

# Selective Mechanochemical Monoarylation of Unbiased Dibromoarenes by *In-situ* Crystallization

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## 1. Chemicals and Instrumentation

The starting materials were obtained from commercial suppliers and used as received. 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. Both jar and ball are made of stainless. NMR spectra were recorded on JEOL JNM-ECX400P, JNM-ECS400 and JNM-ECZ400S spectrometers ( $^1\text{H}$ : 392 or 396 or 399 or 401 MHz,  $^{13}\text{C}$ : 99 or 100 MHz). Tetramethylsilane ( $^1\text{H}$ ),  $\text{CDCl}_3$  ( $^{13}\text{C}$ ) was employed as the external standards, respectively. Multiplicity was recorded as follows: s = singlet, brs = broad singlet, d = doublet, t = triplet, q = quartet, quint = quintet, sept = septet, o = octet, m = multiplet. 1,1,2,2-Tetrachloroethane and fluorobenzene were used as an internal standard to determine NMR yields. Recycle preparative gel permeation chromatography (GPC) was conducted with a JAI LC-9101 using  $\text{CHCl}_3$  as an eluent with JAIGEL-1H. GLC analyses were conducted with a Shimadzu GC-2014 or GC-2025 equipped with ULBON HR-1 glass capillary column (Shinwa Chemical Industries) or SH-Rtx-5MS glass capillary column (Shimadzu Corporation) and a FID detector. High-resolution mass spectra were recorded at the Global Facility Center, Hokkaido University. Powder diffraction data were recorded on a Rigaku SmartLab diffractometer with  $\text{Cu-K}\alpha$  radiation and D/teX Ultra detector covering  $5\text{-}60^\circ$  ( $2\theta$ ).

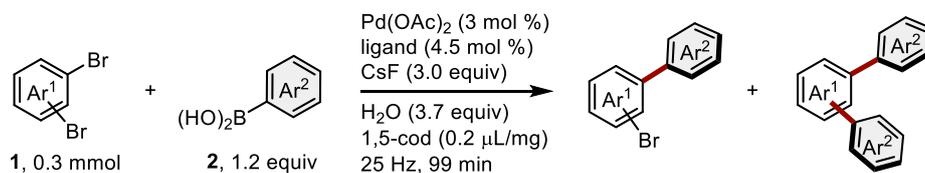


**Figure S1.** Retsch MM400 used in this study.

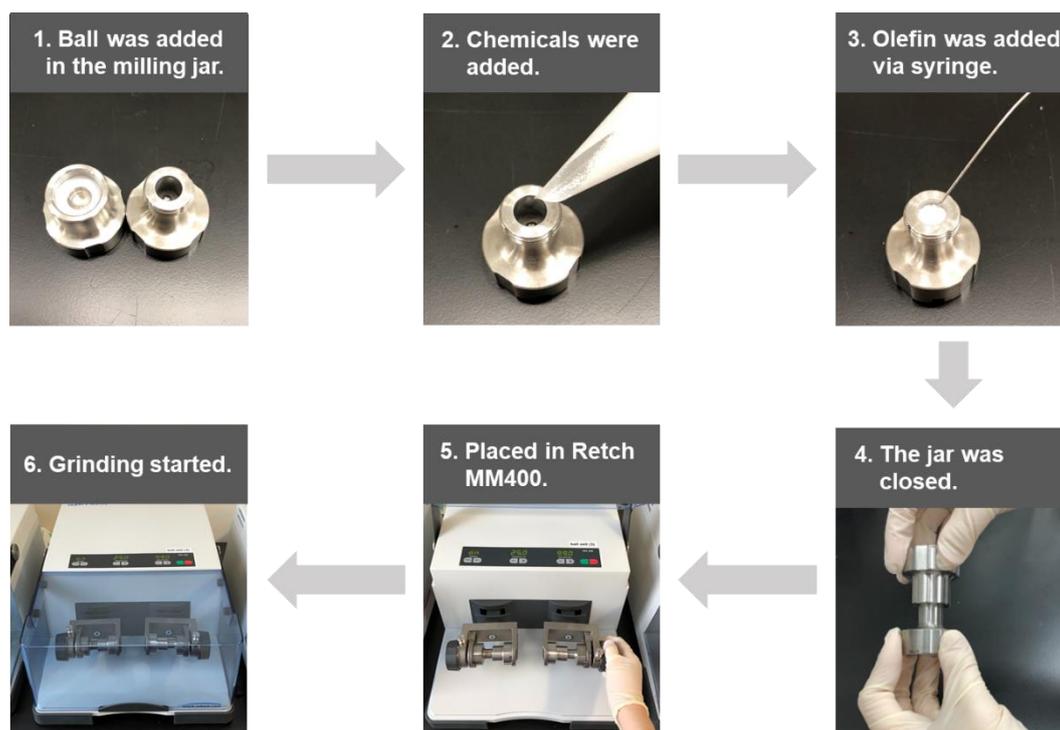


**Figure S2.** Stainless jar and ball used in this study.

## 2. General Procedure for Mechanochemical Cross-Coupling Reactions

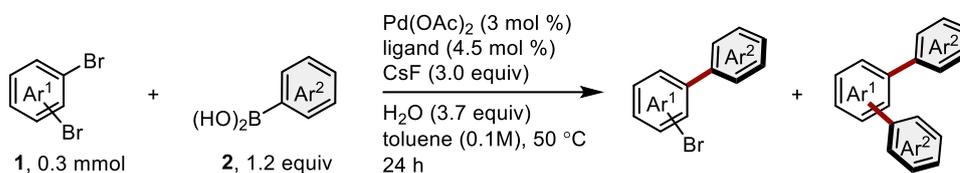


Arylboronic acid **2** (0.36 mmol, 1.2 equiv), Pd(OAc)<sub>2</sub> (0.009 mmol, 3 mol %) and ligand (0.0135 mmol, 4.5 mol %), CsF (0.9 mmol, 3.0 equiv) were placed in a ball milling vessel (stainless, 1.5 mL) loaded with one grinding ball (stainless, diameter: 3 mm). Then aryl halide **1** (0.3 mmol), H<sub>2</sub>O (20 μL, 3.7 equiv) and 1,5-cod (0.2 μL/mg) were added via syringe. After the vessel was closed in air without purging with inert gas, the vessel was placed in the ball mill (Retch MM400, 99 min at 25 Hz). After 99 min, the mixture was extracted with CH<sub>2</sub>Cl<sub>2</sub> three times. The solution was dried over MgSO<sub>4</sub>. After filtration, CH<sub>2</sub>Cl<sub>2</sub> was then removed by rotary evaporation. The crude mixture was then purified by flash column chromatography to give the corresponding monoarylated product.



**Figure S3.** Set-up procedure for the mechanochemical monoarylation.

### 3. General Procedure for Cross-Coupling Reactions in Solution



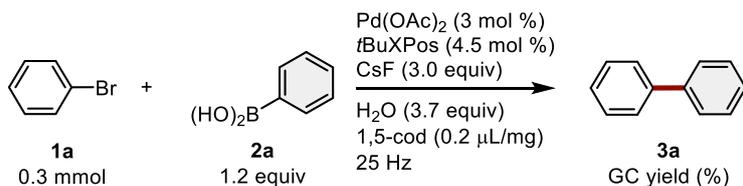
Arylboronic acid **2** (0.36 mmol, 1.2 equiv), Pd(OAc)<sub>2</sub> (0.009 mmol, 3 mol %) and ligand (0.0135 mmol, 4.5 mol %) and CsF (0.9 mmol, 3.0 equiv) were placed in an oven-dried reaction vial. After the vial was sealed with a screw cap containing a teflon-coated rubber septum, the vial was connected to a vacuum/nitrogen manifold through a needle. It was evacuated and then backfilled with nitrogen. This cycle was repeated three times. After toluene (3.0 mL, 0.1 M) was added, aryl halide **1** (0.3 mmol) was added in the vial through the rubber septum. After H<sub>2</sub>O (20 μL, 3.7 equiv) was added to the mixture, the mixture was heated to 50 °C using oil bath. After 24 hours, the mixture was extracted with CH<sub>2</sub>Cl<sub>2</sub> three times. The solution was dried over MgSO<sub>4</sub>. After filtration, CH<sub>2</sub>Cl<sub>2</sub> was then removed by rotary evaporation. <sup>1</sup>H NMR or GC analysis of the resulting crude mixture was measured to determine the yield of products.

#### 4. Details of Kinetic Studies

Reactions were conducted in a Retch MM400 ball mill in a stainless-steel milling jar (1.5 mL) at 25 Hz using one stainless-steel ball (diameter: 3 mm). As periodic sampling of the mechanochemical reaction runs would require stopping the mill and opening the jar, each data point was obtained from an individual reaction. Yields were determined by GC analysis with an internal standard.

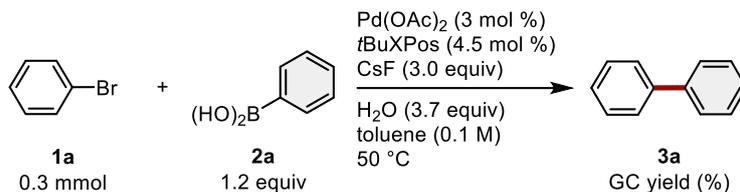
- The reaction **1a** with **2a** under mechanochemical and solution conditions

##### ball mill



Time (min)	0	20	40	60	90
GC yield (%)	0	10	14	62	70

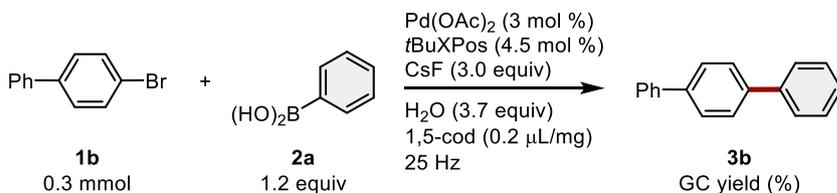
##### in solution



Time (h)	0	1	2	3	4
GC yield (%)	0	32	44	45	46

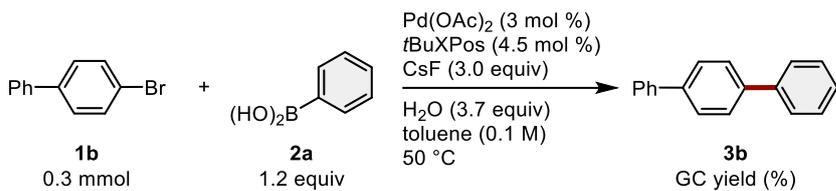
- The reaction of **1b** with **2a** under mechanochemical and solution conditions

##### ball mill



Time (min)	0	20	40	60	90
GC yield (%)	0	4	4	5	5

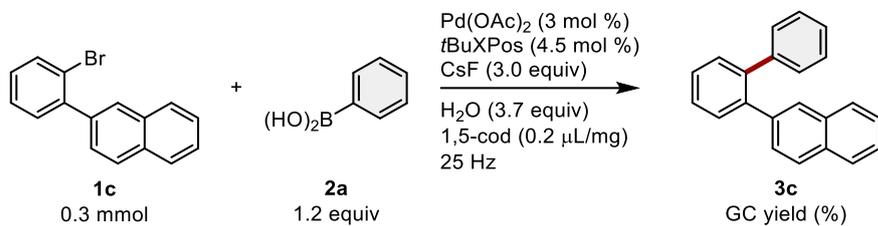
**in solution**



Time (h)	0	1	2	3	4
GC yield (%)	0	33	36	36	36

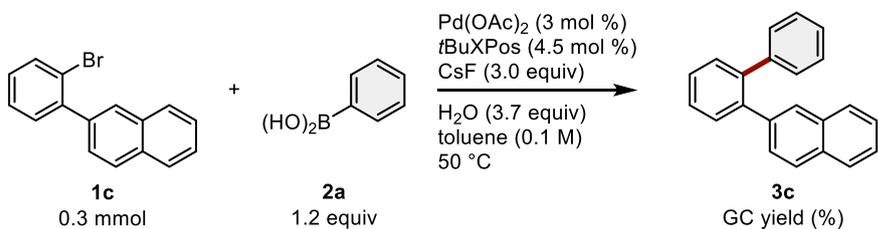
• The reaction of **1c** with **2a** under mechanochemical and solution conditions

**ball mill**



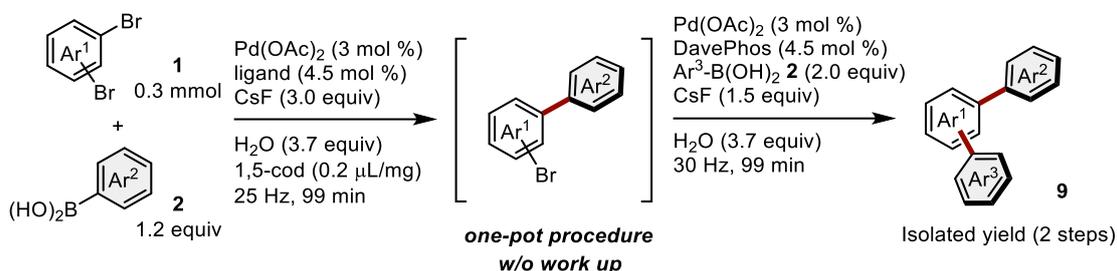
Time (min)	0	20	40	60	90
GC yield (%)	0	11	18	18	19

**in solution**



Time (h)	0	1	2	3	4
GC yield (%)	0	40	42	43	43

## 5. Procedure for One-Pot Sequential Arylations of Unbiased Dibromoarenes

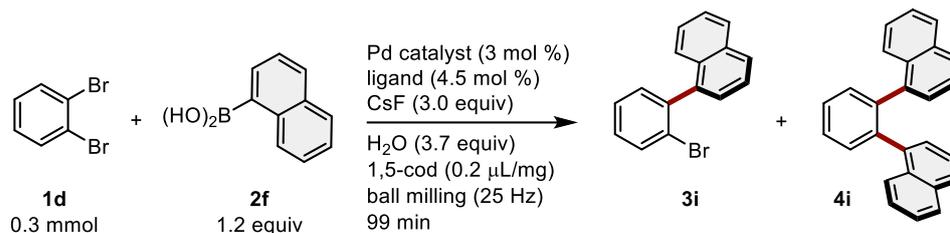


Aryl boronic acid **2** (0.36 mmol, 1.2 equiv),  $\text{Pd(OAc)}_2$  (0.009 mmol, 3 mol %) and ligand (0.0135 mmol, 4.5 mol %), CsF (0.9 mmol, 3.0 equiv) were placed in a ball milling vessel (stainless, 1.5 mL) loaded with one grinding ball (stainless, diameter: 3 mm). Then aryl halide **1** (0.3 mmol),  $\text{H}_2\text{O}$  (20  $\mu\text{L}$ , 3.7 equiv) and 1,5-cod (0.2  $\mu\text{L}/\text{mg}$ ) were added via syringe. After the vessel was closed in air without purging with inert gas, the vessel was placed in the ball mill (Retch MM400, 99 min at 25 Hz). After 99 min, the jar was opened and charged with  $\text{Pd(OAc)}_2$  (0.03 mmol, 3 mol %), DavePhos (0.045 mmol, 4.5 mol %), CsF (0.45 mmol, 1.5 equiv), aryl boronic acid **2** (0.6 mmol, 2.0 equiv) and  $\text{H}_2\text{O}$  (20  $\mu\text{L}$ , 3.7 equiv). After the jar was closed without the purge with inert gas, the jar was placed in the ball mill (Retsch MM 400, 99 min, 30 Hz). After 99 min, the mixture was extracted with  $\text{CH}_2\text{Cl}_2$  three times. The solution was dried over  $\text{MgSO}_4$ . After filtration,  $\text{CH}_2\text{Cl}_2$  was then removed by rotary evaporation. The crude mixture was then purified by flash column chromatography to give the corresponding coupling product **9**. In some cases, the product **9** was further purified by recrystallization and recycle gel permeation chromatography (GPC).

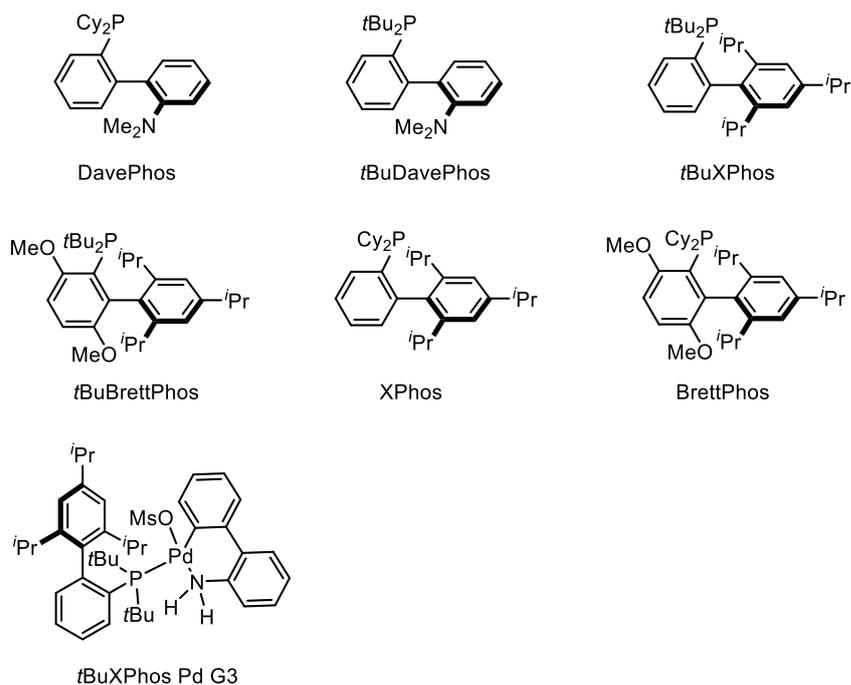
## 6. Results of Optimization Study

### Optimization of Palladium Catalyst

We have initiated the optimization study with **1d** as a substrate and 1,5-cod<sup>1</sup> as a grinding additive. Investigation on the ligand effect revealed that the use of *t*BuXPhos afforded the desired product **3i** in the highest yield with excellent monoarylation selectivity. We found that Pd(OAc)<sub>2</sub> was the best precatalyst for the mechanochemical monoarylation reaction.

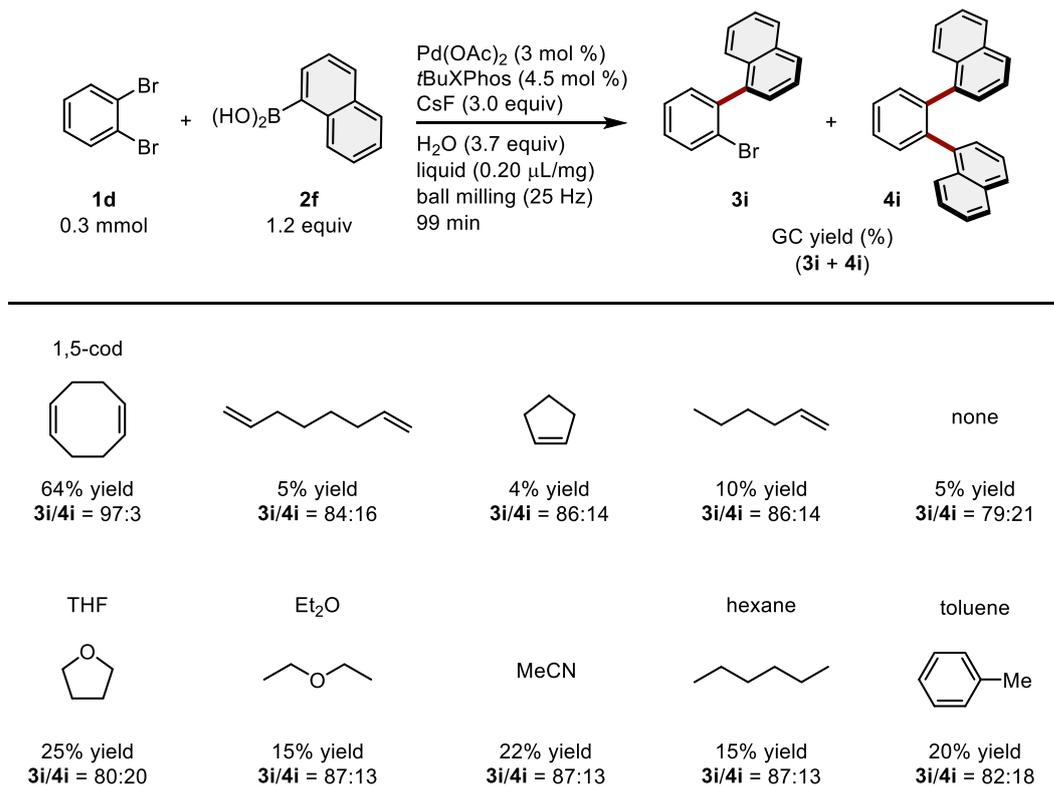


Pd catalyst	ligand	GC yield (%)	3i/4i (3i + 4i)
Pd(OAc) <sub>2</sub>	DavePhos	39%	98:2
Pd(OAc) <sub>2</sub>	<i>t</i> BuDavePhos	33%	95:5
<b>Pd(OAc)<sub>2</sub></b>	<b><i>t</i>BuXPhos</b>	<b>64%</b>	<b>97:3</b>
Pd(OAc) <sub>2</sub>	<i>t</i> BuBrettPhos	55%	97:3
Pd(OAc) <sub>2</sub>	XPhos	18%	87:13
Pd(OAc) <sub>2</sub>	BrettPhos	46%	89:11
Pd <sub>2</sub> (dba) <sub>3</sub>	<i>t</i> BuXPhos	6%	75:25
<i>t</i> BuXPhos G3	none	25%	97:3



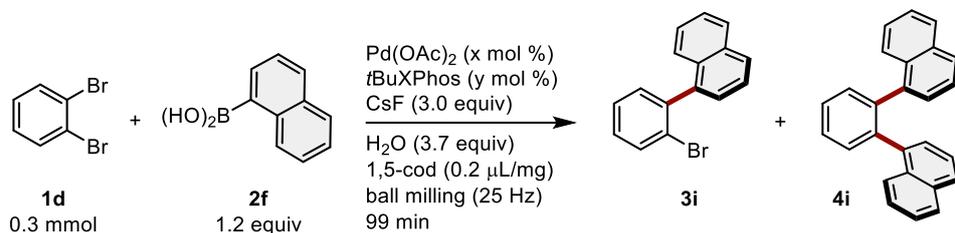
## Optimization of Liquid Additive

We found that the use of 1,5-cod improves the efficiency of the mechanochemical monoarylation reaction. Our previous study suggests that 1,5-cod might act as dispersants for the palladium-based catalyst to suppress higher aggregation of the nanoparticles, and also as stabilizer for the active monomeric palladium(0) species, thus facilitating the solvent-less mechanochemical coupling reaction.<sup>1</sup>

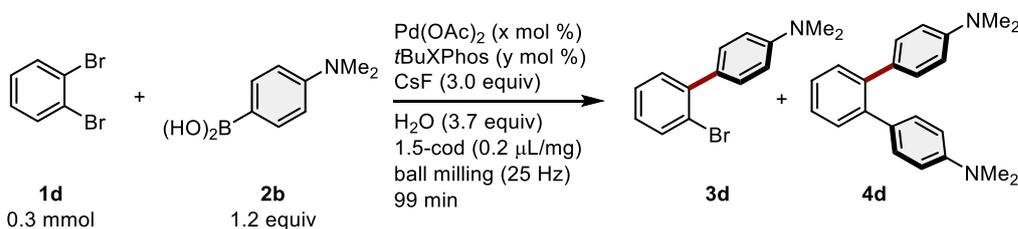


## Optimization of Catalyst Loading

Increasing catalyst loading did not lead to higher yield of the products.

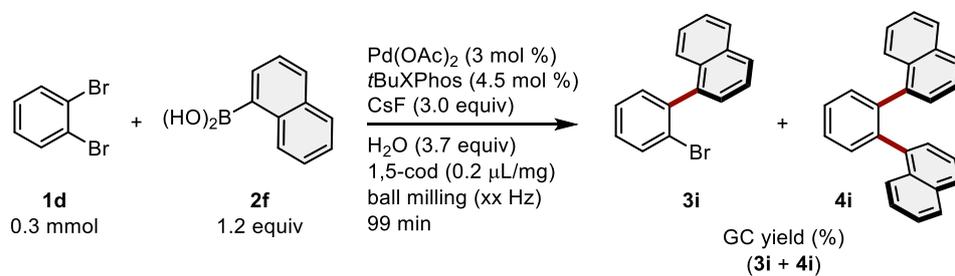


$\text{Pd(OAc)}_2$  (3 mol %),  $t\text{BuXPhos}$  (4.5 mol %): 64% (**3i** + **4i**), **3i/4i** = 97:3  
 $\text{Pd(OAc)}_2$  (5 mol %),  $t\text{BuXPhos}$  (7.5 mol %): 61% (**3i** + **4i**), **3i/4i** = 97:3



$\text{Pd(OAc)}_2$  (3 mol %),  $t\text{BuXPhos}$  (4.5 mol %): 78% (**3d** + **4d**), **3d/4d** = 90:10  
 $\text{Pd(OAc)}_2$  (5 mol %),  $t\text{BuXPhos}$  (7.5 mol %): 79% (**3d** + **4d**), **3d/4d** = 91:9

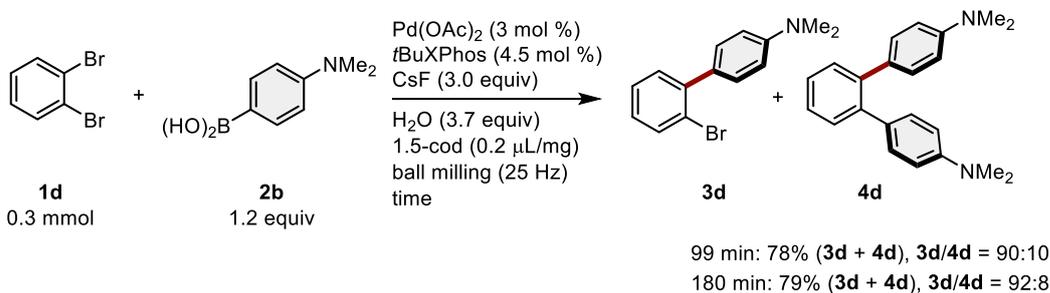
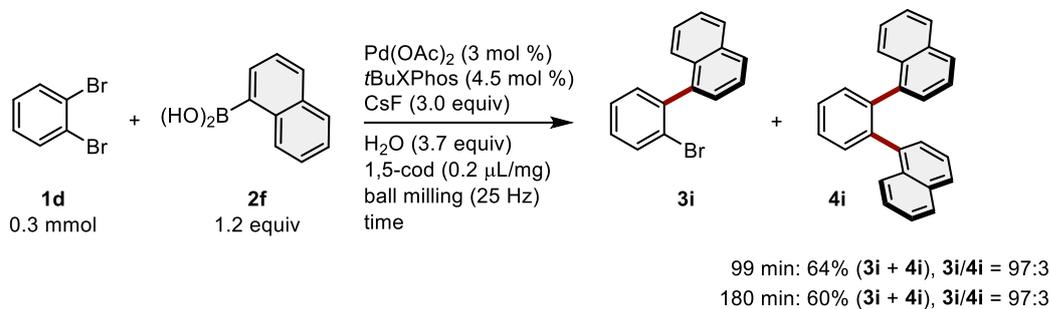
## Optimization of Frequency



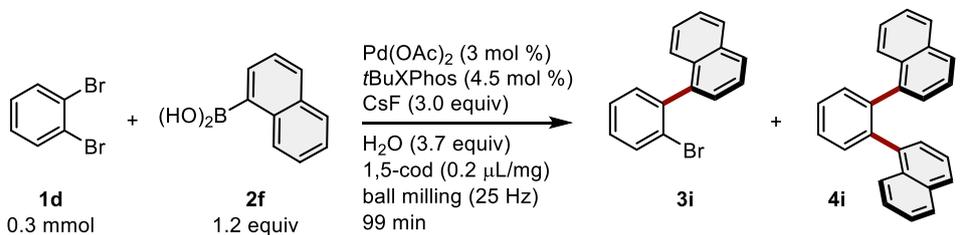
frequency (Hz)	GC yield (%) ( <b>3i</b> + <b>4i</b> )	<b>3i/4i</b>
25	64	97:3
30	60	98:2
20	37	97:3

## Optimization of Reaction Time

Prolonging the reaction time did not lead to higher yield of the products.



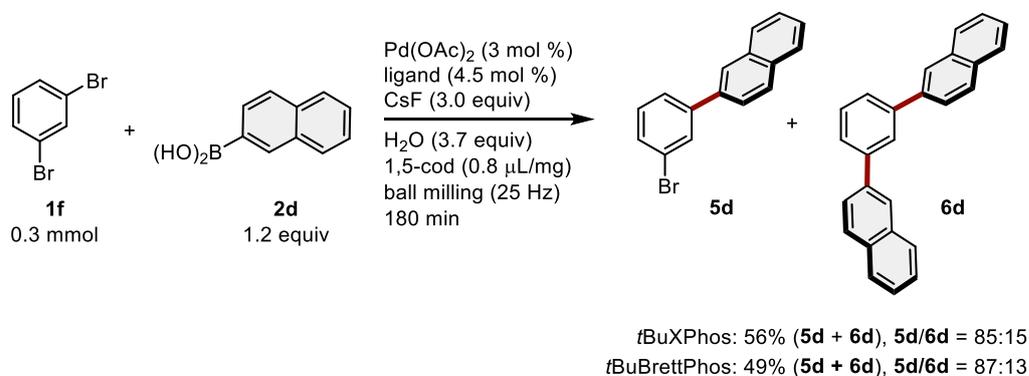
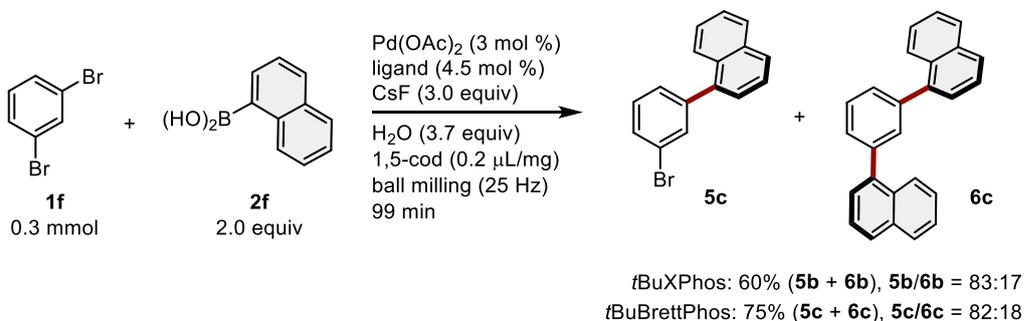
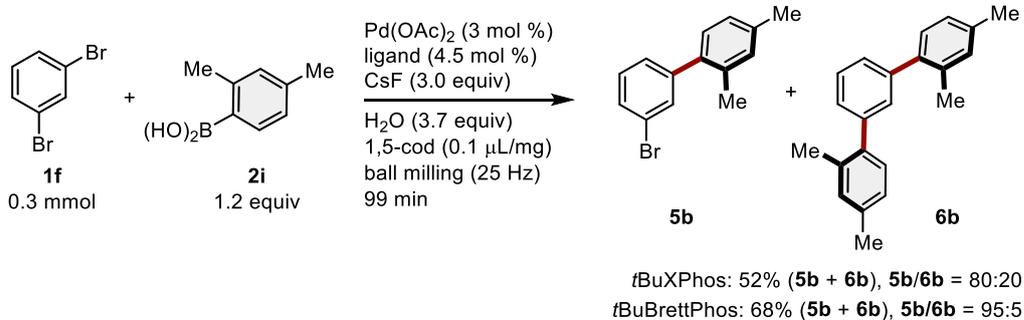
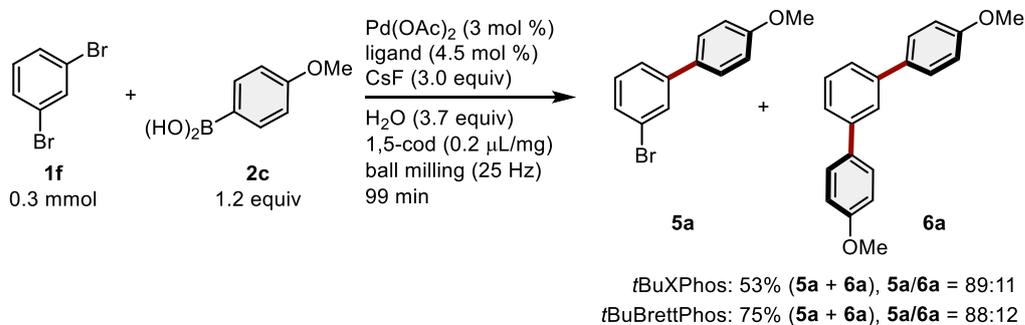
## Optimization of Jar and Ball



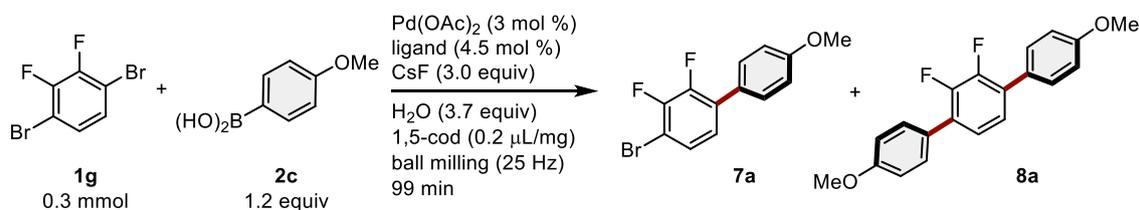
stainless 1.5 mm ball x 2, 1.5 mL jar: 38% (**3i** + **4i**), **3i/4i** = 95:5  
stainless 3 mm ball x 1, 1.5 mL jar: 64% (**3i** + **4i**), **3i/4i** = 97:3  
stainless 5 mm ball x 1, 1.5 mL jar: 63% (**3i** + **4i**), **3i/4i** = 97:3  
stainless 5 mm ball x 1, 5.0 mL jar: 54% (**3i** + **4i**), **3i/4i** = 98:2  
agate 5 mm ball x 2, 5.0 mL jar (30 Hz): 48% (**3i** + **4i**), **3i/4i** = 97:3

## Ligand Effect on Other Classes of Dibromoarenes

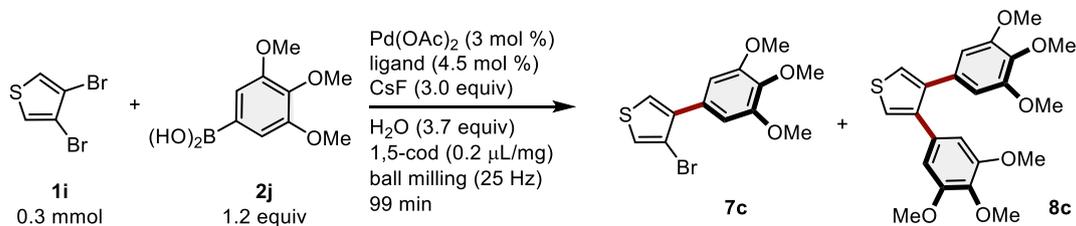
As for the reactions of 1,3-dibromobenzene (**1f**), the use of *t*BuBrettPhos instead of *t*BuXPhos generally gave higher yield of the monoarylation product **5**.



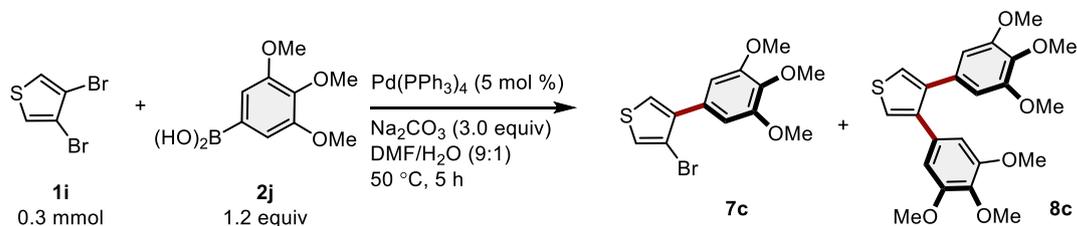
As for the reactions of **1g** and **1i**, the use of *t*BuBrettPhos instead of *t*BuXPhos generally gave higher yields of the monoarylation products **7a** and **7c**. The reported solution conditions with Pd(PPh<sub>3</sub>)<sub>4</sub> as a catalyst require an excess of **1i**,<sup>2</sup> and the catalyst amount was reduced to one equivalent, only a very low selectivity toward monoarylation was observed.



