Solid-State Suzuki-Miyaura Cross-Coupling Reactions: Olefin-Accelerated C–C Coupling Using Mechanochemistry

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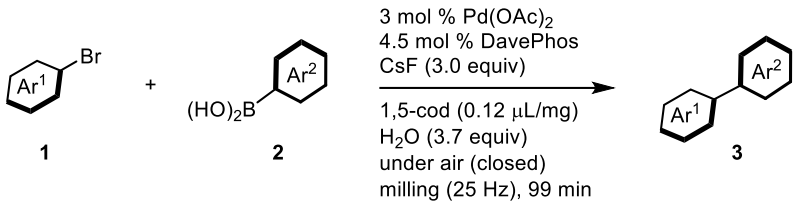
Table of Contents

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 jars (1.5 mL or 25 mL) and balls are made of stainless. NMR spectra were recorded on JEOL JNM-ECX400P and JNM-ECS400 spectrometers (^{1}H: 392 or 396 or 399 or 401 MHz, ^{13}C: 99 or 100 MHz). Tetramethylsilane (^{1}H), $CDCl_3$ (^{13}C) was employed as external standards, respectively. Multiplicity was recorded as follows: s = singlet, brs = broad singlet, d = doublet, t = triplet, q = quartet, quint = quintet, sept = septet, o = octet, m = multiplet. 1,1,2,2-Tetrachloroethane was used as an internal standard to determine NMR yields. Magic angle spinning (MAS) spectra were recorded on a Bruker MSL-300 spectrometer, operating at 121.5 MHz for ^{31}P NMR (spinning rate 8kHz). GLC analyses were conducted with a Shimazu GC-2014 or GC-2025 equipped with ULBON HR-1 glass capillary column (Shinwa Chemical Industries) 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 Cu-K_α radiation and D/teX Ultra detector covering 5-60° (2θ). Transmission electron microscopy analysis was carried out at “Joint-Use Facilities: Laboratory of Nano-Micro Material Analysis”, Hokkaido University. ICP-AES analyses were made ICPE-9000 using at the Global Facility Center, Hokkaido University.

2. General Procedure for Solid-State Cross-Coupling.



Aryl halide **1** (0.3 mmol), aryl boronic acid **2** (0.36 mmol, 1.2 equiv), $Pd(OAc)_2$ (0.009 mmol, 3 mol %) and DavePhos (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: 5 mm). Then H_2O (20 μL, 3.7 equiv) and 1,5-cod (0.12 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 passed through a short silica gel column eluting with CH_2Cl_2 to remove inorganic salts. The crude mixture was then purified by flash column chromatography (SiO_2, typically CH_2Cl_2/hexane, typically 0-15:85) to give the corresponding coupling product **3**.

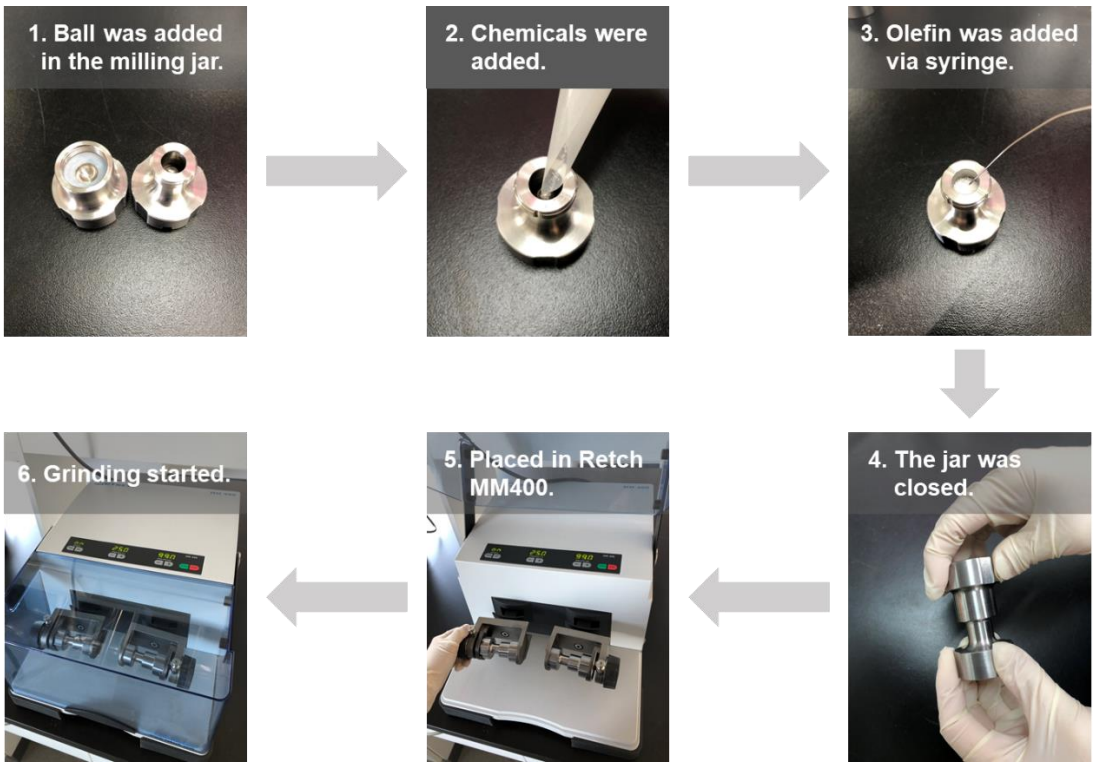
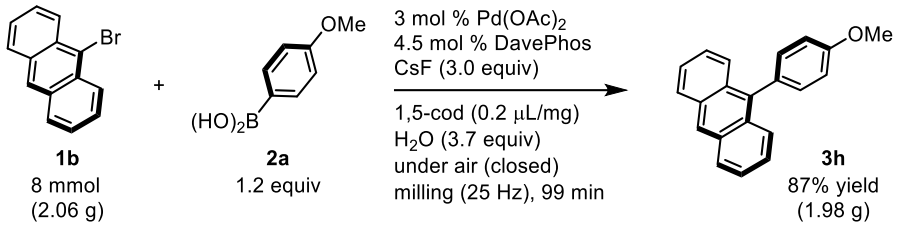


Figure S1. Set-up procedure for the solid-state cross-coupling.

3. Procedure for Solid-State Cross-Coupling at Gram Scale.

Solid-State Conditions



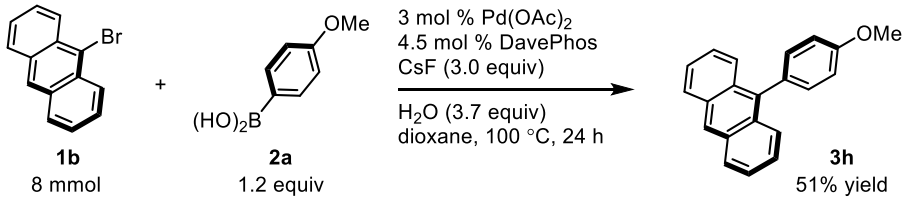
1b
8 mmol
(2.06 g)

2a
1.2 equiv

3h
87% yield
(1.98 g)

1b (8.0 mmol, 2.06 g, 1.0 equiv), **2a** (9.6 mmol, 1.46 g, 1.2 equiv), $Pd(OAc)_2$ (0.24 mmol, 53.9 mg, 3 mol %) and DavePhos (0.36 mmol, 141.7 mg, 4.5 mol %), CsF (24 mmol, 3.65 g, 3.0 equiv) were placed in a ball milling vessel (stainless, 25 mL) loaded with four grinding balls (stainless, diameter: 10 mm). Then H_2O (0.60 mL, 3.7 equiv) and 1,5-cod (1.5 ml, 0.20 μl/mg) was added. After the vessel was closed without purging with inert gas, the vessel was placed in the ball mill (Retch MM400, 99 min at 25Hz). After 99 min, the mixture was passed through a short silica gel column eluting with CH_2Cl_2 to remove inorganic salts. The crude mixture was then purified by reprecipitation from CH_2Cl_2/MeOH to give the corresponding product **3h** as a white solid (1.98 g, 87% yield).

Solution-State Conditions



1b
8 mmol
(2.06 g)

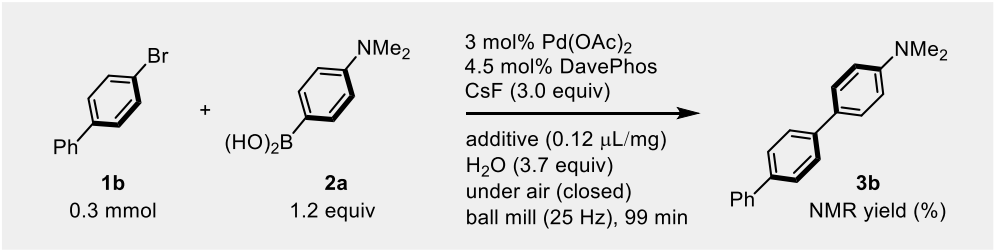
2a
1.2 equiv

3h
51% yield
(1.19 g)

A 500 ml of three necked round bottomed flask was equipped with a stir bar. The vessel was oven dried and then allowed to cool to room temperature. Then **1b** (8.0 mmol, 2.06 g, 1.0 equiv), **2a** (9.6 mmol, 1.46 g, 1.2 equiv), $Pd(OAc)_2$ (0.24 mmol, 53.9 mg, 3 mol %) and DavePhos (0.36 mmol, 141.7 mg, 4.5 mol %), CsF (24 mmol, 3.65 g, 3.0 equiv) were added to a flask. Under nitrogen atmosphere, H_2O (0.53 mL, 3.7 equiv) and dioxane (0.05 M, 160 ml) were added, and the temperature was increased to 100 °C. After 24 hours, the mixture was extracted with CH_2Cl_2 three times. The solution was dried over $MgSO_4$. After filtration, the CH_2Cl_2 was then removed by rotary evaporation. The crude mixture was purified by column chromatography (SiO_2, CH_2Cl_2/Hexane, 0:100–50:50) to give the corresponding product **3h** as a white solid (1.19 g, 51% yield).

4. Results of Optimization Study.

We found that the solid-state cross-coupling reaction with 1,5-cod was dramatically accelerated to form the coupling product in quantitative yield (97% yield). The use of cyclooctene (coe) as an additive also effectively promoted the reaction (88% yield). Other olefins such as 1,7-octadiene, 1-octene, cyclopentene and cyclohexene could also be used to facilitate the solid-state cross-coupling reaction (87–93% yields). In sharp contrast, the use of corresponding alkanes as LAG additives consistently provided lower yields compared to those of the reaction with the olefins. Although a small amount of organic solvents such as dimethyl ether (DME) and toluene improve the yields of product (78% and 84% yield, respectively), full conversion of substrate was not observed in both cases. The use of acetonitrile (MeCN) and dimethylsulfoxide (DMSO) did not or poorly promote the solid-state cross-coupling (12% and 39% yield, respectively). Interestingly, norbornadiene decreased the catalytic activity of this reaction.



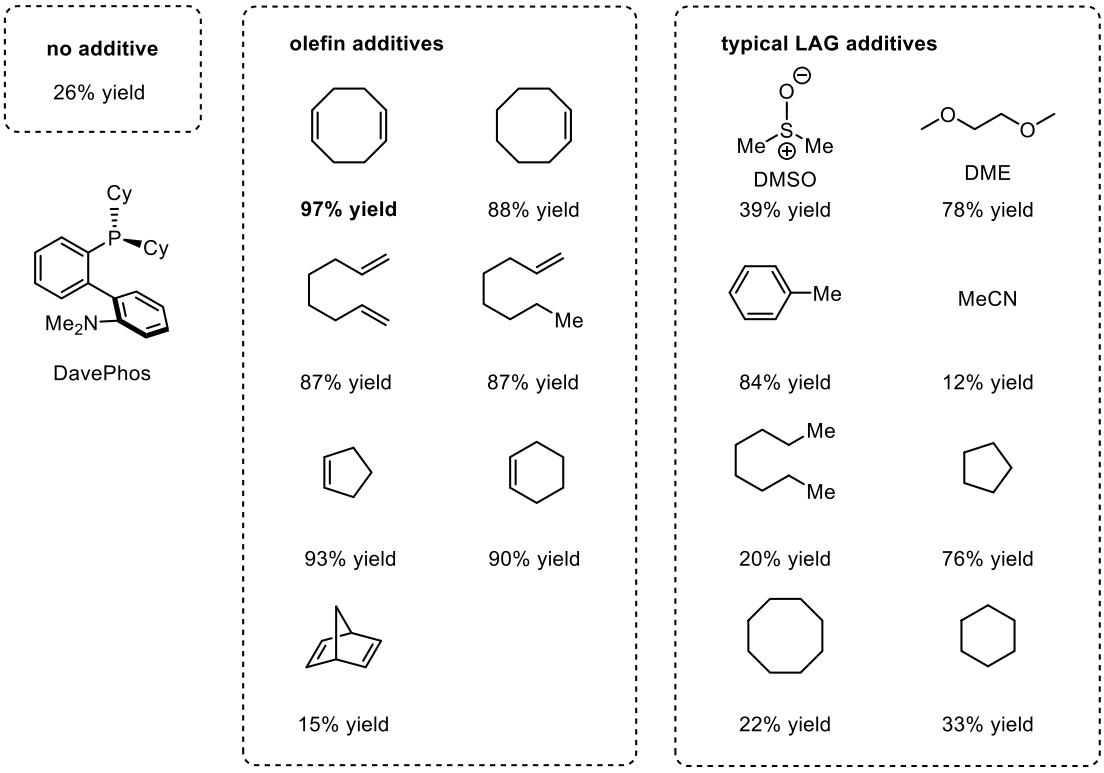
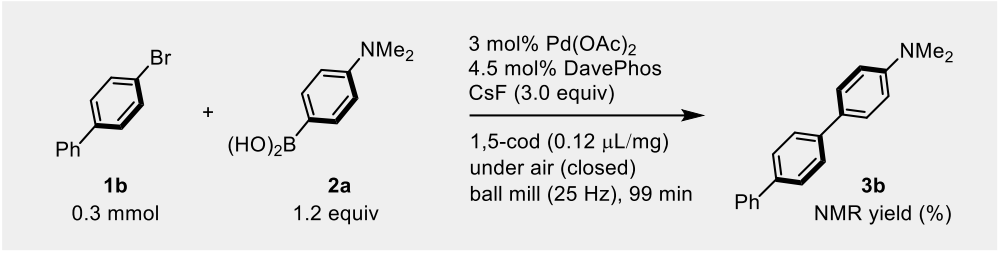
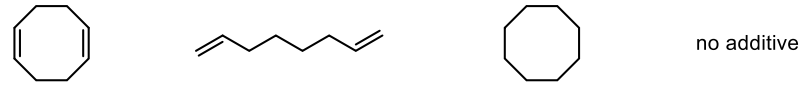


Table S1. Effect of LAG additives on the solid-state cross-coupling.

We found that small amount water is also important for the high reactivity. The reaction without water provided the lower yield of the product. The several reasons can be considered; 1) H_2O could act as dispersant for CsF or boronic acids in the solid-state medium. 2) H_2O could suppress the formation of less reactive boroxines from the corresponding boronic acids during the reaction.





64% yield | 51% yield | 20% yield | 28% yield

Table S2. Effect of water on the solid-state cross-coupling.

5. Details of Transmission Electron Microscopy.

The crude mixtures were prepared by the following conditions: 0.3 mmol of **1b**; 0.36 mmol of **2a**; 0.009 mmol of $Pd(OAc)_2$; 0.0135 mmol of DavePhos; 0.9 mmol of CsF; H_2O (20 μL) and 1,5-cod (33 μL) or cyclooctane (33 μL) in a stainless-steel ball-milling jar (1.5 mL) with a stainless-steel ball (5 mm); 25 Hz; 99 min. The samples for the characterization by transmission electron microscopy (TEM) were prepared by dropping the colloidal solution of hexane onto a copper grid covered with thin carbon film.

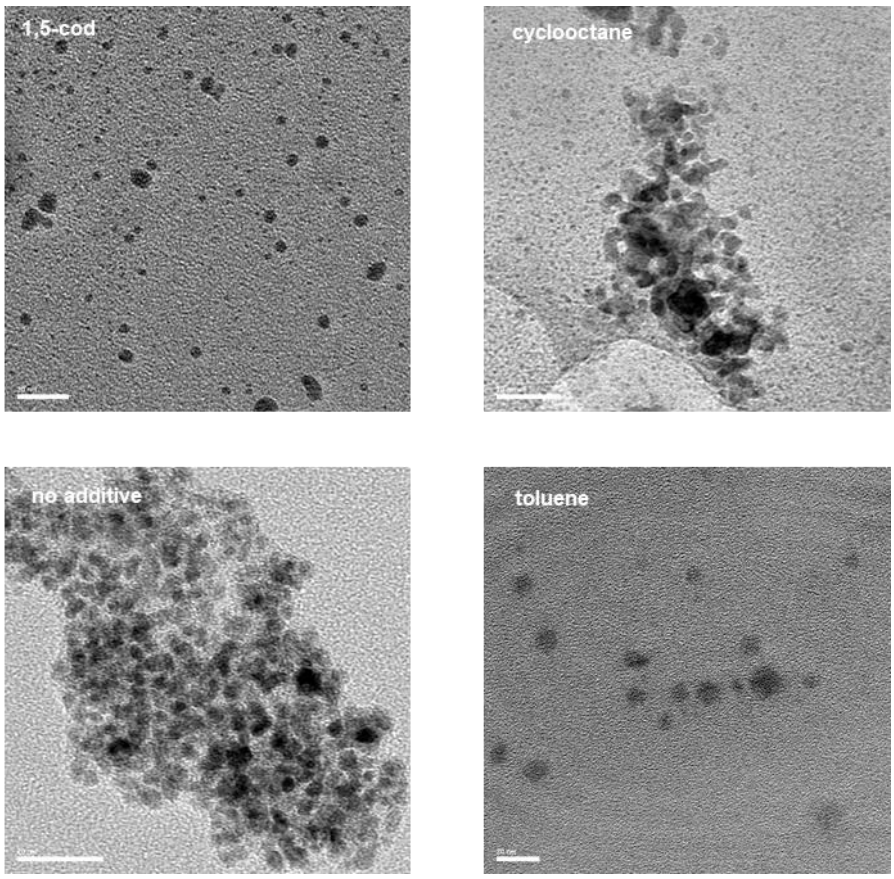


Figure S2. TEM images of palladium nanoparticles in the crude reaction mixtures. Scale bars in the TEM images (bottom left): 20 nm.

6. Solid-State ^{31}P NMR Studies

Figure S3. Solid-state NMR spectra of DavePhos.

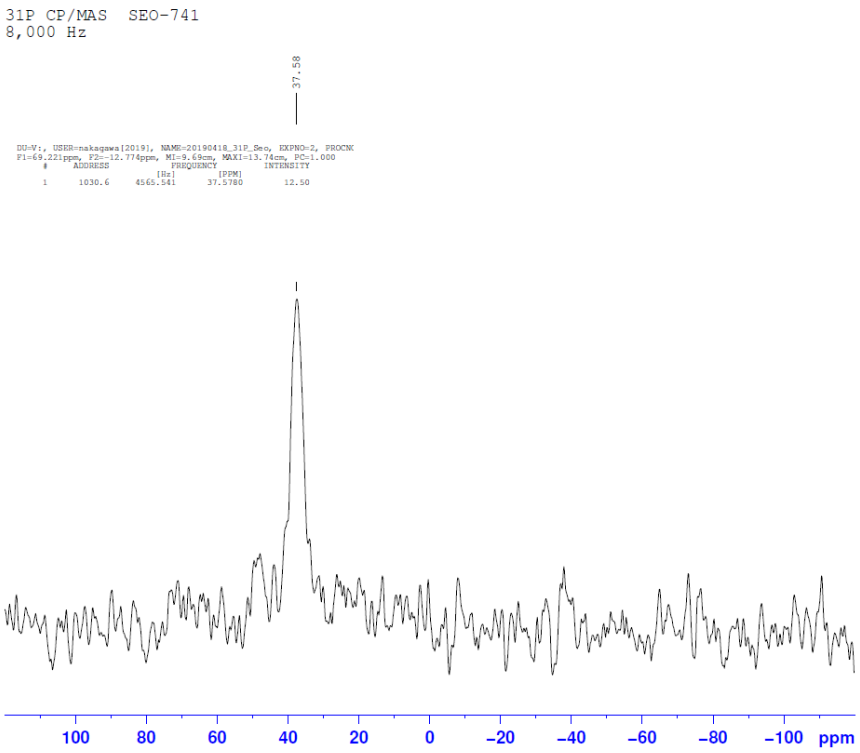


Figure S4. Solid-state NMR spectra of the reaction mixtures of **1c** and **2b** after grinding for 99 min in

a ball mill in the presence of 1,5-cod.

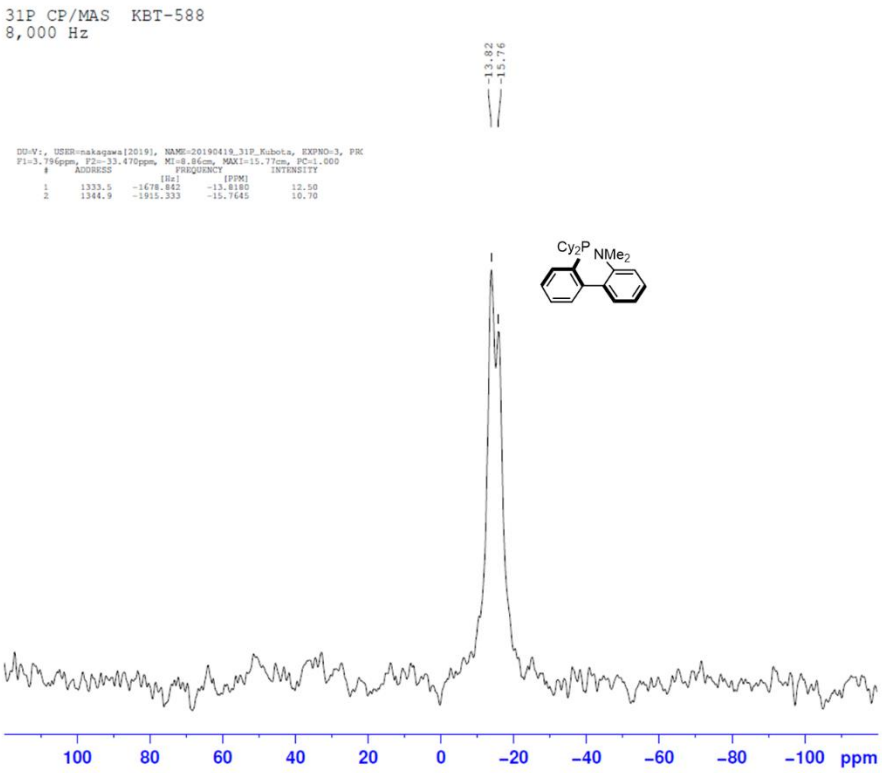


Figure S5. Solid-state NMR spectra of the reaction mixtures of **1c** and **2b** after grinding for 99 min in a ball mill in the absence of 1,5-cod.

7. Reaction Temperature Confirmed by Thermography

The temperature inside the milling jar after the solid-state coupling reaction was confirmed by thermography. The crude mixtures were prepared by the following conditions: 0.3 mmol of **1b**; 0.36 mmol of **2a**; 0.009 mmol of $Pd(OAc)_2$; 0.0135 mmol of DavePhos, 0.9 mmol of CsF, H_2O (20 μL), 1,5-cod (0.12 μL/mg) in a stainless-steel ball milling jar (1.5 mL) with a stainless-steel ball (5 mm); 25Hz; 99 min. The obtained image showed that the temperature was around 35 °C.

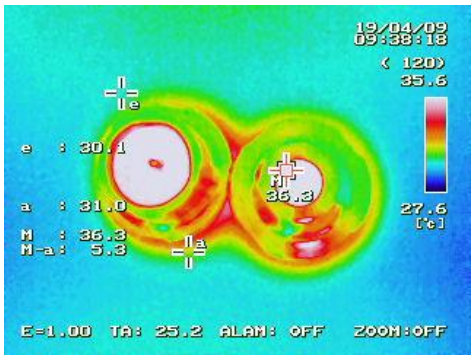


Figure S6. Temperature inside the milling jar confirmed by thermography.

8. ICP-AES Analysis

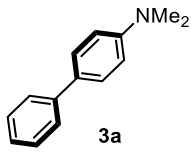
We have carried out ICP-AES analysis using two samples, **3c** and **3h**, to investigate the levels of residual palladium in the products. While no presence of residual palladium in the product **3c** was confirmed (detection limit: 5 ppm), trace amount of residual palladium (560 ppm) was detected in the product **3h**.

Product	Residual palladium
3c	below detection limit (5 ppm)
3h	560 ppm

Table S3. Summary of ICP-AES analysis

9. Characterization of Obtained Coupling Products.

***N*,*N*-Dimethyl-(1,1'-biphenyl)-4-amine (3a).**

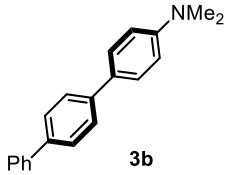


3a

The reaction was carried out with 47.1 mg (0.30 mmol) of **1a** and 59.4 mg (0.36 mmol) of **2a**. The product **3a** was obtained as a white powder (54.4 mg, 0.276 mmol, 92% yield). ^{1}H and ^{13}C NMR were in agreement with the literature.[1]

^{1}H NMR (392 MHz, $CDCl_3$, δ): 3.00 (s, 6H), 6.81 (d, J = 8.7 Hz, 2H), 7.21–7.28 (m, 1H), 7.39 (t, J = 7.2 Hz, 2H), 7.51 (d, J = 8.5 Hz, 2H), 7.56 (d, J = 7.6 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 40.5 (CH_3), 112.9 (*C*H), 125.9 (*C*H), 126.2 (*C*H), 127.7 (*C*H), 128.6 (*C*H), 129.2 (*C*), 141.2 (*C*), 149.9 (*C*). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{14}H_{15}N$, 197.1205; found, 197.1208.

***N*,*N*-Dimethyl-(1,1':4',1''-terphenyl)-4-amine (3b).**

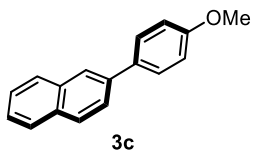


3b

The reaction was carried out with 69.9 mg (0.30 mmol) of **1b** and 59.4 mg (0.36 mmol) of **2a**. The product **3b** was obtained as a white powder (74.6 mg, 0.273 mmol, 91% yield). ^{1}H and ^{13}C NMR were in agreement with the literature.[2]

^{1}H NMR (392 MHz, $CDCl_3$, δ): 3.00 (s, 6H), 6.83 (d, J = 9.0 Hz, 2H), 7.31–7.37 (m, 1H), 7.42–7.48 (m, 2H), 7.54–7.58 (m, 2H), 7.61–7.66 (m, 6H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 40.5 (CH_3), 112.9 (*C*H), 126.6 (*C*H), 126.9 (*C*H), 127.0 (*C*H), 127.4 (*C*H), 127.6 (*C*H), 128.7 (*C*H), 128.8 (*C*), 138.8 (*C*), 140.3 (*C*), 141.1 (*C*), 150.2 (*C*). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{20}H_{19}N$, 273.1518; found, 273.1521.

2-(4-Methoxyphenyl)naphthalene (3c).



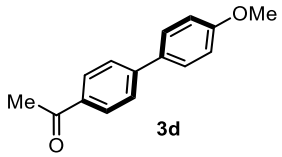
3c

The reaction was carried out with 66.6 mg (0.32 mmol) of **1c** and 54.7 mg (0.36 mmol) of **2b**. The product **3c** was obtained as a white powder (7.02 mg, 0.30 mmol, 93% yield). ^{1}H and ^{13}C NMR were

in agreement with the literature.[3]

^{1}H NMR (401 MHz, $CDCl_3$, δ): 3.88 (s, 3H), 7.01–7.06 (m, 2H), 7.43–7.53 (m, 2H), 7.64–7.70 (m, 2H), 7.72 (dd, *J* = 1.8, 8.6 Hz, 1H), 7.83–7.92 (m, 3H), 7.98–8.01 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 55.5 (*C*H_3), 114.4 (*C*H), 125.1 (*C*H), 125.5 (*C*H), 125.7 (*C*H), 126.3 (*C*H), 127.7 (*C*H), 128.2 (*C*H), 128.47 (*C*H), 128.53 (*C*H), 132.4 (*C*), 133.7 (*C*), 133.9 (*C*), 138.2 (*C*), 159.3 (*C*). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{17}H_{14}O$, 234.1045; found, 234.1043.

1-[4'-Methoxy-(1,1'-biphenyl)-4-yl]ethan-1-one (3d).

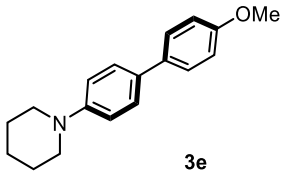


3d

The reaction was carried out with 61.6 mg (0.31 mmol) of **1d** and 54.7 mg (0.36 mmol) of **2b**. The product **3d** was obtained as a white powder (66.8 mg, 0.29 mmol, 95% yield). ^{1}H and ^{13}C NMR were in agreement with the literature.[4]

^{1}H NMR (401 MHz, $CDCl_3$, δ): 2.64 (s, 3H), 3.87 (s, 3H), 6.98–7.04 (m, 2H), 7.55–7.62 (m, 2H), 7.62–7.69 (m, 2H), 7.99–8.04 (m, 2H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 26.7 (*C*H_3), 55.4 (*C*H_3), 114.5 (*C*H), 126.7 (*C*H), 128.4 (*C*H), 129.0 (*C*H), 132.2 (*C*), 135.3 (*C*), 145.4 (*C*), 160.0 (*C*), 197.8 (*C*). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{15}H_{14}O_2$, 226.0994; found, 226.0992.

1-[4'-Methoxy-(1,1'-biphenyl)-4-yl]piperidine (3e).

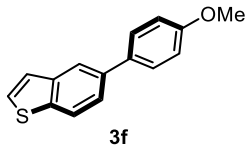


3e

The reaction was carried out with 73.6 mg (0.31 mmol) of **1e** and 54.7 mg (0.36 mmol) of **2b**. The product **3e** was obtained as a white powder (57.6 mg, 0.22 mmol, 70% yield).

^{1}H NMR (392 MHz, $CDCl_3$, δ): 1.54–1.63 (m, 2H), 1.68–1.77 (m, 4H), 3.19 (t, *J* = 4.9 Hz, 4H), 3.83 (d, *J* = 1.2 Hz, 3H), 6.90–7.02 (m, 4H), 7.40–7.52 (m, 4H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 24.4 (*C*H_2), 25.9 (*C*H_2), 50.7 (*C*H_2), 55.4 (*C*H_3), 114.2 (*C*H), 116.7 (*C*H), 127.3 (*C*H), 127.6 (*C*H), 131.6 (*C*), 133.8 (*C*), 151.2 (*C*), 158.5 (*C*). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{18}H_{21}NO$, 267.1610; found, 267.1612.

5-(4-Methoxyphenyl)benzo[b]thiophene (3f).

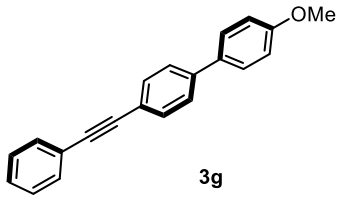


3f

The reaction was carried out with 75.4 mg (0.35 mmol) of **1f** and 54.7 mg (0.36 mmol) of **2b**. The product **3f** was obtained as a white powder (82.0 mg, 0.34 mmol, 96% yield). ^{1}H and ^{13}C NMR were in agreement with the literature.[5]

^{1}H NMR (401 MHz, $CDCl_3$, δ): 3.87 (s, 3H), 6.97–7.03 (m, 2H), 7.37 (d, J = 5.6 Hz, 1H), 7.47 (d, J = 5.6 Hz, 1H), 7.55 (dd, J = 1.6, 8.4 Hz, 1H), 7.57–7.63 (m, 2H), 7.91 (d, J = 8.8 Hz, 1H), 7.98 (d, J = 1.6 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 55.5 (*C*H$_3$), 114.4 (*C*H), 121.6 (*C*H), 122.8 (*C*H), 123.8 (*C*H), 124.2 (*C*H), 127.1 (*C*H), 128.5 (*C*H), 134.0 (*C*), 137.4 (*C*), 138.3 (*C*), 140.3 (*C*), 159.2 (*C*). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{15}H_{12}OS$, 240.0609; found, 240.0606.

4-Methoxy-4'-(phenylethynyl)-1,1'-biphenyl (3g).

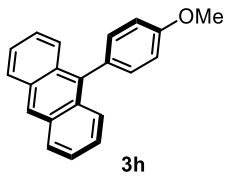


3g

The reaction was carried out with 77.7 mg (0.30 mmol) of **1g** and 54.7 mg (0.36 mmol) of **2b**. The product **3g** was obtained as a white powder (81.1 mg, 0.29 mmol, 84% yield).

^{1}H NMR (399 MHz, $CDCl_3$, δ): 3.86 (s, 3H), 6.96–7.02 (m, 2H), 7.30–7.40 (m, 3H) 7.51–7.62 (m, 8H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 55.5 (*C*H$_3$), 89.6 (*C*), 90.0 (*C*), 114.4 (*C*H), 121.6 (*C*), 123.5 (*C*), 126.6 (*C*H), 128.2 (*C*H), 128.3 (*C*H), 128.5 (*C*H), 131.7 (*C*H), 132.1 (*C*H), 132.9 (*C*), 140.7 (*C*), 159.6 (*C*). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{21}H_{16}O$, 284.1201; found, 284.1198.

9-(4-Methoxyphenyl)anthracene (3h).



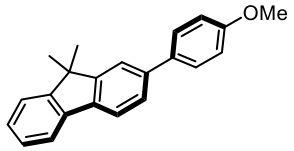
3h

The reaction was carried out with 77.0 mg (0.30 mmol) of **1h** and 54.7 mg (0.36 mmol) of **2b**. The product **3h** was obtained as a white powder (80.0 mg, 0.28 mmol, 94% yield). ^{1}H and ^{13}C NMR were in agreement with the literature.[6]

^{1}H NMR (399 MHz, $CDCl_3$, δ): 3.95 (s, 3H), 7.08–7.15 (m, 2H), 7.30–7.39 (m, 4H) 7.41–7.49 (m,

2H), 7.71 (d, J = 8.8 Hz, 2H), 8.04 (d, J = 8.4 Hz, 2H), 8.48 (s, 1H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 55.5 (*C*H_3), 113.9 (*C*H), 125.2 (*C*H), 125.3 (*C*H), 126.5 (*C*H), 127.0 (*C*H), 128.4 (*C*H), 130.6 (*C*), 130.9 (*C*), 131.5 (*C*), 132.4 (*C*H), 136.9 (*C*), 159.1 (*C*). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{21}H_{16}O$, 284.1201; found, 284.1194.

2-(4-Methoxyphenyl)-9,9-dimethyl-9H-fluorene (3i).

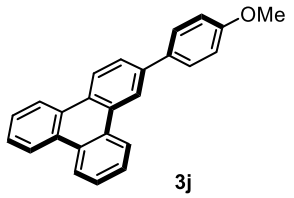


3i

The reaction was carried out with 83.2 mg (0.30 mmol) of **1i** and 54.7 mg (0.36 mmol) of **2b**. The product **3i** was obtained as a white powder (73.6 mg, 0.25 mmol, 80% yield).

^{1}H NMR (401 MHz, $CDCl_3$, δ): 1.53 (s, 6H), 3.86 (s, 3H), 6.95–7.04 (m, 2H), 7.28–7.38 (m, 2H), 7.40–7.48 (m, 1H), 7.49–7.55 (m, 1H), 7.55–7.64 (m, 3H), 7.74 (t, J = 8.4 Hz, 2H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 27.4 (*C*H_3), 47.0 (*C*), 55.5 (*C*H_3), 114.3 (*C*H), 120.1 (*C*H), 120.4 (*C*H), 121.1 (*C*H), 122.7 (*C*H), 125.9 (*C*H), 127.1 (*C*H), 127.2 (*C*H), 128.3 (*C*H), 134.3 (*C*), 138.0 (*C*), 139.1 (*C*), 140.1 (*C*), 153.9 (*C*), 154.3 (*C*), 159.2 (*C*). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{22}H_{20}O$, 300.1514; found, 300.1504.

2-(4-Methoxyphenyl)triphenylene (3j).

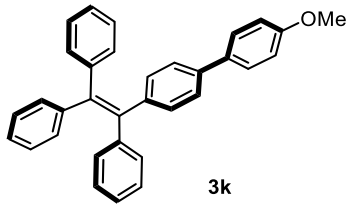


3j

The reaction was carried out with 92.8 mg (0.30 mmol) of **1j** and 54.7 mg (0.36 mmol) of **2b**. The product **3j** was obtained as a white powder (78.5 mg, 0.23 mmol, 78% yield).

^{1}H NMR (401 MHz, $CDCl_3$, δ): 3.09 (s, 3H), 7.05–7.11 (m, 2H), 7.63–7.71 (m, 4H) 7.71–7.78 (m, 2H), 7.87 (dd, J = 1.8, 8.2 Hz, 1H), 8.64–8.71 (m, 4H), 8.71–8.78 (m, 1H), 8.81 (d, J = 2.0 Hz, 1H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 55.6 (*C*H_3), 114.5 (*C*H), 121.3 (*C*H), 123.4 (*C*H), 123.46 (*C*H), 123.51 (*C*H), 124.0 (*C*H), 126.2 (*C*H), 127.2 (*C*H), 127.3 (*C*H), 127.4 (*C*H), 128.6 (*C*H), 129.8 (*C*), 130.0 (*C*), 130.16 (*C*), 130.20 (*C*), 133.8 (*C*), 139.6 (*C*), 159.5 (*C*). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{25}H_{18}O$, 334.1358; found, 334.1343.

4-Methoxy-4'-(1,2,2-triphenylvinyl)-1,1'-biphenyl (3k).

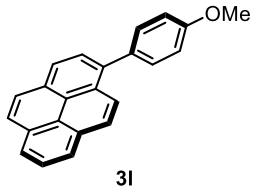


3k

The reaction was carried out with 125.2 mg (0.30 mmol) of **1k** and 54.7 mg (0.36 mmol) of **2b**. The product **3k** was obtained as a white powder (57.6 mg, 0.13 mmol, 43% yield).

^{1}H NMR (401 MHz, $CDCl_3$, δ): 3.83 (s, 3H), 6.93 (d, J = 8.8 Hz, 2H), 7.00–7.15 (m, 17H), 7.30 (d, J = 7.6 Hz, 2H), 7.49 (d, J = 8.8 Hz, 2H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 55.4 (*C*H$_3$), 114.2 (*C*H), 125.8 (*C*H), 126.5 (*C*H), 126.6 (*C*H), 127.76 (*C*H), 127.79 (*C*H), 127.9 (*C*H), 128.0 (*C*H), 131.5 (*C*H), 131.6 (*C*H), 131.9 (*C*H), 133.3 (*C*), 138.6 (*C*), 140.7 (*C*), 141.0 (*C*), 142.2 (*C*), 143.9 (*C*), 144.0 (*C*), 159.2 (*C*). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{33}H_{26}O$, 438.1984; found, 438.1968.

1-(4-Methoxyphenyl)pyrene (3l).

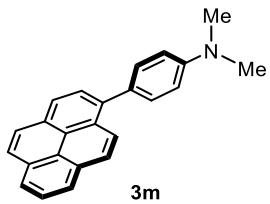


3l

The reaction was carried out with 85.6 mg (0.30 mmol) of **1l** and 54.7 mg (0.36 mmol) of **2b**. The product **3l** was obtained as a white powder (83.8 mg, 0.27 mmol, 89% yield). ^{1}H and ^{13}C NMR were in agreement with the literature.[7]

^{1}H NMR (401 MHz, $CDCl_3$, δ): 3.93 (s, 3H), 7.08–7.14 (m, 2H), 7.53–7.60 (m, 2H), 7.94–8.04 (m, 3H), 8.09 (s, 2H), 8.13–8.23 (m, 4H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 55.5 (*C*H$_3$), 113.9 (*C*H), 124.76 (*C*H), 124.82 (*C*H), 125.0 (*C*), 125.1 (*C*H), 125.5 (*C*H), 126.1 (*C*H), 127.3 (*C*H), 127.4 (*C*H), 127.5 (*C*H), 127.8 (*C*H), 128.7 (*C*), 130.4 (*C*), 131.1 (*C*), 131.6 (*C*), 131.8 (*C*H), 133.6 (*C*), 137.5 (*C*), 159.1 (*C*). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{23}H_{16}O$, 308.1201; found, 308.1197.

***N*,*N*-Dimethyl-4-(pyren-1-yl)aniline (3m).**



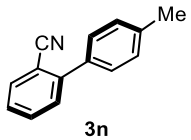
3m

The reaction was carried out with 87.9 mg (0.31 mmol) of **1m** and 59.4 mg (0.36 mmol) of **2a**. The

product **3m** was obtained as a yellow powder (73.6 mg, 0.23 mmol, 73% yield). ^{1}H and ^{13}C NMR were in agreement with the literature.[8]

^{1}H NMR (401 MHz, $CDCl_3$, δ): 3.07 (s, 6H), 6.93 (d, *J* = 8.0 Hz, 2H), 7.54 (d, *J* = 7.6 Hz, 2H), 7.95–8.02 (m, 3H), 8.03–8.10 (m, 2H), 8.10–8.25 (m, 3H), 8.29 (d, *J* = 9.2 Hz, 1H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 40.7 (*C*H_3), 112.4 (*C*H), 124.6 (*C*H), 124.8 (*C*H), 124.9 (*C*H), 125.16 (*C*), 125.23 (*C*), 125.8 (*C*H), 126.0 (*C*H), 127.07 (*C*H), 127.14 (*C*H), 127.6 (*C*H), 127.8 (*C*H), 128.6 (*C*), 129.2 (*C*), 130.1 (*C*), 131.2 (*C*), 131.5 (*C*H), 131.7 (*C*), 138.3 (*C*), 149.9 (*C*). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{24}H_{19}N$, 321.1518; found, 321.1513.

4'-Methyl-[1,1'-biphenyl]-2-carbonitrile (3n).

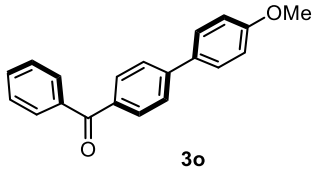


3n

The reaction was carried out with 41.3 mg (0.3 mmol) of **1n** and 48.9 mg (0.36 mmol) of *p*-tolylboronic acid. The product **3n** was obtained as a white powder (51.9 mg, 0.27 mmol, 91% yield). ^{1}H and ^{13}C NMR were in agreement with the literature.[9H)]

^{1}H NMR (401 MHz, $CDCl_3$, δ): 2.42 (s, 3H), 7.30 (d, *J* = 7.6 Hz, 2H), 7.42 (td, *J* = 1.1, 7.6 Hz, 1H), 7.46 (d, *J* = 8.4 Hz, 2H), 7.50 (d, *J* = 7.6 Hz, 1H), 7.63 (td, *J* = 1.2, 7.7 Hz, 1H), 7.75 (dd, *J* = 0.8, 7.6 Hz, 1H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 21.3 (*C*H_3), 111.2 (*C*), 119.0 (*C*), 127.4 (*C*H), 128.7 (*C*H), 129.5 (*C*H), 130.1 (*C*H), 132.9 (*C*H), 133.8 (*C*H), 135.3 (*C*), 138.8 (*C*), 145.6 (*C*). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{14}H_{11}N$, 193.0892; found, 193.0892.

(4'-Methoxy-[1,1'-biphenyl]-4-yl)(phenyl)methanone (3o).

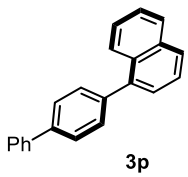


3o

The reaction was carried out with 65.2 mg (0.3 mmol) of **1o** and 54.7 mg (0.36 mmol) of **2b**. The product **3o** was obtained as a white powder (82.7 mg, 0.29 mmol, 95% yield). ^{1}H and ^{13}C NMR were in agreement with the literature.[10]

^{1}H NMR (401 MHz, $CDCl_3$, δ): 3.88 (s, 3H), 6.98–7.05 (m, 2H), 7.50 (t, *J* = 7.4 Hz, 2H), 7.57–7.64 (m, 3H), 7.64–7.70 (m, 2H), 781–7.87 (m, 2H), 7.87–7.91 (m, 2H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 55.5 (*C*H_3), 114.5 (*C*H), 126.5 (*C*H), 128.4 (*C*H), 128.5 (*C*H), 130.1 (*C*H), 130.9 (*C*H), 132.4 (*C*H), 135.7 (*C*), 138.0 (*C*), 145.0 (*C*), 160.0 (*C*), 196.5 (*C*). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{20}H_{16}O_2$, 288.1150; found, 288.1148.

1-[(1,1'-Biphenyl)-4-yl]naphthalene (3p).

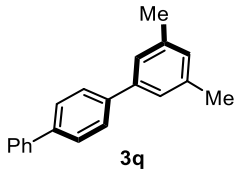


3p

The reaction was carried out with 69.9 mg (0.30 mmol) of **1p** and 61.9 mg (0.36 mmol) of 1-naphthaleneboronic acid. The product **3p** was obtained as a white powder (68.1 mg, 0.243 mmol, 81% yield). ^{1}H and ^{13}C NMR were in agreement with the literature.[11]

^{1}H NMR (392 MHz, $CDCl_3$, δ): 7.39 (t, J = 7.4 Hz, 1H), 7.42–7.61 (m, 8H), 7.66–7.76 (m, 4H), 7.88 (d, J = 8.5 Hz, 1H), 7.93 (d, J = 7.6 Hz, 1H), 7.99 (d, J = 8.1 Hz, 1H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 125.4 (*C*H), 125.8 (*C*H), 126.0 (*C*H), 126.1 (*C*H), 126.9 (*C*H), 127.0 (*C*H), 127.1 (*C*H), 127.3 (*C*H), 127.7 (*C*H), 128.3 (*C*H), 128.8 (*C*H), 130.5 (*C*H), 131.6 (*C*), 133.8 (*C*), 139.7 (*C*), 139.8 (*C*), 140.1 (*C*), 140.8 (*C*). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{22}H_{16}$, 280.1252; found, 280.1262.

3,5-Dimethyl-1,1':4',1''-terphenyl (3q).

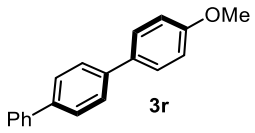


3q

The reaction was carried out with 77.1 mg (0.33 mmol) of **1q** and 54.0 mg (0.36 mmol) of 3,5-dimethylphenylboronic acid. The product **3q** was obtained as a white powder (50.0 mg, 0.19 mmol, 58% yield). ^{1}H and ^{13}C NMR were in agreement with the literature.[12]

^{1}H NMR (399 MHz, $CDCl_3$, δ): 2.31 (s, 3H), 2.38 (s, 3H), 7.08 (d, J = 8.4 Hz, 1H), 7.12 (s, 1H), 7.19 (d, J = 8.0 Hz, 1H), 7.32–7.42 (m, 3H), 7.46 (t, J = 7.4 Hz, 2H), 7.60–7.69 (m, 4H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 20.6 (CH_3), 21.2 (CH_3), 126.7 (*C*H), 126.9 (*C*H), 127.2 (*C*H), 127.4 (*C*H), 128.9 (*C*H), 129.8 (*C*H), 129.9 (*C*H), 131.3 (*C*H), 135.3 (*C*), 137.1 (*C*), 138.7 (*C*), 139.5 (*C*), 141.01 (*C*), 141.03 (*C*). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{20}H_{18}$, 258.1409; found, 258.1407.

