Synthesis of hydrosilylboronates via the monoborylation of a dihydrosilane Si–H bond and their application for the generation of dialkylhydrosilyl anions

Takumi Takeuchi, [†] Ryosuke Shishido, [†] Koji Kubota*, [†,‡] and Hajime Ito*,[†,‡]

[†]*Division of Applied Chemistry and Frontier Chemistry Center, Faculty of Engineering, Hokkaido University, Sapporo, Hokkaido, 060-8628, Japan.*

[‡]*Institute for Chemical Reaction Design and Discovery (WPI-ICReDD), Hokkaido University, Sapporo, Hokkaido 060-8628, Japan.*

e-mail: hajito@eng.hokudai.ac.jp

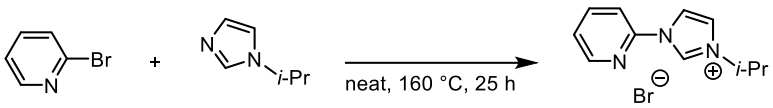
Table of Contents

1. Instrumentation and Chemicals

All reactions were performed in oven-dried glassware using conventional Schlenk techniques under a static pressure of nitrogen or argon. Materials were obtained from commercial suppliers and used as received unless otherwise noted. Dry solvents for the reactions were purchased from commercial suppliers, degassed via three freeze-pump-thaw cycles, and further dried over molecular sieves (MS4A) before use. $[Ir(cod)Cl]_2$ (>93%), $Ni(cod)_2$ (>97%), K(O-*t*-Bu) (>97%), ICy·HCl (>98.0%) and di-*tert*-butylsilane (**1a**) were purchased from TCI and used as received. Bis(pinacolato)diboron $[B_2(pin)_2]$ was recrystallized prior to use. Silica Gel 60 N (40–100 μm, spherical, neutral) purchased from Kanto Chemical Co. was used as received. GLC analyses were conducted with a Shimadzu GC-2014 or GC-2025 equipped with ULBON HR-1 glass capillary column (Shinwa Chemical Industries) and an FID detector. *n*-$C_{13}H_{28}$ was used as an internal standard for determining GC yield. Recycle preparative gel chromatography (GPC) was conducted with JAILC-9101 using $CHCl_3$ as an eluent. NMR spectra were recorded on JEOL JNM-ECX400P, ECS-400 (^{1}H: 400 MHz, ^{13}C: 100 MHz, ^{29}Si: 79.5 MHz), JNM-ECA600, and ECZ600R/S3 (^{29}Si: 120 MHz). Tetramethylsilane (δ = 0.00 ppm for ^{1}H-NMR and ^{29}Si-NMR) and $CDCl_3$ (δ = 77.0 ppm for ^{13}C-NMR) were employed as external standards, respectively. $BF_3·Et_2O$ was used as an external standard for ^{11}B NMR analysis. Multiplicity was reported as follows: s = singlet, brs = broad singlet, d = doublet, t = triplet, q = quartet, quint = quintet, sept = septet, m = multiplet. High-resolution mass spectra were recorded at the Global Facility Center for Instrumental Analysis, Hokkaido University. Single crystal X-ray structural analyses were carried out on a Rigaku XtaLAB AFC11 (RCD3) and XtaLAB PRO MM007 diffractometer using graphite monochromated Mo-Kα or Cu- Kα radiation. The structure was solved by direct methods and expanded using Fourier techniques. Non-hydrogen atoms were refined anisotropically. Hydrogen atoms were refined using the riding model. All calculations were performed using the Olex2 crystallographic software package except for refinement, which was performed using SHELXL-2013.

2. Preparation Procedures of L3 and Substrates

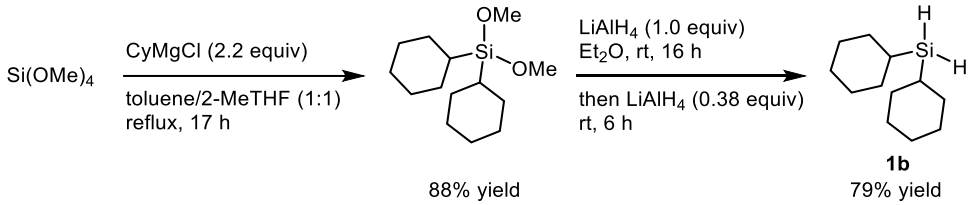
Preparation of L3



This reaction was performed according to the literature procedure.[1] 2-Bromopyridine (1.00 mL, 10.0 mmol) was added dropwise to 1-isopropylimidazole (1.10 g, 10.0 mmol, 1.00 equiv) under nitrogen atmosphere. The reaction mixture was allowed to warm to 160 °C and stirred for 25 h. After cooling to room temperature, the mixture was washed with hexane. The resulting solid was purified by recrystallization from $Et_2O/CHCl_3$ to afford the corresponding imidazolium salt **L3** (0.718 g, 2.68 mmol, 27% yield) as a brown needle crystal.

^{1}H NMR (399 MHz, $CDCl_3$, δ): 1.74 (d, J = 6.8 Hz, 6H), 5.25 (sept, J = 6.7 Hz, 1H), 7.39 (q, J = 1.7 Hz, 1H), 7.47 (dd, J = 4.8, 7.6 Hz, 1H), 8.10 (td, J = 1.6, 8.1 Hz, 1H), 8.33 (t, J = 1.8 Hz, 1H), 8.48–8.55 (m, 1H), 8.80 (d, J = 8.0 Hz, 1H), 12.02 (t, J = 1.6 Hz, 1H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 23.2 (CH_3), 54.1 (CH_2), 115.2 (*C*H), 119.0 (*C*H), 120.0 (*C*H), 125.0 (*C*H), 134.6 (*C*H), 140.5 (*C*H), 145.9 (*C*), 148.8 (*C*H). HRMS-ESI (m/z): $[M–Br]^+$ calcd for $C_{11}H_{14}N_3$, 188.1182; found 188.1184.

Preparation of 1b



The reactions were performed according to the literature procedure.[2] Cyclohexylmagnesium chloride (1.0 M in 2-MeTHF, 55.0 mL, 55.0 mmol, 2.20 equiv) was added dropwise to tetramethyl orthosilicate (3.83 g, 25.0 mmol) in toluene (55.0 mL) under nitrogen atmosphere. The reaction mixture was stirred for 17 h at 120 °C (reflux). After cooling to room temperature, the reaction was quenched with saturated NH_4Cl aqueous solution and extracted with Et_2O three times. The combined organic layer was dried over $MgSO_4$, followed by filtration and evaporation. The residue was purified by Kugelrohr distillation under reduced pressure (36 Pa, bath temp. 130 °C) to afford dicyclohecyldimethoxysilane (5.68 g, 22.2 mmol, 88% yield) as a colorless oil.

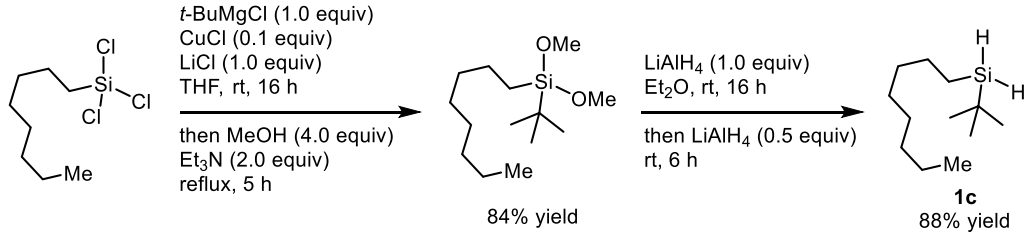
^{1}H NMR (391 MHz, $CDCl_3$, δ): 0.81–0.91 (m, 2H), 1.12–1.35 (m, 10H), 1.62–1.82 (m, 10H),

3.57 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 24.1 (*C*H), 26.9 (*C*H_2), 27.1 (*C*H_2), 27.9 (*C*H_2), 50.7 (*C*H_3). HRMS-EI (m/z): $[M]^+$ calcd for $C_{14}H_{28}O_3Si$, 256.1859; found 256.1854.

Dicyclohexyldimethoxysilane (5.18 g, 20.0 mmol) was added dropwise to a suspension of $LiAlH_4$ (0.761 g, 20.0 mmol, 1.00 equiv) in Et_2O (20.0 mL) under nitrogen atmosphere. The reaction mixture was stirred for 16 h at room temperature. Then, $LiAlH_4$ (0.286 g, 7.53 mmol, 0.375 equiv) was added to the reaction mixture in one portion. After stirring for 6 h, the reaction was quenched by water. The mixture was filtered through a celite pad. The resulting solution was dried over $MgSO_4$, followed by filtration and evaporation. The residue was purified by Kugelrohr distillation under reduced pressure (50 Pa, bath temp. 110 °C) to afford the corresponding silane **1b** (3.12 g, 15.9 mmol, 79% yield) as a colorless oil.

^{1}H NMR (401 MHz, $CDCl_3$, δ): 0.82–0.98 (m, 2H), 1.13–1.34 (m, 10H), 1.60–1.81 (m, 10H), 3.38 (t, *J* = 3.0 Hz, 2H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 20.5 (*C*H), 26.7 (*C*H_2), 27.8 (*C*H_2), 29.6 (*C*H_2). HRMS-EI (m/z): $[M]^+$ calcd for $C_{12}H_{24}Si$, 196.1647; found 196.1646.

Preparation of 1c



The reactions were performed using a modified literature procedure.[3] *tert*-Butylmagnesium chloride (2.0 M in THF, 15.0 mL, 30.0 mmol, 1.00 equiv) was added dropwise to the mixture of *n*-octyltrichlorosilane (7.27 g, 29.4 mmol), copper(I) chloride (0.302 g, 3.05 mmol, 0.104 equiv), and lithium chloride (1.27 g, 30.0 mmol, 1.02 equiv) in THF (30.0 mL) under nitrogen atmosphere. The reaction was stirred for 16 h at room temperature. Then, MeOH (5.00 mL, 120 mmol, 4.08 equiv) and Et_3N (8.50 mL, 60.0 mmol, 2.04 equiv) were added to the reaction mixture. The resulting mixture was stirred for 5 h at 85 °C (reflux). After cooling to room temperature, the reaction mixture was filtered and extracted with hexane three times. The combined organic layer was dried over $MgSO_4$, followed by filtration and evaporation. The residue was purified by Kugelrohr distillation under reduced pressure (63 Pa, bath temp. 130 °C) to afford *tert*-butyldimethoxy(octyl)silane (6.46 g, 24.8 mmol, 84% yield) as a colorless oil.

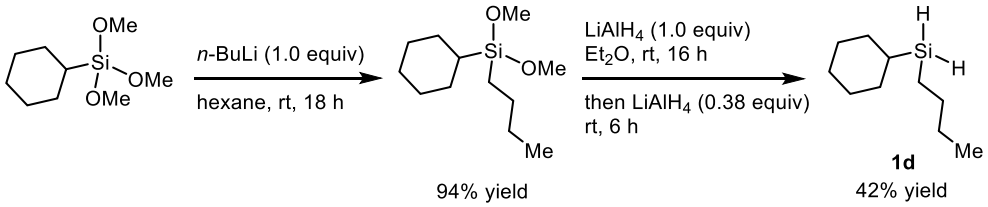
^{1}H NMR (401 MHz, $CDCl_3$, δ): 0.63–0.69 (m, 2H), 0.88 (t, *J* = 6.8 Hz, 3H), 0.94 (s, 9H), 1.22–1.37 (m, 10 H), 1.38–1.48 (m, 2H), 3.58 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 10.1

(CH_2), 14.1 (CH_3), 19.2 (C), 22.7 (CH_2), 23.2 (CH_2), 26.4 (CH_3), 29.2 (CH_2), 29.3 (CH_2), 31.9 (CH_2), 33.8 (CH_2), 51.1 (CH_3). HRMS-EI (m/z): $[M-{}^tBu]^+$ calcd for $C_{10}H_{23}O_2Si$, 203.1467; found 203.1463.

tert-Butyldimethoxy(octyl)silane (6.24 g, 24.0 mmol) was added dropwise to a suspension of $LiAlH_4$ (0.913 mg, 24.0 mmol, 1.00 equiv) in Et_2O (24.0 mL) under nitrogen atmosphere. The reaction mixture was stirred for 16 h at room temperature. Then, $LiAlH_4$ (0.452 mg, 12.0 mmol, 0.500 equiv) was added to the reaction mixture in one portion. After stirring for 6 h at 30 °C, the reaction was quenched by water. The mixture was filtered through a celite pad. The resulting solution was dried over $MgSO_4$, followed by filtration and evaporation. The residue was passed through silica-gel column chromatography (hexane as eluent). The crude product was purified by Kugelrohr distillation under a reduced pressure further purified by distillation (7.0 hPa, bath temp. 150 °C) to afford the corresponding silane **1c** (4.30 g, 21.2 mmol, 88% yield) as a colorless oil.

^1H NMR (401 MHz, $CDCl_3$, δ): 0.64–0.72 (m, 2H), 0.88 (t, J = 7.0 Hz, 3H), 0.99 (s, 9H), 1.20–1.46 (m, 12H), 3.51 (t, J = 4.4 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 7.73 (CH_2), 14.2 (CH_3), 15.8 (C), 22.8 (CH_2), 25.7 (CH_2), 28.0 (CH_3), 29.3 (CH_2), 29.4 (CH_2), 32.0 (CH_2), 33.2 (CH_2). HRMS-EI (m/z): $[M]^+$ calcd for $C_{12}H_{28}Si$, 200.1960; found 200.1954.

Preparation of 1d



n-Butyllithium (1.57 M in hexane, 16.0 mL, 25.1 mmol, 1.00 equiv) was added dropwise to a hexane solution (250 mL) of cyclohexyltrimethoxysilane (5.13 g, 25.1 mmol) under nitrogen atmosphere. The reaction was stirred for 18 h at room temperature. After the reaction was quenched by saturated NH_4Cl aqueous solution, the resulting mixture was extracted by hexane three times. The combined organic layer was dried over $MgSO_4$, followed by filtration and evaporation. The residue was purified by Kugelrohr distillation under reduced pressure (66 Pa, bath temp. 110 °C) to afford butyl(cyclohexyl)dimethoxysilane (5.44 g, 23.6 mmol, 94% yield) as a colorless oil.

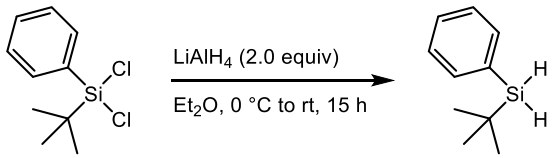
^1H NMR (401 MHz, $CDCl_3$, δ): 0.59–0.67 (m, 2H), 0.77–0.87 (m, 1H), 0.90 (t, J = 6.8 Hz, 3H), 1.13–1.28 (m, 5H), 1.31–1.43 (m, 4H), 1.64–1.81 (m, 5H), 3.54 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 10.2 (CH_2), 13.6 (CH), 24.4 (CH_3), 25.0 (CH_2), 26.5 (CH_2), 26.7 (CH_2), 26.8

(CH_2), 27.8 (CH_2), 50.4 (CH_3). HRMS-EI (m/z): $[M]^+$ calcd for $C_{12}H_{26}O_2Si$, 230.1702; found 230.1691.

Butyl(cyclohexyl)dimethoxysilane (4.60 g, 20.0 mmol) was added dropwise to a suspension of $LiAlH_4$ (0.762 g, 20.1 mmol, 1.00 equiv) in Et_2O (40.0 mL) under nitrogen atmosphere. The reaction mixture was stirred for 16 h at room temperature. After diluting with Et_2O, the reaction was quenched by MeOH. The resulting mixture was filtered through a celite pad, followed by evaporation. The residue was purified by Kugelrohr distillation under reduced pressure (60 Pa, bath temp. 100 °C) to afford the crude product. The crude product was passed through silica-gel column chromatography (hexane as eluent) to afford the corresponding silane **1d** (1.43 g, 8.39 mmol, 42% yield) as a colorless oil.

^1H NMR (401 MHz, $CDCl_3$, δ): 0.59–0.76 (m, 2H), 0.78–0.97 (m, 4H), 1.10–1.30 (m, 5H), 1.31–1.45 (m, 4H), 1.61–1.83 (m, 5H), 3.51 (quint, J = 3.1 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 7.5 (CH_2), 13.8 (CH), 21.3 (CH_3), 26.0 (CH_2), 26.8 (CH_2), 27.8 (CH_2), 27.9 (CH_2), 29.3 (CH_2). HRMS-EI (m/z): $[M]^+$ calcd for $C_{10}H_{22}Si$, 170.1491; found 170.1497.

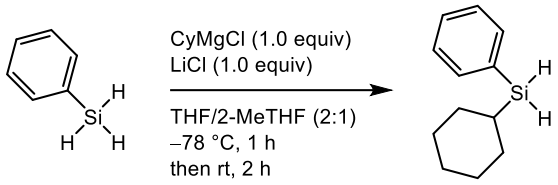
Preparation of 1e



1e
84% yield

The reaction was performed according to the literature procedure.[4] *tert*-Butyldichloro(phenyl)silane (1.02 g, 4.38 mmol) was added dropwise to a suspension of $LiAlH_4$ (0.334 g, 8.80 mmol, 2.0 equiv) in Et_2O (40.0 mL) under nitrogen atmosphere. The reaction mixture was stirred for 15 h at room temperature. After diluting with Et_2O, the reaction mixture was quenched by MeOH. After the resulting mixture was filtered through a celite pad, the filtrate was extracted by Et_2O three times. The combined organic layer was dried over $MgSO_4$, followed by filtration and evaporation. The residue was purified by silica-gel column chromatography (hexane as eluent) to afford the corresponding silane **1e** (0.607 g, 3.69 mmol, 84% yield) as a colorless oil. The NMR spectra of **1e** were in agreement with the literature.[4]

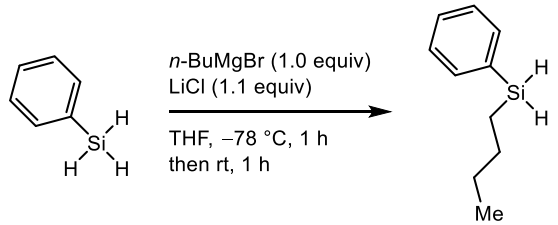
Preparation of 1f



1f
82% yield

The reaction was performed according to the literature procedure.[5] Cyclohexylmagnesium chloride (1.0 M in 2-MeTHF, 10 mL, 1.0 equiv) was added dropwise to a solution of phenylsilane (1.09 g, 10.1 mmol) and lithium chloride (0.430 g, 10.2 mmol, 1.0 equiv) in THF (20.0 mL) at –78 °C under nitrogen atmosphere, and stirred for 1 h. Then, the reaction mixture was allowed to warm to room temperature slowly and stirred for 2 h. The reaction mixture was quenched by a saturated aqueous NH_4Cl. The resulting mixture was extracted by Et_2O three times. The combined organic layer was dried over $MgSO_4$, followed by filtration and evaporation. The residue was purified by silica-gel column chromatography (hexane as eluent) to afford the corresponding silane **1f** (1.58 g, 8.31 mmol, 82%) as a colorless oil. The NMR spectra of **1f** were in agreement with the literature.[6]

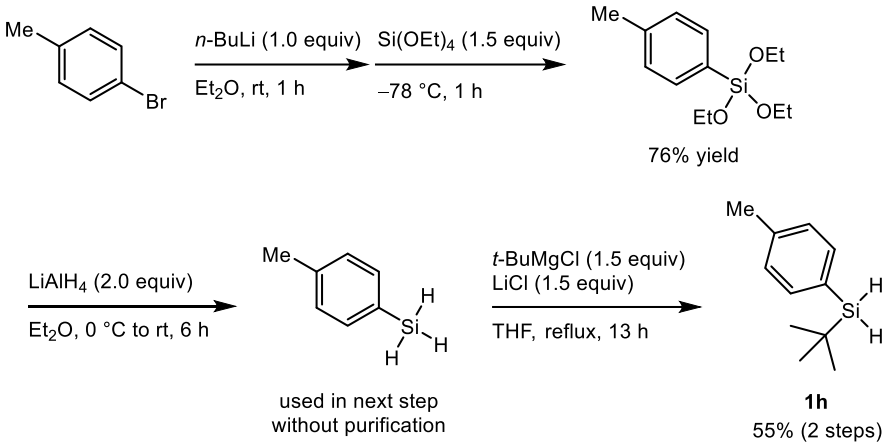
Preparation of 1g



1g
74% yield

The reaction was performed according to the literature procedure.[5] *n*-Butylmagnesium bromide (1.0 M in THF, 10.0 mL, 1.0 equiv) was added dropwise to a solution of phenylsilane (1.07 g, 9.92 mmol) and lithium chloride (0.443 g, 10.5 mmol, 1.1 equiv) in THF (20.0 mL) at –78 °C under nitrogen atmosphere, and stirred for 1 h. Then, the reaction mixture was allowed to warm to room temperature slowly and stirred for 1 h. The reaction mixture was quenched by a saturated aqueous NH_4Cl. The resulting mixture was extracted by Et_2O three times. The combined organic layer was dried over $MgSO_4$, followed by filtration and evaporation. The residue was purified by silica-gel column chromatography (hexane as eluent) to afford the corresponding silane **1g** (1.21 g, 7.37 mmol, 74%) as a colorless oil. The NMR spectra of **1g** were in agreement with the literature.[7]

Preparation of 1h



The reaction was performed according to the literature procedure.[8] *n*-Butyllithium (1.57 M, 6.4 mL, 1.0 equiv) was added dropwise to a solution of 4-bromotoluene (1.73 g, 10.1 mmol) in Et_2O (14.0 mL) at room temperature and stirred for 1 h. After cooling to –78 °C, the reaction mixture was added via cannula to the solution of tetraethyl orthosilicate (3.4 mL, 15.0 mmol, 1.5 equiv) in Et_2O (14.0 mL) at –78 °C. The reaction mixture was stirred for 1 h. After warming to room temperature, the reaction mixture was quenched by a saturated aqueous NH_4Cl. The resulting mixture was extracted by Et_2O three times. The combined organic layer was dried over $MgSO_4$, followed by filtration and evaporation. The residue was purified by Kugelrohr distillation under reduced pressure (50 Pa, bath temp. 125 °C) to afford triethoxy(*p*-tolyl)silane (1.93 g, 7.58 mmol, 76% yield) as a colorless oil.

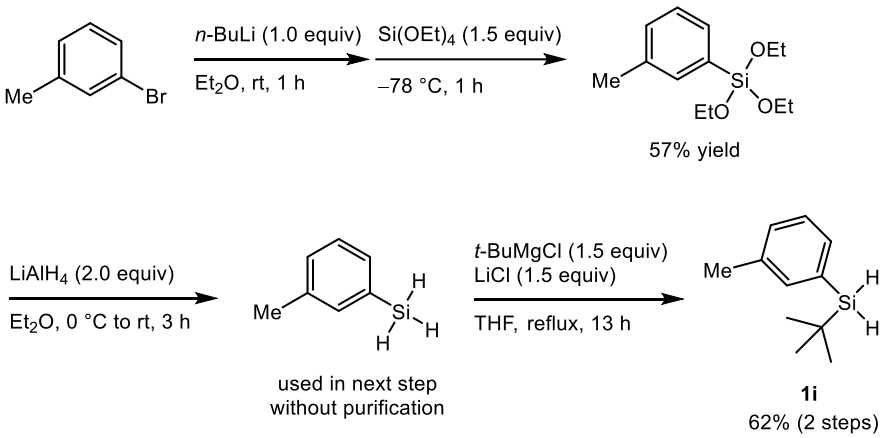
The hydride reduction of triethoxy(*p*-tolyl)silane, followed by reaction with *t*-BuMgCl, were performed according to the literature procedure.[5,9] Triethoxy(*p*-tolyl)silane (1.29 g, 5.07 mmol) was added dropwise to a suspension of $LiAlH_4$ (0.377 g, 9.9 mmol, 2.0 equiv) in Et_2O (10.0 mL) under nitrogen atmosphere. The reaction mixture was stirred for 6 h at room temperature. After diluting with pentane (100 mL), the reaction mixture was filtered through a celite pad, followed by evaporation (150 hPa 0 °C). *Be careful with fires caused by the precipitated hydride species.* The residue was passed through a silica-gel column (Et_2O as an eluent), followed by evaporation (150 hPa, 0 °C). The crude mixture was employed for the next reaction without further purification.

The crude mixture of *p*-tolylsilane was added to the solution of lithium chloride (0.319 g, 7.5 mmol, 1.5 equiv) in THF (10.0 mL). After *tert*-butylmagnesium chloride (2.0 M, 3.8 mL, 7.6 mmol, 1.5 equiv) was added, the reaction mixture was warmed to 80 °C (reflux) and stirred for 13 h. After cooling to room temperature, the reaction mixture was quenched by a saturated aqueous NH_4Cl. The resulting mixture was extracted by Et_2O three times. The combined organic layer was dried over $MgSO_4$, followed by filtration and evaporation. The residue was

purified by silica-gel column chromatography (hexane as eluent) to afford **1h** [0.495 g, 2.78 mmol, 55% (over two steps)] as a colorless oil.

^{1}H NMR (401 MHz, $CDCl_3$, δ): 1.00 (s, 9H), 2.36 (s, 3H), 4.12 (s, 2H), 7.18 (d, J = 6.8 Hz, 2H), 7.46 (d, J = 6.4 Hz, 2H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 16.4 (*C*), 21.5 (*C*H$_3$), 27.4 (*C*H$_3$), 128.5 (*C*), 128.7 (*C*H), 135.9 (*C*H), 139.5 (*C*). HRMS-EI (m/z): $[M]^+$ calcd for $C_{11}H_{18}Si$, 178.1178; found 178.1185.

Preparation of 1i



The reaction was performed according to the literature procedure.[8] *n*-Butyllithium (1.57 M, 6.4 mL, 1.0 equiv) was added dropwise to a solution of 3-bromotoluene (1.72 g, 10.1 mmol) in Et_2O (14.0 mL) at room temperature and stirred for 1 h. After cooling to –78 °C, the reaction mixture was added via cannula to the solution of tetraethyl orthosilicate (3.4 mL, 15.0 mmol, 1.5 equiv) in Et_2O (14.0 mL) at –78 °C. The reaction mixture was stirred for 1 h. After warming to room temperature, the reaction mixture was quenched by a saturated aqueous NH_4Cl. The resulting mixture was extracted by Et_2O three times. The combined organic layer was dried over $MgSO_4$, followed by filtration and evaporation. The residue was purified by Kugelrohr distillation under reduced pressure (31 Pa, bath temp. 160 °C) to afford triethoxy(*m*-tolyl)silane (1.46 g, 5.73 mmol, 57% yield) as a colorless oil.

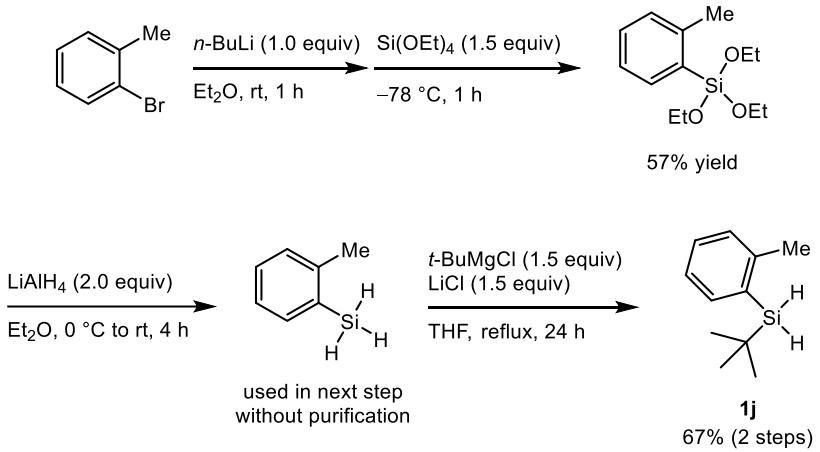
The hydride reduction of triethoxy(*m*-tolyl)silane, followed by reaction with *t*-BuMgCl, were performed according to the literature procedure.[5,9] Triethoxy(*m*-tolyl)silane (1.26 g, 4.97 mmol) was added dropwise to a suspension of $LiAlH_4$ (0.381 g, 10.0 mmol, 2.0 equiv) in Et_2O (10.0 mL) under nitrogen atmosphere. The reaction mixture was stirred for 3 h at room temperature. After diluting with pentane (100 mL), the reaction mixture was filtered through a celite pad, followed by evaporation (150 hPa, 0 °C). *Be careful with fires caused by the precipitated hydride species.* The residue was passed through a silica-gel column (Et_2O as an eluent), followed by evaporation (150 hPa, 0 °C). The crude mixture was employed for the next reaction

without further purification.

The crude mixture of *m*-tolylsilane was added to the solution of lithium chloride (0.335 g, 7.9 mmol, 1.6 equiv) in THF (10.0 mL). After *tert*-butylmagnesium chloride (2.0 M, 3.8 mL, 7.6 mmol, 1.5 equiv) was added, the reaction mixture was warmed to 80 °C (reflux) and stirred for 15 h. After cooling to room temperature, the reaction mixture was quenched by a saturated aqueous NH_4Cl. The resulting mixture was extracted by Et_2O three times. The combined organic layer was dried over $MgSO_4$, followed by filtration and evaporation. The residue was purified by silica-gel column chromatography (hexane as eluent) to afford **1i** [0.546 g, 3.06 mmol, 62% (over two steps)] as a colorless oil.

^1H NMR (399 MHz, $CDCl_3$, δ): 1.02 (s, 9H), 2.36 (s, 3H), 4.13 (s, 2H), 7.20–7.28 (m, 2H), 7.35 –7.40 (m, 2H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 16.4 (*C*), 21.5 (*C*H_3), 27.5 (*C*H_3), 127.7 (*C*H), 130.3 (*C*H), 132.0 (*C*), 132.9 (*C*H), 136.6 (*C*H), 137.1 (*C*). HRMS-EI (m/z): $[M]^+$ calcd for $C_{11}H_{18}Si$, 178.1178; found 178.1178.

Preparation of 1j



The reaction was performed according to the literature procedure.[8] *n*-Butyllithium (1.57 M, 6.4 mL, 1.0 equiv) was added dropwise to a solution of 2-bromotoluene (1.73 g, 10.1 mmol) in Et_2O (14.0 mL) at room temperature and stirred for 1 h. After cool to –78 °C, the reaction mixture was added via cannula to the solution of tetraethyl orthosilicate (3.4 mL, 15.0 mmol, 1.5 equiv) in Et_2O (14.0 mL) at –78 °C. The reaction mixture was stirred for 1 h. After warm to room temperature, the reaction mixture was quenched by a saturated aqueous NH_4Cl. The resulting mixture was extracted by Et_2O three times. The combined organic layer was dried over $MgSO_4$, followed by filtration and evaporation. The residue was purified by Kugelrohr distillation under reduced pressure (35 Pa, bath temp. 110 °C) to afford triethoxy(*o*-tolyl)silane (1.46 g, 5.74 mmol, 57% yield) as a colorless oil.

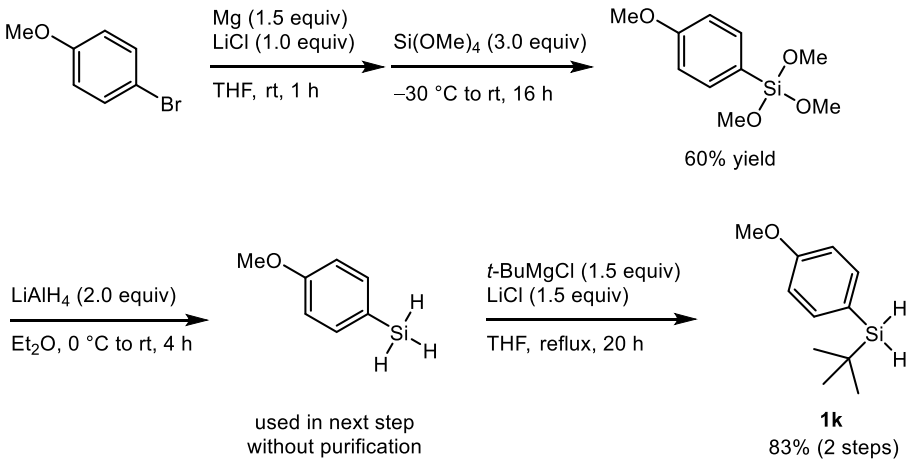
The hydride reduction of triethoxy(*o*-tolyl)silane, followed by reaction with *t*-BuMgCl, were

performed according to the literature procedure.[5,9] Triethoxy(*o*-tolyl)silane (1.27 g, 5.00 mmol) was added dropwise to a suspension of $LiAlH_4$ (0.382 g, 10.1 mmol, 2.0 equiv) in Et_2O (10.0 mL) under nitrogen atmosphere. The reaction mixture was stirred for 4 h at room temperature. After dilut with pentane (100 mL), the reaction mixture was filtered through a celite pad, followed by evaporation (150 hPa, 0 ℃). *Be careful with fires caused by the precipitated hydride species.* The residue was passed through a silica-gel column (Et_2O as an eluent), followed by evaporation (150 hPa, 0 ℃). The crude mixture was employed for the next reaction without further purification.

The crude mixture of *o*-tolylsilane was added to the solution of lithium chloride (0.317 g, 7.5 mmol, 1.5 equiv) in THF (10.0 mL). After *tert*-butylmagnesium chloride (2.0 M, 3.8 mL, 7.6 mmol, 1.5 equiv) was added, the reaction mixture was warmed to 80 ℃ (reflux) and stirred for 24 h. After cool to room temperature, the reaction mixture was quenched by a saturated aqueous NH_4Cl. The resulting mixture was extracted by Et_2O three times. The combined organic layer was dried over $MgSO_4$, followed by filtration and evaporation. The residue was purified by silica-gel column chromatography (hexane as eluent) to afford **1j** [0.594 g, 3.33 mmol, 67% (over two steps)] as a colorless oil.

^{1}H NMR (401 MHz, $CDCl_3$, δ): 1.03 (s, 9H), 2.47 (s, 3H), 4.22 (s, 2H), 7.14–7.21 (m, 2H), 7.30 (td, J = 1.6, 7.5 Hz, 1H), 7.51 (dd = 1.4, 7.4 z, 1H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 17.2 (*C*), 23.4 (*C*H_3), 27.9 (*C*H_3), 124.8 (*C*H), 129.6 (*C*H), 130.0 (*C*H), 131.5 (*C*), 137.5 (*C*H), 144.1 (*C*). HRMS-EI (m/z): $[M]^+$ calcd for $C_{11}H_{18}Si$, 178.1178; found 178.1174.

Preparation of 1k



The reaction was performed according to the literature procedure.[9] 4-bromoanisole (3.65 g, 19.5 mmol) was added to a mixture of Mg (0.732 g, 30.1 mmol, 1.5 equiv), LiCl (0.850 g, 20.1 mmol, 1.0 equiv), and THF (20.0 mL) at room temperature. After stirr for 1 h, the solution of the Grignard reagent was added dropwise via cannula to the solution of tetramethyl orthosilicate

(8.9 mL, 60 mmol, 3.0 equiv) in THF (20.0 mL) at –30 °C. Then, the reaction mixture was allowed to warm to room temperature and stirred for 16 h. The reaction mixture was quenched by a saturated aqueous NH_4Cl. The resulting mixture was extracted by Et_2O three times. The combined organic layer was dried over $MgSO_4$, followed by filtration and evaporation. The residue was purified by Kugelrohr distillation under reduced pressure (34 Pa, bath temp. 120 °C) to afford trimethoxy(4-methoxyphenyl)silane (2.67 g, 11.7 mmol, 60% yield) as a colorless oil.

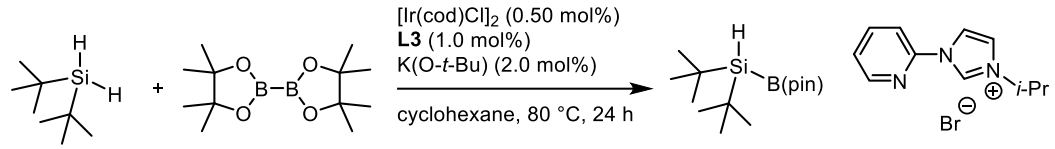
The hydride reduction of triethoxy(*o*-tolyl)silane, followed by reaction with *t*-BuMgCl, were performed according to the literature procedure.[5,9] Trimethoxy(4-methoxyphenyl)silane (1.14 g, 4.99 mmol) was added dropwise to a suspension of $LiAlH_4$ (0.381 g, 10.0 mmol, 2.0 equiv) in Et_2O (10.0 mL) under nitrogen atmosphere. The reaction mixture was stirred for 4 h at room temperature. After diluting with pentane (100 mL), the reaction mixture was filtered through a celite pad, followed by evaporation (150 hPa, 0 °C). *Be careful with fires caused by the precipitated hydride species.* The residue was passed through a silica-gel column (Et_2O as an eluent), followed by evaporation (150 hPa, 0 °C). The crude mixture was employed for the next reaction without further purification.

The crude mixture of (4-methoxyphenyl)silane was added to the solution of lithium chloride (0.323 g, 7.6 mmol, 1.5 equiv) in THF (10.0 mL). After *tert*-butylmagnesium chloride (2.0 M, 3.8 mL, 7.6 mmol, 1.5 equiv) was added, the reaction mixture was warmed to 80 °C (reflux) and stirred for 20 h. After cooling to room temperature, the reaction mixture was quenched by a saturated aqueous NH_4Cl. The resulting mixture was extracted by Et_2O three times. The combined organic layer was dried over $MgSO_4$, followed by filtration and evaporation. The residue was purified by silica-gel column chromatography (hexane as eluent) to afford **1k** [0.804 g, 4.14 mmol, 83% (over two steps)] as a colorless oil.

^{1}H NMR (401 MHz, $CDCl_3$, δ): 1.00 (s, 9H), 3.83 (s, 3H), 4.12 (s, 2H), 6.92 (dt, J = 2.1, 8.6 Hz, 2H), 7.50 (dt, J = 2.2, 8.8 Hz, 2H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 16.4 (*C*), 27.4 (*C*H_3), 54.9 (*C*H_3), 113.6 (*C*H), 122.9 (*C*), 137.3 (*C*H), 160.8 (*C*). HRMS-EI (m/z): $[M]^+$ calcd for $C_{11}H_{18}OSi$, 194.1127; found 194.1127.

3. General Procedures for Si–H Borylation

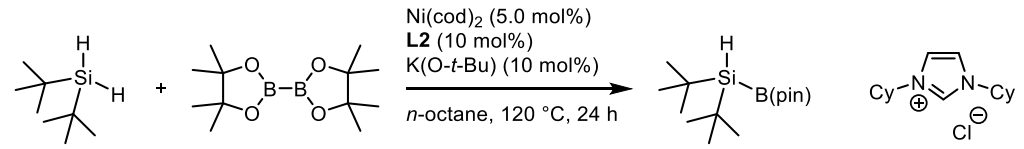
General Procedure for Iridium-Catalyzed Si–H Borylation of Dialkylsilanes: Procedure A



1a (1.0 mmol) **2** (2.0 equiv) **3a** 63% yield **L3**

Bis(pinacolato)diboron **2** (507.1 mg, 2.00 mmol, 2.0 equiv) and **L3** (2.8 mg, 0.010 mmol, 1.0 mol%) were placed in a vial with a screw cap containing a Teflon®-coated rubber septum under air. The vial was placed in a glove box under an argon atmosphere, and then $[Ir(cod)Cl]_2$ (3.4 mg, 0.0051 mmol, 0.51 mol%) and K(O-*t*-Bu) (2.3 mg, 0.020 mmol, 2.0 mol%) were added to the vial. After the reaction vial was sealed with the screw cap, it was removed from the glove box. Then, cyclohexane (2.0 mL) was added to the vial via a syringe. The resulting mixture was allowed to warm at 80 °C and stirred for 1 h. Then, di-*tert*-butylsilane **1a** (144.5 mg, 1.00 mmol, 1.00 equiv) was added dropwise via a syringe. After the reaction mixture was stirred at 80 °C for 24 h, the reaction mixture was analyzed by GC to determine the product's GC yield (71%). The mixture was directly filtered through a silica-gel pad with pentane/Et_2O (9:1) as an eluent, and then the resulting solution was concentrated under reduced pressure. The crude product was purified by silica-gel column chromatography with hexane/Et_2O (100:0 to 98:2) as an eluent to afford the corresponding product **3a** (171.1 mg, 0.633 mmol, 63% yield) as a colorless oil.

General Procedure for Nickel-Catalyzed Si–H Borylation: Procedure B

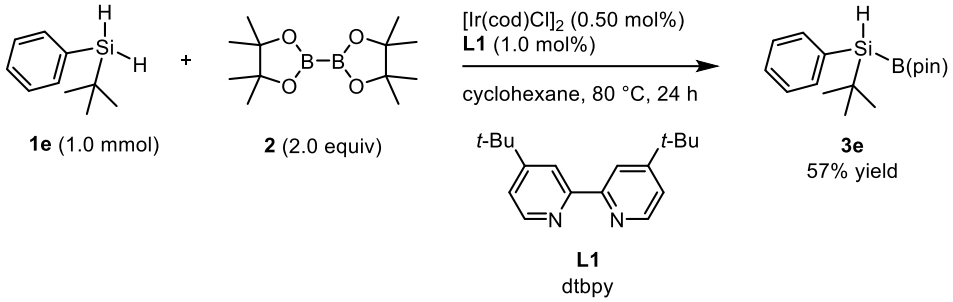


1a (0.5 mmol) **2** (2.0 equiv) **3a** 49% yield **L2** ICy•HCl

Bis(pinacolato)diboron **2** (254.5 mg, 1.00 mmol, 2.0 equiv) was placed in a vial with a screw cap containing a Teflon®-coated rubber septum under air. The vial was placed in a glove box under an argon atmosphere, and then $Ni(cod)_2$ (6.8 mg, 0.025 mmol, 5.0 mol%), **L2** (13.5 mg, 0.0502 mmol, 10.0 mol%), and K(O-*t*-Bu) (5.7 mg, 0.51 mmol, 10 mol%) were added to the vial. After the vial was sealed with the screw cap, it was removed from the glove box. Then, *n*-octane (1.0 mL) was added to the vial via a syringe. The resulting mixture was allowed to warm at 120 °C and stirred for 1 h. Then, di-*tert*-butylsilane **1a** (72.1 mg, 0.500 mmol, 1.00 equiv) was added dropwise via a syringe. After the reaction mixture was stirred at 120 °C for 24 h, the

reaction mixture was analyzed by GC to determine the product's GC yield (59%). The mixture was directly filtered through a silica-gel pad with pentane/Et_2O (9:1) as an eluent, and then the resulting solution was concentrated under reduced pressure. The crude product was purified by silica-gel column chromatography with hexane/Et_2O (100:0 to 98:2) as an eluent to afford the corresponding product **3a** (66.8 mg, 0.247 mmol, 49% yield) as a colorless oil.

General Procedure for Iridium-Catalyzed Si–H Borylation of Alkylarylsilanes: Procedure C

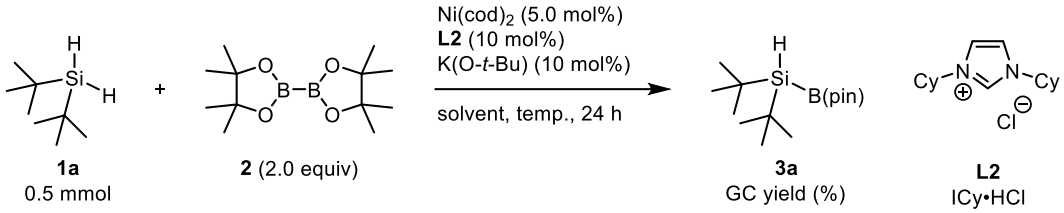


Bis(pinacolato)diboron **2** (255.7 mg, 1.01 mmol, 2.0 equiv) and **L1** (1.4 mg, 0.0052 mmol, 1.0 mol%) were placed in a vial with a screw cap containing a Teflon®-coated rubber septum under air. The vial was placed in a glove box under an argon atmosphere, and then $[Ir(cod)Cl]_2$ (1.8 mg, 0.0027 mmol, 0.5 mol%) was added to the vial. After the reaction vial was sealed with the screw cap, it was removed from the glove box. Then, cyclohexane (1.0 mL) was added to the vial via a syringe. The resulting mixture was allowed to warm at 80 ℃ and stirred for 1 h. Then, *tert*-butylphenylsilane **1e** (82.0 mg, 0.499 mmol, 1.00 equiv) was added dropwise via a syringe. After the reaction mixture was stirred at 80 ℃ for 24 h, the mixture was directly filtered through a silica-gel pad with pentane/Et_2O (9:1) as an eluent. The resulting solution was concentrated under reduced pressure. The crude product was purified by silica-gel column chromatography with hexane/Et_2O (100:0 to 97:3) as an eluent to afford the corresponding product **3e** (81.9 mg, 0.282 mmol, 57% yield) as a colorless oil.

4. Details of Optimization Study

The nickel-catalyzed borylation reaction in cyclohexane at 80 °C afforded **3a** in 50% yield (average of four runs, Table S1). However, the reproducibility of the reaction was unsatisfactory under these conditions. After an extensive screening of the reaction conditions, we found that when the reaction was carried out in *n*-octane at 120 °C, **3a** was obtained in 54% yield (average of four runs, Table S1) with better reproducibility.

Table S1. Optimization on Reaction of 1a



1a
0.5 mmol

2 (2.0 equiv)

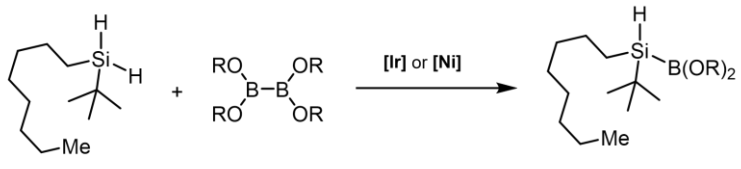
3a
GC yield (%)

L2
ICy•HCl

conditions: cyclohexane, 80 °C	conditions: *n*-octane, 120 °C
1st run 55%	1st run 51%
2nd run 48%	2nd run 54%
3rd run 43%	3rd run 59%
4th run 55%	4th run 54%

The borylations using more bulky diborons (**B1** and **B2**) were carried out to improve the yield (Table S2). Although the iridium-based catalyst produced the borylated product, the nickel-based catalyst did not work well. Unfortunately, the yield was not satisfactory when other boron sources were used.

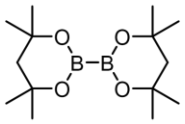
Table S2. Investigation of other boron sources



1c (2.0 equiv) NMR yield (%)

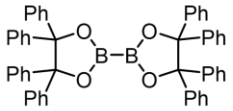
[Ir] : [Ir(cod)Cl]$_2$ (2.5 mol%), **L3** (5.0 mol%), K(O-*t*-Bu) (10 mol%), cyclohexane, 80°C, 24 h

[Ni] : Ni(cod)$_2$ (5.0 mol%), **L2** (10 mol%), K(O-*t*-Bu) (10 mol%), ^{n}octane, 120°C, 24 h



B1

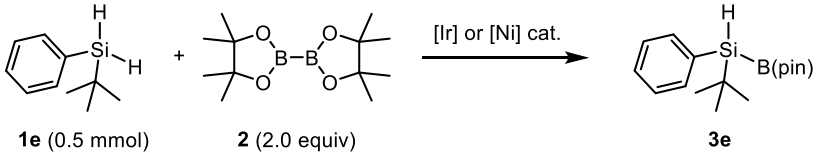
entry	$B_2(OR)_4$	conditions	NMR yield (%)
1	**B1**	**[Ir]**	8
2	**B1**	**[Ni]**	trace
3	**B2**	**[Ir]**	11
4	**B2**	**[Ni]**	no reaction



B2

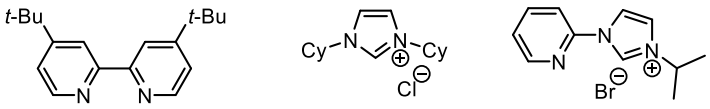
The monoborylation of **1e** was carried out under the developed conditions (Table S3). Although the Ir/**L3** catalytic system produced the desired product in low yield (11%, entry 1), the Ir/dtbpy (**L1**) catalytic system resulted in a good yield (57%, entry 2). The nickel-based catalyst also produced the borylated product (31%, entry 3).

