A Mechanochemical [2+2+2] Cycloaddition Facilitated by a Cobalt(II) Catalyst and Piezoelectric Materials

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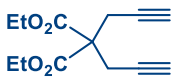
1. Instrumentation and Chemicals

Materials were obtained from commercial suppliers and purified by standard procedures unless otherwise noted. $BaTiO_3$ (tetragonal powder, <3 μm particle size, 99%, product No. 208108) and $BaTiO_3$ (cubic powder, <75 μm particle size, 99%, product No. 467634) were purchased from Sigma-Aldrich Co. LLC. All reactions were performed using grinding vessels in a Retsch MM 400. Both jars (5 mL) and balls (10 mm) are made of stainless steel (SUS400B and SUS420J2, respectively). Solvents for reactions were purchased from commercial suppliers. NMR spectra were recorded on JNM-ECZ400S spectrometers (^1H: 401 MHz, ^{13}C: 99 MHz, ^{19}F: 376 MHz). Tetramethylsilane (^1H) 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, m = multiplet. Mesitylene was used as an internal standard to determine NMR yields. Medium-pressure column chromatography was carried out on a Biotage Flash Purification System Isolera, which is equipped with a UV detector. High-resolution mass spectra were recorded at the Global Facility Center, Hokkaido University.

2. List of Substrates



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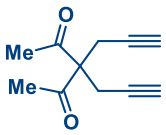

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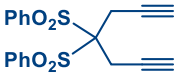

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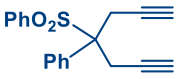

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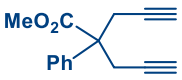

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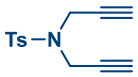
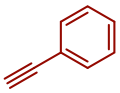


1f

1g



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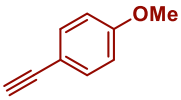

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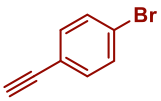

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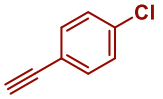

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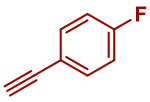

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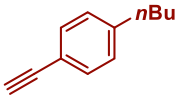

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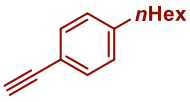

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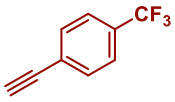

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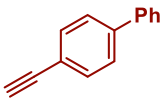

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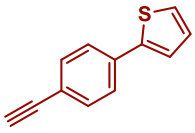

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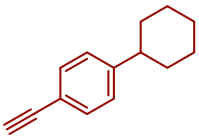

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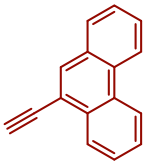

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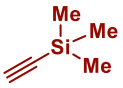
2m



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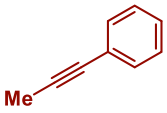
2o



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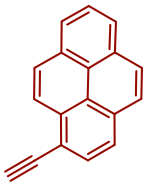
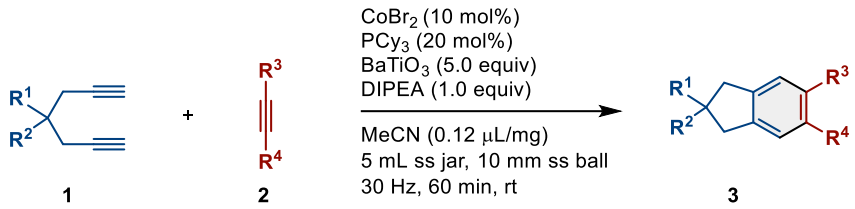


2q

All substrates are commercially available except the diynes **1a-1f**. **1a-1f** were prepared according to the reported procedure.[1]

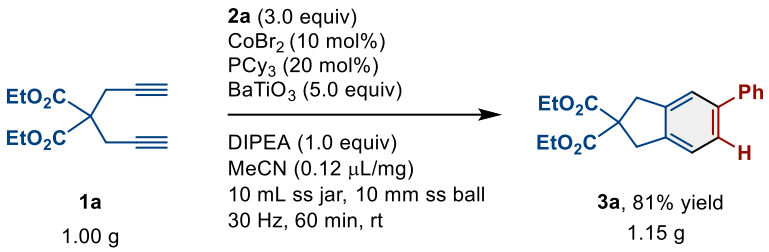
3. General Experimental Procedure for [2+2+2] Cycloaddition



Diyne **1** (0.2 mmol) and $BaTiO_3$ (233.2 mg, 1.0 mmol, 5.0 equiv) were placed in a stainless-steel ball milling vessel (stainless steel, 5 mL) along with a single grinding ball (stainless steel, diameter: 10 mm). The vessel was then transferred to a glovebox, where $CoBr_2$ (4.3 mg, 0.02 mmol, 10 mol%), PCy_3 (11.3 mg, 0.04 mmol, 20 mol%), DIPEA (25.9 mg, 0.2 mmol, 1.0 equiv), alkyne **2** (0.6 mmol, 3.0 equiv), and MeCN (0.12 μL/mg) were added. After sealing the vessel inside the glovebox, the vessel was removed from the glovebox. Then, it was placed in a Retsch MM400 ball mill and subjected to milling at 30 Hz for 60 minutes. The jar was opened upon completion, and the reaction mixture was passed through a short silica gel column using EtOAc as the eluent. The crude product was then purified by flash column chromatography to afford the corresponding product **3**.

**Since $CoBr_2$ is highly moisture-sensitive, it should be stored and handled inside a glovebox.*

4. Scale-up Experiment Procedure of 3a

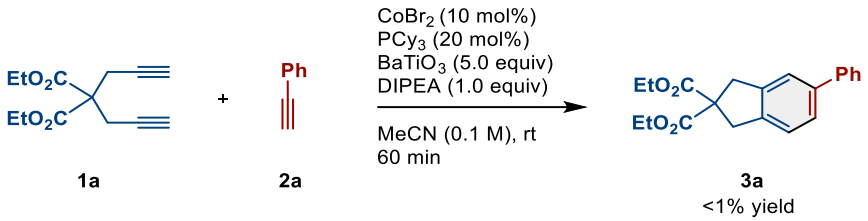


1a
1.00 g

3a, 81% yield
1.15 g

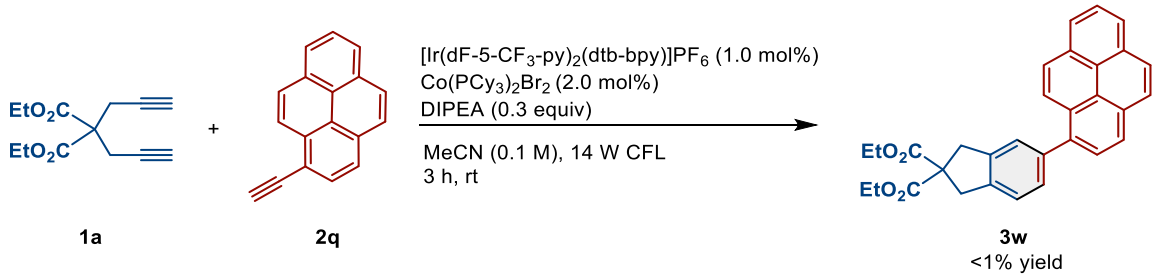
1a (1.00 g, 4.23 mmol) and $BaTiO_3$ (4.94 g, 21.1 mmol, 5.0 equiv) were placed in a stainless-steel ball milling vessel (stainless steel, 10 mL) along with a single grinding ball (stainless steel, 10 mm). The vessel as then transferred to a glovebox, where $CoBr_2$ (93.4 mg, 0.42 mmol, 10 mol%), PCy_3 (238.3 mg, 0.04 mmol, 20 mol%), DIPEA (735 μL, 4.23 mmol, 1.0 equiv), **2a** (1.4 mL, 12.6 mmol, 3.0 equiv), and MeCN (0.12 μL/mg) were added. After sealing the vessel inside the glovebox, the vessel was removed from the glovebox. Then, it was placed in a Retsch MM400 ball mill and subjected to milling at 30 Hz for 60 minutes. The jar was opened upon completion, and the reaction mixture was passed through a short silica gel column using EtOAc as the eluent. The crude product was then purified by flash column chromatography (SiO_2, Et_2O/hexane, 0:100 to 10:90) to afford the corresponding product **3a** in 81% yield (1.16 g, 3.38 mmol) as a yellowish oil.

5. Reaction in Test Tube



$BaTiO_3$ (233.4 mg, 1.0 mmol, 5.0 equiv) and **1a** (47.1 mg, 0.2 mmol) were placed in an oven-dried reaction test tube equipped with a magnetic stir bar. After the tube was sealed with a screw cap containing a Teflon-coated rubber septum, it was transferred to a glovebox. In a glovebox, $CoBr_2$ (4.1 mg, 0.02 mmol, 0.1 equiv) and PCy_3 (11.3 mg, 0.04 mmol, 0.2 equiv) were placed in the test tube. After sealing the test tube inside the glovebox, it was removed from the glovebox. Then, the test tube was connected to a vacuum/nitrogen manifold through a needle. DIPEA (35 μL, 0.2 mmol, 1.0 equiv), **2a** (65 μL, 0.6 mmol, 3.0 equiv), and MeCN (2.0 mL) were introduced to the mixture. The reaction mixture was stirred for 1 hour at room temperature before passing through a short silica gel column using EtOAc as the eluent. The crude mixture was analyzed by ^1H NMR analysis using mesitylene as an internal standard. In this case, no product formation was observed.

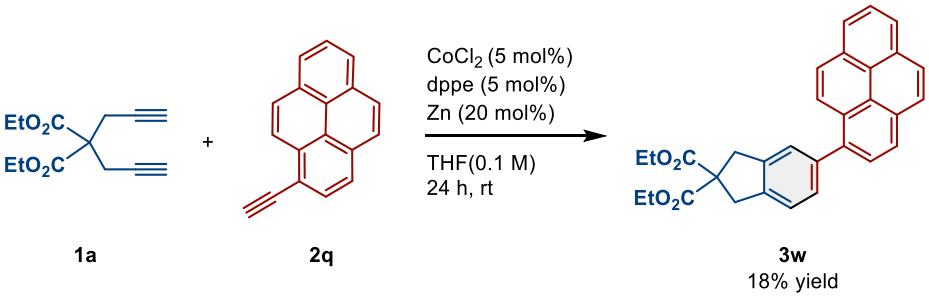
6. [2+2+2] Cycloaddition of 3w Mediated by Photoredox Catalysis



1a **2q** **3w**
<1% yield

The reaction was performed according to the reported procedure.[2] **1a** (23.8 mg, 0.1 mmol), **2q** (45.2 mg, 0.3 mmol, 3.0 equiv) and $[Ir(dF\text{-}5\text{-}CF_3\text{-}py)_2(dtbbpy)]PF_6$ (1.4 mg, 1.0 μmol, 1 mol%) were placed in an oven-dried reaction test tube. After the vial was sealed with a screw cap containing a Teflon-coated rubber septum, the test tube was connected to a vacuum/nitrogen manifold through a needle. It was evacuated and then backfilled with nitrogen. This cycle was repeated three times. Then, $CoBr_2(PCy_3)_2$ [0.1 mL, 0.1 M stock solution in MeCN (2 μmol of the catalyst)], DIPEA (5 μL, 30.0 μmol, 0.3 equiv) and MeCN (1.0 mL) were introduced to the mixture. The reaction mixture was stirred for 3 hours under irradiation with a 14 W CFL bulb. Then, the solvent was removed under reduced pressure. The crude mixture was analyzed by ^1H NMR analysis using mesitylene as an internal standard. In this case, no product formation was observed.

7. [2+2+2] Cycloaddition of 3w under Solution-based Conditions using Zinc

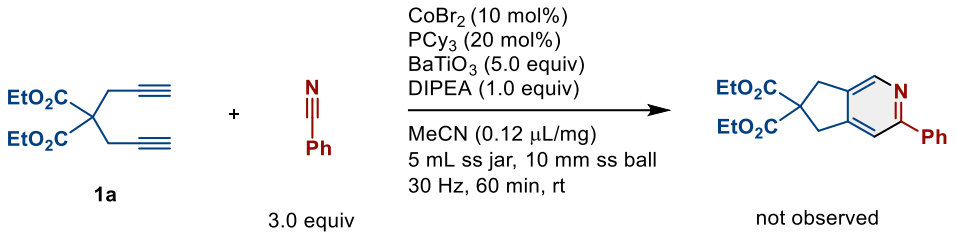


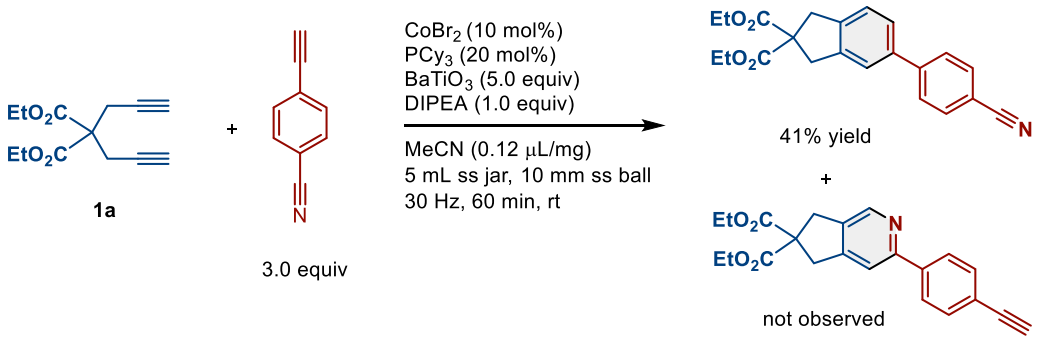
1a **2q** **3w**
18% yield

1a (23.5 mg, 0.1 mmol), zinc (1.3 mg, 0.01 mmol, 20 mol%), **2q** (29.4 mg, 0.13 mmol, 1.3 equiv), $CoCl_2$ (1.2 mg, 5.0 mmol, 5 mol%) and dppe (2.1 mg, 5.0 mmol, 5 mol%) were placed in an oven-dried reaction test tube. After the vial was sealed with a screw cap containing a Teflon-coated rubber septum, the test tube was connected to a vacuum/nitrogen manifold through a needle. It was evacuated and then backfilled with nitrogen. THF (0.4 mL) was then introduced to the mixture. The reaction mixture was stirred for 24 hours before passing through a short silica gel column using EtOAc as the eluent. The crude yield of **3w** was determined by ^1H NMR analysis using mesitylene as an internal standard. In this case, 18% yield of **3w** was obtained.

8. Unsuccessful Examples

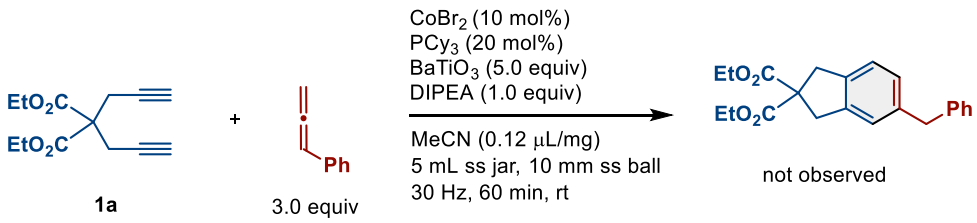
Reactions with nitriles





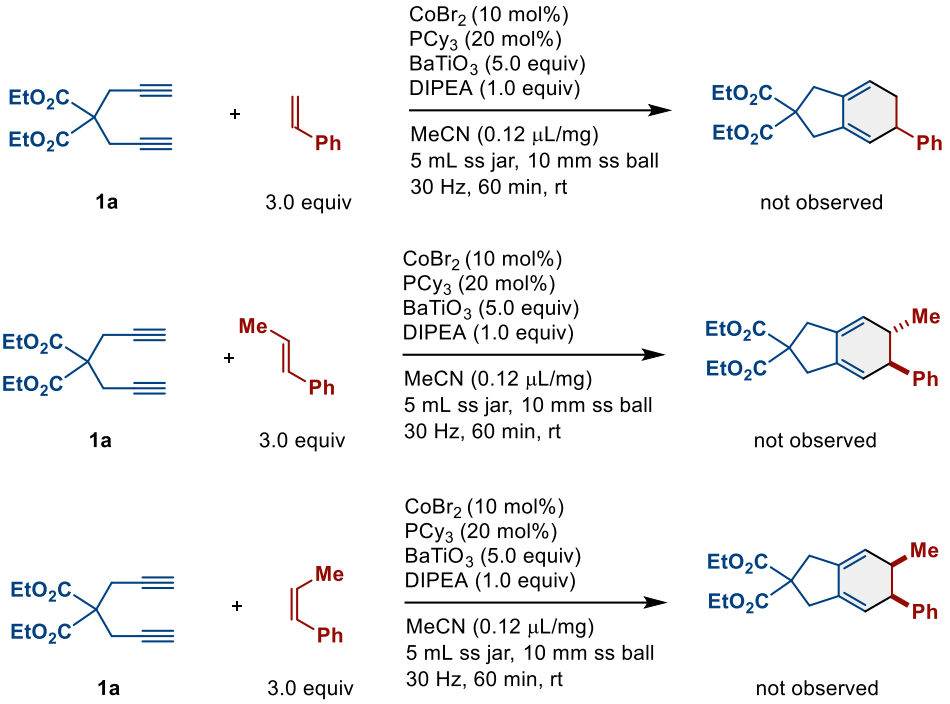
We examined benzonitrile as a coupling partner with **1a**. However, no desired product was formed. Instead, we obtained a homocoupled product of **1a**. To explore the chemoselectivity, we then tested 4-ethynylbenzonitrile as the coupling partner. In this case, the alkyne selectively underwent the cycloaddition reaction, affording the corresponding product in moderate yield. Generally, alkynes are more reactive than cyano groups in [2+2+2] cycloadditions. Therefore, the observed chemoselectivity aligns with established reactivity trends, and no unusual selectivity specific to mechanochemical conditions was observed.

Reactions with an allene



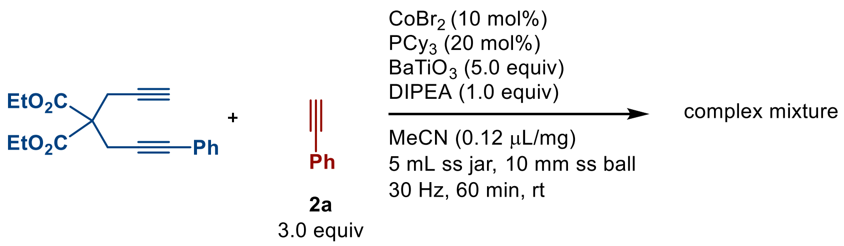
To assess the reactivity of allenes, we tested propa-1,2-dien-1-ylbenzene with **1a**. However, no coupling product was observed in this case. Instead, we obtained a homocoupled product of **1a**.

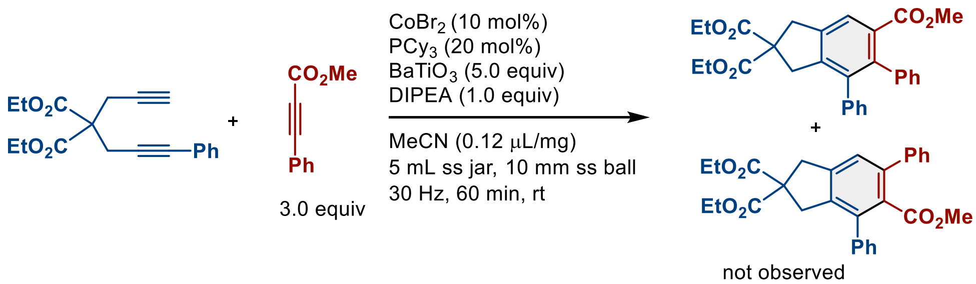
Reactions with alkenes

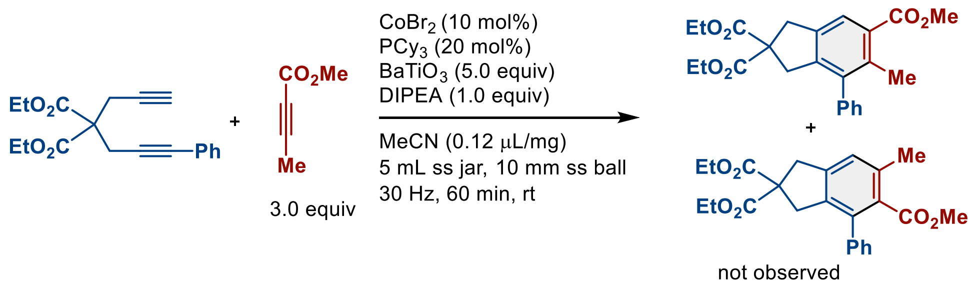


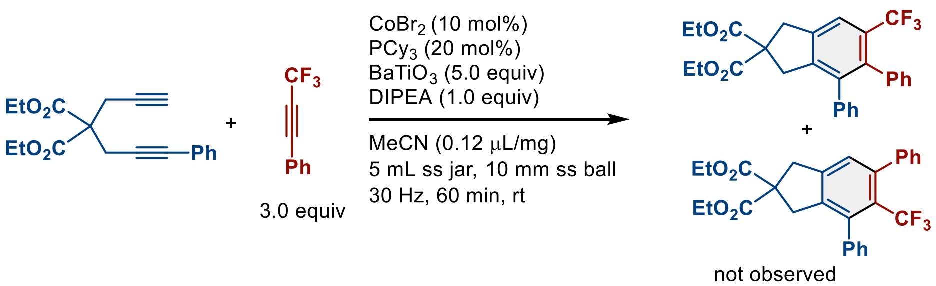
To evaluate the reactivity of alkenes, we conducted the reaction between styrene and **1a**. However, no coupling product was observed. Instead, we obtained a homocoupled product of **1a**. We further tested both (*E*)-prop-1-en-1-ylbenzene and (*Z*)-prop-1-en-1-ylbenzene under the optimized conditions, but neither yielded the desired product.

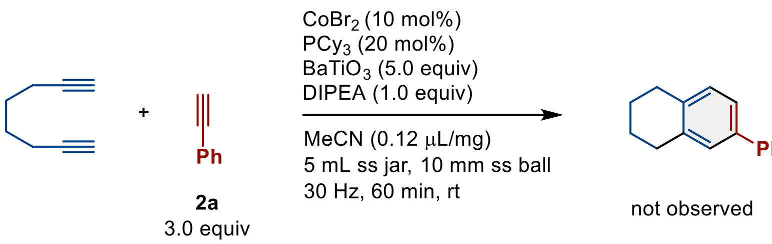
Reactions with various alkynes











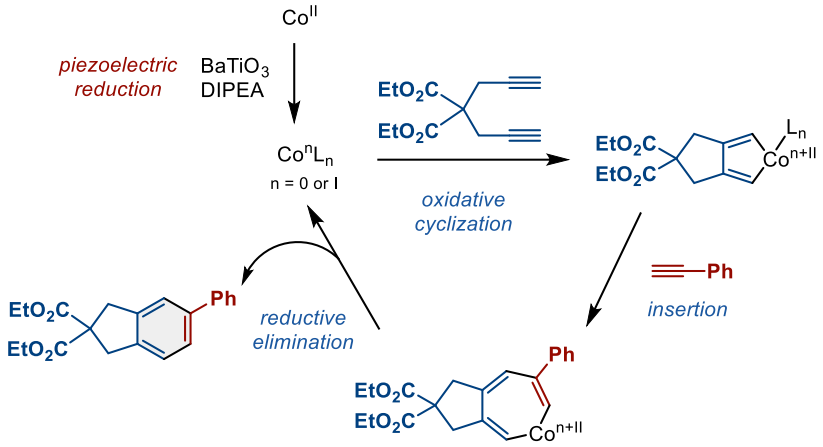
We investigated the reaction using diethyl 2-(3-phenylprop-2-yn-1-yl)-2-(prop-2-yn-1-yl)malonate as a representative monoaryl-substituted diyne and ethynylbenzene (**2a**) as the alkyne partner. However, the reaction yielded a complex mixture that was difficult to purify by column chromatography. Furthermore, the NMR spectra displayed overlapping signals, making it challenging to identify or confirm the formation of any specific product. We also tested other alkynes, including (3,3,3-trifluoroprop-1-yn-1-yl)benzene, methyl

3-phenylpropiolate, and methyl but-2-ynoate, but in all cases, the desired product was not observed. Instead, we mainly obtained homocoupled products with low conversion. We also tested octa-1,7-diyne under the optimized conditions. However, no desired product was obtained, and the starting material was consumed.

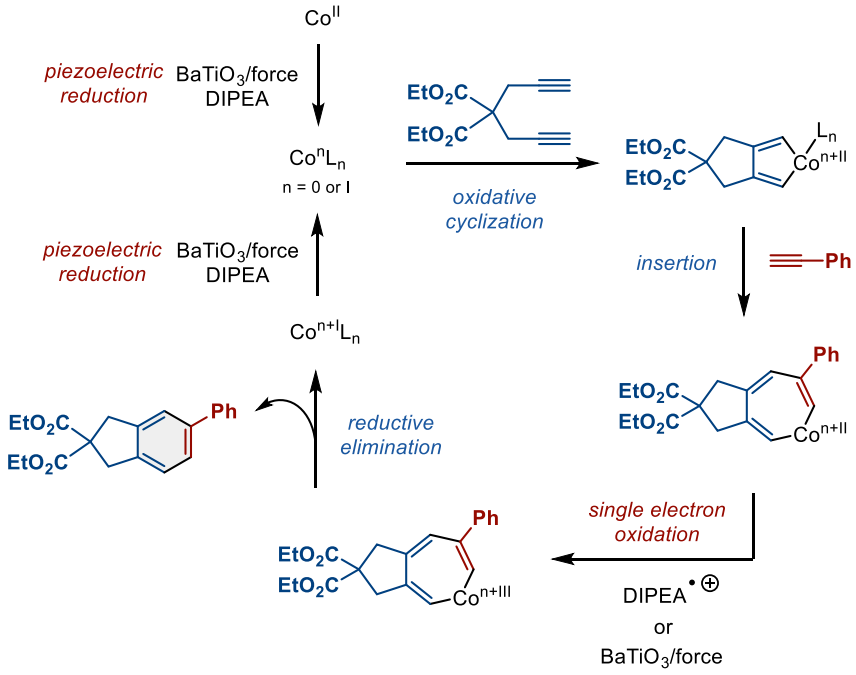
9. Proposed Mechanism

Based on prior literature, we propose that this low-valent cobalt species undergoes oxidative cyclization, followed by alkyne insertion and reductive elimination to afford the desired product (Mechanism A). Thus, we believe that $BaTiO_3$ is not involved in the cyclization step. However, it is also possible that the organocobalt intermediate undergoes single-electron oxidation by either a tertiary amine radical cation or piezoelectric $BaTiO_3$ to form a high-valent cobalt species, which may facilitate the reductive elimination step (Mechanism B). Further mechanistic studies are needed to evaluate these possibilities and will be pursued in future work.

Mechanism A

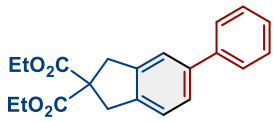


Mechanism B



10. Characterization of Products

Diethyl 5-phenyl-1,3-dihydro-2H-indene-2,2-dicarboxylate (3a)

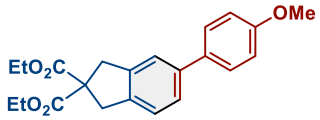


3a

The reaction was conducted with **1a** (47.3 mg, 0.2 mmol) and **2a** (65 μL, 0.6 mmol). The resulting crude mixture was purified by silica-gel column chromatography (SiO_2, Et_2O/hexane, 0:100–10:90) to obtain **3a** in 86% yield (58.4 mg, 0.17 mmol) as a yellowish oil. ^1H and ^{13}C NMR of **3a** were in agreement with the literature.[3]

^1H NMR (401 MHz, $CDCl_3$, δ) 1.26 (t, *J* = 7.1 Hz, 6H), 3.63 (d, *J* = 8.2 Hz, 4H), 4.22 (q, *J* = 7.1 Hz, 4H), 7.25 (d, *J* = 7.6 Hz, 1H), 7.32 (t, *J* = 7.2 Hz, 1H), 7.37–7.44 (m, 4H), 7.52–7.58 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$, δ) 14.2 (*C*H_3), 40.3 (*C*H_2), 40.6 (*C*H_2), 60 .6 (*C*), 61.9 (*C*H_2), 123.1 (*C*H), 124.6 (*C*H), 126.2 (*C*H), 127.16 (*C*H), 127.23 (*C*H), 128.8 (*C*), 139.3 (*C*), 140.4 (*C*), 140.8 (*C*), 141.4 (*C*), 171.8 (*C*). ESI (m/z): $[M+Na]^+$ calcd for $C_{21}H_{22}O_4Na$: 361.1410, found: 361.1401.

Diethyl 5-(4-methoxyphenyl)-1,3-dihydro-2H-indene-2,2-dicarboxylate (3b)

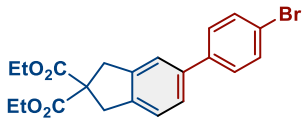


3b

The reaction was conducted with **1a** (47.4 mg, 0.2 mmol) and **2b** (80 μL, 0.6 mmol). The resulting crude mixture was purified by silica-gel column chromatography (SiO_2, EtOAc/hexane, 0:100–5:95) to obtain **3b** in 81% yield (60.2 mg, 0.16 mmol) as a colorless gum. ^1H and ^{13}C NMR of **3b** were in agreement with the literature.[3]

^1H NMR (401 MHz, $CDCl_3$, δ) 1.26 (t, *J* = 7.1 Hz, 6H), 3.62 (d, *J* = 8.2 Hz, 4H), 3.84 (s, 3H), 4.22 (q, *J* = 7.1 Hz, 4H), 6.93–6.98 (m, 2H), 7.24 (t, *J* = 7.6 Hz, 1H), 7.35 (d, *J* = 10.0 Hz , 2H), 7.46–7.52 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$, δ) 14.1 (*C*H_3), 40.3 (*C*H_2), 40.6 (*C*H_2), 55.4 (*C*H_3), 60.6 (*C*), 61.8 (*C*H_2), 114.2 (*C*H), 122.7 (*C*H), 124.5 (*C*H), 125.8 (*C*H), 128.2 (*C*H), 134.0 (*C*), 138.6 (*C*), 140.0 (*C*), 140.8 (*C*), 159.1 (*C*), 171.8 (*C*). ESI (m/z): $[M+Na]^+$ calcd for $C_{22}H_{24}O_5Na$: 391.1516, found: 391.1504.

Diethyl 5-(4-bromophenyl)-1,3-dihydro-2H-indene-2,2-dicarboxylate (3c)

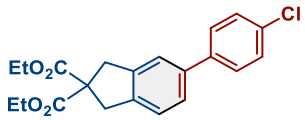


3c

The reaction was conducted with **1a** (47.1 mg, 0.2 mmol) and **2c** (108.2 mg, 0.6 mmol). The resulting crude mixture was purified by silica-gel column chromatography (SiO_2, Et_2O/hexane, 0:100–5:95) to obtain **3c** in 75% yield (62.4 mg, 0.15 mmol) as a yellowish oil.

^{1}H NMR (401 MHz, $CDCl_3$, δ) 1.27 (t, *J* = 7.2 Hz, 6H), 3.63 (d, *J* = 8.0 Hz, 4H), 4.22 (q, *J* = 7.1 Hz, 4H), 7.25–7.28 (m, 1H), 7.33–7.38 (m, 2H), 7.39–7.45 (m, 2H), 7.51–7.56 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$, δ) 14.2 (*C*H_3), 40.3 (*C*H_2), 40.5 (*C*H_2), 60.6 (*C*), 61.9 (*C*H_2), 121.4 (*C*), 122.9 (*C*H), 124.7 (*C*H), 126.0 (*C*H), 128.8 (*C*H), 131.9 (*C*H), 139.1 (*C*), 139.8 (*C*), 140.3 (*C*), 141.0 (*C*), 171.7 (*C*). ESI (m/z): $[M+Na]^+$ calcd for $C_{21}H_{21}BrO_4Na$: 439.0515, found: 439.0510.

Diethyl 5-(4-chlorophenyl)-1,3-dihydro-2H-indene-2,2-dicarboxylate (3d)

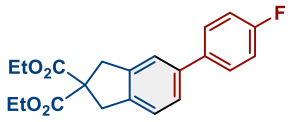


3d

The reaction was conducted with **1a** (47.4 mg, 0.2 mmol) and **2d** (82.2 mg, 0.6 mmol). The resulting crude mixture was purified by silica-gel column chromatography (SiO_2, Et_2O/hexane, 0:100–10:90) to obtain **3d** in 75% yield (56.5 mg, 0.15 mmol) as a yellowish oil.

^{1}H NMR (401 MHz, $CDCl_3$, δ) δ 1.26 (t, *J* = 7.1 Hz, 6H), 3.63 (d, *J* = 8.0 Hz, 4H), 4.22 (q, *J* = 7.1 Hz, 4H), 7.23–7.27 (m, 1H), 7.32–7.39 (m, 4H), 7.44–7.49 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$, δ) 14.1 (*C*H_3), 40.3 (*C*H_2), 40.5 (*C*H_2), 60.6 (*C*), 61.9 (*C*H_2), 122.9 (*C*H), 124.7 (*C*H), 126.1 (*C*H), 128.4 (*C*H), 128.9 (*C*H), 133.2 (*C*), 139.1 (*C*), 139.7 (*C*), 139.8 (*C*), 141.0 (*C*), 171.7 (*C*). ESI (m/z): $[M+Na]^+$ calcd for $C_{21}H_{21}O_4ClNa$: 395.1021, found: 395.1013.