4-Methoxy-1,1':4',1''-terphenyl (3r).



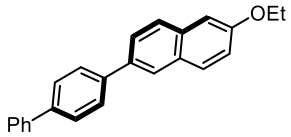
3r

The reaction was carried out with 71.2 mg (0.31 mmol) of **1r** and 54.7 mg (0.36 mmol) of **2b**. The product **3r** was obtained as a white powder (69.3 mg, 0.27 mmol, 87% yield). ^{1}H and ^{13}C NMR were in agreement with the literature.[13]

^{1}H NMR (392 MHz, $CDCl_3$, δ): 3.87 (s, 3H), 6.97–7.03 (m, 2H), 7.33–7.39 (m, 1H), 7.46 (t, J = 7.4

Hz, 2H), 7.55–7.61 (m, 2H), 7.61–7.69 (m, 6H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 55.5 (*C*H$_3$), 114.4 (*C*H), 127.1 (*C*H), 127.2 (*C*H), 127.4 (*C*H), 127.6 (*C*H), 128.2 (*C*H), 128.9 (*C*H), 133.3 (*C*), 139.6 (*C*), 139.9 (*C*), 140.9 (*C*), 159.4 (*C*). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{19}H_{16}O$, 260.1201; found, 260.1201.

2-[(1,1'-Biphenyl)-4-yl]-6-ethoxynaphthalene (3s).

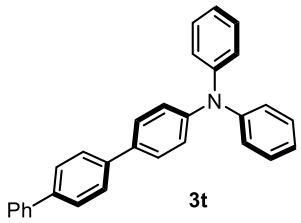


3s

The reaction was carried out with 70.0 mg (0.30 mmol) of **1s** and 77.8 mg (0.36 mmol) of 6-ethoxynaphthalen-2-ylboronic acid. The product **3s** was obtained as a white powder (88.7 mg, 0.27 mmol, 91% yield).

^{1}H NMR (399 MHz, $CDCl_3$, δ): 1.50 (t, *J* = 7.0 Hz, 3H), 4.18 (q, *J* = 6.9 Hz, 2H), 7.14–7.21 (m, 2H), 7.34–7.40 (m, 1H), 7.47 (t, *J* = 7.8 Hz, 2H), 7.64–7.68 (m, 2H), 7.69–7.74 (m, 2H), 7.74–7.84 (m, 5H), 8.00–8.08 (m, 1H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 15.0 (*C*H$_3$), 63.8 (*C*H$_2$), 107.0 (*C*H), 119.7 (*C*H), 125.7 (*C*H), 126.0 (*C*H), 127.2 (*C*H), 127.5 (*C*H), 127.7 (*C*H), 129.0 (*C*H), 129.5 (*C*), 129.9 (*C*H), 134.2 (*C*), 136.1 (*C*), 140.2 (*C*), 140.4 (*C*), 141.1 (*C*), 157.4 (*C*). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{24}H_{20}O$, 324.1514; found, 324.1508.

***N*,*N*-Diphenyl-(1,1':4',1''-terphenyl)-4-amine (3t).**

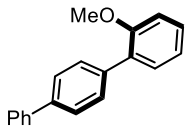


3t

The reaction was carried out with 69.9 mg (0.30 mmol) of **1t** and 104.1 mg (0.36 mmol) of 4-(diphenylamino)phenylboronic acid. The product **3t** was obtained as a white powder (110.9 mg, 0.279 mmol, 93% yield). ^{1}H and ^{13}C NMR were in agreement with the literature.[14]

^{1}H NMR (392 MHz, $CDCl_3$, δ): 7.04 (t, *J* = 7.4 Hz, 2H), 7.12–7.18 (m, 6H), 7.24–7.31 (m, 4H), 7.35 (t, *J* = 7.4 Hz, 1H), 7.46 (t, *J* = 7.6 Hz, 2H), 7.52 (d, *J* = 9.0 Hz, 2H), 7.61–7.68 (m, 6H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 123.0 (*C*H), 123.9 (*C*H), 124.5 (*C*H), 127.0 (*C*H), 127.2 (*C*H), 127.4 (*C*H), 127.7 (*C*H), 128.8 (*C*H), 129.3 (*C*H), 134.6 (*C*), 139.6 (*C*), 139.7 (*C*), 140.8 (*C*), 147.4 (*C*), 147.8 (*C*). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{30}H_{23}N$, 397.1831; found, 397.1819.

2-Methoxy-1,1':4',1''-terphenyl (3u).

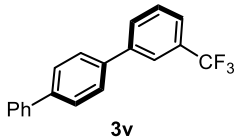


3u

The reaction was carried out with 72.5 mg (0.31 mmol) of **1u** and 54.7 mg (0.36 mmol) of 3-methoxyphenylboronic acid. The product **3u** was obtained as a white powder (73.9 mg, 0.28 mmol, 91% yield). ^{1}H and ^{13}C NMR were in agreement with the literature.[15]

^{1}H NMR (399 MHz, $CDCl_3$, δ): 3.85 (s, 3H), 7.01 (d, J = 8.4 Hz, 1H), 7.06 (t, J = 7.6 Hz, 1H), 7.31–7.40 (m, 3H), 7.45 (t, J = 7.6 Hz, 2H), 7.59–7.69 (m, 6H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 55.6 (*C*H$_3$), 111.3 (*C*H), 121.0 (*C*H), 126.9 (*C*H), 127.2 (*C*H), 127.3 (*C*H), 128.8 (*C*H), 128.9 (*C*H), 130.0 (*C*H), 130.3 (*C*), 130.9 (*C*H), 137.6 (*C*), 139.8 (*C*), 141.1 (*C*), 156.6 (*C*). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{19}H_{16}O$, 260.1201; found, 260.1198.

3-(Trifluoromethyl)-1,1':4',1''-terphenyl (3v).

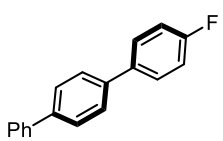


3v

The reaction was carried out with 74.0 mg (0.32 mmol) of **1v** and 68.4 mg (0.36 mmol) of 3-(trifluoromethyl)phenylboronic acid. The product **3v** was obtained as a white powder (95.8 mg, 0.32 mmol, 99% yield).

^{1}H NMR (396 MHz, $CDCl_3$, δ): 7.38 (tt, J = 1.5, 7.3 Hz, 1H), 7.48 (t, J = 7.5 Hz, 2H), 7.54–7.74 (m, 8H), 7.82 (d, J = 7.9 Hz, 1H), 7.89 (s, 1H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 124.0 (dd, J = 3.7, 19.7 Hz, *C*H), 124.4 (q, J = 271.9 Hz, *C*F$_3$), 127.2 (*C*H), 127.67 (*C*H), 127.71 (*C*H), 127.8 (*C*H), 129.0 (*C*H), 129.4 (*C*H), 130.4 (*C*H), 131.3 (q, J = 32.2 Hz, *C*), 138.7 (*C*), 140.5 (*C*), 141.0 (*C*), 141.6 (*C*). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{19}H_{13}F_3$, 298.0970; found, 298.0966.

4-Fluoro-1,1':4',1''-terphenyl (3w).

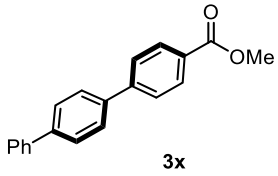


3w

The reaction was carried out with 70.5 mg (0.30 mmol) of **1w** and 50.4 mg (0.36 mmol) of 4-fluorophenylboronic acid. The product **3w** was obtained as a white powder (42.9 mg, 0.17 mmol, 57% yield). ^{1}H and ^{13}C NMR were in agreement with the literature.[16]

^{1}H NMR (401 MHz, $CDCl_3$, δ): 7.11–7.19 (m, 2H), 7.33–7.40 (m, 1H), 7.47 (t, *J* = 7.4 Hz, 2H), 7.56–7.74 (m, 8H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 115.7 (*C*H), 115.9 (*C*H), 127.2 (*C*H), 127.49 (*C*H), 127.54 (*C*H), 127.7 (*C*H), 128.7 (*C*H), 128.8 (*C*H), 129.0 (*C*H), 136.9 (*C*), 137.0 (*C*), 139.2 (*C*), 140.3 (*C*), 140.7 (*C*). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{18}H_{13}F$, 248.1000; found, 248.0997.

Methyl (1,1':4',1''-terphenyl)-4-carboxylate (3x).

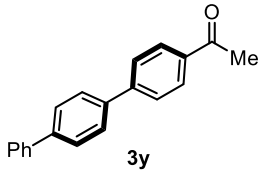


3x

The reaction was carried out with 74.6 mg (0.32 mmol) of **1x** and 64.8 mg (0.36 mmol) of 4-(methoxycarbonyl)phenylboronic acid. The product **3x** was obtained as a white powder (76.5 mg, 0.27 mmol, 83% yield). ^{1}H and ^{13}C NMR were in agreement with the literature.[17]

^{1}H NMR (399 MHz, $CDCl_3$, δ): 3.95 (s, 3H), 7.38 (tt, *J* = 1.5, 7.3 Hz, 1H), 7.47 (t, *J* = 7.4 Hz, 2H), 7.62–7.68 (m, 2H), 7.69–7.76 (m, 6H), 8.10–8.15 (m, 2H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 52.3 (CH_3), 127.0 (*C*H), 127.2 (*C*H), 127.7 (*C*H), 127.8 (*C*H), 129.0 (*C*H), 129.1 (*C*), 130.3 (*C*H), 138.9 (*C*), 140.6 (*C*), 141.2 (*C*), 145.2 (*C*), 167.2 (*C*). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{20}H_{16}O_2$, 288.1150; found, 288.1149.

1-(1,1':4',1''-Terphenyl)-4-ylethan-1-one (3y).

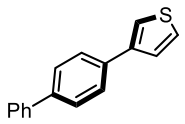


3y

The reaction was carried out with 71.0 mg (0.30 mmol) of **1y** and 59.0 mg (0.36 mmol) of 4-acetylphenylboronic acid. The product **3y** was obtained as a white powder (72.3 mg, 0.27 mmol, 87% yield). ^{1}H and ^{13}C NMR were in agreement with the literature.[18]

^{1}H NMR (401 MHz, $CDCl_3$, δ): 2.68 (s, 3H), 7.38 (t, *J* = 7.2 Hz, 1H), 7.48 (t, *J* = 7.6 Hz, 2H), 7.57 (t, *J* = 7.8 Hz, 1H), 7.66 (d, *J* = 8.0 Hz, 2H), 7.71 (s, 4H), 7.85 (d, *J* = 8.0 Hz, 1H), 7.95 (d, *J* = 7.6 Hz, 1H), 8.24 (s, 1H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 28.9 (CH_3), 126.9 (*C*H), 127.1 (*C*H), 127.4 (*C*H), 127.6 (*C*H), 127.7 (*C*H), 129.0 (*C*H), 129.2 (*C*H), 131.7 (*C*H), 137.7 (*C*), 139.1 (*C*), 140.5 (*C*), 140.7 (*C*), 141.2 (*C*), 198.2 (*C*). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{20}H_{16}O$, 272.1201; found, 272.1198.

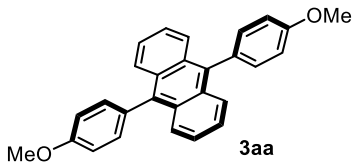
3-[(1,1'-Biphenyl)-4-yl]thiophene (3z).



3z

The reaction was carried out with 71.2 mg (0.31 mmol) of **1z** and 46.1 mg (0.36 mmol) of thiophen-3-ylboronic acid. The product **3z** was obtained as a white powder (73.6 mg, 0.31 mmol, 99% yield). ^{1}H NMR (401 MHz, $CDCl_3$, δ): 7.32–7.38 (m, 1H), 7.39–7.53 (m, 5H), 7.59–7.71 (m, 6H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 120.4 (*C*H), 126.4 (*C*H), 126.9 (*C*H), 127.1 (*C*H), 127.5 (*C*H), 127.6 (*C*H), 128.9 (*C*H), 134.9 (*C*), 140.0 (*C*), 140.8 (*C*), 142.0 (*C*). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{16}H_{12}S$, 236.0660; found, 236.0659.

9,10-Bis(4-methoxyphenyl)anthracene (3aa).

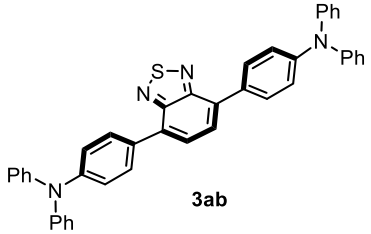


3aa

The reaction was carried out with 51.4 mg (0.15 mmol) of **1aa** and 54.7 mg (0.36 mmol) of **2b**. The product **3aa** was obtained as a yellow powder (59.3 mg, 0.15 mmol, 99% yield). ^{1}H and ^{13}C NMR were in agreement with the literature.[19]

^{1}H NMR (399 MHz, $CDCl_3$, δ): 3.97 (s, 6H), 7.11–7.17 (m, 4H), 7.30–7.36 (m, 4H), 7.36–7.42 (m, 4H), 7.70–7.77 (m, 4H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 55.5 (CH_3), 114.0 (*C*H), 125.0 (*C*H), 127.2 (*C*H), 130.4 (*C*), 131.3 (*C*), 132.5 (*C*H), 136.9 (*C*), 159.1 (*C*). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{28}H_{22}O_2$, 390.1620; found, 390.1614.

4,4'-(Benzo[c][1,2,5]thiadiazole-4,7-diyl)bis(*N*,*N*-diphenylaniline) (3ab).



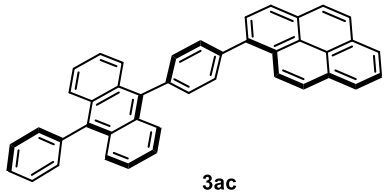
3ab

The reaction was carried out with 45.8 mg (0.16 mmol) of **1ab** and 104.1 mg (0.36 mmol) of 4-(diphenylamino)phenylboronic acid. The product **3ab** was obtained as a red powder (58.0 mg, 0.09 mmol, 60% yield). ^{1}H and ^{13}C NMR were in agreement with the literature.[20]

^{1}H NMR (399 MHz, $CDCl_3$, δ): 7.04–7.11 (m, 4H), 7.16–7.24 (m, 12H), 7.27–7.33 (m, 7H), 7.55 (d, *J* = 7.6 Hz, 1H) 7.75 (s, 1H), 7.77–7.83 (m, 2H), 7.85–7.92 (m, 3H). ^{13}C NMR (99 MHz, $CDCl_3$, δ):

122.7 (*C*H), 123.1 (*C*H), 123.4 (*C*H), 123.6 (*C*H), 125.0 (*C*H), 125.2 (*C*H), 127.5 (*C*H), 127.6 (*C*H), 129.49 (*C*H), 129.55 (*C*H), 129.96 (*C*), 130.03 (*C*H), 131.1 (*C*), 132.3 (*C*), 132.5 (*C*H), 133.7 (*C*), 147.4 (*C*), 147.6 (*C*). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{42}H_{30}N_4S$, 622.2191; found, 622.2204.

1-[4-(10-Phenylanthracen-9-yl)phenyl]pyrene (3ac).

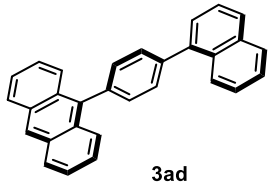


3ac

The reaction was carried out with 99.8 mg (0.30 mmol) of **1ac** and 116.0 mg (0.36 mmol) of 4-(1-pyrenyl)phenylboronic acid. The product **3ac** was obtained as a white powder (146.3 mg, 0.276 mmol, 92% yield).

^{1}H NMR (392 MHz, $CDCl_3$, δ): 7.37–7.47 (m, 4H), 7.49–7.66 (m, 5H), 7.69 (d, *J* = 8.1 Hz, 2H), 7.74 (d, *J* = 8.5 Hz, 2H), 7.88 (d, *J* = 8.1 Hz, 2H), 7.92 (d, *J* = 8.5 Hz, 2H), 8.04 (t, *J* = 7.4 Hz, 1H), 8.09–8.25 (m, 6H), 8.30 (d, *J* = 8.1 Hz, 1H), 8.44 (d, *J* = 9.4 Hz, 1H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 124.8 (*C*H), 125.0 (*C*H), 125.10 (*C*H), 125.14 (*C*H), 125.18 (*C*H), 125.21 (*C*H), 125.4 (*C*H), 126.1 (*C*H), 127.07 (*C*H), 127.12 (*C*H), 127.5 (*C*H), 127.7 (*C*H), 127.8 (*C*H), 128.5 (*C*H), 128.8 (*C*H), 130.1 (*C*), 130.2 (*C*), 130.7 (*C*H), 130.9 (*C*), 131.2 (*C*), 131.4 (*C*H), 131.5 (*C*H), 131.7 (*C*), 136.9 (*C*), 137.4 (*C*), 137.6 (*C*), 138.2 (*C*), 139.2 (*C*), 140.5 (*C*). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{42}H_{26}$, 530.2035; found, 530.2025.

9-[4-(Naphthalen-1-yl)phenyl]anthracene (3ad).

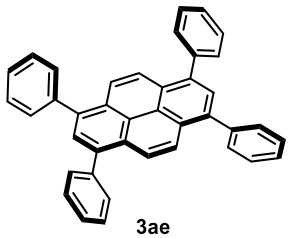


3ad

The reaction was carried out with 51.3 mg (0.20 mmol) of **1ad** and 59.5 mg (0.24 mmol) of 4-(naphthalen-1-yl)phenylboronic acid. The product **3ad** was obtained as a white powder (51.2 mg, 0.13 mmol, 67% yield). ^{1}H and ^{13}C NMR were in agreement with the literature.[21]

^{1}H NMR (401 MHz, $CDCl_3$, δ): 7.39–7.46 (m, 2H), 7.50 (t, *J* = 7.4 Hz, 3H), 7.53–7.59 (m, 3H), 7.59–7.65 (m, 2H), 7.72 (d, *J* = 8.0 Hz, 2H), 7.80–7.87 (m, 2H), 7.87–8.04 (m, 2H), 8.09 (d, *J* = 8.4 Hz, 2H), 8.13–8.20 (m, 1H), 8.54 (s, 1H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 125.3 (*C*H), 125.58 (*C*H), 125.63 (*C*H), 126.0 (*C*H), 126.2 (*C*H), 126.3 (*C*H), 126.8 (*C*H), 127.0 (*C*H), 127.3 (*C*H), 127.9 (*C*H), 128.5 (*C*H), 130.2 (*C*H), 130.4 (*C*), 131.3 (*C*H), 131.6 (*C*), 131.8 (*C*), 134.1 (*C*), 136.9 (*C*), 137.8 (*C*), 140.0 (*C*), 140.2 (*C*). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{30}H_{20}$, 380.1565; found, 380.1563.

1,3,6,8-Tetraphenylpyrene (3ae).

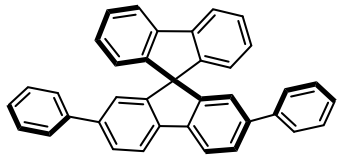


3ae

The reaction was carried out with 159.4 mg (0.31 mmol) of **1ae** and 175.6 mg (1.44 mmol) of phenylboronic acid. The product **3ae** was obtained as a yellow powder (131.1 mg, 0.26 mmol, 84% yield). ^{1}H and ^{13}C NMR were in agreement with the literature.[22]

^{1}H NMR (401 MHz, $CDCl_3$, δ): 7.43–7.50 (m, 4H), 7.50–7.58 (m, 8H), 7.64–7.70 (m, 8H), 8.01 (s, 2H), 8.18 (s, 4H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 125.5 (*C*H), 126.1 (*C*), 127.4 (*C*H), 128.2 (*C*), 128.5 (*C*H), 129.7 (*C*H), 130.8 (*C*H), 137.4 (*C*), 141.2 (*C*). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{40}H_{26}$, 506.2035; found, 506.2027.

2,7-Diphenyl-9,9'-spirobi(fluorene) (3af).

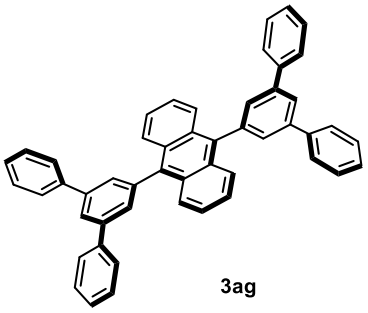


3af

The reaction was carried out with 143.3 mg (0.30 mmol) of **1af** and 87.8 mg (0.72 mmol) of phenylboronic acid. The product **3af** was obtained as a white powder (114.7 mg, 0.24 mmol, 81% yield). ^{1}H and ^{13}C NMR were in agreement with the literature.[23]

^{1}H NMR (401 MHz, $CDCl_3$, δ): 6.82 (d, J = 8.0 Hz, 2H), 6.94 (s, 2H), 7.08–7.15 (m, 2H), 7.20–7.27 (m, 2H), 7.30 (t, J = 7.4 Hz, 4H), 7.37 (t, J = 7.4 Hz, 2H), 7.40–7.45 (m, 4H), 7.63 (dd, J = 2.0, 7.6 Hz, 2H), 7.86 (d, J = 7.6 Hz, 2H), 7.92 (d, J = 8.0 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$, δ): 66.2 (*C*), 120.2 (*C*H), 120.5 (*C*H), 122.8 (*C*H), 124.4 (*C*H), 127.1 (*C*H), 127.2 (*C*H), 127.3 (*C*H), 127.9 (*C*H), 128.0 (*C*H), 128.7 (*C*H), 140.8 (*C*), 141.0 (*C*), 141.9 (*C*), 148.8 (*C*), 150.0 (*C*). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{37}H_{24}$, 468.1878; found, 468.1875.

9,10-Di[(1,1':3',1''-terphenyl)-5'-yl]anthracene (3ag).



3ag

The reaction was carried out with 101.4 mg (0.30 mmol) of **1ag** and 197.4 mg (0.72 mmol) of [1,1':3',1''-terphenyl]-5'-ylboronic acid. The product **3ag** was obtained as a white powder (113.0 mg, 0.18 mmol, 59% yield). ^{1}H and ^{13}C NMR were in agreement with the literature.[24]

^{1}H NMR (401 MHz, $CDCl_3$, δ): 7.35–7.43 (m, 8H), 7.48 (t, *J* = 7.6 Hz, 8H), 7.73–7.80 (m, 12H), 7.86–7.92 (m, 4H), 8.04 (s, 2H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 125.2 (*C*H), 125.5 (*C*H), 127.2 (*C*H), 127.5 (*C*H), 127.8 (*C*H), 129.0 (*C*H), 129.2 (*C*H), 130.1 (*C*), 137.1 (*C*), 140.2 (*C*), 140.9 (*C*), 142.0 (*C*). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{50}H_{34}$, 634.2661; found, 634.2671.

10. References.

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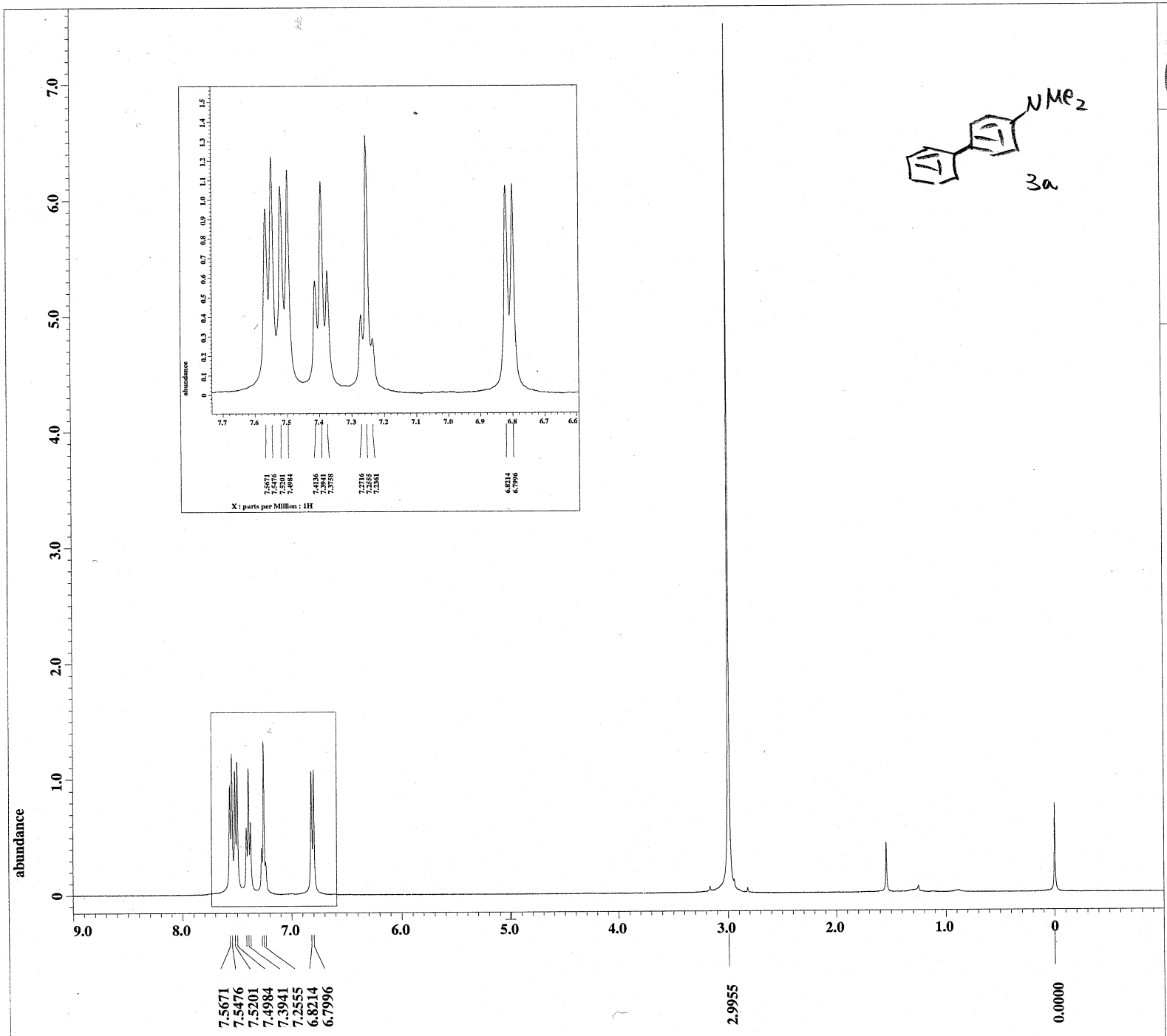

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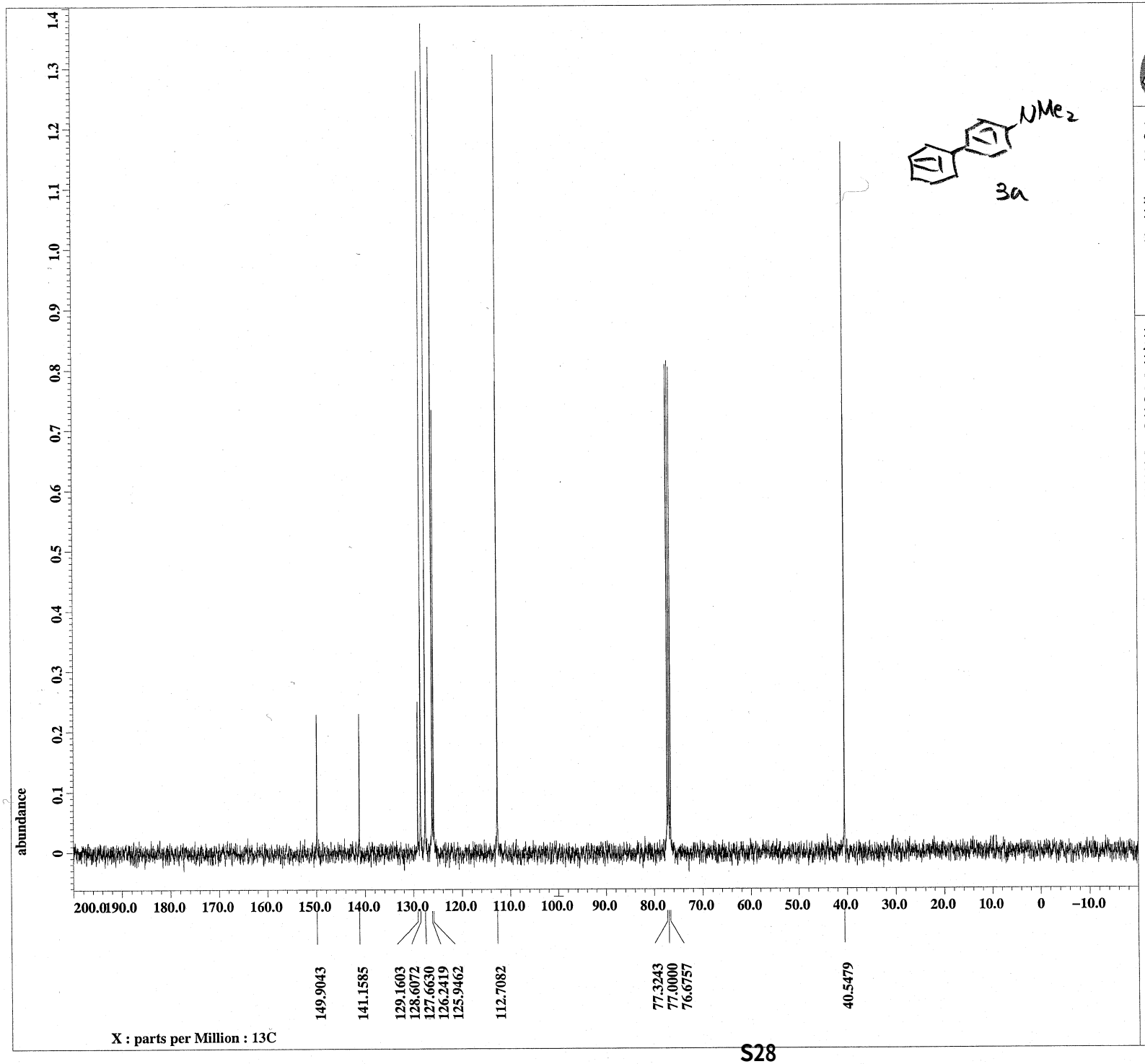

