Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Synthesis of (*Z*)-alkenyl boronates via a copper(I)-catalyzed linear-selective alkylboration of terminal allenes

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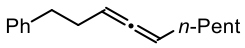
1. Instrumentation and Chemicals

Materials were obtained from commercial suppliers and purified by standard procedures unless otherwise noted. Solvents were also purchased from commercial suppliers, degassed via three freeze-pump-thaw cycles, and further dried over molecular sieves (MS 4A). NMR spectra were recorded on JEOL JNM-ECX400P, JNM-ECS400 and JNM-ECA600 spectrometers (^{1}H: 400 MHz, ^{13}C: 100 MHz). Tetramethylsilane (^{1}H, δ 0.00) and $CDCl_3$ (^{13}C, δ 77.0) were employed as the external standards, respectively. CuCl (224332-25G, ≥99%) and K(O-*t*-Bu) (659878-5G, 99.99%) were purchased from Sigma-Aldrich Co. and used as received. GLC analyses were conducted with a Shimadzu GC-2014 or GC-2025 equipped with a ULBON HR-1 glass capillary column (Shinwa Chemical Industries) and an FID detector. Recycle preparative gel chromatography (GPC) was conducted with JAILC-9101 using $CHCl_3$ as an eluent. High-resolution mass spectra were recorded at the Global Facility Center, Hokkaido University and GC-MS & NMR Lab., Faculty of Agriculture, Hokkaido University.

2. Substrate Preparation and Characterization

Terminal allenes (**1a**–**1j**,[1] **1k**,[2] **1l**,[3] **1m**,[4] **1n**[5] and **1o**[6]), an internal alkyne (**7**[7]), and an internal allene (**9**[8]) were prepared according to literature procedures. The ^{1}H and ^{13}C NMR spectra of known compounds were confirmed with literatures (**1a**,[9] **1b**,[10] **1c**,[11] **1d**,[11] **1e**,[12] **1f**,[13] **1g**,[14] **1h**,[9] **1i**,[15] **1j**,[16] **1k**,[2] **1l**,[3] **1m**,[4] **1n**,[5] **1o**,[6] and **7**[17]). All alkyl iodides (**2a**–**2h**) were purchased from commercial suppliers (Tokyo Chemical Industry Co. and Sigma-Aldrich Co.).

1-Phenyl-3,4-decadiene (9)



9

The internal allene **9** was synthesized according to literature procedure.[8] The product **9** was obtained in 88% yield (521 mg, 2.43 mmol, colorless oil).

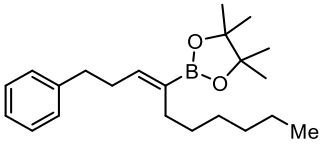
^{1}H NMR (392 MHz, $CDCl_3$, δ): 0.89 (t, J = 6.7 Hz, 3H), 1.22–1.42 (m, 6H), 1.88–1.99 (m, 2H), 2.26–2.35 (m, 2H), 2.72 (t, J = 7.6 Hz, 2H), 5.04–5.16 (m, 2H), 7.14–7.33 (m, 5H). ^{13}C NMR (98 MHz, $CDCl_3$, δ): 14.1 (CH_3), 22.5 (CH_2), 28.8 (CH_2), 30.7 (CH_2), 31.3 (CH_2), 35.5 (CH_2), 90.2 (*C*H), 91.5 (*C*H), 125.7 (*C*H), 128.2 (*C*H), 128.5 (*C*H), 141.9 (*C*), 203.9 (*C*). HRMS-EI (m/z): $[M]^+$ calcd for $C_{16}H_{22}$, 214.1722; found, 214.1720.

3. General Borylation Procedure

IMesCuCl was prepared according to the literature.[18] In an argon-filled grove-box, IMesCuCl (4.1 mg, 0.010 mmol), bis(pinacolato)diboron (**3**) (152.4 mg, 0.60 mmol), and K(O-*t*-Bu) (67.3 mg, 0.60 mmol) were placed in an oven-dried reaction vial. After the vial was sealed with a screw cap containing a Teflon™-coated rubber septum, dry DMF (1.0 mL) was added in the vial through the rubber septum using a syringe. After stirred for 15 min, the reaction mixture was cooled to 0 ℃. After stirred at 0 ℃ for 10 min, **1a** (0.50 mmol) and **2a** (1.0 mmol) were added to the mixture. The reaction mixture was stirred at 0 ℃ for 24 h. After the reaction was completed, the reaction mixture was passed through a short silica gel column (*Φ*: 10 mm, height of the silica-gel column: 90 mm) eluting with Et_2O/hexane (10/90). The crude material was purified by flash column chromatography (SiO_2, Et_2O/hexane, 0:100–20:80) to give the corresponding alkenyl boronate (*Z*)-**4aa** as a colorless oil. Then, the regioselectivity and stereoselectivity were determined by ^1H NMR analysis and ^{13}C NMR analysis.

4. Borylation Product Characterization

(*Z*)-4,4,5,5-Tetramethyl-2-(1-phenyldec-3-en-4-yl)-1,3,2-dioxaborolane [(*Z*)-4aa].

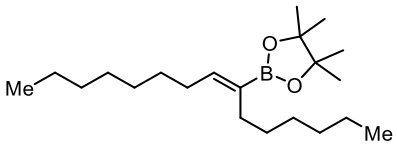


(*Z*)-**4aa**

The borylation reaction was conducted with 72.1 mg (0.500 mmol) of **1a**. The product (*Z*)-**4aa** was obtained in 90% yield with *E*/*Z* = 1:99, **4**:**5** = >99:1 (154.0 mg, 0.450 mmol, colorless oil).

^{1}H NMR (392 MHz, $CDCl_3$, δ): 0.87 (t, *J* = 7.0 Hz, 3H), 1.17–1.34 (m, 8H), 1.26 (s, 12H), 2.06–2.14 (m, 2H), 2.40–2.47 (m, 2H), 2.66–2.73 (m, 2H), 6.35 (t, *J* = 7.0 Hz, 1H), 7.15–7.22 (m, 3H), 7.24–7.32 (m, 2H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 14.1 (*C*H_3), 22.6 (*C*H_2), 24.7 (*C*H_3), 28.5 (*C*H_2), 29.2 (*C*H_2), 30.0 (*C*H_2), 30.7 (*C*H_2), 31.8 (*C*H_2), 35.6 (*C*H_2), 83.0 (*C*), 125.8 (*C*H_2, 128.3 (*C*H), 133.1 (br, B–*C*), 142.2 (*C*), 144.4 (*C*H). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{22}H_{35}O_2{}^{11}B$, 342.2734; found, 342.2726.

(*Z*)-4,4,5,5-Tetramethyl-2-(pentadec-7-en-7-yl)-1,3,2-dioxaborolane [(*Z*)-4ba].

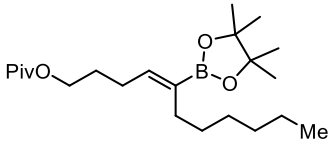


(*Z*)-**4ba**

The borylation reaction was conducted with 68.9 mg (0.498 mmol) of **1b**. The product (*Z*)-**4ba** was obtained in 54% yield with *E*/*Z* = <5:95, **4**:**5** = >95:5 (96.4 mg, 0.269 mmol, colorless oil).

^{1}H NMR (400 MHz, $CDCl_3$, δ): 0.88 (t, *J* = 6.7 Hz, 6H), 1.21–1.34 (m, 18H), 1.25 (s, 12H), 2.08–2.14 (m, 4H), 6.27 (t, *J* = 6.7 Hz, 1H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 14.1 (*C*H_3), 22.7 (*C*H_2), 24.7 (*C*H_3), 24.8 (*C*H_2), 28.49 (*C*H_2), 28.53 (*C*H_2), 29.2 (*C*H_2), 29.5 (*C*H_2), 30.2 (*C*H_2), 31.8 (*C*H_2), 31.9 (*C*H_2), 82.9 (*C*), 146.0 (*C*H). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{21}H_{41}O_2{}^{11}B$, 336.3203; found, 336.3199.

(*Z*)-5-(4,4,5,5-Tetramethyl-1,3,2-dioxaborolan-2-yl)undec-4-en-1-yl pivalate [(*Z*)-4ca].



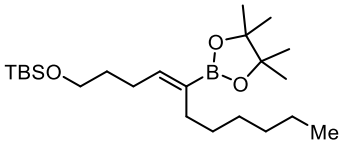
(*Z*)-**4ca**

The borylation reaction was conducted with 91.1 mg (0.500 mmol) of **1c**. The product (*Z*)-**4ca** was obtained in 52% yield with *E*/*Z* = <5:95, **4**:**5** = >95:5 (99.5 mg, 0.260 mmol, colorless oil).

^{1}H NMR (392 MHz, $CDCl_3$, δ): 0.87 (t, *J* = 6.7 Hz, 3H), 1.20 (s, 9H), 1.22–1.33 (m, 8H), 1.25 (s,

12H), 1.73 (quintet, J = 7.0 Hz, 2H), 2.11 (t, J = 6.8 Hz, 2H), 2.21 (q, J = 7.0 Hz, 2H), 4.06 (t, J = 6.7 Hz, 2H), 6.25 (t, J = 7.0 Hz, 1H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 14.1 (*C*H$_3$), 22.6 (*C*H$_2$), 24.7 (*C*H$_3$), 24.9 (*C*H$_2$), 27.2 (*C*H$_3$), 28.2 (*C*H$_2$), 28.5 (*C*H$_2$), 29.3 (*C*H$_2$), 30.1 (*C*H$_2$), 31.8 (*C*H$_2$), 38.7 (*C*), 64.0 (*C*H$_2$), 83.0 (*C*), 144.0 (*C*H), 178.6 (*C*). HRMS-ESI (*m*/*z*): [M+Na]$^+$ calcd for $C_{22}H_{41}O_4{}^{11}BNa$, 403.2994; found, 403.2993.

(*Z*)-*tert*-Butyldimethyl{[5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)undec-4-en-1-yl]oxy}silane [(*Z*)-4da].

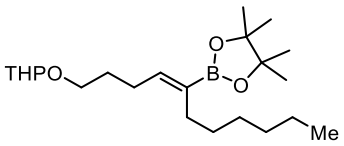


(*Z*)-**4da**

The borylation reaction was conducted with 106.1 mg (0.500 mmol) of **1d**. The product (*Z*)-**4da** was obtained in 86% yield with *E*/*Z* = <5:95, **4**:**5** = >95:5 (177.0 mg, 0.431 mmol, colorless oil).

^{1}H NMR (392 MHz, $CDCl_3$, δ): 0.04 (s, 6H), 0.85–0.91 (m, 3H), 0.89 (s, 9H), 1.21–1.33 (m, 8H), 1.25 (s, 12H), 1.60 (quintet, J = 6.7 Hz, 2H), 2.10–2.21 (m, 4H), 3.61 (t, J = 6.7 Hz, 2H), 6.28 (t, J = 7.0 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): –5.3 (*C*H$_3$), 14.1 (*C*H$_3$), 18.3 (*C*), 22.7 (*C*H$_2$), 24.7 (*C*H$_3$), 24.9 (*C*H$_2$), 25.9 (*C*H$_3$), 28.4 (*C*H$_2$), 29.2 (*C*H$_2$), 30.1 (*C*H$_2$), 31.9 (*C*H$_2$), 32.4 (*C*H$_2$), 62.8 (*C*H$_2$), 82.9 (*C*), 145.2 (*C*H). HRMS-EI (*m*/*z*): [M–Me]$^+$ calcd for $C_{22}H_{44}O_3Si^{11}B$, 395.3157; found, 395.3153.

(*Z*)-2-[1-(Benzyloxy)undec-4-en-5-yl]-4,4,5,5-tetramethyl-1,3,2-dioxaborolane [(*Z*)-4ea].

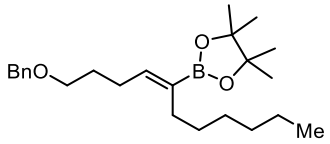


(*Z*)-**4ea**

The borylation reaction was conducted with 91.4 mg (0.501 mmol) of **1e**. The product (*Z*)-**4ea** was obtained in 84% yield with *E*/*Z* = <5:95, **4**:**5** = >95:5 (159.5 mg, 0.421 mmol, colorless oil).

^{1}H NMR (392 MHz, $CDCl_3$, δ): 0.87 (t, J = 6.7 Hz, 3H), 1.20–1.34 (m, 8H), 1.25 (s, 12H), 1.47–1.62 (m, 4H), 1.66–1.74 (m, 3H), 1.78–1.88 (m, 1H), 2.12 (t, J = 6.7 Hz, 2H), 2.16–2.28 (m, 2H), 3.40 (dt, J = 12.9 and 6.7 Hz, 1H), 3.47–3.52 (m, 1H), 3.74 (dt, J = 12.9 and 6.7 Hz, 1H), 3.84–3.90 (m, 1H), 4.57–4.59 (m, 1H), 6.28 (t, J = 6.7 Hz, 1H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 14.1 (*C*H$_3$), 19.6 (*C*H$_2$), 22.7 (*C*H$_2$), 24.7 (*C*H$_3$), 25.2 (*C*H$_2$), 25.5 (*C*H$_2$), 28.5 (*C*H$_2$), 29.22 (*C*H$_2$), 29.25 (*C*H$_2$), 30.1 (*C*H$_2$), 30.7 (*C*H$_2$), 31.9 (*C*H$_2$), 62.2 (*C*H$_2$), 67.1 (*C*H$_2$), 82.9 (*C*), 98.7 (*C*H), 144.9 (*C*H). HRMS-ESI (*m*/*z*): [M+Na]$^+$ calcd for $C_{22}H_{41}O_4{}^{11}BNa$, 403.2994; found, 403.2993.

(*Z*)-2-[1-(Benzyloxy)undec-4-en-5-yl]-4,4,5,5-tetramethyl-1,3,2-dioxaborolane [(*Z*)-4fa].

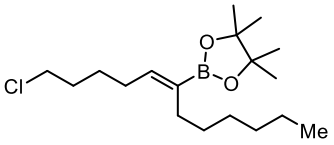


(*Z*)-**4fa**

The borylation reaction was conducted with 94.2 mg (0.500 mmol) of **1f**. The product (*Z*)-**4fa** was obtained in 70% yield with *E*/*Z* = <5:95, **4**:**5** = >95:5 (135.3 mg, 0.350 mmol, colorless oil).

^{1}H NMR (392 MHz, $CDCl_3$, δ): 0.87 (t, *J* = 7.0 Hz, 3H), 1.20–1.34 (m, 8H), 1.25 (s, 12H), 1.72 (quintet, *J* = 7.0 Hz, 2H), 2.12 (t, *J* = 6.8 Hz, 2H), 2.22 (q, *J* = 7.0 Hz, 2H), 3.48 (t, *J* = 6.7 Hz, 2H), 4.50 (s, 2H), 6.26 (t, *J* = 7.0 Hz, 1H), 7.26–7.34 (m, 5H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 14.1 (*C*H_3), 22.6 (*C*H_2), 24.7 (*C*H_3), 25.1 (*C*H_2), 28.5 (*C*H_2), 29.16 (*C*H_2), 29.24 (*C*H_2), 30.1 (*C*H_2), 31.9 (*C*H_2), 70.0 (*C*H_2), 72.8 (*C*H_2), 83.0 (*C*), 127.4 (*C*H), 127.6 (*C*H), 128.3 (*C*H), 138.6 (*C*), 144.8 (*C*H). HRMS-EI (*m*/*z*): $[M–Me]^+$ calcd for $C_{23}H_{36}O_3{}^{11}B$, 371.2762; found, 371.2758.

(*Z*)-2-(1-Chlorododec-5-en-6-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane [(*Z*)-4ga].

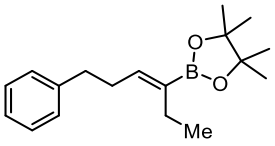


(*Z*)-**4ga**

The borylation reaction was conducted with 65.9 mg (0.504 mmol) of **1g**. The product (*Z*)-**4ga** was obtained in 91% yield with *E*/*Z* = <5:95, **4**:**5** = >95:5 (150.4 mg, 0.458 mmol, colorless oil).

^{1}H NMR (392 MHz, $CDCl_3$, δ): 0.88 (t, *J* = 6.7 Hz, 3H), 1.23–1.33 (m, 8H), 1.25 (s, 12H), 1.50–1.58 (m, 2H), 1.76–1.83 (m, 2H), 2.09–2.19 (m, 4H), 3.53 (t, *J* = 6.7 Hz, 2H), 6.24 (t, *J* = 6.7 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 14.1 (*C*H_3), 22.6 (*C*H_2), 24.7 (*C*H_3), 26.4 (*C*H_2), 27.6 (*C*H_2), 28.5 (*C*H_2), 29.2 (*C*H_2), 30.1 (*C*H_2), 31.9 (*C*H_2), 32.3 (*C*H_2), 45.0 (*C*H_2), 83.0 (*C*), 144.6 (*C*H). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{18}H_{34}O_2Cl^{11}B$, 328.2344; found, 328.2349.

(*Z*)-4,4,5,5-Tetramethyl-2-(6-phenylhex-3-en-3-yl)-1,3,2-dioxaborolane [(*Z*)-4ab].



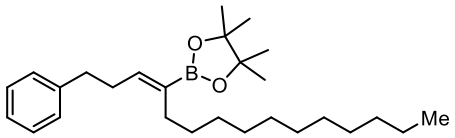
(*Z*)-**4ab**

The borylation reaction was conducted with 71.8 mg (0.498 mmol) of **1a**. The product (*Z*)-**4ab** was obtained in 70% yield with *E*/*Z* = <5:95, **4**:**5** = >95:5 (100.4 mg, 0.349 mmol, colorless oil).

^{1}H NMR (392 MHz, $CDCl_3$, δ): 0.91 (t, *J* = 7.4 Hz, 3H), 1.27 (s, 12H), 2.12 (q, *J* = 7.4 Hz, 2H), 2.42–2.48 (m, 2H), 2.68–2.72 (m, 2H), 6.34 (t, *J* = 7.0 Hz, 1H), 7.16–7.22 (m, 3H), 7.25–7.31 (m, 2H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 14.7 (*C*H_3), 21.8 (*C*H_2), 24.7 (*C*H_3), 30.4 (*C*H_2), 35.6 (*C*H_2), 83.0 (*C*),

125.8 (*C*H), 128.3 (*C*H), 142.1 (*C*), 144.0 (*C*H). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{18}H_{27}O_2{}^{11}B$, 286.2107; found, 286.2102.

(*Z*)-4,4,5,5-Tetramethyl-2-(1-phenylpentadec-3-en-4-yl)-1,3,2-dioxaborolane [(*Z*)-4ac].

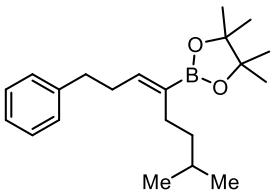


(*Z*)-**4ac**

The borylation reaction was conducted with 72.1 mg (0.500 mmol) of **1a**. The product (*Z*)-**4ac** was obtained in 85% yield with *E*/*Z* = <5:95, **4**:**5** = >95:5 (174.9 mg, 0.424 mmol, colorless oil).

^{1}H NMR (392 MHz, $CDCl_3$, δ): 0.88 (t, *J* = 6.9 Hz, 3H), 1.17–1.35 (m, 18H), 1.26 (s, 12H), 2.06–2.15 (m, 2H), 2.39–2.48 (m, 2H), 2.65–2.73 (m, 2H), 6.35 (t, *J* = 6.9 Hz, 1H), 7.15–7.22 (m, 3H), 7.25–7.32 (m, 2H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 14.1 (*C*H_3), 22.7 (*C*H_2), 24.7 (*C*H_3), 28.5 (*C*H_2), 29.3 (*C*H_2), 29.5 (*C*H_2), 29.6 (*C*H_2), 29.7 (*C*H_2), 30.1 (*C*H_2), 30.7 (*C*H_2), 31.9 (*C*H_2), 35.6 (*C*H_2), 82.9 (*C*), 125.7 (*C*H), 128.3 (*C*H), 133.2 (br, B–*C*), 142.2 (*C*), 144.4 (*C*H). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{27}H_{45}O_2{}^{11}B$, 412.3517; found, 412.3511.

(*Z*)-4,4,5,5-Tetramethyl-2-(7-methyl-1-phenyloct-3-en-4-yl)-1,3,2-dioxaborolane [(*Z*)-4ad].

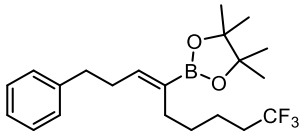


(*Z*)-**4ad**

The borylation reaction was conducted with 72.1 mg (0.500 mmol) of **1a**. The product (*Z*)-**4ad** was obtained in 79% yield with *E*/*Z* = <5:95, **4**:**5** = 94:6 (129.6 mg, 0.395 mmol, colorless oil).

^{1}H NMR (400 MHz, $CDCl_3$, δ): 0.87 (d, *J* = 6.8 Hz, 6H), 1.12–1.20 (m, 2H), 1.26 (s, 12H), 1.45–1.56 (m, 1H), 2.04–2.17 (m, 2H), 2.38–2.49 (m, 2H), 2.63–2.76 (m, 2H), 6.33 (t, *J* = 7.2 Hz, 1H), 7.12–7.23 (m, 3H), 7.23–7.32 (m, 2H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 22.6 (*C*H_3), 24.7 (*C*H_3), 26.4 (*C*H_2), 27.9 (*C*H), 30.6 (*C*H_2), 35.6 (*C*H_2), 39.3 (*C*H_2), 82.9 (*C*), 125.8 (*C*H), 128.3 (*C*H), 133.2 (br, B–*C*), 142.2 (*C*), 144.1 (*C*H). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{21}H_{33}O_2{}^{11}B$, 328.2577; found, 328.2578.

(*Z*)-4,4,5,5-Tetramethyl-2-(9,9,9-trifluoro-1-phenylnon-3-en-4-yl)-1,3,2-dioxaborolane [(*Z*)-4ae].

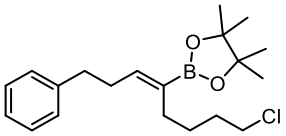


(*Z*)-**4ae**

The borylation reaction was conducted with 72.1 mg (0.500 mmol) of **1a**. The product (*Z*)-**4ae** was obtained in 84% yield with *E*/*Z* = <5:95, **4**:**5** = >95:5 (158.7 mg, 0.415 mmol, colorless oil).

^{1}H NMR (392 MHz, $CDCl_3$, δ): 1.25 (s, 12H), 1.28–1.37 (m, 2H), 1.45–1.53 (m, 2H), 1.96–2.08 (m, 2H), 2.12 (t, *J* = 7.6 Hz, 2H), 2.39–2.47 (m, 2H), 2.67–2.74 (m, 2H), 6.40 (t, *J* = 7.0 Hz, 1H), 7.16–7.22 (m, 3H), 7.24–7.31 (m, 2H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 21.6 (q, *J* = 3.0 Hz, *C*H_2), 24.7 (*C*H_3), 27.9 (*C*H_2), 29.0 (*C*H_2), 30.8 (*C*H_2), 33.7 (q, *J* = 28.3 Hz, *C*H_2), 35.5 (*C*H_2), 83.1 (*C*), 125.8 (*C*), 127.4 (q, *J* = 294.6 Hz, *C*), 128.3 (*C*), 132.0 (br, B–*C*), 142.0 (*C*), 145.4 (*C*H). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{21}H_{30}F_3O_2{}^{11}B$, 382.2295; found, 382.2288.

(*Z*)-2-(8-Chloro-1-phenyloct-3-en-4-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane [(*Z*)-4af].

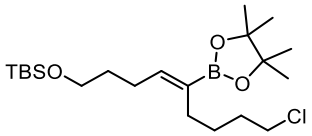


(*Z*)-**4af**

The borylation reaction was conducted with 72.2 mg (0.500 mmol) of **1a**. The product (*Z*)-**4af** was obtained in 85% yield with *E*/*Z* = <5:95, **4**:**5** = >95:5 (148.8 mg, 0.425 mmol, colorless oil).

^{1}H NMR (392 MHz, $CDCl_3$, δ): 1.26 (s, 12H), 1.42 (quintet, *J* = 7.0 Hz, 2H), 1.72 (quintet, *J* = 7.0 Hz, 2H), 2.13 (t, *J* = 7.0 Hz, 2H), 2.41–2.47 (m, 2H), 2.68–2.72 (m, 2H), 3.51 (t, *J* = 7.0 Hz, 1H), 6.39 (t, *J* = 7.0 Hz, 1H), 7.17–7.20 (m, 3H), 7.26–7.30 (m, 2H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 24.7 (*C*H_3), 27.2 (*C*H_2), 27.5 (*C*H_2), 30.8 (*C*H_2), 32.3 (*C*H_2), 35.5 (*C*H_2), 45.1 (*C*H_2), 83.1 (*C*), 125.8 (*C*H), 128.3 (*C*H), 142.0 (*C*), 145.3 (*C*H). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{20}H_{30}O_2Cl{}^{11}B$, 348.2031; found, 348.2025.

(*Z*)-*tert*-Butyl{[9-chloro-5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)non-4-en-1-yl]oxy}dimethylsilane [(*Z*)-4df].



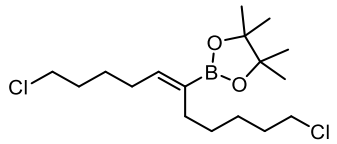
(*Z*)-**4df**

The borylation reaction was conducted with 104.4 mg (0.492 mmol) of **1d**. The product (*Z*)-**4df** was obtained in 60% yield with *E*/*Z* = <5:95, **4**:**5** = >95:5 (125.0 mg, 0.300 mmol, colorless oil).

^{1}H NMR (392 MHz, $CDCl_3$, δ): 0.04 (s, 6H), 0.89 (s, 9H), 1.25 (s, 12H), 1.48 (dt, *J* = 15.3, 7.0 Hz,

2H), 1.57–1.64 (m, 3H), 1.76 (dt, J = 15.3, 7.0 Hz, 2H), 2.16 (dt, J = 14.1, 7.0 Hz, 4H), 3.54 (t, J = 6.7 Hz, 2H), 3.61 (t, J = 6.7 Hz, 2H), 6.32 (t, J = 7.0 Hz, 1H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): –5.3 (*C*H$_3$), 18.3 (*C*), 24.7 (*C*H$_3$), 25.0 (*C*H$_2$), 25.9 (*C*H$_3$), 27.3 (*C*H$_2$), 27.5 (*C*H$_2$), 32.3 (*C*H$_2$), 32.4 (*C*H$_2$), 45.1 (*C*H$_2$), 62.7 (*C*H$_2$), 83.0 (*C*), 146.1 (*C*H). HRMS-EI (*m*/*z*): [M–Me]$^+$ calcd for $C_{20}H_{39}O_3SiCl^{11}B$, 401.2454; found, 401.2445.

(*Z*)-2-(1,11-Dichloroundec-5-en-6-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane [(*Z*)-4gg].

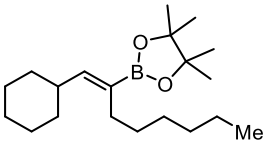


(*Z*)-**4gg**

The borylation reaction was conducted with 65.5 mg (0.501 mmol) of **1g**. The product (*Z*)-**4gg** was obtained in 85% yield with *E*/*Z* = <5:95, **4**:**5** = >95:5 (148.3 mg, 0.426 mmol, colorless oil).

^{1}H NMR (392 MHz, $CDCl_3$, δ): 1.26 (s, 12H), 1.31–1.46 (m, 4H), 1.51–1.58 (m, 2H), 1.74–1.83 (m, 4H), 2.13 (t, J = 7.0 Hz, 2H), 2.17 (t, J = 7.0 Hz, 2H), 3.53 (t, J = 6.8 Hz, 2H), 3.54 (t, J = 6.8 Hz, 2H), 6.27 (t, J = 7.0 Hz, 1H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 24.7 (*C*H$_3$), 26.4 (*C*H$_2$), 26.7 (*C*H$_2$), 27.6 (*C*H$_2$), 28.2 (*C*H$_2$), 29.2 (*C*H$_2$), 32.3 (*C*H$_2$), 32.6 (*C*H$_2$), 44.9 (*C*H$_2$), 45.1 (*C*H$_2$), 83.1 (*C*), 145.0 (*C*H). HRMS-EI (*m*/*z*): [M]$^+$ calcd for $C_{17}H_{31}O_2Cl_2^{11}B$, 348.1797; found, 348.1796.

(*Z*)-2-(1-Cyclohexyloct-1-en-2-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane [(*Z*)-4ha].

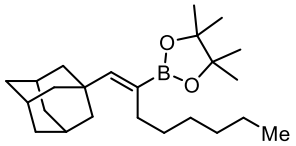


(*Z*)-**4ha**

The borylation reaction was conducted with 62.0 mg (0.507 mmol) of **1h**. The product (*Z*)-**4ha** was obtained in 84% yield with *E*/*Z* = <5:95, **4**:**5** = >95:5 (134.6 mg, 0.420 mmol, colorless oil).

^{1}H NMR (392 MHz, $CDCl_3$, δ): 0.88 (t, J = 6.3 Hz, 3H), 1.05–1.34 (m, 13H), 1.25 (s, 12H), 1.53–1.74 (m, 5H), 2.11 (t, J = 6.3 Hz, 2H), 2.29–2.40 (m, 1H), 6.06 (d, J = 9.4 Hz, 1H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 14.1 (*C*H$_3$), 22.6 (*C*H$_2$), 24.7 (*C*H$_3$), 25.9 (*C*H$_2$), 26.1 (*C*H$_2$), 28.7 (*C*H$_2$), 29.2 (*C*H$_2$), 30.6 (*C*H$_2$), 31.8 (*C*H$_2$), 32.7 (*C*H$_2$), 37.4 (*C*H), 82.9 (*C*), 151.1 (*C*H). HRMS-EI (*m*/*z*): [M]$^+$ calcd for $C_{20}H_{37}O_2^{11}B$, 320.2890; found, 320.2885.

(*Z*)-2-[1-(Adamantan-1-yl)oct-1-en-2-yl]-4,4,5,5-tetramethyl-1,3,2-dioxaborolane [(*Z*)-4ia].

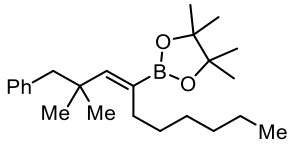


(*Z*)-**4ia**

The borylation reaction was conducted with 87.8 mg (0.504 mmol) of **1i**. The product (*Z*)-**4ia** was obtained in 64% yield with *E*/*Z* = <5:95, **4**:**5** = >95:5 (121.0 mg, 0.325 mmol, colorless oil).

^{1}H NMR (392 MHz, $CDCl_3$, δ): 0.86–0.90 (m, 3H), 1.22–1.35 (m, 8H), 1.24 (s, 12H), 1.65–1.70 (m, 6H), 1.79–1.83 (m, 6H), 1.93–1.97 (m, 3H), 2.24–2.28 (m, 2H), 5.94 (s, 1H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 14.1 (*C*H_3), 22.6 (*C*H_2), 24.7 (*C*H_3), 24.8 (*C*), 28.8 (*C*H), 29.6 (*C*H_2), 29.8 (*C*H_2), 31.1 (*C*H_2), 31.8 (*C*H_2), 36.8 (*C*H_2), 42.6 (*C*H_2), 82.9 (*C*), 153.6 (*C*H). HRMS-ESI (*m*/*z*): $[M+Na]^+$ calcd for $C_{24}H_{41}O_2{}^{11}BNa$, 395.3096; found, 395.3092.

(*Z*)-2-(2,2-Dimethyl-1-phenyldec-3-en-4-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane [(*Z*)-4ja].

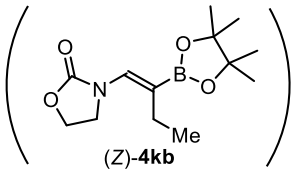


(*Z*)-**4ja**

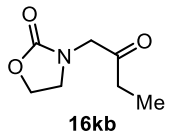
The borylation reaction was conducted with 86.1 mg (0.500 mmol) of **1j**. The product (*Z*)-**4ja** was obtained in 52% yield with *E*/*Z* = <5:95, **4**:**5** = >95:5 (96.4 mg, 0.260 mmol, colorless oil).

^{1}H NMR (392 MHz, $CDCl_3$, δ): 0.87 (t, *J* = 6.8 Hz, 3H), 1.11 (s, 6H), 1.23–1.31 (m, 8H), 1.25 (s, 12H), 2.19–2.24 (m, 2H), 2.72 (s, 2H), 6.18 (s, 1H), 7.12–7.26 (m, 5H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 14.1 (*C*H_3), 22.6 (*C*H_2), 24.7 (*C*H_3), 28.3 (*C*H_3), 29.5 (*C*H_2), 29.7 (*C*H_2), 30.6 (*C*H_2), 31.8 (*C*H_2), 38.7 (*C*), 49.2 (*C*H_2), 83.0 (*C*), 125.8 (*C*H), 127.5 (*C*H), 130.7 (*C*H), 139.1 (*C*), 152.3 (*C*H). HRMS-EI (*m*/*z*): $[M–Me]^+$ calcd for $C_{23}H_{36}O_2{}^{11}B$, 355.2813; found, 355.2809.

3-(2-Oxobutyl)oxazolidin-2-one (16kb)



(*Z*)-**4kb**



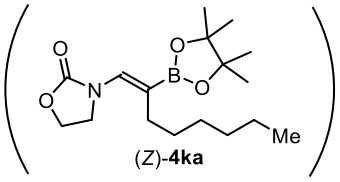
16kb

The borylation reaction was conducted with 62.6 mg (0.500 mmol) of **1k**. In order to remove an undesired boryl substitution product of the alkyl halide and protoboration product of the allene for the further purification and the determination of the regioselectivities, the oxidation of the boryl groups was performed. The corresponding ketone product **16kb** was obtained in 51% yield (40.4 mg, 0.257 mmol, colorless oil).

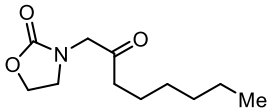
^{1}H NMR (392 MHz, $CDCl_3$, δ): 1.12 (t, *J* = 7.3 Hz, 3H), 2.47 (q, *J* = 7.4 Hz, 2H), 3.68 (t, *J* = 8.0

Hz, 2H), 4.10 (s, 2H), 4.41 (t, J = 8.0 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 7.4 (*C*H_3), 33.2 (*C*H_2), 45.2 (*C*H_2), 52.6 (*C*H_2), 62.3 (*C*H_2), 158.9 (*C*), 205.3 (*C*). HRMS-ESI (*m*/*z*): $[M+Na]^+$ calcd for $C_7H_{11}O_3NNa$, 180.0631; found, 180.0628.

3-(2-Oxooctyl)-1,3-oxazolidin-2-one (16ka)



(*Z*)-**4ka**

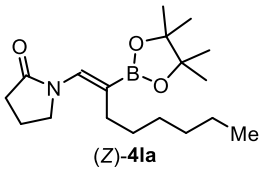


16ka

The borylation reaction was conducted with 62.6 mg (0.500 mmol) of **1k**. In order to remove an undesired boryl substitution product of the alkyl halide and protoboration product of the allene for the further purification and the determination of the regioselectivities, the oxidation of the boryl groups was performed. The corresponding ketone product **16ka** was obtained in 51% yield (54.8 mg, 0.257 mmol, colorless oil).

^{1}H NMR (392 MHz, $CDCl_3$, δ): 0.88 (t, J = 7.0 Hz, 3H), 1.22–1.36 (m, 6H), 1.61 (quintet, J = 7.2 Hz, 2H), 2.42 (t, J = 7.4 Hz, 2H), 3.67 (t, J = 7.8 Hz, 2H), 4.08 (s, 2H), 4.40 (t, J = 8.0 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 14.0 (*C*H_3), 22.4 (*C*H_2), 23.3 (*C*H_2), 28.7 (*C*H_2), 31.4 (*C*H_2), 39.9 (*C*H_2), 45.0 (*C*H_2), 52.7 (*C*H_2), 62.1 (*C*H), 158.7 (*C*), 204.8 (*C*). HRMS-ESI (*m*/*z*): $[M+Na]^+$ calcd for $C_{11}H_{19}O_3NNa$, 236.1257; found, 236.1260.

1-[(*Z*)-2-(4,4,5,5-Tetramethyl-1,3,2-dioxaborolan-2-yl)oct-1-en-1-yl]pyrrolidin-2-one [(*Z*)-4la]

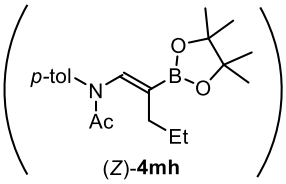


(*Z*)-**4la**

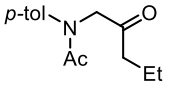
The borylation reaction was conducted with 61.6 mg (0.500 mmol) of **1l**. The product (*Z*)-**4la** was obtained in 48% yield with *E*/*Z* = <5:95, **4**:**5** = >95:5 (76.8 mg, 0.239 mmol, colorless solid).

^{1}H NMR (392 MHz, $CDCl_3$, δ): 0.88 (t, J = 7.0 Hz, 3H), 1.21–1.40 (m, 20H), 2.08 (quintet, J = 7.6 Hz, 2H), 2.22 (t, J = 7.1 Hz, 2H), 2.42 (t, J = 8.2 Hz, 2H), 3.85 (t, J = 7.1 Hz, 2H), 7.23 (s, 1H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 13.9 (*C*H_3), 18.6 (*C*H_2), 22.4 (*C*H_2), 24.5 (*C*H_3), 27.5 (*C*H_2), 29.1 (*C*H_2), 30.0 (*C*H_2), 31.4 (*C*H_2), 31.6 (*C*H_2), 48.0 (*C*H_2), 83.0 (*C*), 113.7 (br, B–*C*), 132.6 (*C*H), 174.9 (*C*). HRMS-ESI (*m*/*z*): $[M+Na]^+$ calcd for $C_{18}H_{32}O_3{}^{11}BNNa$, 344.2371; found, 344.2371.

***N*-(2-Oxobutyl)-*N*-(*p*-tolyl)acetamide (16mh)**



(*Z*)-**4mh**

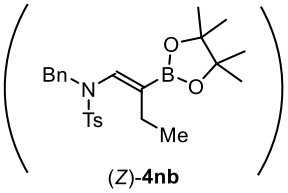


16mh

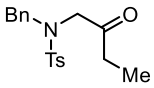
The borylation reaction was conducted with 93.6 mg (0.500 mmol) of **1m**. In order to remove an undesired boryl substitution product of the alkyl halide and protoboration product of the allene for the further purification and the determination of the regioselectivities, the oxidation of the boryl groups was performed. The corresponding ketone product **16mh** was obtained in 48% yield (55.9 mg, 0.240 mmol, colorless oil).

^{1}H NMR (399 MHz, $CDCl_3$, δ): 0.91 (t, *J* = 7.4 Hz, 3H), 1.63 (sixtet, *J* = 7.3 Hz, 2H), 1.91 (s, 3H), 2.36 (s, 3H), 2.40 (t, *J* = 7.4 Hz, 2H), 4.39 (s, 2H), 7.19 (s, *J* = 8.0 Hz, 4H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 13.6 (*C*H_3), 16.9 (*C*H_2), 21.0 (*C*H_3), 21.9 (*C*H_3), 41.8 (*C*H_2), 58.8 (*C*H_2), 127.6 (*C*H), 130.2 (*C*H), 137.9 (*C*), 141.0 (*C*), 170.8 (*C*), 204.9 (*C*). HRMS-ESI (*m*/*z*): $[M+Na]^+$ calcd for $C_{14}H_{19}O_2NNa$, 256.1308; found, 256.1312.

***N*-Benzyl-*N*-(2-oxobutyl)-4-methylbenzenesulfonamide (16nb)**



(*Z*)-**4nb**

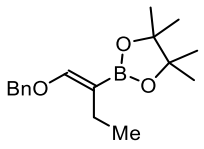


16nb

The borylation reaction was conducted with 149.7 mg (0.500 mmol) of **1n**. In order to remove an undesired boryl substitution product of the alkyl halide and protoboration product of the allene for the further purification and the determination of the regioselectivities, the oxidation of the boryl groups was performed. The corresponding ketone product **16nb** was obtained in 60% yield (99.6 mg, 0.301 mmol, colorless oil).

^{1}H NMR (392 MHz, $CDCl_3$, δ): 0.90 (t, *J* = 7.2 Hz, 3H), 2.25 (q, *J* = 7.4 Hz, 2H), 2.45 (s, 3H), 3.86 (s, 2H), 4.37 (s, 2H), 7.20–7.38 (m, 7H), 7.75 (d, *J* = 6.7 Hz, 2H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 7.2 (*C*H_3), 21.5 (*C*H_3), 32.5 (*C*H_2), 52.0 (*C*H_2), 54.5 (*C*H_2), 127.4 (*C*H), 128.1 (*C*H), 128.7 (*C*H), 128.8 (*C*H), 129.6 (*C*H), 134.9 (*C*), 136.1 (*C*), 143.6 (*C*), 206.4 (*C*). HRMS-ESI (*m*/*z*): $[M+Na]^+$ calcd for $C_{18}H_{21}O_3NNaS$, 354.1134; found, 354.1137.

(*Z*)-2-(1-(Benzyloxy)prop-1-ene-2-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane [(*Z*)-4ob]



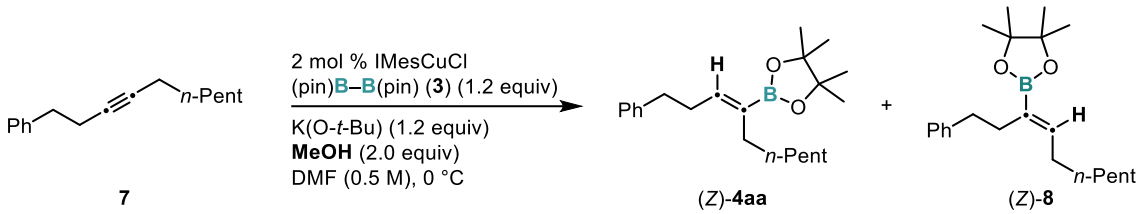
(*Z*)-**4ob**

The borylation reaction was conducted with 74.6 mg (0.500 mmol) of **1o**. The product (*Z*)-**4ob** was obtained in 63% yield with *E*/*Z* = 10:90, **4**:**5** = >95:5 (91.3 mg, 0.317 mmol, colorless oil).

^{1}H NMR (392 MHz, $CDCl_3$, δ): 0.98 (t, *J* = 7.4 Hz, 3H), 1.24 (s, 12H), 2.16 (q, *J* = 7.4 Hz, 2H), 4.92 (s, 2H), 6.74 (s, 1H), 7.27–7.38 (m, 5H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 14.7 (*C*H_3), 18.4 (*C*H_2), 24.6 (*C*H_3), 74.0 (*C*H_2), 82.5 (*C*), 108.4 (Br, B–*C*), 126.9 (*C*H), 127.7 (*C*H), 128.4 (*C*H), 137.5 (*C*), 156.3 (*C*H). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{17}H_{25}O_3{}^{11}B$, 288.1900; found, 288.1894.

5. Comparison Experiments

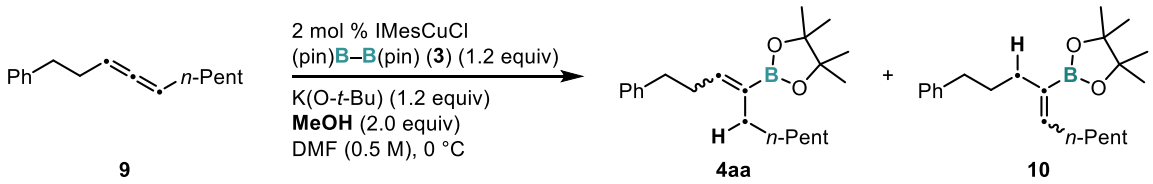
5.1. Protoboration of an internal alkyne 7



82% yield, 1:1 mixture of (*Z*)-**4aa**/(*Z*)-**8**

In an argon-filled grove-box, IMesCuCl (2.0 mg, 0.0050 mmol), bis(pinacolato)diboron (**3**) (76.2 mg, 0.300 mmol) and K(O-*t*-Bu) (33.7 mg, 0.300 mmol) were placed in a round-bottomed flask. Dry DMF (0.5 mL) was added in the flask through the rubber septum using a syringe. After stirring for 30 min at room temperature, **7** (54.0 mg, 0.252 mmol) and MeOH (16.0 mg, 0.500 mmol) were added to the mixture at 0 ℃. After the reaction was completed, the reaction mixture was passed through a short silica gel column (Φ: 10 mm, height of the silica-gel column: 90 mm) eluting with Et_2O/hexane (10/90). The crude material was purified by flash column chromatography (SiO_2, Et_2O/hexane, 0:100–20:80) to give 1:1 mixture of (*Z*)-**4aa**/(*Z*)-**8** in 82% yield (70.7 mg, 0.207 mmol, colorless oil).

5.2. Protoboration of an internal allene 9

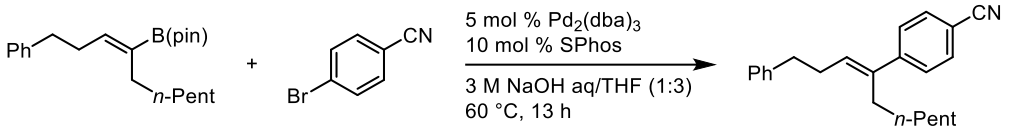


78% yield, 3:2:2:1 mixture of isomers

In an argon-filled grove-box, IMesCuCl (2.0 mg, 0.0050 mmol), bis(pinacolato)diboron (**3**) (76.2 mg, 0.300 mmol) and K(O-*t*-Bu) (33.7 mg, 0.300 mmol) were placed in a round-bottomed flask. Dry DMF (0.5 mL) was added in the flask through the rubber septum using a syringe. After stirring for 30 min at room temperature, **9** (53.6 mg, 0.250 mmol) and MeOH (16.0 mg, 0.500 mmol) were added to the mixture at 0 ℃. After the reaction was completed, the reaction mixture was passed through a short silica gel column (Φ: 10 mm, height of the silica-gel column: 90 mm) eluting with Et2O/hexane (10/90). The crude material was purified by flash column chromatography (SiO_2, Et_2O/hexane, 0:100–20:80) to give 3:2:2:1 mixture of isomers in 78% yield (66.4 mg, 0.194 mmol, colorless oil).

