A Glove-box- and Schlenk-line-free Protocol for Solid-state C–N Cross-coupling Reactions Using Mechanochemistry

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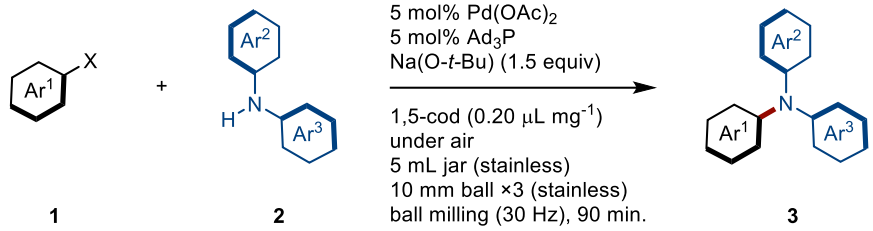
1. Chemicals and Instrumentation.

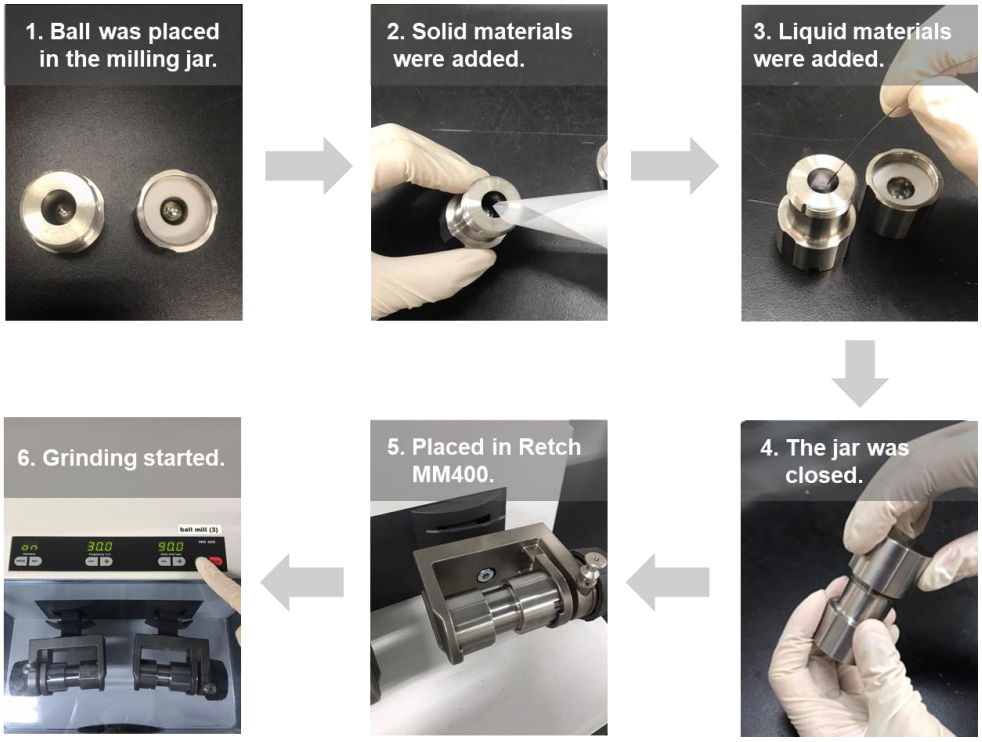
The starting materials were obtained from commercial suppliers and used as received. Tri(1-adamantyl)phosphine was obtained from Strem Chemicals, Inc. (product No. 15-0935) and used as received. All mechanochemical reactions were carried out using grinding vessels in a Retsch MM400 mill jars (1.5 mL, 5 mL or 10 mL) and balls are made of stainless (SUS440B and SUS420J2, respectively). 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. Dibromomethane was used as an internal standard to determine NMR yields. Recycle preparative gel permeation chromatography (GPC) was conducted with a JAI LaboACE LC-5060 using $CHCl_3$ as an eluent. Thermography was recorded with an NEC Avio Thermo GEAR G120. Scanning electron microscopy (SEM) analysis was carried out with JEOL JSM-6510LV. High-resolution mass spectra were recorded at the Global Facility Center, Hokkaido University.

2. General Procedure for Solid-State C–N Coupling Using a Ball Mill.

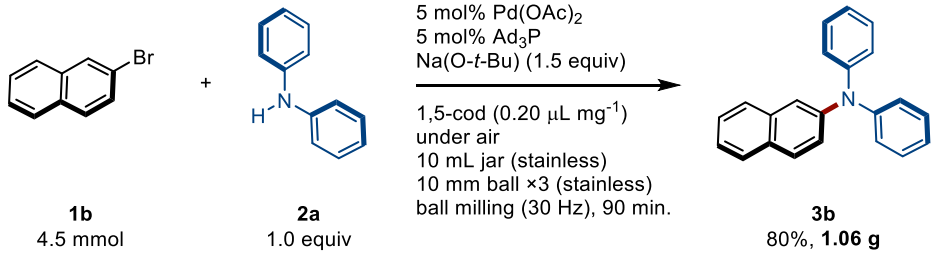


Aryl halide **1** (0.5 mmol), diarylamine **2** (0.5 mmol, 1.0 equiv), $Pd(OAc)_2$ (0.025 mmol, 5 mol %), Ad_3P (0.025 mmol, 5 mol %) and Na(O-*t*-Bu) (0.75 mmol, 1.5 equiv) were placed in a ball milling vessel [stainless (SUS440B), 5 mL] loaded with three grinding balls [stainless (SUS420J2), diameter: 10 mm] in air. Then 1,5-cod (0.20 μl/mg) was added via syringe. After the vessel was closed in air, the vessel was placed in the ball mill (Retch MM400, 30Hz). After 90 min, the mixture was passed through a short silica gel column eluting with EtOAc to remove inorganic salts. The crude mixture was then purified by flash column chromatography (SiO_2, CH_2Cl_2/hexane, typically 0:100-15:85) to give the corresponding arylamines **3**.

Figure S1. Set-up procedure for solid-state C–N coupling reactions using ball milling.



3. Procedure for Solid-State C–N Coupling on a Gram Scale.



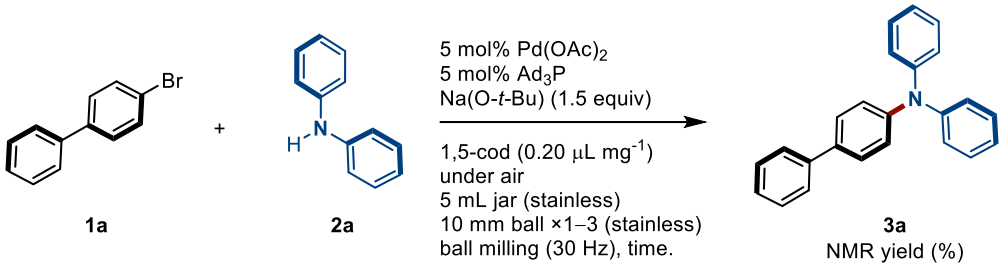
1b
4.5 mmol

2a
1.0 equiv

3b
80%, **1.06 g**

1b (4.5 mmol, 931.8 mg), **2a** (4.5 mmol, 761.7 mg, 1.0 equiv), $Pd(OAc)_2$ (0.225 mmol, 50.5 mg, 5 mol %), Ad_3P (0.225 mmol, 98.2 mg, 5 mol %) and Na(O-*t*-Bu) (6.75 mmol, 648.3 mg, 1.5 equiv) were placed in a ball milling vessel [stainless (SUS440B), 10 mL] loaded with 3 grinding balls [stainless (SUS420J2), diameter: 10 mm] in air. Then 1,5-cod (0.20 μl/mg) was added via syringe. After the vessel was closed in air, the vessel was placed in the ball mill (Retch MM400, 30Hz). After 90 min, the mixture was extracted with CH_2Cl_2 three times. The combined organic layer was then dried over $MgSO_4$. After filtration, the solvents were removed by evaporation. The crude mixture was then purified by flash column chromatography (SiO_2, CH_2Cl_2/hexane, 0:100-15:85) to give the arylamine **3b** as a white solid (1.065 g, 80% yield).

4. Results of Kinetics Study.



The kinetics of the reactions under the conditions using different number of balls were measured. All sampling data were measured individually. The yields were determined by ^{1}H NMR analysis with an internal standard. The data in the figure is the average value of the results of two measurements.

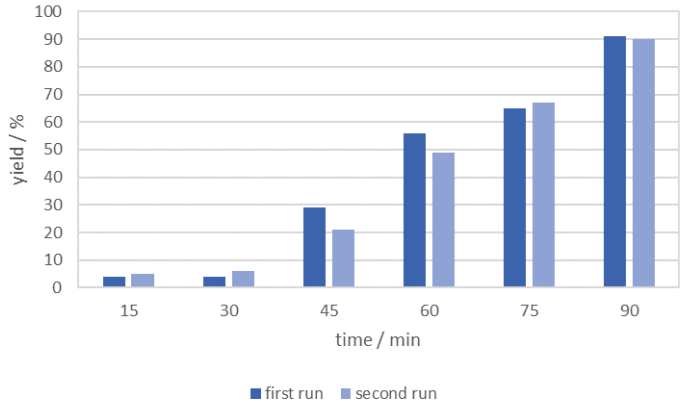


Figure S2. Result of kinetics study using three stainless balls.

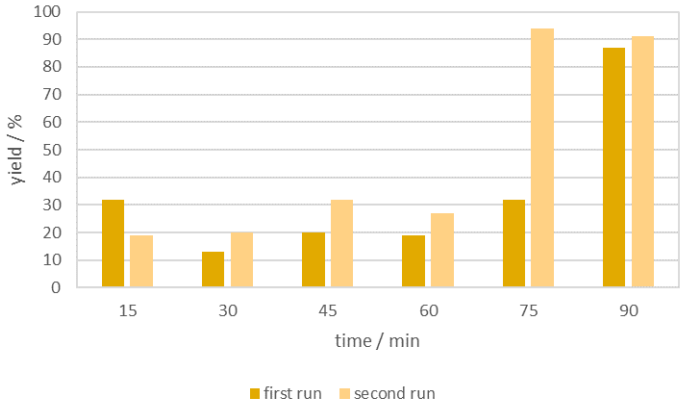


Figure S3. Results of kinetics study using two stainless balls.

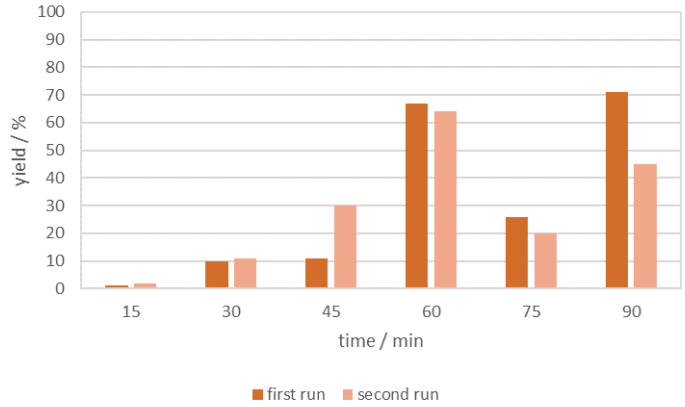


Figure S4. Result of kinetics study using one stainless ball.

Table S1. Result of kinetics study using three stainless balls.

time (min)	NMR yield (%)		average (%)
0	0	0	0
15	4	5	4.5
30	4	6	5
45	29	21	25
60	56	49	52.5
75	65	67	66
90	91	90	90.5

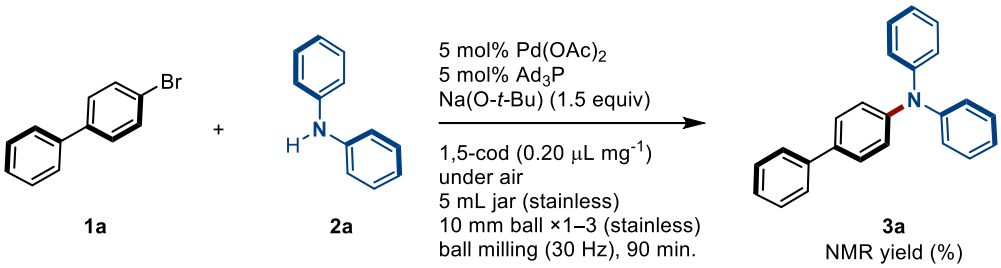
Table S2. Result of kinetics study using two stainless balls.

time (min)	NMR yield (%)		average (%)
0	0	0	0
15	32	19	25.5
30	13	20	16.5
45	20	32	26
60	19	27	23
75	32	94	63
90	87	91	89

Table S3. Result of kinetics study using one stainless ball.

Time (min)	NMR yield (%)		average (%)
0	0	0	0
15	1	2	1.5
30	10	11	10.5
45	11	30	20.5
60	67	64	65.5
75	26	20	23
90	71	45	58

5. Thermographic Analysis.



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: 0.5 mmol of **1a**; 0.5 mmol of **2a**; 0.025 mmol of $Pd(OAc)_2$; 0.025 mmol of ligand; 0.75 mmol of Na(O-*t*-Bu); 1.5-cod (58 μl) in a stainless ball milling jar (SUS440B, 5 mL) with 1–3 stainless-steel balls (SUS420J2, 10 mm); 30 Hz; 90 min. The obtained image showed that the temperature was around 40 °C.

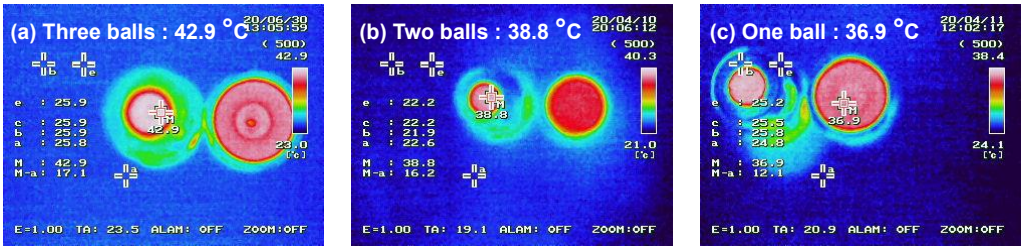
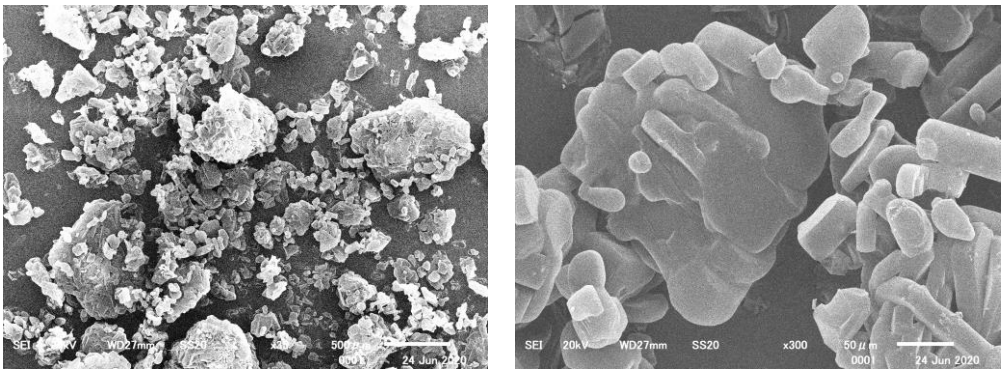


Figure S5. Thermography images of the reaction mixtures after the ball milling at 30 Hz for 90 min.

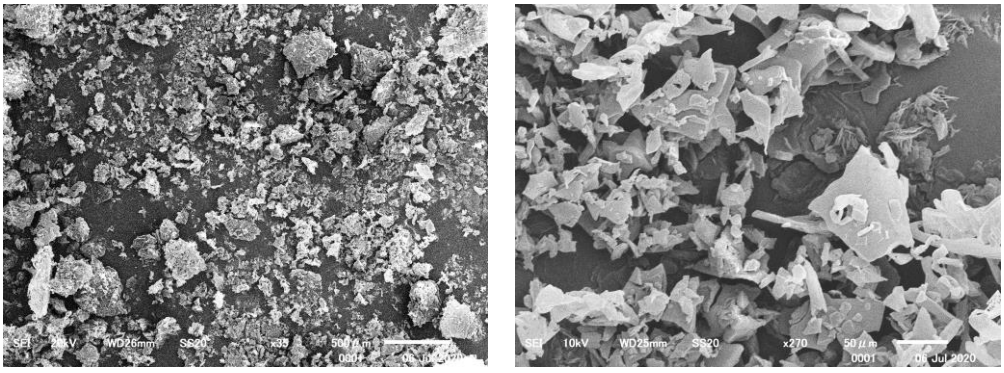
6. Observation of Substrate Particles by Scanning Electron Microscopy

The samples were prepared by the following conditions: 0.5 mmol of **1a** or **2a** in a stainless ball milling jar (SUS440B, 5 mL) with 1~3 stainless-steel balls (SUS420J2, 10 mm); 30 Hz; 60 min. The samples for the characterization by scanning electron microscopy (SEM) were prepared by platinum coating with thin carbon film.



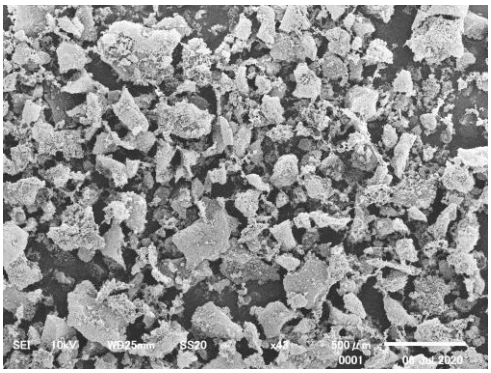
Scale bar : 500 µm **Scale bar : 50 µm**

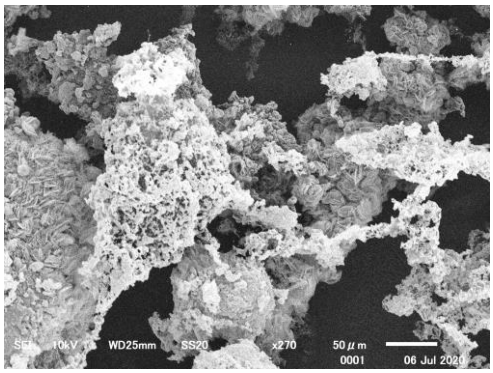
Figure S6. SEM images of 2a before ball milling. Scale bars in SEM images (bottom right).



Scale bar : 500 µm **Scale bar : 50 µm**

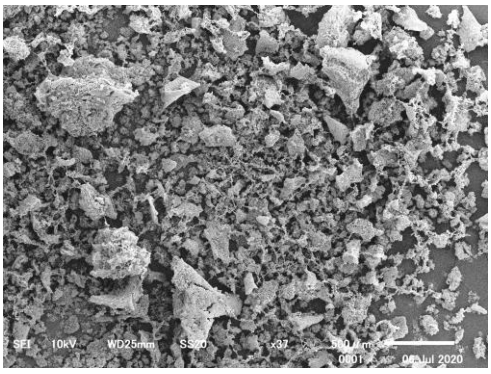
Figure S7. SEM images of 2a upon ball milling with one ball. Scale bars in SEM images (bottom right).

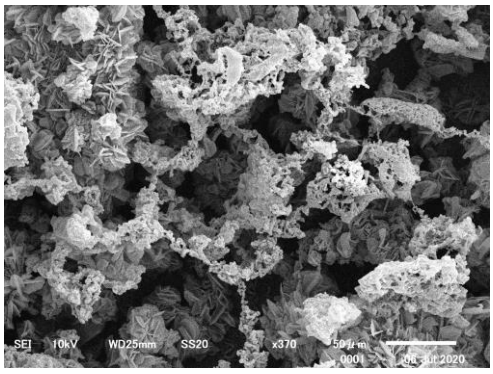




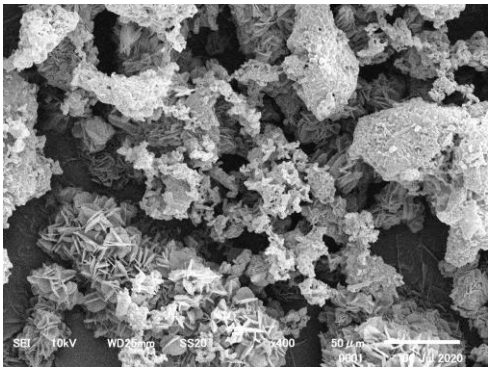
Scale bar : 500 µm **Scale bar : 50 µm**

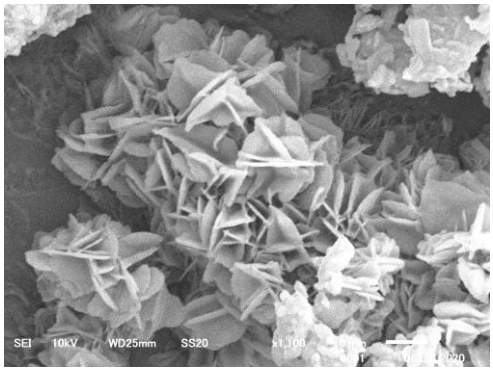
Figure S8. SEM images of 2a upon ball milling with two balls. Scale bars in SEM images (bottom right).





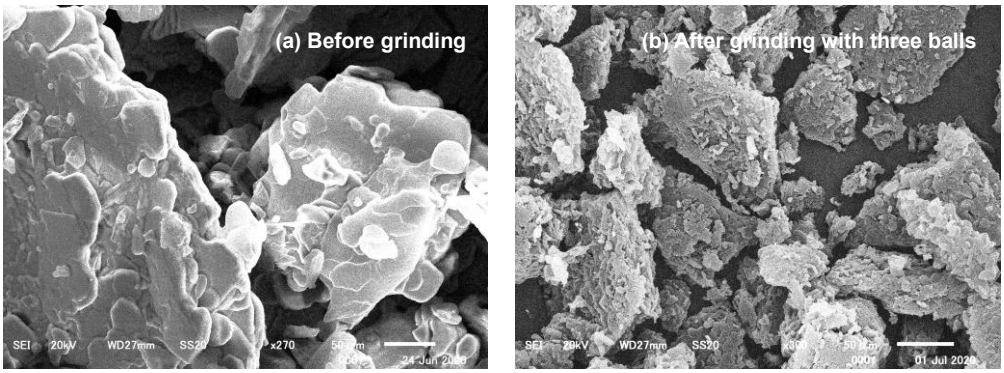
Scale bar : 500 µm **Scale bar : 50 µm**





Scale bar : 50 µm **Scale bar : 10 µm**

Figure S9. SEM images of 2a upon ball milling with three balls. Scale bars in SEM images (bottom right).



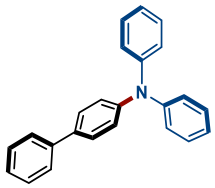
Scale bar : 50 µm **Scale bar : 50 µm**

Figure S10. SEM images of 1a (a) before ball milling and (b) upon ball milling with three balls. Scale bars in SEM images (bottom right).

7. Characterization of Obtained Arylamines.

All arylamines (**3a**–**3r**) synthesized in this study are known compounds. ^{1}H and ^{13}C NMR of the arylamines (**3a**–**3o**[1], **3p**[2], **3q**[3], and **3r**[4]) were in agreement with the corresponding literature.

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

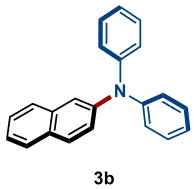


3a

The reaction was carried out with 117.1 mg (0.50 mmol) of **1a** and 84.6 mg (0.50 mmol) of **2a**. The product **3a** was obtained as a white powder (139.4 mg, 0.433 mmol, 87% yield) after purification by silica-gel column chromatography (SiO_2, CH_2Cl_2/hexane, 0:100–5:95).

^{1}H NMR (396 MHz, $CDCl_3$, δ): 7.03 (t, J = 7.1 Hz, 2H), 7.14 (d, J = 8.7 Hz, 6H), 7.25–7.27 (m, 3H), 7.28–7.32 (m, 2H), 7.42 (t, J = 7.7 Hz, 2H), 7.46–7.49 (m, 2H), 7.57 (d, J = 7.7 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$, δ): 123.0 (*C*H), 124.0 (*C*H), 124.5 (*C*H), 126.8 (*C*H), 126.9 (*C*H), 127.9 (*C*H), 128.9 (*C*H), 129.4 (*C*H), 135.2 (*C*), 140.7 (*C*), 147.3 (*C*), 147.8 (*C*). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{24}H_{19}N$, 321.1518; found, 321.1530.

***N,N*-Diphenylnaphthalen-2-amine (3b).**

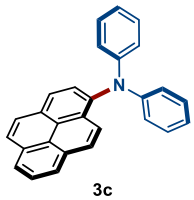


3b

The reaction was carried out with 103.3 mg (0.50 mmol) of **1b** and 84.6 mg (0.50 mmol) of **2a**. The product **3b** was obtained as a white powder (138.6 mg, 0.47 mmol, 96% yield) after purification by silica-gel column chromatography (SiO_2, CH_2Cl_2/hexane, 0:100–5:95).

^{1}H NMR (400 MHz, $CDCl_3$, δ): 7.04 (t, J = 7.1 Hz, 2H), 7.12–7.14 (m, 4H), 7.24–7.28 (m, 5H), 7.32–7.40 (m, 2H), 7.42 (s, 1H), 7.58 (d, J = 8.3 Hz, 1H), 7.71 (d, J = 9.2 Hz, 1H), 7.74 (d, J = 8.0 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$, δ): 120.3 (*C*H), 123.0 (*C*H), 124.46 (*C*H), 124.52 (*C*H), 124.6 (*C*H), 126.4 (*C*H), 127.0 (*C*H), 127.7 (*C*H), 129.0 (*C*H), 129.4 (*C*H), 130.1 (*C*), 134.5 (*C*), 145.6 (*C*), 147.9 (*C*). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{22}H_{17}N$, 295.1361; found, 295.1364.

***N*,*N*-Diphenylpyren-1-amine (3c).**

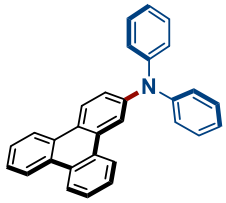


3c

The reaction was carried out with 140.6 mg (0.50 mmol) of **1c** and 84.3 mg (0.50 mmol) of **2a**. The product **3c** was obtained as a yellow powder (147.8 mg, 0.40 mmol, 80% yield) after purification by silica-gel column chromatography (SiO_2, CH_2Cl_2/hexane, 0:100–5:95).

^{1}H NMR (400 MHz, $CDCl_3$, δ): 6.92–6.97 (m, 2H), 7.05–7.10 (m, 4H), 7.18–7.24 (m, 4H), 7.83 (d, *J* = 7.9 Hz, 1H), 7.93 (d, *J* = 9.1 Hz, 1H), 7.98 (t, *J* = 7.5 Hz, 1H), 8.06 (br, s, 2H), 8.10–8.18 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$, δ): 121.9 (*C*H), 122.2 (*C*H), 123.4 (*C*H), 124.9 (*C*), 125.2 (*C*H), 125.3 (*C*H), 126.1 (*C*H), 126.3 (*C*H), 126.5 (*C*), 127.2 (*C*H), 127.3 (*C*H), 127.8 (*C*H), 128.0 (*C*H), 128.3 (*C*), 129.3 (*C*H), 129.6 (*C*), 131.1 (*C*), 131.3 (*C*), 141.0 (*C*), 148.8 (*C*). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{28}H_{19}N$, 369.1518; found, 369.1501.

