Mechanochemistry enabling highly efficient Birch reduction using sodium lumps and D-(+)-glucose

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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 were also purchased from commercial suppliers and dried over molecular sieves (MS 4A) prior to use. 1,3-Dimethyl-2-imidazolidinone (DMI), which is a liquid additive for the Birch reduction, was used as received. All mechanochemical reactions were carried out using grinding vessels in a Retsch MM400 mill (Figure S1). Both jars (10 mL) and balls (10 mm) are made of stainless (SUS400B and SUS420J2, respectively) (Figure S2). NMR spectra were recorded on JEOL JNM-EC X400P and JNM-ECS400 spectrometers (^{1}H: 396 or 399 or 401 MHz, ^{13}C: 99 or 100 or 101 MHz). Tetramethylsilane (^{1}H), $CDCl_3$ (^{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. High-resolution mass spectra were recorded at the Global Facility Center, Hokkaido University.

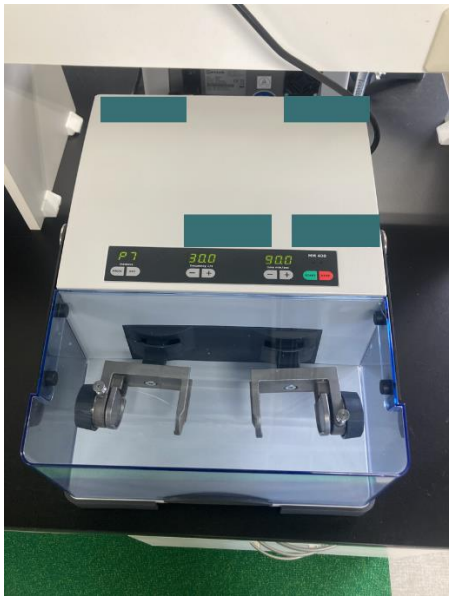
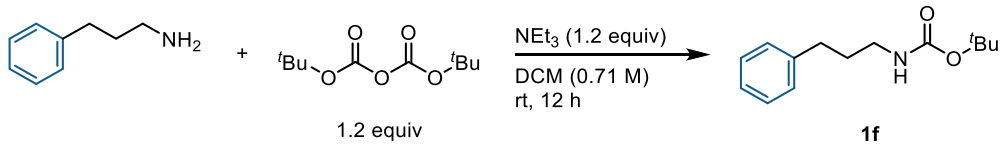


Figure S1. Retsch MM400 used in this study.

Figure S2. Stainless jar (10 mL) and balls (10 mm) used in this study.

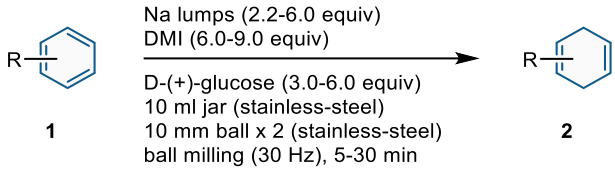
2. Synthesis of 1f



In a vacuum-dried screw nacked, 2-phenylethan-1-amine (5.0 mmol, 676.1 mg) and NEt_3 (6.0 mmol, 0.84 ml) were dissolved in dichloromethane (3.0 mL). *tert*-Butyl dicarbonate (6.0 mmol, 1.38ml) dissolved in dichloromethane (4.0 ml) was added to the mixture and then stirred at room temperature for 12 hours. After the reaction was completed, the resulting suspension was diluted by H_2O. The mixture was extracted with EtOAc three times and dried over Mg_2SO_4. After filtration, the solvents were removed using a rotary evaporator. The crude mixture was then purified by flash column chromatography (SiO_2, EtOAc/hexane, 0:100–10:90) to give **1f** as a colorless oil (1.099 g, 4.67 mmol, 93% yield).

^{1}H NMR (399 MHz, $CDCl_3$, δ): 1.45 (s, 9H), 1.81 (quint, J = 7.5 Hz, 2H), 2.64 (t, J = 7.8 Hz, 2H), 3.06–3.22 (m, 2H), 4.53 (brs, 1H), 7.19 (t, J = 7.2 Hz, 3H), 7.26–7.31 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 28.6 (CH_3), 31.9 (CH_2), 33.3 (CH_2), 40.3 (CH_2), 78.8 (*C*), 126.0 (*C*H), 128.5 (*C*H), 141.8 (*C*), 156.3 (*C*). HRMS-ESI (*m*/*z*): $[M+Na]^+$ calcd for $C_{14}H_{21}O_2NNa$, 258.1465; found, 258,1460.

3. General procedure of mechanochemical Birch reduction



Arene (1.0 mmol, 1.0 equiv) and D-(+)-glucose (3.0–6.0 equiv) were placed in a stainless-steel milling jar (10 mL) with two stainless-steel balls (10 mm, diameter) in air. Sodium lumps (2.2–6.0 equiv) were cut off and weighed in air after wiping off the mineral oil on it with paper, which was then cut into small pieces (diameter: ca. 4–5 mm) and directly added into the jar. Then, 1,3-dimethyl-2-imidazolidinone (DMI) (6.0–9.0 equiv) was added to the jar via syringes. After the jar was closed without purging with inert gas, the jar was placed in the ball mill (Retsch MM 400, 5–30 min, 30 Hz). After grinding, the jar was opened in air. The mixture was quenched with MeOH and H_2O in the jar, transferred into a funnel, and extracted with typically EtOAc (20 mL × 3). The resultant solution was dried over $MgSO_4$, filtrated, and evaporated in vacuo. Crude yields of the corresponding products were determined by ^1H NMR analysis with 1,1,2,2-tetrachloroethane as the internal standard. For compounds that were able to be isolated, the crude mixture was purified by flash column chromatography to obtain the desired products with isolated yield.

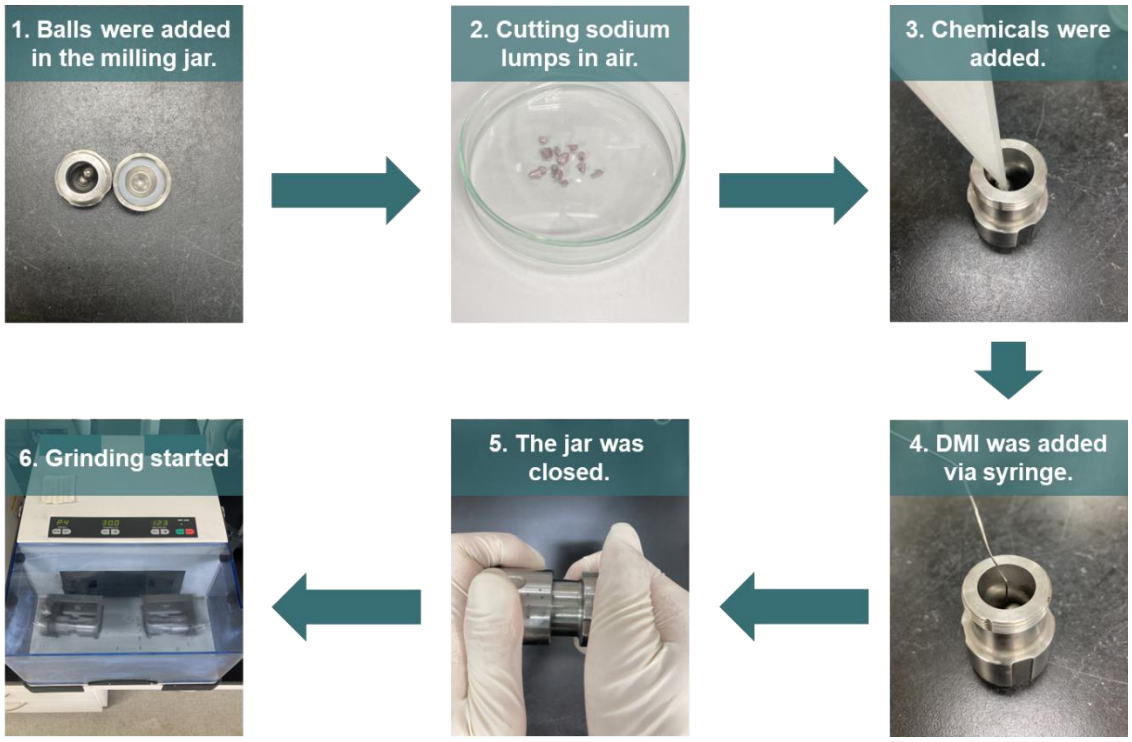
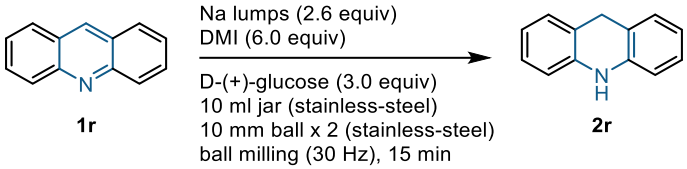


Figure S3. Set-up procedure for mechanochemical Birch reduction.

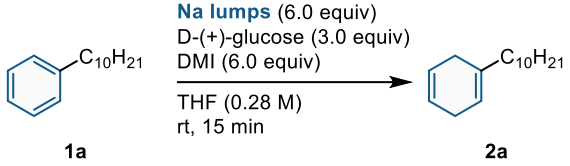
4. Scale-up synthesis of 2r



Scale-up synthesis was carried out by conducting two 3 mmol scale reactions simultaneously according to general procedure. **1r** (3.0 mmol, 537.1 mg), sodium lumps (7.7 mmol, 176.7 mg), D-(+)-glucose (1624.3 mg, 9.0 mmol) and DMI (2.1 ml, 18.0 mmol) were placed in a one stainless-steel milling jar (10 mL) with two stainless-steel balls (10 mm, diameter) in air. In another jar with two balls, **1r** (3.0 mmol, 536.0 mg), sodium lumps (7.8 mmol, 179.2 mg), D-(+)-glucose (1621.7 mg, 9.0 mmol), and DMI (2.1 mL, 18.0 mmol) were placed. After two jars were closed without purging with inert gas, the jars were placed in one ball mill (Retsch MM 400, 15 min, 30 Hz). After grinding simultaneously, the jars were opened in air. The mixtures were quenched with MeOH and H_2O in the jars, transferred into one funnel, and extracted with EtOAc. The resultant solution was dried over $MgSO_4$, filtrated, and evaporated in vacuo. The crude product was purified by flash column chromatography (SiO_2, hexane/EtOAc, 10:90) to obtain **2r** (1029.9 mg, 5.7 mmol, 95%) as a white solid.

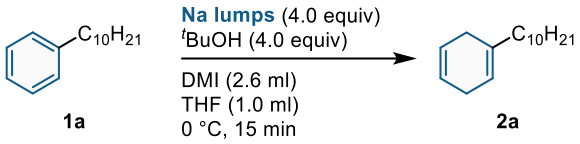
5. Experimental procedures with test tube

Procedure A: Our developed conditions in THF



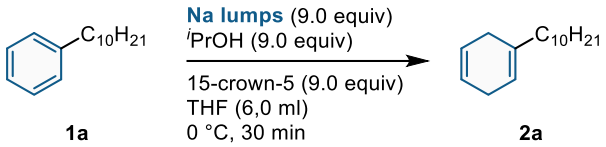
D-(+)-Glucose (3.0 mmol, 543.7 mg) was placed in an oven-dried reaction vial. Sodium lump (6.0 mmol, 139.0 mg) was cut off and weighed in air after wiping off the mineral oil on it with paper, which was then cut into small pieces and directly added to the vial. After the vial was sealed with a screw 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. THF (3.6 mL), **1a** (1.0 mmol, 218.0 mg), and DMI (6.0 mmol, 0.69 mL) were added into the vial via a syringe through the rubber septum. After stirring at room temperature for 15 min, the mixture was quenched with MeOH and H_2O and then extracted with pentane. The resultant solution was dried over $MgSO_4$, filtrated, and evaporated in vacuo. The crude yield of the corresponding products was determined by ^1H NMR analysis with 1,1,2,2-tetrachloroethane as the internal standard. In this case, no product formation was observed.

Procedure B: Using Na lumps instead of sodium dispersion under Takai and Asako's conditions



The reaction was performed according to the literature procedure using sodium lumps with sodium dispersion.[1] Sodium lump (4.0 mmol, 92.0 mg) was cut off and weighed in air after wiping off the mineral oil on it with paper, which was then cut into small pieces and directly added to the 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. THF (1.0 mL), DMI (2.6 mL), and **1a** (1.0 mmol, 219.5 mg) were added into the vial via a syringe through the rubber septum at 0 °C. Next, ^{t}BuOH (4.0 mmol, 380 μL) was added dropwise at the same temperature. After stirring at 0 °C for 15 min, the mixture was quenched with MeOH and H_2O and then extracted with pentane. The resultant solution was dried over $MgSO_4$, filtrated, and evaporated in vacuo. The crude yield of the corresponding products was determined by ^1H NMR analysis with 1,1,2,2-tetrachloroethane as the internal standard. In this case, no product formation was observed.

Procedure C: Using Na lumps instead of sodium dispersion under An's conditions



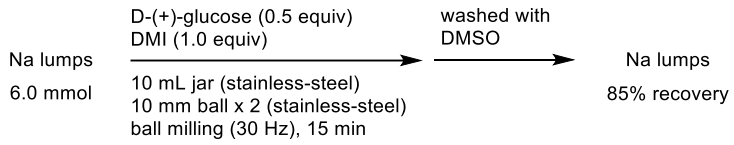
The reaction was performed according to the literature procedure using sodium lumps with sodium dispersion.[2] Sodium lump (9.0 mmol, 210.0 mg) was cut off and weighed in air after wiping off the mineral oil on it with paper, which was then cut into small pieces and directly added to the oven-dried reaction 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. THF (6.0 mL), 15-crown-5 (9.0 mmol, 1.78 mL), and **1a** (1.0 mmol, 219.5 mg) were added into the vial via a syringe through the rubber septum at 0 °C. Next, ^{i}PrOH (9.0 mmol, 680 µL) was added dropwise at the same temperature. After stirring at 0 °C for 30 min, the mixture was quenched with MeOH and H_2O and then extracted with pentane. The resultant solution was dried over $MgSO_4$, filtrated, and evaporated in vacuo. The crude yield of the corresponding products was determined by ^{1}H NMR analysis with 1,1,2,2-tetrachloroethane as the internal standard. In this case, 9% of **2a** was observed.

6. Additional experimental results

a. Reaction in the absence of substrates

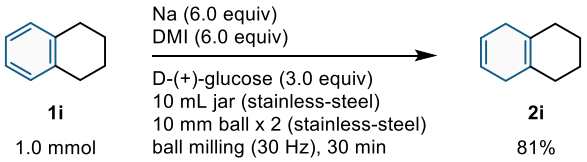
A reaction in the absence of substrates was carried out in order to examine how much sodium might react with D-(+)-glucose (Scheme S1). After ball-milling, the obtained mixture was washed with dimethyl sulfoxide (DMSO) to remove unreacted D-(+)-glucose and its sodiated derivatives. We found that 85% of sodium metal could be recovered, suggesting that sodium metal does not suffer from significant consumption due to reacting with D-(+)-glucose. Therefore, we suggest that the excess of sodium metal is required under the applied mechanochemical conditions due to the relatively moderate reducing properties of sodium metal and not on account of its reaction with D-(+)-glucose.

Scheme S1. Reaction of sodium metal with D-(+)-glucose in the absence of substrates.



b. Product isolation by simple washing

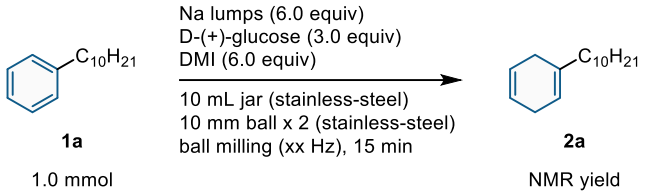
Although most of the products were isolated by column chromatography on silica gel, non-polar products such as **2i** can be isolated by simple washing the crude mixture with water. This result highlights the practical utility of this mechanochemical protocol.



1i (0.98 mmol, 129.6 mg) and D-(+)-glucose (3.0 mmol, 543.3 mg) were placed in a stainless-steel milling jar (10 mL) with two stainless-steel balls (diameter: 10 mm) in air. Sodium lumps (6.0 mmol, 138.1 mg) were cut off and weighed in air after wiping off the residual mineral oil with a paper towel, before they were cut into small pieces (diameter: ~4–5 mm) and directly added to the jar. Then, 1,3-dimethyl-2-imidazolidinone (DMI) (6.0 mmol, 0.69 mL) was added to the jar via syringe. After the jar was closed without purging with inert gas, the jar was placed in the ball-mill (Retsch MM 400, 30 min, 30 Hz). After grinding, the jar was opened and exposed to air. The mixture was quenched with MeOH and H_2O in the jar, transferred into a funnel, and extracted with pentane (3 × 20 mL). The resultant solution was washed by H_2O (3 × 20 mL) and brine (20 mL), dried over $MgSO_4$, and filtered, before all volatiles were removed from the filtrate under reduced pressure to afford pure **2i** as a colorless oil (106.7 mg, 0.80 mmol, 81% yield).

c. Effect of frequency

We investigated the effect of the ball-milling frequency to examine the importance of the mechanical impact on this Birch reduction. We found that lowering the ball-milling frequency led to a decrease in product yield (30 Hz: 96%; 25 Hz: 72%; 20 Hz: 60%; 15 Hz: 55%). These results support our hypothesis that mechanical impact provided by ball milling is crucial to activate the sodium metal and thus facilitates the Birch reduction.



entry	frequency (Hz)	NMR yield of **2a** (%)
1	30	96
2	25	72
3	20	60
4	15	55

Table S1. Effect of frequency.

d. Use of other sugars

The reaction of **1a** using sucrose instead of D-(+)-glucose gave **2a** in 34% yield, while the use of cellulose furnished **2a** in 13% yield. Although further in-depth studies are required, we assume at present that these polysaccharides have a lower proton-donor ability in the solid mixture due to a stronger hydrogen-bonding network in the solid state than that of D-(+)-glucose.

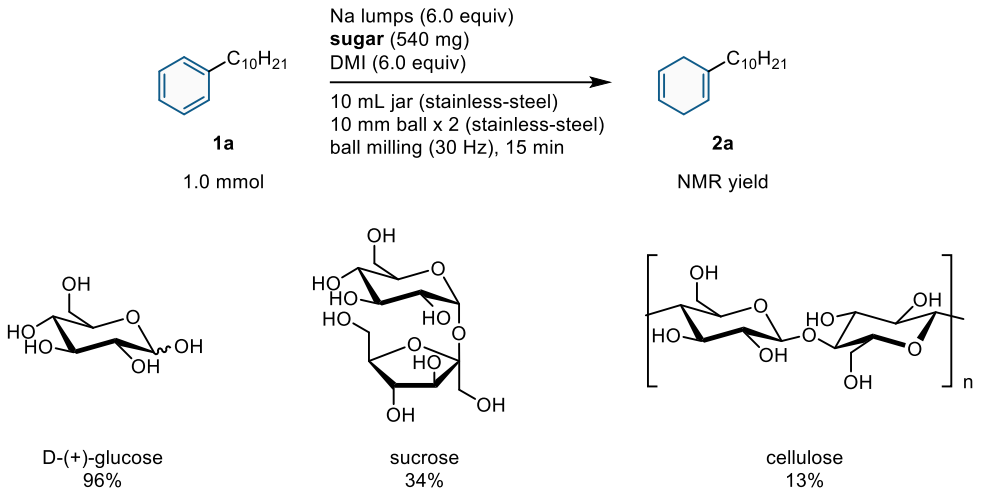
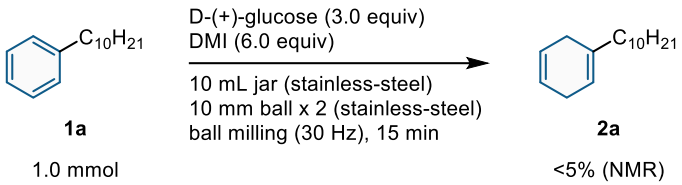


Table S2. Use of other sugars.

e. Reaction without sodium

The reaction without sodium resulted in no product formation, suggesting that the stainless-steel vial is not contributing to the reaction.

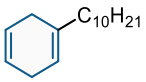
Scheme S2. Reaction without using sodium metal.



7. Characterization of products

Caution: Due to the poor stability of dearomatization product **2**, we sometimes observed that **2** was decomposed or isomerized after column chromatography on silica gel. Therefore, the NMR spectra of the isolated product **2** may contain a small amount of impurities. This phenomenon has commonly been observed in Birch-type reactions.[1-3]

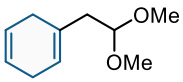
1-Decylcyclohexa-1,4-diene (2a).



The reaction was carried out with 208.4 mg (0.95 mmol) of **1a**, 140.1 mg (6.1 mmol) of sodium lumps, 0.69 ml (6.0 mmol) of DMI, and 541.0 mg (3.0 mmol) of D-(+) glucose. After ball milling for 15 min, the resulting mixture was quenched by MeOH and H_2O and then extracted with pentane. The resultant solution was dried over $MgSO_4$, filtrated, and evaporated in vacuo. The crude mixture was purified by silica-gel column chromatography (SiO_2, pentane only) to afford **2a** as a colorless oil (207.5 mg, 0.94 mmol, 99% yield) containing a small amount of impurities. ^1H and ^{13}C NMR agreed with the literature.[3]

^1H NMR (401 MHz, $CDCl_3$, δ): 0.88 (t, J = 6.8 Hz, 3H), 1.20–1.34 (m, 14H), 1.34–1.45 (m, 2H), 1.94 (t, J = 7.8 Hz, 2H), 2.53–2.63 (m, 2H), 2.64–2.73 (m, 2H), 5.36–5.44 (m, 1H), 5.65–5.77 (m, 2H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 14.3 (CH_3), 22.9 (CH_2), 26.9 (CH_2), 27.6 (CH_2), 29.1 (CH_2), 29.57 (CH_2), 29.62 (CH_2), 29.8 (CH_2), 29.9 (CH_2), 32.1 (CH_2), 37.7 (CH_2), 118.1 (*C*H), 124.4 (*C*H), 124.5 (*C*H), 135.3 (*C*). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{16}H_{28}$, 220.2186; found, 220.2182.

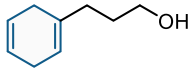
1-(2,2-Dimethoxyethyl)cyclohexa-1,4-diene (2b).