6. Suzuki–Miyaura Cross-coupling Reaction of Borylation Products

6.1. Reaction of (*Z*)-4aa with an aryl halide

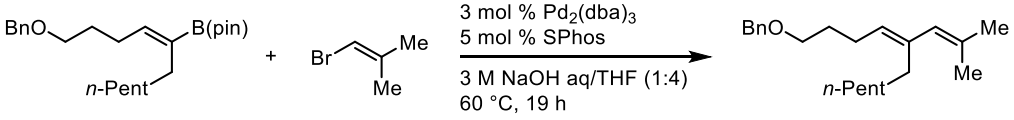


(*Z*)-**4aa** (1.5 equiv) (*E*)-**12a**

The Suzuki–Miyaura cross-coupling reaction of (*Z*)-**4aa** was conducted according to the literature procedure.[19] In an oven-dried reaction vial, (*Z*)-**4aa** (85.9 mg, 0.251 mmol), 4-bromobenzonitrile (68.7 mg, 0.375 mmol), $Pd_2(dba)_3$ (4.6 mg, 0.005 mmol) and SPhos (4.1 mg, 0.01 mmol) were dissolved in THF (2.25 mL) under a nitrogen atmosphere. After the addition of 3 M NaOH aqueous solution (0.75 mL) into the vial, the mixture was stirred at 60 °C for 13 h. The mixture was then quenched by addition of water (5 mL) and extracted three times with Et_2O (10 mL ×3). The combined organic layer was washed with brine, dried over $MgSO_4$ followed by filtration. After evaporation, the crude material was purified by silica gel chromatography (Et_2O/hexane, 0:100–3:97) to give the corresponding coupling product (*E*)-**12a** as a mixture with 4-bromobenzonitrile (75.5 mg). The product ratio was calculated from ^{1}H NMR analysis of the purified material [(*E*)-**12a**: 0.206 mmol, 82% yield, 4-bromobenzonitrile: 0.055 mmol].

^{1}H NMR (392 MHz, $CDCl_3$, δ): 0.85 (t, *J* = 6.9 Hz, 3H), 1.16–1.28 (m, 8H), 2.38–2.46 (m, 2H), 2.53 (q, *J* = 7.6 Hz, 2H), 2.77 (t, *J* = 7.6 Hz, 2H), 5.76 (t, *J* = 7.4 Hz, 1H), 7.18–7.24 (m, 3H), 7.28–7.33 (m, 2H), 7.37–7.40 (m, 2H), 7.56–7.60 (m, 2H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 14.0 (*C*H_3), 22.5 (*C*H_2), 28.4 (*C*H_2), 29.1 (*C*H_2), 29.3 (*C*H_2), 30.6 (*C*H_2), 31.5 (*C*H_2), 35.8 (*C*H_2), 109.9 (*C*), 119.1 (*C*), 126.0 (*C*H), 126.8 (*C*H), 128.35 (*C*H), 128.41 (*C*H), 130.7 (*C*H), 132.0 (*C*H), 139.7 (*C*), 141.5 (*C*), 147.9 (*C*). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{23}H_{27}N$, 317.2144; found, 317.2143.

6.2. Reaction of (*Z*)-4fa with an alkenyl halide



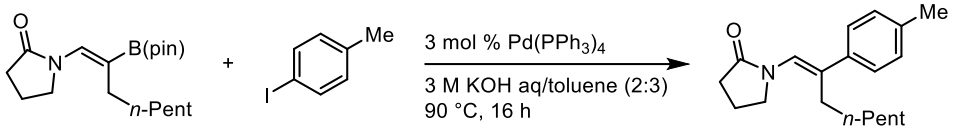
(*Z*)-**4fa** (1.7 equiv) (*E*)-**12b**

The Suzuki–Miyaura cross-coupling reaction of (*Z*)-**4fa** was conducted according to the literature procedure.[19] 1-Bromo-2-methylprop-1-ene (46.2 mg, 0.342 mmol), $Pd_2(dba)_3$ (5.1 mg, 0.006 mmol), SPhos (4.0 mg, 0.010 mmol) were placed in an oven-dried reaction vial under a nitrogen atmosphere. A solution of (*Z*)-**4fa** (77.6 mg, 0.201 mmol) in dry THF (2.0 mL) was added to the vial followed by addition of 3 M NaOH aq (0.70 mL). Then, the mixture was warmed to 60 °C with stirring for 19 h. After the reaction mixture was cooled to room temperature, the reaction mixture was quenched by H_2O and extracted with Et_2O three times. The combined organic layer was then dried over MgSO4.

After filtration, the solvents were removed by evaporation. The crude mixture was purified by flash column chromatography (SiO_2, Et_2O/hexane, 0:100–5:95) to give the corresponding coupling product (*E*)-**12b** (64.8 mg, 0.198 mmol, 99%) as colorless oil.

^{1}H NMR (392 MHz, $CDCl_3$, δ): 0.87 (t, *J* = 6.3 Hz, 3H), 1.22–1.33 (m, 8H), 1.70–1.75 (m, 8H), 2.03 (t, *J* = 7.0 Hz, 2H), 2.18 (q, *J* = 7.0 Hz, 2H), 3.50 (t, *J* = 6.3 Hz, 2H), 4.51 (s, 2H), 5.15 (t, *J* = 7.0 Hz, 1H), 5.55 (s, 1H), 7.26–7.35 (m, 5H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 14.1 (*C*H_3), 19.3 (*C*H_3), 22.6 (*C*H_2), 24.5 (*C*H_2), 26.4 (*C*H_3), 28.6 (*C*H_2), 29.2 (*C*H_2), 30.0 (*C*H_2), 31.0 (*C*H_2), 31.8 (*C*H_2), 69.9 (*C*H_2), 72.9 (*C*H_2), 127.4 (*C*H), 127.6 (*C*H), 127.8 (*C*H), 128.3 (*C*H), 132.7 (*C*), 138.0 (*C*), 138.6 (*C*). HRMS-EI (*m*/*z*): $[M–Me]^+$ calcd for $C_{21}H_{31}O$, 299.2375; found, 299.2376.

6.3. Reaction of (*Z*)-4la with an aryl halide

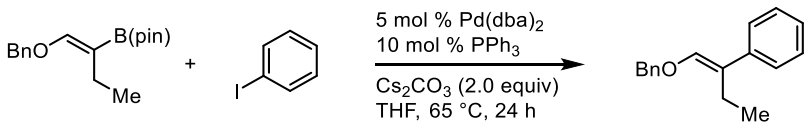


(*Z*)-**4la** (3.0 equiv) (*E*)-**12c**

The Suzuki–Miyaura cross-coupling reaction of (*Z*)-**4la** was conducted according to the literature procedure.[4] In an argon-filled grove-box, (*Z*)-**4la** (32.1 mg, 0.100 mmol) and $Pd(PPh_3)_4$ (3.5 mg, 0.0030 mmol) were placed in an oven-dried reaction vial. After the vial was sealed with a screw cap containing a Teflon^{TM}-coated rubber septum, dry toluene (0.3 mL) was added in the vial through the rubber septum using a syringe. After the addition of 4-tolyl iodide (65.4 mg, 0.300 mmol) and 3 M KOH aqueous solution (0.2 mL) into the vial, the mixture was stirred at 90 ℃ for 16 h. After celite filtration, the celite washed with DCM and the mixture of the filtrate dried over $MgSO_4$ followed by filtration. After evaporation, the crude material was purified by silica gel chromatography (AcOEt/hexane, 15:85–25:75) to give the corresponding coupling product (*E*)-**12c** in 73% yield (20.9 mg, 0.0732 mmol, colorless oil).

^{1}H NMR (392 MHz, $CDCl_3$, δ): 0.85 (t, *J* = 6.7 Hz, 3H), 1.16–1.47 (m, 8H), 2.14 (quintet, *J* = 7.5 Hz, 2H), 2.34 (s, 3H), 2.40–2.58 (m, 4H), 3.77 (t, *J* = 7.1 Hz, 2H), 6.49 (s, 1H), 7.12 (d, *J* = 8.6 Hz, 3H), 7.24 (m, *J* = 8.2 Hz, 2H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 14.0 (*C*H_3), 19.0 (*C*H_2), 21.1 (*C*H_3), 22.6 (*C*H_2), 28.8 (*C*H_2), 29.5 (*C*H_2), 30.0 (*C*H_2), 30.6 (*C*H_2), 31.6 (*C*H_2), 49.3 (*C*H_2), 121.7 (*C*H), 126.6 (*C*H), 128.9 (*C*H), 132.7 (*C*), 136.7 (*C*), 138.0 (*C*), 175.1 (*C*). HRMS-ESI (*m*/*z*): $[M+Na]^+$ calcd for $C_{19}H_{27}ONNa$, 308.1985; found, 308.1986.

6.4. Reaction of (*Z*)-4ob with an aryl halide



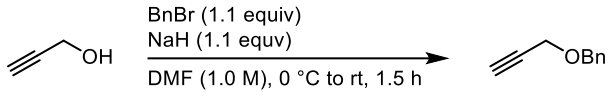
(*Z*)-**4ob** (1.2 equiv) (*E*)-**12d**

The Suzuki–Miyaura cross-coupling reaction of (*Z*)-**4ob** was conducted according to the literature procedure.[20] $Pd_2(dba)_3$ (3.5 mg, 0.0030 mmol), PPh_3 (2.6 mg, 0.010 mmol) and Cs_2CO_3 (65.2 mg, 0.200 mmol) were placed in an oven-dried reaction vial under a nitrogen atmosphere. After the vial was sealed with a screw cap containing a Teflon™-coated rubber septum, dry THF (0.5 mL) was added in the vial through the rubber septum using a syringe. After the addition of iodobenzene (24.3 mg, 0.119 mmol) and (*Z*)-**4ob** (28.8 mg, 0.100 mmol) into the vial, the mixture was stirred at 65 °C for 24 h. After the reaction was completed, the reaction mixture was passed through a short silica gel column (*Φ*: 10 mm, height of the silica-gel column: 90 mm) eluting with Et_2O/hexane (10/90). The crude material was purified by flash column chromatography (SiO_2, Et_2O/hexane, 0:100–2:98) to give the corresponding coupling product (*E*)-**12d** in 76% yield (21.4 mg, 0.0755 mmol, colorless oil).

^{1}H NMR (392 MHz, $CDCl_3$, δ): 1.02 (t, *J* = 7.4 Hz, 3H), 2.58 (q, *J* = 7.6 Hz, 2H), 4.91 (s, 2H), 6.42 (s, 1H), 7.15–7.40 (m, 10H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 13.1 (*C*H_3), 20.4 (*C*H_2), 74.0 (*C*H_2), 112.1 (*C*), 125.7 (*C*H), 125.9 (*C*H), 127.3 (*C*H), 127.9 (*C*H), 128.3 (*C*H), 128.5 (*C*H), 137.6 (*C*), 139.5 (*C*), 143.1 (*C*H). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{17}H_{18}O$, 238.1358; found, 238.1356.

7. Formal Total Synthesis of schizol A

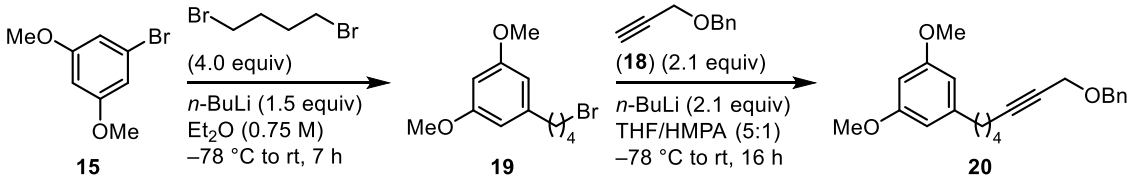
7.1. Synthesis of allene 1p



17 **18**
87% yield

In a vacuum dried 50 mL two-neck round-bottomed flask, NaH (60% paraffin liquid dispersion, 880 mg, 22.0 mmol) was suspended in DMF (20 mL) at 0 ºC. To the suspension, propargyl alcohol **17** (1.12 g, 20.0 mmol) was slowly added and stirred for 30 min. Then, benzyl bromide (2.6 mL, 22.0 mmol) was added, and the mixture was warmed up to room temperature. After stirring for 1.5 h at room temperature, the reaction mixture was quenched by 1 M HCl aqueous solution (40 mL) and extracted with AcOEt three times (40 mL ×3). The combined organic layer was then dried over $MgSO_4$. After filtration, the solvents were removed by evaporation. The crude product was purified by flash column chromatography to obtain the corresponding propargyl ether **18** (2.54 g, 17.4 mmol, 87%) as a colorless oil.

^{1}H NMR (392 MHz, $CDCl_3$, δ): 2.48 (t, J = 2.2 Hz, 1H), 4.18 (d, J = 2.7 Hz, 2H), 4.62 (s, 2H), 7.28–7.40 (m, 5H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 57.0 (*C*H_2), 71.5 (*C*), 74.6 (*C*H_2), 79.6 (*C*H), 127.9 (*C*H), 128.1 (*C*H), 128.4 (*C*H), 137.2 (*C*). HRMS-ESI (*m*/*z*): $[M]^+$ calcd for $C_{10}H_{10}O_1$, 146.0732; found, 146.0730.

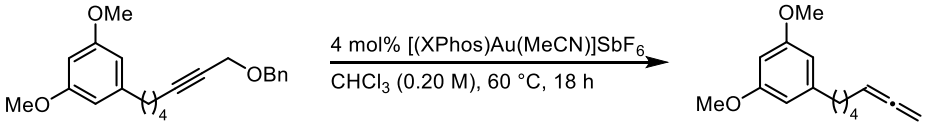


In a vacuum dried 50 mL two-neck round-bottomed flask, aryl bromide **15** (3.26 g, 15.0 mmol) was dissolved in Et_2O (20 mL) under a nitrogen atmosphere. After cooled to −78 °C, to this solution was added *n*-BuLi (14.1 mL, 1.6 M solution in THF, 22.5 mmol) dropwise and the mixture was warmed up to 0 °C. After stirred for 30 min, the reaction mixture was cooled to −78 °C again. Then, to the reaction mixture was added 1,4-dibromobutane (7.1 ml, 60 mmol) dropwise and the mixture was warmed up to room temperature. After 7 h, the resulting mixture was diluted with water (30 ml) and extracted with Et_2O three times. The combined organic layer was then dried over Mg_2SO_4. After filtration, the solvents were removed by evaporation. The crude product was purified by flash column chromatography to give the mixture of corresponding coupling product **19** and 1,3-dimethoxybenzene (colorless oil).

In a vacuum dried 50 mL two-neck round-bottomed flask, propargyl ether **18** was dissolved in THF

(30 mL) under a nitrogen atmosphere. After cooled to −78 °C, to this solution was added *n*-BuLi (10.5 mL, 1.6 M solution in THF, 16.2 mmol) dropwise and the mixture was warmed up to 0 °C. After stirred for 30 min, to the reaction mixture was added HMPA (7.7 ml) and alkyl bromide **19** solution in THF (10 ml). The reaction mixture was warmed up to room temperature and stirred for 16 h. After the reaction was completed, the reaction mixture was cooled to 0 °C and diluted with water (20 ml). The resulting mixture was extracted with Et_2O three times, and the combined organic layer was then dried over Mg_2SO_4. After filtration, the solvents were removed by evaporation. The crude product was purified by flash column chromatography to give the corresponding inner alkyne **20** in 36% yield (1.84 g, 5.43 mmol, colorless oil) in 2 steps.

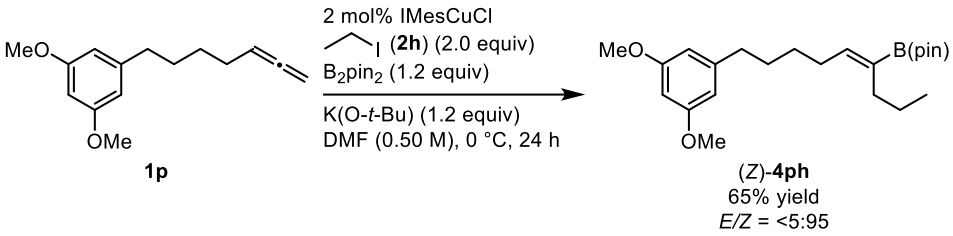
^{1}H NMR (400 MHz, $CDCl_3$, δ): 1.52–1.63 (m, 2H), 1.74 (quintet, J = 7.4 Hz, 2H), 2.27 (tt, J = 6.6 Hz, 2.2 Hz, 2H), 2.58 (t, J = 7.6 Hz, 2H), 3.77 (s, 6H), 4.15 (t, J = 2.2 Hz, 2H), 4.58 (s, 2H) , 6.30 (t, J = 2.0 Hz, 1H) , 6.35 (d, J = 2.0 Hz, 2H), 7.25–7.39 (m, 5H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 18.6 (*C*H_2), 28.0 (*C*H_2), 30.2 (*C*H_2), 35.6 (*C*H_2), 55.1 (*C*H_3), 57.6 (*C*H_2), 71.2 (*C*H_2), 76.0 (*C*), 86.8 (*C*), 97.5 (*C*H), 106.3 (*C*H), 127.6 (*C*H), 128.0 (*C*H), 128.3 (*C*H), 137.5 (*C*), 144.6 (*C*), 160.6 (*C*). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{22}H_{26}O_3$, 338.1882; found, 338.1879.



[(XPhos)Au(MeCN)]SbF_6 (33.8 mg, 0.0356 mmol) were placed in an oven-dried reaction vial. 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. Dry $CHCl_3$ (4.5 mL) and inner alkyne **20** were added to the vial through the rubber septum using a syringe and the reaction mixture was warmed up to 60 °C. After stirring for 24 h, the reaction mixture was cooled to room temperature and passed through a short silica gel column (Φ: 10 mm, the height of the silica-gel column: ca. 30 mm) eluting with Et_2O/hexane (10/90). The crude material was purified by flash column chromatography to give the corresponding allene product **1p** in 62% yield (129.1 mg, 0.556 mmol, colorless oil).

^{1}H NMR (392 MHz, $CDCl_3$, δ): 1.46 (quintet, J = 7.5 Hz, 2H), 1.65 (quintet, J = 7.6 Hz, 2H), 1.99–2.08 (m, 2H), 2.56 (t, J = 7.6 Hz, 2H), 3.78 (s, 6H), 4.62–4.68 (m, 2H), 5.09 (quintet, J = 6.7 Hz, 1H), 6.30 (t, J = 2.3 Hz, 1H), 6.34 (d, J = 2.3 Hz, 2H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 28.0 (*C*H_2), 28.7 (*C*H_2), 30.6 (*C*H_2), 36.0 (*C*H_2), 55.1 (*C*H_3), 74.6 (*C*H_2), 89.8 (*C*H), 97.5 (*C*H), 106.4 (*C*H), 145.0 (*C*), 160.6 (*C*), 208.4 (*C*). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{15}H_{20}O_2$, 232.1463; found, 232.1459.

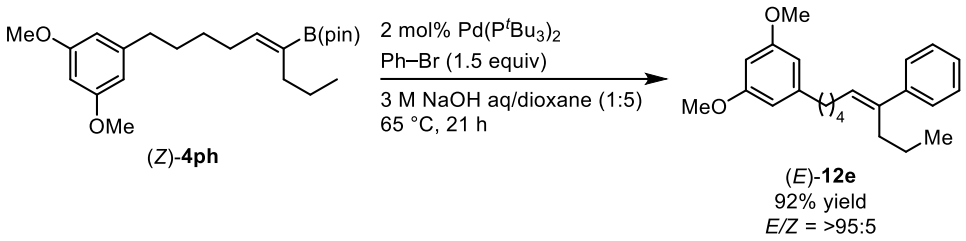
7.2. Synthesis of alkenyl boronate (*Z*)-4ph



IMesCuCl was prepared according to the literature.[18] In an argon-filled grove-box, IMesCuCl (4.5 mg, 0.0111 mmol), bis(pinacolato)diboron (**3**) (169.6 mg, 0.668 mmol), and K(O-*t*-Bu) (75.0 mg, 0.668 mmol) were placed in an oven-dried reaction vial. After the vial was sealed with a screw cap containing a Teflon™-coated rubber septum, dry DMF (1.11 mL) was added in the vial through the rubber septum using a syringe. After stirred for 15 min, the reaction mixture was cooled to 0 ℃. After stirred at 0 ℃ for 10 min, **1p** (129.1 mg, 0.556 mmol) and **2h** (173.1 mg, 1.11 mmol) were added to the mixture. The reaction mixture was stirred at 0 ℃ for 24 h. After the reaction was completed, the reaction mixture was passed through a short silica gel column (*Φ*: 10 mm, height of the silica-gel column: 90 mm) eluting with Et_2O/hexane (10/90). The crude material was purified by flash column chromatography (SiO_2, Et_2O/hexane, 0:100–20:80) to give the corresponding alkenyl boronate (*Z*)-**4ph** in 65% yield with *E*/*Z* = <5:95, **4**:**5** = >95:5 (141.1 mg, 0.363 mmol, colorless oil).

^{1}H NMR (400 MHz, $CDCl_3$, δ): 0.88 (t, *J* = 7.0 Hz, 3H), 1.29 (s, 12H), 1.30–1.49 (m, 4H), 1.63 (quintet, *J* = 7.5 Hz, 2H), 2.04–2.20 (m, 4H), 2.55 (t, *J* = 7.6 Hz, 2H), 3.78 (s, 6H), 6.25–6.32 (m, 2H), 6.32–6.37 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 14.0 (*C*H_3), 23.3 (*C*H_2), 24.7 (*C*H_3), 28.3 (*C*H_2), 28.8 (*C*H_2), 30.5 (*C*H_2), 31.0 (*C*H_2), 36.1 (*C*H_2), 55.2 (*C*H_3), 82.9 (*C*), 97.6 (*C*H), 106.4 (*C*H), 132.3 (br, B–*C*), 145.1 (*C*), 145.7 (*C*H), 160.6 (*C*). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{23}H_{37}O_4{}^{11}B$, 388.2789; found, 388.2779.

7.3. Synthesis of (*E*)-12e



The Suzuki–Miyaura cross-coupling reaction of (*Z*)-**4ph** was conducted according to the literature procedure.[4] In an argon-filled grove-box, $Pd(P^tBu_3)_4$ (1.0 mg, 0.0020 mmol) were placed in an oven-dried reaction vial. After the vial was sealed with a screw cap containing a Teflon™-coated rubber septum, dry 1,4-dioxane (0.5 mL) was added in the vial through the rubber septum using a syringe.

After the addition of (*Z*)-**4ph** (38.8 mg, 0.100 mmol), bromobenzene (18.8 mg, 0.120 mmol) and 3 M NaOH aqueous solution (0.1 mL) into the vial, the mixture was warmed to 65 ℃. After stirred for 21 h, the reaction mixture was cooled to room temperature and passed through a short silica gel column (*Φ*: 10 mm, height of the silica-gel column: 90 mm) eluting with Et_2O/hexane (10/90). The crude material was purified by flash column chromatography to give the corresponding coupling product (*E*)-**12e** in 92% yield with *E*/*Z* = >95:5 (31.0 mg, 0.0916 mmol, colorless oil).

^{1}H NMR (392 MHz, $CDCl_3$, δ): 0.87 (t, *J* = 7.4 Hz, 3H), 1.35 (sextet, *J* = 3.5 Hz, 2H), 1.49 (quintet, *J* = 7.0 Hz, 2H) ,1.68 (quintet, *J* = 8.2 Hz, 2H), 2.22 (q, *J* = 7.2 Hz, 2H), 2.46 (t, *J* = 7.6 Hz, 2H), 2.58 (t, *J* = 7.6 Hz, 2H), 3.78 (s, 6H) , 5.64 (t, *J* = 7.2 Hz, 1H), 6.30 (t, *J* = 2.5 Hz, 1H), 6.35 (d, *J* = 2.0 Hz, 2H), 7.18–7.24 (m, 1H), 7.26–7.35 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 14.0 (*C*H_3), 21.8 (*C*H_2), 28.4 (*C*H_2), 29.5 (*C*H_2), 30.9 (*C*H_2), 31.7 (*C*H_2), 36.2 (*C*H_2), 55.2 (*C*H_3), 97.6 (*C*H), 106.4 (*C*H), 126.3 (*C*H), 126.4 (*C*H), 128.1 (*C*H), 129.0 (*C*H), 140.0 (*C*), 143.4 (*C*), 145.1 (*C*), 160.7 (*C*). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{23}H_{30}O_2$, 338.2246; found, 338.2244.

8. Computational Study

8.1. Calculation method details

All geometry optimizations and thermal energy correction calculations (frequency analyses) using density functional theory (DFT) were performed with the Gaussian 16 (revision C.01)[21] suite of programs. The thresholds defined in Gaussian 16 were used. The geometry optimizations were carried out at ωB97X-D[22] level of theory with a mixed basis set [SDD[23] for Cu atom, and 6-31G(d)[24] for the other atoms]. The solvation effect of DMF was included in the calculations using SMD solvation model.[25] Harmonic frequency calculations were conducted at the same level of theory on the optimized geometries to check all the stationary points as either minima or first-order saddle points. Intrinsic reaction coordinate (IRC)[26] calculations were carried out to confirm the transition states connecting the correct reactants and products on the potential energy surface. Then, the self-consistent field (SCF) energies of the optimized molecular systems were corrected at a higher level of theory. For this purpose, we chose ωB97X-D[22] functional with another mixed basis set [SDD[23] for Cu atom, and 6-311+G(d,p)[24] for the other atoms]. The solvation effect of DMF was included in the calculations using SMD solvation model.[25]

Summary: ωB97X-D/SDD, 6-311+G(d,p)/SMD(DMF)//ωB97X-D/SDD, 6-31G(d)/SMD(DMF).

8.2. Calculated properties of all structures

Table S1. Calculated energies and thermochemical parameters of the optimized structures.

Structure	SCF energy [hartree]	*H* [hartree]	*TS* [hartree]	*G* [hartree]
Substrate **1**	–155.962079	–155.872210	0.032649	–155.904859
Catalyst **Int2**	–155.873154	–1532.181045	0.103293	–1532.284338
TS$^{\text{alkenyl-}Z}$	–1688.762278	–1688.054519	0.111634	–1688.166153
TS$^{\text{alkenyl-}E}$	–1688.757495	–1688.049891	0.110283	–1688.160174
(*Z*)-**Int3**	–1688.846123	–1688.135629	0.112073	–1688.247702
(*E*)-**Int3**	–1688.840612	–1688.129926	0.110694	–1688.240620
Int3'	–1688.838475	–1688.128026	0.110235	–1688.238261

9. References

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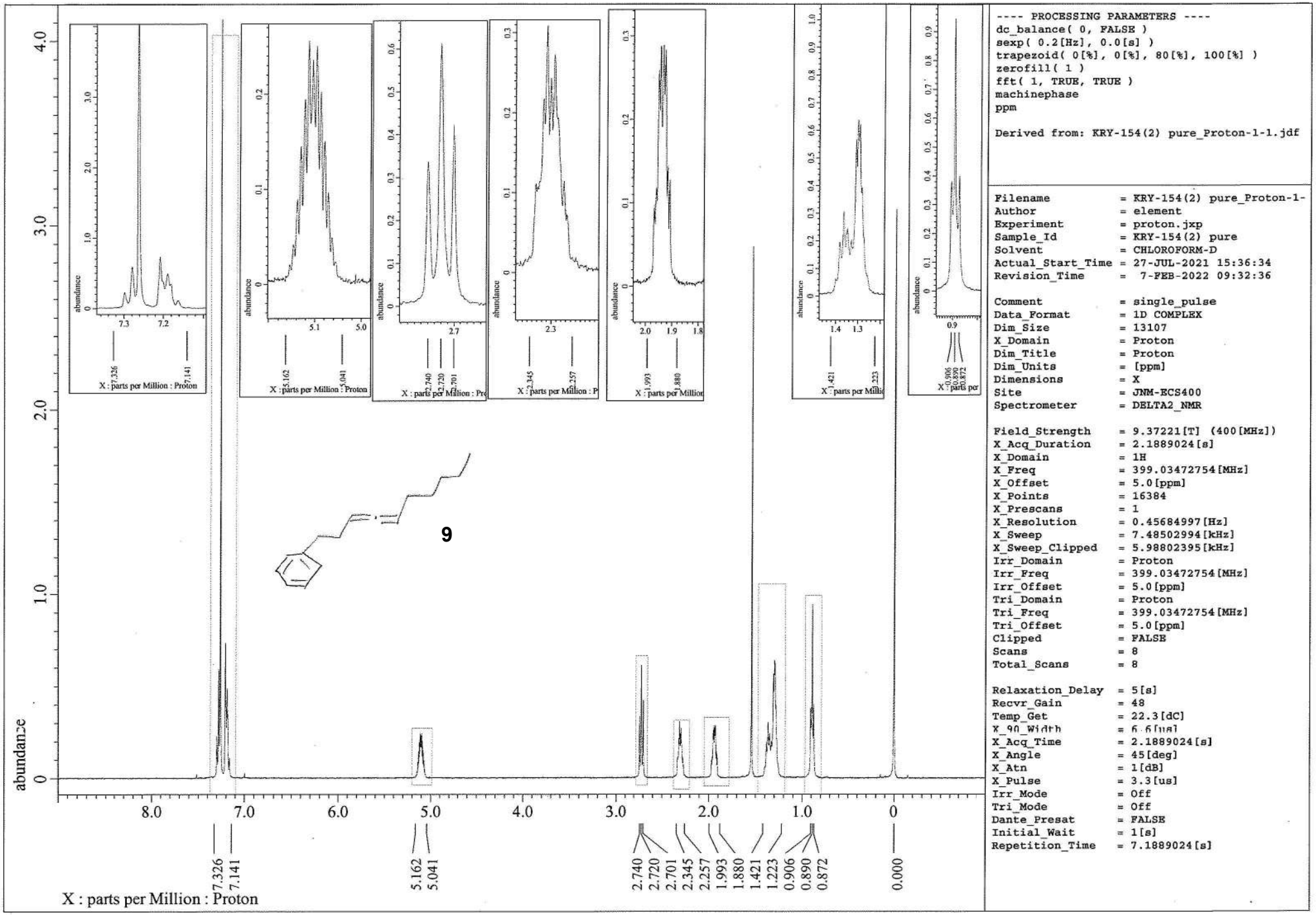


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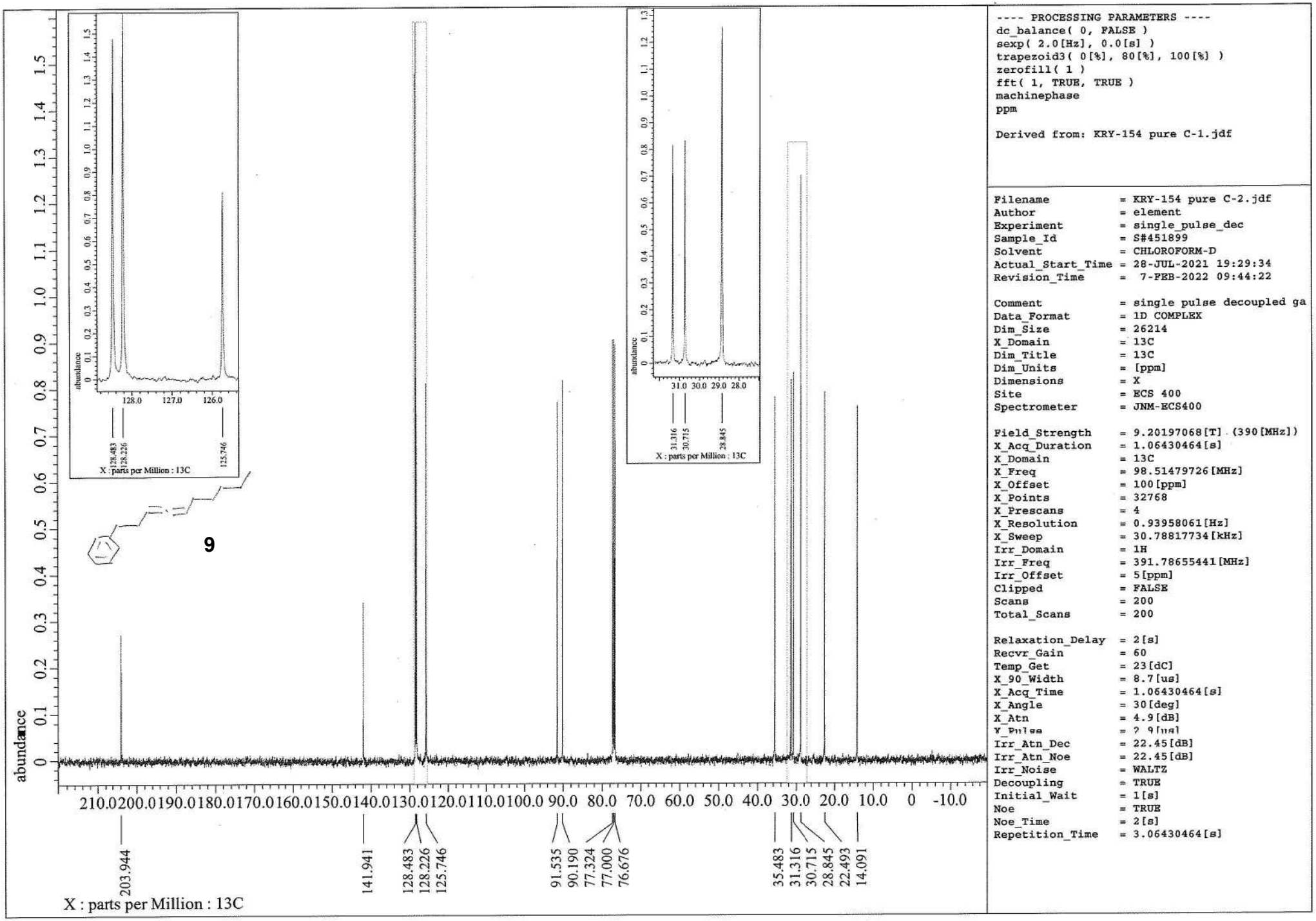
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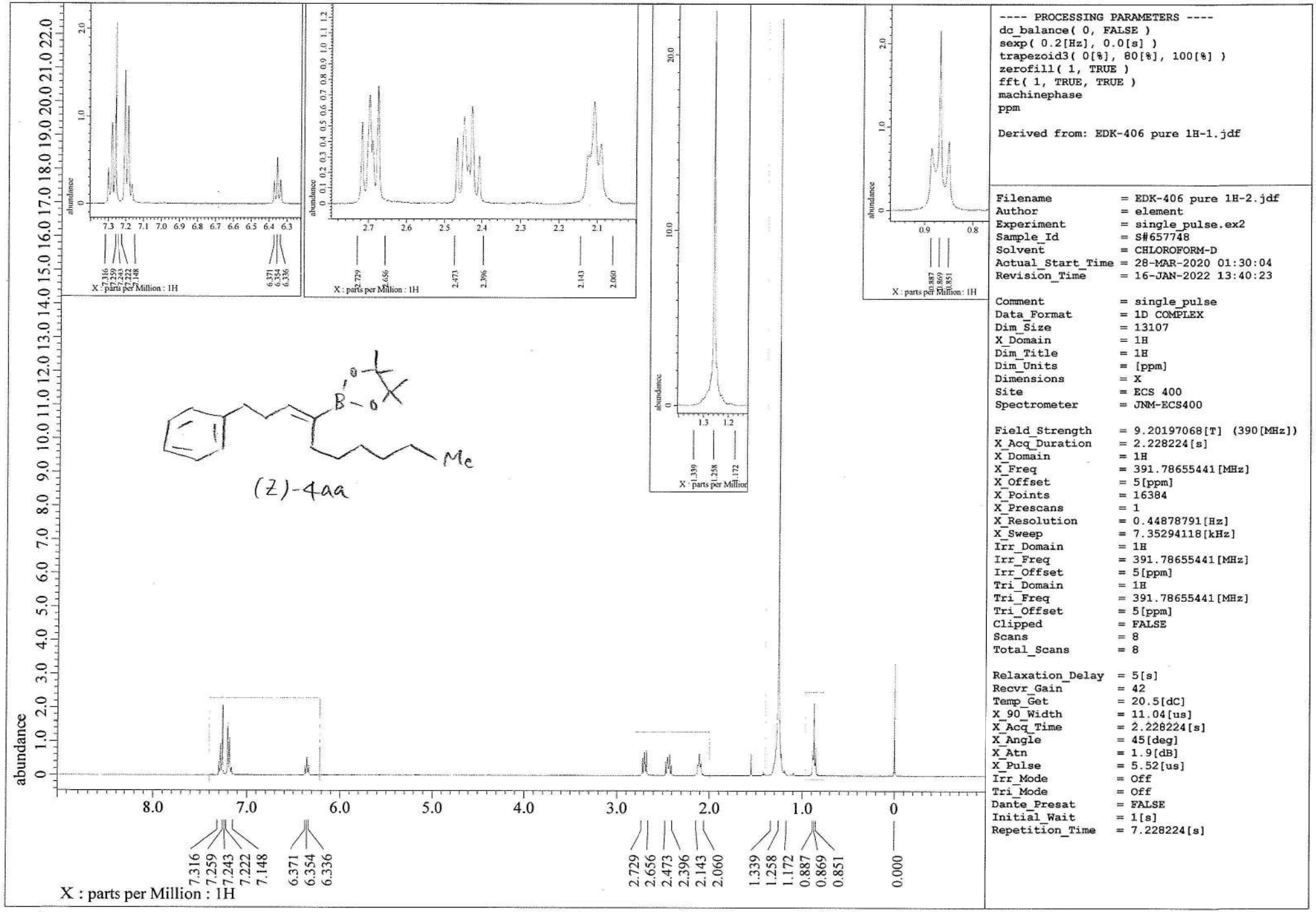


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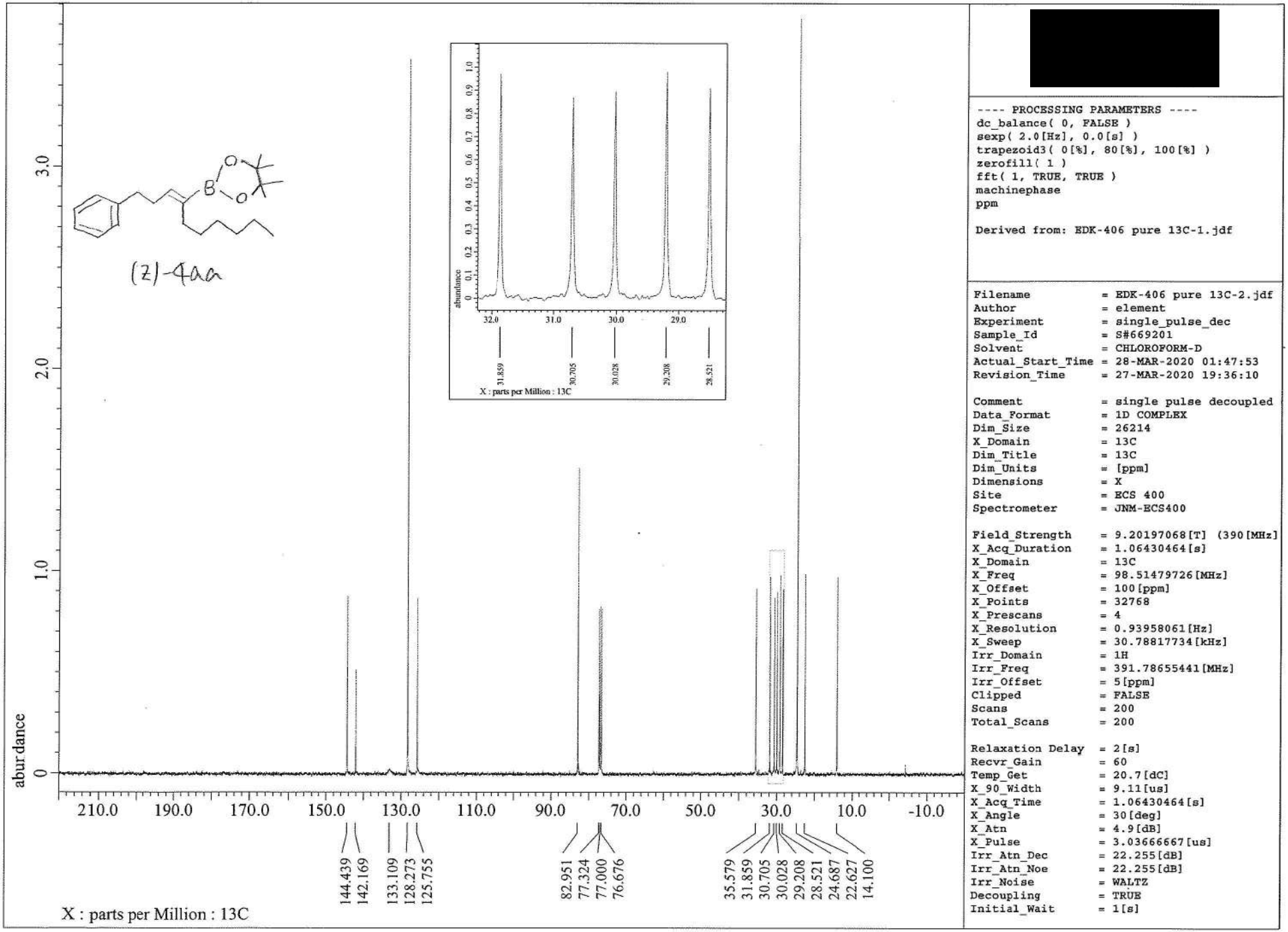

