Efficient Access to Materials-Oriented Aromatic Alkynes via the Mechanochemical Sonogashira Coupling of Solid Aryl Halides with Large Polycyclic Conjugated Systems

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1. Chemicals and Instrumentation.

The starting materials were obtained from commercial suppliers and used as received. Alkyne **1d** was prepared by our ball milling method. **2j** was prepared according to the literature.[1] Solvents were purchased from commercial suppliers and further dried over molecular sieve (MS 4Å). All mechanochemical reactions were carried out using grinding vessels in a Retsch MM400 mill (Figure S1). Both jars (1.5 mL, 10 mL) and balls (5 mm, 15 mm) are made of stainless (SUS400B and SUS420J2, respectively) (Figure S2). The heat gun Takagi HG-1450B with temperature control function was used for high-temperature ball-milling reactions (Figure S3). NMR spectra were recorded on JEOL JNM-ECS400 spectrometers (^{1}H: 400 MHz, ^{13}C: 100 MHz). $CDCl_3$ was employed as external standards. Multiplicity was recorded as follows: s = singlet, brs = broad singlet, d = doublet, t = triplet, q = quartet, quint = quintet, sept = septet, o = octet, m = multiplet. Dibromomethane was used as an internal standard to determine NMR yields. Recycle preparative gel permeation chromatography (GPC) was conducted with a JAI LaboACE LC-5060 using $CHCl_3$ as an eluent with JAIGEL-1H. Thermography was recorded with an NEC Avio Thermo GEAR G120. Single crystal X-ray structural analyses were carried out on a Rigaku XtaLAB PRO MM007 diffractometer using graphite monochromated Cu-K_a radiation and PILATUS-200K detector. The structure was solved by direct methods and expanded using Fourier techniques. Non-hydrogen atoms were refined anisotropically. Hydrogen atoms were refined using the riding model. All calculations were performed using the Olex2 crystallographic software package except for refinement, which was performed using SHELXL-2018.[2] Emission spectra were recorded on a Hitachi F-7000 spectrometer. Absorption spectra were recorded on a Hitachi U-2910 spectrometer. The emission quantum yields were recorded on a Hamamatsu Quantaurus-QY spectrometer with an integrating sphere. High-resolution mass spectra were recorded at the Global Facility Center, Hokkaido University.

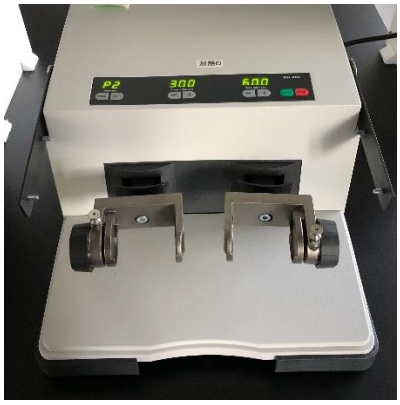


Figure S1. Retsch MM400 used in this study.

Figure S2. Stainless jar (1.5 mL, left; 5 mL, right) and ball (5 mm, left; 15 mm, right) used in this study.

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

2. List of Aryl Halides and Alkynes Used in This Study

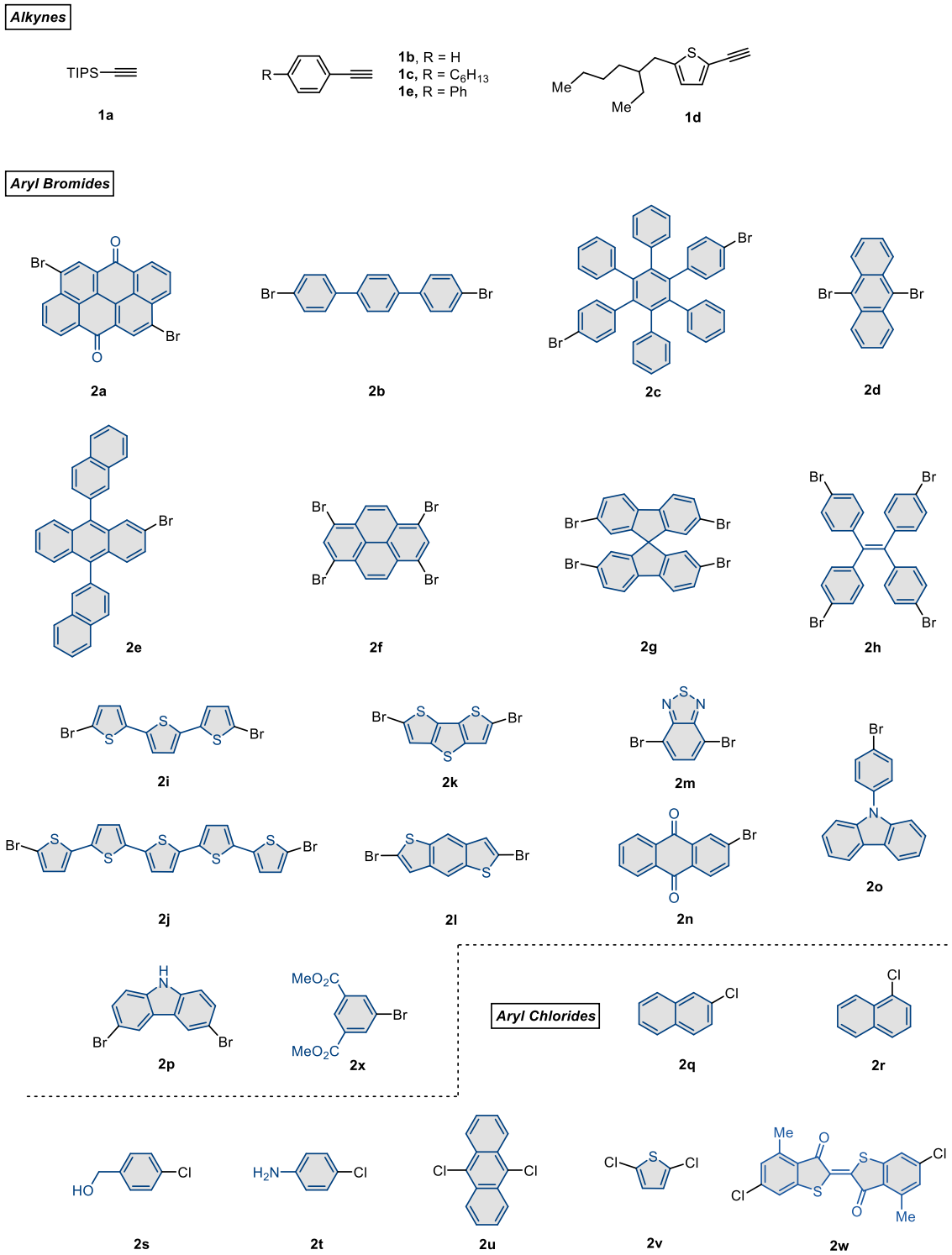


Figure S4. List of aryl halides and alkynes used in this study.

3. Set-Up Procedure for High-Temperature Ball Milling

The heat gun was fixed with clamps and placed directly above the ball milling jar (distance between the heat gun and ball milling jar: ca. 1 cm). The set-up procedure for high-temperature ball-milling reactions is shown in Figure S5. After the ball milling jar was closed, the jar was placed in the ball mill (Retsch MM400), and a heat gun was placed directly above the ball milling jar. The mechanochemical cross-coupling reactions were conducted while applying heated air to the outside of the milling jar (the preset temperature at 150 or 250 °C).

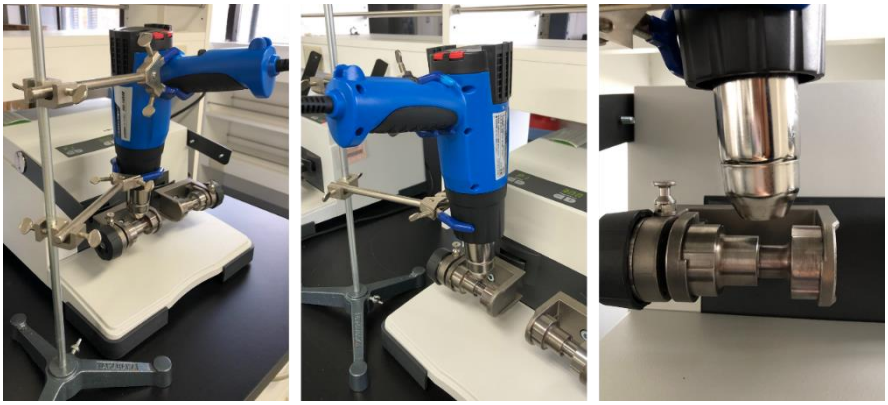
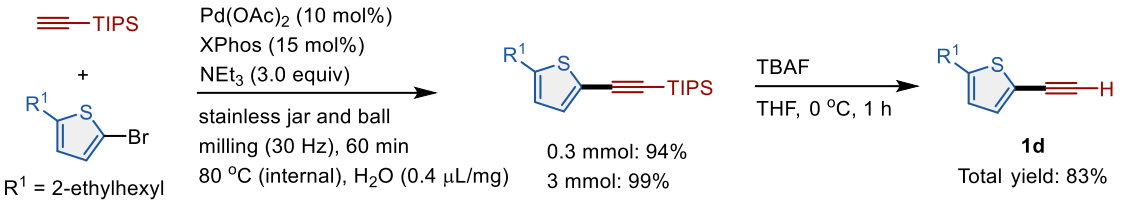


Figure S5. The set-up procedure for a heat gun on MM400.

4. Substrate Preparation

Synthesis of terminal alkyne 1d

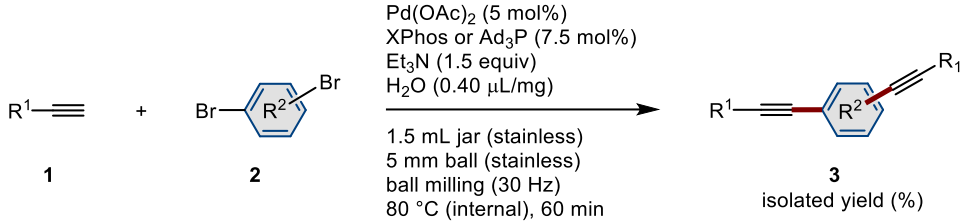


$Pd(OAc)_2$ (3.4 mg, 0.015 mmol, 5 mol %) and XPhos (10.7 mg, 0.023 mmol, 7.5 mol %) were placed in a ball milling vessel (stainless, 1.5 mL) loaded with one grinding ball (stainless, diameter: 5 mm). Then H_2O (0.40 μL/mg), 2-(2-ethylhexyl)-5-ethynylthiophene (82.6 mg, 0.30 mmol, 1.0 equiv), TIPS acetylene (82.1 mg, 0.45 mmol, 1.5 equiv) and NEt_3 (45.5 mg, 0.45 mmol, 1.5 equiv) were added via syringe. After the vessel was closed in air without purging with inert gas, the vessel was placed in the ball mill (Retsch MM400, 60 min at 30 Hz) and a heat gun (the preset temperature at 150 °C). After 60 min, the jar was then cooled rapidly with cold water and opened. The mixture was passed through a short silica pad and eluted with $CHCl_3$. The filtrate was then concentrated under vacuum. The crude mixture was then purified by flash column chromatography (SiO_2, hexane) to give the corresponding coupling product (105.9 mg, 94%). For a 3 mmol scale reaction, 10 mL stainless jar and one 15 mm stainless ball were used (yield: 99%).

Silyl alkyne (1.2 g, 3.2 mmol) was dissolved in THF (35 mL). TBAF solution (9.7 mL, 1.0 M in THF, 3.0 equiv) was added dropwise via syringe at 0 °C. After 1 h of stirring, saturated NH_4Cl aqueous solution (70 mL) was added into the mixture for quenching. The mixture was extracted with Et_2O three times. The organic layer was separated and washed with brine. The resultant solution was dried over $MgSO_4$, filtrated and evaporated under vacuum. The crude mixture was then purified by flash column chromatography (SiO_2, pentane) to give **1d** (total yield after two steps: 83%). ^1H and ^{13}C NMR spectra of the product were in agreement with the literature.[3]

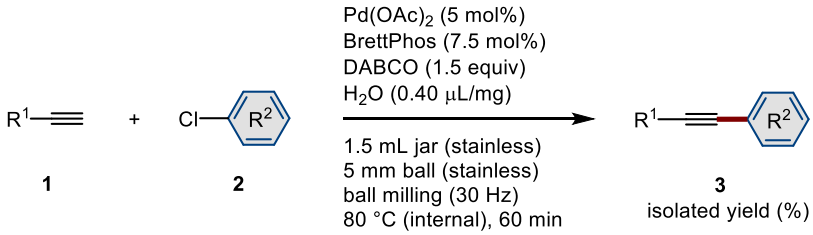
5. General Procedure for Mechanochemical Sonogashira Cross-Coupling.

1) Procedure A: Mechanochemical Sonogashira cross-coupling of aryl bromides



The typical procedure is based on single substituted aryl bromides (**2e**, **2n**, **2o**). For multi-substituted aryl bromides, the equivalents of other reagents are determined by the number of bromide substituents. Aryl bromide **2** (0.30 mmol, 1.0 equiv), $Pd(OAc)_2$ (0.015 mmol, 5 mol %) and ligand (Ad_3P or XPhos) (0.023 mmol, 7.5 mol %) were placed in a ball milling vessel (stainless, 1.5 mL) loaded with one grinding ball (stainless, diameter: 5 mm). Then H_2O (0.40 μL/mg), terminal alkyne **1** (0.45 mmol, 1.5 equiv) and NEt_3 (0.45 mmol, 1.5 equiv) were added via syringe. After the vessel was closed in air without purging with inert gas, the vessel was placed in the ball mill (Retsch MM400, 60 min at 30 Hz) and a heat gun (the preset temperature at 150 °C). After 60 min, the jar was then cooled rapidly with cold water and opened. The mixture was passed through a short silica pad and eluted with $CHCl_3$. The filtrate was then concentrated under vacuum. The crude mixture was then purified by flash column chromatography (SiO_2, typically $CHCl_3$/hexane, typically 0:100–50:50) or recycle preparative GPC to give the corresponding coupling product **3**.

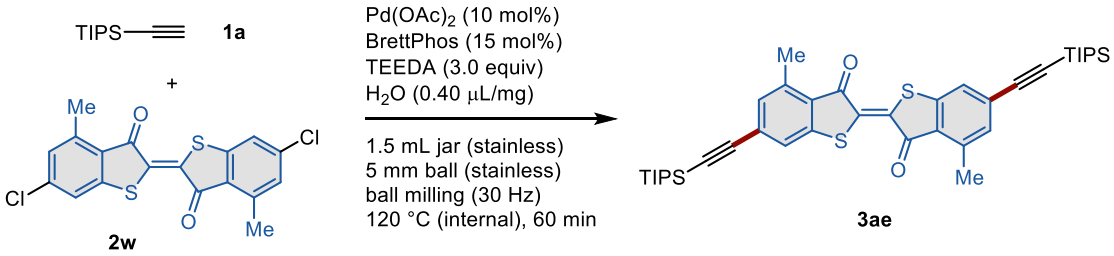
2) Procedure B: Mechanochemical Sonogashira cross-coupling of aryl chlorides



Typical procedure is based on single substituted aryl chlorides. For disubstituted aryl chlorides, the equivalents of other reagents are determined by the number of chloride substituents. Terminal alkyne **1** (0.45 mmol, 1.5 equiv), aryl chloride **2** (0.30 mmol, 1.0 equiv), $Pd(OAc)_2$ (0.015 mmol, 5 mol %), BrettPhos (0.023 mmol, 7.5 mol %) and 1,4-diazabicyclo[2.2.2]octane (DABCO) (0.45 mmol, 1.5 equiv) were placed in a ball milling vessel (stainless, 1.5 mL) loaded with one grinding ball (stainless, diameter: 5 mm). Then H_2O (0.40 μL/mg) was added via syringe. After the vessel was closed in air without purging with inert gas, the vessel was placed in the ball mill (Retsch MM400, 60 min at 30 Hz) and a heat gun (the preset temperature at 150 °C). After 60 min, the jar was then cooled rapidly with cold water and opened. The mixture was passed through a short silica pad and eluted with $CHCl_3$.

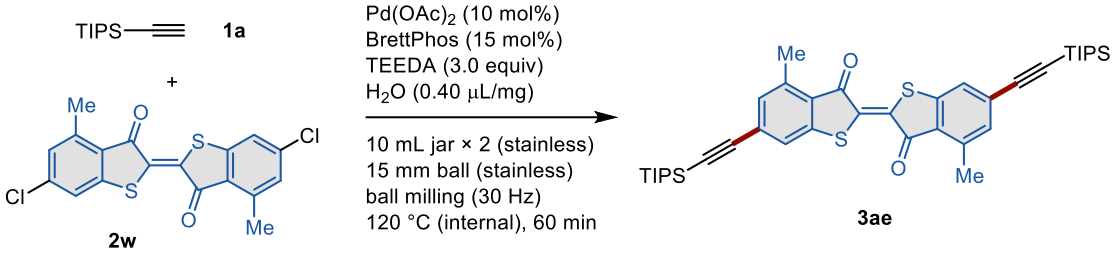
The filtrate was then concentrated under vacuum. The crude mixture was then purified by flash column chromatography (SiO_2, typically $CHCl_3$/hexane, typically 0:100–50:50) to give the corresponding coupling product **3**.

3) Procedure C: Mechanochemical Sonogashira cross-coupling of Vat Red 1 (2w)



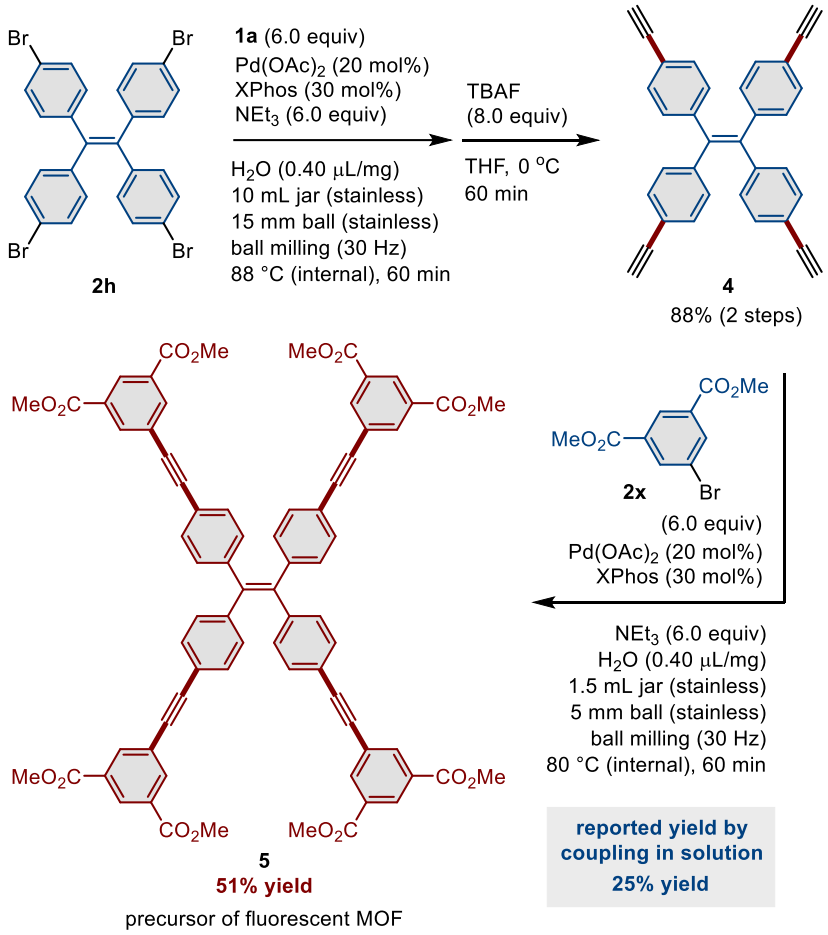
Vat Red 1 (**2w**) (59.0 mg, 0.15 mmol, 1.0 equiv), $Pd(OAc)_2$ (3.4 mg, 0.015 mmol, 10 mol %) and BrettPhos (12.1 mg, 0.023 mmol, 15 mol %) were placed in a ball milling vessel (stainless, 1.5 mL) loaded with one grinding ball (stainless, diameter: 5 mm). Then H_2O (0.40 μL/mg), TIPS acetylene (82.1 mg, 0.45 mmol, 3.0 equiv) and tetraethylethylenediamine (TEEDA) (77.5 mg, 0.45 mmol, 3.0 equiv) were added via syringe. After the vessel was closed in air without purging with inert gas, the vessel was placed in the ball mill (Retsch MM400, 60 min at 30 Hz) and a heat gun (the preset temperature at 250 °C). After 60 min, the jar was then cooled rapidly with cold water and opened. The mixture was passed through a short silica pad and eluted with $CHCl_3$. The filtrate was then concentrated under vacuum. The crude mixture was then purified by flash column chromatography (SiO_2, typically $CHCl_3$/hexane, 0:100–50:50) to give the corresponding coupling product **3ae** (56.1 mg, 55%).

6. Procedure for Gram Scale Synthesis of 3ae



The large-scale synthesis of **3ae** was conducted in two batches using a 10 mL stainless jar. For every batch, Vat Red 1 (**2w**) (511 mg, 1.3 mmol, 1.0 equiv), $Pd(OAc)_2$ (29.2 mg, 0.13 mmol, 10 mol %) and BrettPhos (104.7 mg, 0.20 mmol, 15 mol %) were placed in a ball milling vessel (stainless, 10 mL) loaded with one grinding ball (stainless, diameter: 15 mm). Then H_2O (0.40 μL/mg), TIPS acetylene (711.4 mg, 3.9 mmol, 3.0 equiv) and TEEDA (672.0 mg, 3.9 mmol, 3.0 equiv) were added via syringe. After the vessel was closed in air without purging with inert gas, the vessel was placed in the ball mill (Retsch MM400, 60 min at 30 Hz) and a heat gun (the preset temperature at 250 °C). After 60 min, the jar was then cooled rapidly with cold water and opened. Two batches of the mixture were combined and then passed through a short silica pad and eluted with $CHCl_3$. The filtrate was then concentrated under vacuum. The crude mixture was then purified by flash column chromatography (SiO_2, typically $CHCl_3$/hexane, 0:100–50:50) to give the corresponding coupling product **3ae** (903.9 mg, 51%).

7. Procedure for Synthesis of MOF Ligand Precursor 5



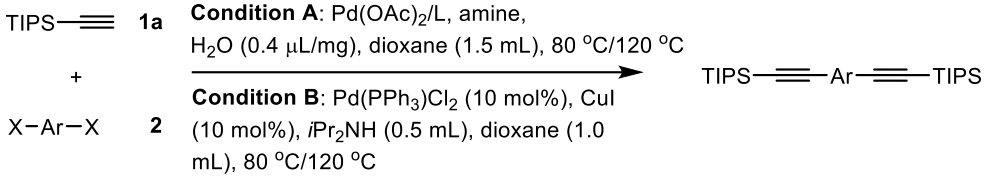
Aryl bromide **2h** (486.0 mg, 0.75 mmol, 1.0 equiv), $Pd(OAc)_2$ (34.0 mg, 0.15 mmol, 20 mol %) and XPhos (107 mg, 0.23 mmol, 30 mol %) were placed in a ball milling vessel (stainless, 10 mL) loaded with one grinding ball (stainless, diameter: 15 mm). Then H_2O (0.40 μL/mg), TIPS acetylene **1a** (821.0 mg, 4.50 mmol, 6.0 equiv) and NEt_3 (455.0 mg, 4.50 mmol, 6.0 equiv) were added via syringe. After the vessel was closed in air without purging with inert gas, the vessel was placed in the ball mill (Retsch MM400, 60 min at 30 Hz) and a heat gun (the preset temperature at 150 °C). After 60 min, the jar was then cooled rapidly with cold water and opened. The mixture was passed through a short silica pad and eluted with $CHCl_3$. The filtrate was then concentrated under vacuum. The crude mixture was directly used in the next step.

The crude product was dissolved in THF (30 mL). TBAF solution (6.0 mL, 1.0 M in THF, 8.0 equiv) was added dropwise via syringe at 0 °C. After 1 h of stirring, saturated NH_4Cl aqueous solution was added into the mixture for quenching. The mixture was extracted with Et_2O three times. The organic layer was separated and washed with brine. The resultant solution was dried over $MgSO_4$, filtrated, and evaporated under vacuum. The crude mixture was then purified by flash column chromatography (SiO_2, $CHCl_3$/hexane, 5:95–25:75). The resultant product was washed with hexane 5 times. Pale

yellow powder was obtained with a total yield of 88% (282 mg) after two steps.

Alkyne **4** (32.1 mg, 0.075 mmol, 1.0 equiv), aryl bromide **2x** (122.9 mg, 0.45 mmol, 6.0 equiv), $Pd(OAc)_2$ (3.4 mg, 0.015 mmol, 20 mol %) and XPhos (10.7 mg, 0.023 mmol, 30 mol %) were placed in a ball milling vessel (stainless, 1.5 mL) loaded with one grinding ball (stainless, diameter: 5 mm). Then H_2O (0.40 μL/mg), and NEt_3 (45.5 mg, 0.45 mmol, 6.0 equiv) were added via syringe. After the vessel was closed in air without purging with inert gas, the vessel was placed in the ball mill (Retsch MM400, 60 min at 30 Hz) and a heat gun (the preset temperature at 150 °C). After 60 min, the jar was then cooled rapidly with cold water and opened. The mixture was passed through a short silica pad and eluted with $CHCl_3$. The filtrate was then concentrated under vacuum. The crude mixture was then purified by flash column chromatography (SiO_2, hexane/ethyl acetate, 90:10–50:50) to give the corresponding product **5** (45.3 mg, 51%). For large-scale reaction (0.66 mmol), 10 mL stainless jar and one 15 mm stainless ball were used (44% yield).

8. General Procedures for Sonogashira Cross-Coupling Reactions in Solution



1) Procedure A: Copper-free conditions

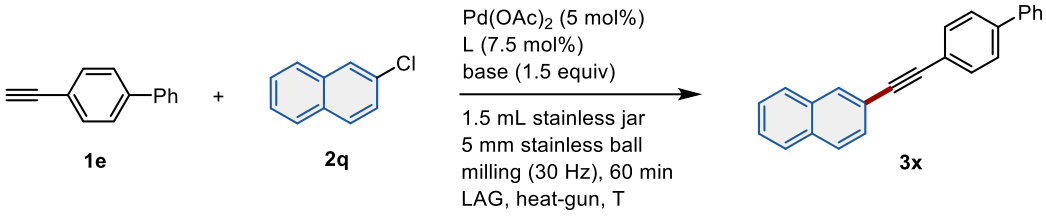
Aryl bromide **2** (0.15 mmol, 1.0 equiv), $Pd(OAc)_2$ (0.015 mmol, 10 mol %) and ligand (XPhos or Ad_3P) (0.023 mmol, 15 mol %) were placed in an oven-dried reaction vial. After the vial was sealed with a screw cap containing a Teflon-coated rubber septum, the vial was connected to a vacuum/nitrogen manifold through a needle. It was evacuated and then backfilled with nitrogen. This cycle was repeated three times. Dioxane (1.5 mL) was added to the vial through the rubber septum. Then H_2O (0.4 μL/mg), TIPS acetylene (0.45 mmol, 3.0 equiv) and Et_3N (0.45 mmol, 3.0 equiv) were added to the mixture via syringe successively. After stirring at 80 °C for 24 hours or 1 hour, the mixture was passed through a short silica pad and eluted with $CHCl_3$. The filtrate was then concentrated under vacuum. The crude mixture was then purified by flash column chromatography (SiO_2, typically $CHCl_3$/hexane, typically 0:100–50:50) to give the corresponding coupling product **3**. For Vat Red 1 (**2w**), BrettPhos and TEEDA were used to replace XPhos/Ad_3P and Et_3N, and the reaction was conducted at 120 °C for 24 hours.

2) Procedure B: Palladium/copper co-catalyzed conditions

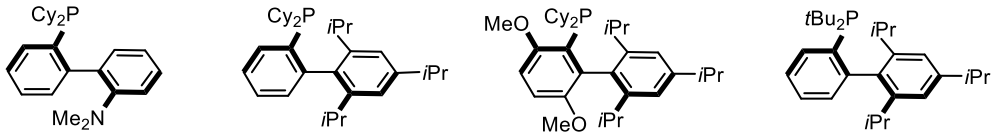
Aryl halide **2** (0.15 mmol, 1.0 equiv), $Pd(PPh_3)_2Cl_2$ (0.015 mmol, 10 mol %) and CuI (0.015 mmol, 10 mol %) were placed in an oven-dried reaction vial. After the vial was sealed with a screw cap containing a Teflon-coated rubber septum, the vial was connected to a vacuum/nitrogen manifold through a needle. It was evacuated and then backfilled with nitrogen. This cycle was repeated three times. Dioxane (1.0 mL) was added into the vial through the rubber septum. Then TIPS acetylene (0.45 mmol, 3.0 equiv) and iPr_2NH (0.5 mL) were added to the mixture via syringe successively. After stirring at 80 °C or 120 °C for 24 hours or 1 hour, the mixture was passed through a short silica pad and eluted with $CHCl_3$. The filtrate was then concentrated under vacuum. The crude mixture was then purified by flash column chromatography (SiO_2, typically $CHCl_3$/hexane, typically 0:100–50:50) to give the corresponding coupling product **3**.

9. Results of Optimization Study for Aryl Chlorides

Table S1. Optimization study of aryl chloride **2q**.



Entry	Ligand	Base	LAG	Amount (µL/mg)	internal temp. (°C)	yield (%)[b]
1	DavePhos	Et_3N	none	-	80	<1
2	XPhos	Et_3N	none	-	80	<1
3	BrettPhos	Et_3N	none	-	80	52
4	*t*BuBrettPhos	Et_3N	none	-	80	<1
5	BrettPhos	DABCO	none	-	80	57
6	BrettPhos	DABCO	none	-	100	54
7	BrettPhos	DABCO	cod	0.2	80	49
8	BrettPhos	DABCO	dioxane	0.2	80	61
9	BrettPhos	DABCO	*n*PrOH	0.2	80	51
10	BrettPhos	DABCO	H_2O	0.2	80	82
11	BrettPhos	DABCO	H_2O	0.1	80	91
12	BrettPhos	DABCO	H_2O	0.4	80	94

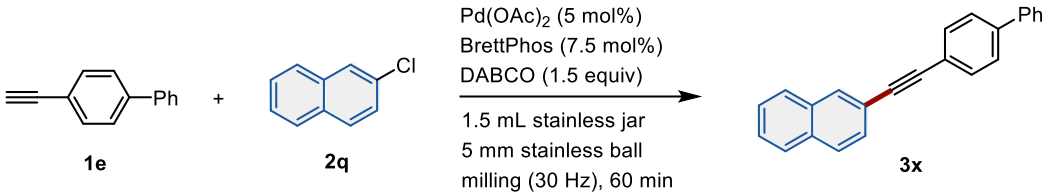


[a]Conditions: **1e** (0.45 mmol), **2q** (0.30 mmol), $Pd(OAc)_2$ (0.015 mmol), ligand (0.0225 mmol), base (0.45 mmol), liquid in a stainless-steel ball-milling jar (1.5 mL). [b]Determined by ^1H NMR analysis of the crude reaction mixture with an internal standard.

10. Details of Kinetic Study of Reaction between 1e and 2q

Reactions were conducted in a Retsch MM400 ball mill in a stainless-steel milling jar (1.5 mL) at 30 Hz using one stainless-steel ball (diameter: 5 mm). Each data point was obtained from an individual reaction. Yields were determined by ^{1}H NMR analysis with an internal standard. In order to reveal the influence of water on this transformation, comparative kinetic research with and without water was performed.

Table S2. Kinetic study of the reaction between **1e** and **2q**.



1e **2q** **3x**

Time (min)	**1e** (equiv)		Conversion of **1e** (%)		Yield (%)	
	w/ H_2O	w/o H_2O	w/ H_2O	w/o H_2O	w/ H_2O	w/o H_2O
0	1.50	1.50	0	0	0	0
2.5	1.40	1.19	6.7	20.7	0	3.5
5	1.22	0.97	18.7	35.3	1.1	5.8
7.5	1.08	0.74	28.0	50.7	7.7	13
10	1.05	0.51	30.0	66.0	11	23
15	0.69	0.19	54.0	87.3	38	44
20	0.41	0	72.7	100	56	62
25	0.18	0	88.0	100	83	66
30	0.10	0	93.3	100	88	66
40	0.07	0	96.0	100	98	66

Appearance of the reaction mixture

In most of the examples presented here, liquid alkynes (**1a**–**1d**) and liquid base (Et_3N) were used as reactants. The liquid reactants can serve as a dispersant for the solid reactants. Therefore, this reaction should not be considered as a prototypical solid-state process. Even for the reactions between solid substrates, the appearance is not 'strictly' solid because we use H_2O as an additive. For example, the appearance of the reaction between **1e** and **2q** is shown in Figure S6. During the first 10 minutes, the solid reactant disperses in water to form small drops. Due to the evaporation of water upon heating, the resulting solid after cooling exhibits a porous structure. After 10 minutes, the porous structure disappears, and the reaction mixture behaves as a black, hard, and crispy solid.

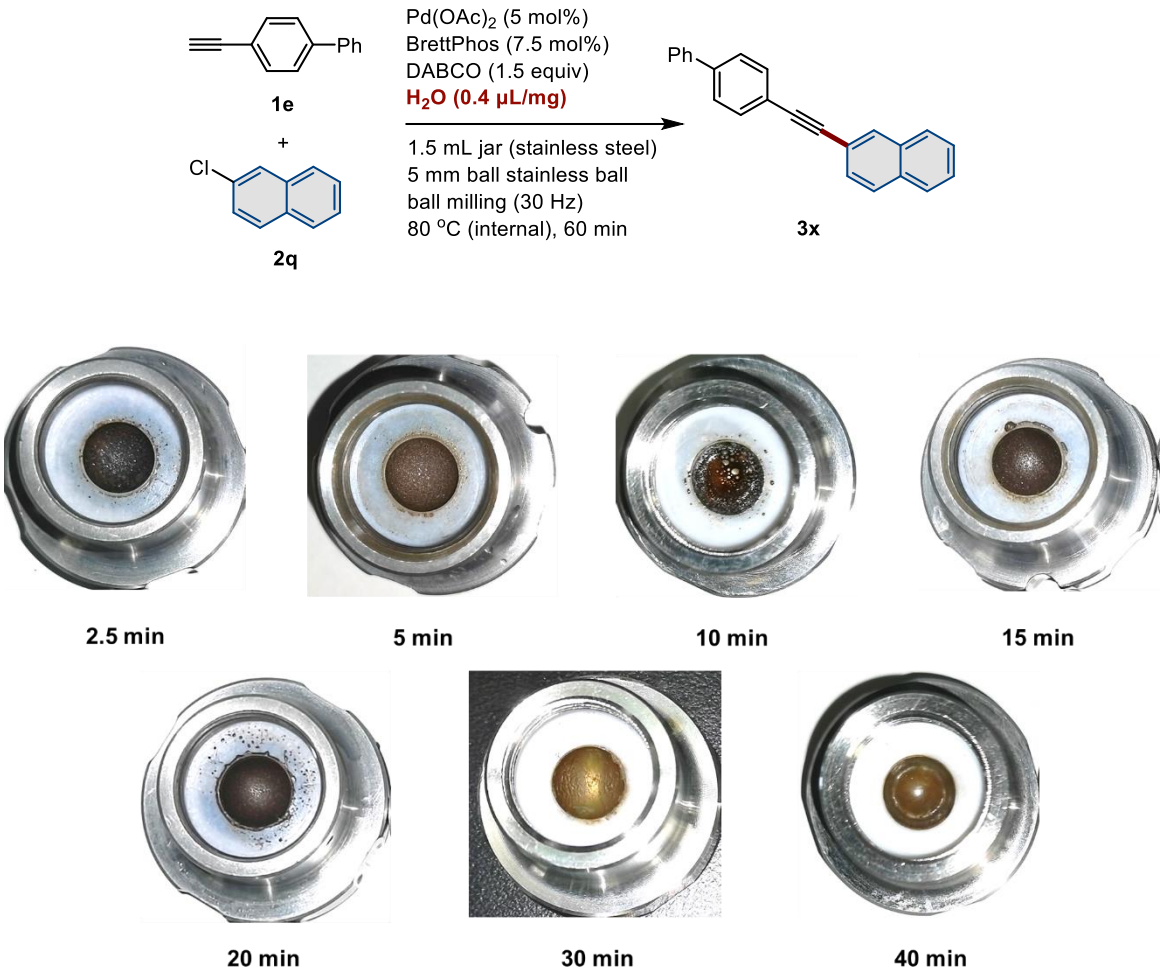


Figure S6. Reaction mixtures of **1e** and **2q** after grinding with water for different periods of time.

11. TEM Characterization of Crude Reaction Mixture of 1e and 2q

Transmission electron microscopy (TEM) experiments were conducted to characterize the palladium nanoparticles generated in situ in the crude reaction mixture of **1e** with **2q**. Both reactions, i.e., with and without H_2O, were checked after 40 minutes of grinding. The images obtained show a different morphology for the palladium nanoparticles generated in these two systems. In the reaction with H_2O, the palladium species behave like a cluster of small dots (Figure S7a). In contrast, in the reaction without H_2O, the palladium species significantly aggregate into dense particles (Figure S7b). Higher aggregation of palladium might lead to the formation of deactivated palladium black. This would explain the lower reaction efficiency under H_2O-free conditions compared to the conditions with H_2O. Although further investigations are needed, we propose that this reaction is catalyzed by phosphine-ligated monomeric palladium(0) species, which could leach from palladium nanoparticles during the reaction. This is consistent with the results summarized in Table 1, which show that the ligands significantly affect the reactivity.

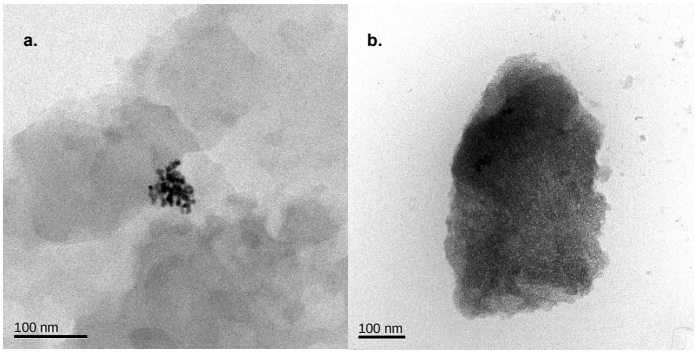


Figure S7. TEM images of palladium particles in the crude reaction mixtures. (a) Crude mixture after 40 min with H_2O, and (b) crude mixture after 99 min without H_2O. Scale bars in the TEM images (bottom left): 100 nm.

12. Thermography Observation for Reaction Temperature

The temperature inside the milling jar after the solid-state coupling reactions was confirmed by observation with a thermography camera immediately after opening the milling jar (Figure S8–S11). All of the pictures were taken after 1 hour of heated ball milling. When the preset temperature of the heat gun is 150 °C, for a 1.5 mL stainless jar, the internal temperature was determined to be 79.2 °C (Figure S8). But when a 10 mL stainless jar was used for large-scale synthesis, the internal temperature was determined to be 87.6 °C (Figure S9). When the preset temperature of the heat gun is 250 °C, for 1.5 mL stainless jar, the internal temperature was determined to be 122.1 °C (Figure S10). But when 10 mL stainless jar was used for large-scale synthesis, the internal temperature was determined to be 140.8 °C (Figure S11).

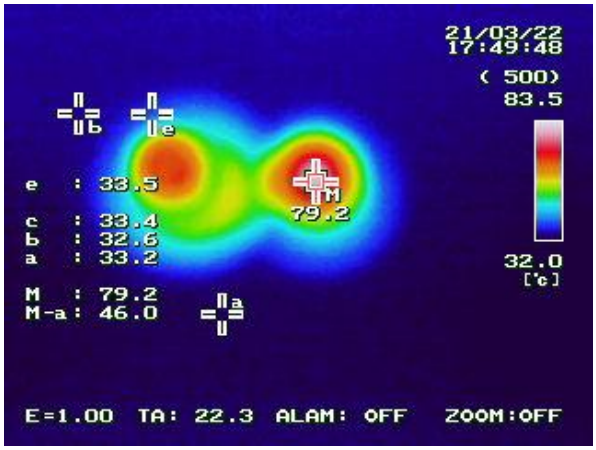


Figure S8. Thermographically derived temperature (79.2 °C) inside the milling jar (1.5 mL) after grinding for 60 min at 30 Hz at a preset temperature of 150 °C.

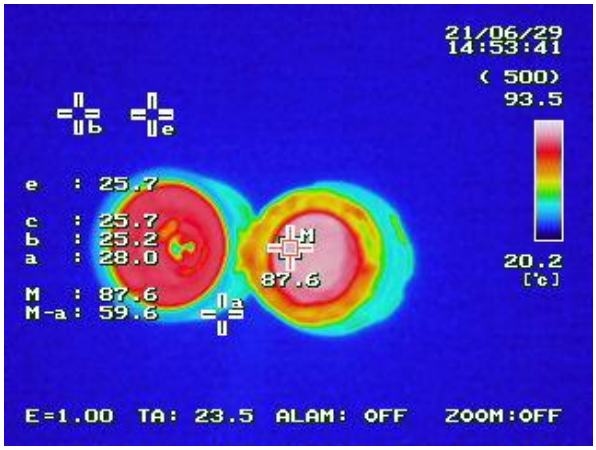


Figure S9. Thermographically derived temperature (87.6 °C) inside the milling jar (10 mL) after grinding for 60 min at 30 Hz at a preset temperature of 150 °C.

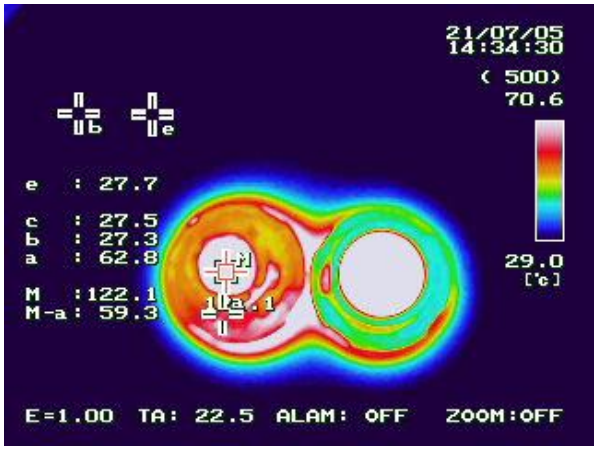


Figure S10. Thermographically derived temperature (122.1 °C) inside the milling jar (1.5 mL) after grinding for 60 min at 30 Hz at a preset temperature of 250 °C.

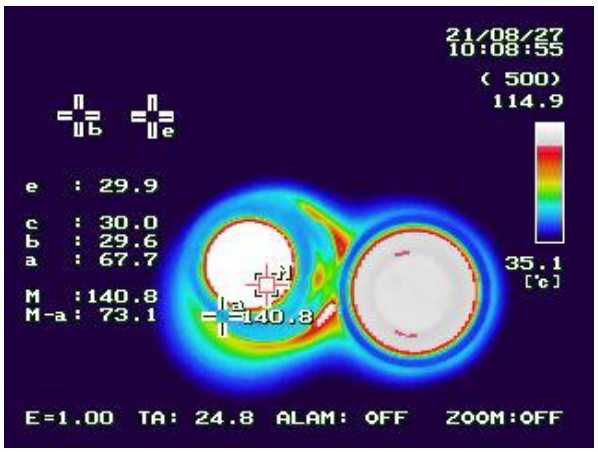


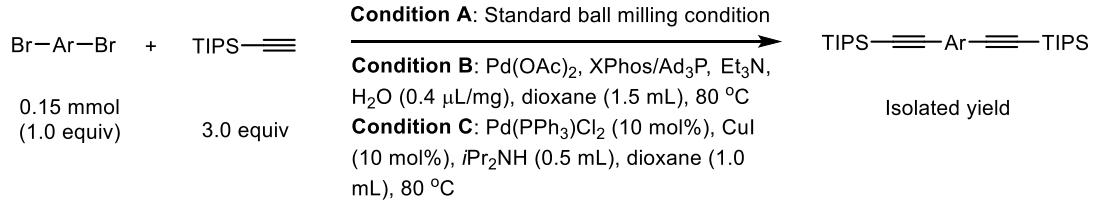
Figure S11. Thermographically derived temperature (140.8 °C) inside the milling jar (10 mL) after grinding for 60 min at 30 Hz at a preset temperature of 250 °C.

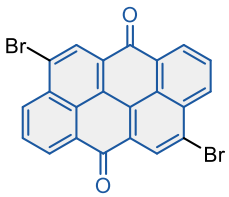
13. Comparative Studies between Ball Milling Conditions and Solution-Based Conditions

Except for the comparative study of Vat Red 1 (**3w**) shown in the main text, three disubstituted aryl bromides were also attempted, including poorly soluble pigment **2a** (Vat Orange 3), oligophenyl substrate **2b**, and fused thiophene substrate **2k**. Two solution-based conditions were selected as standard: the same copper-free catalytic system we utilized in ball milling reactions and the classical palladium/copper co-catalyzed system. Reactions were conducted in dioxane with a concentration of 0.1 M.

For **2a**, the copper-free solution-based method only afforded less than 20% yield after 24 hours. The low conversion could be ascribed to the low solubility of the pigment. Classical palladium/copper co-catalyzed system gave a similar yield with ball milling condition after 12 hours. But the efficiency of the ball milling method still outcompeted the solution-based method. When the reaction time was limited to 1 hour, a significantly decreased yield was obtained under solution-based conditions. A similar phenomenon was observed when **2b** was subjected to this comparative study. The solubility of **2b** is enough for high conversion for the copper-free condition after sufficient time. But the reaction rate in solution is obviously lower than that under ball milling conditions. For fused thiophene substrate **2k**, the copper-free solution-based method led to only 15% yield after 24 hours. Although the palladium/copper co-catalyzed system behaved better than the copper-free system, the yield was still lower than that observed under the ball milling condition. This diversity could be attributed to the side reactions in solution-based conditions. In conclusion, in comparison with solution-based reactions, ball milling is a more efficient and general method for Sonogashira coupling of substrates bearing large π-conjugated structures.

Table S3. Comparative studies between ball milling conditions and solution-based conditions.



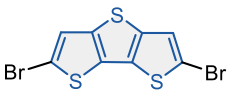


2a

Condition A: 75% (1 h)
Condition B: 16% (24 h)
Condition C: 76% (12 h)
31% (1 h)

2b

Condition A: 83% (1 h)
Condition B: 90% (24 h)
51% (1 h)
Condition C: 88% (24 h)
41% (1 h)



2k

Condition A: 87% (1 h)
Condition B: 15% (24 h)
Condition C: 70% (24 h)

14. Optical Measurements

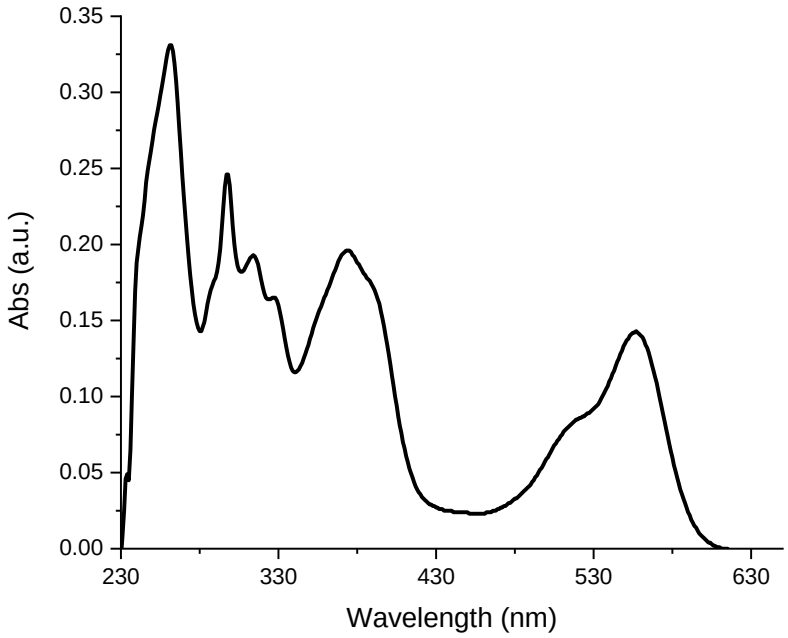


Figure S12. Absorption spectra of the dilute solution of **3ae** (10^{-5} M) in $CHCl_3$.

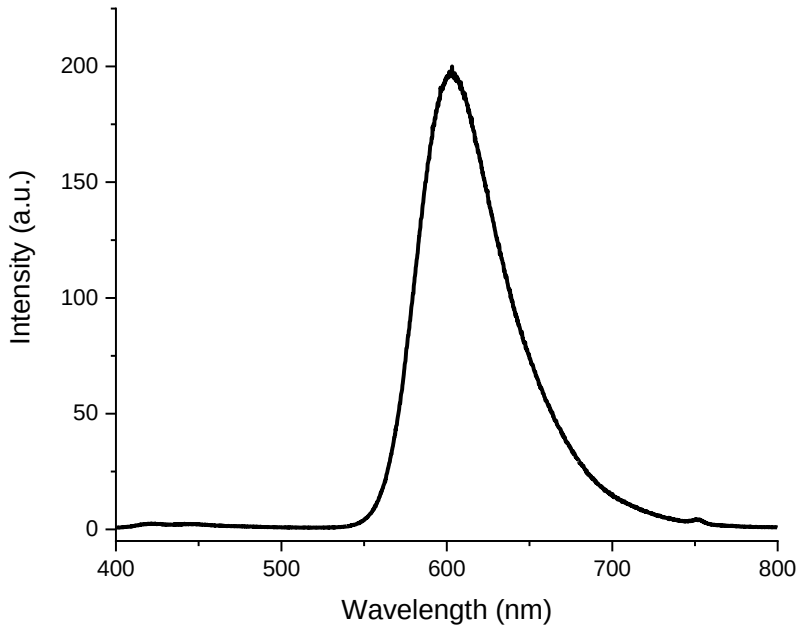


Figure S13. Emission spectra of the dilute solution of **3ae** (10^{-5} M) in $CHCl_3$ (λ_{ex} = 373 nm).

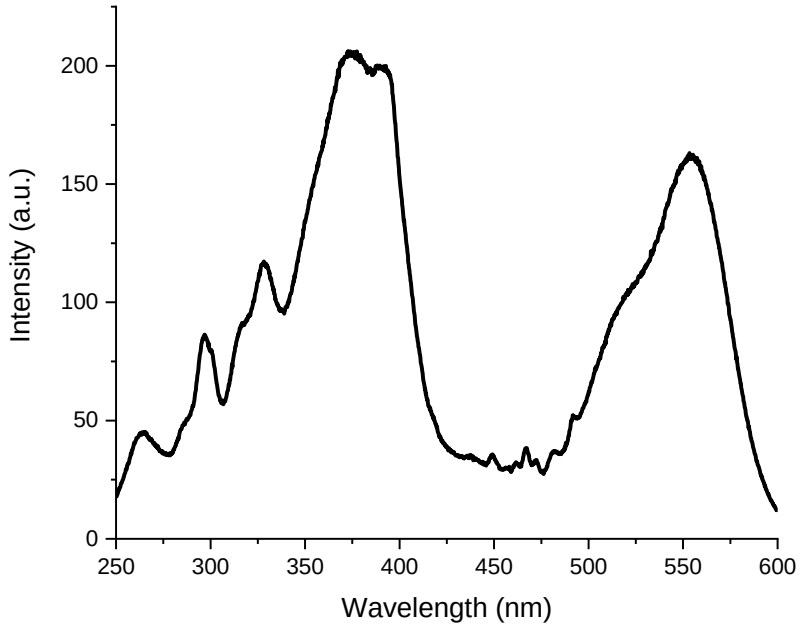


Figure S14. Excitation spectra of the dilute solution of **3ae** (10^{-5} M) in $CHCl_3$ (λ_{em} = 608 nm).

