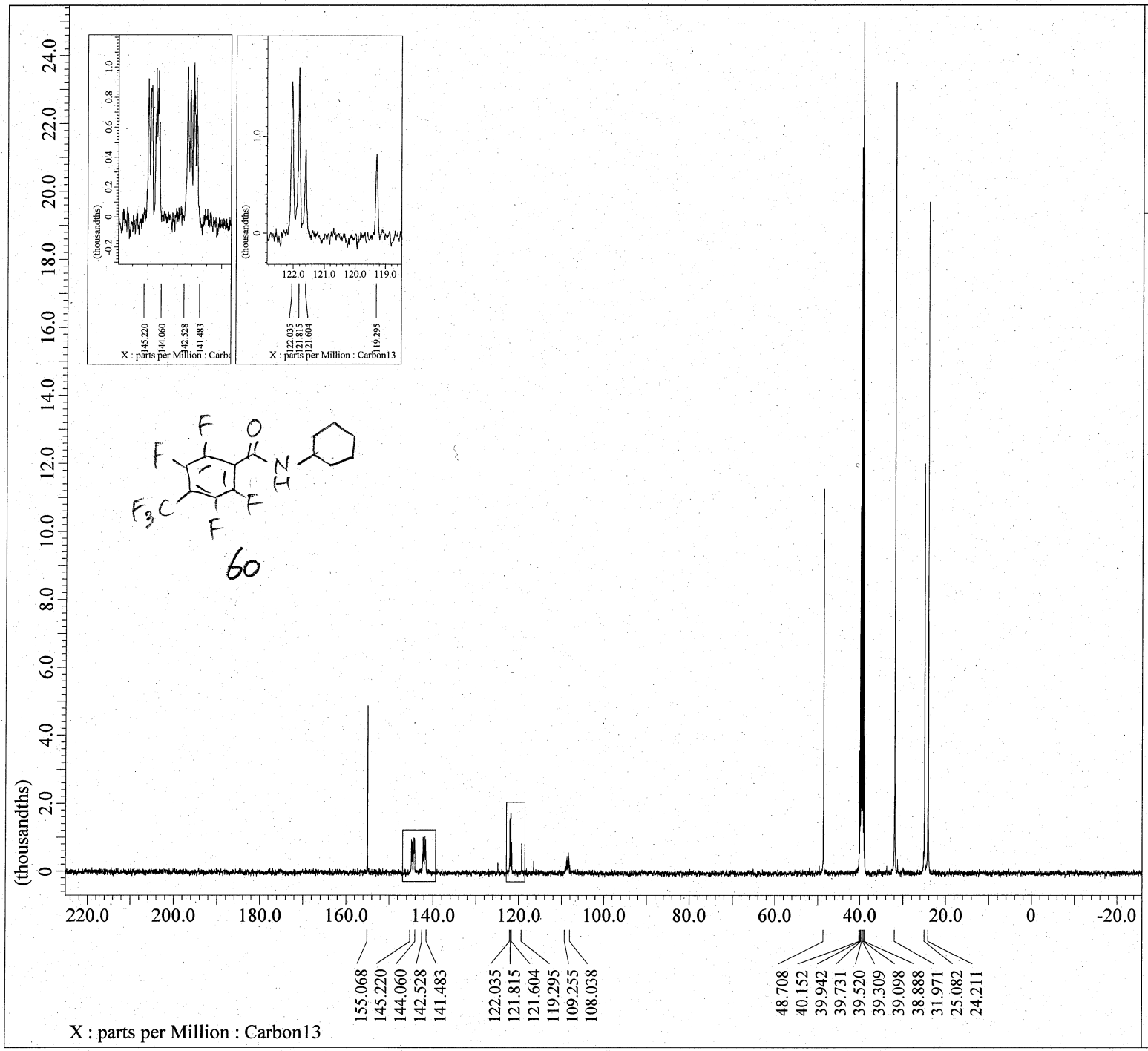
以下に由来:: TKH-1525column_Proton-1-1.jdf

Filename           = TKH-1525column_Proton-1-2
Author             = element
Experiment         = proton.jxp
Sample_Id          = TKH-1525column
Solvent            = CHLOROFORM-D
Actual_Start_Time  =  8-JAN-2022 18:28:33
Revision_Time      = 11-MAR-2022 13:23:25

Comment            = single_pulse
Data_Format        = 1D COMPLEX
Dim_Size           = 13107
X_Domain           = Proton
Dim_Title          = Proton
Dim_Units          = [ppm]
Dimensions         = X
Spectrometer       = DELTA2_NMR

Field_Strength     = 9.4073814[T] (400[MHz])
X_Acq_Duration     = 2.18103808[s]
X_Domain           = 1H
X_Freq             = 400.53219825[MHz]
X_Offset           = 5[ppm]
X_Points           = 16384
X_Prescans         = 1
X_Resolution       = 0.45849727[Hz]
X_Sweep            = 7.51201923[kHz]
X_Sweep_Clipped    = 6.00961538[kHz]
Irr_Domain         = Proton
Irr_Freq           = 400.53219825[MHz]
Irr_Offset         = 5[ppm]
Tri_Domain         = Proton
Tri_Freq           = 400.53219825[MHz]
Tri_Offset         = 5[ppm]
Clipped            = FALSE
Scans              = 8
Total_Scans        = 8