Diethyl 5-(4-fluorophenyl)-1,3-dihydro-2H-indene-2,2-dicarboxylate (3e)

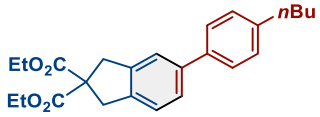


3e

The reaction was conducted with **1a** (47.1 mg, 0.2 mmol) and **2e** (72.3 mg, 0.6 mmol). The resulting crude mixture was purified by silica-gel column chromatography (SiO_2, Et_2O/hexane, 0:100–10:90) to obtain **3e** in 86% yield (61.2 mg, 0.17 mmol) as a yellowish oil.

^{1}H NMR (401 MHz, $CDCl_3$, δ) 1.27 (t, *J* = 7.3 Hz, 6H), 3.63 (d, *J* = 6.6 Hz, 4H), 4.22 (q, *J* = 7.3 Hz, 4H), 7.09 (t, *J* = 8.0 Hz, 2H), 7.24 (d, *J* = 7.6 Hz, 1H), 7.30–7.38 (m, 2H), 7.45–7.54 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$, δ) 14.1 (*C*H_3), 40.3 (*C*H_2), 40.5 (*C*H_2), 60.6 (*C*), 61.9 (*C*H_2), 115.6 (d, *J* = 21.4 Hz, *C*H), 123.0 (*C*H), 124.6 (*C*H), 126.1 (*C*H), 128.7 (d, *J* = 7.9 Hz, *C*H), 137.5 (*C*), 139.3 (*C*), 139.4 (*C*), 140.9 (*C*), 162.4 (d, *J* = 246.0 Hz, *C*), 171.7 (*C*). ^{19}F NMR (377 MHz, $CDCl_3$) δ –116.7. ESI (m/z): $[M+Na]^+$ calcd for $C_{21}H_{21}FO_4Na$: 379.1316, found: 379.1304.

Diethyl 5-(4-butylphenyl)-1,3-dihydro-2H-indene-2,2-dicarboxylate (3f)

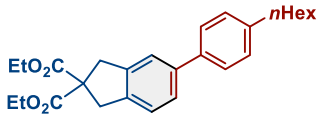


3f

The reaction was conducted with **1a** (47.4 mg, 0.2 mmol) and **2f** (105 μL, 0.6 mmol). The resulting crude mixture was purified by silica-gel column chromatography (SiO_2, Et_2O/hexane, 0:100–10:90) to obtain **3f** in 72% yield (57.2 mg, 0.14 mmol) as a colorless oil.

^{1}H NMR (401 MHz, $CDCl_3$, δ) 0.94 (t, *J* = 7.2 Hz, 3H), 1.26 (t, *J* = 7.6 Hz, 6H), 1.38 (sext, *J* = 7.6 Hz, 2H), 1.58–1.67 (m, 2H), 2.63 (t, *J* = 7.2 Hz, 2H), 3.63 (d, *J* = 8.0 Hz, 4H), 4.21 (q, *J* = 7.2 Hz, 4H), 7.19–7.26 (m, 3H), 7.38 (d, *J* = 9.6 , 2H), 7.46 (d, *J* = 8.0 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$, δ) 14.09 (*C*H_3), 14.15 (*C*H_3), 22.5 (*C*H_2), 33.8 (*C*H_2), 35.4 (*C*H_2), 40.3 (*C*H_2), 40.6 (*C*H_2), 60.6 (*C*), 61.8 (*C*H_2), 122.9 (*C*H), 124.5 (*C*H), 126.1 (*C*H), 127.0 (*C*H), 128.9 (*C*H), 138.7 (*C*), 138.9 (*C*), 140.4 (*C*), 140.7 (*C*), 142.0 (*C*), 171.8 (*C*). ESI (m/z): $[M+Na]^+$ calcd for $C_{25}H_{30}O_4Na$: 417.2036, found: 417.2026.

Diethyl 5-(4-hexylphenyl)-1,3-dihydro-2H-indene-2,2-dicarboxylate (3g)

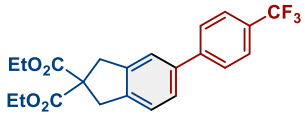


3g

The reaction was conducted with **1a** (47.3 mg, 0.2 mmol) and **2g** (125 µL, 0.6 mmol). The resulting crude mixture was purified by silica-gel column chromatography (SiO_2, Et_2O/hexane, 0:100–10:90) to obtain **3g** in 67% yield (58.2 mg, 0.13 mmol) as a yellowish oil.

^{1}H NMR (401 MHz, $CDCl_3$, δ) δ 0.89 (t, J = 6.8 Hz, 3H), 1.26 (t, J = 7.1 Hz, 6H), 1.31–1.41 (m, 6H), 1.59–1.69 (m, 2H), 2.63 (t, J = 7.2 Hz, 2H), 3.63 (d, J = 7.8 Hz, 4H), 4.21 (q, J = 7.1 Hz, 4H), 7.20–7.26 (m, 3H), 7.38 (d, J = 8.1 Hz, 2H), 7.45 (d, J = 8.1 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$, δ) 14.1 (*C*H_3), 14.2 (*C*H_3), 22.7 (*C*H_2), 29.2 (*C*H_2), 31.6 (*C*H_2), 31.9 (*C*H_2), 35.7 (*C*H_2), 40.3 (*C*H_2), 40.6 (*C*H_2), 60.6 (*C*), 61.8 (*C*H_2), 123.0 (*C*), 124.5 (*C*H), 126.1 (*C*H), 127.0 (*C*H), 128.8 (*C*H), 138.7 (*C*), 138.9 (*C*), 140.4 (*C*), 140.7 (*C*), 142.0 (*C*), 171.8 (*C*). ESI (m/z): $[M+Na]^+$ calcd for $C_{25}H_{30}O_4Na$: 445.2350, found: 445.2339.

Diethyl 5-[4-(trifluoromethyl)phenyl]-1,3-dihydro-2H-indene-2,2-dicarboxylate (3h)

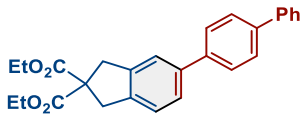


3h

The reaction was conducted with **1a** (47.3 mg, 0.2 mmol) and **2h** (86 µL, 0.6 mmol). The resulting crude mixture was purified by silica-gel column chromatography (SiO_2, Et_2O/hexane, 0:100–10:90) to obtain **3h** in 70% yield (57.2 mg, 0.14 mmol) as a yellowish oil. ^{1}H and ^{13}C NMR of **3h** were in agreement with the literature.[3]

^{1}H NMR (401 MHz, $CDCl_3$, δ) 1.27 (t, J = 7.1 Hz, 6H), 3.65 (d, J = 6.4 Hz, 4H), 4.23 (q, J = 7.1 Hz, 4H), 7.25–7.31 (m, 1H), 7.38–7.44 (m, 2H), 7.62–7.69 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$, δ) 14.1 (*C*H_3), 40.3 (*C*H_2), 40.5 (*C*H_2), 60.6 (C), 61.9 (*C*H_2), 123.2 (*C*H), 124.8 (*C*H), 125.7 (d, J = 3.8 Hz, *C*H), 126.4 (*C*H), 127.4 (*C*H), 129.0 (d, J = 32.8 Hz, *C*), 138.9 (*C*), 140.4 (*C*), 141.1 (*C*), 144.9 (*C*), 171.6 (*C*). The CF_3 carbon signal was not found due to splitting. ^{19}F NMR (377 MHz, $CDCl_3$) δ –62.87. ESI (m/z): $[M+Na]^+$ calcd for $C_{22}H_{21}F_3O_4Na$: 429.1284, found: 429.1272.

Diethyl 5-[(1,1'-biphenyl)-4-yl]1,3-dihydro-2H-indene-2,2-dicarboxylate (3i)

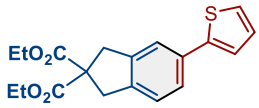


3i

The reaction was conducted with **1a** (47.3 mg, 0.2 mmol) and **2i** (106.8 mg, 0.6 mmol). The resulting crude mixture was purified by silica-gel column chromatography (SiO_2, EtOAc/hexane, 0:100–5:95) to obtain **3i** in 66% yield (54.8 mg, 0.13 mmol) as a yellowish solid.

^{1}H NMR (401 MHz, $CDCl_3$, δ) 1.27 (t, J = 7.1, 6H), 3.65 (d, J = 9.3 Hz, 4H), 4.23 (q, J = 7.1, 4H), 7.28 (d, J = 7.8 Hz, 1H), 7.36 (t, J = 6.8 Hz, 1H), 7.42–7.50 (m, 4H), 7.60–7.70 (m, 6H). ^{13}C NMR (101 MHz, $CDCl_3$, δ) 14.2 (CH_3), 40.3 (CH_2), 40.6 (CH_2), 60.6 (C), 61.9 (CH_2), 123.0 (*C*H), 124.6 (*C*H), 126.1 (*C*H), 127.1 (*C*H), 127.4 (*C*H), 127.5 (*C*H), 127.6 (*C*H), 128.9 (*C*H), 139.4 (C), 139.9 (C), 140.3 (C), 140.8 (C), 140.9 (C), 171.8 (C). ESI (m/z): $[M+Na]^+$ calcd for $C_{27}H_{26}O_4Na$: 437.1723, found: 437.1716.

Diethyl 5-(thiophen-2-yl)-1,3-dihydro-2H-indene-2,2-dicarboxylate (3j)

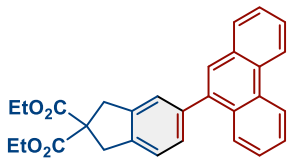


3j

The reaction was conducted with **1a** (47.2 mg, 0.2 mmol) and **2j** (60.1 mg, 0.57 mmol). The resulting crude mixture was purified by silica-gel column chromatography (SiO_2, Et_2O/hexane, 0:100–10:90) to obtain **3j** in 70% yield (48.6 mg, 0.14 mmol) as a colorless oil.

^{1}H NMR (401 MHz, $CDCl_3$, δ) 1.26 (t, J = 7.1 Hz, 6H), 3.61 (d, J = 8.9 Hz, 4H), 4.21 (q, J = 7.1 Hz, 4H), 7.21 (d, J = 7.7 Hz, 1H), 7.33–7.37 (m, 2H), 7.38–7.43 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$, δ) 14.1 (CH_3), 40.3 (CH_2), 40.5 (CH_2), 60.6 (*C*), 61.9 (CH_2), 120.0 (*C*H), 122.4 (*C*H), 124.6 (*C*H), 125.5 (*C*H), 126.2 (*C*H), 126.5 (*C*H), 135.0 (*C*), 139.1 (*C*), 140.8 (*C*), 142.5 (*C*), 171.7 (*C*). ESI (m/z): $[M+Na]^+$ calcd for $C_{19}H_{20}O_4SNa$: 367.0975, found: 367.0988.

Diethyl 5-(phenanthren-9-yl)-1,3-dihydro-2H-indene-2,2-dicarboxylate (3k)

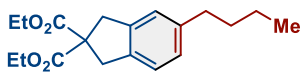


3k

The reaction was conducted with **1a** (47.3 mg, 0.2 mmol) and **2k** (121.2 mg, 0.6 mmol). The resulting crude mixture was purified by silica-gel column chromatography (SiO_2, Et_2O/hexane, 0:100–10:90) to obtain **3k** in 82% yield (72.4 mg, 0.16 mmol) as a yellowish oil.

^{1}H NMR (401 MHz, $CDCl_3$, δ) 1.29 (t, *J* = 7.1 Hz, 6H), 3.71 (d, *J* = 5.7 Hz, 4H), 4.25 (q, *J* = 7.1 Hz, 4H), 7.30–7.38 (m, 3H), 7.49–7.55 (m, 1H), 7.57–7.68 (m, 4H), 7.85–7.94 (m, 2H), 8.70 (d, *J* = 8.1 Hz, 1H), 8.75 (d, *J* = 7.2 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$, δ) 14.2 (*C*H_3), 40.5 (*C*H_2), 40.6 (*C*H_2), 60.6 (*C*), 61.9 (*C*H_2), 122.6 (*C*H), 123.0 (*C*H), 124.1 (*C*H), 125.9 (*C*H), 126.5 (*C*H), 126.57 (*C*H), 126.61 (*C*H), 126.9 (*C*H), 127.1 (*C*H), 127.6 (*C*H), 128.7 (*C*H), 129.0 (*C*H), 130.0 (*C*), 130.7 (*C*), 131.3 (*C*), 131.7 (*C*), 138.9 (*C*), 139.3 (*C*), 139.7 (*C*), 140.3 (*C*), 171.9 (*C*). ESI (m/z): $[M+Na]^+$ calcd for $C_{29}H_{26}O_4Na$: 461.1723, found: 461.1717.

Diethyl 5-butyl-1,3-dihydro-2H-indene-2,2-dicarboxylate (3l)

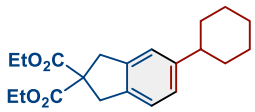


3l

The reaction was conducted with **1a** (47.1 mg, 0.2 mmol) and **2l** (68 μL, 0.6 mmol). The resulting crude mixture was purified by silica-gel column chromatography (SiO_2, Et_2O/hexane, 0:100–10:90) to obtain **3l** in 81% yield (51.4 mg, 0.16 mmol) as a yellowish oil. ^{1}H and ^{13}C NMR of the product **3l** were in agreement with the literature.[4]

^{1}H NMR (401 MHz, $CDCl_3$, δ) 0.92 (t, *J* = 7.3 Hz, 3H), 1.25 (t, *J* = 7.1 Hz, 6H), 1.30–1.39 (m, 2H), 1.52–1.61 (m, 2H), 2.56 (t, *J* = 7.6 Hz, 2H), 3.55 (d, *J* = 3.0 Hz, 4H), 4.19 (q, *J* = 7.1 Hz, 4H), 6.97 (d, *J* = 7.2 Hz, 1H), 7.00 (s, 1H), 7.08 (d, *J* = 7.6 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$, δ) 14.06 (*C*H_3), 14.11 (*C*H_3), 22.5 (*C*H_2), 34.0 (*C*H_2), 35.6 (*C*H_2), 40.3 (*C*H_2), 40.5 (*C*H_2), 60.6 (*C*), 61.7 (*C*H_2), 124.0 (*C*H), 124.3 (*C*H), 127.2 (*C*H), 137.2 (*C*), 140.1 (*C*), 141.8 (*C*), 171.9 (*C*). ESI (m/z): $[M+Na]^+$ calcd for $C_{19}H_{26}O_4Na$: 341.1723, found: 341.1713.

Diethyl 5-cyclohexyl-1,3-dihydro-2H-indene-2,2-dicarboxylate (3m)

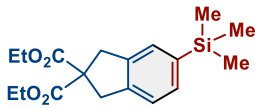


3m

The reaction was conducted with **1a** (47.4 mg, 0.2 mmol) and **2m** (65.2 mg, 0.6 mmol). The resulting crude mixture was purified by silica-gel column chromatography (SiO_2, Et_2O/hexane, 0:100–10:90) to obtain **3m** in 80% yield (55.6 mg, 0.16 mmol) as a yellowish oil.

^{1}H NMR (401 MHz, $CDCl_3$, δ) 1.19–1.24 (m, 1H), 1.25 (t, J = 7.2 Hz, 6H), 1.32–1.44 (m, 4H), 1.73 (d, J = 12.0 Hz, 1H), 1.78–1.89 (m, 4H), 2.40–2.49 (m, 1H), 3.55 (d, J = 8.02 Hz, 4H), 4.20 (q, J = 7.20 Hz, 4H), 7.00 (d, J = 8.0 Hz, 1H), 7.03 (s, 1H), 7.10 (d, J = 7.6 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$, δ) 14.1 (CH_3), 26.3 (CH_2), 27.0 (CH_2), 34.7 (CH_2), 40.3 (CH_2), 40.6 (CH_2), 44.6 (*C*H), 60.5 (*C*), 61.7 (CH_2), 122.6 (*C*H), 124.0 (*C*H), 125.7 (*C*H), 140.1 (*C*), 147.1 (*C*), 171.9 (*C*). ESI (m/z): $[M+Na]^+$ calcd for $C_{21}H_{28}O_4Na$: 367.1880, found: 367.1869.

Diethyl 5-(trimethylsilyl)-1,3-dihydro-2H-indene-2,2-dicarboxylate (3n)

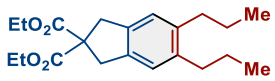


3n

The reaction was conducted with **1a** (47.1 mg, 0.2 mmol) and **2n** (58.2 mg, 0.6 mmol). The resulting crude mixture was purified by silica-gel column chromatography (SiO_2, Et_2O/hexane, 0:100–5:95) to obtain **3n** in 50% yield (33.4 mg, 0.10 mmol) as a yellowish oil. ^{1}H and ^{13}C NMR of **3n** were in agreement with the literature.[3]

^{1}H NMR (401 MHz, $CDCl_3$, δ) 0.24 (s, 9H), 1.26 (t, J = 7.6 Hz, 6H), 3.59 (d, J = 7.6 Hz, 4H), 4.20 (q, J = 6.8 Hz, 4H), 7.14–7.23 (d, J = 7.6 Hz, 1H), 7.30–7.40 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$, δ) –0.90 (CH_3), 14.1 (CH_3), 14.2 (CH_3), 40.5 (CH_2), 40.6 (CH_2), 60.2 (*C*), 61.8 (CH_2), 123.8 (*C*H), 129.2 (*C*H), 132.1 (*C*H), 138.9 (*C*), 139.5 (*C*), 140.9 (*C*), 171.8 (*C*). ESI (m/z): $[M+Na]^+$ calcd for $C_{18}H_{26}O_4SiNa$: 357.1493, found: 357.1482.

Diethyl 5,6-dipropyl-1,3-dihydro-2H-indene-2,2-dicarboxylate (3o)

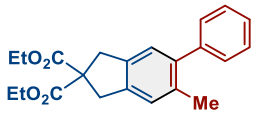


3o

The reaction was conducted with **1a** (47.3 mg, 0.2 mmol) and **2o** (66.3 mg, 0.6 mmol). The resulting crude mixture was purified by silica-gel column chromatography (SiO_2, Et_2O/hexane, 0:100–10:90) to obtain **3o** in 44% yield (30.8 mg, 0.09 mmol) as a colorless oil.

^{1}H NMR (401 MHz, $CDCl_3$, δ) 0.97 (t, J = 7.2 Hz, 6H), 1.25 (t, J = 7.6 Hz, 6H), 1.52–1.62 (m, 4H), 2.52 (t, J = 7.6 Hz, 4H), 3.53 (s, 4H), 4.18 (q, J = 7.2 Hz, 4H), 6.96 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$, δ) 14.1 (*C*H$_3$), 14.4 (*C*H$_3$), 24.6 (*C*H$_2$), 34.9 (*C*H$_2$), 40.4 (*C*H$_2$), 60.5 (*C*), 61.7 (*C*H$_2$), 124.8 (*C*H), 137.5 (*C*), 139.2 (*C*), 172.0 (*C*). ESI (m/z): $[M+Na]^+$ calcd for $C_{21}H_{30}O_4Na$: 369.2036, found: 369.2027.

Diethyl 5-methyl-6-phenyl-1,3-dihydro-2H-indene-2,2-dicarboxylate (3p)

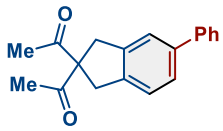


3p

The reaction was conducted with **1a** (47.2 mg, 0.2 mmol) and **2p** (70.2 mg, 0.6 mmol). The resulting crude mixture was purified by silica-gel column chromatography (SiO_2, Et_2O/hexane, 0:100–10:90) to obtain **3p** in 52% yield (36.5 mg, 0.10 mmol) as a colorless oil. ^{1}H and ^{13}C NMR of **3p** were in agreement with the literature.[5]

^{1}H NMR (401 MHz, $CDCl_3$, δ) 1.26 (t, J = 7.1 Hz, 6H), 2.21 (s, 3H), 3.59 (d, J = 5.8 Hz, 4H), 4.22 (q, J = 7.1 Hz, 4H), 7.05 (s, 1H), 7.10 (s, 1H), 7.25–7.33 (m, 3H), 7.37–7.42 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$, δ) 14.1 (*C*H$_3$), 20.5 (*C*H$_3$), 40.3 (*C*H$_2$), 40.4 (*C*H$_2$), 60.6 (*C*), 61.8 (*C*H$_2$), 125.6 (*C*H), 126.0 (*C*H), 126.7 (*C*H), 128.1 (*C*H), 129.3 (*C*H), 134.2 (*C*), 137.6 (*C*), 139.2 (*C*), 140.9 (*C*), 142.2 (*C*), 171.9 (*C*). ESI (m/z): $[M+Na]^+$ calcd for $C_{22}H_{24}O_4Na$: 375.1567, found: 375.1558.

1,1'-(5-Phenyl-2,3-dihydro-1H-indene-2,2-diyl)bis(ethan-1-one) (3q)

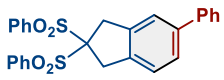


3q

The reaction was conducted with **1b** (35.4 mg, 0.2 mmol) and **2a** (65 μL, 0.6 mmol). The resulting crude mixture was purified by silica-gel column chromatography (SiO_2, EtOAc/hexane, 0:100–10:90) to obtain **3q** in 64% yield (35.6 mg, 0.13 mmol) as a colorless oil.[6]

^{1}H NMR (401 MHz, $CDCl_3$, δ) 2.19 (s, 6H), 3.55 (d, *J* = 7.8 Hz, 4H), 7.25 (d, *J* = 6.8 Hz, 1H), 7.29–7.35 (m, 1H), 7.37–7.45 (m, 4H), 7.54 (d, *J* = 7.6 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$, δ) 26.7 (*C*H_3), 37.4 (*C*H_2), 37.7 (*C*H_2), 75.1 (*C*), 123.3 (*C*H), 124.8 (*C*H), 126.4 (*C*H), 127.2 (*C*H), 127.3 (*C*H), 128.8 (*C*H), 138.9 (*C*), 140.5 (*C*), 140.6 (*C*), 141.2 (*C*), 204.9 (*C*). ESI (m/z): $[M+Na]^+$ calcd for $C_{19}H_{18}O_2Na$: 301.1199, found: 301.1193.

5-Phenyl-2,2-bis(phenylsulfonyl)-2,3-dihydro-1H-indene (3r)

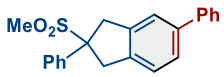


3r

The reaction was conducted with **1c** (74.3 mg, 0.2 mmol) and **2a** (65 μL, 0.6 mmol). The resulting crude mixture was purified by silica-gel column chromatography (SiO_2, EtOAc/hexane, 0:100–40:60) to obtain **3r** in 89% yield (84.1 mg, 0.18 mmol) as a colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$, δ) 3.97 (d, *J* = 4.0 Hz, 4H), 6.97 (d, *J* = 7.6 Hz, 1H), 7.07 (s, 1H), 7.20 (d, *J* = 7.6 Hz, 1H), 7.30–7.50 (m, 9H), 7.54–7.62 (m, 2H), 7.96 (d, *J* = 8.4 Hz, 4H). ^{13}C NMR (101 MHz, $CDCl_3$, δ) 38.5 (*C*H_2), 38.7 (*C*H_2), 92.7 (*C*), 122.6 (*C*H), 124.2 (*C*H), 126.7 (*C*H), 127.1 (*C*H), 127.5 (*C*H), 128.8 (*C*H), 128.9 (*C*H), 130.9 (*C*H), 134.7 (*C*H), 136.8 (*C*), 137.2 (*C*), 138.7 (*C*), 140.8 (*C*), 140.9 (*C*). ESI (m/z): [M + Na]+ calcd for $C_{27}H_{22}O_4S_2Na$: 497.0852, found: 497.0838.

2-(Methylsulfonyl)-2,5-diphenyl-2,3-dihydro-1H-indene (3s)

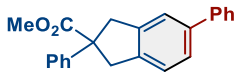


3s

The reaction was conducted with **1d** (49.1 mg, 0.2 mmol) and **2a** (65 μL, 0.6 mmol). The resulting crude mixture was purified by silica-gel column chromatography (SiO_2, EtOAc/hexane, 0:100–30:70) to obtain **3s** in 92% yield (64.2 mg, 0.18 mmol) as a yellowish oil.

^{1}H NMR (400 MHz, $CDCl_3$, δ) 2.48 (s, 3H), 3.81 (dd, *J* = 7.6, 10.0 Hz, 2H), 4.19 (dd, *J* = 7.6, 10.0 Hz, 2H), 7.31–7.37 (m, 2H), 7.38–7.47 (m, 6H), 7.49 (s, 1H), 7.54–7.63 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$, δ) 36.8 (*C*H_3), 40.8 (*C*H_2), 41.1 (*C*H_2), 76.6 (*C*), 123.0 (*C*H), 124.6 (*C*H), 126.8 (*C*H), 127.2 (*C*H), 127.5 (*C*H), 128.6 (*C*H), 128.9 (*C*H), 129.0 (*C*H), 129.9 (*C*H), 136.1 (*C*), 138.9 (*C*), 140.5 (*C*), 140.9 (*C*), 141.0 (*C*). ESI (m/z): $[M+Na]^+$ calcd for $C_{22}H_{20}O_2SNa$: 371.1076, found: 371.1067.

Methyl 2,5-diphenyl-2,3-dihydro-1H-indene-2-carboxylate (3t)

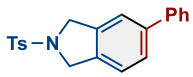


3t

The reaction was conducted with **1e** (45.4 mg, 0.2 mmol) and **2a** (65 μL, 0.6 mmol). The resulting crude mixture was purified by silica-gel column chromatography (SiO_2, EtOAc/hexane, 0:100–10:90) to obtain **3t** in 91% yield (59.8 mg, 0.18 mmol) as a colorless oil.

^{1}H NMR (401 MHz, $CDCl_3$, δ) 3.38 (dd, *J* = 8.2, 15.6 Hz, 2H), 3.62 (s, 3H), 4.03 (dd, *J* = 6.9, 15.6 Hz, 2H), 7.24–7.28 (m, 1H), 7.29–7.38 (m, 4H), 7.39–7.45 (m, 5H), 7.47 (s, 1H), 7.56 (d, *J* = 8.0 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$, δ) 42.6 (*C*H_2), 42.9 (*C*H_2), 52.8 (*C*H_3), 59.9 (*C*), 123.2 (*C*H), 124.6 (*C*H), 126.0 (*C*H), 126.8 (*C*H), 127.1 (*C*H), 127.2 (*C*H), 128.7 (*C*H), 128.8 (*C*H), 129.2 (*C*H), 140.2 (*C*), 140.4 (*C*), 141.5 (*C*), 141.9 (*C*), 142.7 (*C*), 176.0 (*C*). ESI (m/z): $[M+Na]^+$ calcd for $C_{23}H_{20}O_2Na$: 351.1356, found: 351.1344.

5-Phenyl-2-tosylisoindoline (3u)

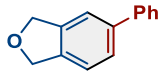


3u

The reaction was conducted with **1f** (49.3 mg, 0.2 mmol) and **2a** (65 μL, 0.6 mmol). The resulting crude mixture was purified by silica-gel column chromatography (SiO_2, EtOAc/hexane, 0:100–10:90) to obtain 0 **3u** in 89% yield (62.1 mg, 0.18 mmol) as a yellowish solid. ^1H and ^{13}C NMR of **3u** were in agreement with the literature.[4]

^1H NMR (401 MHz, $CDCl_3$, δ) 2.40 (s, 3H). 4.67 (d, J = 4.2 Hz, 4H), 7.20–7.28 (m, 1H), 7.29–7.38 (m, 4H), 7.43 (q, J = 8.1 Hz, 3H), 7.51 (d, J = 8.0 Hz, 2H), 7.79 (d, J = 7.9 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$, δ) 21.6 (CH_3), 53.6 (CH_2), 53.8 (CH_2), 121.4 (*C*H), 123.0 (*C*H), 127.0 (*C*H), 127.2 (*C*H), 127.6 (*C*H), 127.7 (*C*H), 128.9 (*C*H), 129.9 (*C*H), 133.7 (*C*), 135.2 (*C*), 136.9 (*C*), 140.6 (*C*), 141.3 (*C*), 143.8 (*C*). ESI (m/z): [M + Na]+ calcd for $C_{21}H_{19}NO_2SNa$: 372.1029, found: 372.1022.

5-Phenyl-1,3-dihydroisobenzofuran (3v)

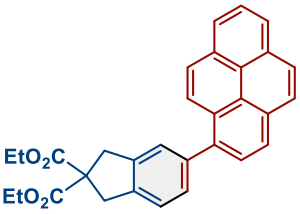


3v

The reaction was conducted with **1g** (18.4 mg, 0.2 mmol) and **2a** (65 μL, 0.6 mmol). The resulting crude mixture was purified by silica-gel column chromatography (SiO_2, Et_2O/hexane, 0:100–10:90) to obtain **3v** in 79% yield (30.2 mg, 0.16 mmol) as a yellowish oil.

^1H NMR (400 MHz, $CDCl_3$, δ) 5.16 (s, 4H), 7.30 (d, J = 8.0 Hz, 1H), 7.33–7.39 (m, 1H), 7.40–7.53 (m, 4H), 7.58 (d, J = 7.2 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$, δ) 73.5 (CH_2), 73.6 (CH_2), 119.8 (*C*H), 121.3 (*C*H), 126.7 (*C*H), 127.3 (*C*H), 127.4 (*C*H), 128.9 (*C*H), 138.3 (*C*), 140.0 (*C*), 140.9 (*C*), 141.1 (*C*). EI (m/z): $[M]^+$ calcd for $C_{14}H_{12}O$: 196.0883, found: 196.0883.

Diethyl 5-(4,6-dihydropyren-1-yl)-1,3-dihydro-2H-indene-2,2-dicarboxylate (3w)



3w

The reaction was conducted with **1a** (47.1 mg, 0.2 mmol) and **2q** (134.2 mg, 0.6 mmol). The resulting crude mixture was purified by silica-gel column chromatography (SiO_2, Et_2O/hexane, 0:100–10:90) to obtain **3w** in 51% yield (47.4 mg, 0.10 mmol) as a yellowish oil.

^{1}H NMR (401 MHz, $CDCl_3$, δ) 1.30 (t, J = 6.8 Hz, 6H), 3.74 (s, 4H), 4.26 (q, J = 6.8 Hz, 4H), 7.37 (d, J = 8.0 Hz, 1H), 7.40–7.46 (m, 2H), 7.94 (d, J = 7.6 Hz, 1H), 7.97–8.02 (m, 2H), 8.07 (s, 2H), 8.13–8.21 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$, δ) 14.2 (CH_3), 40.5 (CH_2), 40.7 (CH_2), 60.6 (C), 61.9 (CH_2), 124.2 (*C*H), 124.7 (*C*H), 124.9 (*C*H), 125.1 (*C*H), 125.5 (*C*H), 126.1 (*C*H), 126.4 (*C*H), 127.4 (*C*H), 127.48 (*C*H), 127.52 (*C*H), 127.7 (*C*H), 128.6 (*C*), 129.6 (*C*H), 130.6 (*C*), 131.1 (*C*), 131.6 (*C*), 137.9 (*C*), 139.2 (*C*), 140.1 (*C*), 140.4 (*C*), 171.9 (*C*). ESI (m/z): $[M+Na]^+$ calcd for $C_{31}H_{26}O_4Na$: 485.1723, found: 485.1714.

11. References

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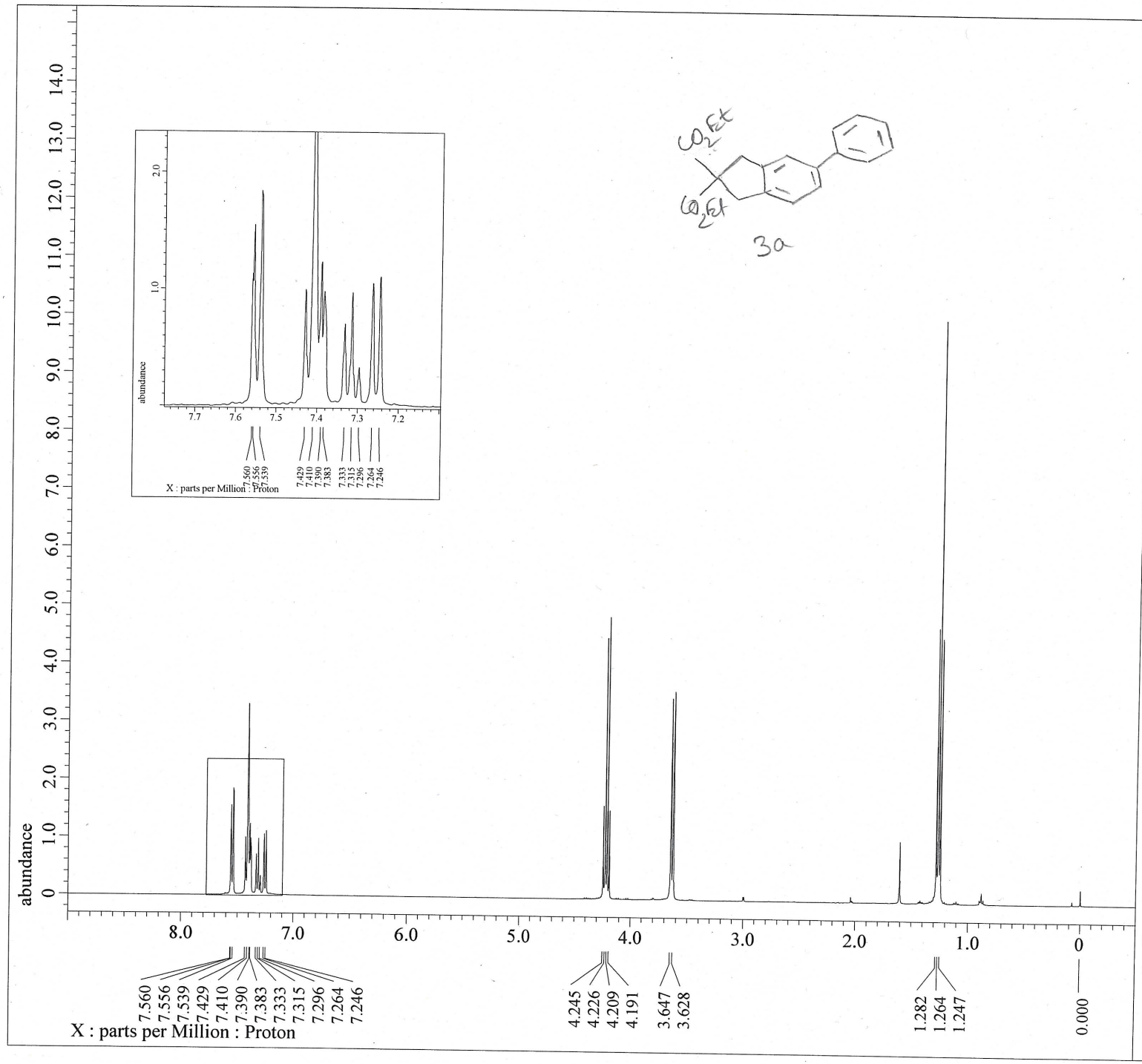
[2] K. E. Ruhl, T. Rovis, *J. Am. Chem. Soc.* **2016**, *138*, 15527–15530.