***N*,*N*-Diphenyltriphenylen-2-amine (3d).**

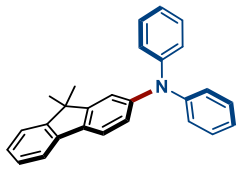


3d

The reaction was carried out with 153.4 mg (0.50 mmol) of **1d** and 84.9 mg (0.50 mmol) of **2a**. The product **3d** was obtained as a white powder (164.3 mg, 0.42 mmol, 83% yield) after purification by silica-gel column chromatography (SiO_2, CH_2Cl_2/hexane, 0:100–5:95).

^{1}H NMR (400 MHz, $CDCl_3$, δ): 7.07 (t, *J* = 7.3 Hz, 2H), 7.20–7.24 (m, 4H), 7.28–7.32 (m, 4H), 7.38 (dd, *J* = 1.6, 8.7 Hz, 1H), 7.52 (t, *J* = 7.5 Hz, 1H), 7.57–7.63 (m, 3H), 8.28 (d, *J* = 8.3 Hz, 1H), 8.32 (d, *J* = 2.0 Hz, 1H), 8.48–8.53 (m, 2H), 8.61 (d, *J* = 7.5 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$, δ): 117.2 (*C*H), 123.0 (*C*H), 123.2 (*C*H), 123.4 (*C*H), 123.5 (*C*H), 124.0 (*C*H), 124.6 (*C*H), 125.1 (*C*), 126.6 (*C*H), 127.1 (*C*H), 127.4 (*C*H), 129.2 (*C*), 129.4 (*C*), 129.5 (*C*H), 129.9 (*C*), 130.2 (*C*), 131.0 (*C*), 147.1 (*C*), 147.8 (*C*). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{30}H_{21}N$, 395.1674; found, 395.1658.

9,9-Dimethyl-*N*,*N*-diphenyl-9*H*-fluoren-2-amine (3e).

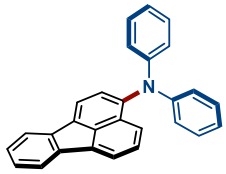


3e

The reaction was carried out with 137.4 mg (0.50 mmol) of **1e** and 84.2 mg (0.50 mmol) of **2a**. The product **3e** was obtained as a white powder (131.7 mg, 0.36 mmol, 73% yield) after purification by silica-gel column chromatography (SiO_2, CH_2Cl_2/hexane, 0:100–30:70).

^{1}H NMR (400 MHz, $CDCl_3$, δ): 1.40 (s, 6H), 6.97–7.05 (m, 3H), 7.13 (d, *J* = 7.5 Hz, 4H), 7.19 (d, *J* = 1.6 Hz, 1H), 7.23–7.32 (m, 6H), 7.38 (d, *J* = 7.1 Hz, 1H), 7.56 (d, *J* = 8.3 Hz, 1H), 7.63 (d, *J* = 7.5 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$, δ): 27.2 (*C*H$_3$), 46.9 (*C*), 118.7 (*C*H), 119.5 (*C*H), 120.7 (*C*H), 122.6 (*C*H), 122.7 (*C*H), 123.4 (*C*H), 124.2 (*C*H), 126.5 (*C*H), 127.1 (*C*H), 129.3 (*C*H), 134.2 (*C*), 139.1 (*C*), 147.4 (*C*), 148.1 (*C*), 153.6 (*C*), 155.1 (*C*). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{27}H_{23}N$, 361.1831; found, 361.1826.

***N*,*N*-Diphenylfluoranthen-3-amine (3f).**

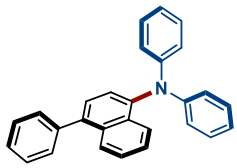


3f

The reaction was carried out with 140.5 mg (0.50 mmol) of **1f** and 84.4 mg (0.50 mmol) of **2a**. The product **3f** was obtained as a yellow powder (171.1 mg, 0.46 mmol, 93% yield) after purification by silica-gel column chromatography (SiO_2, CH_2Cl_2/hexane, 0:100–5:95).

^{1}H NMR (400 MHz, $CDCl_3$, δ): 6.98 (dt, *J* = 3.6, 10.0 Hz, 2H), 7.1 (dd, *J* = 0.8, 7.5 Hz, 4H), 7.23 (t, *J* = 7.5 Hz, 4H), 7.31–7.42 (m, 4H), 7.62 (d, *J* = 7.7 Hz, 1H), 7.83–7.88 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$, δ): 120.2 (*C*H), 121.2 (*C*H), 121.3 (*C*H), 121.6 (*C*H), 122.3 (*C*H), 123.1 (*C*H), 124.5 (*C*H), 127.2 (*C*H), 127.3 (*C*H), 127.76 (*C*H), 127.79 (*C*H), 127.9 (*C*), 129.3 (*C*H), 134.25 (*C*), 134.31 (*C*), 137.4 (*C*), 139.1 (*C*), 139.6 (*C*), 144.8 (*C*), 149.0 (*C*). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{28}H_{19}N$, 369.1518; found, 369.1516.

***N,N*,4-Triphenylnaphthalen-1-amine (3g).**

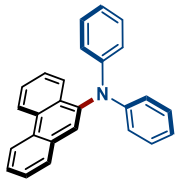


3g

The reaction was carried out with 141.5 mg (0.50 mmol) of **1g** and 84.6 mg (0.5 mmol) of **2a**. The product **3g** was obtained as a yellow powder (68.5 mg, 0.18 mmol, 37% yield) after purification by silica-gel column chromatography (SiO_2, CH_2Cl_2/hexane, 0:100–5:95).

^{1}H NMR (400 MHz, $CDCl_3$, δ): 6.94 (t, *J* = 7.3 Hz, 2H), 7.08 (dd, *J* = 1.2, 7.5 Hz, 4H), 7.21 (t, *J* = 7.9 Hz, 4H), 7.34–7.46 (m, 5H), 7.48–7.54 (m, 4H), 7.93 (dd, *J* = 1.8, 7.3 Hz, 1H), 8.04 (d, *J* = 7.5 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$, δ): 121.8 (*C*H), 122.0 (*C*H), 124.7 (*C*H), 126.3 (*C*H), 126.4 (*C*H), 126.8 (*C*H), 126.9 (*C*H), 127.4 (*C*H), 127.6 (*C*H), 128.4 (*C*H), 129.3 (*C*H), 130.3 (*C*H), 131.5 (*C*), 133.4 (*C*), 138.8 (*C*), 140.7 (*C*), 143.2 (*C*), 148.6 (*C*). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{28}H_{21}N$, 371.1674; found, 371.1658.

***N,N*-Diphenylphenanthren-9-amine (3h).**

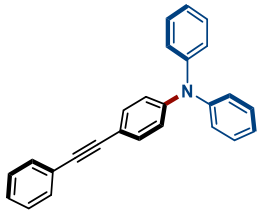


3h

The reaction was carried out with 128.6 mg (0.50 mmol) of **1h** and 84.9 mg (0.50 mmol) of **2a**. The product **3h** was obtained as a white powder (51.7 mg, 0.15 mmol, 30% yield) after purification by silica-gel column chromatography (SiO_2, CH_2Cl_2/hexane, 0:100–5:95).

^{1}H NMR (400 MHz, $CDCl_3$, δ): 6.95 (t, *J* = 7.1 Hz, 2H), 7.10 (d, *J* = 8.7 Hz, 4H), 7.20 (t, *J* = 7.5 Hz, 4H), 7.47 (t, *J* = 7.5 Hz, 1H), 7.57 (t, *J* = 7.3 Hz, 1H), 7.60 (s, 1H), 7.64 (t, *J* = 7.1 Hz, 2H), 7.76 (d, *J* = 7.5 Hz, 1H), 8.05 (d, *J* = 7.9 Hz, 1H), 8.70 (d, *J* = 8.3 Hz, 1H), 8.74 (d, *J* = 8.3 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$, δ): 121.9 (*C*H), 122.0 (*C*H), 122.7 (*C*H), 123.2 (*C*H), 125.2 (*C*H), 126.6 (*C*H), 126.95 (*C*H), 126.99 (*C*H), 127.1 (*C*H), 127.7 (*C*H), 128.4 (*C*H), 129.3 (*C*H), 129.5 (*C*), 130.6 (*C*), 132.3 (*C*), 132.6 (*C*), 142.2 (*C*), 148.4 (*C*). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{26}H_{19}N$, 345.1518; found, 345.1510.

***N*,*N*-Diphenyl-4-(phenylethynyl)aniline (3j).**

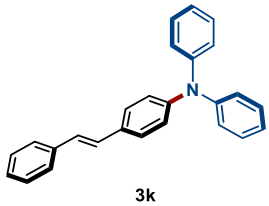


3j

The reaction was carried out with 128.5 mg (0.50 mmol) of **1j** and 84.9 mg (0.50 mmol) of **2a**. The product **3j** was obtained as a white powder (144.8 mg, 0.42 mmol, 84% yield) after purification by silica-gel column chromatography (SiO_2, CH_2Cl_2/hexane, 0:100–3:97).

^{1}H NMR (400 MHz, $CDCl_3$, δ): 7.00 (d, J = 1.6 Hz, 2H), 7.06 (t, J = 7.3 Hz, 2H), 7.11 (d, J = 7.9 Hz, 4H), 7.25–7.39 (m, 9H), 7.51 (dd, J = 1.8, 7.7 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$, δ): 88.8 (*C*), 89.8 (*C*), 116.2 (*C*), 122.4 (*C*H), 123.6 (*C*H), 123.7 (*C*), 125.0 (*C*H), 128.0 (*C*H), 128.4 (*C*H), 129.5 (*C*H), 131.5 (*C*H), 132.6 (*C*H), 147.2 (*C*), 147.9 (*C*). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{26}H_{19}N$, 345.1518; found, 345.1501.

(*E*)-*N*,*N*-Diphenyl-4-styrylaniline (3k).

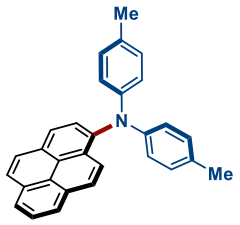


3k

The reaction was carried out with 129.9 mg (0.50 mmol) of **1k** and 84.0 mg (0.50 mmol) of **2a**. The product **3k** was obtained as a orange powder (153.0 mg, 0.44 mmol, 89% yield) after purification by reprecipitation (CH_2Cl_2→MeOH).

^{1}H NMR (400 MHz, $CDCl_3$, δ): 7.01–7.07 (m, 5H), 7.08–7.12 (m, 4H), 7.22–7.29 (m, 6H), 7.33–7.40 (m, 4H), 7.49 (d, J = 7.1 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$, δ): 123.1 (*C*H), 123.7 (*C*H), 124.5 (*C*H), 126.4 (*C*H), 127.1 (*C*H), 127.4 (*C*H), 127.5 (*C*H), 128.2 (*C*H), 128.7 (*C*H), 129.4 (*C*H), 131.5 (*C*), 137.6 (*C*), 147.4 (*C*), 147.6 (*C*). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{26}H_{21}N$, 347.1674; found, 347.1662.

***N*,*N*-Di-*p*-tolylpyren-1-amine (3l).**

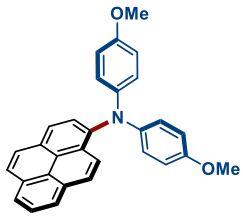


3l

The reaction was carried out with 140.6 mg (0.50 mmol) of **1c** and 98.3 mg (0.50 mmol) of **2b**. The product **3l** was obtained as a yellow-green powder (172.7 mg, 0.43 mmol, 87% yield) after purification by silica-gel column chromatography (SiO_2, CH_2Cl_2/hexane, 0:100–3:97).

^{1}H NMR (400 MHz, $CDCl_3$, δ): 2.28 (s, 6H), 6.93–7.01 (m, 8H), 7.79 (d, J = 8.3 Hz, 1H), 7.92 (d, J = 8.7 Hz, 1H), 7.97 (t, J = 7.5 Hz, 1H), 8.04 (s, 2H), 8.09 (d, J = 7.1 Hz, 1H), 8.13–8.16 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$, δ): 20.8 (*C*H$_3$), 122.2 (*C*H), 123.6 (*C*H), 124.96 (*C*), 125.05 (*C*H), 125.1 (*C*H), 126.1 (*C*H), 126.2 (*C*H), 126.4 (*C*), 126.9 (*C*H), 127.3 (*C*H), 127.5 (*C*H), 127.8 (*C*H), 128.0 (*C*), 129.3 (*C*), 129.9 (*C*H), 131.1 (*C*), 131.2 (*C*), 131.3 (*C*), 141.5 (*C*), 146.7 (*C*). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{30}H_{23}N$, 397.1831; found, 397.1814.

***N*,*N*-Bis(4-methoxyphenyl)pyren-1-amine (3m).**

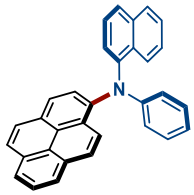


3m

The reaction was carried out with 140.7 mg (0.50 mmol) of **1c** and 114.5 mg (0.50 mmol) of **2c**. The product **3m** was obtained as a yellow powder (199.6 mg, 0.46 mmol, 93% yield) after purification by silica-gel column chromatography (SiO_2, CH_2Cl_2/hexane, 0:100–30:70).

^{1}H NMR (392 MHz, $CDCl_3$, δ): 3.76 (s, 6H), 6.76 (d, J = 9.1 Hz, 4H), 6.97 (d, J = 8.7 Hz, 4H), 7.75 (d, J = 7.9 Hz, 1H), 7.90 (d, J = 9.1 Hz, 1H), 7.96 (t, J = 7.7 Hz, 1H), 8.02 (s, 2H), 8.08–8.17 (m, 4H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 55.5 (*C*H$_3$), 114.6 (*C*H), 123.66 (*C*H), 123.71 (*C*H), 124.91 (*C*H), 124.96 (*C*), 125.0 (*C*H), 126.0 (*C*H), 126.2 (*C*H), 126.5 (*C*), 126.7 (*C*H), 126.8 (*C*H), 127.3 (*C*H), 127.4 (*C*), 127.5 (*C*H), 128.9 (*C*), 131.1 (*C*), 131.4 (*C*), 142.1 (*C*), 143.1 (*C*), 154.7 (*C*). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{30}H_{23}NO_2$, 429.1729; found, 429.1709.

***N*-(Naphthalen-1-yl)-*N*-phenylpyren-1-amine (3n).**

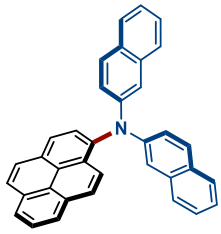


3n

The reaction was carried out with 140.3 mg (0.50 mmol) of **1c** and 109.3 mg (0.50 mmol) of **2d**. The product **3n** was obtained as a yellow powder (134.0 mg, 0.32 mmol, 64% yield) after purification by silica-gel column chromatography (SiO_2, CH_2Cl_2/hexane, 0:100–25:75).

^{1}H NMR (392 MHz, $CDCl_3$, δ): 6.77 (d, *J* = 7.5 Hz, 2H), 6.89 (t, *J* = 6.9 Hz, 1H), 7.13 (t, *J* = 7.5 Hz, 2H), 7.26–7.27 (m, 1H), 7.33–7.39 (m, 2H), 7.46 (t, *J* = 7.7 Hz, 1H), 7.71 (d, *J* = 7.9 Hz, 1H), 7.77 (dd, *J* = 1.4, 8.1 Hz, 1H), 7.89–7.92 (m, 2H), 7.98 (dt, *J* = 4.0, 10.7 Hz, 1H), 8.02 (br, s, 2H), 8.05–8.17 (m, 4H), 8.25 (d, *J* = 8.7 Hz, 1H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 120.5 (*C*H), 120.9 (*C*H), 123.6 (*C*H), 124.6 (*C*H), 125.0 (*C*), 125.1 (*C*H), 125.2 (*C*H), 125.6 (*C*H), 125.8 (*C*H), 125.87 (*C*H), 125.94 (*C*H), 126.2 (*C*H), 126.27 (*C*H), 126.29 (*C*H), 126.42 (*C*H), 126.45 (*C*), 126.8 (*C*H), 126.9 (*C*), 127.4 (*C*H), 127.9 (*C*H), 128.7 (*C*H), 129.1 (*C*), 129.2 (*C*H), 130.4 (*C*), 131.2 (*C*), 131.5 (*C*), 135.4 (*C*), 142.5 (*C*), 145.0 (*C*), 150.8 (*C*). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{32}H_{21}N$, 419.1674; found, 419.1656.

***N*,*N*-Di(naphthalen-2-yl)pyren-1-amine (3o).**

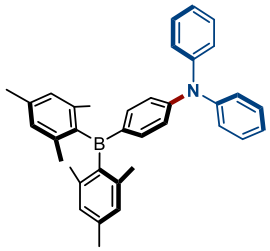


3o

The reaction was carried out with 140.6 mg (0.50 mmol) of **1c** and 109.6 mg (0.50 mmol) of **2e**. The product **3o** was obtained as a yellow powder (140.2 mg, 0.30 mmol, 60% yield) after purification by silica-gel column chromatography (SiO_2, CH_2Cl_2/hexane, 0:100–30:70).

^{1}H NMR (392 MHz, $CDCl_3$, δ): 7.30–7.40 (m, 8H), 7.47–7.50 (m, 2H), 7.71–7.77 (m, 4H), 7.88 (d, *J* = 3.2 Hz, 1H), 7.91 (d, *J* = 2.0 Hz, 1H), 7.99 (t, *J* = 7.7 Hz, 1H), 8.09–8.11 (m, 3H), 8.19–8.22 (m, 3H). ^{13}C NMR (99 MHz, $CDCl_3$, δ): 118.5 (*C*H), 123.3 (*C*H), 123.4 (*C*H), 124.4 (*C*H), 124.9 (*C*), 125.3 (*C*H), 125.4 (*C*H), 126.2 (*C*H), 126.4 (*C*H), 126.48 (*C*H), 126.53 (*C*), 127.0 (*C*H), 127.3 (*C*H), 127.7 (*C*H), 127.8 (*C*H), 128.15 (*C*), 128.20 (*C*H), 129.1 (*C*H), 129.8 (*C*), 129.9 (*C*), 131.2 (*C*), 131.3 (*C*), 134.6 (*C*), 140.9 (*C*), 146.5 (*C*). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{36}H_{23}N$, 469.1831; found, 469.1826.

4-(Dimesitylboraneyl)-*N*,*N*-diphenylaniline (3p).

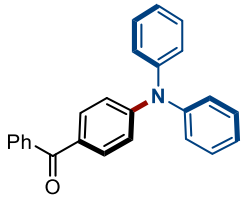


3p

The reaction was carried out with 202.2 mg (0.50 mmol) of **1l** and 84.3 mg (0.50 mmol) of **2a**. The product **3p** was obtained as a yellow powder (91.1 mg, 0.21 mmol, 42% yield) after purification by silica-gel column chromatography (SiO_2, CH_2Cl_2/hexane, 0:100–2:98) and GPC.

^{1}H NMR (400 MHz, $CDCl_3$, δ): 2.06 (s, 12H), 2.28 (s, 6H), 6.79 (s, 4H), 6.90 (d, J = 8.8 Hz, 2H), 7.08 (t, J = 6.9 Hz, 2H), 7.15 (d, J = 6.9 Hz, 4H), 7.25–7.30 (m, 4H), 7.35 (d, J = 8.8 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$, δ): 21.3 (*C*H_3), 23.6 (*C*H_3), 119.8 (*C*H), 124.3 (*C*H), 126.0 (*C*H), 128.2 (*C*H), 129.5 (*C*H), 138.1 (*C*), 138.8 (*C*H), 140.8 (*C*), 146.9 (*C*), 151.4 (*C*). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{36}H_{36}BN$, 492.2977; found, 492.2958.

[4-(Diphenylamino)phenyl](phenyl)methanone (3q).

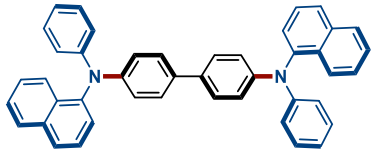


3q

The reaction was carried out with 131.0 mg (0.50 mmol) of **1m** and 84.1 mg (0.50 mmol) of **2a**. The product **3q** was obtained as a white powder (167.1 mg, 0.48 mmol, 96% yield) after purification by silica-gel column chromatography (SiO_2, CH_2Cl_2/hexane, 0:100–70:30).

^{1}H NMR (400 MHz, $CDCl_3$, δ): 6.98–7.04 (m, 2H), 7.12–7.19 (m, 6H), 7.33 (t, J = 7.9 Hz, 4H), 7.46 (t, J = 7.5 Hz, 2H), 7.52–7.58 (m, 1H), 7.68–7.73 (m, 2H), 7.75–7.79 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$, δ): 119.5 (*C*H), 124.6 (*C*H), 125.9 (*C*H), 128.1 (*C*H), 129.5 (*C*H), 131.7 (*C*H), 131.9 (*C*H), 138.4 (*C*), 146.4 (*C*), 151.8 (*C*). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{25}H_{19}NO$, 349.1467; found, 349.1476.

N^4,$N^{4'}$-Di(naphthalen-1-yl)-N^4,$N^{4'}$-diphenyl-(1,1'-biphenyl)-4,4'-diamine (3r).



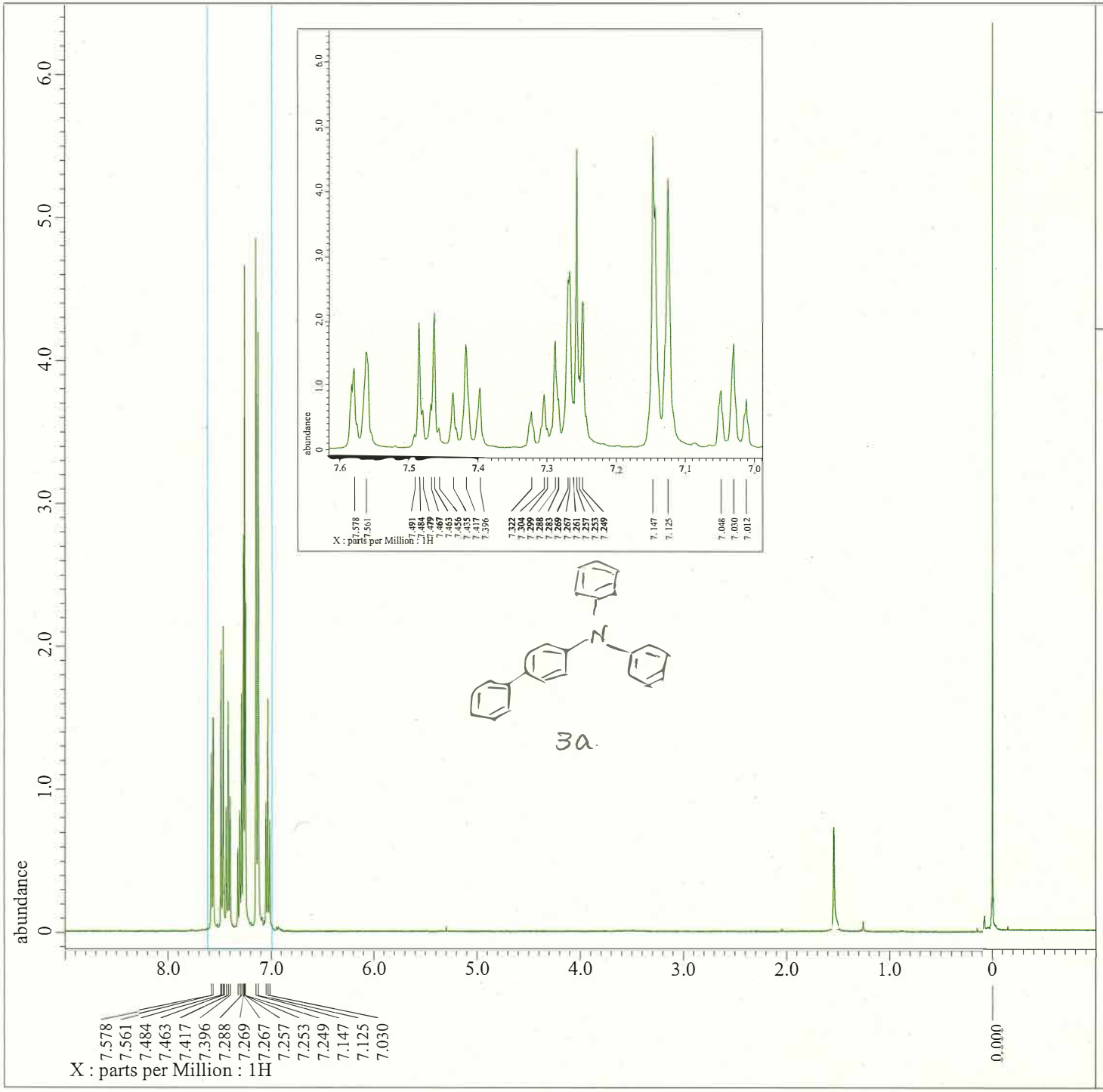
3r

The reaction was carried out with 93.2 mg (0.30 mmol) of **1o** and 131.0 mg (0.60 mmol) of **2d**. The product **3r** was obtained as a yellow powder (169.9 mg, 0.29 mmol, 96% yield) after purification by silica-gel column chromatography (SiO_2, CH_2Cl_2/hexane, 0:100–30:70).

^{1}H NMR (400 MHz, $CDCl_3$, δ): 6.93 (t, J = 7.3 Hz, 2H), 7.04 (t, J = 7.5 Hz, 8H), 7.20 (t, J = 7.7 Hz, 4H), 7.33–7.39 (m, 8H), 7.46 (q, J = 7.9 Hz, 4H), 7.77 (d, J = 8.3 Hz, 2H), 7.80 (d, J = 7.9 Hz, 2H), 7.94 (d, J = 8.3 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$, δ): 121.9 (*C*H), 122.0 (*C*H), 122.1 (*C*H), 124.4 (*C*H), 126.3 (*C*H), 126.5 (*C*H), 126.6 (*C*H), 127.2 (*C*H), 127.4 (*C*H), 128.5 (*C*H), 129.2 (*C*H), 131.3 (*C*), 133.9 (*C*), 135.4 (*C*), 143.6 (*C*), 147.3 (*C*), 148.4 (*C*). HRMS-EI (*m*/*z*): $[M]^+$ calcd for $C_{44}H_{32}N_2$, 588.2566; found, 588.2561.

8. References

1. Kubota, K.; Seo, T.; Koide, K.; Hasegawa, Y.; Ito, H. *Nat. Commun.* **2019**, *10*, 1–11.
2. Proń, A.; Baumgarten, M.; Müllen, K. *Org. Lett.* **2010**, *12*, 4236–4239.
3. Matsubara, K.; Ueno, K.; Koga, Y.; Hara, K. *J. Org. Chem.* **2007**, *72*, 5069–5076.
4. Smith, C. J.; Tsang, M. W. S.; Holmes, A. B.; Danheiser, L.; Tester, J. W. *Org. Biomol. Chem.* **2005**, *3*, 3767–3781.