Table S3. Investigation of the borylation of 1e



1e (0.5 mmol) **2** (2.0 equiv) **3e**

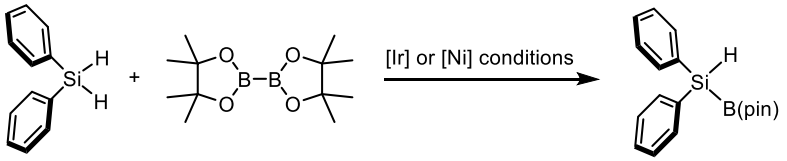
entry	conditions	isolated yield (%)
1	$[Ir(cod)Cl]_2$ (0.5 mol%) **L3** (1 mol%) K(O-*t*-Bu) (2 mol%) cyclohexane, 80 °C, 24 h	11
2	$[Ir(cod)Cl]_2$ (0.5 mol%) **L1** (1 mol%) cyclohexane, 80 °C, 24 h	57
3	$Ni(cod)_2$ (5 mol%) **L2** (1 mol%) K(O-*t*-Bu) (10 mol%) *n*-octane, 120 °C, 24 h	31



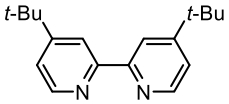
L1 dtbpy **L2** ICy•HCl **L3**

The borylation of diarylsilanes did not produce the desired silylboronates (Table S4). In the case of the iridium-based catalyst, dehydrogenative homo-coupling afforded oligosilanes. On the other hand, the reactions using the nickel-based catalyst resulted in the production of complex mixtures.

Table S4. Investigation of the borylation of diarylsilanes

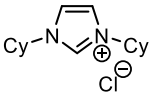


[Ir] conditions:
$[Ir(cod)Cl]_2$ (2.5 mol%)
L1 (5.0 mol%)
cyclohexane, 80°C, 24 h

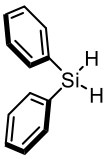
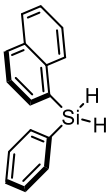
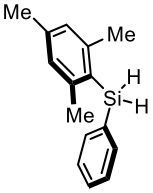


L1
dtbpy

[Ni] conditions:
$Ni(cod)_2$ (5.0 mol%)
L2 (10 mol%)
K(O-*t*-Bu) (10 mol%)
n-octane, 120°C, 24 h

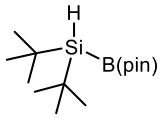


L2
ICy•HCl

entry	dihydrosilane	conditions	result
1		[Ir]	oligosilanes
		[Ni]	complex mixture
2		[Ir]	oligosilanes
		[Ni]	complex mixture
3		[Ir]	oligosilanes
		[Ni]	complex mixture

5. Characterization of Borylation Products 3a–3c, 3e, and 3h–3k

Di-*tert*-butyl(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)silane (3a).



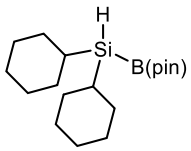
3a

Procedure **A**: The reaction was performed with **1a** (144.5 mg, 1.00 mmol). The crude product was purified by silica-gel column chromatography with hexane/Et_2O (100:0 to 97:3) as an eluent to afford the corresponding silylboronate **3a** in 63% isolated yield (171.1 mg, 0.633 mmol) as a colorless oil.

Procedure **B**: The reaction was performed with **1a** (72.1 mg, 0.500 mmol). The crude product was purified by silica-gel column chromatography with hexane/Et_2O (100:0 to 97:3) as an eluent to afford the corresponding silylboronate **3a** in 49% isolated yield (66.8 mg, 0.247 mmol) as a colorless oil.

^{1}H NMR (401 MHz, $CDCl_3$, δ): 1.06 (s, 18H), 1.25 (s, 12H), 3.25 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 18.4 (*C*), 24.9 (*C*H_3), 29.5 (*C*H_3), 83.1 (*C*). ^{11}B{^{1}H} NMR (126 MHz, $CDCl_3$, δ): 34.5. ^{29}Si{^{1}H} NMR (119 MHz, $CDCl_3$, δ): –8.45 (brs). The broad signal of ^{29}Si was caused by the quadrupolar boron atom. HRMS-EI (m/z): $[M–Me]^+$ calcd for $C_{13}H_{28}{}^{11}BO_2Si$, 255.1951; found 255.1954.

Dicyclohexyl(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)silane (3b).



3b

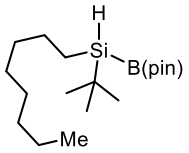
Procedure **A**: The reaction was performed with **1b** (192.4 mg, 0.980 mmol). The crude product was purified by silica-gel column chromatography with hexane/Et_2O (100:0 to 97:3) as an eluent to afford the corresponding silylboronate **3b** in 24% GC yield.

Procedure **B**: The reaction was performed with **1b** (99.7 mg, 0.508 mmol). The crude product was purified by silica-gel column chromatography with hexane/Et_2O (100:0 to 97:3) as an eluent to afford the corresponding silylboronate **3b** in 29% isolated yield (48.0 mg, 0.149 mmol) as a colorless oil.

^{1}H NMR (401 MHz, $CDCl_3$, δ): 0.87–1.04 (m, 2H), 1.13–1.34 (m, 22H), 1.62–1.84 (m, 10H), 3.21 (brs, 1H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 20.9 (*C*H), 25.0 (*C*H_3), 26.8 (*C*H_2), 28.0 (*C*H_2), 29.8 (*C*H_2), 30.1 (*C*H_2), 83.2 (*C*). ^{11}B{^{1}H} NMR (127 MHz, $CDCl_3$, δ): 34.6. The signal derived

from the silicon directly attached to the boron atom was not detected by $^{29}Si\{^{1}H\}$ NMR, which is likely due to quadrupolar relaxation. HRMS-EI (m/z): $[M–Me]^+$ calcd for $C_{17}H_{32}{}^{11}BO_2Si$, 307.2273; found 307.2268.

***tert*-Butyl(octyl)(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)silane (3c).**



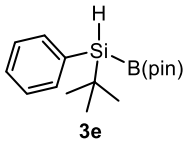
3c

Procedure **A**: The reaction was performed with **1c** (200.7 mg, 1.00 mmol). The crude product was purified by silica-gel column chromatography with hexane/Et_2O (100:0 to 97:3) as an eluent to afford the corresponding silylboronate **3c** in 11% isolated yield (36.3 mg, 0.111 mmol) as a colorless oil.

Procedure **B**: The reaction was performed with **1c** (100.2 mg, 0.500 mmol). The crude product was purified by silica-gel column chromatography with hexane/Et_2O (100:0 to 97:3) as an eluent to afford the corresponding silylboronate **3c** in 43% isolated yield (69.9 mg, 0.214 mmol) as a colorless oil.

^{1}H NMR (396 MHz, $CDCl_3$, δ): 0.65–0.75 (m, 2H), 0.86 (t, J = 7.2 Hz, 3H), 0.99 (s, 9H), 1.20–1.45 (m, 24H), 3.35 (t, J = 4.4 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 8.04 (CH_2), 14.1 (CH_3), 16.4 (C), 22.7 (CH_2), 25.0 (CH_3), 26.1 (CH_2), 28.5 (CH_3), 29.2 (CH_2), 29.3 (CH_2), 31.9 (CH_2), 33.3 (CH_2), 83.2 (C). $^{11}B\{^{1}H\}$ NMR (126 MHz, $CDCl_3$, δ): 34.7. $^{29}Si\{^{1}H\}$ NMR (119 MHz, $CDCl_3$, δ): –22.0 (brs). The broad signal of ^{29}Si was caused by the quadrupolar boron atom. HRMS-EI (m/z): $[M–Me]^+$ calcd for $C_{17}H_{36}{}^{11}BO_2Si$, 311.2582; found 311.2581.

***tert*-Butyl(phenyl)(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)silane (3e).**



3e

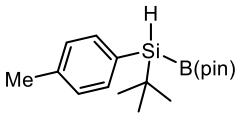
Procedure **C**: The reaction was performed with **1e** (82.0 mg, 0.499 mmol). The crude product was purified by silica-gel column chromatography with hexane/Et_2O (100:0 to 97:3) as an eluent to afford the corresponding silylboronate **3e** in 57% isolated yield (81.9 mg, 0.282 mmol) as a colorless oil.

Procedure **B**: The reaction was performed with **1e** (82.0 mg, 0.499 mmol). The crude product was purified by silica-gel column chromatography with hexane/Et_2O (100:0 to 97:3) as an

eluent to afford the corresponding silylboronate **3e** in 31% isolated yield (45.1 mg, 0.155 mmol) as a colorless oil.

^{1}H NMR (401 MHz, $CDCl_3$, δ): 1.00 (s, 9H), 1.28 (s, 12H), 3.98 (s, 1H), 7.29–7.39 (m, 3H), 7.60–7.69 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 17.1 (*C*), 25.0 (*C*H_3), 28.0 (*C*H_3), 83.6 (*C*), 127.5 (*C*H), 128.8 (*C*H), 133.8 (*C*), 136.4 (*C*H). ^{11}B{^{1}H} NMR (126 MHz, $CDCl_3$, δ): 34.0. The signal derived from the silicon directly attached to the boron atom was not detected by ^{29}Si{^{1}H} NMR, which is likely due to quadrupolar relaxation. HRMS-EI (m/z): $[M–Me]^+$ calcd for $C_{15}H_{24}{}^{11}BO_2Si$, 275.1639; found 275.1632.

***tert*-Butyl(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)(*p*-tolyl)silane (3h).**



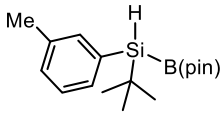
3h

Procedure **C**: The reaction was performed with **1h** (89.7 mg, 0.503 mmol). The crude product was purified by silica-gel column chromatography with hexane/Et_2O (100:0 to 97:3) as an eluent to afford the corresponding silylboronate **3h** in 61% isolated yield (92.9 mg, 0.305 mmol) as a white solid.

Procedure **B**: The reaction was performed with **1h** (90.3 mg, 0.506 mmol). The crude product was purified by silica-gel column chromatography with hexane/Et_2O (100:0 to 97:3) as an eluent to afford the corresponding silylboronate **3h** in 29% isolated yield (45.1 mg, 0.148 mmol) as a white solid.

^{1}H NMR (401 MHz, $CDCl_3$, δ): 0.99 (s, 9H), 1.28 (s, 12H), 2.35 (s, 3H), 3.96 (s, 1H), 7.16 (d, J = 7.2 Hz, 2H), 7.53 (d, J = 7.2 Hz, 2H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 17.1 (*C*), 21.5 (*C*H_3), 25.0 (*C*H_3), 28.0 (*C*H_3), 83.6 (*C*), 128.4 (*C*H), 130.1 (*C*), 136.4 (*C*H), 138.7 (*C*). ^{11}B{^{1}H} NMR (126 MHz, $CDCl_3$, δ): 34.1. The signal derived from the silicon directly attached to the boron atom was not detected by ^{29}Si{^{1}H} NMR, which is likely due to quadrupolar relaxation. HRMS-EI (m/z): $[M–Me]^+$ calcd for $C_{16}H_{26}{}^{11}BO_2Si$, 289.1795; found 289.1786. mp 50–58 °C.

***tert*-Butyl(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)(*m*-tolyl)silane (3i).**



3i

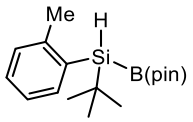
Procedure **C**: The reaction was performed with **1i** (89.7 mg, 0.503 mmol). The crude product was purified by silica-gel column chromatography with hexane/Et_2O (100:0 to 97:3) as an

eluent to afford the corresponding silylboronate **3i** in 58% isolated yield (88.5 mg, 0.291 mmol) as a white solid.

Procedure **B**: The reaction was performed with **1i** (89.2 mg, 0.500 mmol). The crude product was purified by silica-gel column chromatography with hexane/Et_2O (100:0 to 97:3) as an eluent to afford the corresponding silylboronate **3i** in 31% isolated yield (46.6 mg, 0.153 mmol) as a white solid.

^1H NMR (401 MHz, $CDCl_3$, δ): 1.00 (s, 9H), 1.278 (s, 6H), 1.282 (s, 6H), 2.34 (s, 3H), 3.96 (s, 1H), 7.15–7.19 (m, 1H), 7.23 (t, J = 7.6 Hz, 1H), 7.41–7.46 (m, 2H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 17.1 (*C*), 21.5 (*C*H_3), 25.0 (*C*H_3), 28.0 (*C*H_3), 83.6 (*C*), 127.5 (*C*H), 130.0 (*C*H), 133.4 (*C*H), 133.6 (*C*), 136.7 (*C*), 137.1 (*C*H). $^{11}B\{^1H\}$ NMR (126 MHz, $CDCl_3$, δ): 34.0. The signal derived from the silicon directly attached to the boron atom was not detected by $^{29}Si\{^1H\}$ NMR, which is likely due to quadrupolar relaxation. HRMS-EI (m/z): $[M–Me]^+$ calcd for $C_{16}H_{26}{}^{11}BO_2Si$, 289.1795; found 289.1796. mp 40–45 °C.

***tert*-Butyl(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)(*o*-tolyl)silane (3j).**

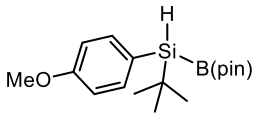


3j

Procedure **B**: The reaction was performed with **1j** (89.3 mg, 0.501 mmol). The crude product was purified by silica-gel column chromatography with hexane/Et_2O (100:0 to 97:3) as an eluent to afford the corresponding silylboronate **3j** in 59% isolated yield (89.7 mg, 0.295 mmol) as a colorless oil.

^1H NMR (401 MHz, $CDCl_3$, δ): 1.03 (s, 9H), 1.27 (s, 6H), 1.28 (s, 6H), 2.47 (s, 3H), 4.16 (s, 1H), 7.11–7.19 (m, 2H), 7.25 (td, J = 1.6, 7.5 Hz, 1H), 7.63 (d, J = 7.2 Hz, 1H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 18.0 (*C*), 23.8 (*C*H_3), 25.0 (*C*H_3), 28.4 (*C*H_3), 83.6 (*C*), 124.6 (*C*H), 129.2 (*C*H), 129.5 (*C*H), 132.9 (*C*), 137.9 (*C*H), 144.2 (*C*). $^{11}B\{^1H\}$ NMR (126 MHz, $CDCl_3$, δ): 34.2. The signal derived from the silicon directly attached to the boron atom was not detected by $^{29}Si\{^1H\}$ NMR, which is likely due to quadrupolar relaxation. HRMS-EI (m/z): $[M–Me]^+$ calcd for $C_{16}H_{26}{}^{11}BO_2Si$, 289.1795; found 289.1794.

***tert*-Butyl(4-methoxyphenyl)(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)silane (3k).**



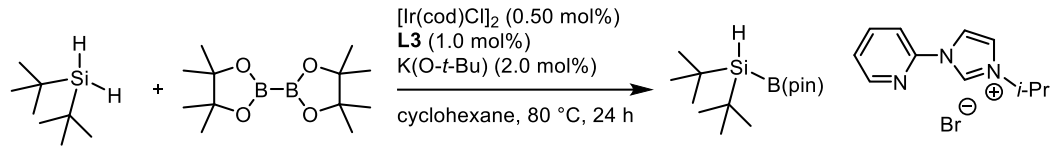
3k

Procedure **C**: The reaction was performed with **1k** (97.3 mg, 0.501 mmol). The crude product was purified by silica-gel column chromatography with hexane/Et_2O (100:0 to 97:3) as an eluent to afford the corresponding silylboronate **3k** in 71% isolated yield (113.1 mg, 0.353 mmol) as a white solid.

Procedure **B**: The reaction was performed with **1k** (97.2 mg, 0.500 mmol). The crude product was purified by silica-gel column chromatography with hexane/Et_2O (100:0 to 97:3) as an eluent to afford the corresponding silylboronate **3k** in 29% isolated yield (45.8 mg, 0.143 mmol) as a white solid.

^{1}H NMR (392 MHz, $CDCl_3$, δ): 0.98 (s, 9H), 1.28 (s, 12H), 3.81 (s, 3H), 4.00 (s, 1H), 6.90 (dt, J = 2.1, 8.6 Hz, 2H), 7.57 (dt, J = 2.2, 8.6 Hz, 2H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 17.2 (*C*), 25.0 (*C*H_3), 27.9 (*C*H_3), 54.9 (*C*H_3), 83.5 (*C*), 113.4 (*C*H), 124.5 (*C*), 137.8 (*C*H), 160.4 (*C*). ^{11}B{^{1}H} NMR (126 MHz, $CDCl_3$, δ): 34.1. The signal derived from the silicon directly attached to the boron atom was not detected by ^{29}Si{^{1}H} NMR, which is likely due to quadrupolar relaxation. HRMS-EI (m/z): $[M–Me]^+$ calcd for $C_{16}H_{26}{}^{11}BO_3Si$, 305.1744; found 305.1747. mp 50–53 °C.

6. Procedure for Gram-Scale Synthesis of 3a



1a (7.0 mmol) **2** (2.0 equiv) **3a** 70% yield **L3**

Bis(pinacolato)diboron **2** (3.56 g, 14.0 mmol, 2.00 equiv) and **L3** (18.8 mg, 0.0701 mmol, 1.00 mol%) were placed in a vial with a screw cap containing a Teflon®-coated rubber septum under air. The vial was placed in a glove box under an argon atmosphere, and then $[Ir(cod)Cl]_2$ (23.5 mg, 0.0350 mmol, 0.500 mol%) and K(O-*t*-Bu) (15.7 mg, 0.140 mmol, 2.00 mol%) were added to the vial. After the vial was sealed with the screw cap, it was removed from the glove box. Then, cyclohexane (7.0 mL) was added to the vial via a syringe. The resulting mixture was allowed to warm at 80 °C and stirred for 1 h. Then, di-*tert*-butylsilane **1a** (1.01 g, 7.01 mmol, 1.00 equiv) was added dropwise via a syringe. After the reaction mixture was stirred at 80 °C for 24 h, the reaction mixture was analyzed by GC to determined the GC yield of the product (73%). The mixture was directly filtered through a silica-gel pad with pentane/Et_2O (9:1) as an eluent, and then the resulting solution was concentrated under reduced pressure. The crude product was purified by silica-gel column chromatography with hexane/Et_2O (100:0 to 98:2) as an eluent to afford the corresponding product **3a** (1.33 g, 4.93 mmol, 70% yield) as a colorless oil.

7. Single Crystal X-ray Structural Analysis of 3a

The molecular structure of **3a** was confirmed by single-crystal X-ray diffraction analysis (Figure S1). Although several conformers of **3a** were observed in the disordered structure, the presence of a silicon-boron bond was confirmed unambiguously.

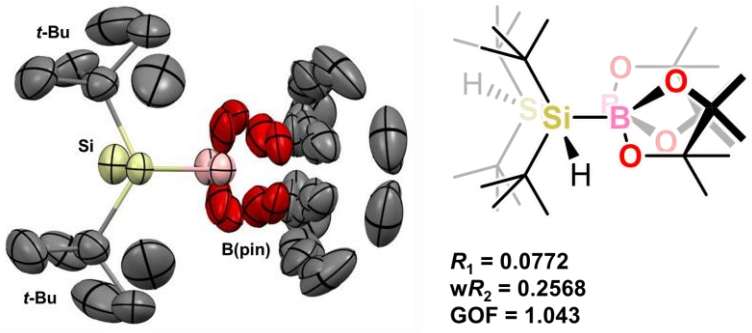


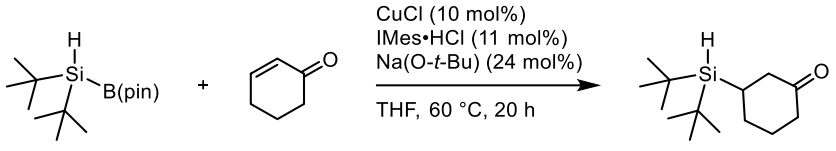
Figure S1. Molecular structure of **3a** with thermal ellipsoids at 50% probability. Hydrogen atoms are omitted for clarity.

Table S5. Summary of X-ray crystallographic data for **3a**.

CCDC	2065033
Empirical formula	$C_{14}H_{31}BO_2Si$
Formula weight	270.29
Temperature/K	173
Crystal system	orthorhombic
Space group	Pnma
a / Å	12.7304(6)
b / Å	14.6636(6)
c / Å	9.7331(4)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	1816.91(14)
Z	4
ρ_{calc} g/cm^3	0.988
μ/mm^{-1}	0.124
F(000)	600.0
Crystal size/mm^3	0.3×0.3×0.02
Radiation	MoKα (λ = 0.71073)
2θ range for data collection/°	5.268 to 58.418
Index ranges	$-15 \leqq h \leqq 16$, $-19 \leqq k \leqq 19$, $-12 \leqq l \leqq 12$
Reflections collected	25184
Independent reflections	2333 [R_{int} = 0.0841, R_{sigma} = 0.0524]
Data/restraints/parameters	2333/449/236
Goodness-of-fit on F^2	1.043
Final *R* indexes [I>=2σ (I)]	R_1 = 0.0772, wR_2 = 0.2346
Final *R* indexes [all data]	R_1 = 0.0948, wR_2 = 0.2568
Largest diff. peak/hole / e Å^{-3}	0.27/–0.59

8. Procedures for Organic Transformations of 3a

Copper-Catalyzed Conjugated Silylation

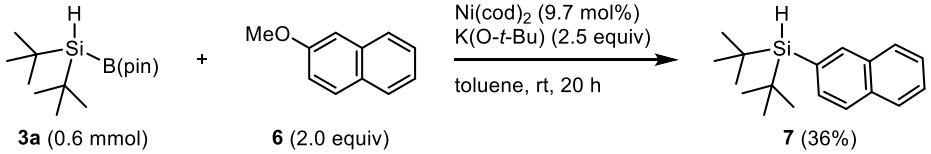


3a (0.2 mmol) **4** (2.0 equiv) **5** 56% yield

Copper(I) chloride (2.0 mg, 0.020 mmol, 10 mol %) and IMes·HCl (7.5 mg, 0.022 mmol, 11 mol %) were placed in a vial under air. The vial was placed in a glove box, and then Na(O-*t*-Bu) (4.5 mg, 0.048 mmol, 24 mol%) was added to the vial under an argon atmosphere. After the vial was sealed with a screw cap containing a Teflon®-coated rubber septum, it was removed from the glove box. Then, THF (1.0 mL) and **3a** (54.8 mg, 0.203 mmol) were added to the vial via syringes. The resulting mixture was stirred for 10 min at room temperature, and then 2-cyclohexen-1-one (**4**) (38.0 μL, 0.400 mmol, 2.00 equiv) and MeOH (16.0 μL, 0.400 mmol, 2.00 equiv) were added dropwise to the vial. After the resulting mixture was stirred at 60 °C for 20 h, the mixture was directly filtered through a silica-gel pad with Et_2O as an eluent. Then, the resultant solution was concentrated under reduced pressure. The crude product was purified by silica-gel column chromatography with hexane/ Et_2O (100:0 to 98:2) to give the corresponding product **5** (26.7 mg, 0.111 mmol, 56% yield) as a colorless oil.

^{1}H NMR (392 MHz, $CDCl_3$, δ): 1.07 (s, 9H), 1.08 (s, 9H), 1.39–1.50 (m, 1H), 1.70 (qt, J = 4.1, 12.6 Hz, 1H), 1.82 (qd, J = 3.2, 12.9 Hz, 1H), 1.97–2.04 (m, 1H), 2.16–2.23 (m, 1H), 2.33 (td, J = 6.0, 13.3 Hz, 1H), 2.39–2.57 (m, 3H), 3.29 (s, 1H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 19.9 (*C*), 20.1 (*C*), 25.3 (*C*H), 28.9 (*C*H_2), 29.4 (*C*H_3), 29.5 (*C*H_3), 30.2 (*C*H_2), 42.0 (*C*H_2), 45.3 (*C*H_2), 211.9 (*C*). HRMS-EI (m/z): [M–^{t}Bu]$^+$ calcd for $C_{10}H_{19}OSi$, 183.1205; found 183.1203.

Nickel-Catalyzed Silylation of Ether



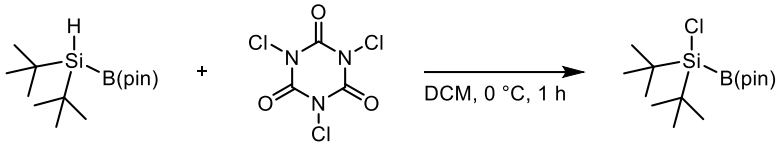
3a (0.6 mmol) **6** (2.0 equiv) **7** (36%)

2-Methoxynaphthalene **6** (189.6 mg, 1.20 mmol, 2.00 equiv) was placed in a vial under air. The vial was placed in a glove box, and then $Ni(cod)_2$ (16.3 mg, 0.0593 mmol, 9.71 mol%) and K(O-*t*-Bu) (167.9 mg, 1.50 mmol, 2.45 equiv) were added to the vial under an argon atmosphere. After the vial was sealed with a screw cap containing a Teflon®-coated rubber septum, it was removed from the glove box. Then, toluene (3.0 mL) and **3a** (165.6 mg, 0.613 mmol) were added to the vial via syringes. After the resulting mixture was stirred for 20 h at room

temperature, the mixture was directly filtered through a silica-gel pad with Et_2O as an eluent. Then the resultant solution was concentrated under reduced pressure. The crude product was purified by silica-gel column chromatography with hexane as eluent and GPC to give the corresponding product **7** (60.1 mg, 0.222 mmol, 36% yield) as a white solid

^{1}H NMR (401 MHz, $CDCl_3$, δ): 1.09 (s, 18H), 4.00 (s, 1H), 7.47–7.51 (m, 2H), 7.65 (dd, J = 1.2, 8.0 Hz, 1H), 7.78–7.87 (m, 3H), 8.09 (s, 1H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 19.2 (*C*), 29.0 (CH_3), 125.8 (*C*H), 126.3 (*C*H), 126.5 (*C*H), 127.7 (*C*H), 128.1 (*C*H), 131.8 (*C*H), 132.8 (*C*), 133.2 (*C*), 133.6 (*C*), 136.8 (*C*H). HRMS-EI (m/z): $[M]^+$ calcd for $C_{18}H_{26}Si$, 270.1804; found 270.1798. mp 50–53 °C.

Chlorination of Si–H Bond



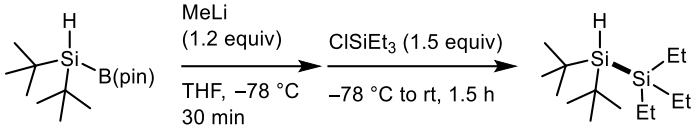
3a (0.6 mmol) **8** (1.1 equiv) **9** 76% yield

This reaction was performed according to the literature procedure.[10] Trichloroisocyanuric acid **8** (763.6 mg, 3.29 mmol, 1.10 equiv) was placed in a vial under air. After the vial was sealed with a screw cap containing a Teflon®-coated rubber septum, it was connected to a vacuum/nitrogen manifold through a needle. It was evacuated and then backfilled with nitrogen. This cycle was repeated three times. CH_2Cl_2 (15.0 mL) was added to the vial via a syringe and allowed to cool at 0 °C. Then, **3a** (809.1 mg, 2.99 mmol) was added dropwise to the mixture via a syringe. After the reaction mixture was stirred for 1 h at 0 °C, the solution was filtered under a nitrogen atmosphere and concentrated under reduced pressure. The crude product was purified by Kugelrohr distillation under reduced pressure (87 Pa, bath temp. 125 °C to 145 °C) to afford the corresponding product **9** (695.9 mg, 2.28 mmol, 76% yield) as a colorless oil.

^{1}H NMR (401 MHz, $CDCl_3$, δ): 1.09 (s, 18H), 1.27 (s, 12H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 21.6 (*C*), 24.9 (CH_3), 27.6 (CH_3), 84.0 (*C*). ^{11}B{^{1}H} NMR (127 MHz, $CDCl_3$, δ): 33.0. ^{29}Si{^{1}H} NMR (79 MHz, $CDCl_3$, δ): 24.1 (brs). The broad signal of ^{29}Si was caused by the quadrupolar boron atom. HRMS-EI (m/z): $[M–Me]^+$ calcd for $C_{13}H_{27}{}^{11}BClO_2Si$, 289.1572; found 289.1565.

9. Procedure for Silicon-Silicon Coupling with 3a

2,2-Di-*tert*-butyl-1,1,1-triethyldisilane (10a).

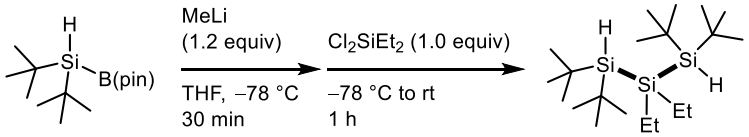


3a (0.5 mmol) **10a** 92% yield

The vial was sealed with a screw cap containing a Teflon®-coated rubber septum and connected to a vacuum/nitrogen manifold through a needle. It was evacuated and then backfilled with nitrogen. This cycle was repeated three times. THF (2.0 mL) and **3a** (135.7 mg, 0.502 mmol) were added to the vial via syringes and allowed to cool at –78 °C. Then MeLi (1.16 M in Et_2O, 500 μL, 0.580 mmol, 1.16 equiv) was added dropwise to the mixture via a syringe. After the reaction mixture was stirred for 30 min at –78 °C, triethylchlorosilane (125.0 μL, 0.750 mmol, 1.50 equiv) was added to the reaction mixture and allowed to warm to room temperature slowly. After stirring for 1.5 h, the mixture was directly filtered through a silica-gel pad with pentane as an eluent. Then, the resultant solution was concentrated under reduced pressure. The crude product was purified by silica-gel column chromatography with hexane as an eluent to afford the corresponding product **10a** (119.7 mg, 0.463 mmol, 92% yield) as a colorless oil.

^{1}H NMR (401 MHz, $CDCl_3$, δ): 0.76 (q, J = 7.6 Hz, 6H), 1.01 (t, J = 7.8 Hz, 9H), 1.09 (s, 18H), 3.43 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 5.47 (CH_2), 8.32 (CH_3), 20.5 (C), 30.9 (CH_3). ^{29}Si{^{1}H} NMR (79 MHz, $CDCl_3$, δ): –7.96, –5.89. HRMS-EI (m/z): $[M]^+$ calcd for $C_{14}H_{34}Si_2$, 258.2199; found 258.2194.

1,1,3,3-Tetra-*tert*-butyl-2,2-diethyltrisilane (10b).



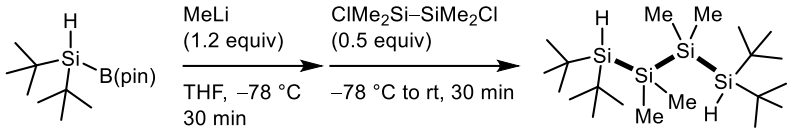
3a (0.5 mmol) **10b** 85% yield

The vial was sealed with a screw cap containing a Teflon®-coated rubber septum and connected to a vacuum/nitrogen manifold through a needle. It was evacuated and then backfilled with nitrogen. This cycle was repeated three times. THF (2.0 mL) and **3a** (135.7 mg, 0.502 mmol) were added to the vial via syringes and allowed to cool at –78 °C. Then MeLi (1.16 M in Et_2O, 500 μL, 0.580 mmol, 1.16 equiv) was added dropwise to the mixture via a syringe. After the reaction mixture was stirred for 30 min at –78 °C, diethyldichlorosilane (37.0

μL, 0.250 mmol, 0.500 equiv) was added to the reaction mixture and allowed to warm to room temperature slowly. After stirring for 1 h, the mixture was directly filtered through a silica-gel pad with pentane as an eluent. Then the resultant solution was concentrated under reduced pressure. The crude product was purified by silica-gel column chromatography with hexane as an eluent to afford the corresponding product **10b** (79.8 mg, 0.214 mmol, 85% yield) as a white solid.

^{1}H NMR (401 MHz, $CDCl_3$, δ): 1.02–1.17 (m, 46H), 3.64 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 4.35 (*C*H_2), 10.5 (*C*H_3), 21.9 (*C*), 31.1 (*C*H_3). ^{29}Si{^{1}H} NMR (79 MHz, $CDCl_3$, δ):–33.0, 3.74. HRMS-EI (m/z): $[M–^{t}Bu]^{+}$ calcd for $C_{16}H_{39}Si_3$, 315.2360; found 315.2350. mp 102–103 °C.

1,1,4,4-Tetra-*tert*-butyl-2,2,3,3-tetramethyltetrasilane (10c).

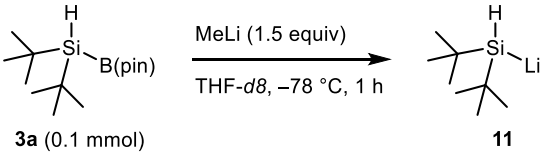


3a (0.5 mmol) **10c** 76% yield

The vial was sealed with a screw cap containing a Teflon®-coated rubber septum and connected to a vacuum/nitrogen manifold through a needle. It was evacuated and then backfilled with nitrogen. This cycle was repeated three times. THF (2.0 mL) and **3a** (134.9 mg, 0.499 mmol) were added to the vial via syringes and allowed to cool at –78 °C. Then MeLi (1.16 M in Et_2O, 500 μL, 0.580 mmol, 1.16 equiv) was added dropwise to the mixture via a syringe. After the reaction mixture was stirred for 30 min at –78 °C, 1,2-dichloro-1,1,2,2-tetramethylsilane (46.0 μL, 0.250 mmol, 0.500 equiv) was added to the reaction mixture and allowed to warm to room temperature slowly. After stirring for 30 min, the mixture was directly filtered through a silica-gel pad with pentane as an eluent. Then the resultant solution was concentrated under reduced pressure. The crude product was purified by silica-gel column chromatography with hexane as an eluent to afford the corresponding product **10c** (76.5 mg, 0.190 mmol, 76% yield) as a white solid.

^{1}H NMR (401 MHz, $CDCl_3$, δ): 0.33 (s, 12 H), 1.09 (s, 36H), 3.55 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): –1.38 (*C*H_3), 21.0 (*C*), 30.7 (*C*H_3). ^{29}Si{1H} NMR (79 MHz, $CDCl_3$, δ): –42.9, –1.58. HRMS-EI (m/z): $[M–^{t}Bu]^{+}$ calcd for $C_{16}H_{41}Si_4$, 345.2285; found 345.2279. mp 108–110 °C.

10. Details of ^{29}Si NMR Experiments



3a (0.1 mmol) **11**

The vial was sealed with a screw cap containing a Teflon®-coated rubber septum and connected to a vacuum/nitrogen manifold through a needle. It was evacuated and then backfilled with nitrogen. This cycle was repeated three times. THF (500 μL) and **3a** (27.0 mg, 0.100 mmol) were added to the vial via syringes and allowed to cool at –78 °C. Then MeLi (1.16 M in Et_2O, 130 μL, 0.151 mmol, 1.51 equiv) was added dropwise to the mixture via a syringe. After the reaction mixture was stirred for 1 h at –78 °C and a further 1 h at room temperature, the resulting mixture was transferred to an NMR tube and analyzed by ^{29}Si{^{1}H} NMR spectroscopy (JEOL JNM-ECZ600R/S3) at room temperature.

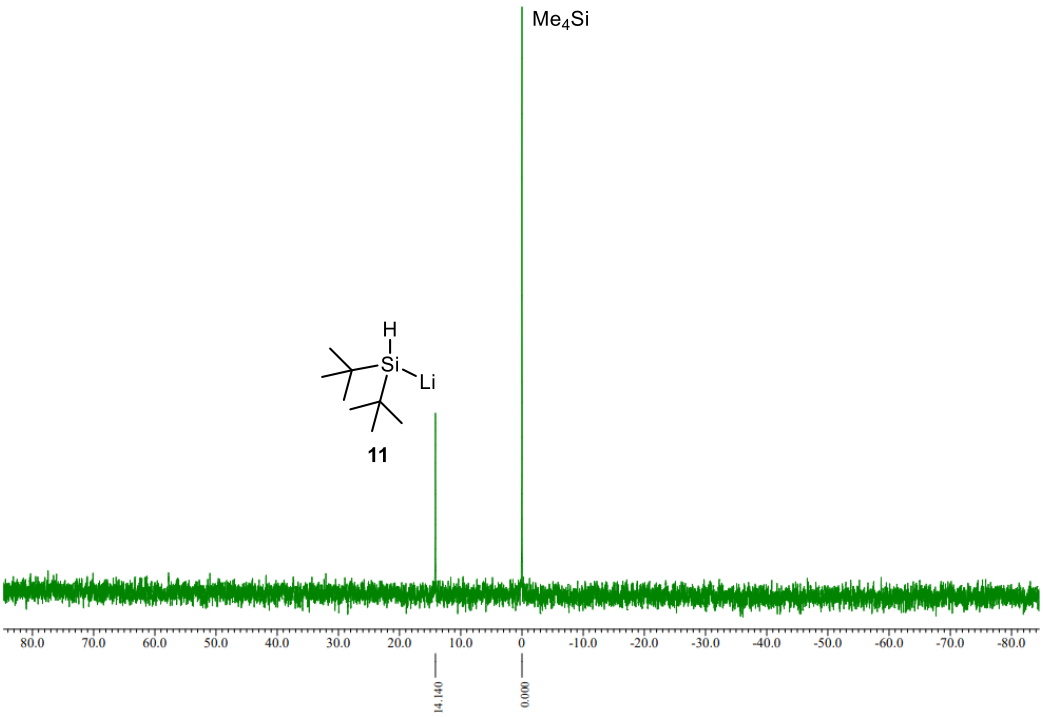


Figure S2. ^{29}Si{^{1}H} NMR spectra of (*t*-Bu)$_2$HSiLi (**11**) at room temperature.

The vial was sealed with a screw cap containing a Teflon®-coated rubber septum and connected to a vacuum/nitrogen manifold through a needle. It was evacuated and then backfilled with nitrogen. This cycle was repeated three times. THF (500 μL) and **3a** (26.7 mg, 0.0988 mmol) were added to the vial via syringes and allowed to cool at –78 °C. Then MeLi (1.16 M in Et_2O, 130 μL, 0.151 mmol, 1.53 equiv) was added dropwise to the mixture via a

syringe. After the reaction mixture was stirred for 1 h at –78 °C, the resulting mixture was transferred to an NMR tube and analyzed by $^{29}Si\{^{1}H\}$ NMR spectroscopy (JEOL JNM-ECA600) at –95°C.

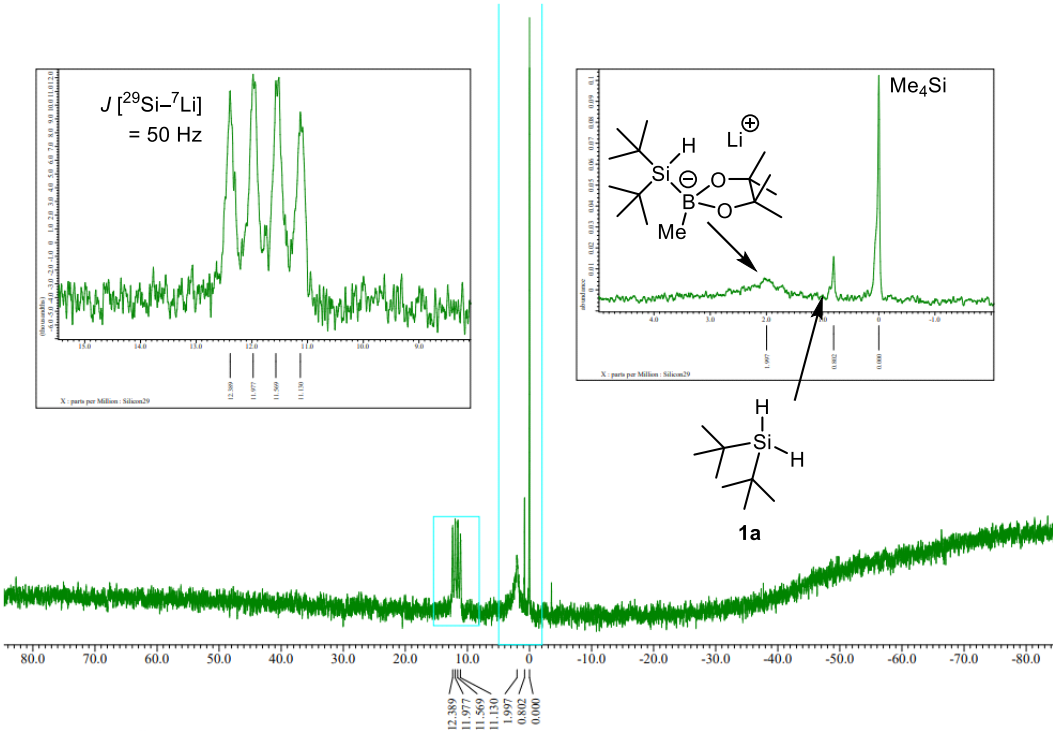
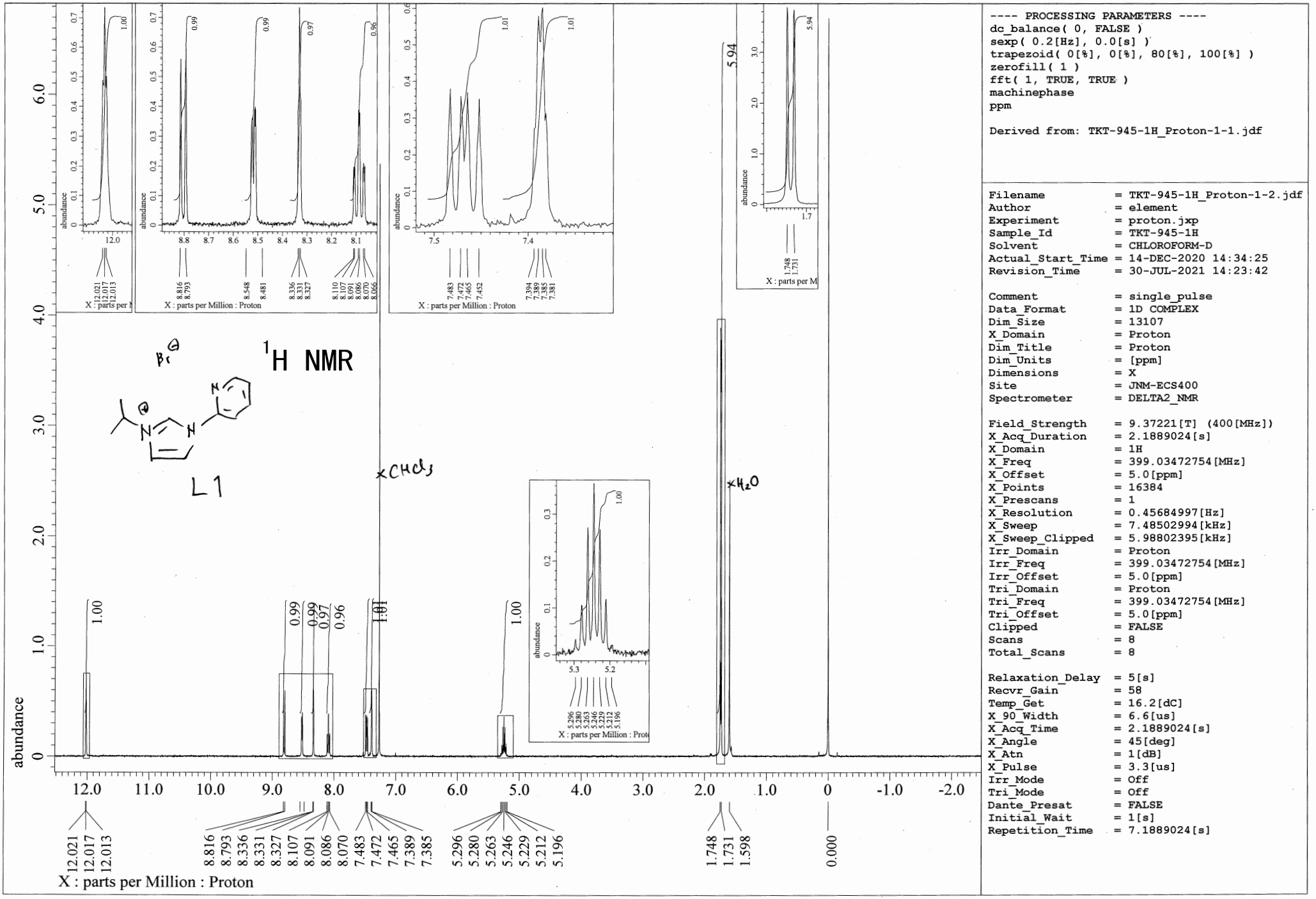


Figure S3. $^{29}Si\{^{1}H\}$ NMR spectra of $(t\text{-Bu})_2HSiLi$ (**11**) at –95°C.

$^{29}Si\{^{1}H\}$ NMR analysis revealed that **11** was generated in the reaction mixture (Figure S2 and S3). Signals derived from the corresponding borate and hydrolyzed dihydrosilane **1a** were also observed at –95°C (Figure S3).

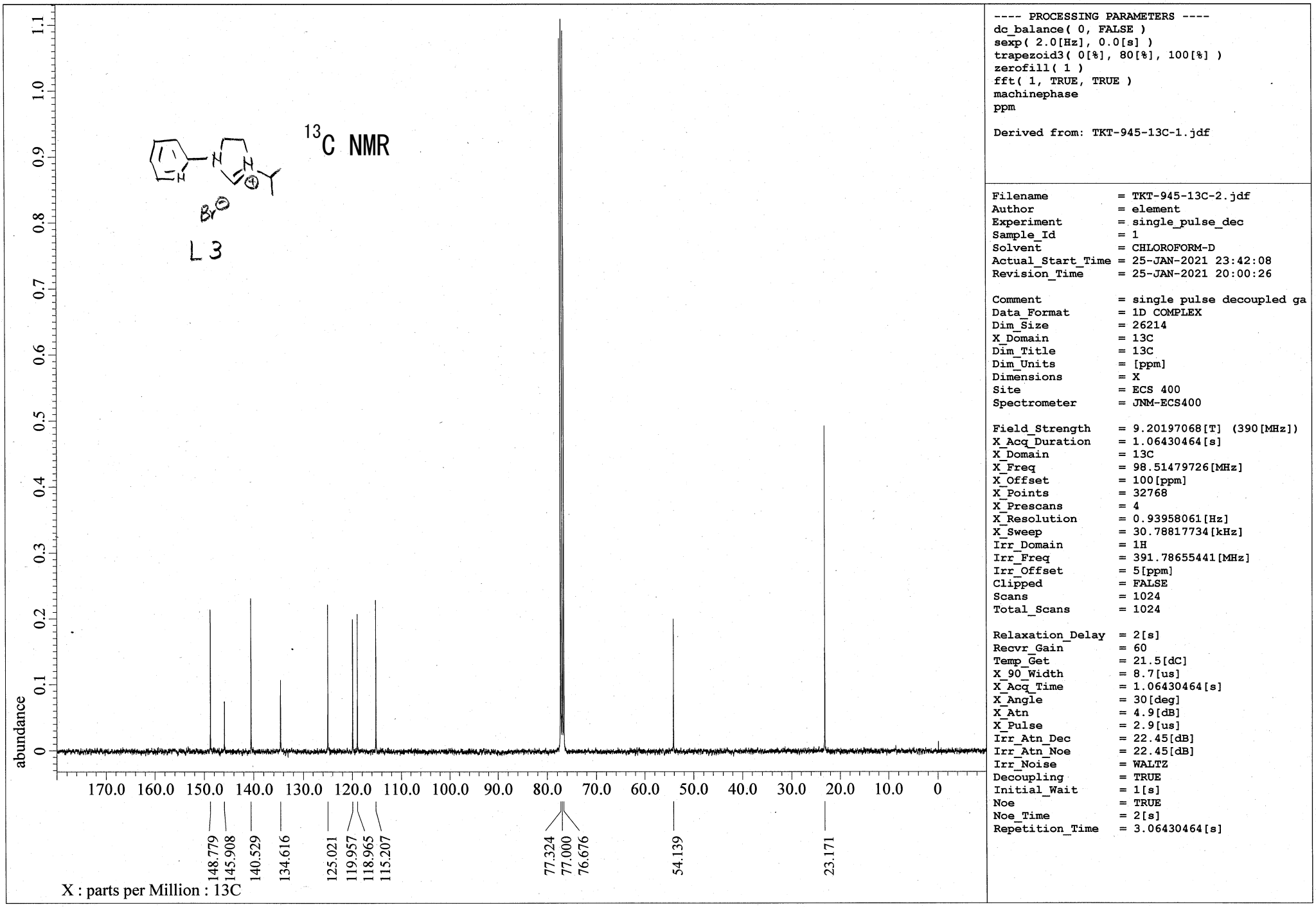
11. References

1) Gründemann, S.; Albrecht, M.; Kovacevic, A.; Faller, J. W.; Crabtree, R. H. *J. Chem. Soc., Dalton Trans.* **2002**, *10*, 2163.
2) Masaoka, S.; Banno, T.; Ishikawa, M. *J. Organomet. Chem.* **2006**, *691*, 182.
3) Iwanaga, K.; Tokuhisa, K. METHOD FOR PRODUCING TERTIARY ALKYLSILANE AND TERTIARY ALKOXYSILANE. Tosoh Corporation Patent JP 2016/138086, Aug 4, 2016.
4) Igawa, K.; Yoshihiro, D.; Ichikawa, N.; Kokan, N.; Tomooka, K. *Angew. Chem., Int. Ed.* **2012**, *51*, 12745.
5) Hirone, N.; Sanjiki, H.; Tanaka, R.; Hata, T.; Urabe, H. *Angew. Chem., Int. Ed.* **2010**, *49*, 7762.
6) Zhu, J.; Chen, S.; He, C. *J. Am. Chem. Soc.* **2021**, *143*, 5301.
7) Shirakawa, E.; Ikeda, D.; Masui, S.; Yoshida, M.; Hayashi, T. *J. Am. Chem. Soc.* **2012**, *134*, 272.
8) Manoso, A. S.; Ahn, C.; Soheili, A.; Handy, C. J.; Correia, R.; Seganish, W. M.; DeShong, P. *J. Org. Chem.* **2004**, *69*, 8305.
9) Visco, M. D.; Wieting, J. M.; Mattson, A. E. *Org. Lett.* **2016**, *18*, 2883.
10) Varaprath, S.; Stutts, D. H. *J. Organomet. Chem.* **2007**, *692*, 1892.