The reaction was carried out with 164.4 mg (0.99 mmol) of **1b**, 140.0 mg (6.1 mmol) of sodium lumps, 0.69 ml (6.0 mmol) of DMI, and 541.2 mg (3.0 mmol) of D-(+) glucose. After ball milling for 15 min, the resulting mixture was quenched by MeOH and H_2O and then extracted with pentane. The resultant solution was dried over $MgSO_4$, filtrated, and evaporated in vacuo. The crude mixture was purified by silica-gel column chromatography (SiO_2, Et_2O/pentane, 0:100-5:95) to afford **2b** as a colorless oil (143.5 mg, 0.85 mmol, 86% yield).

^1H NMR (401 MHz, $CDCl_3$, δ): 2.29 (d, J = 5.2 Hz, 2H), 2.60–2.76 (m, 4H), 3.33 (s, 6H), 4.50 (t, J = 6.0 Hz, 1H), 5.47–5.55 (m, 1H), 5.63–5.75 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$, δ): 26.8 (CH_2), 29.4 (CH_2), 40.8 (CH_2), 52.6 (CH_3), 103.3 (*C*H), 121.4 (*C*H), 123.9 (*C*H), 124.2 (*C*H), 130.6 (*C*). HRMS-ESI (*m*/*z*): $[M+Na]^+$ calcd for $C_{10}H_{16}O_2Na$, 191.1043; found, 191.1041.

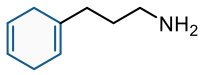
3-(Cyclohexa-1,4-dien-1-yl)propan-1-ol (2c).



The reaction was carried out with 138.9 mg (1.02 mmol) of **1c**, 140.1 mg (6.1 mmol) of sodium lumps, 0.69 ml (6.0 mmol) of DMI, and 1081.0 mg (6.0 mmol) of D-(+) glucose. After ball milling for 5 min, the resulting mixture was quenched by MeOH and H_2O and then extracted with Et_2O. The resultant solution was dried over $MgSO_4$, filtrated, and evaporated in vacuo. The resulting crude mixture was analyzed by ^1H NMR with 1,1,2,2-tetrachloroethane (96.0 mg) as an internal standard to obtain the NMR yield of **2c** in 76% yield. **2c** was easily aromatized during silica gel column chromatography, and 3-(cyclohex-1-en-1-yl)propan-1-ol was inseparable as a byproduct, resulting in the unsuccessful isolation of **2c**. **2c** was characterized by crude ^1H NMR analysis and HRMS. ^1H NMR was in agreement with the literature.[3]

^1H NMR (396 MHz, $CDCl_3$, δ): 1.66–1.75 (m, 3H), 2.05 (t, J = 7.5 Hz, 2H), 2.55–2.74 (m, 4H), 3.60–3.71 (m, 2H), 5.40–5.50 (m, 1H), 5.66–5.77 (m, 2H). HRMS-EI (m/z): $[M]^+$ calcd for $C_9H_{14}O$, 138.1039; found, 138.1040.

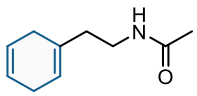
3-(Cyclohexa-1,4-dien-1-yl)propan-1-amine (2d).



The reaction was carried out with 135.5 mg (1.0 mmol) of **1d**, 138.1 mg (6.0 mmol) of sodium lumps, 0.69 ml (6.0 mmol) of DMI, and 1081.6 mg (6.0 mmol) of D-(+) glucose. After ball milling for 15 min, the resulting mixture was quenched by MeOH and H_2O and then extracted with Et_2O. The resultant solution was dried over $MgSO_4$, filtrated, and evaporated in vacuo. The crude mixture was purified by silica-gel column chromatography (SiO_2, DCM/MeOH, 0:100-30:70) to afford **2d** as a white solid (82.7 mg, 0.60 mmol, 60% yield). ^1H and ^{13}C NMR agreed with the literature.[1]

^1H NMR (401 MHz, $CDCl_3$, δ): 1.82–1.93 (m, 2H), 2.09 (t, J = 7.2 Hz, 2H), 2.54–2.62 (m, 2H), 2.63–2.72 (m, 2H), 2.96 (t, J = 7.6 Hz, 2H), 5.43–5.52 (m, 1H), 5.64–5.73 (m, 2H). The two protons on the amino group were not detected in the ^1H NMR spectrum. ^{13}C NMR (101 MHz, $CDCl_3$, δ): 25.8 (CH_2), 26.8 (CH_2), 28.7 (CH_2), 34.3 (CH_2), 39.9 (CH_2), 120.0 (CH), 124.1 (CH), 124.3 (CH), 132.9 (C). HRMS-ESI (m/z): $[M+H]^+$ calcd for $C_9H_{16}N$, 138.1277; found, 138.1276.

***N*-[2-(Cyclohexa-1,4-dien-1-yl)ethyl]acetamide (2e).**

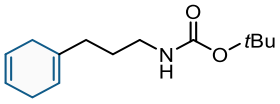


The reaction was carried out with 163.0 mg (1.0 mmol) of **1e**, 140.1 mg (6.1 mmol) of sodium lumps, 0.69 ml (6.0 mmol) of DMI, and 1085.3 mg (6.0 mmol) of D-(+) glucose. After ball milling for 15

min, the resulting mixture was quenched by MeOH and H_2O and then extracted with EtOAc. The resultant solution was dried over $MgSO_4$, filtrated, and evaporated in vacuo. The crude mixture was purified by silica-gel column chromatography (SiO_2, DCM/EtOAc, 70:30-30:70) to afford **2e** as a white solid (135.5 mg, 0.82 mmol, 82% yield). ^1H and ^{13}C NMR agreed with the literature.[1]

^1H NMR (392 MHz, $CDCl_3$, δ): 1.97 (s, 3H), 2.17 (t, J = 6.5 Hz, 2H), 2.56–2.64 (m, 2H), 2.67–2.76 (m, 2H), 3.36 (q, J = 6.5 Hz, 2H), 5.46 (brs, 1H), 5.48–5.54 (m, 1H), 5.67–5.76 (m, 2H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 23.5 (*C*H_3), 26.8 (*C*H_2), 28.7 (*C*H_2), 37.0 (*C*H_2), 37.1 (*C*H_2), 120.9 (*C*H), 124.1 (*C*H), 124.2 (*C*H), 132.0 (*C*), 170.1 (*C*). HRMS-ESI (*m*/*z*): $[M+Na]^+$ calcd for $C_{10}H_{15}ONNa$, 188.1046; found, 188.1046.

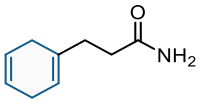
tert-Butyl (3-(cyclohexa-1,4-dien-1-yl)propyl)carbamate (2f).



The reaction was carried out with 229.3 mg (0.97 mmol) of **1f**, 138.1 mg (6.0 mmol) of sodium lumps, 0.69 ml (6.0 mmol) of DMI, and 1082.1 mg (6.0 mmol) of D-(+) glucose. After ball milling for 15 min, the resulting mixture was quenched by MeOH and H_2O and then extracted with EtOAc. The resultant solution was dried over $MgSO_4$, filtrated, and evaporated in vacuo. The crude mixture was purified by silica-gel column chromatography (SiO_2, DCM/EtOAc, 100:0-95:5) to afford **2f** as a colorless oil (154.1 mg, 0.65 mmol, 67% yield).

^1H NMR (401 MHz, $CDCl_3$, δ): 1.44 (s, 9H), 1.58–1.66 (m, 2H), 1.99 (t, J = 7.6 Hz, 2H), 2.53–2.63 (m, 2H), 2.63–2.74 (m, 2H), 3.04–3.20 (m, 2H), 4.53 (brs, 1H), 5.39–5.46 (m, 1H), 5.63–5.76 (m, 2H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 26.8 (*C*H_2), 27.7 (*C*H_2), 28.5 (*C*H_3), 28.9 (*C*H_2), 34.7 (*C*H_2), 40.4 (*C*H_2), 79.1 (*C*), 118.9 (*C*H), 124.26 (*C*H), 124.31 (*C*H), 134.2 (*C*), 156.0 (*C*). HRMS-ESI (*m*/*z*): $[M+Na]^+$ calcd for $C_{14}H_{23}O_2NNa$, 260.1621; found, 260.1615.

3-(Cyclohexa-1,4-dien-1-yl)propenamide (2g).

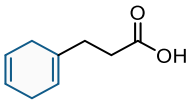


The reaction was carried out with 141.5 mg (1.0 mmol) of **1g**, 137.8 mg (6.0 mmol) of sodium lumps, 0.69 ml (6.0 mmol) of DMI, and 1082.4 mg (6.0 mmol) of D-(+) glucose. After ball milling for 15 min, the resulting mixture was quenched by MeOH and H_2O and then extracted with EtOAc. The resultant solution was dried over $MgSO_4$, filtrated, and evaporated in vacuo. The resulting crude mixture was analyzed by ^1H NMR with 1,1,2,2-tetrachloroethane (96.9 mg) as an internal standard to obtain the NMR yield of **2g** in 51% yield. **2g** was easily aromatized during silica gel column

chromatography, resulting in the unsuccessful isolation of **2g**. **2g** was characterized by crude ^{1}H NMR analysis and HRMS. ^{1}H NMR agreed with the literature.[1]

^{1}H NMR (399 MHz, $CDCl_3$, δ): 2.24–2.42 (m, 4H), 2.59–2.72 (m, 4H), 5.45–5.52 (m, 1H), 5.69–5.73 (m, 2H). The two protons on the amide group were not detected in the ^{1}H NMR spectrum. HRMS-ESI (*m*/*z*): $[M+H]^+$ calcd for $C_9H_{13}NO$, 152.1070; found, 151.1069.

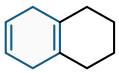
3-(Cyclohexa-1,4-dien-1-yl)propanoic acid (2h).



The reaction was carried out with 151.4 mg (1.0 mmol) of **1h**, 138.4 mg (6.0 mmol) of sodium lumps, 0.69 ml (6.0 mmol) of DMI, and 542.1 mg (3.0 mmol) of D-(+) glucose. After ball milling for 30 min, the resulting mixture was quenched by MeOH and 1M HCl and then extracted with EtOAc. The resultant solution was dried over $MgSO_4$, filtrated, and evaporated in vacuo. The resulting crude mixture was analyzed by ^{1}H NMR with 1,1,2,2-tetrachloroethane (151.0 mg) as an internal standard to obtain the NMR yield of **2h** in 88% yield. Some byproducts could not be separated by silica-gel column chromatography, resulting in the unsuccessful isolation of **2h**. **2h** was characterized by crude ^{1}H NMR analysis and HRMS. ^{1}H NMR agreed with the literature.[1]

^{1}H NMR (399 MHz, $CDCl_3$, δ): 2.30 (t, J = 7.6 Hz, 2H), 2.42–2.53 (m, 2H), 2.56–2.64 (m, 2H), 2.64–2.73 (m, 2H), 5.44–5.49 (m, 1H), 5.64–5.75 (m, 2H). The proton on the carboxylic acid moiety was not detected in the ^{1}NMR spectrum. HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_9H_{12}O_2$, 152.0831; found, 152.0833.

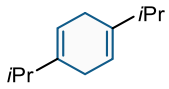
1,2,3,4,5,8-Hexahydronaphthalene (2i).



The reaction was carried out with 132.4 mg (1.0 mmol) of **1i**, 140.1 mg (6.1 mmol) of sodium lumps, 0.69 ml (6.0 mmol) of DMI, and 540.0 mg (3.0 mmol) of D-(+) glucose. After ball milling for 30 min, the resulting mixture was quenched by MeOH and H_2O and then extracted with pentane. The resultant solution was dried over $MgSO_4$, filtrated, and evaporated in vacuo. The crude mixture was purified by silica-gel column chromatography (SiO_2, pentane only) to afford **2i** as a colorless oil (115.1 mg, 0.86 mmol, 86% yield). ^{1}H and ^{13}C NMR agreed with the literature.[1]

^{1}H NMR (401 MHz, $CDCl_3$, δ): 1.61–1.69 (m, 4H), 1.80–1.91 (m, 4H), 2.53 (s, 4H), 5.72 (s, 2H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 23.3 (*C*H_2), 30.0 (*C*H_2), 31.7 (*C*H_2), 124.7 (*C*H), 125.7 (*C*). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{10}H_{14}$, 134.1090; found, 134.1089.

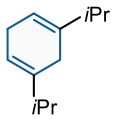
1,4-Diisopropylcyclohexa-1,4-diene (2j).



The reaction was carried out with 163.1 mg (1.0 mmol) of **1j**, 136.3 mg (5.9 mmol) of sodium lumps, 0.69 ml (6.0 mmol) of DMI, and 1080.0 mg (6.0 mmol) of D-(+) glucose. After ball milling for 30 min, the resulting mixture was quenched by MeOH and H_2O and then extracted with pentane. The resultant solution was dried over $MgSO_4$, filtrated, and evaporated in vacuo. The crude mixture was purified by silica-gel column chromatography (SiO_2, pentane only) to afford **2j** as a colorless oil (147.4 mg, 0.90 mmol, 89% yield). ^1H and ^{13}C NMR agreed with the literature.[3]

^1H NMR (401 MHz, $CDCl_3$, δ): 1.02 (d, J = 7.2 Hz, 12H), 2.20 (sept, J = 6.9 Hz, 2H), 2.59–2.68 (m, 4H), 5.42–5.49 (m, 2H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 21.4 (CH_2), 27.7 (CH_2), 34.6 (*C*H), 116.3 (*C*H), 140.8 (*C*). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{12}H_{20}$, 164.1560; found, 164.1561.

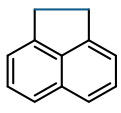
1,5-Diisopropylcyclohexa-1,4-diene (2k).



The reaction was carried out with 162.4 mg (1.0 mmol) of **1k**, 138.0 mg (6.0 mmol) of sodium lumps, 0.69 ml (6.0 mmol) of DMI and 1081.6 mg (6.0 mmol) of D-(+) glucose. After ball milling for 30 min, the resulting mixture was quenched by MeOH and H_2O and then extracted with pentane. The resultant solution was dried over $MgSO_4$, filtrated, and evaporated in vacuo. The resulting crude mixture was analyzed by ^1H NMR with 1,1,2,2-tetrachloroethane (94.5 mg) as an internal standard to obtain the NMR yield of **2k** in 44% yield. The remaining **1k** was inseparable by silica-gel column chromatography, resulting in the unsuccessful isolation of **2k**. **2k** was characterized by crude ^1H NMR analysis and HRMS. ^1H NMR agreed with the literature.[3]

^1H NMR (396 MHz, $CDCl_3$, δ): 1.04 (d, J = 6.7 Hz, 12H), 2.10–2.29 (m, 2H), 2.51–2.62 (m, 2H), 2.66–2.75 (m, 2H), 5.40–5.48 (m, 2H). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{12}H_{20}$, 164.1560; found, 164.1562.

1,2-Dihydroacenaphthylene (2l).

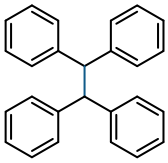


The reaction was carried out with 151.9 mg (1.0 mmol) of **1l**, 53.0 mg (2.3 mmol) of sodium lumps, 0.69 ml (6.0 mmol) of DMI, and 540.7 mg (3.0 mmol) of D-(+) glucose. After ball milling for 10 min, the resulting mixture was quenched by MeOH and H_2O and then extracted with hexane. The resultant

solution was dried over $MgSO_4$, filtrated, and evaporated in vacuo. The crude mixture was purified by silica-gel column chromatography (SiO_2, hexane only) to afford **2l** as a white solid (124.1 mg, 0.80 mmol, 81% yield). ^1H and ^{13}C NMR agreed with the literature.[2]

^1H NMR (401 MHz, $CDCl_3$, δ): 3.40 (s, 4H), 7.27 (d, J = 7.2 Hz, 2H), 7.43 (t, J = 7.6 Hz, 2H), 7.58 (d, J = 8.4 Hz, 2H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 30.4 (*C*H_2), 119.2 (*C*H), 122.3 (*C*H), 127.9 (*C*H), 131.7 (*C*), 139.4 (*C*), 146.1 (*C*). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{12}H_{10}$, 154.0777; found, 154.0777.

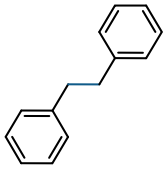
1,1,2,2-Tetraphenylethane (2m).



The reaction was carried out with 332.6 mg (1.0 mmol) of **1m**, 73.7 mg (3.2 mmol) of sodium lumps, 0.69 ml (6.0 mmol) of DMI, and 541.0 mg (3.0 mmol) of D-(+) glucose. After ball milling for 15 min, the resulting mixture was quenched by MeOH and H_2O and then extracted with EtOAc. The resultant solution was dried over $MgSO_4$, filtrated, and evaporated in vacuo. The crude mixture was purified by silica-gel column chromatography (SiO_2, hexane/DCM, 90:10-50:50) to afford **2m** as a white solid (261.0 mg, 0.78 mmol, 78% yield). ^1H and ^{13}C NMR agreed with the literature.[3]

^1H NMR (401 MHz, $CDCl_3$, δ): 4.77 (s, 2H), 7.01 (t, J = 7.0 Hz, 4H), 7.10 (t, J = 7.4 Hz, 8H), 7.16 (d, J = 7.2 Hz, 8H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 56.5 (*C*H), 126.0 (*C*H), 128.3 (*C*H), 128.6 (*C*H), 143.6 (*C*). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{26}H_{22}$, 334.1716; found, 334.1744.

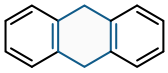
1,2-Diphenylethane (2n).



The reaction was carried out with 177.7 mg (1.0 mmol) of **1n**, 142.2 mg (6.2 mmol) of sodium lumps, 1.0 ml (9.0 mmol) of DMI, and 1089.1 mg (6.0 mmol) of D-(+) glucose. After ball milling for 30 min, the resulting mixture was quenched by MeOH and H_2O and then extracted with hexane. The resultant solution was dried over $MgSO_4$, filtrated, and evaporated in vacuo. The crude mixture was purified by silica-gel column chromatography (SiO_2, hexane only) to afford **2n** as a colorless oil (100.3 mg, 0.55 mmol, 55% yield). ^1H and ^{13}C NMR agreed with the literature.[2]

^1H NMR (401 MHz, $CDCl_3$, δ): 2.93 (s, 4H), 7.20 (t, J = 6.6 Hz, 6H), 7.25–7.32 (m, 4H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 38.1 (*C*H_2), 126.0 (*C*H), 128.5 (*C*H), 128.6 (*C*H), 141.9 (*C*). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{14}H_{14}$, 182.1090; found, 182.1085.

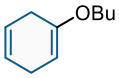
9,10-Dihydroanthracene (2o).



The reaction was carried out with 177.9 mg (1.0 mmol) of **1o**, 59.2 mg (2.6 mmol) of sodium lumps, 0.69 ml (6.0 mmol) of DMI, and 541.2 mg (3.0 mmol) of D-(+) glucose. After ball milling for 15 min, the resulting mixture was quenched by MeOH and H_2O and then extracted with EtOAc. The resultant solution was dried over $MgSO_4$, filtrated, and evaporated in vacuo. The crude mixture was purified by silica-gel column chromatography (SiO_2, hexane only) to afford **2o** as a white solid (163.9 mg, 0.91 mmol, 91% yield). ^{1}H and ^{13}C NMR agreed with the literature.[3]

^{1}H NMR (401 MHz, $CDCl_3$, δ): 3.94 (s, 4H), 7.16–7.23 (m, 4H), 7.26–7.33 (m, 4H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 36.2 (*C*H_2), 126.2 (*C*H), 127.5 (*C*H), 136.7 (*C*). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{14}H_{12}$, 180.0934; found, 180.0934.

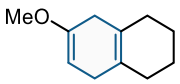
1-Butoxycyclohexa-1,4-diene (2p)



The reaction was carried out with 150.1 mg (1.0 mmol) of **1p**, 138.1 mg (6.0 mmol) of sodium lumps, 0.69 ml (6.0 mmol) of DMI, and 1079.1 mg (6.0 mmol) of D-(+) glucose. After ball milling for 10 min, the resulting mixture was quenched by MeOH and H_2O and then extracted with pentane. The resultant solution was dried over $MgSO_4$, filtrated, and evaporated in vacuo. The crude mixture was purified by silica-gel column chromatography (SiO_2, pentane only) to afford **2p** as a colorless oil (88.8 mg, 0.58 mmol, 58% yield) with a small amount of impurities. ^{1}H and ^{13}C NMR agreed with the literature.[3]

^{1}H NMR (401 MHz, $CDCl_3$, δ): 0.94 (t, J = 7.4 Hz, 3H), 1.42 (sext, J = 7.4 Hz, 2H), 1.65 (quint, J = 7.1 Hz, 2H), 2.67–2.76 (m, 2H), 2.76–2.85 (m, 2H), 3.68 (t, J = 6.4 Hz, 2H), 4.57–4.65 (m, 1H), 5.64–5.73 (m, 2H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 14.0 (*C*H_3), 19.5 (*C*H_2), 26.5 (*C*H_2), 28.8 (*C*H_2), 31.4 (*C*H_2), 66.0 (*C*H_2), 91.1 (*C*H), 123.4 (*C*H), 124.7 (*C*H), 152.2 (*C*). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{10}H_{16}O$, 152.1196; found, 152.1193.

6-Methoxy-1,2,3,4,5,8-hexahydronaphthalene (2q).

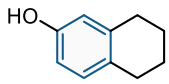


The reaction was carried out with 162.4 mg (1.0 mmol) of **1q**, 136.7 mg (5.9 mmol) of sodium lumps, 0.69 ml (6.0 mmol) of DMI and 1086.3 mg (6.0 mmol) of D-(+) glucose. After ball milling for 15 min, the resulting mixture was quenched by MeOH and H_2O and then extracted with pentane. The resultant solution was dried over $MgSO_4$, filtrated, and evaporated in vacuo. The resulting crude mixture was

analyzed by ^{1}H NMR with 1,1,2,2-tetrachloroethane (95.7 mg) as an internal standard to obtain the NMR yield of **2q** in 34% yield. Some byproducts could not be separated by silica-gel column chromatography, resulting in the unsuccessful isolation of **2q**. **2q** was characterized by crude ^{1}H NMR analysis and HRMS. ^{1}H NMR agreed with the literature.[3]

^{1}H NMR (401 MHz, $CDCl_3$, δ): 1.58–1.67 (m, 4H), 1.87–1.94 (m, 4H), 2.54–2.74 (m, 4H), 3.55 (s, 3H), 4.63 (t, J = 3.4 Hz, 1H). HRMS-EI (m/z): $[M]^+$ calcd for $C_{11}H_{16}O$, 164.1196; found, 164.1196.