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machinephase
ppm

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Dim_Units           = [ppm]
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Spectrometer        = DELTA2_NMR

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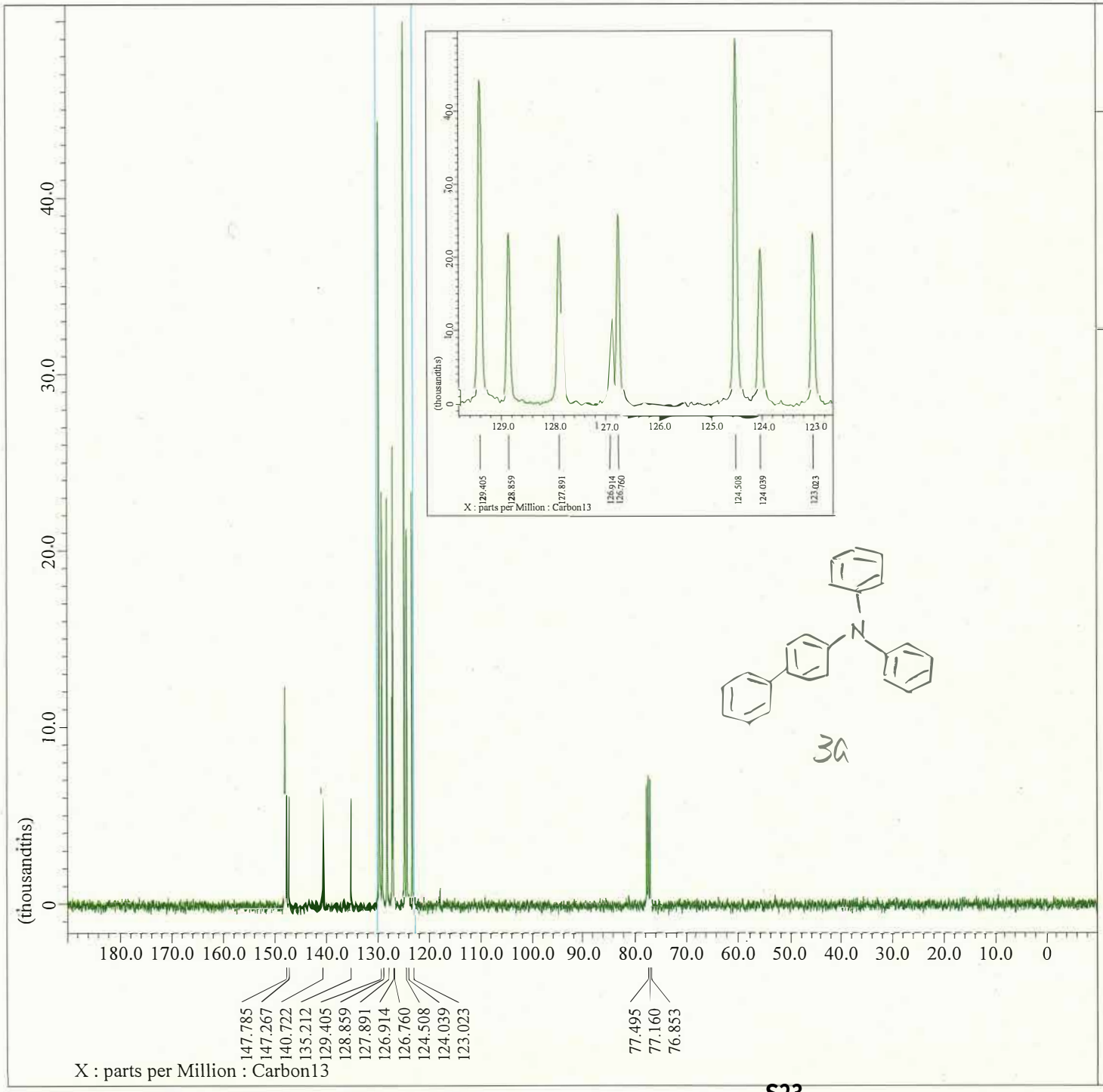


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machinephase
ppm
thresh( 5[%], 1 )
peak_pick( 0[Hz], 0.1[ppm], Peaks, 0[Hz] )

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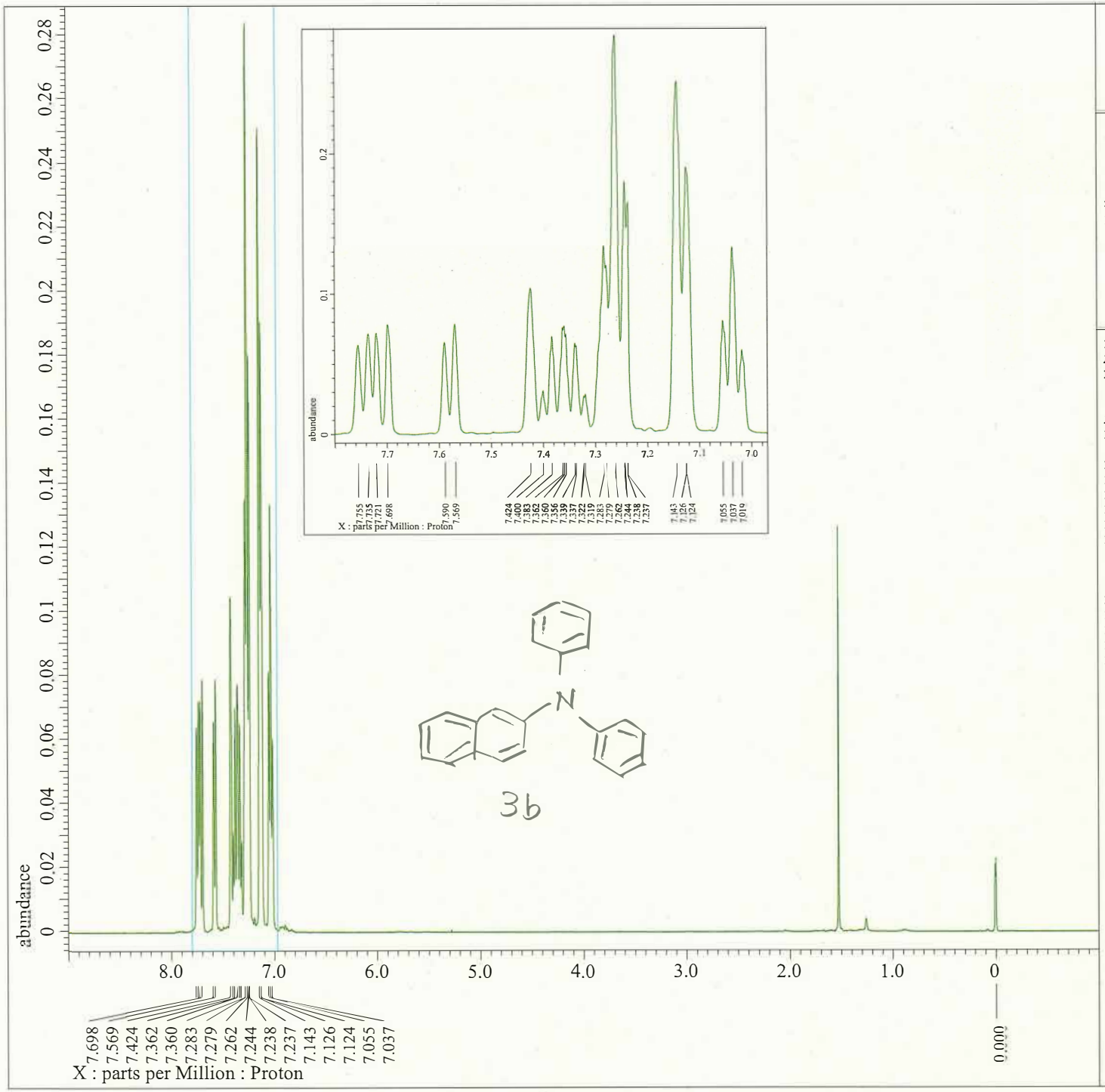
Author                      = delta
Experiment                  = carbon.jxp
Sample_Id                   = RIK-311-pureC
Solvent                     = CHLOROFORM-D
Actual_Start_Time           =  5-JUN-2020 12:5
Revision_Time               =  7-AUG-2020 16:5

Data_Format                 = 1D COMPLEX
Dim_Size                    = 26214
X_Domain                    = Carbon13
Dim_Title                   = Carbon13
Dim_Units                   = [ppm]
Dimensions                  = X
Spectrometer                = JNM-ECZ400S/L1

Field_Strength              = 9.389766[T] (400
X_Acq_Duration              = 1.03809024[s]
X_Domain                    = Carbon13
X_Freq                      = 100.52530333[MHz
X_Offset                    = 100[ppm]
X_Points                    = 32768
X_Prescans                  = 4
X_Resolution                = 0.96330739[Hz]
X_Sweep                     = 31.56565657[kHz]
X_Sweep_Clipped             = 25.25252525[kHz]
Irr_Domain                  = Proton
Irr_Freq                    = 399.78219838[MHz
Irr_Offset                  = 5[ppm]
Blanking                    = 5[us]
Clipped                     = FALSE
Scans                       = 64
Total_Scans                 = 64

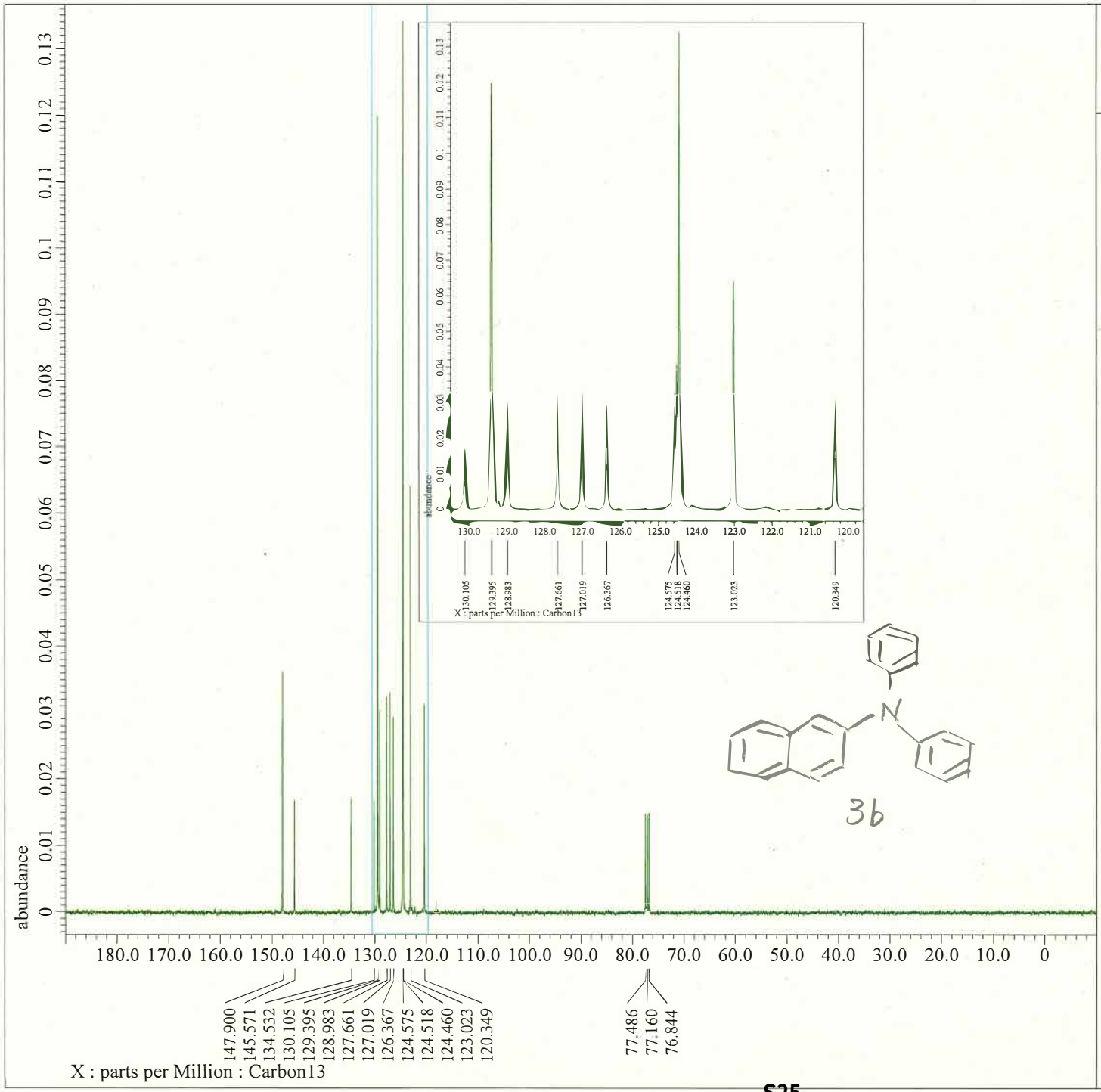
Relaxation_Delay            = 2[s]
Recvr_Gain                  = 52
Temp_Get                    = 19.9[dC]
X_90_Width                  = 10.6[us]
X_Acq_Time                  = 1.03809024[s]
X_Angle                     = 30[deg]
X_Atn                       = 8.8[dB]
X_Pulse                     = 3.53333333[us]
Irr_Atn_Dec                 = 31.25[dB]
Irr_Atn_Dec_Calc            = 31.25[dB]
Irr_Atn_Dec_Default_Calc    = 31.25[dB]
Irr_Atn_Noe                 = 31.25[dB]
Irr_Dec_Bandwidth_Hz        = 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm       = 11.96303566[ppm]
Irr_Dec_Freq                = 399.78219838[MHz
```




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

以下に由来:: RIK-313-pureH_PROTON-1-1.jdf
```

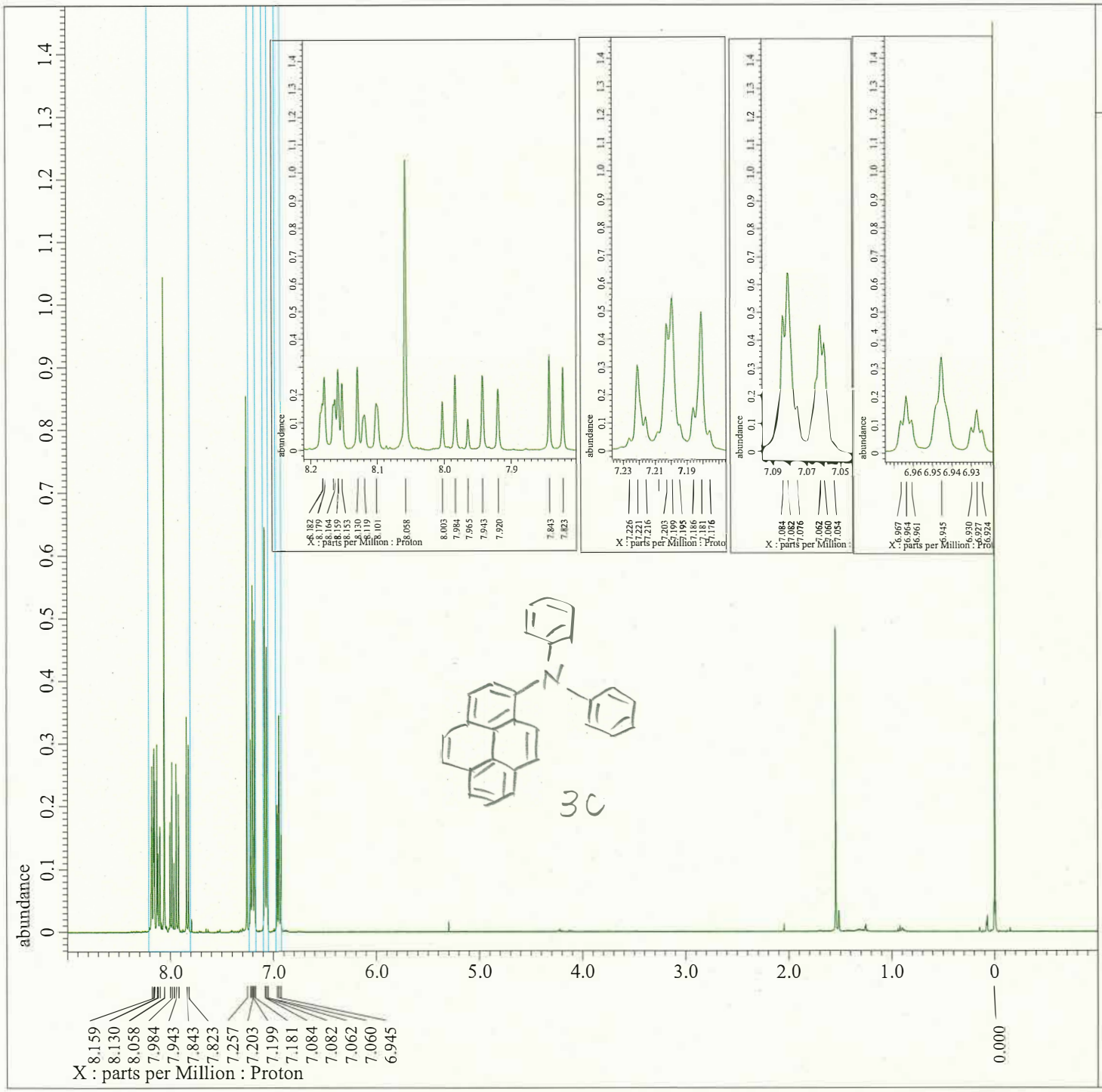
Filename	= RIK-313-pureH_PROTO
Author	= delta
Experiment	= proton.jxp
Sample_Id	= RIK-313-pureH
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 3-JUN-2020 12:22:4
Revision_Time	= 7-AUG-2020 15:01:5
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ400S/L1
Field_Strength	= 9.389766[T] (400[MH
X_Acq_Duration	= 4.37256192[s]
X_Domain	= Proton
X_Freq	= 399.78219838[MHz]
X_Offset	= 5[ppm]
X_Points	= 32768
X_Prescans	= 0
X_Resolution	= 0.22869888[Hz]
X_Sweep	= 7.4940048[kHz]
X_Sweep_Clipped	= 5.99520384[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.78219838[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 399.78219838[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 4[s]
Recvr_Gain	= 42
Temp_Get	= 21.4[dC]
X_90_Width	= 5.6[us]
X_Acq_Time	= 4.37256192[s]
X_Angle	= 45[deg]
X_Atn	= 5[dB]
X_Pulse	= 2.8[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 400
Dante_Presat	= FALSE




```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
thresh( 5[%], 1 )
peak_pick( 0[Hz], 0.1[ppm], Peaks, 0[Hz] )

以下に由来:: RIK-313-pureC_CARBON-1-1.jdf
```

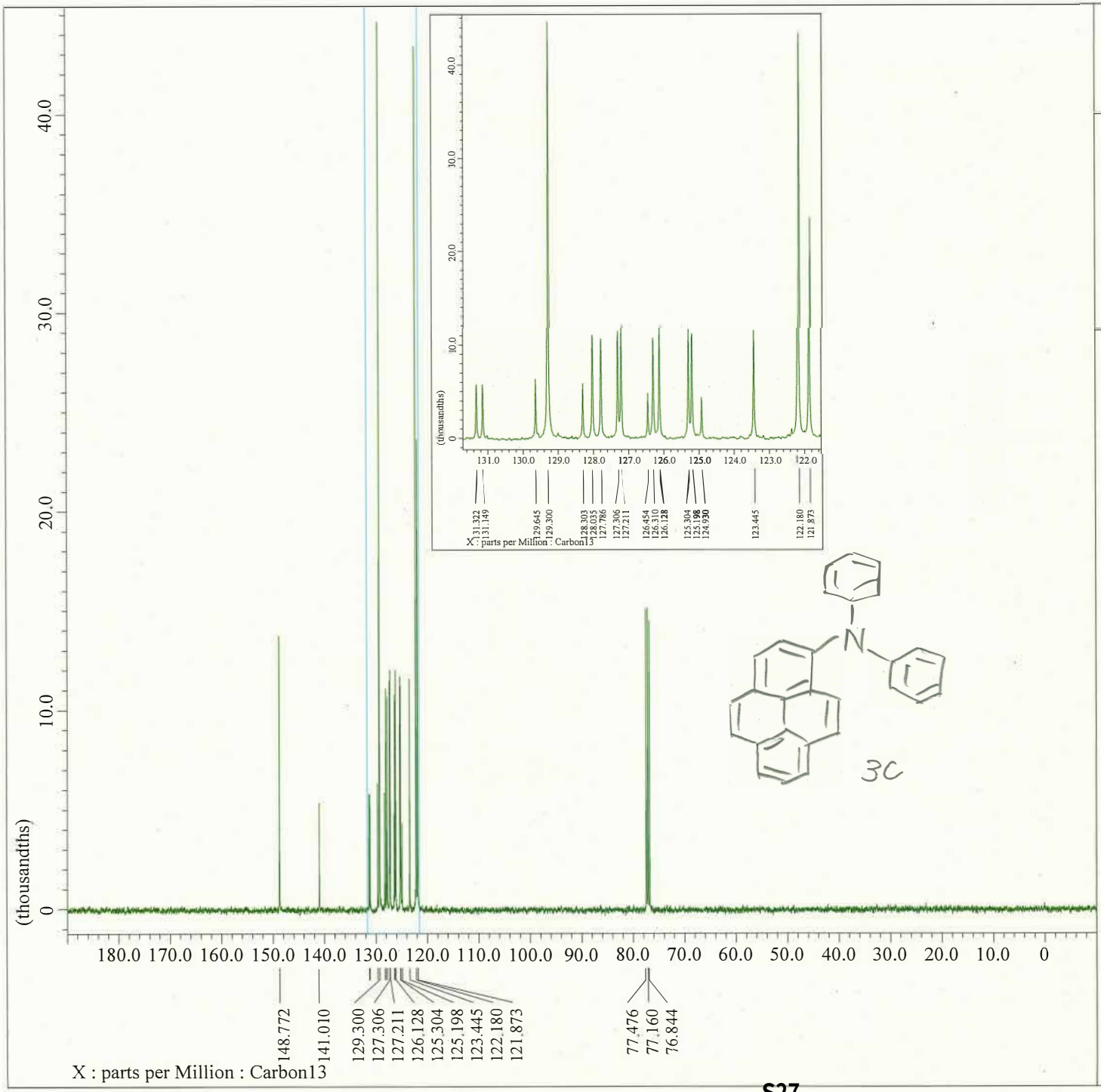
Filename	= RIK-313-pureC_CA
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= RIK-313-pureC
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 3-JUN-2020 12:2
Revision_Time	= 7-AUG-2020 16:5
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ400S/L1
Field_Strength	= 9.389766[T] (400
X_Acq_Duration	= 1.03809024[s]
X_Domain	= Carbon13
X_Freq	= 100.52530333[MHz
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.96330739[Hz]
X_Sweep	= 31.56565657[kHz]
X_Sweep_Clipped	= 25.25252525[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.78219838[MHz
Irr_Offset	= 5[ppm]
Blanking	= 5[us]
Clipped	= FALSE
Scans	= 64
Total_Scans	= 64
Relaxation_Delay	= 2[s]
Recvr_Gain	= 52
Temp_Get	= 20.9[dC]
X_90_Width	= 10.6[us]
X_Acq_Time	= 1.03809024[s]
X_Angle	= 30[deg]
X_Atn	= 8.8[dB]
X_Pulse	= 3.53333333[us]
Irr_Atn_Dec	= 31.25[dB]
Irr_Atn_Dec_Calc	= 31.25[dB]
Irr_Atn_Dec_Default_Calc	= 31.25[dB]
Irr_Atn_Noe	= 31.25[dB]
Irr_Dec_Bandwidth_Hz	= 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm	= 11.96303566[ppm]
Irr_Dec_Freq	= 399.78219838[MHz




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

以下に由来:: RIK-324-pureH_PROTON-1-1.jdf
```

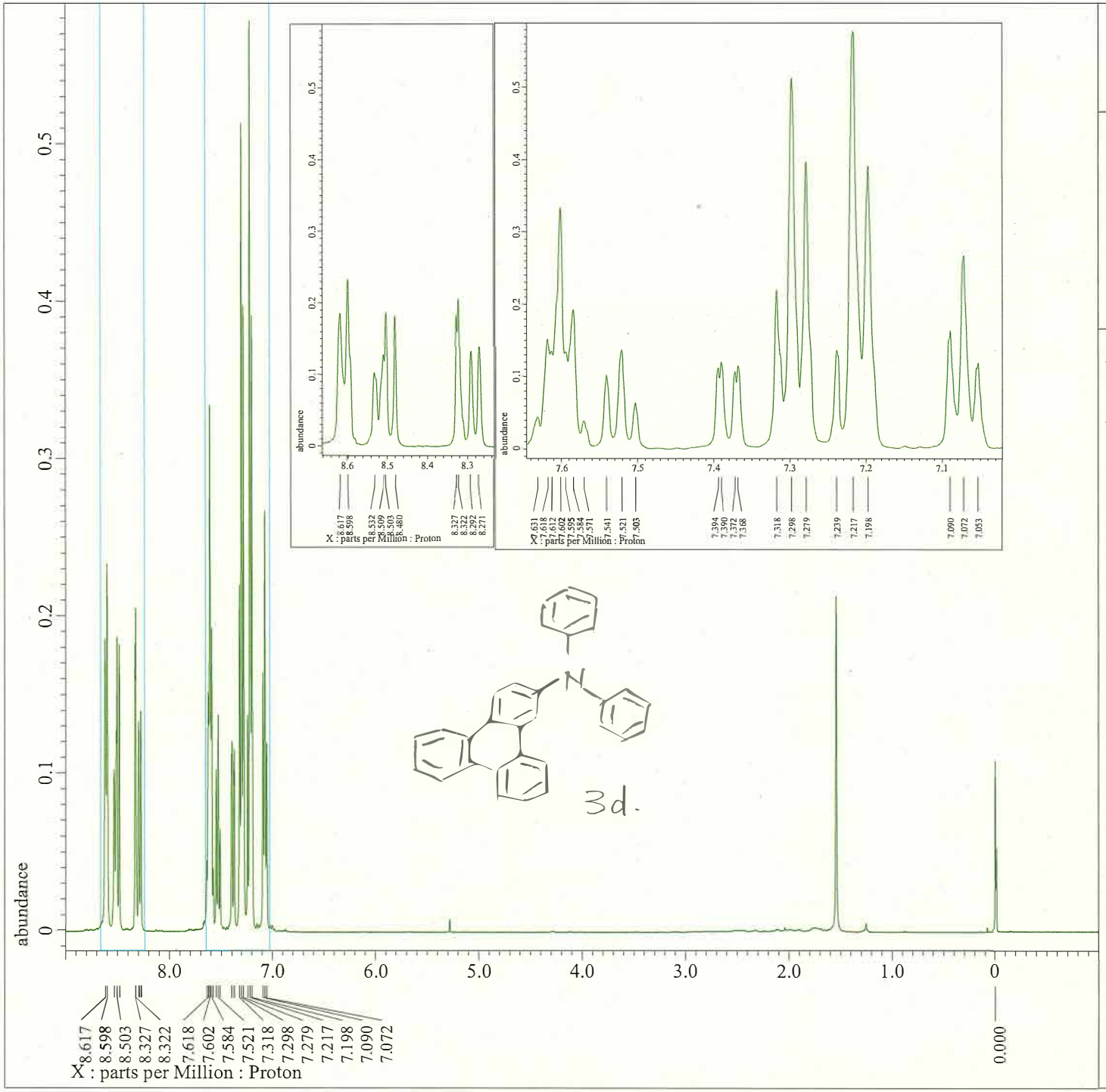
Filename	= RIK-324-pureH_PROTO
Author	= delta
Experiment	= proton.jxp
Sample_Id	= RIK-324-pureH
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 30-JUL-2020 12:14:1
Revision_Time	= 7-AUG-2020 15:07:3
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ400S/L1
Field_Strength	= 9.389766[T] (400[MH
X_Acq_Duration	= 4.37256192[s]
X_Domain	= Proton
X_Freq	= 399.78219838[MHz]
X_Offset	= 5[ppm]
X_Points	= 32768
X_Prescans	= 0
X_Resolution	= 0.22869888[Hz]
X_Sweep	= 7.4940048[kHz]
X_Sweep_Clipped	= 5.99520384[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.78219838[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 399.78219838[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 4[s]
Recvr_Gain	= 62
Temp_Get	= 19.5[dC]
X_90_Width	= 5.6[us]
X_Acq_Time	= 4.37256192[s]
X_Angle	= 45[deg]
X_Atn	= 5[dB]
X_Pulse	= 2.8[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 400
Dante_Presat	= FALSE




```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
thresh( 5[%], 1 )
peak_pick( 0[Hz], 0.1[ppm], Peaks, 0[Hz] )