*t*BuXPhos: 58% (**7a** + **8a**), **7a/8a** = 90:10  
*t*BuBrettPhos: 72% (**7a** + **8a**), **7a/8a** = 90:10

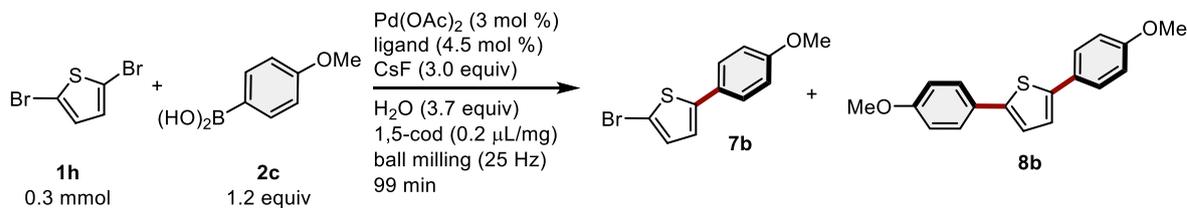


*t*BuXPhos: 14% (**7c** + **8c**), **7c/8c** = 97:3  
*t*BuBrettPhos: 71% (**7c** + **8c**), **7c/8c** = 88:12



45% (**7c** + **8c**), **7c/8c** = 25:75

As for the reactions of **1h**, the use of *t*BuXPhos gave higher yield of the monoarylation product **7b**.



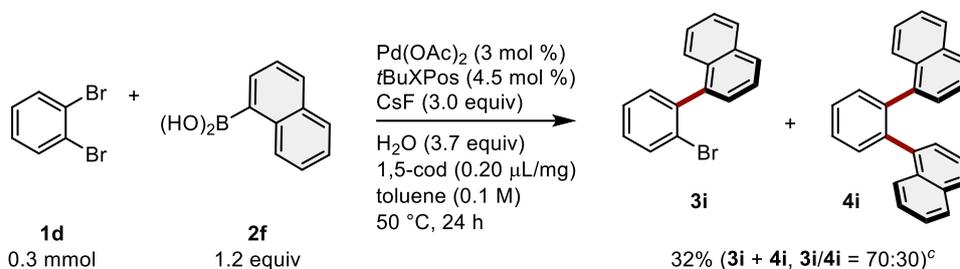
*t*BuXPhos: 55% (**7b** + **8b**), **7b/8b** = 91:9  
*t*BuBrettPhos: 45% (**7b** + **8b**), **7b/8b** = 85:15

The ligand effects on the mechanochemical monoarylation reactions were summarized as followed:

1. *t*BuXPhos is the best ligand for the reactions of 1,2-dibromobenzenes.
2. *t*BuBrettPhos generally provides better yield for the reactions of other classes of dibromoarenes compared to *t*BuXPhos. We would recommend that both ligands (*t*BuXPhos and *t*BuBrettPhos) should be tested to find optimal conditions when substrates other than 1,2-dibromobenzenes are used for the mono-selective mechanochemical coupling reactions.

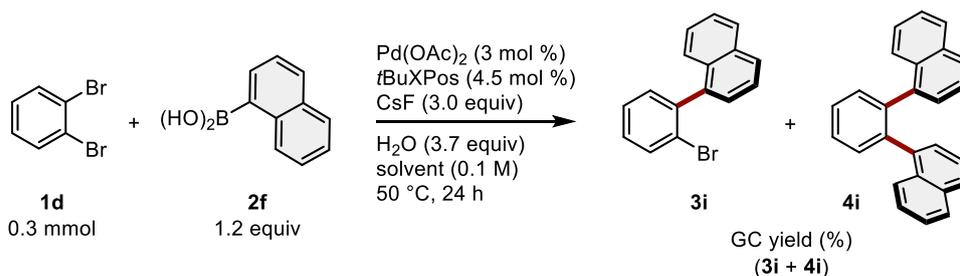
### Solution-based Coupling Reaction in the Presence of 1,5-Cod

The coupling reaction was performed in the presence of 1,5-cod in solution, and the selectivity toward monoarylation was not changed (32%, **3i/4i** = 70:30). This result suggests that 1,5-cod should not be a factor in the observed selectivity.



### Effect of Solvent on Solution-based Coupling Reaction

We investigated the effect of solvent on the solution-based cross-coupling reactions. The results showed that the choice of solvent did not significantly affect the selectivity toward monoarylation.

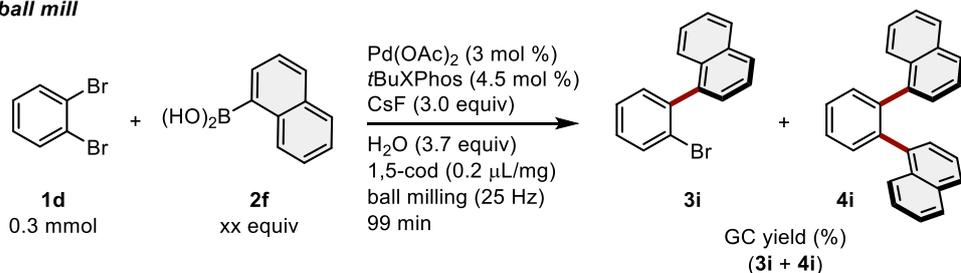


solvent	GC yield (%) ( <b>3i</b> + <b>4i</b> )	<b>3i/4i</b>
toluene	30	70:30
THF	10	79:21
dioxane	12	75:25
MeCN	48	73:27

## Reactions Using Excess Amount of Arylboronic Acid

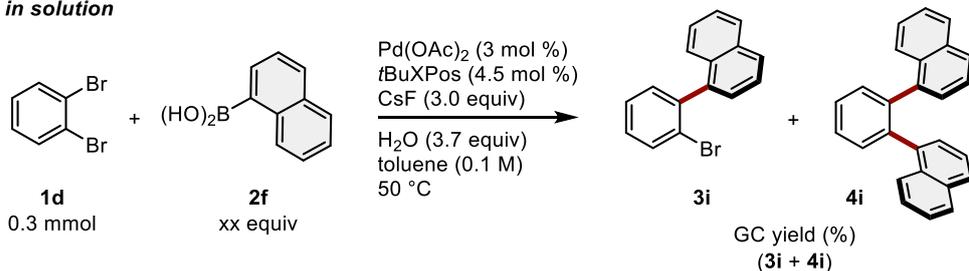
The reactions using 2.0 equivalents of arylboronic acid under both mechanochemical conditions and solution-based conditions were investigated. We found that increasing amount of arylboronic acid did not affect the monoarylation selectivity under mechanochemical conditions (50%, **3i/4i** = 98:2). In contrast, the selectivity became lower under solution-based conditions (35%, **3i/4i** = 63:37).

### ball mill



equiv of <b>2f</b>	GC yield (%) ( <b>3i</b> + <b>4i</b> )	<b>3i/4i</b>
1.2	64	97:3
2.0	50	98:2

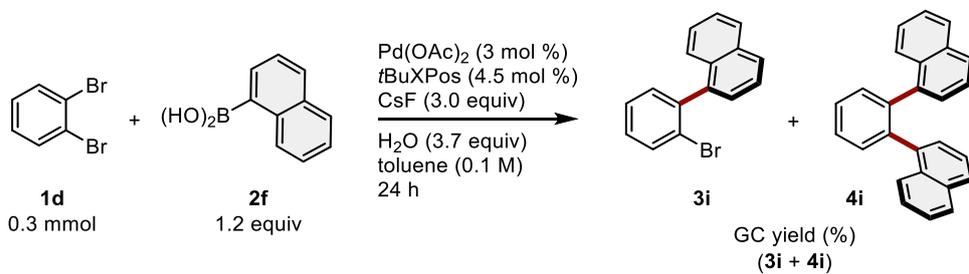
### in solution



equiv of <b>2f</b>	GC yield (%) ( <b>3i</b> + <b>4i</b> )	<b>3i/4i</b>
1.2	30	70:30
2.0	35	63:37

### Effect of Temperature on Solution-based Coupling Reaction

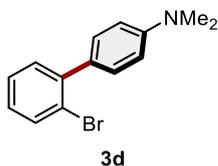
The coupling reactions in toluene at 50°C and 30 °C were carried out. The result showed that reaction temperature did not affect the selectivity toward monoarylation (27%, **3i/4i** = 70:30).



temp. (°C)	GC yield (%) ( <b>3i</b> + <b>4i</b> )	<b>3i/4i</b>
50	30	70:30
30	27	70:30

## 7. Characterization of Obtained Coupling Products

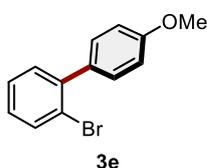
### 2'-Bromo-*N,N*-dimethyl-[1,1'-biphenyl]-4-amine (3d).



The reaction was carried out with 70.8 mg (0.30 mmol) of **1d** and 59.4 mg (0.36 mmol) of **2b**. The product **3d** was obtained as a white solid (56.0 mg, 0.203 mmol, 68% yield) after purification by silica-gel column chromatography (SiO<sub>2</sub>, CH<sub>2</sub>Cl<sub>2</sub>/hexane, 0:100–50:50). <sup>1</sup>H and <sup>13</sup>C NMR were in agreement with the literature.<sup>3</sup>

<sup>1</sup>H NMR (392 MHz, CDCl<sub>3</sub>, δ): 3.01 (s, 6H), 6.75–6.81 (m, 2H), 7.09–7.18 (m, 1H), 7.29–7.37 (m, 4H), 7.64 (d, *J* = 7.8 Hz, 1H). <sup>13</sup>C NMR (99 MHz, CDCl<sub>3</sub>, δ): 40.6 (CH<sub>3</sub>), 111.7 (CH), 123.1 (C), 127.4 (CH), 128.0 (CH), 129.1 (C), 130.3 (CH), 131.5 (CH), 133.2 (CH), 142.7 (C), 149.9 (C). HRMS-ESI (*m/z*): [M+H]<sup>+</sup> calcd for C<sub>14</sub>H<sub>15</sub>NBr, 276.0382; found, 276.0383.

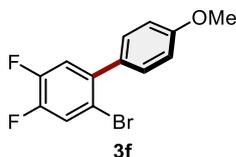
### 2-Bromo-4'-methoxy-1,1'-biphenyl (3e).



The reaction was carried out with 70.8 mg (0.30 mmol) of **1d** and 91.2 mg (0.6 mmol) of **2c**. The product **3e** was obtained as a white solid (56.5 mg, 0.216 mmol, 72% yield) after purification by silica-gel column chromatography (SiO<sub>2</sub>, CH<sub>2</sub>Cl<sub>2</sub>/hexane, 0:100–30:70). <sup>1</sup>H and <sup>13</sup>C NMR were in agreement with the literature.<sup>4</sup>

<sup>1</sup>H NMR (392 MHz, CDCl<sub>3</sub>, δ): 3.86 (s, 3H), 6.94–7.00 (m, 2H), 7.14–7.21 (m, 1H), 7.29–7.39 (m, 4H), 7.66 (d, *J* = 9.0 Hz, 1H). <sup>13</sup>C NMR (99 MHz, CDCl<sub>3</sub>, δ): 55.4 (CH<sub>3</sub>), 113.5 (CH), 123.0 (C), 127.5 (CH), 128.5 (CH), 130.7 (CH), 131.5 (CH), 133.2 (CH), 133.6 (C), 142.3 (C), 159.2 (C). HRMS-EI (*m/z*): [M]<sup>+</sup> calcd for C<sub>13</sub>H<sub>11</sub>BrO, 261.9993; found, 262.0004.

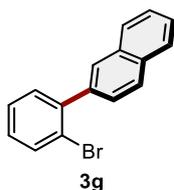
### 2-Bromo-4,5-difluoro-4'-methoxy-1,1'-biphenyl (**3f**).



The reaction was carried out with 81.6 mg (0.30 mmol) of **1e** and 54.7 mg (0.36 mmol) of **2c**. The product **3f** was obtained as a white solid (60.7 mg, 0.203 mmol, 68% yield) after purification by silica-gel column chromatography (SiO<sub>2</sub>, Et<sub>2</sub>O/hexane, 0:100–2:98).

<sup>1</sup>H NMR (396 MHz, CDCl<sub>3</sub>, δ): 3.86 (s, 3H), 6.93–6.99 (m, 2H), 7.15 (dd, *J* = 8.1, 10.9 Hz, 1H), 7.27–7.33 (m, 2H), 7.48 (dd, *J* = 7.5, 9.9 Hz, 1H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>, δ): 55.4 (CH<sub>3</sub>), 113.7 (CH), 116.4 (q, *J* = 3.8 Hz, C), 119.6 (d, *J* = 18.1 Hz, CH), 121.9 (d, *J* = 20.0 Hz, CH), 130.6 (CH), 131.9 (C), 139.2 (t, *J* = 4.7 Hz, C), 148.1 (q, *J* = 12.4 Hz, C), 150.6 (q, *J* = 11.4 Hz, C), 159.6 (C). HRMS-EI (*m/z*): [M]<sup>+</sup> calcd for C<sub>13</sub>H<sub>9</sub>BrF<sub>2</sub>O, 297.9805; found, 297.9806.

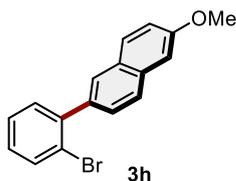
### 2-(2-Bromophenyl)naphthalene (**3g**).



The reaction was carried out with 70.8 mg (0.30 mmol) of **1d** and 61.9 mg (0.36 mmol) of **2d**. The product **3g** was obtained as a white solid (56.2 mg, 0.199 mmol, 66% yield) after purification by silica-gel column chromatography (SiO<sub>2</sub>, hexane only) and GPC. <sup>1</sup>H and <sup>13</sup>C NMR were in agreement with the literature.<sup>5</sup>

<sup>1</sup>H NMR (396 MHz, CDCl<sub>3</sub>, δ): 7.21–7.28 (m, 1H), 7.37–7.45 (m, 2H), 7.49–7.54 (m, 2H), 7.57 (dd, *J* = 1.8, 8.1 Hz, 1H), 7.71 (d, *J* = 7.7 Hz, 1H), 7.84–7.92 (m, 4H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>, δ): 122.9 (C), 126.4 (CH), 127.5 (CH), 127.6 (CH), 127.7 (CH), 127.8 (CH), 128.3 (CH), 128.4 (CH), 129.0 (CH), 131.7 (CH), 132.7 (C), 133.2 (C), 133.3 (C), 138.7 (C), 142.6 (C). HRMS-EI (*m/z*): [M]<sup>+</sup> calcd for C<sub>16</sub>H<sub>11</sub>Br, 282.0044; found, 282.0045.

### 2-(2-Bromophenyl)-6-methoxynaphthalene (**3h**).



The reaction was carried out with 70.8 mg (0.30 mmol) of **1d** and 72.7 mg (0.36 mmol) of **2e**. The

product **3h** was obtained as a white solid (60.7 mg, 0.195 mmol, 65% yield) after purification by silica-gel column chromatography (SiO<sub>2</sub>, CH<sub>2</sub>Cl<sub>2</sub>/hexane, 0:100–50:50) and GPC. <sup>1</sup>H and <sup>13</sup>C NMR were in agreement with the literature.<sup>6</sup>

<sup>1</sup>H NMR (392 MHz, CDCl<sub>3</sub>, δ): 3.95 (s, 3H), 7.15–7.28 (m, 3H), 7.35–7.45 (m, 2H), 7.53 (d, *J* = 8.6 Hz, 1H), 7.70 (d, *J* = 7.8 Hz, 1H), 7.74–7.82 (m, 3H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>, δ): 55.5 (CH<sub>3</sub>), 105.7 (CH), 119.2 (CH), 123.0 (C), 126.3 (CH), 127.5 (CH), 128.19 (CH), 128.22 (CH), 128.6 (C), 128.8 (CH), 129.8 (CH), 131.7 (CH), 133.3 (CH), 133.9 (C), 136.5 (C), 142.7 (C), 158.1 (C). HRMS-EI (*m/z*): [M]<sup>+</sup> calcd for C<sub>17</sub>H<sub>13</sub>BrO, 312.0150; found, 312.0148.

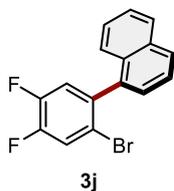
### 1-(2-Bromophenyl)naphthalene (**3i**).



The reaction was carried out with 70.8 mg (0.30 mmol) of **1d** and 61.9 mg (0.36 mmol) of **2f**. The product **3i** was obtained as a white solid (46.0 mg, 0.162 mmol, 54% yield) after purification by silica-gel column chromatography (SiO<sub>2</sub>, hexane only) and GPC. <sup>1</sup>H and <sup>13</sup>C NMR were in agreement with the literature.<sup>7</sup>

<sup>1</sup>H NMR (392 MHz, CDCl<sub>3</sub>, δ): 7.31 (td, *J* = 2.0, 7.6 Hz, 1H), 7.34–7.52 (m, 6H), 7.55 (t, *J* = 7.6 Hz, 1H), 7.74 (d, *J* = 7.4 Hz, 1H), 7.92 (d, *J* = 8.2 Hz, 2H). <sup>13</sup>C NMR (99 MHz, CDCl<sub>3</sub>, δ): 124.5 (C), 125.3 (CH), 126.0 (CH), 126.1 (CH), 126.3 (CH), 127.1 (CH), 127.3 (CH), 128.3 (CH), 128.4 (CH), 129.2 (CH), 131.7 (C), 132.1 (CH), 132.9 (CH), 133.5 (C), 139.2 (C), 141.4 (C). HRMS-EI (*m/z*): [M]<sup>+</sup> calcd for C<sub>16</sub>H<sub>11</sub>Br, 282.0044; found, 282.0042.

### 1-(2-Bromo-4,5-difluorophenyl)naphthalene (**3j**).

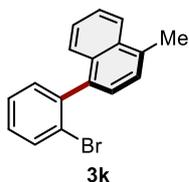


The reaction was carried out with 81.6 mg (0.30 mmol) of **1e** and 61.9 mg (0.36 mmol) of **2f**. The product **3j** was obtained as a white solid (48.0 mg, 0.150 mmol, 50% yield) after purification by silica-gel column chromatography (SiO<sub>2</sub>, hexane only) and GPC.

<sup>1</sup>H NMR (396 MHz, CDCl<sub>3</sub>, δ): 7.22 (dd, *J* = 8.3, 10.3 Hz, 1H), 7.33 (dd, *J* = 1.2, 7.1 Hz, 1H), 7.40–7.48 (m, 2H), 7.48–7.55 (m, 2H), 7.55–7.60 (m, 1H), 7.93 (dt, *J* = 1.4, 8.2 Hz, 2H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>, δ): 118.2 (q, *J* = 3.5 Hz, C), 120.4 (d, *J* = 18.1 Hz, CH), 121.6 (d, *J* = 20.0 Hz, CH), 125.2

(CH), 125.5 (CH), 126.2 (CH), 126.6 (CH), 127.3 (CH), 128.5 (CH), 128.9 (CH), 131.3 (C), 133.5 (C), 137.3 (C), 138.2 (t,  $J = 4.8$  Hz, C), 148.4 (q,  $J = 14.3$  Hz, C), 150.9 (q,  $J = 14.6$  Hz, C). HRMS-EI ( $m/z$ ):  $[M]^+$  calcd for  $C_{16}H_9BrF_2$ , 317.9856; found, 317.9849.

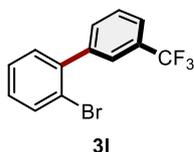
### 1-(2-Bromophenyl)-4-methylnaphthalene (**3k**).



The reaction was carried out with 70.8 mg (0.30 mmol) of **1d** and 67.0 mg (0.36 mmol) of **2g**. The product **3k** was obtained as a white solid (52.0 mg, 0.175 mmol, 58% yield) after purification by silica-gel column chromatography ( $SiO_2$ , hexane only) and GPC.

$^1H$  NMR (401 MHz,  $CDCl_3$ ,  $\delta$ ): 2.76 (s, 3H), 7.26–7.33 (m, 2H), 7.35 (dd,  $J = 1.8, 7.8$  Hz, 1H), 7.37–7.45 (m, 3H), 7.47 (d,  $J = 7.6$  Hz, 1H), 7.50–7.56 (m, 1H), 7.73 (d,  $J = 8.4$  Hz, 1H), 8.07 (d,  $J = 8.8$  Hz, 1H).  $^{13}C$  NMR (99 MHz,  $CDCl_3$ ,  $\delta$ ): 19.8 ( $CH_3$ ), 124.6 (CH), 124.7 (C), 125.87 (CH), 125.94 (CH), 126.1 (CH), 126.7 (CH), 126.8 (CH), 127.3 (CH), 129.1 (CH), 131.7 (C), 132.3 (CH), 132.6 (C), 132.8 (CH), 134.7 (C), 137.6 (C), 141.7 (C). HRMS-EI ( $m/z$ ):  $[M]^+$  calcd for  $C_{17}H_{13}Br$ , 296.0201; found, 296.0207.

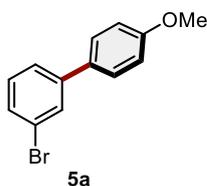
### 2-Bromo-3'-(trifluoromethyl)-1,1'-biphenyl (**3l**).



The reaction was carried out with 70.8 mg (0.30 mmol) of **1d** and 68.4 mg (0.36 mmol) of **2h**. The product **3l** was obtained as an oil (47.0 mg, 0.156 mmol, 52% yield) after purification by silica-gel column chromatography ( $SiO_2$ , hexane only) and GPC.

$^1H$  NMR (401 MHz,  $CDCl_3$ ,  $\delta$ ): 7.22–7.28 (m, 1H), 7.33 (dd,  $J = 2.0, 7.2$  Hz, 1H), 7.39 (td,  $J = 1.5, 7.3$  Hz, 1H), 7.55 (t,  $J = 7.6$  Hz, 1H), 7.59–7.71 (m, 4H).  $^{13}C$  NMR (99 MHz,  $CDCl_3$ ,  $\delta$ ): 122.6 (C), 124.1 (q,  $J = 216.4$  Hz,  $CF_3$ ), 124.6 (q,  $J = 3.7$  Hz, CH), 126.4 (q,  $J = 3.8$  Hz, CH), 127.3 (CH), 127.7 (CH), 128.6 (CH), 129.5 (CH), 130.6 (d,  $J = 30.0$  Hz, C), 131.3 (CH), 133.0 (CH), 133.5 (CH), 141.2 (C), 141.8 (C). HRMS-EI ( $m/z$ ):  $[M]^+$  calcd for  $C_{13}H_8BrF_3$ , 299.9762; found, 299.9766.

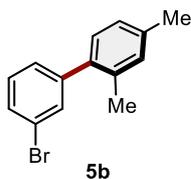
### 3-Bromo-4'-methoxy-1,1'-biphenyl (**5a**).



The reaction was carried out with 70.8 mg (0.30 mmol) of **1f** and 54.7 mg (0.36 mmol) of **2c**. The product **5a** was obtained as a white solid (49.7 mg, 0.189 mmol, 63% yield) after purification by silica-gel column chromatography (SiO<sub>2</sub>, CH<sub>2</sub>Cl<sub>2</sub>/hexane, 0:100–10:90) and GPC. <sup>1</sup>H and <sup>13</sup>C NMR were in agreement with the literature.<sup>8</sup>

<sup>1</sup>H NMR (396 MHz, CDCl<sub>3</sub>, δ): 3.85 (s, 3H), 6.95–7.00 (m, 2H), 7.24–7.30 (m, 1H), 7.40–7.53 (m, 4H), 7.69 (t, *J* = 1.8 Hz, 1H). <sup>13</sup>C NMR (99 MHz, CDCl<sub>3</sub>, δ): 55.5 (CH<sub>3</sub>), 114.5 (CH), 123.0 (C), 125.4 (CH), 128.3 (CH), 129.7 (CH), 129.9 (CH), 130.4 (CH), 132.3 (C), 143.1 (C), 159.7 (C). HRMS-EI (*m/z*): [M]<sup>+</sup> calcd for C<sub>13</sub>H<sub>11</sub>BrO, 261.9993; found, 261.9994.

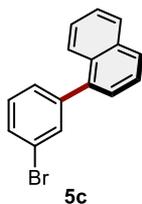
### 3'-Bromo-2,4-dimethyl-1,1'-biphenyl (**5b**).



The reaction was carried out with 70.8 mg (0.30 mmol) of **1f** and 54.0 mg (0.36 mmol) of **2i**. The product **5b** was obtained as a white solid (44.4 mg, 0.170 mmol, 56% yield) after purification by silica-gel column chromatography (SiO<sub>2</sub>, hexane only) and GPC.

<sup>1</sup>H NMR (396 MHz, CDCl<sub>3</sub>, δ): 2.23 (s, 3H), 2.36 (s, 3H), 7.03–7.11 (m, 3H), 7.21–7.29 (m, 2H), 7.43–7.48 (m, 2H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>, δ): 20.4 (CH<sub>3</sub>), 21.2 (CH<sub>3</sub>), 122.2 (C), 126.7 (CH), 128.1 (CH), 129.7 (CH), 129.8 (CH), 131.3 (CH), 132.4 (CH), 135.1 (C), 137.6 (C), 137.7 (C), 144.2 (C). HRMS-EI (*m/z*): [M]<sup>+</sup> calcd for C<sub>14</sub>H<sub>13</sub>Br, 260.0201; found, 260.0202.

### 1-(3-Bromophenyl)naphthalene (**5c**).

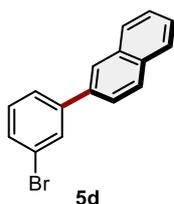


The reaction was carried out with 70.8 mg (0.30 mmol) of **1f** and 103.2 mg (0.60 mmol) of **2f**. The product **5c** was obtained as a white solid (46.9 mg, 0.166 mmol, 55% yield) after purification by silica-

gel column chromatography (SiO<sub>2</sub>, hexane only) and GPC.

<sup>1</sup>H NMR (392 MHz, CDCl<sub>3</sub>, δ): 7.33–7.60 (m, 7H), 7.65 (t, *J* = 1.6 Hz, 1H), 7.81–7.94 (m, 3H). <sup>13</sup>C NMR (99 MHz, CDCl<sub>3</sub>, δ): 122.5 (C), 125.4 (CH), 125.7 (CH), 126.0 (CH), 126.5 (CH), 127.1 (CH), 128.3 (CH), 128.5 (CH), 128.8 (CH), 129.9 (CH), 130.4 (CH), 131.4 (C), 133.0 (CH), 133.8 (C), 138.7 (C), 142.9 (C). HRMS-EI (*m/z*): [M]<sup>+</sup> calcd for C<sub>16</sub>H<sub>11</sub>Br, 282.0044; found, 282.0049.

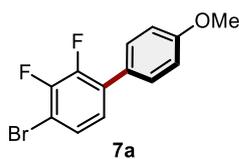
#### 2-(3-Bromophenyl)naphthalene (**5d**).



The reaction was carried out with 70.8 mg (0.30 mmol) of **1f** and 103.2 mg (0.60 mmol) of **2d**. The product **5d** was obtained as a white solid (34.7 mg, 0.123 mmol, 41% yield) after purification by silica-gel column chromatography (SiO<sub>2</sub>, hexane only) and GPC. <sup>1</sup>H and <sup>13</sup>C NMR were in agreement with the literature.<sup>9</sup>

<sup>1</sup>H NMR (401 MHz, CDCl<sub>3</sub>, δ): 7.35 (t, *J* = 7.8 Hz, 1H), 7.47–7.56 (m, 3H), 7.64 (dd, *J* = 1.2, 7.6 Hz, 1H), 7.70 (dd, *J* = 1.8, 8.2 Hz, 1H), 7.84–7.96 (m, 4H), 8.02 (s, 1H). <sup>13</sup>C NMR (99 MHz, CDCl<sub>3</sub>, δ): 123.1 (C), 125.3 (CH), 126.1 (CH), 126.4 (CH), 126.6 (CH), 127.8 (CH), 128.4 (CH), 128.7 (CH), 130.35 (CH), 130.45 (CH), 130.51 (CH), 132.9 (C), 133.7 (C), 137.1 (C), 143.3 (C). HRMS-EI (*m/z*): [M]<sup>+</sup> calcd for C<sub>16</sub>H<sub>11</sub>Br, 282.0044; found, 282.0047.

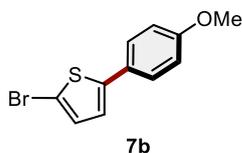
#### 4-Bromo-2,3-difluoro-4'-methoxy-1,1'-biphenyl (**7a**).



The reaction was carried out with 81.6 mg (0.30 mmol) of **1g** and 91.2 mg (0.60 mmol) of **2c**. The product **7a** was obtained as a white solid (47.5 mg, 0.159 mmol, 53% yield) after purification by silica-gel column chromatography (SiO<sub>2</sub>, CH<sub>2</sub>Cl<sub>2</sub>/hexane, 0:100–10:90).

<sup>1</sup>H NMR (392 MHz, CDCl<sub>3</sub>, δ): 3.86 (s, 3H), 6.99 (d, *J* = 7.4 Hz, 2H), 7.08 (t, *J* = 3.6 Hz, 1H), 7.34 (t, *J* = 3.8 Hz, 1H), 7.46 (d, *J* = 8.6 Hz, 2H). <sup>13</sup>C NMR (99 MHz, CDCl<sub>3</sub>, δ): 55.5 (CH<sub>3</sub>), 108.3 (d, *J* = 17.9 Hz, C), 114.3 (CH), 125.3 (t, *J* = 3.7 Hz, CH), 126.4 (C), 127.7 (d, *J* = 3.7 Hz, CH), 130.1 (d, *J* = 2.9 Hz, CH), 130.3 (d, *J* = 10.3 Hz, C), 147.3 (q, *J* = 22.7 Hz, C), 149.9 (q, *J* = 20.7 Hz, C), 159.9 (C). HRMS-EI (*m/z*): [M]<sup>+</sup> calcd for C<sub>13</sub>H<sub>9</sub>BrF<sub>2</sub>O, 297.9805; found, 297.9807.

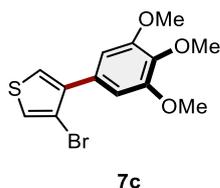
### 2-Bromo-5-(4-methoxyphenyl)thiophene (**7b**).



The reaction was carried out with 72.6 mg (0.30 mmol) of **1h** and 91.0 mg (0.60 mmol) of **2c**. The product **7b** was obtained as a yellow solid (38.8 mg, 0.144 mmol, 48% yield) after purification by silica-gel column chromatography (SiO<sub>2</sub>, CH<sub>2</sub>Cl<sub>2</sub>/hexane, 0:100–20:80). <sup>1</sup>H and <sup>13</sup>C NMR were in agreement with the literature.<sup>10</sup>

<sup>1</sup>H NMR (401 MHz, CDCl<sub>3</sub>, δ): 3.83 (s, 3H), 6.88–6.92 (m, 2H), 6.93 (d, *J* = 3.6 Hz, 1H), 6.99 (d, *J* = 3.6 Hz, 1H), 7.41–7.47 (m, 2H). <sup>13</sup>C NMR (99 MHz, CDCl<sub>3</sub>, δ): 55.5 (CH<sub>3</sub>) 110.3 (C), 114.5 (CH), 122.3 (CH), 126.7 (C), 127.1 (CH), 130.9 (CH), 146.0 (C), 159.6 (C). HRMS-EI (*m/z*): [M]<sup>+</sup> calcd for C<sub>11</sub>H<sub>9</sub>BrOS, 267.9558; found, 267.9558.

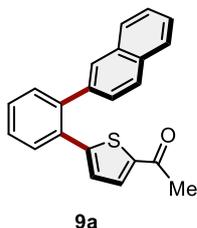
### 3-Bromo-4-(3,4,5-trimethoxyphenyl)thiophene (**7c**).



The reaction was carried out with 72.6 mg (0.30 mmol) of **1i** and 76.3 mg (0.60 mmol) of **2j**. The product **7c** was obtained as a white solid (60.2 mg, 0.183 mmol, 61% yield) after purification by silica-gel column chromatography (SiO<sub>2</sub>, EtOAc/hexane, 0:100–20:80). <sup>1</sup>H and <sup>13</sup>C NMR were in agreement with the literature.<sup>2</sup>

<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, δ): 3.90 (s, 9H), 6.71 (s, 2H), 7.27 (d, *J* = 3.6 Hz, 1H), 7.37 (d, *J* = 3.6 Hz, 1H). <sup>13</sup>C NMR (99 MHz, CDCl<sub>3</sub>, δ): 56.1 (CH<sub>3</sub>), 60.9 (CH<sub>3</sub>), 106.2 (CH), 111.0 (C), 123.2 (CH), 124.2 (CH), 130.6 (C), 137.6 (C), 141.8 (C), 152.9 (C). HRMS-EI (*m/z*): [M]<sup>+</sup> calcd for C<sub>13</sub>H<sub>13</sub>BrO<sub>3</sub>S, 327.9769; found, 327.9764.

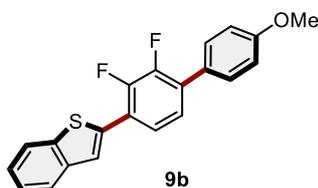
**1-{5-[2-(Naphthalen-2-yl)phenyl]thiophen-2-yl}ethan-1-one (9a).**



The reaction was carried out with 70.7 mg (0.30 mmol) of **1d**. The product **9a** was obtained as a white solid (65.9 mg, 0.201 mmol, 67% yield) after purification by silica-gel column chromatography (SiO<sub>2</sub>, EtOAc/hexane, 25:75) and recrystallization from Et<sub>2</sub>O.

<sup>1</sup>H NMR (392 MHz, CDCl<sub>3</sub>, δ): 2.45 (s, 3H), 6.53–6.58 (m, 1H), 7.23–7.28 (m, 1H), 7.34 (d, *J* = 4.0 Hz, 1H), 7.41–7.52 (m, 5H), 7.57–7.62 (m, 1H), 7.72 (d, *J* = 8.4 Hz, 1H), 7.78–7.86 (m, 3H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>, δ): 26.5 (CH<sub>3</sub>), 126.1 (CH), 126.2 (CH), 127.6 (CH), 127.7 (CH), 127.9 (CH), 128.0 (CH), 128.2 (CH), 128.5 (CH), 129.0 (CH), 130.6 (CH), 131.4 (CH), 132.3 (C), 132.4 (C), 132.6 (CH), 133.3 (C), 138.5 (C), 140.9 (C), 143.6 (C), 152.0 (C), 190.6 (C). HRMS-EI (*m/z*): [M]<sup>+</sup> calcd for C<sub>22</sub>H<sub>16</sub>OS, 328.0922; found, 328.0921.

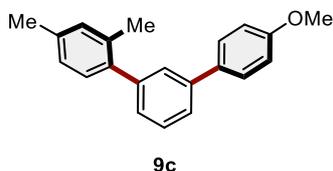
**2-[2,3-Difluoro-4'-methoxy-(1,1'-biphenyl)-4-yl]benzo[b]thiophene (9b).**



The reaction was carried out with 81.6 mg (0.30 mmol) of **1g**. The product **9b** was obtained as a white solid (64.5 mg, 0.183 mmol, 61% yield) after purification by silica-gel column chromatography (SiO<sub>2</sub>, CH<sub>2</sub>Cl<sub>2</sub>/hexane, 0:100–40:60).

<sup>1</sup>H NMR (392 MHz, CDCl<sub>3</sub>, δ): 3.78 (s, 3H), 6.78–6.83 (m, 2H), 6.97 (s, 1H), 7.12–7.21 (m, 3H), 7.23–7.32 (m, 2H), 7.41 (dd, *J* = 8.1, 11.2 Hz, 1H), 7.63 (dd, *J* = 1.8, 6.7 Hz, 1H), 7.71 (d, *J* = 7.7 Hz, 1H). <sup>13</sup>C NMR (99 MHz, CDCl<sub>3</sub>, δ): 55.2 (CH<sub>3</sub>), 113.7 (CH), 119.4 (CH), 119.58 (CH), 119.61 (CH), 122.0 (CH), 123.6 (CH), 123.8 (CH), 124.3 (CH), 129.8 (dd, *J* = 3.4, 6.4 Hz, C), 130.6 (CH), 131.4 (C), 137.7 (dd, *J* = 3.7, 5.6 Hz, C), 139.7 (C), 140.4 (C), 141.6 (C), 148.1 (dd, *J* = 12.2, 68.6 Hz, C), 150.6 (dd, *J* = 12.7, 70.9 Hz, C), 159.2 (C). HRMS-EI (*m/z*): [M]<sup>+</sup> calcd for C<sub>21</sub>H<sub>14</sub>F<sub>2</sub>OS, 352.0733; found, 352.0732.

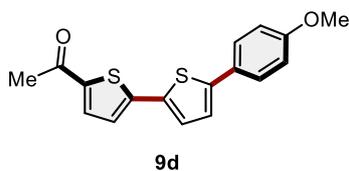
**4''-Methoxy-2,4-dimethyl-1,1':3',1''-terphenyl (9c).**



The reaction was carried out with 70.8 mg (0.30 mmol) of **1f**. The product **9c** was obtained as a white solid (54.5 mg, 0.189 mmol, 63% yield) after purification by silica-gel column chromatography (SiO<sub>2</sub>, CH<sub>2</sub>Cl<sub>2</sub>/hexane, 0:100–60:40).

<sup>1</sup>H NMR (392 MHz, CDCl<sub>3</sub>, δ): 2.29 (s, 3H), 2.37 (s, 3H), 3.84 (s, 3H), 6.97 (dt, *J* = 2.5, 9.2 Hz, 2H), 7.08 (d, *J* = 7.6 Hz, 1H), 7.11 (s, 1H), 7.19 (d, *J* = 8.1 Hz, 1H), 7.25 (dt, *J* = 1.6, 7.6 Hz, 1H), 7.41–7.47 (m, 1H), 7.48–7.58 (m, 4H). <sup>13</sup>C NMR (99 MHz, CDCl<sub>3</sub>, δ): 20.5 (CH<sub>3</sub>), 21.1 (CH<sub>3</sub>), 55.3 (CH<sub>3</sub>), 114.2 (CH), 124.9 (CH), 126.5 (CH), 127.6 (CH), 127.7 (CH), 128.2 (CH), 128.4 (CH), 129.7 (CH), 131.1 (CH), 133.6 (C), 135.2 (C), 137.0 (C), 139.0 (C), 140.5 (C), 142.3 (C), 159.1 (C). HRMS-EI (*m/z*): [M]<sup>+</sup> calcd for C<sub>21</sub>H<sub>20</sub>O, 288.1514; found, 288.1514.