[3] N. Saino, F. Amemiya, E. Tanabe, K. Kase, S. Okamoto, *Org. Lett.* **2006**, *8*, 1439–1442.

[4] J. García-Lacuna, G. Domínguez, J. Blanco-Urgoiti, J. Pérez-Castells, *Org. Lett.* **2018**, *20*, 5219–5223.

[5] D. Brenna, M. Villa, T. N. Gieshoff, F. Fischer, M. Hapke, A. Jacobi von Wangelin, *Angew. Chem. Int. Ed.* **2017**, *56*, 8451–8454.

[6] B. D. Ravetz, J. Y. Wang, K. E. Ruhl, T. Rovis, *ACS Catal.* **2019**, *9*, 200–204.

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machinephase
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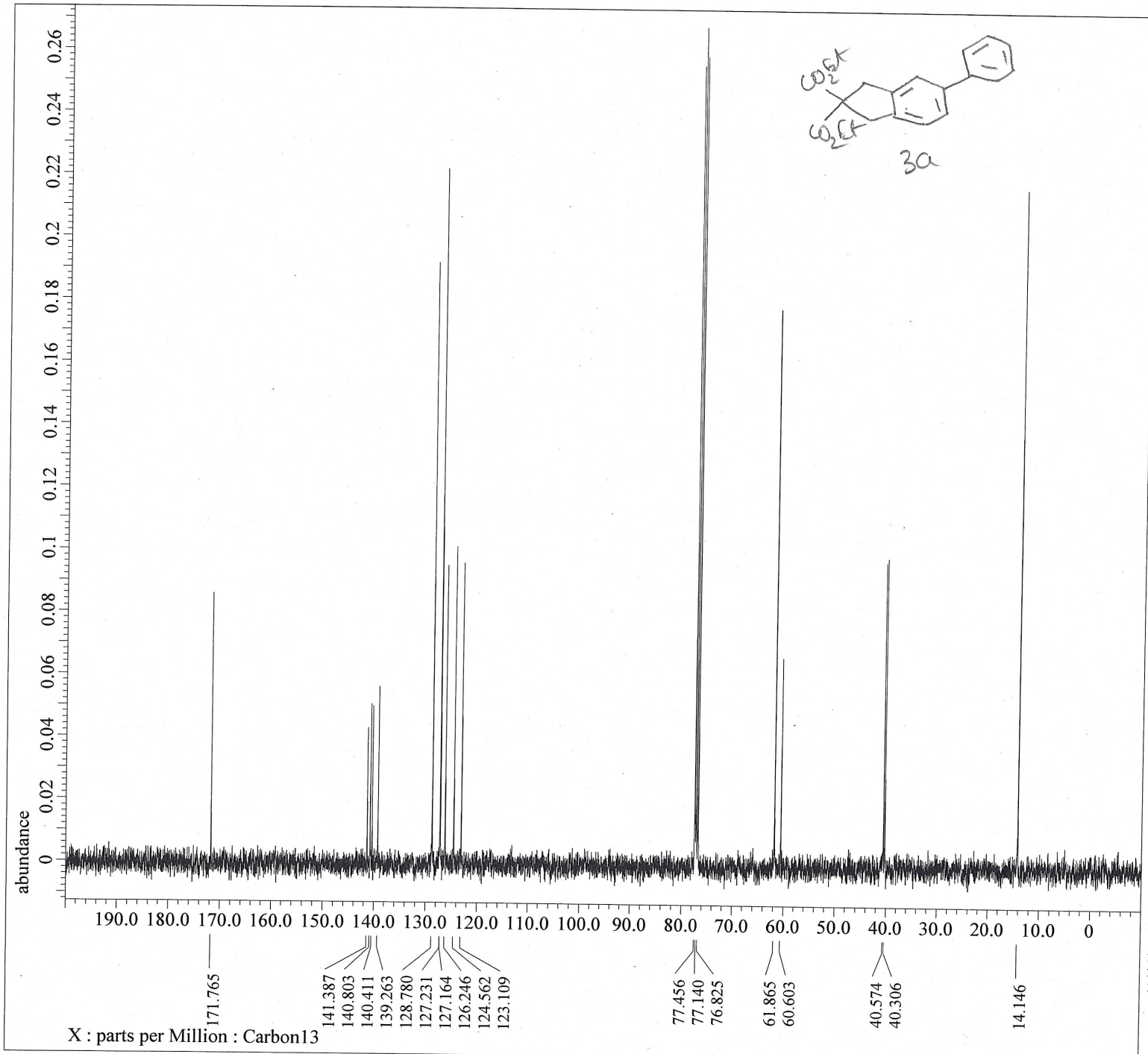


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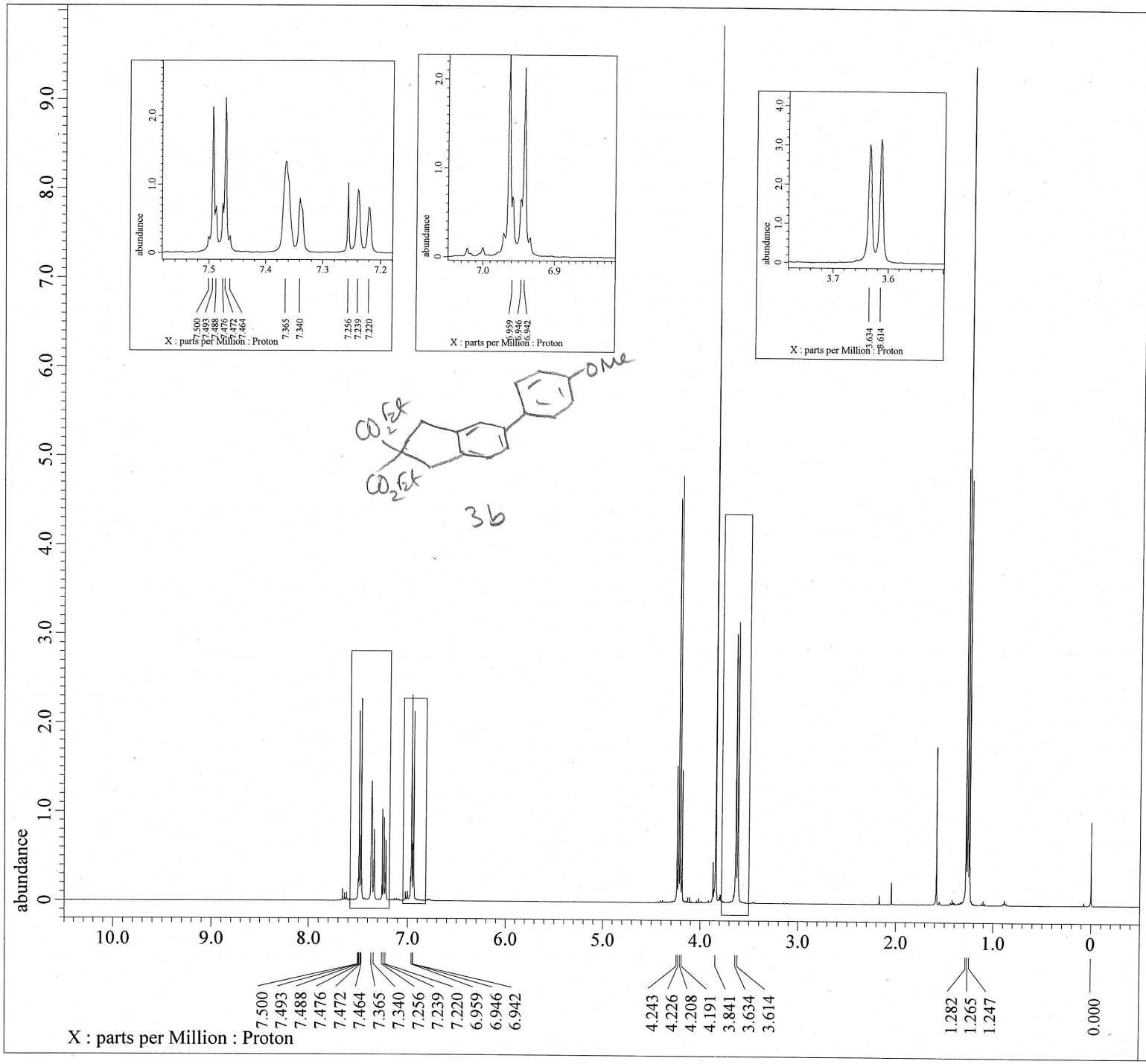


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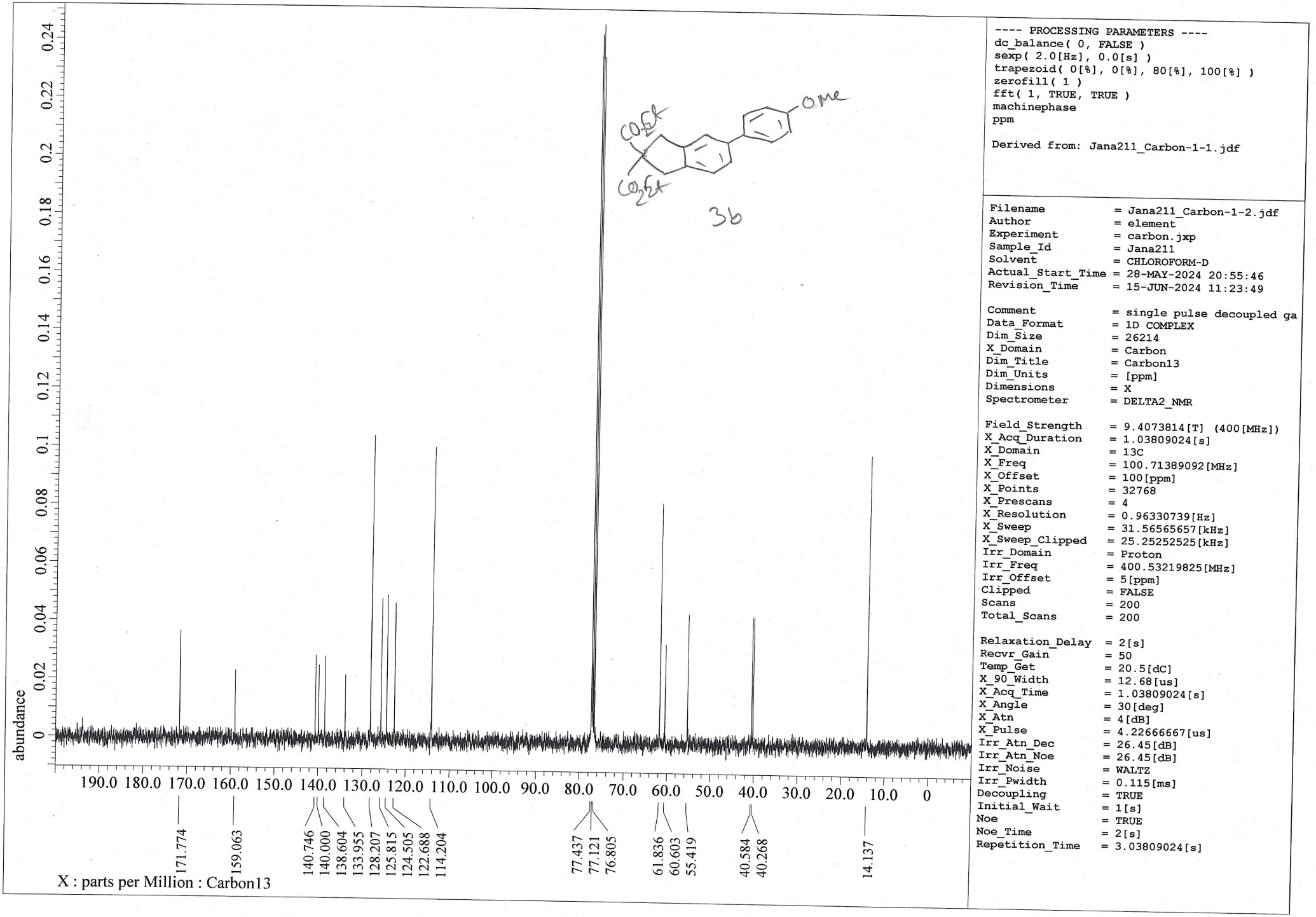
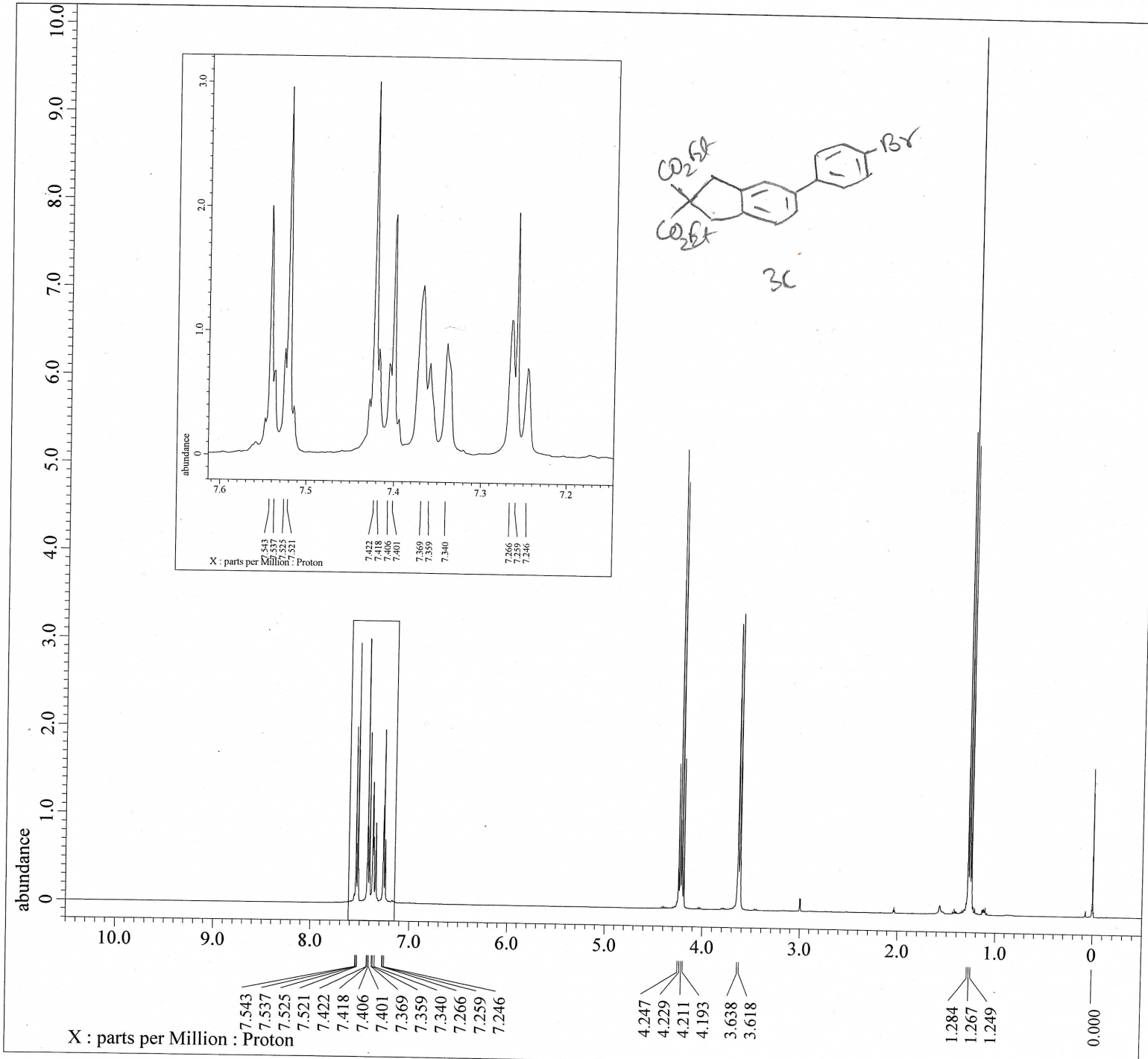
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.4073814[T] (400[MHz])
X_Acq_Duration	= 2.18103808[s]
X_Domain	= 1H
X_Freq	= 400.53219825[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45849727[Hz]
X_Sweep	= 7.51201923[kHz]
X_Sweep_Clipped	= 6.00961538[kHz]
Irr_Domain	= 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	= 20.3[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]



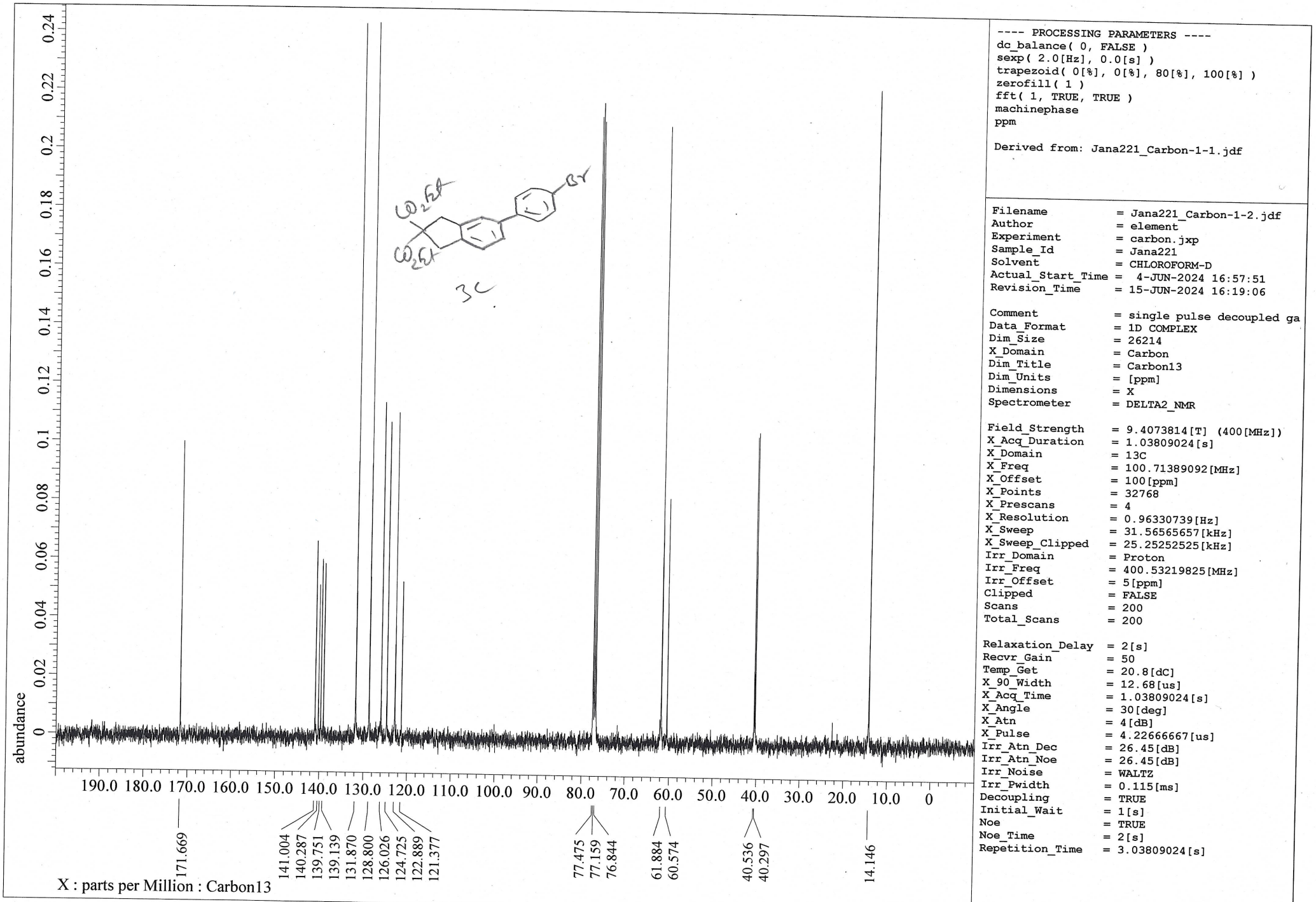

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: Jana211_Carbon-1-1.jdf
```

Filename	= Jana211_Carbon-1-2.jdf
Author	= element
Experiment	= carbon.jxp
Sample_Id	= Jana211
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 28-MAY-2024 20:55:46
Revision_Time	= 15-JUN-2024 11:23:49
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	= 200
Total_Scans	= 200
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 20.5[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]



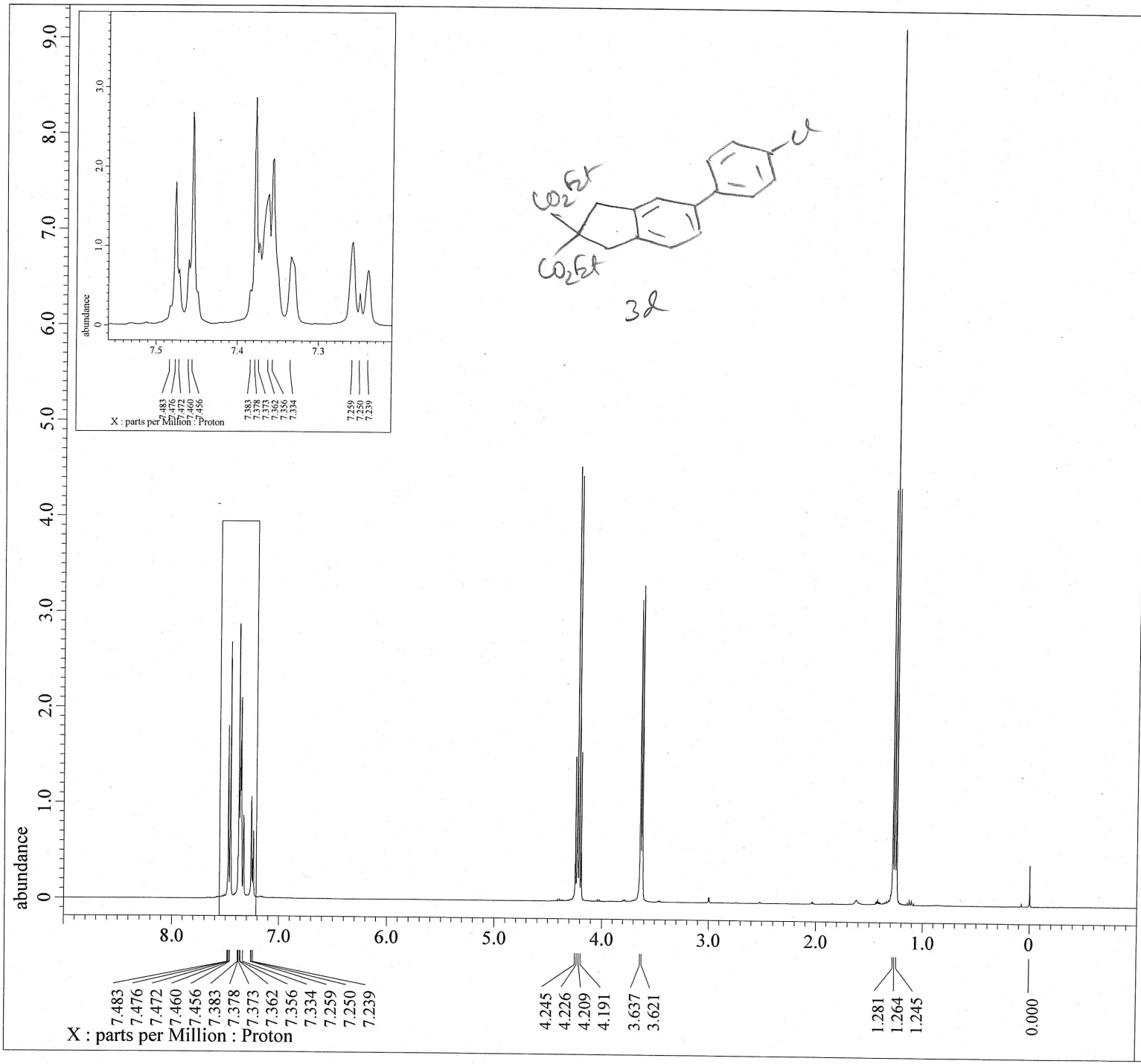

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: Jana221r_Proton-1-1.jdf
```

Filename	= Jana221r_Proton-1-2.jdf
Author	= element
Experiment	= proton.jxp
Sample_Id	= Jana221r
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 21-FEB-2025 12:42:59
Revision_Time	= 21-FEB-2025 12:12:28
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.4073814[T] (400[MHz])
X_Acq_Duration	= 2.18103808[s]
X_Domain	= 1H
X_Freq	= 400.53219825[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45849727[Hz]
X_Sweep	= 7.51201923[kHz]
X_Sweep_Clipped	= 6.00961538[kHz]
Irr_Domain	= Proton
Irr_Freq	= 400.53219825[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 400.53219825[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 38
Temp_Get	= 18.4[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]



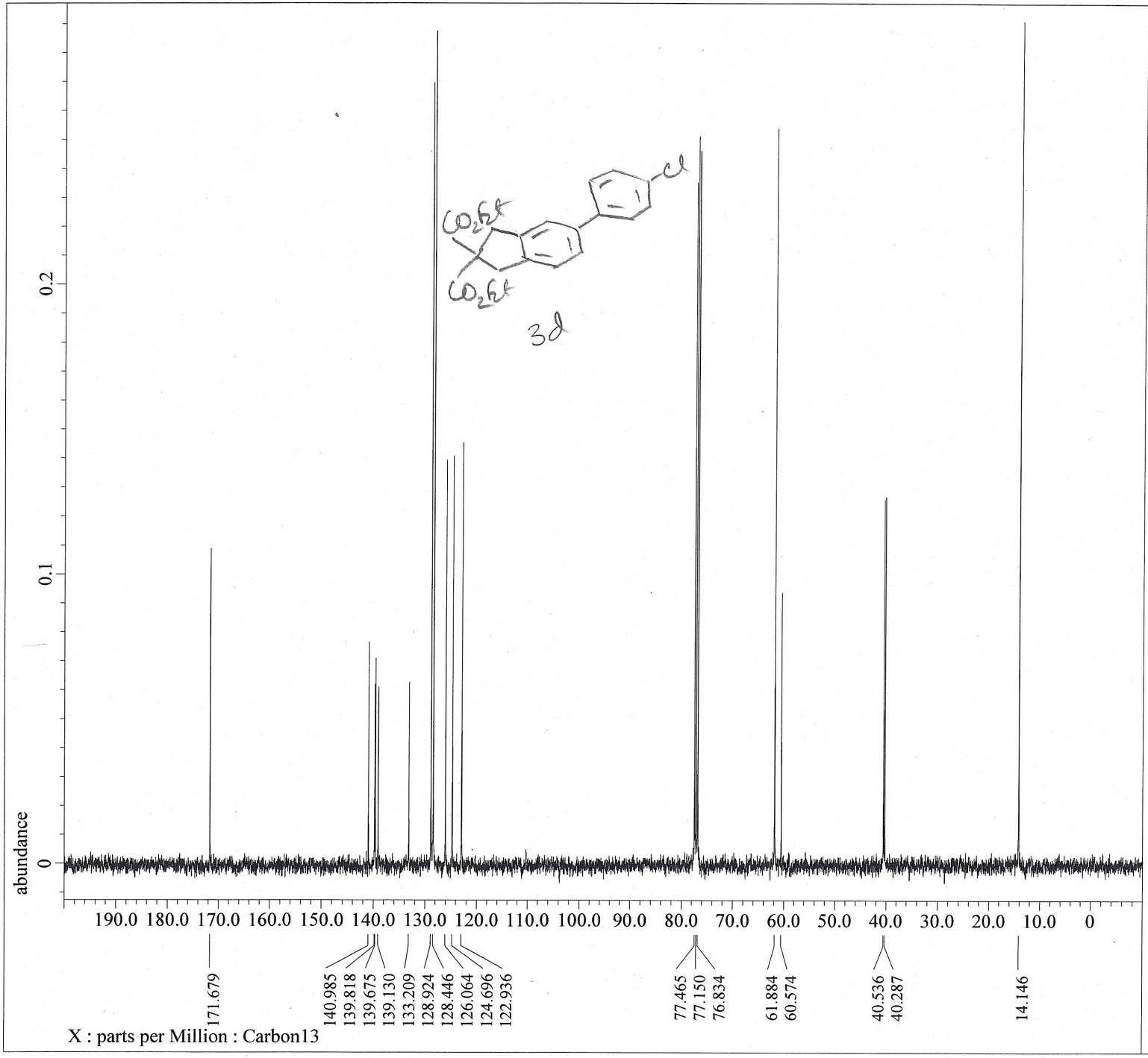

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: Jana221_Carbon-1-1.jdf
```

Filename	= Jana221_Carbon-1-2.jdf
Author	= element
Experiment	= carbon.jxp
Sample_Id	= Jana221
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 4-JUN-2024 16:57:51
Revision_Time	= 15-JUN-2024 16:19:06
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	= 200
Total_Scans	= 200
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 20.8[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]



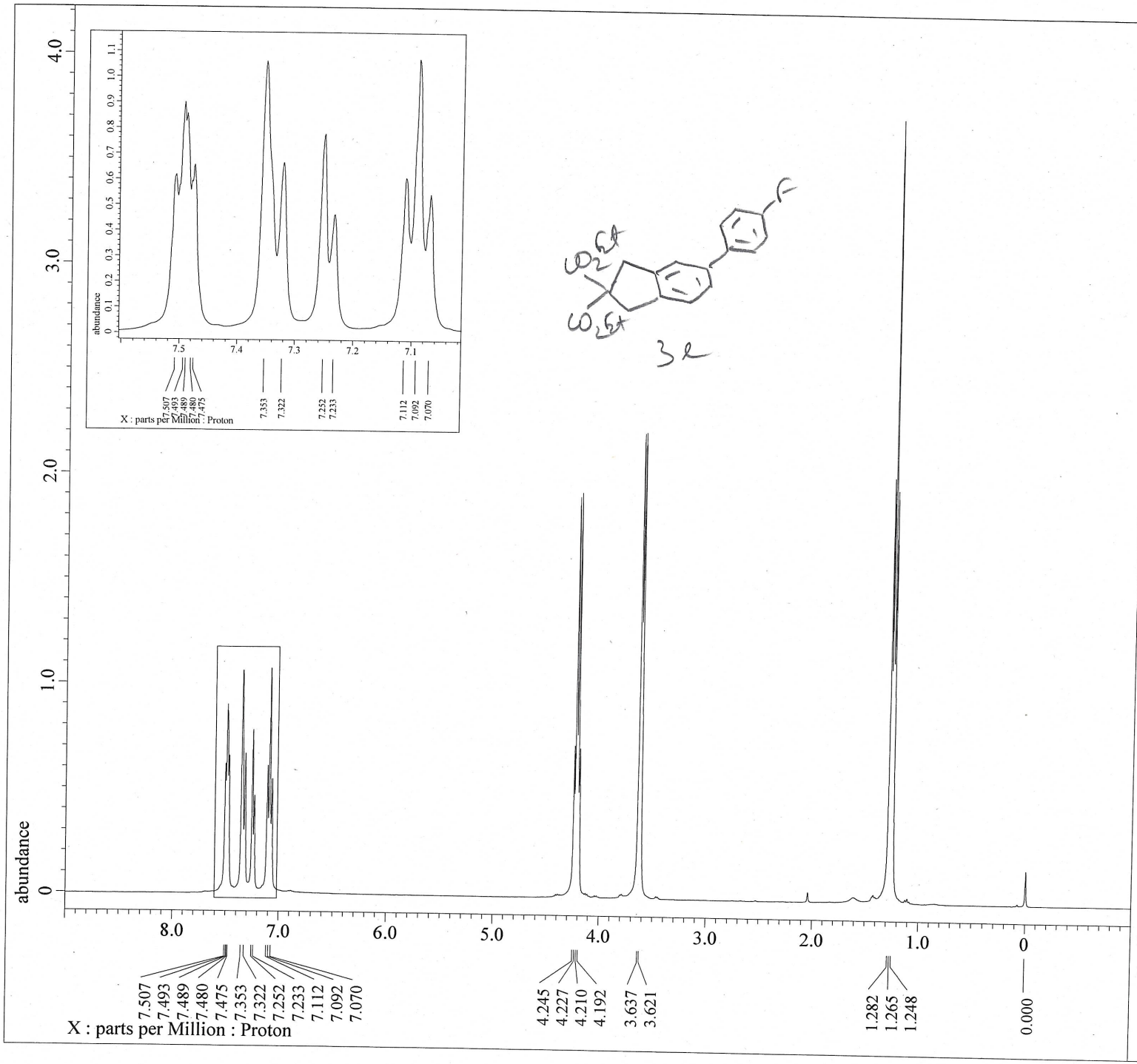

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: Jana223_Proton-1-1.jdf
```