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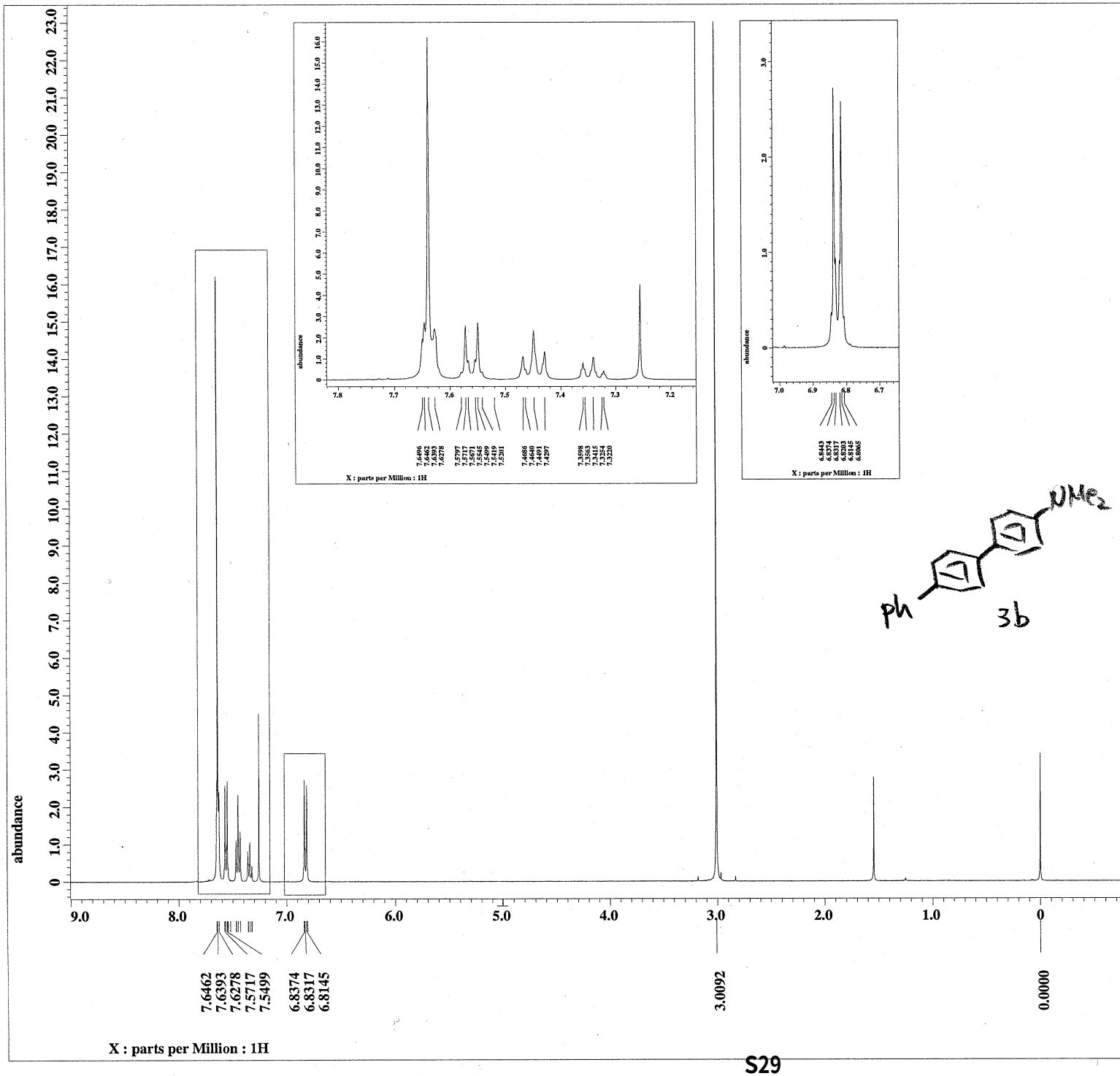
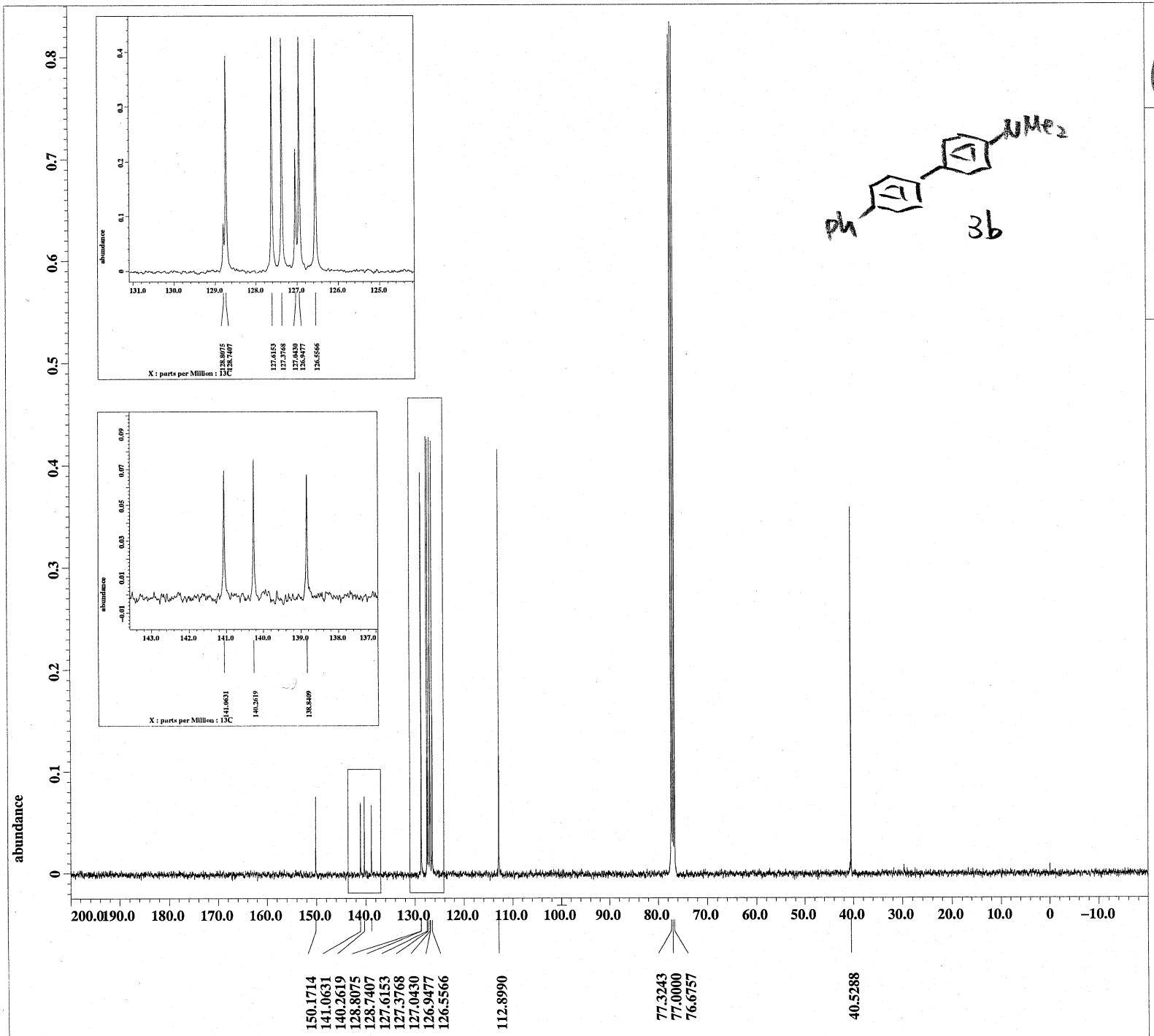
X_points	= 32768
X_prescans	= 4
X_resolution	= 0.93958061[Hz]
X_sweep	= 30.78817734[kHz]
Irr_domain	= 1H
Irr_freq	= 391.78655441[MHz]
Irr_offset	= 5[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 66
Total_scans	= 66
X_90_width	= 9.11[us]
X_acq_time	= 1.06430464[s]
X_angle	= 30[deg]
X_atn	= 4.9[dB]
X_pulse	= 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	= 18.7[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: Ph-Ph-Ph-NMe2-1H-1.jdf
```

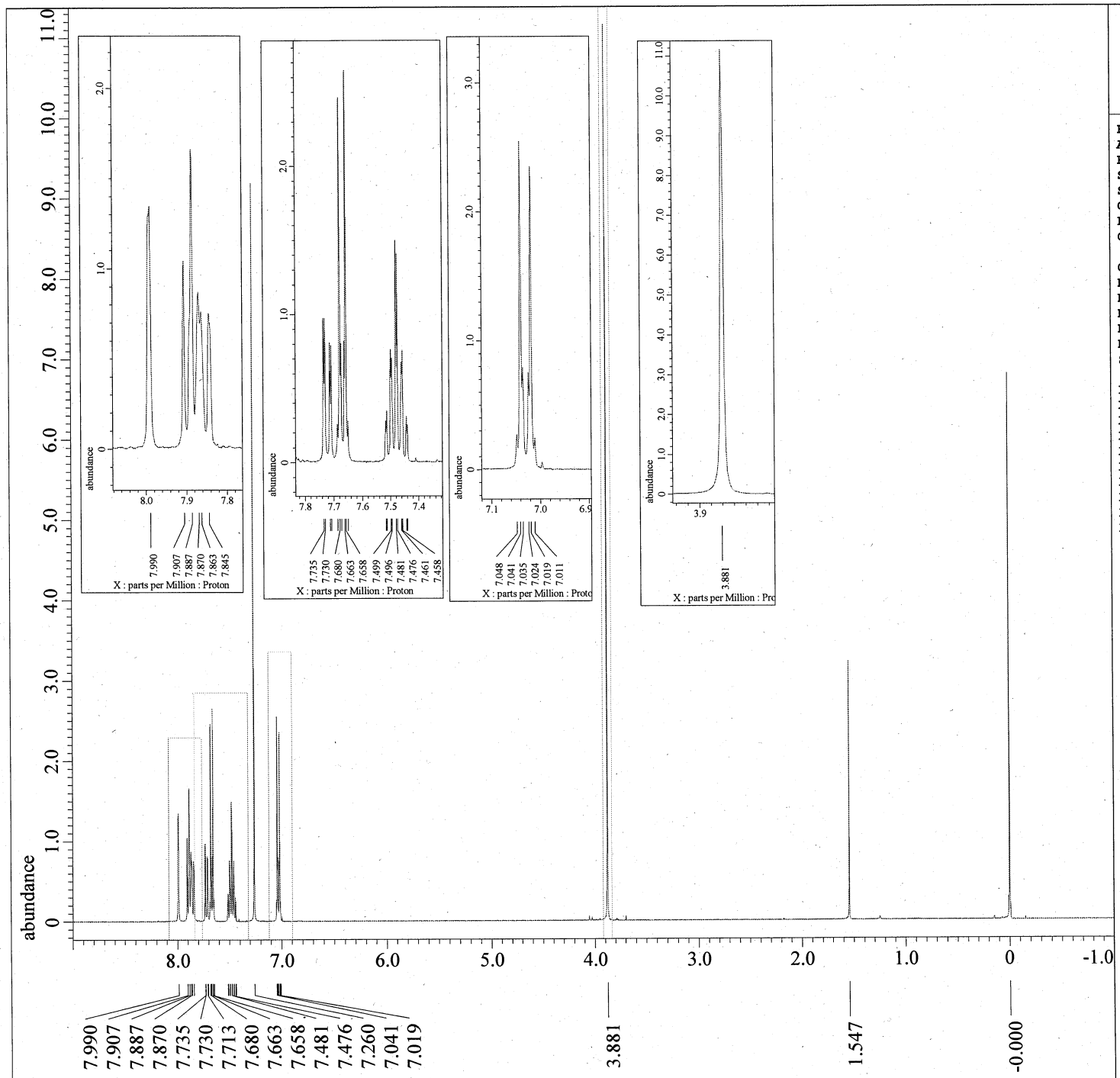
Filename	= Ph-Ph-Ph-NMe2-1H-3.jd
Author	= element
Experiment	= single_pulse.ex2
Sample_id	= S#576266
Solvent	= CHLOROFORM-D
Creation_time	= 12-JAN-2019 14:31:10
Revision_time	= 7-FEB-2019 19:51:58
Current_time	= 7-FEB-2019 19:53:22
Comment	= single_pulse
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 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	= 18.7[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

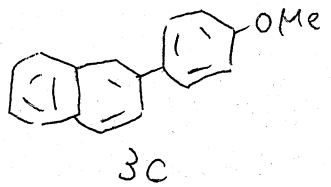
Derived from: Ph-Ph-Ph-NMe2-13C-1.jdf

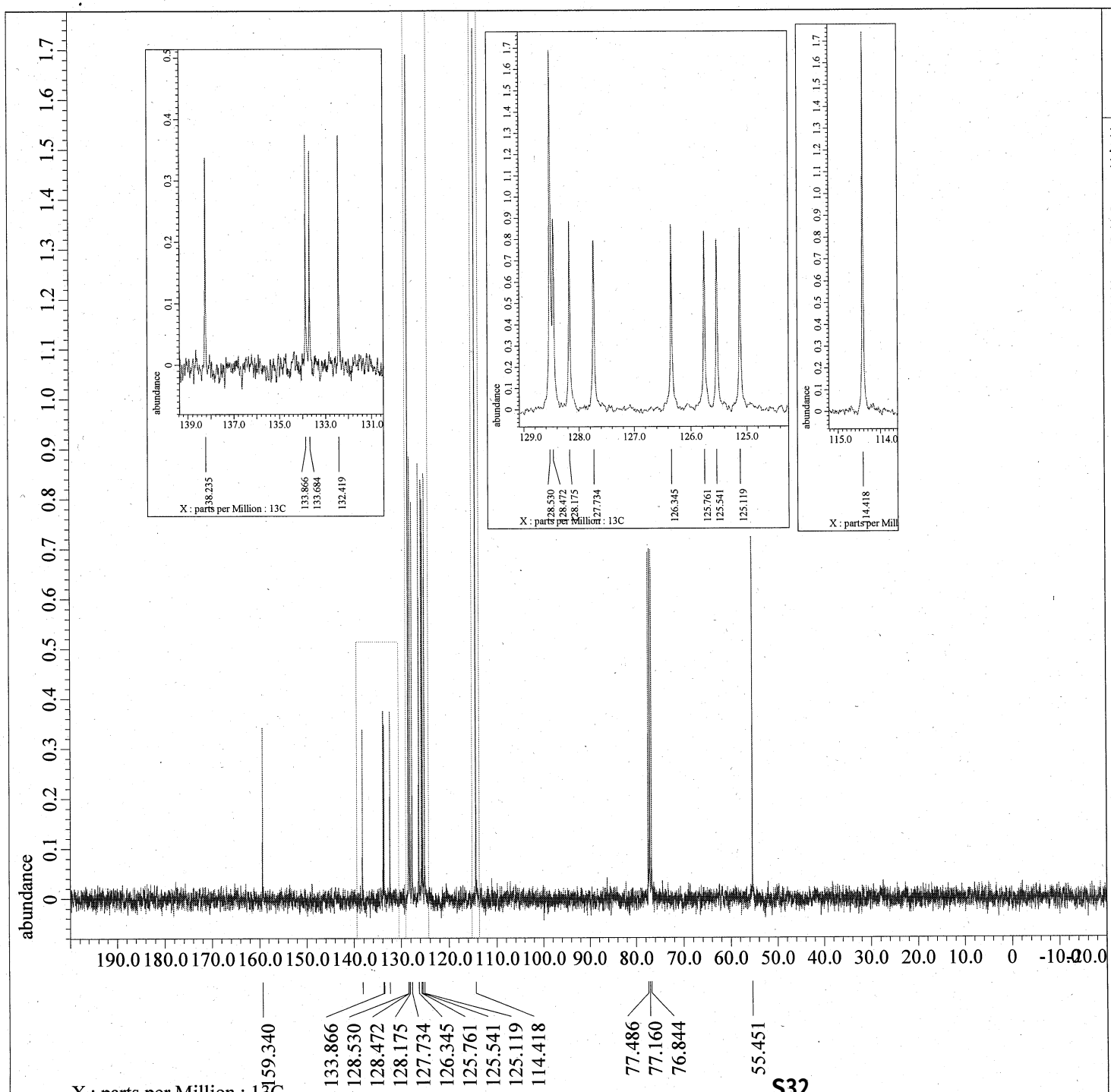
Filename	= Ph-Ph-Ph-NMe2-13C-3.j
Author	= element
Experiment	= single_pulse_dec
Sample_id	= S#585817
Solvent	= CHLOROFORM-D
Creation_time	= 12-JAN-2019 16:11:28
Revision_time	= 7-FEB-2019 19:53:57
Current_time	= 7-FEB-2019 19:55:26
Comment	= single pulse decouple
Data_format	= 1D COMPLEX
Dim_size	= 26214
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	= 1674
Total_scans	= 1674
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	= 50[dC]



JEOL
Solutions for Innovation

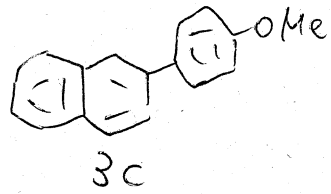
Filename	= SEO-429-1-pure_Proton-1-
Author	= element
Experiment	= proton.jxp
Sample_Id	= SEO-429-1-pure
Solvent	= CHLOROFORM-D
Creation_Time	= 5-SEP-2018 18:27:59
Revision_Time	= 7-FEB-2019 17:44:32
Current_Time	= 7-FEB-2019 17:46:04
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
Dim_Title	= 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	= 18.9[dC]
X_90_Width	= 6.22[us]
X_Acq_Time	= 2.18103808[s]
X_Angle	= 45[deg]
X_Atn	= 0.8[dB]
X_Pulse	= 3.11[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.18103808[s]

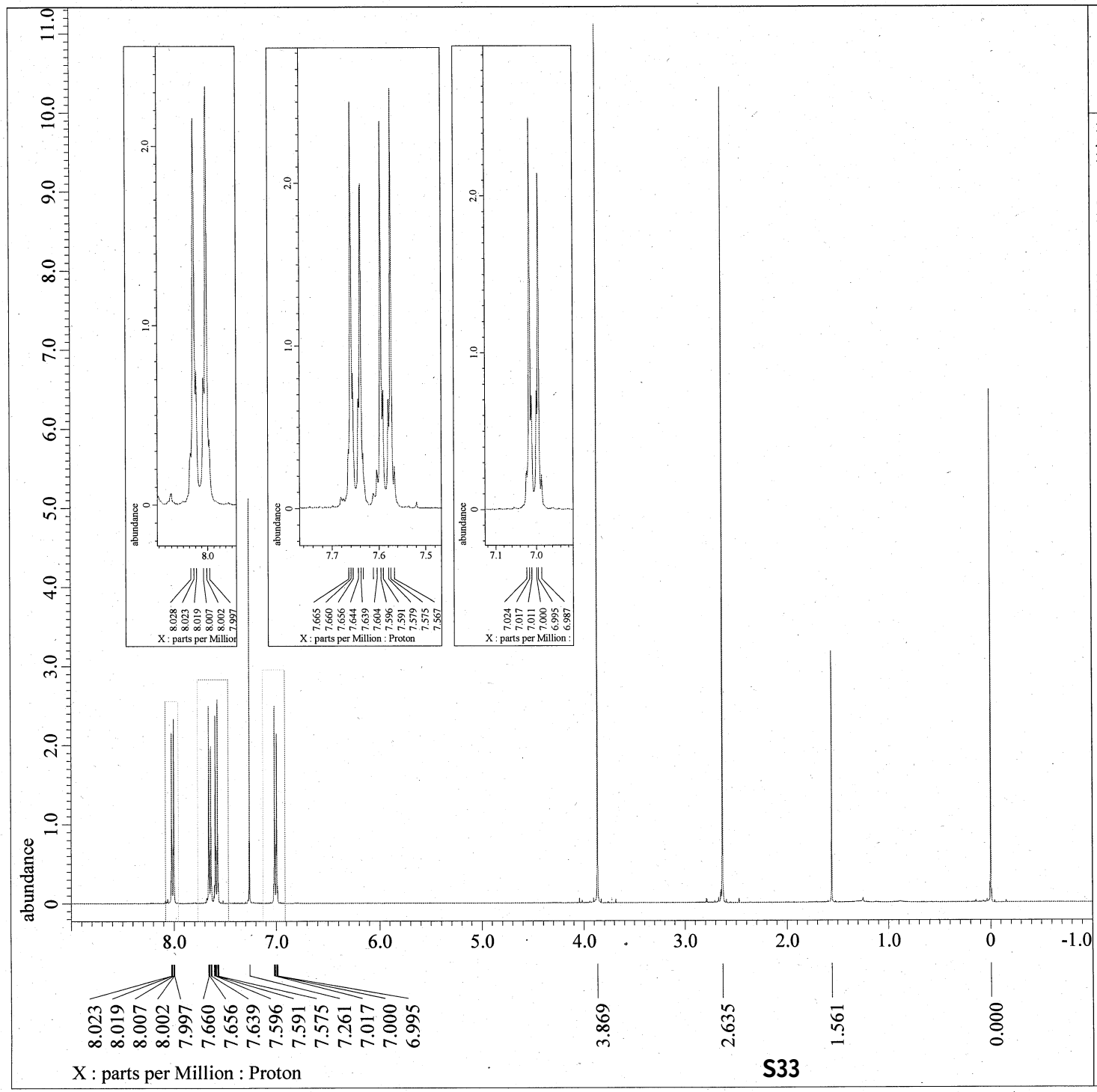




JEOL
Solutions for Innovation

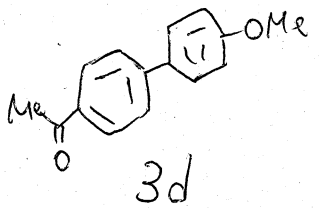
Filename	= SEO-429-1-pure-13C-4.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= 1
Solvent	= CHLOROFORM-D
Creation_Time	= 5-SEP-2018 17:58:44
Revision_Time	= 7-FEB-2019 18:18:35
Current_Time	= 7-FEB-2019 18:20:30
Comment	= single pulse decoupled g
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
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	= 21
Total_Scans	= 21
Relaxation_Delay	= 2[s]
Recvr_Gain	= 56
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_Noe	= 22.3[dB]
Irr_Noise	= WALTZ
Decoupling	= TRUE
Initial_Wait	= 1[s]
Noe	= TRUE
Noe_Time	= 2[s]
Repetition_Time	= 3.048576[s]



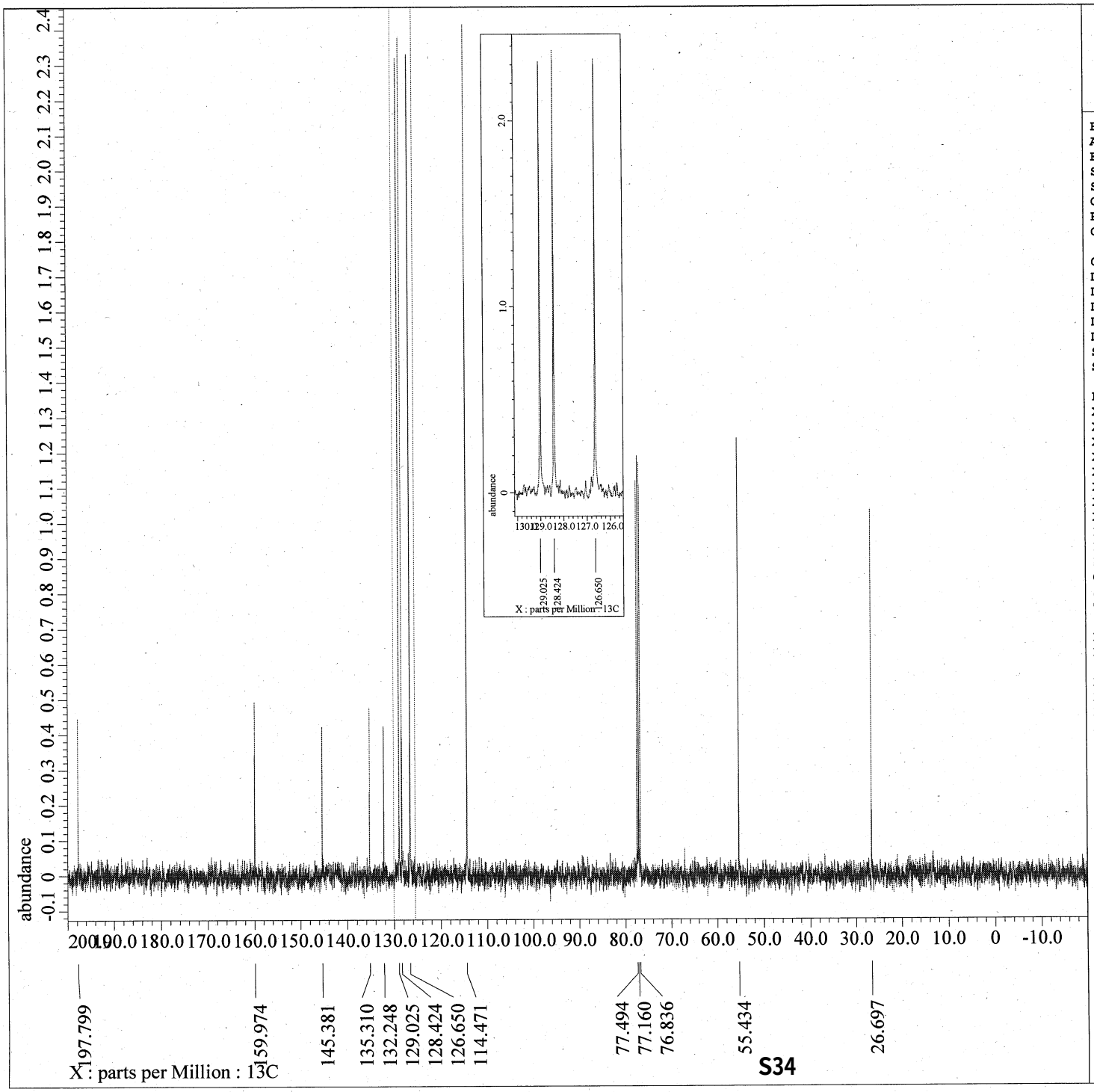


JEOL
Solutions for Innovation

Filename	= SEO-435-1-pure_Proton-1-
Author	= element
Experiment	= proton.jxp
Sample_Id	= SEO-435-1-pure
Solvent	= CHLOROFORM-D
Creation_Time	= 14-SEP-2018 14:43:00
Revision_Time	= 7-FEB-2019 17:54:05
Current_Time	= 7-FEB-2019 17:55:50
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.4073814[T] (400[MHz])
X_Acq_Duration	= 2.18103808[s]
X_Domain	= 1H
X_Freq	= 400.53219825[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45849727[Hz]
X_Sweep	= 7.51201923[kHz]
X_Sweep_Clipped	= 6.00961538[kHz]
Irr_Domain	= Proton
Irr_Freq	= 400.53219825[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 400.53219825[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 46
Temp_Get	= 19[dC]
X_90_Width	= 6.22[us]
X_Acq_Time	= 2.18103808[s]
X_Angle	= 45[deg]
X_Atn	= 0.8[dB]
X_Pulse	= 3.11[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.18103808[s]

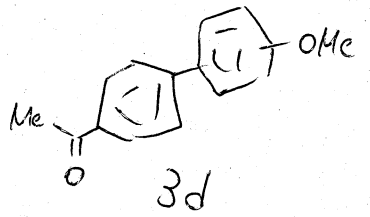


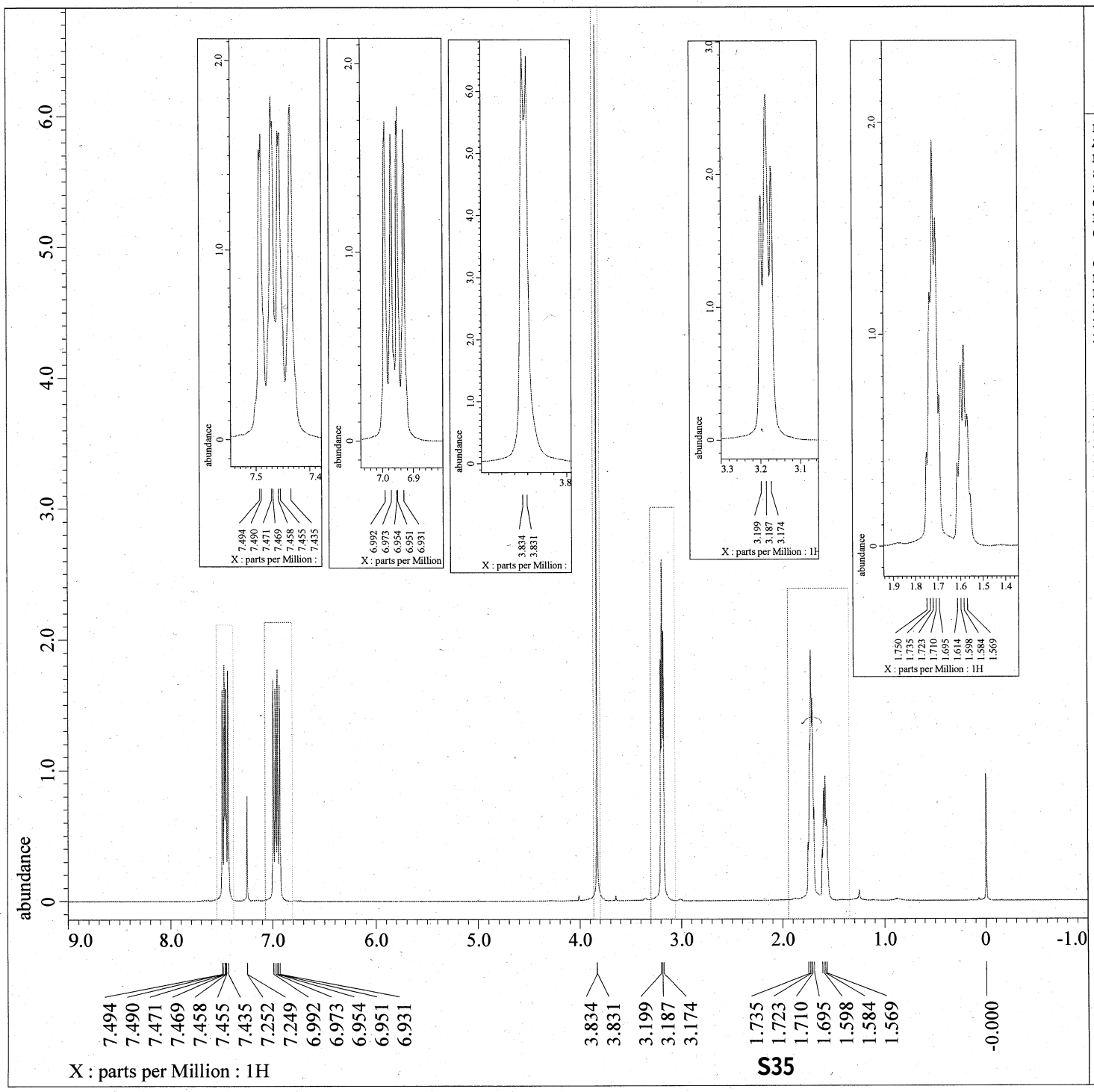
3d



JEOL
Solutions for Innovation

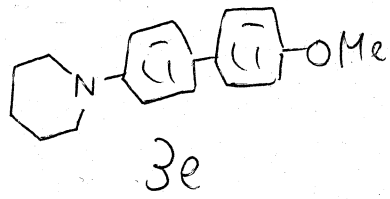
Filename	= SEO-435-1-pure-13C-4.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= 1
Solvent	= CHLOROFORM-D
Creation_Time	= 14-SEP-2018 13:15:13
Revision_Time	= 7-FEB-2019 18:21:24
Current_Time	= 7-FEB-2019 18:22:15
Comment	= single pulse decoupled g
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
Dim_Title	= 13C
Dim_Units	= [ppm]
Dimensions	= X
Site	= ECS 400
Spectrometer	= JNM-ECS400
Field_Strength	= 9.20197068[T] (390[MHz])
X_Acq_Duration	= 1.06430464[s]
X_Domain	= 13C
X_Freq	= 98.51479726[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.93958061[Hz]
X_Sweep	= 30.78817734[kHz]
Irr_Domain	= 1H
Irr_Freq	= 391.78655441[MHz]
Irr_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 13
Total_Scans	= 13
Relaxation_Delay	= 2[s]
Recvr_Gain	= 60
Temp_Get	= 20.5[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
Noe_Time	= 2[s]
Repetition_Time	= 3.06430464[s]



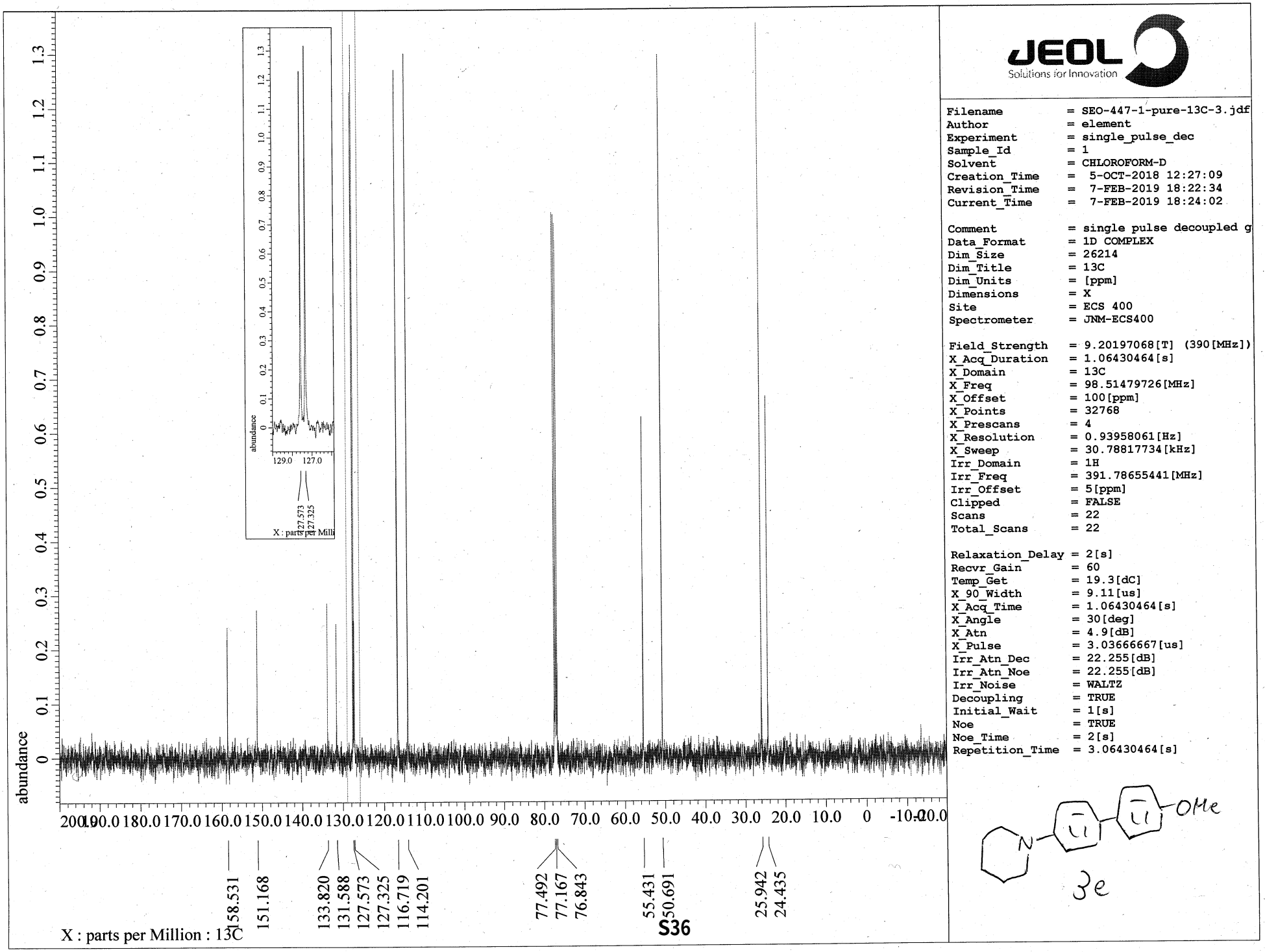


JEOL
Solutions for Innovation

Filename	= SEO-447-1-pure-4.jdf
Author	= element
Experiment	= single_pulse.ex2
Sample_Id	= S#493617
Solvent	= CHLOROFORM-D
Creation_Time	= 5-OCT-2018 12:16:12
Revision_Time	= 7-FEB-2019 18:03:23
Current_Time	= 7-FEB-2019 18:03:36
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[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	= 42
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
Initial_Wait	= 1[s]
Repetition_Time	= 7.228224[s]

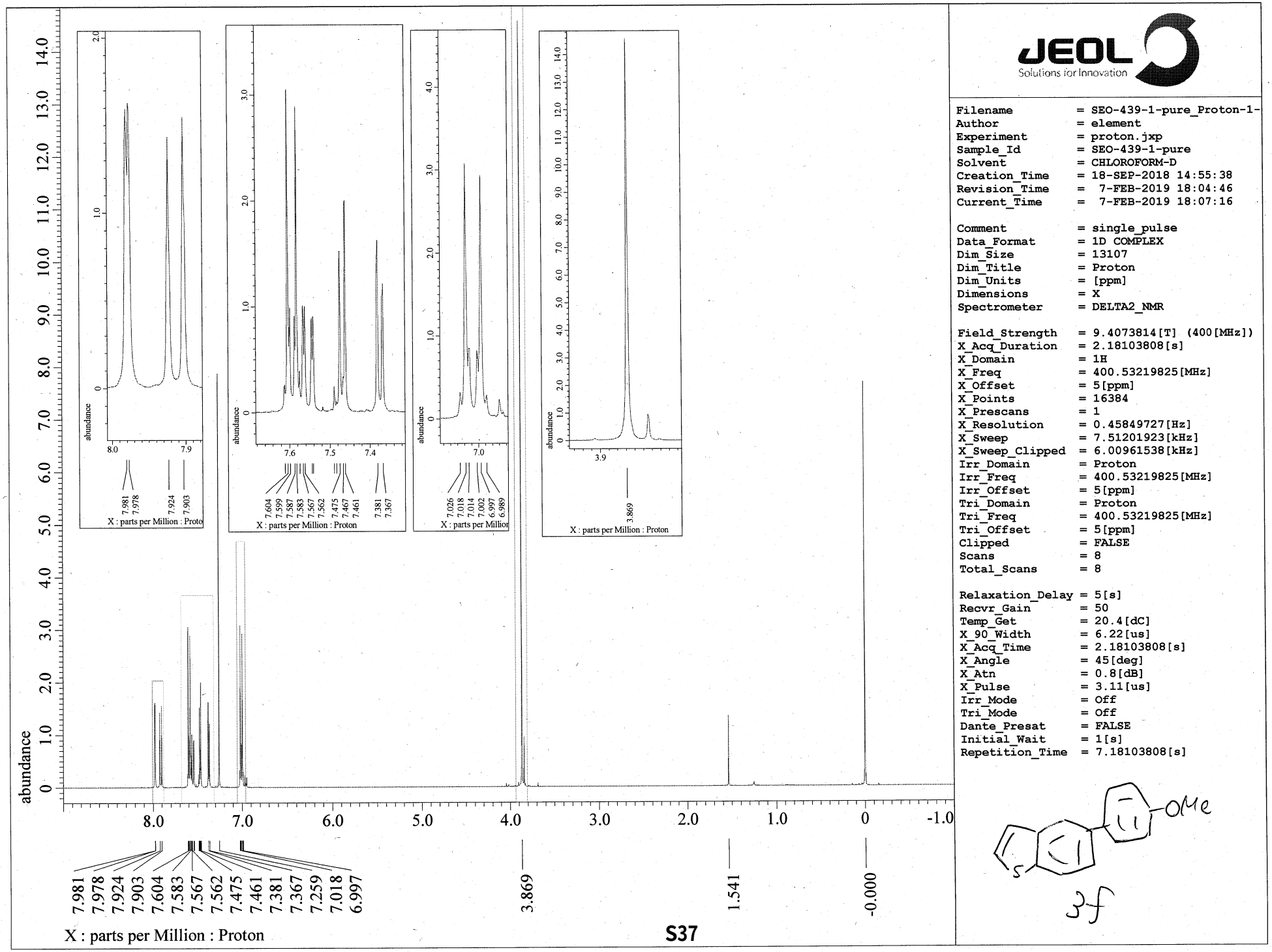


3e



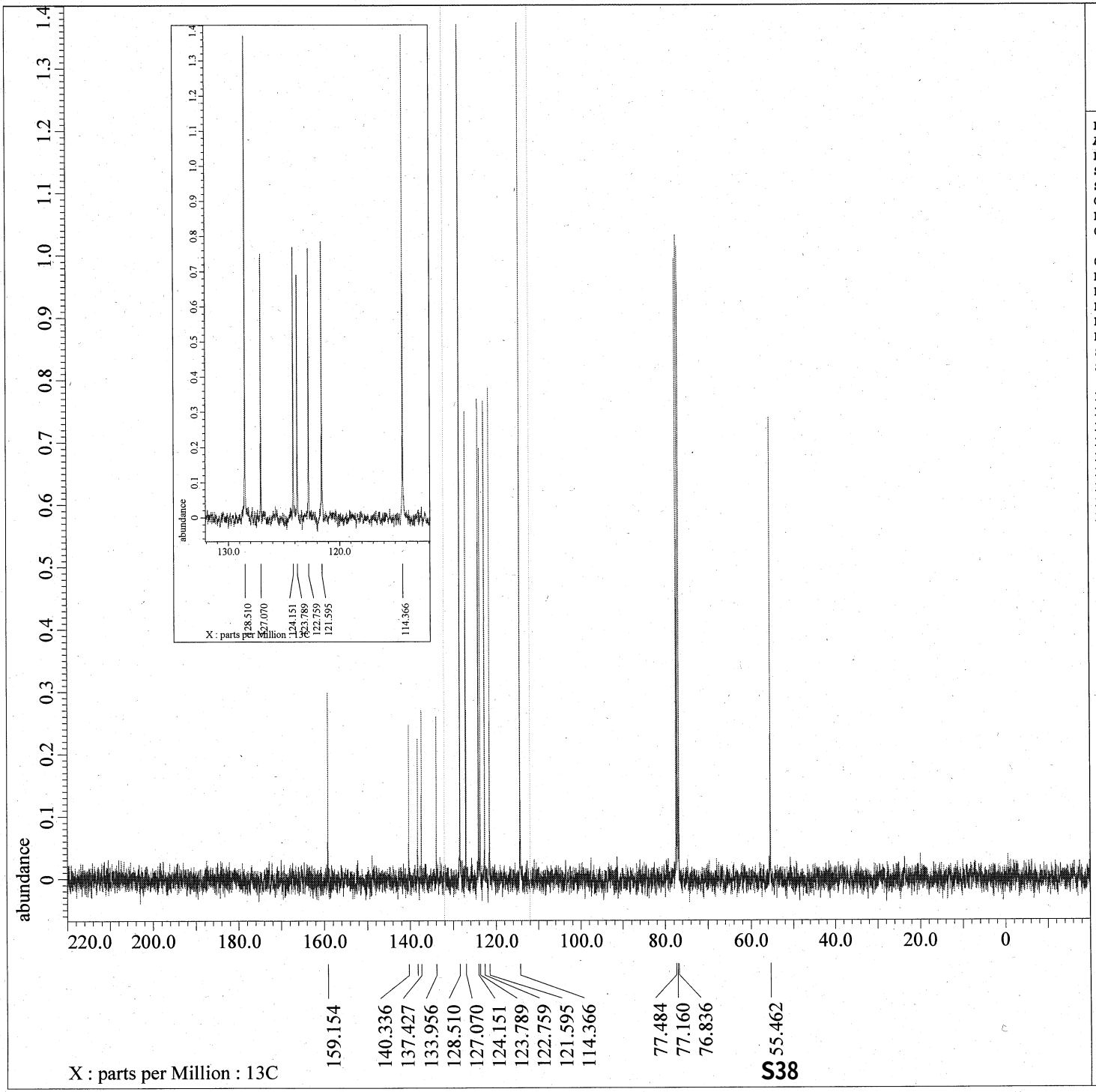
JEOL
Solutions for Innovation

Filename	= SEO-447-1-pure-13C-3.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= 1
Solvent	= CHLOROFORM-D
Creation_Time	= 5-OCT-2018 12:27:09
Revision_Time	= 7-FEB-2019 18:22:34
Current_Time	= 7-FEB-2019 18:24:02
Comment	= single pulse decoupled g
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[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	= 22
Total_Scans	= 22
Relaxation_Delay	= 2[s]
Recvr_Gain	= 60
Temp_Get	= 19.3[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
Noe_Time	= 2[s]
Repetition_Time	= 3.06430464[s]



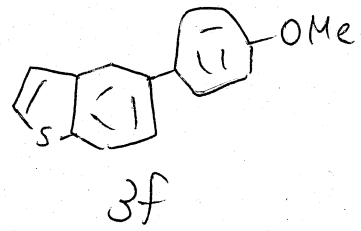
JEOL
Solutions for Innovation

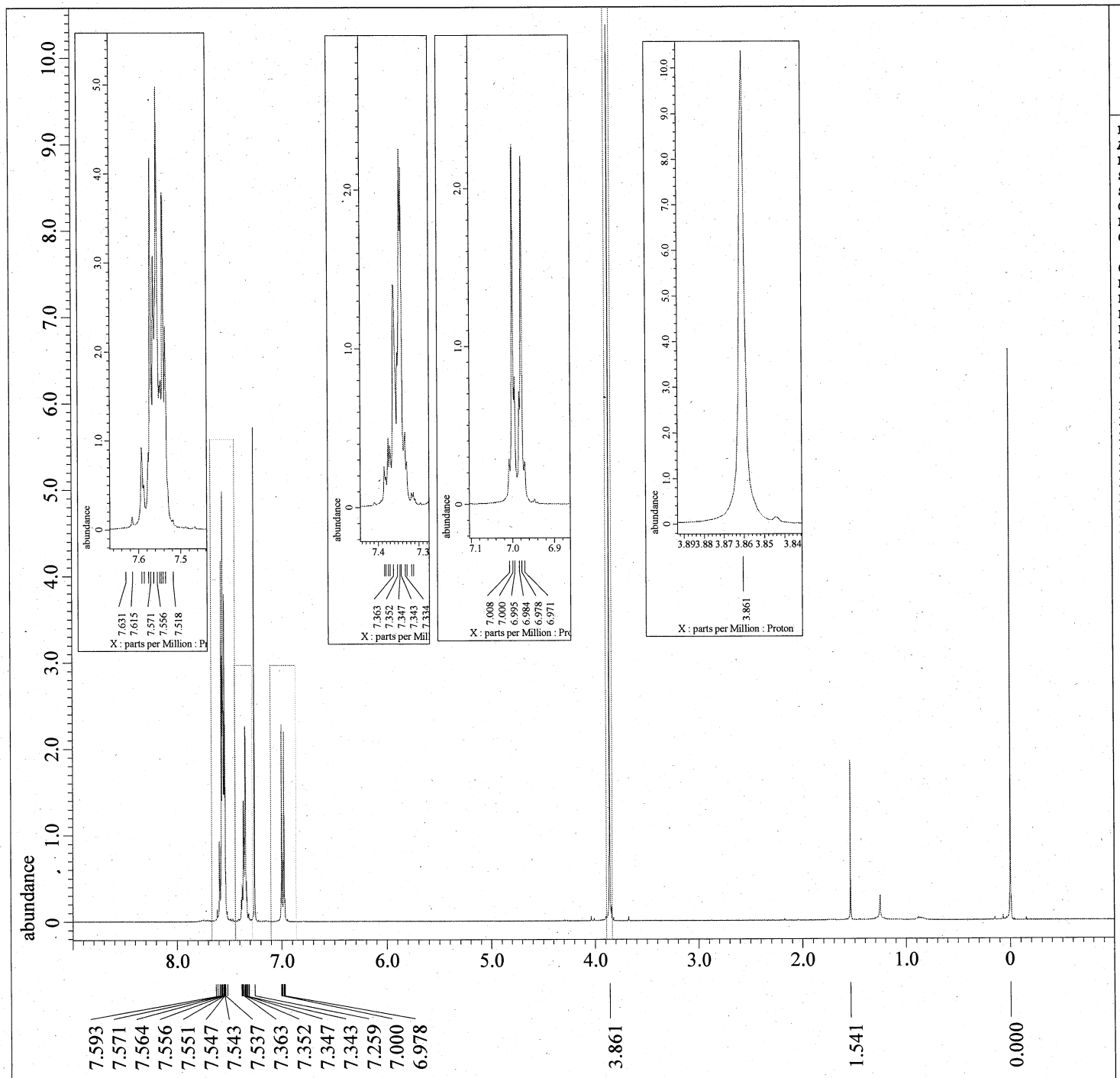
Filename	= SEO-439-1-pure_Proton-1-
Author	= element
Experiment	= proton.jxp
Sample_Id	= SEO-439-1-pure
Solvent	= CHLOROFORM-D
Creation_Time	= 18-SEP-2018 14:55:38
Revision_Time	= 7-FEB-2019 18:04:46
Current_Time	= 7-FEB-2019 18:07:16
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
Dim_Title	= 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	= 20.4[dC]
X_90_Width	= 6.22[us]
X_Acq_Time	= 2.18103808[s]
X_Angle	= 45[deg]
X_Atn	= 0.8[dB]
X_Pulse	= 3.11[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.18103808[s]



JEOL
Solutions for Innovation

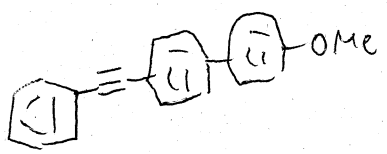
```
Filename          = SEO-439-2-pure-13C-4.jdf
Author            = element
Experiment        = single_pulse_dec
Sample_Id         = 1
Solvent           = CHLOROFORM-D
Creation_Time     = 14-JAN-2019 14:39:03
Revision_Time     =  7-FEB-2019 18:25:18
Current_Time      =  7-FEB-2019 18:25:55

Comment           = single pulse decoupled g
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[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             = 34
Total_Scans       = 34