以下に由来:: RIK-324-pureC_CARBON-1-1.jdf
```

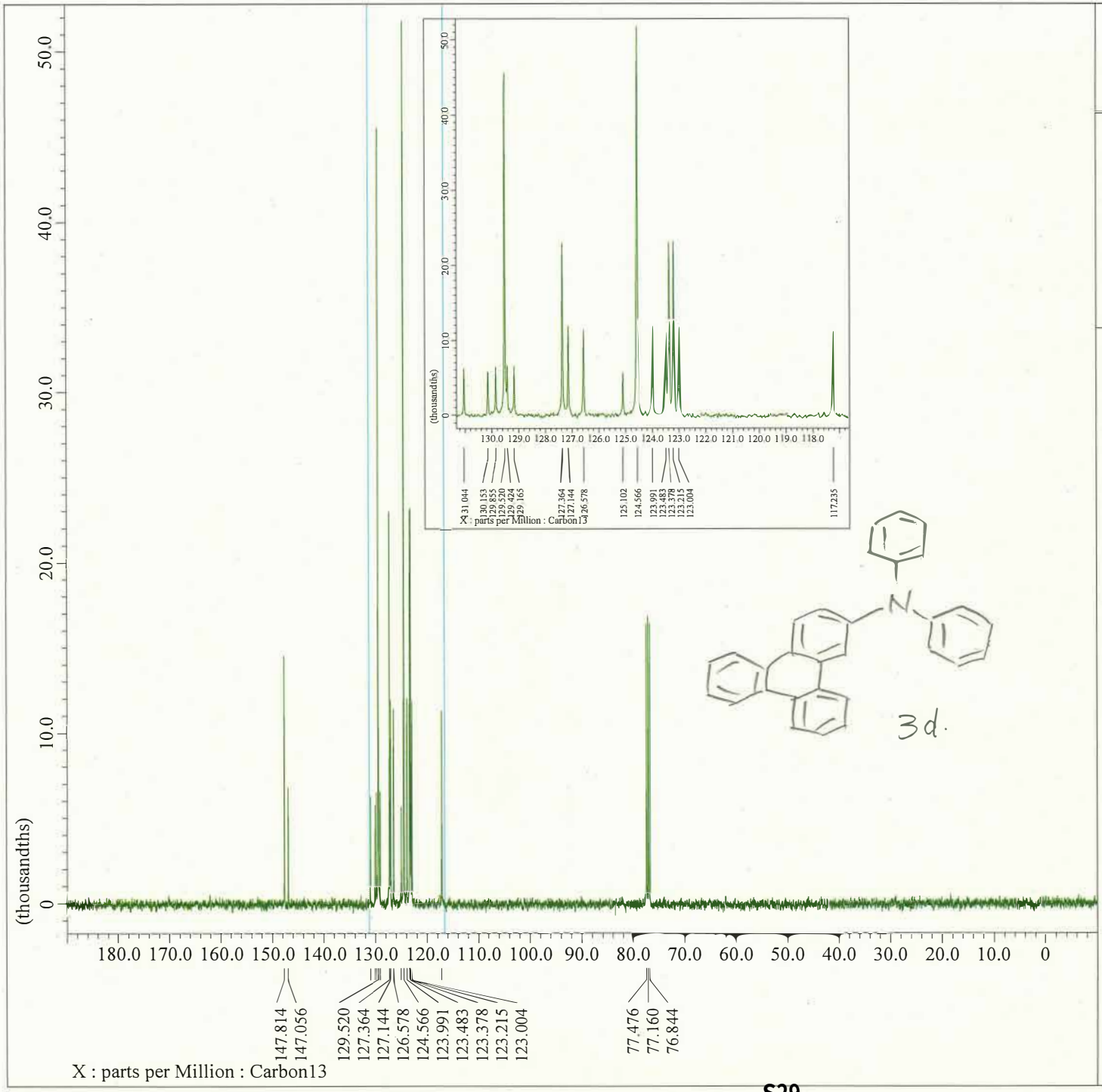
Filename	= RIK-324-pureC_CA
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= RIK-324-pureC
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 3-JUN-2020 10:2
Revision_Time	= 7-AUG-2020 16:5
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ400S/L1
Field_Strength	= 9.389766[T] (400
X_Acq_Duration	= 1.03809024[s]
X_Domain	= Carbon13
X_Freq	= 100.52530333[MHz
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.96330739[Hz]
X_Sweep	= 31.56565657[kHz]
X_Sweep_Clipped	= 25.25252525[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.78219838[MHz
Irr_Offset	= 5[ppm]
Blanking	= 5[us]
Clipped	= FALSE
Scans	= 256
Total_Scans	= 256
Relaxation_Delay	= 2[s]
Recvr_Gain	= 52
Temp_Get	= 20.6[dC]
X_90_Width	= 10.6[us]
X_Acq_Time	= 1.03809024[s]
X_Angle	= 30[deg]
X_Atn	= 8.8[dB]
X_Pulse	= 3.53333333[us]
Irr_Atn_Dec	= 31.25[dB]
Irr_Atn_Dec_Calc	= 31.25[dB]
Irr_Atn_Dec_Default_Calc	= 31.25[dB]
Irr_Atn_Noe	= 31.25[dB]
Irr_Dec_Bandwidth_Hz	= 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm	= 11.96303566[ppm]
Irr_Dec_Freq	= 399.78219838[MHz




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

以下に由来:: RIK-318-pureH_PROTON-1-1.jdf
```

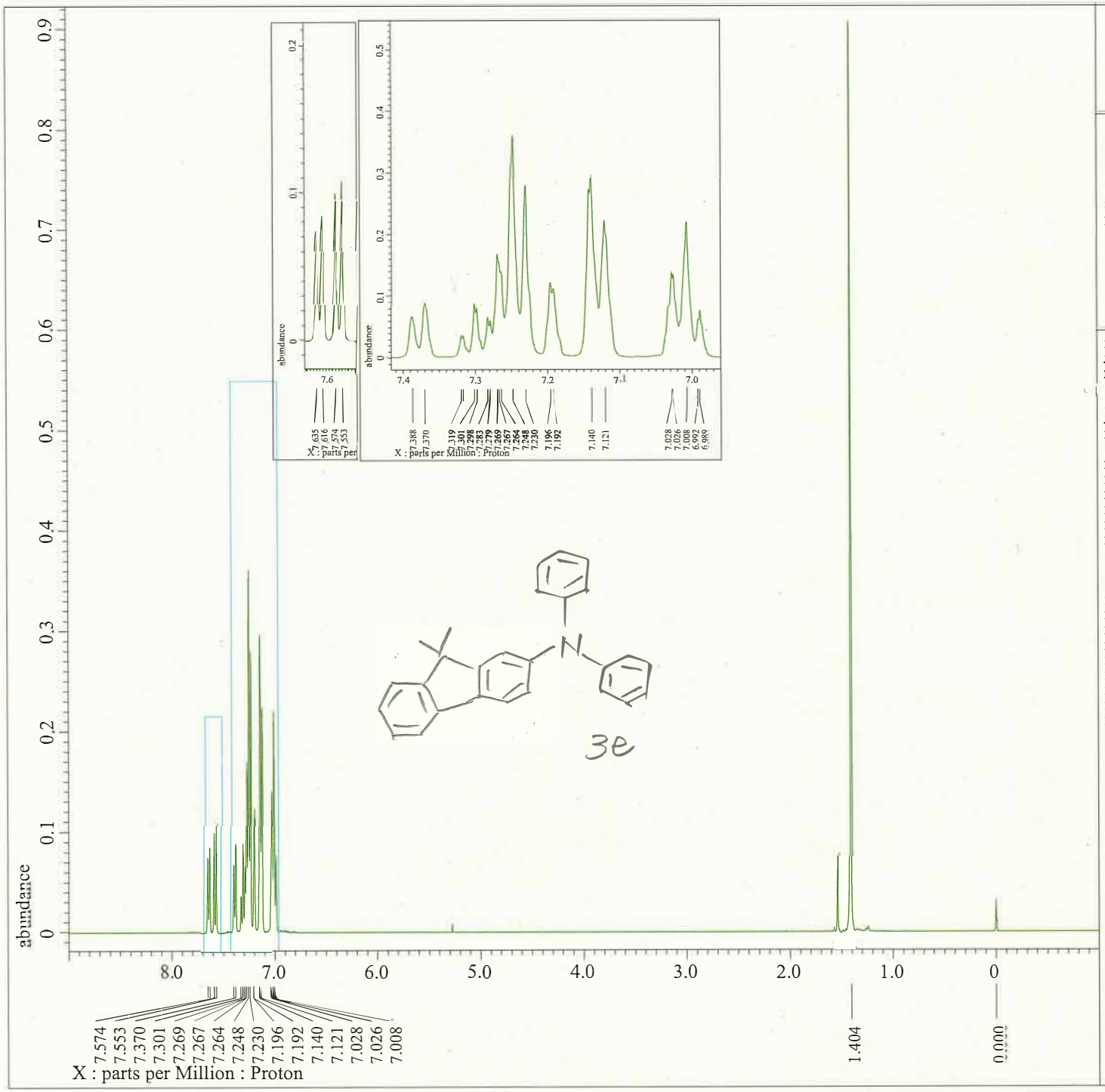
Filename	= RIK-318-pureH_PROTO
Author	= delta
Experiment	= proton.jxp
Sample_Id	= RIK-318-pureH
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 5-JUN-2020 13:12:5
Revision_Time	= 7-AUG-2020 15:26:2
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ400S/L1
Field_Strength	= 9.389766[T] (400[MH
X_Acq_Duration	= 4.37256192[s]
X_Domain	= Proton
X_Freq	= 399.78219838[MHz]
X_Offset	= 5[ppm]
X_Points	= 32768
X_Prescans	= 0
X_Resolution	= 0.22869888[Hz]
X_Sweep	= 7.4940048[kHz]
X_Sweep_Clipped	= 5.99520384[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.78219838[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 399.78219838[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 4[s]
Recvr_Gain	= 52
Temp_Get	= 19.8[dC]
X_90_Width	= 5.6[us]
X_Acq_Time	= 4.37256192[s]
X_Angle	= 45[deg]
X_Atn	= 5[dB]
X_Pulse	= 2.8[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 400
Dante_Presat	= FALSE




```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
thresh( 5[%], 1 )
peak_pick( 0[Hz], 0.1[ppm], Peaks, 0[Hz] )

以下に由来:: RIK-318-pureC_CARBON-1-1.jdf
```

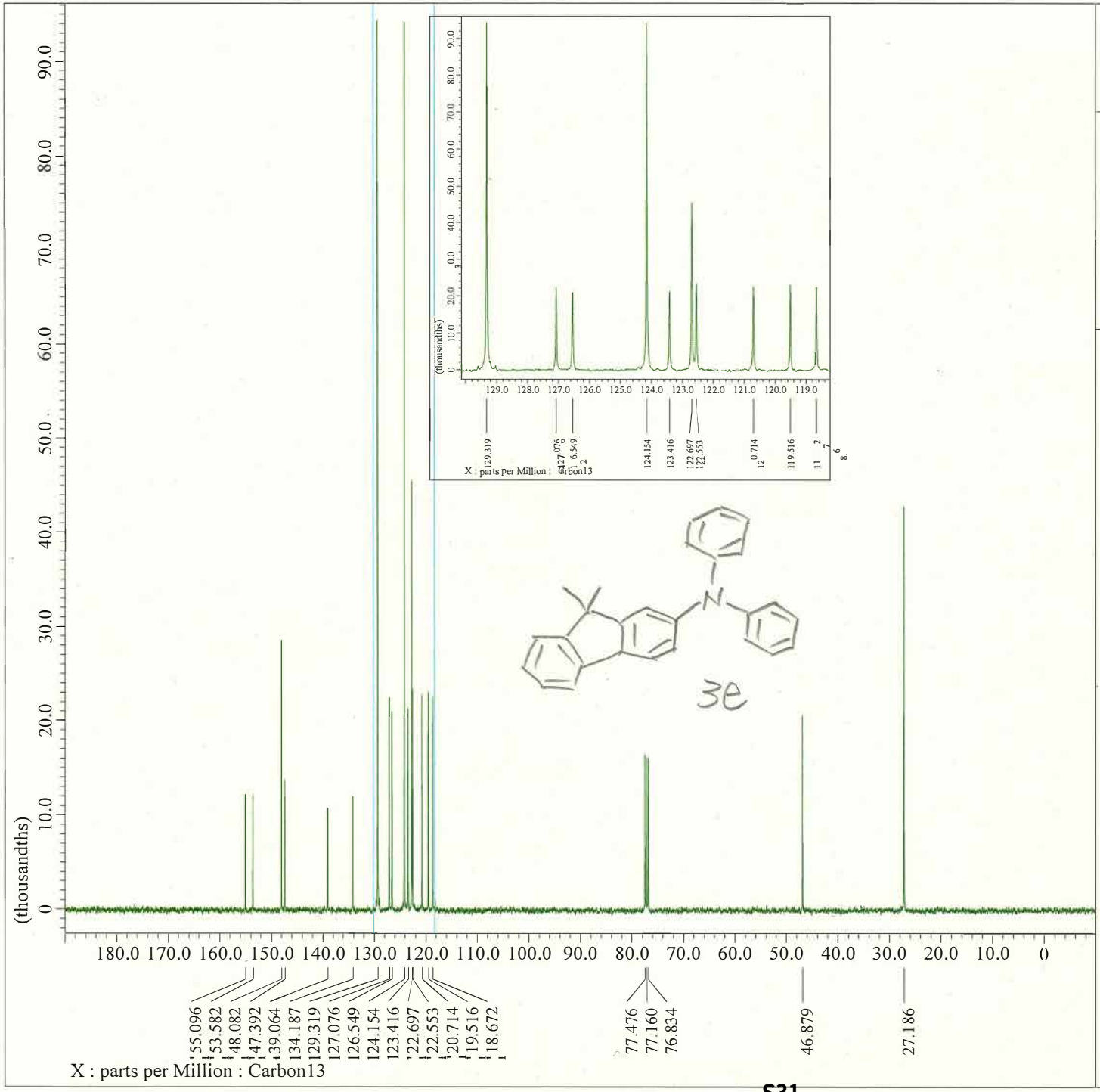
Filename	= RIK-318-pureC_CA
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= RIK-318-pureC
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 5-JUN-2020 13:1
Revision_Time	= 7-AUG-2020 16:4
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ400S/L1
Field_Strength	= 9.389766[T] (400
X_Acq_Duration	= 1.03809024[s]
X_Domain	= Carbon13
X_Freq	= 100.52530333[MHz
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.96330739[Hz]
X_Sweep	= 31.56565657[kHz]
X_Sweep_Clipped	= 25.25252525[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.78219838[MHz
Irr_Offset	= 5[ppm]
Blanking	= 5[us]
Clipped	= FALSE
Scans	= 64
Total_Scans	= 64
Relaxation_Delay	= 2[s]
Recvr_Gain	= 52
Temp_Get	= 19.8[dC]
X_90_Width	= 10.6[us]
X_Acq_Time	= 1.03809024[s]
X_Angle	= 30[deg]
X_Atn	= 8.8[dB]
X_Pulse	= 3.53333333[us]
Irr_Atn_Dec	= 31.25[dB]
Irr_Atn_Dec_Calc	= 31.25[dB]
Irr_Atn_Dec_Default_Calc	= 31.25[dB]
Irr_Atn_Noe	= 31.25[dB]
Irr_Dec_Bandwidth_Hz	= 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm	= 11.96303566[ppm]
Irr_Dec_Freq	= 399.78219838[MHz




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

以下に由来:: RIK-319-pureH_PROTON-1-1.jdf
```

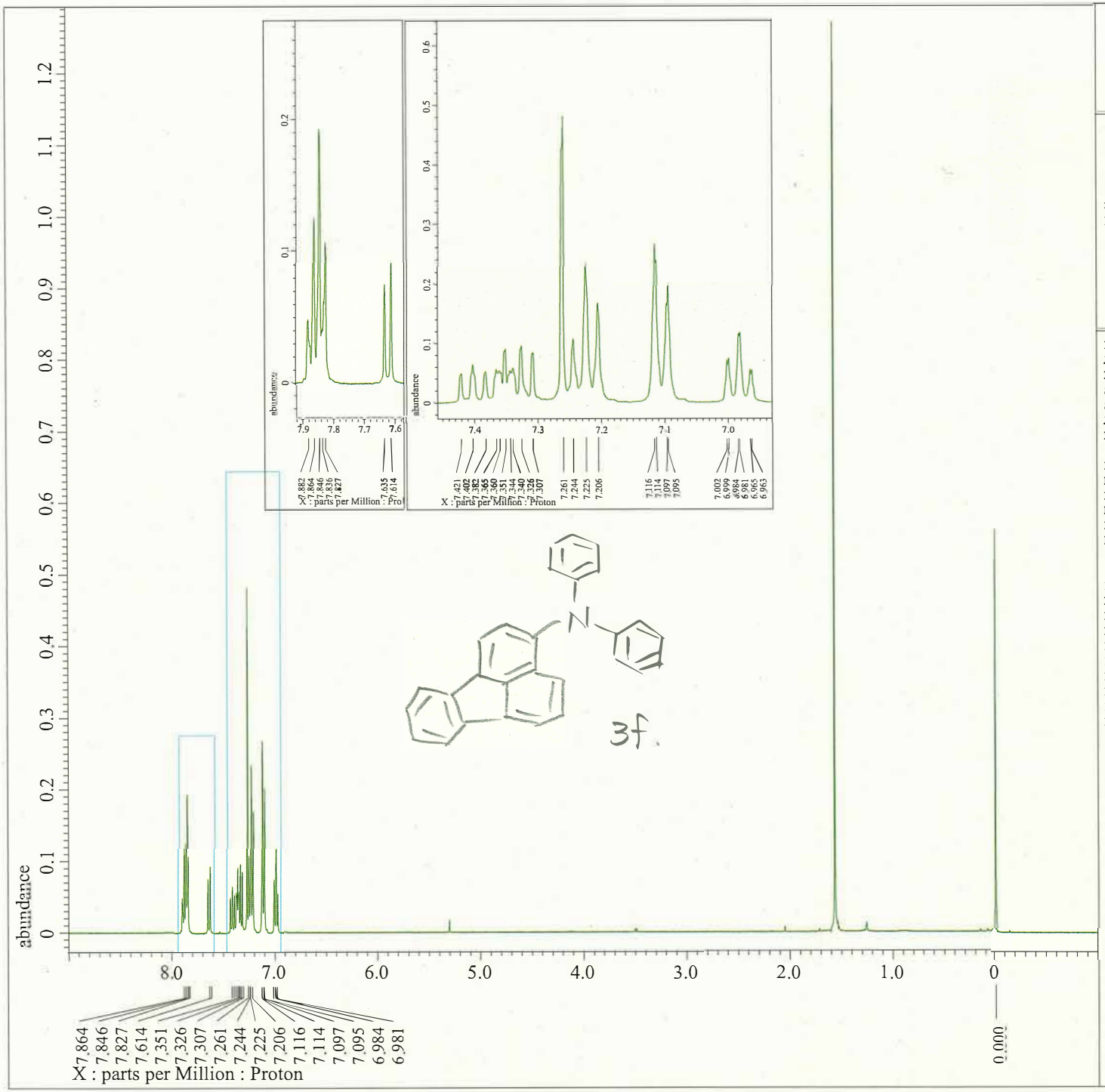
Filename	= RIK-319-pureH_PROTO
Author	= delta
Experiment	= proton.jxp
Sample_Id	= RIK-319-pureH
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 8-JUN-2020 09:13:3
Revision_Time	= 7-AUG-2020 15:32:1
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ400S/L1
Field_Strength	= 9.389766[T] (400[MH
X_Acq_Duration	= 4.37256192[s]
X_Domain	= Proton
X_Freq	= 399.78219838[MHz]
X_Offset	= 5[ppm]
X_Points	= 32768
X_Prescans	= 0
X_Resolution	= 0.22869888[Hz]
X_Sweep	= 7.4940048[kHz]
X_Sweep_Clipped	= 5.99520384[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.78219838[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 399.78219838[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 4[s]
Recvr_Gain	= 42
Temp_Get	= 19[dC]
X_90_Width	= 5.6[us]
X_Acq_Time	= 4.37256192[s]
X_Angle	= 45[deg]
X_Atn	= 5[dB]
X_Pulse	= 2.8[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 400
Dante_Presat	= FALSE




```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
thresh( 5[%], 1 )
peak_pick( 0[Hz], 0.1[ppm], Peaks, 0[Hz] )

以下に由来:: RIK-319-pureC_CARBON-1-1.jdf
```

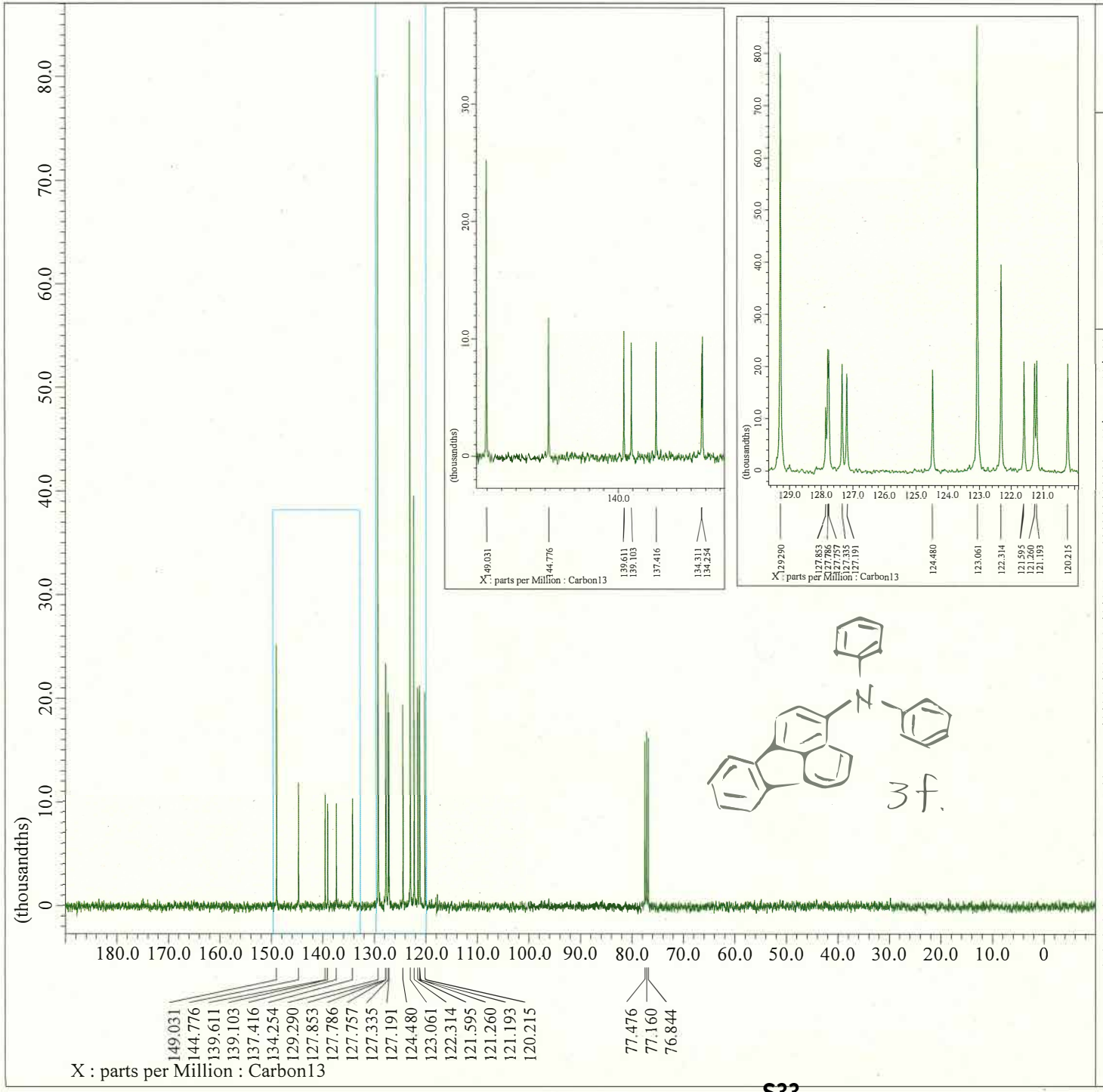
Filename	= RIK-319-pureC_CA
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= RIK-319-pureC
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 8-JUN-2020 09:1
Revision_Time	= 7-AUG-2020 16:4
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ400S/L1
Field_Strength	= 9.389766[T] (400
X_Acq_Duration	= 1.03809024[s]
X_Domain	= Carbon13
X_Freq	= 100.52530333[MHz
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.96330739[Hz]
X_Sweep	= 31.56565657[kHz]
X_Sweep_Clipped	= 25.25252525[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.78219838[MHz
Irr_Offset	= 5[ppm]
Blanking	= 5[us]
Clipped	= FALSE
Scans	= 64
Total_Scans	= 64
Relaxation_Delay	= 2[s]
Recvr_Gain	= 52
Temp_Get	= 19.1[dC]
X_90_Width	= 10.6[us]
X_Acq_Time	= 1.03809024[s]
X_Angle	= 30[deg]
X_Atn	= 8.8[dB]
X_Pulse	= 3.53333333[us]
Irr_Atn_Dec	= 31.25[dB]
Irr_Atn_Dec_Calc	= 31.25[dB]
Irr_Atn_Dec_Default_Calc	= 31.25[dB]
Irr_Atn_Noe	= 31.25[dB]
Irr_Dec_Bandwidth_Hz	= 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm	= 11.96303566[ppm]
Irr_Dec_Freq	= 399.78219838[MHz




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

以下に由来:: RIK-317-pureH_PROTON-2-1.jdf
```