Filename	= Jana223_Proton-1-2.jdf
Author	= element
Experiment	= proton.jxp
Sample_Id	= Jana223
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 5-JUN-2024 20:55:19
Revision_Time	= 15-JUN-2024 16:48:48
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.4073814[T] (400[MHz])
X_Acq_Duration	= 2.18103808[s]
X_Domain	= 1H
X_Freq	= 400.53219825[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45849727[Hz]
X_Sweep	= 7.51201923[kHz]
X_Sweep_Clipped	= 6.00961538[kHz]
Irr_Domain	= Proton
Irr_Freq	= 400.53219825[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 400.53219825[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 26
Temp_Get	= 20[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]



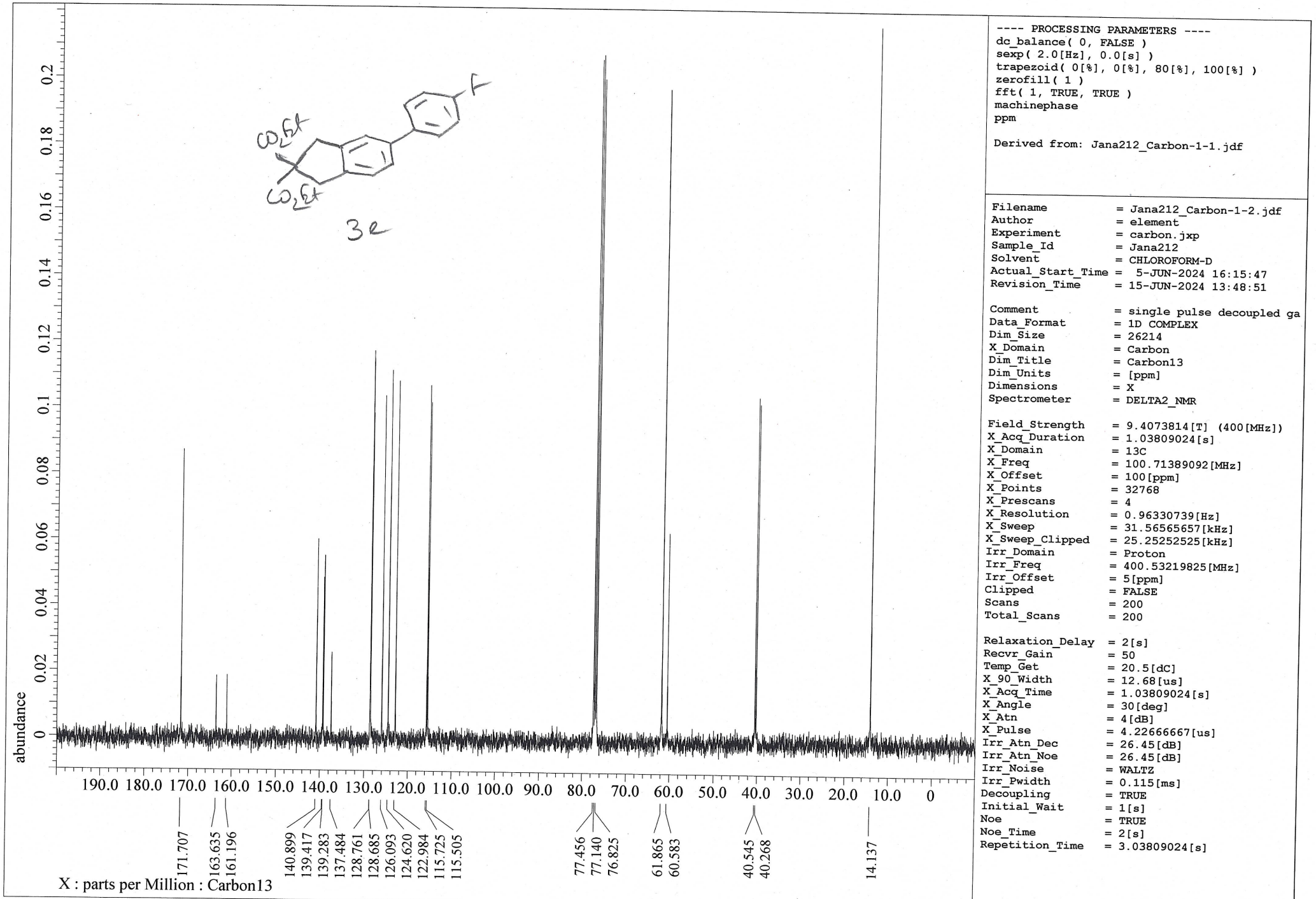

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: Jana223_Carbon-1-1.jdf
```

```
Filename            = Jana223_Carbon-1-2.jdf
Author              = element
Experiment          = carbon.jxp
Sample_Id           = Jana223
Solvent             = CHLOROFORM-D
Actual_Start_Time   =  5-JUN-2024 20:56:38
Revision_Time       = 15-JUN-2024 16:49:37

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               = 200
Total_Scans         = 200

Relaxation_Delay    = 2[s]
Recvr_Gain          = 50
Temp_Get            = 19.9[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]
```



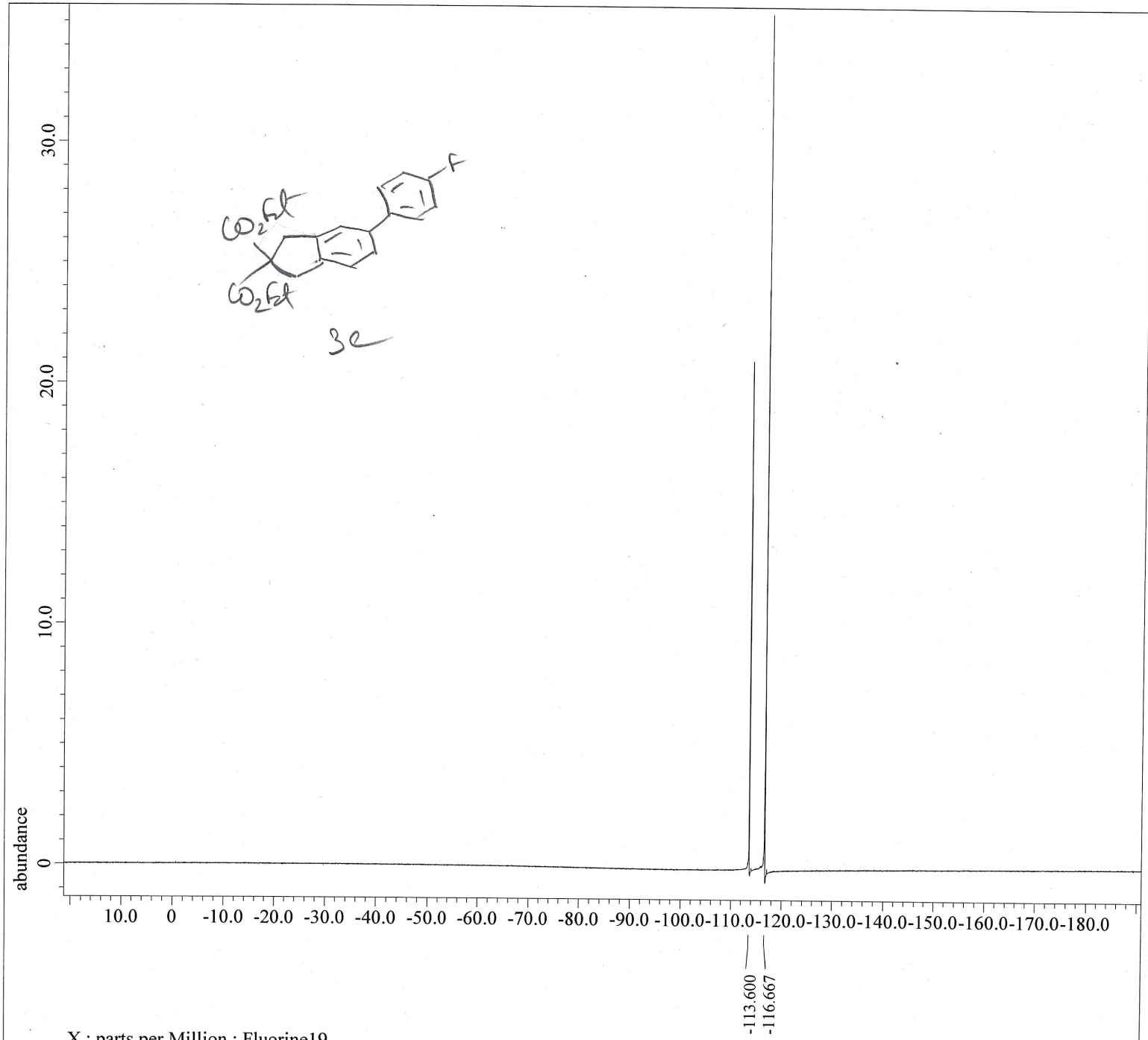

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: Jana212_Proton-1-1.jdf
```

Filename	= Jana212_Proton-1-2.jdf
Author	= element
Experiment	= proton.jxp
Sample_Id	= Jana212
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 5-JUN-2024 16:14:27
Revision_Time	= 15-JUN-2024 13:44:45
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.4073814[T] (400[MHz])
X_Acq_Duration	= 2.18103808[s]
X_Domain	= 1H
X_Freq	= 400.53219825[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45849727[Hz]
X_Sweep	= 7.51201923[kHz]
X_Sweep_Clipped	= 6.00961538[kHz]
Irr_Domain	= Proton
Irr_Freq	= 400.53219825[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 400.53219825[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 28
Temp_Get	= 20.5[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]



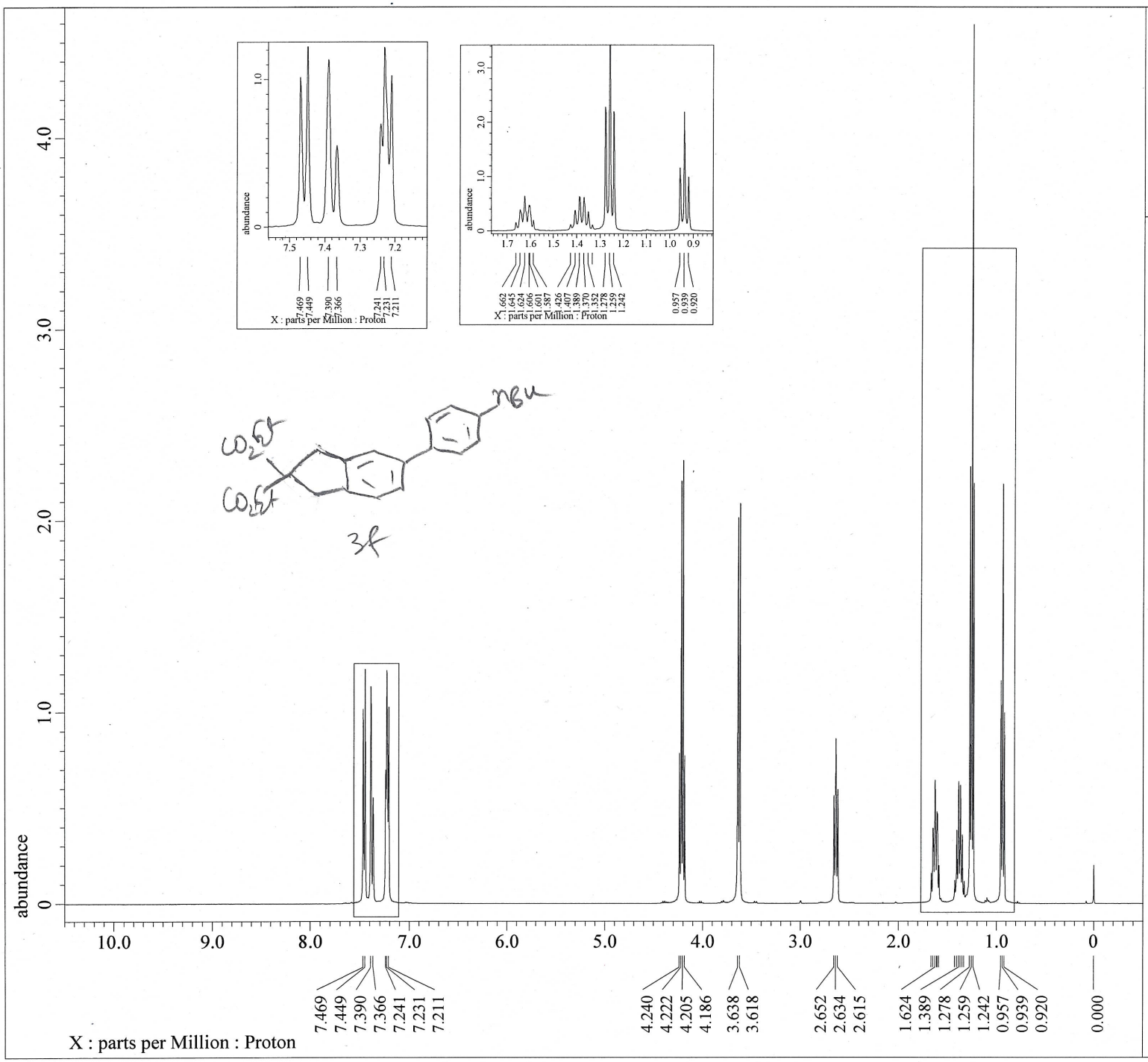

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: Jana212_Carbon-1-1.jdf
```

Filename	= Jana212_Carbon-1-2.jdf
Author	= element
Experiment	= carbon.jxp
Sample_Id	= Jana212
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 5-JUN-2024 16:15:47
Revision_Time	= 15-JUN-2024 13:48:51
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	= 200
Total_Scans	= 200
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 20.5[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]



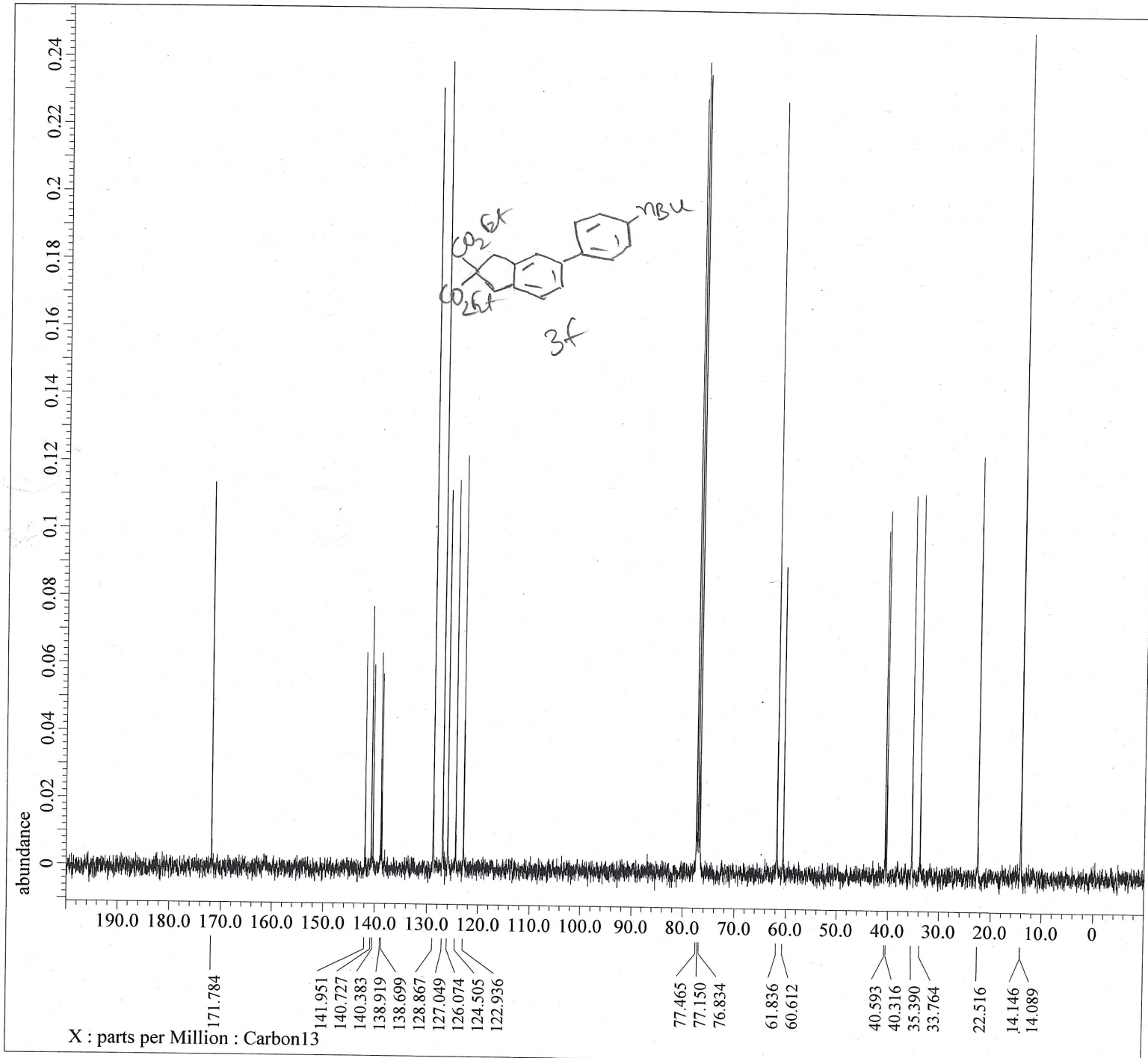

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
reference( -112.96619[ppm], 0[ppm] )
reference( 0.0[ppm], -113.6[ppm] )
phase( -90.59421, 0, 78.91042[%] )

Derived from: Jana212f_single_pulse-1-1.jdf
```

```
Filename            = Jana212f_single_pulse-1-2
Author              = element
Experiment          = single_pulse.jxp
Sample_Id           = Jana212f
Solvent             = CHLOROFORM-D
Actual_Start_Time   =  7-FEB-2025 18:51:07
Revision_Time       =  7-FEB-2025 18:32:40

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

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

Relaxation_Delay    = 5[s]
Recvr_Gain          = 46
Temp_Get            = 18.3[dC]
X_90_Width          = 7.59[us]
X_Acq_Time          = 86.50752[ms]
X_Angle             = 45[deg]
X_Atn               = 3[dB]
X_Pulse             = 3.795[us]
Irr_Mode            = Off
Tri_Mode            = Off
Dante_Presat        = FALSE
Initial_Wait        = 1[s]
Repetition_Time     = 5.08650752[s]
```



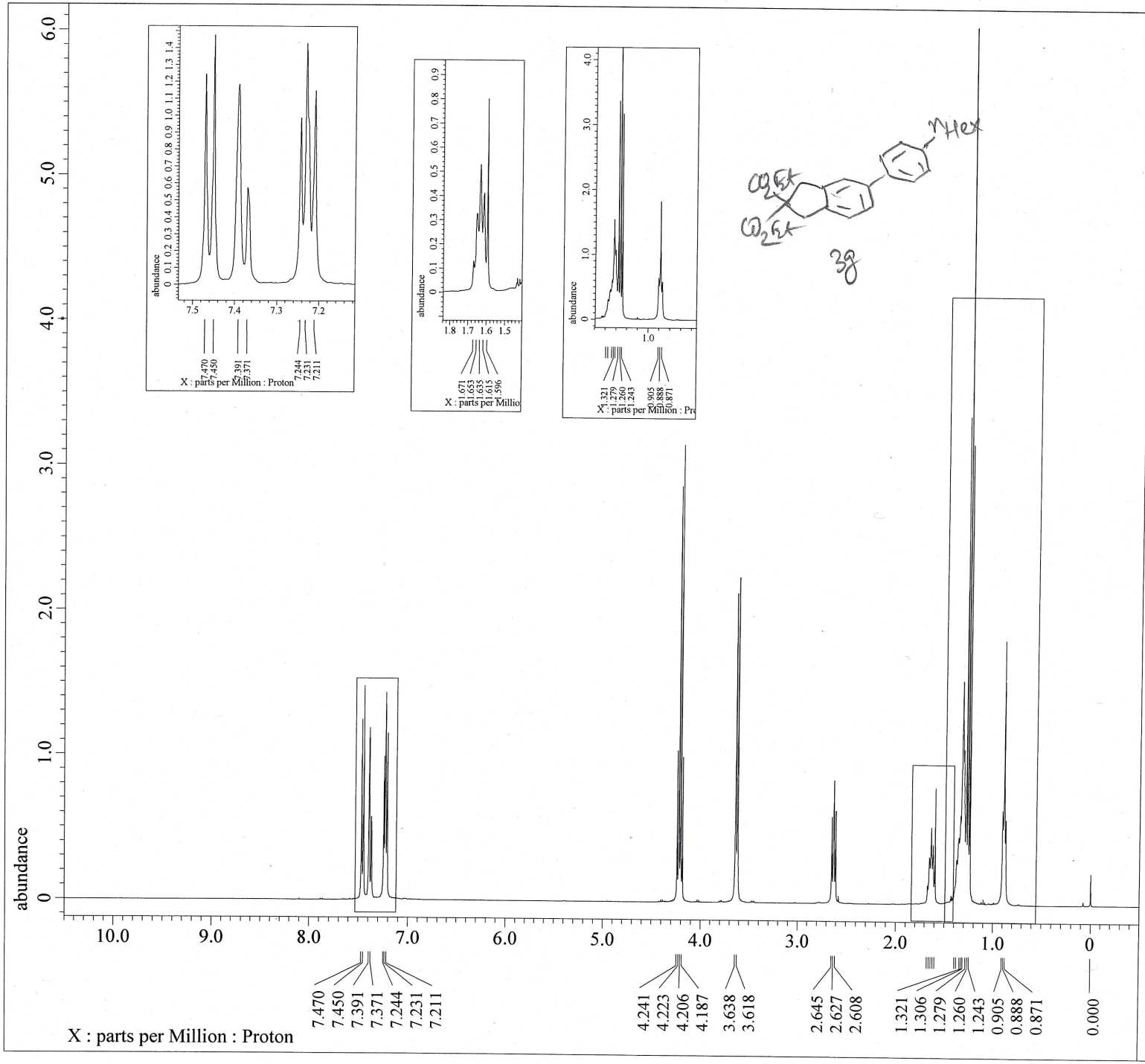

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: Jana225_Proton-1-1.jdf
```

```
Filename            = Jana225_Proton-1-2.jdf
Author              = element
Experiment          = proton.jxp
Sample_Id           = Jana225
Solvent             = CHLOROFORM-D
Actual_Start_Time   =  7-JUN-2024 13:53:54
Revision_Time       = 10-FEB-2025 20:18:56

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          = 24
Temp_Get            = 20.8[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]
```



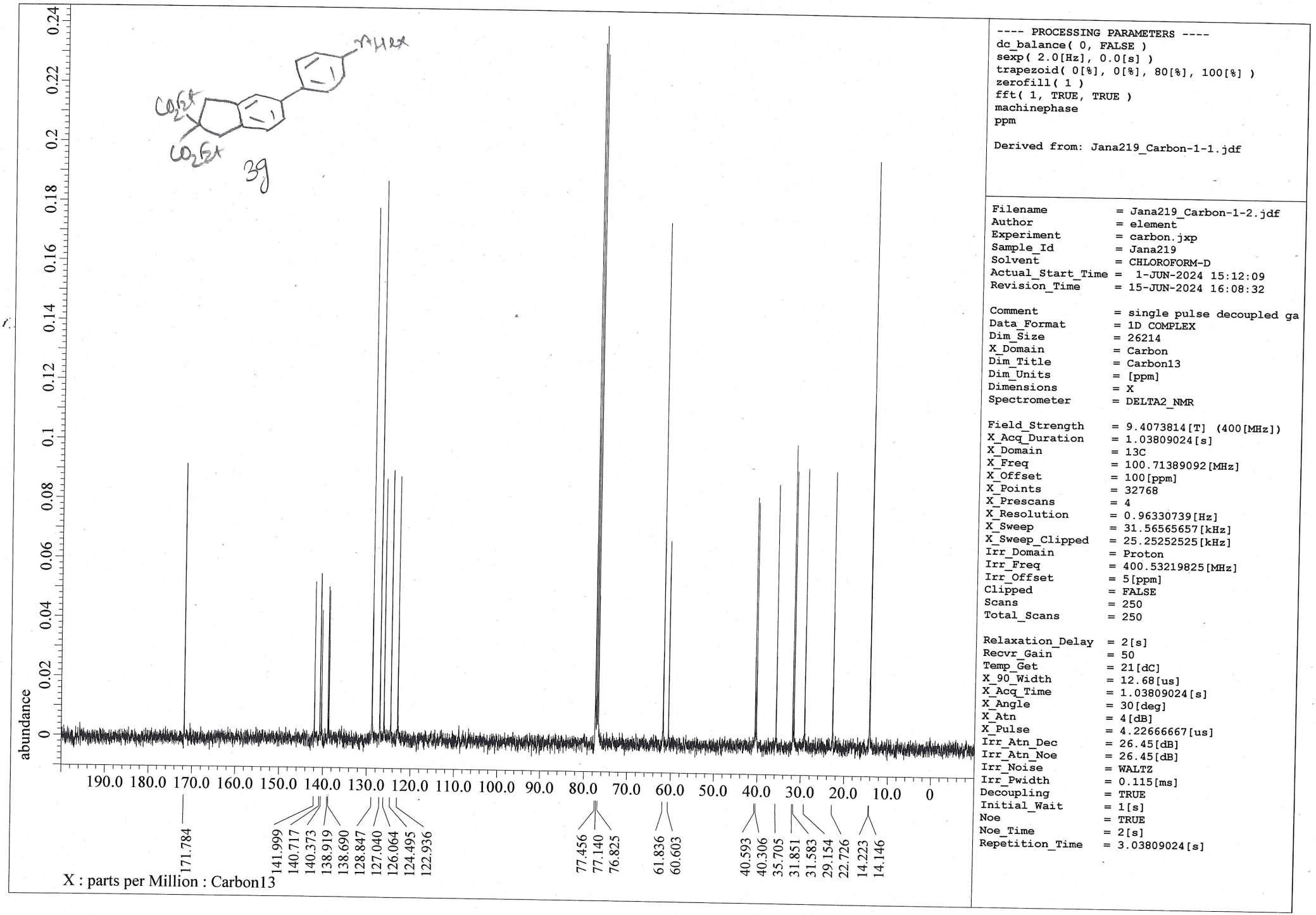

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: Jana225_Carbon-1-1.jdf
```

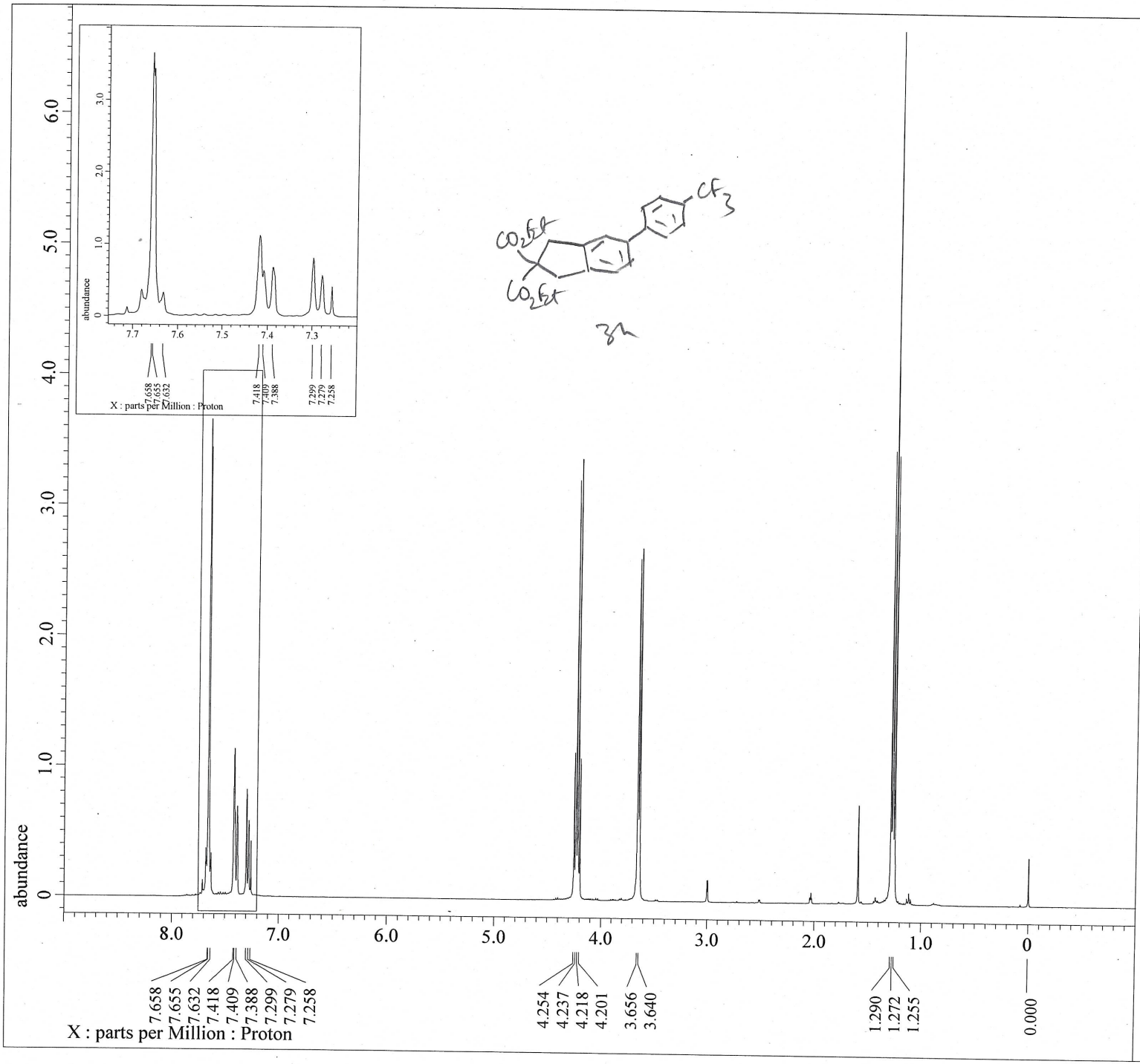
Filename	= Jana225_Carbon-1-2.jdf
Author	= element
Experiment	= carbon.jxp
Sample_Id	= Jana225
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 7-JUN-2024 13:55:14
Revision_Time	= 24-JUN-2024 18:28:02
Comment	= single pulse decoupled ga
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon
Dim_Title	= 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	= 200
Total_Scans	= 200
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 ----
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: Jana219_Proton-1-1.jdf
```

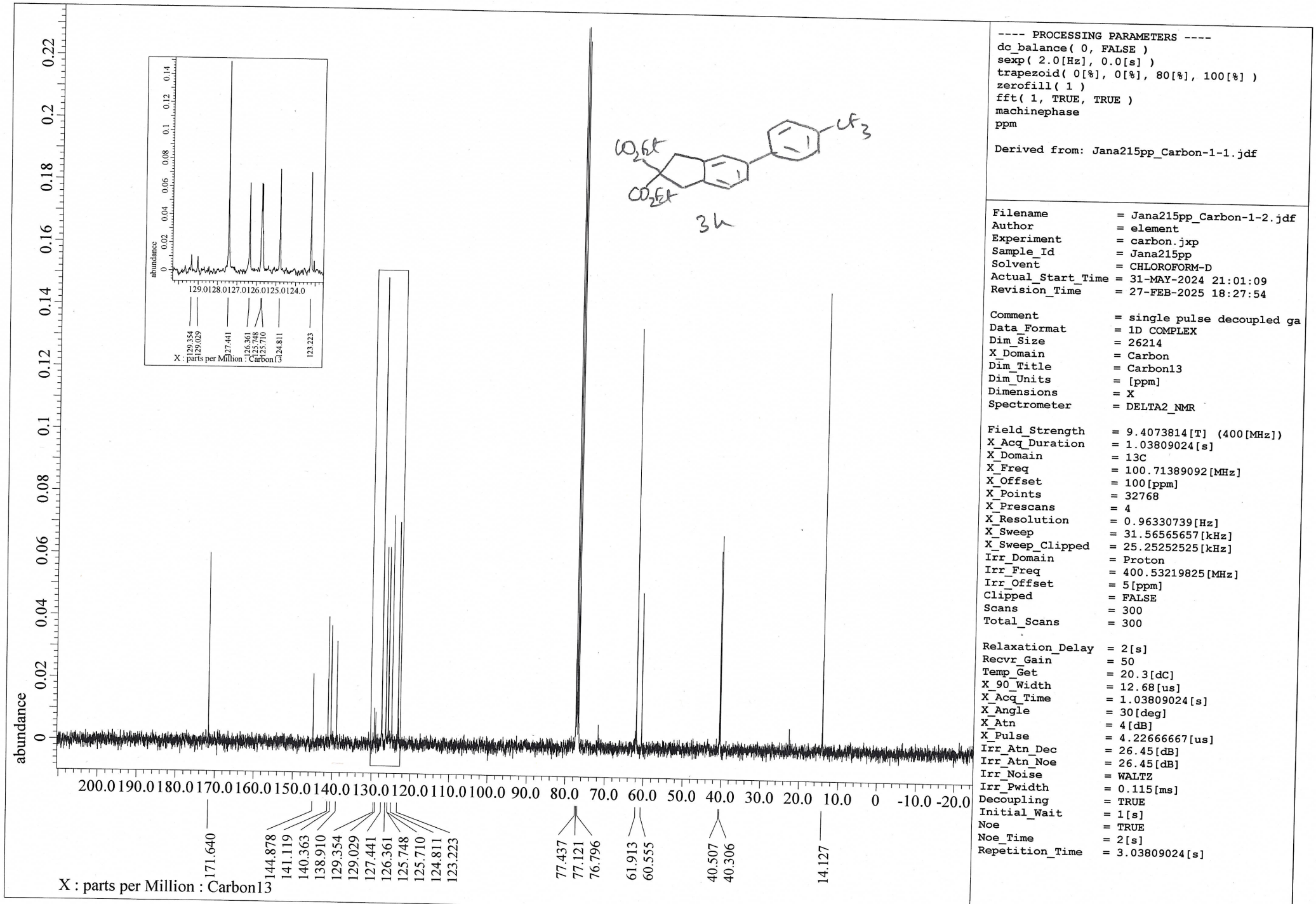
Filename	= Jana219_Proton-1-2.jdf
Author	= element
Experiment	= proton.jxp
Sample_Id	= Jana219
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 1-JUN-2024 15:10:49
Revision_Time	= 10-FEB-2025 20:56:57
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.4073814[T] (400[MHz])
X_Acq_Duration	= 2.18103808[s]
X_Domain	= 1H
X_Freq	= 400.53219825[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45849727[Hz]
X_Sweep	= 7.51201923[kHz]
X_Sweep_Clipped	= 6.00961538[kHz]
Irr_Domain	= Proton
Irr_Freq	= 400.53219825[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 400.53219825[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 26
Temp_Get	= 20.8[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]

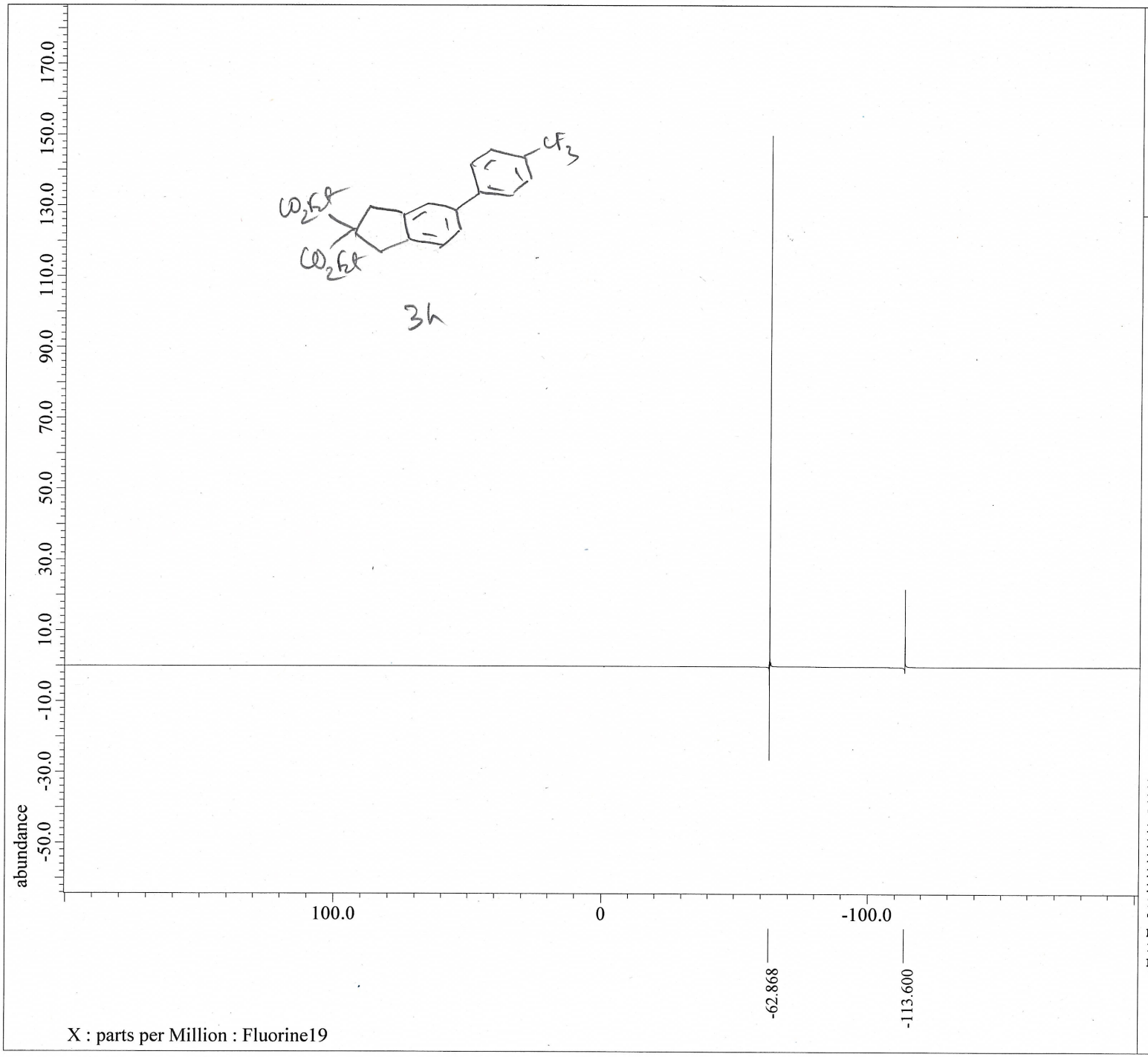

abundance
0
0.02
0.04
0.06
0.08
0.1
0.12
0.14
0.16
0.18
0.2
0.22
0.24
190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
171.784
141.999
140.717
140.373
138.919
138.690
128.847
127.040
126.064
124.495
122.936
77.456
77.140
76.825
61.836
60.603
40.593
40.306
35.705
31.851
31.583
29.154
22.726
14.223
14.146
X : parts per Million : Carbon13
3g
---- 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: Jana219_Carbon-1-1.jdf
Filename = Jana219_Carbon-1-2.jdf
Author = element
Experiment = carbon.jxp
Sample_Id = Jana219
Solvent = CHLOROFORM-D
Actual_Start_Time = 1-JUN-2024 15:12:09
Revision_Time = 15-JUN-2024 16:08:32
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 = 250
Total_Scans = 250
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 21[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: Jana215pp_Proton-1-1.jdf
```