15. Single Crystal X-ray Structure Analyses

1) 5,5''''-Bis((triisopropylsilyl)ethynyl)-2,2':5',2'':5'',2''':5''',2''''-quinquethiophene (3j)

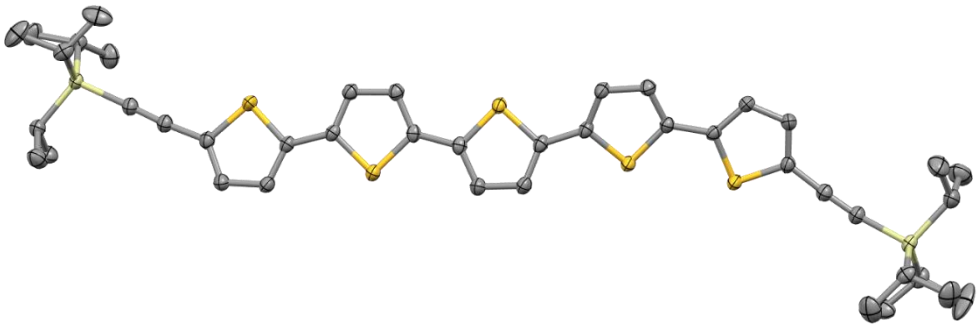


Figure S15. Molecular structure of **3j** (H atoms omitted. Thermal ellipsoids at 50% probability).

Table S4. Summary of X-ray crystallographic data for **3j**.

CCDC Number	2106265
Empirical Formula	$C_{42}H_{52}S_5Si_2$
Formula Weight	773.31
Crystal Size / mm	0.3×0.2×0.04
Crystal System	monoclinic
a / Å	39.5034(4)
b / Å	9.23520(10)
c / Å	23.1512(3)
α / °	90
β / °	96.9160(10)
γ / °	90
V / Å^3	8384.60(17)
Space Group	*C2/c*
Z value	8
D_{calc} / g cm^{-3}	1.225
Temperature / K	123
$2\theta_{max}$ / °	153.106
μ / mm^{-1}	3.301 (Cu K$_\alpha$)
No. of reflections	Total: 19756 Unique: 8430 R_{int} = 0.0337
R_1[a]	0.0343
wR_2[b]	0.0988
GOF[c]	1.075
Max./Mini. peak *I* / Å^3	0.34 e$^-$/−0.26 e$^-$

[a]For data with $I > 2.00\sigma(I)$. [b]For all reflection data. [c]Goodness of Fit.

2) (*E*)-4,4'-Dimethyl-6,6'-bis[(triisopropylsilyl)ethynyl]-3H,3'H-[2,2'-bibenzo[b]thiophenylidene]-3,3'-dione (3ae)

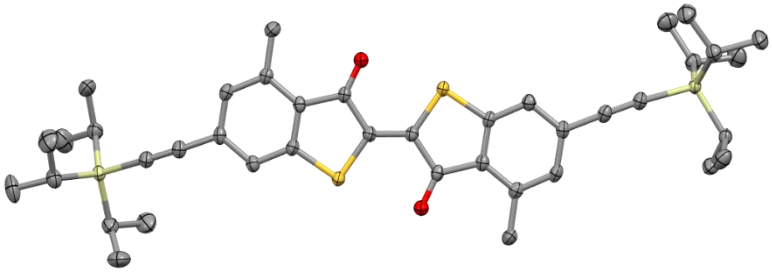


Figure S16. Molecular structure of **3ae** (H atoms omitted. Thermal ellipsoids at 50% probability).

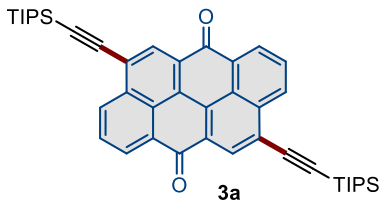
Table S5. Summary of X-ray crystallographic data for **3ae**.

CCDC Number	2106264
Empirical Formula	$C_{40}H_{52}O_2S_2Si_2$
Formula Weight	685.11
Crystal Size / mm	0.25×0.2×0.04
Crystal System	triclinic
a / Å	14.2639(6)
b / Å	14.5005(4)
c / Å	20.4969(7)
α / °	105.307(3)
β / °	109.588(4)
γ / °	90.479(3)
V / Å^3	3830.5(3)
Space Group	*P*-1
Z value	4
D_{calc} / g cm^{-3}	1.188
Temperature / K	123
$2\theta_{max}$ / °	153.044
μ / mm^{-1}	2.101 (Cu K$_\alpha$)
No. of reflections	Total: 22451 Unique: 11884 R_{int} = 0.0243
R_1[a]	0.0408
wR_2[b]	0.1148
GOF[c]	1.048
Max./Mini. peak *I* / Å^3	0.57 e$^-$/−0.28 e$^-$

[a]For data with $I > 2.00\sigma(I)$. [b]For all reflection data. [c]Goodness of Fit.

16. Characterization of Coupling Products.

4,10-Bis[(triisopropylsilyl)ethynyl]naphtho[7,8,1,2,3-nopqr]tetraphene-6,12-dione (3a).



3a

The reaction was performed according to the general procedure A using Ad_3P as the ligand. The reaction was carried out with 82.1 mg (0.45 mmol) of **1a** and 69.6 mg (0.15 mmol) of **2a**. Product **3a** was obtained as a red powder (74.9 mg, 0.112 mmol, 75% yield) after purification by silica-gel column chromatography (SiO_2, $CHCl_3$/hexane, 0:100–50:50). ^1H and ^{13}C NMR were in agreement with the literature.[4]

^1H NMR (400 MHz, $CDCl_3$, δ): 1.23–1.31 (m, 42H), 7.90 (t, J = 7.9 Hz, 2H), 8.52 (s, 2H), 8.70 (d, J = 8.2 Hz, 4H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 11.4 (*C*H), 18.8 (*C*H$_3$), 100.7 (*C*), 103.5 (*C*), 124.2 (*C*), 126.8 (*C*), 126.9 (*C*), 128.6 (*C*H), 128.7 (*C*), 128.9 (*C*), 129.4 (*C*H), 131.0 (*C*H), 133.5 (*C*H), 133.7 (*C*), 181.6 (*C*). HRMS-ESI (*m*/*z*): $[M+Na]^+$ calcd for $C_{44}H_{50}O_2NaSi_2$, 689.3242; found, 689.3256.

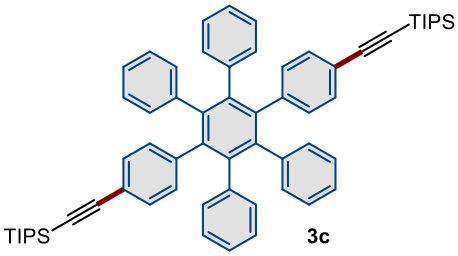
4,4''-Bis[(triisopropylsilyl)ethynyl]-1,1':4',1''-terphenyl (3b).

3b

The reaction was performed according to the general procedure A using XPhos as the ligand. The reaction was carried out with 82.1 mg (0.45 mmol) of **1a** and 58.2 mg (0.15 mmol) of **2b**. Product **3b** was obtained as a white powder (73.7 mg, 0.125 mmol, 83% yield) after purification by silica-gel column chromatography (SiO_2, $CHCl_3$/hexane, 0:100–5:95).

^1H NMR (400 MHz, $CDCl_3$, δ): 1.15 (s, 42H), 7.55–7.60 (m, 8H), 7.67 (s, 4H). ^{13}C NMR (101 MHz, $CDCl_3$, δ): 11.3 (*C*H), 18.7 (*C*H$_3$), 91.5 (*C*), 106.9 (*C*), 122.6 (*C*), 126.7 (*C*H), 127.4 (*C*H), 132.5 (*C*H), 139.6 (*C*), 140.3 (*C*). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{40}H_{54}Si_2$, 590.3764; found, 590.3744. mp 158–159 °C.

{[2',3',5',6'-Tetraphenyl-(1,1':4',1''-terphenyl)-4,4''-diyl]bis(ethyne-2,1-diyl)}bis(triisopropyl-silane) (3c).

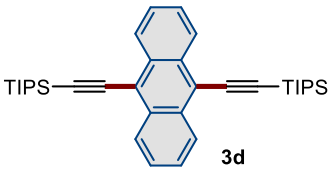


3c

The reaction was performed according to the general procedure A using XPhos as the ligand. The reaction was carried out with 82.1 mg (0.45 mmol) of **1a** and 103.9 mg (0.15 mmol) of **2c**. Product **3c** was obtained as a white powder (52.9 mg, 0.059 mmol, 39% yield) after purification by silica-gel column chromatography (SiO_2, hexane).

^{1}H NMR (400 MHz, $CDCl_3$, δ): 1.06 (s, 42H), 6.75–6.83 (m, 12H), 6.85–6.91 (m, 12H), 6.98 (d, J = 8.6 Hz, 4H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 11.3 (*C*H), 18.6 (*C*H$_3$), 89.6 (*C*), 107.4 (*C*), 120.2 (*C*), 125.4 (*C*H), 126.8 (*C*H), 130.5 (*C*H), 131.2 (*C*H), 131.3 (*C*H), 139.7 (*C*), 140.2 (*C*), 140.4 (*C*), 140.8 (*C*). HRMS-ESI (*m*/*z*): $[M+Na]^+$ calcd for $C_{64}H_{70}NaSi_2$, 917.4908; found, 917.4904. mp > 300 °C.

9,10-Bis[(triisopropylsilyl)ethynyl]anthracene (3d).

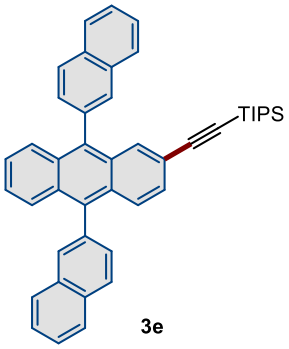


3d

For aryl bromide substrate **2d**, the reaction was performed according to the general procedure A using Ad_3P as the ligand. The reaction was carried out with 82.1 mg (0.45 mmol) of **1a** and 50.4 mg (0.15 mmol) of **2d**. Product **3d** was obtained as an orange powder (77.1 mg, 0.143 mmol, 95% yield) after purification by silica-gel column chromatography (SiO_2, hexane). For aryl chloride substrate **2u**, the reaction was performed according to the general procedure B. The reaction was carried out with 82.1 mg (0.45 mmol) of **1a** and 37.1 mg (0.15 mmol) of **2u**. Product **3d** was obtained as a white powder (36.7 mg, 0.068 mmol, 45% yield) after purification by silica-gel column chromatography (SiO_2, hexane). ^{1}H and ^{13}C NMR were in agreement with the literature.[5]

^{1}H NMR (400 MHz, $CDCl_3$, δ): 1.23–1.35 (m, 42H), 7.56–7.63 (m, 4H), 8.61–8.66 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 11.5 (*C*H), 18.9 (*C*H$_3$), 103.3 (*C*), 104.8 (*C*), 118.7 (*C*), 126.8 (*C*H), 127.2 (*C*H), 132.4 (*C*). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{36}H_{50}Si_2$, 538.3451; found, 538.3436.

{[9,10-Di(naphthalen-2-yl)anthracen-2-yl]ethynyl}triisopropylsilane (3e).

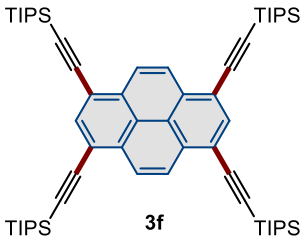


3e

The reaction was performed according to the general procedure A using Ad_3P as the ligand. The reaction was carried out with 82.1 mg (0.45 mmol) of **1a** and 152.9 mg (0.30 mmol) of **2e**. Product **3e** was obtained as a yellow powder (180.9 mg, 0.296 mmol, 99% yield) after purification by silica-gel column chromatography (SiO_2, hexane).

^{1}H NMR (400 MHz, $CDCl_3$, δ): 1.03–1.13 (m, 21H), 7.30–7.38 (m, 3H), 7.58–7.78 (m, 9H), 7.91–8.15 (m, 9H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 11.3 (*C*H), 18.6 (*C*H$_3$), 92.3 (*C*), 107.8 (*C*), 120.1 (*C*), 125.5 (*C*H), 125.6 (*C*H), 126.27 (*C*H), 126.31 (*C*H), 126.4 (*C*H), 126.5 (*C*H), 127.1 (*C*H), 127.2 (*C*H), 127.9 (*C*H), 128.1 (*C*H), 128.2 (*C*H), 129.0 (*C*), 129.1 (*C*), 129.3 (*C*H), 129.41 (*C*H), 129.44 (*C*), 129.6 (*C*H), 130.2 (*C*H), 130.4 (*C*H), 130.59 (*C*), 130.63 (*C*H), 132.79 (*C*), 132.83 (*C*), 133.4 (*C*), 136.0 (*C*), 136.2 (*C*), 137.1 (*C*), 137.2 (*C*). HRMS-ESI (*m*/*z*): $[M+Na]^+$ calcd for $C_{45}H_{42}NaSi$, 633.2948; found, 633.2951. mp 136–138 °C.

1,3,6,8-Tetrakis[(triisopropylsilyl)ethynyl]pyrene (3f).

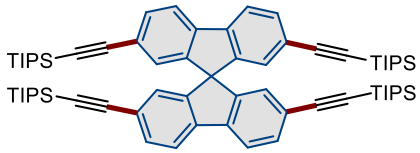


3f

The reaction was performed according to the general procedure A using Ad_3P as the ligand. The reaction was carried out with 82.1 mg (0.45 mmol) of **1a** and 38.8 mg (0.075 mmol) of **2f**. Product **3f** was obtained as a yellow powder (57.5 mg, 0.062 mmol, 83% yield) after purification by silica-gel column (hexane) and recycle preparative GPC. ^{1}H and ^{13}C NMR were in agreement with the literature.[6]

^{1}H NMR (400 MHz, $CDCl_3$, δ): 1.20–1.33 (m, 84H), 8.28 (s, 2H), 8.67 (s, 4H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 11.5 (*C*H), 18.8 (*C*H$_3$), 98.2 (*C*), 104.7 (*C*), 119.0 (*C*), 123.7 (*C*), 127.0 (*C*H), 132.1 (*C*), 134.5 (*C*H). HRMS-ESI (*m*/*z*): $[M+Na]^+$ calcd for $C_{60}H_{90}NaSi_4$, 945.6012; found, 945.6020.

2,2',7,7'-Tetrakis[(triisopropylsilyl)ethynyl]-9,9'-spirobi(fluorene) (3g).

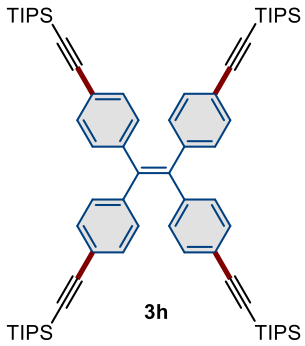


3g

The reaction was performed according to the general procedure A using XPhos as the ligand. The reaction was carried out with 82.1 mg (0.45 mmol) of **1a** and 47.4 mg (0.075 mmol) of **2g**. Product **3g** was obtained as a yellow powder (70.4 mg, 0.068 mmol, 91% yield) after purification by silica-gel column chromatography (SiO_2, pentane).

^{1}H NMR (400 MHz, $CDCl_3$, δ): 1.10 (s, 84H), 6.79 (s, 4H), 7.57 (dd, J = 1.4, 7.7 Hz, 4H), 7.79 (d, J = 8.2 Hz, 4H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 11.3 (*C*H), 18.7 (*C*H$_3$), 65.2 (*C*), 91.6 (*C*), 107.0 (*C*), 120.2 (*C*H), 123.2 (*C*), 127.4 (*C*H), 132.9 (*C*H), 141.1 (*C*), 147.8 (*C*). HRMS-ESI (*m*/*z*): [M+Na]$^+$ calcd for $C_{69}H_{96}NaSi_4$, 1059.6481; found, 1059.6479. mp > 300 °C.

1,1,2,2-Tetrakis{4-[(triisopropylsilyl)ethynyl]phenyl}ethene (3h).

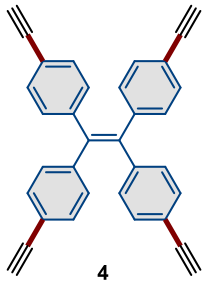


3h

The reaction was performed according to the general procedure A using XPhos as the ligand. The reaction was carried out with 82.1 mg (0.45 mmol) of **1a** and 48.6 mg (0.075 mmol) of **2h**. Product **3h** was obtained as a white powder (72.9 mg, 0.069 mmol, 92% yield) after purification by silica-gel column chromatography (SiO_2, hexane). ^{1}H and ^{13}C NMR were in agreement with the literature.[7]

^{1}H NMR (400 MHz, $CDCl_3$, δ): 1.13 (s, 84H), 6.93 (d, J = 8.6 Hz, 8H), 7.24 (d, J = 8.6 Hz, 8H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 11.3 (*C*H), 18.7 (*C*H$_3$), 91.2 (*C*), 107.0 (*C*), 121.9 (*C*), 131.2 (*C*H), 131.7 (*C*H), 140.6 (*C*), 143.1 (*C*). HRMS-ESI (*m*/*z*): [M+Na]$^+$ calcd for $C_{70}H_{100}NaSi_4$, 1075.6794; found, 1075.6798.

1,1,2,2-Tetrakis(4-ethynylphenyl)ethene (4).



4

The reaction was performed according to section 6. The reaction was carried out with 821 mg (4.5 mmol) of **1a**, about 0.75 mmol of crude **2h**, and 6 mL of TBAF solution (1 M in THF). Product **4** was obtained as a yellow powder (282 mg, 0.658 mmol, 88% yield after two steps) after purification by silica-gel column chromatography (SiO_2, $CHCl_3$/hexane, 5:95–25:75), which was then washed with hexane for 5 times. ^1H and ^{13}C NMR were in agreement with the literature.[8]

^1H NMR (400 MHz, $CDCl_3$, δ): 3.06 (s, 4H), 6.94 (d, J = 8.2 Hz, 8H), 7.25 (d, J = 8.2 Hz, 8H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 77.8 (*C*H), 83.4 (*C*), 120.7 (*C*), 131.2 (*C*H), 131.8 (*C*H), 140.8 (*C*), 143.2 (*C*). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{34}H_{20}$, 428.1565; found, 428.1550.

5,5''-Bis[(triisopropylsilyl)ethynyl]-2,2':5',2''-terthiophene (3i).

3i

The reaction was performed according to the general procedure A using Ad_3P as the ligand. The reaction was carried out with 82.1 mg (0.45 mmol) of **1a** and 60.9 mg (0.15 mmol) of **2i**. Product **3i** was obtained as an orange oil (85.8 mg, 0.141 mmol, 94% yield) after purification by silica-gel column chromatography (SiO_2, hexane).

^1H NMR (400 MHz, $CDCl_3$, δ): 1.12–1.16 (m, 42H), 7.00 (d, J = 4.1 Hz, 2H), 7.05–7.08 (m, 2H), 7.12 (d, J = 3.6 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 11.3 (*C*H), 18.6 (*C*H_3), 97.2 (*C*), 99.1 (*C*), 122.5 (*C*), 123.3 (*C*H), 124.8 (*C*H), 133.2 (*C*H), 136.0 (*C*), 137.9 (*C*). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{34}H_{48}S_3Si_2$, 608.2457; found, 608.2443.

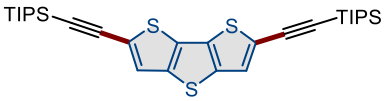
5,5''''-Bis[(triisopropylsilyl)ethynyl]-2,2':5',2'':5'',2''':5''',2''''-quinquethiophene (3j).

3j

The reaction was performed according to the general procedure A using Ad_3P as the ligand. The reaction was carried out with 41.0 mg (0.225 mmol) of **1a** and 42.8 mg (0.075 mmol) of **2j**. Product **3j** was obtained as a brown powder (21.2 mg, 0.027 mmol, 37% yield) after purification by silica-gel column chromatography (SiO_2, $CHCl_3$/hexane, 5:95–20:80).

^{1}H NMR (400 MHz, $CDCl_3$, δ): 1.12–1.15 (m, 42H), 7.00 (d, J = 3.7 Hz, 2H), 7.05–7.09 (m, 6H), 7.12 (d, J = 3.7 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 11.3 (*C*H), 18.6 (*C*H$_3$), 97.2 (*C*), 99.1 (*C*), 122.4 (*C*), 123.2 (*C*H), 124.4 (*C*H), 124.5 (*C*H), 124.8 (*C*H), 133.3 (*C*H), 135.7 (*C*), 135.9 (*C*), 136.3 (*C*), 138.1 (*C*). HRMS-ESI (*m*/*z*): $[M+Na]^+$ calcd for $C_{42}H_{52}NaS_5Si_2$, 795.2103; found, 795.2123. mp 141–143 °C.

2,6-Bis[(triisopropylsilyl)ethynyl]dithieno[3,2-b:2',3'-d]thiophene (3k).

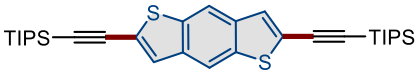


3k

The reaction was performed according to the general procedure A using Ad_3P as the ligand. The reaction was carried out with 82.1 mg (0.45 mmol) of **1a** and 53.1 mg (0.15 mmol) of **2k**. Product **3k** was obtained as a yellow powder (72.8 mg, 0.131 mmol, 87% yield) after purification by silica-gel column chromatography (SiO_2, hexane).

^{1}H NMR (400 MHz, $CDCl_3$, δ): 1.13–1.16 (m, 42H), 7.40 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 11.3 (*C*H), 18.6 (*C*H$_3$), 98.0 (*C*), 99.5 (*C*), 124.4 (*C*), 125.6 (*C*H), 130.9 (*C*), 141.5 (*C*). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{30}H_{44}S_3Si_2$, 556.2144; found, 556.2141. mp 95–97 °C.

2,6-Bis[(triisopropylsilyl)ethynyl]benzo[1,2-b:4,5-b']dithiophene (3l).

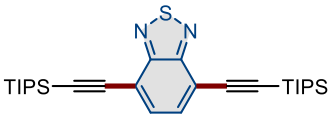


3l

The reaction was performed according to the general procedure A using Ad_3P as the ligand. The reaction was carried out with 82.1 mg (0.45 mmol) of **1a** and 52.2 mg (0.15 mmol) of **2l**. Product **3l** was obtained as a yellow powder (69.7 mg, 0.126 mmol, 84% yield) after purification by silica-gel column chromatography (SiO_2, hexane).

^{1}H NMR (400 MHz, $CDCl_3$, δ): 1.14–1.18 (m, 42H), 7.46 (s, 2H), 8.07 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 11.3 (*C*H), 18.6 (*C*H$_3$), 98.8 (*C*), 99.6 (*C*), 116.4 (*C*H), 124.3 (*C*), 128.2 (*C*H), 137.7 (*C*). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{32}H_{46}S_2Si_2$, 550.2579; found, 550.2580. mp 177–179 °C.

4,7-Bis[(triisopropylsilyl)ethynyl]benzo[c][1,2,5]thiadiazole (3m).

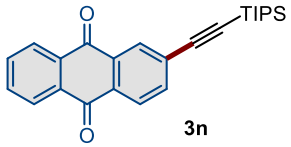


3m

The reaction was performed according to the general procedure A using XPhos as the ligand. The reaction was carried out with 82.1 mg (0.45 mmol) of **1a** and 44.1 mg (0.15 mmol) of **2m**. **3m** was obtained as a yellow powder (73.3 mg, 0.148 mmol, 99% yield) after purification by silica-gel column (SiO_2, $CHCl_3$/hexane, 0:100−15:85). ^{1}H and ^{13}C NMR were in agreement with the literature.[9]

^{1}H NMR (400 MHz, $CDCl_3$, δ): 1.17–1.24 (m, 42H), 7.67 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 11.3 (*C*H), 18.7 (*C*H$_3$), 100.2 (*C*), 102.3 (*C*), 117.5 (*C*), 132.7 (*C*H), 154.6 (*C*). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{28}H_{44}N_2SSi_2$, 496.2764; found, 496.2776.

2-[(Triisopropylsilyl)ethynyl]anthracene-9,10-dione (3n).

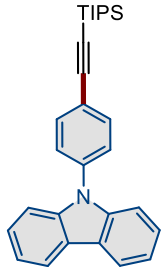


3n

The reaction was performed according to the general procedure A using XPhos as the ligand. The reaction was carried out with 82.1 mg (0.45 mmol) of **1a** and 86.1 mg (0.30 mmol) of **2n**. Product **3n** was obtained as a yellow powder (113.0 mg, 0.291 mmol, 97% yield) after purification by silica-gel column chromatography (SiO_2, CH_2Cl_2/hexane, 0:100–50:50).

^{1}H NMR (400 MHz, $CDCl_3$, δ): 1.13–1.17 (m, 21H), 7.77–7.86 (m, 3H), 8.23 (d, *J* = 8.2 Hz, 1H), 8.26–8.32 (m, 2H), 8.32–8.37 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 11.2 (*C*H), 18.6 (CH_3), 96.9 (*C*), 105.2 (*C*), 127.20 (*C*H), 127.25 (*C*H), 127.3 (*C*H), 129.6 (*C*), 130.6 (*C*H), 132.3 (*C*), 133.28 (*C*), 133.34 (*C*), 133.5 (*C*), 134.1 (*C*H), 134.3 (*C*H), 137.0 (*C*H), 182.4 (*C*), 182.6 (*C*). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{25}H_{28}O_2Si$, 388.1859; found, 388.1857. mp 121–123 °C.

9-{4-[(Triisopropylsilyl)ethynyl]phenyl}-9H-carbazole (3o).

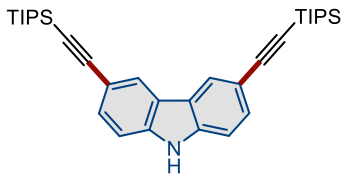


3o

The reaction was performed according to the general procedure A using Ad_3P as the ligand. The reaction was carried out with 82.1 mg (0.45 mmol) of **1a** and 96.7 mg (0.30 mmol) of **2o**. Product **3o** was obtained as a yellow oil (132.7 mg, 0.313 mmol, >99% yield) after purification by silica-gel column chromatography (SiO_2, hexane).

^{1}H NMR (400 MHz, $CDCl_3$, δ): 1.27 (s, 21H), 7.36 (sept, *J* = 3.6 Hz, 2H), 7.47 (d, *J* = 3.6 Hz, 4H), 7.57 (dt, *J* = 2.0, 8.6 Hz, 2H), 7.78 (dt, *J* = 2.0, 8.6 Hz, 2H), 8.20 (d, *J* = 8.0 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 11.3 (*C*H), 18.7 (CH_3), 91.8 (*C*), 106.3 (*C*), 109.6 (*C*H), 120.1 (*C*H), 120.3 (*C*H), 122.4 (*C*), 123.5 (*C*), 126.0 (*C*H), 126.7 (*C*H), 133.5 (*C*H), 137.5 (*C*), 140.5 (*C*). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{29}H_{33}NSi$, 423.2382; found, 423.2389.

3,6-Bis((triisopropylsilyl)ethynyl)-9H-carbazole (3p).

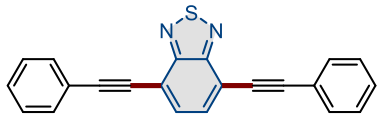


3p

The reaction was performed according to the general procedure A using Ad_3P as the ligand. The reaction was carried out with 82.1 mg (0.45 mmol) of **1a** and 48.8 mg (0.15 mmol) of **2p**. Product **3p** was obtained as a yellow powder (54.8 mg, 0.104 mmol, 69% yield) after purification by silica-gel column chromatography (SiO_2, CH_2Cl_2/hexane, 10:90–20:80). ^1H and ^{13}C NMR were in agreement with the literature.[10]

^1H NMR (400 MHz, $CDCl_3$, δ): 1.18 (s, 42H), 7.31 (d, J = 8.2 Hz, 2H), 7.55 (dd, J = 8.5, 1.6 Hz, 2H), 8.09 (s, 1H), 8.21 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 11.4 (*C*H), 18.7 (*C*H$_3$), 88.3 (*C*), 108.1 (*C*), 110.5 (*C*H), 114.9 (*C*), 122.7 (*C*), 124.6 (*C*H), 130.4 (*C*H), 139.3 (*C*). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{34}H_{49}NSi_2$, 527.3404; found, 527.3390.

4,7-Bis(phenylethynyl)benzo[c][1,2,5]thiadiazole (3q).

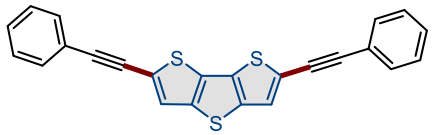


3q

The reaction was performed according to the general procedure A using XPhos as the ligand. The reaction was carried out with 45.9 mg (0.45 mmol) of **1b** and 44.1 mg (0.15 mmol) of **2m**. Product **3q** was obtained as a yellow powder (51.0 mg, 0.152 mmol, >99% yield) after purification by silica-gel column chromatography (SiO_2, $CHCl_3$/hexane, 0:100–20:80). ^1H and ^{13}C NMR were in agreement with the literature.[11]

^1H NMR (400 MHz, $CDCl_3$, δ): 7.37–7.43 (m, 6H), 7.64–7.71 (m, 4H), 7.78 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 85.3 (*C*), 97.4 (*C*), 117.1 (*C*), 122.4 (*C*), 128.4 (*C*H), 129.1 (*C*H), 132.0 (*C*H), 132.4 (*C*H), 154.3 (*C*). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{22}H_{12}N_2S$, 336.0721; found, 336.0711.

2,6-Bis(phenylethynyl)dithieno[3,2-b:2',3'-d]thiophene (3r).

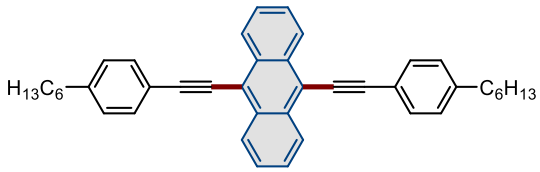


3r

The reaction was performed according to the general procedure A using Ad_3P as the ligand. The reaction was carried out with 45.9 mg (0.45 mmol) of **1b** and 53.1 mg (0.15 mmol) of **2k**. Product **3r** was obtained as a yellow powder (38.9 mg, 0.098 mmol, 65% yield) after purification by silica-gel column chromatography (SiO_2, hexane). ^1H and ^{13}C NMR were in agreement with the literature.[12]

^1H NMR (400 MHz, $CDCl_3$, δ): 7.34–7.41 (m, 6H), 7.44 (s, 2H), 7.53–7.59 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 83.0 (*C*), 95.0 (*C*), 122.5 (*C*), 124.2 (*C*), 125.1 (*C*H), 128.4 (*C*H), 128.7 (*C*H), 131.3 (*C*), 131.4 (*C*H), 141.7 (*C*). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{24}H_{12}S_3$, 396.0101; found, 396.0094.

9,10-Bis[(4-hexylphenyl)ethynyl]anthracene (3s).

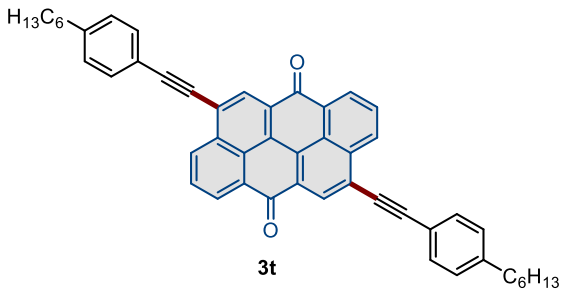


3s

The reaction was performed according to the general procedure A using Ad_3P as the ligand. The reaction was carried out with 83.8 mg (0.45 mmol) of **1c** and 50.4 mg (0.15 mmol) of **2d**. Product **3s** was obtained as a yellow powder (77.1 mg, 0.141 mmol, 94% yield) after purification by silica-gel column chromatography (SiO_2, $CHCl_3$/hexane, 0:100–10:90).

^1H NMR (400 MHz, $CDCl_3$, δ): 0.95 (t, J = 6.6 Hz, 6H), 1.29–1.45 (m, 12H), 1.68 (quint, J = 7.6 Hz, 4H), 2.69 (t, J = 7.7 Hz, 4H), 7.28 (d, J = 8.2 Hz, 4H), 7.62–7.67 (m, 4H), 7.71 (d, J = 8.2 Hz, 4H), 8.69–8.74 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 14.1 (CH_3), 22.6 (CH_2), 28.9 (CH_2), 31.2 (CH_2), 31.7 (CH_2), 36.0 (CH_2), 86.0 (*C*), 102.6 (*C*), 118.5 (*C*), 120.6 (*C*), 126.6 (*C*H), 127.2 (*C*H), 128.6 (*C*H), 131.6 (*C*H), 132.0 (*C*), 143.9 (*C*). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{42}H_{42}$, 546.3287; found, 546.3287. mp 146–148 °C.

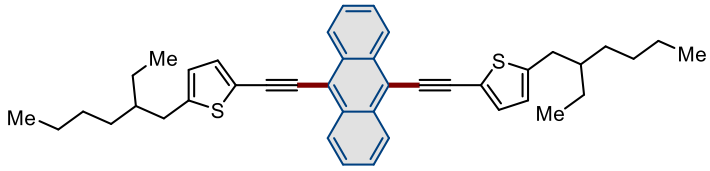
4,10-Bis[(4-hexylphenyl)ethynyl]naphtho[7,8,1,2,3-nopqr]tetraphene-6,12-dione (3t).



3t

The reaction was performed according to the general procedure A using Ad_3P as the ligand. The reaction was carried out with 83.8 mg (0.45 mmol) of **1c** and 69.6 mg (0.15 mmol) of **2a**. Product **3t** was obtained as a purple powder (85.2 mg, 0.126 mmol, 84% yield) after purification by silica-gel column (SiO_2, $CHCl_3$/hexane, 0:100–100:0). ^1H and ^{13}C NMR were in agreement with the literature.[13] ^1H NMR (400 MHz, $CDCl_3$, δ): 0.91 (t, J = 6.8 Hz, 6H), 1.28–1.42 (m, 12H), 1.62–1.71 (m, 4H), 2.67 (t, J = 7.9 Hz, 4H), 7.24 (d, J = 8.0 Hz, 4H), 7.60 (d, J = 8.2 Hz, 4H), 7.89 (t, J = 7.7 Hz, 2H), 8.58 (s, 2H), 8.73 (d, J = 7.7 Hz, 4H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 14.1 (*C*H_3), 22.6 (*C*H_2), 29.0 (*C*H_2), 31.2 (*C*H_2), 31.7 (*C*H_2), 36.1 (*C*H_2), 86.1 (*C*), 98.3 (*C*), 119.7 (*C*), 124.3 (*C*), 126.6 (*C*), 127.1 (*C*), 127.9 (*C*H), 128.6 (*C*H), 128.9 (*C*), 129.0 (*C*), 129.1 (*C*H), 131.0 (*C*H), 131.9 (*C*H), 133.4 (*C*), 133.6 (*C*H), 144.4 (*C*), 181.8 (*C*). HRMS-ESI (*m*/*z*): $[M+Na]^+$ calcd for $C_{50}H_{42}O_2Na$, 697.3077; found, 697.3091.

9,10-Bis{[5-(2-ethylhexyl)thiophen-2-yl]ethynyl}anthracene (3u).

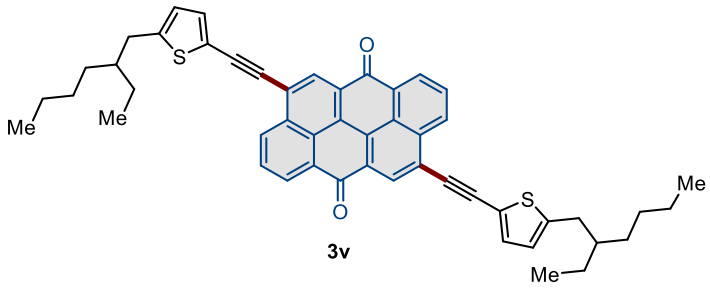


3u

The reaction was performed according to the general procedure A using Ad_3P as the ligand. The reaction was carried out with 98.6 mg (0.45 mmol) of **1d** and 50.4 mg (0.15 mmol) of **2d**. Product **3u** was obtained as a brown powder (78.6 mg, 0.128 mmol, 85% yield) after purification by silica-gel column chromatography (SiO_2, $CHCl_3$/hexane, 0:100–5:95).

^1H NMR (400 MHz, $CDCl_3$, δ): 0.88–1.01 (m, 12H), 1.26–1.48 (m, 16H), 1.60–1.71 (m, 2H), 2.82 (d, J = 6.8 Hz, 4H), 6.78 (d, J = 3.6 Hz, 2H), 7.34 (d, J = 3.6 Hz, 2H), 7.60–7.68 (m, 4H), 8.59–8.66 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 10.8 (*C*H_3), 14.1 (*C*H_3), 23.0 (*C*H_2), 25.5 (*C*H_2), 28.9 (*C*H_2), 32.4 (*C*H_2), 34.3 (*C*H_2), 41.5 (*C*H), 89.9 (*C*), 96.2 (*C*), 118.2 (*C*), 120.8 (*C*), 125.6 (*C*H), 126.7 (*C*H), 127.2 (*C*H), 131.8 (*C*), 132.2 (*C*H), 147.8 (*C*). HRMS-ESI (*m*/*z*): $[M+Na]^+$ calcd for $C_{42}H_{46}NaS_2$, 637.2933; found, 637.2937. mp 55–56 °C.

4,10-Bis{[5-(2-ethylhexyl)thiophen-2-yl]ethynyl}naphtho[7,8,1,2,3-nopqr]tetraphene-6,12-dione (3v).

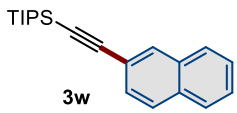


3v

The reaction was performed according to the general procedure A using Ad_3P as the ligand. The reaction was carried out with 98.6 mg (0.45 mmol) of **1d** and 69.6 mg (0.15 mmol) of **2a**. Product **3v** was obtained as a purple powder (69.4 mg, 0.093 mmol, 62% yield) after purification by silica-gel column chromatography (SiO_2, $CHCl_3$/hexane, 5:95–50:50).

^{1}H NMR (400 MHz, $CDCl_3$, δ): 0.90–0.98 (m, 12H), 1.29–1.45 (m, 16H), 1.61–1.70 (m, 2H), 2.81 (d, *J* = 6.9 Hz, 4H), 6.76 (d, *J* = 3.7 Hz, 2H), 7.29 (d, *J* = 3.7 Hz, 2H), 7.84 (t, *J* = 7.8 Hz, 2H), 8.44 (s, 2H), 8.59 (dd, *J* = 0.9, 8.3 Hz, 2H), 8.65 (dd, *J* = 0.9, 7.3 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 10.8 (*C*H_3), 14.2 (*C*H_3), 23.0 (*C*H_2), 25.5 (*C*H_2), 28.9 (*C*H_2), 32.4 (*C*H_2), 34.3 (*C*H_2), 41.5 (*C*H), 90.0 (*C*), 91.8 (*C*), 120.0 (*C*), 123.5 (*C*), 125.6 (*C*H), 125.8 (*C*), 126.5 (*C*), 127.1 (*C*H), 128.36 (*C*), 128.43 (*C*), 128.8 (*C*H), 130.7 (*C*H), 132.5 (*C*), 133.0 (*C*H), 133.1 (*C*H), 148.4 (*C*), 181.0 (*C*). HRMS-ESI (*m*/*z*): $[M+Na]^+$ calcd for $C_{50}H_{46}O_2NaS_2$, 765.2831; found, 765.2850. mp 179–180 °C.

Triisopropyl(naphthalen-2-ylethynyl)silane (3w).

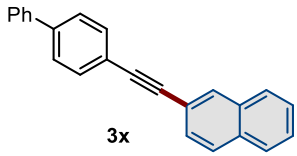


3w

The reaction was performed according to the general procedure B. The reaction was carried out with 82.1 mg (0.45 mmol) of **1a** and 48.8 mg (0.30 mmol) of **2q**. Product **3w** was obtained as a colorless liquid (93.9 mg, 0.304 mmol, >99% yield) after purification by silica-gel column chromatography (SiO_2, pentane). ^{1}H and ^{13}C NMR were in agreement with the literature.[14]

^{1}H NMR (400 MHz, $CDCl_3$, δ): 1.21 (s, 21H), 7.48–7.53 (m, 2H), 7.56 (dd, *J* = 1.6, 8.4 Hz, 1H), 7.75–7.88 (m, 3H), 8.04 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 11.4 (*C*), 18.7 (*C*), 90.9 (*C*), 107.5 (*C*), 120.8 (*C*), 126.5 (*C*H), 126.6 (*C*H), 127.68 (*C*H), 127.70 (*C*H), 127.8 (*C*H), 128.8 (*C*H), 131.8 (*C*H), 132.8 (*C*), 132.9 (*C*). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{21}H_{28}Si$, 308.1960; found, 308.1951.

2-[(1,1'-Biphenyl)-4-ylethynyl]naphthalene (3x).

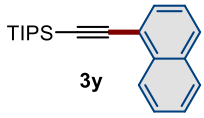


3x

The reaction was performed according to the general procedure B. The reaction was carried out with 80.2 mg (0.45 mmol) of **1e** and 48.8 mg (0.30 mmol) of **2q**. Product **3x** was obtained as a white powder (83.3 mg, 0.273 mmol, 91% yield) after purification by silica-gel column chromatography (SiO_2, $CHCl_3$/hexane, 0:100–10:90). ^1H and ^{13}C NMR were in agreement with the literature.[15]

^1H NMR (400 MHz, $CDCl_3$, δ): 7.37–7.42 (m, 1H), 7.45–7.56 (m, 4H), 7.60–7.71 (m, 7H), 7.82–7.89 (m, 3H), 8.10 (d, J = 0.9 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 89.7 (*C*), 90.5 (*C*), 120.6 (*C*), 122.2 (*C*), 126.5 (*C*H), 126.7 (*C*H), 127.01 (*C*H), 127.04 (*C*H), 127.6 (*C*H), 127.8 (*C*H), 128.0 (*C*H), 128.4 (*C*H), 128.8 (*C*H), 131.4 (*C*H), 132.1 (*C*H), 132.8 (*C*), 132.9 (*C*H), 133.0 (*C*), 140.3 (*C*), 141.0 (*C*). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{24}H_{16}$, 304.1252; found, 304.1250.

Triisopropyl(naphthalen-1-ylethynyl)silane (3y).

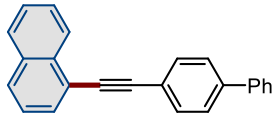


3y

The reaction was performed according to the general procedure B. The reaction was carried out with 82.1 mg (0.45 mmol) of **1a** and 48.8 mg (0.30 mmol) of **2r**. Product **3y** was obtained as a colorless liquid (91.8 mg, 0.298 mmol, 99% yield) after purification by silica-gel column chromatography (SiO_2, pentane). ^1H and ^{13}C NMR were in agreement with the literature.[14]

^1H NMR (400 MHz, $CDCl_3$, δ): 1.21–1.29 (m, 21H), 7.45 (t, J = 7.7 Hz, 1H), 7.55 (dd, J = 7.0, 7.9 Hz, 1H), 7.60–7.65 (m, 1H), 7.77 (d, J = 7.2 Hz, 1H), 7.86 (t, J = 9.1 Hz, 2H), 8.46 (d, J = 8.2 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 11.4 (*C*H), 18.8 (*C*H_3), 95.7 (*C*), 105.0 (*C*), 121.2 (*C*), 125.1 (*C*H), 126.27 (*C*H), 126.32 (*C*H), 126.8 (*C*H), 128.2 (*C*H), 128.8 (*C*H), 131.0 (*C*H), 133.1 (*C*), 133.5 (*C*). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{21}H_{28}Si$, 308.1960; found, 308.1960.

1-[(1,1'-Biphenyl)-4-ylethynyl]naphthalene (3z).

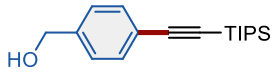


3z

The reaction was performed according to the general procedure B. The reaction was carried out with 80.2 mg (0.45 mmol) of **1e** and 48.8 mg (0.30 mmol) of **2r**. Product **3z** was obtained as a white powder (83.9 mg, 0.276 mmol, 92% yield) after purification by silica-gel column chromatography (SiO_2, hexane). ^1H and ^{13}C NMR were in agreement with the literature.[15]

^1H NMR (400 MHz, $CDCl_3$, δ): 7.39 (t, J = 7.2 Hz, 1H), 7.48 (t, J = 7.9 Hz, 3H), 7.56 (t, J = 7.5 Hz, 1H), 7.60–7.66 (m, 5H), 7.74 (d, J = 7.7 Hz, 2H), 7.80 (d, J = 7.2 Hz, 1H), 7.88 (t, J = 8.8 Hz, 2H), 8.49 (d, J = 8.2 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 88.2 (*C*), 94.2 (*C*), 120.9 (*C*), 122.3 (*C*), 125.3 (*C*H), 126.2 (*C*H), 126.4 (*C*H), 126.8 (*C*H), 127.0 (*C*H), 127.1 (*C*H), 127.7 (*C*H), 128.3 (*C*H), 128.8 (*C*H), 128.9 (*C*H), 130.4 (*C*H), 132.1 (*C*H), 133.21 (*C*), 133.25 (*C*), 140.3 (*C*), 141.1 (*C*). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{24}H_{16}$, 304.1252; found, 304.1250.

(4-((Triisopropylsilyl)ethynyl)phenyl)methanol (3aa).

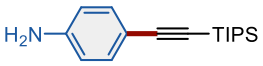


3aa

The reaction was performed according to the general procedure B. The reaction was carried out with 82.1 mg (0.45 mmol) of **1a** and 42.8 mg (0.30 mmol) of **2s**. Product **3aa** was obtained as a colorless oil (77.1 mg, 0.267 mmol, 90% yield) after purification by silica-gel column chromatography (SiO_2, CH_2Cl_2/hexane, 20:80–66:33). ^1H and ^{13}C NMR were in agreement with the literature.[16]

^1H NMR (400 MHz, $CDCl_3$, δ): 1.13 (s, 21H), 2.28 (s, 1H), 4.62 (s, 2H), 7.26 (d, J = 8.2 Hz, 2H), 7.43–7.49 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 11.3 (*C*H), 18.6 (*C*H_3), 64.7 (*C*H_2), 90.5 (*C*), 106.8 (*C*), 122.7 (*C*), 126.6 (*C*H), 132.1 (*C*H), 141.0 (*C*). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{18}H_{28}OSi$, 288.1909; found, 288.1909.

4-((Triisopropylsilyl)ethynyl)aniline (3ab).



3ab

The reaction was performed according to the general procedure B. The reaction was carried out with 82.1 mg (0.45 mmol) of **1a** and 38.3 mg (0.30 mmol) of **2t**. Product **3ab** was obtained as a pale yellow oil (58.9 mg, 0.215 mmol, 72% yield) after purification by silica-gel column chromatography (SiO_2, CH_2Cl_2/hexane, 10:90–50:50). ^1H and ^{13}C NMR were in agreement with the literature.[17]

^1H NMR (400 MHz, $CDCl_3$, δ): 1.16–1.09 (m, 21H), 3.78 (s, 2H), 6.56–6.60 (m, 2H), 7.27–7.32 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 11.4 (*C*H), 18.7 (*C*H$_3$), 87.4 (*C*), 107.8 (*C*), 113.0 (*C*), 114.5 (*C*H), 133.4 (*C*H), 146.6 (*C*). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{17}H_{27}NSi$, 273.1913; found, 273.1914.

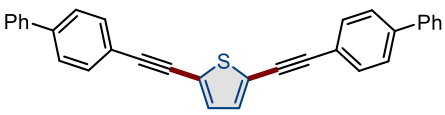
2,5-Bis[(triisopropylsilyl)ethynyl]thiophene (3ac).

3ac

The reaction was performed according to the general procedure B. The reaction was carried out with 82.1 mg (0.45 mmol) of **1a** and 23.0 mg (0.15 mmol) of **2v**. Product **3ac** was obtained as a yellow oil (57.9 mg, 0.130 mmol, 87% yield) after purification by silica-gel column chromatography (SiO_2, hexane). ^1H and ^{13}C NMR were in agreement with the literature.[18]

^1H NMR (400 MHz, $CDCl_3$, δ): 1.10–1.13 (m, 42H), 7.04 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 11.3 (*C*H), 18.6 (*C*H$_3$), 96.6 (*C*), 98.8 (*C*), 124.6 (*C*), 131.8 (*C*H). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{26}H_{44}SSi_2$, 444.2702; found, 444.2686.

2,5-Bis[(1,1'-biphenyl)-4-ylethynyl]thiophene (3ad).

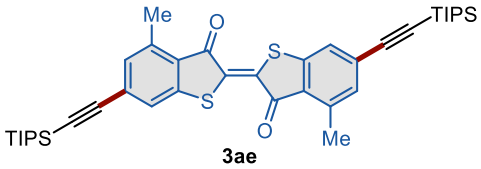


3ad

The reaction was performed according to the general procedure B. The reaction was carried out with 80.2 mg (0.45 mmol) of **1e** and 23.0 mg (0.15 mmol) of **2v**. Product **3ad** was obtained as a yellow powder (56.0 mg, 0.128 mmol, 86% yield) after purification by silica-gel column chromatography (SiO_2, $CHCl_3$/hexane, 5:95–30:70) and preparative recycle GPC.

^{1}H NMR (400 MHz, $CDCl_3$, δ): 7.19 (s, 2H), 7.38 (tt, J = 1.6, 6.0 Hz, 2H), 7.44–7.48 (m, 4H), 7.59–7.64 (m, 12H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 83.0 (*C*), 94.1 (*C*), 121.4 (*C*), 124.7 (*C*), 127.0 (*C*H), 127.1 (*C*H), 127.7 (*C*H), 128.9 (*C*H), 131.9 (*C*H), 140.2 (*C*), 141.4 (*C*). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{32}H_{20}S$, 436.1286; found, 436.1267. mp 220–221 °C.

(*E*)-4,4'-Dimethyl-6,6'-bis[(triisopropylsilyl)ethynyl]-3H,3'H-[2,2'-bibenzo[b]thiophenylidene]-3,3'-dione (3ae).

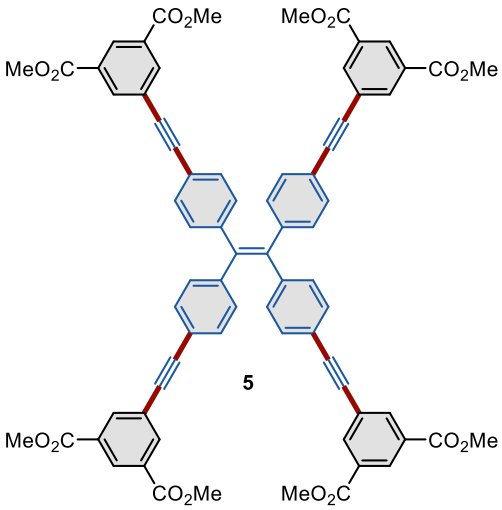


3ae

The reaction was performed according to the general procedure C. The reaction was carried out with 82.1 mg (0.45 mmol) of **1a** and 59.0 mg (0.15 mmol) of **2w**. Product **3ae** was obtained as a red powder (56.1 mg, 0.082 mmol, 55% yield) after purification by silica-gel column chromatography (SiO_2, $CHCl_3$/hexane, 5:95–30:70).

^{1}H NMR (400 MHz, $CDCl_3$, δ): 1.08–1.19 (m, 42H), 2.67 (s, 6H), 7.09 (s, 2H), 7.38 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 11.2 (*C*H), 18.6 (*C*H$_3$), 18.7 (*C*H$_3$), 96.8 (*C*), 105.7 (*C*), 124.9 (*C*H), 125.7 (*C*), 130.1 (*C*), 132.0 (*C*H), 132.9 (*C*), 141.7 (*C*), 149.1 (*C*), 190.0 (*C*). HRMS-ESI (*m*/*z*): $[M+Na]^+$ calcd for $C_{40}H_{52}O_2NaS_2Si_2$, 707.2840; found, 707.2843. mp 293–296 °C.

Octamethyl 5,5',5'',5'''-{[ethene-1,1,2,2-tetrayltetrakis(benzene-4,1-diyl)]tetrakis(ethyne-2,1-diyl)}tetraisophthalate (5).



5

The reaction was performed according to the section 6. The reaction was carried out with 32.1 mg

(0.075 mmol) of **4**, 122.9 mg (0.45 mmol) of **2x**. Product **5** was obtained as a yellow powder (45.3 mg, 0.038 mmol, 51% yield) after purification by silica-gel column chromatography (SiO_2, ethyl acetate/hexane, 10:90−50:50). ^{1}H and ^{13}C NMR were in agreement with the literature.[8]

^{1}H NMR (400 MHz, $CDCl_3$, δ): 3.94 (s, 24H), 7.05 (d, *J* = 8.2 Hz, 8H), 7.34 (d, *J* = 8.2 Hz, 8H), 8.32 (d, *J* = 1.8 Hz, 8H), 8.60 (d, *J* = 1.8 Hz, 4H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 52.5 (*C*H_3), 88.1 (*C*), 91.1 (*C*), 121.1 (*C*), 124.2 (*C*), 130.0 (*C*H), 130.9 (*C*), 131.42 (*C*H), 131.44 (*C*H), 136.4 (*C*H), 141.1 (*C*), 143.3 (*C*), 165.5 (*C*). HRMS-ESI (*m*/*z*): $[M+Na]^+$ calcd for $C_{74}H_{52}O_{16}Na$, 1219.3148; found, 1219.3173.