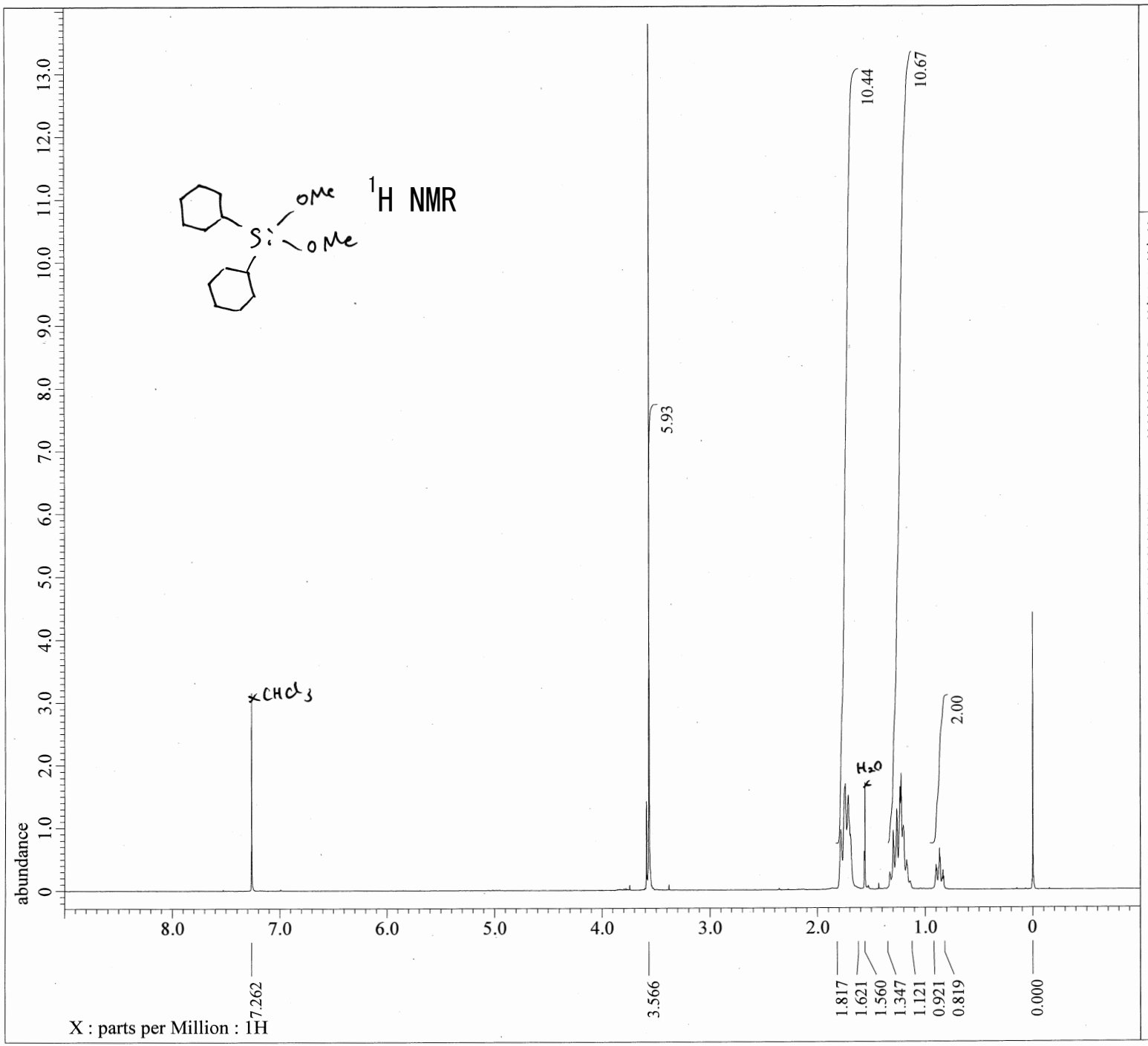

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: TKT-945-1H_Proton-1-1.jdf
```

Filename	= TKT-945-1H_Proton-1-2.jdf
Author	= element
Experiment	= proton.jxp
Sample_Id	= TKT-945-1H
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 14-DEC-2020 14:34:25
Revision_Time	= 30-JUL-2021 14:23:42
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	= 58
Temp_Get	= 16.2[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]



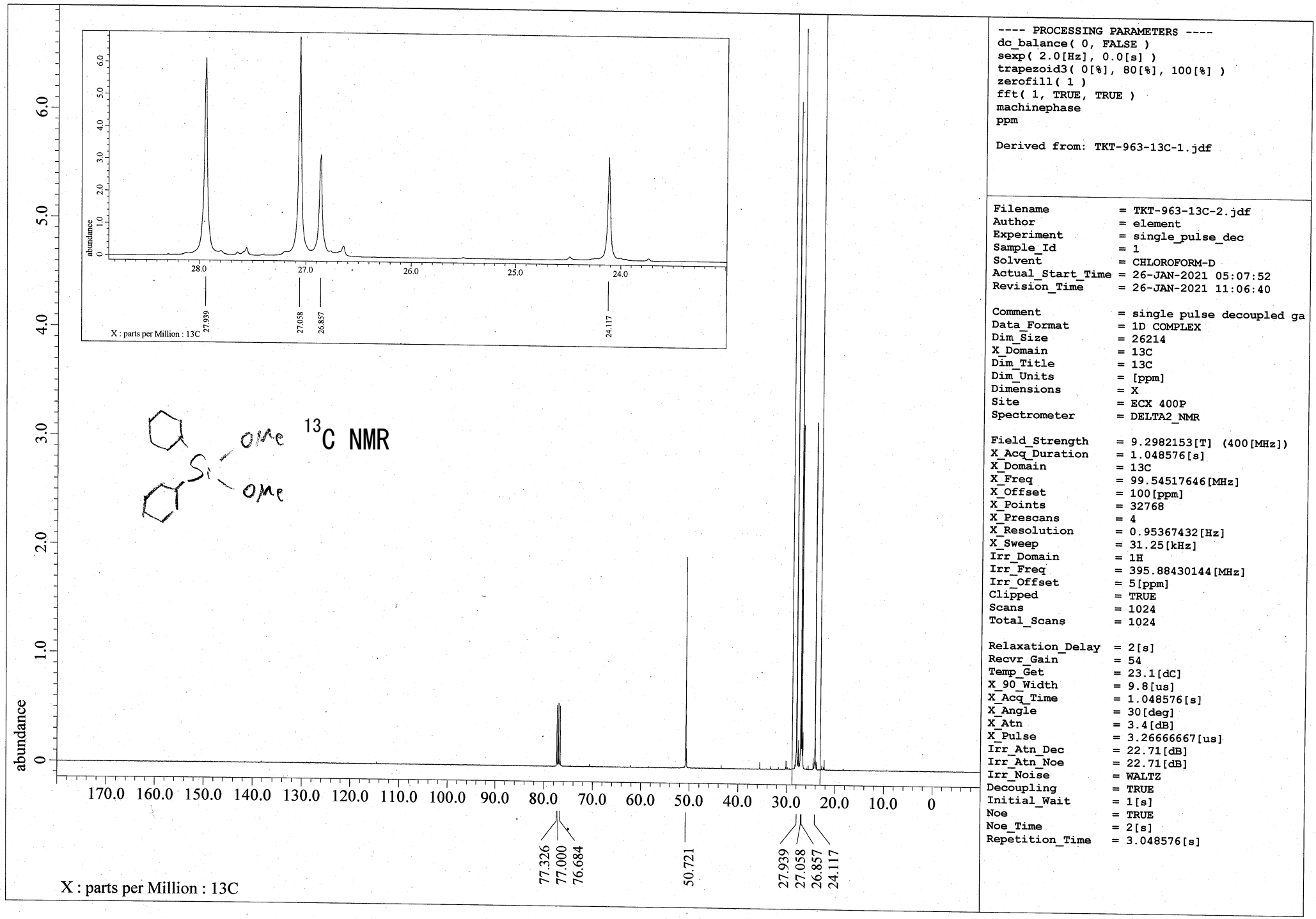

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: TKT-945-13C-1.jdf
```

Filename	= TKT-945-13C-2.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= 1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 25-JAN-2021 23:42:08
Revision_Time	= 25-JAN-2021 20:00:26
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	= 1024
Total_Scans	= 1024
Relaxation_Delay	= 2[s]
Recvr_Gain	= 60
Temp_Get	= 21.5[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]



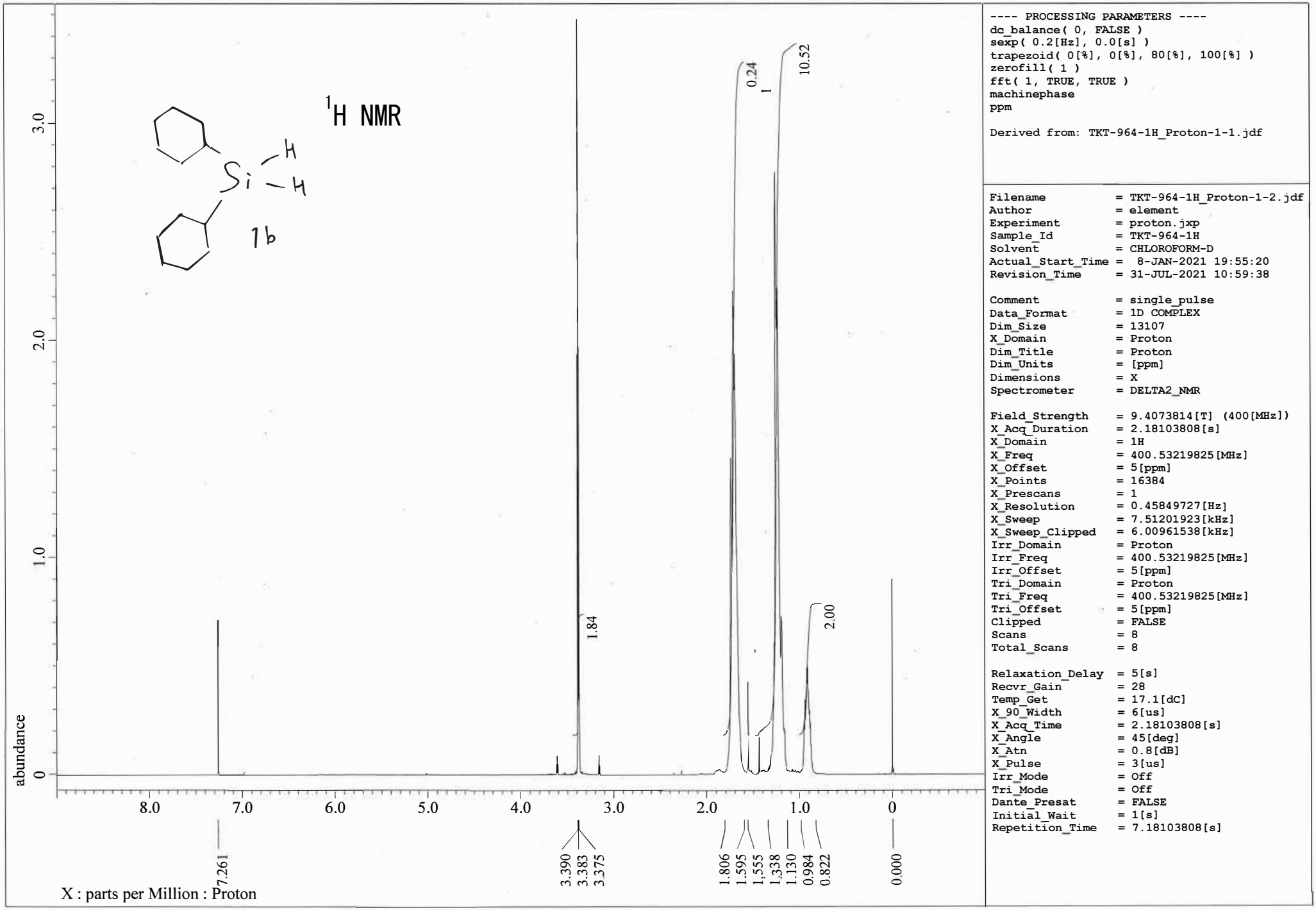

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: TKT-963-1H-1.jdf
```

```
Filename            = TKT-963-1H-2.jdf
Author              = element
Experiment          = single_pulse.ex2
Sample_Id           = S#576991
Solvent             = CHLOROFORM-D
Actual_Start_Time   =  7-JAN-2021 23:04:13
Revision_Time       = 30-JUL-2021 14:29:28

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          = 48
Temp_Get            = 18.3[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]
```



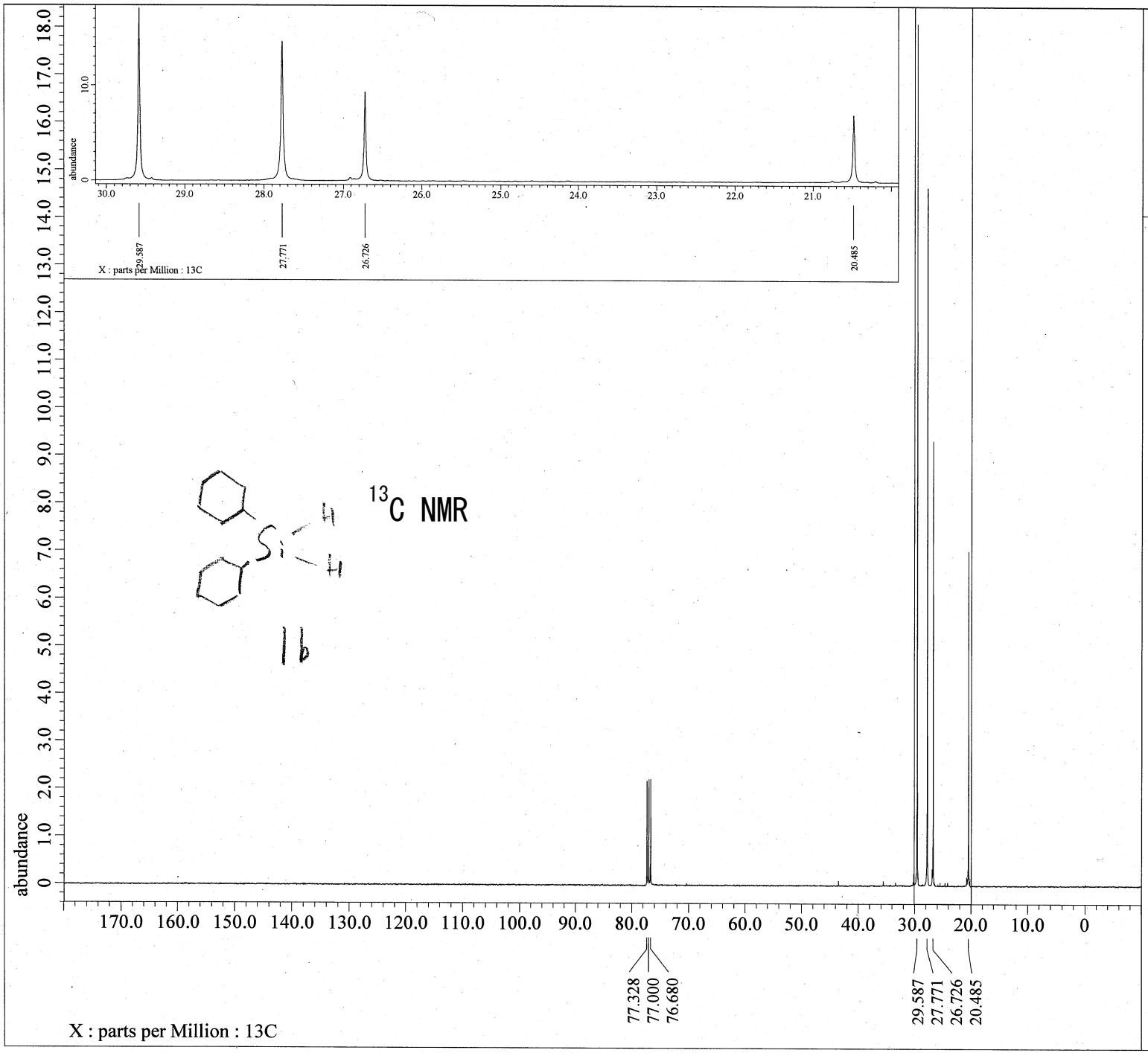

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: TKT-963-13C-1.jdf
```

Filename	= TKT-963-13C-2.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= 1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 26-JAN-2021 05:07:52
Revision_Time	= 26-JAN-2021 11:06:40
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	= TRUE
Scans	= 1024
Total_Scans	= 1024
Relaxation_Delay	= 2[s]
Recvr_Gain	= 54
Temp_Get	= 23.1[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] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: TKT-964-1H_Proton-1-1.jdf
```

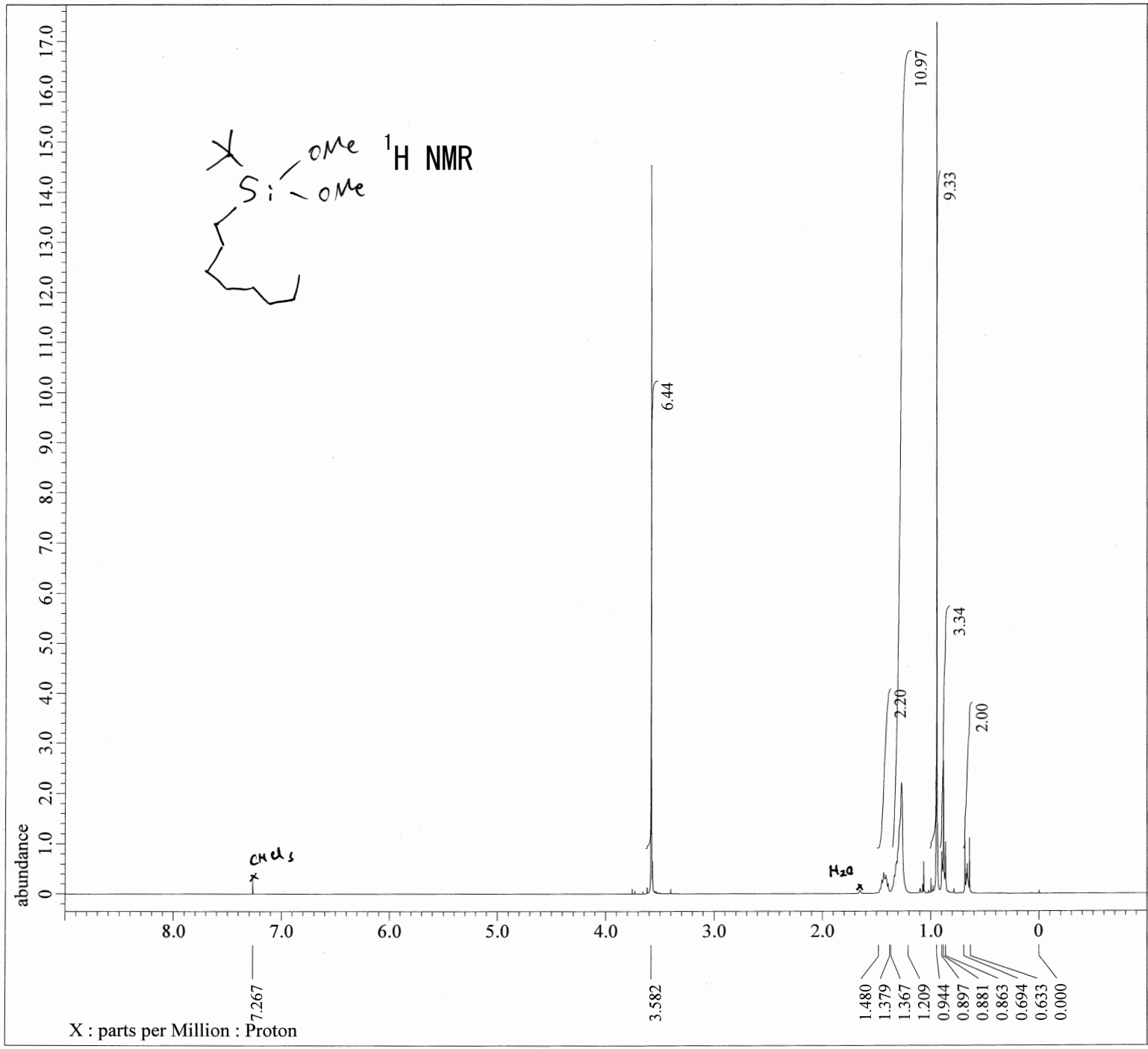
```
Filename            = TKT-964-1H_Proton-1-2.jdf
Author              = element
Experiment          = proton.jxp
Sample_Id           = TKT-964-1H
Solvent             = CHLOROFORM-D
Actual_Start_Time   =  8-JAN-2021 19:55:20
Revision_Time       = 31-JUL-2021 10:59:38

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          = 28
Temp_Get            = 17.1[dC]
X_90_Width          = 6[us]
X_Acq_Time          = 2.18103808[s]
X_Angle             = 45[deg]
X_Atn               = 0.8[dB]
X_Pulse             = 3[us]
Irr_Mode            = Off
Tri_Mode            = Off
Dante_Presat        = FALSE
Initial_Wait        = 1[s]
Repetition_Time     = 7.18103808[s]
```



^{13}C NMR

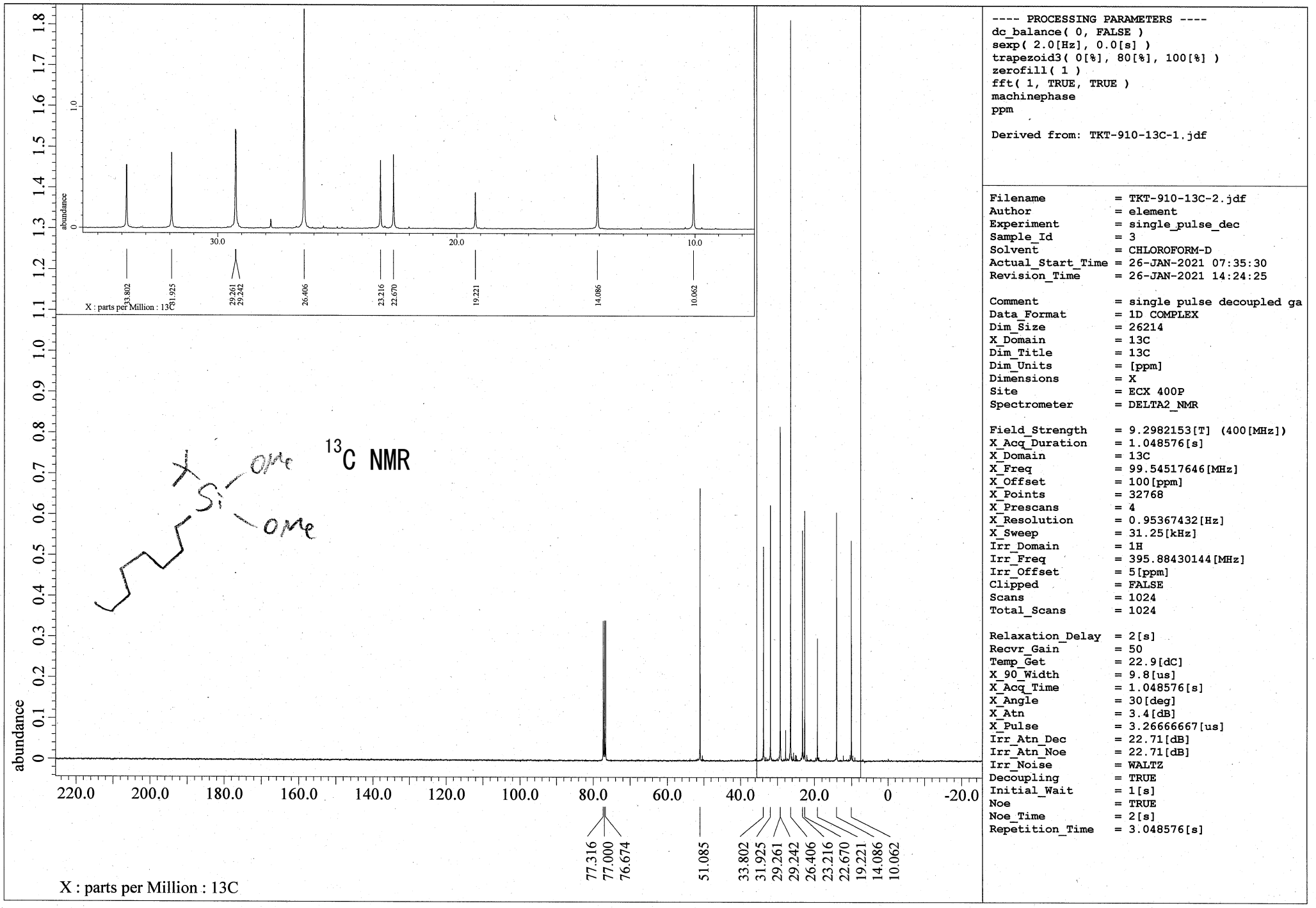
```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: TKT-964-13C-1.jdf
```

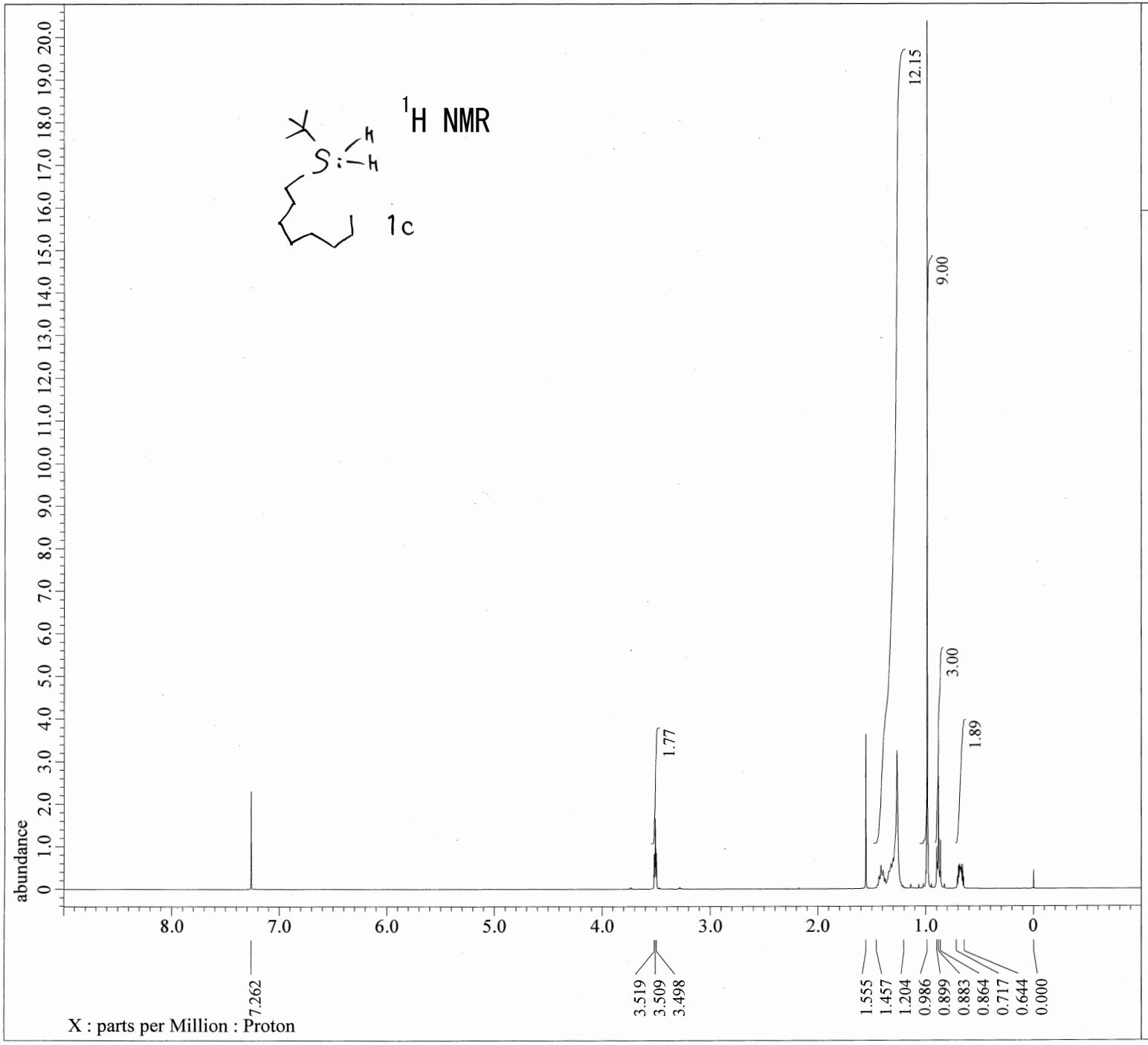
Filename	= TKT-964-13C-2.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= 1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 26-JAN-2021 17:43:46
Revision_Time	= 26-JAN-2021 14:10:53
Comment	= single pulse decoupled ga
Data_Format	= 1D COMPLEX
Dim_Size	= 32768
X_Domain	= 13C
Dim_Title	= 13C
Dim_Units	= [ppm]
Dimensions	= X
Site	= ECS 400
Spectrometer	= JNM-ECS400
Field_Strength	= 9.20197068[T] (390[MHz])
X_Acq_Duration	= 1.3303808[s]
X_Domain	= 13C
X_Freq	= 98.51479726[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.75166449[Hz]
X_Sweep	= 24.63054187[kHz]
Irr_Domain	= 1H
Irr_Freq	= 391.78655441[MHz]
Irr_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 512
Total_Scans	= 512
Relaxation_Delay	= 2[s]
Recvr_Gain	= 68
Temp_Get	= 20.7[dC]
X_90_Width	= 8.7[us]
X_Acq_Time	= 1.3303808[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	= 3.3303808[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: TKT-910-1H_Proton-1-1.jdf
```

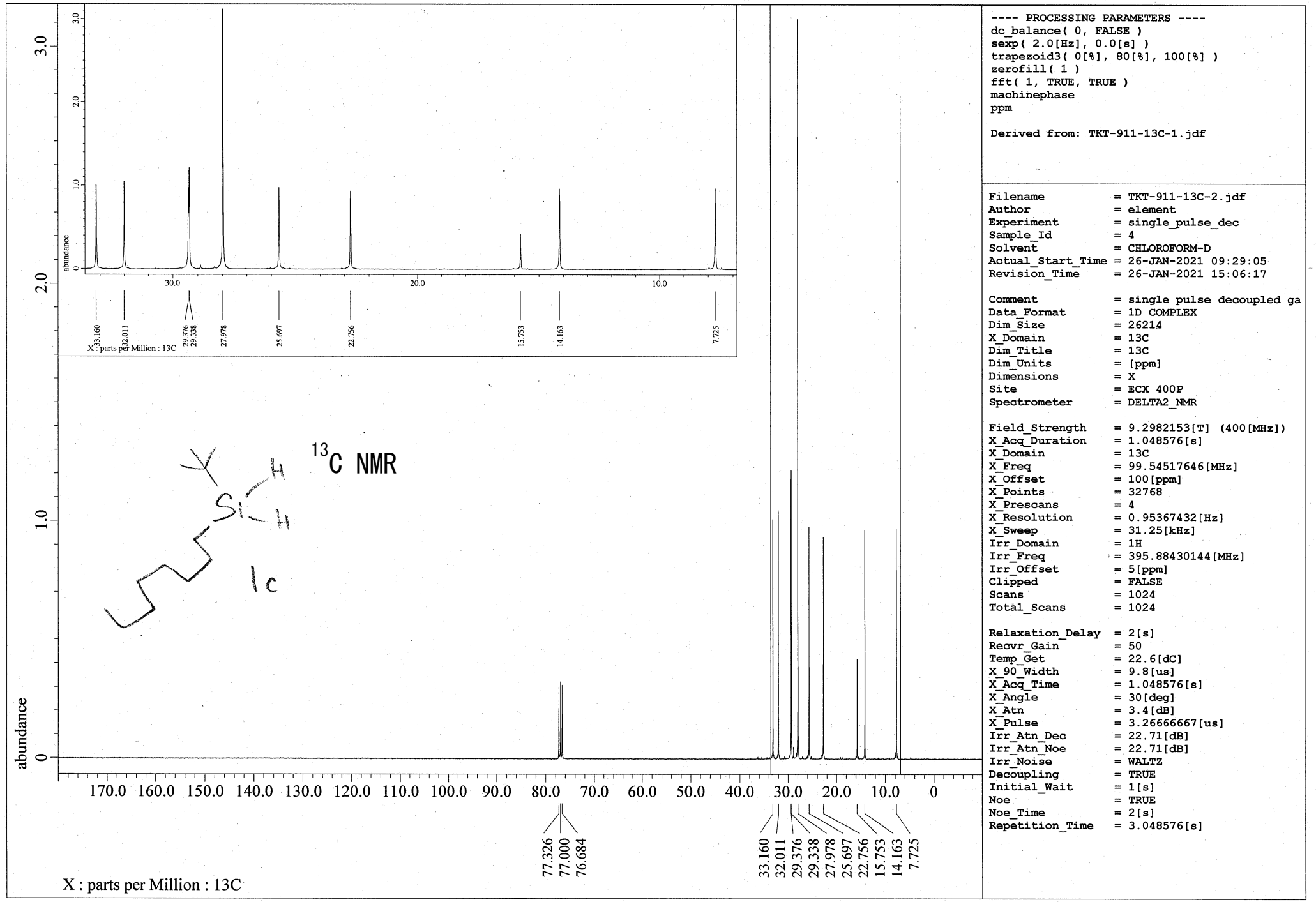
```
Filename            = TKT-910-1H_Proton-1-2.jdf
Author              = element
Experiment          = proton.jxp
Sample_Id           = TKT-910-1H
Solvent             = CHLOROFORM-D
Actual_Start_Time   =  5-NOV-2020 19:04:23
Revision_Time       = 30-JUL-2021 14:39:33

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          = 24
Temp_Get            = 19.1[dC]
X_90_Width          = 6[us]
X_Acq_Time          = 2.18103808[s]
X_Angle             = 45[deg]
X_Atn               = 0.8[dB]
X_Pulse             = 3[us]
Irr_Mode            = Off
Tri_Mode            = Off
Dante_Presat        = FALSE
Initial_Wait        = 1[s]
Repetition_Time     = 7.18103808[s]
```

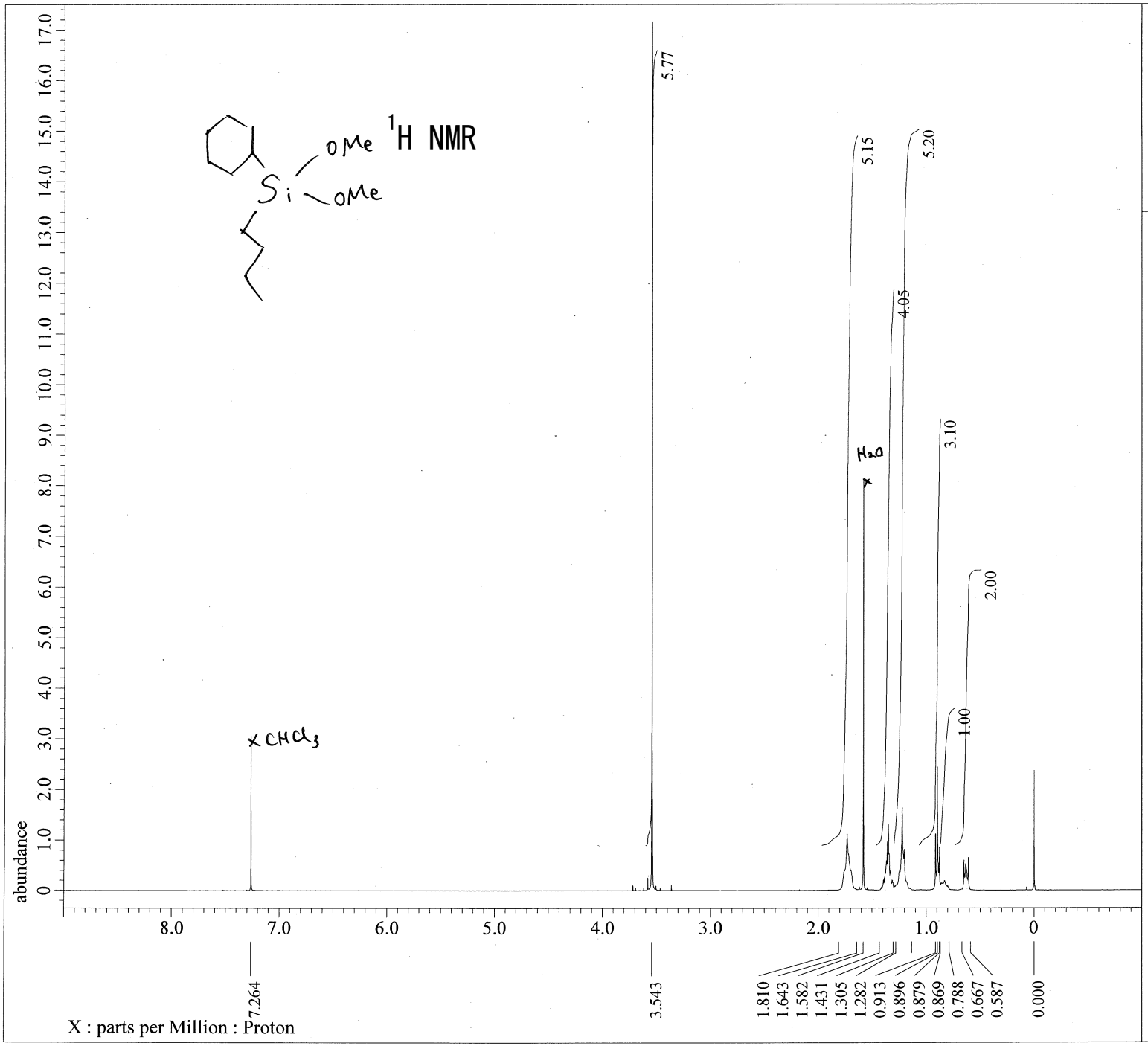

13C NMR
abundance
X : parts per Million : 13C
77.316
77.000
76.674
51.085
33.802
31.925
29.261
29.242
26.406
23.216
22.670
19.221
14.086
10.062
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid3(0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: TKT-910-13C-1.jdf
Filename = TKT-910-13C-2.jdf
Author = element
Experiment = single_pulse_dec
Sample_Id = 3
Solvent = CHLOROFORM-D
Actual_Start_Time = 26-JAN-2021 07:35:30
Revision_Time = 26-JAN-2021 14:24:25
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 = 1024
Total_Scans = 1024
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 22.9[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] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: TKT-911-1H_Proton-1-1.jdf
```

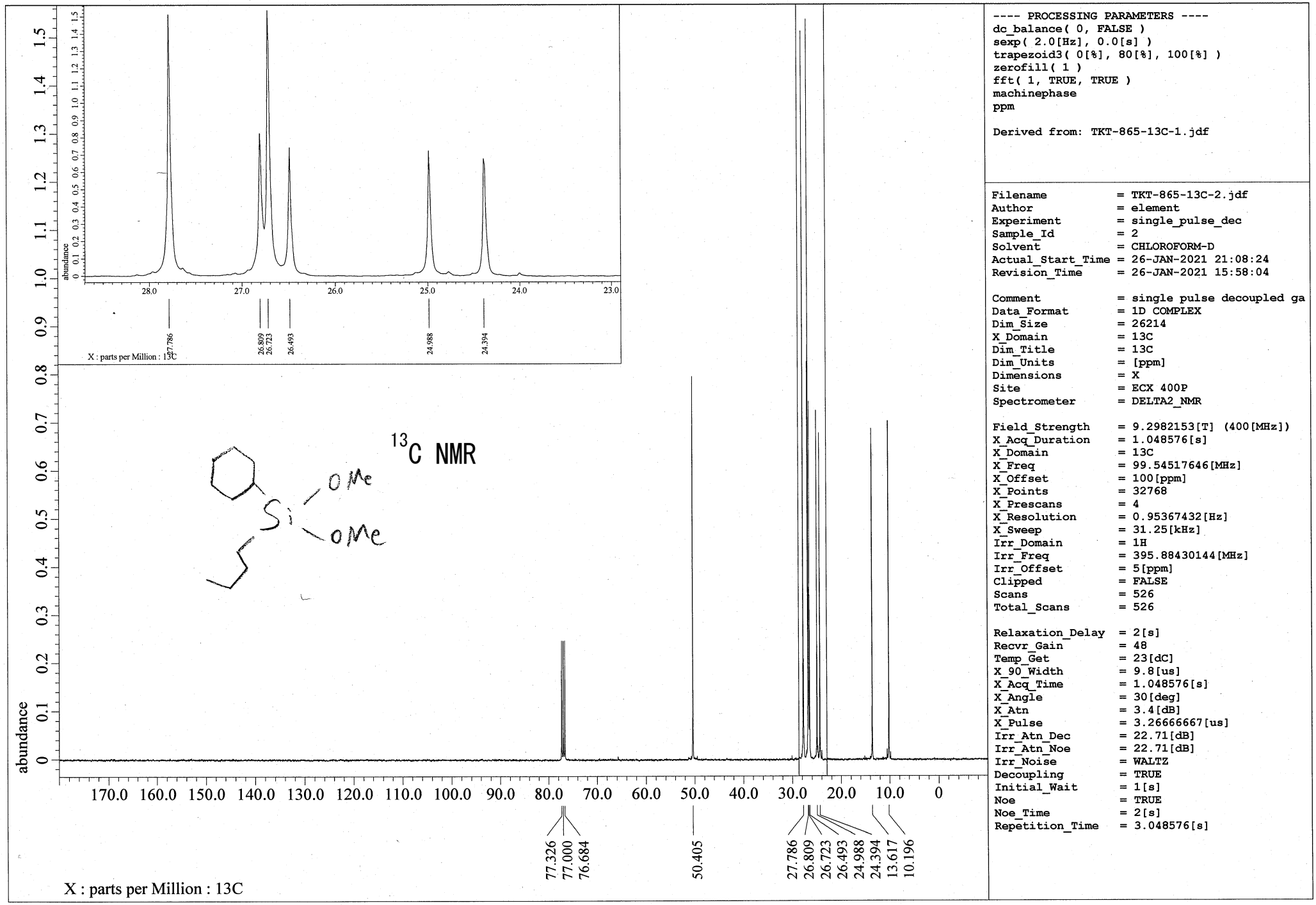
```
Filename            = TKT-911-1H_Proton-1-2.jdf
Author              = element
Experiment          = proton.jxp
Sample_Id           = TKT-911-1H
Solvent             = CHLOROFORM-D
Actual_Start_Time   =  7-NOV-2020 18:14:21
Revision_Time       = 30-JUL-2021 14:44:02

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            = 19.5[dC]
X_90_Width          = 6[us]
X_Acq_Time          = 2.18103808[s]
X_Angle             = 45[deg]
X_Atn               = 0.8[dB]
X_Pulse             = 3[us]
Irr_Mode            = Off
Tri_Mode            = Off
Dante_Presat        = FALSE
Initial_Wait        = 1[s]
Repetition_Time     = 7.18103808[s]
```

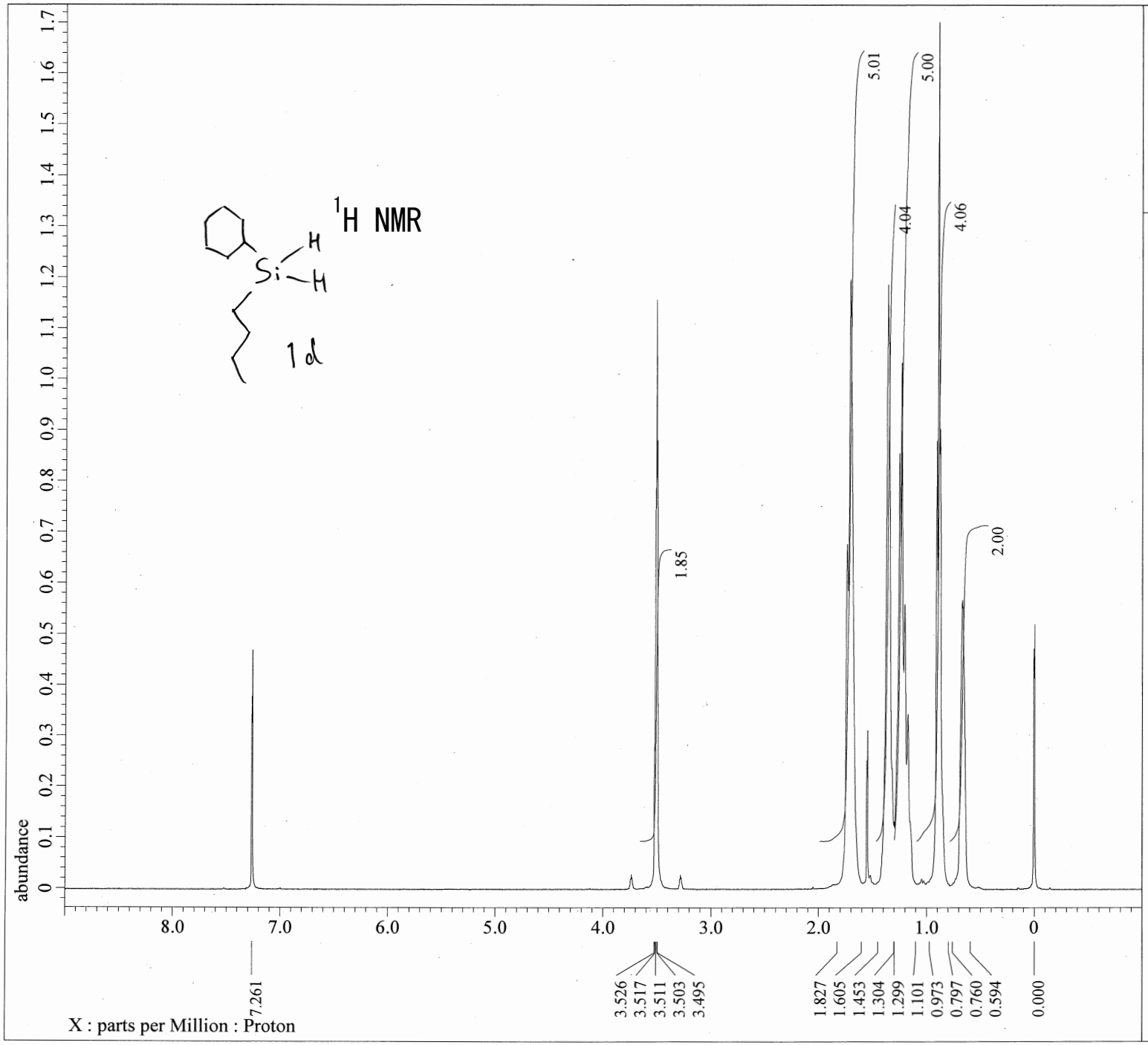

13C NMR
1c
abundance
X : parts per Million : 13C
77.326
77.000
76.684
33.160
32.011
29.376
29.338
27.978
25.697
22.756
15.753
14.163
7.725
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid3(0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: TKT-911-13C-1.jdf
Filename = TKT-911-13C-2.jdf
Author = element
Experiment = single_pulse_dec
Sample_Id = 4
Solvent = CHLOROFORM-D
Actual_Start_Time = 26-JAN-2021 09:29:05
Revision_Time = 26-JAN-2021 15:06:17
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = 13C
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Site = 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 = 1024
Total_Scans = 1024
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 22.6[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] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: TKT-865-1H_Proton-1-1.jdf
```