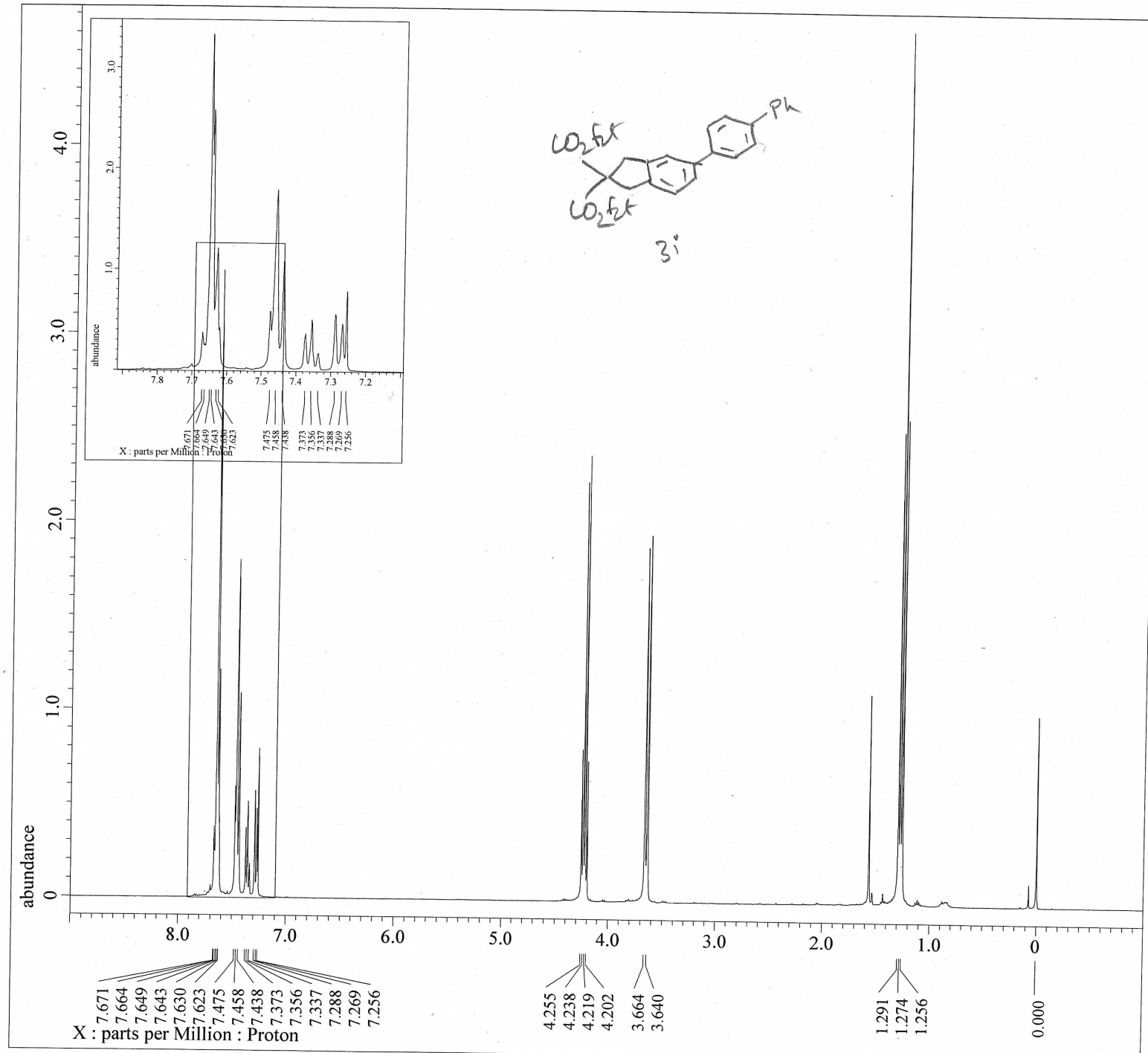
Filename	= Jana215pp_Proton-1-2.jdf
Author	= element
Experiment	= proton.jxp
Sample_Id	= Jana215pp
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 31-MAY-2024 20:59:49
Revision_Time	= 15-JUN-2024 15:20:59
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.4073814[T] (400[MHz])
X_Acq_Duration	= 2.18103808[s]
X_Domain	= 1H
X_Freq	= 400.53219825[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45849727[Hz]
X_Sweep	= 7.51201923[kHz]
X_Sweep_Clipped	= 6.00961538[kHz]
Irr_Domain	= Proton
Irr_Freq	= 400.53219825[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 400.53219825[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 30
Temp_Get	= 20.5[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]


abundance
X : parts per Million : Carbon13
171.640
144.878
141.119
140.363
138.910
129.354
129.029
127.441
126.361
125.748
125.710
124.811
123.223
77.437
77.121
76.796
61.913
60.555
40.507
40.306
14.127
3h
---- 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: Jana215pp_Carbon-1-1.jdf
Filename = Jana215pp_Carbon-1-2.jdf
Author = element
Experiment = carbon.jxp
Sample_Id = Jana215pp
Solvent = CHLOROFORM-D
Actual_Start_Time = 31-MAY-2024 21:01:09
Revision_Time = 27-FEB-2025 18:27:54
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 = 300
Total_Scans = 300
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 20.3[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]



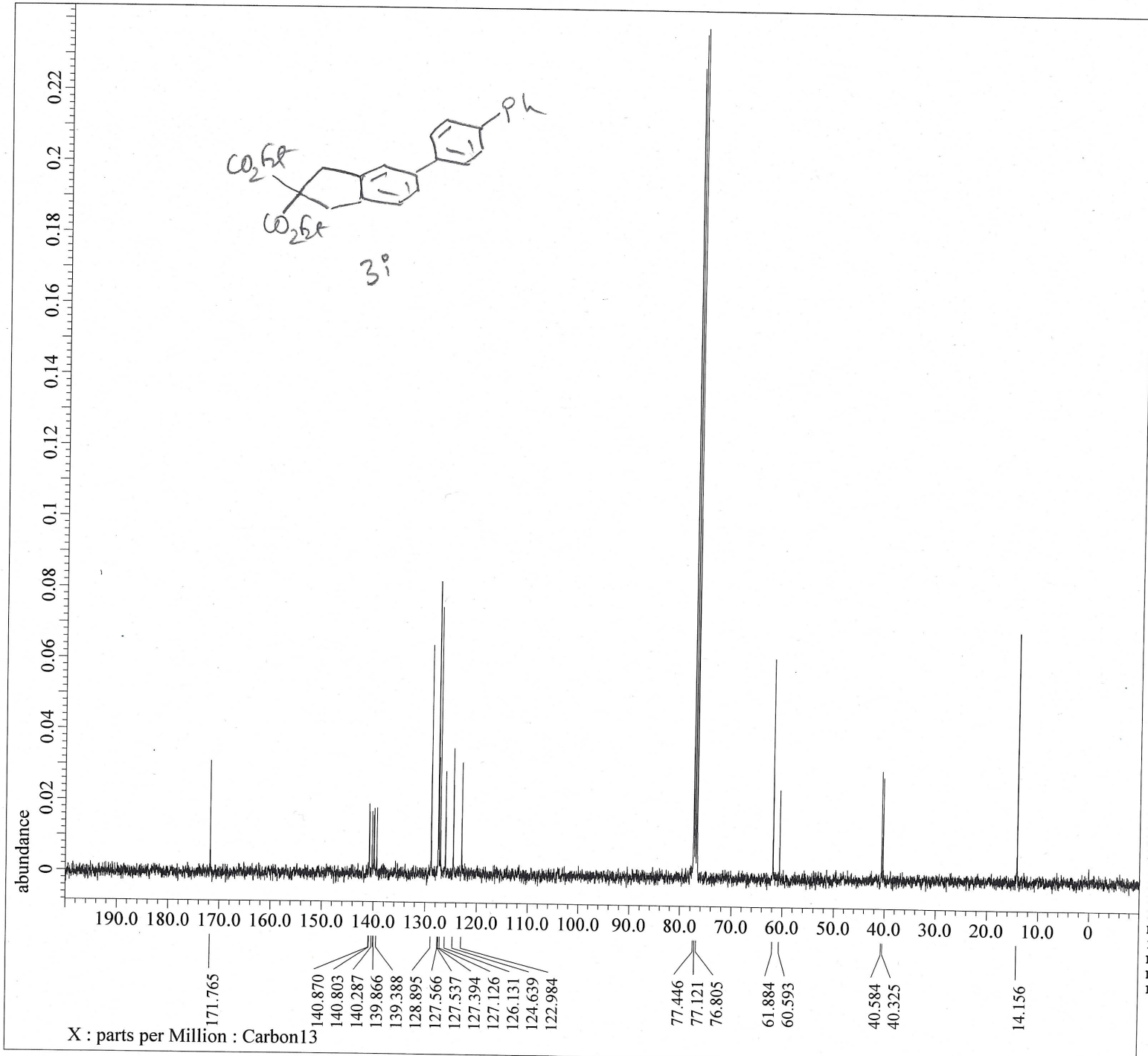

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: Jana215f_single_pulse-1-1.jdf
```

```
Filename            = Jana215f_single_pulse-1-2
Author              = element
Experiment          = single_pulse.jxp
Sample_Id           = Jana215f
Solvent             = CHLOROFORM-D
Actual_Start_Time   =  7-FEB-2025 19:02:03
Revision_Time       =  7-FEB-2025 18:35:04

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

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

Relaxation_Delay    = 5[s]
Recvr_Gain          = 42
Temp_Get            = 18[dC]
X_90_Width          = 7.59[us]
X_Acq_Time          = 86.50752[ms]
X_Angle             = 45[deg]
X_Atn               = 3[dB]
X_Pulse             = 3.795[us]
Irr_Mode            = Off
Tri_Mode            = Off
Dante_Presat        = FALSE
Initial_Wait        = 1[s]
Repetition_Time     = 5.08650752[s]
```



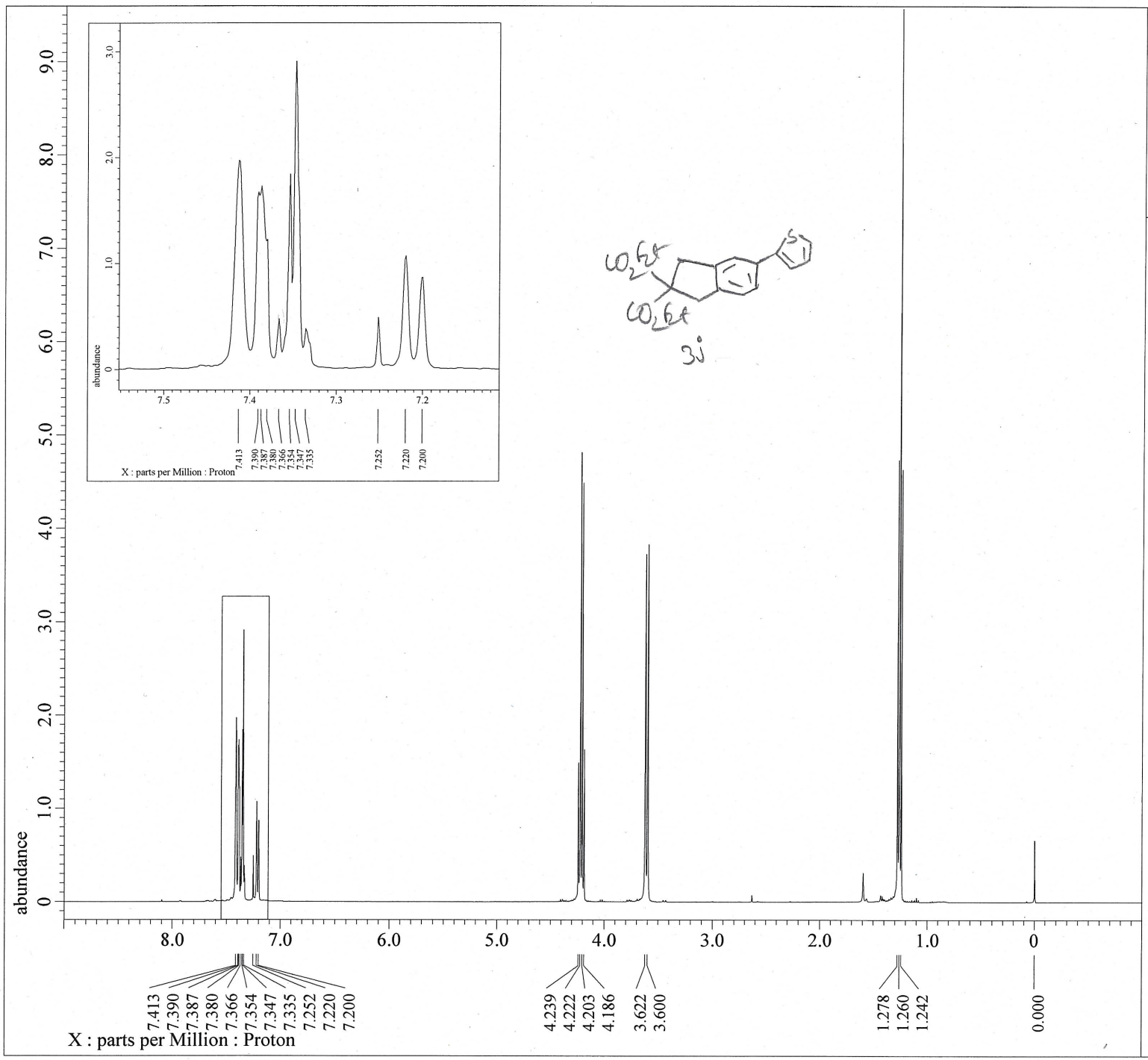

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: Jana216pp_Proton-1-1.jdf
```

Filename	= Jana216pp_Proton-1-2.jdf
Author	= element
Experiment	= proton.jxp
Sample_Id	= Jana216pp
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 31-MAY-2024 14:46:18
Revision_Time	= 15-JUN-2024 13:34:48
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.4073814[T] (400[MHz])
X_Acq_Duration	= 2.18103808[s]
X_Domain	= 1H
X_Freq	= 400.53219825[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45849727[Hz]
X_Sweep	= 7.51201923[kHz]
X_Sweep_Clipped	= 6.00961538[kHz]
Irr_Domain	= Proton
Irr_Freq	= 400.53219825[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 400.53219825[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 36
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]



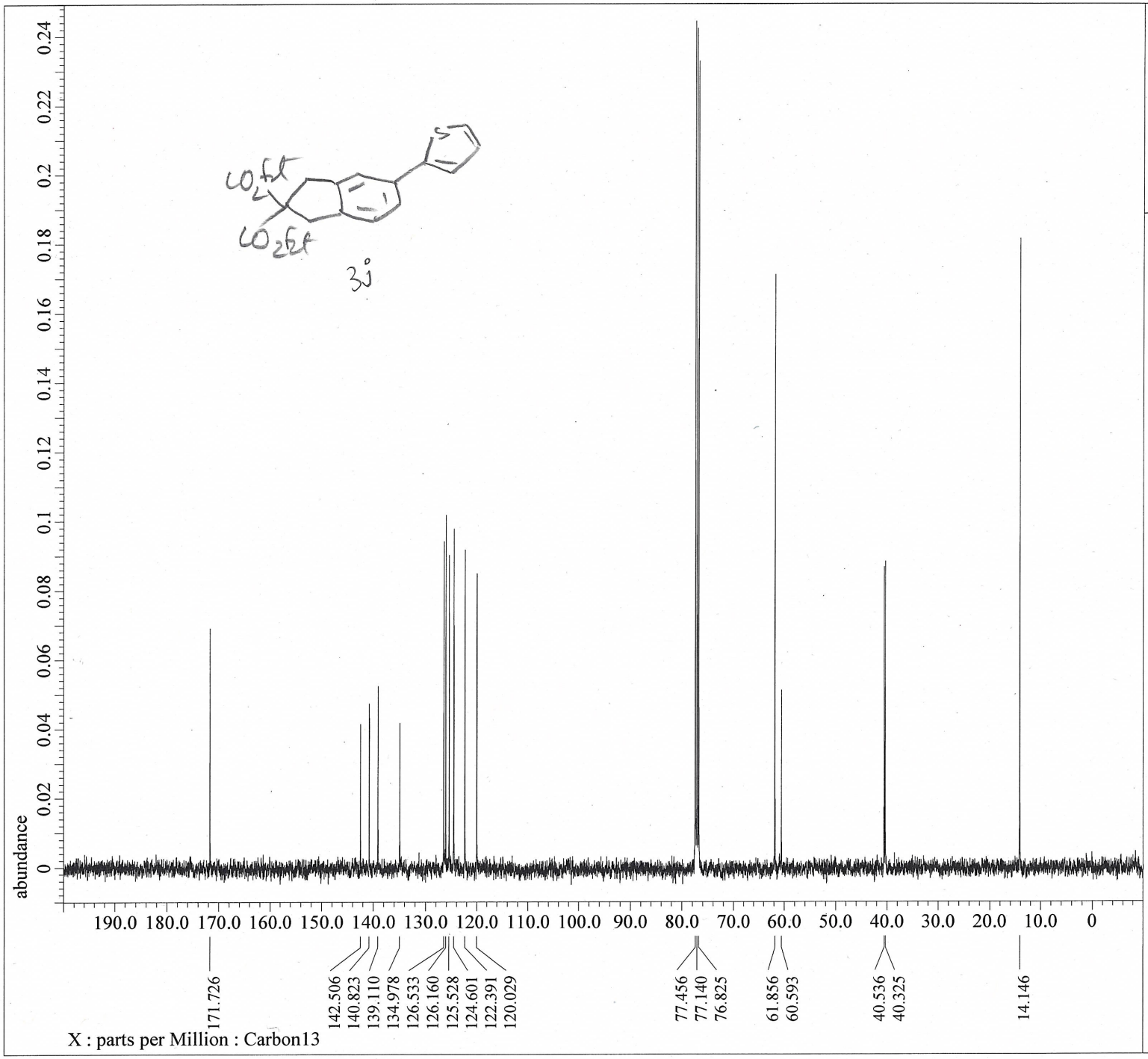

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: Jana216_Carbon-1-1.jdf
```

Filename	= Jana216_Carbon-1-2.jdf
Author	= element
Experiment	= carbon.jxp
Sample_Id	= Jana216
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 30-JAN-2025 20:01:39
Revision_Time	= 30-JAN-2025 19:57:28
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	= 500
Total_Scans	= 500
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 18[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]



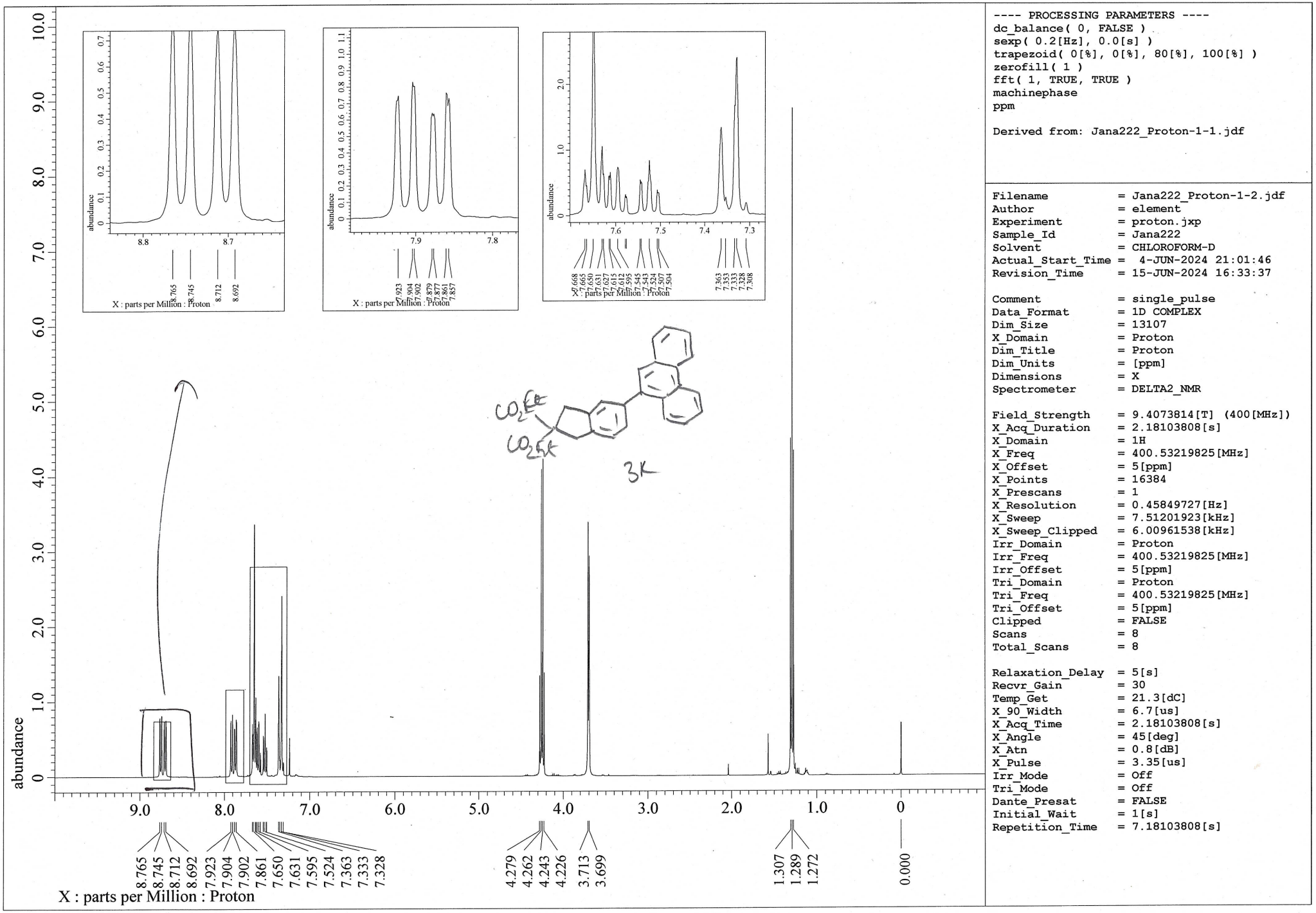

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: Jana224_Proton-1-1.jdf
```

Filename	= Jana224_Proton-1-2.jdf
Author	= element
Experiment	= proton.jxp
Sample_Id	= Jana224
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 6-JUN-2024 15:09:13
Revision_Time	= 15-JUN-2024 17:02:04
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	= 20.3[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]



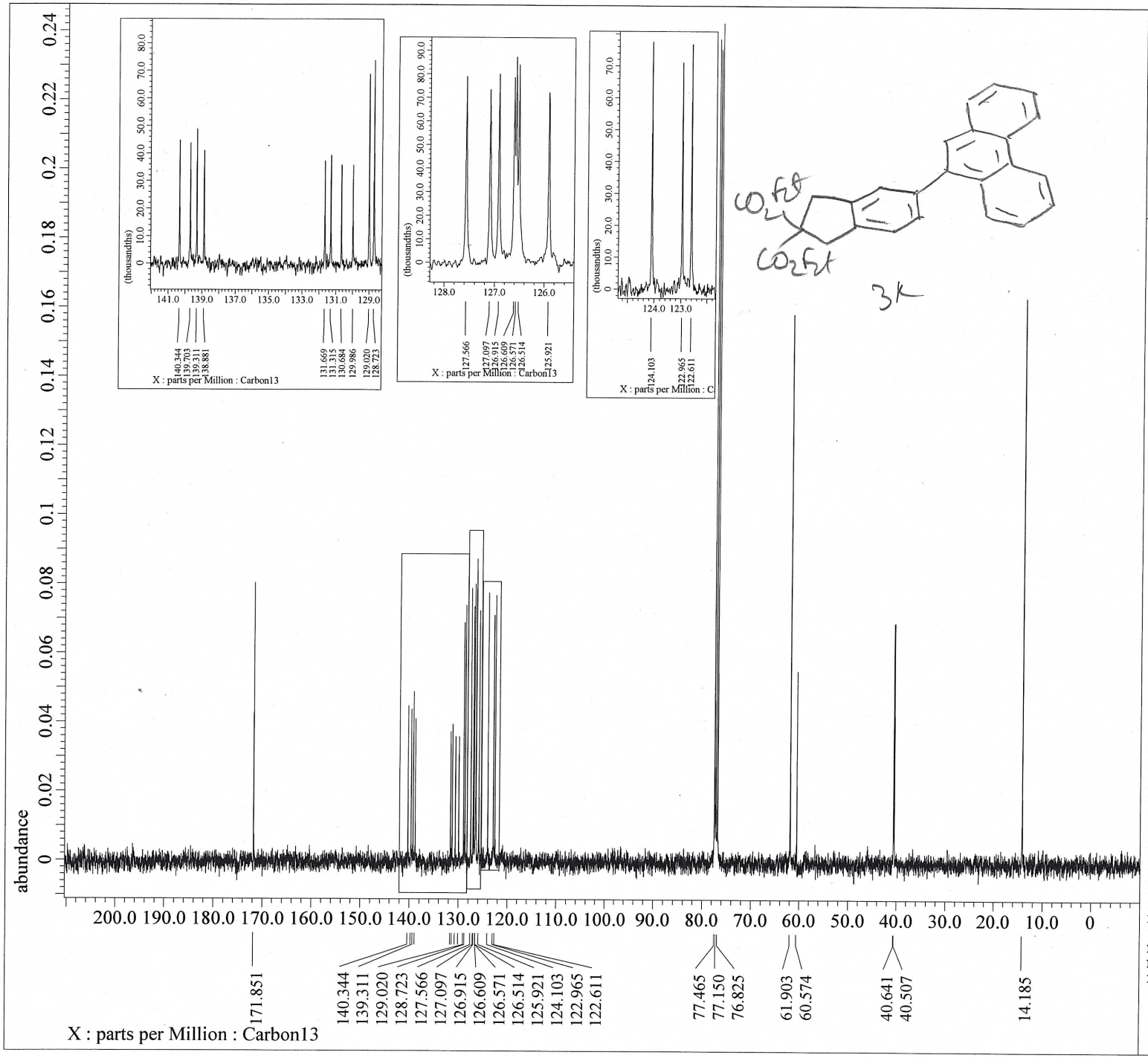

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: Jana224_Carbon-1-1.jdf
```

Filename	= Jana224_Carbon-1-2.jdf
Author	= element
Experiment	= carbon.jxp
Sample_Id	= Jana224
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 6-JUN-2024 15:10:32
Revision_Time	= 15-JUN-2024 17:03:47
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	= 250
Total_Scans	= 250
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 20.3[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]



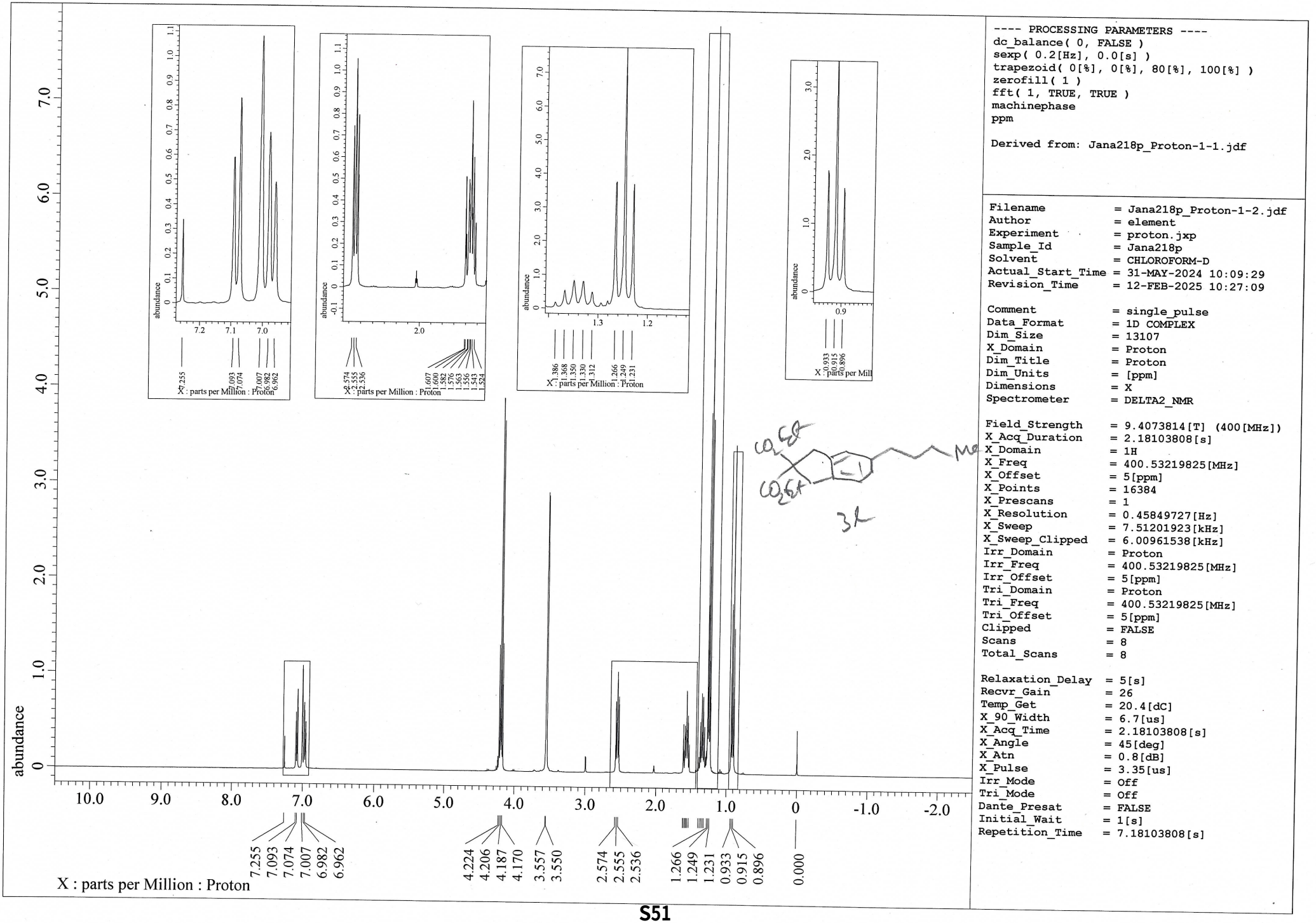

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: Jana222_Proton-1-1.jdf
```