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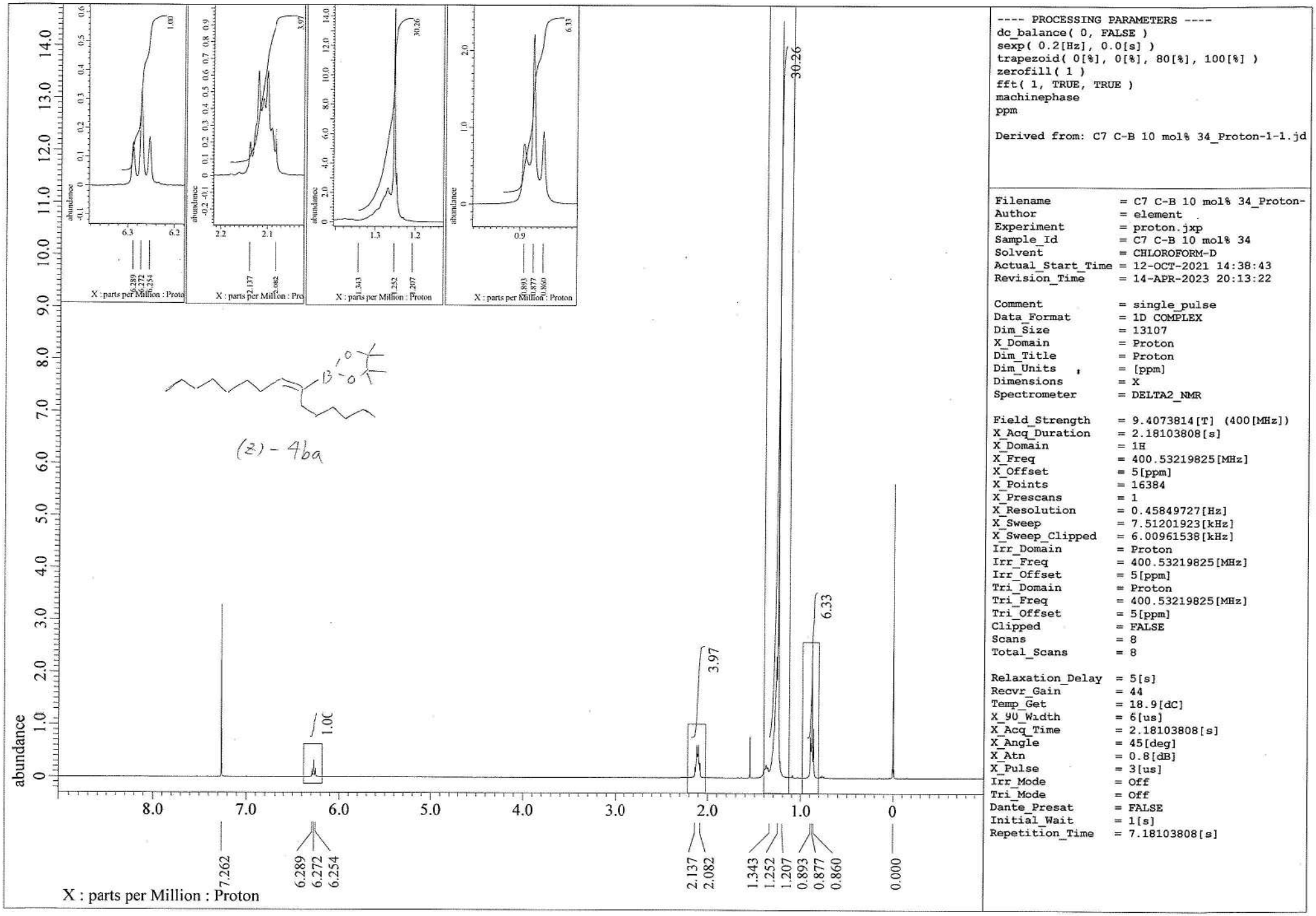
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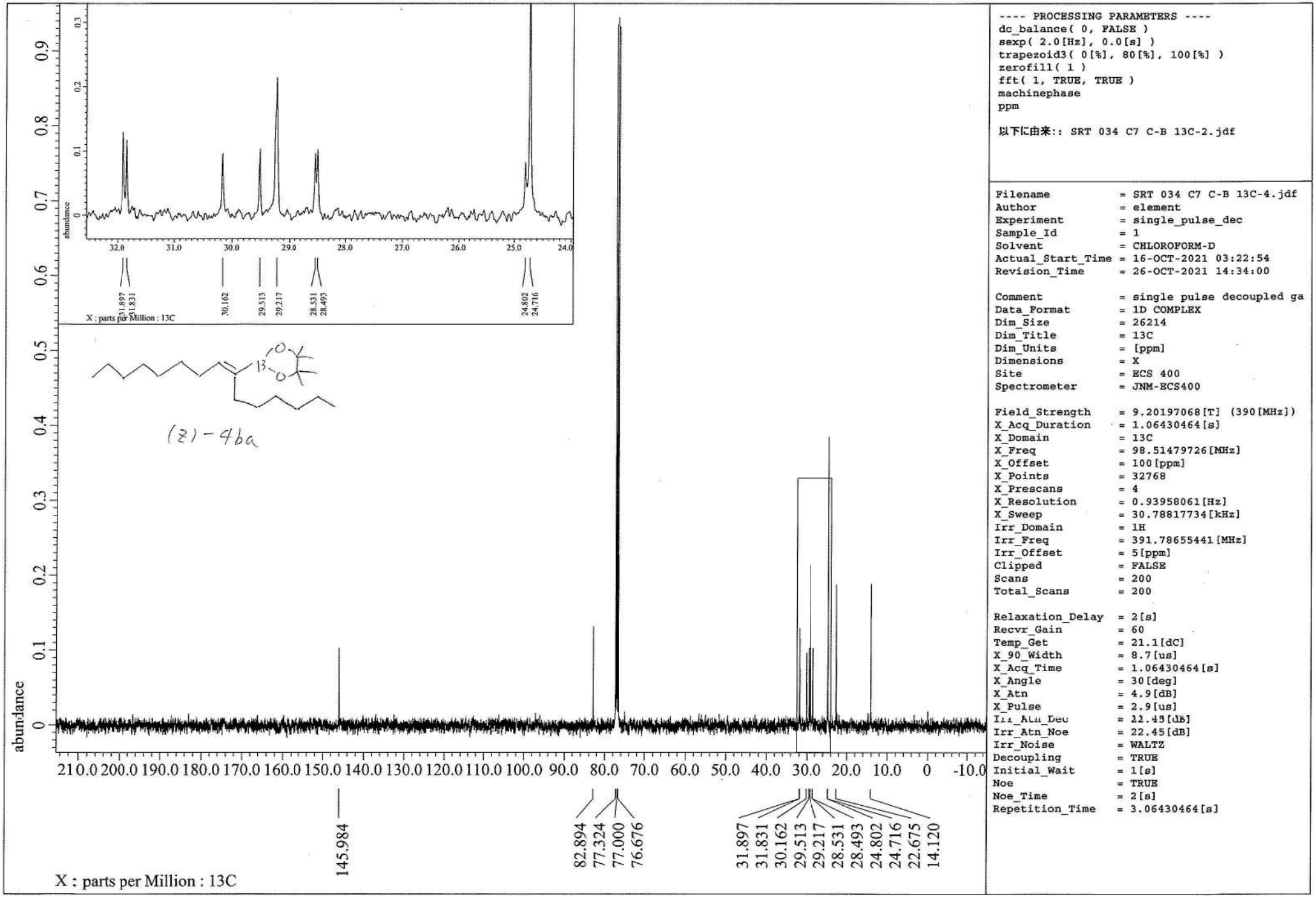
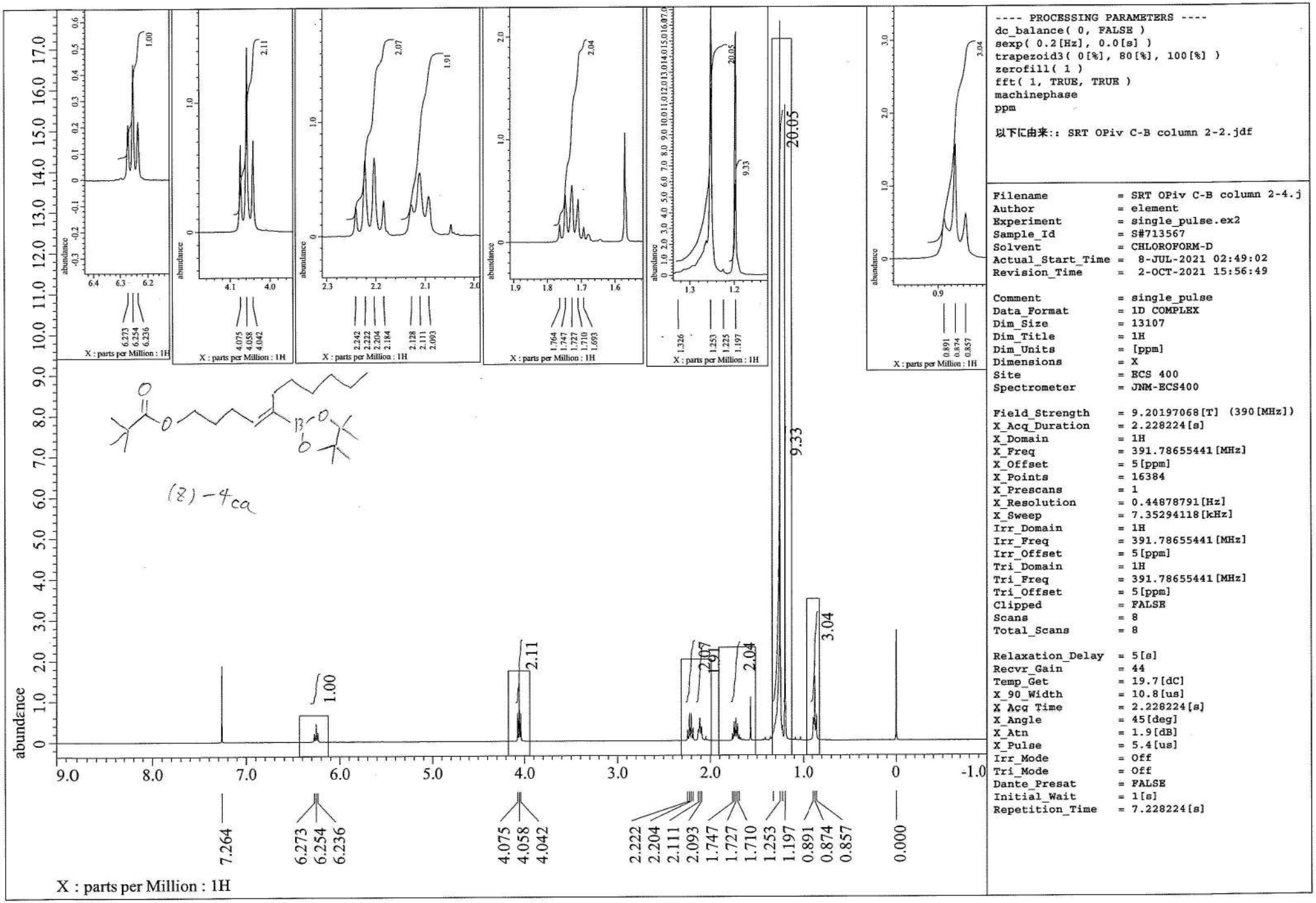
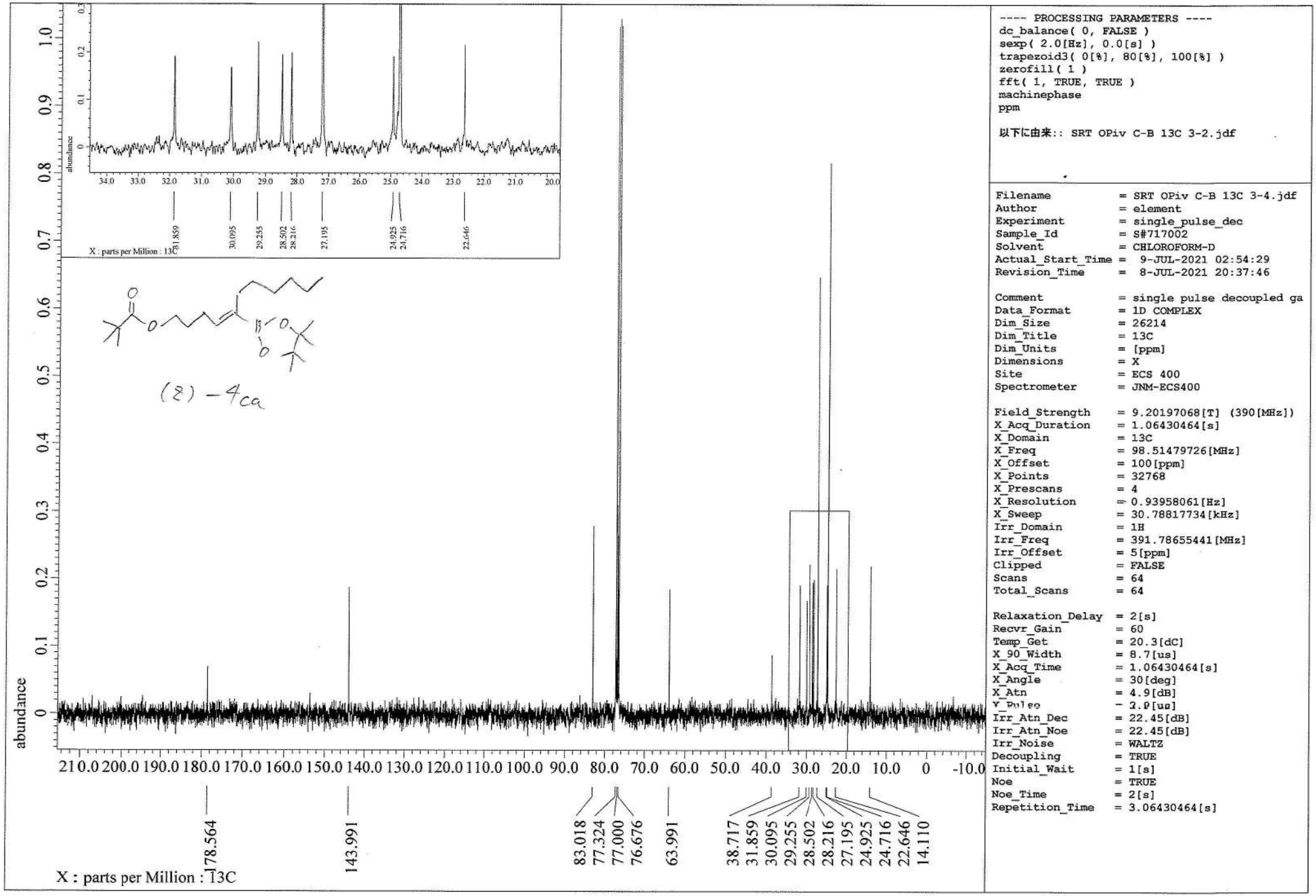
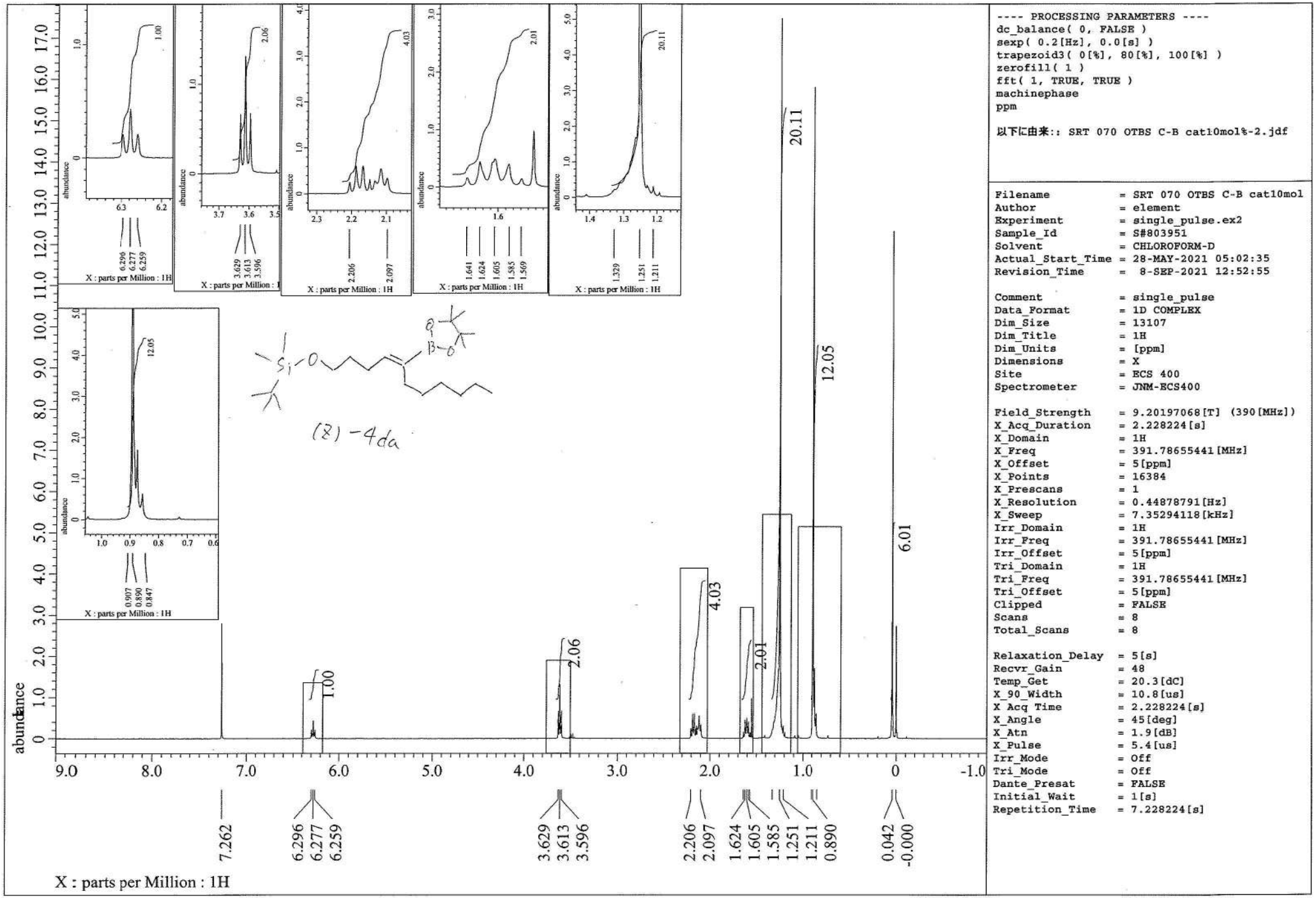
6.33
1.00


---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid3(0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
以下に由来:: SRT 034 C7 C-B 13C-2.jdf
Filename = SRT 034 C7 C-B 13C-4.jdf
Author = element
Experiment = single_pulse_dec
Sample_Id = 1
Solvent = CHLOROFORM-D
Actual_Start_Time = 16-OCT-2021 03:22:54
Revision_Time = 26-OCT-2021 14:34:00
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_Strength = 9.20197068[T] (390[MHz])
X_Acq_Duration = 1.06430464[s]
X_Domain = 13C
X_Freq = 98.51479726[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.93958061[Hz]
X_Sweep = 30.78817734[kHz]
Irr_Domain = 1H
Irr_Freq = 391.78655441[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 200
Total_Scans = 200
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 21.1[dC]
X_90_Width = 8.7[us]
X_Acq_Time = 1.06430464[s]
X_Angle = 30[deg]
X_Atn = 4.9[dB]
X_Pulse = 2.9[us]
Irr_Atn_Dec = 22.45[dB]
Irr_Atn_Noe = 22.45[dB]
Irr_Noise = WALTZ
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.06430464[s]
(Z)-4ba
abundance
X : parts per Million : 13C
145.984
82.894
77.324
77.000
76.676
31.897
31.831
30.162
29.513
29.217
28.531
28.493
24.802
24.716
22.675
14.120

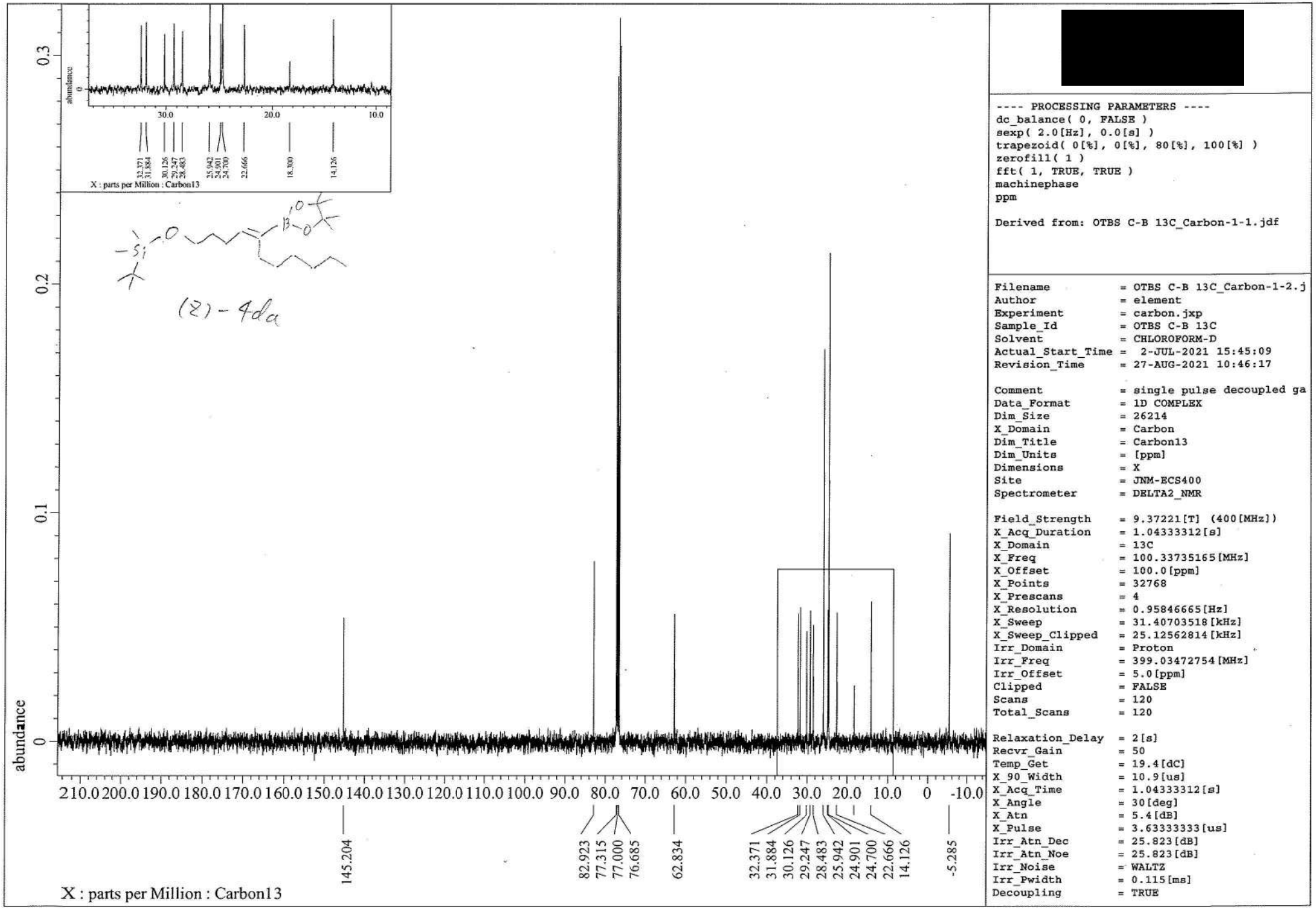

(Z)-4ca
X : parts per Million : 1H
abundance
7.264
6.273
6.254
6.236
4.075
4.058
4.042
2.222
2.204
2.111
2.093
1.747
1.727
1.710
1.253
1.197
0.891
0.874
0.857
0.000
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid3(0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
以下に由来:: SRT OPiv C-B column 2-2.jdf
Filename = SRT OPiv C-B column 2-4.j
Author = element
Experiment = single_pulse.ex2
Sample_Id = S#713567
Solvent = CHLOROFORM-D
Actual_Start_Time = 8-JUL-2021 02:49:02
Revision_Time = 2-OCT-2021 15:56:49
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
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 = 44
Temp_Get = 19.7[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]

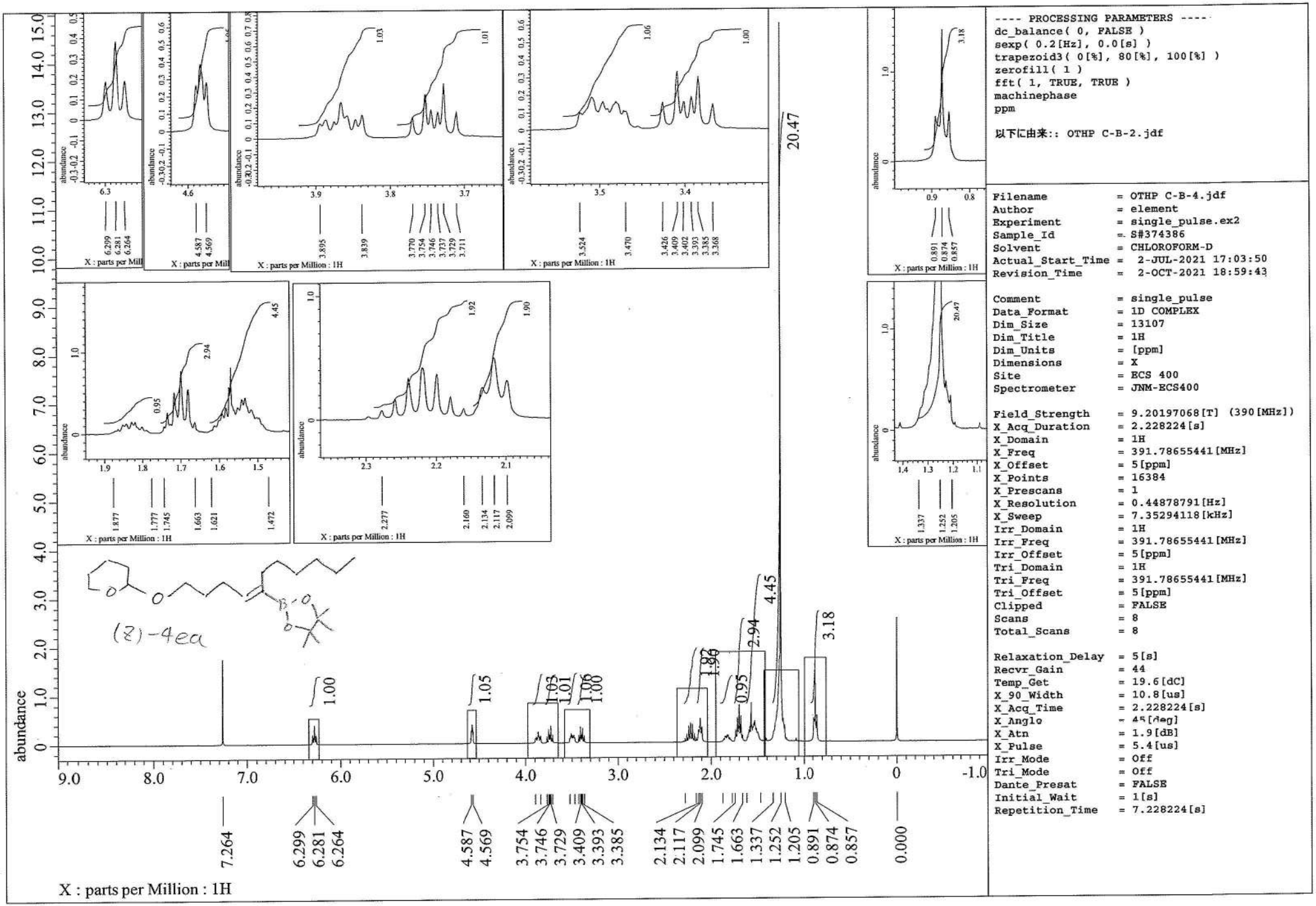

---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid3(0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
以下に由来:: SRT OPiv C-B 13C 3-2.jdf
Filename = SRT OPiv C-B 13C 3-4.jdf
Author = element
Experiment = single_pulse_dec
Sample_Id = S#717002
Solvent = CHLOROFORM-D
Actual_Start_Time = 9-JUL-2021 02:54:29
Revision_Time = 8-JUL-2021 20:37:46
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_Strength = 9.20197068[T] (390[MHz])
X_Acq_Duration = 1.06430464[s]
X_Domain = 13C
X_Freq = 98.51479726[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.93958061[Hz]
X_Sweep = 30.78817734[kHz]
Irr_Domain = 1H
Irr_Freq = 391.78655441[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 64
Total_Scans = 64
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 20.3[dC]
X_90_Width = 8.7[us]
X_Acq_Time = 1.06430464[s]
X_Angle = 30[deg]
X_Atn = 4.9[dB]
Irr_Atn_Dec = 22.45[dB]
Irr_Atn_Noe = 22.45[dB]
Irr_Noise = WALTZ
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.06430464[s]
(E)-4ca
abundance
X : parts per Million : 13C
178.564
143.991
83.018
77.324
77.000
76.676
63.991
38.717
31.859
30.095
29.255
28.502
28.216
27.195
24.925
24.716
22.646
14.110

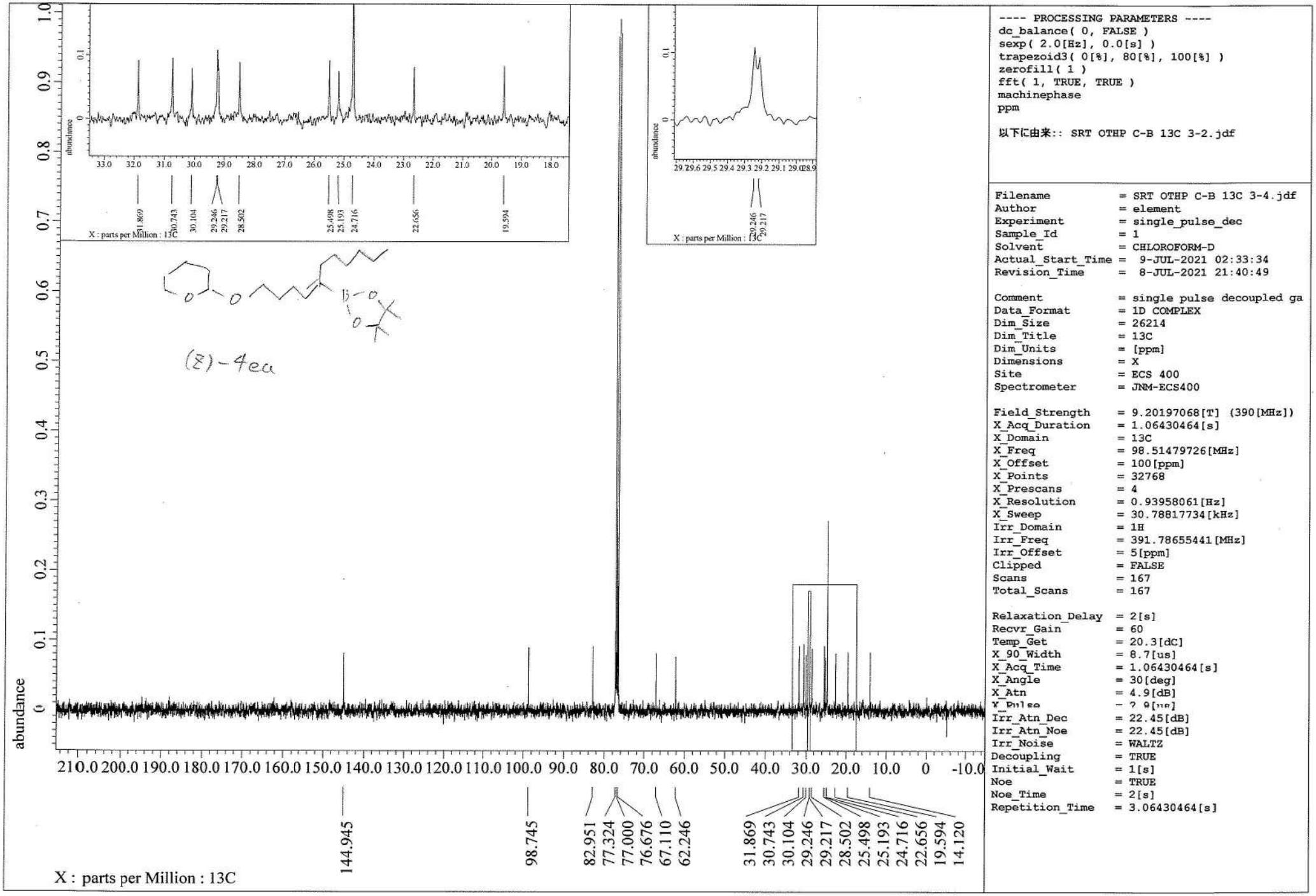


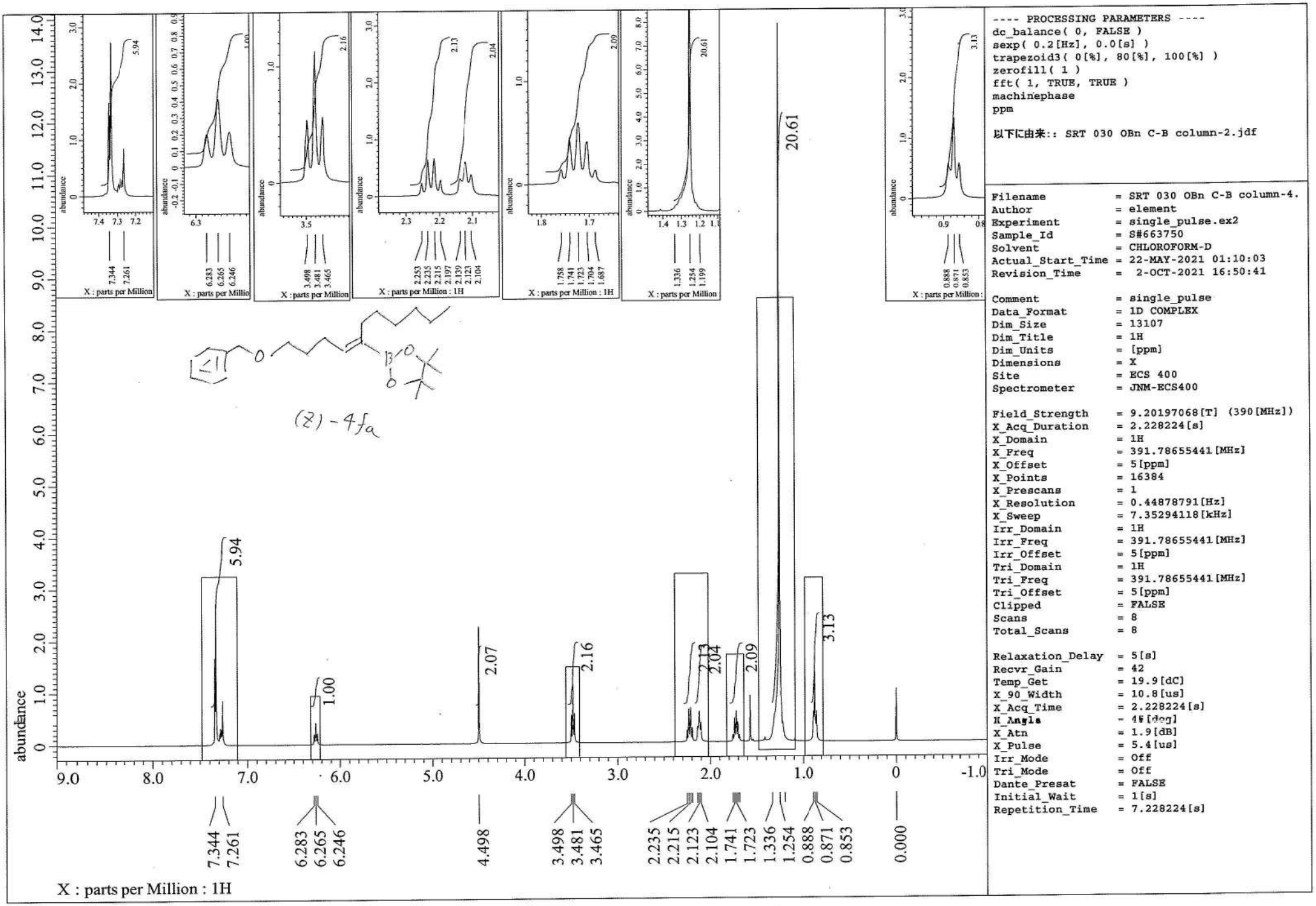

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

以下に由来:: SRT 070 OTBS C-B cat10mol%-2.jdf
```

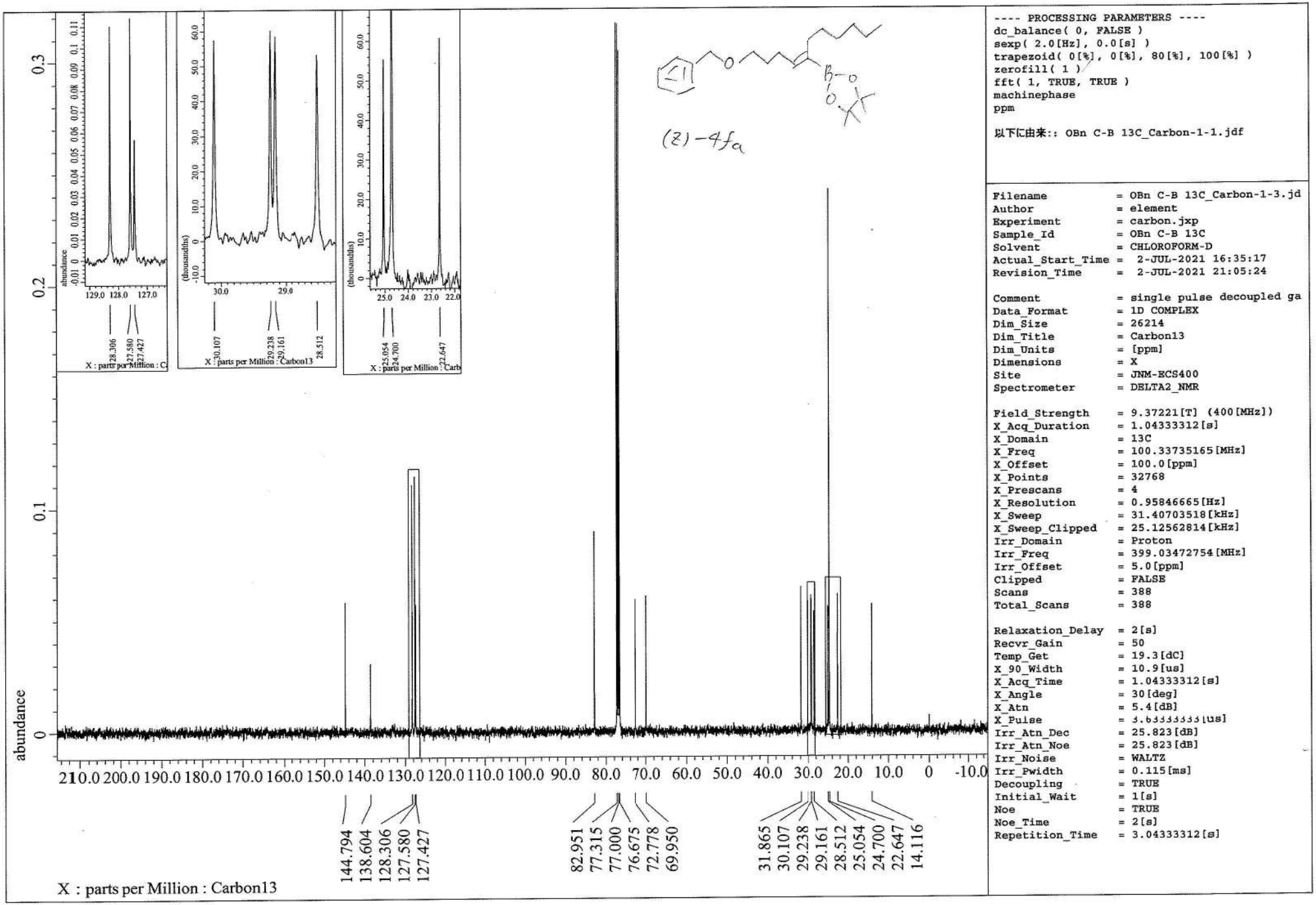
Filename	= SRT 070 OTBS C-B cat10mol
Author	= element
Experiment	= single_pulse.ex2
Sample_Id	= S#803951
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 28-MAY-2021 05:02:35
Revision_Time	= 8-SEP-2021 12:52:55
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
Dim_Title	= 1H
Dim_Units	= [ppm]
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	= 48
Temp_Get	= 20.3[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]

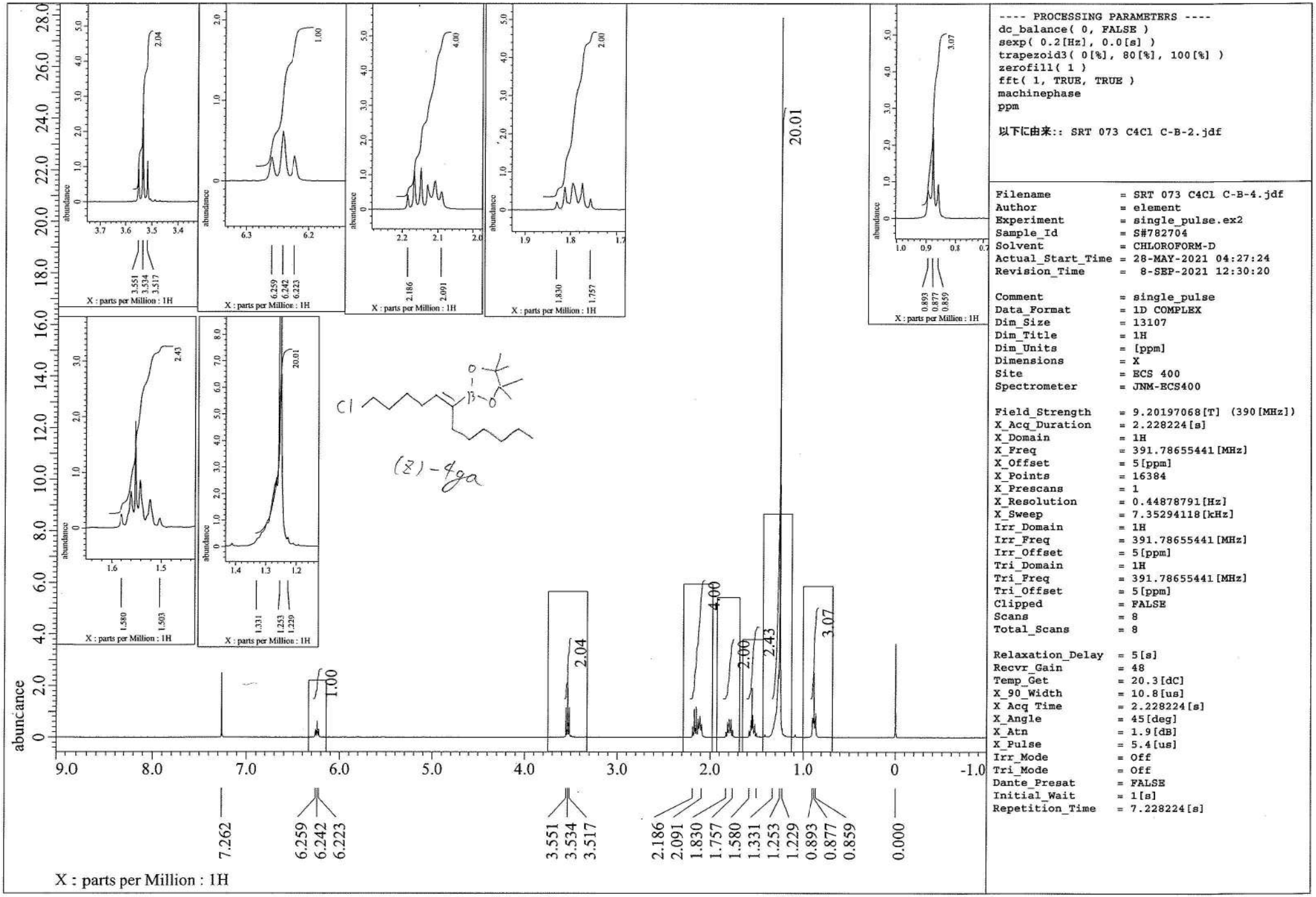

[redacted]
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: OTBS C-B 13C_Carbon-1-1.jdf
Filename = OTBS C-B 13C_Carbon-1-2.j
Author = element
Experiment = carbon.jxp
Sample_Id = OTBS C-B 13C
Solvent = CHLOROFORM-D
Actual_Start_Time = 2-JUL-2021 15:45:09
Revision_Time = 27-AUG-2021 10:46:17
Comment = single pulse decoupled ga
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 = 120
Total_Scans = 120
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 19.4[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
(E)-4da
abundance
X : parts per Million : Carbon13
145.204
82.923
77.315
77.000
76.685
62.834
32.371
31.884
30.126
29.247
28.483
25.942
24.901
24.700
22.666
14.126
-5.285


(Z)-4ea
X : parts per Million : 1H
abundance
20.47
4.45
3.18
2.94
1.92
1.96
1.00
1.05
1.03
1.01
1.06
0.95
7.264
6.299
6.281
6.264
4.587
4.569
3.754
3.746
3.729
3.409
3.393
3.385
2.134
2.117
2.099
1.745
1.663
1.337
1.252
1.205
0.891
0.874
0.857
0.000
---- 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:: OTHP C-B-2.jdf
Filename = OTHP C-B-4.jdf
Author = element
Experiment = single_pulse.ex2
Sample_Id = S#374386
Solvent = CHLOROFORM-D
Actual_Start_Time = 2-JUL-2021 17:03:50
Revision_Time = 2-OCT-2021 18:59:43
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
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 = 44
Temp_Get = 19.6[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]


abundance
X : parts per Million : 13C
144.945
98.745
82.951
77.324
77.000
76.676
67.110
62.246
31.869
30.743
30.104
29.246
29.217
28.502
25.498
25.193
24.716
22.656
19.594
14.120
(E)-4ea
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid3(0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
以下に由来:: SRT OTHP C-B 13C 3-2.jdf
Filename = SRT OTHP C-B 13C 3-4.jdf
Author = element
Experiment = single_pulse_dec
Sample_Id = 1
Solvent = CHLOROFORM-D
Actual_Start_Time = 9-JUL-2021 02:33:34
Revision_Time = 8-JUL-2021 21:40:49
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_Strength = 9.20197068[T] (390[MHz])
X_Acq_Duration = 1.06430464[s]
X_Domain = 13C
X_Freq = 98.51479726[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.93958061[Hz]
X_Sweep = 30.78817734[kHz]
Irr_Domain = 1H
Irr_Freq = 391.78655441[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 167
Total_Scans = 167
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 20.3[dC]
X_90_Width = 8.7[us]
X_Acq_Time = 1.06430464[s]
X_Angle = 30[deg]
X_Atn = 4.9[dB]
Irr_Atn_Dec = 22.45[dB]
Irr_Atn_Noe = 22.45[dB]
Irr_Noise = WALTZ
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.06430464[s]

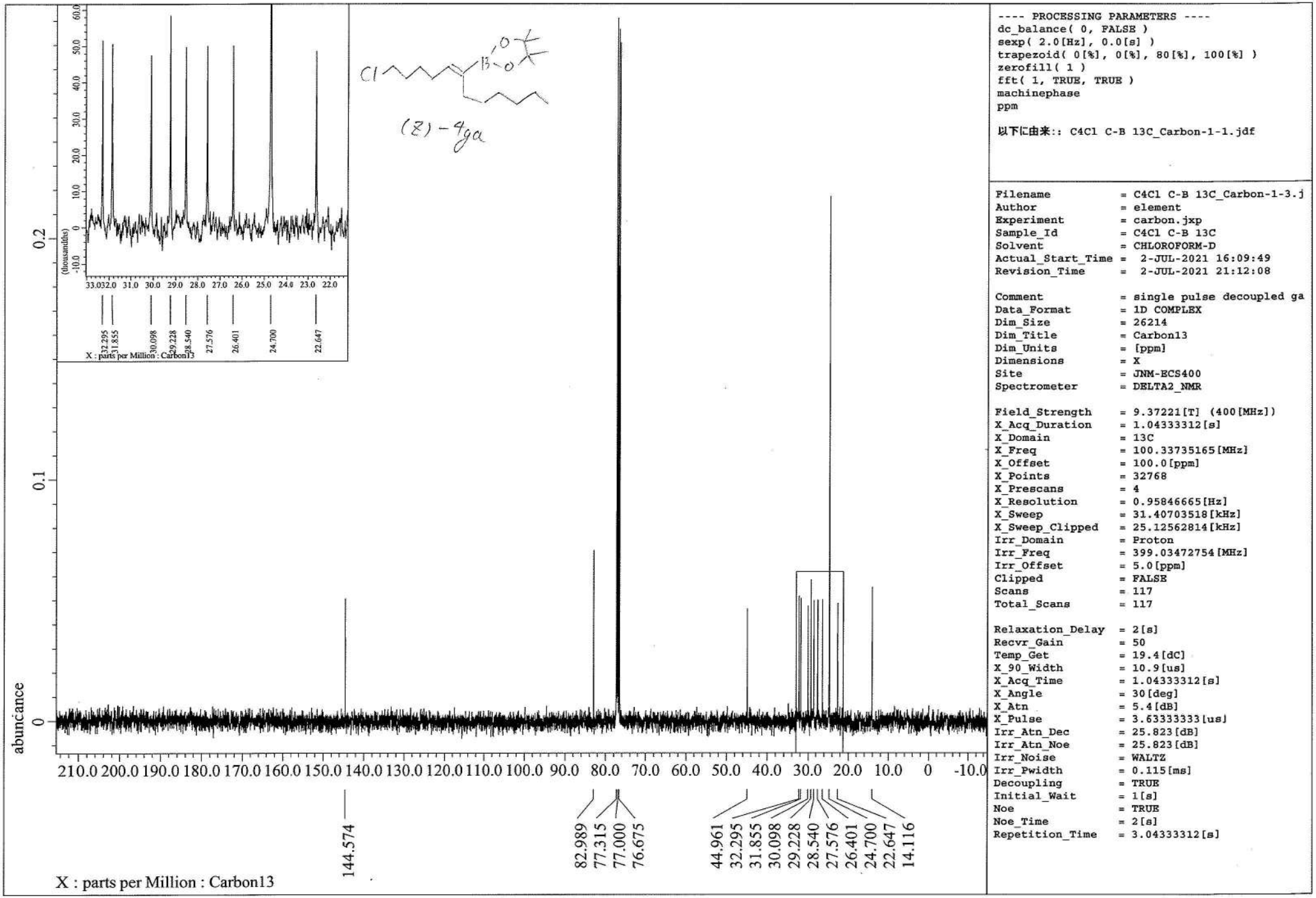

(Z)-4fa
X : parts per Million : 1H
abundance
5.94
1.00
2.07
2.16
2.13
2.04
2.09
20.61
3.13
7.344
7.261
6.283
6.265
6.246
4.498
3.498
3.481
3.465
2.235
2.215
2.123
2.104
1.741
1.723
1.336
1.254
0.888
0.871
0.853
0.000
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid3(0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
以下に由来:: SRT 030 OBn C-B column-2.jdf
Filename = SRT 030 OBn C-B column-4.
Author = element
Experiment = single_pulse.ex2
Sample_Id = S#663750
Solvent = CHLOROFORM-D
Actual_Start_Time = 22-MAY-2021 01:10:03
Revision_Time = 2-OCT-2021 16:50:41
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
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 = 42
Temp_Get = 19.9[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]

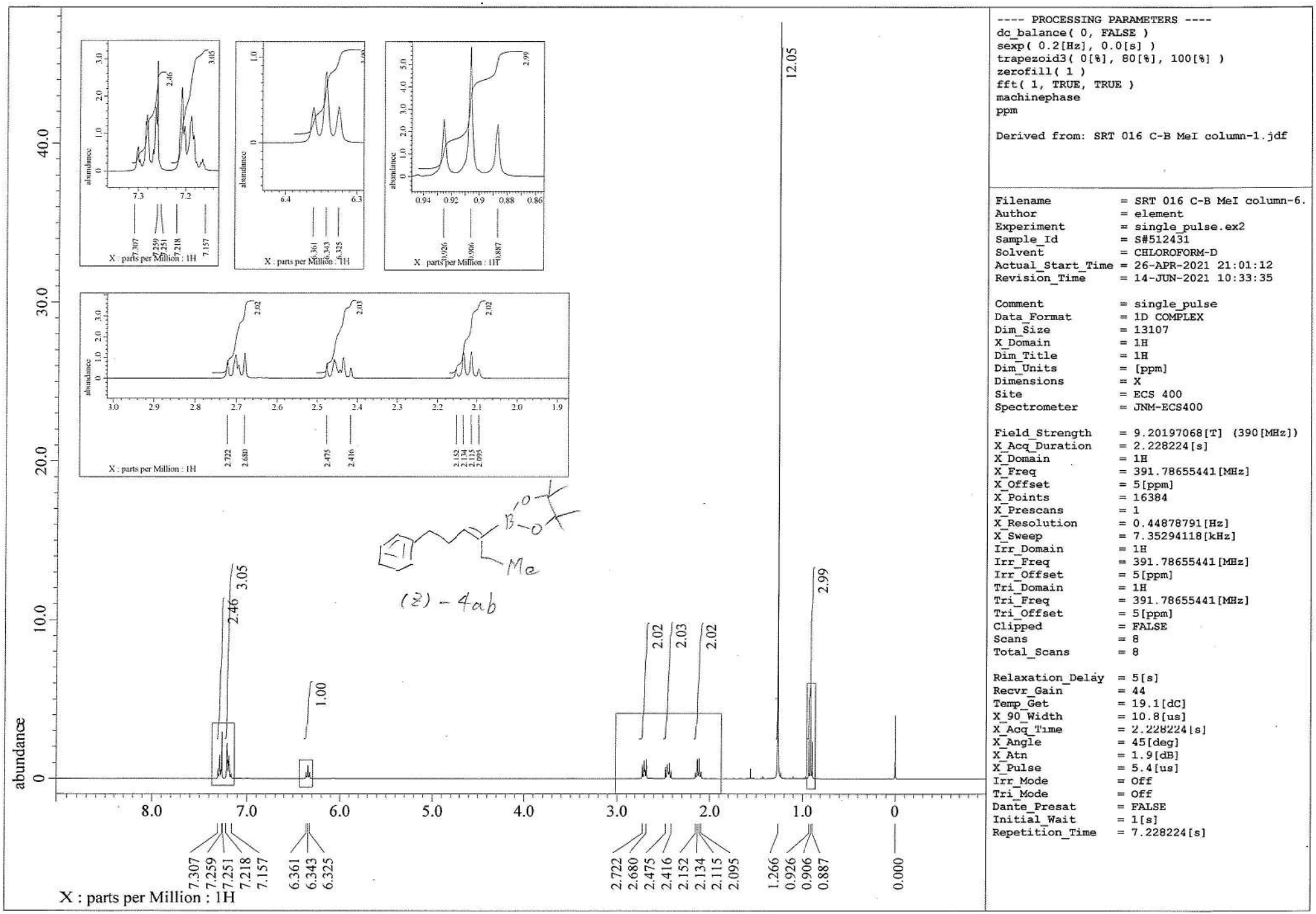

(Z)-4fa
abundance
X : parts per Million : Carbon13
144.794
138.604
128.306
127.580
127.427
82.951
77.315
77.000
76.675
72.778
69.950
31.865
30.107
29.238
29.161
28.512
25.054
24.700
22.647
14.116
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
以下に由来:: OBn C-B 13C_Carbon-1-1.jdf
Filename = OBn C-B 13C_Carbon-1-3.jd
Author = element
Experiment = carbon.jxp
Sample_Id = OBn C-B 13C
Solvent = CHLOROFORM-D
Actual_Start_Time = 2-JUL-2021 16:35:17
Revision_Time = 2-JUL-2021 21:05:24
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
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 = 388
Total_Scans = 388
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 19.3[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] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

以下に由来:: SRT 073 C4Cl C-B-2.jdf
```