Relaxation_Delay  = 2[s]
Recvr_Gain        = 60
Temp_Get          = 19[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
Noe_Time          = 2[s]
Repetition_Time   = 3.06430464[s]
```



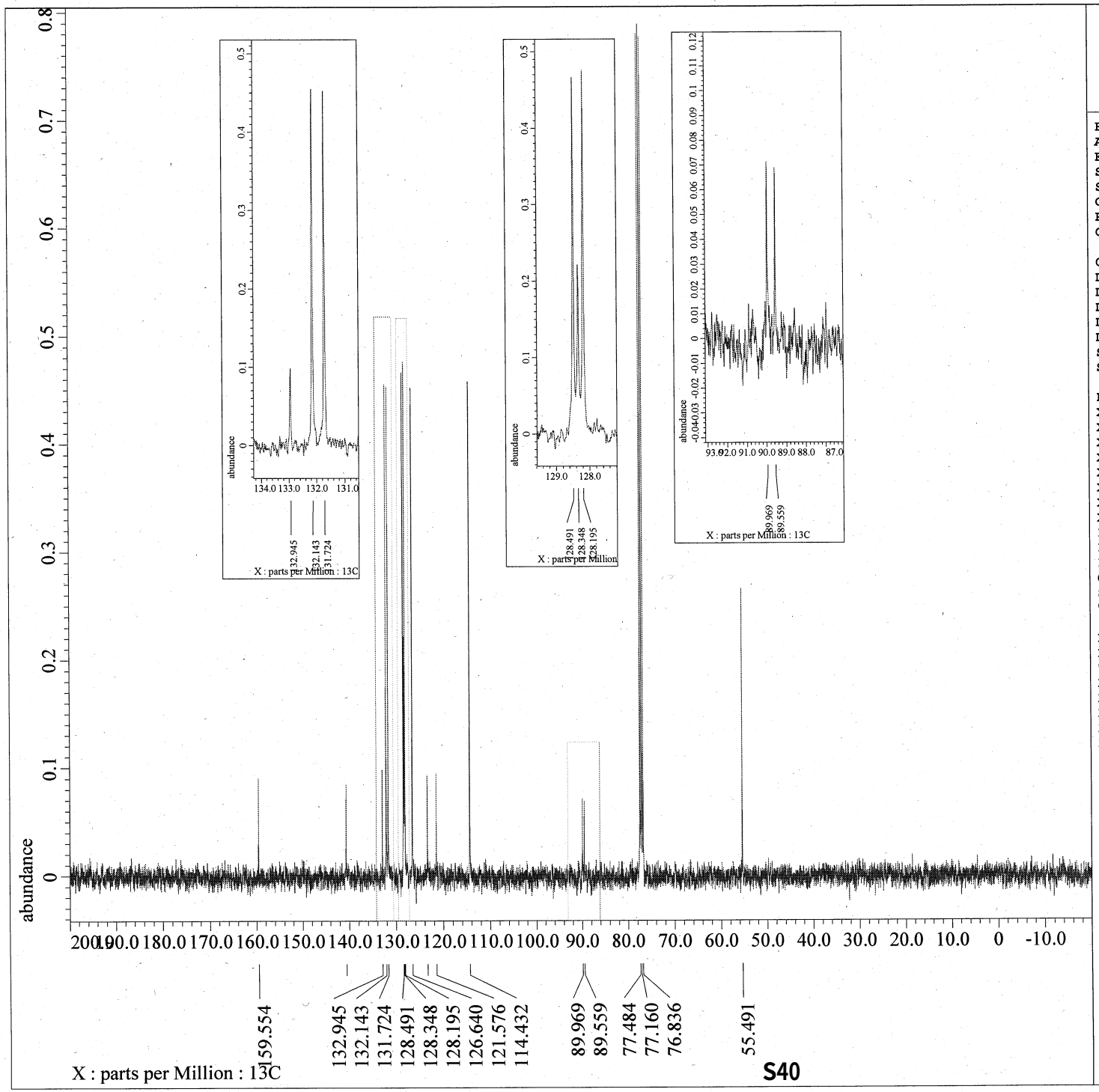


JEOL
Solutions for Innovation

Filename	= SEO-446-2-pure_Proton-1-
Author	= element
Experiment	= proton.jxp
Sample_Id	= SEO-446-2-pure
Solvent	= CHLOROFORM-D
Creation_Time	= 8-OCT-2018 13:45:25
Revision_Time	= 7-FEB-2019 18:10:06
Current_Time	= 7-FEB-2019 18:15:59
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECS400
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.37221[T] (400[MHz])
X_Acq_Duration	= 2.1889024[s]
X_Domain	= 1H
X_Freq	= 399.03472754[MHz]
X_Offset	= 5.0[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45684997[Hz]
X_Sweep	= 7.48502994[kHz]
X_Sweep_Clipped	= 5.98802395[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.03472754[MHz]
Irr_Offset	= 5.0[ppm]
Tri_Domain	= Proton
Tri_Freq	= 399.03472754[MHz]
Tri_Offset	= 5.0[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 48
Temp_Get	= 21[dC]
X_90_Width	= 6.6[us]
X_Acq_Time	= 2.1889024[s]
X_Angle	= 45[deg]
X_Atn	= 1[dB]
X_Pulse	= 3.3[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.1889024[s]

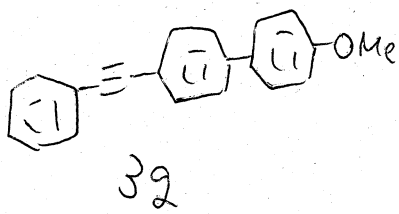


39

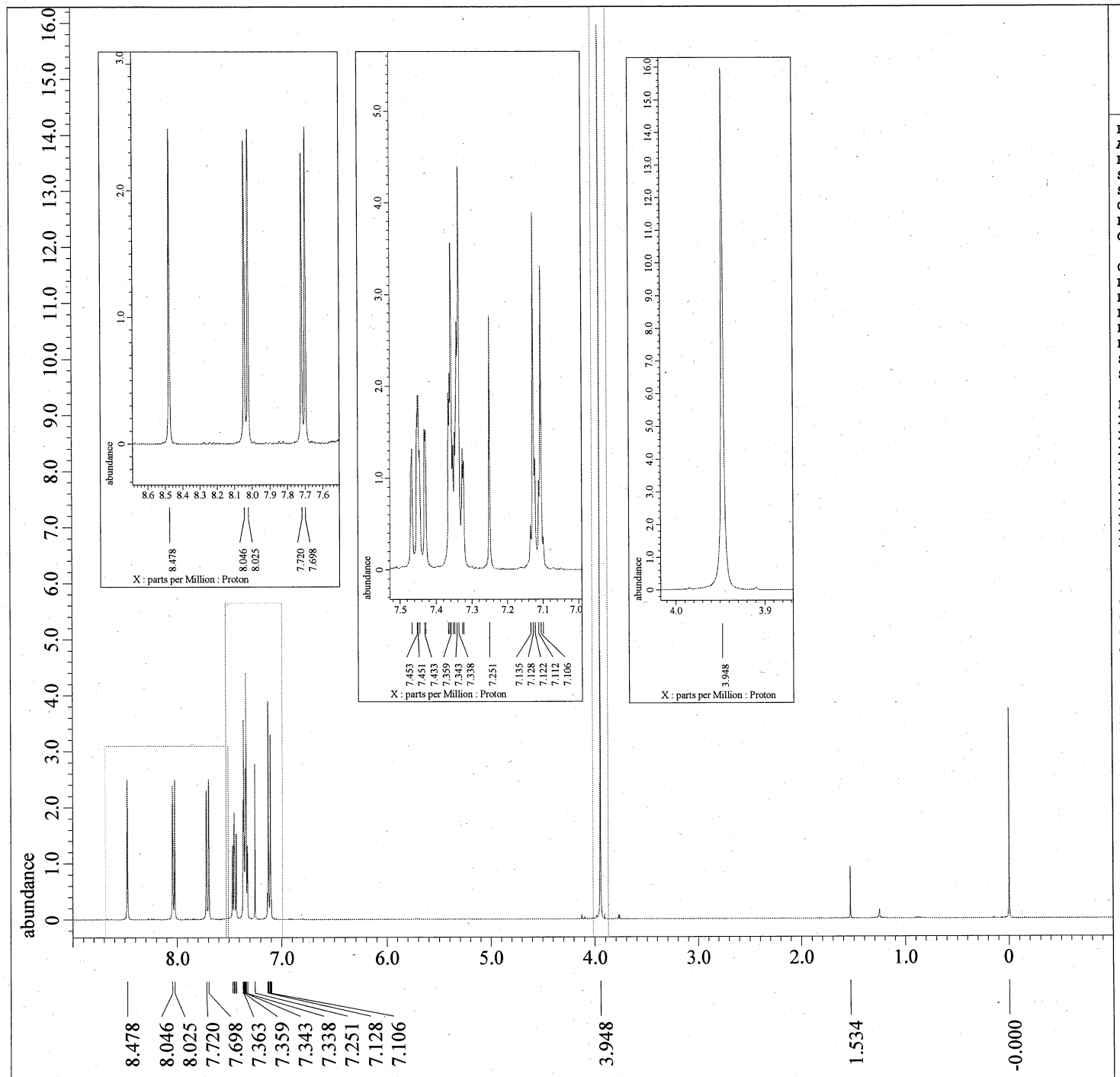


JEOL
Solutions for Innovation

Filename	= SEO-446-2-pure-13C-4.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= 1
Solvent	= CHLOROFORM-D
Creation_Time	= 8-OCT-2018 12:24:35
Revision_Time	= 7-FEB-2019 18:26:48
Current_Time	= 7-FEB-2019 18:28:48
Comment	= single pulse decoupled g
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[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	= 133
Total_Scans	= 133
Relaxation_Delay	= 2[s]
Recvr_Gain	= 60
Temp_Get	= 20.5[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
Noe_Time	= 2[s]
Repetition_Time	= 3.06430464[s]

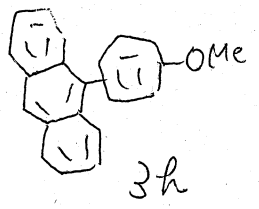


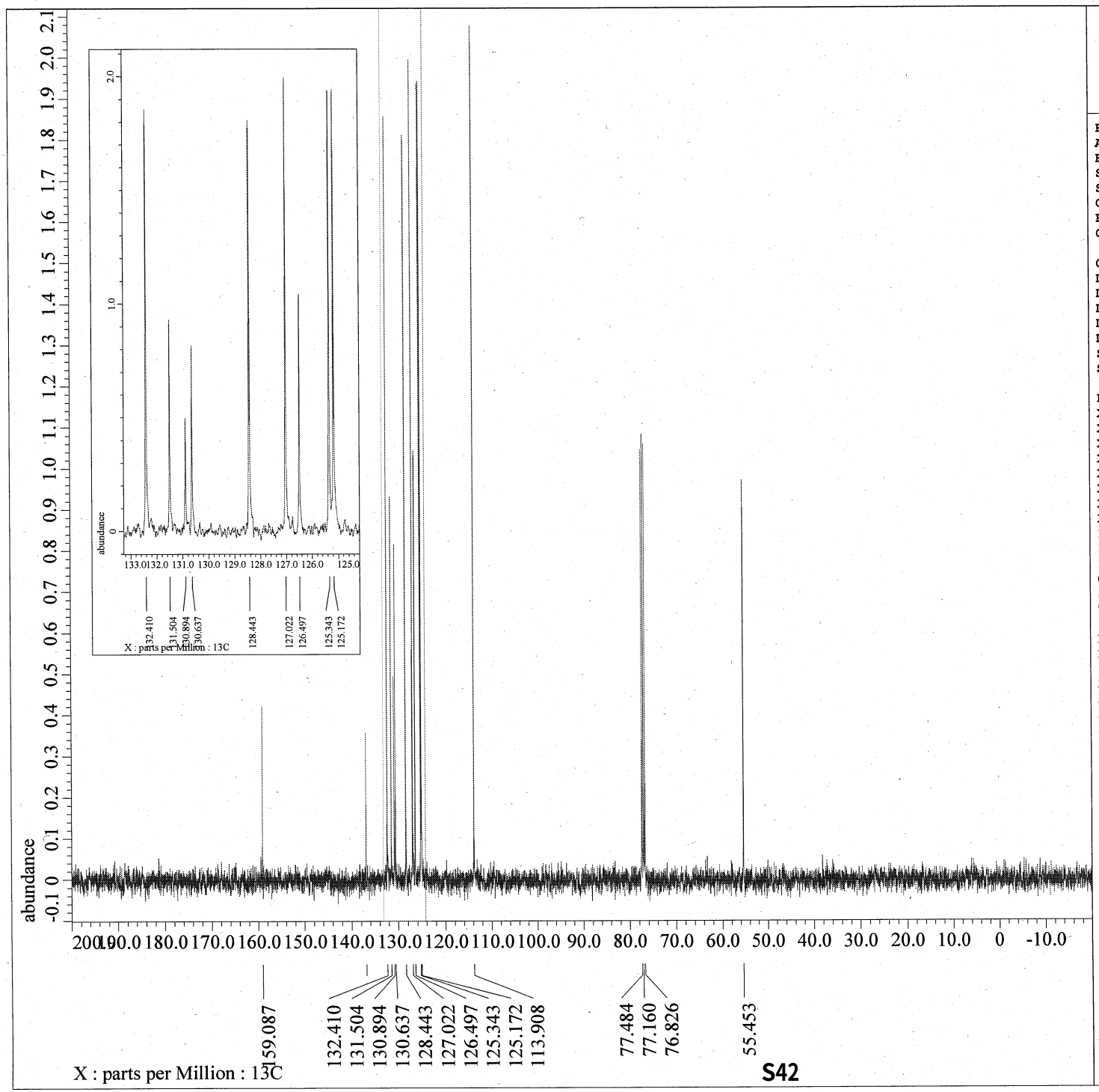
32



JEOL
Solutions for Innovation

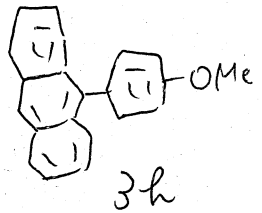
Filename	= SEO-448-1-pure_Proton-1-
Author	= element
Experiment	= proton.jxp
Sample_Id	= SEO-448-1-pure
Solvent	= CHLOROFORM-D
Creation_Time	= 8-OCT-2018 13:50:58
Revision_Time	= 7-FEB-2019 18:30:56
Current_Time	= 7-FEB-2019 18:32:11
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECS400
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.37221[T] (400[MHz])
X_Acq_Duration	= 2.1889024[s]
X_Domain	= 1H
X_Freq	= 399.03472754[MHz]
X_Offset	= 5.0[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45684997[Hz]
X_Sweep	= 7.48502994[kHz]
X_Sweep_Clipped	= 5.98802395[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.03472754[MHz]
Irr_Offset	= 5.0[ppm]
Tri_Domain	= Proton
Tri_Freq	= 399.03472754[MHz]
Tri_Offset	= 5.0[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 42
Temp_Get	= 21.2[dC]
X_90_Width	= 6.6[us]
X_Acq_Time	= 2.1889024[s]
X_Angle	= 45[deg]
X_Atn	= 1[dB]
X_Pulse	= 3.3[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.1889024[s]

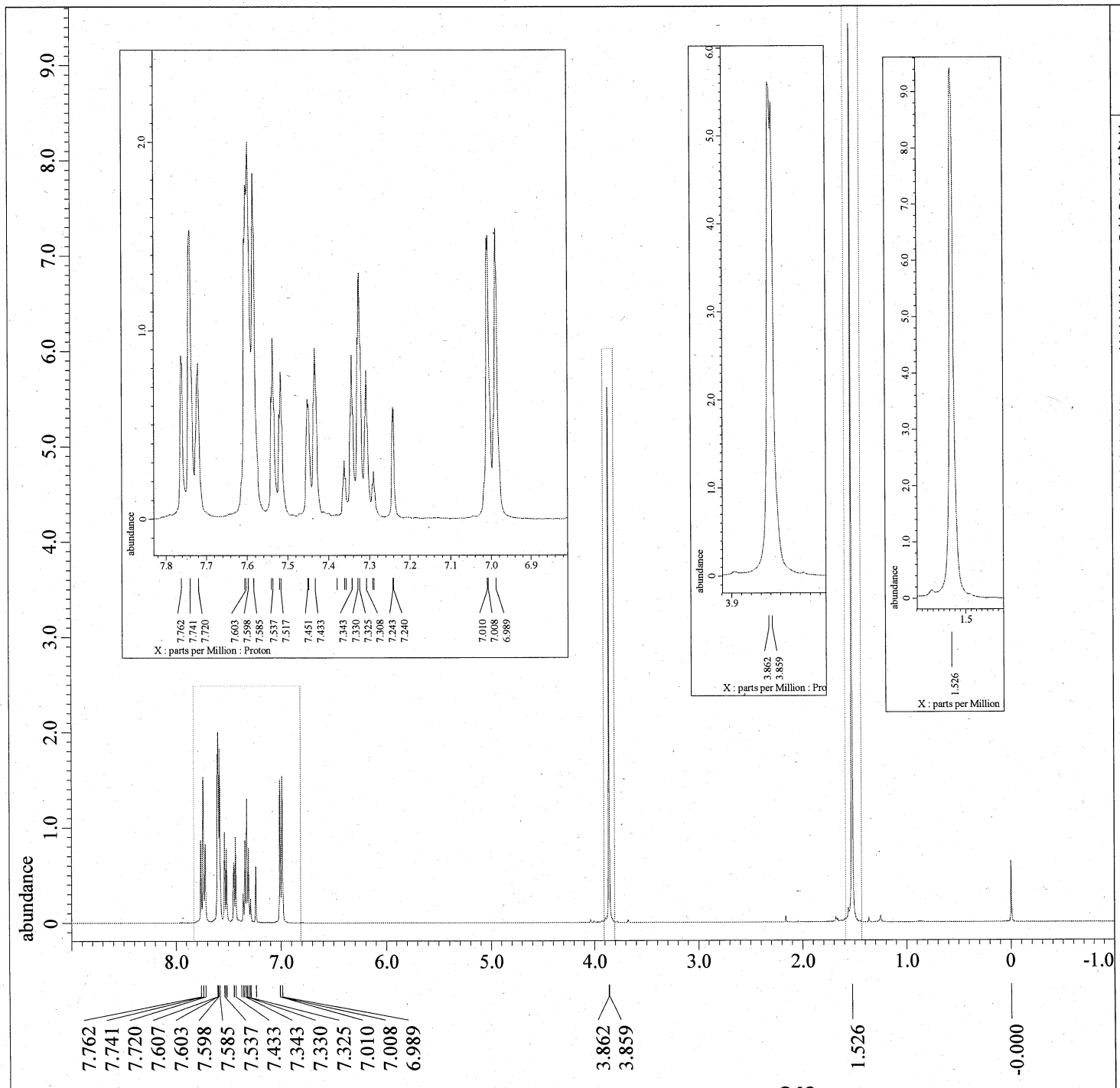




JEOL
Solutions for Innovation

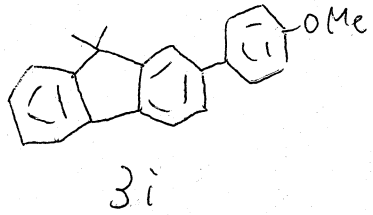
Filename	= SEO-448-1-pure-13C-4.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= 1
Solvent	= CHLOROFORM-D
Creation_Time	= 8-OCT-2018 12:34:49
Revision_Time	= 7-FEB-2019 18:32:31
Current_Time	= 7-FEB-2019 18:33:08
Comment	= single pulse decoupled g
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
Dim_Title	= 13C
Dim_Units	= [ppm]
Dimensions	= X
Site	= ECS 400
Spectrometer	= JNM-ECS400
Field_Strength	= 9.20197068[T] (390[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	= 18
Total_Scans	= 18
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
Noe_Time	= 2[s]
Repetition_Time	= 3.06430464[s]



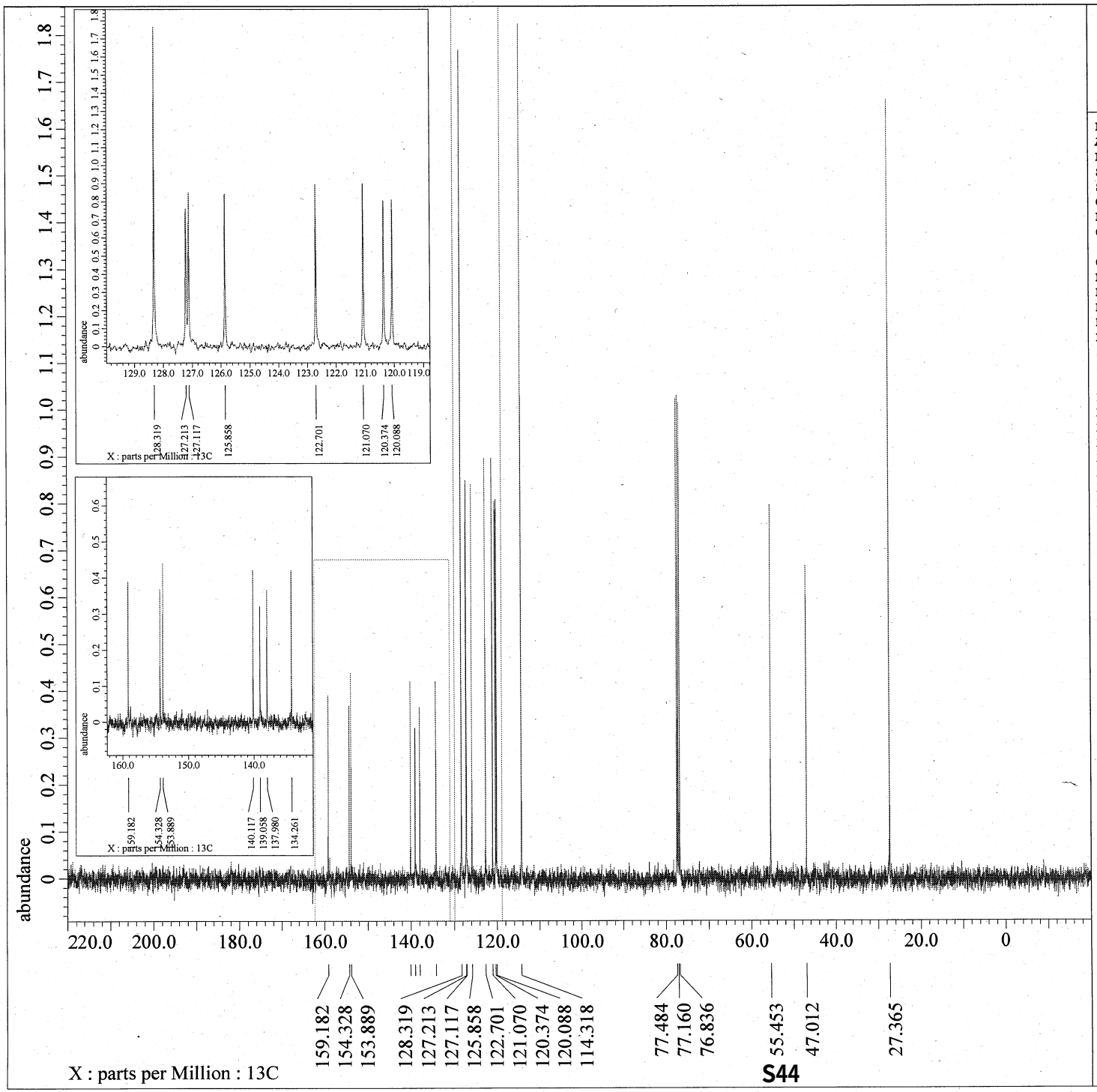


JEOL
Solutions for Innovation

Filename	= SEO-454-1-pure_Proton-1-
Author	= element
Experiment	= proton.jxp
Sample_Id	= SEO-454-1-pure
Solvent	= CHLOROFORM-D
Creation_Time	= 11-OCT-2018 20:46:11
Revision_Time	= 7-FEB-2019 18:36:33
Current_Time	= 7-FEB-2019 18:36:57
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.4073814[T] (400[MHz])
X_Acq_Duration	= 2.18103808[s]
X_Domain	= 1H
X_Freq	= 400.53219825[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45849727[Hz]
X_Sweep	= 7.51201923[kHz]
X_Sweep_Clipped	= 6.00961538[kHz]
Irr_Domain	= Proton
Irr_Freq	= 400.53219825[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 400.53219825[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 36
Temp_Get	= 19.4[dC]
X_90_Width	= 6.22[us]
X_Acq_Time	= 2.18103808[s]
X_Angle	= 45[deg]
X_Atn	= 0.8[dB]
X_Pulse	= 3.11[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.18103808[s]

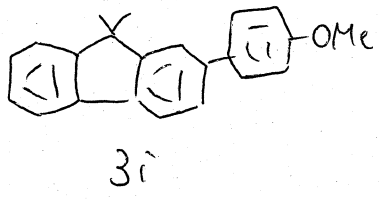


3i

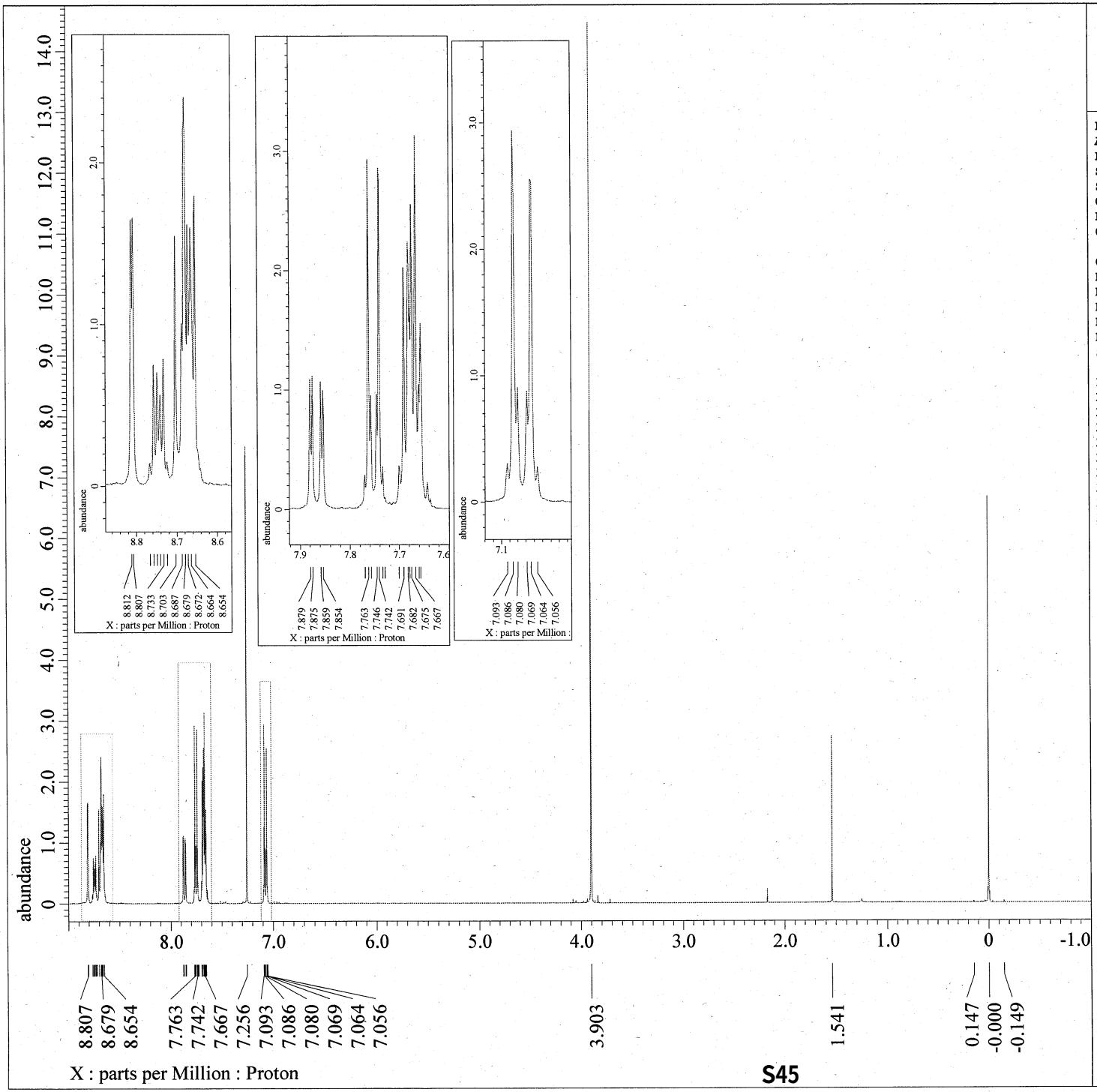


JEOL
Solutions for Innovation

Filename	= SEO-454-1-pure-13C-4.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= 1
Solvent	= CHLOROFORM-D
Creation_Time	= 11-OCT-2018 19:22:17
Revision_Time	= 7-FEB-2019 18:37:13
Current_Time	= 7-FEB-2019 18:38:44
Comment	= single pulse decoupled g
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[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	= 31
Total_Scans	= 31
Relaxation_Delay	= 2[s]
Recvr_Gain	= 60
Temp_Get	= 19.6[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
Noe_Time	= 2[s]
Repetition_Time	= 3.06430464[s]

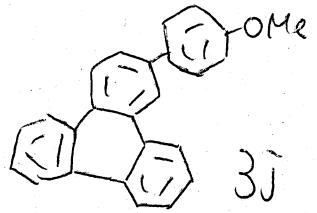


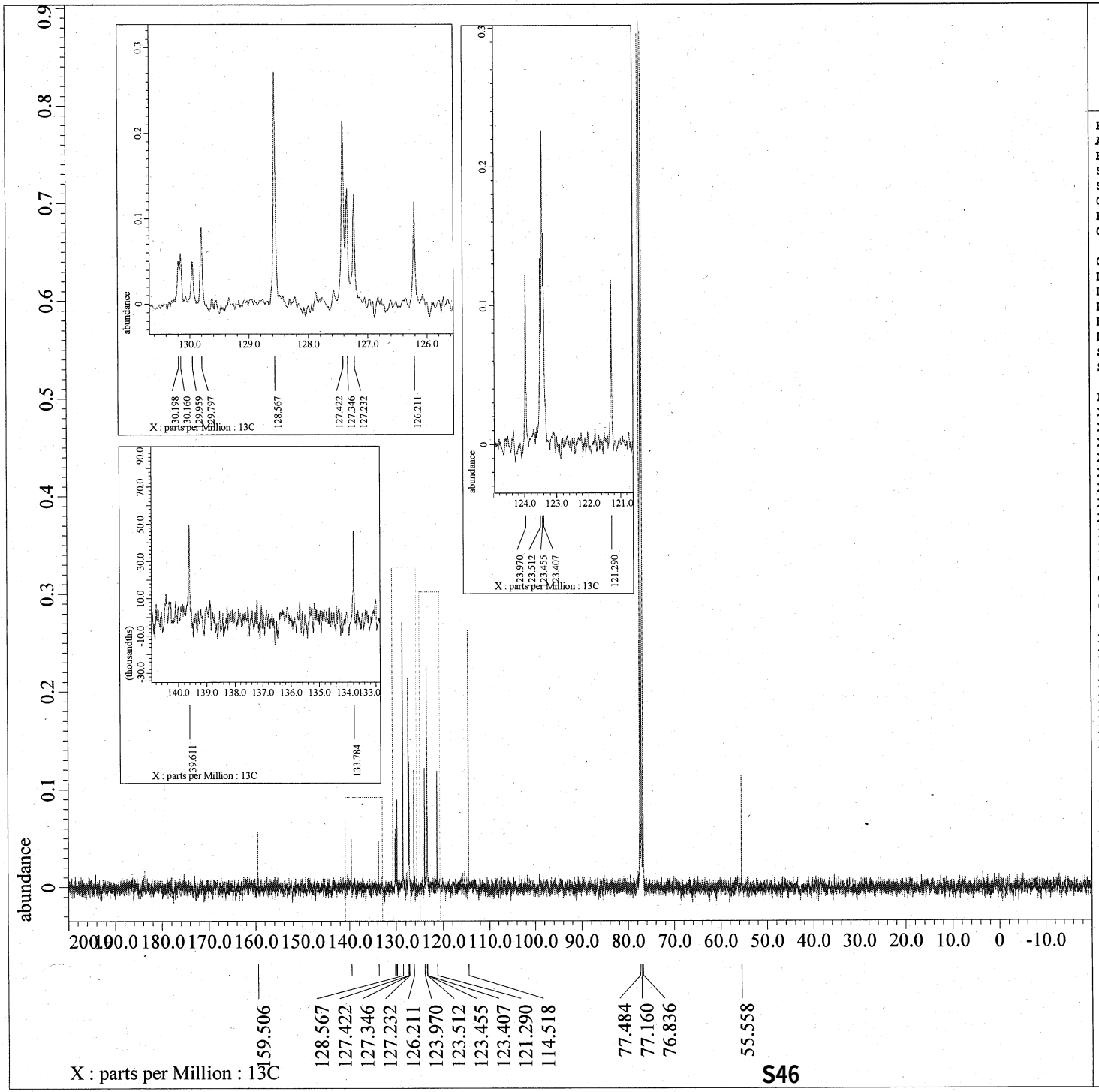
3i



JEOL
Solutions for Innovation

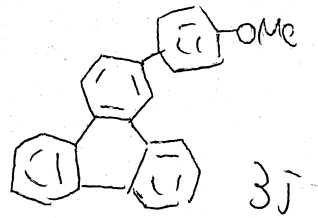
Filename	= SEO-455-1-pure_Proton-1-
Author	= element
Experiment	= proton.jxp
Sample_Id	= SEO-455-1-pure
Solvent	= CHLOROFORM-D
Creation_Time	= 12-OCT-2018 08:42:42
Revision_Time	= 7-FEB-2019 18:41:08
Current_Time	= 7-FEB-2019 18:42:54
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.4073814[T] (400[MHz])
X_Acq_Duration	= 2.18103808[s]
X_Domain	= 1H
X_Freq	= 400.53219825[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45849727[Hz]
X_Sweep	= 7.51201923[kHz]
X_Sweep_Clipped	= 6.00961538[kHz]
Irr_Domain	= Proton
Irr_Freq	= 400.53219825[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 400.53219825[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 48
Temp_Get	= 19.6[dC]
X_90_Width	= 6.22[us]
X_Acq_Time	= 2.18103808[s]
X_Angle	= 45[deg]
X_Atn	= 0.8[dB]
X_Pulse	= 3.11[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.18103808[s]

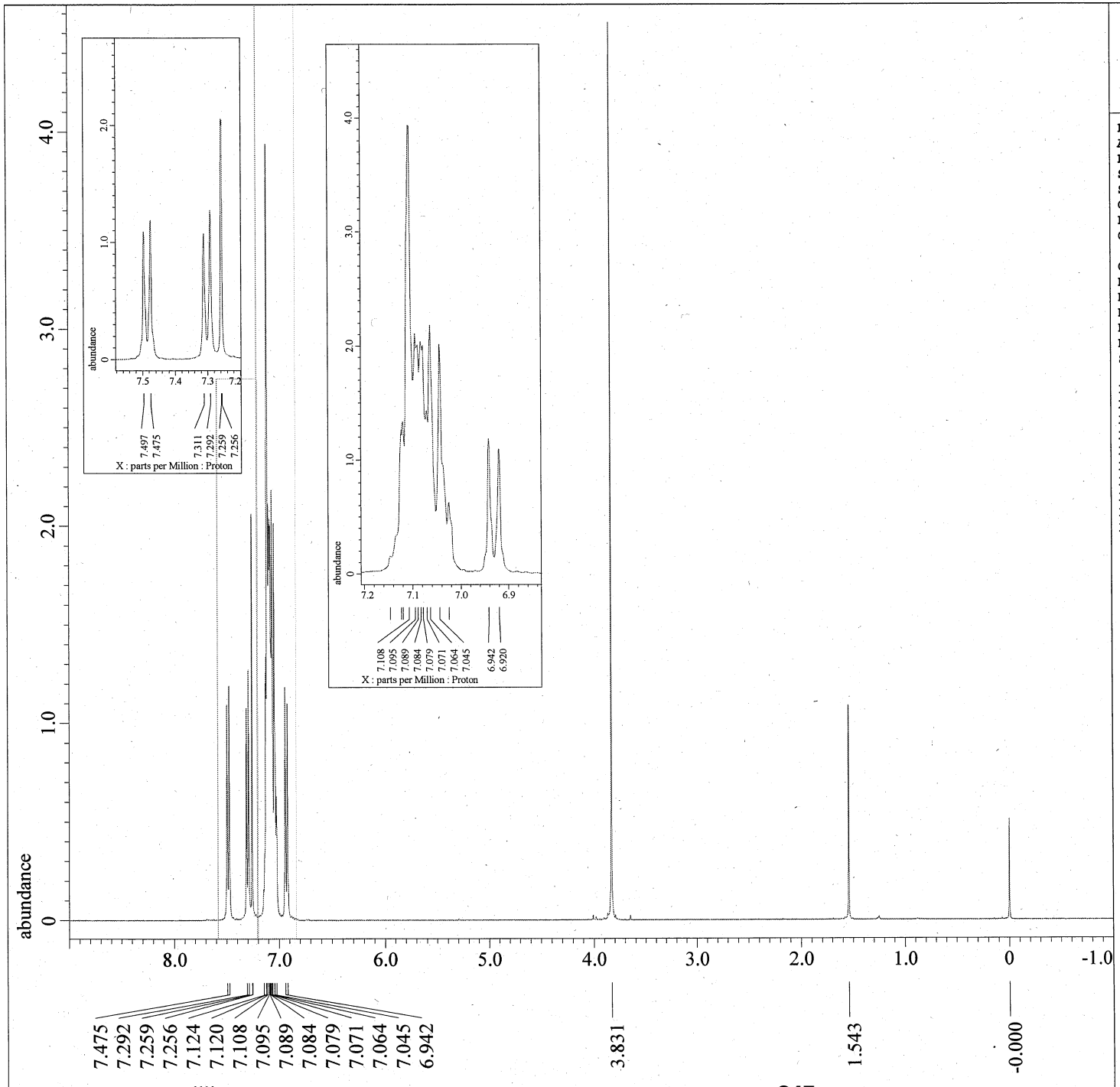




JEOL
Solutions for Innovation

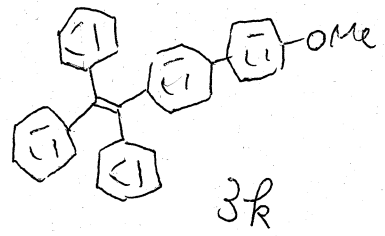
```
Filename          = SEO-455-1-pure-13C-4.jdf
Author            = element
Experiment        = single_pulse_dec
Sample_Id         = 1
Solvent           = CHLOROFORM-D
Creation_Time     = 12-OCT-2018 07:48:48
Revision_Time     =  7-FEB-2019 18:45:12
Current_Time      =  7-FEB-2019 18:46:44

Comment           = single pulse decoupled g
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[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             = 200
Total_Scans       = 200

Relaxation_Delay  = 2[s]
Recvr_Gain        = 60
Temp_Get          = 19.7[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
Noe_Time          = 2[s]
Repetition_Time   = 3.06430464[s]
```

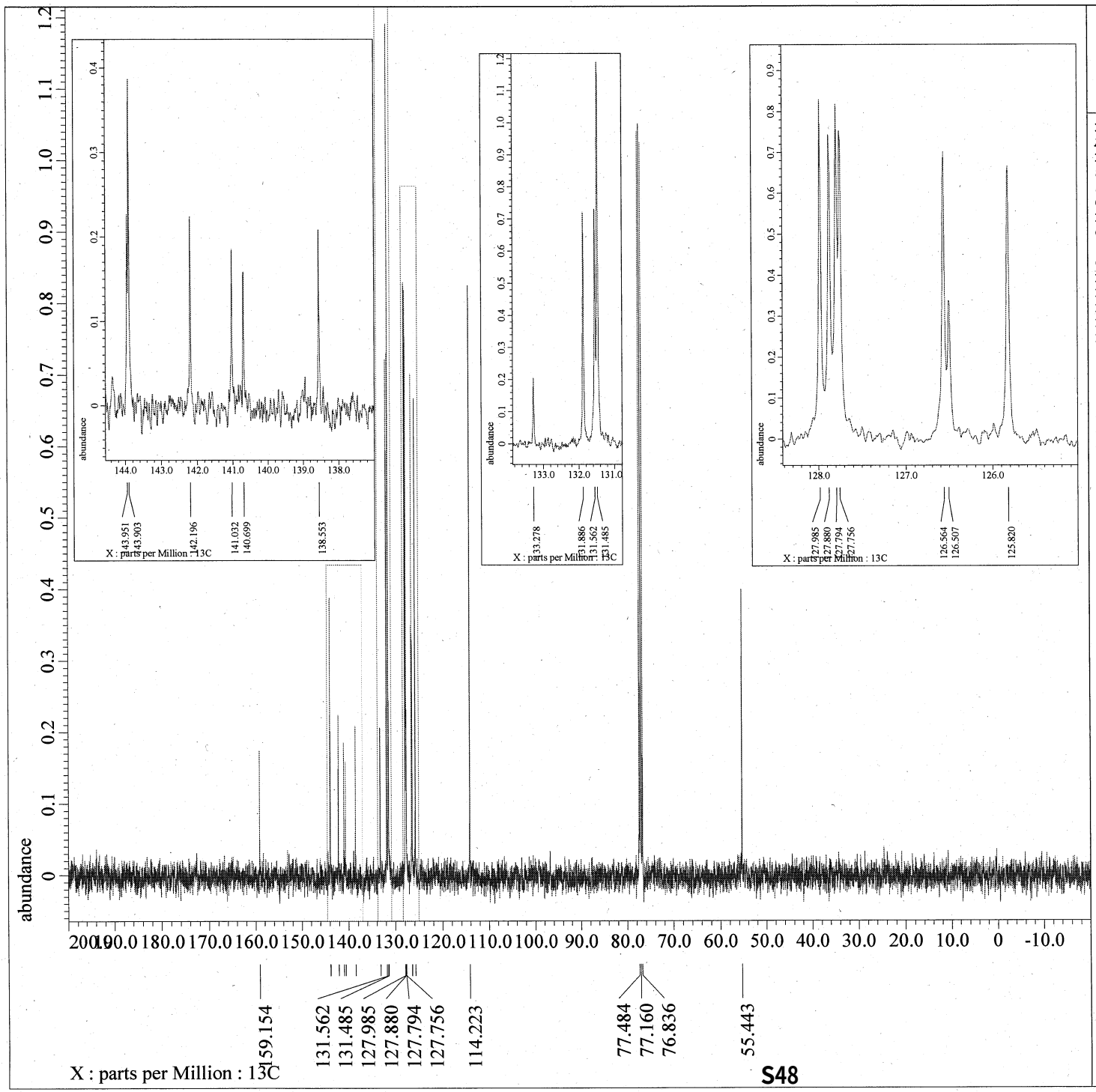




JEOL
Solutions for Innovation

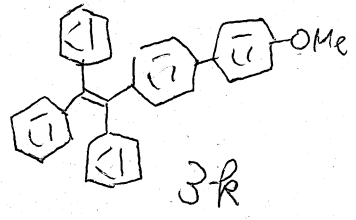
Filename	= SEO-432-2-pure_Proton-1-
Author	= element
Experiment	= proton.jxp
Sample_Id	= SEO-432-2-pure
Solvent	= CHLOROFORM-D
Creation_Time	= 14-JAN-2019 16:12:55
Revision_Time	= 7-FEB-2019 18:49:33
Current_Time	= 7-FEB-2019 18:51:33
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.4073814[T] (400[MHz])
X_Acq_Duration	= 2.18103808[s]
X_Domain	= 1H
X_Freq	= 400.53219825[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45849727[Hz]
X_Sweep	= 7.51201923[kHz]
X_Sweep_Clipped	= 6.00961538[kHz]
Irr_Domain	= Proton
Irr_Freq	= 400.53219825[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 400.53219825[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 44
Temp_Get	= 18.9[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
Initial_Wait	= 1[s]
Repetition_Time	= 7.18103808[s]

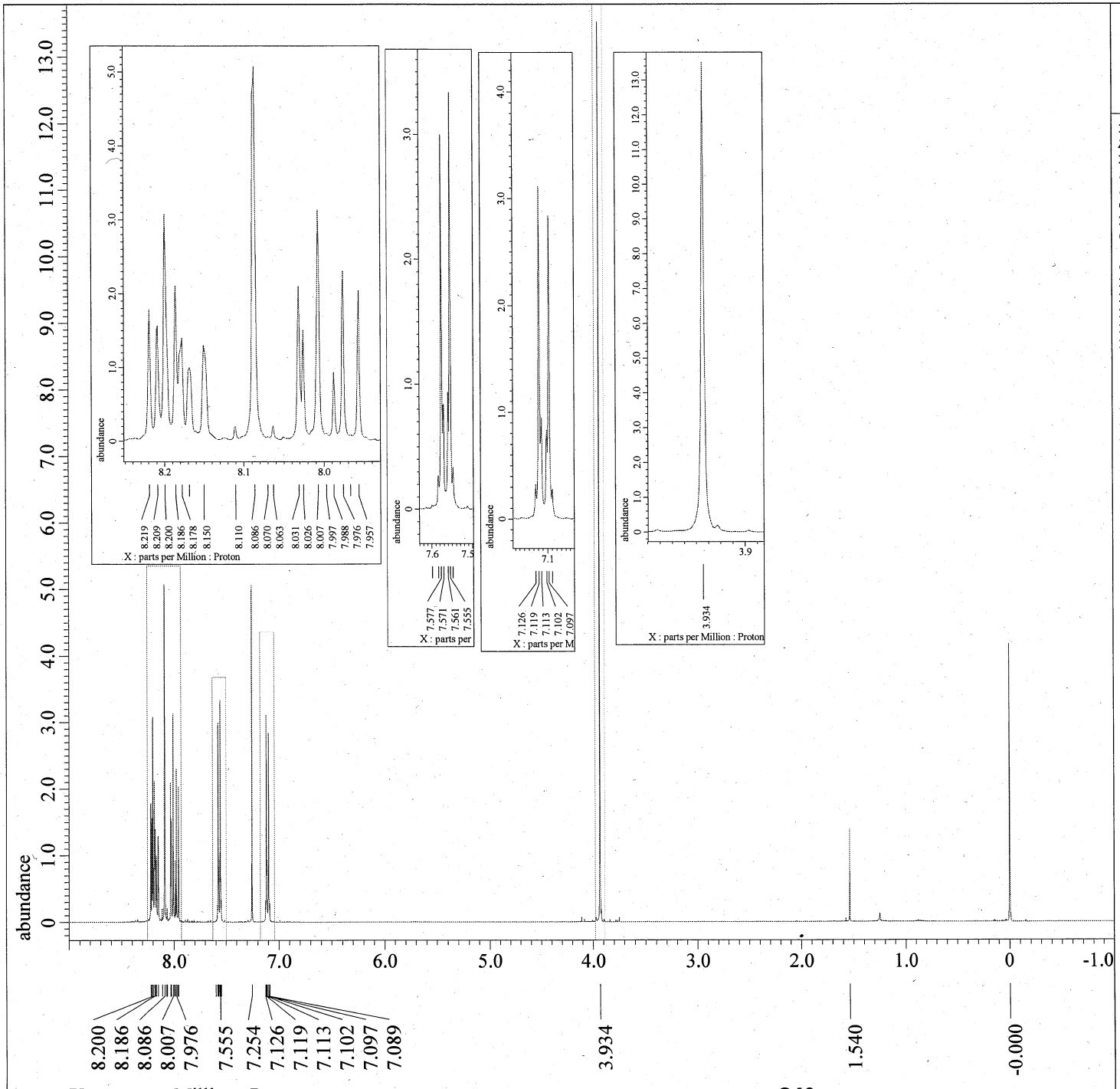




JEOL
Solutions for Innovation

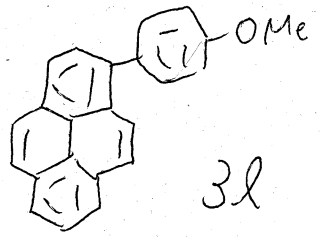
Filename	= SEO-432-2-pure-13C-4.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= 1
Solvent	= CHLOROFORM-D
Creation_Time	= 14-JAN-2019 14:47:10
Revision_Time	= 7-FEB-2019 18:51:56
Current_Time	= 7-FEB-2019 18:53:52
Comment	= single pulse decoupled g
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
Dim_Title	= 13C
Dim_Units	= [ppm]
Dimensions	= X
Site	= ECS 400
Spectrometer	= JNM-ECS400
Field_Strength	= 9.20197068[T] (390[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	= 34
Total_Scans	= 34
Relaxation_Delay	= 2[s]
Recvr_Gain	= 60
Temp_Get	= 18.7[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
Noe_Time	= 2[s]
Repetition_Time	= 3.06430464[s]

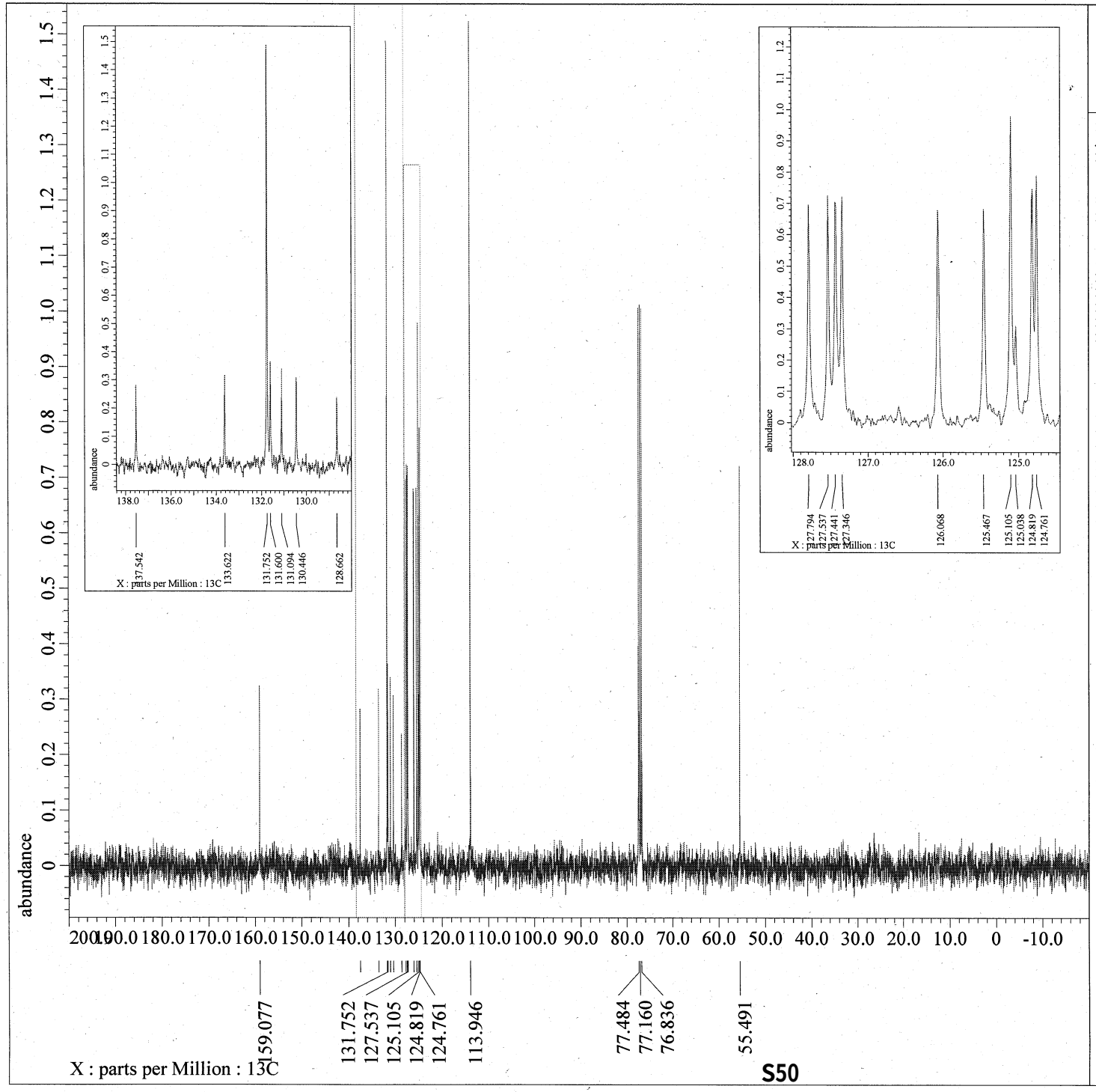




JEOL
Solutions for Innovation

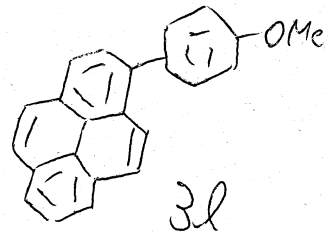
Filename	= SEO-444-1-pure_Proton-1-
Author	= element
Experiment	= proton.jxp
Sample_Id	= SEO-445-1-pure
Solvent	= CHLOROFORM-D
Creation_Time	= 5-OCT-2018 13:06:52
Revision_Time	= 7-FEB-2019 18:56:37
Current_Time	= 7-FEB-2019 18:58:21
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.4073814[T] (400[MHz])
X_Acq_Duration	= 2.18103808[s]
X_Domain	= 1H
X_Freq	= 400.53219825[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45849727[Hz]
X_Sweep	= 7.51201923[kHz]
X_Sweep_Clipped	= 6.00961538[kHz]
Irr_Domain	= Proton
Irr_Freq	= 400.53219825[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 400.53219825[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 46
Temp_Get	= 19.5[dC]
X_90_Width	= 6.22[us]
X_Acq_Time	= 2.18103808[s]
X_Angle	= 45[deg]
X_Atn	= 0.8[dB]
X_Pulse	= 3.11[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.18103808[s]

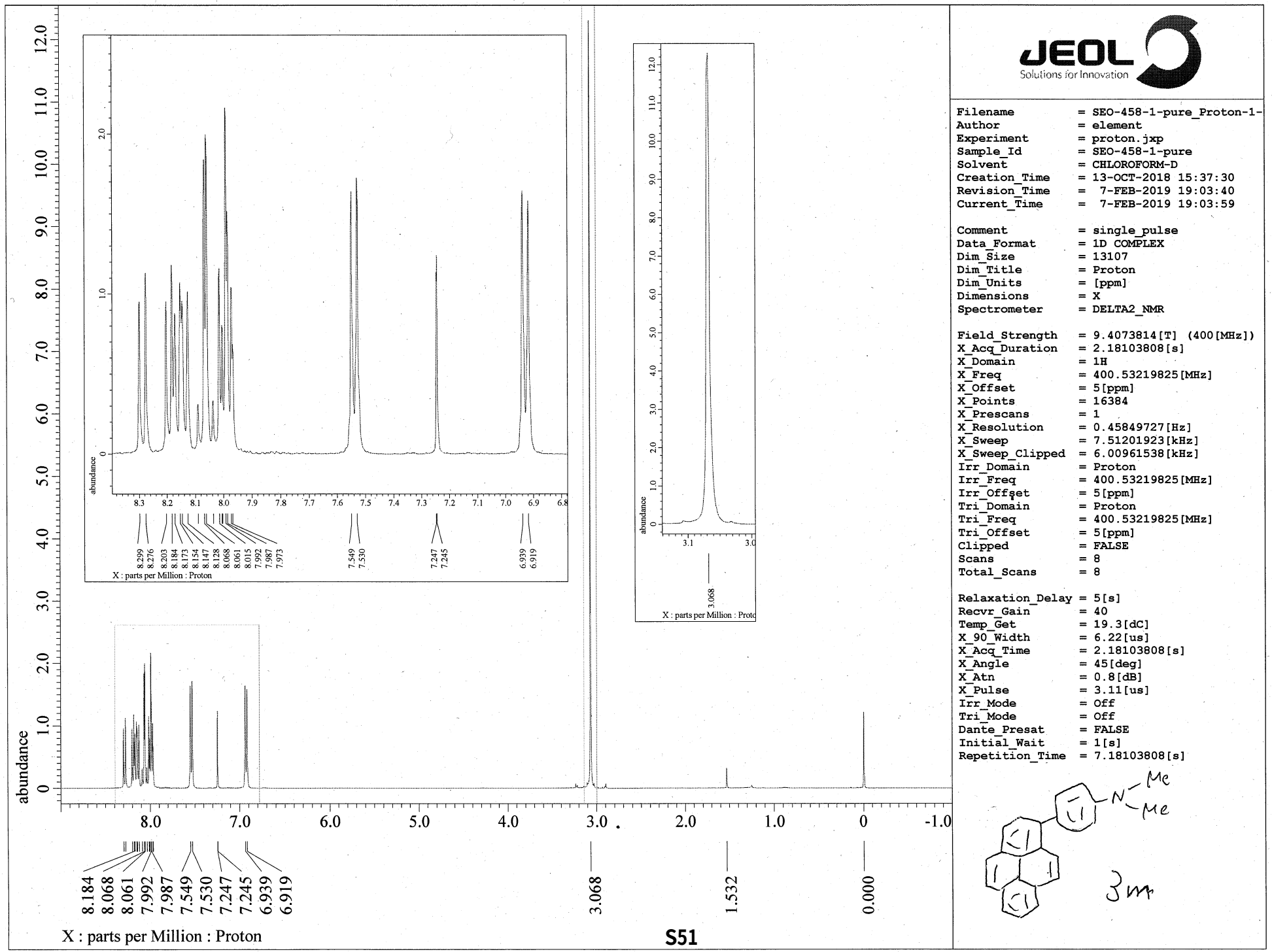




JEOL
Solutions for Innovation

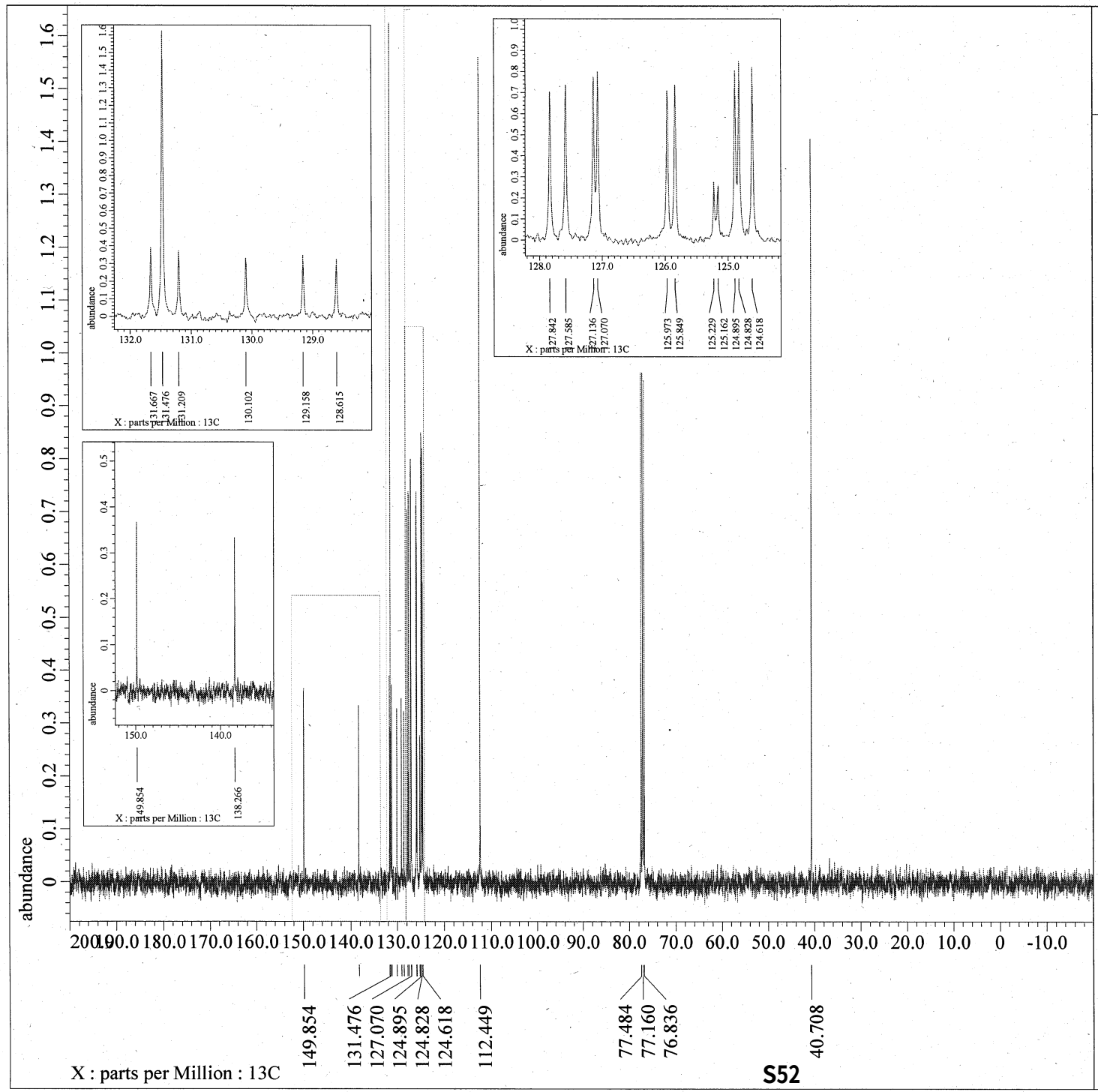
Filename	= SEO-444-1-pure-13C-4.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= 1
Solvent	= CHLOROFORM-D
Creation_Time	= 5-OCT-2018 12:07:10
Revision_Time	= 7-FEB-2019 18:58:37
Current_Time	= 7-FEB-2019 19:00:24
Comment	= single pulse decoupled g
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
Dim_Title	= 13C
Dim_Units	= [ppm]
Dimensions	= X
Site	= ECS 400
Spectrometer	= JNM-ECS400
Field_Strength	= 9.20197068[T] (390[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	= 16
Total_Scans	= 16
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_Noe	= 22.255[dB]
Irr_Noise	= WALTZ
Decoupling	= TRUE
Initial_Wait	= 1[s]
Noe	= TRUE
Noe_Time	= 2[s]
Repetition_Time	= 3.06430464[s]





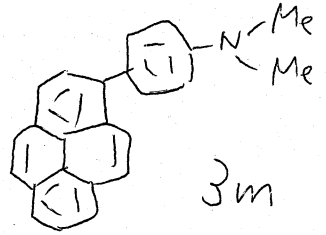
JEOL
Solutions for Innovation

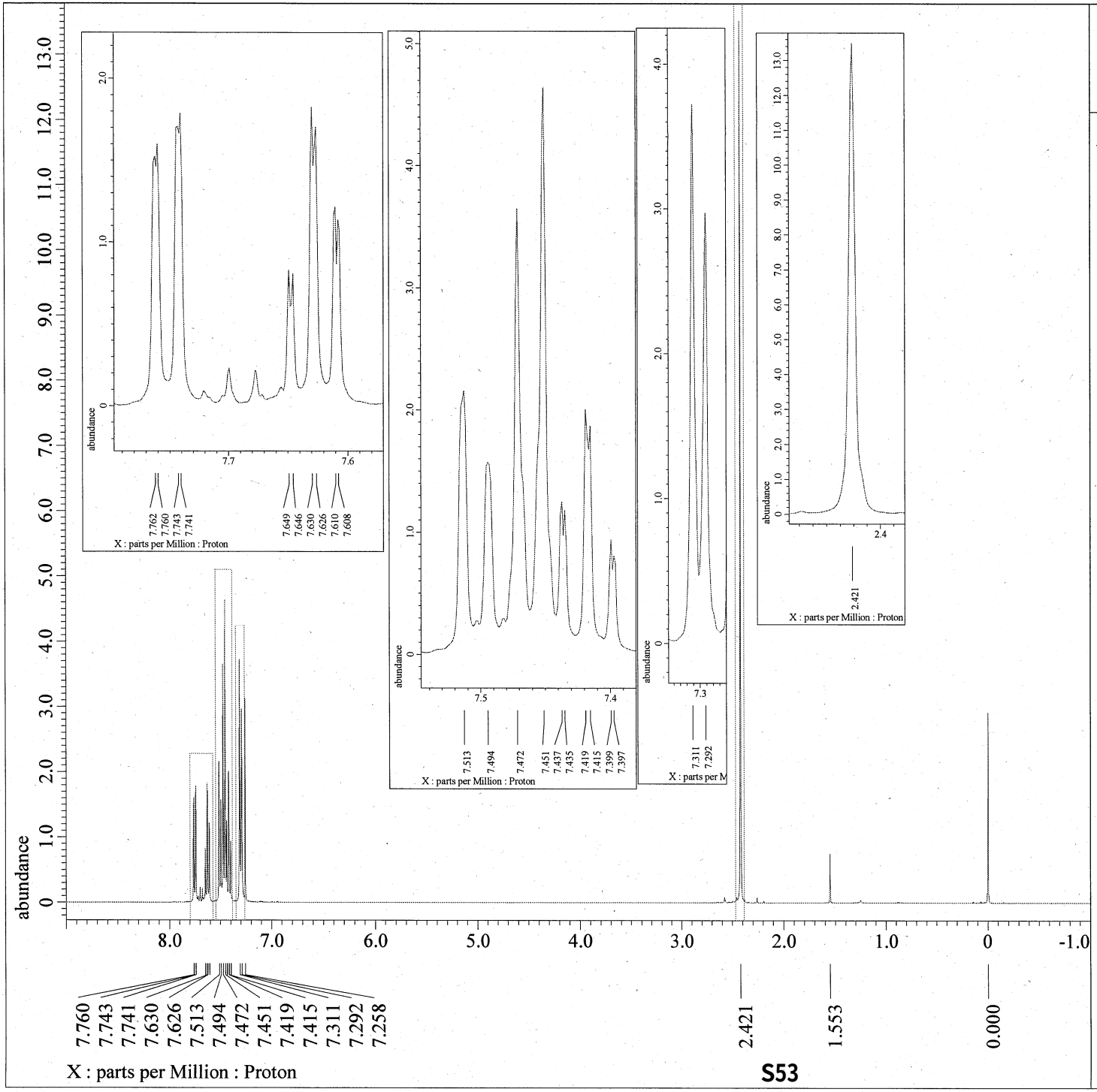
Filename	= SEO-458-1-pure_Proton-1-
Author	= element
Experiment	= proton.jxp
Sample_Id	= SEO-458-1-pure
Solvent	= CHLOROFORM-D
Creation_Time	= 13-OCT-2018 15:37:30
Revision_Time	= 7-FEB-2019 19:03:40
Current_Time	= 7-FEB-2019 19:03:59
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.4073814[T] (400[MHz])
X_Acq_Duration	= 2.18103808[s]
X_Domain	= 1H
X_Freq	= 400.53219825[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45849727[Hz]
X_Sweep	= 7.51201923[kHz]
X_Sweep_Clipped	= 6.00961538[kHz]
Irr_Domain	= Proton
Irr_Freq	= 400.53219825[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 400.53219825[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 40
Temp_Get	= 19.3[dC]
X_90_Width	= 6.22[us]
X_Acq_Time	= 2.18103808[s]
X_Angle	= 45[deg]
X_Atn	= 0.8[dB]
X_Pulse	= 3.11[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.18103808[s]



JEOL
Solutions for Innovation

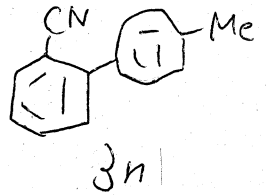
```
Filename          = SEO-458-1-pure-13C-4.jdf
Author            = element
Experiment        = single_pulse_dec
Sample_Id         = 1
Solvent           = CHLOROFORM-D
Creation_Time     = 13-OCT-2018 14:05:56
Revision_Time     =  7-FEB-2019 19:04:15
Current_Time      =  7-FEB-2019 19:06:11