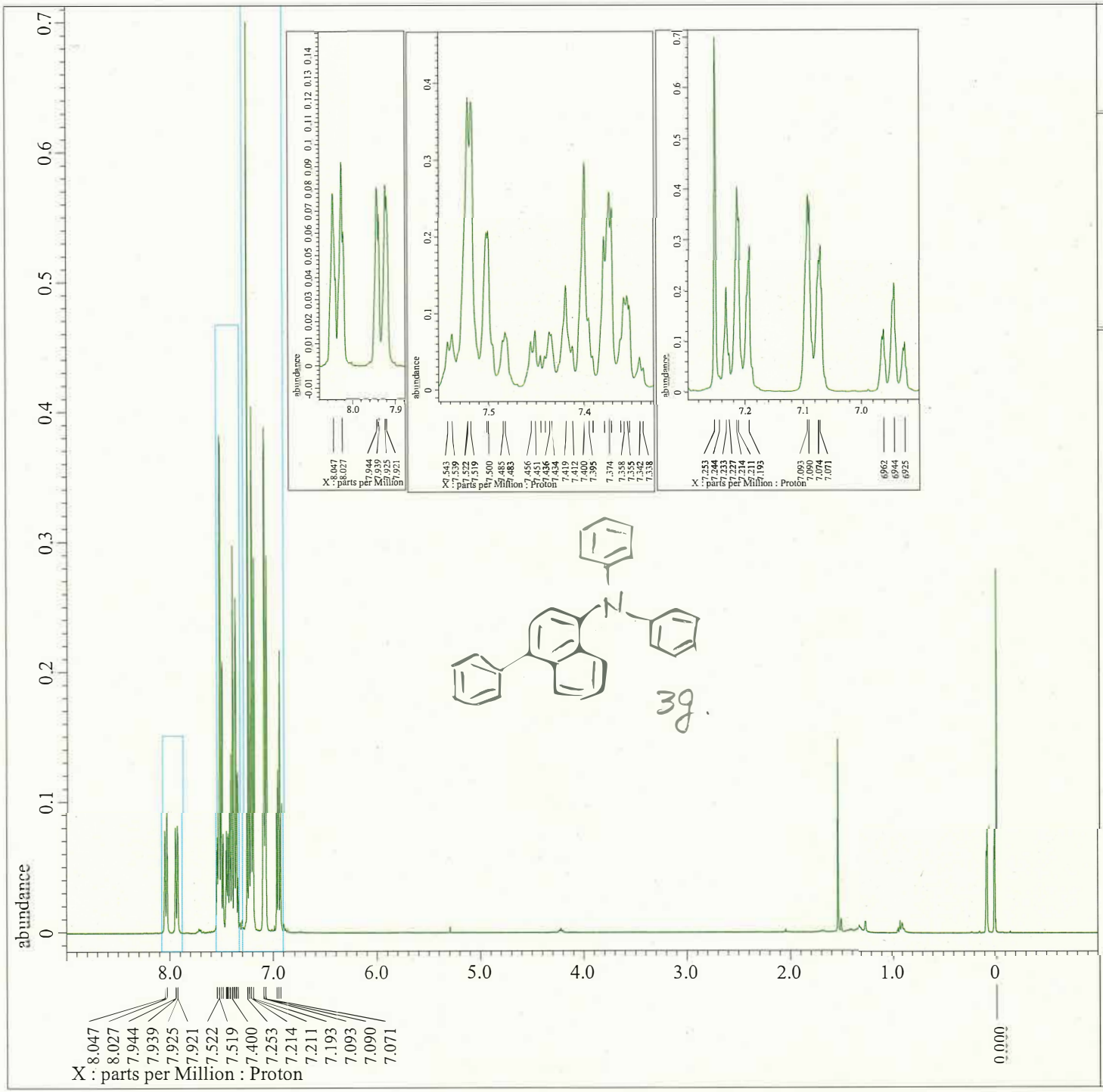
Filename	= RIK-317-pureH_PROTO
Author	= delta
Experiment	= proton.jxp
Sample_Id	= RIK-317-pureH
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 8-JUN-2020 12:59:2
Revision_Time	= 7-AUG-2020 15:37:1
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ400S/L1
Field_Strength	= 9.389766[T] (400[MH
X_Acq_Duration	= 4.37256192[s]
X_Domain	= Proton
X_Freq	= 399.78219838[MHz]
X_Offset	= 5[ppm]
X_Points	= 32768
X_Prescans	= 0
X_Resolution	= 0.22869888[Hz]
X_Sweep	= 7.4940048[kHz]
X_Sweep_Clipped	= 5.99520384[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.78219838[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 399.78219838[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 4[s]
Recvr_Gain	= 62
Temp_Get	= 19.5[dC]
X_90_Width	= 5.6[us]
X_Acq_Time	= 4.37256192[s]
X_Angle	= 45[deg]
X_Atn	= 5[dB]
X_Pulse	= 2.8[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 400
Dante_Presat	= FALSE




```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
thresh( 5[%], 1 )
peak_pick( 0[Hz], 0.1[ppm], Peaks, 0[Hz] )

以下に由来:: RIK-317-pureC_CARBON-2-1.jdf
```

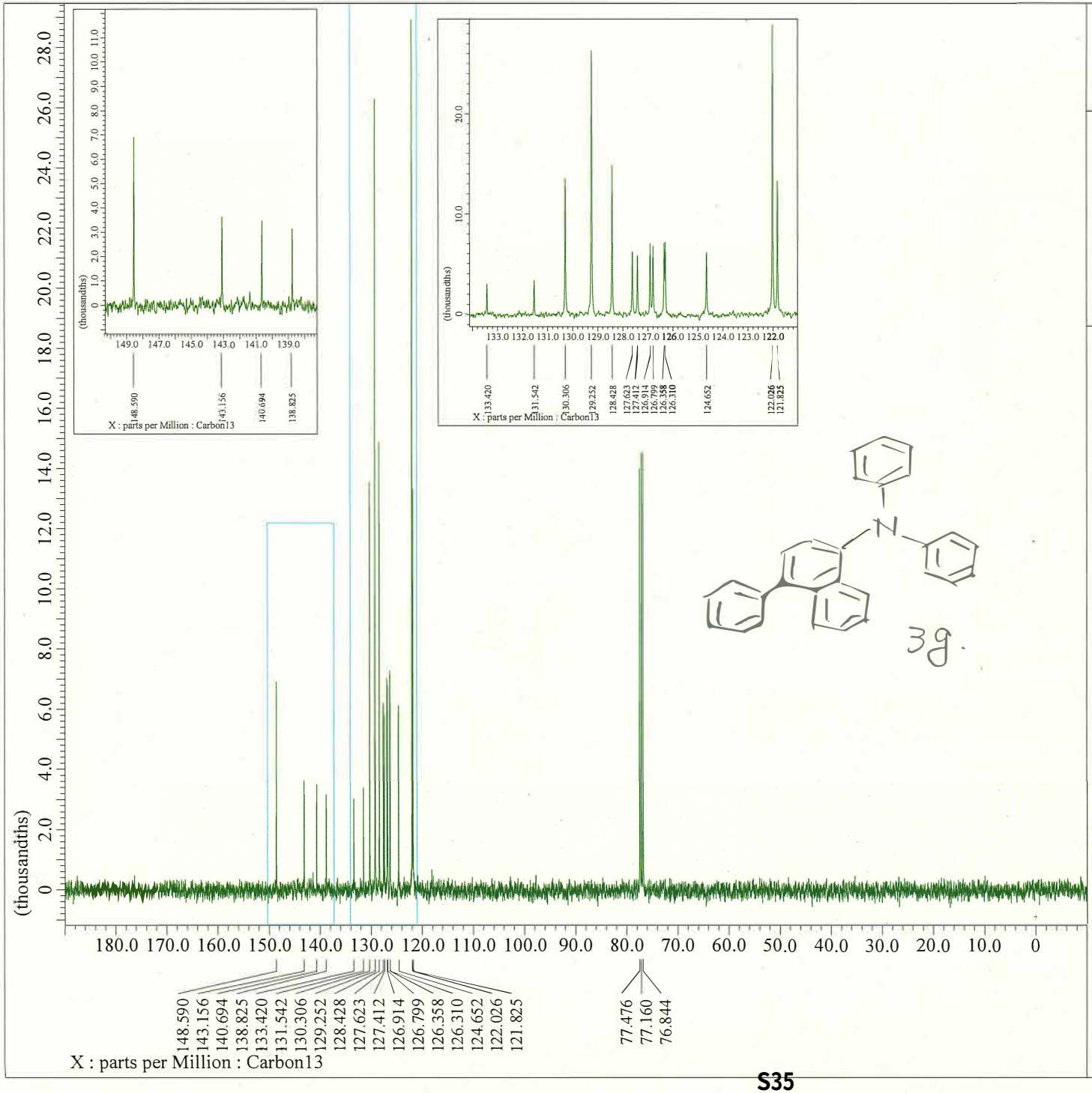
Filename	= RIK-317-pureC_CA
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= RIK-317-pureC
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 8-JUN-2020 13:4
Revision_Time	= 26-JUL-2020 16:0
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ400S/L1
Field_Strength	= 9.389766[T] (400
X_Acq_Duration	= 1.03809024[s]
X_Domain	= Carbon13
X_Freq	= 100.52530333[MHz
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.96330739[Hz]
X_Sweep	= 31.56565657[kHz]
X_Sweep_Clipped	= 25.25252525[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.78219838[MHz
Irr_Offset	= 5[ppm]
Blanking	= 5[us]
Clipped	= FALSE
Scans	= 32
Total_Scans	= 32
Relaxation_Delay	= 2[s]
Recvr_Gain	= 52
Temp_Get	= 19.9[dC]
X_90_Width	= 10.6[us]
X_Acq_Time	= 1.03809024[s]
X_Angle	= 30[deg]
X_Atn	= 8.8[dB]
X_Pulse	= 3.53333333[us]
Irr_Atn_Dec	= 31.25[dB]
Irr_Atn_Dec_Calc	= 31.25[dB]
Irr_Atn_Dec_Default_Calc	= 31.25[dB]
Irr_Atn_Noe	= 31.25[dB]
Irr_Dec_Bandwidth_Hz	= 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm	= 11.96303566[ppm]
Irr_Dec_Freq	= 399.78219838[MHz




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

以下に由来:: RIK-320-pureH_PROTON-2-1.jdf
```

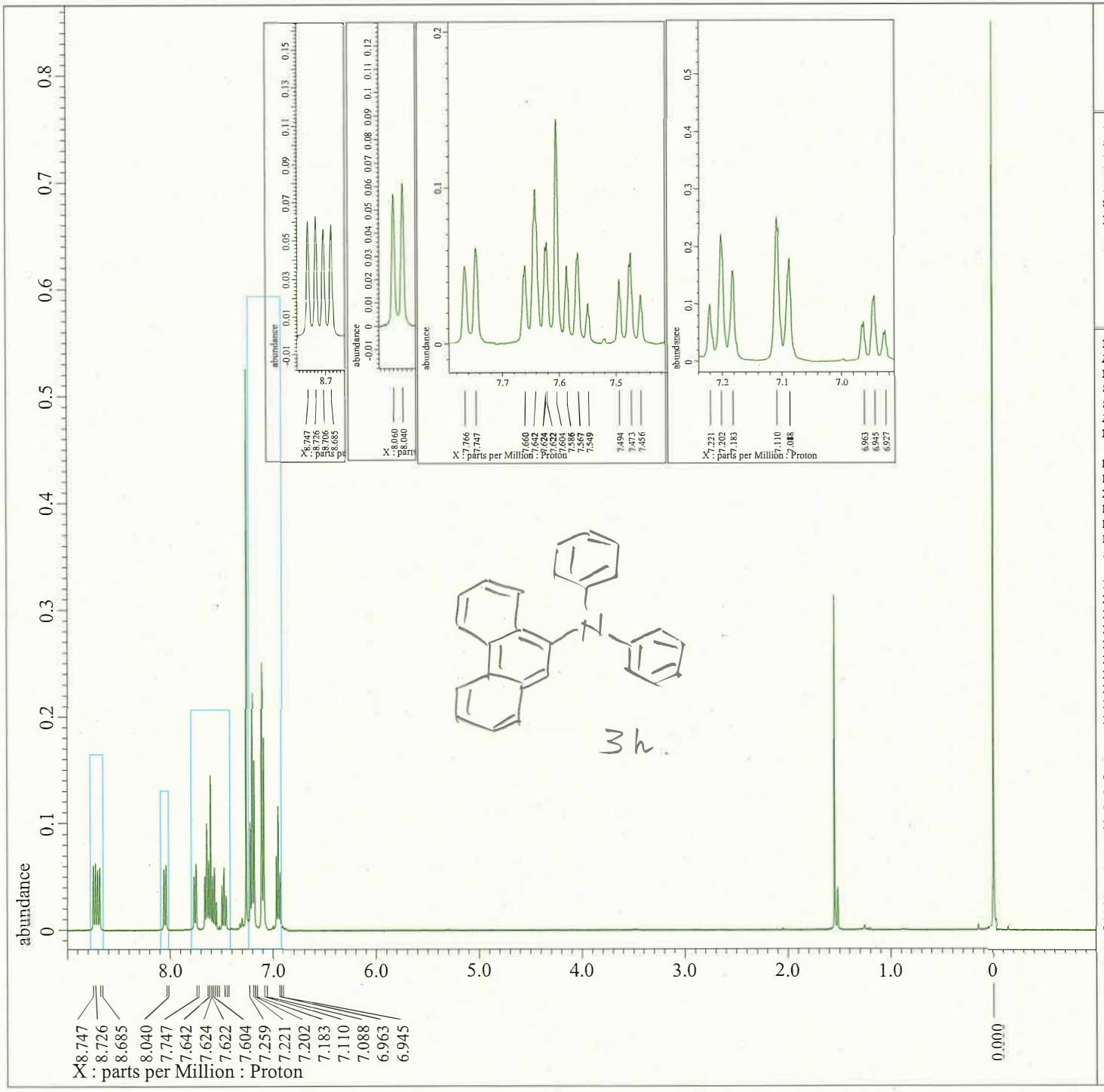
Filename	= RIK-320-pureH_PROTO
Author	= delta
Experiment	= proton.jxp
Sample_Id	= RIK-320-pureH
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 30-JUL-2020 12:09:2
Revision_Time	= 7-AUG-2020 15:43:4
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ400S/L1
Field_Strength	= 9.389766[T] (400[MH
X_Acq_Duration	= 4.37256192[s]
X_Domain	= Proton
X_Freq	= 399.78219838[MHz]
X_Offset	= 5[ppm]
X_Points	= 32768
X_Prescans	= 0
X_Resolution	= 0.22869888[Hz]
X_Sweep	= 7.4940048[kHz]
X_Sweep_Clipped	= 5.99520384[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.78219838[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 399.78219838[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 4[s]
Recvr_Gain	= 52
Temp_Get	= 19.6[dC]
X_90_Width	= 5.6[us]
X_Acq_Time	= 4.37256192[s]
X_Angle	= 45[deg]
X_Atn	= 5[dB]
X_Pulse	= 2.8[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 400
Dante_Presat	= FALSE




```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
thresh( 5[%], 1 )
peak_pick( 0[Hz], 0.1[ppm], Peaks, 0[Hz] )

以下に由来:: RIK-320-pureC_CARBON-1-1.jdf
```

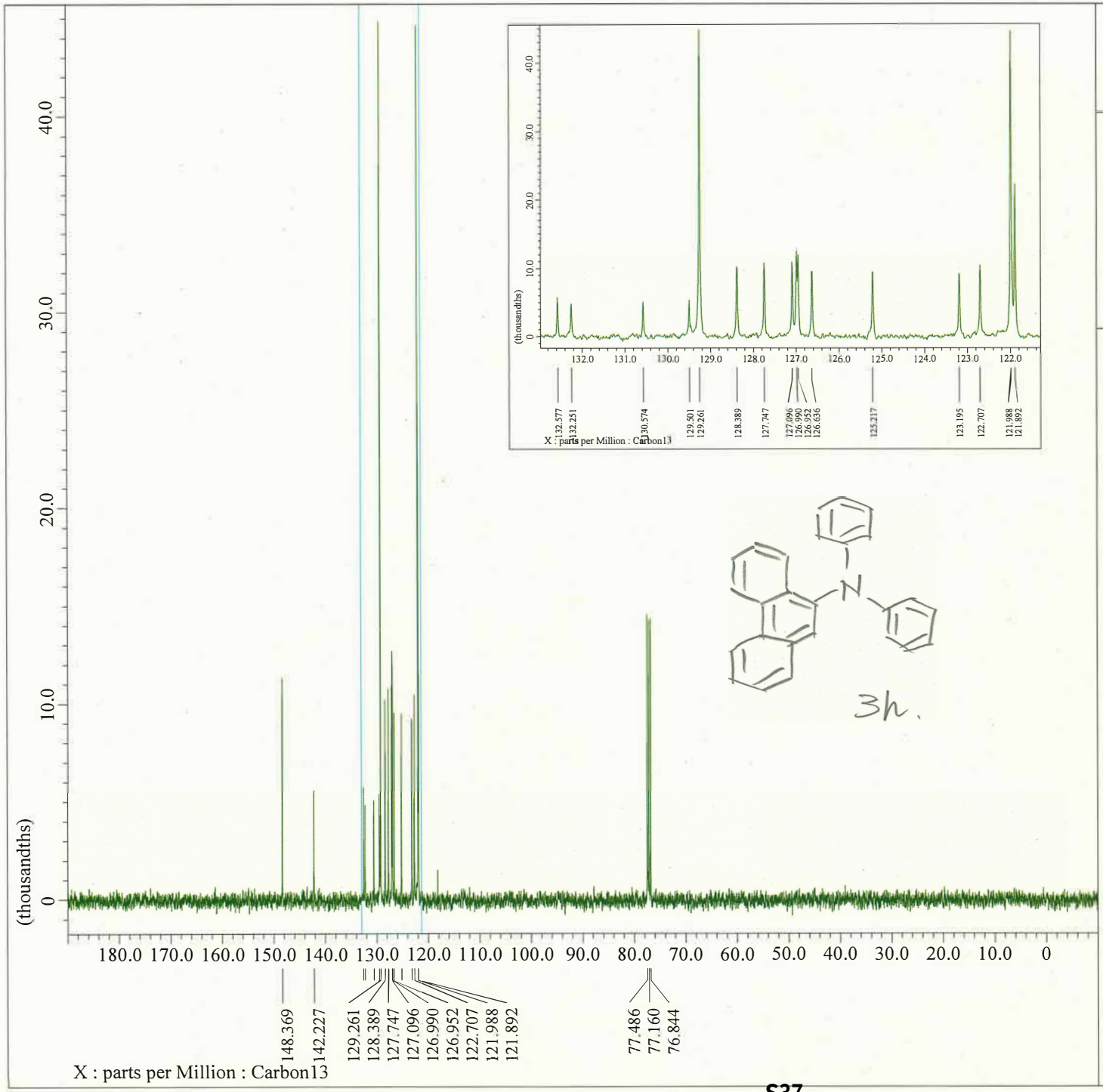
Filename	= RIK-320-pureC_CA
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= RIK-320-pureC
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 3-JUN-2020 12:5
Revision_Time	= 26-JUL-2020 16:0
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ400S/L1
Field_Strength	= 9.389766[T] (400
X_Acq_Duration	= 1.03809024[s]
X_Domain	= Carbon13
X_Freq	= 100.52530333[MHz
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.96330739[Hz]
X_Sweep	= 31.56565657[kHz]
X_Sweep_Clipped	= 25.25252525[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.78219838[MHz
Irr_Offset	= 5[ppm]
Blanking	= 5[us]
Clipped	= FALSE
Scans	= 64
Total_Scans	= 64
Relaxation_Delay	= 2[s]
Recvr_Gain	= 52
Temp_Get	= 20.4[dC]
X_90_Width	= 10.6[us]
X_Acq_Time	= 1.03809024[s]
X_Angle	= 30[deg]
X_Atn	= 8.8[dB]
X_Pulse	= 3.53333333[us]
Irr_Atn_Dec	= 31.25[dB]
Irr_Atn_Dec_Calc	= 31.25[dB]
Irr_Atn_Dec_Default_Calc	= 31.25[dB]
Irr_Atn_Noe	= 31.25[dB]
Irr_Dec_Bandwidth_Hz	= 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm	= 11.96303566[ppm]
Irr_Dec_Freq	= 399.78219838[MHz




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

以下に由来:: RIK-331-pureH_PROTON-1-1.jdf
```

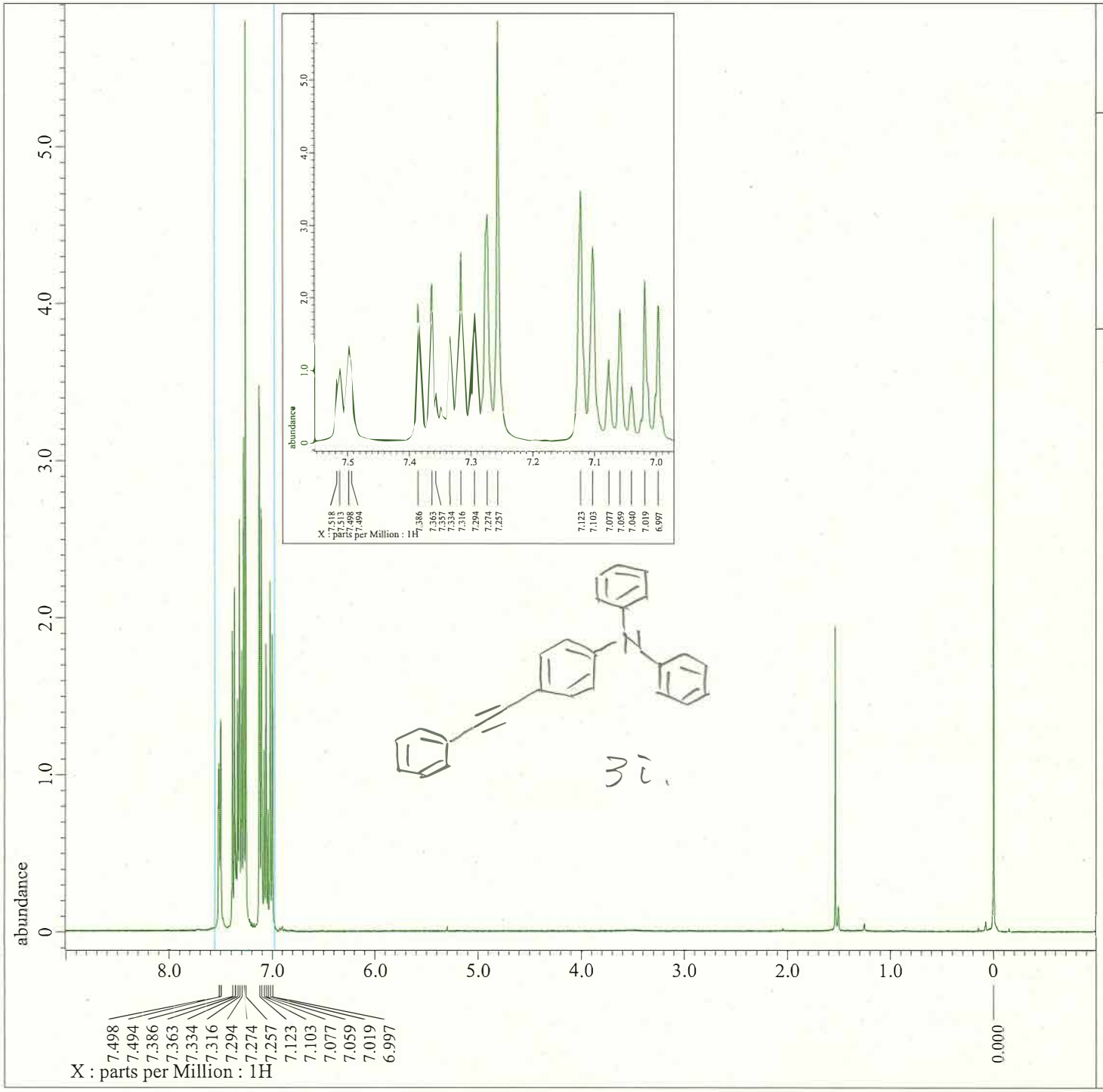
Filename	= RIK-331-pureH_PROTO
Author	= delta
Experiment	= proton.jxp
Sample_Id	= RIK-331-pure
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 14-JUN-2020 16:28:5
Revision_Time	= 7-AUG-2020 15:51:5
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ400S/L1
Field_Strength	= 9.389766[T] (400[MH
X_Acq_Duration	= 4.37256192[s]
X_Domain	= Proton
X_Freq	= 399.78219838[MHz]
X_Offset	= 5[ppm]
X_Points	= 32768
X_Prescans	= 0
X_Resolution	= 0.22869888[Hz]
X_Sweep	= 7.4940048[kHz]
X_Sweep_Clipped	= 5.99520384[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.78219838[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 399.78219838[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 4[s]
Recvr_Gain	= 62
Temp_Get	= 19.8[dC]
X_90_Width	= 5.6[us]
X_Acq_Time	= 4.37256192[s]
X_Angle	= 45[deg]
X_Atn	= 5[dB]
X_Pulse	= 2.8[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 400
Dante_Presat	= FALSE




```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
thresh( 5[%], 1 )
peak_pick( 0[Hz], 0.1[ppm], Peaks, 0[Hz] )

以下に由来:: RIK-331-pureC_CARBON-1-1.jdf
```

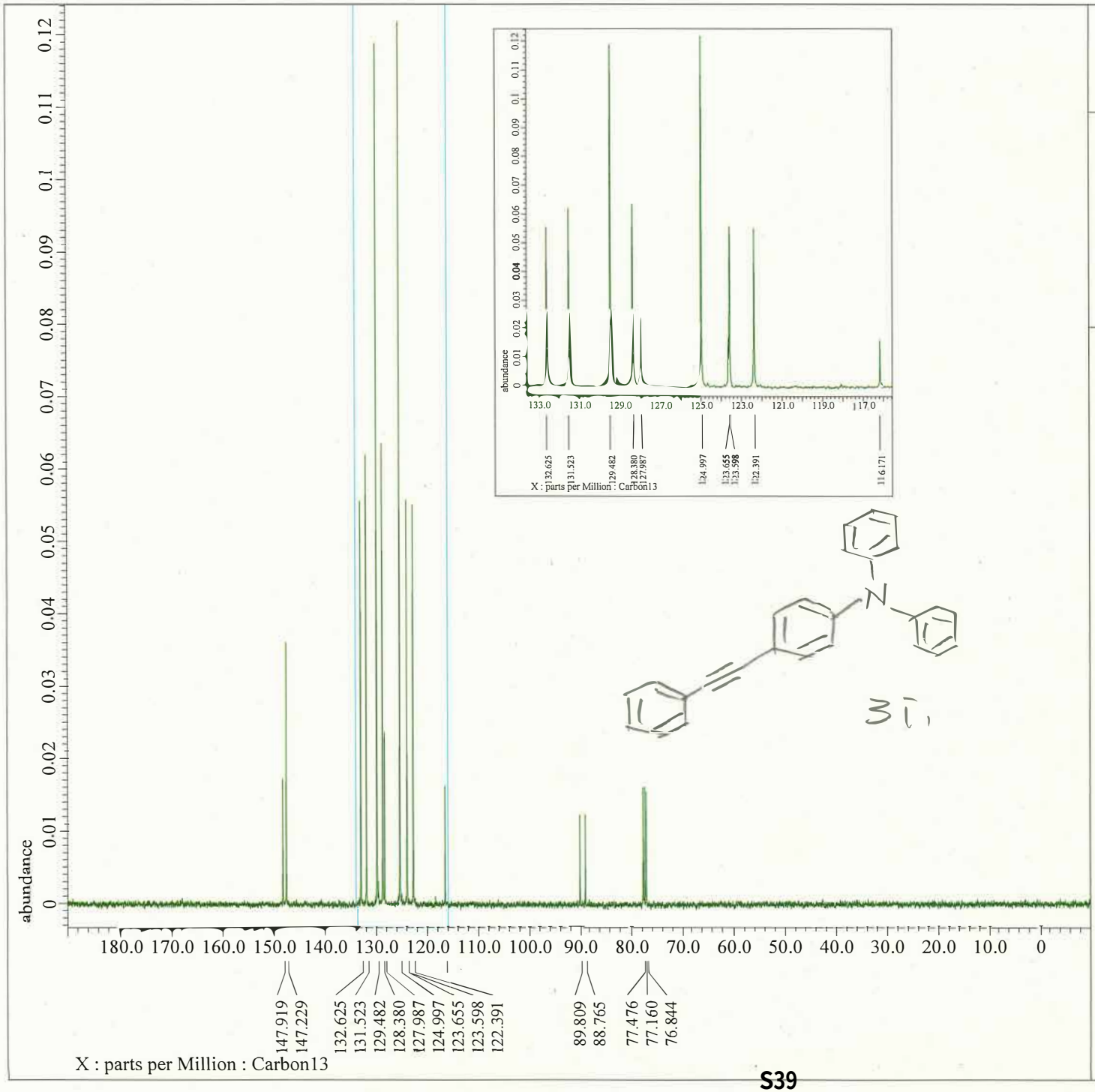
Filename	= RIK-331-pureC_CA
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= RIK-331-pureC
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 14-JUN-2020 16:4
Revision_Time	= 28-JUL-2020 18:5
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ400S/L1
Field_Strength	= 9.389766[T] (400
X_Acq_Duration	= 1.03809024[s]
X_Domain	= Carbon13
X_Freq	= 100.52530333[MHz
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.96330739[Hz]
X_Sweep	= 31.56565657[kHz]
X_Sweep_Clipped	= 25.25252525[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.78219838[MHz
Irr_Offset	= 5[ppm]
Blanking	= 5[us]
Clipped	= FALSE
Scans	= 32
Total_Scans	= 32
Relaxation_Delay	= 2[s]
Recvr_Gain	= 52
Temp_Get	= 19.9[dC]
X_90_Width	= 10.6[us]
X_Acq_Time	= 1.03809024[s]
X_Angle	= 30[deg]
X_Atn	= 8.8[dB]
X_Pulse	= 3.53333333[us]
Irr_Atn_Dec	= 31.25[dB]
Irr_Atn_Dec_Calc	= 31.25[dB]
Irr_Atn_Dec_Default_Calc	= 31.25[dB]
Irr_Atn_Noe	= 31.25[dB]
Irr_Dec_Bandwidth_Hz	= 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm	= 11.96303566[ppm]
Irr_Dec_Freq	= 399.78219838[MHz