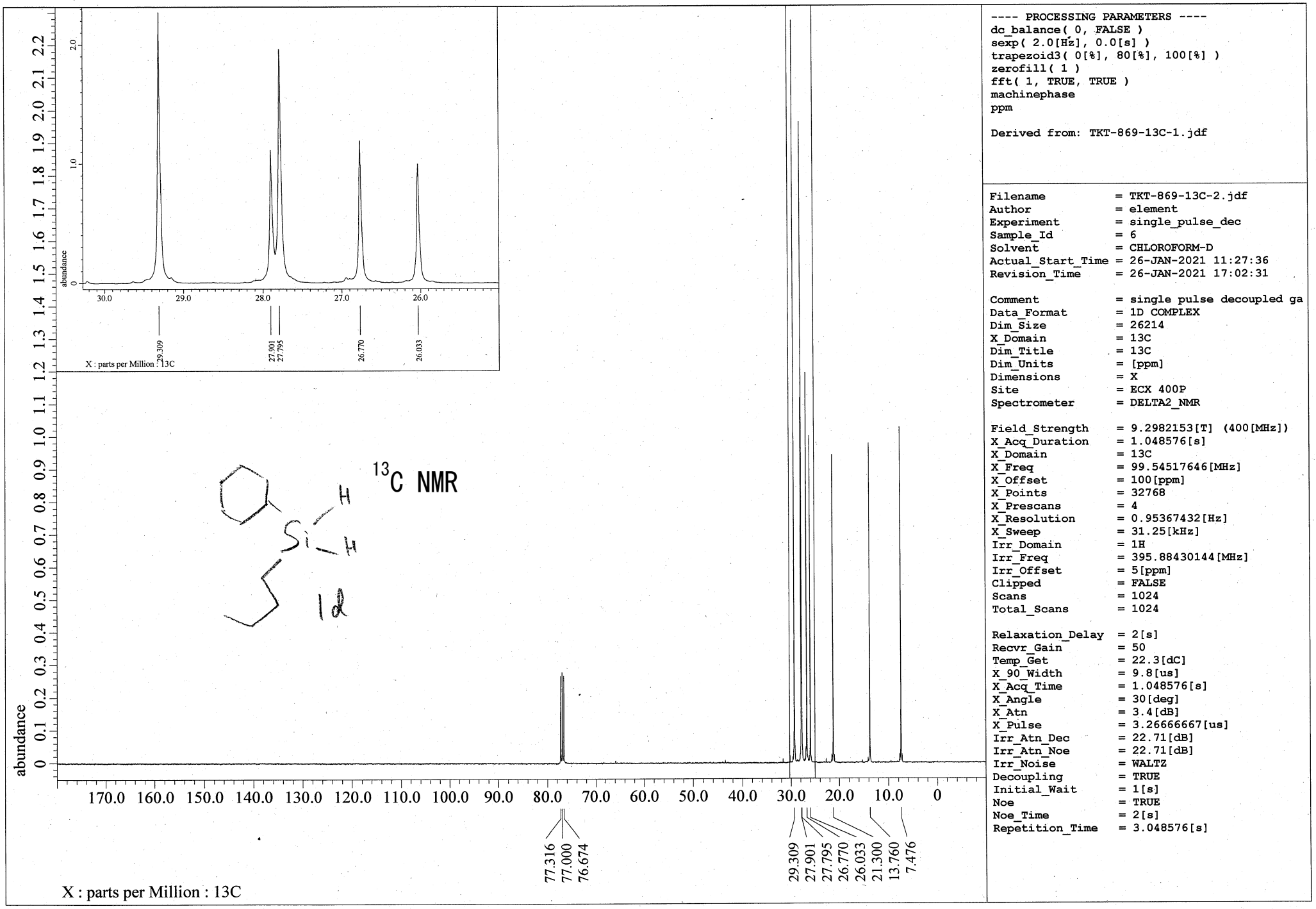
Filename	= TKT-865-1H_Proton-1-2.jdf
Author	= element
Experiment	= proton.jxp
Sample_Id	= TKT-865-1H
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 1-OCT-2020 17:16:10
Revision_Time	= 30-JUL-2021 14:49:00
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
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]

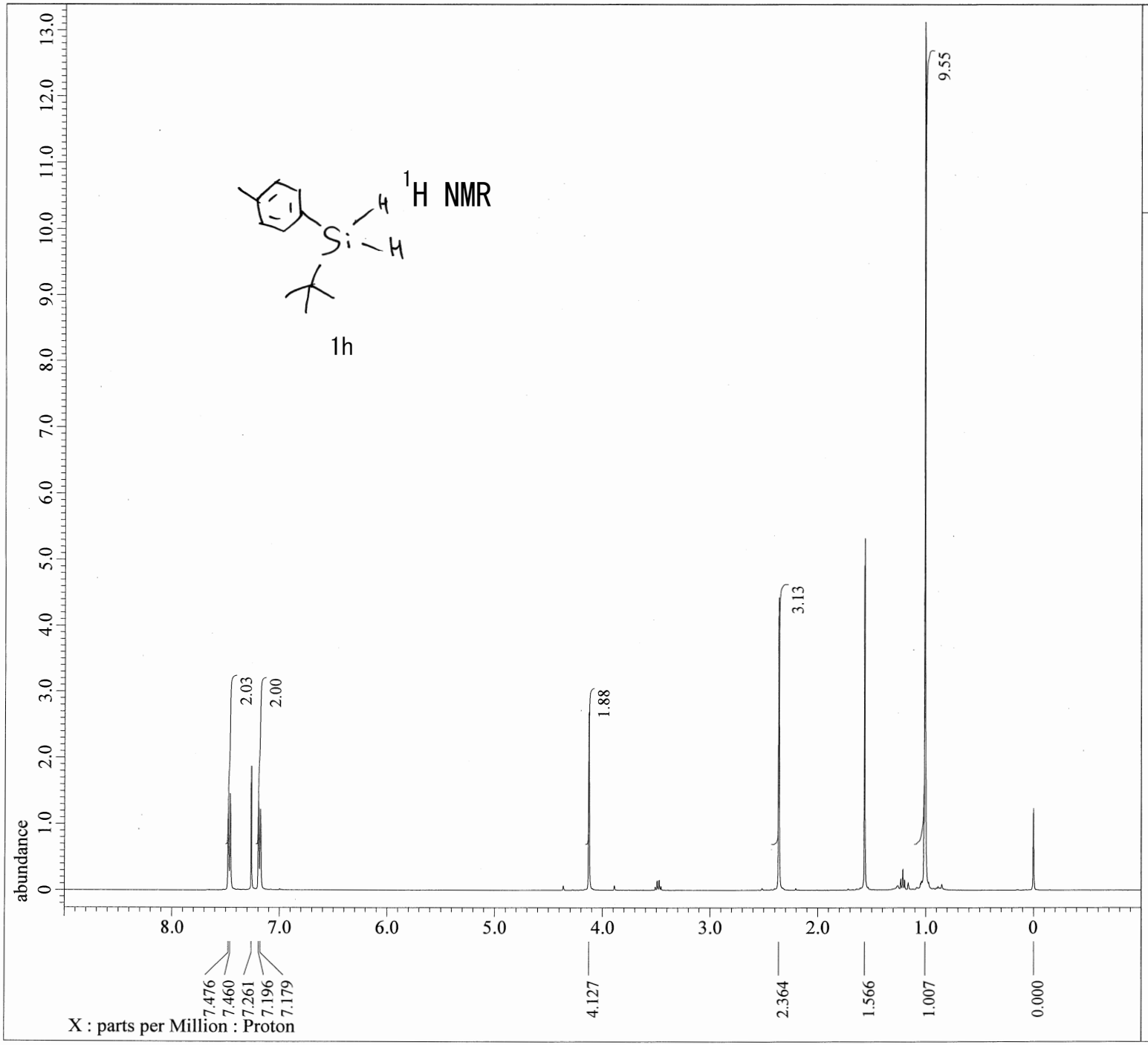

---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid3(0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: TKT-865-13C-1.jdf
Filename = TKT-865-13C-2.jdf
Author = element
Experiment = single_pulse_dec
Sample_Id = 2
Solvent = CHLOROFORM-D
Actual_Start_Time = 26-JAN-2021 21:08:24
Revision_Time = 26-JAN-2021 15:58:04
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 = 526
Total_Scans = 526
Relaxation_Delay = 2[s]
Recvr_Gain = 48
Temp_Get = 23[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]
13C NMR
OMe
OMe
Si
abundance
X : parts per Million : 13C
77.326
77.000
76.684
50.405
27.786
26.809
26.723
26.493
24.988
24.394
13.617
10.196




```
---- 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: TKT-869-1H_Proton-2-1.jdf
```

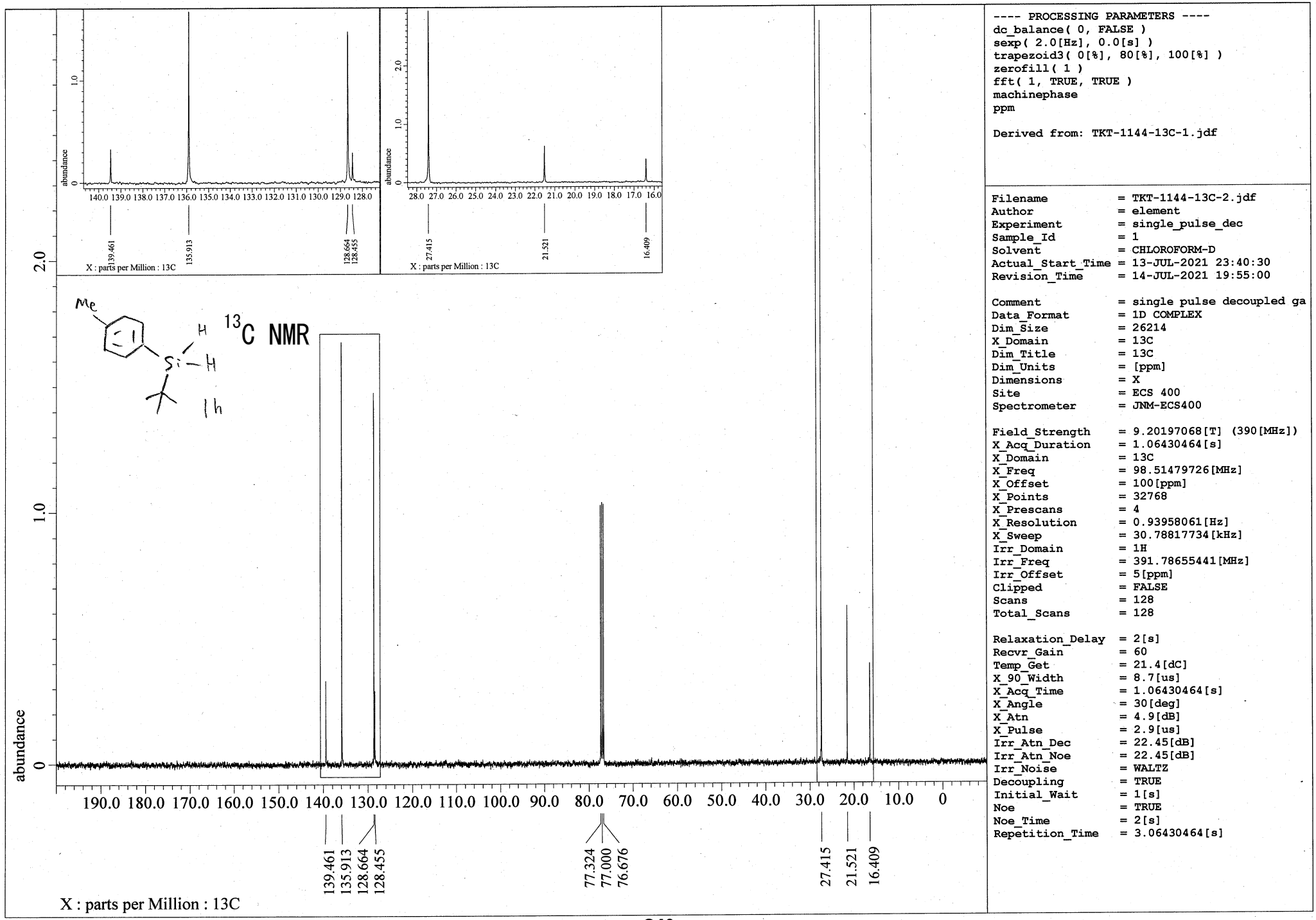
```
Filename            = TKT-869-1H_Proton-2-2.jdf
Author              = element
Experiment          = proton.jxp
Sample_Id           = TKT-869-1H
Solvent             = CHLOROFORM-D
Actual_Start_Time   = 25-JAN-2021 22:05:30
Revision_Time       = 30-JUL-2021 14:53:57

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          = 42
Temp_Get            = 18.6[dC]
X_90_Width          = 6[us]
X_Acq_Time          = 2.18103808[s]
X_Angle             = 45[deg]
X_Atn               = 0.8[dB]
X_Pulse             = 3[us]
Irr_Mode            = Off
Tri_Mode            = Off
Dante_Presat        = FALSE
Initial_Wait        = 1[s]
Repetition_Time     = 7.18103808[s]
```


---- 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: TKT-869-13C-1.jdf
Filename = TKT-869-13C-2.jdf
Author = element
Experiment = single_pulse_dec
Sample_Id = 6
Solvent = CHLOROFORM-D
Actual_Start_Time = 26-JAN-2021 11:27:36
Revision_Time = 26-JAN-2021 17:02:31
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 = 1024
Total_Scans = 1024
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 22.3[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]
13C NMR
1d
abundance
X : parts per Million : 13C
77.316
77.000
76.674
29.309
27.901
27.795
26.770
26.033
21.300
13.760
7.476



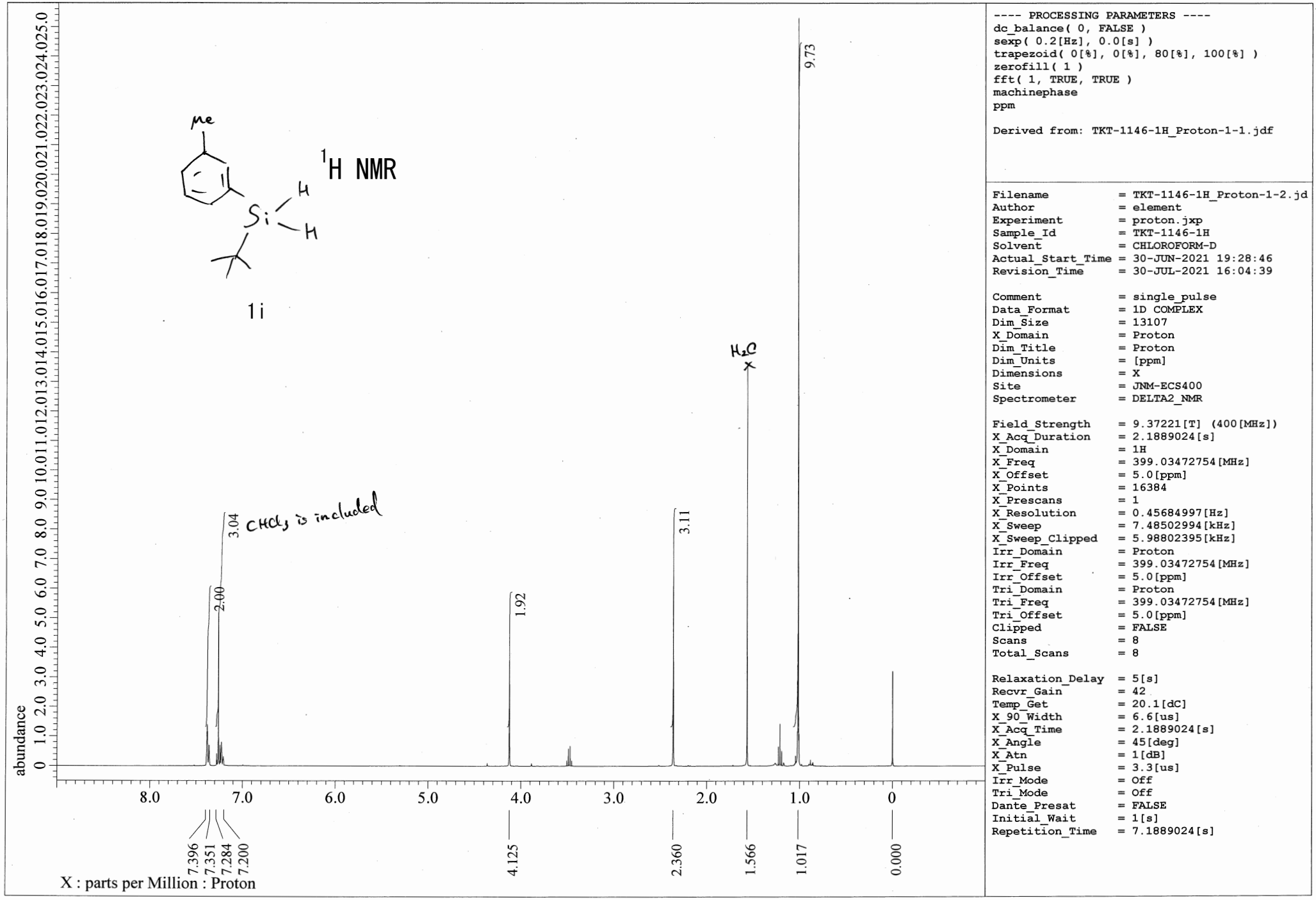

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: TKT-1144-1H_Proton-1-1.jdf
```

```
Filename            = TKT-1144-1H_Proton-1-2.jd
Author              = element
Experiment          = proton.jxp
Sample_Id           = TKT-1144-1H
Solvent             = CHLOROFORM-D
Actual_Start_Time   = 29-JUN-2021 18:48:10
Revision_Time       = 30-JUL-2021 15:58:16

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            = 19.3[dC]
X_90_Width          = 6[us]
X_Acq_Time          = 2.18103808[s]
X_Angle             = 45[deg]
X_Atn               = 0.8[dB]
X_Pulse             = 3[us]
Irr_Mode            = Off
Tri_Mode            = Off
Dante_Presat        = FALSE
Initial_Wait        = 1[s]
Repetition_Time     = 7.18103808[s]
```



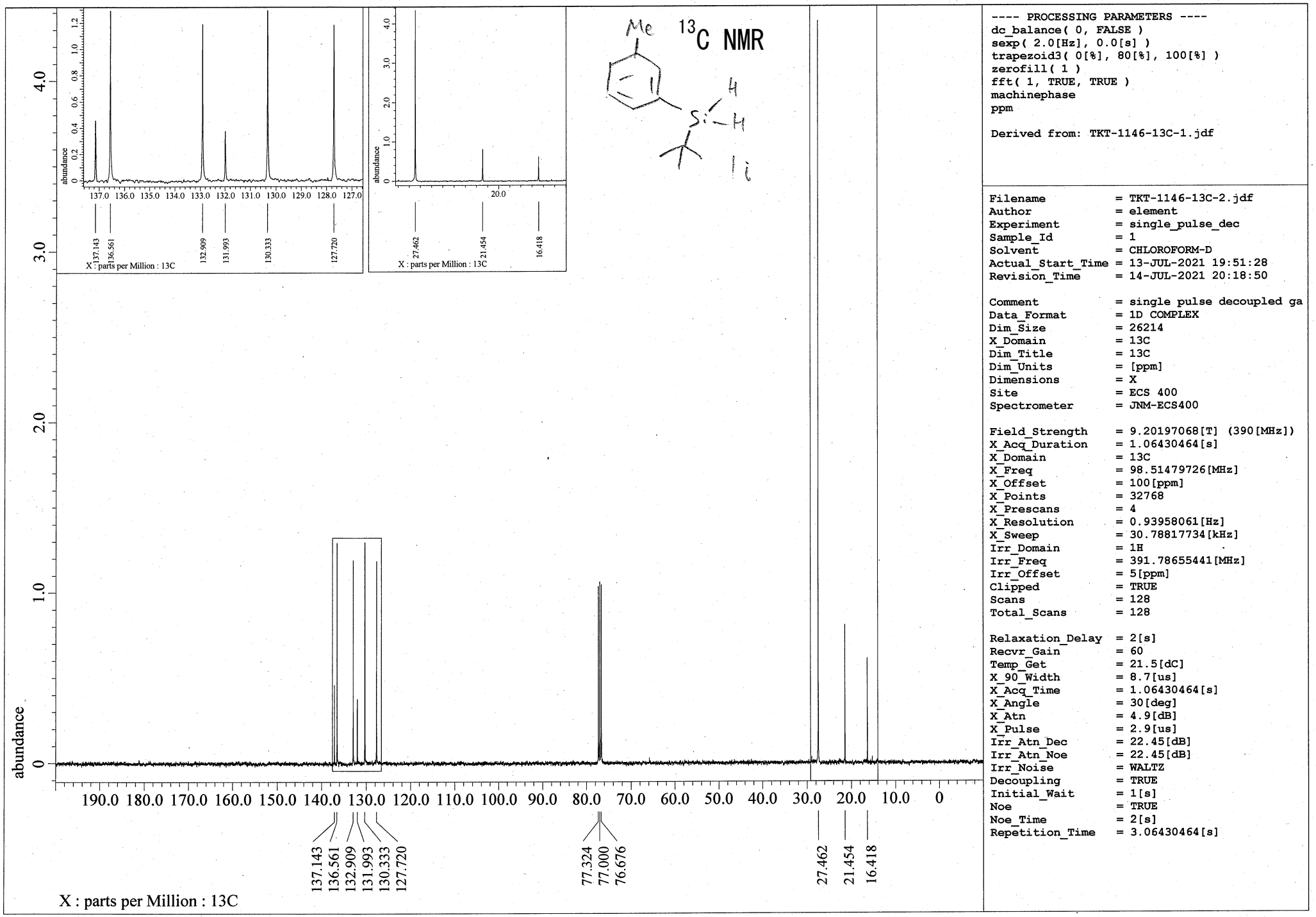

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: TKT-1144-13C-1.jdf
```

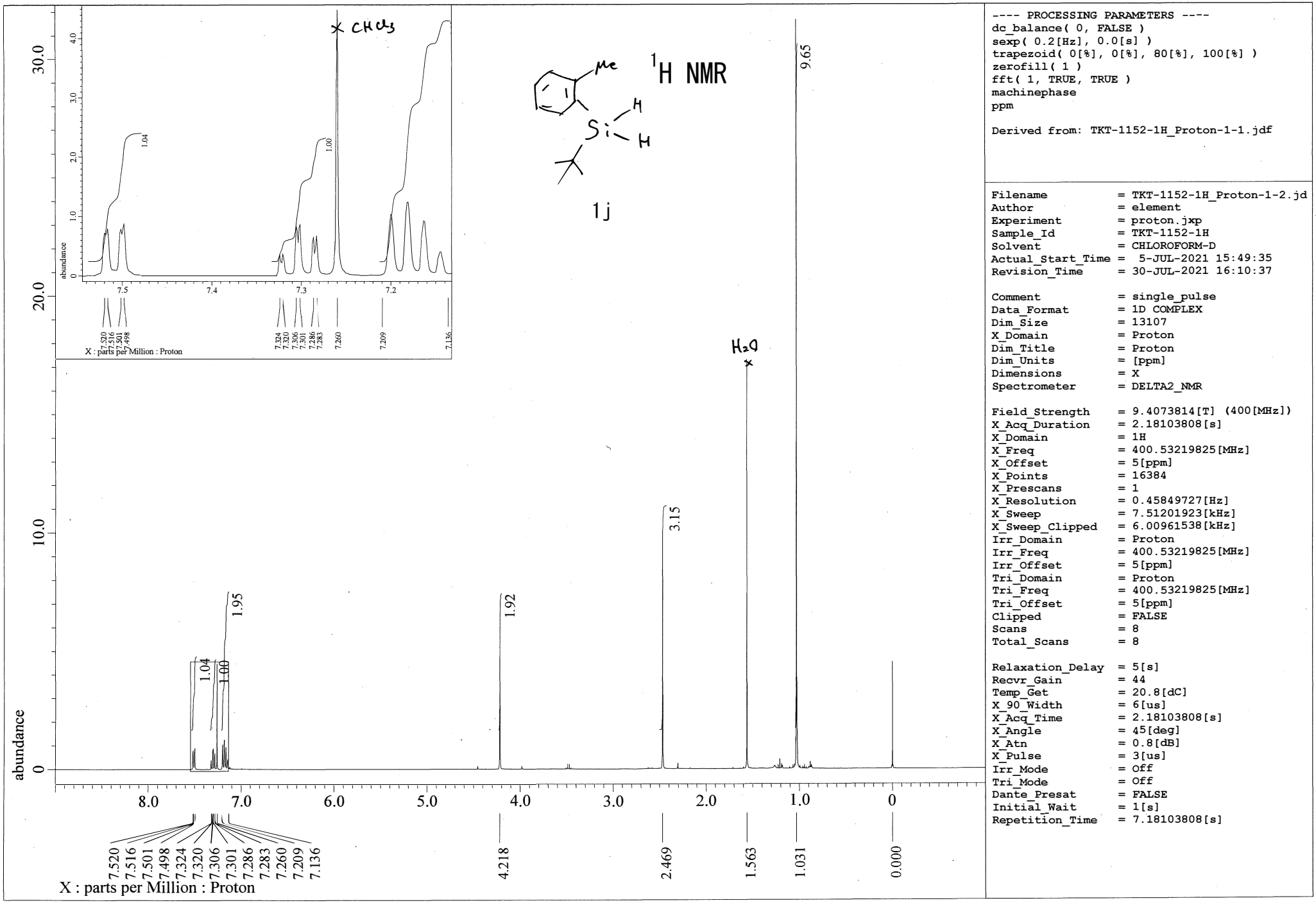
```
Filename            = TKT-1144-13C-2.jdf
Author              = element
Experiment          = single_pulse_dec
Sample_Id           = 1
Solvent             = CHLOROFORM-D
Actual_Start_Time   = 13-JUL-2021 23:40:30
Revision_Time       = 14-JUL-2021 19:55:00

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               = 128
Total_Scans         = 128

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

Derived from: TKT-1146-1H_Proton-1-1.jdf
```

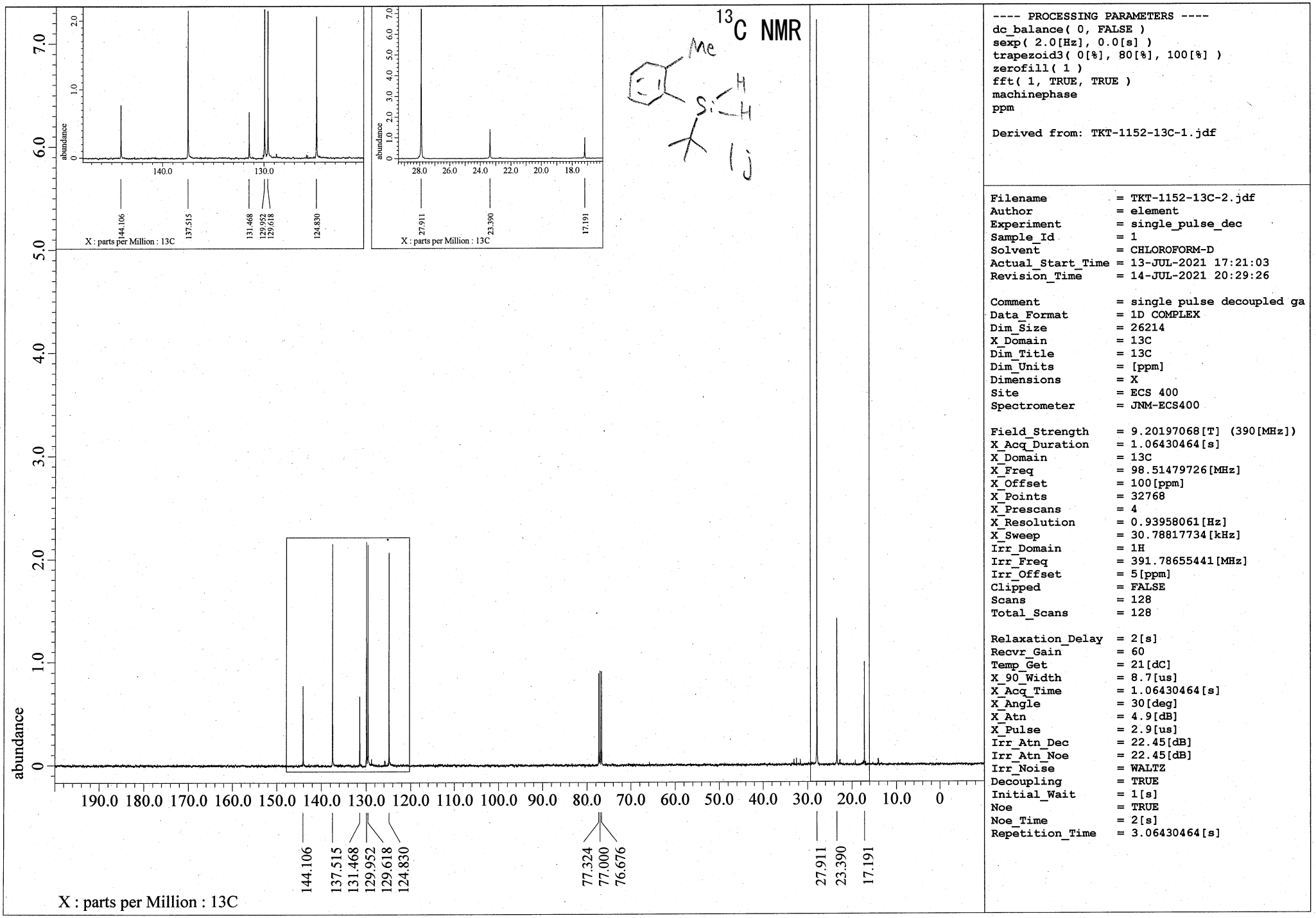
```
Filename            = TKT-1146-1H_Proton-1-2.jd
Author              = element
Experiment          = proton.jxp
Sample_Id           = TKT-1146-1H
Solvent             = CHLOROFORM-D
Actual_Start_Time   = 30-JUN-2021 19:28:46
Revision_Time       = 30-JUL-2021 16:04:39

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

Field_Strength      = 9.37221[T] (400[MHz])
X_Acq_Duration      = 2.1889024[s]
X_Domain            = 1H
X_Freq              = 399.03472754[MHz]
X_Offset            = 5.0[ppm]
X_Points            = 16384
X_Prescans          = 1
X_Resolution        = 0.45684997[Hz]
X_Sweep             = 7.48502994[kHz]
X_Sweep_Clipped     = 5.98802395[kHz]
Irr_Domain          = Proton
Irr_Freq            = 399.03472754[MHz]
Irr_Offset          = 5.0[ppm]
Tri_Domain          = Proton
Tri_Freq            = 399.03472754[MHz]
Tri_Offset          = 5.0[ppm]
Clipped             = FALSE
Scans               = 8
Total_Scans         = 8

Relaxation_Delay    = 5[s]
Recvr_Gain          = 42
Temp_Get            = 20.1[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]
```


13C NMR
Me
Si
H
H
abundance
X : parts per Million : 13C
137.143
136.561
132.909
131.993
130.333
127.720
77.324
77.000
76.676
27.462
21.454
16.418
---- 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: TKT-1146-13C-1.jdf
Filename = TKT-1146-13C-2.jdf
Author = element
Experiment = single_pulse_dec
Sample_Id = 1
Solvent = CHLOROFORM-D
Actual_Start_Time = 13-JUL-2021 19:51:28
Revision_Time = 14-JUL-2021 20:18:50
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 = TRUE
Scans = 128
Total_Scans = 128
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 21.5[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]



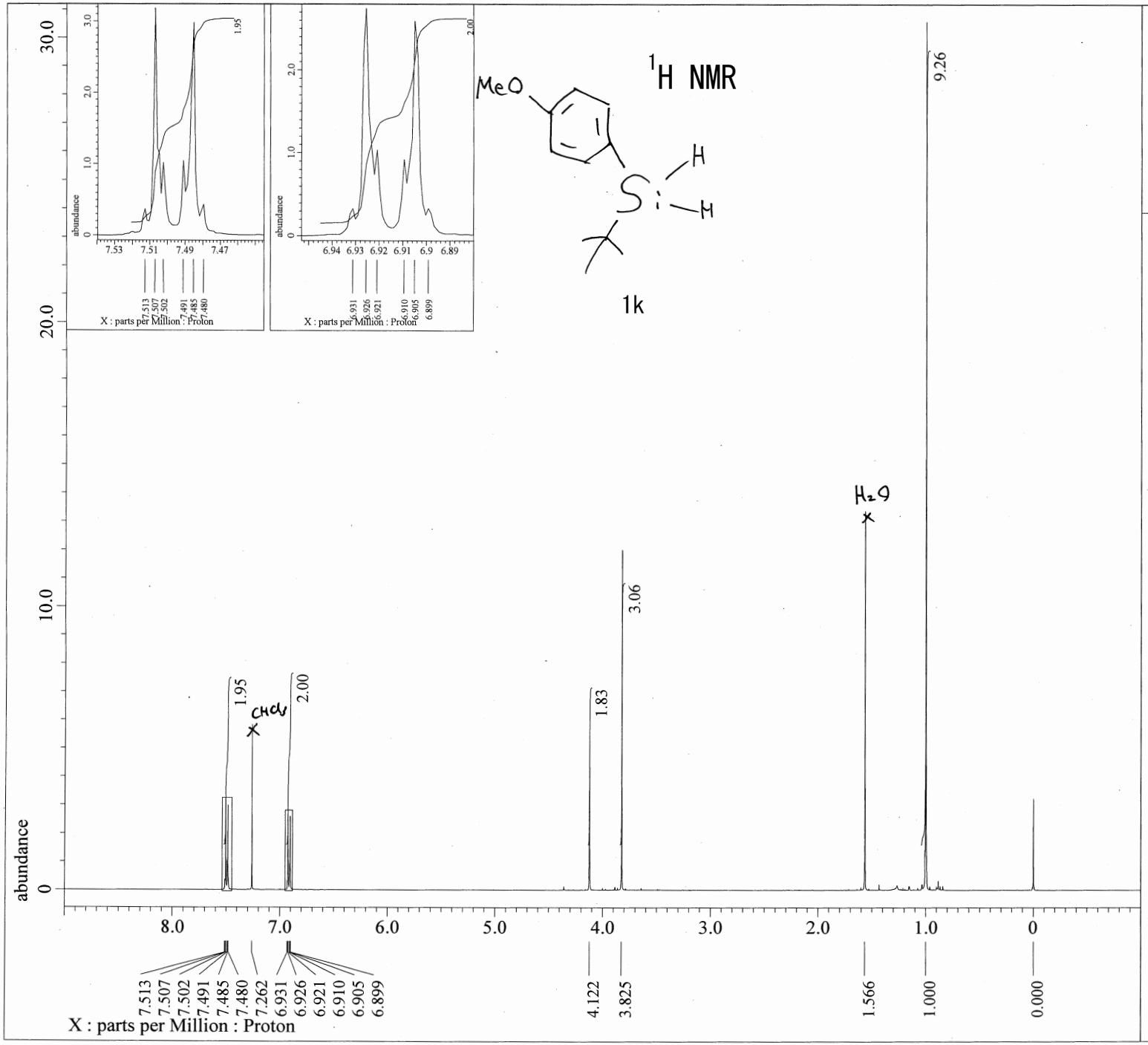

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: TKT-1152-1H_Proton-1-1.jdf
```

```
Filename            = TKT-1152-1H_Proton-1-2.jd
Author              = element
Experiment          = proton.jxp
Sample_Id           = TKT-1152-1H
Solvent             = CHLOROFORM-D
Actual_Start_Time   =  5-JUL-2021 15:49:35
Revision_Time       = 30-JUL-2021 16:10:37

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            = 20.8[dC]
X_90_Width          = 6[us]
X_Acq_Time          = 2.18103808[s]
X_Angle             = 45[deg]
X_Atn               = 0.8[dB]
X_Pulse             = 3[us]
Irr_Mode            = Off
Tri_Mode            = Off
Dante_Presat        = FALSE
Initial_Wait        = 1[s]
Repetition_Time     = 7.18103808[s]
```



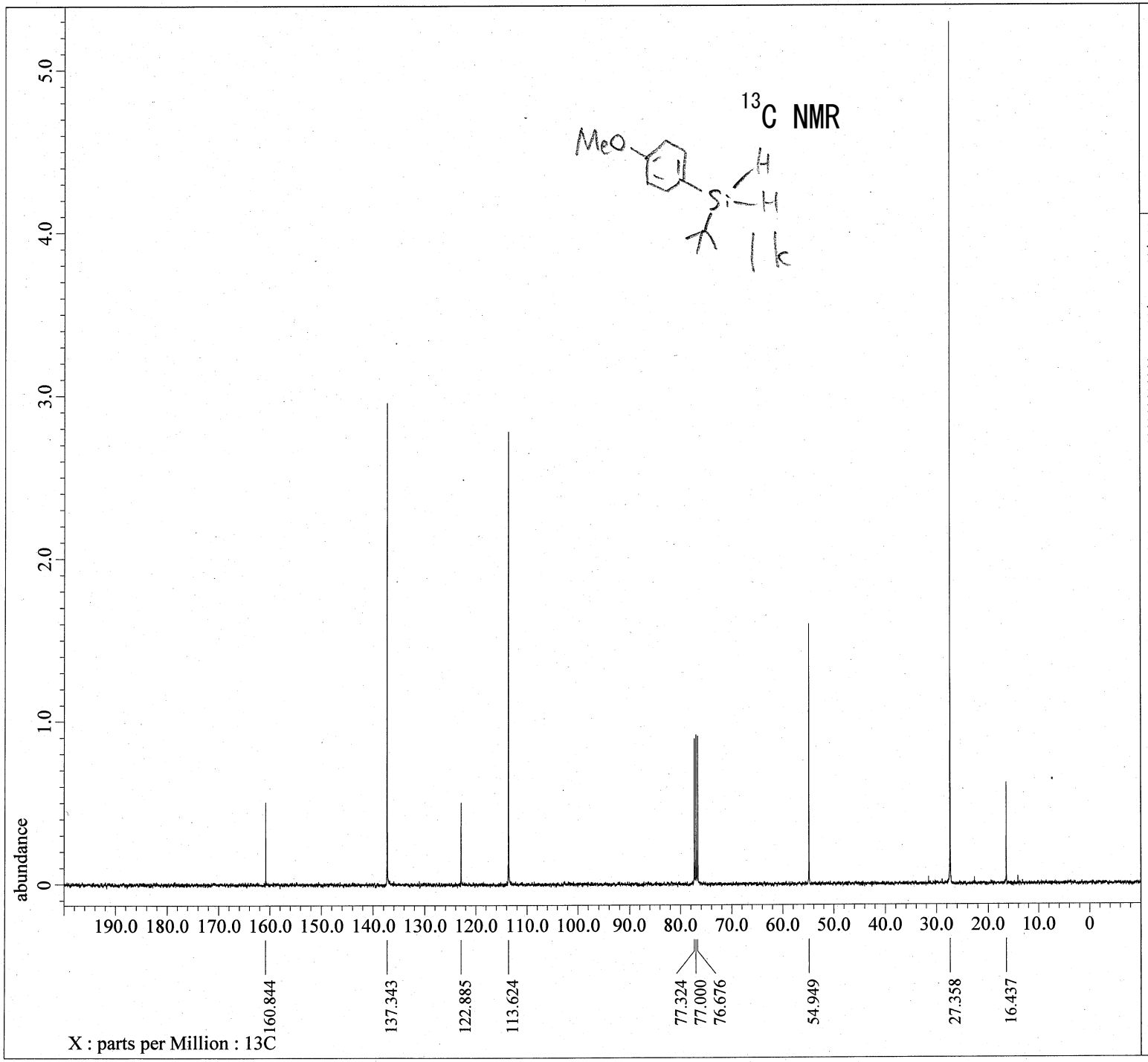

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: TKT-1152-13C-1.jdf
```

Filename	= TKT-1152-13C-2.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= 1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 13-JUL-2021 17:21:03
Revision_Time	= 14-JUL-2021 20:29:26
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	= 128
Total_Scans	= 128
Relaxation_Delay	= 2[s]
Recvr_Gain	= 60
Temp_Get	= 21[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]



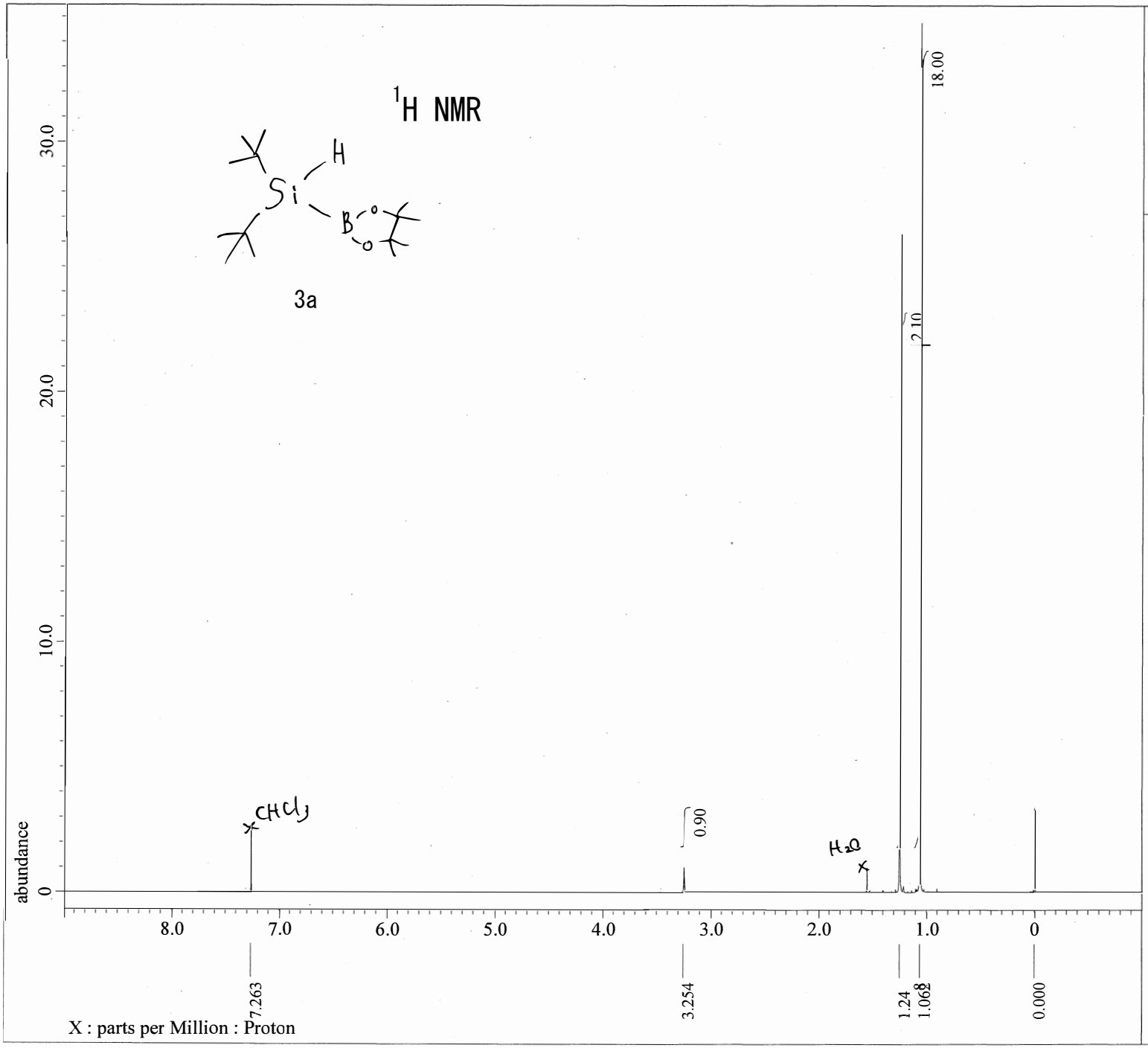

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: TKT-1149-1H_Proton-1-1.jdf
```

```
Filename            = TKT-1149-1H_Proton-1-2.jd
Author              = element
Experiment          = proton.jxp
Sample_Id           = TKT-1149-1H
Solvent             = CHLOROFORM-D
Actual_Start_Time   =  1-JUL-2021 22:43:27
Revision_Time       = 30-JUL-2021 16:14:39

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

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

Relaxation_Delay    = 5[s]
Recvr_Gain          = 44
Temp_Get            = 20.6[dC]
X_90_Width          = 6[us]
X_Acq_Time          = 2.18103808[s]
X_Angle             = 45[deg]
X_Atn               = 0.8[dB]
X_Pulse             = 3[us]
Irr_Mode            = Off
Tri_Mode            = Off
Dante_Presat        = FALSE
Initial_Wait        = 1[s]
Repetition_Time     = 7.18103808[s]
```



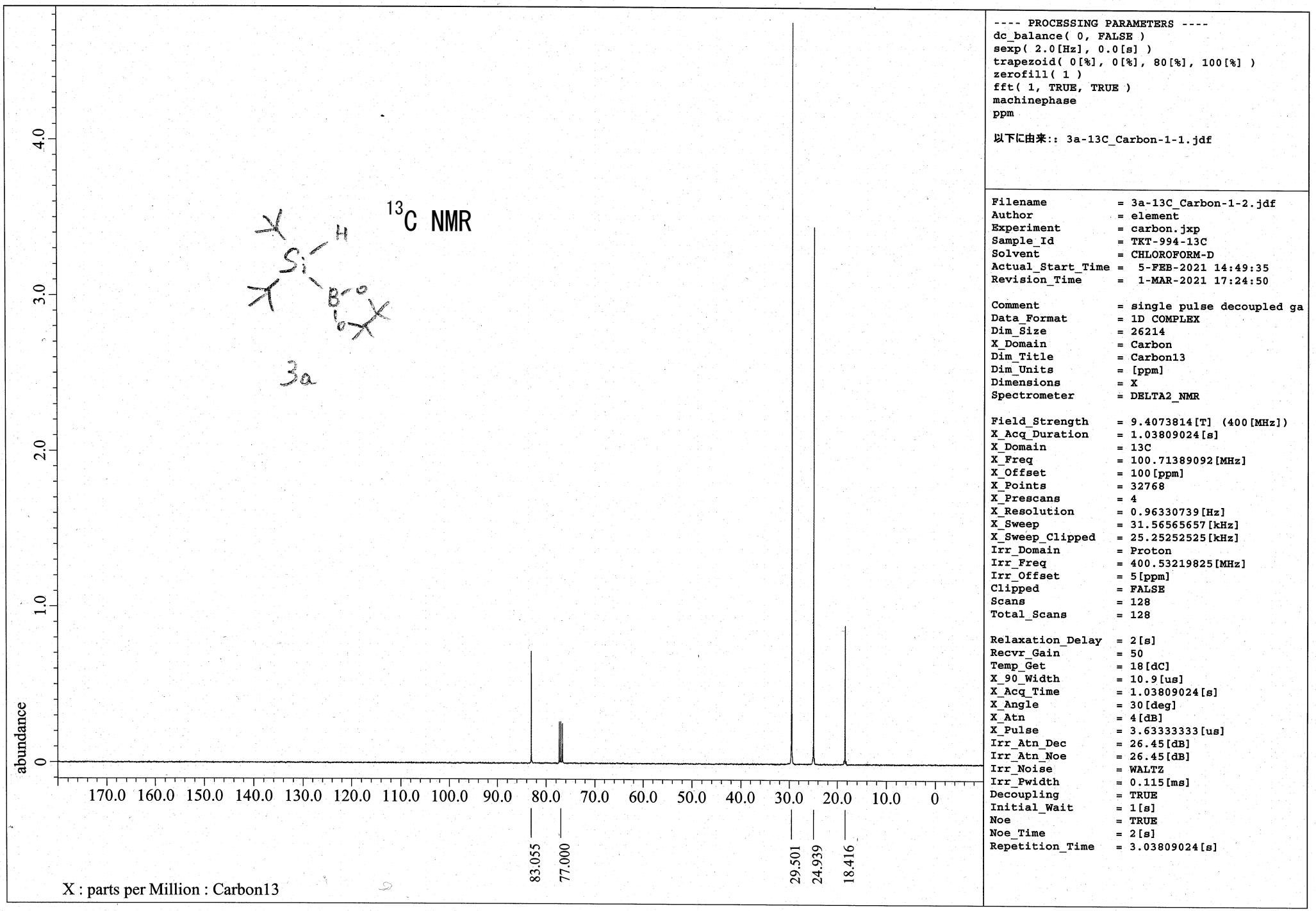

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: TKT-1149-13C-1.jdf
```

```
Filename            = TKT-1149-13C-2.jdf
Author              = element
Experiment          = single_pulse_dec
Sample_Id           = 1
Solvent             = CHLOROFORM-D
Actual_Start_Time   = 14-JUL-2021 00:26:24
Revision_Time       = 14-JUL-2021 20:43:34

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               = 128
Total_Scans         = 128

Relaxation_Delay    = 2[s]
Recvr_Gain          = 60
Temp_Get            = 21.5[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]
```