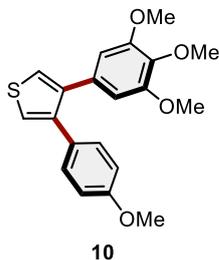
**1-[5'-(4-Methoxyphenyl)-(2,2'-bithiophen)-5-yl]ethan-1-one (9d).**



The reaction was carried out with 72.6 mg (0.30 mmol) of **1h**. The product **9d** was obtained as a yellow solid (45.3 mg, 0.144 mmol, 48% yield) after purification by silica-gel column chromatography (SiO<sub>2</sub>, CH<sub>2</sub>Cl<sub>2</sub>/hexane, 0:100–100:0).

<sup>1</sup>H NMR (392 MHz, CDCl<sub>3</sub>, δ): 2.55 (s, 3H), 3.85 (s, 3H), 6.93 (d, *J* = 7.6 Hz, 2H), 7.10–7.18 (m, 2H), 7.24–7.28 (m, 1H), 7.54 (d, *J* = 8.1 Hz, 2H), 7.59 (dd, *J* = 0.9, 4.0 Hz, 1H). <sup>13</sup>C NMR (99 MHz, CDCl<sub>3</sub>, δ): 26.5 (CH<sub>3</sub>), 55.4 (CH<sub>3</sub>), 114.4 (CH), 123.0 (CH), 123.6 (CH), 126.4 (C), 126.6 (CH), 127.1 (CH), 133.4 (CH), 134.4 (C), 142.0 (C), 145.5 (C), 146.0 (C), 159.7 (C), 190.3 (C). HRMS-EI (*m/z*): [M]<sup>+</sup> calcd for C<sub>17</sub>H<sub>14</sub>O<sub>2</sub>S<sub>2</sub>, 314.0435; found, 314.0431.

**3-(4-Methoxyphenyl)-4-(3,4,5-trimethoxyphenyl)thiophene (10).**

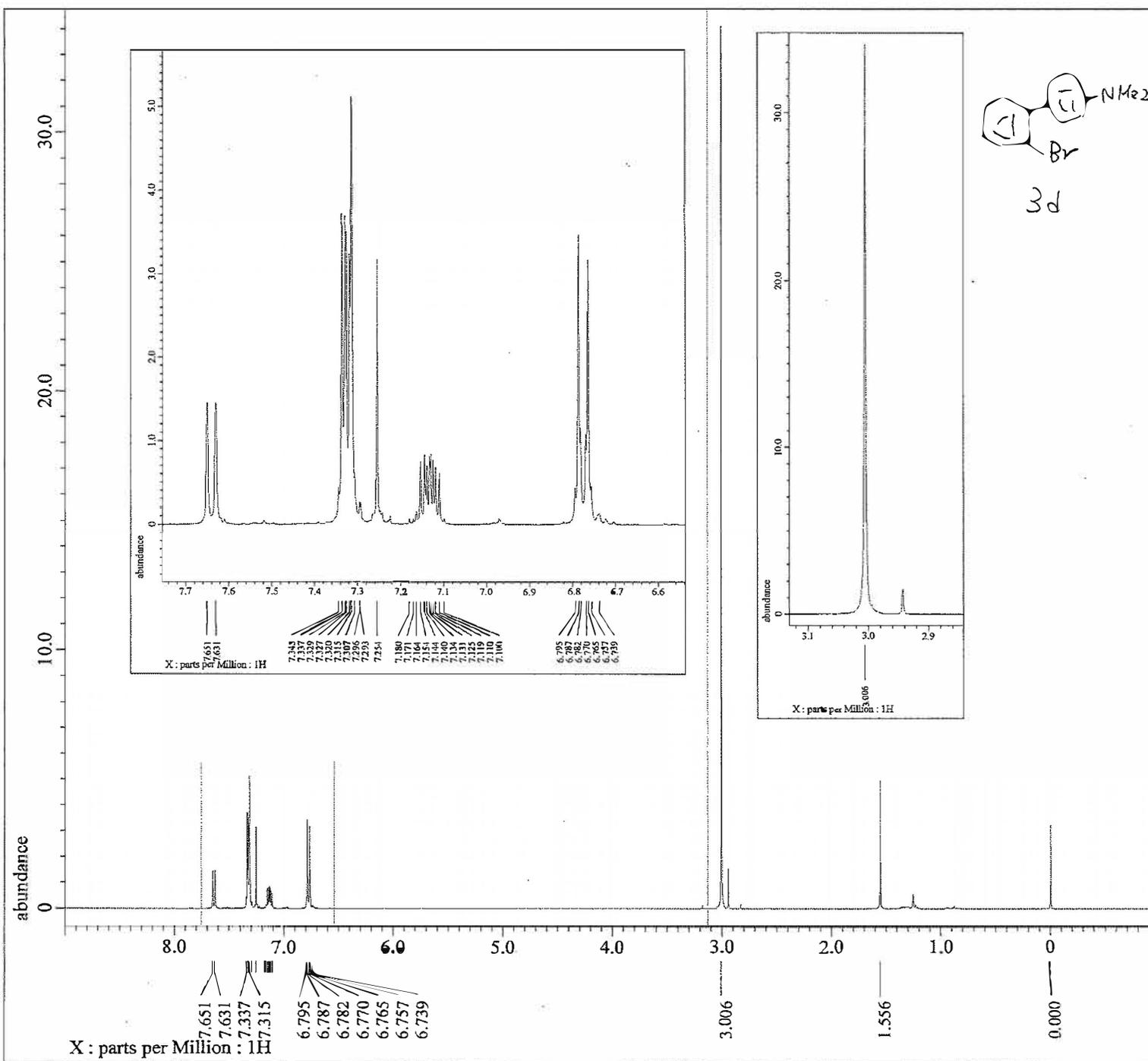


The reaction was carried out with 72.6 mg (0.30 mmol) of **1i**. The product **10** was obtained as a white solid (57.7 mg, 0.162 mmol, 54% yield) after purification by silica-gel column chromatography (SiO<sub>2</sub>, EtOAc/hexane, 0:100–20:80) and GPC. <sup>1</sup>H and <sup>13</sup>C NMR were in agreement with the literature.<sup>2</sup>

<sup>1</sup>H NMR (392 MHz, CDCl<sub>3</sub>, δ): 3.65 (s, 6H), 3.79 (s, 3H), 3.85 (s, 3H), 6.40 (s, 2H), 6.82 (dt, *J* = 2.4, 9.4 Hz, 2H), 7.14 (dt, *J* = 2.5, 9.2 Hz, 2H), 7.25 (d, *J* = 3.1 Hz, 1H), 7.31 (d, *J* = 3.6 Hz, 1H). <sup>13</sup>C NMR (99 MHz, CDCl<sub>3</sub>, δ): 55.2 (CH<sub>3</sub>), 55.8 (CH<sub>3</sub>), 60.9 (CH<sub>3</sub>), 106.1 (CH), 113.5 (CH), 123.20 (CH), 123.24 (CH), 129.0 (C), 130.2 (C), 132.0 (C), 136.9 (C), 141.3 (C), 141.5 (C), 152.7 (C), 158.6 (C). HRMS-EI (*m/z*): [M]<sup>+</sup> calcd for C<sub>20</sub>H<sub>20</sub>O<sub>4</sub>S, 356.1082; found, 356.1071.

## 8. References

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dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
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ppm

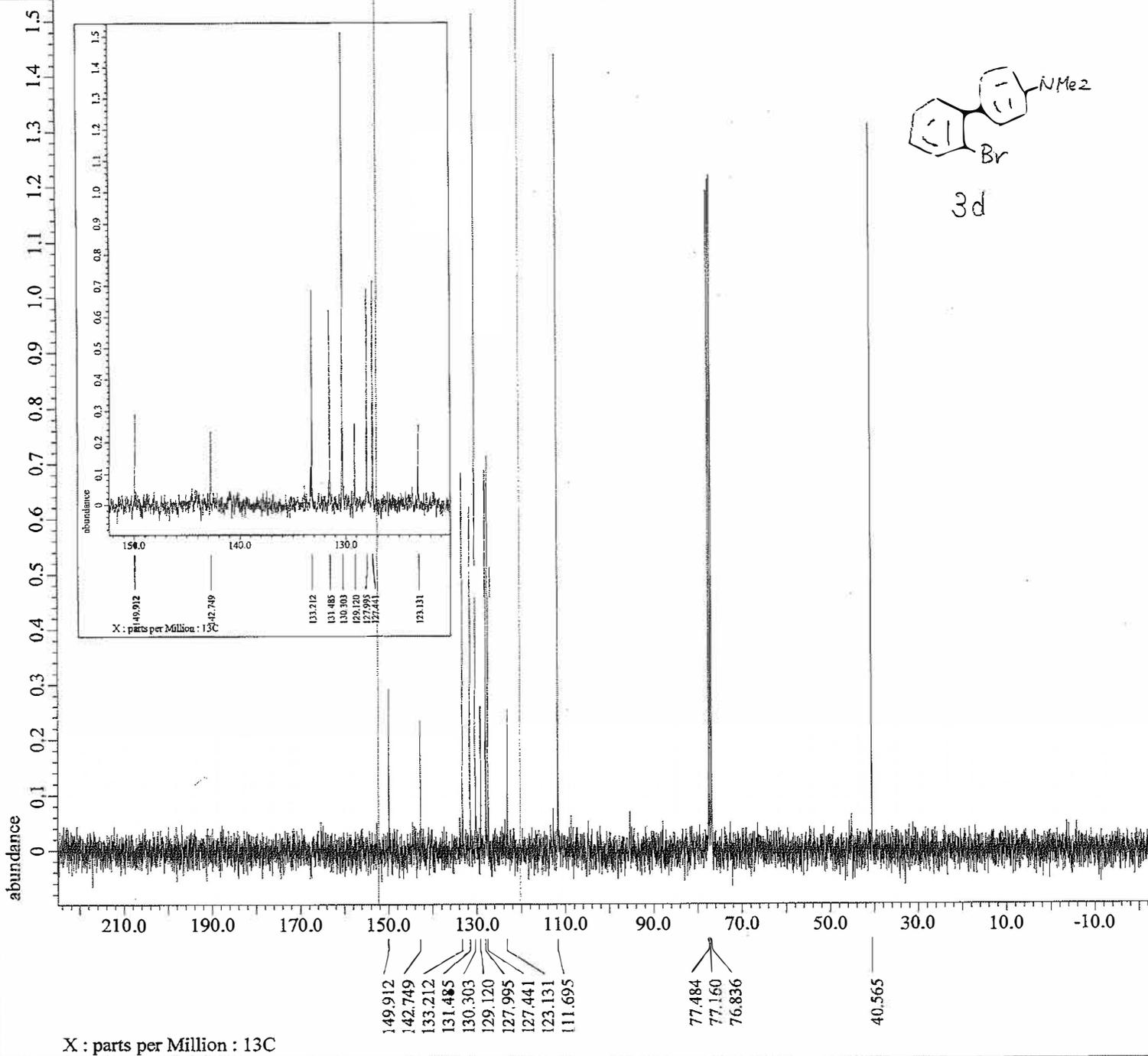
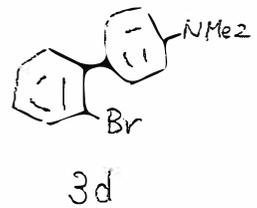
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Revision_Time   = 25-JUL-2019 20:41:28

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Dim Title    = 1H
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X Domain       = 1H
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X Offset      = 5[ppm]
X Points      = 16384
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Irr Freq     = 391.78655441[MHz]
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Dante_Presat   = FALSE
  
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```

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

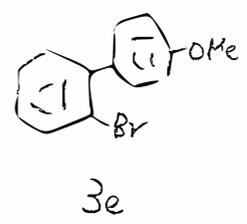
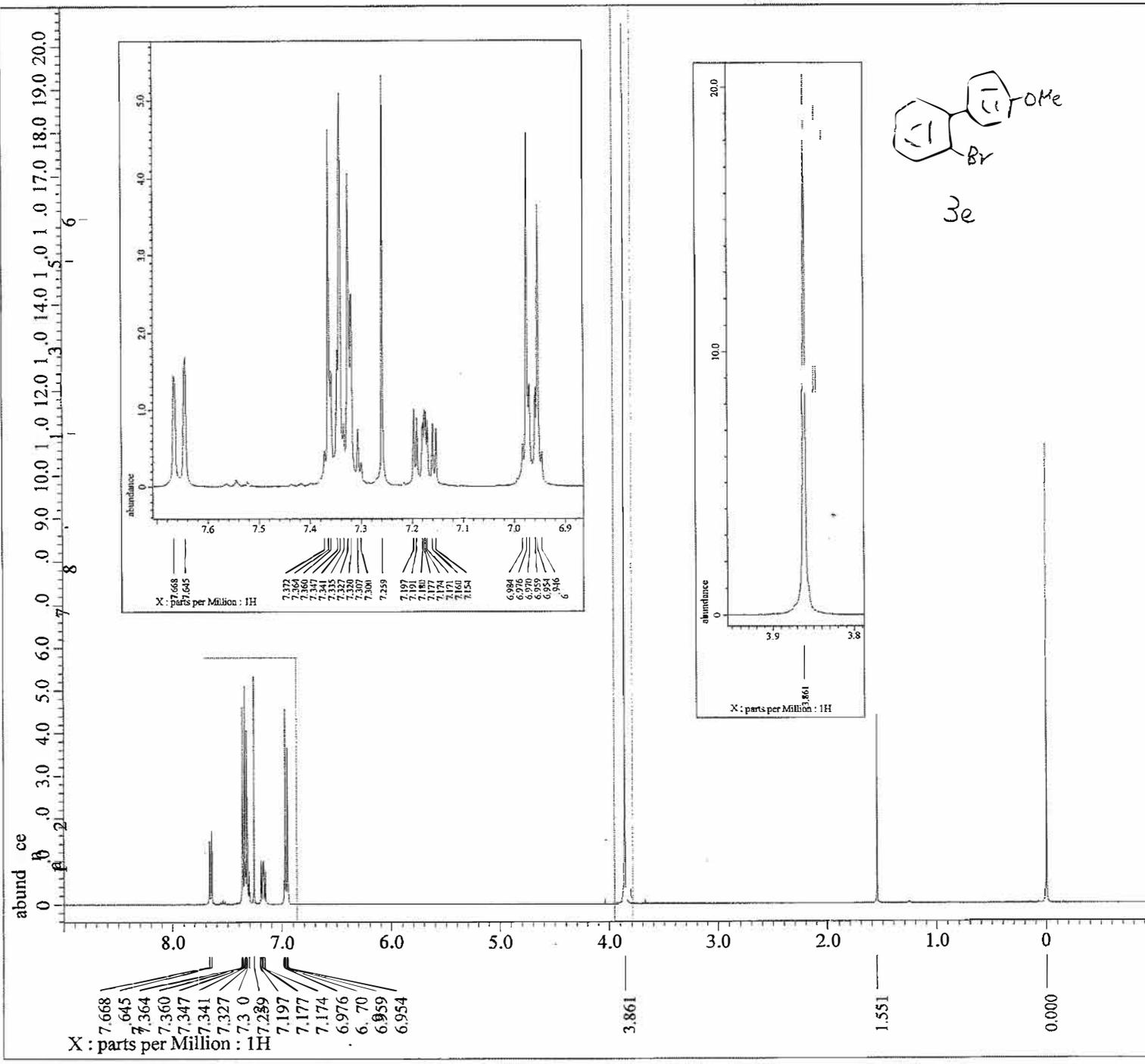
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Author            = element
Experiment        = single_pulse_dec
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Revision_Time     = 25-JUL-2019 20:43:56

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Dim Title        = 13C
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Spectrometer     = JNM-ECS400

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X_Domain         = 13C
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X_Offset         = 100[ppm]
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X_Prescans       = 4
X_Resolution     = 0.93958061[Hz]
X_Sweep          = 30.78817734[kHz]
Irr_Domain       = 1H
Irr_Freq         = 391.78655441[MHz]
Irr_Offset       = 5[ppm]
Clipped          = FALSE
Scans            = 15
Total_Scans      = 15

Relaxation_Delay = 2[s]
Recvr_Gain       = 60
Temp_Get         = 20.7[dC]
X_90_Width       = 9.11[us]
X_Acq_Time       = 1.06430464[s]
X_Angle          = 30[deg]
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X_Pulse          = 3.03666667[us]
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Irr_Atn_Noise    = 22.255[dB]
Irr_Noise        = WALTZ
Decoupling       = TRUE
Initial_Wait     = 1[s]
Noe              = TRUE
  
```



```

---- PROCESSED PARAMETERS ----
dc_balance 0 ( FALS E )
sexp( 0.2[H z] 0.0[s ] )
trap ezoi d3( @C[M], 100[%] )
ze f0 l[ 1 ]
fft( 1, TRU E, TRUE )
machi hape
ppm

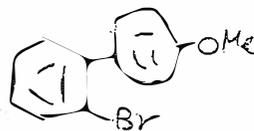
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R exon Time   = 25-JUL-2019 20:28:57

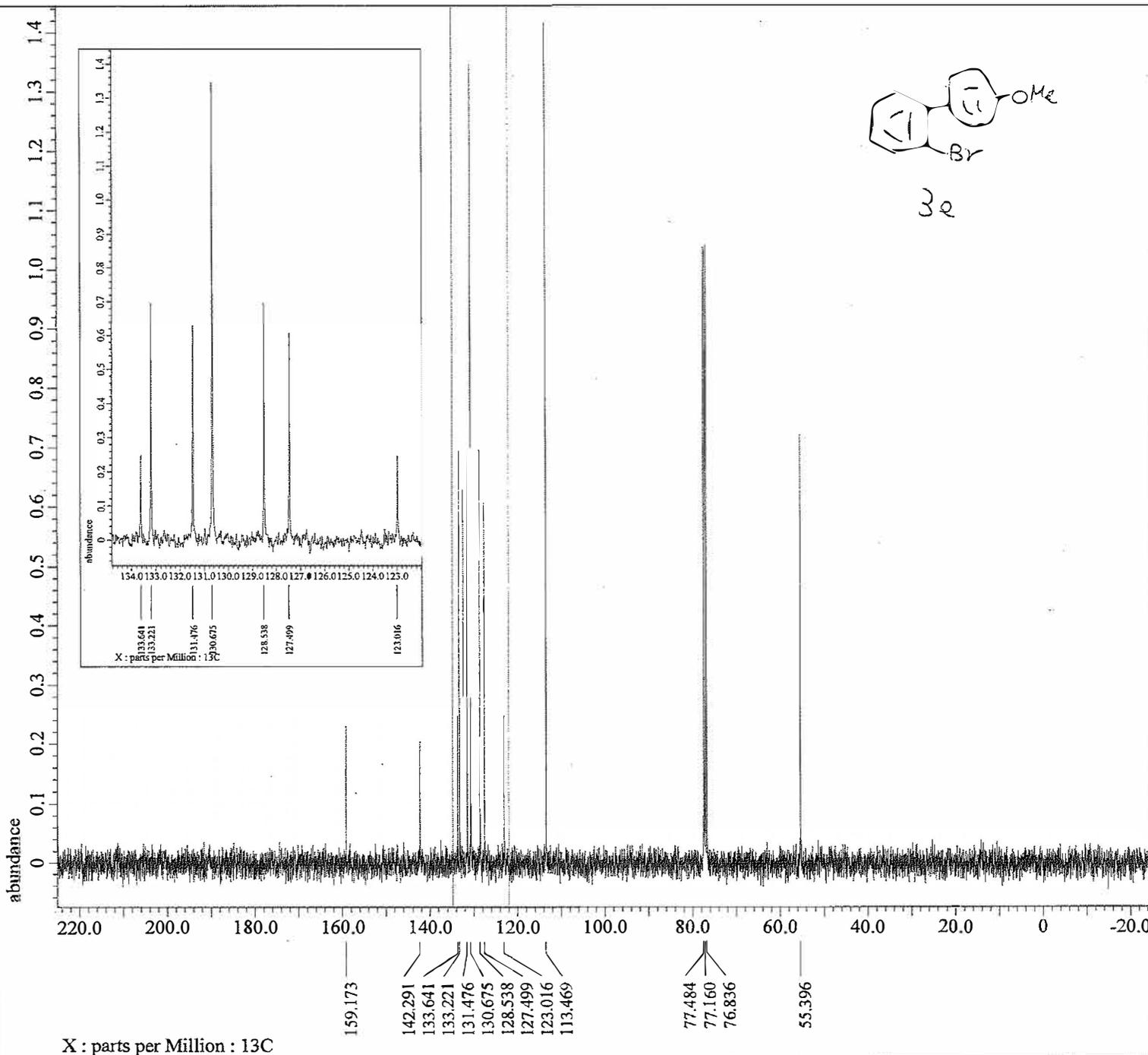
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Dim Units    = [ppm]
Dimensions   = X
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Spectromet  = JNM- EC S400

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X Doma n      = 1H
X Freq       = 391.78655441[MHz]
X Off set    = 5[ppm]
X Points     = 16384
X Prescans   = 1
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X Sweep     = 7.35294118[kHz]
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Irr Freq    = 391.78655441[MHz ]
Irr Offset   = 5[ppm]
Tri Domain   = 1H
Tri Freq    = 391.78655441[MHz]
Tri Offset   = 5[ppm]
Clipped     = FALS E
Scans       = 8
Tot astans  = 8

Relaxation   = 2.5[s ]
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X Acq Time   = 2.228224[s]
X Angle     = 45[deg ]
X Atn       = 1.9[dB ]
X Pulse     = 5.52[us]
Irr Mode     = Off
Tri Mode     = Off
Dante Pres at = FALS E
  
```



3e



```

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

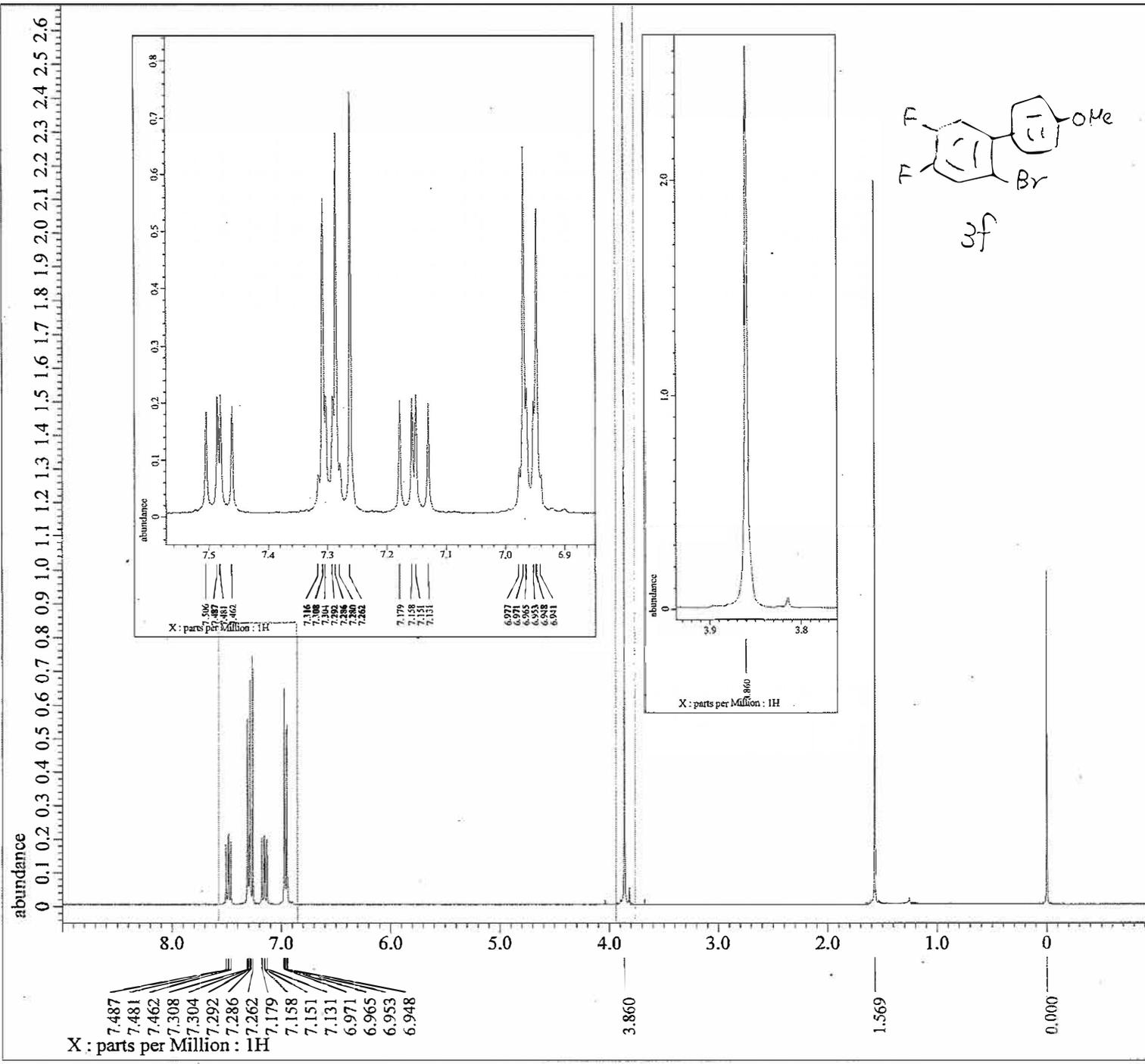
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Author        = element
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Revision_Time  = 25-JUL-2019 20:29:56

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X_Domain       = 13C
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X_Offset       = 100[ppm]
X_Points       = 32768
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X_Resolution   = 0.93958061[Hz]
X_Sweep        = 30.78817734[kHz]
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Initial_Wait    = 1[s]
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----- PROCESSING PARAMETERS -----

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dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s] )
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zerofill( 1 )
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machinephase
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以下に由来: SEO-829-1-pure-1H-1.jdf

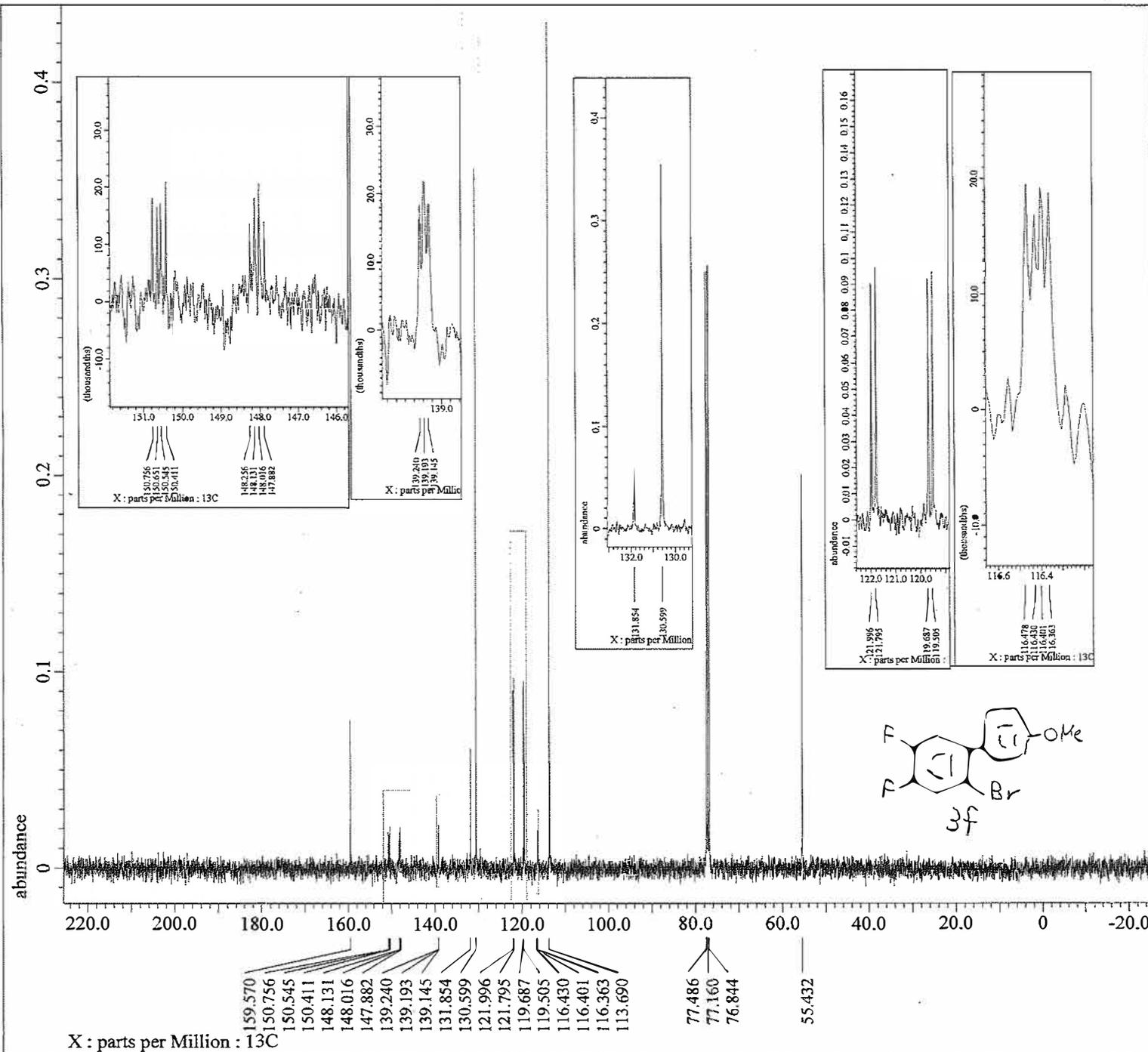
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Revision_Time   = 25-JUL-2019 20:50:47

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Dim_Size     = 13107
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Tri_Offset   = 5[ppm]
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Scans       = 8
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```

---- PROCESSING PARAMETERS ----
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machinephase
ppm

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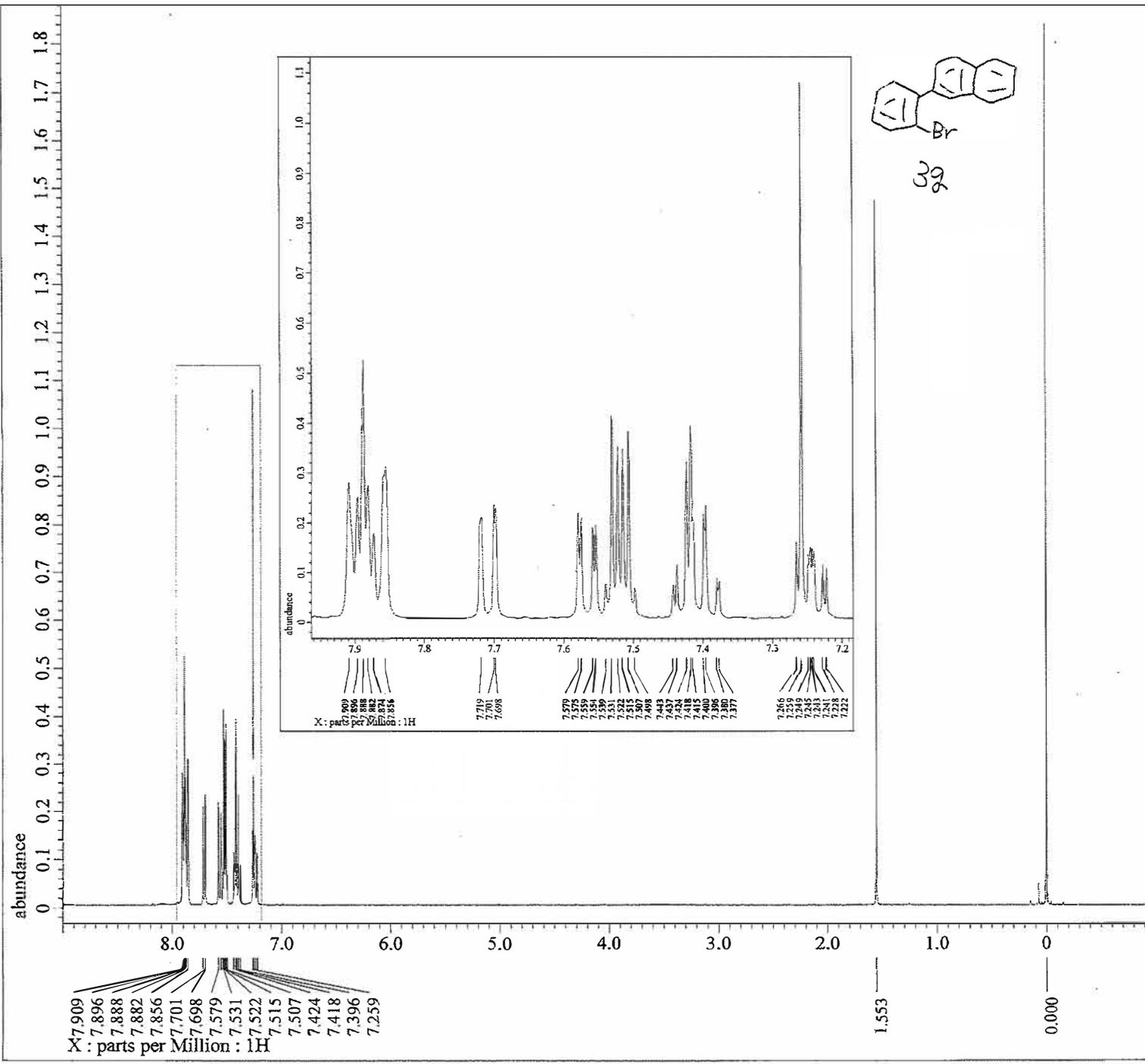
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Scans          = 100
Total_Scans    = 100

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```

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Irr_Atn_Dec     = 22.3 [dB]
Irr_Atn_Noise   = 22.3 [dB]
Irr_Noise       = WALTZ
Decoupling      = TRUE
Initial_Wait    = 1[s]
Noe             = TRUE

```



```

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

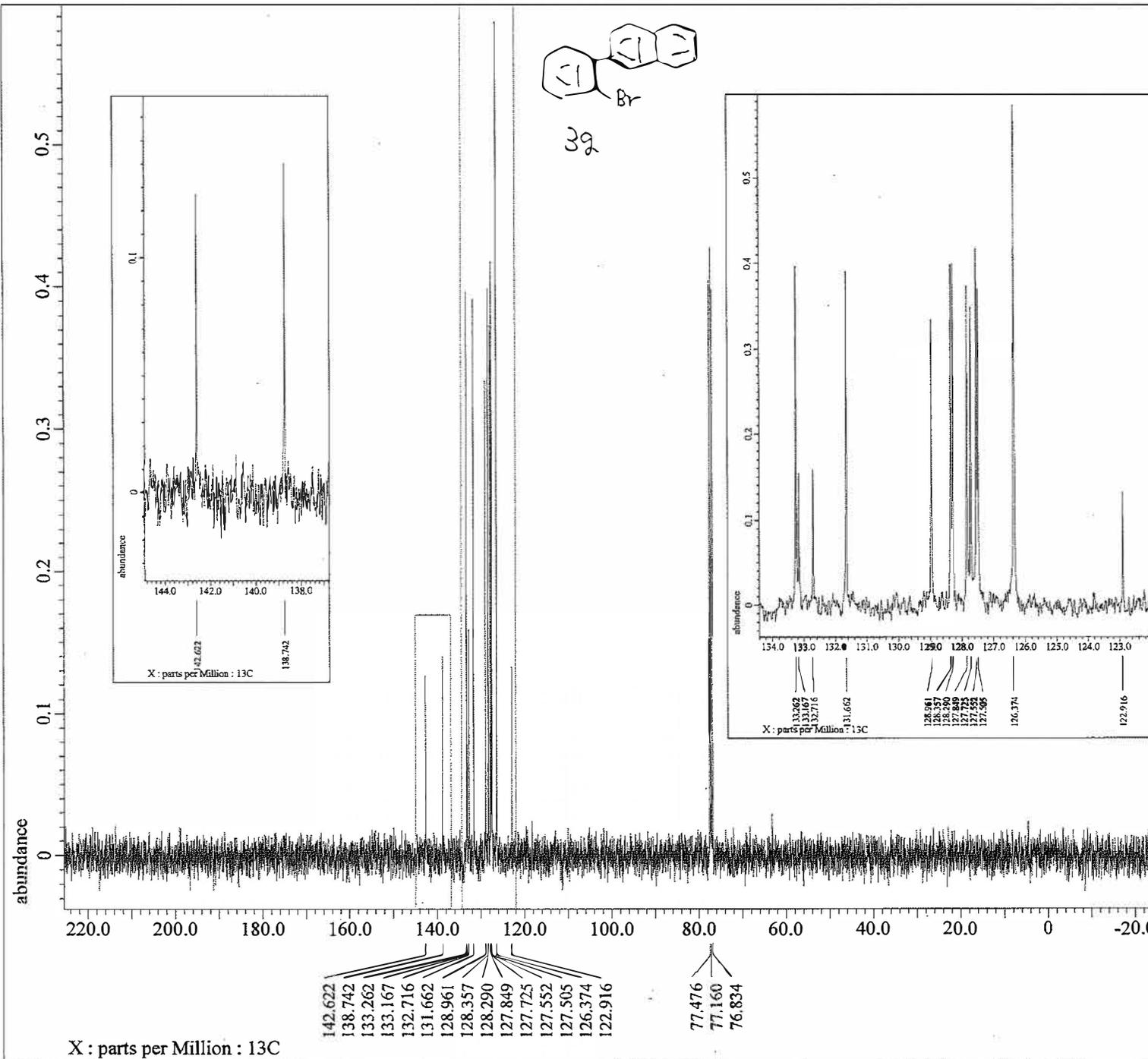
以下に由来: SEO-743-1-pure-1H-1.jdf

Filename           = SEO-743-1-pure-1H-2.jdf
Author             = element
Experiment         = single_pulse.ex2
Sample_Id         = S#313690
Solvent           = CHLOROFORM-D
Actual_Start_Time = 21-MAY-2019 17:03:04
Revision_Time     = 25-JUL-2019 21:36:51