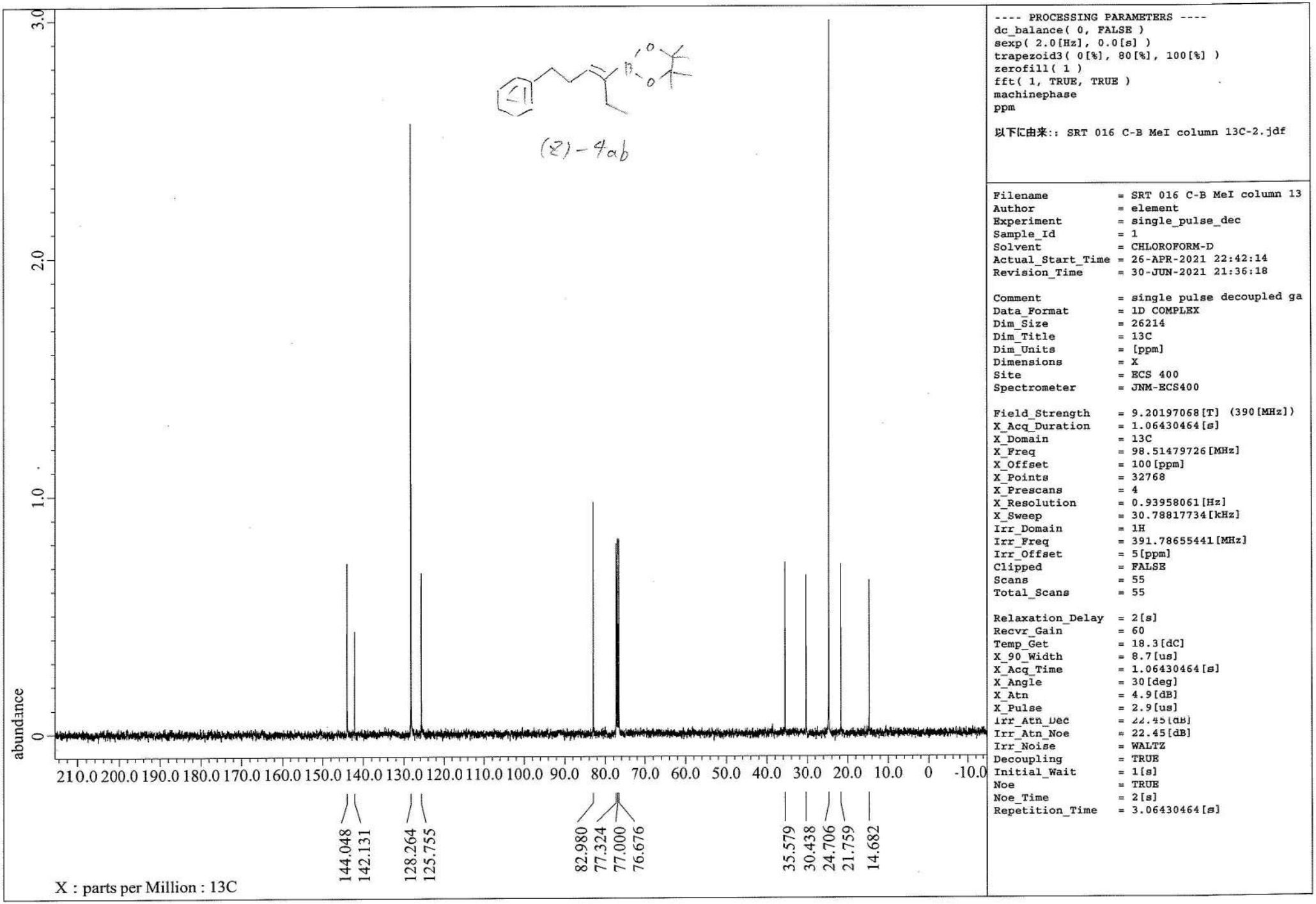
Filename	= SRT 073 C4Cl C-B-4.jdf
Author	= element
Experiment	= single_pulse.ex2
Sample_Id	= S#782704
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 28-MAY-2021 04:27:24
Revision_Time	= 8-SEP-2021 12:30:20
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
Dim_Title	= 1H
Dim_Units	= [ppm]
Dimensions	= 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	= 48
Temp_Get	= 20.3[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]


(Z)-4ga
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
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:: C4Cl C-B 13C_Carbon-1-1.jdf
Filename = C4Cl C-B 13C_Carbon-1-3.j
Author = element
Experiment = carbon.jxp
Sample_Id = C4Cl C-B 13C
Solvent = CHLOROFORM-D
Actual_Start_Time = 2-JUL-2021 16:09:49
Revision_Time = 2-JUL-2021 21:12:08
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
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 = 117
Total_Scans = 117
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 19.4[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]
abundance
0
0.1
0.2
210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0
144.574
82.989
77.315
77.000
76.675
44.961
32.295
31.855
30.098
29.228
28.540
27.576
26.401
24.700
22.647
14.116
X : parts per Million : Carbon13
(thousandths)
33.0 32.0 31.0 30.0 29.0 28.0 27.0 26.0 25.0 24.0 23.0 22.0
32.295
31.855
30.098
29.228
28.540
27.576
26.401
24.700
22.647
X : parts per Million : Carbon13



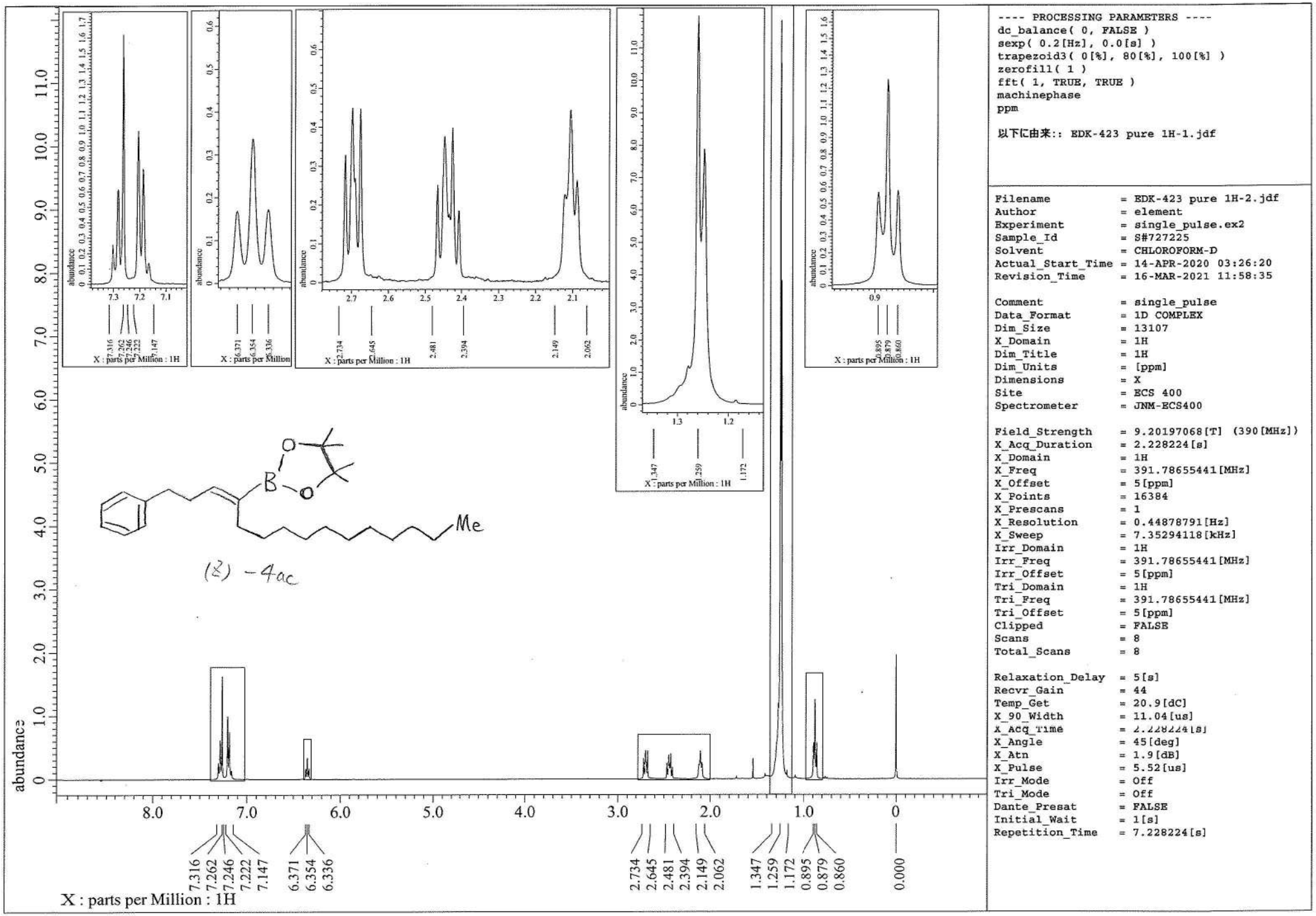

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: SRT 016 C-B MeI column-1.jdf
```

```
Filename            = SRT 016 C-B MeI column-6.
Author              = element
Experiment          = single_pulse.ex2
Sample_Id           = S#512431
Solvent             = CHLOROFORM-D
Actual_Start_Time   = 26-APR-2021 21:01:12
Revision_Time       = 14-JUN-2021 10:33:35

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          = 44
Temp_Get            = 19.1[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]
```



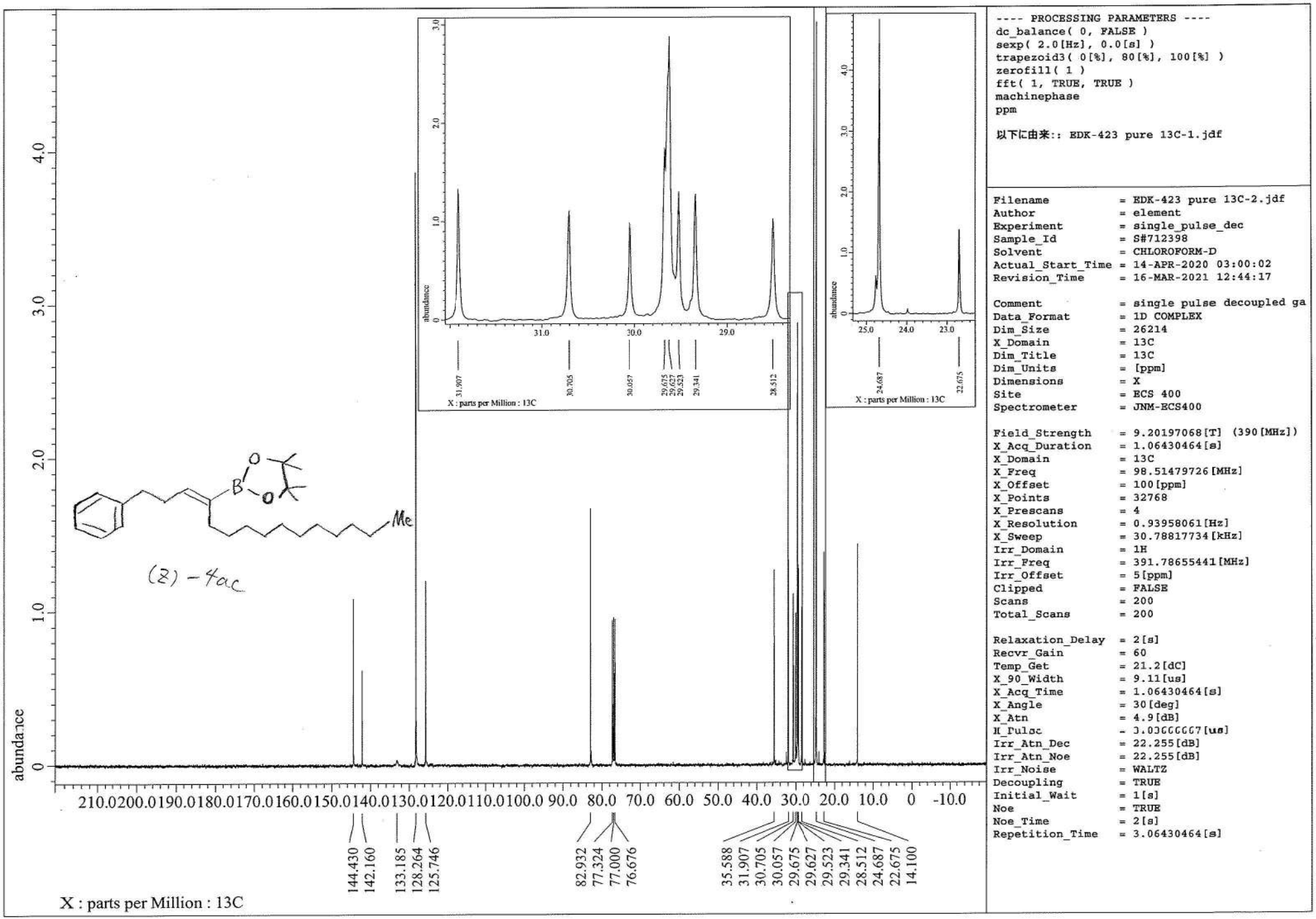

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

以下に由来:: SRT 016 C-B MeI column 13C-2.jdf
```

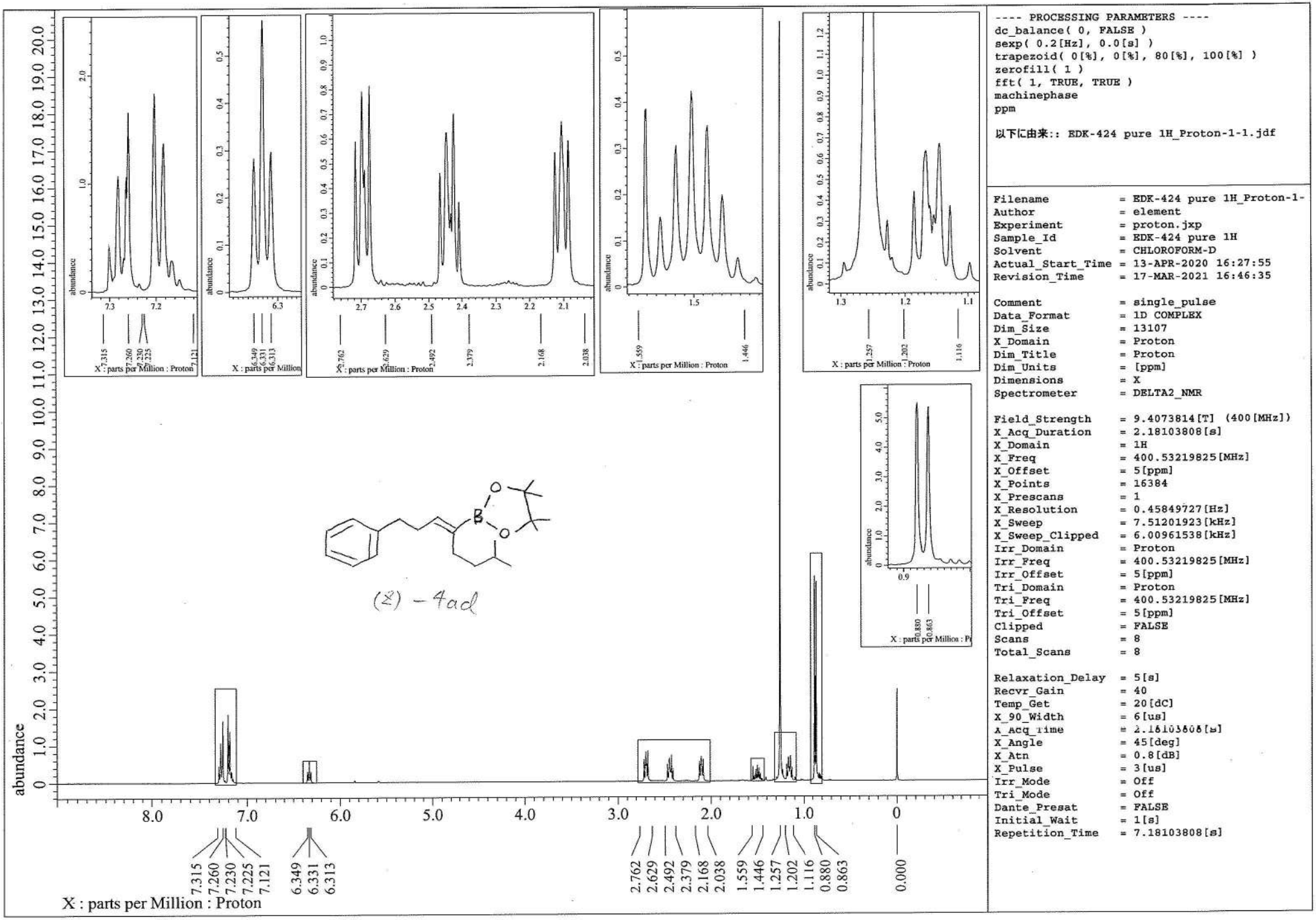
Filename	= SRT 016 C-B MeI column 13
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= 1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 26-APR-2021 22:42:14
Revision_Time	= 30-JUN-2021 21:36:18
Comment	= single pulse decoupled ga
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
Dim_Title	= 13C
Dim_Units	= [ppm]
Dimensions	= X
Site	= ECS 400
Spectrometer	= JNM-ECS400
Field_Strength	= 9.20197068[T] (390[MHz])
X_Acq_Duration	= 1.06430464[s]
X_Domain	= 13C
X_Freq	= 98.51479726[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.93958061[Hz]
X_Sweep	= 30.78817734[kHz]
Irr_Domain	= 1H
Irr_Freq	= 391.78655441[MHz]
Irr_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 55
Total_Scans	= 55
Relaxation_Delay	= 2[s]
Recvr_Gain	= 60
Temp_Get	= 18.3[dC]
X_90_Width	= 8.7[us]
X_Acq_Time	= 1.06430464[s]
X_Angle	= 30[deg]
X_Atn	= 4.9[dB]
X_Pulse	= 2.9[us]
Irr_Atn_Dec	= 22.45[dB]
Irr_Atn_Noe	= 22.45[dB]
Irr_Noise	= WALTZ
Decoupling	= TRUE
Initial_Wait	= 1[s]
Noe	= TRUE
Noe_Time	= 2[s]
Repetition_Time	= 3.06430464[s]

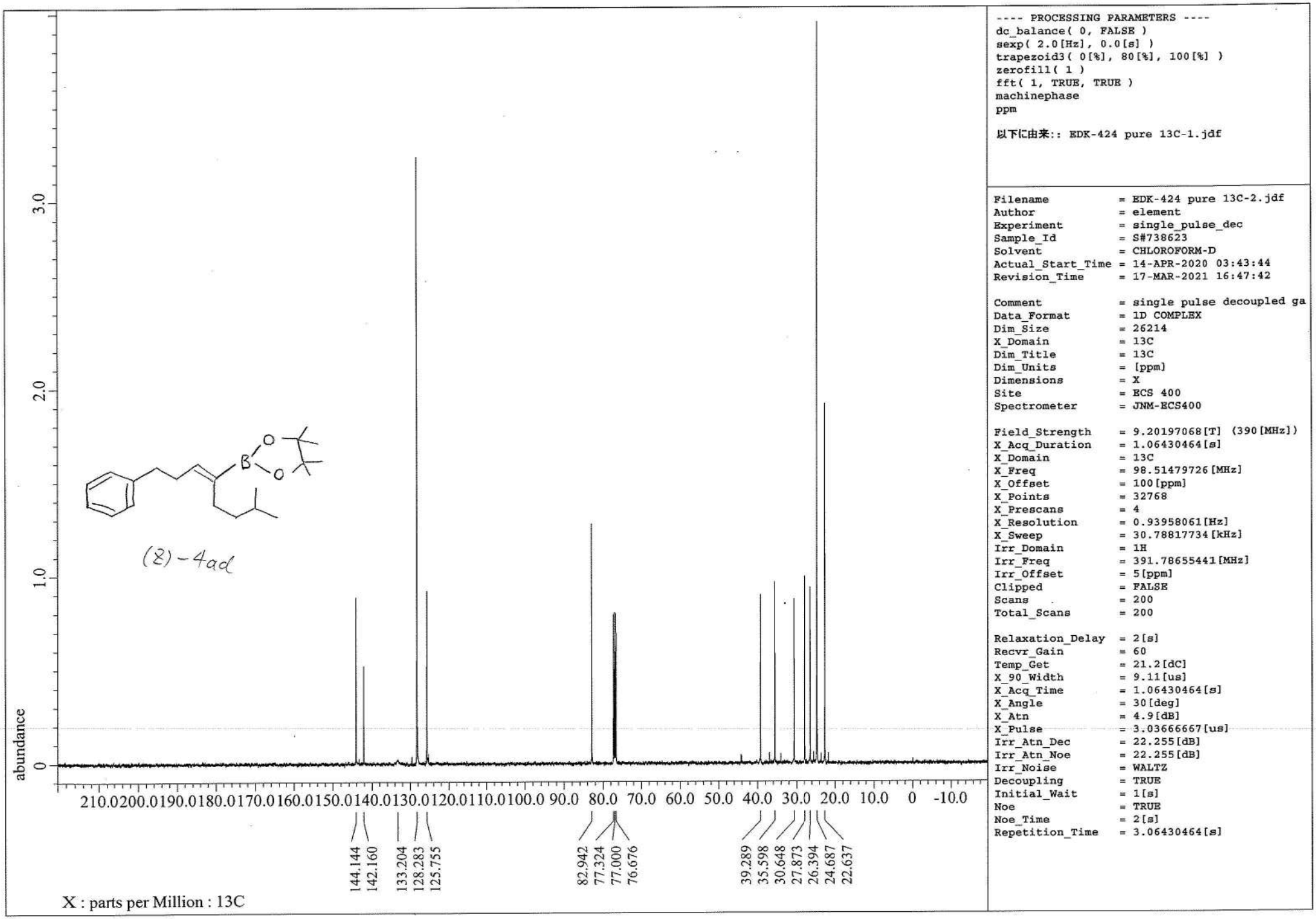


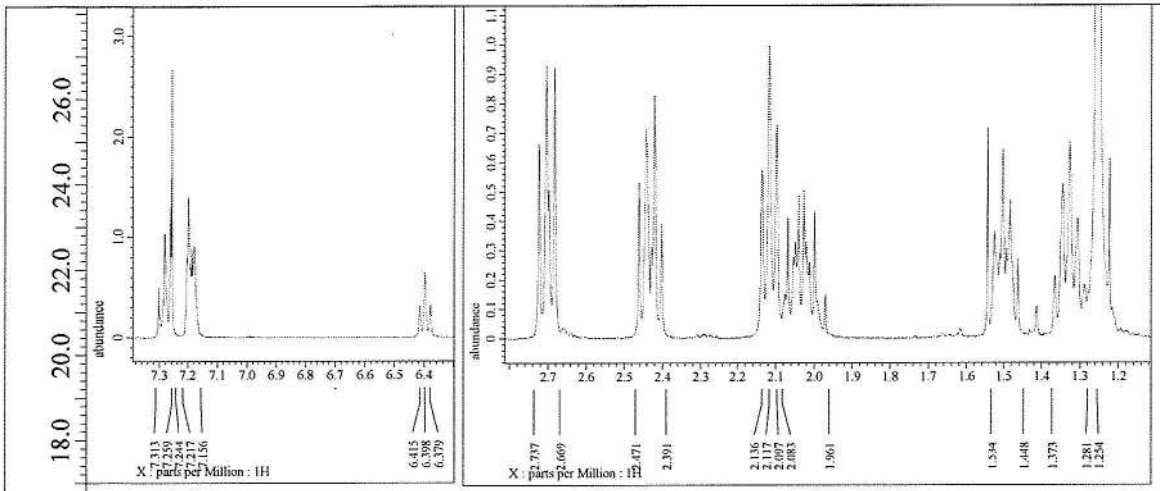

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

以下に由来:: EDK-423 pure 1H-1.jdf
```

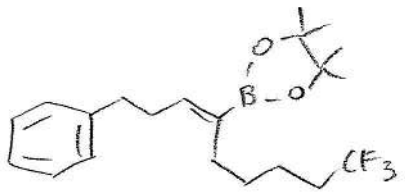
Filename	= EDK-423 pure 1H-2.jdf
Author	= element
Experiment	= single_pulse.ex2
Sample_Id	= S#727225
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 14-APR-2020 03:26:20
Revision_Time	= 16-MAR-2021 11:58:35
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= 1H
Dim_Title	= 1H
Dim_Units	= [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	= 44
Temp_Get	= 20.9[dC]
X_90_Width	= 11.04[us]
X_Acq_Time	= 2.228224[s]
X_Angle	= 45[deg]
X_Atn	= 1.9[dB]
X_Pulse	= 5.52[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.228224[s]


---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid3(0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
以下に由来:: EDK-423 pure 13C-1.jdf
Filename = EDK-423 pure 13C-2.jdf
Author = element
Experiment = single_pulse_dec
Sample_Id = S#712398
Solvent = CHLOROFORM-D
Actual_Start_Time = 14-APR-2020 03:00:02
Revision_Time = 16-MAR-2021 12:44:17
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = 13C
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_Strength = 9.20197068[T] (390[MHz])
X_Acq_Duration = 1.06430464[s]
X_Domain = 13C
X_Freq = 98.51479726[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.93958061[Hz]
X_Sweep = 30.78817734[kHz]
Irr_Domain = 1H
Irr_Freq = 391.78655441[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 200
Total_Scans = 200
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 21.2[dC]
X_90_Width = 9.11[us]
X_Acq_Time = 1.06430464[s]
X_Angle = 30[deg]
X_Atn = 4.9[dB]
X_Pulse = 3.03666667[us]
Irr_Atn_Dec = 22.255[dB]
Irr_Atn_Noe = 22.255[dB]
Irr_Noise = WALTZ
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.06430464[s]
(Z)-4ac
Me
abundance
X : parts per Million : 13C
144.430
142.160
133.185
128.264
125.746
82.932
77.324
77.000
76.676
35.588
31.907
30.705
30.057
29.675
29.627
29.523
29.341
28.512
24.687
22.675
14.100


---- 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:: EDK-424 pure 1H_Proton-1-1.jdf
Filename = EDK-424 pure 1H_Proton-1-
Author = element
Experiment = proton.jxp
Sample_Id = EDK-424 pure 1H
Solvent = CHLOROFORM-D
Actual_Start_Time = 13-APR-2020 16:27:55
Revision_Time = 17-MAR-2021 16:46:35
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 = 40
Temp_Get = 20[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]
(±) -4ad
abundance
X : parts per Million : Proton
7.315
7.260
7.230
7.225
7.121
6.349
6.331
6.313
2.762
2.629
2.492
2.379
2.168
2.038
1.559
1.446
1.257
1.202
1.116
0.880
0.863
0.000


---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid3(0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
以下に由来:: EDK-424 pure 13C-1.jdf
Filename = EDK-424 pure 13C-2.jdf
Author = element
Experiment = single_pulse_dec
Sample_Id = S#738623
Solvent = CHLOROFORM-D
Actual_Start_Time = 14-APR-2020 03:43:44
Revision_Time = 17-MAR-2021 16:47:42
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = 13C
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_Strength = 9.20197068[T] (390[MHz])
X_Acq_Duration = 1.06430464[s]
X_Domain = 13C
X_Freq = 98.51479726[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.93958061[Hz]
X_Sweep = 30.78817734[kHz]
Irr_Domain = 1H
Irr_Freq = 391.78655441[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 200
Total_Scans = 200
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 21.2[dC]
X_90_Width = 9.11[us]
X_Acq_Time = 1.06430464[s]
X_Angle = 30[deg]
X_Atn = 4.9[dB]
X_Pulse = 3.03666667[us]
Irr_Atn_Dec = 22.255[dB]
Irr_Atn_Noe = 22.255[dB]
Irr_Noise = WALTZ
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.06430464[s]
abundance
0
1.0
2.0
3.0
(E)-4ad
210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0
144.144
142.160
133.204
128.283
125.755
82.942
77.324
77.000
76.676
39.289
35.598
30.648
27.873
26.394
24.687
22.637
X : parts per Million : 13C

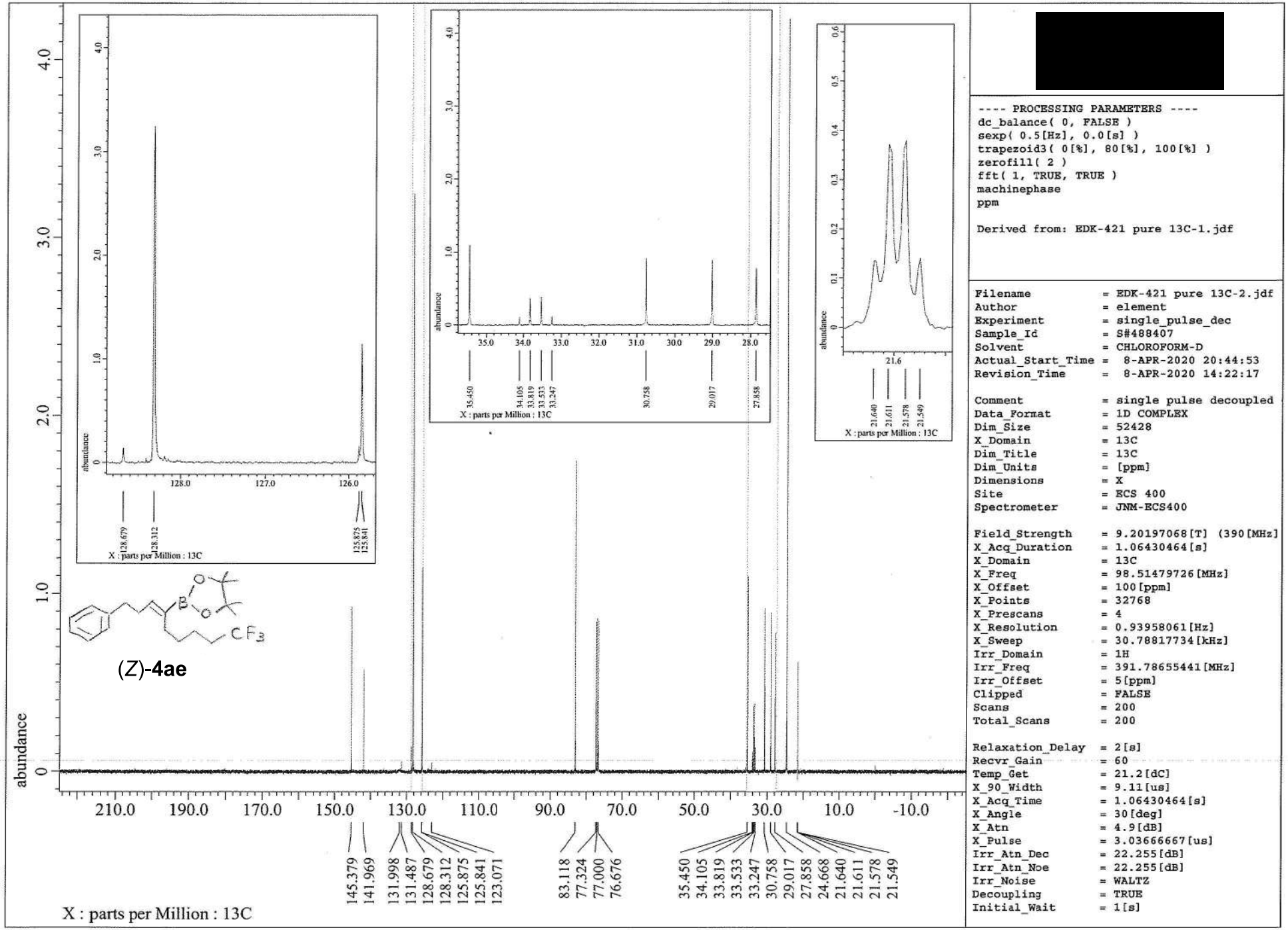




(*Z*)-**4ae**


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

Derived from: EDK-421 pure 1H-1.jdf
```

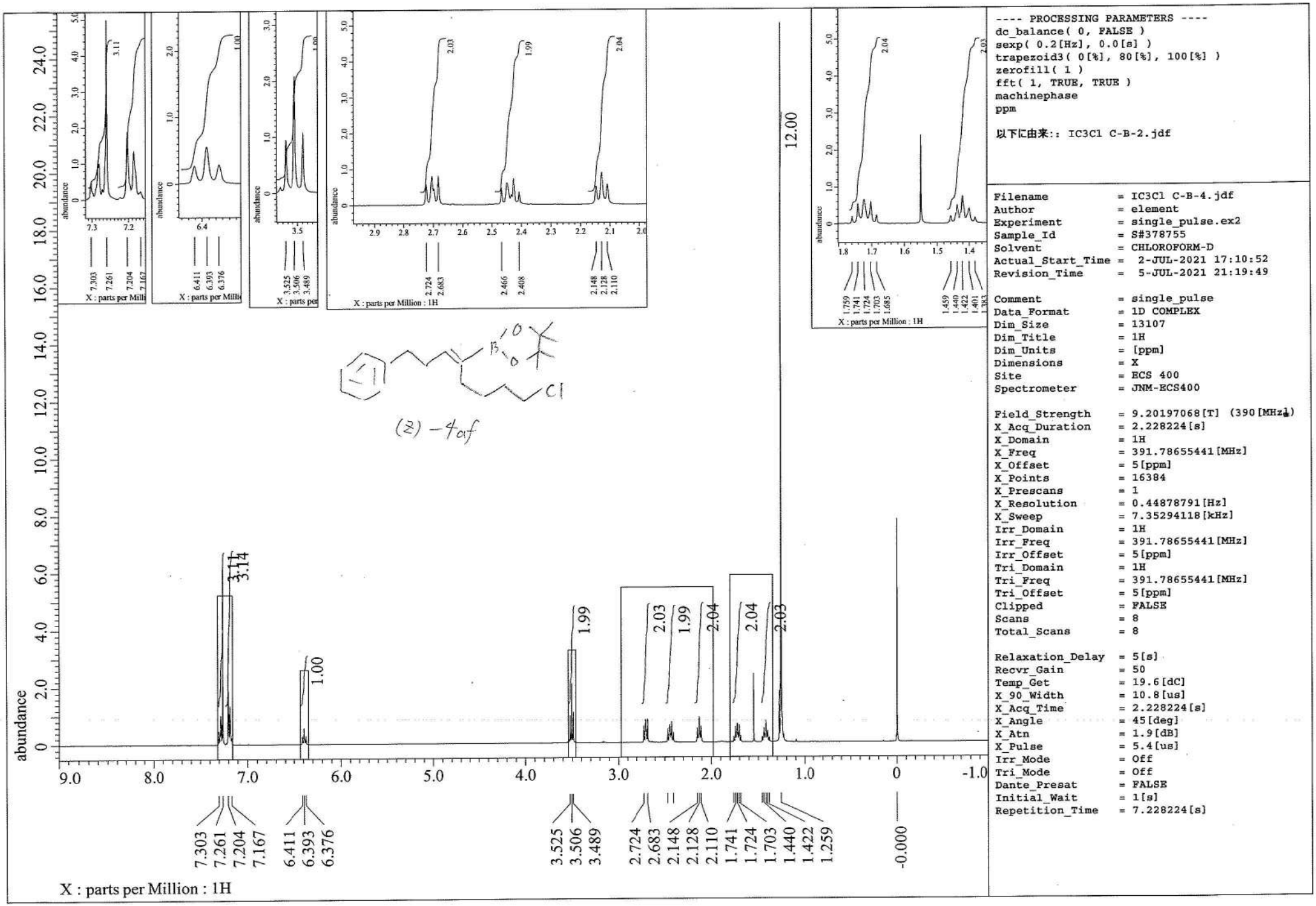
Filename	= EDK-421 pure 1H-2.jdf
Author	= element
Experiment	= single_pulse.ex2
Sample_Id	= S#476803
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 8-APR-2020 20:26:34
Revision_Time	= 16-JAN-2022 14:27:59
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= 1H
Dim_Title	= 1H
Dim_Units	= [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	= 44
Temp_Get	= 20.9[dC]
X_90_Width	= 11.04[us]
X_Acq_Time	= 2.228224[s]
X_Angle	= 45[deg]
X_Atn	= 1.9[dB]
X_Pulse	= 5.52[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.228224[s]

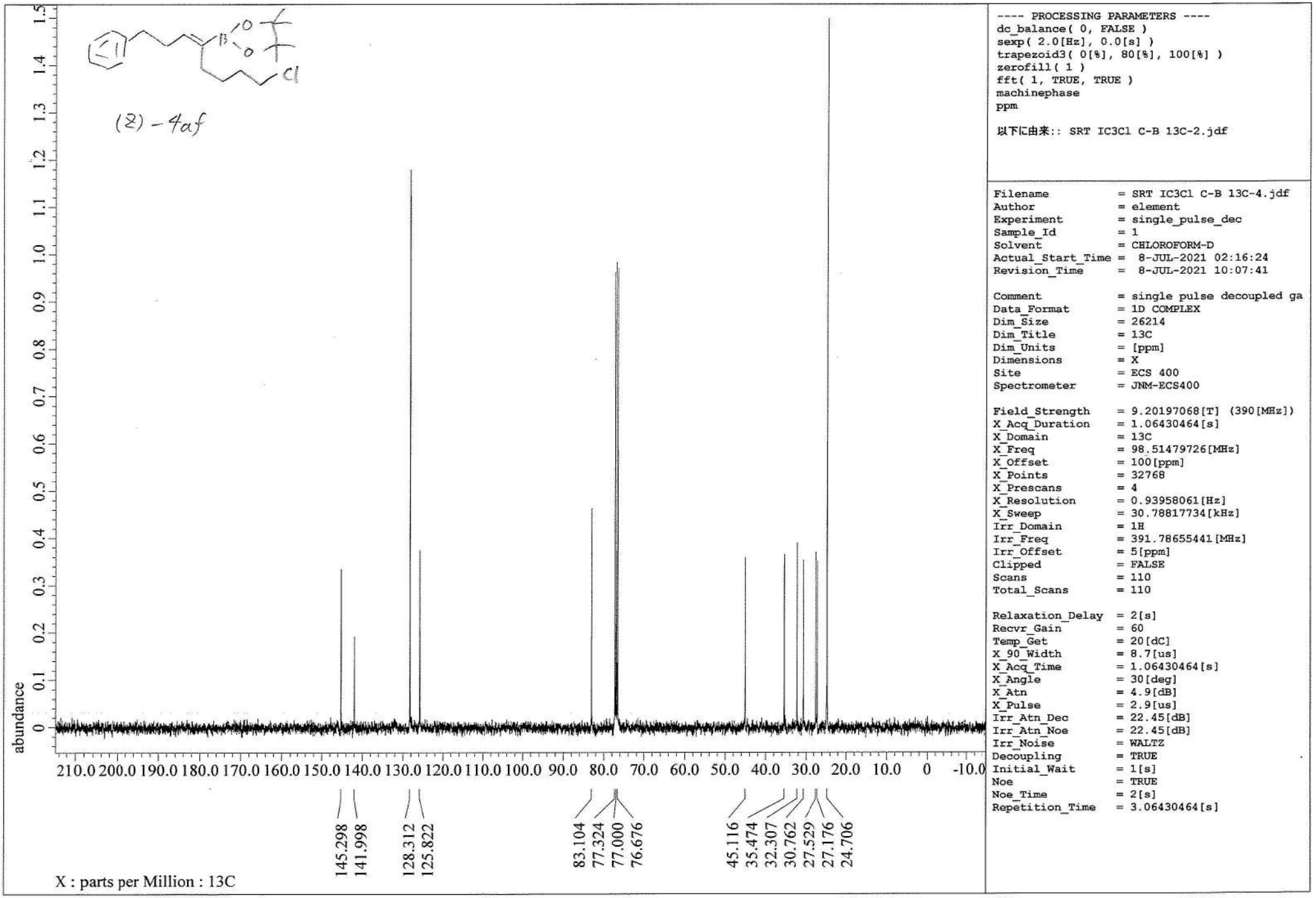


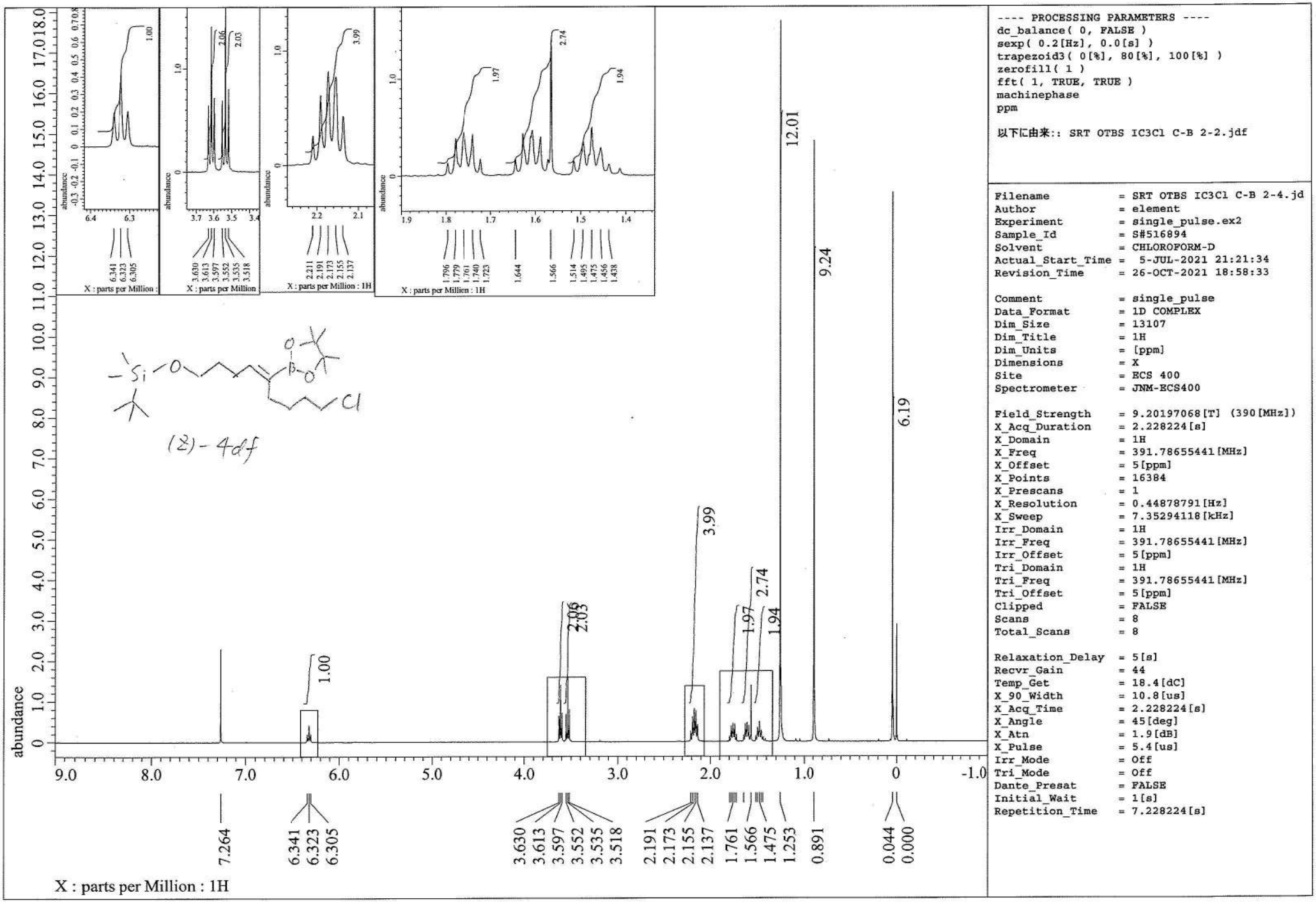
[redacted]