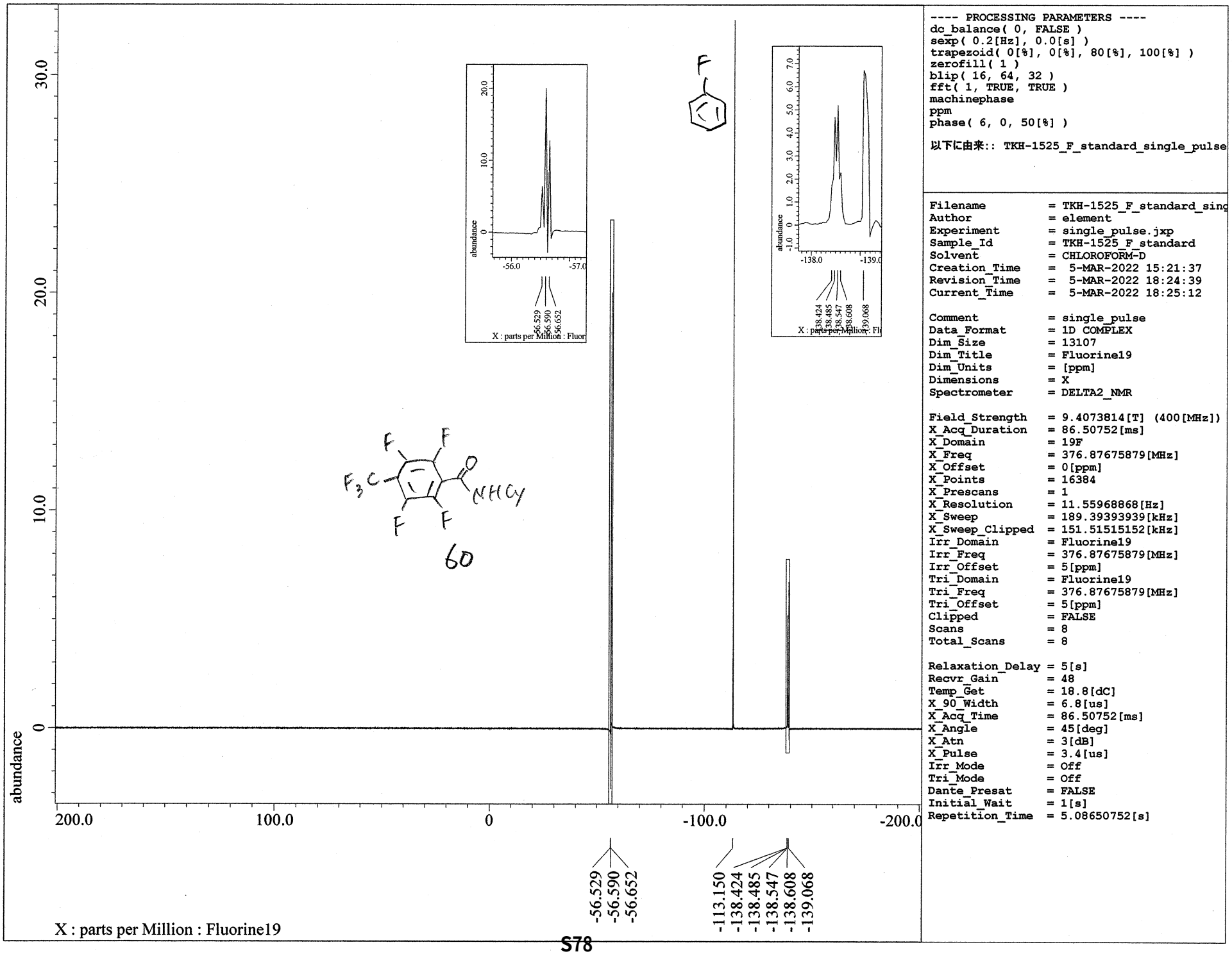
Relaxation_Delay   = 5[s]
Recvr_Gain         = 44
Temp_Get           = 18.7[dC]
X_90_Width         = 6[us]
X_Acq_Time         = 2.18103808[s]
X_Angle            = 45[deg]
X_Atn              = 0.8[dB]
X_Pulse            = 3[us]
Irr_Mode           = Off
Tri_Mode           = Off
Dante_Presat       = FALSE
Initial_Wait       = 1[s]
Repetition_Time    = 7.18103808[s]
```




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

以下に由来:: TKH-1525_DMSO_carbon-1-1.jdf
```