Comment           = single_pulse
Data Format       = 1D COMPLEX
Dim_Size         = 13107
X_Domain        = 1H
Dim_Title       = 1H
Dim_Units       = [ppm]
Dimensions      = X
Site            = ECX 400P
Spectrometer    = DELTA2_NMR

Field_Strength   = 9.2982153[T] (400[MHz])
X_Acq_Duration  = 2.20725248[s]
X_Domain        = 1H
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]
Irr_Domain     = 1H
Irr_Freq      = 395.88430144[MHz]
Irr_Offset    = 5[ppm]
Tri_Domain    = 1H
Tri_Freq     = 395.88430144[MHz]
Tri_Offset   = 5[ppm]
Clipped      = FALSE
Scans        = 8
Total_Scans  = 8

Relaxation_Delay = 5[s]
Recvr_Gain       = 38
Temp_Get        = 19.9[dc]
X_90_Width     = 13.2[us]
X_Acq_Time     = 2.20725248[s]
X_Angle       = 45[deg]
X_Atn         = 3.5[db]
X_Pulse       = 6.6[us]
Irr_Mode      = Off
Tri_Mode      = Off
Dante_Presat  = FALSE
  
```



```

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

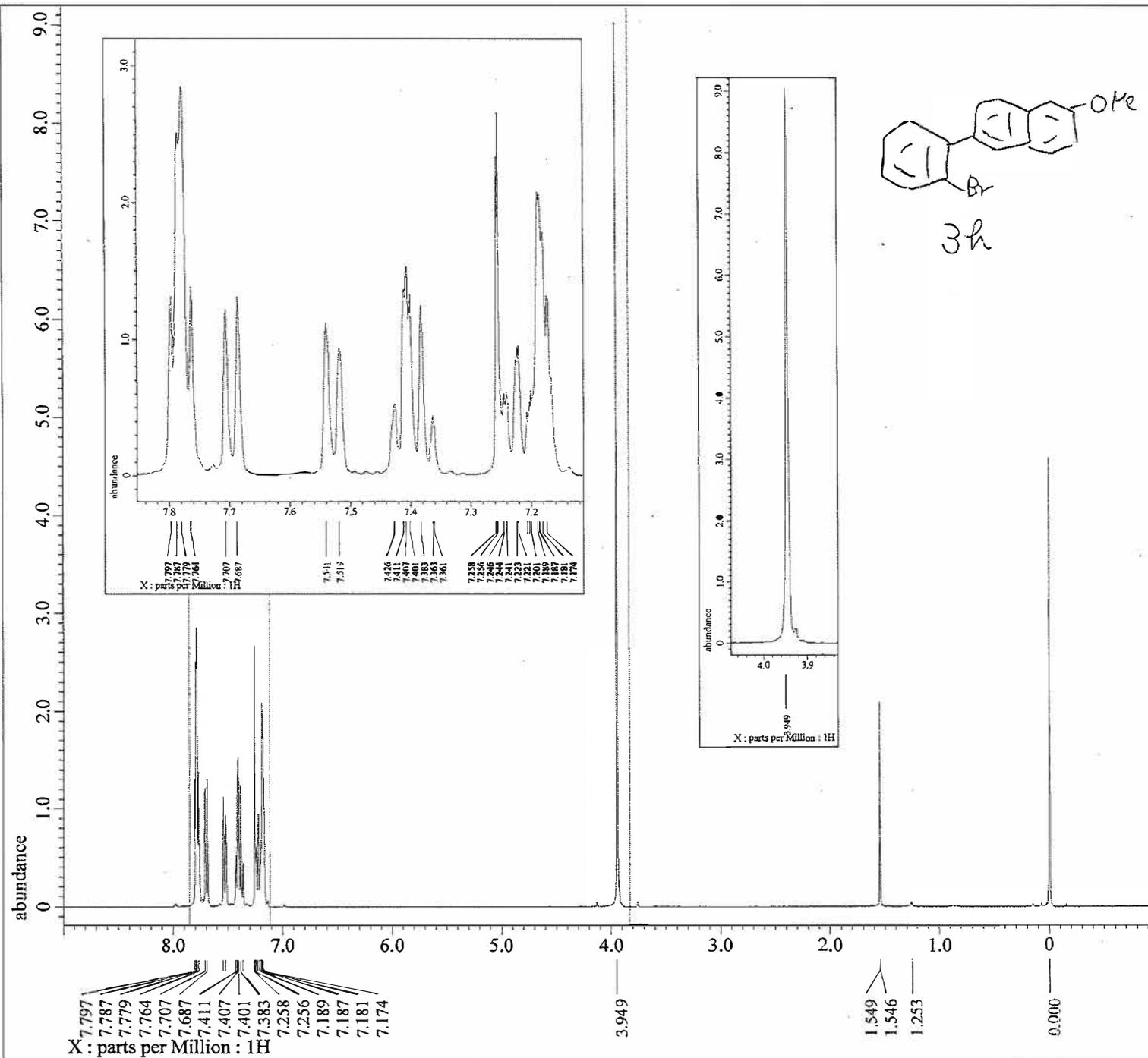
以下に由来: SEO-743-1-pure-13C-1.jdf

Filename      = SEO-743-1-pure-13C-2.jdf
Author       = element
Experiment   = single_pulse_dec
Sample_Id    = 1
Solvent      = CHLOROFORM-D
Actual_Start_Time = 21-MAY-2019 17:07:45
Revision_Time   = 25-JUL-2019 21:39:12

Comment      = single pulse decoupled ga
Data Format   = 1D COMPLEX
Dim_Size     = 26214
X_Domain     = 13C
Dim_Title    = 13C
Dim_Units    = [ppm]
Dimensions   = X
Site         = ECX 400P
Spectrometer = DELTA2_NMR

Field Strength = 9.2982153[T] (400[MHz])
X_Acq_Duration = 1.048576[s]
X_Domain       = 13C
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]
Irr_Domain    = 1H
Irr_Freq     = 395.88430144[MHz]
Irr_Offset    = 5[ppm]
Clipped      = FALSE
Scans        = 14
Total_Scans   = 14

Relaxation_Delay = 2[s]
Recvr_Gain      = 50
Temp_Get       = 20.2[dC]
X_90_Width     = 10.1[us]
X_Acq_Time     = 1.048576[s]
X_Angle        = 30[deg]
X_Atn         = 3.4[dB]
X_Pulse       = 3.366666667[us]
Irr_Atn_Dec   = 22.3[dB]
Irr_Atn_Noe   = 22.3[dB]
Irr_Noise     = WALTZ
Decoupling    = TRUE
Initial_Wait  = 1[s]
Noe           = TRUE
  
```



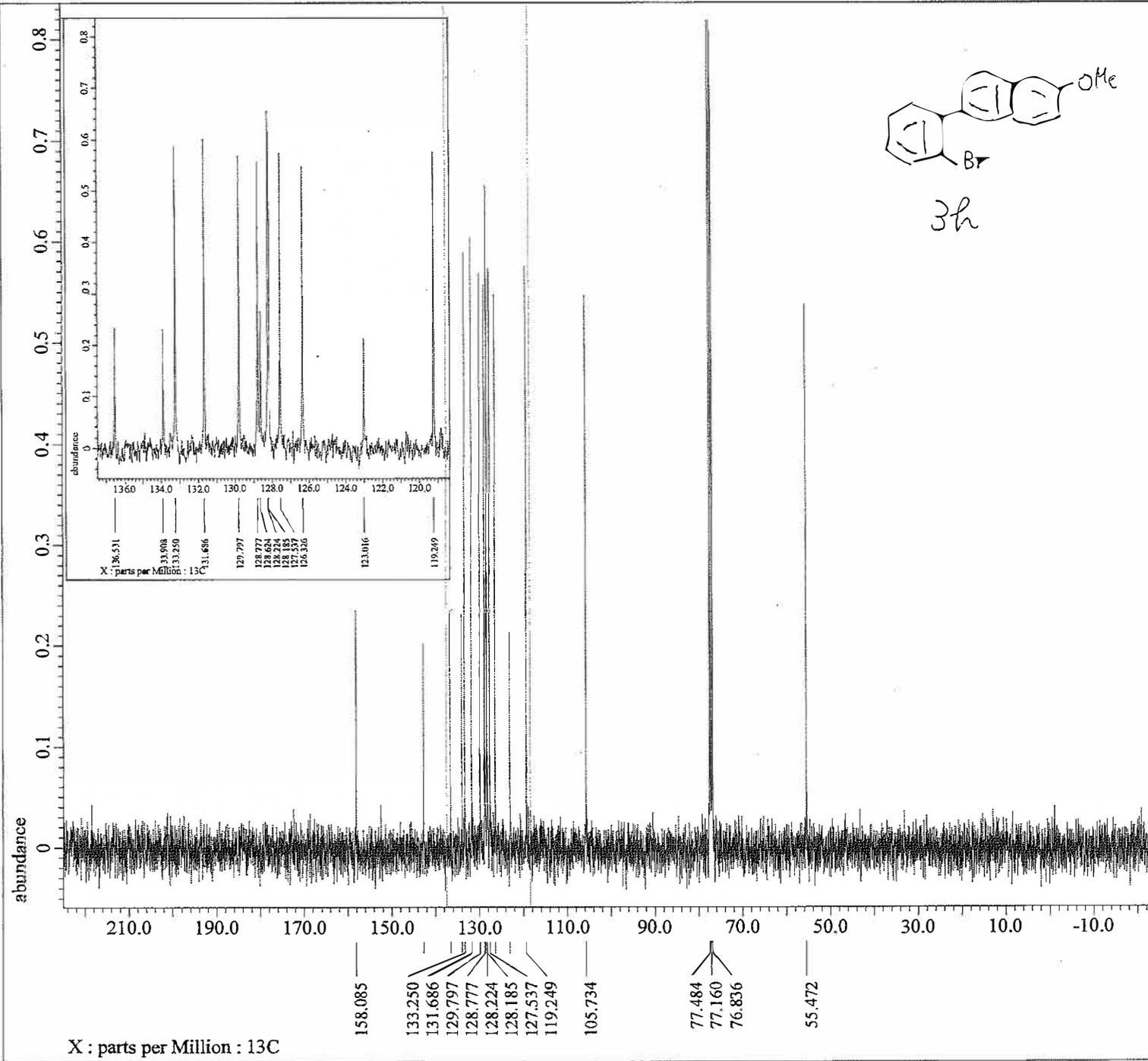
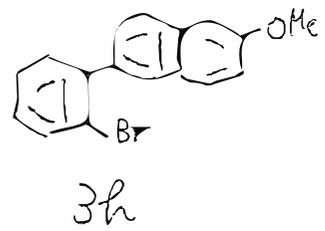
----- PROCESSING PARAMETERS -----  
 dc\_balance( 0, FALSE )  
 sexp( 0.2[Hz], 0.0[s] )  
 trapezoid3( 0[%], 80[%], 100[%] )  
 zerofill( 1 )  
 fft( 1, TRUE, TRUE )  
 machinephase  
 ppm  
 以下に由来: SEO-797-1-pure-1H-1.jdf

Filename = SEO-797-1-pure-1H-2.jdf  
 Author = element  
 Experiment = single\_pulse.ex2  
 Sample\_Id = S#441064  
 Solvent = CHLOROFORM-D  
 Actual\_Start\_Time = 18-MAY-2019 19:34:04  
 Revision\_Time = 25-JUL-2019 21:21:23

Comment = single\_pulse  
 Data\_Format = 1D\_COMPLEX  
 Dim\_Size = 13107  
 X\_Domain = 1H  
 Dim\_Title = 1H  
 Dim\_Units = [ppm]  
 Dimensions = X  
 Site = ECS 400  
 Spectrometer = JNM-ECS400

Field\_Strength = 9.20197068[T] (390[MHz])  
 X\_Acq\_Duration = 2.228224[s]  
 X\_Domain = 1H  
 X\_Freq = 391.78655441[MHz]  
 X\_Offset = 5[ppm]  
 X\_Points = 16384  
 X\_Prescans = 1  
 X\_Resolution = 0.44878791[Hz]  
 X\_Sweep = 7.35294118[kHz]  
 Irr\_Domain = 1H  
 Irr\_Freq = 391.78655441[MHz]  
 Irr\_Offset = 5[ppm]  
 Tri\_Domain = 1H  
 Tri\_Freq = 391.78655441[MHz]  
 Tri\_Offset = 5[ppm]  
 Clipped = FALSE  
 Scans = 8  
 Total\_Scans = 8

Relaxation\_Delay = 5[s]  
 Recvr\_Gain = 50  
 Temp\_Get = 19.2[dC]  
 X\_90\_Width = 11.04[us]  
 X\_Acq\_Time = 2.228224[s]  
 X\_Angle = 45[deg]  
 X\_Atn = 1.9[dB]  
 X\_Pulse = 5.52[us]  
 Irr\_Mode = Off  
 Tri\_Mode = Off  
 Dante\_Presat = FALSE



```

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

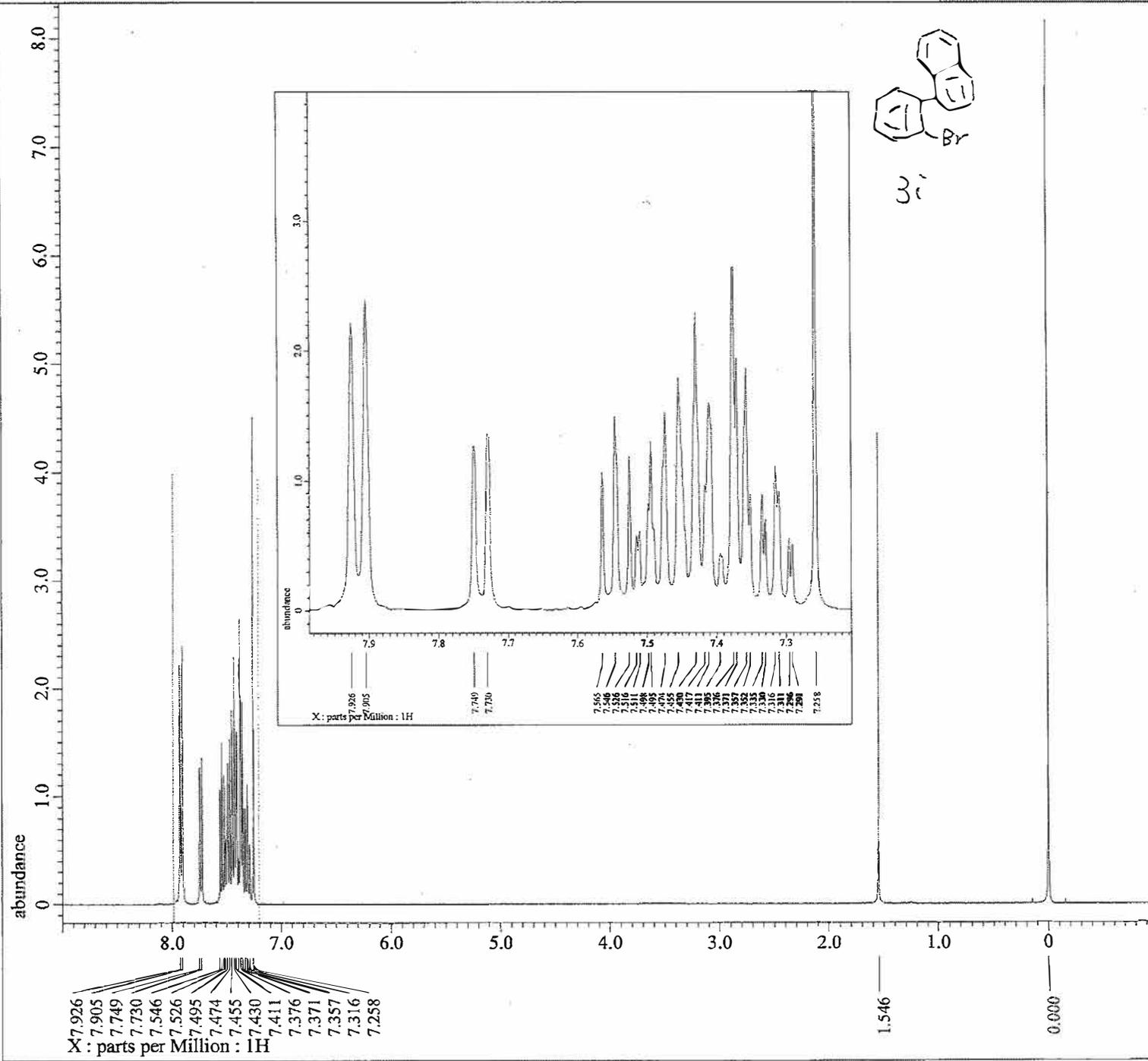
以下に由来: SEO-797-1-pure-13C-1.jdf

Filename      = SEO-797-1-pure-13C-2.jdf
Author       = element
Experiment   = single_pulse_dec
Sample_Id    = 1
Solvent      = CHLOROFORM-D
Actual_Start_Time = 18-MAY-2019 19:39:33
Revision_Time   = 25-JUL-2019 21:24:18

Comment      = single pulse decoupled ga
Data Format   = 1D COMPLEX
Dim Size     = 26214
X Domain     = 13C
Dim Title    = 13C
Dim Units    = [ppm]
Dimensions   = X
Site         = ECS 400
Spectrometer = JNM-ECS400

Field_Strength = 9.20197068[T] (390[MHz])
X_Acq_Duration = 1.06430464[s]
X_Domain       = 13C
X_Freq        = 98.51479726[MHz]
X_Offset      = 100[ppm]
X_Points      = 32768
X_Prescans    = 4
X_Resolution  = 0.93958061[Hz]
X_Sweep       = 30.78817734[kHz]
Irr_Domain    = 1H
Irr_Freq      = 391.78655441[MHz]
Irr_Offset    = 5[ppm]
Clipped       = FALSE
Scans         = 32
Total_Scans   = 32

Relaxation_Delay = 2[s]
Recvr_Gain       = 60
Temp_Get         = 19.4[dC]
X_90_Width      = 9.11[us]
X_Acq_Time      = 1.06430464[s]
X_Angle         = 30[deg]
X_Atn           = 4.9[dB]
X_Pulse         = 3.03666667[us]
Irr_Atn_Dec     = 22.255[dB]
Irr_Atn_Noise  = 22.255[dB]
Irr_Noise       = WALTZ
Decoupling      = TRUE
Initial_wait    = 1[s]
Noe              = TRUE
  
```



```

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

以下に由来: SEO-757-1-pure-1H-1.jdf

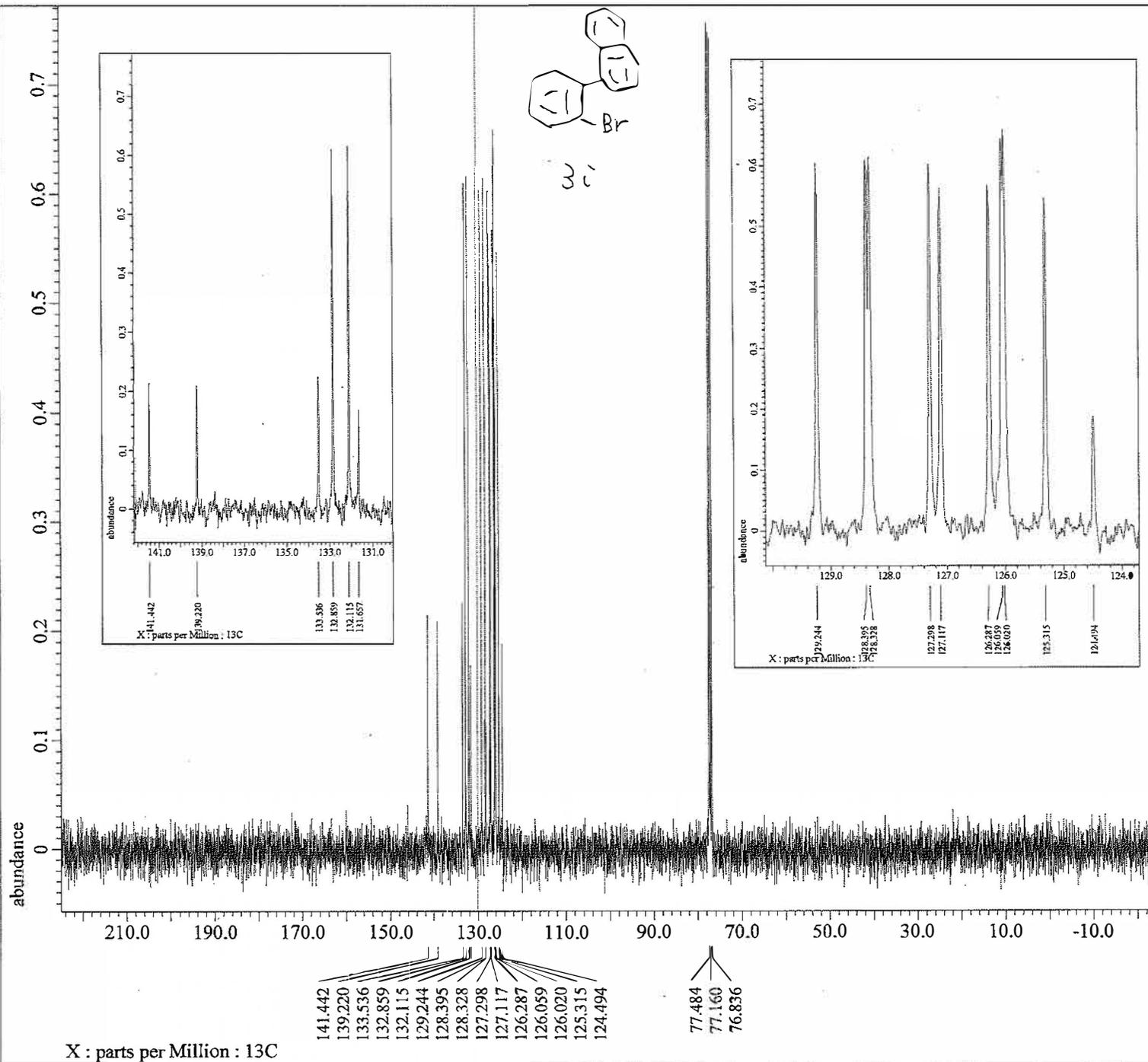
Filename      = SEO-757-1-pure-1H-2.jdf
Author       = element
Experiment   = single_pulse.ex2
Sample_Id    = S#539971
Solvent      = CHLOROFORM-D
Actual_Start_Time = 17-MAY-2019 22:19:13
Revision_Time   = 25-JUL-2019 21:15:03

Comment      = single_pulse
Data Format   = 1D COMPLEX
Dim Size     = 13107
X Domain     = 1H
Dim Title    = 1H
Dim Units    = [ppm]
Dimensions   = X
Site         = ECS 400
Spectrometer = JNM-ECS400

Field_Strength = 9.20197068[T] (390[MHz])
X_Acq_Duration = 2.228224[s]
X_Domain       = 1H
X_Freq        = 391.78655441[MHz]
X_Offset      = 5[ppm]
X_Points      = 16384
X_Prescans    = 1
X_Resolution  = 0.44878791[Hz]
X_Sweep       = 7.3294118[kHz]
Irr_Domain    = 1H
Irr_Freq     = 391.78655441[MHz]
Irr_Offset    = 5[ppm]
Tri_Domain    = 1H
Tri_Freq     = 391.78655441[MHz]
Tri_Offset    = 5[ppm]
Clipped      = FALSE
Scans        = 8
Total_Scans  = 8

Relaxation_Delay = 5[s]
Recvr_Gain       = 52
Temp_Get         = 19.1[dC]
X_90_Width      = 11.04[us]
X_Acq_Time      = 2.228224[s]
X_Angle         = 45[deg]
X_Atn           = 1.9[dB]
X_Pulse        = 5.52[us]
Irr_Mode        = Off
Tri_Mode        = Off
Dante_Presat    = FALSE

```



```

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

```

以下に由来: SEO-757-1-pure-13C-1.jdf

```

Filename      = SEO-757-1-pure-13C-2.jdf
Author       = element
Experiment    = single_pulse_dec
Sample_Id    = 1
Solvent      = CHLOROFORM-D
Actual_Start_Time = 17-MAY-2019 22:24:45
Revision_Time = 25-JUL-2019 21:17:02

```

```

Comment      = single pulse decoupled ga
Data Format   = 1D COMPLEX
Dim Size     = 26214
X_Domain     = 13C
Dim Title    = 13C
Dim Units    = [ppm]
Dimensions   = X
Site         = ECS 400
Spectrometer = JNM-ECS400

```

```

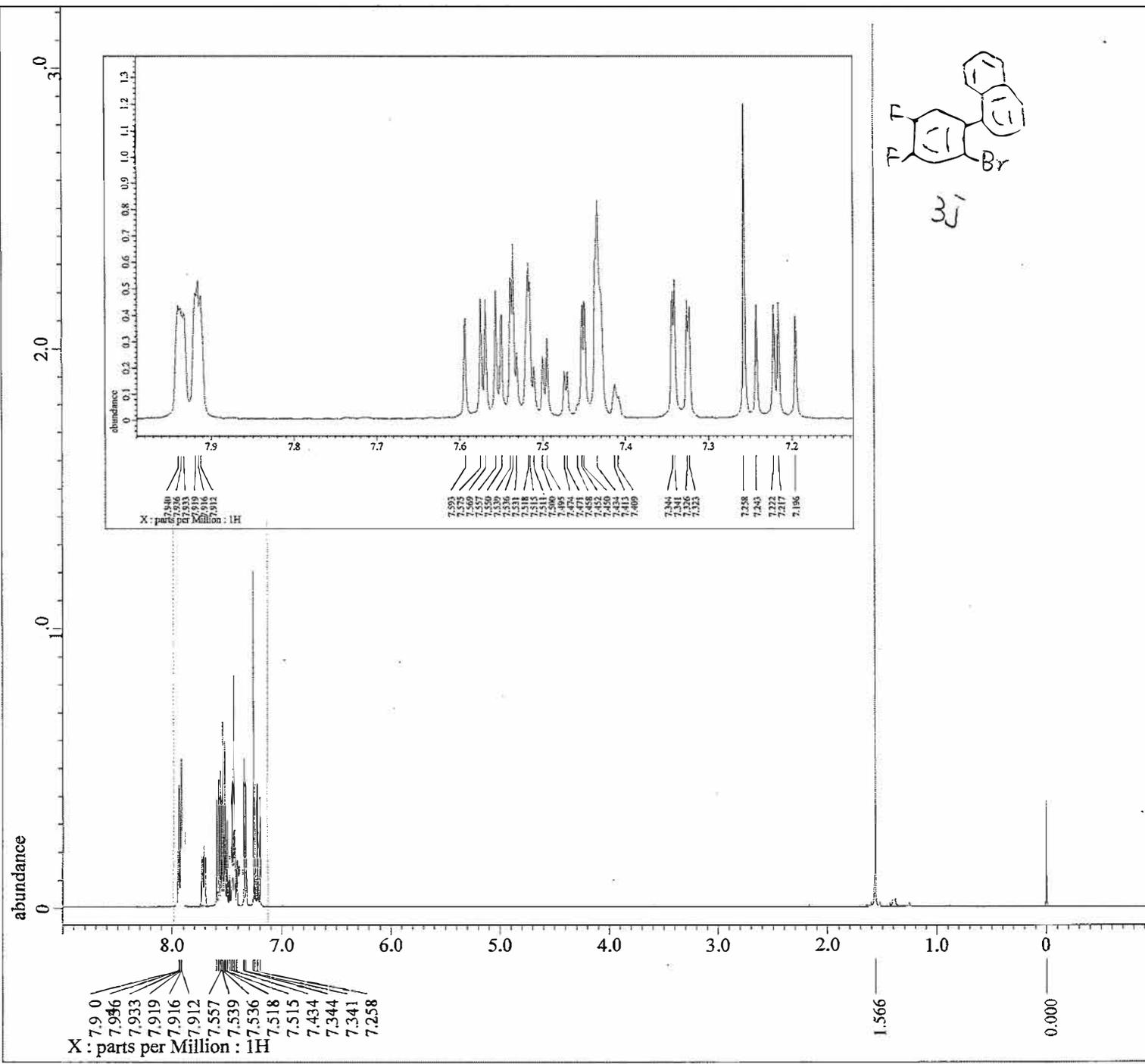
Field Strength = 9.20197068[T] (390[MHz])
X_Acq_Duration = 1.06430464[s]
X_Domain       = 13C
X_Freq         = 98.51479726[MHz]
X_Offset       = 100[ppm]
X_Points       = 32768
X_Prescans     = 4
X_Resolution   = 0.93958061[Hz]
X_Sweep        = 30.78817734[kHz]
Irr_Domain     = 1B
Irr_Freq       = 391.78655441[MHz]
Irr_Offset     = 5[ppm]
Clipped        = FALSE
Scans          = 39
Total_Scans    = 39

```

```

Relaxation_Delay = 2[s]
Recvr_Gain       = 60
Temp_Get         = 19.4[dC]
X_90_Width       = 9.11[us]
X_Acq_Time       = 1.06430464[s]
X_Angle          = 30[deg]
X_Atn            = 4.9[dB]
X_Pulse          = 3.03666667[us]
Irr_Atn_Dec      = 22.255[dB]
Irr_Atn_Noise   = 22.255[dB]
Irr_Noise        = WALTZ
Decoupling       = TRUE
Initial_Wait     = 1[s]
Noe              = TRUE

```



```

----- PROCESSING PARAMETERS -----
dc_balance( 0, FALSE )
sexp( 0.2[Hz], 0.0[s ] )
t_apezoid3( 0[%], 80[%], 100[%] )
zer_ofill( 1 )
fft( 1, TRUE, TRUE )
machin ep3a
ppm

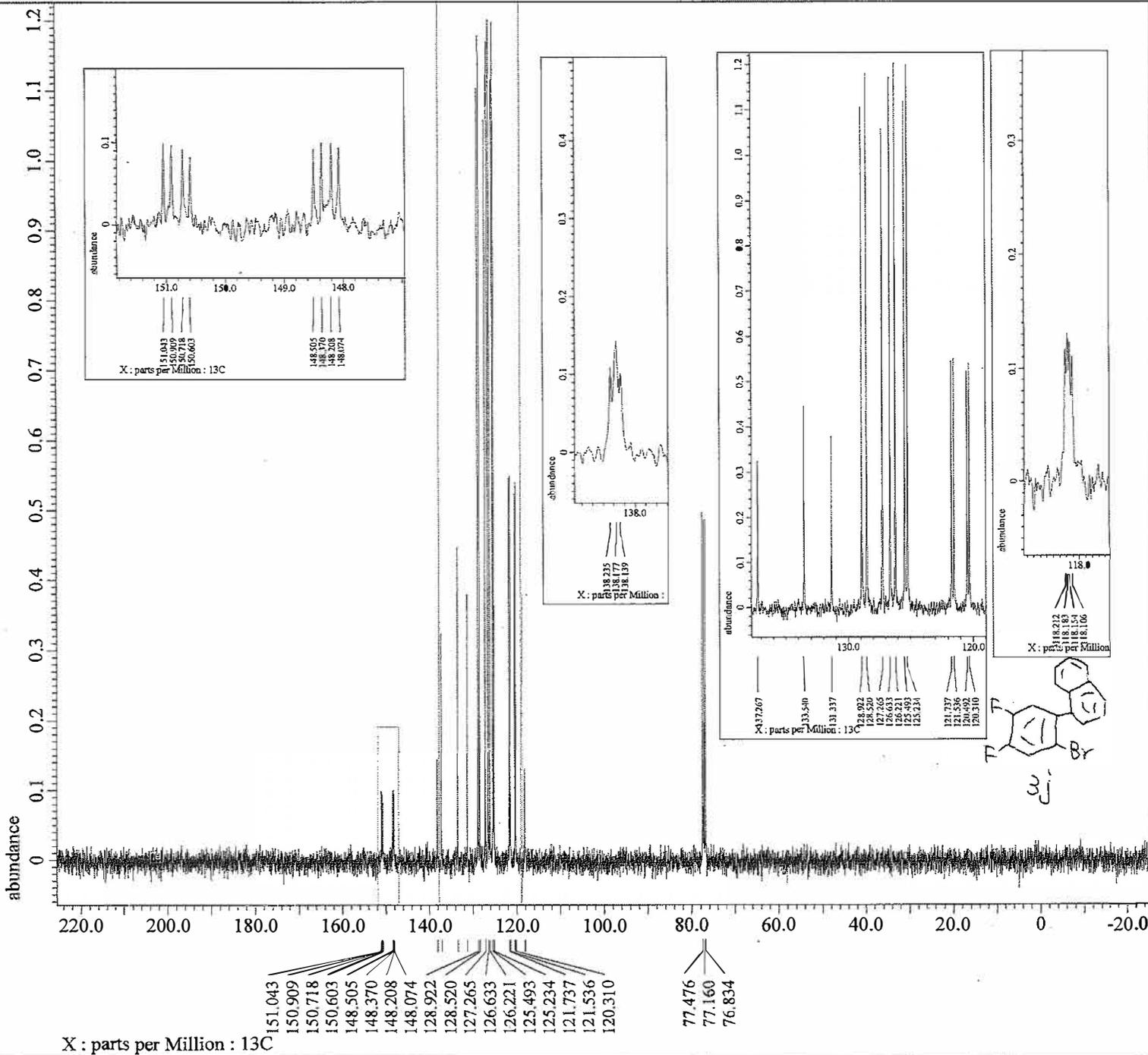
以下に由来: SE 0-812-1-pur-1H-1.jdf

F i lename      = SE 0812-1-pure-1H-2.jdf
Author         = element
Experiment t   = singl epulse. ex2
Sample Id     = 1
Solvent       = CHLOR OF O RM-D
Ac t uaStart Time = 6-JUN-2019 16:39:43
Revision Time  = 25-JUL-2019 21:55:27

Comment       = single pulse
Dat aFormat   = 1D COMPLEX
Dim Size      = 13107
X Domain      = 1H
Dim Title     = 1H
Dim Units     = [ppm]
Dimensions    = X
Site         = ECX 400P
Spectrometer  = DE LTA2_NMR

Field Strength = 9.2982153[T I400[MH z]]
X Acq Duration = 2.20725248[s]
X Domain      = 1H
X Freq       = 395.88430144[MH z]
X Offset     = 5[ppm]
X Points     = 16384
X Prescans   = 1
X Resolution = 0.45305193[Hz]
X Sweep     = 7.42280285[k Hz]
Irr Domain   = 1H
Irr Freq     = 395.88430144[M Hz]
Irr Offset   = 5[ppm]
Tri Domain   = 1H
Tri Freq     = 395.88430144[MHz]
Tri Offset   = 5[ppm]
Clipped      = FALSE
Scans        = 8
Total Scans  = 8

Relaxation_Delay = 5[s]
Recvr Gain      = 38
Temp Get       = 21.2[dC]
X 90 Width     = 13.2[us]
X Acq Time     = 2.20725248[s ]
X Angle       = 45[deg]
X Atn         = 3.5[dB]
X Pulse       = 6.6[us ]
Irr Mode      = 0 ff
Tri Mode      = Off
Dante Pres #  = FALSE
  
```



```

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

```

以下に由来: SEO-812-1-pure-13C-1.jdf

```

Filename      = SEO-812-1-pure-13C-2.jdf
Author       = element
Experiment    = single_pulse_dec
Sample Id    = 1
Solvent      = CHLOROFORM-D
Actual_Start_Time = 6-JUN-2019 16:50:08
Revision_Time  = 25-JUL-2019 21:59:47

```

```

Comment      = single pulse decoupled ga
Data Format   = 1D COMPLEX
Dir Size     = 26214
X Domain     = 13C
Dim Title    = 13C
Dim Units    = [ppm]
Dimensions   = X
Site         = ECX 400P
Spectrometer = DELTA2_NMR

```

