Mechanochemistry-directed ligand design for enhanced reactivity and enantioselectivity in solvent-less palladium-catalyzed conjugate arylations

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1. Chemicals and instrumentation

Materials were obtained from commercial suppliers and used as received. Solvents for the synthesis of starting materials and liquid additives for mechanochemical reactions were also purchased from commercial suppliers and dried over molecular sieves (MS 4A) prior to use. All mechanochemical reactions were carried out using grinding vessels in a Retsch MM400 mill (Figure S1). Both jars (1.5 mL) and balls (7 mm) are made of stainless (SUS400B and SUS420J2, respectively) (Figure S2). The heat gun Takagi HG-1450B with a temperature control function was used for high-temperature ball-milling reactions (Figure S3). NMR spectra were recorded on JEOL JNM-EC X400P and JNM-ECS400 spectrometers (^{1}H: 392 or 396 or 399 or 401 MHz, ^{13}C: 99 or 100 or 101 MHz). Tetramethylsilane (^{1}H) and $CDCl_3$ (^{13}C) were employed as external standards, respectively. Multiplicity was recorded as follows: s = singlet, brs = broad singlet, d = doublet, t = triplet, q = quartet, quint = quintet, sept = septet, o = octet, m = multiplet. 1,1,2,2-Tetrachloroethane was used as an internal standard to determine NMR yields. HPLC analyses with chiral stationary phase were carried out using a Hitachi LaChrome Elite HPLC system with a L-2400 UV detector. Specific optical rotations were measured with HORIBA SEPA-300 and a Rudolph Research Analytical Autopol IV Polarimeter. Size exclusion chromatography (SEC) was performed at 40 °C using a Jasco high-performance liquid chromatography system using THF as an eluent. The number-average molecular weight (M_n) and polydispersity index (PDI) of the PEGylated ligands were calculated based on a polystyrene calibration. Transmission electron microscopy analysis was carried out at "Joint-Use Facilities: Laboratory of Nano-Micro Material Analysis", Hokkaido University. High-resolution mass spectra were recorded at the Global Facility Center, Hokkaido University.

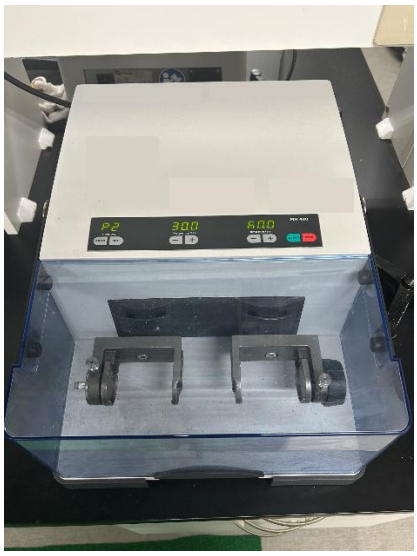


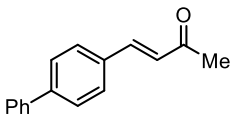
Figure S1. Retsch MM400 used in this study.

Figure S2. Stainless jar (1.5 mL) and balls (7 mm) used in this study.

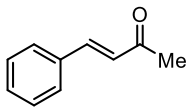
Figure S3. The temperature-controllable heat gun Takagi HG-1450B used in this study.

2. List of substrates

(a) conjugate ketones



1a



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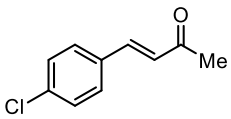

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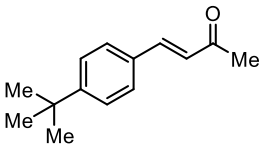

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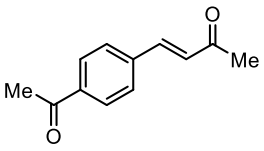

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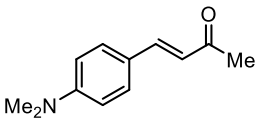

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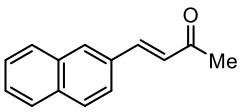

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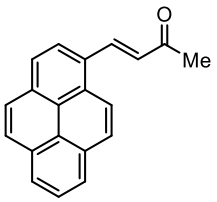
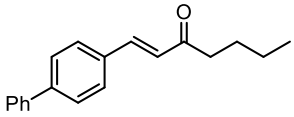
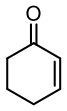


1h



1i



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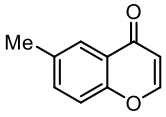

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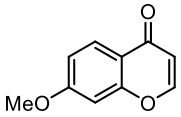
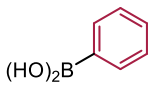


4b

(b) boronic acids



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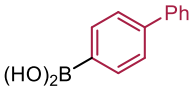

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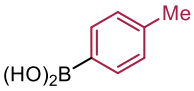

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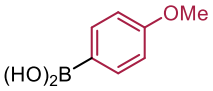

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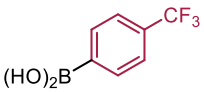

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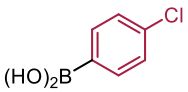

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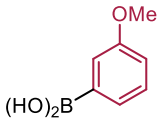

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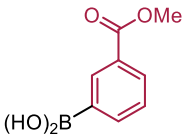

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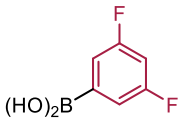

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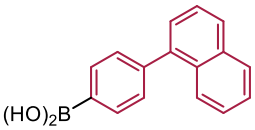

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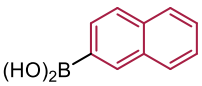

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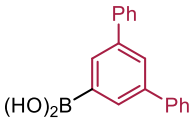
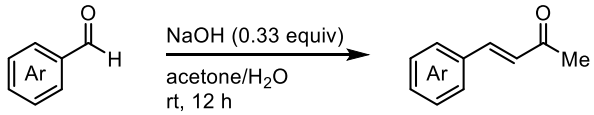


2l

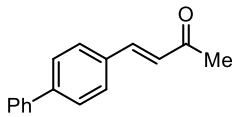
3. Substrate preparation

Preparation of conjugated ketones (1a, 1c, 1d, 1f, 1g and 1h).



In a 50 mL two-neck round-bottomed flask, the corresponding aldehyde (5.0 mmol) and NaOH (1.7 mmol) were dissolved in acetone (3.3 mL) and H_2O (5.0 mL) under a nitrogen atmosphere at room temperature. After stirring for 12 hours, the reaction mixture was transferred to a funnel, and the organic layer was extracted with CH_2Cl_2 (30 mL×3). The solution was dried over $MgSO_4$, filtered, and evaporated in vacuo. The crude material was purified by recrystallization from ethanol or flash chromatography (SiO_2, typically EtOAc/hexane, typically 0–10:90) to give the corresponding product.

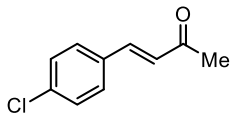
(*E*)-4-[(1,1'-Biphenyl)-4-yl]but-3-en-2-one (1a).



The reaction was carried out with 911.0 mg (5.0 mmol) of biphenyl-4-carboxaldehyde. **1a** was obtained as a white solid (553.9 mg, 2.5 mmol, 50% yield) after purification by silica-gel column chromatography (SiO_2, EtOAc/hexane, 0:100–40:60). The ^1H and ^{13}C NMR spectra were consistent with the literature.[1]

^1H NMR (399 MHz, $CDCl_3$, δ): 2.41 (s, 3H), 6.77 (d, J = 16.4 Hz, 1H), 7.35–7.42 (m, 1H), 7.47 (t, J = 7.6 Hz, 2H), 7.56 (d, J = 16.4 Hz, 1H), 7.59–7.67 (m, 6H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 27.7 (*C*H_3), 127.07 (*C*H), 127.15 (*C*H), 127.7 (*C*H), 128.0 (*C*H), 128.9 (*C*H), 129.0 (*C*H), 133.4 (*C*H), 140.1 (*C*), 143.1 (*C*), 143.4 (*C*), 198.5 (*C*). HRMS-ESI (m/z): $[M+H]^+$ calcd for $C_{16}H_{15}O$, 223.1117; found, 223.1115.

(*E*)-4-(4-Chlorophenyl)but-3-en-2-one (1c).

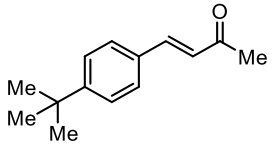


The reaction was carried out with 711.2 mg (5.1 mmol) of 4-chlorobenzaldehyde. **1c** was obtained as a white solid (445.3 mg, 2.5 mmol, 49% yield) after purification by recrystallization from ethanol. The ^1H and ^{13}C NMR spectra were consistent with the literature.[1]

^1H NMR (392 MHz, $CDCl_3$, δ): 2.39 (s, 3H), 6.69 (d, J = 16.1 Hz, 1H), 7.33–7.41 (m, 2H), 7.44–

7.51 (m, 3H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 27.8 (*C*H_3), 127.5 (*C*H), 129.3 (*C*H), 129.5 (*C*H), 133.0 (*C*), 136.5 (*C*), 142.0 (*C*H), 198.2 (*C*). HRMS-ESI (*m*/*z*): $[M+H]^+$ calcd for $C_{10}H_{10}ClO$, 181.0415; found, 181.0416.

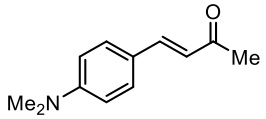
(*E*)-4-[4-(t*ert*-Butyl)phenyl]but-3-en-2-one (1d).



The reaction was carried out with 809.1 mg (5.0 mmol) of 4-*tert*-butylbenzaldehyde. **1d** was obtained as a white solid (403.2 mg, 2.0 mmol, 40% yield) after purification by recrystallization from ethanol. The ^{1}H and ^{13}C NMR spectra were consistent with the literature.[2]

^{1}H NMR (401 MHz, $CDCl_3$, δ): 1.33 (s, 9H), 2.38 (s, 3H), 6.70 (d, *J* = 16.0 Hz, 1H), 7.40–7.46 (m, 2H), 7.47–7.54 (m, 3H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 27.6 (*C*H_3), 31.3 (*C*H_3), 35.1 (*C*), 126.1 (*C*H), 126.6 (*C*H), 128.3 (*C*H), 131.8 (*C*), 143.6 (*C*H), 154.3 (*C*), 198.7 (*C*). HRMS-ESI (*m*/*z*): $[M+H]^+$ calcd for $C_{14}H_{19}O$, 203.1430; found, 203.1428.

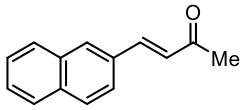
(*E*)-4-[4-(Dimethylamino)phenyl]but-3-en-2-one (1f).



The reaction was carried out with 745.3 mg (5.0 mmol) of 4-dimethylaminobenzaldehyde. **1f** was obtained as a yellow solid (797.8 mg, 4.2 mmol, 84% yield) after purification by silica-gel column chromatography (SiO_2, EtOAc/hexane, 0:100–40:60). The ^{1}H and ^{13}C NMR spectra were consistent with the literature.[3]

^{1}H NMR (401 MHz, $CDCl_3$, δ): 2.35 (s, 3H), 3.04 (s, 6H), 6.55 (d, *J* = 15.8 Hz, 1H), 6.66–6.71 (m, 2H), 7.42–7.50 (m, 3H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 27.0 (*C*H_3), 39.9 (*C*H_3), 111.7 (*C*H), 121.7 (*C*), 122.0 (*C*H), 129.9 (*C*H), 144.3 (*C*H), 151.8 (*C*), 198.2 (*C*). HRMS-EI (m/z): $[M]^+$ calcd for $C_{12}H_{15}NO$, 189.1148; found, 189.1147.

(*E*)-4-(Naphthalen-2-yl)but-3-en-2-one (1g).

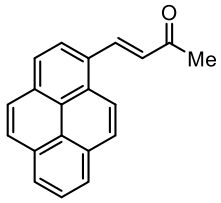


The reaction was carried out with 782.4 mg (5.0 mmol) of 2-naphthaldehyde. **1g** was obtained as a white solid (359.3 mg, 1.9 mmol, 39% yield) after purification by recrystallization from

ethanol. The ^{1}H and ^{13}C NMR spectra were consistent with the literature.[4]

^{1}H NMR (399 MHz, $CDCl_3$, δ): 2.43 (s, 3H), 6.84 (d, J = 15.8 Hz, 1H), 7.49–7.58 (m, 2H), 7.65–7.73 (m, 2H), 7.79–7.91 (m, 3H), 7.96 (s, 1H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 27.5 (*C*H_3), 123.4 (*C*H), 126.7 (*C*H), 127.1 (*C*H), 127.3 (*C*H), 127.7 (*C*H), 128.5 (*C*H), 128.7 (*C*H), 130.3 (*C*H), 131.8 (*C*), 133.1 (*C*), 134.2 (*C*), 143.4 (*C*H), 198.2 (*C*). HRMS-EI (m/z): $[M]^+$ calcd for $C_{14}H_{12}O$, 196.0883; found, 196.0881.

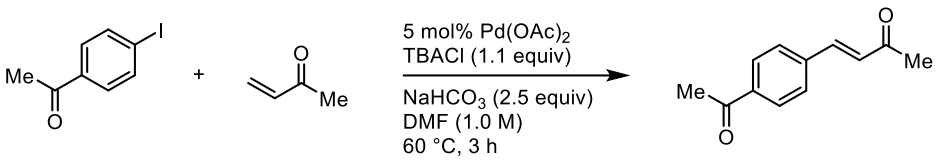
(*E*)-4-(Pyren-1-yl)but-3-en-2-one (1h).



The reaction was carried out with 3.45 g (15.0 mmol) of 1-pyrenecarboxaldehyde. **1h** was obtained as a yellow solid (3.57 g, 13.2 mmol, 88% yield) after purification by recrystallization from ethanol. The ^{1}H and ^{13}C NMR spectra were consistent with the literature.[5]

^{1}H NMR (401 MHz, $CDCl_3$, δ): 2.54 (s, 3H), 7.03 (d, J = 16.0 Hz, 1H), 8.00–8.29 (m, 7H), 8.31 (d, J = 8.0 Hz, 1H), 8.48 (d, J = 9.2 Hz, 1H), 8.70 (d, J = 16.0 Hz, 1H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 28.3 (*C*H_3), 122.2 (*C*H), 124.2 (*C*H), 124.6 (*C*), 124.9 (*C*), 125.1 (*C*H), 126.0 (*C*H), 126.2 (*C*H), 126.4 (*C*H), 127.4 (*C*H), 128.1 (*C*), 128.70 (*C*H), 128.74 (*C*H), 128.8 (*C*H), 130.0 (*C*), 130.7 (*C*), 131.3 (*C*), 132.9 (*C*), 139.9 (*C*H), 198.3 (*C*). HRMS-ESI (*m*/*z*): $[M+H]^+$ calcd for $C_{20}H_{15}O$, 271.1117; found, 271.1113.

Preparation of (*E*)-4-(4-acetylphenyl)but-3-en-2-one (1e).

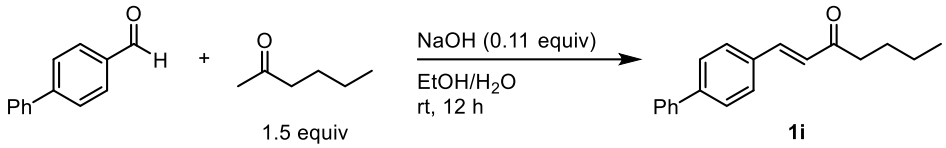


In a 50 mL two-neck round-bottomed flask, 4'-iodoacetophenone (1.24 g, 5.0 mmol) and $Pd(OAc)_2$ (58.1 mg, 0.26 mmol), TBACl (1.47 g, 5.3 mmol), and $NaHCO_3$ (1.07 g, 12.8 mmol) were dissolved in DMF (5.0 mL) under a nitrogen atmosphere. To the mixture, methyl vinyl ketone (820 μL, 10.0 mmol) was added, then stirred at 60 °C for 3 hours. After cooling the reaction mixture to room temperature, the reaction was quenched with H_2O. The reaction mixture was transferred to a funnel and the organic layer was extracted with EtOAc (30 mL×3). The solution was dried over $MgSO_4$, filtered, and evaporated in vacuo. The crude material was purified by silica-gel column chromatography (SiO_2, EtOAc/hexane, 0:100–50:50) to give **1e** (807.0 mg, 4.3

mmol, 85% yield) as a white solid. The ^{1}H and ^{13}C NMR spectra were consistent with the literature.[6]

^{1}H NMR (401 MHz, $CDCl_3$, δ): 2.42 (s, 3H), 2.63 (s, 3H), 6.80 (d, J = 16.0 Hz, 1H), 7.53 (d, J = 16.0 Hz, 1H), 7.64 (d, J = 8.4 Hz, 2H), 7.99 (d, J = 8.0 Hz, 2H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 26.8 (*C*H_3), 27.9 (*C*H_3), 128.4 (*C*H), 129.0 (*C*H), 129.2 (*C*H), 138.2 (*C*), 138.9 (*C*), 141.8 (*C*H), 197.4 (*C*), 198.2 (*C*). HRMS-ESI (*m*/*z*): $[M+H]^+$ calcd for $C_{12}H_{13}O_2$, 189.0910; found, 189.0909.

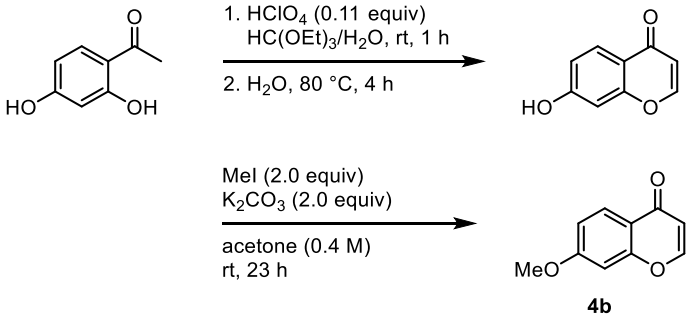
Preparation of (*E*)-1-[(1,1'-biphenyl)-4-yl]hex-1-en-3-one (1i).



In a 50 mL two-neck round-bottomed flask, biphenyl-4-carboxaldehyde (922.0 mg, 5.1 mmol) and NaOH (23.0 mg, 0.58 mmol) were dissolved in EtOH (9.0 mL) and H_2O (200 μL) under a nitrogen atmosphere. To the mixture, 2-hexanone (930 μL, 7.5 mmol) was added, then stirred at room temperature for 12 hours. The reaction mixture was transferred to a funnel and the organic layer was extracted with CH_2Cl_2 (30 mL×3). The solution was dried over $MgSO_4$, filtered, and evaporated in vacuo. The crude material was purified by recrystallization from ethanol to give **1i** (731.8 mg, 2.8 mmol, 55% yield) as a white solid.

^{1}H NMR (392 MHz, $CDCl_3$, δ): 0.96 (t, J = 7.4 Hz, 3H), 1.40 (sxt, J = 7.4 Hz, 2H), 1.68 (quint, J = 7.5 Hz, 2H), 2.69 (t, J = 7.4 Hz, 2H), 6.79 (d, J = 16.1 Hz, 1H), 7.35–7.41 (m, 1H), 7.46 (t, J = 7.2 Hz, 2H), 7.55–7.67 (m, 7H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 14.1 (*C*H_3), 22.6 (*C*H_2), 26.6 (*C*H_2), 40.9 (*C*H_2), 126.2 (*C*H), 127.2 (*C*H), 127.7 (*C*H), 128.0 (*C*H), 128.89 (*C*H), 129.04 (*C*H), 133.7 (*C*), 140.2 (*C*), 142.0 (*C*H), 143.3 (*C*), 200.8 (*C*). HRMS-ESI (*m*/*z*): $[M+H]^+$ calcd for $C_{19}H_{21}O$, 265.1587; found, 265.1581.

Preparation of 7-methoxy-4*H*-chromen-4-one (4b).



In a 100 mL round-bottomed flask, 1-(2,4-dihydroxyphenyl)ethan-1-one (998.4 mg, 6.6 mmol) was dissolved in triethyl orthoformate (5.8 mL) under a nitrogen atmosphere. To the mixture,

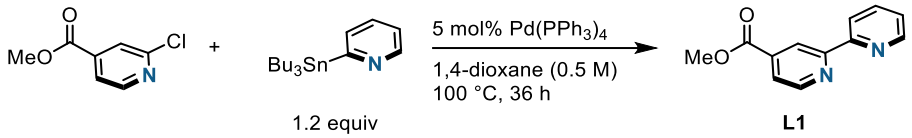
perchloric acid (60% in H_2O, 770 μL) was added dropwise, then stirred at room temperature for 1 hour. 50 mL of Et_2O was added to the reaction mixture, and a large amount of red solid precipitated. After suction filtration, the red solid was dissolved in 30 mL of water to form a suspension and stirred at 80 ℃ for 4 hours. After cooling the reaction mixture, the mixture was transferred to a funnel and the organic layer was extracted with EtOAc (30 mL×3). The solution was dried over $MgSO_4$, filtered, and evaporated in vacuo. The crude material was purified by silica-gel column chromatography (SiO_2, EtOAc/hexane, 0:100–10:90) to give 7-hydroxy-4*H*-chromen-4-one (687.6 mg, 4.2 mmol, 65% yield) as a brown solid.

In an oven-dried 100 mL two-neck round-bottomed flask, 7-hydroxy-4*H*-chromen-4-one (687.6 mg, 4.2 mmol) and K_2CO_3 (1.16 g, 8.4 mmol) were dissolved in acetone (10.5 mL) under a nitrogen atmosphere. To the mixture, methyl iodide (520 μL, 8.4 mmol) was added, then stirred at room temperature for 23 hours. The resulting suspension was quenched by H_2O. The mixture was extracted with EtOAc three times (30 mL×3). The solution was dried over $MgSO_4$, filtered, and evaporated in vacuo. The crude material was purified by silica-gel column chromatography (SiO_2, EtOAc/hexane, 0:100–50:50) to give **4b** (526.0 mg, 3.0 mmol, 71% yield) as a brown solid. The ^1H and ^{13}C NMR spectra were consistent with the literature.[7]

^1H NMR (401 MHz, $CDCl_3$, δ): 3.91 (s, 3H), 6.29 (d, J = 6.0 Hz, 1H), 6.85 (d, J = 2.4 Hz, 1H), 6.98 (dd, J = 2.2, 8.6 Hz, 1H), 7.78 (d, J = 6.0 Hz, 1H), 8.12 (d, J = 8.8 Hz, 1H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 55.9 (*C*H_3), 100.4 (*C*H), 113.1 (*C*H), 114.6 (*C*H), 118.9 (*C*), 127.3 (*C*H), 155.0 (*C*H), 158.4 (*C*), 164.2 (*C*), 177.2 (*C*). HRMS-ESI (*m*/*z*): $[M+H]^+$ calcd for $C_{10}H_9O_3$, 177.0546; found, 177.0545.

4. Ligand synthesis

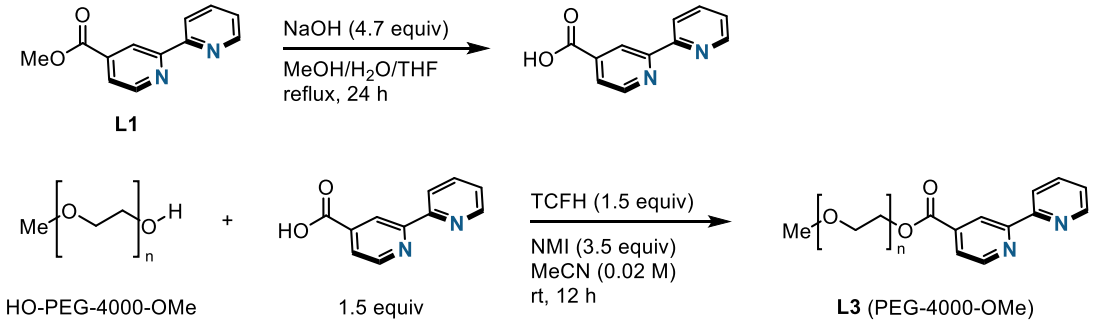
Preparation of L1.



In an oven-dried 100 mL two-neck round-bottomed flask, methyl 2-chloroisonicotinate (862.0 mg, 5.0 mmol) and $Pd(PPh_3)_4$ (304.1 mg, 0.26 mmol) were dissolved in 1,4-dioxane (10 mL) under a nitrogen atmosphere. To the reaction mixture, tributyl(2-pyridyl)tin (1.92 mL, 6.0 mmol) was added, then stirred at 100 °C for 36 hours. After cooling the reaction mixture to room temperature, the reaction was quenched with H_2O. The mixture was extracted with EtOAc three times (30 mL×3), and the solution was dried over $MgSO_4$, filtered, and evaporated in vacuo. The crude material was purified by silica-gel column chromatography (SiO_2, EtOAc/CH_2Cl_2, 0:100–30:70) to give **L1** (706.7 mg, 3.3 mmol, 66% yield) as a white solid. The ^1H and ^{13}C NMR spectra were consistent with the literature.[8]

^1H NMR (399 MHz, $CDCl_3$, δ): 3.99 (s, 3H), 7.32–7.41 (m, 1H), 7.81–7.94 (m, 2H), 8.43 (d, J = 8.0 Hz, 1H), 8.73 (d, J = 4.0 Hz, 1H), 8.83 (d, J = 4.8 Hz, 1H), 8.95 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 52.7 (*C*H_3), 120.4 (*C*H), 121.3 (*C*H), 122.8 (*C*H), 124.2 (*C*H), 137.1 (*C*H), 138.5 (*C*), 149.4 (*C*H), 150.0 (*C*H), 155.3 (*C*), 157.3 (*C*), 165.8 (*C*). HRMS-ESI (*m*/*z*): $[M+H]^+$ calcd for $C_{12}H_{11}O_2N_2$, 215.0815; found, 215.0812.

Preparation of L3 (PEG-4000).



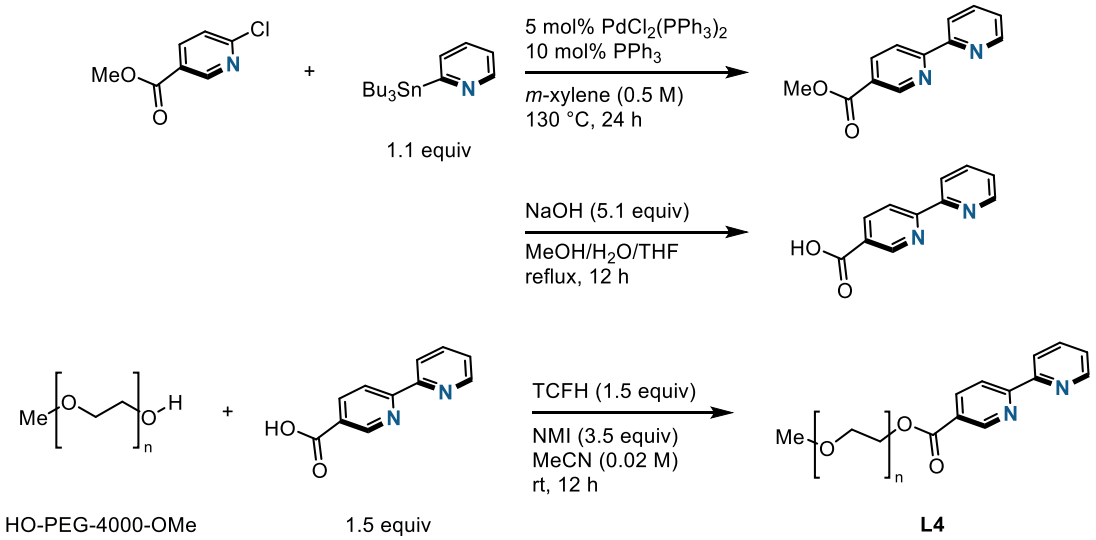
In an oven-dried 100 mL two-neck round-bottomed flask, **L1** (619.1 mg, 2.9 mmol) and NaOH (54.0 mg, 13.5 mmol) were dissolved in MeOH (1.7 mL), H_2O (6.6 mL), and THF (11 mL), and the reaction mixture was heated at reflux for 24 h under a nitrogen atmosphere. After cooling the reaction mixture to room temperature, the solvent was removed under reduced pressure, and the aqueous phase was acidified with 1 N HCl to pH 3.5−4.0. Upon cooling, a white precipitate formed and was collected by filtration. The obtained solid was washed with water and Et_2O, then dried under vacuum to afford the desired product as a white solid (373.8 mg, 1.9 mmol, 65% yield).

In a 100 mL round-bottomed flask, (2,2'-bipyridine)-4-carboxylic acid (152.5 mg, 0.76 mmol), HO-PEG-4000-OMe (2.00 g, 0.50 mmol), chloro-*N*,*N*,*N*',*N*'-tetramethylformamidinium hexafluorophosphate (TCFH) (210.1 mg, 0.75 mmol) and 1-methylimidazole (NMI) (140 μL, 1.8 mmol) were added in MeCN (25 mL) at room temperature for 12 hours. After completion of the reaction, the mixture was quenched with water and extracted with CH_2Cl_2 (3×30 mL). The combined organic layers were dried over anhydrous $MgSO_4$, filtered, and concentrated under reduced pressure. The resulting residue was treated with Et_2O, forming the precipitation of the product **L3**. The solid was collected by filtration and dried under vacuum to afford the desired PEGylated ligand **L3** as a white solid (1.72 g, 0.39 mmol, 77% yield). The absence of HO-PEG-4000-OMe in the product was confirmed by ^{1}H NMR analysis.

^{1}H NMR (401MHz, $CDCl_3$, δ): 3.38 (s, 3H), 3.47 (t, J = 5.0 Hz, 2H), 3.53–3.86 (m, 418H), 3.87 (t, J = 4.8 Hz, 2H), 4.55 (t, J = 4.8 Hz, 2H), 7.34–7.40 (m, 1H), 7.82–7.92 (m, 2H), 8.42 (d, J = 7.6 Hz, 1H), 8.73 (d, J = 4.4 Hz, 1H), 8.83 (d, J = 4.8 Hz, 1H), 8.95 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 58.6 (*C*H_3), 64.4 (*C*H_2), 68.5 (*C*H_2), 70.1 (*C*H_2), 71.5 (*C*H_2), 120.0 (*C*H), 120.8 (*C*H), 122.5 (*C*H), 123.8 (*C*H), 136.6 (*C*H), 138.1 (*C*), 149.0 (*C*H), 149.6 (*C*H), 154.8 (*C*H), 156.8 (*C*), 167.7 (*C*).

SEC was also performed, and the number-average molecular weight (M_n) and polydispersity index (PDI) of **L3** were calculated based on a polystyrene calibration; M_n of **L3**: 3.1 × 10^3 kg/mol, PDI: 1.30. The loading amount of **L3** for mechanochemical cross-coupling reactions was calculated based on the median of molecular weight dispersity.

Preparation of L4 (PEG-4000)



In an oven-dried 100 mL two-neck round-bottomed flask, methyl 6-chloronicotinate (1.73 g, 10.0 mmol), $PdCl_2(PPh_3)_2$ (355.2 mg, 0.51 mmol), and PPh_3 (275.9 mg, 1.1 mmol) were dissolved

in *m*-xylene (20 mL) under a nitrogen atmosphere. To the reaction mixture, tributyl(2-pyridyl)tin (3.52 mL, 11.0 mmol) was added, then stirred at 130 ℃ for 24 hours. After cooling the reaction mixture to room temperature, the reaction was quenched with H_2O. The mixture was extracted with EtOAc three times (30 mL×3), and the solution was dried over $MgSO_4$, filtered, and evaporated in vacuo. The crude material was purified by silica-gel column chromatography (SiO_2, EtOAc/CH_2Cl_2, 0:100–30:70) to give methyl (2,2'-bipyridine)-5-carboxylate (852.5 mg, 4.0 mmol, 40% yield) as a white solid.

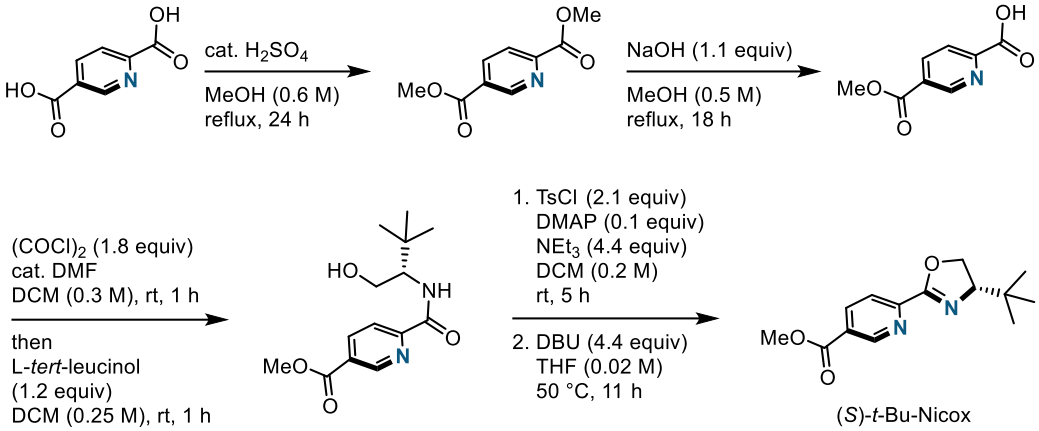
In an oven-dried 100 mL two-neck round-bottomed flask, methyl (2,2'-bipyridine)-5-carboxylate (240.2 mg, 1.1 mmol) and NaOH (206.2 mg, 5.2 mmol) were dissolved in MeOH (0.6 mL), H_2O (2.6 mL) and THF (4.3 mL), and the reaction mixture was heated at reflux for 12 h under a nitrogen atmosphere. After cooling the reaction mixture to room temperature, the solvent was removed under reduced pressure, and the aqueous phase was acidified with 1 N HCl to pH 3.5−4.0. A white precipitate separated upon cooling. It was collected by filtration, washed with water and Et_2O. The collected solids were dried under vacuum to afford the desired product as a white solid (168.5 mg, 0.84 mmol, 75% yield).

In a 50 mL round-bottomed flask, (2,2'-bipyridine)-5-carboxylic acid (61.2 mg, 0.31 mmol), HO-PEG-4000-OMe (798.1 g, 0.2 mmol), TCFH (84.3 mg, 0.3 mmol), and NMI (60 μL, 0.71 mmol) were added in MeCN (10 mL) at room temperature for 12 hours. After the reaction, the reaction was quenched by saturated $NaHCO_3$ aqueous solution. The mixture was extracted with CH_2Cl_2 three times (30 mL×3), and the solution was dried over $MgSO_4$, filtered, and evaporated in vacuo. The resulting residue was treated with Et_2O, forming the precipitation of the product **L4**. The solid was collected by filtration and dried under vacuum to afford the desired PEGylated ligand **L4** as a white solid (683.7 mg, 0.15 mmol, 77% yield). The absence of HO-PEG-4000-OMe in the product was confirmed by ^{1}H NMR analysis.

^{1}H NMR (401MHz, $CDCl_3$, δ): 3.38 (s, 3H), 3.44–3.49 (m, 2H), 3.53–3.76 (m, 402H), 3.79–3.84 (m, 2H), 3.87 (t, J = 4.8 Hz, 2H), 4.52–4.56 (m, 2H), 7.35–7.40 (m, 1H), 7.86 (td, J = 1.6, 7.8 Hz, 1H), 8.43 (dd, J = 2.4, 8.0 Hz, 1H), 8.50 (t, J = 9.2 Hz, 2H), 8.69–8.74 (m, 1H), 9.28–9.31 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 59.0 (*C*H_3), 64.5 (*C*H_2), 69.0 (*C*H_2), 70.5 (*C*H_2), 70.7 (*C*H_2), 71.9 (*C*H_2), 120.4 (*C*H), 121.9 (*C*H), 124.5 (*C*H), 125.6 (*C*), 137.0 (*C*H), 138.1 (*C*H), 149.4 (*C*H), 150.6 (*C*H), 155.0 (*C*), 159.4 (*C*), 165.2 (*C*).

SEC was also performed, and the number-average molecular weight (M_n) and polydispersity index (PDI) of **L4** were calculated based on a polystyrene calibration; M_n of **L4**: 3.7×10^3 kg/mol, PDI: 1.24. The loading amount of **L4** for mechanochemical cross-coupling reactions was calculated based on the median of molecular weight dispersity.

Preparation of (*S*)-*t*-BuNicox.



(*S*)-*t*-BuNicox was synthesized according to the literature procedure.[9] In a 500 mL two-neck round-bottomed flask, catalytic amounts of concentrated H_2SO_4 (2.1 mL) were added to a suspension of pyridine-2,5-dicarboxylic acid (16.1 g, 96.0 mmol) in MeOH (170 mL), and the reaction mixture was heated at reflux for 24 h under a nitrogen atmosphere. After cooling the mixture to room temperature, the mixture was diluted with CH_2Cl_2, washed with saturated $NaHCO_3$ aqueous solution, and dried over $MgSO_4$. Evaporation of the solvents under reduced pressure afforded dimethyl pyridine-2,5-dicarboxylate (12.2 g, 62.4 mmol, 65% yield) as a white solid, which was used without further purification.

In an oven-dried 200 mL two-neck round-bottomed flask, sodium hydroxide (1.70 g, 42.5 mmol) was added to a suspension of dimethyl pyridine-2,5-dicarboxylate (6.40 g, 32.8 mmol) in MeOH (66 mL) and the reaction mixture was heated at reflux for 18 h under a nitrogen atmosphere. At 60 °C, the reaction was carefully quenched by slow addition of 1M HCl aqueous solution (45.9 mL). The reaction mixture was cooled to 0 °C, and a precipitate was formed. After 10 min, filtration of the precipitate and washing with MeOH afforded 5-(methoxycarbonyl)picolinic acid (5.91 g, 32.6 mmol, 99% yield) as a white solid, which was used without further purification.

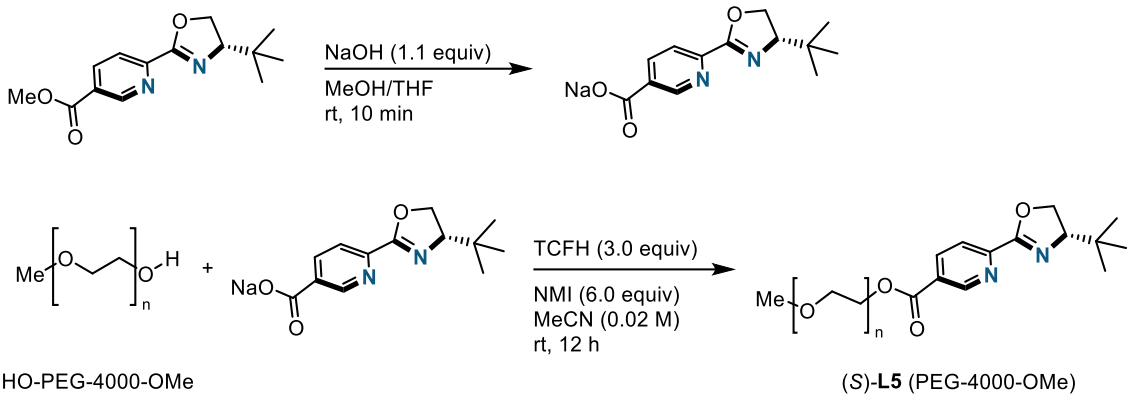
In an oven-dried 100 mL two-neck round-bottomed flask, DMF (1.0 mL) was added to a suspension of 5-(methoxycarbonyl)picolinic acid (1.81 g, 10.0 mmol) in CH_2Cl_2 (33 mL) at room temperature under a nitrogen atmosphere. Oxalyl chloride (1.5 mL, 17.5 mmol) was added dropwise over 1 h at room temperature, forming a homogenous solution. After evaporation of the solvent and the excess of oxalyl chloride, the residue was dissolved in CH_2Cl_2 (50 mL) and slowly added via syringe to a solution of L-*tert*-leucinol (1.39 g, 11.8 mmol) and Et_3N (7.0 mL, 50.0 mmol) in CH_2Cl_2 (40 mL) under a nitrogen atmosphere. The reaction mixture was stirring at a room temperature for 60 min and then washed with saturated $NaHCO_3$ aqueous solution. The aqueous layer was extracted with CH_2Cl_2, and the combined organic phases were dried over $MgSO_4$, filtered, and evaporated in vacuo. The crude material was purified by silica-gel column

chromatography (SiO_2, EtOAc/CH_2Cl_2, 0:100–50:50) to give methyl (*S*)-6-[(1-hydroxy-3-methylbutan-2-yl)carbamoyl]nicotinate (2.07 g, 7.4 mmol, 74% yield) as a white solid.

In an oven-dried 50 mL two-neck round-bottomed flask, Et_3N (4.5 mL, 32.5 mmol) was added to the solution of methyl (*S*)-6-[(1-hydroxy-3-methylbutan-2-yl)carbamoyl]nicotinate (2.01 g, 7.17 mmol) and 4-dimethylaminopyridine (DMAP) (98.8 mg, 0.81 mmol) in CH_2Cl_2 (50 mL) at room temperature under a nitrogen atmosphere. TsCl (2.85 g, 14.9 mmol) was added to the mixture. After stirring the reaction mixture for 5 hours at room temperature, the mixture was diluted with H_2O and extracted with CH_2Cl_2. The combined organic phase was dried over $MgSO_4$, filtered, and evaporated in vacuo. The resulting crude product was used without further purification.

In an oven-dried 200 mL two-neck round-bottomed flask, DBU (4.8 mL, 32.0 mmol) was added to the solution of the tosylate in THF (364 mL), and the reaction mixture was heated to 50 °C for 11 hours under a nitrogen atmosphere. After cooling to room temperature, the solvent was removed under reduced pressure. The resulting residue was diluted with H_2O, transferred into a funnel, and extracted with CH_2Cl_2 three times. The combined organic phase was dried over $MgSO_4$, and the solvents were removed under reduced pressure. The crude material was purified by silica-gel column chromatography (SiO_2, EtOAc/CH_2Cl_2, 0:100–60:40) to give (*S*)-*t*-Bu-Nicox (1.49 g, 5.7 mmol, 79% yield) as a white solid. The ^1H and ^{13}C NMR spectra were consistent with the literature.[91]H NMR (401 MHz, $CDCl_3$, δ): 0.99 (s, 9H), 3.98 (s, 3H), 4.12–4.20 (m, 1H), 4.34 (t, *J* = 8.8 Hz, 1H), 4.45–4.52 (m, 1H), 8.17 (d, *J* = 8.4 Hz, 1H), 8.38 (dd, *J* = 2.0, 8.0 Hz, 1H), 9.25–9.31 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 26.0 (*C*H_3), 34.1 (*C*), 52.7 (*C*H_3), 69.6 (*C*H_2), 76.8 (*C*H), 123.7 (*C*H), 127.3 (*C*), 137.8 (*C*H), 150.2 (*C*), 150.8 (*C*H), 162.0 (*C*), 165.3 (*C*). HRMS-ESI (*m*/*z*): $[M+H]^+$ calcd for $C_{14}H_{19}O_3N_2$, 269.1390; found, 269.1383. $[\alpha]_D^{23}$ −85.6 (c 1.0, $CHCl_3$).

Preparation of (*S*)-L5 (PEG-4000).



In an oven-dried 100 mL two-neck round-bottomed flask, (*S*)-*t*-BuNicox (262.2 mg, 1.0 mmol) and NaOH (44.2 mg, 1.1 mmol) were dissolved in MeOH (0.5 mL) and THF (3.6 mL) under a nitrogen atmosphere. After stirring for 10 minutes, the white powder was precipitated. The precipitated solid was collected by filtration and dried in vacuo. The resulting crude product was used without further purification.

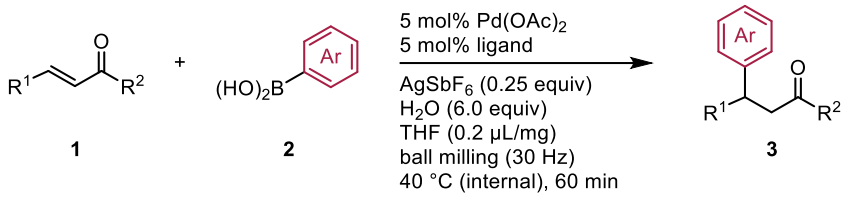
In a 100 mL round-bottomed flask, the sodium carboxylate, HO-PEG-4000-OMe (2.01 g, 0.5 mmol), TCFH (424.7 mg, 1.5 mmol), and NMI (240 μL, 3.0 mmol) were added in MeCN (25 mL) at room temperature for 12 hours. After completing the reaction, the mixture was quenched by H_2O. The resulting mixture was extracted with CH_2Cl_2 three times (30 mL×3), and the solution was dried over $MgSO_4$, filtered, and evaporated in vacuo. The obtained residue was dissolved in Et_2O to give the product (*S*)-**L5** as a precipitate. The collected solid was dried under vacuum to afford the desired product (*S*)-**L5** as a white solid (1.13 g, 0.25 mmol, 50% yield). The absence of HO-PEG-4000-OMe in the product was confirmed by ^{1}H NMR analysis.

^{1}H NMR (396 MHz, $CDCl_3$, δ): 1.05 (s, 9H), 3.38 (s, 3H), 3.44–3.48 (m, 2H), 3.53–3.90 (m, 414H), 3.95–4.04 (m, 2H), 4.51–4.57 (m, 2H), 8.29 (dd, J = 0.8, 8.3 Hz, 1H), 8.48 (dd, J = 2.4, 8.3 Hz, 1H), 9.18–9.20 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$, δ): 27.0 (*C*H_3), 33.9 (*C*), 58.9 (*C*H), 60.0 (*C*H_3), 62.8 (*C*H_2), 64.7 (*C*H_2), 68.9 (*C*H_2), 70.5 (*C*H_2), 70.6 (*C*H_2), 71.8 (*C*H_2), 121.9 (*C*H), 128.0 (*C*), 138.6 (*C*H), 149.4 (*C*H), 152.6 (*C*), 164.1 (*C*), 164.5 (*C*). $[\alpha]_D^{24}$ −0.9 (c 10.0, $CHCl_3$).

SEC was also performed, and the number-average molecular weight (M_n) and polydispersity index (PDI) of (*S*)-**L5** were calculated based on a polystyrene calibration; M_n of (*S*)-**L5**: 5.4×10^3 kg/mol, PDI: 1.21. The loading amount of (*S*)-**L5** for mechanochemical cross-coupling reactions was calculated based on the median of molecular weight dispersity.

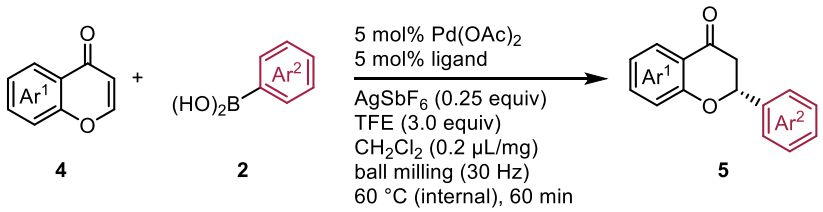
5. General procedure for the mechanochemical palladium-catalyzed conjugate addition

Procedure A: Conjugate addition to α,β-conjugated ketones



α,β-Conjugated ketones **1** (0.20 mmol), aryl boronic acid **2** (0.30 mmol, 1.5 equiv), $Pd(OAc)_2$ (0.01 mmol, 5 mol %), and ligand (0.01 mmol, 5 mol %), $AgSbF_6$ (0.05 mmol, 25 mol%) were placed in a ball milling vessel (stainless, 1.5 mL) loaded with one grinding ball (stainless, diameter: 7 mm). Then H_2O (22 μL, 6.0 equiv) and THF (0.2 μL/mg) were added via a syringe. After the vessel was closed in air without purging with inert gas, the vessel was placed in the ball mill (Retsch MM400, 60 min at 30 Hz) and a heat gun (the preset temperature at 70 °C). After 60 min, the jar was then cooled rapidly with cold water and opened. The mixture was passed through a short silica gel column eluting with CH_2Cl_2/EtOAc (100:0–50:50) to remove inorganic salts. The crude mixture was purified by flash column chromatography (SiO_2, typically CH_2Cl_2/hexane, typically 30:70–70:30) to give the corresponding conjugate addition product **3**.

Procedure B: Asymmetric conjugate addition to chromone derivatives



Chromone derivatives **4** (0.20 mmol), aryl boronic acid **2** (0.40 mmol, 2.0 equiv), $Pd(OAc)_2$ (0.01 mmol, 5 mol %), and ligand (0.01 mmol, 5 mol %), $AgSbF_6$ (0.05 mmol, 25 mol%) were placed in a ball milling vessel (stainless, 1.5 mL) loaded with one grinding ball (stainless, diameter: 7 mm). Then TFE (43 mL, 3.0 equiv) and CH_2Cl_2 (0.2 μL/mg) were added via a syringe. After the vessel was closed in air without purging with inert gas, the vessel was placed in the ball mill (Retsch MM400, 60 min at 30 Hz) and a heat gun (the preset temperature at 120 °C). After 60 min, the jar was then cooled rapidly with cold water and opened. The mixture was passed through a short silica gel column eluting with CH_2Cl_2/EtOAc (80:20) to remove inorganic salts. The crude mixture was purified by flash column chromatography (SiO_2, typically EtOAc/hexane, typically 0:100–10:90) to give the corresponding conjugate addition product **5**. The racemic sample was prepared using 2,2-bipyridyl for the ligand.

The heat gun was fixed with clamps and placed directly above the ball milling jar (distance between the heat gun and ball milling jar: ca. 1 cm) (Figure S4). The setup procedure for high-temperature ball-milling reactions was shown in Figure S5. First, one grinding ball (stainless, diameter: 7 mm) was loaded in a ball milling jar (stainless, 1.5 mL). Then, solid and liquid materials were added to the jar. After the ball-milling jar was closed, the jar was placed in the ball mill (Retsch MM400), and a heat gun was placed directly above the ball-milling jar. The mechanochemical cross-coupling reactions were conducted while applying heated air to the outside of the milling jar (the preset temperature at 70 °C or 120 °C).

Figure S4. The setup procedure for a heat gun on MM400.

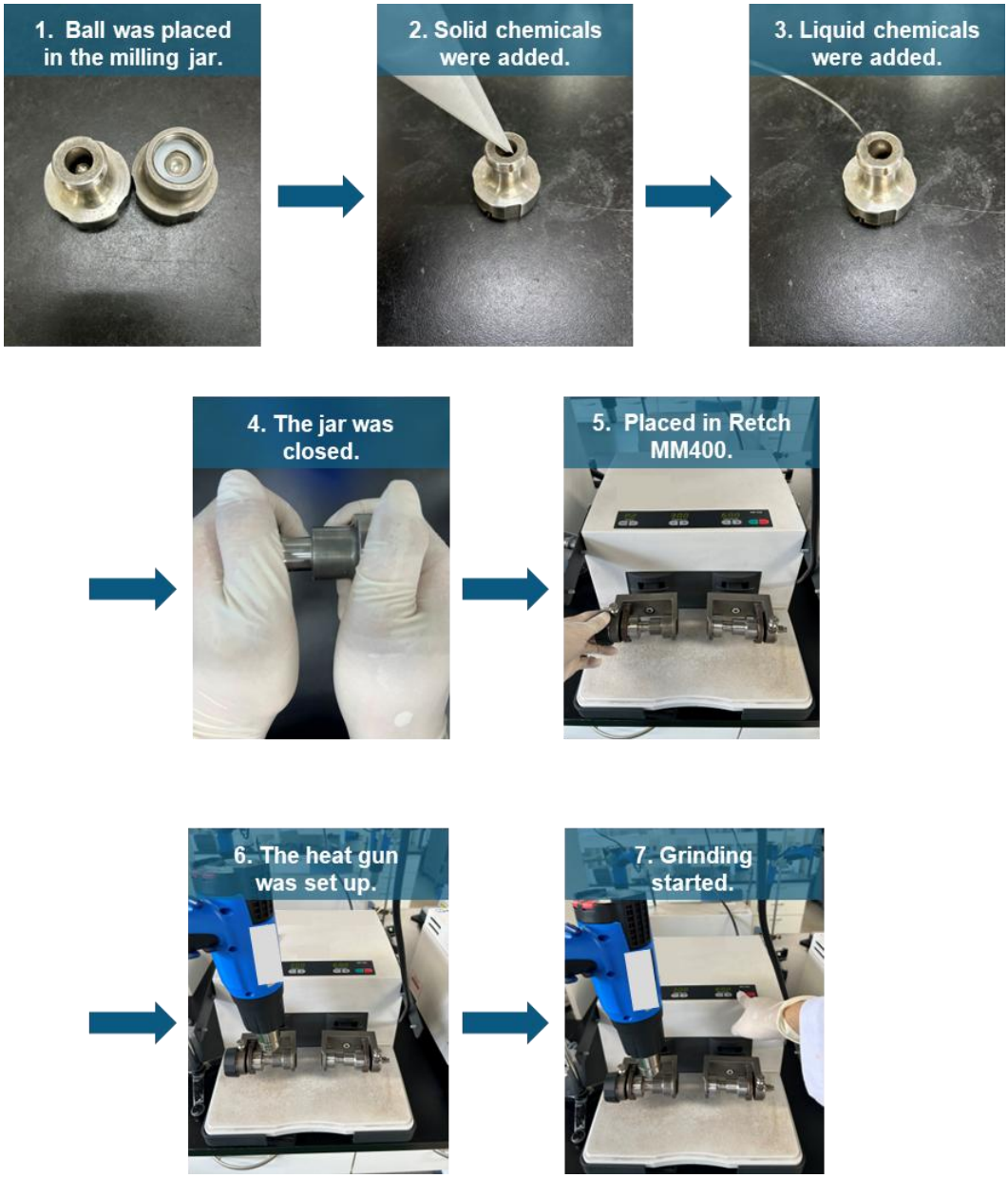
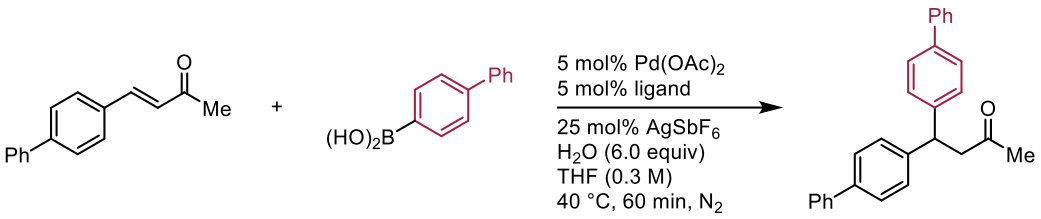


Figure S5. The setup procedure of mechanochemical cross-coupling reactions using the heat gun.