Comment           = single pulse decoupled g
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[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          = 20.6[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
Noe_Time          = 2[s]
Repetition_Time   = 3.06430464[s]
```

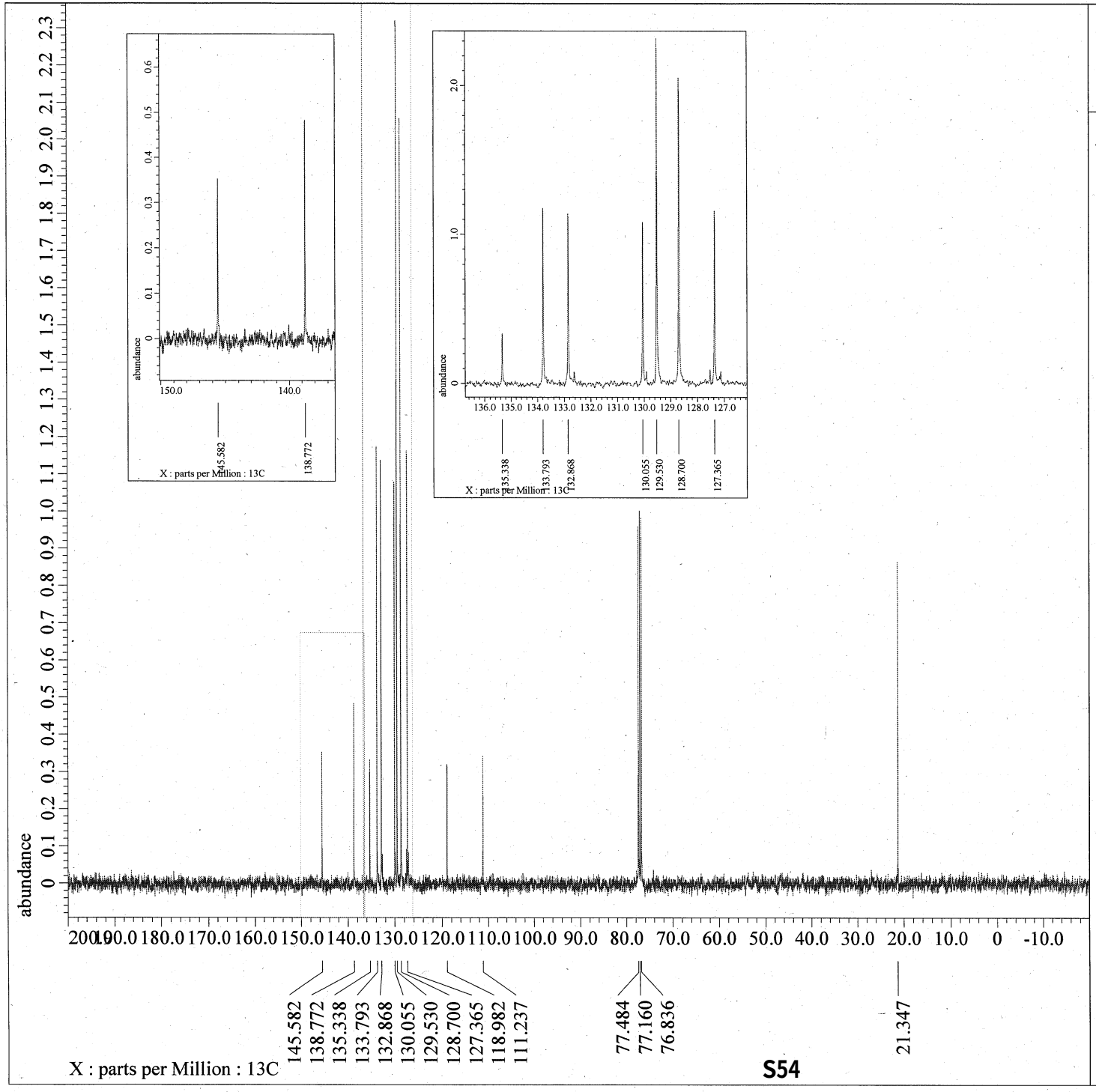




JEOL
Solutions for Innovation

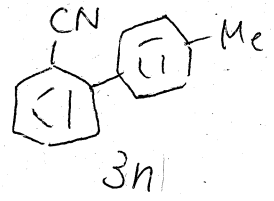
Filename	= SEO-502-1-pure_Proton-1-
Author	= element
Experiment	= proton.jxp
Sample_Id	= SEO-502-1-pure
Solvent	= CHLOROFORM-D
Creation_Time	= 16-NOV-2018 11:48:27
Revision_Time	= 7-FEB-2019 19:08:59
Current_Time	= 7-FEB-2019 19:11:57
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.4073814[T] (400[MHz])
X_Acq_Duration	= 2.18103808[s]
X_Domain	= 1H
X_Freq	= 400.53219825[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45849727[Hz]
X_Sweep	= 7.51201923[kHz]
X_Sweep_Clipped	= 6.00961538[kHz]
Irr_Domain	= Proton
Irr_Freq	= 400.53219825[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 400.53219825[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 44
Temp_Get	= 19.5[dC]
X_90_Width	= 6.22[us]
X_Acq_Time	= 2.18103808[s]
X_Angle	= 45[deg]
X_Atn	= 0.8[dB]
X_Pulse	= 3.11[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.18103808[s]

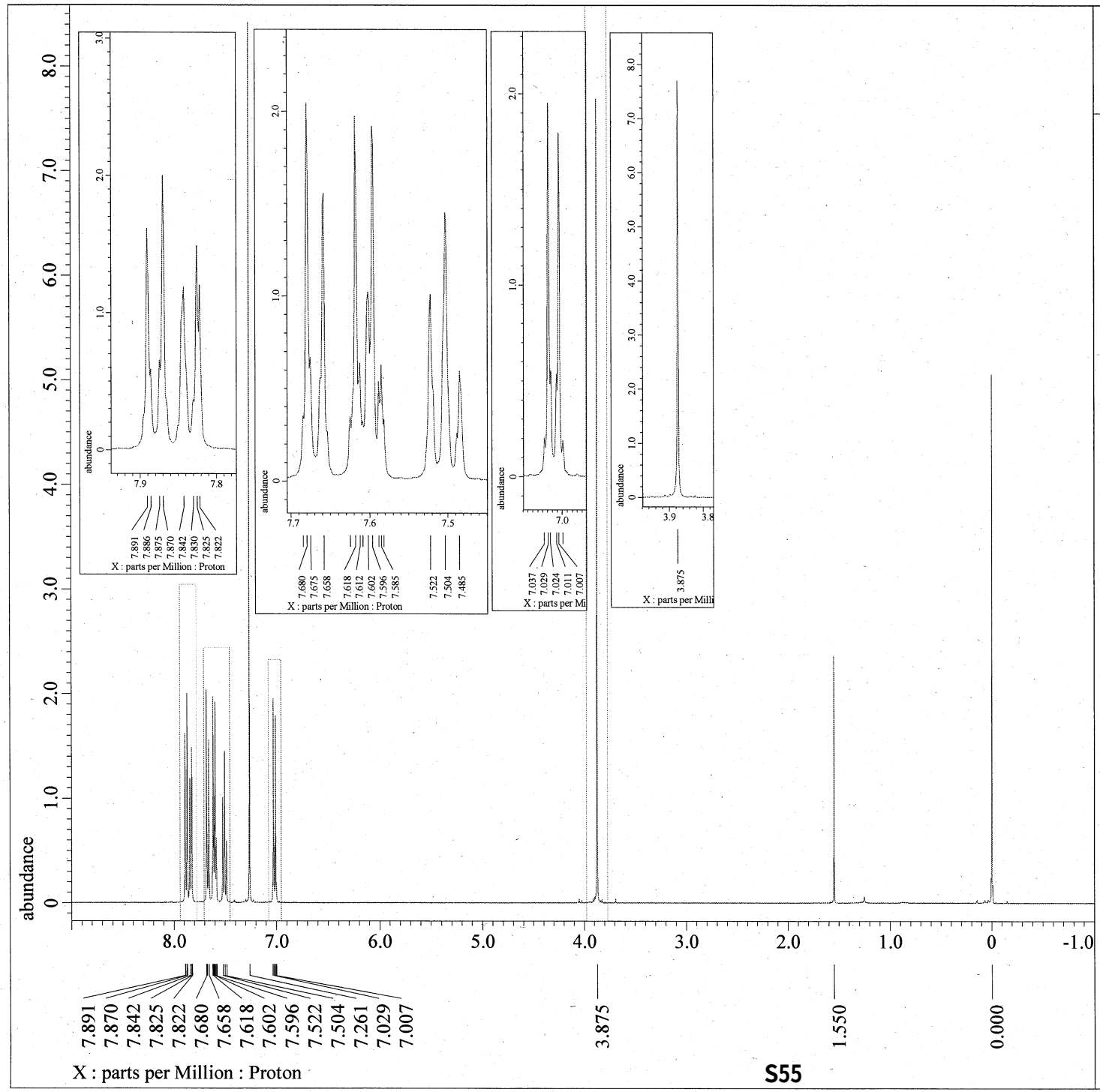




JEOL
Solutions for Innovation

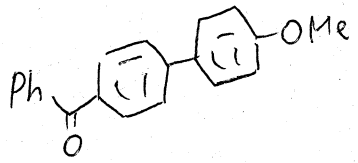
Filename	= SEO-502-1-pure-13C-7.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= 1
Solvent	= CHLOROFORM-D
Creation_Time	= 16-NOV-2018 10:24:45
Revision_Time	= 7-FEB-2019 19:10:49
Current_Time	= 7-FEB-2019 19:11:26
Comment	= single pulse decoupled g
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
Dim_Title	= 13C
Dim_Units	= [ppm]
Dimensions	= X
Site	= ECS 400
Spectrometer	= JNM-ECS400
Field_Strength	= 9.20197068[T] (390[MHz])
X_Acq_Duration	= 1.06430464[s]
X_Domain	= 13C
X_Freq	= 98.51479726[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.93958061[Hz]
X_Sweep	= 30.78817734[kHz]
Irr_Domain	= 1H
Irr_Freq	= 391.78655441[MHz]
Irr_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 38
Total_Scans	= 38
Relaxation_Delay	= 2[s]
Recvr_Gain	= 60
Temp_Get	= 21.2[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
Noe_Time	= 2[s]
Repetition_Time	= 3.06430464[s]



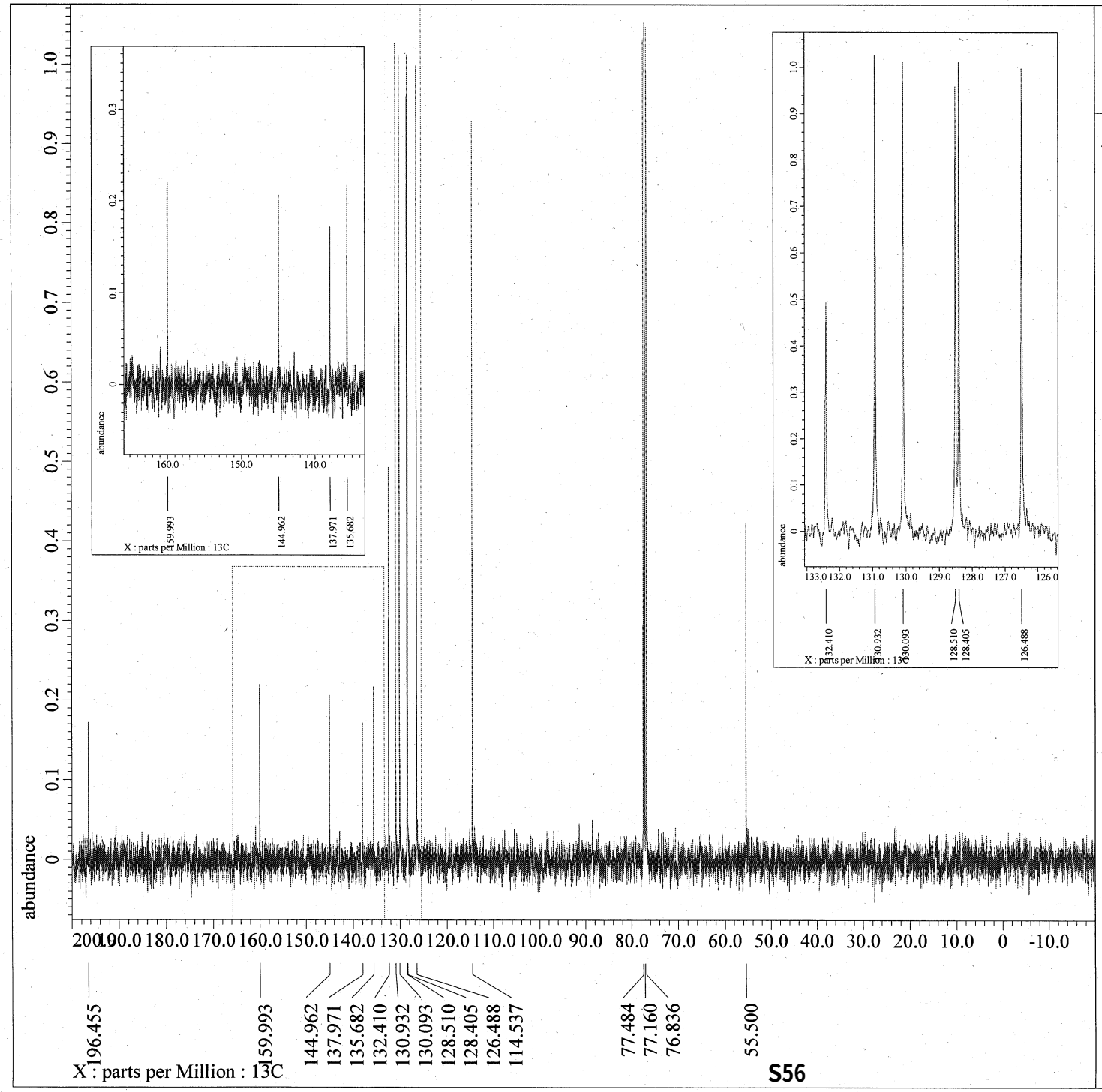


JEOL
Solutions for Innovation

Filename	= SEO-494-2-pure_Proton-1-
Author	= element
Experiment	= proton.jxp
Sample_Id	= SEO-494-2-pure
Solvent	= CHLOROFORM-D
Creation_Time	= 13-NOV-2018 10:17:04
Revision_Time	= 7-FEB-2019 19:14:28
Current_Time	= 7-FEB-2019 19:17:53
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
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	= 19.5[dC]
X_90_Width	= 6.22[us]
X_Acq_Time	= 2.18103808[s]
X_Angle	= 45[deg]
X_Atn	= 0.8[dB]
X_Pulse	= 3.11[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.18103808[s]

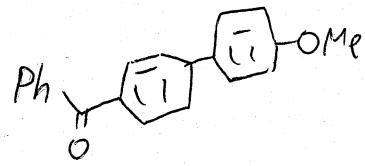


30

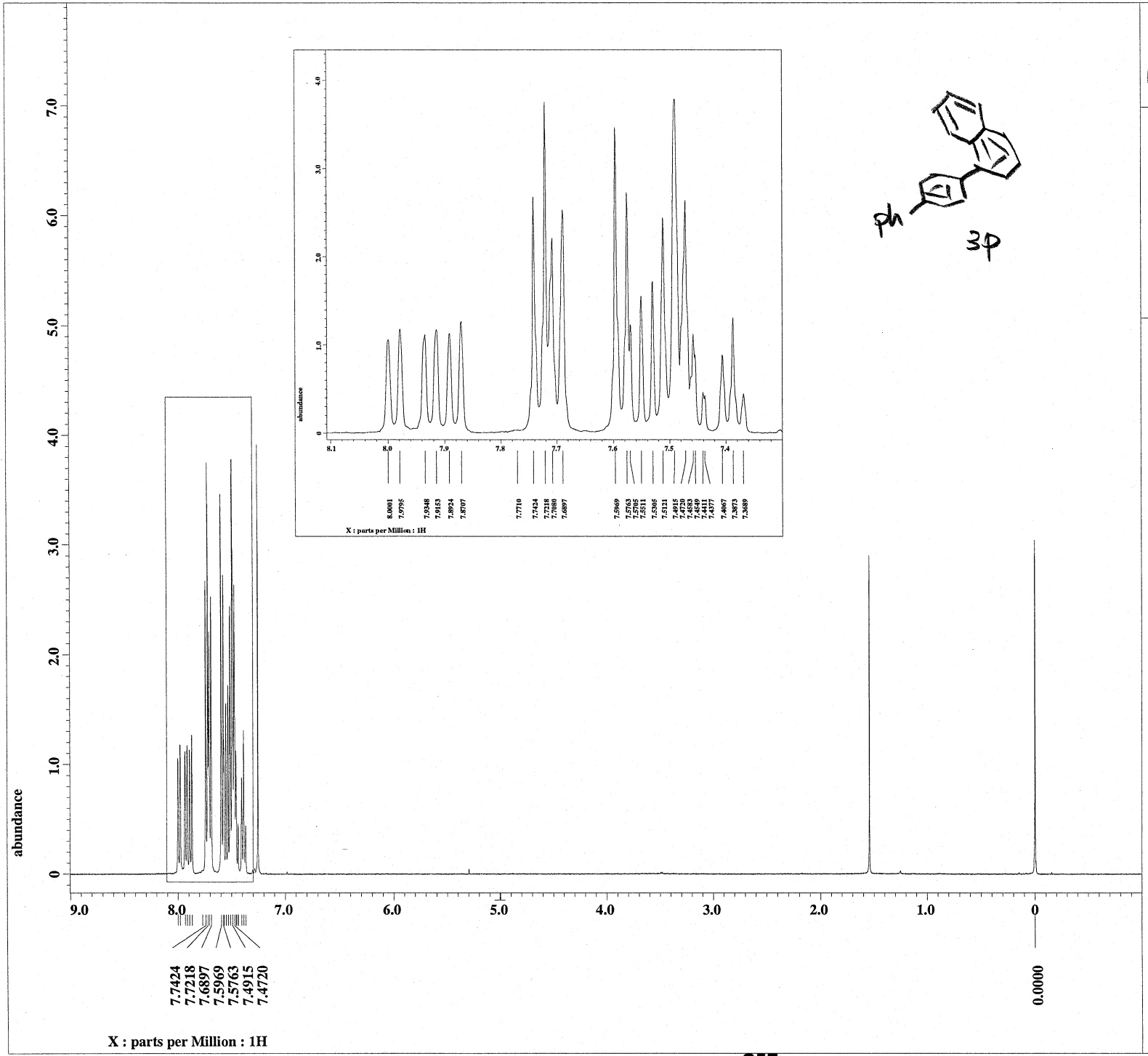


JEOL
Solutions for Innovation

Filename	= SEO-494-2-pure-13C-6.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= 1
Solvent	= CHLOROFORM-D
Creation_Time	= 13-NOV-2018 08:55:28
Revision_Time	= 7-FEB-2019 19:17:12
Current_Time	= 7-FEB-2019 19:18:29
Comment	= single pulse decoupled g
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[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	= 25
Total_Scans	= 25
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
Noe_Time	= 2[s]
Repetition_Time	= 3.06430464[s]



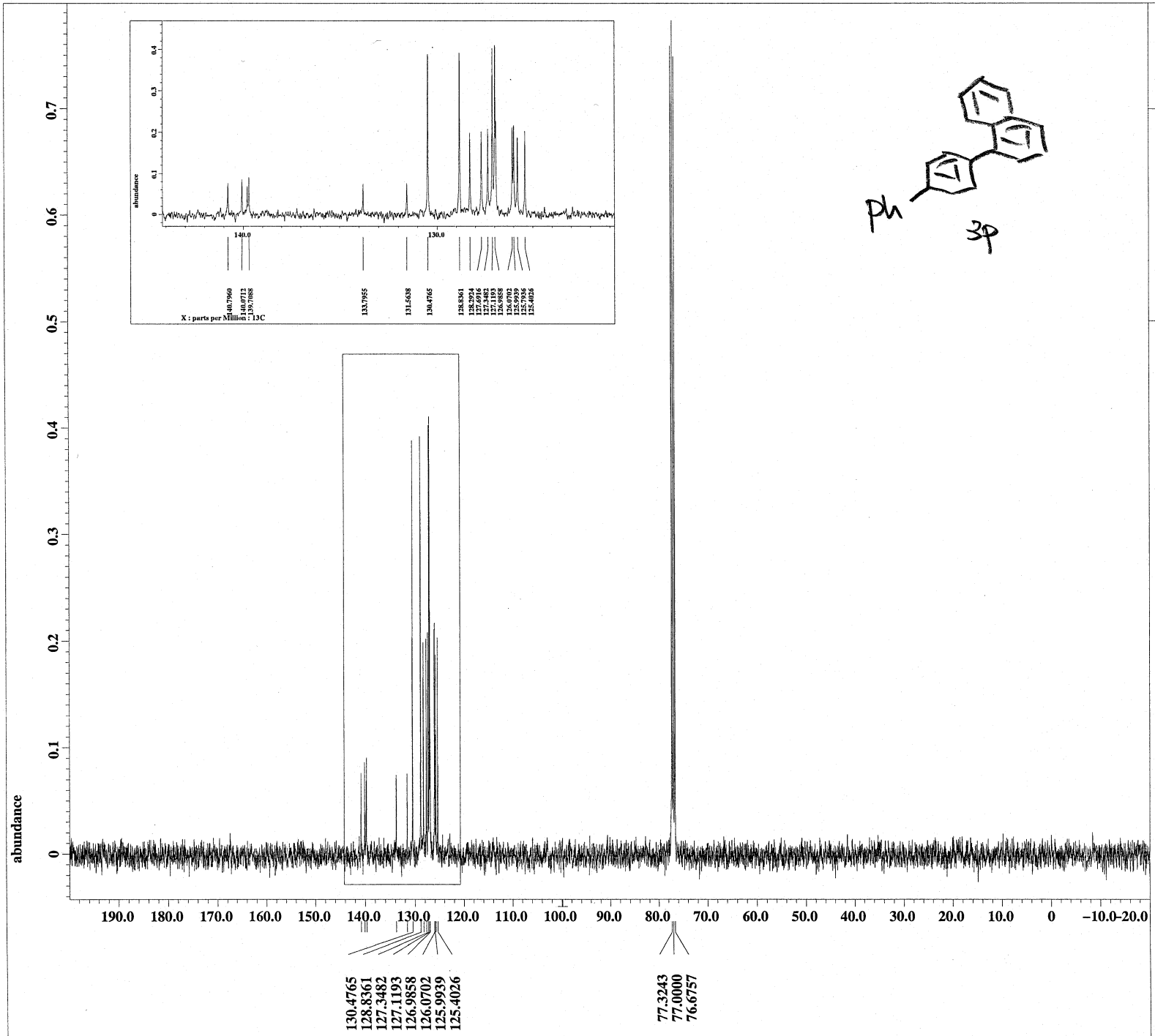
30



JEOL

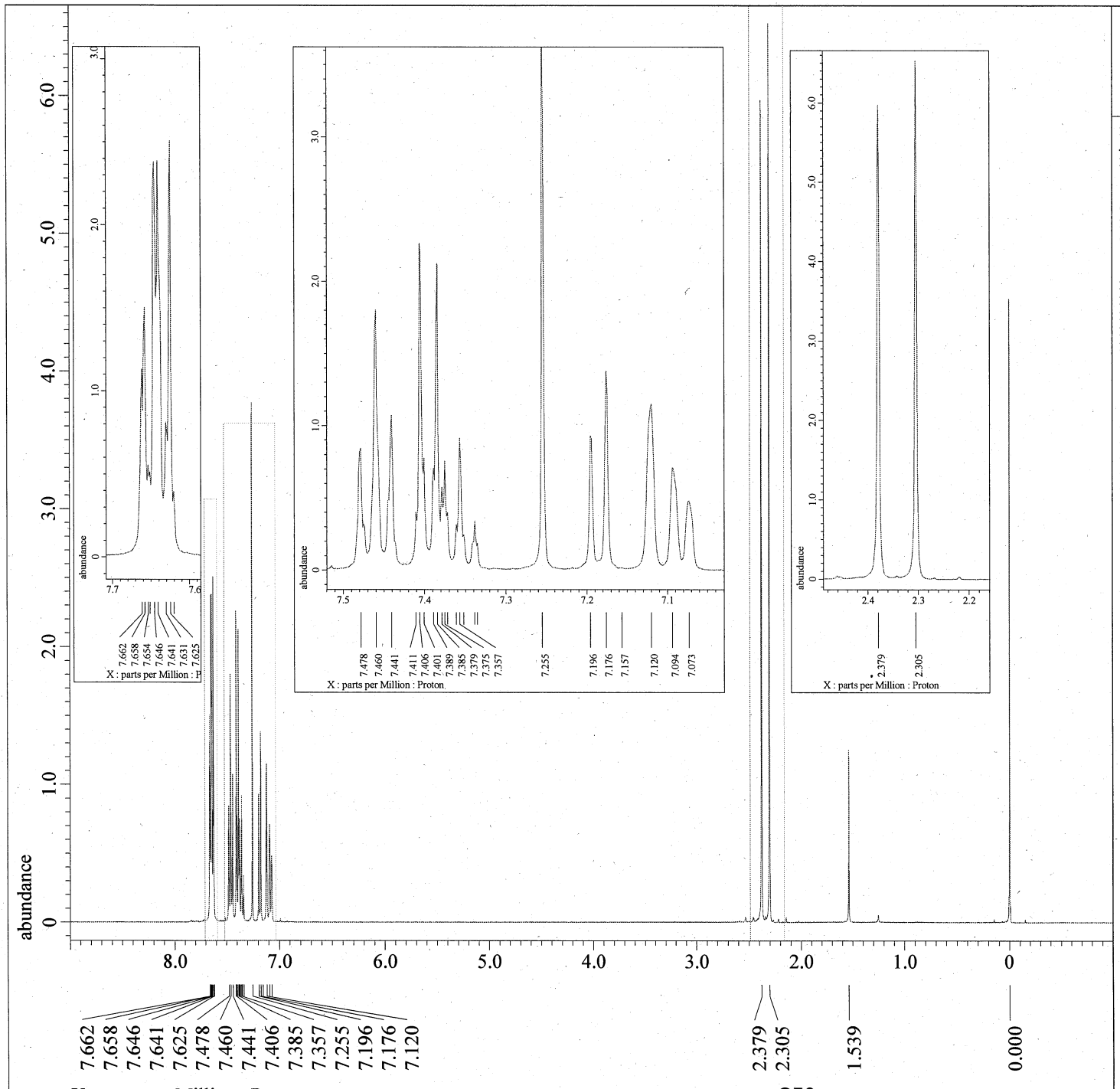
```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 0.2[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: Ph-Ph-Naph-1H-4_copy-1.jdf
```

```
Filename            = Ph-Ph-Naph-1H-4_copy-
Author              = element
Experiment          = single_pulse.ex2
Sample_id           = S#417615
Solvent             = CHLOROFORM-D
Creation_time       =  7-FEB-2019 10:02:42
Revision_time       =  7-FEB-2019 19:56:56
Current_time        =  7-FEB-2019 19:57:18

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
Incomplete_copy     = TRUE
Mod_return          = 1
Scans               = 5
Total_scans         = 5

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            = 18.5[dC]
```



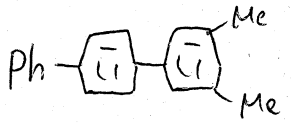
```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 2.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: Ph-Ph-Naph-13C-1.jdf
```

Filename	= Ph-Ph-Naph-13C-3.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_id	= S#397964
Solvent	= CHLOROFORM-D
Creation_time	= 19-JAN-2019 09:37:05
Revision_time	= 7-FEB-2019 19:57:57
Current_time	= 7-FEB-2019 19:58:32
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	= 114.0
Total_scans	= 114.0
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	= 19.2[dC]

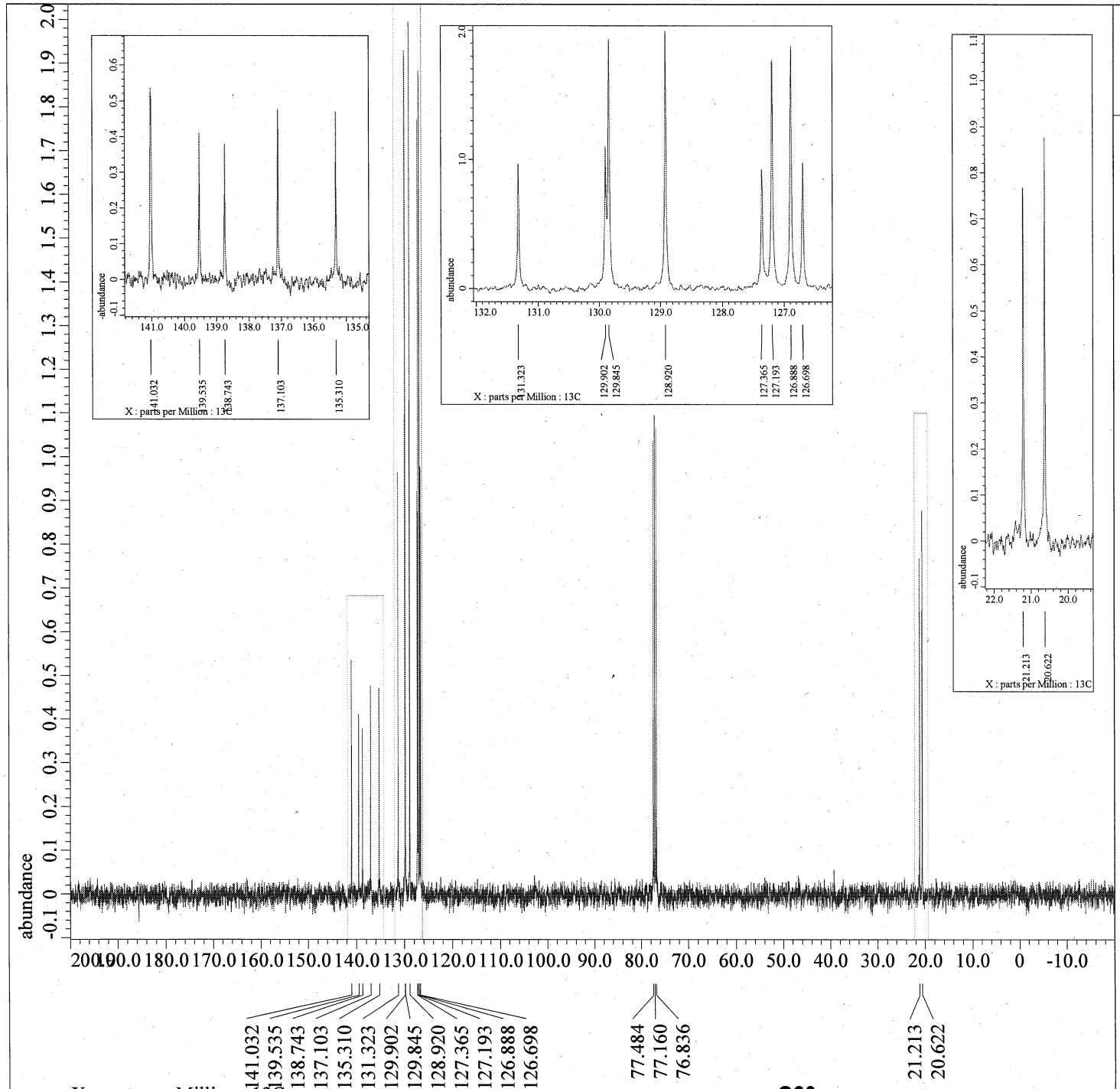


JEOL
Solutions for Innovation

Filename	= SEO-416-1-pure_Proton-1-
Author	= element
Experiment	= proton.jxp
Sample_Id	= SEO-416-1-pure
Solvent	= CHLOROFORM-D
Creation_Time	= 29-AUG-2018 09:28:04
Revision_Time	= 7-FEB-2019 19:23:53
Current_Time	= 7-FEB-2019 19:24:30
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECS400
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.37221[T] (400[MHz])
X_Acq_Duration	= 2.1889024[s]
X_Domain	= 1H
X_Freq	= 399.03472754[MHz]
X_Offset	= 5.0[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45684997[Hz]
X_Sweep	= 7.48502994[kHz]
X_Sweep_Clipped	= 5.98802395[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.03472754[MHz]
Irr_Offset	= 5.0[ppm]
Tri_Domain	= Proton
Tri_Freq	= 399.03472754[MHz]
Tri_Offset	= 5.0[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 44
Temp_Get	= 20.3[dC]
X_90_Width	= 6.6[us]
X_Acq_Time	= 2.1889024[s]
X_Angle	= 45[deg]
X_Atn	= 1[dB]
X_Pulse	= 3.3[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.1889024[s]

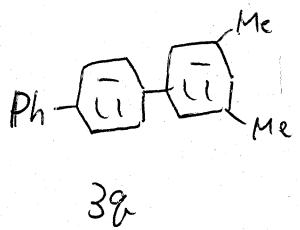


38

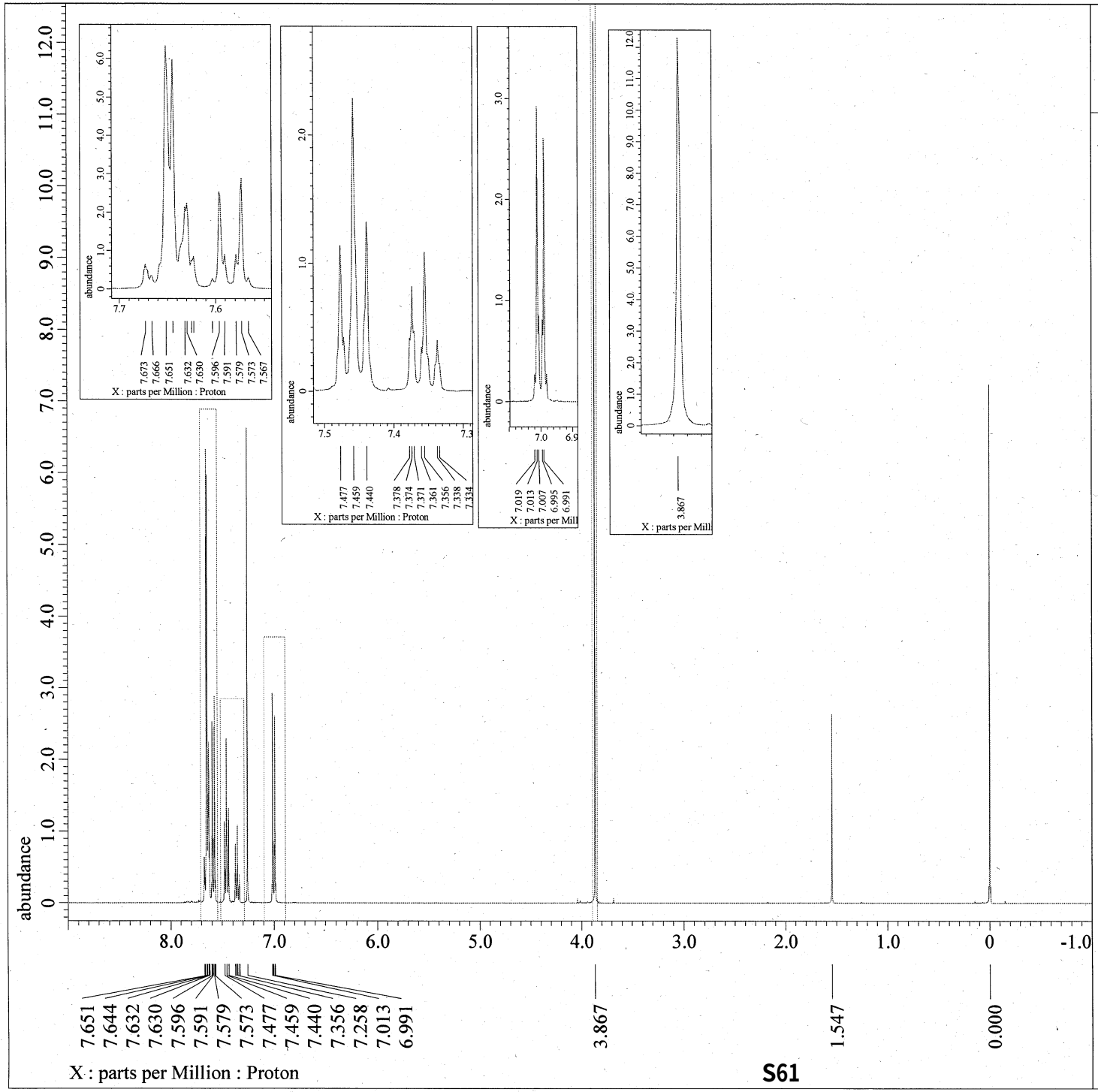


JEOL
Solutions for Innovation

Filename	= SEO-416-1-pure-13C-4.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= 1
Solvent	= CHLOROFORM-D
Creation_Time	= 29-AUG-2018 07:59:30
Revision_Time	= 7-FEB-2019 19:24:49
Current_Time	= 7-FEB-2019 19:26:31
Comment	= single pulse decoupled g
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[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	= 22
Total_Scans	= 22
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]
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]
Repetition_Time	= 3.06430464[s]

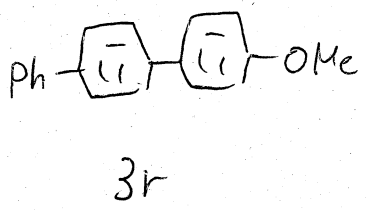


3g

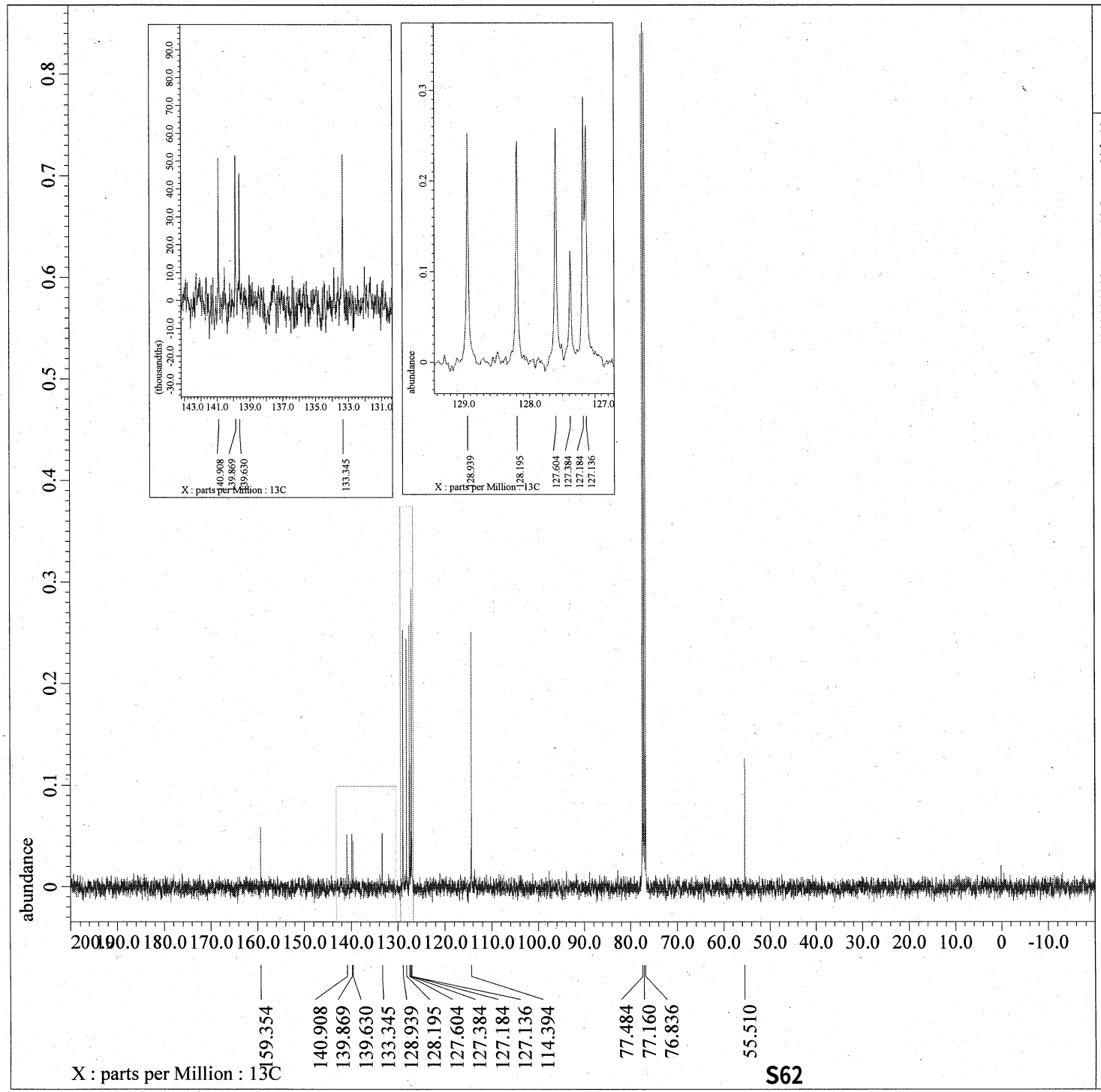


JEOL
Solutions for Innovation

```
Filename          = SEO-412-1-pure_Proton-1-
Author            = element
Experiment        = proton.jxp
Sample_Id         = SEO-412-1-pure
Solvent           = CHLOROFORM-D
Creation_Time     = 27-AUG-2018 11:30:21
Revision_Time     =  7-FEB-2019 19:32:08
Current_Time      =  7-FEB-2019 19:33:32

