Solid-State Aromatic Nucleophilic Fluorination: A Rapid, Practical, and Environmentally Friendly Route to *N*-Heteroaryl Fluorides

Koji Kubota,*[a,b] Tetsu Makino,[a] Keisuke Kondo,[a] Tamae Seo,[a] Mingoo Jin[b] and Hajime Ito*[a,b]

[a]*Division of Applied Chemistry, Graduate School of Engineering, Hokkaido University, Sapporo, Hokkaido, 060-8628, Japan.*
[b]*Institute for Chemical Reaction Design and Discovery (WPI-ICReDD), Hokkaido University, Sapporo, Hokkaido, 001-0021, Japan.*

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

Table of Contents

1. Chemicals and Instrumentation

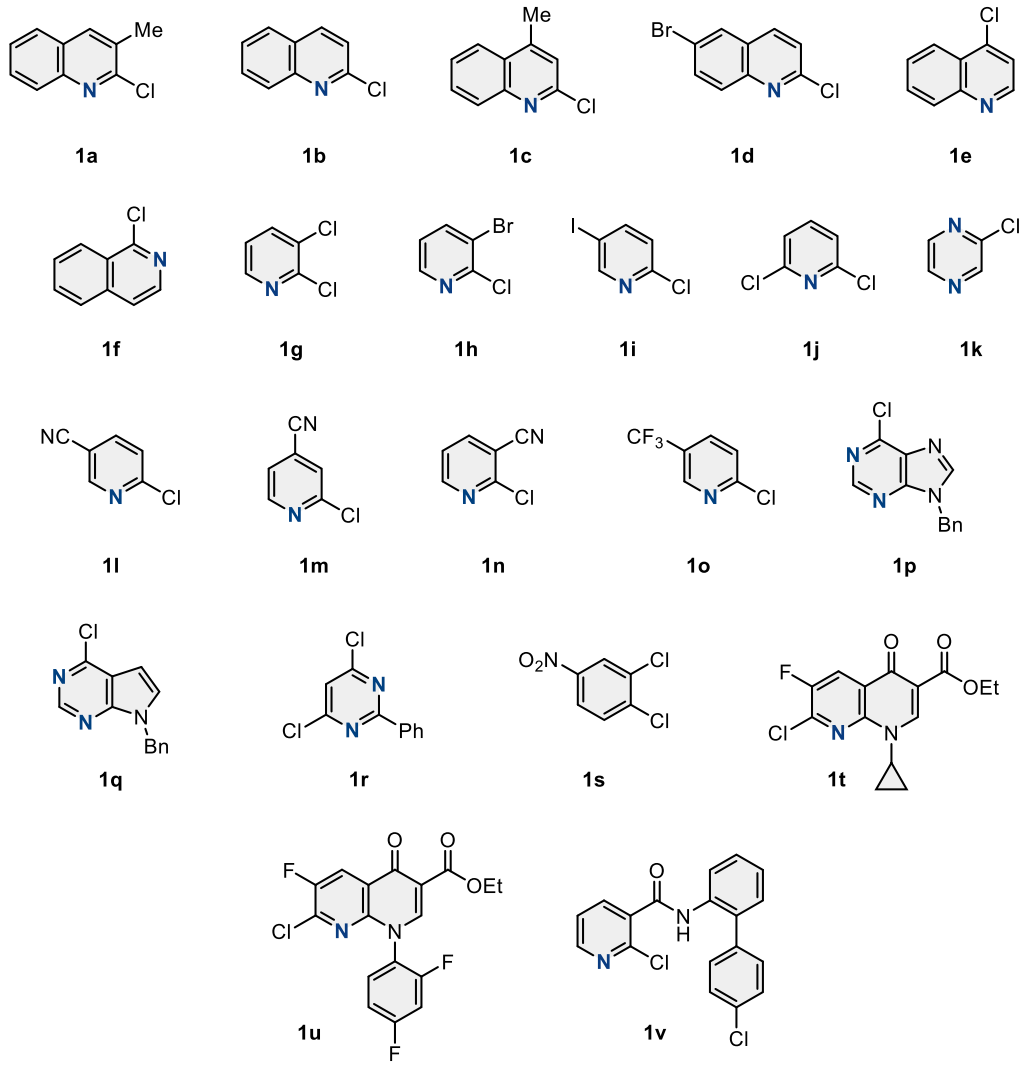
Solvents and liquid additives were purchased from commercial suppliers and further dried over molecular sieve (MS 4Å). KF (spray-dried) was purchased from Wako Chemicals (166-13241). All mechanochemical reactions were carried out using grinding vessels in a Retsch MM400 mill. Both jars (1.5 mL, 5.0 mL, and 10 mL) and balls (7 mm, 10 mm, and 15 mm, diameter) are made of stainless (SUS400B and SUS420J2, respectively) (Figure S1 and S2). The heat gun Takagi, HG-1450B, with temperature control function was used (Figure S3). NMR spectra were recorded on JEOL JNM-ECZ400S and JNM-ECS400 spectrometers (^{1}H: 396 or 399 or 401 MHz, ^{13}C: 99 or 100 or 101 MHz, ^{19}F: 369 or 373 or 375 or 377 MHz). Tetramethylsilane (^{1}H, δ: 0.00), $CDCl_3$ (^{13}C, δ: 77.0), and fluorobenzene (^{19}F, δ: –113.6) were employed as external standards, respectively. Multiplicity was recorded as follows: s = singlet, brs = broad singlet, d = doublet, t = triplet, q = quartet, quint = quintet, sept = septet, o = octet, m = multiplet. Recycle preparative gel permeation chromatography (GPC) was conducted with a JAI LC-9101 using $CHCl_3$ as an eluent with JAIGEL-1H. Thermography was recorded with an NEC Avio Thermo GEAR G120. High-resolution mass spectra were recorded at the Global Facility Center, Hokkaido University.

Figure S1. Retsch MM 400 used in this study.

Figure S2. Stainless jars and balls used in this study.

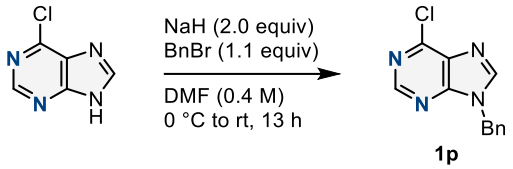
Figure S3. The temperature-controllable heat gun used in this study.

2. Substrate Preparation



1a–1o, **1r**, **1s**, **1u** and **1v** were purchased from commercial suppliers and used as received. **1p**, **1q,** and **1t** were prepared through the following procedures.

Preparation of 9-benzyl-6-chloro-9H-purine (1p).

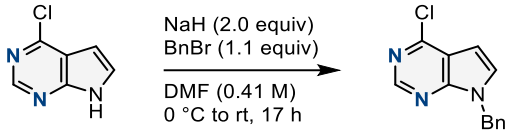


In a vacuum-dried reaction vial equipped with a magnetic stirring bar, 6-chloro-9H-purine (463.8 mg, 3.0 mmol) was dissolved in DMF (7.5 mL). NaH (60% dispersal in mineral oil, 358.5 mg, 6.5 mmol)

was added to the solution at 0 °C, and then stirred for 30 min. After 30 min, benzyl bromide (0.39 mL, 3.3 mmol) was added to the mixture. The mixture was allowed to warm to room temperature and stirred for 13 h. After the reaction, the mixture was quenched with water and extracted with 20% EtOAc/hexane three times. The organic layer was washed with brine and dried over anhydrous $MgSO_4$. After filtration, the solvent was removed under vacuum, and the residue was purified by silica gel column chromatography (EtOAc/hexane, 30:70–40:60) to afford compound **1p** (250.9 mg, 1.0 mmol, 34%) as a white solid. ^{1}H and ^{13}C NMR were in agreement with the literature.[1]

^{1}H NMR (396 MHz, $CDCl_3$, δ): 5.47 (s, 2H), 7.30–7.41 (m, 5H), 8.11 (s, 1H), 8.80 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 47.8 (*C*H_2), 127.9 (*C*H), 128.8 (*C*H), 129.2 (*C*H), 131.5 (*C*), 134.5 (*C*), 144.9 (*C*H), 151.1 (*C*), 151.8 (*C*), 152.1 (*C*H). HRMS-ESI (m/z): $[M+Na]^+$ calcd for $C_{12}H_9ClN_4Na$, 267.0408; found, 267.0405.

Preparation of 7-benzyl-4-chloro-7H-pyrrolo[2,3-d]pyrimidine (1q).

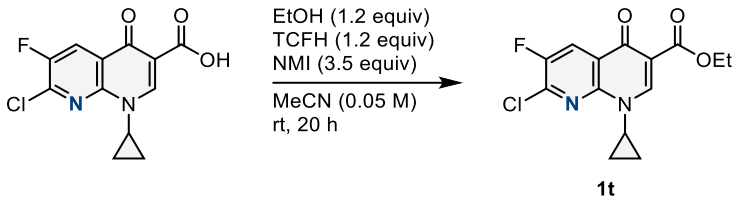


1q

In a vacuum-dried reaction vial equipped with a magnetic stirring bar, 4-chloro-1H-pyrrolo[2,3-d]pyrimidine (500.3 mg, 3.3 mmol) was dissolved in DMF (8.0 mL). NaH (60% dispersal in mineral oil, 262.8 mg, 6.6 mmol) was added to the solution at 0 °C, and then stirred for 30 min. After 30 min, benzyl bromide (0.43 mL, 3.6 mmol) was added to the mixture. The mixture was allowed to warm to room temperature and stirred for 17 h. After the reaction, the mixture was quenched with water and extracted with 20% EtOAc/hexane three times. The organic layer was washed with brine and dried over anhydrous $MgSO_4$. After filtration, the solvent was removed under vacuum, and the residue was purified by silica gel column chromatography (Et_2O/hexane, 0:100–15:85) to afford compound **1q** (561.5 mg, 2.3 mmol, 71%) as a white solid. ^{1}H and ^{13}C NMR were in agreement with the literature.[2]

^{1}H NMR (401 MHz, $CDCl_3$, δ): 5.46 (s, 2H), 6.62 (d, *J* = 3.6 Hz, 1H), 7.21–7.23 (m, 3H), 7.30–7.36. (m, 3H), 8.68 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 48.2 (*C*H_2), 99.7 (*C*H), 117.2 (*C*), 127.4 (*C*H), 127.9 (*C*H), 128.7 (*C*H), 128.9 (*C*H), 136.0 (*C*), 150.6 (*C*H), 150.9 (*C*), 151.9 (*C*). HRMS-ESI (m/z): $[M+H]^+$ calcd for $C_{13}H_{11}ClN_3$, 244.0636; found, 244.0635.

Preparation of ethyl-7-chloro-6-fluoro-1-cyclopropyl-1,4-dihydro-4-oxo-1,8-naphthyridine-3-carboxylate (1t).



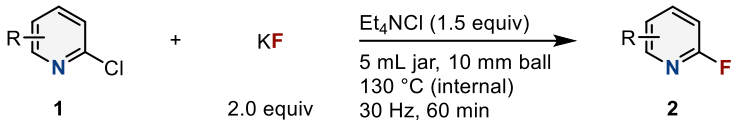
1t

In a 100 mL two-necked round-bottomed flask equipped with a magnetic stirring bar, 7-chloro-1-cyclopropyl-6-fluoro-1,4-dihydro-4-oxo-1,8-naphthyridine-3-carboxylic acid (565.4 mg, 2.0 mmol) was dissolved in MeCN (38 mL). EtOH (0.14 mL, 2.4 mmol), *N*-methylimidazole (NMI) (0.56 mL, 7.0 mmol), and chloro-*N*,*N*,*N*′,*N*′-tetramethylformamidinium hexafluorophosphate (TCFH) (673.9 mg, 2.4 mmol) were added to the solution, then stirred at room temperature for 20 h. After the reaction, the solution was diluted with water and extracted with CH_2Cl_2 three times. The organic layer was washed with brine and dried over $MgSO_4$. After filtration, the solvent was removed under vacuum. The residue was washed with water to remove tetramethylurea and purified by silica gel column chromatography (EtOAc/hexane, 20:80–100:0) to afford compound **1t** (533.4 mg, 1.7 mmol, 86%) as a white powder. ^{1}H NMR was in agreement with the literature.[3]

^{1}H NMR (401 MHz, $CDCl_3$, δ): 1.04–1.09 (m, 2H), 1.29–1.36 (m, 2H), 1.41 (t, *J* = 7.2 Hz, 3H), 3.66 (tt, *J* = 3.2, 4.0 Hz, 1H), 4.41 (q, *J* = 7.2 Hz, 2H), 8.44 (d, *J* = 7.2 Hz, 1H), 8.66 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 7.5 (*C*H_2), 14.2 (*C*H_3), 34.3 (*C*H), 61.0 (*C*H_2), 111.8 (*C*), 122.8 (d, *J* = 21.0 Hz, *C*H), 123.6 (d, *J* = 2.8 Hz, *C*), 142.2 (d, *J* = 21.9 Hz, *C*), 145.7 (d, *J* = 1.9 Hz, *C*), 148.8 (*C*H), 152.4 (d, *J* = 261.3 Hz, *C*), 164.5 (*C*), 173.0 (*C*). HRMS-EI (m/z): $[M]^+$ calcd for $C_{14}H_{12}ClFN_2O_3$, 310.0515; found, 310.0516.

3. General Experimental Procedure

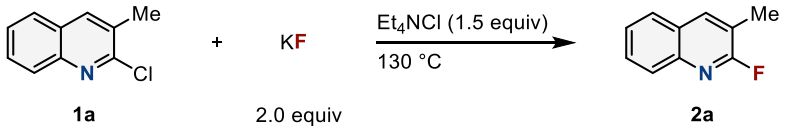
1) Mechanochemical S_NAr fluorination



Procedure A: Heteroaryl chloride **1** (0.50 mmol), KF (1.0 mmol, 2.0 equiv), and Et_4NCl (0.75 mmol, 1.5 equiv) were placed in a ball milling vessel (stainless, 5 mL) loaded with one grinding ball (stainless, diameter: 10 mm). After the vessel was closed in air without purging with inert gas, the vessel was placed in the ball mill (Retsch MM400, 60 min at 30 Hz) and a heat gun (preset temperature at 250 °C). After 60 min, the jar was cooled rapidly with cold water and opened. The mixture was passed through a short silica gel column eluting with 50% EtOAc/CH_2Cl_2. The crude mixture was purified by flash column chromatography (SiO_2, Et_2O/hexane, typically 0:100–5:95) to give the corresponding fluorinated product **2**.

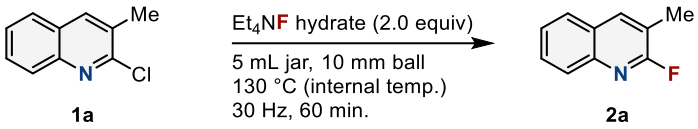
Procedure B: Heteroaryl chloride **1** (0.50 mmol), KF (1.0 mmol, 2.0 equiv), and Et_4NCl (0.75 mmol, 1.5 equiv) were placed in a ball milling vessel (stainless, 1.5 mL) loaded with one grinding ball (stainless, diameter: 7 mm). After the vessel was closed in air without purging with inert gas, the vessel was placed in the ball mill (Retsch MM400, 30–60 min at 30 Hz) and a heat gun (preset temperature at 250 °C). After 30–60 min, the jar was then cooled and opened. The mixture was passed through a short silica gel column eluting with 50% EtOAc/CH_2Cl_2. The crude mixture was purified by flash column chromatography (SiO_2, Et_2O/hexane, typically 0:100–20:80) to give the corresponding fluorinated product **2**.

2) S_NAr fluorination reaction under neat conditions



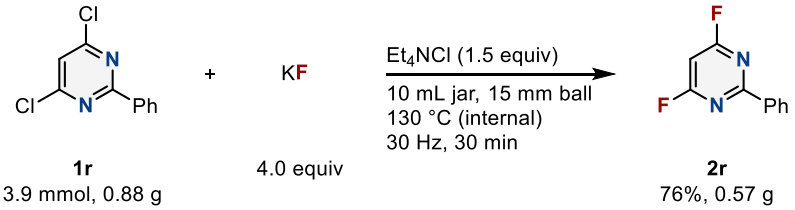
In a vacuum-dried test tube equipped with a magnetic stirring bar, 2-chloro-3-methylquinoline **1a** (0.50 mmol), KF (1.0 mmol, 2.0 equiv) and Et_4NCl (0.75 mmol, 1.5 equiv) were added. The mixture was warmed to 130 °C and stirred for 60 min or 24 h. After the reaction, the mixture was cooled to room temperature and diluted with water, then extracted with Et_2O three times. The organic layer was washed with brine and dried over anhydrous $MgSO_4$. The yield was determined by ^{19}F NMR analysis with fluorobenzene as an internal standard.

3) Mechanochemical S_NAr fluorination reaction using ammonium fluoride



2-Chloro-3-methylquinoline **1a** (88.6 mg, 0.50 mmol) and Et_4NF hydrate (150 mg, 1.0 mmol, 2.0 equiv based on anhydrous) were placed in a ball milling vessel (stainless, 5 mL) loaded with one grinding ball (stainless, diameter: 10 mm) in a glovebox. After the vessel was closed purging with inert gas, the vessel was placed in the ball mill (Retsch MM400, 60 min at 30 Hz) and heat gun (preset temperature at 250 °C). After 60 min, the jar was then cooled rapidly with cold water and opened. The mixture was passed through a short silica gel column eluting with 50% EtOAc/CH_2Cl_2. The crude mixture was analyzed using ^{19}F NMR with fluorobenzene (15.5 mg) as an internal standard to obtain a NMR yield of **2a** in 61% yield.

4. Scaled-up Synthesis of 2r



1r
3.9 mmol, 0.88 g

4.0 equiv

2r
76%, 0.57 g

Fenclorim **1r** (0.877 g, 3.9 mmol), KF (0.907 g, 15.6 mmol, 4.0 equiv) and Et_4NCl (0.970 g, 5.85 mmol, 1.5 equiv) were placed in a ball milling vessel (stainless, 10 mL) loaded with grinding ball (stainless, diameter: 15 mm). After the vessel was closed in air without purging with inert gas, the vessel was placed in the ball mill (Retsch MM400, 30 min at 30 Hz) and a heat gun (preset temperature at 250 °C). After 30 min, the jar was then cooled rapidly with cold water and opened. The mixture was diluted with water and then extracted with EtOAc three times. The organic layer was combined and dried over anhydrous $MgSO_4$. After filtration, the solvent was removed under vacuum, and the residue was purified by silica gel column chromatography (Et_2O/hexane, 0:100–2:98) to afford compound **2r** (569.6 mg, 2.96 mmol, 76%) as a white solid.

5. Thermography Observation for Reaction Temperature

The temperature inside the milling jar after the mechanochemical S_NAr fluorination reactions were confirmed by observation with a thermography camera immediately after opening the milling jar. When the pre-set temperature of the heat gun was 250 °C for a 5 mL stainless jar with a 10 mm ball (30 Hz, 60 min), the internal temperature was determined to be 129.5 °C (Figure S4). Similarly, for a 10 mL stainless jar with a 15 mm ball (30 Hz, 30 min), the internal temperature was 131.2 °C (Figure S5). For a 1.5 mL stainless jar with a 7 mm ball (30 Hz, 30 min), the internal temperature was 125.4 °C (Figure S6).

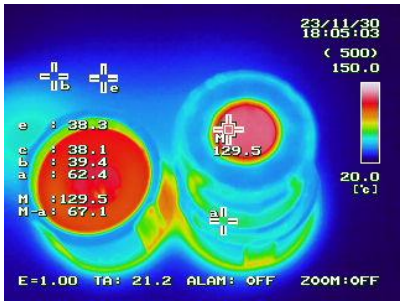


Figure S4. Thermography image inside the milling jar (5 mL) after grinding for 60 min at 30 Hz.

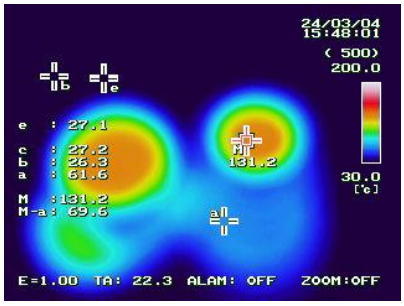


Figure S5. Thermography image inside the milling jar (10 mL) after grinding for 30 min at 30 Hz.

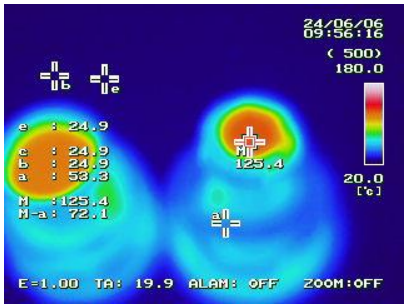


Figure S6. Thermography image inside the milling jar (1.5 mL) after grinding for 30 min at 30 Hz.

6. Calculation of E-factors

The E-factors were calculated for the present solid-state conditions and compared to those of Bland's and Sanford's conditions following literature procedures.[4,5]

< **Our solid-state fluorination conditions** >

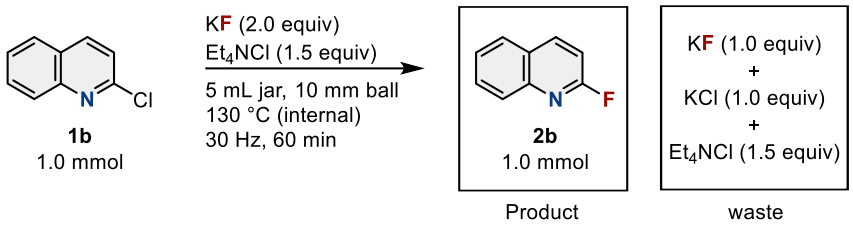


Table S1. E-factor of our solid-state fluorination conditions.

this work	Mw	mmol	mg
product			
2b	147.15	1.0	147.15
waste			
KF	58.1	1.0	58.1
KCl	74.55	1.0	74.55
Et_4NCl	165.71	1.5	248.565
total			381.215
E-factor			2.6

< **Bland's fluorination conditions**[4] >

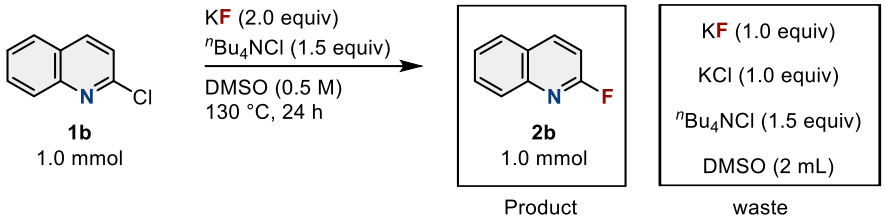


Table S2. E-factor of Bland's fluorination conditions.

Bland, 2014	Mw	mmol	mg
product			
2b	147.15	1.0	147.15
waste			
KF	58.1	1.0	58.1
KCl	74.55	1.0	74.55
$^{n}Bu_4NCl$	277.92	1.5	416.88
DMSO			2200
total			2749.52
E-factor			18.7

< **Sanford's fluorination conditions**[5] >

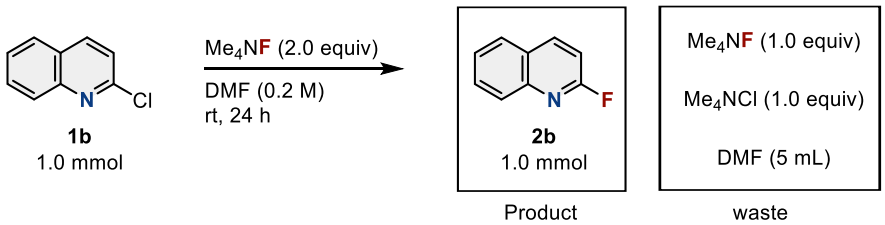


Table S3. E-factor of Sanford's fluorination conditions.

Sanford, 2015	Mw	mmol	mg
product			
2b	147.15	1.0	147.15
waste			
Me_4NF	93.14	1.0	93.14
Me_4NCl	109.6	1.0	109.6
DMF			4720
total			4922.74
E-factor			33.5

We recalculated the E-factor for the reaction of **1b**, taking into account the purification step. As shown below, the E-factor is 3019.92. We also calculated the E-factor for the large-scale mechanochemical synthesis of **2r** and its purification, which is 1252.73. Importantly, it should be noted here that our research aims to reduce the quantity of reaction solvents, and the current workup/purification procedure is not optimal from a sustainability perspective. Although this was not the focus of this study, it must be considered when developing industrial mechanochemical protocols.

< **E-factor for the reaction of 1b considering the purification process** >

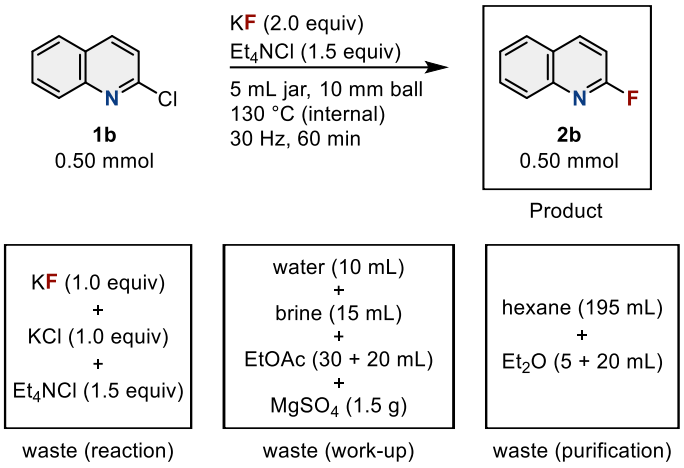


Table S4. E-factor of our solid-state fluorination conditions considering the purification step.

this work	Mw	mmol	g
product			
2b	147.15	0.50	0.074
waste (Reaction)			
KF	58.10	0.50	0.029
KCl	74.55	0.50	0.037
Et_4NCl	165.71	0.75	0.124
waste (work-up)			
water			10
brine			18
EtOAc			45
$MgSO_4$			1.5
waste (purification)			
hexane			130
Et_2O			17.5
total waste			222.191
E-factor (total)			3019.92

< **E-factor for the reaction of 1r considering the purification process** >

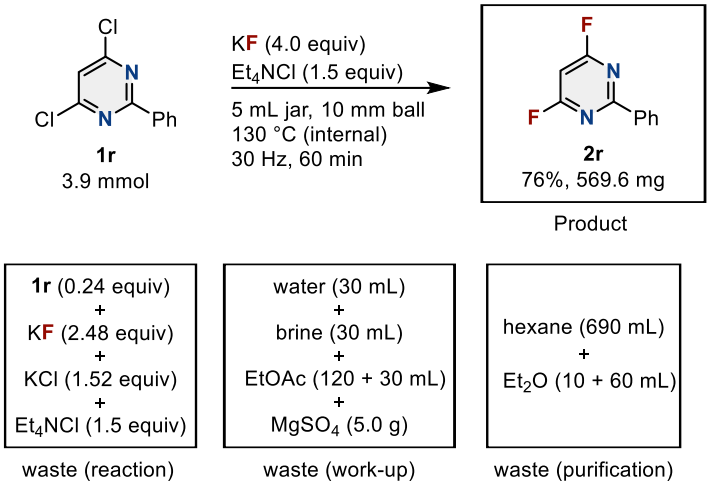


Table S5. E-factor of our solid-state fluorination conditions on a gram scale considering the purification step.

this work	Mw	mmol	g
product			
2r	192.17	2.96	0.569
waste (Reaction)			
1r	225.07	0.94	0.211
KF	58.10	9.67	0.562
KCl	74.55	5.93	0.442
Et_4NCl	165.71	5.85	0.969
waste (work-up)			
water			30
brine			36
EtOAc			135
$MgSO_4$			5
waste (purification)			
hexane			455.4
Et_2O			49
total waste			712.584
E-factor (reaction)			3.839
E-factor (total)			1252.73

7. Calculation of Reagents Cost

The reagent costs were calculated on a 1.0 mol scale reaction under the present solid-state conditions and compared to those of Bland's and Sanford's conditions.[4,5] Retail prices are for July 2024. The results showed that our method is much less inexpensive S_NAr fluorination system.

< **Our solid-state fluorination conditions** >

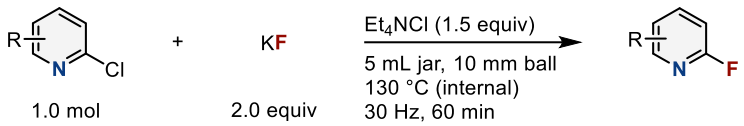


Table S6. Total reagents cost of our solid-state fluorination conditions.

This work	amount (mol or L)	cost (JPY)
KF (Wako, 166-13241)	2	2092
Et_4NCl (TCI, T0095)	1.5	12279
Total cost		14371 (ca. US $89)

< **Bland's fluorination conditions**[4] >

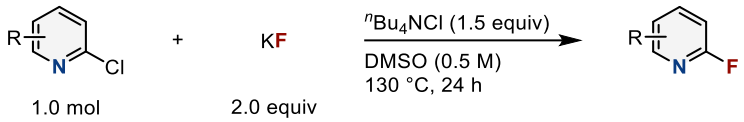


Table S7. Total reagents cost of Bland's conditions.

Bland, 2014	amount (mol or L)	cost (JPY)
KF (Wako, 166-13241)	2	2092
$^nBu_4NCl$ (TCI, T0055)	1.5	121729
DMSO (KANTO, 10380-05)	2	34000
Total cost		157821 (ca. US $977)

< **Sanford's fluorination conditions**[5] >

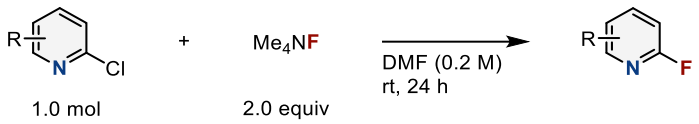


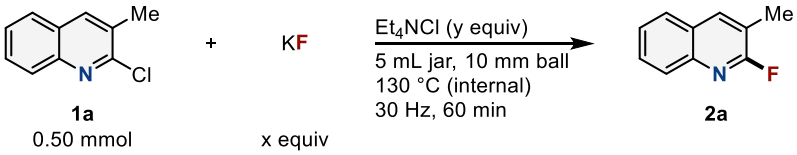
Table S8. Total reagents cost of Sanford's conditions.

Sanford, 2015	amount (mol or L)	cost (JPY)
Me_4NF (Sigma-Aldrich, 459135)	2	1818093
DMF (KANTO, 11339-05)	5	51000
Total cost		1869093 (ca. US $11571)

8. Additional Optimization Study

2-Chloro-3-methylquinoline (**1a**, 0.50 mmol), KF (1.0–2.0 equiv), and Et_4NCl (0–1.5 equiv) were placed in a ball-milling vessel (stainless steel, 5 mL) loaded with one grinding ball (stainless steel, diameter: 10 mm). After the vessel was closed in air without purging with inert gas, the vessel was placed in the ball mill (Retsch MM400, 60 min, 30 Hz) and a heat gun (preset temperature: 250 °C). After 60 min, the jar was cooled rapidly with cold water and opened. The mixture was passed through a short column of silica gel using EtOAc/CH_2Cl_2 (1/1, v/v). The crude mixture was analyzed using ^{19}F NMR spectroscopy with fluorobenzene as the internal standard. When reducing the amount of KF and Et_4NCl, the yield of **2a** decreased. The use of KF (2.0 equiv) and Et_4NCl (1.5 equiv) is required for an efficient fluorination.

Table S9. Additional optimization study.



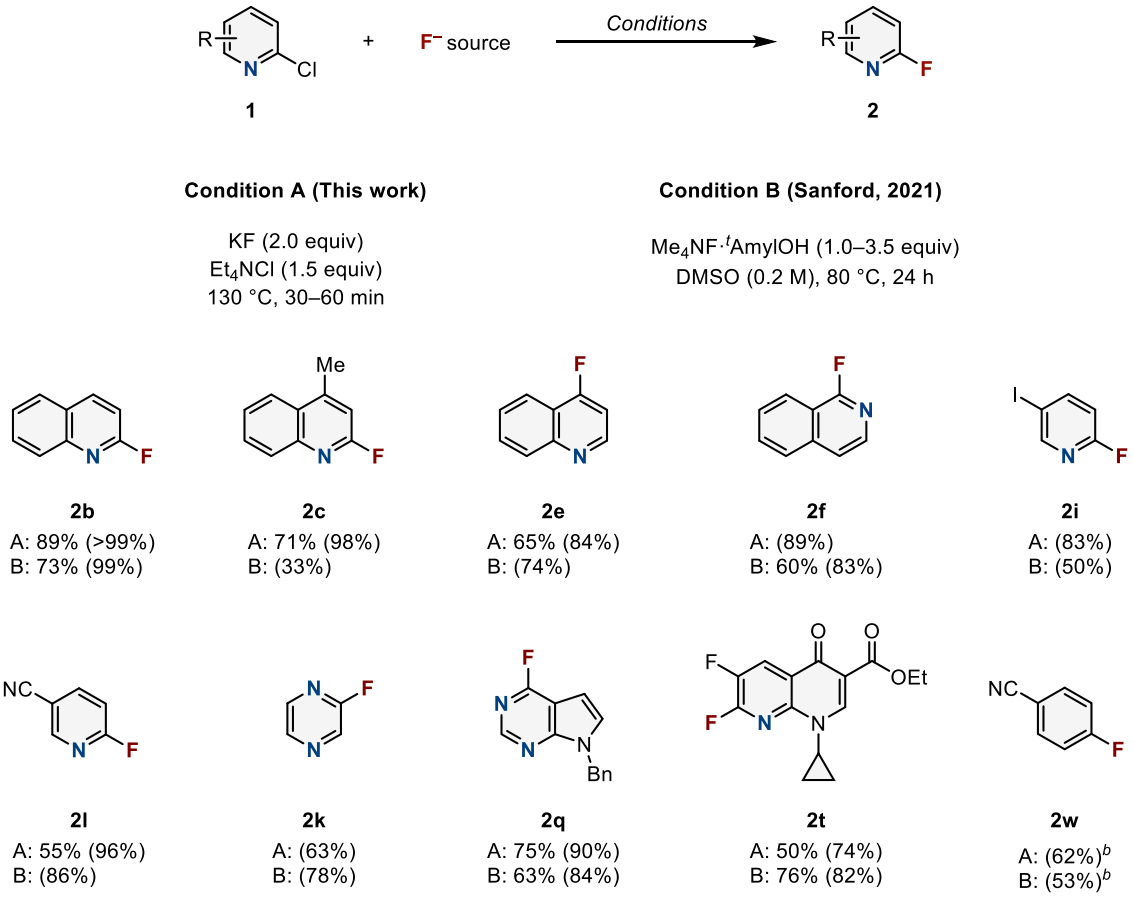
Entry	KF (x equiv)	Et_4NCl (y equiv)	yield of **2a** (%)[a]
1	2.0	1.5	>99
2	1.5	1.5	70
3	1.0	1.5	27
4	2.0	0.5	79
5	2.0	0.1	29
6	2.0	0	n.d.

[a] ^{19}F NMR yields determined with fluorobenzene as an internal standard.

9. Comparison with Solution-based Protocols

We compared the yields of the present mechanochemical conditions, and the solution-based conditions reported by Sanford, which is one of the most practical S_NAr fluorination protocols.[6] As shown below, in these ten examples, there are no significant differences in yield between mechanochemical (condition A) and solution-based (condition B) reactions. For **2c** and **2i**, the mechanochemical protocol is much better than the solution-based method.

Table S10. Comparison with solution-based protocols.

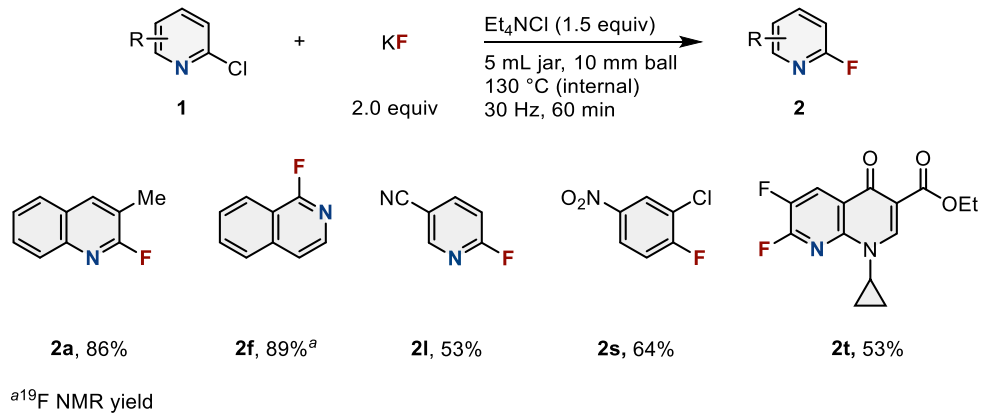


2b	**2c**	**2e**	**2f**	**2i**
A: 89% (>99%) B: 73% (99%)	A: 71% (98%) B: (33%)	A: 65% (84%) B: (74%)	A: (89%) B: 60% (83%)	A: (83%) B: (50%)
2l	**2k**	**2q**	**2t**	**2w**
A: 55% (96%) B: (86%)	A: (63%) B: (78%)	A: 75% (90%) B: 63% (84%)	A: 50% (74%) B: 76% (82%)	A: (62%)[b] B: (53%)[b]

[a]Isolated yields.[19]F NMR yields are given in parentheses. [b]From nitroarene

10. Purification Without Using Dichloromethane

To enhance the sustainability of this mechanochemical protocol, we conducted the purification process without using dichloromethane. We used EtOAc for the purification step in reactions involving five different substrates. The results showed that the yields of these products were similar to those of the reactions using dichloromethane (±5%), suggesting that dichloromethane can be replaced by EtOAc in the purification step.



a19F NMR yield

Procedure C (for 1a and 1t): Heteroaryl chloride **1** (0.50 mmol), KF (1.0 mmol, 2.0 equiv), and Et_4NCl (0.75 mmol, 1.5 equiv) were placed in a ball-milling vessel (stainless steel, 5 mL) loaded with one grinding ball (stainless steel, diameter: 10 mm). After the vessel was closed in air without purging with inert gas, the vessel was placed in the ball mill (Retsch MM400, 60 min, 30 Hz) and a heat gun (preset temperature: 250 °C). After 60 min, the jar was cooled rapidly with cold water and opened. The mixture was transferred to a separatory funnel with EtOAc (10 mL) and water (10 mL) and then extracted with EtOAc (3 ×10 mL). The combined organic layer was washed with brine (15 mL) and dried over anhydrous $MgSO_4$. After filtration, the solvent was removed from the filtrate under reduced pressure. The crude mixture was purified by flash column chromatography (SiO_2, Et_2O/hexane) to give the corresponding fluorinated product (**2**).

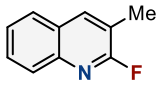
Procedure D (for 1f): **1f** (0.50 mmol), KF (1.0 mmol, 2.0 equiv), and Et_4NCl (0.75 mmol, 1.5 equiv) were placed in a ball milling vessel (stainless steel, 5 mL) loaded with one grinding ball (stainless steel, diameter: 10 mm). After the vessel was closed in air without purging with inert gas, the vessel was placed in the ball mill (Retsch MM400, 60 min, 30 Hz) and a heat gun (preset temperature: 250 °C). After 60 min, the jar was cooled rapidly with cold water and opened. The mixture was transferred to a separatory funnel with EtOAc (10 mL) and water (10 mL), then extracted with EtOAc (3 × 10 mL). The combined organic layer was washed with brine (15 mL) and dried over anhydrous $MgSO_4$. After

filtration, the solvent was removed from the filtrate under reduced pressure. The resulting crude mixture was analyzed by ^{19}F NMR spectroscopy with fluorobenzene as the internal standard.

Procedure E (for 1l and 1s): Heteroaryl chloride **1** (0.50 mmol), KF (1.0 mmol, 2.0 equiv), and Et_4NCl (0.75 mmol, 1.5 equiv) were placed in a ball-milling vessel (stainless steel, 1.5 mL) loaded with one grinding ball (stainless steel, diameter: 7 mm). After the vessel was closed in air without purging with inert gas, the vessel was placed in the ball mill (Retsch MM400, 30 or 45 min, 30 Hz) and a heat gun (preset temperature: 250 °C). After 30 or 45 min, the jar was then cooled and opened. The mixture was transferred to a separatory funnel with EtOAc (10 mL) and water (10 mL), and extracted with EtOAc (3 × 10 mL). The combined organic layers were washed with brine (15 mL) and dried over anhydrous $MgSO_4$. After filtration, the solvent was removed from the filtrate under reduced pressure. The crude mixture was purified by flash column chromatography (SiO_2, Et_2O/hexane) to give the corresponding fluorinated product (**2**).

11. Characterization of Obtained Fluorinated Products

2-Fluoro-3-methylquinoline (2a).