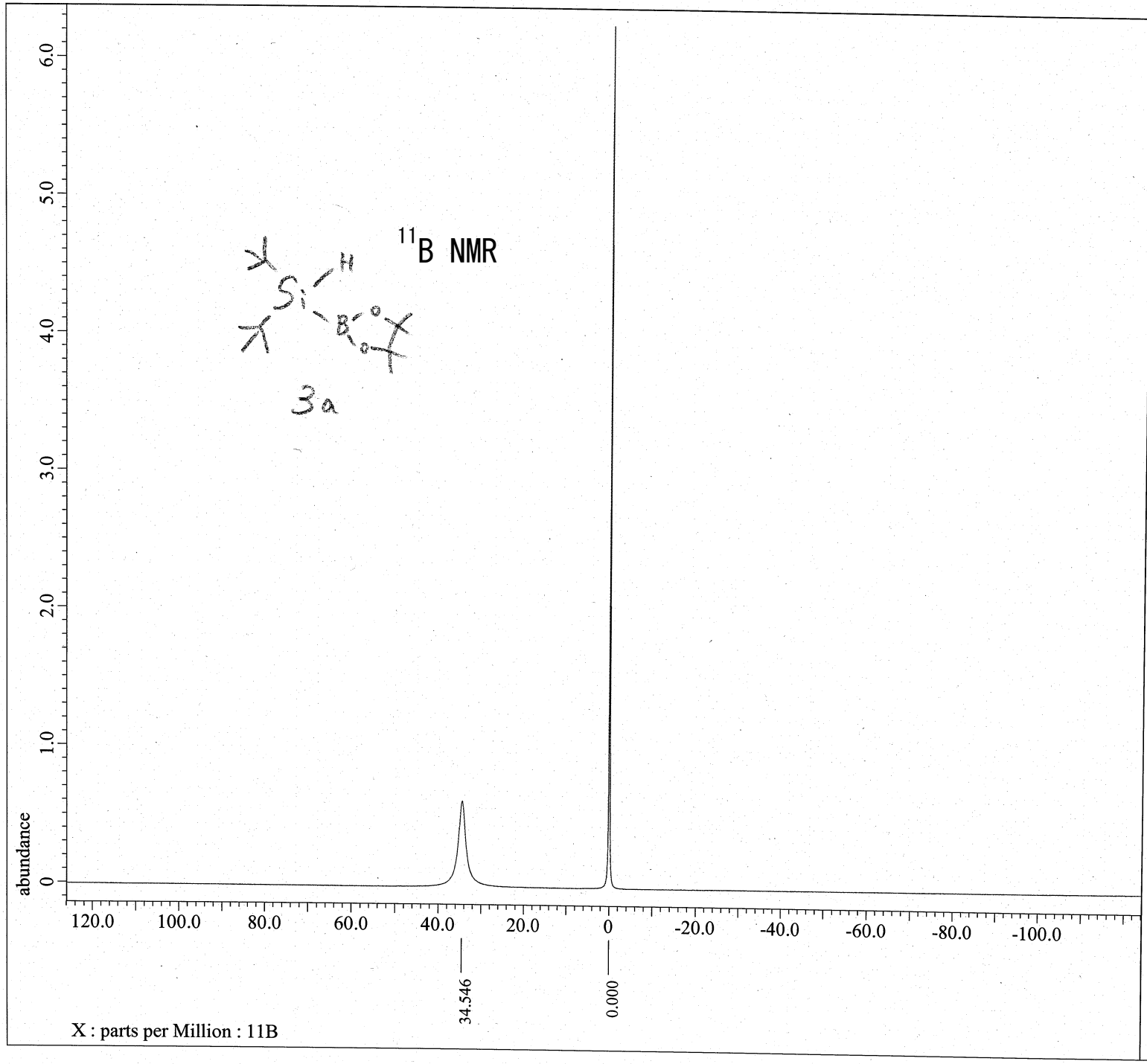

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: 3a-1H.jdf
```

```
Filename            = 3a-1H-1.jdf
Author              = element
Experiment          = proton.jxp
Sample_Id           = TKT-929-1H
Solvent             = CHLOROFORM-D
Actual_Start_Time   =  1-DEC-2020 17:38:51
Revision_Time       = 30-JUL-2021 16:49:59

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



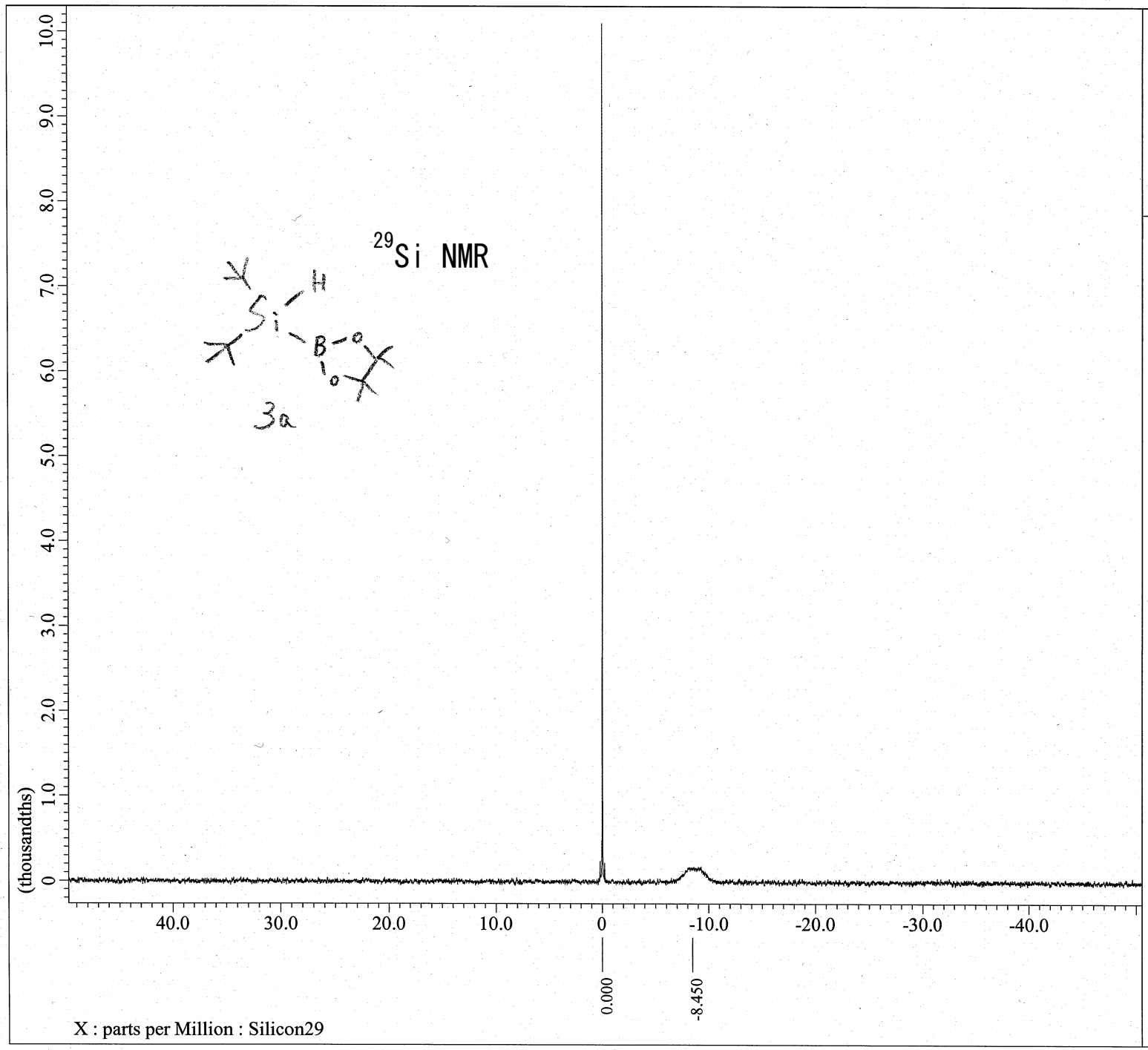

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

以下に由来:: 3a-13C_Carbon-1-1.jdf
```

Filename	= 3a-13C_Carbon-1-2.jdf
Author	= element
Experiment	= carbon.jxp
Sample_Id	= TKT-994-13C
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 5-FEB-2021 14:49:35
Revision_Time	= 1-MAR-2021 17:24:50
Comment	= single pulse decoupled ga
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.4073814[T] (400[MHz])
X_Acq_Duration	= 1.03809024[s]
X_Domain	= 13C
X_Freq	= 100.71389092[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.96330739[Hz]
X_Sweep	= 31.56565657[kHz]
X_Sweep_Clipped	= 25.25252525[kHz]
Irr_Domain	= Proton
Irr_Freq	= 400.53219825[MHz]
Irr_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 128
Total_Scans	= 128
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 18[dC]
X_90_Width	= 10.9[us]
X_Acq_Time	= 1.03809024[s]
X_Angle	= 30[deg]
X_Atn	= 4[dB]
X_Pulse	= 3.63333333[us]
Irr_Atn_Dec	= 26.45[dB]
Irr_Atn_Noe	= 26.45[dB]
Irr_Noise	= WALTZ
Irr_Pwidth	= 0.115[ms]
Decoupling	= TRUE
Initial_Wait	= 1[s]
Noe	= TRUE
Noe_Time	= 2[s]
Repetition_Time	= 3.03809024[s]



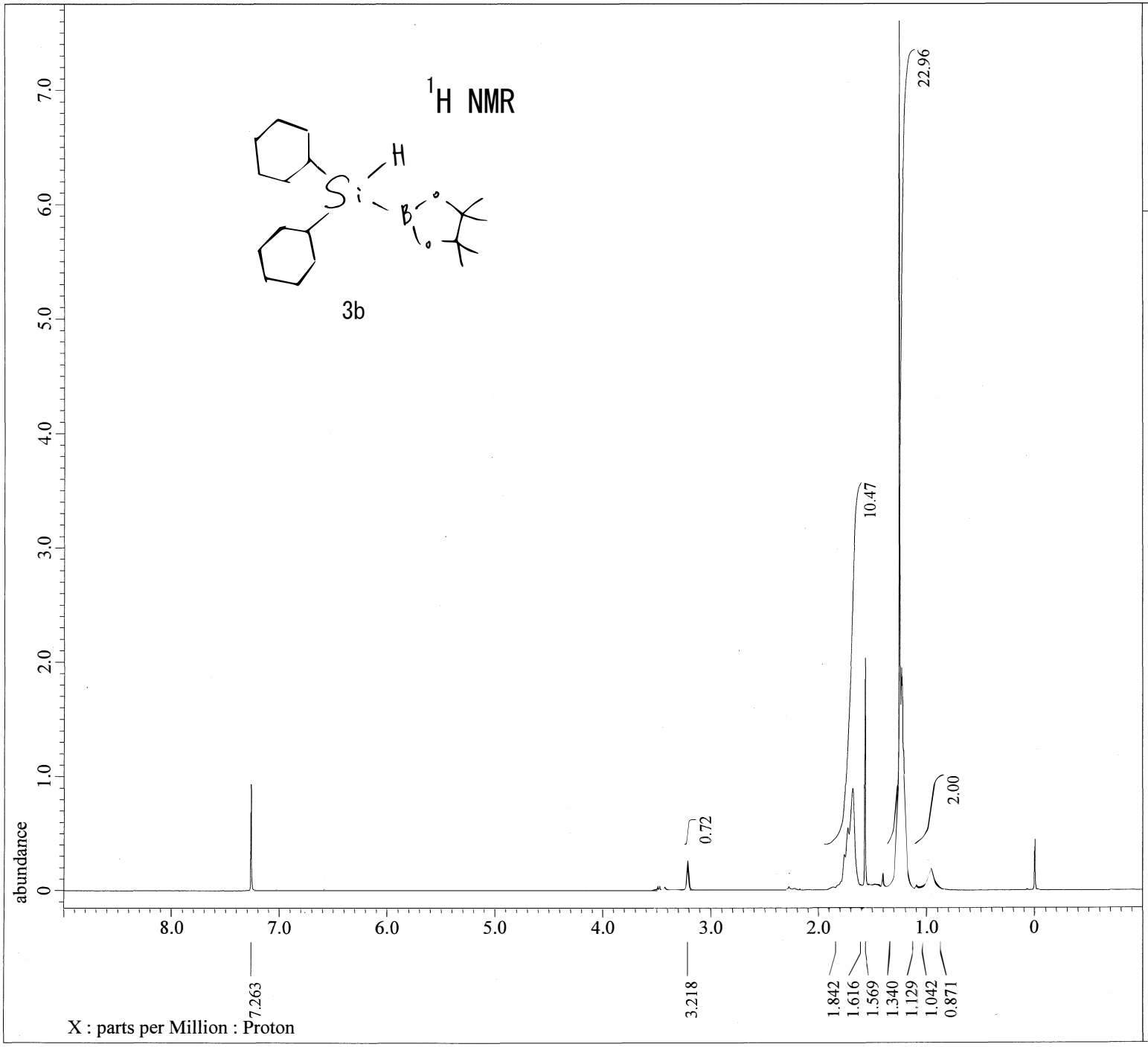

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

以下に由来:: 3a-11B-1.jdf
```

Filename	= 3a-11B-2.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= 1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 5-FEB-2021 21:53:15
Revision_Time	= 1-MAR-2021 17:25:56
Comment	= single pulse decoupled ga
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= 11B
Dim_Title	= 11B
Dim_Units	= [ppm]
Dimensions	= X
Site	= ECS 400
Spectrometer	= JNM-ECS400
Field_Strength	= 9.20197068[T] (390[MHz])
X_Acq_Duration	= 0.83361792[s]
X_Domain	= 11B
X_Freq	= 125.70081325[MHz]
X_Offset	= 0[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 1.19959034[Hz]
X_Sweep	= 39.3081761[kHz]
Irr_Domain	= 1H
Irr_Freq	= 391.78655441[MHz]
Irr_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 962
Total_Scans	= 962
Relaxation_Delay	= 2[s]
Recvr_Gain	= 42
Temp_Get	= 18.4[dC]
X_90_Width	= 10[us]
X_Acq_Time	= 0.83361792[s]
X_Angle	= 30[deg]
X_Atn	= 5.5[dB]
X_Pulse	= 3.33333333[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	= 2.83361792[s]



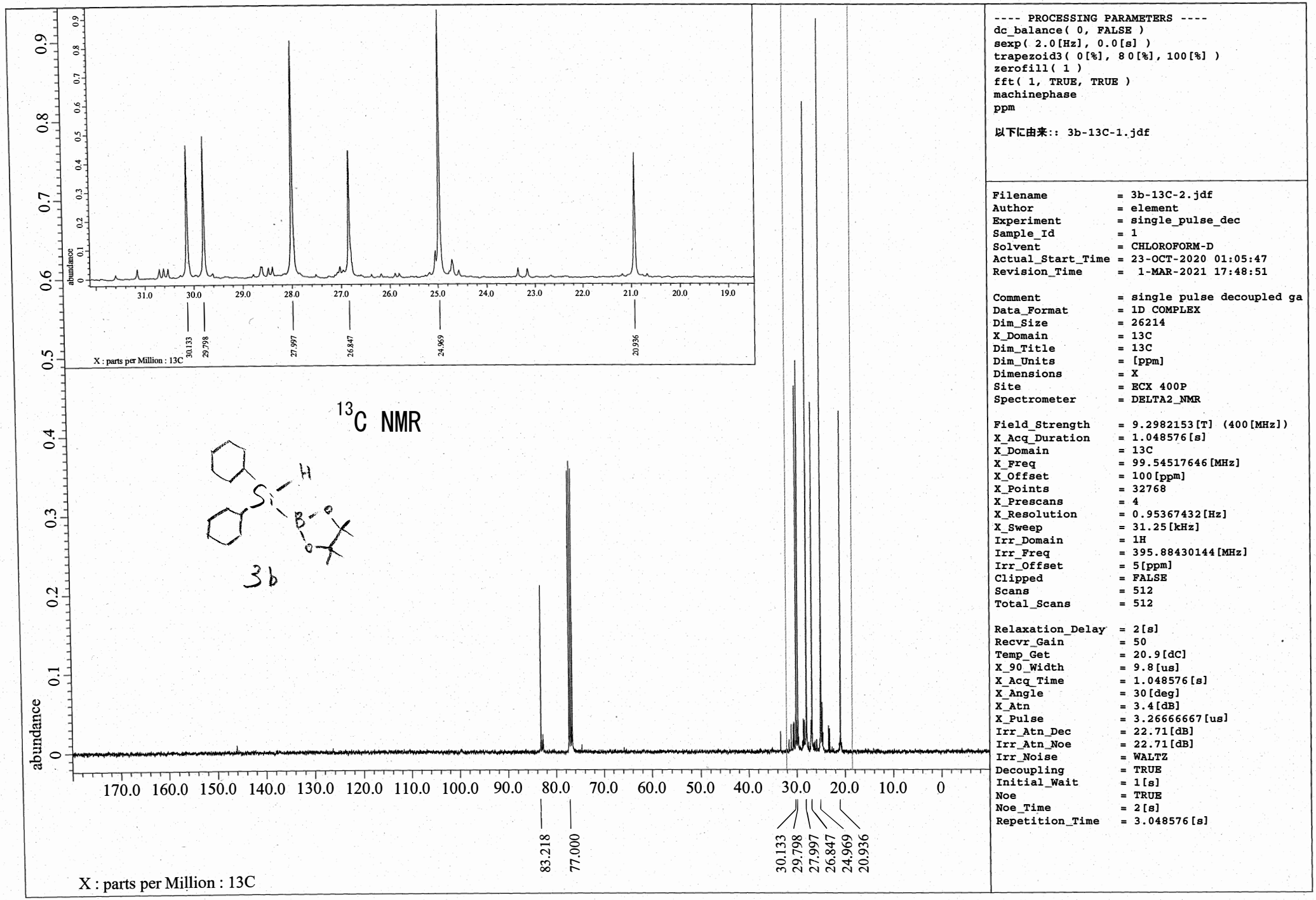

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

以下に由来:: 3a-29Si-re_single_pulse_dec-1-1.jdf
```

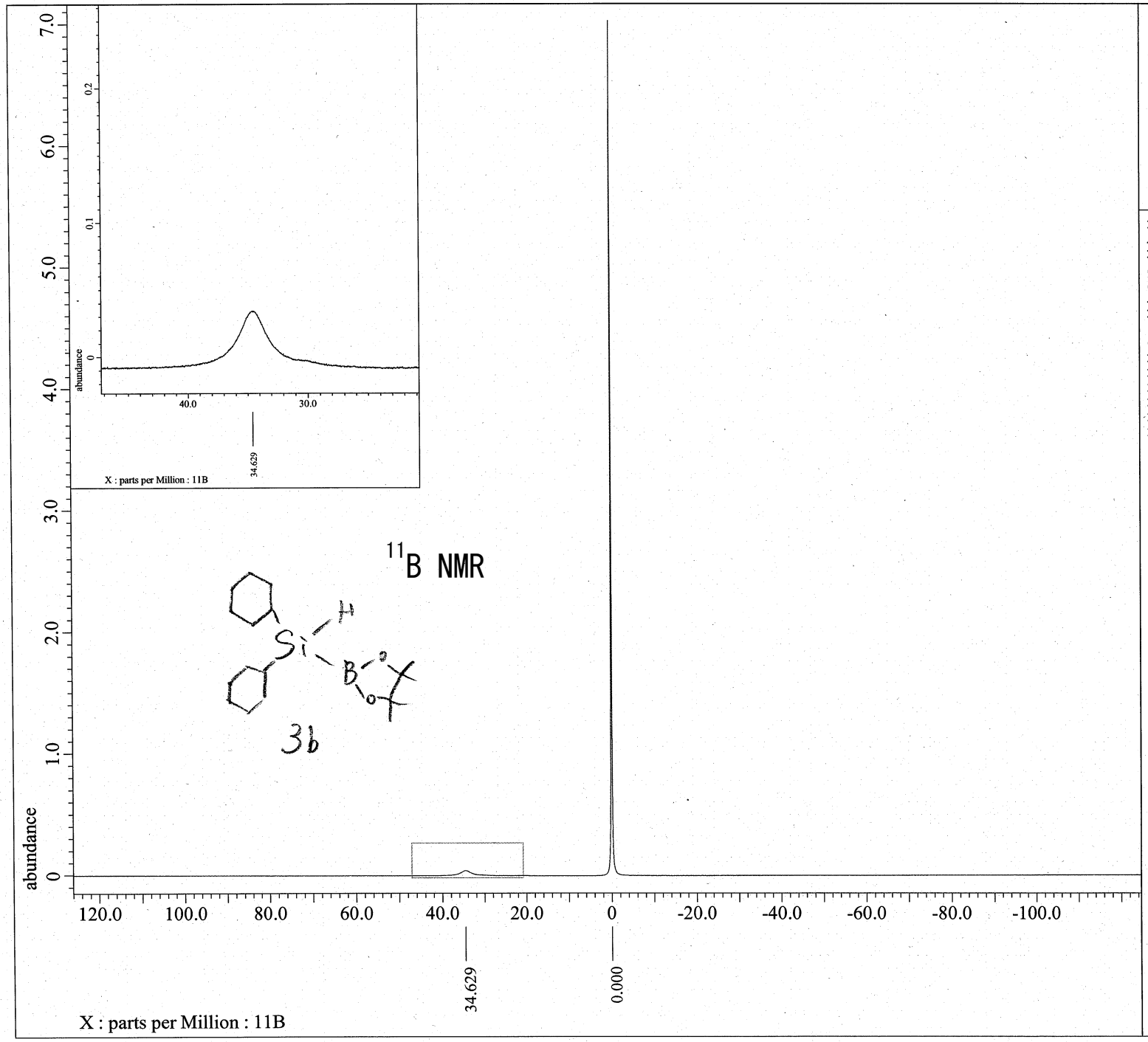
Filename	= 3a-29Si-re_single_
Author	= element
Experiment	= single_pulse_dec.j
Sample_Id	= TKT-994-29Si-re
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 12-FEB-2021 18:06:
Revision_Time	= 1-MAR-2021 17:27:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Silicon29
Dim_Title	= Silicon29
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (60
X_Acq_Duration	= 2.19152384[s]
X_Domain	= Silicon29
X_Freq	= 119.23728868[MHz]
X_Offset	= 0[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.4563035[Hz]
X_Sweep	= 14.95215311[kHz]
X_Sweep_Clipped	= 11.96172249[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 5[us]
Clipped	= FALSE
Scans	= 5000
Total_Scans	= 5000
Relaxation_Delay	= 10[s]
Recvr_Gain	= 56
Temp_Get	= 16.7[dC]
X_90_Width	= 10[us]
X_Acq_Time	= 2.19152384[s]
X_Angle	= 30[deg]
X_Atn	= 9[dB]
X_Pulse	= 3.33333333[us]
Irr_Atn_Dec	= 26.628[dB]
Irr_Atn_Dec_Calc	= 26.628[dB]
Irr_Atn_Dec_Default_Calc	= 26.628[dB]
Irr_Dec_Bandwidth_Hz	= 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.05794078[ppm]
Irr_Dec_Freq	= 600.1723046[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= FALSE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]




```
---- 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: 3b-1H_Proton-1-1.jdf
```

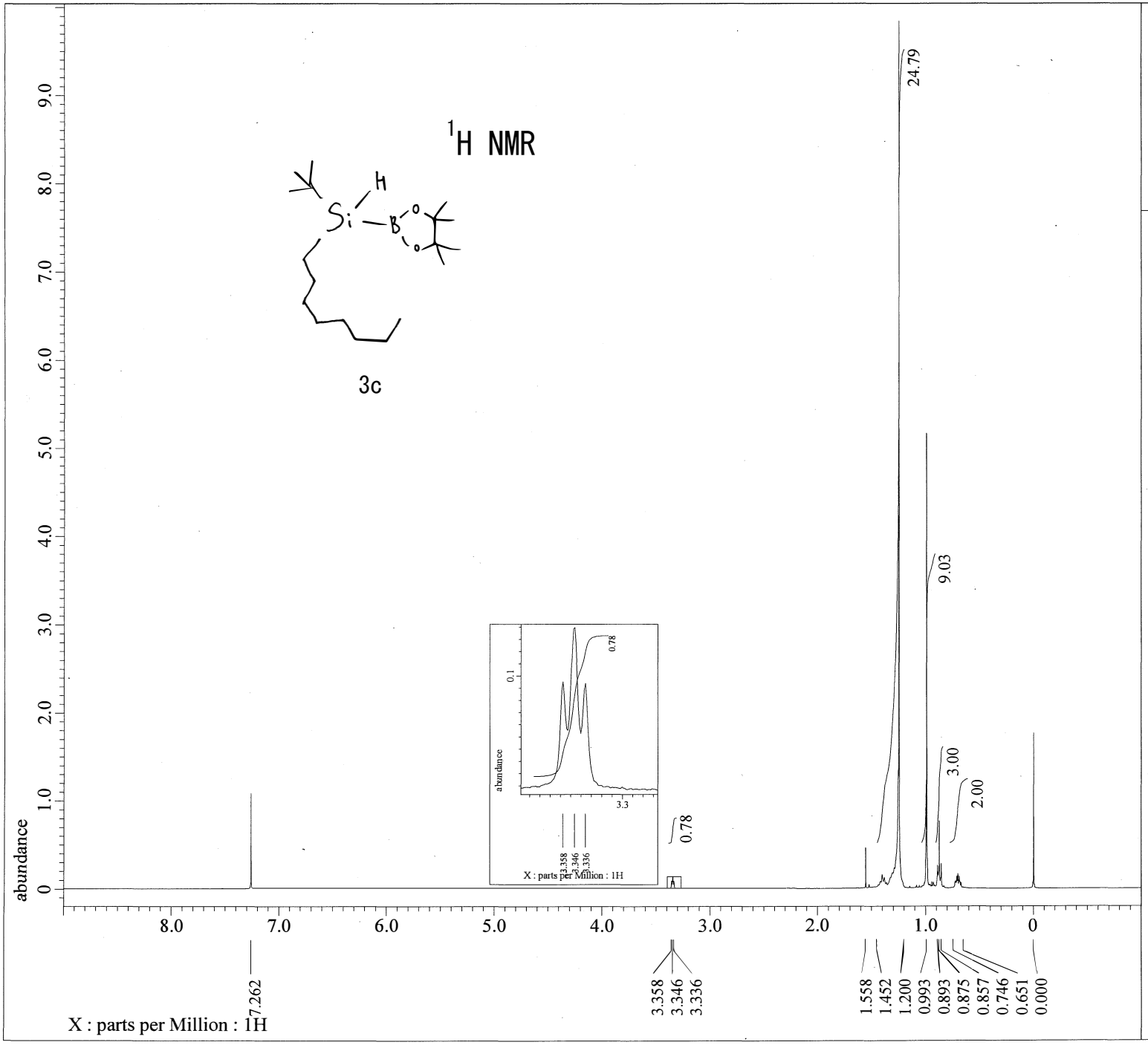
```
Filename            = 3b-1H_Proton-1-2.jdf
Author              = element
Experiment          = proton.jxp
Sample_Id           = TKT-893-1H
Solvent             = CHLOROFORM-D
Actual_Start_Time   = 22-OCT-2020 16:55:25
Revision_Time       = 30-JUL-2021 16:54:27

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            = 19.6[dC]
X_90_Width          = 6[us]
X_Acq_Time          = 2.18103808[s]
X_Angle             = 45[deg]
X_Atn               = 0.8[dB]
X_Pulse             = 3[us]
Irr_Mode            = Off
Tri_Mode            = Off
Dante_Presat        = FALSE
Initial_Wait        = 1[s]
Repetition_Time     = 7.18103808[s]
```


13C NMR
3b
abundance
X : parts per Million : 13C
83.218
77.000
30.133
29.798
27.997
26.847
24.969
20.936
---- 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:: 3b-13C-1.jdf
Filename = 3b-13C-2.jdf
Author = element
Experiment = single_pulse_dec
Sample_Id = 1
Solvent = CHLOROFORM-D
Actual_Start_Time = 23-OCT-2020 01:05:47
Revision_Time = 1-MAR-2021 17:48:51
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 = 512
Total_Scans = 512
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 20.9[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]



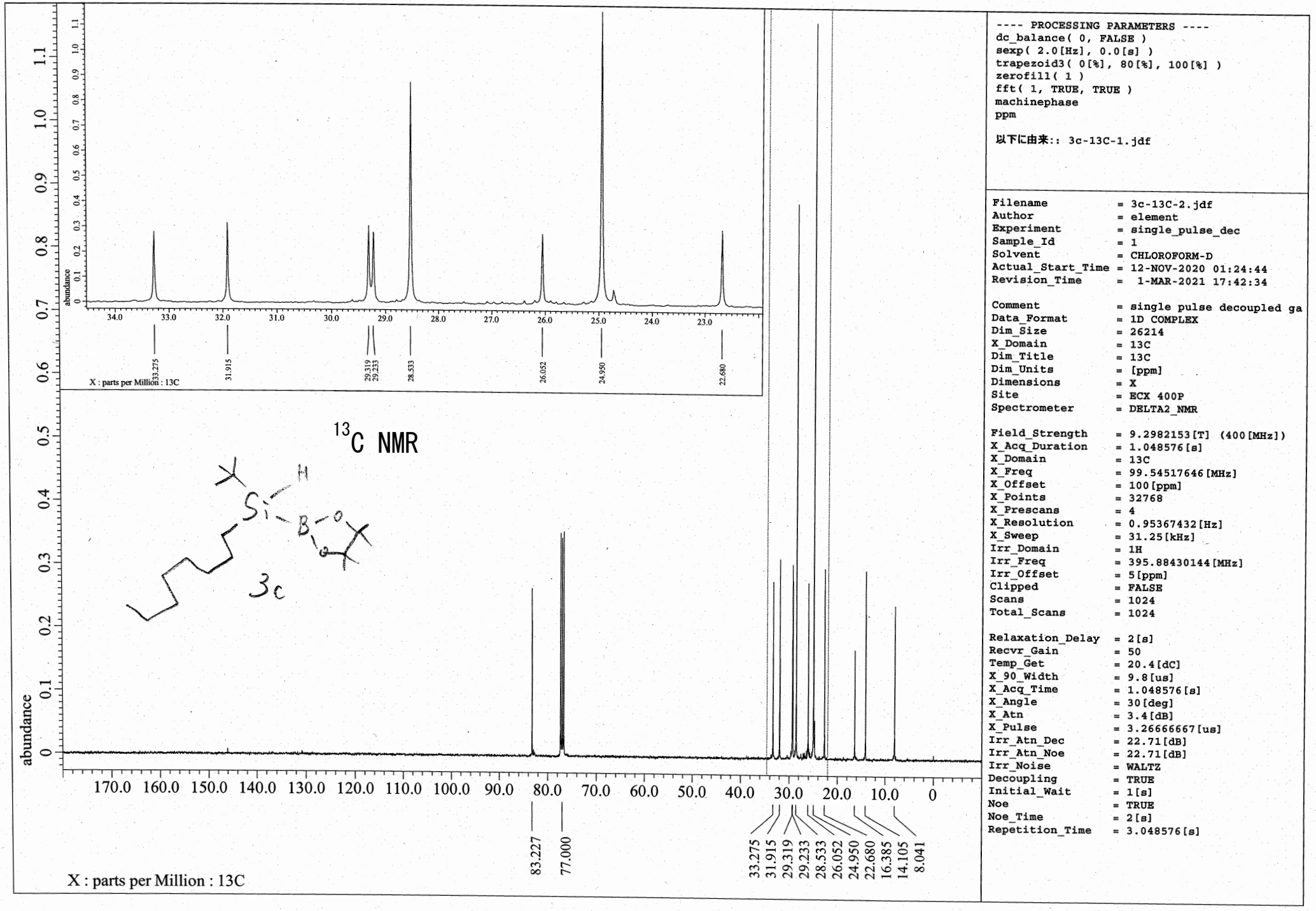

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

以下に由来:: 3b-11B-1.jdf
```

```
Filename            = 3b-11B-2.jdf
Author              = element
Experiment          = single_pulse_dec
Sample_Id           = S#624409
Solvent             = CHLOROFORM-D
Actual_Start_Time   = 25-FEB-2021 01:30:25
Revision_Time       =  1-MAR-2021 17:50:06

Comment             = single pulse decoupled ga
Data_Format         = 1D COMPLEX
Dim_Size            = 52428
X_Domain            = 11B
Dim_Title           = 11B
Dim_Units           = [ppm]
Dimensions          = X
Site                = ECX 400P
Spectrometer        = DELTA2_NMR

Field_Strength      = 9.2982153[T] (400[MHz])
X_Acq_Duration      = 1.64626432[s]
X_Domain            = 11B
X_Freq              = 127.01553457[MHz]
X_Offset            = 0[ppm]
X_Points            = 65536
X_Prescans          = 4
X_Resolution        = 0.60743587[Hz]
X_Sweep             = 39.8089172[kHz]
Irr_Domain          = 1H
Irr_Freq            = 395.88430144[MHz]
Irr_Offset          = 5[ppm]
Clipped             = FALSE
Scans               = 1883
Total_Scans         = 1883

Relaxation_Delay    = 2[s]
Recvr_Gain          = 50
Temp_Get            = 19.5[dC]
X_90_Width          = 10[us]
X_Acq_Time          = 1.64626432[s]
X_Angle             = 30[deg]
X_Atn               = 4.8[dB]
X_Pulse             = 3.33333333[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     = 3.64626432[s]
```



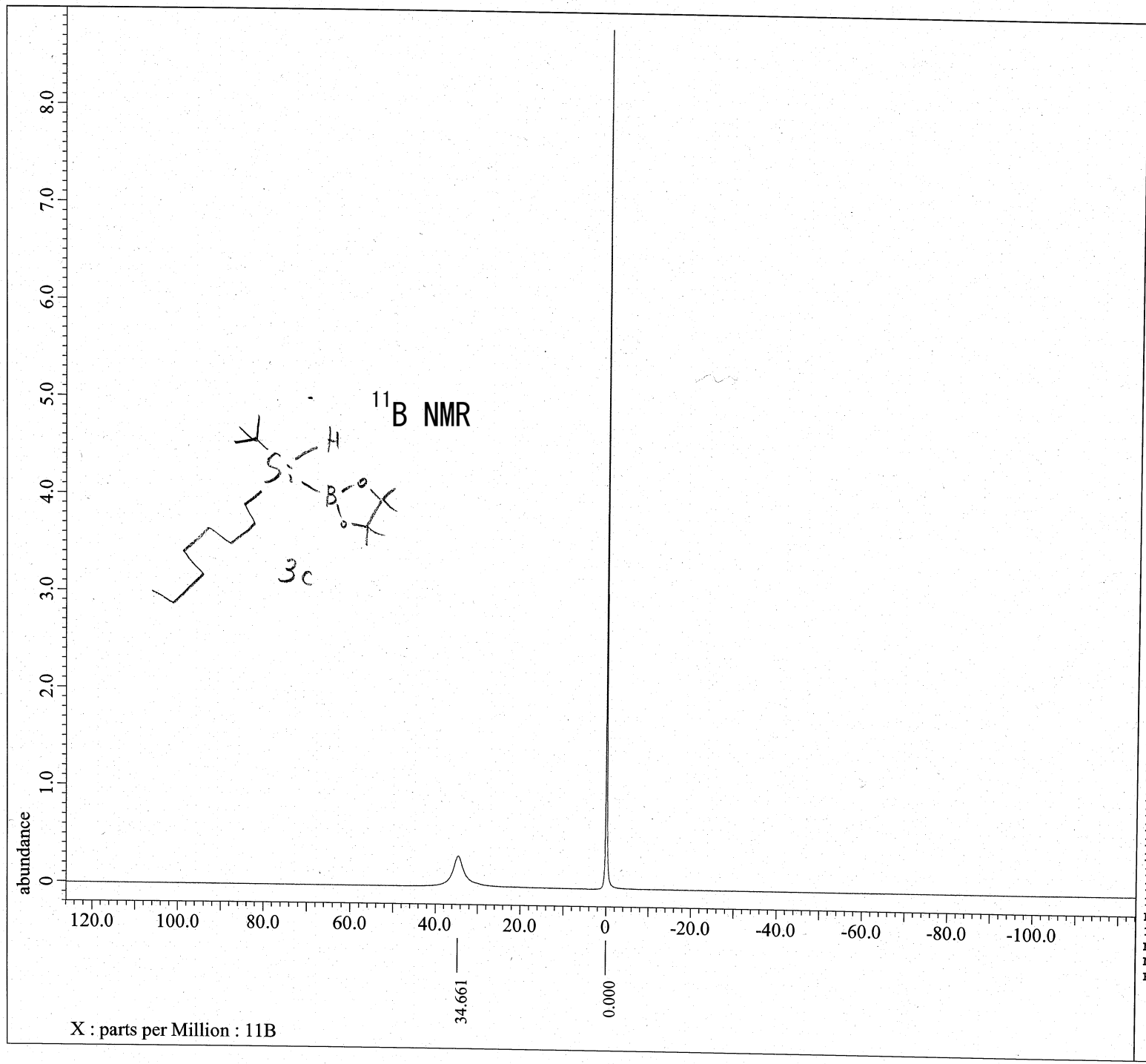

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: 3c-1H-1.jdf
```

Filename	= 3c-1H-2.jdf
Author	= element
Experiment	= single_pulse.ex2
Sample_Id	= S#617266
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 12-NOV-2020 01:19:32
Revision_Time	= 30-JUL-2021 17:01:59
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= 1H
Dim_Title	= 1H
Dim_Units	= [ppm]
Dimensions	= X
Site	= ECX 400P
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.2982153[T] (400[MHz])
X_Acq_Duration	= 2.20725248[s]
X_Domain	= 1H
X_Freq	= 395.88430144[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45305193[Hz]
X_Sweep	= 7.42280285[kHz]
Irr_Domain	= 1H
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= 1H
Tri_Freq	= 395.88430144[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 38
Temp_Get	= 19.7[dC]
X_90_Width	= 12.6[us]
X_Acq_Time	= 2.20725248[s]
X_Angle	= 45[deg]
X_Atn	= 3.5[dB]
X_Pulse	= 6.3[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.20725248[s]



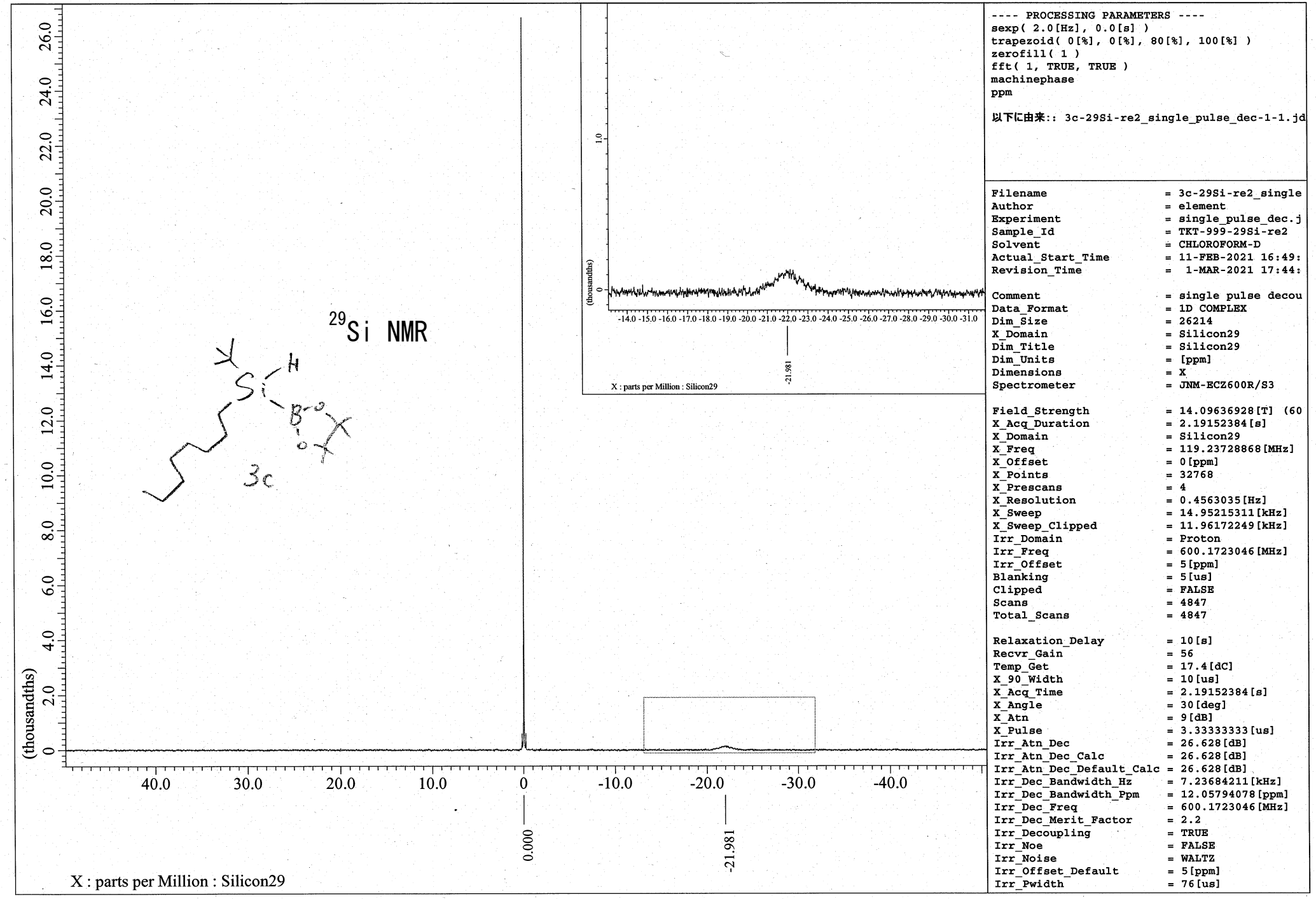

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

以下に由来:: 3c-13C-1.jdf
```

Filename	= 3c-13C-2.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= 1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 12-NOV-2020 01:24:44
Revision_Time	= 1-MAR-2021 17:42:34
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	= 1024
Total_Scans	= 1024
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 20.4[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]



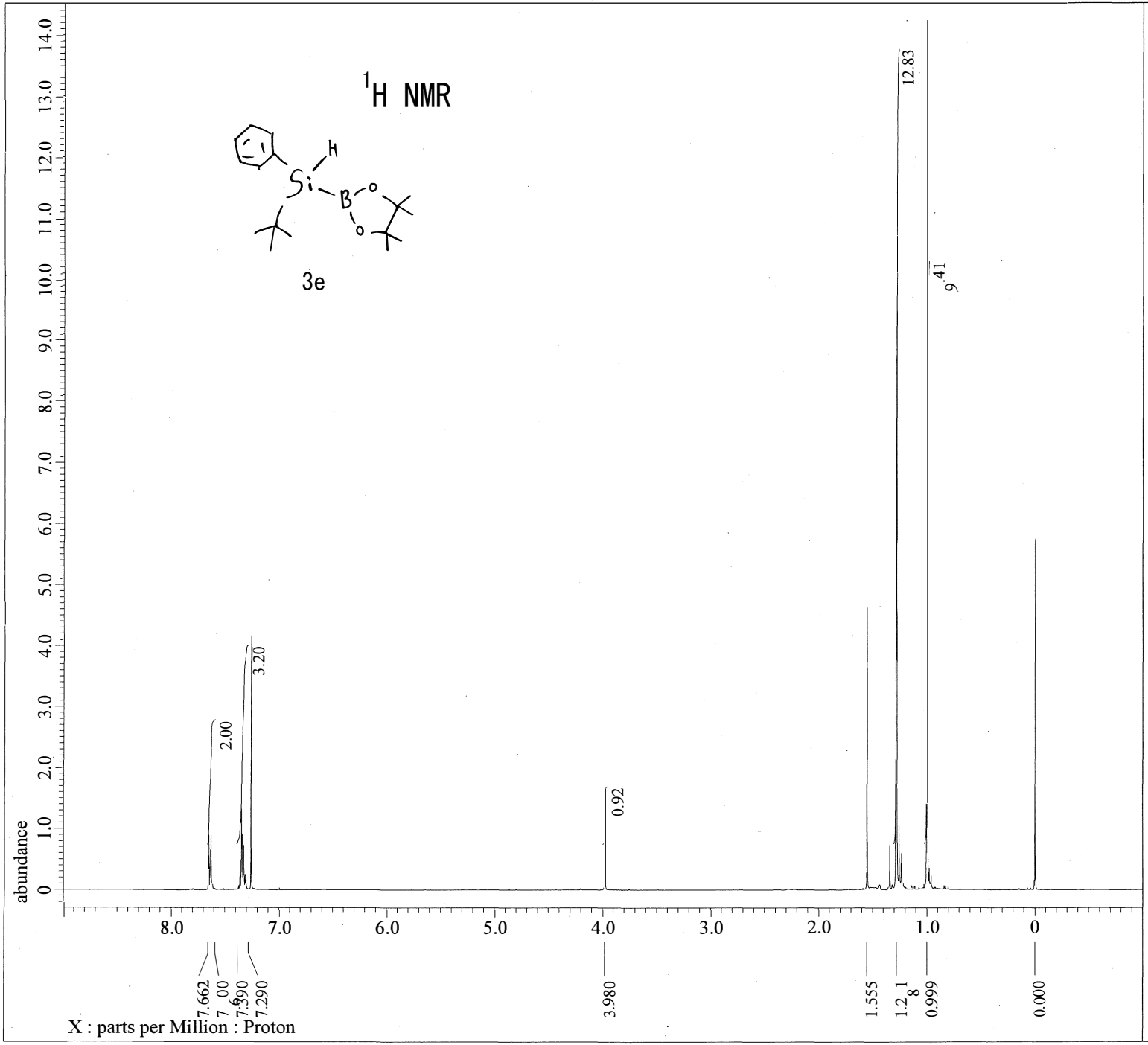

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

以下に由来:: 3c-11B-re-1.jdf
```

Filename	= 3c-11B-re-2.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= S#525422
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 10-FEB-2021 21:34:35
Revision_Time	= 1-MAR-2021 17:44:09
Comment	= single pulse decoupled ga
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= 11B
Dim_Title	= 11B
Dim_Units	= [ppm]
Dimensions	= X
Site	= ECS 400
Spectrometer	= JNM-ECS400
Field_Strength	= 9.20197068[T] (390[MHz])
X_Acq_Duration	= 0.83361792[s]
X_Domain	= 11B
X_Freq	= 125.70081325[MHz]
X_Offset	= 0[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 1.19959034[Hz]
X_Sweep	= 39.3081761[kHz]
Irr_Domain	= 1H
Irr_Freq	= 391.78655441[MHz]
Irr_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 512
Total_Scans	= 512
Relaxation_Delay	= 2[s]
Recvr_Gain	= 44
Temp_Get	= 17.1[dC]
X_90_Width	= 10[us]
X_Acq_Time	= 0.83361792[s]
X_Angle	= 30[deg]
X_Atn	= 5.5[dB]
X_Pulse	= 3.33333333[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	= 2.83361792[s]



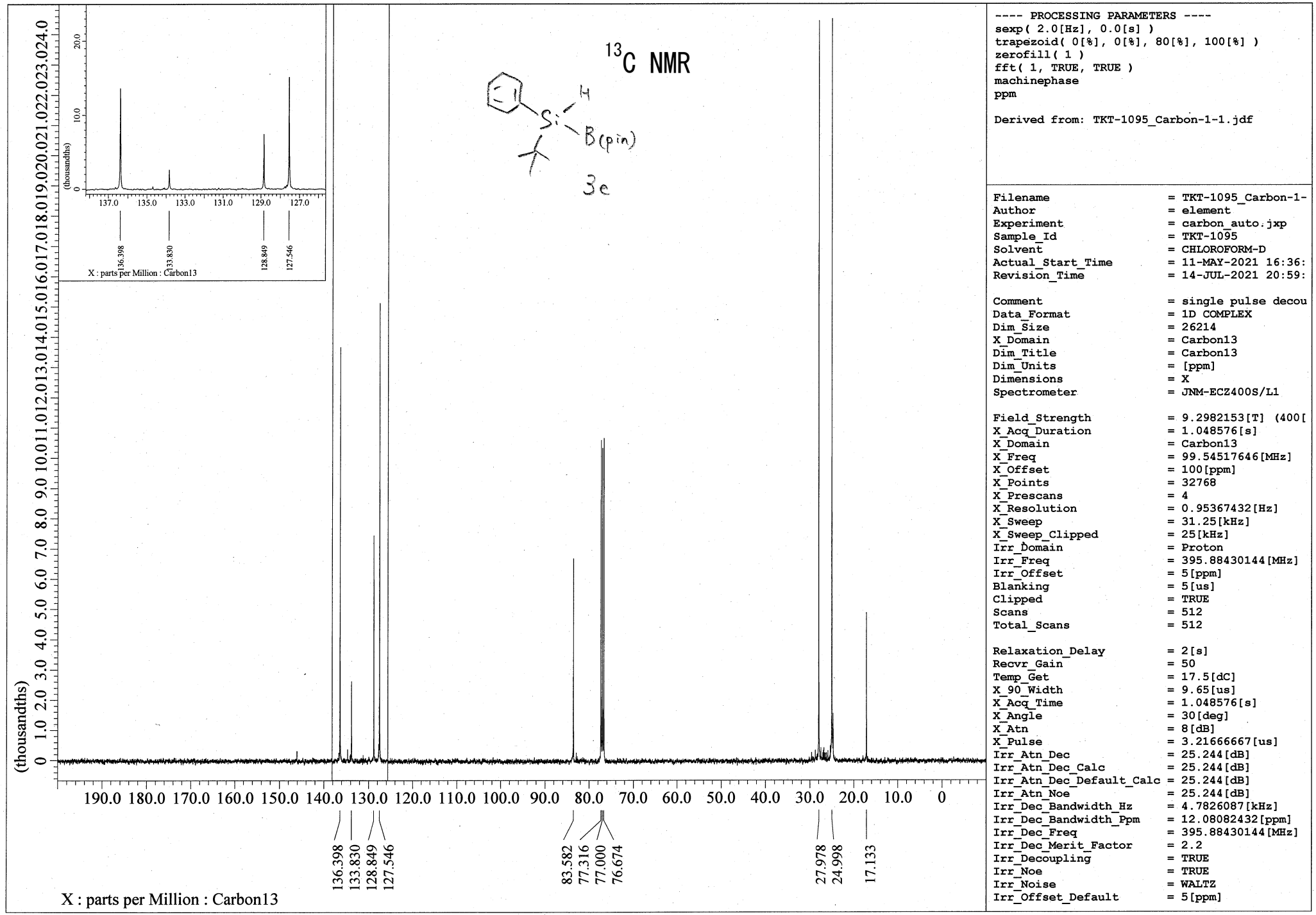

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

以下に由来:: 3c-29Si-re2_single_pulse_dec-1-1.jd
```