6. General procedure for the palladium-catalyzed conjugate addition in solution

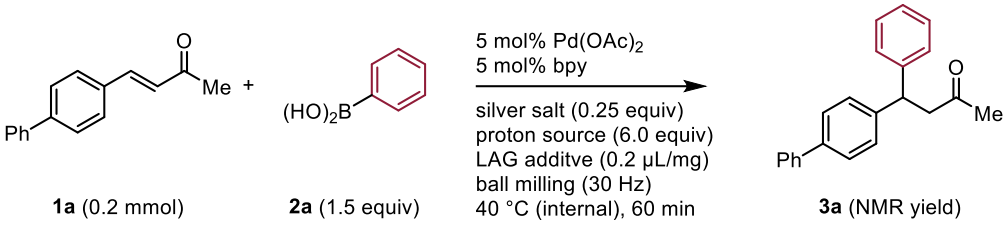


1a **2b** **3b**

1a (0.20 mmol), **2b** (0.30 mmol, 1.5 equiv), $Pd(OAc)_2$ (0.01 mmol, 5 mol%), and ligand (0.01 mmol, 5 mol% %), $AgSbF_6$ (0.05 mmol, 25 mol%) were placed in an oven-dried reaction vial. After the vial was sealed with a screw cap containing a Teflon-coated rubber septum, the vial was connected to a vacuum/nitrogen manifold through a needle. It was evacuated and then backfilled with nitrogen. This cycle was repeated three times. After THF (0.3 M, 0.67 mL) was added to the vial through the rubber septum. Then H_2O (22 μL, 6.0 equiv) was added to the mixture at 40 °C using an oil bath. After 60 minutes, the mixture was passed through a short silica gel column eluting with CH_2Cl to remove inorganic salts. ^1H NMR analysis of the resulting crude mixture was performed to determine the yield of **3b**.

7. Initial optimization studies

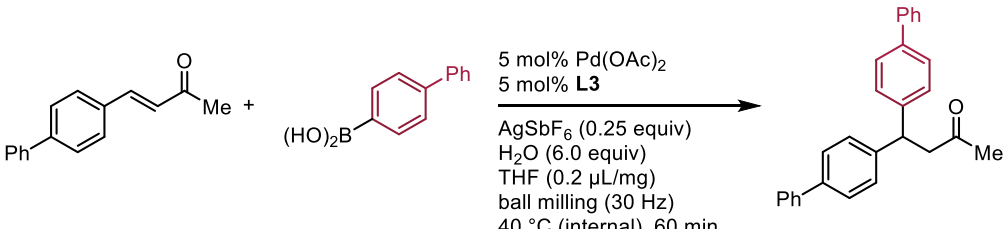
Optimization of the silver salt, proton source, and LAG additive



1a (0.2 mmol) **2a** (1.5 equiv) **3a** (NMR yield)

entry	silver salt	proton source	LAG additive	NMR yield / %
1	none	H_2O/CH_3CO_2H (1:1)	THF	32
2	none	H_2O	THF	47
3	none	H_2O	CH_2Cl_2	22
4	none	H_2O	hexane	11
5	none	H_2O	DMSO	44
6	none	H_2O	none	17
7	$AgBF_4$	H_2O	THF	60
8	$AgSbF_6$	H_2O	THF	61

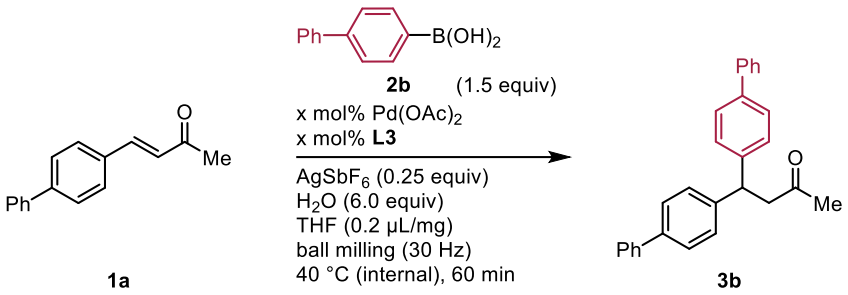
Effect of the LAG additive on the conjugate addition using L3



1a (0.2 mmol) **2b** (1.5 equiv)

3b
91%
(w/o THF: 72%)

Optimization of the catalyst loading

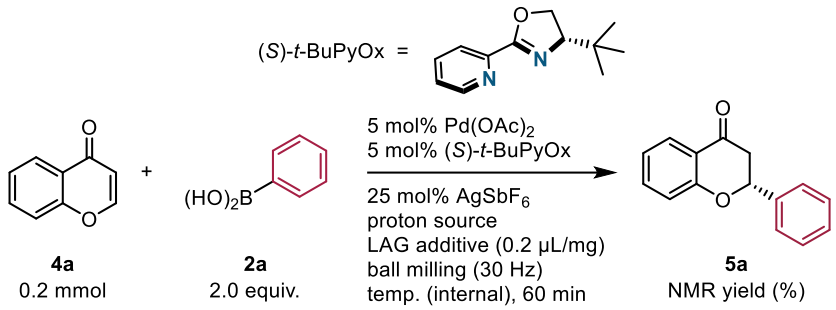


1a
0.2 mmol

3b
NMR yield (%)

entry	x / mol%	NMR yield / %
1	5	91
2	3	88
3	1	29

Preliminary optimization of asymmetric conjugate addition



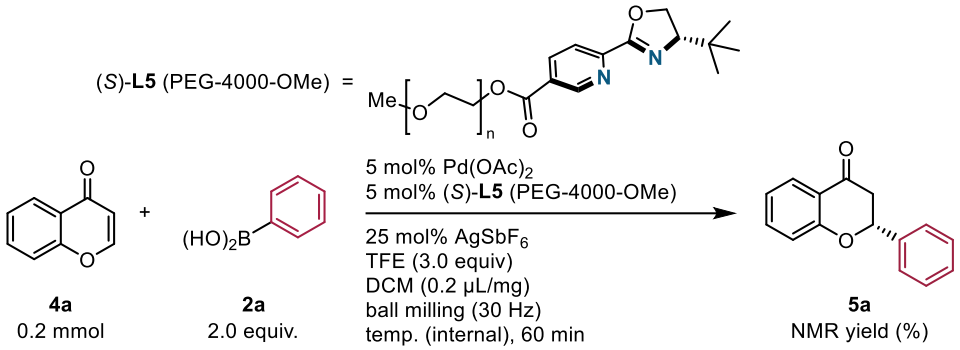
4a
0.2 mmol

2a
2.0 equiv.

5a
NMR yield (%)

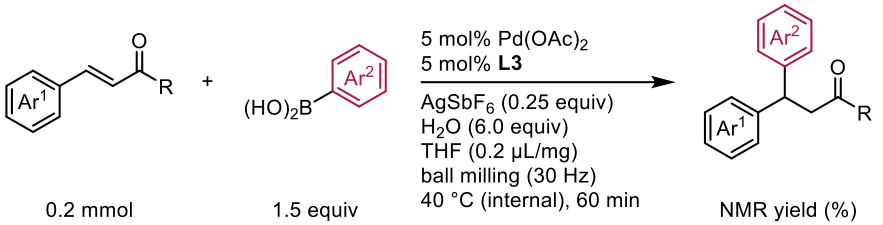
entry	proton source	LAG additive	temp. / °C	NMR yield / %	ee / %
1	H_2O (6.0 equiv)	THF	40	18	94
2	TFE (3.0 equiv)	THF	40	38	93
3	TFE (3.0 equiv)	CH_2Cl_2	40	44	92
4	TFE (3.0 equiv)	*n*-hexane	40	12	72
5	TFE (3.0 equiv)	1,4-dioxane	40	13	63
6	TFE (6.0 equiv)	CH_2Cl_2	40	21	60
7	TFE (3.0 equiv)	CH_2Cl_2	rt	7	60
8	TFE (3.0 equiv)	CH_2Cl_2	60	50	90

Investigation of the reaction temperature of asymmetric conjugate addition using (*S*)-L5 (PEG-4000)

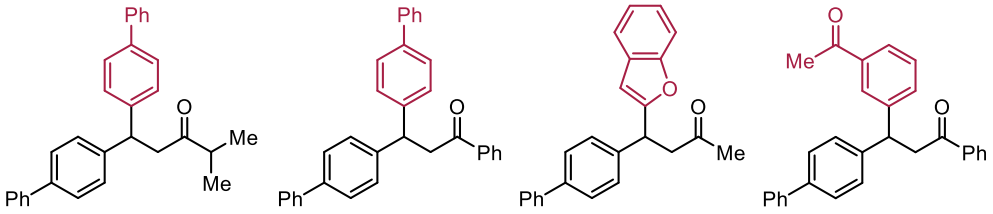


entry	temp. / °C	NMR yield / %	ee / %
1	60	71	90
2	40	23	92
3	rt	<5	-

8. Unsuccessful substrates

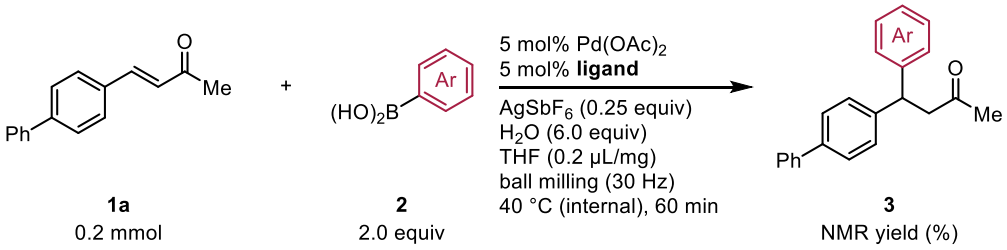


0.2 mmol | 1.5 equiv | NMR yield (%)



31% | 26% | 10% | 29%

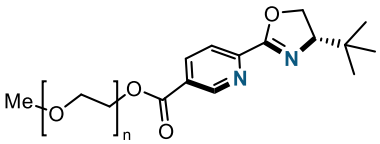
9. Initial attempts of an enantioselective conjugate addition of arylboronic acids to acyclic conjugate ketone



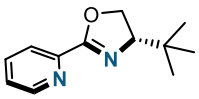
1a
0.2 mmol

2
2.0 equiv

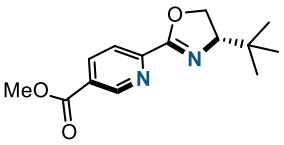
3
NMR yield (%)



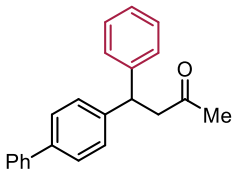
(*S*)-**L5** (PEG-4000-OMe)



(*S*)-*t*-BuPyOx

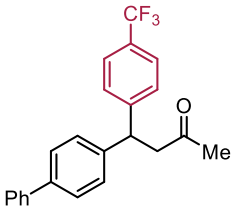


(*S*)-*t*-BuNicox



3a

(*S*)-**L5**: 24%, <5% ee
(*S*)-*t*-BuPyOx: 14%, 8% ee
(*S*)-*t*-BuNicox: <5%, -



3e

(*S*)-**L5**: <5%, -
(*S*)-*t*-BuPyOx: 21%, 12% ee
(*S*)-*t*-BuNicox: <5%, -

10. Thermography observation for reaction temperature

The temperature inside the milling jar after the mechanochemical cross-coupling reactions was confirmed by observation with a thermography camera immediately after the milling jar (Figures S6 and S7). The crude mixture was prepared by the following conditions: 0.2 mmol of **1a**; 0.30 mmol of **2a**; 0.01 mmol of $Pd(OAc)_2$; 0.01 mmol of 2,2-bipyridyl; 0.05 mmol of $AgSbF_6$; H_2O (22 μL) and THF (0.2 μL/mg) in a stainless-steel ball-milling jar (1.5 mL) with a stainless-steel ball (7 mm); heat gun (set temp.; 70 °C); 30 Hz; 60 min (Figure S6). 0.2 mmol of **1a**; 0.4 mmol of **2a**; 0.01 mmol of $Pd(OAc)_2$; 0.01 mmol of (*S*)-*t*-BuPyOx; 0.05 mmol of $AgSbF_6$; TFE (43 μL) and CH_2Cl_2 (0.2 μL/mg) in a stainless-steel ball-milling jar (1.5 mL) with a stainless-steel ball (7 mm); heat gun (set temp.; 120 °C); 30 Hz; 60 min (Figure S7).

Figure S6. Thermographically derived temperature (41.6 °C) inside the milling jar after grinding for 60 min at 30 Hz.

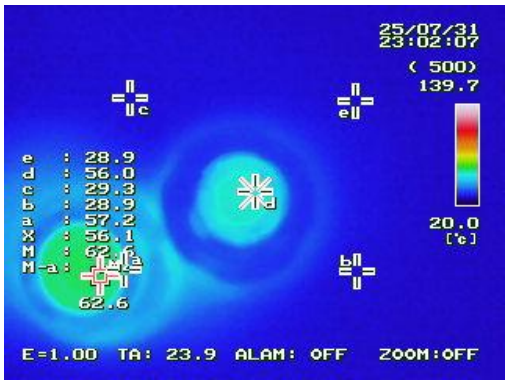


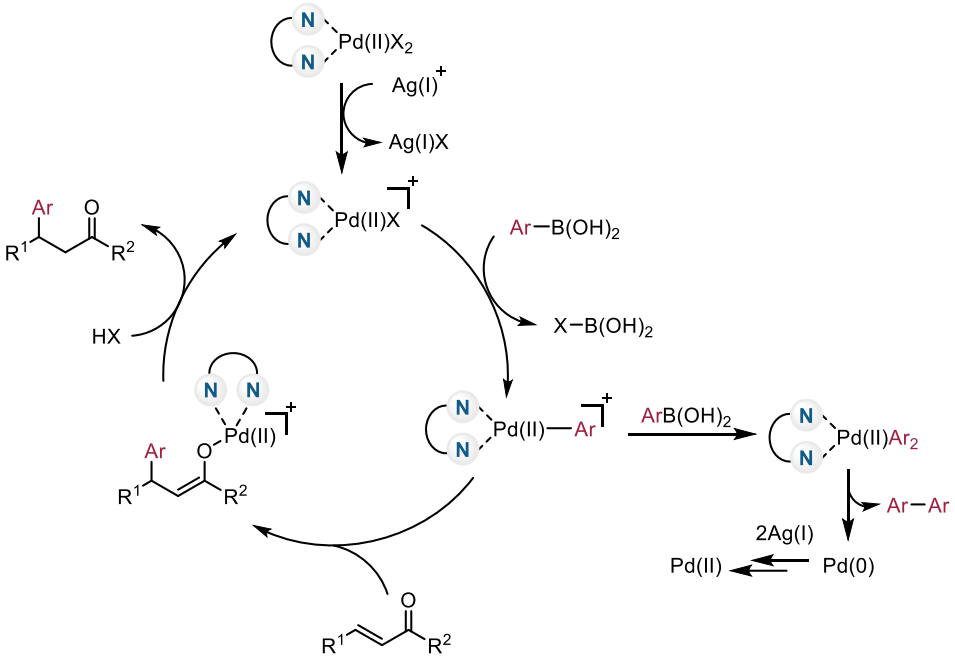
Figure S7. Thermographically derived temperature (62.6 °C) inside the milling jar after grinding for 60 min at 30 Hz.

11. ICP-MS analysis

We carried out ICP-AES analysis on two samples, i.e., **3a** and **3e**, to determine the levels of residual palladium in the products. The results confirmed that no residual palladium (detection limit: 5 ppm) is present in either **3a** or **3e**.

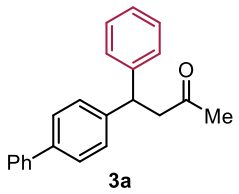
Product	Residual palladium
3a	below detection limit (5 ppm)
3e	below detection limit (5 ppm)

12. Proposed catalytic cycle



13. Characterization of conjugate addition products

4-[(1,1'-Biphenyl)-4-yl]-4-phenylbutan-2-one (3a).



3a

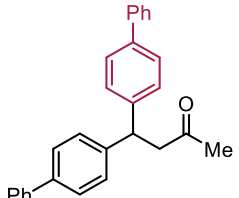
3a was synthesized from two different pathways, as described in the main text.

From 1a and 2a: The reaction was performed according to the general procedure A. The reaction was carried out with 44.2 mg (0.20 mmol) of **1a** and 36.5 mg (0.30 mmol) of **2a**. Product **3a** was obtained as a white powder (45.9 mg, 0.15 mmol, 77% yield). The ^{1}H and ^{13}C NMR spectra were consistent with the literature.[10]

From 1b and 2b: The reaction was performed according to the general procedure A. The reaction was carried out with 29.2 mg (0.20 mmol) of **1b** and 59.4 mg (0.30 mmol) of **2b**. Product **3a** was obtained as a white powder (43.7 mg, 0.15 mmol, 73% yield).

^{1}H NMR (396 MHz, $CDCl_3$, δ): 2.11 (s, 3H), 3.22 (d, J = 7.9 Hz, 2H), 4.64 (t, J = 7.5 Hz, 1H), 7.16–7.22 (m, 1H), 7.23–7.35 (m, 7H), 7.38–7.44 (m, 2H), 7.47–7.57 (m, 4H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 30.8 (*C*H$_3$), 45.8 (*C*H), 49.8 (*C*H$_2$), 126.6 (*C*H), 127.1 (*C*H), 127.3 (*C*H), 127.4 (*C*H), 127.8 (*C*H), 128.2 (*C*H), 128.78 (*C*H), 128.84 (*C*H), 139.4 (*C*), 140.9 (*C*), 143.1 (*C*), 143.9 (*C*), 207.0 (*C*). HRMS-EI (m/z): $[M]^+$ calcd for $C_{22}H_{20}O$, 300.1509; found, 300.1508.

4,4-Di[(1,1'-biphenyl)-4-yl]butan-2-one (3b).

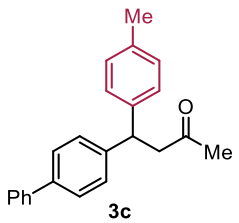


3b

The reaction was performed according to the general procedure A. The reaction was carried out with 44.2 mg (0.20 mmol) of **1a** and 59.5 mg (0.30 mmol) of **2b**. Product **3b** was obtained as a white powder (61.6 mg, 0.16 mmol, 81% yield).

^{1}H NMR (399 MHz, $CDCl_3$, δ): 2.14 (s, 3H), 3.26 (d, J = 7.2 Hz, 2H), 4.68 (t, J = 7.6 Hz, 1H), 7.29–7.37 (m, 6H), 7.38–7.45 (m, 4H), 7.50–7.59 (m, 8H). ^{13}C NMR (101 MHz, $CDCl_3$, δ): 30.8 (*C*H$_3$), 45.5 (*C*H), 49.8 (*C*H$_2$), 127.1 (*C*H), 127.3 (*C*H), 127.5 (*C*H), 128.2 (*C*H), 128.9 (*C*H), 139.5 (*C*), 140.9 (*C*), 143.0 (*C*), 206.9 (*C*). HRMS-EI (m/z): $[M+Na]^+$ calcd for $C_{28}H_{24}ONa$, 399.1719; found, 399.1712.

4-[(1,1'-Biphenyl)-4-yl]-4-(p-tolyl)butan-2-one (3c).

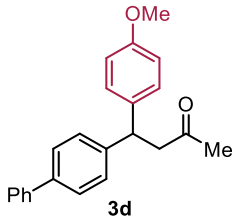


3c

The reaction was performed according to the general procedure A. The reaction was carried out with 44.3 mg (0.20 mmol) of **1a** and 40.7 mg (0.30 mmol) of **2c**. Product **3c** was obtained as a white powder (50.3 mg, 0.16 mmol, 80% yield).

^{1}H NMR (392 MHz, $CDCl_3$, δ): 2.11 (s, 3H), 2.30 (s, 3H), 3.20 (d, J = 7.8 Hz, 2H), 4.59 (t, J = 7.6 Hz, 1H), 7.13 (q, J = 9.1 Hz, 4H), 7.26–7.35 (m, 3H), 7.41 (t, J = 7.2 Hz, 2H), 7.47–7.57 (m, 4H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 21.1 (CH_3), 30.8 (CH_3), 45.5 (*C*H), 49.8 (CH_2), 127.1 *C*H), 127.2 (*C*H), 127.4 (*C*H), 127.7 (*C*H), 128.1 (*C*H), 128.8 (*C*H), 129.5 (*C*H), 136.2 (*C*), 139.4 (*C*), 140.88 (*C*), 140.92 (*C*), 143.3 (*C*), 207.1 (*C*). HRMS-ESI (m/z): $[M+Na]^+$ calcd for $C_{23}H_{22}ONa$, 337.1563; found, 337.1554.

4-[(1,1'-Biphenyl)-4-yl]-4-(4-methoxyphenyl)butan-2-one (3d).

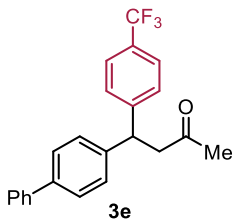


3d

The reaction was performed according to the general procedure A. The reaction was carried out with 44.4 mg (0.20 mmol) of **1a** and 46.1 mg (0.30 mmol) of **2d**. Product **3d** was obtained as a white powder (43.6 mg, 0.13 mmol, 66% yield).

^{1}H NMR (399 MHz, $CDCl_3$, δ): 2.10 (s, 3H), 3.19 (d, J = 7.2 Hz, 2H), 3.77 (s, 3H), 4.58 (t, J = 7.4 Hz, 1H), 6.83 (d, J = 8.8 Hz, 2H), 7.17 (d, J = 8.4 Hz, 2H), 7.23–7.35 (m, 3H), 7.41 (t, J = 7.6 Hz, 2H), 7.52 (dd, J = 8.0, 17.6 Hz, 4H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 30.8 (CH_3), 45.1 (*C*H), 50.0 (CH_2), 55.3 (CH_3), 114.1 (*C*H), 127.1 (*C*H), 127.3 (*C*H), 127.4 (*C*H), 128.1 (*C*H), 128.80 (*C*H), 128.84 (*C*H), 136.0 (*C*), 139.4 (*C*), 140.9 (*C*), 143.4 (*C*), 158.3 (*C*), 207.1 (*C*). HRMS-ESI (m/z): $[M+Na]^+$ calcd for $C_{23}H_{22}O_2Na$, 353.1512; found, 353.1502.

4-[(1,1'-Biphenyl)-4-yl]-4-[4-(trifluoromethyl)phenyl]butan-2-one (3e).

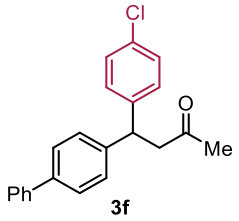


3e

The reaction was performed according to the general procedure A. The reaction was carried out with 44.6 mg (0.20 mmol) of **1a** and 57.0 mg (0.30 mmol) of **2e**. Product **3e** was obtained as a white powder (60.6 mg, 0.17 mmol, 82% yield).

^{1}H NMR (399 MHz, $CDCl_3$, δ): 2.14 (s, 3H), 3.24 (d, J = 7.6 Hz, 2H), 4.70 (t, J = 7.4 Hz, 1H), 7.25–7.29 (m, 2H), 7.33 (tt, J = 1.5, 7.3 Hz, 1H), 7.35–7.45 (m, 4H), 7.49–7.58 (m, 6H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 30.7 (*C*H_3), 45.4 (*C*H), 49.4 (*C*H_2), 122.9 (*C*), 125.5–125.9 (m, *C*H, (observed complexity is due to C–F coupling), 127.1 (*C*H), 127.4 (*C*H), 127.6 (*C*H), 128.17 (*C*H), 128.20 (*C*H), 128.9 (*C*H), 139.9 (*C*), 140.7 (*C*), 142.0 (*C*), 148.0 (*C*), 206.2 (*C*). One carbon is missing, likely due to overlapping with the other signals. HRMS-ESI (m/z): $[M+Na]^+$ calcd for $C_{23}H_{19}OF_3Na$, 391.1280; found, 391.1276.

4-[(1,1'-Biphenyl)-4-yl]-4-(4-chlorophenyl)butan-2-one (3f).



3f

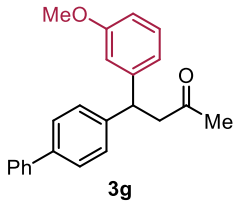
3f was synthesized from two different pathways, as described in the main text.

From 1a and 2f: The reaction was performed according to the general procedure A. The reaction was carried out with 44.2 mg (0.20 mmol) of **1a** and 46.9 mg (0.30 mmol) of **2f**. Product **3f** was obtained as a white powder (65.0 mg, 0.19 mmol, 98% yield).

From 1c and 2b: The reaction was performed according to the general procedure A. The reaction was carried out with 36.0 mg (0.20 mmol) of **1c** and 60.0 mg (0.30 mmol) of **2b**. Product **3f** was obtained as a white powder (57.3 mg, 0.17 mmol, 86% yield).

^{1}H NMR (392 MHz, $CDCl_3$, δ): 2.11 (s, 3H), 3.19 (d, J = 7.6 Hz, 2H), 4.61 (t, J = 7.6 Hz, 1H), 7.19 (d, J = 8.7 Hz, 2H), 7.20–7.29 (m, 4H), 7.32 (t, J = 7.3 Hz, 1H), 7.41 (t, J = 7.6 Hz, 2H), 7.47–7.58 (m, 4H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 30.8 (*C*H_3), 45.0 (*C*H), 49.5 (*C*H_2), 127.1 (*C*H), 127.4 (*C*H), 127.5 (*C*H), 128.1 (*C*H), 128.9 (*C*H), 129.2 (*C*H), 132.4 (*C*), 139.6 (*C*), 140.7 (*C*), 142.45 (*C*), 142.53 (*C*), 206.5 (*C*). HRMS-EI (m/z): $[M]^+$ calcd for $C_{22}H_{19}ClO$, 334.1119; found, 334.1116.

4-[(1,1'-Biphenyl)-4-yl]-4-(3-methoxyphenyl)butan-2-one (3g).

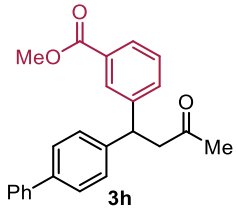


3g

The reaction was performed according to the general procedure A. The reaction was carried out with 44.2 mg (0.20 mmol) of **1a** and 45.5 mg (0.30 mmol) of **2g**. Product **3g** was obtained as a white powder (49.1 mg, 0.15 mmol, 75% yield).

^{1}H NMR (401 MHz, $CDCl_3$, δ): 2.12 (s, 3H), 3.21 (d, J = 7.6 Hz, 2H), 3.78 (s, 3H), 4.60 (t, J = 7.4 Hz, 1H), 6.74 (dd, J = 2.4, 8.0 Hz, 1H), 6.78–6.82 (m, 1H), 6.86 (d, J = 7.6 Hz, 1H), 7.22 (t, J = 8.0 Hz, 1H), 7.27–7.36 (m, 3H), 7.41 (t, J = 7.4 Hz, 2H), 7.47–7.58 (m, 4H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 30.8 (*C*H_3), 45.8 (*C*H), 49.7 (*C*H_2), 55.3 (*C*H_3), 111.5 (*C*H), 114.1 (*C*H), 120.2 (*C*H), 127.1 (*C*H), 127.3 (*C*H), 127.4 (*C*H), 128.2 (*C*H), 128.8 (*C*H), 129.7 (*C*H), 139.5 (*C*), 140.9 (*C*), 142.9 (*C*), 145.5 (*C*), 159.8 (*C*), 206.9 (*C*). HRMS-ESI (m/z): $[M+Na]^+$ calcd for $C_{23}H_{22}O_2Na$, 353.1512; found, 353.1505.

Methyl 3-[1-{(1,1'-biphenyl)-4-yl}-3-oxobutyl]benzoate (3h).

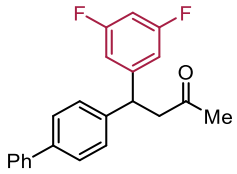


3h

The reaction was performed according to the general procedure A with a preset temperature of 120 °C. The reaction was carried out with 44.5 mg (0.20 mmol) of **1a** and 54.0 mg (0.30 mmol) of **2h**. Product **3h** was obtained as a white powder (57.2 mg, 0.16 mmol, 80% yield).

^{1}H NMR (396 MHz, $CDCl_3$, δ): 2.13 (s, 3H), 3.26 (d, J = 7.9 Hz, 2H), 3.90 (s, 3H), 4.69 (t, J = 7.3 Hz, 1H), 7.28–7.35 (m, 3H), 7.36–7.44 (m, 3H), 7.45–7.58 (m, 5H), 7.88 (dt, J = 1.4, 7.8 Hz, 1H), 7.95–7.99 (m, 1H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 30.8 (*C*H_3), 45.4 (*C*H), 49.4 (*C*H_2), 52.3 (*C*H_3), 127.1 (*C*H), 127.3 (*C*H), 127.5 (*C*H), 127.9 (*C*H), 128.2 (*C*H), 128.6 (*C*H), 128.8 (*C*H), 130.6 (*C*), 132.8 (*C*H), 139.6 (*C*), 140.7 (*C*), 142.5 (*C*), 144.3 (*C*), 167.1 (*C*), 206.5 (*C*). HRMS-EI (m/z): $[M]^+$ calcd for $C_{24}H_{22}O_3$, 358.1564; found, 358.1563.

4-[(1,1'-Biphenyl)-4-yl]-4-(3,5-difluorophenyl)butan-2-one (3i).

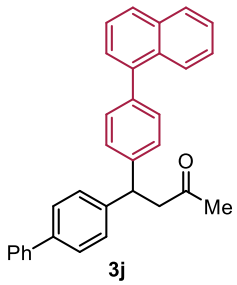


3i

The reaction was performed according to the general procedure A. The reaction was carried out with 44.5 mg (0.20 mmol) of **1a** and 47.3 mg (0.30 mmol) of **2i**. Product **3i** was obtained as a white powder (50.3 mg, 0.15 mmol, 75% yield).

^{1}H NMR (399 MHz, $CDCl_3$, δ): 2.14 (s, 3H), 3.19 (d, J = 7.6 Hz, 2H), 4.61 (t, J = 7.2 Hz, 1H), 6.64 (tt, J = 2.3, 8.9 Hz, 1H), 6.73–6.83 (m, 2H), 7.23–7.29 (m, 2H), 7.33 (tt, J = 1.6, 7.3 Hz, 1H), 7.39–7.46 (m, 2H), 7.50–7.57 (m, 4H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 30.8 (CH_3), 45.2 (*C*H), 49.2 (CH_2), 102.1 (t, J = 25.5 Hz, *C*H), 110.8 (dd, J = 7.0, 18.4 Hz, *C*H), 127.1 (*C*H), 127.5 (*C*H), 127.7 (*C*H), 128.1 (*C*H), 128.9 (*C*H), 140.0 (*C*), 140.6 (*C*), 141.7 (*C*), 148.0 (t, J = 8.5 Hz, *C*), 163.2 (dd, J = 15.6, 252.5 Hz, *C*), 206.0 (*C*). HRMS-EI (m/z): $[M]^+$ calcd for $C_{22}H_{18}F_2O$, 336.1320; found, 336.1318.

4-[(1,1'-Biphenyl)-4-yl]-4-[4-(naphthalen-1-yl)phenyl]butan-2-one (3j).

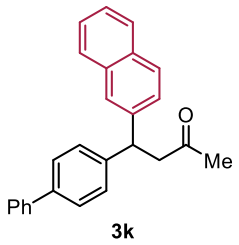


3j

The reaction was performed according to the general procedure A. The reaction was carried out with 44.5 mg (0.20 mmol) of **1a** and 74.4 mg (0.30 mmol) of **2j**. Product **3j** was obtained as a white powder (55.0 mg, 0.13 mmol, 64% yield).

^{1}H NMR (396 MHz, $CDCl_3$, δ): 2.17 (s, 3H), 3.31 (d, J = 7.9 Hz, 2H), 4.74 (t, J = 7.7 Hz, 1H), 7.33 (tt, J = 1.5, 7.4 Hz, 1H), 7.35–7.53 (m, 12H), 7.54–7.60 (m, 4H), 7.84 (d, J = 7.9, 1H), 7.89 (d, J = 7.9, 2H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 30.9 (CH_3), 45.6 (*C*H), 49.8 (CH_2), 125.5 (*C*H), 125.9 (*C*H), 126.1 (*C*H), 127.0 (*C*H), 127.1 (*C*H), 127.3 (*C*H), 127.5 (*C*H), 127.7 (*C*H), 128.3 (*C*H), 128.4 (*C*H), 128.9 (*C*H), 130.4 (*C*H), 131.6 (*C*), 133.9 (*C*), 139.0 (*C*), 139.5 (*C*), 139.9 (*C*), 140.8 (*C*), 142.9 (*C*), 143.0 (*C*), 206.9 (*C*). HRMS-EI (m/z): $[M]^+$ calcd for $C_{32}H_{26}O$, 426.1978; found, 426.1974.

4-[(1,1'-Biphenyl)-4-yl]-4-(naphthalen-2-yl)butan-2-one (3k).



3k

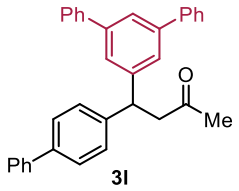
3k was synthesized from two different pathways, as described in the main text.

From 1a and 2k: The reaction was performed according to the general procedure A. The reaction was carried out with 44.5 mg (0.20 mmol) of **1a** and 51.6 mg (0.30 mmol) of **2k**. Product **3k** was obtained as a white powder (46.3 mg, 0.15 mmol, 62% yield).

From 1g and 2b: The reaction was performed according to the general procedure A. The reaction was carried out with 39.2 mg (0.20 mmol) of **1g** and 59.4 mg (0.30 mmol) of **2b**. Product **3k** was obtained as a pale yellow powder (22.0 mg, 0.064 mmol, 31% yield).

^{1}H NMR (396 MHz, $CDCl_3$, δ): 2.13 (s, 3H), 3.29 (dd, J = 4.9, 14.1 Hz, 1H), 3.35 (dd, J = 5.1, 14.3 Hz, 1H), 4.81 (t, J = 7.5 Hz, 1H), 7.29–7.36 (m, 3H), 7.37–7.47 (m, 5H), 7.48–7.57 (m, 4H), 7.71 (s, 1H), 7.74–7.83 (m, 3H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 30.8 (*C*H_3), 45.8 (*C*H), 49.6 (*C*H_2), 125.76 (*C*H), 125.84 (*C*H), 126.2 (*C*H), 126.7 (*C*H), 127.1 (*C*H), 127.3 (*C*H), 127.4 (*C*H), 127.7 (*C*H), 127.9 (*C*H), 128.3 (*C*H), 128.5 (*C*H), 128.8 (*C*H), 132.3 (*C*), 133.6 (*C*), 139.5 (*C*), 140.8 (*C*), 141.3 (*C*), 142.9 (*C*), 206.9 (*C*). HRMS-EI (m/z): $[M]^+$ calcd for $C_{26}H_{22}O$, 350.1665; found, 350.1663.

4-[(1,1'-Biphenyl)-4-yl]-4-[(1,1':3',1''-terphenyl)-5'-yl]butan-2-one (3l).



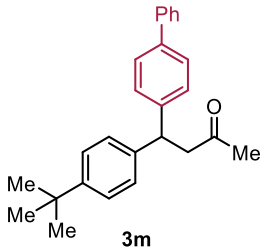
3l

The reaction was performed according to the general procedure A. The reaction was carried out with 44.3 mg (0.20 mmol) of **1a** and 82.6 mg (0.30 mmol) of **2l**. Product **3l** was obtained as a white powder (73.4 mg, 0.16 mmol, 81% yield).

^{1}H NMR (399 MHz, $CDCl_3$, δ): 2.15 (s, 3H), 3.32 (d, J = 8.0 Hz, 2H), 4.78 (t, J = 7.6 Hz, 1H), 7.28–7.49 (m, 13H), 7.50–7.57 (m, 4H), 7.58–7.65 (m, 5H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 30.9 (*C*H_3), 46.0 (*C*H), 49.8 (*C*H_2), 124.7 (*C*H), 125.8 (*C*H), 127.1 (*C*H), 127.3 (*C*H), 127.4 (*C*H), 127.5 (*C*H), 127.6 (*C*H), 128.2 (*C*H), 128.8 (*C*H), 128.9 (*C*H), 139.6 (*C*), 140.8 (*C*), 141.2 (*C*),

142.3 (*C*) 142.9 (*C*), 145.0 (*C*), 206.8 (*C*). HRMS-ESI (m/z): $[M+Na]^+$ calcd for $C_{34}H_{28}ONa$, 475.2032; found, 475.2024.

4-[(1,1'-Biphenyl)-4-yl]-4-[4-(tert-butyl)phenyl]butan-2-one (3m).

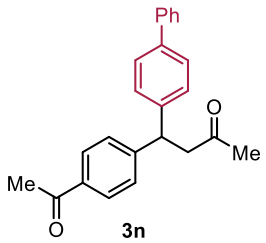


3m

The reaction was performed according to the general procedure A. The reaction was carried out with 40.4 mg (0.20 mmol) of **1d** and 59.6 mg (0.30 mmol) of **2b**. Product **3m** was obtained as a white powder (51.0 mg, 0.14 mmol, 72% yield).

^{1}H NMR (399 MHz, $CDCl_3$, δ): 1.28 (s, 9H), 2.11 (s, 3H), 3.19 (dd, *J* = 5.2, 14.4 Hz, 1H), 3.24 (dd, *J* = 5.8, 14.6 Hz, 1H), 4.60 (t, *J* = 7.6 Hz, 1H), 7.18 (d, *J* = 8.0 Hz, 2H), 7.28–7.35 (m, 5H), 7.41 (t, *J* = 7.2 Hz, 2H), 7.48–7.57 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 30.8 (*C*H_3), 31.5 (*C*H_3), 34.5 (*C*), 45.4 (*C*H), 49.9 (*C*H_2), 125.7 (*C*H), 127.1 (*C*H), 127.2 (*C*H), 127.37 (*C*H), 127.41 (*C*H), 128.2 (*C*H), 128.8 (*C*H), 139.4 (*C*), 140.8 (*C*), 140.9 (*C*), 143.3 (*C*), 149.3 (*C*), 207.1 (*C*). HRMS-ESI (m/z): $[M+Na]^+$ calcd for $C_{26}H_{28}ONa$, 379.2032; found, 379.2019.

4-[(1,1'-Biphenyl)-4-yl]-4-(4-acetylphenyl)butan-2-one (3n).

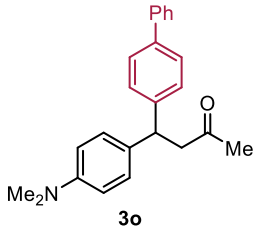


3n

The reaction was performed according to the general procedure A. The reaction was carried out with 37.8 mg (0.20 mmol) of **1e** and 60.2 mg (0.30 mmol) of **2b**. Product **3n** was obtained as a white powder (61.3 mg, 0.17 mmol, 85% yield).

^{1}H NMR (399 MHz, $CDCl_3$, δ): 2.14 (s, 3H), 2.57 (s, 3H), 3.26 (d, *J* = 7.2 Hz, 2H), 4.70 (t, *J* = 7.6 Hz, 1H), 7.26–7.39 (m, 5H), 7.42 (t, *J* = 7.6 Hz, 2H), 7.48–7.57 (m, 4H), 7.90 (d, *J* = 8.4 Hz, 2H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 26.7 (*C*H_3), 30.8 (*C*H_3), 45.6 (*C*H), 49.3 (*C*H_2), 127.1 (*C*H), 127.4 (*C*H), 127.6 (*C*H), 128.1 (*C*H), 128.2 (*C*H), 128.87 (*C*H), 128.93 (*C*H), 135.6 (*C*), 139.8 (*C*), 140.7 (*C*), 142.1 (*C*), 149.4 (*C*), 197.8 (*C*), 206.3 (*C*). HRMS-ESI (m/z): $[M+Na]^+$ calcd for $C_{24}H_{22}O_2Na$, 365.1512; found, 365.1500.

4-[(1,1'-Biphenyl)-4-yl]-4-[4-(dimethylamino)phenyl]butan-2-one (3o).

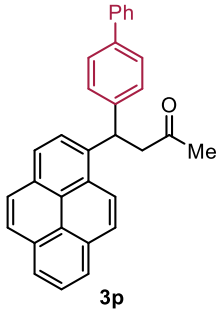


3o

The reaction was performed according to the general procedure A. The reaction was carried out with 37.8 mg (0.20 mmol) of **1f** and 59.4 mg (0.30 mmol) of **2b**. Product **3o** was obtained as a yellow powder (38.2 mg, 0.11 mmol, 56% yield).

^{1}H NMR (396 MHz, $CDCl_3$, δ): 2.10 (s, 3H), 2.90 (s, 6H), 3.18 (d, J = 7.9 Hz, 2H), 4.53 (t, J = 7.7 Hz, 1H), 6.64–6.71 (m, 2H), 7.09–7.16 (m, 2H), 7.24–7.35 (m, 3H), 7.37–7.44 (m, 2H), 7.46–7.51 (m, 2H), 7.52–7.57 (m, 2H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 30.8 (CH_3), 40.7 (CH_3), 45.0 (*C*H), 50.1 (CH_2), 112.9 (*C*H), 127.1 (*C*H), 127.2 (*C*H), 127.3 (*C*H), 128.1 (*C*H), 128.4 (*C*H), 128.8 (*C*H), 131.7 (*C*), 139.1 (*C*), 141.0 (*C*), 143.9 (*C*), 149.3 (*C*), 207.5 (*C*). HRMS-EI (m/z): $[M]^+$ calcd for $C_{24}H_{25}NO$, 343.1931; found, 343.1933.

4-[(1,1'-Biphenyl)-4-yl]-4-(pyren-1-yl)butan-2-one (3p).

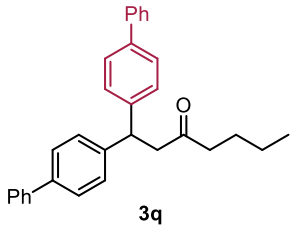


3p

The reaction was performed according to the general procedure A. The reaction was carried out with 54.2 mg (0.20 mmol) of **1h** and 60.1 mg (0.30 mmol) of **2b**. Product **3p** was obtained as a yellow powder (79.6 mg, 0.19 mmol, 94% yield).

^{1}H NMR (401 MHz, $CDCl_3$, δ): 2.17 (s, 3H), 3.46 (dd, J = 6.8, 17.2 Hz, 1H), 3.55 (dd, J = 7.8, 17.0 Hz, 1H), 5.81 (t, J = 7.4 Hz, 1H), 7.27–7.33 (m, 1H), 7.35–7.42 (m, 4H), 7.46–7.55 (m, 4H), 7.94 (d, J = 7.6 Hz, 1H), 7.99 (t, J = 7.4 Hz, 1H), 8.04 (s, 2H), 8.12 (d, J = 9.6 Hz, 1H), 8.17 (d, J = 7.2 Hz, 3H), 8.48 (d, J = 9.6 Hz, 1H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 30.8 (CH_3), 41.3 (*C*H), 50.3 (CH_2), 123.1 (*C*H), 124.9 (*C*H), 124.96 (*C*), 125.03 (*C*H), 125.1 (*C*H), 125.3 (*C*), 125.4 (*C*), 126.1 (*C*H), 127.1 (*C*H), 127.3 (*C*H), 127.4 (*C*H), 127.5 (*C*H), 128.0 (*C*H), 128.4 (*C*H), 128.7 (*C*), 128.8 (*C*H), 130.2 (*C*), 130.8 (*C*), 131.5 (*C*), 137.4 (*C*), 139.3 (*C*), 140.8 (*C*), 143.3 (*C*), 206.9 (*C*). HRMS-ESI (m/z): $[M+K]^+$ calcd for $C_{32}H_{24}OK$, 463.1459; found, 463.1449.

1,1-Di[(1,1'-biphenyl)-4-yl]hexan-3-one (3q).

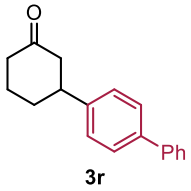


3q

The reaction was performed according to the general procedure A. The reaction was carried out with 52.9 mg (0.20 mmol) of **1i** and 59.2 mg (0.30 mmol) of **2b**. Product **3q** was obtained as a white powder (49.6 mg, 0.12 mmol, 59% yield).

^{1}H NMR (399 MHz, $CDCl_3$, δ): 0.83 (t, J = 7.4 Hz, 3H), 1.21 (sxt, J = 7.4 Hz, 2H), 1.49 (quint, J = 7.5 Hz, 2H), 2.37 (t, J = 7.2 Hz, 2H), 3.23 (d, J = 7.6 Hz, 2H), 4.70 (t, J = 7.4 Hz, 1H), 7.29–7.36 (m, 6H), 7.41 (t, J = 7.8 Hz, 4H), 7.49–7.58 (m, 8H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 13.9 (*C*H_3), 22.3 (*C*H_2), 25.8 (*C*H_2), 43.5 (*C*H_2), 45.4 (*C*H), 48.9 (*C*H_2), 127.1 (*C*H), 127.3 (*C*H), 127.5 (*C*H), 128.3 (*C*H), 128.9 (*C*H), 139.5 (*C*), 140.9 (*C*), 143.1 (*C*), 209.3 (*C*). HRMS-ESI (m/z): $[M+Na]^+$ calcd for $C_{31}H_{30}ONa$, 441.2189; found, 441.2179.

3-[(1,1'-Biphenyl)-4-yl]cyclohexan-1-one (3r).

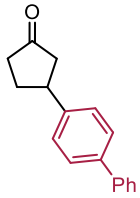


3r

The reaction was performed according to the general procedure A. The reaction was carried out with 19.5 mg (0.20 mmol) of **1j** and 59.5 mg (0.30 mmol) of **2b**. Product **3r** was obtained as a white powder (37.9 mg, 0.15 mmol, 75% yield). The ^{1}H and ^{13}C NMR spectra were consistent with the literature.[11]

^{1}H NMR (396 MHz, $CDCl_3$, δ): 1.72–1.97 (m, 2H), 2.08–2.23 (m, 2H), 2.34–2.54 (m, 2H), 2.54–2.61 (m, 1H), 2.62–2.69 (m, 1H), 3.06 (tt, J = 4.0, 11.7 Hz, 1H), 7.27–7.31 (m, 2H), 7.34 (tt, J = 1.6, 7.3 Hz, 1H), 7.40–7.47 (m, 2H), 7.54–7.61 (m, 4H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 25.7 (*C*H_2), 32.9 (*C*H_2), 41.3 (*C*H_2), 44.5 (*C*H), 49.0 (*C*H_2), 127.1 (*C*H), 127.3 (*C*H), 127.5 (*C*H), 128.9 (*C*H), 139.8 (*C*), 140.8 (*C*), 143.5 (*C*), 211.1 (*C*). HRMS-EI (m/z): $[M]^+$ calcd for $C_{18}H_{18}O$, 250.1352; found, 250.1352.

3-[(1,1'-Biphenyl)-4-yl]cyclopentan-1-one (3s).

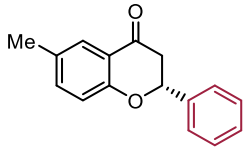


3s

The reaction was performed according to the general procedure A. The reaction was carried out with 16.3 mg (0.20 mmol) of **1k** and 59.4 mg (0.30 mmol) of **2b**. Product **3s** was obtained as a pale yellow powder (29.6 mg, 0.13 mmol, 63% yield). The ^{1}H and ^{13}C NMR spectra were consistent with the literature.[12]

^{1}H NMR (396 MHz, $CDCl_3$, δ): 1.96–2.11 (m, 1H), 2.26–2.44 (m, 2H), 2.45–2.56 (m, 2H), 2.71 (dd, *J* = 7.9, 18.2 Hz, 1H), 3.40–3.53 (m, 1H), 7.31–7.38 (m, 3H), 7.41–7.48 (m, 2H), 7.54–7.63 (m, 4H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 31.4 (*C*H_2), 39.0 (*C*H_2), 42.1 (*C*H), 45.9 (*C*H_2), 127.1 (*C*H), 127.3 (*C*H), 127.4 (*C*H), 127.5 (*C*H), 128.9 (*C*H), 139.9 (*C*), 140.8 (*C*), 142.2 (*C*), 218.5 (*C*). HRMS-EI (m/z): $[M]^+$ calcd for $C_{17}H_{16}O$, 236.1196; found, 236.1195.

(*R*)-6-Methyl-2-phenylchroman-4-one (5a).

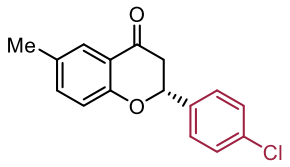


5a

The reaction was performed according to the general procedure B. The reaction was carried out with 32.0 mg (0.20 mmol) of **4a** and 49.5 mg (0.41 mmol) of **2a**. Product **5a** was obtained as a white powder (30.5 mg, 0.13 mmol, 64% yield).

^{1}H NMR (399 MHz, $CDCl_3$, δ): 2.33 (s, 3H), 2.88 (dd, *J* = 3.2, 16.8 Hz, 1H), 3.08 (dd, *J* = 13.2, 16.8 Hz, 1H), 5.46 (dd, *J* = 2.8, 13.2 Hz, 1H), 6.97 (d, *J* = 8.4 Hz, 1H), 7.33 (dd, *J* = 2.2, 8.6 Hz, 1H), 7.36–7.41 (m, 1H), 7.41–7.47 (m, 2H), 7.48–7.52 (m, 2H), 7.73 (d, *J* = 1.6 Hz, 1H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 20.6 (*C*H_3), 44.8 (*C*H_2), 79.7 (*C*H), 118.0 (*C*H), 120.6 (*C*), 126.3 (*C*H), 126.7 (*C*H), 128.8 (*C*H), 128.9 (*C*H), 131.2 (*C*), 137.4 (*C*H), 139.0 (*C*), 159.8 (*C*), 192.4 (*C*). HRMS-ESI (m/z): $[M+H]^+$ calcd for $C_{16}H_{15}O_2$, 239.1067; found, 239.1062. $[\alpha]_D^{23.3}$ +41.9 (*c* 1.0 in $CHCl_3$, 90% ee). Daicel CHIRALPAK® IBN-3, 2-PrOH/Hexane = 5/95, 0.5 mL/min, 40 °C, *S* isomer: t_S = 14.95 min., *R* isomer: t_R = 16.97 min.

(*R*)-2-(4-Chlorophenyl)-6-methylchroman-4-one (5b).

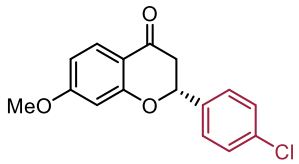


5b

The reaction was performed according to the general procedure B. The reaction was carried out with 31.9 mg (0.20 mmol) of **4a** and 62.3 mg (0.40 mmol) of **2f**. Product **5b** was obtained as a white powder (35.9 mg, 0.13 mmol, 65% yield).

^{1}H NMR (399 MHz, $CDCl_3$, δ): 2.33 (s, 3H), 2.86 (dd, J = 2.8, 16.8 Hz, 1H), 3.02 (dd, J = 13.2, 16.8 Hz, 1H), 5.44 (dd, J = 2.8, 13.2 Hz, 1H), 6.96 (d, J = 8.0 Hz, 1H), 7.33 (dd, J = 2.4, 8.8 Hz, 1H), 7.38–7.46 (m, 4H), 7.72 (d, J = 1.6 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$, δ): 20.6 (CH_3), 44.8 (CH_2), 78.9 (*C*H), 118.0 (*C*H), 120.6 (*C*), 126.8 (*C*H), 127.6 (*C*H), 129.1 (*C*H), 131.4 (*C*), 134.6 (*C*), 137.5 (*C*H), 159.5 (*C*), 191.9 (*C*). HRMS-EI (m/z): $[M+H]^+$ calcd for $C_{16}H_{14}O_2Cl$, 273.0677; found, 273.0670. $[\alpha]_D^{22.9}$ +51.3 (*c* 1.0 in $CHCl_3$, 94% ee). Daicel CHIRALPAK® IBN-3, 2-PrOH/Hexane = 5/95, 0.5 mL/min, 40 °C, *S* isomer: t_S = 16.69 min., *R* isomer: t_R = 18.95 min.

(*R*)-2-(4-Chlorophenyl)-7-methoxychroman-4-one (5c).



5c

The reaction was performed according to the general procedure B. The reaction was carried out with 35.2 mg (0.20 mmol) of **4b** and 62.6 mg (0.40 mmol) of **2f**. Product **5c** was obtained as a white powder (38.3 mg, 0.13 mmol, 66% yield).

^{1}H NMR (399 MHz, $CDCl_3$, δ): 2.82 (dd, J = 3.2, 16.6 Hz, 1H), 2.99 (dd, J = 13.3, 16.8 Hz, 1H), 3.85 (s, 3H), 5.46 (dd, J = 3.2, 13.1 Hz, 1H), 6.50 (d, J = 2.4 Hz, 1H), 6.63 (dd, J = 2.6, 8.9 Hz, 1H), 7.42 (s, 4H), 7.87 (d, J = 8.7 Hz, 1H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 44.3 (CH_2), 55.8 (CH_3) 79.3 (*C*H), 101.0 (*C*H), 110.5 (*C*H), 114.9 (*C*), 127.6 (*C*H), 128.9 (*C*H), 129.1 (*C*H), 134.7 (*C*), 137.4 (*C*), 163.4 (*C*), 166.4 (*C*), 190.3 (*C*). HRMS-ESI (m/z): $[M+H]^+$ calcd for $C_{16}H_{14}O_3Cl$, 289.0626; found, 289.0620. $[\alpha]_D^{23.1}$ +102.6 (*c* 1.0 in $CHCl_3$, 94% ee). Daicel CHIRALPAK® IBN-3, 2-PrOH/Hexane = 5/95, 0.5 mL/min, 40 °C, *S* isomer: t_S = 25.44 min., *R* isomer: t_R = 29.13 min.