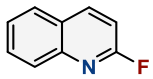


2a

The reaction was performed according to the general procedure A. The reaction was carried out with 88.9 mg (0.50 mmol) of **1a**. The resulting crude mixture was analyzed using ^{19}F NMR with fluorobenzene (15.3 mg) as an internal standard to obtain the NMR yield of **2a** in >99% yield. Product **2a** was obtained as a white solid (68.8 mg, 0.43 mmol, 85% yield) after purification by silica-gel column chromatography (SiO_2, Et_2O/hexane, 0:100–5:95).

^{1}H NMR (396 MHz, $CDCl_3$, δ): 2.45 (s, 3H), 7.48–7.54 (m, 1H), 7.63–7.70 (m, 1H), 7.77 (d, J = 7.9 Hz, 1H), 7.91 (d, J = 8.7 Hz, 1H), 8.02 (d, J = 9.9 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 15.1 (*C*H$_3$), 120.0 (d, J = 36.2 Hz, *C*), 125.9 (d, J = 2.0 Hz, *C*H), 126.6 (*C*H), 127.3 (d, J = 2.0 Hz, *C*), 127.6 (*C*H), 129.3 (*C*H), 140.4 (d, J = 7.6 Hz, *C*H), 144.2 (d, J = 17.2 Hz, *C*), 160.4 (d, J = 243.2 Hz, *C*). ^{19}F NMR (373 MHz, $CDCl_3$, δ): –66.5 (s). HRMS-APCI (m/z): $[M+H]^+$ calcd for $C_{10}H_9FN$, 161.0714; found, 161.0708.

2-Fluoroquinoline (2b).



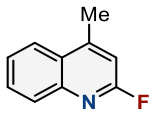
2b

The reaction was performed according to the general procedure A. The reaction was carried out with 81.8 mg (0.50 mmol) of **1b**. The resulting crude mixture was analyzed using ^{19}F NMR with fluorobenzene (14.6 mg) as an internal standard to obtain the NMR yield of **2b** in >99% yield. Product **2b** was obtained as a colorless oil (65.3 mg, 0.44 mmol, 89% yield) after purification by silica-gel column chromatography (SiO_2, Et_2O/hexane, 0:100–10:90) and recycling preparative GPC. ^{1}H, ^{13}C, and ^{19}F NMR were in agreement with the literature.[6]

The reaction was carried out with 104.2 mg (0.50 mmol) of 2-bromoquinoline (**1b'**). The resulting crude mixture was analyzed using ^{19}F NMR with fluorobenzene (15.2 mg) as an internal standard to obtain the NMR yield of **2b** in >99% yield. ^{19}F NMR was in agreement with the literature.[6] ^{1}H NMR (401 MHz, $CDCl_3$, δ): 7.09 (dd, J = 2.8, 8.8 Hz, 1H), 7.55 (t, J = 7.6 Hz, 1H), 7.74 (t, J = 7.4 Hz, 1H), 7.85 (d, J = 8.0 Hz, 1H), 7.96 (d, J = 8.8 Hz, 1H), 8.26 (t, J = 8.6 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 110.0 (d, J = 42.2 Hz, *C*H), 126.1 (d, J = 2.9 Hz, *C*H), 126.8 (d, J = 1.9 Hz, *C*), 127.5 (*C*H), 128.0 (*C*H), 130.6 (*C*H), 141.9 (d, J = 10.5 Hz, *C*H), 145.7 (d, J = 16.3 Hz, *C*), 161.1 (d, J = 241.6 Hz, *C*). ^{19}F NMR (377 MHz, $CDCl_3$, δ): –62.2 (s). HRMS-EI (m/z): $[M]^+$ calcd for C_9H_6FN,

147.0479; found, 147.0479.

2-Fluoro-4-methylquinoline (2c).

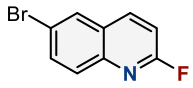


2c

The reaction was performed according to the general procedure A. The reaction was carried out with 88.8 mg (0.50 mmol) of **1c**. The resulting crude mixture was analyzed by ^{19}F NMR with fluorobenzene (15.2 mg) as an internal standard to obtain the NMR yield of **2c** in 98% yield. Product **2c** was obtained as a colorless oil (57.6 mg, 0.36 mmol, 71% yield, isolated along with approximately 6% of starting material) after purification by silica-gel column chromatography (SiO_2, Et_2O/hexane, 0:100–5:95). ^{1}H and ^{19}F NMR were in agreement with the literature.[7]

^{1}H NMR (396 MHz, $CDCl_3$, δ): 2.73 (s, 3H), 6.93 (s, 1H), 7.52–7.57 (m, 1H), 7.72 (t, J = 7.5 Hz, 1H), 7.96 (t, J = 9.3 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 18.9 (d, J = 2.9 Hz, *C*H$_3$), 109.9 (d, J = 41.9 Hz, *C*H), 123.7 (*C*H), 125.73 (*C*H), 125.75 (*C*), 128.5 (*C*H), 130.2 (*C*H), 145.5 (d, J = 17.2 Hz, *C*), 151.0 (d, J = 10.0 Hz, *C*), 160.9 (d, J = 241.3 Hz, *C*). ^{19}F NMR (377 MHz, $CDCl_3$, δ): –63.5 (s). HRMS-EI (m/z): $[M]^+$ calcd for $C_{10}H_8FN$, 161.0635; found, 161.0636.

6-Bromo-2-fluoroquinoline (2d).

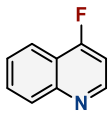


2d

The reaction was performed according to the general procedure A. The reaction was carried out with 121.9 mg (0.50 mmol) of **1d**. The resulting crude mixture was analyzed by ^{19}F NMR with fluorobenzene (15.1 mg) as an internal standard to obtain the NMR yield of **2d** in 88% yield. Product **2d** was obtained as a white solid (80.2 mg, 0.35 mmol, 71% yield) after purification by silica-gel column chromatography (SiO_2, Et_2O/hexane, 0:100–5:95). ^{1}H, ^{13}C, and ^{19}F NMR were in agreement with the literature.[6]

^{1}H NMR (396 MHz, $CDCl_3$, δ): 7.13 (dd, J = 2.8, 9.1 Hz, 1H), 7.79–7.85 (m, 2H), 8.02 (d, J = 2.0 Hz, 1H), 8.18 (t, J = 8.5 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 111.0 (d, J = 42.0 Hz, *C*H), 119.8 (d, J = 2.9 Hz, *C*), 127.8 (d, J = 1.9 Hz, *C*), 129.5 (*C*H), 129.6 (d, J = 16.2 Hz, *C*H), 133.9 (*C*H), 140.9 (d, J = 9.6 Hz, *C*H), 144.3 (d, J = 17.2 Hz, *C*), 161.1 (d, J = 244.1 Hz, *C*). ^{19}F NMR (373 MHz, $CDCl_3$, δ): –61.3 (s). HRMS-EI (m/z): $[M]^+$ calcd for C_9H_5BrFN, 224.9584; found, 224.9589.

4-Fluoroquinoline (2e).

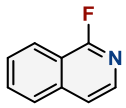


2e

The reaction was performed according to the general procedure A. The reaction was carried out with 81.8 mg (0.50 mmol) of **1e**. The resulting crude mixture was analyzed using ^{19}F NMR with fluorobenzene (15.3 mg) as an internal standard to obtain the NMR yield of **2e** in 84% yield. Product **2e** was obtained as a yellow oil (48.2 mg, 0.33 mmol, 65% yield, isolated along with approximately 3% of starting material) after purification by silica-gel column chromatography (SiO_2, Et_2O/hexane, 0:100–20:80). ^1H, ^{13}C, and ^{19}F NMR were in agreement with the literature.[8]

^1H NMR (396 MHz, $CDCl_3$, δ): 7.11 (dd, J = 5.1, 9.5 Hz, 1H), 7.59–7.65 (m, 1H), 7.76–7.82 (ddd, J = 1.6, 6.9, 8.5 Hz, 1H), 8.11–8.15 (m, 2H), 8.88 (dd, J = 4.9, 8.1 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 105.6 (d, J = 15.4 Hz, *C*H), 119.5 (d, J = 12.5 Hz, *C*), 120.4 (d, J = 4.8 Hz, *C*H), 126.8 (*C*H), 129.1 (d, J = 3.8 Hz, *C*H), 130.5 (*C*H), 150.4 (d, J = 4.8 Hz, *C*), 151.4 (d, J = 7.7 Hz, *C*H), 165.2 (d, J = 268.4 Hz, *C*).^{19}F NMR (373 MHz, $CDCl_3$, δ): –113.2 (s). HRMS-EI (m/z): $[M]^+$ calcd for C_9H_6FN, 147.0479; found, 147.0482.

1-Fluoroisoquinoline (2f).



2f

The reaction was performed according to the general procedure A. The reaction was carried out with 81.8 mg (0.50 mmol) of **1f**. The resulting crude mixture was analyzed by ^{19}F NMR with fluorobenzene (15.1 mg) as an internal standard to obtain the NMR yield of **2f** in 89% yield. ^{19}F NMR was in agreement with the literature.[6]

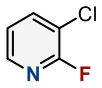
The reaction was carried out with 104.1 mg (0.50 mmol) of 1-bromoisoquinoline (**1f'**). The resulting crude mixture was analyzed by ^{19}F NMR with fluorobenzene (15.0 mg) as an internal standard to obtain the NMR yield of **2f** in 82% yield. ^{19}F NMR was in agreement with the literature.[6]

The reaction was carried out with 127.6 mg (0.50 mmol) of 1-iodoisoquinoline (**1f''**). The resulting crude mixture was analyzed by ^{19}F NMR with fluorobenzene (15.4 mg) as an internal standard to obtain the NMR yield of **2f** in >99% yield. Product **2f** was obtained as a yellow oil (62.7 mg, 0.43 mmol, 85% yield) after purification by silica-gel column chromatography (SiO_2, Et_2O/pentane, 0:100–10:90). ^1H, ^{13}C, and ^{19}F NMR were in agreement with the literature.[6]

^1H NMR (399 MHz, $CDCl_3$, δ): 7.53 (dd, J = 1.4, 5.8 Hz, 1H), 7.63–7.69 (m, 1H), 7.74–7.80 (m, 1H),

7.87 (d, J = 8.0 Hz, 1H), 8.06 (dd, J = 1.2, 5.6 Hz, 1H), 8.17 (d, J = 8.4 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 117.6 (d, J = 31.7 Hz, *C*), 119.3 (d, J = 4.8 Hz, *C*H), 123.0 (*C*H), 126.3 (d, J = 3.8 Hz, *C*H), 127.9 (*C*H), 131.4 (*C*H), 139.1 (d, J = 16.3 Hz, *C*H), 139.5 (d, J = 5.7 Hz, *C*), 159.9 (d, J = 246.3 Hz, *C*). ^{19}F NMR (375 MHz, $CDCl_3$, δ): –71.7 (s). HRMS-EI (m/z): $[M]^+$ calcd for C_9H_6FN, 147.0479; found, 147.0483.

3-Chloro-2-fluoropyridine (2g).

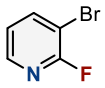


2g

The reaction was performed according to the general procedure A. The reaction was carried out with 73.8 mg (0.50 mmol) of **1g**. The resulting crude mixture was diluted with $CDCl_3$ and then analyzed using ^{19}F NMR with fluorobenzene (15.5 mg) as an internal standard to obtain the NMR yield of **2g** in 66% yield. ^{19}F NMR was in agreement with the literature.[7] Since **2g** is a volatile compound, only the NMR yield was reported.

^{19}F NMR (377 MHz, $CDCl_3$, δ): –71.1 (s).

3-Bromo-2-fluoropyridine (2h).

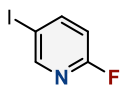


2h

The reaction was performed according to the general procedure A. The reaction was carried out with 96.0 mg (0.50 mmol) of **1h**. The resulting crude mixture was diluted with $CDCl_3$ and then analyzed by ^{19}F NMR with fluorobenzene (14.9 mg) as an internal standard to obtain the NMR yield of **2h** in 82% yield. ^{19}F NMR was in agreement with the literature.[9] Since **2h** is a volatile compound, only the NMR yield was reported.

^{19}F NMR (377 MHz, $CDCl_3$, δ): –65.1 (s).

2-Fluoro-4-iodopyridine (2i).



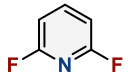
2i

The reaction was performed according to the general procedure A. The reaction was carried out with 119.7 mg (0.50 mmol) of **1i**. The resulting crude mixture was analyzed using ^{19}F NMR with fluorobenzene (15.1 mg) as an internal standard to obtain the NMR yield of **2i** in 83% yield. ^{19}F NMR was in agreement with an authentic sample (F0773, Tokyo Chemical Industry Co.). Since **2i** is a

volatile compound, only the NMR yield was reported.

^{19}F NMR (373 MHz, $CDCl_3$, δ): –70.1 (s).

2,6-Difluoropyridine (2j).



2j

The reaction was performed according to the general procedure A. The reaction was carried out with 74.0 mg (0.50 mmol) of **1j**, 116.7 mg (2.0 mmol) of KF, and 248.8 mg (1.5 mmol) of Et_4NCl. The resulting crude mixture was diluted with $CDCl_3$ and then analyzed using ^{19}F NMR with fluorobenzene (15.1 mg) as an internal standard to obtain the NMR yield of **2j** in 75% yield. ^{19}F NMR was in agreement with the literature.[10] Since **2j** is a volatile compound, only the NMR yield was reported.

^{19}F NMR (373 MHz, $CDCl_3$, δ): –68.1 (s).

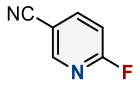
2-Fluoropyrazine (2k).

2k

The reaction was performed according to the general procedure A. The reaction was carried out with 57.4 mg (0.50 mmol) of **1k**. The resulting crude mixture was diluted with $CDCl_3$ and then analyzed using ^{19}F NMR with fluorobenzene (14.9 mg) as an internal standard to obtain the NMR yield of **2k** in 63% yield. ^{19}F NMR was in agreement with the literature.[11] Since **2k** is a volatile compound, only the NMR yield was reported.

^{19}F NMR (377 MHz, $CDCl_3$, δ): –79.4 (s).

5-Cyano-2-fluoropyridine (2l).



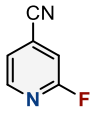
2l

The reaction was performed according to the general procedure B. The reaction was carried out with 69.2 mg (0.50 mmol) of **1l** for 30 min. The resulting crude mixture was analyzed by ^{19}F NMR with fluorobenzene (15.1 mg) as an internal standard to obtain the NMR yield of **2l** in 96% yield. Product **2l** was obtained as a colorless solid (33.5 mg, 0.27 mmol, 55% yield) after purification by silica-gel column chromatography (SiO_2, Et_2O/hexane, 0:100–20:80). ^{1}H, ^{13}C, and ^{19}F NMR were in agreement with the literature.[12]

^{1}H NMR (396 MHz, $CDCl_3$, δ): 7.08–7.13 (m, 1H), 8.05–8.13 (m, 1H), 8.59 (d, J = 2.4 Hz, 1H). ^{13}C

NMR (100 MHz, $CDCl_3$, δ): 108.0 (d, *J* = 4.8 Hz, *C*), 110.8 (d, *J* = 37.3 Hz, *C*H), 115.5 (*C*), 144.4 (d, *J* = 9.6 Hz, *C*H), 152.2 (d, *J* = 17.3 Hz, *C*H), 164.9 (d, *J* = 249.2 Hz, *C*). ^{19}F NMR (373 MHz, $CDCl_3$, δ): –57.8 (s). HRMS-APCI (m/z): $[M+H]^+$ calcd for $C_6H_4FN_2$, 123.0353; found, 123.0354.

4-Cyano-2-fluoropyridine (2m).

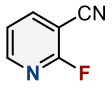


2m

The reaction was performed according to the general procedure B. The reaction was carried out with 69.3 mg (0.50 mmol) of **1m** for 30 min. The resulting crude mixture was analyzed using ^{19}F NMR with fluorobenzene (15.2 mg) as an internal standard to obtain a NMR yield of **2m** in a 73% yield. ^{19}F NMR was in agreement with an authentic sample (C3383, Tokyo Chemical Industry Co.). Since **2m** is a volatile compound, only the NMR yield was reported.

^{19}F NMR (369 MHz, $CDCl_3$, δ): –63.5 (s).

3-Cyano-2-fluoropyridine (2n).

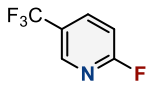


2n

The reaction was performed according to the general procedure B. The reaction was carried out with 69.3 mg (0.50 mmol) of **1n** for 30 min. The resulting crude mixture was analyzed using ^{19}F NMR with fluorobenzene (15.3 mg) as an internal standard to obtain a NMR yield of **2n** in 92% yield. Product **2n** was obtained as a colorless solid (32.9 mg, 0.27 mmol, 54% yield) after purification by silica-gel column chromatography (SiO_2, Et_2O/hexane, 0:100–30:70). ^1H, ^{13}C, and ^{19}F NMR were in agreement with the literature.[9]

^1H NMR (396 MHz, $CDCl_3$, δ): 7.38 (ddd, *J* = 1.6, 4.9, 7.3 Hz, 1H), 8.12 (ddd, *J* = 1.6, 6.9, 9.1 Hz, 1H), 8.48–8.50 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 97.3 (d, *J* = 31.6 Hz, *C*), 112.5 (d, *J* = 5.7 Hz, *C*), 121.6 (d, *J* = 3.8 Hz, *C*H), 144.4 (*C*H), 152.0 (d, *J* = 14.3 Hz, *C*H), 162.6 (d, *J* = 247.2 Hz, *C*). ^{19}F NMR (373 MHz, $CDCl_3$, δ): –60.4 (s). HRMS-APCI (m/z): $[M+H]^+$ calcd for $C_6H_4FN_2$, 123.0353; found, 123.0354.

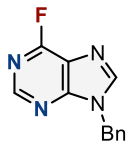
2-Fluoro-5-(trifluoromethyl)pyridine (2o).



2o

The reaction was performed according to the general procedure B. The reaction was carried out with 90.6 mg (0.50 mmol) of **1o** for 30 min. The resulting crude mixture was analyzed using ^{1}H NMR with dibromomethane (18.5 mg) as an internal standard to obtain a ^{1}H NMR yield of **2o** in 76% yield. ^{1}H NMR was in agreement with an authentic sample (F0995, Tokyo Chemical Industry Co.). Since **2o** is a volatile compound, only the NMR yield was reported.

9-Benzyl-6-floro-9*H*-purine (2p).

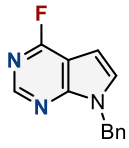


2p

The reaction was performed according to the general procedure B. The reaction was carried out with 122.0 mg (0.50 mmol) of **1p** for 60 min. The resulting crude mixture was analyzed using ^{19}F NMR with fluorobenzene (15.0 mg) as an internal standard to obtain a NMR yield of **2p** in 46% yield. Product **2p** was obtained as a white solid (46.4 mg, 0.20 mmol, 41% yield) after purification by silica-gel column chromatography (SiO_2, EtOAc/hexane, 25:75–35:65). ^{1}H, ^{13}C, and ^{19}F NMR were in agreement with the literature.[8]

^{1}H NMR (396 MHz, $CDCl_3$, δ): 5.48 (s, 2H), 7.29–7.42 (m, 5H), 8.08 (s, 1H), 8.68 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 47.9 (*C*H$_2$), 120.1 (d, *J* = 29.6 Hz, *C*), 127.9 (*C*H), 128.8 (*C*H), 129.2 (*C*H), 134.5 (*C*), 144.8 (*C*H), 152.0 (d, *J* = 14.2 Hz, *C*H), 155.6 (d, *J* = 11.4 Hz, *C*), 159.8 (d, *J* = 260.3 Hz, *C*). ^{19}F NMR (373 MHz, $CDCl_3$, δ): –70.3 (s). HRMS-ESI (m/z): $[M+H]^+$ calcd for $C_{12}H_{10}FN_4$, 229.0884; found, 229.0882.

7-Benzyl-4-fluoro-7H-pyrrolo[2,3-d]pyrimidine (2q).



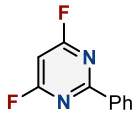
2q

The reaction was performed according to the general procedure B. The reaction was carried out with 121.4 mg (0.50 mmol) of **1q** for 60 min. The resulting crude mixture was analyzed using ^{19}F NMR with fluorobenzene (15.1 mg) as an internal standard to obtain the NMR yield of **2q** in 90% yield. Product **2q** was obtained as a white solid (85.1 mg, 0.37 mmol, 75% yield) after purification by silica-

gel column chromatography (SiO_2, Et_2O/hexane, 0:100–20:80). ^1H, ^{13}C, and ^{19}F NMR were in agreement with the literature.[6]

^1H NMR (401 MHz, $CDCl_3$, δ): 5.48 (s, 2H), 6.61 (d, J = 3.2 Hz, 1H). 7.18–7.24 (m, 3H), 7.29–7.38 (m, 3H), 8.57 (d, J = 0.8 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 48.6 (CH_2), 98.0 (d, J = 4.8 Hz, *C*H), 104.2 (d, J = 33.3 Hz, *C*), 127.5 (*C*H), 128.1 (*C*H), 128.4 (d, J = 2.0 Hz, *C*H), 128.9 (*C*H), 136.3 (*C*), 150.6 (d, J = 14.3 Hz, *C*H), 154.7 (d, J = 12.3 Hz, *C*), 162.3 (d, J = 252.7 Hz, *C*). ^{19}F NMR (373 MHz, $CDCl_3$, δ): –66.5 (s). HRMS-ESI (m/z): $[M+H]^+$ calcd for $C_{13}H_{11}FN_3$, 228.0932; found, 228.0928.

4,6-Difluoro-2-phenylpyrimidine (2r).

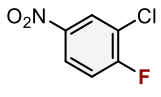


2r

The reaction was performed according to the general procedure B. The reaction was carried out with 112.6 mg (0.50 mmol) of **1r**, 116.1 mg (2.0 mmol) of KF, and 123.9 mg (0.75 mmol) of Et_4NCl for 30 min. The resulting crude mixture was analyzed by ^{19}F NMR with fluorobenzene (15.1 mg) as an internal standard to obtain the NMR yield of **2r** in 65% yield. Product **2r** was obtained as a white solid (53.2 mg, 0.28 mmol, 55% yield) after purification by silica-gel column chromatography (SiO_2, Et_2O/hexane, 0:100–2:98). ^1H, ^{13}C, and ^{19}F NMR were in agreement with the literature.[6]

^1H NMR (401 MHz, $CDCl_3$, δ): 6.44 (t, J = 2.2 Hz, 1H), 7.45–7.60 (m, 3H), 8.39–8.47 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$, δ): 89.9 (t, J = 37.1 Hz, *C*H), 128.73 (*C*H), 128.75 (*C*H), 132.4 (*C*H), 134.7 (*C*), 166.0 (t, J = 17.3 Hz, *C*), 172.2 (dd, J = 18.8, 256.7 Hz, *C*). ^{19}F NMR (377 MHz, $CDCl_3$, δ): –56.5 (s). HRMS-APCI (m/z): $[M+H]^+$ calcd for $C_{10}H_7F_2N_2$, 193.0572; found, 193.0566.

3-Chloro-4-fluoronitrobenzene (2s).



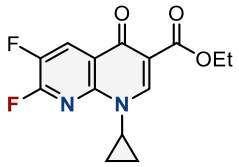
2s

The reaction was performed according to the general procedure B. The reaction was carried out with 95.8 mg (0.50 mmol) of **1s** for 45 min. The resulting crude mixture was analyzed using ^{19}F NMR with fluorobenzene (15.2 mg) as an internal standard to obtain an NMR yield of **2s** in 80% yield. Product **2s** was obtained as a yellow solid (58.0 mg, 0.33 mmol, 66% yield, isolated along with approximately 3% of starting material) after purification by silica-gel column chromatography (SiO_2, Et_2O/pentane, 0:100–3:97). ^1H, ^{13}C, and ^{19}F NMR were in agreement with the literature.[13]

^1H NMR (401 MHz, $CDCl_3$, δ): 7.33 (dd, J = 8.2, 9.0 Hz, 1H), 8.19 (ddd, J = 2.7, 4.3, 9.1 Hz, 1H),

8.37 (dd, J = 2.8, 6.0 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$, δ): 117.2 (d, J = 24.1 Hz, *C*H), 122.5 (d, J = 19.2 Hz, *C*), 124.0 (d, J = 8.7 Hz, *C*H), 126.7 (*C*H), 144.2 (*C*), 161.9 (d, J = 260.0 Hz, *C*). ^{19}F NMR (377 MHz, $CDCl_3$, δ): –104.4 (s). HRMS-EI (m/z): $[M]^+$ calcd for $C_6H_3ClFNO_2$, 174.9831; found, 174.9832.

Ethyl 1-cyclopropyl-6,7-difluoro-4-oxo-1,4-dihydro-1,8-naphthyridine-3-carboxylate (2t).

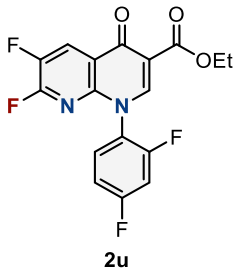


2t

The reaction was performed according to the general procedure A. The reaction was carried out with 155.3 mg (0.50 mmol) of **1t**. The resulting crude mixture was analyzed using ^{19}F NMR with fluorobenzene (14.7 mg) as an internal standard to obtain the NMR yield of **2t** in 74% yield. Product **2t** was obtained as a white solid (73.1 mg, 0.25 mmol, 50% yield) after purification by silica-gel column chromatography (SiO_2, EtOAc/hexane, 40:60–50:50). ^{1}H, ^{13}C, and ^{19}F NMR were in agreement with the literature.[6]

^{1}H NMR (399 MHz, $CDCl_3$, δ): 1.04–1.08 (m, 2H), 1.32 (q, J = 6.8 Hz, 2H), 1.41 (t, J = 7.0 Hz, 3H), 3.59 (tt, J = 3.7, 7.4 Hz, 1H), 4.41 (q, J = 7.0 Hz, 2H), 8.55 (t, J = 9.0 Hz, 1H), 8.65 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 7.6 (CH_2), 14.3 (CH_3), 34.3 (*C*H), 61.2 (CH_2), 112.3 (*C*), 122.8 (d, J = 2.8 Hz, *C*), 126.0 (dd, J = 5.2, 16.8 Hz, *C*H), 143.5 (dd, J = 27.8, 261.6 Hz, *C*), 144.3 (d, J = 14.3 Hz, *C*), 148.7 (*C*H), 152.3 (dd, J = 16.7, 249.7 Hz, *C*), 164.6 (*C*), 172.8 (*C*). ^{19}F NMR (375 MHz, $CDCl_3$, δ): –142.4 (d, J = 23.3 Hz, 1F), –77.3 (d, J = 34.5 Hz, 1F). HRMS-EI (m/z): $[M]^+$ calcd for $C_{14}H_{12}F_2N_2O_3$, 294.0811; found, 294.0814.

Ethyl 1-(2,4-difluorophenyl)-6,7-difluoro-1,4-dihydro-4-oxo-1,8-naphthyridine-3-carboxylate (2u).



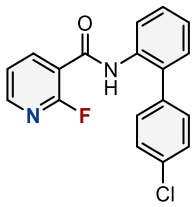
2u

The reaction was performed according to the general procedure A. The reaction was carried out with 191.3 mg (0.50 mmol) of **1u**. The resulting crude mixture was analyzed using ^{19}F NMR with fluorobenzene (15.3 mg) as an internal standard to obtain the NMR yield of **2u** in 78% yield. Product

2u was obtained as a white solid (116.2 mg, 0.32 mmol, 63% yield) after purification by silica-gel column chromatography (SiO_2, EtOAc/hexane, 40:60).

^{1}H NMR (399 MHz, $CDCl_3$, δ): 1.41 (t, *J* = 7.0 Hz, 3H), 4.41 (q, *J* = 7.2 Hz, 2H), 7.08–7.15 (m, 2H), 7.41–7.46 (m, 1H), 8.53(s, 1H), 8.60 (t, *J* = 8.8 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 14.2 (CH_3), 61.4 (CH_2), 105.6 (dd, *J* = 23.0, 26.8 Hz, *C*H), 112.6 (dd, *J* = 3.4, 22.5 Hz, *C*H), 113.6 (*C*), 122.3 (d, *J* = 2.9 Hz, *C*), 123.3 (dd, *J* = 3.8, 13.4 Hz, *C*), 126.2 (dd, *J* = 5.3, 16.8 Hz, *C*H), 129.9 (d, *J* = 10.6 Hz, *C*H), 143.2 (d, *J* = 13.4 Hz, *C*), 143.8 (dd, *J* = 27.3, 262.2 Hz, *C*), 149.1 (*C*H), 152.6 (dd, *J* = 17.3, 252.1 Hz, *C*), 157.9 (dd, *J* = 12.4, 255.9 Hz, *C*), 163.4 (dd, *J* = 10.5, 254.1 Hz, *C*), 164.1 (*C*), 172.9 (*C*). ^{19}F NMR (375 MHz, $CDCl_3$, δ): –141.4 (d, *J* = 34.9 Hz, 1F), –115.0 (s, 1F), –105.2 (s, 1F), –76.8 (d, *J* = 22.9 Hz, 1F). HRMS-EI (m/z): $[M]^+$ calcd for $C_{17}H_{10}F_4N_2O_3$, 366.0622; found, 366.0629.

***N*-(4'-Chlorobiphenyl-2-yl)-2-fluoronicotinamide (2v).**

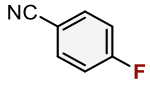


2v

The reaction was performed according to the general procedure A. The reaction was carried out with 171.5 mg (0.50 mmol) of **1v**. The resulting crude mixture was analyzed using ^{19}F NMR with fluorobenzene (15.5 mg) as an internal standard to obtain a NMR yield of **2v** in 55%. Product **2v** was obtained as a white solid (48.2 mg, 0.15 mmol, 30% yield) after purification by silica-gel column chromatography (SiO_2, Et_2O/hexane, 0:100–25:75) and recycling preparative GPC.

^{1}H NMR (396 MHz, $CDCl_3$, δ): 7.21–7.31 (m, 2H), 7.31–7.42 (m, 3H), 7.42–7.52 (m, 3H), 8.31–8.33 (m, 1H), 8.49 (d, *J* = 8.2 Hz, 1H), 8.58 (brs, 1H), 8.62 (ddd, *J* = 2.2, 7.5, 9.9 Hz, 1H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 116.2 (d, *J* = 28.2 Hz, *C*), 121.9 (*C*H), 122.6 (d, *J* = 4.7 Hz, *C*H), 125.1 (*C*H), 128.8 (*C*H), 129.3 (*C*H), 130.2 (*C*H), 130.6 (*C*H), 132.0 (*C*), 134.4 (*C*), 134.5 (*C*), 136.0 (*C*), 143.7 (d, *J* = 1.9 Hz, *C*H), 150.6 (d, *J* = 16.9 Hz, *C*H), 159.4 (d, *J* = 235.8 Hz, *C*), 159.5 (d, *J* = 8.5 Hz, *C*). ^{19}F NMR (377 MHz, $CDCl_3$, δ): –65.0 (s). HRMS-EI (m/z): $[M]^+$ calcd for $C_{18}H_{12}ClFN_2O$, 326.0617; found, 326.0617.

4-Fluorobenzonitrile (2w).



2w

The reaction was performed according to the general procedure B. The reaction was carried out with 68.7 mg (0.50 mmol) of 4-chlorobenzonitrile (**1w)** for 30 min. The resulting crude mixture was

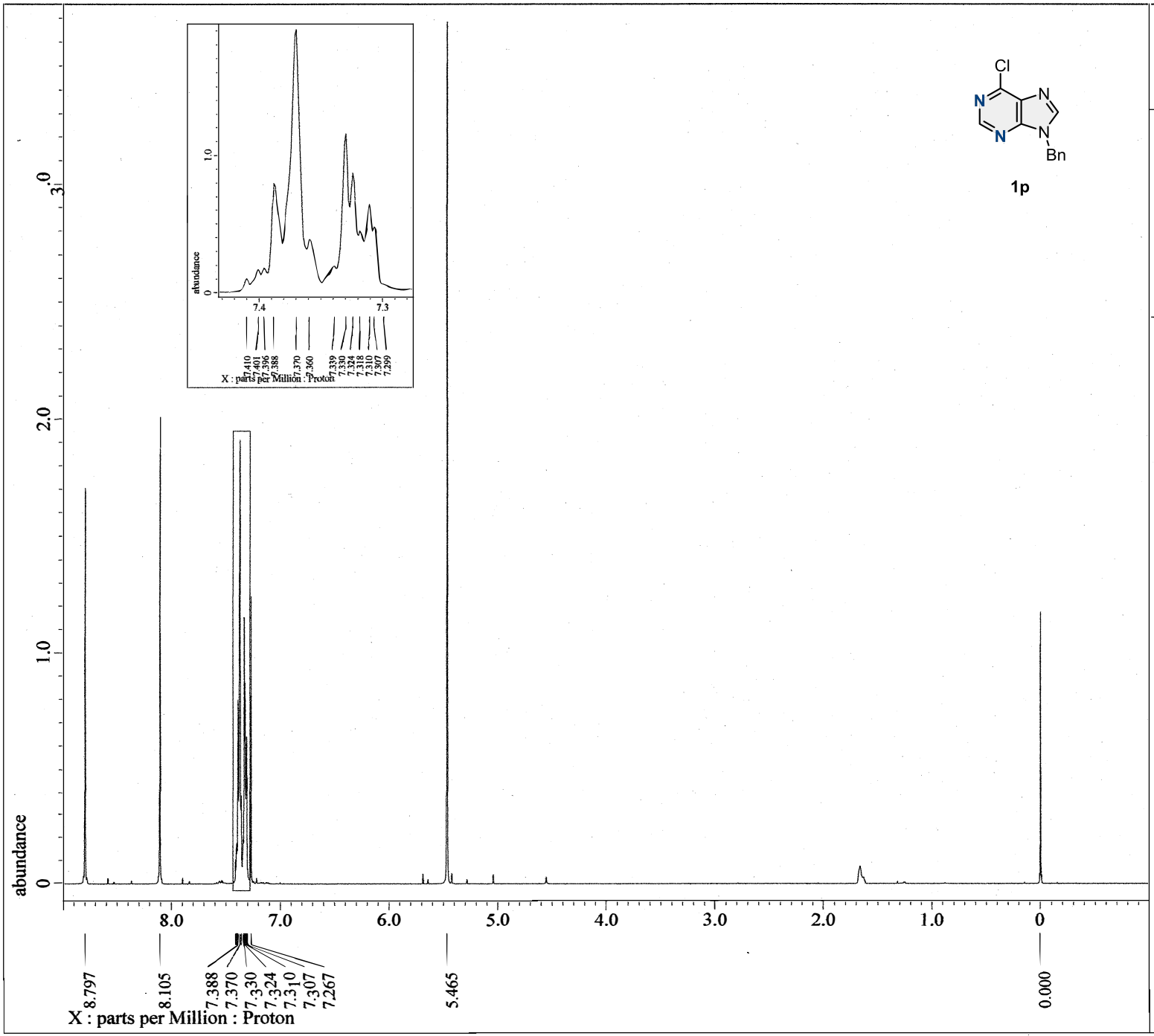
analyzed by ^{19}F NMR with fluorobenzene (15.1 mg) as an internal standard to obtain the NMR yield of **2w** in 3% yield. ^{19}F NMR was in agreement with the literature.[14]

The reaction was carried out with 74.0 mg (0.50 mmol) of 4-nitrobenzonitrile (**1w'**) for 30 min. The resulting crude mixture was analyzed by ^{19}F NMR with fluorobenzene (15.3 mg) as an internal standard to obtain the NMR yield of **2w** in 62% yield. ^{19}F NMR was in agreement with the literature.[14] Since **2w** is a volatile compound, only the NMR yield was reported.

^{19}F NMR (373 MHz, $CDCl_3$, δ): –102.8 (s).

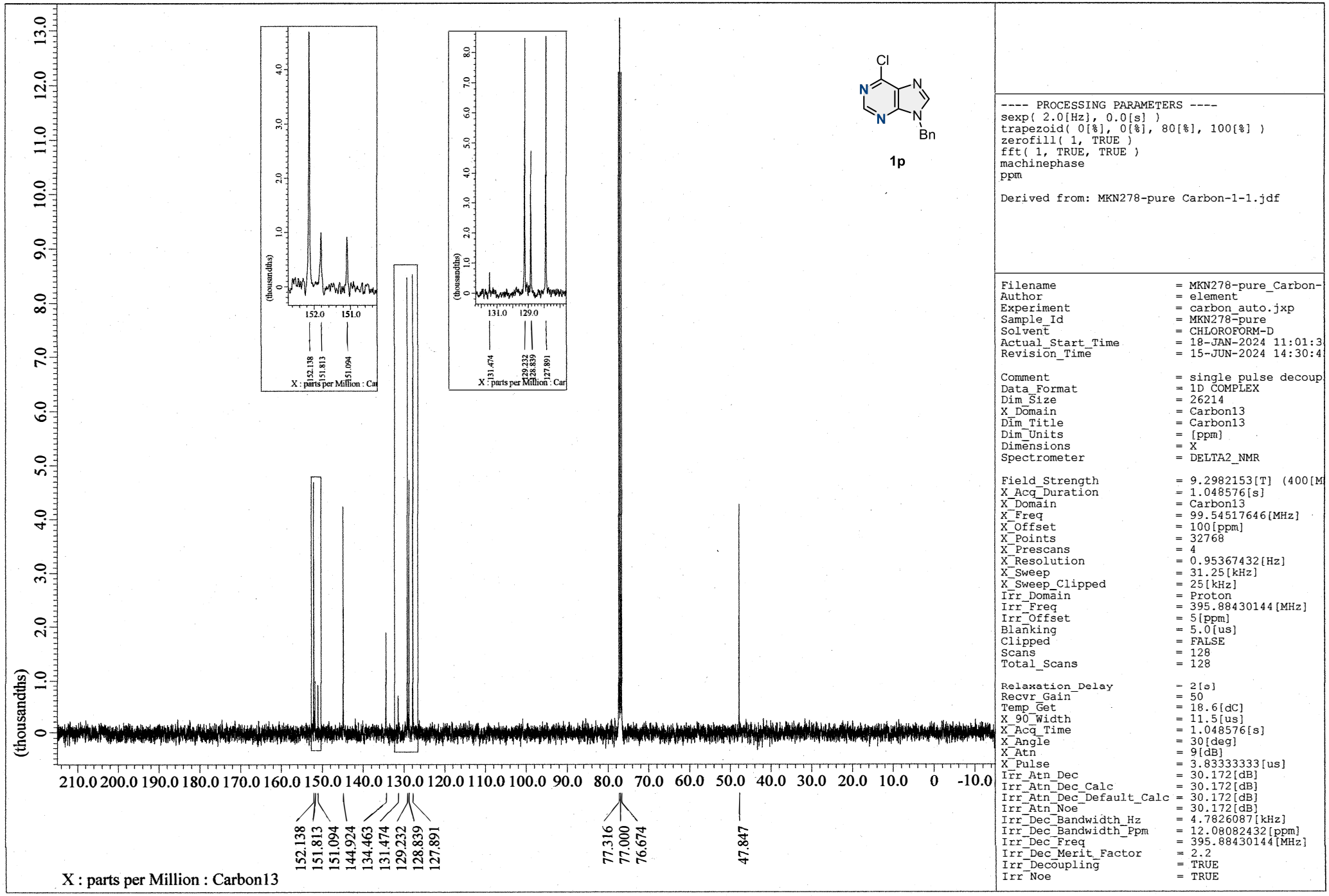
12. References

1. Bliman, D.; Pettersson, M.; Bood, M.; Grotli, M. *Tetrahedron Lett.* **2014**, *55*, 2929.
2. Wood, A. B.; Nandiwale, K. Y.; Mo, Y.; Jin, B.; Pomberger, A.; Schultz, V.; Gallou, F.; Jensen, K. F.; Lipshutz, B. H. *Green Chem.* **2020**, *22*, 3441.
3. Karoli, T.; Mamidyala, S. K.; Zuegg, J.; Fry, S. R.; Tee, E. H. L.; Bradford, T. A.; Madala, P. K.; Huang, J. X.; Ramu, S.; Butler, M. S.; Cooper, M. A. *Bioorg. Med. Chem. Lett.* **2012**, *22*, 2428.
4. Allen, L. J.; Lee, S. H.; Cheng, Y.; Hanley, P. S.; Muhuhi, J. M.; Kane, E.; Powers, S. L.; Anderson, J. E.; Bell, B. M.; Roth, G. A.; Sanford, M. S.; Bland, D. C. *Org. Process Res. Dev.* **2014**, *18*, 1045.
5. Schimler, S. D.; Ryan, S. J.; Bland, D. C.; Anderson, J. E.; Sanford, M. S. *J. Org. Chem.* **2015**, *80*, 12137.
6. Morales-Colón, M. T.; See, Y. Y.; Lee, S. J.; Scott, P. J. H.; Bland, D. C.; Sanford, M. S. *Org. Lett.* **2021**, *23*, 4493.
7. Roger, J.; Royer, S.; Cattey, H.; Savateev, A.; Smaliy, R. V.; Kostyuk, A. N.; Hierso, J.-C. *Eur. J. Inorg. Chem.* **2017**, *2017*, 330.
8. Taylor, N. J.; Emer, E.; Preshlock, S.; Schedler, M.; Tredwell, M.; Verhoog, S.; Mercier, J.; Genicot, C.; Gouverneur, V. *J. Am. Chem. Soc.* **2017**, *139*, 8267.
9. Katoh, T.; Tomata, Y.; Tsukamoto, T.; Nakada, Y. *Tetrahedron Lett*. **2015**, *56*, 6043.
10. Ryan, S. J.; Schimler, S. D.; Bland, D. C.; Sanford, M. S. *Org. Lett.* **2015**, *17*, 1866.
11. Plé, N.; Turck, A.; Heynderickx, A.; Quéguiner, G. *Tetrahedron* 1998, *54*, 4899.
12. Johansen, M. B.; Lindhardt, A. T. *Chem. Commun.* **2018**, *54*, 825.
13. Lacour, M.-A.; Zablocka, M.; Duhayon, C.; Majoral, J.-P.; Taillefer, M. *Adv. Synth. Catal.* **2008**, *350*, 2677.
14. Wood, A. B.; Kincaid, J. R. A.; Lipshutz, B. H. *Green Chem.* **2022**, *24*, 2853.