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

以下に由来:: RIK-323-pureH-1.jdf
```

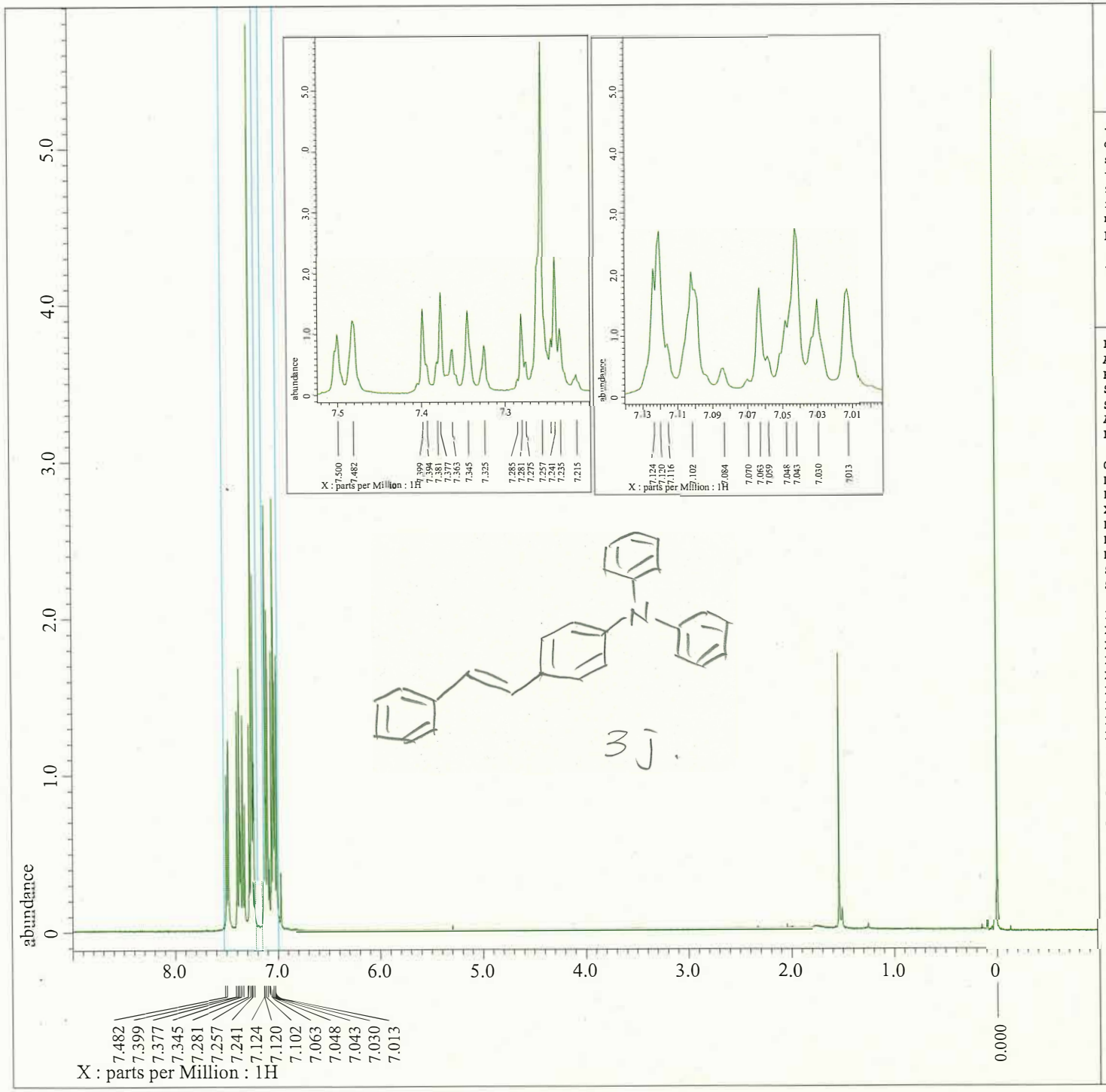
Filename	= RIK-323-pureH-2.jdf
Author	= delta
Experiment	= single_pulse.ex2
Sample_Id	= S#720404
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 29-JUL-2020 04:44:23
Revision_Time	= 7-AUG-2020 15:53:40
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= 1H
Dim_Title	= 1H
Dim_Units	= [ppm]
Dimensions	= X
Site	= ECX 400
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	= 50
Temp_Get	= 22.8[dC]
X_90_Width	= 11.5[us]
X_Acq_Time	= 2.20725248[s]
X_Angle	= 45[deg]
X_Atn	= 9[dB]
X_Pulse	= 5.75[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Presat	= FALSE
Initial_Wait	= 1[s]




```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
thresh( 5[%], 1 )
peak_pick( 0[Hz], 0.1[ppm], Peaks, 0[Hz] )

以下に由来:: RIK-323-pureC_CARBON-1-1.jdf
```

Filename	= RIK-323-pureC_CA
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= RIK-323-pureC
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 8-JUN-2020 11:3
Revision_Time	= 28-JUL-2020 21:3
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ400S/L1
Field_Strength	= 9.389766[T] (400
X_Acq_Duration	= 1.03809024[s]
X_Domain	= Carbon13
X_Freq	= 100.52530333[MHz
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.96330739[Hz]
X_Sweep	= 31.56565657[kHz]
X_Sweep_Clipped	= 25.25252525[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.78219838[MHz
Irr_Offset	= 5[ppm]
Blanking	= 5[us]
Clipped	= FALSE
Scans	= 32
Total_Scans	= 32
Relaxation_Delay	= 2[s]
Recvr_Gain	= 52
Temp_Get	= 19.7[dC]
X_90_Width	= 10.6[us]
X_Acq_Time	= 1.03809024[s]
X_Angle	= 30[deg]
X_Atn	= 8.8[dB]
X_Pulse	= 3.53333333[us]
Irr_Atn_Dec	= 31.25[dB]
Irr_Atn_Dec_Calc	= 31.25[dB]
Irr_Atn_Dec_Default_Calc	= 31.25[dB]
Irr_Atn_Noe	= 31.25[dB]
Irr_Dec_Bandwidth_Hz	= 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm	= 11.96303566[ppm]
Irr_Dec_Freq	= 399.78219838[MHz




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

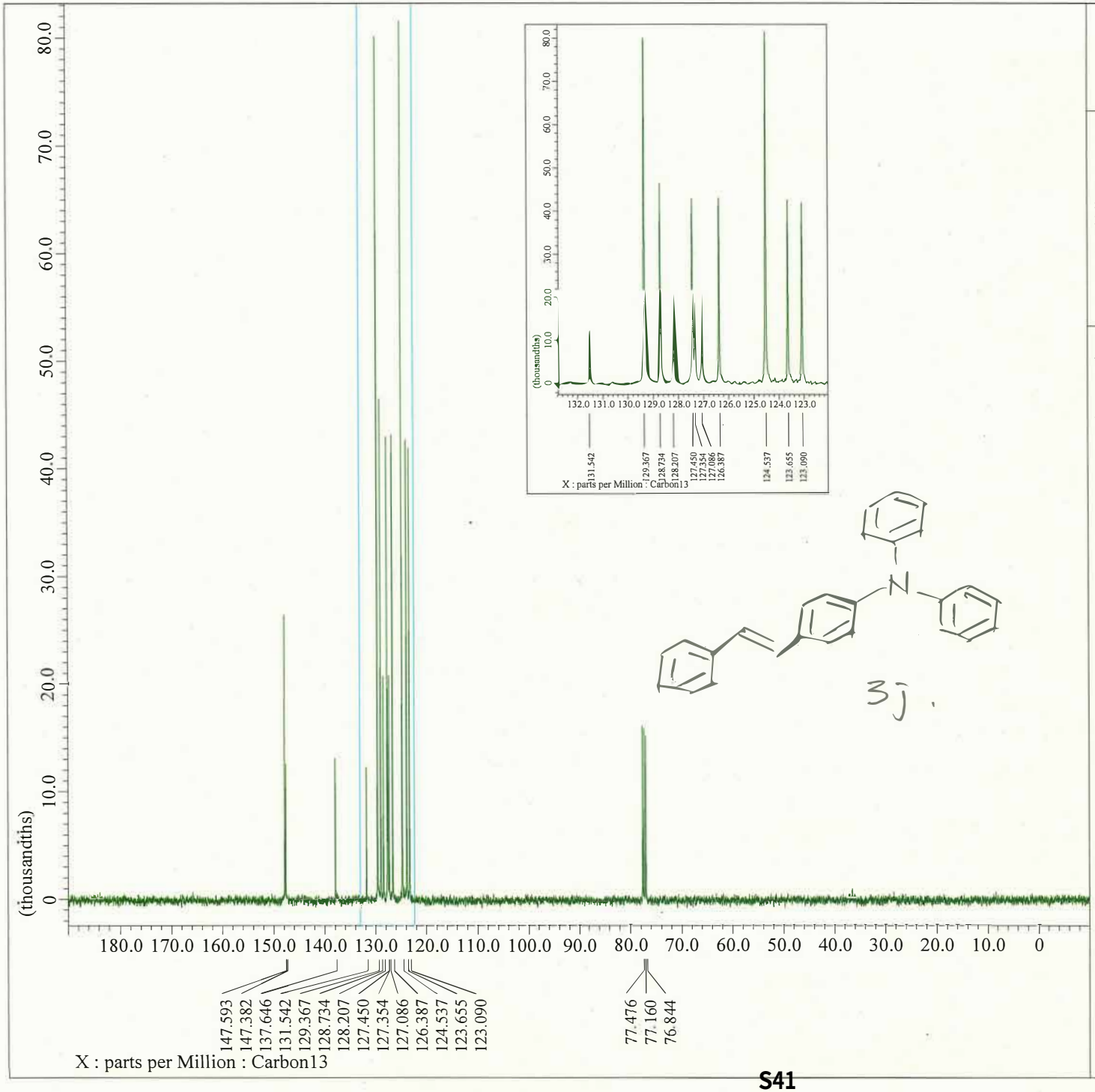
以下に由来:: RIK-322-pureH-1.jdf
```

```
Filename            = RIK-322-pureH-2.jdf
Author              = delta
Experiment          = single_pulse.ex2
Sample_Id           = S#723356
Solvent             = CHLOROFORM-D
Actual_Start_Time   = 29-JUL-2020 04:49:19
Revision_Time       =  7-AUG-2020 15:58:11

Comment             = single_pulse
Data_Format         = 1D COMPLEX
Dim_Size            = 13107
X_Domain            = 1H
Dim_Title           = 1H
Dim_Units           = [ppm]
Dimensions          = X
Site                = ECX 400
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

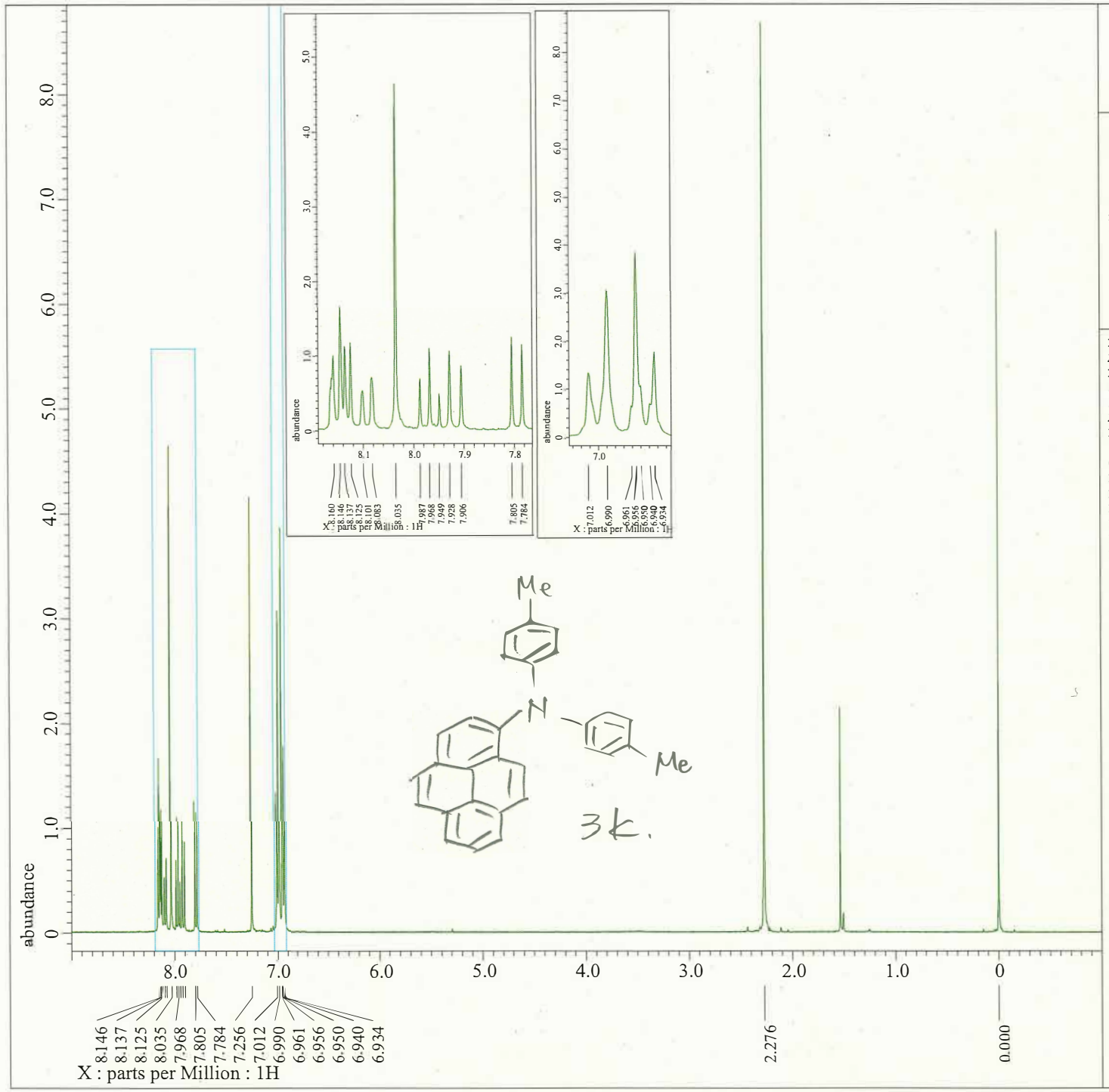
Relaxation_Delay    = 5[s]
Recvr_Gain          = 50
Temp_Get            = 22.7[dC]
X_90_Width          = 11.5[us]
X_Acq_Time          = 2.20725248[s]
X_Angle             = 45[deg]
X_Atn               = 9[dB]
X_Pulse             = 5.75[us]
Irr_Mode            = Off
Tri_Mode            = Off
Dante_Presat        = FALSE
Initial_Wait        = 1[s]
```




```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
thresh( 5[%], 1 )
peak_pick( 0[Hz], 0.1[ppm], Peaks, 0[Hz] )

以下に由来:: RIK-322-pureC_CARBON-1-1.jdf
```

Filename	= RIK-322-pureC_CA
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= RIK-322-pureC
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 8-JUN-2020 09:5
Revision_Time	= 28-JUL-2020 21:3
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ400S/L1
Field_Strength	= 9.389766[T] (400
X_Acq_Duration	= 1.03809024[s]
X_Domain	= Carbon13
X_Freq	= 100.52530333[MHz
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.96330739[Hz]
X_Sweep	= 31.56565657[kHz]
X_Sweep_Clipped	= 25.25252525[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.78219838[MHz
Irr_Offset	= 5[ppm]
Blanking	= 5[us]
Clipped	= FALSE
Scans	= 32
Total_Scans	= 32
Relaxation_Delay	= 2[s]
Recvr_Gain	= 52
Temp_Get	= 19.4[dC]
X_90_Width	= 10.6[us]
X_Acq_Time	= 1.03809024[s]
X_Angle	= 30[deg]
X_Atn	= 8.8[dB]
X_Pulse	= 3.53333333[us]
Irr_Atn_Dec	= 31.25[dB]
Irr_Atn_Dec_Calc	= 31.25[dB]
Irr_Atn_Dec_Default_Calc	= 31.25[dB]
Irr_Atn_Noe	= 31.25[dB]
Irr_Dec_Bandwidth_Hz	= 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm	= 11.96303566[ppm]
Irr_Dec_Freq	= 399.78219838[MHz




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

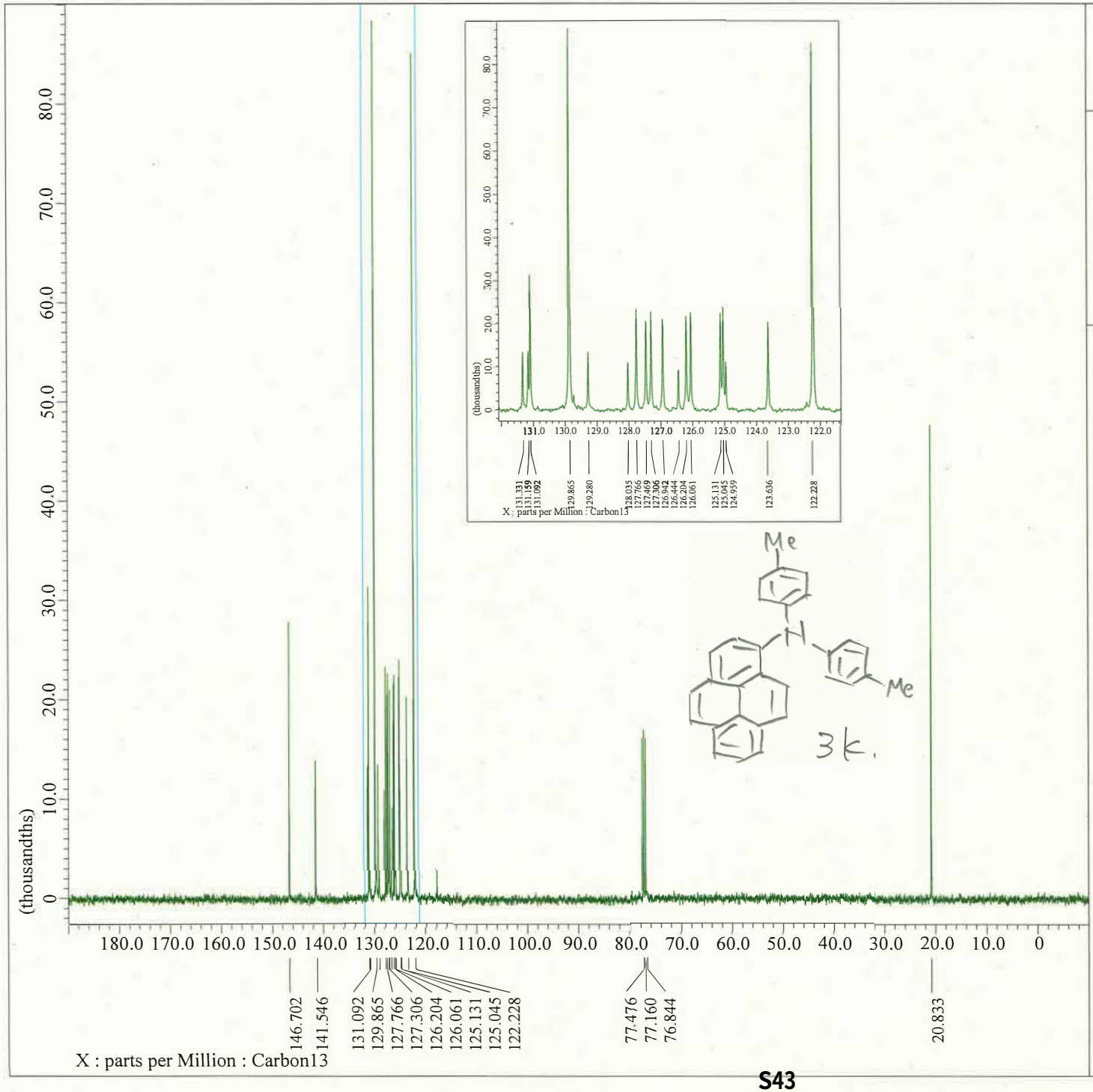
以下に由来:: RIK-326-pureH-1.jdf
```

```
Filename           = RIK-326-pureH-2.jdf
Author             = delta
Experiment         = single_pulse.ex2
Sample_Id          = S#736035
Solvent            = CHLOROFORM-D
Actual_Start_Time  = 29-JUL-2020 05:10:26
Revision_Time      =  7-AUG-2020 16:02:36

Comment            = single_pulse
Data_Format        = 1D COMPLEX
Dim_Size           = 13107
X_Domain           = 1H
Dim_Title          = 1H
Dim_Units          = [ppm]
Dimensions         = X
Site               = ECX 400
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

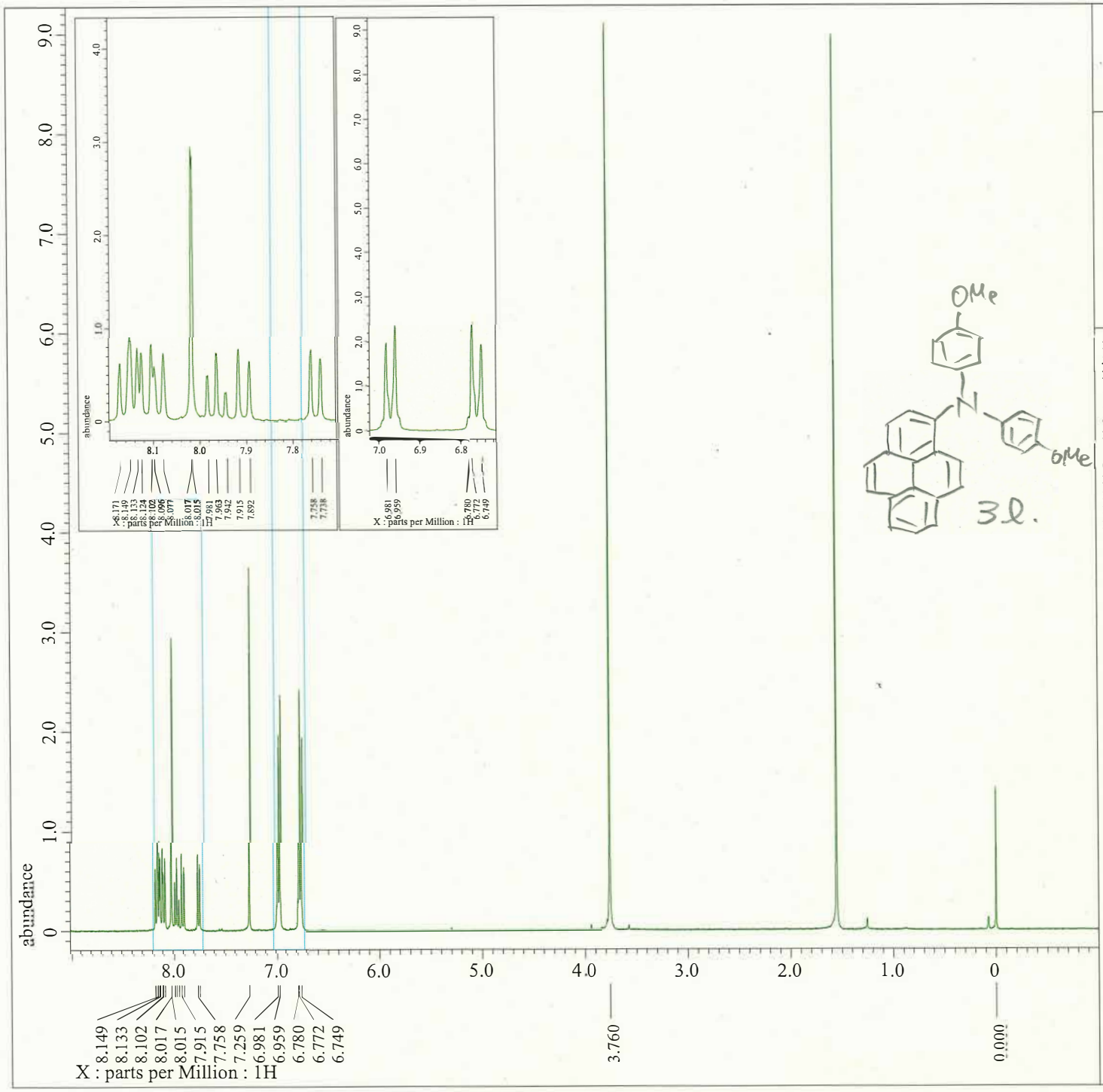
Relaxation_Delay   = 5[s]
Recvr_Gain         = 50
Temp_Get           = 21.9[dC]
X_90_Width         = 11.5[us]
X_Acq_Time         = 2.20725248[s]
X_Angle            = 45[deg]
X_Atn              = 9[dB]
X_Pulse            = 5.75[us]
Irr_Mode           = Off
Tri_Mode           = Off
Dante_Presat       = FALSE
Initial_Wait       = 1[s]
```




```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
thresh( 5[%], 1 )
peak_pick( 0[Hz], 0.1[ppm], Peaks, 0[Hz] )