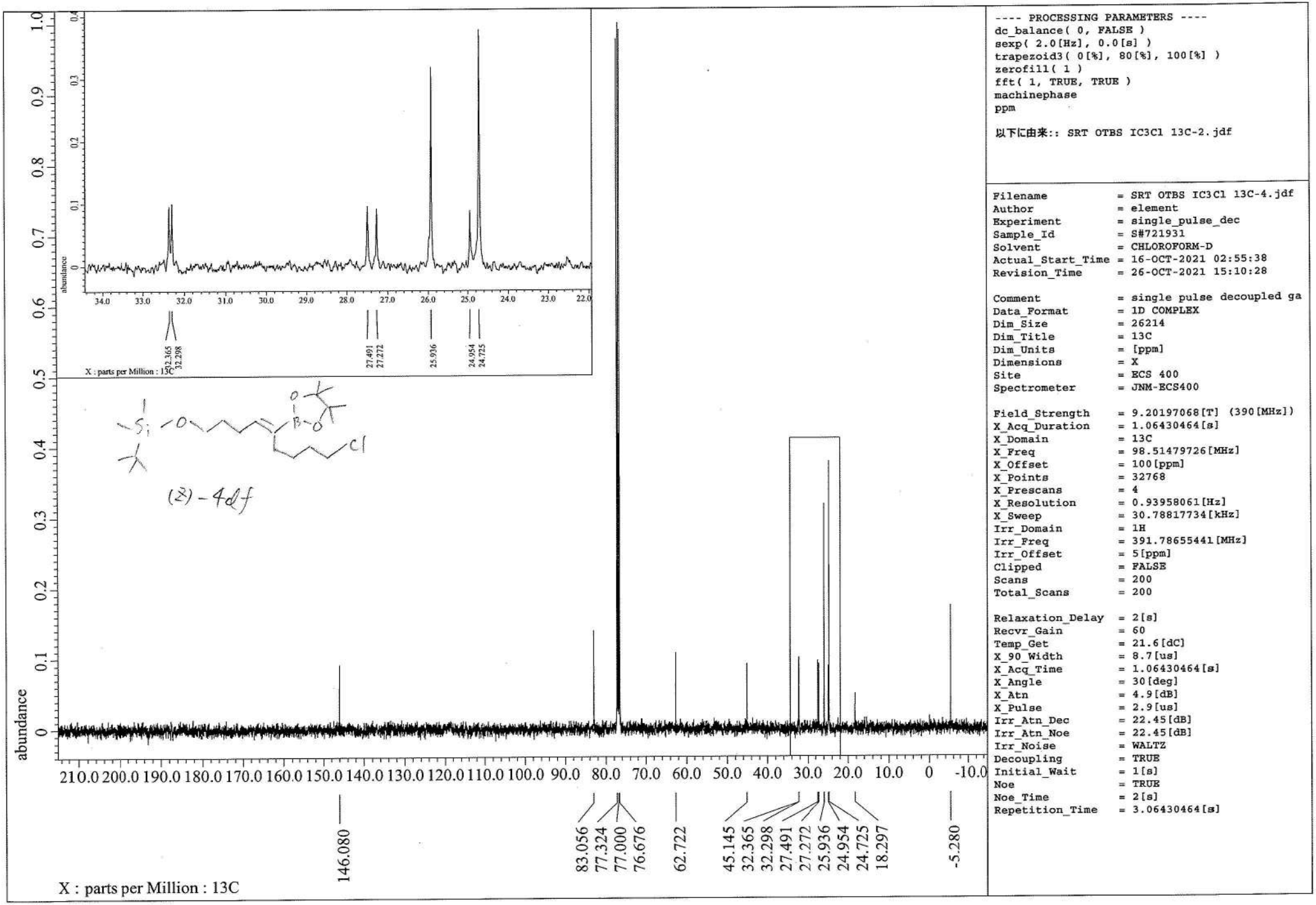
```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.5[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 2 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: EDK-421 pure 13C-1.jdf
```

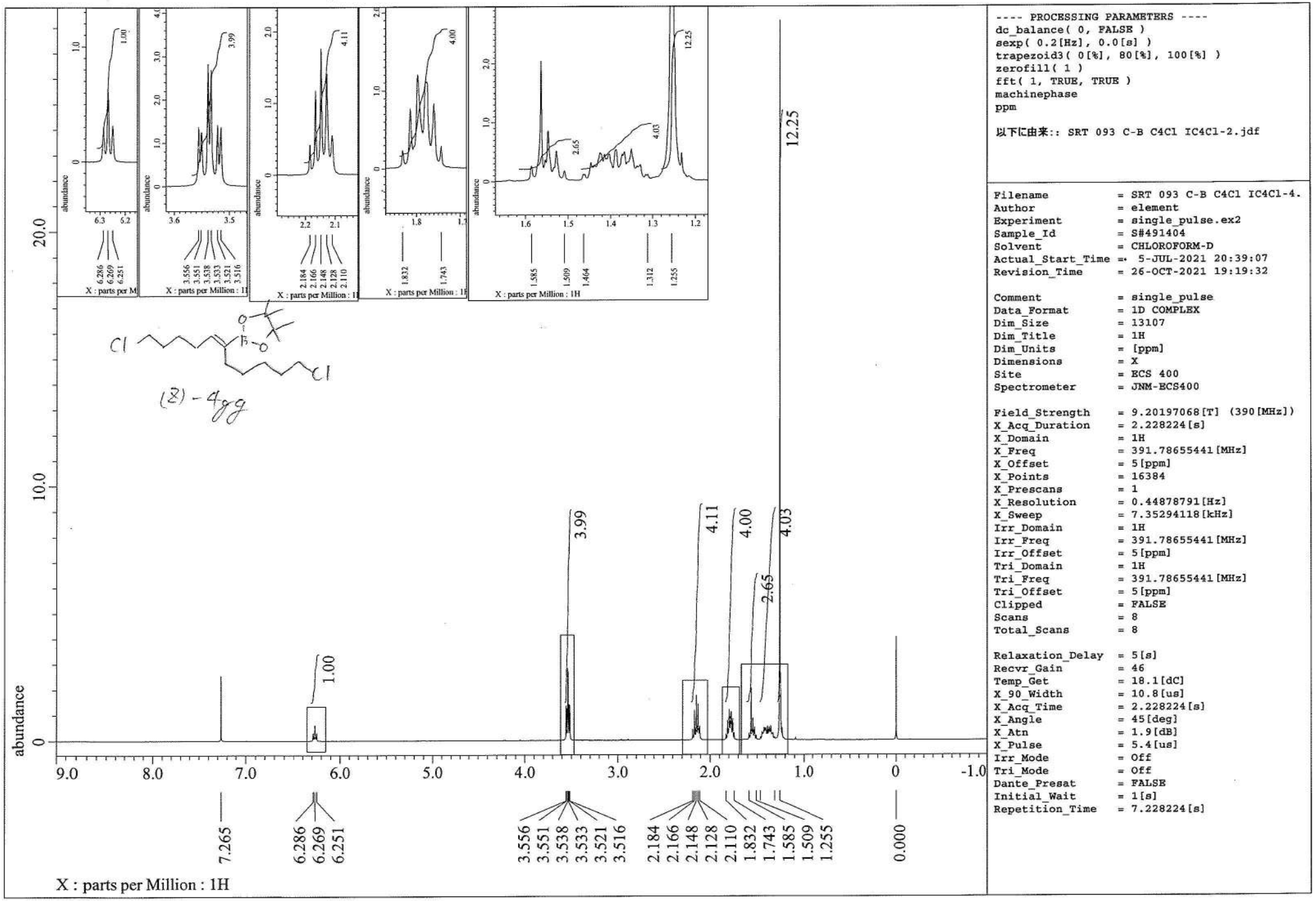
Filename	= EDK-421 pure 13C-2.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= S#488407
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 8-APR-2020 20:44:53
Revision_Time	= 8-APR-2020 14:22:17
Comment	= single pulse decoupled
Data_Format	= 1D COMPLEX
Dim_Size	= 52428
X_Domain	= 13C
Dim_Title	= 13C
Dim_Units	= [ppm]
Dimensions	= X
Site	= ECS 400
Spectrometer	= JNM-ECS400
Field_Strength	= 9.20197068[T] (390[MHz]
X_Acq_Duration	= 1.06430464[s]
X_Domain	= 13C
X_Freq	= 98.51479726[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.93958061[Hz]
X_Sweep	= 30.78817734[kHz]
Irr_Domain	= 1H
Irr_Freq	= 391.78655441[MHz]
Irr_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 200
Total_Scans	= 200
Relaxation_Delay	= 2[s]
Recvr_Gain	= 60
Temp_Get	= 21.2[dC]
X_90_Width	= 9.11[us]
X_Acq_Time	= 1.06430464[s]
X_Angle	= 30[deg]
X_Atn	= 4.9[dB]
X_Pulse	= 3.03666667[us]
Irr_Atn_Dec	= 22.255[dB]
Irr_Atn_Noe	= 22.255[dB]
Irr_Noise	= WALTZ
Decoupling	= TRUE
Initial_Wait	= 1[s]

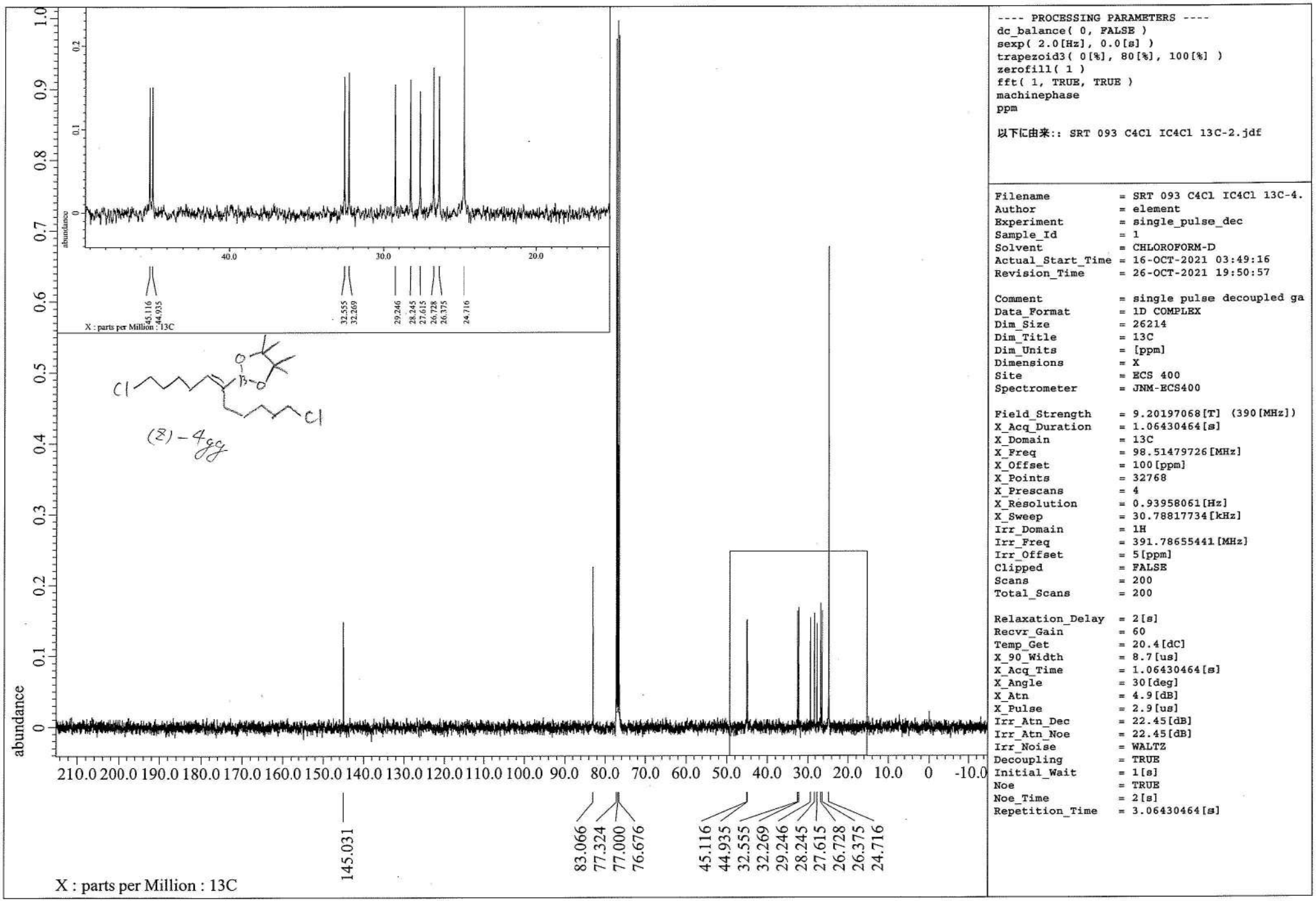

---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid3(0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
以下に由来:: IC3Cl C-B-2.jdf
Filename = IC3Cl C-B-4.jdf
Author = element
Experiment = single_pulse.ex2
Sample_Id = S#378755
Solvent = CHLOROFORM-D
Actual_Start_Time = 2-JUL-2021 17:10:52
Revision_Time = 5-JUL-2021 21:19:49
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
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 = 50
Temp_Get = 19.6[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]
(Z) -4af
abundance
X : parts per Million : 1H

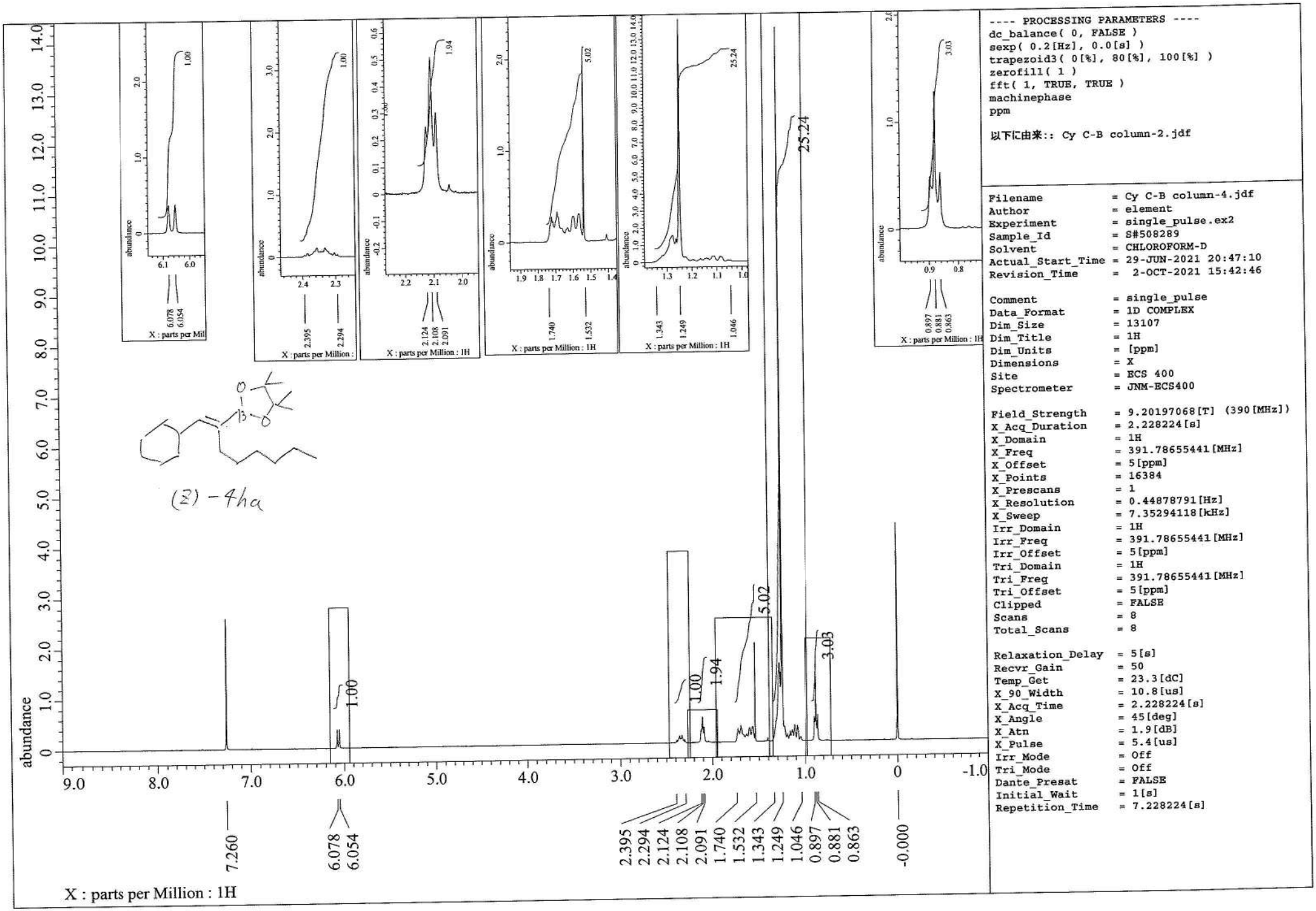

(Z)-4af
abundance
X : parts per Million : 13C
145.298
141.998
128.312
125.822
83.104
77.324
77.000
76.676
45.116
35.474
32.307
30.762
27.529
27.176
24.706
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid3(0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
以下に由来:: SRT IC3Cl C-B 13C-2.jdf
Filename = SRT IC3Cl C-B 13C-4.jdf
Author = element
Experiment = single_pulse_dec
Sample_Id = 1
Solvent = CHLOROFORM-D
Actual_Start_Time = 8-JUL-2021 02:16:24
Revision_Time = 8-JUL-2021 10:07:41
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_Strength = 9.20197068[T] (390[MHz])
X_Acq_Duration = 1.06430464[s]
X_Domain = 13C
X_Freq = 98.51479726[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.93958061[Hz]
X_Sweep = 30.78817734[kHz]
Irr_Domain = 1H
Irr_Freq = 391.78655441[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 110
Total_Scans = 110
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 20[dC]
X_90_Width = 8.7[us]
X_Acq_Time = 1.06430464[s]
X_Angle = 30[deg]
X_Atn = 4.9[dB]
X_Pulse = 2.9[us]
Irr_Atn_Dec = 22.45[dB]
Irr_Atn_Noe = 22.45[dB]
Irr_Noise = WALTZ
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.06430464[s]

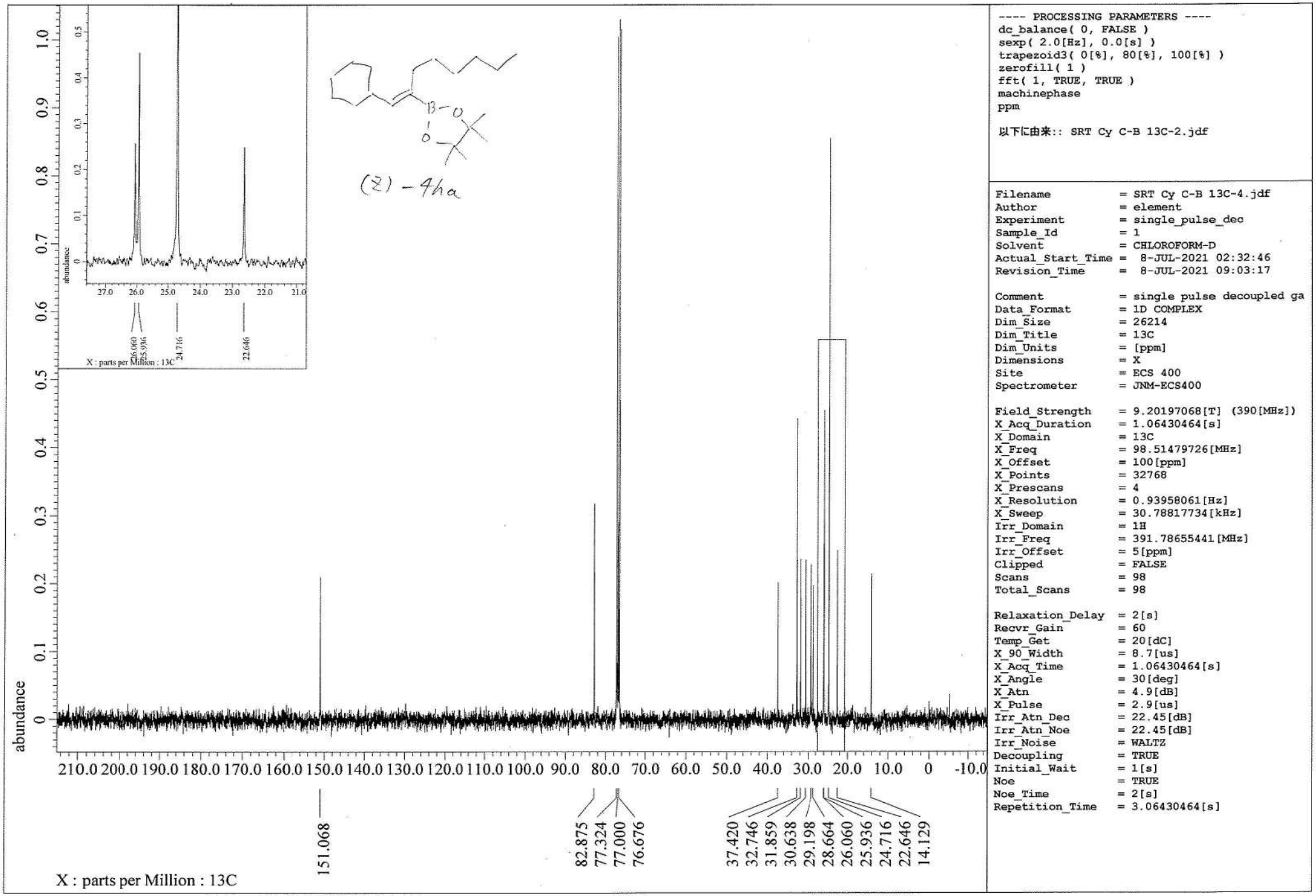

---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid3(0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
以下に由来:: SRT OTBS IC3Cl C-B 2-2.jdf
Filename = SRT OTBS IC3Cl C-B 2-4.jd
Author = element
Experiment = single_pulse.ex2
Sample_Id = S#516894
Solvent = CHLOROFORM-D
Actual_Start_Time = 5-JUL-2021 21:21:34
Revision_Time = 26-OCT-2021 18:58:33
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
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 = 44
Temp_Get = 18.4[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]
(E)-4df
abundance
X : parts per Million : 1H
7.264
6.341
6.323
6.305
3.630
3.613
3.597
3.552
3.535
3.518
2.191
2.173
2.155
2.137
1.761
1.566
1.475
1.253
0.891
0.044
0.000
1.00
2.06
2.03
3.99
1.97
2.74
1.94
12.01
9.24
6.19

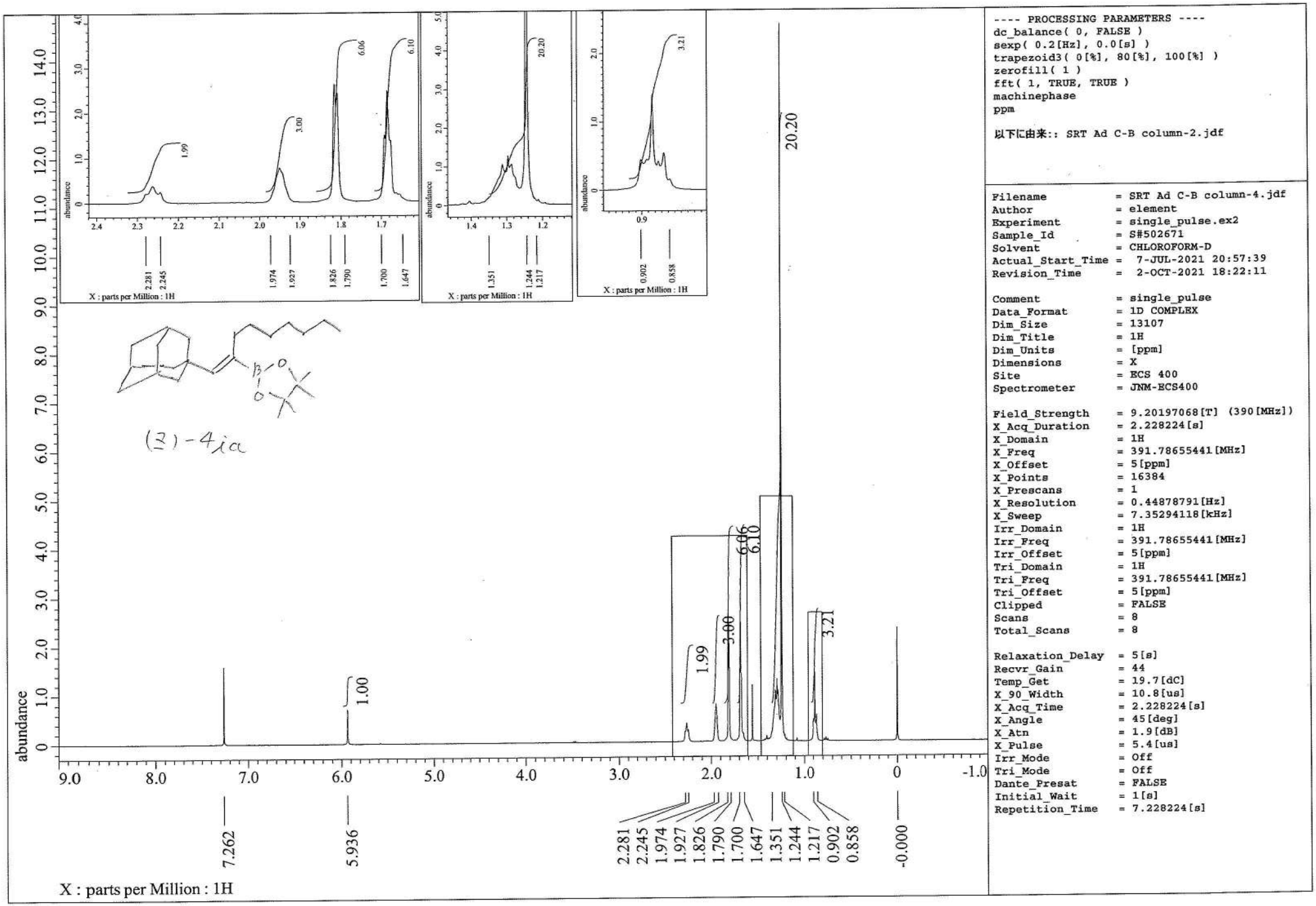

---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid3(0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
以下に由来:: SRT OTBS IC3Cl 13C-2.jdf
Filename = SRT OTBS IC3Cl 13C-4.jdf
Author = element
Experiment = single_pulse_dec
Sample_Id = S#721931
Solvent = CHLOROFORM-D
Actual_Start_Time = 16-OCT-2021 02:55:38
Revision_Time = 26-OCT-2021 15:10:28
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_Strength = 9.20197068[T] (390[MHz])
X_Acq_Duration = 1.06430464[s]
X_Domain = 13C
X_Freq = 98.51479726[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.93958061[Hz]
X_Sweep = 30.78817734[kHz]
Irr_Domain = 1H
Irr_Freq = 391.78655441[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 200
Total_Scans = 200
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 21.6[dC]
X_90_Width = 8.7[us]
X_Acq_Time = 1.06430464[s]
X_Angle = 30[deg]
X_Atn = 4.9[dB]
X_Pulse = 2.9[us]
Irr_Atn_Dec = 22.45[dB]
Irr_Atn_Noe = 22.45[dB]
Irr_Noise = WALTZ
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.06430464[s]
(Z)-4df
abundance
X : parts per Million : 13C
146.080
83.056
77.324
77.000
76.676
62.722
45.145
32.365
32.298
27.491
27.272
25.936
24.954
24.725
18.297
-5.280


---- 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:: SRT 093 C-B C4Cl IC4Cl-2.jdf
Filename = SRT 093 C-B C4Cl IC4Cl-4.
Author = element
Experiment = single_pulse.ex2
Sample_Id = S#491404
Solvent = CHLOROFORM-D
Actual_Start_Time = 5-JUL-2021 20:39:07
Revision_Time = 26-OCT-2021 19:19:32
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
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 = 46
Temp_Get = 18.1[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]
(Z)-4gg
abundance
X : parts per Million : 1H
7.265
6.286
6.269
6.251
3.556
3.551
3.538
3.533
3.521
3.516
2.184
2.166
2.148
2.128
2.110
1.832
1.743
1.585
1.509
1.255
0.000


abundance
X : parts per Million : 13C
145.031
83.066
77.324
77.000
76.676
45.116
44.935
32.555
32.269
29.246
28.245
27.615
26.728
26.375
24.716
(Z)-4gg
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid3(0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
以下に由来:: SRT 093 C4Cl IC4Cl 13C-2.jdf
Filename = SRT 093 C4Cl IC4Cl 13C-4.
Author = element
Experiment = single_pulse_dec
Sample_Id = 1
Solvent = CHLOROFORM-D
Actual_Start_Time = 16-OCT-2021 03:49:16
Revision_Time = 26-OCT-2021 19:50:57
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_Strength = 9.20197068[T] (390[MHz])
X_Acq_Duration = 1.06430464[s]
X_Domain = 13C
X_Freq = 98.51479726[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.93958061[Hz]
X_Sweep = 30.78817734[kHz]
Irr_Domain = 1H
Irr_Freq = 391.78655441[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 200
Total_Scans = 200
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 20.4[dC]
X_90_Width = 8.7[us]
X_Acq_Time = 1.06430464[s]
X_Angle = 30[deg]
X_Atn = 4.9[dB]
X_Pulse = 2.9[us]
Irr_Atn_Dec = 22.45[dB]
Irr_Atn_Noe = 22.45[dB]
Irr_Noise = WALTZ
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.06430464[s]

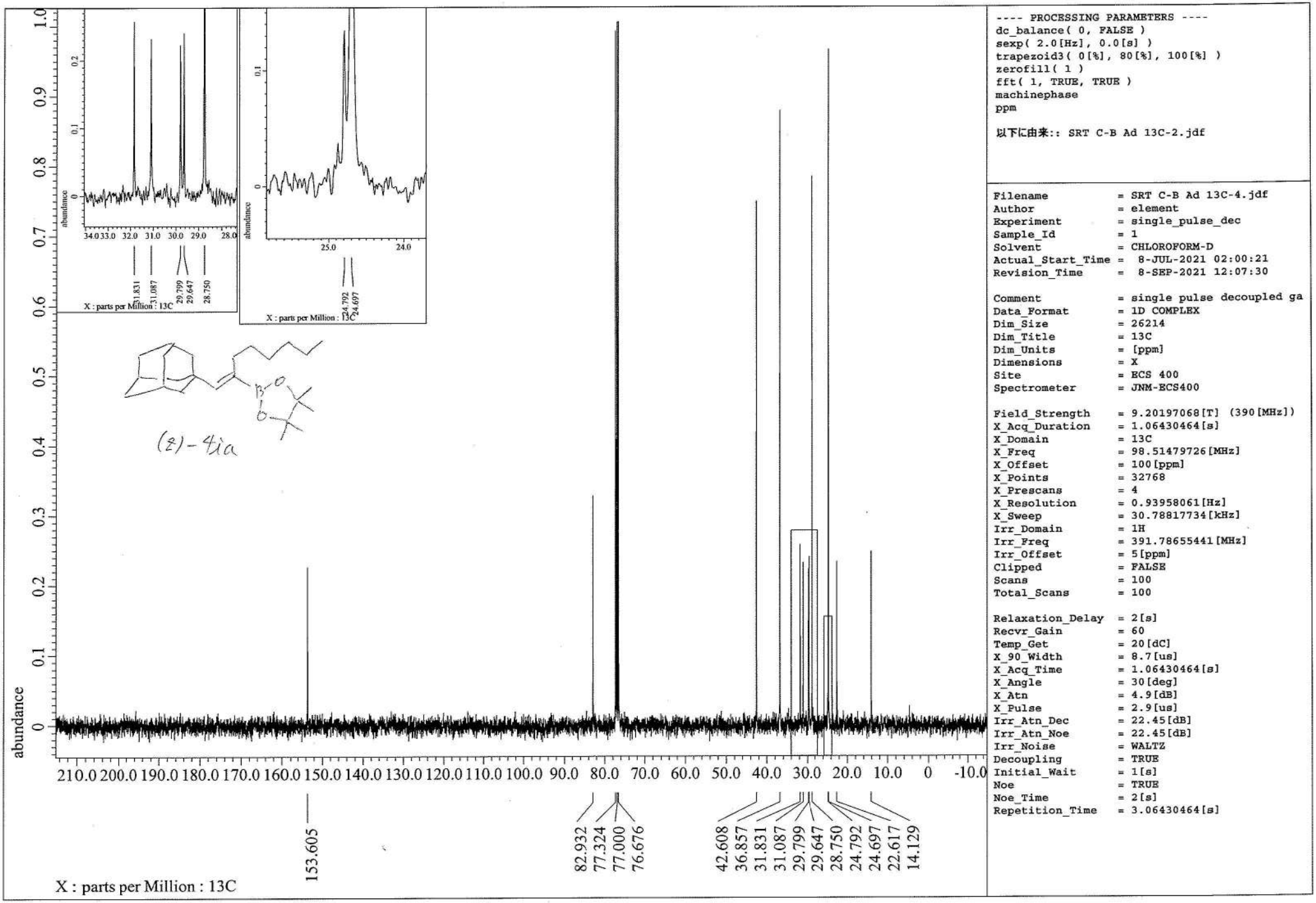

(Z)-4ha
X : parts per Million : 1H
abundance
7.260
6.078
6.054
2.395
2.294
2.124
2.108
2.091
1.740
1.532
1.343
1.249
1.046
0.897
0.881
0.863
-0.000
25.24
5.02
3.03
1.94
1.00
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid3(0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
以下に由来:: Cy C-B column-2.jdf
Filename = Cy C-B column-4.jdf
Author = element
Experiment = single_pulse.ex2
Sample_Id = S#508289
Solvent = CHLOROFORM-D
Actual_Start_Time = 29-JUN-2021 20:47:10
Revision_Time = 2-OCT-2021 15:42:46
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
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 = 50
Temp_Get = 23.3[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]

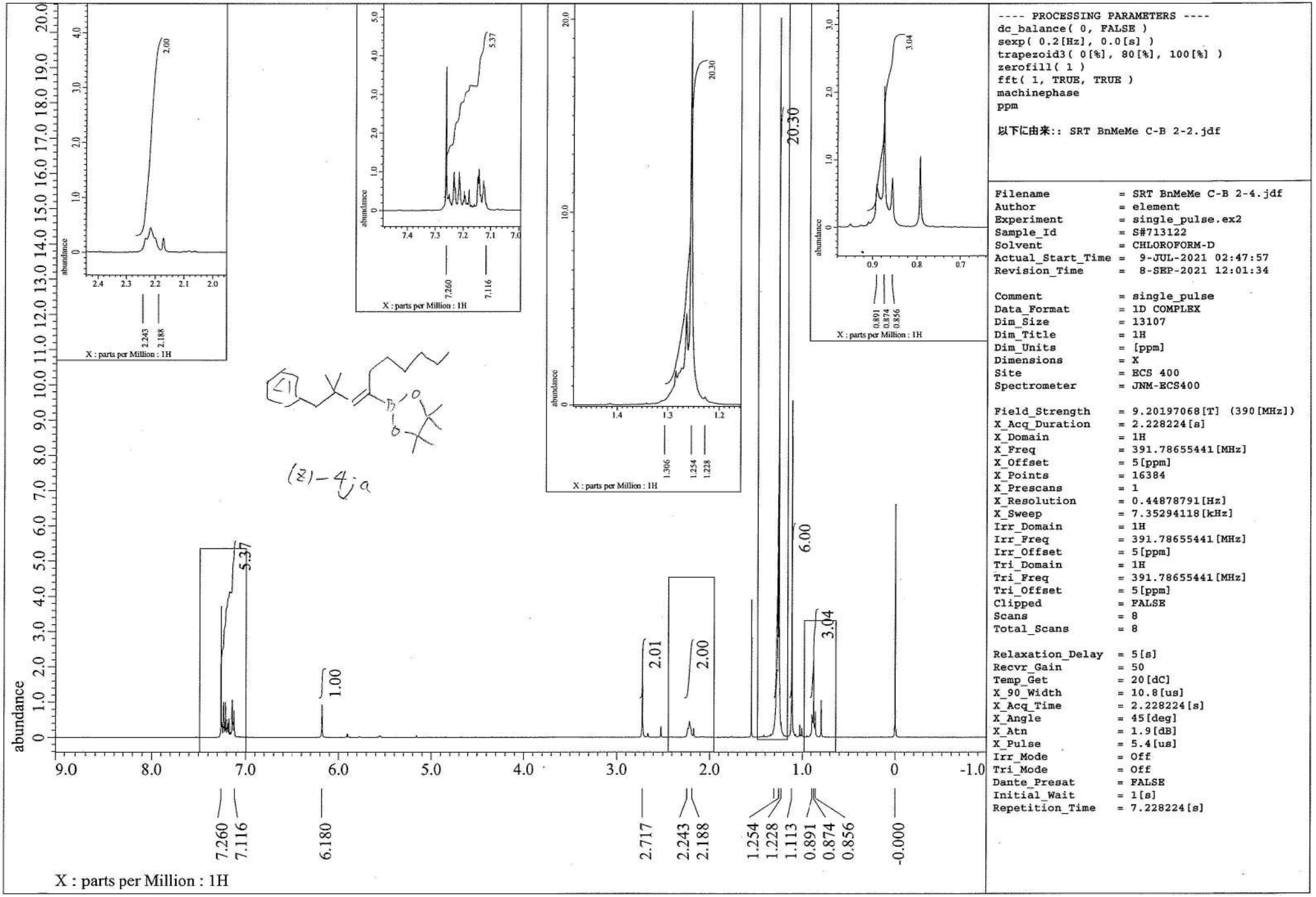

(Z)-4ha
abundance
X : parts per Million : 13C
151.068
82.875
77.324
77.000
76.676
37.420
32.746
31.859
30.638
29.198
28.664
26.060
25.936
24.716
22.646
14.129
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid3(0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
以下に由来:: SRT Cy C-B 13C-2.jdf
Filename = SRT Cy C-B 13C-4.jdf
Author = element
Experiment = single_pulse_dec
Sample_Id = 1
Solvent = CHLOROFORM-D
Actual_Start_Time = 8-JUL-2021 02:32:46
Revision_Time = 8-JUL-2021 09:03:17
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_Strength = 9.20197068[T] (390[MHz])
X_Acq_Duration = 1.06430464[s]
X_Domain = 13C
X_Freq = 98.51479726[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.93958061[Hz]
X_Sweep = 30.78817734[kHz]
Irr_Domain = 1H
Irr_Freq = 391.78655441[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 98
Total_Scans = 98
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 20[dC]
X_90_Width = 8.7[us]
X_Acq_Time = 1.06430464[s]
X_Angle = 30[deg]
X_Atn = 4.9[dB]
X_Pulse = 2.9[us]
Irr_Atn_Dec = 22.45[dB]
Irr_Atn_Noe = 22.45[dB]
Irr_Noise = WALTZ
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.06430464[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:: SRT Ad C-B column-2.jdf
```

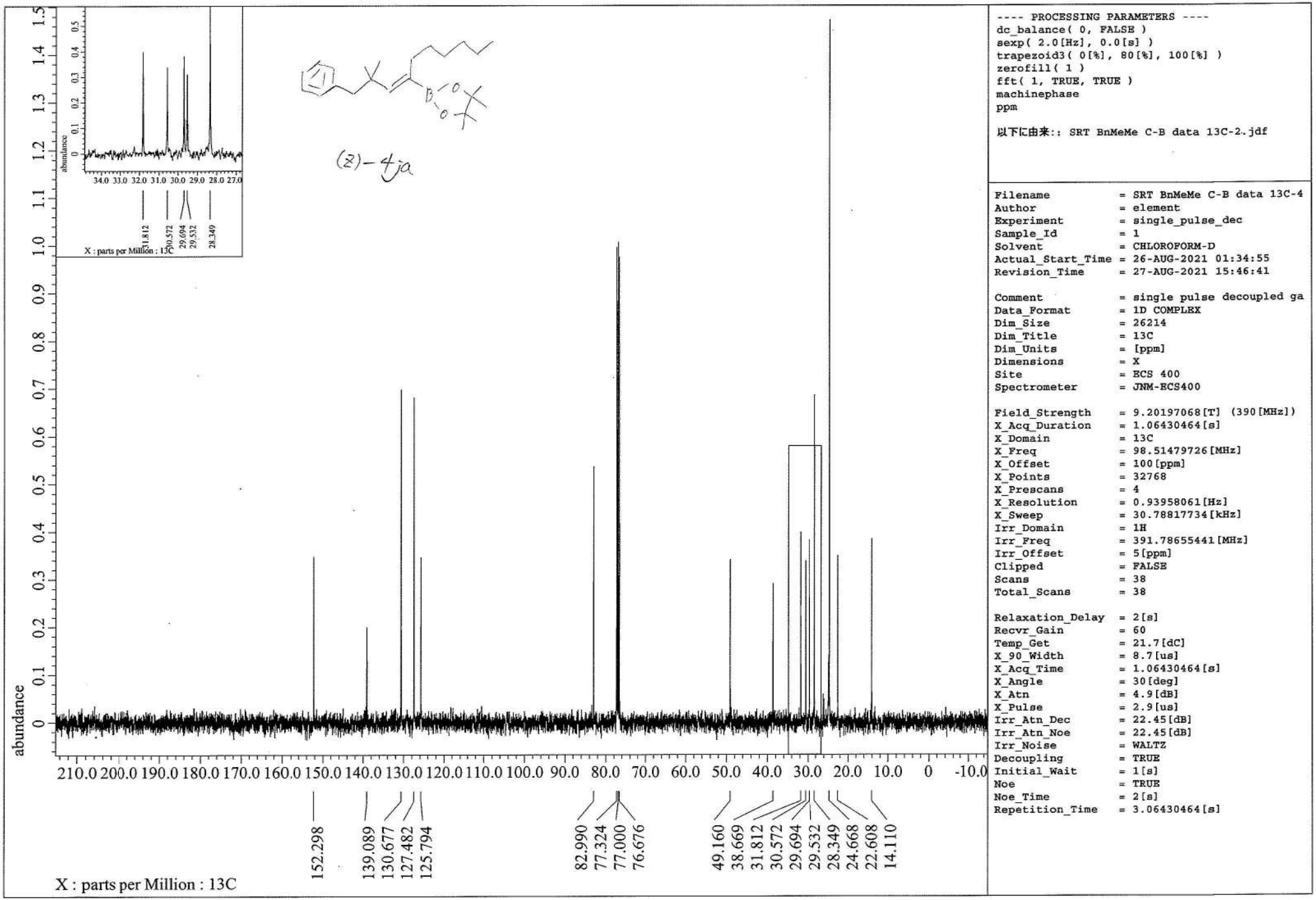
```
Filename            = SRT Ad C-B column-4.jdf
Author              = element
Experiment          = single_pulse.ex2
Sample_Id           = S#502671
Solvent             = CHLOROFORM-D
Actual_Start_Time   =  7-JUL-2021 20:57:39
Revision_Time       =  2-OCT-2021 18:22:11