17. References.

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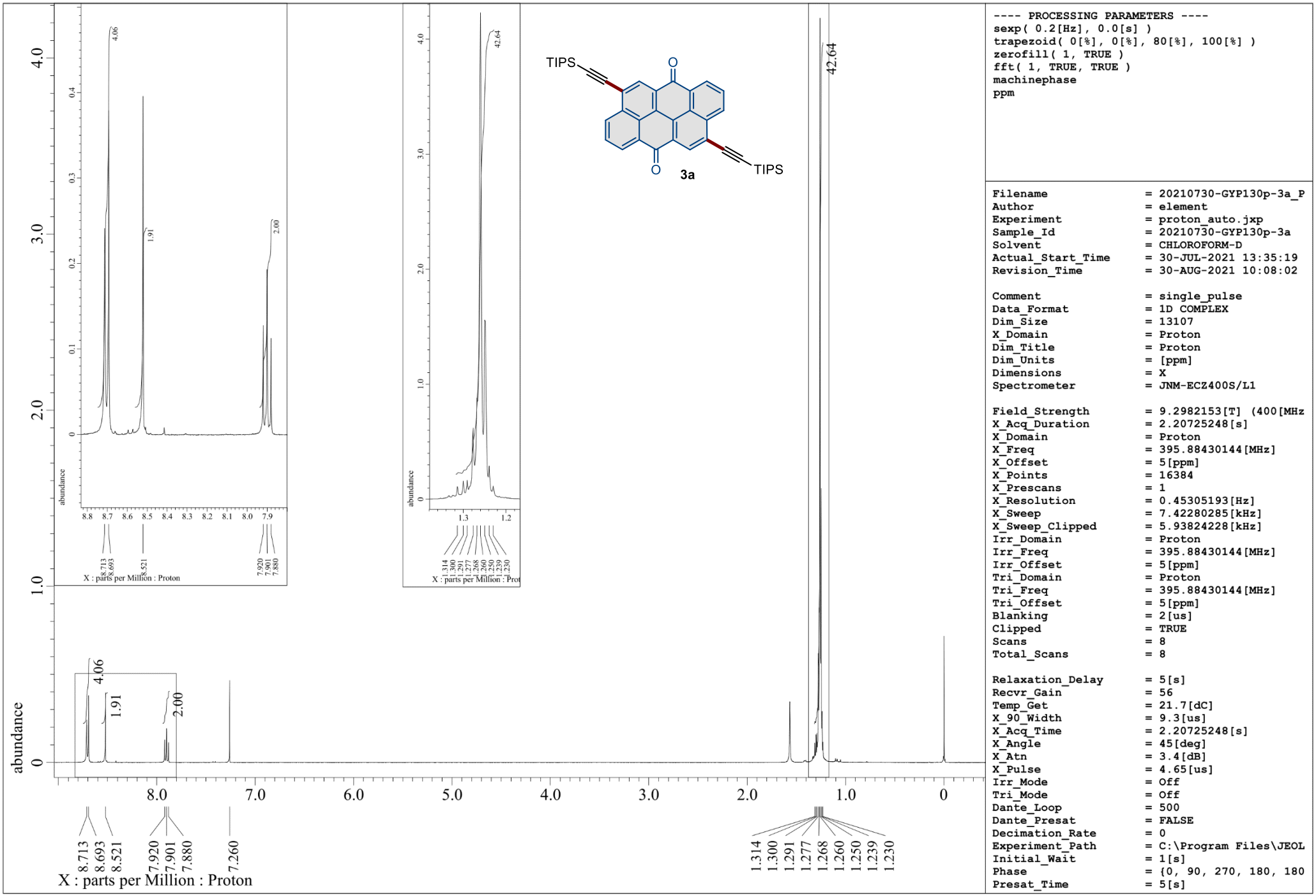


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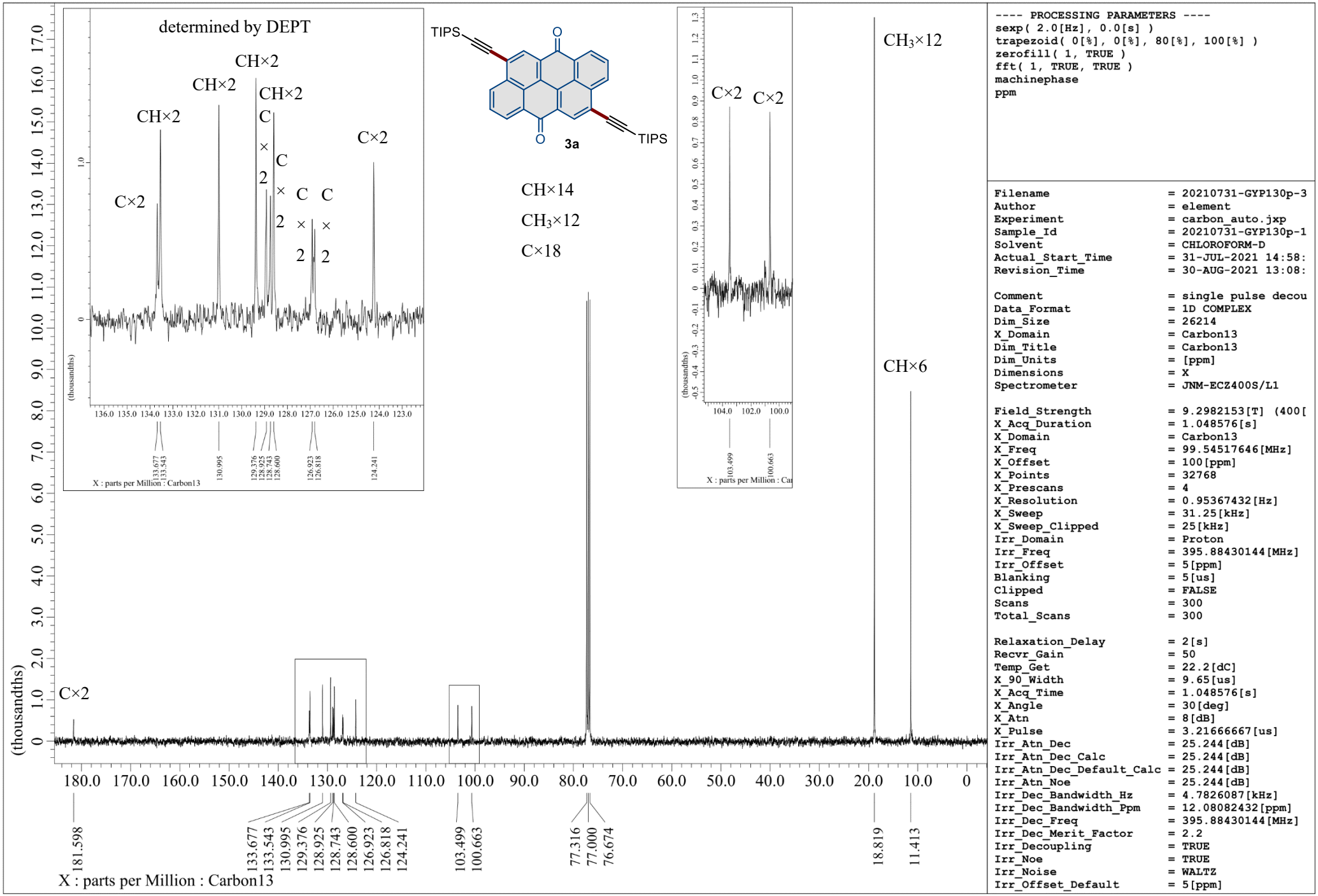


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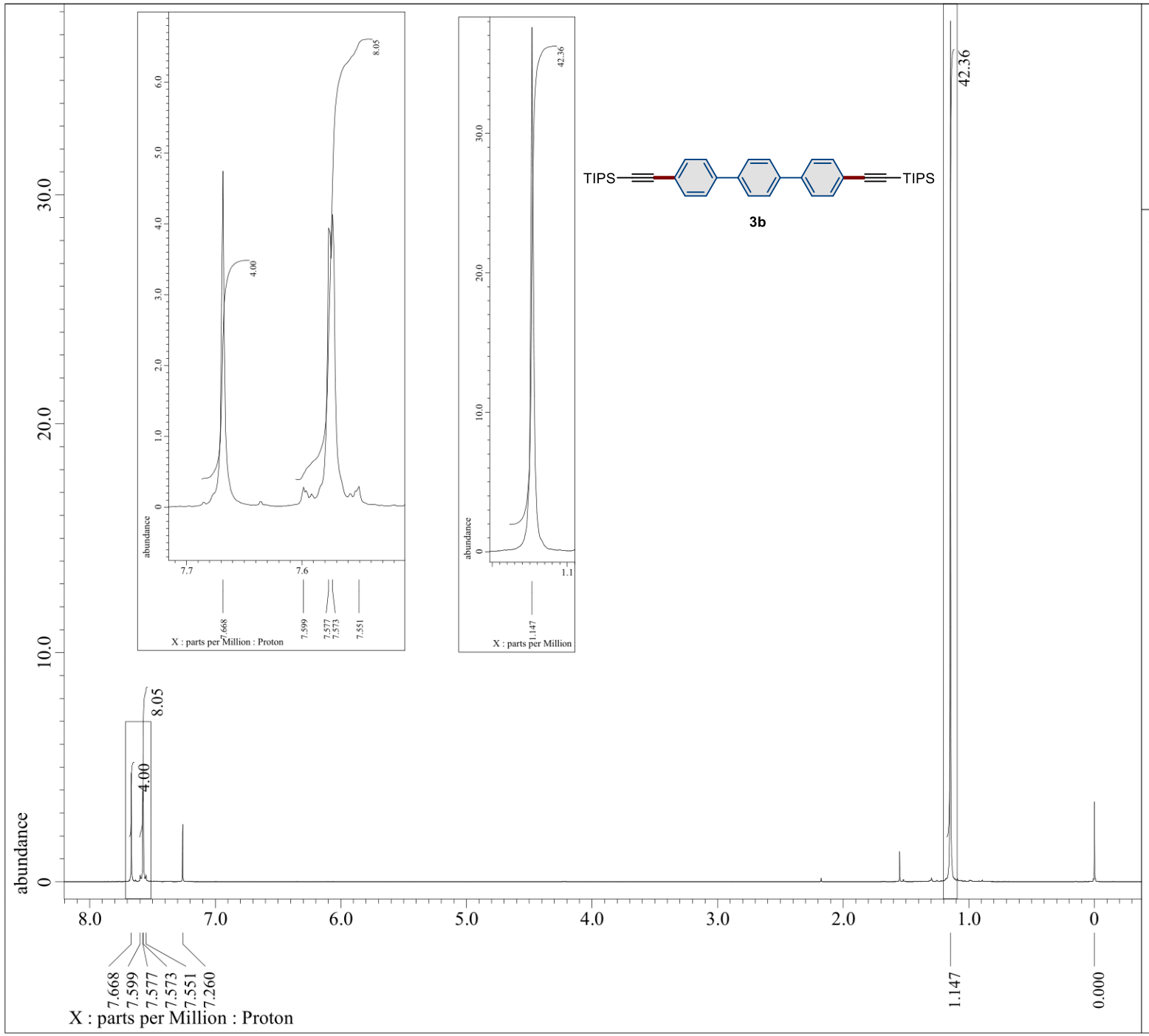

3b

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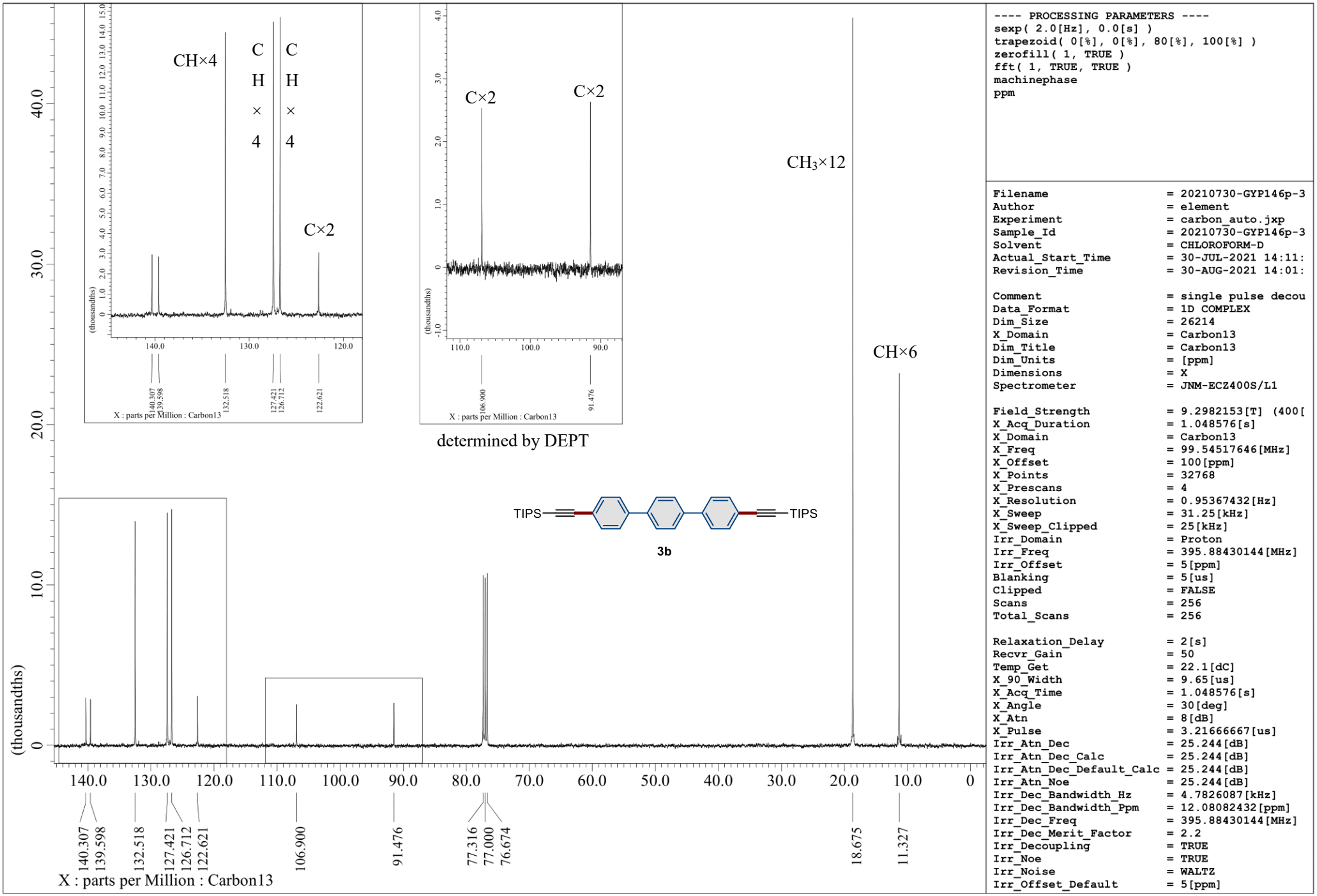
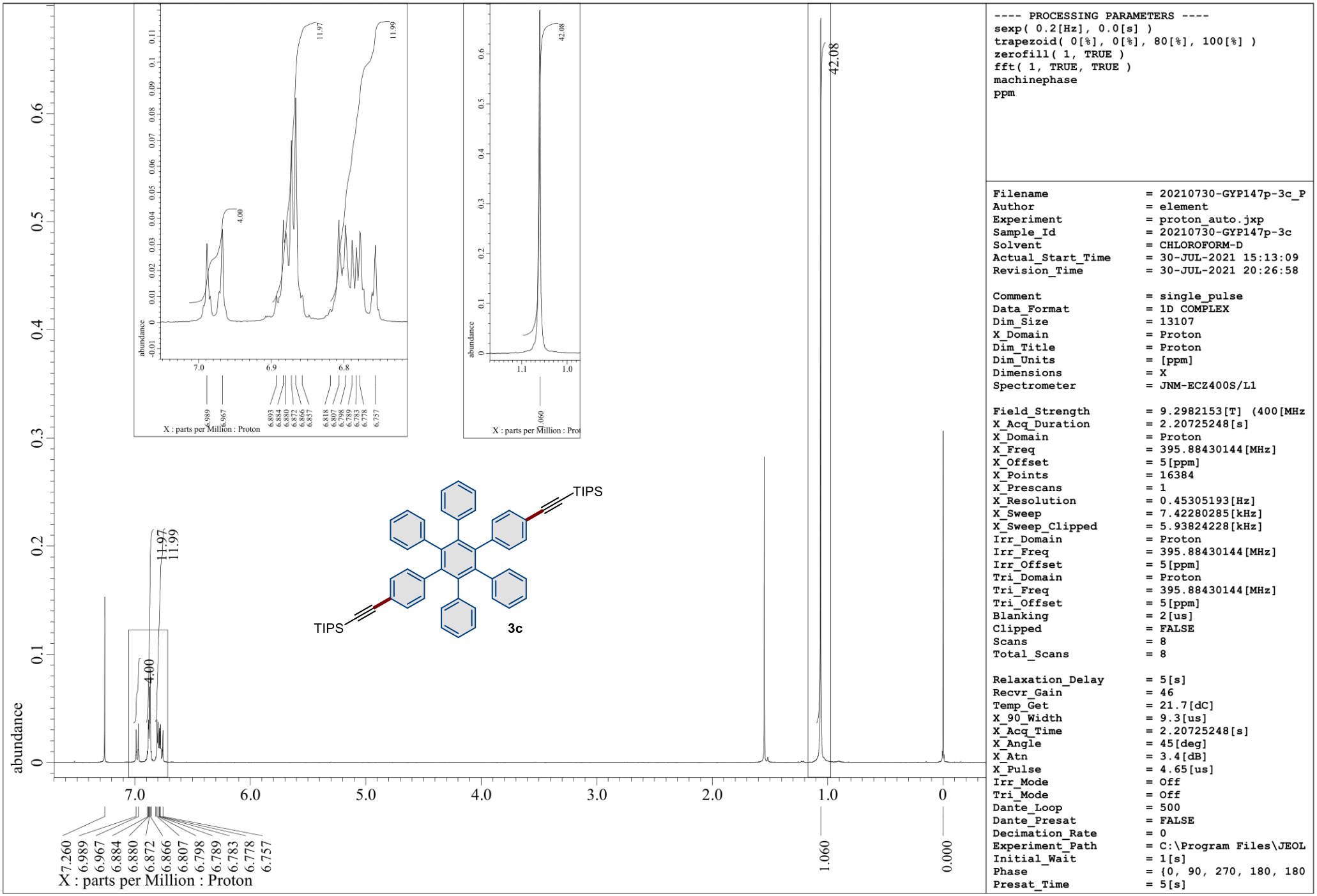
Repetition_Time     = 7.1889024[s]
```



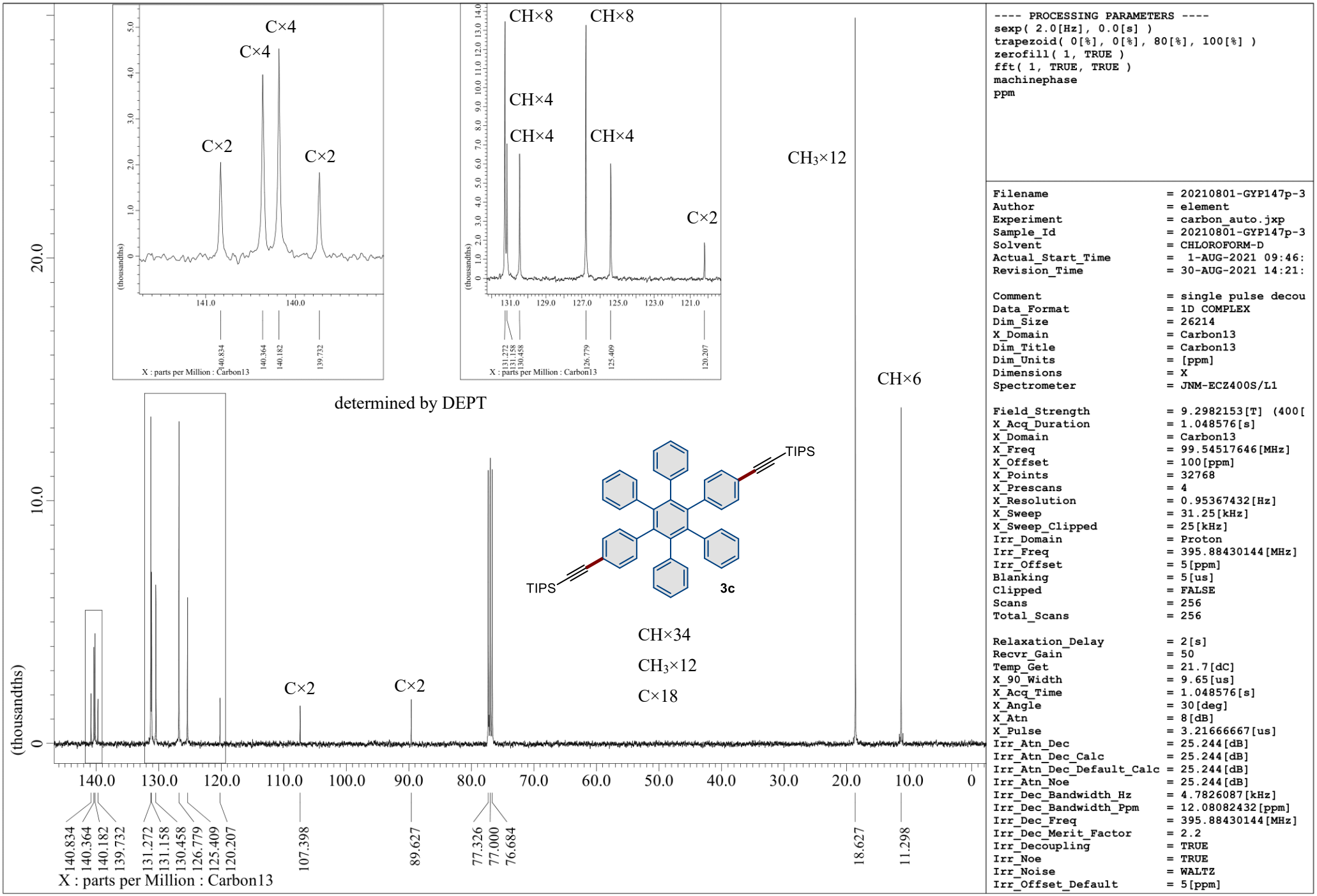

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

Filename	= 20210730-GYP146p-3
Author	= element
Experiment	= carbon_auto.jxp
Sample_Id	= 20210730-GYP146p-3
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 30-JUL-2021 14:11:
Revision_Time	= 30-AUG-2021 14:01:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ400S/L1
Field_Strength	= 9.2982153[T] (400[
X_Acq_Duration	= 1.048576[s]
X_Domain	= Carbon13
X_Freq	= 99.54517646[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.95367432[Hz]
X_Sweep	= 31.25[kHz]
X_Sweep_Clipped	= 25[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 5[us]
Clipped	= FALSE
Scans	= 256
Total_Scans	= 256
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 22.1[dC]
X_90_Width	= 9.65[us]
X_Acq_Time	= 1.048576[s]
X_Angle	= 30[deg]
X_Atn	= 8[dB]
X_Pulse	= 3.21666667[us]
Irr_Atn_Dec	= 25.244[dB]
Irr_Atn_Dec_Calc	= 25.244[dB]
Irr_Atn_Dec_Default_Calc	= 25.244[dB]
Irr_Atn_Noe	= 25.244[dB]
Irr_Dec_Bandwidth_Hz	= 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.08082432[ppm]
Irr_Dec_Freq	= 395.88430144[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]



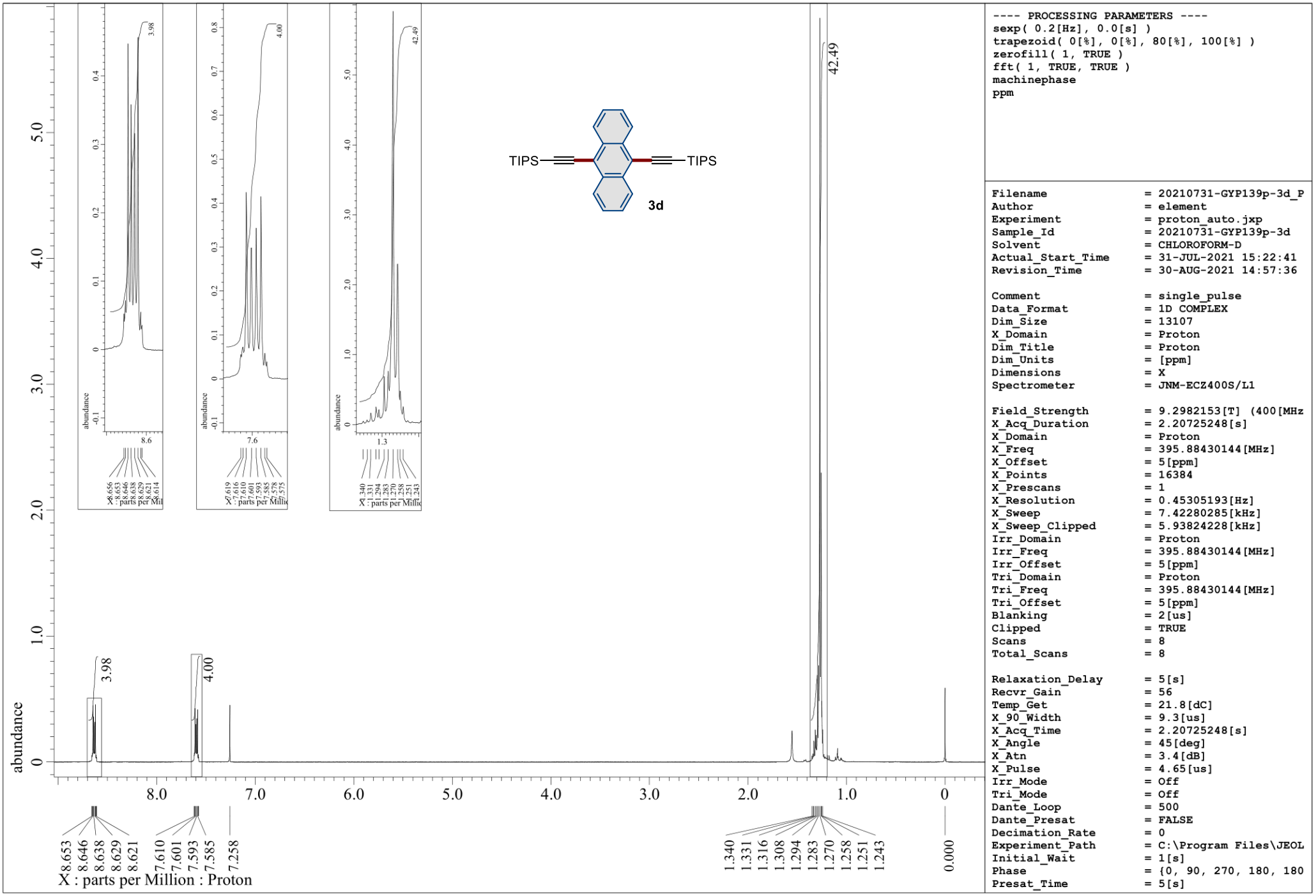

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

Filename	= 20210730-GYP147p-3c_P
Author	= element
Experiment	= proton_auto.jxp
Sample_Id	= 20210730-GYP147p-3c
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 30-JUL-2021 15:13:09
Revision_Time	= 30-JUL-2021 20:26:58
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ400S/L1
Field_Strength	= 9.2982153[T] (400[MHz
X_Acq_Duration	= 2.20725248[s]
X_Domain	= Proton
X_Freq	= 395.88430144[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45305193[Hz]
X_Sweep	= 7.42280285[kHz]
X_Sweep_Clipped	= 5.93824228[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 395.88430144[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 46
Temp_Get	= 21.7[dC]
X_90_Width	= 9.3[us]
X_Acq_Time	= 2.20725248[s]
X_Angle	= 45[deg]
X_Atn	= 3.4[dB]
X_Pulse	= 4.65[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 500
Dante_Presat	= FALSE
Decimation_Rate	= 0
Experiment_Path	= C:\Program Files\JEOL
Initial_Wait	= 1[s]
Phase	= {0, 90, 270, 180, 180
Presat_Time	= 5[s]



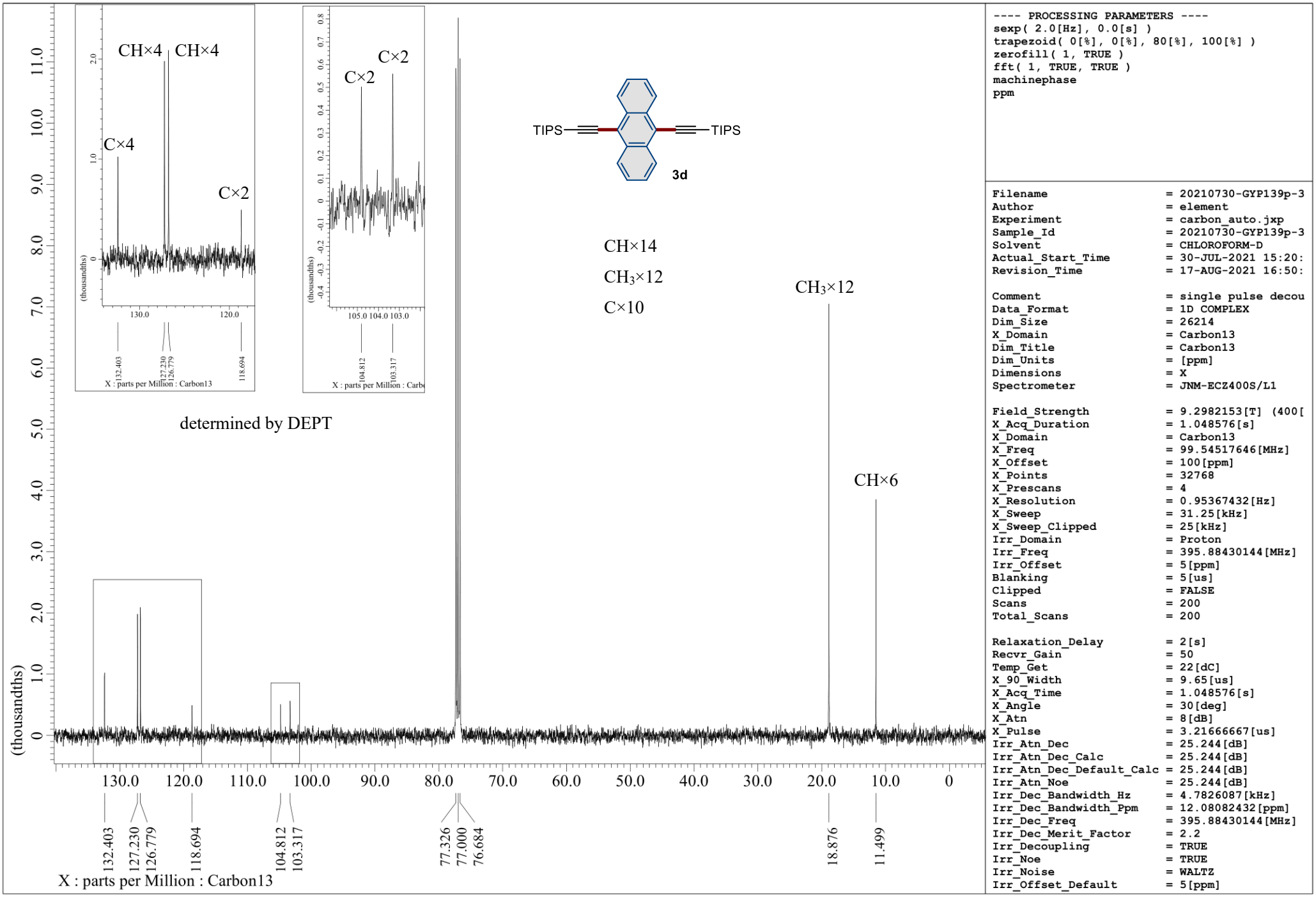

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

Filename	= 20210801-GYP147p-3
Author	= element
Experiment	= carbon_auto.jxp
Sample_Id	= 20210801-GYP147p-3
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 1-AUG-2021 09:46:
Revision_Time	= 30-AUG-2021 14:21:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ400S/L1
Field_Strength	= 9.2982153[T] (400[
X_Acq_Duration	= 1.048576[s]
X_Domain	= Carbon13
X_Freq	= 99.54517646[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.95367432[Hz]
X_Sweep	= 31.25[kHz]
X_Sweep_Clipped	= 25[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 5[us]
Clipped	= FALSE
Scans	= 256
Total_Scans	= 256
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 21.7[dC]
X_90_Width	= 9.65[us]
X_Acq_Time	= 1.048576[s]
X_Angle	= 30[deg]
X_Atn	= 8[dB]
X_Pulse	= 3.21666667[us]
Irr_Atn_Dec	= 25.244[dB]
Irr_Atn_Dec_Calc	= 25.244[dB]
Irr_Atn_Dec_Default_Calc	= 25.244[dB]
Irr_Atn_Noe	= 25.244[dB]
Irr_Dec_Bandwidth_Hz	= 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.08082432[ppm]
Irr_Dec_Freq	= 395.88430144[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]



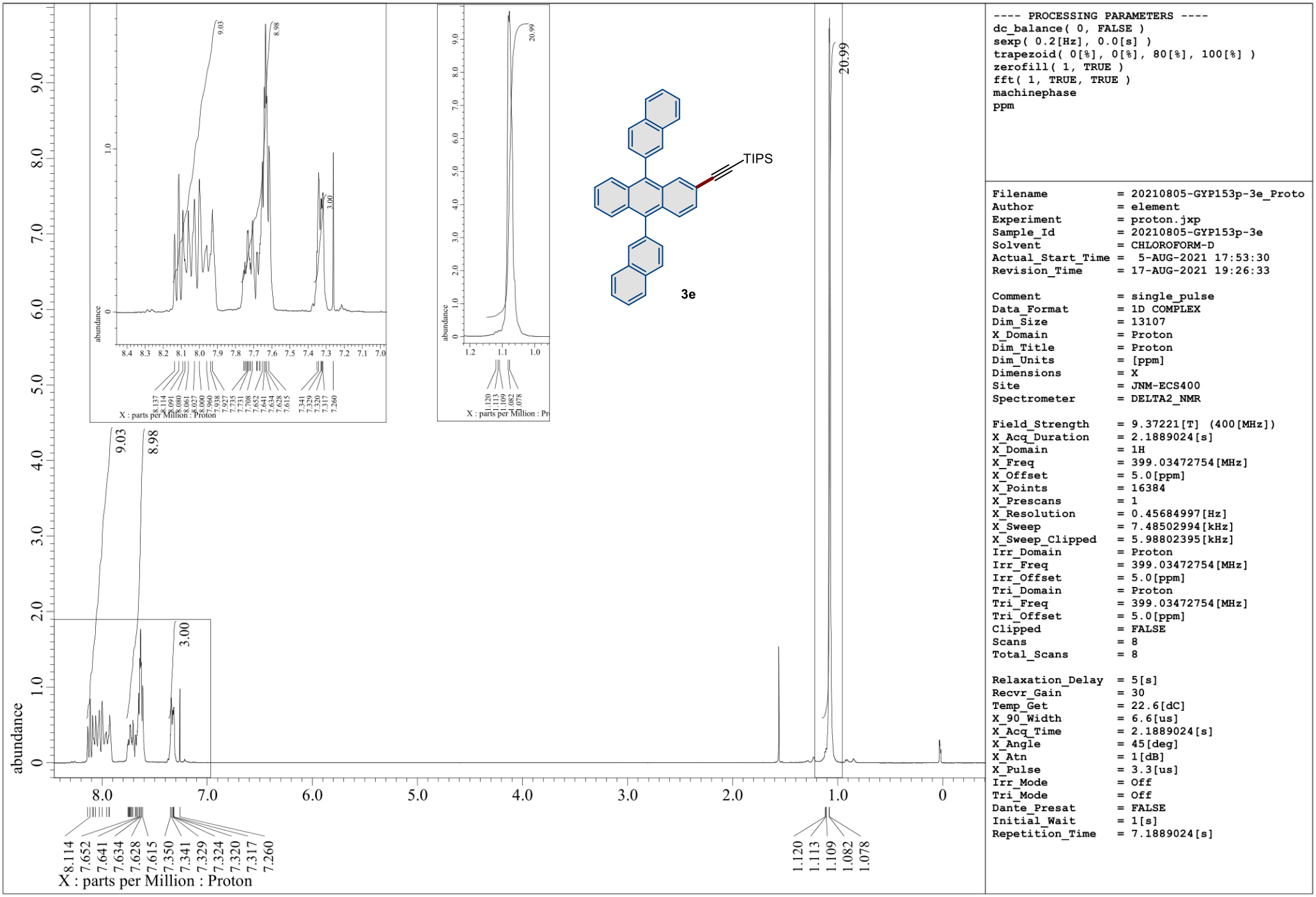

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

Filename	= 20210731-GYP139p-3d_P
Author	= element
Experiment	= proton_auto.jxp
Sample_Id	= 20210731-GYP139p-3d
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 31-JUL-2021 15:22:41
Revision_Time	= 30-AUG-2021 14:57:36
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ400S/L1
Field_Strength	= 9.2982153[T] (400[MHz
X_Acq_Duration	= 2.20725248[s]
X_Domain	= Proton
X_Freq	= 395.88430144[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45305193[Hz]
X_Sweep	= 7.42280285[kHz]
X_Sweep_Clipped	= 5.93824228[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 395.88430144[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= TRUE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 56
Temp_Get	= 21.8[dC]
X_90_Width	= 9.3[us]
X_Acq_Time	= 2.20725248[s]
X_Angle	= 45[deg]
X_Atn	= 3.4[dB]
X_Pulse	= 4.65[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 500
Dante_Presat	= FALSE
Decimation_Rate	= 0
Experiment_Path	= C:\Program Files\JEOL
Initial_Wait	= 1[s]
Phase	= {0, 90, 270, 180, 180
Presat_Time	= 5[s]




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

Filename	= 20210730-GYP139p-3
Author	= element
Experiment	= carbon_auto.jxp
Sample_Id	= 20210730-GYP139p-3
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 30-JUL-2021 15:20:
Revision_Time	= 17-AUG-2021 16:50:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ400S/L1
Field_Strength	= 9.2982153[T] (400[
X_Acq_Duration	= 1.048576[s]
X_Domain	= Carbon13
X_Freq	= 99.54517646[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.95367432[Hz]
X_Sweep	= 31.25[kHz]
X_Sweep_Clipped	= 25[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 5[us]
Clipped	= FALSE
Scans	= 200
Total_Scans	= 200
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 22[dC]
X_90_Width	= 9.65[us]
X_Acq_Time	= 1.048576[s]
X_Angle	= 30[deg]
X_Atn	= 8[dB]
X_Pulse	= 3.21666667[us]
Irr_Atn_Dec	= 25.244[dB]
Irr_Atn_Dec_Calc	= 25.244[dB]
Irr_Atn_Dec_Default_Calc	= 25.244[dB]
Irr_Atn_Noe	= 25.244[dB]
Irr_Dec_Bandwidth_Hz	= 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.08082432[ppm]
Irr_Dec_Freq	= 395.88430144[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]



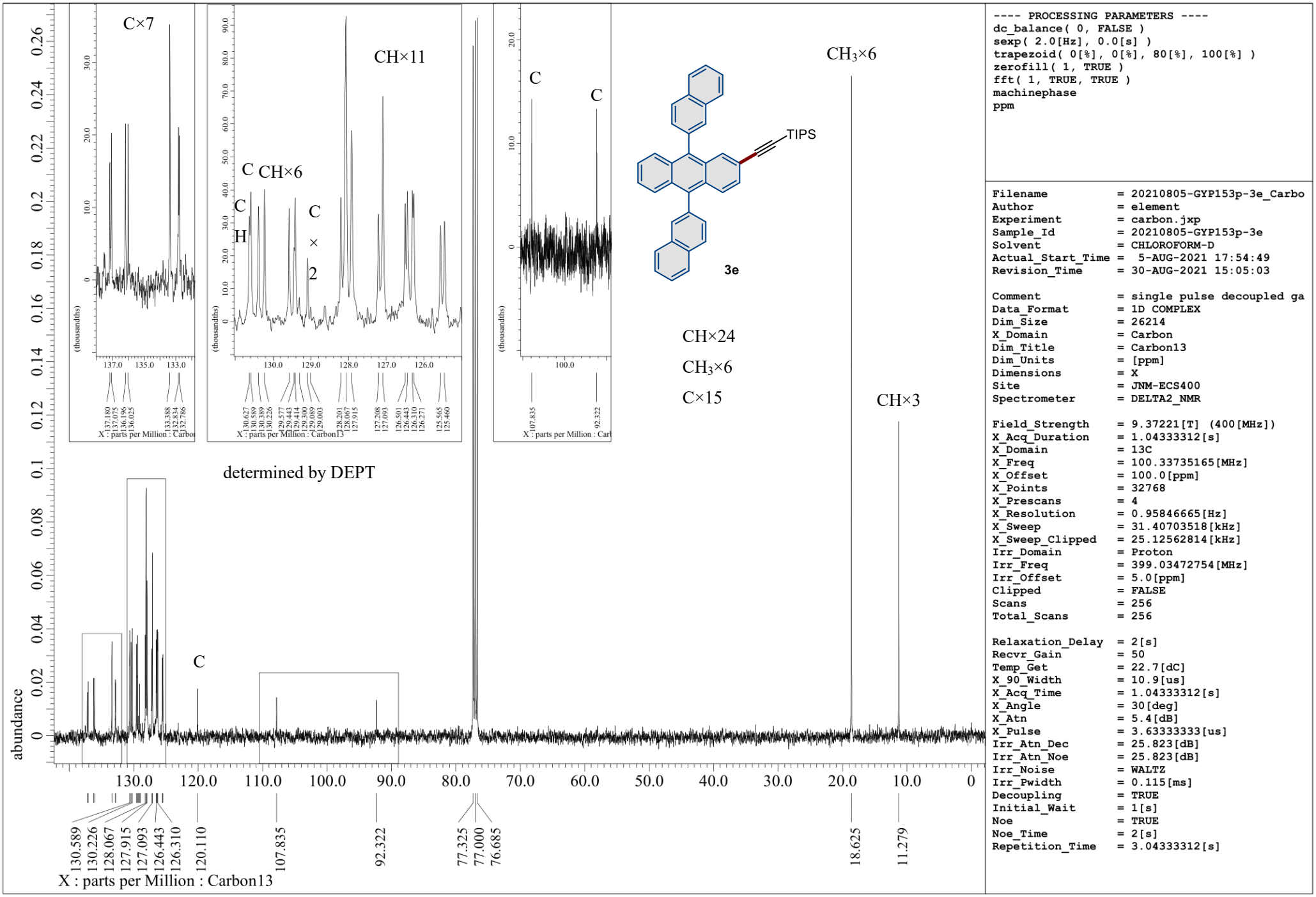

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename            = 20210805-GYP153p-3e_Proto
Author              = element
Experiment          = proton.jxp
Sample_Id           = 20210805-GYP153p-3e
Solvent             = CHLOROFORM-D
Actual_Start_Time   =  5-AUG-2021 17:53:30
Revision_Time       = 17-AUG-2021 19:26:33

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

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

Relaxation_Delay    = 5[s]
Recvr_Gain          = 30
Temp_Get            = 22.6[dC]
X_90_Width          = 6.6[us]
X_Acq_Time          = 2.1889024[s]
X_Angle             = 45[deg]
X_Atn               = 1[dB]
X_Pulse             = 3.3[us]
Irr_Mode            = Off
Tri_Mode            = Off
Dante_Presat        = FALSE
Initial_Wait        = 1[s]
Repetition_Time     = 7.1889024[s]
```



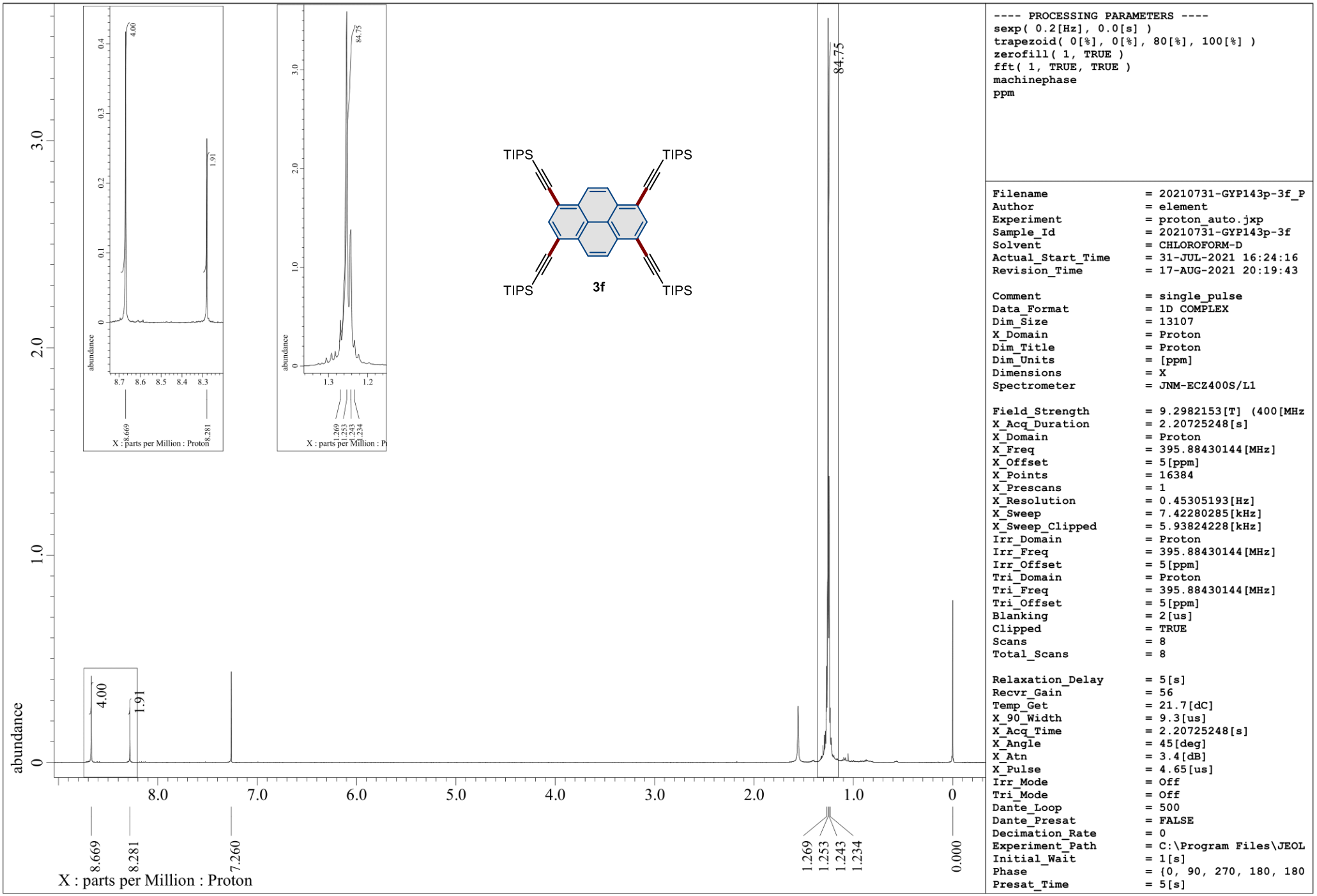

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename            = 20210805-GYP153p-3e_Carbo
Author              = element
Experiment          = carbon.jxp
Sample_Id           = 20210805-GYP153p-3e
Solvent             = CHLOROFORM-D
Actual_Start_Time   =  5-AUG-2021 17:54:49
Revision_Time       = 30-AUG-2021 15:05:03

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

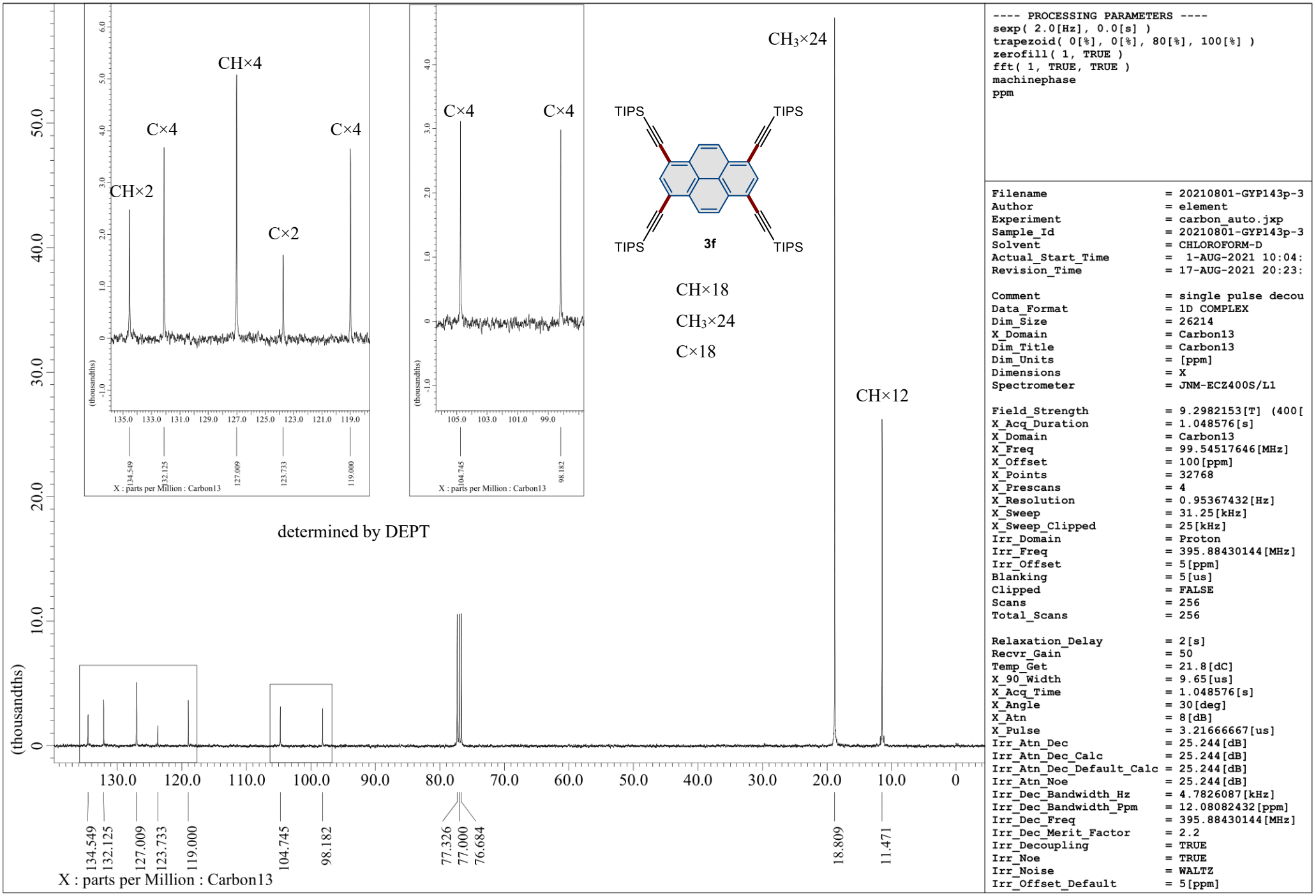
Field_Strength      = 9.37221[T] (400[MHz])
X_Acq_Duration      = 1.04333312[s]
X_Domain            = 13C
X_Freq              = 100.33735165[MHz]
X_Offset            = 100.0[ppm]
X_Points            = 32768
X_Prescans          = 4
X_Resolution        = 0.95846665[Hz]
X_Sweep             = 31.40703518[kHz]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