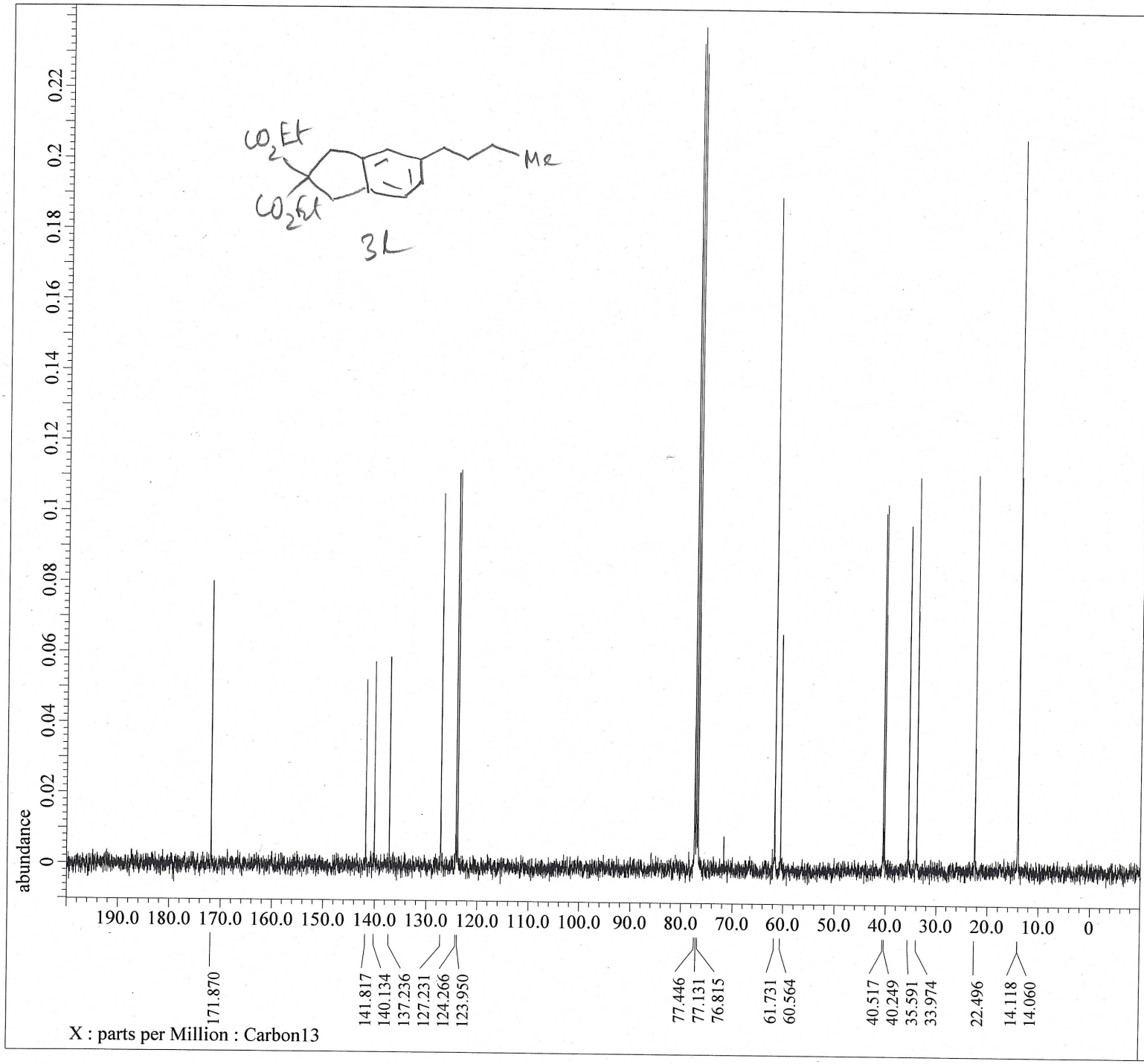
```
Filename            = Jana222_Proton-1-2.jdf
Author              = element
Experiment          = proton.jxp
Sample_Id           = Jana222
Solvent             = CHLOROFORM-D
Actual_Start_Time   =  4-JUN-2024 21:01:46
Revision_Time       = 15-JUN-2024 16:33:37

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

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

Relaxation_Delay    = 5[s]
Recvr_Gain          = 30
Temp_Get            = 21.3[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: Jana222_Carbon-1-1.jdf
```

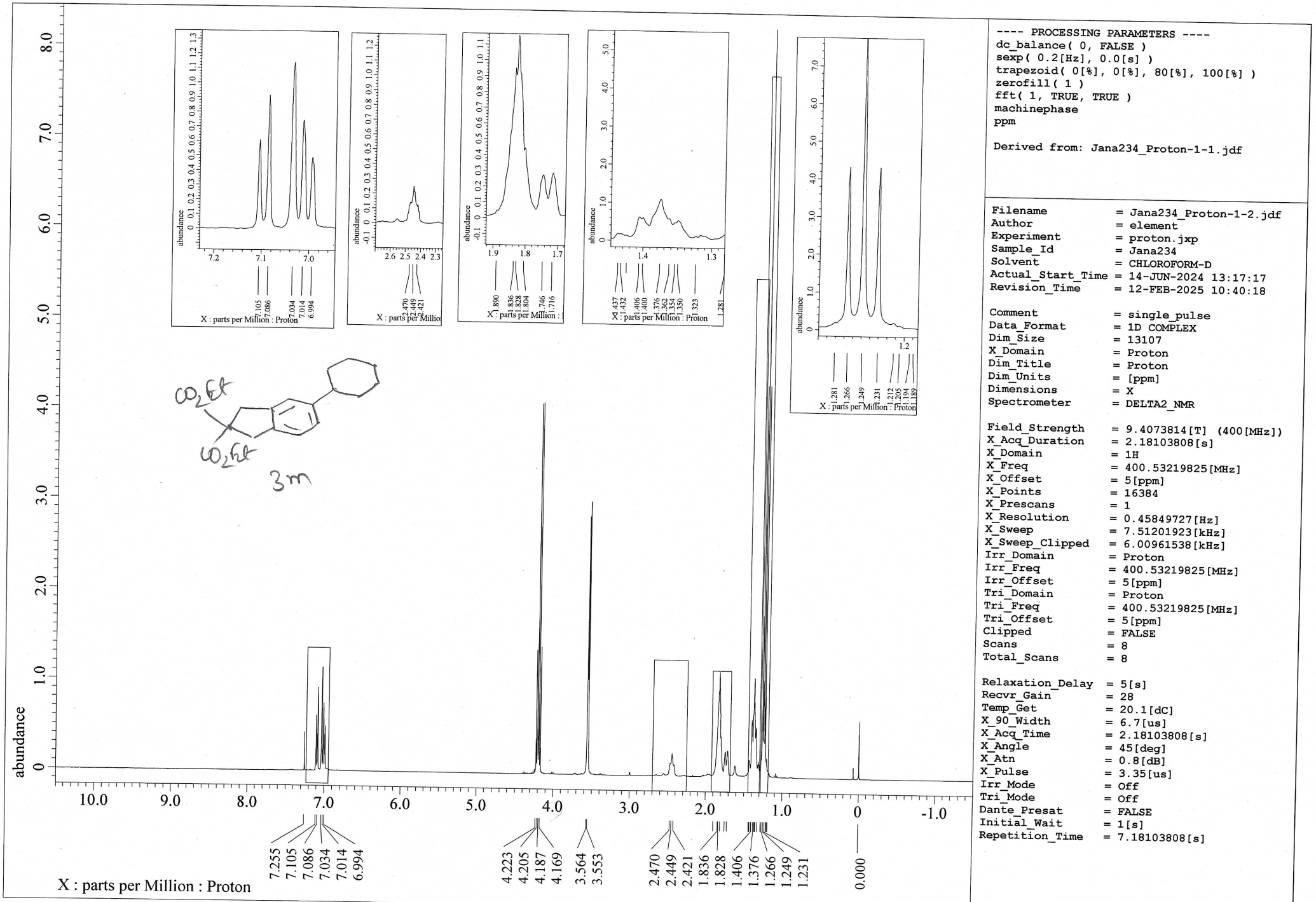
Filename	= Jana222_Carbon-1-2.jdf
Author	= element
Experiment	= carbon.jxp
Sample_Id	= Jana222
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 4-JUN-2024 21:03:06
Revision_Time	= 12-FEB-2025 09:59:45
Comment	= single pulse decoupled ga
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon
Dim_Title	= 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	= 200
Total_Scans	= 200
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 21[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]


abundance
X : parts per Million : Proton
7.255
7.093
7.074
7.007
6.982
6.962
4.224
4.206
4.187
4.170
3.557
3.550
2.574
2.555
2.536
1.266
1.249
1.231
0.933
0.915
0.896
0.000
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: Jana218p_Proton-1-1.jdf
Filename = Jana218p_Proton-1-2.jdf
Author = element
Experiment = proton.jxp
Sample_Id = Jana218p
Solvent = CHLOROFORM-D
Actual_Start_Time = 31-MAY-2024 10:09:29
Revision_Time = 12-FEB-2025 10:27:09
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 = 26
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]



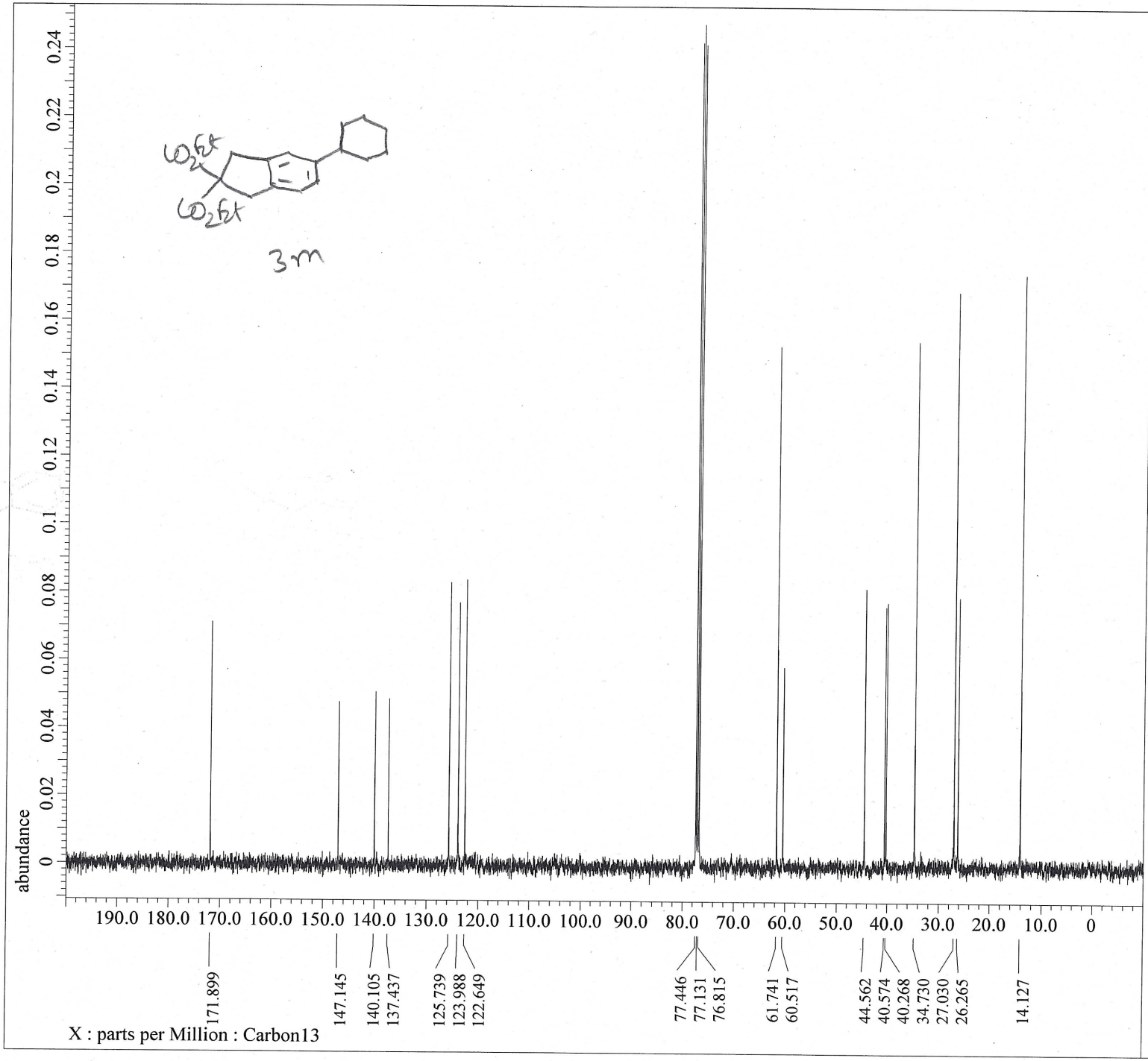

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: Jana218p_Carbon-1-1.jdf
```

Filename	= Jana218p_Carbon-1-2.jdf
Author	= element
Experiment	= carbon.jxp
Sample_Id	= Jana218p
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 31-MAY-2024 10:16:19
Revision_Time	= 15-JUN-2024 15:52:57
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	= 250
Total_Scans	= 250
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 20[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]



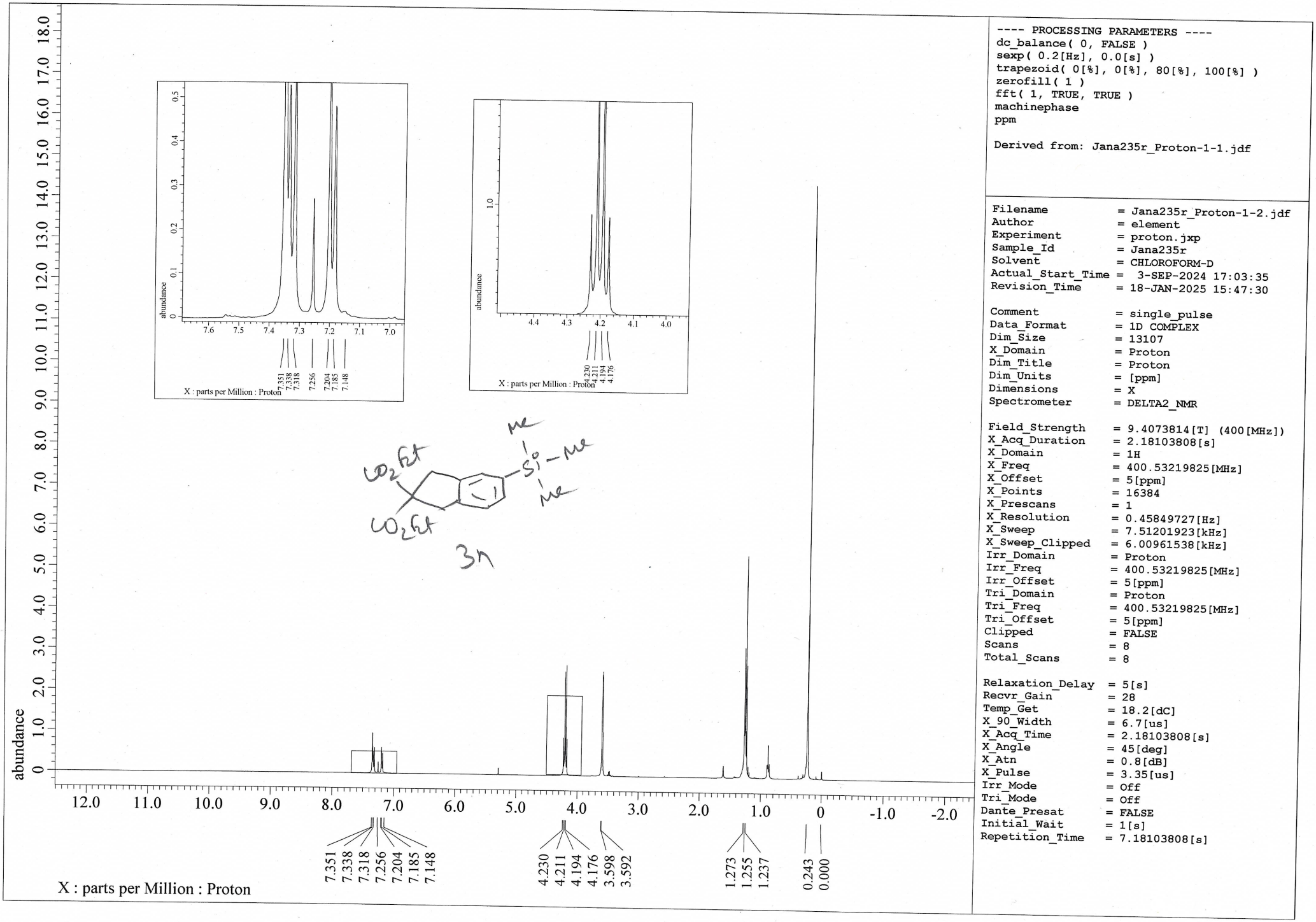

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: Jana234_Proton-1-1.jdf
```

Filename	= Jana234_Proton-1-2.jdf
Author	= element
Experiment	= proton.jxp
Sample_Id	= Jana234
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 14-JUN-2024 13:17:17
Revision_Time	= 12-FEB-2025 10:40:18
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.4073814[T] (400[MHz])
X_Acq_Duration	= 2.18103808[s]
X_Domain	= 1H
X_Freq	= 400.53219825[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45849727[Hz]
X_Sweep	= 7.51201923[kHz]
X_Sweep_Clipped	= 6.00961538[kHz]
Irr_Domain	= Proton
Irr_Freq	= 400.53219825[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 400.53219825[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 28
Temp_Get	= 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]



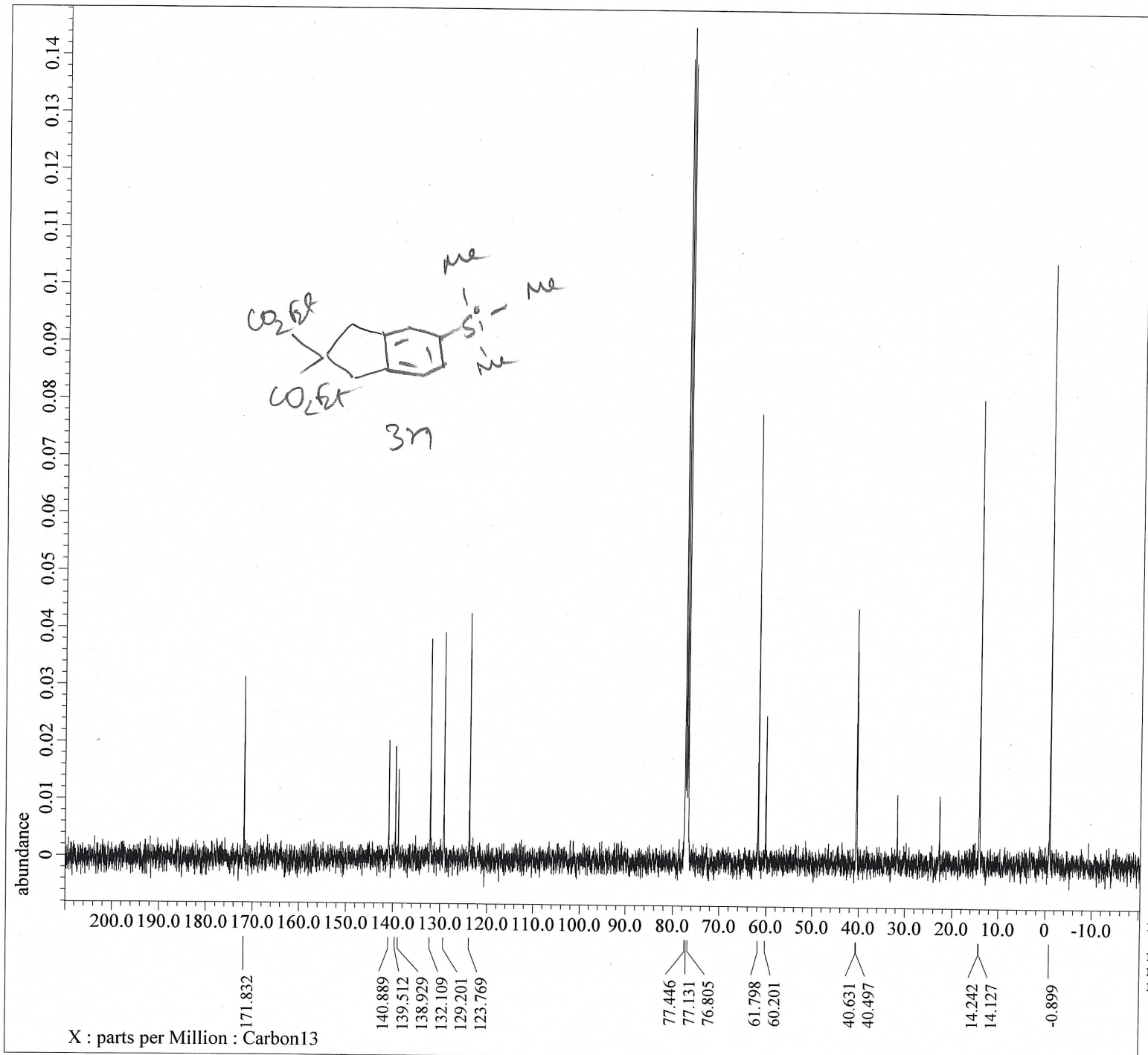

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: Jana234_Carbon-1-1.jdf
```

```
Filename            = Jana234_Carbon-1-2.jdf
Author              = element
Experiment          = carbon.jxp
Sample_Id           = Jana234
Solvent             = CHLOROFORM-D
Actual_Start_Time   = 14-JUN-2024 13:18:37
Revision_Time       = 24-JUN-2024 18:44:54

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               = 300
Total_Scans         = 300

Relaxation_Delay    = 2[s]
Recvr_Gain          = 50
Temp_Get            = 20[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]
```



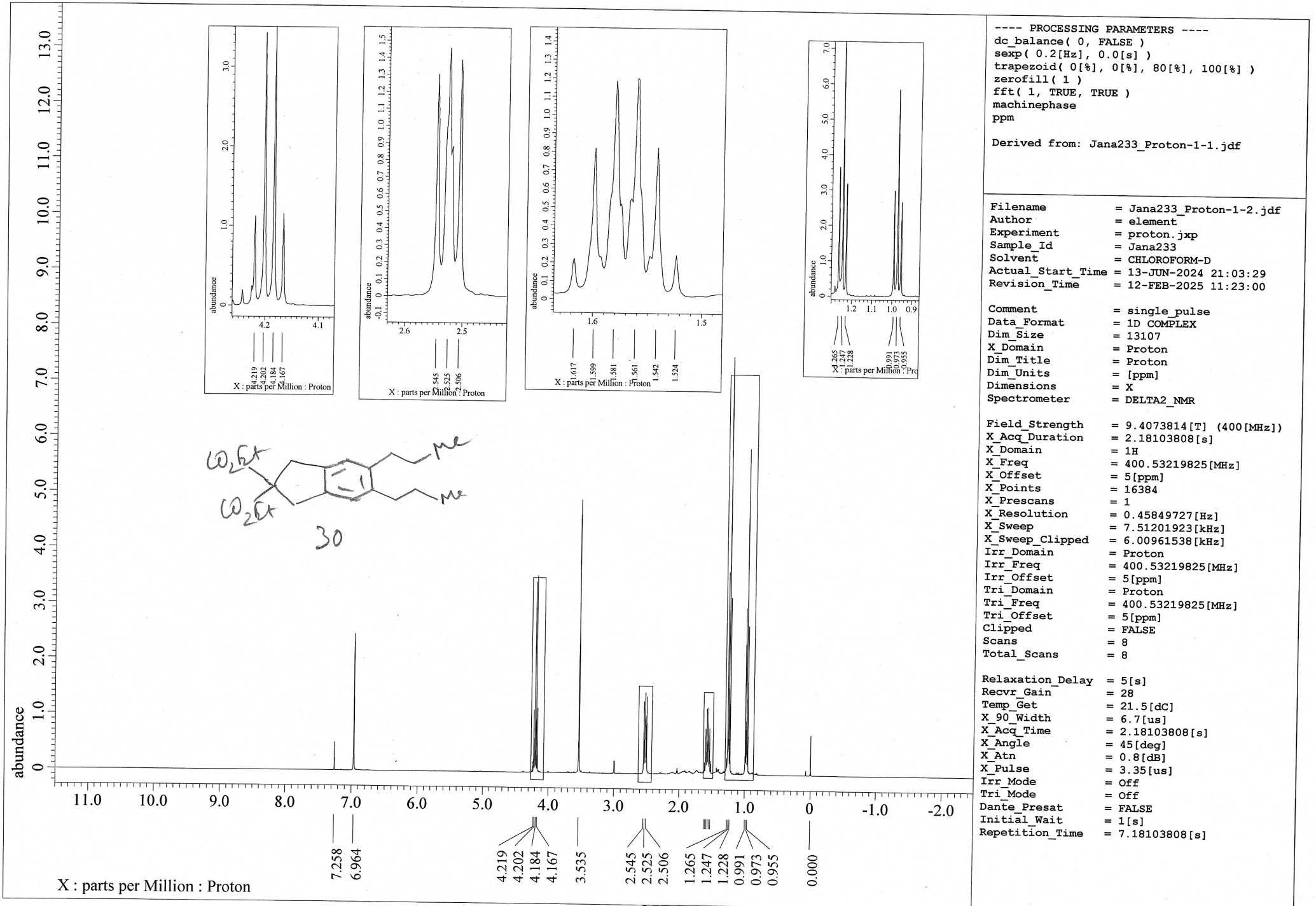

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: Jana235r_Proton-1-1.jdf
```

Filename	= Jana235r_Proton-1-2.jdf
Author	= element
Experiment	= proton.jxp
Sample_Id	= Jana235r
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 3-SEP-2024 17:03:35
Revision_Time	= 18-JAN-2025 15:47:30
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	= 28
Temp_Get	= 18.2[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]



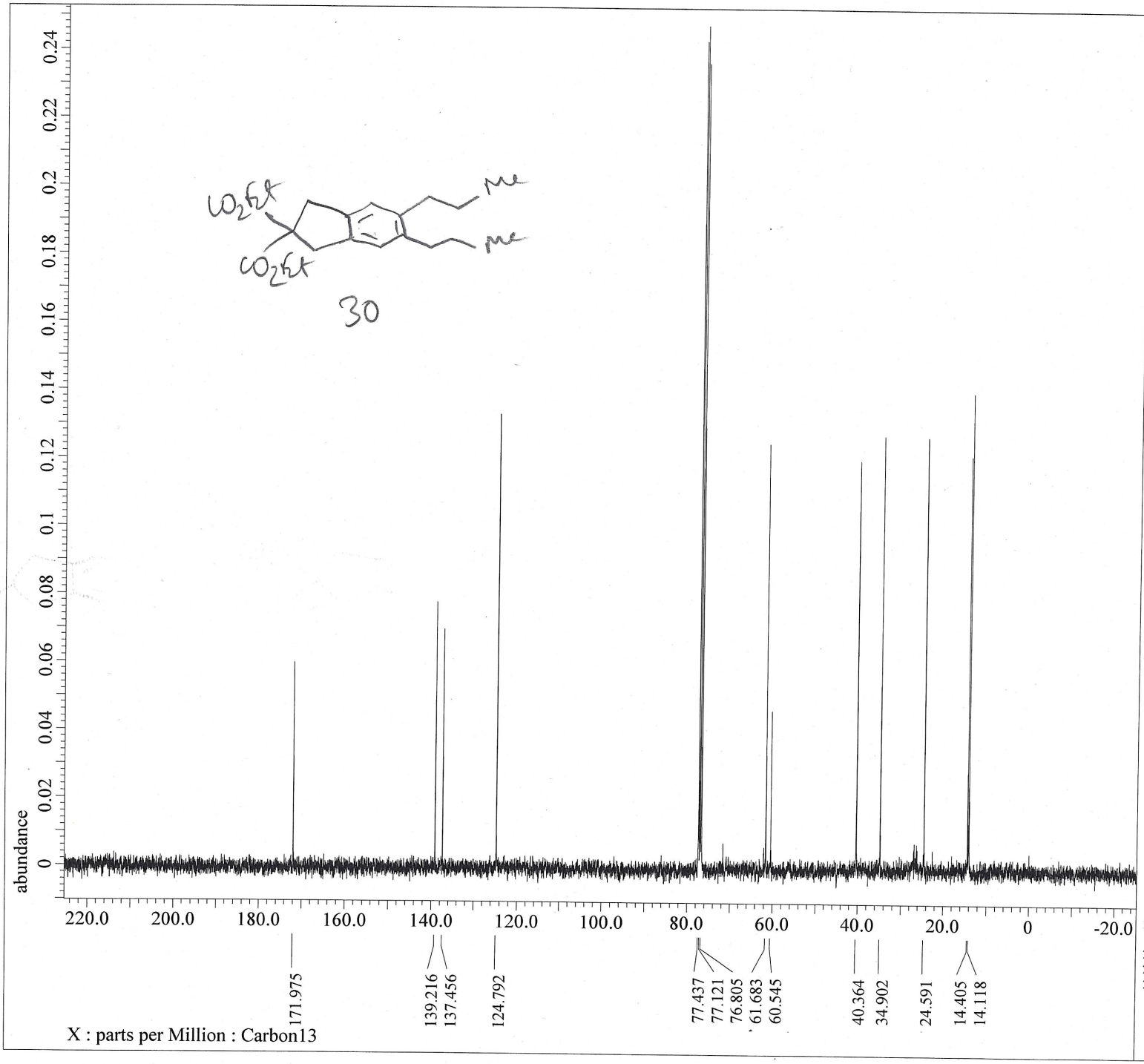

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: Jana235r_Carbon-1-1.jdf
```

Filename	= Jana235r_Carbon-1-2.jdf
Author	= element
Experiment	= carbon.jxp
Sample_Id	= Jana235r
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 3-SEP-2024 17:08:54
Revision_Time	= 12-FEB-2025 11:10:55
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	= 300
Total_Scans	= 300
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 18.2[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]



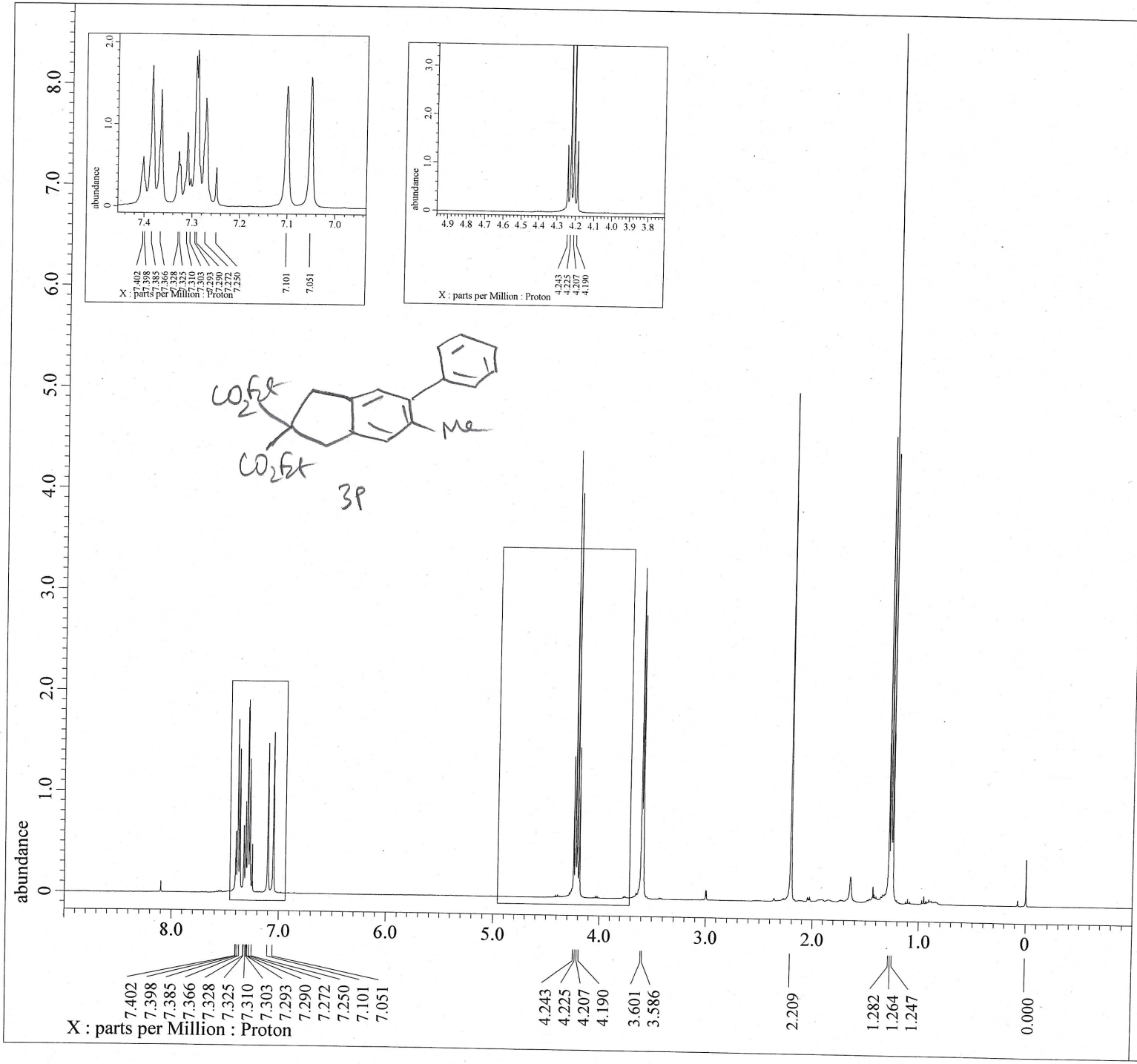

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: Jana233_Proton-1-1.jdf
```