Comment             = single_pulse
Data_Format         = 1D COMPLEX
Dim_Size            = 13107
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          = 44
Temp_Get            = 19.7[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]
```

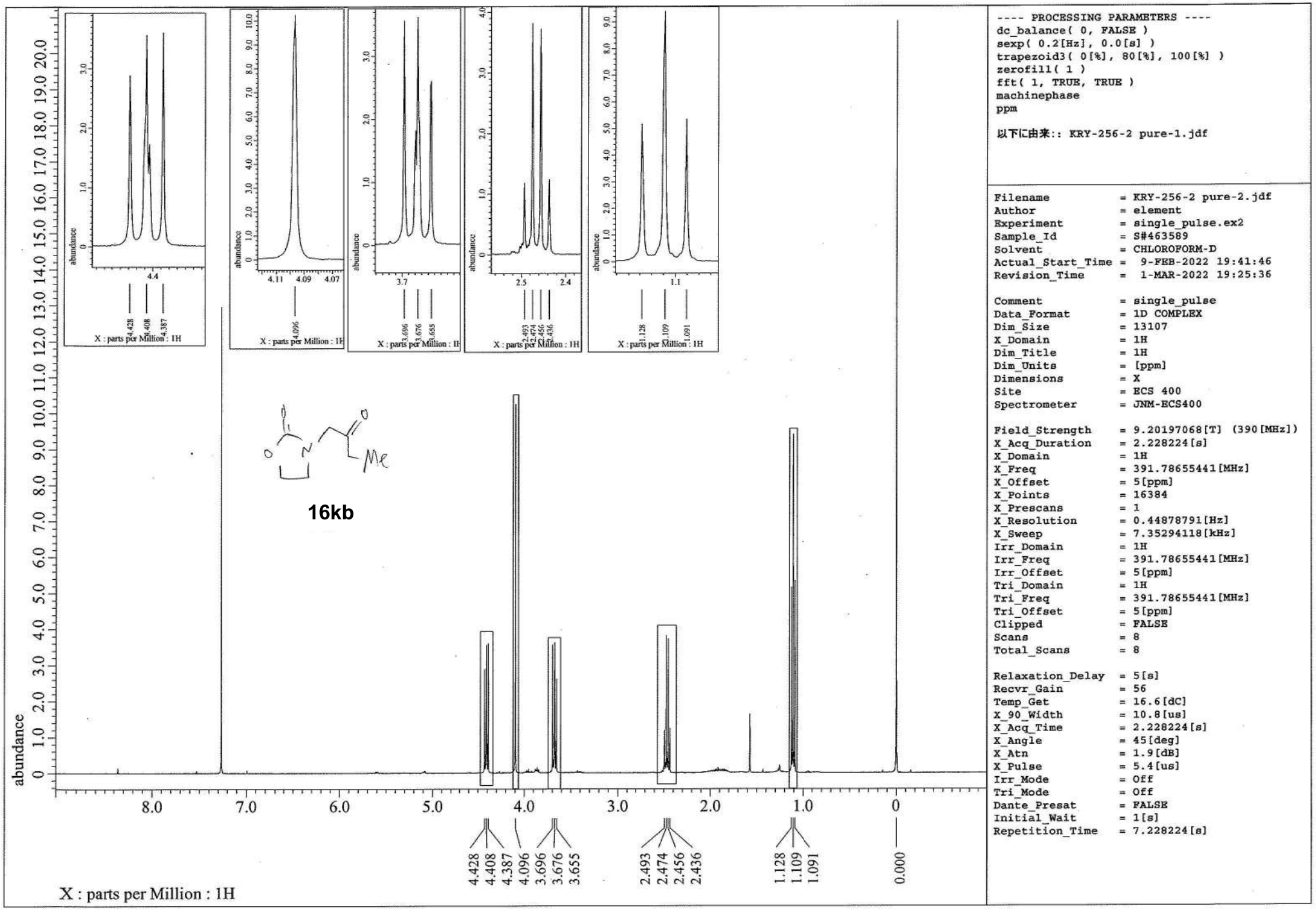

---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid3(0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
以下に由来:: SRT C-B Ad 13C-2.jdf
Filename = SRT C-B Ad 13C-4.jdf
Author = element
Experiment = single_pulse_dec
Sample_Id = 1
Solvent = CHLOROFORM-D
Actual_Start_Time = 8-JUL-2021 02:00:21
Revision_Time = 8-SEP-2021 12:07:30
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_Strength = 9.20197068[T] (390[MHz])
X_Acq_Duration = 1.06430464[s]
X_Domain = 13C
X_Freq = 98.51479726[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.93958061[Hz]
X_Sweep = 30.78817734[kHz]
Irr_Domain = 1H
Irr_Freq = 391.78655441[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 100
Total_Scans = 100
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 20[dC]
X_90_Width = 8.7[us]
X_Acq_Time = 1.06430464[s]
X_Angle = 30[deg]
X_Atn = 4.9[dB]
X_Pulse = 2.9[us]
Irr_Atn_Dec = 22.45[dB]
Irr_Atn_Noe = 22.45[dB]
Irr_Noise = WALTZ
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.06430464[s]
(E)-4ia
abundance
X : parts per Million : 13C
153.605
82.932
77.324
77.000
76.676
42.608
36.857
31.831
31.087
29.799
29.647
28.750
24.792
24.697
22.617
14.129




```
---- 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:: SRT BnMeMe C-B 2-2.jdf
```

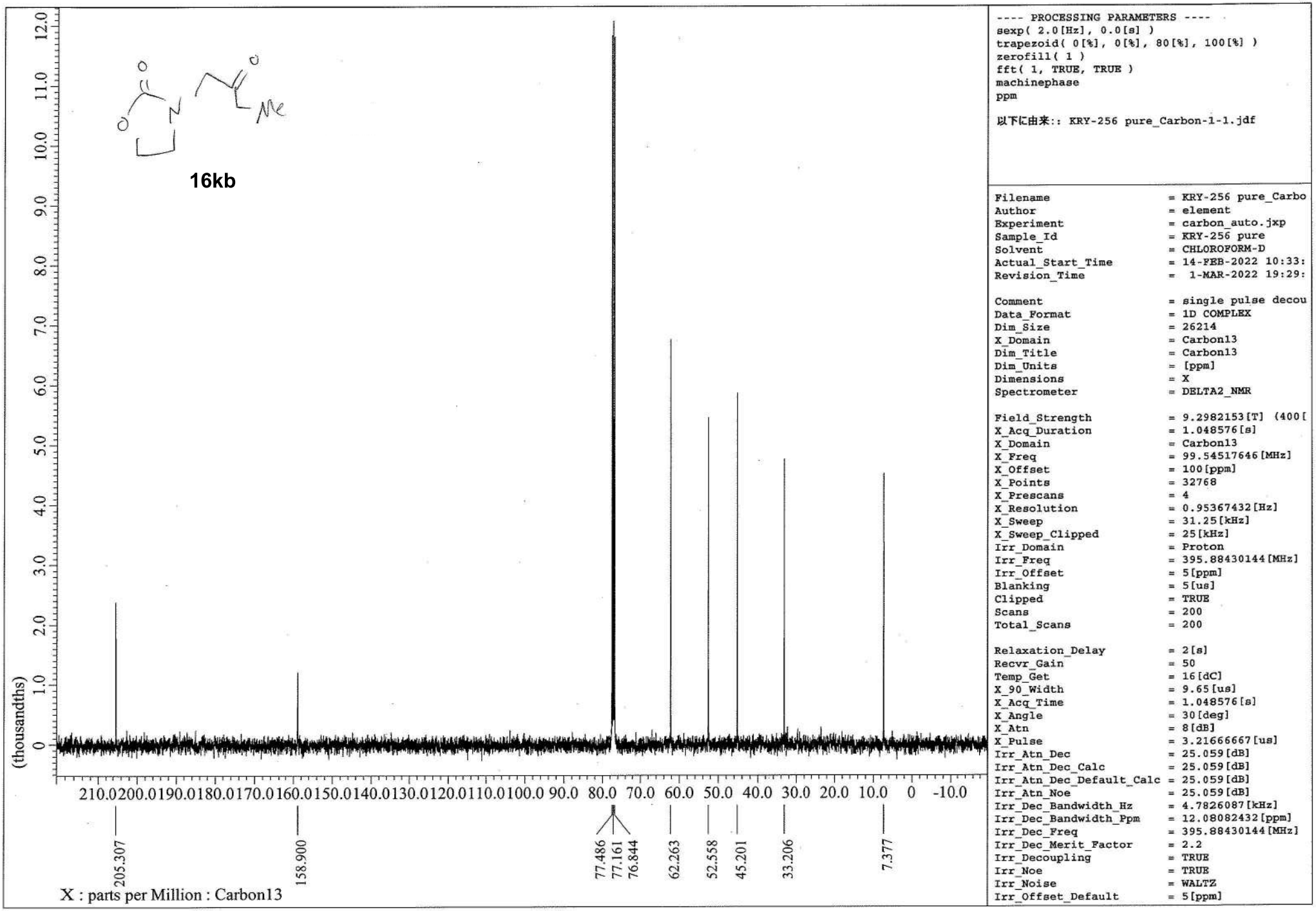
Filename	= SRT BnMeMe C-B 2-4.jdf
Author	= element
Experiment	= single_pulse.ex2
Sample_Id	= S#713122
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 9-JUL-2021 02:47:57
Revision_Time	= 8-SEP-2021 12:01:34
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
Dim_Title	= 1H
Dim_Units	= [ppm]
Dimensions	= 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	= 50
Temp_Get	= 20[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]


(Z)-4ja
X : parts per Million : 13C
abundance
152.298
139.089
130.677
127.482
125.794
82.990
77.324
77.000
76.676
49.160
38.669
31.812
30.572
29.694
29.532
28.349
24.668
22.608
14.110
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid3(0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
以下に由来:: SRT BnMeMe C-B data 13C-2.jdf
Filename = SRT BnMeMe C-B data 13C-4
Author = element
Experiment = single_pulse_dec
Sample_Id = 1
Solvent = CHLOROFORM-D
Actual_Start_Time = 26-AUG-2021 01:34:55
Revision_Time = 27-AUG-2021 15:46:41
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_Strength = 9.20197068[T] (390[MHz])
X_Acq_Duration = 1.06430464[s]
X_Domain = 13C
X_Freq = 98.51479726[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.93958061[Hz]
X_Sweep = 30.78817734[kHz]
Irr_Domain = 1H
Irr_Freq = 391.78655441[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 38
Total_Scans = 38
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 21.7[dC]
X_90_Width = 8.7[us]
X_Acq_Time = 1.06430464[s]
X_Angle = 30[deg]
X_Atn = 4.9[dB]
X_Pulse = 2.9[us]
Irr_Atn_Dec = 22.45[dB]
Irr_Atn_Noe = 22.45[dB]
Irr_Noise = WALTZ
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.06430464[s]



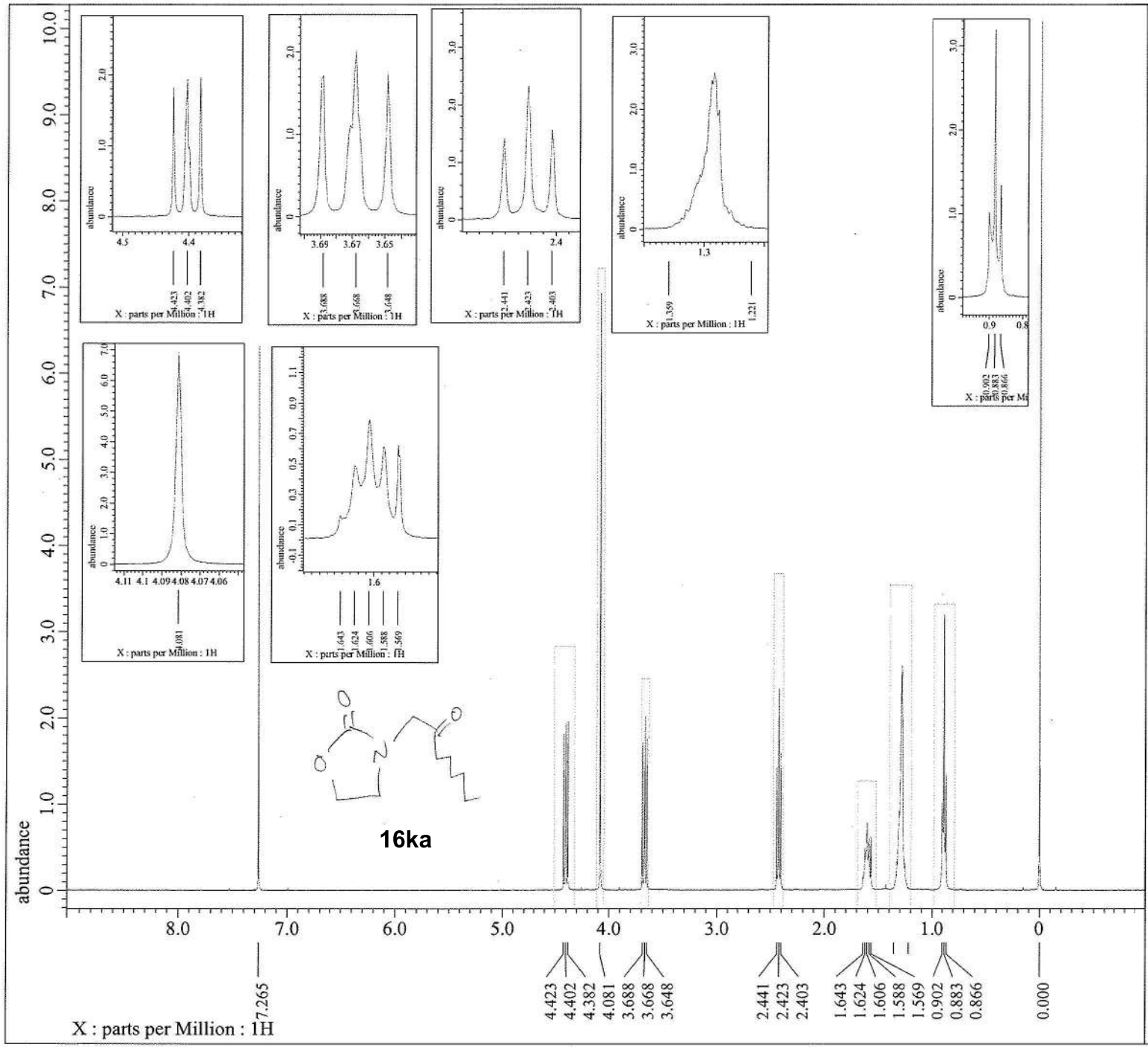

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

以下に由来:: KRY-256-2 pure-1.jdf
```

Filename	= KRY-256-2 pure-2.jdf
Author	= element
Experiment	= single_pulse.ex2
Sample_Id	= S#463589
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 9-FEB-2022 19:41:46
Revision_Time	= 1-MAR-2022 19:25:36
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	= 16.6[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]



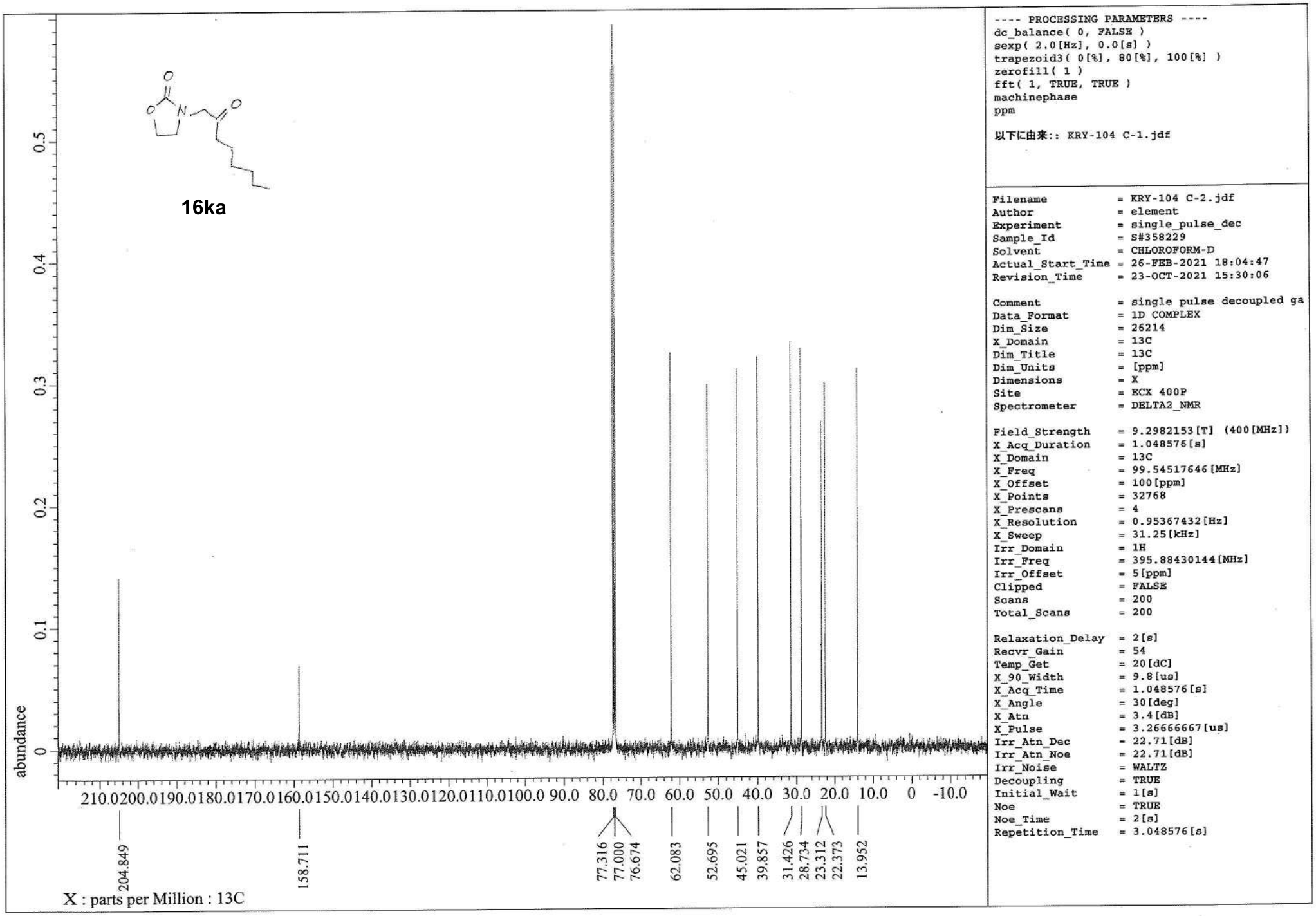

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

以下に由来:: KRY-256 pure_Carbon-1-1.jdf
```

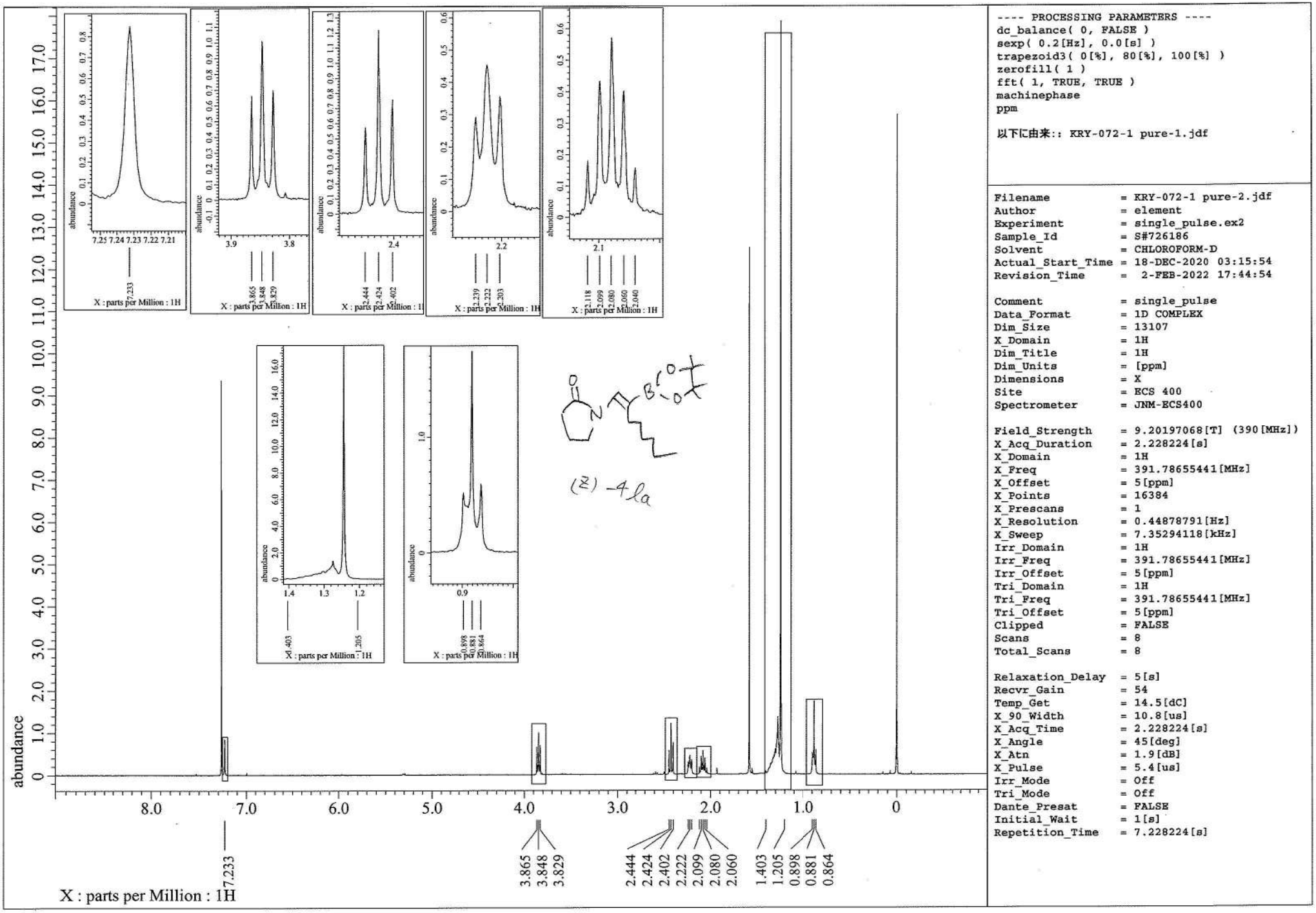
Filename	= KRY-256 pure_Carbo
Author	= element
Experiment	= carbon_auto.jxp
Sample_Id	= KRY-256 pure
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 14-FEB-2022 10:33:
Revision_Time	= 1-MAR-2022 19:29:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
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	= 200
Total_Scans	= 200
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 16[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] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

以下に由来:: KRY-104 pure-1.jdf
```

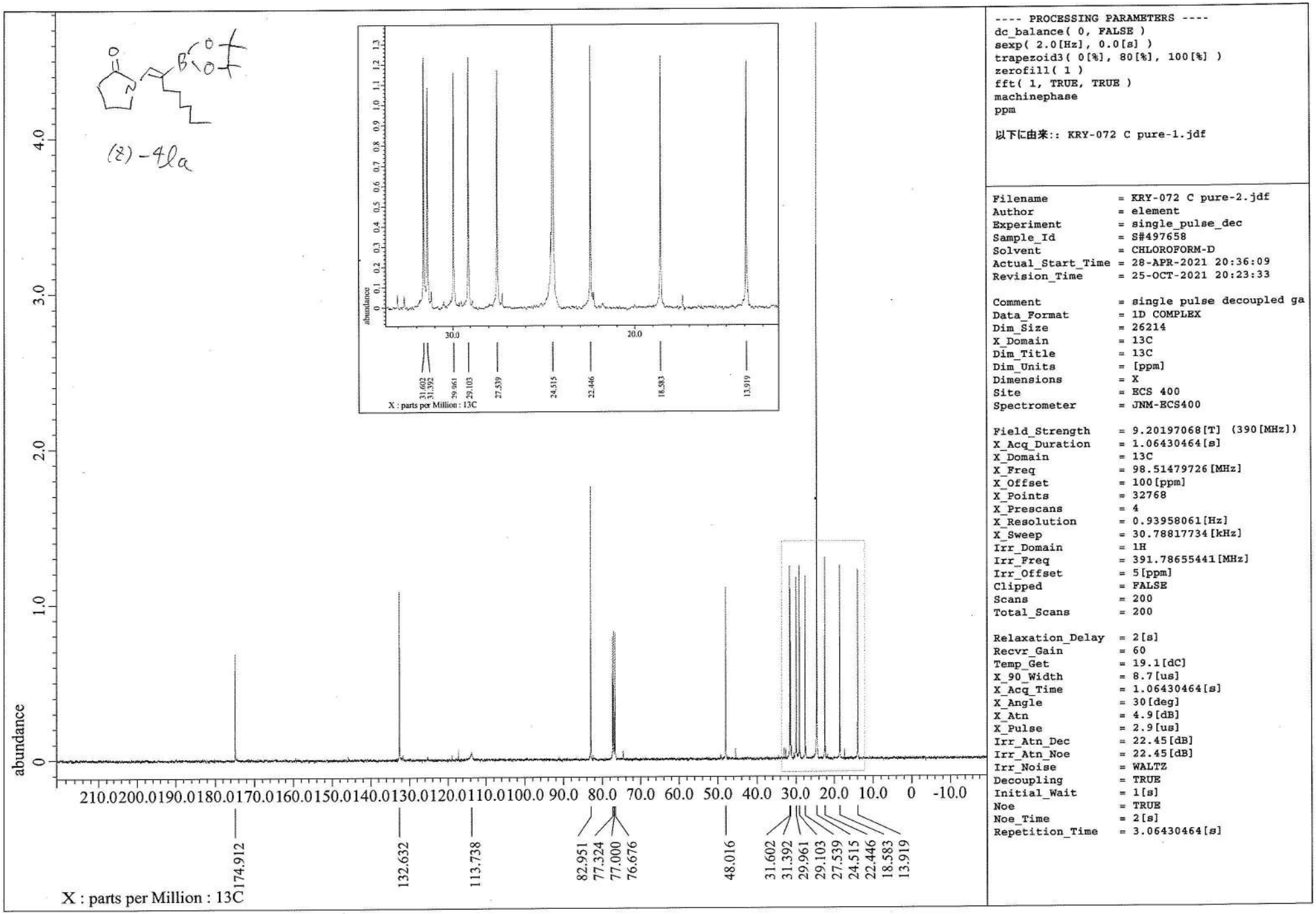
Filename	= KRY-104 pure-2.jdf
Author	= element
Experiment	= single_pulse.ex2
Sample_Id	= S#338441
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 26-FEB-2021 16:19:36
Revision_Time	= 2-AUG-2021 18:43:45
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= 1H
Dim_Title	= 1H
Dim_Units	= [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	= 52
Temp_Get	= 17.6[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]

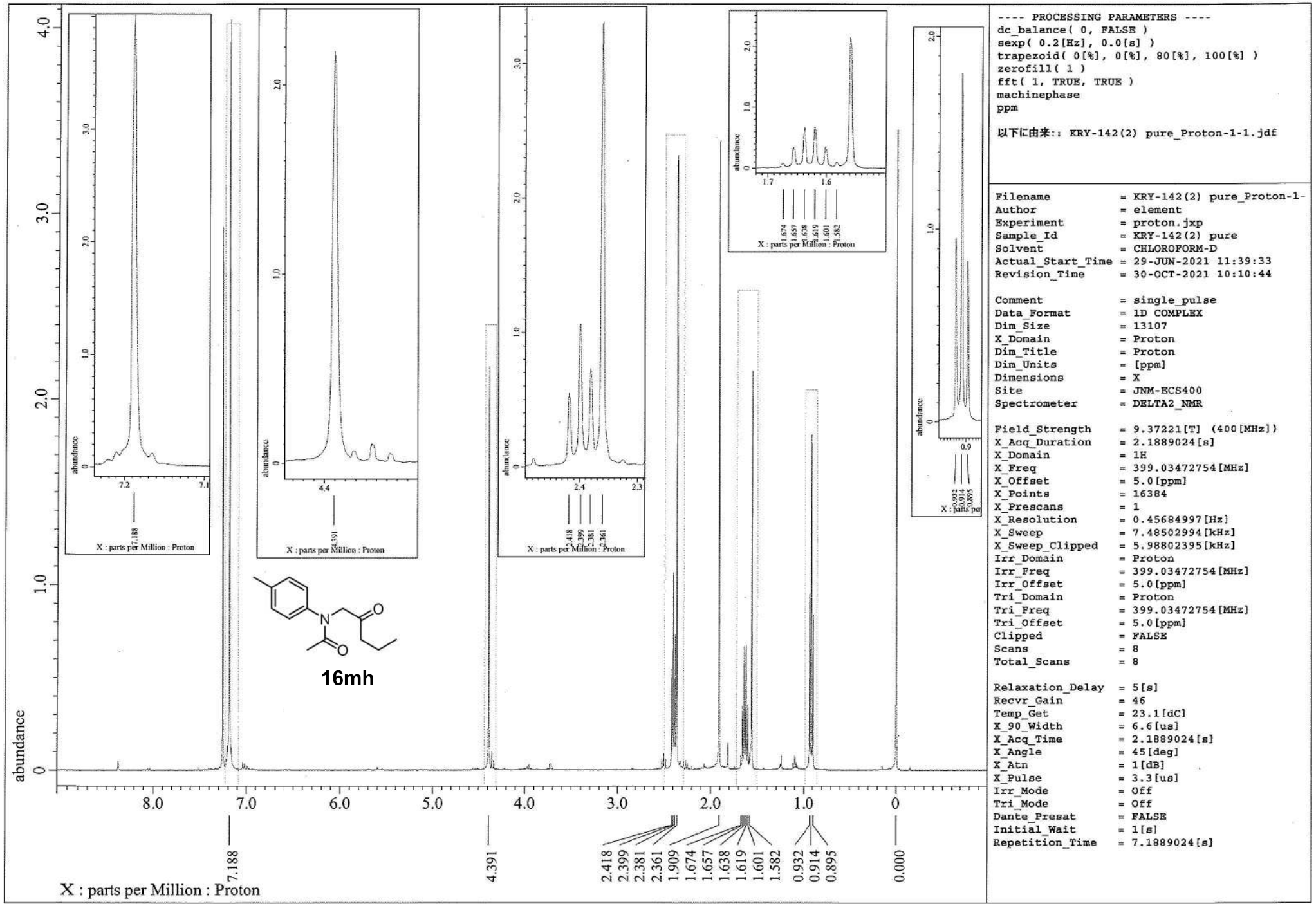

16ka
abundance
0
0.1
0.2
0.3
0.4
0.5
210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0
204.849
158.711
77.316
77.000
76.674
62.083
52.695
45.021
39.857
31.426
28.734
23.312
22.373
13.952
X : parts per Million : 13C
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid3(0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
以下に由来:: KRY-104 C-1.jdf
Filename = KRY-104 C-2.jdf
Author = element
Experiment = single_pulse_dec
Sample_Id = S#358229
Solvent = CHLOROFORM-D
Actual_Start_Time = 26-FEB-2021 18:04:47
Revision_Time = 23-OCT-2021 15:30:06
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = 13C
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400P
Spectrometer = DELTA2_NMR
Field_Strength = 9.2982153[T] (400[MHz])
X_Acq_Duration = 1.048576[s]
X_Domain = 13C
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]
Irr_Domain = 1H
Irr_Freq = 395.88430144[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 200
Total_Scans = 200
Relaxation_Delay = 2[s]
Recvr_Gain = 54
Temp_Get = 20[dC]
X_90_Width = 9.8[us]
X_Acq_Time = 1.048576[s]
X_Angle = 30[deg]
X_Atn = 3.4[dB]
X_Pulse = 3.26666667[us]
Irr_Atn_Dec = 22.71[dB]
Irr_Atn_Noe = 22.71[dB]
Irr_Noise = WALTZ
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.048576[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:: KRY-072-1 pure-1.jdf
```

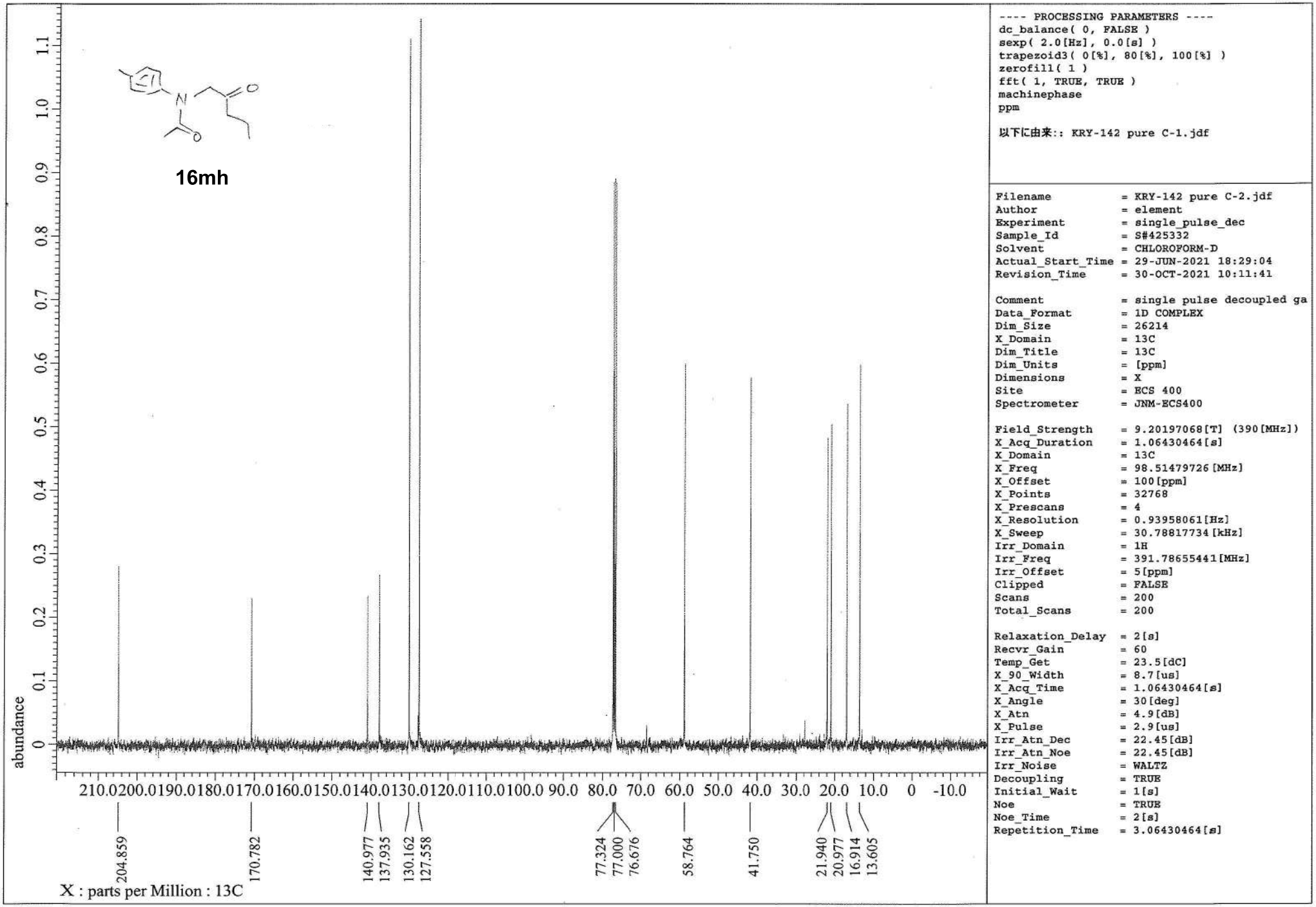
Filename	= KRY-072-1 pure-2.jdf
Author	= element
Experiment	= single_pulse.ex2
Sample_Id	= S#726186
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 18-DEC-2020 03:15:54
Revision_Time	= 2-FEB-2022 17:44:54
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= 1H
Dim_Title	= 1H
Dim_Units	= [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	= 54
Temp_Get	= 14.5[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]


(E)-4la
abundance
X : parts per Million : 13C
174.912
132.632
113.738
82.951
77.324
77.000
76.676
48.016
31.602
31.392
29.961
29.103
27.539
24.515
22.446
18.583
13.919
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid3(0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
以下に由来:: KRY-072 C pure-1.jdf
Filename = KRY-072 C pure-2.jdf
Author = element
Experiment = single_pulse_dec
Sample_Id = S#497658
Solvent = CHLOROFORM-D
Actual_Start_Time = 28-APR-2021 20:36:09
Revision_Time = 25-OCT-2021 20:23:33
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = 13C
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_Strength = 9.20197068[T] (390[MHz])
X_Acq_Duration = 1.06430464[s]
X_Domain = 13C
X_Freq = 98.51479726[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.93958061[Hz]
X_Sweep = 30.78817734[kHz]
Irr_Domain = 1H
Irr_Freq = 391.78655441[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 200
Total_Scans = 200
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 19.1[dC]
X_90_Width = 8.7[us]
X_Acq_Time = 1.06430464[s]
X_Angle = 30[deg]
X_Atn = 4.9[dB]
X_Pulse = 2.9[us]
Irr_Atn_Dec = 22.45[dB]
Irr_Atn_Noe = 22.45[dB]
Irr_Noise = WALTZ
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.06430464[s]



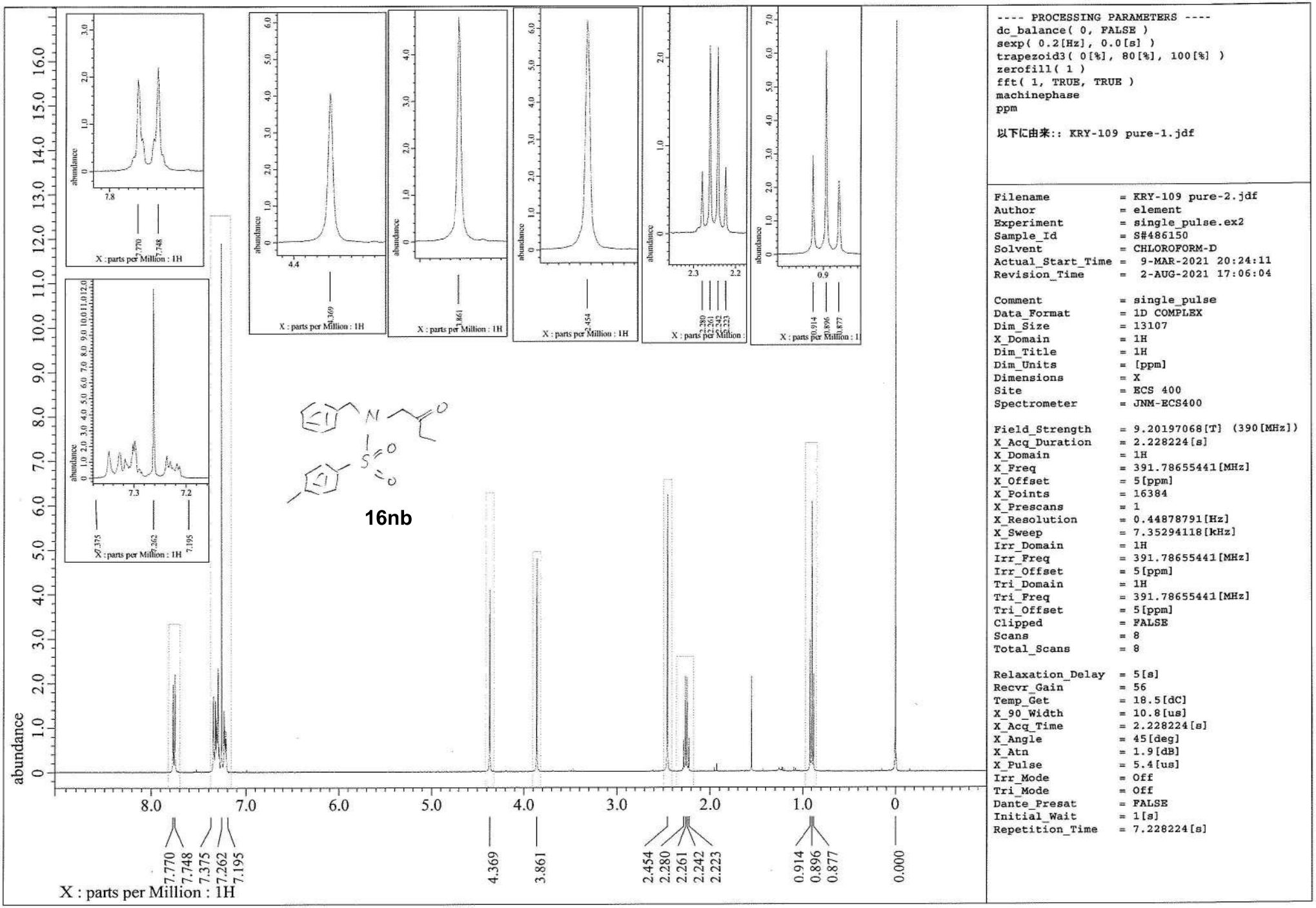

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

以下に由来:: KRY-142(2) pure_Proton-1-1.jdf
```

Filename	= KRY-142(2) pure_Proton-1-
Author	= element
Experiment	= proton.jxp
Sample_Id	= KRY-142(2) pure
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 29-JUN-2021 11:39:33
Revision_Time	= 30-OCT-2021 10:10:44
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	= 23.1[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]



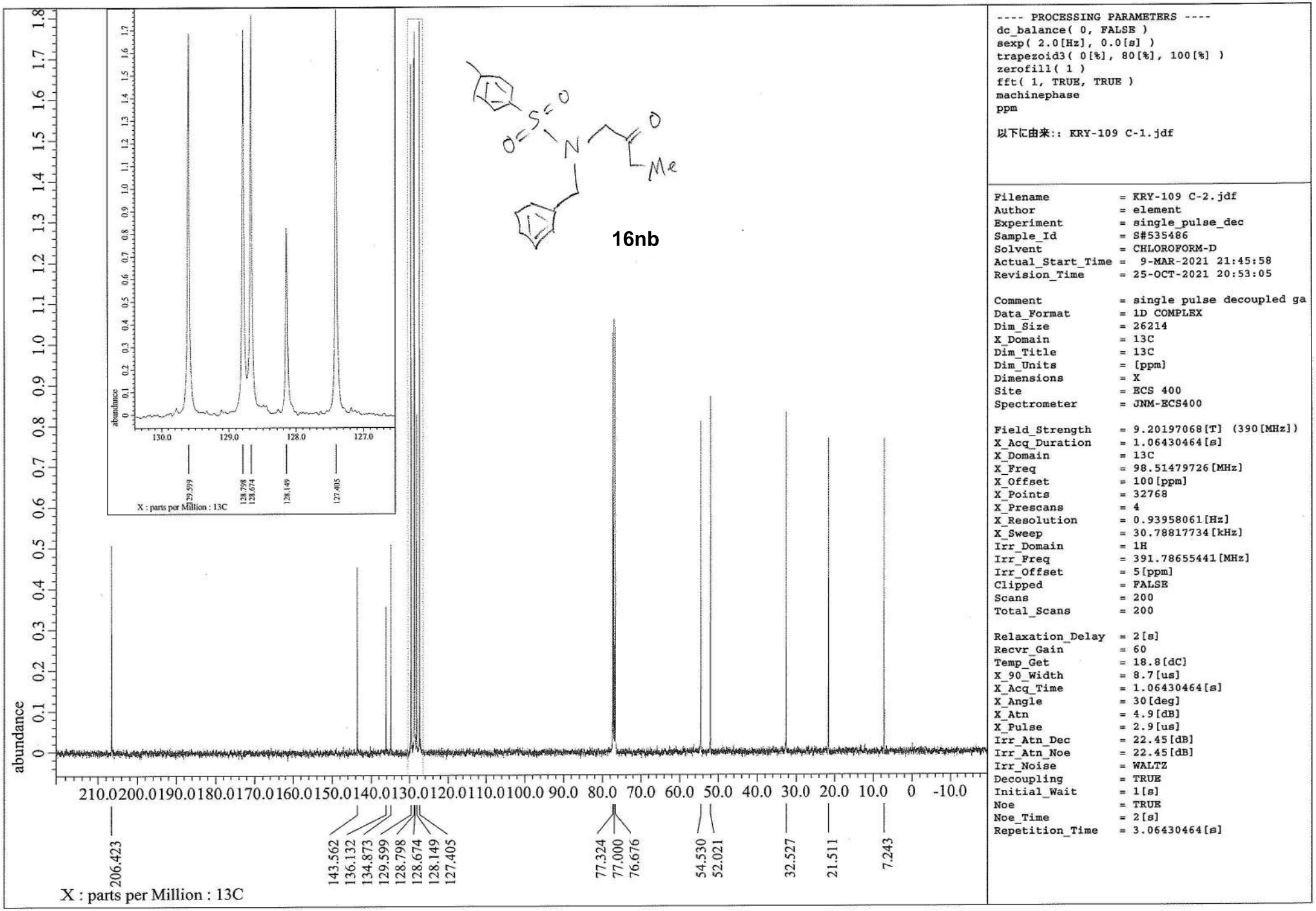

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

以下に由来:: KRY-142 pure C-1.jdf
```

Filename	= KRY-142 pure C-2.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= S#425332
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 29-JUN-2021 18:29:04
Revision_Time	= 30-OCT-2021 10:11:41
Comment	= single pulse decoupled ga
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= 13C
Dim_Title	= 13C
Dim_Units	= [ppm]
Dimensions	= X
Site	= ECS 400
Spectrometer	= JNM-ECS400
Field_Strength	= 9.20197068[T] (390[MHz])
X_Acq_Duration	= 1.06430464[s]
X_Domain	= 13C
X_Freq	= 98.51479726[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.93958061[Hz]
X_Sweep	= 30.78817734[kHz]
Irr_Domain	= 1H
Irr_Freq	= 391.78655441[MHz]
Irr_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 200
Total_Scans	= 200
Relaxation_Delay	= 2[s]
Recvr_Gain	= 60
Temp_Get	= 23.5[dC]
X_90_Width	= 8.7[us]
X_Acq_Time	= 1.06430464[s]
X_Angle	= 30[deg]
X_Atn	= 4.9[dB]
X_Pulse	= 2.9[us]
Irr_Atn_Dec	= 22.45[dB]
Irr_Atn_Noe	= 22.45[dB]
Irr_Noise	= WALTZ
Decoupling	= TRUE
Initial_Wait	= 1[s]
Noe	= TRUE
Noe_Time	= 2[s]
Repetition_Time	= 3.06430464[s]



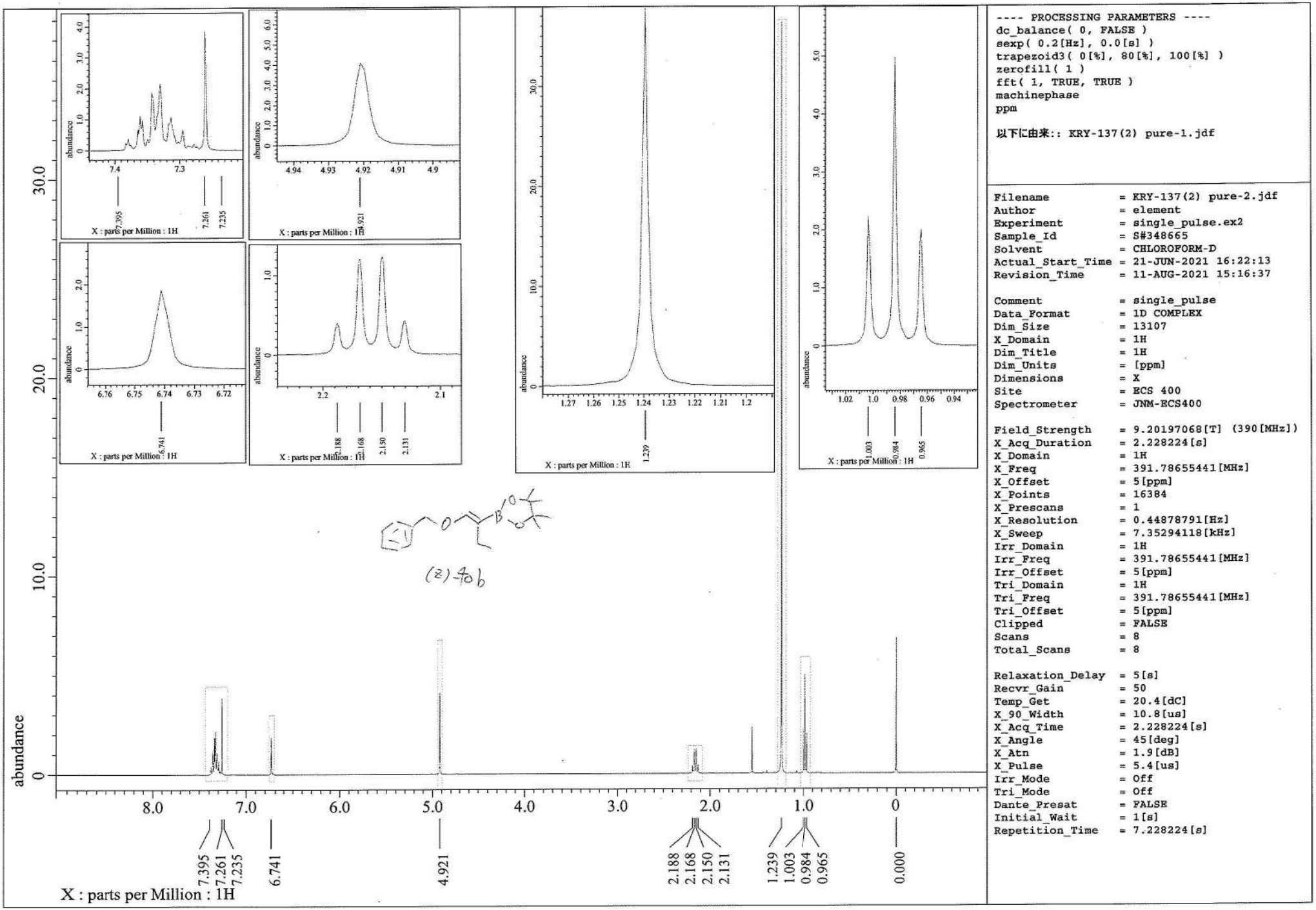

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

以下に由来:: KRY-109 pure-1.jdf
```

```
Filename            = KRY-109 pure-2.jdf
Author              = element
Experiment          = single_pulse.ex2
Sample_Id           = S#486150
Solvent             = CHLOROFORM-D
Actual_Start_Time   =  9-MAR-2021 20:24:11
Revision_Time       =  2-AUG-2021 17:06:04

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            = 18.5[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]
```