Relaxation_Delay    = 2[s]
Recvr_Gain          = 50
Temp_Get            = 22.7[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]
```



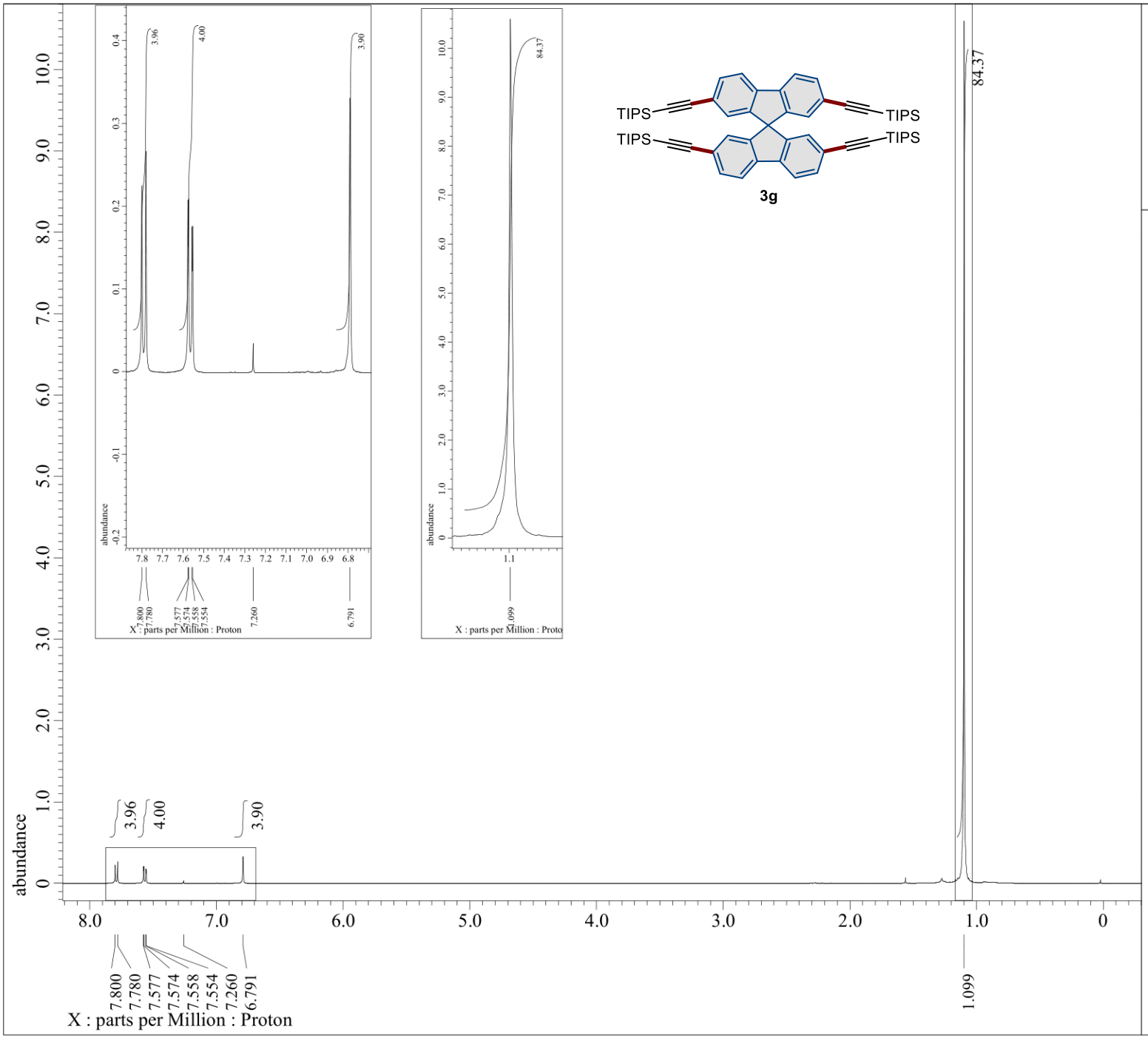

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

Filename	= 20210731-GYP143p-3f_P
Author	= element
Experiment	= proton_auto.jxp
Sample_Id	= 20210731-GYP143p-3f
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 31-JUL-2021 16:24:16
Revision_Time	= 17-AUG-2021 20:19:43
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ400S/L1
Field_Strength	= 9.2982153[T] (400[MHz
X_Acq_Duration	= 2.20725248[s]
X_Domain	= Proton
X_Freq	= 395.88430144[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45305193[Hz]
X_Sweep	= 7.42280285[kHz]
X_Sweep_Clipped	= 5.93824228[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 395.88430144[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= TRUE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 56
Temp_Get	= 21.7[dC]
X_90_Width	= 9.3[us]
X_Acq_Time	= 2.20725248[s]
X_Angle	= 45[deg]
X_Atn	= 3.4[dB]
X_Pulse	= 4.65[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 500
Dante_Presat	= FALSE
Decimation_Rate	= 0
Experiment_Path	= C:\Program Files\JEOL
Initial_Wait	= 1[s]
Phase	= {0, 90, 270, 180, 180
Presat_Time	= 5[s]



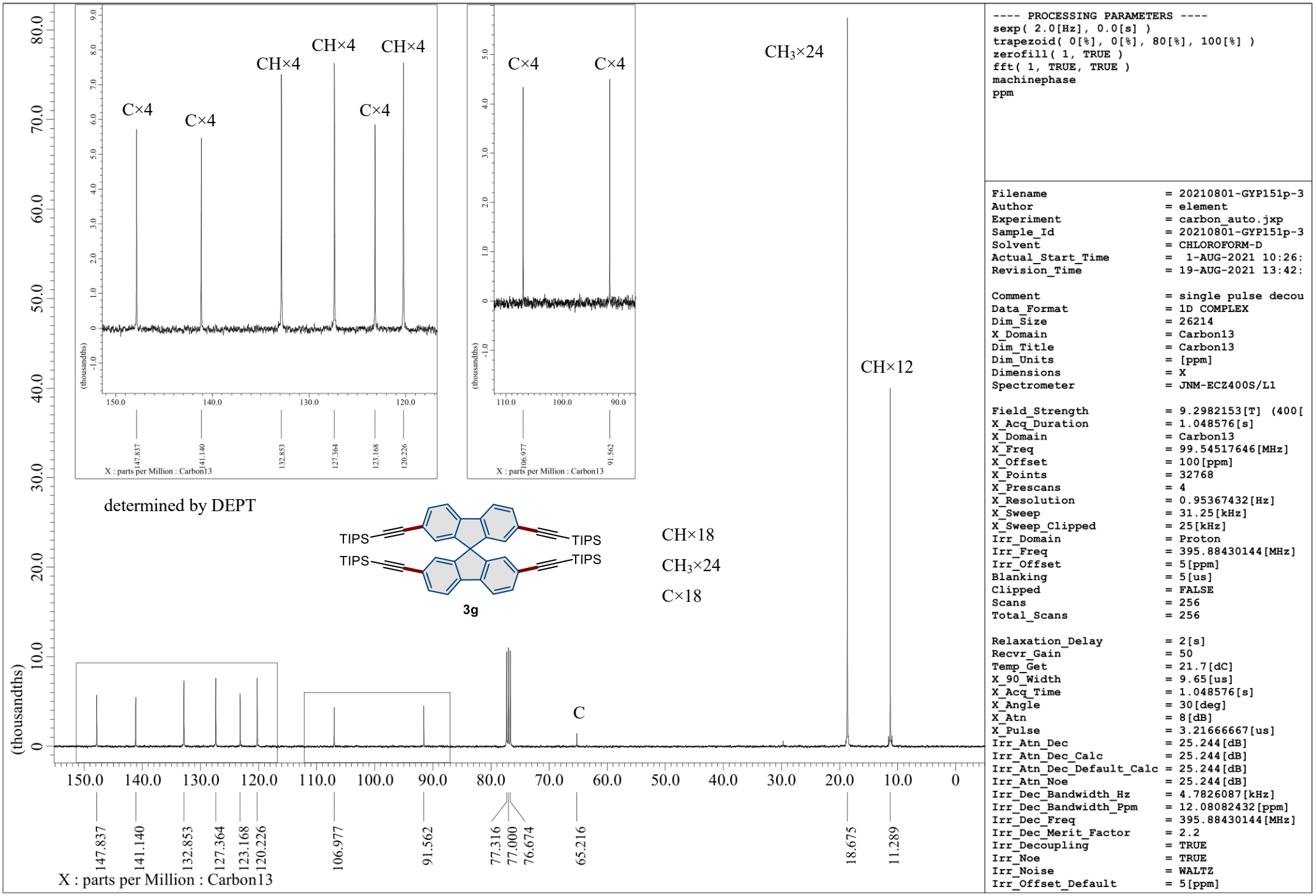

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

Filename	= 20210801-GYP143p-3
Author	= element
Experiment	= carbon_auto.jxp
Sample_Id	= 20210801-GYP143p-3
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 1-AUG-2021 10:04:
Revision_Time	= 17-AUG-2021 20:23:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ400S/L1
Field_Strength	= 9.2982153[T] (400[
X_Acq_Duration	= 1.048576[s]
X_Domain	= Carbon13
X_Freq	= 99.54517646[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.95367432[Hz]
X_Sweep	= 31.25[kHz]
X_Sweep_Clipped	= 25[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 5[us]
Clipped	= FALSE
Scans	= 256
Total_Scans	= 256
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 21.8[dC]
X_90_Width	= 9.65[us]
X_Acq_Time	= 1.048576[s]
X_Angle	= 30[deg]
X_Atn	= 8[dB]
X_Pulse	= 3.21666667[us]
Irr_Atn_Dec	= 25.244[dB]
Irr_Atn_Dec_Calc	= 25.244[dB]
Irr_Atn_Dec_Default_Calc	= 25.244[dB]
Irr_Atn_Noe	= 25.244[dB]
Irr_Dec_Bandwidth_Hz	= 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.08082432[ppm]
Irr_Dec_Freq	= 395.88430144[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]



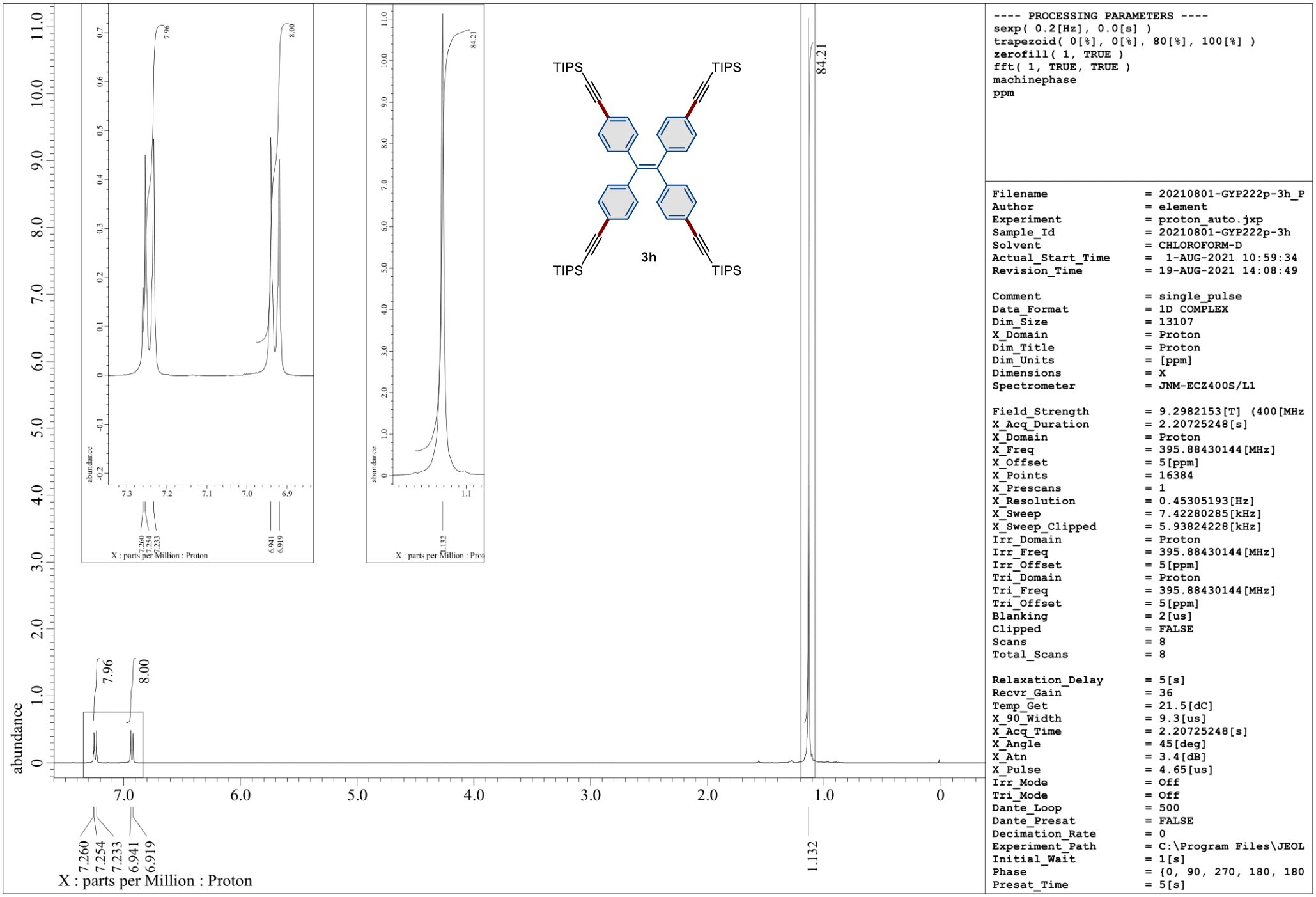

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

Filename	= 20210801-GYP151p-3g_P
Author	= element
Experiment	= proton_auto.jxp
Sample_Id	= 20210801-GYP151p-3g
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 1-AUG-2021 10:25:11
Revision_Time	= 19-AUG-2021 13:39:21
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ400S/L1
Field_Strength	= 9.2982153[T] (400[MHz
X_Acq_Duration	= 2.20725248[s]
X_Domain	= Proton
X_Freq	= 395.88430144[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45305193[Hz]
X_Sweep	= 7.42280285[kHz]
X_Sweep_Clipped	= 5.93824228[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 395.88430144[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 36
Temp_Get	= 21.5[dC]
X_90_Width	= 9.3[us]
X_Acq_Time	= 2.20725248[s]
X_Angle	= 45[deg]
X_Atn	= 3.4[dB]
X_Pulse	= 4.65[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 500
Dante_Presat	= FALSE
Decimation_Rate	= 0
Experiment_Path	= C:\Program Files\JEOL
Initial_Wait	= 1[s]
Phase	= {0, 90, 270, 180, 180
Presat_Time	= 5[s]



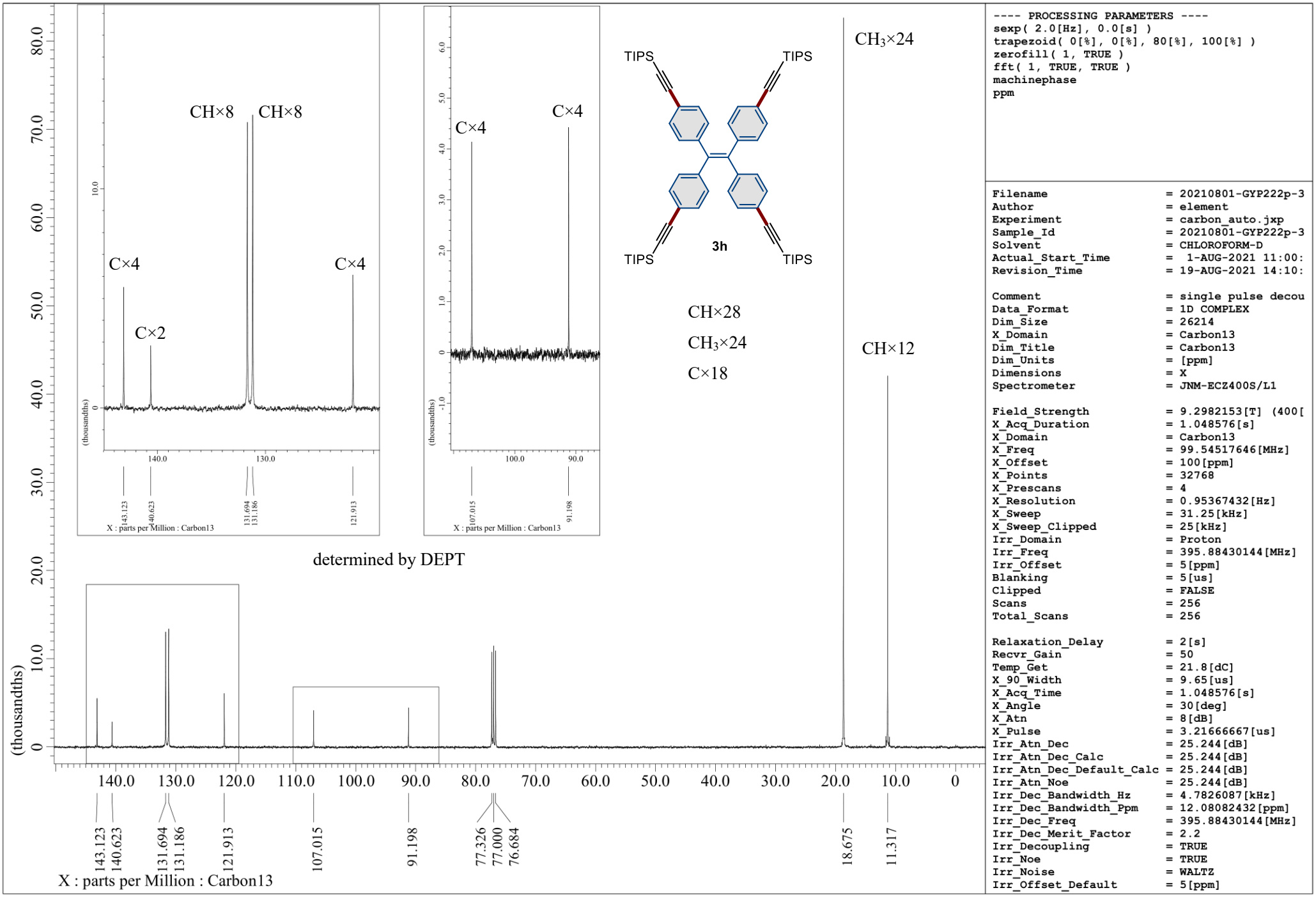

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

Filename	= 20210801-GYP151p-3
Author	= element
Experiment	= carbon_auto.jxp
Sample_Id	= 20210801-GYP151p-3
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 1-AUG-2021 10:26:
Revision_Time	= 19-AUG-2021 13:42:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ400S/L1
Field_Strength	= 9.2982153[T] (400[
X_Acq_Duration	= 1.048576[s]
X_Domain	= Carbon13
X_Freq	= 99.54517646[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.95367432[Hz]
X_Sweep	= 31.25[kHz]
X_Sweep_Clipped	= 25[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 5[us]
Clipped	= FALSE
Scans	= 256
Total_Scans	= 256
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 21.7[dC]
X_90_Width	= 9.65[us]
X_Acq_Time	= 1.048576[s]
X_Angle	= 30[deg]
X_Atn	= 8[dB]
X_Pulse	= 3.21666667[us]
Irr_Atn_Dec	= 25.244[dB]
Irr_Atn_Dec_Calc	= 25.244[dB]
Irr_Atn_Dec_Default_Calc	= 25.244[dB]
Irr_Atn_Noe	= 25.244[dB]
Irr_Dec_Bandwidth_Hz	= 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.08082432[ppm]
Irr_Dec_Freq	= 395.88430144[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]



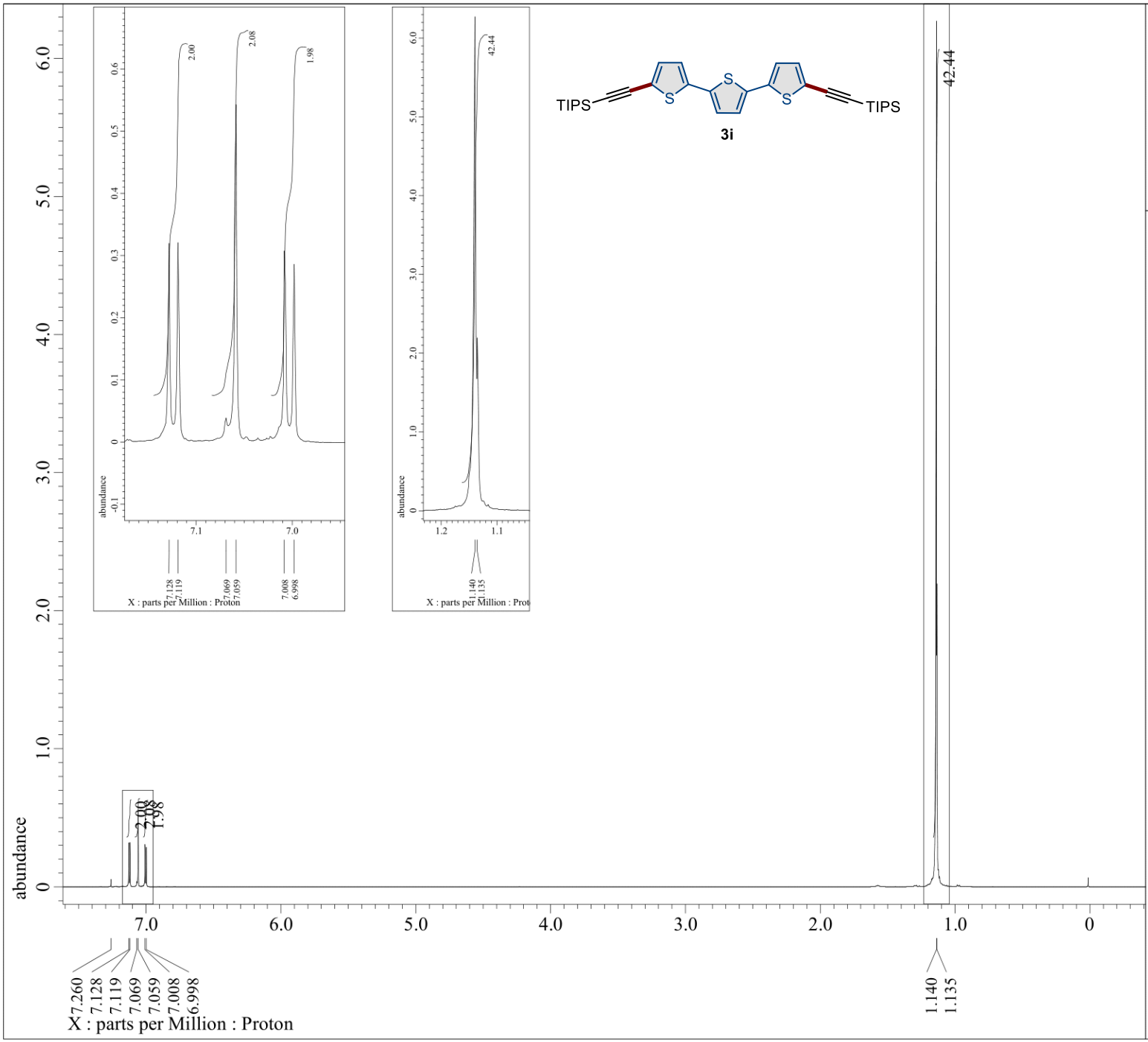

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

Filename	= 20210801-GYP222p-3h_P
Author	= element
Experiment	= proton_auto.jxp
Sample_Id	= 20210801-GYP222p-3h
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 1-AUG-2021 10:59:34
Revision_Time	= 19-AUG-2021 14:08:49
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ400S/L1
Field_Strength	= 9.2982153[T] (400[MHz
X_Acq_Duration	= 2.20725248[s]
X_Domain	= Proton
X_Freq	= 395.88430144[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45305193[Hz]
X_Sweep	= 7.42280285[kHz]
X_Sweep_Clipped	= 5.93824228[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 395.88430144[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 36
Temp_Get	= 21.5[dC]
X_90_Width	= 9.3[us]
X_Acq_Time	= 2.20725248[s]
X_Angle	= 45[deg]
X_Atn	= 3.4[dB]
X_Pulse	= 4.65[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 500
Dante_Presat	= FALSE
Decimation_Rate	= 0
Experiment_Path	= C:\Program Files\JEOL
Initial_Wait	= 1[s]
Phase	= {0, 90, 270, 180, 180
Presat_Time	= 5[s]



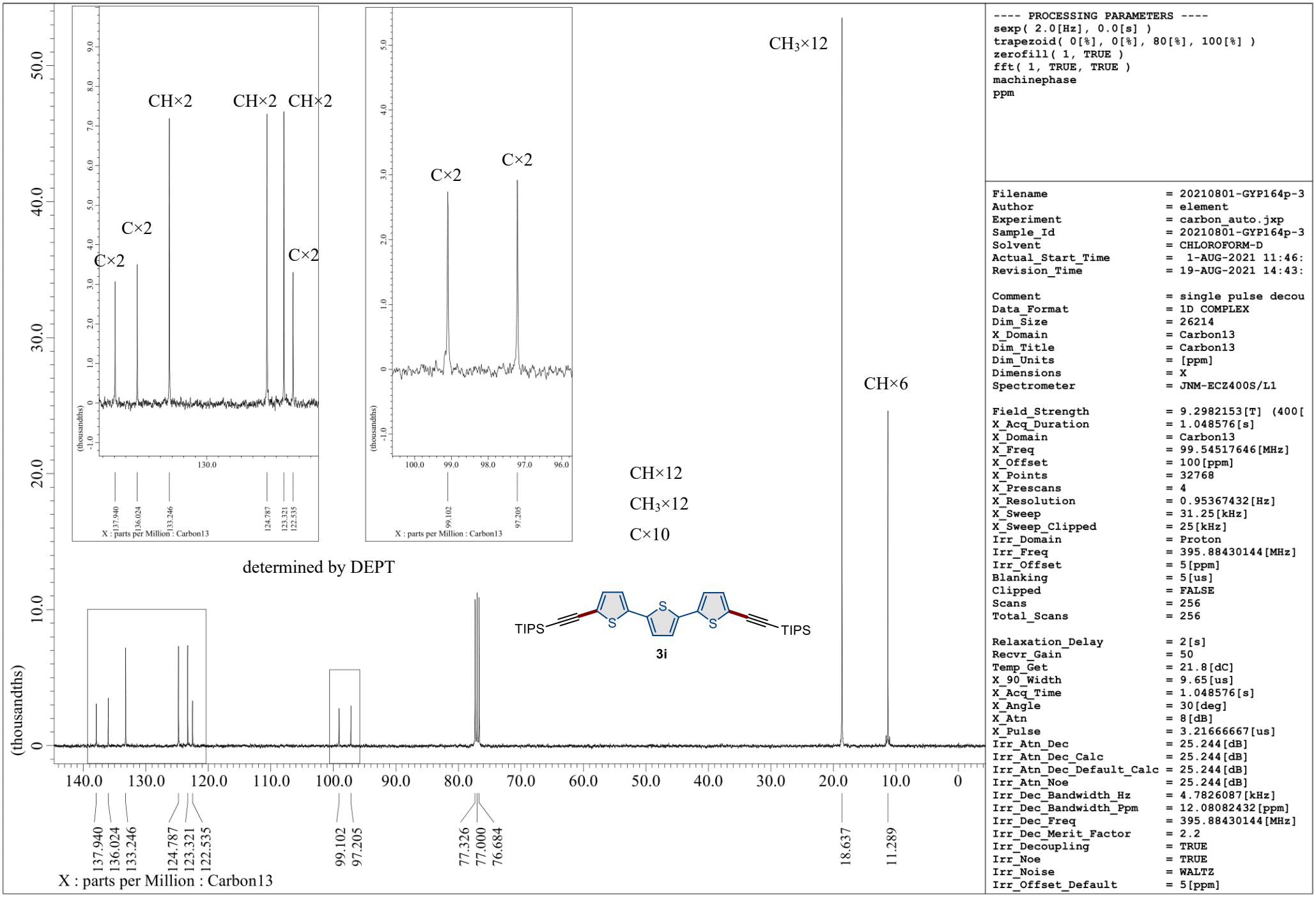

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

Filename	= 20210801-GYP222p-3
Author	= element
Experiment	= carbon_auto.jxp
Sample_Id	= 20210801-GYP222p-3
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 1-AUG-2021 11:00:
Revision_Time	= 19-AUG-2021 14:10:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ400S/L1
Field_Strength	= 9.2982153[T] (400[
X_Acq_Duration	= 1.048576[s]
X_Domain	= Carbon13
X_Freq	= 99.54517646[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.95367432[Hz]
X_Sweep	= 31.25[kHz]
X_Sweep_Clipped	= 25[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 5[us]
Clipped	= FALSE
Scans	= 256
Total_Scans	= 256
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 21.8[dC]
X_90_Width	= 9.65[us]
X_Acq_Time	= 1.048576[s]
X_Angle	= 30[deg]
X_Atn	= 8[dB]
X_Pulse	= 3.21666667[us]
Irr_Atn_Dec	= 25.244[dB]
Irr_Atn_Dec_Calc	= 25.244[dB]
Irr_Atn_Dec_Default_Calc	= 25.244[dB]
Irr_Atn_Noe	= 25.244[dB]
Irr_Dec_Bandwidth_Hz	= 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.08082432[ppm]
Irr_Dec_Freq	= 395.88430144[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]



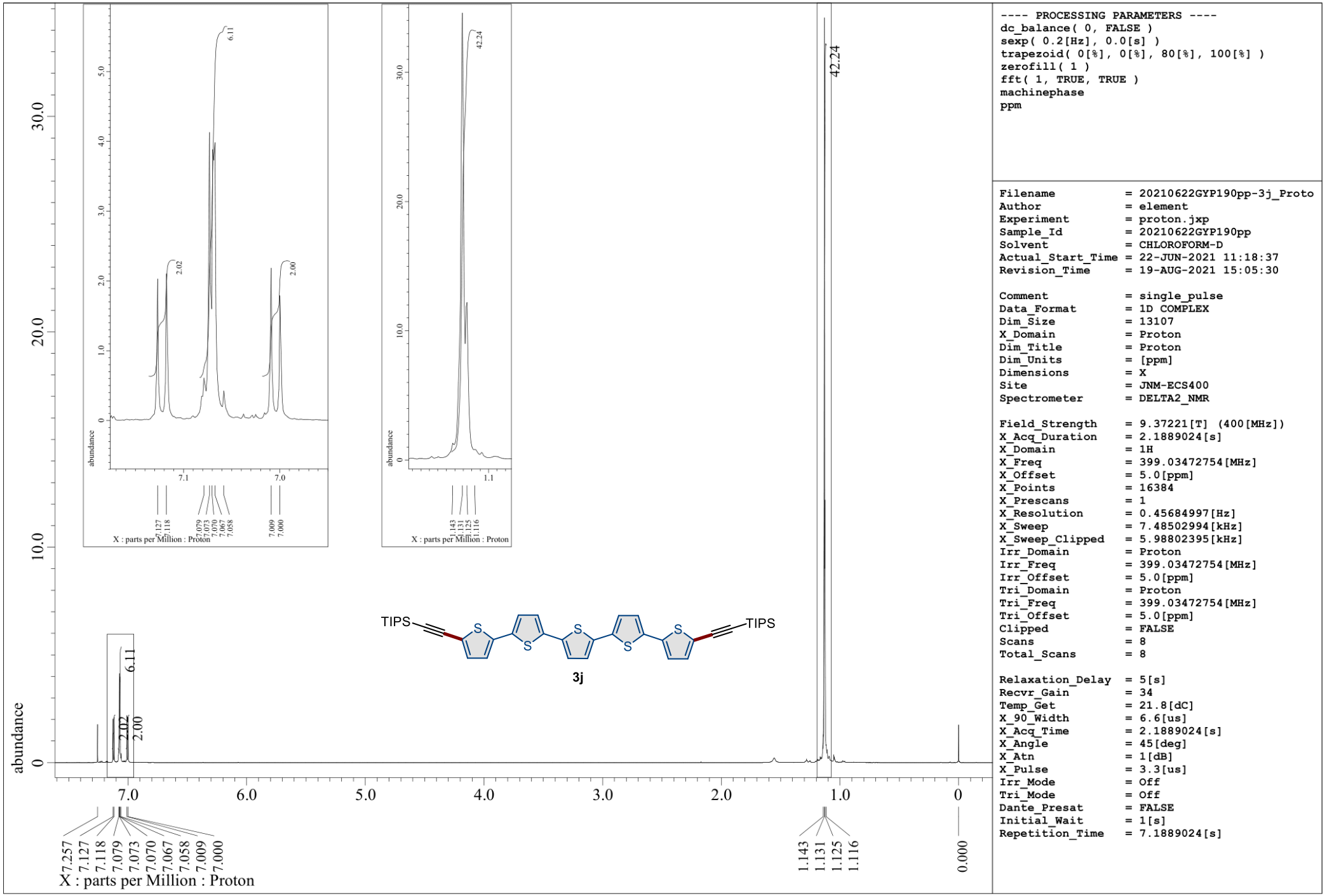

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

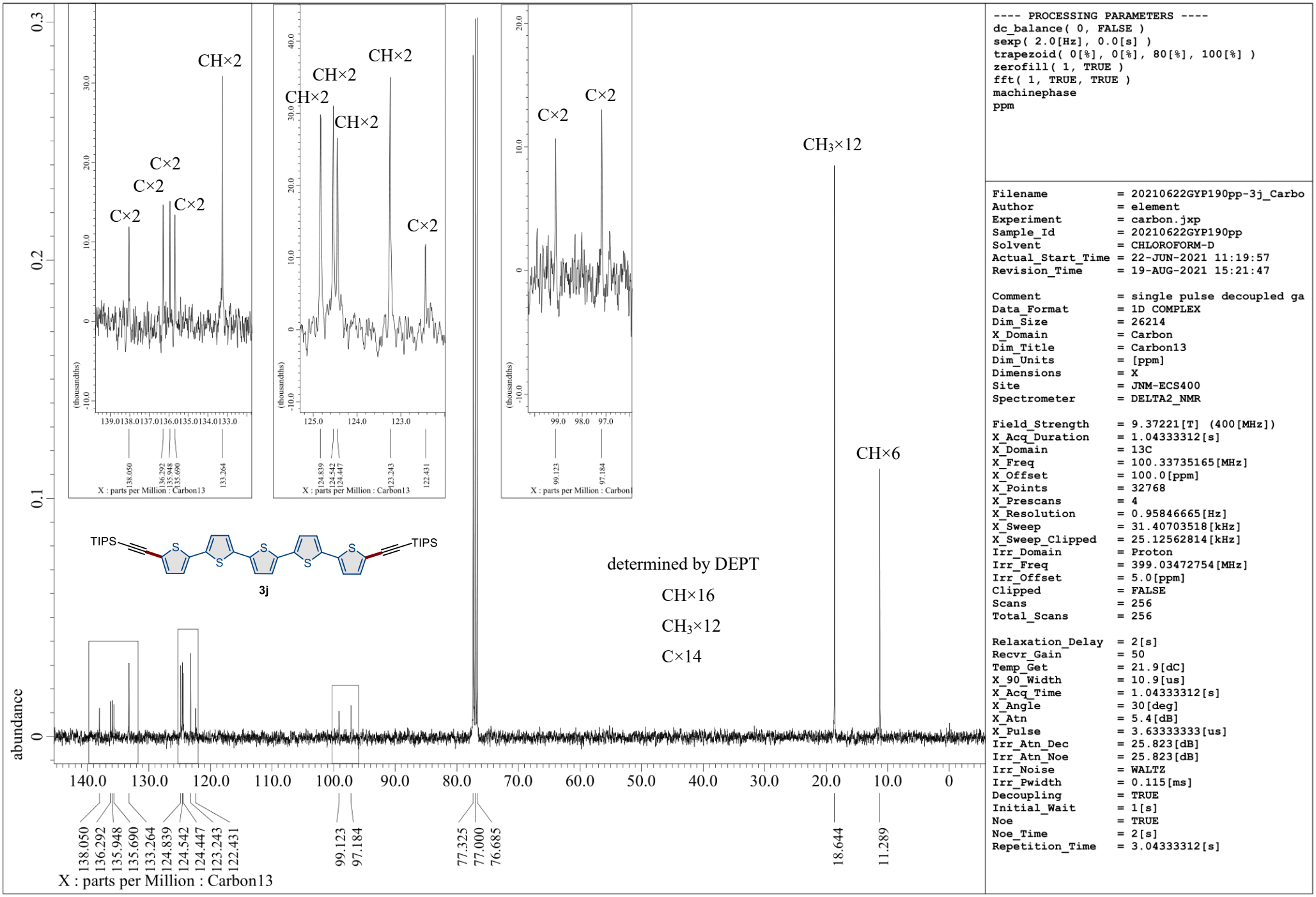
Filename	= 20210801-GYP164p-3i_P
Author	= element
Experiment	= proton_auto.jxp
Sample_Id	= 20210801-GYP164p-3i
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 1-AUG-2021 11:45:17
Revision_Time	= 19-AUG-2021 14:41:20
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ400S/L1
Field_Strength	= 9.2982153[T] (400[MHz
X_Acq_Duration	= 2.20725248[s]
X_Domain	= Proton
X_Freq	= 395.88430144[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45305193[Hz]
X_Sweep	= 7.42280285[kHz]
X_Sweep_Clipped	= 5.93824228[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 395.88430144[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 36
Temp_Get	= 21.5[dC]
X_90_Width	= 9.3[us]
X_Acq_Time	= 2.20725248[s]
X_Angle	= 45[deg]
X_Atn	= 3.4[dB]
X_Pulse	= 4.65[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 500
Dante_Presat	= FALSE
Decimation_Rate	= 0
Experiment_Path	= C:\Program Files\JEOL
Initial_Wait	= 1[s]
Phase	= {0, 90, 270, 180, 180
Presat_Time	= 5[s]




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

Filename	= 20210801-GYP164p-3
Author	= element
Experiment	= carbon_auto.jxp
Sample_Id	= 20210801-GYP164p-3
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 1-AUG-2021 11:46:
Revision_Time	= 19-AUG-2021 14:43:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ400S/L1
Field_Strength	= 9.2982153[T] (400[
X_Acq_Duration	= 1.048576[s]
X_Domain	= Carbon13
X_Freq	= 99.54517646[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.95367432[Hz]
X_Sweep	= 31.25[kHz]
X_Sweep_Clipped	= 25[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 5[us]
Clipped	= FALSE
Scans	= 256
Total_Scans	= 256
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 21.8[dC]
X_90_Width	= 9.65[us]
X_Acq_Time	= 1.048576[s]
X_Angle	= 30[deg]
X_Atn	= 8[dB]
X_Pulse	= 3.21666667[us]
Irr_Atn_Dec	= 25.244[dB]
Irr_Atn_Dec_Calc	= 25.244[dB]
Irr_Atn_Dec_Default_Calc	= 25.244[dB]
Irr_Atn_Noe	= 25.244[dB]
Irr_Dec_Bandwidth_Hz	= 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.08082432[ppm]
Irr_Dec_Freq	= 395.88430144[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]


---- PROCESSING PARAMETERS ----
dc_balance(0, FALSE)
sexp(0.2[Hz], 0.0[s])
trapezoid(0[%], 0[%], 80[%], 100[%])
zerofill(1)
fft(1, TRUE, TRUE)
machinephase
ppm
Filename = 20210622GYP190pp-3j_Proto
Author = element
Experiment = proton.jxp
Sample_Id = 20210622GYP190pp
Solvent = CHLOROFORM-D
Actual_Start_Time = 22-JUN-2021 11:18:37
Revision_Time = 19-AUG-2021 15:05:30
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 = 34
Temp_Get = 21.8[dC]
X_90_Width = 6.6[us]
X_Acq_Time = 2.1889024[s]
X_Angle = 45[deg]
X_Atn = 1[dB]
X_Pulse = 3.3[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 7.1889024[s]
TIPS
TIPS
S
3j
abundance
X : parts per Million : Proton
6.11
2.02
2.00
42.24
7.257
7.127
7.118
7.079
7.073
7.070
7.067
7.058
7.009
7.000
1.143
1.131
1.125
1.116
0.000



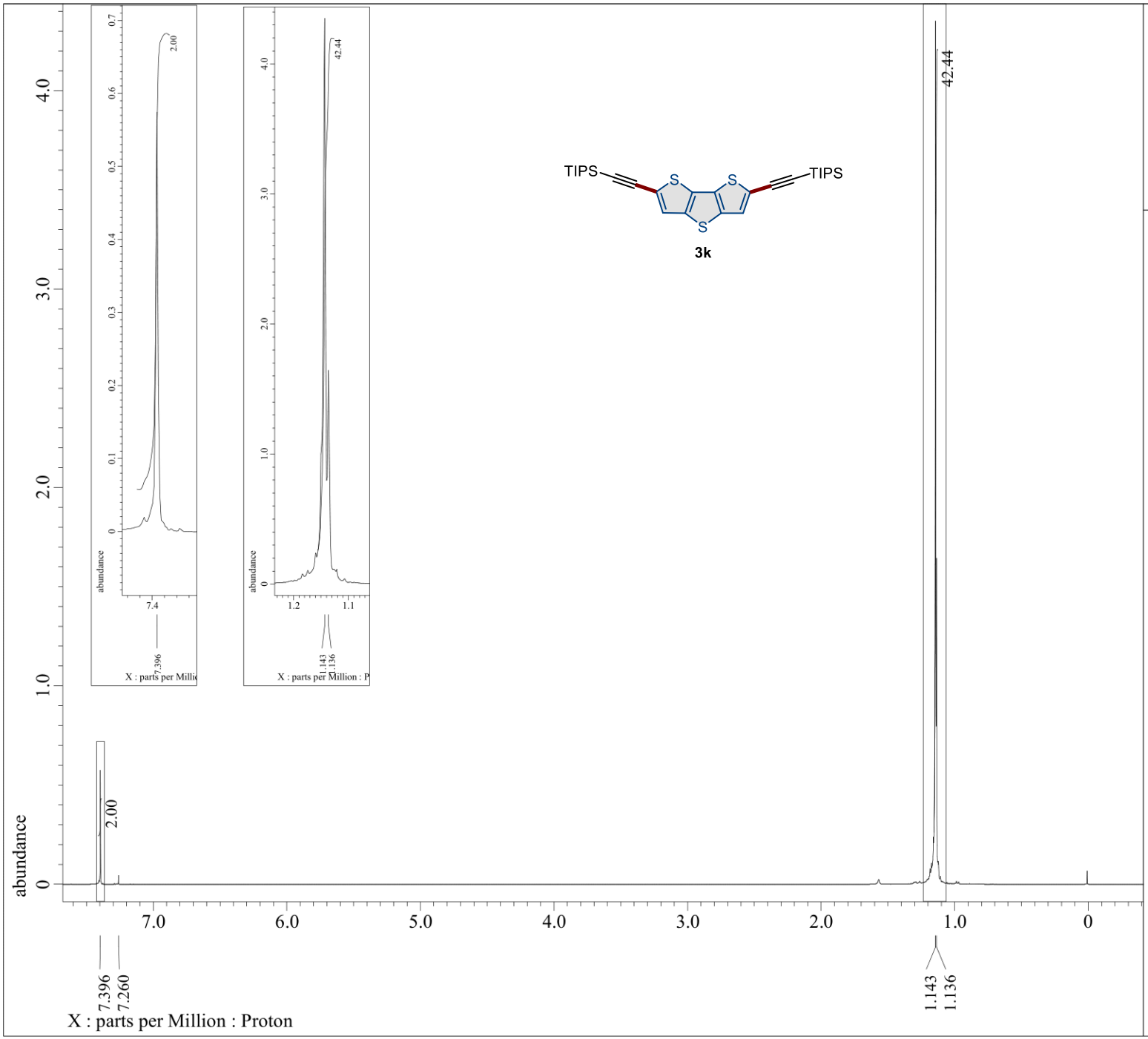

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename           = 20210622GYP190pp-3j_Carbo
Author             = element
Experiment         = carbon.jxp
Sample_Id          = 20210622GYP190pp
Solvent            = CHLOROFORM-D
Actual_Start_Time  = 22-JUN-2021 11:19:57
Revision_Time      = 19-AUG-2021 15:21:47

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

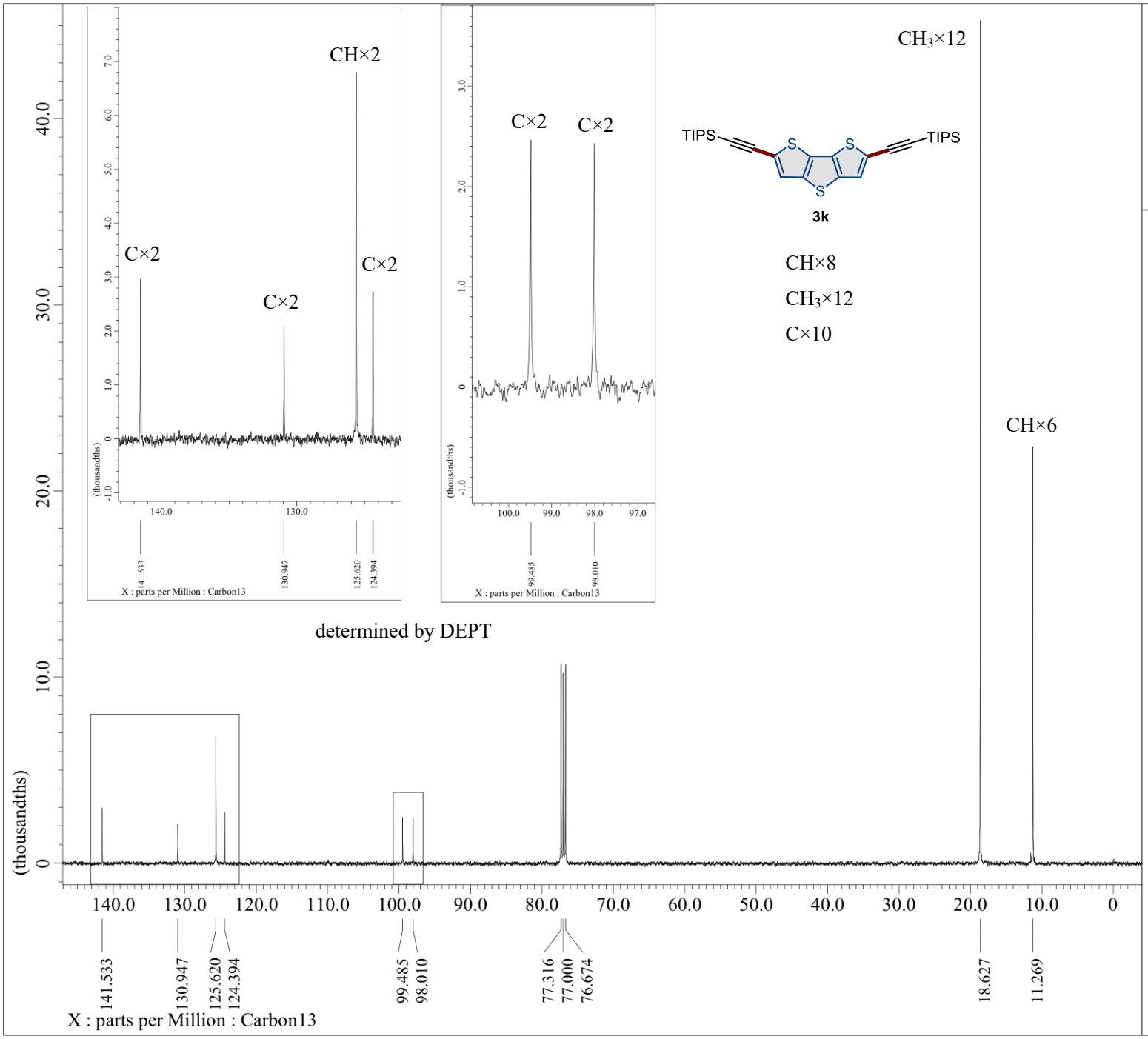
Field_Strength     = 9.37221[T] (400[MHz])
X_Acq_Duration     = 1.04333312[s]
X_Domain           = 13C
X_Freq             = 100.33735165[MHz]
X_Offset           = 100.0[ppm]
X_Points           = 32768
X_Prescans         = 4
X_Resolution       = 0.95846665[Hz]
X_Sweep            = 31.40703518[kHz]
X_Sweep_Clipped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

Relaxation_Delay   = 2[s]
Recvr_Gain         = 50
Temp_Get           = 21.9[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]
```



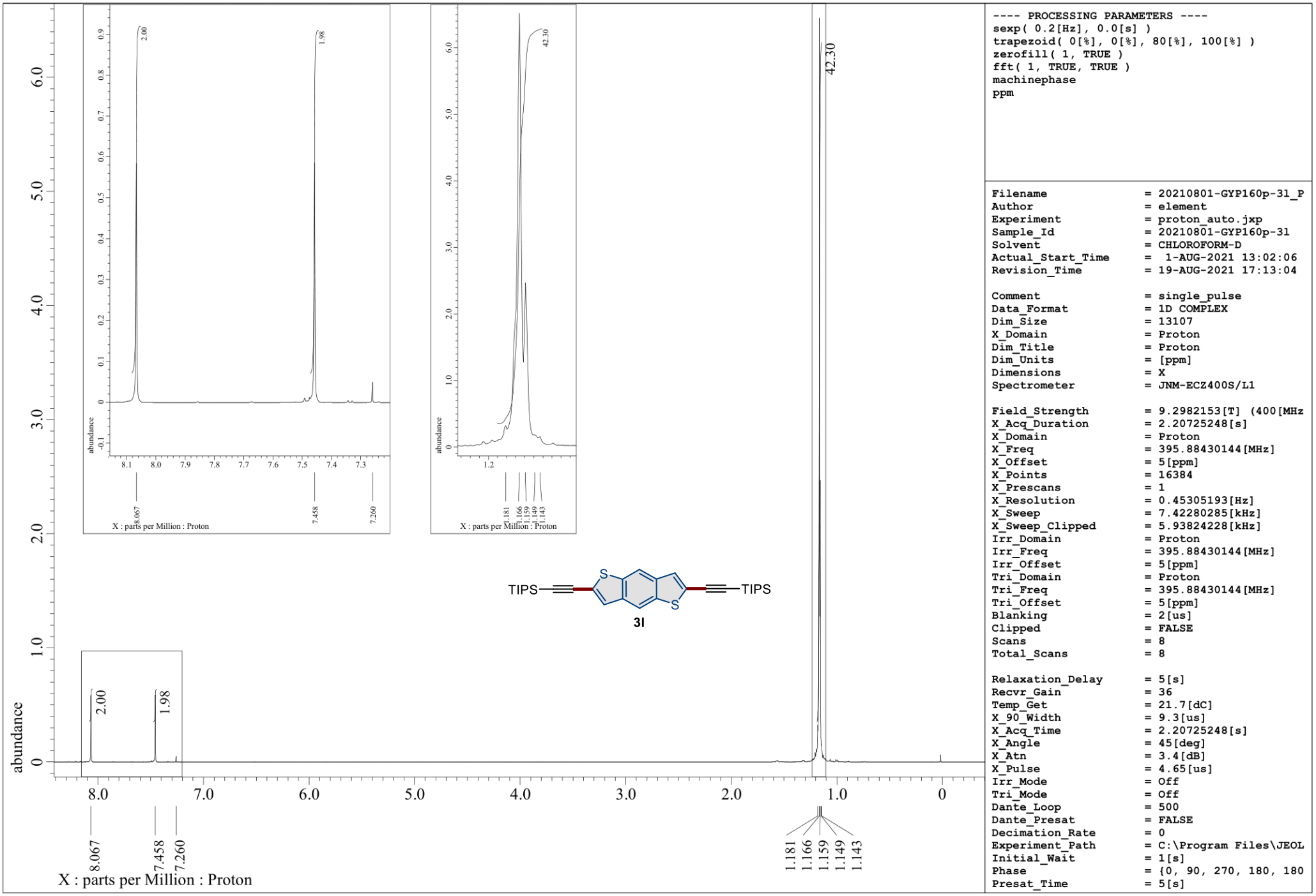

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

Filename	= 20210801-GYP166p-3k_P
Author	= element
Experiment	= proton_auto.jxp
Sample_Id	= 20210801-GYP166p-3k
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 1-AUG-2021 12:25:33
Revision_Time	= 19-AUG-2021 15:47:42
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ400S/L1
Field_Strength	= 9.2982153[T] (400[MHz
X_Acq_Duration	= 2.20725248[s]
X_Domain	= Proton
X_Freq	= 395.88430144[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45305193[Hz]
X_Sweep	= 7.42280285[kHz]
X_Sweep_Clipped	= 5.93824228[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 395.88430144[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 36
Temp_Get	= 21.6[dC]
X_90_Width	= 9.3[us]
X_Acq_Time	= 2.20725248[s]
X_Angle	= 45[deg]
X_Atn	= 3.4[dB]
X_Pulse	= 4.65[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 500
Dante_Presat	= FALSE
Decimation_Rate	= 0
Experiment_Path	= C:\Program Files\JEOL
Initial_Wait	= 1[s]
Phase	= {0, 90, 270, 180, 180
Presat_Time	= 5[s]