11. References

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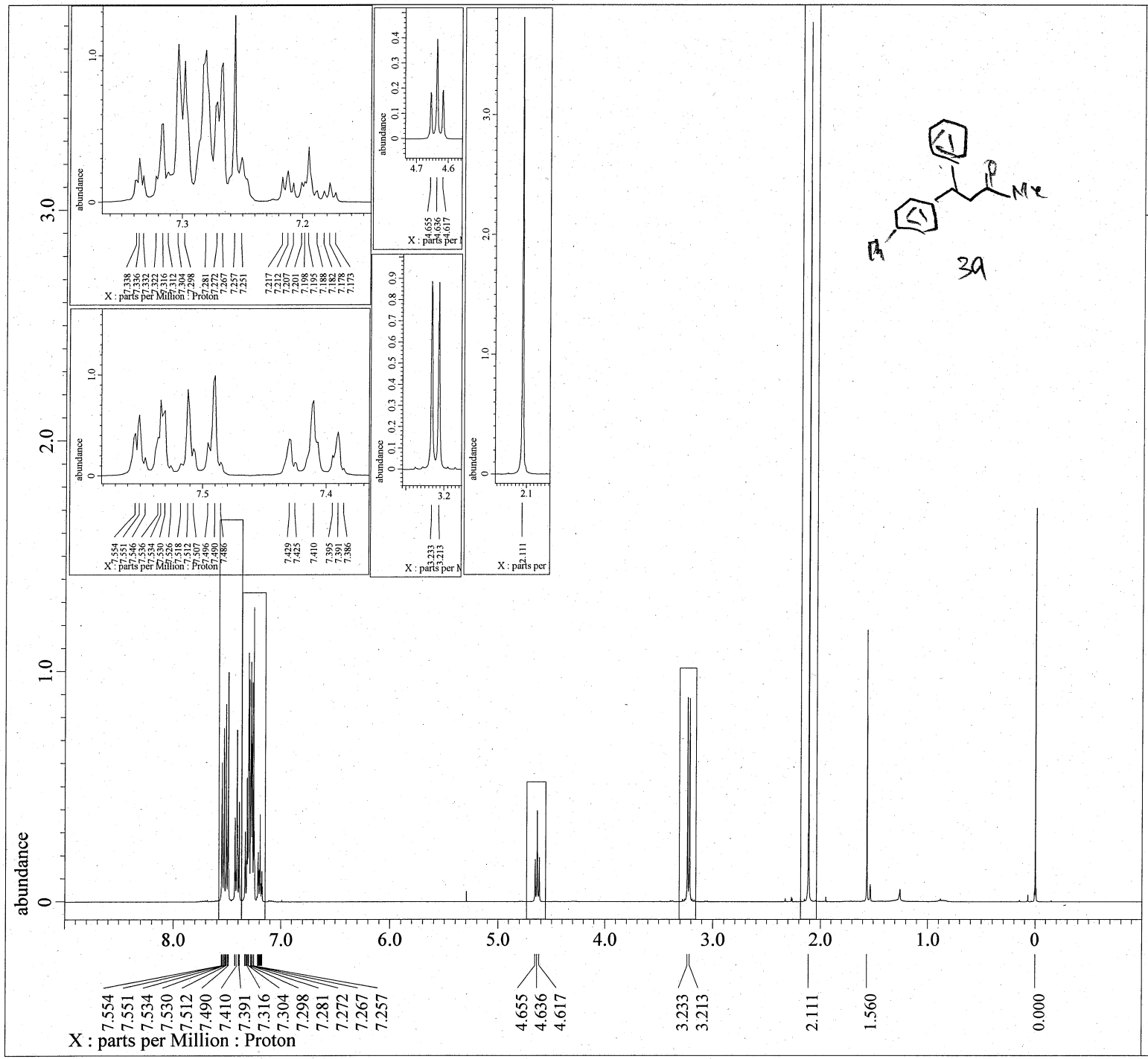


```
---- PROCESSING PARAMETERS ----
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trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: SHO-071-pure2_Proton-1-1.jdf
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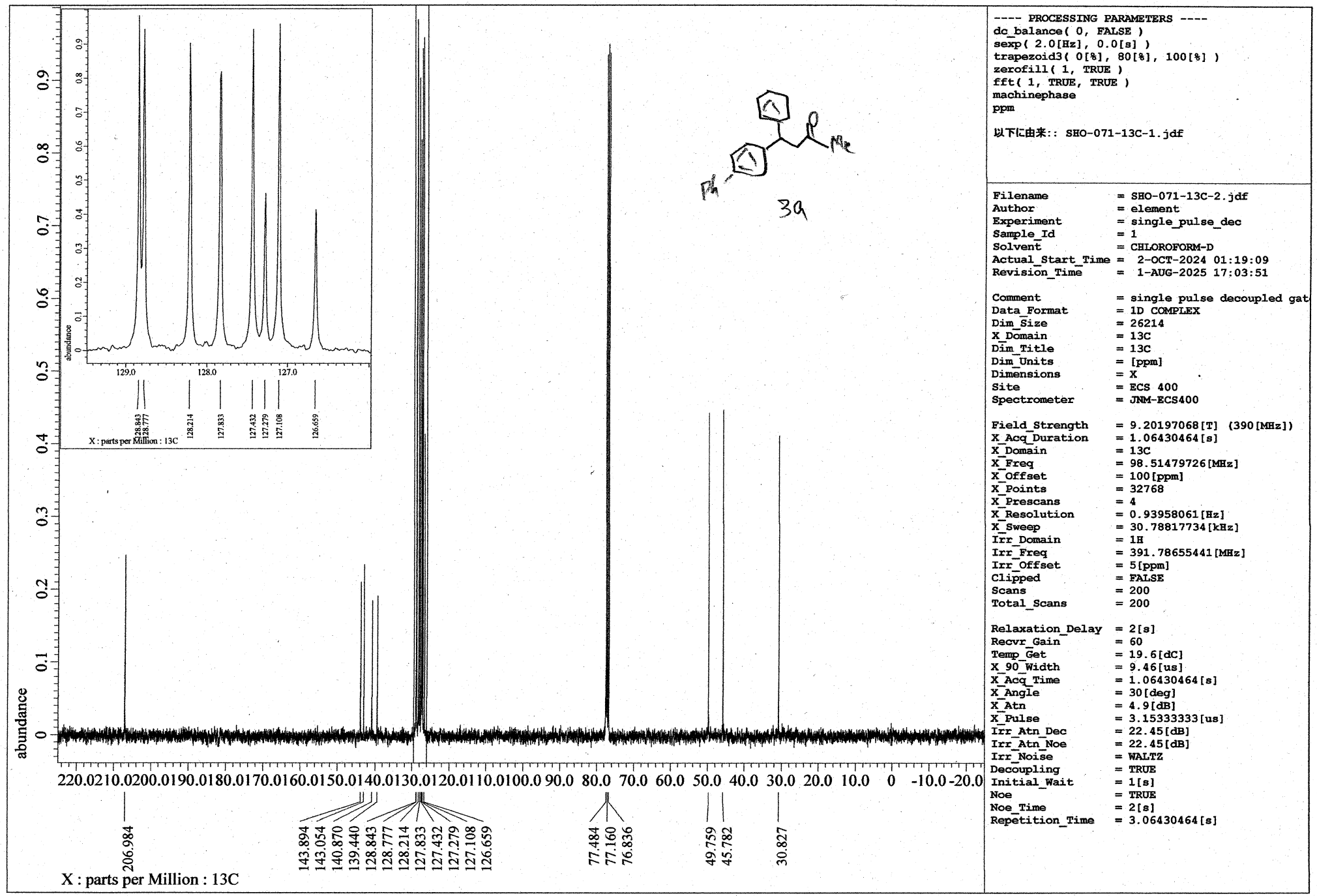
Author	= element
Experiment	= proton_auto.jxp
Sample_Id	= SHO-071-pure2
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 6-JUL-2024 12:01:04
Revision_Time	= 9-OCT-2024 10:52:15
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.2982153[T] (400[MHz
X_Acq_Duration	= 2.20725248[s]
X_Domain	= Proton
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]
X_Sweep_Clipped	= 5.93824228[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 395.88430144[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 56
Temp_Get	= 19.9[dC]
X_90_Width	= 6.34[us]
X_Acq_Time	= 2.20725248[s]
X_Angle	= 45[deg]
X_Atn	= 5[dB]
X_Pulse	= 3.17[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 500
Dante_Presat	= FALSE
Decimation_Rate	= 0
Experiment_Path	= C:\Program Files\JEOL
Initial_Wait	= 1[s]
Phase	= {0, 90, 270, 180, 180
Presat_Time	= 5[s]




```
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trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm

以下に由来:: SHO-071-13C-1.jdf
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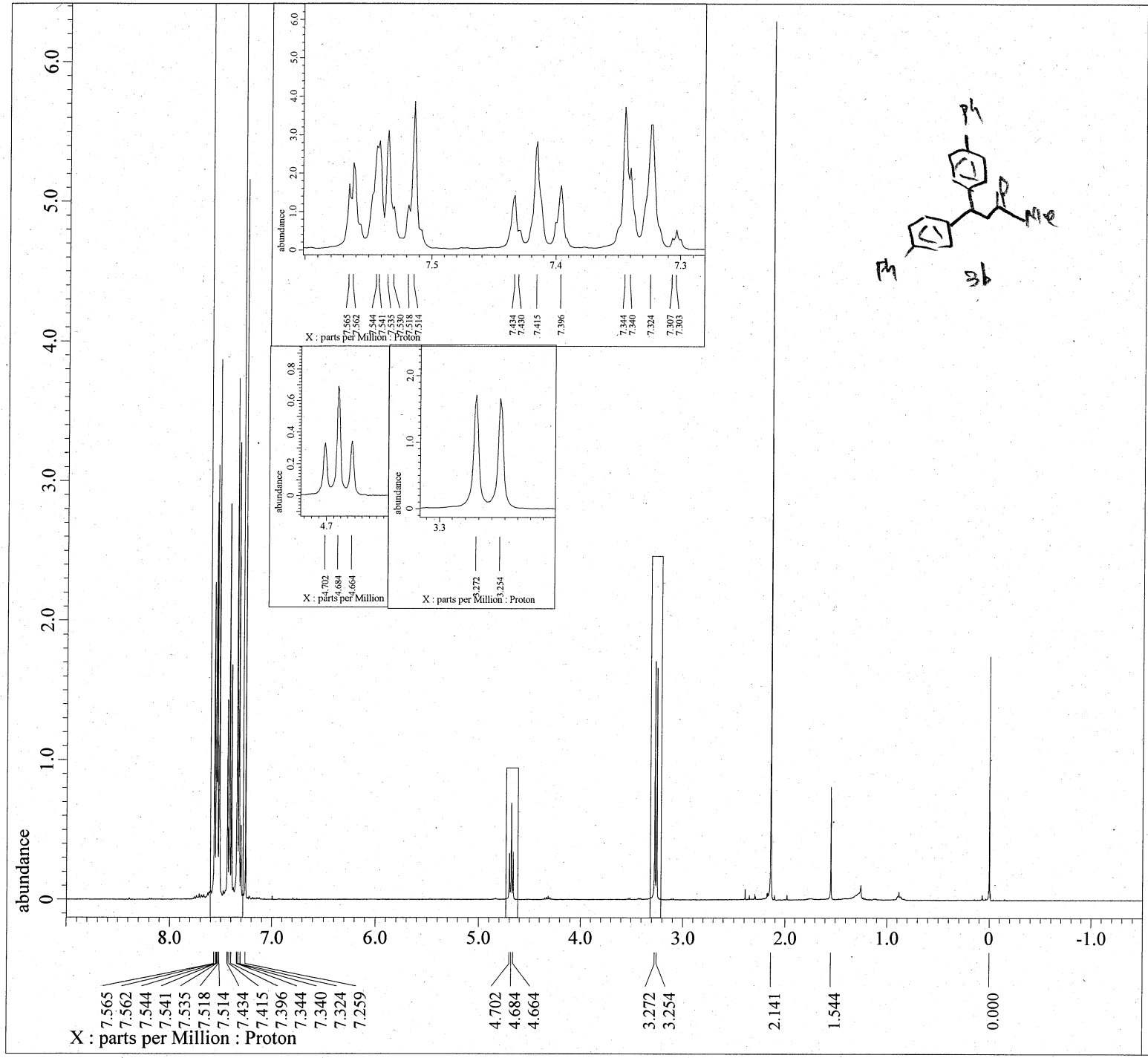
Filename	= SHO-071-13C-2.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= 1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 2-OCT-2024 01:19:09
Revision_Time	= 1-AUG-2025 17:03:51
Comment	= single pulse decoupled gat
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= 13C
Dim_Title	= 13C
Dim_Units	= [ppm]
Dimensions	= X
Site	= ECS 400
Spectrometer	= JNM-ECS400
Field_Strength	= 9.20197068[T] (390[MHz])
X_Acq_Duration	= 1.06430464[s]
X_Domain	= 13C
X_Freq	= 98.51479726[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.93958061[Hz]
X_Sweep	= 30.78817734[kHz]
Irr_Domain	= 1H
Irr_Freq	= 391.78655441[MHz]
Irr_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 200
Total_Scans	= 200
Relaxation_Delay	= 2[s]
Recvr_Gain	= 60
Temp_Get	= 19.6[dC]
X_90_Width	= 9.46[us]
X_Acq_Time	= 1.06430464[s]
X_Angle	= 30[deg]
X_Atn	= 4.9[dB]
X_Pulse	= 3.15333333[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: KND_2044_pure_Proton-1-1.jdf
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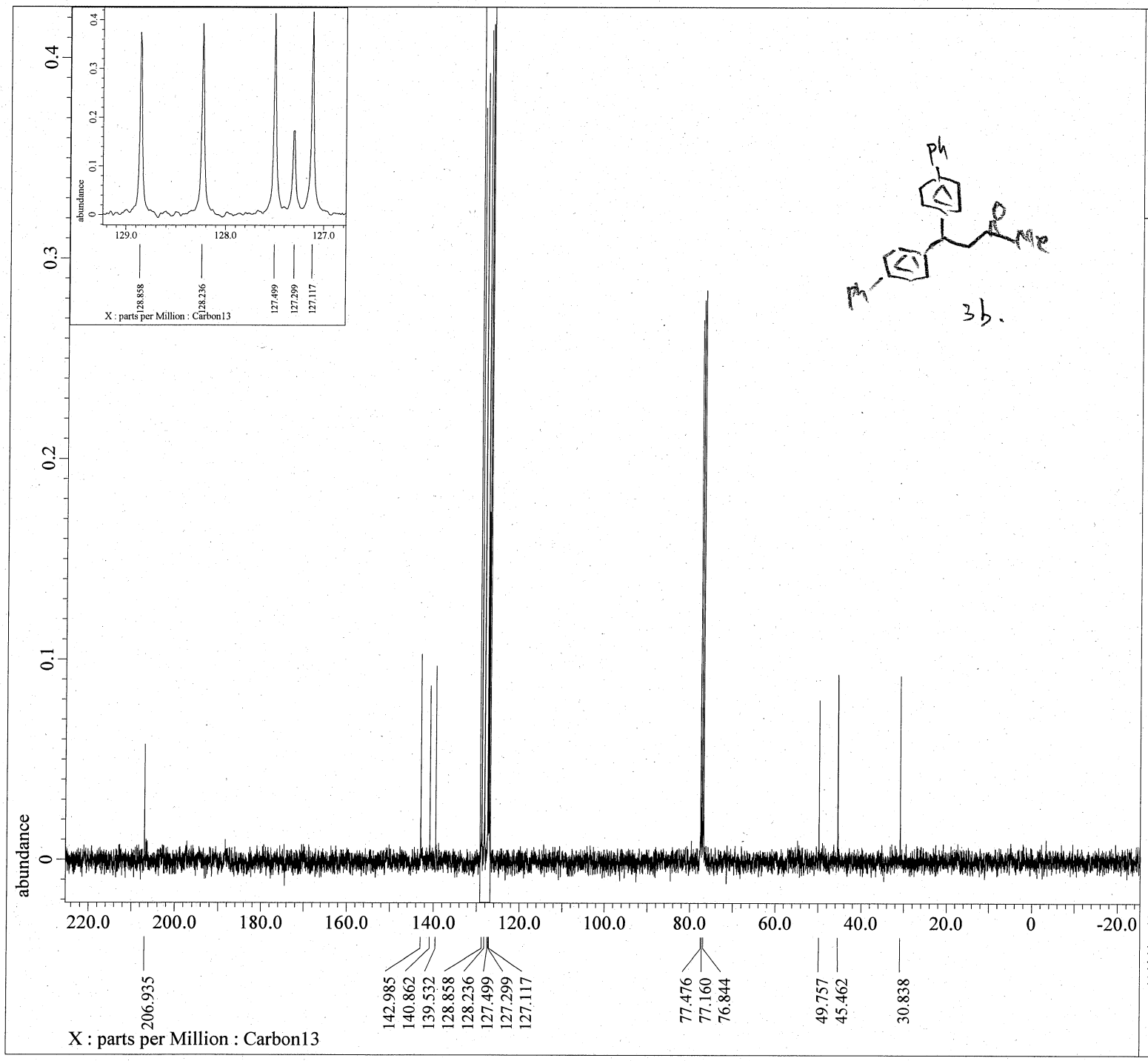
Filename	= KND_2044_pure_Proton-1-2.
Author	= element
Experiment	= proton.jxp
Sample_Id	= KND_2044_pure
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 7-NOV-2024 00:10:34
Revision_Time	= 6-NOV-2024 23:11:05
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECS400
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.37221[T] (400[MHz])
X_Acq_Duration	= 2.1889024[s]
X_Domain	= 1H
X_Freq	= 399.03472754[MHz]
X_Offset	= 5.0[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45684997[Hz]
X_Sweep	= 7.48502994[kHz]
X_Sweep_Clipped	= 5.98802395[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.03472754[MHz]
Irr_Offset	= 5.0[ppm]
Tri_Domain	= Proton
Tri_Freq	= 399.03472754[MHz]
Tri_Offset	= 5.0[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 46
Temp_Get	= 20.8[dC]
X_90_Width	= 6.6[us]
X_Acq_Time	= 2.1889024[s]
X_Angle	= 45[deg]
X_Atn	= 1[dB]
X_Pulse	= 3.3[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.1889024[s]




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

Derived from: KND_2044_13C_Carbon-1-1.jdf
```

Filename	= KND_2044_13C_Carbon-1-2.j
Author	= element
Experiment	= carbon.jxp
Sample_Id	= KND_2044_13C
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 21-AUG-2024 13:07:40
Revision_Time	= 6-NOV-2024 23:13:14
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	= 48
Total_Scans	= 48
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 21.1[dC]
X_90_Width	= 12.68[us]
X_Acq_Time	= 1.03809024[s]
X_Angle	= 30[deg]
X_Atn	= 4[dB]
X_Pulse	= 4.22666667[us]
Irr_Atn_Dec	= 26.45[dB]
Irr_Atn_Noe	= 26.45[dB]
Irr_Noise	= WALTZ
Irr_Pwidth	= 0.115[ms]
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Initial_Wait	= 1[s]
Noe	= TRUE
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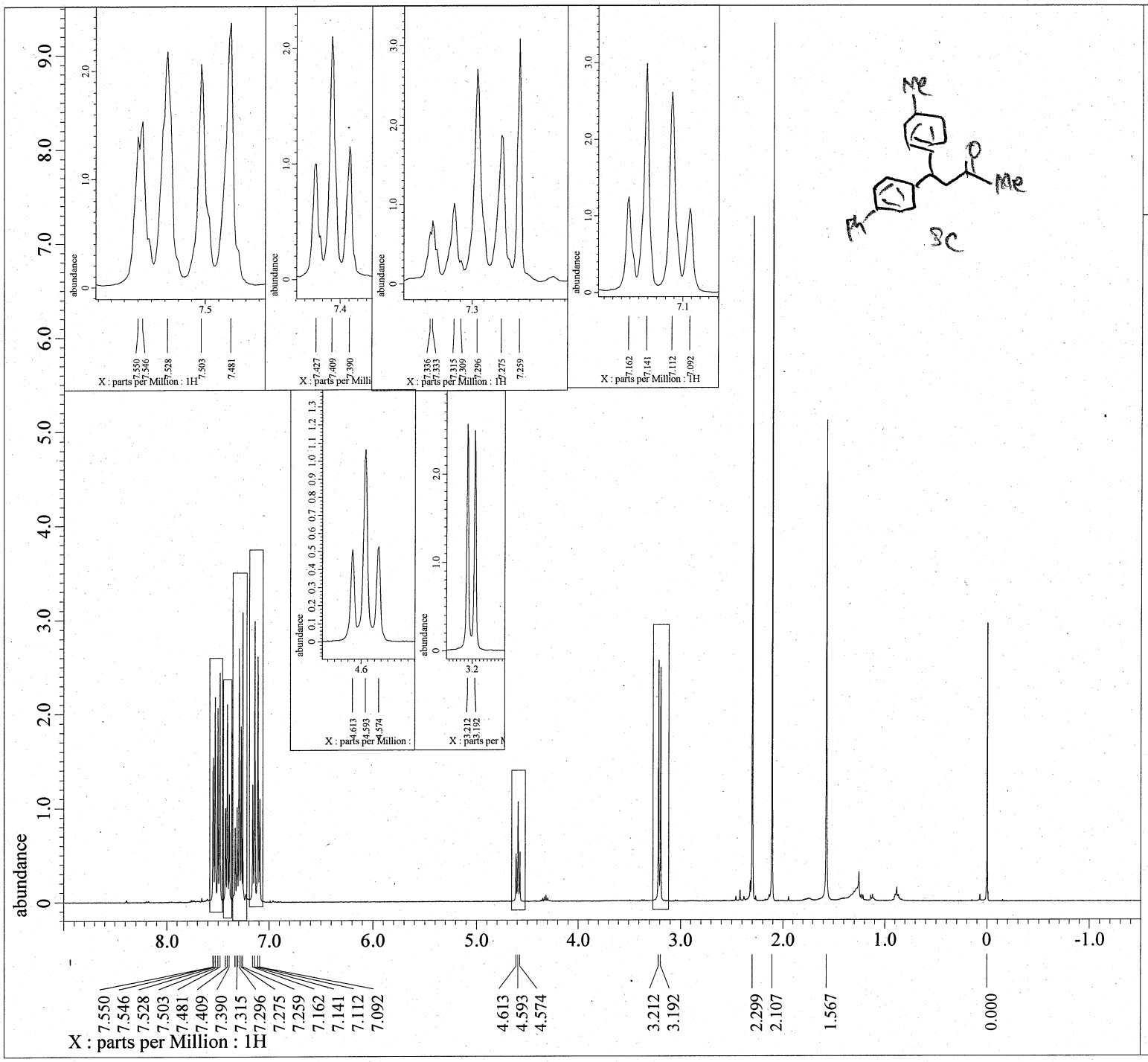
Repetition_Time	= 3.03809024[s]




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

Derived from: KND_2031_pure.jdf
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Filename	= KND_2031_pure-1.jdf
Author	= element
Experiment	= single_pulse.ex2
Sample_Id	= S#804693
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 3-OCT-2024 04:37:32
Revision_Time	= 7-OCT-2024 21:33:50
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= 1H
Dim_Title	= 1H
Dim_Units	= [ppm]
Dimensions	= X
Site	= ECS 400
Spectrometer	= JNM-ECS400
Field_Strength	= 9.20197068[T] (390[MHz])
X_Acq_Duration	= 2.228224[s]
X_Domain	= 1H
X_Freq	= 391.78655441[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.44878791[Hz]
X_Sweep	= 7.35294118[kHz]
Irr_Domain	= 1H
Irr_Freq	= 391.78655441[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= 1H
Tri_Freq	= 391.78655441[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 52
Temp_Get	= 20.3[dC]
X_90_Width	= 10.79[us]
X_Acq_Time	= 2.228224[s]
X_Angle	= 45[deg]
X_Atn	= 1.9[dB]
X_Pulse	= 5.395[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
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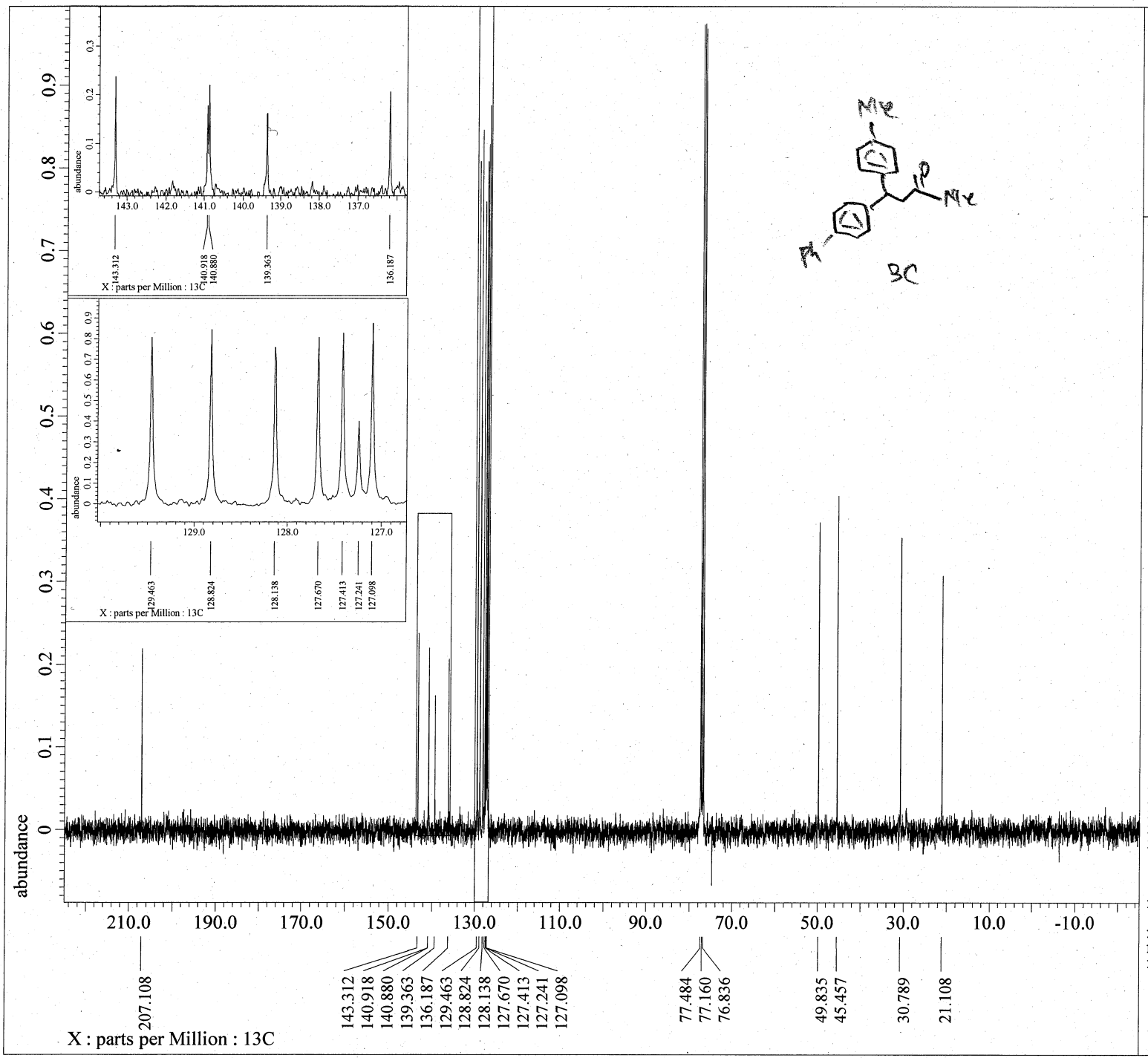


```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KND_2031_13C-1.jdf
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Author	= element
Experiment	= single_pulse_dec
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Solvent	= CHLOROFORM-D
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Revision_Time	= 7-OCT-2024 22:21:57
Comment	= single pulse decoupled ga
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Dim_Size	= 26214
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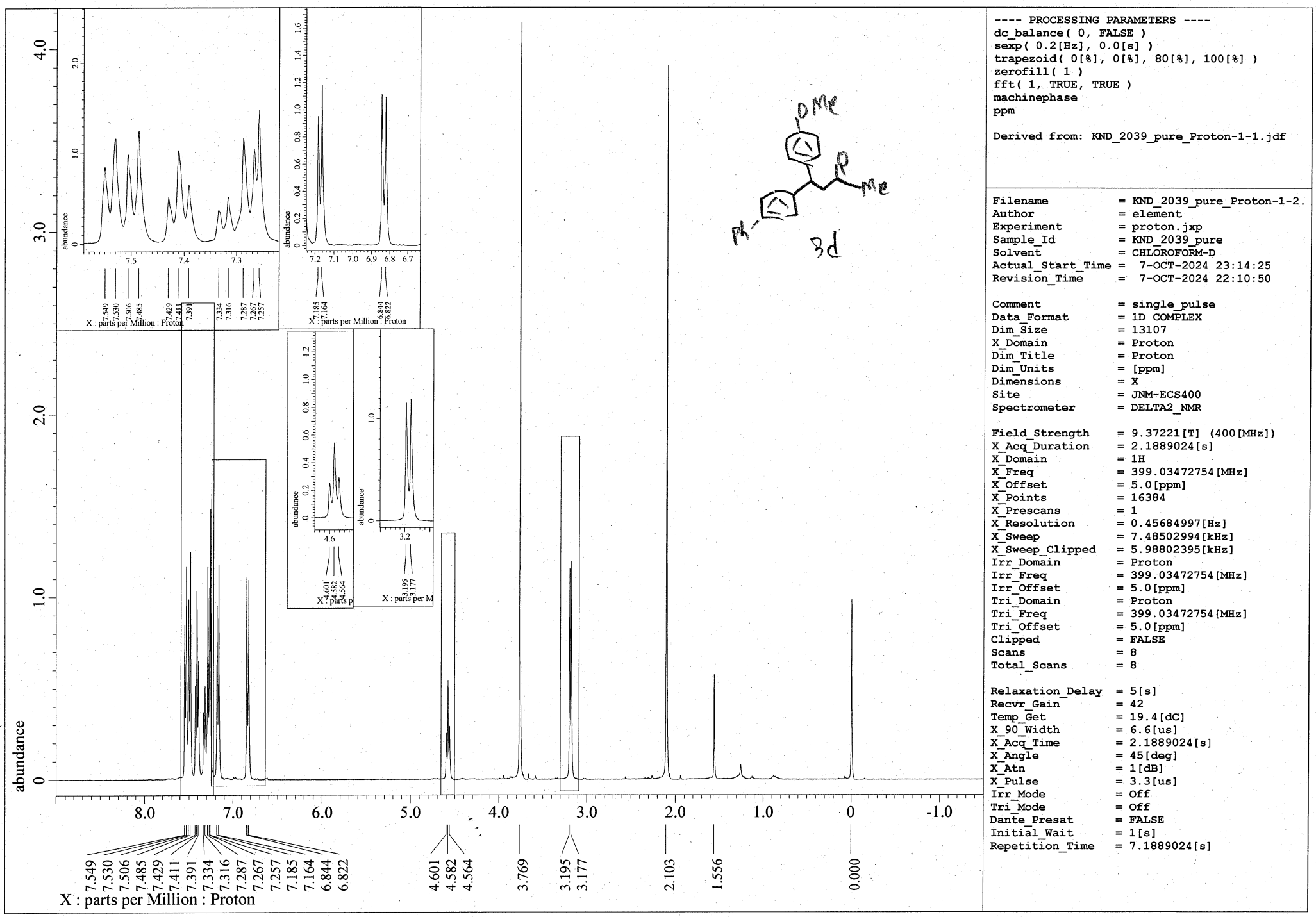
Dim_Title	= 13C
Dim_Units	= [ppm]
Dimensions	= X
Site	= ECS 400
Spectrometer	= JNM-ECS400
Field_Strength	= 9.20197068[T] (390[MHz])
X_Acq_Duration	= 1.06430464[s]
X_Domain	= 13C
X_Freq	= 98.51479726[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.93958061[Hz]
X_Sweep	= 30.78817734[kHz]
Irr_Domain	= 1H
Irr_Freq	= 391.78655441[MHz]
Irr_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 68
Total_Scans	= 68
Relaxation_Delay	= 2[s]
Recvr_Gain	= 60
Temp_Get	= 22.3[dC]
X_90_Width	= 9.46[us]
X_Acq_Time	= 1.06430464[s]
X_Angle	= 30[deg]
X_Atn	= 4.9[dB]
X_Pulse	= 3.15333333[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 ----
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sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
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machinephase
ppm

Derived from: KND_2039_pure_Proton-1-1.jdf
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Revision_Time	= 7-OCT-2024 22:10:50
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Dim_Size	= 13107
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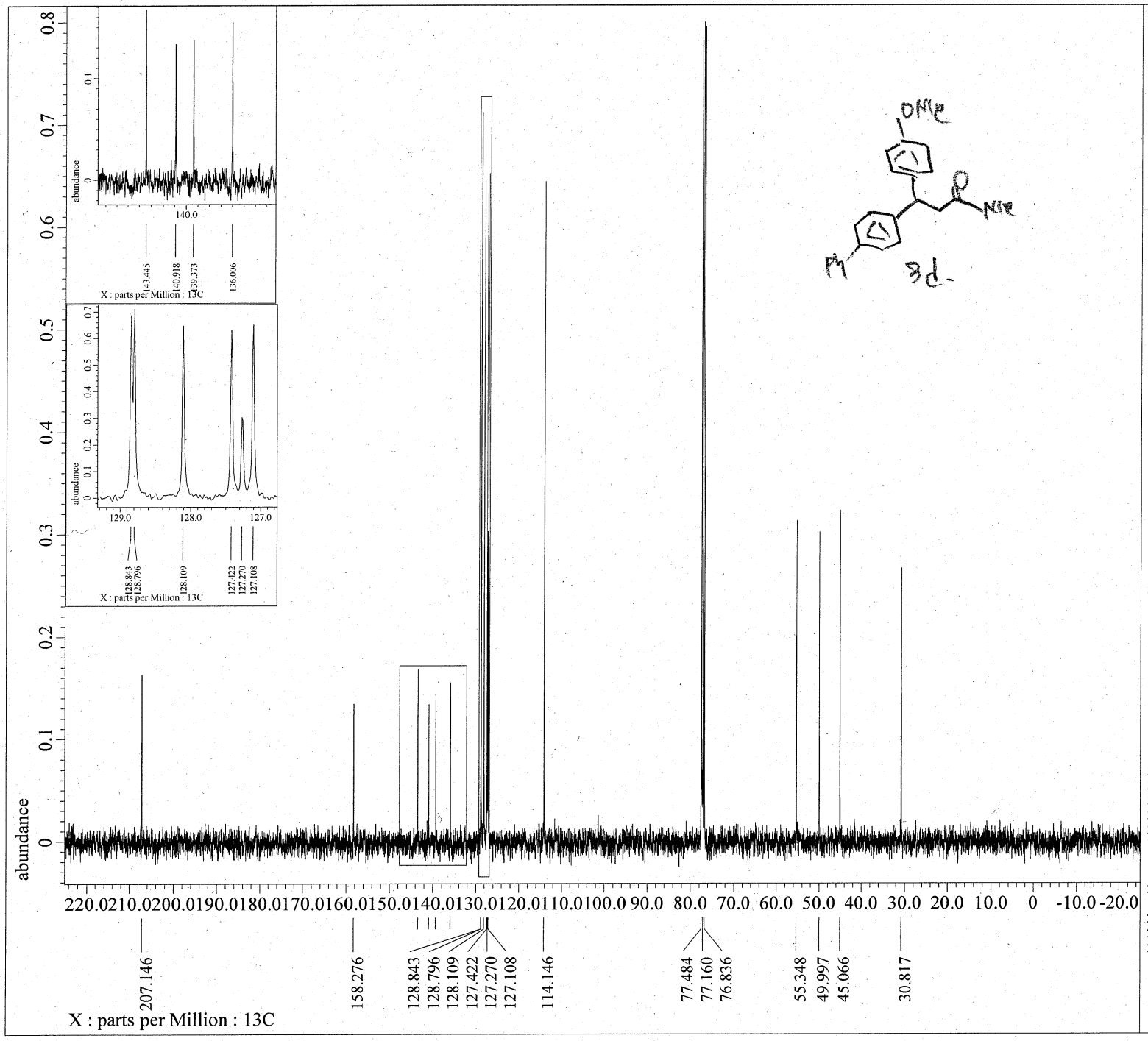
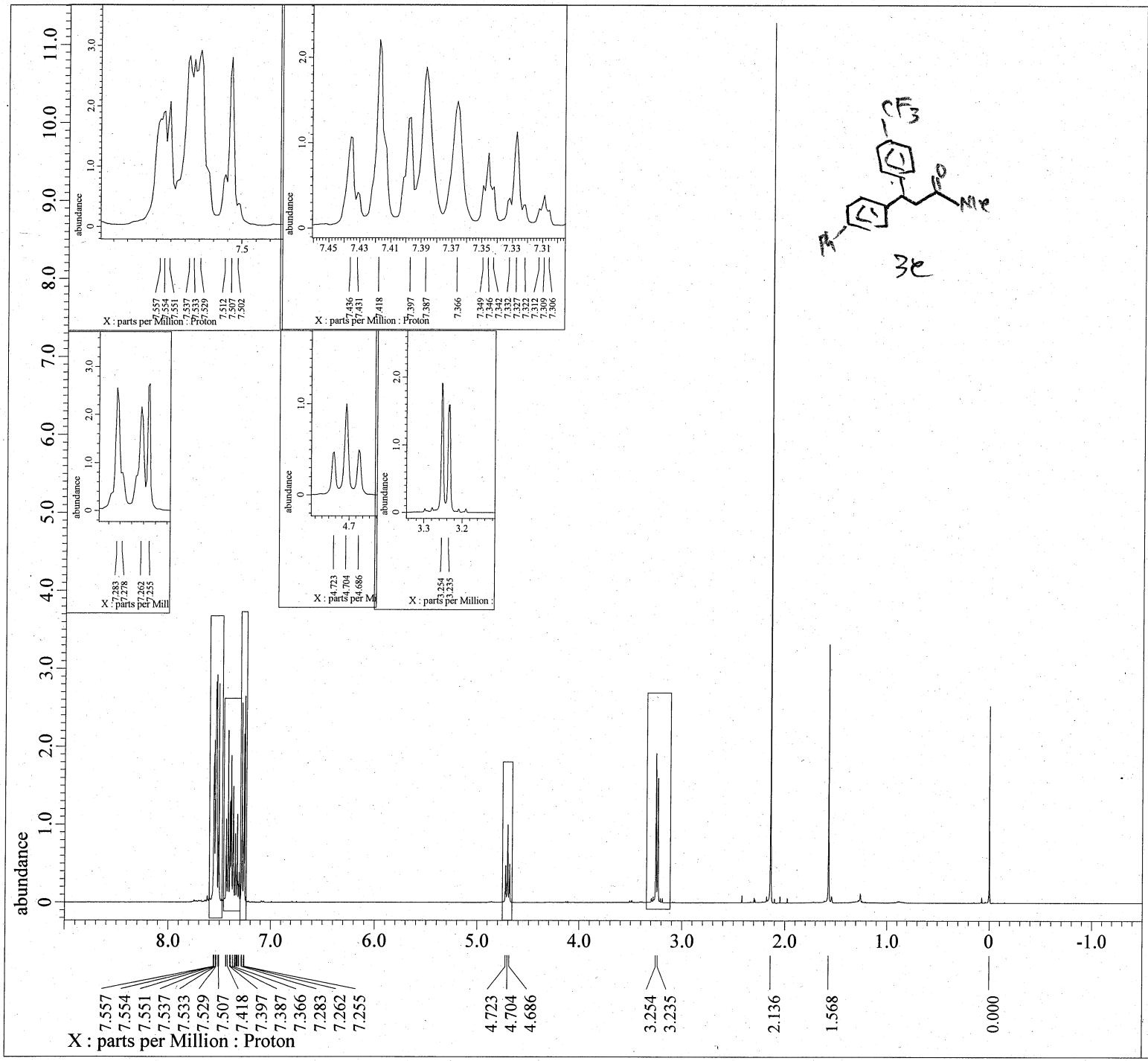
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECS400
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.37221[T] (400[MHz])
X_Acq_Duration	= 2.1889024[s]
X_Domain	= 1H
X_Freq	= 399.03472754[MHz]
X_Offset	= 5.0[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45684997[Hz]
X_Sweep	= 7.48502994[kHz]
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	= 19.4[dC]
X_90_Width	= 6.6[us]
X_Acq_Time	= 2.1889024[s]
X_Angle	= 45[deg]
X_Atn	= 1[dB]
X_Pulse	= 3.3[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.1889024[s]



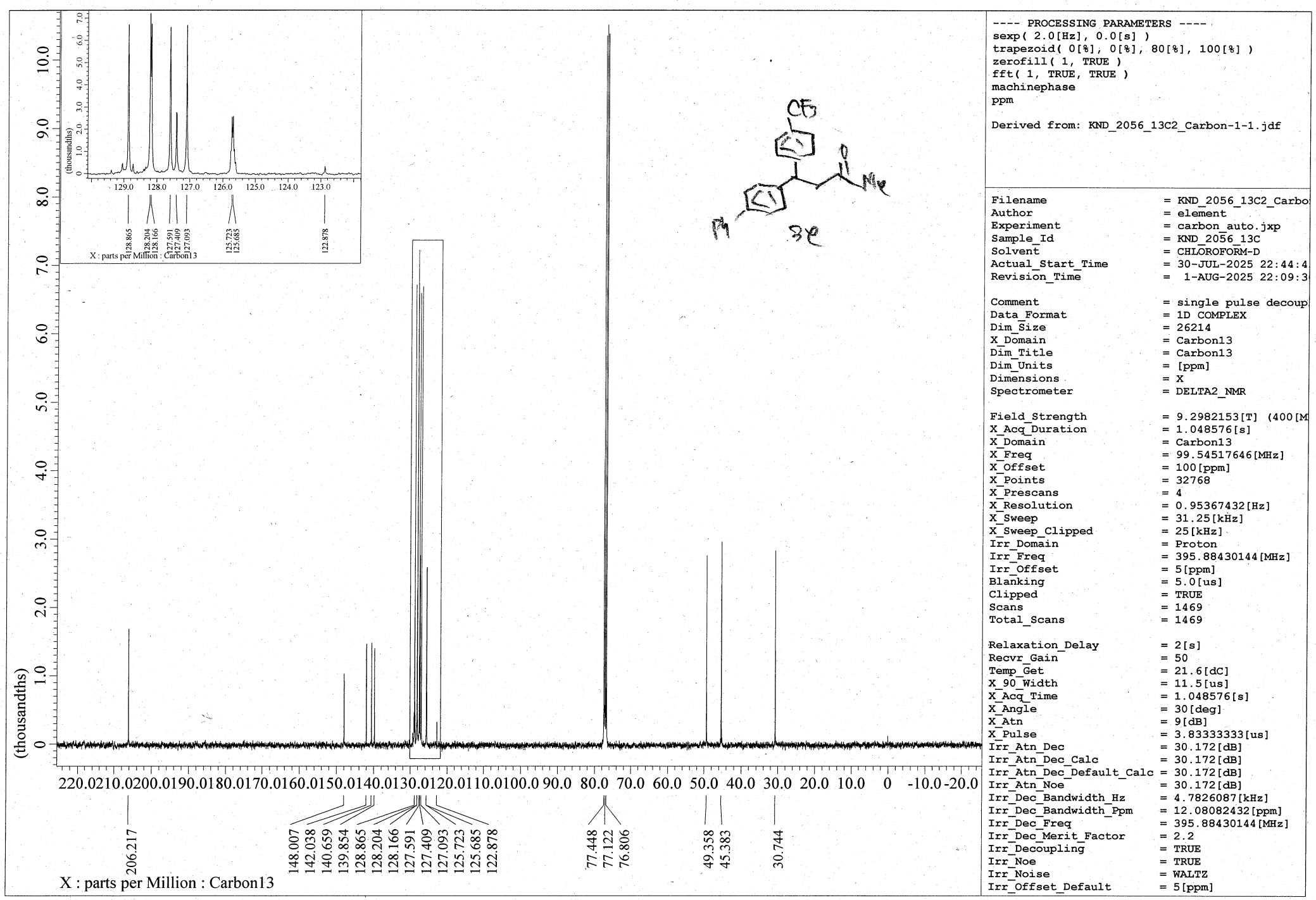

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KND_2039_13C-1.jdf
```

Filename	= KND_2039_13C-2.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= 1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 27-AUG-2024 01:02:42
Revision_Time	= 7-AUG-2025 22:07:14
Comment	= single pulse decoupled gat
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	= 99
Total_Scans	= 99
Relaxation_Delay	= 2[s]
Recvr_Gain	= 60
Temp_Get	= 22.9[dC]
X_90_Width	= 9.46[us]
X_Acq_Time	= 1.06430464[s]
X_Angle	= 30[deg]
X_Atn	= 4.9[dB]
X_Pulse	= 3.15333333[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]



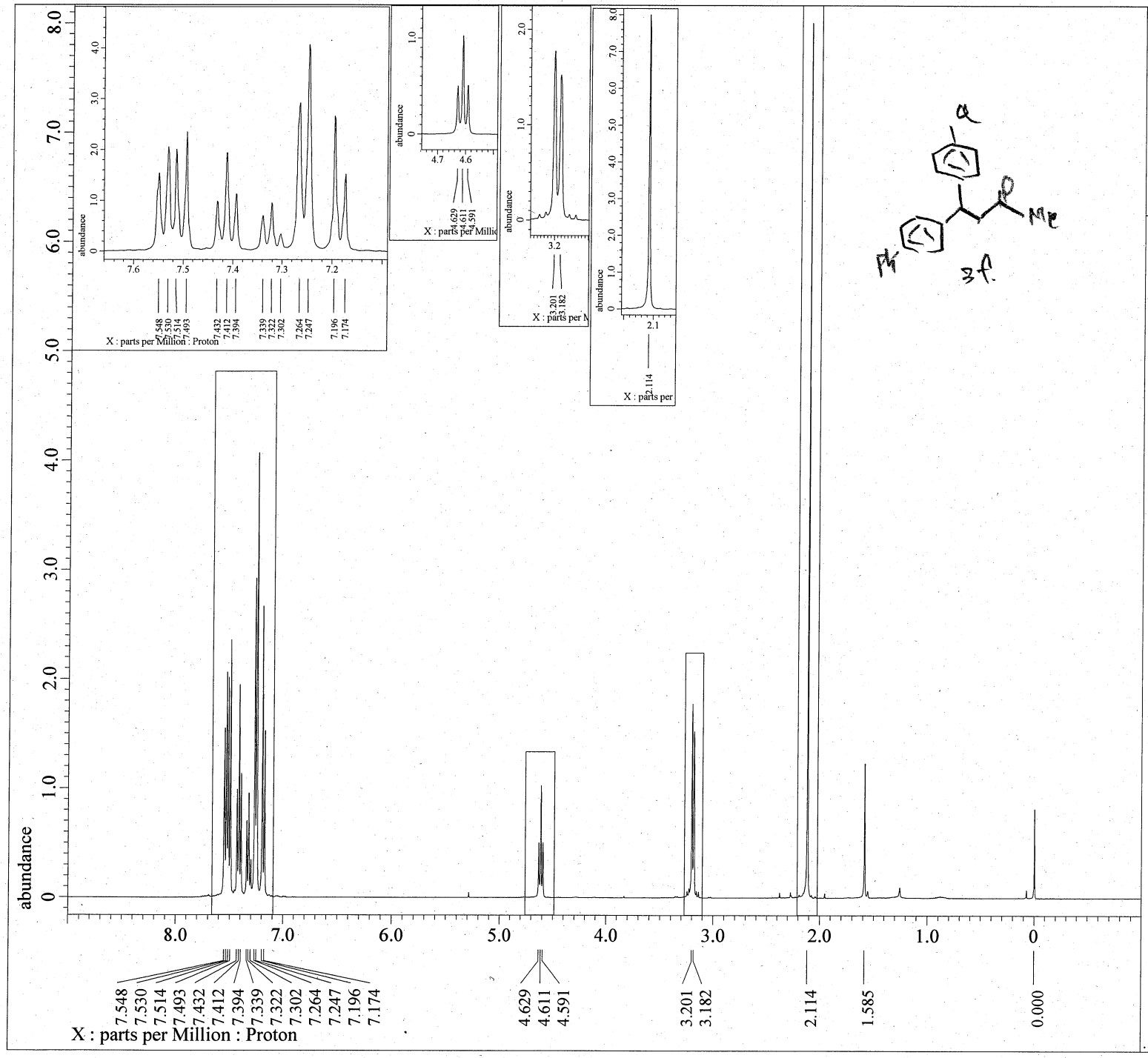

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KND_2056_pure_Proton-1-1.jdf
```

Filename	= KND_2056_pure_Proton-1-2.
Author	= element
Experiment	= proton.jxp
Sample_Id	= KND_2056_pure
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 4-SEP-2024 22:30:25
Revision_Time	= 21-OCT-2024 22:53:24
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECS400
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.37221[T] (400[MHz])
X_Acq_Duration	= 2.1889024[s]
X_Domain	= 1H
X_Freq	= 399.03472754[MHz]
X_Offset	= 5.0[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45684997[Hz]
X_Sweep	= 7.48502994[kHz]
X_Sweep_Clipped	= 5.98802395[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.03472754[MHz]
Irr_Offset	= 5.0[ppm]
Tri_Domain	= Proton
Tri_Freq	= 399.03472754[MHz]
Tri_Offset	= 5.0[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 38
Temp_Get	= 22[dC]
X_90_Width	= 6.6[us]
X_Acq_Time	= 2.1889024[s]
X_Angle	= 45[deg]
X_Atn	= 1[dB]
X_Pulse	= 3.3[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.1889024[s]



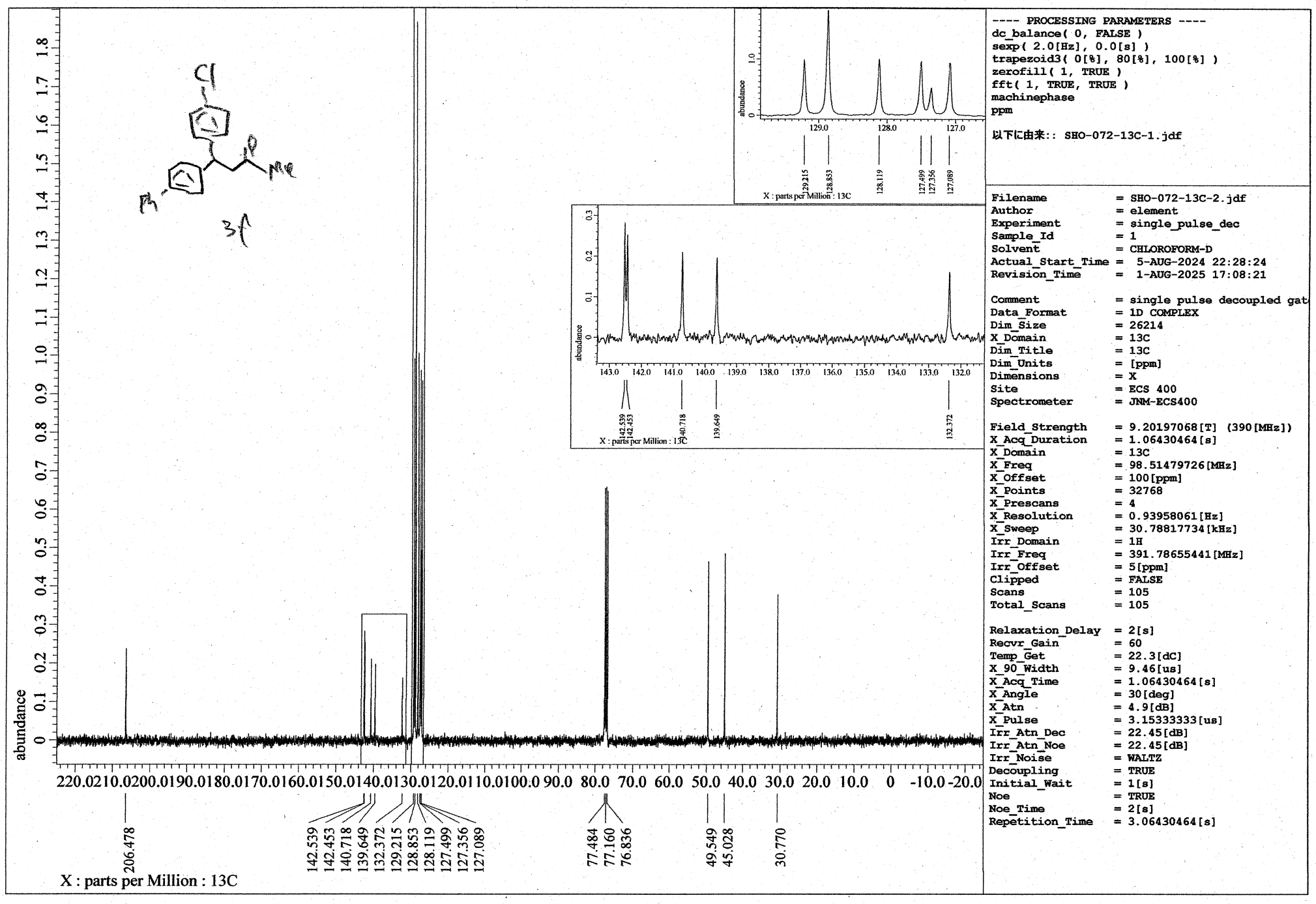

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KND_2056_13C2_Carbon-1-1.jdf
```

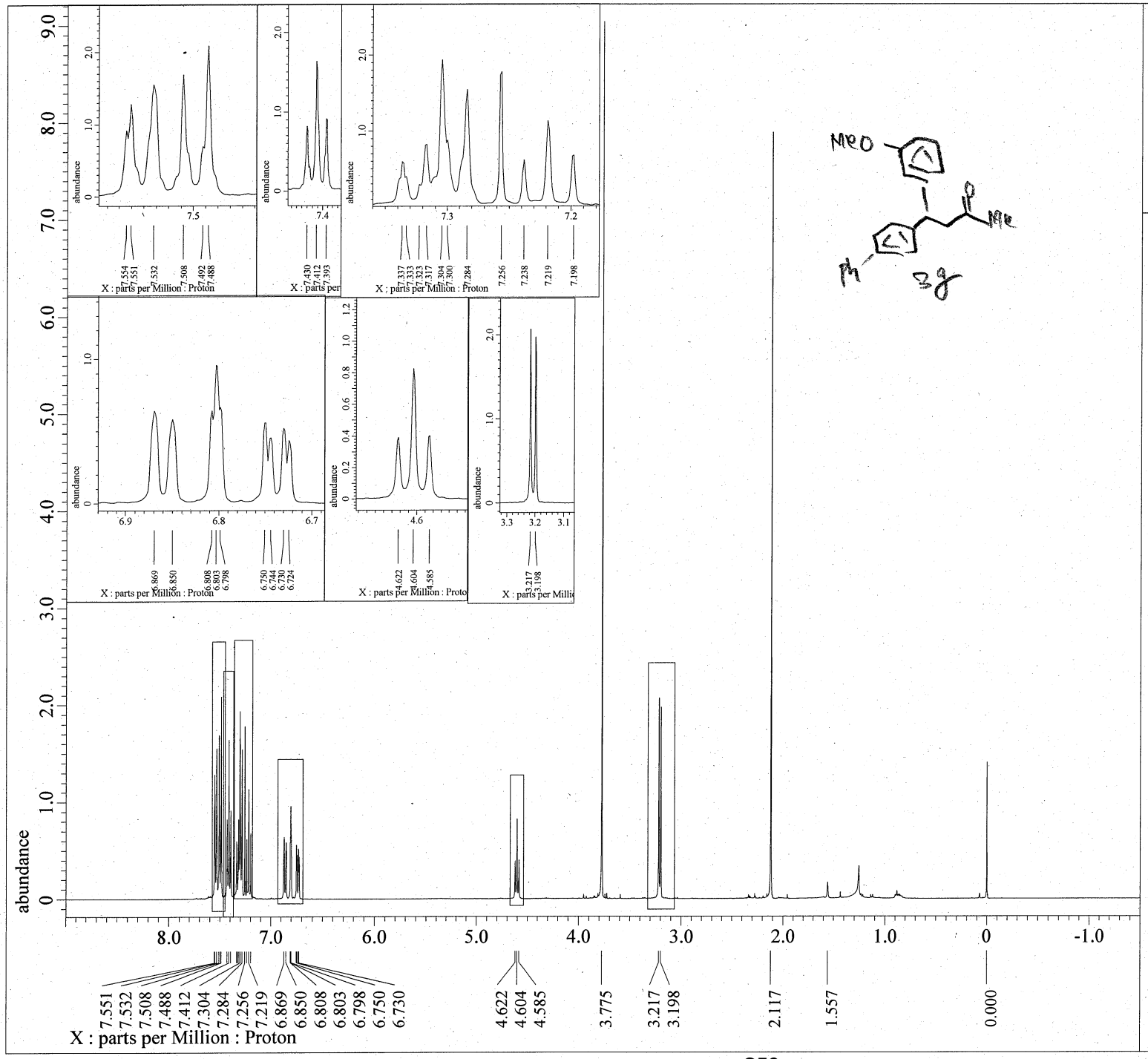
Filename	= KND_2056_13C2_Carbo
Author	= element
Experiment	= carbon_auto.jxp
Sample_Id	= KND_2056_13C
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 30-JUL-2025 22:44:4
Revision_Time	= 1-AUG-2025 22:09:3
Comment	= single pulse decoup
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.2982153[T] (400[M
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	= 5.0[us]
Clipped	= TRUE
Scans	= 1469
Total_Scans	= 1469
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 21.6[dC]
X_90_Width	= 11.5[us]
X_Acq_Time	= 1.048576[s]
X_Angle	= 30[deg]
X_Atn	= 9[dB]
X_Pulse	= 3.83333333[us]
Irr_Atn_Dec	= 30.172[dB]
Irr_Atn_Dec_Calc	= 30.172[dB]
Irr_Atn_Dec_Default_Calc	= 30.172[dB]
Irr_Atn_Noe	= 30.172[dB]
Irr_Dec_Bandwidth_Hz	= 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.08082432[ppm]
Irr_Dec_Freq	= 395.88430144[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]




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

Derived from: SHO-072-pure2_Proton-1-1.jdf
```