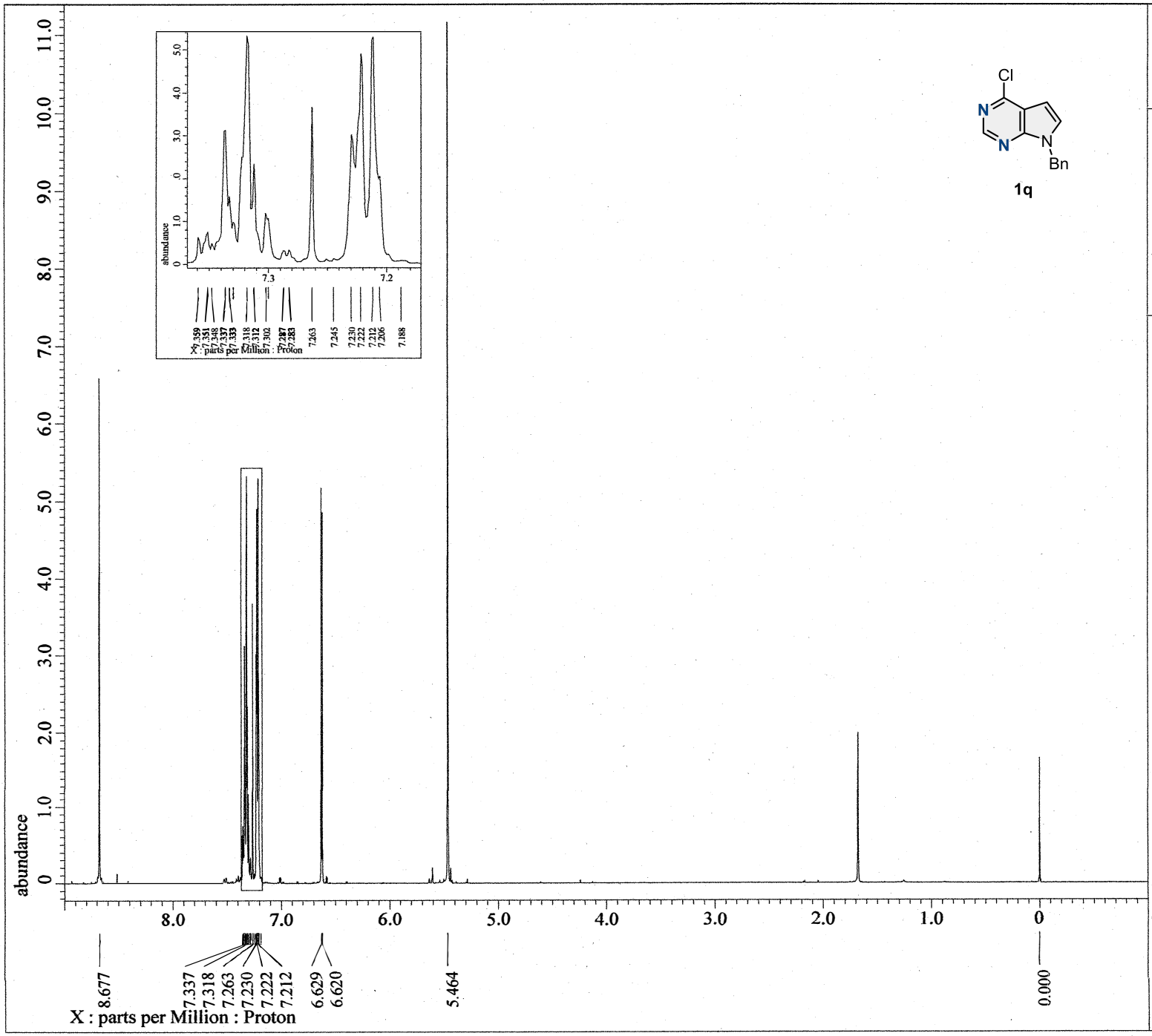

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
ma chiephase
ppm

Derived from: MKN278-pure Proton-1-1.jdf
```

Filename	= MKN278-pure_Proton-1-2
Author	= element
Experiment	= proton_a utojxp
Sa mple_Id	= MKN278-pu re
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 18-JAN-2024 10:47:11
Revision_Time	= 15-JUN-2024 12:17:08
Comment	= single_pulse
Data_Forma t	= 1D COMPLEX
Dim_Size	= 13107
X_Doma in	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.2982153[T] (400[MHz]
X_Acq_Duration	= 2.20725248[s]
X_Domain	= Proton
X_Freq	= 395.88430144[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolu tion	= 0.45305193[Hz]
X_Sweep	= 7.42280285[kHz]
X_Sweep_Clipped	= 5.93824228[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 395.88430144[MHz]
Tri_Offset	= 5[ppm]
Bl ankin	= 2.0[us]
Cli pped	= FALSE
Scans	= 8
Tota lSca ns	= 8
Rela xa tion_De y	= 5[s]
Recvr_Gain	= 56
Temp_Get	= 19.1[dC]
X_90_Width	= 6.34[us]
X_Acq_Time	= 2.20725248[s]
X_Angle	= 45[deg]
X_Atn	= 5[dB]
X_Pulse	= 3.17[u s]
I rr_Mode	= Off
Tri_Mode	= Off
Da ne_Loop	= 500
Dante_Presa t	= FALSE
Decimation_Rate	= 0
Initia lWait	= 1[s]
Phase	= {0, 90, 270, 180, 180,



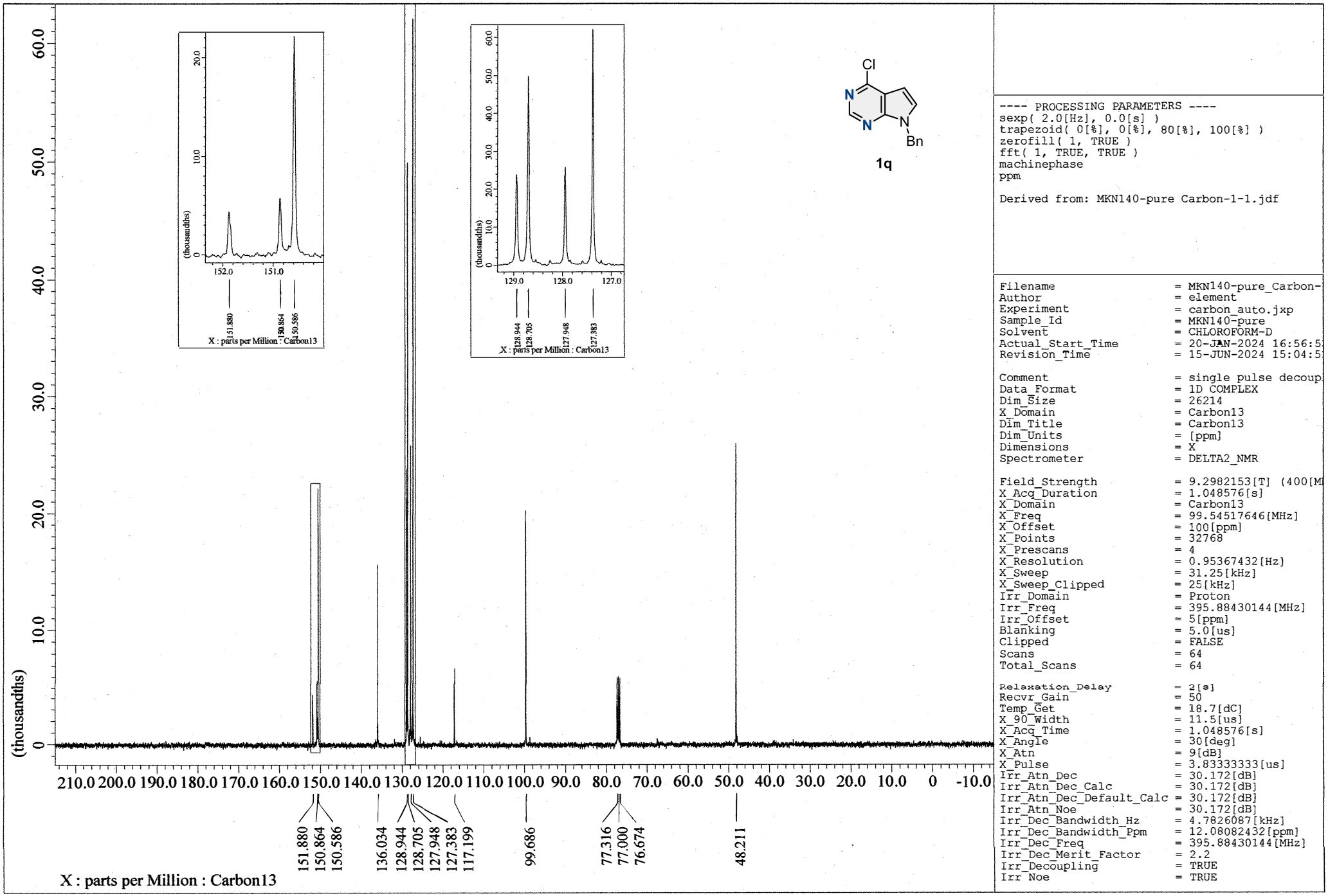

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: MKN278-pure Carbon-1-1.jdf
```

Filename	= MKN278-pure_Carbon-
Author	= element
Experiment	= carbon_auto.jxp
Sample_Id	= MKN278-pure
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 18-JAN-2024 11:01:3
Revision_Time	= 15-JUN-2024 14:30:4
Comment	= single pulse decoup
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.2982153[T] (400[M
X_Acq_Duration	= 1.048576[s]
X_Domain	= Carbon13
X_Freq	= 99.54517646[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.95367432[Hz]
X_Sweep	= 31.25[kHz]
X_Sweep_Clipped	= 25[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 5.0[us]
Clipped	= FALSE
Scans	= 128
Total_Scans	= 128
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 18.6[dC]
X_90_Width	= 11.5[us]
X_Acq_Time	= 1.048576[s]
X_Angle	= 30[deg]
X_Atn	= 9[dB]
X_Pulse	= 3.83333333[us]
Irr_Atn_Dec	= 30.172[dB]
Irr_Atn_Dec_Calc	= 30.172[dB]
Irr_Atn_Dec_Default_Calc	= 30.172[dB]
Irr_Atn_Noe	= 30.172[dB]
Irr_Dec_Bandwidth_Hz	= 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.08082432[ppm]
Irr_Dec_Freq	= 395.88430144[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE



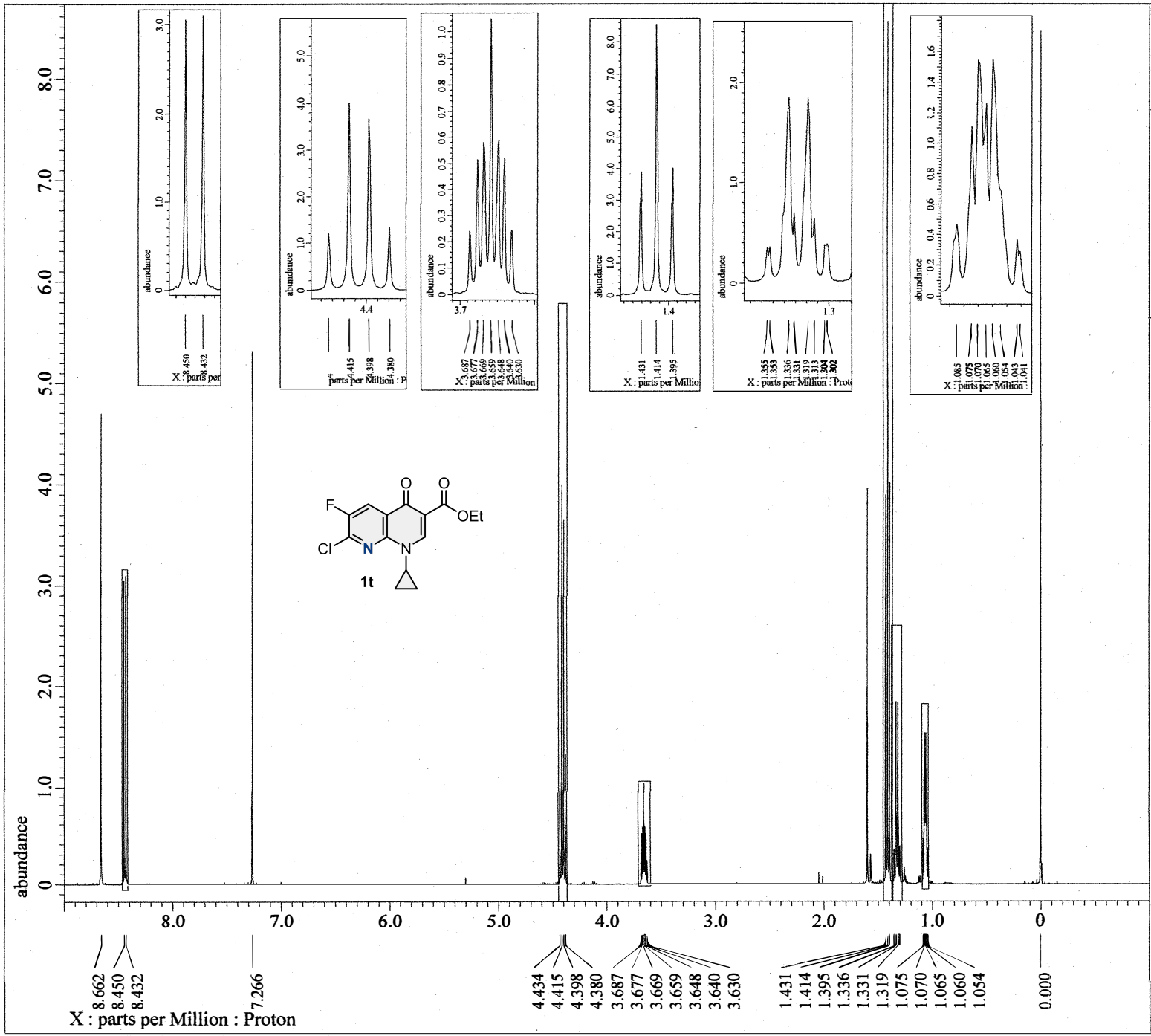

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: MKN140-pure2 Proton-1-1.jdf
```

Filename	= MKN140-pure2_Proton-1-2.jd
Author	= element
Experiment	= proton.jxp
Sample_Id	= MKN140-pure2
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 7-SEP-2023 13:04:21
Revision_Time	= 15-JUN-2024 14:48:25
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.4073814[T] (400[MHz])
X_Acq_Duration	= 2.18103808[s]
X_Domain	= 1H
X_Freq	= 400.53219825[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45849727[Hz]
X_Sweep	= 7.51201923[kHz]
X_Sweep_Clipped	= 6.00961538[kHz]
Irr_Domain	= Proton
Irr_Freq	= 400.53219825[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 400.53219825[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 40
Temp_Get	= 19.5[dC]
X_90_Width	= 6.7[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]



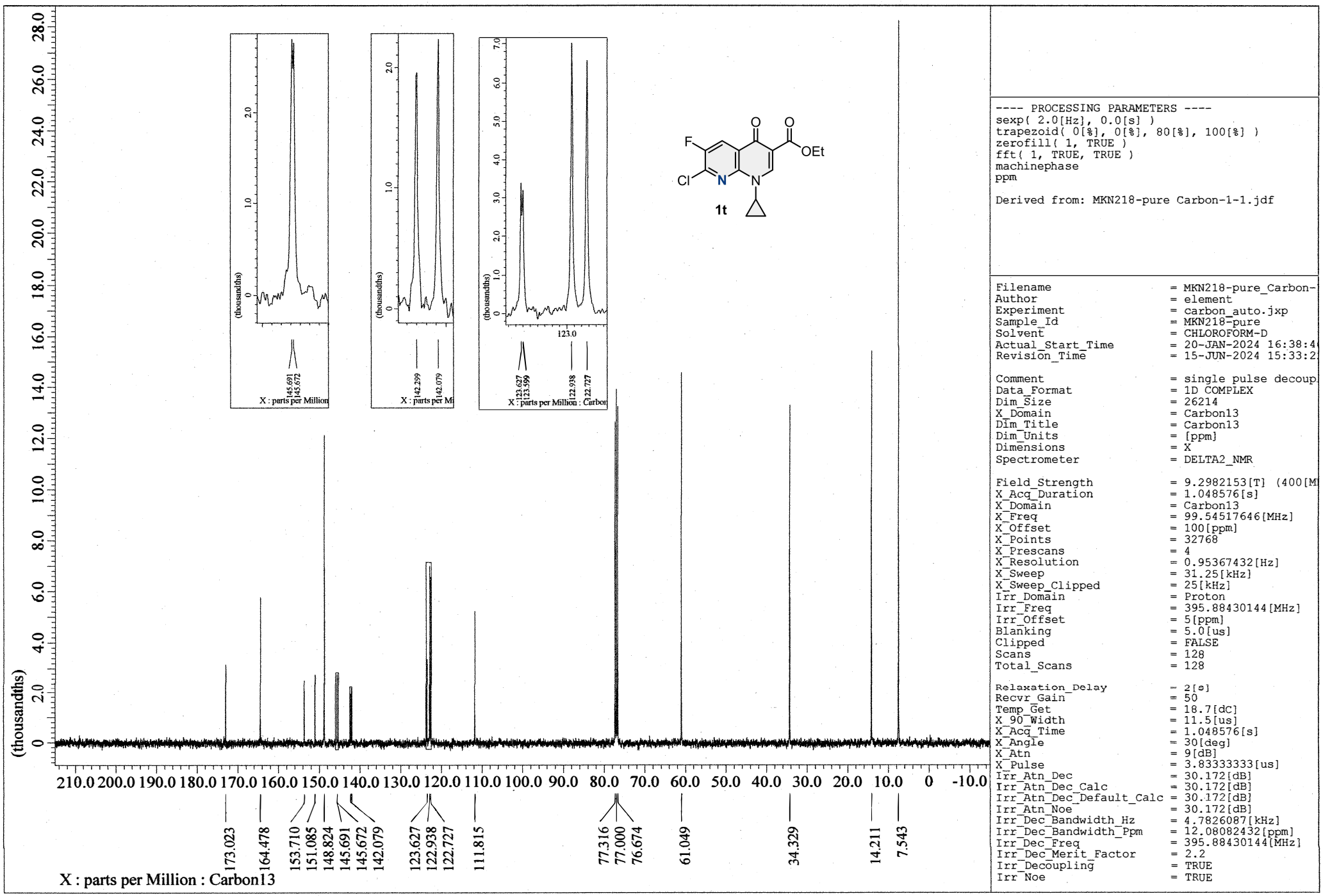

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: MKN140-pure Carbon-1-1.jdf
```

Filename	= MKN140-pure_Carbon-
Author	= element
Experiment	= carbon_auto.jxp
Sample_Id	= MKN140-pure
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 20-JAN-2024 16:56:5
Revision_Time	= 15-JUN-2024 15:04:5
Comment	= single pulse decoup
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.2982153[T] (400[M
X_Acq_Duration	= 1.048576[s]
X_Domain	= Carbon13
X_Freq	= 99.54517646[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.95367432[Hz]
X_Sweep	= 31.25[kHz]
X_Sweep_Clipped	= 25[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 5.0[us]
Clipped	= FALSE
Scans	= 64
Total_Scans	= 64
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 18.7[dC]
X_90_Width	= 11.5[us]
X_Acq_Time	= 1.048576[s]
X_Angle	= 30[deg]
X_Atn	= 9[dB]
X_Pulse	= 3.83333333[us]
Irr_Atn_Dec	= 30.172[dB]
Irr_Atn_Dec_Calc	= 30.172[dB]
Irr_Atn_Dec_Default_Calc	= 30.172[dB]
Irr_Atn_Noe	= 30.172[dB]
Irr_Dec_Bandwidth_Hz	= 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.08082432[ppm]
Irr_Dec_Freq	= 395.88430144[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE



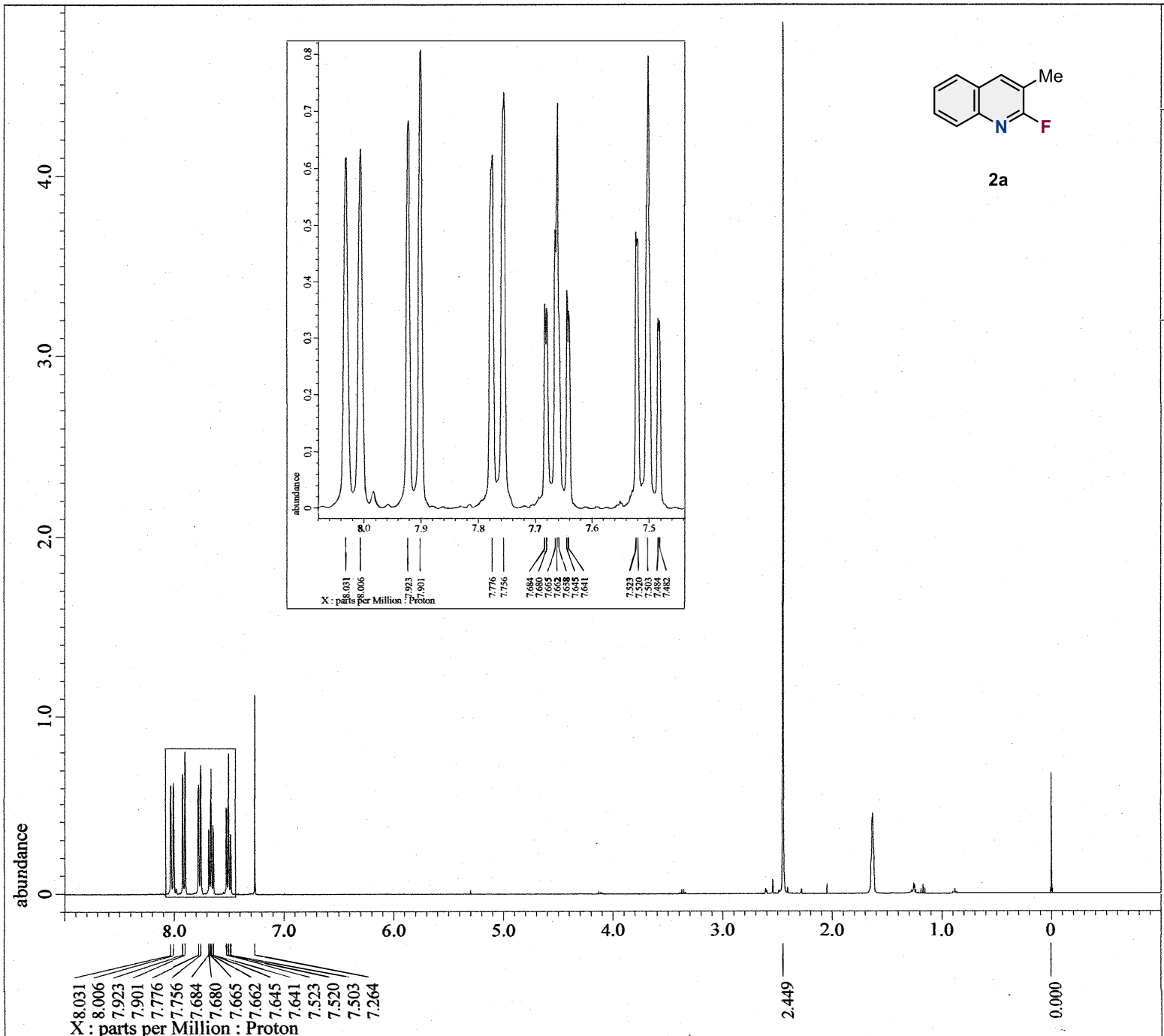

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: MKN218-pure2 Proton-1-1.jdf
```

Filename	= MKN218-pure2_Proton-1-2.jd
Author	= element
Experiment	= proton.jxp
Sample_Id	= MKN218-pure2
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 16-NOV-2023 12:42:18
Revision_Time	= 15-JUN-2024 15:13:57
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	= 46
Temp_Get	= 19.7[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 ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: MKN218-pure Carbon-1-1.jdf
```

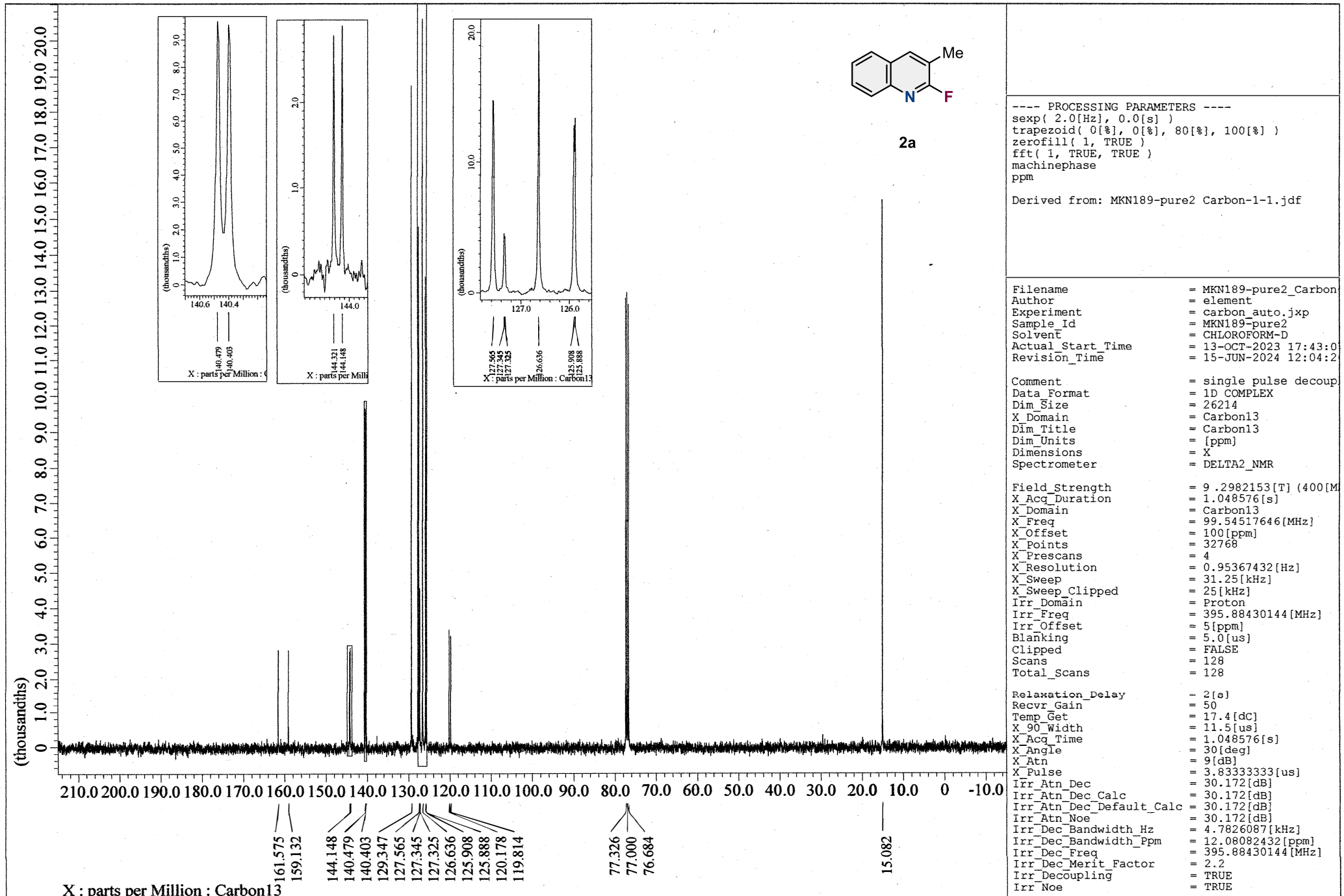
Filename	= MKN218-pure_Carbon-
Author	= element
Experiment	= carbon_auto.jxp
Sample_Id	= MKN218-pure
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 20-JAN-2024 16:38:4
Revision_Time	= 15-JUN-2024 15:33:2
Comment	= single pulse decoup
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.2982153[T] (400[M
X_Acq_Duration	= 1.048576[s]
X_Domain	= Carbon13
X_Freq	= 99.54517646[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.95367432[Hz]
X_Sweep	= 31.25[kHz]
X_Sweep_Clipped	= 25[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 5.0[us]
Clipped	= FALSE
Scans	= 128
Total_Scans	= 128
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 18.7[dC]
X_90_Width	= 11.5[us]
X_Acq_Time	= 1.048576[s]
X_Angle	= 30[deg]
X_Atn	= 9[dB]
X_Pulse	= 3.83333333[us]
Irr_Atn_Dec	= 30.172[dB]
Irr_Atn_Dec_Calc	= 30.172[dB]
Irr_Atn_Dec_Default_Calc	= 30.172[dB]
Irr_Atn_Noe	= 30.172[dB]
Irr_Dec_Bandwidth_Hz	= 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.08082432[ppm]
Irr_Dec_Freq	= 395.88430144[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr Noe	= TRUE



2a

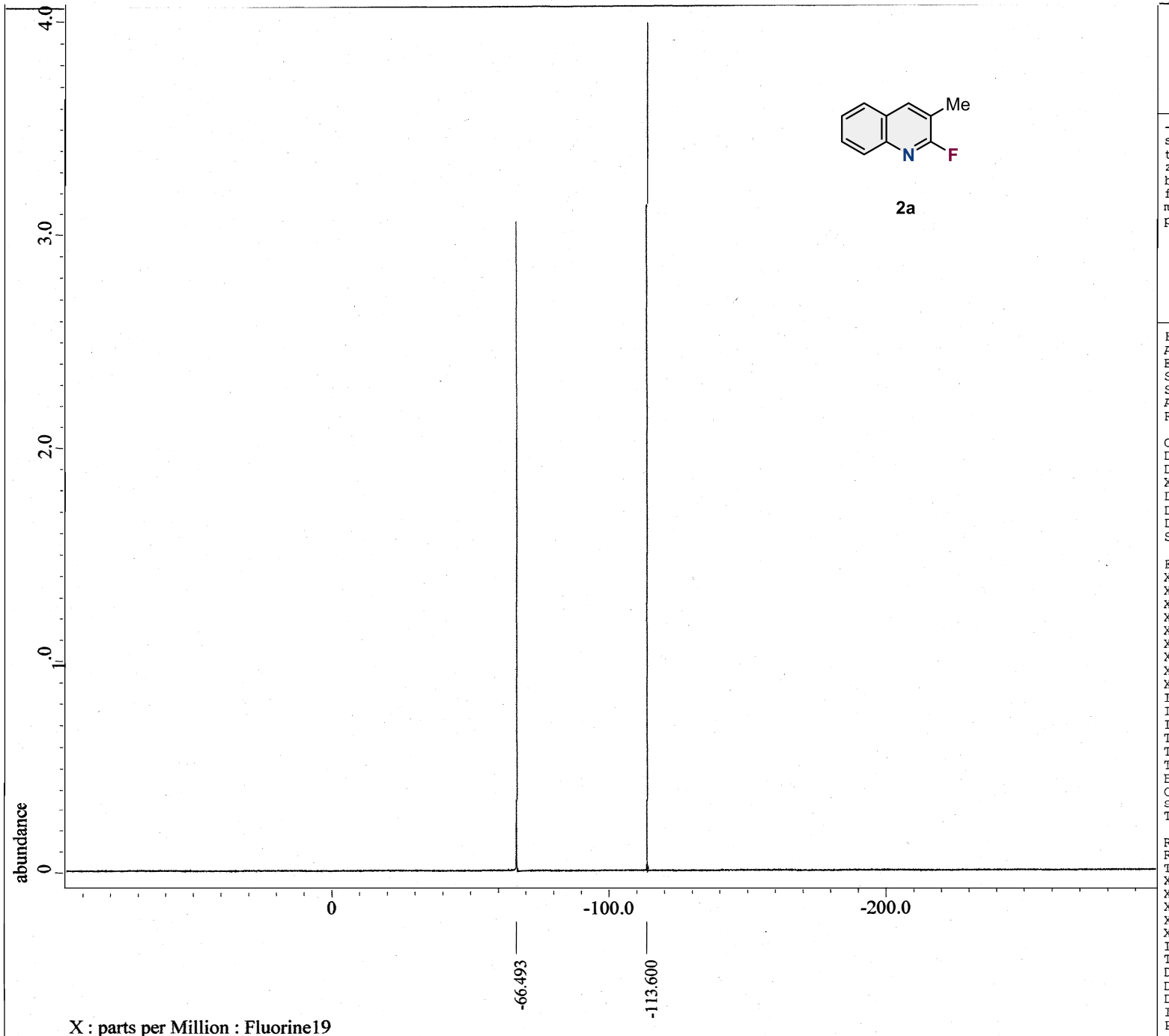
```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: MKN189-pure2 Proton-1-1.jdf
```

Filename	= MKN189-pure2_Proton-1-
Author	= element
Experiment	= proton_auto.jxp
Sample_Id	= MKN189-pure2
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 2-OCT-2023 14:48:28
Revision_Time	= 15-JUN-2024 11:12:55
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	= 9.2982153[T] (400[MHz]
X_Acq_Duration	= 2.20725248[s]
X_Domain	= Proton
X_Freq	= 395.88430144[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45305193[Hz]
X_Sweep	= 7.42280285[kHz]
X_Sweep_Clipped	= 5.93824228[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 395.88430144[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2.0[us]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 56
Temp_Get	= 18.2[dC]
X_90_Width	= 6.34[us]
X_Acq_Time	= 2.20725248[s]
X_Angle	= 45[deg]
X_Atn	= 5[dB]
X_Pulse	= 3.17[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 500
Dante_Presat	= FALSE
Decimation_Rate	= 0
Initial_Wait	= 1[s]
Phase	= {0, 90, 270, 180, 180,



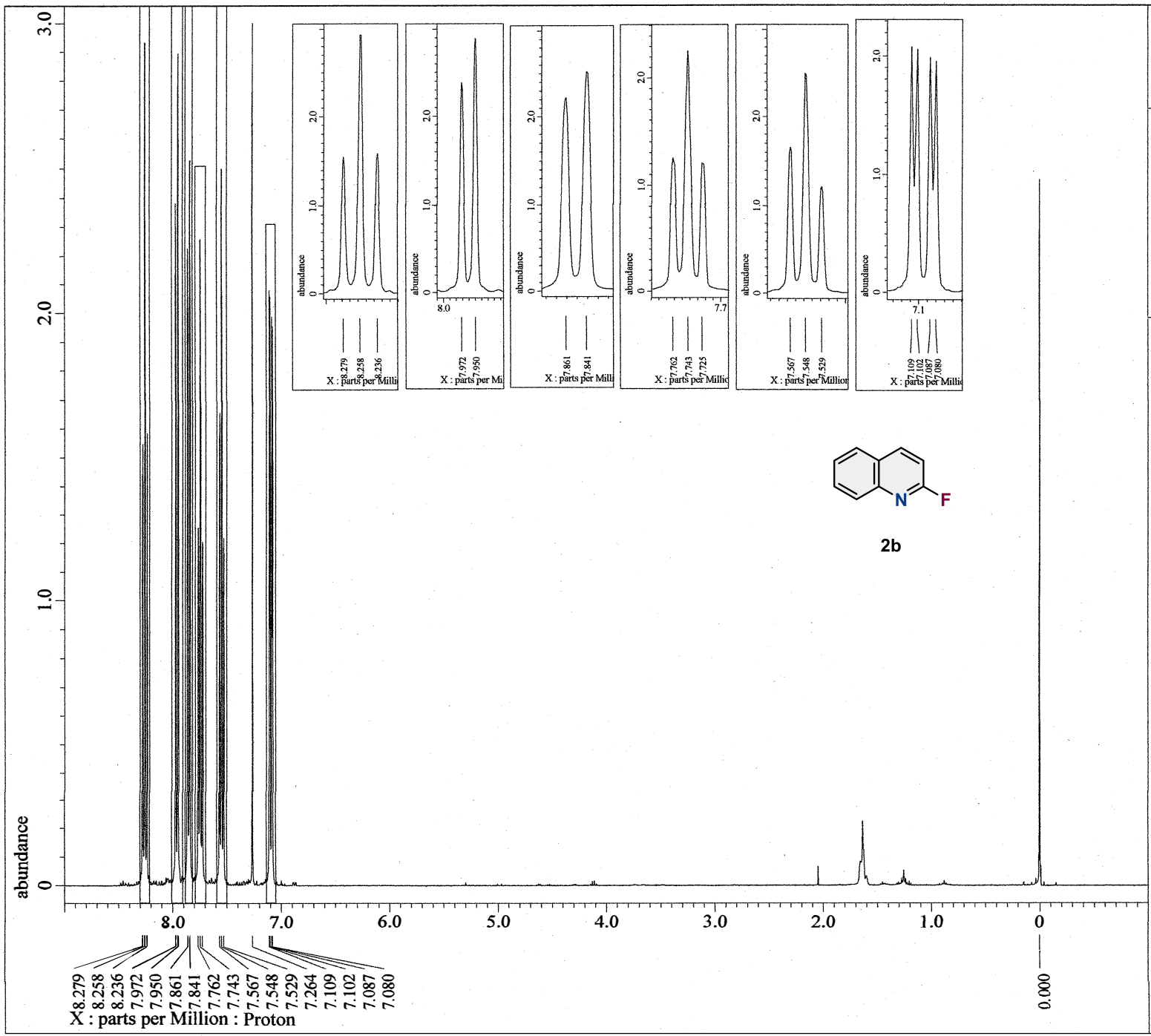

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: MKN189-pure2 Carbon-1-1.jdf
```

Filename	= MKN189-pure2_Carbon
Author	= element
Experiment	= carbon_auto.jxp
Sample_Id	= MKN189-pure2
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 13-OCT-2023 17:43:0
Revision_Time	= 15-JUN-2024 12:04:2
Comment	= single pulse decoup
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9 .2982153[T] (400[M
X_Acq_Duration	= 1.048576[s]
X_Domain	= Carbon13
X_Freq	= 99.54517646[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.95367432[Hz]
X_Sweep	= 31.25[kHz]
X_Sweep_Clipped	= 25[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 5.0[us]
Clipped	= FALSE
Scans	= 128
Total_Scans	= 128
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 17.4[dC]
X_90_Width	= 11.5[us]
X_Acq_Time	= 1.048576[s]
X_Angle	= 30[deg]
X_Atn	= 9[dB]
X_Pulse	= 3.83333333[us]
Irr_Atn_Dec	= 30.172[dB]
Irr_Atn_Dec_Calc	= 30.172[dB]
Irr_Atn_Dec_Default_Calc	= 30.172[dB]
Irr_Atn_Noe	= 30.172[dB]
Irr_Dec_Bandwidth_Hz	= 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.08082432[ppm]
Irr_Dec_Freq	= 395.88430144[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE