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

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

Relaxation_Delay  = 5[s]
Recvr_Gain        = 46
Temp_Get          = 19.2[dC]
X_90_Width        = 6.22[us]
X_Acq_Time        = 2.18103808[s]
X_Angle           = 45[deg]
X_Atn             = 0.8[dB]
X_Pulse           = 3.11[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 7.18103808[s]
```

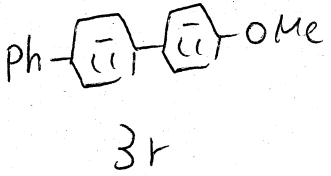


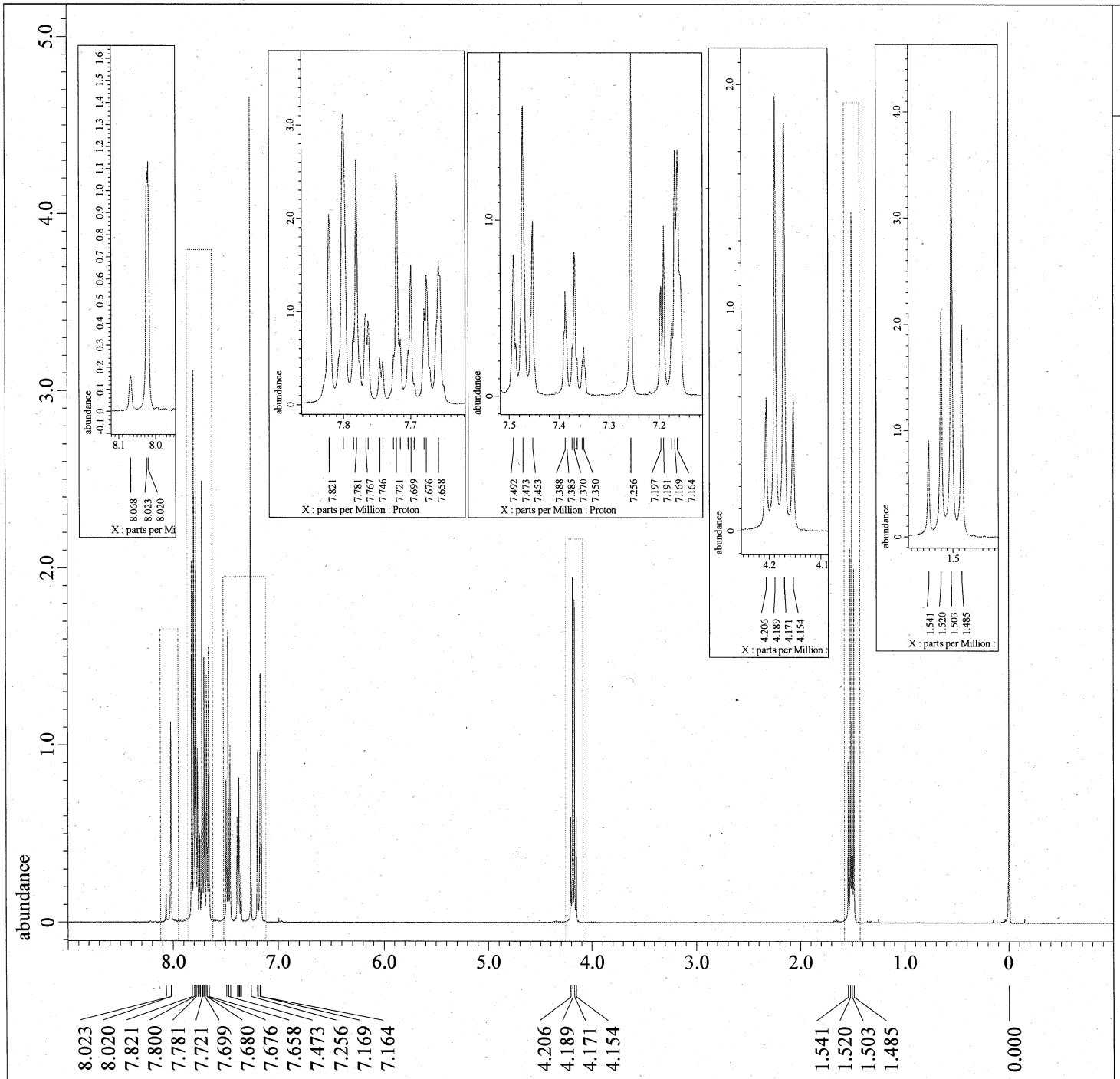
3r



JEOL
Solutions for Innovation

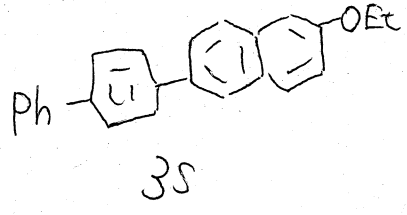
Filename	= SEO-412-1-pure-13C-4.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= 1
Solvent	= CHLOROFORM-D
Creation_Time	= 27-AUG-2018 10:17:24
Revision_Time	= 7-FEB-2019 19:33:50
Current_Time	= 7-FEB-2019 19:35:37
Comment	= single pulse decoupled g
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
Dim_Title	= 13C
Dim_Units	= [ppm]
Dimensions	= X
Site	= ECS 400
Spectrometer	= JNM-ECS400
Field_Strength	= 9.20197068[T] (390[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	= 200
Total_Scans	= 200
Relaxation_Delay	= 2[s]
Recvr_Gain	= 60
Temp_Get	= 21[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
Noe_Time	= 2[s]
Repetition_Time	= 3.06430464[s]

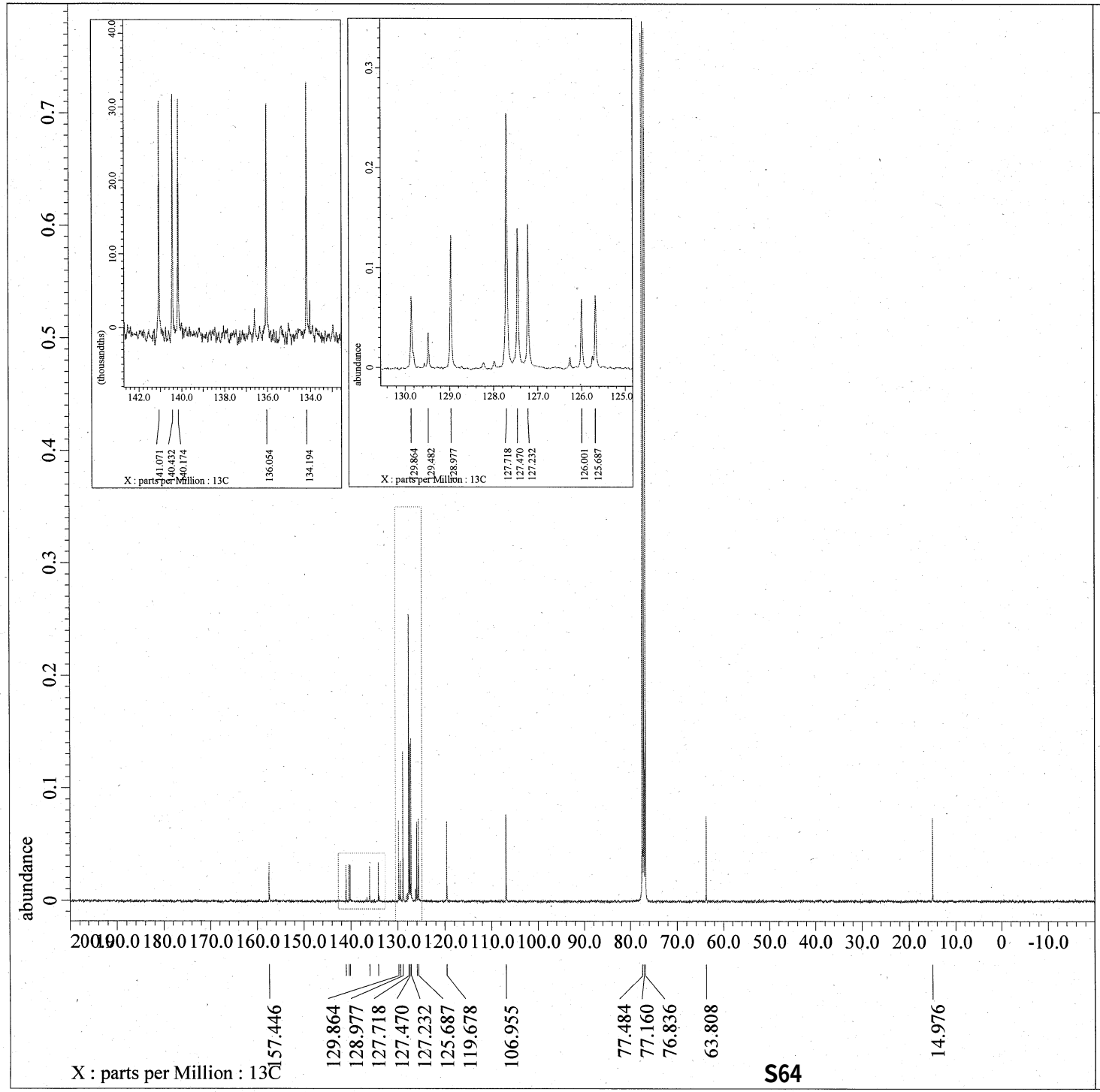




JEOL
Solutions for Innovation

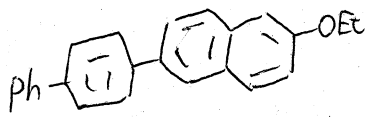
```
Filename          = SEO-452-2-pure_Proton-1-
Author            = element
Experiment        = proton.jxp
Sample_Id         = SEO-452-2-pure
Solvent           = CHLOROFORM-D
Creation_Time     = 10-OCT-2018 15:52:17
Revision_Time     =  7-FEB-2019 19:37:16
Current_Time      =  7-FEB-2019 19:39:27

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

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

Relaxation_Delay  = 5[s]
Recvr_Gain        = 44
Temp_Get          = 19.5[dC]
X_90_Width        = 6.6[us]
X_Acq_Time        = 2.1889024[s]
X_Angle           = 45[deg]
X_Atn             = 1[dB]
X_Pulse           = 3.3[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 7.1889024[s]
```


OEt
Ph
3s

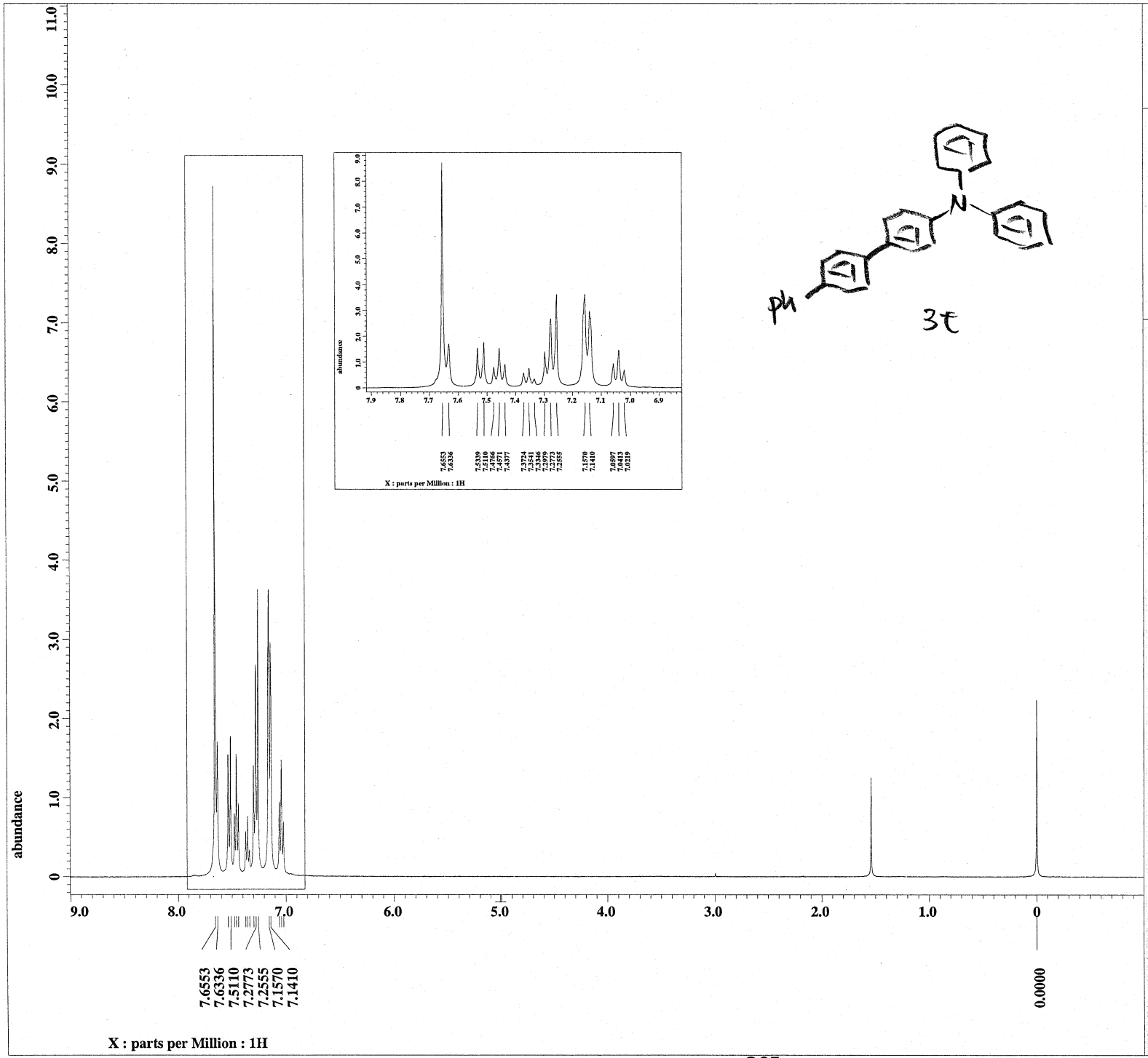


JEOL
Solutions for Innovation

```
Filename          = SEO-452-2-pure-13C-7.jdf
Author            = element
Experiment        = single_pulse_dec
Sample_Id         = S#699612
Solvent           = CHLOROFORM-D
Creation_Time     = 15-JAN-2019 07:21:49
Revision_Time     =  7-FEB-2019 19:44:21
Current_Time      =  7-FEB-2019 19:44:55

Comment           = single pulse decoupled g
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[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             = 15787
Total_Scans       = 15787

Relaxation_Delay  = 2[s]
Recvr_Gain        = 60
Temp_Get          = 55[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
Noe_Time          = 2[s]
Repetition_Time   = 3.06430464[s]
```



3S

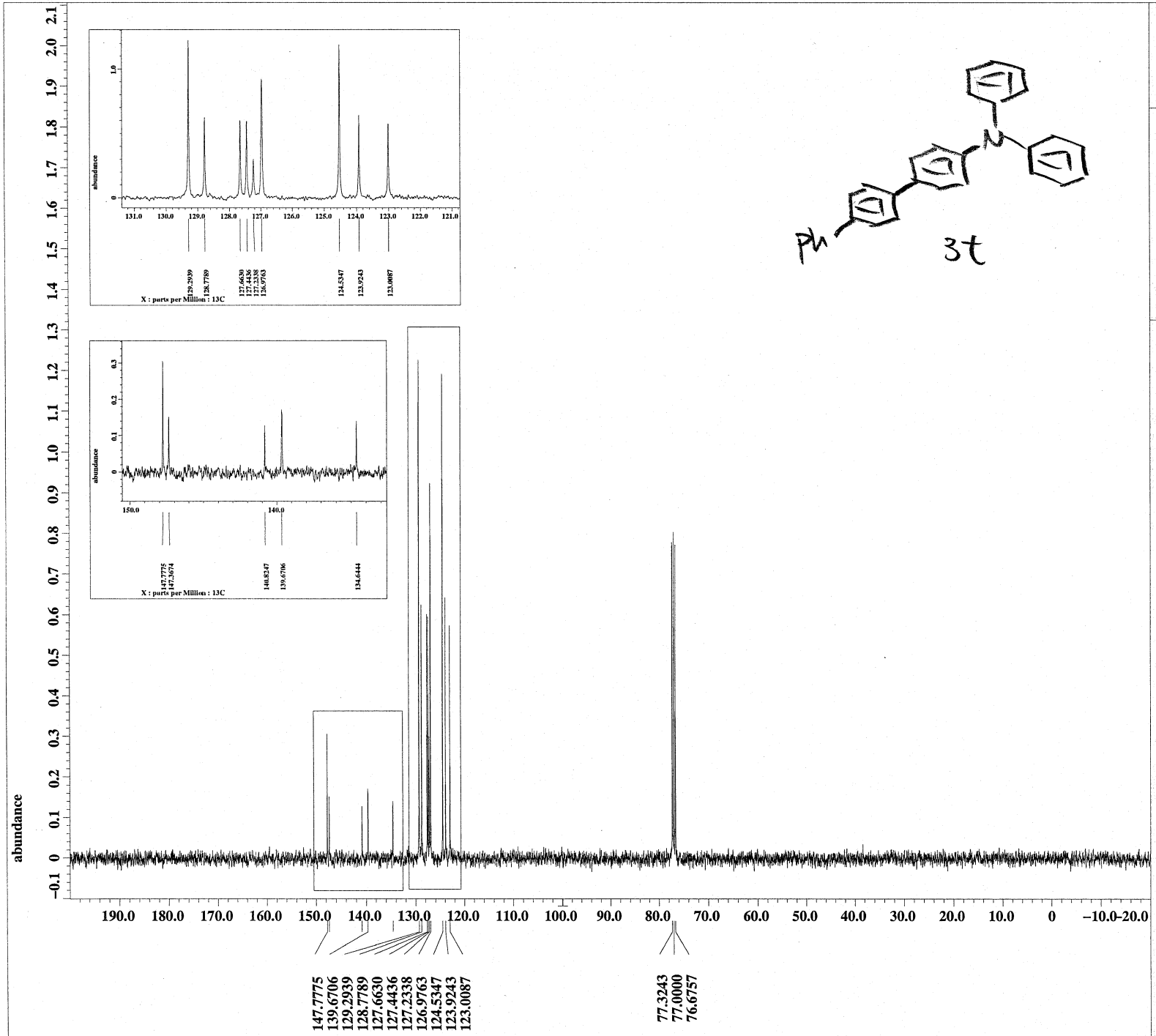


3t

---- 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

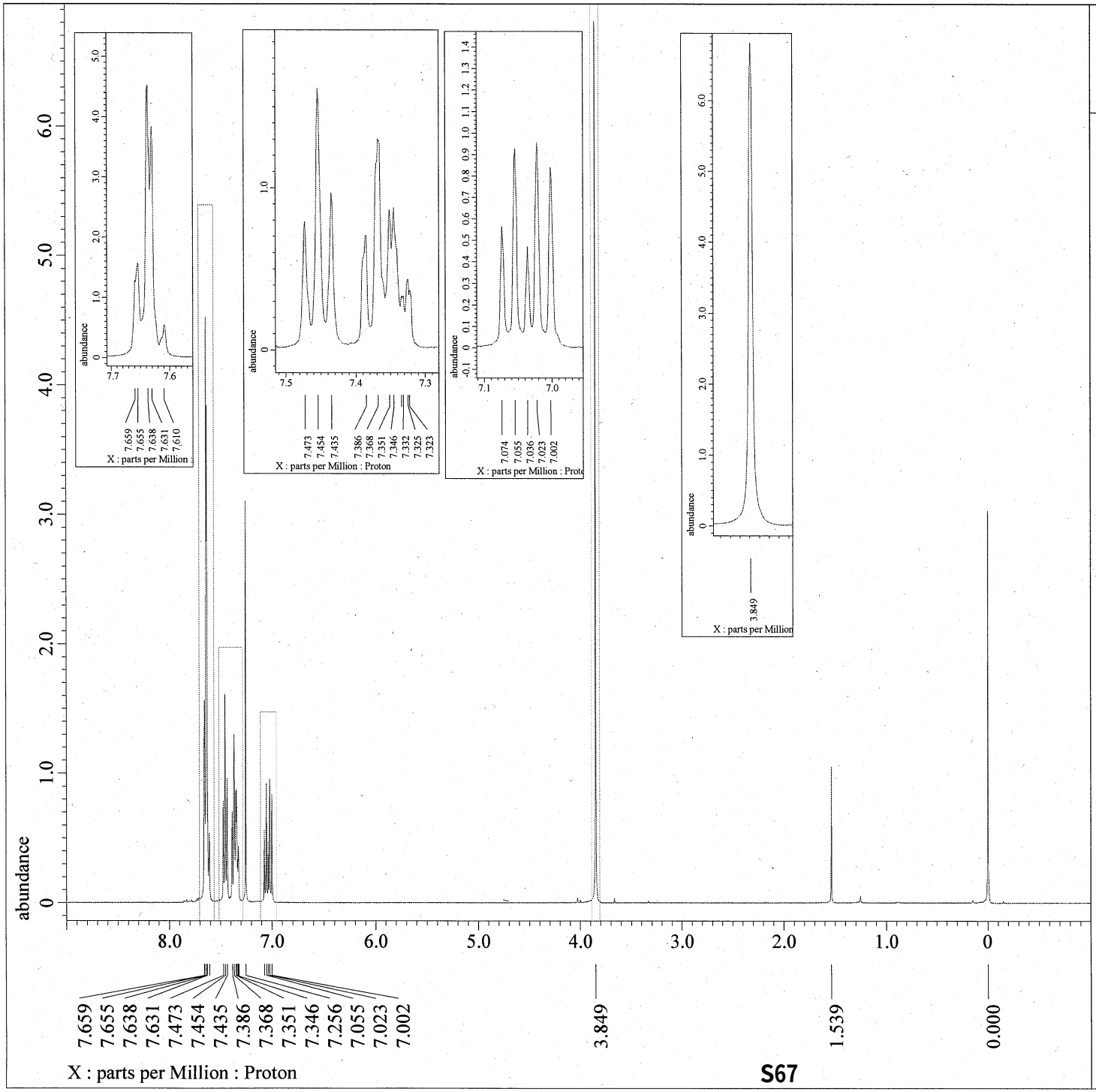
Derived from: Ph-Ph-Ph-NPh2-1H-1.jdf

Filename	= Ph-Ph-Ph-NPh2-1H-3.jd
Author	= element
Experiment	= single_pulse.ex2
Sample_id	= S#728110
Solvent	= CHLOROFORM-D
Creation_time	= 16-JAN-2019 18:43:38
Revision_time	= 7-FEB-2019 19:59:43
Current_time	= 7-FEB-2019 20:01:01
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	= 18.8[dC]



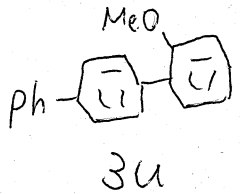