```

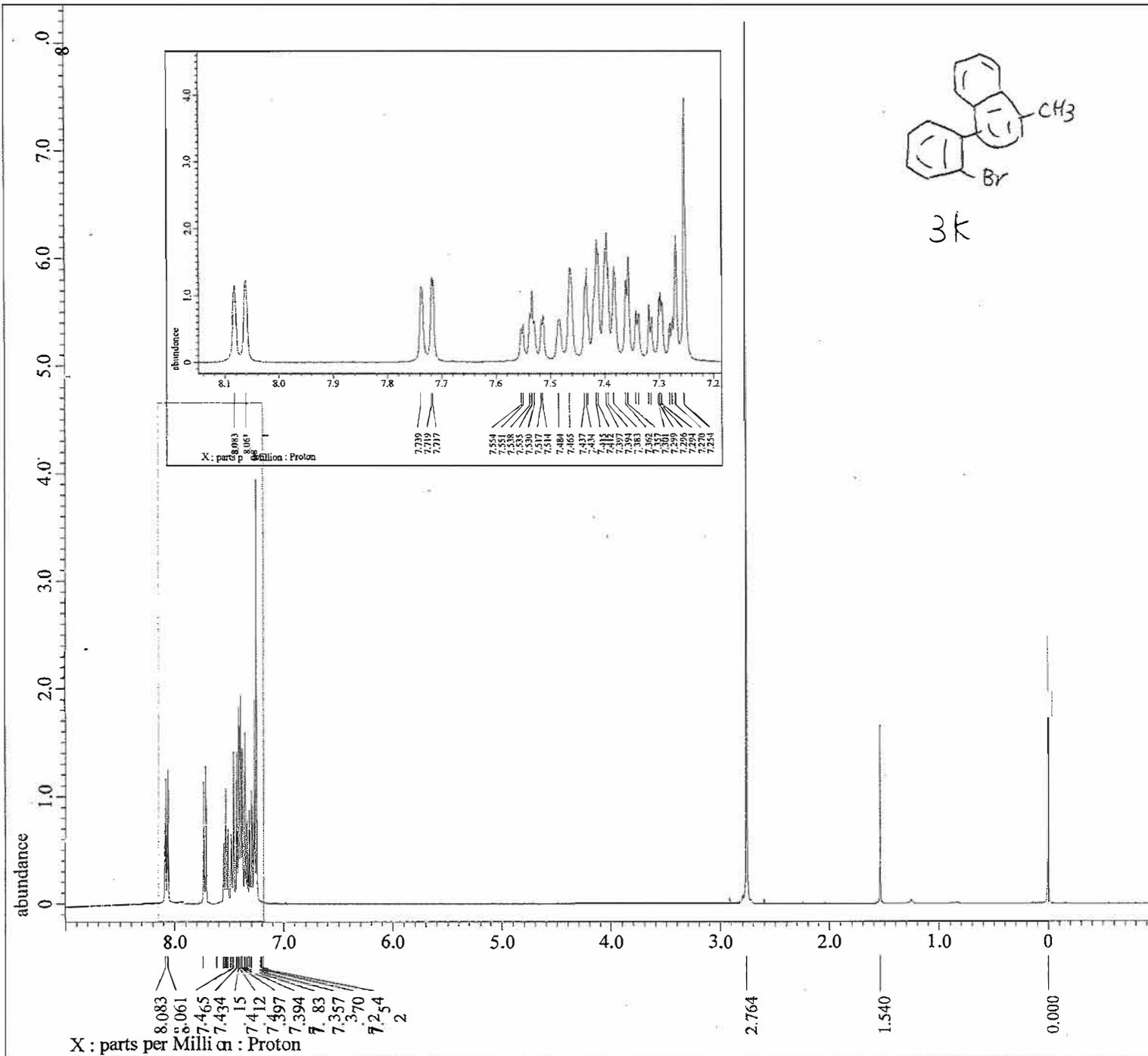
Field Strength = 9.2982153[T] (400[MHz])
X Acq Duration = 1.048576[s]
X Domain       = 13C
X Freq        = 99.54517646[MHz]
X Offset      = 100[ppm]
X Points      = 32768
X Prescans    = 4
X Resolution  = 0.95367432[Hz]
X Sweep       = 31.25[kBz]
Irr Domain    = 1H
Irr Freq     = 395.88430144[MHz]
Irr Offset    = 5[ppm]
Clipped      = FALSE
Scans        = 22
Total Scans  = 22

```

```

Relaxation_Delay = 2[s]
Recvr Gain       = 54
Temp_Get        = 21.5[dc]
X 90 Width      = 10.1[us]
X Acq Time      = 1.048576[s]
X Angle         = 30[deg]
X Atn           = 3.4[db]
X Pulse        = 3.36666667[us]
Irr Atn Dec     = 22.3[db]
Irr Atn Noe    = 22.3[db]
Irr Noise       = WALTZ
Decoupling      = TRUE
Initial_Wait    = 1[s]
Noe             = TRUE

```



```

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

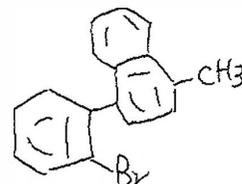
以下に由来: SEO-713-2-pure_Proton-1-1.jdf

Filename      = SEO-713-2-pure_Proton-1-2
Author        = element
Experiment    = proton_jxp
Sample_Id     = SEO-713-2-pure
Solvent       = CHLOROFORM-D
Actual_Start Time = 12-APR-2019 17:10:48
Revision_Time = 25-JUL-2019 21:42:47

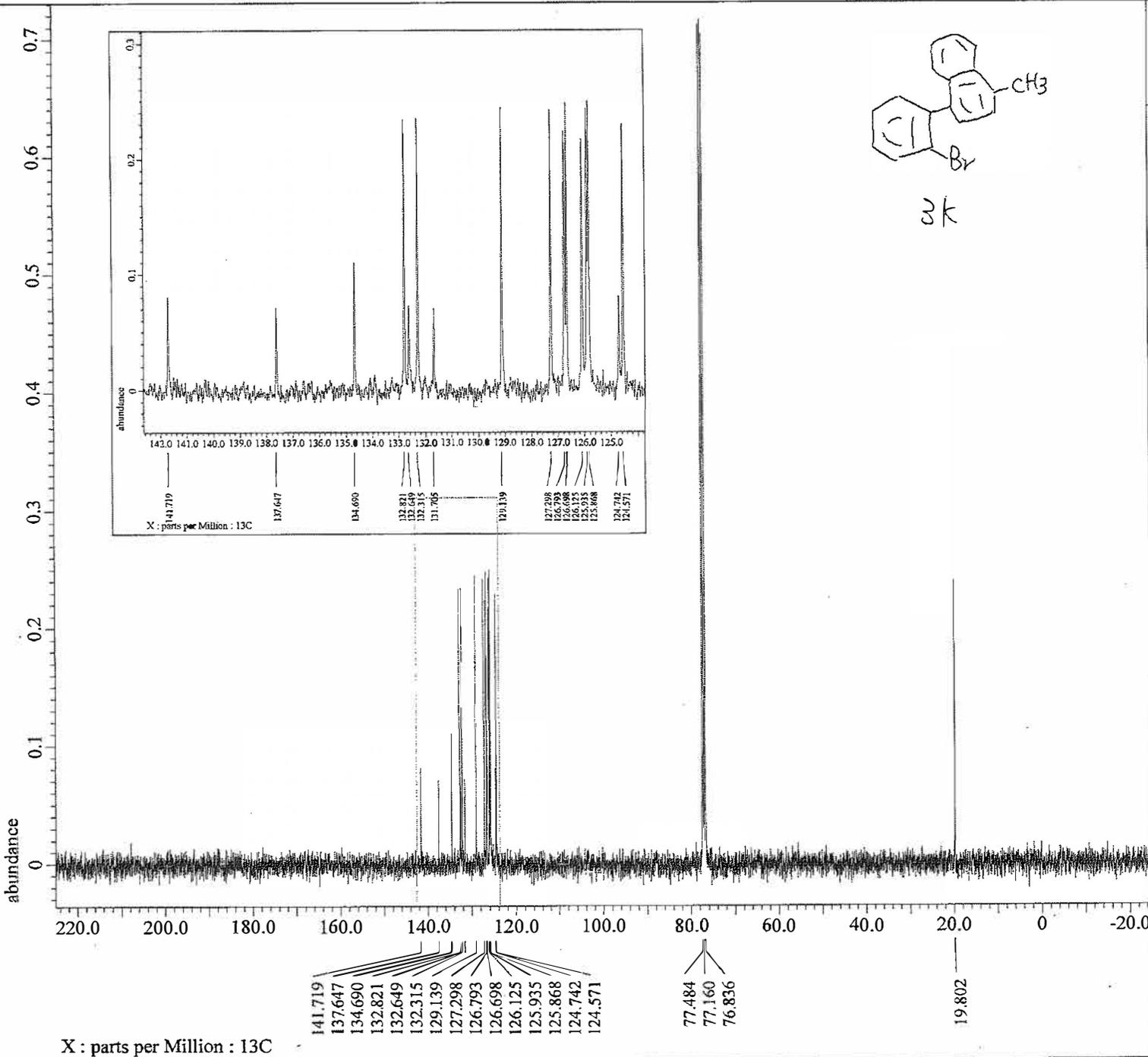
Comment       = single_pulse
Data_Format   = 1D COMPLEX
Dim_Size      = 13107
X_Domain      = Proton
Dim_Title     = Proton
Dim_Units     = [ppm]
Dimensions    = X
Spectrometer  = DELTA2_NMR

Field_Strength = 9.4073814[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_Clippped = 6.00961538 [kHz]
Irr_Domain     = Proton
Irr_Freq       = 400.53219825 [MHz]
Irr_Offset     = 5 [ppm]
Tri_Domain     = Proton
Tri_Freq       = 400.53219825 [MHz]
Tri_Offset     = 5 [ppm]
Clipped        = FALSE
Scans          = 8
Total_Scans    = 8

Relaxation_Delay = 5[s]
Recvr_Gain       = 44
Temp_Get         = 19.6 [dC]
X_90_W_dth      = 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
  
```



3k



```

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

以下に由来: SEO-713-2-pure-13C-1.jdf

```

Filename      = SEO-713-2-pure-13C-2.jdf
Author        = element
Experiment     = single_pulse_dec
Sample Id     = 1
Solvent       = CHLOROFORM-D
Actual_Start_Time = 13-APR-2019 01:06:22
Revision_Time  = 25-JUL-2019 21:48:57
  
```

```

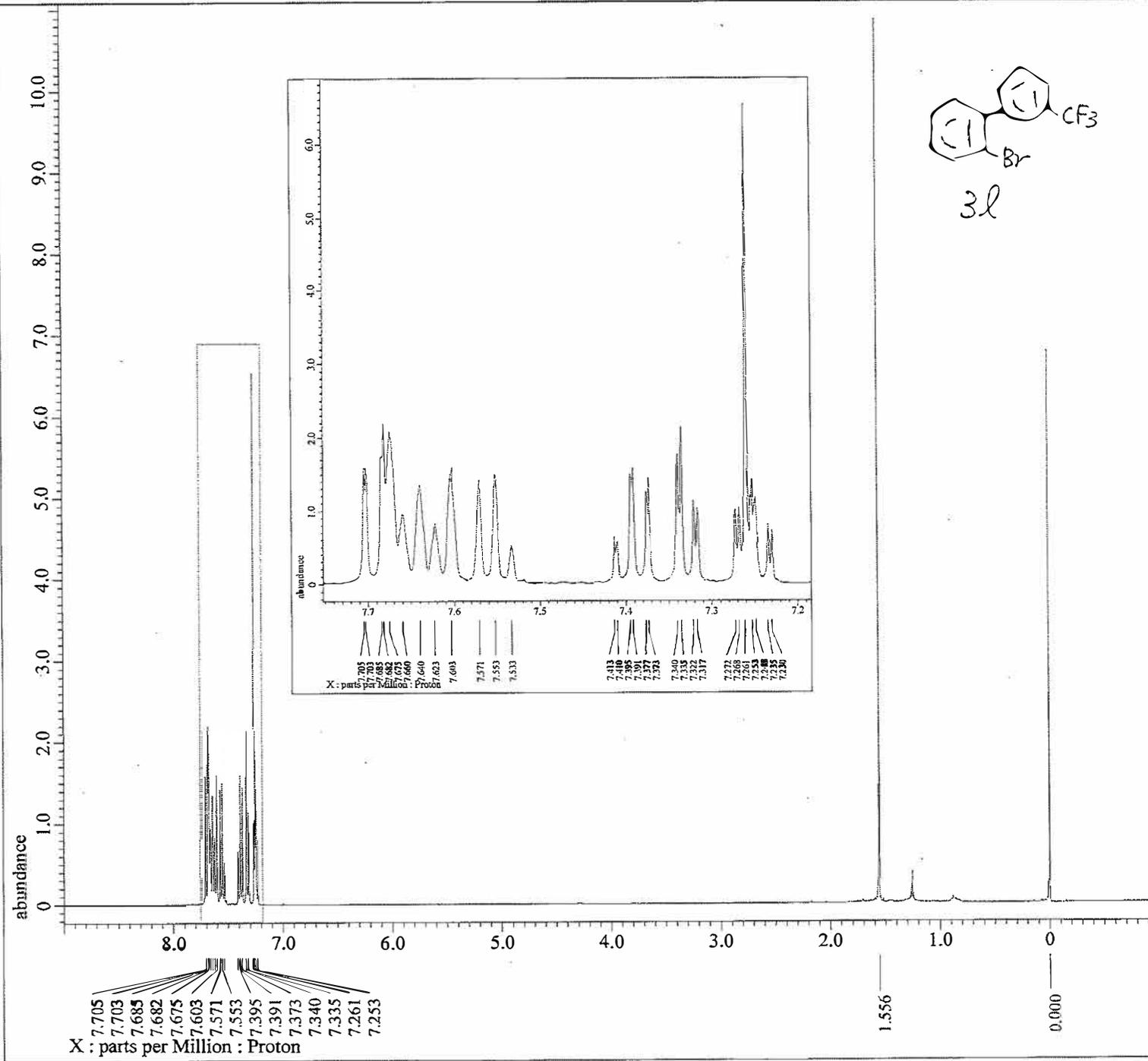
Comment       = single pulse decoupled ga
Data Format    = 1D COMPLEX
Dim Size      = 26214
X Domain      = 13C
Dim Title     = 13C
Dim Units     = [ppm]
Dimensions    = X
Site          = ECS 400
Spectrometer  = JNM-ECS400
  
```

```

Field_Strength = 9.20197068[T] (390[MHz])
X Acq Duration = 1.06430464[s]
X Domain       = 13C
X Freq         = 98.51479726[MHz]
X Offset       = 100 [ppm]
X Points       = 32768
X Prescans     = 4
X Resolution   = 0.93958061 [Hz]
X Sweep       = 30.78817734 [kHz]
Irr Domain     = 1H
Irr Freq       = 391.78655441 [MHz]
Irr Offset     = 5 [ppm]
Clipped        = FALSE
Scans          = 164
Total_Scans    = 164
  
```

```

Relaxation_Delay = 2[s]
Recvr Gain       = 60
Temp_Get         = 20.2 [dC]
X 90 Width       = 9.11 [us]
X Acq Time       = 1.06430464 [s]
X Angle          = 30 [deg]
X Atn            = 4.9 [dB]
X Pulse         = 3.03666667 [us]
Irr Atn Dec      = 22.255 [dB]
Irr Atn Noe     = 22.255 [dB]
Irr Noise        = WALTZ
Decoupling       = TRUE
Initial_Wait     = 1[s]
Noe              = TRUE
  
```



```

---- 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

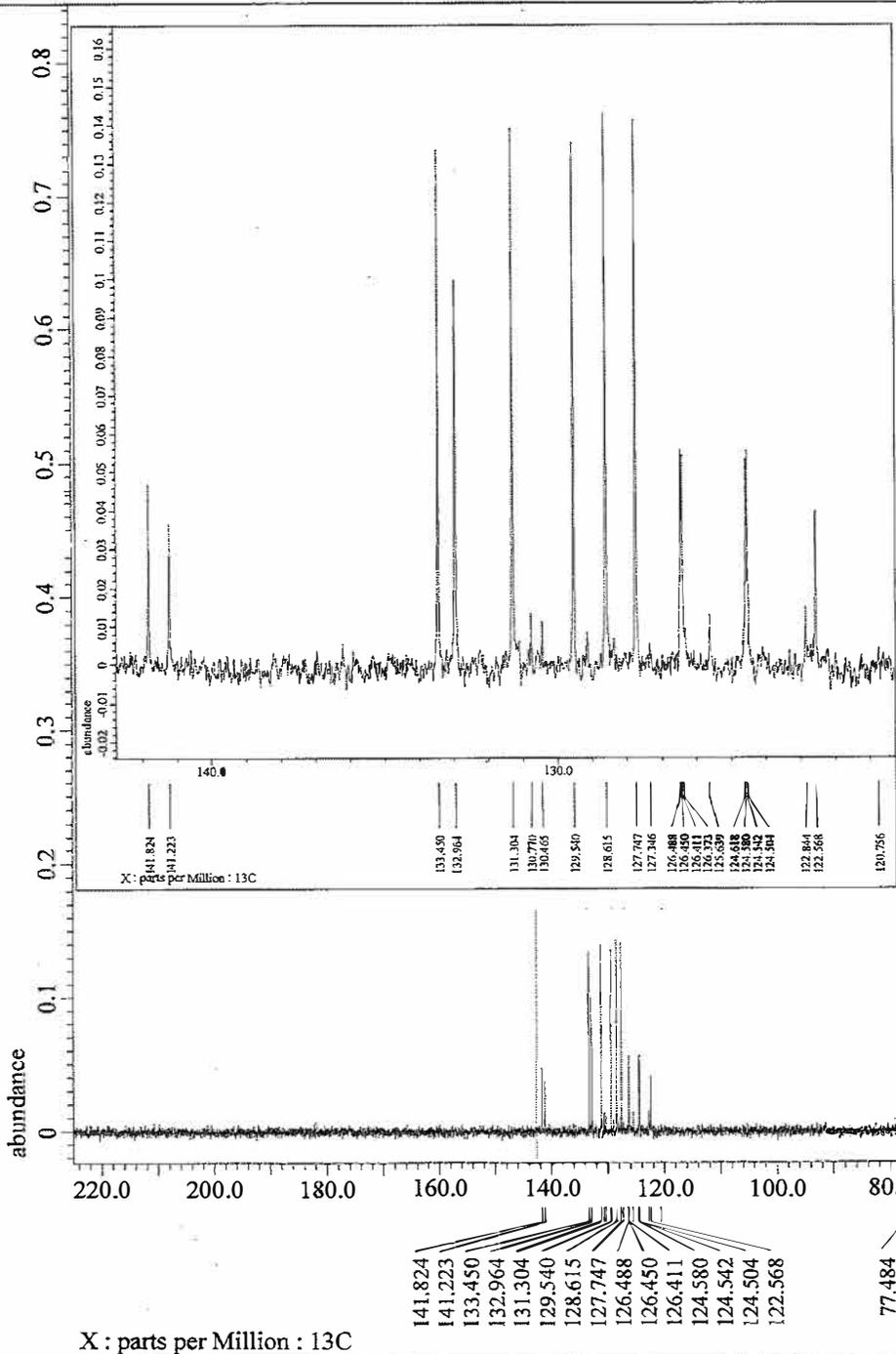
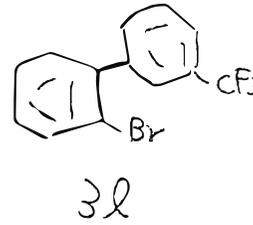
以下に由来: SEO-810-3-pure_Proton-1-1.jdf

Filename      = SEO-810-3-pure_Proton-1-2
Author        = element
Experiment     = proton.jxp
Sample_Id     = SEO-810-3-pure
Solvent       = CHLOROFORM-D
Actual_Start_Time = 31-MAY-2019 14:52:01
Revision_Time  = 25-JUL-2019 22:31:47

Comment       = single_pulse
Data Format    = 1D COMPLEX
Dim Size      = 13107
X_Domain     = Proton
Dim Title     = Proton
Dim Units     = [ppm]
Dimensions    = X
Spectrometer  = DELTA2_NMR

Field Strength = 9.4073814[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_Clip = 6.00961538[kHz]
Irr_Domain    = Proton
Irr Freq      = 400.53219825[MHz]
Irr Offset    = 5[ppm]
Tri_Domain    = Proton
Tri Freq      = 400.53219825[MHz]
Tri Offset    = 5[ppm]
Clipped       = FALSE
Scans         = 8
Total Scans   = 8

Relaxation_Delay = 5[s]
Recvr Gain       = 48
Temp_Get         = 20.2[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
  
```



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

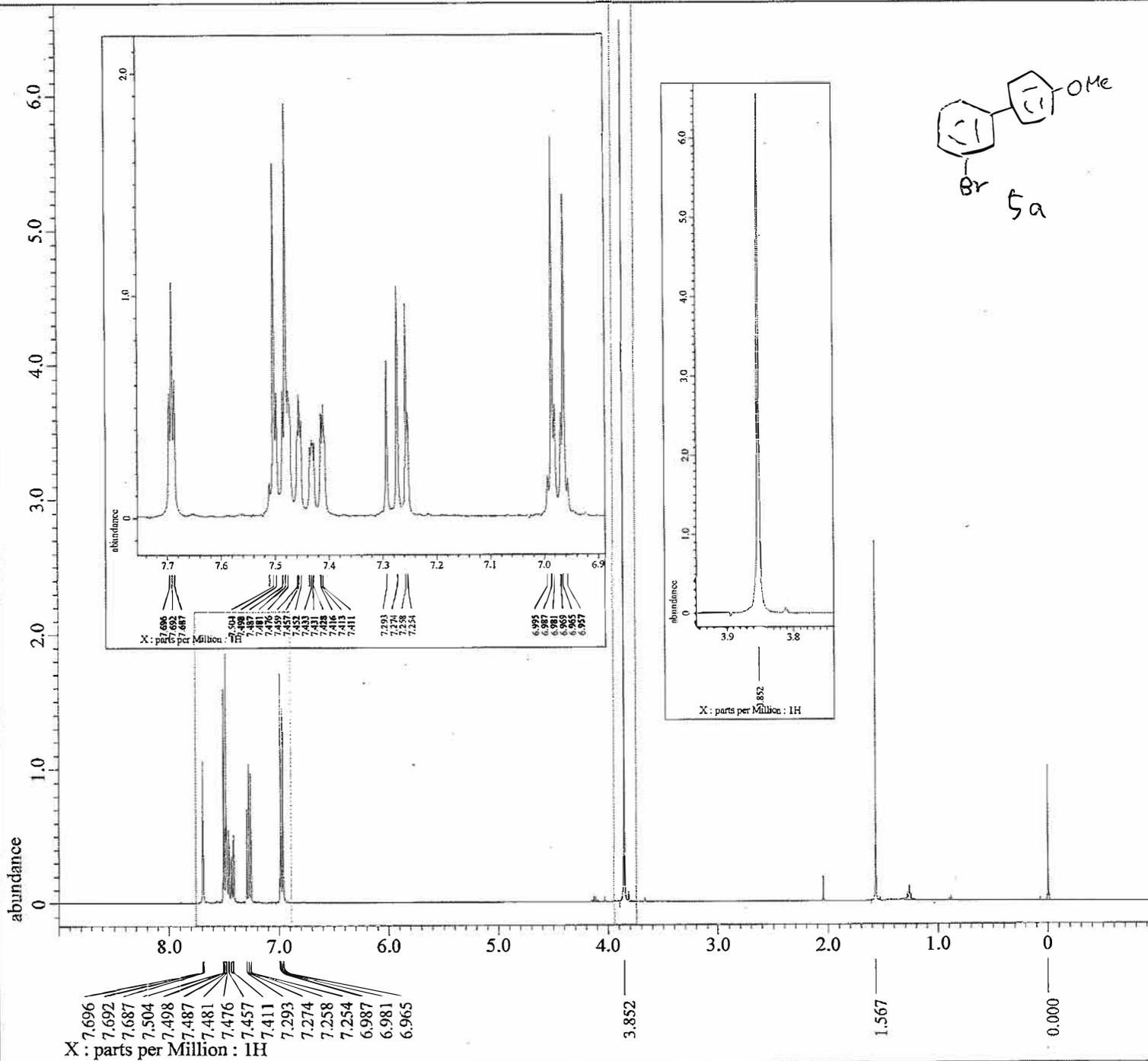
以下に由来: SEO-810-2-pure-13C-1.jdf

Filename = SEO-810-2-pure-13C-2.jdf  
 Author = element  
 Experiment = single\_pulse\_dec  
 Sample\_Id = S#368330  
 Solvent = CHLOROFORM-D  
 Actual\_Start\_Time = 5-AUG-2019 17:24:02  
 Revision\_Time = 5-AUG-2019 14:33:31

Comment = single pulse decoupled ga  
 Data\_Format = 1D\_COMPLEX  
 Dim\_Size = 26214  
 X\_Domain = 13C  
 Dim\_Title = 13C  
 Dim\_Units = [ppm]  
 Dimensions = X  
 Site = ECS 400  
 Spectrometer = JNM-ECS400

Field\_Strength = 9.20197068[T] (390[MHz])  
 X\_Acq\_Duration = 1.06430464[s]  
 X\_Domain = 13c  
 X\_Freq = 98.51479726[MHz]  
 X\_Offset = 100[ppm]  
 X\_Points = 32768  
 X\_Prescans = 4  
 X\_Resolution = 0.93958061[Hz]  
 X\_Sweep = 30.78817734[kHz]  
 Irr\_Domain = 1H  
 Irr\_Freq = 391.78655441[MHz]  
 Irr\_Offset = 5[ppm]  
 Clipped = FALSE  
 Scans = 1100  
 Total\_Scans = 1100

Relaxation\_Delay = 2[s]  
 Recvr\_Gain = 60  
 Temp\_Get = 23.3[dc]  
 X\_90\_Width = 9.11[us]  
 X\_Acq\_Time = 1.06430464[s]  
 X\_Angle = 30[deg]  
 X\_Atn = 4.9[db]  
 X\_Pulse = 3.03666667[us]  
 Irr\_Atn\_Dec = 22.255[db]  
 Irr\_Atn\_Noe = 22.255[db]  
 Irr\_Noise = WALTZ  
 Decoupling = TRUE  
 Initial\_Wait = 1[s]  
 Noe = TRUE



----- PROCESSING PARAMETERS -----

```

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

以下に由来: SE0-835-1-pure-1.jdf

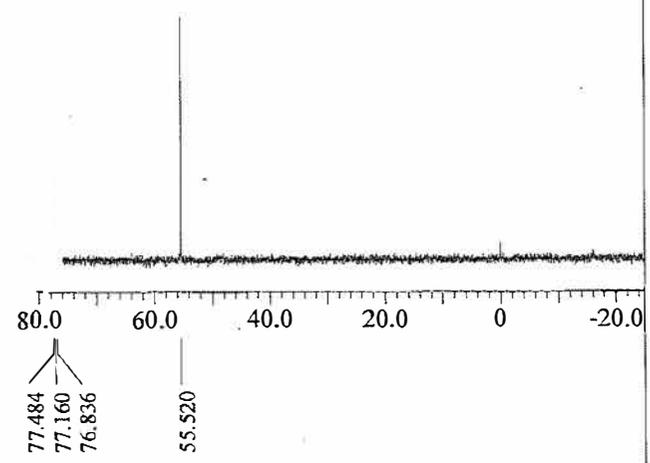
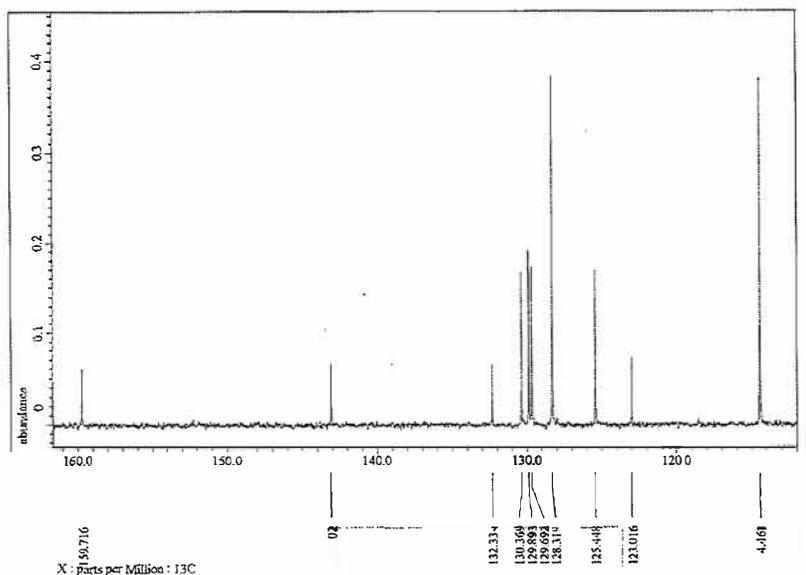
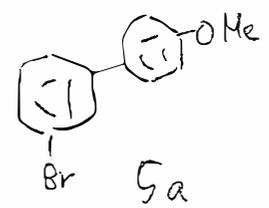
Filename      = SE0-835-1-pure-2.jdf
Author       = element
Experiment   = single_pulse.ex2
Sample_Id    = S#515031
Solvent      = CHLOROFORM-D
Actual_Start_Time = 20-JUN-2019 22:38:52
Revision_Time   = 25-JUL-2019 22:04:06

Comment      = single_pulse
Data Format   = 1D COMPLEX
Dim Size     = 13107
X Domain     = 1H
Dim Title    = 1H
Dim Units    = [ppm]
Dimensions   = X
Site         = ECX 400P
Spectrometer = DELTA2_NMR

Field Strength = 9.2982153[T] (400[MHz])
X Acq_Duration = 2.20725248[s]
X Domain       = 1H
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]
Irr Domain    = 1H
Irr Freq     = 395.88430144[MHz]
Irr Offset    = 5[ppm]
Tri Domain    = 1H
Tri Freq     = 395.88430144[MHz]
Tri Offset    = 5[ppm]
Clipped      = FALSE
Scans        = 8
Total_Scans  = 8

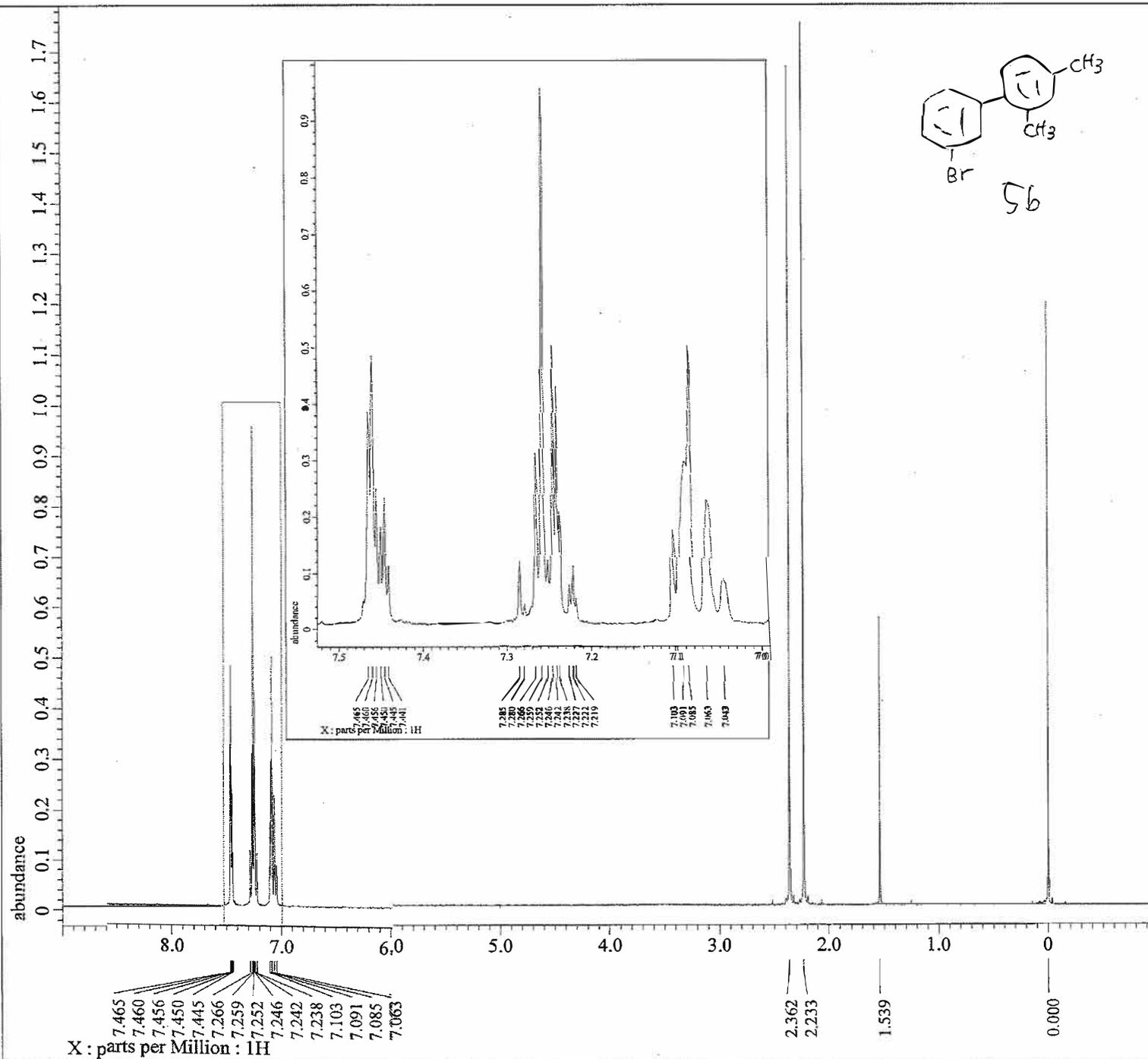
Relaxation_Delay = 5[s]
Recvr_gain       = 38
Temp_Get         = 21.8[dC]
X 90_Width      = 13.2[us]
X Acq_Time      = 2.20725248[s]
X Angle         = 45[deg]
X Atn           = 3.5[dB]
X Pulse        = 6.6[us]
Irr_Mode       = Off
Tri_Mode       = Off
Dante_Presat   = FALSE

```



----- PROCESSING PARAMETERS -----  
 dc\_balance( 0, FALSE )  
 sexp( 2.0[Hz], 0.0[s] )  
 trapezoid3( 0[%], 80[%], 100[%] )  
 zerofill( 1 )  
 fft( 1, TRUE, TRUE )  
 machinephase  
 ppm  
 以下に由来: SEO-851-1-pure-13C-1.jdf