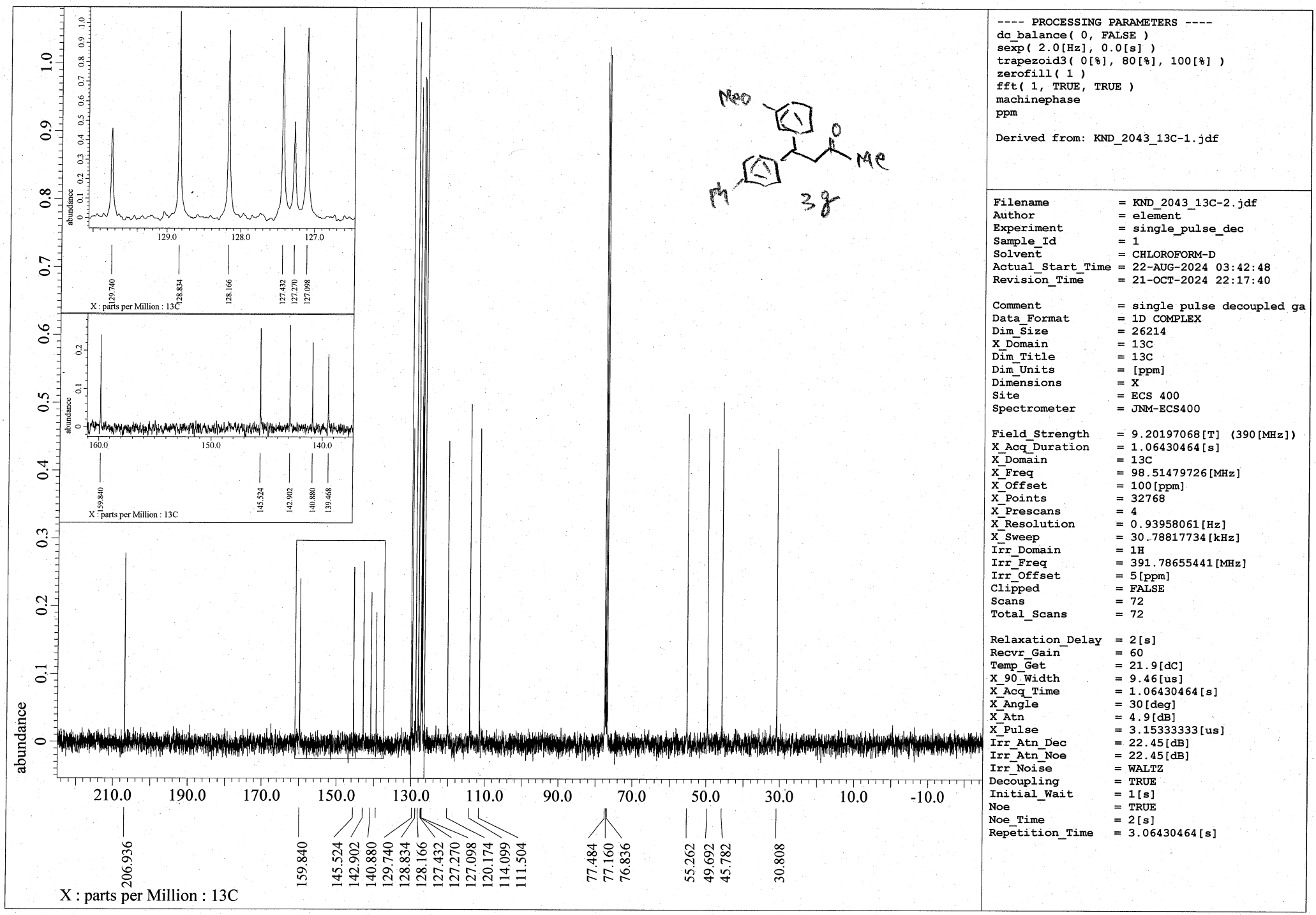
Filename	= SHO-072-pure2_Proton-1-2.
Author	= element
Experiment	= proton.jxp
Sample_Id	= SHO-072-pure2
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 8-JUL-2024 22:20:49
Revision_Time	= 9-OCT-2024 11:03:07
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
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	= 36
Temp_Get	= 18.9[dC]
X_90_Width	= 6.7[us]
X_Acq_Time	= 2.18103808[s]
X_Angle	= 45[deg]
X_Atn	= 0.8[dB]
X_Pulse	= 3.35[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.18103808[s]


3f
abundance
X : parts per Million : 13C
206.478
142.539
142.453
140.718
139.649
132.372
129.215
128.853
128.119
127.499
127.356
127.089
77.484
77.160
76.836
49.549
45.028
30.770
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid3(0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
以下に由来:: SHO-072-13C-1.jdf
Filename = SHO-072-13C-2.jdf
Author = element
Experiment = single_pulse_dec
Sample_Id = 1
Solvent = CHLOROFORM-D
Actual_Start_Time = 5-AUG-2024 22:28:24
Revision_Time = 1-AUG-2025 17:08:21
Comment = single pulse decoupled gat
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 = 105
Total_Scans = 105
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 22.3[dC]
X_90_Width = 9.46[us]
X_Acq_Time = 1.06430464[s]
X_Angle = 30[deg]
X_Atn = 4.9[dB]
X_Pulse = 3.15333333[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]



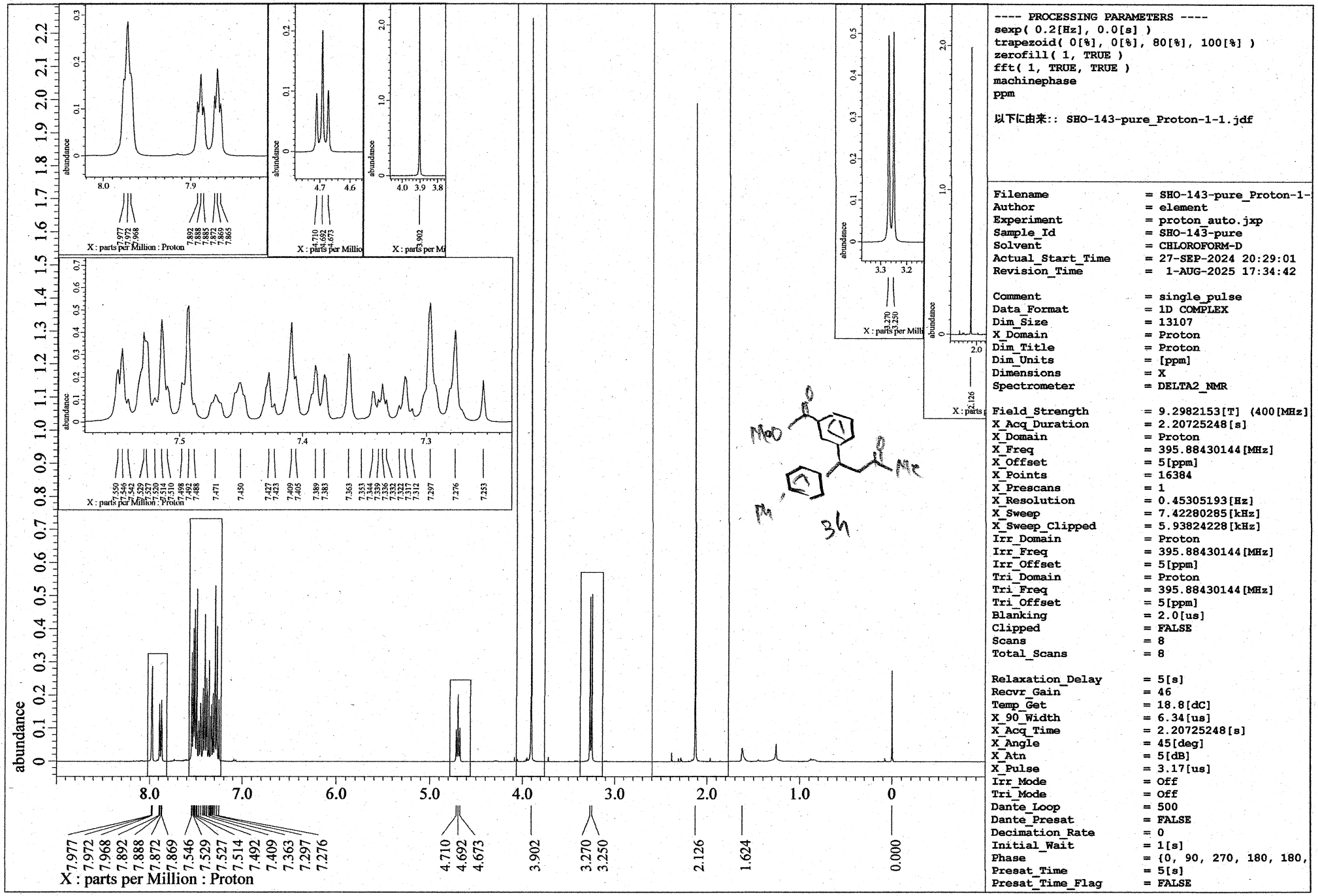

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KND_2034_2Proton-1-1.jdf
```

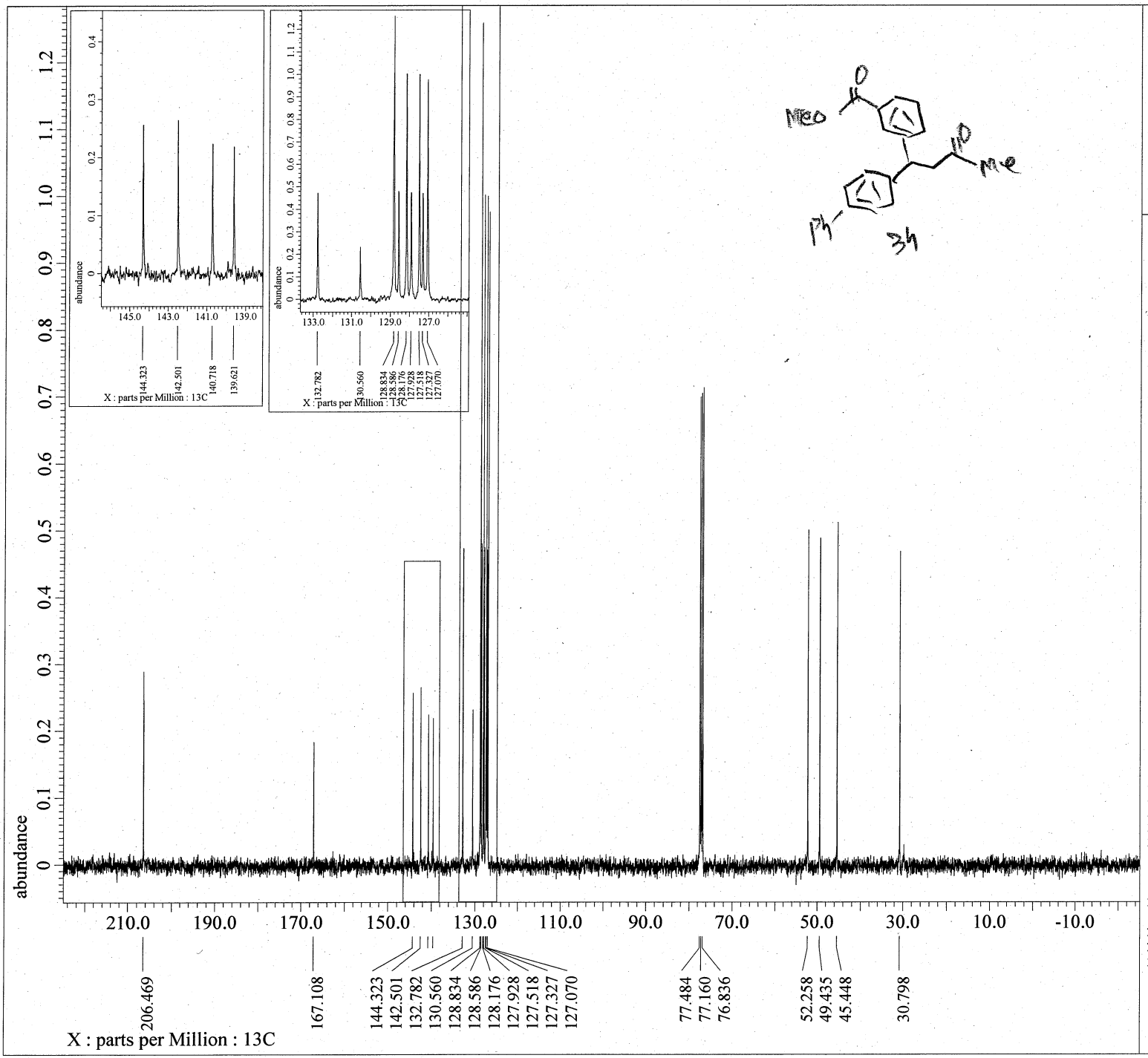
Filename	= KND_2034_2Proton-1-2.jdf
Author	= element
Experiment	= proton.jxp
Sample_Id	= KND_
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 9-OCT-2024 23:52:06
Revision_Time	= 21-OCT-2024 22:09:02
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [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	= 18.9[dC]
X_90_Width	= 6.7[us]
X_Acq_Time	= 2.18103808[s]
X_Angle	= 45[deg]
X_Atn	= 0.8[dB]
X_Pulse	= 3.35[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: KND_2043_13C-1.jdf
```

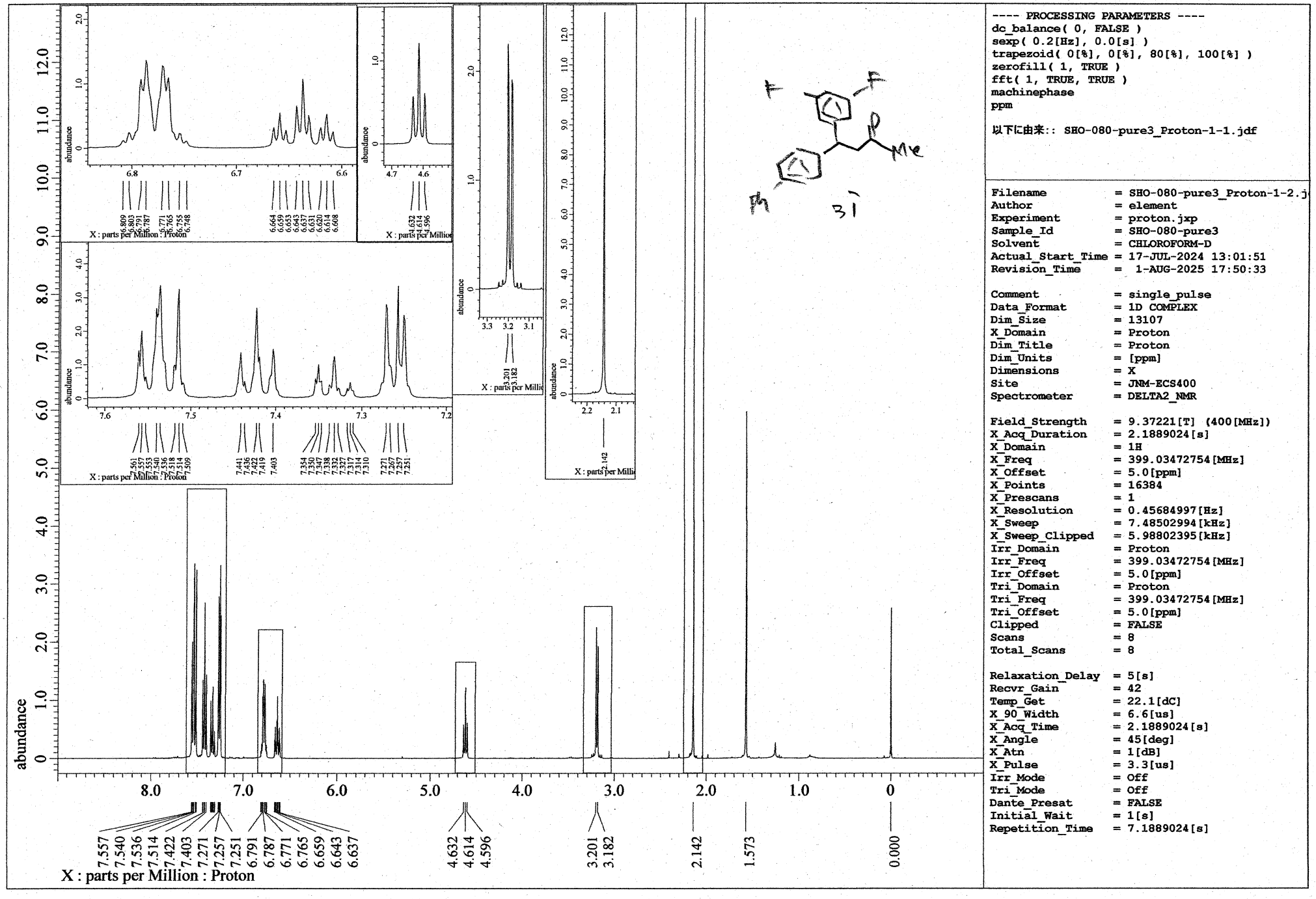
Filename	= KND_2043_13C-2.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= 1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 22-AUG-2024 03:42:48
Revision_Time	= 21-OCT-2024 22:17:40
Comment	= single pulse decoupled ga
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= 13C
Dim_Title	= 13C
Dim_Units	= [ppm]
Dimensions	= X
Site	= 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	= 72
Total_Scans	= 72
Relaxation_Delay	= 2[s]
Recvr_Gain	= 60
Temp_Get	= 21.9[dC]
X_90_Width	= 9.46[us]
X_Acq_Time	= 1.06430464[s]
X_Angle	= 30[deg]
X_Atn	= 4.9[dB]
X_Pulse	= 3.15333333[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]


X : parts per Million : Proton
abundance
7.977
7.972
7.968
7.892
7.888
7.885
7.872
7.869
7.865
7.550
7.546
7.542
7.529
7.527
7.514
7.510
7.498
7.492
7.488
7.471
7.450
7.427
7.423
7.409
7.405
7.389
7.383
7.363
7.353
7.344
7.339
7.336
7.332
7.322
7.317
7.312
7.297
7.276
7.253
4.710
4.692
4.673
3.902
3.270
3.250
2.126
1.624
0.000
---- PROCESSING PARAMETERS ----
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
以下に由来:: SHO-143-pure_Proton-1-1.jdf
Filename = SHO-143-pure_Proton-1-
Author = element
Experiment = proton_auto.jxp
Sample_Id = SHO-143-pure
Solvent = CHLOROFORM-D
Actual_Start_Time = 27-SEP-2024 20:29:01
Revision_Time = 1-AUG-2025 17:34:42
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 = 9.2982153[T] (400[MHz]
X_Acq_Duration = 2.20725248[s]
X_Domain = Proton
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]
X_Sweep_Clipped = 5.93824228[kHz]
Irr_Domain = Proton
Irr_Freq = 395.88430144[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 395.88430144[MHz]
Tri_Offset = 5[ppm]
Blanking = 2.0[us]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 18.8[dC]
X_90_Width = 6.34[us]
X_Acq_Time = 2.20725248[s]
X_Angle = 45[deg]
X_Atn = 5[dB]
X_Pulse = 3.17[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = {0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE



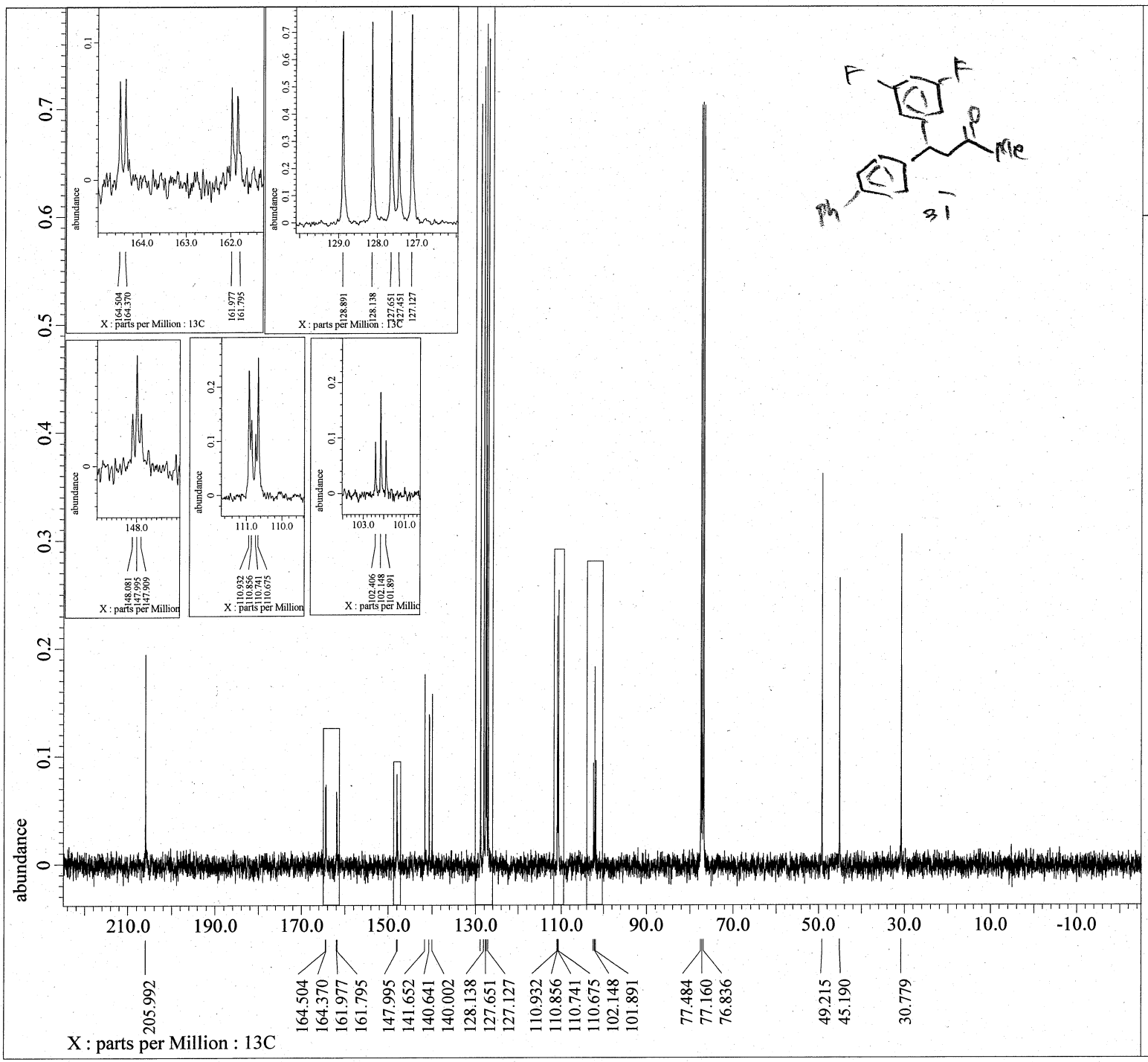

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: SHO-143-13C-1.jdf
```

Filename	= SHO-143-13C-2.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= 1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 2-OCT-2024 19:20:03
Revision_Time	= 5-OCT-2024 13:33:17
Comment	= single pulse decoupled ga
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= 13C
Dim_Title	= 13C
Dim_Units	= [ppm]
Dimensions	= X
Site	= ECS 400
Spectrometer	= JNM-ECS400
Field_Strength	= 9.20197068[T] (390[MHz])
X_Acq_Duration	= 1.06430464[s]
X_Domain	= 13C
X_Freq	= 98.51479726[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.93958061[Hz]
X_Sweep	= 30.78817734[kHz]
Irr_Domain	= 1H
Irr_Freq	= 391.78655441[MHz]
Irr_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 119
Total_Scans	= 119
Relaxation_Delay	= 2[s]
Recvr_Gain	= 60
Temp_Get	= 19.7[dC]
X_90_Width	= 9.46[us]
X_Acq_Time	= 1.06430464[s]
X_Angle	= 30[deg]
X_Atn	= 4.9[dB]
X_Pulse	= 3.15333333[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]



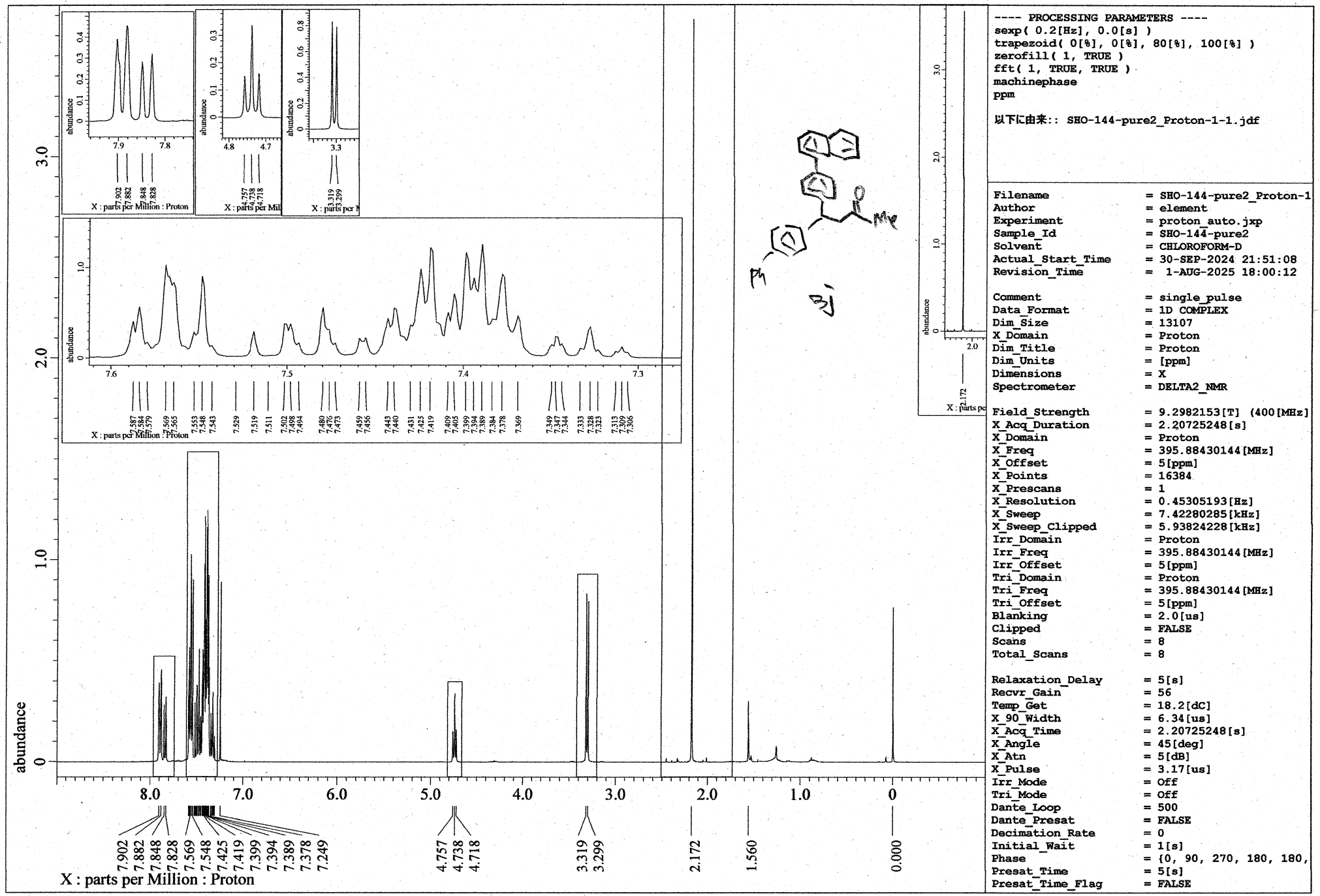

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm

以下に由来:: SHO-080-pure3_Proton-1-1.jdf
```

Filename	= SHO-080-pure3_Proton-1-2.j
Author	= element
Experiment	= proton.jxp
Sample_Id	= SHO-080-pure3
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 17-JUL-2024 13:01:51
Revision_Time	= 1-AUG-2025 17:50:33
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	= 22.1[dC]
X_90_Width	= 6.6[us]
X_Acq_Time	= 2.1889024[s]
X_Angle	= 45[deg]
X_Atn	= 1[dB]
X_Pulse	= 3.3[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.1889024[s]



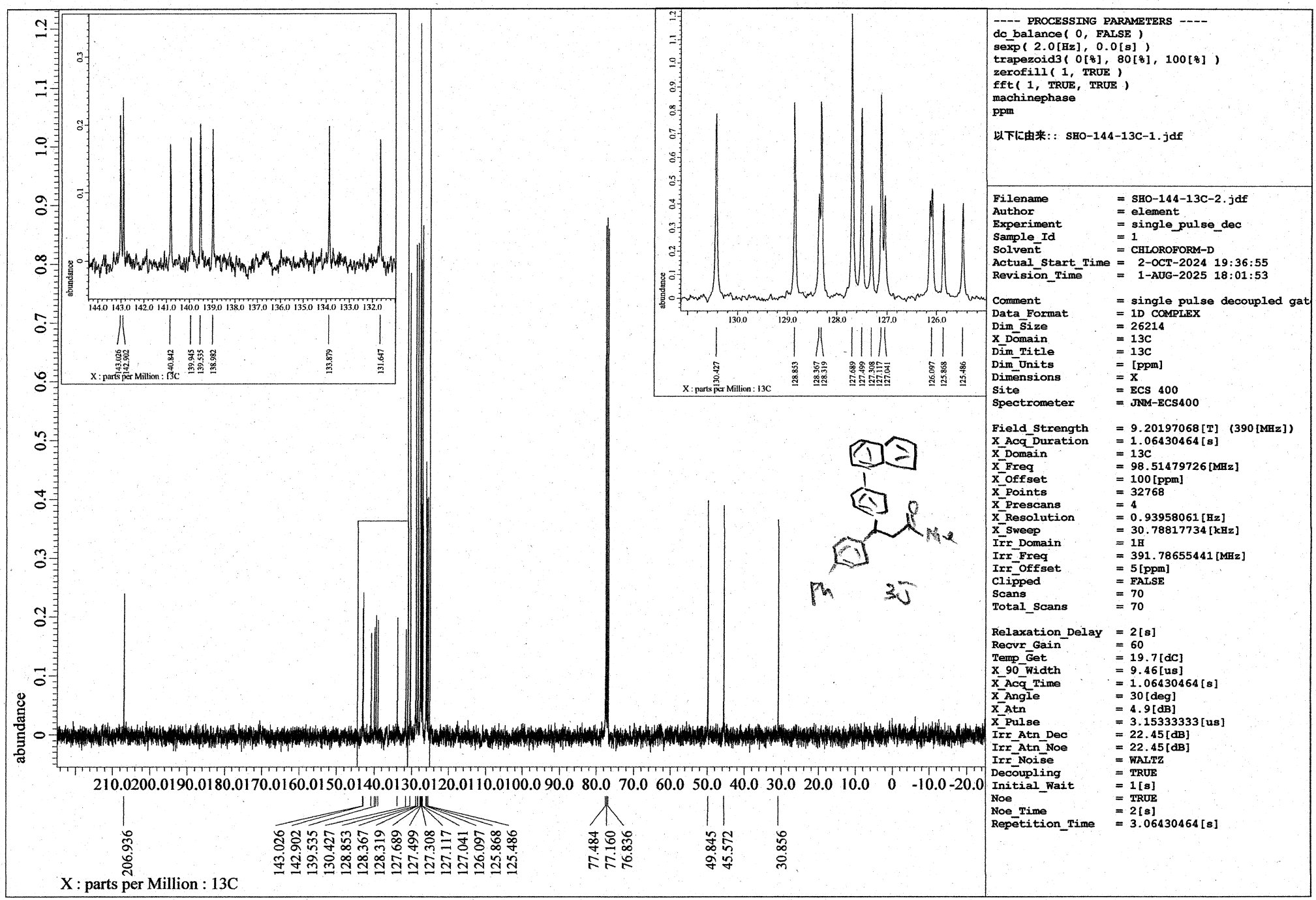

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: SHO-080-13C-1.jdf
```

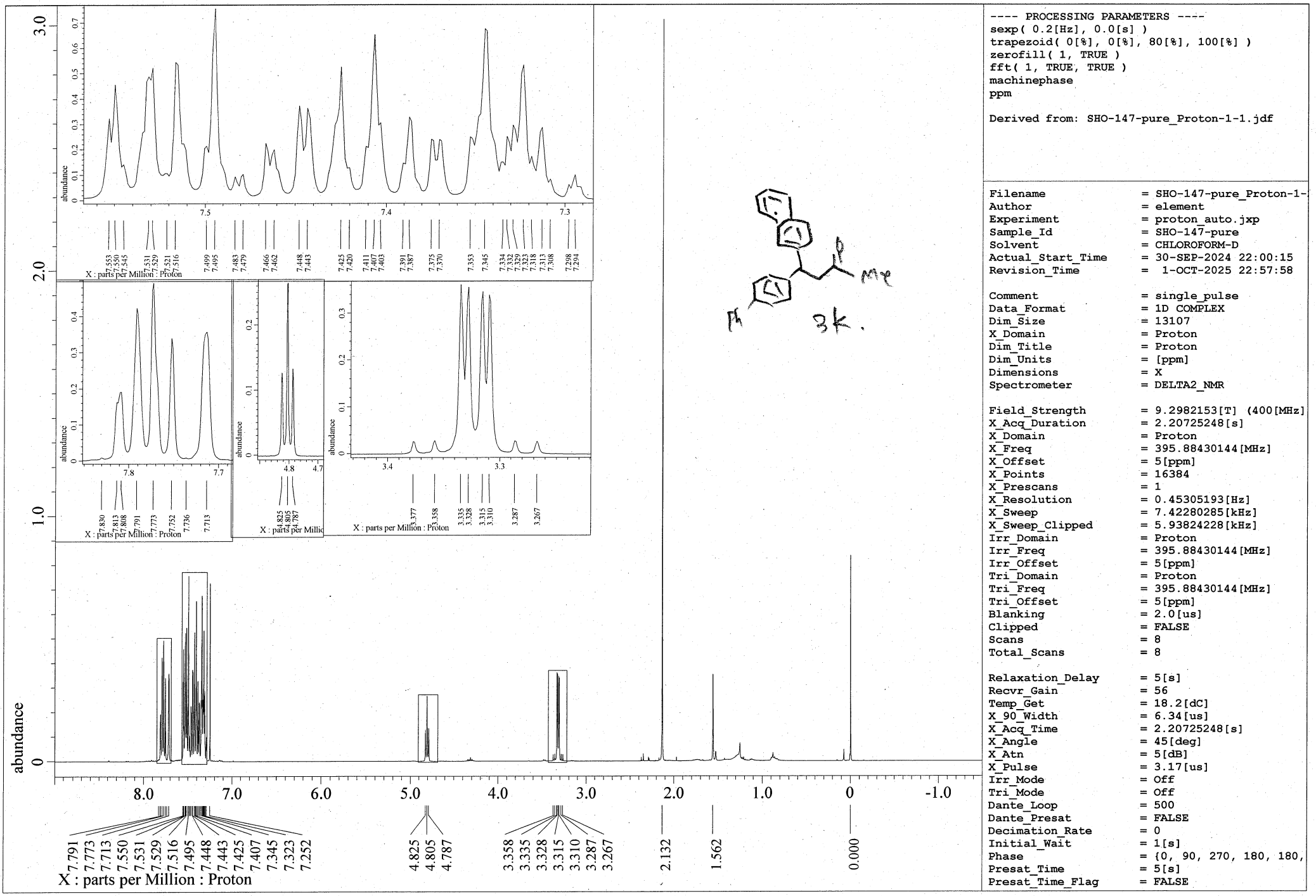
Filename	= SHO-080-13C-2.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= S#462744
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 2-OCT-2024 19:07:50
Revision_Time	= 5-OCT-2024 13:29:48
Comment	= single pulse decoupled ga
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= 13C
Dim_Title	= 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	= 146
Total_Scans	= 146
Relaxation_Delay	= 2[s]
Recvr_Gain	= 60
Temp_Get	= 19.8[dC]
X_90_Width	= 9.46[us]
X_Acq_Time	= 1.06430464[s]
X_Angle	= 30[deg]
X_Atn	= 4.9[dB]
X_Pulse	= 3.15333333[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 ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm

以下に由来:: SHO-144-pure2_Proton-1-1.jdf
```

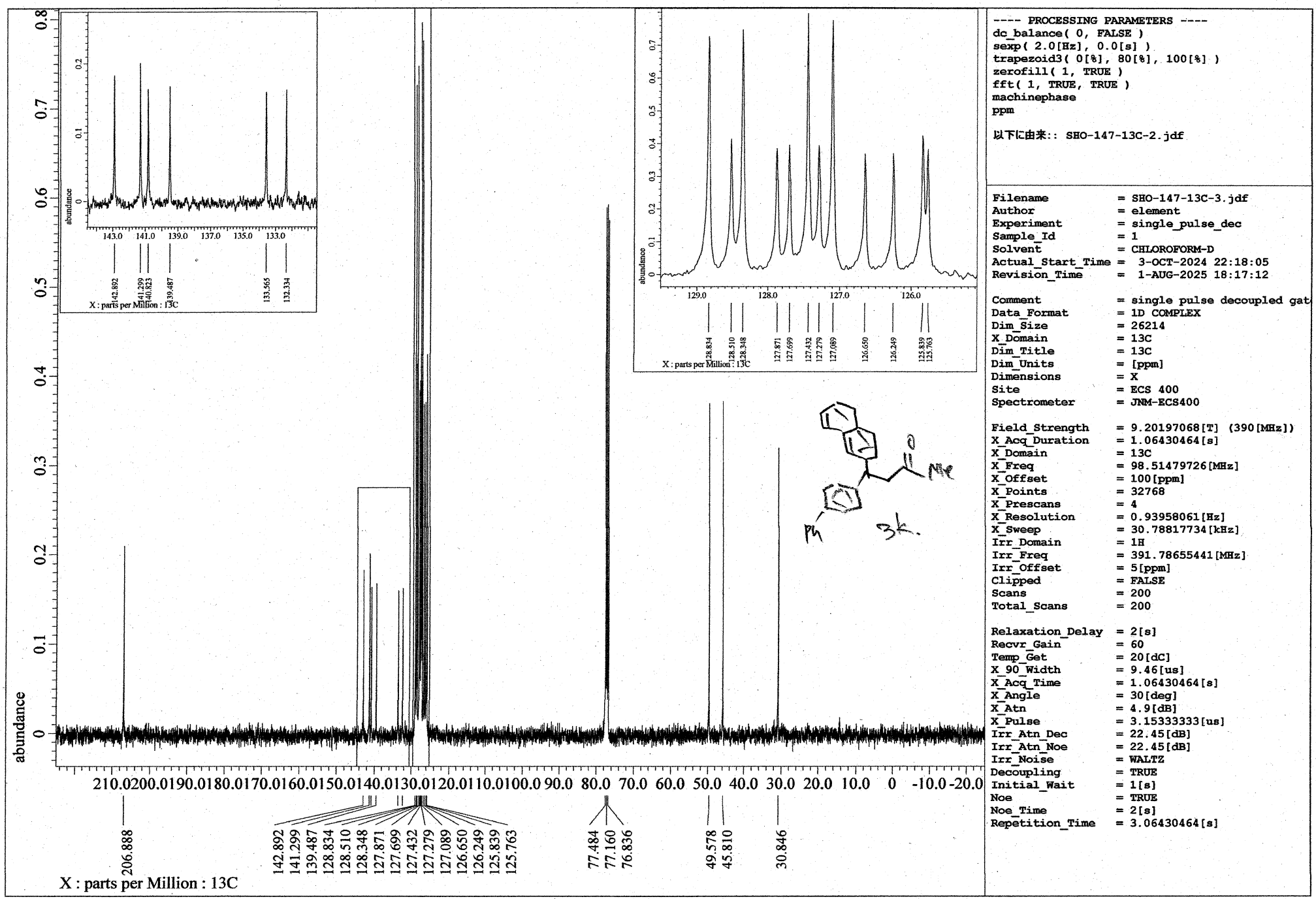
Filename	= SHO-144-pure2_Proton-1
Author	= element
Experiment	= proton_auto.jxp
Sample_Id	= SHO-144-pure2
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 30-SEP-2024 21:51:08
Revision_Time	= 1-AUG-2025 18:00:12
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.2982153[T] (400[MHz]
X_Acq_Duration	= 2.20725248[s]
X_Domain	= Proton
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]
X_Sweep_Clipped	= 5.93824228[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 395.88430144[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2.0[us]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 56
Temp_Get	= 18.2[dC]
X_90_Width	= 6.34[us]
X_Acq_Time	= 2.20725248[s]
X_Angle	= 45[deg]
X_Atn	= 5[dB]
X_Pulse	= 3.17[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 500
Dante_Presat	= FALSE
Decimation_Rate	= 0
Initial_Wait	= 1[s]
Phase	= {0, 90, 270, 180, 180,
Presat_Time	= 5[s]
Presat_Time_Flag	= FALSE


---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid3(0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
以下に由来:: SHO-144-13C-1.jdf
Filename = SHO-144-13C-2.jdf
Author = element
Experiment = single_pulse_dec
Sample_Id = 1
Solvent = CHLOROFORM-D
Actual_Start_Time = 2-OCT-2024 19:36:55
Revision_Time = 1-AUG-2025 18:01:53
Comment = single pulse decoupled gat
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 = 70
Total_Scans = 70
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 19.7[dC]
X_90_Width = 9.46[us]
X_Acq_Time = 1.06430464[s]
X_Angle = 30[deg]
X_Atn = 4.9[dB]
X_Pulse = 3.15333333[us]
Irr_Atn_Dec = 22.45[dB]
Irr_Atn_Noe = 22.45[dB]
Irr_Noise = WALTZ
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.06430464[s]
abundance
X : parts per Million : 13C
206.936
143.026
142.902
139.535
130.427
128.853
128.367
128.319
127.689
127.499
127.308
127.117
127.041
126.097
125.868
125.486
77.484
77.160
76.836
49.845
45.572
30.856



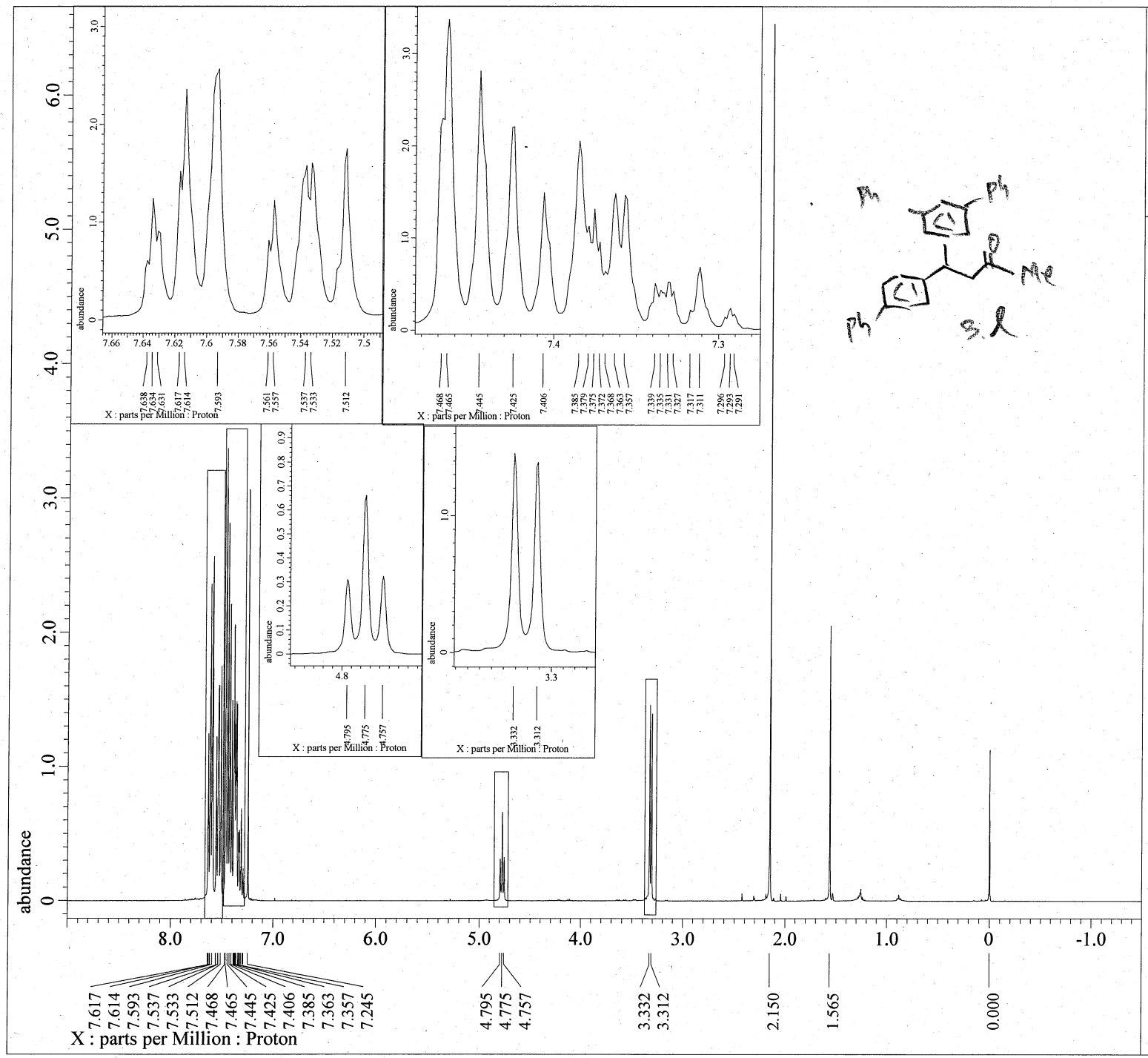

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: SHO-147-pure_Proton-1-1.jdf
```

Filename	= SHO-147-pure_Proton-1-
Author	= element
Experiment	= proton_auto.jxp
Sample_Id	= SHO-147-pure
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 30-SEP-2024 22:00:15
Revision_Time	= 1-OCT-2025 22:57:58
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	= 9.2982153[T] (400[MHz]
X_Acq_Duration	= 2.20725248[s]
X_Domain	= Proton
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]
X_Sweep_Clipped	= 5.93824228[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 395.88430144[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2.0[us]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 56
Temp_Get	= 18.2[dC]
X_90_Width	= 6.34[us]
X_Acq_Time	= 2.20725248[s]
X_Angle	= 45[deg]
X_Atn	= 5[dB]
X_Pulse	= 3.17[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 500
Dante_Presat	= FALSE
Decimation_Rate	= 0
Initial_Wait	= 1[s]
Phase	= {0, 90, 270, 180, 180,
Presat_Time	= 5[s]
Presat_Time_Flag	= FALSE



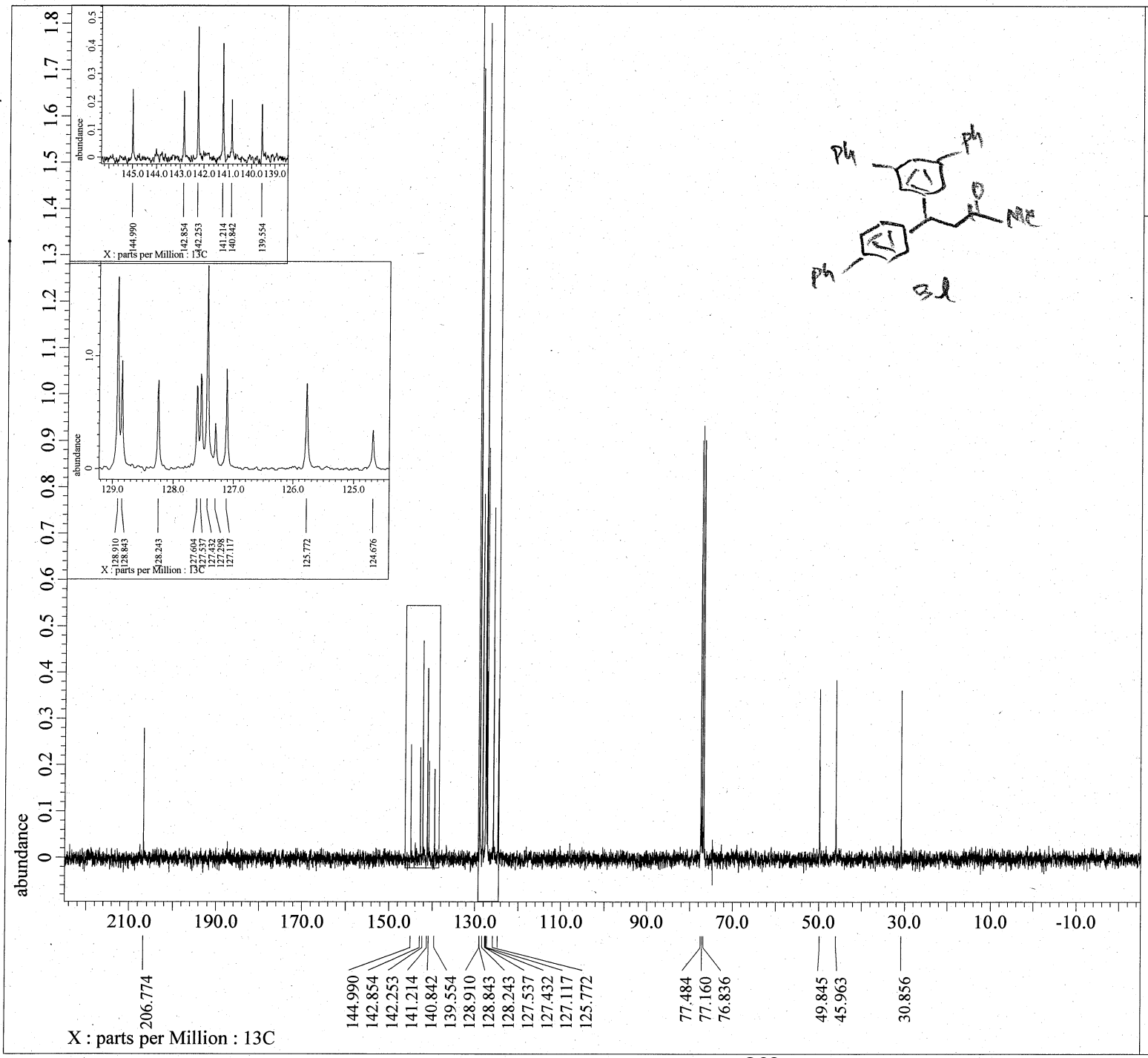

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm

以下に由来:: SHO-147-13C-2.jdf
```

Filename	= SHO-147-13C-3.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= 1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 3-OCT-2024 22:18:05
Revision_Time	= 1-AUG-2025 18:17:12
Comment	= single pulse decoupled gat
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= 13C
Dim_Title	= 13C
Dim_Units	= [ppm]
Dimensions	= X
Site	= ECS 400
Spectrometer	= JNM-ECS400
Field_Strength	= 9.20197068[T] (390[MHz])
X_Acq_Duration	= 1.06430464[s]
X_Domain	= 13C
X_Freq	= 98.51479726[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.93958061[Hz]
X_Sweep	= 30.78817734[kHz]
Irr_Domain	= 1H
Irr_Freq	= 391.78655441[MHz]
Irr_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 200
Total_Scans	= 200
Relaxation_Delay	= 2[s]
Recvr_Gain	= 60
Temp_Get	= 20[dC]
X_90_Width	= 9.46[us]
X_Acq_Time	= 1.06430464[s]
X_Angle	= 30[deg]
X_Atn	= 4.9[dB]
X_Pulse	= 3.15333333[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]