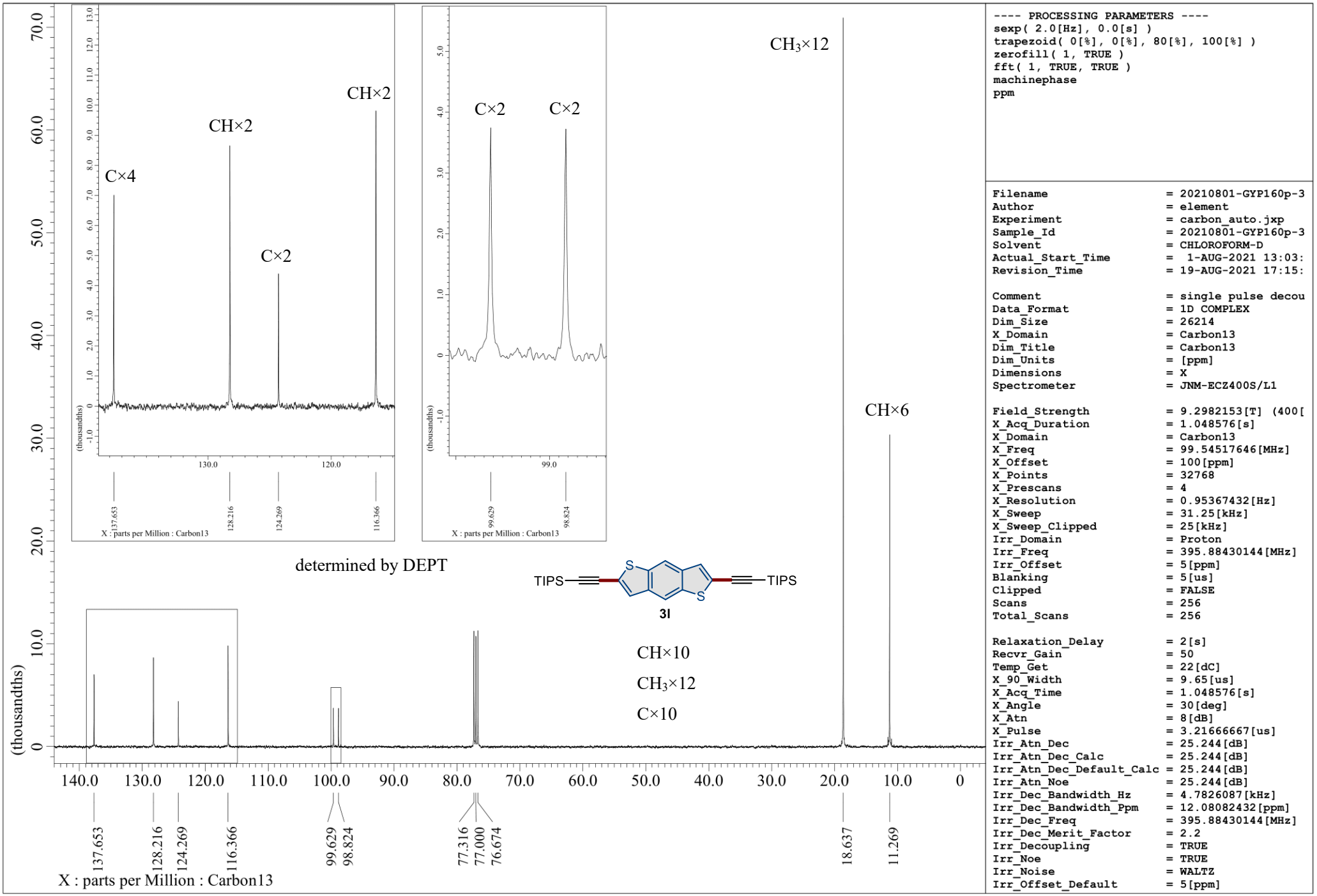

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

Filename	= 20210801-GYP166p-3
Author	= element
Experiment	= carbon_auto.jxp
Sample_Id	= 20210801-GYP166p-3
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 1-AUG-2021 12:26:
Revision_Time	= 19-AUG-2021 15:50:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ400S/L1
Field_Strength	= 9.2982153[T] (400[
X_Acq_Duration	= 1.048576[s]
X_Domain	= Carbon13
X_Freq	= 99.54517646[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.95367432[Hz]
X_Sweep	= 31.25[kHz]
X_Sweep_Clipped	= 25[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 5[us]
Clipped	= FALSE
Scans	= 256
Total_Scans	= 256
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 21.9[dC]
X_90_Width	= 9.65[us]
X_Acq_Time	= 1.048576[s]
X_Angle	= 30[deg]
X_Atn	= 8[dB]
X_Pulse	= 3.21666667[us]
Irr_Atn_Dec	= 25.244[dB]
Irr_Atn_Dec_Calc	= 25.244[dB]
Irr_Atn_Dec_Default_Calc	= 25.244[dB]
Irr_Atn_Noe	= 25.244[dB]
Irr_Dec_Bandwidth_Hz	= 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.08082432[ppm]
Irr_Dec_Freq	= 395.88430144[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]



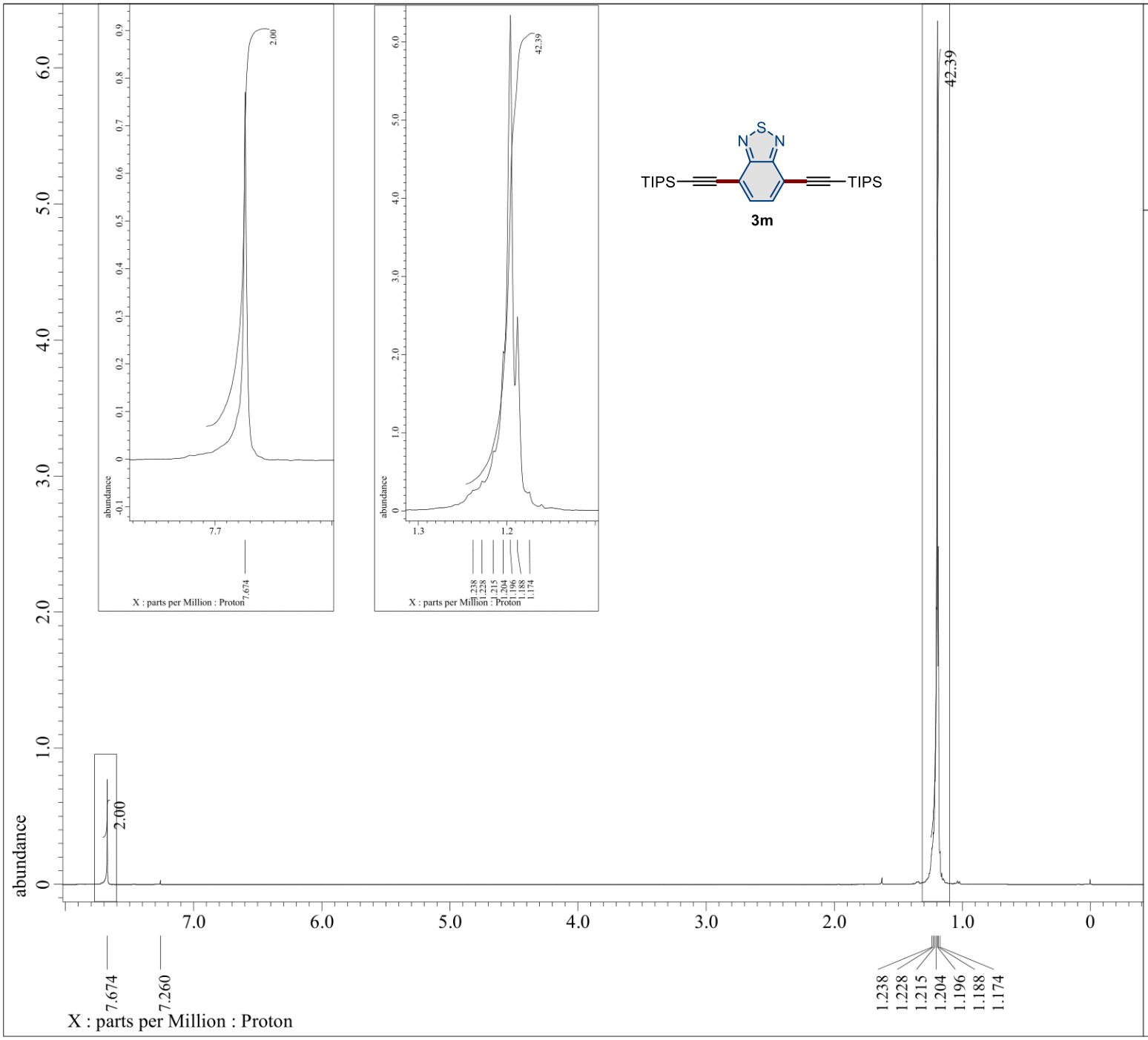

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

Filename	= 20210801-GYP160p-3l_P
Author	= element
Experiment	= proton_auto.jxp
Sample_Id	= 20210801-GYP160p-3l
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 1-AUG-2021 13:02:06
Revision_Time	= 19-AUG-2021 17:13:04
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ400S/L1
Field_Strength	= 9.2982153[T] (400[MHz
X_Acq_Duration	= 2.20725248[s]
X_Domain	= Proton
X_Freq	= 395.88430144[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45305193[Hz]
X_Sweep	= 7.42280285[kHz]
X_Sweep_Clipped	= 5.93824228[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 395.88430144[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 36
Temp_Get	= 21.7[dC]
X_90_Width	= 9.3[us]
X_Acq_Time	= 2.20725248[s]
X_Angle	= 45[deg]
X_Atn	= 3.4[dB]
X_Pulse	= 4.65[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 500
Dante_Presat	= FALSE
Decimation_Rate	= 0
Experiment_Path	= C:\Program Files\JEOL
Initial_Wait	= 1[s]
Phase	= {0, 90, 270, 180, 180
Presat_Time	= 5[s]




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

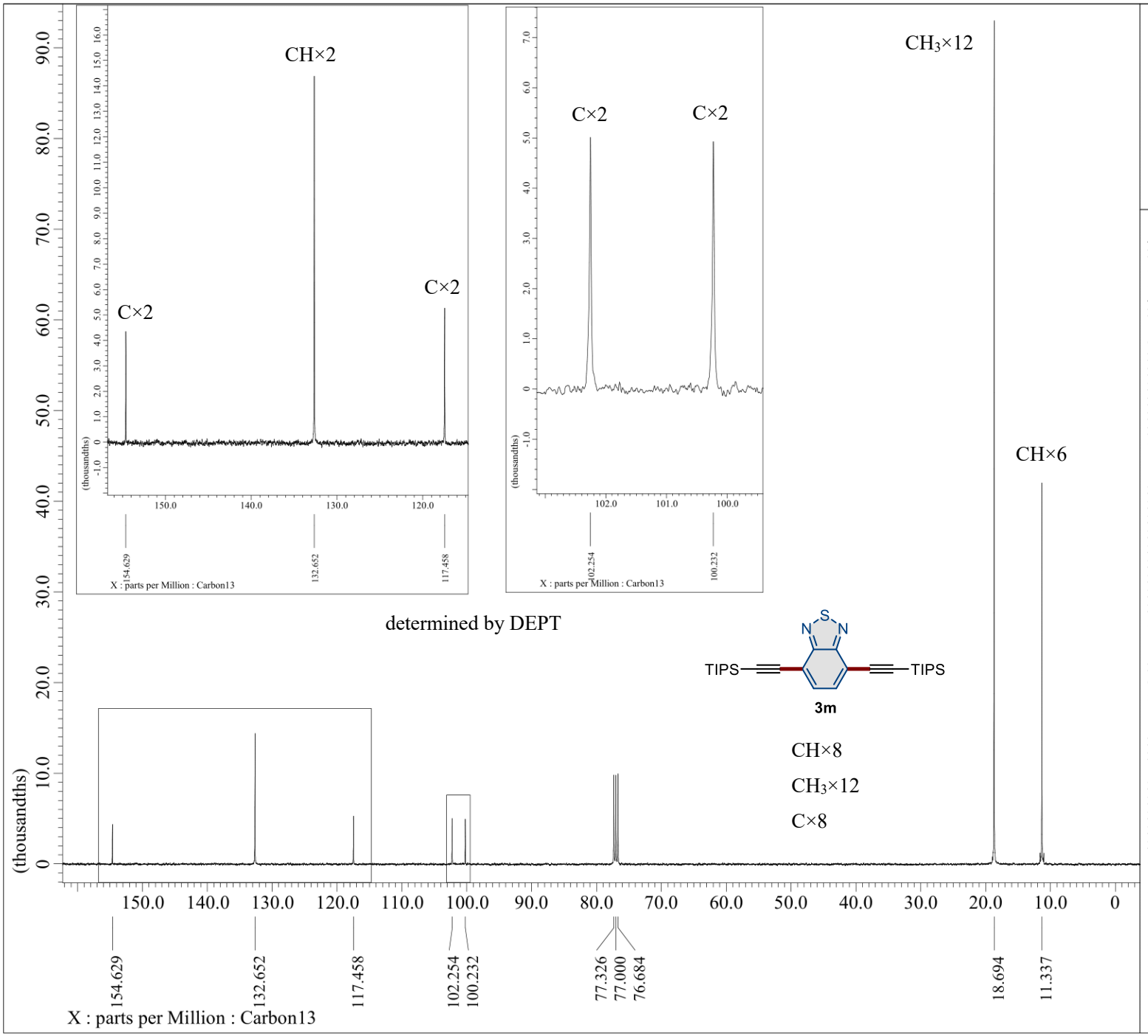
Filename	= 20210801-GYP160p-3
Author	= element
Experiment	= carbon_auto.jxp
Sample_Id	= 20210801-GYP160p-3
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 1-AUG-2021 13:03:
Revision_Time	= 19-AUG-2021 17:15:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ400S/L1
Field_Strength	= 9.2982153[T] (400[
X_Acq_Duration	= 1.048576[s]
X_Domain	= Carbon13
X_Freq	= 99.54517646[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.95367432[Hz]
X_Sweep	= 31.25[kHz]
X_Sweep_Clipped	= 25[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 5[us]
Clipped	= FALSE
Scans	= 256
Total_Scans	= 256
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 22[dC]
X_90_Width	= 9.65[us]
X_Acq_Time	= 1.048576[s]
X_Angle	= 30[deg]
X_Atn	= 8[dB]
X_Pulse	= 3.21666667[us]
Irr_Atn_Dec	= 25.244[dB]
Irr_Atn_Dec_Calc	= 25.244[dB]
Irr_Atn_Dec_Default_Calc	= 25.244[dB]
Irr_Atn_Noe	= 25.244[dB]
Irr_Dec_Bandwidth_Hz	= 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.08082432[ppm]
Irr_Dec_Freq	= 395.88430144[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]



3m

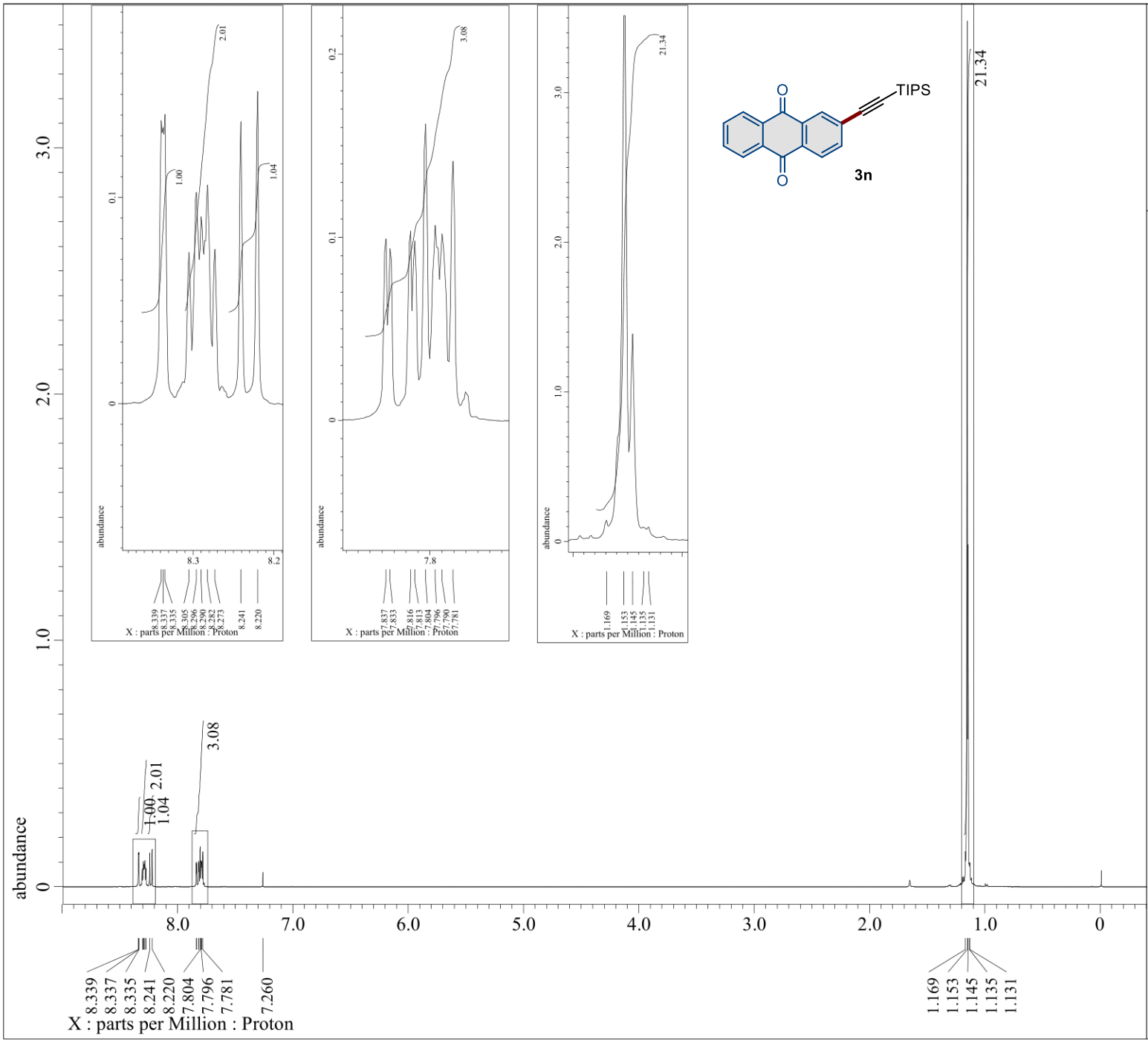
```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

Filename	= 20210801-GYP156p-3m_P
Author	= element
Experiment	= proton_auto.jxp
Sample_Id	= 20210801-GYP156p-3m
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 1-AUG-2021 13:37:08
Revision_Time	= 19-AUG-2021 18:58:48
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ400S/L1
Field_Strength	= 9.2982153[T] (400[MHz
X_Acq_Duration	= 2.20725248[s]
X_Domain	= Proton
X_Freq	= 395.88430144[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45305193[Hz]
X_Sweep	= 7.42280285[kHz]
X_Sweep_Clipped	= 5.93824228[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 395.88430144[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 36
Temp_Get	= 21.8[dC]
X_90_Width	= 9.3[us]
X_Acq_Time	= 2.20725248[s]
X_Angle	= 45[deg]
X_Atn	= 3.4[dB]
X_Pulse	= 4.65[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 500
Dante_Presat	= FALSE
Decimation_Rate	= 0
Experiment_Path	= C:\Program Files\JEOL
Initial_Wait	= 1[s]
Phase	= {0, 90, 270, 180, 180
Presat_Time	= 5[s]



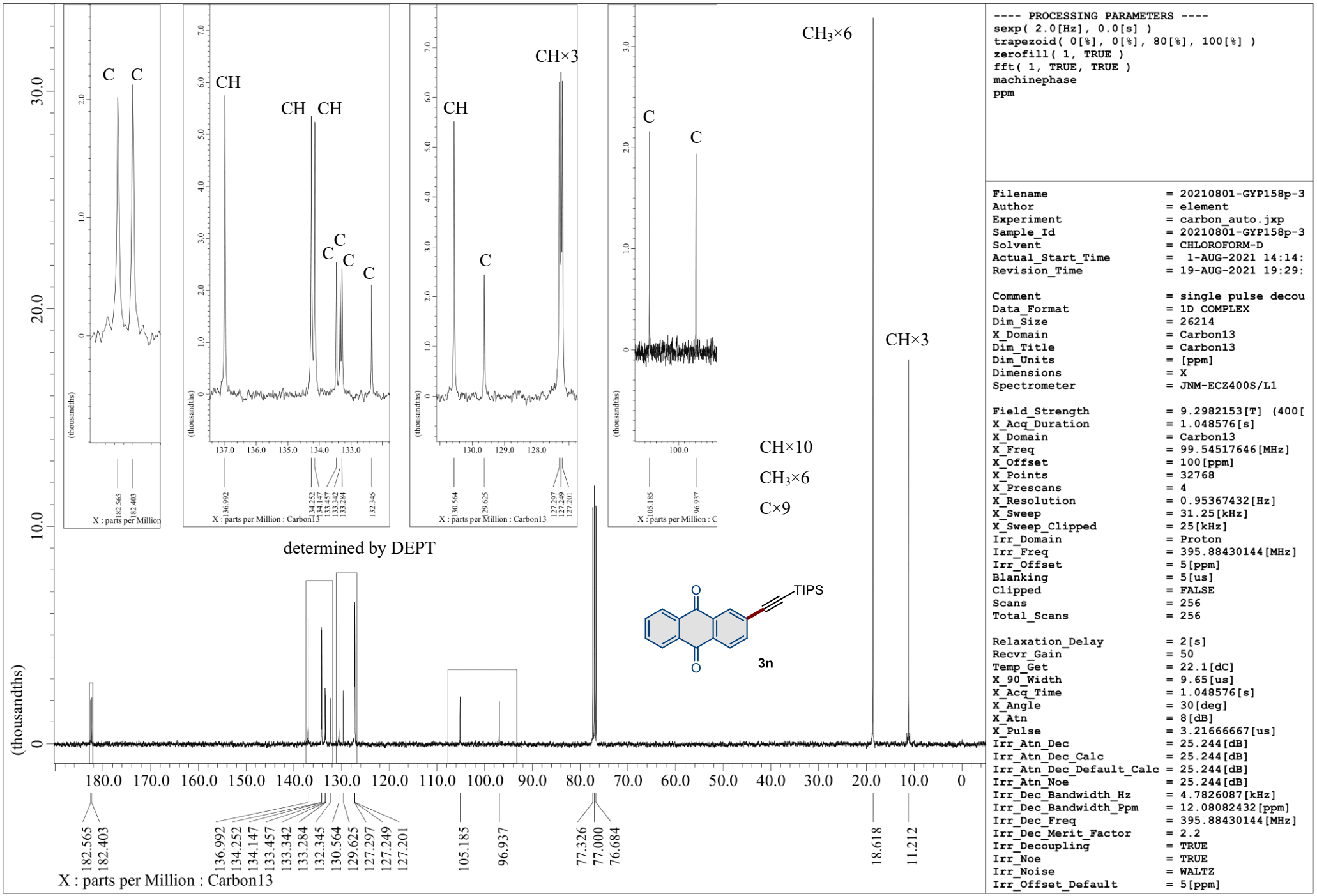

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

Filename	= 20210801-GYP156p-3
Author	= element
Experiment	= carbon_auto.jxp
Sample_Id	= 20210801-GYP156p-3
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 1-AUG-2021 13:38:
Revision_Time	= 19-AUG-2021 19:00:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ400S/L1
Field_Strength	= 9.2982153[T] (400[
X_Acq_Duration	= 1.048576[s]
X_Domain	= Carbon13
X_Freq	= 99.54517646[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.95367432[Hz]
X_Sweep	= 31.25[kHz]
X_Sweep_Clipped	= 25[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 5[us]
Clipped	= FALSE
Scans	= 256
Total_Scans	= 256
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 22[dC]
X_90_Width	= 9.65[us]
X_Acq_Time	= 1.048576[s]
X_Angle	= 30[deg]
X_Atn	= 8[dB]
X_Pulse	= 3.21666667[us]
Irr_Atn_Dec	= 25.244[dB]
Irr_Atn_Dec_Calc	= 25.244[dB]
Irr_Atn_Dec_Default_Calc	= 25.244[dB]
Irr_Atn_Noe	= 25.244[dB]
Irr_Dec_Bandwidth_Hz	= 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.08082432[ppm]
Irr_Dec_Freq	= 395.88430144[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]



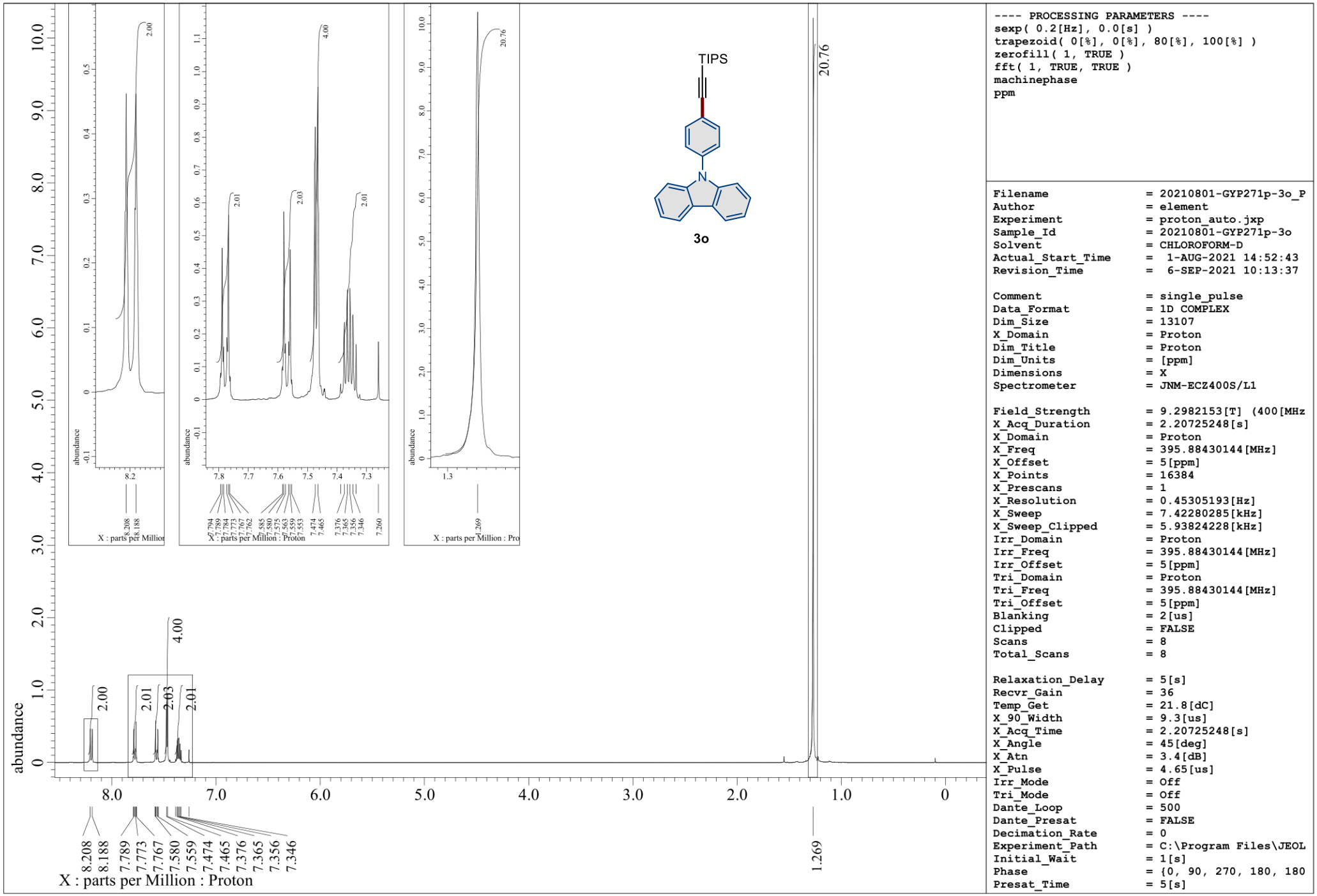

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

Filename	= 20210801-GYP158p-3n_P
Author	= element
Experiment	= proton_auto.jxp
Sample_Id	= 20210801-GYP158p-3n
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 1-AUG-2021 14:13:40
Revision_Time	= 30-AUG-2021 15:48:30
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ400S/L1
Field_Strength	= 9.2982153[T] (400[MHz
X_Acq_Duration	= 2.20725248[s]
X_Domain	= Proton
X_Freq	= 395.88430144[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45305193[Hz]
X_Sweep	= 7.42280285[kHz]
X_Sweep_Clipped	= 5.93824228[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 395.88430144[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 36
Temp_Get	= 21.7[dC]
X_90_Width	= 9.3[us]
X_Acq_Time	= 2.20725248[s]
X_Angle	= 45[deg]
X_Atn	= 3.4[dB]
X_Pulse	= 4.65[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 500
Dante_Presat	= FALSE
Decimation_Rate	= 0
Experiment_Path	= C:\Program Files\JEOL
Initial_Wait	= 1[s]
Phase	= {0, 90, 270, 180, 180
Presat_Time	= 5[s]



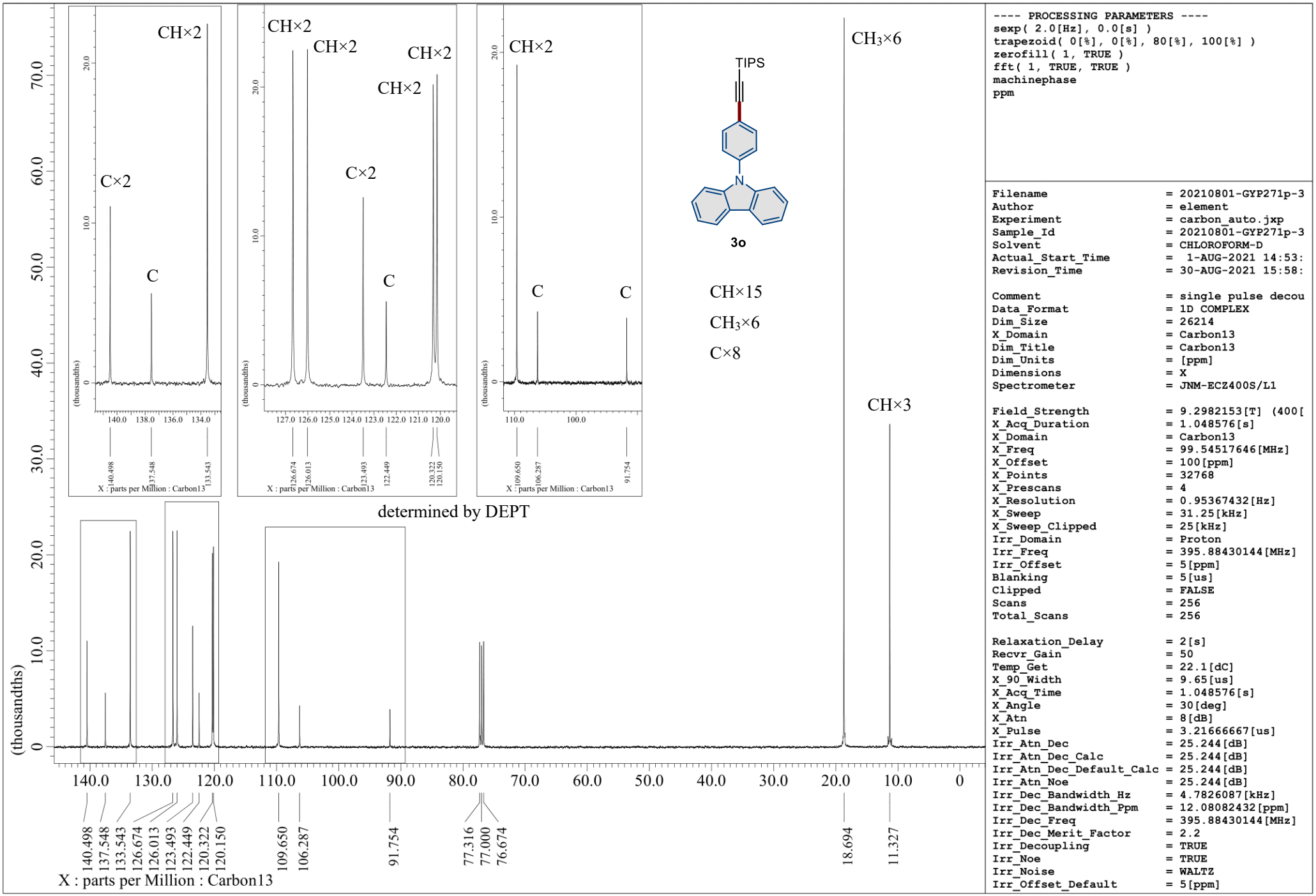

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

Filename	= 20210801-GYP158p-3
Author	= element
Experiment	= carbon_auto.jxp
Sample_Id	= 20210801-GYP158p-3
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 1-AUG-2021 14:14:
Revision_Time	= 19-AUG-2021 19:29:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ400S/L1
Field_Strength	= 9.2982153[T] (400[
X_Acq_Duration	= 1.048576[s]
X_Domain	= Carbon13
X_Freq	= 99.54517646[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.95367432[Hz]
X_Sweep	= 31.25[kHz]
X_Sweep_Clipped	= 25[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 5[us]
Clipped	= FALSE
Scans	= 256
Total_Scans	= 256
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 22.1[dC]
X_90_Width	= 9.65[us]
X_Acq_Time	= 1.048576[s]
X_Angle	= 30[deg]
X_Atn	= 8[dB]
X_Pulse	= 3.21666667[us]
Irr_Atn_Dec	= 25.244[dB]
Irr_Atn_Dec_Calc	= 25.244[dB]
Irr_Atn_Dec_Default_Calc	= 25.244[dB]
Irr_Atn_Noe	= 25.244[dB]
Irr_Dec_Bandwidth_Hz	= 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.08082432[ppm]
Irr_Dec_Freq	= 395.88430144[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]



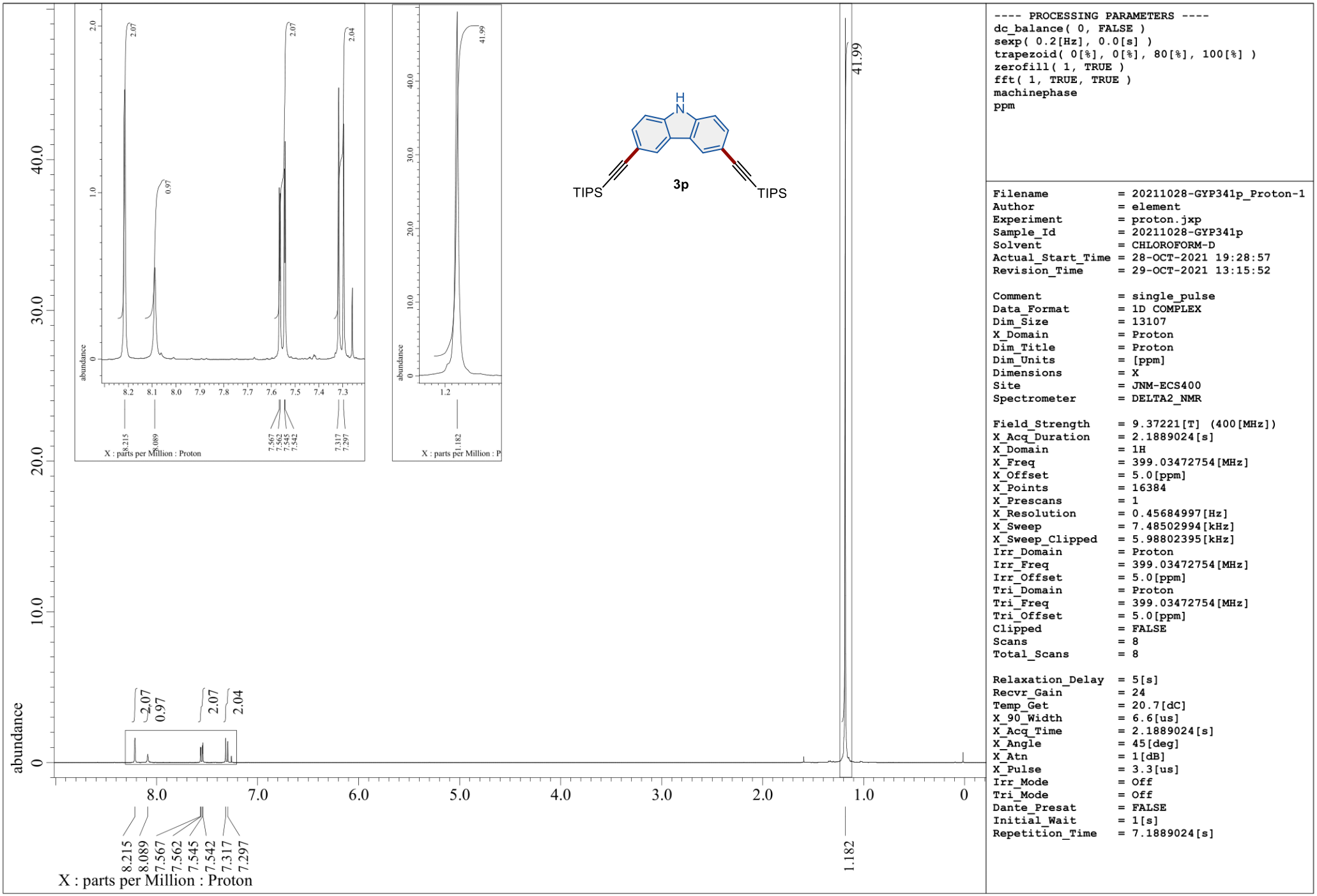

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

Filename	= 20210801-GYP271p-3o_P
Author	= element
Experiment	= proton_auto.jxp
Sample_Id	= 20210801-GYP271p-3o
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 1-AUG-2021 14:52:43
Revision_Time	= 6-SEP-2021 10:13:37
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ400S/L1
Field_Strength	= 9.2982153[T] (400[MHz
X_Acq_Duration	= 2.20725248[s]
X_Domain	= Proton
X_Freq	= 395.88430144[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45305193[Hz]
X_Sweep	= 7.42280285[kHz]
X_Sweep_Clipped	= 5.93824228[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 395.88430144[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 36
Temp_Get	= 21.8[dC]
X_90_Width	= 9.3[us]
X_Acq_Time	= 2.20725248[s]
X_Angle	= 45[deg]
X_Atn	= 3.4[dB]
X_Pulse	= 4.65[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 500
Dante_Presat	= FALSE
Decimation_Rate	= 0
Experiment_Path	= C:\Program Files\JEOL
Initial_Wait	= 1[s]
Phase	= {0, 90, 270, 180, 180
Presat_Time	= 5[s]




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

Filename	= 20210801-GYP271p-3
Author	= element
Experiment	= carbon_auto.jxp
Sample_Id	= 20210801-GYP271p-3
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 1-AUG-2021 14:53:
Revision_Time	= 30-AUG-2021 15:58:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ400S/L1
Field_Strength	= 9.2982153[T] (400[
X_Acq_Duration	= 1.048576[s]
X_Domain	= Carbon13
X_Freq	= 99.54517646[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.95367432[Hz]
X_Sweep	= 31.25[kHz]
X_Sweep_Clipped	= 25[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 5[us]
Clipped	= FALSE
Scans	= 256
Total_Scans	= 256
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 22.1[dC]
X_90_Width	= 9.65[us]
X_Acq_Time	= 1.048576[s]
X_Angle	= 30[deg]
X_Atn	= 8[dB]
X_Pulse	= 3.21666667[us]
Irr_Atn_Dec	= 25.244[dB]
Irr_Atn_Dec_Calc	= 25.244[dB]
Irr_Atn_Dec_Default_Calc	= 25.244[dB]
Irr_Atn_Noe	= 25.244[dB]
Irr_Dec_Bandwidth_Hz	= 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.08082432[ppm]
Irr_Dec_Freq	= 395.88430144[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]



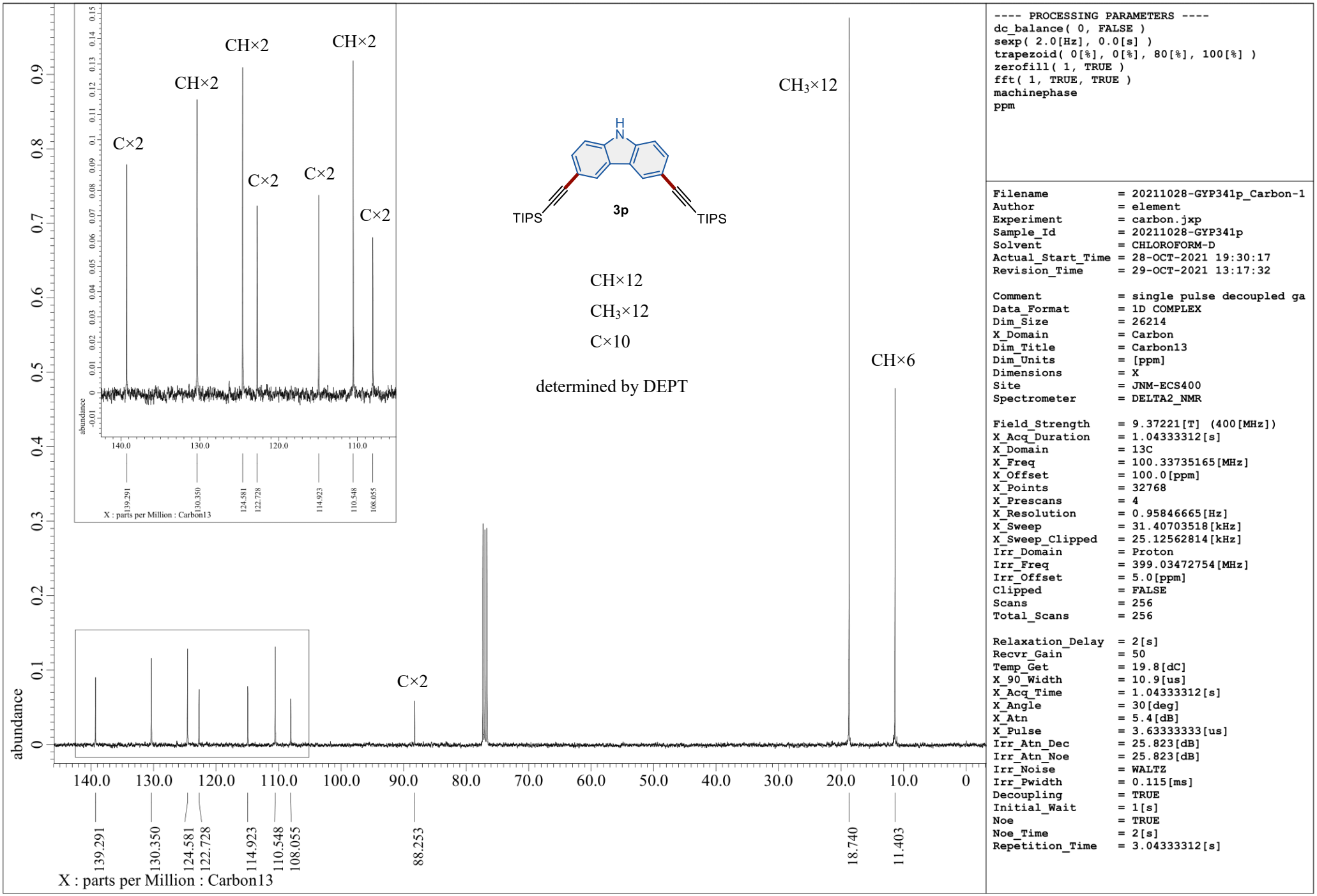

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename            = 20211028-GYP341p_Proton-1
Author              = element
Experiment          = proton.jxp
Sample_Id           = 20211028-GYP341p
Solvent             = CHLOROFORM-D
Actual_Start_Time   = 28-OCT-2021 19:28:57
Revision_Time       = 29-OCT-2021 13:15:52

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

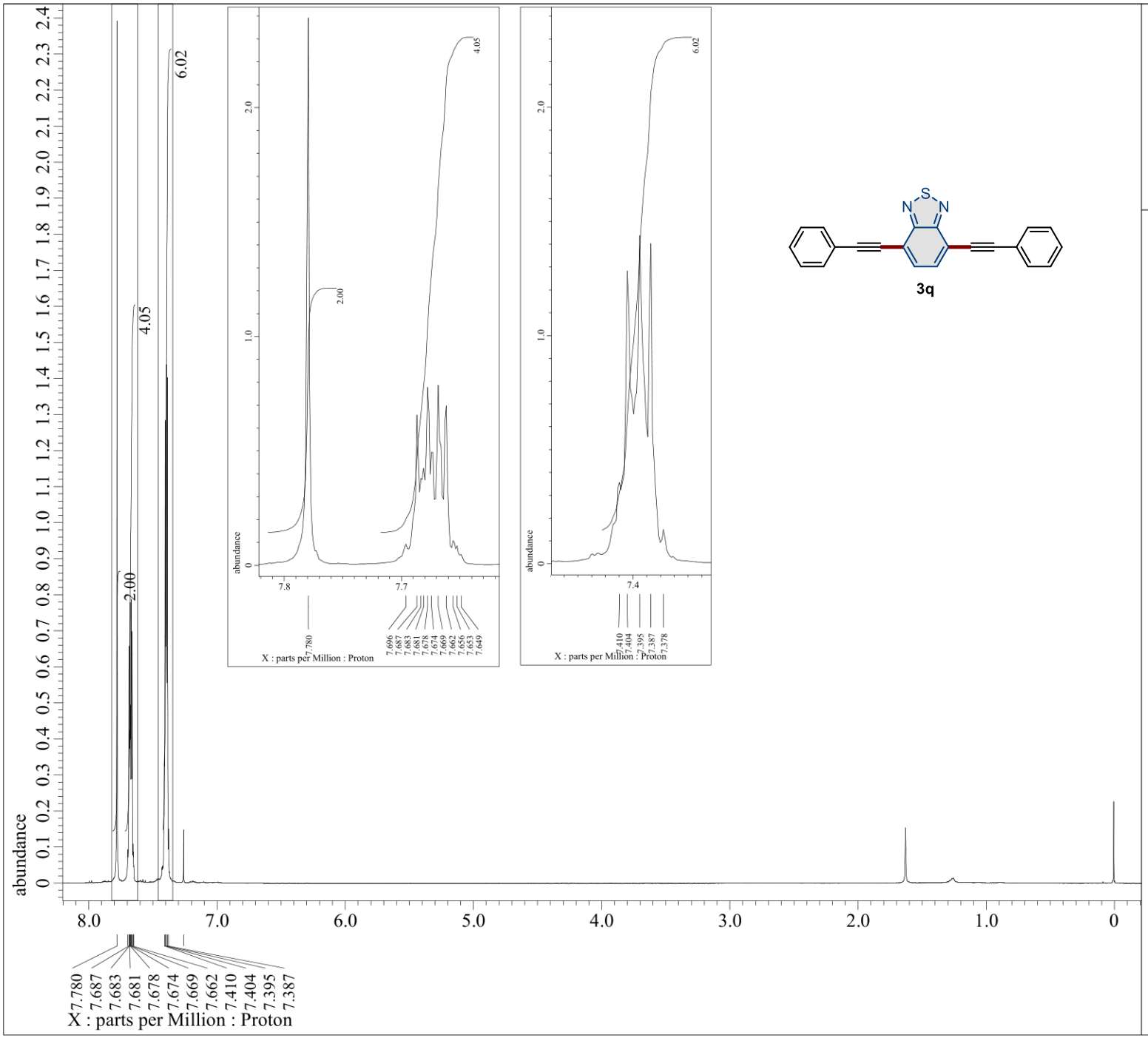
Field_Strength      = 9.37221[T] (400[MHz])
X_Acq_Duration      = 2.1889024[s]
X_Domain            = 1H
X_Freq              = 399.03472754[MHz]
X_Offset            = 5.0[ppm]
X_Points            = 16384
X_Prescans          = 1
X_Resolution        = 0.45684997[Hz]
X_Sweep             = 7.48502994[kHz]
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          = 24
Temp_Get            = 20.7[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
```

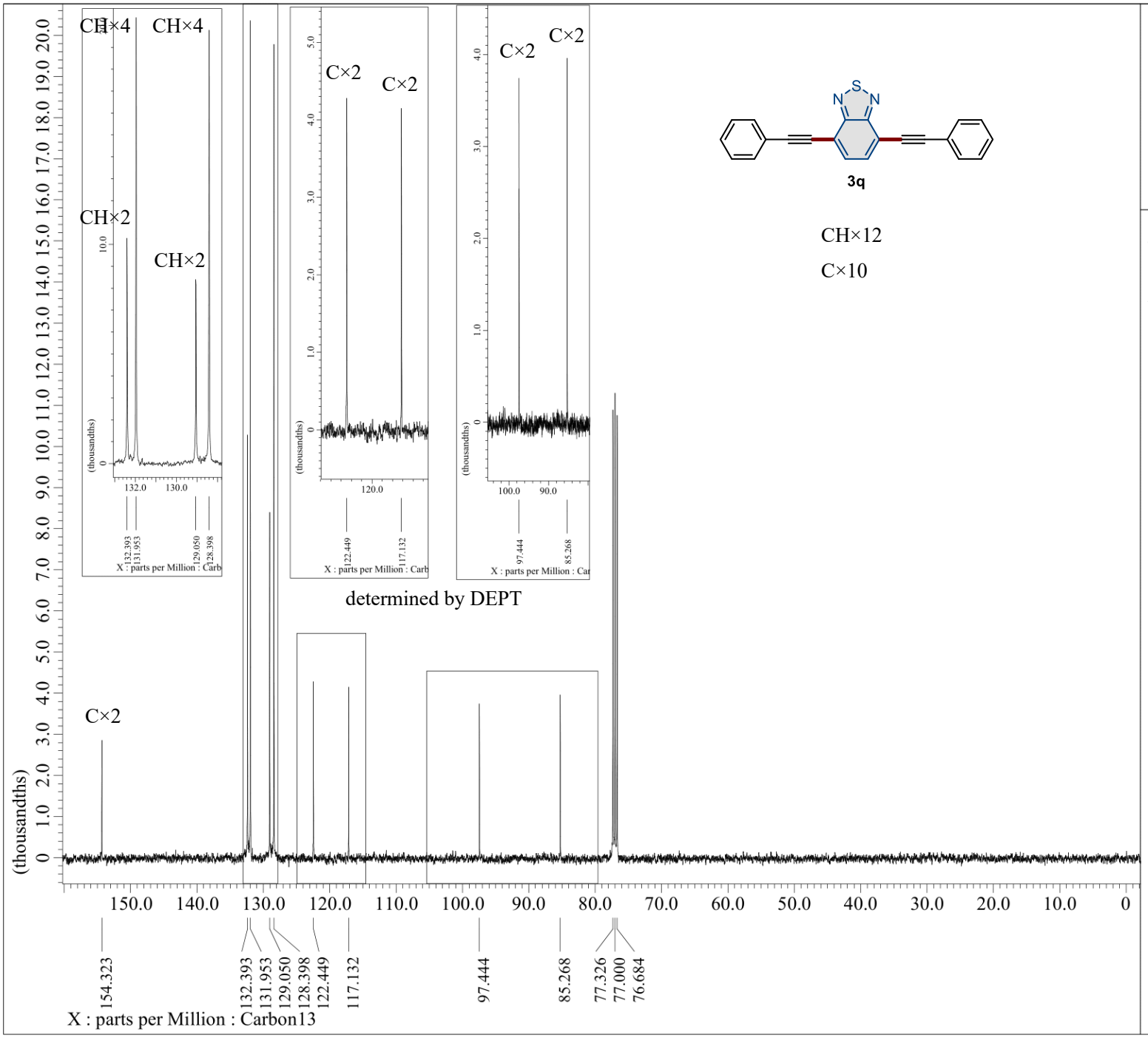
Filename	= 20211028-GYP341p_Carbon-1
Author	= element
Experiment	= carbon.jxp
Sample_Id	= 20211028-GYP341p
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 28-OCT-2021 19:30:17
Revision_Time	= 29-OCT-2021 13:17:32
Comment	= single pulse decoupled ga
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECS400
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.37221[T] (400[MHz])
X_Acq_Duration	= 1.04333312[s]
X_Domain	= 13C
X_Freq	= 100.33735165[MHz]
X_Offset	= 100.0[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.95846665[Hz]
X_Sweep	= 31.40703518[kHz]
X_Sweep_Clipped	= 25.12562814[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.03472754[MHz]
Irr_Offset	= 5.0[ppm]
Clipped	= FALSE
Scans	= 256
Total_Scans	= 256
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 19.8[dC]
X_90_Width	= 10.9[us]
X_Acq_Time	= 1.04333312[s]
X_Angle	= 30[deg]
X_Atn	= 5.4[dB]
X_Pulse	= 3.63333333[us]
Irr_Atn_Dec	= 25.823[dB]
Irr_Atn_Noe	= 25.823[dB]
Irr_Noise	= WALTZ
Irr_Pwidth	= 0.115[ms]
Decoupling	= TRUE
Initial_Wait	= 1[s]
Noe	= TRUE
Noe_Time	= 2[s]
Repetition_Time	= 3.04333312[s]