Filename	= Jana233_Proton-1-2.jdf
Author	= element
Experiment	= proton.jxp
Sample_Id	= Jana233
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 13-JUN-2024 21:03:29
Revision_Time	= 12-FEB-2025 11:23:00
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.4073814[T] (400[MHz])
X_Acq_Duration	= 2.18103808[s]
X_Domain	= 1H
X_Freq	= 400.53219825[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45849727[Hz]
X_Sweep	= 7.51201923[kHz]
X_Sweep_Clipped	= 6.00961538[kHz]
Irr_Domain	= Proton
Irr_Freq	= 400.53219825[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 400.53219825[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 28
Temp_Get	= 21.5[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]



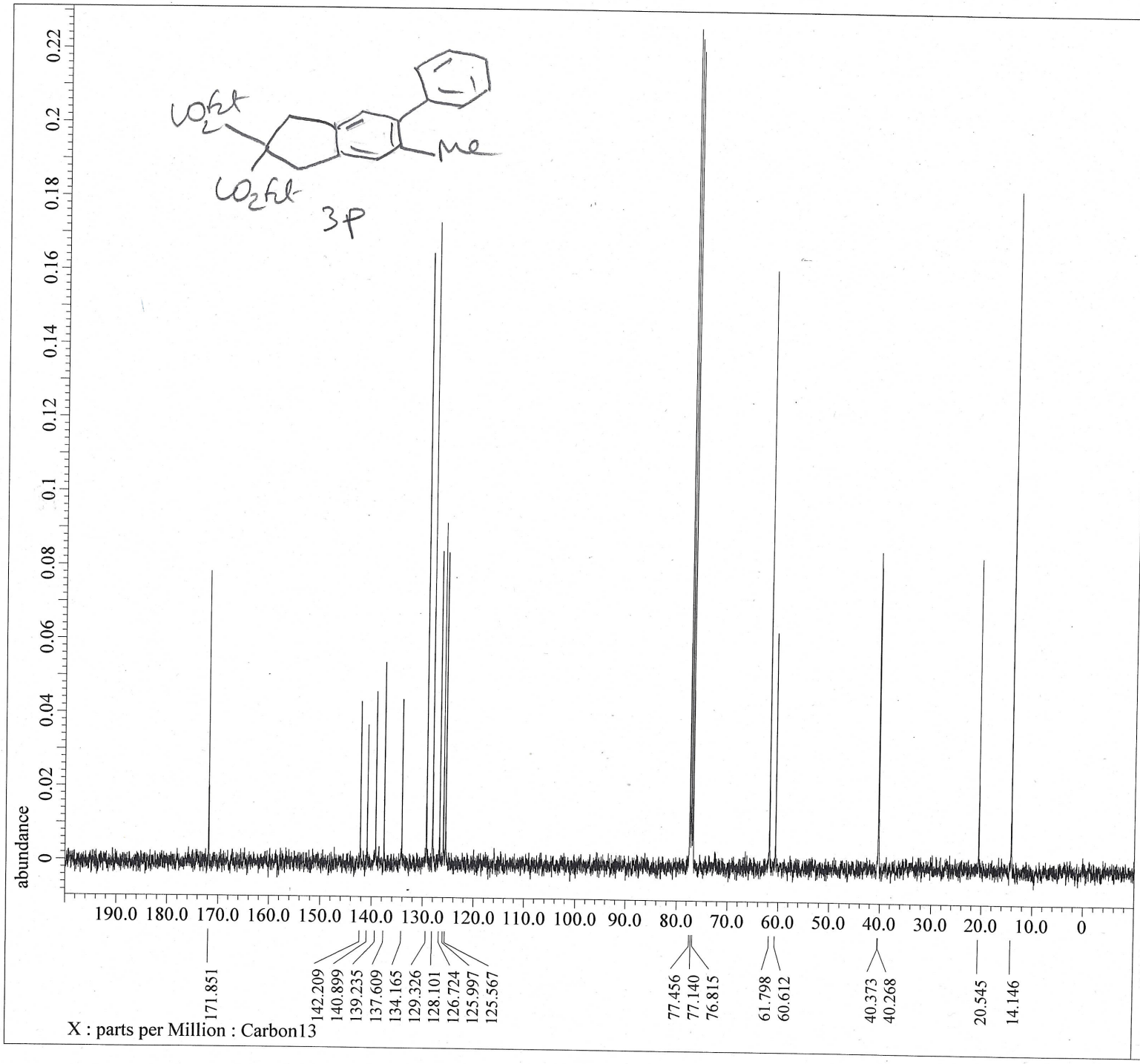

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: Jana233_Carbon-1-1.jdf
```

Filename	= Jana233_Carbon-1-2.jdf
Author	= element
Experiment	= carbon.jxp
Sample_Id	= Jana233
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 13-JUN-2024 21:04:49
Revision_Time	= 18-JAN-2025 15:56:22
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	= 250
Total_Scans	= 250
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 21.5[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]



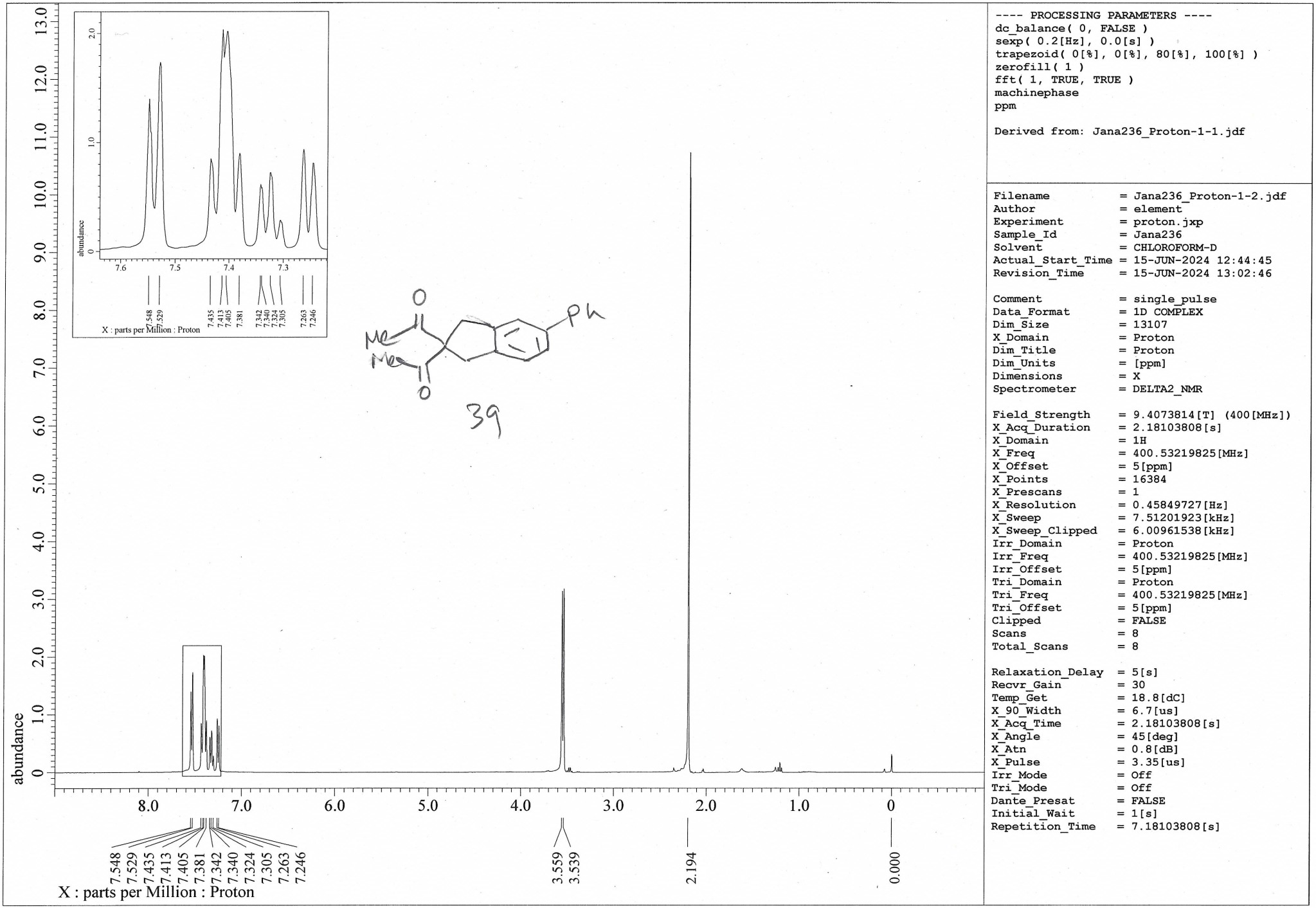

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: Jana232_Proton-1-1.jdf
```

Filename	= Jana232_Proton-1-2.jdf
Author	= element
Experiment	= proton.jxp
Sample_Id	= Jana232
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 12-JUN-2024 14:38:19
Revision_Time	= 15-JUN-2024 10:52:27
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.4073814[T] (400[MHz])
X_Acq_Duration	= 2.18103808[s]
X_Domain	= 1H
X_Freq	= 400.53219825[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45849727[Hz]
X_Sweep	= 7.51201923[kHz]
X_Sweep_Clipped	= 6.00961538[kHz]
Irr_Domain	= Proton
Irr_Freq	= 400.53219825[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 400.53219825[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 30
Temp_Get	= 21.3[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]



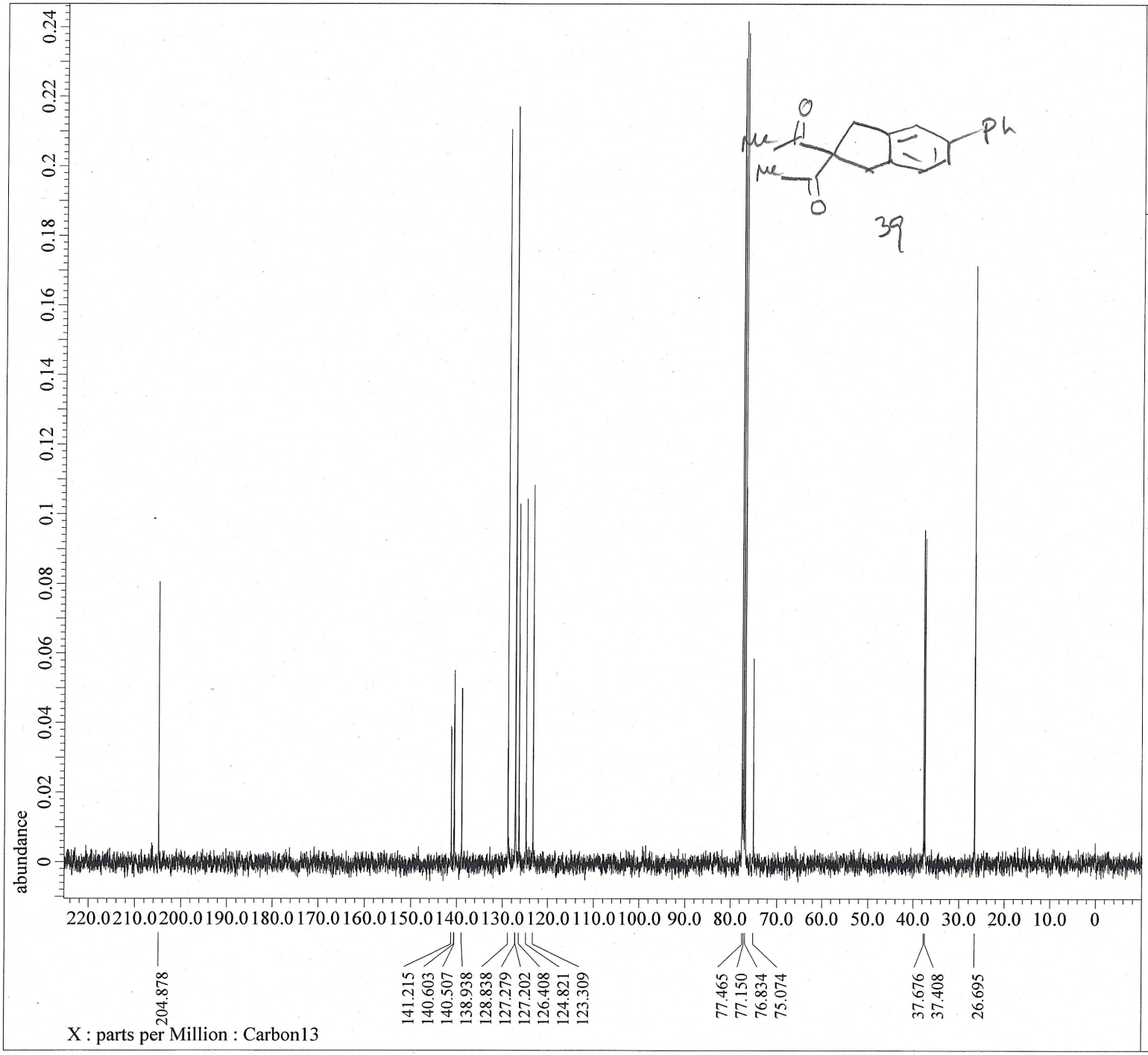

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: Jana232_Carbon-1-1.jdf
```

Filename	= Jana232_Carbon-1-2.jdf
Author	= element
Experiment	= carbon.jxp
Sample_Id	= Jana232
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 12-JUN-2024 14:53:01
Revision_Time	= 15-JUN-2024 11:00:30
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	= 250
Total_Scans	= 250
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 21.3[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]



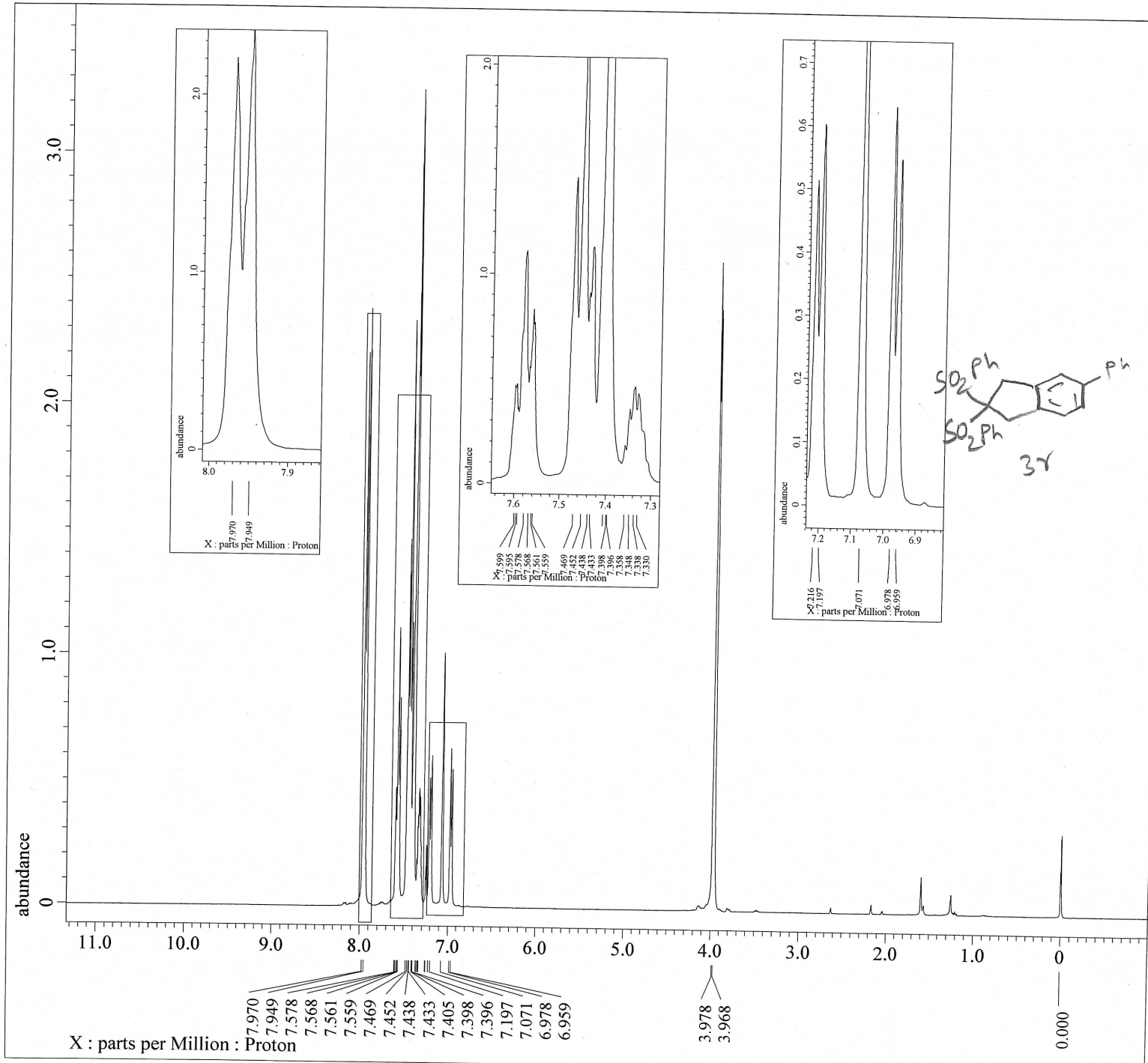

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: Jana236_Proton-1-1.jdf
```

Filename	= Jana236_Proton-1-2.jdf
Author	= element
Experiment	= proton.jxp
Sample_Id	= Jana236
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 15-JUN-2024 12:44:45
Revision_Time	= 15-JUN-2024 13:02:46
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	= 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]



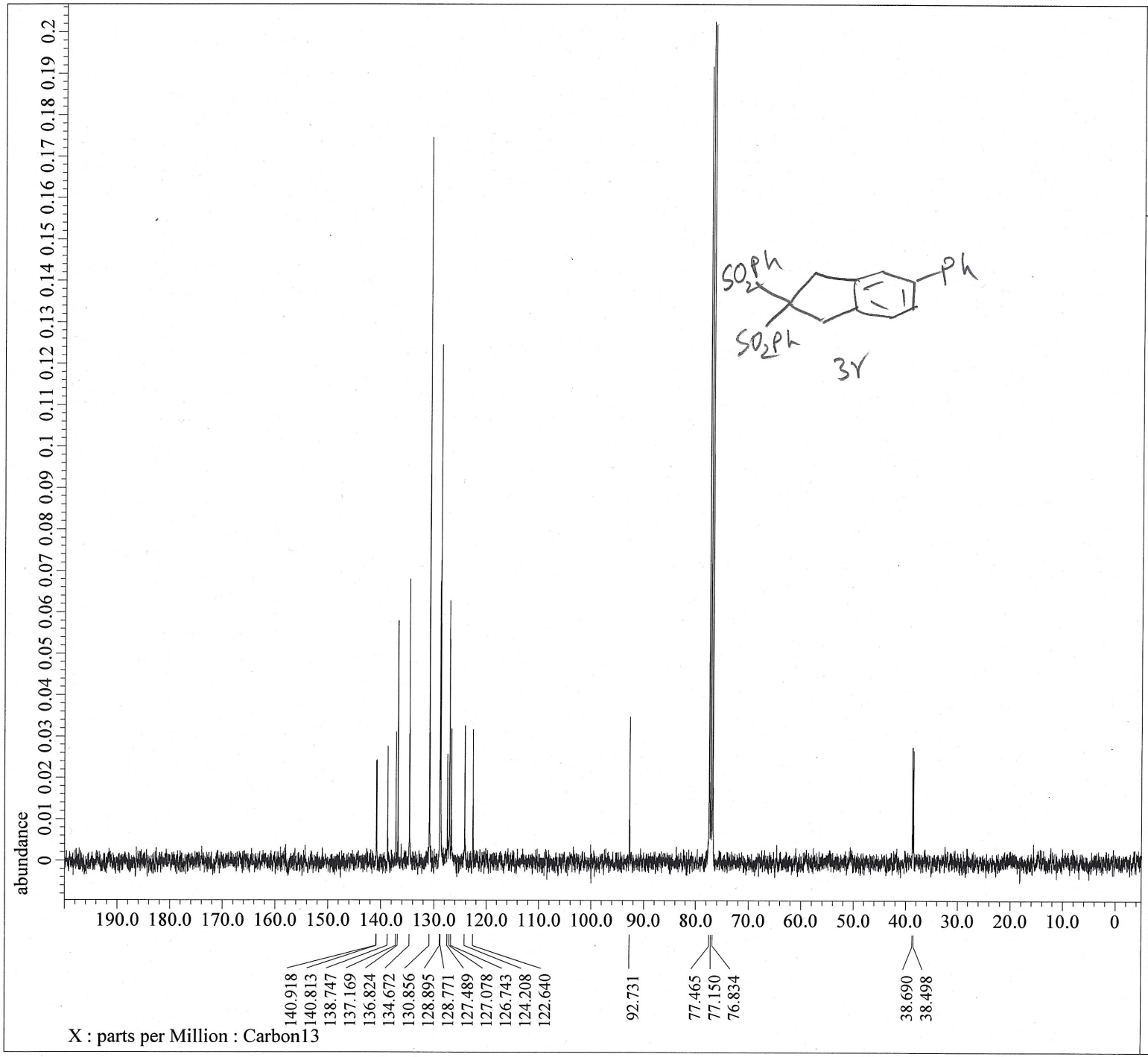

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: Jana236_Carbon-1-1.jdf
```

Filename	= Jana236_Carbon-1-2.jdf
Author	= element
Experiment	= carbon.jxp
Sample_Id	= Jana236
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 15-JUN-2024 12:46:05
Revision_Time	= 15-JUN-2024 12:58:20
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	= 200
Total_Scans	= 200
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 18.4[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]



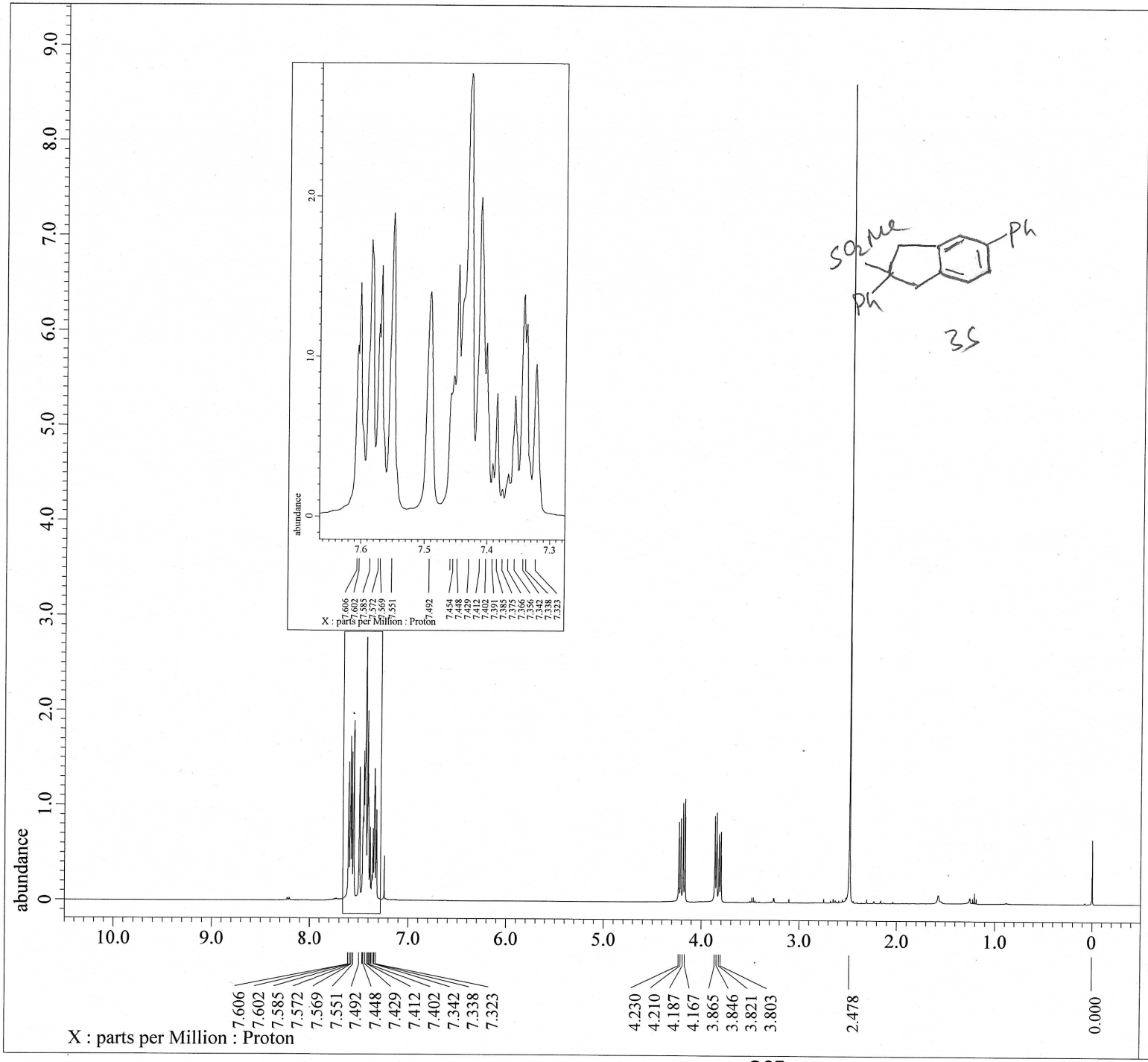

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: Jana259_Proton-1-1.jdf
```

Filename	= Jana259_Proton-1-2.jdf
Author	= element
Experiment	= proton.jxp
Sample_Id	= Jana259
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 29-JUN-2024 18:13:14
Revision_Time	= 12-FEB-2025 11:39:02
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	= 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]



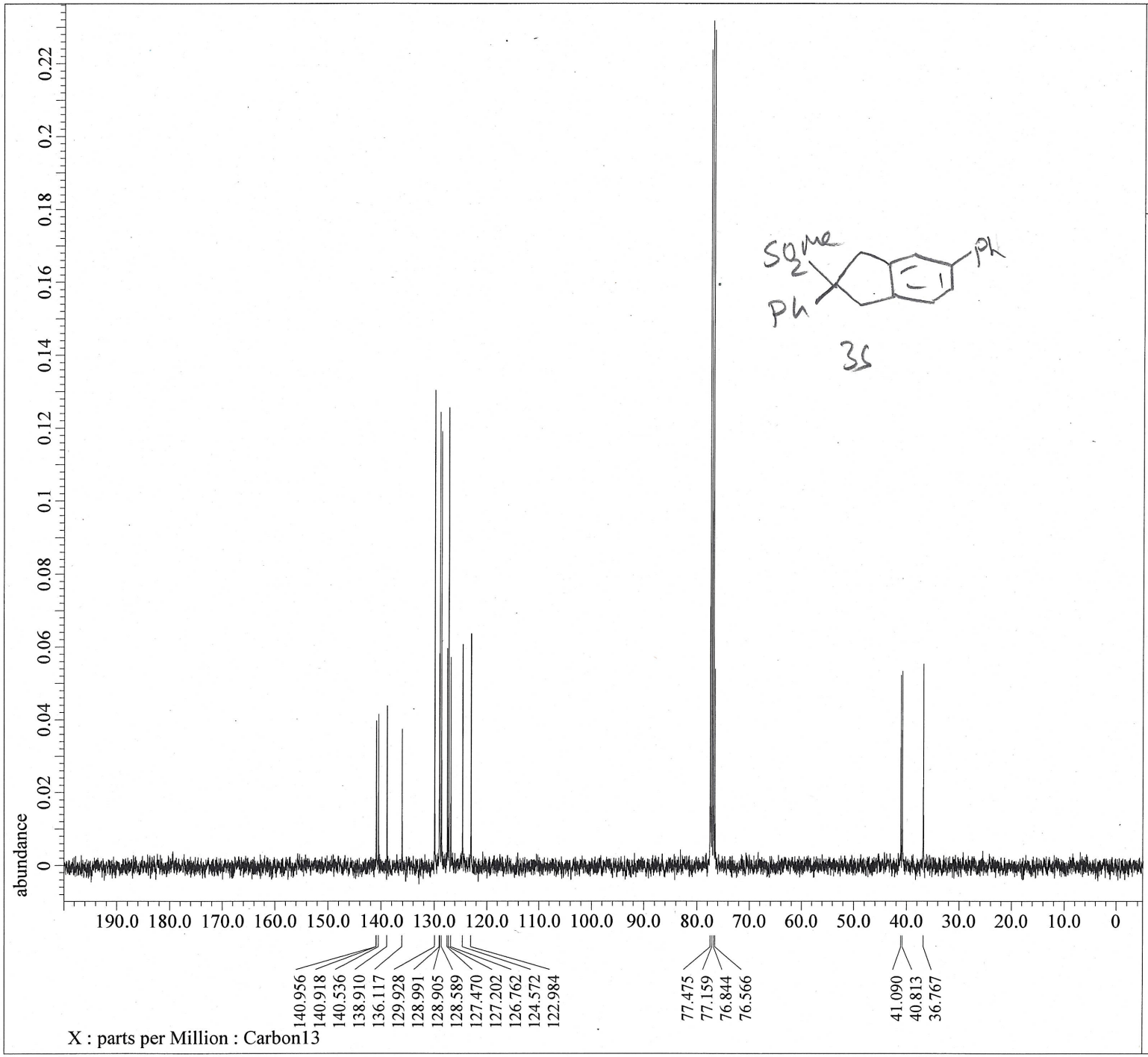

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: Jana259_Carbon-1-1.jdf
```

```
Filename            = Jana259_Carbon-1-2.jdf
Author              = element
Experiment          = carbon.jxp
Sample_Id           = Jana259
Solvent             = CHLOROFORM-D
Actual_Start_Time   = 29-JUN-2024 18:14:34
Revision_Time       = 16-OCT-2024 18:43:05

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               = 250
Total_Scans         = 250