```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
blip( 16, 64, 30 )
fft( 1, TRUE, TRUE )
machineph ase
ppm
```

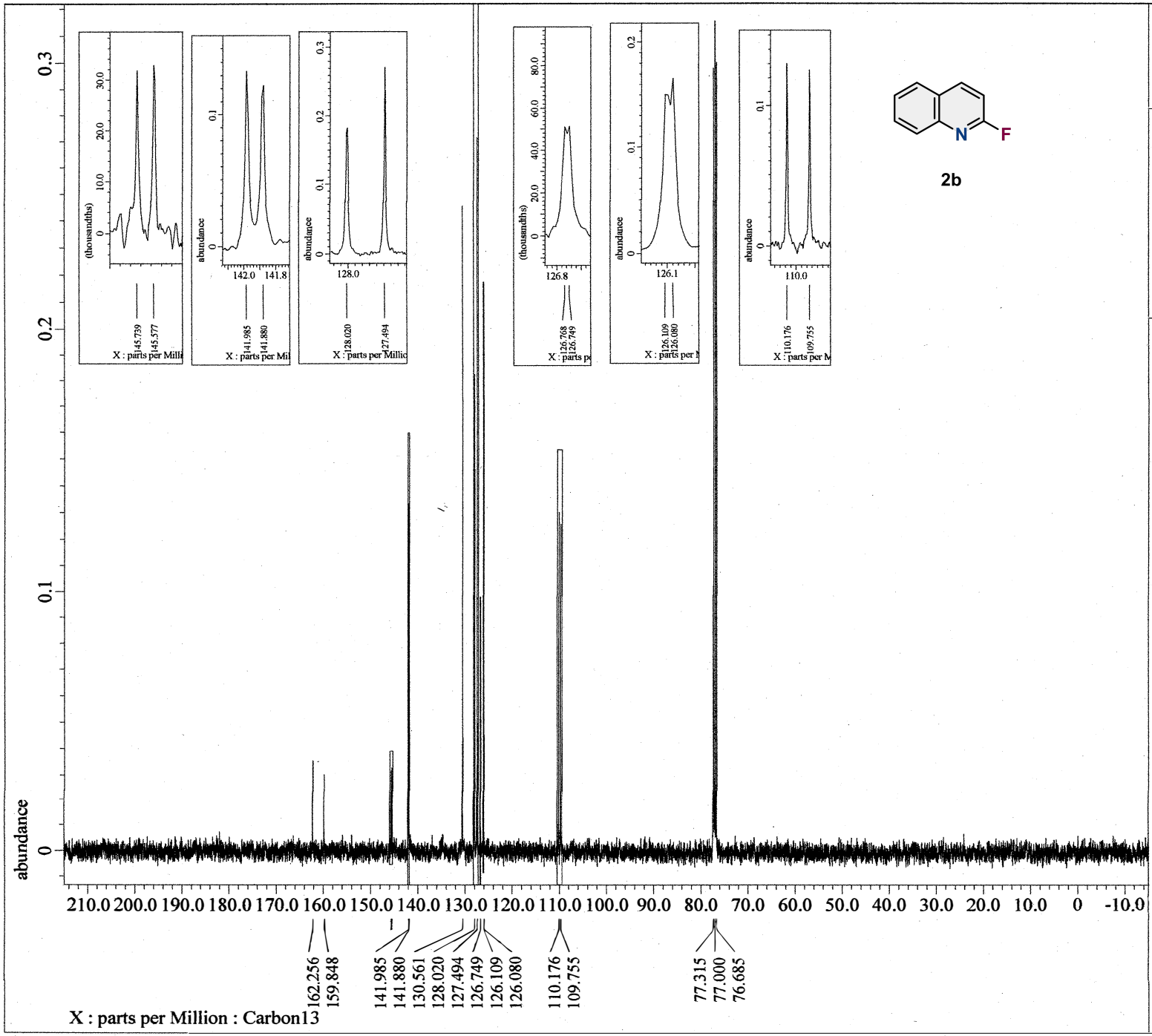
Filename	= MKN189-pure2_int_singl
Author	= element
Experiment	= single_pulse.jxp
Sample_Id	= MKN189-pure2_int
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 14-OCT-2023 11:09:07
Revision_Time	= 24-JAN-2024 11:39:29
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Fluorine19
Dim_Title	= Fluorine19
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.2982153[T] (400[MHz]
X_Acq_Duration	= 89.12896[ms]
X_Domain	= Fluorine19
X_Freq	= 372.50336686[MHz]
X_Offset	= -100[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 11.21969784[Hz]
X_Sweep	= 183.82352941[kHz]
X_Sweep_Clipped	= 147.05882353[kHz]
Irr_Domain	= Fluorine19
Irr_Freq	= 372.50336686[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Fluorine19
Tri_Freq	= 372.50336686[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2.0[us]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 56
Temp_Get	= 18.9[dC]
X_90_Width	= 8.03[us]
X_Acq_Time	= 89.12896[ms]
X_Angle	= 45[deg]
X_Atn	= 5[dB]
X_Pulse	= 4.015[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 500
Dante_Presat	= FALSE
Decimation_Rate	= 0
Initial_Wait	= 1[s]
Phase	= {0, 90, 270, 180, 180,



2b

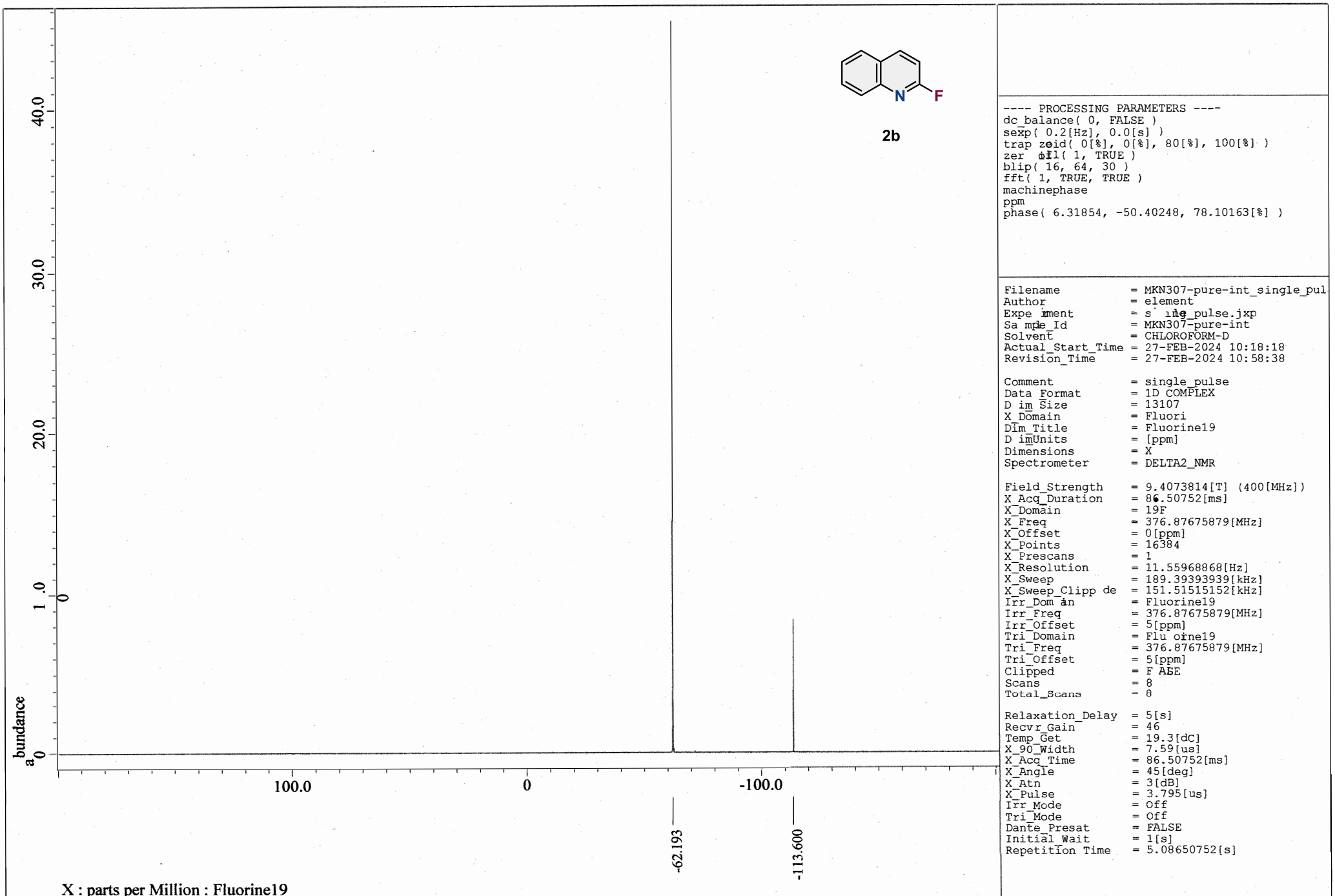
```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: MKN307-pure Proton-1-1.jdf
```

Filename	= MKN307-pure_Proton-1-2.jdf
Author	= element
Experiment	= proton.jxp
Sample_Id	= MKN307-pure
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 27-FEB-2024 10:07:26
Revision_Time	= 17-JUN-2024 13:15:45
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	= 40
Temp_Get	= 19.6[dC]
X_90_Width	= 6.7[us]
X_Acq_Time	= 2.18103808[s]
X_Angle	= 45[deg]
X_Atn	= 0.8[dB]
X_Pulse	= 3.35[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.18103808[s]



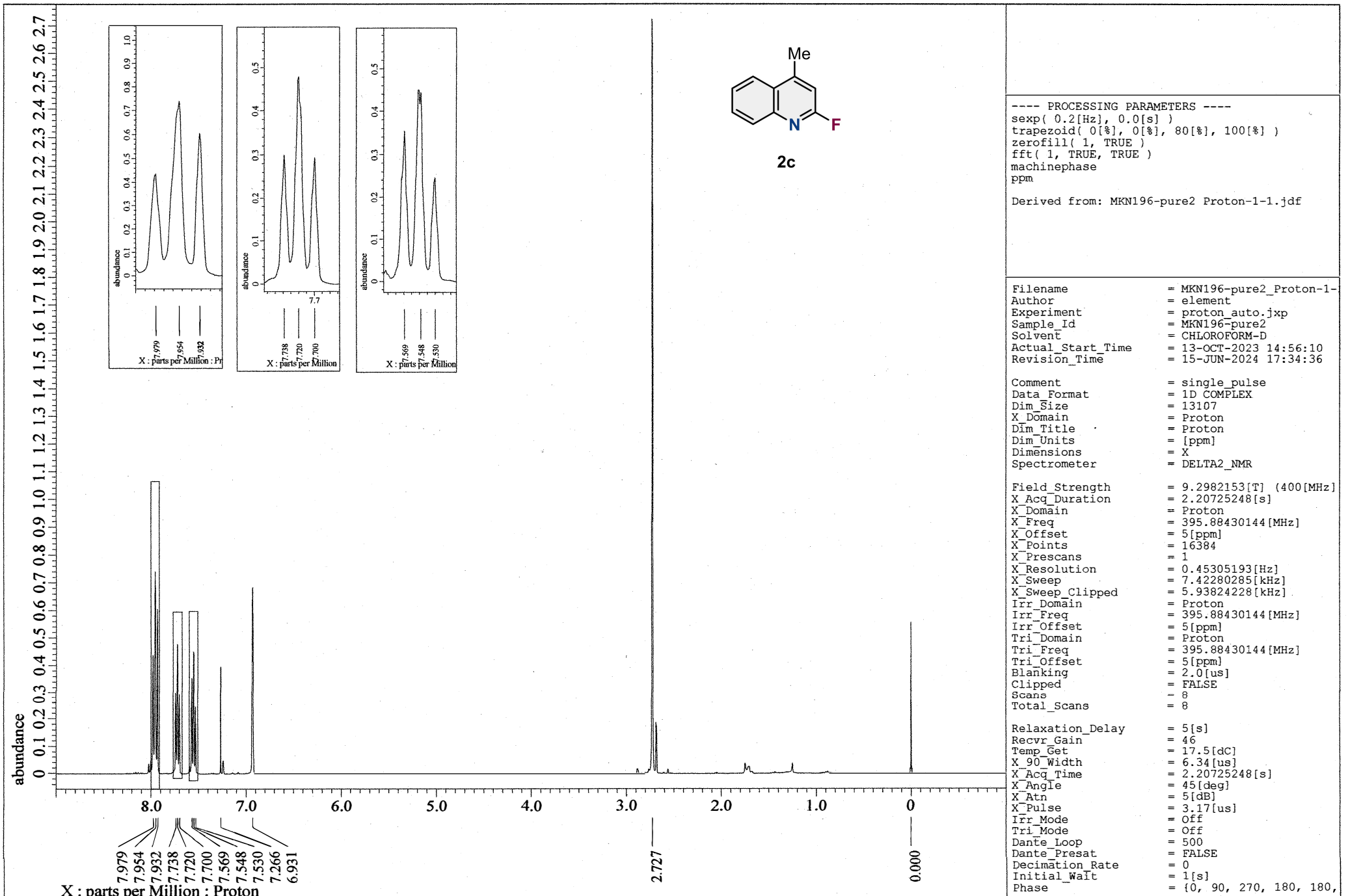

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: MKN307-pure Carbon-1-1.jdf
```

```
Filename            = MKN307-pure_Carbon-1-3.jdf
Author              = element
Experiment          = carbon.jxp
Sample_Id           = MKN307-pure
Solvent             = CHLOROFORM-D
Actual_Start_Time   = 27-FEB-2024 11:08:31
Revision_Time       = 17-JUN-2024 13:30:42

Comment             = single pulse decoupled gat
Data_Format         = 1D COMPLEX
Dim_Size            = 26214
X_Domain            = Carbon
Dim_Title           = Carbon13
Dim_Units           = [ppm]
Dimensions          = X
Site                = JNM-ECS400
Spectrometer        = DELTA2_NMR

Field_Strength      = 9.37221[T] (400[MHz])
X_Acq_Duration      = 1.04333312[s]
X_Domain            = 13C
X_Freq              = 100.33735165[MHz]
X_Offset            = 100.0[ppm]
X_Points            = 32768
X_Prescans          = 4
X_Resolution        = 0.95846665[Hz]
X_Sweep             = 31.40703518[kHz]
X_Sweep_Clipped     = 25.12562814[kHz]
Irr_Domain          = Proton
Irr_Freq            = 399.03472754[MHz]
Irr_Offset          = 5.0[ppm]
Clipped             = FALSE
Scans               = 128
Total_Scans         = 128

Relaxation_Delay    = 2[s]
Recvr_Gain          = 50
Temp_Get            = 18.6[dC]
X_90_Width          = 10.9[us]
X_Acq_Time          = 1.04333312[s]
X_Angle             = 30[deg]
X_Atn               = 5.4[dB]
X_Pulse             = 3.63333333[us]
Irr_Atn_Dec         = 25.823[dB]
Irr_Atn_Noe         = 25.823[dB]
Irr_Noise           = WALTZ
Irr_Pwidth          = 0.115[ms]
Decoupling          = TRUE
Initial_Wait        = 1[s]
Noe                 = TRUE
Noe_Time            = 2[s]
Repetition Time     = 3.04333312[s]
```



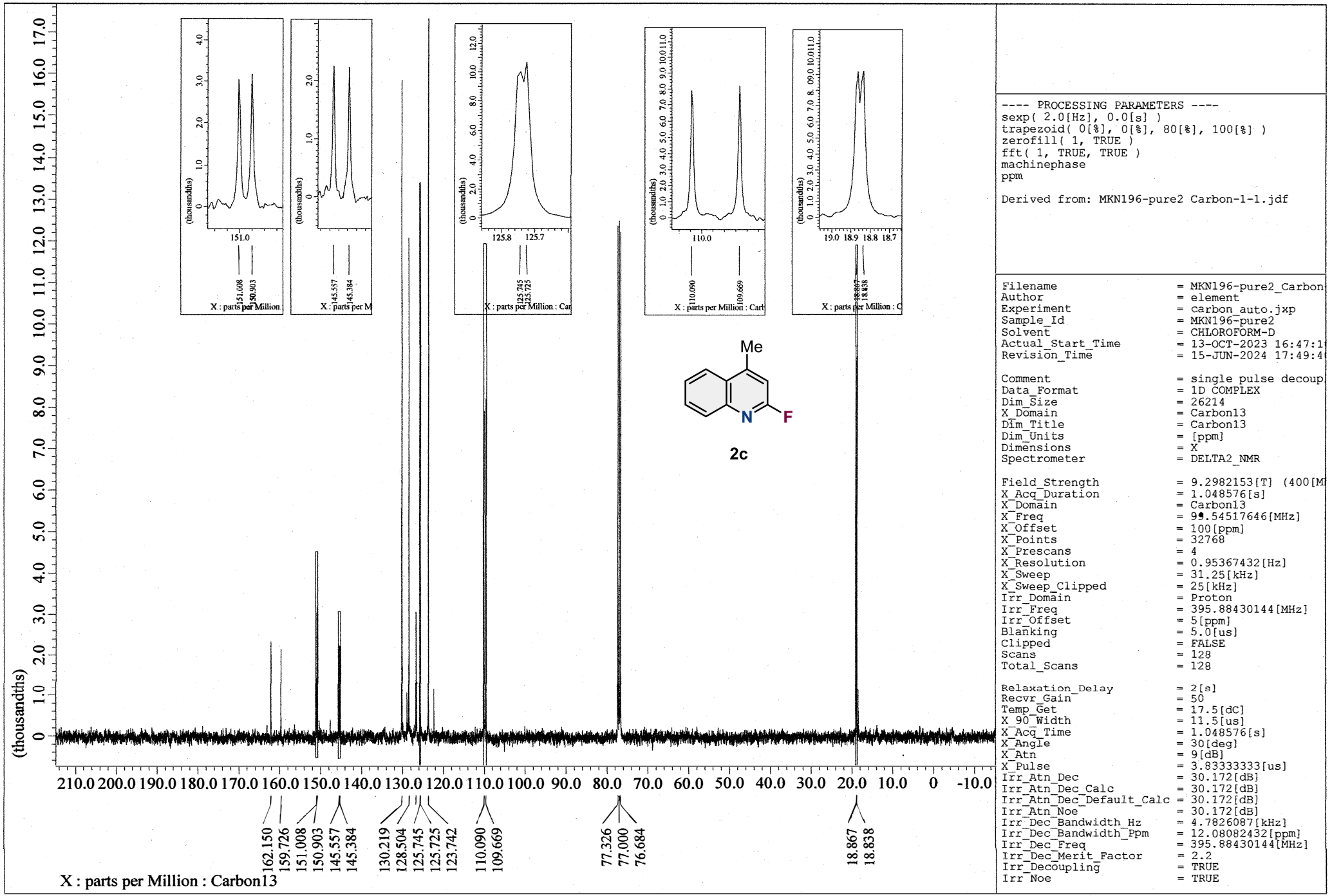

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trap zeid( 0[%], 0[%], 80[%], 100[%] )
zer  oil( 1, TRUE )
blip( 16, 64, 30 )
fft( 1, TRUE, TRUE )
machinephase
ppm
phase( 6.31854, -50.40248, 78.10163[%] )
```

```
Filename            = MKN307-pure-int_single_pul
Author              = element
Expe iment          = s  ingle_pulse.jxp
Sa mple_Id          = MKN307-pure-int
Solvent             = CHLOROFORM-D
Actual_Start_Time   = 27-FEB-2024 10:18:18
Revision_Time       = 27-FEB-2024 10:58:38

Comment             = single_pulse
Data Format         = 1D COMPLEX
D im Size           = 13107
X_Domain            = Fluori
Dim_Title           = Fluorine19
D imUnits           = [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_Clipp de    = 151.51515152[kHz]
Irr_Dom ain         = Fluorine19
Irr_Freq            = 376.87675879[MHz]
Irr_Offset          = 5[ppm]
Tri_Domain          = Flu orne19
Tri_Freq            = 376.87675879[MHz]
Tri_Offset          = 5[ppm]
Clipped             = F ALSE
Scans               = 8
Total_Scans         = 8

Relaxation_Delay    = 5[s]
Recvr_Gain          = 46
Temp_Get            = 19.3[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]
```



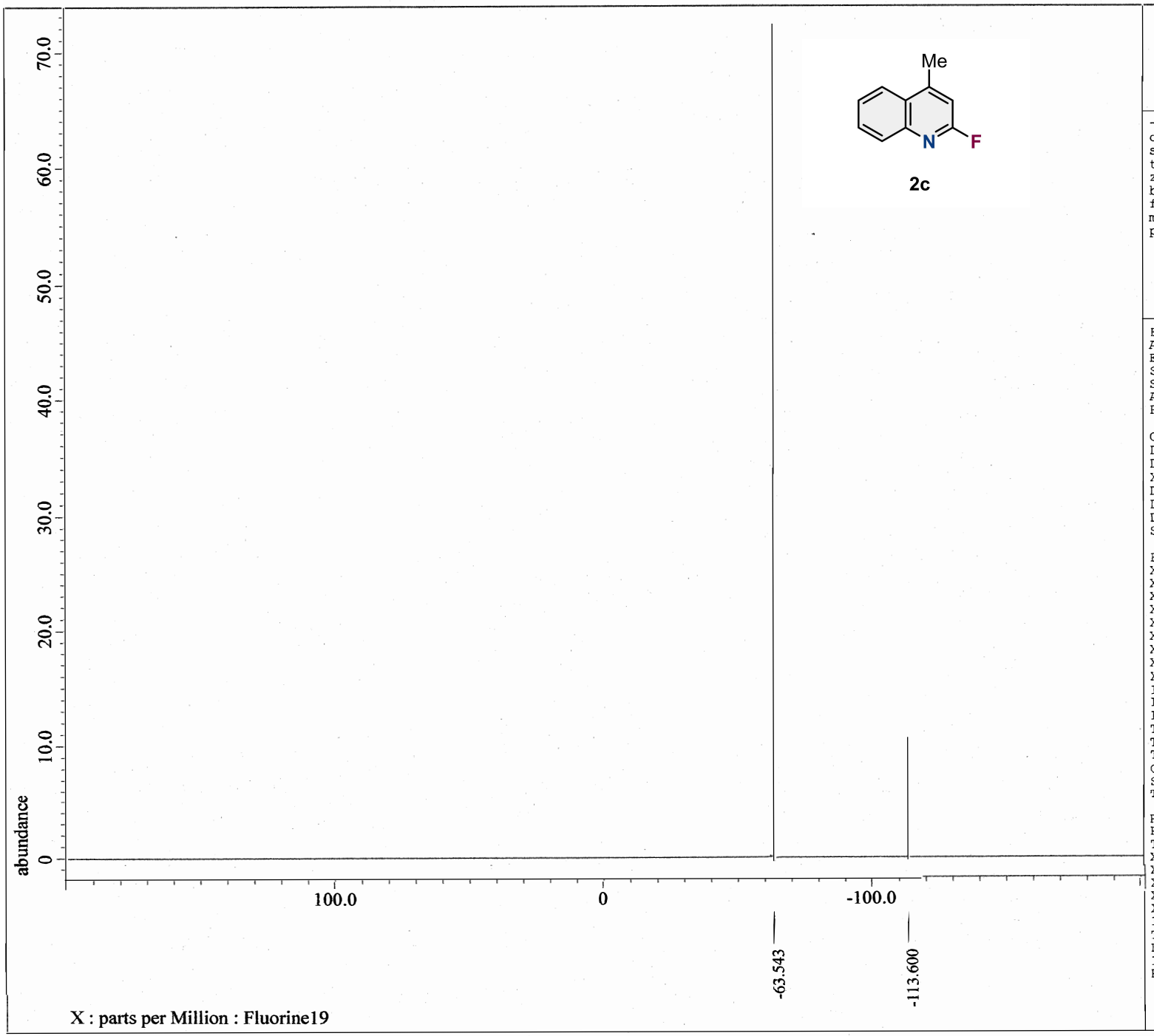

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: MKN196-pure2 Proton-1-1.jdf
```

Filename	= MKN196-pure2_Proton-1-
Author	= element
Experiment	= proton_auto.jxp
Sample_Id	= MKN196-pure2
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 13-OCT-2023 14:56:10
Revision_Time	= 15-JUN-2024 17:34:36
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.2982153[T] (400[MHz]
X_Acq_Duration	= 2.20725248[s]
X_Domain	= Proton
X_Freq	= 395.88430144[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45305193[Hz]
X_Sweep	= 7.42280285[kHz]
X_Sweep_Clipped	= 5.93824228[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 395.88430144[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2.0[us]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 46
Temp_Get	= 17.5[dC]
X_90_Width	= 6.34[us]
X_Acq_Time	= 2.20725248[s]
X_Angle	= 45[deg]
X_Atn	= 5[dB]
X_Pulse	= 3.17[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 500
Dante_Presat	= FALSE
Decimation_Rate	= 0
Initial_Wait	= 1[s]
Phase	= {0, 90, 270, 180, 180,




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

Derived from: MKN196-pure2 Carbon-1-1.jdf
```

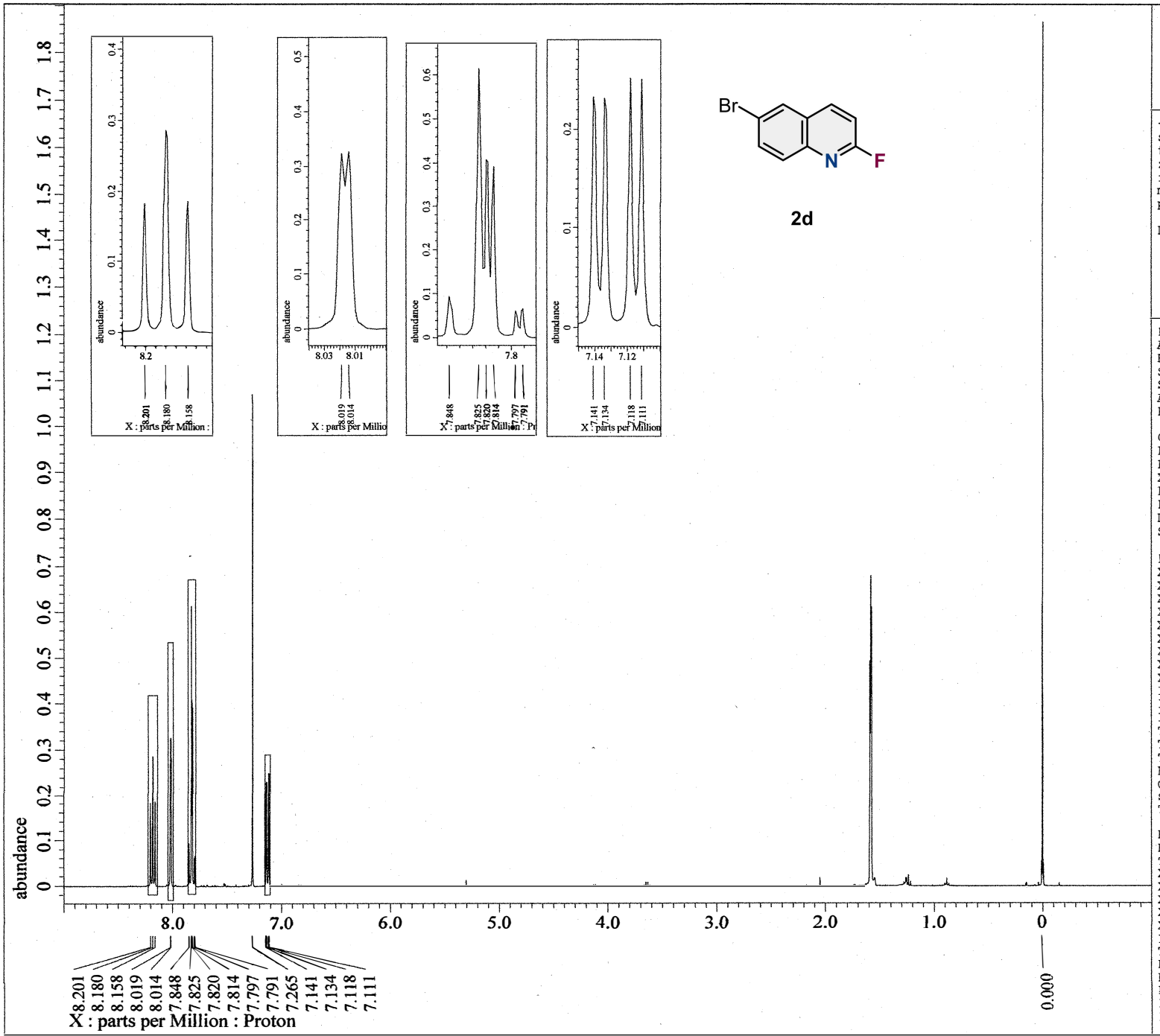
Filename	= MKN196-pure2_Carbon
Author	= element
Experiment	= carbon_auto.jxp
Sample_Id	= MKN196-pure2
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 13-OCT-2023 16:47:1
Revision_Time	= 15-JUN-2024 17:49:4
Comment	= single pulse decoup
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.2982153[T] (400[M
X_Acq_Duration	= 1.048576[s]
X_Domain	= Carbon13
X_Freq	= 99.54517646[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.95367432[Hz]
X_Sweep	= 31.25[kHz]
X_Sweep_Clipped	= 25[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 5.0[us]
Clipped	= FALSE
Scans	= 128
Total_Scans	= 128
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 17.5[dC]
X_90_Width	= 11.5[us]
X_Acq_Time	= 1.048576[s]
X_Angle	= 30[deg]
X_Atn	= 9[dB]
X_Pulse	= 3.83333333[us]
Irr_Atn_Dec	= 30.172[dB]
Irr_Atn_Dec_Calc	= 30.172[dB]
Irr_Atn_Dec_Default_Calc	= 30.172[dB]
Irr_Atn_Noe	= 30.172[dB]
Irr_Dec_Bandwidth_Hz	= 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.08082432[ppm]
Irr_Dec_Freq	= 395.88430144[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE



2c

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
blip( 16, 64, 30 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

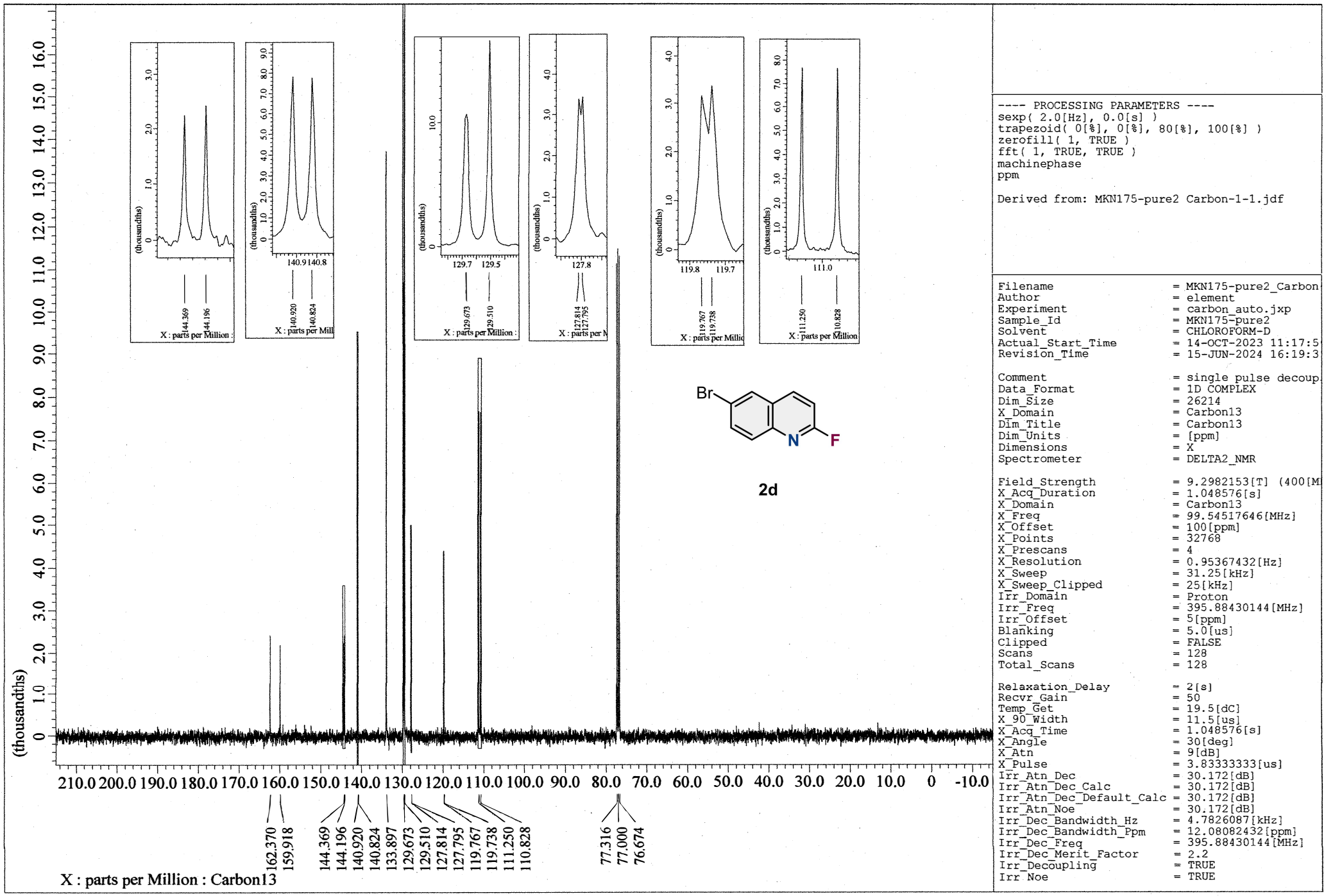
```
Filename            = MKN196-pure_int _singlepul
Author              = element
Experiment          = single_pulse.jxp
Sample_Id           = MKN196-pure_int
Solvent             = CHLOROFORM-D
Actual_Start_Time   = 13-OCT-2023 15:58:23
Revision_Time       = 24-JAN-2024 11:41:04

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          = 44
Temp_Get            = 19.6[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]
```



2d

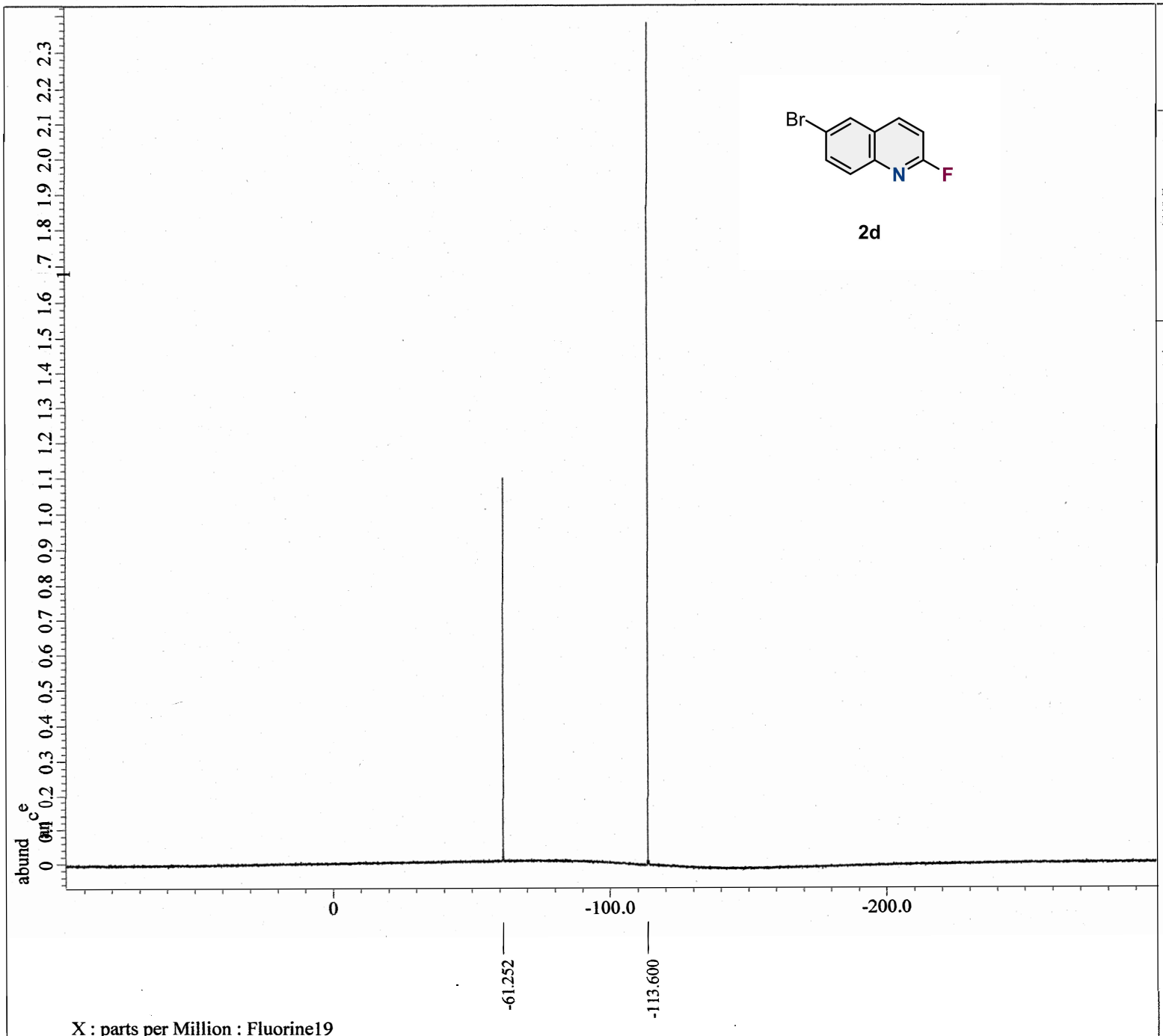
```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: MKN175-pure2 Proton-1-1.jdf
```

Filename	= MKN175-pure2_Proton-1-
Author	= element
Experiment	= proton_auto.jxp
Sample_Id	= MKN175-pure2
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 29-SEP-2023 13:08:04
Revision_Time	= 15-JUN-2024 16:06:04
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	= 9.2982153[T] (400[MHz]
X_Acq_Duration	= 2.20725248[s]
X_Domain	= Proton
X_Freq	= 395.88430144[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45305193[Hz]
X_Sweep	= 7.42280285[kHz]
X_Sweep_Clipped	= 5.93824228[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 395.88430144[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2.0[us]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 56
Temp_Get	= 19[dC]
X_90_Width	= 6.34[us]
X_Acq_Time	= 2.20725248[s]
X_Angle	= 45[deg]
X_Atn	= 5[dB]
X_Pulse	= 3.17[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 500
Dante_Presat	= FALSE
Decimation_Rate	= 0
Initial_Wait	= 1[s]
Phase	= {0, 90, 270, 180, 180,



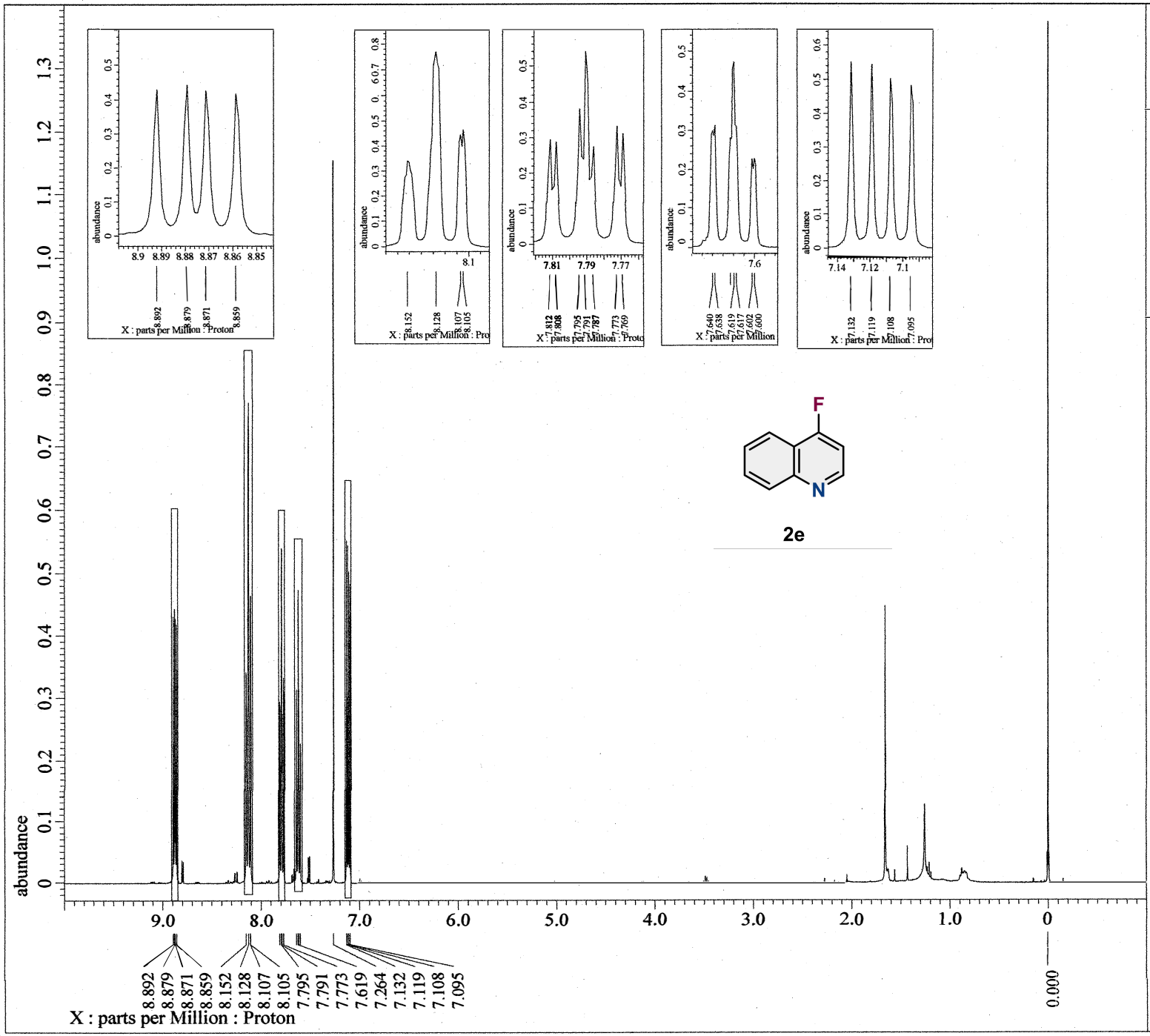

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: MKN175-pure2 Carbon-1-1.jdf
```