3q

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

Filename	= 20210801-GYP169p-3p_P
Author	= element
Experiment	= proton_auto.jxp
Sample_Id	= 20210801-GYP169p-3p
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 1-AUG-2021 15:29:41
Revision_Time	= 30-AUG-2021 16:00:54
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ400S/L1
Field_Strength	= 9.2982153[T] (400[MHz
X_Acq_Duration	= 2.20725248[s]
X_Domain	= Proton
X_Freq	= 395.88430144[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45305193[Hz]
X_Sweep	= 7.42280285[kHz]
X_Sweep_Clipped	= 5.93824228[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 395.88430144[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 46
Temp_Get	= 21.7[dC]
X_90_Width	= 9.3[us]
X_Acq_Time	= 2.20725248[s]
X_Angle	= 45[deg]
X_Atn	= 3.4[dB]
X_Pulse	= 4.65[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 500
Dante_Presat	= FALSE
Decimation_Rate	= 0
Experiment_Path	= C:\Program Files\JEOL
Initial_Wait	= 1[s]
Phase	= {0, 90, 270, 180, 180
Presat_Time	= 5[s]



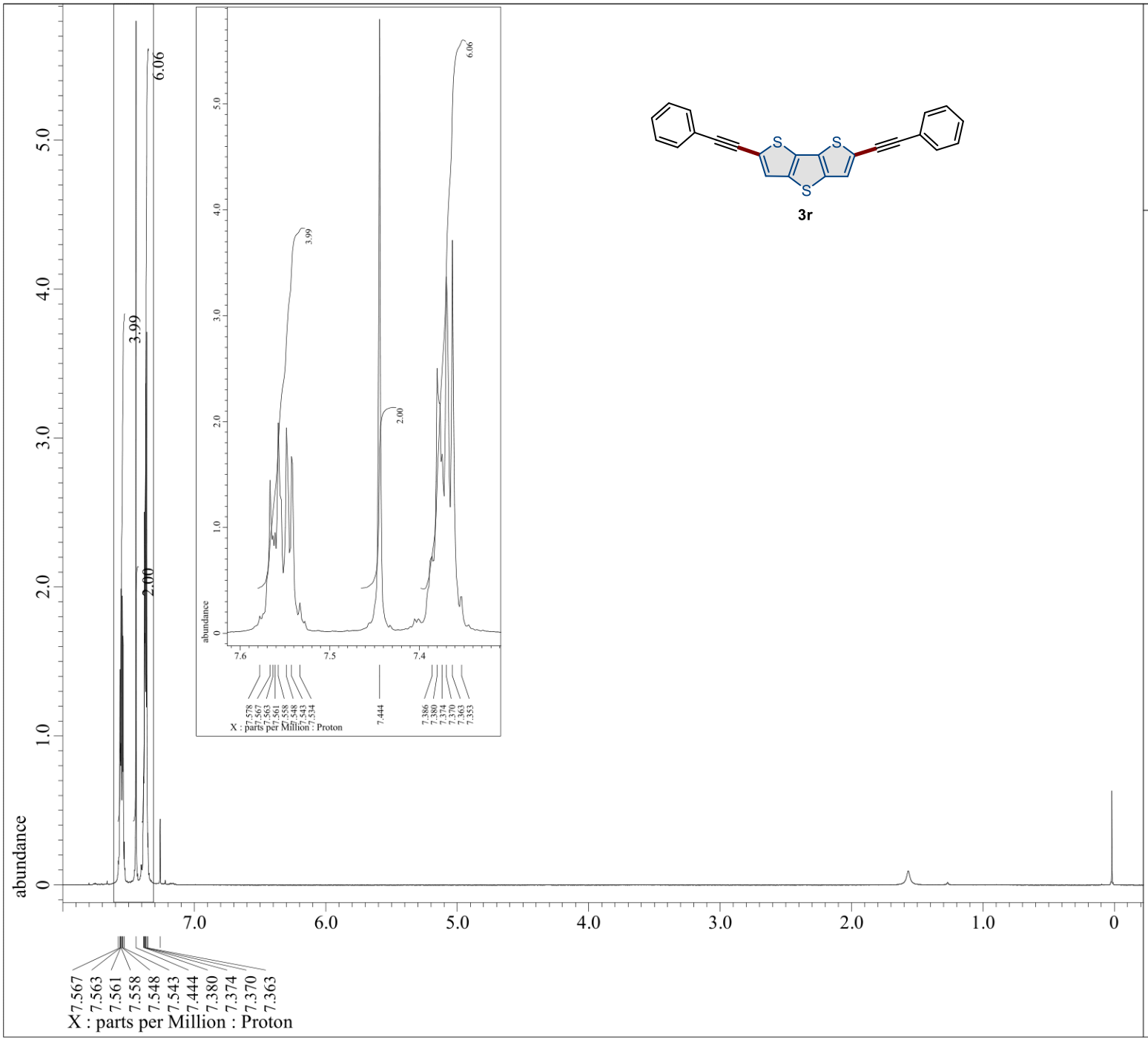
3q

CH×12

C×10

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

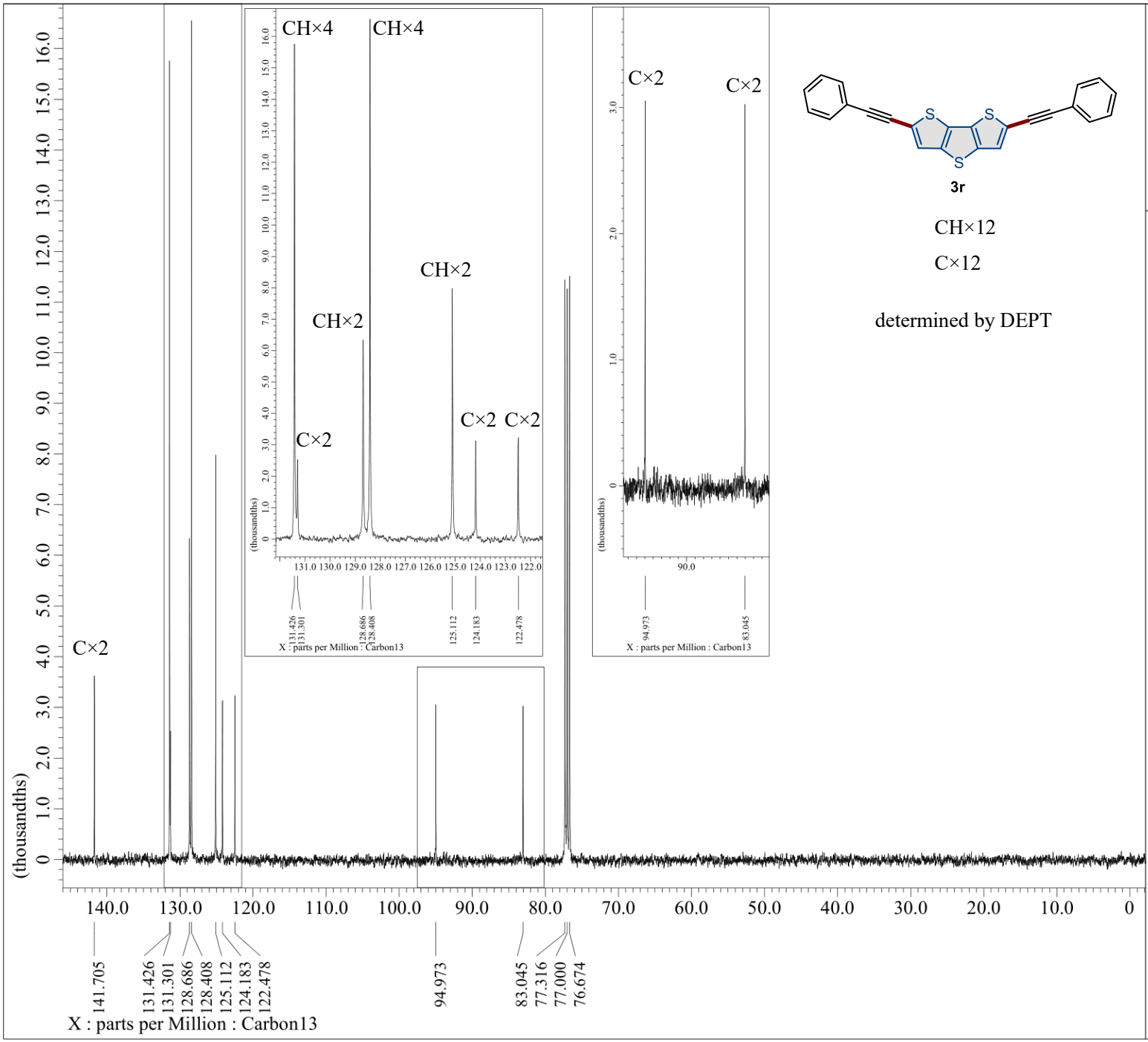
Filename	= 20210801-GYP169p-3
Author	= element
Experiment	= carbon_auto.jxp
Sample_Id	= 20210801-GYP169p-3
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 1-AUG-2021 15:30:
Revision_Time	= 30-AUG-2021 16:07:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ400S/L1
Field_Strength	= 9.2982153[T] (400[
X_Acq_Duration	= 1.048576[s]
X_Domain	= Carbon13
X_Freq	= 99.54517646[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.95367432[Hz]
X_Sweep	= 31.25[kHz]
X_Sweep_Clipped	= 25[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 5[us]
Clipped	= FALSE
Scans	= 256
Total_Scans	= 256
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 22[dC]
X_90_Width	= 9.65[us]
X_Acq_Time	= 1.048576[s]
X_Angle	= 30[deg]
X_Atn	= 8[dB]
X_Pulse	= 3.21666667[us]
Irr_Atn_Dec	= 25.244[dB]
Irr_Atn_Dec_Calc	= 25.244[dB]
Irr_Atn_Dec_Default_Calc	= 25.244[dB]
Irr_Atn_Noe	= 25.244[dB]
Irr_Dec_Bandwidth_Hz	= 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.08082432[ppm]
Irr_Dec_Freq	= 395.88430144[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]



3r

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

Filename	= 20210801-GYP177p-3q_P
Author	= element
Experiment	= proton_auto.jxp
Sample_Id	= 20210801-GYP177p-3q
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 1-AUG-2021 16:07:54
Revision_Time	= 20-AUG-2021 09:54:49
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ400S/L1
Field_Strength	= 9.2982153[T] (400[MHz
X_Acq_Duration	= 2.20725248[s]
X_Domain	= Proton
X_Freq	= 395.88430144[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45305193[Hz]
X_Sweep	= 7.42280285[kHz]
X_Sweep_Clipped	= 5.93824228[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 395.88430144[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= TRUE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 56
Temp_Get	= 21.8[dC]
X_90_Width	= 9.3[us]
X_Acq_Time	= 2.20725248[s]
X_Angle	= 45[deg]
X_Atn	= 3.4[dB]
X_Pulse	= 4.65[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 500
Dante_Presat	= FALSE
Decimation_Rate	= 0
Experiment_Path	= C:\Program Files\JEOL
Initial_Wait	= 1[s]
Phase	= {0, 90, 270, 180, 180
Presat_Time	= 5[s]



3r

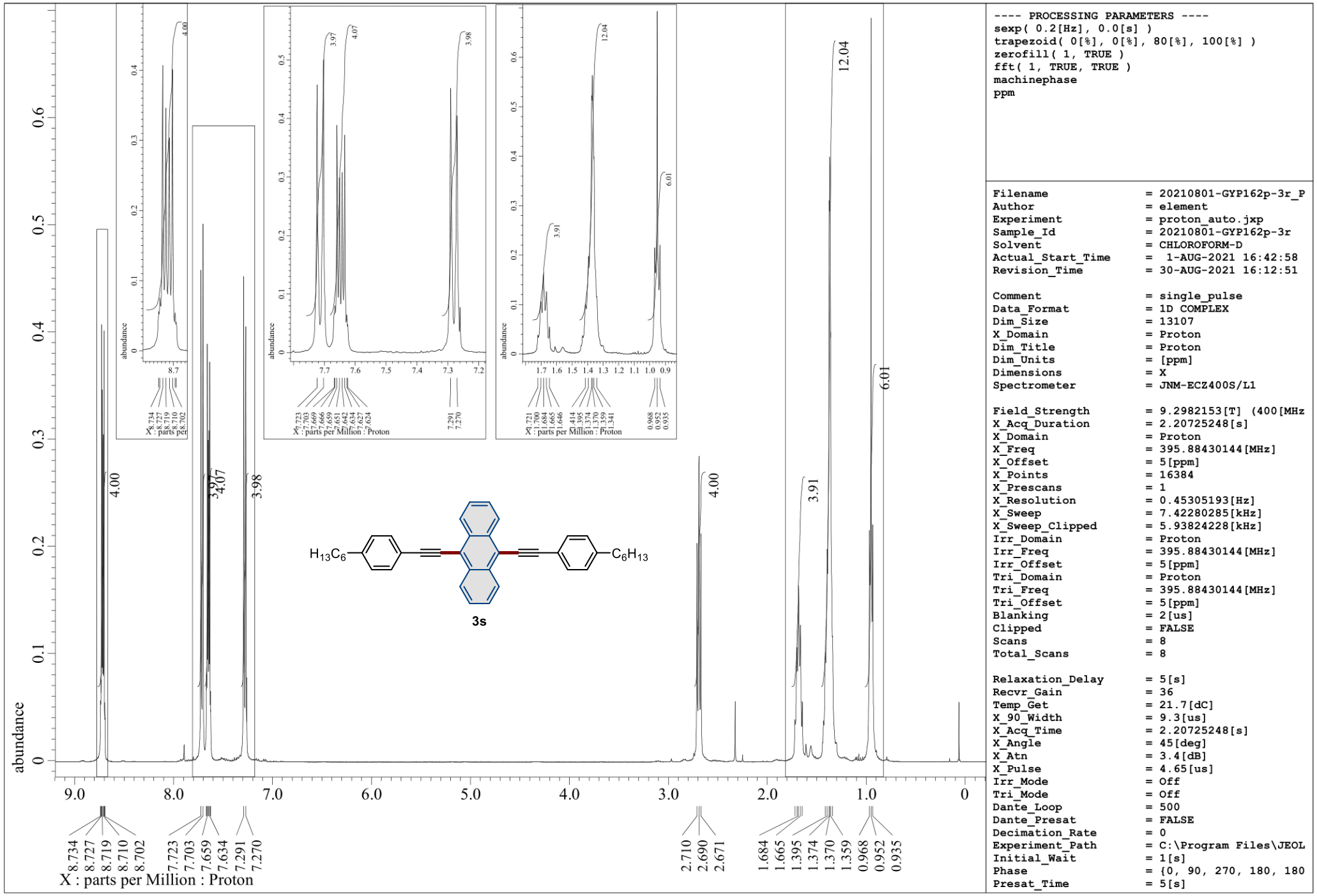
CH×12

C×12

determined by DEPT

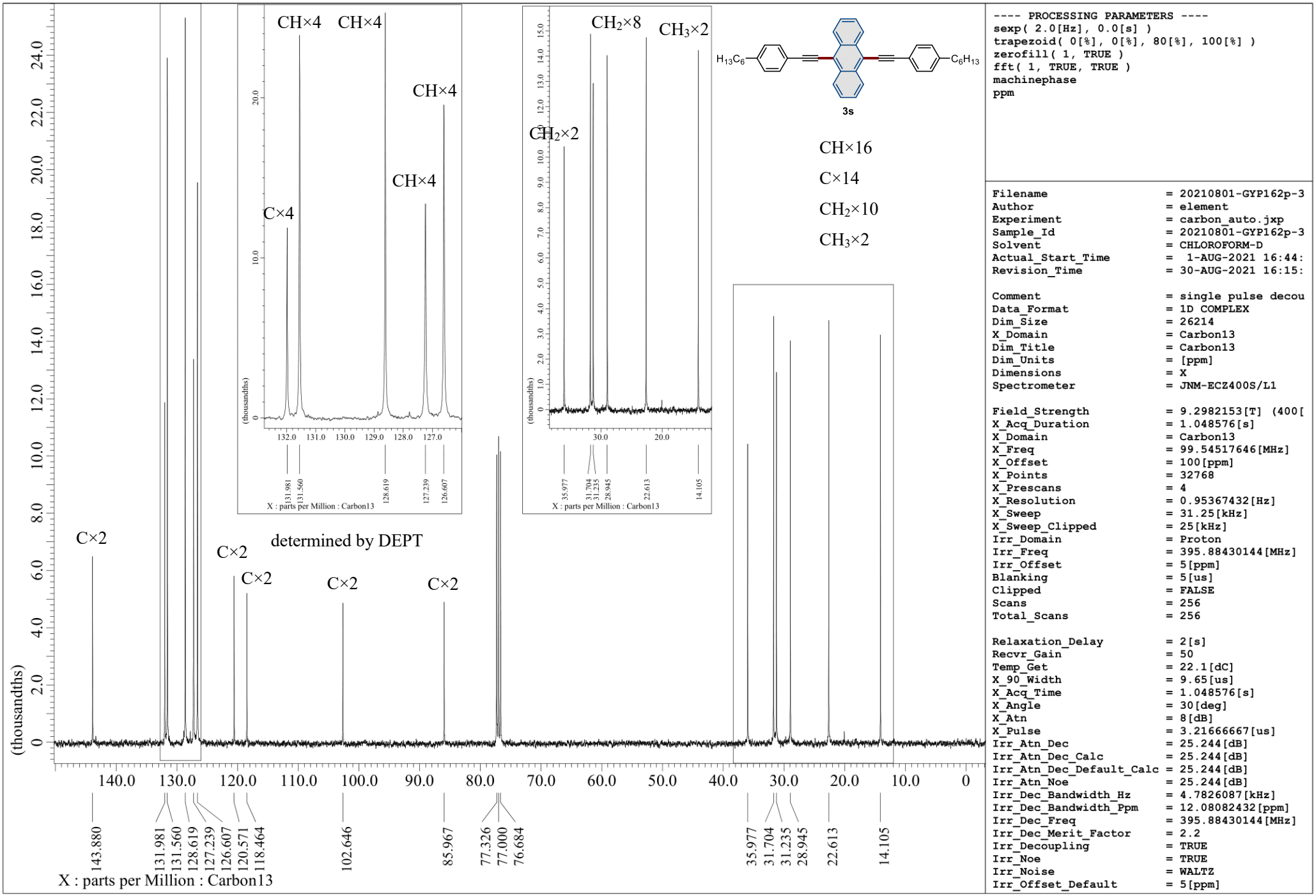
```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

Filename	= 20210801-GYP177p-3
Author	= element
Experiment	= carbon_auto.jxp
Sample_Id	= 20210801-GYP177p-3
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 1-AUG-2021 16:09:
Revision_Time	= 20-AUG-2021 09:56:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ400S/L1
Field_Strength	= 9.2982153[T] (400[
X_Acq_Duration	= 1.048576[s]
X_Domain	= Carbon13
X_Freq	= 99.54517646[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.95367432[Hz]
X_Sweep	= 31.25[kHz]
X_Sweep_Clipped	= 25[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 5[us]
Clipped	= FALSE
Scans	= 256
Total_Scans	= 256
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 22.1[dC]
X_90_Width	= 9.65[us]
X_Acq_Time	= 1.048576[s]
X_Angle	= 30[deg]
X_Atn	= 8[dB]
X_Pulse	= 3.21666667[us]
Irr_Atn_Dec	= 25.244[dB]
Irr_Atn_Dec_Calc	= 25.244[dB]
Irr_Atn_Dec_Default_Calc	= 25.244[dB]
Irr_Atn_Noe	= 25.244[dB]
Irr_Dec_Bandwidth_Hz	= 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.08082432[ppm]
Irr_Dec_Freq	= 395.88430144[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]



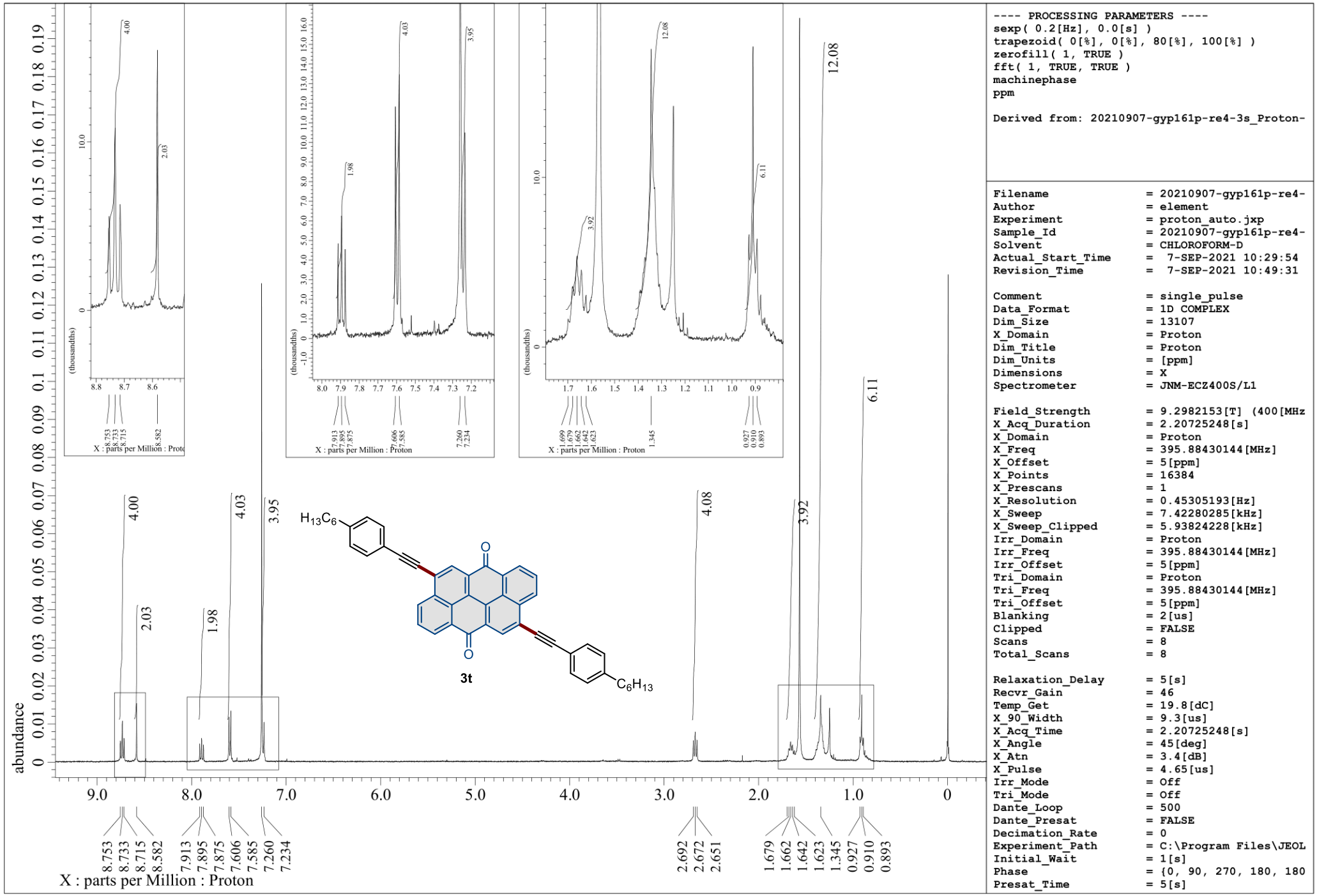

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

Filename	= 20210801-GYP162p-3r_P
Author	= element
Experiment	= proton_auto.jxp
Sample_Id	= 20210801-GYP162p-3r
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 1-AUG-2021 16:42:58
Revision_Time	= 30-AUG-2021 16:12:51
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ400S/L1
Field_Strength	= 9.2982153[T] (400[MHz
X_Acq_Duration	= 2.20725248[s]
X_Domain	= Proton
X_Freq	= 395.88430144[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45305193[Hz]
X_Sweep	= 7.42280285[kHz]
X_Sweep_Clipped	= 5.93824228[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 395.88430144[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 36
Temp_Get	= 21.7[dC]
X_90_Width	= 9.3[us]
X_Acq_Time	= 2.20725248[s]
X_Angle	= 45[deg]
X_Atn	= 3.4[dB]
X_Pulse	= 4.65[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 500
Dante_Presat	= FALSE
Decimation_Rate	= 0
Experiment_Path	= C:\Program Files\JEOL
Initial_Wait	= 1[s]
Phase	= {0, 90, 270, 180, 180
Presat_Time	= 5[s]




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

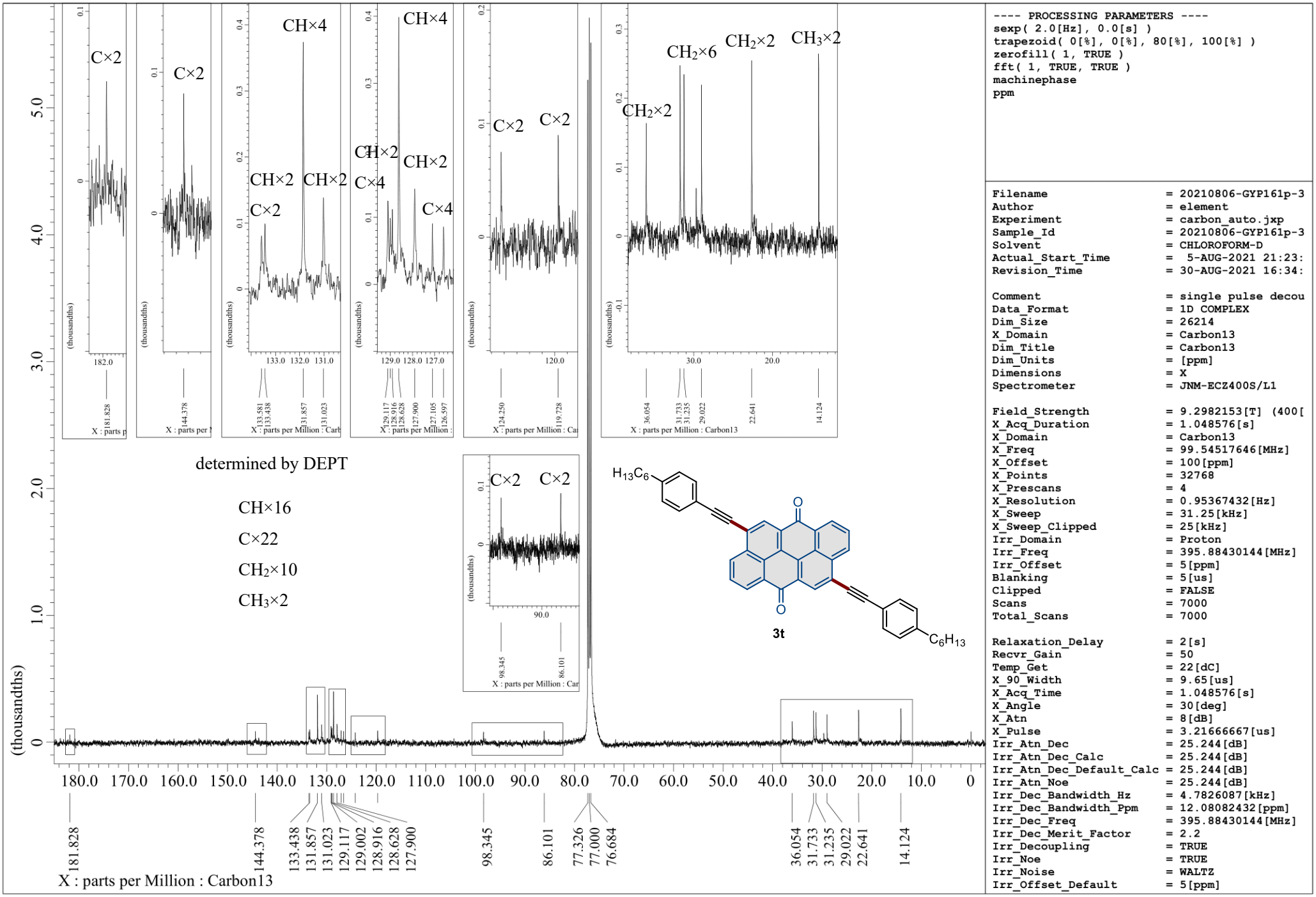
Filename	= 20210801-GYP162p-3
Author	= element
Experiment	= carbon_auto.jxp
Sample_Id	= 20210801-GYP162p-3
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 1-AUG-2021 16:44:
Revision_Time	= 30-AUG-2021 16:15:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ400S/L1
Field_Strength	= 9.2982153[T] (400[
X_Acq_Duration	= 1.048576[s]
X_Domain	= Carbon13
X_Freq	= 99.54517646[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.95367432[Hz]
X_Sweep	= 31.25[kHz]
X_Sweep_Clipped	= 25[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 5[us]
Clipped	= FALSE
Scans	= 256
Total_Scans	= 256
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 22.1[dC]
X_90_Width	= 9.65[us]
X_Acq_Time	= 1.048576[s]
X_Angle	= 30[deg]
X_Atn	= 8[dB]
X_Pulse	= 3.21666667[us]
Irr_Atn_Dec	= 25.244[dB]
Irr_Atn_Dec_Calc	= 25.244[dB]
Irr_Atn_Dec_Default_Calc	= 25.244[dB]
Irr_Atn_Noe	= 25.244[dB]
Irr_Dec_Bandwidth_Hz	= 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.08082432[ppm]
Irr_Dec_Freq	= 395.88430144[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]




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

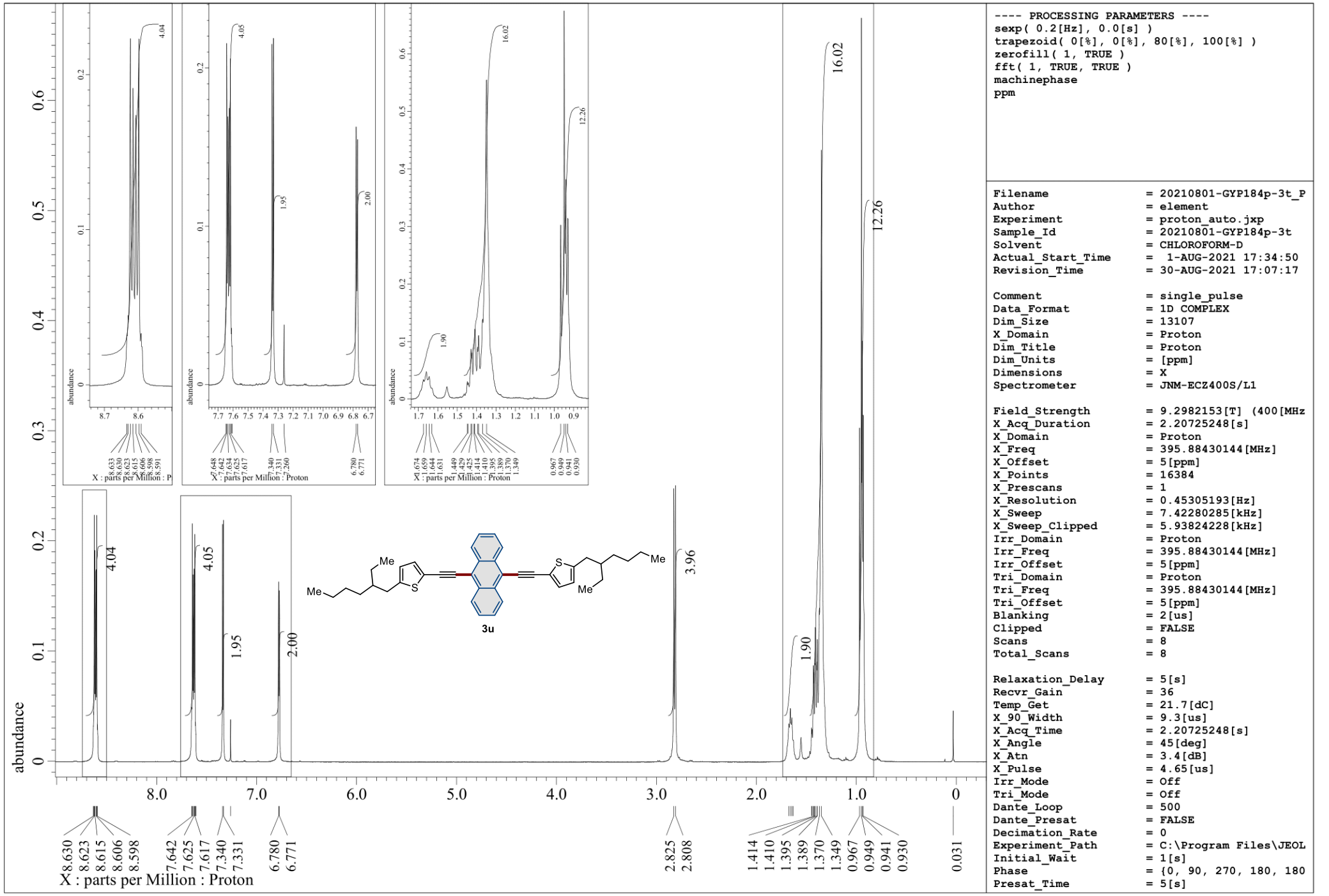
Derived from: 20210907-gyp161p-re4-3s_Proton-
```

Filename	= 20210907-gyp161p-re4-
Author	= element
Experiment	= proton_auto.jxp
Sample_Id	= 20210907-gyp161p-re4-
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 7-SEP-2021 10:29:54
Revision_Time	= 7-SEP-2021 10:49:31
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ400S/L1
Field_Strength	= 9.2982153[T] (400[MHz
X_Acq_Duration	= 2.20725248[s]
X_Domain	= Proton
X_Freq	= 395.88430144[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45305193[Hz]
X_Sweep	= 7.42280285[kHz]
X_Sweep_Clipped	= 5.93824228[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 395.88430144[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 46
Temp_Get	= 19.8[dC]
X_90_Width	= 9.3[us]
X_Acq_Time	= 2.20725248[s]
X_Angle	= 45[deg]
X_Atn	= 3.4[dB]
X_Pulse	= 4.65[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 500
Dante_Presat	= FALSE
Decimation_Rate	= 0
Experiment_Path	= C:\Program Files\JEOL
Initial_Wait	= 1[s]
Phase	= {0, 90, 270, 180, 180
Presat_Time	= 5[s]



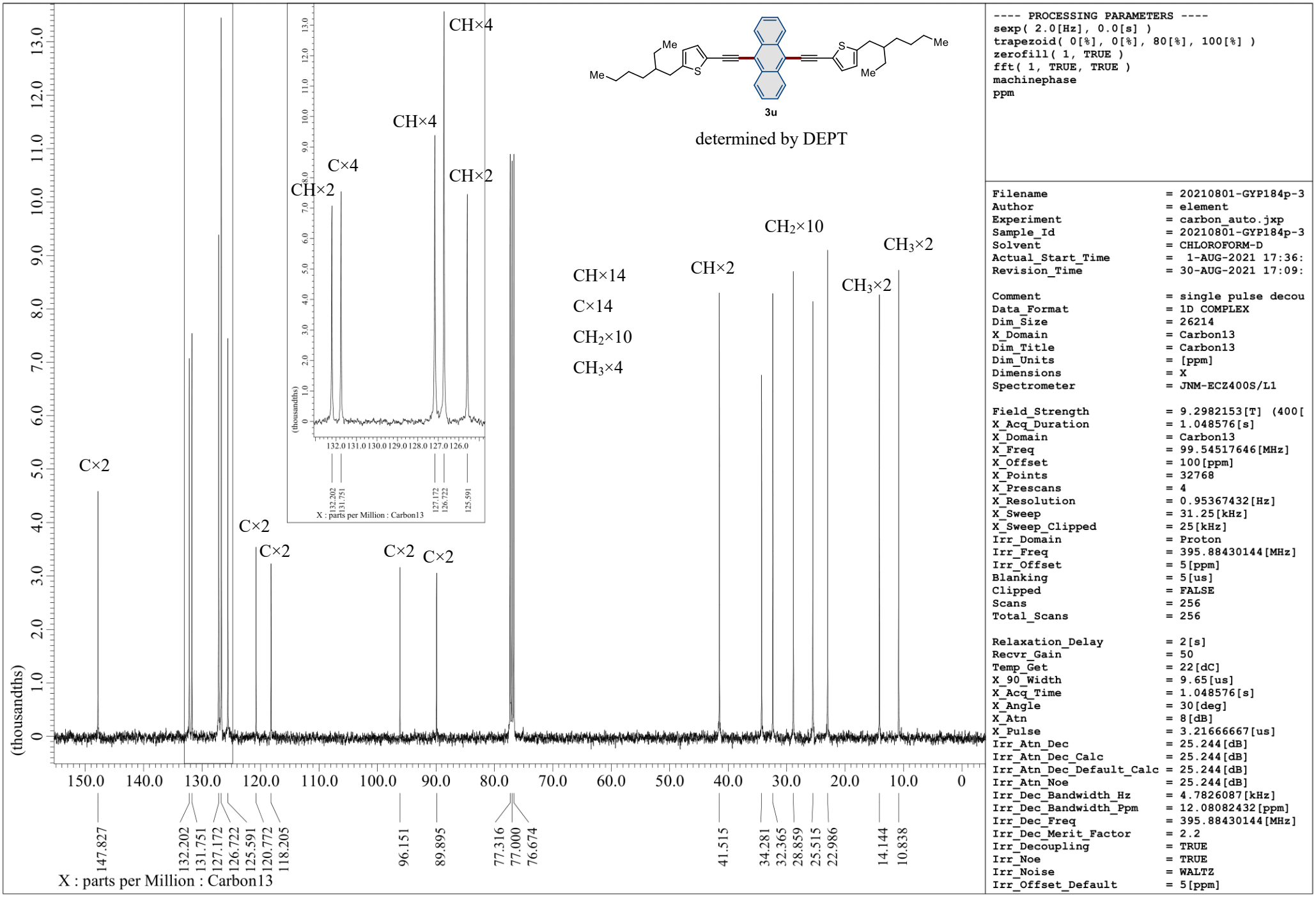

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

Filename	= 20210806-GYP161p-3
Author	= element
Experiment	= carbon_auto.jxp
Sample_Id	= 20210806-GYP161p-3
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 5-AUG-2021 21:23:
Revision_Time	= 30-AUG-2021 16:34:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ400S/L1
Field_Strength	= 9.2982153[T] (400[
X_Acq_Duration	= 1.048576[s]
X_Domain	= Carbon13
X_Freq	= 99.54517646[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.95367432[Hz]
X_Sweep	= 31.25[kHz]
X_Sweep_Clipped	= 25[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 5[us]
Clipped	= FALSE
Scans	= 7000
Total_Scans	= 7000
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 22[dC]
X_90_Width	= 9.65[us]
X_Acq_Time	= 1.048576[s]
X_Angle	= 30[deg]
X_Atn	= 8[dB]
X_Pulse	= 3.21666667[us]
Irr_Atn_Dec	= 25.244[dB]
Irr_Atn_Dec_Calc	= 25.244[dB]
Irr_Atn_Dec_Default_Calc	= 25.244[dB]
Irr_Atn_Noe	= 25.244[dB]
Irr_Dec_Bandwidth_Hz	= 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.08082432[ppm]
Irr_Dec_Freq	= 395.88430144[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]



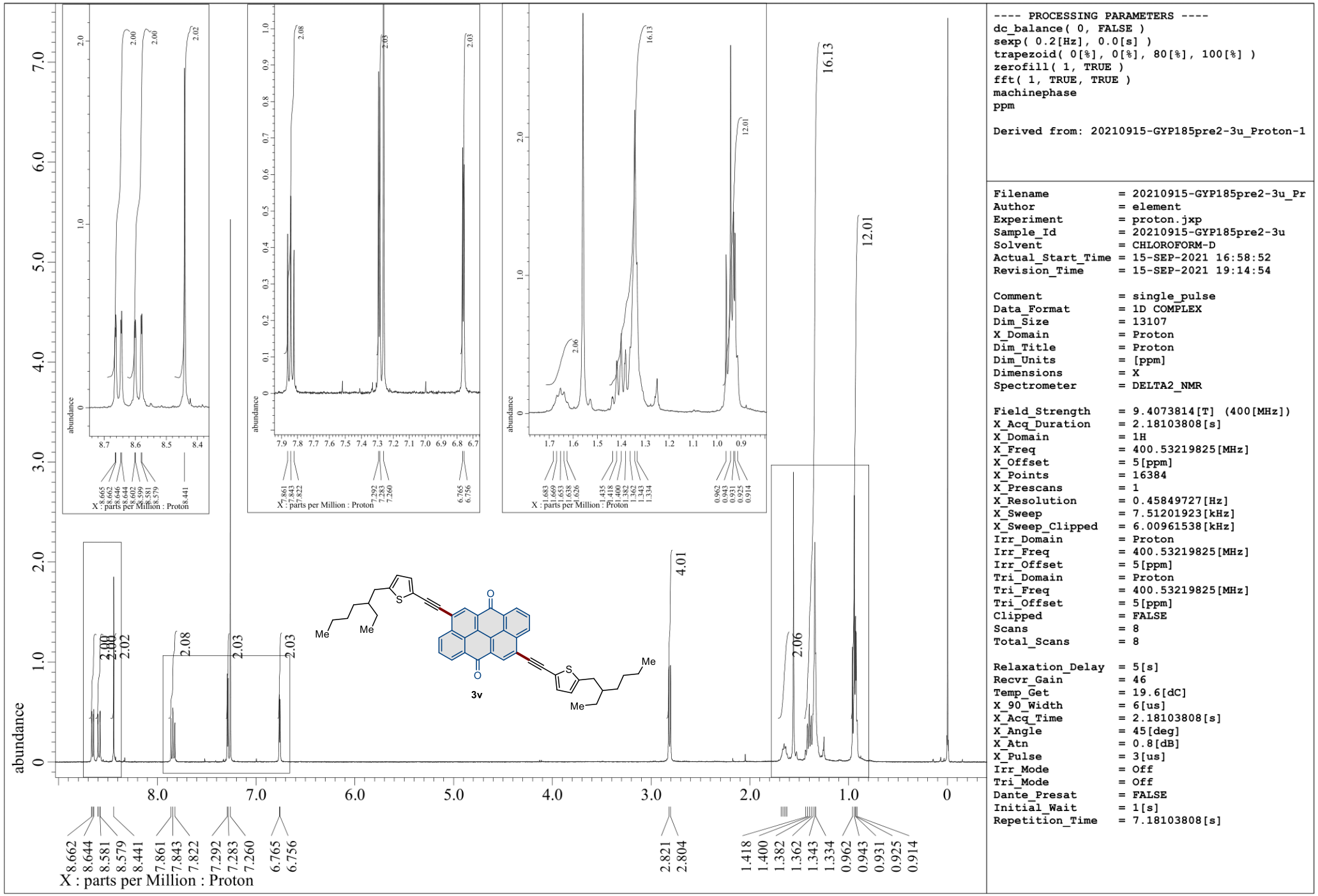

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

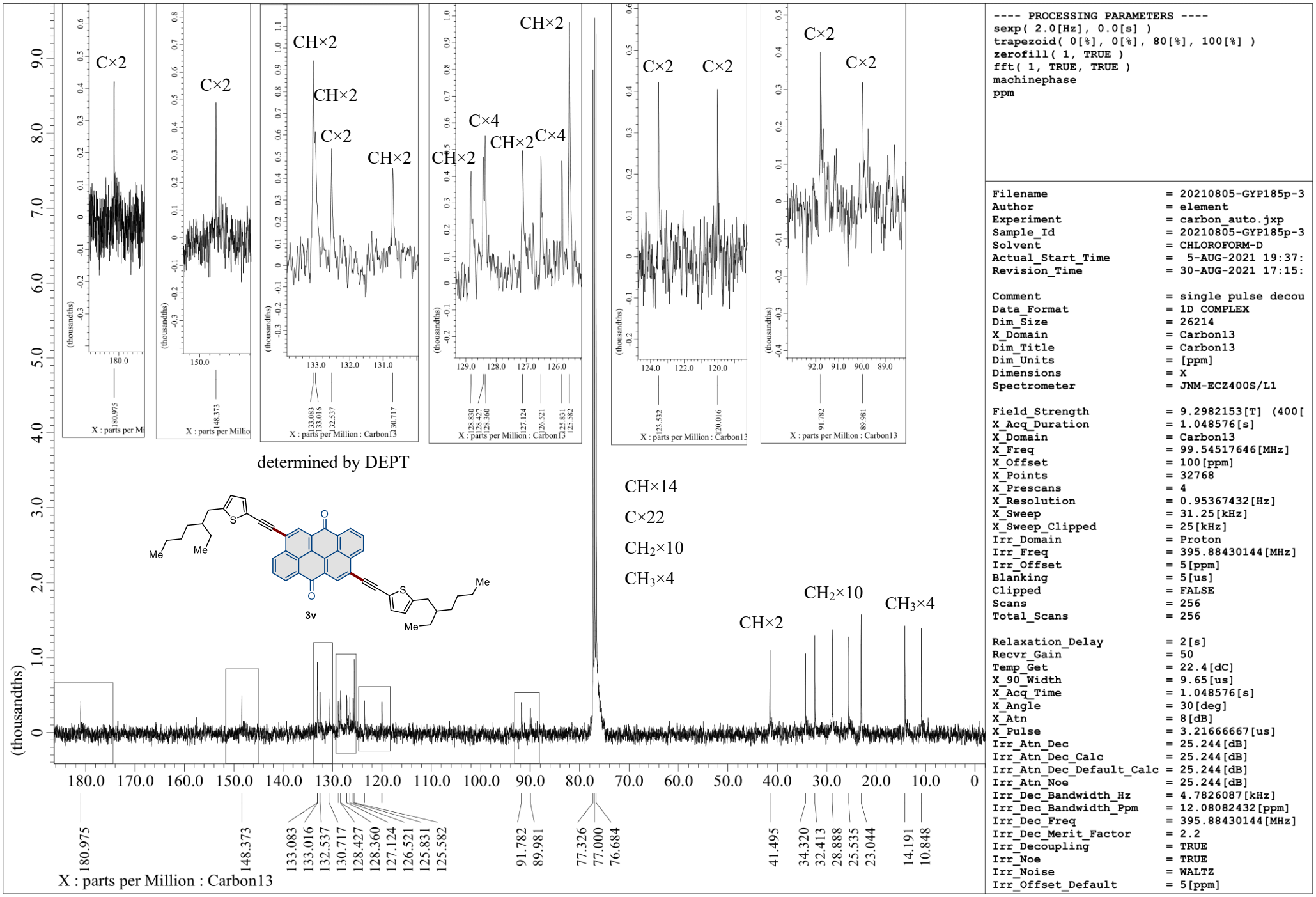
Filename	= 20210801-GYP184p-3t_P
Author	= element
Experiment	= proton_auto.jxp
Sample_Id	= 20210801-GYP184p-3t
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 1-AUG-2021 17:34:50
Revision_Time	= 30-AUG-2021 17:07:17
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ400S/L1
Field_Strength	= 9.2982153[T] (400[MHz
X_Acq_Duration	= 2.20725248[s]
X_Domain	= Proton
X_Freq	= 395.88430144[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45305193[Hz]
X_Sweep	= 7.42280285[kHz]
X_Sweep_Clipped	= 5.93824228[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 395.88430144[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 36
Temp_Get	= 21.7[dC]
X_90_Width	= 9.3[us]
X_Acq_Time	= 2.20725248[s]
X_Angle	= 45[deg]
X_Atn	= 3.4[dB]
X_Pulse	= 4.65[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 500
Dante_Presat	= FALSE
Decimation_Rate	= 0
Experiment_Path	= C:\Program Files\JEOL
Initial_Wait	= 1[s]
Phase	= {0, 90, 270, 180, 180
Presat_Time	= 5[s]




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

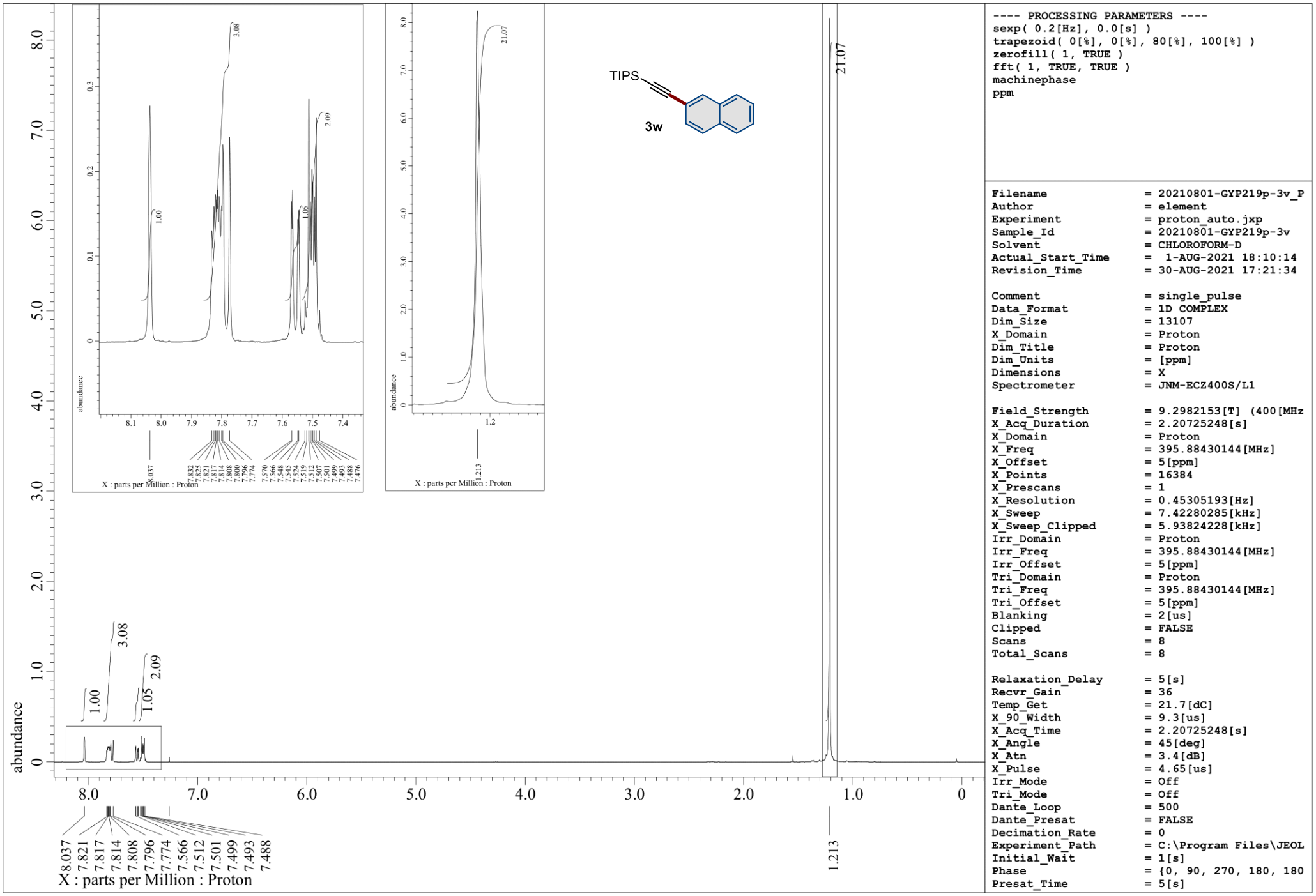
Filename	= 20210801-GYP184p-3
Author	= element
Experiment	= carbon_auto.jxp
Sample_Id	= 20210801-GYP184p-3
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 1-AUG-2021 17:36:
Revision_Time	= 30-AUG-2021 17:09:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ400S/L1
Field_Strength	= 9.2982153[T] (400[
X_Acq_Duration	= 1.048576[s]
X_Domain	= Carbon13
X_Freq	= 99.54517646[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.95367432[Hz]
X_Sweep	= 31.25[kHz]
X_Sweep_Clipped	= 25[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 5[us]
Clipped	= FALSE
Scans	= 256
Total_Scans	= 256
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 22[dC]
X_90_Width	= 9.65[us]
X_Acq_Time	= 1.048576[s]
X_Angle	= 30[deg]
X_Atn	= 8[dB]
X_Pulse	= 3.21666667[us]
Irr_Atn_Dec	= 25.244[dB]
Irr_Atn_Dec_Calc	= 25.244[dB]
Irr_Atn_Dec_Default_Calc	= 25.244[dB]
Irr_Atn_Noe	= 25.244[dB]
Irr_Dec_Bandwidth_Hz	= 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.08082432[ppm]
Irr_Dec_Freq	= 395.88430144[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]