以下に由来:: RIK-326-pureC_CARBON-1-1.jdf
```

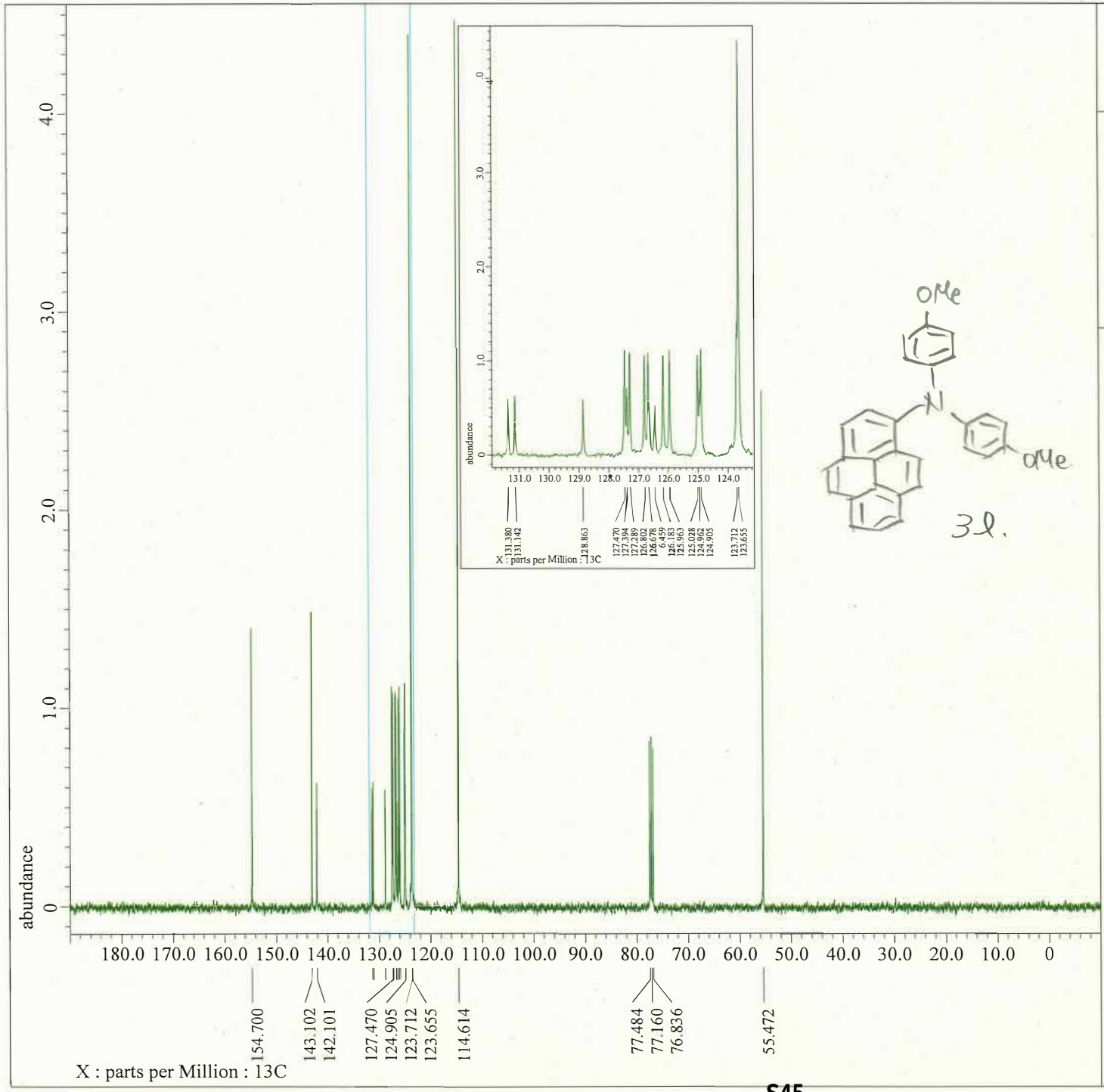
Filename	= RIK-326-pureC_CA
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= RIK-326-pureC
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 8-JUN-2020 13:5
Revision_Time	= 28-JUL-2020 21:4
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ400S/L1
Field_Strength	= 9.389766[T] (400
X_Acq_Duration	= 1.03809024[s]
X_Domain	= Carbon13
X_Freq	= 100.52530333[MHz
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.96330739[Hz]
X_Sweep	= 31.56565657[kHz]
X_Sweep_Clipped	= 25.25252525[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.78219838[MHz
Irr_Offset	= 5[ppm]
Blanking	= 5[us]
Clipped	= FALSE
Scans	= 32
Total_Scans	= 32
Relaxation_Delay	= 2[s]
Recvr_Gain	= 52
Temp_Get	= 19.8[dC]
X_90_Width	= 10.6[us]
X_Acq_Time	= 1.03809024[s]
X_Angle	= 30[deg]
X_Atn	= 8.8[dB]
X_Pulse	= 3.53333333[us]
Irr_Atn_Dec	= 31.25[dB]
Irr_Atn_Dec_Calc	= 31.25[dB]
Irr_Atn_Dec_Default_Calc	= 31.25[dB]
Irr_Atn_Noe	= 31.25[dB]
Irr_Dec_Bandwidth_Hz	= 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm	= 11.96303566[ppm]
Irr_Dec_Freq	= 399.78219838[MHz




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

以下に由来:: RIK-327-pureH-1.jdf
```

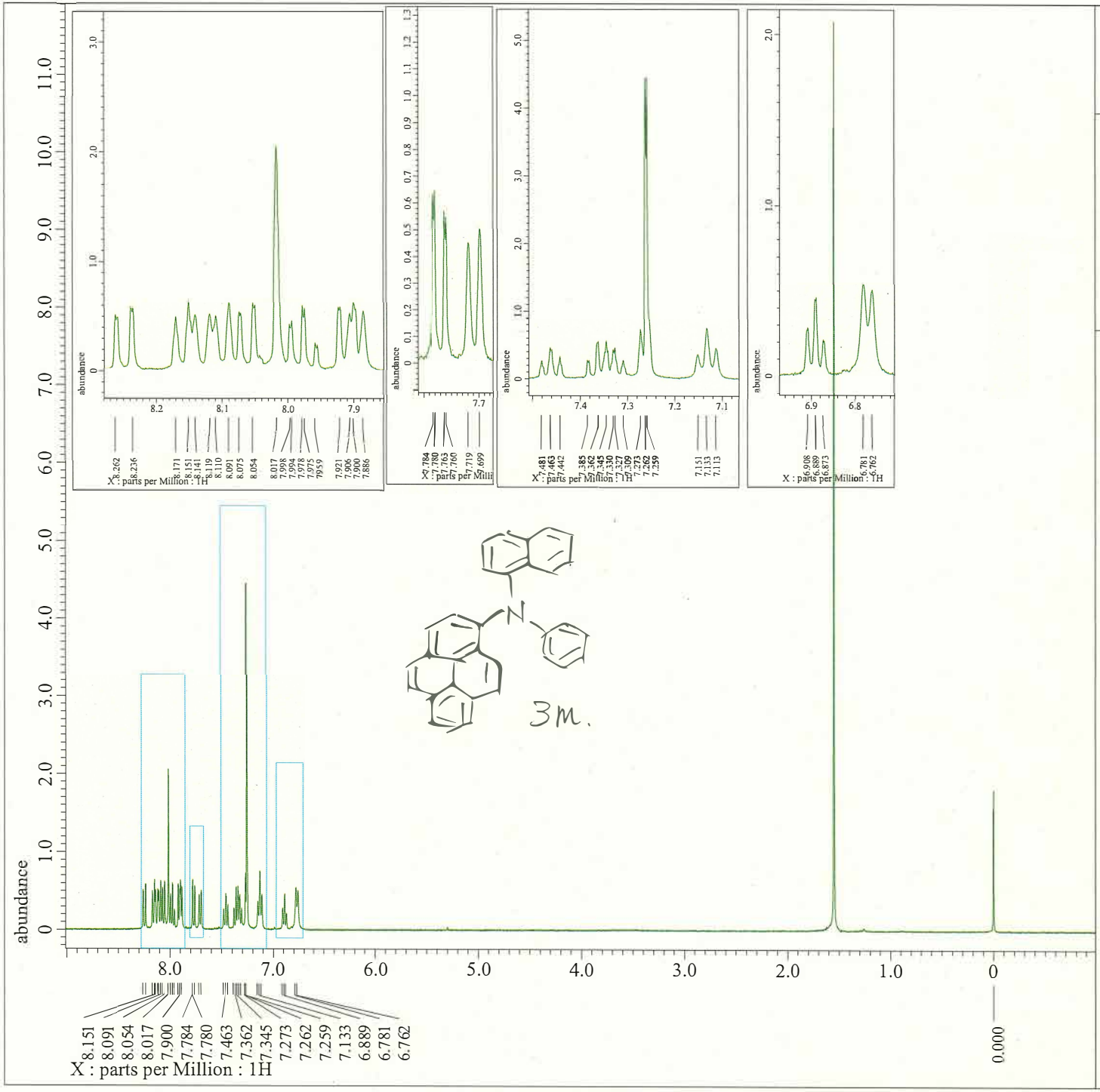
Filename	= RIK-327-pureH-2.jdf
Author	= element
Experiment	= single_pulse.ex2
Sample_Id	= S#549711
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 9-JUN-2020 22:24:32
Revision_Time	= 7-AUG-2020 16:07:16
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= 1H
Dim_Title	= 1H
Dim_Units	= [ppm]
Dimensions	= X
Site	= ECS 400
Spectrometer	= JNM-ECS400
Field_Strength	= 9.20197068[T] (390[MHz]
X_Acq_Duration	= 2.228224[s]
X_Domain	= 1H
X_Freq	= 391.78655441[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.44878791[Hz]
X_Sweep	= 7.35294118[kHz]
Irr_Domain	= 1H
Irr_Freq	= 391.78655441[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= 1H
Tri_Freq	= 391.78655441[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 54
Temp_Get	= 23.7[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]




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

以下に由来:: RIK-327-pureC-1.jdf
```

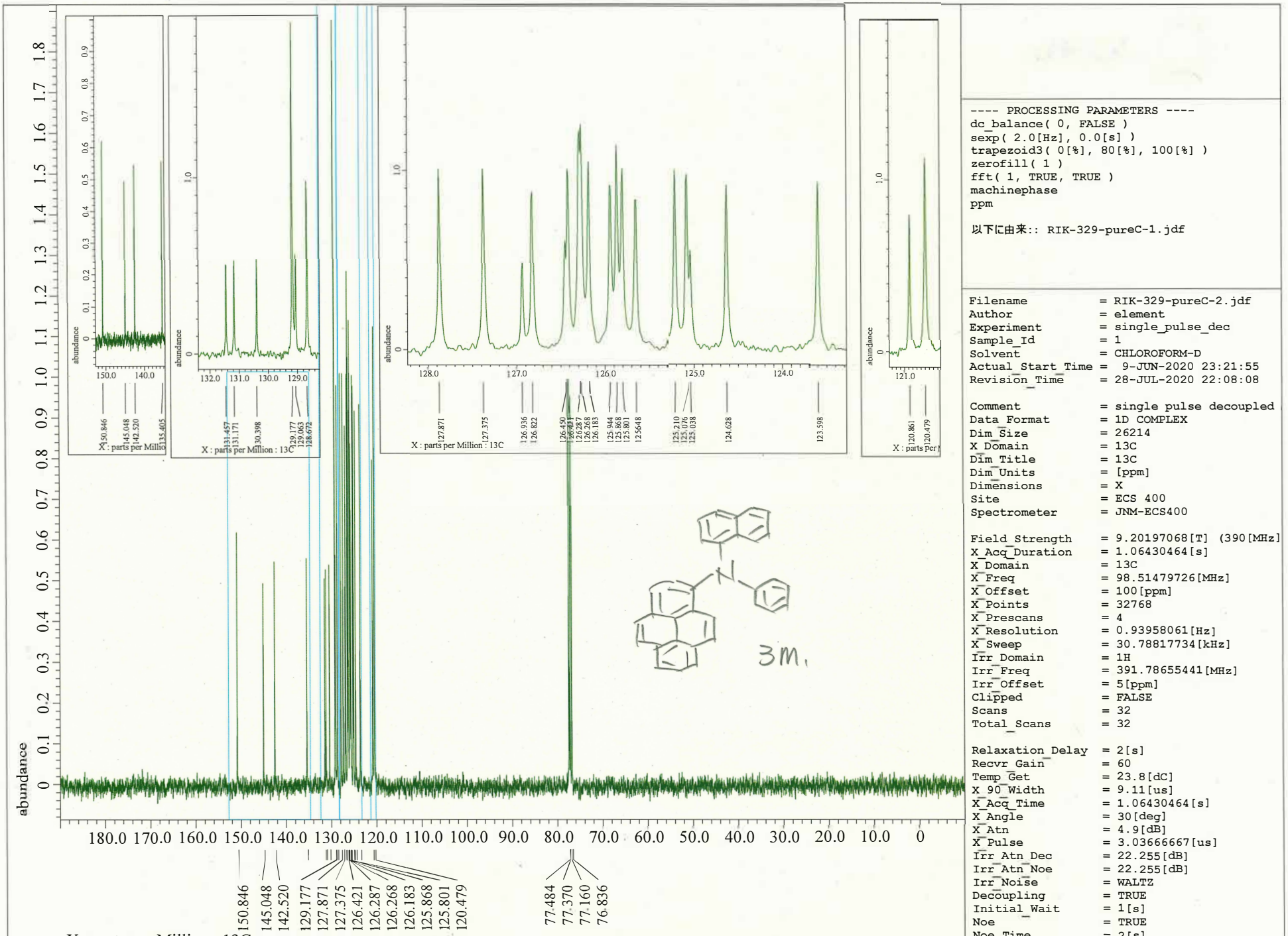
Filename	= RIK-327-pureC-2.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= 1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 9-JUN-2020 22:58:38
Revision_Time	= 7-AUG-2020 16:54:03
Comment	= single pulse decoupled
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= 13C
Dim_Title	= 13C
Dim_Units	= [ppm]
Dimensions	= X
Site	= ECS 400
Spectrometer	= JNM-ECS400
Field_Strength	= 9.20197068[T] (390[MHz]
X_Acq_Duration	= 1.06430464[s]
X_Domain	= 13C
X_Freq	= 98.51479726[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.93958061[Hz]
X_Sweep	= 30.78817734[kHz]
Irr_Domain	= 1H
Irr_Freq	= 391.78655441[MHz]
Irr_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 32
Total_Scans	= 32
Relaxation_Delay	= 2[s]
Recvr_Gain	= 60
Temp_Get	= 23.9[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]




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

以下に由来:: RIK-329-pureH-1.jdf
```

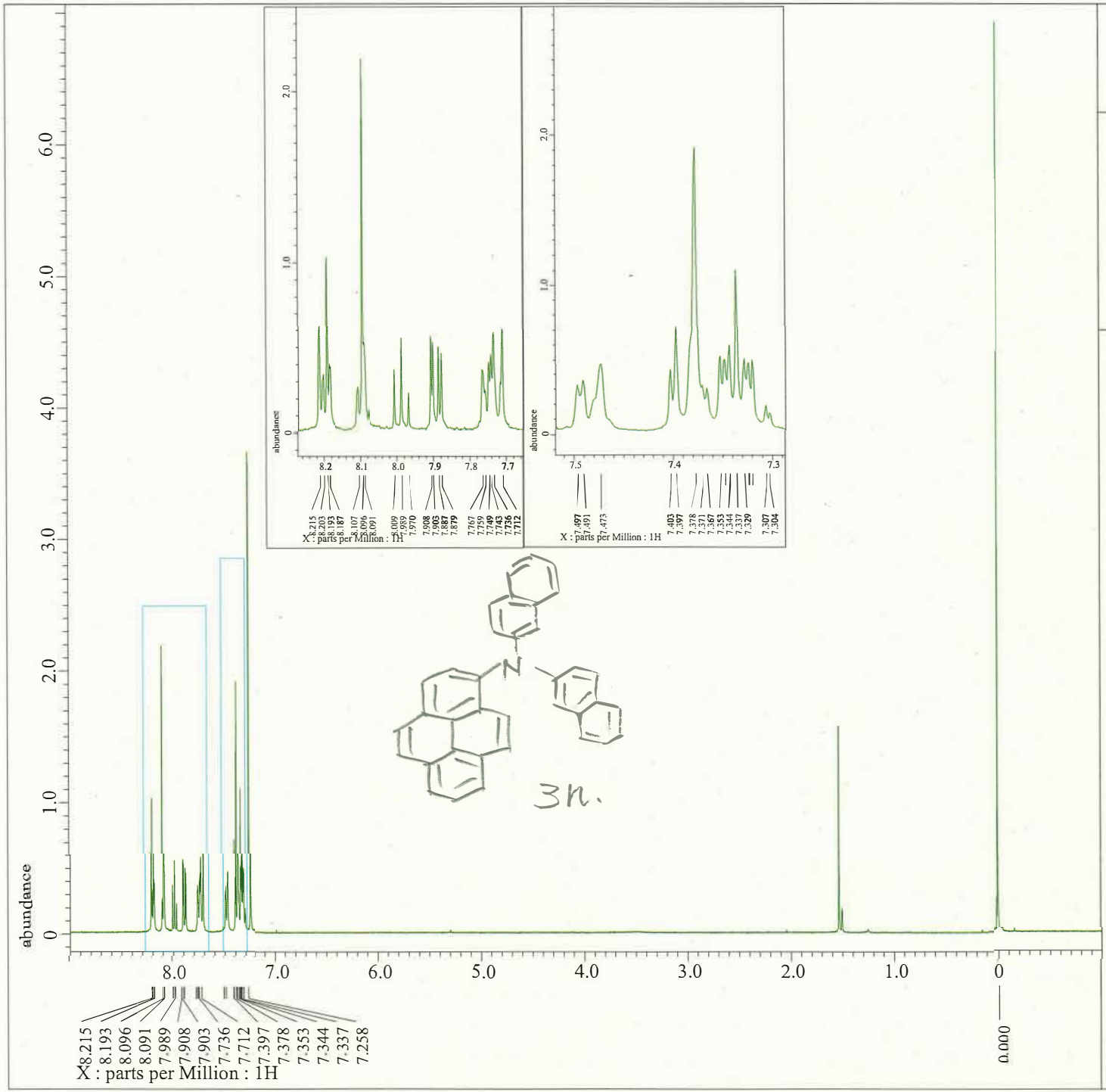
Filename	= RIK-329-pureH-2.jdf
Author	= element
Experiment	= single_pulse.ex2
Sample_Id	= S#557812
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 9-JUN-2020 22:38:00
Revision_Time	= 7-AUG-2020 16:10:42
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= 1H
Dim_Title	= 1H
Dim_Units	= [ppm]
Dimensions	= X
Site	= ECS 400
Spectrometer	= JNM-ECS400
Field_Strength	= 9.20197068[T] (390[MHz]
X_Acq_Duration	= 2.228224[s]
X_Domain	= 1H
X_Freq	= 391.78655441[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.44878791[Hz]
X_Sweep	= 7.35294118[kHz]
Irr_Domain	= 1H
Irr_Freq	= 391.78655441[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= 1H
Tri_Freq	= 391.78655441[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 56
Temp_Get	= 23.7[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]




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

以下に由来:: RIK-329-pureC-1.jdf
```

Filename	= RIK-329-pureC-2.jdf
Author	= element
Experiment	= single_pulse_dec
Sample_Id	= 1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 9-JUN-2020 23:21:55
Revision_Time	= 28-JUL-2020 22:08:08
Comment	= single pulse decoupled
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= 13C
Dim_Title	= 13C
Dim_Units	= [ppm]
Dimensions	= X
Site	= ECS 400
Spectrometer	= JNM-ECS400
Field_Strength	= 9.20197068[T] (390[MHz]
X_Acq_Duration	= 1.06430464[s]
X_Domain	= 13C
X_Freq	= 98.51479726[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.93958061[Hz]
X_Sweep	= 30.78817734[kHz]
Irr_Domain	= 1H
Irr_Freq	= 391.78655441[MHz]
Irr_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 32
Total_Scans	= 32
Relaxation_Delay	= 2[s]
Recvr_Gain	= 60
Temp_Get	= 23.8[dC]
X_90_Width	= 9.11[us]
X_Acq_Time	= 1.06430464[s]
X_Angle	= 30[deg]
X_Atn	= 4.9[dB]
X_Pulse	= 3.03666667[us]
Irr_Atn_Dec	= 22.255[dB]
Irr_Atn_Noe	= 22.255[dB]
Irr_Noise	= WALTZ
Decoupling	= TRUE
Initial_Wait	= 1[s]
Noe	= TRUE
Noe_Time	= 2[s]




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

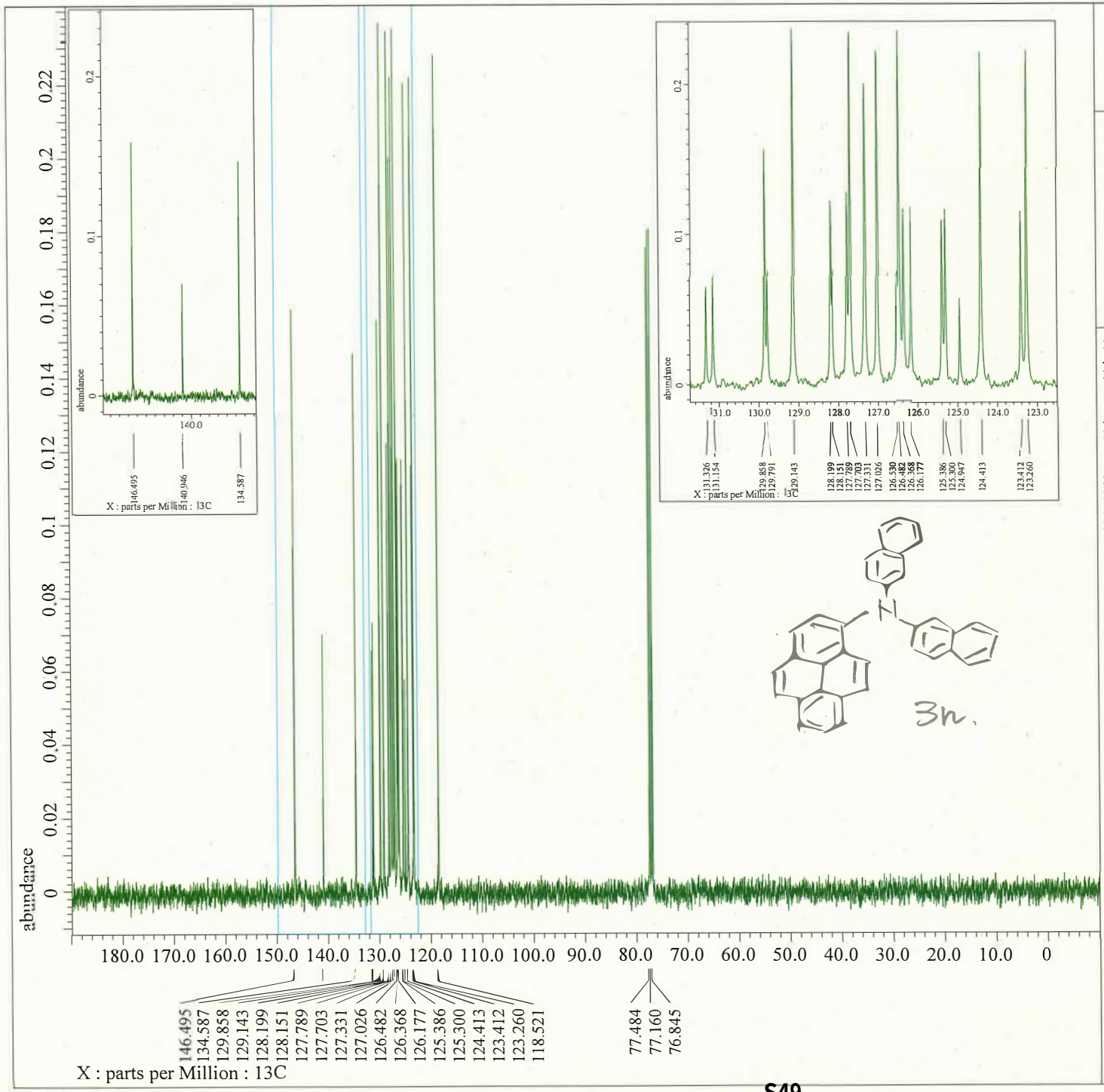
以下に由来:: RIK-328-pureH-2.jdf
```

```
Filename            = RIK-328-pureH-3.jdf
Author              = delta
Experiment          = single_pulse.ex2
Sample_Id           = S#739626
Solvent             = CHLOROFORM-D
Actual_Start_Time   = 29-JUL-2020 05:16:26
Revision_Time       =  7-AUG-2020 16:15:35

Comment             = single_pulse
Data_Format         = 1D COMPLEX
Dim_Size            = 13107
X_Domain            = 1H
Dim_Title           = 1H
Dim_Units           = [ppm]
Dimensions          = X
Site                = ECX 400
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

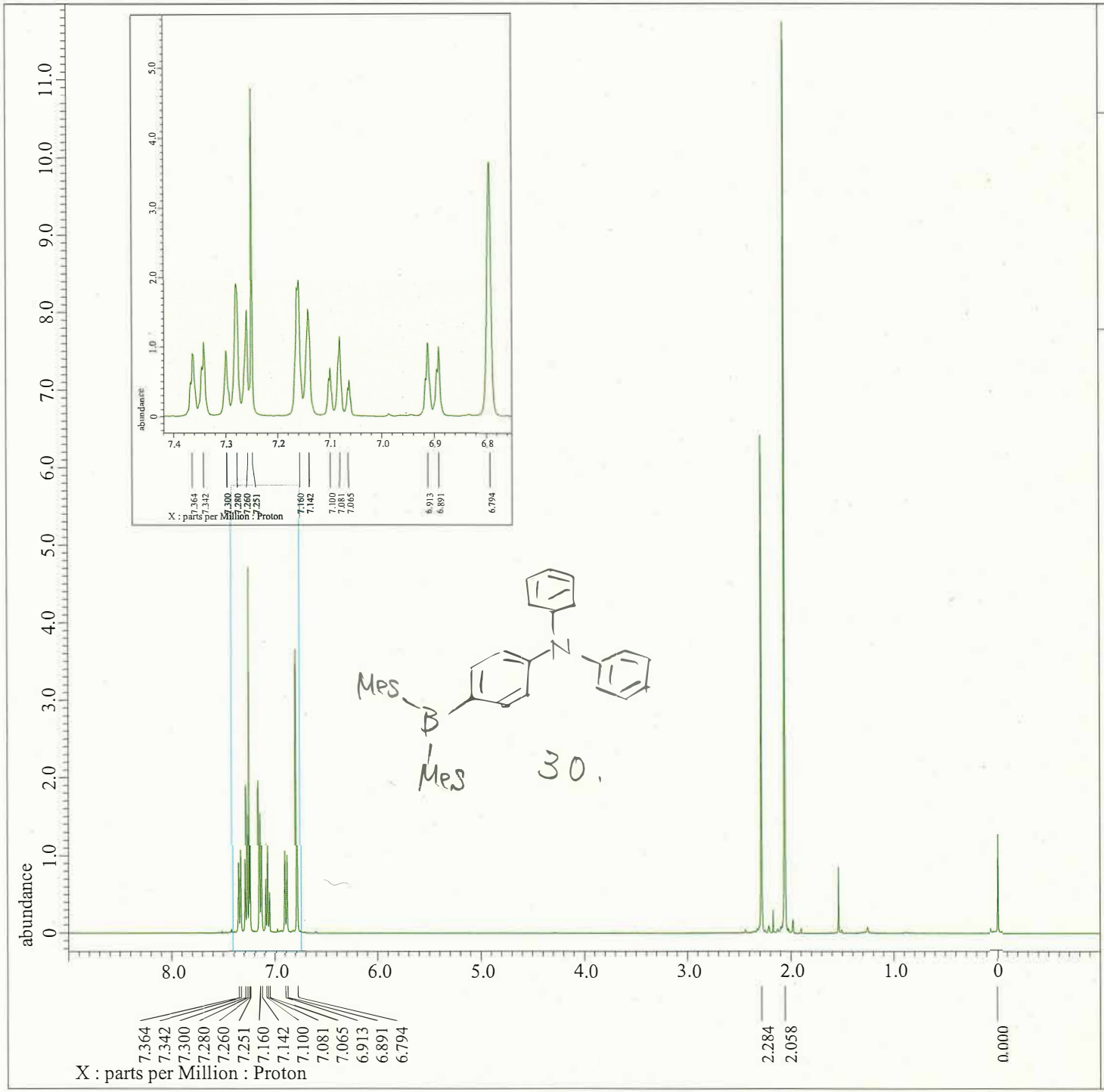
Relaxation_Delay    = 5[s]
Recvr_Gain          = 50
Temp_Get            = 22.7[dC]
X_90_Width          = 11.5[us]
X_Acq_Time          = 2.20725248[s]
X_Angle             = 45[deg]
X_Atn               = 9[dB]
X_Pulse             = 5.75[us]
Irr_Mode            = Off
Tri_Mode            = Off
Dante_Presat        = FALSE
Initial_Wait        = 1[s]
```