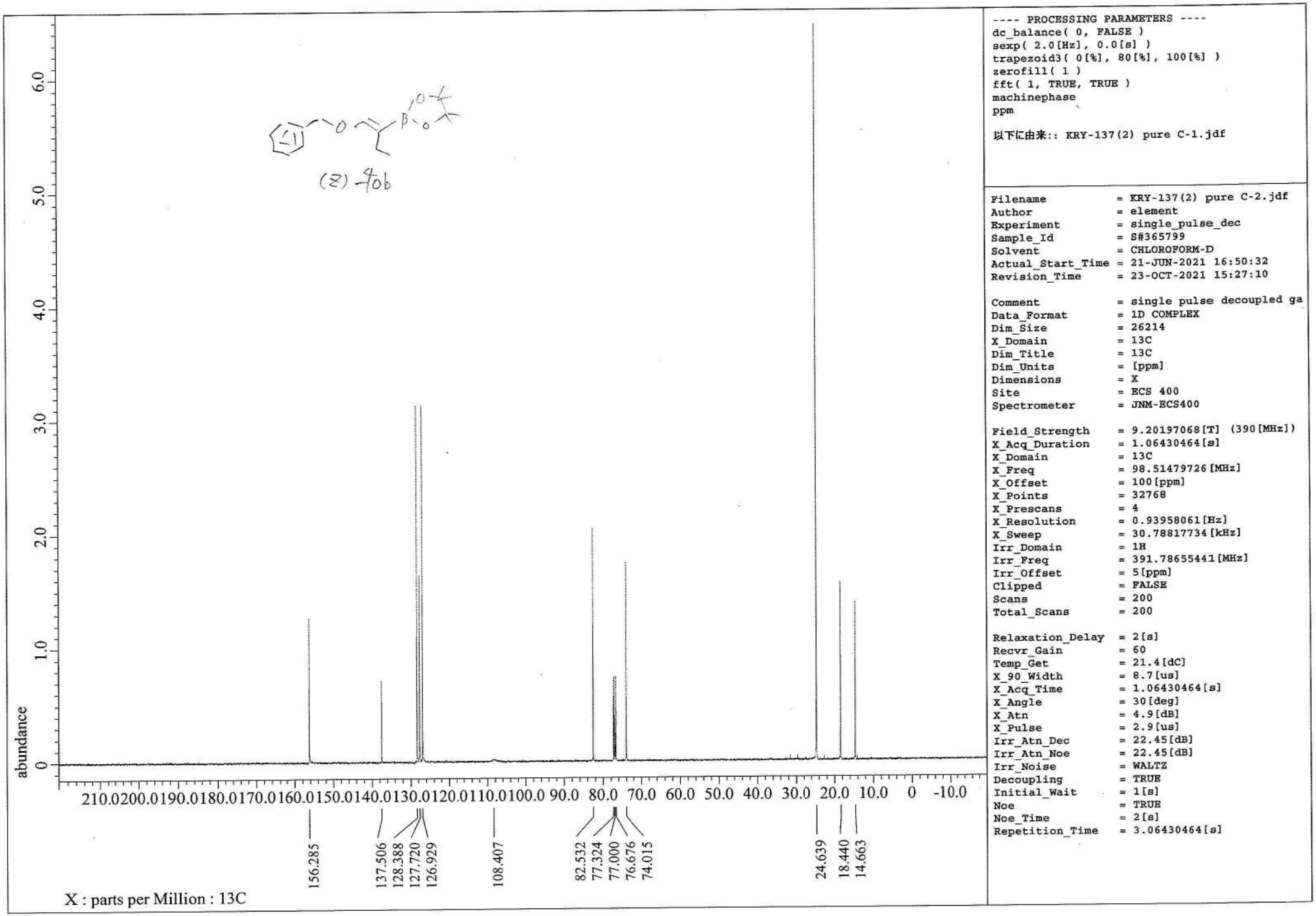

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

以下に由来:: KRY-109 C-1.jdf
```

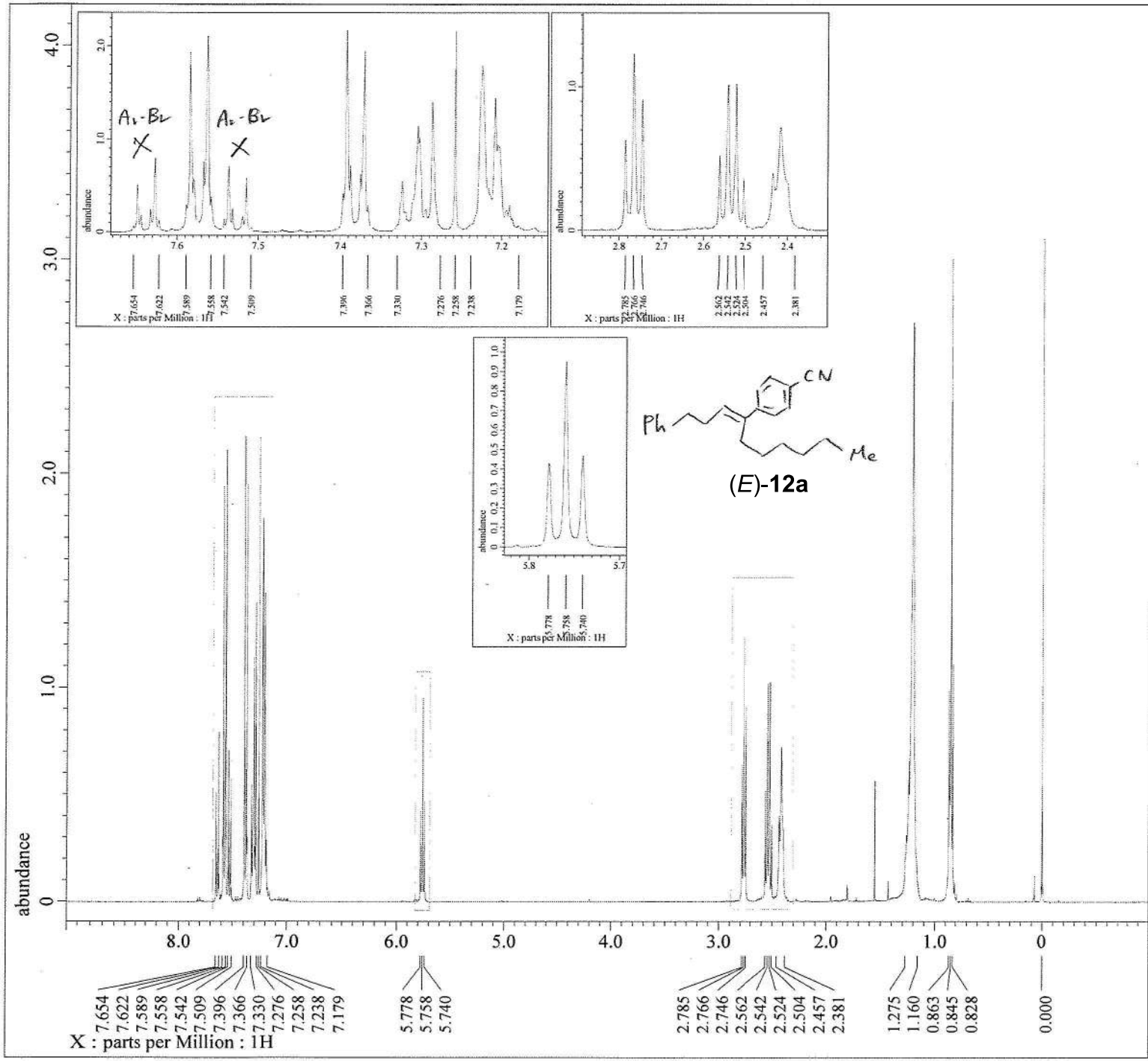
Filename	= KRY-109 C-2.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= S#535486
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 9-MAR-2021 21:45:58
Revision_Time	= 25-OCT-2021 20:53:05
Comment	= single pulse decoupled ga
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= 13C
Dim_Title	= 13C
Dim_Units	= [ppm]
Dimensions	= X
Site	= ECS 400
Spectrometer	= JNM-ECS400
Field_Strength	= 9.20197068[T] (390[MHz])
X_Acq_Duration	= 1.06430464[s]
X_Domain	= 13C
X_Freq	= 98.51479726[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.93958061[Hz]
X_Sweep	= 30.78817734[kHz]
Irr_Domain	= 1H
Irr_Freq	= 391.78655441[MHz]
Irr_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 200
Total_Scans	= 200
Relaxation_Delay	= 2[s]
Recvr_Gain	= 60
Temp_Get	= 18.8[dC]
X_90_Width	= 8.7[us]
X_Acq_Time	= 1.06430464[s]
X_Angle	= 30[deg]
X_Atn	= 4.9[dB]
X_Pulse	= 2.9[us]
Irr_Atn_Dec	= 22.45[dB]
Irr_Atn_Noe	= 22.45[dB]
Irr_Noise	= WALTZ
Decoupling	= TRUE
Initial_Wait	= 1[s]
Noe	= TRUE
Noe_Time	= 2[s]
Repetition_Time	= 3.06430464[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:: KRY-137(2) pure-1.jdf
```

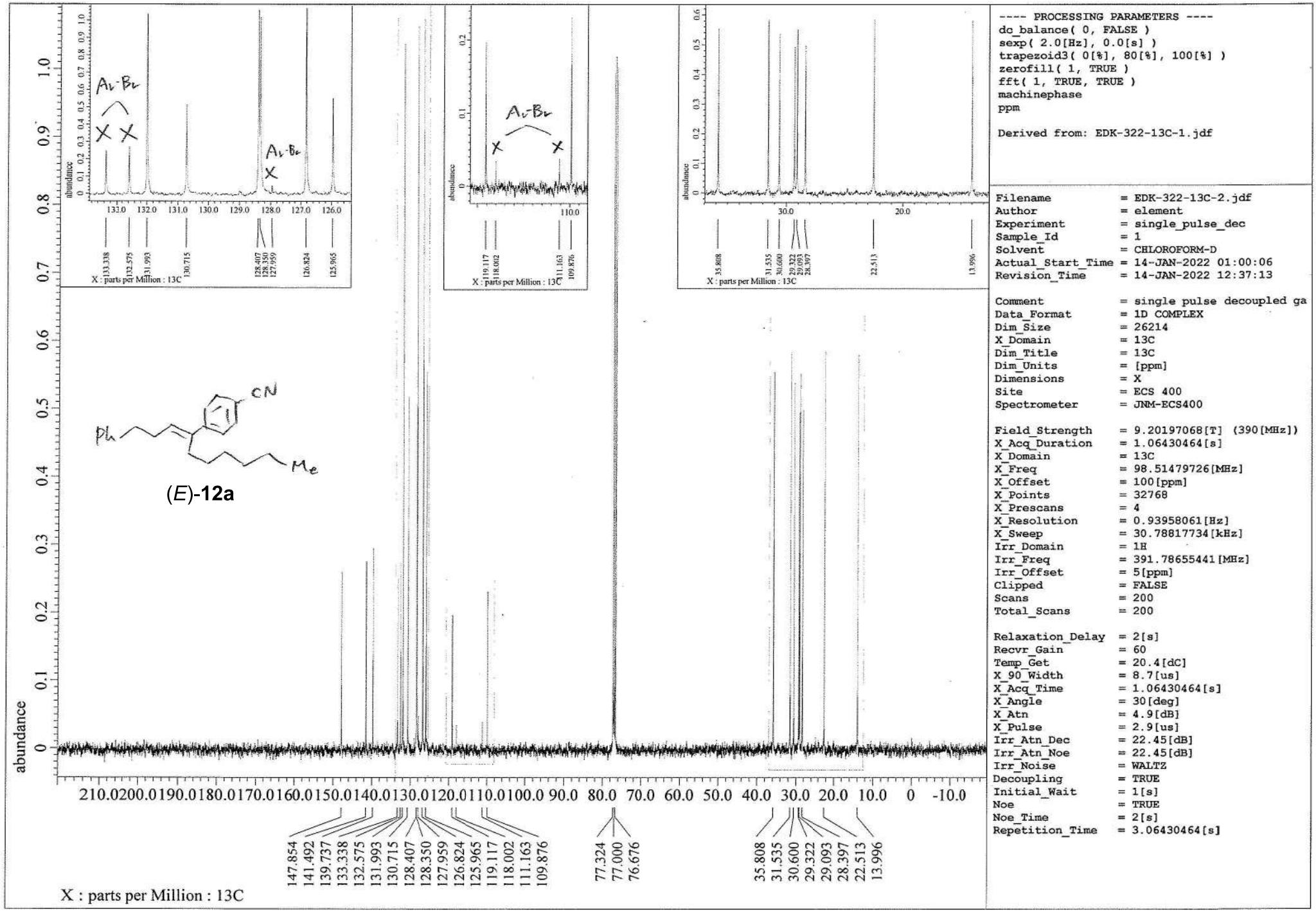
```
Filename            = KRY-137(2) pure-2.jdf
Author              = element
Experiment          = single_pulse.ex2
Sample_Id           = S#348665
Solvent             = CHLOROFORM-D
Actual_Start_Time   = 21-JUN-2021 16:22:13
Revision_Time       = 11-AUG-2021 15:16:37

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          = 50
Temp_Get            = 20.4[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]
```

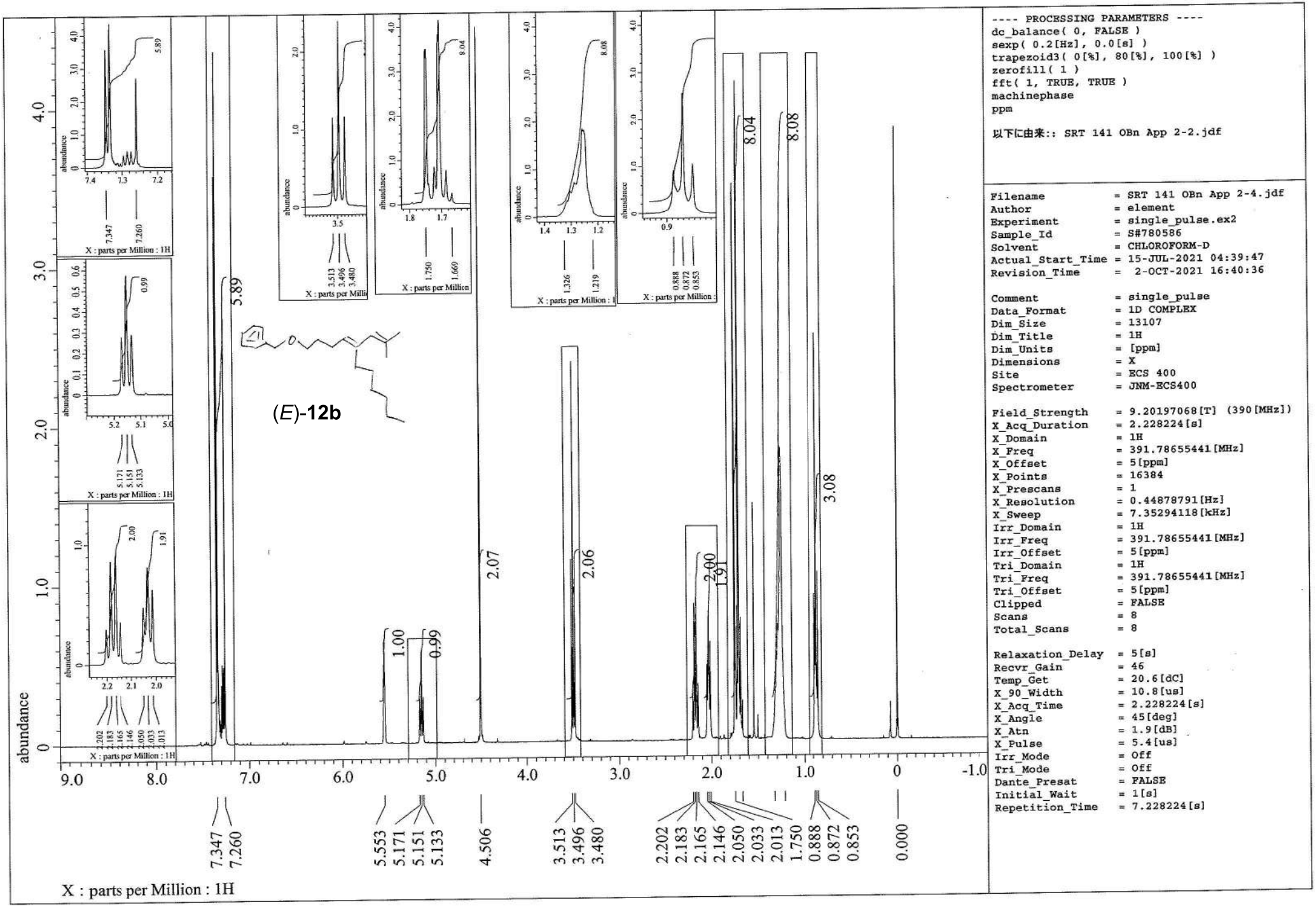

(E)-4ob
abundance
X : parts per Million : 13C
156.285
137.506
128.388
127.720
126.929
108.407
82.532
77.324
77.000
76.676
74.015
24.639
18.440
14.663
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid3(0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
以下に由来:: KRY-137(2) pure C-1.jdf
Filename = KRY-137(2) pure C-2.jdf
Author = element
Experiment = single_pulse_dec
Sample_Id = S#365799
Solvent = CHLOROFORM-D
Actual_Start_Time = 21-JUN-2021 16:50:32
Revision_Time = 23-OCT-2021 15:27:10
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = 13C
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_Strength = 9.20197068[T] (390[MHz])
X_Acq_Duration = 1.06430464[s]
X_Domain = 13C
X_Freq = 98.51479726[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.93958061[Hz]
X_Sweep = 30.78817734[kHz]
Irr_Domain = 1H
Irr_Freq = 391.78655441[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 200
Total_Scans = 200
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 21.4[dC]
X_90_Width = 8.7[us]
X_Acq_Time = 1.06430464[s]
X_Angle = 30[deg]
X_Atn = 4.9[dB]
X_Pulse = 2.9[us]
Irr_Atn_Dec = 22.45[dB]
Irr_Atn_Noe = 22.45[dB]
Irr_Noise = WALTZ
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.06430464[s]

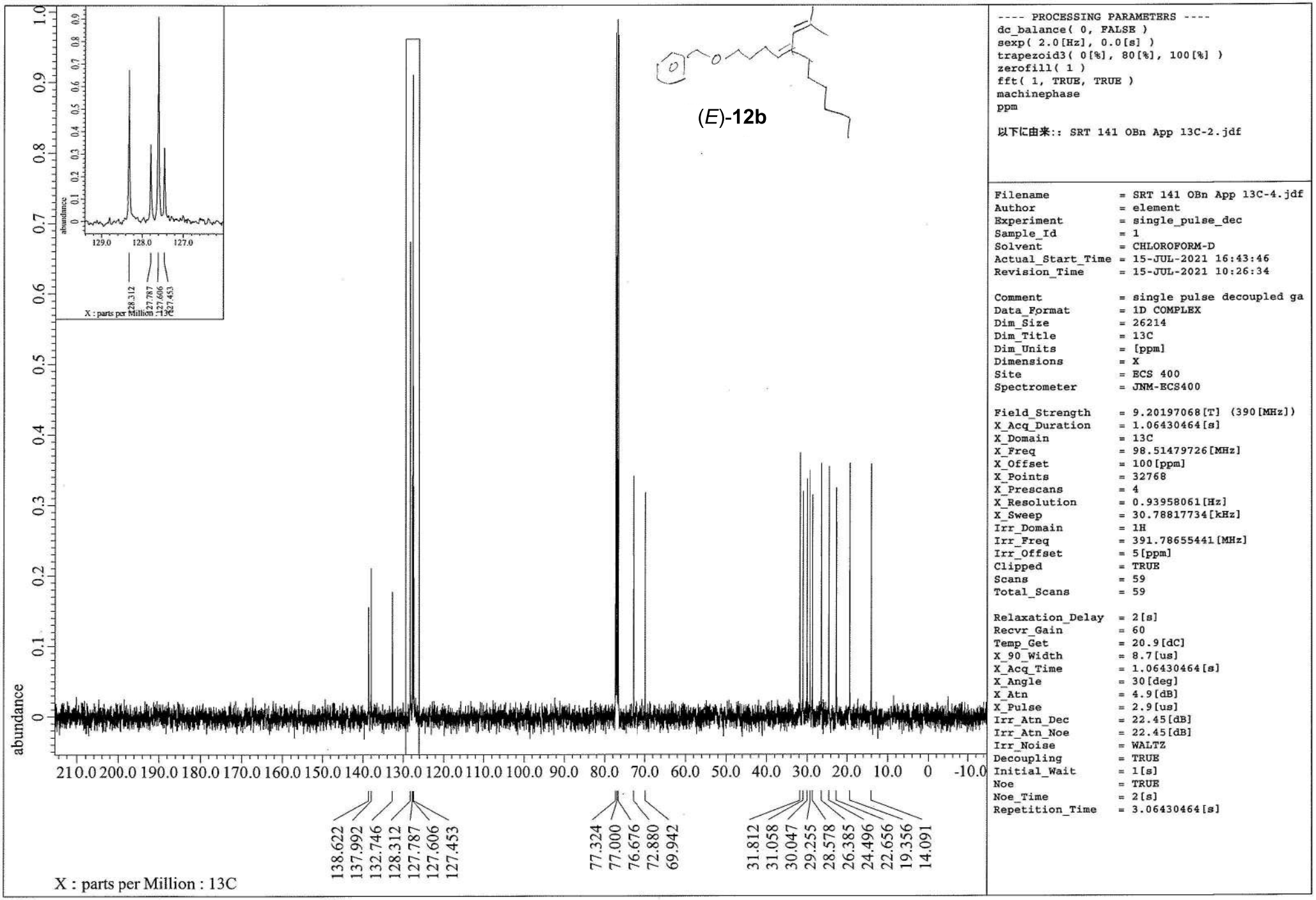


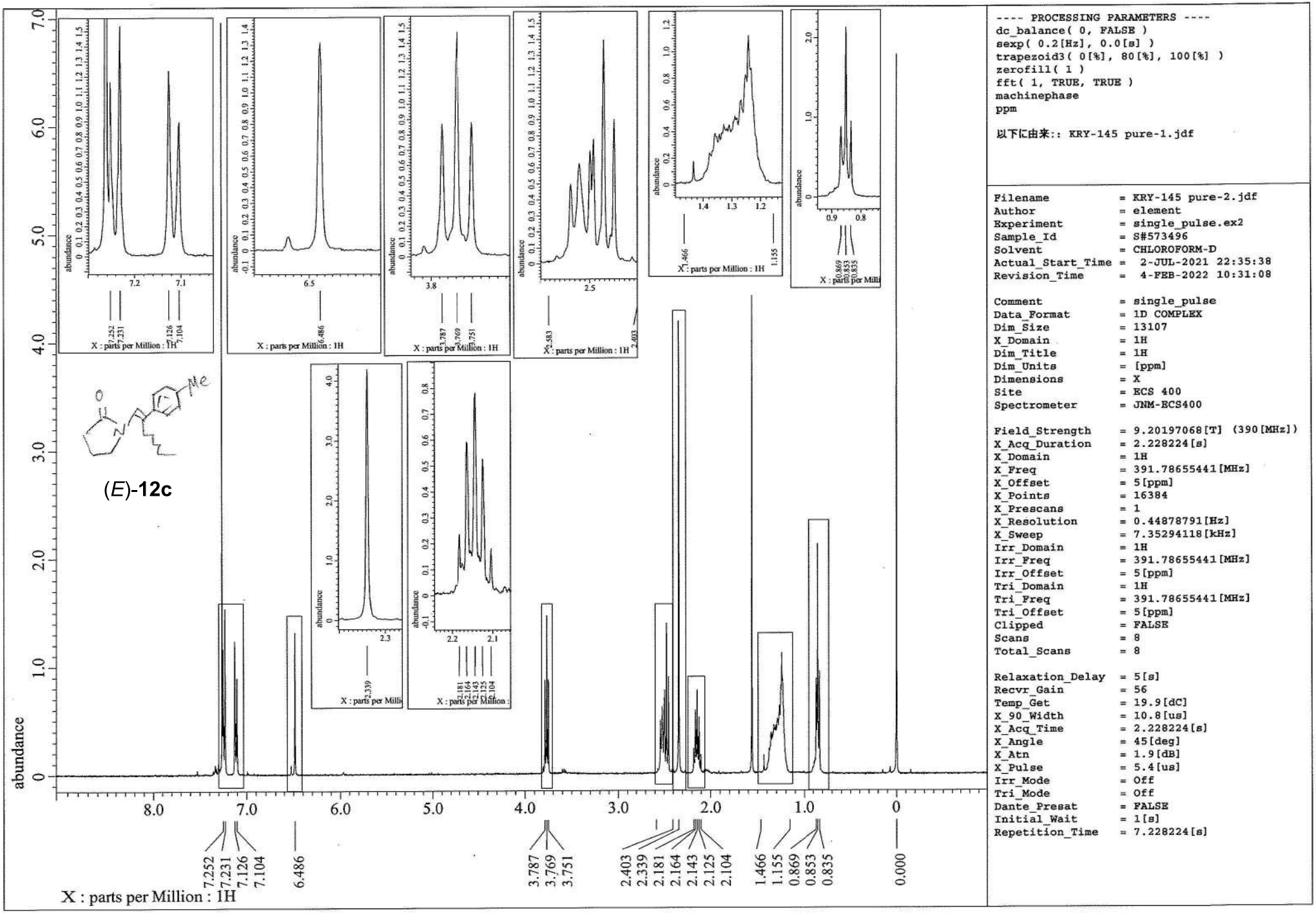

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: EDK-322-pure-1.jdf
```

Filename	= EDK-322-pure-2.jdf
Author	= element
Experiment	= single_pulse.ex2
Sample_Id	= S#599477
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 13-JAN-2022 23:32:14
Revision_Time	= 14-JAN-2022 13:03:19
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	= 40
Temp_Get	= 19.6[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]


Ar-Br
Ar-Br
CN
Ph
Me
(E)-12a
X : parts per Million : 13C
abundance
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid3(0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: EDK-322-13C-1.jdf
Filename = EDK-322-13C-2.jdf
Author = element
Experiment = single_pulse_dec
Sample_Id = 1
Solvent = CHLOROFORM-D
Actual_Start_Time = 14-JAN-2022 01:00:06
Revision_Time = 14-JAN-2022 12:37:13
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = 13C
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_Strength = 9.20197068[T] (390[MHz])
X_Acq_Duration = 1.06430464[s]
X_Domain = 13C
X_Freq = 98.51479726[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.93958061[Hz]
X_Sweep = 30.78817734[kHz]
Irr_Domain = 1H
Irr_Freq = 391.78655441[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 200
Total_Scans = 200
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 20.4[dC]
X_90_Width = 8.7[us]
X_Acq_Time = 1.06430464[s]
X_Angle = 30[deg]
X_Atn = 4.9[dB]
X_Pulse = 2.9[us]
Irr_Atn_Dec = 22.45[dB]
Irr_Atn_Noe = 22.45[dB]
Irr_Noise = WALTZ
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.06430464[s]

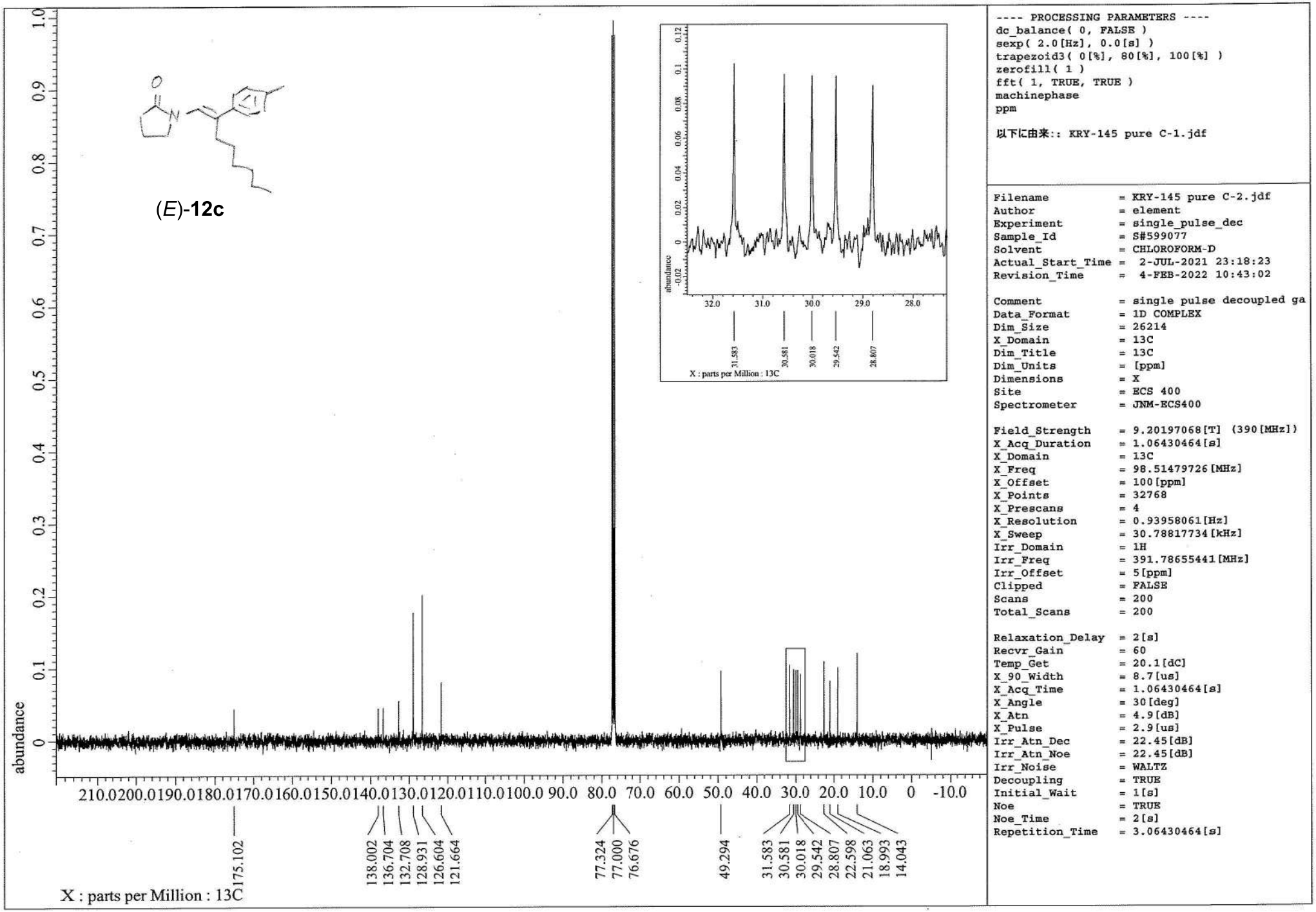

(E)-12b
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid3(0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
以下に由来:: SRT 141 OBn App 2-2.jdf
Filename = SRT 141 OBn App 2-4.jdf
Author = element
Experiment = single_pulse.ex2
Sample_Id = S#780586
Solvent = CHLOROFORM-D
Actual_Start_Time = 15-JUL-2021 04:39:47
Revision_Time = 2-OCT-2021 16:40:36
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
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 = 46
Temp_Get = 20.6[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]
abundance
X : parts per Million : 1H

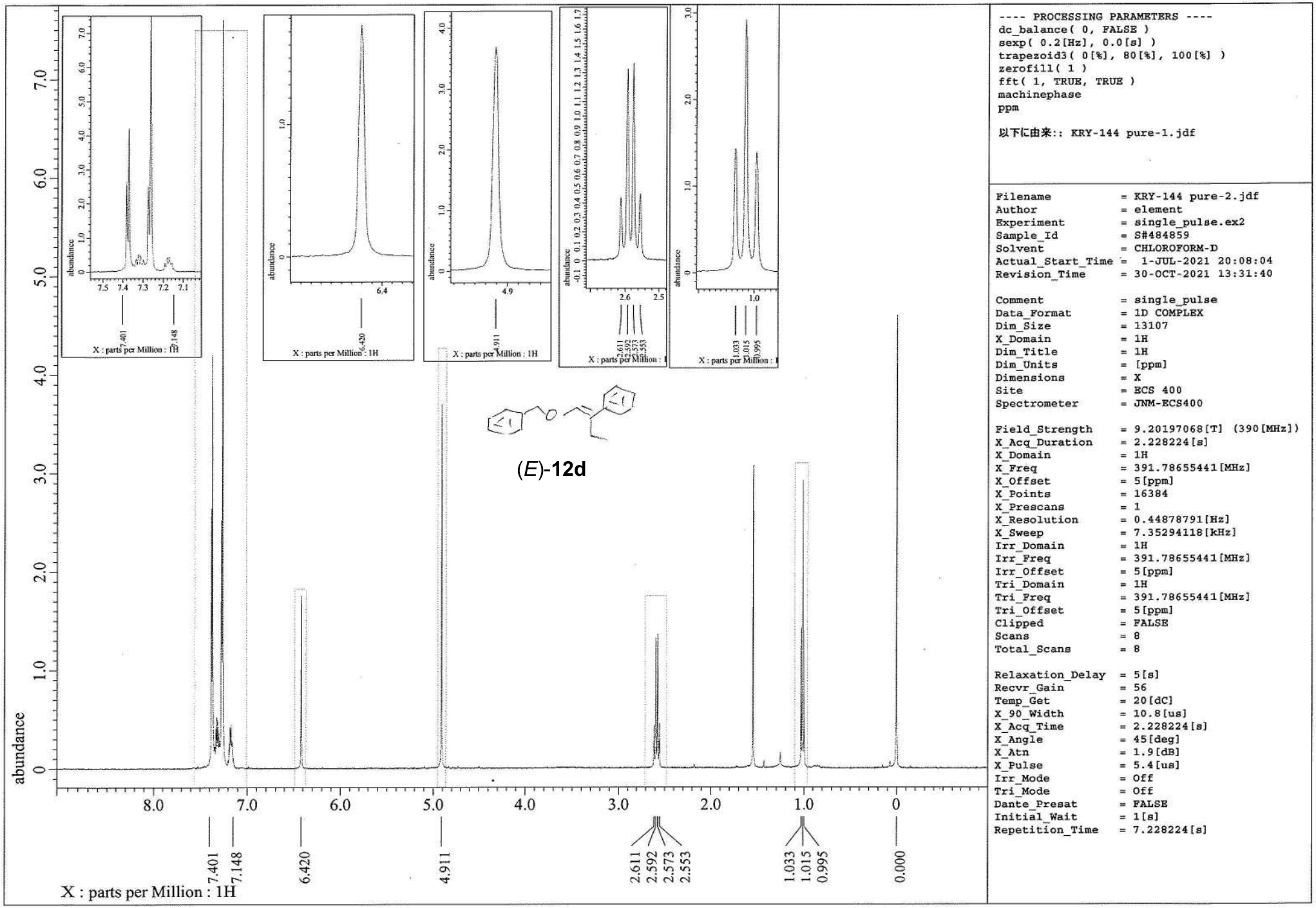

(E)-12b
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid3(0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
以下に由来:: SRT 141 OBn App 13C-2.jdf
Filename = SRT 141 OBn App 13C-4.jdf
Author = element
Experiment = single_pulse_dec
Sample_Id = 1
Solvent = CHLOROFORM-D
Actual_Start_Time = 15-JUL-2021 16:43:46
Revision_Time = 15-JUL-2021 10:26:34
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_Strength = 9.20197068[T] (390[MHz])
X_Acq_Duration = 1.06430464[s]
X_Domain = 13C
X_Freq = 98.51479726[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.93958061[Hz]
X_Sweep = 30.78817734[kHz]
Irr_Domain = 1H
Irr_Freq = 391.78655441[MHz]
Irr_Offset = 5[ppm]
Clipped = TRUE
Scans = 59
Total_Scans = 59
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 20.9[dC]
X_90_Width = 8.7[us]
X_Acq_Time = 1.06430464[s]
X_Angle = 30[deg]
X_Atn = 4.9[dB]
X_Pulse = 2.9[us]
Irr_Atn_Dec = 22.45[dB]
Irr_Atn_Noe = 22.45[dB]
Irr_Noise = WALTZ
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.06430464[s]
abundance
X : parts per Million : 13C
138.622
137.992
132.746
128.312
127.787
127.606
127.453
77.324
77.000
76.676
72.880
69.942
31.812
31.058
30.047
29.255
28.578
26.385
24.496
22.656
19.356
14.091




```
---- 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:: KRY-145 pure-1.jdf
```

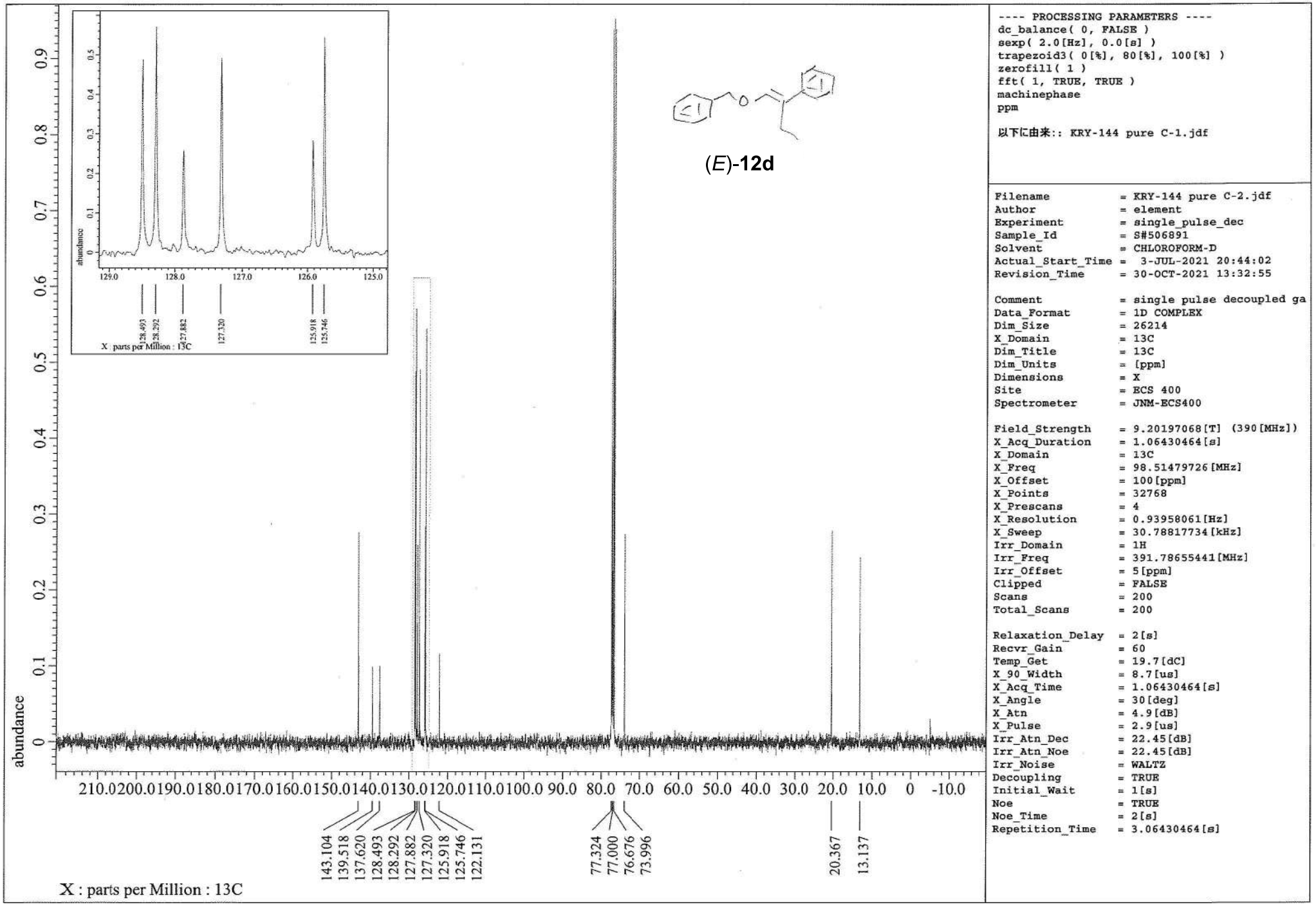
```
Filename            = KRY-145 pure-2.jdf
Author              = element
Experiment          = single_pulse.ex2
Sample_Id           = S#573496
Solvent             = CHLOROFORM-D
Actual_Start_Time   =  2-JUL-2021 22:35:38
Revision_Time       =  4-FEB-2022 10:31:08