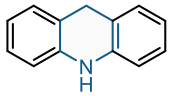
5,6,7,8-Tetrahydronaphthalen-2-ol (2q')



The resulting crude mixture of the reaction with **1q** was analyzed by ^{1}H NMR with 1,1,2,2-tetrachloroethane (95.7 mg) as an internal standard to obtain the NMR yield of **2q'** in 43% yield. **2q'** was characterized by crude ^{1}H NMR analysis and HRMS. ^{1}H NMR agreed with the literature.[4]

^{1}H NMR (401 MHz, $CDCl_3$, δ): 1.74–1.79 (m, 4H), 2.77–2.80 (m, 4H), 5.08 (brs, 1H), 6.53–6.57 (m, 1H), 6.57–6.62 (m, 1H), 6.92 (d, J = 8.0 Hz, 1H). HRMS-EI (m/z): $[M]^+$ calcd for $C_{10}H_{12}O$, 148.0883; found, 148.0878.

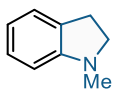
9,10-Dihydroacridine (2r).



The reaction was carried out with 179.3 mg (1.0 mmol) of **1r**, 59.0 mg (2.6 mmol) of sodium lumps, 0.69 ml (6.0 mmol) of DMI, and 543.3 mg (3.0 mmol) of D-(+) glucose. After ball milling for 15 min, the resulting mixture was quenched by MeOH and H_2O and then extracted with Et_2O. The resultant solution was dried over $MgSO_4$, filtrated, and evaporated in vacuo. The crude mixture was purified by silica-gel column chromatography (SiO_2, hexane/EtOAc, 90:10) to afford **2r** as a white solid (174.1 mg, 0.96 mmol, 96% yield). ^{1}H and ^{13}C NMR agreed with the literature.[3]

^{1}H NMR (401 MHz, $CDCl_3$, δ): 4.06 (s, 2H), 5.96 (brs, 1H), 6.67 (d, J = 7.6 Hz, 2H), 6.85 (t, J = 7.6 Hz, 2H), 7.04–7.13 (m, 4H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 31.5 (CH_2), 113.5 (CH), 120.1 (C), 120.7 (CH), 127.1 (CH), 128.7 (CH), 140.2 (C). HRMS-APCI (m/z): $[M+H]^+$ calcd for $C_{13}H_{12}N$, 182.0964; found, 182.0964.

1-Methylindoline (2s).

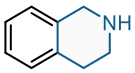


The reaction was carried out with 130.7 mg (1.0 mmol) of **1s**, 91.1 mg (4.0 mmol) of sodium lumps, 0.69 ml (6.0 mmol) of DMI, and 1081.3 mg (6.0 mmol) of D-(+) glucose. After ball milling for 15

min, the resulting mixture was quenched by MeOH and H_2O and then extracted with Et_2O. The resultant solution was dried over $MgSO_4$, filtrated, and evaporated in vacuo. The crude mixture was purified by silica-gel column chromatography (SiO_2, pentane/Et_2O, 100:0-97:3) to afford **2s** as a colorless oil (66.3 mg, 0.50 mmol, 50% yield). ^1H and ^{13}C NMR agreed with the literature.[3]

^1H NMR (401 MHz, $CDCl_3$, δ): 2.75 (s, 3H), 2.94 (t, *J* = 8.2 Hz, 2H), 3.28 (t, *J* = 8.4 Hz, 2H), 6.49 (d, *J* = 8.4 Hz, 1H), 6.67 (t, *J* = 7.2 Hz, 1H), 7.03–7.13 (m, 2H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 28.8 (*C*H_2), 36.4 (*C*H_3), 56.2 (*C*H_2), 107.3 (*C*H), 117.9 (*C*H), 124.3 (*C*H), 127.4 (*C*H), 130.4 (*C*), 153.5 (*C*). HRMS-ESI (*m*/*z*): $[M+H]^+$ calcd for $C_9H_{12}N$, 134.0964; found, 134.0965.

1,2,3,4-Tetrahydroisoquinoline (2t).

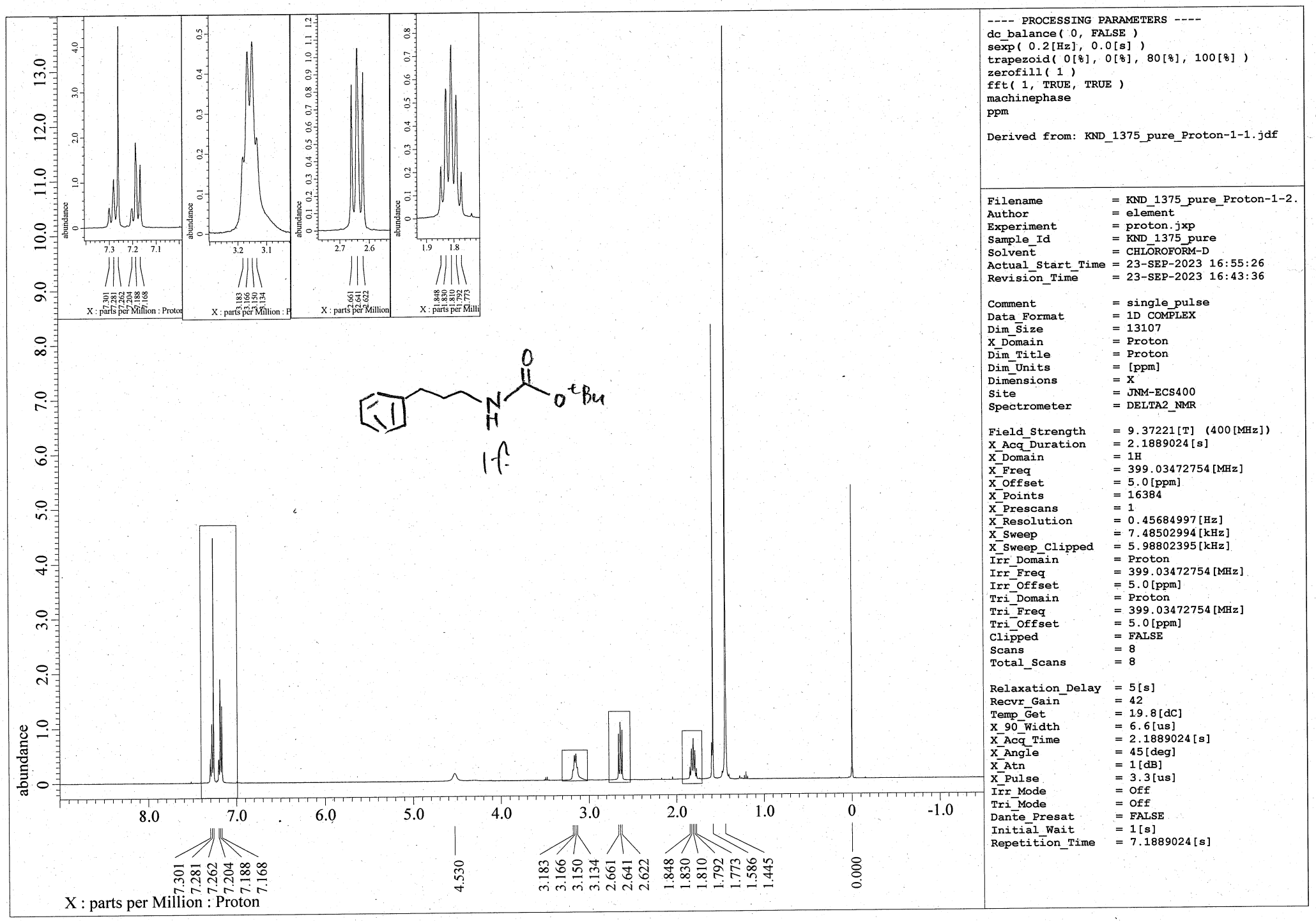


The reaction was carried out with 130.3 mg (1.0 mmol) of **1t**, 140.0 mg (6.1 mmol) of sodium lumps, 0.69 ml (6.0 mmol) of DMI, and 1081.3 mg (6.0 mmol) of D-(+) glucose. After ball milling for 15 min, the resulting mixture was quenched by MeOH and H_2O and then extracted with Et_2O. The resultant solution was dried over $MgSO_4$, filtrated, and evaporated in vacuo. The resulting crude mixture was analyzed by ^1H NMR with 1,1,2,2-tetrachloroethane (96.1 mg) as an internal standard to obtain the NMR yield of **2t** in 49% yield. Separation of **2t** from DMI by silica-gel column chromatography was unsuccessful. **2t** was characterized by crude ^1H NMR analysis and HRMS. ^1H NMR was in agreement with the literature.[3]

^1H NMR (396 MHz, $CDCl_3$, δ): 2.77–2.84 (m, 4H), 4.02 (s, 2H), 6.97–7.05 (m, 1H), 7.07–7.16 (m, 3H). HRMS-ESI (*m*/*z*): $[M+H]^+$ calcd for $C_9H_{12}N$, 134.0964; found, 134.0964.

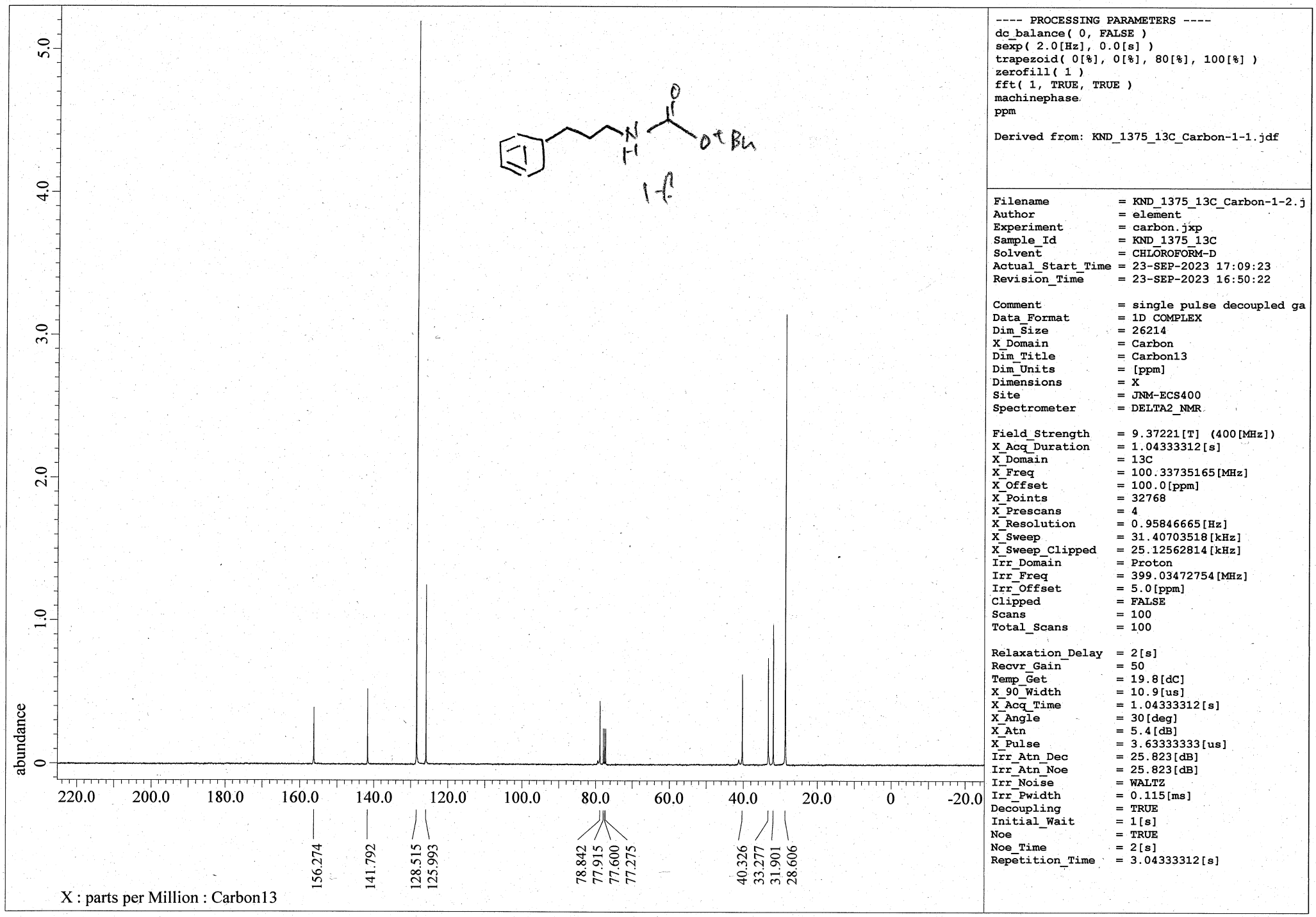
8. References

1. Asako, S.; Takahashi, I.; Kurogi, T.; Murakami, Y.; Llies, L.; Takai, K. *Chem. Lett.* **2022**, *51*, 38.
2. Lei, P.; Ding, Y.; Zhang, X.; Adijiang, A.; Li, H.; Ling, Y.; An, J. *Org. Lett.* **2018**, *20*, 3439.
3. Gao, Y.; Kubota, K.; Ito, H. *Angew. Chem. Int. Ed.* **2023**, *62*, e202217723.
4. Chen, G.; Shi, Y.; Tian, W.; Xie, H.; Yan, Z.; Yu, J. *Tetrahedron. Lett.* **2023**, *117*, 154365.



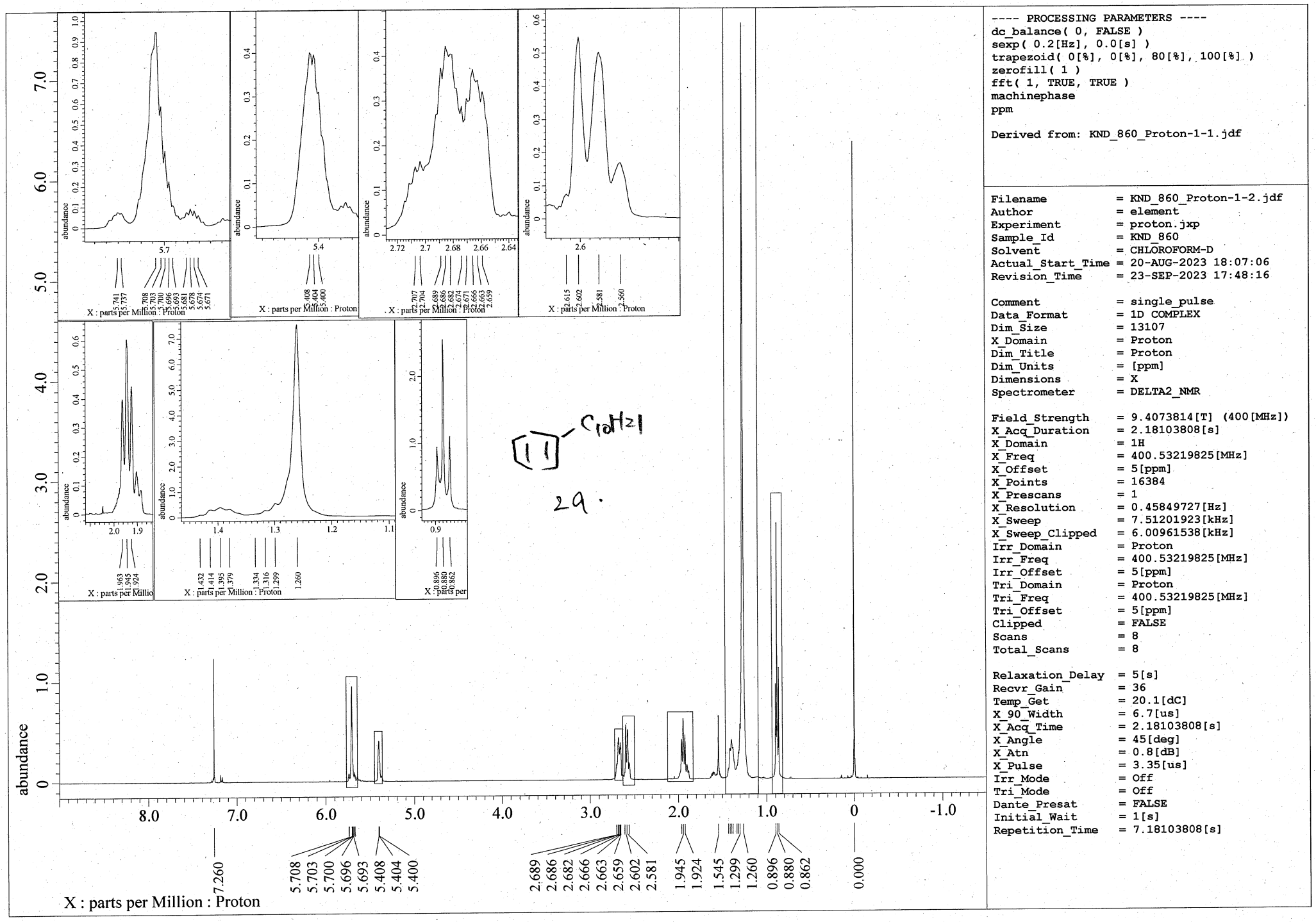

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KND_1375_pure_Proton-1-1.jdf
```

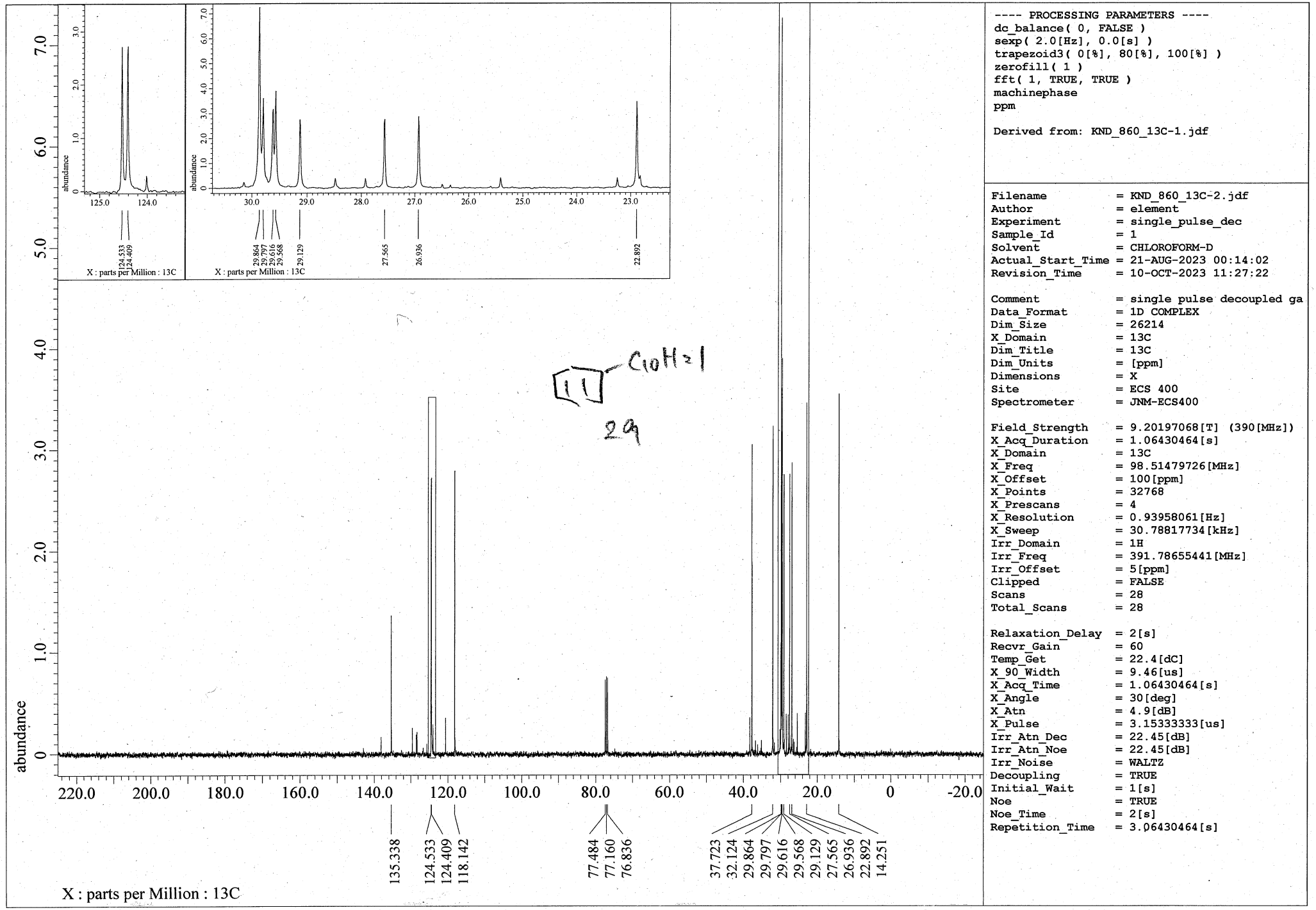
Filename	= KND_1375_pure_Proton-1-2.
Author	= element
Experiment	= proton.jxp
Sample_Id	= KND_1375_pure
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 23-SEP-2023 16:55:26
Revision_Time	= 23-SEP-2023 16:43:36
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
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	= 19.8[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_1375_13C_Carbon-1-1.jdf
```