Filename	= TKH-1525_DMSO_carb
Author	= element
Experiment	= carbon.jxp
Sample_Id	= TKH-1525_DMSO
Solvent	= DMSO-D6
Actual_Start_Time	= 16-MAR-2022 21:20:
Revision_Time	= 17-MAR-2022 09:09:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.2982153[T] (400[
X_Acq_Duration	= 1.048576[s]
X_Domain	= Carbon13
X_Freq	= 99.54517646[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.95367432[Hz]
X_Sweep	= 31.25[kHz]
X_Sweep_Clipped	= 25[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 5[us]
Clipped	= TRUE
Scans	= 512
Total_Scans	= 512
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 19.4[dC]
X_90_Width	= 9.65[us]
X_Acq_Time	= 1.048576[s]
X_Angle	= 30[deg]
X_Atn	= 8[dB]
X_Pulse	= 3.21666667[us]
Irr_Atn_Dec	= 25.059[dB]
Irr_Atn_Dec_Calc	= 25.059[dB]
Irr_Atn_Dec_Default_Calc	= 25.059[dB]
Irr_Atn_Noe	= 25.059[dB]
Irr_Dec_Bandwidth_Hz	= 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.08082432[ppm]
Irr_Dec_Freq	= 395.88430144[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]




```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
blip( 16, 64, 32 )
fft( 1, TRUE, TRUE )
machinephase
ppm
phase( 6, 0, 50[%] )

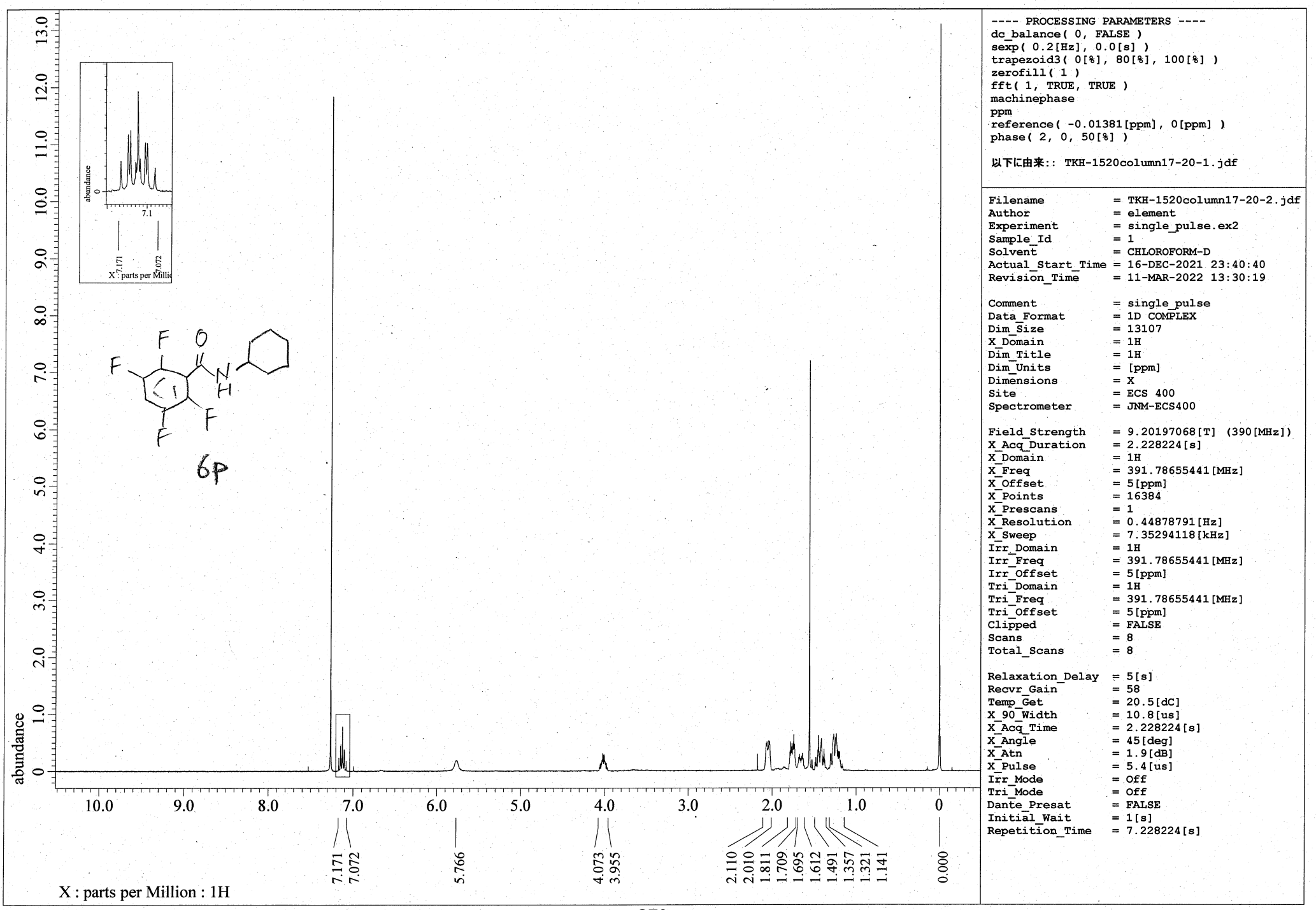
以下に由来:: TKH-1525_F_standard_single_pulse
```

```
Filename          = TKH-1525_F_standard_sing
Author            = element
Experiment        = single_pulse.jxp