```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 2.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: Ph-Ph-Ph-NPh2-13c-1.jdf
```

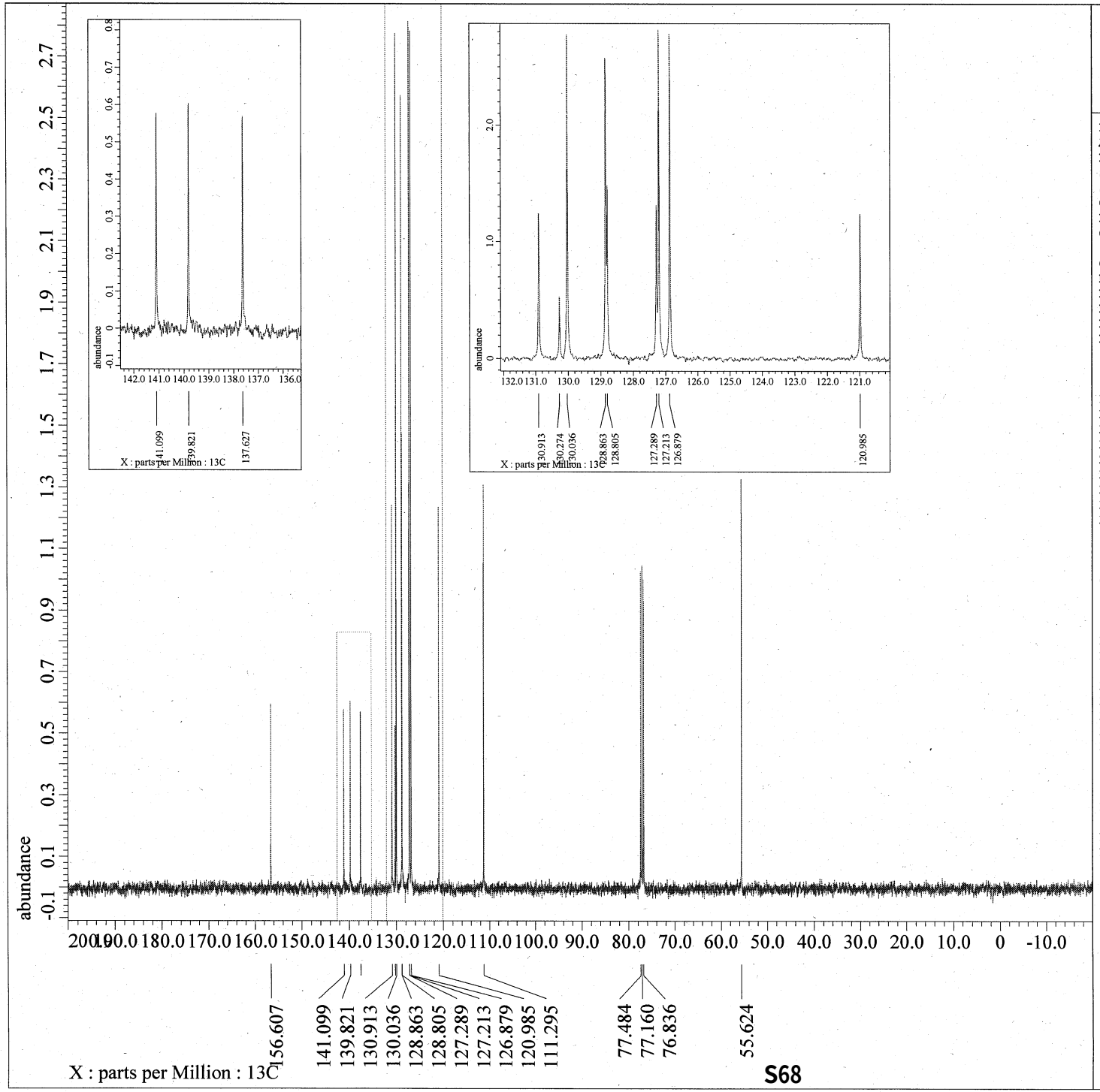
Filename	= Ph-Ph-Ph-NPh2-13c-3.j
Author	= element
Experiment	= single_pulse_dec
Sample_id	= S#735129
Solvent	= CHLOROFORM-D
Creation_time	= 16-JAN-2019 18:57:07
Revision_time	= 7-FEB-2019 20:01:21
Current_time	= 7-FEB-2019 20:02:52
Comment	= single pulse decouple
Data_format	= 1D COMPLEX
Dim_size	= 26214
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	= 57
Total_scans	= 57
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	= 50[dC]



JEOL
Solutions for Innovation

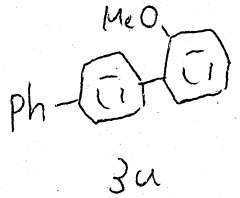
Filename	= SEO-415-1-pure_Proton-1-
Author	= element
Experiment	= proton.jxp
Sample_Id	= SEO-415-1-pure
Solvent	= CHLOROFORM-D
Creation_Time	= 29-AUG-2018 09:22:45
Revision_Time	= 7-FEB-2019 19:49:58
Current_Time	= 7-FEB-2019 19:51:11
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECS400
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.37221[T] (400[MHz])
X_Acq_Duration	= 2.1889024[s]
X_Domain	= 1H
X_Freq	= 399.03472754[MHz]
X_Offset	= 5.0[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45684997[Hz]
X_Sweep	= 7.48502994[kHz]
X_Sweep_Clipped	= 5.98802395[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.03472754[MHz]
Irr_Offset	= 5.0[ppm]
Tri_Domain	= Proton
Tri_Freq	= 399.03472754[MHz]
Tri_Offset	= 5.0[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 46
Temp_Get	= 20.3[dC]
X_90_Width	= 6.6[us]
X_Acq_Time	= 2.1889024[s]
X_Angle	= 45[deg]
X_Atn	= 1[dB]
X_Pulse	= 3.3[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.1889024[s]



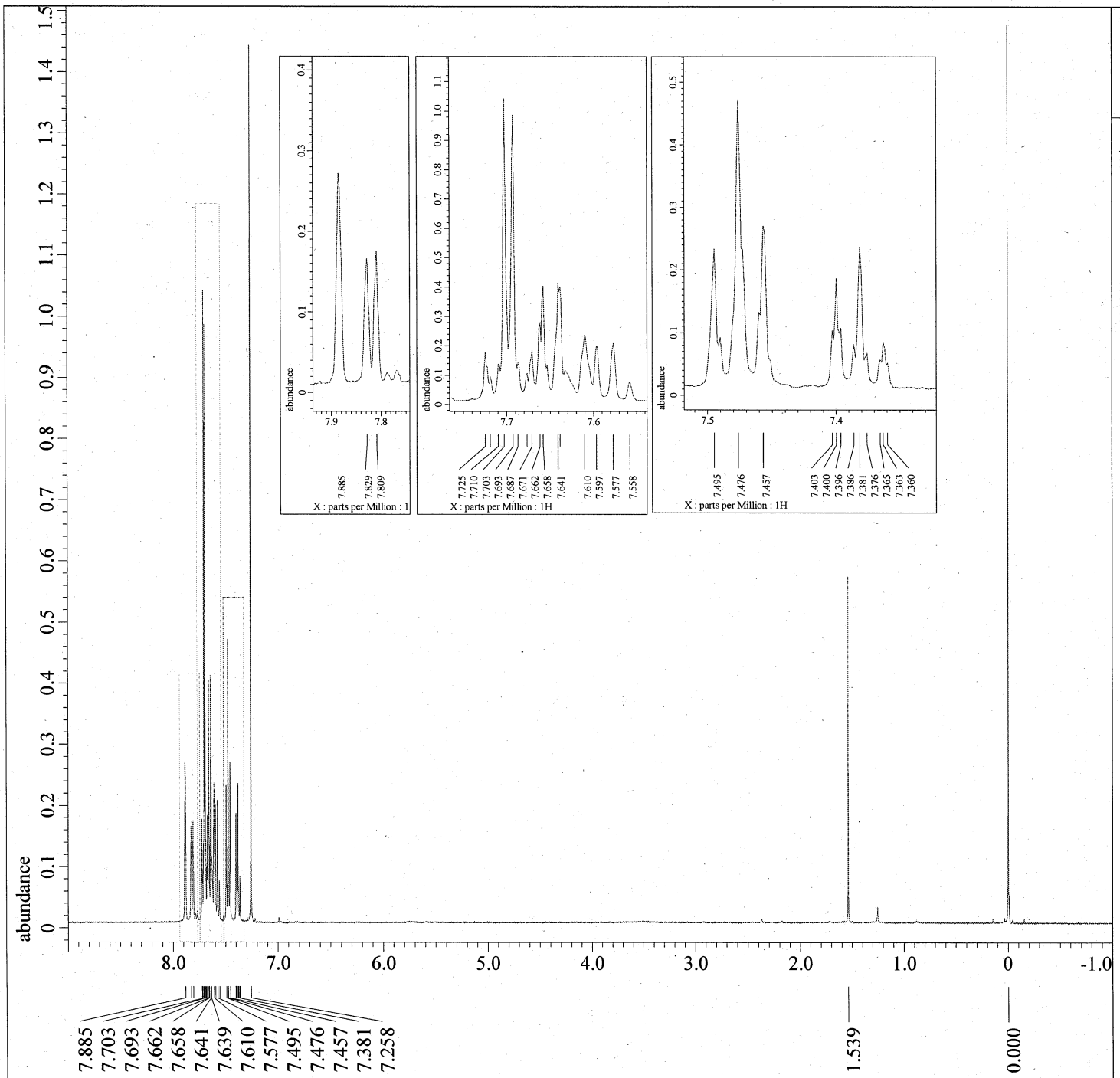


JEOL
Solutions for Innovation

Filename	= SEO-415-1-pure-13C-4.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= 1
Solvent	= CHLOROFORM-D
Creation_Time	= 29-AUG-2018 07:51:54
Revision_Time	= 7-FEB-2019 19:51:30
Current_Time	= 7-FEB-2019 19:53:49
Comment	= single pulse decoupled g
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[MHz])
X_Acq_Duration	= 1.06430464[s]
X_Domain	= 13C
X_Freq	= 98.51479726[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.93958061[Hz]
X_Sweep	= 30.78817734[kHz]
Irr_Domain	= 1H
Irr_Freq	= 391.78655441[MHz]
Irr_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 38
Total_Scans	= 38
Relaxation_Delay	= 2[s]
Recvr_Gain	= 60
Temp_Get	= 20.7[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
Noe_Time	= 2[s]
Repetition_Time	= 3.06430464[s]

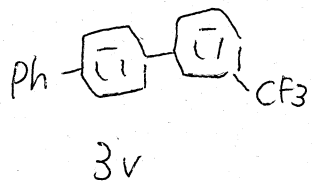


3u

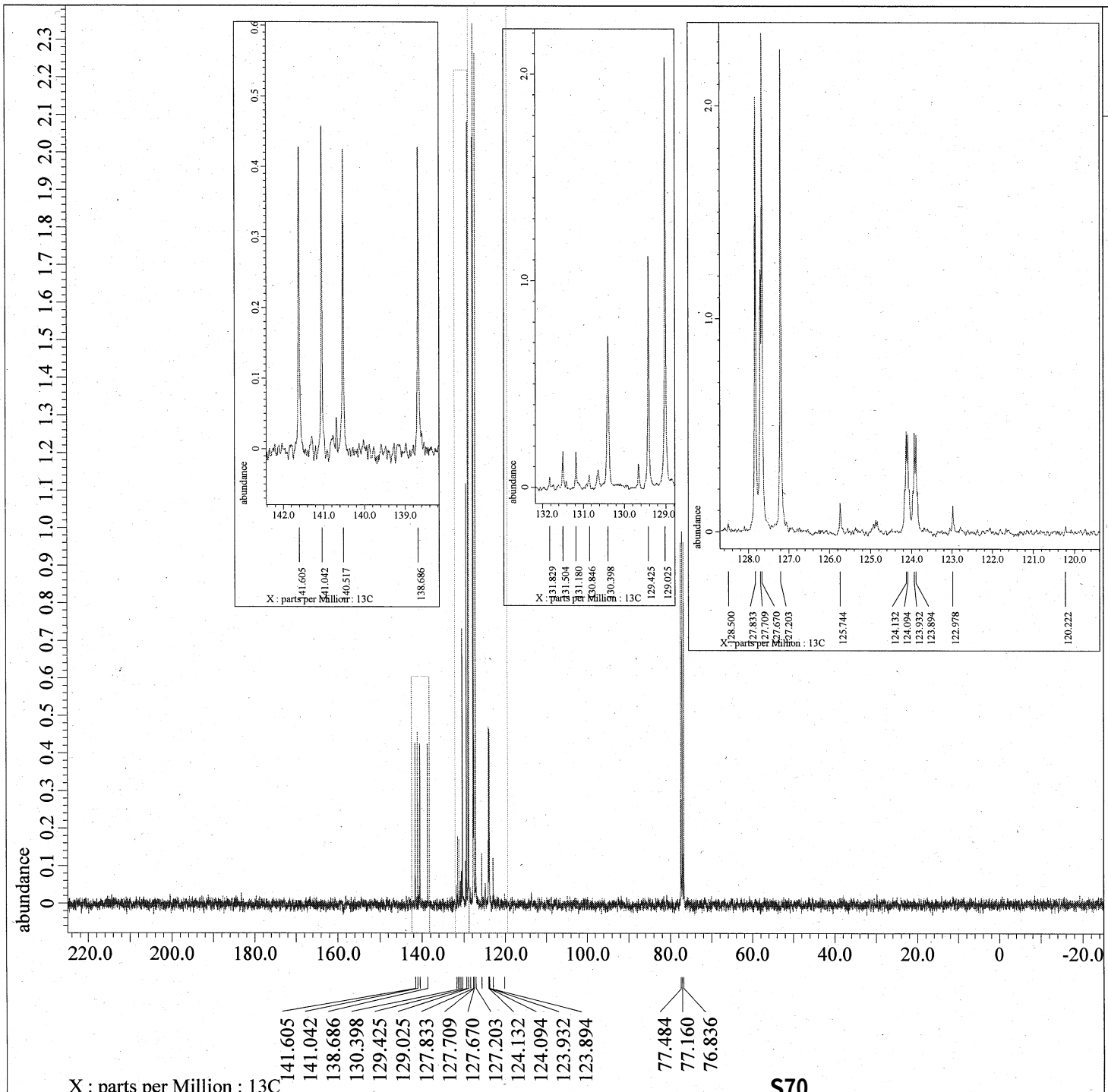


JEOL
Solutions for Innovation

Filename	= SEO-427-1-pure-4.jdf
Author	= element
Experiment	= single_pulse.ex2
Sample_Id	= S#521416
Solvent	= CHLOROFORM-D
Creation_Time	= 4-SEP-2018 14:04:08
Revision_Time	= 7-FEB-2019 19:55:46
Current_Time	= 7-FEB-2019 19:57:05
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
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	= 22.2[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	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.20725248[s]

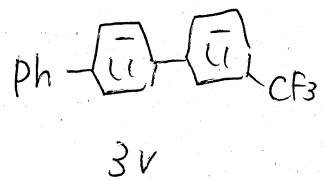


3v

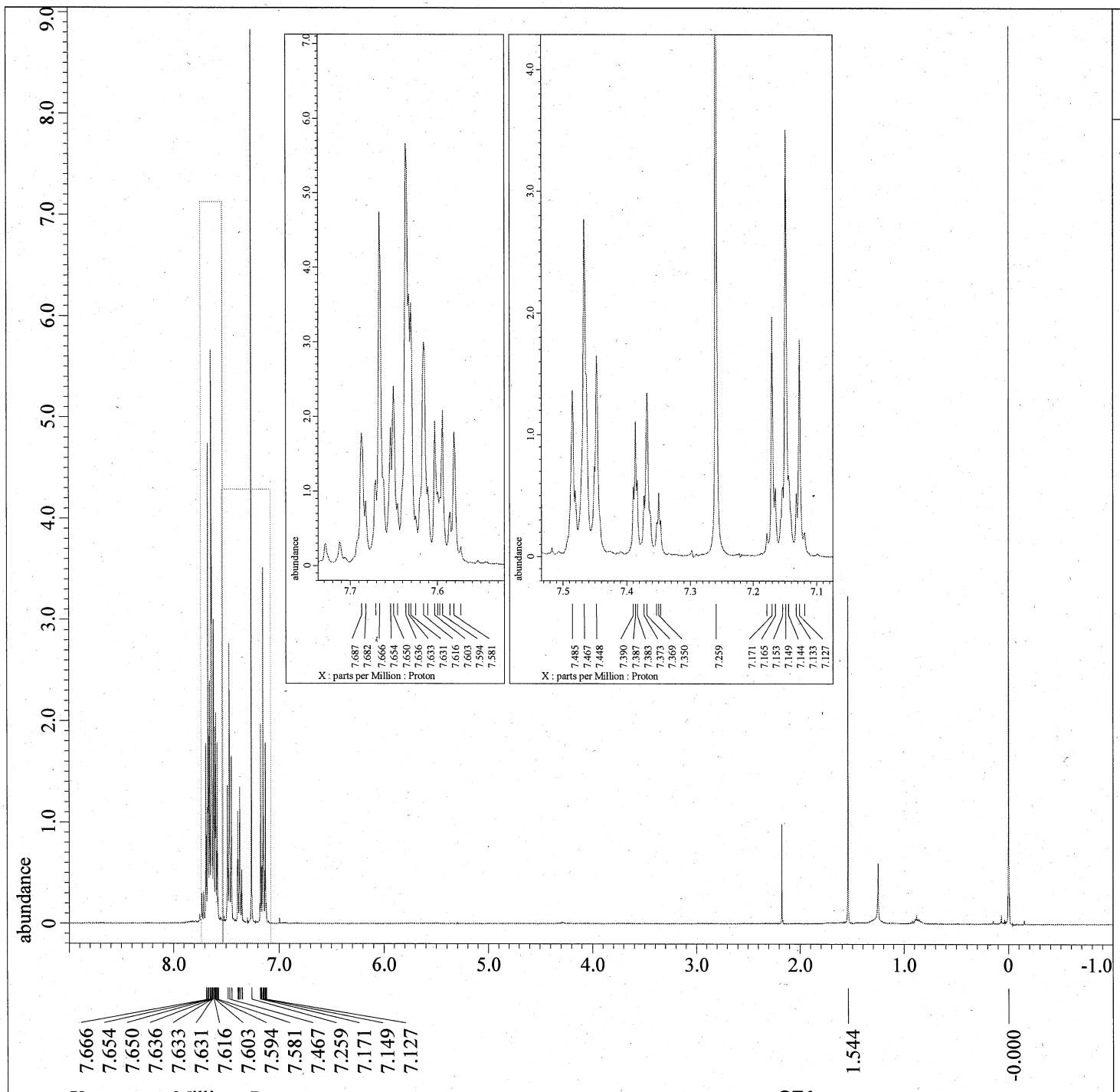


JEOL
Solutions for Innovation

Filename	= SEO-427-1-pure-13C-4.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= 1
Solvent	= CHLOROFORM-D
Creation_Time	= 4-SEP-2018 13:43:59
Revision_Time	= 7-FEB-2019 20:02:53
Current_Time	= 7-FEB-2019 20:03:07
Comment	= single pulse decoupled g
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[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	= 66
Total_Scans	= 66
Relaxation_Delay	= 2[s]
Recvr_Gain	= 60
Temp_Get	= 21.3[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
Noe_Time	= 2[s]
Repetition_Time	= 3.06430464[s]

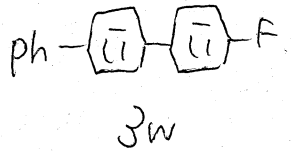


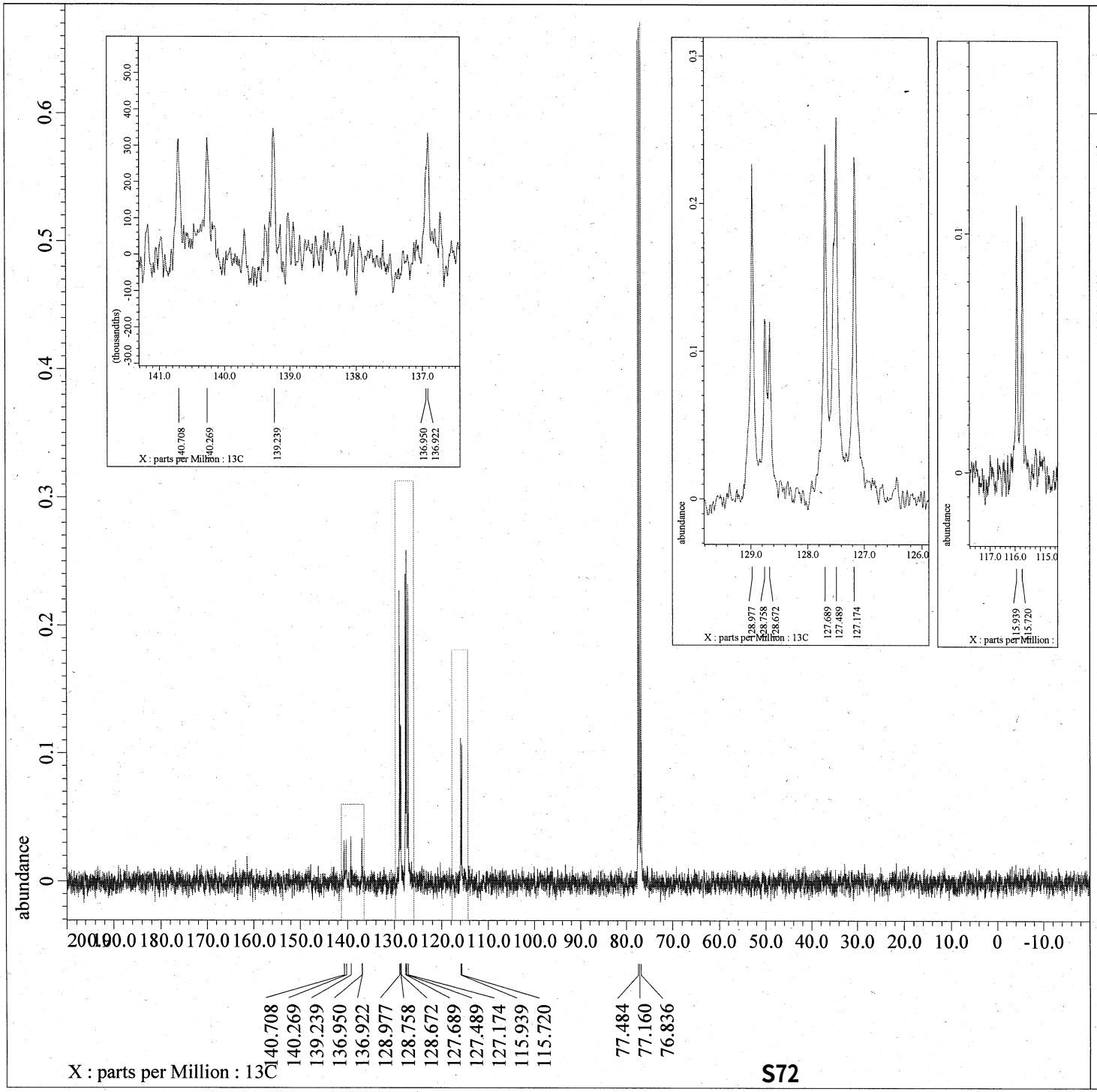
3v



JEOL
Solutions for Innovation

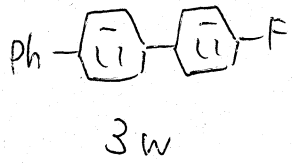
Filename	= SEO-456-1-pure_Proton-1-
Author	= element
Experiment	= proton.jxp
Sample_Id	= SEO-456-1-pure
Solvent	= CHLOROFORM-D
Creation_Time	= 12-OCT-2018 08:54:22
Revision_Time	= 7-FEB-2019 20:05:51
Current_Time	= 7-FEB-2019 20:06:39
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
Dim_Title	= 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	= 19.6[dC]
X_90_Width	= 6.22[us]
X_Acq_Time	= 2.18103808[s]
X_Angle	= 45[deg]
X_Atn	= 0.8[dB]
X_Pulse	= 3.11[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.18103808[s]



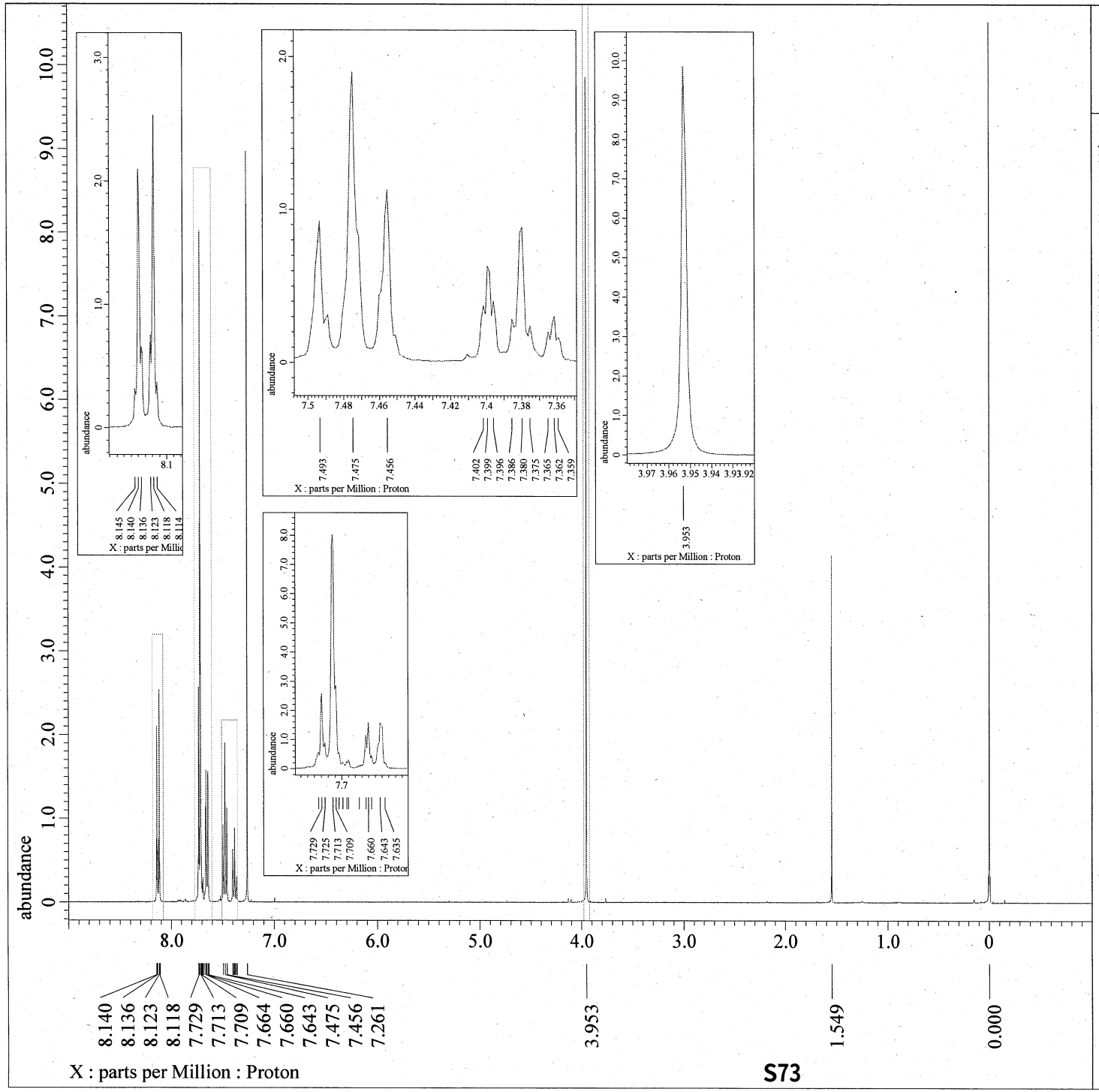


JEOL Solutions for Innovation

Filename	= SEO-456-1-pure-13C-4.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= 1
Solvent	= CHLOROFORM-D
Creation_Time	= 12-OCT-2018 08:06:24
Revision_Time	= 7-FEB-2019 20:09:12
Current_Time	= 7-FEB-2019 20:09:45
Comment	= single pulse decoupled g
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[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	= 200
Total_Scans	= 200
Relaxation_Delay	= 2[s]
Recvr_Gain	= 60
Temp_Get	= 19.7[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
Noe_Time	= 2[s]
Repetition_Time	= 3.06430464[s]

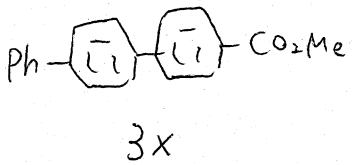


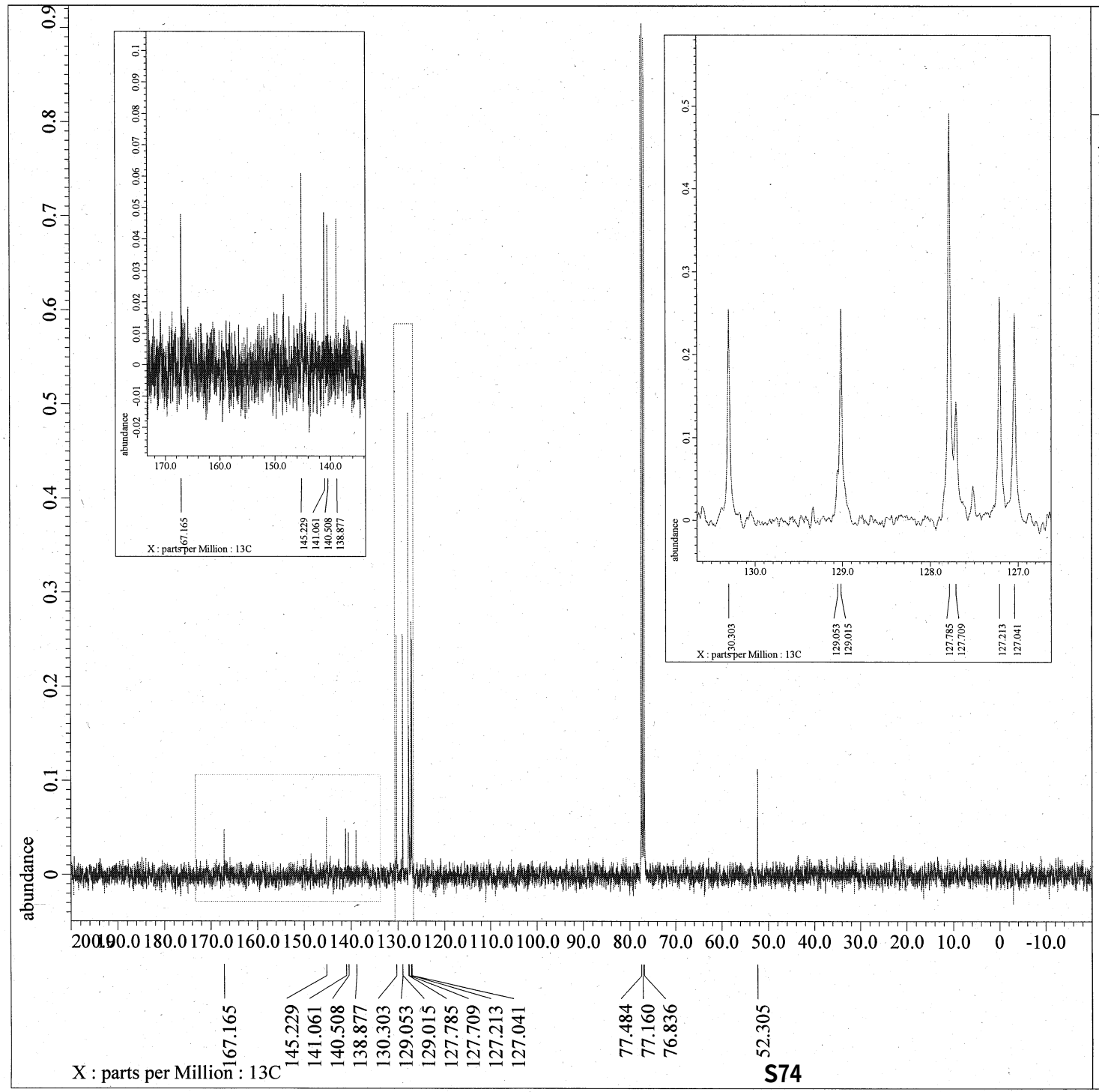
3w



JEOL
Solutions for Innovation

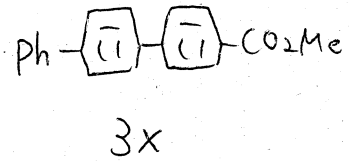
Filename	= SEO-418-1-pure_Proton-1-
Author	= element
Experiment	= proton.jxp
Sample_Id	= SEO-418-1-pure
Solvent	= CHLOROFORM-D
Creation_Time	= 29-AUG-2018 20:14:24
Revision_Time	= 7-FEB-2019 20:11:46
Current_Time	= 7-FEB-2019 20:16:04
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECS400
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.37221[T] (400[MHz])
X_Acq_Duration	= 2.1889024[s]
X_Domain	= 1H
X_Freq	= 399.03472754[MHz]
X_Offset	= 5.0[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45684997[Hz]
X_Sweep	= 7.48502994[kHz]
X_Sweep_Clipped	= 5.98802395[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.03472754[MHz]
Irr_Offset	= 5.0[ppm]
Tri_Domain	= Proton
Tri_Freq	= 399.03472754[MHz]
Tri_Offset	= 5.0[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 50
Temp_Get	= 20.4[dC]
X_90_Width	= 6.6[us]
X_Acq_Time	= 2.1889024[s]
X_Angle	= 45[deg]
X_Atn	= 1[dB]
X_Pulse	= 3.3[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.1889024[s]



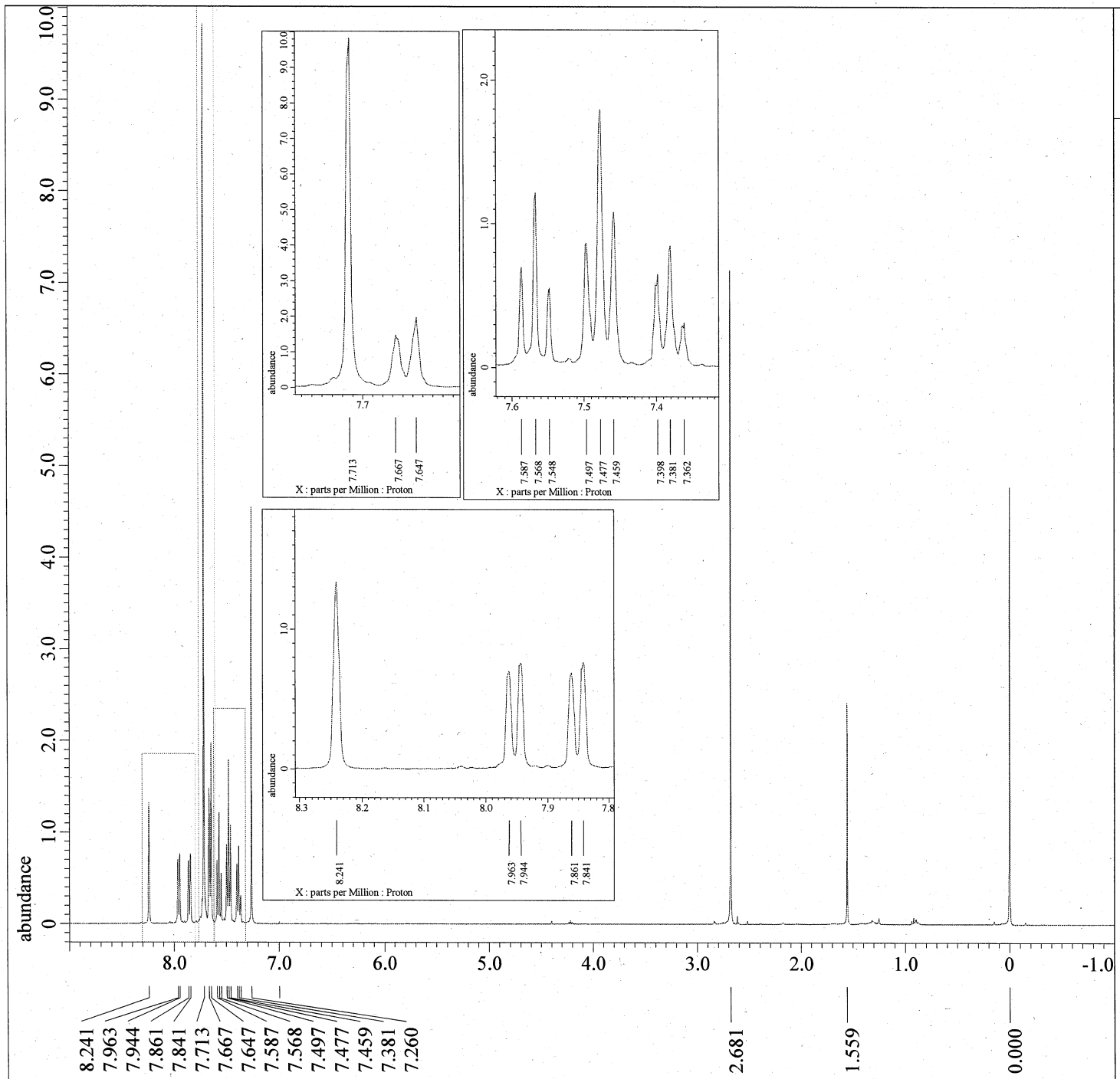


JEOL
Solutions for Innovation

Filename	= SEO-418-1-pure-13C-7.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= 1
Solvent	= CHLOROFORM-D
Creation_Time	= 29-AUG-2018 18:43:45
Revision_Time	= 7-FEB-2019 20:20:31
Current_Time	= 7-FEB-2019 20:21:27
Comment	= single pulse decoupled g
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[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	= 100
Total_Scans	= 100
Relaxation_Delay	= 2[s]
Recvr_Gain	= 60
Temp_Get	= 21[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
Noe_Time	= 2[s]
Repetition_Time	= 3.06430464[s]

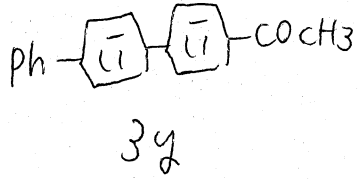


3x

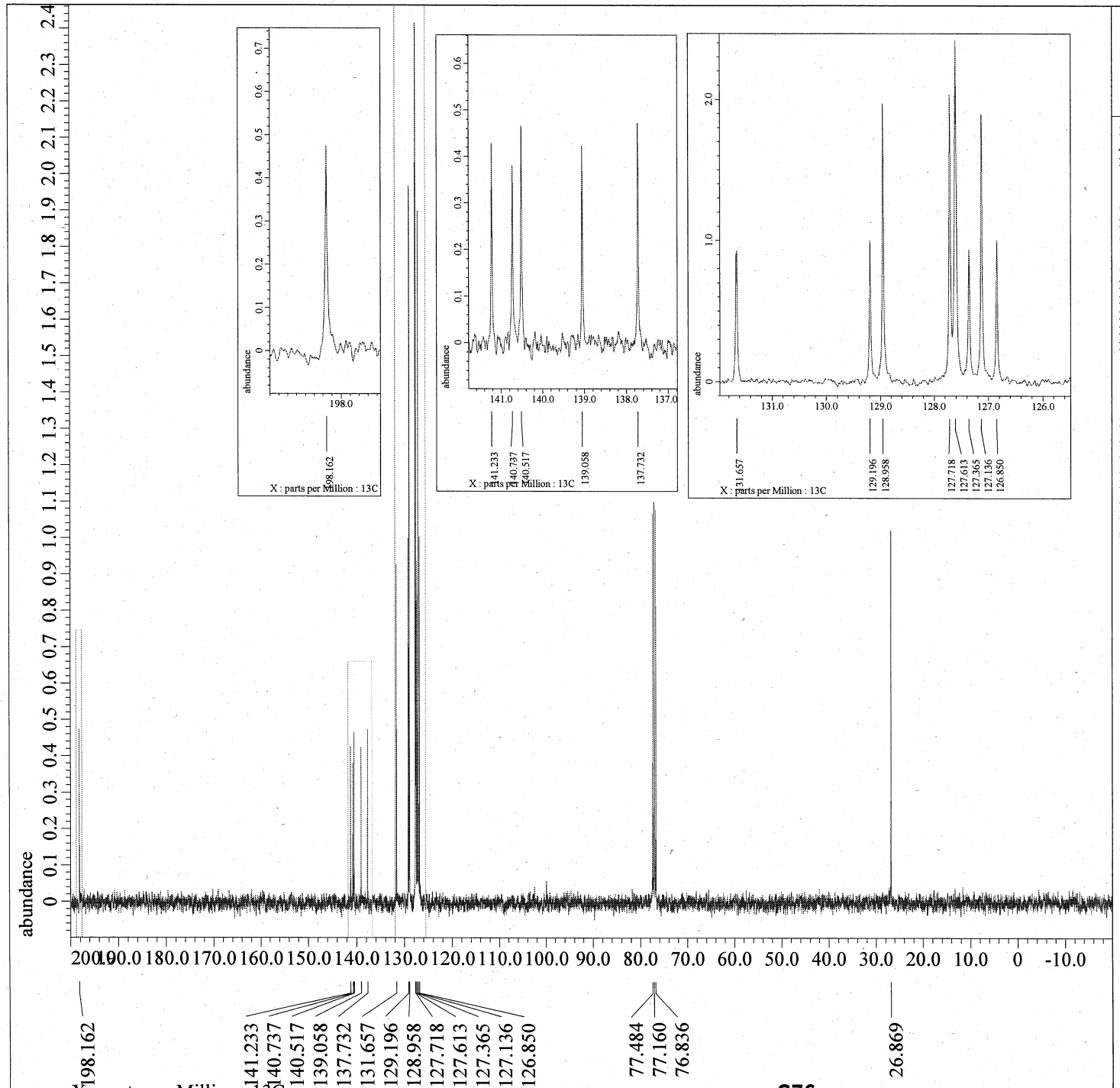


JEOL
Solutions for Innovation

Filename	= SEO-420-1-pure_Proton-1-
Author	= element
Experiment	= proton.jxp
Sample_Id	= SEO-420-1-pure
Solvent	= CHLOROFORM-D
Creation_Time	= 31-AUG-2018 10:07:11
Revision_Time	= 7-FEB-2019 20:25:33
Current_Time	= 7-FEB-2019 20:26:03
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
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	= 19.3[dC]
X_90_Width	= 6.22[us]
X_Acq_Time	= 2.18103808[s]
X_Angle	= 45[deg]
X_Atn	= 0.8[dB]
X_Pulse	= 3.11[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.18103808[s]

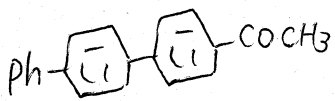


3y

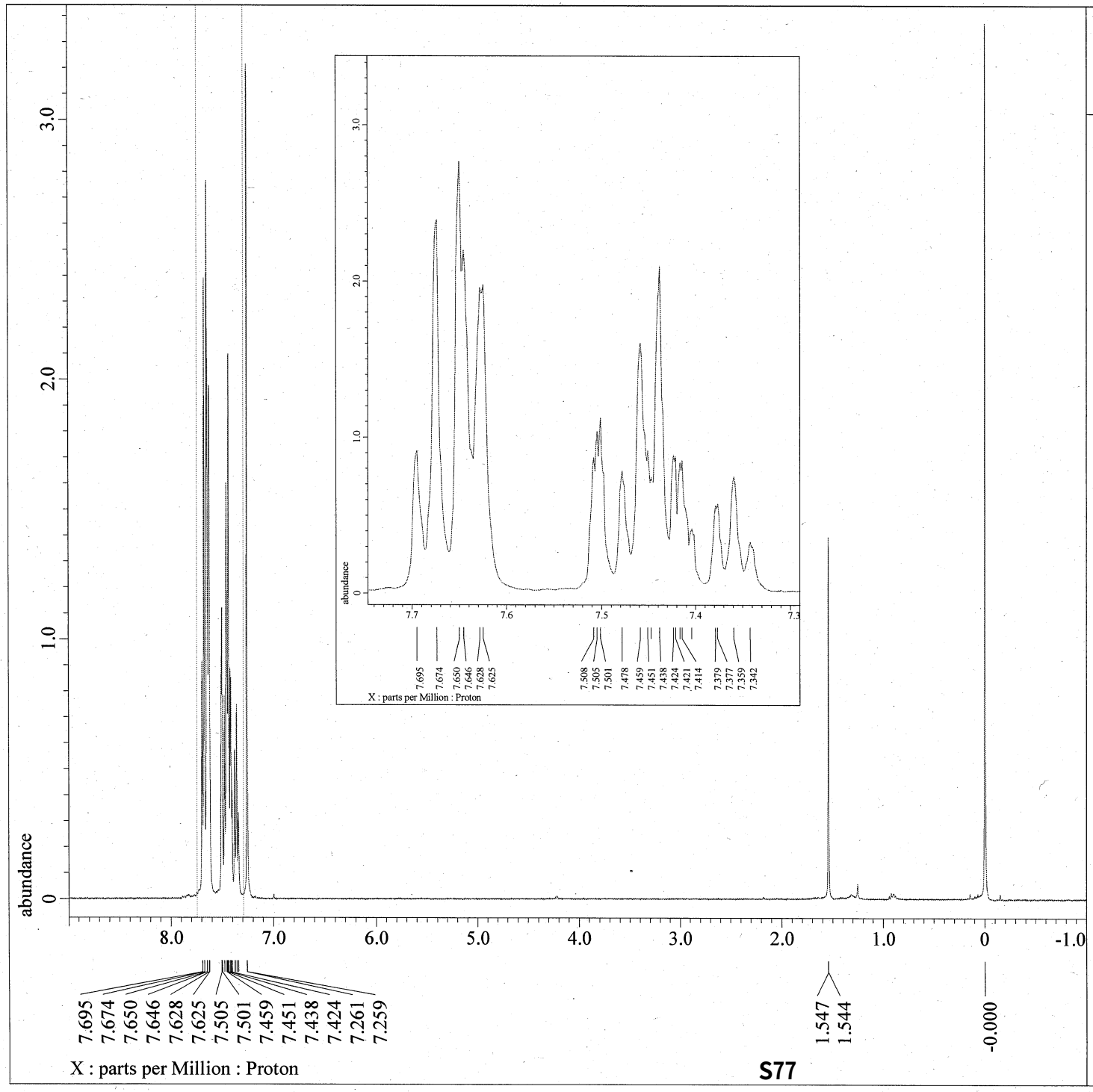


JEOL
Solutions for Innovation

Filename	= SEO-420-1-pure-13C-4.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= 1
Solvent	= CHLOROFORM-D
Creation_Time	= 31-AUG-2018 08:36:25
Revision_Time	= 7-FEB-2019 20:26:20
Current_Time	= 7-FEB-2019 20:27:43
Comment	= single pulse decoupled g
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[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	= 20.9[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_Noe	= 22.255[dB]
Irr_Noise	= WALTZ
Decoupling	= TRUE
Initial_Wait	= 1[s]
Noe	= TRUE
Noe_Time	= 2[s]
Repetition_Time	= 3.06430464[s]

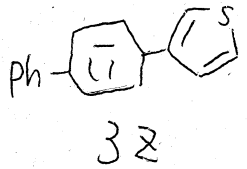


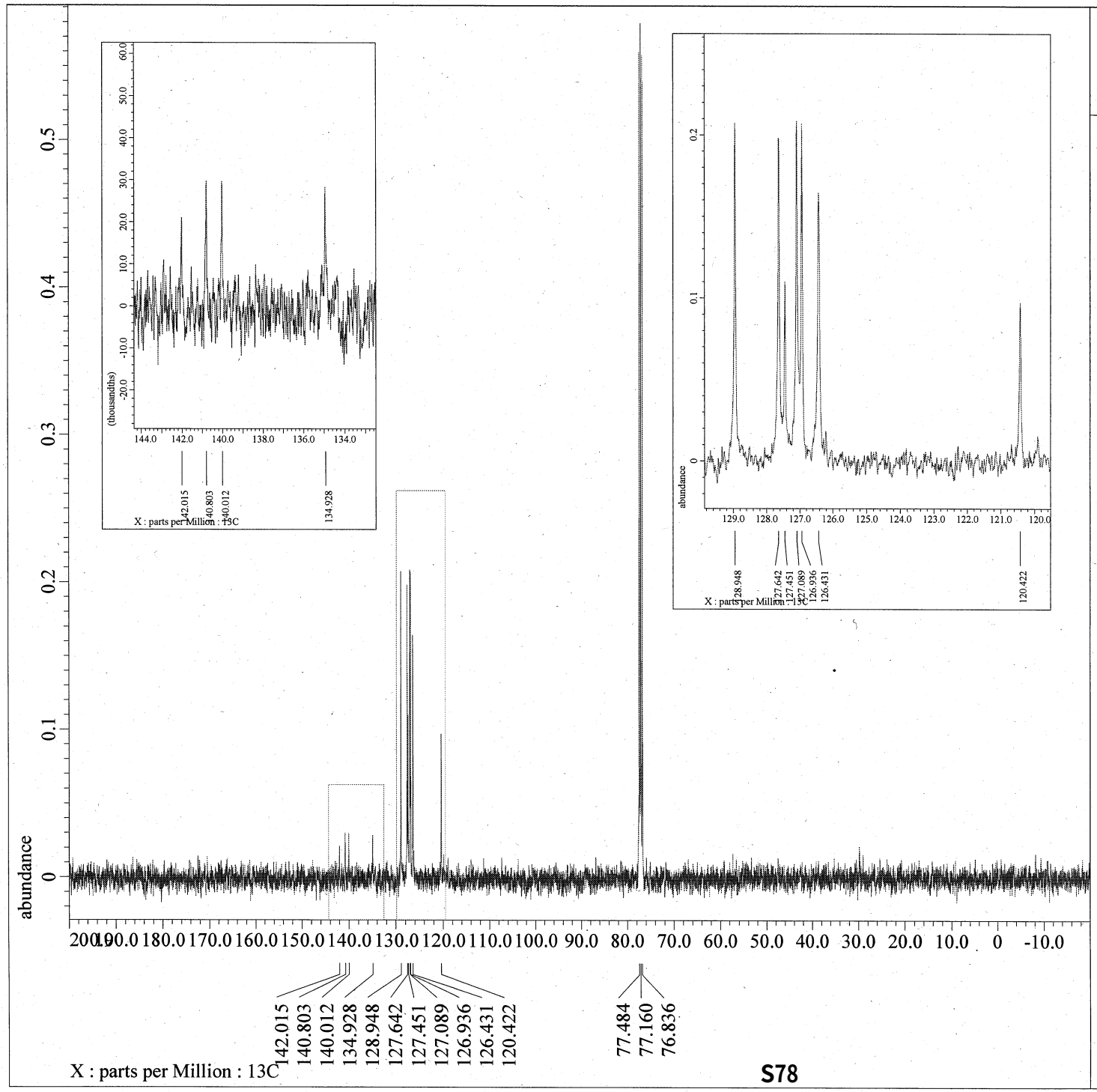
3y



JEOL
Solutions for Innovation

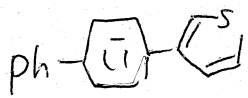
Filename	= SEO-419-1-pure_Proton-1-
Author	= element
Experiment	= proton.jxp
Sample_Id	= SEO-419-1-pure
Solvent	= CHLOROFORM-D
Creation_Time	= 31-AUG-2018 09:12:39
Revision_Time	= 7-FEB-2019 20:29:47
Current_Time	= 7-FEB-2019 20:30:37
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
Dim_Title	= 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[dC]
X_90_Width	= 6.22[us]
X_Acq_Time	= 2.18103808[s]
X_Angle	= 45[deg]
X_Atn	= 0.8[dB]
X_Pulse	= 3.11[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.18103808[s]



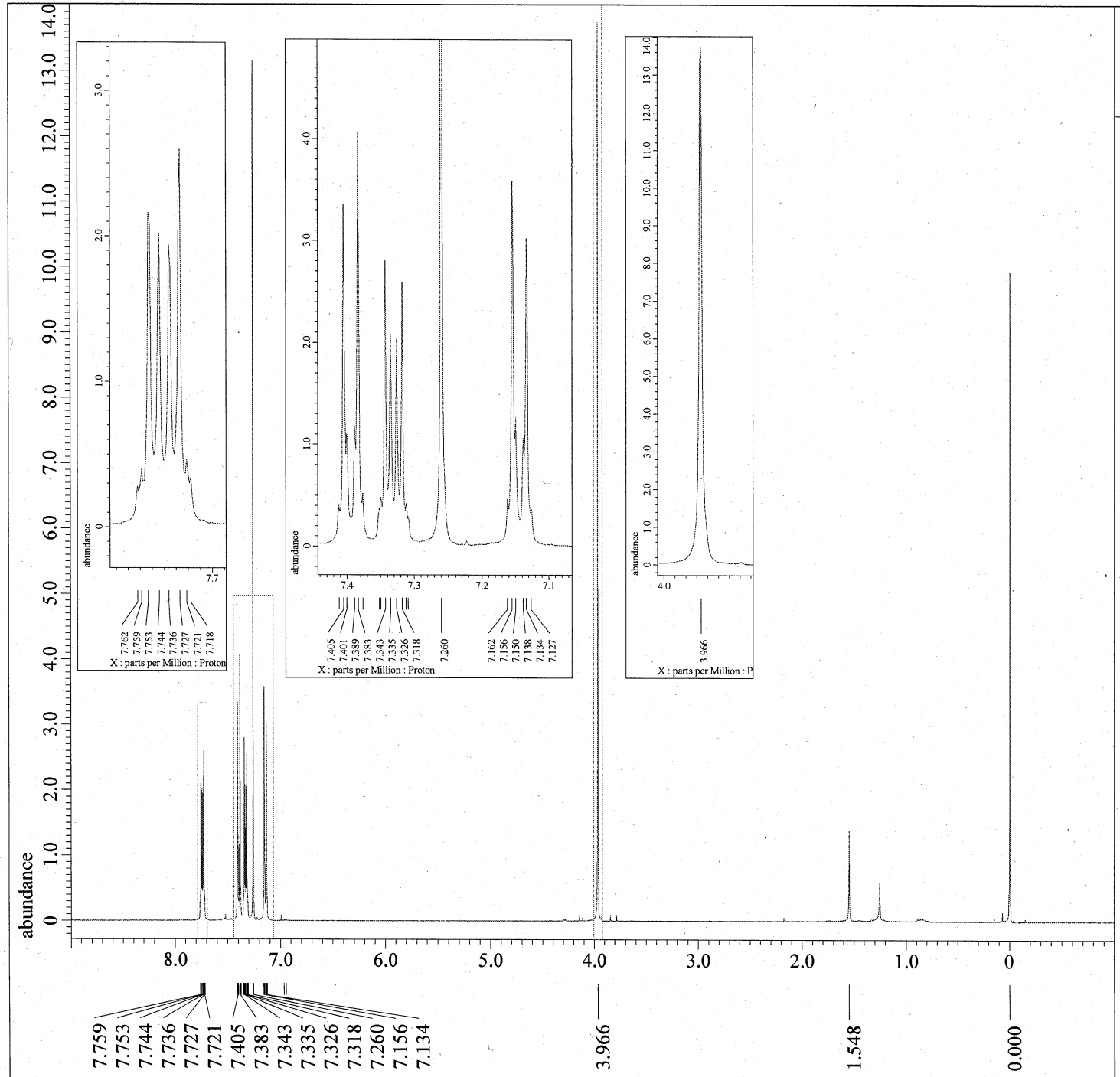


JEOL
Solutions for Innovation

Filename	= SEO-419-1-pure-13C-4.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= 1
Solvent	= CHLOROFORM-D
Creation_Time	= 31-AUG-2018 07:59:44
Revision_Time	= 7-FEB-2019 20:31:19
Current_Time	= 7-FEB-2019 20:32:07
Comment	= single pulse decoupled g
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[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	= 200
Total_Scans	= 200
Relaxation_Delay	= 2[s]
Recvr_Gain	= 60
Temp_Get	= 20.9[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_Noe	= 22.255[dB]
Irr_Noise	= WALTZ
Decoupling	= TRUE
Initial_Wait	= 1[s]
Noe	= TRUE
Noe_Time	= 2[s]
Repetition_Time	= 3.06430464[s]

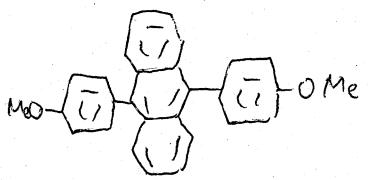


32

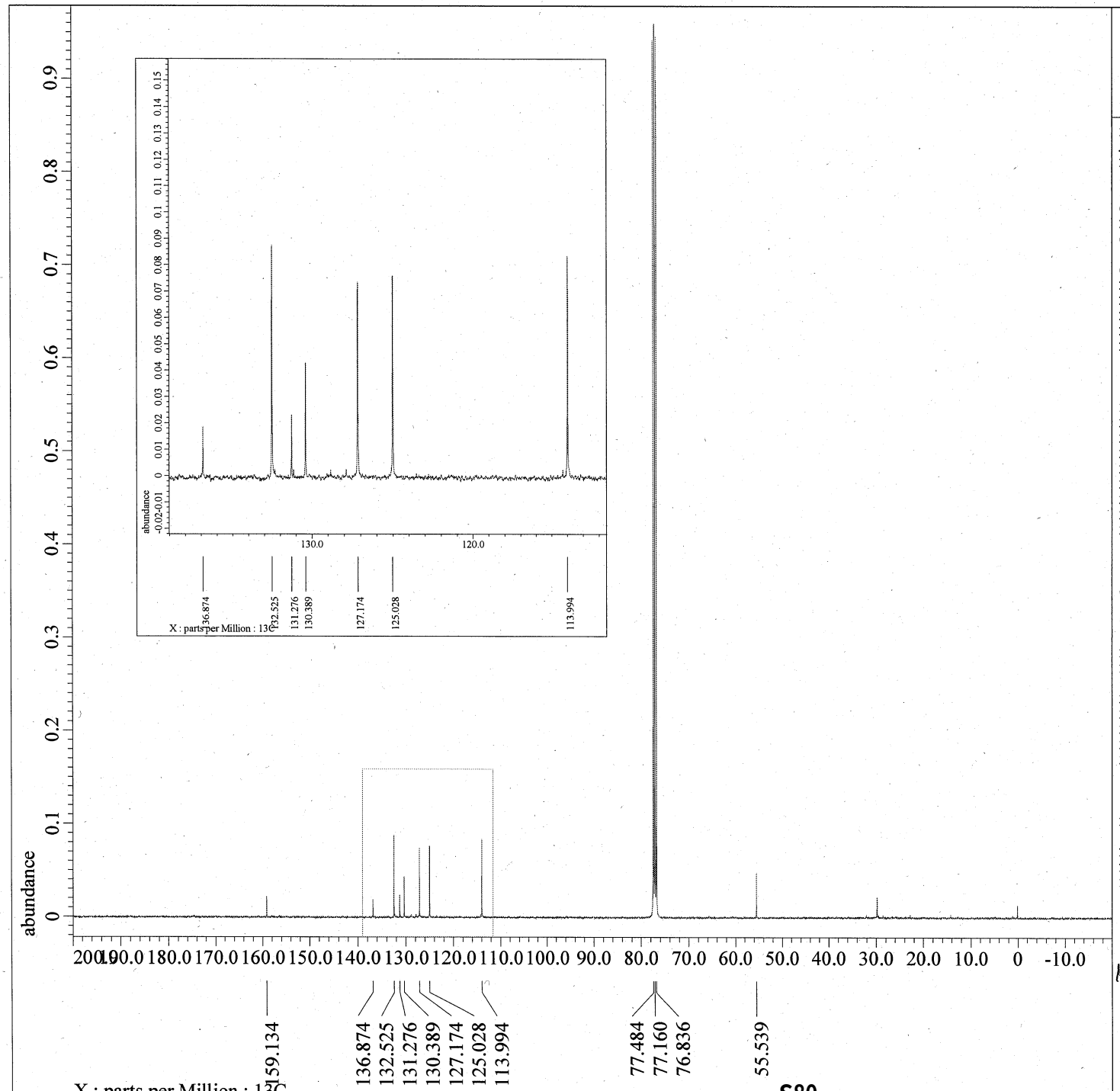


JEOL
Solutions for Innovation

Filename	= SEO-459-1-pure_Proton-1-
Author	= element
Experiment	= proton.jxp
Sample_Id	= SEO-459-1-pure
Solvent	= CHLOROFORM-D
Creation_Time	= 13-OCT-2018 18:41:25
Revision_Time	= 7-FEB-2019 20:34:03
Current_Time	= 7-FEB-2019 20:35:22
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECS400
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.37221[T] (400[MHz])
X_Acq_Duration	= 2.1889024[s]
X_Domain	= 1H
X_Freq	= 399.03472754[MHz]
X_Offset	= 5.0[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45684997[Hz]
X_Sweep	= 7.48502994[kHz]
X_Sweep_Clipped	= 5.98802395[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.03472754[MHz]
Irr_Offset	= 5.0[ppm]
Tri_Domain	= Proton
Tri_Freq	= 399.03472754[MHz]
Tri_Offset	= 5.0[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 50
Temp_Get	= 19.3[dC]
X_90_Width	= 6.6[us]
X_Acq_Time	= 2.1889024[s]
X_Angle	= 45[deg]
X_Atn	= 1[dB]
X_Pulse	= 3.3[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.1889024[s]

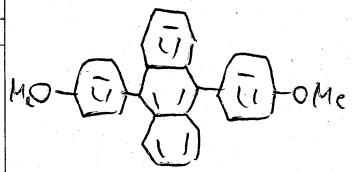


3aa

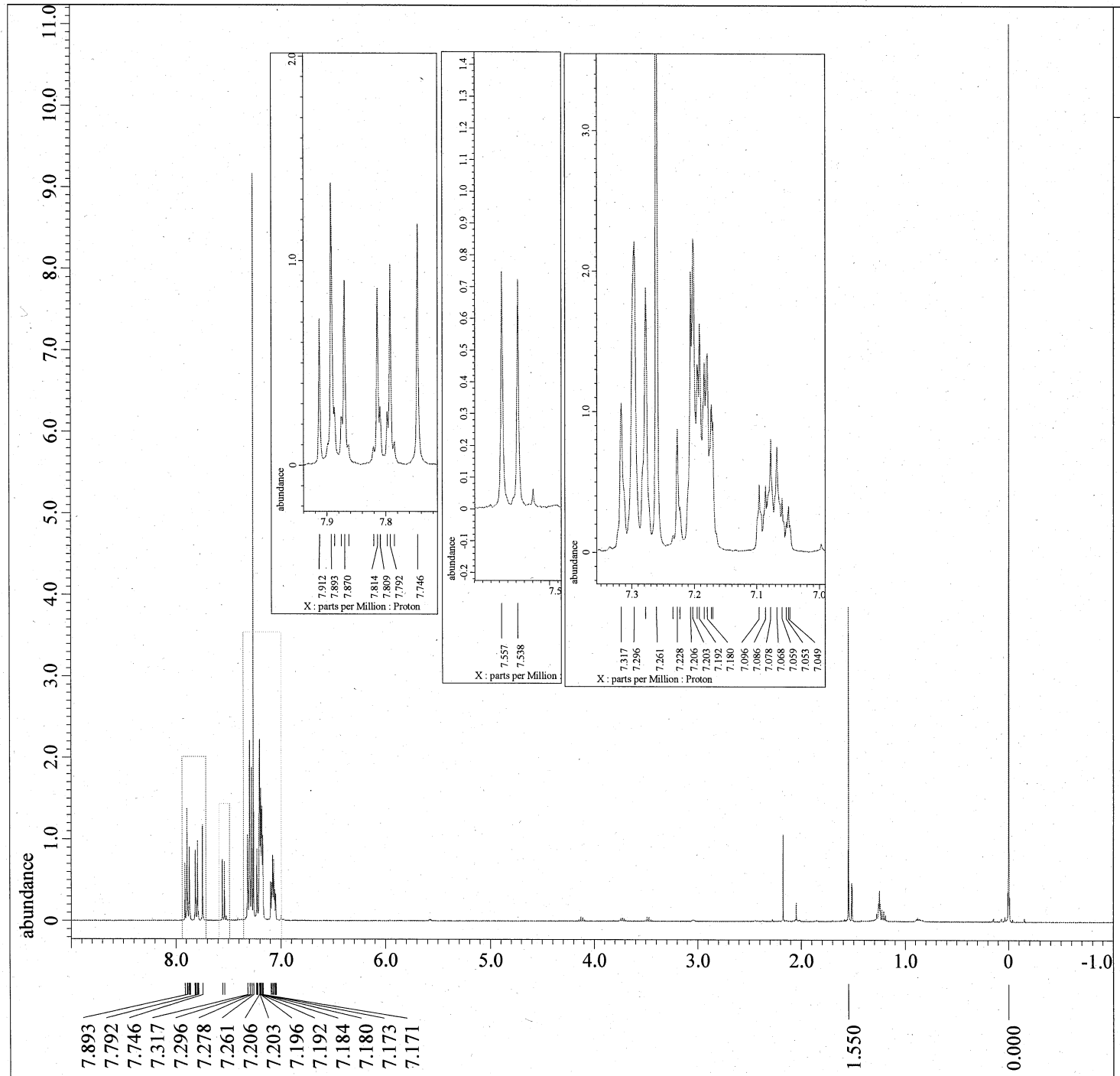


JEOL
Solutions for Innovation

Filename	= SEO-459-2-13C-6.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= S#646671
Solvent	= CHLOROFORM-D
Creation_Time	= 15-OCT-2018 06:53:31
Revision_Time	= 7-FEB-2019 20:36:07
Current_Time	= 7-FEB-2019 20:37:42
Comment	= single pulse decoupled g
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[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	= 16953
Total_Scans	= 16953
Relaxation_Delay	= 2[s]
Recvr_Gain	= 60
Temp_Get	= 20.3[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
Noe_Time	= 2[s]
Repetition_Time	= 3.06430464[s]

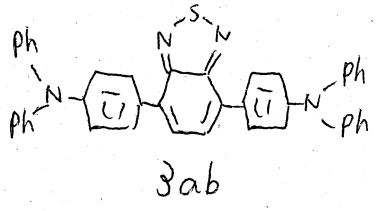


3aa

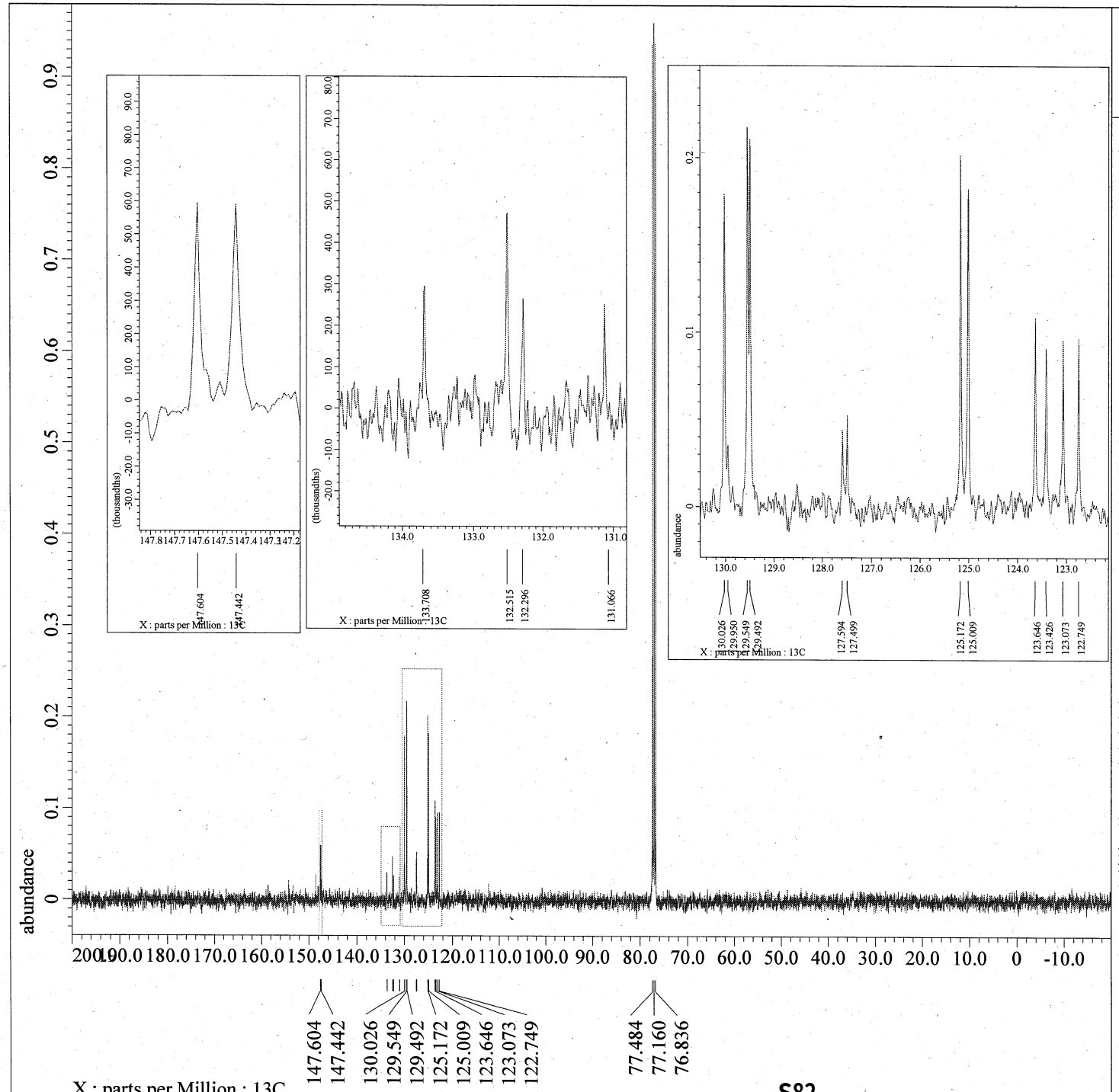


JEOL
Solutions for Innovation

Filename	= SEO-460-1-pure_Proton-1-
Author	= element
Experiment	= proton.jxp
Sample_Id	= SEO-460-1-pure
Solvent	= CHLOROFORM-D
Creation_Time	= 16-OCT-2018 14:02:04
Revision_Time	= 7-FEB-2019 20:39:50
Current_Time	= 7-FEB-2019 20:41:02
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.4073814[T] (400[MHz])
X_Acq_Duration	= 2.18103808[s]
X_Domain	= 1H
X_Freq	= 400.53219825[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45849727[Hz]
X_Sweep	= 7.51201923[kHz]
X_Sweep_Clipped	= 6.00961538[kHz]
Irr_Domain	= Proton
Irr_Freq	= 400.53219825[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 400.53219825[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 48
Temp_Get	= 19.5[dC]
X_90_Width	= 6.22[us]
X_Acq_Time	= 2.18103808[s]
X_Angle	= 45[deg]
X_Atn	= 0.8[dB]
X_Pulse	= 3.11[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.18103808[s]

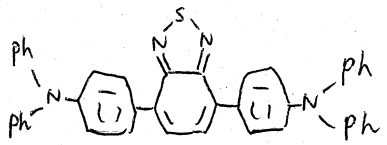


3ab

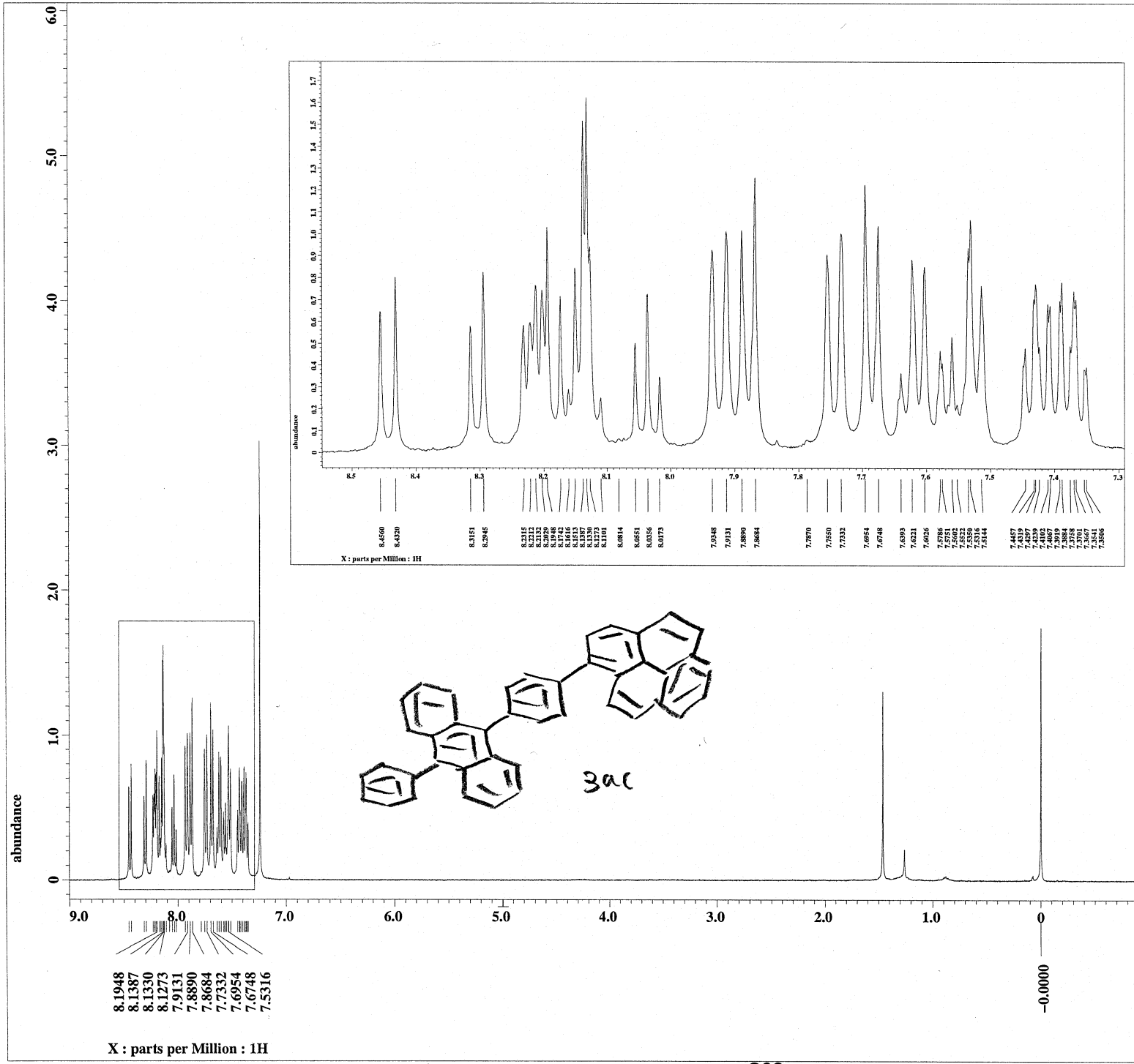


JEOL
Solutions for Innovation

Filename	= SEO-460-1-pure-13C-4.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= 1
Solvent	= CHLOROFORM-D
Creation_Time	= 16-OCT-2018 12:39:51
Revision_Time	= 7-FEB-2019 20:46:55
Current_Time	= 7-FEB-2019 20:47:56
Comment	= single pulse decoupled g
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[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	= 200
Total_Scans	= 200
Relaxation_Delay	= 2[s]
Recvr_Gain	= 60
Temp_Get	= 18.9[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_Noe	= 22.255[dB]
Irr_Noise	= WALTZ
Decoupling	= TRUE
Initial_Wait	= 1[s]
Noe	= TRUE
Noe_Time	= 2[s]
Repetition_Time	= 3.06430464[s]



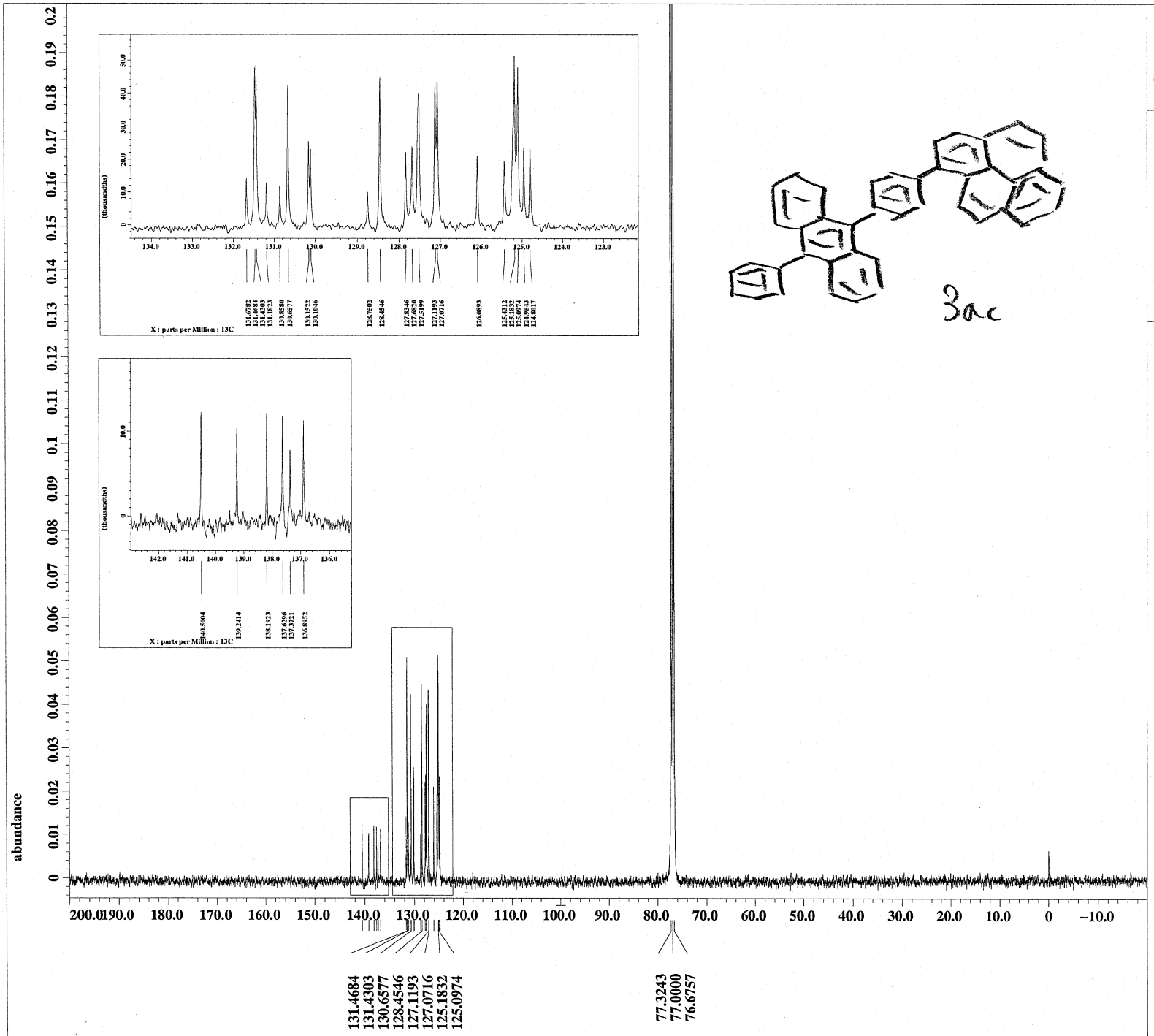
3ab



JEOL

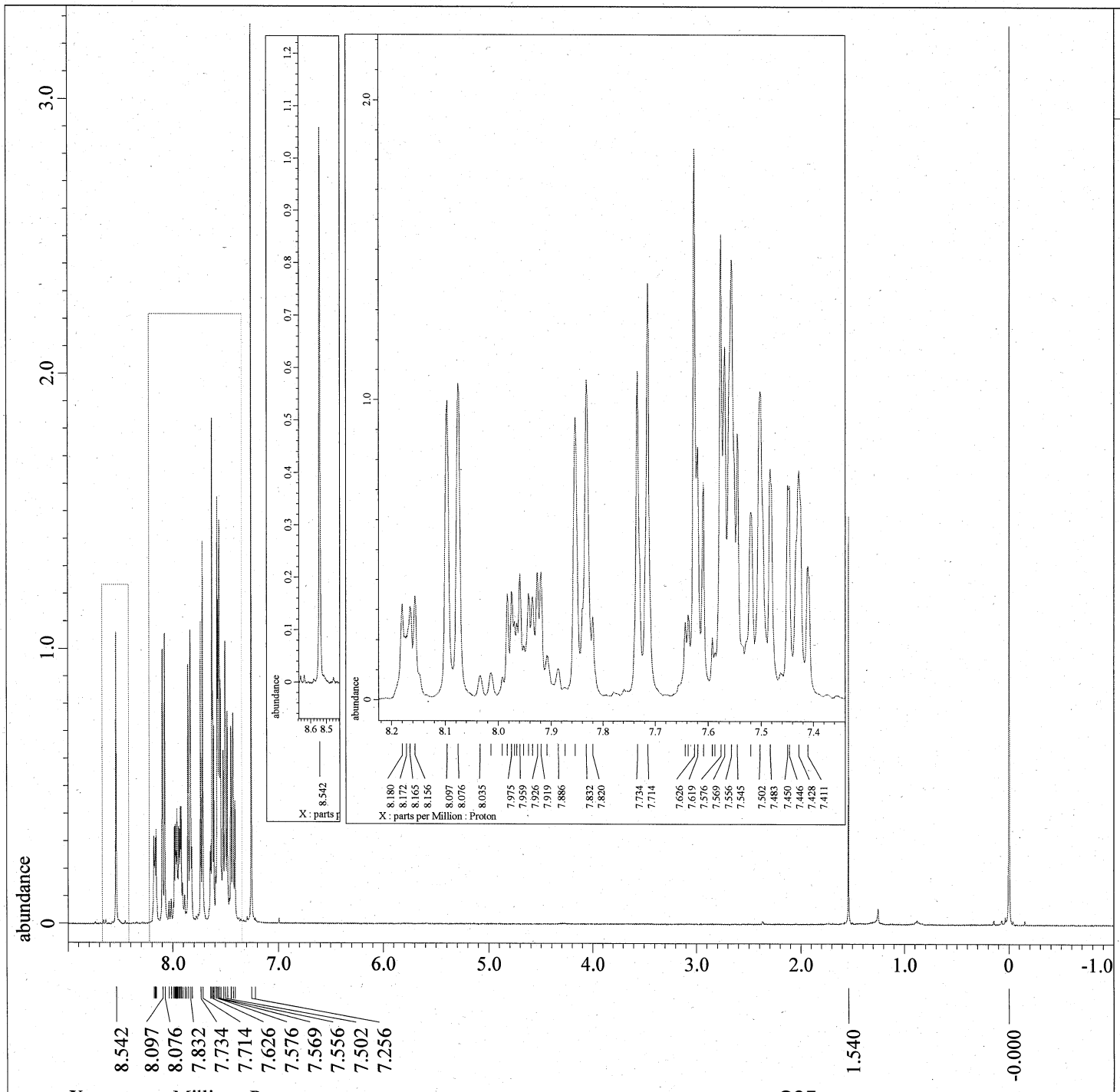
```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 0.2[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: Ph-ant-Ph-pyrene-2-CHECK-1
```

Filename	= Ph-ant-Ph-pyrene-2-CH
Author	= element
Experiment	= single_pulse.ex2
Sample_id	= S#412532
Solvent	= CHLOROFORM-D
Creation_time	= 19-JAN-2019 09:57:20
Revision_time	= 7-FEB-2019 20:04:05
Current_time	= 7-FEB-2019 20:05:50
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	= 50[dC]



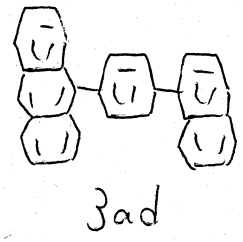