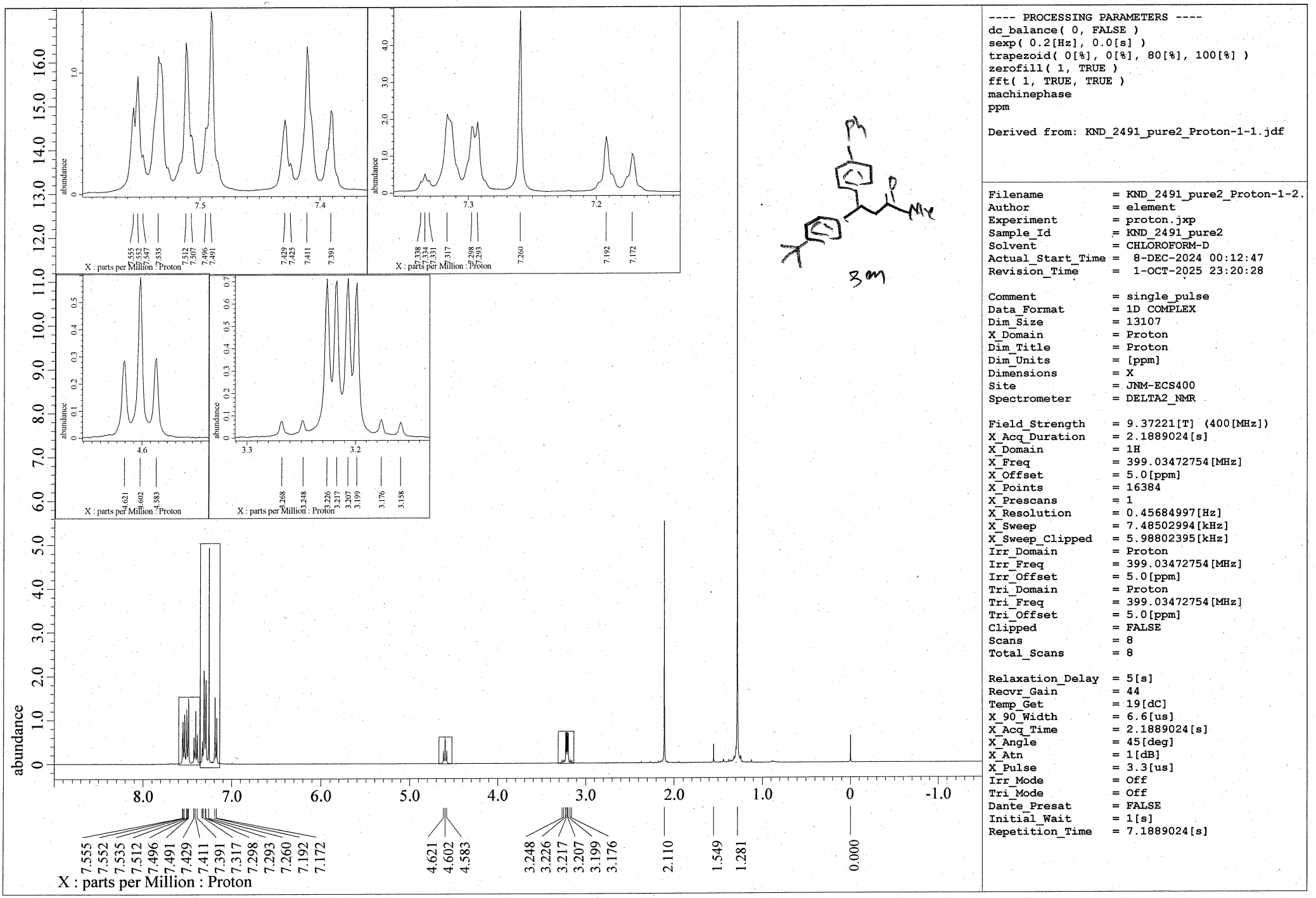

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KND_2049_Proton-1-1.jdf
```

Filename	= KND_2049_Proton-1-2.jdf
Author	= element
Experiment	= proton.jxp
Sample_Id	= KND_2049
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 5-SEP-2024 23:40:34
Revision_Time	= 21-OCT-2024 22:33:18
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	= 36
Temp_Get	= 22[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]



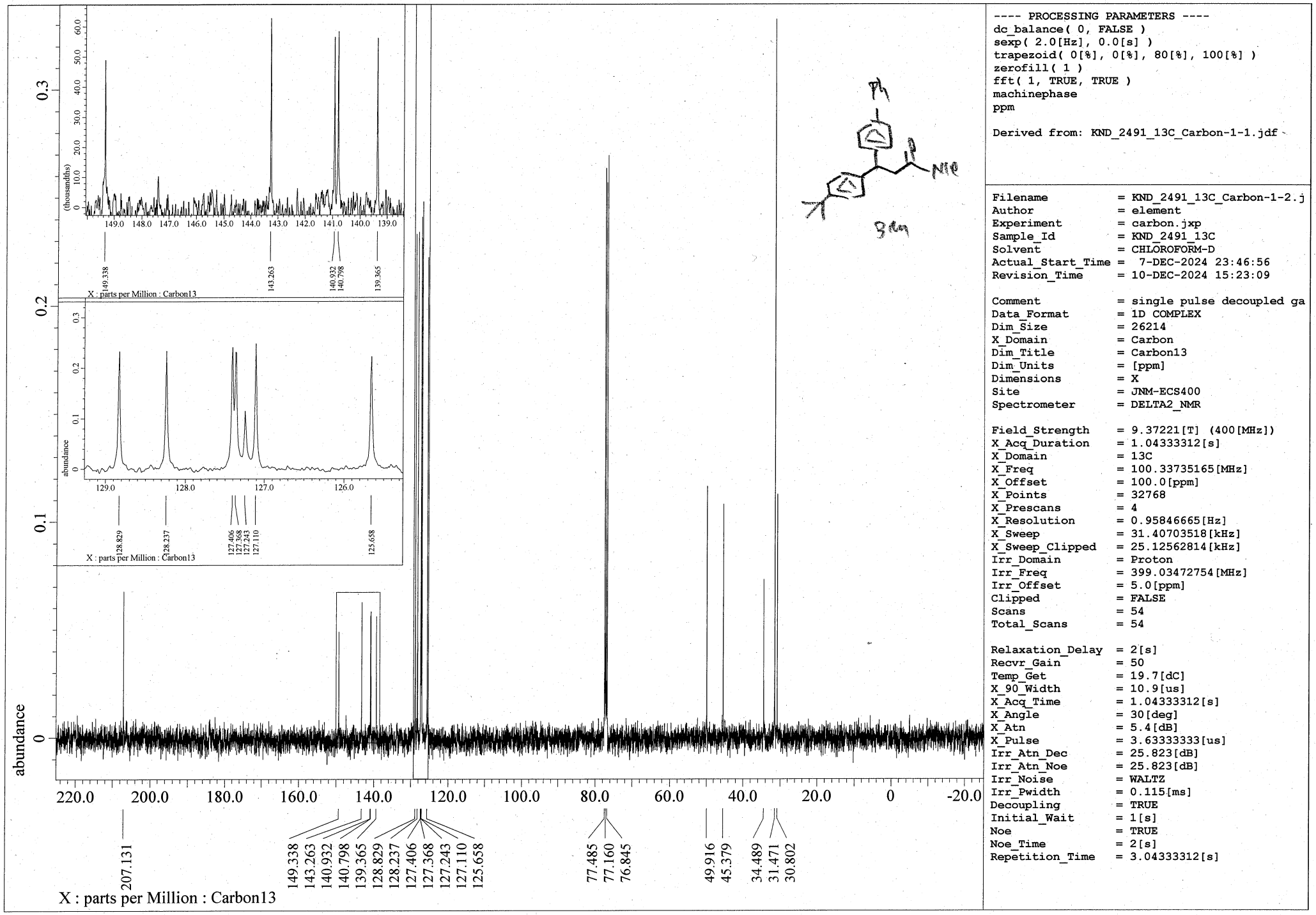

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KND_2049_13C-2.jdf
```

Filename	= KND_2049_13C-3.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= S#531842
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 6-SEP-2024 21:06:09
Revision_Time	= 21-OCT-2024 22:42:58
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	= 54
Total_Scans	= 54
Relaxation_Delay	= 2[s]
Recvr_Gain	= 60
Temp_Get	= 22.2[dC]
X_90_Width	= 9.46[us]
X_Acq_Time	= 1.06430464[s]
X_Angle	= 30[deg]
X_Atn	= 4.9[dB]
X_Pulse	= 3.15333333[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]



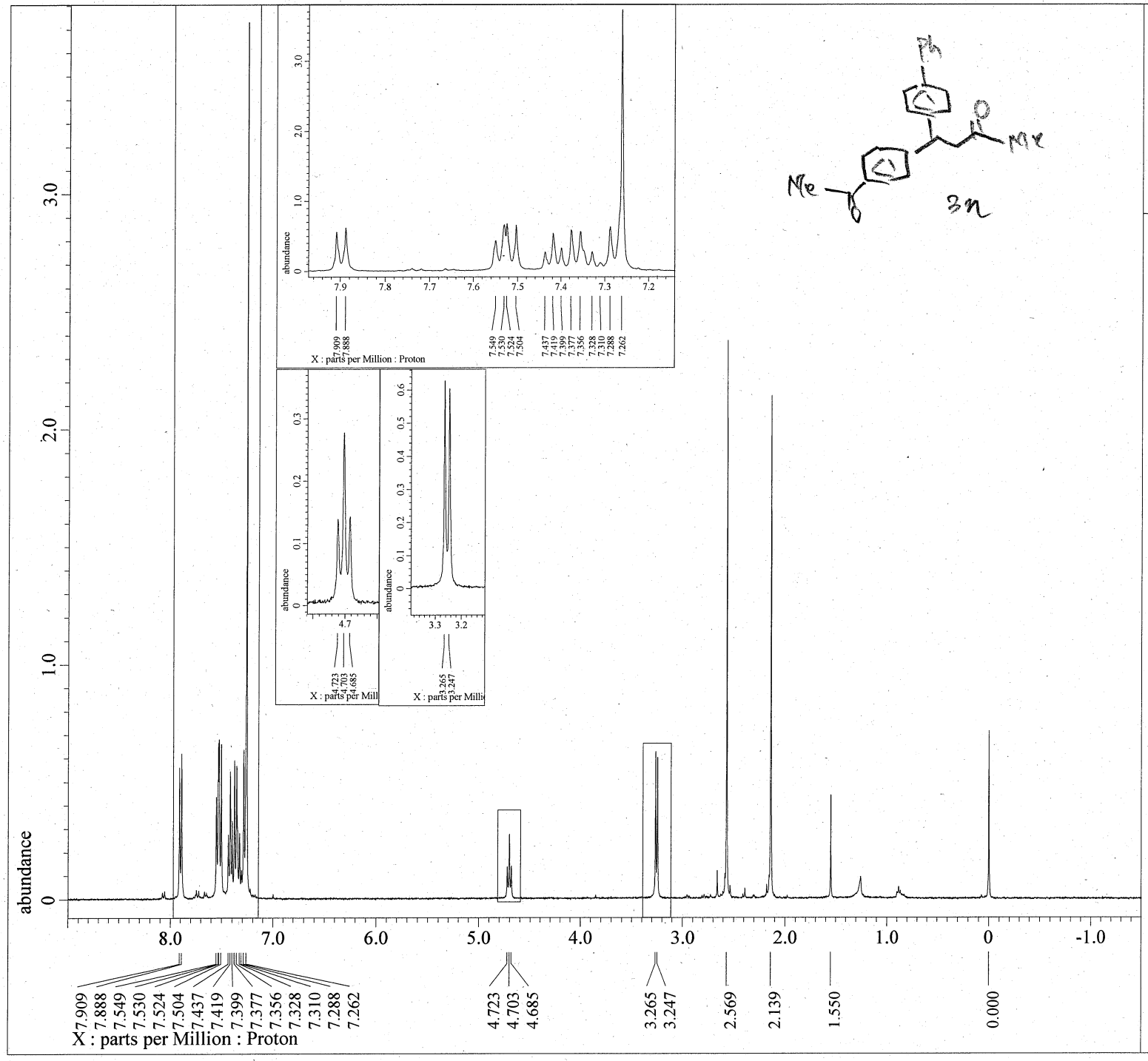

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KND_2491_pure2_Proton-1-1.jdf
```

Filename	= KND_2491_pure2_Proton-1-2.
Author	= element
Experiment	= proton.jxp
Sample_Id	= KND_2491_pure2
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 8-DEC-2024 00:12:47
Revision_Time	= 1-OCT-2025 23:20:28
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	= 44
Temp_Get	= 19[dC]
X_90_Width	= 6.6[us]
X_Acq_Time	= 2.1889024[s]
X_Angle	= 45[deg]
X_Atn	= 1[dB]
X_Pulse	= 3.3[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.1889024[s]



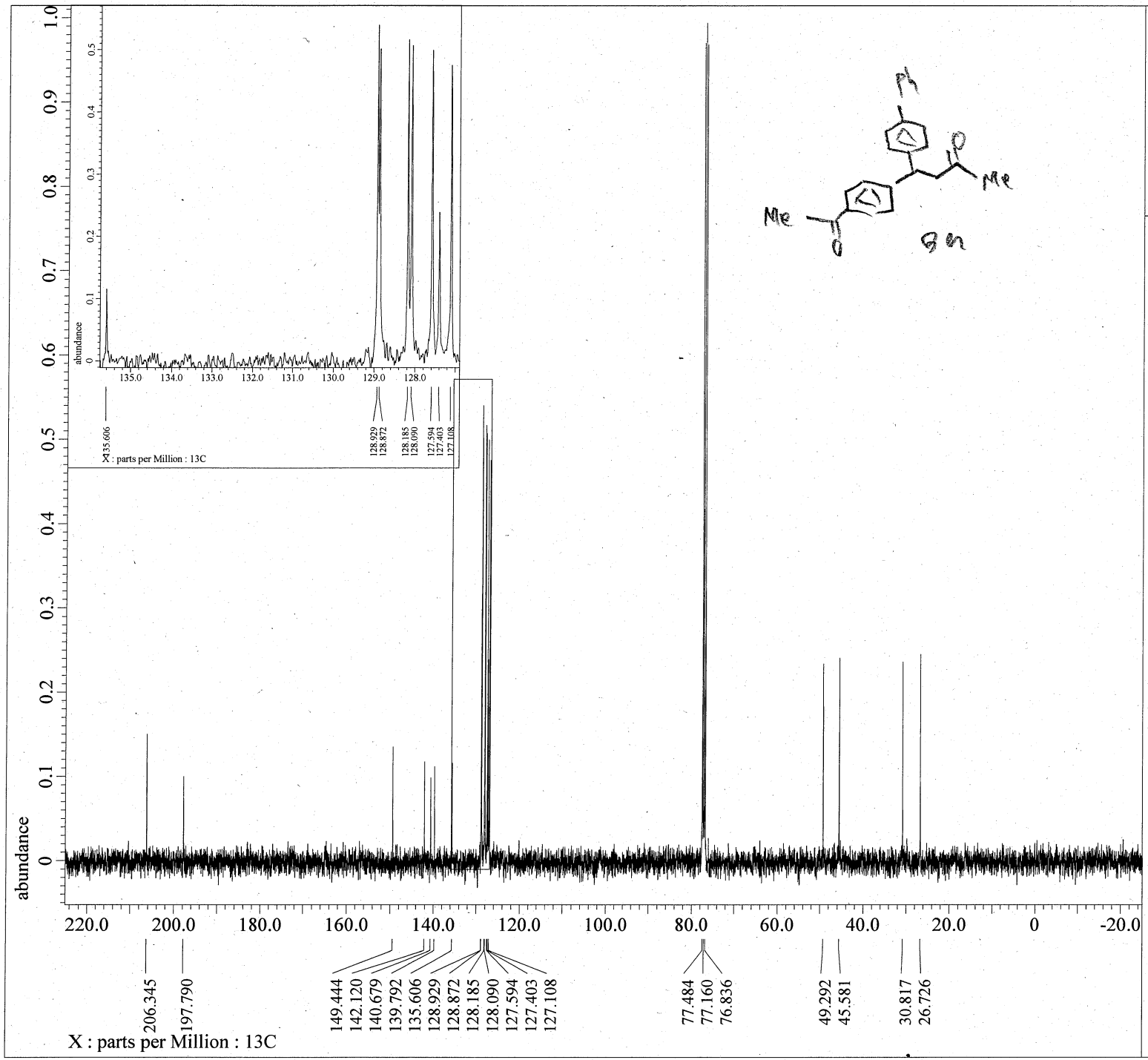

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KND_2491_13C_Carbon-1-1.jdf
```

Filename	= KND_2491_13C_Carbon-1-2.j
Author	= element
Experiment	= carbon.jxp
Sample_Id	= KND_2491_13C
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 7-DEC-2024 23:46:56
Revision_Time	= 10-DEC-2024 15:23:09
Comment	= single pulse decoupled ga
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECS400
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.37221[T] (400[MHz])
X_Acq_Duration	= 1.04333312[s]
X_Domain	= 13C
X_Freq	= 100.33735165[MHz]
X_Offset	= 100.0[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.95846665[Hz]
X_Sweep	= 31.40703518[kHz]
X_Sweep_Clipped	= 25.12562814[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.03472754[MHz]
Irr_Offset	= 5.0[ppm]
Clipped	= FALSE
Scans	= 54
Total_Scans	= 54
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 19.7[dC]
X_90_Width	= 10.9[us]
X_Acq_Time	= 1.04333312[s]
X_Angle	= 30[deg]
X_Atn	= 5.4[dB]
X_Pulse	= 3.63333333[us]
Irr_Atn_Dec	= 25.823[dB]
Irr_Atn_Noe	= 25.823[dB]
Irr_Noise	= WALTZ
Irr_Pwidth	= 0.115[ms]
Decoupling	= TRUE
Initial_Wait	= 1[s]
Noe	= TRUE
Noe_Time	= 2[s]
Repetition_Time	= 3.04333312[s]



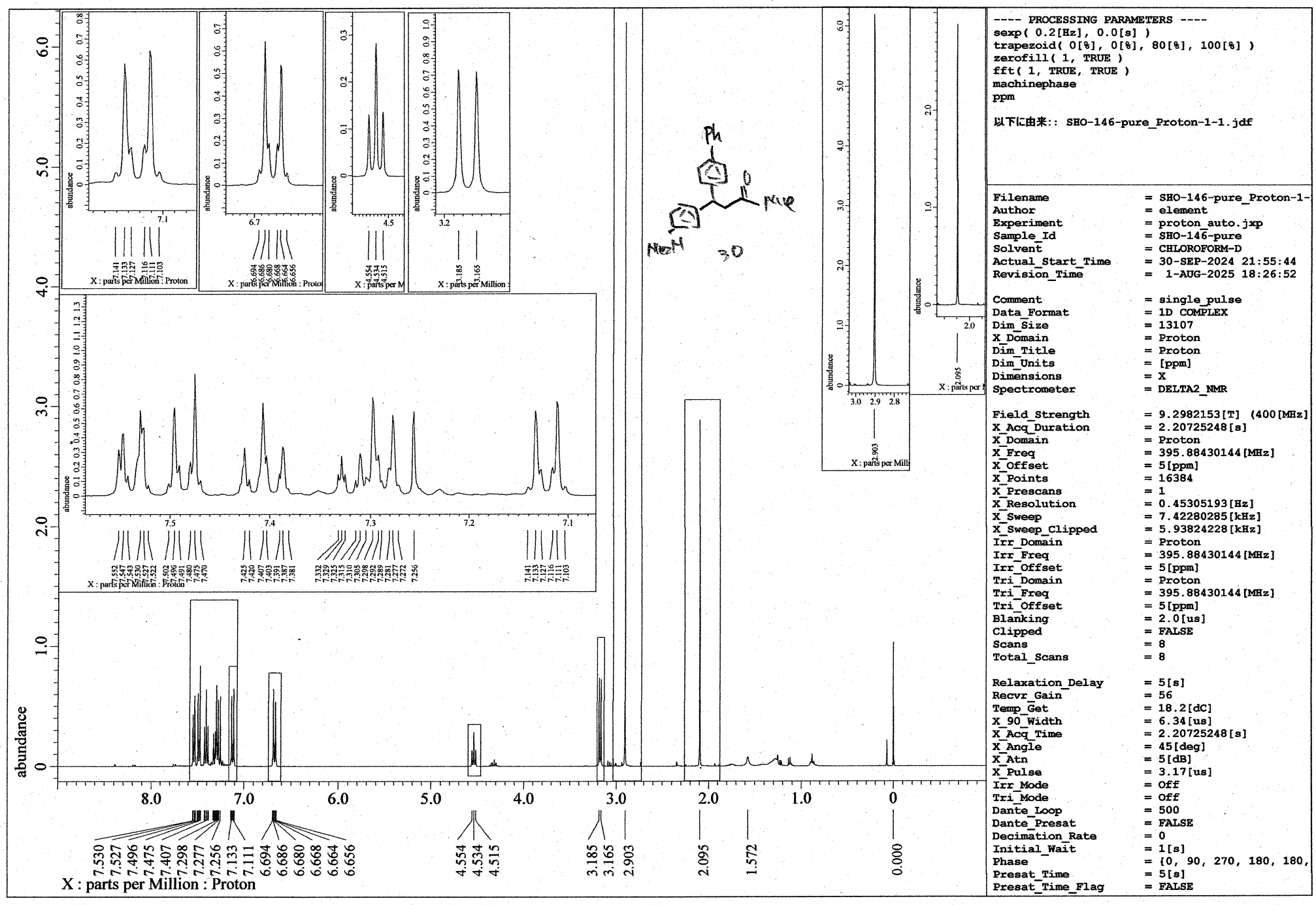

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KND_2078_pure_Proton-1-1.jdf
```

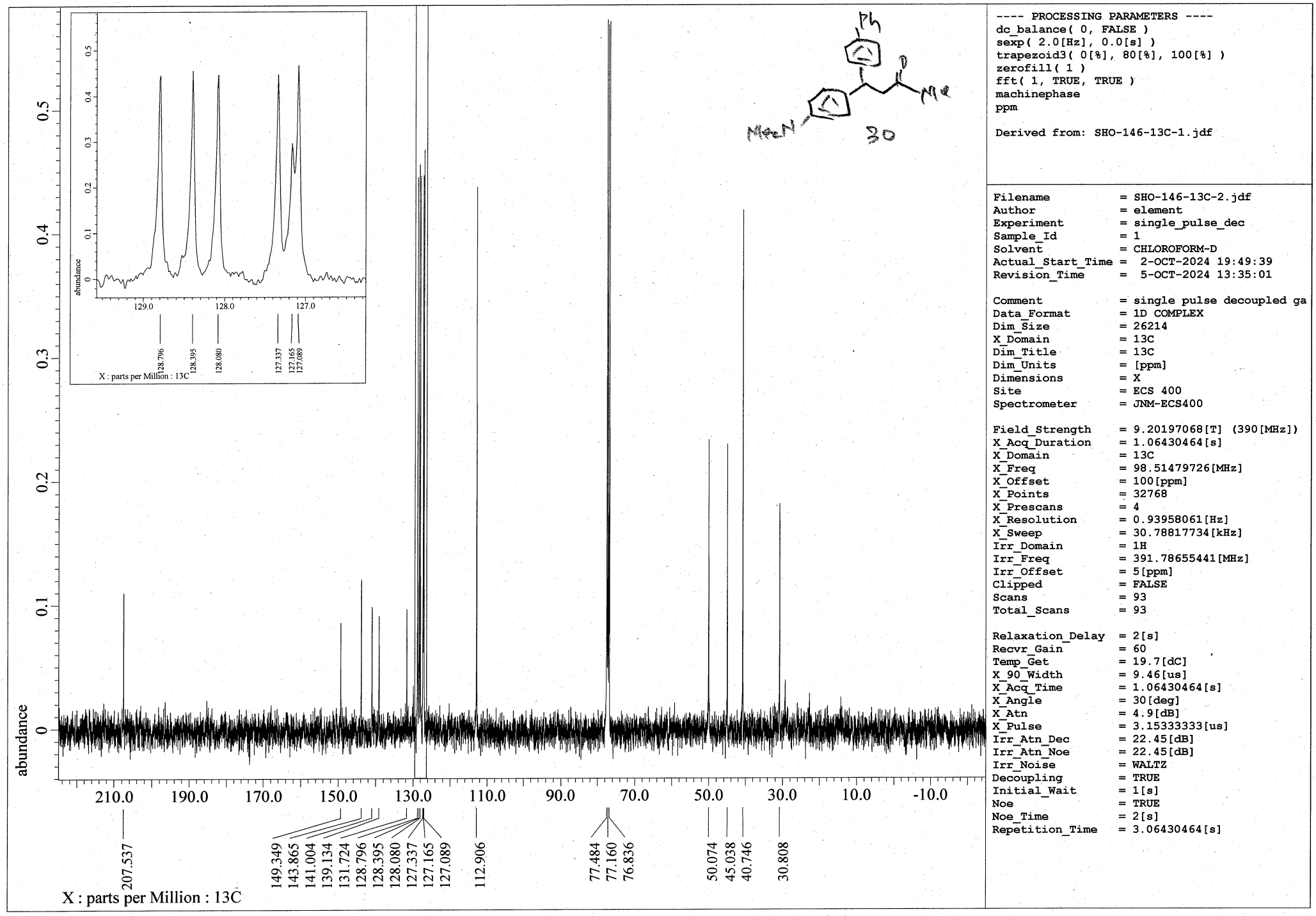
Filename	= KND_2078_pure_Proton-1-2.
Author	= element
Experiment	= proton.jxp
Sample_Id	= KND_2078_pure
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 9-DEC-2024 11:07:28
Revision_Time	= 10-DEC-2024 15:58:37
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
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	= 50
Temp_Get	= 19.3[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]

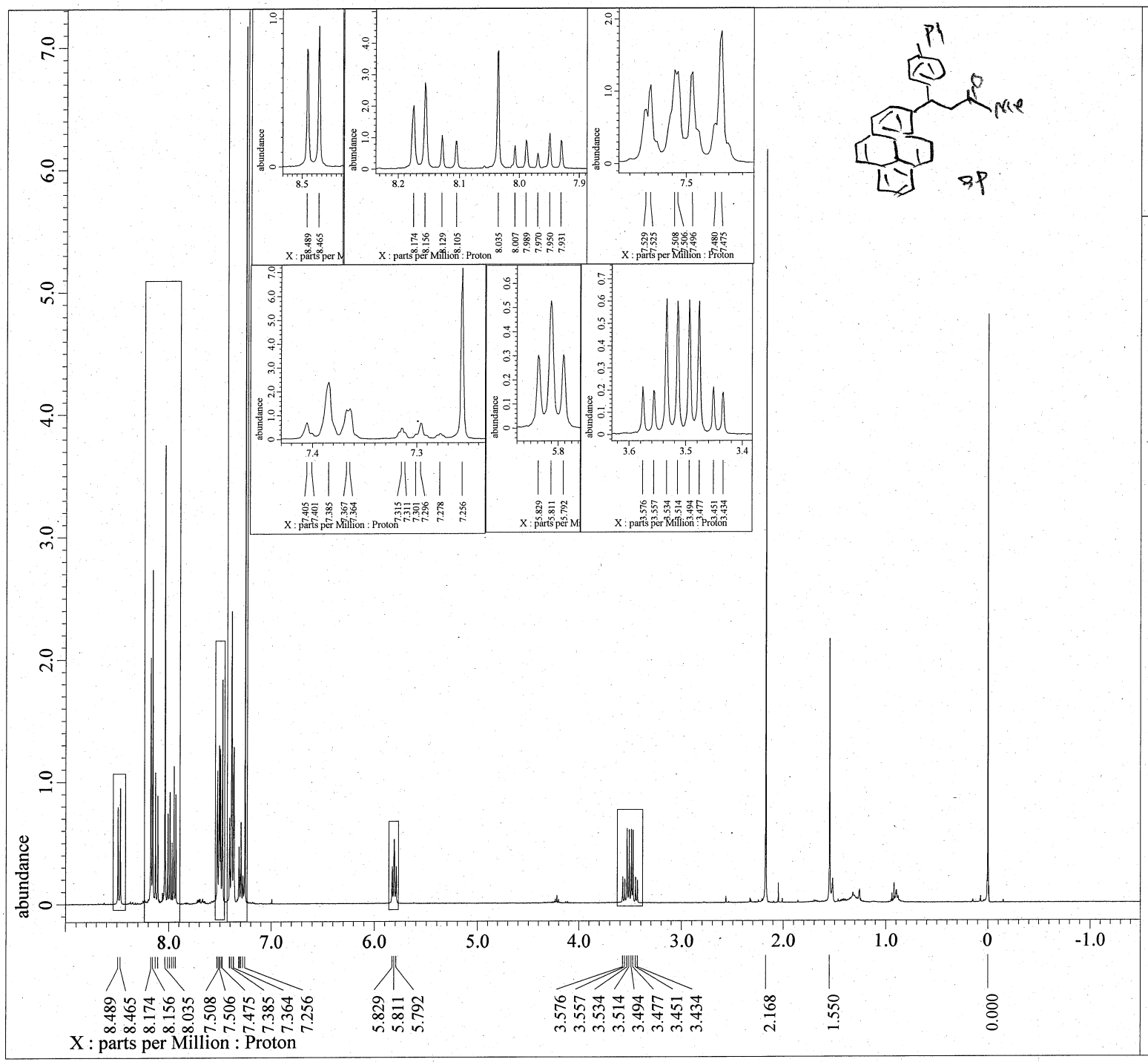



```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KND_2078_13C-1.jdf
```

Filename	= KND_2078_13C-2.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= 1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 9-DEC-2024 16:11:56
Revision_Time	= 10-DEC-2024 16:00:26
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	= 68
Total_Scans	= 68
Relaxation_Delay	= 2[s]
Recvr_Gain	= 60
Temp_Get	= 18.4[dC]
X_90_Width	= 9.46[us]
X_Acq_Time	= 1.06430464[s]
X_Angle	= 30[deg]
X_Atn	= 4.9[dB]
X_Pulse	= 3.15333333[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]

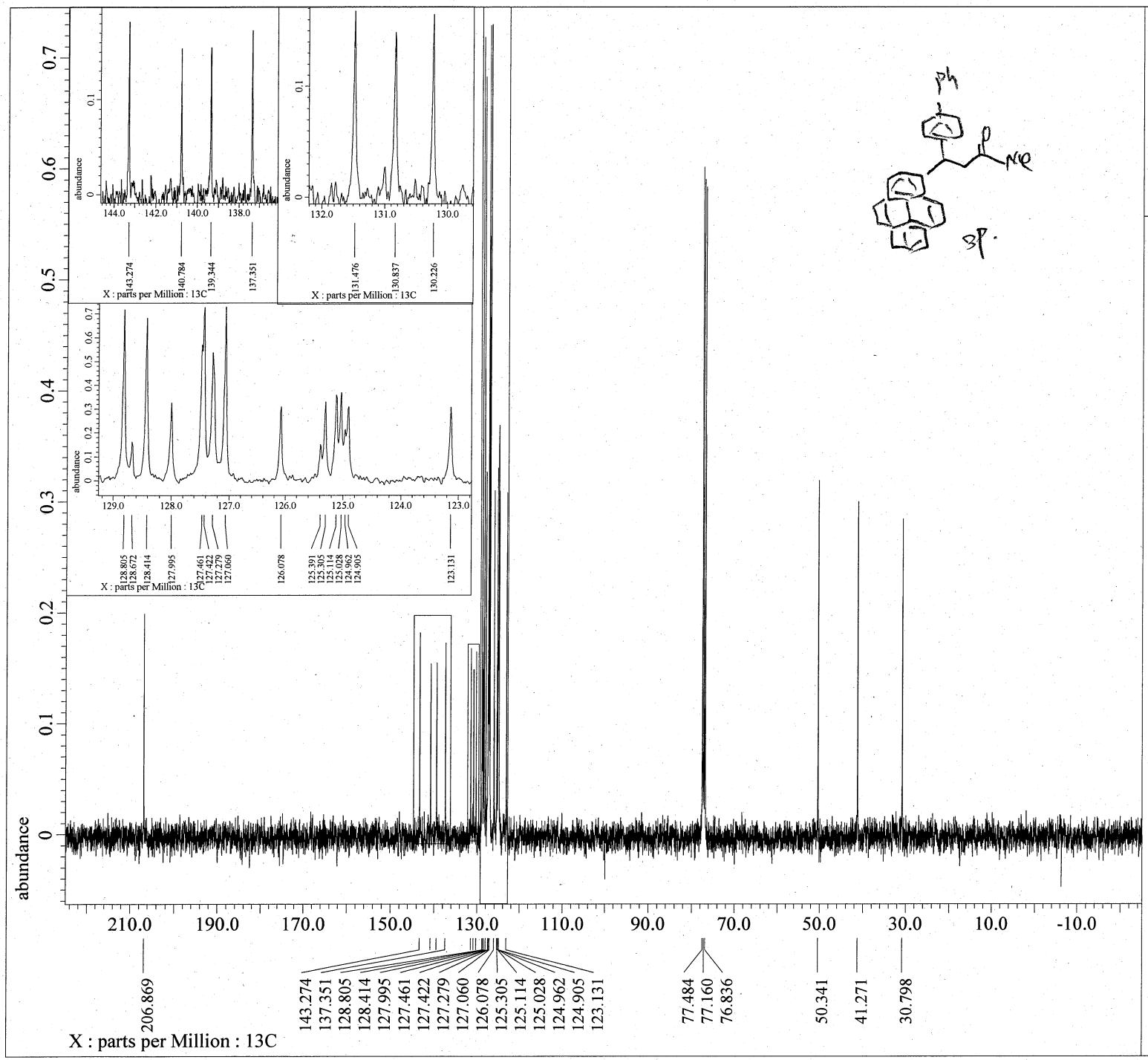

X : parts per Million : Proton
abundance
7.530
7.527
7.496
7.475
7.407
7.298
7.277
7.256
7.133
7.111
6.694
6.686
6.680
6.668
6.664
6.656
4.554
4.534
4.515
3.185
3.165
2.903
2.095
1.572
0.000
---- PROCESSING PARAMETERS ----
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
以下に由来:: SHO-146-pure_Proton-1-1.jdf
Filename = SHO-146-pure_Proton-1-
Author = element
Experiment = proton_auto.jxp
Sample_Id = SHO-146-pure
Solvent = CHLOROFORM-D
Actual_Start_Time = 30-SEP-2024 21:55:44
Revision_Time = 1-AUG-2025 18:26:52
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = DELTA2_NMR
Field_Strength = 9.2982153[T] (400[MHz]
X_Acq_Duration = 2.20725248[s]
X_Domain = Proton
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]
X_Sweep_Clipped = 5.93824228[kHz]
Irr_Domain = Proton
Irr_Freq = 395.88430144[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 395.88430144[MHz]
Tri_Offset = 5[ppm]
Blanking = 2.0[us]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 56
Temp_Get = 18.2[dC]
X_90_Width = 6.34[us]
X_Acq_Time = 2.20725248[s]
X_Angle = 45[deg]
X_Atn = 5[dB]
X_Pulse = 3.17[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = {0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE


---- 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: SHO-146-13C-1.jdf
Filename = SHO-146-13C-2.jdf
Author = element
Experiment = single_pulse_dec
Sample_Id = 1
Solvent = CHLOROFORM-D
Actual_Start_Time = 2-OCT-2024 19:49:39
Revision_Time = 5-OCT-2024 13:35:01
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 = 93
Total_Scans = 93
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 19.7[dC]
X_90_Width = 9.46[us]
X_Acq_Time = 1.06430464[s]
X_Angle = 30[deg]
X_Atn = 4.9[dB]
X_Pulse = 3.15333333[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]
30
abundance
X : parts per Million : 13C
207.537
149.349
143.865
141.004
139.134
131.724
128.796
128.395
128.080
127.337
127.165
127.089
112.906
77.484
77.160
76.836
50.074
45.038
40.746
30.808



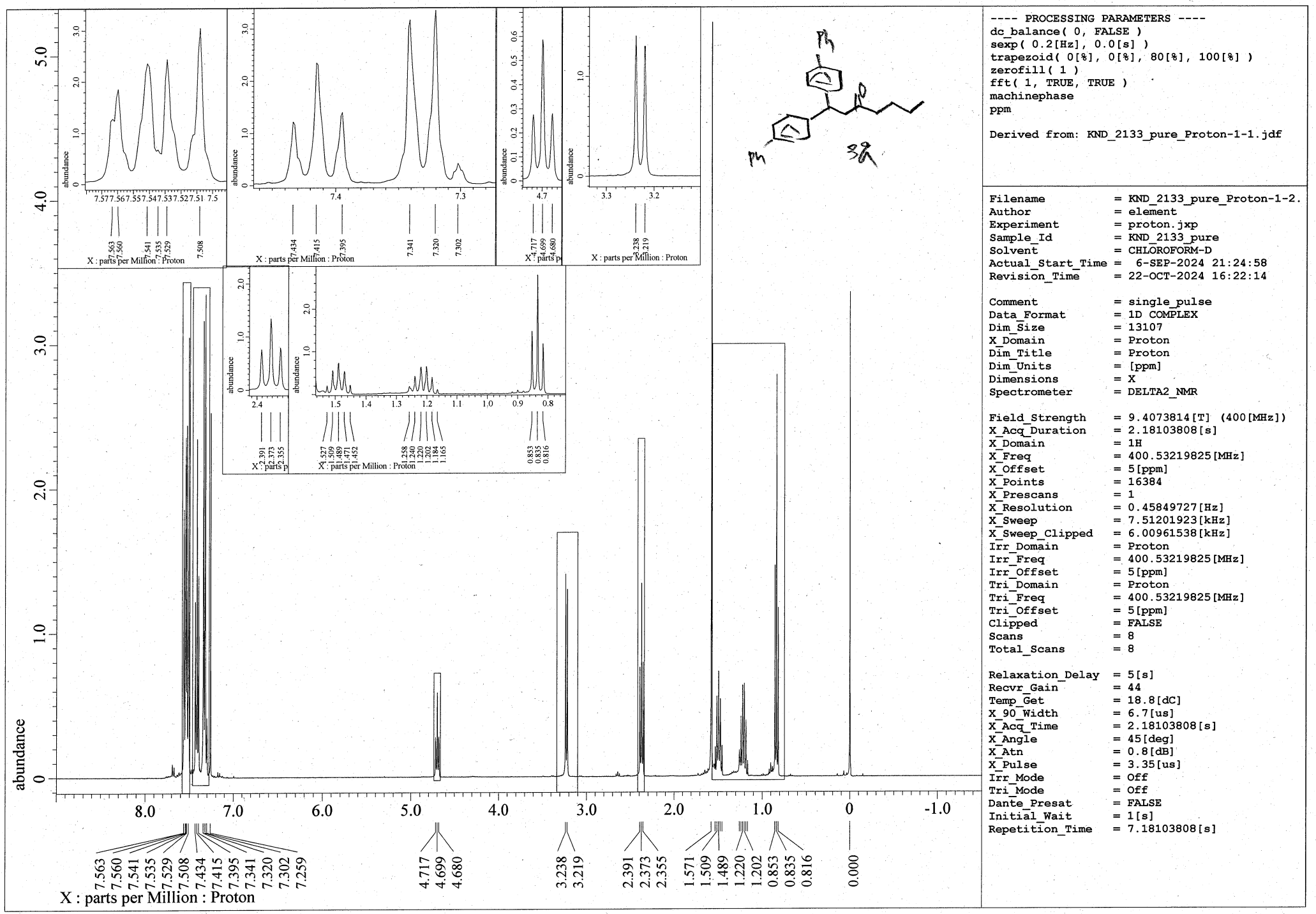

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KND_2066_Proton-1-1.jdf
```

Filename	= KND_2066_Proton-1-2.jdf
Author	= element
Experiment	= proton.jxp
Sample_Id	= KND_1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 25-AUG-2024 01:58:55
Revision_Time	= 21-OCT-2024 23:19:30
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	= 20.9[dC]
X_90_Width	= 6.7[us]
X_Acq_Time	= 2.18103808[s]
X_Angle	= 45[deg]
X_Atn	= 0.8[dB]
X_Pulse	= 3.35[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.18103808[s]



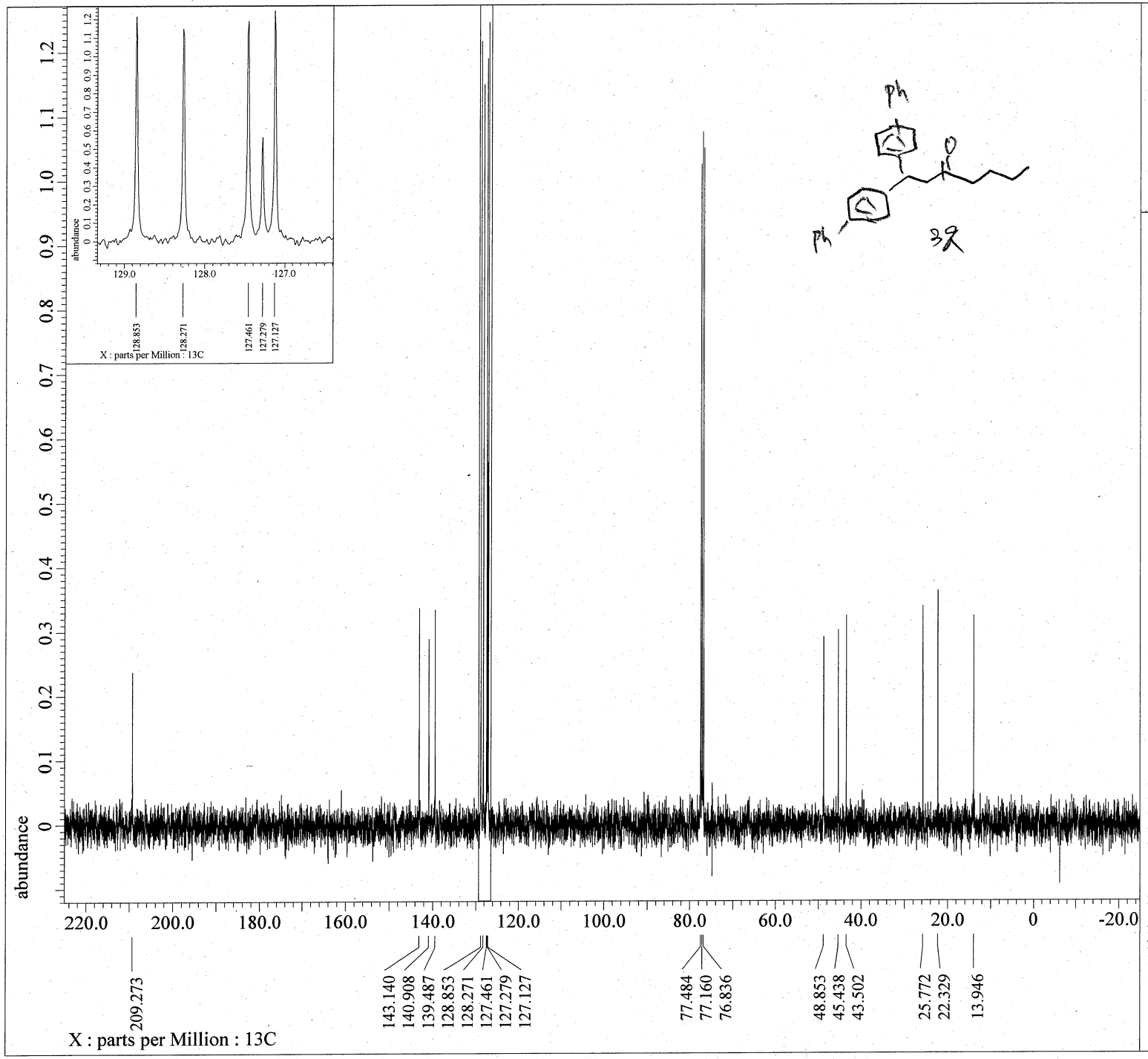

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KND_2066_13C-1.jdf
```

Filename	= KND_2066_13C-2.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= 1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 25-AUG-2024 21:07:27
Revision_Time	= 22-OCT-2024 15:56:40
Comment	= single pulse decoupled ga
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= 13C
Dim_Title	= 13C
Dim_Units	= [ppm]
Dimensions	= X
Site	= 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	= 83
Total_Scans	= 83
Relaxation_Delay	= 2[s]
Recvr_Gain	= 60
Temp_Get	= 22.3[dC]
X_90_Width	= 9.46[us]
X_Acq_Time	= 1.06430464[s]
X_Angle	= 30[deg]
X_Atn	= 4.9[dB]
X_Pulse	= 3.15333333[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]



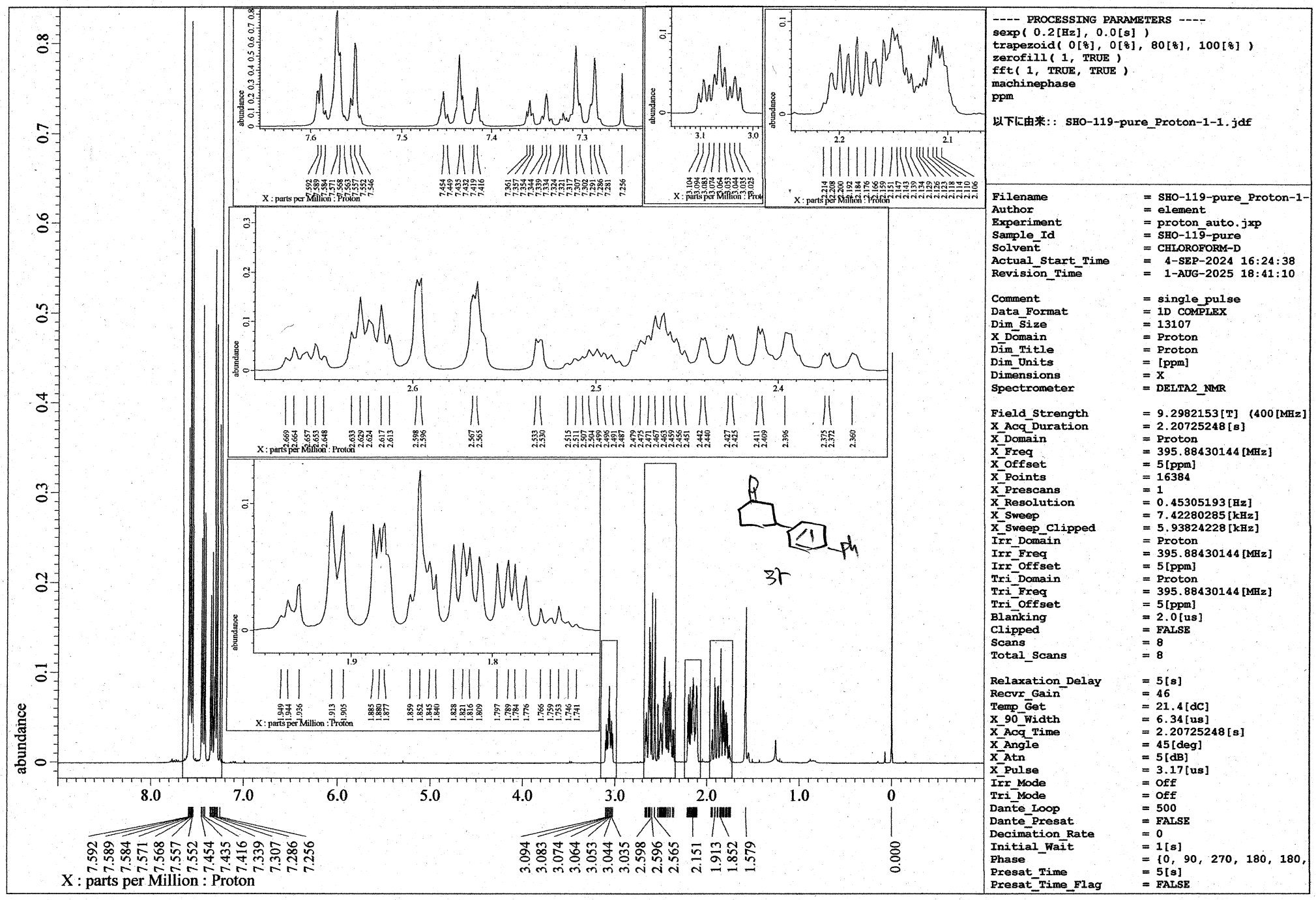

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KND_2133_pure_Proton-1-1.jdf
```

Filename	= KND_2133_pure_Proton-1-2.
Author	= element
Experiment	= proton.jxp
Sample_Id	= KND_2133_pure
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 6-SEP-2024 21:24:58
Revision_Time	= 22-OCT-2024 16:22:14
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.4073814[T] (400[MHz])
X_Acq_Duration	= 2.18103808[s]
X_Domain	= 1H
X_Freq	= 400.53219825[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45849727[Hz]
X_Sweep	= 7.51201923[kHz]
X_Sweep_Clipped	= 6.00961538[kHz]
Irr_Domain	= Proton
Irr_Freq	= 400.53219825[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 400.53219825[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 44
Temp_Get	= 18.8[dC]
X_90_Width	= 6.7[us]
X_Acq_Time	= 2.18103808[s]
X_Angle	= 45[deg]
X_Atn	= 0.8[dB]
X_Pulse	= 3.35[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.18103808[s]



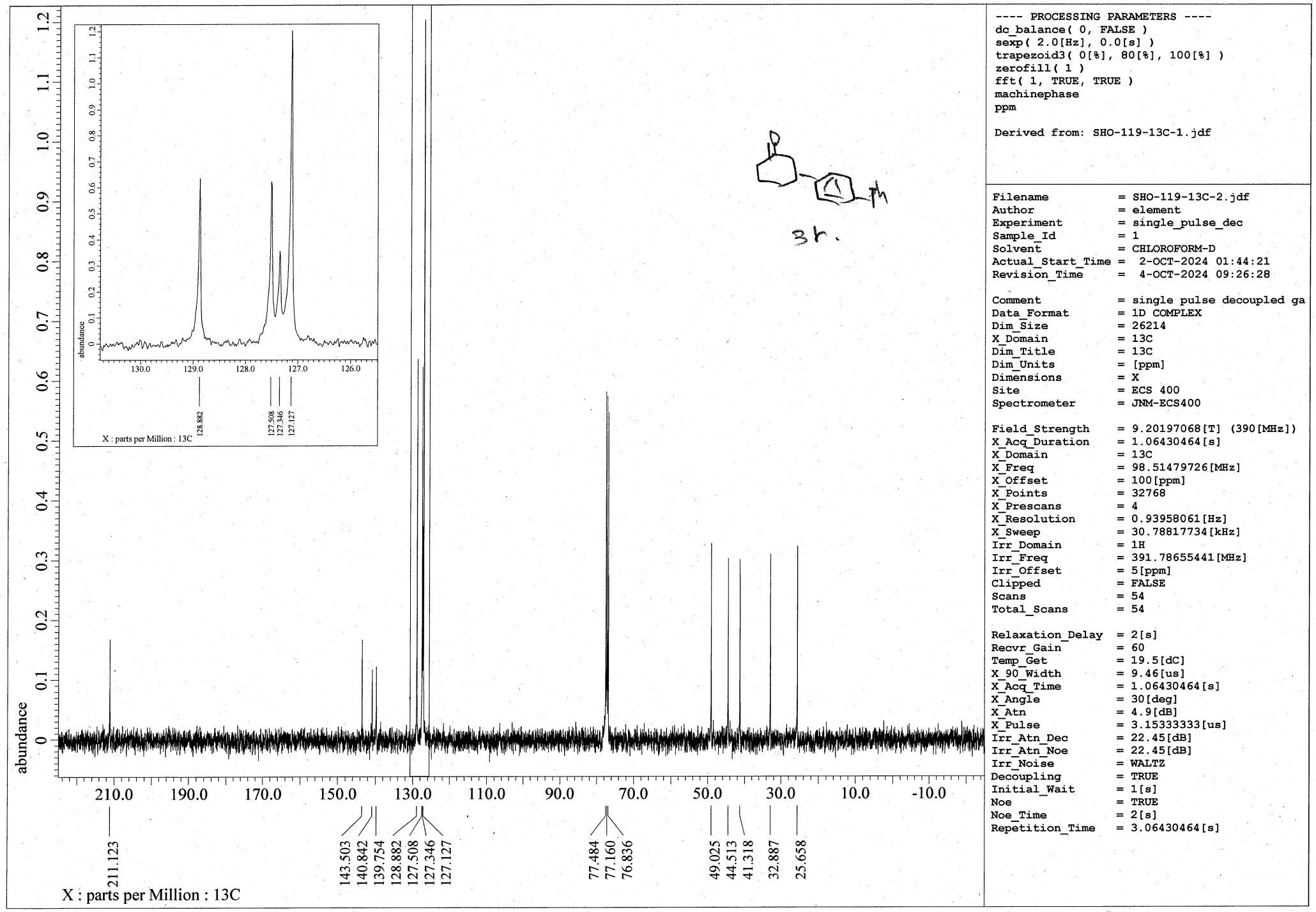

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KND_2133_13C-3.jdf
```

Filename	= KND_2133_13C-4.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= 1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 7-SEP-2024 03:27:28
Revision_Time	= 22-OCT-2024 16:24:17
Comment	= single pulse decoupled ga
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= 13C
Dim_Title	= 13C
Dim_Units	= [ppm]
Dimensions	= X
Site	= ECS 400
Spectrometer	= JNM-ECS400
Field_Strength	= 9.20197068[T] (390[MHz])
X_Acq_Duration	= 1.06430464[s]
X_Domain	= 13C
X_Freq	= 98.51479726[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.93958061[Hz]
X_Sweep	= 30.78817734[kHz]
Irr_Domain	= 1H
Irr_Freq	= 391.78655441[MHz]
Irr_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 18
Total_Scans	= 18
Relaxation_Delay	= 2[s]
Recvr_Gain	= 60
Temp_Get	= 21.6[dC]
X_90_Width	= 9.46[us]
X_Acq_Time	= 1.06430464[s]
X_Angle	= 30[deg]
X_Atn	= 4.9[dB]
X_Pulse	= 3.15333333[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]



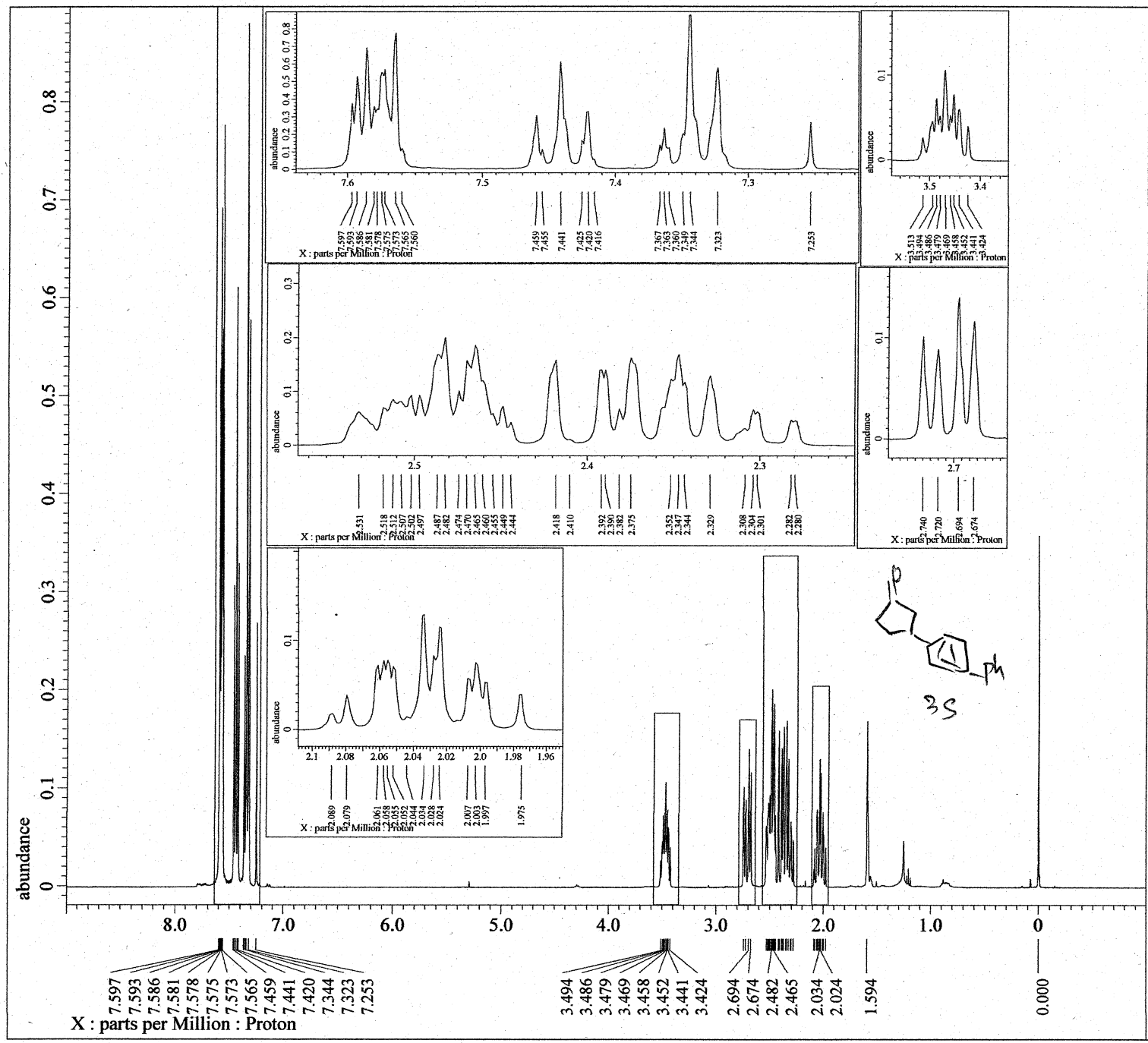

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm

以下に由来:: SHO-119-pure_Proton-1-1.jdf
```