Filename	= MKN175-pure2_Carbon
Author	= element
Experiment	= carbon_auto.jxp
Sample_Id	= MKN175-pure2
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 14-OCT-2023 11:17:5
Revision_Time	= 15-JUN-2024 16:19:3
Comment	= single pulse decoup
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.2982153[T] (400[M
X_Acq_Duration	= 1.048576[s]
X_Domain	= Carbon13
X_Freq	= 99.54517646[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.95367432[Hz]
X_Sweep	= 31.25[kHz]
X_Sweep_Clipped	= 25[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 5.0[us]
Clipped	= FALSE
Scans	= 128
Total_Scans	= 128
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 19.5[dC]
X_90_Width	= 11.5[us]
X_Acq_Time	= 1.048576[s]
X_Angle	= 30[deg]
X_Atn	= 9[dB]
X_Pulse	= 3.83333333[us]
Irr_Atn_Dec	= 30.172[dB]
Irr_Atn_Dec_Calc	= 30.172[dB]
Irr_Atn_Dec_Default_Calc	= 30.172[dB]
Irr_Atn_Noe	= 30.172[dB]
Irr_Dec_Bandwidth_Hz	= 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.08082432[ppm]
Irr_Dec_Freq	= 395.88430144[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE



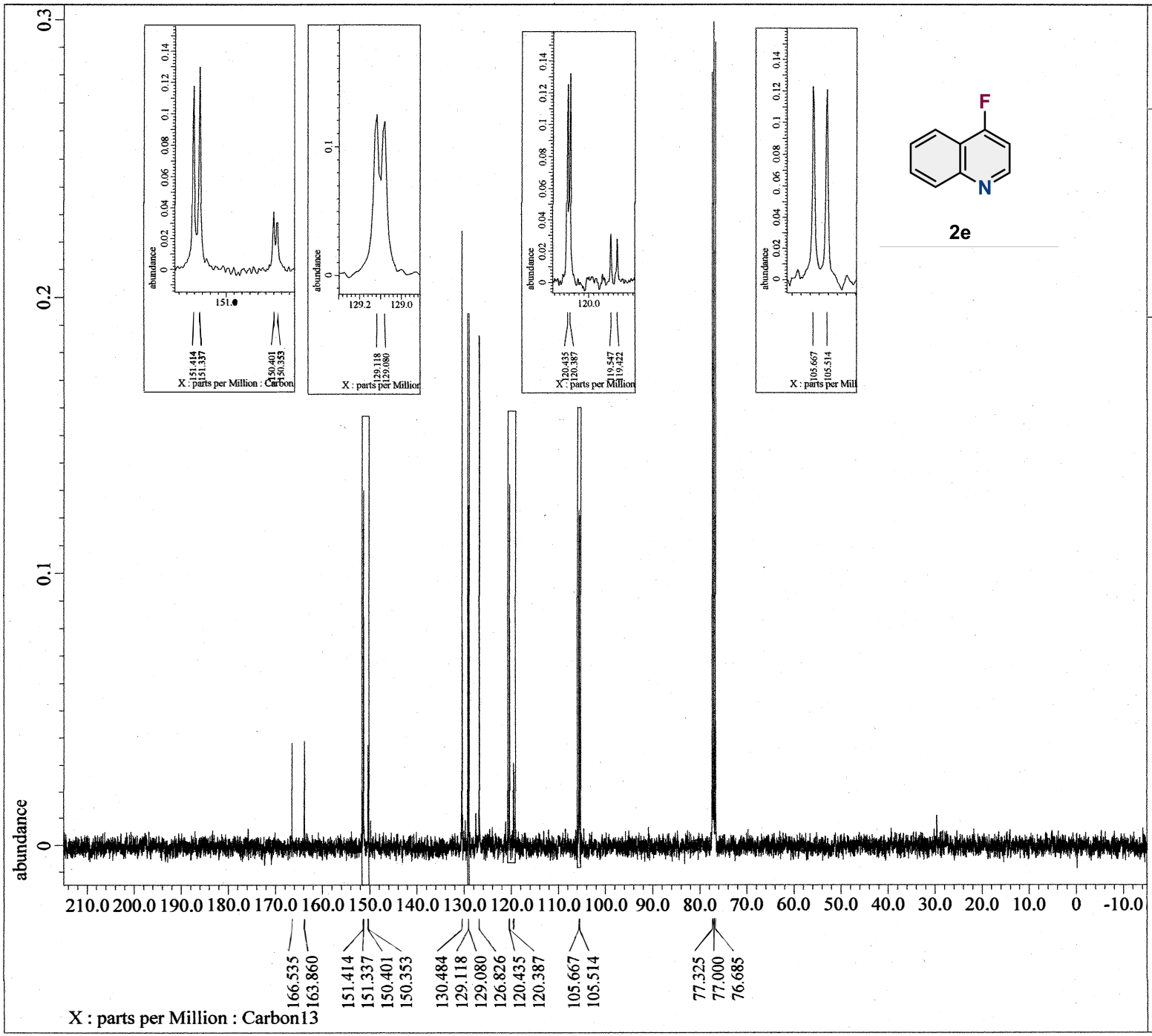

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
phase( 83.95055, 0, 50[%] )
```

```
Filename              = MKN175-pure2_int_singl
Author                = element
Experiment            = single_pulse.jxp
Sample_Id             = MKN175-pure2_int
Solvent               = CHLOROFORM-D
Actual_Start_Time     = 14-OCT-2023 11:13:30
Revision_Time         = 24-JAN-2024 11:35:11

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

Field_Strength        = 9.2982153[T] (400[MHz]
X_Acq_Duration        = 89.12896[ms]
X_Domain              = Fluorine19
X_Freq                = 372.50336686[MHz]
X_Offset              = -100[ppm]
X_Points              = 16384
X_Prescans            = 1
X_Resolution          = 11.21969784[Hz]
X_Sweep               = 183.82352941[kHz]
X_Sweep_Clipped       = 147.05882353[kHz]
Irr_Domain            = Fluorine19
Irr_Freq              = 372.50336686[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Fluorine19
Tri_Freq              = 372.50336686[MHz]
Tri_Offset            = 5[ppm]
Blanking              = 2.0[us]
Clipped               = FALSE
Scans                 = 8
Total_Scans           = 8

Relaxation_Delay      = 5[s]
Recvr_Gain            = 56
Temp_Get              = 19.1[dC]
X_90_Width            = 8.03[us]
X_Acq_Time            = 89.12896[ms]
X_Angle               = 45[deg]
X_Atn                 = 5[dB]
X_Pulse               = 4.015[us]
Irr_Mode              = Off
Tri_Mode              = Off
Dante_Loop            = 500
Dante_Presat          = FALSE
Decimation_Rate       = 0
Initial_Wait          = 1[s]
Phase                 = {0, 90, 270, 180, 180,
```



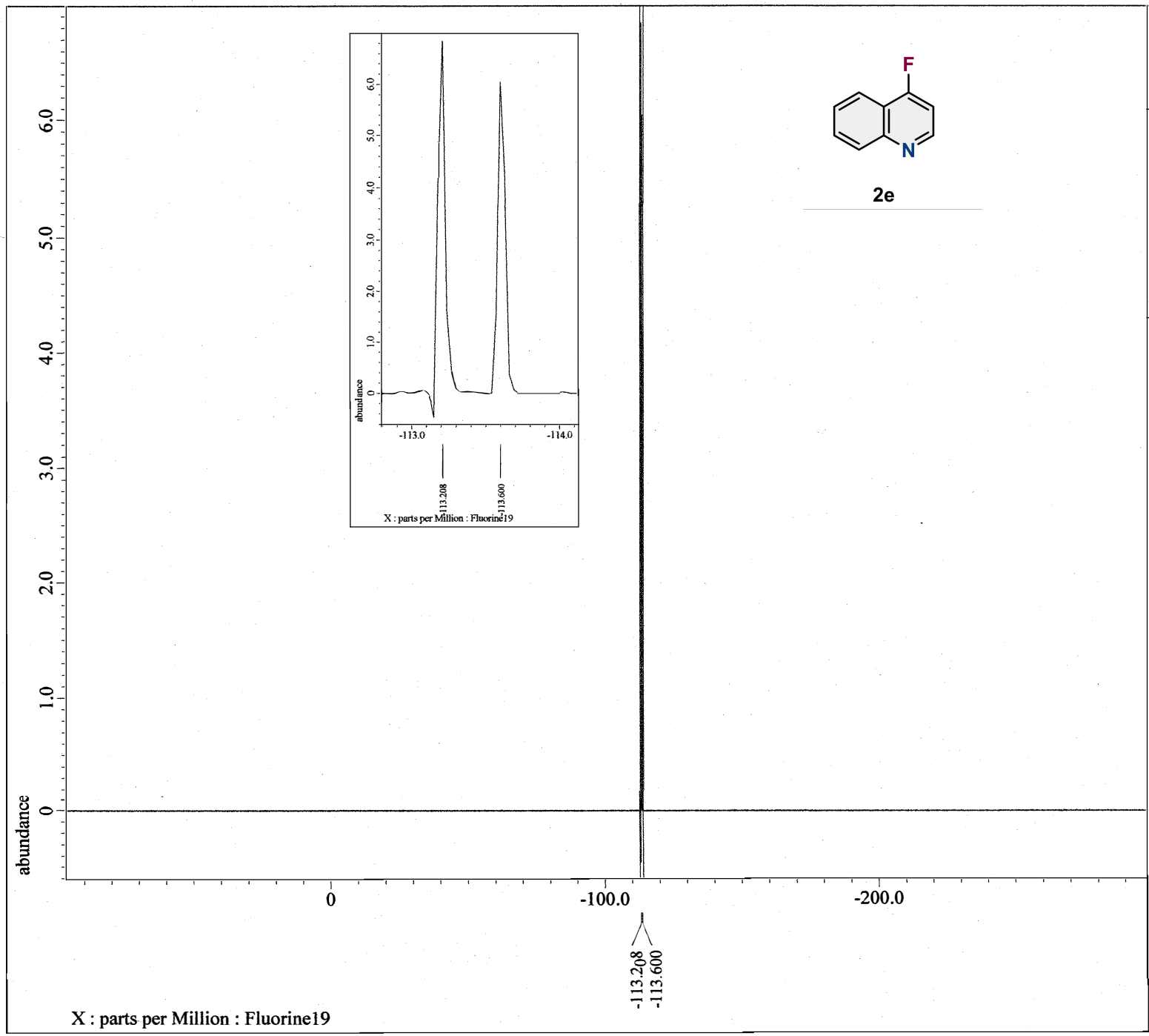

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: MKN281-pure Proton-1-1.jdf
```

Filename	= MKN281-pure_Proton-1-2
Author	= element
Experiment	= proton_auto.jxp
Sample_Id	= MKN281-column
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 25-JAN-2024 20:22:45
Revision_Time	= 15-JUN-2024 16:42:20
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.2982153[T] (400[MHz]
X_Acq_Duration	= 2.20725248[s]
X_Domain	= Proton
X_Freq	= 395.88430144[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45305193[Hz]
X_Sweep	= 7.42280285[kHz]
X_Sweep_Clipped	= 5.93824228[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 395.88430144[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2.0[us]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 56
Temp_Get	= 19.6[dC]
X_90_Width	= 6.34[us]
X_Acq_Time	= 2.20725248[s]
X_Angle	= 45[deg]
X_Atn	= 5[dB]
X_Pulse	= 3.17[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 500
Dante_Presat	= FALSE
Decimation_Rate	= 0
Initial_Wait	= 1[s]
Phase	= {0, 90, 270, 180, 180,




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

Derived from: MKN281-pure Carbon-1-1.jdf
```

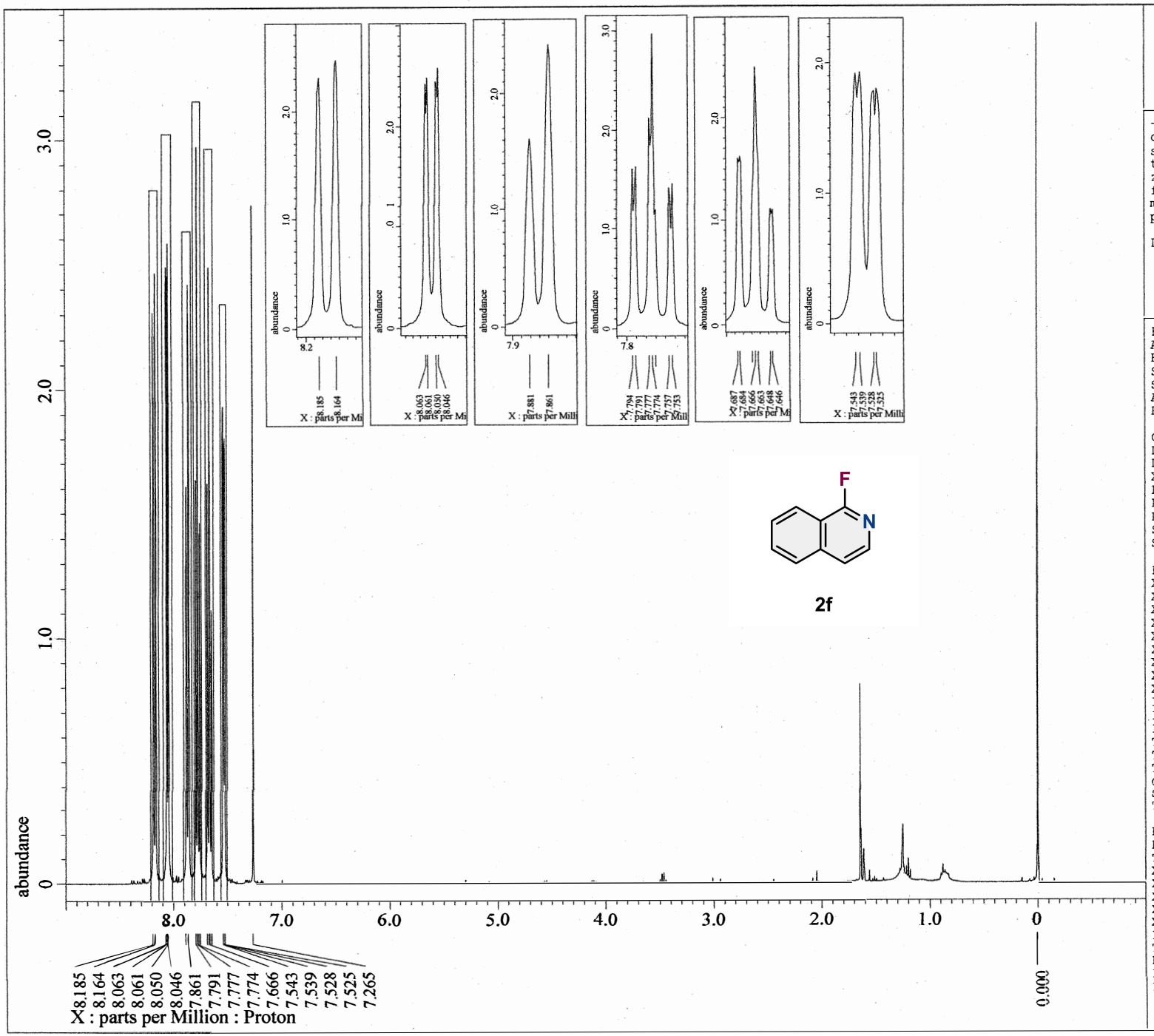
Filename	= MKN281-pure_Carbon-1-3.jdf
Author	= element
Experiment	= carbon.jxp
Sample_Id	= MKN281-pure
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 3-FEB-2024 12:56:29
Revision_Time	= 15-JUN-2024 17:12:39
Comment	= single pulse decoupled gat
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECS400
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.37221[T] (400[MHz])
X_Acq_Duration	= 1.04333312[s]
X_Domain	= 13C
X_Freq	= 100.33735165[MHz]
X_Offset	= 100.0[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.95846665[Hz]
X_Sweep	= 31.40703518[kHz]
X_Sweep_Clipped	= 25.12562814[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.03472754[MHz]
Irr_Offset	= 5.0[ppm]
Clipped	= FALSE
Scans	= 128
Total_Scans	= 128
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 19.1[dC]
X_90_Width	= 10.9[us]
X_Acq_Time	= 1.04333312[s]
X_Angle	= 30[deg]
X_Atn	= 5.4[dB]
X_Pulse	= 3.63333333[us]
Irr_Atn_Dec	= 25.823[dB]
Irr_Atn_Noe	= 25.823[dB]
Irr_Noise	= WALTZ
Irr_Pwidth	= 0.115[ms]
Decoupling	= TRUE
Initial_Wait	= 1[s]
Noe	= TRUE
Noe_Time	= 2[s]
Repetition Time	= 3.04333312[s]



2e

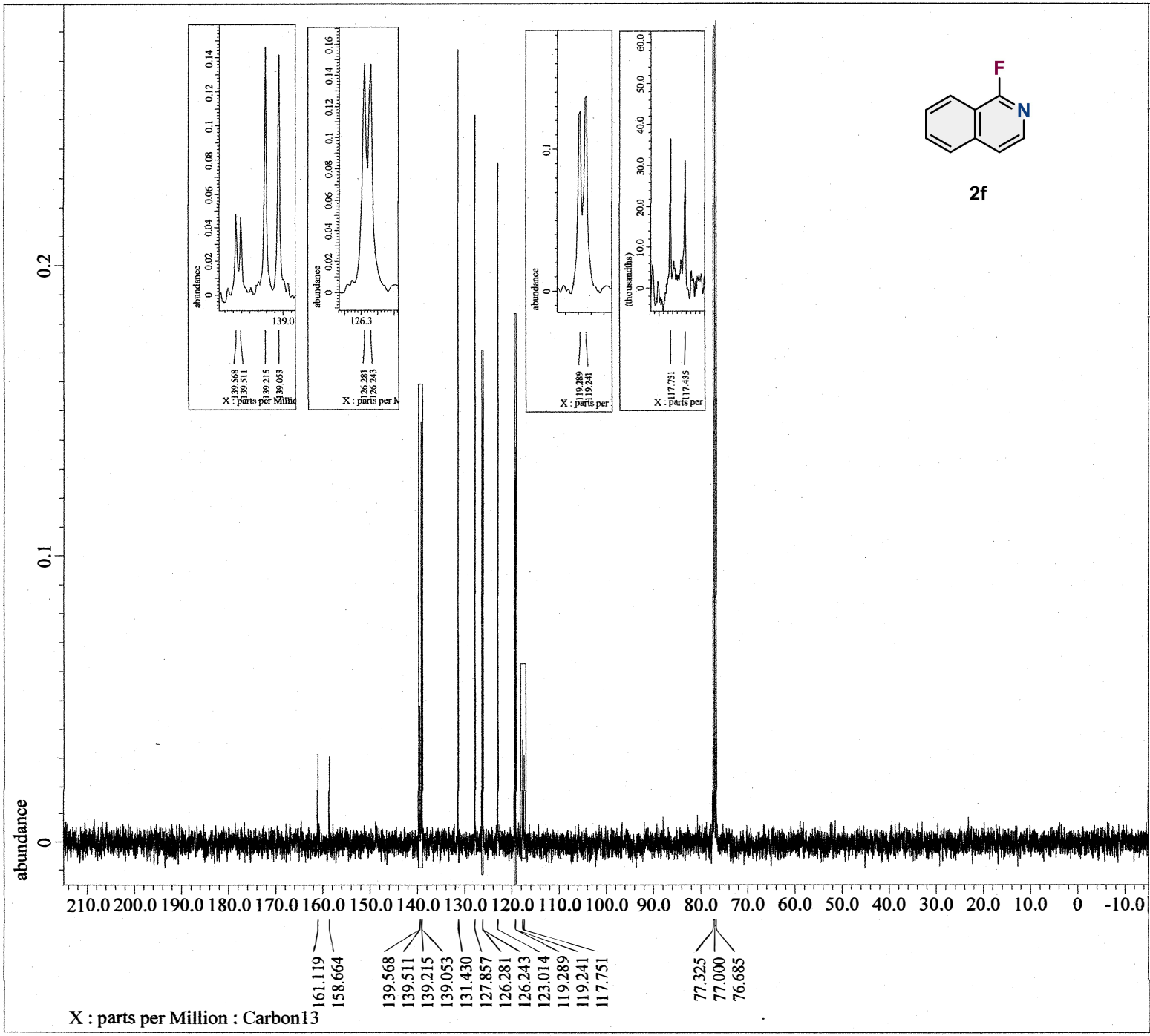
```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
blip( 16, 64, 30 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: MKN281-pure-int single pulse-1-1
```

Filename	= MKN281-pure-int_single
Author	= element
Experiment	= single_pulse.jxp
Sample_Id	= MKN281-pure-int
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 1-FEB-2024 15:22:36
Revision_Time	= 15-JUN-2024 17:19:58
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Fluorine19
Dim_Title	= Fluorine19
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.2982153[T] (400[MHz]
X_Acq_Duration	= 89.12896[ms]
X_Domain	= Fluorine19
X_Freq	= 372.50336686[MHz]
X_Offset	= -100[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 11.21969784[Hz]
X_Sweep	= 183.82352941[kHz]
X_Sweep_Clipped	= 147.05882353[kHz]
Irr_Domain	= Fluorine19
Irr_Freq	= 372.50336686[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Fluorine19
Tri_Freq	= 372.50336686[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2.0[us]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 56
Temp_Get	= 18.8[dC]
X_90_Width	= 8.03[us]
X_Acq_Time	= 89.12896[ms]
X_Angle	= 45[deg]
X_Atn	= 5[dB]
X_Pulse	= 4.015[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 500
Dante_Presat	= FALSE
Decimation_Rate	= 0
Initial_Wait	= 1[s]
Phase	= {0, 90, 270, 180, 180,



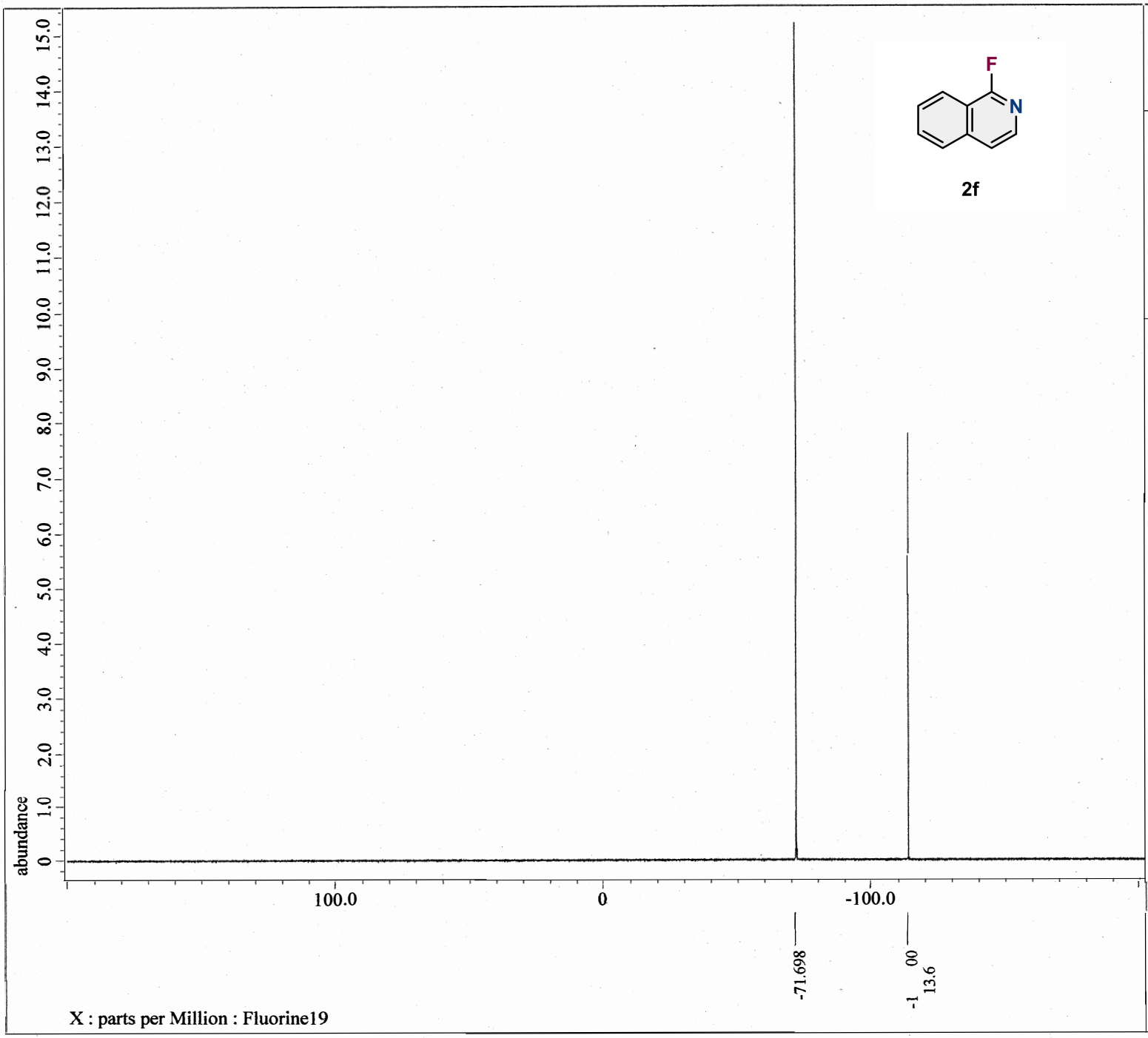

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: MKN306 pure Proton-1-1.jdf
```

Filename	= MKN306_pure_Proton-1-3.jdf
Author	= element
Experiment	= proton.jxp
Sample_Id	= MKN306_column
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 22-FEB-2024 19:59:20
Revision_Time	= 17-JUN-2024 12:12:47
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECS400
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.37221[T] (400[MHz])
X_Acq_Duration	= 2.1889024[s]
X_Domain	= 1H
X_Freq	= 399.03472754[MHz]
X_Offset	= 5.0[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45684997[Hz]
X_Sweep	= 7.48502994[kHz]
X_Sweep_Clipped	= 5.98802395[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.03472754[MHz]
Irr_Offset	= 5.0[ppm]
Tri_Domain	= Proton
Tri_Freq	= 399.03472754[MHz]
Tri_Offset	= 5.0[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 40
Temp_Get	= 18.2[dC]
X_90_Width	= 6.6[us]
X_Acq_Time	= 2.1889024[s]
X_Angle	= 45[deg]
X_Atn	= 1[dB]
X_Pulse	= 3.3[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition Time	= 7.1889024[s]



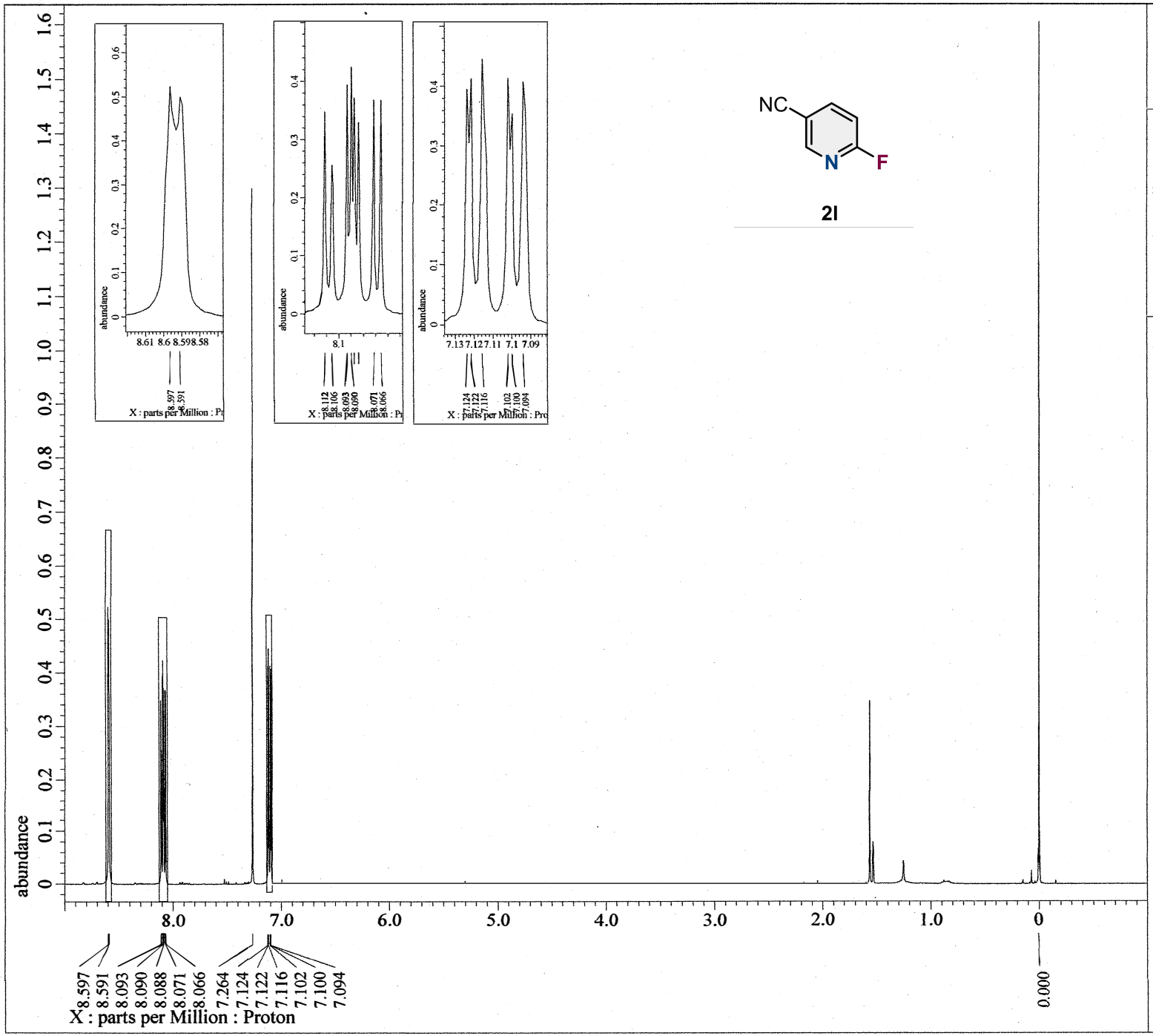

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: MKN306-pure Carbon-3-1.jdf
```

Filename	= MKN306-pure_Carbon-3-2.jdf
Author	= element
Experiment	= carbon.jxp
Sample_Id	= MKN306-pure
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 24-FEB-2024 14:10:38
Revision_Time	= 17-JUN-2024 12:25:05
Comment	= single pulse decoupled gat
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECS400
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.37221[T] (400[MHz])
X_Acq_Duration	= 1.04333312[s]
X_Domain	= 13C
X_Freq	= 100.33735165[MHz]
X_Offset	= 100.0[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.95846665[Hz]
X_Sweep	= 31.40703518[kHz]
X_Sweep_Clipped	= 25.12562814[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.03472754[MHz]
Irr_Offset	= 5.0[ppm]
Clipped	= FALSE
Scans	= 64
Total_Scans	= 64
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 18.3[dC]
X_90_Width	= 10.9[us]
X_Acq_Time	= 1.04333312[s]
X_Angle	= 30[deg]
X_Atn	= 5.4[dB]
X_Pulse	= 3.63333333[us]
Irr_Atn_Dec	= 25.823[dB]
Irr_Atn_Noe	= 25.823[dB]
Irr_Noise	= WALTZ
Irr_Pwidth	= 0.115[ms]
Decoupling	= TRUE
Initial_Wait	= 1[s]
Noe	= TRUE
Noe_Time	= 2[s]
Repetition Time	= 3.04333312[s]




```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
blip( 16, 64, 30 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: MKN 306-pure-int single pulse-1-1
```

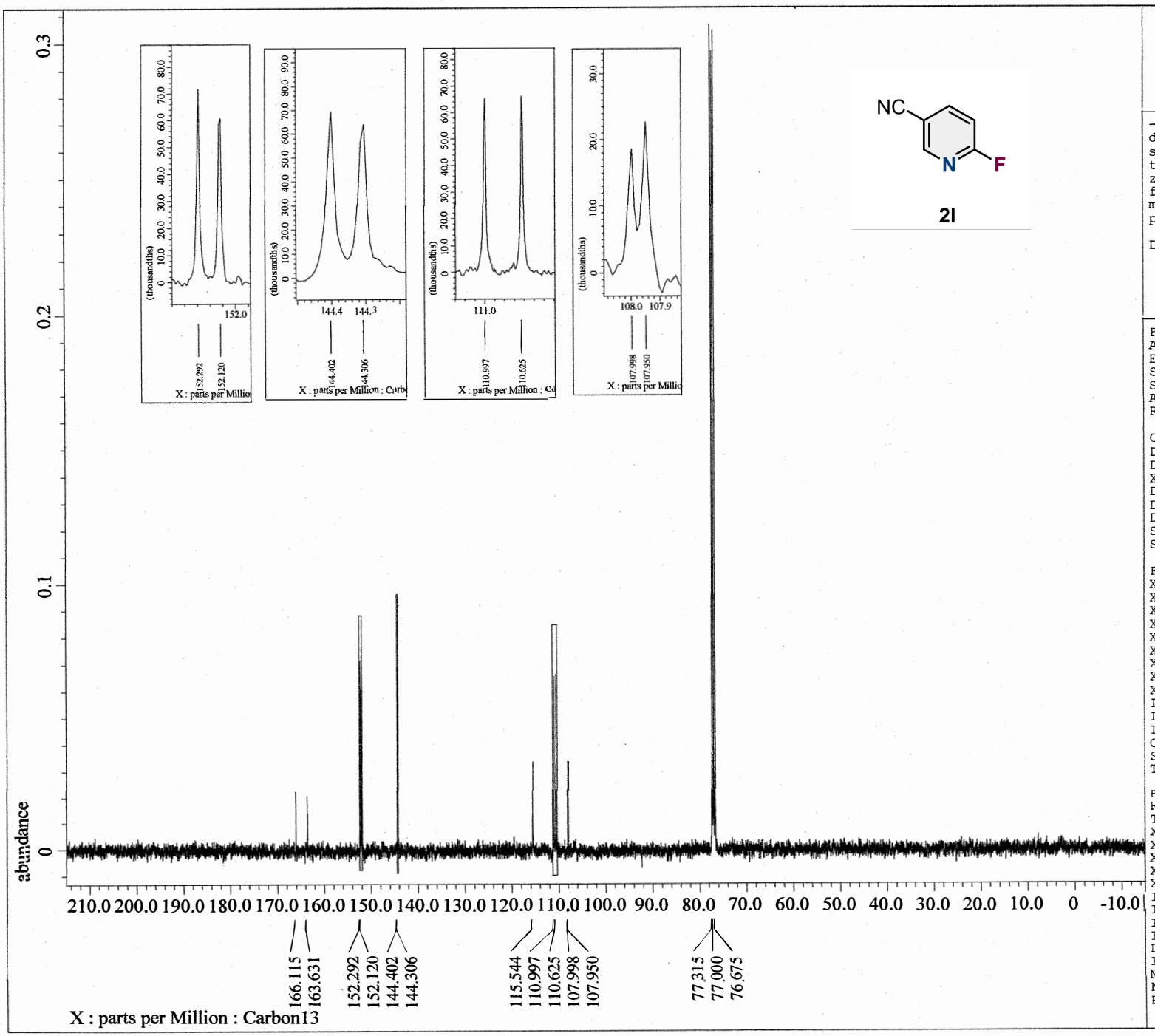
Filename	= MKN 306-pure-int_single_pul
Author	= element
Experiment	= single_pulse.jxp
Sample_Id	= MKN 306-pure-int
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 24-FEB-2024 13:18:27
Revision_Time	= 17-JUN-2024 12:29:14
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Fluori
Dim_Title	= Fluorine19
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECS400
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.37221[T] (400[MHz])
X_Acq_Duration	= 86.50752[ms]
X_Domain	= 19F
X_Freq	= 375.46772873[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	= 375.46772873[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Fluorine19
Tri_Freq	= 375.46772873[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 44
Temp_Get	= 18.4[dC]
X_90_Width	= 7.6[us]
X_Acq_Time	= 86.50752[ms]
X_Angle	= 45[deg]
X_Atn	= 2.5[dB]
X_Pulse	= 3.8[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition Time	= 5.08650752[s]



2l

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

Derived from: MKN221-pure Proton-1-1.jdf
```

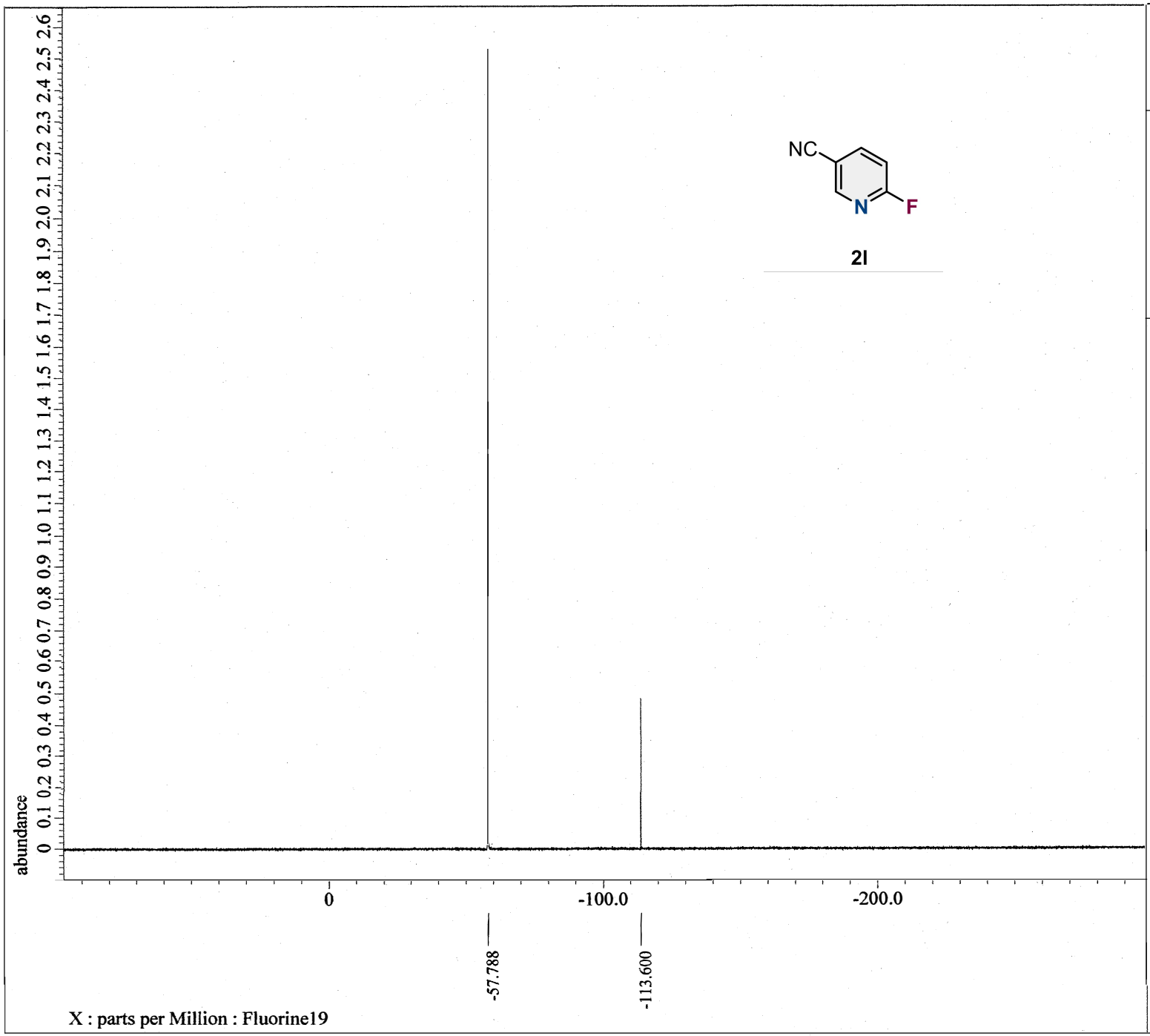
Filename	= MKN221-pure_Proton-1-2
Author	= element
Experiment	= proton_auto.jxp
Sample_Id	= MKN221-pure
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 23-JAN-2024 17:15:19
Revision_Time	= 17-JUN-2024 11:44:47
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.2982153[T] (400[MHz]
X_Acq_Duration	= 2.20725248[s]
X_Domain	= Proton
X_Freq	= 395.88430144[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45305193[Hz]
X_Sweep	= 7.42280285[kHz]
X_Sweep_Clipped	= 5.93824228[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 395.88430144[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2.0[us]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 56
Temp_Get	= 19.3[dC]
X_90_Width	= 6.34[us]
X_Acq_Time	= 2.20725248[s]
X_Angle	= 45[deg]
X_Atn	= 5[dB]
X_Pulse	= 3.17[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 500
Dante_Presat	= FALSE
Decimation_Rate	= 0
Initial_Wait	= 1[s]
Phase	= {0, 90, 270, 180, 180,