Sample_Id         = TKH-1525_F_standard
Solvent           = CHLOROFORM-D
Creation_Time     =  5-MAR-2022 15:21:37
Revision_Time     =  5-MAR-2022 18:24:39
Current_Time      =  5-MAR-2022 18:25:12

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
Dim_Title         = Fluorine19
Dim_Units         = [ppm]
Dimensions        = X
Spectrometer      = DELTA2_NMR

Field_Strength    = 9.4073814[T] (400[MHz])
X_Acq_Duration    = 86.50752[ms]
X_Domain          = 19F
X_Freq            = 376.87675879[MHz]
X_Offset          = 0[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 11.55968868[Hz]
X_Sweep           = 189.39393939[kHz]
X_Sweep_Clipped   = 151.51515152[kHz]
Irr_Domain        = Fluorine19
Irr_Freq          = 376.87675879[MHz]
Irr_Offset        = 5[ppm]
Tri_Domain        = Fluorine19
Tri_Freq          = 376.87675879[MHz]
Tri_Offset        = 5[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay = 5[s]
Recvr_Gain        = 48
Temp_Get          = 18.8[dC]
X_90_Width        = 6.8[us]
X_Acq_Time        = 86.50752[ms]
X_Angle           = 45[deg]
X_Atn             = 3[dB]
X_Pulse           = 3.4[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 5.08650752[s]
```




```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
reference( -0.01381[ppm], 0[ppm] )
phase( 2, 0, 50[%] )

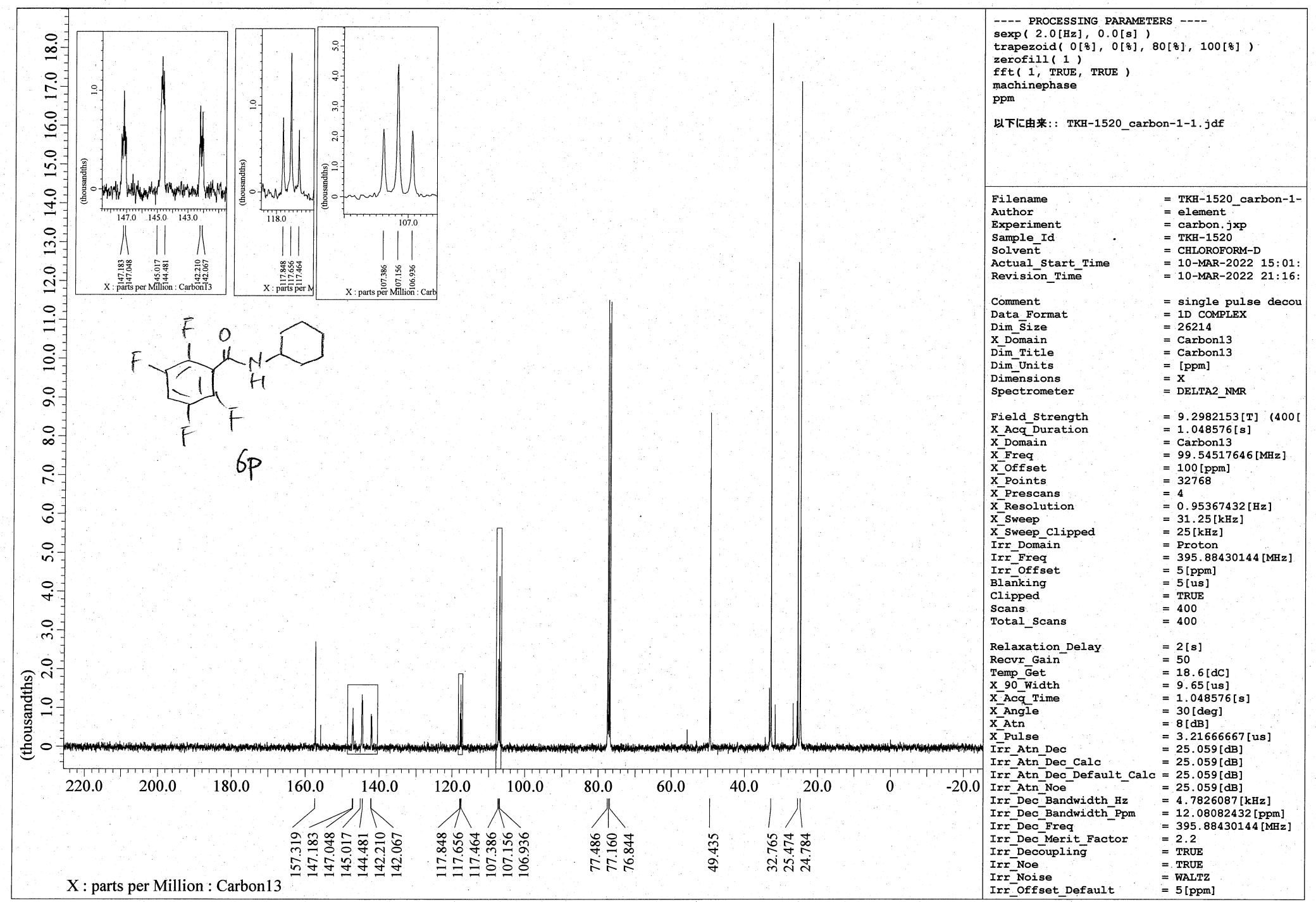
以下に由来:: TKH-1520column17-20-1.jdf
```