Filename	= SHO-119-pure_Proton-1-
Author	= element
Experiment	= proton_auto.jxp
Sample_Id	= SHO-119-pure
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 4-SEP-2024 16:24:38
Revision_Time	= 1-AUG-2025 18:41:10
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	= 9.2982153[T] (400[MHz]
X_Acq_Duration	= 2.20725248[s]
X_Domain	= Proton
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]
X_Sweep_Clipped	= 5.93824228[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 395.88430144[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2.0[us]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 46
Temp_Get	= 21.4[dC]
X_90_Width	= 6.34[us]
X_Acq_Time	= 2.20725248[s]
X_Angle	= 45[deg]
X_Atn	= 5[dB]
X_Pulse	= 3.17[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 500
Dante_Presat	= FALSE
Decimation_Rate	= 0
Initial_Wait	= 1[s]
Phase	= {0, 90, 270, 180, 180,
Presat_Time	= 5[s]
Presat_Time_Flag	= FALSE



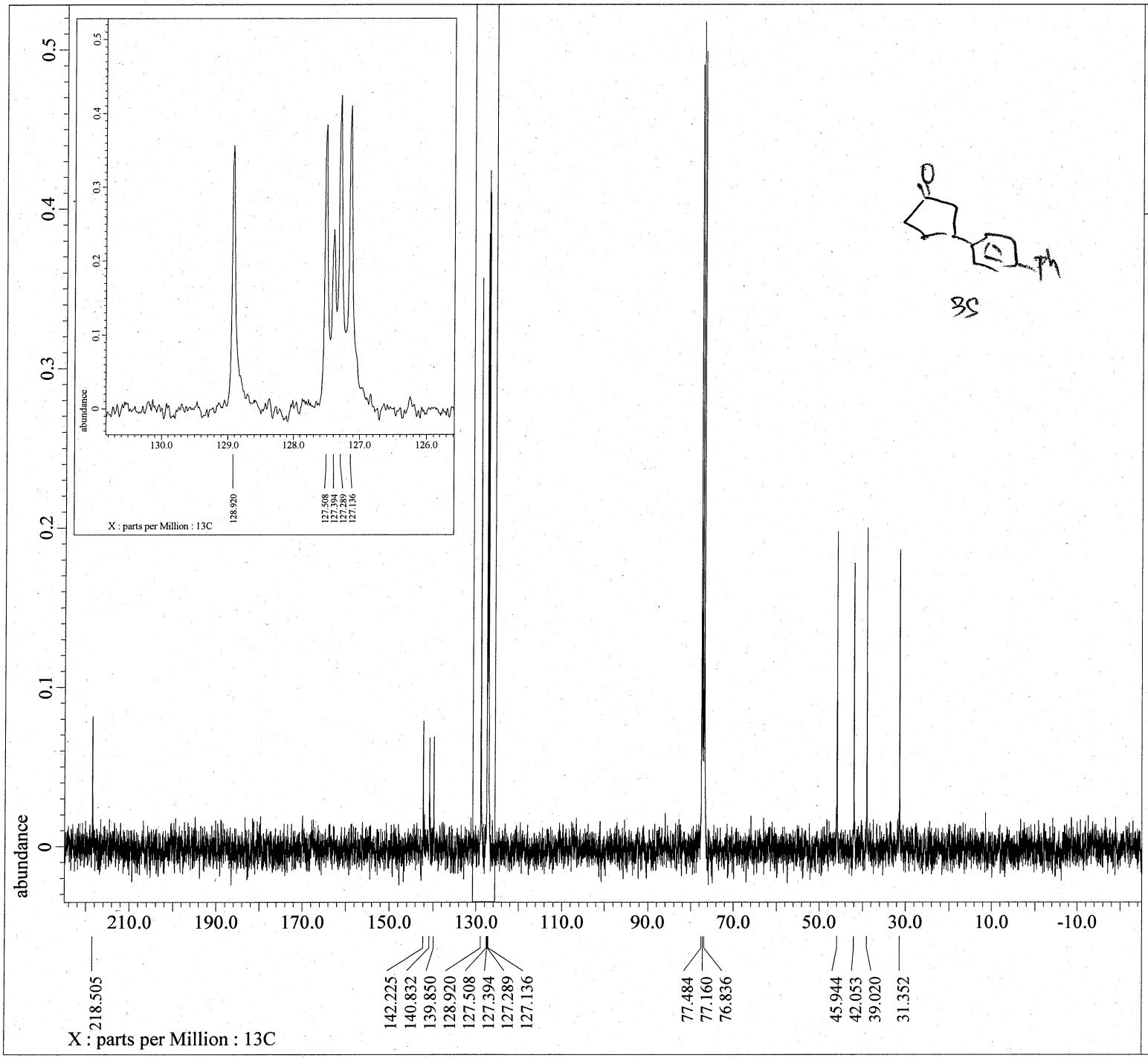

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: SHO-119-13C-1.jdf
```

Filename	= SHO-119-13C-2.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= 1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 2-OCT-2024 01:44:21
Revision_Time	= 4-OCT-2024 09:26:28
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	= 54
Total_Scans	= 54
Relaxation_Delay	= 2[s]
Recvr_Gain	= 60
Temp_Get	= 19.5[dC]
X_90_Width	= 9.46[us]
X_Acq_Time	= 1.06430464[s]
X_Angle	= 30[deg]
X_Atn	= 4.9[dB]
X_Pulse	= 3.15333333[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]



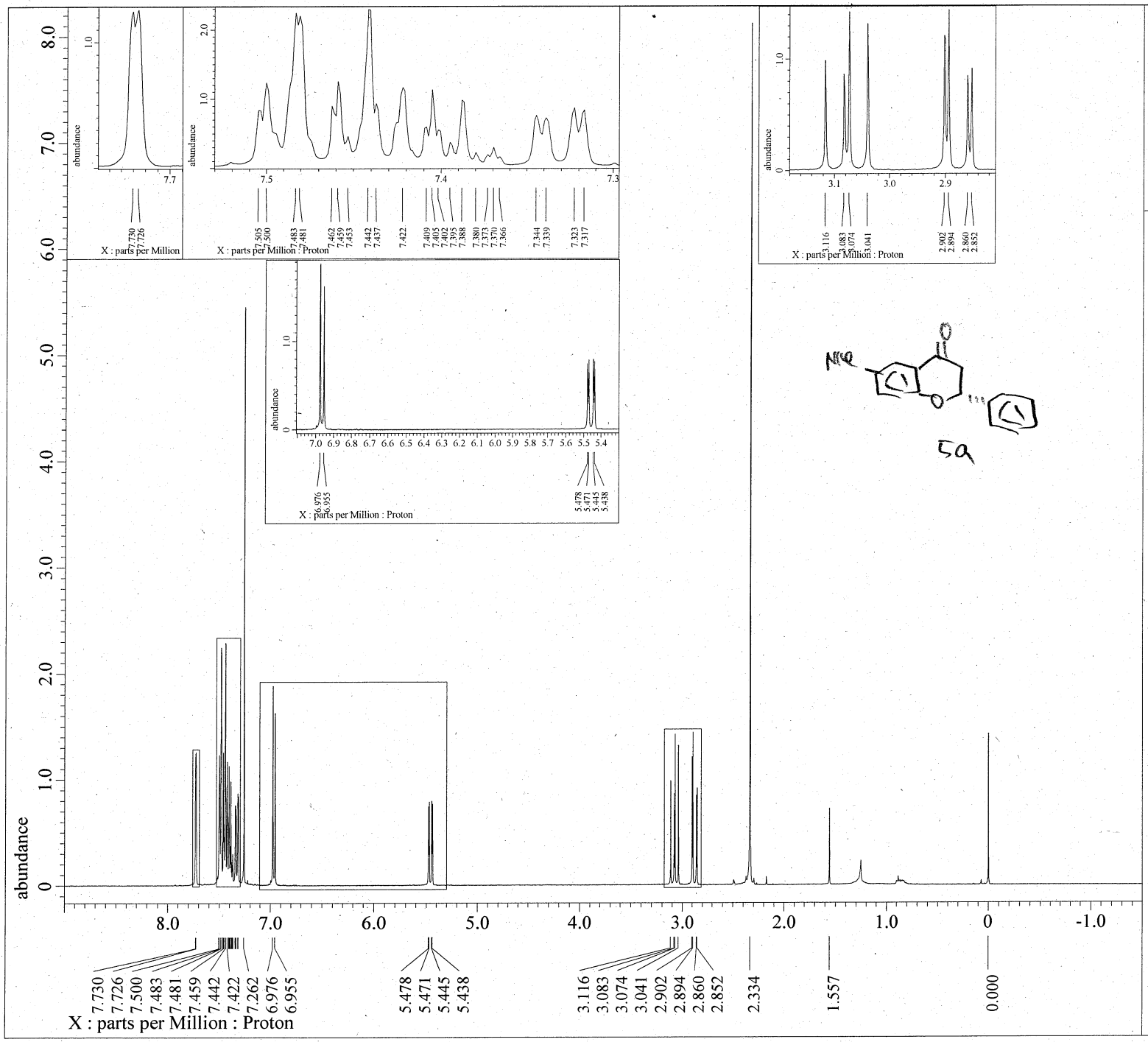

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm

以下に由来:: SHO-122-pure_Proton-1-1.jdf
```

Filename	= SHO-122-pure_Proton-1-
Author	= element
Experiment	= proton_auto.jxp
Sample_Id	= SHO-122-pure
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 10-SEP-2024 13:14:51
Revision_Time	= 1-AUG-2025 18:47:08
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	= 9.2982153[T] (400[MHz]
X_Acq_Duration	= 2.20725248[s]
X_Domain	= Proton
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]
X_Sweep_Clipped	= 5.93824228[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 395.88430144[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2.0[us]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 46
Temp_Get	= 21.2[dC]
X_90_Width	= 6.34[us]
X_Acq_Time	= 2.20725248[s]
X_Angle	= 45[deg]
X_Atn	= 5[dB]
X_Pulse	= 3.17[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 500
Dante_Presat	= FALSE
Decimation_Rate	= 0
Initial_Wait	= 1[s]
Phase	= {0, 90, 270, 180, 180,
Presat_Time	= 5[s]
Presat_Time_Flag	= FALSE



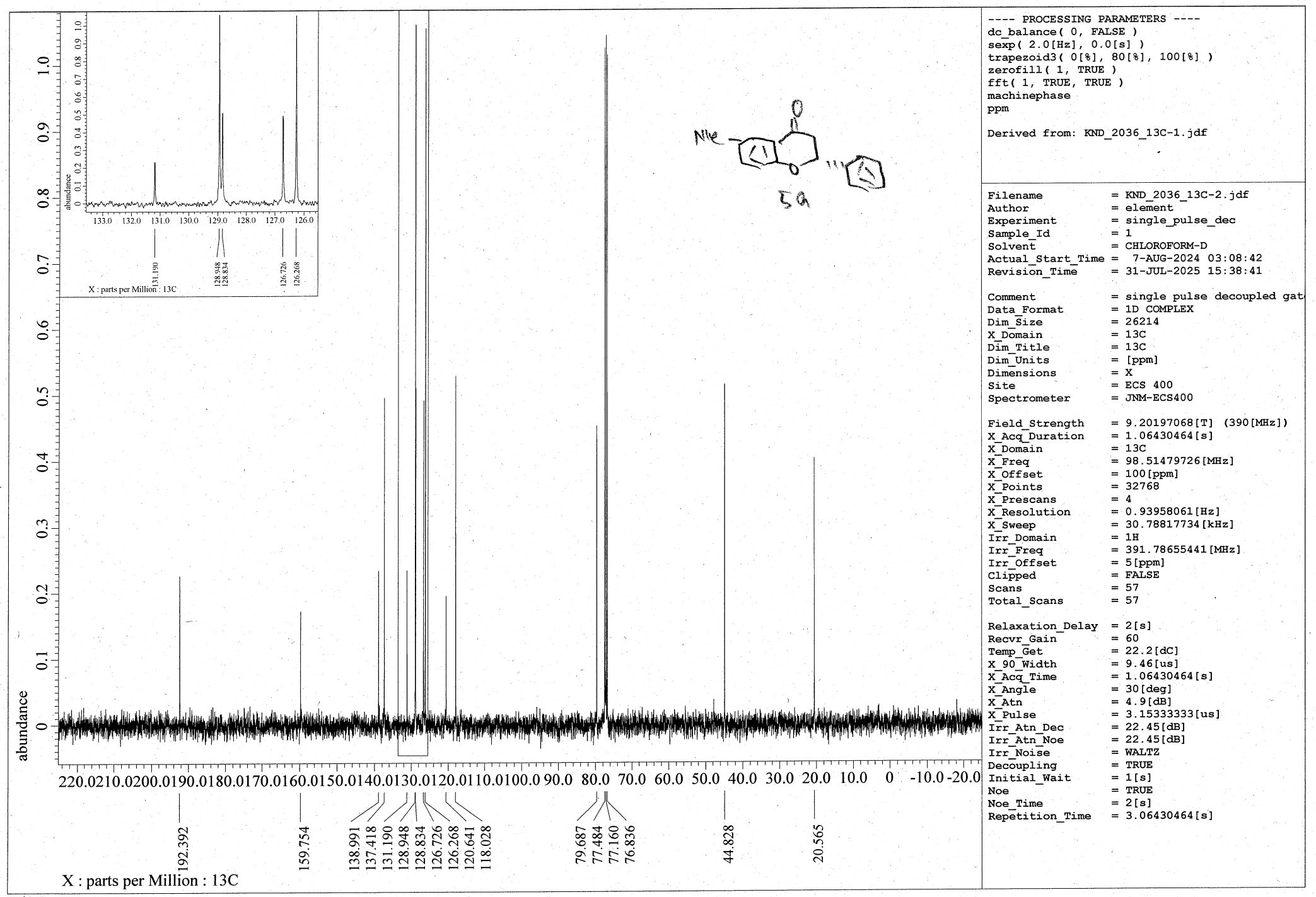

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: SHO-122-13C-1.jdf
```

Filename	= SHO-122-13C-2.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= 1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 2-OCT-2024 02:05:17
Revision_Time	= 4-OCT-2024 09:27:07
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	= 103
Total_Scans	= 103
Relaxation_Delay	= 2[s]
Recvr_Gain	= 60
Temp_Get	= 19.6[dC]
X_90_Width	= 9.46[us]
X_Acq_Time	= 1.06430464[s]
X_Angle	= 30[deg]
X_Atn	= 4.9[dB]
X_Pulse	= 3.15333333[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]



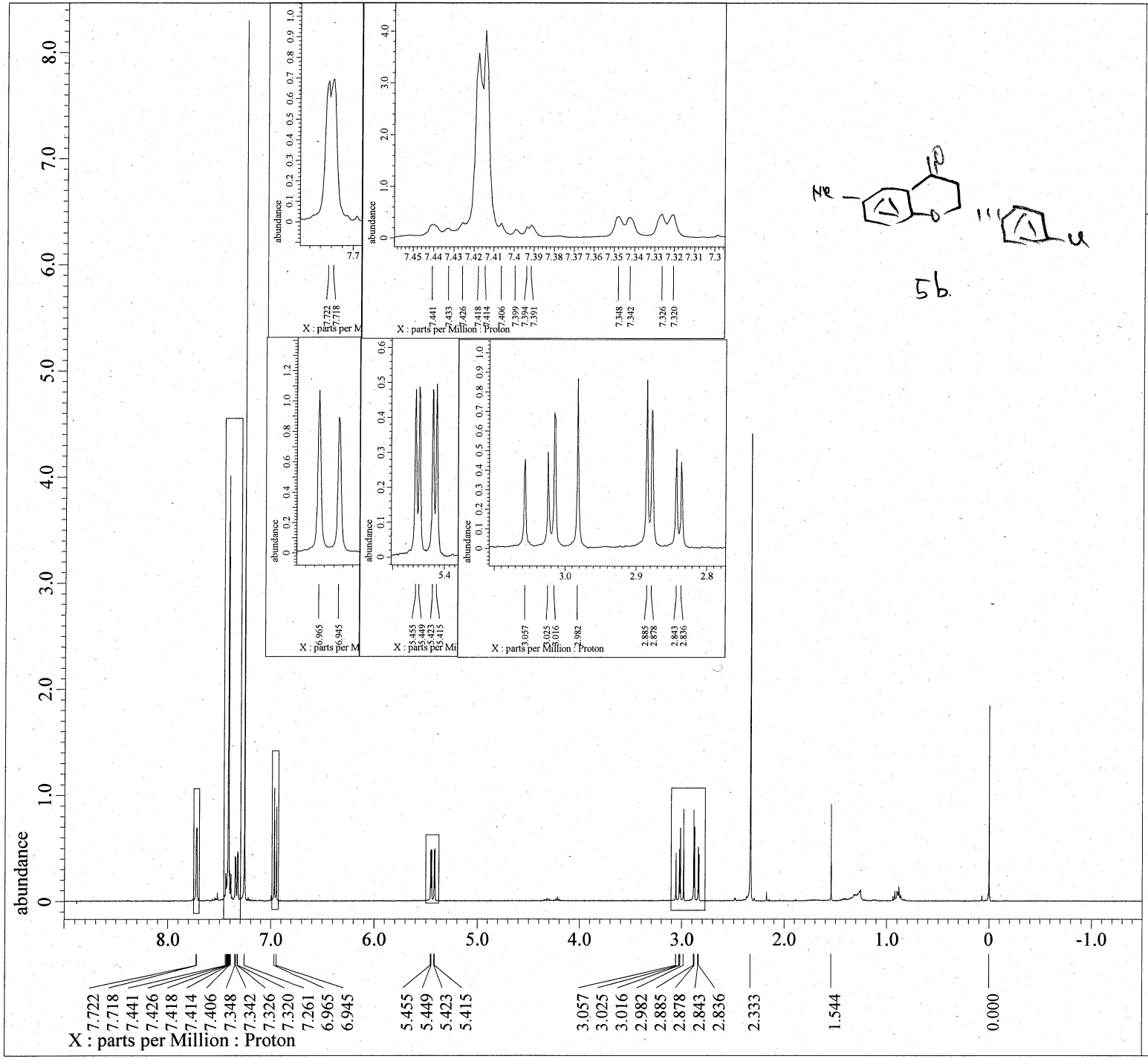

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KND_2036_pure_Proton-1-1.jdf
```

Filename	= KND_2036_pure_Proton-1-2.j
Author	= element
Experiment	= proton.jxp
Sample_Id	= KND_2164_pure
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 7-DEC-2024 22:56:00
Revision_Time	= 31-JUL-2025 15:29:09
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	= 48
Temp_Get	= 18.6[dC]
X_90_Width	= 6.6[us]
X_Acq_Time	= 2.1889024[s]
X_Angle	= 45[deg]
X_Atn	= 1[dB]
X_Pulse	= 3.3[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.1889024[s]




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

Derived from: KND_2036_13C-1.jdf
```

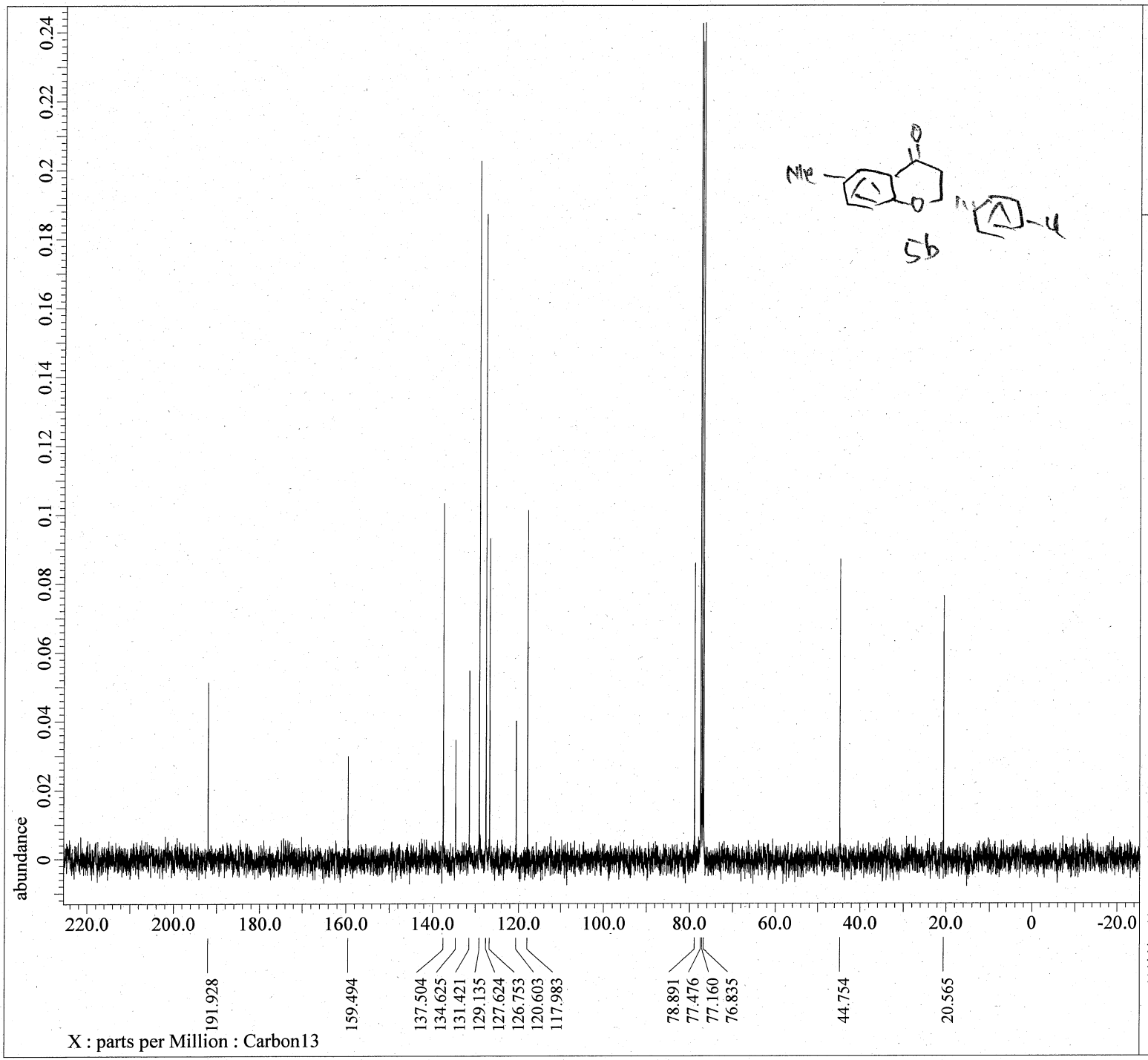
Filename	= KND_2036_13C-2.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= 1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 7-AUG-2024 03:08:42
Revision_Time	= 31-JUL-2025 15:38:41
Comment	= single pulse decoupled gat
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= 13C
Dim_Title	= 13C
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	= 57
Total_Scans	= 57
Relaxation_Delay	= 2[s]
Recvr_Gain	= 60
Temp_Get	= 22.2[dC]
X_90_Width	= 9.46[us]
X_Acq_Time	= 1.06430464[s]
X_Angle	= 30[deg]
X_Atn	= 4.9[dB]
X_Pulse	= 3.15333333[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]



5b.

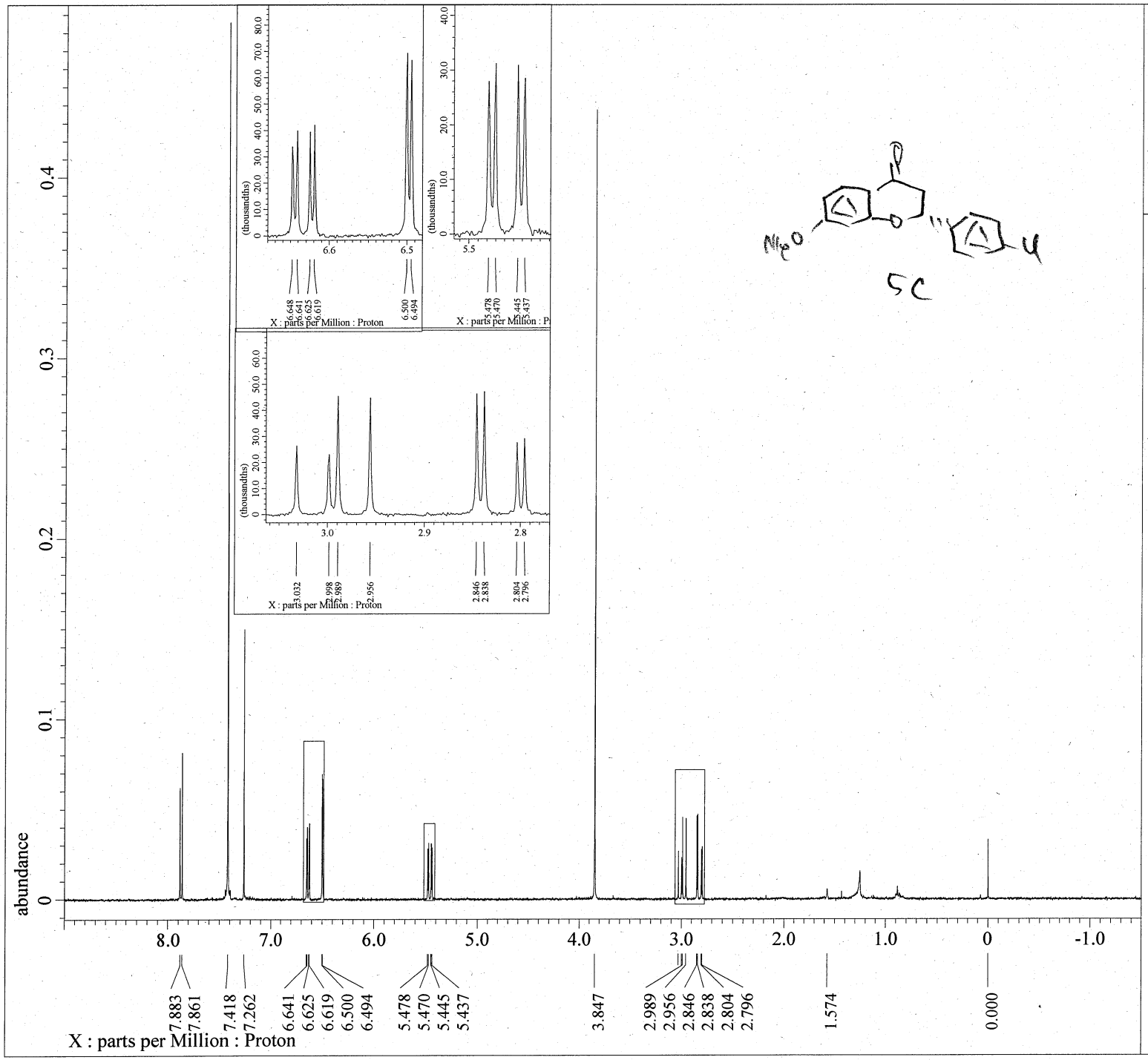
```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KND_2151_pure2_Proton-1-1.jdf
```

Filename	= KND_2151_pure2_Proton-1-2
Author	= element
Experiment	= proton.jxp
Sample_Id	= KND_2151_pure
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 9-DEC-2024 10:40:36
Revision_Time	= 10-DEC-2024 20:09:57
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	= 50
Temp_Get	= 20.8[dC]
X_90_Width	= 6.6[us]
X_Acq_Time	= 2.1889024[s]
X_Angle	= 45[deg]
X_Atn	= 1[dB]
X_Pulse	= 3.3[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.1889024[s]



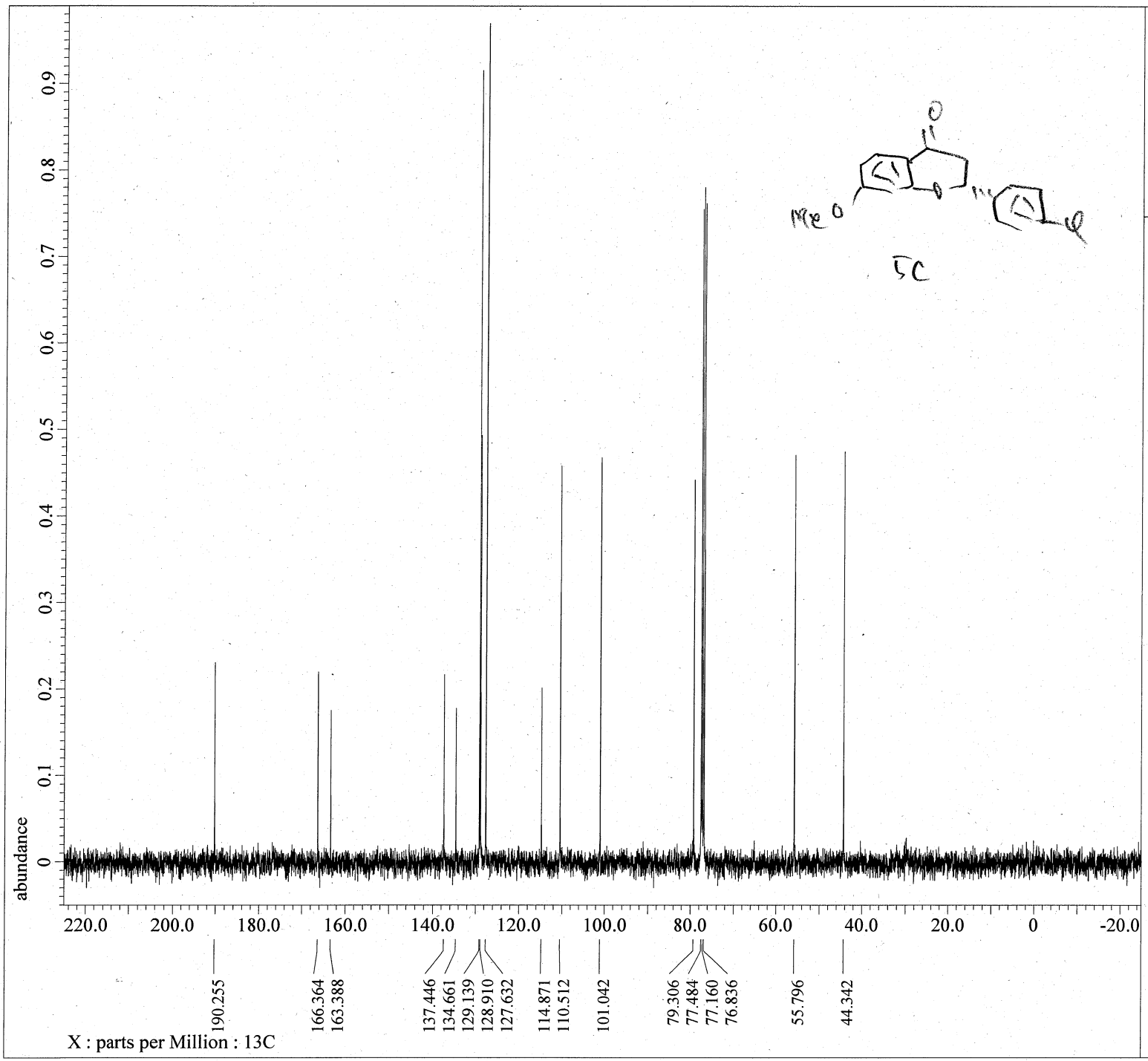

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KND_2151_13C_Carbon-1-1.jdf
```

Filename	= KND_2151_13C_Carbon-1-2.j
Author	= element
Experiment	= carbon.jxp
Sample_Id	= KND_2151_13C
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 1-AUG-2024 23:55:50
Revision_Time	= 10-DEC-2024 20:11:49
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	= 88
Total_Scans	= 88
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 20.9[dC]
X_90_Width	= 12.68[us]
X_Acq_Time	= 1.03809024[s]
X_Angle	= 30[deg]
X_Atn	= 4[dB]
X_Pulse	= 4.22666667[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]



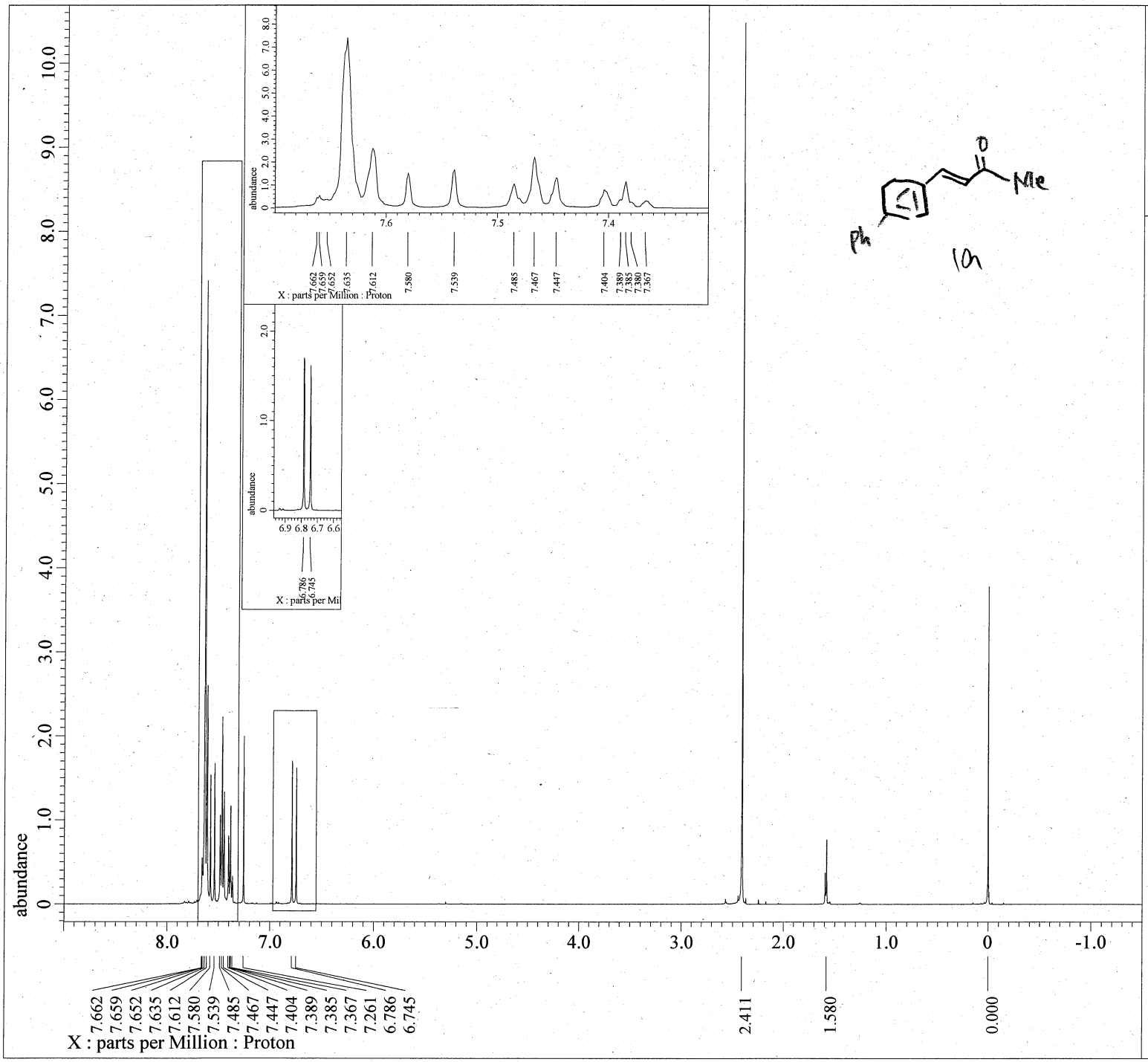

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KND_2152_pure_Proton-1-1.jdf
```

Filename	= KND_2152_pure_Proton-
Author	= element
Experiment	= proton_auto.jxp
Sample_Id	= KND_2142_pure
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 9-DEC-2024 10:43:11
Revision_Time	= 10-DEC-2024 20:48:25
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	= 9.2982153[T] (400[MHz
X_Acq_Duration	= 2.20725248[s]
X_Domain	= Proton
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]
X_Sweep_Clipped	= 5.93824228[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 395.88430144[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 66
Temp_Get	= 17.1[dC]
X_90_Width	= 6.34[us]
X_Acq_Time	= 2.20725248[s]
X_Angle	= 45[deg]
X_Atn	= 5[dB]
X_Pulse	= 3.17[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 500
Dante_Presat	= FALSE
Decimation_Rate	= 0
Experiment_Path	= C:\Program Files\JEOL
Initial_Wait	= 1[s]
Phase	= {0, 90, 270, 180, 180
Presat_Time	= 5[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: KND_2152_13C-1.jdf
```

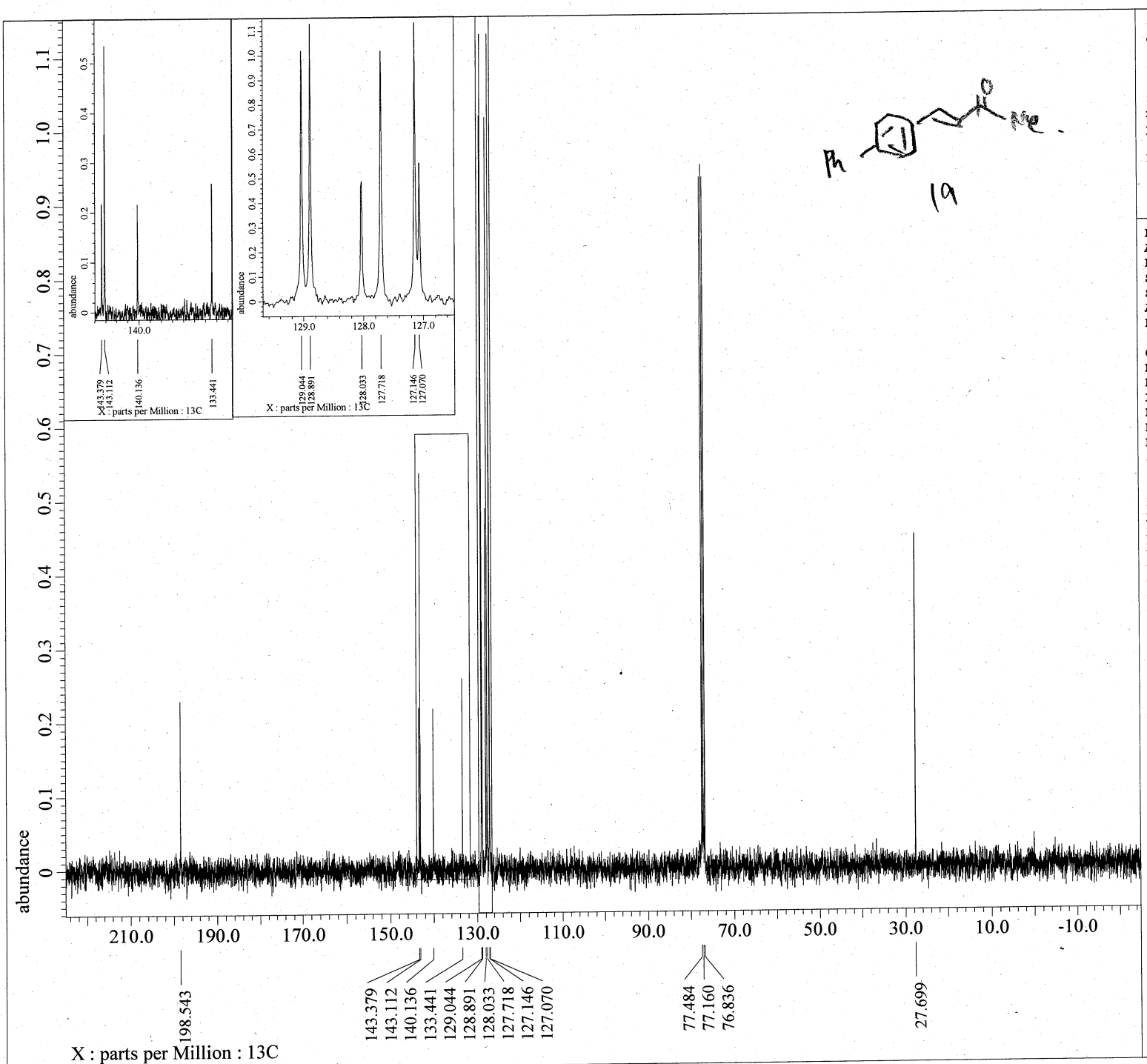
Filename	= KND_2152_13C-2.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= 1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 31-JUL-2024 03:36:26
Revision_Time	= 10-DEC-2024 20:52:04
Comment	= single pulse decoupled ga
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= 13C
Dim_Title	= 13C
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	= 77
Total_Scans	= 77
Relaxation_Delay	= 2[s]
Recvr_Gain	= 60
Temp_Get	= 22.6[dC]
X_90_Width	= 9.46[us]
X_Acq_Time	= 1.06430464[s]
X_Angle	= 30[deg]
X_Atn	= 4.9[dB]
X_Pulse	= 3.15333333[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]



10h

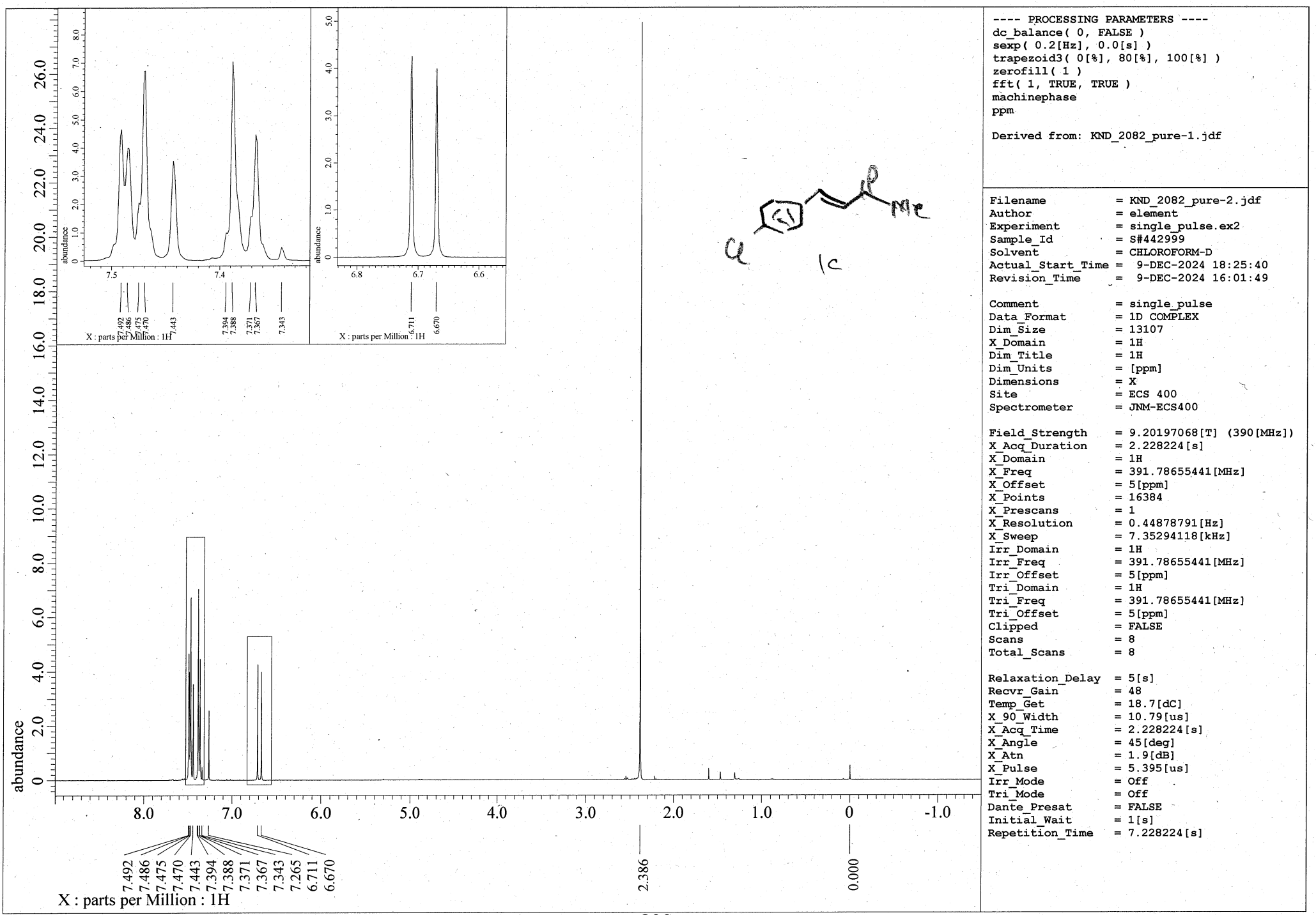
```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KND_2502_pure_Proton-1-1.jdf
```

Filename	= KND_2502_pure_Proton-1-2.
Author	= element
Experiment	= proton.jxp
Sample_Id	= KND_2502_pure
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 13-DEC-2024 17:30:12
Revision_Time	= 13-DEC-2024 18:36:56
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	= 18.4[dC]
X_90_Width	= 6.6[us]
X_Acq_Time	= 2.1889024[s]
X_Angle	= 45[deg]
X_Atn	= 1[dB]
X_Pulse	= 3.3[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.1889024[s]



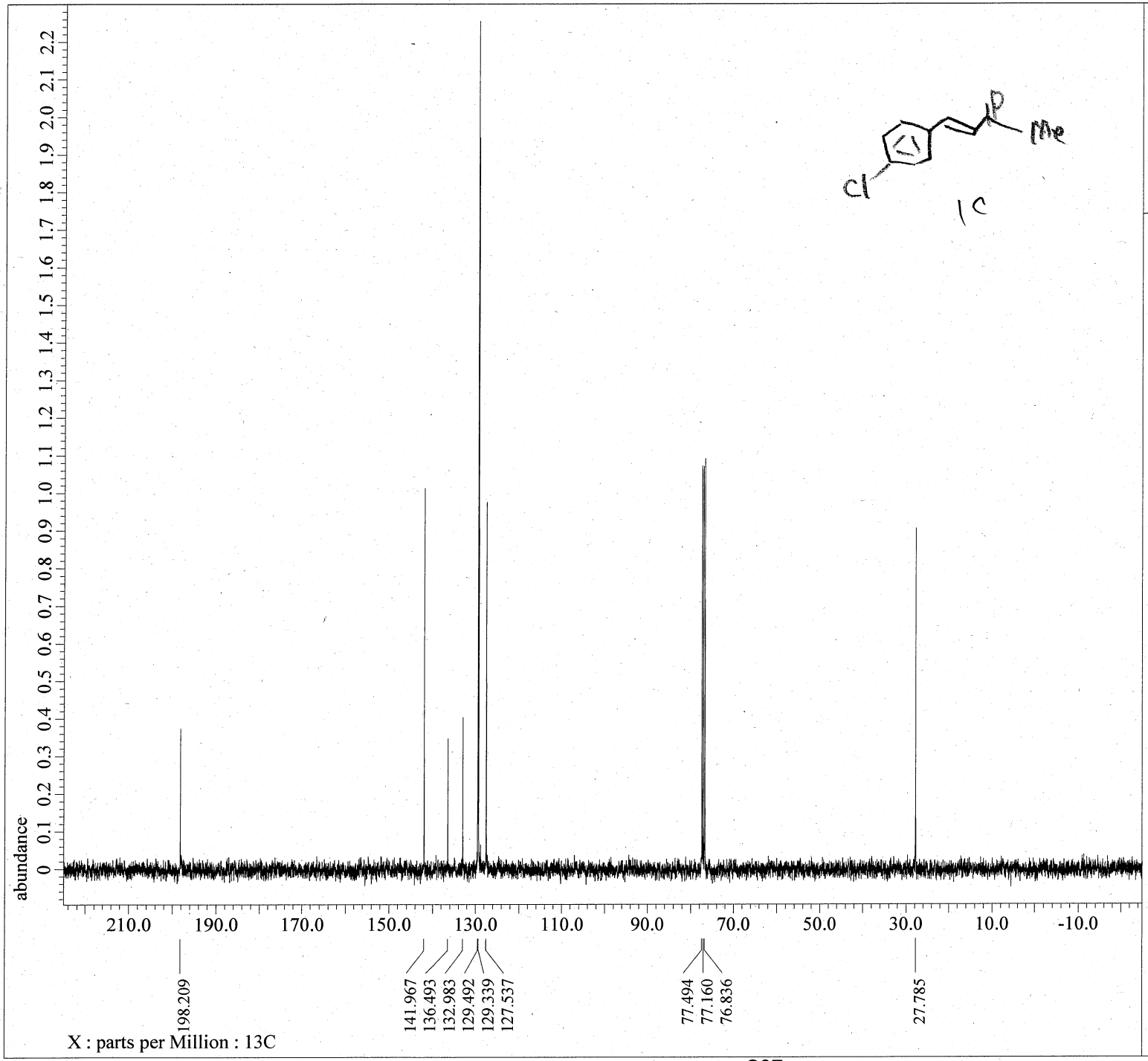

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KND_2502_13C-1.jdf
```

Filename	= KND_2502_13C-2.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= 1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 13-DEC-2024 22:42:32
Revision_Time	= 13-DEC-2024 18:40:07
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	= 45
Total_Scans	= 45
Relaxation_Delay	= 2[s]
Recvr_Gain	= 60
Temp_Get	= 18.3[dC]
X_90_Width	= 9.46[us]
X_Acq_Time	= 1.06430464[s]
X_Angle	= 30[deg]
X_Atn	= 4.9[dB]
X_Pulse	= 3.15333333[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]



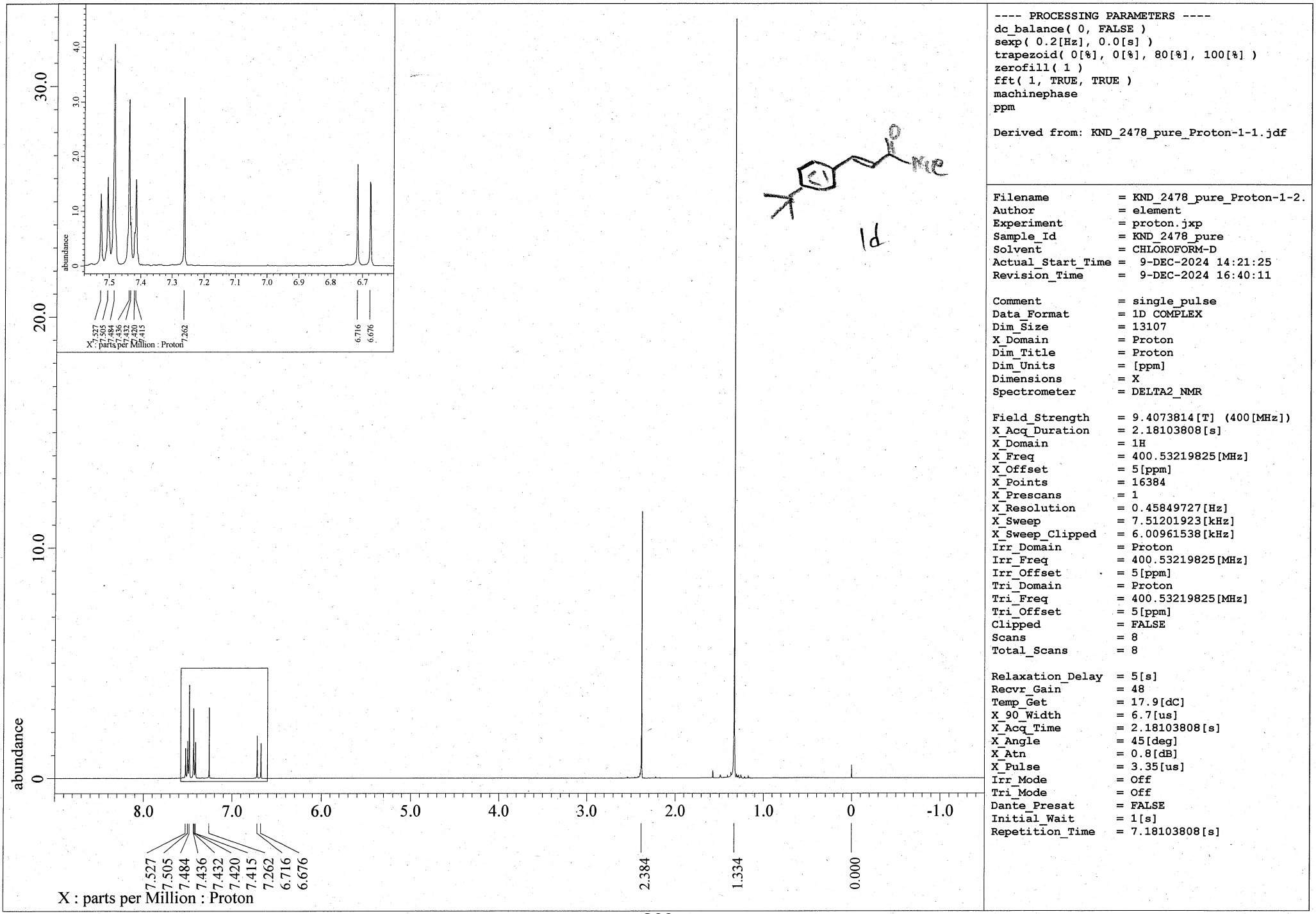

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KND_2082_pure-1.jdf
```