Filename = SEO-851-1-pure-13C-2.jdf  
 Author = element  
 Experiment = single\_pulse\_dec  
 Sample\_Id = 1  
 Solvent = CHLOROFORM-D  
 Actual\_Start\_Time = 26-JUL-2019 01:01:32  
 Revision\_Time = 25-JUL-2019 22:07:42  
 Comment = single pulse decoupled ga  
 Data Format = 1D COMPLEX  
 Dim Size = 26214  
 X Domain = 13C  
 Dim Title = 13C  
 Dim Units = [ppm]  
 Dimensions = X  
 Site = ECS 400  
 Spectrometer = JNM-ECS400  
 Field Strength = 9.20197068[T] (390[MHz])  
 X Acq Duration = 1.06430464[s]  
 X Domain = 13C  
 X Freq = 98.51479726[MHz]  
 X Offset = 100[ppm]  
 X Points = 32768  
 X Prescans = 4  
 X Resolution = 0.93958061[Hz]  
 X Sweep = 30.78817734[kHz]  
 Irr Domain = 1H  
 Irr Freq = 391.78655441[MHz]  
 Irr Offset = 5[ppm]  
 Clipped = FALSE  
 Scans = 1500  
 Total\_Scans = 1500  
 Relaxation\_Delay = 2[s]  
 Recvr Gain = 60  
 Temp Get = 22.1[dC]  
 X\_90\_Width = 9.11[us]  
 X\_Acq\_Time = 1.06430464[s]  
 X\_Angle = 30[deg]  
 X\_Atn = 4.9[dB]  
 X\_Pulse = 3.03666667[us]  
 Irr\_Atn\_Dec = 22.255[dB]  
 Irr\_Atn\_Noise = 22.255[dB]  
 Irr\_Noise = WALTZ  
 Decoupling = TRUE  
 Initial\_Wait = 1[s]  
 Noe = TRUE



```

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

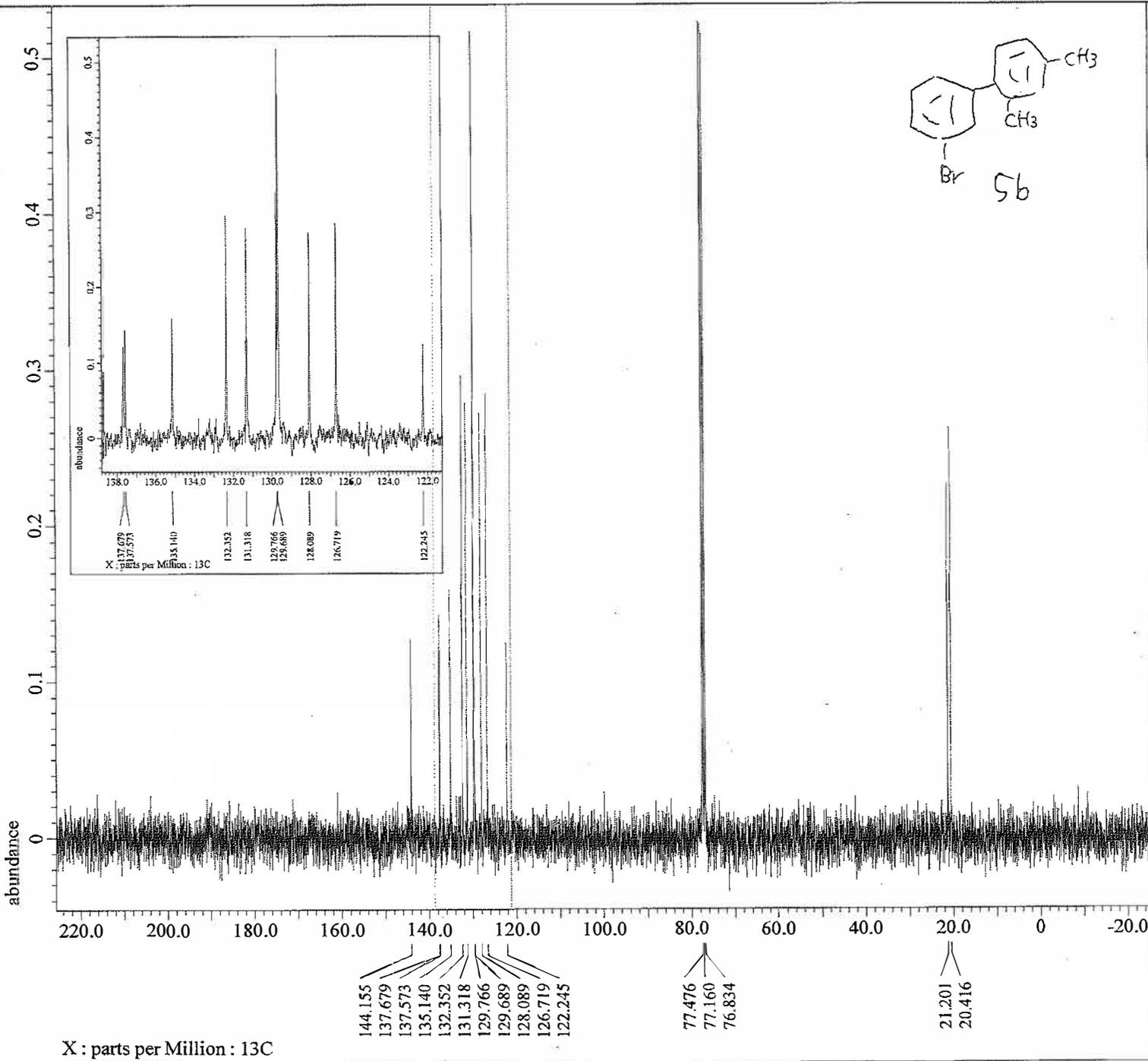
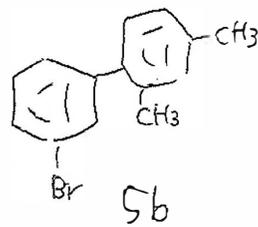
以下に由来: SEO-885-1-pure-1H-1.jdf

Filename      = SEO-885-1-pure-1H-2.jdf
Author        = element
Experiment    = single_pulse.ex2
Sample_Id     = S#306738
Solvent       = CHLOROFORM-D
Actual_Start_Time = 22-JUL-2019 16:51:52
Revision_Time  = 25-JUL-2019 22:10:33

Comment       = single_pulse
Data Format    = 1D COMPLEX
Dim_Size      = 13107
X_Domain      = 1H
Dim Title     = 1H
Dim Units     = [ppm]
Dimensions    = X
Site          = ECX 400P
Spectrometer  = DELTA2_NMR

Field_Strength = 9.2982153[T] (400[MHz])
X_Acq_Duration = 2.20725248[s]
X_Domain       = 1H
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]
Irr_Domain    = 1H
Irr_Freq      = 395.88430144 [MHz]
Irr_Offset    = 5[ppm]
Tri_Domain    = 1H
Tri_Freq      = 395.88430144 [MHz]
Tri_Offset    = 5[ppm]
Clipped       = FALSE
Scans         = 8
Total_Scans   = 8

Relaxation_Delay = 5[s]
Recvr Gain      = 40
Temp_Get       = 22.4[dc]
X_90_Width     = 13.2[us]
X_Acq_Time     = 2.20725248[s]
X_Angle        = 45[deg]
X_Atn         = 3.5[db]
X_Pulse       = 6.6[us]
Irr_Mode       = Off
Tri_Mode       = Off
Dante_Presat   = FALSE
  
```



```

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

```

以下に由来: SEO-885-1-pure-13C-1.jdf

```

Filename      = SEO-885-1-pure-13C-2.jdf
Author        = element
Experiment    = single_pulse_dec
Sample_Id     = 1
Solvent       = CHLOROFORM-D
Actual_Start_Time = 22-JUL-2019 16:57:33
Revision_Time = 25-JUL-2019 22:12:40

```

```

Comment       = single pulse decoupled ga
Data_Format   = 1D COMPLEX
Dim Size      = 26214
X Domain      = 13C
Dim Title     = 13C
Dim Units     = [ppm]
Dimensions    = X
Site          = ECX 400P
Spectrometer  = DELTA2_NMR

```

```

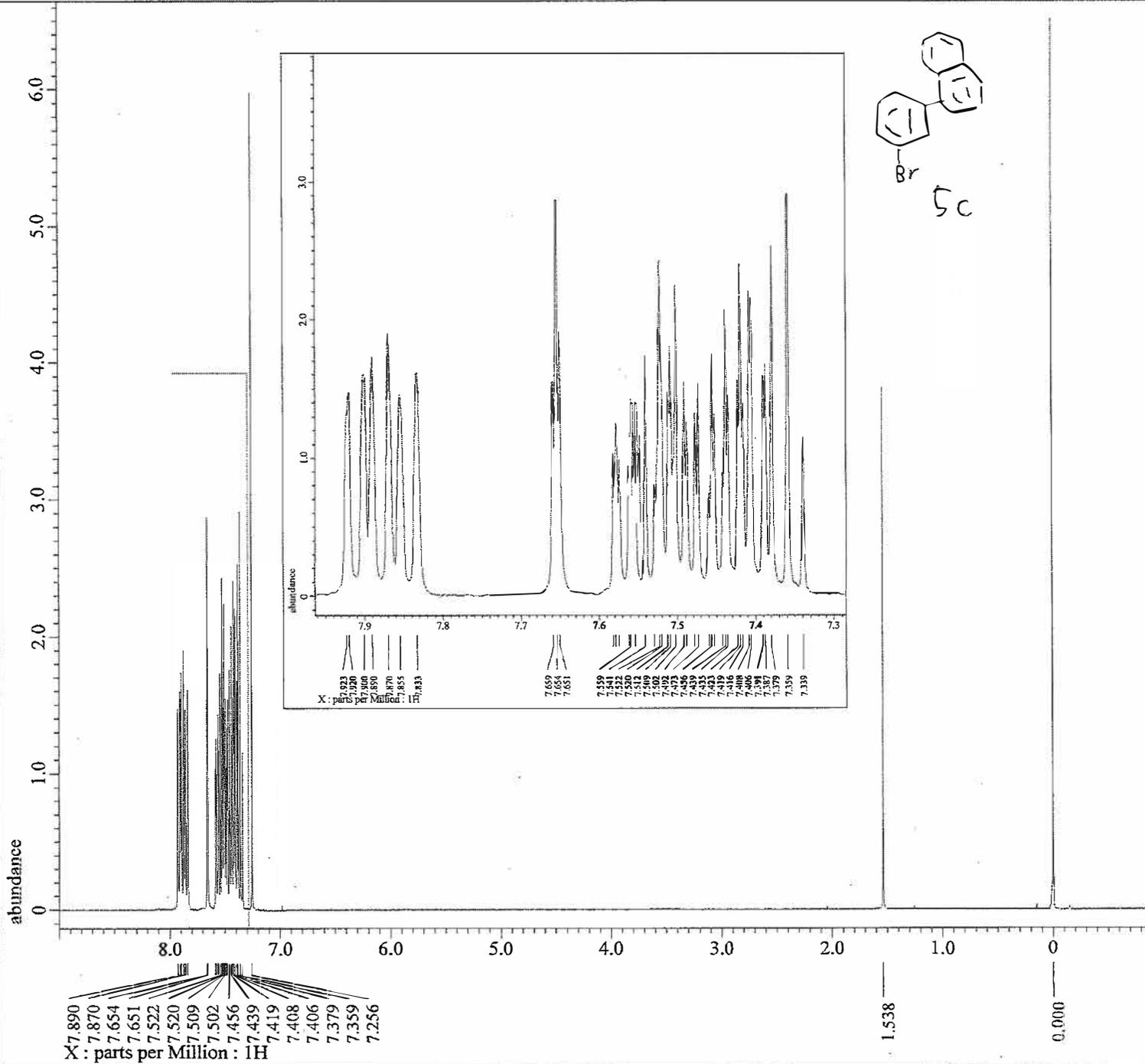
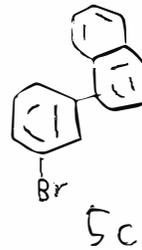
Field Strength = 9.2982153[T] (400[MHz])
X Acq_Duration = 1.048576[s]
X Domain       = 13C
X_Freq        = 99.54517646[MHz]
X_Offset      = 100[ppm]
X Points      = 32768
X_Prescans    = 4
X_Resolution  = 0.95367432[Hz]
X_Sweep       = 31.25[kHz]
Irr_Domain    = 1H
Irr_Freq      = 395.88430144[MHz]
Irr_Offset    = 5[ppm]
Clipped       = FALSE
Scans         = 25
Total_Scans   = 25

```

```

Relaxation_Delay = 2[s]
Recvr_Gain       = 54
Temp_Get         = 22.7[dC]
X_90_Width      = 10.1[us]
X_Acq_Time       = 1.048576[s]
X_Angle          = 30[deg]
X_Atn            = 3.4[dB]
X_Pulse          = 3.36666667[us]
Irr_Atn_Dec      = 22.3[dB]
Irr_Atn_Noise   = 22.3[dB]
Irr_Noise       = WALTZ
Decoupling       = TRUE
Initial_Wait     = 1[s]
Noe              = TRUE

```



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

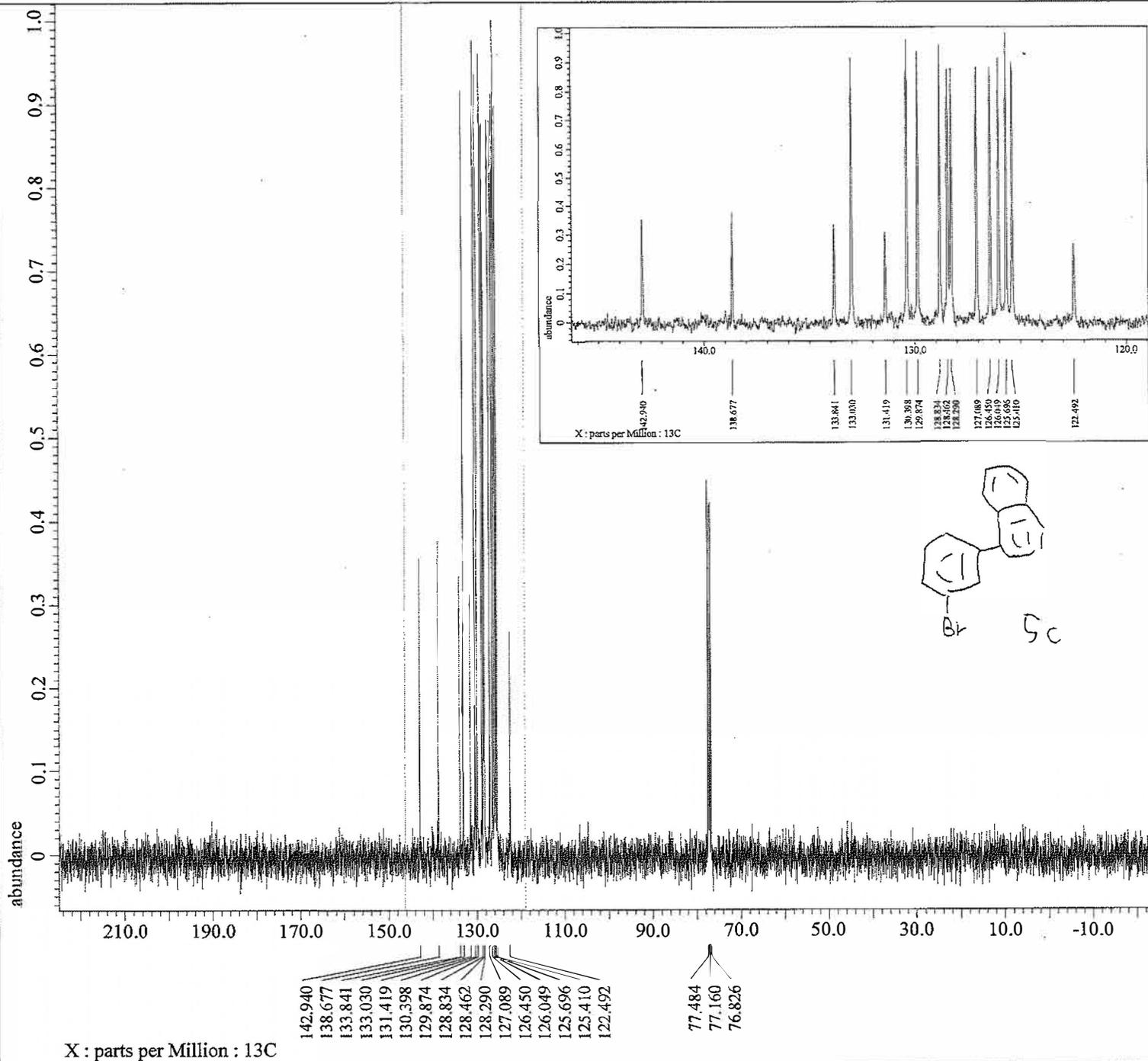
以下に由来: SEO-869-1-pure-1.jdf

Filename = SEO-869-1-pure-2.jdf  
 Author = element  
 Experiment = single pulse.ex2  
 Sample Id = S#584654  
 Solvent = CHLOROFORM-D  
 Actual\_Start\_Time = 15-JUL-2019 23:28:22  
 Revision\_Time = 25-JUL-2019 22:17:46

Comment = single pulse  
 Data Format = 1D COMPLEX  
 Dim Size = 13107  
 X Domain = 1H  
 Dim Title = 1H  
 Dim Units = [ppm]  
 Dimensions = X  
 Site = ECS 400  
 Spectrometer = JNM-ECS400

Field\_Strength = 9.20197068[T] (390[MHz])  
 X Acq\_Duration = 2.228224[s]  
 X Domain = 1H  
 X Freq = 391.78655441[MHz]  
 X Offset = 5[ppm]  
 X Points = 16384  
 X Prescans = 1  
 X Resolution = 0.44878791[Hz]  
 X Sweep = 7.35294118[kHz]  
 Irr\_Domain = 1H  
 Irr\_Freq = 391.78655441[MHz]  
 Irr\_Offset = 5[ppm]  
 Tri\_Domain = 1H  
 Tri\_Freq = 391.78655441[MHz]  
 Tri\_Offset = 5[ppm]  
 Clipped = FALSE  
 Scans = 8  
 Total\_Scans = 8

Relaxation\_Delay = 5[s]  
 Recvr\_Gain = 50  
 Temp\_Get = 21.2[dC]  
 X 90\_Width = 11.04[us]  
 X Acq\_Time = 2.228224[s]  
 X Angle = 45[deg]  
 X Atn = 1.9[dB]  
 X Pulse = 5.52[us]  
 Irr\_Mode = Off  
 Tri\_Mode = Off  
 Dante\_Presat = FALSE



```

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

```

以下に由来: SEO-869-1-pure-13C-1.jdf

```

Filename      = SEO-869-1-pure-13C-2.jdf
Author        = element
Experiment    = single_pulse_dec
Sample_Id     = 1
Solvent       = CHLOROFORM-D
Actual_Start_Time = 15-JUL-2019 23:42:02
Revision_Time = 25-JUL-2019 22:20:40

```

```

Comment       = single pulse decoupled ga
Data Format    = 1D COMPLEX
Dim Size      = 26214
X_Domain      = 13C
Dim Title     = 13C
Dim Units     = [ppm]
Dimensions    = X
Site          = ECS 400
Spectrometer  = JNM-ECS400

```

```

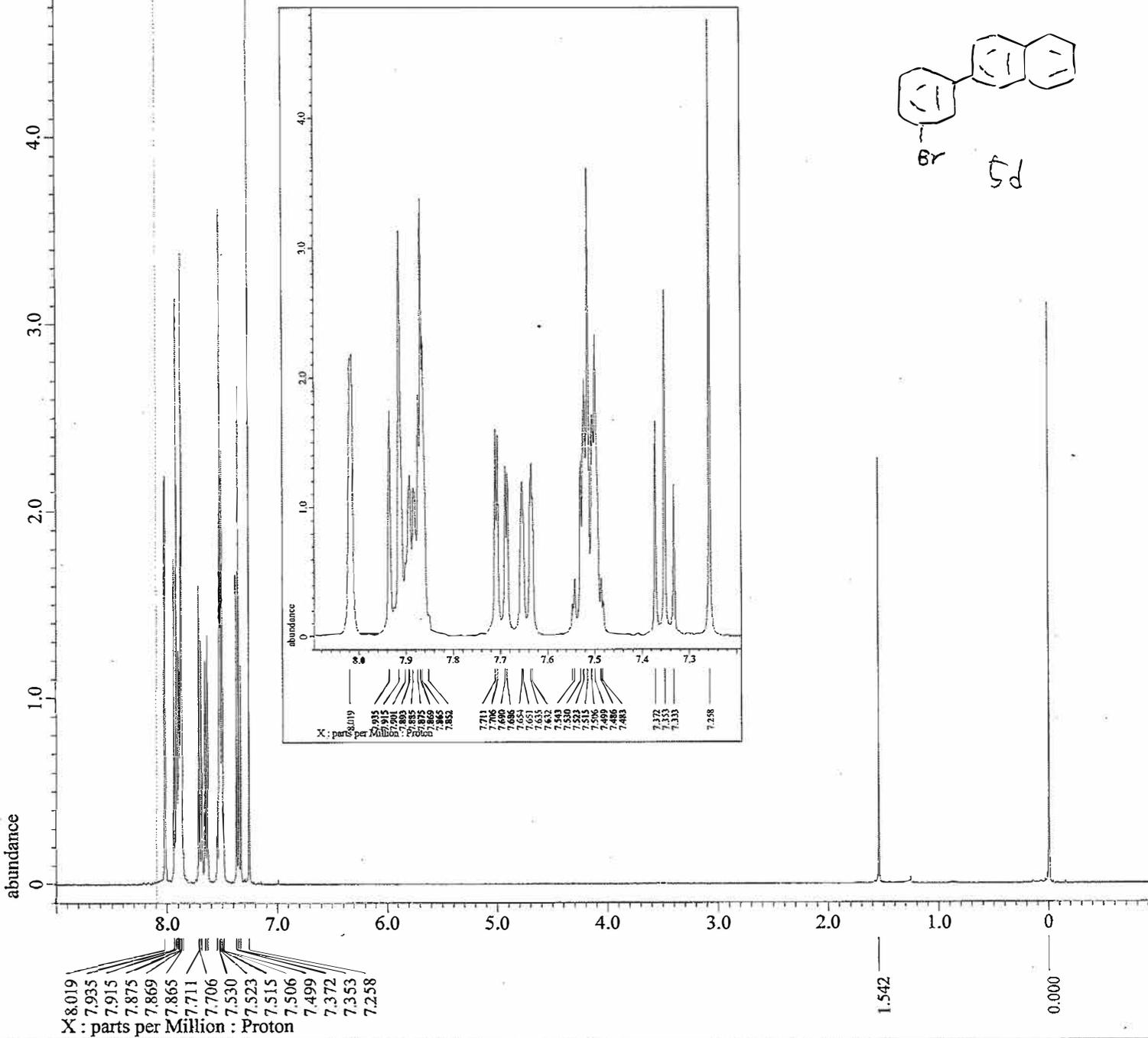
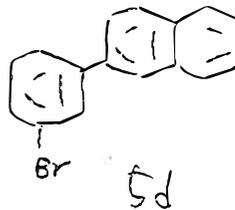
Field Strength = 9.20197068[T] (390[MHz])
X_Acq Duration = 1.06430464[s]
X_Domain       = 13C
X_Freq         = 98.51479726[MHz]
X_Offset       = 100[ppm]
X_Points       = 32768
X_Prescans     = 4
X_Resolution   = 0.93958061[Hz]
X_Sweep        = 30.78817734[kHz]
Irr_Domain     = 1H
Irr_Freq       = 391.78655441[MHz]
Irr_Offset     = 5[ppm]
Clipped        = FALSE
Scans          = 29
Total_Scans    = 29

```

```

Relaxation_Delay = 2[s]
Recvr Gain       = 60
Temp_Get         = 21.4[dC]
X_90_Width      = 9.11[us]
X_Acq Time       = 1.06430464[s]
X_Angle         = 30[deg]
X_Atn           = 4.9[dB]
X_Pulse         = 3.03666667[us]
Irr_Atn_Dec     = 22.255[dB]
Irr_Atn_Noise   = 22.255[dB]
Irr_Noise       = WALTZ
Decoupling      = TRUE
Initial_Wait    = 1[s]
Noe              = TRUE

```



```

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

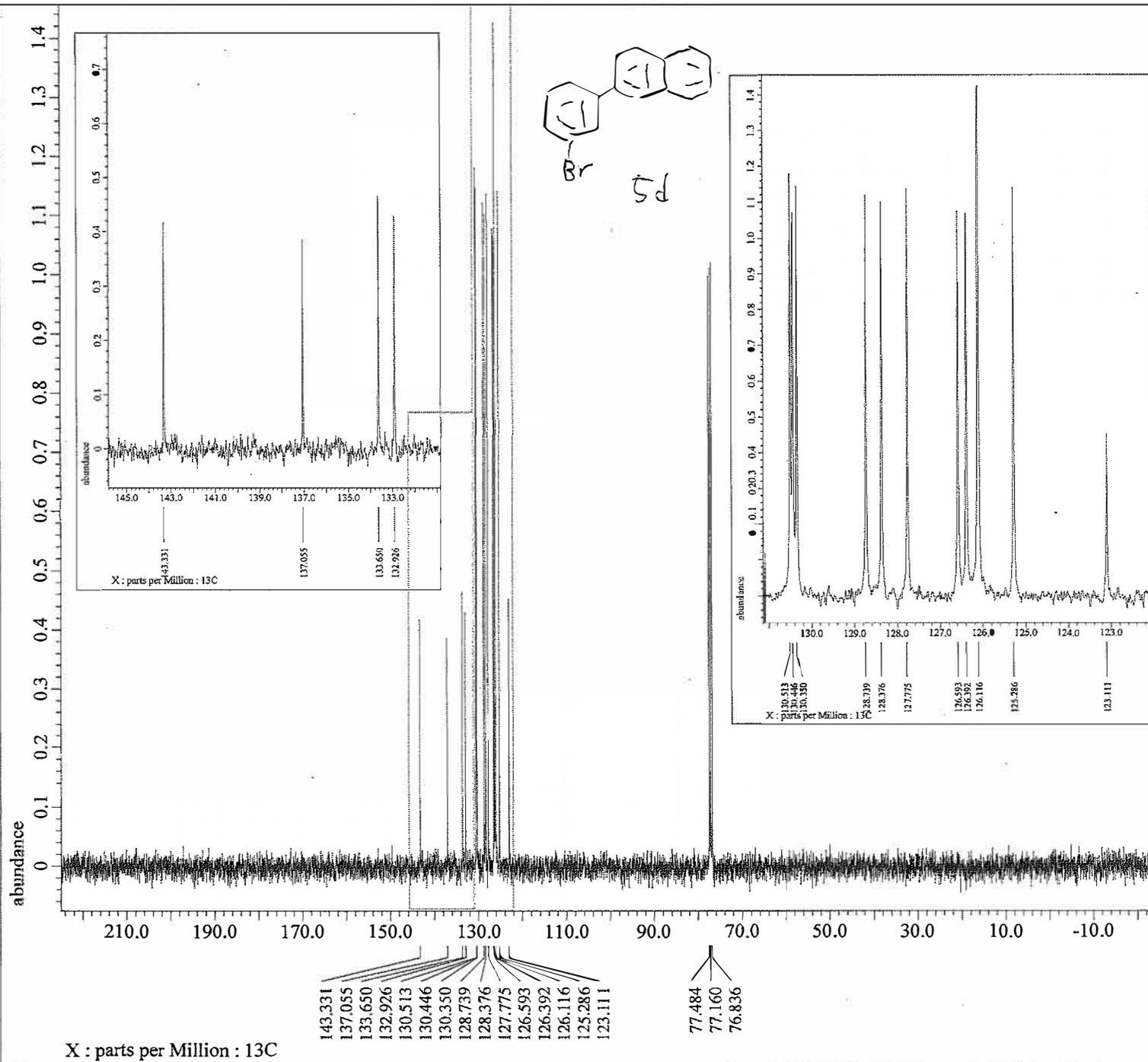
以下に由来: SEO-898-2-pure_Proton-1-1.jdf

Filename      = SEO-898-2-pure_Proton-1-2
Author        = element
Experiment    = proton.jxp
Sample_Id     = SEO-898-2-pure
Solvent       = CHLOROFORM-D
Actual_Start_Time = 5-AUG-2019 10:21:12
Revision_Time  = 5-AUG-2019 10:33:09

Comment       = single_pulse
Data Format    = 1D COMPLEX
Dim_Size      = 13107
X_Domain      = Proton
Dim Title     = Proton
Dim Units     = [ppm]
Dimensions    = X
Spectrometer  = DELTA2_NMR

Field Strength = 9.4073814 [T] (400 [MHz])
X Acq Duration = 2.18103808 [s]
X Domain       = 1H
X Freq         = 400.53219825 [MHz]
X Offset       = 5 [ppm]
X Points       = 16384
X Prescans     = 1
X Resolution   = 0.45849727 [Hz]
X Sweep        = 7.51201923 [kHz]
X Sweep_Clippped = 6.00961538 [kHz]
Irr_Domain     = Proton
Irr Freq       = 400.53219825 [MHz]
Irr_Offset     = 5 [ppm]
Tri_Domain     = Proton
Tri Freq       = 400.53219825 [MHz]
Tri_Offset     = 5 [ppm]
Clipped        = FALSE
Scans          = 8
Total_Scans    = 8

Relaxation_Delay = 5 [s]
Recvr Gain       = 48
Temp_Get         = 19.5 [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
  
```



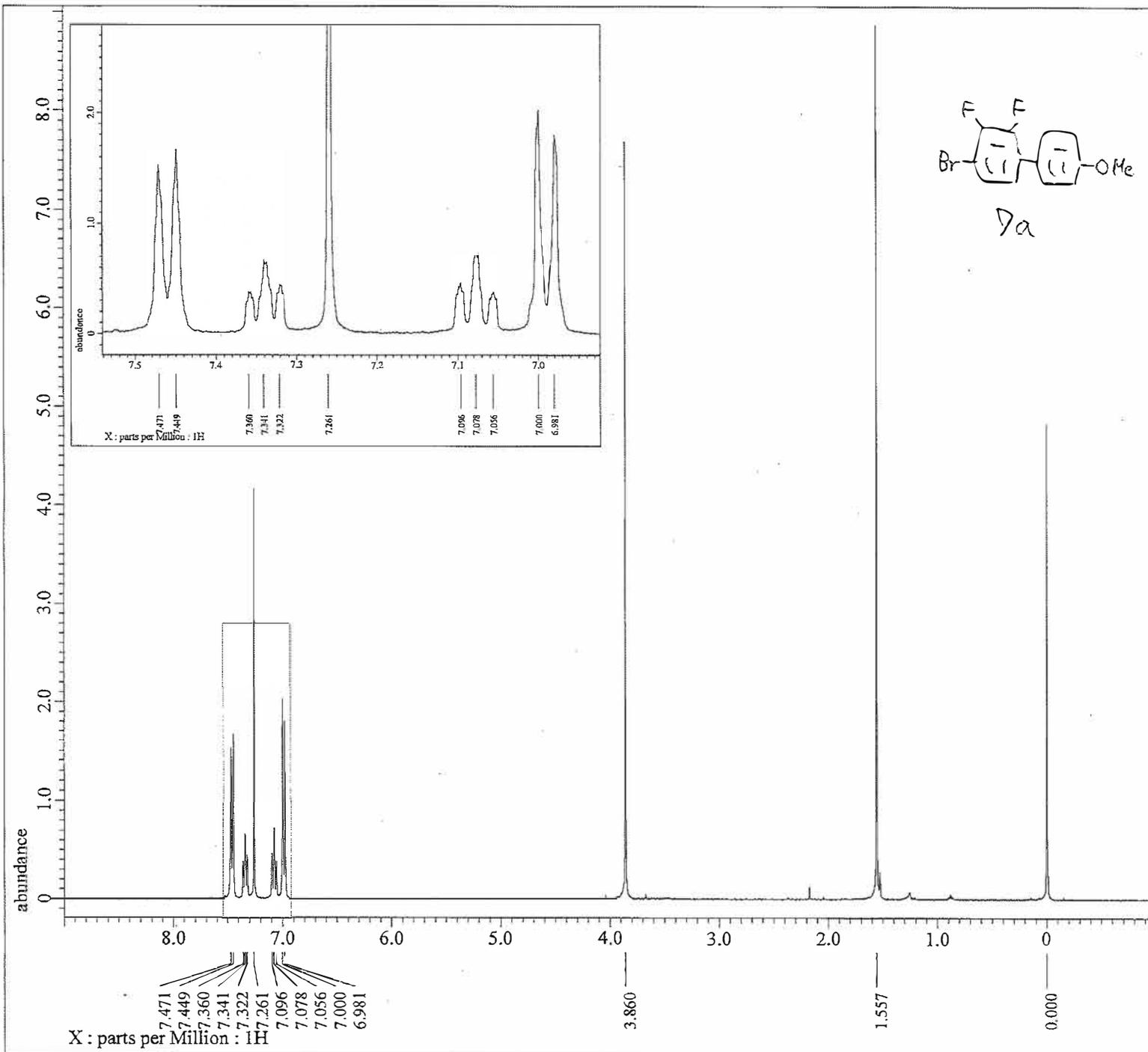
----- PROCESSING PARAMETERS -----  
 dc\_balance( 0, FALSE )  
 sexp( 2.0[Hz], 0.0[s] )  
 trapezoid3( 0[%], 80[%], 100[%] )  
 zerofill( 1 )  
 fft( 1, TRUE, TRUE )  
 machinephase  
 ppm  
 以下に由来: SEO-881-1-pure-13C-1.jdf

Filename = SEO-881-1-pure-13C-2.jdf  
 Author = element  
 Experiment = single\_pulse\_dec  
 Sample\_Id = 1  
 Solvent = CHLOROFORM-D  
 Actual\_Start\_Time = 25-JUL-2019 19:16:53  
 Revision\_Time = 25-JUL-2019 22:25:40

Comment = single pulse decoupled ga  
 Data Format = 1D COMPLEX  
 Dim\_Size = 26214  
 X\_Domain = 13C  
 Dim\_Title = 13C  
 Dim\_Units = [ppm]  
 Dimensions = X  
 Site = ECS 400  
 Spectrometer = JNM-ECS400

Field Strength = 9.20197068 [T] (390 [MHz])  
 X\_Acq\_Duration = 1.06430464 [s]  
 X\_Domain = 13C  
 X\_Freq = 98.51479726 [MHz]  
 X\_Offset = 100 [ppm]  
 X\_Points = 32768  
 X\_Prescans = 4  
 X\_Resolution = 0.93958061 [Hz]  
 X\_Sweep = 30.78817734 [kHz]  
 Irr\_Domain = 1H  
 Irr\_Freq = 391.78655441 [MHz]  
 Irr\_Offset = 5 [ppm]  
 Clipped = FALSE  
 Scans = 32  
 Total\_Scans = 32

Relaxation\_Delay = 2 [s]  
 Recvr\_Gain = 60  
 Temp\_Get = 21.8 [dC]  
 X\_90\_Width = 9.11 [us]  
 X\_Acq\_Time = 1.06430464 [s]  
 X\_Angle = 30 [deg]  
 X\_Atn = 4.9 [dB]  
 X\_Pulse = 3.03666667 [us]  
 Irr\_Atn\_Dec = 22.255 [dB]  
 Irr\_Atn\_Noise = 22.255 [dB]  
 Irr\_Noise = WALTZ  
 Decoupling = TRUE  
 Initial\_Wait = 1 [s]  
 Noe = TRUE



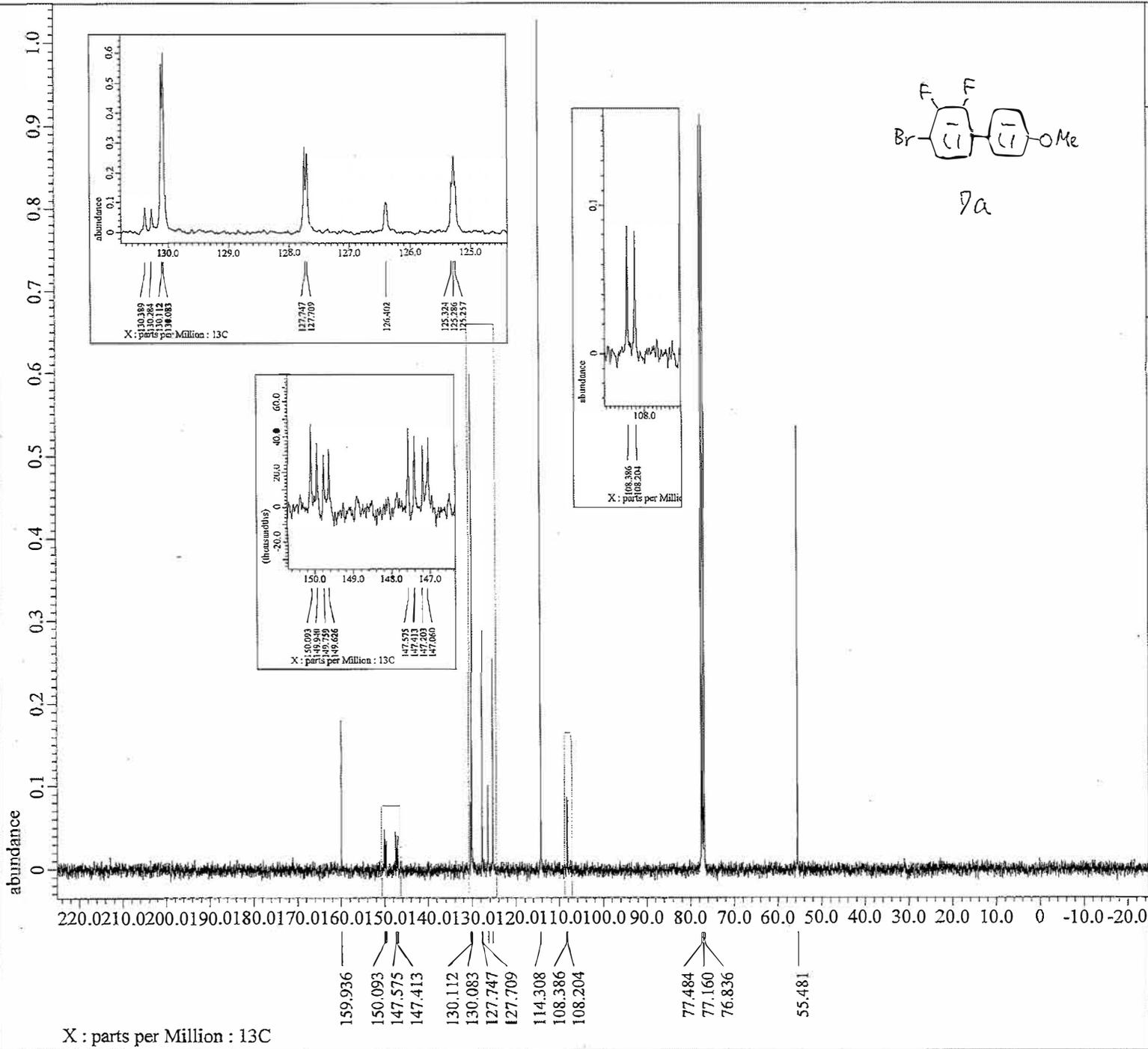
----- PROCESSING PARAMETERS -----  
 dc\_balance( 0, FALSE )  
 sexp( 0.2[Hz], 0.0[s] )  
 trapezoid3( 0[%], 80[%], 100[%] )  
 zerofill( 1, TRUE )  
 fft( 1, TRUE, TRUE )  
 machinephase  
 ppm  
 以下に由来: SEO-936-1-pure-1H-1.jdf

Filename = SEO-936-1-pure-1H-2.jdf  
 Author = element  
 Experiment = single\_pulse.ex2  
 Sample\_Id = S#712539  
 Solvent = CHLOROFORM-D  
 Actual\_Start\_Time = 6-SEP-2019 03:10:35  
 Revision\_Time = 8-NOV-2019 20:37:40