```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 2.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: Ph-ant-Ph-pyrene-13C-3-1.j
```

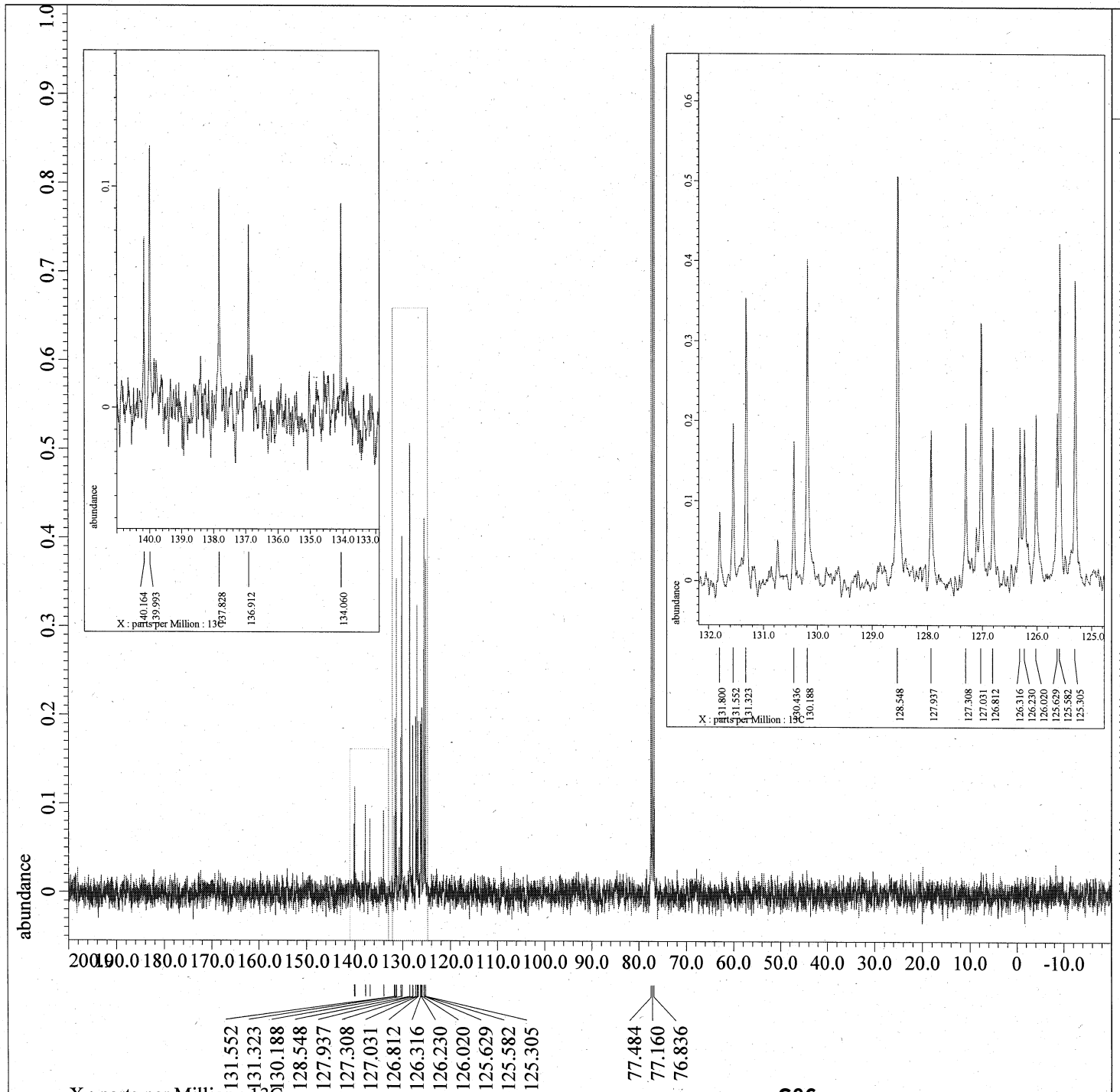
Filename	= Ph-ant-Ph-pyrene-13C-
Author	= element
Experiment	= single_pulse_dec
Sample_id	= S#759109
Solvent	= CHLOROFORM-D
Creation_time	= 22-JAN-2019 06:37:24
Revision_time	= 7-FEB-2019 20:06:30
Current_time	= 7-FEB-2019 20:07:42
Comment	= single pulse decouple
Data_format	= 1D COMPLEX
Dim_size	= 26214
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	= 13000
Total_scans	= 13000
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	= 50[dC]



JEOL
Solutions for Innovation

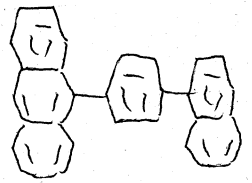
Filename	= SEO-510-1-pure_Proton-1-
Author	= element
Experiment	= proton.jxp
Sample_Id	= SEO-510-1-pure
Solvent	= CHLOROFORM-D
Creation_Time	= 29-NOV-2018 11:19:02
Revision_Time	= 7-FEB-2019 20:51:53
Current_Time	= 7-FEB-2019 20:52:45
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.4073814[T] (400[MHz])
X_Acq_Duration	= 2.18103808[s]
X_Domain	= 1H
X_Freq	= 400.53219825[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45849727[Hz]
X_Sweep	= 7.51201923[kHz]
X_Sweep_Clipped	= 6.00961538[kHz]
Irr_Domain	= Proton
Irr_Freq	= 400.53219825[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 400.53219825[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 44
Temp_Get	= 19.5[dC]
X_90_Width	= 6.22[us]
X_Acq_Time	= 2.18103808[s]
X_Angle	= 45[deg]
X_Atn	= 0.8[dB]
X_Pulse	= 3.11[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.18103808[s]



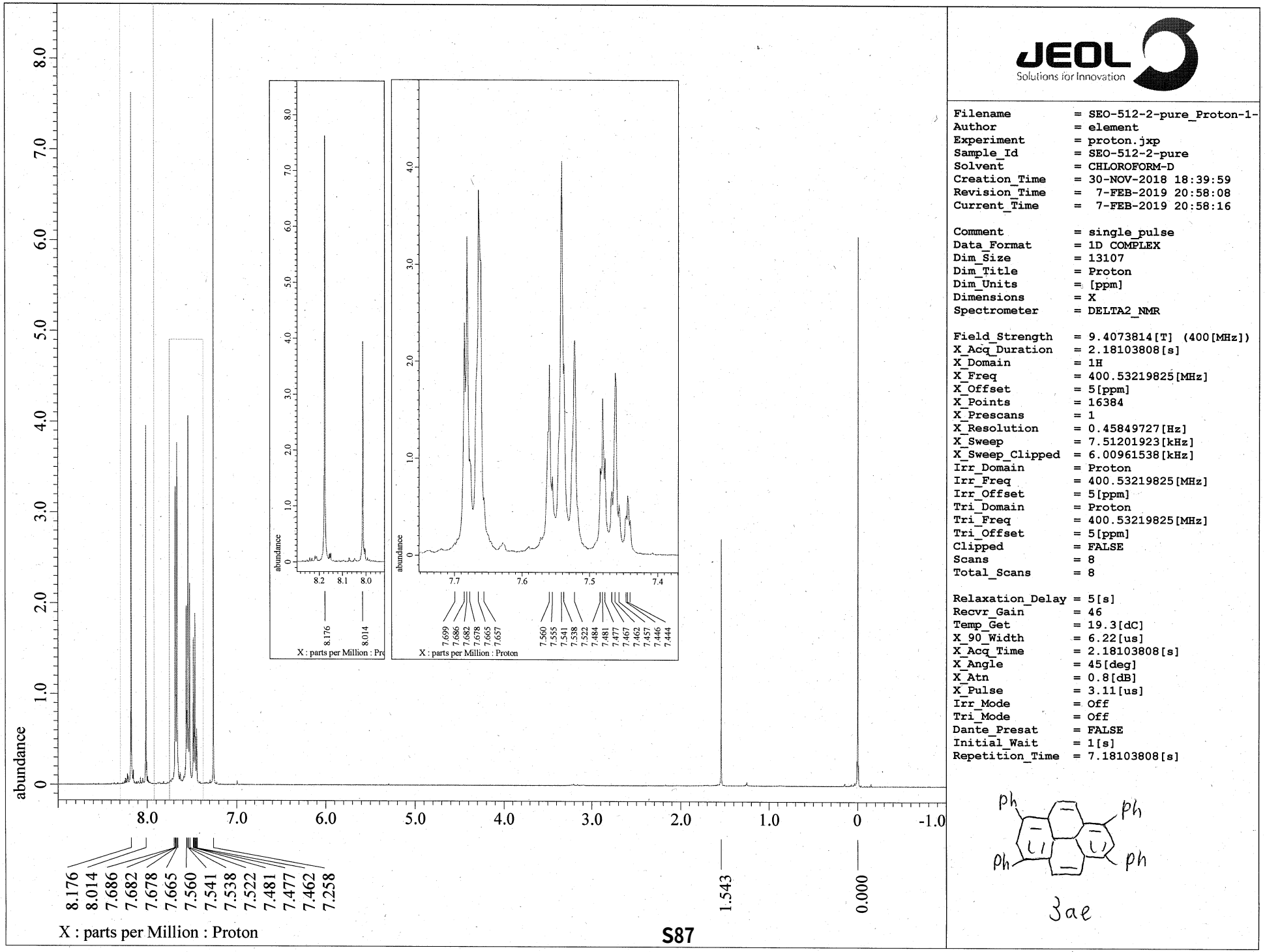


JEOL
Solutions for Innovation

Filename	= SEO-510-1-pure-13C-7.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= 1
Solvent	= CHLOROFORM-D
Creation_Time	= 29-NOV-2018 18:55:22
Revision_Time	= 7-FEB-2019 20:53:03
Current_Time	= 7-FEB-2019 20:54:42
Comment	= single pulse decoupled g
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[MHz])
X_Acq_Duration	= 1.06430464[s]
X_Domain	= 13C
X_Freq	= 98.51479726[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.93958061[Hz]
X_Sweep	= 30.78817734[kHz]
Irr_Domain	= 1H
Irr_Freq	= 391.78655441[MHz]
Irr_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 53
Total_Scans	= 53
Relaxation_Delay	= 2[s]
Recvr_Gain	= 60
Temp_Get	= 21.4[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_Noe	= 22.255[dB]
Irr_Noise	= WALTZ
Decoupling	= TRUE
Initial_Wait	= 1[s]
Noe	= TRUE
Noe_Time	= 2[s]
Repetition_Time	= 3.06430464[s]



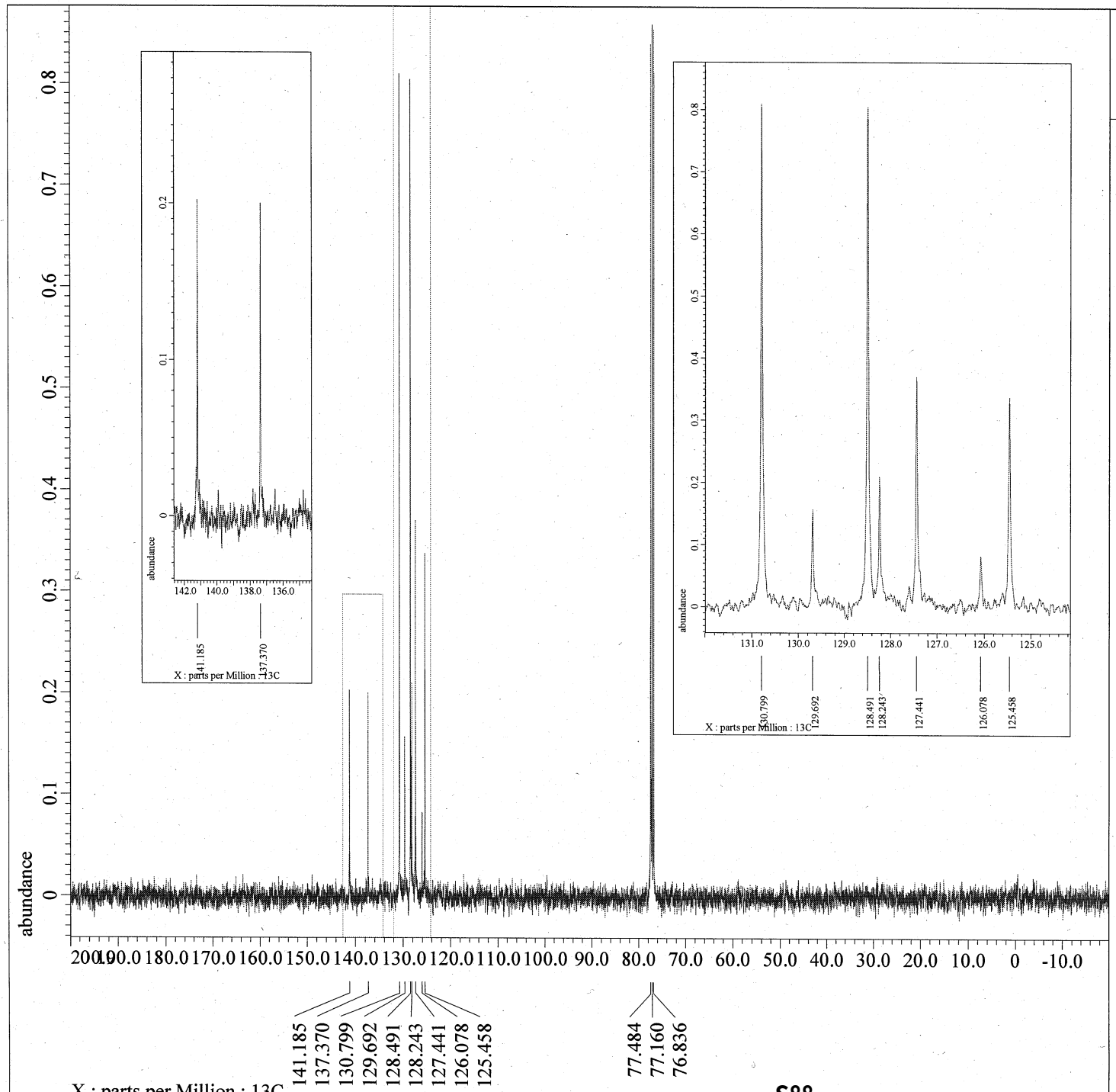
3ad



JEOL
Solutions for Innovation

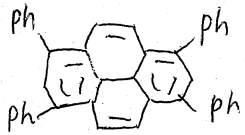
Filename	= SEO-512-2-pure_Proton-1-
Author	= element
Experiment	= proton.jxp
Sample_Id	= SEO-512-2-pure
Solvent	= CHLOROFORM-D
Creation_Time	= 30-NOV-2018 18:39:59
Revision_Time	= 7-FEB-2019 20:58:08
Current_Time	= 7-FEB-2019 20:58:16
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.4073814[T] (400[MHz])
X_Acq_Duration	= 2.18103808[s]
X_Domain	= 1H
X_Freq	= 400.53219825[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45849727[Hz]
X_Sweep	= 7.51201923[kHz]
X_Sweep_Clipped	= 6.00961538[kHz]
Irr_Domain	= Proton
Irr_Freq	= 400.53219825[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 400.53219825[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 46
Temp_Get	= 19.3[dC]
X_90_Width	= 6.22[us]
X_Acq_Time	= 2.18103808[s]
X_Angle	= 45[deg]
X_Atn	= 0.8[dB]
X_Pulse	= 3.11[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.18103808[s]

3ae

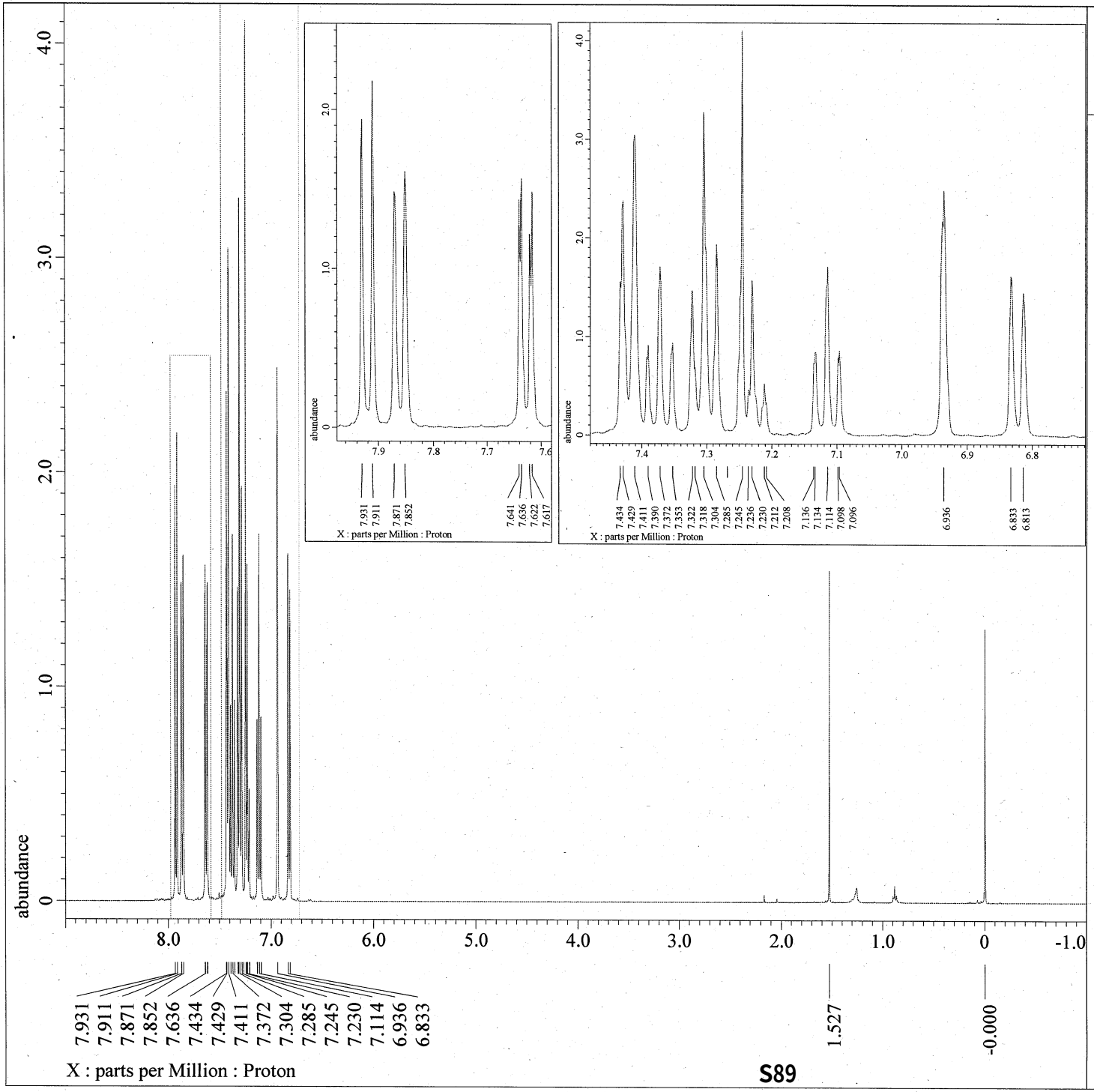


JEOL
Solutions for Innovation

Filename	= SEO-512-2-pure-13C-4.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= 1
Solvent	= CHLOROFORM-D
Creation_Time	= 30-NOV-2018 17:13:11
Revision_Time	= 7-FEB-2019 20:58:34
Current_Time	= 7-FEB-2019 20:59:32
Comment	= single pulse decoupled g
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[MHz])
X_Acq_Duration	= 1.06430464[s]
X_Domain	= 13C
X_Freq	= 98.51479726[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.93958061[Hz]
X_Sweep	= 30.78817734[kHz]
Irr_Domain	= 1H
Irr_Freq	= 391.78655441[MHz]
Irr_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 109
Total_Scans	= 109
Relaxation_Delay	= 2[s]
Recvr_Gain	= 60
Temp_Get	= 19.5[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
Noe_Time	= 2[s]
Repetition_Time	= 3.06430464[s]

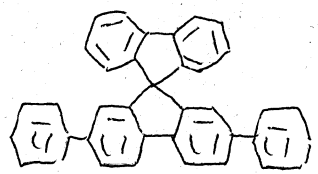


3ae

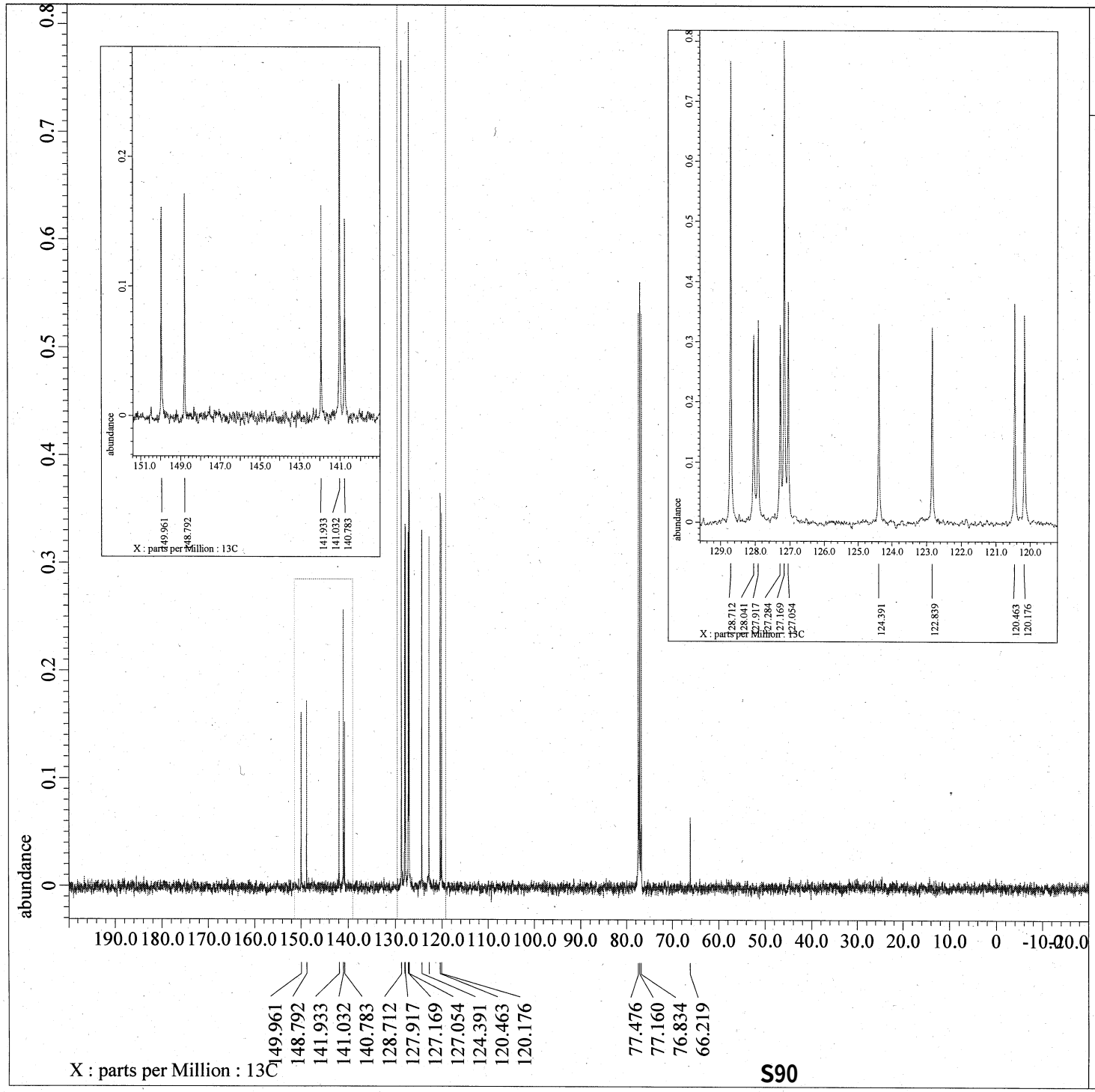


JEOL
Solutions for Innovation

Filename	= SEO-520-1-pure_Proton-1-
Author	= element
Experiment	= proton.jxp
Sample_Id	= SEO-520-1-pure
Solvent	= CHLOROFORM-D
Creation_Time	= 12-DEC-2018 09:43:10
Revision_Time	= 7-FEB-2019 21:08:23
Current_Time	= 7-FEB-2019 21:09:35
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.4073814[T] (400[MHz])
X_Acq_Duration	= 2.18103808[s]
X_Domain	= 1H
X_Freq	= 400.53219825[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45849727[Hz]
X_Sweep	= 7.51201923[kHz]
X_Sweep_Clipped	= 6.00961538[kHz]
Irr_Domain	= Proton
Irr_Freq	= 400.53219825[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 400.53219825[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 40
Temp_Get	= 19.5[dC]
X_90_Width	= 6.22[us]
X_Acq_Time	= 2.18103808[s]
X_Angle	= 45[deg]
X_Atn	= 0.8[dB]
X_Pulse	= 3.11[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.18103808[s]

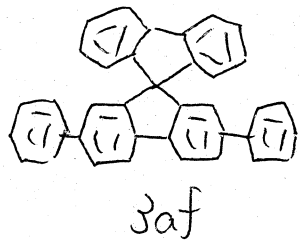


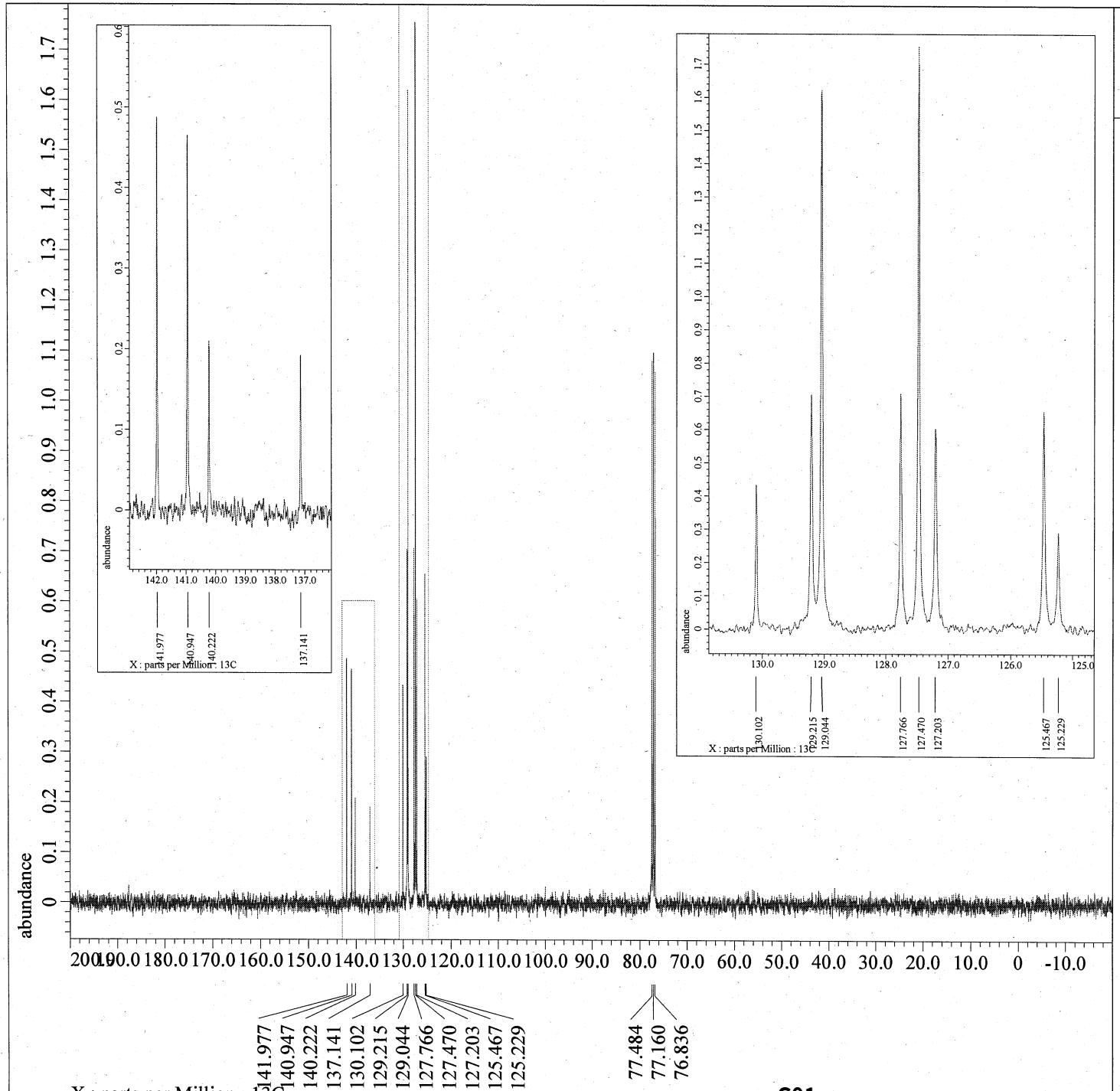
3af



JEOL
Solutions for Innovation

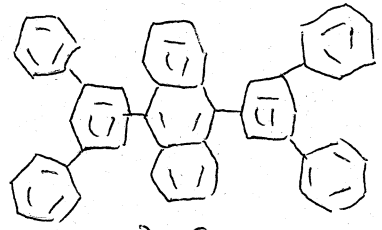
Filename	= SEO-517-3-pure-13C-4.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= 1
Solvent	= CHLOROFORM-D
Creation_Time	= 10-DEC-2018 16:25:04
Revision_Time	= 7-FEB-2019 21:16:01
Current_Time	= 7-FEB-2019 21:16:46
Comment	= single pulse decoupled g
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
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	= 200
Total_Scans	= 200
Relaxation_Delay	= 2[s]
Recvr_Gain	= 54
Temp_Get	= 23.4[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
Noe_Time	= 2[s]
Repetition_Time	= 3.048576[s]





JEOL
Solutions for Innovation

Filename	= SEO-513-4-pure-13C-4.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= 1
Solvent	= CHLOROFORM-D
Creation_Time	= 1-DEC-2018 16:54:14
Revision_Time	= 7-FEB-2019 21:20:26
Current_Time	= 7-FEB-2019 21:21:32
Comment	= single pulse decoupled g
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[MHz])
X_Acq_Duration	= 1.06430464[s]
X_Domain	= 13C
X_Freq	= 98.51479726[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.93958061[Hz]
X_Sweep	= 30.78817734[kHz]
Irr_Domain	= 1H
Irr_Freq	= 391.78655441[MHz]
Irr_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 53
Total_Scans	= 53
Relaxation_Delay	= 2[s]
Recvr_Gain	= 60
Temp_Get	= 19.5[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
Noe_Time	= 2[s]
Repetition_Time	= 3.06430464[s]



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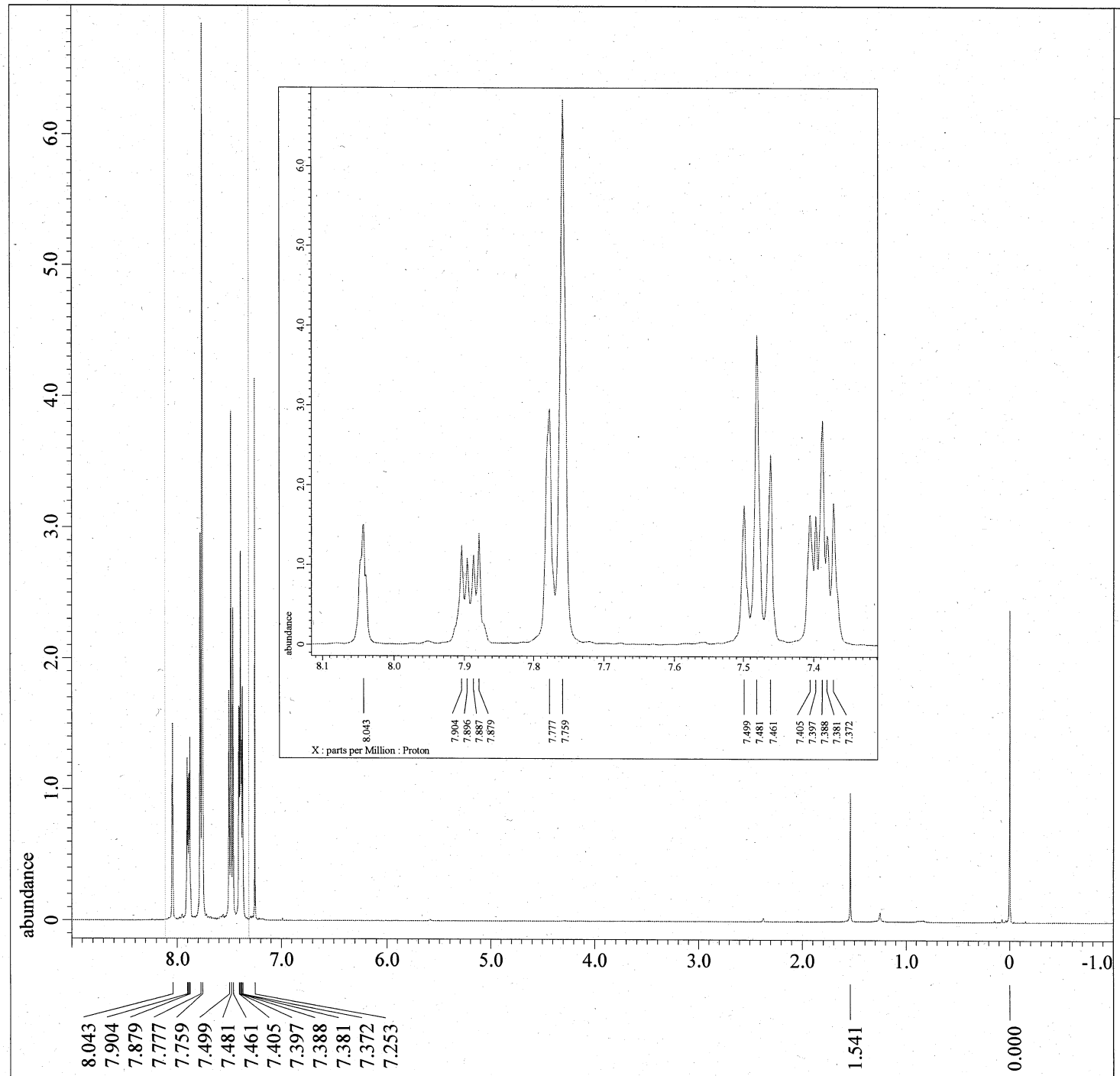
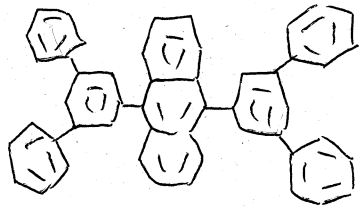


JEOL
Solutions for Innovation

Filename	= SEO-513-3-pure_Proton-1-
Author	= element
Experiment	= proton.jxp
Sample_Id	= SEO-513-3-pure
Solvent	= CHLOROFORM-D
Creation_Time	= 1-DEC-2018 18:22:51
Revision_Time	= 7-FEB-2019 21:20:52
Current_Time	= 7-FEB-2019 21:21:44
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.4073814[T] (400[MHz])
X_Acq_Duration	= 2.18103808[s]
X_Domain	= 1H
X_Freq	= 400.53219825[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45849727[Hz]
X_Sweep	= 7.51201923[kHz]
X_Sweep_Clipped	= 6.00961538[kHz]
Irr_Domain	= Proton
Irr_Freq	= 400.53219825[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 400.53219825[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 42
Temp_Get	= 18.7[dC]
X_90_Width	= 6.22[us]
X_Acq_Time	= 2.18103808[s]
X_Angle	= 45[deg]
X_Atn	= 0.8[dB]
X_Pulse	= 3.11[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]
Repetition_Time	= 7.18103808[s]



3aq