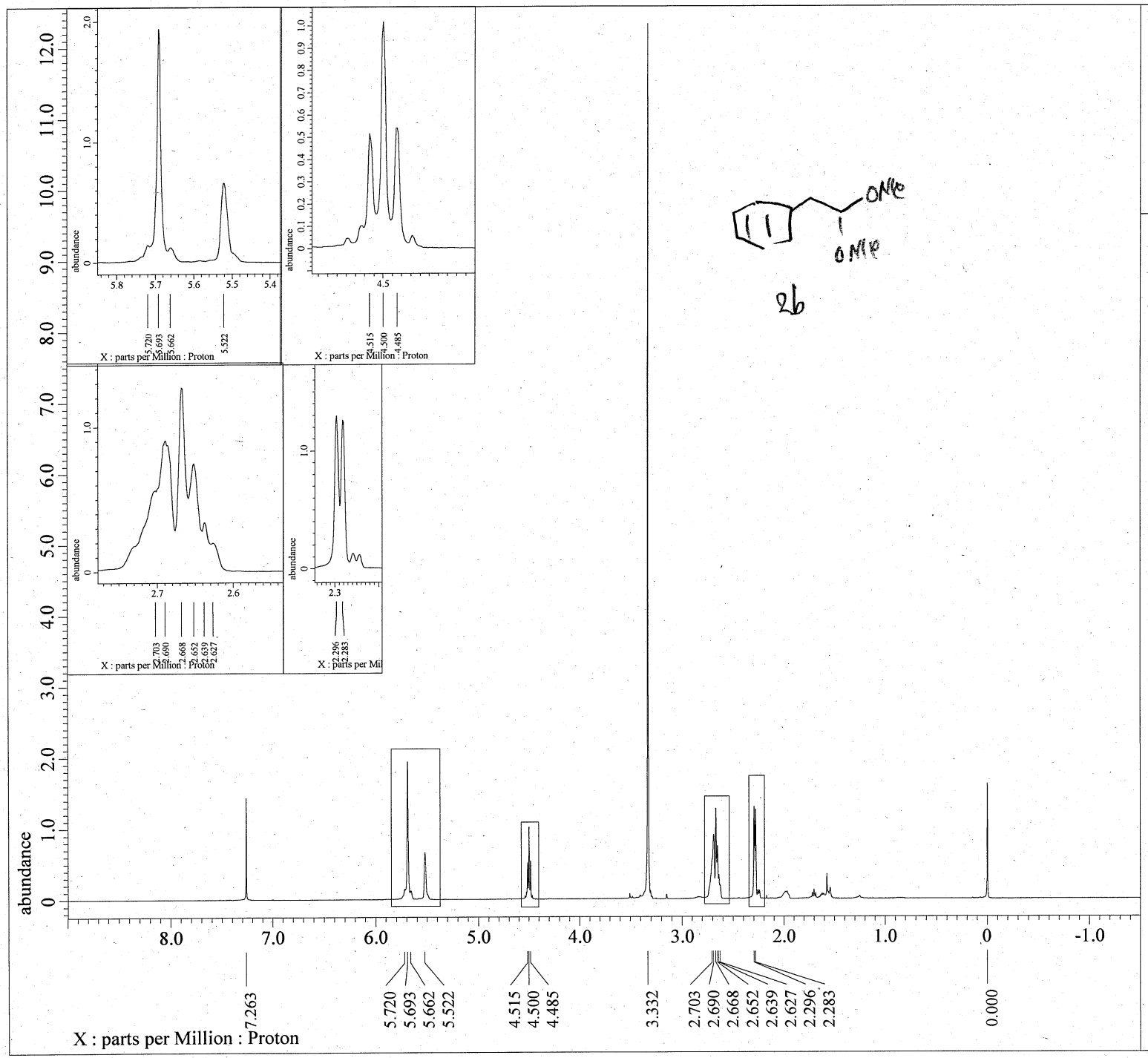
Filename	= KND_1375_13C_Carbon-1-2.j
Author	= element
Experiment	= carbon.jxp
Sample_Id	= KND_1375_13C
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 23-SEP-2023 17:09:23
Revision_Time	= 23-SEP-2023 16:50:22
Comment	= single pulse decoupled ga
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon
Dim_Title	= 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	= 100
Total_Scans	= 100
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 19.8[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_860_Proton-1-1.jdf
Filename = KND_860_Proton-1-2.jdf
Author = element
Experiment = proton.jxp
Sample_Id = KND_860
Solvent = CHLOROFORM-D
Actual_Start_Time = 20-AUG-2023 18:07:06
Revision_Time = 23-SEP-2023 17:48:16
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = DELTA2_NMR
Field_Strength = 9.4073814[T] (400[MHz])
X_Acq_Duration = 2.18103808[s]
X_Domain = 1H
X_Freq = 400.53219825[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45849727[Hz]
X_Sweep = 7.51201923[kHz]
X_Sweep_Clipped = 6.00961538[kHz]
Irr_Domain = Proton
Irr_Freq = 400.53219825[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 400.53219825[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 36
Temp_Get = 20.1[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]
abundance
X : parts per Million : Proton
7.260
5.708
5.703
5.700
5.696
5.693
5.408
5.404
5.400
2.689
2.686
2.682
2.666
2.663
2.659
2.602
2.581
1.945
1.924
1.545
1.299
1.260
0.896
0.880
0.862
0.000
C10H21
29.



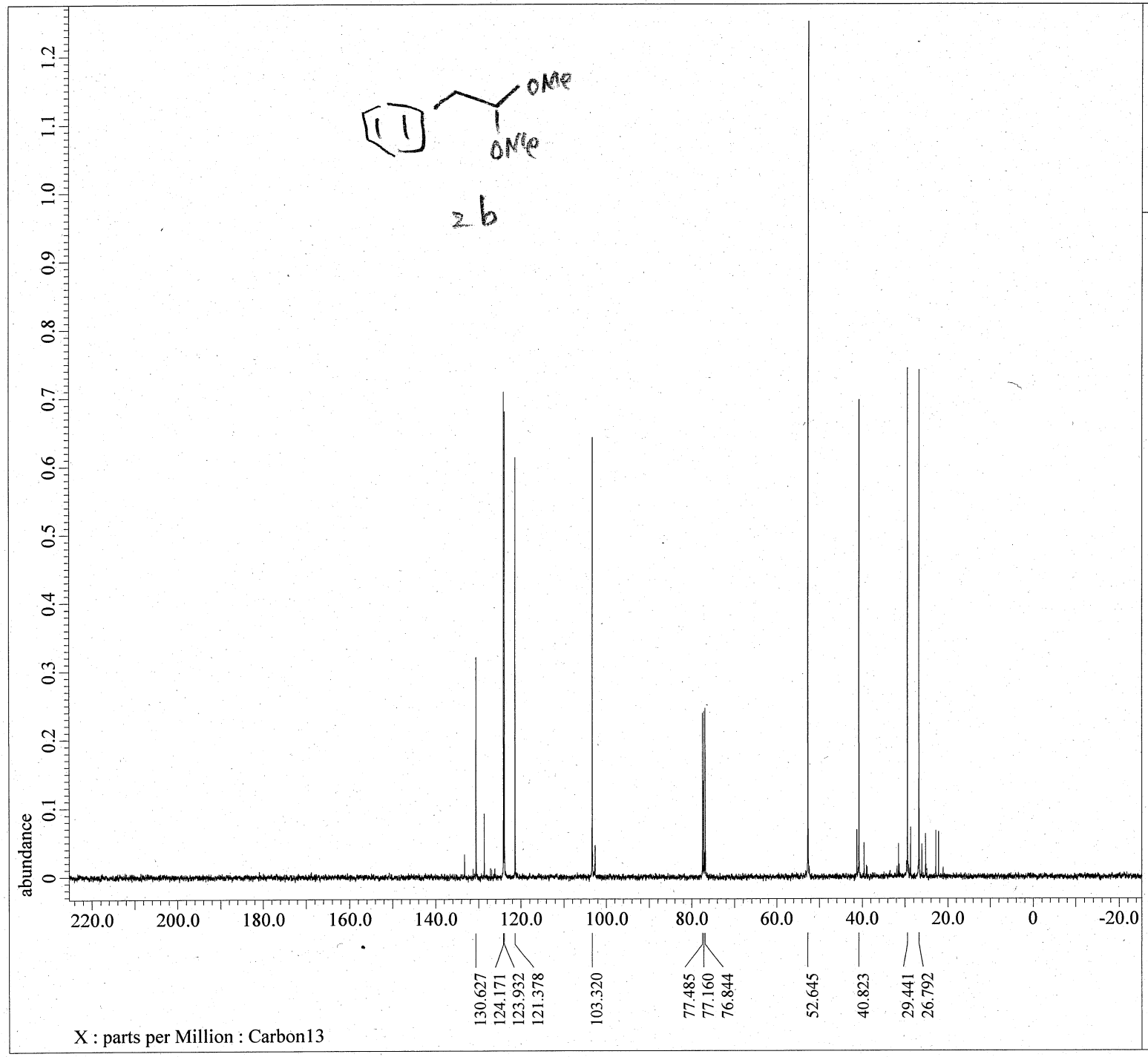

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KND_860_13C-1.jdf
```

Filename	= KND_860_13C-2.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= 1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 21-AUG-2023 00:14:02
Revision_Time	= 10-OCT-2023 11:27:22
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	= 28
Total_Scans	= 28
Relaxation_Delay	= 2[s]
Recvr_Gain	= 60
Temp_Get	= 22.4[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]



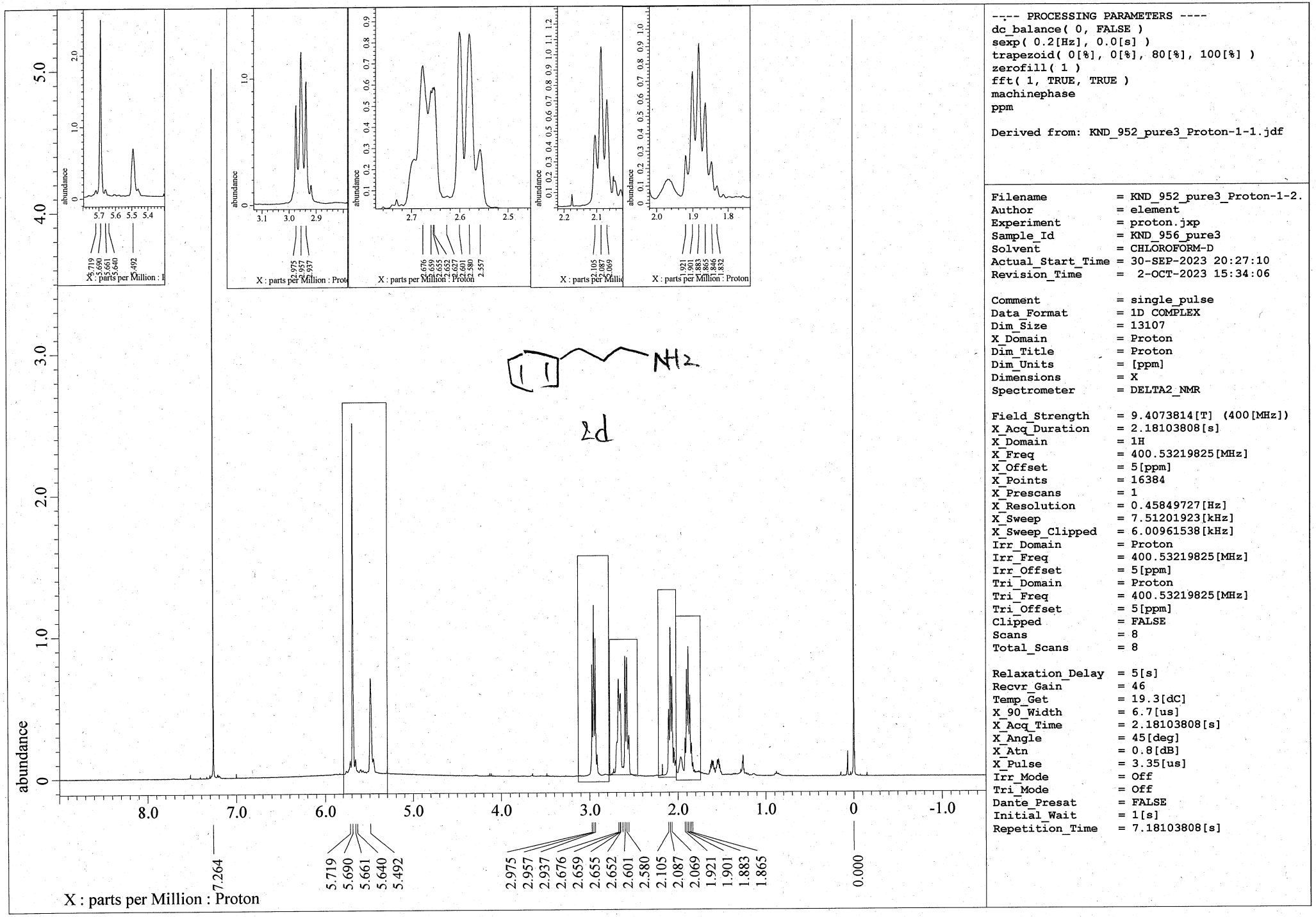

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KND_869_pure_Proton-1-1.jdf
```

Filename	= KND_869_pure_Proton-1-2.j
Author	= element
Experiment	= proton.jxp
Sample_Id	= KND_869_pure
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 4-MAY-2023 17:11:03
Revision_Time	= 23-SEP-2023 18:21:42
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	= 9.4073814[T] (400[MHz])
X_Acq_Duration	= 2.18103808[s]
X_Domain	= 1H
X_Freq	= 400.53219825[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45849727[Hz]
X_Sweep	= 7.51201923[kHz]
X_Sweep_Clipped	= 6.00961538[kHz]
Irr_Domain	= Proton
Irr_Freq	= 400.53219825[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 400.53219825[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 40
Temp_Get	= 19.6[dC]
X_90_Width	= 6.7[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]



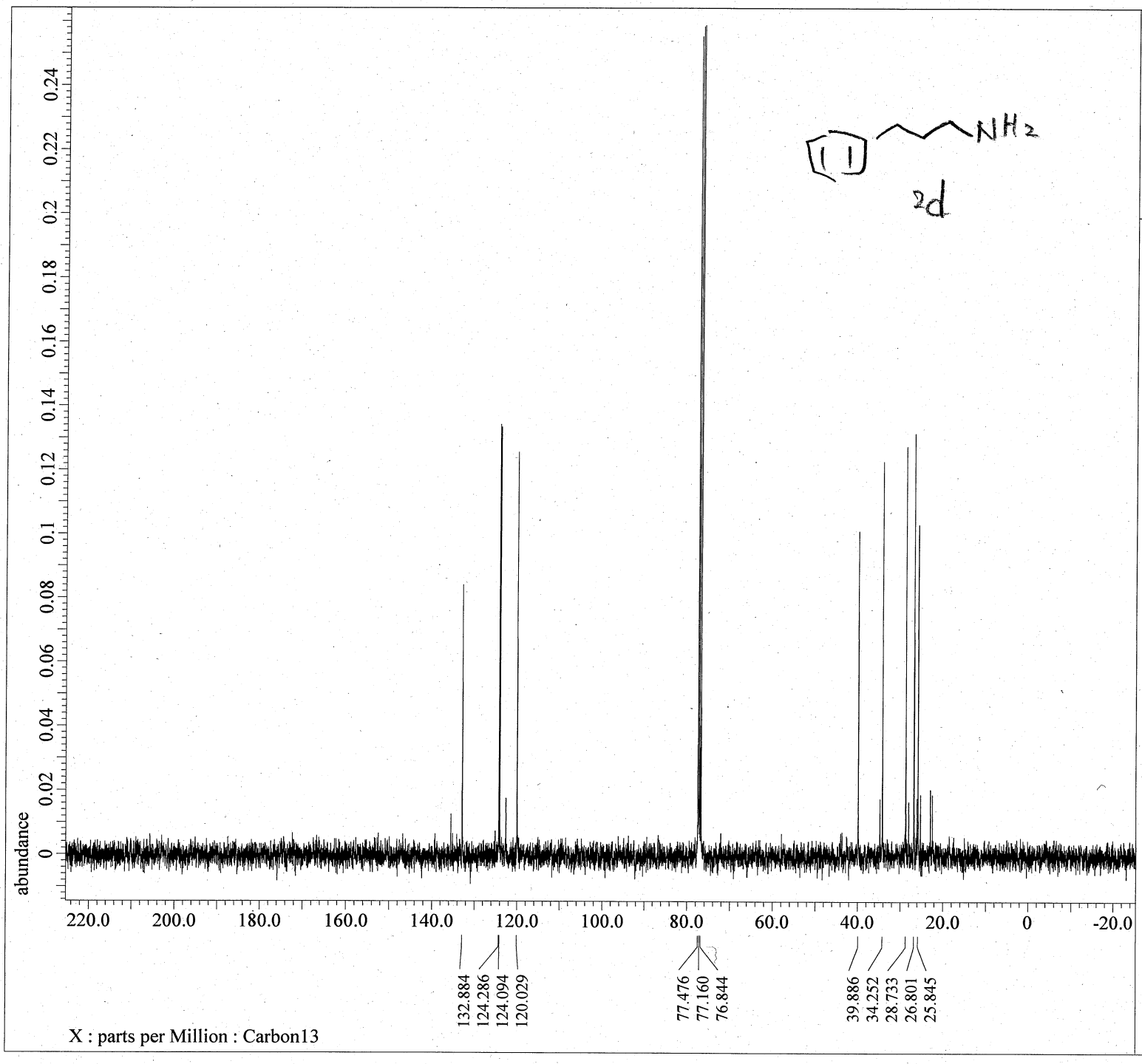

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KND_869_13C_Carbon-1-1.jdf
```

```
Filename            = KND_869_13C_Carbon-1-2.jd
Author              = element
Experiment          = carbon.jxp
Sample_Id           = KND_869_13C
Solvent             = CHLOROFORM-D
Actual_Start_Time   =  4-MAY-2023 17:23:46
Revision_Time       = 23-SEP-2023 18:23:26

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               = 100
Total_Scans         = 100

Relaxation_Delay    = 2[s]
Recvr_Gain          = 50
Temp_Get            = 19.5[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]
```



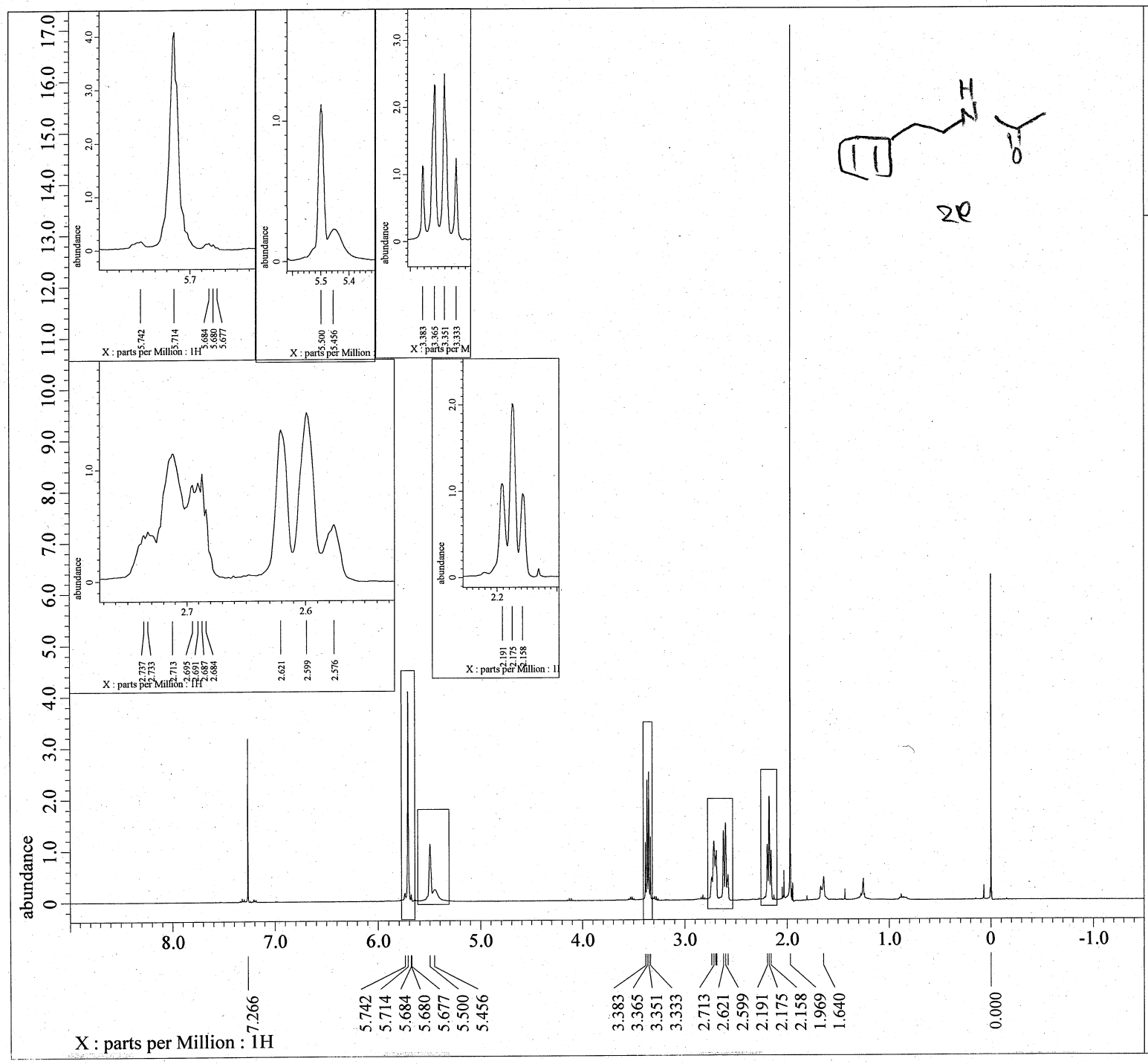

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KND_952_pure3_Proton-1-1.jdf
```