Filename	= 3c-29Si-re2_single
Author	= element
Experiment	= single_pulse_dec.j
Sample_Id	= TKT-999-29Si-re2
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 11-FEB-2021 16:49:
Revision_Time	= 1-MAR-2021 17:44:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Silicon29
Dim_Title	= Silicon29
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (60
X_Acq_Duration	= 2.19152384[s]
X_Domain	= Silicon29
X_Freq	= 119.23728868[MHz]
X_Offset	= 0[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.4563035[Hz]
X_Sweep	= 14.95215311[kHz]
X_Sweep_Clipped	= 11.96172249[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 5[us]
Clipped	= FALSE
Scans	= 4847
Total_Scans	= 4847
Relaxation_Delay	= 10[s]
Recvr_Gain	= 56
Temp_Get	= 17.4[dC]
X_90_Width	= 10[us]
X_Acq_Time	= 2.19152384[s]
X_Angle	= 30[deg]
X_Atn	= 9[dB]
X_Pulse	= 3.33333333[us]
Irr_Atn_Dec	= 26.628[dB]
Irr_Atn_Dec_Calc	= 26.628[dB]
Irr_Atn_Dec_Default_Calc	= 26.628[dB]
Irr_Dec_Bandwidth_Hz	= 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.05794078[ppm]
Irr_Dec_Freq	= 600.1723046[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= FALSE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]



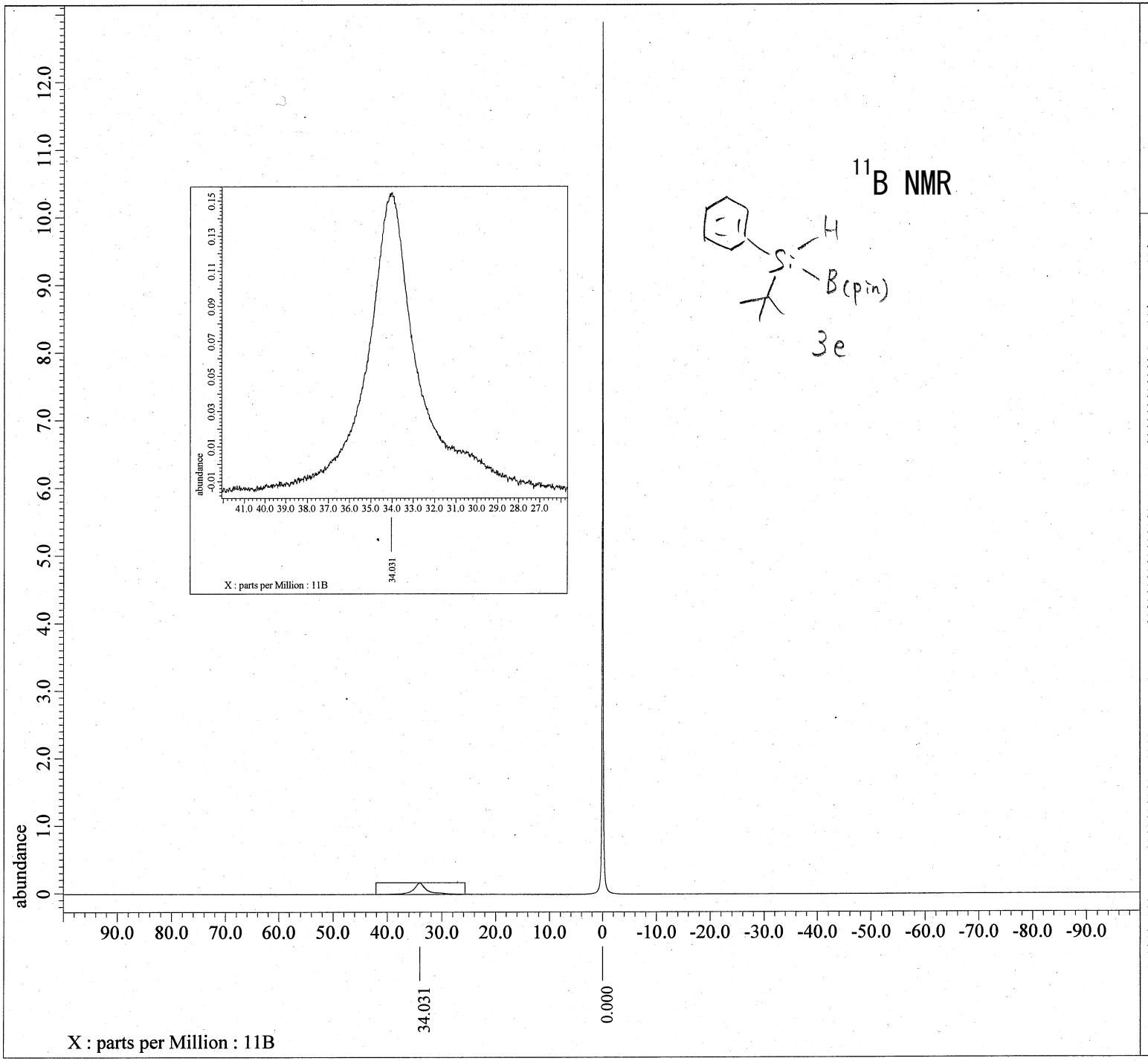

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: TKT-1095-1H_Proton-1-1.jdf
```

```
Filename            = TKT-1095-1H_Proton-1-2.jd
Author              = element
Experiment          = proton.jxp
Sample_Id           = TKT-1095-1H
Solvent             = CHLOROFORM-D
Actual_Start_Time   = 11-MAY-2021 16:51:20
Revision_Time       = 30-JUL-2021 17:08:03

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            = 19.4[dC]
X_90_Width          = 6[us]
X_Acq_Time          = 2.18103808[s]
X_Angle             = 45[deg]
X_Atn               = 0.8[dB]
X_Pulse             = 3[us]
Irr_Mode            = Off
Tri_Mode            = Off
Dante_Presat        = FALSE
Initial_Wait        = 1[s]
Repetition_Time     = 7.18103808[s]
```




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

Derived from: TKT-1095_Carbon-1-1.jdf
```

Filename	= TKT-1095_Carbon-1-
Author	= element
Experiment	= carbon_auto.jxp
Sample_Id	= TKT-1095
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 11-MAY-2021 16:36:
Revision_Time	= 14-JUL-2021 20:59:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ400S/L1
Field_Strength	= 9.2982153[T] (400[
X_Acq_Duration	= 1.048576[s]
X_Domain	= Carbon13
X_Freq	= 99.54517646[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.95367432[Hz]
X_Sweep	= 31.25[kHz]
X_Sweep_Clipped	= 25[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 5[us]
Clipped	= TRUE
Scans	= 512
Total_Scans	= 512
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 17.5[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	= 25.244[dB]
Irr_Atn_Dec_Calc	= 25.244[dB]
Irr_Atn_Dec_Default_Calc	= 25.244[dB]
Irr_Atn_Noe	= 25.244[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]

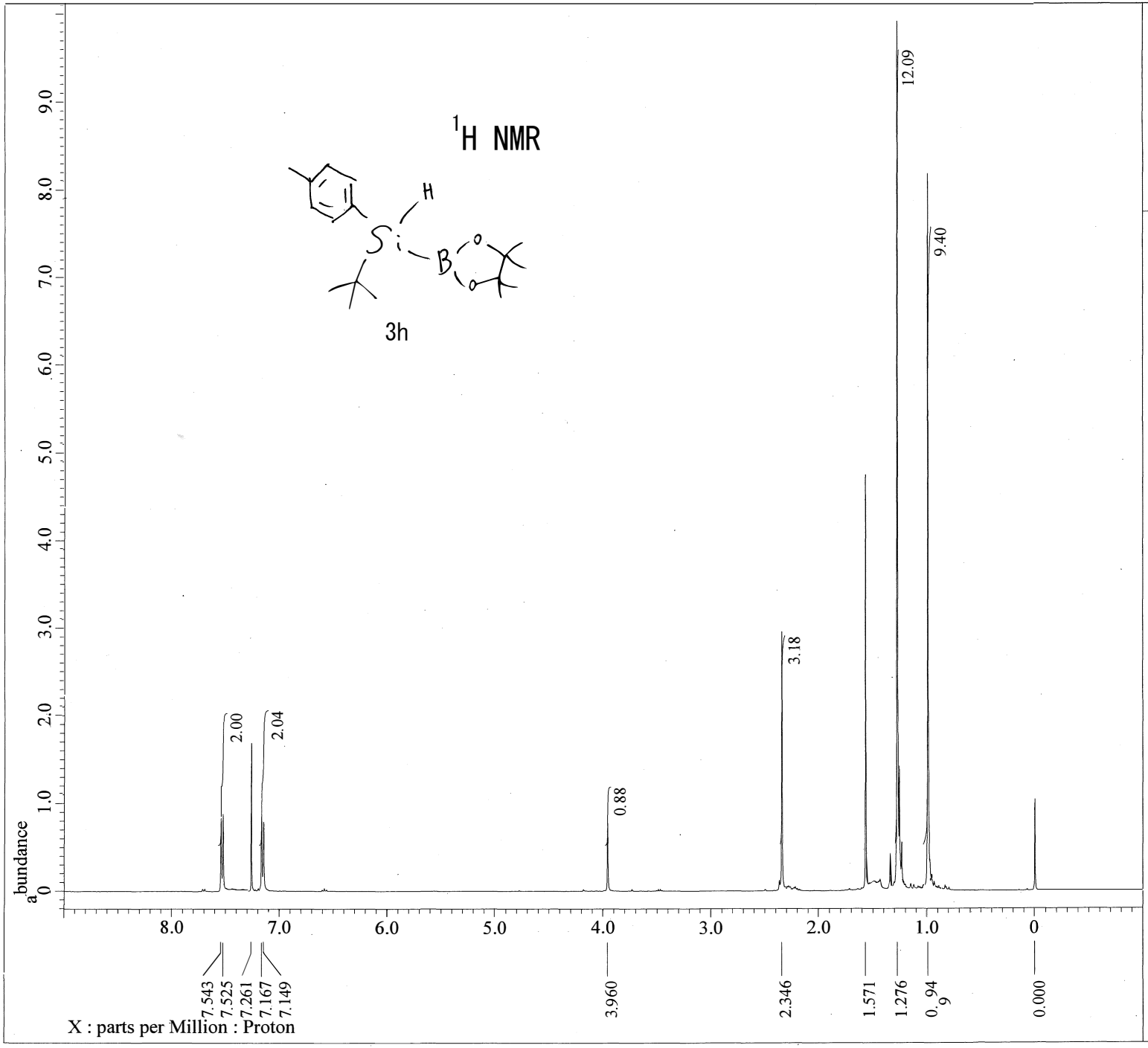


^{11}B NMR

3e

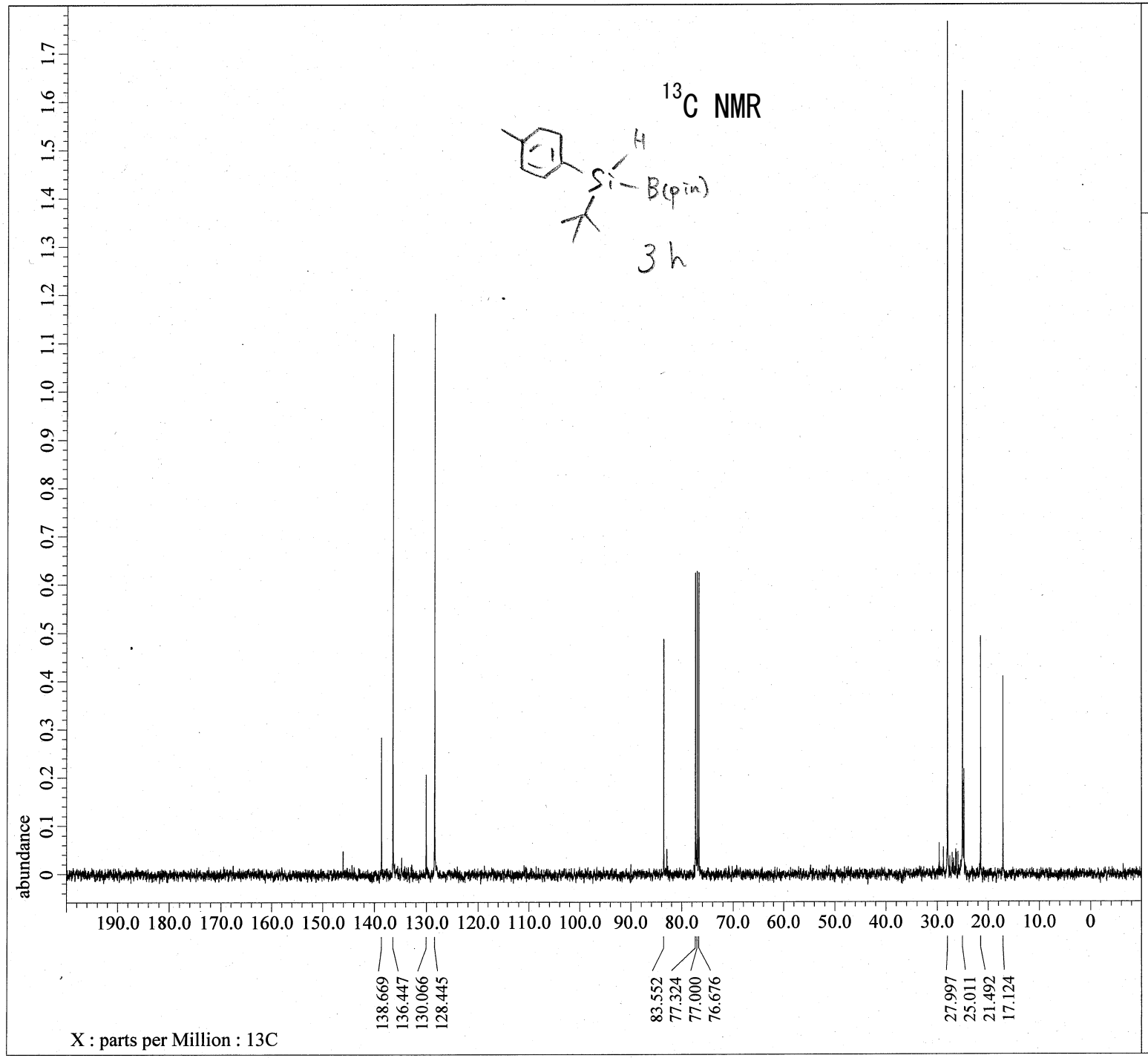
```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: TKT-1095-11B-1.jdf
```

```
Filename            = TKT-1095-11B-2.jdf
Author              = element
Experiment          = single_pulse_dec
Sample_Id           = S#635888
Solvent             = CHLOROFORM-D
Actual_Start_Time   = 12-MAY-2021 00:25:45
Revision_Time       = 14-JUL-2021 21:54:03

Comment             = single pulse decoupled ga
Data_Format         = 1D COMPLEX
Dim_Size            = 26214
X_Domain            = 11B
Dim_Title           = 11B
Dim_Units           = [ppm]
Dimensions          = X
Site                = ECS 400
Spectrometer        = JNM-ECS400

Field_Strength      = 9.20197068[T] (390[MHz])
X_Acq_Duration      = 0.83361792[s]
X_Domain            = 11B
X_Freq              = 125.70081325[MHz]
X_Offset            = 0[ppm]
X_Points            = 32768
X_Prescans          = 4
X_Resolution        = 1.19959034[Hz]
X_Sweep             = 39.3081761[kHz]
Irr_Domain          = 1H
Irr_Freq            = 391.78655441[MHz]
Irr_Offset          = 5[ppm]
Clipped             = FALSE
Scans               = 256
Total_Scans         = 256

Relaxation_Delay    = 2[s]
Recvr_Gain          = 44
Temp_Get            = 18.9[dC]
X_90_Width          = 10[us]
X_Acq_Time          = 0.83361792[s]
X_Angle             = 30[deg]
X_Atn               = 5.5[dB]
X_Pulse             = 3.33333333[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     = 2.83361792[s]
```



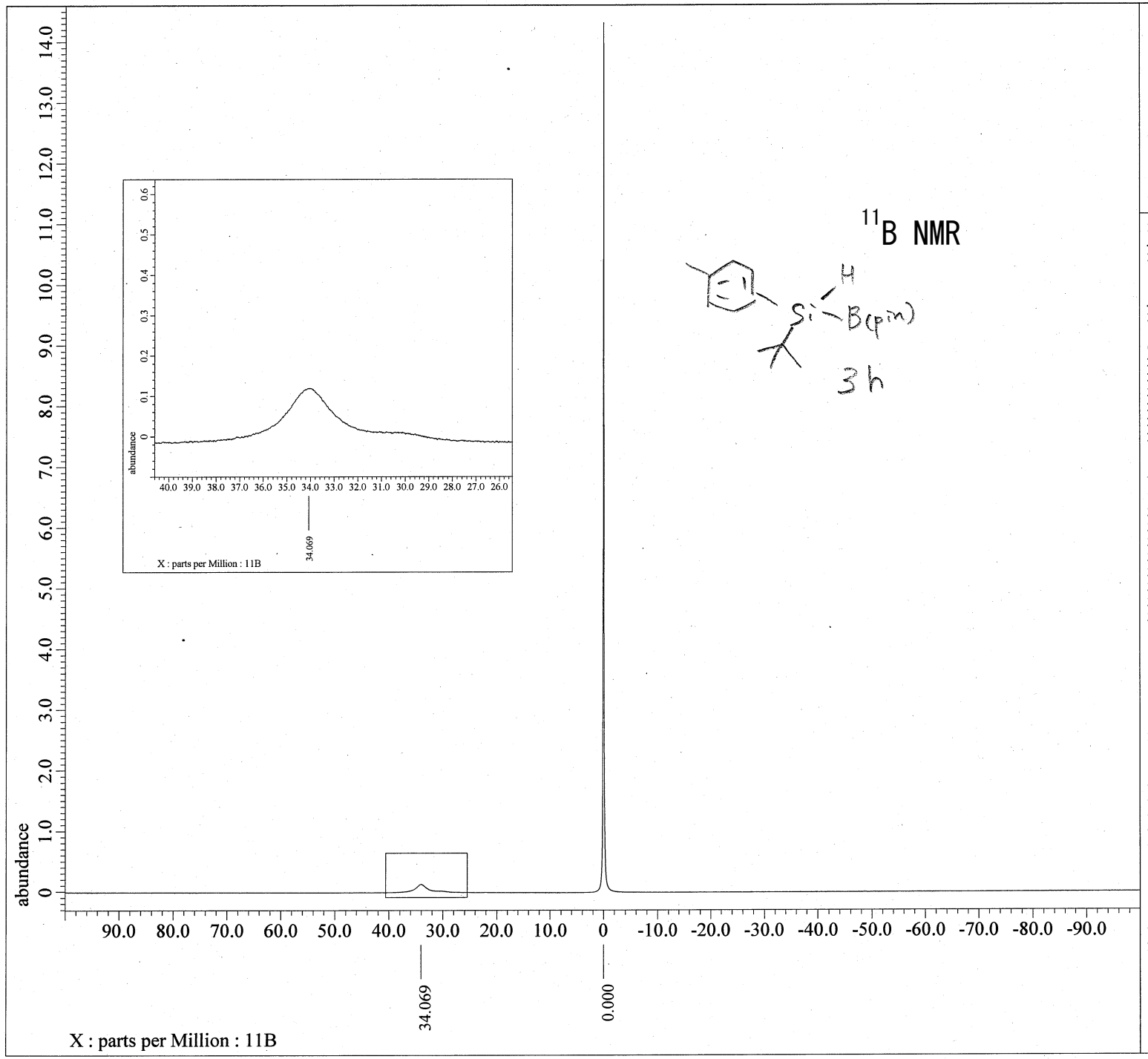

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: TKT-1150-1H_Proton-1-1.jdf
```

```
Filename            = TKT-1150-1H_Proton-1-3.jd
Author              = element
Experiment          = proton.jxp
Sample_Id           = TKT-1150-1H
Solvent             = CHLOROFORM-D
Actual_Start_Time   =  3-JUL-2021 18:44:35
Revision_Time       = 30-JUL-2021 17:15:25

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

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

Relaxation_Delay    = 5[s]
Recvr_Gain          = 42
Temp_Get            = 20.7[dC]
X_90_Width          = 6[us]
X_Acq_Time          = 2.18103808[s]
X_Angle             = 45[deg]
X_Atn               = 0.8[dB]
X_Pulse             = 3[us]
Irr_Mode            = Off
Tri_Mode            = Off
Dante_Presat        = FALSE
Initial_Wait        = 1[s]
Repetition_Time     = 7.18103808[s]
```



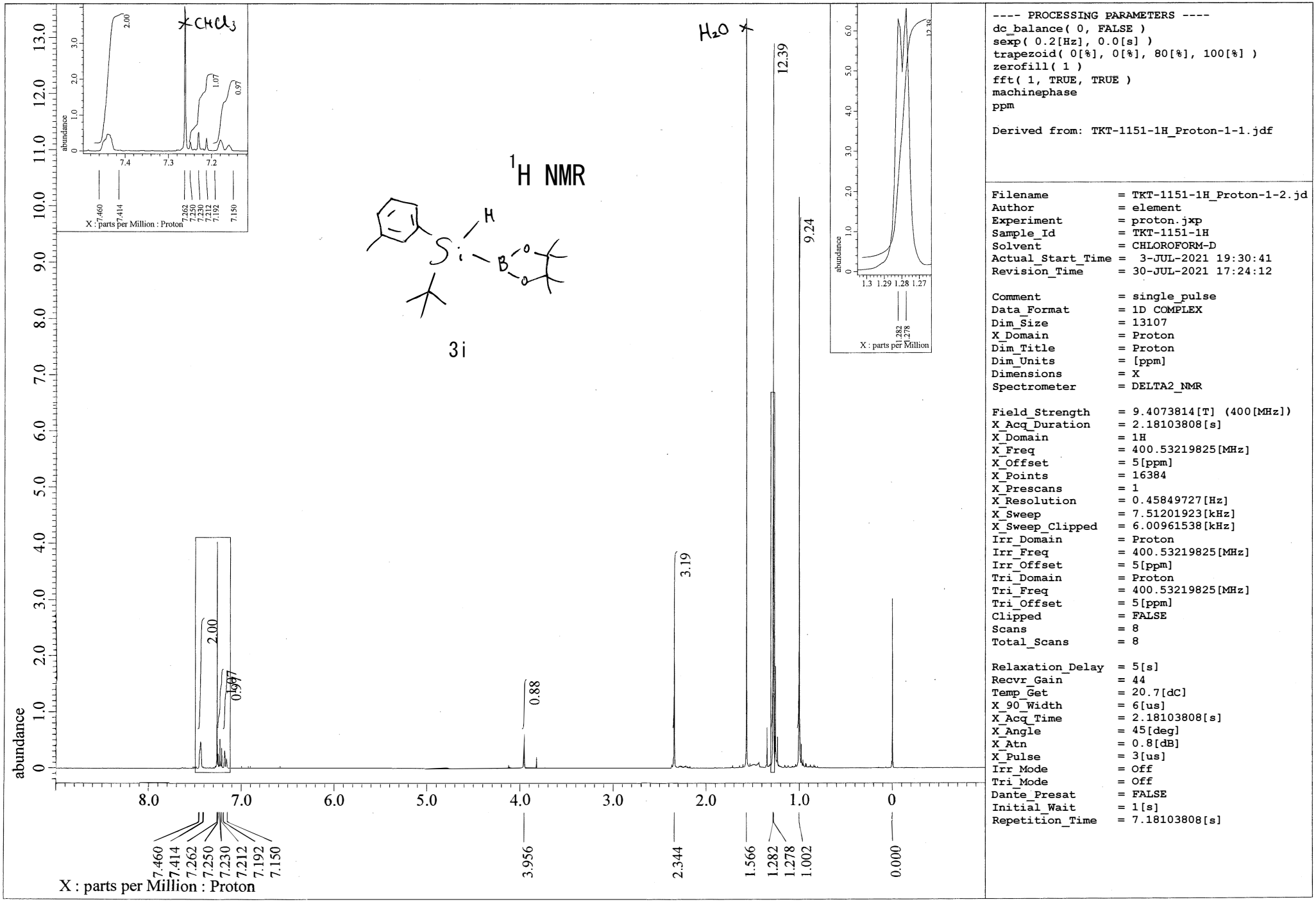

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: TKT-1150-13C-1.jdf
```

```
Filename            = TKT-1150-13C-2.jdf
Author              = element
Experiment          = single_pulse_dec
Sample_Id           = 1
Solvent             = CHLOROFORM-D
Actual_Start_Time   = 14-JUL-2021 22:04:15
Revision_Time       = 14-JUL-2021 22:04:42

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             = TRUE
Scans               = 128
Total_Scans         = 128

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]
```



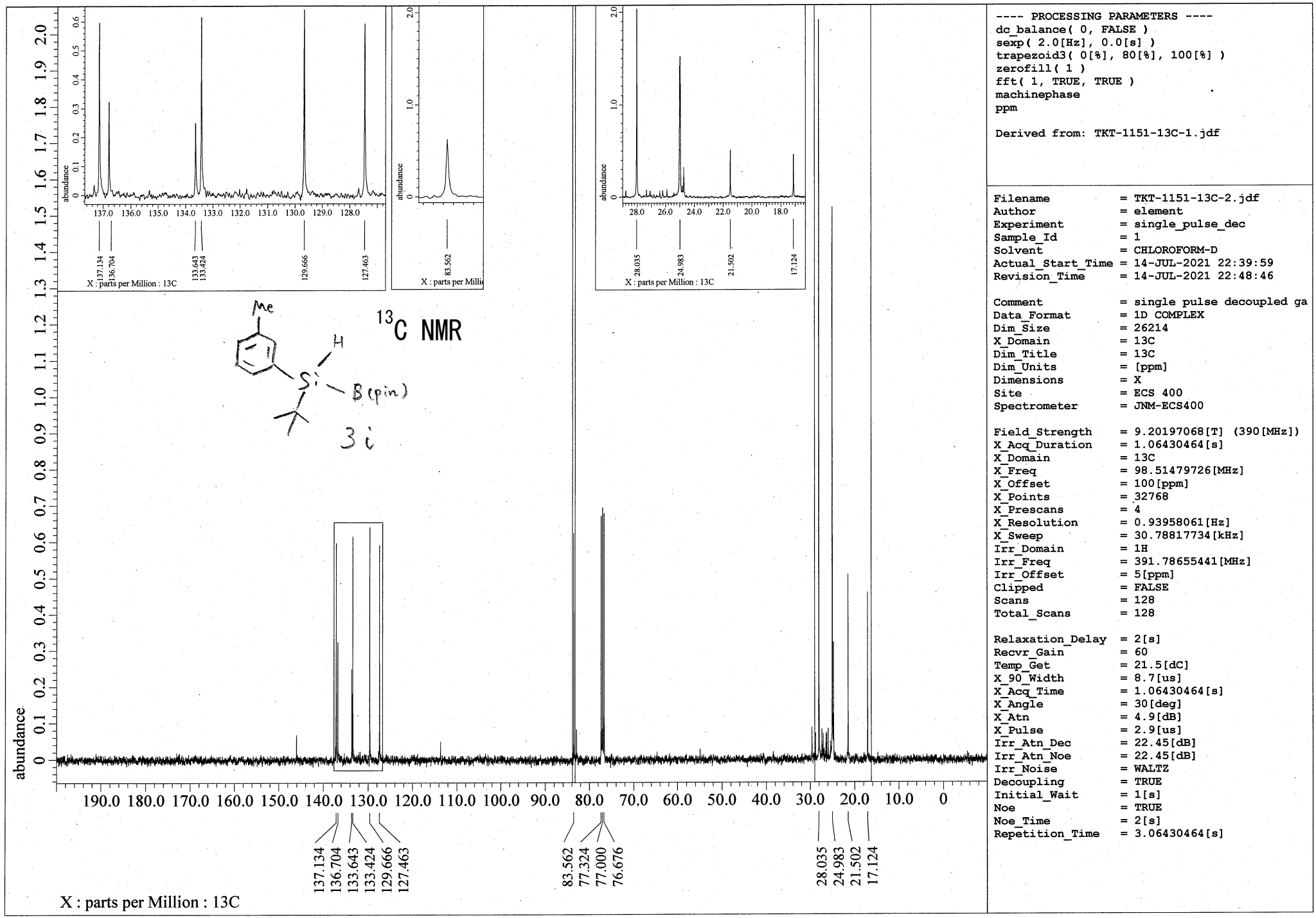

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: TKT-1150-11B-1.jdf
```

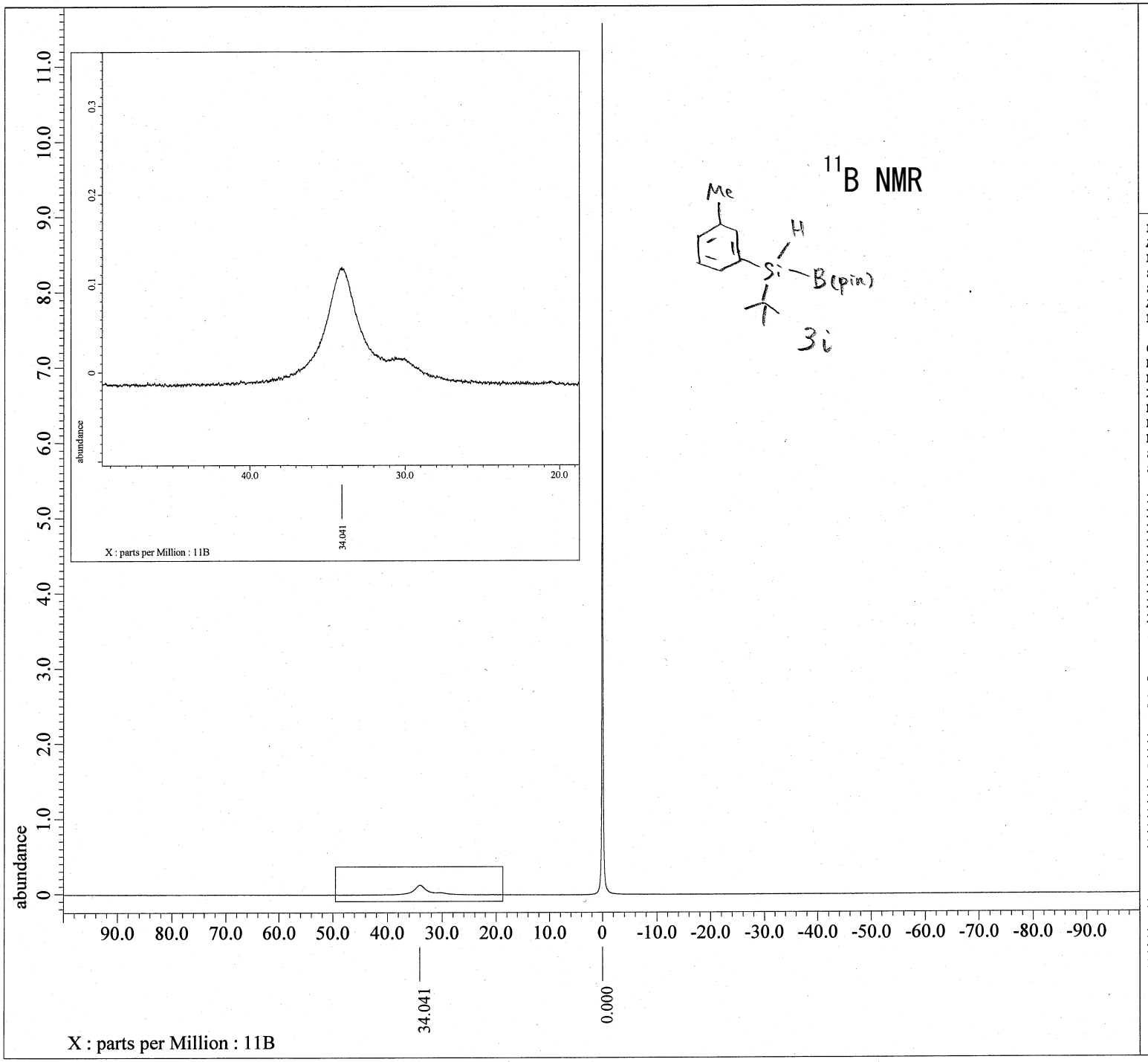
```
Filename            = TKT-1150-11B-2.jdf
Author              = element
Experiment          = single_pulse_dec
Sample_Id           = 1
Solvent             = CHLOROFORM-D
Actual_Start_Time   = 14-JUL-2021 22:22:23
Revision_Time       = 14-JUL-2021 22:05:48

Comment             = single pulse decoupled ga
Data_Format         = 1D COMPLEX
Dim_Size            = 26214
X_Domain            = 11B
Dim_Title           = 11B
Dim_Units           = [ppm]
Dimensions          = X
Site                = ECS 400
Spectrometer        = JNM-ECS400

Field_Strength      = 9.20197068[T] (390[MHz])
X_Acq_Duration      = 0.83361792[s]
X_Domain            = 11B
X_Freq              = 125.70081325[MHz]
X_Offset            = 0[ppm]
X_Points            = 32768
X_Prescans          = 4
X_Resolution        = 1.19959034[Hz]
X_Sweep             = 39.3081761[kHz]
Irr_Domain          = 1H
Irr_Freq            = 391.78655441[MHz]
Irr_Offset          = 5[ppm]
Clipped             = FALSE
Scans               = 256
Total_Scans         = 256

Relaxation_Delay    = 2[s]
Recvr_Gain          = 46
Temp_Get            = 21.6[dC]
X_90_Width          = 10[us]
X_Acq_Time          = 0.83361792[s]
X_Angle             = 30[deg]
X_Atn               = 5.5[dB]
X_Pulse             = 3.33333333[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     = 2.83361792[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: TKT-1151-1H_Proton-1-1.jdf
```

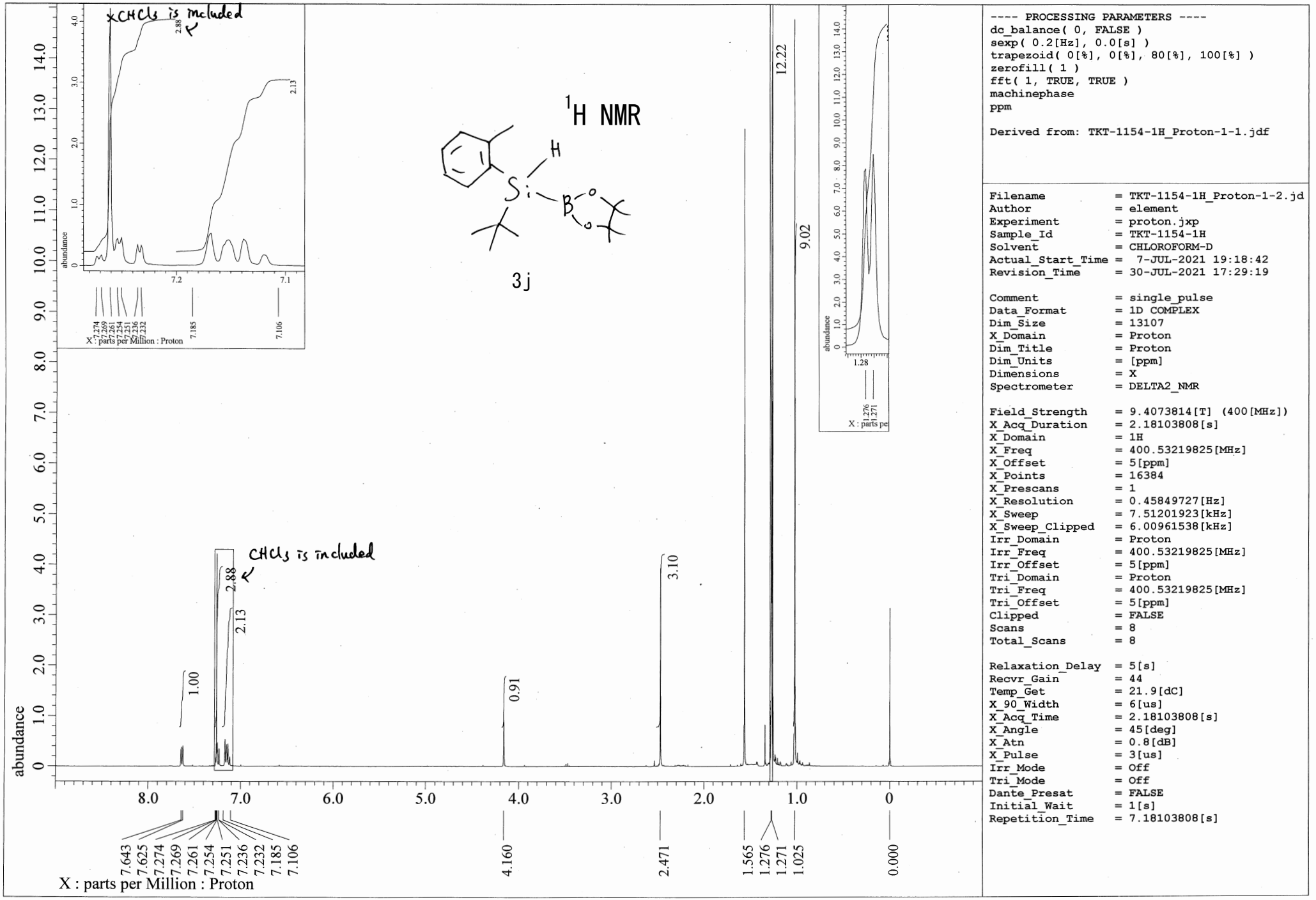
Filename	= TKT-1151-1H_Proton-1-2.jd
Author	= element
Experiment	= proton.jxp
Sample_Id	= TKT-1151-1H
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 3-JUL-2021 19:30:41
Revision_Time	= 30-JUL-2021 17:24:12
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
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	= 20.7[dC]
X_90_Width	= 6[us]
X_Acq_Time	= 2.18103808[s]
X_Angle	= 45[deg]
X_Atn	= 0.8[dB]
X_Pulse	= 3[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.18103808[s]


Me
H
Si
B(pin)
3i
^{13}C NMR
abundance
X : parts per Million : 13C
137.134
136.704
133.643
133.424
129.666
127.463
83.562
77.324
77.000
76.676
28.035
24.983
21.502
17.124
---- 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: TKT-1151-13C-1.jdf
Filename = TKT-1151-13C-2.jdf
Author = element
Experiment = single_pulse_dec
Sample_Id = 1
Solvent = CHLOROFORM-D
Actual_Start_Time = 14-JUL-2021 22:39:59
Revision_Time = 14-JUL-2021 22:48:46
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 = 128
Total_Scans = 128
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 21.5[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]



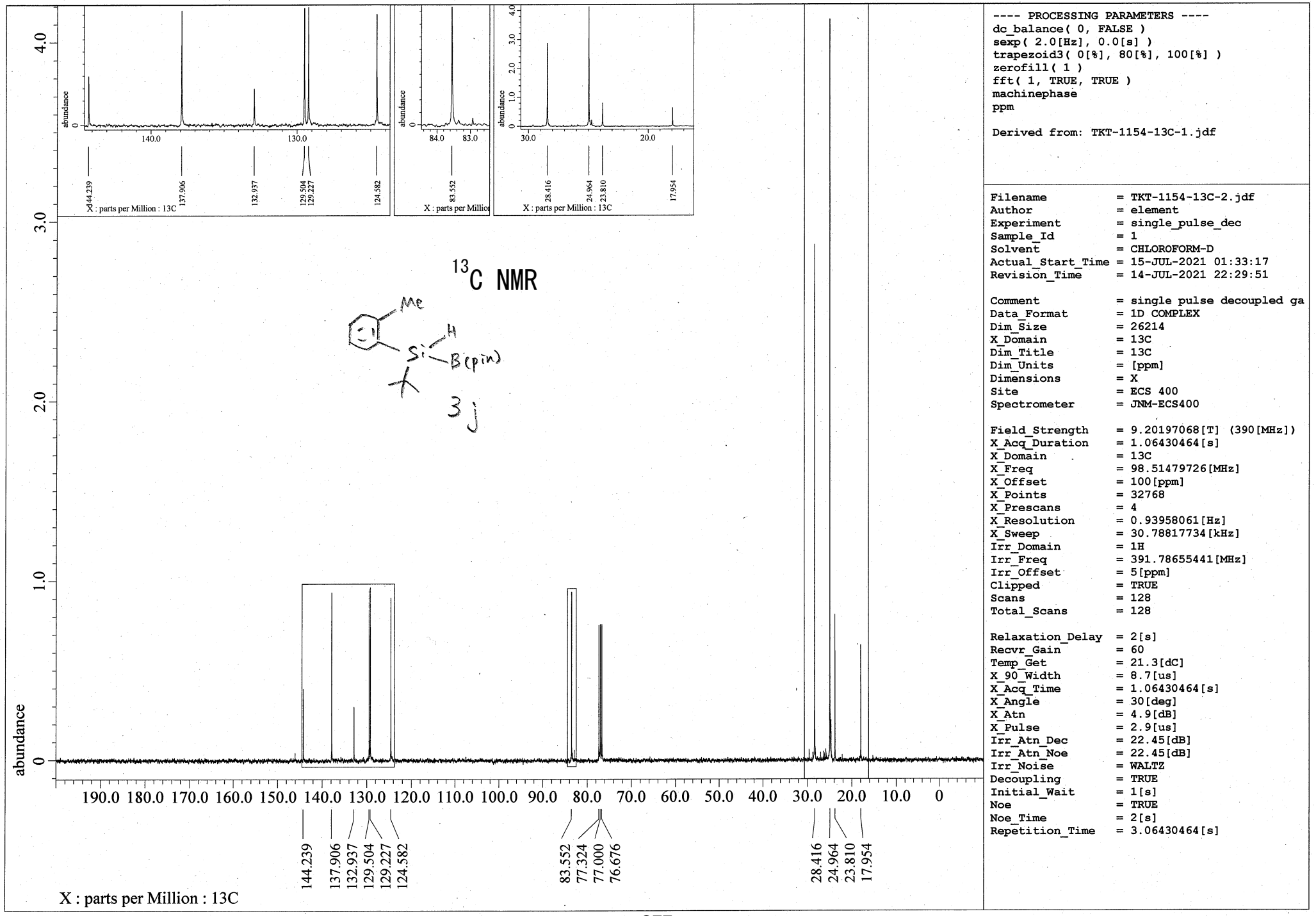

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: TKT-1151-11B-1.jdf
```

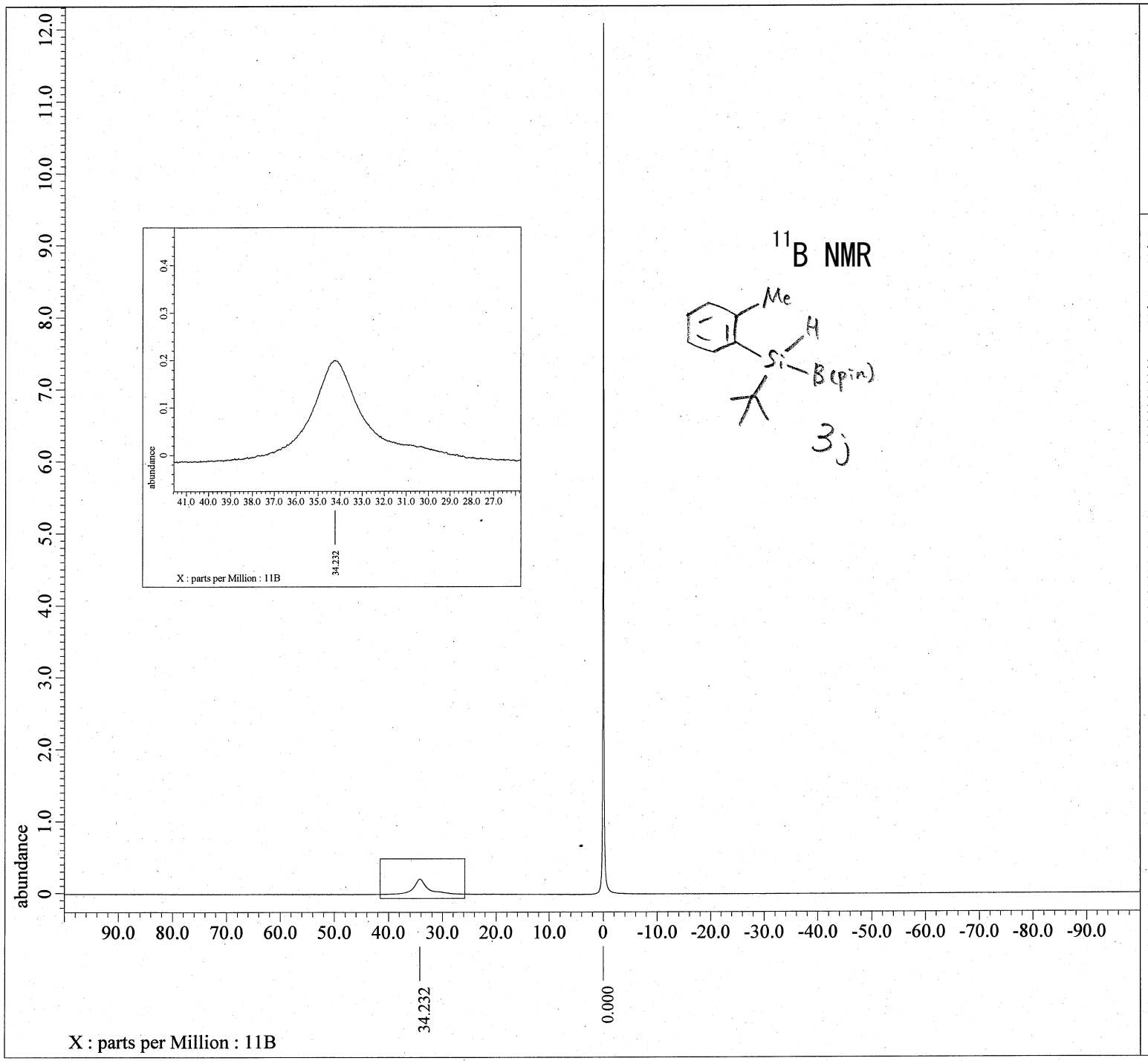
```
Filename            = TKT-1151-11B-2.jdf
Author              = element
Experiment          = single_pulse_dec
Sample_Id           = 1
Solvent             = CHLOROFORM-D
Actual_Start_Time   = 14-JUL-2021 22:57:28
Revision_Time       = 14-JUL-2021 22:51:25

Comment             = single pulse decoupled ga
Data_Format         = 1D COMPLEX
Dim_Size            = 26214
X_Domain            = 11B
Dim_Title           = 11B
Dim_Units           = [ppm]
Dimensions          = X
Site                = ECS 400
Spectrometer        = JNM-ECS400

Field_Strength      = 9.20197068[T] (390[MHz])
X_Acq_Duration      = 0.83361792[s]
X_Domain            = 11B
X_Freq              = 125.70081325[MHz]
X_Offset            = 0[ppm]
X_Points            = 32768
X_Prescans          = 4
X_Resolution        = 1.19959034[Hz]
X_Sweep             = 39.3081761[kHz]
Irr_Domain          = 1H
Irr_Freq            = 391.78655441[MHz]
Irr_Offset          = 5[ppm]
Clipped             = FALSE
Scans               = 183
Total_Scans         = 183

Relaxation_Delay    = 2[s]
Recvr_Gain          = 44
Temp_Get            = 21.5[dC]
X_90_Width          = 10[us]
X_Acq_Time          = 0.83361792[s]
X_Angle             = 30[deg]
X_Atn               = 5.5[dB]
X_Pulse             = 3.33333333[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     = 2.83361792[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: TKT-1154-1H_Proton-1-1.jdf
```