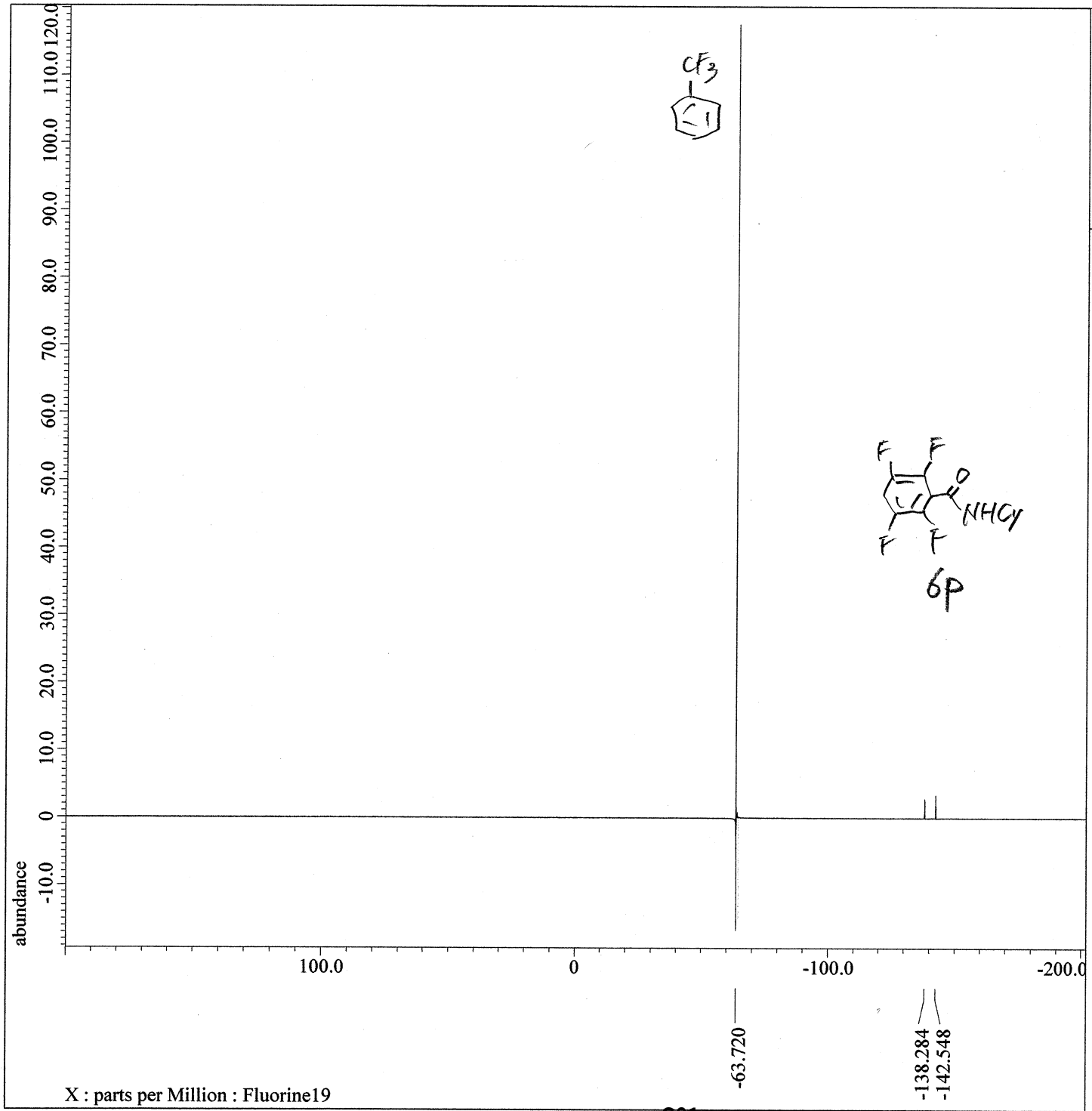
```
Filename            = TKH-1520column17-20-2.jdf
Author              = element
Experiment          = single_pulse.ex2
Sample_Id           = 1
Solvent             = CHLOROFORM-D
Actual_Start_Time   = 16-DEC-2021 23:40:40
Revision_Time       = 11-MAR-2022 13:30:19

Comment             = single_pulse
Data_Format         = 1D COMPLEX
Dim_Size            = 13107
X_Domain            = 1H
Dim_Title           = 1H
Dim_Units           = [ppm]
Dimensions          = X
Site                = ECS 400
Spectrometer        = JNM-ECS400

Field_Strength      = 9.20197068[T] (390[MHz])
X_Acq_Duration      = 2.228224[s]
X_Domain            = 1H
X_Freq              = 391.78655441[MHz]
X_Offset            = 5[ppm]
X_Points            = 16384
X_Prescans          = 1
X_Resolution        = 0.44878791[Hz]
X_Sweep             = 7.35294118[kHz]
Irr_Domain          = 1H
Irr_Freq            = 391.78655441[MHz]
Irr_Offset          = 5[ppm]
Tri_Domain          = 1H
Tri_Freq            = 391.78655441[MHz]
Tri_Offset          = 5[ppm]
Clipped             = FALSE
Scans               = 8
Total_Scans         = 8

Relaxation_Delay    = 5[s]
Recvr_Gain          = 58
Temp_Get            = 20.5[dC]
X_90_Width          = 10.8[us]
X_Acq_Time          = 2.228224[s]
X_Angle             = 45[deg]
X_Atn               = 1.9[dB]
X_Pulse             = 5.4[us]
Irr_Mode            = Off
Tri_Mode            = Off
Dante_Presat        = FALSE
Initial_Wait        = 1[s]
Repetition_Time     = 7.228224[s]
```