---- 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: 20210915-GYP185pre2-3u_Proton-1
Filename = 20210915-GYP185pre2-3u_Pr
Author = element
Experiment = proton.jxp
Sample_Id = 20210915-GYP185pre2-3u
Solvent = CHLOROFORM-D
Actual_Start_Time = 15-SEP-2021 16:58:52
Revision_Time = 15-SEP-2021 19:14:54
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = DELTA2_NMR
Field_Strength = 9.4073814[T] (400[MHz])
X_Acq_Duration = 2.18103808[s]
X_Domain = 1H
X_Freq = 400.53219825[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45849727[Hz]
X_Sweep = 7.51201923[kHz]
X_Sweep_Clipped = 6.00961538[kHz]
Irr_Domain = Proton
Irr_Freq = 400.53219825[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 400.53219825[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 19.6[dC]
X_90_Width = 6[us]
X_Acq_Time = 2.18103808[s]
X_Angle = 45[deg]
X_Atn = 0.8[dB]
X_Pulse = 3[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 7.18103808[s]
abundance
X : parts per Million : Proton
Me
S
O
3v
16.13
12.01
4.01
2.08
2.06
2.03
2.02
2.00



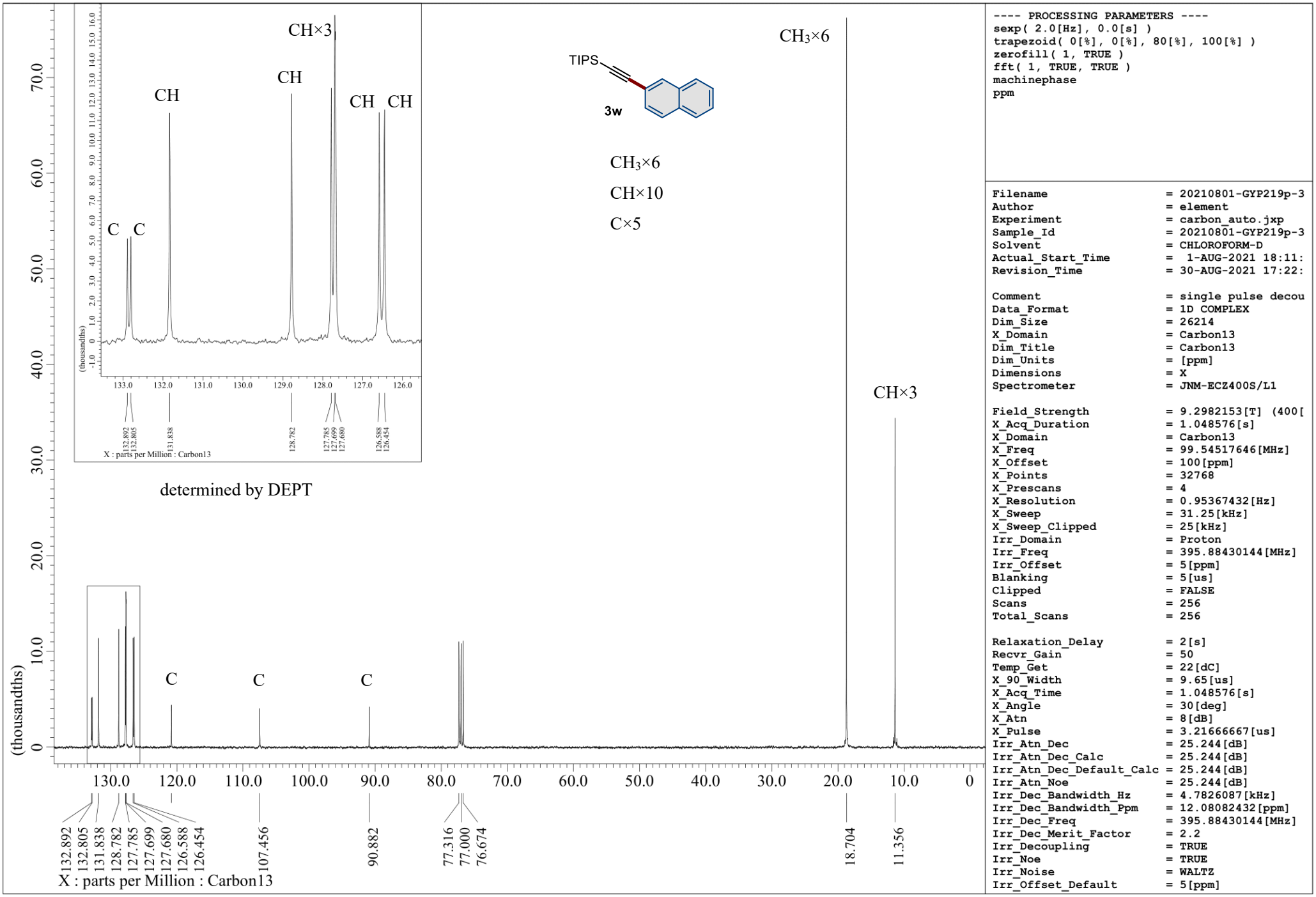

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

Filename	= 20210805-GYP185p-3
Author	= element
Experiment	= carbon_auto.jxp
Sample_Id	= 20210805-GYP185p-3
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 5-AUG-2021 19:37:
Revision_Time	= 30-AUG-2021 17:15:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ400S/L1
Field_Strength	= 9.2982153[T] (400[
X_Acq_Duration	= 1.048576[s]
X_Domain	= Carbon13
X_Freq	= 99.54517646[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.95367432[Hz]
X_Sweep	= 31.25[kHz]
X_Sweep_Clipped	= 25[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 5[us]
Clipped	= FALSE
Scans	= 256
Total_Scans	= 256
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 22.4[dC]
X_90_Width	= 9.65[us]
X_Acq_Time	= 1.048576[s]
X_Angle	= 30[deg]
X_Atn	= 8[dB]
X_Pulse	= 3.21666667[us]
Irr_Atn_Dec	= 25.244[dB]
Irr_Atn_Dec_Calc	= 25.244[dB]
Irr_Atn_Dec_Default_Calc	= 25.244[dB]
Irr_Atn_Noe	= 25.244[dB]
Irr_Dec_Bandwidth_Hz	= 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.08082432[ppm]
Irr_Dec_Freq	= 395.88430144[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]



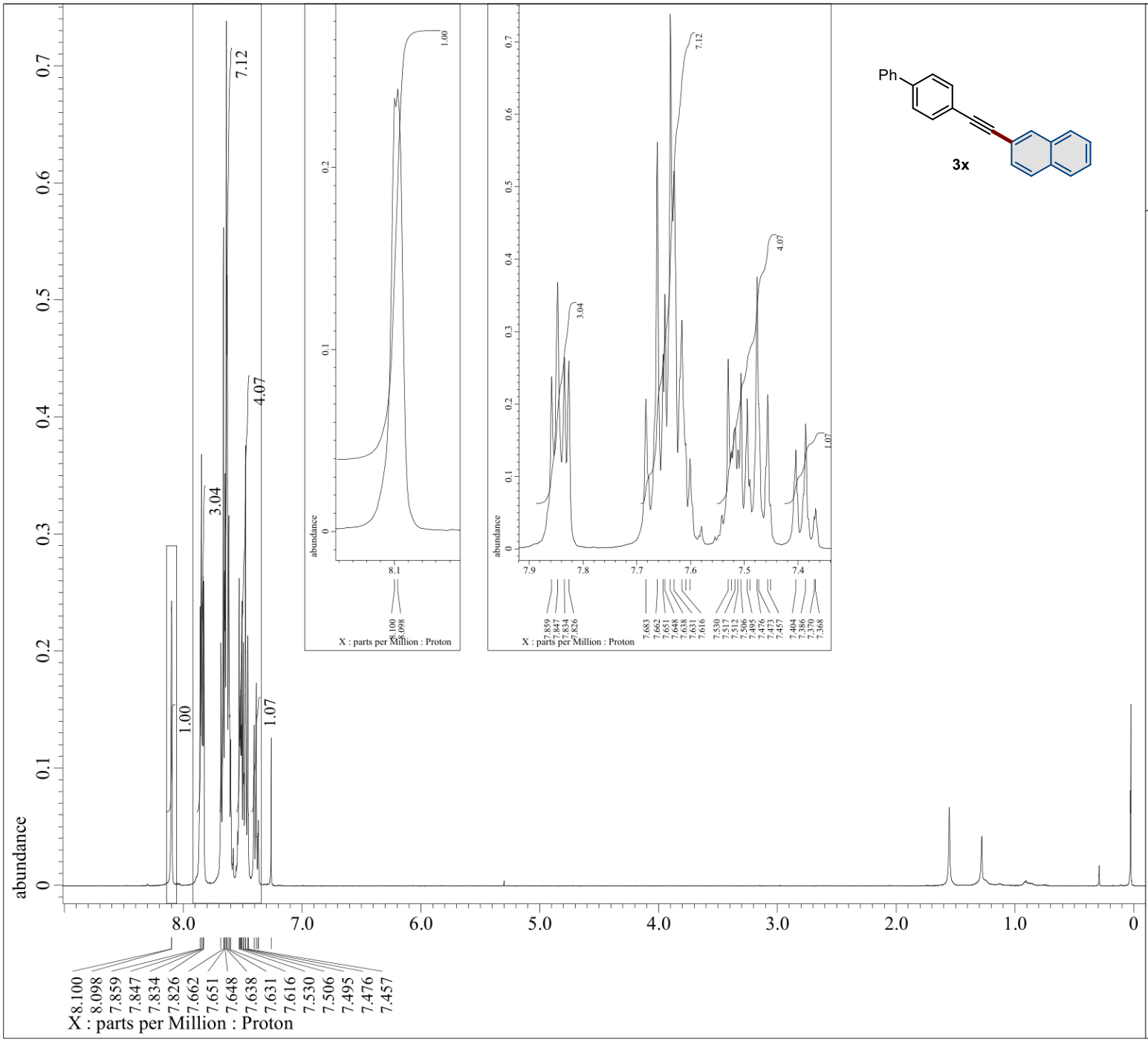

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

Filename	= 20210801-GYP219p-3v_P
Author	= element
Experiment	= proton_auto.jxp
Sample_Id	= 20210801-GYP219p-3v
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 1-AUG-2021 18:10:14
Revision_Time	= 30-AUG-2021 17:21:34
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ400S/L1
Field_Strength	= 9.2982153[T] (400[MHz
X_Acq_Duration	= 2.20725248[s]
X_Domain	= Proton
X_Freq	= 395.88430144[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45305193[Hz]
X_Sweep	= 7.42280285[kHz]
X_Sweep_Clipped	= 5.93824228[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 395.88430144[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 36
Temp_Get	= 21.7[dC]
X_90_Width	= 9.3[us]
X_Acq_Time	= 2.20725248[s]
X_Angle	= 45[deg]
X_Atn	= 3.4[dB]
X_Pulse	= 4.65[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 500
Dante_Presat	= FALSE
Decimation_Rate	= 0
Experiment_Path	= C:\Program Files\JEOL
Initial_Wait	= 1[s]
Phase	= {0, 90, 270, 180, 180
Presat_Time	= 5[s]




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

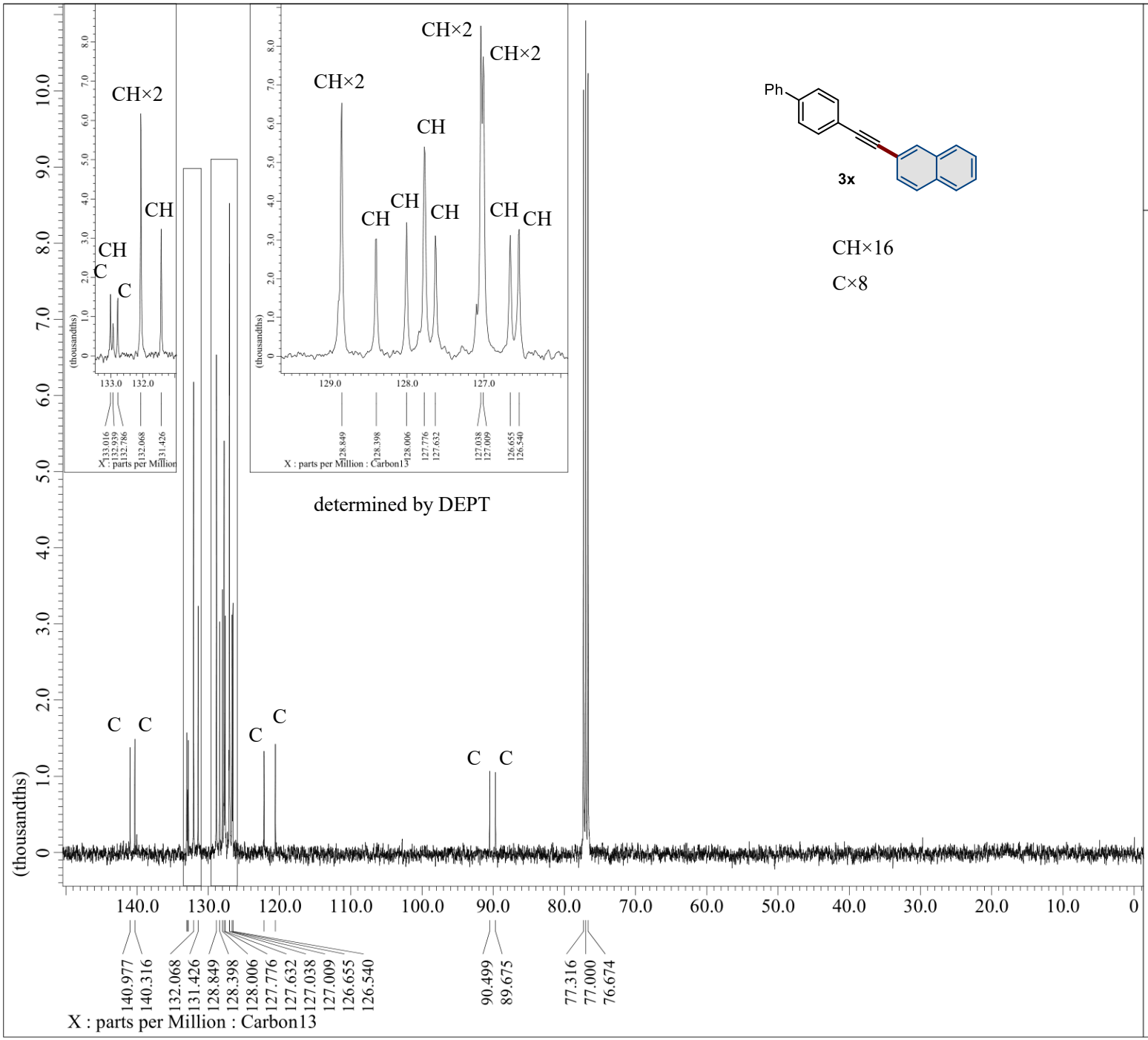
Filename	= 20210801-GYP219p-3
Author	= element
Experiment	= carbon_auto.jxp
Sample_Id	= 20210801-GYP219p-3
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 1-AUG-2021 18:11:
Revision_Time	= 30-AUG-2021 17:22:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ400S/L1
Field_Strength	= 9.2982153[T] (400[
X_Acq_Duration	= 1.048576[s]
X_Domain	= Carbon13
X_Freq	= 99.54517646[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.95367432[Hz]
X_Sweep	= 31.25[kHz]
X_Sweep_Clipped	= 25[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 5[us]
Clipped	= FALSE
Scans	= 256
Total_Scans	= 256
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 22[dC]
X_90_Width	= 9.65[us]
X_Acq_Time	= 1.048576[s]
X_Angle	= 30[deg]
X_Atn	= 8[dB]
X_Pulse	= 3.21666667[us]
Irr_Atn_Dec	= 25.244[dB]
Irr_Atn_Dec_Calc	= 25.244[dB]
Irr_Atn_Dec_Default_Calc	= 25.244[dB]
Irr_Atn_Noe	= 25.244[dB]
Irr_Dec_Bandwidth_Hz	= 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.08082432[ppm]
Irr_Dec_Freq	= 395.88430144[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]



3x

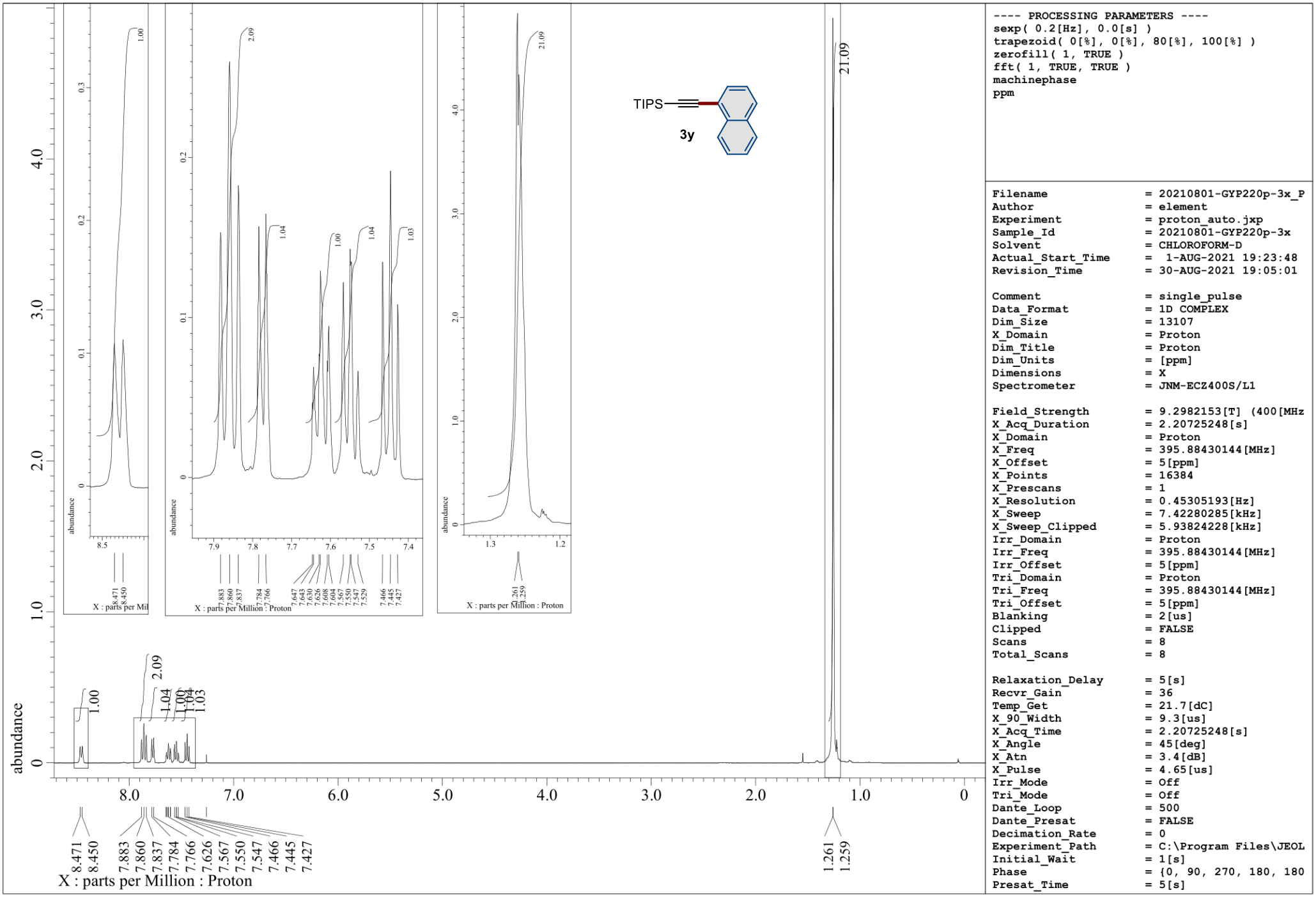
```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

Filename	= 20210801-GYP047p-3w_P
Author	= element
Experiment	= proton_auto.jxp
Sample_Id	= 20210801-GYP047p-3w
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 1-AUG-2021 18:45:26
Revision_Time	= 30-AUG-2021 18:57:35
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ400S/L1
Field_Strength	= 9.2982153[T] (400[MHz
X_Acq_Duration	= 2.20725248[s]
X_Domain	= Proton
X_Freq	= 395.88430144[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45305193[Hz]
X_Sweep	= 7.42280285[kHz]
X_Sweep_Clipped	= 5.93824228[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 395.88430144[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 46
Temp_Get	= 21.7[dC]
X_90_Width	= 9.3[us]
X_Acq_Time	= 2.20725248[s]
X_Angle	= 45[deg]
X_Atn	= 3.4[dB]
X_Pulse	= 4.65[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 500
Dante_Presat	= FALSE
Decimation_Rate	= 0
Experiment_Path	= C:\Program Files\JEOL
Initial_Wait	= 1[s]
Phase	= {0, 90, 270, 180, 180
Presat_Time	= 5[s]



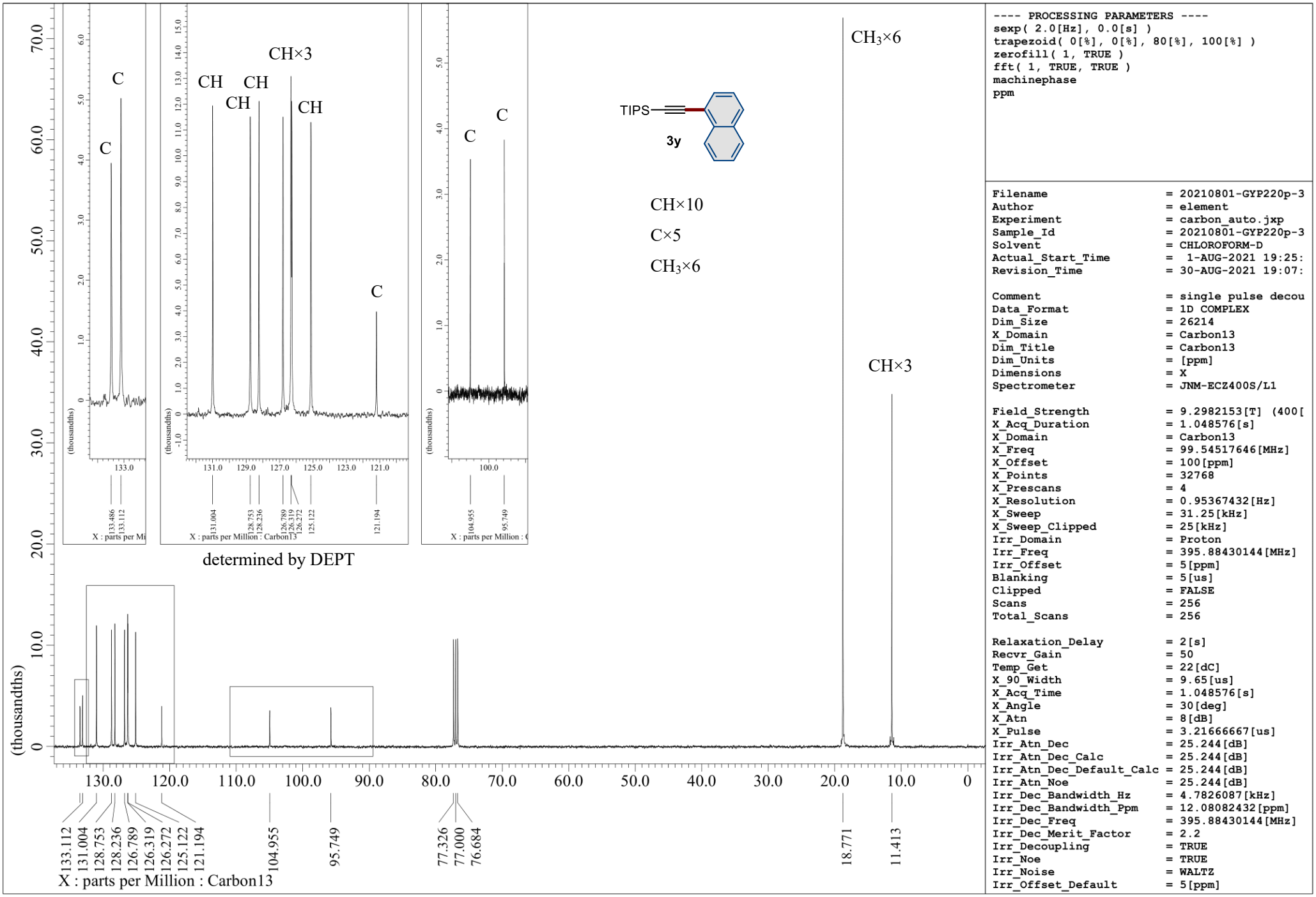

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

Filename	= 20210801-GYP047p-3
Author	= element
Experiment	= carbon_auto.jxp
Sample_Id	= 20210801-GYP047p-3
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 1-AUG-2021 18:46:
Revision_Time	= 30-AUG-2021 19:00:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ400S/L1
Field_Strength	= 9.2982153[T] (400[
X_Acq_Duration	= 1.048576[s]
X_Domain	= Carbon13
X_Freq	= 99.54517646[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.95367432[Hz]
X_Sweep	= 31.25[kHz]
X_Sweep_Clipped	= 25[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 5[us]
Clipped	= FALSE
Scans	= 256
Total_Scans	= 256
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 22[dC]
X_90_Width	= 9.65[us]
X_Acq_Time	= 1.048576[s]
X_Angle	= 30[deg]
X_Atn	= 8[dB]
X_Pulse	= 3.21666667[us]
Irr_Atn_Dec	= 25.244[dB]
Irr_Atn_Dec_Calc	= 25.244[dB]
Irr_Atn_Dec_Default_Calc	= 25.244[dB]
Irr_Atn_Noe	= 25.244[dB]
Irr_Dec_Bandwidth_Hz	= 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.08082432[ppm]
Irr_Dec_Freq	= 395.88430144[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]



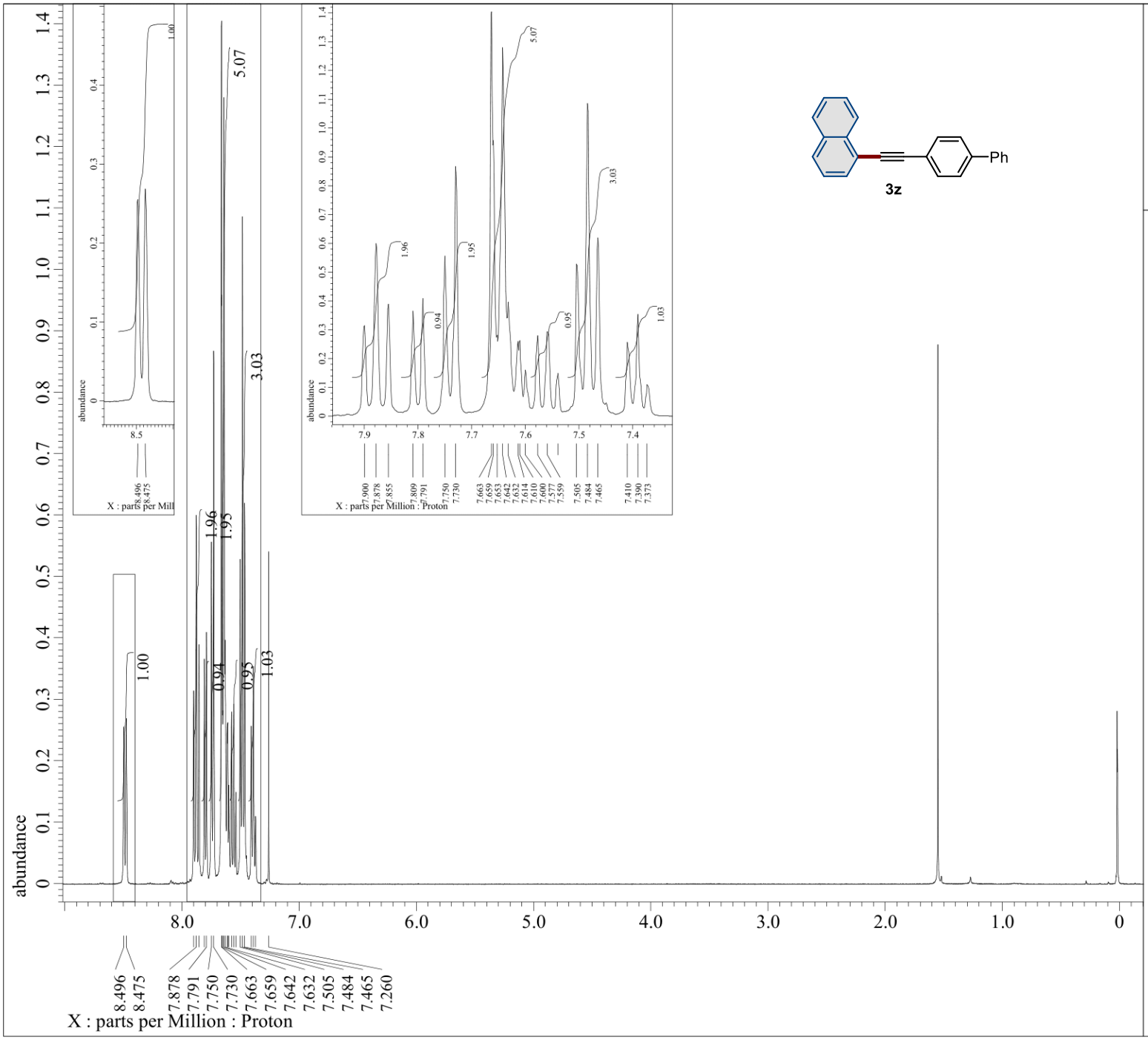

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

Filename	= 20210801-GYP220p-3x_P
Author	= element
Experiment	= proton_auto.jxp
Sample_Id	= 20210801-GYP220p-3x
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 1-AUG-2021 19:23:48
Revision_Time	= 30-AUG-2021 19:05:01
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ400S/L1
Field_Strength	= 9.2982153[T] (400[MHz
X_Acq_Duration	= 2.20725248[s]
X_Domain	= Proton
X_Freq	= 395.88430144[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45305193[Hz]
X_Sweep	= 7.42280285[kHz]
X_Sweep_Clipped	= 5.93824228[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 395.88430144[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 36
Temp_Get	= 21.7[dC]
X_90_Width	= 9.3[us]
X_Acq_Time	= 2.20725248[s]
X_Angle	= 45[deg]
X_Atn	= 3.4[dB]
X_Pulse	= 4.65[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 500
Dante_Presat	= FALSE
Decimation_Rate	= 0
Experiment_Path	= C:\Program Files\JEOL
Initial_Wait	= 1[s]
Phase	= {0, 90, 270, 180, 180
Presat_Time	= 5[s]




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

Filename	= 20210801-GYP220p-3
Author	= element
Experiment	= carbon_auto.jxp
Sample_Id	= 20210801-GYP220p-3
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 1-AUG-2021 19:25:
Revision_Time	= 30-AUG-2021 19:07:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ400S/L1
Field_Strength	= 9.2982153[T] (400[
X_Acq_Duration	= 1.048576[s]
X_Domain	= Carbon13
X_Freq	= 99.54517646[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.95367432[Hz]
X_Sweep	= 31.25[kHz]
X_Sweep_Clipped	= 25[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 5[us]
Clipped	= FALSE
Scans	= 256
Total_Scans	= 256
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 22[dC]
X_90_Width	= 9.65[us]
X_Acq_Time	= 1.048576[s]
X_Angle	= 30[deg]
X_Atn	= 8[dB]
X_Pulse	= 3.21666667[us]
Irr_Atn_Dec	= 25.244[dB]
Irr_Atn_Dec_Calc	= 25.244[dB]
Irr_Atn_Dec_Default_Calc	= 25.244[dB]
Irr_Atn_Noe	= 25.244[dB]
Irr_Dec_Bandwidth_Hz	= 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.08082432[ppm]
Irr_Dec_Freq	= 395.88430144[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]

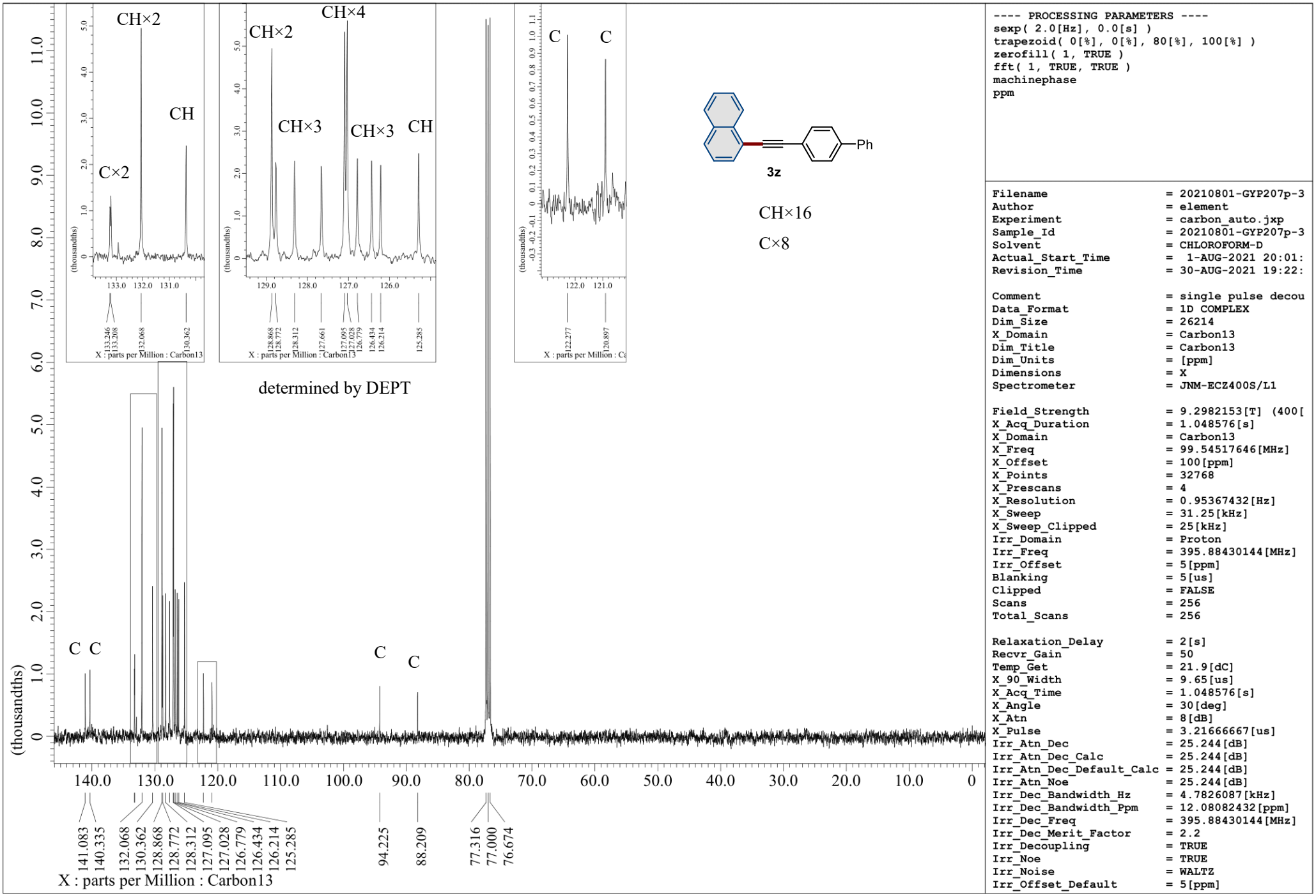


3z

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

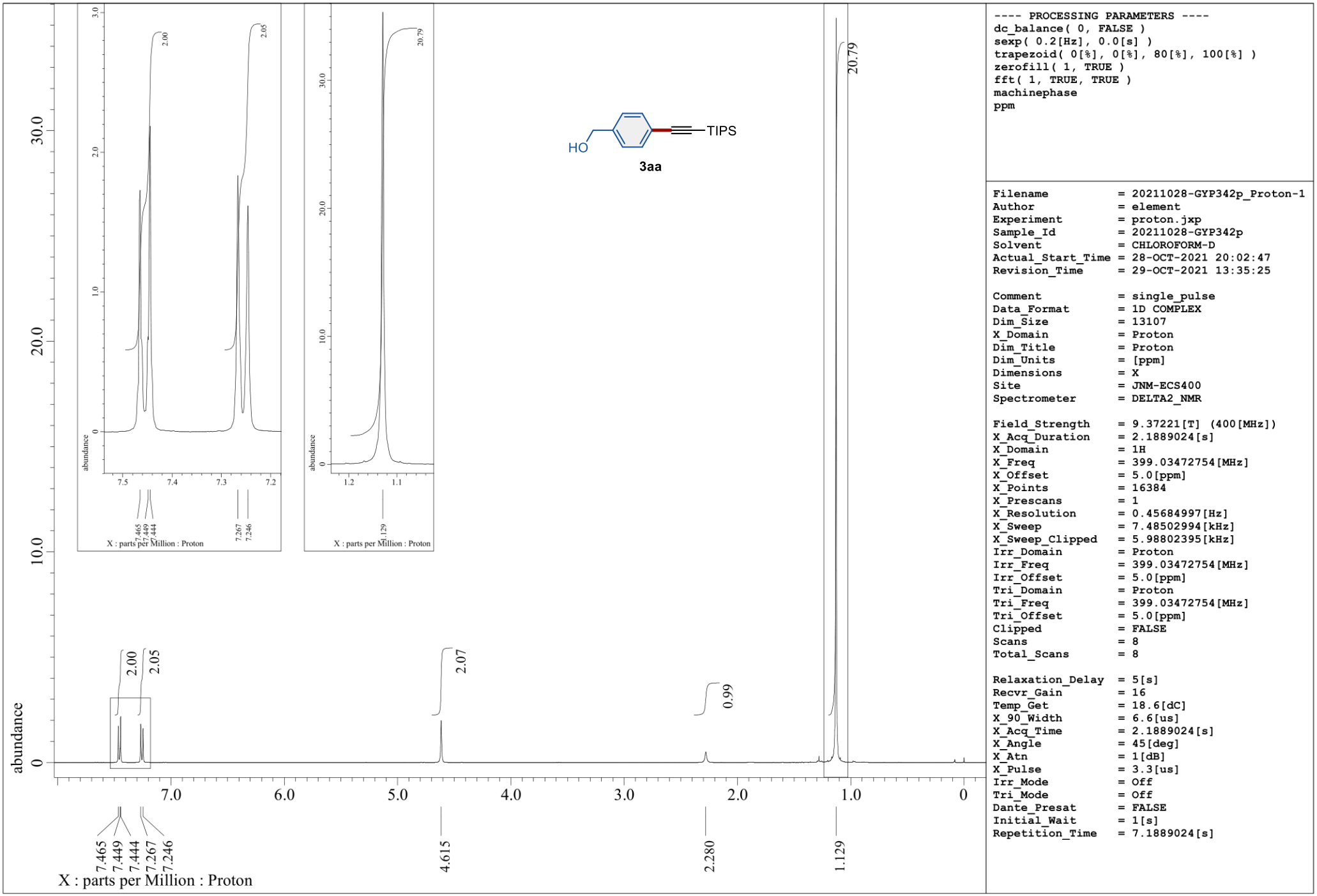
Derived from: 20210801-GYP207p-3y_Proton-1-1.
```

Filename	= 20210801-GYP207p-3y_P
Author	= element
Experiment	= proton_auto.jxp
Sample_Id	= 20210801-GYP207p-3y
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 1-AUG-2021 20:00:36
Revision_Time	= 30-AUG-2021 19:18:47
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ400S/L1
Field_Strength	= 9.2982153[T] (400[MHz
X_Acq_Duration	= 2.20725248[s]
X_Domain	= Proton
X_Freq	= 395.88430144[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45305193[Hz]
X_Sweep	= 7.42280285[kHz]
X_Sweep_Clipped	= 5.93824228[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 395.88430144[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= TRUE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 56
Temp_Get	= 21.7[dC]
X_90_Width	= 9.3[us]
X_Acq_Time	= 2.20725248[s]
X_Angle	= 45[deg]
X_Atn	= 3.4[dB]
X_Pulse	= 4.65[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 500
Dante_Presat	= FALSE
Decimation_Rate	= 0
Experiment_Path	= C:\Program Files\JEOL
Initial_Wait	= 1[s]
Phase	= {0, 90, 270, 180, 180
Presat_Time	= 5[s]




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

Filename	= 20210801-GYP207p-3
Author	= element
Experiment	= carbon_auto.jxp
Sample_Id	= 20210801-GYP207p-3
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 1-AUG-2021 20:01:
Revision_Time	= 30-AUG-2021 19:22:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ400S/L1
Field_Strength	= 9.2982153[T] (400[
X_Acq_Duration	= 1.048576[s]
X_Domain	= Carbon13
X_Freq	= 99.54517646[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.95367432[Hz]
X_Sweep	= 31.25[kHz]
X_Sweep_Clipped	= 25[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 5[us]
Clipped	= FALSE
Scans	= 256
Total_Scans	= 256
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 21.9[dC]
X_90_Width	= 9.65[us]
X_Acq_Time	= 1.048576[s]
X_Angle	= 30[deg]
X_Atn	= 8[dB]
X_Pulse	= 3.21666667[us]
Irr_Atn_Dec	= 25.244[dB]
Irr_Atn_Dec_Calc	= 25.244[dB]
Irr_Atn_Dec_Default_Calc	= 25.244[dB]
Irr_Atn_Noe	= 25.244[dB]
Irr_Dec_Bandwidth_Hz	= 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.08082432[ppm]
Irr_Dec_Freq	= 395.88430144[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]



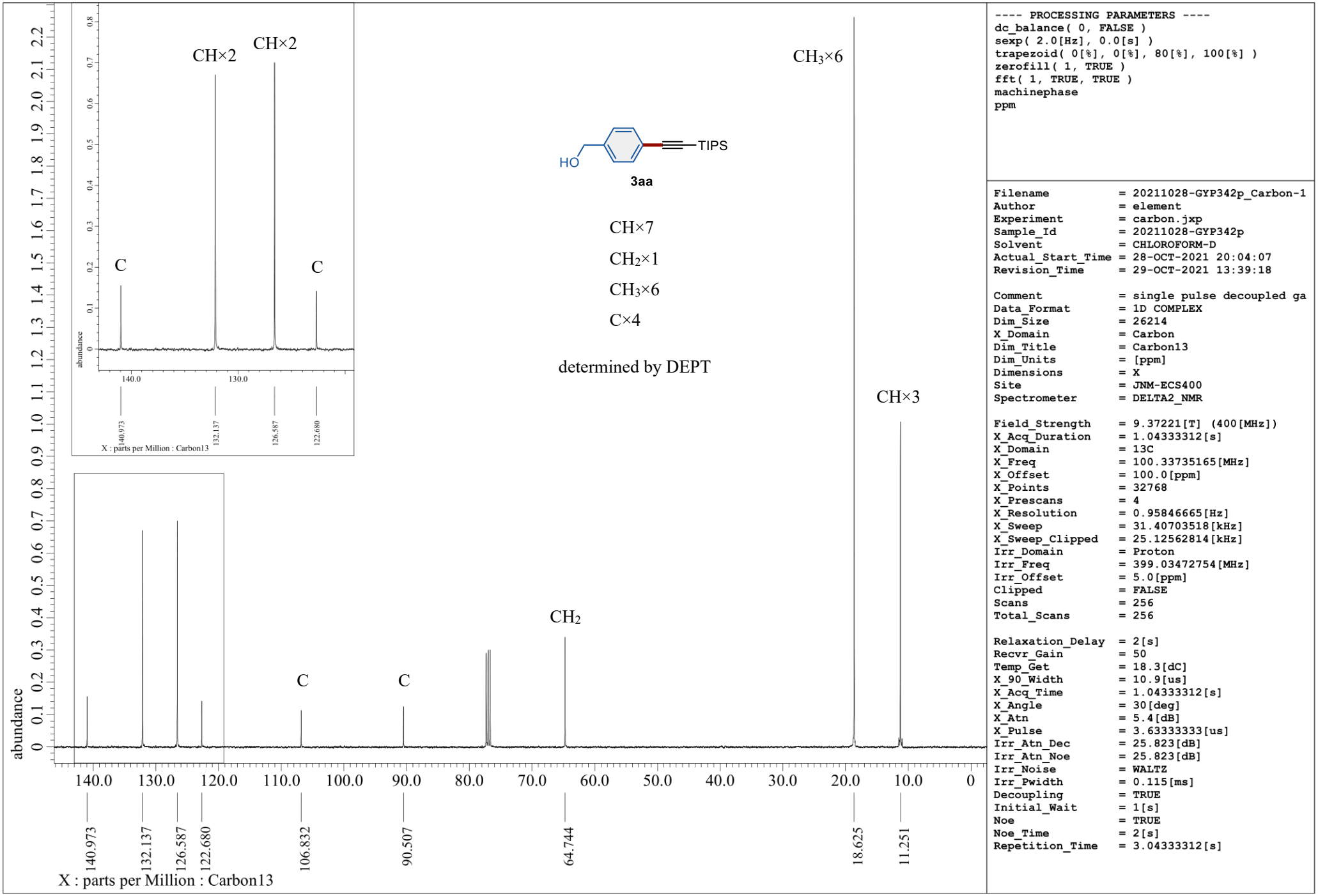

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename           = 20211028-GYP342p_Proton-1
Author             = element
Experiment         = proton.jxp
Sample_Id          = 20211028-GYP342p
Solvent            = CHLOROFORM-D
Actual_Start_Time  = 28-OCT-2021 20:02:47
Revision_Time      = 29-OCT-2021 13:35:25

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         = 16
Temp_Get           = 18.6[dC]
X_90_Width         = 6.6[us]
X_Acq_Time         = 2.1889024[s]
X_Angle            = 45[deg]
X_Atn              = 1[dB]
X_Pulse            = 3.3[us]
Irr_Mode           = Off
Tri_Mode           = Off
Dante_Presat       = FALSE
Initial_Wait       = 1[s]
Repetition_Time    = 7.1889024[s]
```



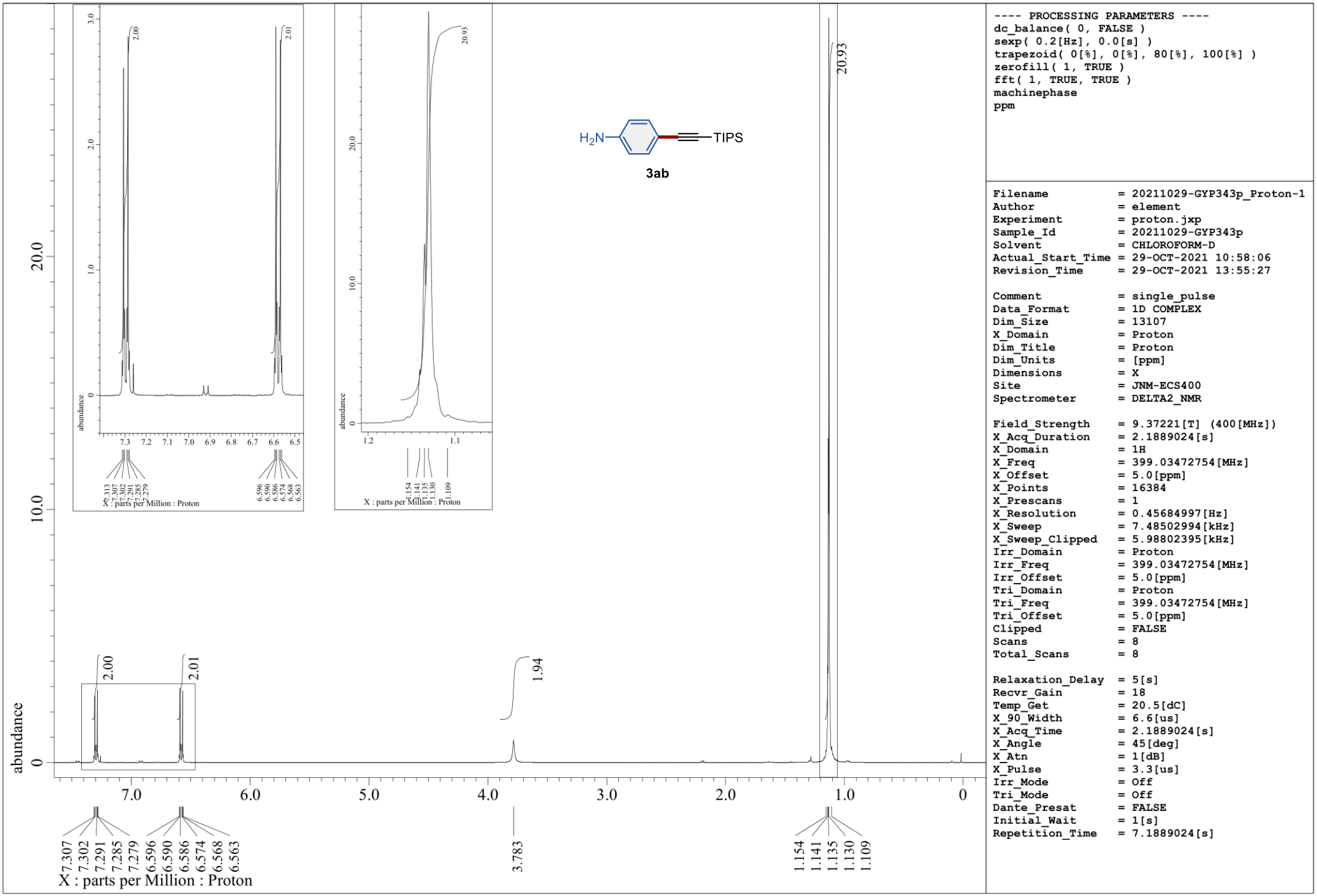

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

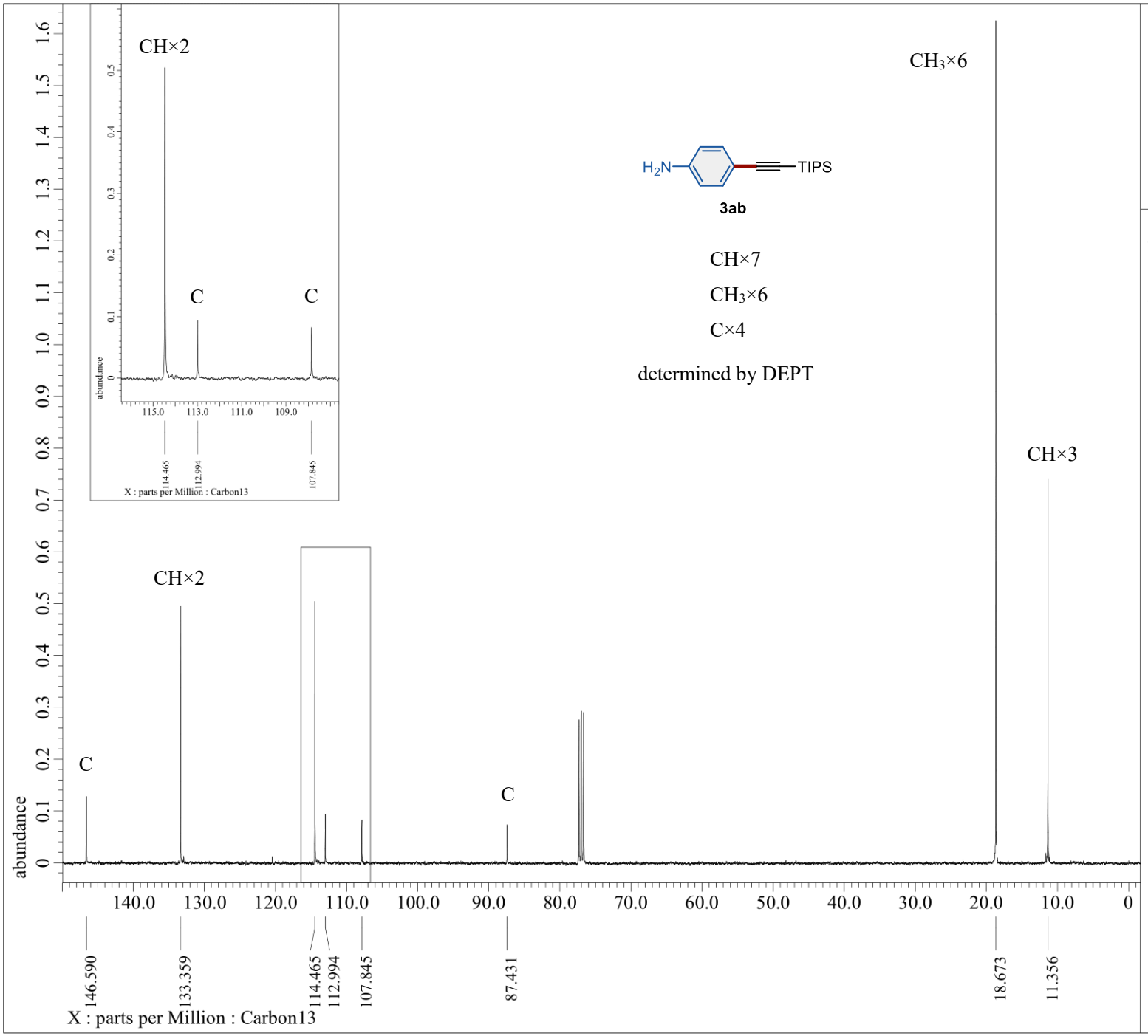
```
Filename            = 20211028-GYP342p_Carbon-1
Author              = element
Experiment          = carbon.jxp
Sample_Id           = 20211028-GYP342p
Solvent             = CHLOROFORM-D
Actual_Start_Time   = 28-OCT-2021 20:04:07
Revision_Time       = 29-OCT-2021 13:39:18