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

以下に由来:: RIK-328-pureC-1.jdf
```

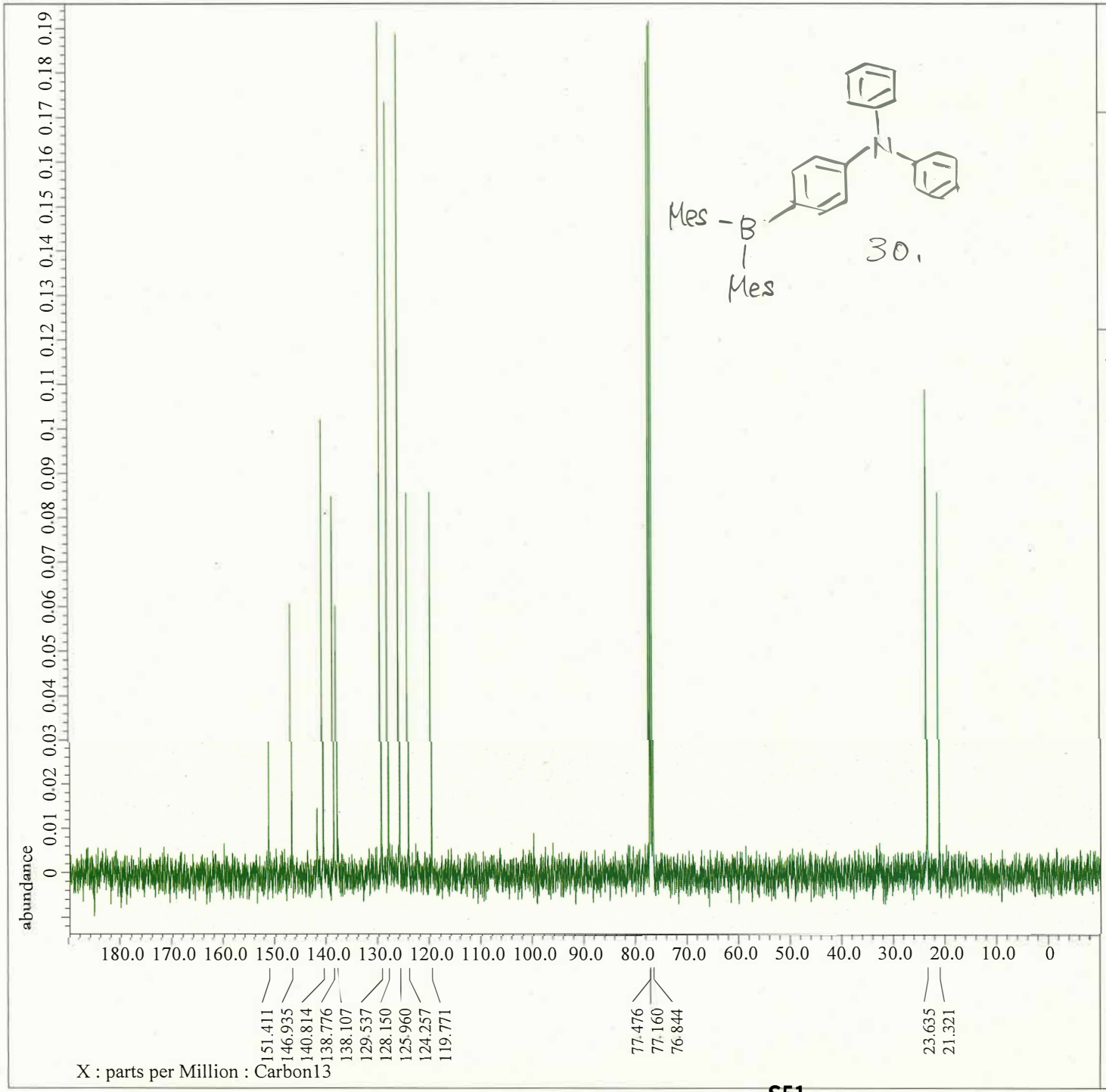
Filename	= RIK-328-pureC-2.jdf
Author	= delta
Experiment	= single_pulse_dec
Sample_Id	= S#771440
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 31-JUL-2020 05:51:55
Revision_Time	= 30-JUL-2020 21:27:41
Comment	= single pulse decoupled
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= 13C
Dim_Title	= 13C
Dim_Units	= [ppm]
Dimensions	= X
Site	= ECA 500 (26)
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.389766[T] (400[MHz])
X_Acq_Duration	= 1.04333312[s]
X_Domain	= 13C
X_Freq	= 100.52530333[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.95846665[Hz]
X_Sweep	= 31.40703518[kHz]
Irr_Domain	= 1H
Irr_Freq	= 399.78219838[MHz]
Irr_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 64
Total_Scans	= 64
Relaxation_Delay	= 2[s]
Recvr_Gain	= 46
Temp_Get	= 28[dC]
X_90_Width	= 10.5[us]
X_Acq_Time	= 1.04333312[s]
X_Angle	= 30[deg]
X_Atn	= 6[dB]
X_Pulse	= 3.5[us]
Irr_Atn_Dec	= 22.5[dB]
Irr_Atn_Noe	= 22.5[dB]
Irr_Noise	= WALTZ
Decoupling	= TRUE
Initial_Wait	= 1[s]
Noe	= TRUE
Noe_Time	= 2[s]




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

以下に由来:: RIK-334-pure_Proton-1-1.jdf
```

Filename	= RIK-334-pure_Proton-1-2
Author	= element
Experiment	= proton.jxp
Sample_Id	= RIK-334-pure
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 19-JUN-2020 20:48:38
Revision_Time	= 7-AUG-2020 16:21:06
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= DELTA2_NMR
Field_Strength	= 9.4073814[T] (400[MHz])
X_Acq_Duration	= 2.18103808[s]
X_Domain	= 1H
X_Freq	= 400.53219825[MHz]
X_Offset	= 5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.45849727[Hz]
X_Sweep	= 7.51201923[kHz]
X_Sweep_Clipped	= 6.00961538[kHz]
Irr_Domain	= Proton
Irr_Freq	= 400.53219825[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 400.53219825[MHz]
Tri_Offset	= 5[ppm]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 5[s]
Recvr_Gain	= 34
Temp_Get	= 20.3[dC]
X_90_Width	= 6[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]




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

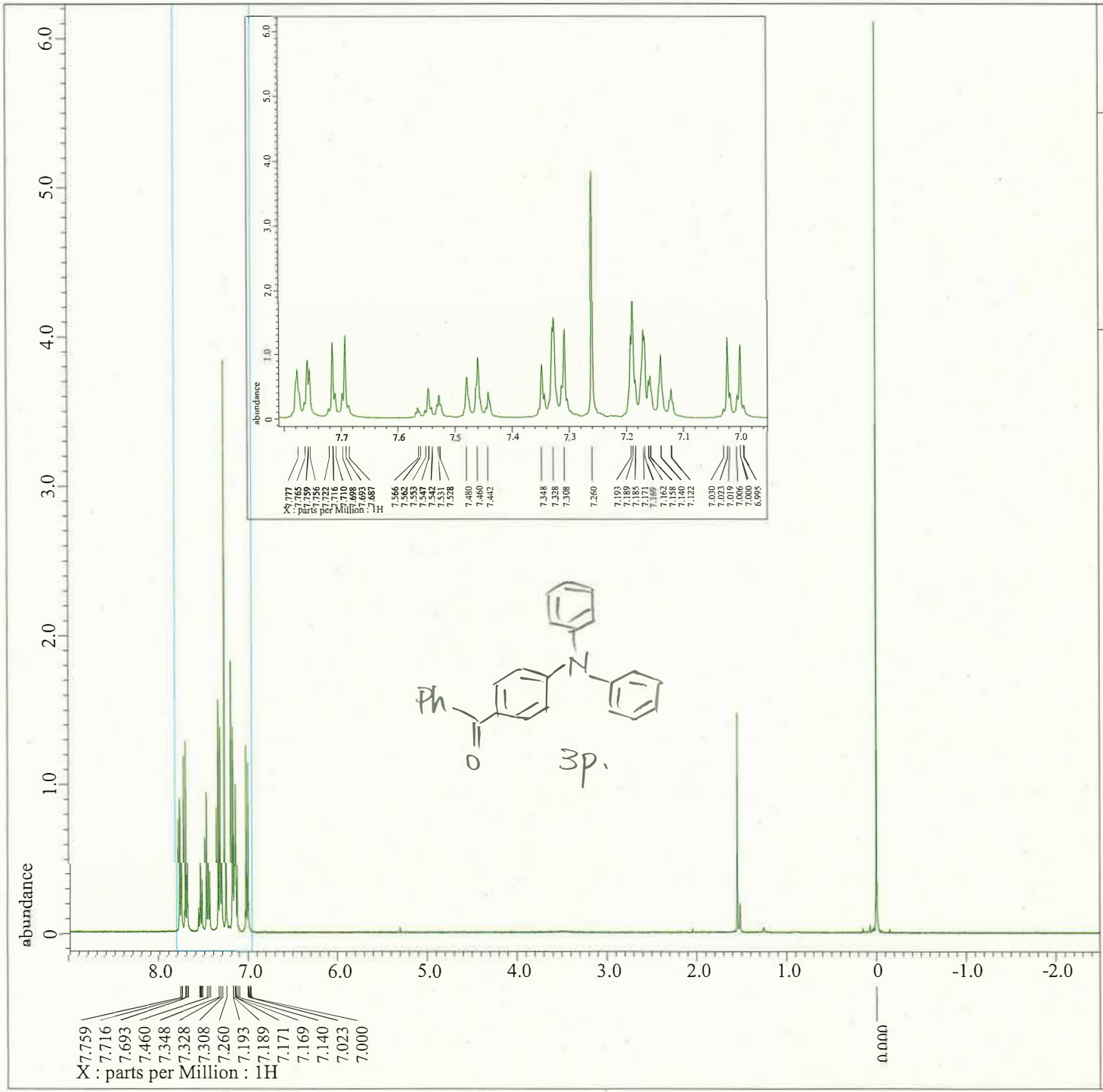
以下に由来:: RIK-334-pureC_Carbon-1-1.jdf
```

```
Filename            = RIK-334-pureC_Carbon-1-
Author              = element
Experiment          = carbon.jxp
Sample_Id           = RIK-334-pureC
Solvent             = CHLOROFORM-D
Actual_Start_Time   = 19-JUN-2020 21:01:37
Revision_Time       =  7-AUG-2020 16:34:25

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

Field_Strength      = 9.4073814[T] (400[MHz])
X_Acq_Duration      = 1.03809024[s]
X_Domain            = 13C
X_Freq              = 100.71389092[MHz]
X_Offset            = 100[ppm]
X_Points            = 32768
X_Prescans          = 4
X_Resolution        = 0.96330739[Hz]
X_Sweep             = 31.56565657[kHz]
X_Sweep_Clipped     = 25.25252525[kHz]
Irr_Domain          = Proton
Irr_Freq            = 400.53219825[MHz]
Irr_Offset          = 5[ppm]
Clipped             = FALSE
Scans               = 64
Total_Scans         = 64

Relaxation_Delay    = 2[s]
Recvr_Gain          = 50
Temp_Get            = 20.5[dC]
X_90_Width          = 10.9[us]
X_Acq_Time          = 1.03809024[s]
X_Angle             = 30[deg]
X_Atn               = 4[dB]
X_Pulse             = 3.63333333[us]
Irr_Atn_Dec         = 26.45[dB]
Irr_Atn_Noe         = 26.45[dB]
Irr_Noise           = WALTZ
Irr_Pwidth          = 0.115[ms]
Decoupling          = TRUE
Initial_Wait        = 1[s]
Noe                 = TRUE
```




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

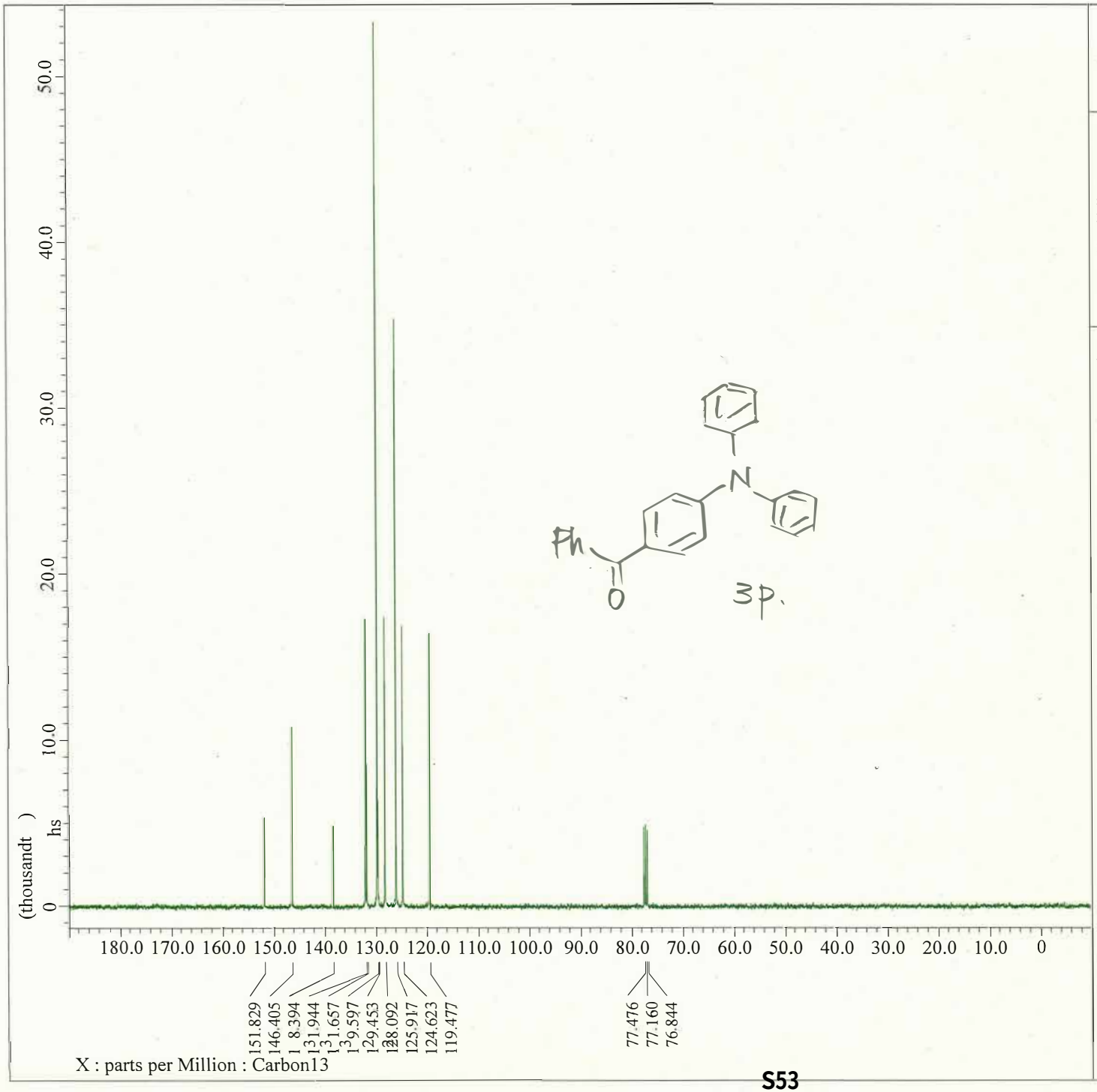
以下に由来:: RIK-405-pureH-1.jdf
```

```
Filename            = RIK-405-pureH-2.jdf
Author              = delta
Experiment          = single_pulse.ex2
Sample_Id           = S#742731
Solvent             = CHLOROFORM-D
Actual_Start_Time   = 29-JUL-2020 05:21:35
Revision_Time       =  7-AUG-2020 16:23:57

Comment             = single_pulse
Data_Format         = 1D COMPLEX
Dim_Size            = 13107
X_Domain            = 1H
Dim_Title           = 1H
Dim_Units           = [ppm]
Dimensions          = X
Site                = ECX 400
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

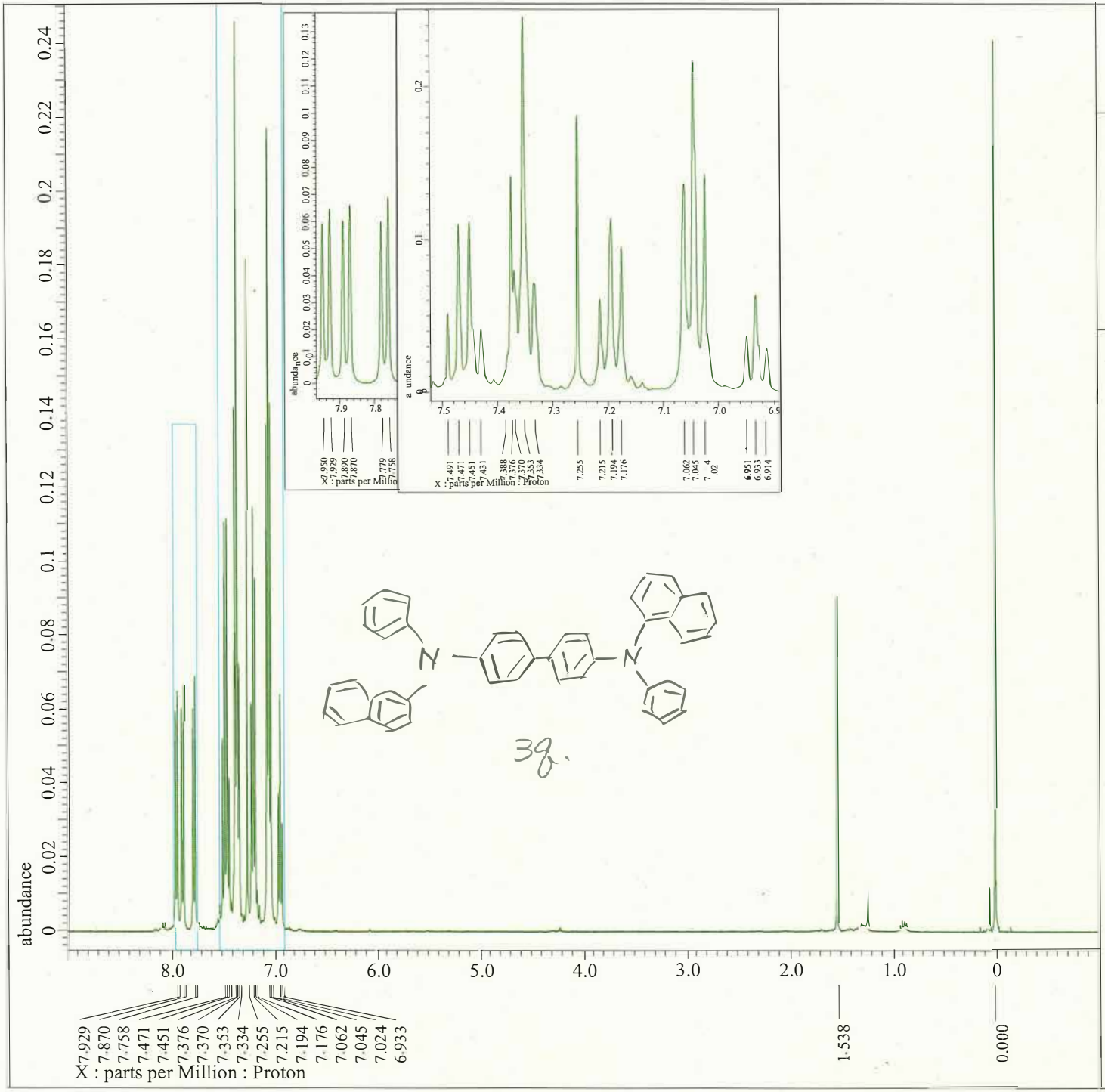
Relaxation_Delay    = 5[s]
Recvr_Gain          = 50
Temp_Get            = 22.7[dC]
X_90_Width          = 11.5[us]
X_Acq_Time          = 2.20725248[s]
X_Angle             = 45[deg]
X_Atn               = 9[dB]
X_Pulse             = 5.75[us]
Irr_Mode            = Off
Tri_Mode            = Off
Dante_Presat        = FALSE
Initial_Wait        = 1[s]
```




```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
thresh( 5[%], 1 )
peak_pick( 0[Hz], 0.1[ppm], Peaks, 0[Hz] )

以下に由来:: RIK-405-pureC_CARBON-1-1.jdf
```

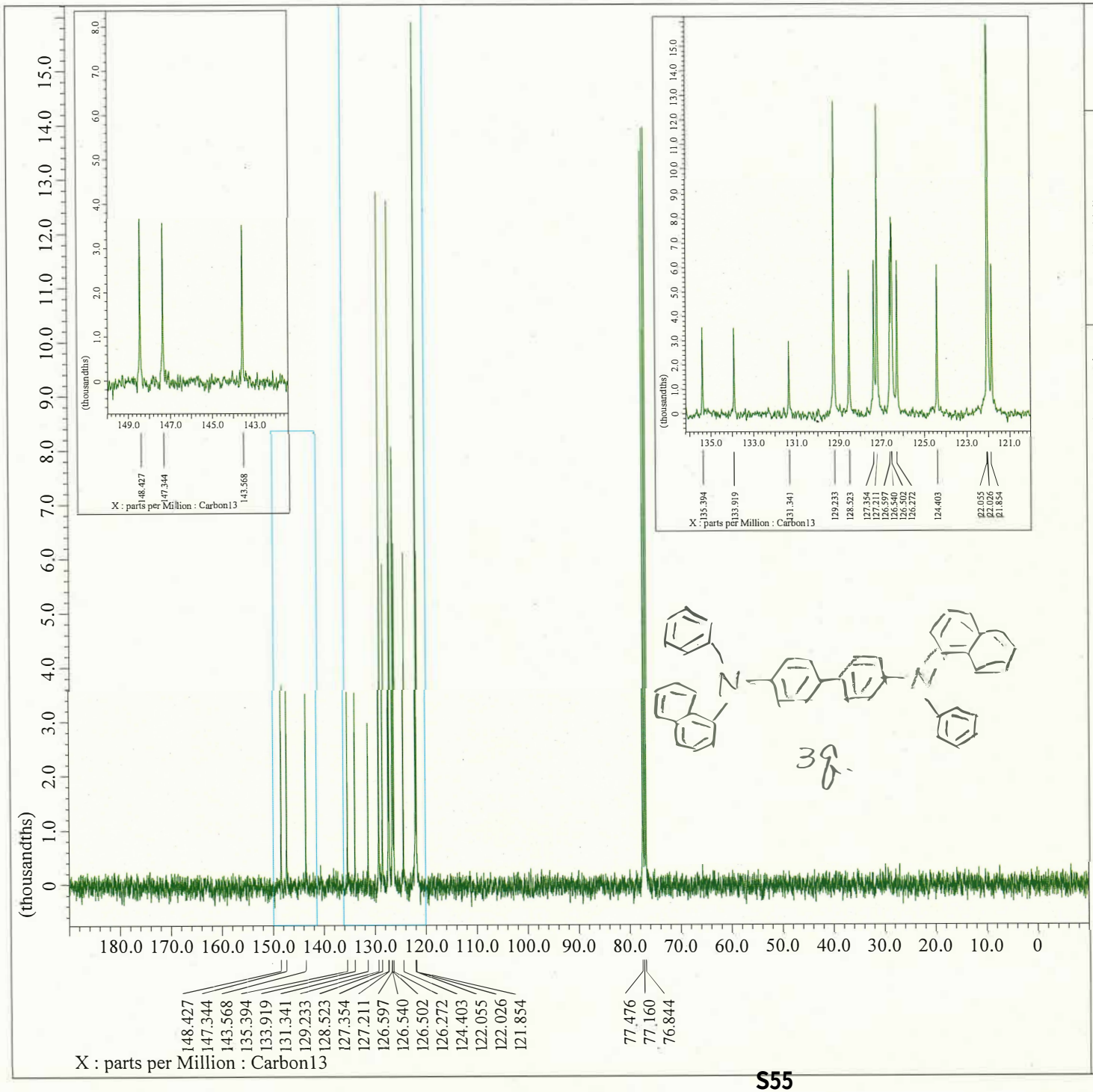
Filename	= RIK-405-pureC_CA
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= RIK-405-pureC
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 5-JUL-2020 15:5
Revision_Time	= 28-JUL-2020 22:3
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ400S/L1
Field_Strength	= 9.389766[T] (400
X_Acq_Duration	= 1.03809024[s]
X_Domain	= Carbon13
X_Freq	= 100.52530333[MHz
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.96330739[Hz]
X_Sweep	= 31.56565657[kHz]
X_Sweep_Clipped	= 25.25252525[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.78219838[MHz
Irr_Offset	= 5[ppm]
Blanking	= 5[us]
Clipped	= FALSE
Scans	= 32
Total_Scans	= 32
Relaxation_Delay	= 2[s]
Recvr_Gain	= 42
Temp_Get	= 19.8[dC]
X_90_Width	= 10.6[us]
X_Acq_Time	= 1.03809024[s]
X_Angle	= 30[deg]
X_Atn	= 8.8[dB]
X_Pulse	= 3.53333333[us]
Irr_Atn_Dec	= 31.25[dB]
Irr_Atn_Dec_Calc	= 31.25[dB]
Irr_Atn_Dec_Default_Calc	= 31.25[dB]
Irr_Atn_Noe	= 31.25[dB]
Irr_Dec_Bandwidth_Hz	= 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm	= 11.96303566[ppm]
Irr_Dec_Freq	= 399.78219838[MHz




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

以下に由来:: RIK-454-pureH_PROTON-2-1.jdf
```

Filename	= RIK-454-pureH_PROTO
Author	= delta
Experiment	= proton.jxp
Sample_Id	= RIK-454-pureH
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 27-JUL-2020 20:03:1
Revision_Time	= 7-AUG-2020 16:26:1
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ400S/L1
Field_Strength	= 9.389766[T] (400[MH
X_Acq_Duration	= 4.37256192[s]
X_Domain	= Proton
X_Freq	= 399.78219838[MHz]
X_Offset	= 5[ppm]
X_Points	= 32768
X_Prescans	= 0
X_Resolution	= 0.22869888[Hz]
X_Sweep	= 7.4940048[kHz]
X_Sweep_Clipped	= 5.99520384[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.78219838[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 399.78219838[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2[us]
Clipped	= FALSE
Scans	= 8
Total_Scans	= 8
Relaxation_Delay	= 4[s]
Recvr_Gain	= 52
Temp_Get	= 19.8[dC]
X_90_Width	= 5.6[us]
X_Acq_Time	= 4.37256192[s]
X_Angle	= 45[deg]
X_Atn	= 5[dB]
X_Pulse	= 2.8[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 400
Dante_Presat	= FALSE




```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid3( 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
thresh( 5[%], 1 )
peak_pick( 0[Hz], 0.1[ppm], Peaks, 0[Hz] )

以下に由来:: RIK-454-pureC_CARBON-1-1.jdf
```

Filename	= RIK-454-pureC_CA
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= RIK-454-pureC
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 27-JUL-2020 20:2
Revision_Time	= 28-JUL-2020 22:4
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ400S/L1
Field_Strength	= 9.389766[T] (400
X_Acq_Duration	= 1.03809024[s]
X_Domain	= Carbon13
X_Freq	= 100.52530333[MHz
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 0.96330739[Hz]
X_Sweep	= 31.56565657[kHz]
X_Sweep_Clipped	= 25.25252525[kHz]
Irr_Domain	= Proton
Irr_Freq	= 399.78219838[MHz
Irr_Offset	= 5[ppm]
Blanking	= 5[us]
Clipped	= FALSE
Scans	= 128
Total_Scans	= 128
Relaxation_Delay	= 2[s]
Recvr_Gain	= 52
Temp_Get	= 19.7[dC]
X_90_Width	= 10.6[us]
X_Acq_Time	= 1.03809024[s]
X_Angle	= 30[deg]
X_Atn	= 8.8[dB]
X_Pulse	= 3.53333333[us]
Irr_Atn_Dec	= 31.25[dB]
Irr_Atn_Dec_Calc	= 31.25[dB]
Irr_Atn_Dec_Default_Calc	= 31.25[dB]
Irr_Atn_Noe	= 31.25[dB]
Irr_Dec_Bandwidth_Hz	= 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm	= 11.96303566[ppm]
Irr_Dec_Freq	= 399.78219838[MHz