Comment = single\_pulse  
 Data\_Format = 1D COMPLEX  
 Dim\_Size = 13107  
 X\_Domain = 1H  
 Dim\_Title = 1H  
 Dim\_Units = [ppm]  
 Dimensions = X  
 Site = ECS 400  
 Spectrometer = JNM-ECS400

Field\_Strength = 9.20197068[T] (390[MHz])  
 X\_Acq\_Duration = 2.228224[s]  
 X\_Domain = 1H  
 X\_Freq = 391.78655441[MHz]  
 X\_Offset = 5[ppm]  
 X\_Points = 16384  
 X\_Prescans = 1  
 X\_Resolution = 0.44878791[Hz]  
 X\_Sweep = 7.35294118[kHz]  
 Irr\_Domain = 1H  
 Irr\_Freq = 391.78655441[MHz]  
 Irr\_Offset = 5[ppm]  
 Tri\_Domain = 1H  
 Tri\_Freq = 391.78655441[MHz]  
 Tri\_Offset = 5[ppm]  
 Clipped = FALSE  
 Scans = 8  
 Total\_Scans = 8

Relaxation\_Delay = 5[s]  
 Recvr\_Gain = 54  
 Temp\_Get = 21.8[dc]  
 X\_90\_Width = 11.04[us]  
 X\_Acq\_Time = 2.228224[s]  
 X\_Angle = 45[deg]  
 X\_Atn = 1.9[db]  
 X\_Pulse = 5.52[us]  
 Irr\_Mode = Off  
 Tri\_Mode = Off  
 Dante\_Presat = FALSE



```

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

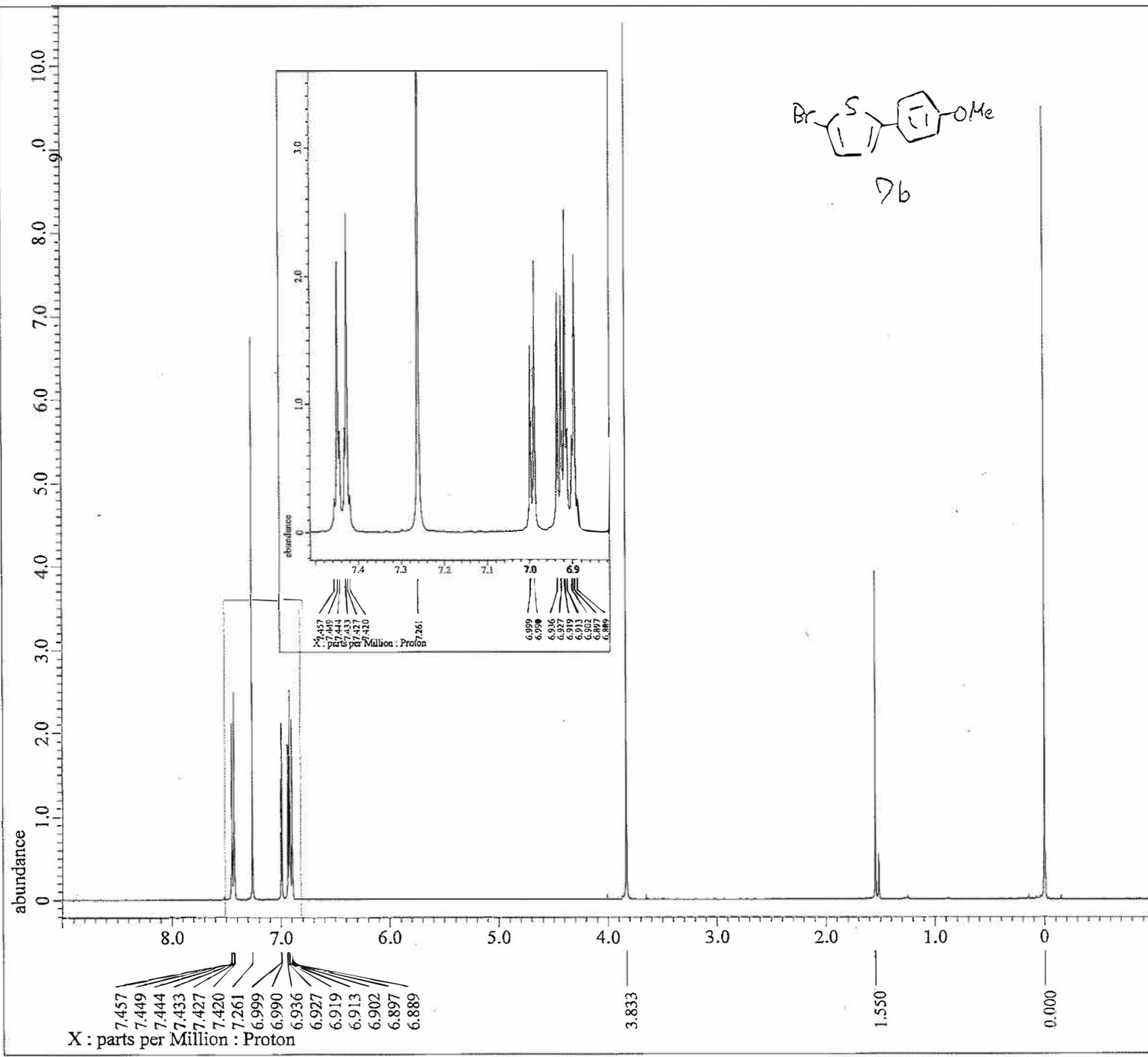
以下に由来: SEO-936-2-pure-13C-1.jdf

Filename      = SEO-936-2-pure-13C-2.jdf
Author        = element
Experiment    = single_pulse_dec
Sample_Id     = 1
Solvent       = CHLOROFORM-D
Actual_Start Time = 6-SEP-2019 03:22:12
Revision_Time = 8-NOV-2019 20:13:43

Comment       = single pulse decoupled ga
Data_Format   = 1D COMPLEX
Dim Size      = 26214
X_Domain      = 13C
Dim Title     = 13C
Dim Units     = [ppm]
Dimensions    = X
Site          = ECS 400
Spectrometer  = JNM-ECS400

Field_Strength = 9.20197068[T] (390 [MHz])
X_Acq_Duration = 1.06430464[s]
X_Domain       = 13C
X_Freq        = 98.51479726[MHz]
X_Offset      = 100[ppm]
X_Points      = 32768
X_Prescans    = 4
X_Resolution  = 0.93958061[Hz]
X_Sweep       = 30.78817734[kHz]
Irr_Domain    = 1H
Irr_Freq      = 391.78655441[MHz]
Irr_Offset    = 5[ppm]
Clipped       = FALSE
Scans         = 300
Total_Scans   = 300

Relaxation_Delay = 2[s]
Recvr_Gain      = 60
Temp_Get       = 22[dC]
X_90_Width     = 9.11[us]
X_Acq_Time     = 1.06430464[s]
X_Angle        = 30[deg]
X_Atn         = 4.9[dB]
X_Pulse        = 3.03666667[us]
Irr_Atn_Dec    = 22.255[dB]
Irr_Atn_Noise = 22.255[dB]
Irr_Noise     = WALTZ
Decoupling     = TRUE
Initial_Wait   = 1[s]
Noe            = TRUE
  
```



```

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

以下に由来: SEO-922-1-pure_Proton-1-1.jdf

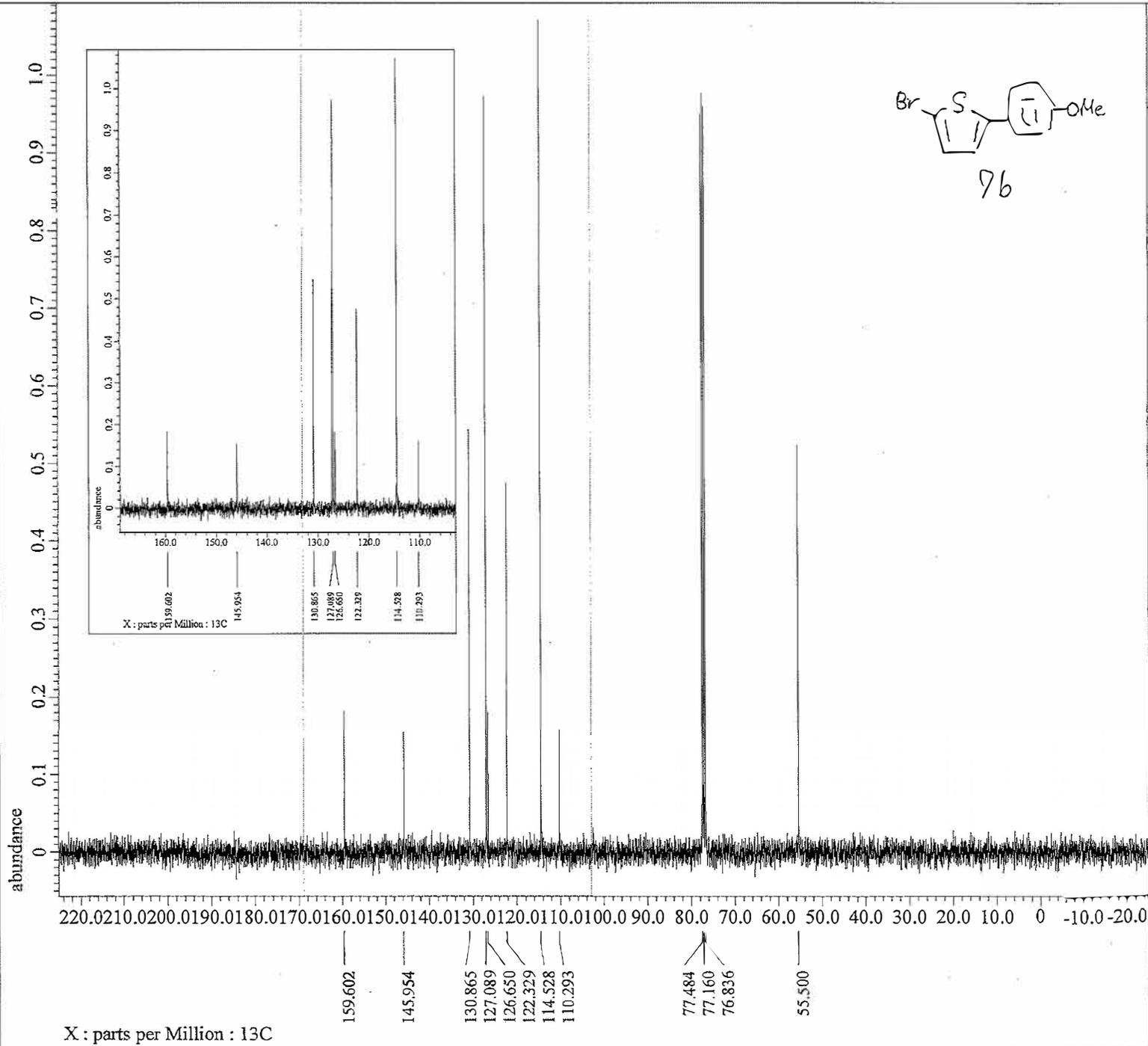
Filename      = SEO-922-1-pure_Proton-1-2
Author        = element
Experiment    = proton.jxp
Sample_Id     = SEO-922-1-pure
Solvent       = CHLOROFORM-D
Actual_Start_Time = 10-AUG-2019 16:40:22
Revision_Time  = 8-NOV-2019 20:01:57

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

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

Relaxation_Delay = 5 [s]
Recvr_Gain       = 50
Temp_Get        = 19.9 [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

```



```

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

以下に由来: SEO-922-1-pure-13C-1.jdf

```

```

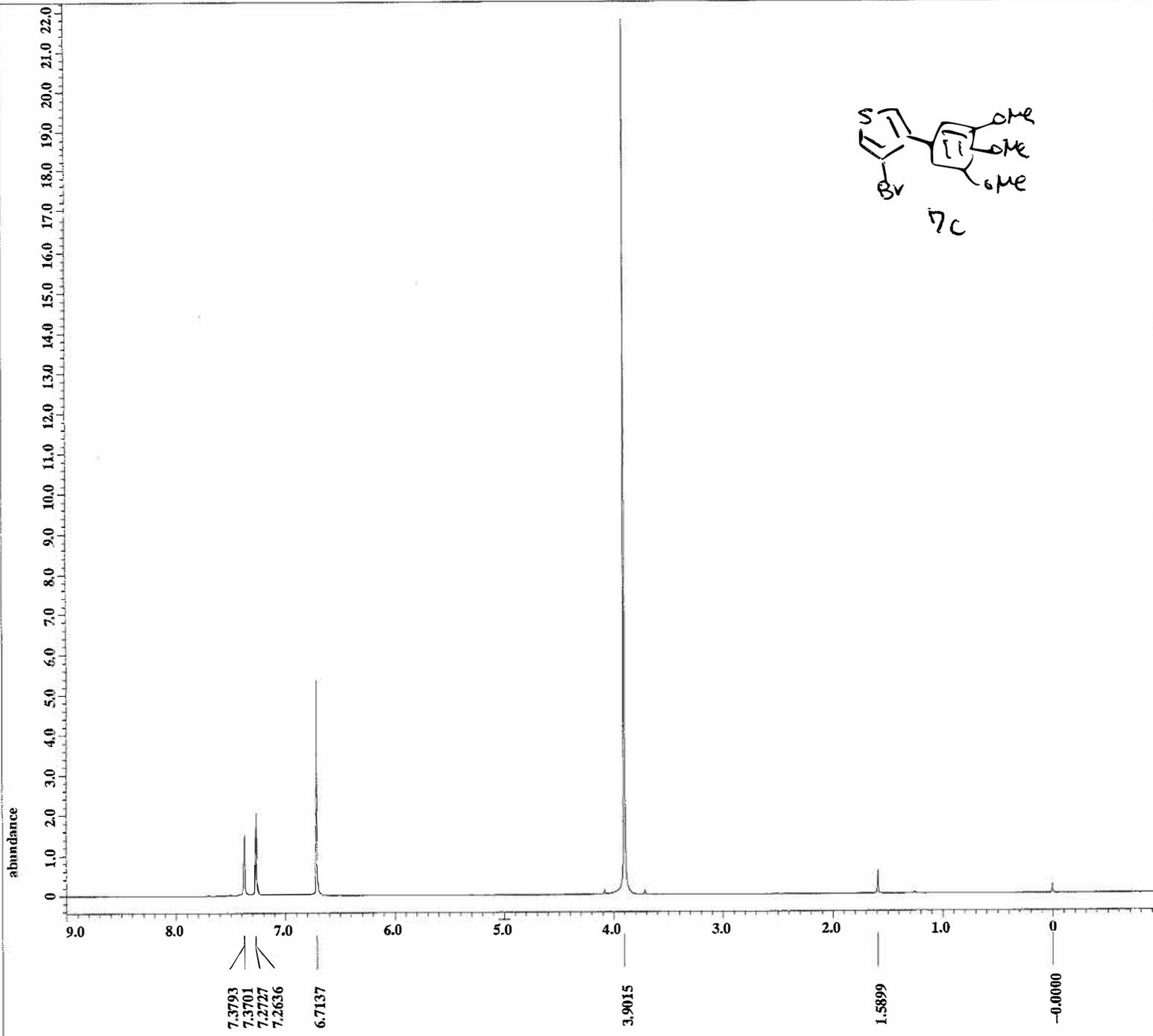
Filename      = SEO-922-1-pure-13C-2.jdf
Author       = element
Experiment   = single_pulse_dec
Sample_Id    = 1
Solvent      = CHLOROFORM-D
Actual_Start Time = 10-AUG-2019 23:41:36
Revision_Time = 8-NOV-2019 20:05:38

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

Field_Strength = 9.20197068[T] (390 [MHz])
X_Acq_Duration = 1.06430464 [s]
X_Domain       = 13C
X_Freq         = 98.51479726 [MHz]
X_Offset       = 100 [ppm]
X_Points       = 32768
X_Prescans    = 4
X_Resolution   = 0.93958061 [Hz]
X_Sweep        = 30.78817734 [kHz]
Irr_Domain     = 1H
Irr_Freq       = 391.78655441 [MHz]
Irr_Offset     = 5 [ppm]
Clipped        = FALSE
Scans          = 59
Total_Scans   = 59

Relaxation_Delay = 2 [s]
Recvr_Gain       = 60
Temp_Get         = 22.9 [dc]
X_90_Width      = 9.11 [us]
X_Acq_Time      = 1.06430464 [s]
X_Angle         = 30 [deg]
X_Atn           = 4.9 [dB]
X_Pulse         = 3.03666667 [us]
Irr_Atn_Dec     = 22.255 [dB]
Irr_Atn_Noise  = 22.255 [dB]
Irr_Noise       = WALTZ
Decoupling      = TRUE
Initial_Wait    = 1 [s]
Noe              = TRUE

```



```

---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 0.2[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm
Derived from: 1H-1.jdf

```

```

Filename      = 1H-3.jdf
Author        = element
Experiment    = single_pulse.ex2
Sample_id     = S#523616
Solvent       = CHLOROFORM-D
Creation_time = 27-JAN-2020 12:37:31
Revision_time = 10-FEB-2020 14:47:29
Current_time  = 10-FEB-2020 14:47:44

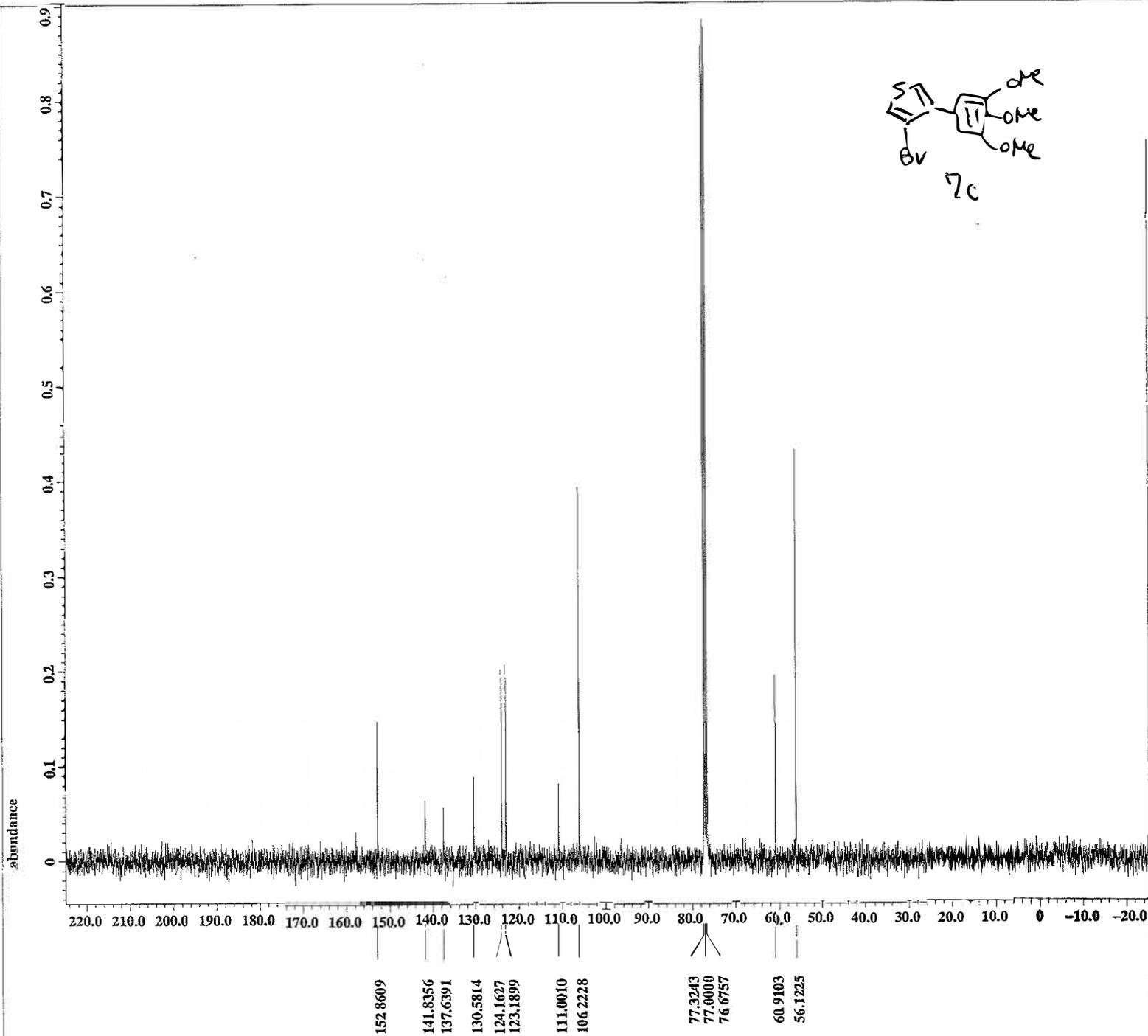
Comment       = single_pulse
Data_format   = 1D COMPLEX
Dim_size      = 13107
Dim_title     = 1H
Dim_units     = [ppm]
Dimensions    = X
Site          = ECS 400
Spectrometer  = JNM-ECS400

Field_strength = 9.20197068[T] (390[MH]
X_acq_duration = 2.228224[s]
X_domain       = 1H
X_freq         = 391.78655441[MHz]
X_offset       = 5[ppm]
X_points       = 16384
X_prescans     = 1
X_resolution   = 0.44878791[Hz]
X_sweep        = 7.35294118[kHz]
Irr_domain     = 1H
Irr_freq       = 391.78655441[MHz]
Irr_offset     = 5[ppm]
Tri_domain     = 1H
Tri_freq       = 391.78655441[MHz]
Tri_offset     = 5[ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 8
Total_scans    = 8

X_90_width    = 11.04[us]
X_acq_time     = 2.228224[s]
X_angle        = 45[deg]
X_atn          = 1.9[db]
X_pulse        = 5.52[us]
Irr_mode       = Off
Tri_mode       = Off
Dante_presat   = FALSE
Initial_wait   = 1[s]
Recvr_gain     = 42
Relaxation_delay = 5[s]
Repetition_time = 7.228224[s]
Temp_get       = 18.3[dc]

```

X : parts per Million : 1H



```

PROCESS PARAMETERS
dc_balance : 0 : FALSE
seXP : 2.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

```

Derived from: 13C-1.jdf

```

Filename = 13C-4.jdf
Author = element
Experiment = single_pulse_dec
Sample_id = S#527219
Solvent = CHLOROFORM-D
Creation_time = 27-JAN-2020 12:46:38
Revision_time = 10-FEB-2020 14:48:44
Current_time = 10-FEB-2020 14:48:59

```

```

Comment = single pulse decouple
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400

```

```

Field_strength = 9.20197068[T] (390[MH
X_acq_duration = 1.06430464[s]
X_domain = 13C
X_freq = 98.51479726[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.93958061[Hz]
X_sweep = 30.78817734[kHz]
Irr_domain = 1H
Irr_freq = 391.78655441[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 100
Total_scans = 100

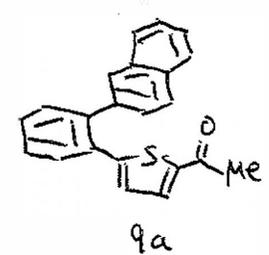
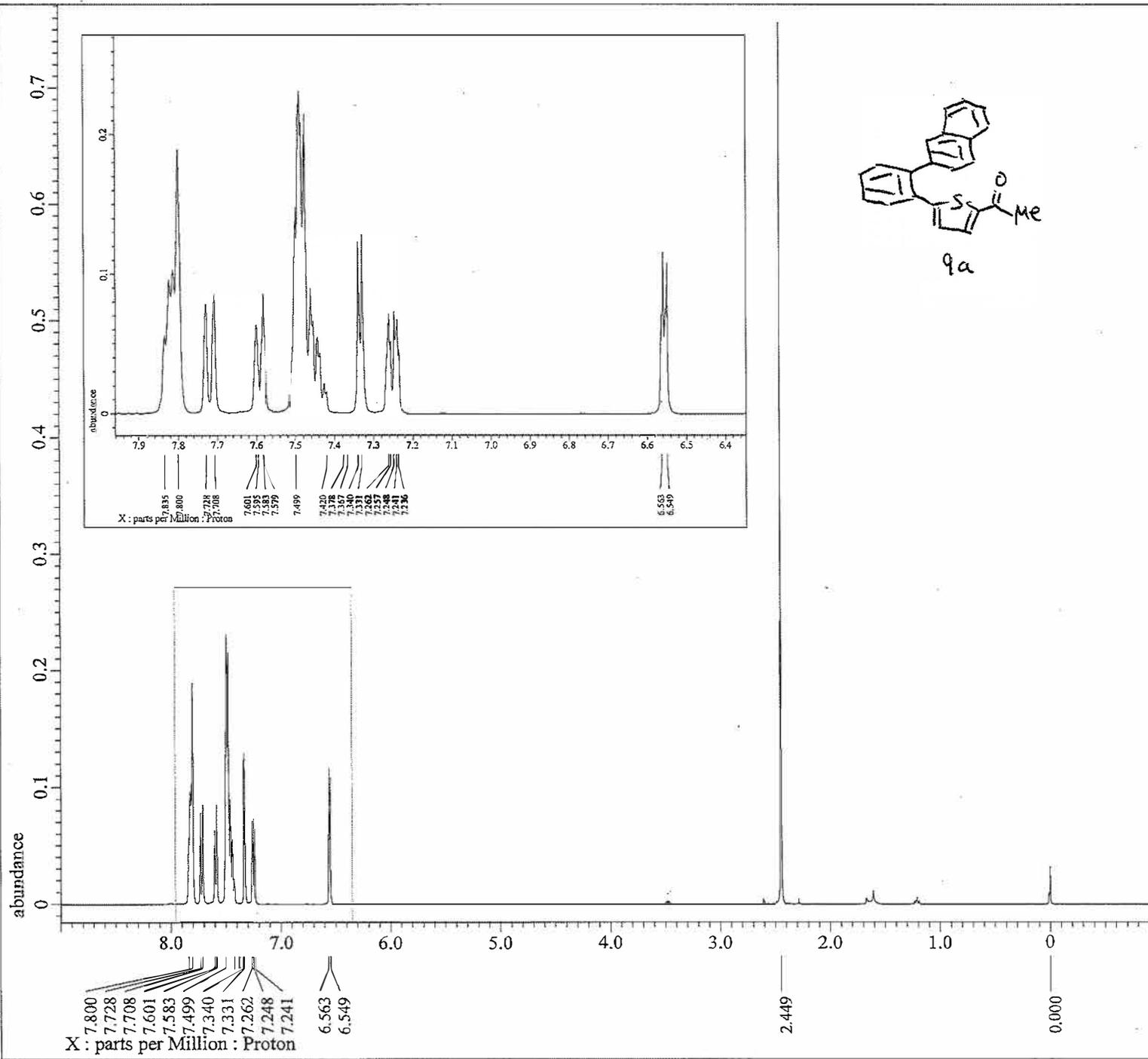
```

```

X_90_width = 9.11[us]
X_acq_time = 1.06430464[s]
X_angle = 30[deg]
X_atn = 4.9[db]
X_pulse = 3.03666667[us]
Irr_atn_dec = 22.255[db]
Irr_atn_noe = 22.255[db]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 60
Relaxation_delay = 2[s]
Repetition_time = 3.06430464[s]
Temp_get = 18.6[dc]

```

X : parts per Million : 13C



```

----- PROCESSING PARAMETERS -----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
以下に由来: KBT-724-recry_PROTON-1-1.jdf

```

```

Filename      = KBT-724-recry_PROTON-
Author        = delta
Experiment     = proton.jxp
Sample Id     = KBT-724-recry
Solvent       = CHLOROFORM-D
Actual Start Time = 13-NOV-2019 17:12:01
Revision Time  = 10-FEB-2020 15:24:52

```

```

Data Format    = 1D COMPLEX
Dim Size      = 26214
X Domain      = Proton
Dim Title     = Proton
Dim Units     = [ppm]
Dimensions    = X
Spectrometer  = JNM-ECZ400S/L1

```

```

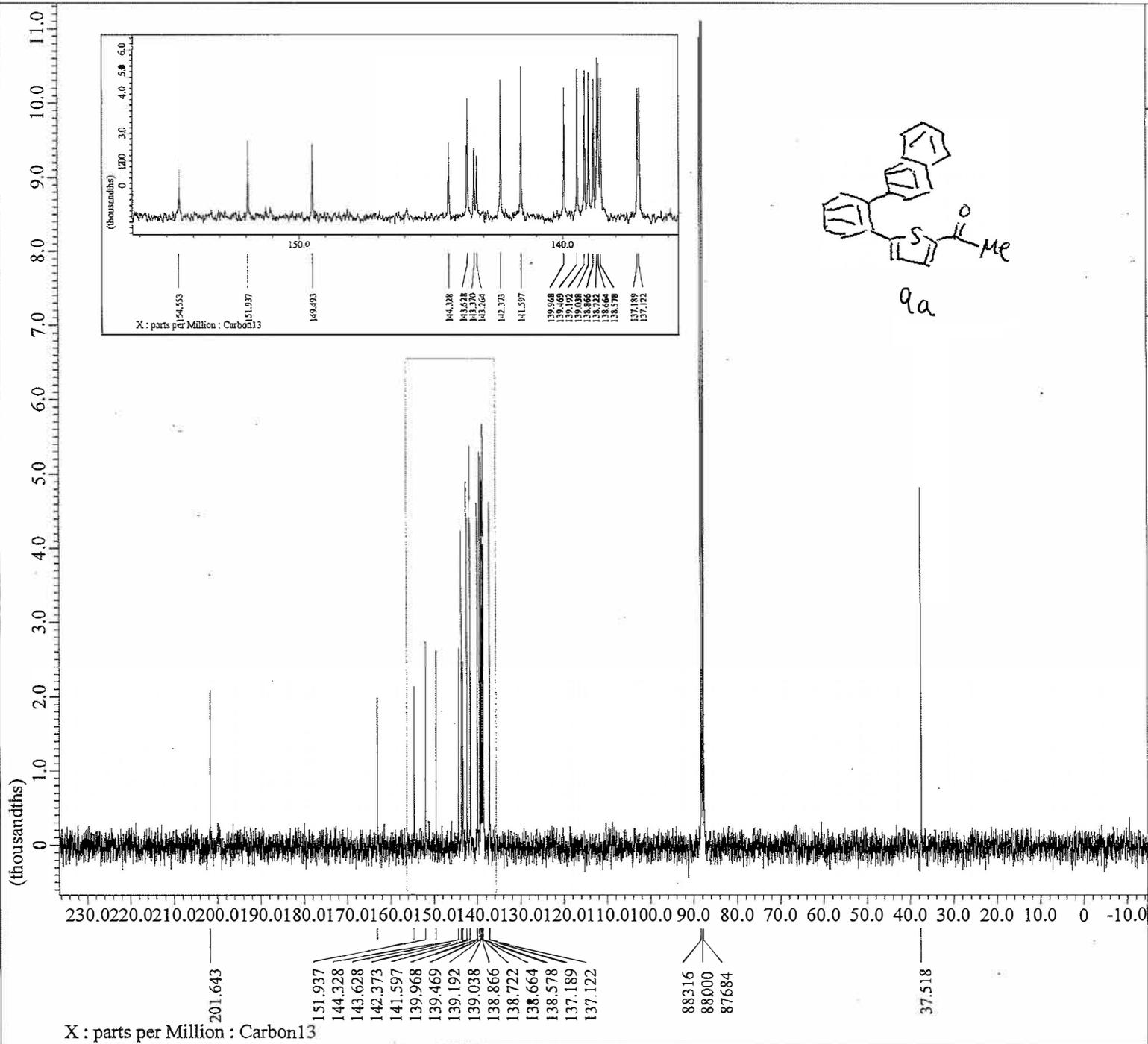
Field Strength = 9.389766[T] (400[MHz])
X Acq Duration = 4.37256192[s]
X Domain       = Proton
X Freq         = 399.78219838[MHz]
X Offset       = 5[ppm]
X Points       = 32768
X Prescans     = 0
X Resolution   = 0.22869888[Hz]
X Sweep        = 7.4940048[kHz]
X Sweep Clipped = 5.99520384[kHz]
Irr Domain     = Proton
Irr Freq       = 399.78219838[MHz]
Irr Offset     = 5[ppm]
Tri Domain     = Proton
Tri Freq       = 399.78219838[MHz]
Tri Offset     = 5[ppm]
Blanking       = 2[us]
Clipped        = FALSE
Scans          = 16
Total Scans    = 16

```

```

Relaxation Delay = 4[s]
Recvr Gain       = 42
Temp Get         = 18.9[dC]
X 90 Width      = 5.6[us]
X Acq Time       = 4.37256192[s]
X Angle          = 45[deg]
X Atn           = 5[dB]
X Pulse         = 2.8[us]
Irr Mode         = Off
Tri Mode         = Off
Dante Loop       = 400

```



```

----- PROCESSING PARAMETERS -----
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1, TRUE )
fft( 1, TRUE, TRUE )
machinephase
ppm
thresh( 5[%], 1 )
peak_pick( 0[Hz], 0.1[ppm], Peaks, 0[Hz] )
以下[由来]: KBT-724-recry_CARBON-1-1.jdf

```

```

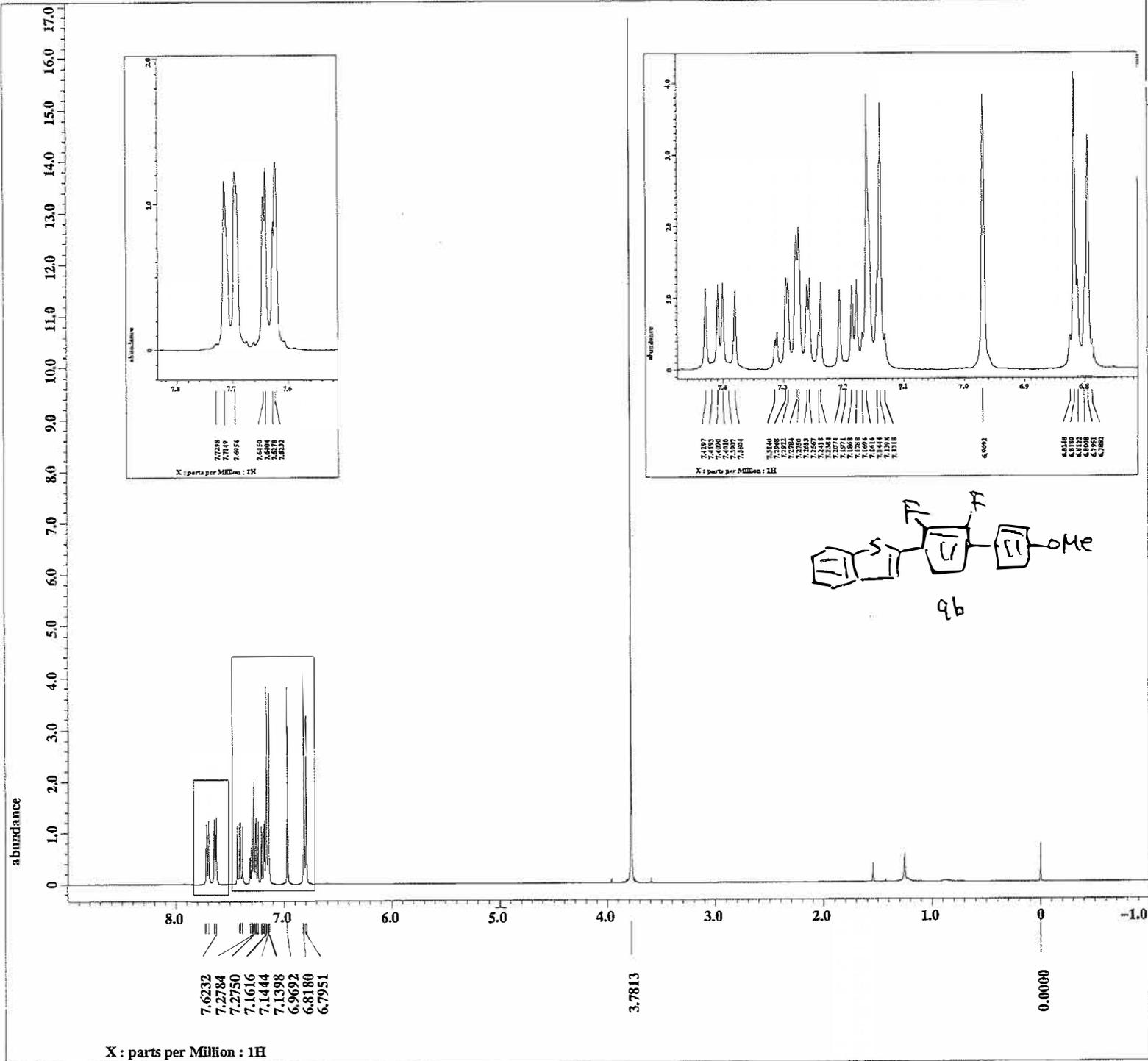
Filename           = KBT-724-recry_CARB
Author             = delta
Experiment         = carbon.jxp
Sample_Id          = KBT-724-recry
Solvent            = CHLOROFORM-D
Actual_Start_Time  = 13-NOV-2019 17:17:
Revision_Time      = 10-FEB-2020 15:26:

Data_Format        = 1D COMPLEX
Dim_Size           = 26214
X_Domain           = Carbon13
Dim_Title          = Carbon13
Dim_Units          = [ppm]
Dimensions         = X
Spectrometer       = JNM-ECZ400s/L1

Field_Strength     = 9.389766[T] (400[M
X_Acq_Duration     = 1.03809024[s]
X_Domain           = Carbon13
X_Freq             = 100.52530333[MHz]
X_Offset           = 100[ppm]
X_Points           = 32768
X_Prescans         = 4
X_Resolution       = 0.96330739[Hz]
X_Sweep            = 31.56565657[kHz]
X_Sweep_Clipped    = 25.25252525[kHz]
Irr_Domain         = Proton
Irr_Freq           = 399.78219838[MHz]
Irr_Offset         = 5[ppm]
Blanking           = 5[us]
Clipped            = TRUE
Scans              = 150
Total_Scans        = 150

Relaxation_Delay   = 2[s]
Recvr_Gain         = 52
Temp_Get           = 18.4[dc]
X_90_Width         = 10.6[us]
X_Acq_Time         = 1.03809024[s]
X_Angle            = 30[deg]
X_Atn              = 8.8[dB]
X_Pulse            = 3.53333333[us]
Irr_Atn_Dec        = 31.25[dB]
Irr_Atn_Dec_Calc   = 31.25[dB]
Irr_Atn_Dec_Default_Calc = 31.25[dB]
Irr_Atn_Noise     = 31.25[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]