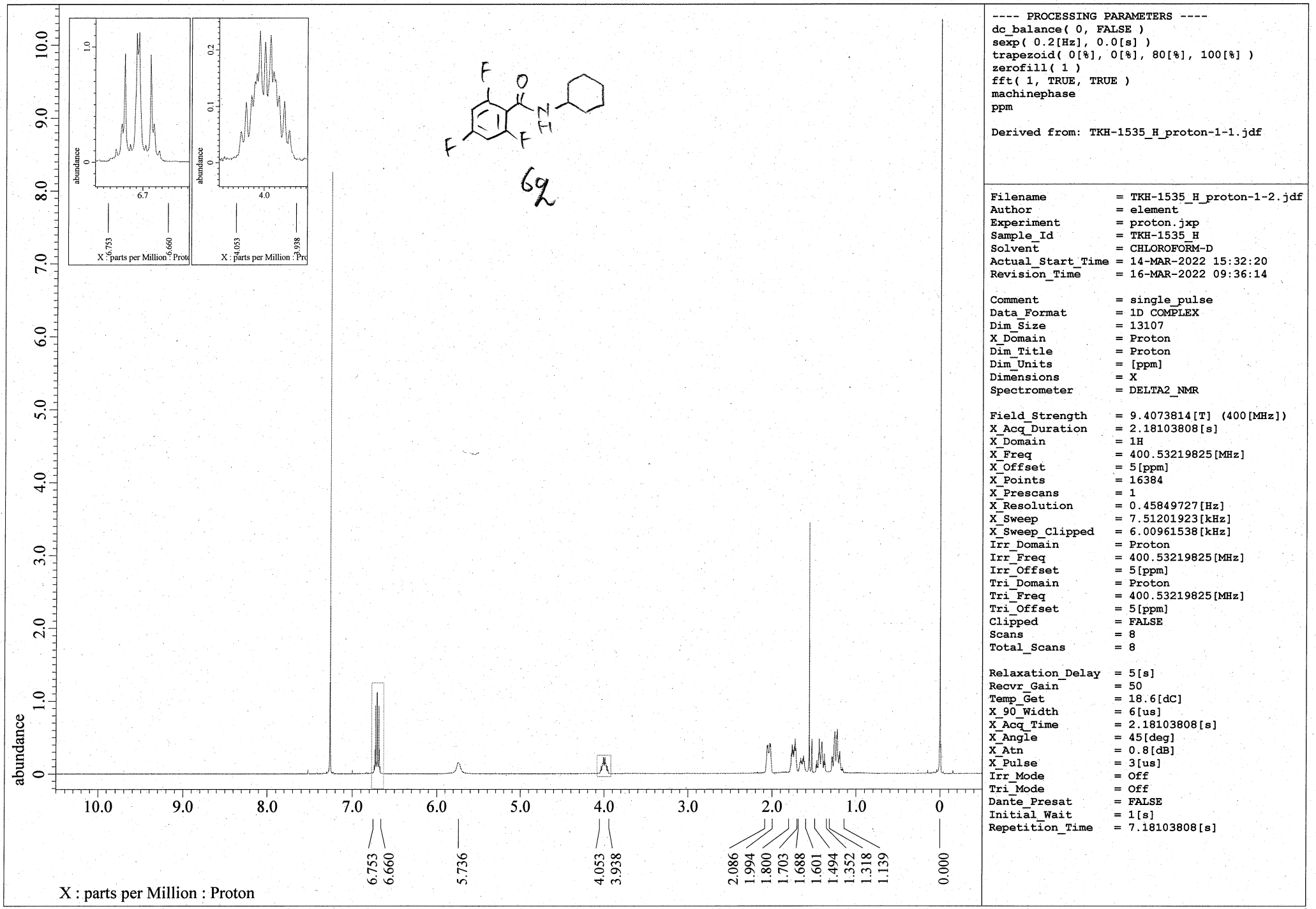

---- PROCESSING PARAMETERS ----
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
以下に由来:: TKH-1520_carbon-1-1.jdf
Filename = TKH-1520_carbon-1-
Author = element
Experiment = carbon.jxp
Sample_Id = TKH-1520
Solvent = CHLOROFORM-D
Actual_Start_Time = 10-MAR-2022 15:01:
Revision_Time = 10-MAR-2022 21:16:
Comment = single pulse decou
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = DELTA2_NMR
Field_Strength = 9.2982153[T] (400[
X_Acq_Duration = 1.048576[s]
X_Domain = Carbon13
X_Freq = 99.54517646[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95367432[Hz]
X_Sweep = 31.25[kHz]
X_Sweep_Clipped = 25[kHz]
Irr_Domain = Proton
Irr_Freq = 395.88430144[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = TRUE
Scans = 400
Total_Scans = 400
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 18.6[dC]
X_90_Width = 9.65[us]
X_Acq_Time = 1.048576[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 3.21666667[us]
Irr_Atn_Dec = 25.059[dB]
Irr_Atn_Dec_Calc = 25.059[dB]
Irr_Atn_Dec_Default_Calc = 25.059[dB]
Irr_Atn_Noe = 25.059[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm = 12.08082432[ppm]
Irr_Dec_Freq = 395.88430144[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
(thousandths)
X : parts per Million : Carbon13
157.319
147.183
147.048
145.017
144.481
142.210
142.067
117.848
117.656
117.464
107.386
107.156
106.936
77.486
77.160
76.844
49.435
32.765
25.474
24.784
6P




```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
blip( 16, 64, 32 )
fft( 1, TRUE, TRUE )
machinephase
ppm
phase( 14, 0, 50[%] )

以下に由来:: TKH-1520_F_standard_single_pulse
```

Filename	= TKH-1520_F_standard_sing
Author	= element
Experiment	= single_pulse.jxp
Sample_Id	= TKH-1520_F_standard
Solvent	= CHLOROFORM-D
Creation_Time	= 5-MAR-2022 15:29:14
Revision_Time	= 5-MAR-2022 18:22:26
Current_Time	= 5-MAR-2022 18:22:30
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
Dim_Title	= Fluorine19
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.4073814[T] (400[MHz])
X_Acq_Duration	= 86.50752[ms]
X_Domain	= 19F
X_Freq	= 376.87675879[MHz]
X_Offset	= 0[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 11.55968868[Hz]
X_Sweep	= 189.39393939[kHz]
X_Sweep_Clipped	= 151.51515152[kHz]
Irr_Domain	= Fluorine19
Irr_Freq	= 376.87675879[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Fluorine19
Tri_Freq	= 376.87675879[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 46
Temp_Get	= 18.8[dC]
X_90_Width	= 6.8[us]
X_Acq_Time	= 86.50752[ms]
X_Angle	= 45[deg]
X_Atn	= 3[dB]
X_Pulse	= 3.4[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 5.08650752[s]