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

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

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]
```


2.00
2.01
20.93
1.94
abundance
7.307
7.302
7.291
7.285
7.279
6.596
6.590
6.586
6.574
6.568
6.563
3.783
1.154
1.141
1.135
1.130
1.109
X : parts per Million : Proton
H2N
TIPS
3ab
---- 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
Filename = 20211029-GYP343p_Proton-1
Author = element
Experiment = proton.jxp
Sample_Id = 20211029-GYP343p
Solvent = CHLOROFORM-D
Actual_Start_Time = 29-OCT-2021 10:58:06
Revision_Time = 29-OCT-2021 13:55:27
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 = 18
Temp_Get = 20.5[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]



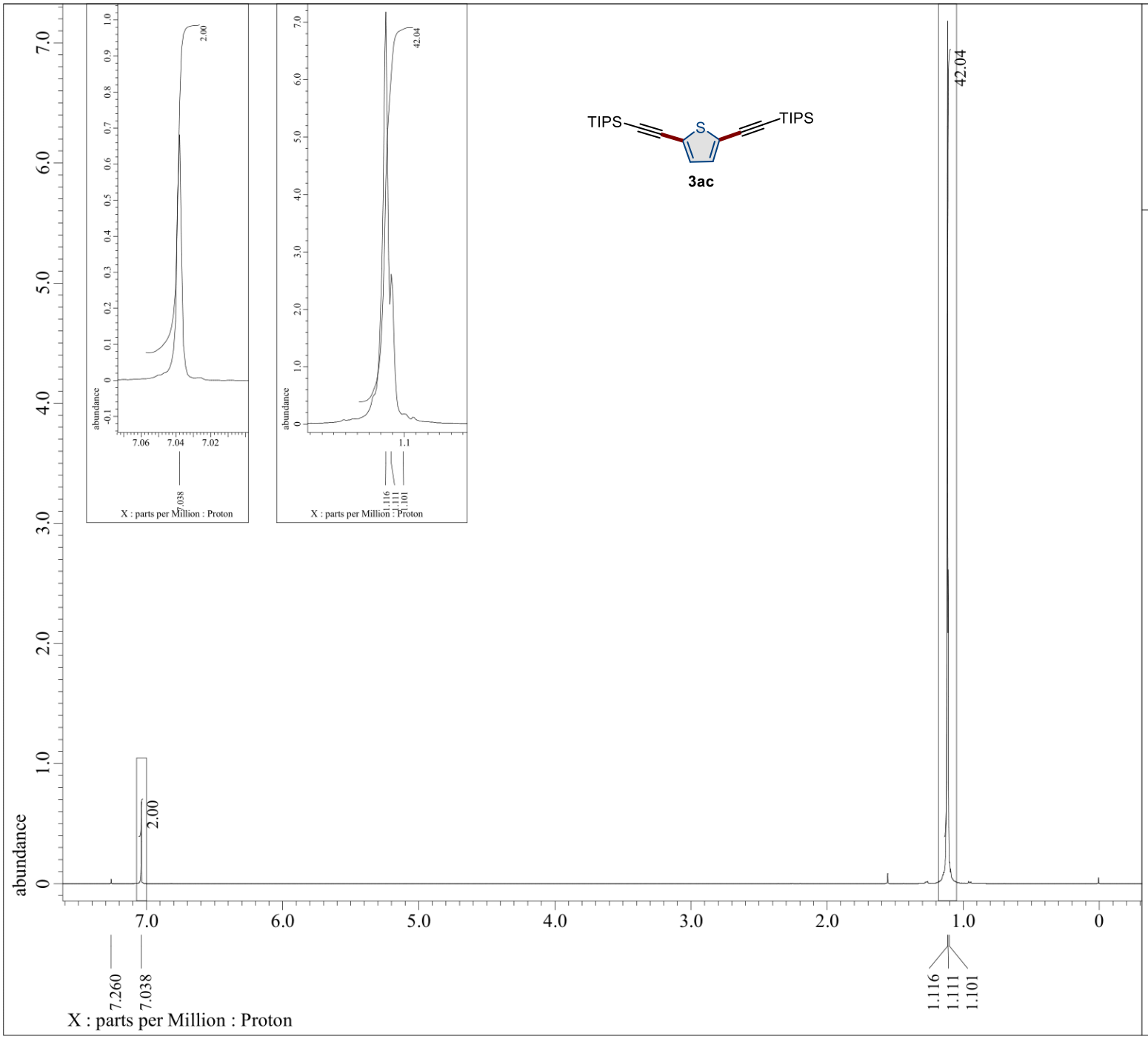

```
---- PROCESSING PARAMETERS ----
dc_balance( 0, FALSE )
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename            = 20211029-GYP343p_Carbon-1
Author              = element
Experiment          = carbon.jxp
Sample_Id           = 20211029-GYP343p
Solvent             = CHLOROFORM-D
Actual_Start_Time   = 29-OCT-2021 10:59:26
Revision_Time       = 29-OCT-2021 13:57:05

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

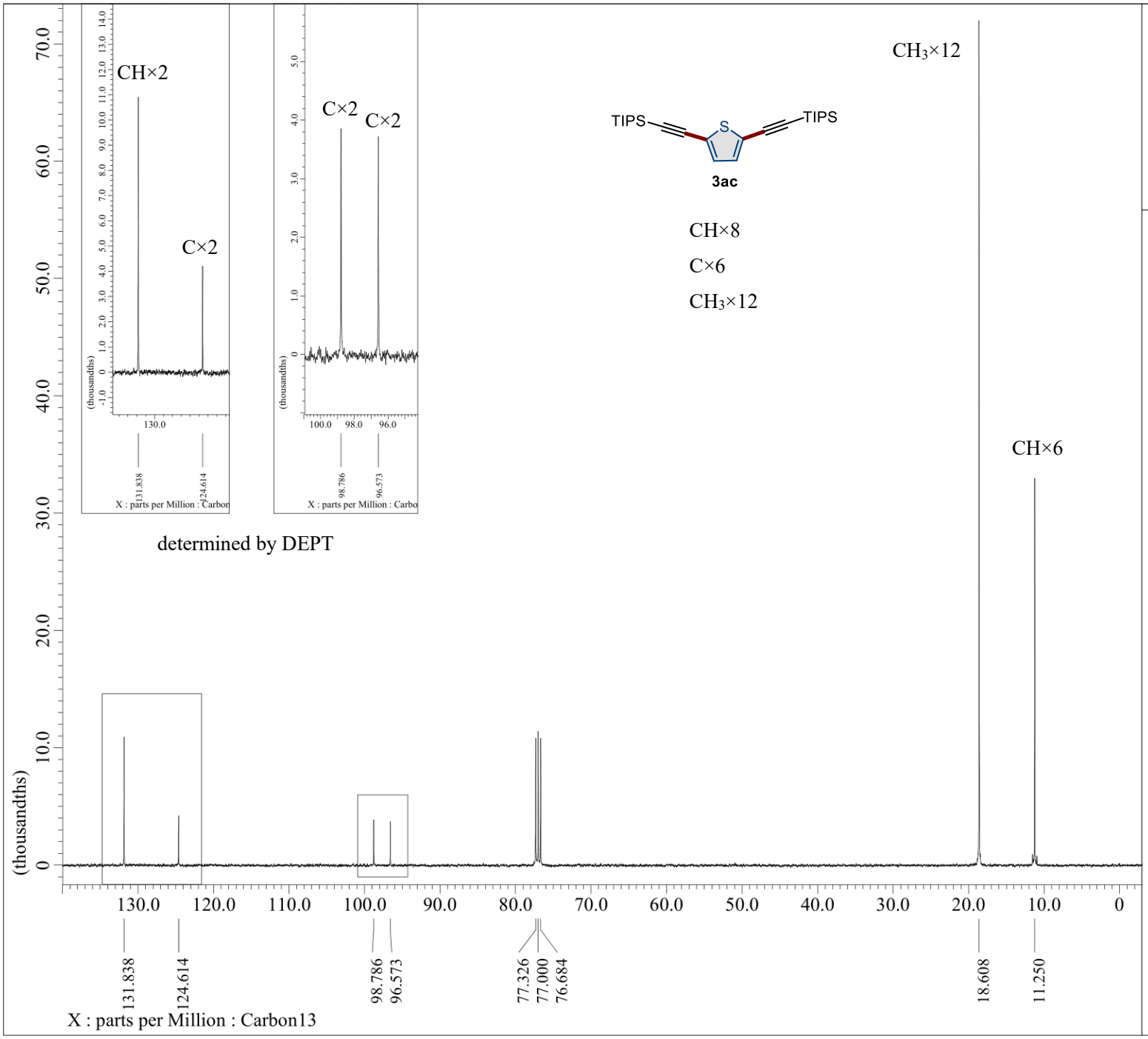
Field_Strength      = 9.37221[T] (400[MHz])
X_Acq_Duration      = 1.04333312[s]
X_Domain            = 13C
X_Freq              = 100.33735165[MHz]
X_Offset            = 100.0[ppm]
X_Points            = 32768
X_Prescans          = 4
X_Resolution        = 0.95846665[Hz]
X_Sweep             = 31.40703518[kHz]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

Relaxation_Delay    = 2[s]
Recvr_Gain          = 50
Temp_Get            = 20.7[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]
```



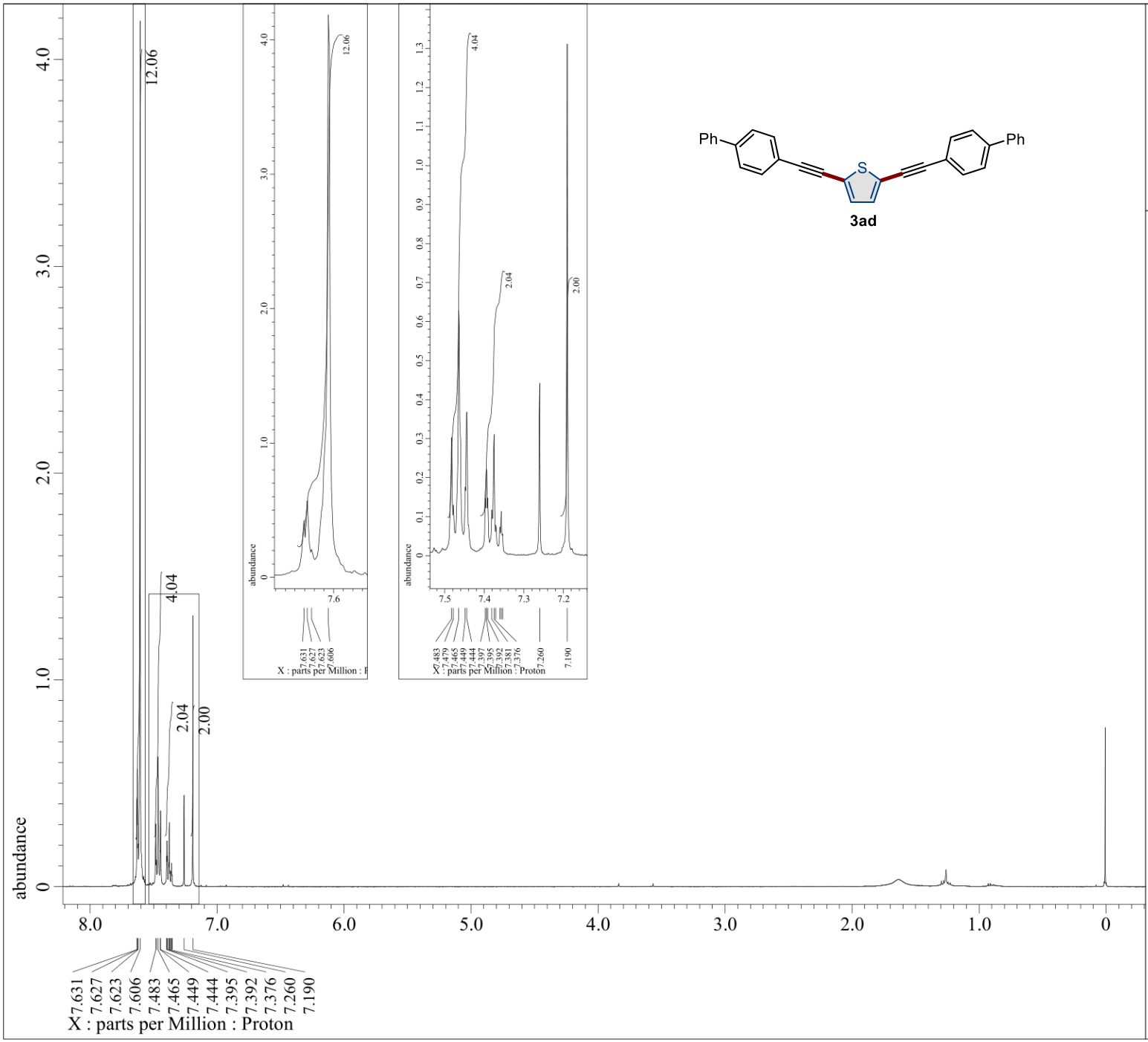

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

Filename	= 20210801-GYP213p-3aa_
Author	= element
Experiment	= proton_auto.jxp
Sample_Id	= 20210801-GYP213p-3aa
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 1-AUG-2021 20:36:37
Revision_Time	= 30-AUG-2021 19:25:40
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ400S/L1
Field_Strength	= 9.2982153[T] (400[MHz
X_Acq_Duration	= 2.20725248[s]
X_Domain	= Proton
X_Freq	= 395.88430144[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45305193[Hz]
X_Sweep	= 7.42280285[kHz]
X_Sweep_Clipped	= 5.93824228[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 395.88430144[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 36
Temp_Get	= 21.6[dC]
X_90_Width	= 9.3[us]
X_Acq_Time	= 2.20725248[s]
X_Angle	= 45[deg]
X_Atn	= 3.4[dB]
X_Pulse	= 4.65[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 500
Dante_Presat	= FALSE
Decimation_Rate	= 0
Experiment_Path	= C:\Program Files\JEOL
Initial_Wait	= 1[s]
Phase	= {0, 90, 270, 180, 180
Presat_Time	= 5[s]




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

Filename	= 20210801-GYP213p-3
Author	= element
Experiment	= carbon_auto.jxp
Sample_Id	= 20210801-GYP213p-3
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 1-AUG-2021 20:37:
Revision_Time	= 21-AUG-2021 10:31:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ400S/L1
Field_Strength	= 9.2982153[T] (400[
X_Acq_Duration	= 1.048576[s]
X_Domain	= Carbon13
X_Freq	= 99.54517646[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.95367432[Hz]
X_Sweep	= 31.25[kHz]
X_Sweep_Clipped	= 25[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 5[us]
Clipped	= FALSE
Scans	= 256
Total_Scans	= 256
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 21.9[dC]
X_90_Width	= 9.65[us]
X_Acq_Time	= 1.048576[s]
X_Angle	= 30[deg]
X_Atn	= 8[dB]
X_Pulse	= 3.21666667[us]
Irr_Atn_Dec	= 25.244[dB]
Irr_Atn_Dec_Calc	= 25.244[dB]
Irr_Atn_Dec_Default_Calc	= 25.244[dB]
Irr_Atn_Noe	= 25.244[dB]
Irr_Dec_Bandwidth_Hz	= 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.08082432[ppm]
Irr_Dec_Freq	= 395.88430144[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]



3ad

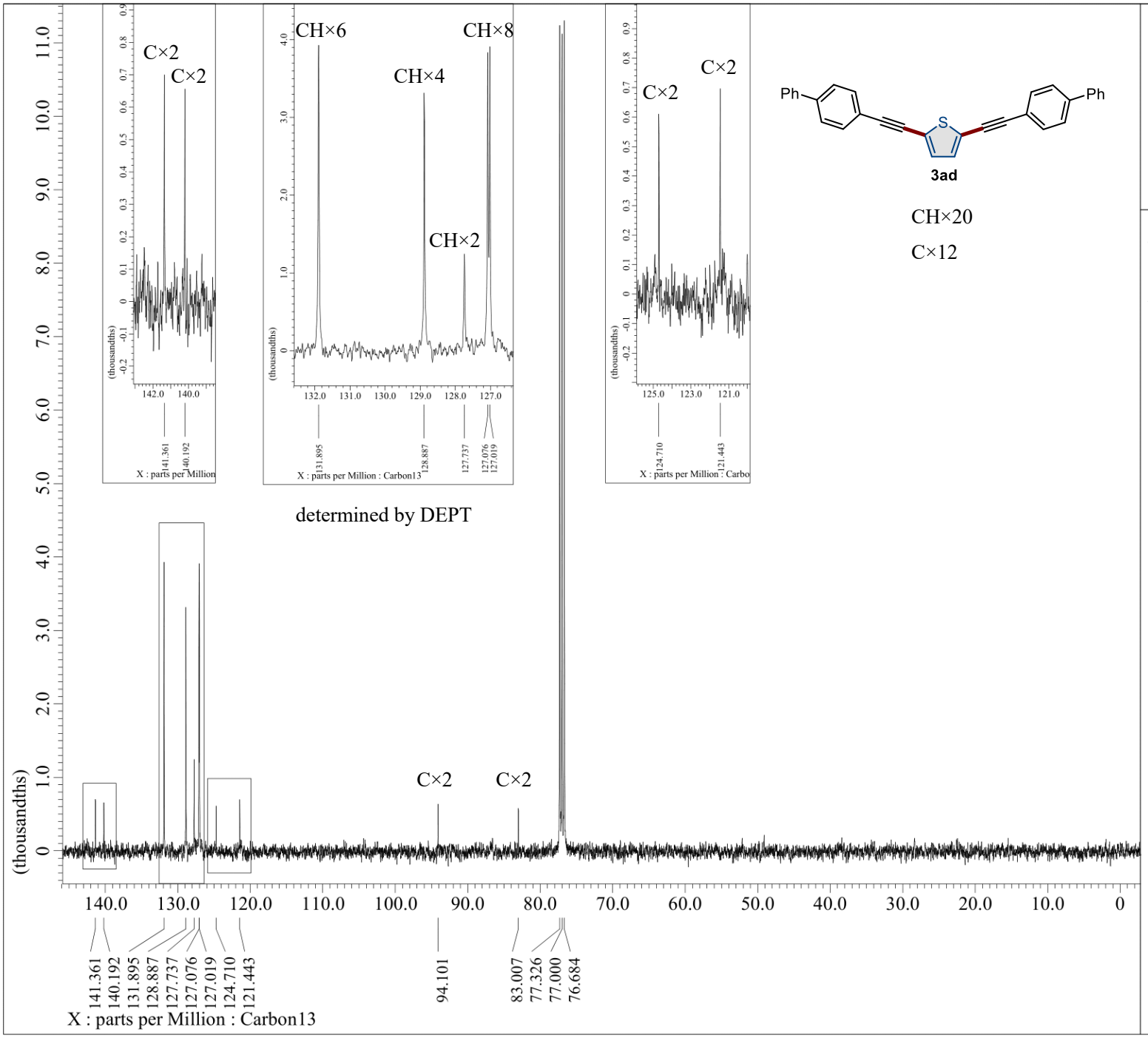
```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename                = 20210802-GYP218p-3ab_
Author                  = element
Experiment              = proton_auto.jxp
Sample_Id               = 20210802-GYP218p-3ab
Solvent                 = CHLOROFORM-D
Actual_Start_Time       =  2-AUG-2021 18:23:08
Revision_Time           = 30-AUG-2021 19:30:02

Comment                 = single_pulse
Data_Format             = 1D COMPLEX
Dim_Size                = 13107
X_Domain                = Proton
Dim_Title               = Proton
Dim_Units               = [ppm]
Dimensions              = X
Spectrometer            = JNM-ECZ400S/L1

Field_Strength          = 9.2982153[T] (400[MHz
X_Acq_Duration          = 2.20725248[s]
X_Domain                = Proton
X_Freq                  = 395.88430144[MHz]
X_Offset                = 5[ppm]
X_Points                = 16384
X_Prescans              = 1
X_Resolution            = 0.45305193[Hz]
X_Sweep                 = 7.42280285[kHz]
X_Sweep_Clipped         = 5.93824228[kHz]
Irr_Domain              = Proton
Irr_Freq                = 395.88430144[MHz]
Irr_Offset              = 5[ppm]
Tri_Domain              = Proton
Tri_Freq                = 395.88430144[MHz]
Tri_Offset              = 5[ppm]
Blanking                = 2[us]
Clipped                 = TRUE
Scans                   = 8
Total_Scans             = 8

Relaxation_Delay        = 5[s]
Recvr_Gain              = 56
Temp_Get                = 21.9[dC]
X_90_Width              = 9.3[us]
X_Acq_Time              = 2.20725248[s]
X_Angle                 = 45[deg]
X_Atn                   = 3.4[dB]
X_Pulse                 = 4.65[us]
Irr_Mode                = Off
Tri_Mode                = Off
Dante_Loop              = 500
Dante_Presat            = FALSE
Decimation_Rate         = 0
Experiment_Path         = C:\Program Files\JEOL
Initial_Wait            = 1[s]
Phase                   = {0, 90, 270, 180, 180
Presat_Time             = 5[s]
```



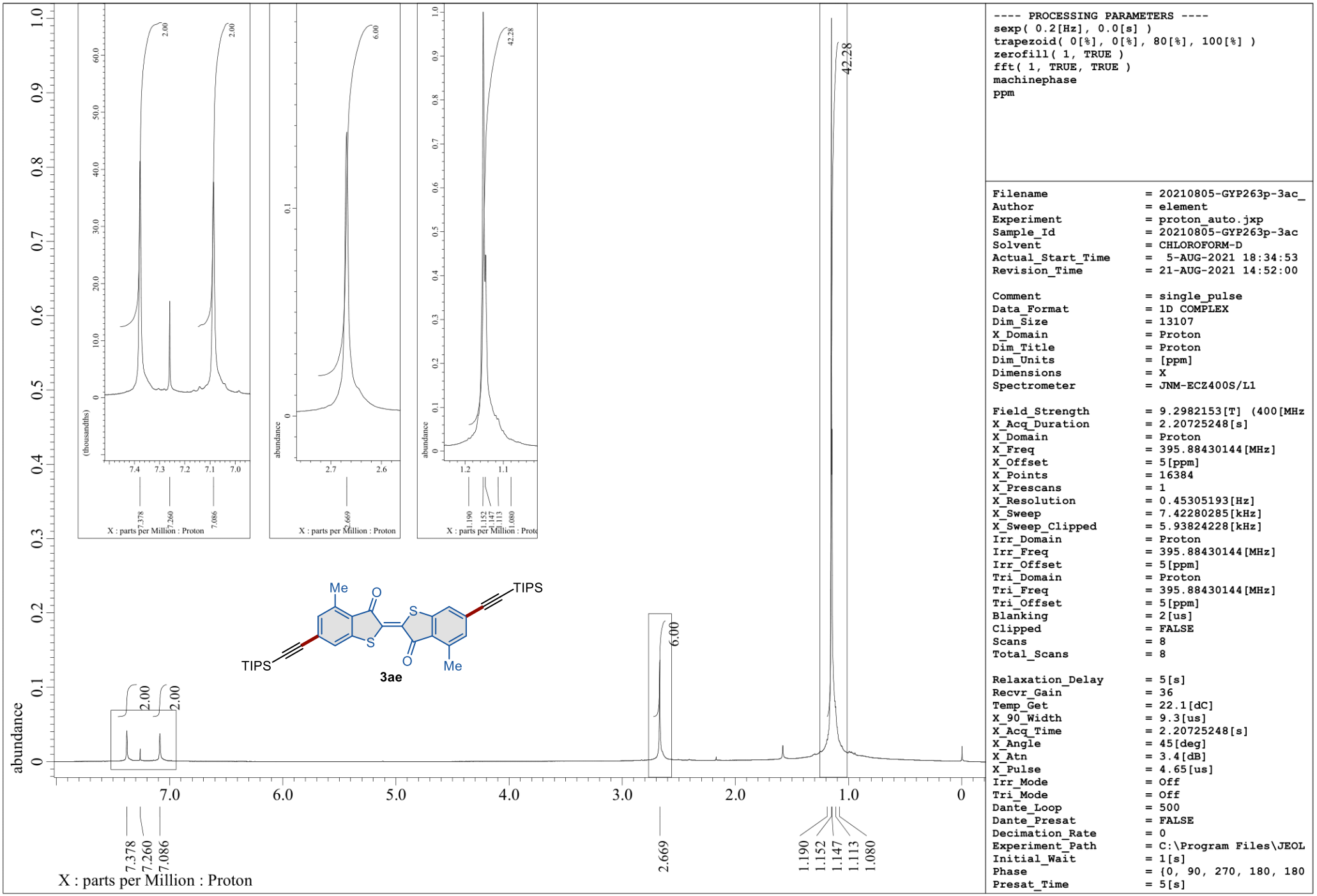
3ad

CH×20

C×12

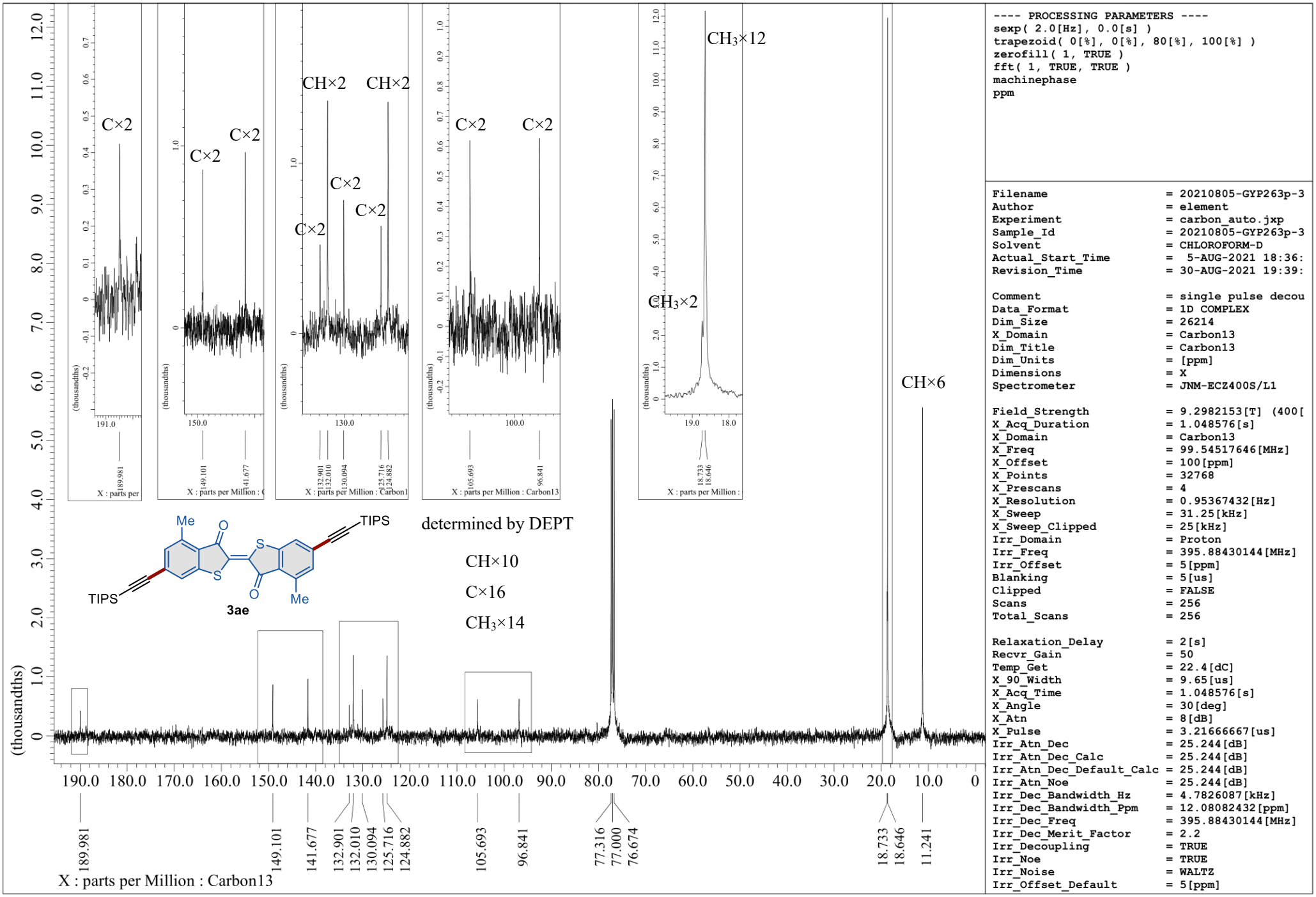
```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

Filename	= 20210802-GYP218p-3
Author	= element
Experiment	= carbon_auto.jxp
Sample_Id	= 20210802-GYP218p-3
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 2-AUG-2021 18:24:
Revision_Time	= 30-AUG-2021 19:32:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ400S/L1
Field_Strength	= 9.2982153[T] (400[
X_Acq_Duration	= 1.048576[s]
X_Domain	= Carbon13
X_Freq	= 99.54517646[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.95367432[Hz]
X_Sweep	= 31.25[kHz]
X_Sweep_Clipped	= 25[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 5[us]
Clipped	= FALSE
Scans	= 256
Total_Scans	= 256
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 22.2[dC]
X_90_Width	= 9.65[us]
X_Acq_Time	= 1.048576[s]
X_Angle	= 30[deg]
X_Atn	= 8[dB]
X_Pulse	= 3.21666667[us]
Irr_Atn_Dec	= 25.244[dB]
Irr_Atn_Dec_Calc	= 25.244[dB]
Irr_Atn_Dec_Default_Calc	= 25.244[dB]
Irr_Atn_Noe	= 25.244[dB]
Irr_Dec_Bandwidth_Hz	= 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.08082432[ppm]
Irr_Dec_Freq	= 395.88430144[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]



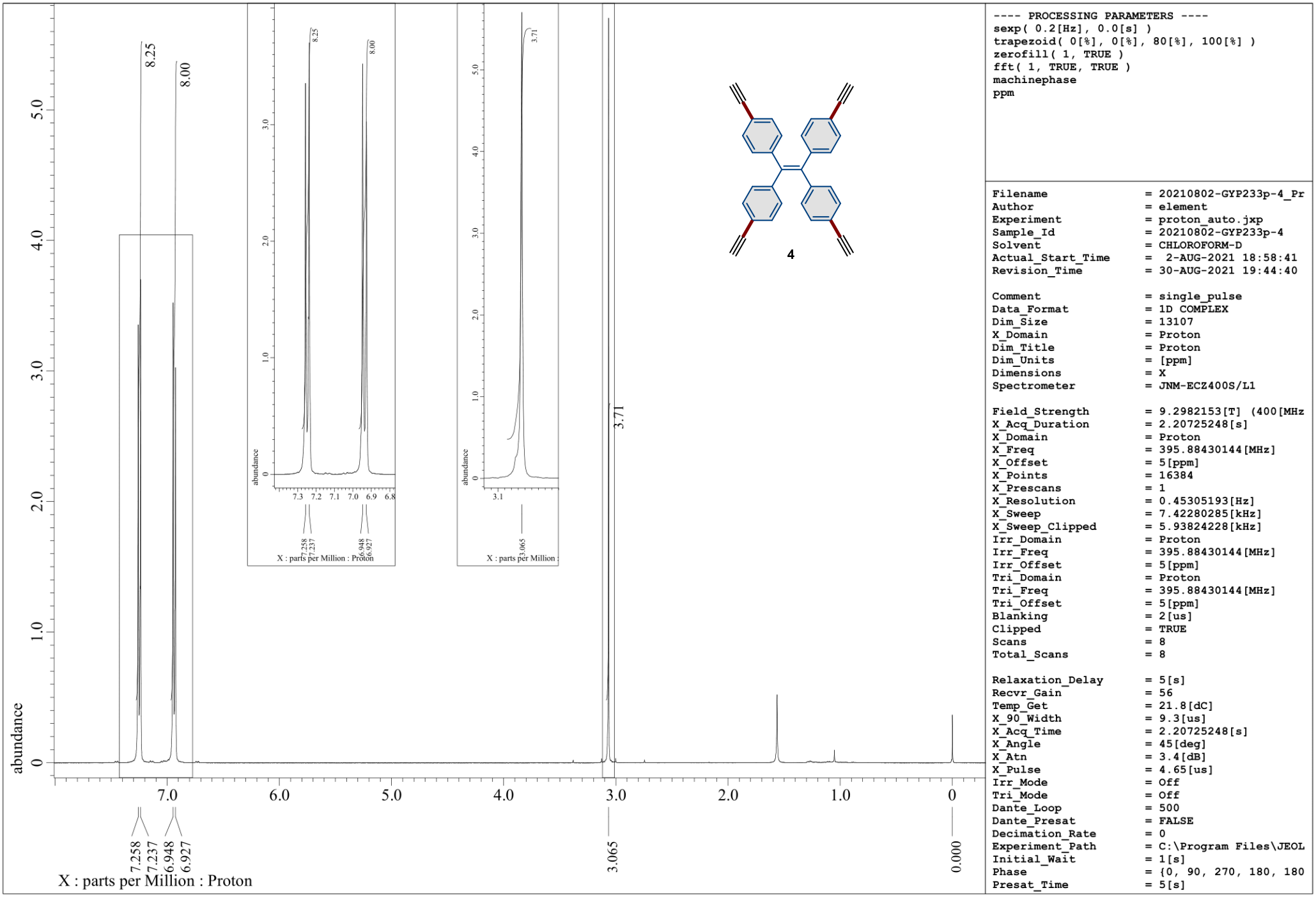

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

Filename	= 20210805-GYP263p-3ac_
Author	= element
Experiment	= proton_auto.jxp
Sample_Id	= 20210805-GYP263p-3ac
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 5-AUG-2021 18:34:53
Revision_Time	= 21-AUG-2021 14:52:00
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ400S/L1
Field_Strength	= 9.2982153[T] (400[MHz
X_Acq_Duration	= 2.20725248[s]
X_Domain	= Proton
X_Freq	= 395.88430144[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45305193[Hz]
X_Sweep	= 7.42280285[kHz]
X_Sweep_Clipped	= 5.93824228[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 395.88430144[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 36
Temp_Get	= 22.1[dC]
X_90_Width	= 9.3[us]
X_Acq_Time	= 2.20725248[s]
X_Angle	= 45[deg]
X_Atn	= 3.4[dB]
X_Pulse	= 4.65[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 500
Dante_Presat	= FALSE
Decimation_Rate	= 0
Experiment_Path	= C:\Program Files\JEOL
Initial_Wait	= 1[s]
Phase	= {0, 90, 270, 180, 180
Presat_Time	= 5[s]



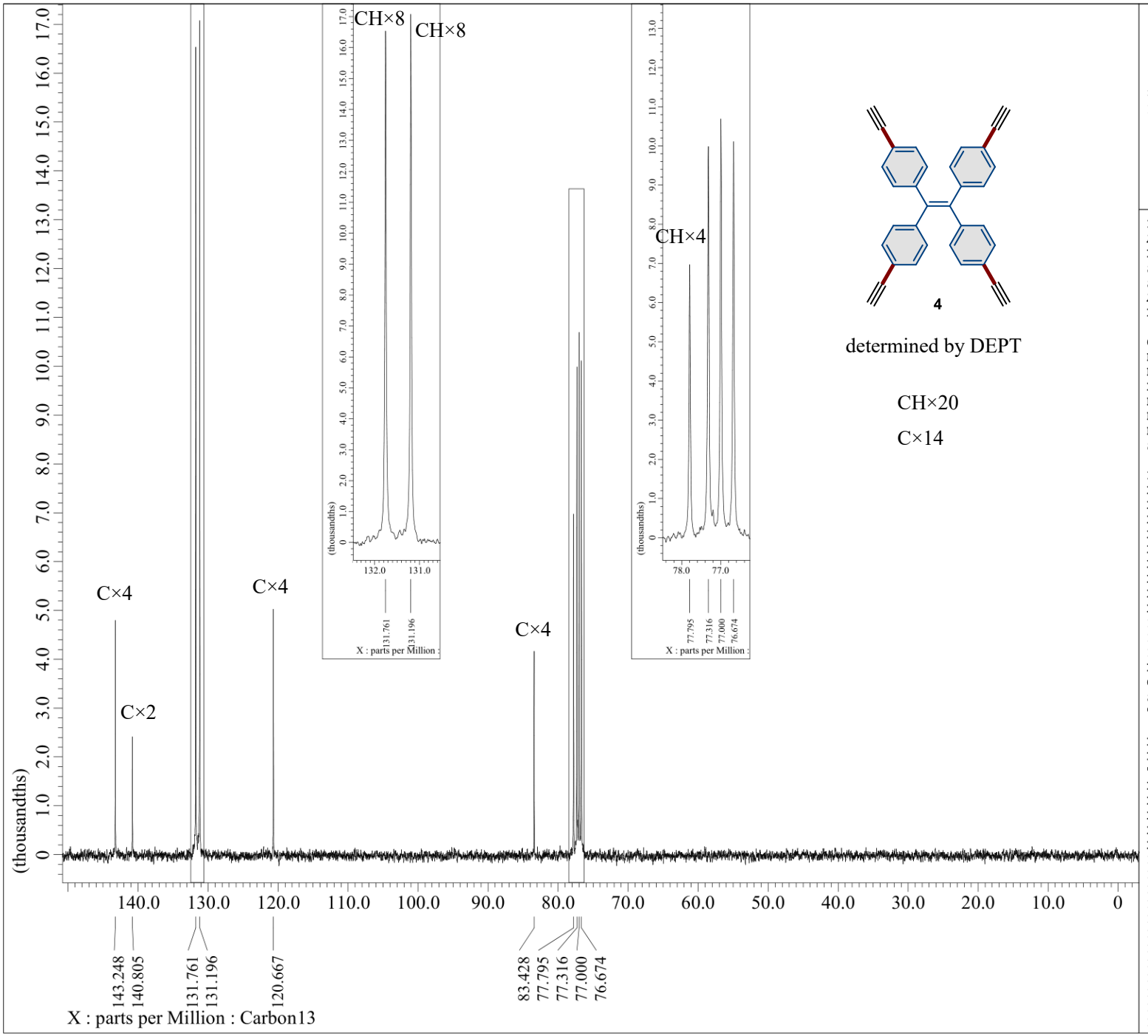

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

Filename	= 20210805-GYP263p-3
Author	= element
Experiment	= carbon_auto.jxp
Sample_Id	= 20210805-GYP263p-3
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 5-AUG-2021 18:36:
Revision_Time	= 30-AUG-2021 19:39:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ400S/L1
Field_Strength	= 9.2982153[T] (400[
X_Acq_Duration	= 1.048576[s]
X_Domain	= Carbon13
X_Freq	= 99.54517646[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.95367432[Hz]
X_Sweep	= 31.25[kHz]
X_Sweep_Clipped	= 25[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 5[us]
Clipped	= FALSE
Scans	= 256
Total_Scans	= 256
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 22.4[dC]
X_90_Width	= 9.65[us]
X_Acq_Time	= 1.048576[s]
X_Angle	= 30[deg]
X_Atn	= 8[dB]
X_Pulse	= 3.21666667[us]
Irr_Atn_Dec	= 25.244[dB]
Irr_Atn_Dec_Calc	= 25.244[dB]
Irr_Atn_Dec_Default_Calc	= 25.244[dB]
Irr_Atn_Noe	= 25.244[dB]
Irr_Dec_Bandwidth_Hz	= 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.08082432[ppm]
Irr_Dec_Freq	= 395.88430144[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]




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

Filename	= 20210802-GYP233p-4_Pr
Author	= element
Experiment	= proton_auto.jxp
Sample_Id	= 20210802-GYP233p-4
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 2-AUG-2021 18:58:41
Revision_Time	= 30-AUG-2021 19:44:40
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ400S/L1
Field_Strength	= 9.2982153[T] (400[MHz
X_Acq_Duration	= 2.20725248[s]
X_Domain	= Proton
X_Freq	= 395.88430144[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45305193[Hz]
X_Sweep	= 7.42280285[kHz]
X_Sweep_Clipped	= 5.93824228[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 395.88430144[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= TRUE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 56
Temp_Get	= 21.8[dC]
X_90_Width	= 9.3[us]
X_Acq_Time	= 2.20725248[s]
X_Angle	= 45[deg]
X_Atn	= 3.4[dB]
X_Pulse	= 4.65[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 500
Dante_Presat	= FALSE
Decimation_Rate	= 0
Experiment_Path	= C:\Program Files\JEOL
Initial_Wait	= 1[s]
Phase	= {0, 90, 270, 180, 180
Presat_Time	= 5[s]



4

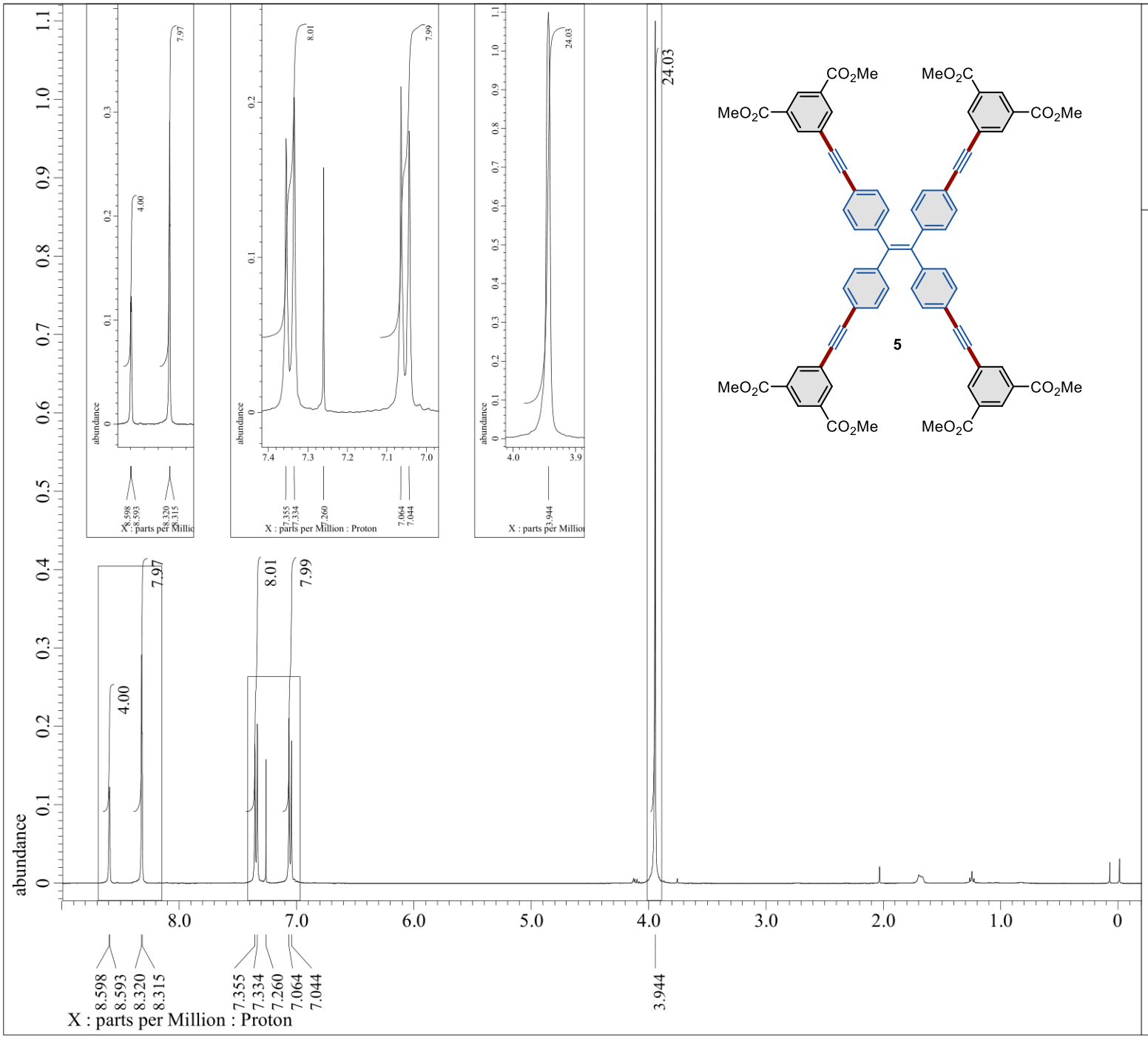
determined by DEPT

CH×20

C×14

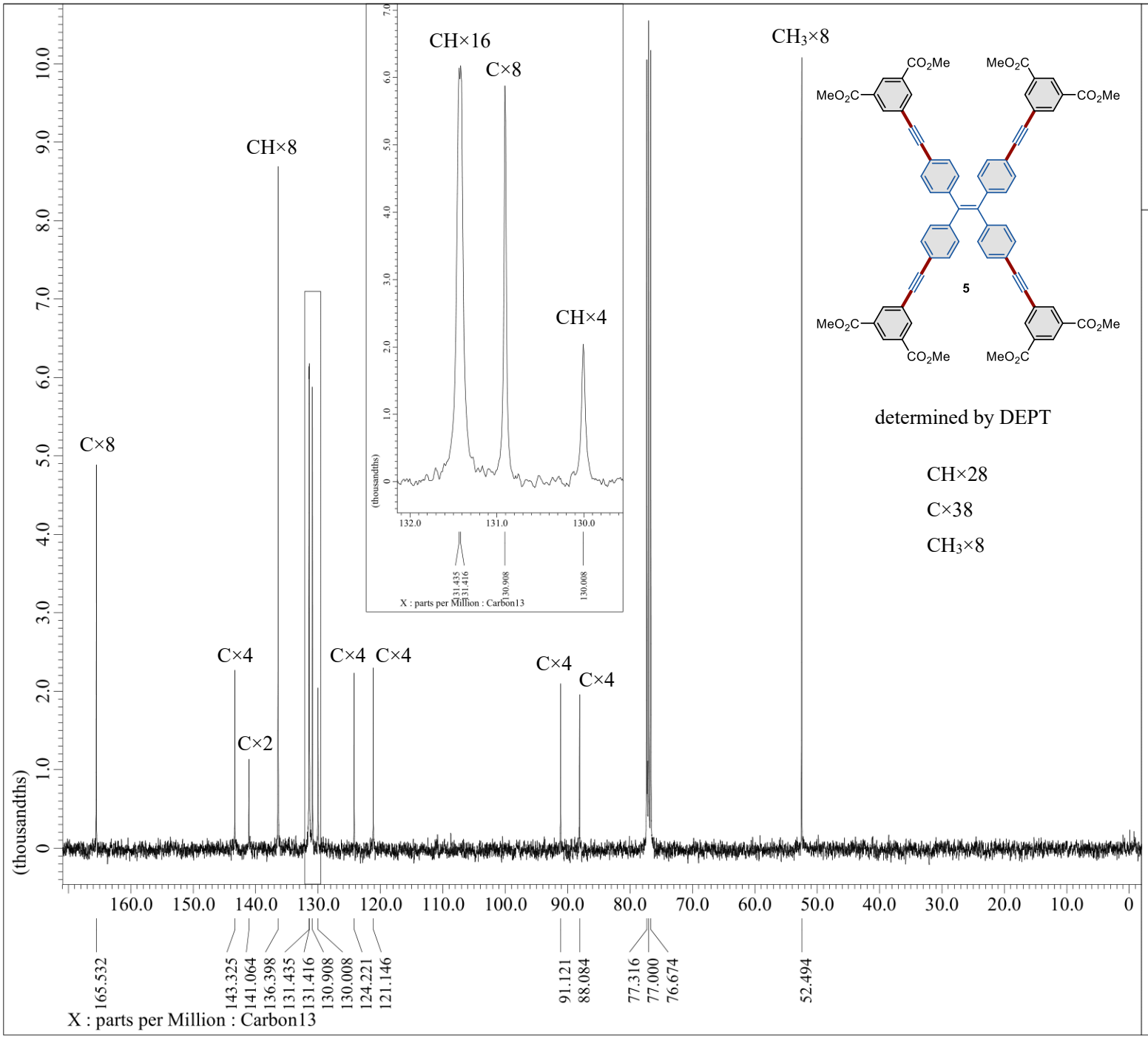
```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

Filename	= 20210802-GYP233p-4
Author	= element
Experiment	= carbon_auto.jxp
Sample_Id	= 20210802-GYP233p-4
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 2-AUG-2021 18:59:
Revision_Time	= 21-AUG-2021 15:18:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ400S/L1
Field_Strength	= 9.2982153[T] (400[
X_Acq_Duration	= 1.048576[s]
X_Domain	= Carbon13
X_Freq	= 99.54517646[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.95367432[Hz]
X_Sweep	= 31.25[kHz]
X_Sweep_Clipped	= 25[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 5[us]
Clipped	= FALSE
Scans	= 256
Total_Scans	= 256
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 22[dC]
X_90_Width	= 9.65[us]
X_Acq_Time	= 1.048576[s]
X_Angle	= 30[deg]
X_Atn	= 8[dB]
X_Pulse	= 3.21666667[us]
Irr_Atn_Dec	= 25.244[dB]
Irr_Atn_Dec_Calc	= 25.244[dB]
Irr_Atn_Dec_Default_Calc	= 25.244[dB]
Irr_Atn_Noe	= 25.244[dB]
Irr_Dec_Bandwidth_Hz	= 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.08082432[ppm]
Irr_Dec_Freq	= 395.88430144[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]




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

Filename	= 20210802-GYP257p-5_Pr
Author	= element
Experiment	= proton_auto.jxp
Sample_Id	= 20210802-GYP257p-5
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 2-AUG-2021 19:36:02
Revision_Time	= 30-AUG-2021 19:49:11
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ400S/L1
Field_Strength	= 9.2982153[T] (400[MHz
X_Acq_Duration	= 2.20725248[s]
X_Domain	= Proton
X_Freq	= 395.88430144[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45305193[Hz]
X_Sweep	= 7.42280285[kHz]
X_Sweep_Clipped	= 5.93824228[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 395.88430144[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 36
Temp_Get	= 21.7[dC]
X_90_Width	= 9.3[us]
X_Acq_Time	= 2.20725248[s]
X_Angle	= 45[deg]
X_Atn	= 3.4[dB]
X_Pulse	= 4.65[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 500
Dante_Presat	= FALSE
Decimation_Rate	= 0
Experiment_Path	= C:\Program Files\JEOL
Initial_Wait	= 1[s]
Phase	= {0, 90, 270, 180, 180
Presat_Time	= 5[s]



determined by DEPT

CH×28

C×38

CH₃×8

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

Filename	= 20210802-GYP257p-5
Author	= element
Experiment	= carbon_auto.jxp
Sample_Id	= 20210802-GYP257p-5
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 2-AUG-2021 19:37:
Revision_Time	= 30-AUG-2021 19:52:
Comment	= single pulse decou
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ400S/L1
Field_Strength	= 9.2982153[T] (400[
X_Acq_Duration	= 1.048576[s]
X_Domain	= Carbon13
X_Freq	= 99.54517646[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.95367432[Hz]
X_Sweep	= 31.25[kHz]
X_Sweep_Clipped	= 25[kHz]
Irr_Domain	= Proton
Irr_Freq	= 395.88430144[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 5[us]
Clipped	= FALSE
Scans	= 256
Total_Scans	= 256
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 22[dC]
X_90_Width	= 9.65[us]
X_Acq_Time	= 1.048576[s]
X_Angle	= 30[deg]
X_Atn	= 8[dB]
X_Pulse	= 3.21666667[us]
Irr_Atn_Dec	= 25.244[dB]
Irr_Atn_Dec_Calc	= 25.244[dB]
Irr_Atn_Dec_Default_Calc	= 25.244[dB]
Irr_Atn_Noe	= 25.244[dB]
Irr_Dec_Bandwidth_Hz	= 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.08082432[ppm]
Irr_Dec_Freq	= 395.88430144[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]