Filename	= KND_952_pure3_Proton-1-2.
Author	= element
Experiment	= proton.jxp
Sample_Id	= KND_956_pure3
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 30-SEP-2023 20:27:10
Revision_Time	= 2-OCT-2023 15:34:06
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.4073814[T] (400[MHz])
X_Acq_Duration	= 2.18103808[s]
X_Domain	= 1H
X_Freq	= 400.53219825[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45849727[Hz]
X_Sweep	= 7.51201923[kHz]
X_Sweep_Clipped	= 6.00961538[kHz]
Irr_Domain	= Proton
Irr_Freq	= 400.53219825[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 400.53219825[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 46
Temp_Get	= 19.3[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] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KND_952_13C_Carbon-1-1.jdf
```

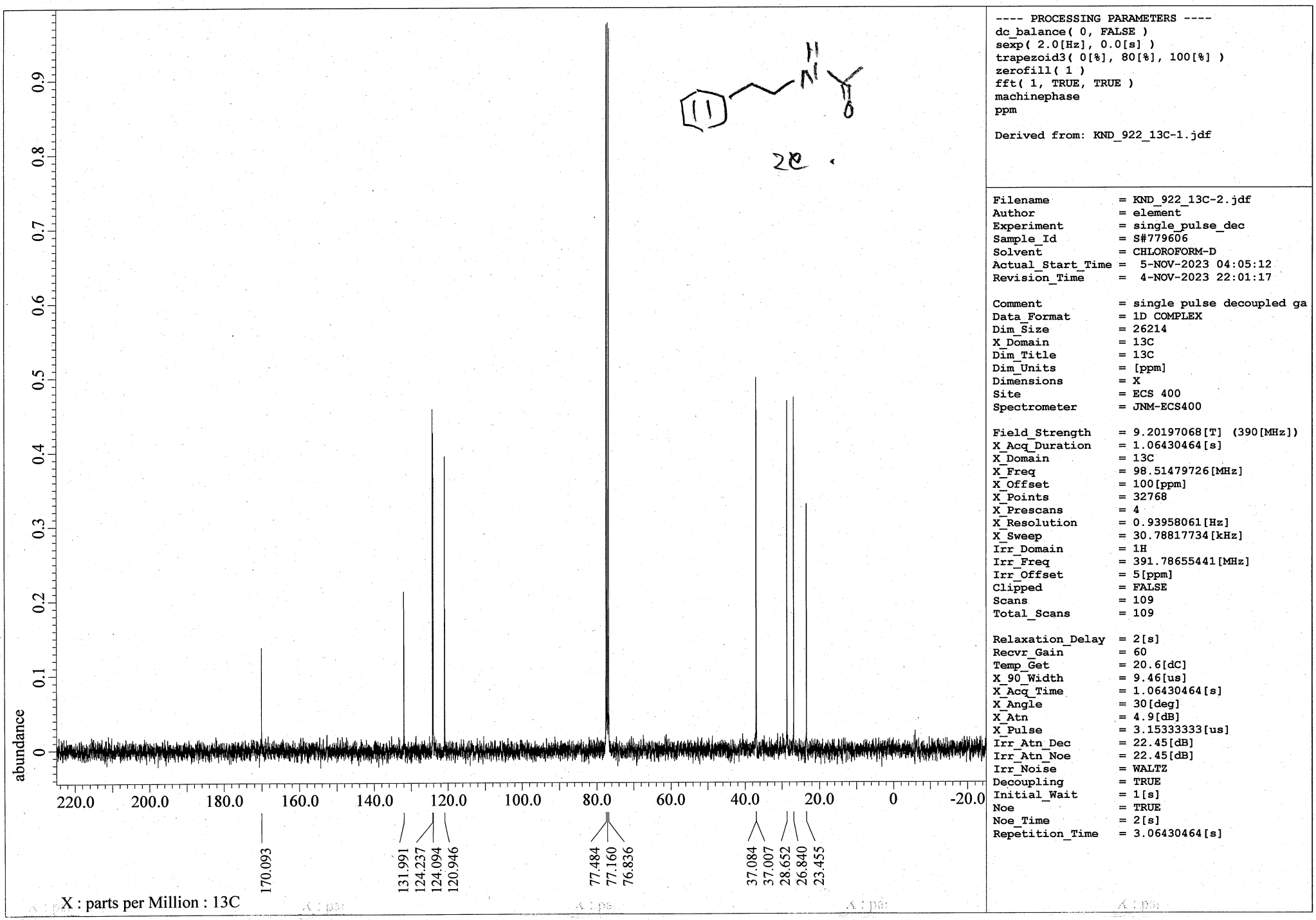
Filename	= KND_952_13C_Carbon-1-2.jd
Author	= element
Experiment	= carbon.jxp
Sample_Id	= KND_952_13C
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 4-MAY-2023 18:30:15
Revision_Time	= 2-OCT-2023 15:36:13
Comment	= single pulse decoupled ga
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon
Dim_Title	= 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	= 100
Total_Scans	= 100
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 19.3[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]



2e

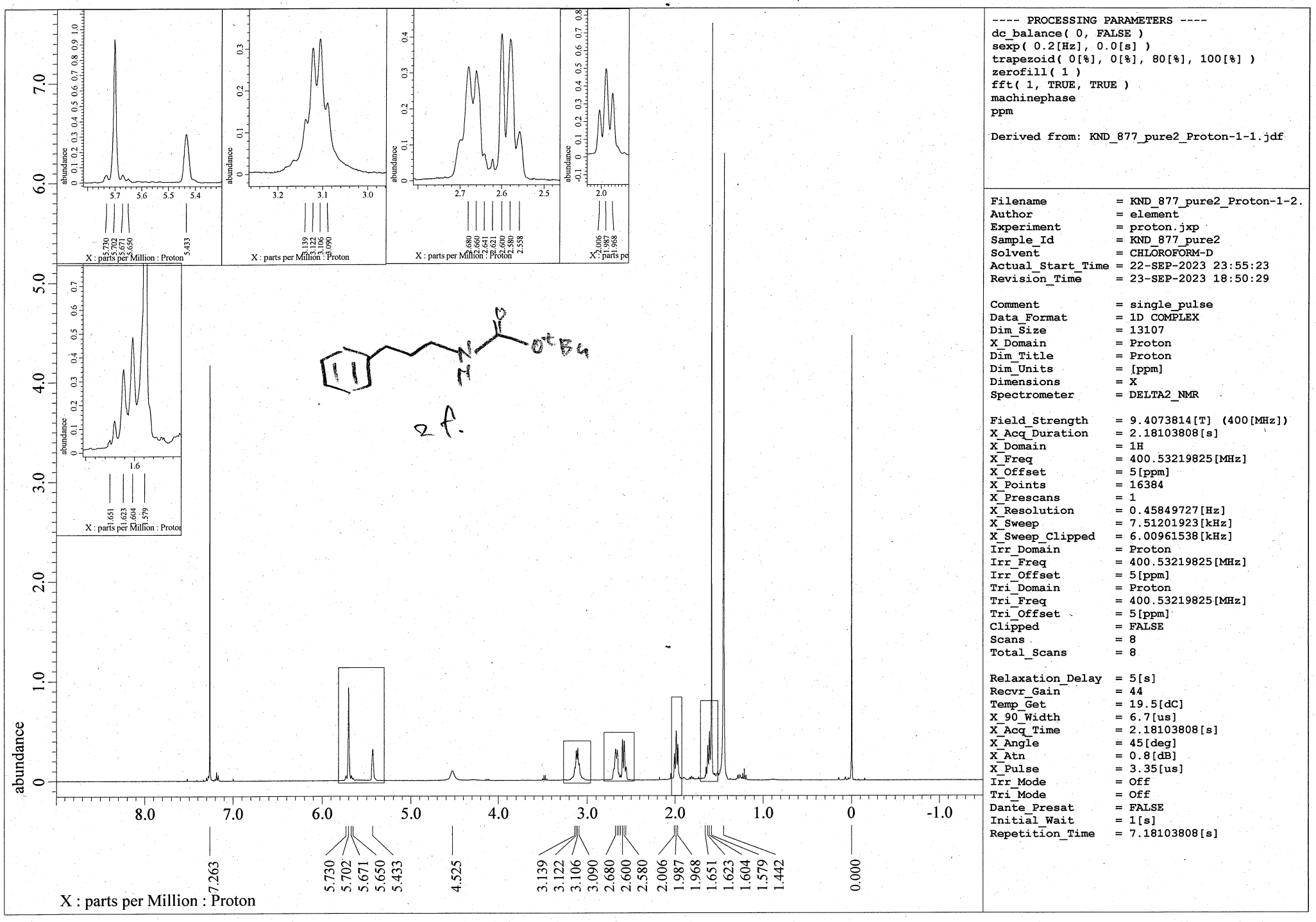
```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KND_922_pure-1.jdf
```

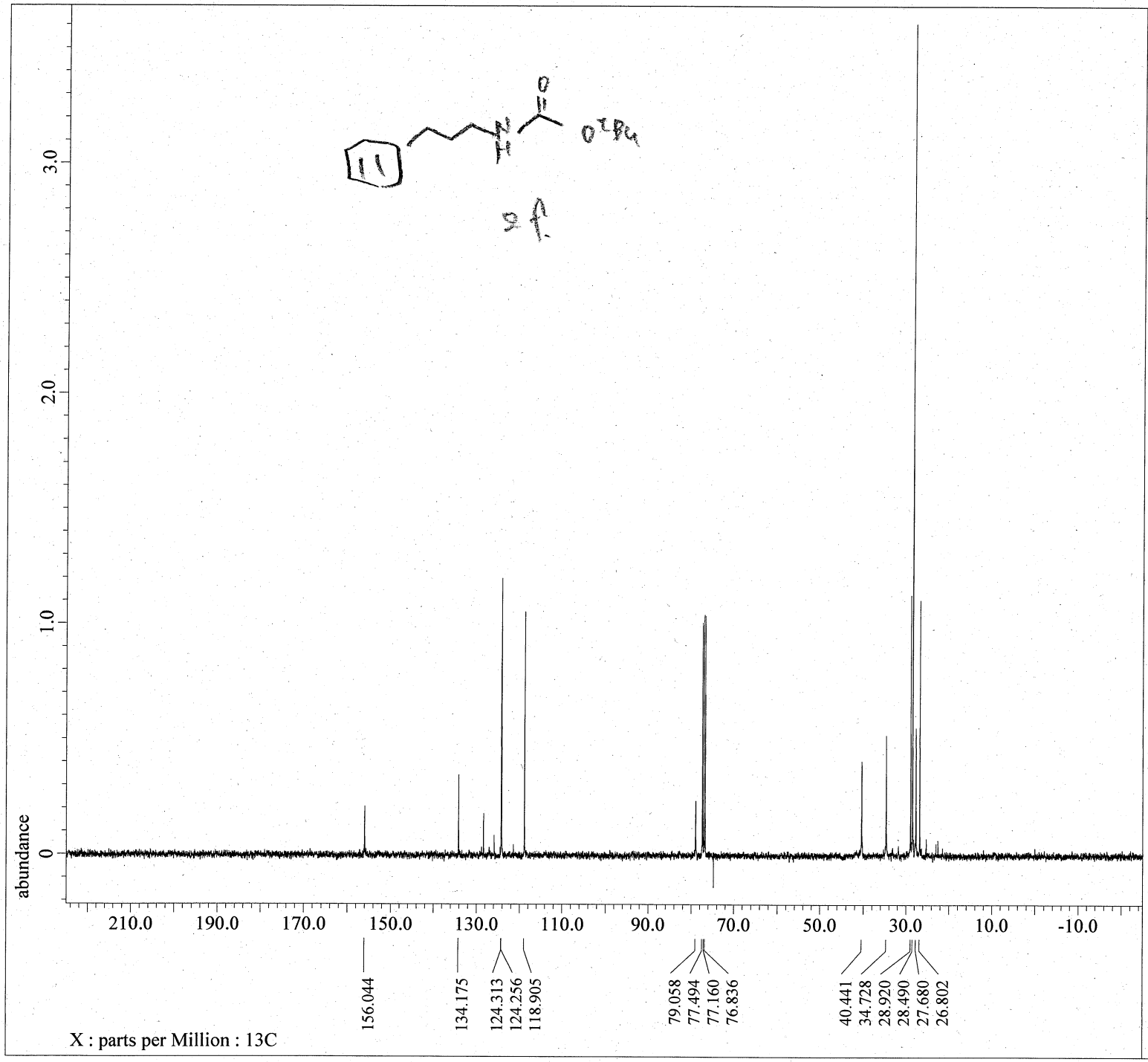
Filename	= KND_922_pure-2.jdf
Author	= element
Experiment	= single_pulse.ex2
Sample_Id	= S#772426
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 5-NOV-2023 03:53:24
Revision_Time	= 4-NOV-2023 21:59:13
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= 1H
Dim_Title	= 1H
Dim_Units	= [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	= 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
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_922_13C-1.jdf
```

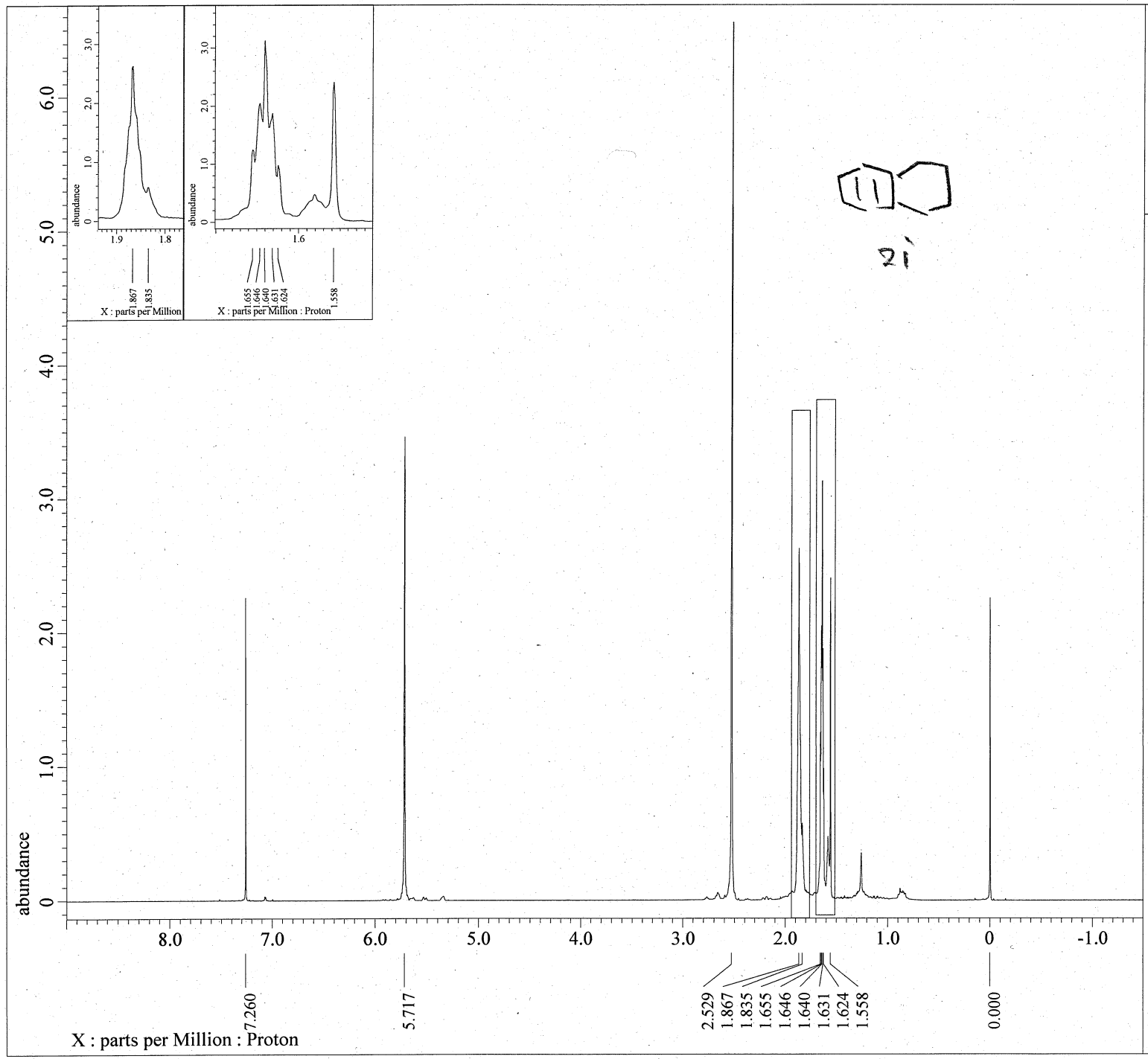
Filename	= KND_922_13C-2.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= S#779606
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 5-NOV-2023 04:05:12
Revision_Time	= 4-NOV-2023 22:01:17
Comment	= single pulse decoupled ga
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= 13C
Dim_Title	= 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	= 109
Total_Scans	= 109
Relaxation_Delay	= 2[s]
Recvr_Gain	= 60
Temp_Get	= 20.6[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_877_pure2_Proton-1-1.jdf
Filename = KND_877_pure2_Proton-1-2.
Author = element
Experiment = proton.jxp
Sample_Id = KND_877_pure2
Solvent = CHLOROFORM-D
Actual_Start_Time = 22-SEP-2023 23:55:23
Revision_Time = 23-SEP-2023 18:50:29
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = DELTA2_NMR
Field_Strength = 9.4073814[T] (400[MHz])
X_Acq_Duration = 2.18103808[s]
X_Domain = 1H
X_Freq = 400.53219825[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45849727[Hz]
X_Sweep = 7.51201923[kHz]
X_Sweep_Clipped = 6.00961538[kHz]
Irr_Domain = Proton
Irr_Freq = 400.53219825[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 400.53219825[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 44
Temp_Get = 19.5[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]
2f.
abundance
X : parts per Million : Proton
7.263
5.730
5.702
5.671
5.650
5.433
4.525
3.139
3.122
3.106
3.090
2.680
2.600
2.580
2.006
1.987
1.968
1.651
1.623
1.604
1.579
1.442
0.000



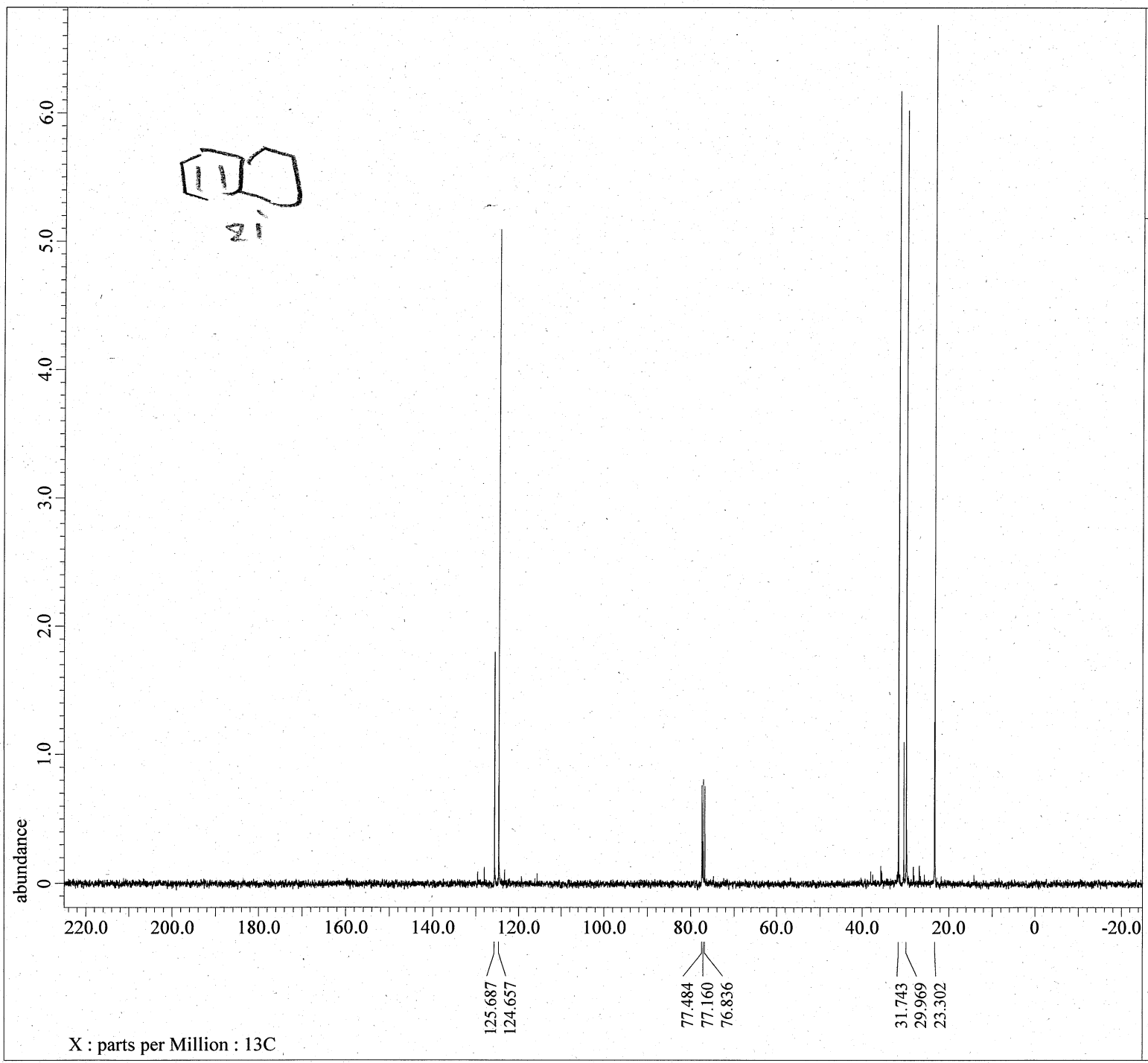

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KND_877_13C-1.jdf
```

Filename	= KND_877_13C-2.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= 1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 23-SEP-2023 06:08:13
Revision_Time	= 23-SEP-2023 18:53:43
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	= 78
Total_Scans	= 78
Relaxation_Delay	= 2[s]
Recvr_Gain	= 60
Temp_Get	= 20.1[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]



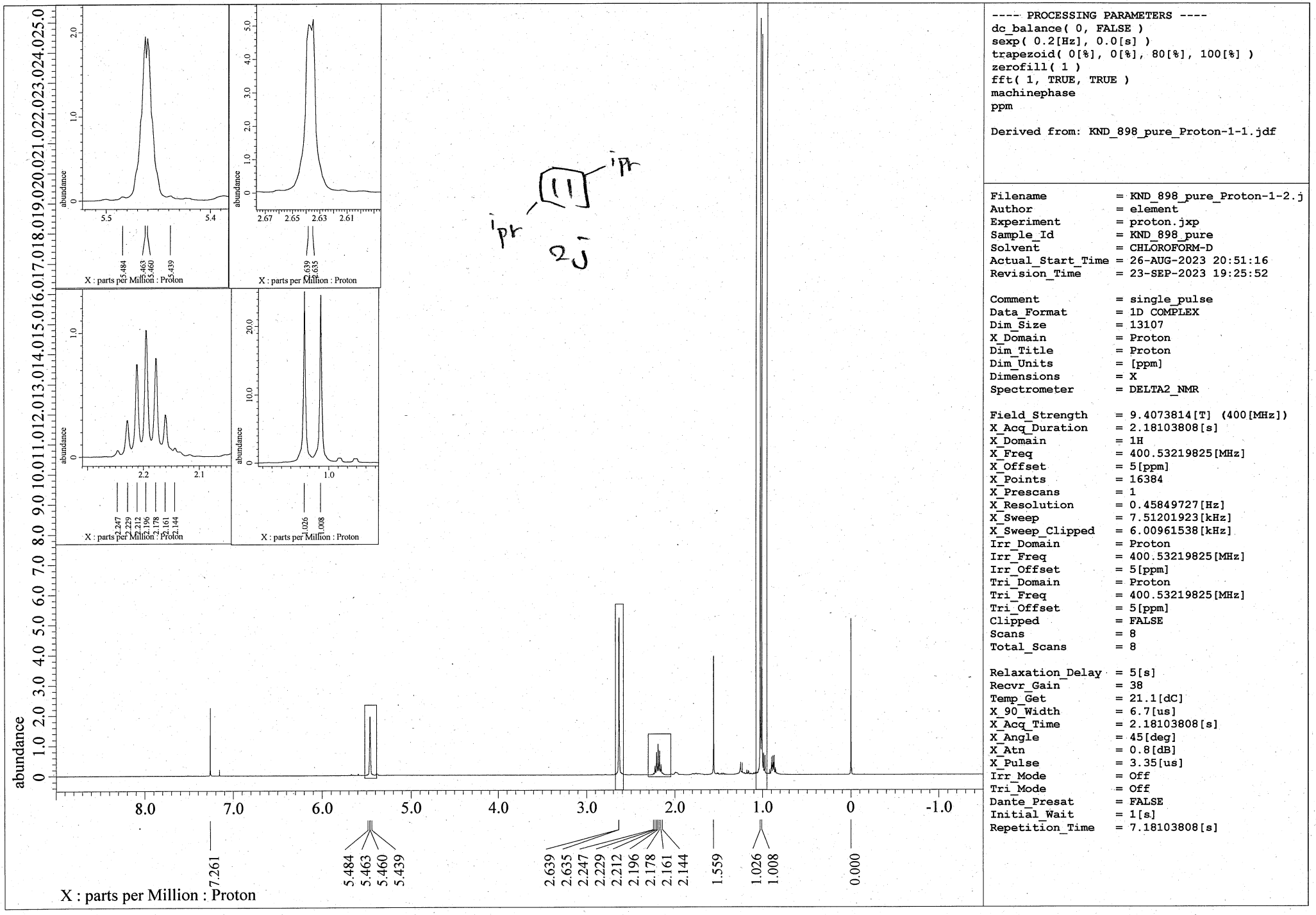

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KND_1054_pure_Proton-1-1.jdf
```