Relaxation_Delay    = 2[s]
Recvr_Gain          = 50
Temp_Get            = 20.3[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]
```



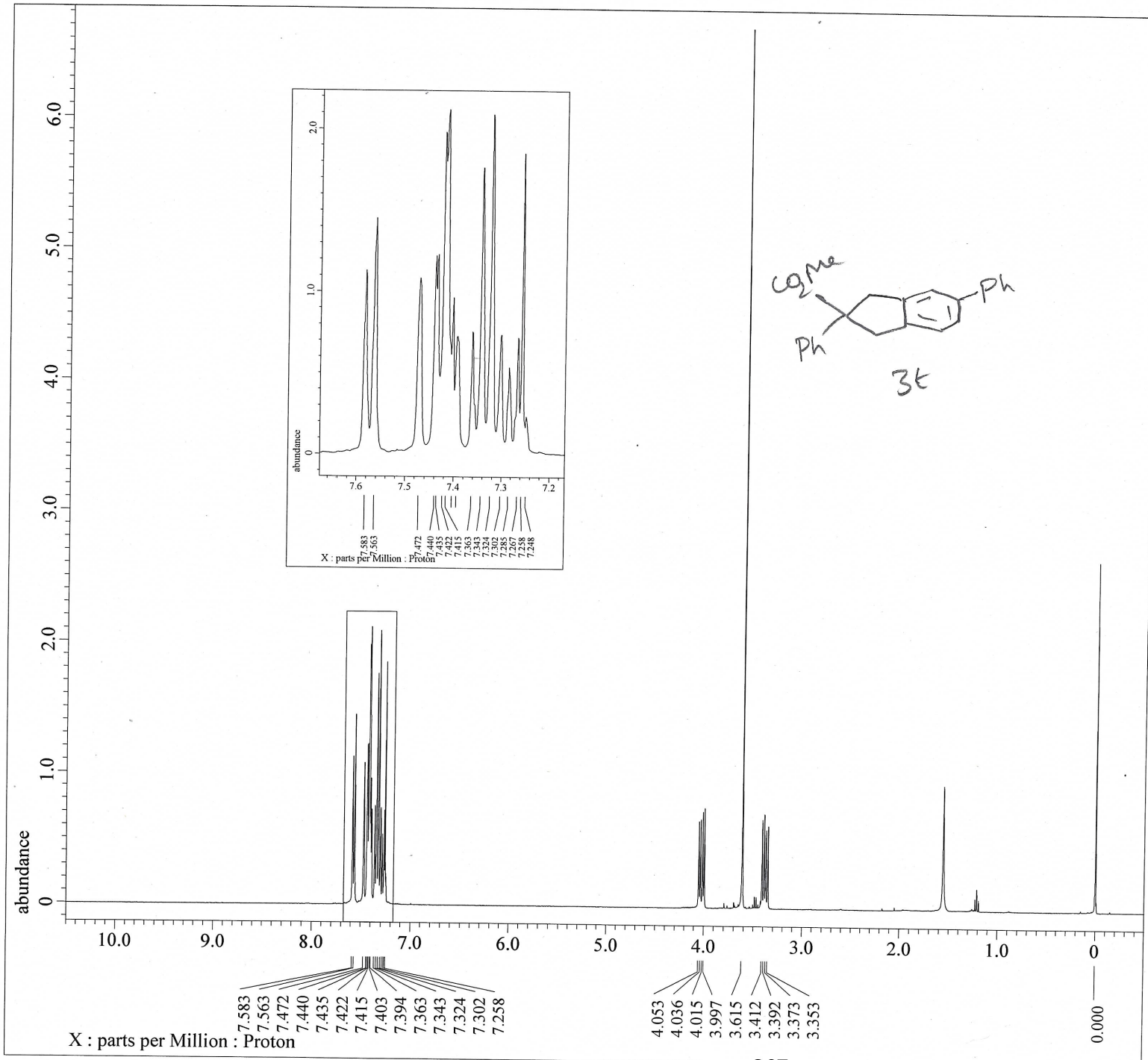

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: Jana260p_Proton-1-1.jdf
```

Filename	= Jana260p_Proton-1-2.jdf
Author	= element
Experiment	= proton.jxp
Sample_Id	= Jana260p
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 29-JUN-2024 17:13:37
Revision_Time	= 12-FEB-2025 12:04:39
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.4073814[T] (400[MHz])
X_Acq_Duration	= 2.18103808[s]
X_Domain	= 1H
X_Freq	= 400.53219825[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45849727[Hz]
X_Sweep	= 7.51201923[kHz]
X_Sweep_Clipped	= 6.00961538[kHz]
Irr_Domain	= Proton
Irr_Freq	= 400.53219825[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 400.53219825[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 36
Temp_Get	= 20.7[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]



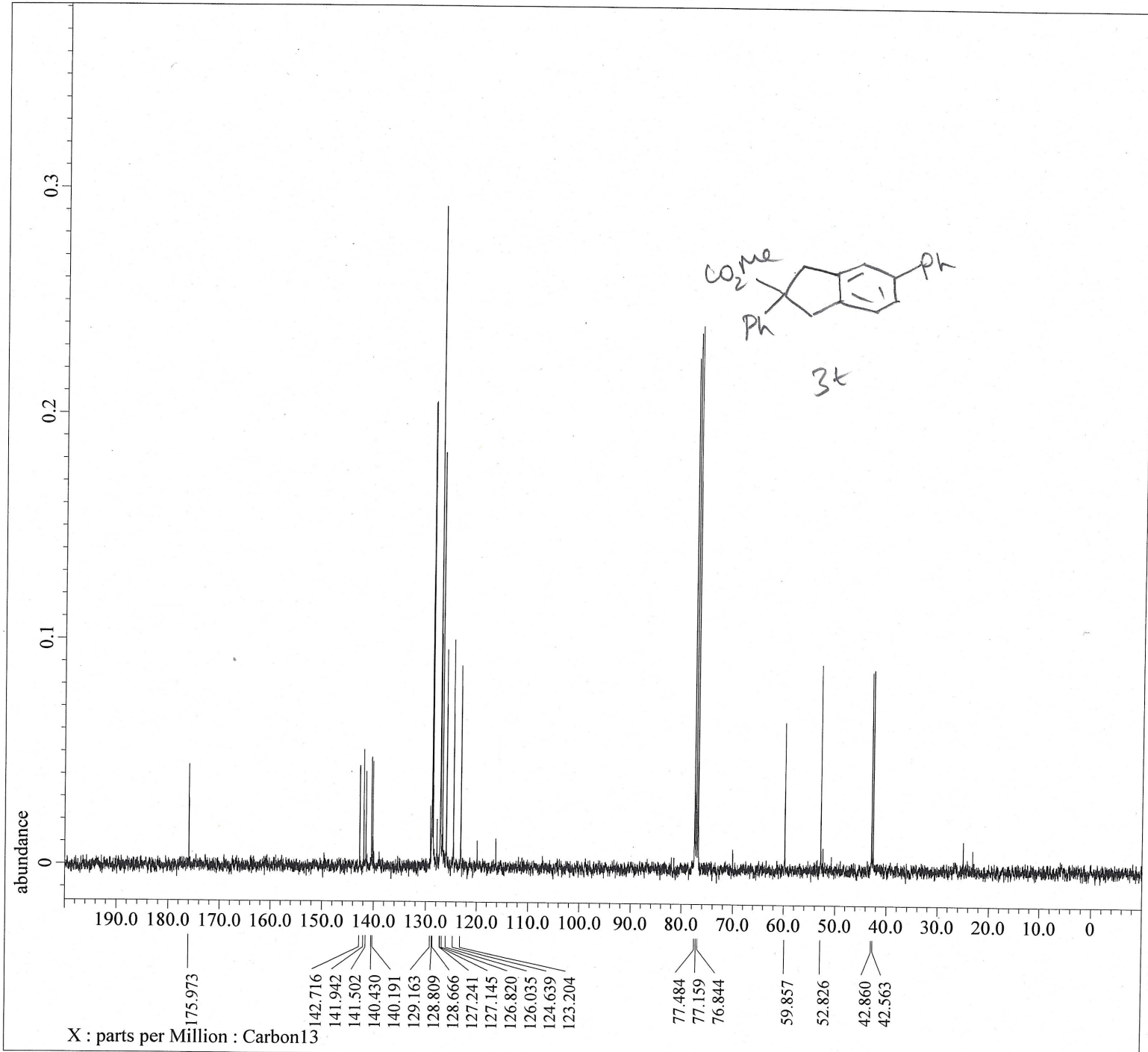

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: Jana260p_Carbon-1-1.jdf
```

Filename	= Jana260p_Carbon-1-2.jdf
Author	= element
Experiment	= carbon.jxp
Sample_Id	= Jana260p
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 29-JUN-2024 17:14:56
Revision_Time	= 16-OCT-2024 13:28:18
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	= 250
Total_Scans	= 250
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 20.8[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]



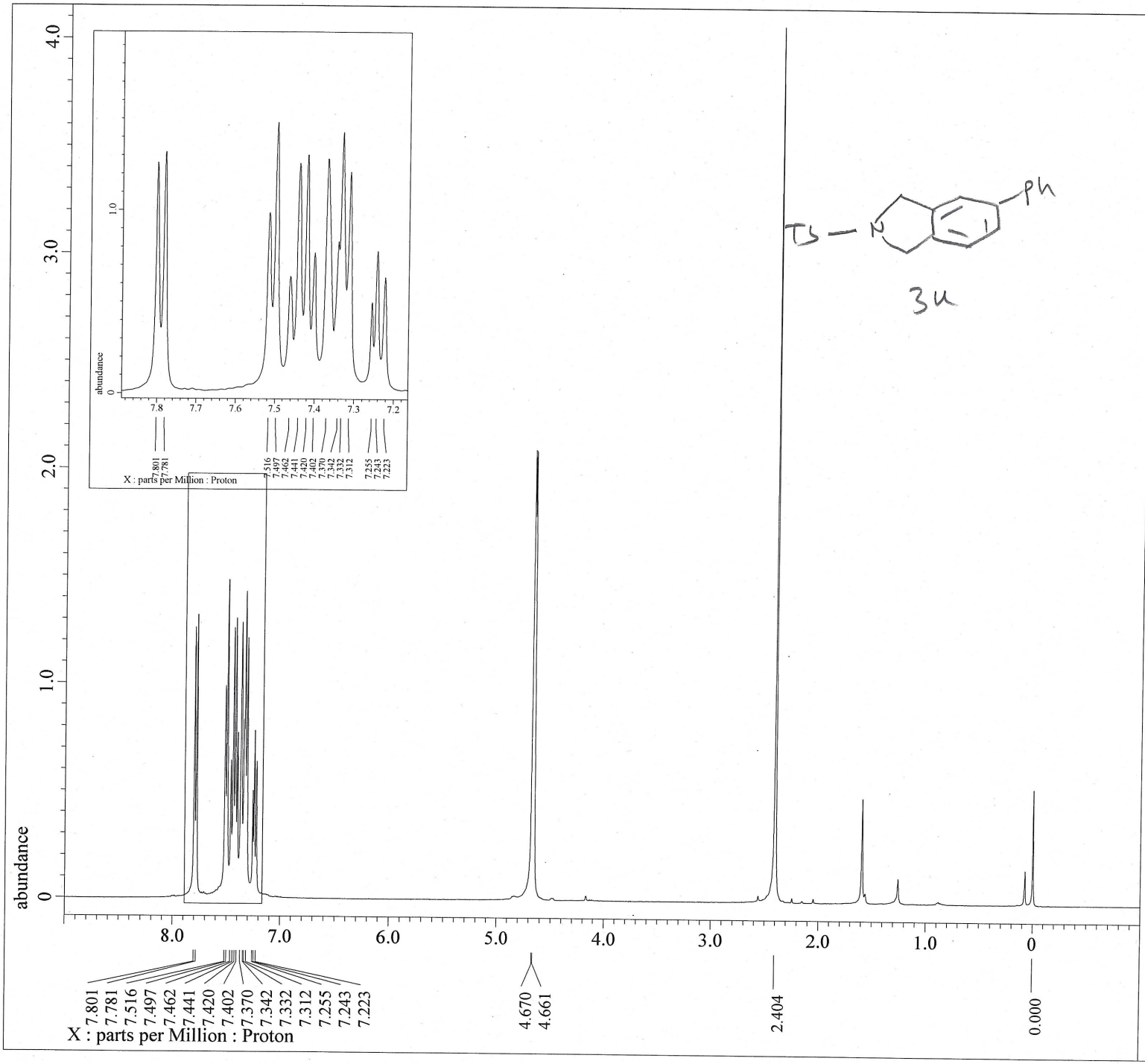

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: Jana229pp_Proton-1-1.jdf
```

Filename	= Jana229pp_Proton-1-2.jdf
Author	= element
Experiment	= proton.jxp
Sample_Id	= Jana229pp
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 15-JUN-2024 13:06:13
Revision_Time	= 12-FEB-2025 12:15:09
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.4073814[T] (400[MHz])
X_Acq_Duration	= 2.18103808[s]
X_Domain	= 1H
X_Freq	= 400.53219825[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45849727[Hz]
X_Sweep	= 7.51201923[kHz]
X_Sweep_Clipped	= 6.00961538[kHz]
Irr_Domain	= Proton
Irr_Freq	= 400.53219825[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 400.53219825[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 42
Temp_Get	= 18.4[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]



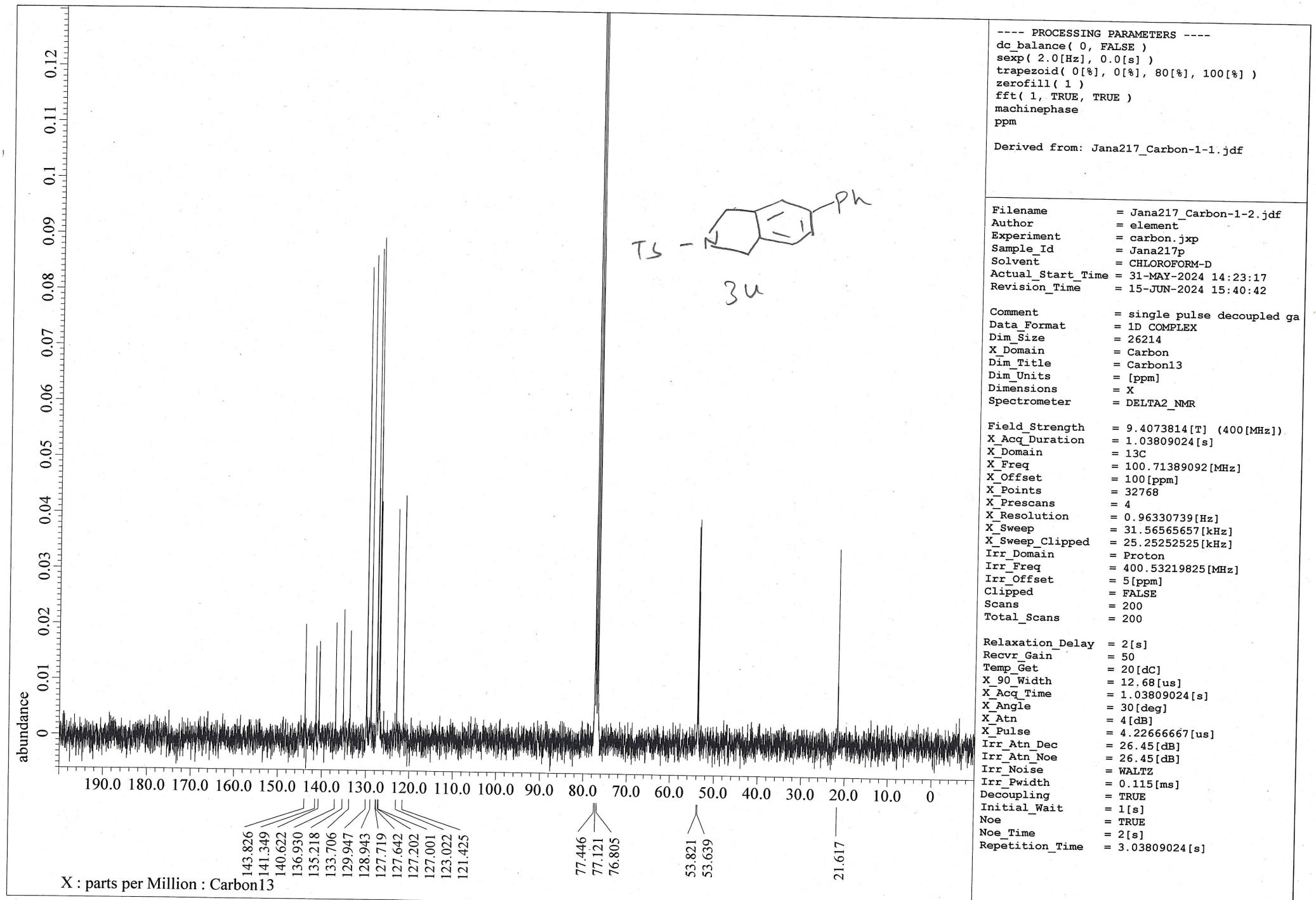

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: Jana229r_Carbon-1-1.jdf
```

Filename	= Jana229r_Carbon-1-2.jdf
Author	= element
Experiment	= carbon.jxp
Sample_Id	= Jana229r
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 14-JUN-2024 19:39:24
Revision_Time	= 15-JUN-2024 13:18:52
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	= 200
Total_Scans	= 200
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 19.7[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]



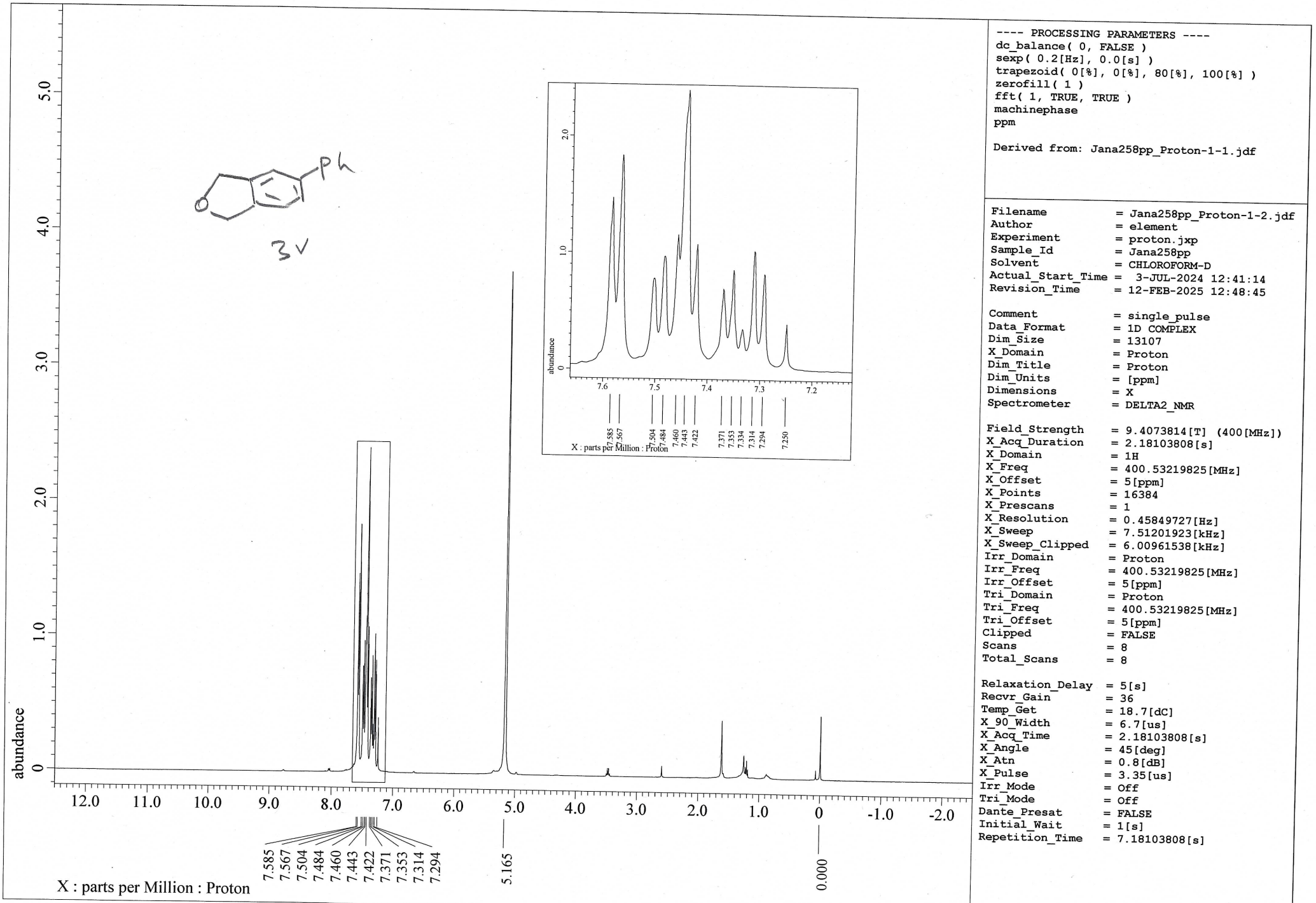

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: Jana217p_Proton-1-1.jdf
```

Filename	= Jana217p_Proton-1-2.jdf
Author	= element
Experiment	= proton.jxp
Sample_Id	= Jana217p
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 31-MAY-2024 14:21:57
Revision_Time	= 15-JUN-2024 15:33:54
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.4073814[T] (400[MHz])
X_Acq_Duration	= 2.18103808[s]
X_Domain	= 1H
X_Freq	= 400.53219825[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45849727[Hz]
X_Sweep	= 7.51201923[kHz]
X_Sweep_Clipped	= 6.00961538[kHz]
Irr_Domain	= Proton
Irr_Freq	= 400.53219825[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 400.53219825[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 36
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]



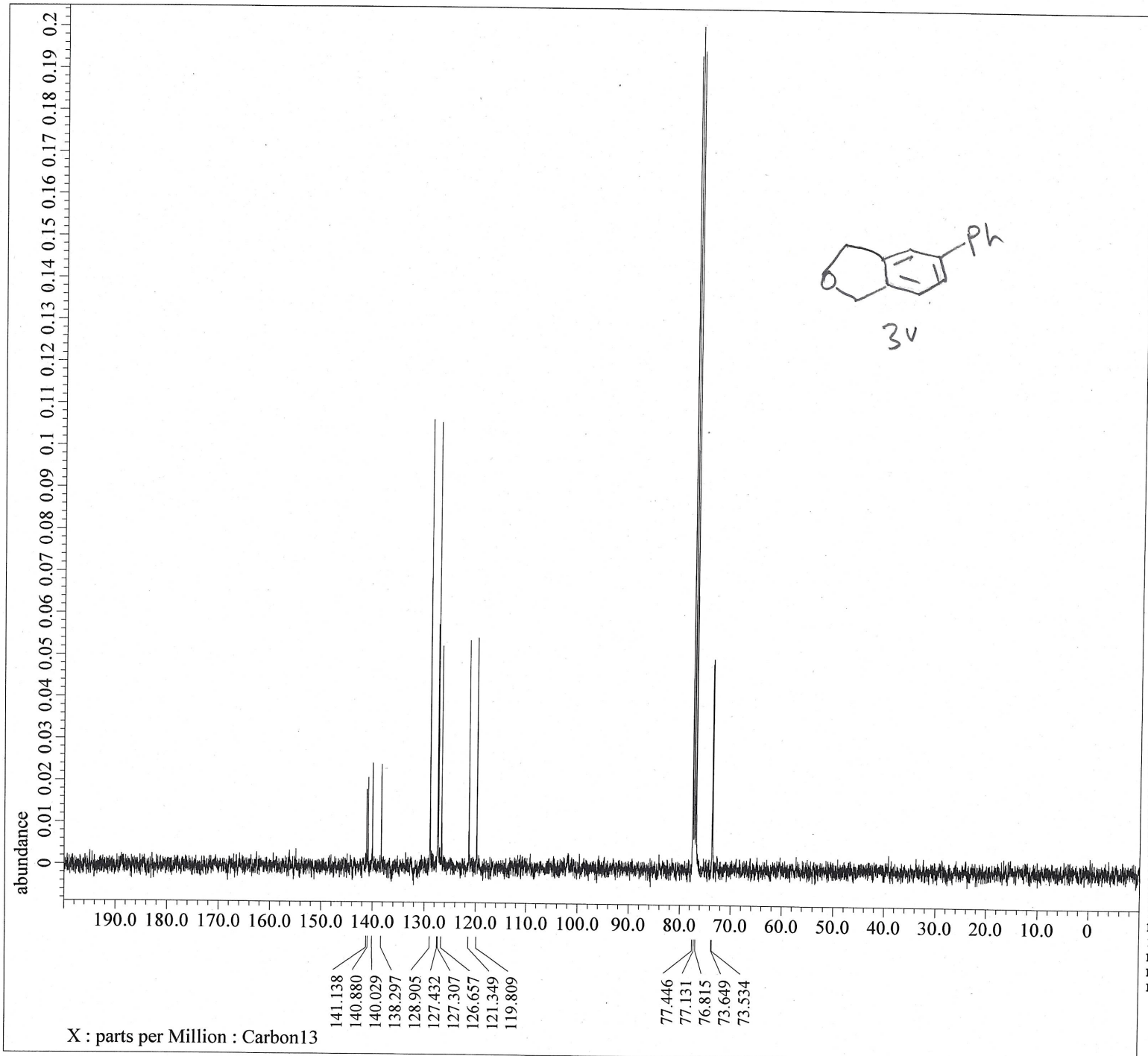

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: Jana217_Carbon-1-1.jdf
```

Filename	= Jana217_Carbon-1-2.jdf
Author	= element
Experiment	= carbon.jxp
Sample_Id	= Jana217p
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 31-MAY-2024 14:23:17
Revision_Time	= 15-JUN-2024 15:40:42
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	= 200
Total_Scans	= 200
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 20[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]



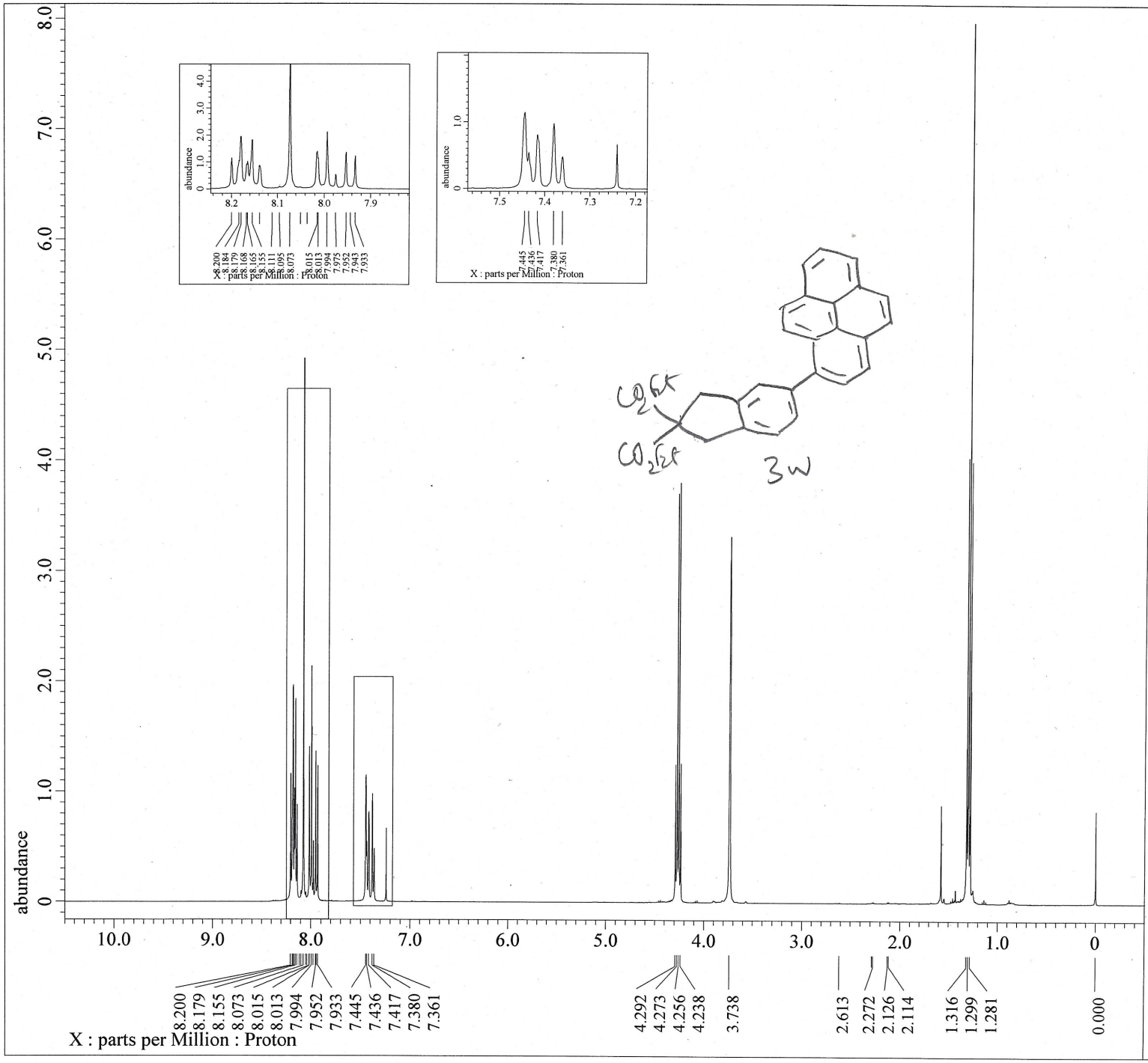

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: Jana258pp_Proton-1-1.jdf
```

Filename	= Jana258pp_Proton-1-2.jdf
Author	= element
Experiment	= proton.jxp
Sample_Id	= Jana258pp
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 3-JUL-2024 12:41:14
Revision_Time	= 12-FEB-2025 12:48:45
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.4073814[T] (400[MHz])
X_Acq_Duration	= 2.18103808[s]
X_Domain	= 1H
X_Freq	= 400.53219825[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45849727[Hz]
X_Sweep	= 7.51201923[kHz]
X_Sweep_Clipped	= 6.00961538[kHz]
Irr_Domain	= Proton
Irr_Freq	= 400.53219825[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 400.53219825[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 36
Temp_Get	= 18.7[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]



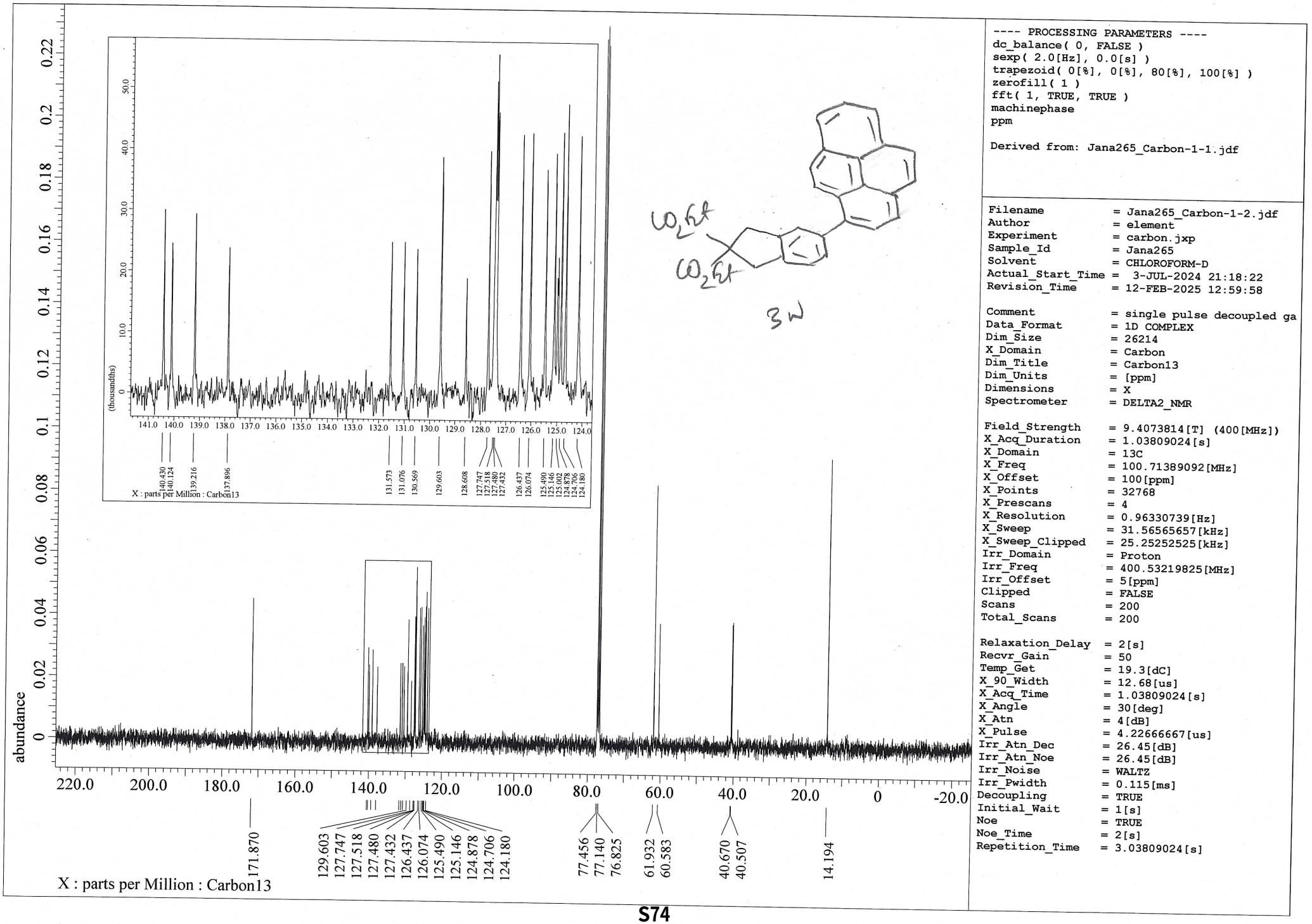

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: Jana258pp_Carbon-1-1.jdf
```

Filename	= Jana258pp_Carbon-1-2.jdf
Author	= element
Experiment	= carbon.jxp
Sample_Id	= Jana258pp
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 3-JUL-2024 12:42:33
Revision_Time	= 19-OCT-2024 17:11:35
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	= 300
Total_Scans	= 300
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 19.2[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: Jana265_Proton-1-1.jdf
```

Filename	= Jana265_Proton-1-2.jdf
Author	= element
Experiment	= proton.jxp
Sample_Id	= Jana265
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 3-JUL-2024 21:17:02
Revision_Time	= 15-OCT-2024 19:54:55
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	= 19.5[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]




```
---- 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: Jana265_Carbon-1-1.jdf
```

Filename	= Jana265_Carbon-1-2.jdf
Author	= element
Experiment	= carbon.jxp
Sample_Id	= Jana265
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 3-JUL-2024 21:18:22
Revision_Time	= 12-FEB-2025 12:59:58
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	= 200
Total_Scans	= 200
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]