Filename	= KND_2082_pure-2.jdf
Author	= element
Experiment	= single_pulse.ex2
Sample_Id	= S#442999
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 9-DEC-2024 18:25:40
Revision_Time	= 9-DEC-2024 16:01:49
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	= 18.7[dC]
X_90_Width	= 10.79[us]
X_Acq_Time	= 2.228224[s]
X_Angle	= 45[deg]
X_Atn	= 1.9[dB]
X_Pulse	= 5.395[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.228224[s]



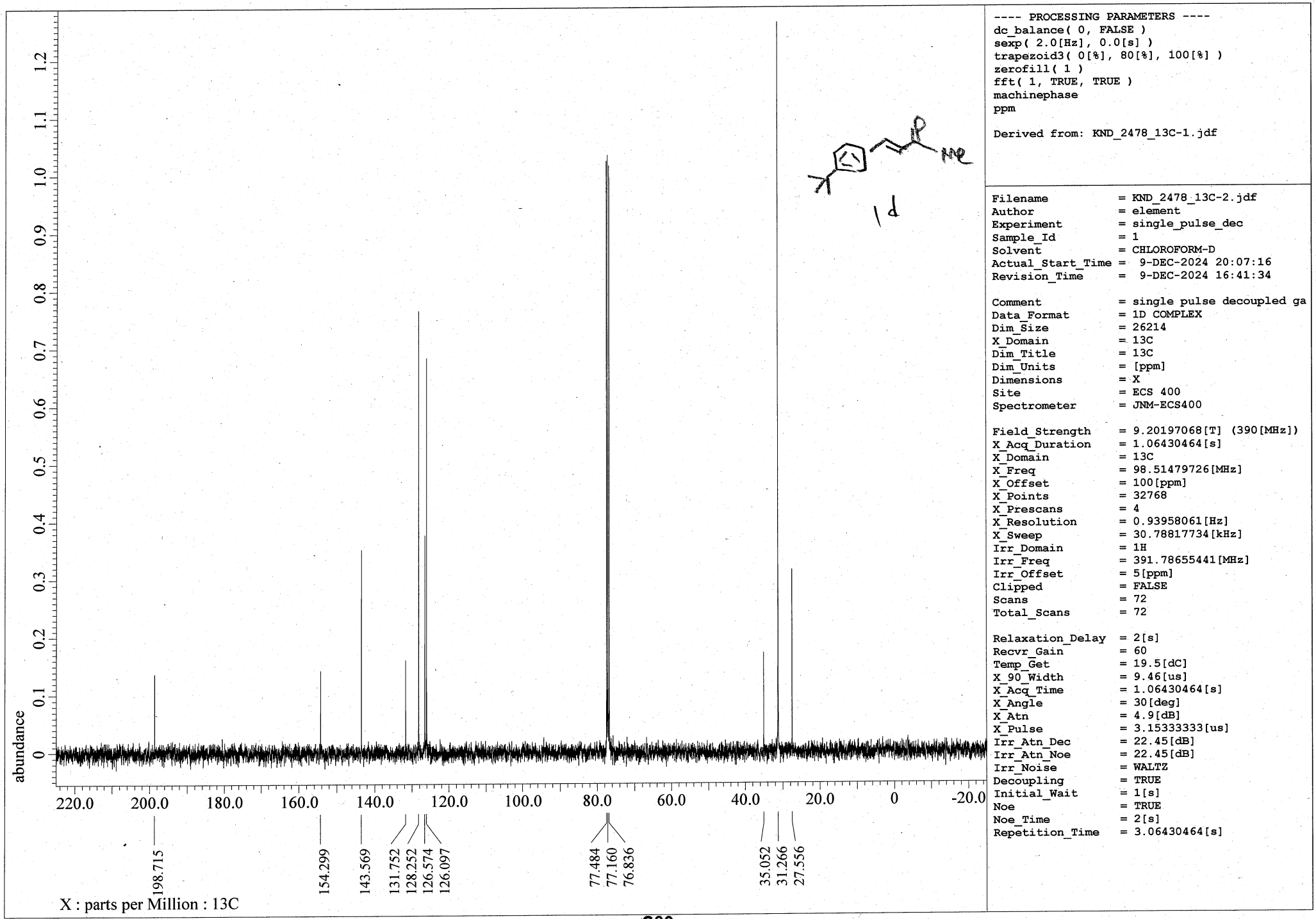

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KND_2082_13C-1.jdf
```

```
Filename            = KND_2082_13C-2.jdf
Author              = element
Experiment          = single_pulse_dec
Sample_Id           = 1
Solvent             = CHLOROFORM-D
Actual_Start_Time   =  9-DEC-2024 18:34:53
Revision_Time       =  9-DEC-2024 16:02:46

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               = 31
Total_Scans         = 31

Relaxation_Delay    = 2[s]
Recvr_Gain          = 60
Temp_Get            = 18.8[dC]
X_90_Width          = 9.46[us]
X_Acq_Time          = 1.06430464[s]
X_Angle             = 30[deg]
X_Atn               = 4.9[dB]
X_Pulse             = 3.15333333[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]
```



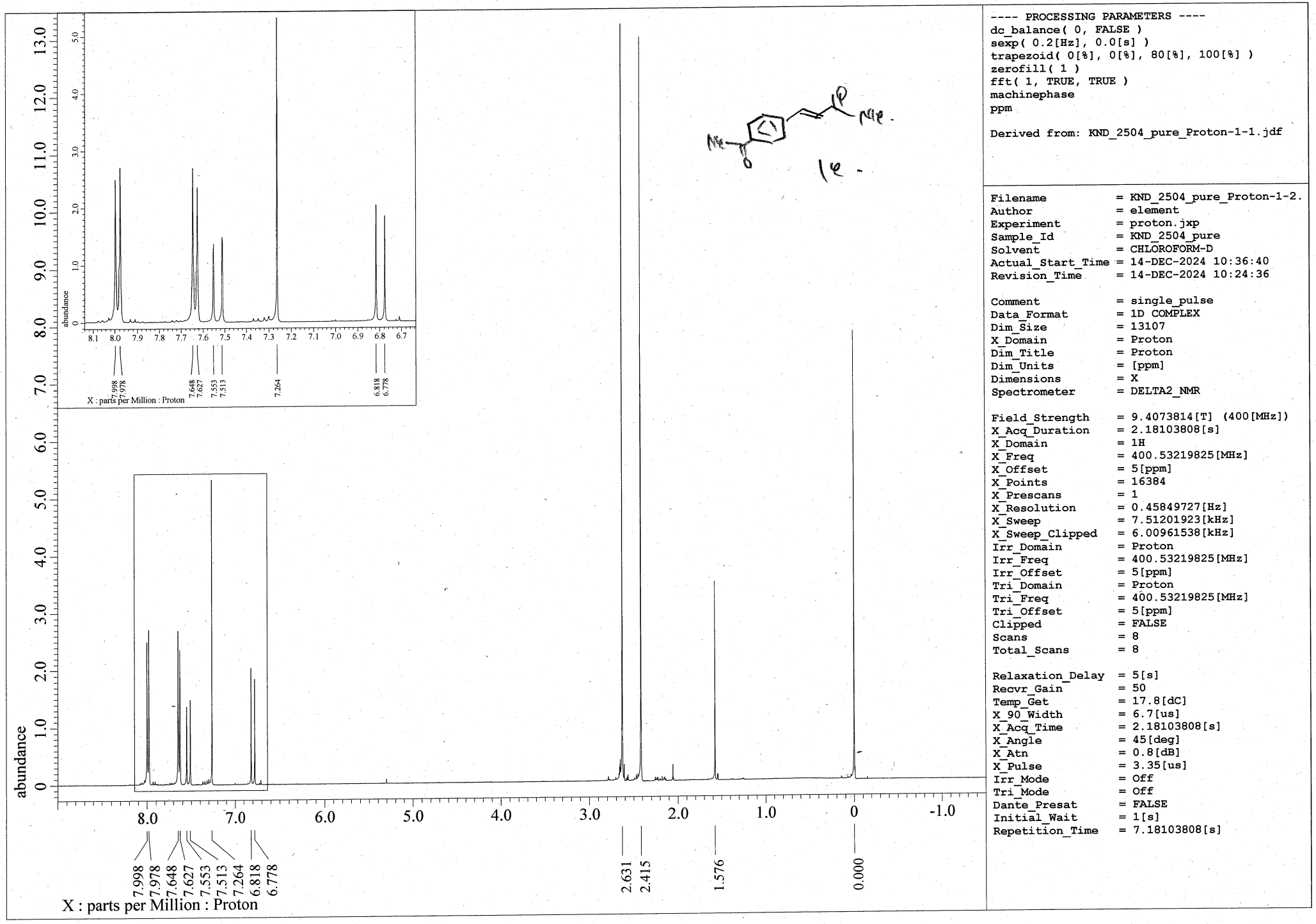

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KND_2478_pure_Proton-1-1.jdf
```

Filename	= KND_2478_pure_Proton-1-2.
Author	= element
Experiment	= proton.jxp
Sample_Id	= KND_2478_pure
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 9-DEC-2024 14:21:25
Revision_Time	= 9-DEC-2024 16:40:11
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	= 17.9[dC]
X_90_Width	= 6.7[us]
X_Acq_Time	= 2.18103808[s]
X_Angle	= 45[deg]
X_Atn	= 0.8[dB]
X_Pulse	= 3.35[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.18103808[s]



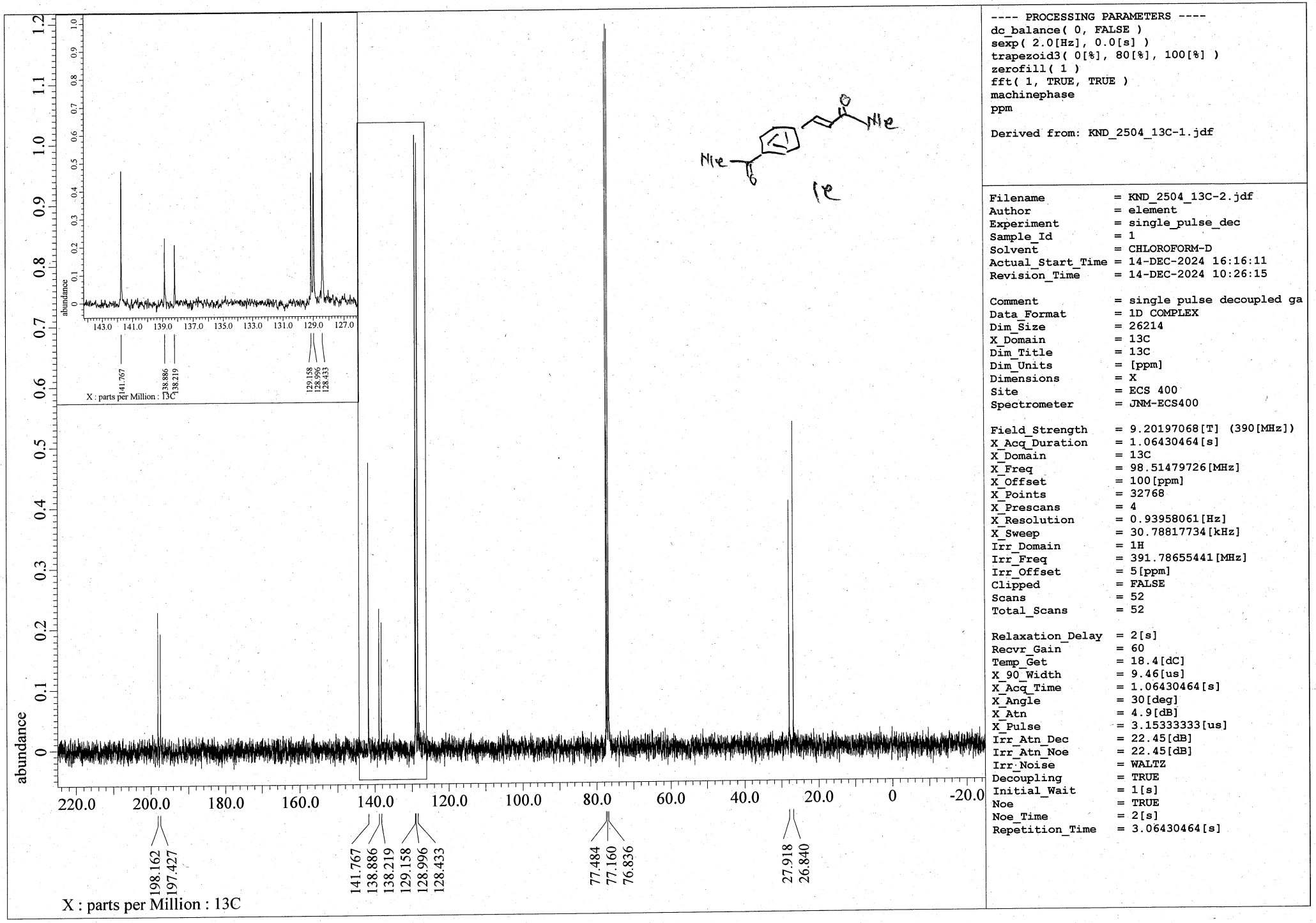

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KND_2478_13C-1.jdf
```

Filename	= KND_2478_13C-2.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= 1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 9-DEC-2024 20:07:16
Revision_Time	= 9-DEC-2024 16:41:34
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	= 72
Total_Scans	= 72
Relaxation_Delay	= 2[s]
Recvr_Gain	= 60
Temp_Get	= 19.5[dC]
X_90_Width	= 9.46[us]
X_Acq_Time	= 1.06430464[s]
X_Angle	= 30[deg]
X_Atn	= 4.9[dB]
X_Pulse	= 3.15333333[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]



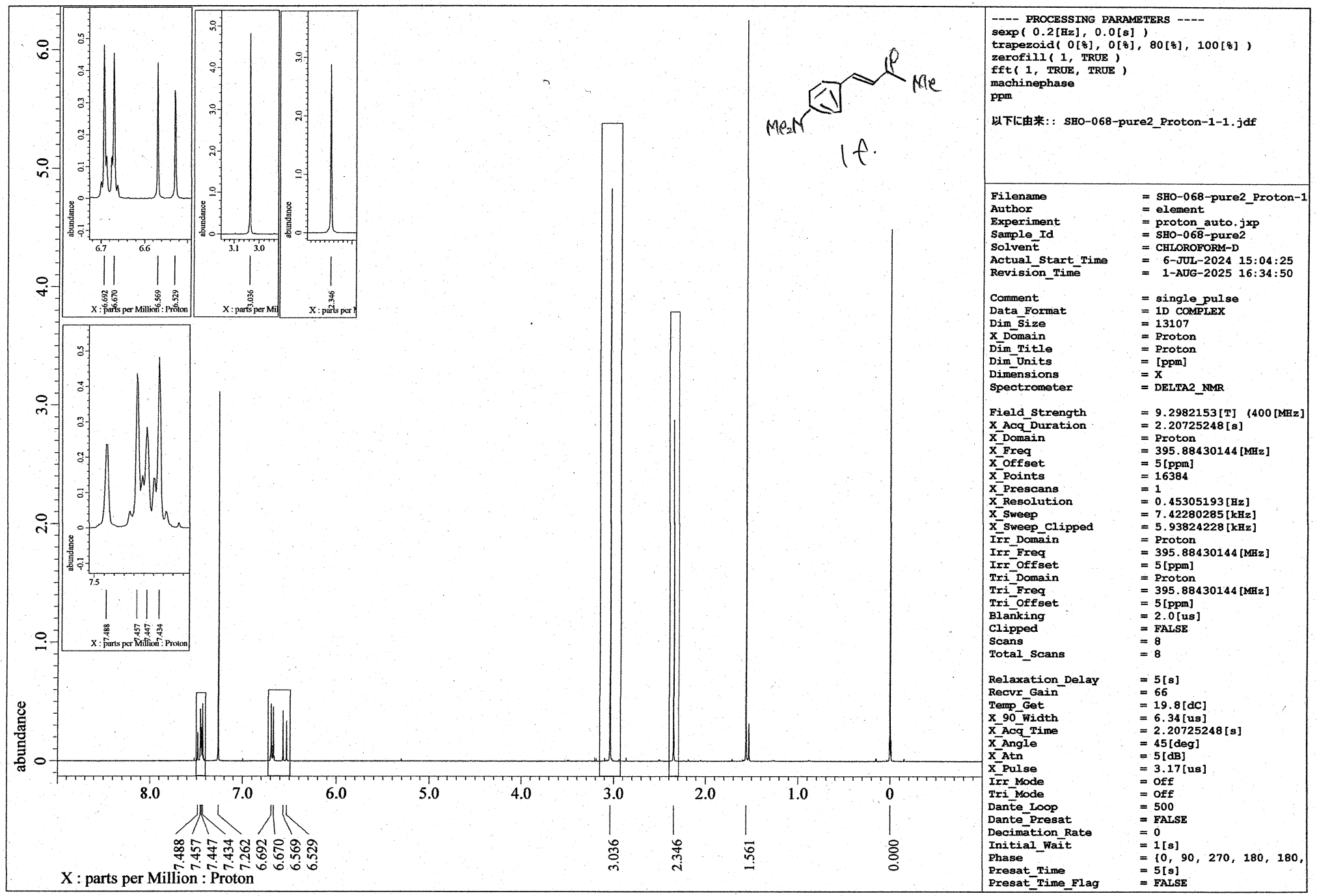

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KND_2504_pure_Proton-1-1.jdf
```

```
Filename            = KND_2504_pure_Proton-1-2.
Author              = element
Experiment          = proton.jxp
Sample_Id           = KND_2504_pure
Solvent             = CHLOROFORM-D
Actual_Start_Time   = 14-DEC-2024 10:36:40
Revision_Time       = 14-DEC-2024 10:24:36

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            = 17.8[dC]
X_90_Width          = 6.7[us]
X_Acq_Time          = 2.18103808[s]
X_Angle             = 45[deg]
X_Atn               = 0.8[dB]
X_Pulse             = 3.35[us]
Irr_Mode            = Off
Tri_Mode            = Off
Dante_Presat        = FALSE
Initial_Wait        = 1[s]
Repetition_Time     = 7.18103808[s]
```



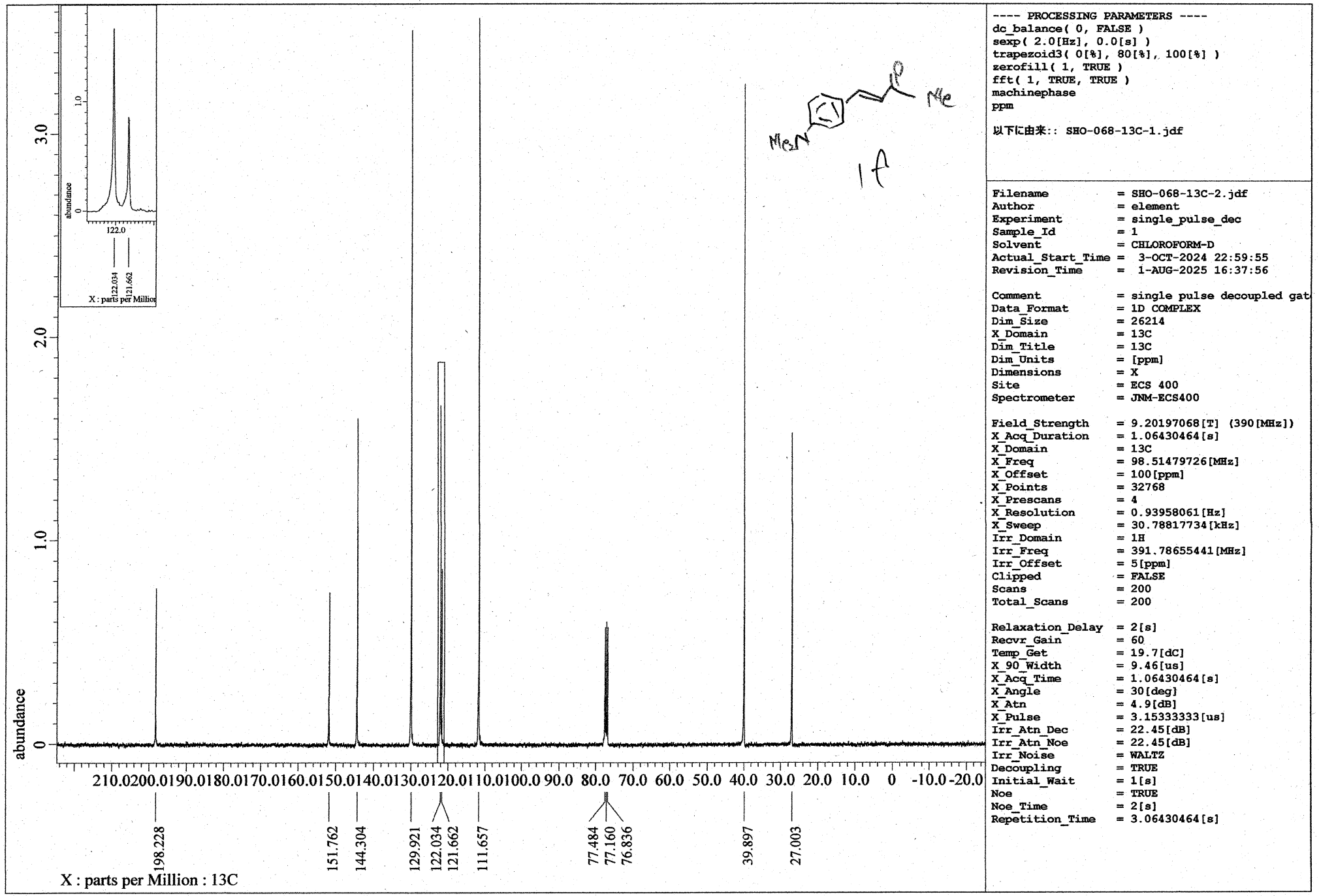

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KND_2504_13C-1.jdf
```

Filename	= KND_2504_13C-2.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= 1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 14-DEC-2024 16:16:11
Revision_Time	= 14-DEC-2024 10:26:15
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	= 52
Total_Scans	= 52
Relaxation_Delay	= 2[s]
Recvr_Gain	= 60
Temp_Get	= 18.4[dC]
X_90_Width	= 9.46[us]
X_Acq_Time	= 1.06430464[s]
X_Angle	= 30[deg]
X_Atn	= 4.9[dB]
X_Pulse	= 3.15333333[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]



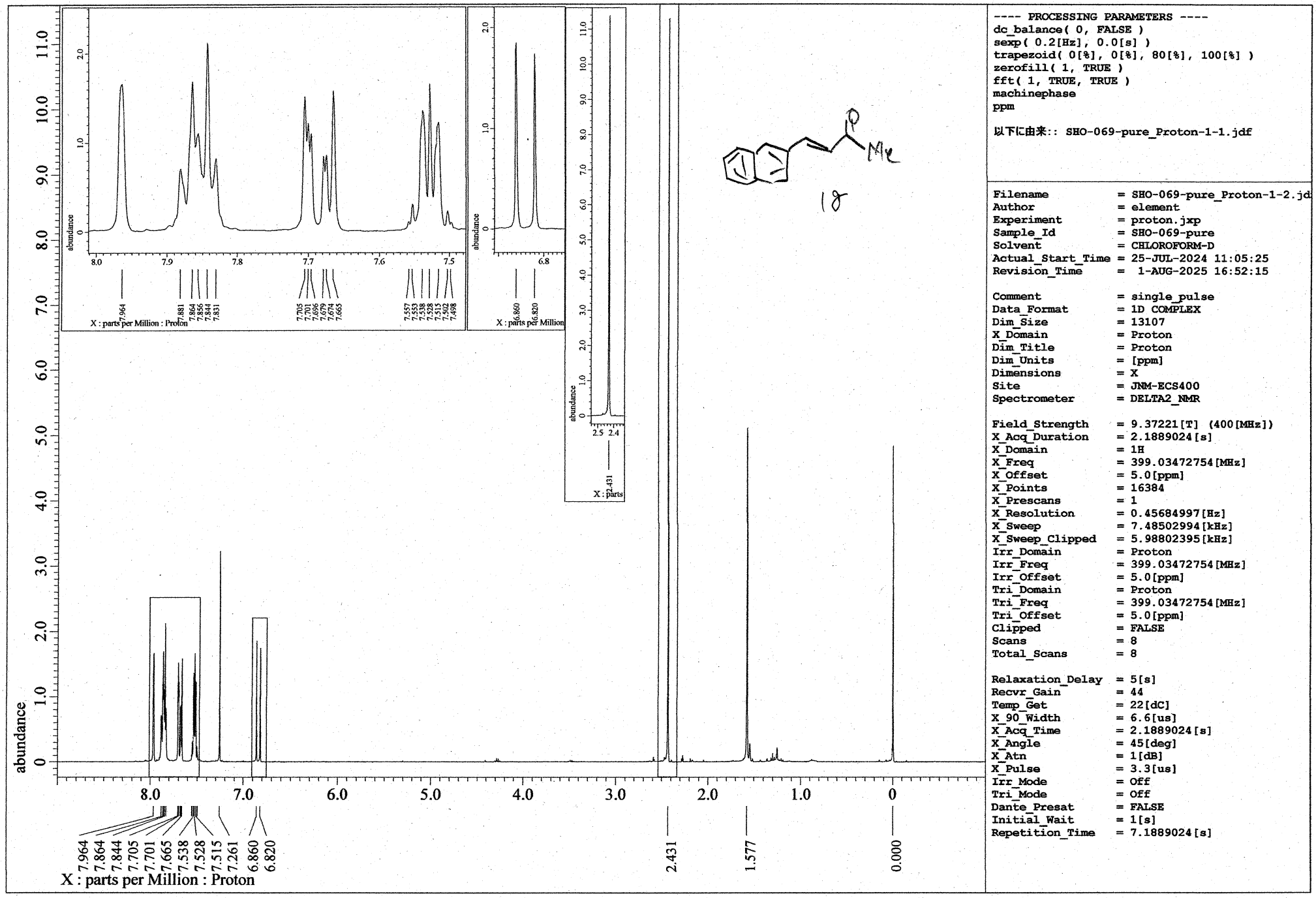

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm

以下に由来:: SHO-068-pure2_Proton-1-1.jdf
```

Filename	= SHO-068-pure2_Proton-1
Author	= element
Experiment	= proton_auto.jxp
Sample_Id	= SHO-068-pure2
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 6-JUL-2024 15:04:25
Revision_Time	= 1-AUG-2025 16:34:50
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	= 9.2982153[T] (400[MHz]
X_Acq_Duration	= 2.20725248[s]
X_Domain	= Proton
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]
X_Sweep_Clipped	= 5.93824228[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 395.88430144[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2.0[us]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 66
Temp_Get	= 19.8[dC]
X_90_Width	= 6.34[us]
X_Acq_Time	= 2.20725248[s]
X_Angle	= 45[deg]
X_Atn	= 5[dB]
X_Pulse	= 3.17[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 500
Dante_Presat	= FALSE
Decimation_Rate	= 0
Initial_Wait	= 1[s]
Phase	= {0, 90, 270, 180, 180,
Presat_Time	= 5[s]
Presat_Time_Flag	= FALSE



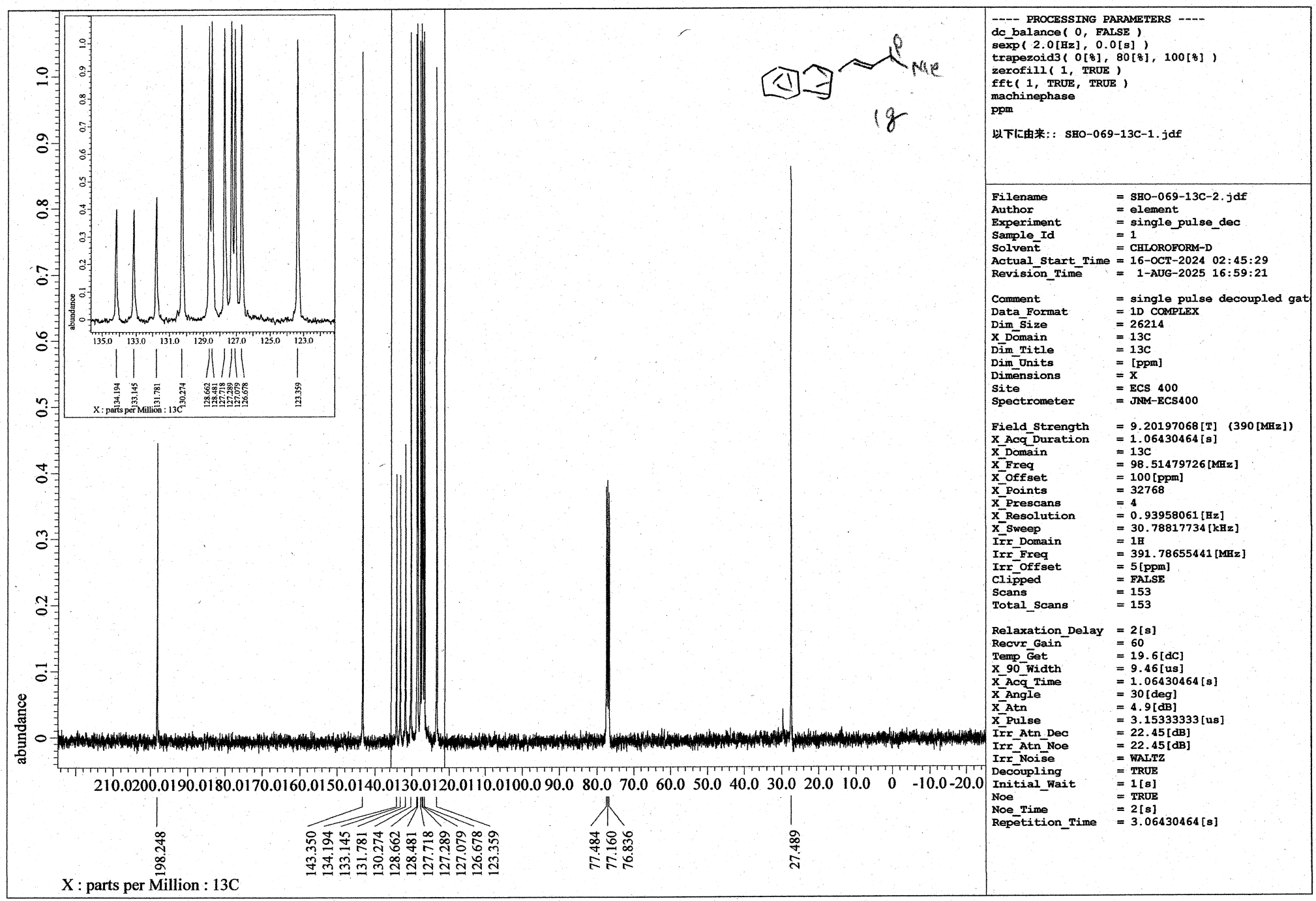

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm

以下に由来:: SHO-068-13C-1.jdf
```

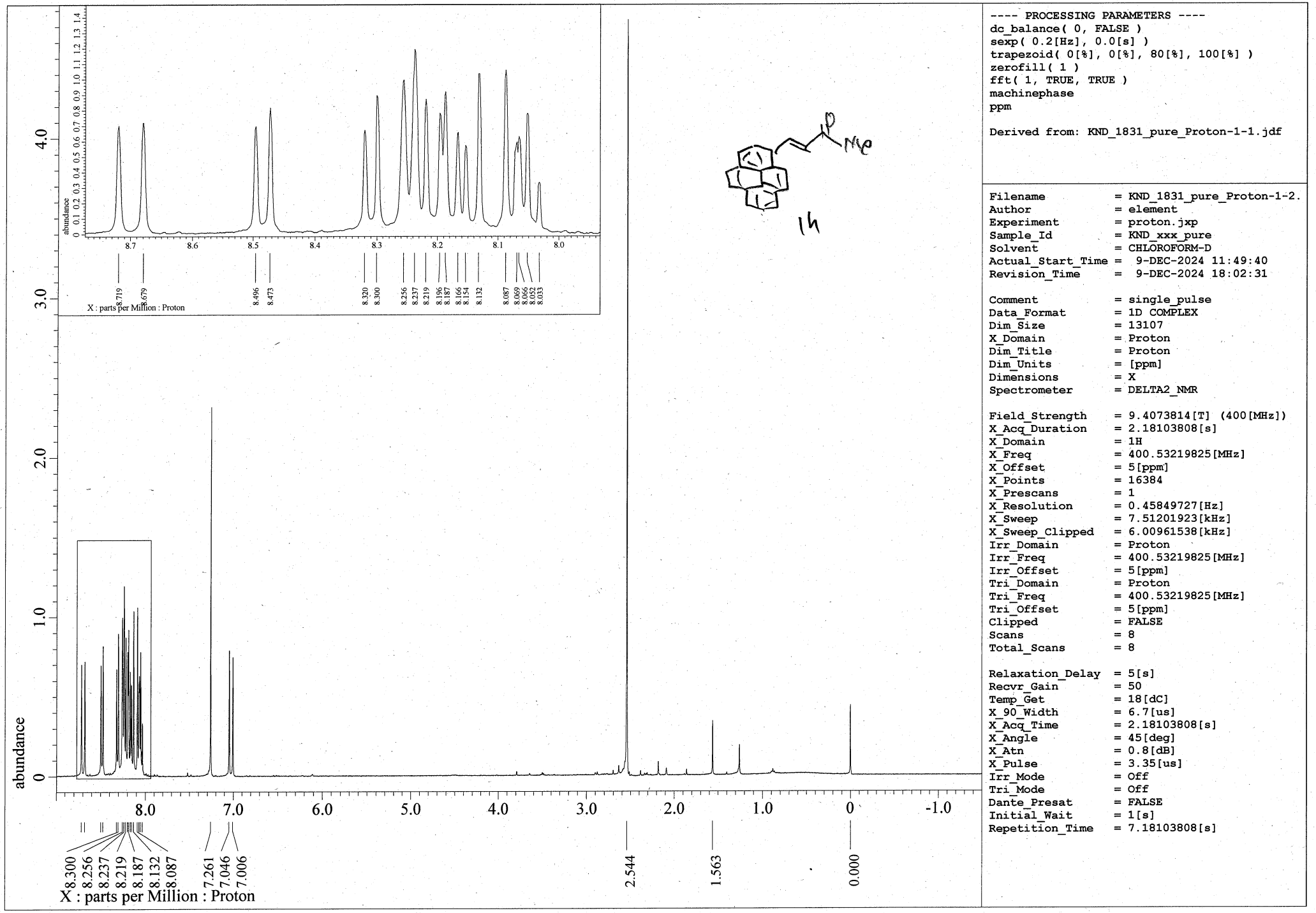
Filename	= SHO-068-13C-2.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= 1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 3-OCT-2024 22:59:55
Revision_Time	= 1-AUG-2025 16:37:56
Comment	= single pulse decoupled gat
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= 13C
Dim_Title	= 13C
Dim_Units	= [ppm]
Dimensions	= X
Site	= ECS 400
Spectrometer	= JNM-ECS400
Field_Strength	= 9.20197068[T] (390[MHz])
X_Acq_Duration	= 1.06430464[s]
X_Domain	= 13C
X_Freq	= 98.51479726[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.93958061[Hz]
X_Sweep	= 30.78817734[kHz]
Irr_Domain	= 1H
Irr_Freq	= 391.78655441[MHz]
Irr_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 200
Total_Scans	= 200
Relaxation_Delay	= 2[s]
Recvr_Gain	= 60
Temp_Get	= 19.7[dC]
X_90_Width	= 9.46[us]
X_Acq_Time	= 1.06430464[s]
X_Angle	= 30[deg]
X_Atn	= 4.9[dB]
X_Pulse	= 3.15333333[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, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm

以下に由来:: SHO-069-pure_Proton-1-1.jdf
```

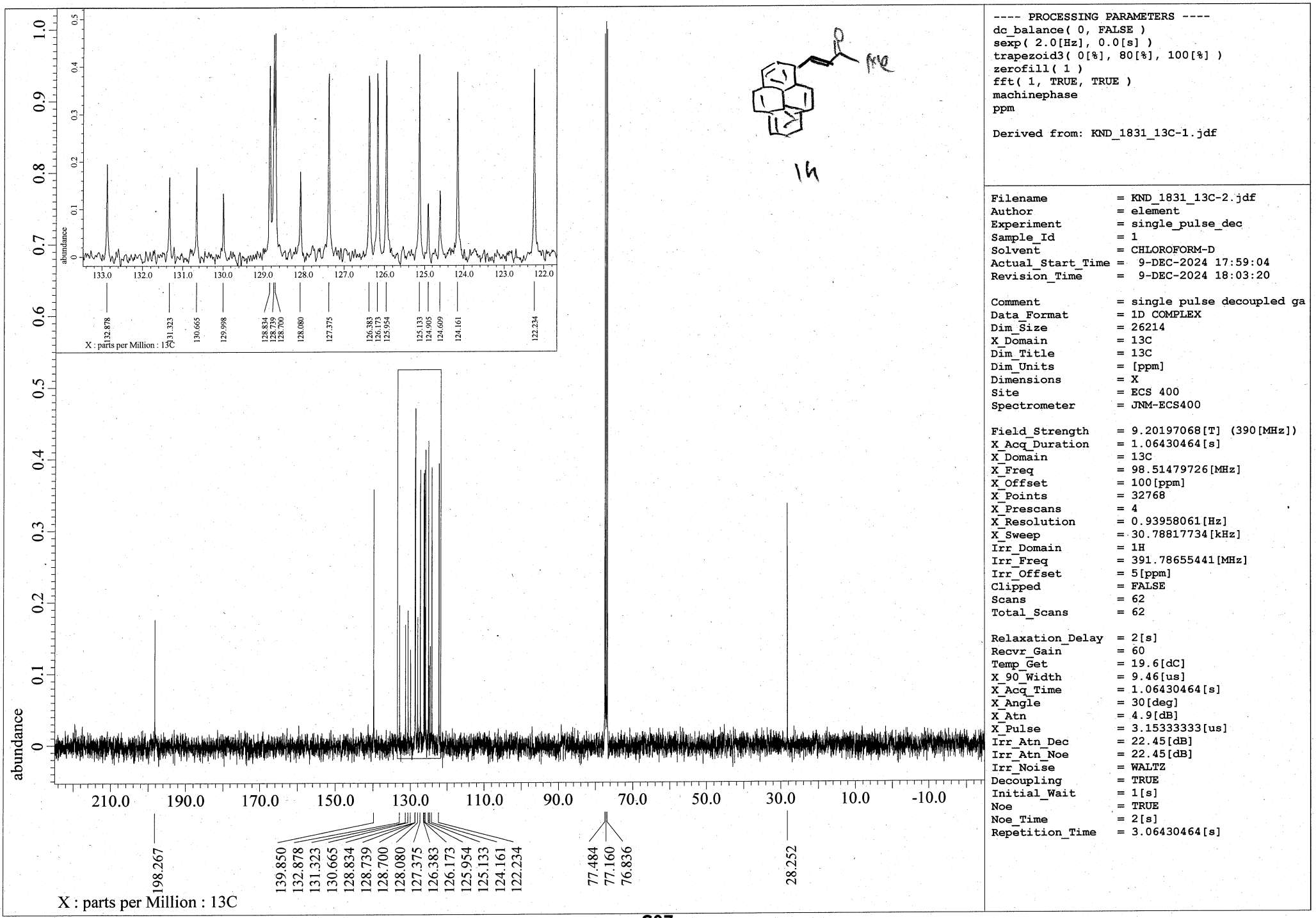
Filename	= SHO-069-pure_Proton-1-2.jd
Author	= element
Experiment	= proton.jxp
Sample_Id	= SHO-069-pure
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 25-JUL-2024 11:05:25
Revision_Time	= 1-AUG-2025 16:52:15
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
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	= 44
Temp_Get	= 22[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]


abundance
X : parts per Million : 13C
198.248
143.350
134.194
133.145
131.781
130.274
128.662
128.481
127.718
127.289
127.079
126.678
123.359
77.484
77.160
76.836
27.489
18
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(2.0[Hz], 0.0[s])
trapezoid3(0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
以下に由来:: SHO-069-13C-1.jdf
Filename = SHO-069-13C-2.jdf
Author = element
Experiment = single_pulse_dec
Sample_Id = 1
Solvent = CHLOROFORM-D
Actual_Start_Time = 16-OCT-2024 02:45:29
Revision_Time = 1-AUG-2025 16:59:21
Comment = single pulse decoupled gat
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 = 153
Total_Scans = 153
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 19.6[dC]
X_90_Width = 9.46[us]
X_Acq_Time = 1.06430464[s]
X_Angle = 30[deg]
X_Atn = 4.9[dB]
X_Pulse = 3.15333333[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]



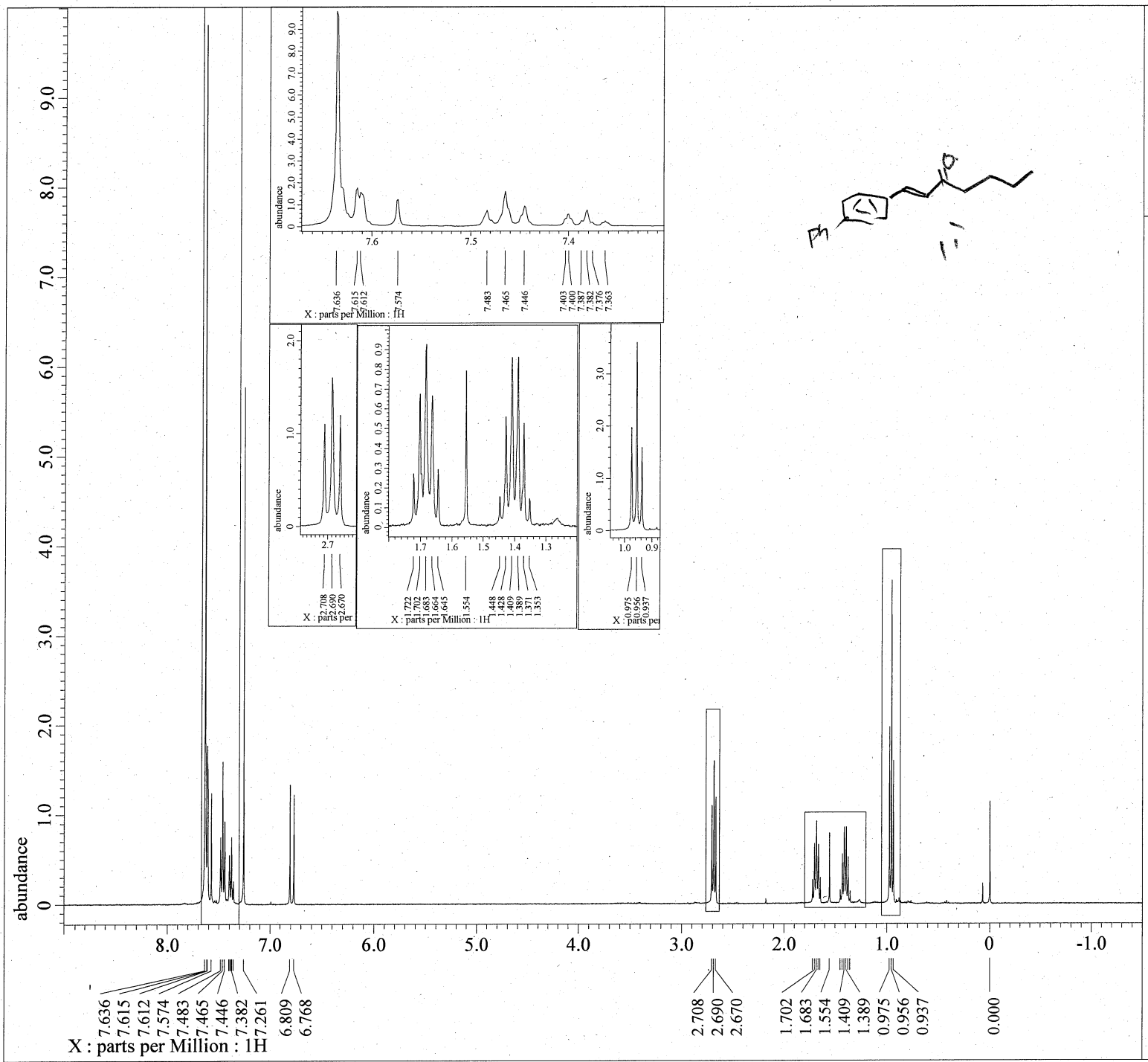

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KND_1831_pure_Proton-1-1.jdf
```

Filename	= KND_1831_pure_Proton-1-2.
Author	= element
Experiment	= proton.jxp
Sample_Id	= KND_xxx_pure
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 9-DEC-2024 11:49:40
Revision_Time	= 9-DEC-2024 18:02:31
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.4073814[T] (400[MHz])
X_Acq_Duration	= 2.18103808[s]
X_Domain	= 1H
X_Freq	= 400.53219825[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45849727[Hz]
X_Sweep	= 7.51201923[kHz]
X_Sweep_Clipped	= 6.00961538[kHz]
Irr_Domain	= Proton
Irr_Freq	= 400.53219825[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 400.53219825[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 50
Temp_Get	= 18[dC]
X_90_Width	= 6.7[us]
X_Acq_Time	= 2.18103808[s]
X_Angle	= 45[deg]
X_Atn	= 0.8[dB]
X_Pulse	= 3.35[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.18103808[s]



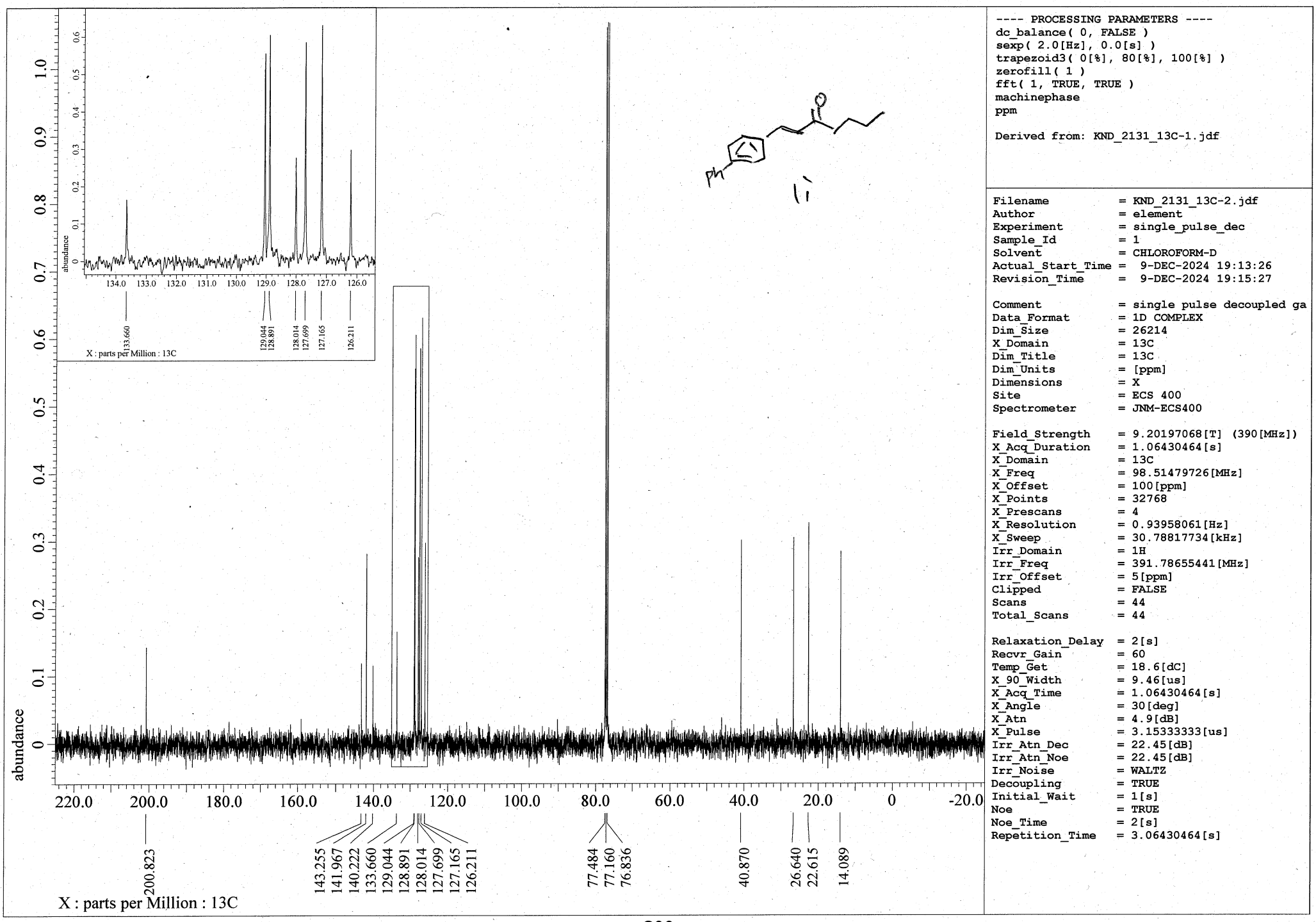

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KND_1831_13C-1.jdf
```

Filename	= KND_1831_13C-2.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= 1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 9-DEC-2024 17:59:04
Revision_Time	= 9-DEC-2024 18:03:20
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	= 62
Total_Scans	= 62
Relaxation_Delay	= 2[s]
Recvr_Gain	= 60
Temp_Get	= 19.6[dC]
X_90_Width	= 9.46[us]
X_Acq_Time	= 1.06430464[s]
X_Angle	= 30[deg]
X_Atn	= 4.9[dB]
X_Pulse	= 3.15333333[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]