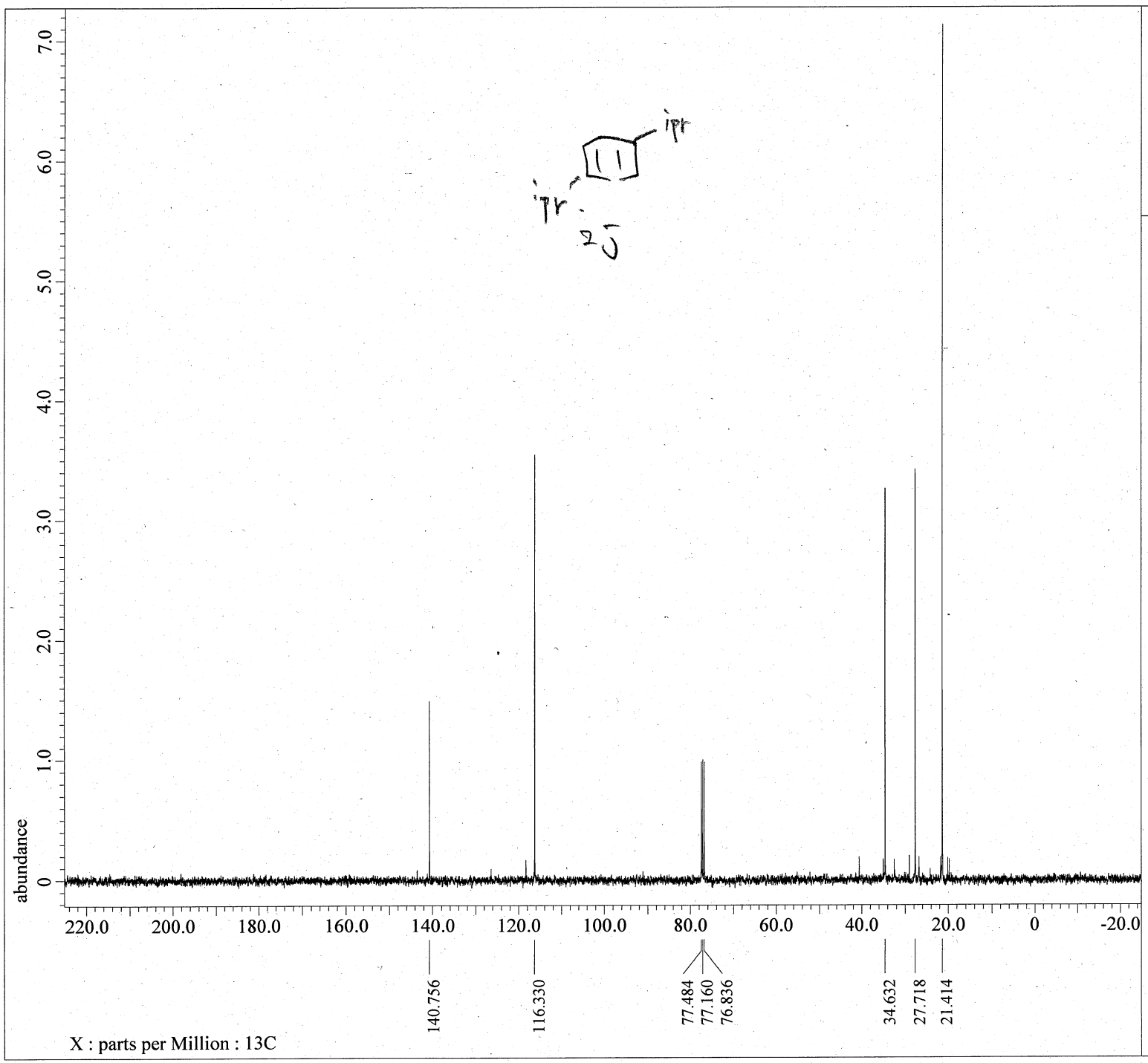
Filename	= KND_1054_pure_Proton-1-2.
Author	= element
Experiment	= proton.jxp
Sample_Id	= KND_1054_pure
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 25-AUG-2023 22:20:14
Revision_Time	= 23-SEP-2023 19:10:05
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.4073814[T] (400[MHz])
X_Acq_Duration	= 2.18103808[s]
X_Domain	= 1H
X_Freq	= 400.53219825[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45849727[Hz]
X_Sweep	= 7.51201923[kHz]
X_Sweep_Clipped	= 6.00961538[kHz]
Irr_Domain	= Proton
Irr_Freq	= 400.53219825[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 400.53219825[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 40
Temp_Get	= 21.6[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 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KND_1054_13C-1.jdf
```

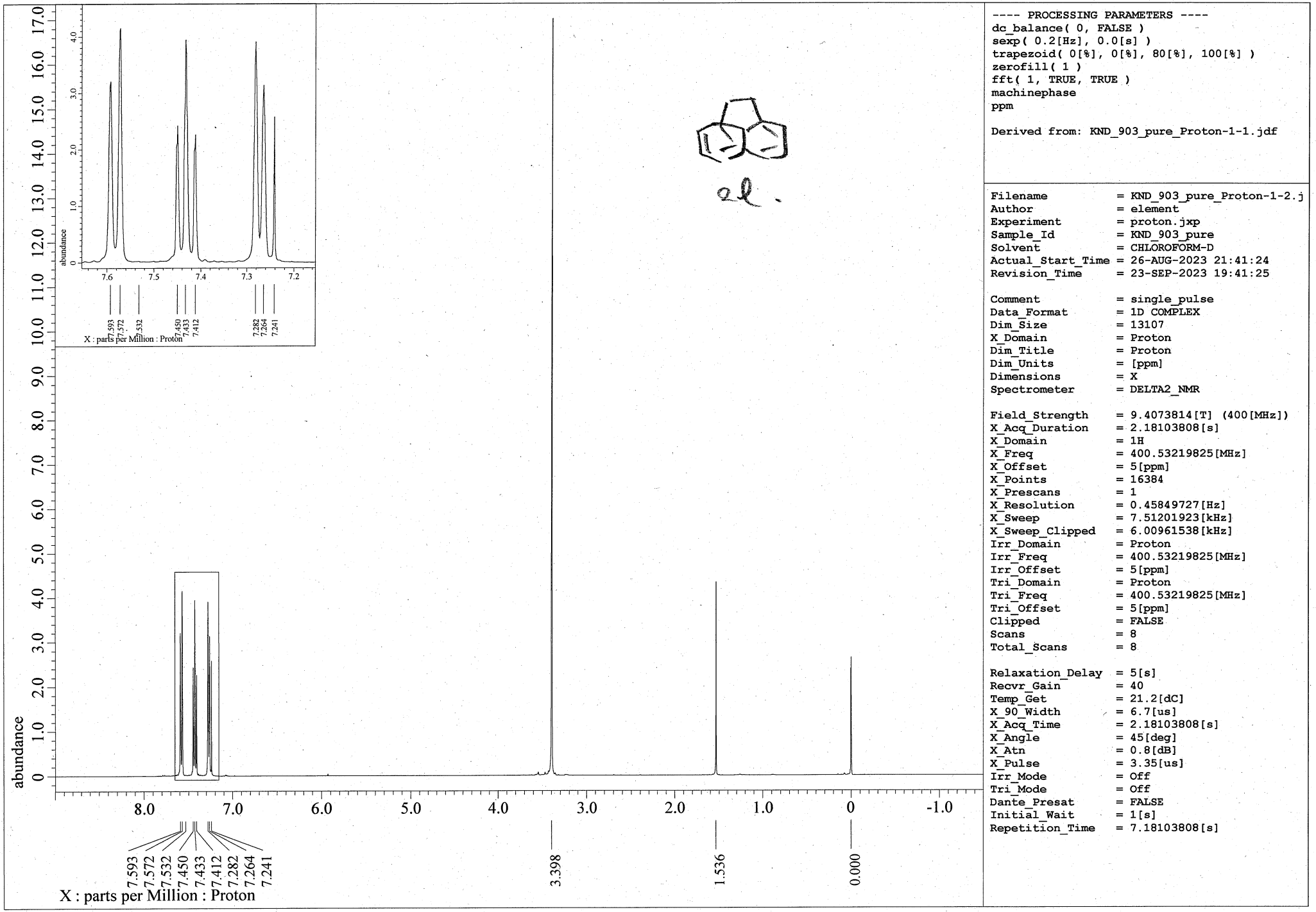
Filename	= KND_1054_13C-2.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= 1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 26-AUG-2023 04:27:05
Revision_Time	= 23-SEP-2023 19:13:03
Comment	= single pulse decoupled ga
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= 13C
Dim_Title	= 13C
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	= 23
Total_Scans	= 23
Relaxation_Delay	= 2[s]
Recvr_Gain	= 60
Temp_Get	= 23.4[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)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: KND_898_pure_Proton-1-1.jdf
Filename = KND_898_pure_Proton-1-2.j
Author = element
Experiment = proton.jxp
Sample_Id = KND_898_pure
Solvent = CHLOROFORM-D
Actual_Start_Time = 26-AUG-2023 20:51:16
Revision_Time = 23-SEP-2023 19:25:52
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = DELTA2_NMR
Field_Strength = 9.4073814[T] (400[MHz])
X_Acq_Duration = 2.18103808[s]
X_Domain = 1H
X_Freq = 400.53219825[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45849727[Hz]
X_Sweep = 7.51201923[kHz]
X_Sweep_Clipped = 6.00961538[kHz]
Irr_Domain = Proton
Irr_Freq = 400.53219825[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 400.53219825[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 38
Temp_Get = 21.1[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]
abundance
X : parts per Million : Proton
7.261
5.484
5.463
5.460
5.439
2.639
2.635
2.247
2.229
2.212
2.196
2.178
2.161
2.144
1.559
1.026
1.008
0.000
iPr
iPr
2J



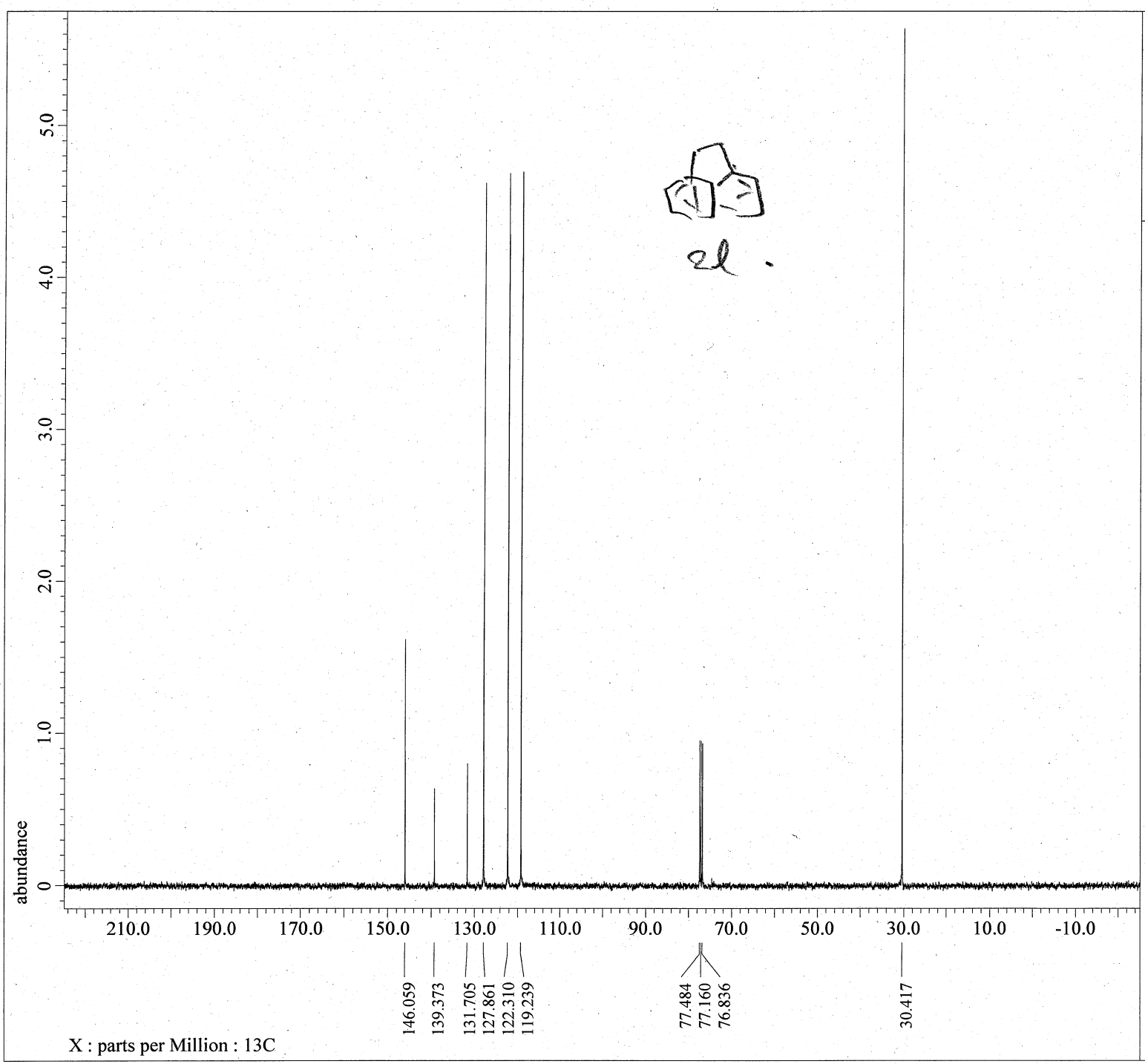

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KND_898_13C-1.jdf
```

Filename	= KND_898_13C-2.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= 1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 27-AUG-2023 02:56:17
Revision_Time	= 23-SEP-2023 19:30:47
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	= 13
Total_Scans	= 13
Relaxation_Delay	= 2[s]
Recvr_Gain	= 60
Temp_Get	= 23.5[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]



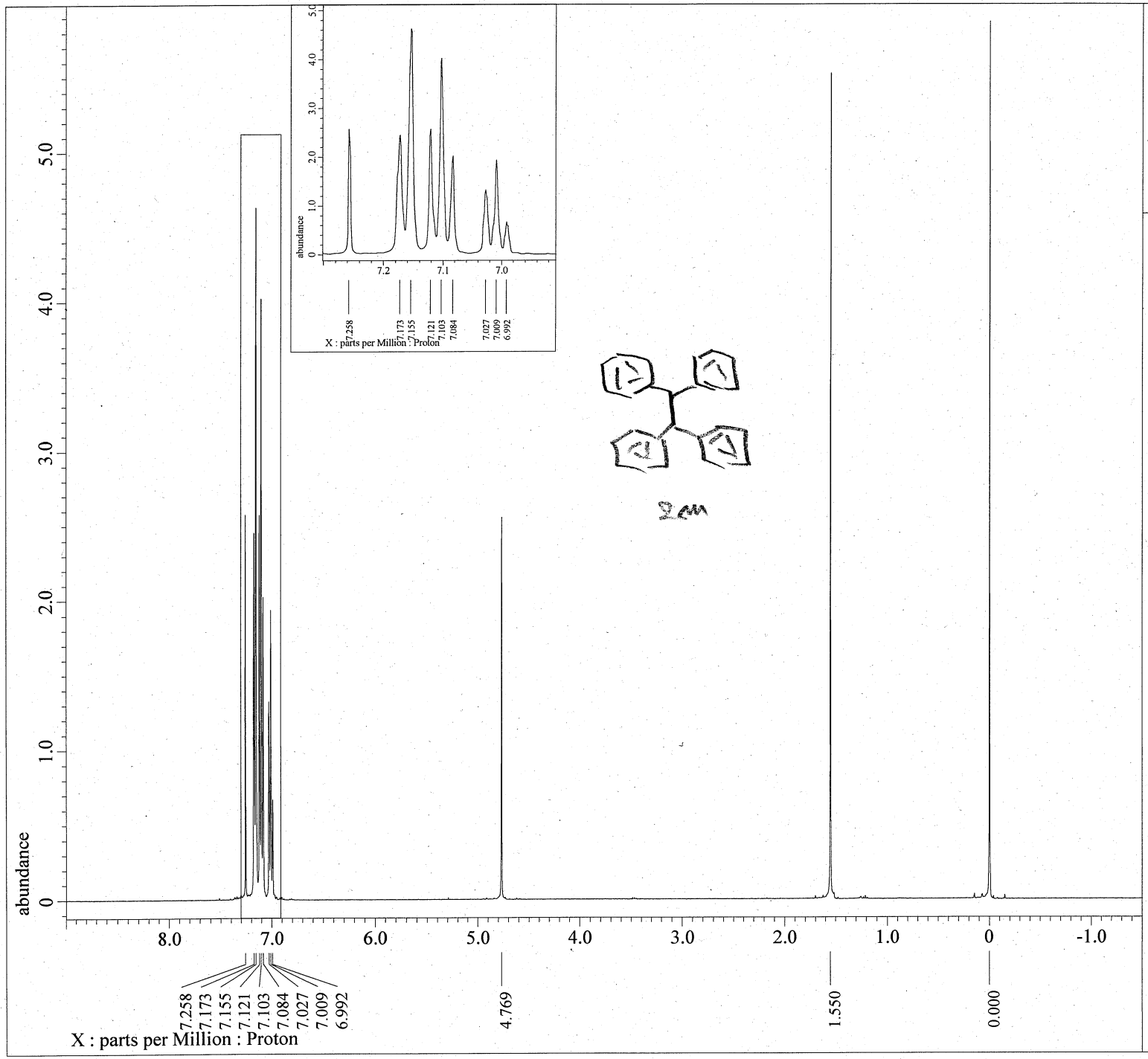

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KND_903_pure_Proton-1-1.jdf
```

Filename	= KND_903_pure_Proton-1-2.j
Author	= element
Experiment	= proton.jxp
Sample_Id	= KND_903_pure
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 26-AUG-2023 21:41:24
Revision_Time	= 23-SEP-2023 19:41:25
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.4073814[T] (400[MHz])
X_Acq_Duration	= 2.18103808[s]
X_Domain	= 1H
X_Freq	= 400.53219825[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45849727[Hz]
X_Sweep	= 7.51201923[kHz]
X_Sweep_Clipped	= 6.00961538[kHz]
Irr_Domain	= Proton
Irr_Freq	= 400.53219825[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 400.53219825[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 40
Temp_Get	= 21.2[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]



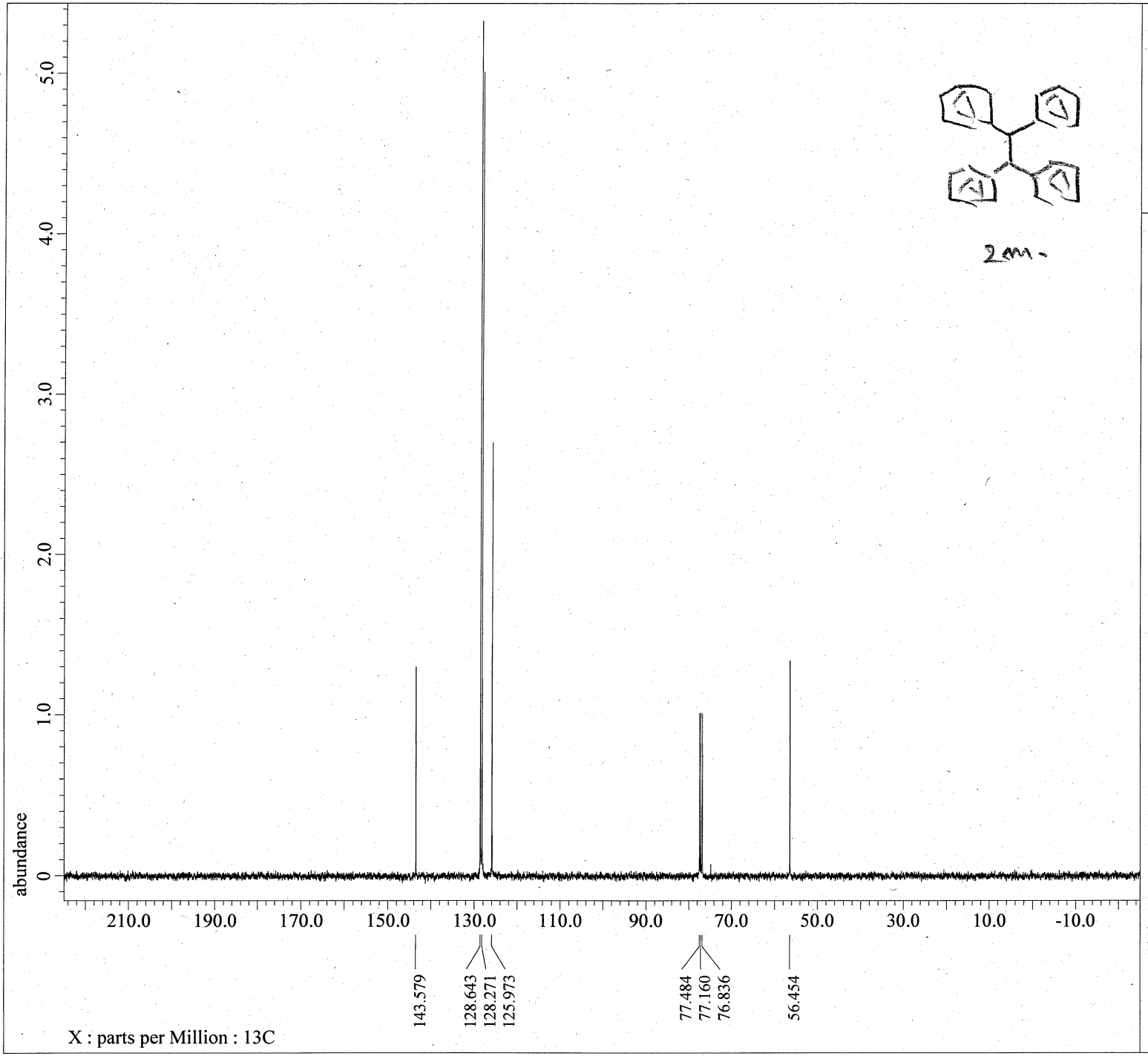

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KND_903_13C-1.jdf
```