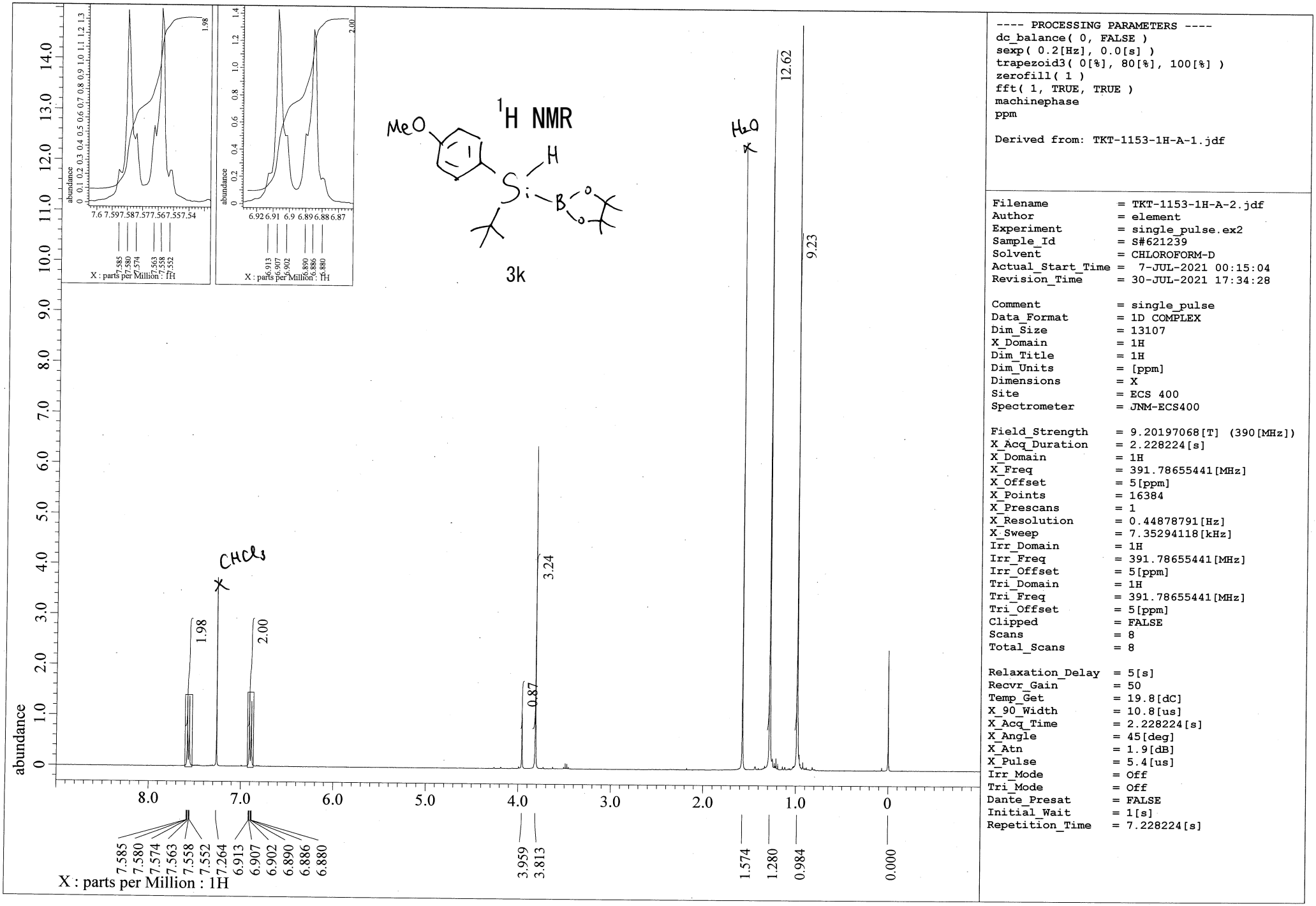
```
Filename            = TKT-1154-1H_Proton-1-2.jd
Author              = element
Experiment          = proton.jxp
Sample_Id           = TKT-1154-1H
Solvent             = CHLOROFORM-D
Actual_Start_Time   =  7-JUL-2021 19:18:42
Revision_Time       = 30-JUL-2021 17:29:19

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            = 21.9[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]
```


^{13}C NMR
Me
H
Si
B(pin)
3j
abundance
X : parts per Million : 13C
144.239
137.906
132.937
129.504
129.227
124.582
83.552
77.324
77.000
76.676
28.416
24.964
23.810
17.954
---- 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: TKT-1154-13C-1.jdf
Filename = TKT-1154-13C-2.jdf
Author = element
Experiment = single_pulse_dec
Sample_Id = 1
Solvent = CHLOROFORM-D
Actual_Start_Time = 15-JUL-2021 01:33:17
Revision_Time = 14-JUL-2021 22:29:51
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 = TRUE
Scans = 128
Total_Scans = 128
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]



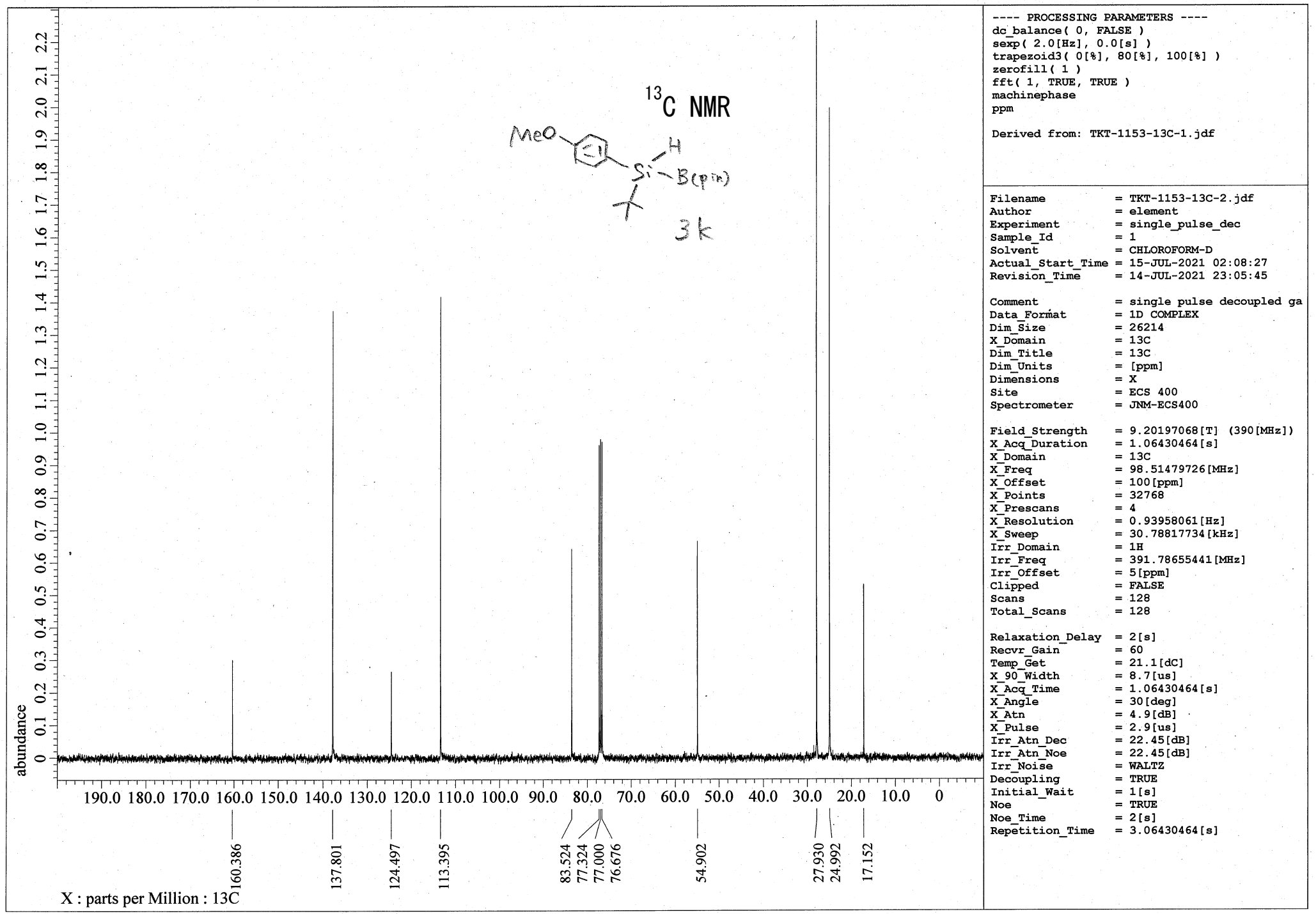

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: TKT-1154-11B-1.jdf
```

Filename	= TKT-1154-11B-2.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= 1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 15-JUL-2021 01:50:46
Revision_Time	= 14-JUL-2021 22:32:50
Comment	= single pulse decoupled ga
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= 11B
Dim_Title	= 11B
Dim_Units	= [ppm]
Dimensions	= X
Site	= ECS 400
Spectrometer	= JNM-ECS400
Field_Strength	= 9.20197068[T] (390[MHz])
X_Acq_Duration	= 0.83361792[s]
X_Domain	= 11B
X_Freq	= 125.70081325[MHz]
X_Offset	= 0[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 1.19959034[Hz]
X_Sweep	= 39.3081761[kHz]
Irr_Domain	= 1H
Irr_Freq	= 391.78655441[MHz]
Irr_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 256
Total_Scans	= 256
Relaxation_Delay	= 2[s]
Recvr_Gain	= 44
Temp_Get	= 21.2[dC]
X_90_Width	= 10[us]
X_Acq_Time	= 0.83361792[s]
X_Angle	= 30[deg]
X_Atn	= 5.5[dB]
X_Pulse	= 3.33333333[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	= 2.83361792[s]



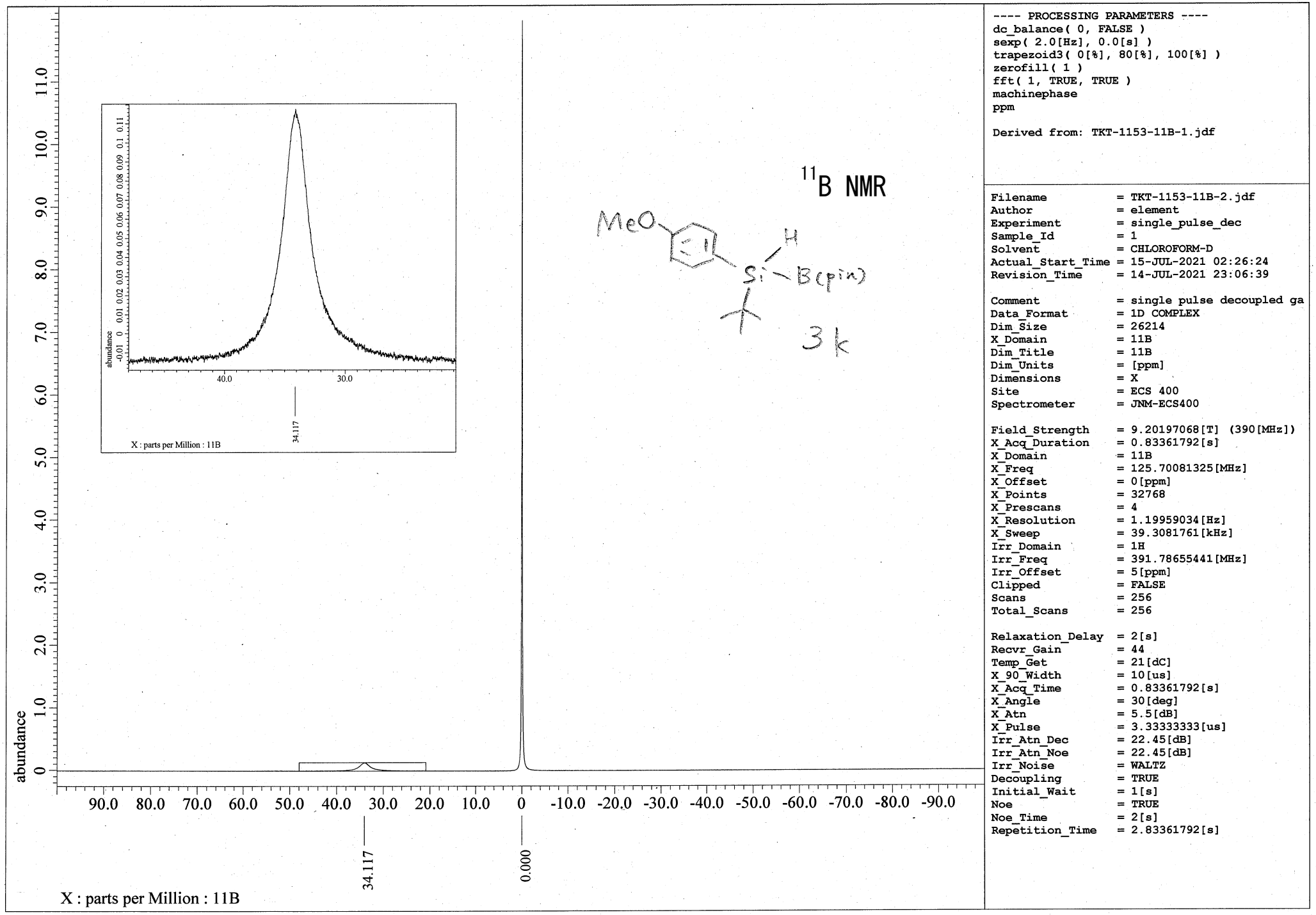

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: TKT-1153-1H-A-1.jdf
```

Filename	= TKT-1153-1H-A-2.jdf
Author	= element
Experiment	= single_pulse.ex2
Sample_Id	= S#621239
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 7-JUL-2021 00:15:04
Revision_Time	= 30-JUL-2021 17:34:28
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	= 19.8[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]



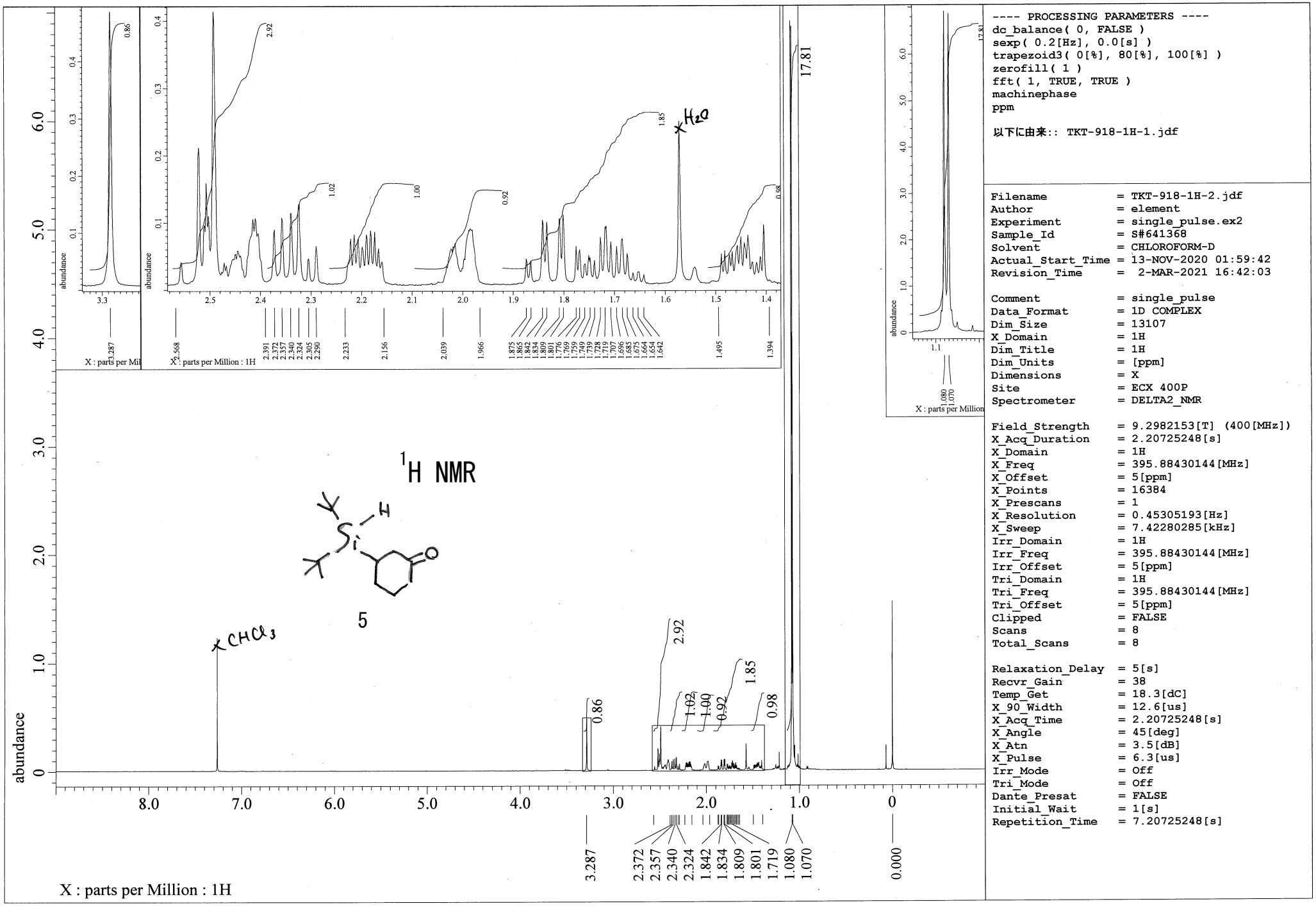

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: TKT-1153-13C-1.jdf
```

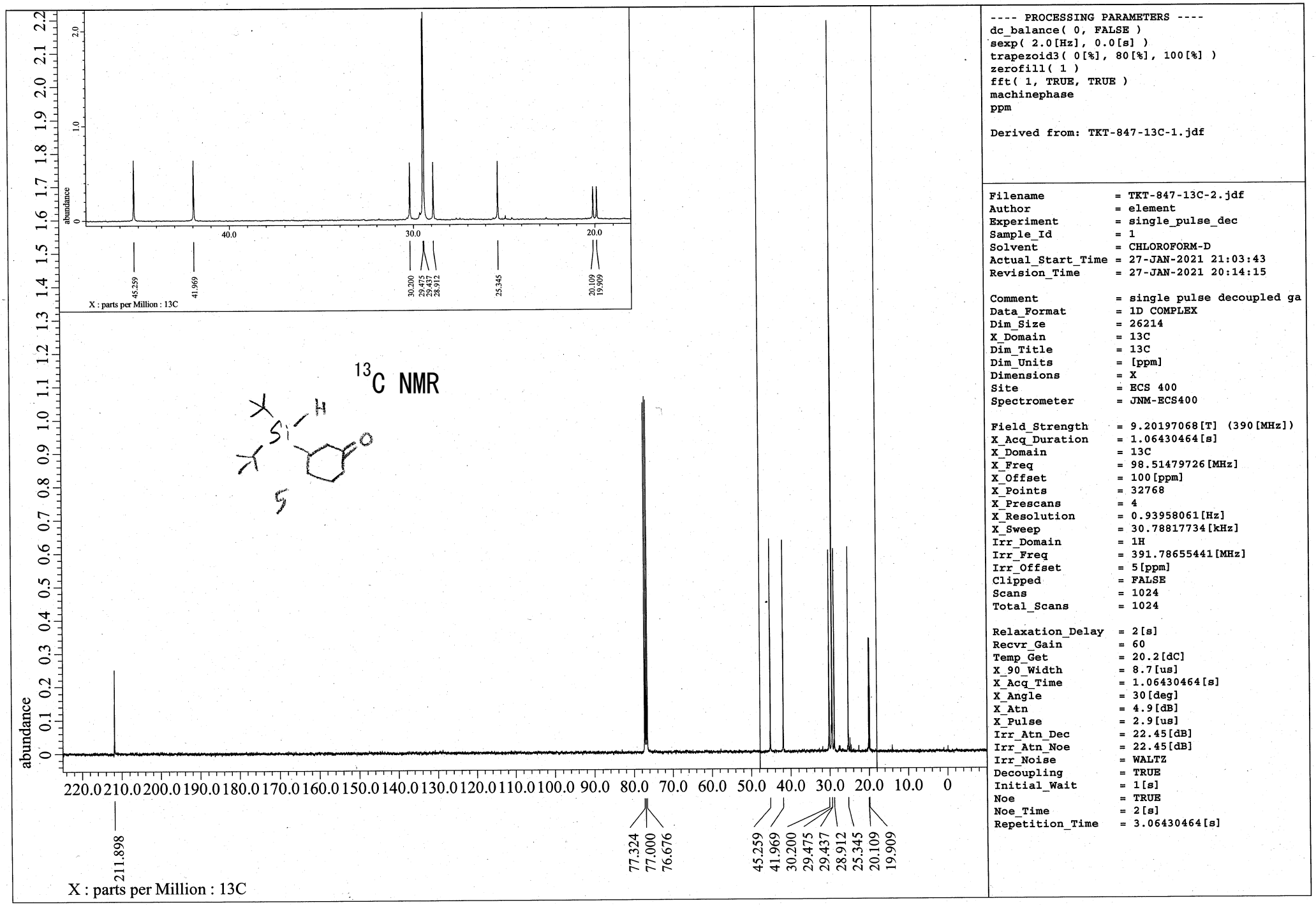
```
Filename            = TKT-1153-13C-2.jdf
Author              = element
Experiment          = single_pulse_dec
Sample_Id           = 1
Solvent             = CHLOROFORM-D
Actual_Start_Time   = 15-JUL-2021 02:08:27
Revision_Time       = 14-JUL-2021 23:05:45

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               = 128
Total_Scans         = 128

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]
```

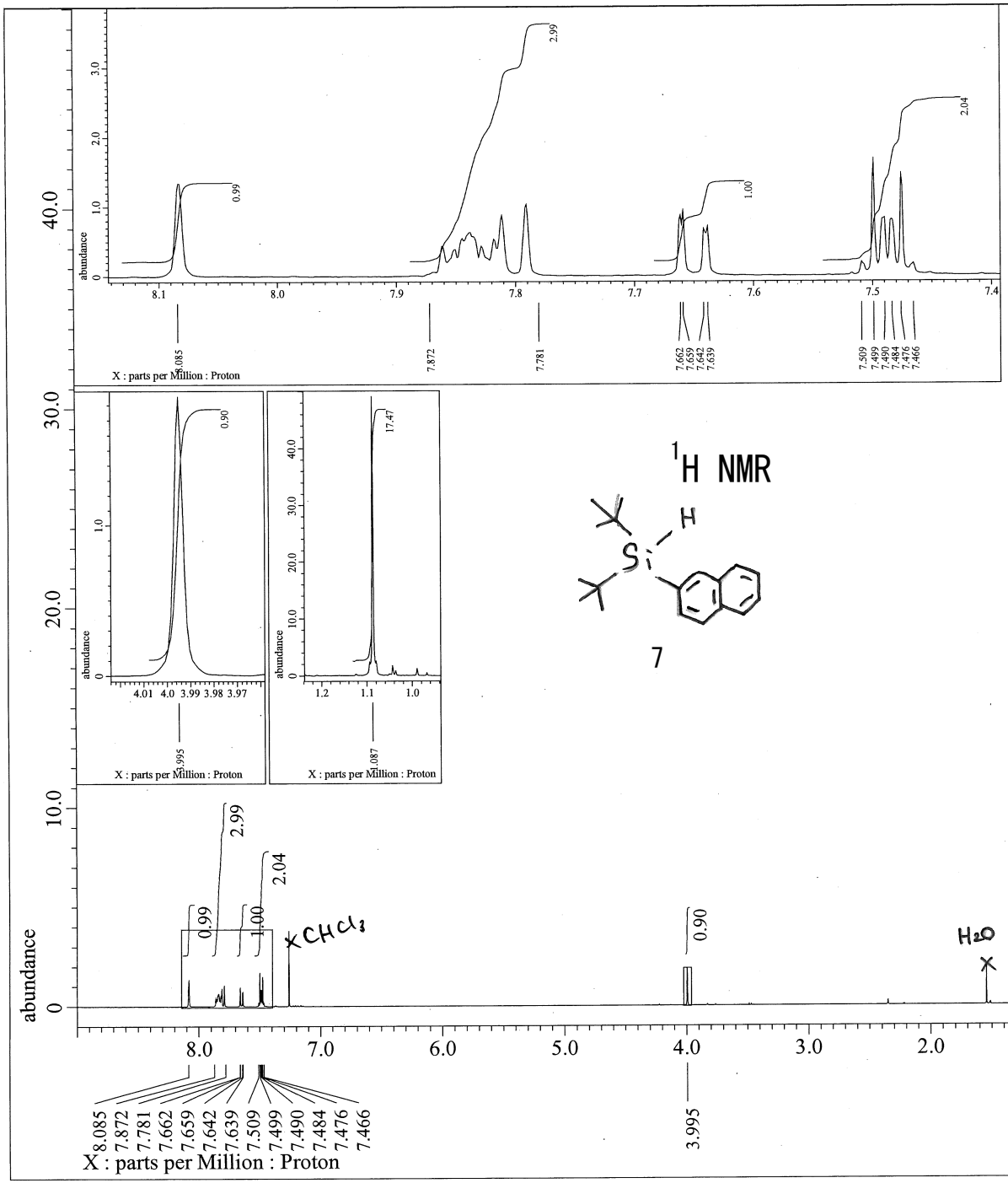



```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: TKT-1153-11B-1.jdf
```

```
Filename            = TKT-1153-11B-2.jdf
Author              = element
Experiment          = single_pulse_dec
Sample_Id           = 1
Solvent             = CHLOROFORM-D
Actual_Start_Time   = 15-JUL-2021 02:26:24
Revision_Time       = 14-JUL-2021 23:06:39

Comment             = single pulse decoupled ga
Data_Format         = 1D COMPLEX
Dim_Size            = 26214
X_Domain            = 11B
Dim_Title           = 11B
Dim_Units           = [ppm]
Dimensions          = X
Site                = ECS 400
Spectrometer        = JNM-ECS400

Field_Strength      = 9.20197068[T] (390[MHz])
X_Acq_Duration      = 0.83361792[s]
X_Domain            = 11B
X_Freq              = 125.70081325[MHz]
X_Offset            = 0[ppm]
X_Points            = 32768
X_Prescans          = 4
X_Resolution        = 1.19959034[Hz]
X_Sweep             = 39.3081761[kHz]
Irr_Domain          = 1H
Irr_Freq            = 391.78655441[MHz]
Irr_Offset          = 5[ppm]
Clipped             = FALSE
Scans               = 256
Total_Scans         = 256

Relaxation_Delay    = 2[s]
Recvr_Gain          = 44
Temp_Get            = 21[dC]
X_90_Width          = 10[us]
X_Acq_Time          = 0.83361792[s]
X_Angle             = 30[deg]
X_Atn               = 5.5[dB]
X_Pulse             = 3.33333333[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     = 2.83361792[s]
```

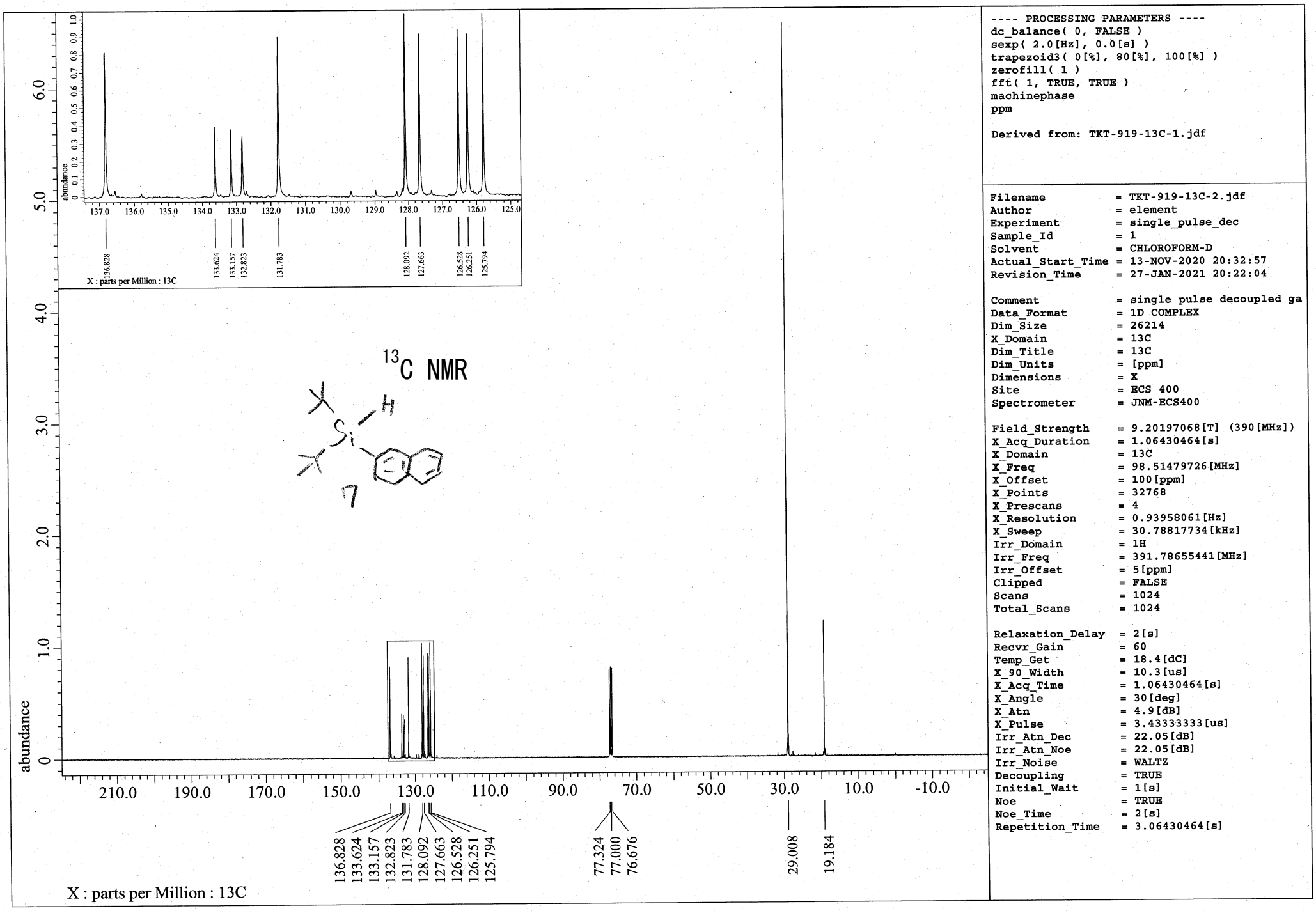

1H NMR
5
CHCl3
H2O
abundance
X : parts per Million : 1H
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid3(0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
以下に由来:: TKT-918-1H-1.jdf
Filename = TKT-918-1H-2.jdf
Author = element
Experiment = single_pulse.ex2
Sample_Id = S#641368
Solvent = CHLOROFORM-D
Actual_Start_Time = 13-NOV-2020 01:59:42
Revision_Time = 2-MAR-2021 16:42:03
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
X_Domain = 1H
Dim_Title = 1H
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400P
Spectrometer = DELTA2_NMR
Field_Strength = 9.2982153[T] (400[MHz])
X_Acq_Duration = 2.20725248[s]
X_Domain = 1H
X_Freq = 395.88430144[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45305193[Hz]
X_Sweep = 7.42280285[kHz]
Irr_Domain = 1H
Irr_Freq = 395.88430144[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = 1H
Tri_Freq = 395.88430144[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 38
Temp_Get = 18.3[dC]
X_90_Width = 12.6[us]
X_Acq_Time = 2.20725248[s]
X_Angle = 45[deg]
X_Atn = 3.5[dB]
X_Pulse = 6.3[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 7.20725248[s]


^{13}C NMR
abundance
X : parts per Million : 13C
211.898
77.324
77.000
76.676
45.259
41.969
30.200
29.475
29.437
28.912
25.345
20.109
19.909
---- 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: TKT-847-13C-1.jdf
Filename = TKT-847-13C-2.jdf
Author = element
Experiment = single_pulse_dec
Sample_Id = 1
Solvent = CHLOROFORM-D
Actual_Start_Time = 27-JAN-2021 21:03:43
Revision_Time = 27-JAN-2021 20:14:15
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 = 1024
Total_Scans = 1024
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 20.2[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]



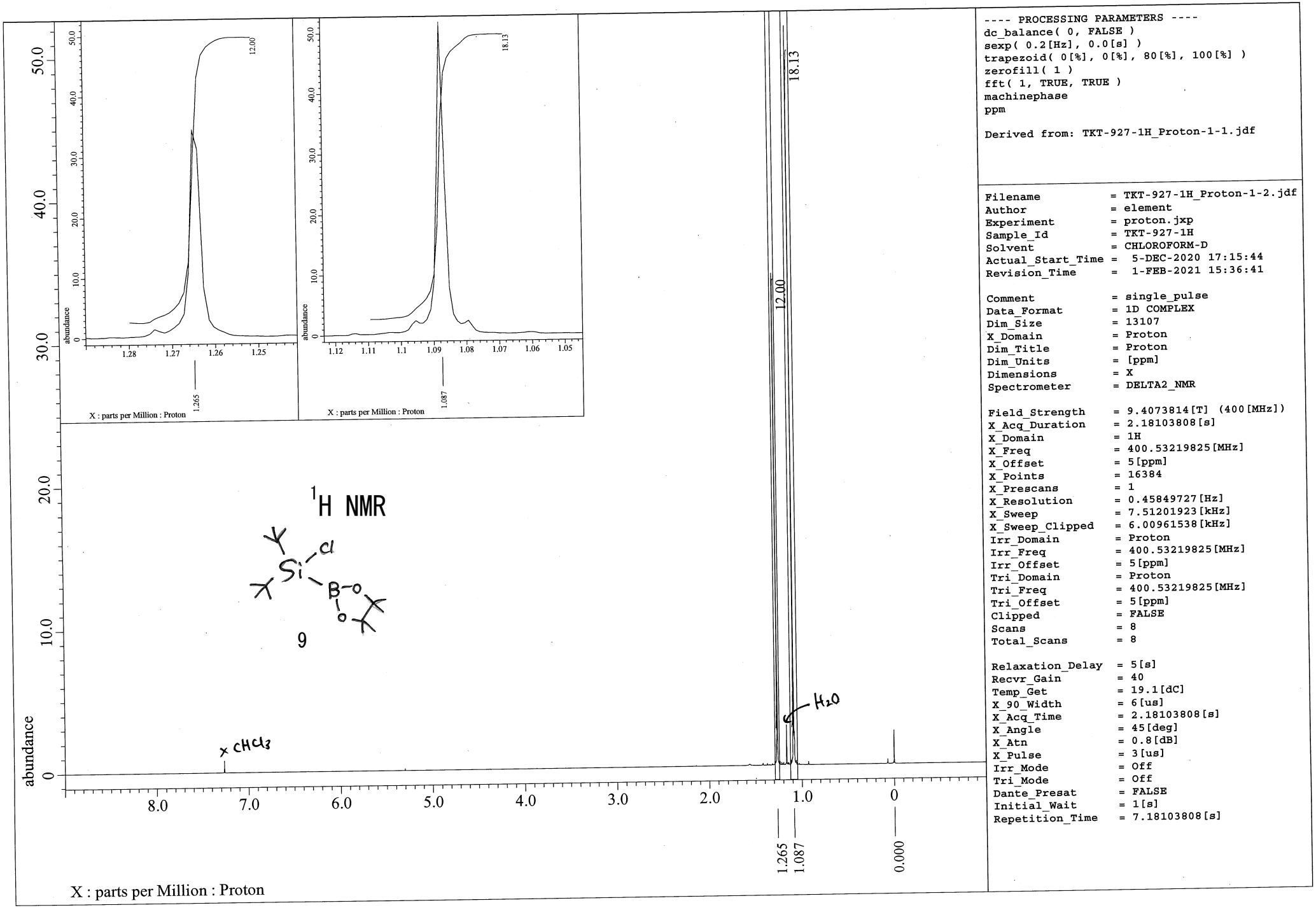

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: TKT-919-1H_GPC_Proton-1-1.jdf
```

Filename	= TKT-919-1H_GPC_Proton-1-2
Author	= element
Experiment	= proton.jxp
Sample_Id	= TKT-919-1H_GPC
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 13-NOV-2020 13:30:08
Revision_Time	= 27-JAN-2021 20:19:48
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	= 44
Temp_Get	= 19.4[dC]
X_90_Width	= 6[us]
X_Acq_Time	= 2.18103808[s]
X_Angle	= 45[deg]
X_Atn	= 0.8[dB]
X_Pulse	= 3[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.18103808[s]



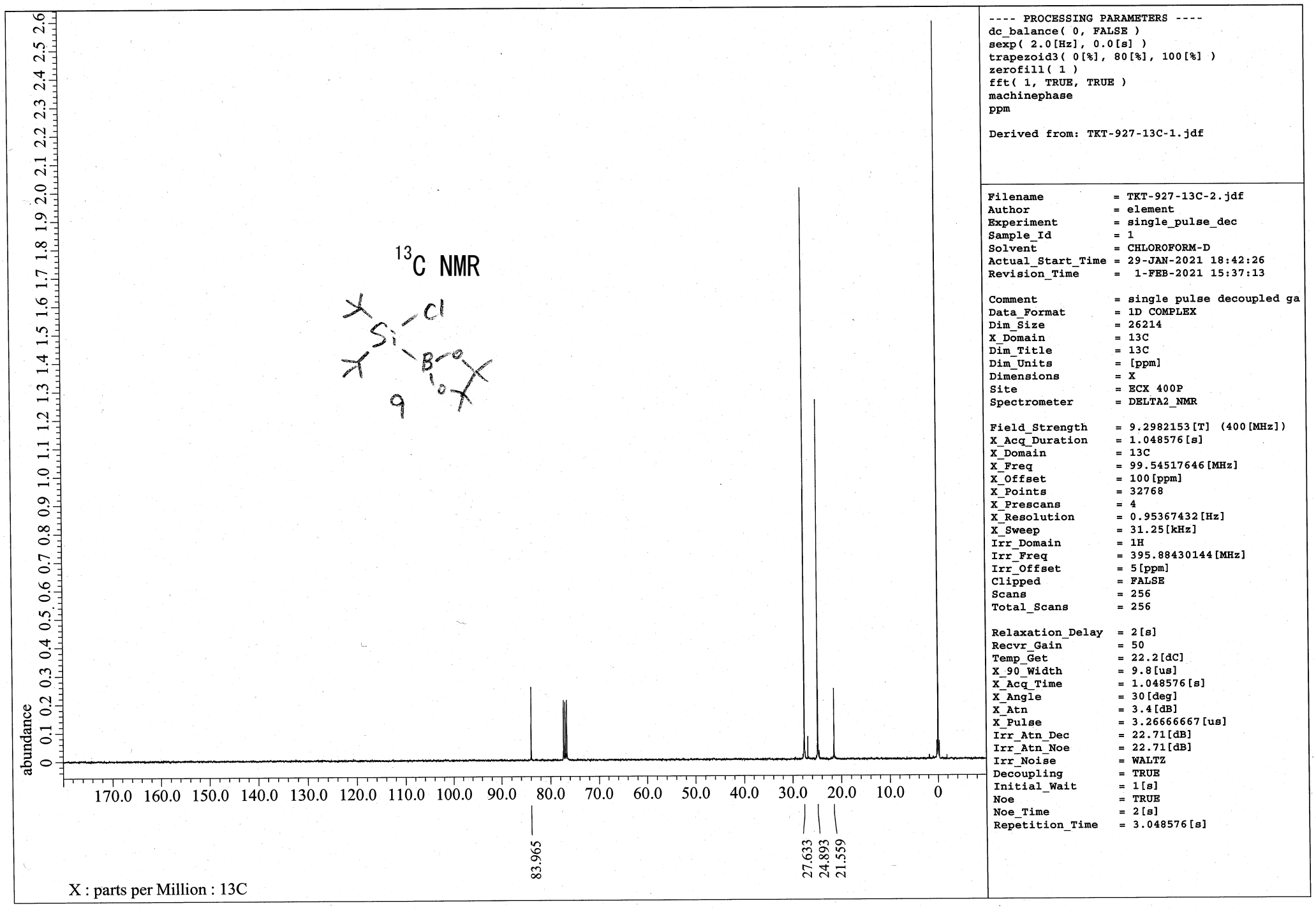

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: TKT-919-13C-1.jdf
```

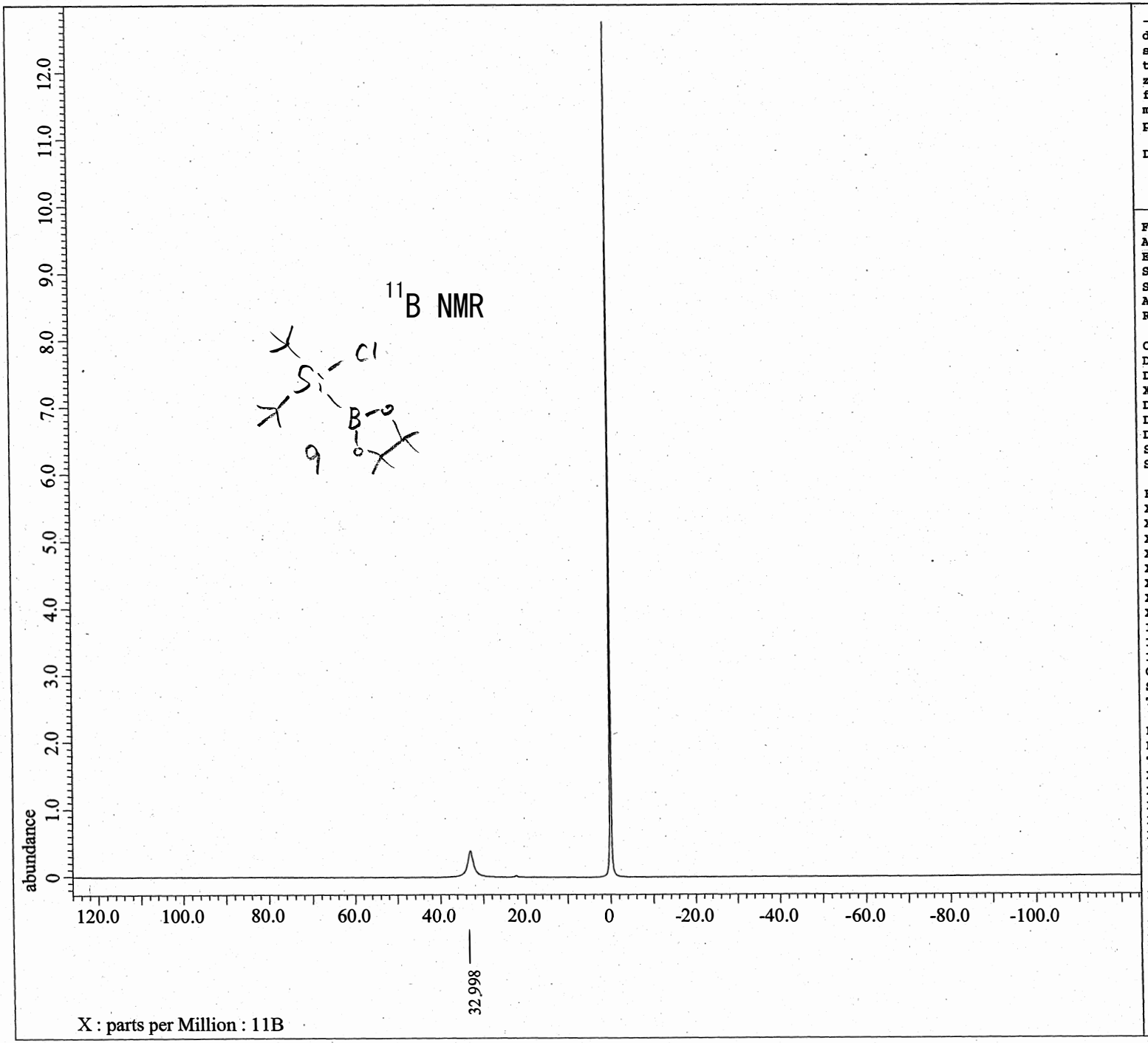
Filename	= TKT-919-13C-2.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= 1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 13-NOV-2020 20:32:57
Revision_Time	= 27-JAN-2021 20:22:04
Comment	= single pulse decoupled ga
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= 13C
Dim_Title	= 13C
Dim_Units	= [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	= 1024
Total_Scans	= 1024
Relaxation_Delay	= 2[s]
Recvr_Gain	= 60
Temp_Get	= 18.4[dC]
X_90_Width	= 10.3[us]
X_Acq_Time	= 1.06430464[s]
X_Angle	= 30[deg]
X_Atn	= 4.9[dB]
X_Pulse	= 3.43333333[us]
Irr_Atn_Dec	= 22.05[dB]
Irr_Atn_Noe	= 22.05[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: TKT-927-1H_Proton-1-1.jdf
```