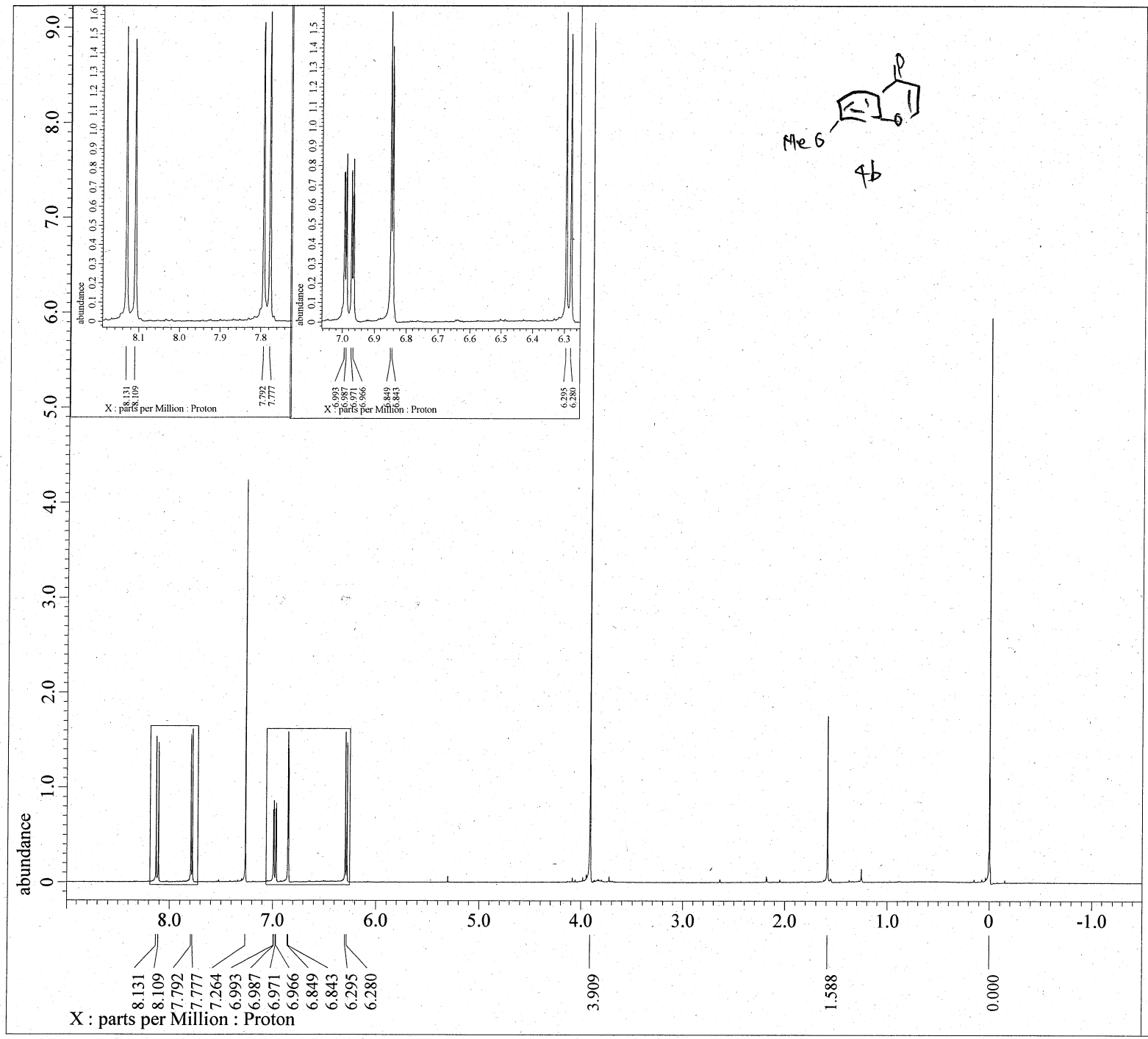

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KND_2131_pure-1.jdf
```

Filename	= KND_2131_pure-2.jdf
Author	= element
Experiment	= single_pulse.ex2
Sample_Id	= S#465571
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 9-DEC-2024 19:03:20
Revision_Time	= 9-DEC-2024 19:12:38
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= 1H
Dim_Title	= 1H
Dim_Units	= [ppm]
Dimensions	= X
Site	= ECS 400
Spectrometer	= JNM-ECS400
Field_Strength	= 9.20197068[T] (390[MHz])
X_Acq_Duration	= 2.228224[s]
X_Domain	= 1H
X_Freq	= 391.78655441[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.44878791[Hz]
X_Sweep	= 7.35294118[kHz]
Irr_Domain	= 1H
Irr_Freq	= 391.78655441[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= 1H
Tri_Freq	= 391.78655441[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 54
Temp_Get	= 18.4[dC]
X_90_Width	= 10.79[us]
X_Acq_Time	= 2.228224[s]
X_Angle	= 45[deg]
X_Atn	= 1.9[dB]
X_Pulse	= 5.395[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.228224[s]



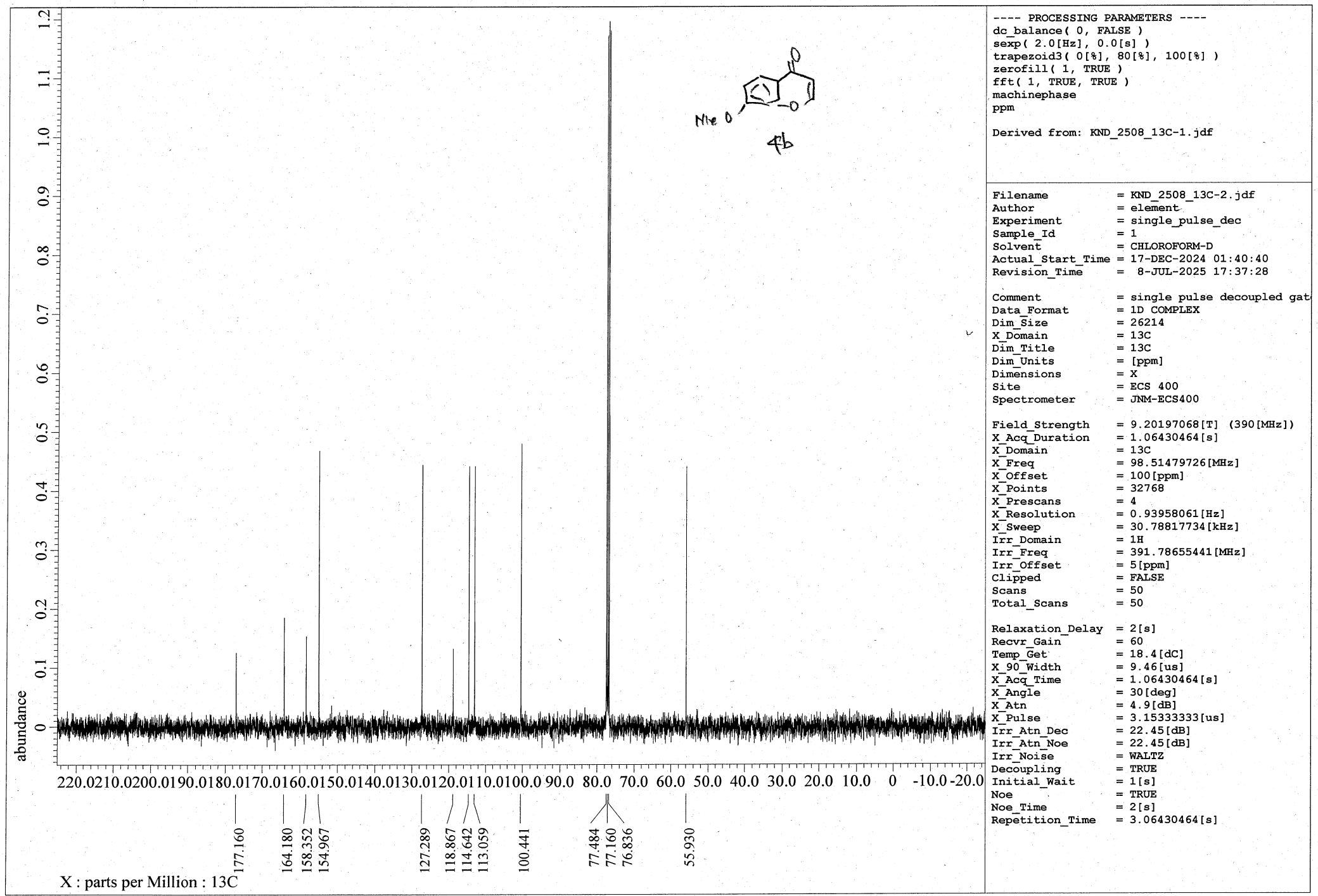

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KND_2131_13C-1.jdf
```

Filename	= KND_2131_13C-2.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= 1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 9-DEC-2024 19:13:26
Revision_Time	= 9-DEC-2024 19:15:27
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	= 44
Total_Scans	= 44
Relaxation_Delay	= 2[s]
Recvr_Gain	= 60
Temp_Get	= 18.6[dC]
X_90_Width	= 9.46[us]
X_Acq_Time	= 1.06430464[s]
X_Angle	= 30[deg]
X_Atn	= 4.9[dB]
X_Pulse	= 3.15333333[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]



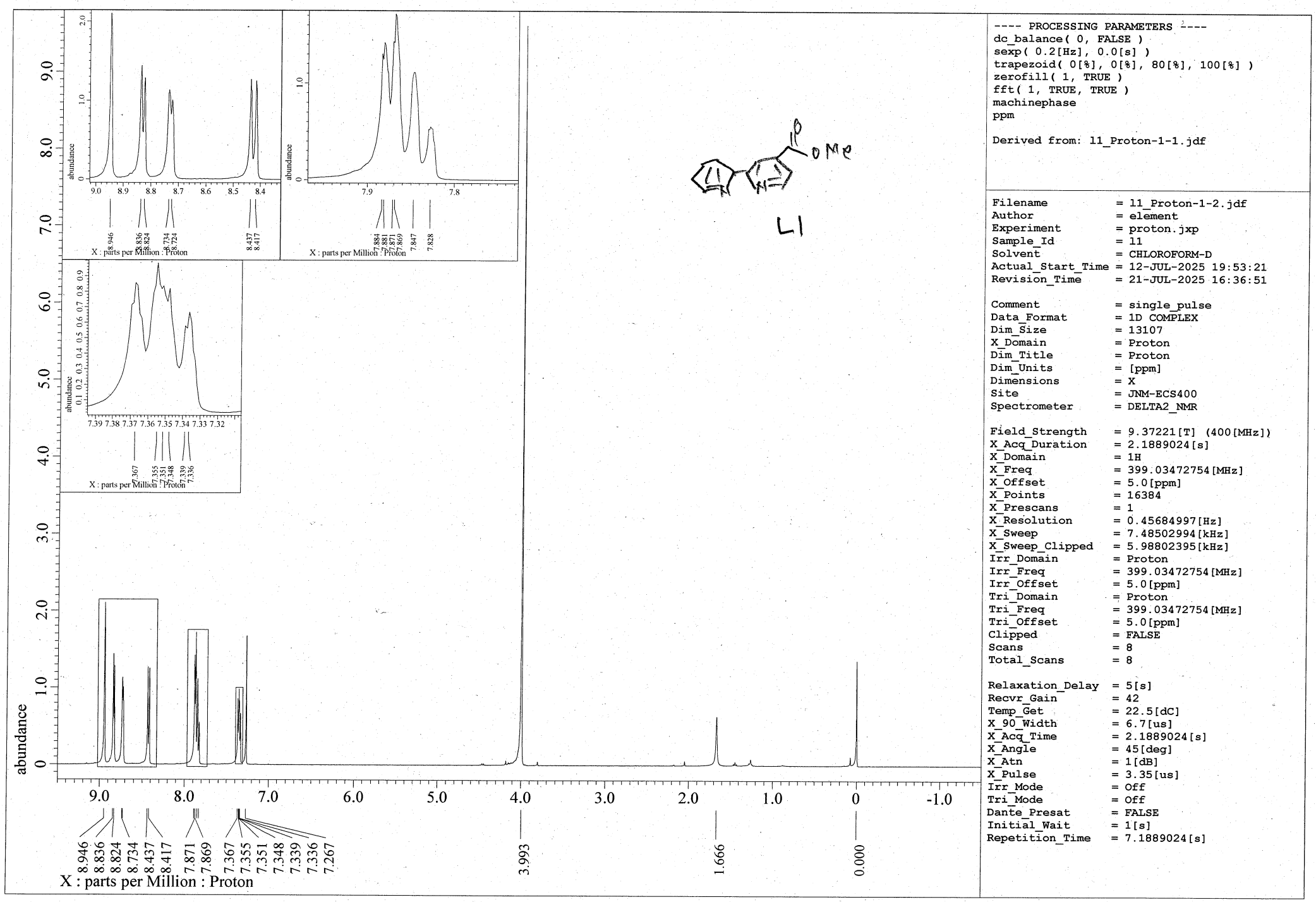

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KND_2508_pure_Proton-1-1.jdf
```

Filename	= KND_2508_pure_Proton-1-2.j
Author	= element
Experiment	= proton.jxp
Sample_Id	= KND_2509_pure
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 16-DEC-2024 19:46:11
Revision_Time	= 8-JUL-2025 16:42:49
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.4073814[T] (400[MHz])
X_Acq_Duration	= 2.18103808[s]
X_Domain	= 1H
X_Freq	= 400.53219825[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45849727[Hz]
X_Sweep	= 7.51201923[kHz]
X_Sweep_Clipped	= 6.00961538[kHz]
Irr_Domain	= Proton
Irr_Freq	= 400.53219825[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 400.53219825[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 46
Temp_Get	= 17.6[dC]
X_90_Width	= 6.7[us]
X_Acq_Time	= 2.18103808[s]
X_Angle	= 45[deg]
X_Atn	= 0.8[dB]
X_Pulse	= 3.35[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.18103808[s]



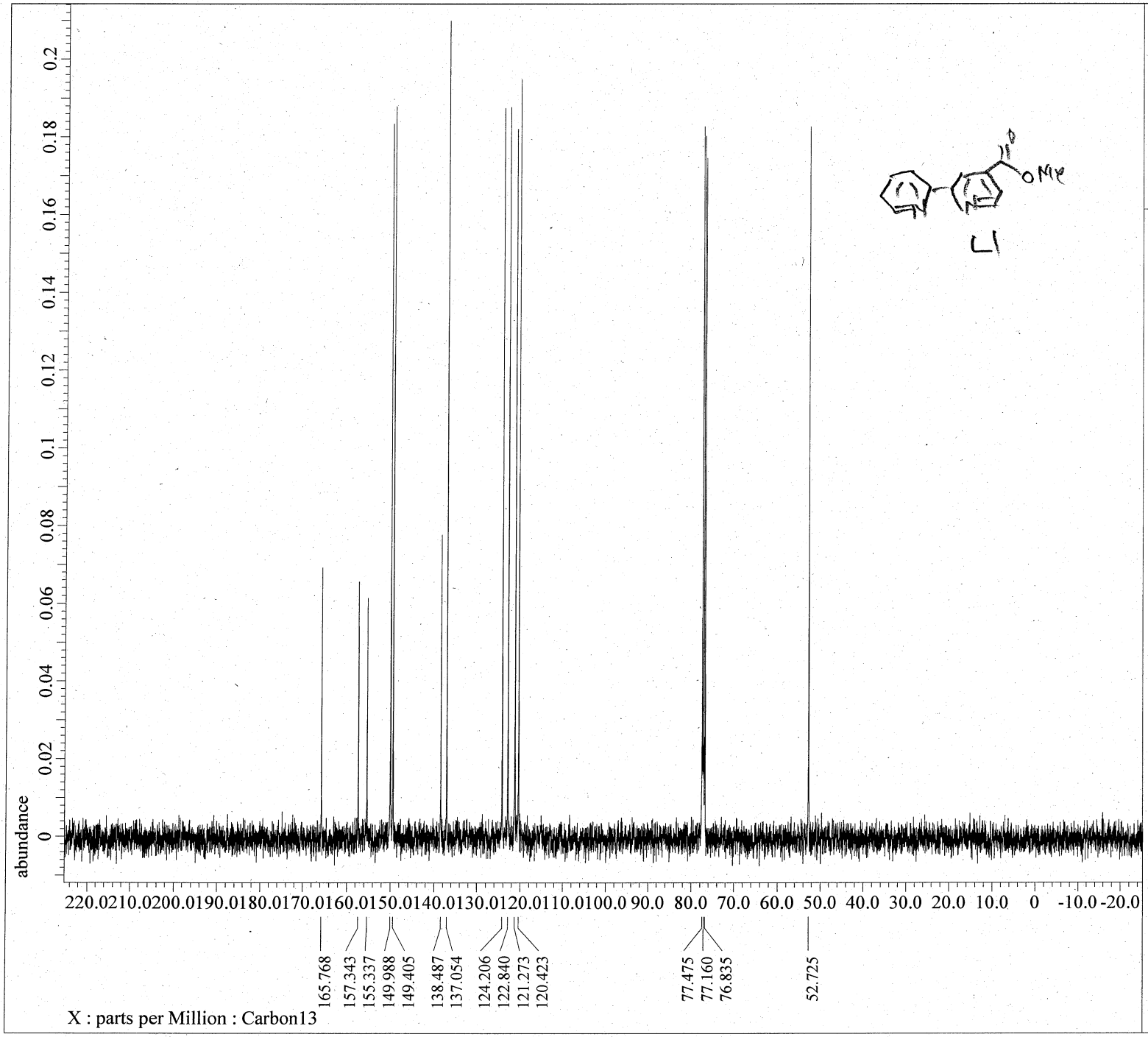

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KND_2508_13C-1.jdf
```

```
Filename            = KND_2508_13C-2.jdf
Author              = element
Experiment          = single_pulse_dec
Sample_Id           = 1
Solvent             = CHLOROFORM-D
Actual_Start_Time   = 17-DEC-2024 01:40:40
Revision_Time       =  8-JUL-2025 17:37:28

Comment             = single pulse decoupled gat
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               = 50
Total_Scans         = 50

Relaxation_Delay    = 2[s]
Recvr_Gain          = 60
Temp_Get            = 18.4[dC]
X_90_Width          = 9.46[us]
X_Acq_Time          = 1.06430464[s]
X_Angle             = 30[deg]
X_Atn               = 4.9[dB]
X_Pulse             = 3.15333333[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, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: 11_Proton-1-1.jdf
```

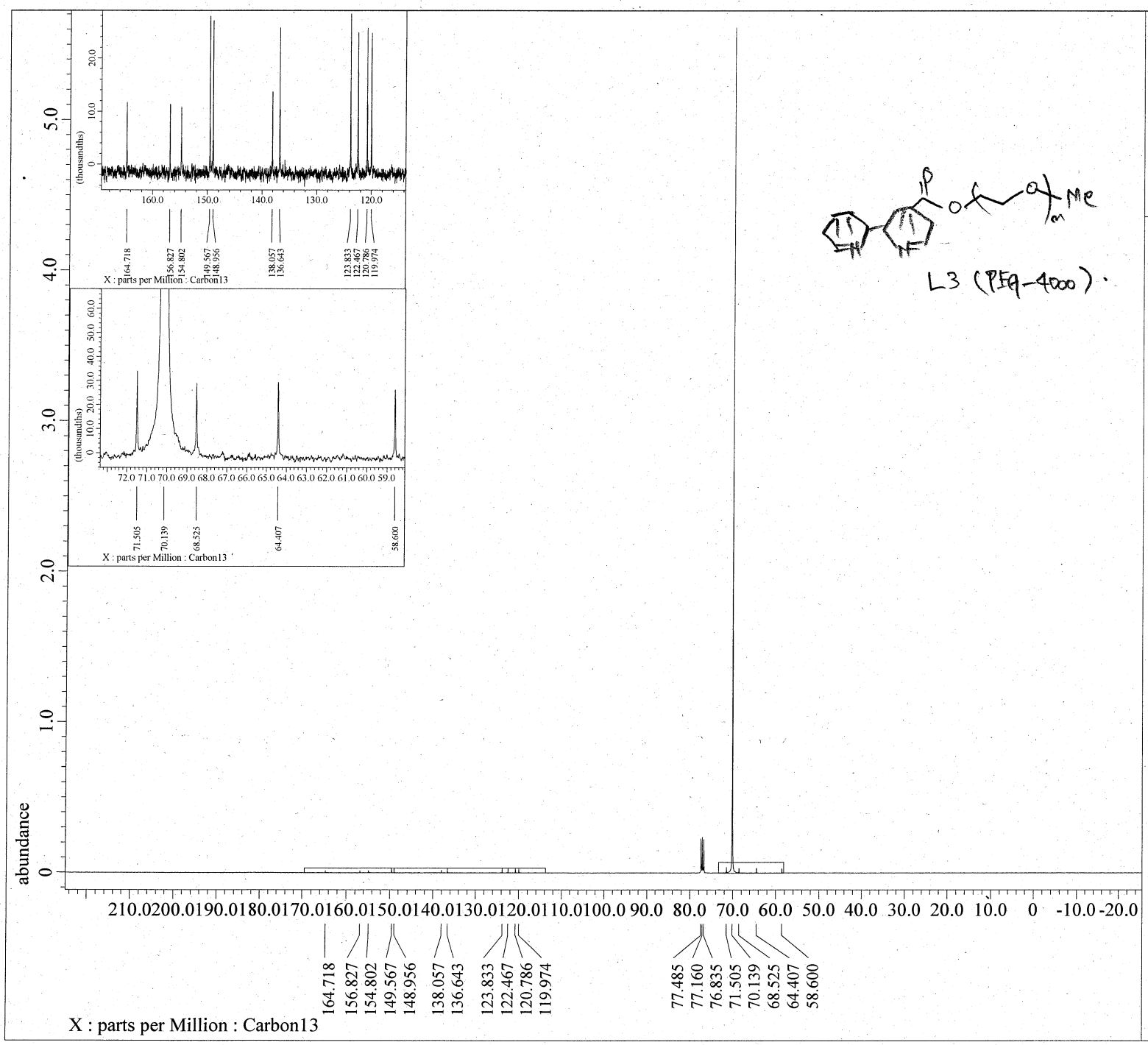
Filename	= 11_Proton-1-2.jdf
Author	= element
Experiment	= proton.jxp
Sample_Id	= 11
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 12-JUL-2025 19:53:21
Revision_Time	= 21-JUL-2025 16:36:51
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
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	= 22.5[dC]
X_90_Width	= 6.7[us]
X_Acq_Time	= 2.1889024[s]
X_Angle	= 45[deg]
X_Atn	= 1[dB]
X_Pulse	= 3.35[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.1889024[s]



L1

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

Derived from: l1_13C_Carbon-1-1.jdf
```

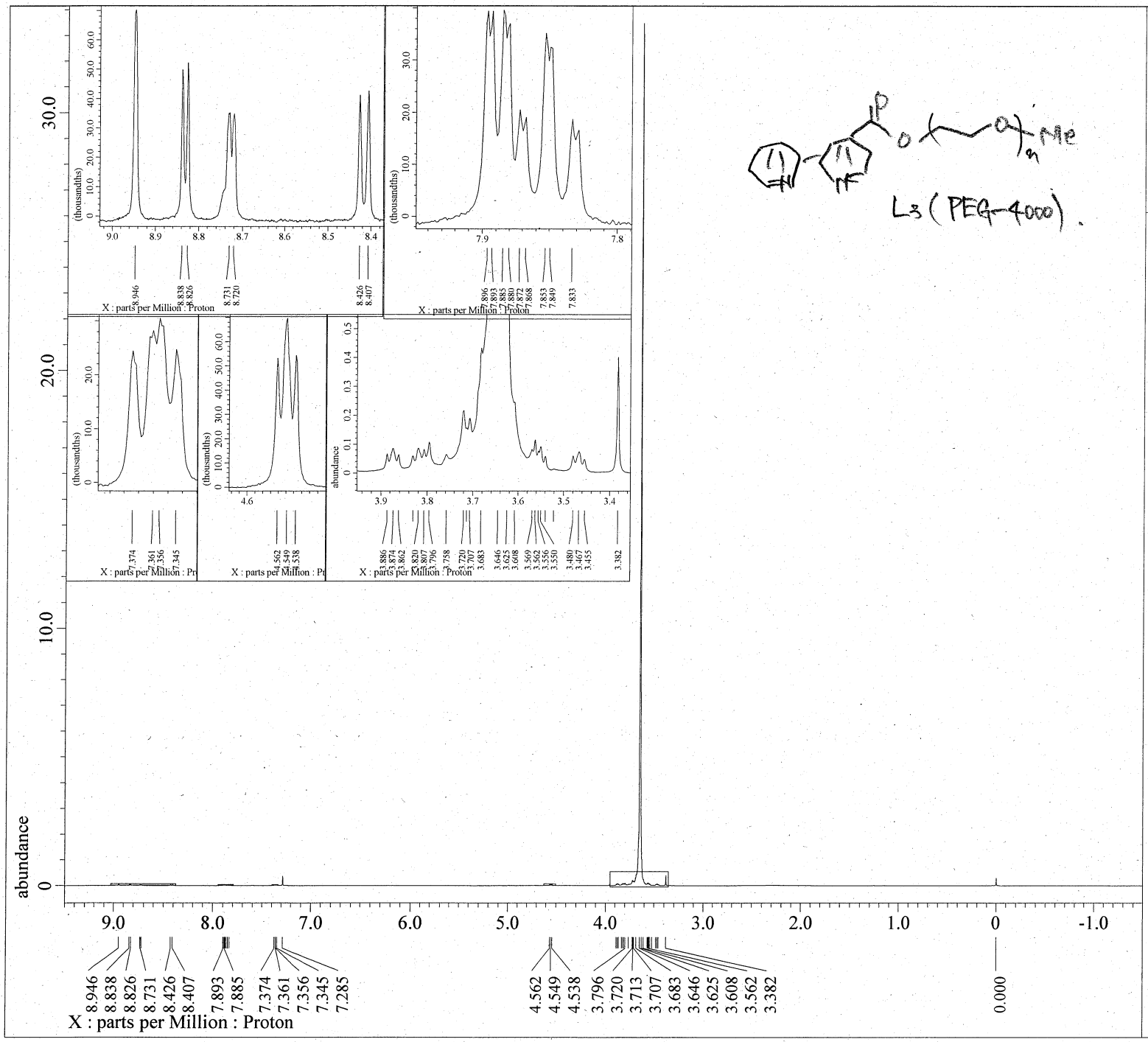
Filename	= l1_13C_Carbon-1-2.jdf
Author	= element
Experiment	= carbon.jxp
Sample_Id	= l1_13C
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 12-JUL-2025 20:09:40
Revision_Time	= 21-JUL-2025 16:42:35
Comment	= single pulse decoupled gat
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECS400
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.37221[T] (400[MHz])
X_Acq_Duration	= 1.04333312[s]
X_Domain	= 13C
X_Freq	= 100.33735165[MHz]
X_Offset	= 100.0[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.95846665[Hz]
X_Sweep	= 31.40703518[kHz]
X_Sweep_Clipped	= 25.12562814[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.03472754[MHz]
Irr_Offset	= 5.0[ppm]
Clipped	= FALSE
Scans	= 123
Total_Scans	= 123
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 22.5[dC]
X_90_Width	= 11.8[us]
X_Acq_Time	= 1.04333312[s]
X_Angle	= 30[deg]
X_Atn	= 5.4[dB]
X_Pulse	= 3.93333333[us]
Irr_Atn_Dec	= 25.823[dB]
Irr_Atn_Noe	= 25.823[dB]
Irr_Noise	= WALTZ
Irr_Pwidth	= 0.115[ms]
Decoupling	= TRUE
Initial_Wait	= 1[s]
Noe	= TRUE
Noe_Time	= 2[s]
Repetition_Time	= 3.04333312[s]



L3 (PEG-4000).

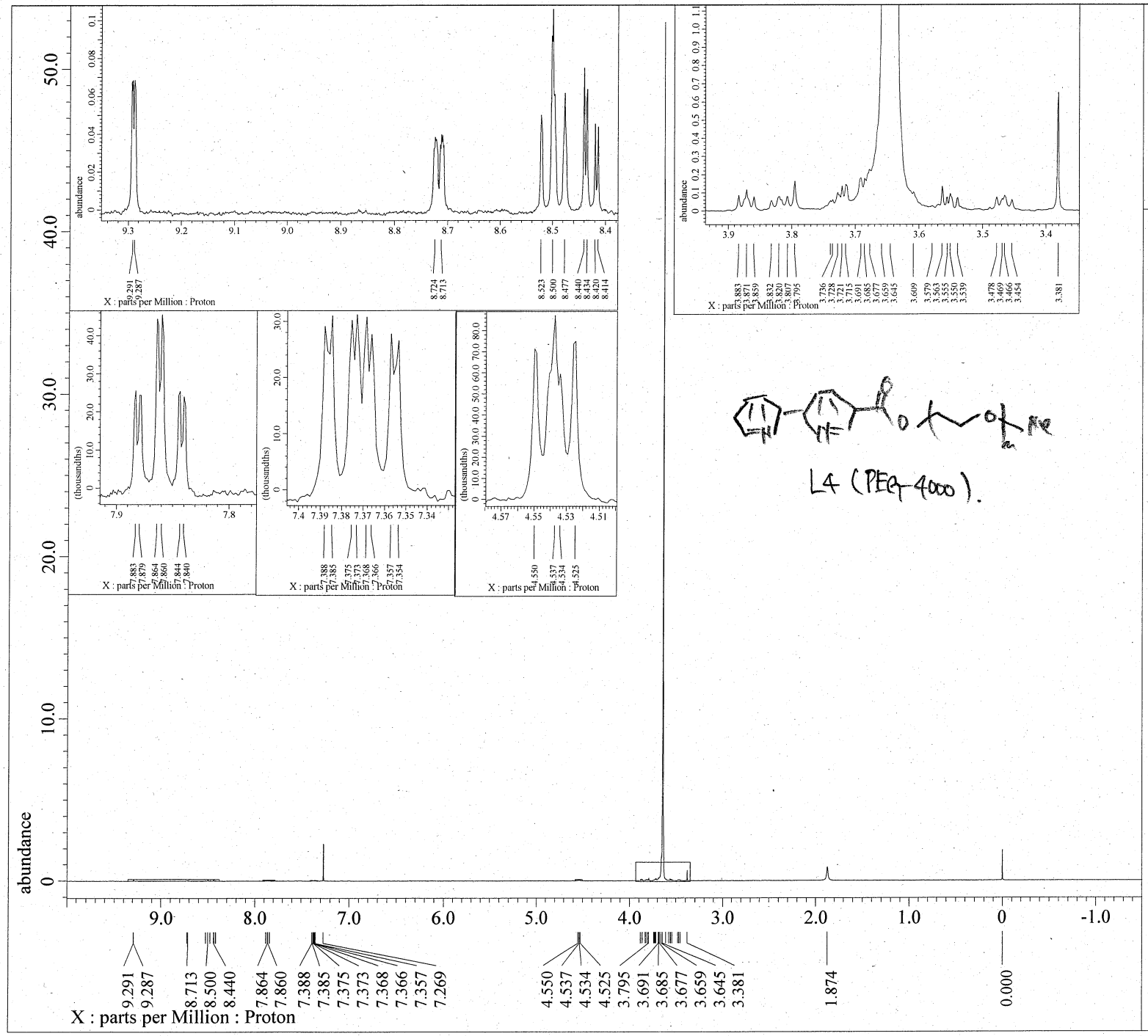
```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: 13_13C_Carbon-1-1.jdf
```

Filename	= 13_13C_Carbon-1-2.jdf
Author	= element
Experiment	= carbon.jxp
Sample_Id	= 13_13C
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 12-JUL-2025 23:08:41
Revision_Time	= 21-JUL-2025 18:42:53
Comment	= single pulse decoupled gat
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECS400
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.37221[T] (400[MHz])
X_Acq_Duration	= 1.04333312[s]
X_Domain	= 13C
X_Freq	= 100.33735165[MHz]
X_Offset	= 100.0[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.95846665[Hz]
X_Sweep	= 31.40703518[kHz]
X_Sweep_Clipped	= 25.12562814[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.03472754[MHz]
Irr_Offset	= 5.0[ppm]
Clipped	= FALSE
Scans	= 1245
Total_Scans	= 1245
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 22.2[dC]
X_90_Width	= 11.8[us]
X_Acq_Time	= 1.04333312[s]
X_Angle	= 30[deg]
X_Atn	= 5.4[dB]
X_Pulse	= 3.93333333[us]
Irr_Atn_Dec	= 25.823[dB]
Irr_Atn_Noe	= 25.823[dB]
Irr_Noise	= WALTZ
Irr_Pwidth	= 0.115[ms]
Decoupling	= TRUE
Initial_Wait	= 1[s]
Noe	= TRUE
Noe_Time	= 2[s]
Repetition_Time	= 3.04333312[s]



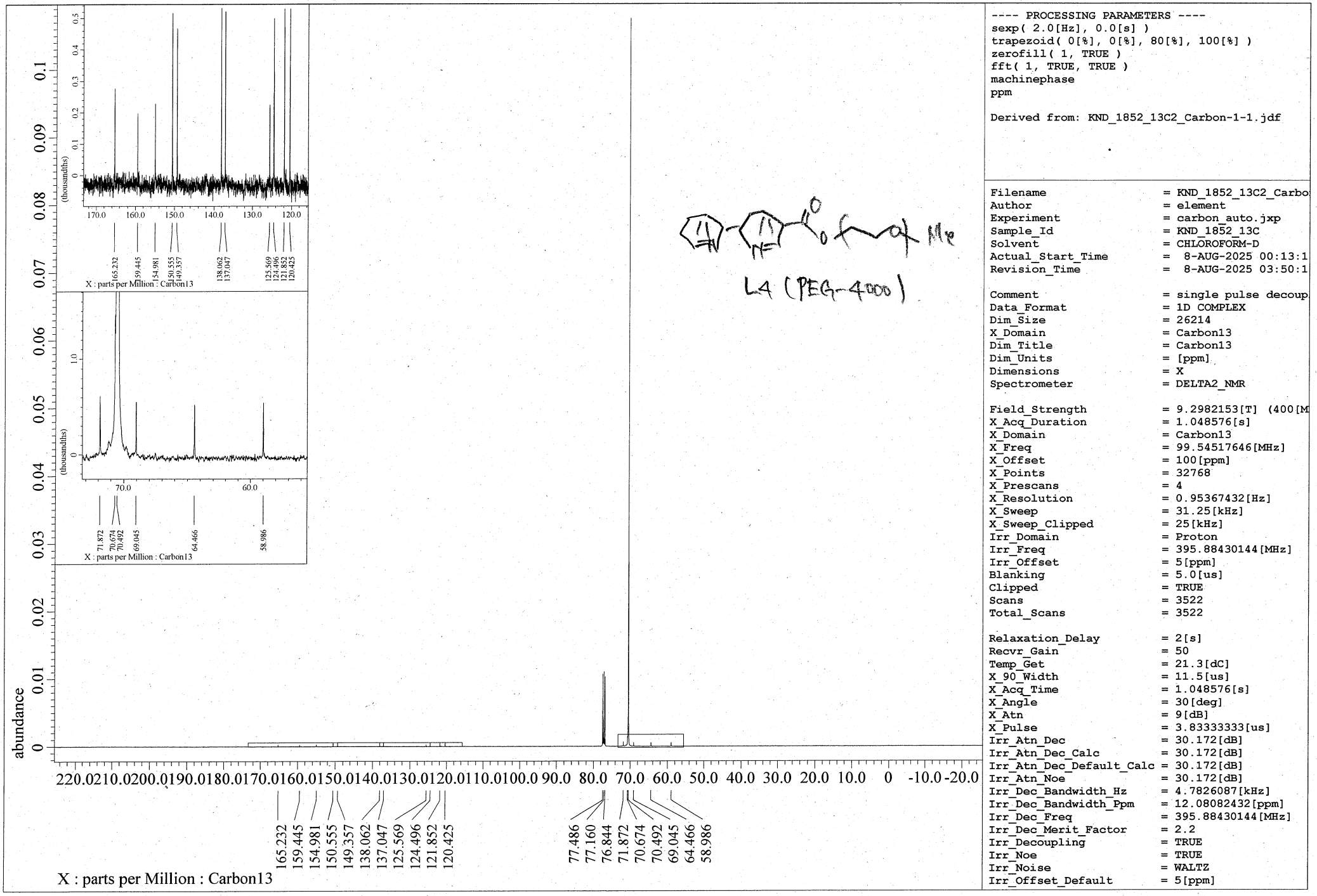

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: 13_Proton-1-1.jdf
```

Filename	= 13_Proton-1-2.jdf
Author	= element
Experiment	= proton.jxp
Sample_Id	= 13
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 12-JUL-2025 22:10:38
Revision_Time	= 21-JUL-2025 18:40:43
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	= 34
Temp_Get	= 19.9[dC]
X_90_Width	= 6.7[us]
X_Acq_Time	= 2.18103808[s]
X_Angle	= 45[deg]
X_Atn	= 0.8[dB]
X_Pulse	= 3.35[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.18103808[s]



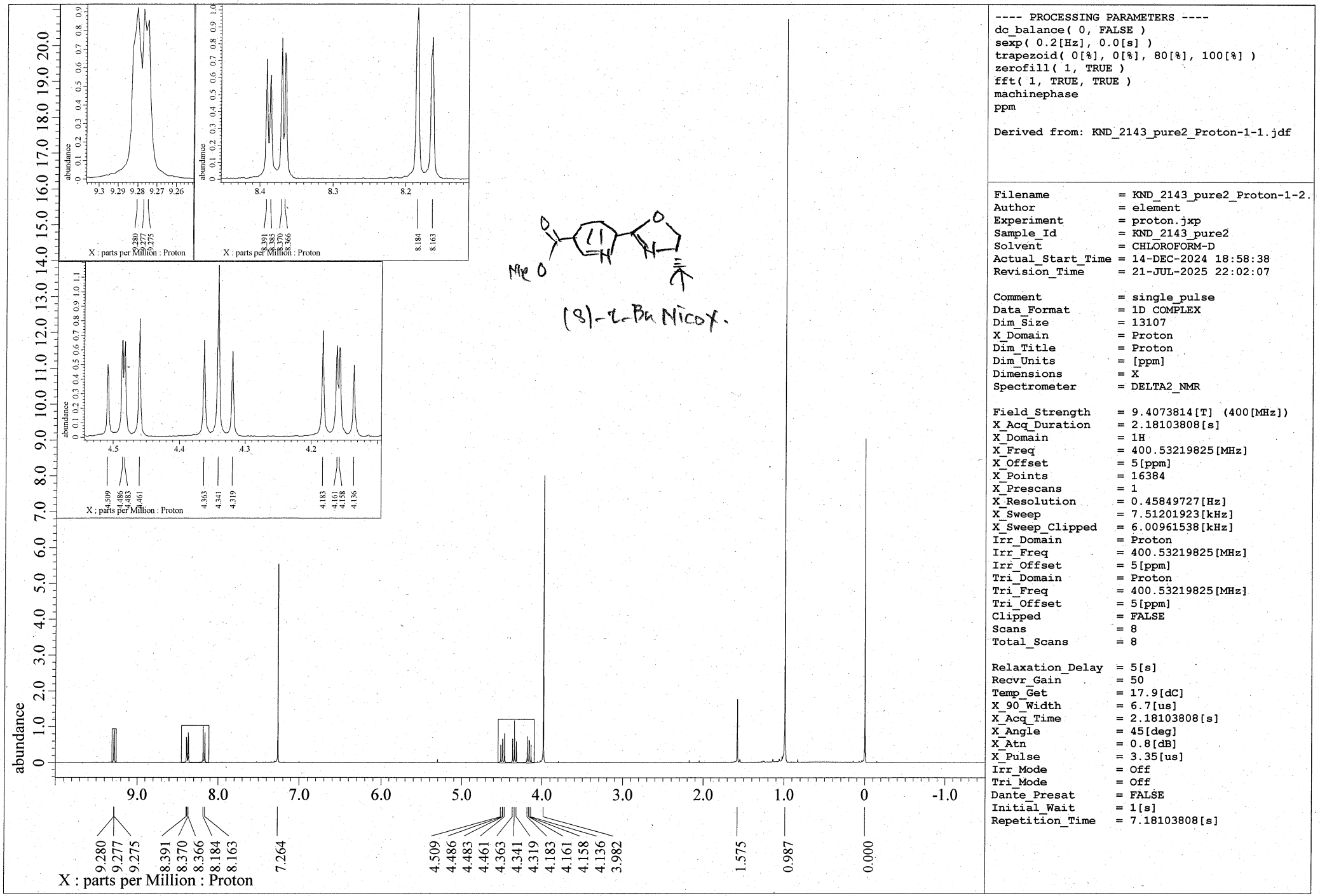

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KND_1852_pure_Proton-1-1.jdf
```

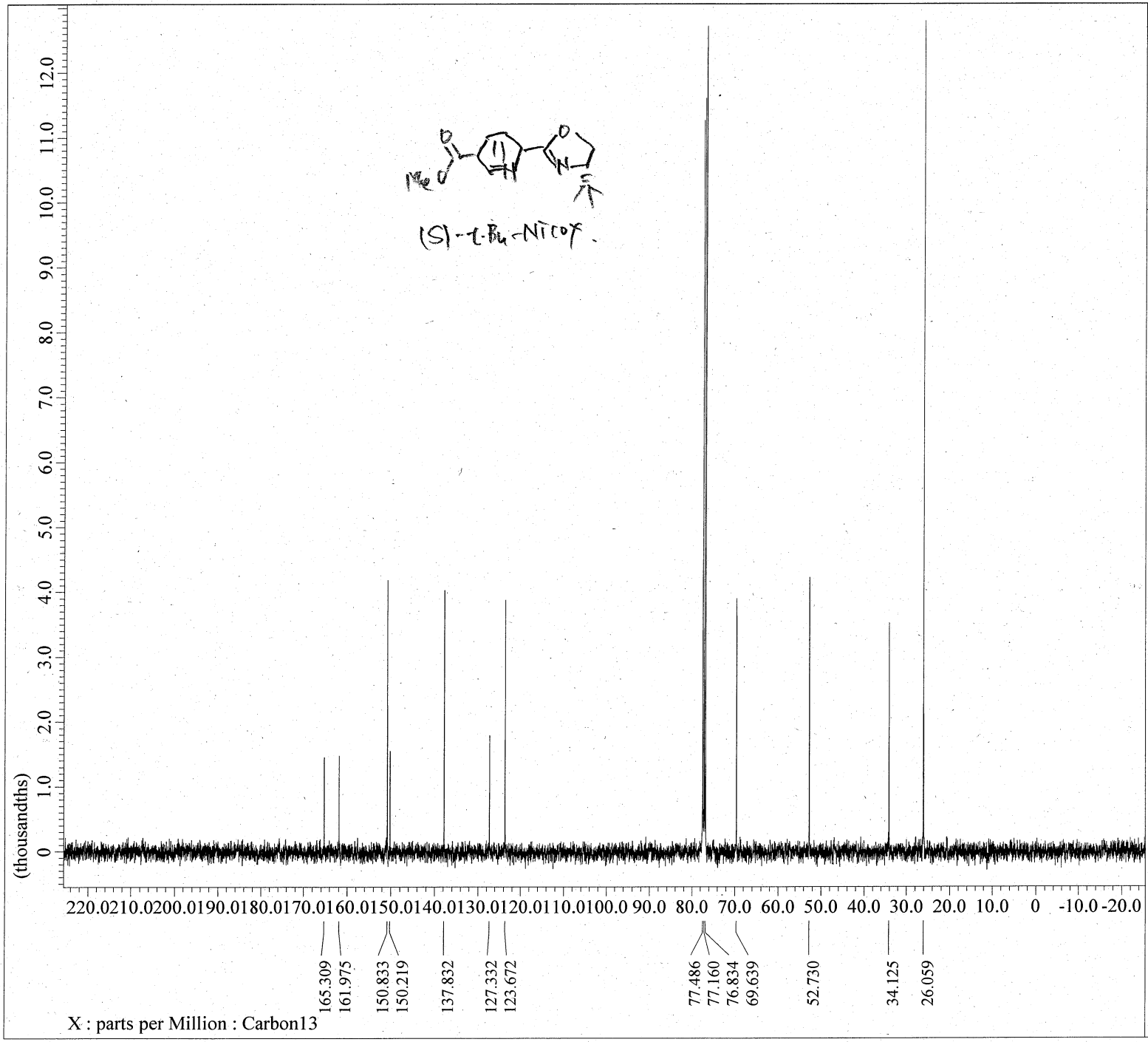
Filename	= KND_1852_pure_Proton-1-2.j
Author	= element
Experiment	= proton.jxp
Sample_Id	= KND_1852_pure
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 15-JUL-2025 00:04:37
Revision_Time	= 21-JUL-2025 21:49:09
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= 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	= 36
Temp_Get	= 23.2[dC]
X_90_Width	= 6.7[us]
X_Acq_Time	= 2.1889024[s]
X_Angle	= 45[deg]
X_Atn	= 1[dB]
X_Pulse	= 3.35[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.1889024[s]




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

Derived from: KND_1852_13C2_Carbon-1-1.jdf
```

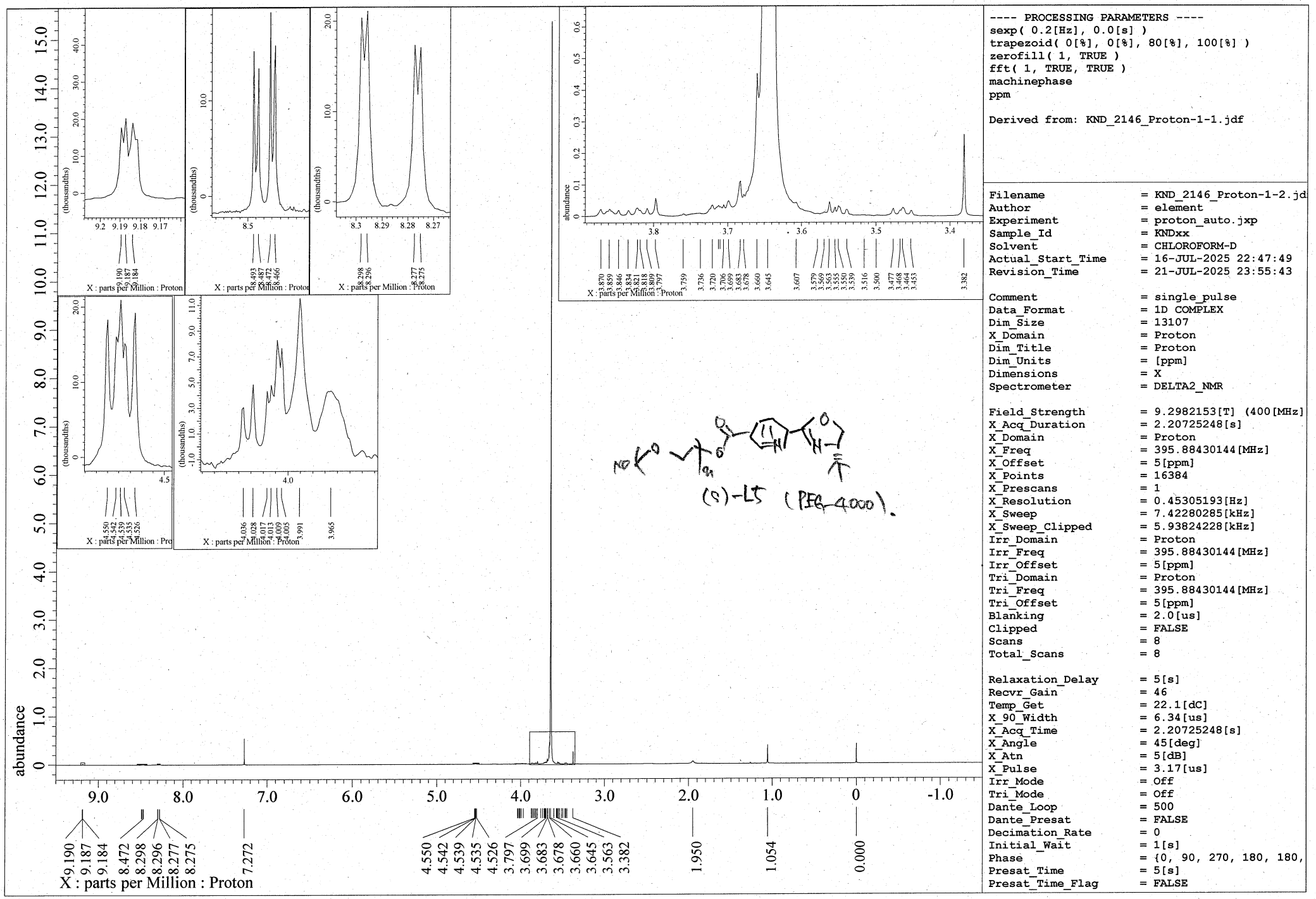
Filename	= KND_1852_13C2_Carbo
Author	= element
Experiment	= carbon_auto.jxp
Sample_Id	= KND_1852_13C
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 8-AUG-2025 00:13:1
Revision_Time	= 8-AUG-2025 03:50:1
Comment	= single pulse decoup
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.2982153[T] (400[M
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	= 5.0[us]
Clipped	= TRUE
Scans	= 3522
Total_Scans	= 3522
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 21.3[dC]
X_90_Width	= 11.5[us]
X_Acq_Time	= 1.048576[s]
X_Angle	= 30[deg]
X_Atn	= 9[dB]
X_Pulse	= 3.83333333[us]
Irr_Atn_Dec	= 30.172[dB]
Irr_Atn_Dec_Calc	= 30.172[dB]
Irr_Atn_Dec_Default_Calc	= 30.172[dB]
Irr_Atn_Noe	= 30.172[dB]
Irr_Dec_Bandwidth_Hz	= 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.08082432[ppm]
Irr_Dec_Freq	= 395.88430144[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]


---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: KND_2143_pure2_Proton-1-1.jdf
Filename = KND_2143_pure2_Proton-1-2.
Author = element
Experiment = proton.jxp
Sample_Id = KND_2143_pure2
Solvent = CHLOROFORM-D
Actual_Start_Time = 14-DEC-2024 18:58:38
Revision_Time = 21-JUL-2025 22:02:07
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 = 17.9[dC]
X_90_Width = 6.7[us]
X_Acq_Time = 2.18103808[s]
X_Angle = 45[deg]
X_Atn = 0.8[dB]
X_Pulse = 3.35[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 7.18103808[s]
(S)-t-Bu NicoX.
abundance
X : parts per Million : Proton
9.280 9.277 9.275 8.391 8.370 8.366 8.184 8.163 7.264 4.509 4.486 4.483 4.461 4.363 4.341 4.319 4.183 4.161 4.158 4.136 3.982 1.575 0.987 0.000



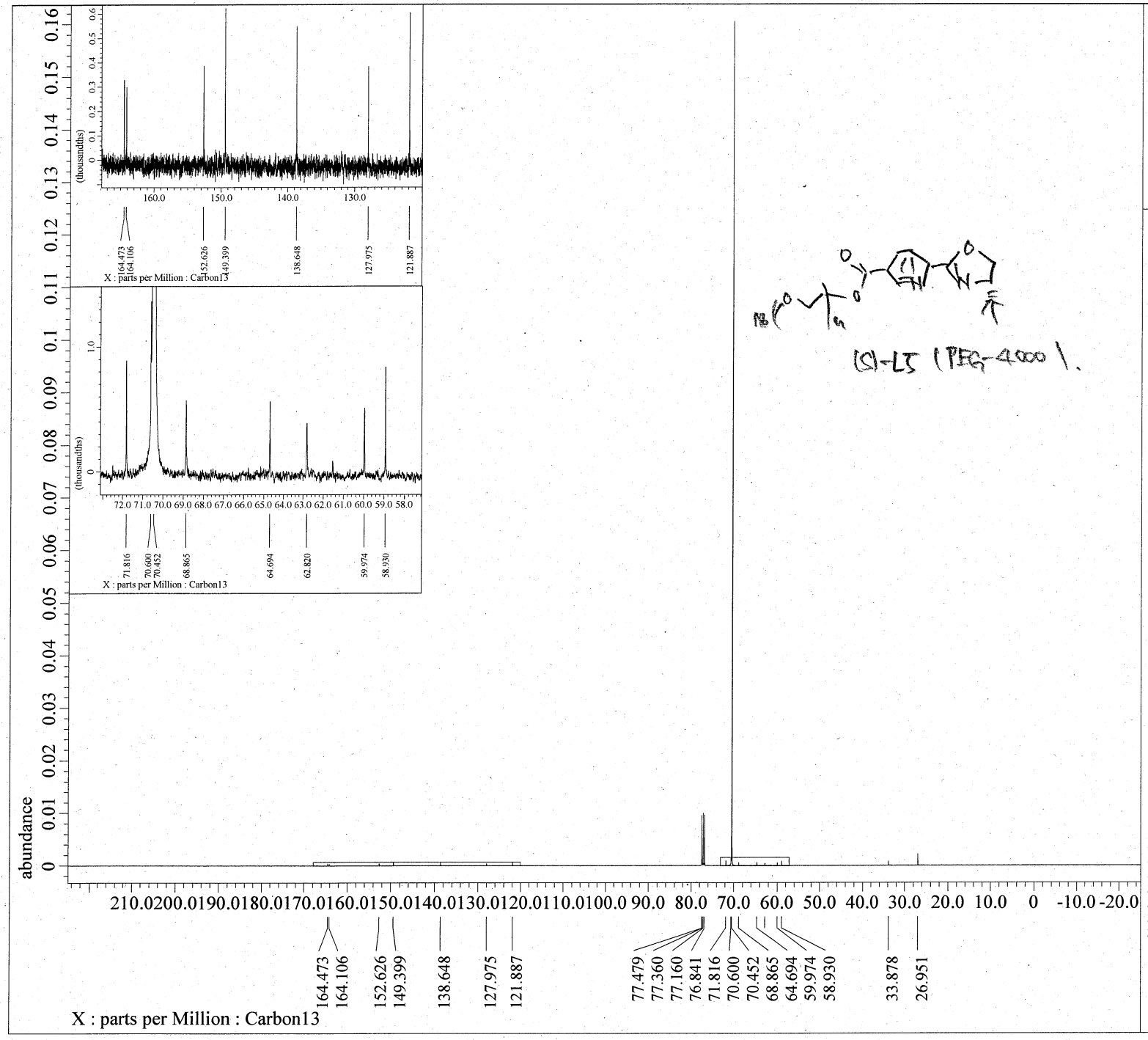

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KND_2143_13C_Carbon-1-1.jdf
```

Filename	= KND_2143_13C_Carbon
Author	= element
Experiment	= carbon_auto.jxp
Sample_Id	= KND_2143_13C
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 24-JUL-2025 22:20:5
Revision_Time	= 29-JUL-2025 22:41:3
Comment	= single pulse decoup
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.2982153[T] (400[M
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	= 5.0[us]
Clipped	= FALSE
Scans	= 152
Total_Scans	= 152
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 22.7[dC]
X_90_Width	= 11.5[us]
X_Acq_Time	= 1.048576[s]
X_Angle	= 30[deg]
X_Atn	= 9[dB]
X_Pulse	= 3.83333333[us]
Irr_Atn_Dec	= 30.172[dB]
Irr_Atn_Dec_Calc	= 30.172[dB]
Irr_Atn_Dec_Default_Calc	= 30.172[dB]
Irr_Atn_Noe	= 30.172[dB]
Irr_Dec_Bandwidth_Hz	= 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.08082432[ppm]
Irr_Dec_Freq	= 395.88430144[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]




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

Derived from: KND_2146_Proton-1-1.jdf
```

Filename	= KND_2146_Proton-1-2.jd
Author	= element
Experiment	= proton_auto.jxp
Sample_Id	= KNDxx
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 16-JUL-2025 22:47:49
Revision_Time	= 21-JUL-2025 23:55:43
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	= 9.2982153[T] (400[MHz]
X_Acq_Duration	= 2.20725248[s]
X_Domain	= Proton
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]
X_Sweep_Clipped	= 5.93824228[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 395.88430144[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2.0[us]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 46
Temp_Get	= 22.1[dC]
X_90_Width	= 6.34[us]
X_Acq_Time	= 2.20725248[s]
X_Angle	= 45[deg]
X_Atn	= 5[dB]
X_Pulse	= 3.17[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 500
Dante_Presat	= FALSE
Decimation_Rate	= 0
Initial_Wait	= 1[s]
Phase	= {0, 90, 270, 180, 180,
Presat_Time	= 5[s]
Presat_Time_Flag	= FALSE




```
---- PROCESSING PARAMETERS ----
sexp( 0.99975[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 2, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KND_2146_13C_Carbon-1-1.jdf
```

Filename	= KND_2146_13C_Carbon
Author	= element
Experiment	= carbon.jxp
Sample_Id	= KND_2146_13C
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 16-JUL-2025 22:50:1
Revision_Time	= 21-JUL-2025 23:45:0
Data_Format	= 1D COMPLEX
Dim_Size	= 52429
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= NM-70010S4L1
Field_Strength	= 9.389766[T] (400[MH
X_Acq_Duration	= 1.0002536[s]
X_Domain	= Carbon13
X_Freq	= 100.52530333[MHz]
X_Offset	= 100[ppm]
X_Points	= 31415
X_Points_Input	= 25132
X_Prescans	= 4
X_Resolution	= 0.99974646[Hz]
X_Sweep	= 31.40703518[kHz]
X_Sweep_Clipped	= 25.12562814[kHz]
X_Sweep_Input	= 250[ppm]
Irr_Domain	= Proton
Irr_Freq	= 399.78219838[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Carbon13
Tri_Freq	= 100.52530333[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 5.0[us]
Clipped	= FALSE
Scans	= 1024
Total_Scans	= 1024
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 21.4[dC]
X_90_Width	= 11.39[us]
X_Acq_Time	= 1.0002536[s]
X_Angle	= 30[deg]
X_Atn	= 8[dB]
X_Data_Points	= 32768
X_Points_Default	= 22434
X_Pulse	= 3.79666667[us]
Irr_Atn_Dec	= 29.13[dB]
Irr_Atn_Dec_Calc	= 29.13[dB]
Irr_Atn_Noe	= 29.13[dB]
Irr_Bandwidth	= 4.7826087[kHz]
Irr_Bandwidth_Ppm	= 11.96303566[ppm]
Irr_Corresp_Pw90	= 0.115[ms]