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            = 19.9[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]
```

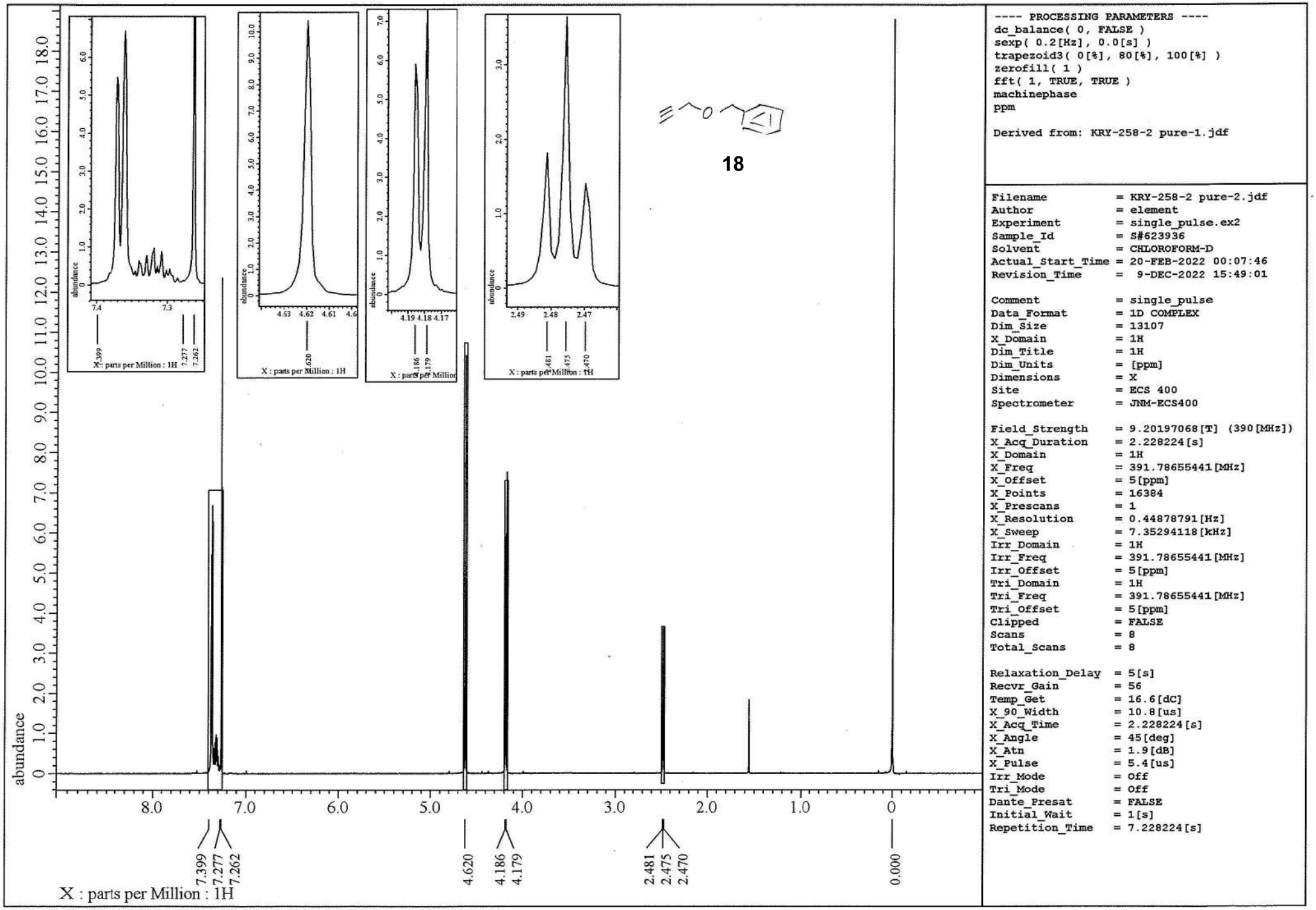

(E)-12c
abundance
X : parts per Million : 13C
175.102
138.002
136.704
132.708
128.931
126.604
121.664
77.324
77.000
76.676
49.294
31.583
30.581
30.018
29.542
28.807
22.598
21.063
18.993
14.043
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid3(0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
以下に由来:: KRY-145 pure C-1.jdf
Filename = KRY-145 pure C-2.jdf
Author = element
Experiment = single_pulse_dec
Sample_Id = S#599077
Solvent = CHLOROFORM-D
Actual_Start_Time = 2-JUL-2021 23:18:23
Revision_Time = 4-FEB-2022 10:43:02
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = 13C
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_Strength = 9.20197068[T] (390[MHz])
X_Acq_Duration = 1.06430464[s]
X_Domain = 13C
X_Freq = 98.51479726[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.93958061[Hz]
X_Sweep = 30.78817734[kHz]
Irr_Domain = 1H
Irr_Freq = 391.78655441[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 200
Total_Scans = 200
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 20.1[dC]
X_90_Width = 8.7[us]
X_Acq_Time = 1.06430464[s]
X_Angle = 30[deg]
X_Atn = 4.9[dB]
X_Pulse = 2.9[us]
Irr_Atn_Dec = 22.45[dB]
Irr_Atn_Noe = 22.45[dB]
Irr_Noise = WALTZ
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.06430464[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:: KRY-144 pure-1.jdf
```

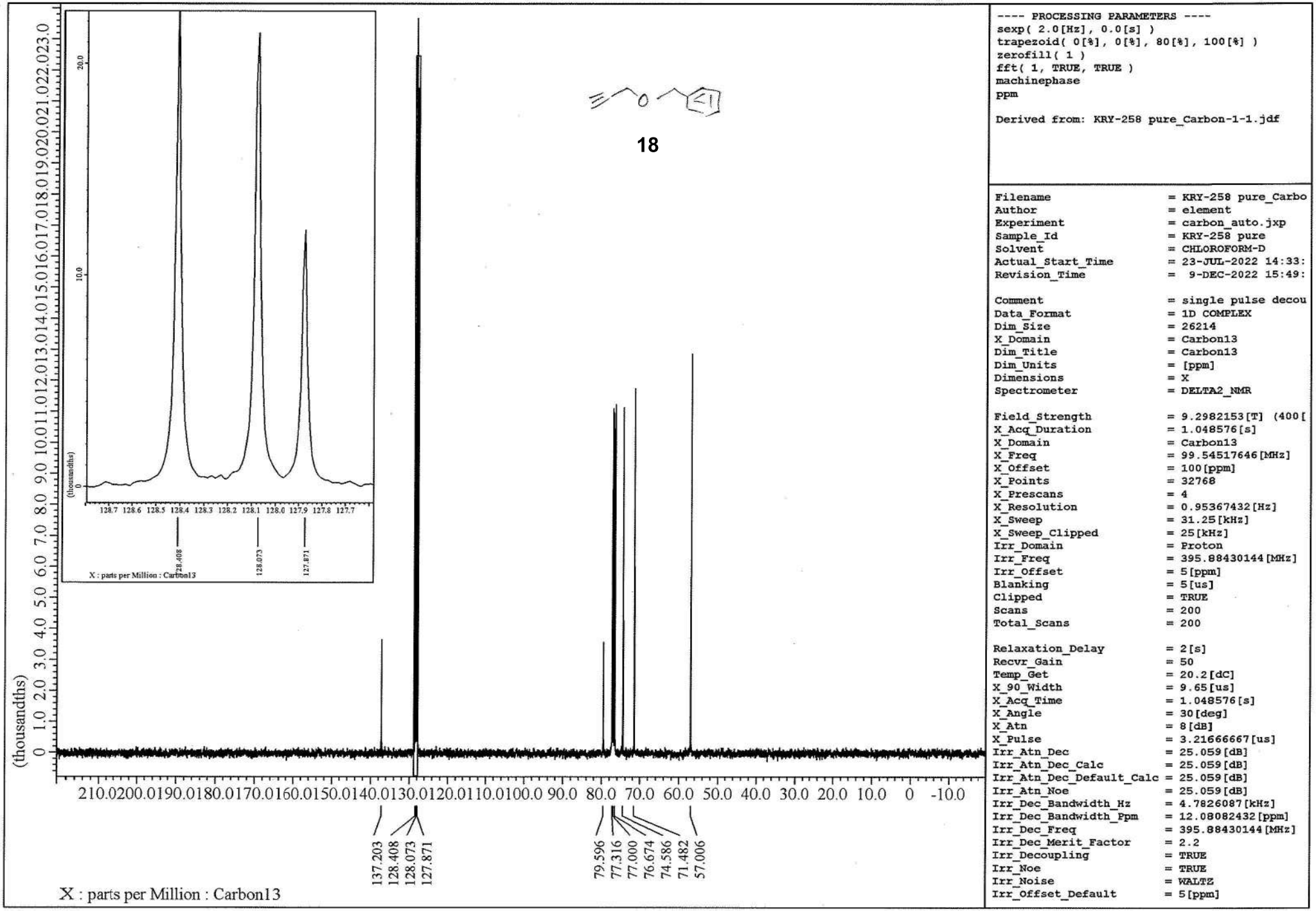
```
Filename            = KRY-144 pure-2.jdf
Author              = element
Experiment          = single_pulse.ex2
Sample_Id           = S#484859
Solvent             = CHLOROFORM-D
Actual_Start_Time   =  1-JUL-2021 20:08:04
Revision_Time       = 30-OCT-2021 13:31:40

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[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]
```

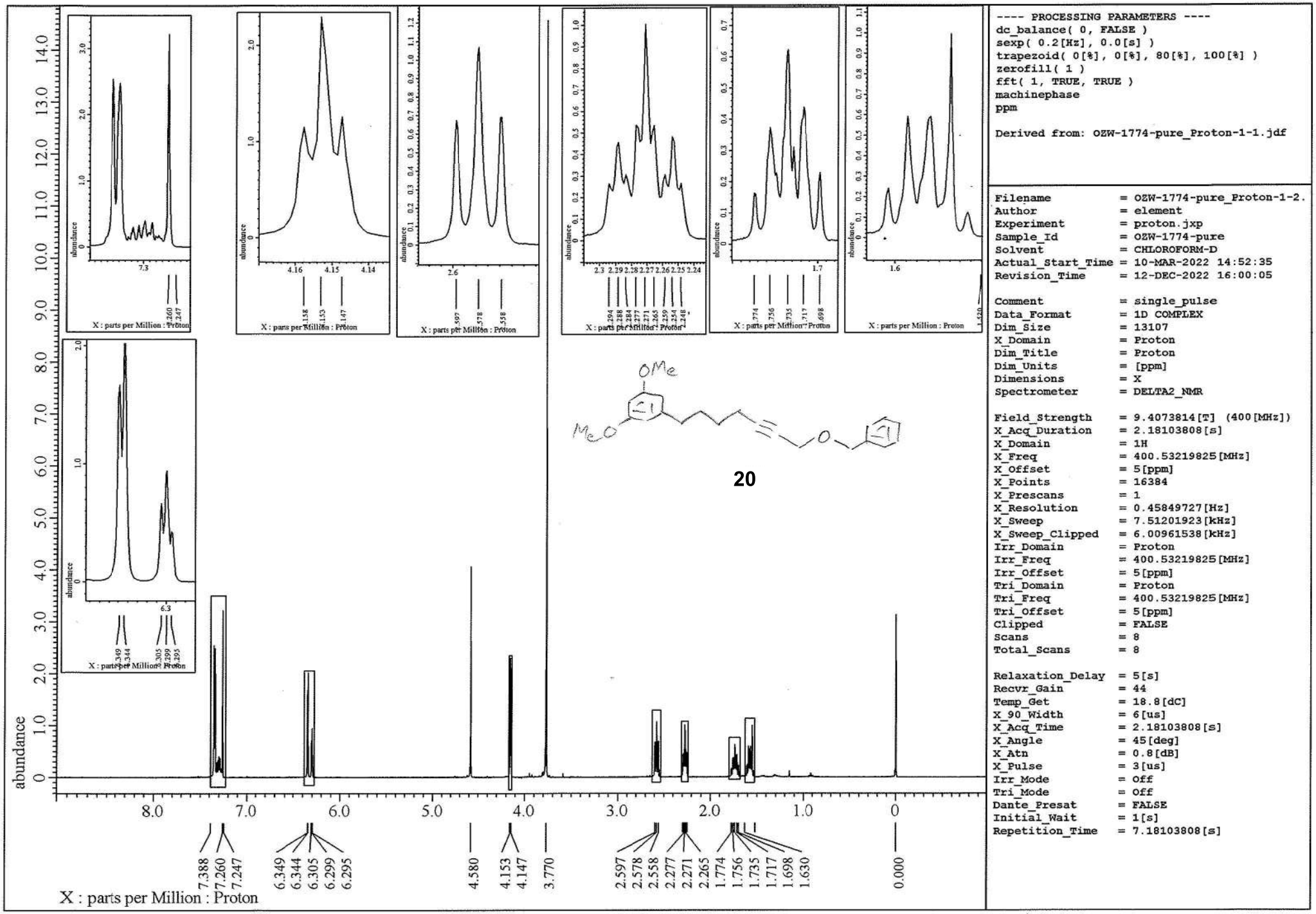

abundance
X : parts per Million : 13C
143.104
139.518
137.620
128.493
128.292
127.882
127.320
125.918
125.746
122.131
77.324
77.000
76.676
73.996
20.367
13.137
X : parts per Million : 13C
(E)-12d
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid3(0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
以下に由来:: KRY-144 pure C-1.jdf
Filename = KRY-144 pure C-2.jdf
Author = element
Experiment = single_pulse_dec
Sample_Id = S#506891
Solvent = CHLOROFORM-D
Actual_Start_Time = 3-JUL-2021 20:44:02
Revision_Time = 30-OCT-2021 13:32:55
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = 13C
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_Strength = 9.20197068[T] (390[MHz])
X_Acq_Duration = 1.06430464[s]
X_Domain = 13C
X_Freq = 98.51479726[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.93958061[Hz]
X_Sweep = 30.78817734[kHz]
Irr_Domain = 1H
Irr_Freq = 391.78655441[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 200
Total_Scans = 200
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 19.7[dC]
X_90_Width = 8.7[us]
X_Acq_Time = 1.06430464[s]
X_Angle = 30[deg]
X_Atn = 4.9[dB]
X_Pulse = 2.9[us]
Irr_Atn_Dec = 22.45[dB]
Irr_Atn_Noe = 22.45[dB]
Irr_Noise = WALTZ
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.06430464[s]

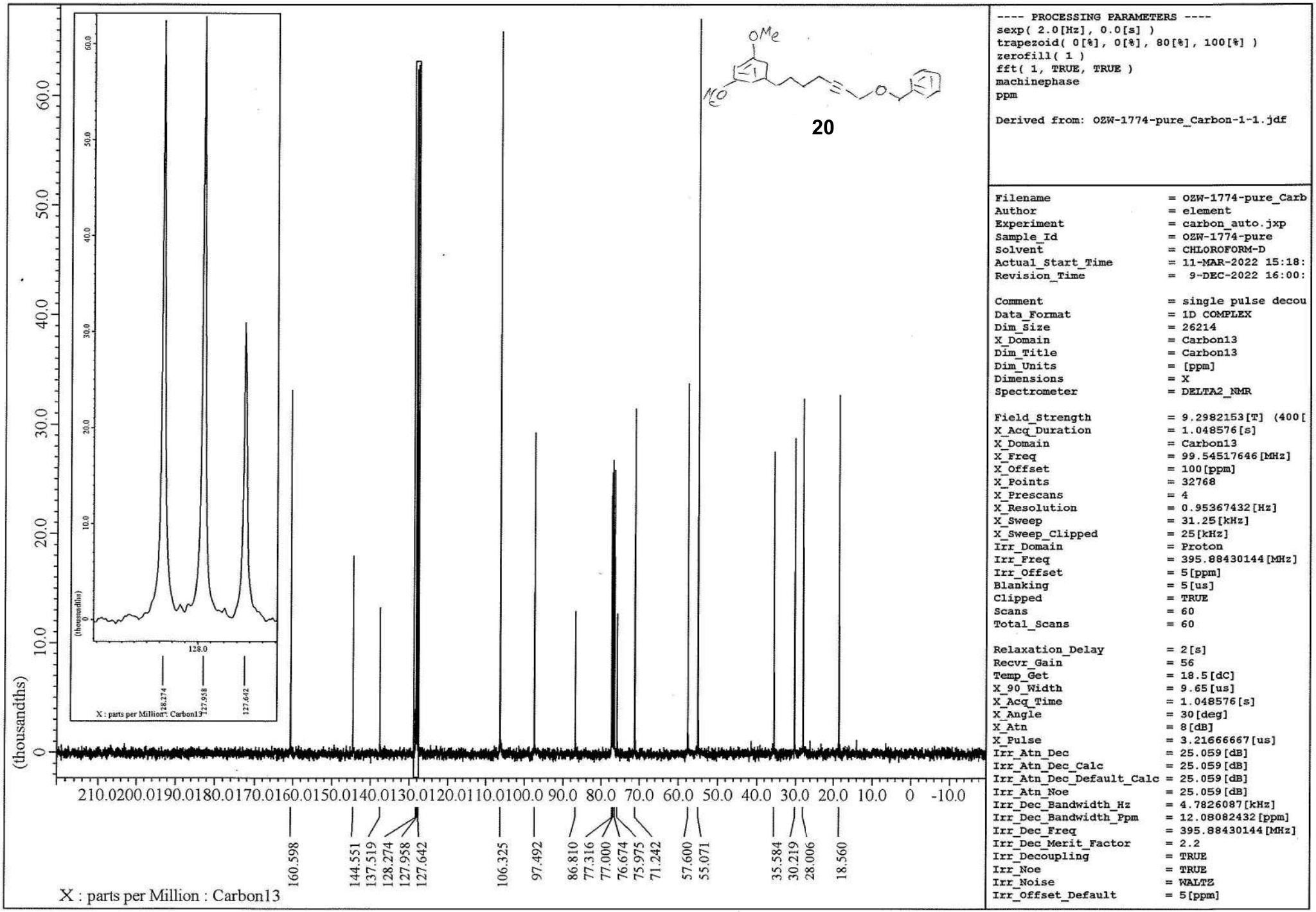


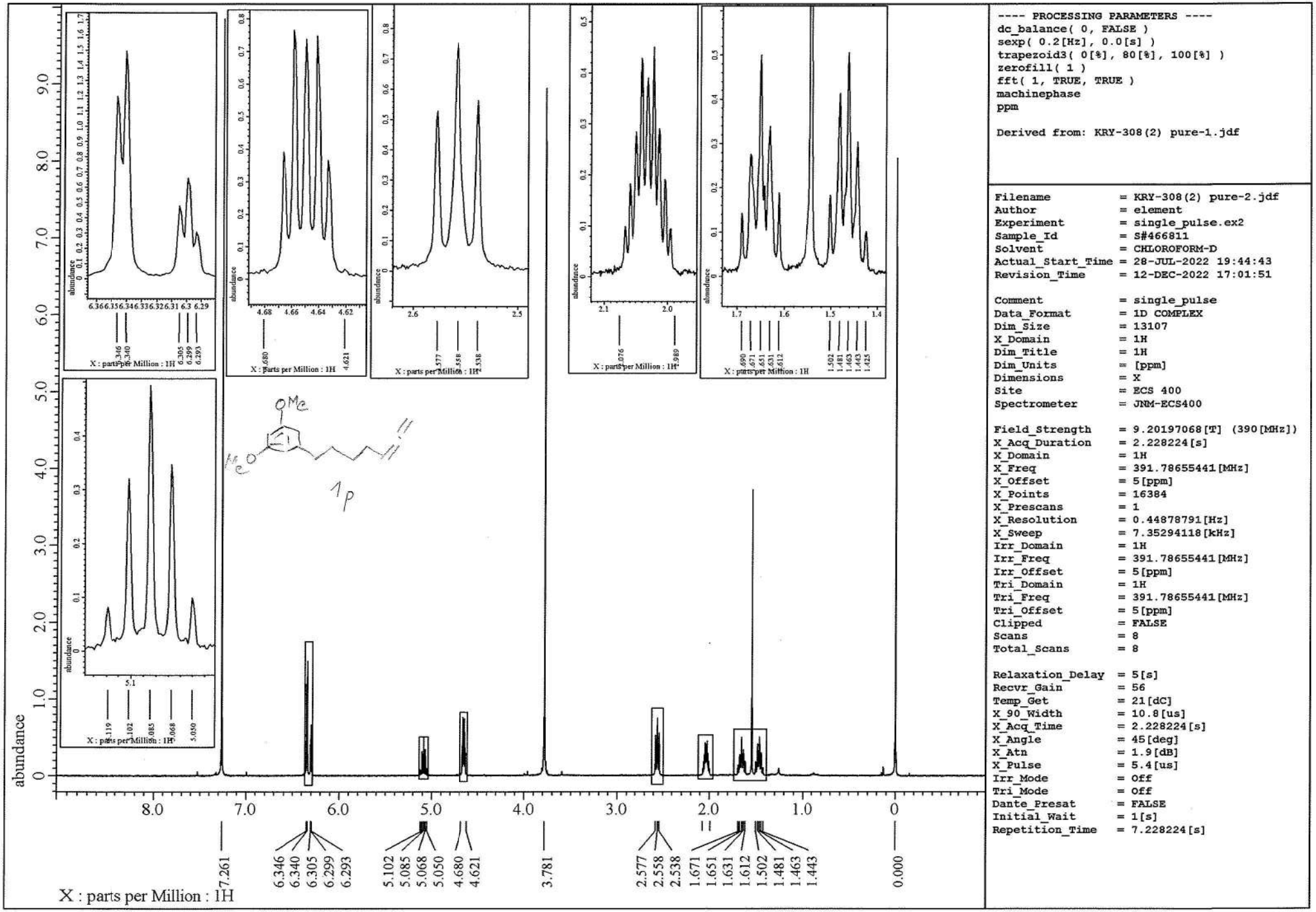

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KRY-258-2 pure-1.jdf
```

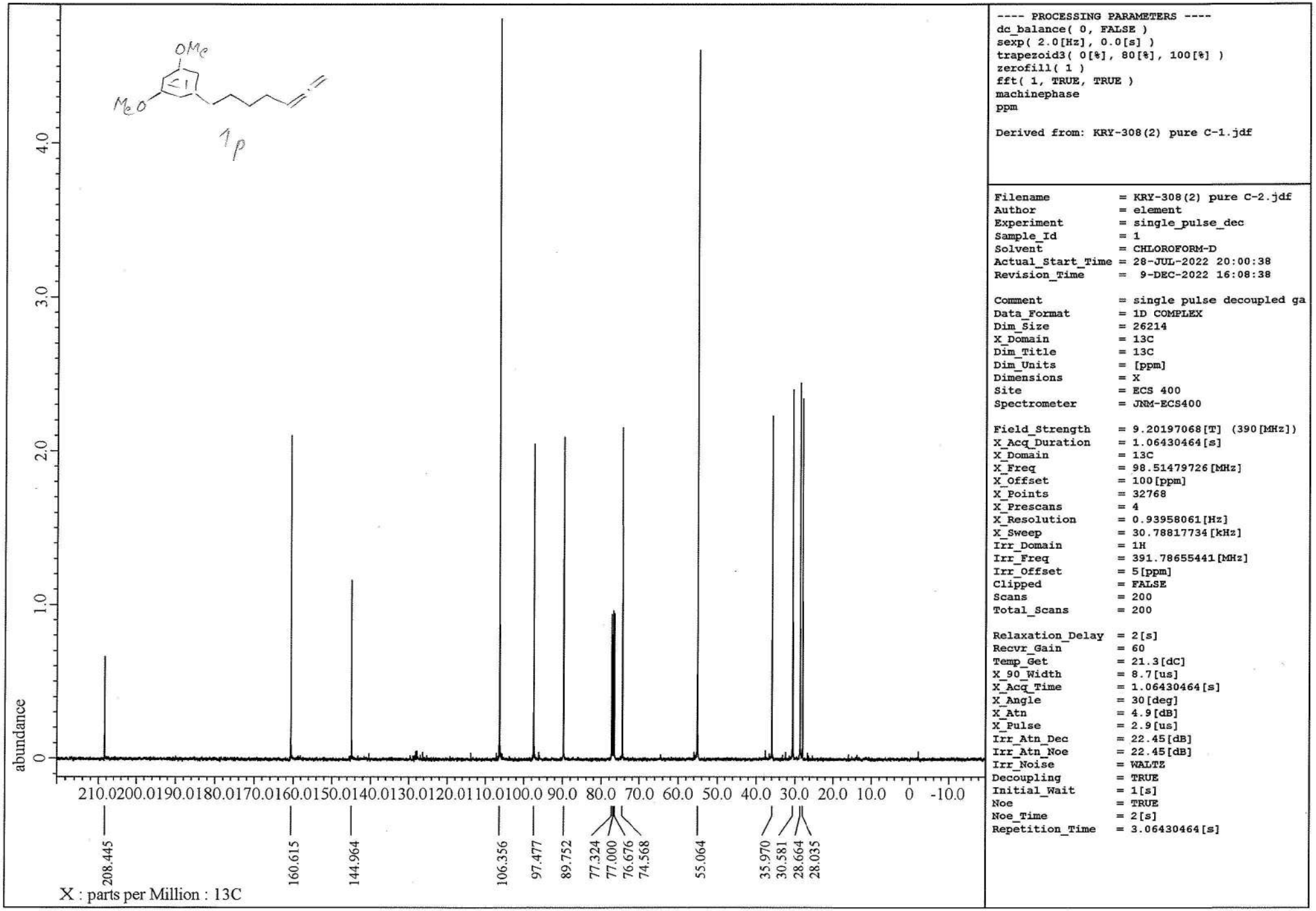
```
Filename            = KRY-258-2 pure-2.jdf
Author              = element
Experiment          = single_pulse.ex2
Sample_Id           = S#623936
Solvent             = CHLOROFORM-D
Actual_Start_Time   = 20-FEB-2022 00:07:46
Revision_Time       =  9-DEC-2022 15:49:01

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            = 16.6[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]
```

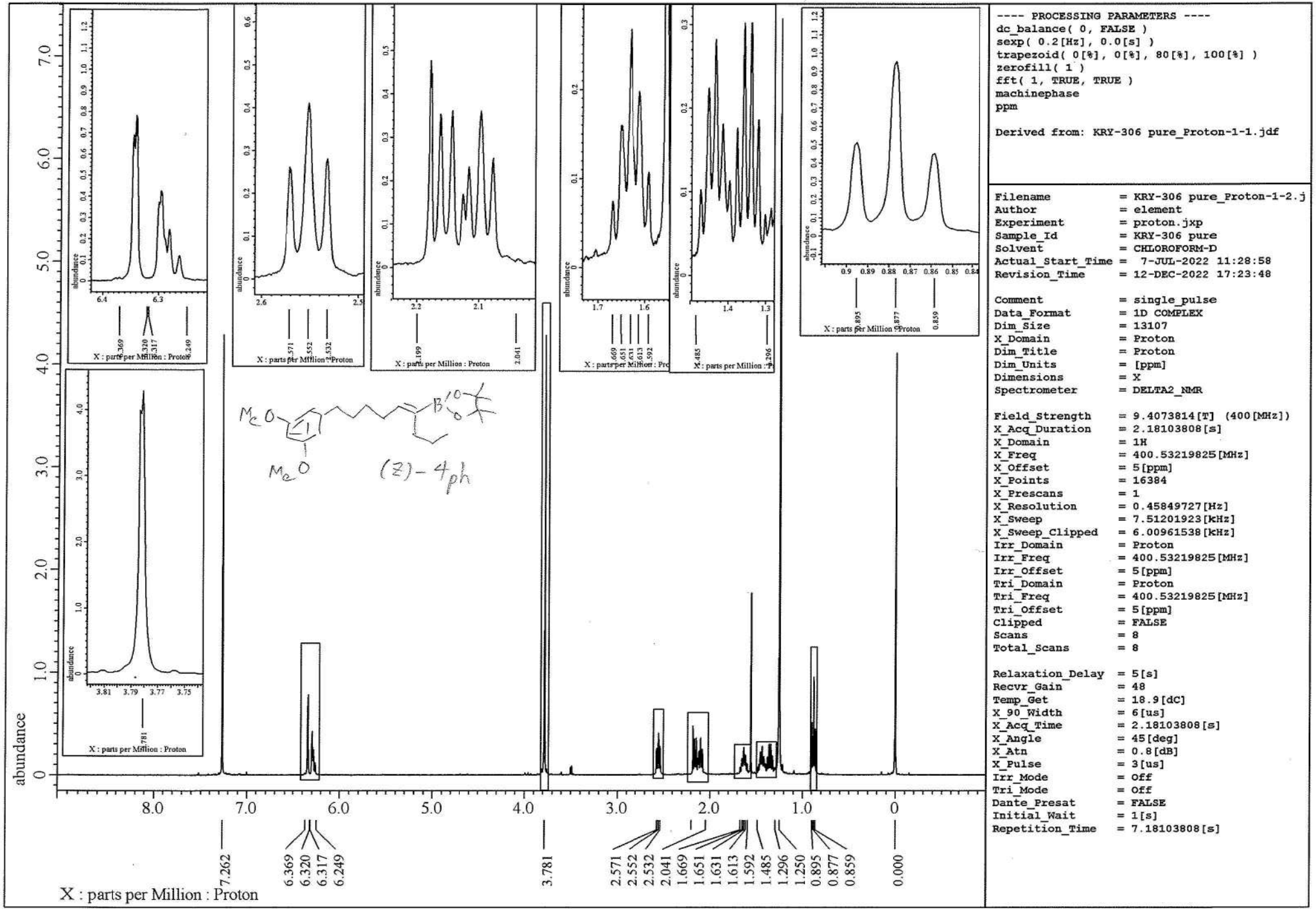

18
---- PROCESSING PARAMETERS ----
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: KRY-258 pure_Carbon-1-1.jdf
Filename = KRY-258 pure_Carbo
Author = element
Experiment = carbon_auto.jxp
Sample_Id = KRY-258 pure
Solvent = CHLOROFORM-D
Actual_Start_Time = 23-JUL-2022 14:33:
Revision_Time = 9-DEC-2022 15:49:
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 = 200
Total_Scans = 200
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 20.2[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
137.203
128.408
128.073
127.871
79.596
77.316
77.000
76.674
74.586
71.482
57.006


OMe
MeO
O
20
X : parts per Million : Proton
7.388
7.260
7.247
6.349
6.344
6.305
6.299
6.295
4.580
4.153
4.147
3.770
2.597
2.578
2.558
2.277
2.271
2.265
1.774
1.756
1.735
1.717
1.698
1.630
0.000
---- 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: OZW-1774-pure_Proton-1-1.jdf
Filename = OZW-1774-pure_Proton-1-2.
Author = element
Experiment = proton.jxp
Sample_Id = OZW-1774-pure
Solvent = CHLOROFORM-D
Actual_Start_Time = 10-MAR-2022 14:52:35
Revision_Time = 12-DEC-2022 16:00:05
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 = 44
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]


OMe
NO
O
20
---- PROCESSING PARAMETERS ----
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: OZW-1774-pure_Carbon-1-1.jdf
Filename = OZW-1774-pure_Carb
Author = element
Experiment = carbon_auto.jxp
Sample_Id = OZW-1774-pure
Solvent = CHLOROFORM-D
Actual_Start_Time = 11-MAR-2022 15:18:
Revision_Time = 9-DEC-2022 16:00:
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 = 60
Total_Scans = 60
Relaxation_Delay = 2[s]
Recvr_Gain = 56
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]
(thousandths)
X : parts per Million : Carbon13
160.598
144.551
137.519
128.274
127.958
127.642
106.325
97.492
86.810
77.316
77.000
76.674
75.975
71.242
57.600
55.071
35.584
30.219
28.006
18.560

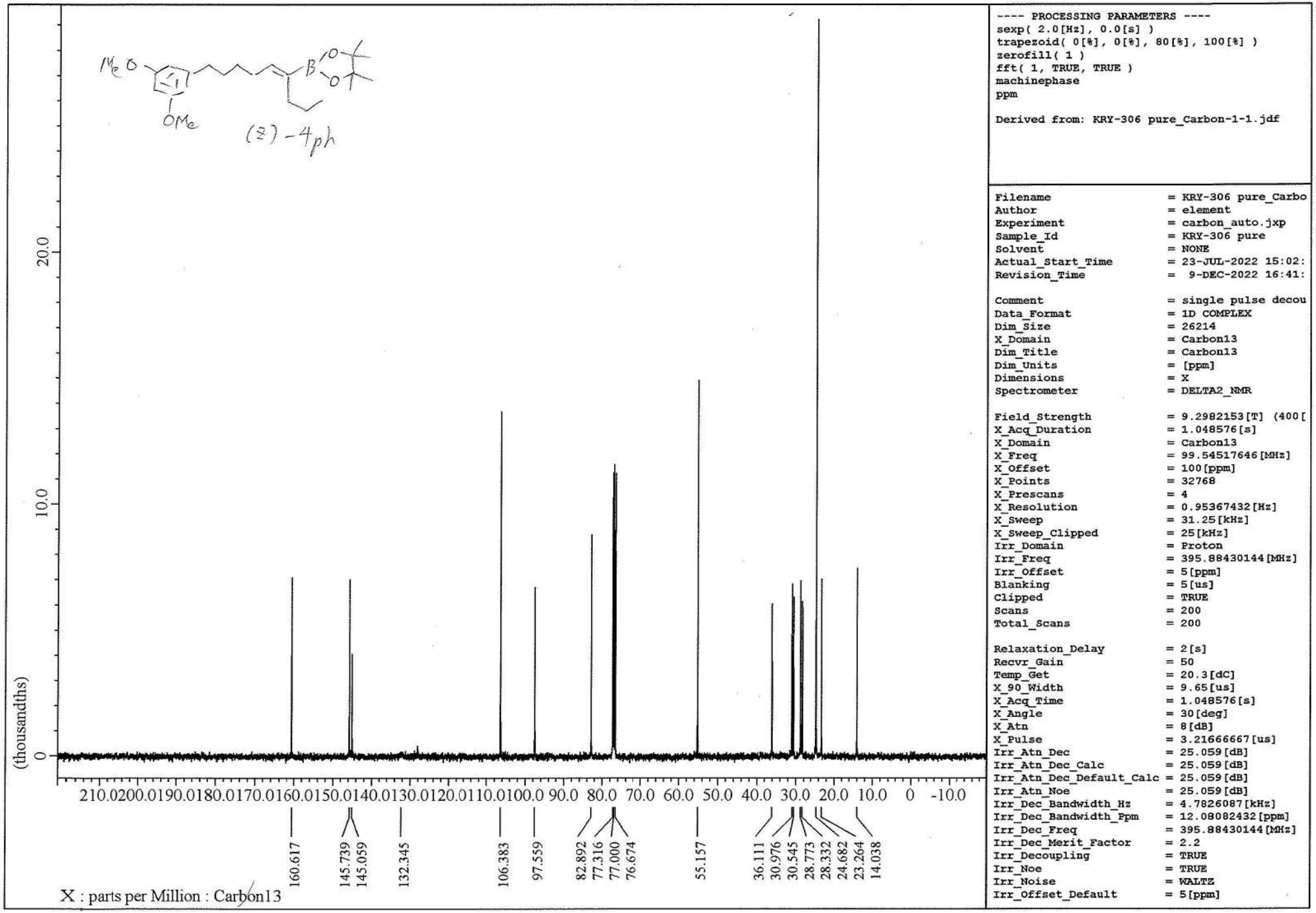

---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid3(0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: KRY-308(2) pure-1.jdf
Filename = KRY-308(2) pure-2.jdf
Author = element
Experiment = single_pulse.ex2
Sample_Id = S#466811
Solvent = CHLOROFORM-D
Actual_Start_Time = 28-JUL-2022 19:44:43
Revision_Time = 12-DEC-2022 17:01:51
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 = 21[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]
OMe
MeO
1p
abundance
X : parts per Million : 1H
7.261
6.346
6.340
6.305
6.299
6.293
5.102
5.085
5.068
5.050
4.680
4.621
3.781
2.577
2.558
2.538
1.671
1.651
1.631
1.612
1.502
1.481
1.463
1.443
0.000

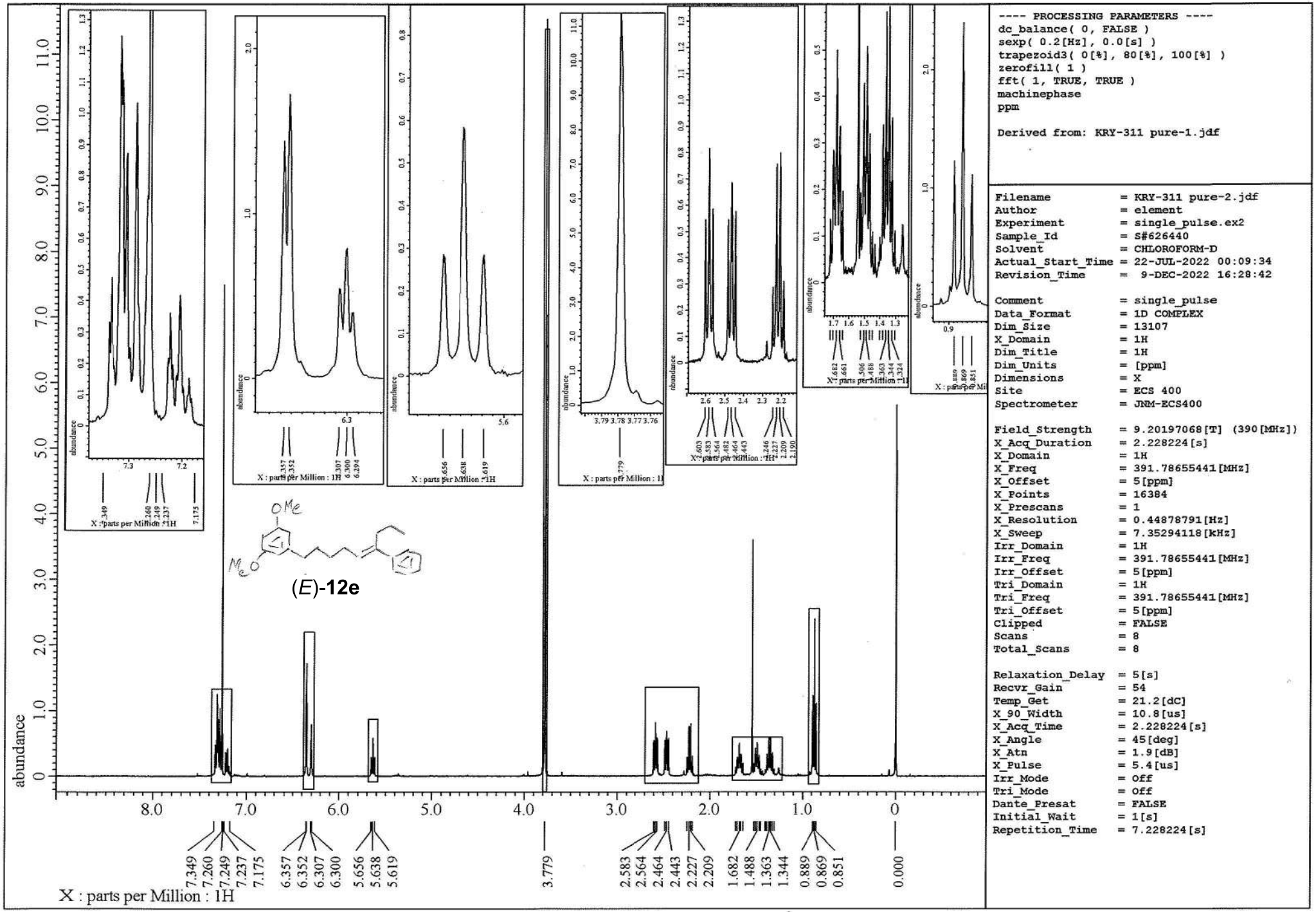

OMe
MeO
1p
abundance
4.0
3.0
2.0
1.0
0
210.0200.0190.0180.0170.0160.0150.0140.0130.0120.0110.0100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0
208.445
160.615
144.964
106.356
97.477
89.752
77.324
77.000
76.676
74.568
55.064
35.970
30.581
28.664
28.035
X : parts per Million : 13C
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid3(0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: KRY-308(2) pure C-1.jdf
Filename = KRY-308(2) pure C-2.jdf
Author = element
Experiment = single_pulse_dec
Sample_Id = 1
Solvent = CHLOROFORM-D
Actual_Start_Time = 28-JUL-2022 20:00:38
Revision_Time = 9-DEC-2022 16:08:38
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = 13C
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_Strength = 9.20197068[T] (390[MHz])
X_Acq_Duration = 1.06430464[s]
X_Domain = 13C
X_Freq = 98.51479726[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.93958061[Hz]
X_Sweep = 30.78817734[kHz]
Irr_Domain = 1H
Irr_Freq = 391.78655441[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 200
Total_Scans = 200
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 21.3[dC]
X_90_Width = 8.7[us]
X_Acq_Time = 1.06430464[s]
X_Angle = 30[deg]
X_Atn = 4.9[dB]
X_Pulse = 2.9[us]
Irr_Atn_Dec = 22.45[dB]
Irr_Atn_Noe = 22.45[dB]
Irr_Noise = WALTZ
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.06430464[s]

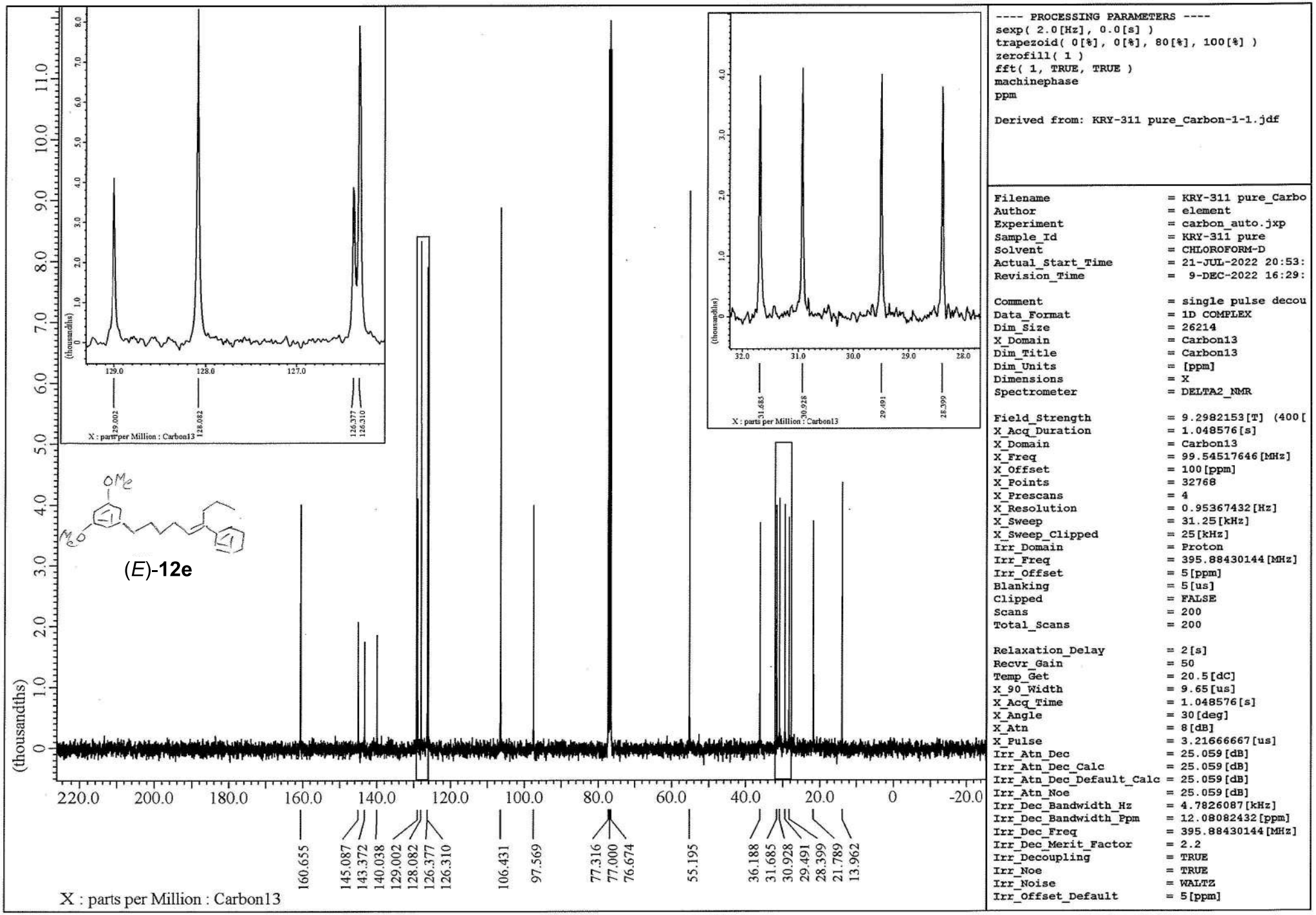



```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KRY-306 pure_Proton-1-1.jdf
```

```
Filename            = KRY-306 pure_Proton-1-2.j
Author              = element
Experiment          = proton.jxp
Sample_Id           = KRY-306 pure
Solvent             = CHLOROFORM-D
Actual_Start_Time   =  7-JUL-2022 11:28:58
Revision_Time       = 12-DEC-2022 17:23:48

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            = 18.9[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]
```


(thousandths)
20.0
10.0
0
210.0200.0190.0180.0170.0160.0150.0140.0130.0120.0110.0100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0
160.617
145.739
145.059
132.345
106.383
97.559
82.892
77.316
77.000
76.674
55.157
36.111
30.976
30.545
28.773
28.332
24.682
23.264
14.038
X : parts per Million : Carbon13
(Z)-4ph
---- PROCESSING PARAMETERS ----
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: KRY-306 pure_Carbon-1-1.jdf
Filename = KRY-306 pure_Carbo
Author = element
Experiment = carbon_auto.jxp
Sample_Id = KRY-306 pure
Solvent = NONE
Actual_Start_Time = 23-JUL-2022 15:02:
Revision_Time = 9-DEC-2022 16:41:
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 = 20.3[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])
trapezoid3(0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: KRY-311 pure-1.jdf
Filename = KRY-311 pure-2.jdf
Author = element
Experiment = single_pulse.ex2
Sample_Id = S#626440
Solvent = CHLOROFORM-D
Actual_Start_Time = 22-JUL-2022 00:09:34
Revision_Time = 9-DEC-2022 16:28:42
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 = 54
Temp_Get = 21.2[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]
OMe
MeO
(E)-12e
abundance
X : parts per Million : 1H
7.349
7.260
7.249
7.237
7.175
6.357
6.352
6.307
6.300
5.656
5.638
5.619
3.779
2.583
2.564
2.464
2.443
2.227
2.209
1.682
1.488
1.363
1.344
0.889
0.869
0.851
0.000


(thousandths)
X : parts per Million : Carbon13
160.655
145.087
143.372
140.038
129.002
128.082
126.377
126.310
106.431
97.569
77.316
77.000
76.674
55.195
36.188
31.685
30.928
29.491
28.399
21.789
13.962
OMe
MeO
(E)-12e
---- PROCESSING PARAMETERS ----
sexp(2.0[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: KRY-311 pure_Carbon-1-1.jdf
Filename = KRY-311 pure_Carbo
Author = element
Experiment = carbon_auto.jxp
Sample_Id = KRY-311 pure
Solvent = CHLOROFORM-D
Actual_Start_Time = 21-JUL-2022 20:53:
Revision_Time = 9-DEC-2022 16:29:
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 = FALSE
Scans = 200
Total_Scans = 200
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 20.5[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]