Filename	= KND_903_13C-2.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= 1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 27-AUG-2023 03:48:43
Revision_Time	= 23-SEP-2023 19:42:59
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	= 42
Total_Scans	= 42
Relaxation_Delay	= 2[s]
Recvr_Gain	= 60
Temp_Get	= 23.5[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_918_pure_Proton-1-1.jdf
```

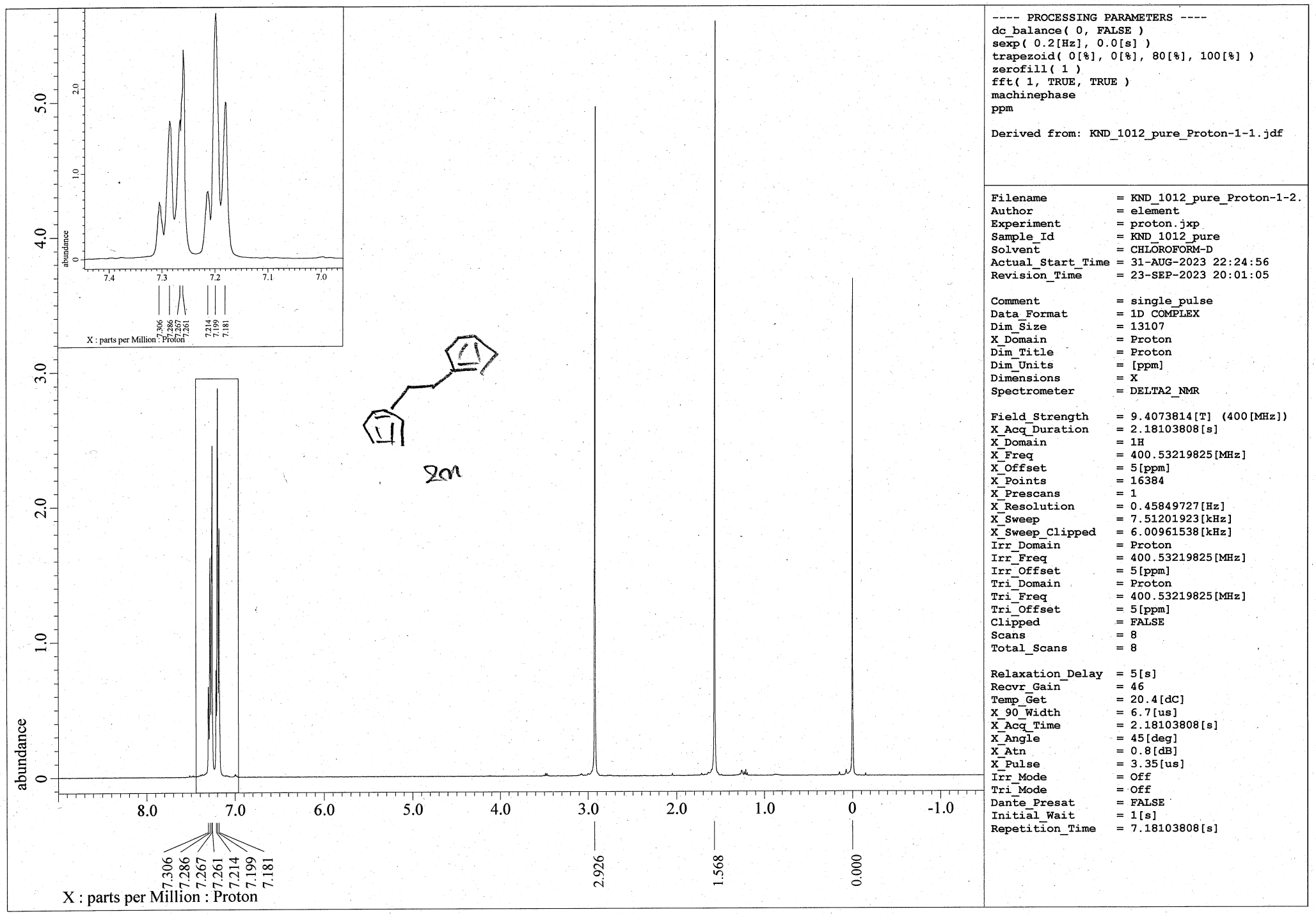
Filename	= KND_918_pure_Proton-1-2.j
Author	= element
Experiment	= proton.jxp
Sample_Id	= KND_918_pure
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 27-AUG-2023 20:35:35
Revision_Time	= 23-SEP-2023 19:51:23
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.4073814[T] (400[MHz])
X_Acq_Duration	= 2.18103808[s]
X_Domain	= 1H
X_Freq	= 400.53219825[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45849727[Hz]
X_Sweep	= 7.51201923[kHz]
X_Sweep_Clipped	= 6.00961538[kHz]
Irr_Domain	= Proton
Irr_Freq	= 400.53219825[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 400.53219825[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 44
Temp_Get	= 20.2[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]



2mm

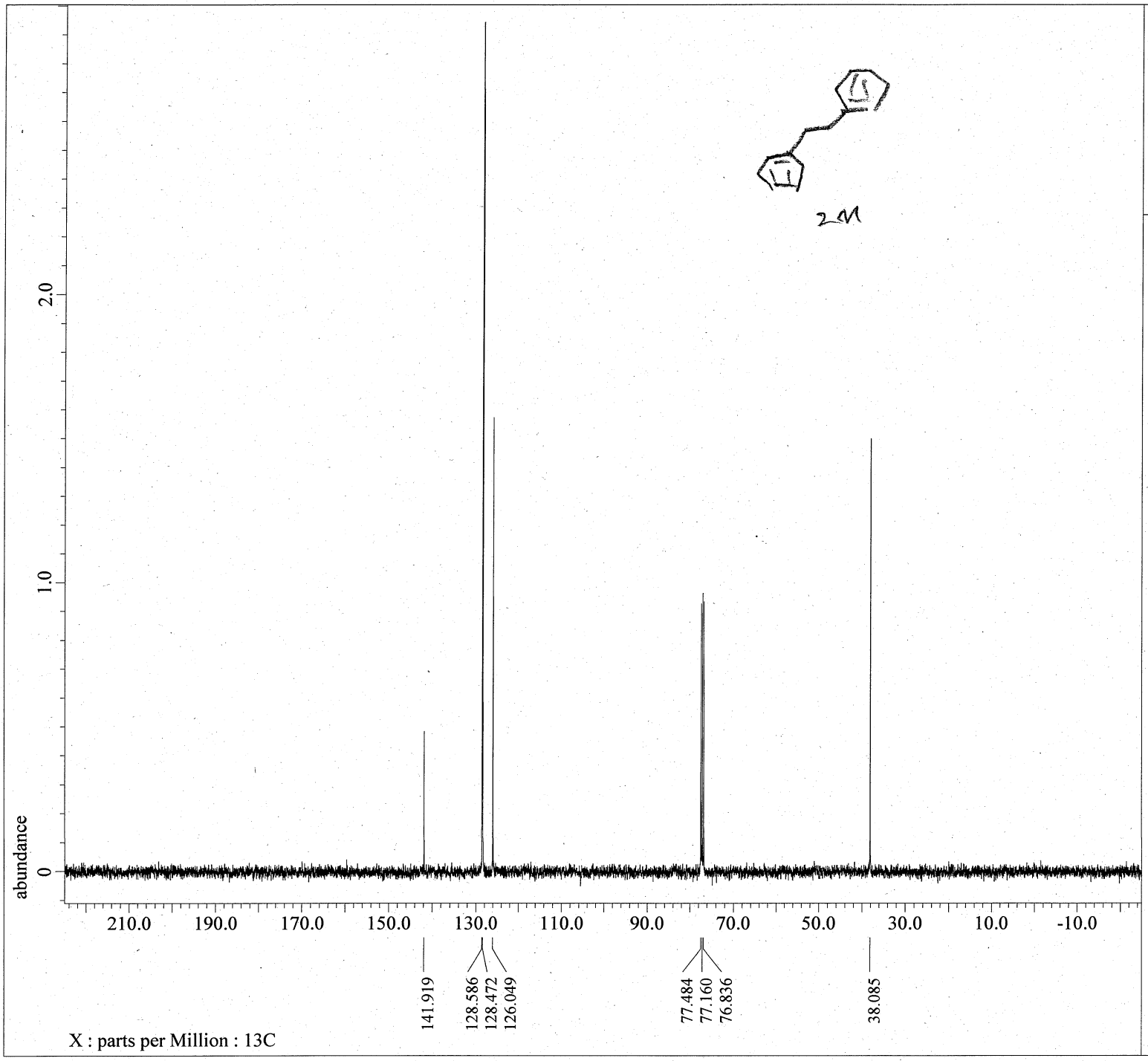
```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KND_918_13C-1.jdf
```

Filename	= KND_918_13C-2.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= 1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 28-AUG-2023 02:39:22
Revision_Time	= 23-SEP-2023 19:52:40
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	= 33
Total_Scans	= 33
Relaxation_Delay	= 2[s]
Recvr_Gain	= 60
Temp_Get	= 22.8[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]



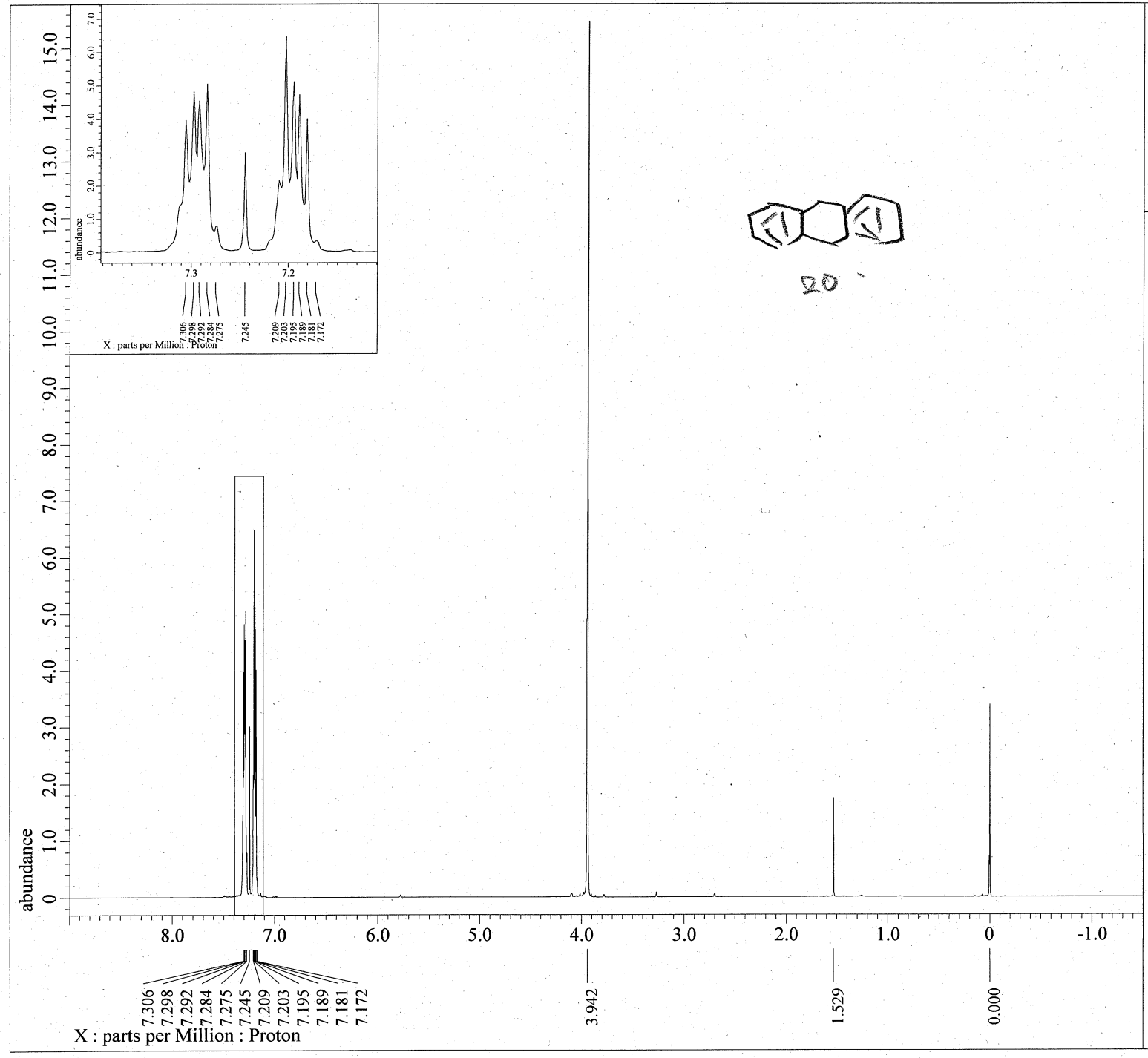

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KND_1012_pure_Proton-1-1.jdf
```

Filename	= KND_1012_pure_Proton-1-2.
Author	= element
Experiment	= proton.jxp
Sample_Id	= KND_1012_pure
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 31-AUG-2023 22:24:56
Revision_Time	= 23-SEP-2023 20:01:05
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.4073814[T] (400[MHz])
X_Acq_Duration	= 2.18103808[s]
X_Domain	= 1H
X_Freq	= 400.53219825[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45849727[Hz]
X_Sweep	= 7.51201923[kHz]
X_Sweep_Clipped	= 6.00961538[kHz]
Irr_Domain	= Proton
Irr_Freq	= 400.53219825[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 400.53219825[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 46
Temp_Get	= 20.4[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]



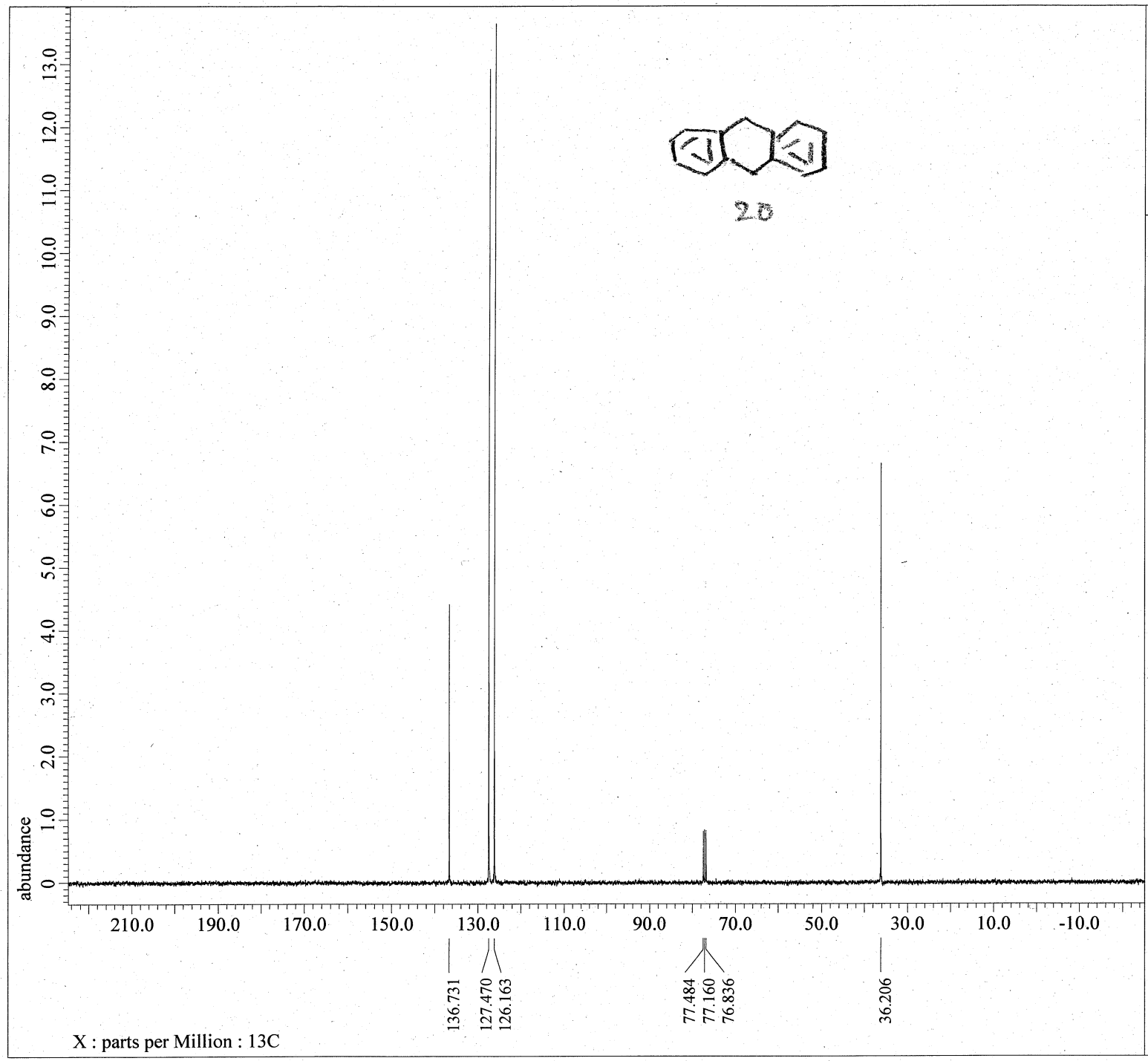

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KND_1012_13C-1.jdf
```

Filename	= KND_1012_13C-2.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= 1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 1-SEP-2023 04:29:12
Revision_Time	= 23-SEP-2023 20:02:28
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	= 38
Total_Scans	= 38
Relaxation_Delay	= 2[s]
Recvr_Gain	= 60
Temp_Get	= 23[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_906_pure_Proton-1-1.jdf
```

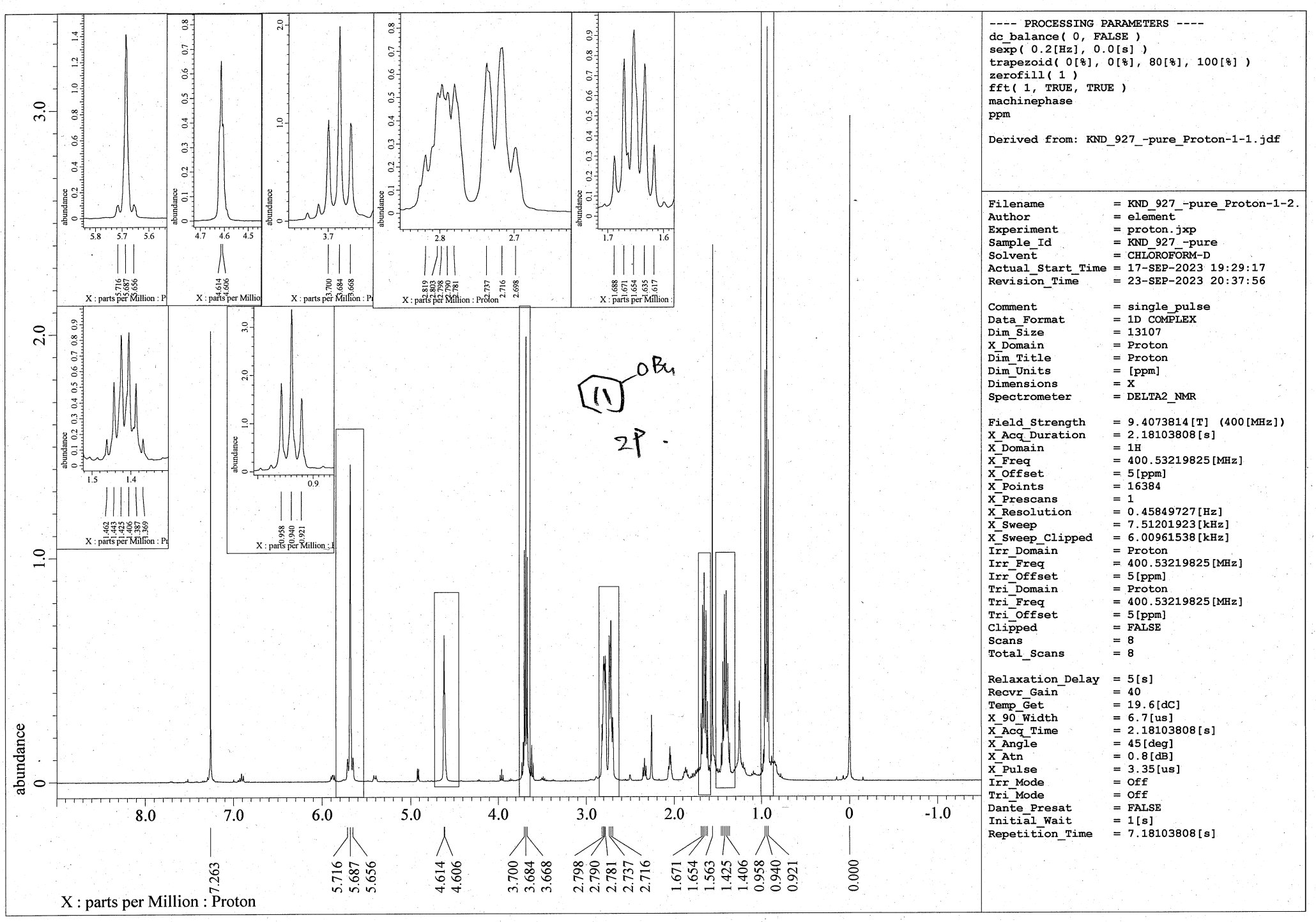
Filename	= KND_906_pure_Proton-1-2.j
Author	= element
Experiment	= proton.jxp
Sample_Id	= KND_906_pure
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 15-SEP-2023 21:54:38
Revision_Time	= 23-SEP-2023 20:20:36
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
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	= 40
Temp_Get	= 19.8[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]