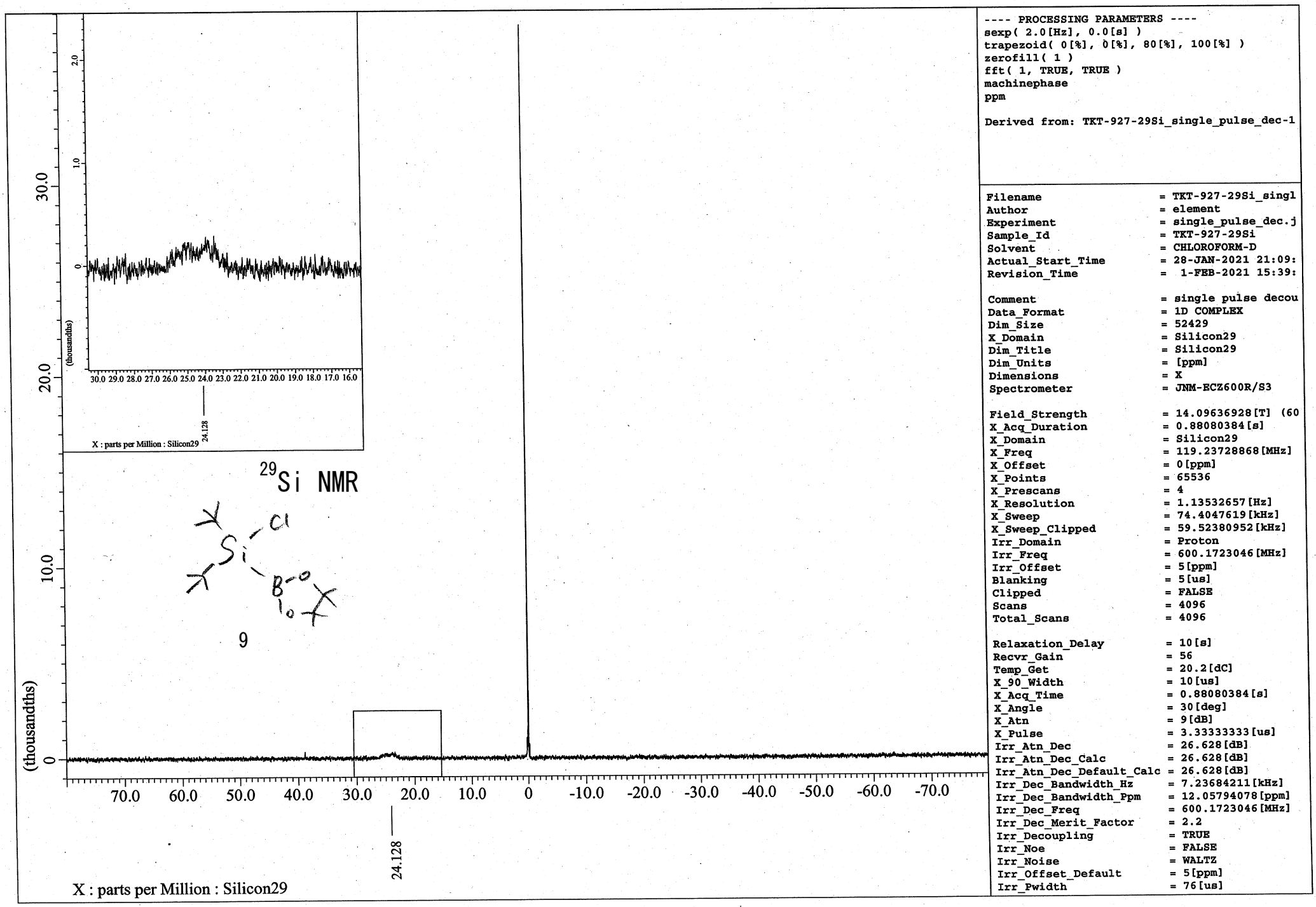
```
Filename            = TKT-927-1H_Proton-1-2.jdf
Author              = element
Experiment          = proton.jxp
Sample_Id           = TKT-927-1H
Solvent             = CHLOROFORM-D
Actual_Start_Time   =  5-DEC-2020 17:15:44
Revision_Time       =  1-FEB-2021 15:36:41

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            = 19.1[dC]
X_90_Width          = 6[us]
X_Acq_Time          = 2.18103808[s]
X_Angle             = 45[deg]
X_Atn               = 0.8[dB]
X_Pulse             = 3[us]
Irr_Mode            = Off
Tri_Mode            = Off
Dante_Presat        = FALSE
Initial_Wait        = 1[s]
Repetition_Time     = 7.18103808[s]
```


13C NMR
abundance
0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0 1.1 1.2 1.3 1.4 1.5 1.6 1.7 1.8 1.9 2.0 2.1 2.2 2.3 2.4 2.5 2.6
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
83.965
27.633
24.893
21.559
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: TKT-927-13C-1.jdf
Filename = TKT-927-13C-2.jdf
Author = element
Experiment = single_pulse_dec
Sample_Id = 1
Solvent = CHLOROFORM-D
Actual_Start_Time = 29-JAN-2021 18:42:26
Revision_Time = 1-FEB-2021 15:37:13
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = 13C
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Site = 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 = 256
Total_Scans = 256
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 22.2[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]



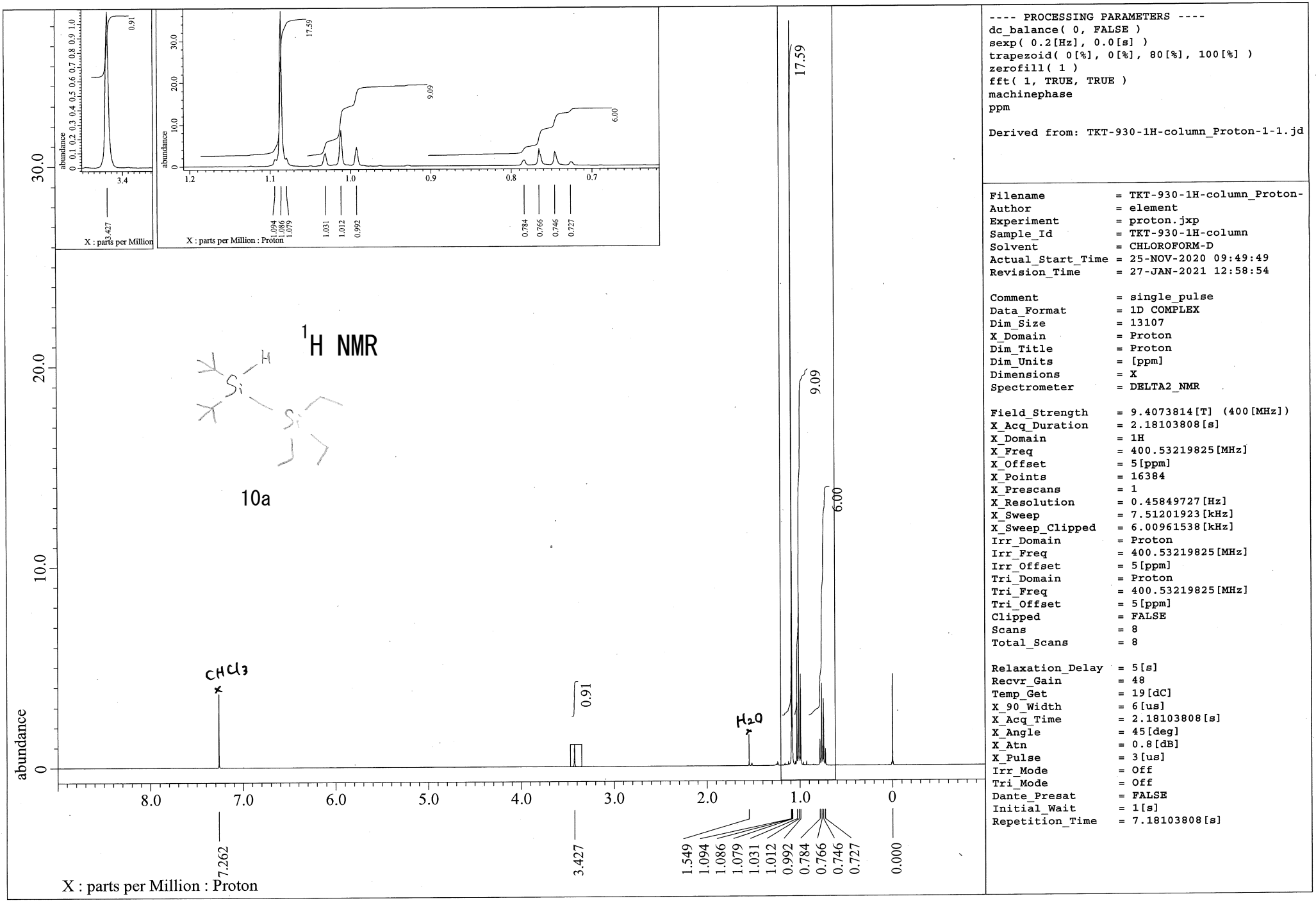

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: TKT-927-11B-1.jdf
```

```
Filename            = TKT-927-11B-2.jdf
Author              = element
Experiment          = single_pulse_dec
Sample_Id           = 1
Solvent             = CHLOROFORM-D
Actual_Start_Time   = 29-JAN-2021 04:14:29
Revision_Time       =  1-FEB-2021 15:38:16

Comment             = single pulse decoupled ga
Data_Format         = 1D COMPLEX
Dim_Size            = 26214
X_Domain            = 11B
Dim_Title           = 11B
Dim_Units           = [ppm]
Dimensions          = X
Site                = ECX 400P
Spectrometer        = DELTA2_NMR

Field_Strength      = 9.2982153[T] (400[MHz])
X_Acq_Duration      = 0.82313216[s]
X_Domain            = 11B
X_Freq              = 127.01553457[MHz]
X_Offset            = 0[ppm]
X_Points            = 32768
X_Prescans          = 4
X_Resolution        = 1.21487174[Hz]
X_Sweep             = 39.8089172[kHz]
Irr_Domain          = 1H
Irr_Freq            = 395.88430144[MHz]
Irr_Offset          = 5[ppm]
Clipped             = FALSE
Scans               = 1024
Total_Scans         = 1024

Relaxation_Delay    = 2[s]
Recvr_Gain          = 50
Temp_Get            = 21.5[dC]
X_90_Width          = 10[us]
X_Acq_Time          = 0.82313216[s]
X_Angle             = 30[deg]
X_Atn               = 4.8[dB]
X_Pulse             = 3.33333333[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     = 2.82313216[s]
```



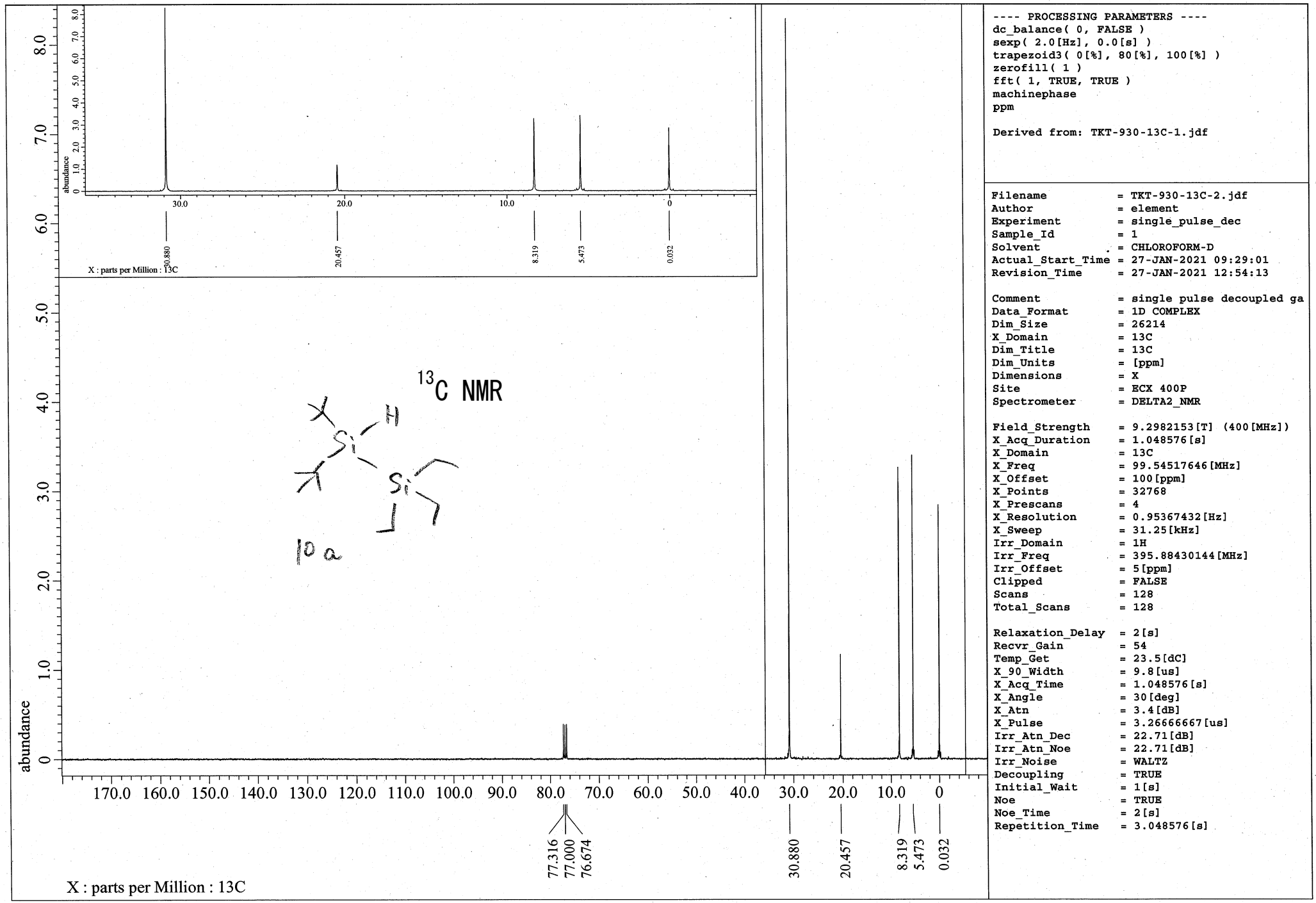

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: TKT-927-29Si_single_pulse_dec-1
```

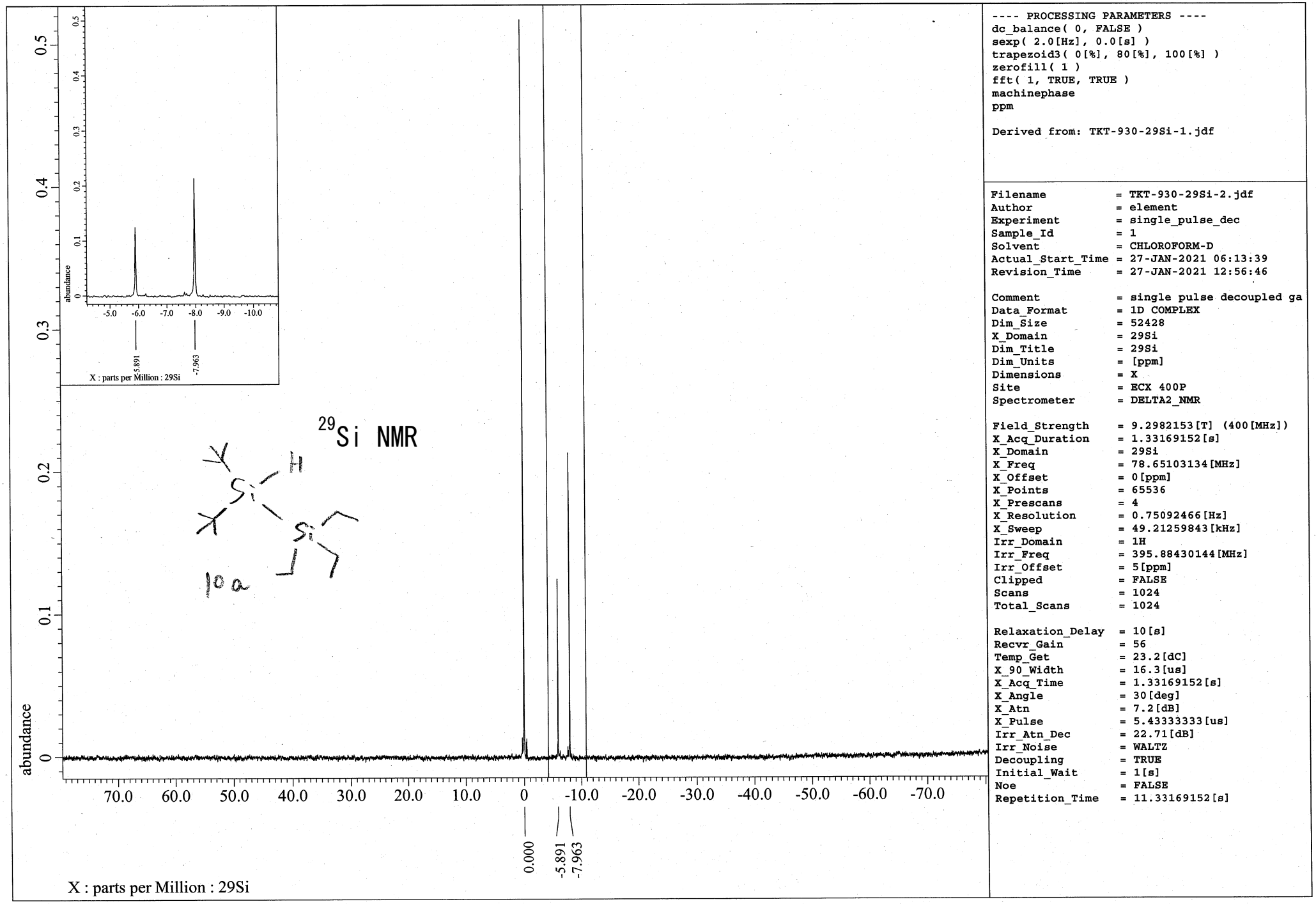
Filename	= TKT-927-29Si_singl
Author	= element
Experiment	= single_pulse_dec.j
Sample_Id	= TKT-927-29Si
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 28-JAN-2021 21:09:
Revision_Time	= 1-FEB-2021 15:39:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 52429
X_Domain	= Silicon29
Dim_Title	= Silicon29
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S3
Field_Strength	= 14.09636928[T] (60
X_Acq_Duration	= 0.88080384[s]
X_Domain	= Silicon29
X_Freq	= 119.23728868[MHz]
X_Offset	= 0[ppm]
X_Points	= 65536
X_Prescans	= 4
X_Resolution	= 1.13532657[Hz]
X_Sweep	= 74.4047619[kHz]
X_Sweep_Clipped	= 59.52380952[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 5[us]
Clipped	= FALSE
Scans	= 4096
Total_Scans	= 4096
Relaxation_Delay	= 10[s]
Recvr_Gain	= 56
Temp_Get	= 20.2[dC]
X_90_Width	= 10[us]
X_Acq_Time	= 0.88080384[s]
X_Angle	= 30[deg]
X_Atn	= 9[dB]
X_Pulse	= 3.33333333[us]
Irr_Atn_Dec	= 26.628[dB]
Irr_Atn_Dec_Calc	= 26.628[dB]
Irr_Atn_Dec_Default_Calc	= 26.628[dB]
Irr_Dec_Bandwidth_Hz	= 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.05794078[ppm]
Irr_Dec_Freq	= 600.1723046[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= FALSE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]

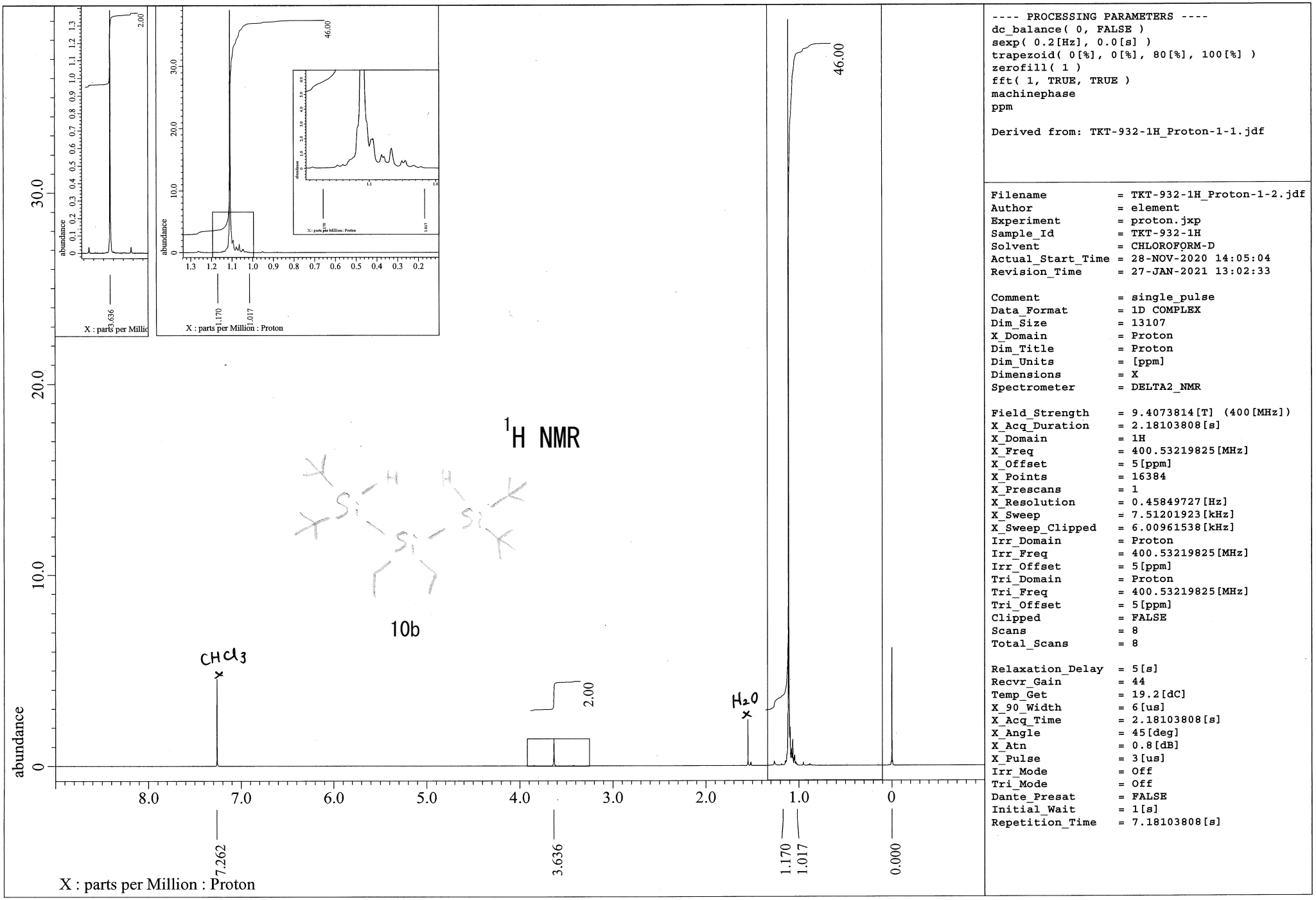


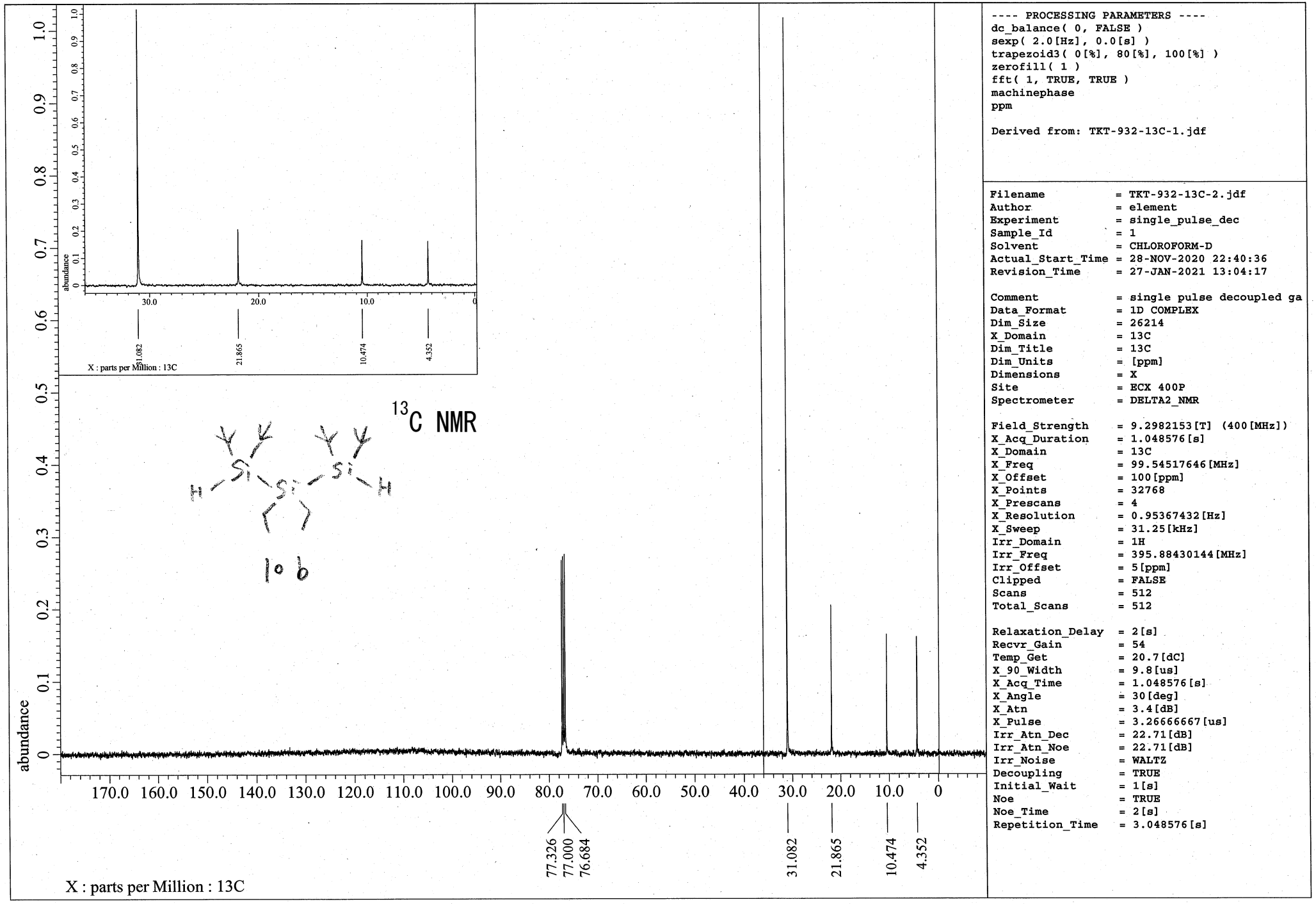

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: TKT-930-1H-column_Proton-1-1.jd
```

Filename	= TKT-930-1H-column_Proton-
Author	= element
Experiment	= proton.jxp
Sample_Id	= TKT-930-1H-column
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 25-NOV-2020 09:49:49
Revision_Time	= 27-JAN-2021 12:58:54
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.4073814[T] (400[MHz])
X_Acq_Duration	= 2.18103808[s]
X_Domain	= 1H
X_Freq	= 400.53219825[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45849727[Hz]
X_Sweep	= 7.51201923[kHz]
X_Sweep_Clipped	= 6.00961538[kHz]
Irr_Domain	= Proton
Irr_Freq	= 400.53219825[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 400.53219825[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 48
Temp_Get	= 19[dC]
X_90_Width	= 6[us]
X_Acq_Time	= 2.18103808[s]
X_Angle	= 45[deg]
X_Atn	= 0.8[dB]
X_Pulse	= 3[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.18103808[s]


13C NMR
10a
abundance
X : parts per Million : 13C
77.316
77.000
76.674
30.880
20.457
8.319
5.473
0.032
---- 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: TKT-930-13C-1.jdf
Filename = TKT-930-13C-2.jdf
Author = element
Experiment = single_pulse_dec
Sample_Id = 1
Solvent = CHLOROFORM-D
Actual_Start_Time = 27-JAN-2021 09:29:01
Revision_Time = 27-JAN-2021 12:54:13
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = 13C
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Site = 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 = 128
Total_Scans = 128
Relaxation_Delay = 2[s]
Recvr_Gain = 54
Temp_Get = 23.5[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]

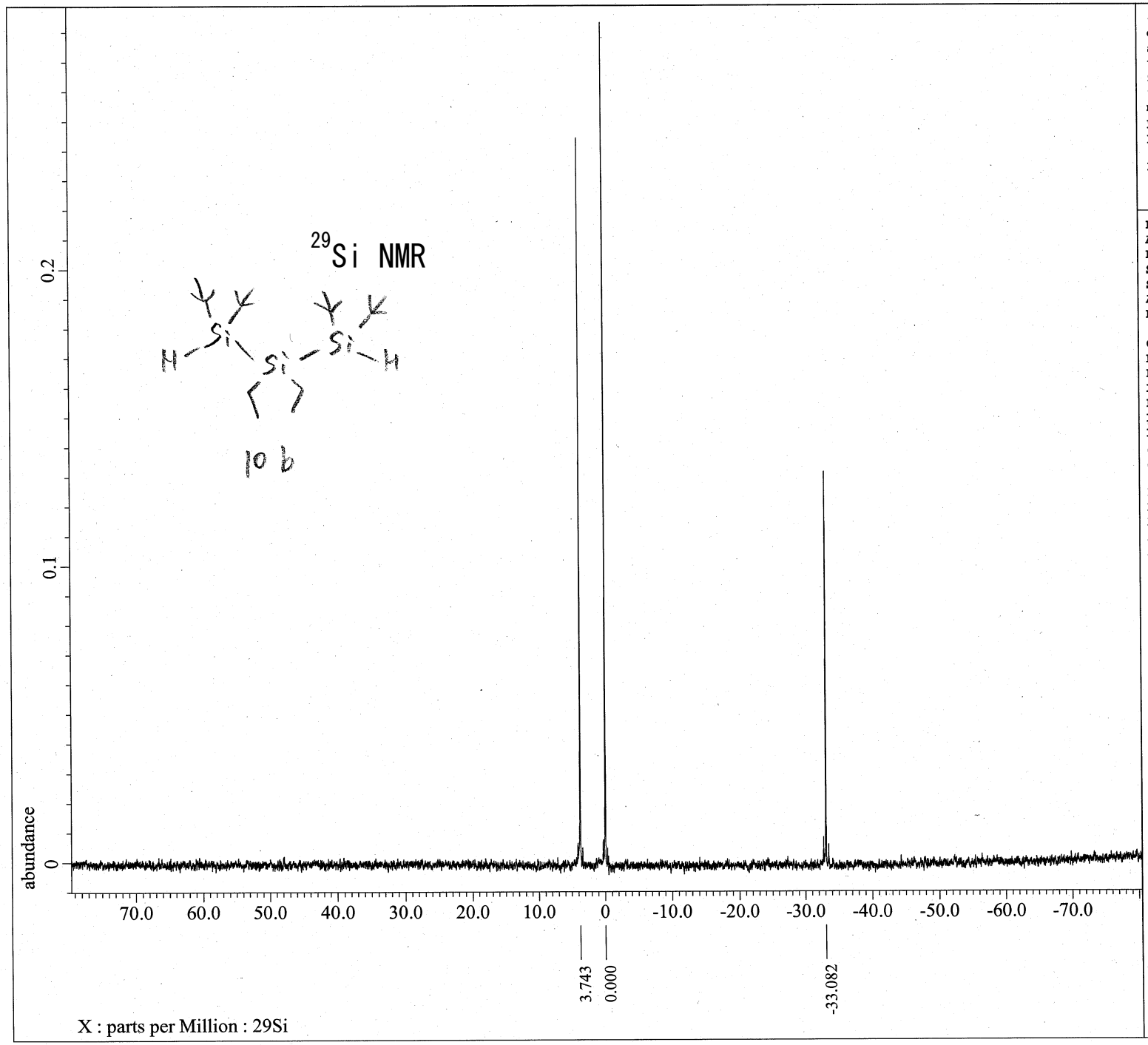

^{29}Si NMR
10a
abundance
X : parts per Million : 29Si
0.000
-5.891
-7.963
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid3(0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: TKT-930-29Si-1.jdf
Filename = TKT-930-29Si-2.jdf
Author = element
Experiment = single_pulse_dec
Sample_Id = 1
Solvent = CHLOROFORM-D
Actual_Start_Time = 27-JAN-2021 06:13:39
Revision_Time = 27-JAN-2021 12:56:46
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 52428
X_Domain = 29Si
Dim_Title = 29Si
Dim_Units = [ppm]
Dimensions = X
Site = ECX 400P
Spectrometer = DELTA2_NMR
Field_Strength = 9.2982153[T] (400[MHz])
X_Acq_Duration = 1.33169152[s]
X_Domain = 29Si
X_Freq = 78.65103134[MHz]
X_Offset = 0[ppm]
X_Points = 65536
X_Prescans = 4
X_Resolution = 0.75092466[Hz]
X_Sweep = 49.21259843[kHz]
Irr_Domain = 1H
Irr_Freq = 395.88430144[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 1024
Total_Scans = 1024
Relaxation_Delay = 10[s]
Recvr_Gain = 56
Temp_Get = 23.2[dC]
X_90_Width = 16.3[us]
X_Acq_Time = 1.33169152[s]
X_Angle = 30[deg]
X_Atn = 7.2[dB]
X_Pulse = 5.43333333[us]
Irr_Atn_Dec = 22.71[dB]
Irr_Noise = WALTZ
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = FALSE
Repetition_Time = 11.33169152[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: TKT-932-1H_Proton-1-1.jdf
Filename = TKT-932-1H_Proton-1-2.jdf
Author = element
Experiment = proton.jxp
Sample_Id = TKT-932-1H
Solvent = CHLOROFORM-D
Actual_Start_Time = 28-NOV-2020 14:05:04
Revision_Time = 27-JAN-2021 13:02:33
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 = 19.2[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]
^{1}H NMR
10b
CHCl3
H2O
2.00
46.00
abundance
X : parts per Million : Proton
7.262
3.636
1.170
1.017
0.000



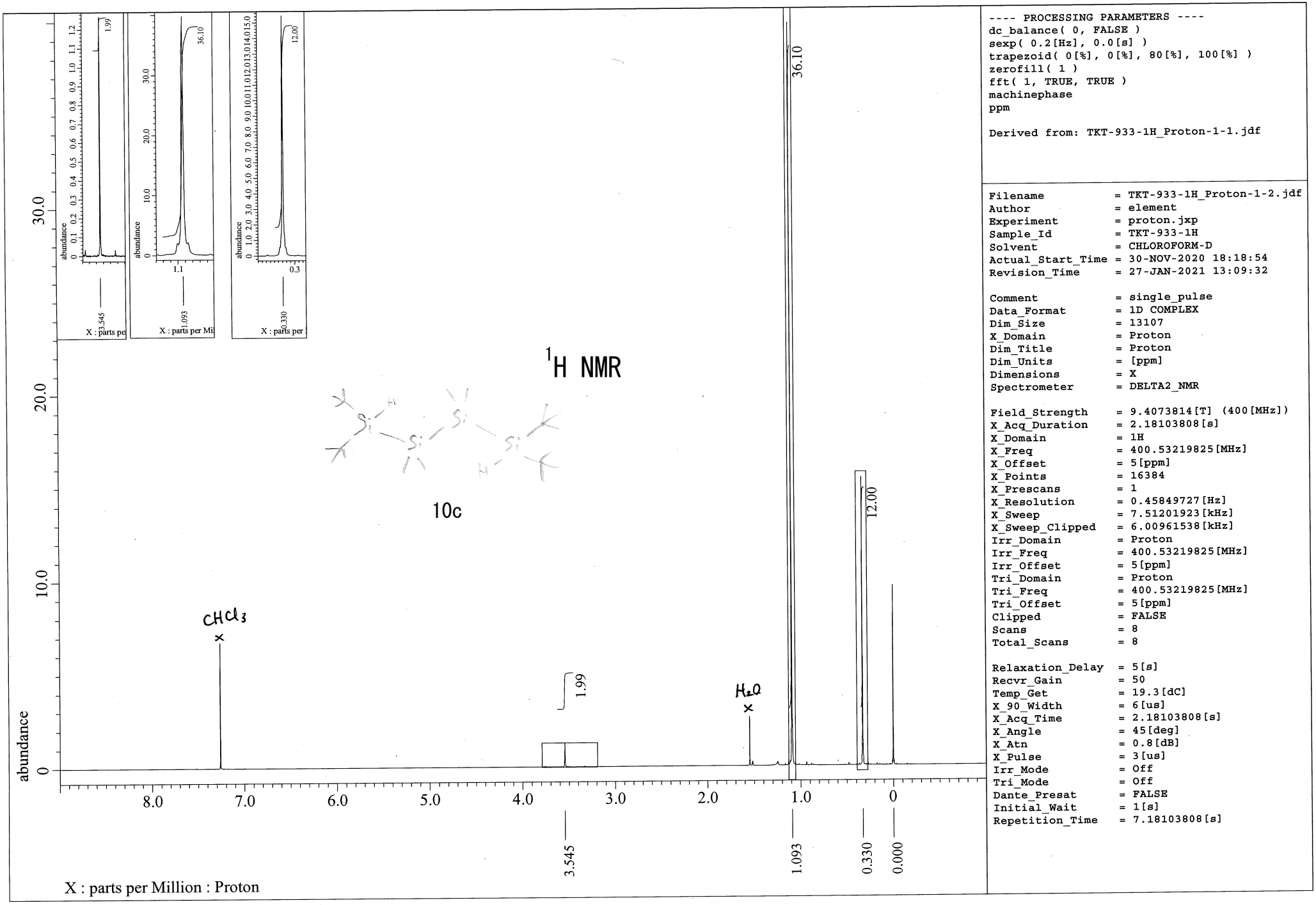

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: TKT-932-13C-1.jdf
```

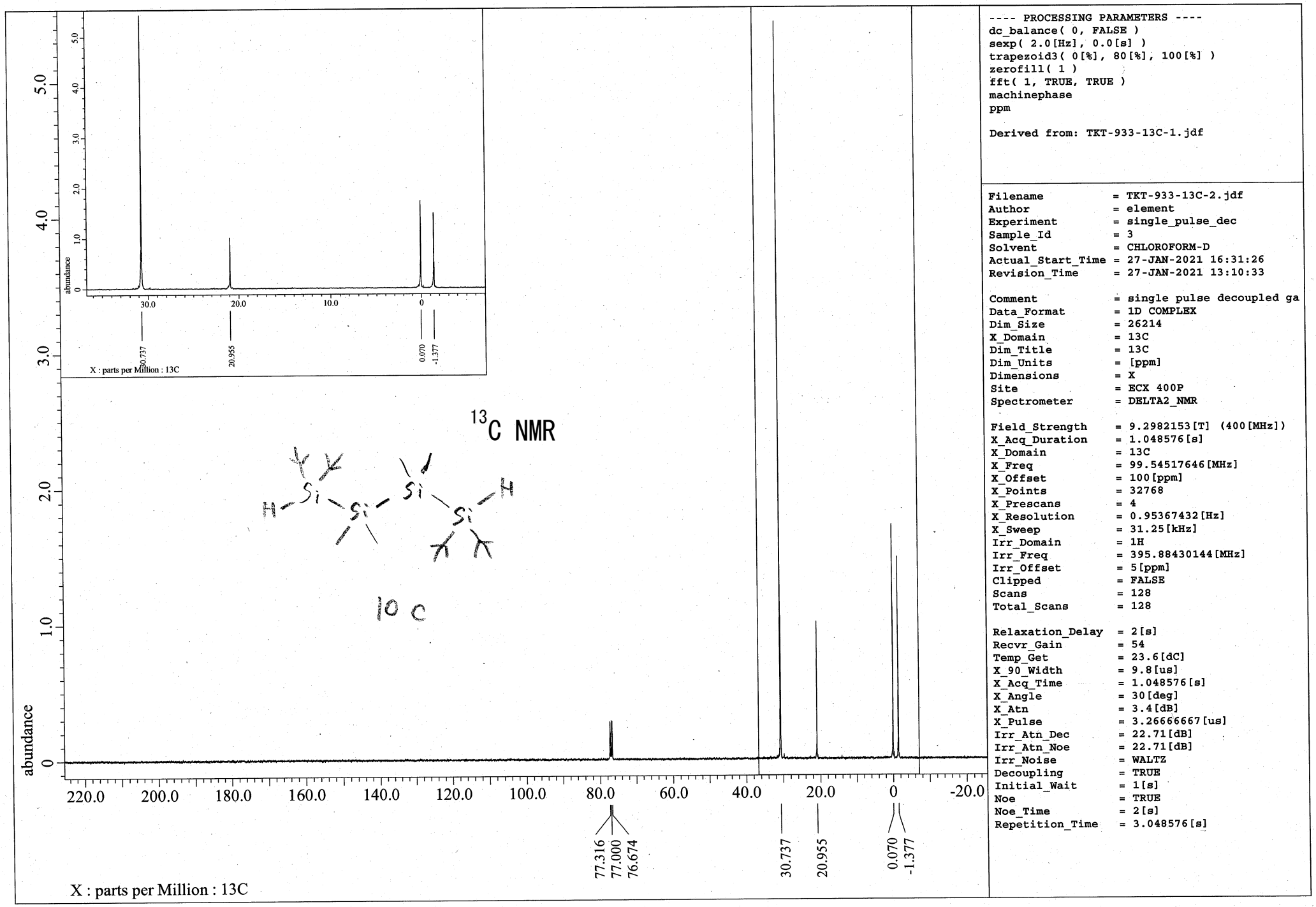
Filename	= TKT-932-13C-2.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= 1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 28-NOV-2020 22:40:36
Revision_Time	= 27-JAN-2021 13:04:17
Comment	= single pulse decoupled ga
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= 13C
Dim_Title	= 13C
Dim_Units	= [ppm]
Dimensions	= X
Site	= 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	= 512
Total_Scans	= 512
Relaxation_Delay	= 2[s]
Recvr_Gain	= 54
Temp_Get	= 20.7[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]

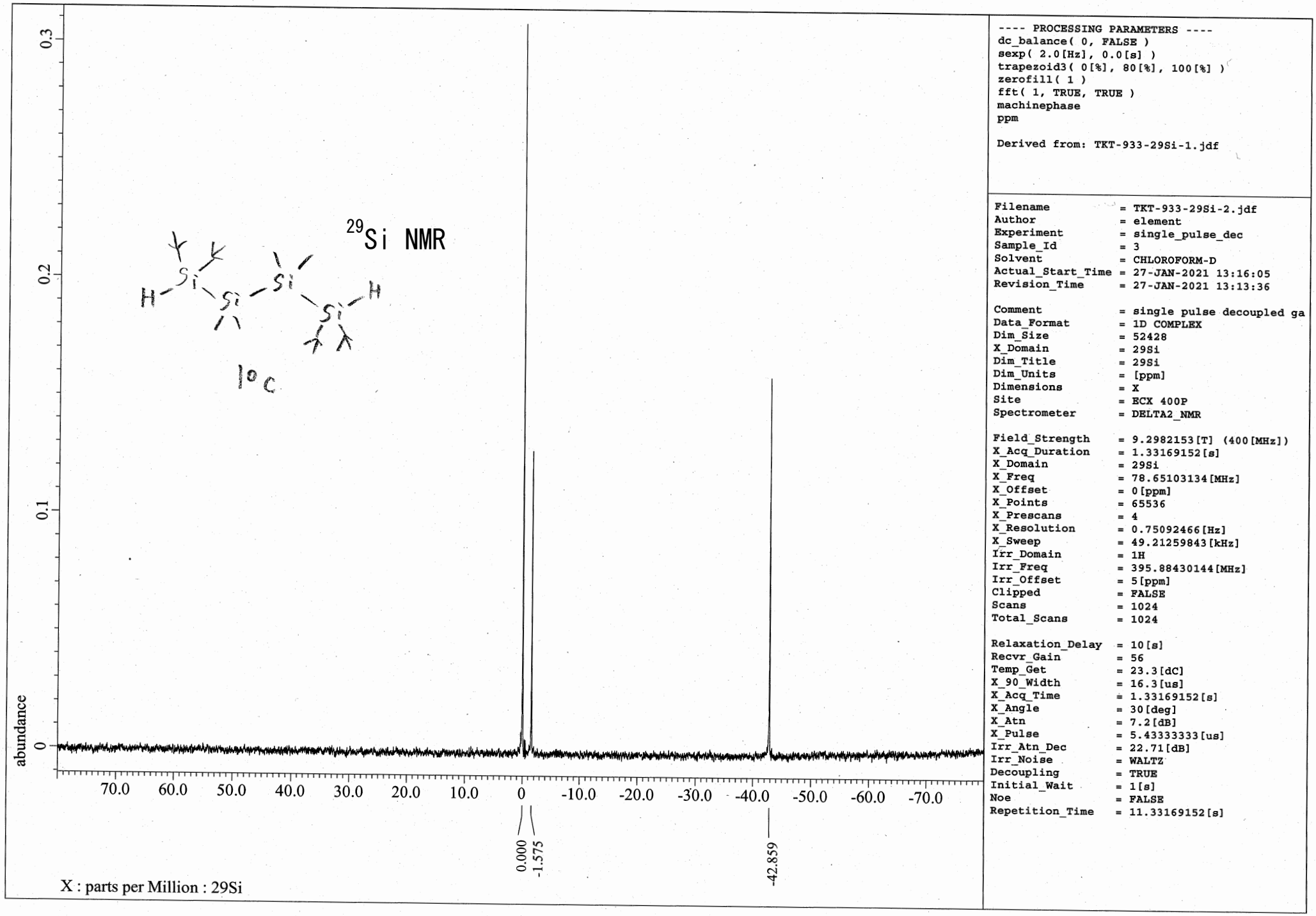



```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
phase( 68.91786, 0, 50[%] )

Derived from: TKT-932-29Si-2.jdf
```

Filename	= TKT-932-29Si-3.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= 2
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 27-JAN-2021 09:52:12
Revision_Time	= 27-JAN-2021 13:05:36
Comment	= single pulse decoupled ga
Data_Format	= 1D COMPLEX
Dim_Size	= 52428
X_Domain	= 29Si
Dim_Title	= 29Si
Dim_Units	= [ppm]
Dimensions	= X
Site	= ECX 400P
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.2982153[T] (400[MHz])
X_Acq_Duration	= 1.33169152[s]
X_Domain	= 29Si
X_Freq	= 78.65103134[MHz]
X_Offset	= 0[ppm]
X_Points	= 65536
X_Prescans	= 4
X_Resolution	= 0.75092466[Hz]
X_Sweep	= 49.21259843[kHz]
Irr_Domain	= 1H
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 1024
Total_Scans	= 1024
Relaxation_Delay	= 10[s]
Recvr_Gain	= 56
Temp_Get	= 23.2[dC]
X_90_Width	= 16.3[us]
X_Acq_Time	= 1.33169152[s]
X_Angle	= 30[deg]
X_Atn	= 7.2[dB]
X_Pulse	= 5.43333333[us]
Irr_Atn_Dec	= 22.71[dB]
Irr_Noise	= WALTZ
Decoupling	= TRUE
Initial_Wait	= 1[s]
Noe	= FALSE
Repetition_Time	= 11.33169152[s]


1H NMR
10c
CHCl3
H2O
1.99
36.10
12.00
3.545
1.093
0.330
0.000
abundance
X : parts per Million : Proton
---- 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: TKT-933-1H_Proton-1-1.jdf
Filename = TKT-933-1H_Proton-1-2.jdf
Author = element
Experiment = proton.jxp
Sample_Id = TKT-933-1H
Solvent = CHLOROFORM-D
Actual_Start_Time = 30-NOV-2020 18:18:54
Revision_Time = 27-JAN-2021 13:09:32
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = DELTA2_NMR
Field_Strength = 9.4073814[T] (400[MHz])
X_Acq_Duration = 2.18103808[s]
X_Domain = 1H
X_Freq = 400.53219825[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45849727[Hz]
X_Sweep = 7.51201923[kHz]
X_Sweep_Clipped = 6.00961538[kHz]
Irr_Domain = Proton
Irr_Freq = 400.53219825[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 400.53219825[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 50
Temp_Get = 19.3[dC]
X_90_Width = 6[us]
X_Acq_Time = 2.18103808[s]
X_Angle = 45[deg]
X_Atn = 0.8[dB]
X_Pulse = 3[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 7.18103808[s]


13C NMR
10 C
abundance
X : parts per Million : 13C
77.316
77.000
76.674
30.737
20.955
0.070
-1.377
---- 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: TKT-933-13C-1.jdf
Filename = TKT-933-13C-2.jdf
Author = element
Experiment = single_pulse_dec
Sample_Id = 3
Solvent = CHLOROFORM-D
Actual_Start_Time = 27-JAN-2021 16:31:26
Revision_Time = 27-JAN-2021 13:10:33
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = 13C
Dim_Title = 13C
Dim_Units = [ppm]
Dimensions = X
Site = 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 = 128
Total_Scans = 128
Relaxation_Delay = 2[s]
Recvr_Gain = 54
Temp_Get = 23.6[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( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: TKT-933-29Si-1.jdf
```

Filename	= TKT-933-29Si-2.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= 3
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 27-JAN-2021 13:16:05
Revision_Time	= 27-JAN-2021 13:13:36
Comment	= single pulse decoupled ga
Data_Format	= 1D COMPLEX
Dim_Size	= 52428
X_Domain	= 29Si
Dim_Title	= 29Si
Dim_Units	= [ppm]
Dimensions	= X
Site	= ECX 400P
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.2982153[T] (400[MHz])
X_Acq_Duration	= 1.33169152[s]
X_Domain	= 29Si
X_Freq	= 78.65103134[MHz]
X_Offset	= 0[ppm]
X_Points	= 65536
X_Prescans	= 4
X_Resolution	= 0.75092466[Hz]
X_Sweep	= 49.21259843[kHz]
Irr_Domain	= 1H
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 1024
Total_Scans	= 1024
Relaxation_Delay	= 10[s]
Recvr_Gain	= 56
Temp_Get	= 23.3[dC]
X_90_Width	= 16.3[us]
X_Acq_Time	= 1.33169152[s]
X_Angle	= 30[deg]
X_Atn	= 7.2[dB]
X_Pulse	= 5.43333333[us]
Irr_Atn_Dec	= 22.71[dB]
Irr_Noise	= WALTZ
Decoupling	= TRUE
Initial_Wait	= 1[s]
Noe	= FALSE
Repetition_Time	= 11.33169152[s]