2l

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

Derived from: MKN221-pure Carbon-1-1.jdf
```

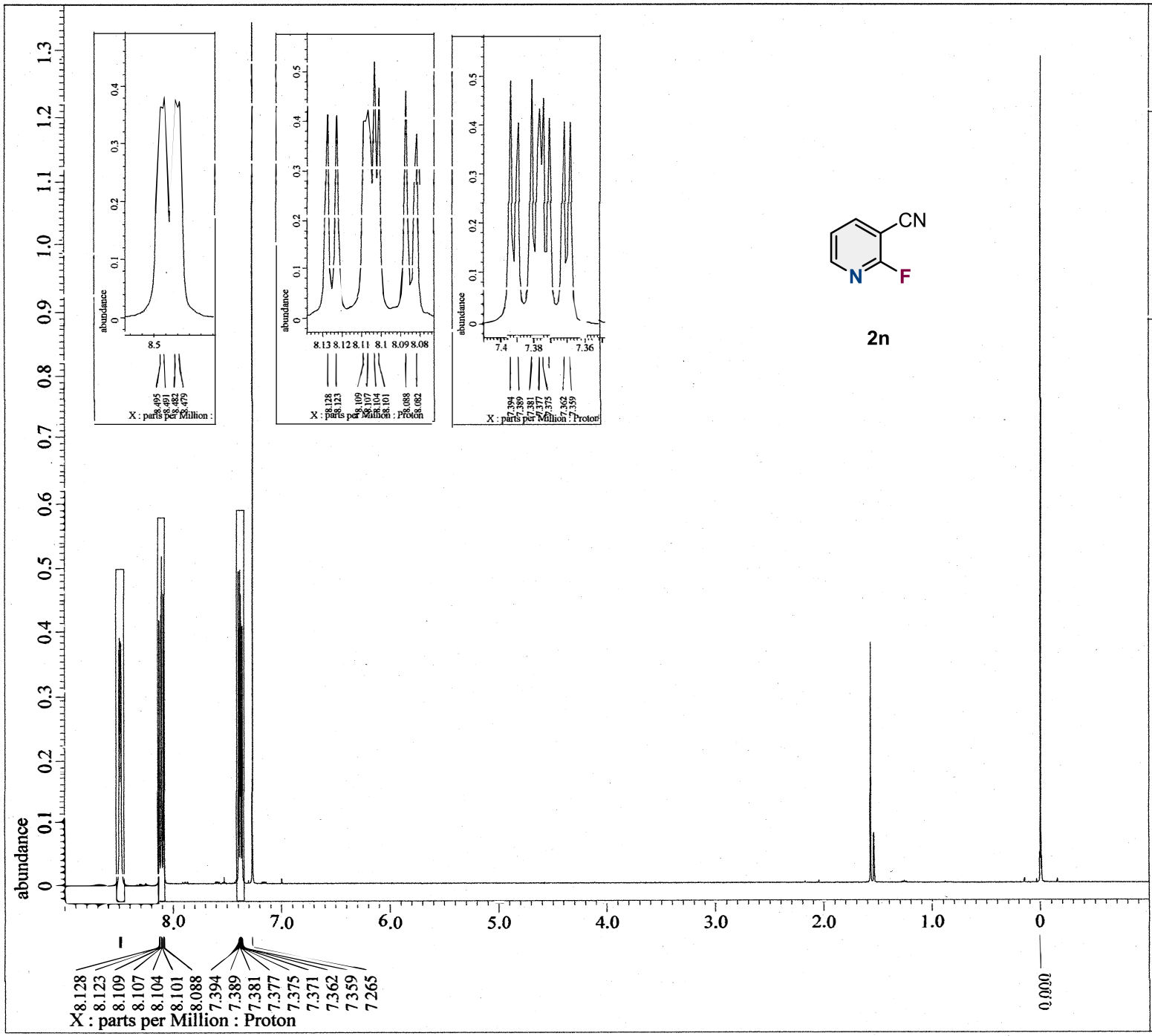
```
Filename            = MKN221-pure_Carbon-1-2.jdf
Author              = element
Experiment          = carbon.jxp
Sample_Id           = MKN221-pure
Solvent             = CHLOROFORM-D
Actual_Start_Time   = 23-JAN-2024 18:56:15
Revision_Time       = 17-JUN -2024 11:53:19

Comment             = single pulse decoupled gat
Data_Format         = 1D COMPLEX
Dim_Size            = 26214
X_Domain            = Carbon
Dim_Title           = Carbon13
Dim_Units           = [ppm]
Dimensions          = X
Site                = JNM-ECS400
Spectrometer        = DELTA2_NMR

Field_Strength      = 9.37221[T] (400[MHz])
X_Acq_Duration      = 1.04333312[s]
X_Domain            = 13C
X_Freq              = 100.33735165[MHz]
X_Offset            = 100.0[ppm]
X_Points            = 32768
X_Prescans          = 4
X_Resolution        = 0.95846665[Hz]
X_Sweep             = 31.40703518[kHz]
X_Sweep_Clipped     = 25.12562814[kHz]
Irr_Domain          = Proton
Irr_Freq            = 399.03472754[MHz]
Irr_Offset          = 5.0[ppm]
Clipped             = FALSE
Scans               = 256
Total_Scans         = 256

Relaxation_Delay    = 2[s]
Recvr_Gain          = 50
Temp_Get            = 19.7[dC]
X_90_Width          = 10.9[us]
X_Acq_Time          = 1.04333312[s]
X_Angle             = 30[deg]
X_Atn               = 5.4[dB]
X_Pulse             = 3.63333333[us]
Irr_Atn_Dec         = 25.823[dB]
Irr_Atn_Noe         = 25.823[dB]
Irr_Noise           = WALTZ
Irr_Pwidth          = 0.115[ms]
Decoupling          = TRUE
Initial_Wait        = 1[s]
Noe                 = TRUE
Noe_Time            = 2[s]
Repetition Time     = 3.04333312[s]
```



2l

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
blip( 16, 64, 30 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

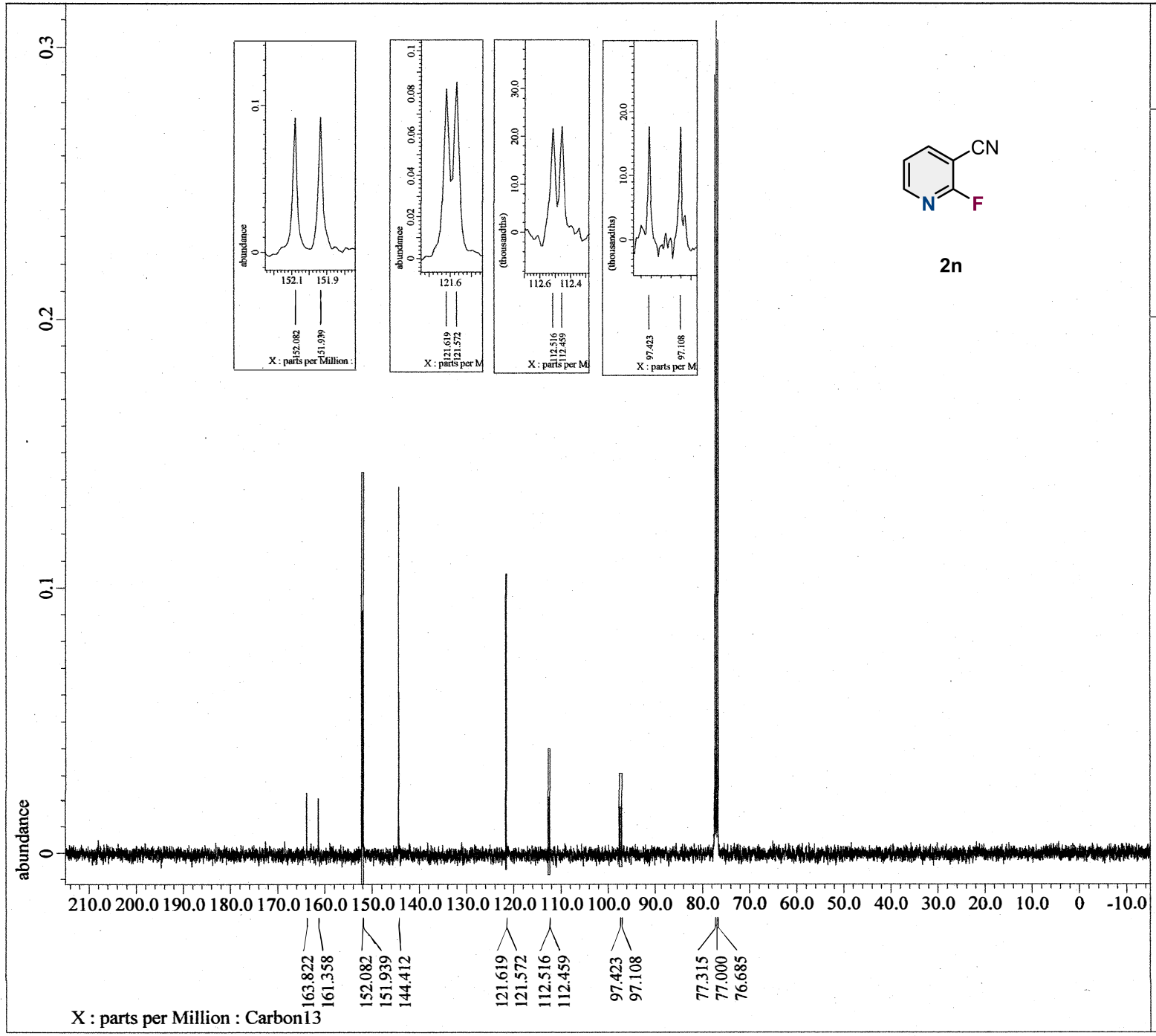
Filename	= MKN221-pure-int_ sigle
Autho r	= element
Experiment	= single_pulse.jxp
Sample_Id	= MKN221-pure-int
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 23-JAN-2024 17:28:53
Revision_T ime	= 17-JUN-2024 11:57:29
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Fluorine19
Dim_Tit le	= Fluorine19
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.2982153[T] (400[MHz
X_Acq_Duration	= 89.12896[ms]
X_Domain	= Fluorine19
X_Freq	= 372.50336686[MHz]
X_Offset	= -100[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 11.21969784[Hz]
X_Sweep	= 183.82352941[kHz]
X_Sweep_Clipped	= 147.05882353[kHz]
Ir r_Domain	= Fluorine19
Irr_Freq	= 372.50336686[MHz]
Irr_Offset	= 5[ppm]
T ri_Domain	= Fluorine19
T ri_Freq	= 372.50336686[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2.0[us]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_ Delay	= 5[s]
Recvr_Gain	= 56
Temp_Get	= 18.8[dC]
X_90_Width	= 8.03[us]
X_Acq_Time	= 89.12896[ms]
X_Angle	= 45[deg]
X_Atn	= 5[dB]
X_Pulse	= 4.015[us]
Irr_Mode	= Off
T ri_ Mode	= Off
Dante_Loop	= 500
Dante_Presat	= FALSE
Decimation_Rate	= 0
Initial_Wait	= 1[s]
Phase	= {0, 90, 270, 180, 180,



2n

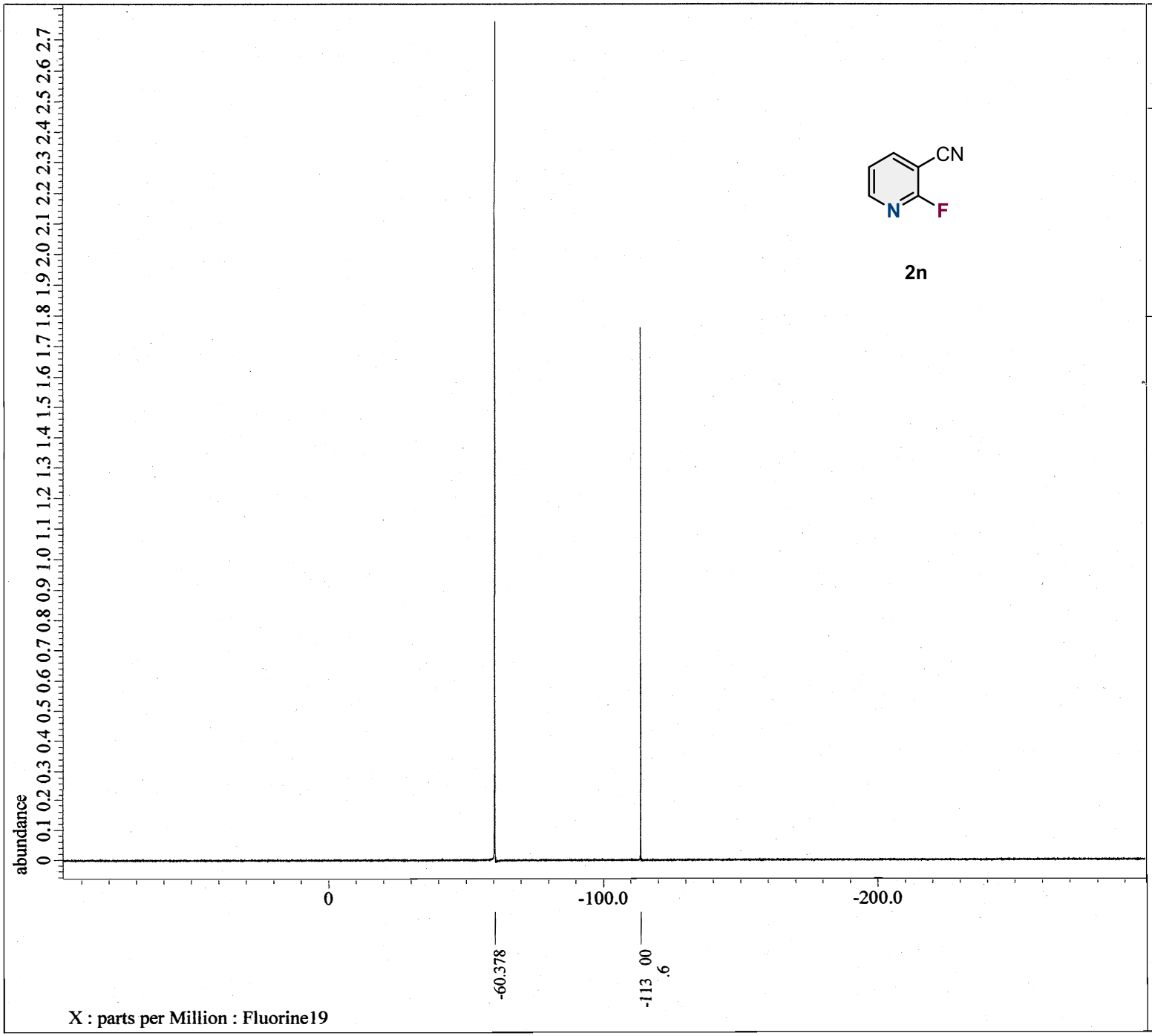
```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: MKN240-pure Proton-1-1.jdf
```

Filename	= MKN240-pure_Proton-1-2
Author	= element
Experiment	= proton_auto.jxp
Sample_Id	= MKN240-pure
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 23-JAN-2024 17:22:40
Revision_Time	= 17-JUN-2024 11:22:06
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.2982153[T] (400[MHz]
X_Acq_Duration	= 2.20725248[s]
X_Domain	= Proton
X_Freq	= 395.88430144[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45305193[Hz]
X_Sweep	= 7.42280285[kHz]
X_Sweep_Clipped	= 5.93824228[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 395.88430144[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2.0[us]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 56
Temp_Get	= 19[dC]
X_90_Width	= 6.34[us]
X_Acq_Time	= 2.20725248[s]
X_Angle	= 45[deg]
X_Atn	= 5[dB]
X_Pulse	= 3.17[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 500
Dante_Presat	= FALSE
Decimation_Rate	= 0
Initial_Wait	= 1[s]
Phase	= {0, 90, 270, 180, 180,




```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
reference( 77.13146[ppm], 77[ppm] )
thresh( 4.48623[%], 1,  )

Derived from: MKN240-pure Carbon-1-1.jdf
```

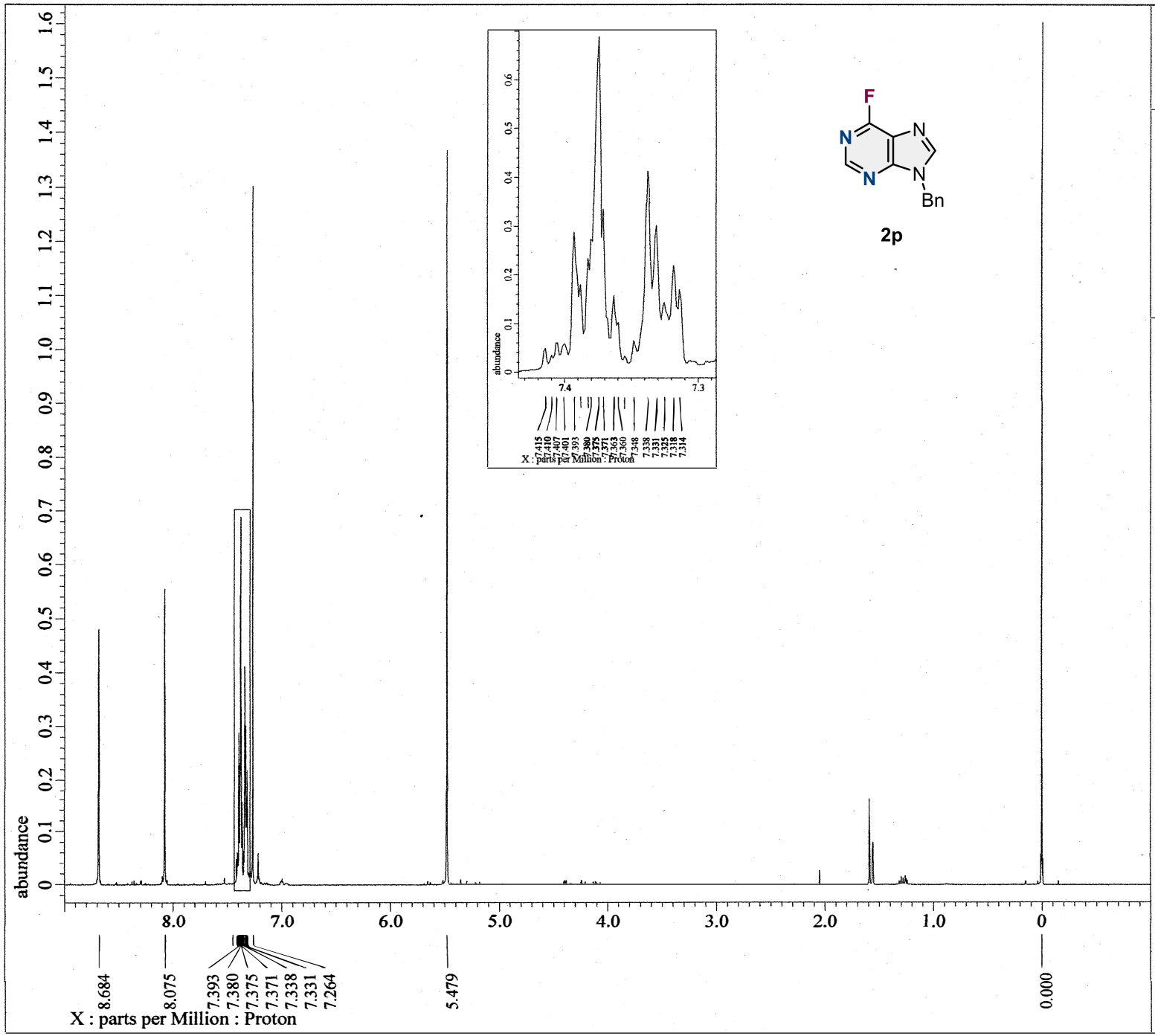
```
Filename            = MKN240-pure_Carbon-1-2.jdf
Author              = element
Experiment          = carbon.jxp
Sample_Id           = MKN240-pure
Solvent             = CHLOROFORM-D
Actual_Start_Time   = 23-JAN-2024 19:31:00
Revision_Time       = 17-JUN-2024 11:29:40

Comment             = single pulse decoupled gat
Data_Format         = 1D COMPLEX
Dim_Size            = 26214
X_Domain            = Carbon
Dim_Title           = Carbon13
Dim_Units           = [ppm]
Dimensions          = X
Site                = JNM-ECS400
Spectrometer        = DELTA2_NMR

Field_Strength      = 9.37221[T] (400[MHz])
X_Acq_Duration      = 1.04333312[s]
X_Domain            = 13C
X_Freq              = 100.33735165[MHz]
X_Offset            = 100.0[ppm]
X_Points            = 32768
X_Prescans          = 4
X_Resolution        = 0.95846665[Hz]
X_Sweep             = 31.40703518[kHz]
X_Sweep_Clipped     = 25.12562814[kHz]
Irr_Domain          = Proton
Irr_Freq            = 399.03472754[MHz]
Irr_Offset          = 5.0[ppm]
Clipped             = FALSE
Scans               = 256
Total_Scans         = 256

Relaxation_Delay    = 2[s]
Recvr_Gain          = 50
Temp_Get            = 19.6[dC]
X_90_Width          = 10.9[us]
X_Acq_Time          = 1.04333312[s]
X_Angle             = 30[deg]
X_Atn               = 5.4[dB]
X_Pulse             = 3.63333333[us]
Irr_Atn_Dec         = 25.823[dB]
Irr_Atn_Noe         = 25.823[dB]
Irr_Noise           = WALTZ
Irr_Pwidth          = 0.115[ms]
Decoupling          = TRUE
Initial_Wait        = 1[s]
Noe                 = TRUE
Noe_Time            = 2[s]
Repetition Time     = 3.04333312[s]
```



2n

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[ %],0[ %],80[ %],100[%] )
zerofill( 1 )
blip( 16, 64, 30 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

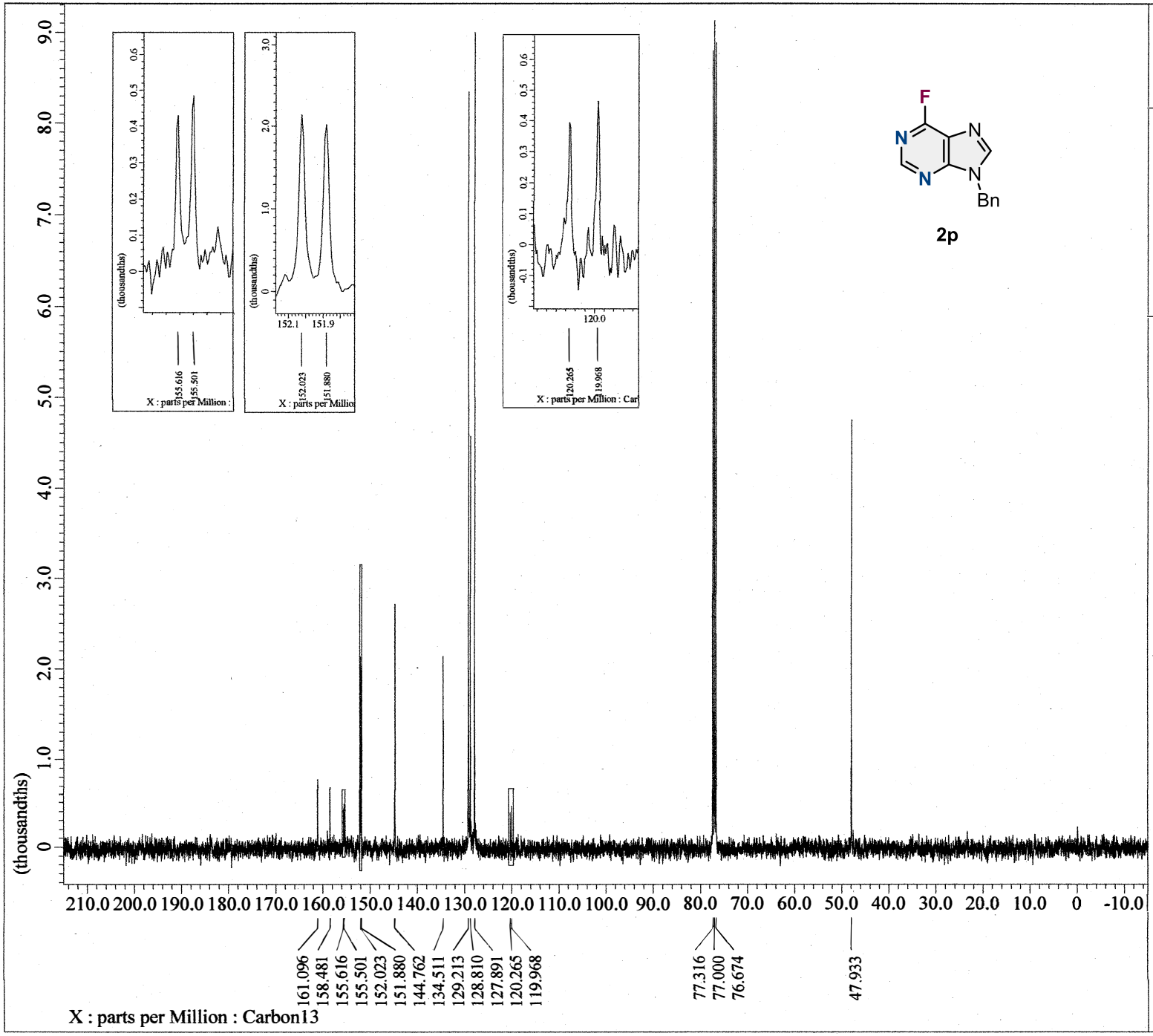
Filename	= MKN240-pure-int_single
Author	= element
Experiment	= single_pulse.jxp
Sample_Id	= MKN240-pure-int
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 23-JAN-2024 17:33:35
Revision_Time	= 24-JAN-2024 11:59:08
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Fluorine19
Dim_Title	= Fluorine19
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9. 298215[T] (400[MHz]
X_Acq_Duration	= 89. 12896 [ms]
X_Domain	= Fluorine19
X_Freq	= 372.50336686[MHz]
X_Offset	= -100[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 11.21969784[Hz]
X_Sweep	= 183.82352941[kHz]
X_Sweep_Clipped	= 147.05 882353[kHz]
Irr_Domain	= Fluorine19
Irr_Freq	= 372.50336686[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Fluorine19
Tri_Freq	= 372.50336686[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2.0[us]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 56
Temp_Get	= 18.7[dC]
X_90_Width	= 8.03[us]
X_Acq_Time	= 89.12896[ms]
X_Angle	= 45[deg]
X_Atn	= 5[dB]
X_Pulse	= 4.0 15[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 500
Dante_Presat	= FALSE
Decimation_Rate	= 0
Initial_Wait	= 1[s]
Phase	= {0, 90, 270, 180, 180,



2p

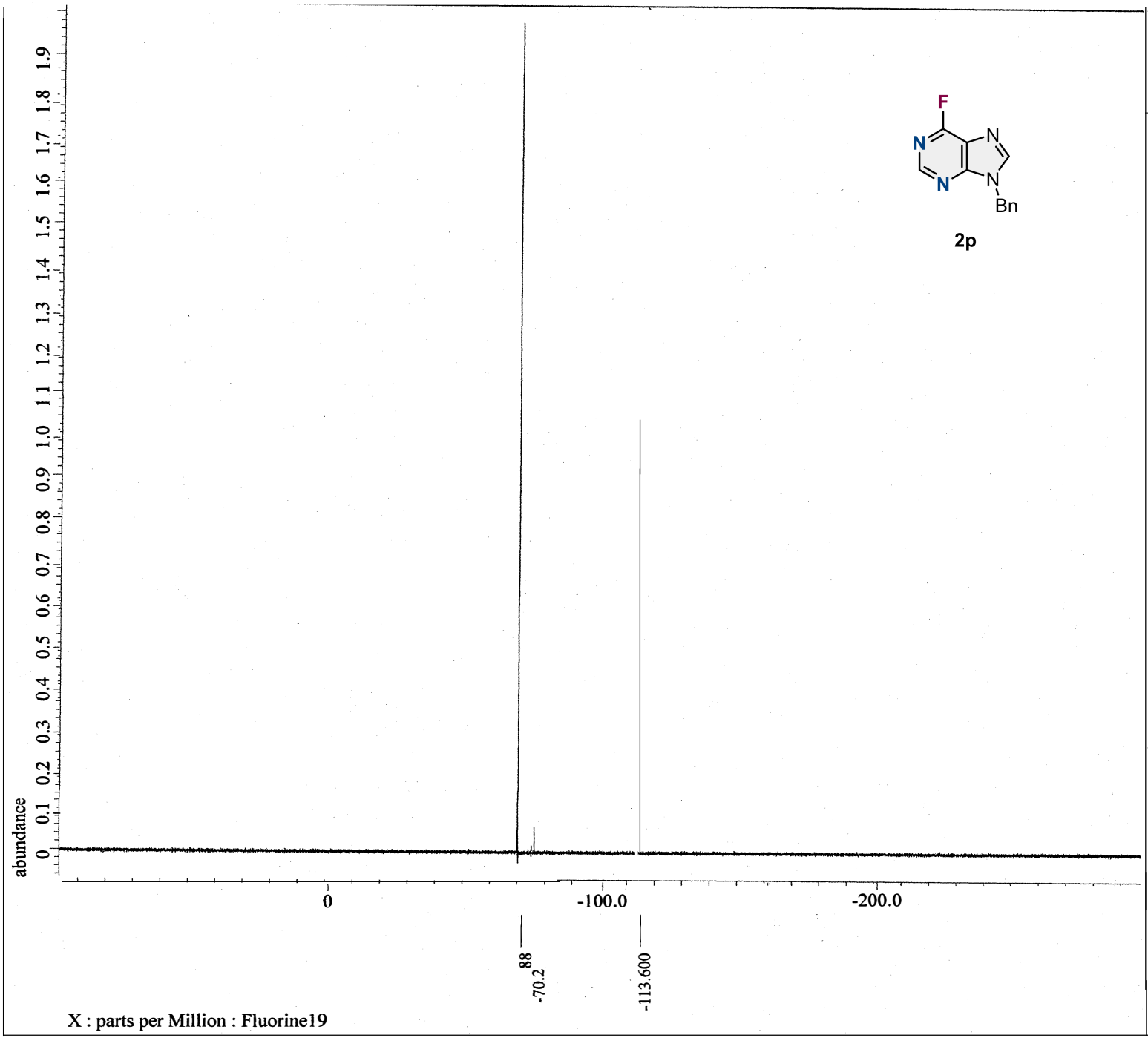
```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: MKN272-pure Proton-1-1.jdf
```

Filename	= MKN272-pure_Proton-1-2
Author	= element
Experiment	= proton_auto.jxp
Sample_Id	= MKN272-pure
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 20-JAN-2024 15:44:09
Revision_Time	= 17-JUN-2024 10:40:04
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	= 9.2982153[T] (400[MHz]
X_Acq_Duration	= 2.20725248[s]
X_Domain	= Proton
X_Freq	= 395.88430144[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45305193[Hz]
X_Sweep	= 7.42280285[kHz]
X_Sweep_Clipped	= 5.93824228[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 395.88430144[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2.0[us]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 56
Temp_Get	= 18.9[dC]
X_90_Width	= 6.34[us]
X_Acq_Time	= 2.20725248[s]
X_Angle	= 45[deg]
X_Atn	= 5[dB]
X_Pulse	= 3.17[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 500
Dante_Presat	= FALSE
Decimation_Rate	= 0
Initial_Wait	= 1[s]
Phase	= {0, 90, 270, 180, 180,



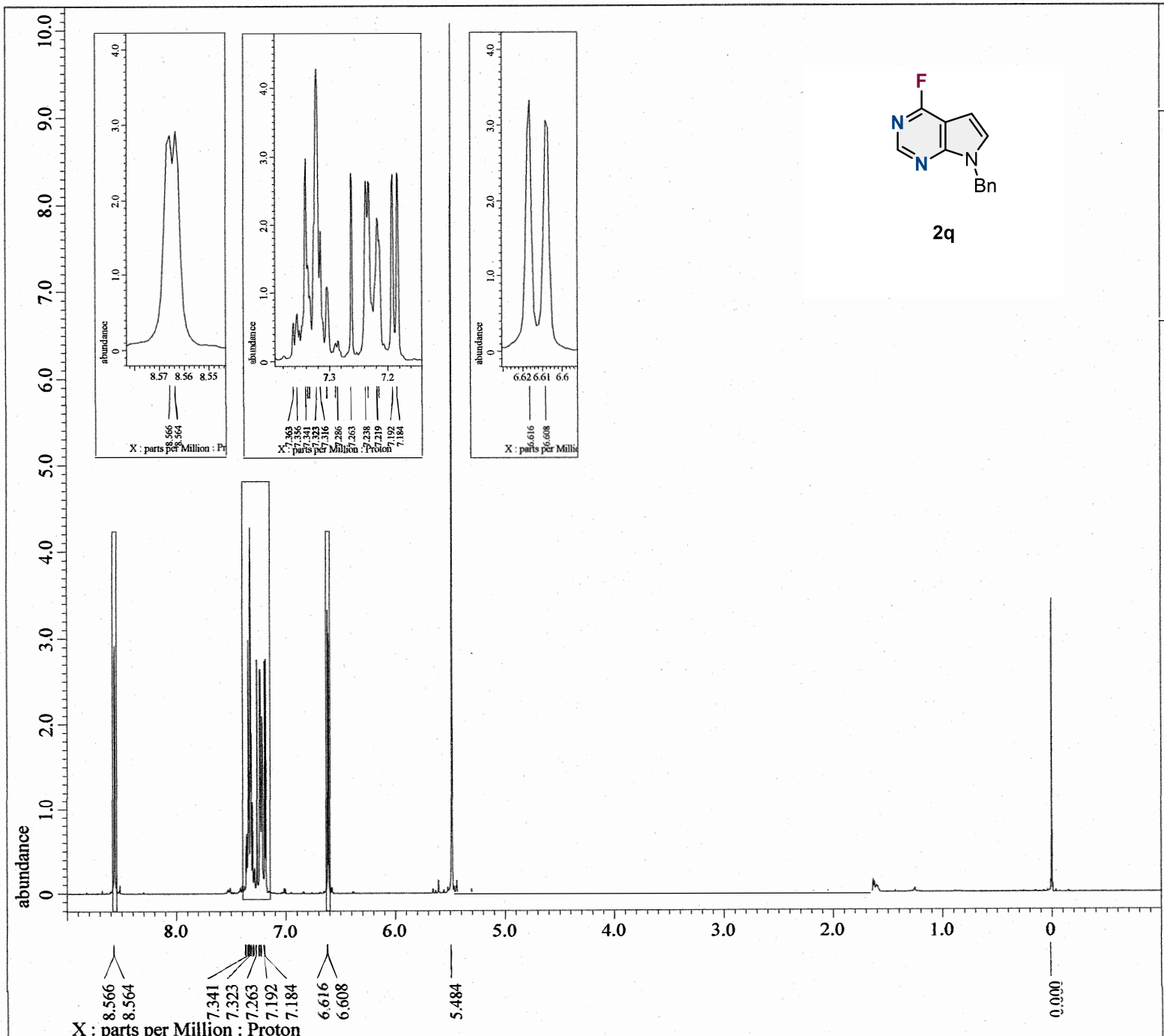

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
reference( 77.15094[ppm], 77[ppm] )
thresh( 2.87842[%], 1,  )

Derived from: MKN272-pure Carbon-1-1.jdf
```

Filename	= MKN272-pure_Carbon-
Author	= element
Experiment	= carbon_auto.jxp
Sample_Id	= MKN272-pure
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 20-JAN-2024 16:03:2
Revision_Time	= 17-JUN-2024 11:12:5
Comment	= single pulse decoup
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.2982153[T] (400[M
X_Acq_Duration	= 1.048576[s]
X_Domain	= Carbon13
X_Freq	= 99.54517646[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.95367432[Hz]
X_Sweep	= 31.25[kHz]
X_Sweep_Clipped	= 25[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 5.0[us]
Clipped	= FALSE
Scans	= 256
Total_Scans	= 256
Relaxation_Delay	= 2[s]
Recvr_Gain	= 5
Temp_Get	= 18.8[dC]
X_90_Width	= 11.5[us]
X_Acq_Time	= 1.048576[s]
X_Angle	= 30[deg]
X_Atn	= 9[dB]
X_Pulse	= 3.83333333[us]
Irr_Atn_Dec	= 30.172[dB]
Irr_Atn_Dec_Calc	= 30.172[dB]
Irr_Atn_Dec_Default_Calc	= 30.172[dB]
Irr_Atn_Noe	= 30.172[dB]
Irr_Dec_Bandwidth_Hz	= 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.08082432[ppm]
Irr_Dec_Freq	= 395.88430144[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE




```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
blip( 16, 64, 30 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: MKN272-pure-int single pulse-1-1
```

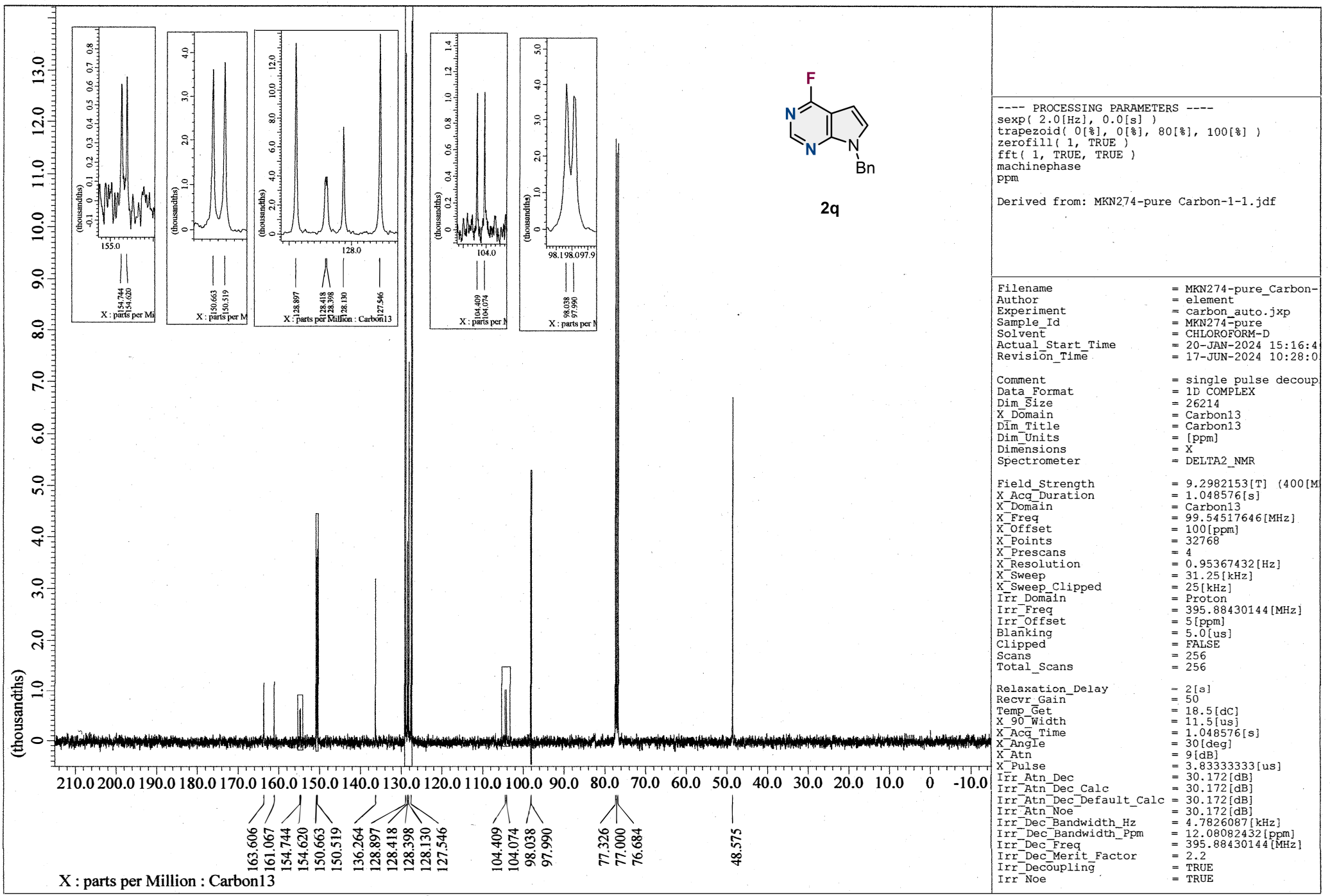
Filename	= MKN272-pure-int_single
Author	= element
Experiment	= single_pulse.jxp
Sa mbe_Id	= MKN272-pure-int
Solvent	= CHLOROFORM-D
Actual Start_Time	= 20-JAN-2024 15:58:51
Revision Time	= 17-JUN-2024 10:45:48
Comment	= single_pulse
Data_Forma t	= 1D COMP EXL
Dim_Size	= 13107
X_Domain	= Fluorine19
Dim Title	= Fluorine19
Dim_Units	= [ppm]
Dimensio ns	= X
Spectrometer	= DELTA2 NMR
Field_Strength	= 9.2982153[T] (400[MHz]
X_Acq_Dura tion	= 89.12896[ms]
X_Domain	= Fluorine19
X_Freq	= 372.50336686[MHz]
X_Offset	= -100[ppm]
X_Points	= 16384
X_Presca ns	= 1
X_Resolution	= 11.21969784[Hz]
X_Sweep	= 183.82352941[kHz]
X_Sweep_Clipped	= 147.05882353[kHz]
Irr_Domain	= Fluorine19
Irr_Freq	= 372.50336686[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Fluorine19
Tri_Freq	= 372.50336686[MHz]
Tri_Offset	= 5[ppm]
Bla nking	= 2.0[us]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxa tionDela y	= 5[s]
Recvr_Gain	= 56
Temp_Get	= 18.3[dC]
X_90_Width	= 8.03[us]
X_Acq_Time	= 89.12896[ms]
X_Angle	= 45[deg]
X_Atn	= 5[dB]
X_Pulse	= 4.015[us]
Irr_Mode	= Off
Tri_Mode	= Off
Da ne_Loop	= 500
Da nte_Presa t	= FALSE
Decima tion_Rate	= 0
Initial Wait	= 1[s]
Phase	= {0, 90, 270, 180, 180,