```



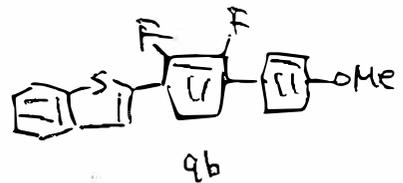
---- PROCESSING PARAMETERS ----  
 dc\_balance : 0 : FALSE  
 sexp : 0.2[Hz] : 0.0[s]  
 trapezoid3 : 0[%] : 80[%] : 100[%]  
 zerofill : 1  
 fft : 1 : TRUE : TRUE  
 machinephase  
 ppm  
 Derived from: benzothio-1H-1.jdf

Filename = benzothio-1H-3.jdf  
 Author = element  
 Experiment = single\_pulse.ex2  
 Sample\_id = S#469950  
 Solvent = CHLOROFORM-D  
 Creation\_time = 25-NOV-2019 11:17:01  
 Revision\_time = 10-FEB-2020 14:32:12  
 Current\_time = 10-FEB-2020 14:32:17

Comment = single\_pulse  
 Data\_format = 1D COMPLEX  
 Dim\_size = 13107  
 Dim\_title = 1H  
 Dim\_units = [ppm]  
 Dimensions = X  
 Site = ECS 400  
 Spectrometer = JNM-ECS400

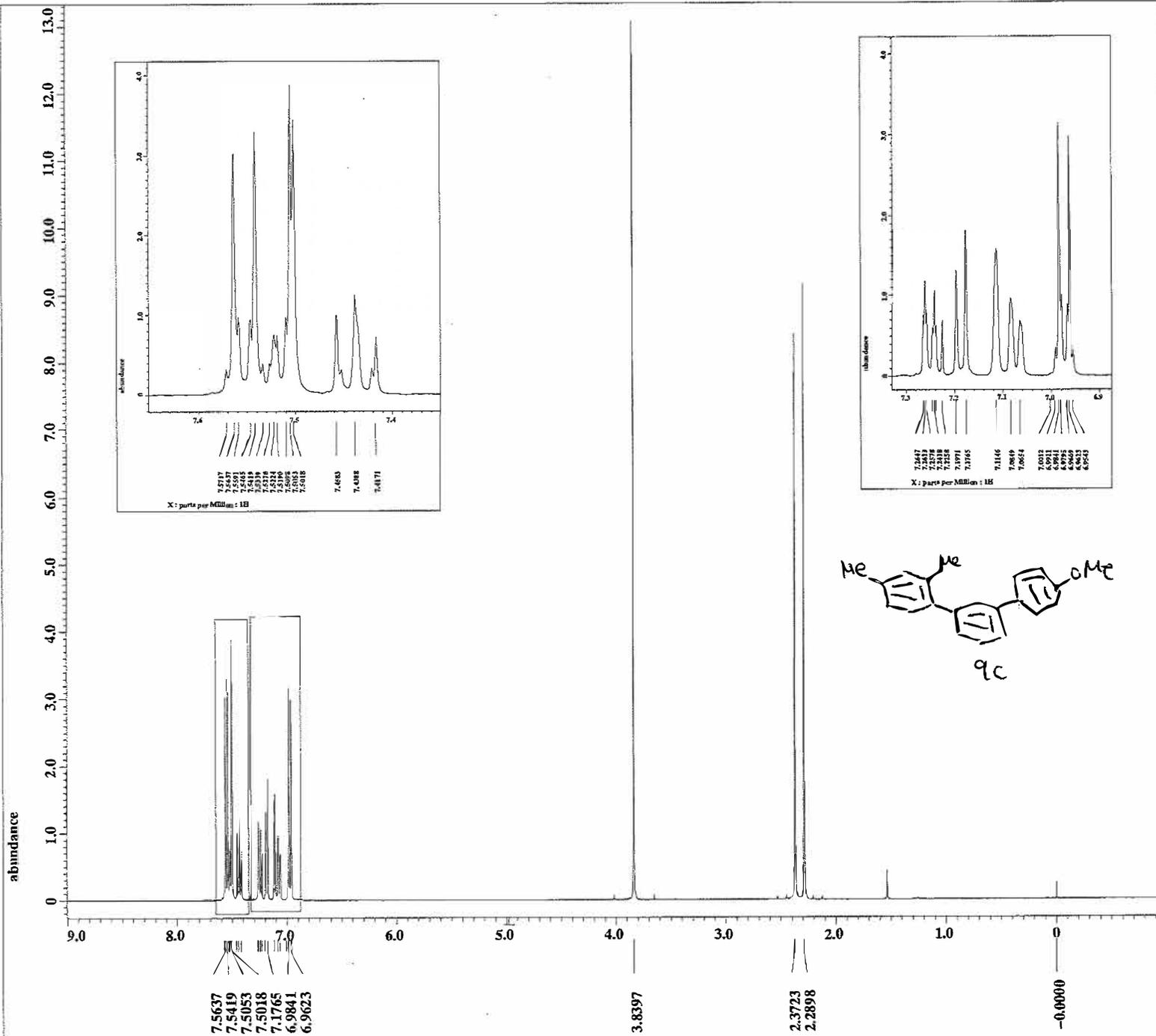
Field\_strength = 9.20197068[T] (390[MH  
 X\_acq\_duration = 2.228224[s]  
 X\_domain = 1H  
 X\_freq = 391.78655441[MHz]  
 X\_offset = 5[ppm]  
 X\_points = 16384  
 X\_prescans = 1  
 X\_resolution = 0.44878791[Hz]  
 X\_sweep = 7.35294118[kHz]  
 Irr\_domain = 1H  
 Irr\_freq = 391.78655441[MHz]  
 Irr\_offset = 5[ppm]  
 Tri\_domain = 1H  
 Tri\_freq = 391.78655441[MHz]  
 Tri\_offset = 5[ppm]  
 Clipped = FALSE  
 Mod\_return = 1  
 Scans = 8  
 Total\_scans = 8

X\_90\_width = 11.04[us]  
 X\_acq\_time = 2.228224[s]  
 X\_angle = 45[deg]  
 X\_atn = 1.9[dB]  
 X\_pulse = 5.52[us]  
 Irr\_mode = Off  
 Tri\_mode = Off  
 Dante\_presat = FALSE  
 Initial\_wait = 1[s]  
 Recvr\_gain = 36  
 Relaxation\_delay = 5[s]  
 Repetition\_time = 7.228224[s]  
 Temp\_get = 18[dc]



X : parts per Million : 1H





```

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

```

Derived from: 1H-1.jdf

```

Filename      = 1H-3.jdf
Author       = element
Experiment   = single_pulse.ex2
Sample_id    = S#404905
Solvent      = CHLOROFORM-D
Creation_time = 21-JAN-2020 09:20:31
Revision_time = 10-FEB-2020 14:43:29
Current_time  = 10-FEB-2020 14:44:27

```

```

Comment       = single_pulse
Data_format   = ID COMPLEX
Dim_size      = 13107
Dim_title     = 1H
Dim_units     = [ppm]
Dimensions    = X
Site          = ECS 400
Spectrometer  = JNM-ECS400

```

```

Field_strength = 9.20197068[T] (390[MH]
X_acq_duration = 2.228224[s]
X_domain       = 1H
X_freq         = 391.78655441[MHz]
X_offset       = 5[ppm]
X_points       = 16384
X_prescans     = 1
X_resolution   = 0.44878791[Hz]
X_sweep        = 7.35294118[kHz]
Irr_domain     = 1H
Irr_freq       = 391.78655441[MHz]
Irr_offset     = 5[ppm]
Tri_domain     = 1H
Tri_freq       = 391.78655441[MHz]
Tri_offset     = 5[ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 8
Total_scans    = 8

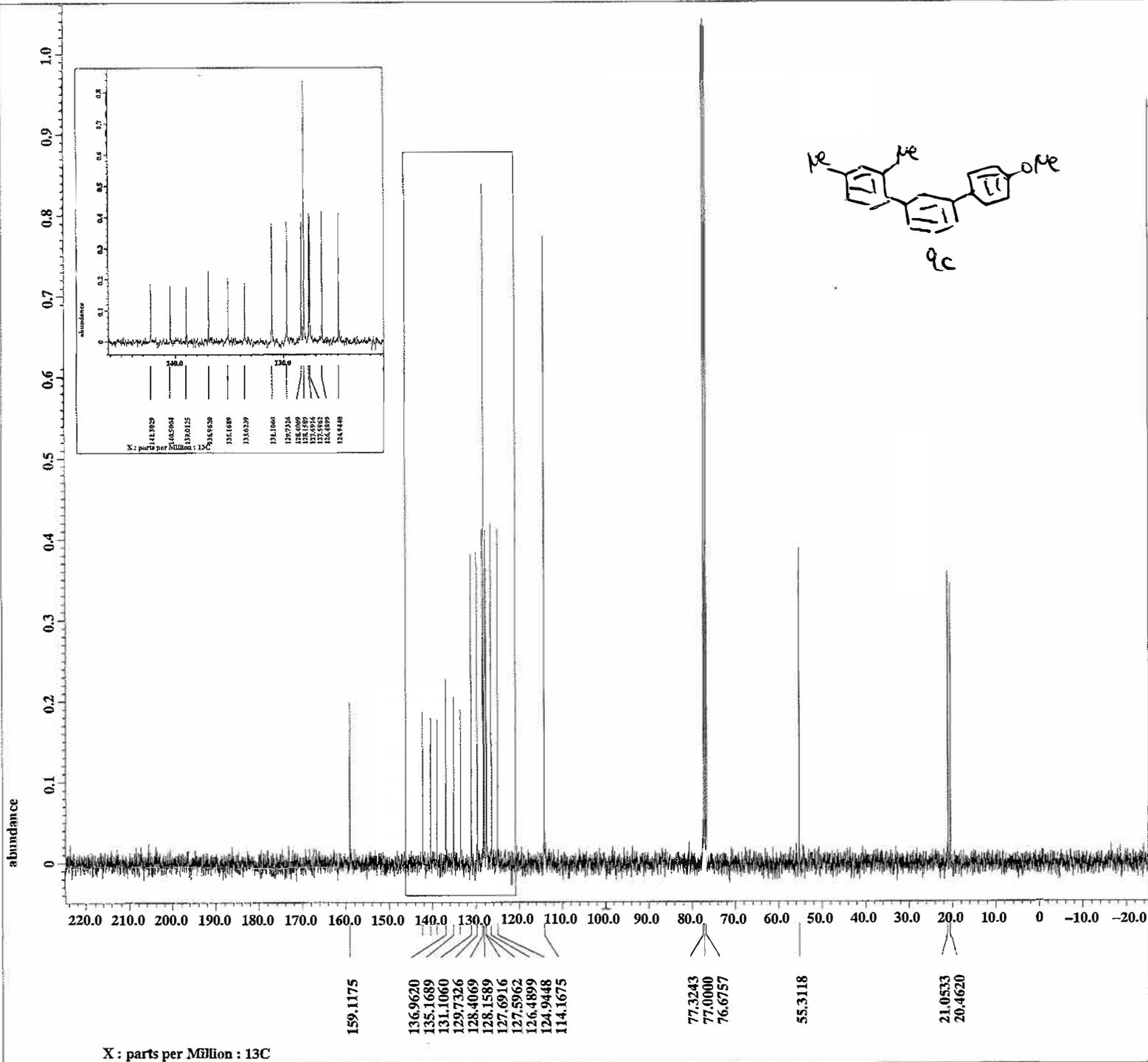
```

```

X_90_width    = 11.04[us]
X_acq_time     = 2.228224[s]
X_angle        = 45[deg]
X_atn          = 1.9[dB]
X_pulse        = 5.52[us]
Irr_mode       = Off
Tri_mode       = Off
Dante_presat   = FALSE
Initial_wait   = 1[s]
Recvr_gain     = 34
Relaxation_delay = 5[s]
Repetition_time = 7.228224[s]
Temp_get       = 18.3[dc]

```

X : parts per Million : 1H



```

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

Derived from: 13C-1.jdf

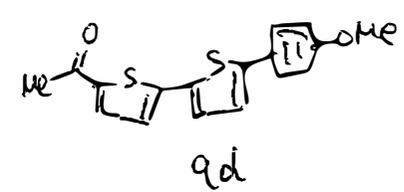
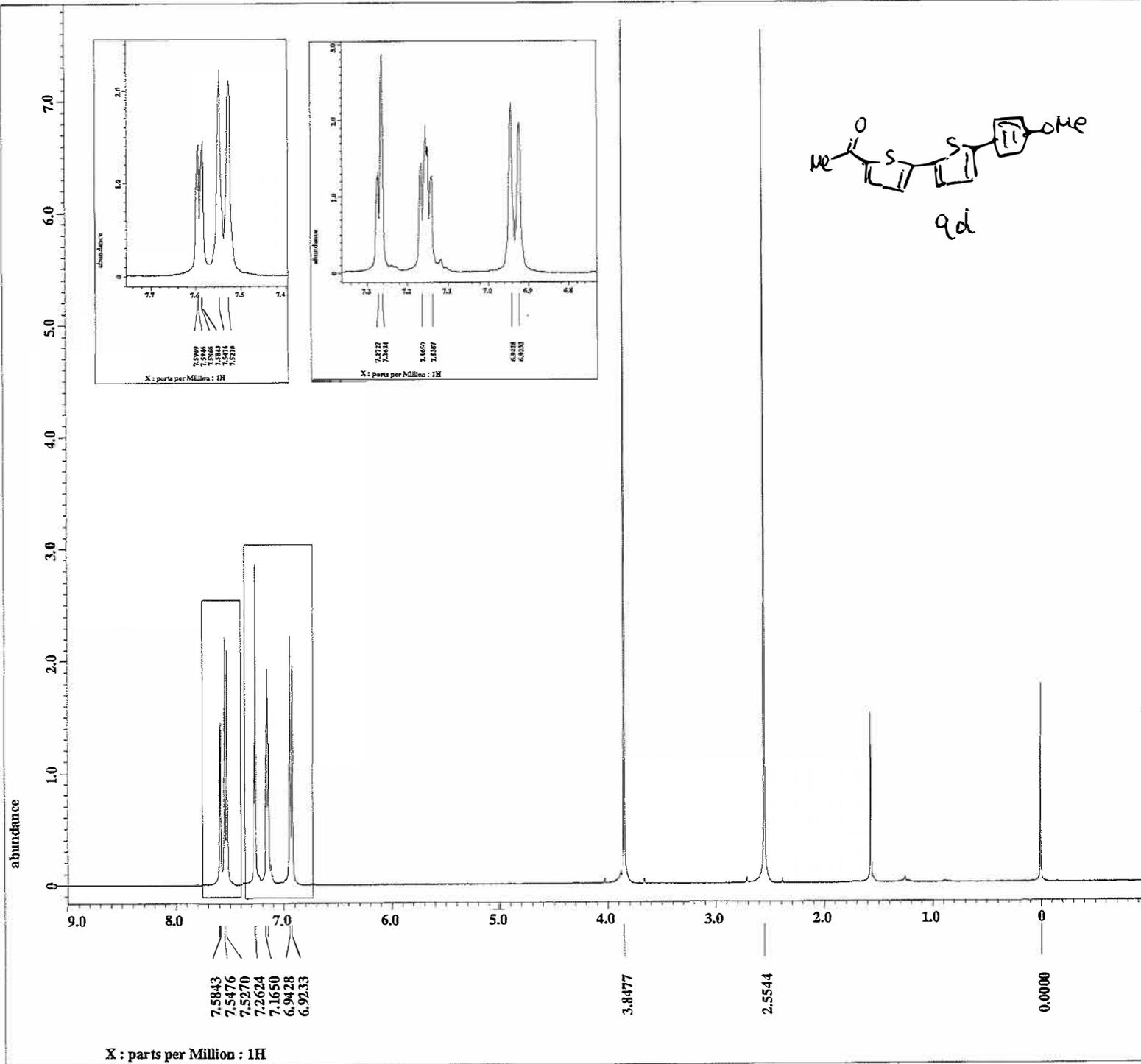
Filename      = 13C-3.jdf
Author       = element
Experiment   = single_pulse_dec
Sample_id    = S#406926
Solvent      = CHLOROFORM-D
Creation_time = 21-JAN-2020 09:26:09
Revision_time = 10-FEB-2020 14:44:47
Current_time  = 10-FEB-2020 14:45:20

Comment      = single pulse decouple
Data_format  = 1D COMPLEX
Dim_size     = 26214
Dim_title    = 13C
Dim_units    = [ppm]
Dimensions   = X
Site         = ECS 400
Spectrometer = JNM-ECS400

Field_strength = 9.20197068[T] (390 [MH]
X_acq_duration = 1.06430464[s]
X_domain       = 13C
X_freq        = 98.51479726[MHz]
X_offset      = 100[ppm]
X_points      = 32768
X_prescans    = 4
X_resolution  = 0.93958061[Hz]
X_sweep       = 30.78817734[kHz]
Irr_domain    = 1H
Irr_freq      = 391.78655441[MHz]
Irr_offset    = 5[ppm]
Clipped       = FALSE
Mod_return    = 1
Scans         = 89
Total_scans   = 89

X_90_width   = 9.11[us]
X_acq_time   = 1.06430464[s]
X_angle      = 30[deg]
X_atn        = 4.9[dB]
X_pulse      = 3.03666667[us]
Irr_atn_dec  = 22.255[dB]
Irr_atn_noe  = 22.255[dB]
Irr_noise    = WALTZ
Decoupling   = TRUE
Initial_wait = 1[s]
Noe          = TRUE
Noe_time     = 2[s]
Recvr_gain   = 60
Relaxation_delay = 2[s]
Repetition_time = 3.06430464[s]
Temp_get     = 18.6[dc]

```



```

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

Derived from: thio-thio-1H-1.jdf

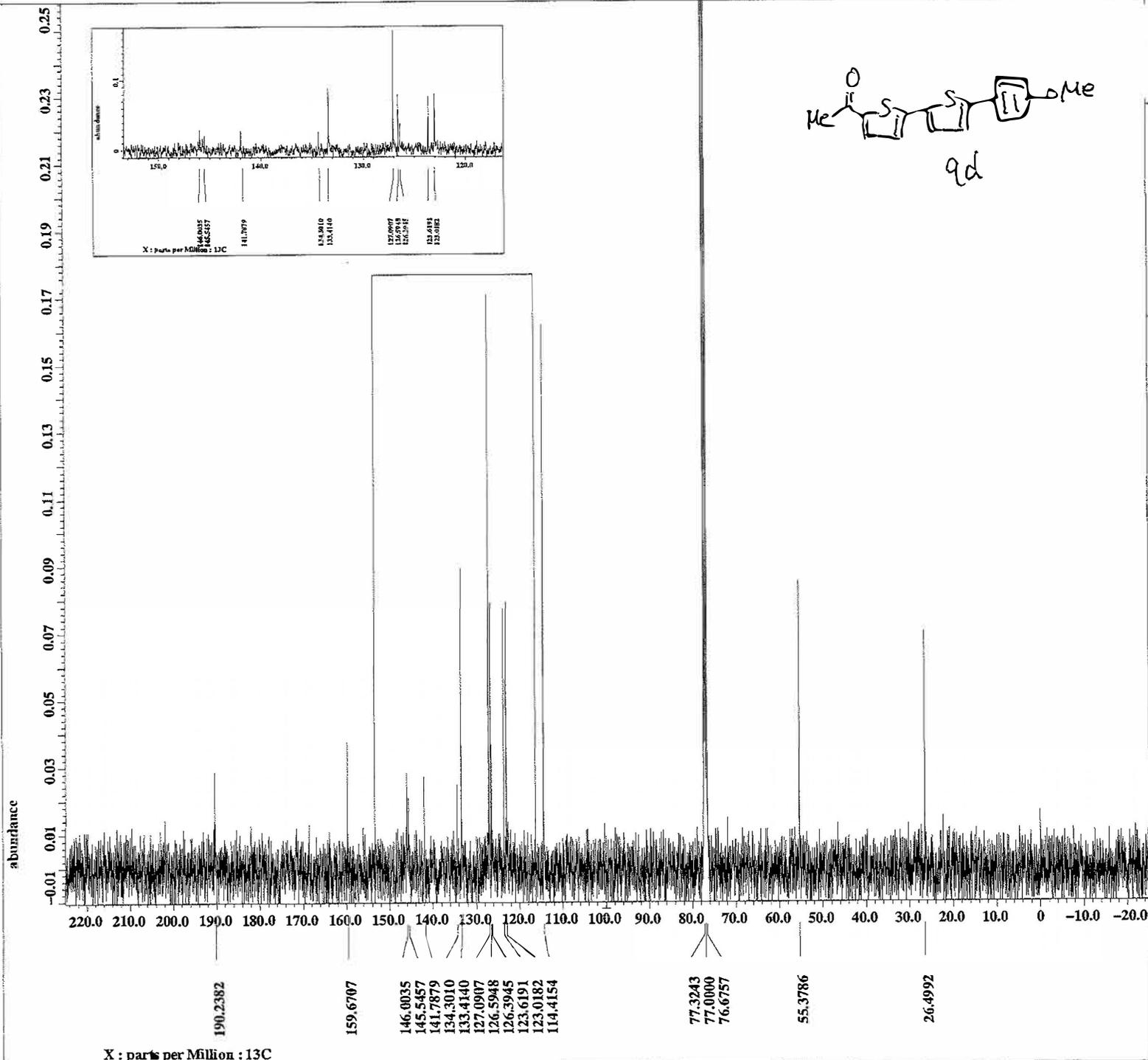
Filename      = thio-thio-1H-3.jdf
Author       = element
Experiment   = single_pulse.ex2
Sample_id    = S#619353
Solvent      = CHLOROFORM-D
Creation_time = 5-DEC-2019 15:24:03
Revision_time = 10-FEB-2020 14:51:21
Current_time  = 10-FEB-2020 14:52:11

Comment      = single_pulse
Data_format  = 1D COMPLEX
Dim_size     = 13107
Dim_title    = 1H
Dim_units    = [ppm]
Dimensions   = X
Site         = ECS 400
Spectrometer = JNM-ECS400

Field_strength = 9.20197068[T] (390[MH]
X_acq_duration = 2.228224[s]
X_domain       = 1H
X_freq         = 391.78655441[MHz]
X_offset       = 5[ppm]
X_points       = 16384
X_prescans     = 1
X_resolution   = 0.44878791[Hz]
X_sweep        = 7.35294118[kHz]
Irr_domain     = 1H
Irr_freq       = 391.78655441[MHz]
Irr_offset     = 5[ppm]
Tri_domain     = 1H
Tri_freq       = 391.78655441[MHz]
Tri_offset     = 5[ppm]
Clipped        = FALSE
Mod_return     = 1
Scans          = 8
Total_scans    = 8

X_90_width    = 11.04[us]
X_acq_time     = 2.228224[s]
X_angle        = 45[deg]
X_atn          = 1.9[dB]
X_pulse        = 5.52[us]
Irr_mode       = Off
Tri_mode       = Off
Dante_presat   = FALSE
Initial_wait   = 1[s]
Recvr_gain     = 50
Relaxation_delay = 5[s]
Repetition_time = 7.228224[s]
Temp_get       = 20.8[dC]

```



```

---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 2.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm
Derived from: thio-thio-13C-1.jdf

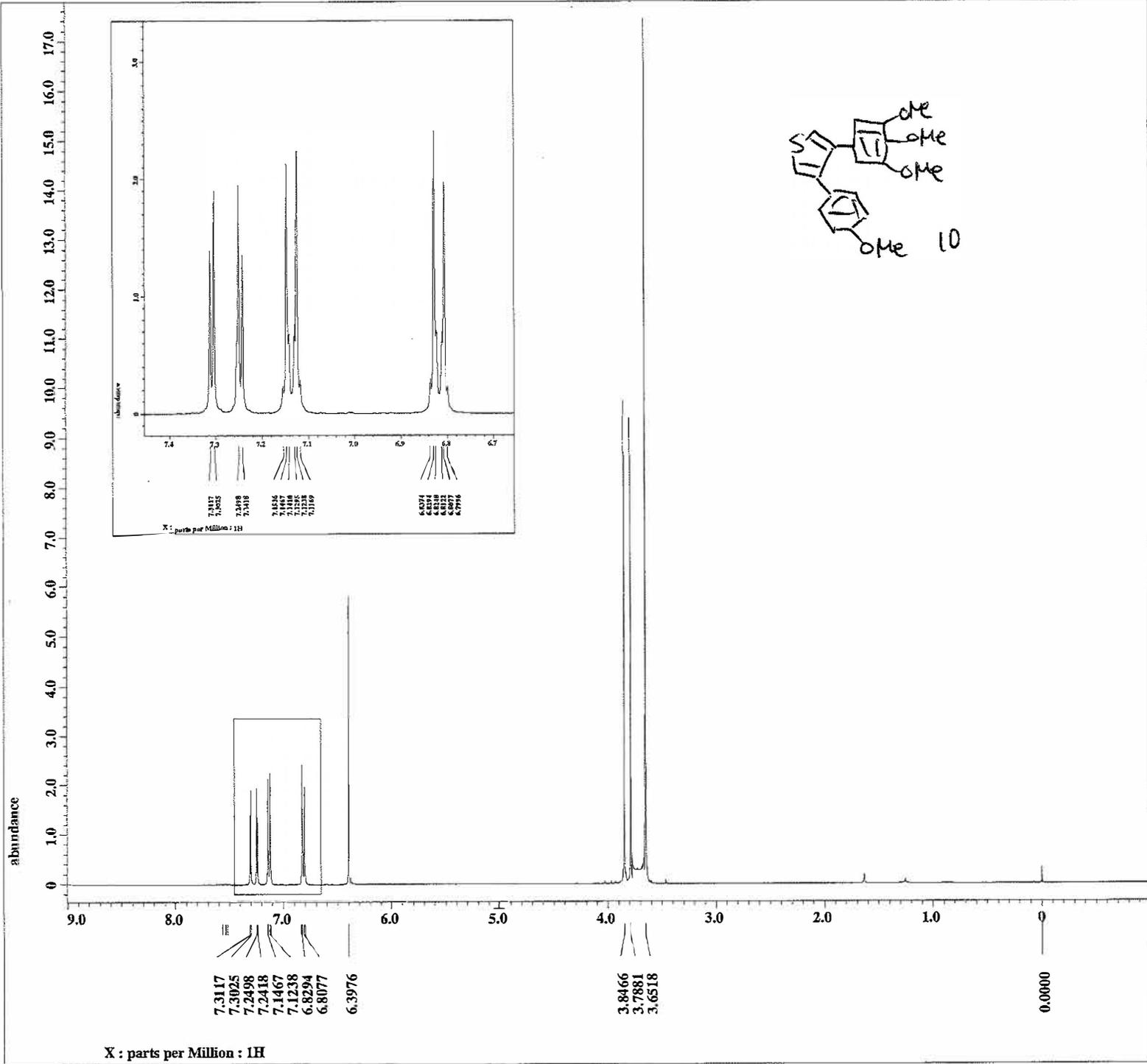
Filename = thio-thio-13C-4.jdf
Author = element
Experiment = single_pulse_dec
Sample_id = S#620988
Solvent = CHLOROFORM-D
Creation_time = 5-DEC-2019 15:35:14
Revision_time = 10-FEB-2020 14:54:21
Current_time = 10-FEB-2020 14:55:34

Comment = single pulse decouple
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400

Field_strength = 9.20197068[T] (390[MH]
X_acq_duration = 1.06430464[s]
X_domain = 13C
X_freq = 98.51479726[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.93958061[Hz]
X_sweep = 30.78817734[kHz]
Irr_domain = 1H
Irr_freq = 391.78655441[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 200
Total_scans = 200

X_90_width = 9.11[us]
X_acq_time = 1.06430464[s]
X_angle = 30[deg]
X_atn = 4.9[dB]
X_pulse = 3.03666667[us]
Irr_atn_dec = 22.255[dB]
Irr_atn_noe = 22.255[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 60
Relaxation_delay = 2[s]
Repetition_time = 3.06430464[s]
Temp_get = 21[dc]

```



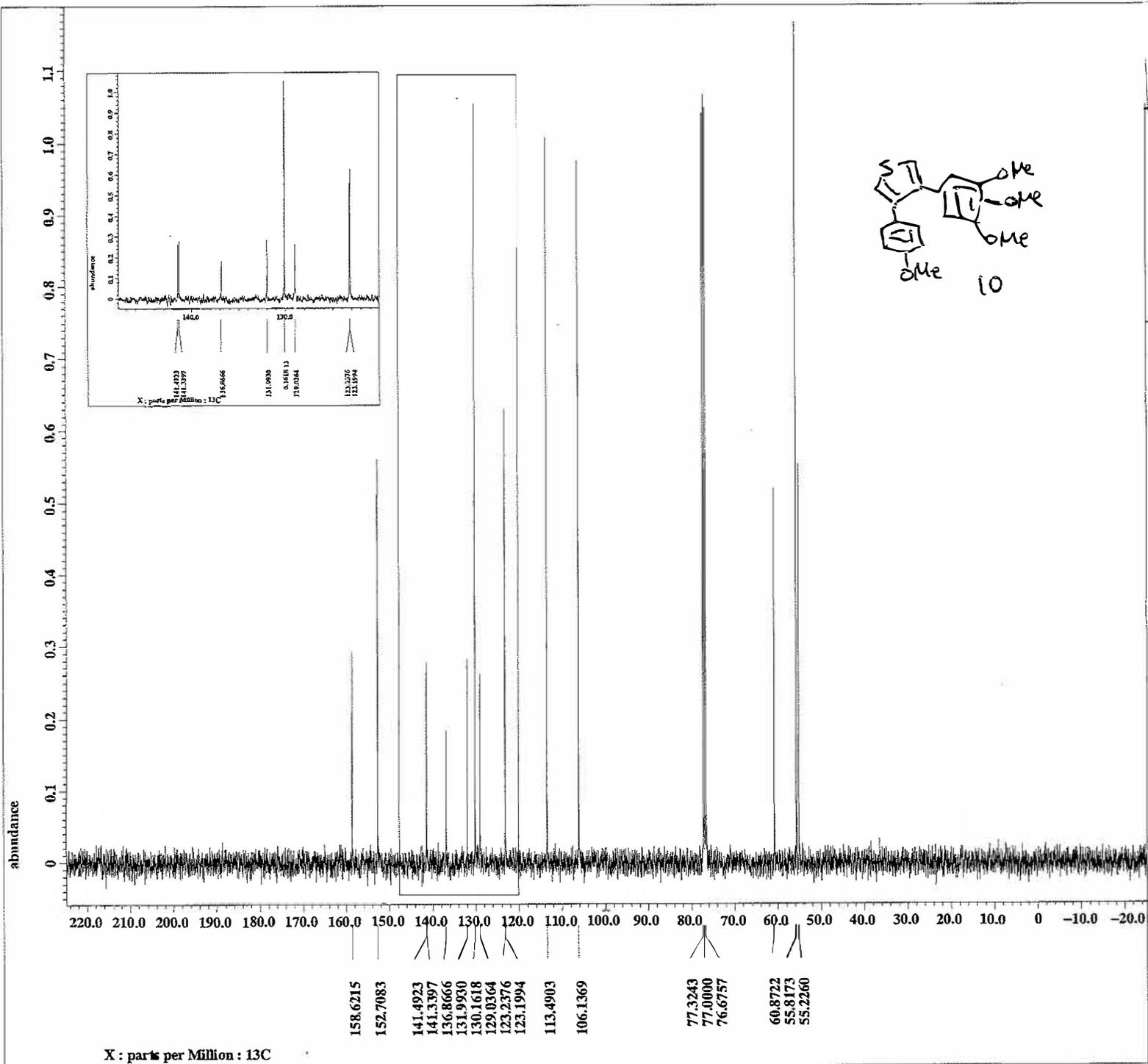
---- PROCESSING PARAMETERS ----  
 dc\_balance : 0 : FALSE  
 secp : 0.2[Hz] : 0.0[s]  
 trapezoid3 : 0[%] : 80[%] : 100[%]  
 zerofill : 1  
 fft : 1 : TRUE : TRUE  
 machinephase  
 ppm  
 Derived from: bioactive-1H-1.jdf

Filename = bioactive-1H-3.jdf  
 Author = element  
 Experiment = single\_pulse.ex2  
 Sample\_id = S#559789  
 Solvent = CHLOROFORM-D  
 Creation\_time = 5-DEC-2019 13:45:04  
 Revision\_time = 10-FEB-2020 14:37:45  
 Current\_time = 10-FEB-2020 14:38:13

Comment = single\_pulse  
 Data\_format = 1D COMPLEX  
 Dim\_size = 13107  
 Dim\_title = 1H  
 Dim\_units = [ppm]  
 Dimensions = X  
 Site = ECS 400  
 Spectrometer = JNM-ECS400

Field\_strength = 9.20197068[T] (390[MH]  
 X\_acq\_duration = 2.228224[s]  
 X\_domain = 1H  
 X\_freq = 391.78655441[MHz]  
 X\_offset = 5[ppm]  
 X\_points = 16384  
 X\_prescans = 1  
 X\_resolution = 0.44878791[Hz]  
 X\_sweep = 7.35294118[kHz]  
 Irr\_domain = 1H  
 Irr\_freq = 391.78655441[MHz]  
 Irr\_offset = 5[ppm]  
 Tri\_domain = 1H  
 Tri\_freq = 391.78655441[MHz]  
 Tri\_offset = 5[ppm]  
 Clipped = FALSE  
 Mod\_return = 1  
 Scans = 8  
 Total\_scans = 8

X\_90\_width = 11.04[us]  
 X\_acq\_time = 2.228224[s]  
 X\_angle = 45[deg]  
 X\_atn = 1.9[dB]  
 X\_pulse = 5.52[us]  
 Irr\_mode = Off  
 Tri\_mode = Off  
 Dante\_presat = FALSE  
 Initial\_wait = 1[s]  
 Recvr\_gain = 30  
 Relaxation\_delay = 5[s]  
 Repetition\_time = 7.228224[s]  
 Temp\_get = 20.8[dc]



----- PROCESSING PARAMETERS -----  
 dc\_balance : 0 : FALSE  
 secp : 2.0[Hz] : 0.0[s]  
 trapezoid3 : 0[%] : 80[%] : 100[%]  
 zeroFill : 1  
 fft : 1 : TRUE : TRUE  
 machinephase  
 ppm  
 Derived from: bioactive-13C-1.jdf

Filename = bioactive-13C-3.jdf  
 Author = element  
 Experiment = single\_pulse\_dec  
 Sample\_id = S#561635  
 Solvent = CHLOROFORM-D  
 Creation\_time = 5-DEC-2019 13:48:56  
 Revision\_time = 10-FEB-2020 14:40:04  
 Current\_time = 10-FEB-2020 14:41:00

Comment = single pulse decouple  
 Data\_format = 1D COMPLEX  
 Dim\_size = 26214  
 Dim\_title = 13C  
 Dim\_units = [ppm]  
 Dimensions = X  
 Site = ECS 400  
 Spectrometer = JNM-ECS400

Field\_strength = 9.20197068[T] (390[MH  
 X\_acq\_duration = 1.06430464[s]  
 X\_domain = 13C  
 X\_freq = 98.51479726[MHz]  
 X\_offset = 100 [ppm]  
 X\_points = 32768  
 X\_prescans = 4  
 X\_resolution = 0.93958061 [Hz]  
 X\_sweep = 30.78817734 [kHz]  
 Irr\_dmain = 1H  
 Irr\_freq = 391.78655441[MHz]  
 Irr\_offset = 5 [ppm]  
 Clipped = FALSE  
 Mod\_return = 1  
 Scans = 55  
 Total\_scans = 55

X\_90\_width = 9.11 [us]  
 X\_acq\_time = 1.06430464 [s]  
 X\_angle = 30 [deg]  
 X\_atn = 4.9 [dB]  
 X\_pulse = 3.03666667 [us]  
 Irr\_atn\_dec = 22.255 [dB]  
 Irr\_atn\_noe = 22.255 [dB]  
 Irr\_noise = WALTZ  
 Decoupling = TRUE  
 Initial\_wait = 1 [s]  
 Noe = TRUE  
 Noe\_time = 2 [s]  
 Recvr\_gain = 60  
 Relaxation\_delay = 2 [s]  
 Repetition\_time = 3.06430464 [s]  
 Temp\_get = 21 [dc]