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

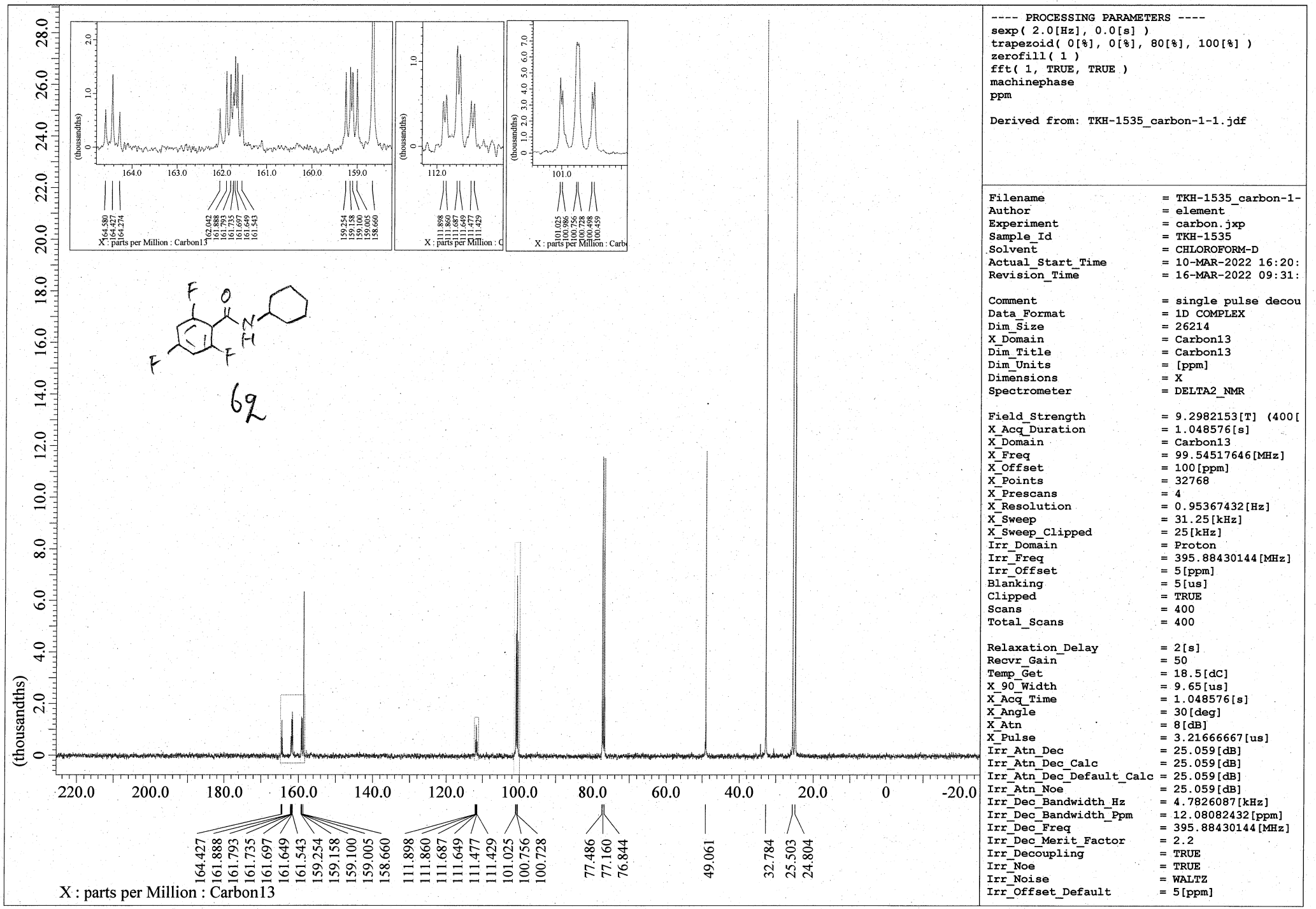
Derived from: TKH-1535_H_proton-1-1.jdf
```

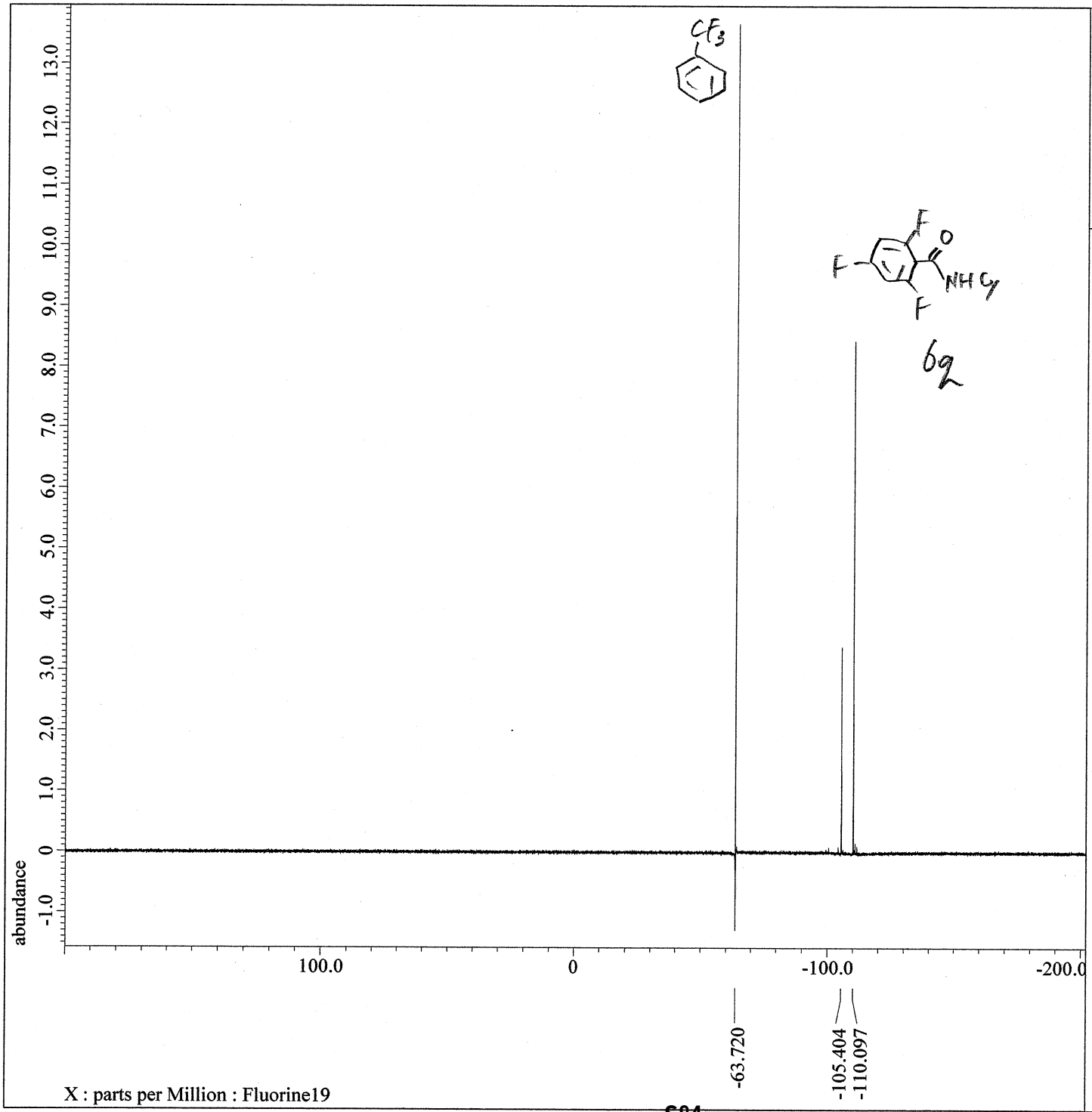
```
Filename            = TKH-1535_H_proton-1-2.jdf
Author              = element
Experiment          = proton.jxp
Sample_Id           = TKH-1535_H
Solvent             = CHLOROFORM-D
Actual_Start_Time   = 14-MAR-2022 15:32:20
Revision_Time       = 16-MAR-2022 09:36:14