2q

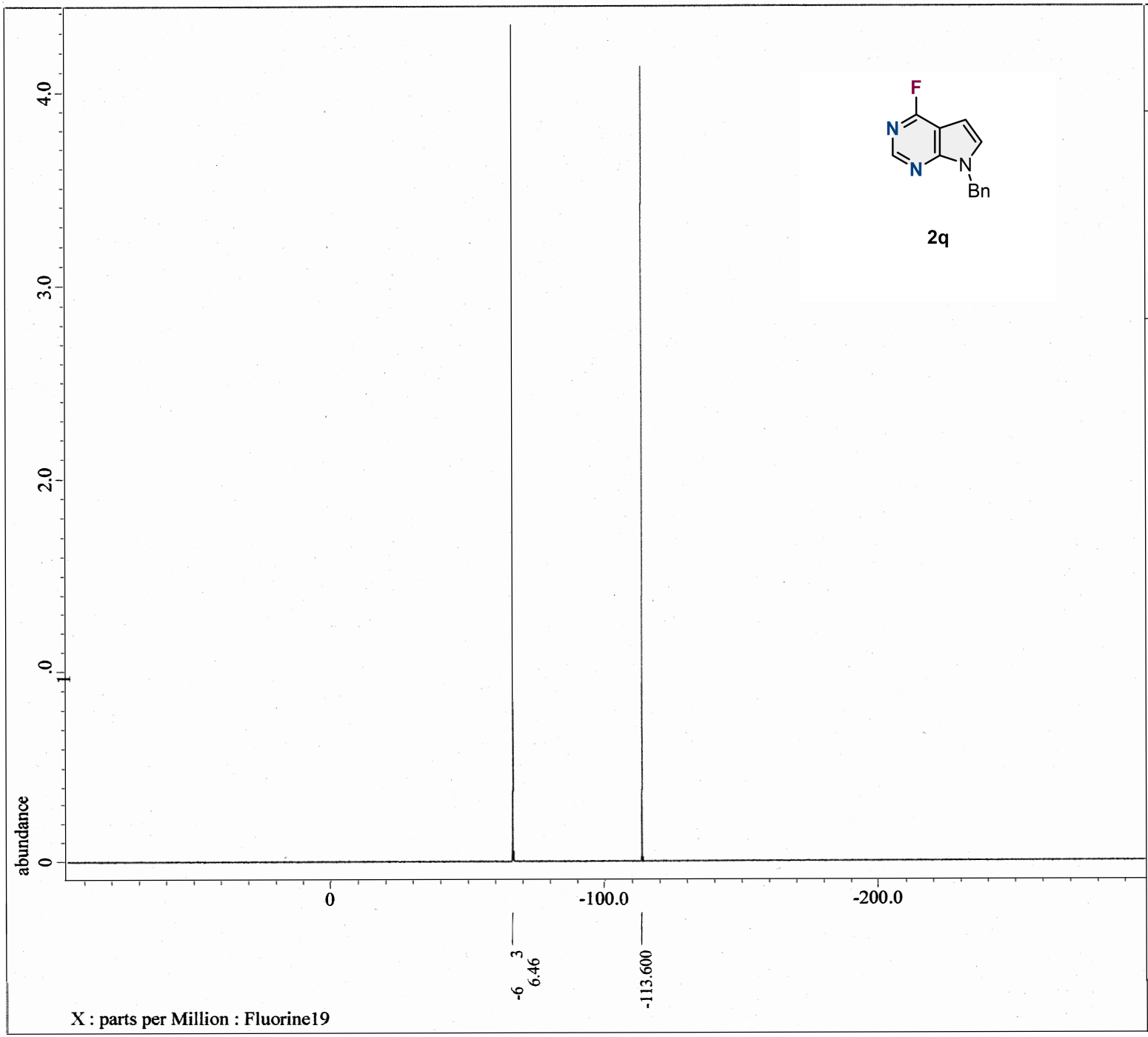
```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: MKN274-pure Proton-1-1.jdf
```

```
Filename            = MKN274-pure_Proton-1-2.jdf
Author              = element
Experiment          = proton.jxp
Sample_Id           = MKN274-pure
Solvent             = CHLOROFORM-D
Actual_Start_Time   = 20-JAN-2024 14:22:21
Revision_Time       = 17-JUN-2024 10:17:13

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            = 19.3[dC]
X_90_Width          = 6.7[us]
X_Acq_Time          = 2.18103808[s]
X_Angle             = 45[deg]
X_Atn               = 0.8[dB]
X_Pulse             = 3.35[us]
Irr_Mode            = Off
Tri_Mode            = Off
Dante_Presat        = FALSE
Initial_Wait        = 1[s]
Repetition Time     = 7.18103808[s]
```



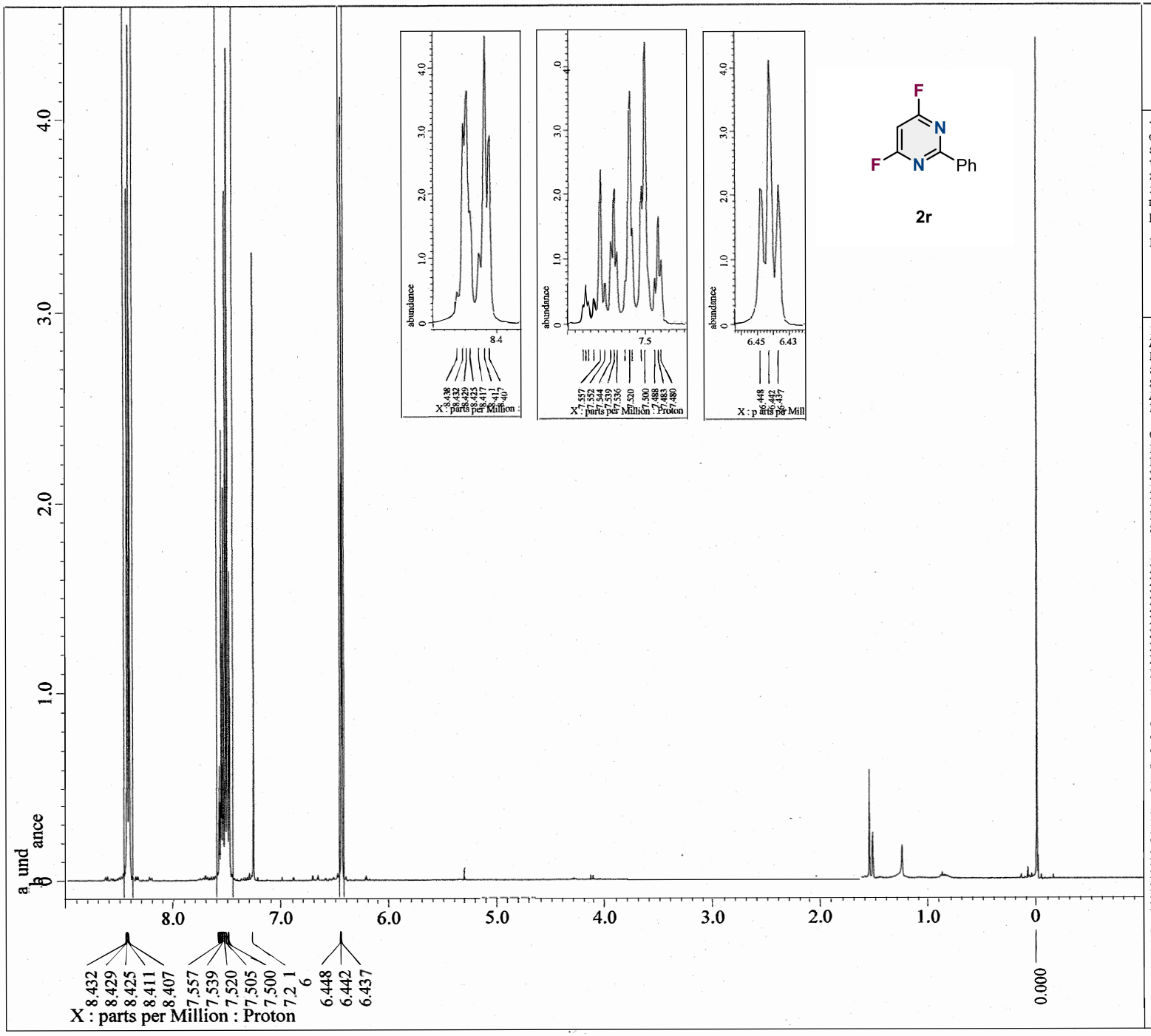

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: MKN274-pure Carbon-1-1.jdf
```

Filename	= MKN274-pure_Carbon-
Author	= element
Experiment	= carbon_auto.jxp
Sample_Id	= MKN274-pure
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 20-JAN-2024 15:16:4
Revision_Time	= 17-JUN-2024 10:28:0
Comment	= single pulse decoup
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.2982153[T] (400[M
X_Acq_Duration	= 1.048576[s]
X_Domain	= Carbon13
X_Freq	= 99.54517646[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.95367432[Hz]
X_Sweep	= 31.25[kHz]
X_Sweep_Clipped	= 25[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 5.0[us]
Clipped	= FALSE
Scans	= 256
Total_Scans	= 256
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 18.5[dC]
X_90_Width	= 11.5[us]
X_Acq_Time	= 1.048576[s]
X_Angle	= 30[deg]
X_Atn	= 9[dB]
X_Pulse	= 3.83333333[us]
Irr_Atn_Dec	= 30.172[dB]
Irr_Atn_Dec_Calc	= 30.172[dB]
Irr_Atn_Dec_Default_Calc	= 30.172[dB]
Irr_Atn_Noe	= 30.172[dB]
Irr_Dec_Bandwidth_Hz	= 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.08082432[ppm]
Irr_Dec_Freq	= 395.88430144[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE




```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
blip( 16, 64 ,30 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

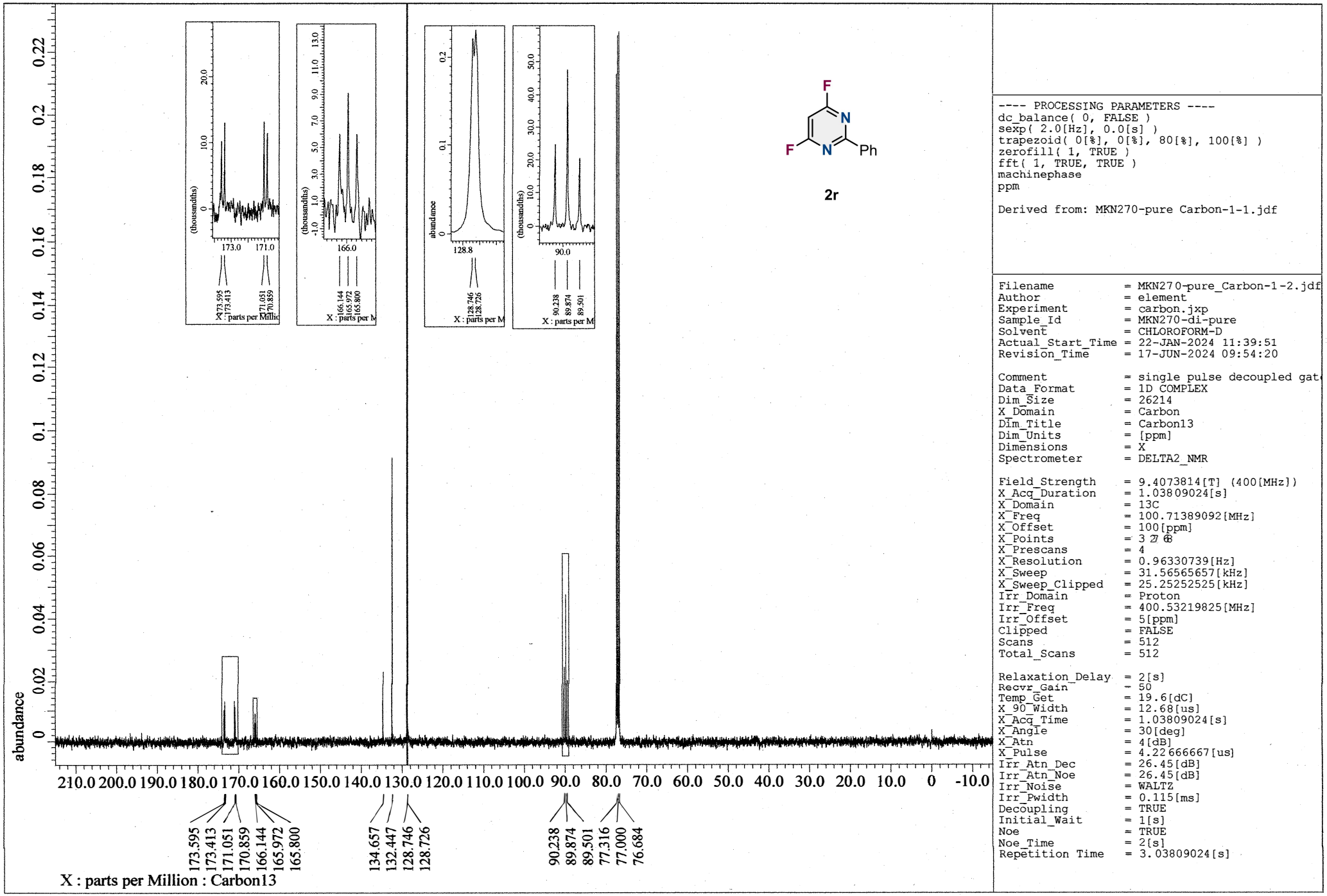
Filename	= MKN274 pure -int_single
Author	= eleme nt
Experiment	= s inge_pulse.jxp
Sample_Id	= MKN274-pure-int
Solv ent	= CHLOROFORM-D
Actual_Start_Time	= 20 -JAN-202415:12:22
Revision_Time	= 17 -JUN -202410:23:33
Comment	= single_pulse
Data_Format	= 1D COMP EX
Dim_Size	= 13107
X_Domain	= Fluorine19
Dim_Title	= Fluorine 19
Dim_Units	= [ppm]
Dimensions	= X
Spe ctome ter	= DELTA2_N MR
Field_Strength	= 9.2982153[T] (400[MHz]
X_Acq_D uration	= 89.12896[ms]
X_Domain	= Fluorine19
X_Freq	= 372.50336686[MHz]
X_Offset	= -100[ppm]
X_Points	= 16384
X_Pre scans	= 1
X_Resolution	= 11.21969784[Hz]
X_Sweep	= 183.82352941[k Hz]
X_Sweep_Clipped	= 147.05882353[kHz]
Irr_Domain	= Fluorine19
Irr_Freq	= 372.50336686[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Fluorine19
Tri_Fre q	= 372.50336686[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2.0[us]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_De lay	= 5[s]
Recvr_Gain	= 56
Temp_Get	= 18.8[dC]
X_90_Width	= 8.03[us]
X_Acq_Time	= 89.12896[ms]
X_Angle	= 45[deg]
X_Atn	= 5[dB]
X_Pulse	= 4.015[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Lo p	= 500
Dante_Pr esat	= FALSE
Decimation_Rate	= 0
Initial_Wait	= 1[s]
Phase	= {0, 90, 270, 180, 180,



2r

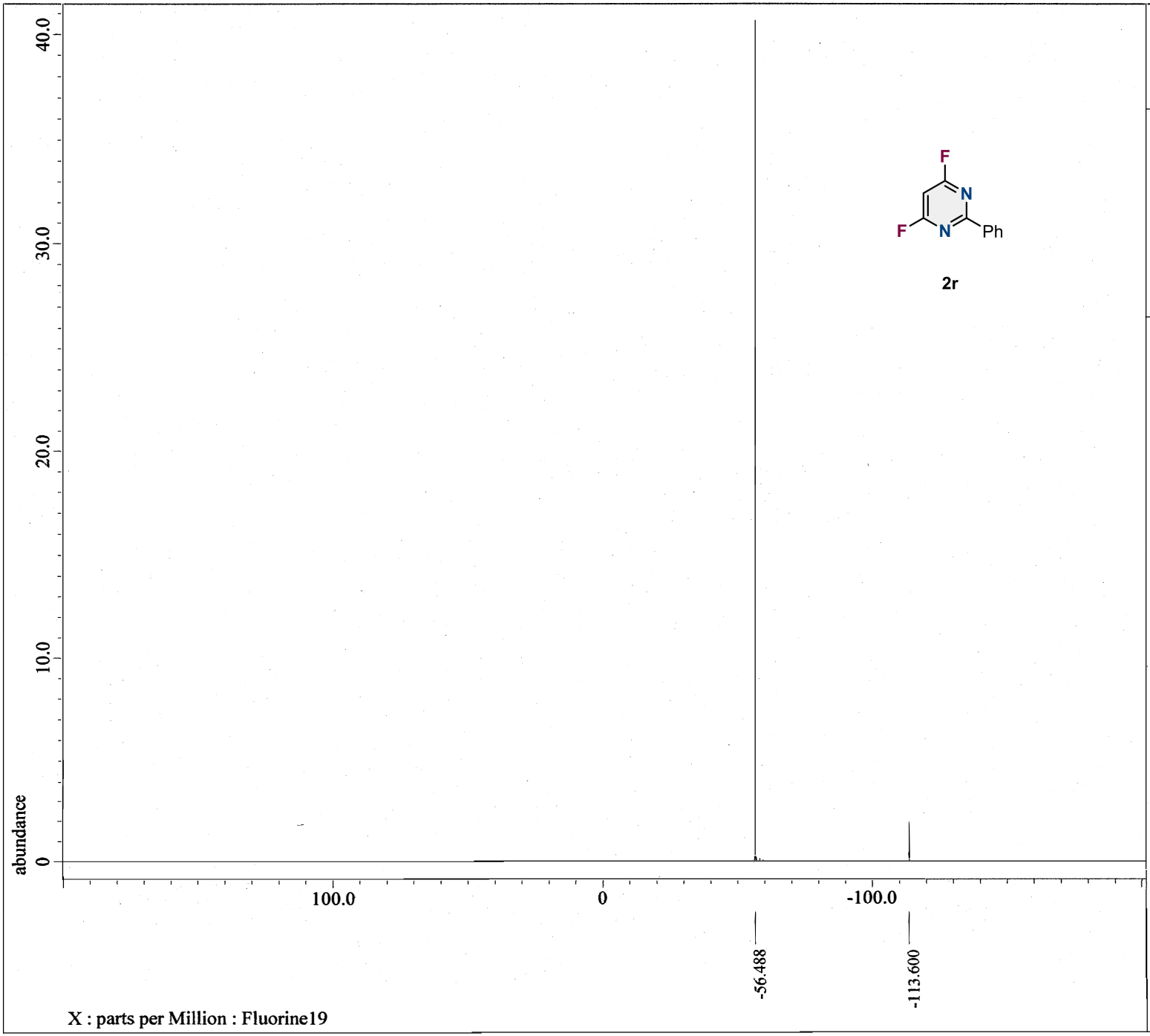
```
-  --PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: MKN270-pure Proton-1-1.jdf
```

```
Filename            = MKN270-pure_Proton-1-2.jdf
Author              = element
Experiment          = proton.jxp
Sample_Id           = MKN270   -pure
Solvent             = CHLOROFORM-D
Actual_Start_Time   = 22   -JUN-2024 11:13:58
Revision_Time       = 17-JUN-2024 09:47:51

Comment             = single_pulse
Data_Format         = 1D COMPLEX
Dim_Size            = 13107
X_Domain            = Proton
Dim_Title           = Proton
Dim_Units           = [ppm]
Dimensions          = X
Spectrometer        = DELTA2_N   MR

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

Relaxation_Delay    = 5[s]
Recvr_Gain          = 44
Temp_Get            = 19.6[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]
```



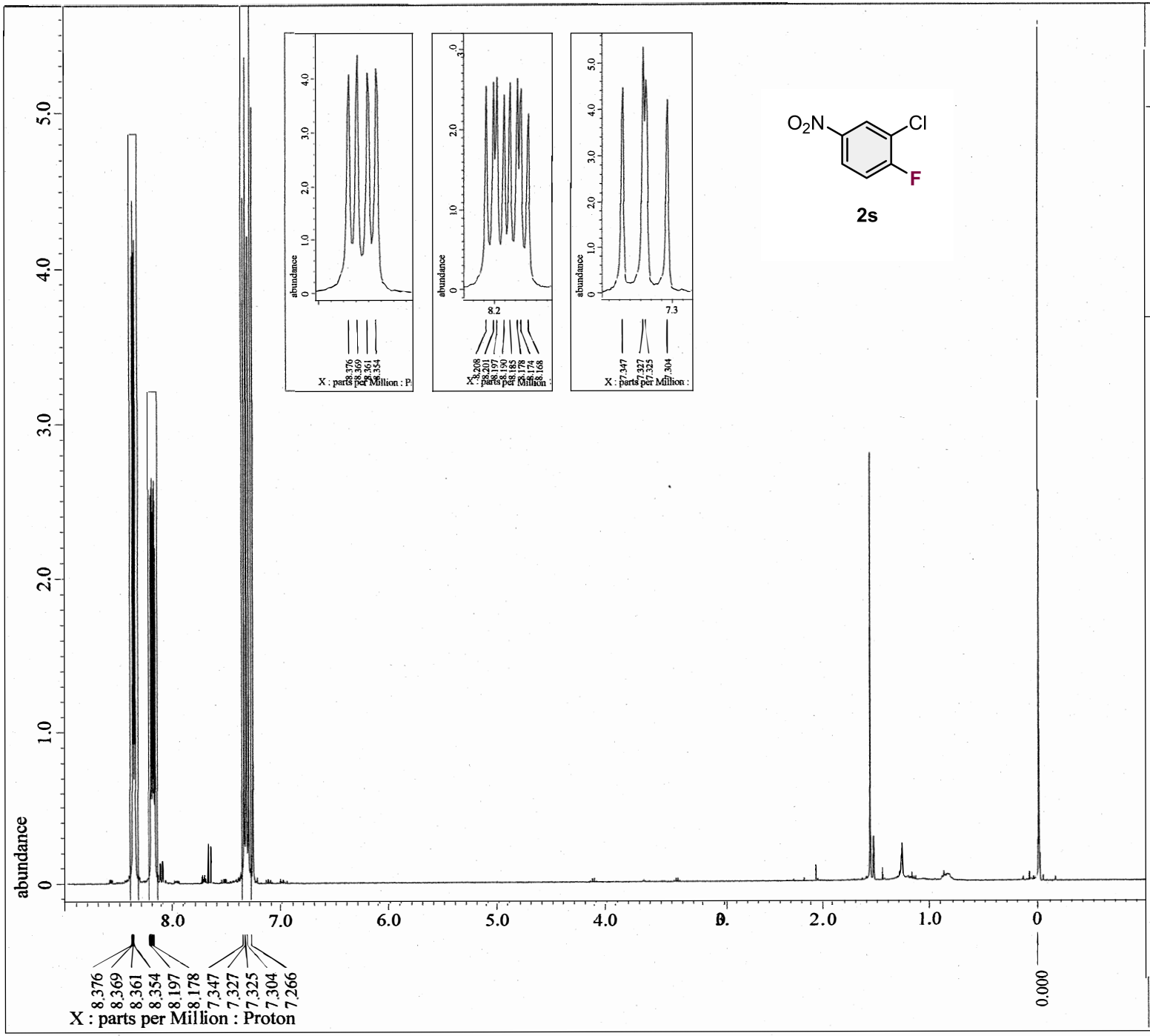

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: MKN270-pure Carbon-1-1.jdf
```

Filename	= MKN270-pure_Carbon-1-2.jdf
Author	= element
Experiment	= carbon.jxp
Sample_Id	= MKN270-di-pure
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 22-JAN-2024 11:39:51
Revision_Time	= 17-JUN-2024 09:54:20
Comment	= single pulse decoupled gat
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	= 512
Total_Scans	= 512
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 19.6[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 )
blip( 16, 64, 30 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

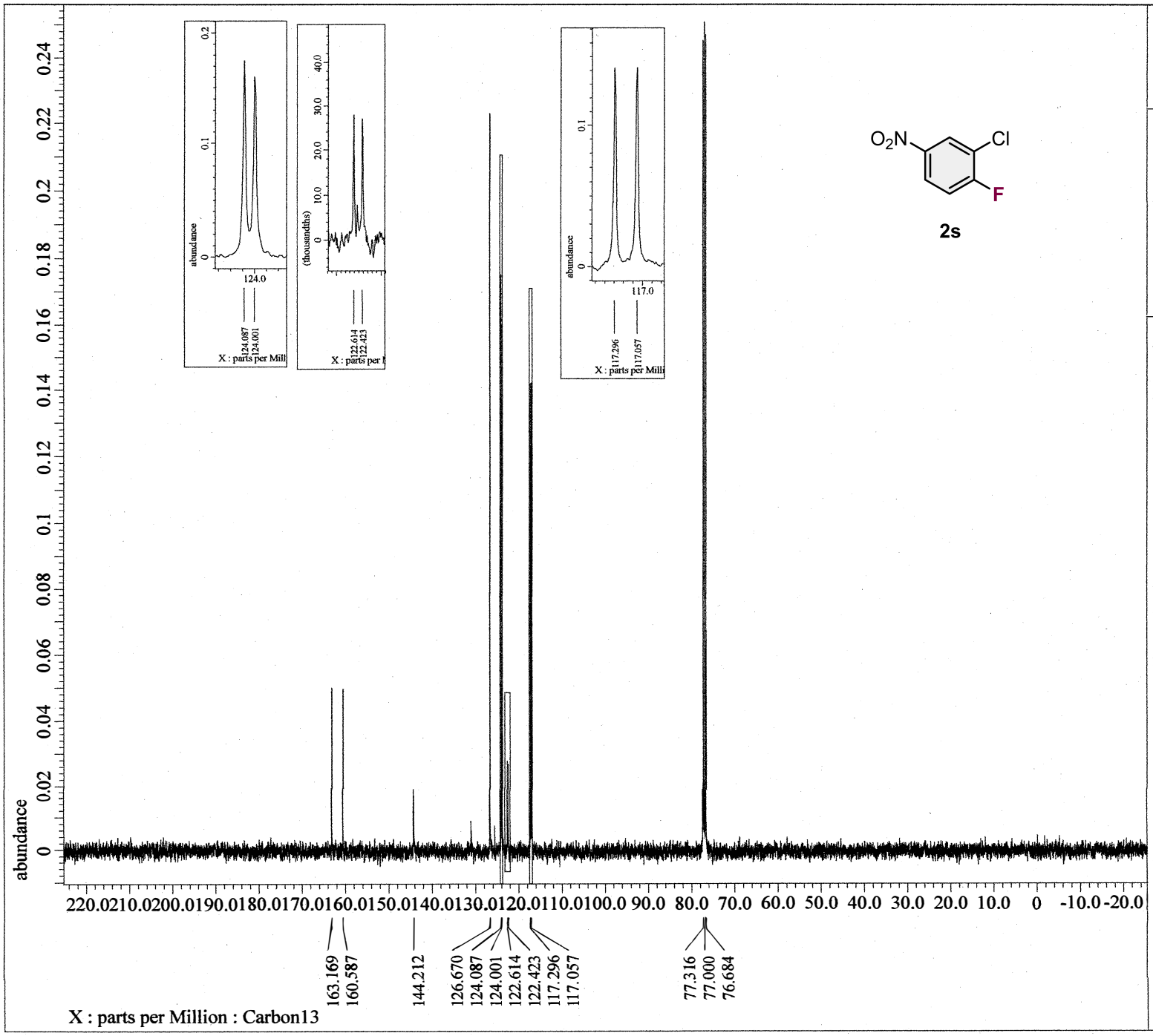
```
Filename            = MKN270-pur eint_single_pul
Author              = element
Experiment          = single_pulse.jxp
Sample_Id           = MKN270-di-pure-int
Solvent             = CHLOROFORM-D
Actual_Start_Time   = 22-JAN-2024 11:25:33
Revision_Time       = 24-JAN-2024 12:15:35

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            = 19.2[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]
```



2s

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

Derived from: MKN283-pure Proton-1-1.jdf
```

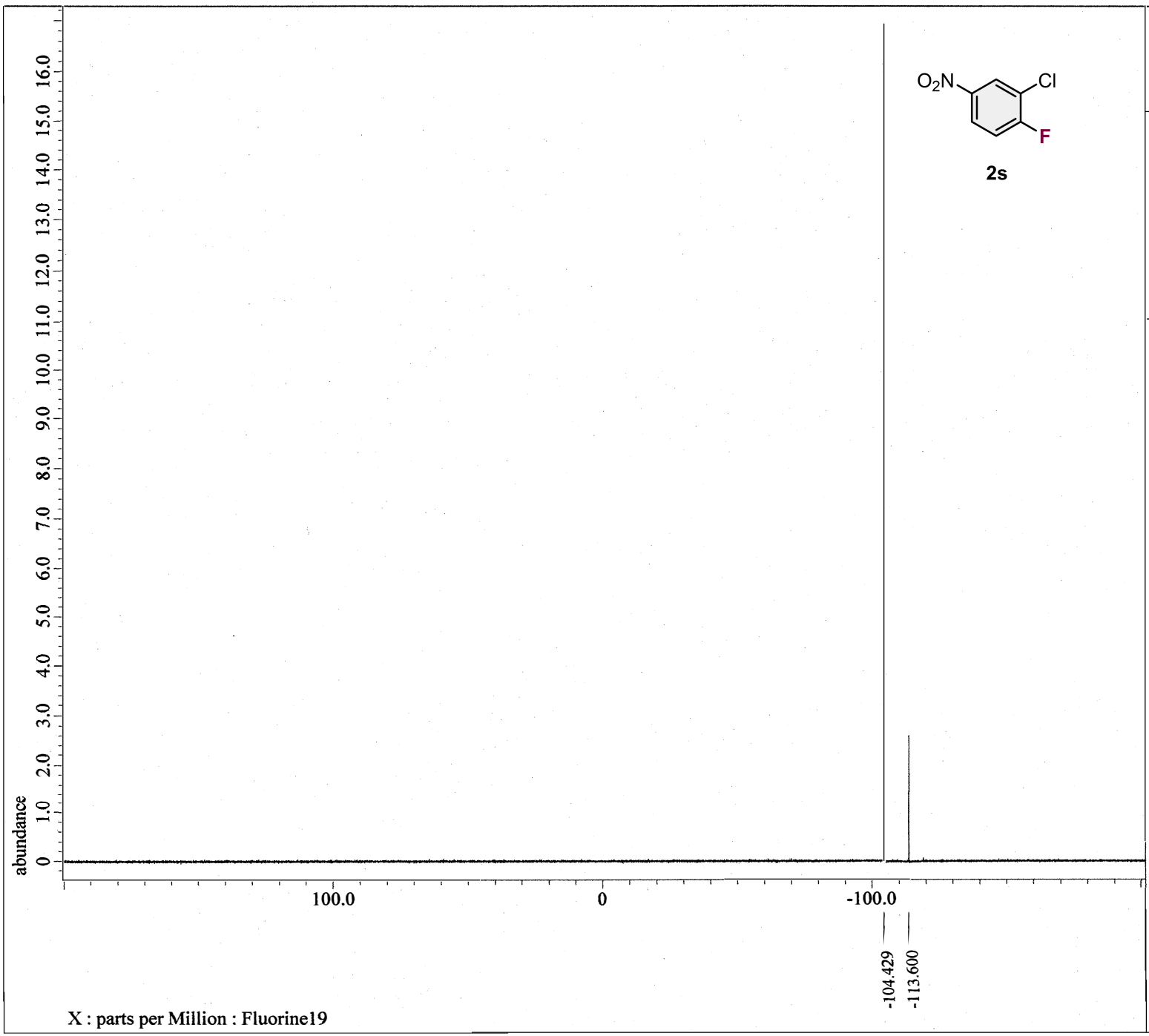
```
Filename            = MKN283-pure_Proton-1-2.jdf
Author              = element
Experiment          = proton.jxp
Sample_Id           = MKN283-pure
Solvent             = CHLOROFORM-D
Actual_Start_Time   = 25-JAN-2024 13:49:52
Revision_Time       = 17-JUN-2024 09:15:08

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

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

Relaxation_Delay    = 5[s]
Recvr_Gain          = 48
Temp_Get            = 19[dC]
X_90_Width          = 6.7[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]
```



2s

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

Derived from: MKN283-pure Carbon-1-1.jdf
```

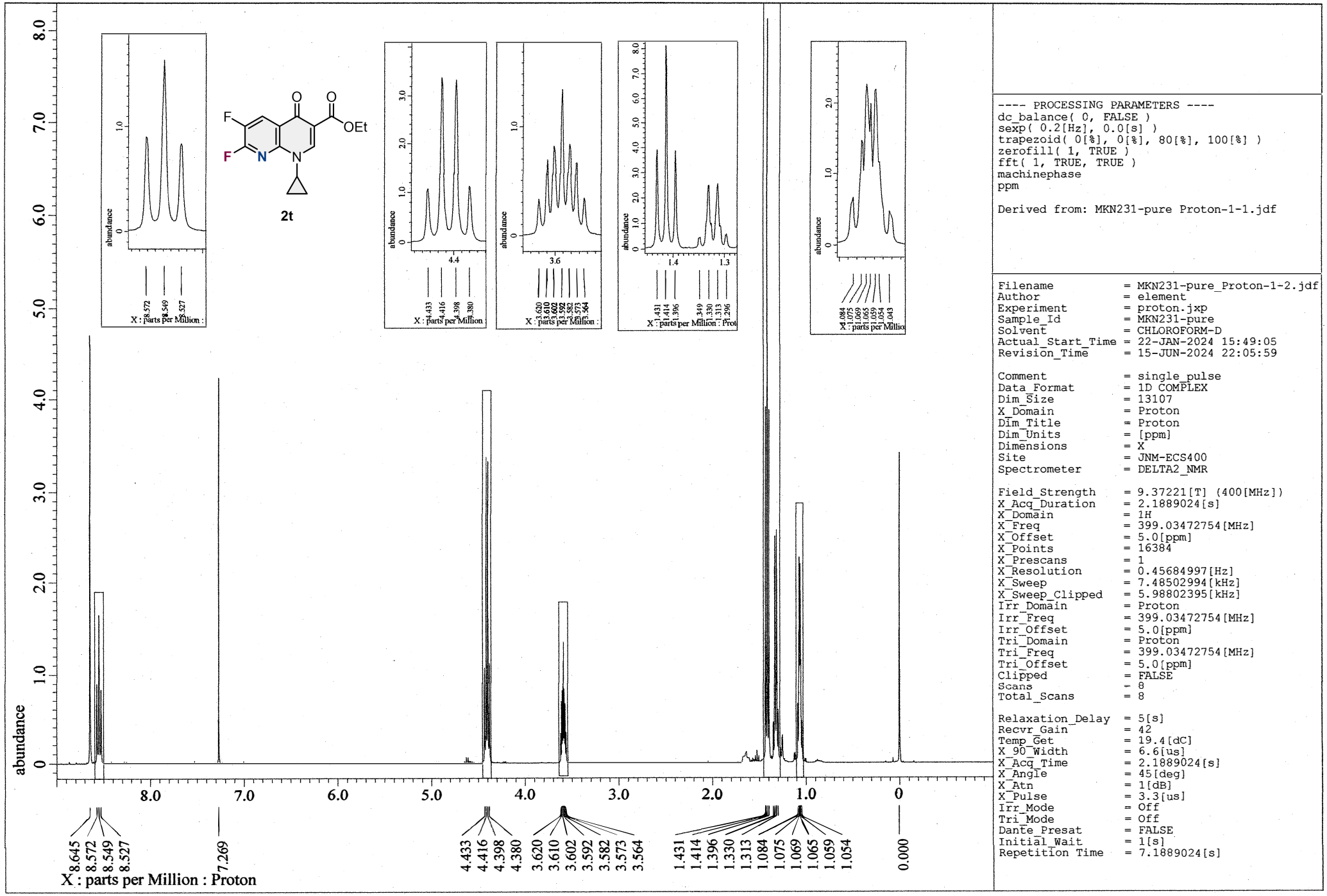
```
Filename            = MKN283-pure_Carbon-1-2.jdf
Author              = element
Experiment          = carbon.jxp
Sample_Id           = MKN283-pure
Solvent             = CHLOROFORM-D
Actual_Start_Time   = 25-JAN-2024 14:19:32
Revision_Time       = 17-JUN-2024 09:34:36

Comment             = single pulse decoupled gat
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               = 257
Total_Scans         = 257