20

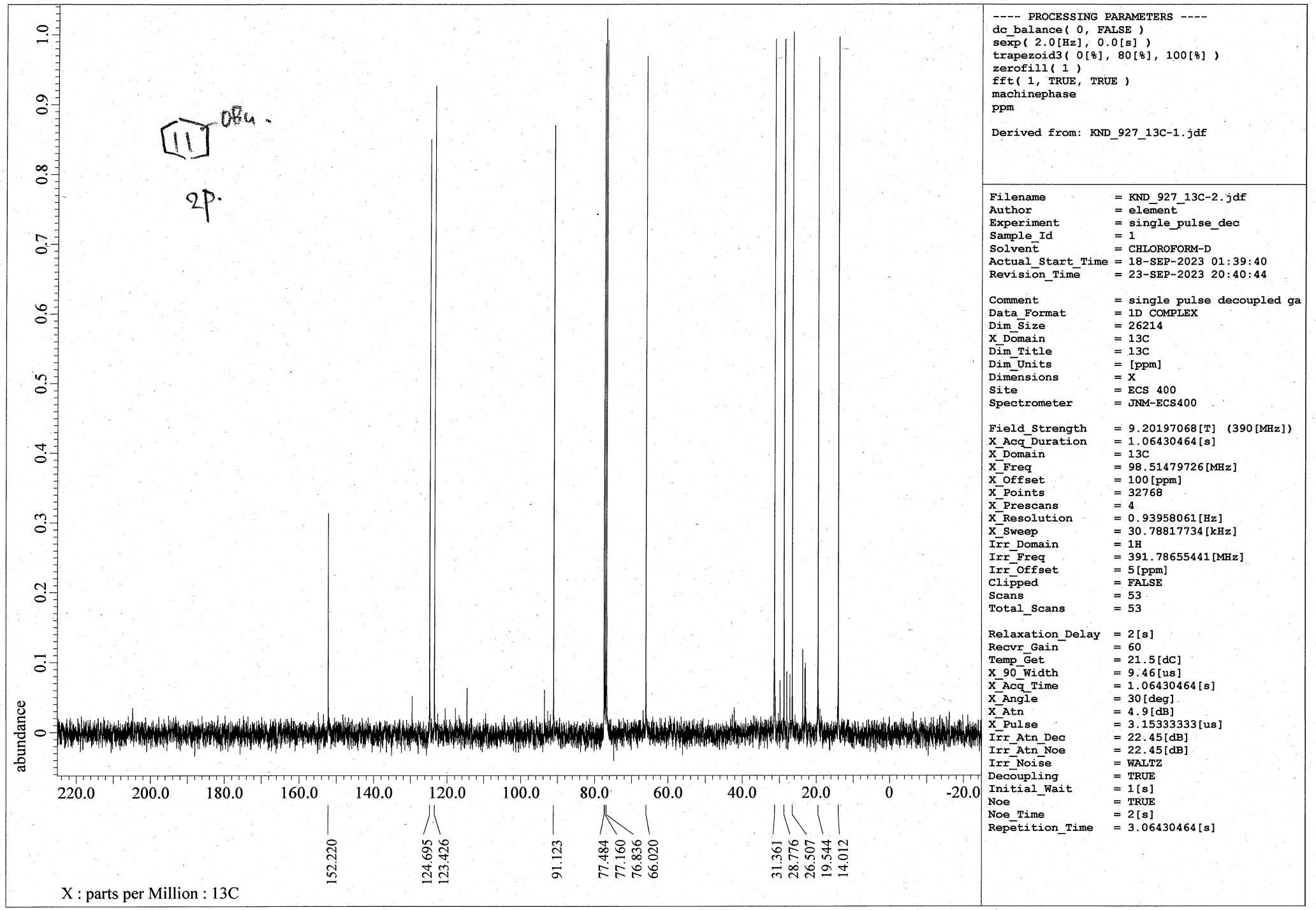
```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KND_906_13C-1.jdf
```

Filename	= KND_906_13C-2.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= 1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 16-SEP-2023 03:32:57
Revision_Time	= 23-SEP-2023 20:22:17
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	= 15
Total_Scans	= 15
Relaxation_Delay	= 2[s]
Recvr_Gain	= 60
Temp_Get	= 21.1[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]



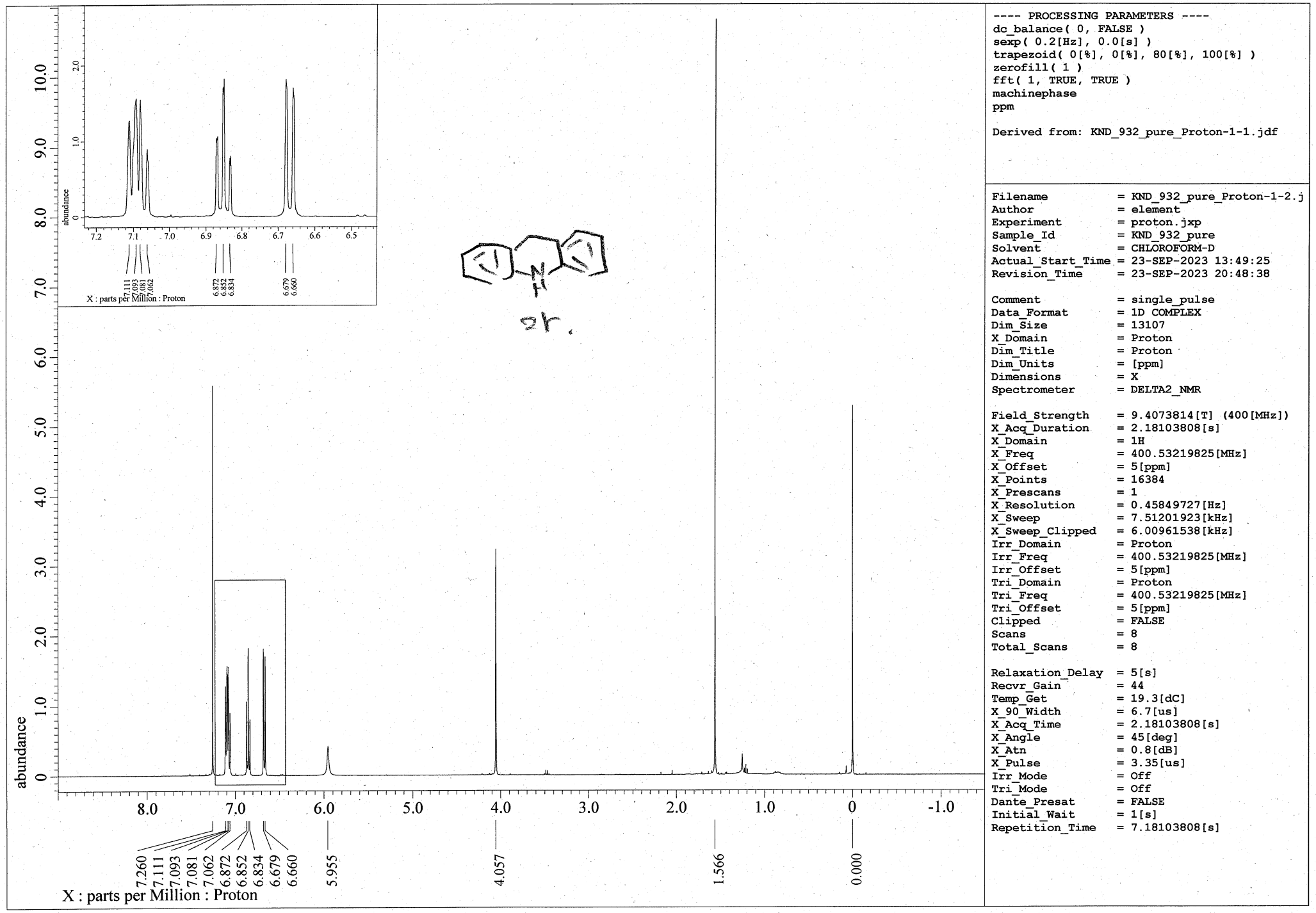

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KND_927_-pure_Proton-1-1.jdf
```

Filename	= KND_927_-pure_Proton-1-2.
Author	= element
Experiment	= proton.jxp
Sample_Id	= KND_927_-pure
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 17-SEP-2023 19:29:17
Revision_Time	= 23-SEP-2023 20:37:56
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.4073814[T] (400[MHz])
X_Acq_Duration	= 2.18103808[s]
X_Domain	= 1H
X_Freq	= 400.53219825[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45849727[Hz]
X_Sweep	= 7.51201923[kHz]
X_Sweep_Clipped	= 6.00961538[kHz]
Irr_Domain	= Proton
Irr_Freq	= 400.53219825[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 400.53219825[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 40
Temp_Get	= 19.6[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]



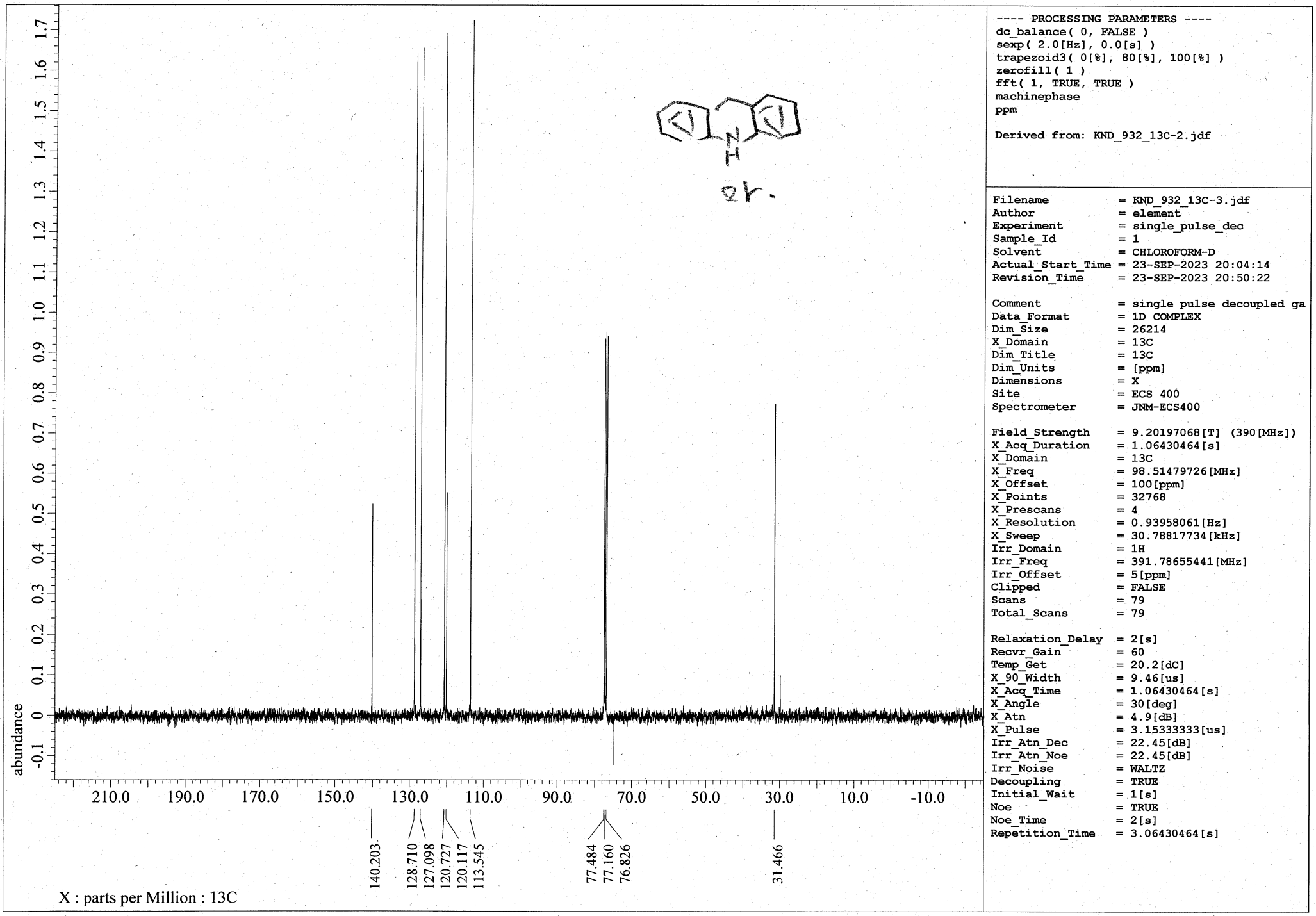

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KND_927_13C-1.jdf
```

Filename	= KND_927_13C-2.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= 1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 18-SEP-2023 01:39:40
Revision_Time	= 23-SEP-2023 20:40:44
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	= 53
Total_Scans	= 53
Relaxation_Delay	= 2[s]
Recvr_Gain	= 60
Temp_Get	= 21.5[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]



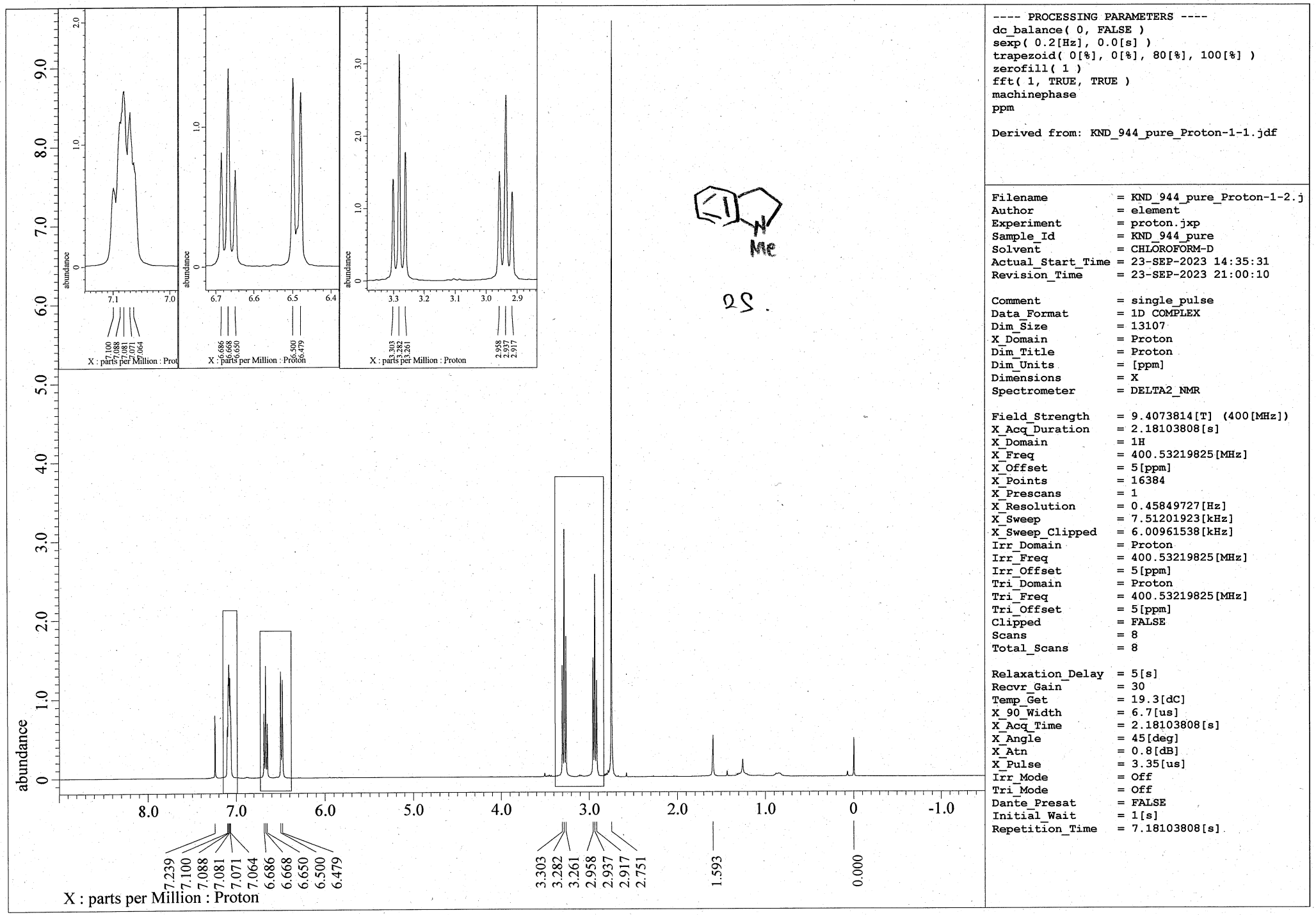

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KND_932_pure_Proton-1-1.jdf
```

Filename	= KND_932_pure_Proton-1-2.j
Author	= element
Experiment	= proton.jxp
Sample_Id	= KND_932_pure
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 23-SEP-2023 13:49:25
Revision_Time	= 23-SEP-2023 20:48:38
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.4073814[T] (400[MHz])
X_Acq_Duration	= 2.18103808[s]
X_Domain	= 1H
X_Freq	= 400.53219825[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45849727[Hz]
X_Sweep	= 7.51201923[kHz]
X_Sweep_Clipped	= 6.00961538[kHz]
Irr_Domain	= Proton
Irr_Freq	= 400.53219825[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 400.53219825[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 44
Temp_Get	= 19.3[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]



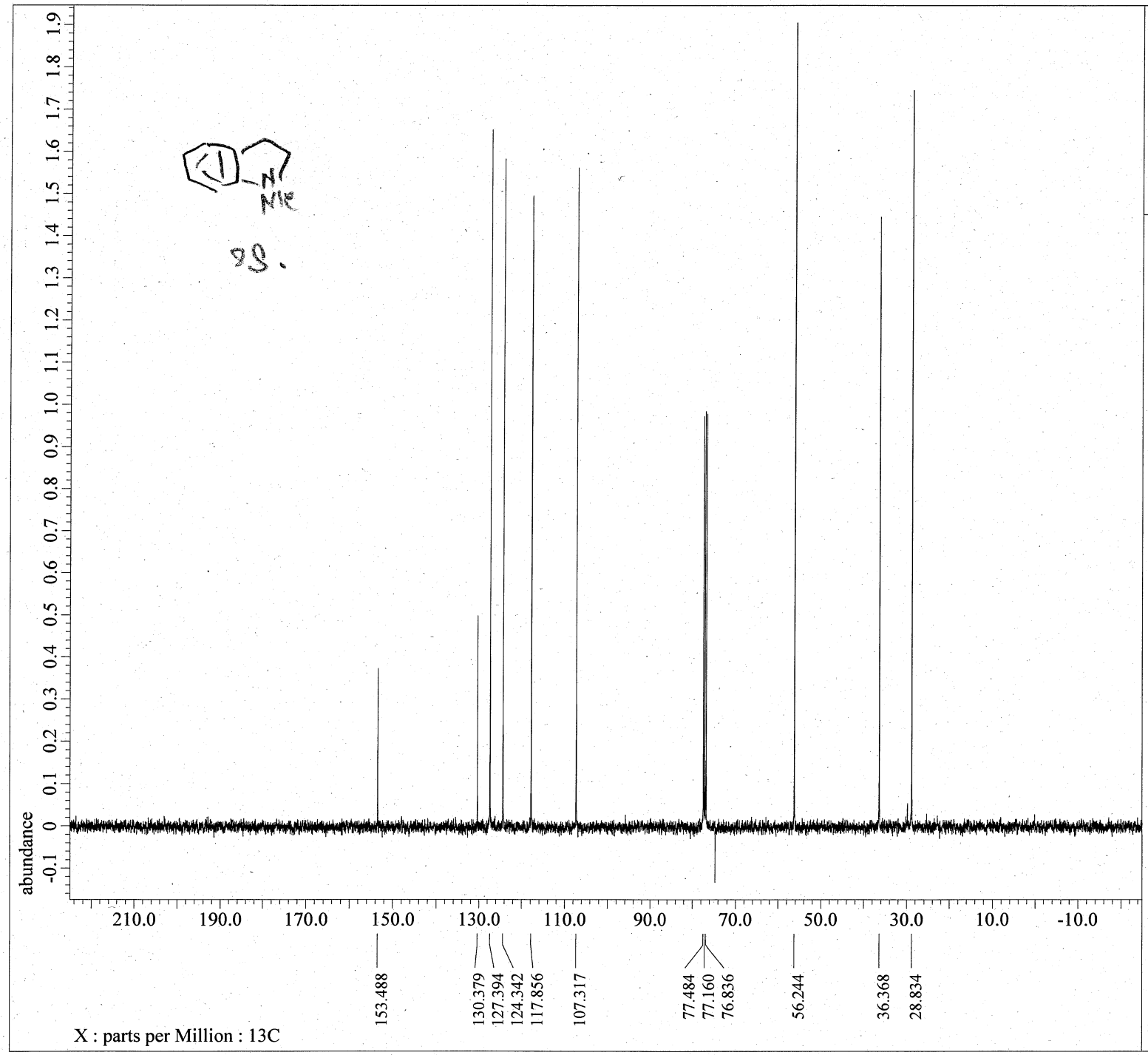

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KND_932_13C-2.jdf
```

Filename	= KND_932_13C-3.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= 1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 23-SEP-2023 20:04:14
Revision_Time	= 23-SEP-2023 20:50:22
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	= 79
Total_Scans	= 79
Relaxation_Delay	= 2[s]
Recvr_Gain	= 60
Temp_Get	= 20.2[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 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: KND_944_pure_Proton-1-1.jdf
```

Filename	= KND_944_pure_Proton-1-2.j
Author	= element
Experiment	= proton.jxp
Sample_Id	= KND_944_pure
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 23-SEP-2023 14:35:31
Revision_Time	= 23-SEP-2023 21:00:10
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	= 9.4073814[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	= 30
Temp_Get	= 19.3[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_944_13C-2.jdf
```

Filename	= KND_944_13C-3.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= 1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 23-SEP-2023 20:50:22
Revision_Time	= 23-SEP-2023 21:01:35
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	= 81
Total_Scans	= 81
Relaxation_Delay	= 2[s]
Recvr_Gain	= 60
Temp_Get	= 20.2[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]