Comment             = single_pulse
Data_Format         = 1D COMPLEX
Dim_Size            = 13107
X_Domain            = Proton
Dim_Title           = Proton
Dim_Units           = [ppm]
Dimensions          = X
Spectrometer        = DELTA2_NMR

Field_Strength      = 9.4073814[T] (400[MHz])
X_Acq_Duration      = 2.18103808[s]
X_Domain            = 1H
X_Freq              = 400.53219825[MHz]
X_Offset            = 5[ppm]
X_Points            = 16384
X_Prescans          = 1
X_Resolution        = 0.45849727[Hz]
X_Sweep             = 7.51201923[kHz]
X_Sweep_Clipped     = 6.00961538[kHz]
Irr_Domain          = Proton
Irr_Freq            = 400.53219825[MHz]
Irr_Offset          = 5[ppm]
Tri_Domain          = Proton
Tri_Freq            = 400.53219825[MHz]
Tri_Offset          = 5[ppm]
Clipped             = FALSE
Scans               = 8
Total_Scans         = 8

Relaxation_Delay    = 5[s]
Recvr_Gain          = 50
Temp_Get            = 18.6[dC]
X_90_Width          = 6[us]
X_Acq_Time          = 2.18103808[s]
X_Angle             = 45[deg]
X_Atn               = 0.8[dB]
X_Pulse             = 3[us]
Irr_Mode            = Off
Tri_Mode            = Off
Dante_Presat        = FALSE
Initial_Wait        = 1[s]
Repetition_Time     = 7.18103808[s]
```


(thousandths)
X : parts per Million : Carbon13
69
---- PROCESSING PARAMETERS ----
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: TKH-1535_carbon-1-1.jdf
Filename = TKH-1535_carbon-1-
Author = element
Experiment = carbon.jxp
Sample_Id = TKH-1535
Solvent = CHLOROFORM-D
Actual_Start_Time = 10-MAR-2022 16:20:
Revision_Time = 16-MAR-2022 09:31:
Comment = single pulse decou
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = DELTA2_NMR
Field_Strength = 9.2982153[T] (400[
X_Acq_Duration = 1.048576[s]
X_Domain = Carbon13
X_Freq = 99.54517646[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.95367432[Hz]
X_Sweep = 31.25[kHz]
X_Sweep_Clipped = 25[kHz]
Irr_Domain = Proton
Irr_Freq = 395.88430144[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = TRUE
Scans = 400
Total_Scans = 400
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 18.5[dC]
X_90_Width = 9.65[us]
X_Acq_Time = 1.048576[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 3.21666667[us]
Irr_Atn_Dec = 25.059[dB]
Irr_Atn_Dec_Calc = 25.059[dB]
Irr_Atn_Dec_Default_Calc = 25.059[dB]
Irr_Atn_Noe = 25.059[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm = 12.08082432[ppm]
Irr_Dec_Freq = 395.88430144[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]




```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
blip( 16, 64, 32 )
fft( 1, TRUE, TRUE )
machinephase
ppm
phase( -6, 0, 50[%] )

以下に由来:: TKH-1535_F_standard_single_pulse
```

Filename	= TKH-1535_F_standard_sing
Author	= element
Experiment	= single_pulse.jxp
Sample_Id	= TKH-1535_F_standard
Solvent	= CHLOROFORM-D
Creation_Time	= 5-MAR-2022 15:37:12
Revision_Time	= 5-MAR-2022 18:21:09
Current_Time	= 5-MAR-2022 18:21:15
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
Dim_Title	= Fluorine19
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.4073814[T] (400[MHz])
X_Acq_Duration	= 86.50752[ms]
X_Domain	= 19F
X_Freq	= 376.87675879[MHz]
X_Offset	= 0[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 11.55968868[Hz]
X_Sweep	= 189.39393939[kHz]
X_Sweep_Clipped	= 151.51515152[kHz]
Irr_Domain	= Fluorine19
Irr_Freq	= 376.87675879[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Fluorine19
Tri_Freq	= 376.87675879[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 46
Temp_Get	= 18.7[dC]
X_90_Width	= 6.8[us]
X_Acq_Time	= 86.50752[ms]
X_Angle	= 45[deg]
X_Atn	= 3[dB]
X_Pulse	= 3.4[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 5.08650752[s]