Relaxation_Delay    = 2[s]
Recvr_Gain          = 50
Temp_Get            = 19.5[dC]
X_90_Width          = 12.68[us]
X_Acq_Time          = 1.03809024[s]
X_Angle             = 30[deg]
X_Atn               = 4[dB]
X_Pulse             = 4.22666667[us]
Irr_Atn_Dec         = 26.45[dB]
Irr_Atn_Noe         = 26.45[dB]
Irr_Noise           = WALTZ
Irr_Pwidth          = 0.115[ms]
Decoupling          = TRUE
Initial_Wait        = 1[s]
Noe                 = TRUE
Noe_Time            = 2[s]
Repetition Time     = 3.03809024[s]
```



2s

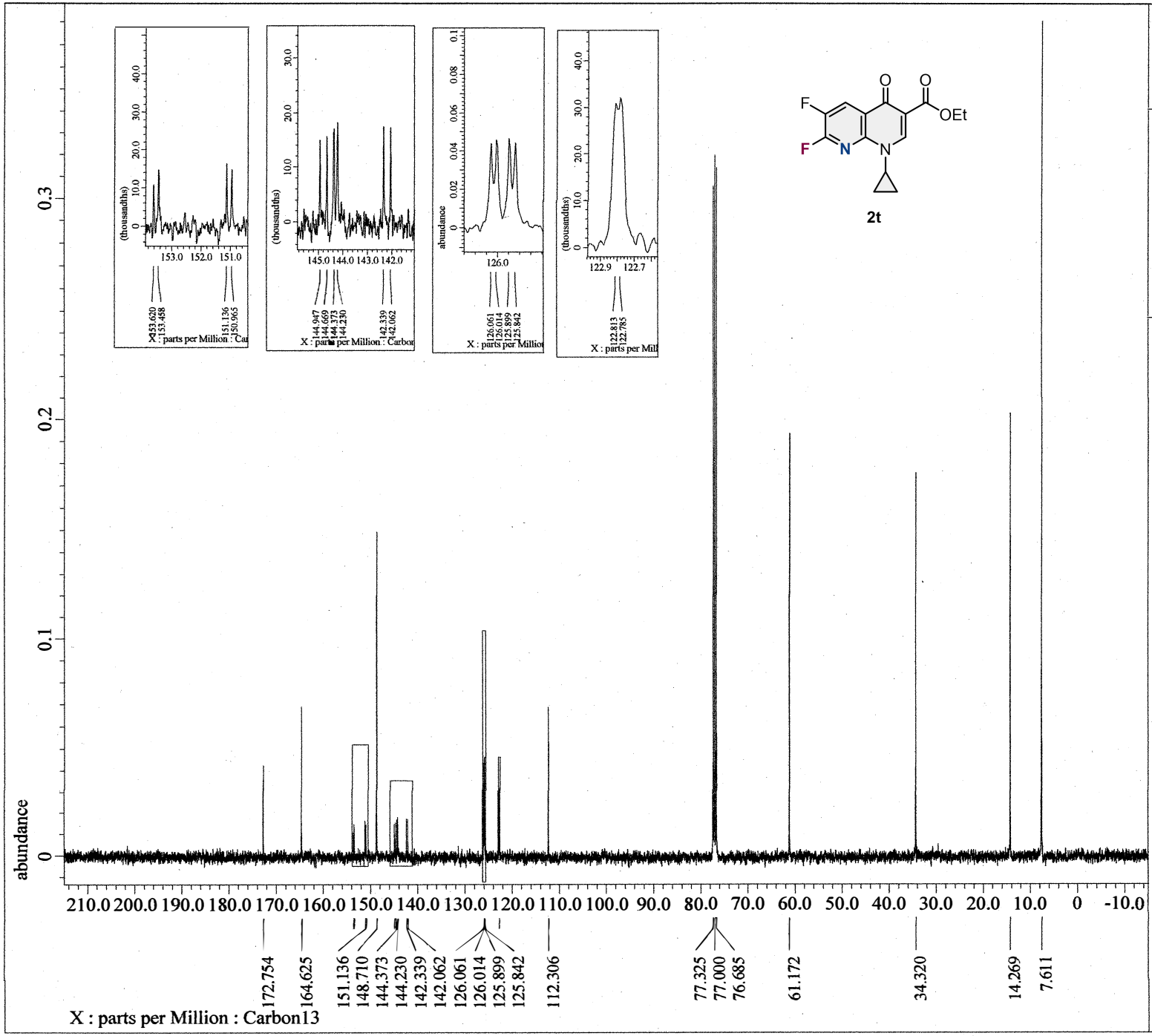
```
---- P ROCESSING PARAMETERS ----
dc balance( 0, FALSE)
sine( 0.2[Hz], 0.0[s])
trapezoid( 0[%], 0[%], 80[%],100[%])
zerofill( 1 )
blip( 16, 64, 30 )
fft( 1, TRUE, TRUE )
machine phase
ppm
```

```
Filename            = MKN283-pure-int_single_pul
Author              = element
Experiment          = single_pulse.jxp
Sample_Id           = MKN283-pure-int
Solvent             = CHLOROFORM-D
Actual_Start_Time   = 25-JAN-2024 13:28:28
Revision_Time       = 17-JUN-2024 09:39:52

Comment             = single_pulse
Data_Format         = 1D COMPLEX
Dim_Size            = 13107
X_Domain            = Fluori
Dim_Title           = Fluorine19
Dim_Units           = [ppm]
Dimension           = 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            = 19[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]
RepetitionTime      = 5.08650752[s]
```




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

Derived from: MKN231-pure Proton-1-1.jdf
```

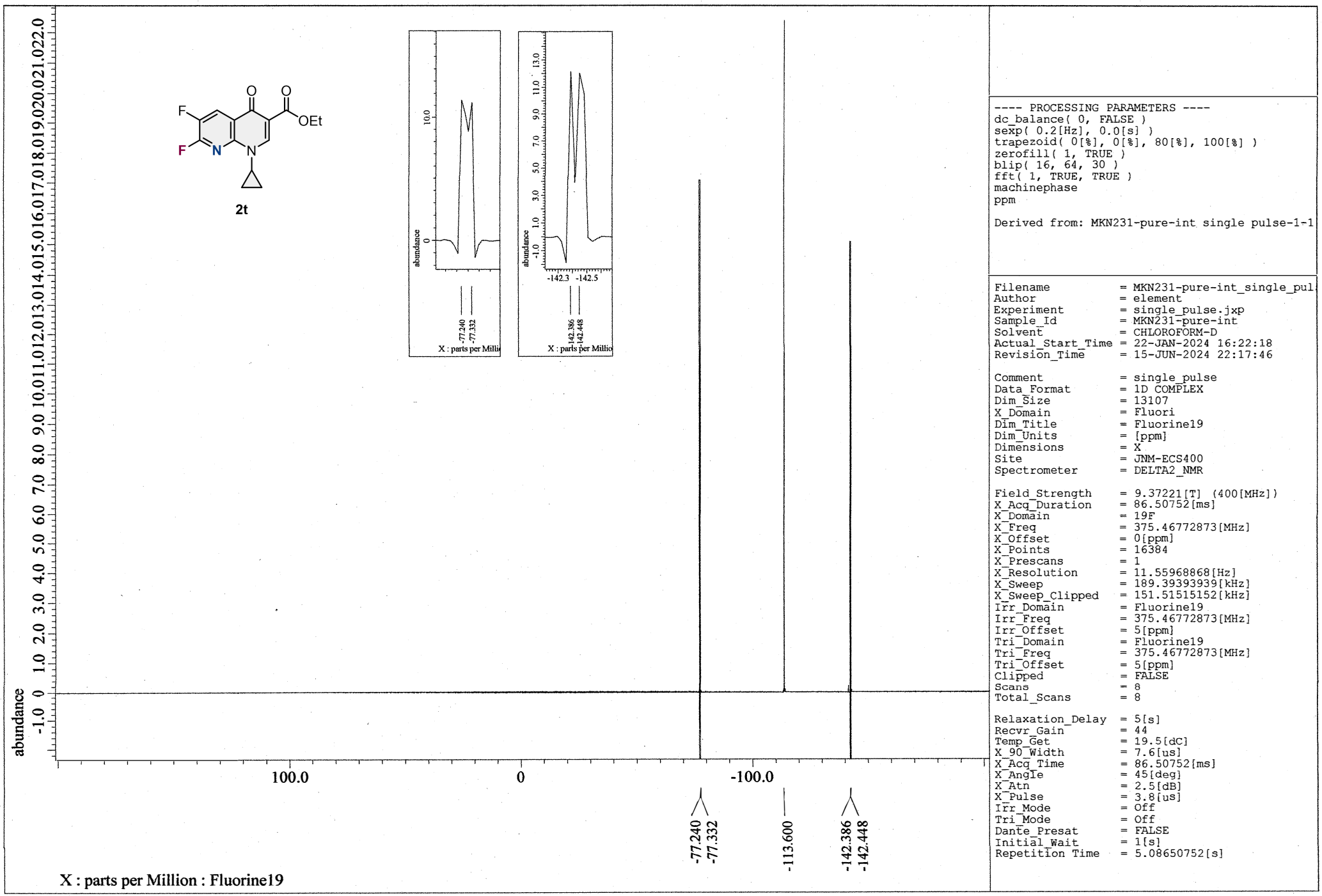
Filename	= MKN231-pure_Proton-1-2.jdf
Author	= element
Experiment	= proton.jxp
Sample_Id	= MKN231-pure
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 22-JAN-2024 15:49:05
Revision_Time	= 15-JUN-2024 22:05:59
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECS400
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.37221[T] (400[MHz])
X_Acq_Duration	= 2.1889024[s]
X_Domain	= 1H
X_Freq	= 399.03472754[MHz]
X_Offset	= 5.0[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45684997[Hz]
X_Sweep	= 7.48502994[kHz]
X_Sweep_Clipped	= 5.98802395[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.03472754[MHz]
Irr_Offset	= 5.0[ppm]
Tri_Domain	= Proton
Tri_Freq	= 399.03472754[MHz]
Tri_Offset	= 5.0[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 42
Temp_Get	= 19.4[dC]
X_90_Width	= 6.6[us]
X_Acq_Time	= 2.1889024[s]
X_Angle	= 45[deg]
X_Atn	= 1[dB]
X_Pulse	= 3.3[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition Time	= 7.1889024[s]



2t

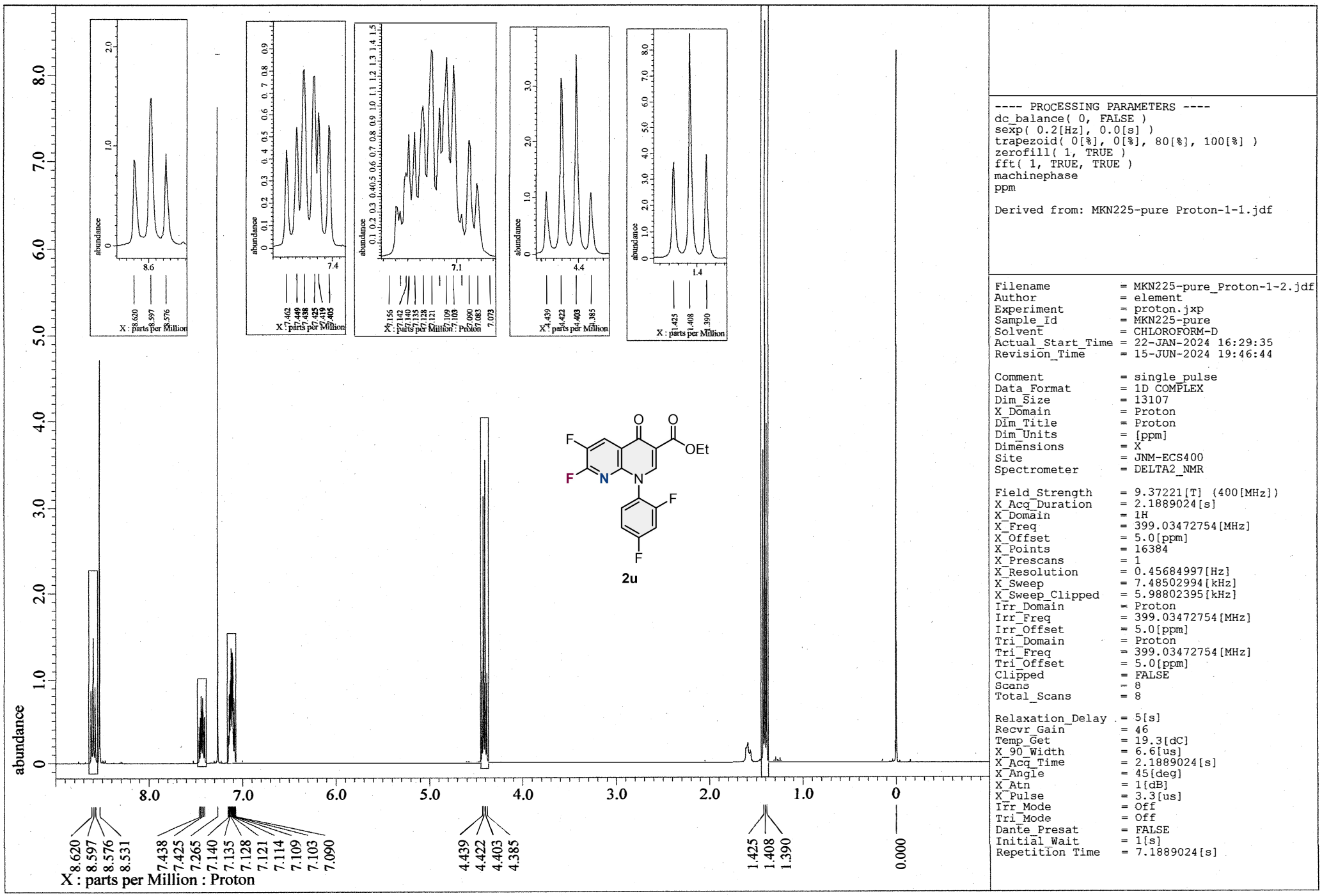
```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: MKN231-pure Carbon-1-1.jdf
```

Filename	= MKN231-pure_Carbon-1-2.jdf
Author	= element
Experiment	= carbon.jxp
Sample_Id	= MKN231-pure
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 22-JAN-2024 16:37:40
Revision_Time	= 15-JUN-2024 22:34:5●
Comment	= single pulse decoupled gat
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECS400
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.37221[T] (400[MHz])
X_Acq_Duration	= 1.04333312[s]
X_Domain	= 13C
X_Freq	= 100.33735165[MHz]
X_Offset	= 100.0[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.95846665[Hz]
X_Sweep	= 31.40703518[kHz]
X_Sweep_Clipped	= 25.12562814[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.03472754[MHz]
Irr_Offset	= 5.0[ppm]
Clipped	= FALSE
Scans	= 256
Total_Scans	= 256
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 19.7[dC]
X_90_Width	= 10.9[us]
X_Acq_Time	= 1.04333312[s]
X_Angle	= 30[deg]
X_Atn	= 5.4[dB]
X_Pulse	= 3.63333333[us]
Irr_Atn_Dec	= 25.823[dB]
Irr_Atn_Noe	= 25.823[dB]
Irr_Noise	= WALTZ
Irr_Pwidth	= 0.115[ms]
Decoupling	= TRUE
Initial_Wait	= 1[s]
Noe	= TRUE
Noe_Time	= 2[s]
Repetition Time	= 3.04333312[s]




```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
blip( 16, 64, 30 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: MKN231-pure-int single pulse-1-1
```

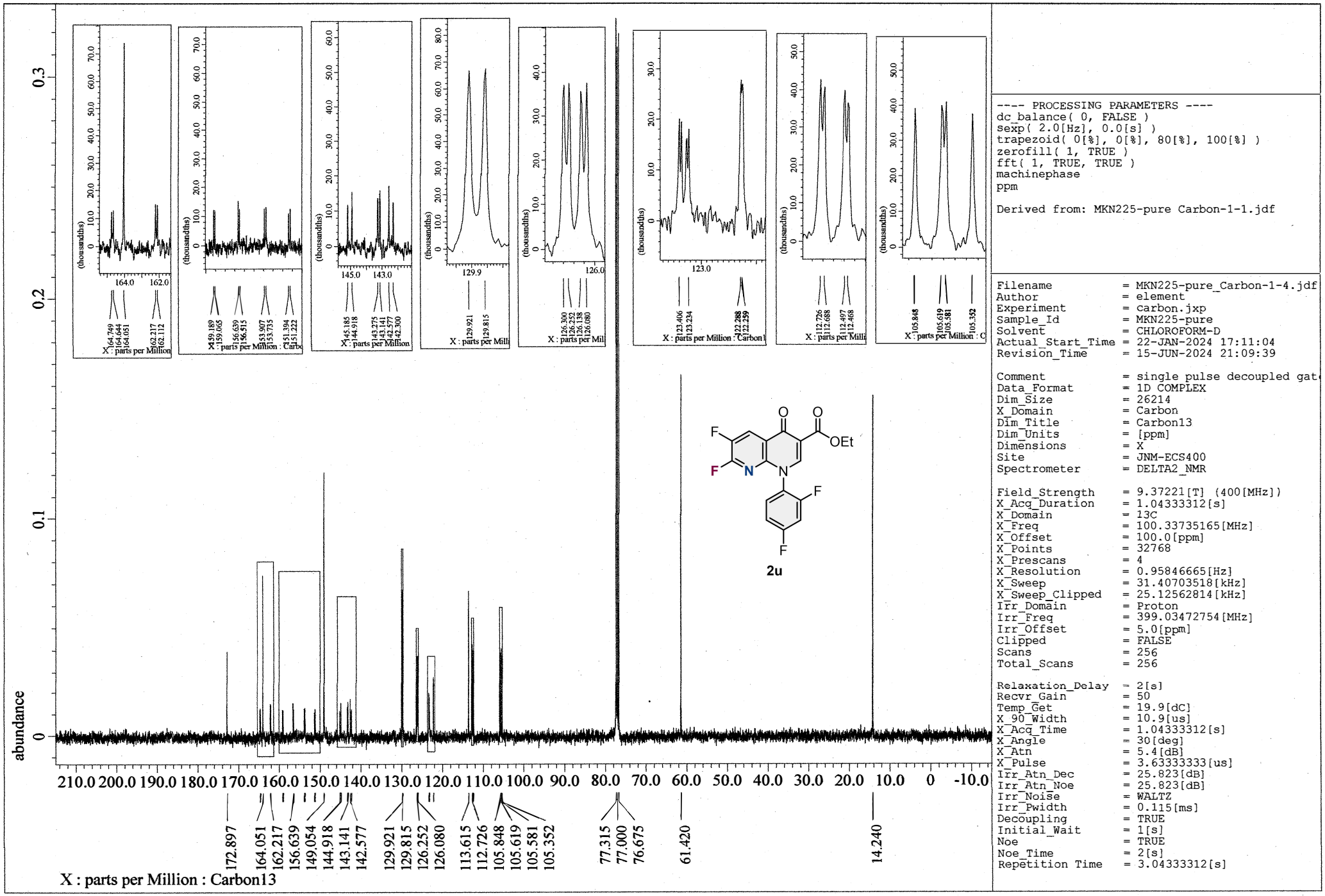
Filename	= MKN231-pure-int_single_pul
Author	= element
Experiment	= single_pulse.jxp
Sample_Id	= MKN231-pure-int
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 22-JAN-2024 16:22:18
Revision_Time	= 15-JUN-2024 22:17:46
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Fluori
Dim_Title	= Fluorine19
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECS400
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.37221[T] (400[MHz])
X_Acq_Duration	= 86.50752[ms]
X_Domain	= 19F
X_Freq	= 375.46772873[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	= 375.46772873[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Fluorine19
Tri_Freq	= 375.46772873[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 44
Temp_Get	= 19.5[dC]
X_90_Width	= 7.6[us]
X_Acq_Time	= 86.50752[ms]
X_Angle	= 45[deg]
X_Atn	= 2.5[dB]
X_Pulse	= 3.8[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition Time	= 5.08650752[s]



2u

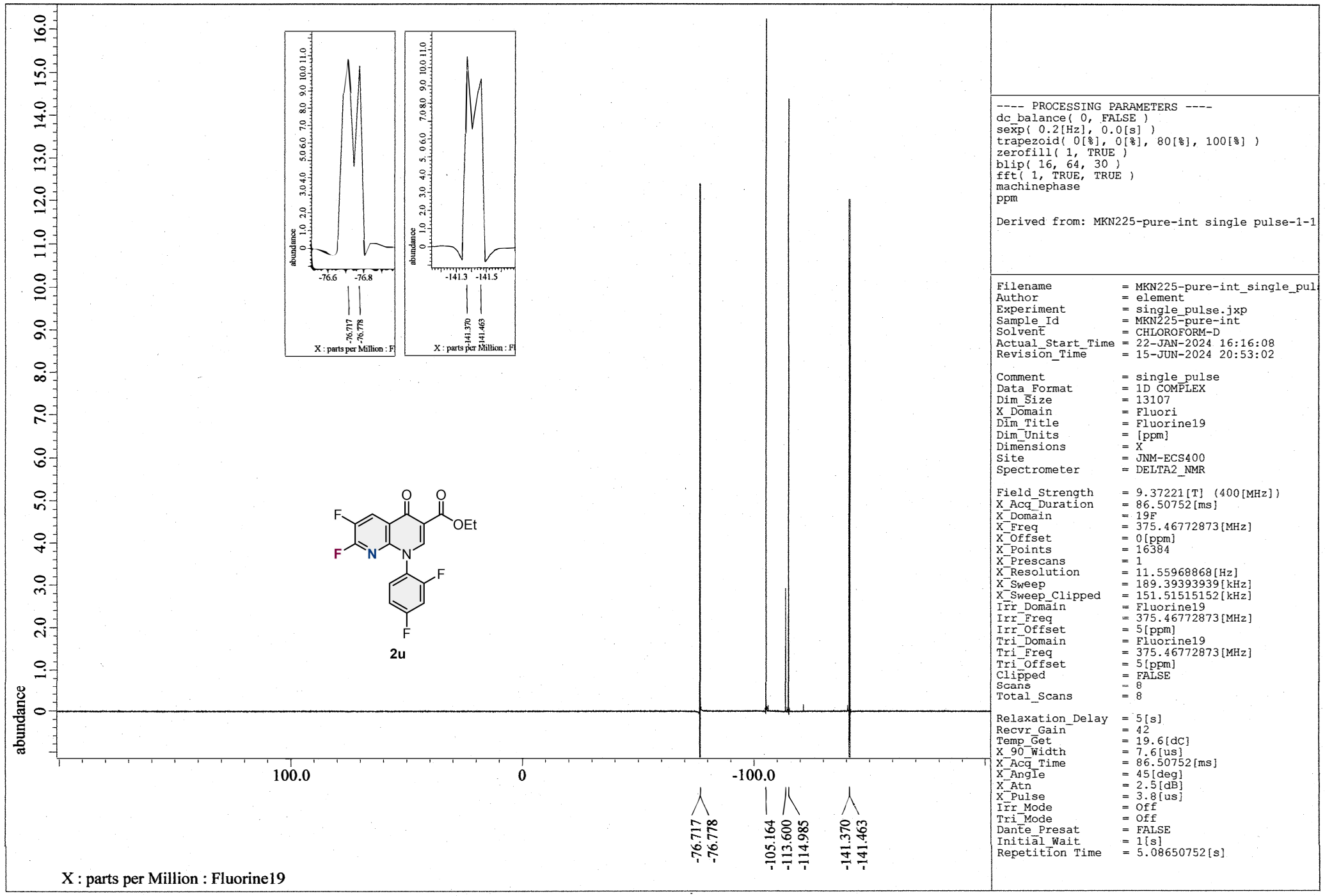
```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: MKN225-pure Proton-1-1.jdf
```

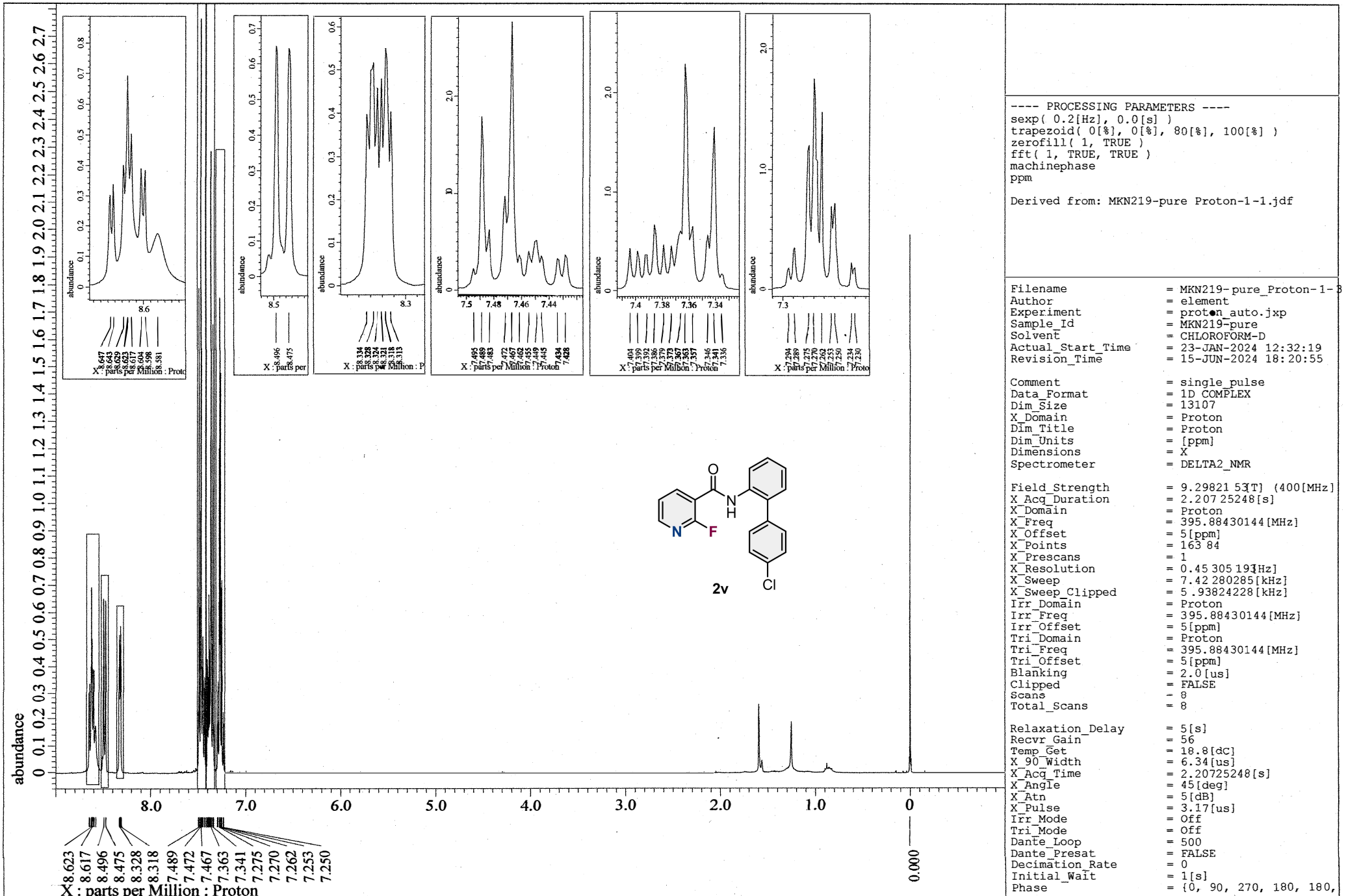
Filename	= MKN225-pure_Proton-1-2.jdf
Author	= element
Experiment	= proton.jxp
Sample_Id	= MKN225-pure
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 22-JAN-2024 16:29:35
Revision_Time	= 15-JUN-2024 19:46:44
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECS400
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.37221[T] (400[MHz])
X_Acq_Duration	= 2.1889024[s]
X_Domain	= 1H
X_Freq	= 399.03472754[MHz]
X_Offset	= 5.0[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45684997[Hz]
X_Sweep	= 7.48502994[kHz]
X_Sweep_Clipped	= 5.98802395[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.03472754[MHz]
Irr_Offset	= 5.0[ppm]
Tri_Domain	= Proton
Tri_Freq	= 399.03472754[MHz]
Tri_Offset	= 5.0[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 46
Temp_Get	= 19.3[dC]
X_90_Width	= 6.6[us]
X_Acq_Time	= 2.1889024[s]
X_Angle	= 45[deg]
X_Atn	= 1[dB]
X_Pulse	= 3.3[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition Time	= 7.1889024[s]




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

Derived from: MKN225-pure Carbon-1-1.jdf
```

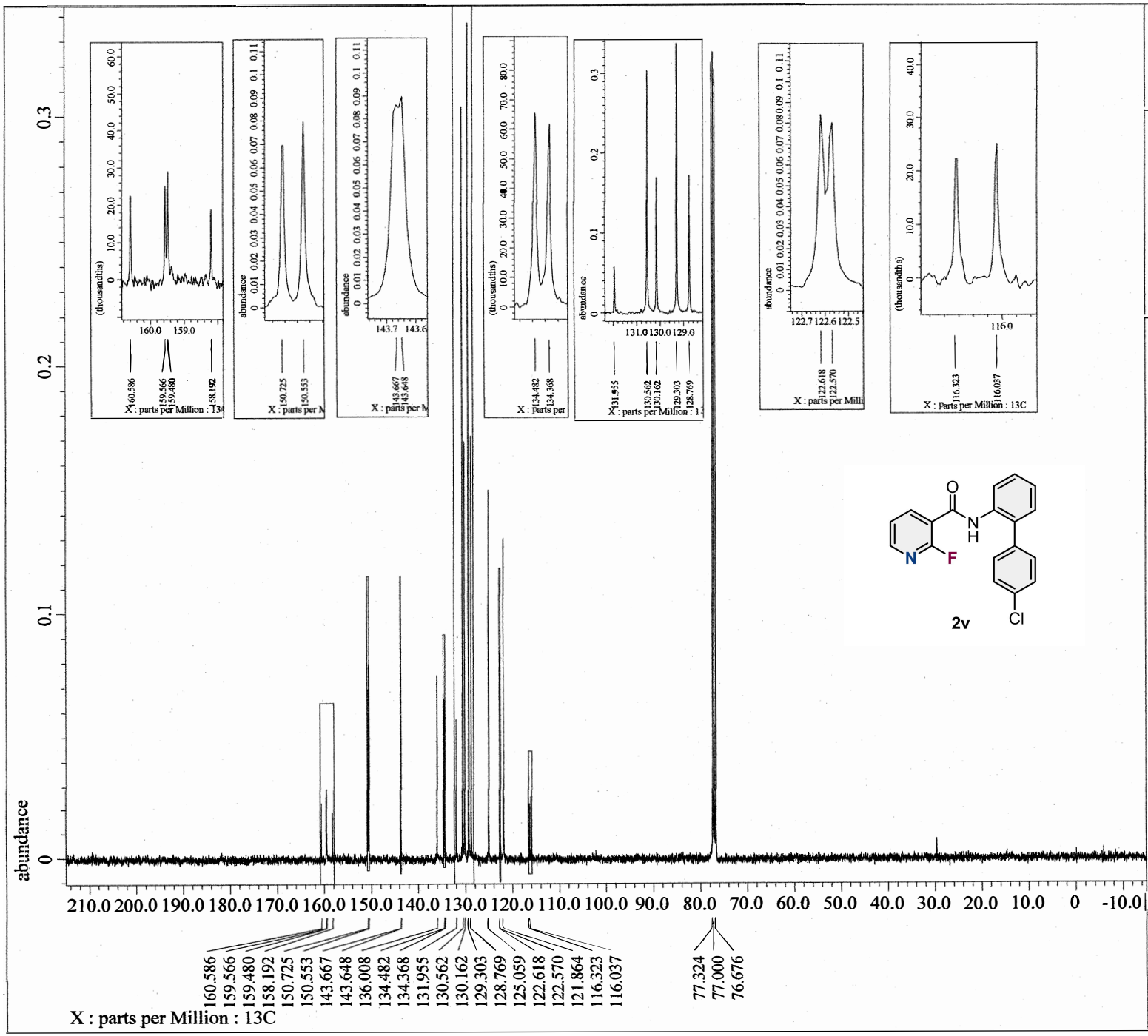
Filename	= MKN225-pure_Carbon-1-4.jdf
Author	= element
Experiment	= carbon.jxp
Sample_Id	= MKN225-pure
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 22-JAN-2024 17:11:04
Revision_Time	= 15-JUN-2024 21:09:39
Comment	= single pulse decoupled gat
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECS400
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.37221[T] (400[MHz])
X_Acq_Duration	= 1.04333312[s]
X_Domain	= 13C
X_Freq	= 100.33735165[MHz]
X_Offset	= 100.0[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.95846665[Hz]
X_Sweep	= 31.40703518[kHz]
X_Sweep_Clipped	= 25.12562814[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.03472754[MHz]
Irr_Offset	= 5.0[ppm]
Clipped	= FALSE
Scans	= 256
Total_Scans	= 256
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 19.9[dC]
X_90_Width	= 10.9[us]
X_Acq_Time	= 1.04333312[s]
X_Angle	= 30[deg]
X_Atn	= 5.4[dB]
X_Pulse	= 3.63333333[us]
Irr_Atn_Dec	= 25.823[dB]
Irr_Atn_Noe	= 25.823[dB]
Irr_Noise	= WALTZ
Irr_Pwidth	= 0.115[ms]
Decoupling	= TRUE
Initial_Wait	= 1[s]
Noe	= TRUE
Noe_Time	= 2[s]
Repetition Time	= 3.04333312[s]


abundance
X : parts per Million : Fluorine19
100.0
0
-100.0
-76.717
-76.778
-105.164
-113.600
-114.985
-141.370
-141.463
2u
---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1, TRUE)
blip(16, 64, 30)
fft(1, TRUE, TRUE)
machinephase
ppm
Derived from: MKN225-pure-int single pulse-1-1
Filename = MKN225-pure-int_single_pul
Author = element
Experiment = single_pulse.jxp
Sample_Id = MKN225-pure-int
Solvent = CHLOROFORM-D
Actual_Start_Time = 22-JAN-2024 16:16:08
Revision_Time = 15-JUN-2024 20:53:02
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
X_Domain = Fluori
Dim_Title = Fluorine19
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_Strength = 9.37221[T] (400[MHz])
X_Acq_Duration = 86.50752[ms]
X_Domain = 19F
X_Freq = 375.46772873[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 = 375.46772873[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Fluorine19
Tri_Freq = 375.46772873[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 42
Temp_Get = 19.6[dC]
X_90_Width = 7.6[us]
X_Acq_Time = 86.50752[ms]
X_Angle = 45[deg]
X_Atn = 2.5[dB]
X_Pulse = 3.8[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition Time = 5.08650752[s]



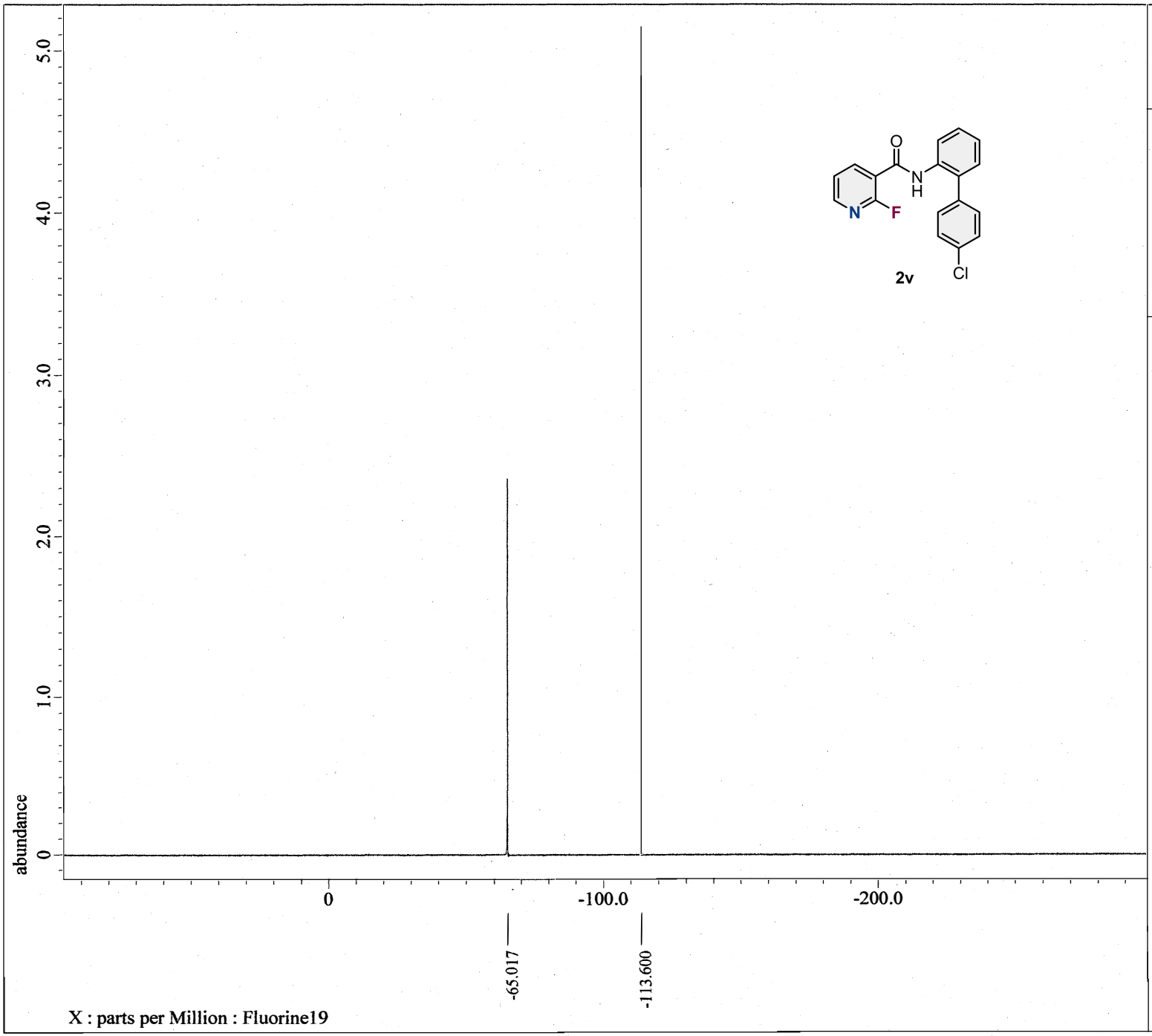

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm

Derived from: MKN219-pure Proton-1-1.jdf
```

Filename	= MKN219-pure_Proton-1-1
Author	= element
Experiment	= proton_auto.jxp
Sample_Id	= MKN219-pure
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 23-JAN-2024 12:32:19
Revision_Time	= 15-JUN-2024 18:20:55
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	= 9.29821 53[T] (400[MHz]
X_Acq_Duration	= 2.207 25248[s]
X_Domain	= Proton
X_Freq	= 395.88430144[MHz]
X_Offset	= 5[ppm]
X_Points	= 163 84
X_Prescans	= 1
X_Resolution	= 0.45 305 193[Hz]
X_Sweep	= 7.42 280285[kHz]
X_Sweep_Clipped	= 5 .93824228[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 395.88430144[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2.0[us]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 56
Temp_Get	= 18.8[dC]
X_90_Width	= 6.34[us]
X_Acq_Time	= 2.20725248[s]
X_Angle	= 45[deg]
X_Atn	= 5[dB]
X_Pulse	= 3.17[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 500
Dante_Presat	= FALSE
Decimation_Rate	= 0
Initial_Wait	= 1[s]
Phase	= {0, 90, 270, 180, 180,




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

Derived from: MKN219-pure Carbon-1.jdf
```

```
Filename            = MKN219-pure_Carbon-2.jdf
Author              = element
Experiment          = single_pulse_dec
Sample_Id           = 1
Solvent             = CHLOROFORM-D
Actual_Start_Time   = 23-JAN-2024 19:20:17
Revision_Time       = 15-JUN-2024 18:49:15

Comment             = single pulse decoupled gat
Data_Format         = 1D COMPLEX
Dim_Size            = 26214
X_Domain            = 13C
Dim_Title           = 13C
Dim_Units           = [ppm]
Dimensions          = X
Site                = ECS 400
Spectrometer        = JNM-ECS400

Field_Strength      = 9.20197068[T] (390[MHz])
X_Acq_Duration      = 1.06430464[s]
X_Domain            = 13C
X_Freq              = 98.51479726[MHz]
X_Offset            = 100[ppm]
X_Points            = 32768
X_Prescans          = 4
X_Resolution        = 0.93958061[Hz]
X_Sweep             = 30.78817734[kHz]
Irr_Domain          = 1H
Irr_Freq            = 391.78655441[MHz]
Irr_Offset          = 5[ppm]
Clipped             = FALSE
Scans               = 509
Total_Scans         = 509

Relaxation_Delay    = 2[s]
Recvr_Gain          = 50
Temp_Get            = 19.9[dC]
X_90_Width          = 9.46[us]
X_Acq_Time          = 1.06430464[s]
X_Angle             = 30[deg]
X_Atn               = 4.9[dB]
X_Pulse             = 3.15333333[us]
Irr_Atn_Dec         = 22.45[dB]
Irr_Atn_Noe         = 22.45[dB]
Irr_Noise           = WALTZ
Decoupling          = TRUE
Initial_Wait        = 1[s]
Noe                 = TRUE
Noe_Time            = 2[s]
Repetition Time     = 3.06430464[s]
```




```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
blip( 16, 64, 30 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

Filename	= MKN219-pure-int_single
Author	= element
Experiment	= single_pulse.jxp
Sample_Id	= MKN219-pure-int
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 23-JAN-2024 12:46:55
Revision_Time	= 15-JUN-2024 19:36:02
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Fluorine19
Dim_Title	= Fluorine19
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.2982153[T] (400[MHz]
X_Acq_Duration	= 89.12896[ms]
X_Domain	= Fluorine19
X_Freq	= 372.50336686[MHz]
X_Offset	= -100[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 11.21969784[Hz]
X_Sweep	= 183.82352941[kHz]
X_Sweep_Clipped	= 147.05882353[kHz]
Irr_Domain	= Fluorine19
Irr_Freq	= 372.50336686[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Fluorine19
Tri_Freq	= 372.50336686[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2.0[us]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 56
Temp_Get	= 19.3[dC]
X_90_Width	= 8.03[us]
X_Acq_Time	= 89.12896[ms]
X_Angle	= 45[deg]
X_Atn	= 5[dB]
X_Pulse	= 4.015[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 500
Dante_Presat	= FALSE
Decimation_Rate	= 0
Initial_Wait	= 1[s]
Phase	= {0, 90, 270, 180, 180,